UNIVERSITÀ DEGLI STUDI DI CATANIA
DIPARTIMENTO DI SCIENZE CHIMICHE

International Doctorate in Chemical Sciences
XXIX cycle

Alessio Paternò

Multivariate design of sustainable and efficient ionic liquids

Ph.D Thesis

Tutor *Prof. G. Musumarra*
Coordinator *Prof. S. Sortino*

2017

Index

1. Introduction

Inductive and deductive approaches are different ways to explore the world around us, and philosophers, or people in general, differently adopt them to explain the principles of their thoughts and opinions. In scientific research both deductive and inductive approaches may be used. Deductive reasoning is a "top-down" approach aimed at testing a hypothesis initially postulated, and then trying to find experimental evidences to support or disprove it. On the contrary, inductive reasoning is a "bottom-up" approach, based on learning from observations; explanatory hypotheses are eventually formulated at the end of the process.

The computer age had an enormous impact on chemical research. Nowadays hundreds molecular modeling softwares adopting different investigational approaches are available in different areas of chemistry. Among them, (as reported in Fig. 1, going from the left to the right) quantum chemistry, which considers mainly problems related to quantum phenomena; theoretical chemistry, traditionally associated to the formulation of new theories and/or approximations; computational chemistry, a branch of theoretical chemistry, whose objective is to build a mathematical model to calculate molecular properties (energy, dipole moments, vibrational frequencies etc.); cheminformatics, which uses computational and chemometric tools to investigate different chemical and biological issues. The term chemometrics was proposed in 1974 by Bruce Kovalski (Seattle, USA) and Svante Wold (Umea, Sweden) and since then several successful chemometric applications have been reported in pharmaceutical, food and analytical chemistry. Although chemometric competence is sought in industry and applied in R&D, chemometrics, probably due to its highly empirical character, which implies adoption of data-driven "soft" models, is still not very popular among organic chemists.

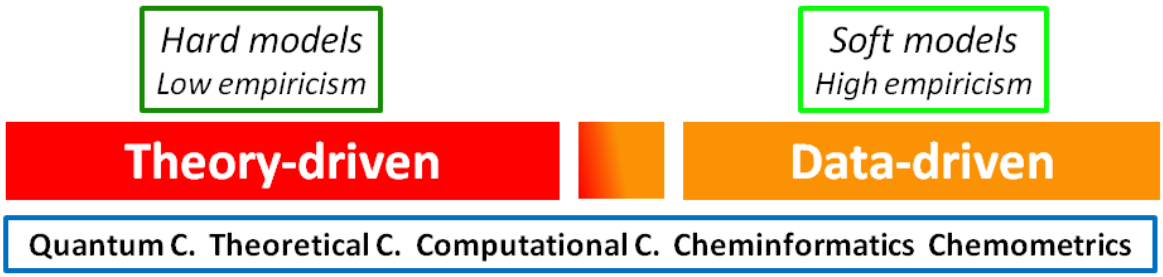


Fig. 1 Hard and soft modelling fields of application.

In a recent paper Martens[1] points out the gap between the mathematics-statistics culture, focusing on formal accuracy, and other sciences cultures producing lots of good raw data, which often treat them using limited and uninformed mathematics and statistics. He states that "chemometrics has a lot to learn from other disciplines, mathematics and statistics [...] but on the other hand chemometrics has a lot to give to other disciplines" and hopes for a culture favouring cooperation rather than competition.

He also points out that in the past forty years science witnessed a big data explosion paralleled by an increasing computer capacity in respect to storage space, memory and CPU, but unfortunately unless we can also interpret these data we are overwhelmed by them. In this context Martens states that chemometrics, in contrast with "black box" approaches, developed a pragmatic science culture attempting to approach the real world letting the data talk to us but at the same time trying to interpret the results in light of prior chemical knowledge and the laws of physics.

The reason for chemometrics being not applied in organic chemistry might be due to the fact that in the past two decades many Universities have not focused on education in physical organic chemistry which led organic chemists to delegate these studies to theoreticians (whose aim is to provide a unique model of high complexity able to fit all the data) and to statisticians (whose cultural background emphasizes the importance of high correlation and predictivity, expressed as R^2 and Q^2 values respectively, which in cases such as biological and physical measurements on ionic liquids are difficult to achieve) both believed to be more suited to the job. In the field of ionic liquids, low melting point salts, formed of an organic cation and an inorganic or organic anion, covering a huge experimental space difficult to be explored, multivariate approaches leading to soft models of local validity might be useful for their applicative potentialities.

Ionic liquids (ILs) exhibited an unprecedented efficiency at a molecular level and showed promising characteristics for the development of green and sustainable technologies. It is important to stress that the characteristics of both cations and anions determine the physico-chemical properties and the process performances of the resulting IL as well as its toxicity. Predicting the efficiency and sustainability of ILs could be presently considered a major issue for the scientific community.

1.1 ILs Descriptors

In theory a suitable IL could be designed for a specific use relating its structural properties to a given application by a quantitative structure-property relationship (QSPR) approach, but in practice experimentally determined physico-chemical properties in the case of ILs are very few, measured under different conditions and scattered in the literature. Since it is hardly possible to experimentally explore such a huge chemical space, available data often cover only a fraction of it. Moreover, synthetic and experimental screening efforts are in general expensive and time-consuming even for relatively small subspaces of ILs structures, and their purity can dramatically affect the experimental determination of their properties.[2] Hence there is a need of *in silico* descriptors for as many ILs as possible, in order to derive QSPR models allowing properties prediction for yet unknown ILs before planning their synthesis and/or carrying out efficiency tests.

Adopting multivariate strategies exhibits great advantages in optimizing desired properties (yield, regio- or stereo-isomeric ratios, etc.) by simultaneous variation of experimental conditions, which may be continuous (temperature, time, concentrations, etc.) or discrete (solvent, catalyst, etc.) variables. The latter variables need parameterization by means of intrinsic properties suitable for experimental design, *i.e.* orthogonal to each other. The above requirement led to the derivation of principal properties (PPs), which are intrinsic properties representative of experimentally observable macroscopic descriptors. PPs are calculated as the principal component analysis (PCA) scores using experimentally measured properties, and are already available for solvents,[3,4] aldehydes and ketones,[5] amines,[6] Lewis acids,[7] lanthanide triflates,[8] aromatic substituents[9] and amino acids.[10-13] First and second-generation PPs for heteroaromatic moieties, based on aromaticity[14] and on 3D-GRID structural parameters[15] respectively, were reported. In addition to statistical orthogonality, PPs derived by PCA models have the advantage of being less influenced by measurement errors and system-specific variations than single descriptors. A typical example of the potentialities of PPs used for optimization purposes was provided by the results of a multivariate experimental design based on the PPs of Lewis acid catalysts and solvents. This approach gave a better understanding of the effects of the above parameters on the isomeric distribution in the reaction of phenylhydrazones derived from unsymmetrical ketones (the Fischer indole synthesis). Multivariate optimization achieved not only regiospecific synthesis of single indole regio-isomers,[16] but almost quantitative yields in a single step reaction.[17] It is worth noting that the above result was achieved for a reaction, the Fischer indole synthesis,[18,19] known for more than a century. Furthermore PPs resulted to be suitable for design in quantitative structure-activity relationships (QSARs),[9] especially for the design of biologically active peptides.[10,11] Dedicated PPs for amino acids were then derived for peptides QSARs,[12] for quantitative sequence-activity modelling[20] and more recently, using MIF (Molecular Interaction Fields) descriptors, for GRID-based description of molecular similarity and ligand-based virtual screening.[13,21] PPs are particularly suited to describe compounds that are the sum of finite building blocks such as ionic liquids (anions and cations as anionic and cationic building blocks).

In spite of the potentialities exhibited in multivariate design of synthetic procedures and in the discovery of novel biologically active compounds, the use of PPs has received little attention in the past decade.

1.2 ILs properties and toxicities

Ionic liquids represent an innovation in the industrial scenario due to their very interesting physico-chemical properties relevant either in academic or industrial fields. They attracted much attention as green solvents as compared to common volatile organic solvents due to their low vapour pressure, resulting in lower air emission, low flammability and non-explosiveness, even though these features are

not sufficient to justify their "greenness". The interest in ILs is highlighted by an exponential increase in publications, which demonstrates that this field has developed beyond the concept of new solvents. A wide variety of ILs applications are examined by recent papers and reviews on their use as reaction media,[22-25] lubricants,[26] surfactants,[27] anticorrosion agents,[28,29] in separation[30-33] and more in general in analytical chemistry,[34] in the cyclization of allenes,[35] on their role in catalysis[36] as well as in major societal issues such as energy, materials and medicine.[37]

The widespread use of ILs makes the study of their impact on human's health and environment an unavoidable priority.[38] In fact, release of ILs from industrial processes into aquatic environments may lead to water pollution due to their high solubility and their high stability in water which might render them persistent pollutants in wastewaters. For this reason it is necessary to determine the environmental risk in aquatic ecosystems first of all, to comply with the terms of the European Union regulation for the Registration, Evaluation, Authorization and Restriction of Chemicals (REACH) requiring a comprehensive knowledge of the properties and hazards of ILs.[39] Such an ambitious task is particularly hard to achieve due to the difficulties in developing procedures for collecting and assessing this kind of information. Predicting the efficiency and sustainability of ILs is presently a major issue for the scientific community.

However, the assessment of eco-toxicity of ILs is quite complicated due to the fact that different biological "sensors" could be considered as representative of their hazard and often these data are available for a numerically limited numbers of ILs.[40] The term "toxicity" refers to a general concept including different biological tests such as cytotoxicity, toxicity towards invertebrates, vertebrates, fungi and bacteria, phytotoxicity, impact on enzymatic activity and protein stability. ILs experimental toxicity data for many ionic liquids in different biological test systems were reported in the UFT-Merck Ionic Liquids Biological Effects Database.[41] Unlikely, this database is no longer operative and, even when it was accessible, single toxicity tests were not available for many ILs. In conclusion, there is a need to accelerate the discovery of biocompatible ILs by identifying safe, non-toxic, environmental friendly ionic liquids by thorough ecotoxicological testing,[42] but this goal is not easy to achieve since, quoting Sir Richard Livingstone, 'danger is not too few, but too many options [...] to be puzzled by innumerable alternatives'. In this context, adoption of multivariate approaches can help to simplify the overall toxicity picture.

1.3 Purposes of this Ph.D thesis

Ionic liquids appeared in the scientific literature in 1914 thanks to the work of Paul Walden[43] who noticed their chemo-physical properties and envisaged their possible catalytic effects. Nevertheless, the scientific community has really appreciated their values since 2000, with an exponential increase of

researches in this very fertile field. This scenario prompted me to select such an innovative and, in many ways, little explored topic for my Ph.D thesis. My interest for ILs arises from their usefulness, and it is due not only to academic purposes but also to the social impact that the potential results of my study could have for the development of sustainable industrial applications.

Given the huge number of cation/anion combinations, a large variety of solvent systems having different properties can be obtained. This may simultaneously represent an advantage and a detriment. Although a wide range of solvents would be in principle available for the same process, the lack of knowledge of solvent properties and the efforts required to perform experimental investigations makes the selection of a suitable solvent for a given process or reaction a hard task. Moreover, the increasing number of industrial applications boosts the knowledge of their potential toxicological and environmental properties, as required by the EU regulation (REACH). In this context priorities have to be established by selecting reliable and representative toxicity tests on a limited number of informative ILs. Hence the need to predict solvents properties by quantitative structure-property relationship (QSPR) models based on *in silico* structural descriptors.

Such *in silico* descriptors can be calculated adopting a cheminformatic tool called VolSurf+.[44,45] It allows to explore the physicochemical space of a molecule from the 3D maps of interaction energy between the molecule and chemical probes (GRID-based Molecular Interaction Fields, or MIFs[46-49]) deriving the resulting physicochemical and ADME molecular descriptors (128 descriptors). The VolSurf+ procedure has been already successfully applied to study structure–permeation relationships,[44] to predict antitumour activities,[50-55] and more recently for modelling phospholipidosis induction,[56,57] representing a fundamental tool for the purposes of this thesis.

This approach would allow to gain a better knowledge on the relationships between *in silico* structural physico-chemical properties and toxicity on different biological targets. However, as a huge number of descriptors cannot be easily handled, we intended to revive interest on principal properties (originally intrinsic properties representative of experimentally observable macroscopic descriptors) by compacting the VolSurf+ parameters into few properties for heterocyclic cations and inorganic or organic anions. These new structural descriptors could be adopted for the selection or the design of ILs for specific green processes or products as well as for the assessment of the toxicity for more than 8000 ILs. The choice between adoption of the entire set of VolSurf+ descriptors, with a higher degree of information, or compacted ILs PPs, with a lower information content but easier to handle, will be data-driven following the ancient motto “Frustra fit per plura quod fieri potest per pauciora” (It is vain to do with many what can be done with few).

Having this in mind, the aim of my research has been to achieve a better and deeper knowledge about the environmental and scientific impact of ILs, in particular exploiting the potentialities of multivariate statistics. These approaches are the best tools to analyze many variables and conditions simultaneously,

with the purpose either to extract the most relevant information describing a dataset structure or to optimize a process, trying in both cases to recognize an eventual “systematic” pattern in the data. Several cheminformatic tools have been developed to achieve this goal, and herein presented and used two ones (PCA and PLS) considered to be the most appropriate for the purposes of this thesis, suitable to deal with many data and variables, resulting basically simple to use and to interpret, little time-consuming and, last but not least, not expensive at all.

2. Methods

2.1 Computational methods

VolSurf+ is a powerful cheminformatic tool aimed at producing and exploring the physico-chemical property space of a library of molecules starting from 3D maps of interaction energies between the molecule and chemical probes.

The interaction of molecules with biological membranes is mediated by surface properties such as shape, electrostatic forces, H-bonds and hydrophobicity. Therefore, the GRID[46] force field can be chosen to characterize potential polar and hydrophobic interaction sites around target molecules by the water (OH2), the hydrophobic (DRY), the carbonyl oxygen (O) and amide nitrogen (N1) probes. The information contained in the resulting MIFs (molecular interaction fields) is translated into a quantitative scale by calculating the volume or the surface of the interaction contours. In fact, in VolSurf+ 3D structures generation is automatically performed generating a bunch of minimized 3D structures of molecules in water and apolar solvents from which the best energy minima conformers are selected. All the remaining structures are used to derive conformational dependent descriptors, such as flexibility parameters, LogP, partition coefficient in non-water solvent, amphiphilic moments.

The VolSurf+ procedure can be summarized as in Fig. 2. In the first step, a three-dimensional map (3D map), is generated from the interactions of the OH2, DRY, O and N1 probes with a target molecule. In this 3D map each pixel contains information about a chemical property. The amount of information contained in a 3D map is related to the interacting molecular partners. The second step consists in the calculation of descriptors from the 3D maps obtained in the first step.

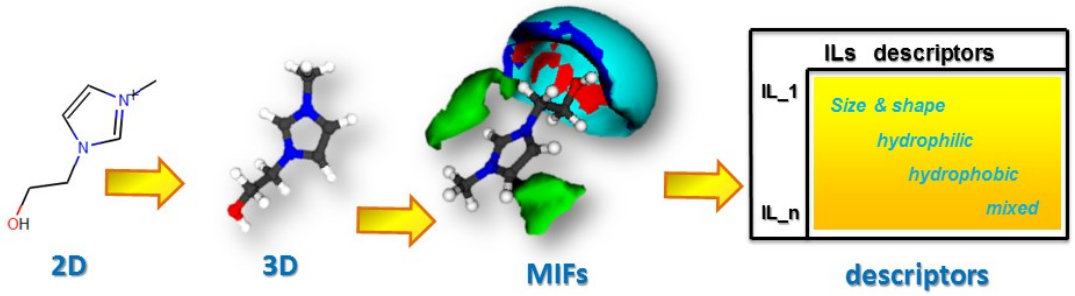


Fig. 2 Scheme showing the sequence of steps in VolSurf+.

The molecular descriptors calculated by means of VolSurf+ refer to molecular size and shape, to hydrophilic and hydrophobic regions and to the balance between them, to molecular diffusion, to partition coefficient in different solvents, to pH-dependent water solubility and molecular flexibility in different solvents, to the “charge state” descriptors, to the new 3D pharmacophoric descriptors and to

some descriptors on some relevant ADME properties. The definition of all 128 VolSurf+ descriptors is given in case studies[44,53-60] with the previous versions of VolSurf+ and reported in detail in Table C1 (in the Appendix section).

The SIMCA (Soft Independent Modelling of Class Analogy) package[61] was then used to derive PCA models as in section 3.2 and PLS models correlating cations and anions VolSurf+ descriptors or PPs to ILs physico-chemical properties or toxicities as below reported.

PCA (Principal Component Analysis)[62] is an extremely useful technique to compact the most relevant information present in a data matrix (containing objects and related variables) into a simplified and more understandable form. Data are pre-processed by autoscaling all variables to unitary variance, *i.e.* by multiplying the variables by appropriate weights (usually the reciprocal of the variable standard deviation) to give them unit variance (*i.e.* the same importance) after subtracting the mean value. PCA works by decomposing the matrix as the product of two smaller matrices (as eq. 1 expresses in a simplified version), the loading and score matrices. The loading matrix (P) contains information about the variables: it is composed of few vectors (Principal Components, PCs) which are linear combinations of the original variables. The score matrix (T) contains information about the objects: each object is described in terms of its projections onto the PCs, representing the scores, instead of the original variables. The information not contained in these matrices remains as "unexplained X-variance" in a residual matrix (E).

$$X = TP + E \qquad \text{(eq. 1)}$$

The PCs, among many others, have two interesting properties: they are extracted in decreasing order of importance: the first PC always containing more information than the second, the second more than the third and so on. Moreover they are orthogonal to each other: there is no correlation between the information contained in different PCs.

In PCA, each new extracted PC increases the amount of information (the variance, expressed by the R^2 parameter indicating the goodness of fit) explained by the model. However, usually the first four of five PCs explain more than 90% of the variance. There is no simple or unique criterion to decide how many PCs should be considered as significant. From a theoretical point of view, it is possible to use cross-validation techniques to decide the number of significant PCs evaluating the predictability of variation (Q^2) of each component and all together (see below).

The Partial Least Squares Projections to Latent Variables (PLS)[63] analysis is a regression technique whose goal is to explain one or more dependent variables (Y's) in terms of a number of explanatory variables (X's, contained in the X-matrix) according to equation 2.

$$Y = f(X) + E \qquad \text{(eq. 2)}$$

It is possible to build many different models that fulfill the above equation. Different methods produce models that "fit" the Y's more or less accurately. Among them, the best one will be able to calculate Y

values that correspond to the experimental ones, even for molecules not included in the building model (or learning) set. Consequently, this model becomes "predictive" and can be used to calculate reliable estimations of Y values for new molecules, prior to their availability. It is important to note that the Y variables, like any other experimental variable, contain an error. The models will try to fit the Y as much as possible (increasing R^2 parameter) but trying to improve too much the fitting, the model will include also some noise. This phenomenon, called overfitting, is very dangerous because overfitted models appear to be statistically very significant (having high R^2) but often prove to be useless in prediction for Y's of objects not included in the learning set (low or negative Q^2). An interesting example on overfitting is given in section 3.4.3-III. Even if the 3D-QSPR models are approximate and are not able to explain the activity values to a full extent, they are extremely valuable to identify the X-variables that contribute most to the activity.

In 3D-QSPR often the X-matrix contains much fewer objects (molecules) than variables. In these situations, the classical regression technique, Multiple Linear Regression (MLR) is not a suitable statistical approach. There are many reasons, but, among others: i) MLR was developed to deal with situations in which the number of objects is three times at least larger than the number of variables. This inconvenience can be overcome by using stepwise MLR, but then there is a high probability of obtaining relationships just by chance. ii) MLR assumes that the X-variables are "independent" and not correlated to each other. It is known that variables do not often fulfill these requirements, especially in real biological or chemical fields. In fact, the only regression method than can deal with the kind of X-matrices used in 3D-QSPR is PLS. It works on pre-treated data, decomposing the X-matrix as the product of two smaller matrices, much like PCA does. The weight (concept similar to the PCA loadings, and often so called) matrix contains information about the variables. It contains few vectors (Latent Variables, LVs) which are linear combinations of the original X-variables. The concept of LV is quite equivalent to the PC in PCA. The score matrix (T) contains information about the objects. Each object is described in terms of the LVs, as in PCA. The main difference is that PCA obtains the PCs that represent at best the structure of the X-matrix and PLS obtains the LVs under the following constraints: they have to represent the structure of the X-matrix and Y-matrix and maximizing the correlation between the X's and the Y's.

The LVs share some important properties with the PCs: they are extracted in decreasing order of importance and each LV is orthogonal to each other. For the purposes of the present work, no distinction will be made between PCs and LVs, and they will be indistinctly named as principal components (PCs) hereinafter.

In PLS selecting the correct dimensionality is of critical importance. When too many PCs are included a serious overfitting danger will result and the model will have little or no validity (high R^2 but low or negative Q^2). To check how many PCs to include it is strictly necessary to test the predictive ability of the model. The predictive ability of a PLS model is usually evaluated by using cross-validation (CV). One

of the main reliable CV process works building reduced models (models for which some of the objects were removed) and using them to predict the Y-variables of the held-out objects. Then the predicted Y is compared with the experimental Y, and for each model the following dimensionality indexes are computed:

-SDEP or Standard Deviation of Errors of Prediction:

$$\text{SDEP} = \sqrt{\sum \frac{(Y-Y')^2}{N}}$$

-Q^2 as Predictive correlation coefficient (referring to the model predictability as the fraction of the total variation of the Y's predicted by each or all PLS components):

$$Q^2 = 1 - \frac{\sum(Y-Y')^2}{\sum(Y-\acute{Y})^2}$$

(Y : Experimental value; Y' : Predicted value; Ý: Average value ; N: Number of objects).

The CV technique is very valuable because it performs an "internal validation" of the model and obtains an estimation of the predictive ability without the help of external datasets. This is particularly important in QSAR studies, where the number of objects available is usually small, and it is not affordable to remove objects from the learning dataset. One of the main inconveniences of CV is that there is not a general agreement on how to build the reduced groups and on the criterion to decide how many objects to keep. SIMCA, by default, divides dataset into *n* (often 7) groups, each one containing an equal (or nearly equal) number of objects. Then models are built keeping one of these groups out of the analysis until all of the objects are kept out once. The procedure should be repeated many times, in order to obtain stable results. For this procedure the Standard Deviation of SDEP gives an estimate of the dispersion of the SDEP values obtained from different runs.

Another or complementary way to evaluate the predictive ability of the model is to use an external prediction set. In this approach the objects in the original dataset are split up into two groups from the very beginning of the analysis. The first one, the learning set, will be used to build the PLS model. The other, the prediction (or validation) set, will be used to compare their experimental Y-values with the predictions made by the PLS model. There is no doubt that this technique is more realistic to test the predictive ability. However it can be argued that the results depend critically upon how many and which objects are assigned to each group. Also, datasets in QSAR often contain too few objects and it is not possible to remove objects from the analysis without a loss of information.

The **OPLS** (Orthogonal PLS),[64-66] a modification of the PLS method,[67] separates the systematic X-variation in two parts, one that is linearly related to Y and one that is unrelated (orthogonal) to Y. This partitioning of the X-data facilitates model interpretation and improves model predictivity.[64-66] The OPLS model comprises two modelled variations, the Y-predictive (TPPp T) and the Y-orthogonal (TOPO T) components. Only the Y-predictive variation is used for the modelling of Y (TPCP T).

Model of X: X= TPPp T + TOPO T +E (eq. 3)

Model of Y: Y= TPCP T +F (eq. 4)

(E and F are the residual matrices of X and Y, respectively).

The statistical results obtained by the PLS or OPLS method are able to detect what variables in the X-block are relevant to determine the dependent variables (Y-block) by means of the VIP (Variables Importance for the Projection) values. The VIP values reflect, in fact, the importance of terms in the model both with respect to Y, *i.e.* its correlation to all the responses, and with respect to X, *i. e.* in explaining X-variation. The VIP values are calculated for each X-variable by summing the squares of the PLS loading weights multiplied by the amount of sum of squares explained in each model component.[61]

In PLS, Q^2 assesses the predictive power of the model and a permutation plot is a further cheminformatic tool (available in SIMCA[61]) useful to check the significance of a PLS model and the reliability of its Y-predictions. In fact, the purpose of this validation tool is to compare the goodness of the original model fit (R^2 and Q^2) with the goodness of fit of several models based on data where the order of the Y-observations has been randomly permuted, while the X-matrix has been kept intact. The permutation plot shows R^2 and Q^2 values on the vertical axis: far to the right the parental PLS model parameters, while the Y-permuted models ones are on the left. The horizontal axis shows the correlation between the permuted Y-vectors and the original Y-vectors. The original parameters have correlation 1 with themselves. In order to have a valid plot[61]

-all Q^2-values on the left should be lower than the original points to the right.

or

-the regression line of the Q^2-points should intersect the vertical axis (on the left) at or below zero.

The R^2-values provide often an optimistic estimate, but when the R^2-values on the left are lower than the original point to the right, this supports the validity of the original model.

For the models presented herein, 50 permutated models were derived for each PLS correlation model.

2.2 Experimental

2.2.1 Materials, synthesis and characterization of ILs

Commercially available compounds were used directly without any preliminary treatment. *1-Butyl-3-methylimidazolium tetrafluoroborate* (IM14 BF4) was purchased from Sigma-Aldrich. *1-Butyl-3-methylimidazolium tricyanomethanide* (IM14 C(CN)3), *1-butyl-3-methylimidazolium dimethylphosphate* (IM14 (1O)2PO2), *1-butyl-4-methylpyridinium tricyanomethanide* (Py4-4Me C(CN)3), *1-butyl-4-methylpyridinium chloride* (Py4-4Me Cl) and *1-hexyl-3-methylimidazolium chloride* (IM16 Cl) were purchased from Io.Li.Tec. Solvents, HBF_4 solution (50/50, w/w) and Amberlite IRA-400 resin were used as purchased without further purification.

The general procedure for the synthesis of *1-butyl-3-methylimidazolium acetate and trifluoroacetate* (IM14 1COO, IM14 CF3COO) and *1-hexyl-3-methylimidazolium* salts (*tetrafluoroborate*, *acetate* and

trifluoroacetate, or IM16 BF4, IM16 1COO, IM16 CF3COO respectively) from the corresponding halides is reported below. All ionic liquids were dried on a vacuum line at 60 °C for at least 2 h before use, then stored in a dryer under argon and over calcium chloride. In all cases, the silver nitrate test, performed to verify the presence of residual halide anion, gave a negative result.

The Amberlite resin IRA-400 (16 g) was converted from chloride form to hydroxide form by eluting an aqueous solution of NaOH (10 mL, 10% w/v) within a column. Subsequently the resin was washed with water until the eluate was neutral. The halide salt(s) (10 mmol), dissolved in methanol/water (70/30, v/v), was eluted, and the eluate collected into a flask containing a solution of the corresponding acid in stoichiometric amount, until neutralization. The resulting solution was concentrated *in vacuo*, then treated with activated charcoal in ethanol. Filtration and removal of the solvent afforded the ionic liquids as viscous oils in high to quantitative yields. The products structures were confirmed by NMR spectra and are in agreement with literature data.[68-72]

1-Hexyl-3-methylimidazolium tetrafluoroborate (IM16 BF4). Pale yellow oil. Yield: 100%. ^{1}H NMR (300 MHz, $CDCl_3$): δ=8.70 (s, 1 H), 7.21 (d, *J*=14 Hz, 2 H), 4.17 (t, *J*=6 Hz, 2 H), 3.94 (s, 3 H), 1.87 (m, 2 H), 1.31 (m, 6 H), 0.87 (t, J=6 Hz, 3 H) ppm. ^{13}C NMR (300 MHz, $CDCl_3$): δ= 135.8, 123.4, 121.9, 50.0, 36.2, 31.1, 29.0, 25.9, 22.3, 13.8 ppm.

1-Hexyl-3-methylimidazolium acetate (IM16 1COO). Pale yellow oil. Yield: 99%. ^{1}H NMR (300 MHz, d_6-DMSO): δ=9.44 (s, 1 H), 7.74 (d, *J*=24 Hz, 2 H), 4.15 (t, *J*=7 Hz, 2 H), 3.85 (s, 3 H), 1.77 (quint, *J*=6.8 Hz 2 H), 1.56 (s, 3 H), 1.26 (m, 6 H), 0.85 (t, *J*=7 Hz, 3 H) ppm. ^{13}C NMR (300 MHz, d_6-DMSO) δ= 173.8, 137.9, 124.1, 122.0, 49.0, 36.0, 31.1, 30.2, 29.8, 25.9, 24.6, 22.4 ppm.

1-Hexyl-3-methylimidazolium trifluoroacetate (IM16 CF3COO). Pale yellow oil. Yield: 96%. ^{1}H NMR (300 MHz, d_6-DMSO): δ=9.15 (s, 1 H), 7.74 (d, *J*=26 Hz, 2 H), 4.13 (t, *J*=8 Hz, 2 H), 3.82 (s, 3 H), 1.73 (quint, *J*=8 Hz, 2 H), 1.25 (m, 6 H), 0.85 (t, *J*=7 Hz, 3 H) ppm. ^{13}C NMR (300 MHz, d_6-DMSO): δ= 158.0, 137.2, 124.1, 122.1, 49.24, 36.1, 30.9, 30.2, 29.9, 25.6, 22.3, 14.2 ppm.

1-Butyl-3-methylimidazolium trifluoroacetate (IM14 CF3COO). Pale yellow oil. Yield: 94%. ^{1}H NMR (300 MHz, d_6-DMSO): δ=9.34 (s, 1 H), 7.91 (d, *J*=24 Hz, 2 H), 4.33 (t, *J*=8 Hz, 2 H), 4.01 (s, 3H), 1.93 (quint, *J*=7.6 Hz, 2 H), 1.40 (quint, *J*=7.6 Hz, 2 H), 1.07 (t, *J*=7.6 Hz, 3 H) ppm. ^{13}C NMR (300 MHz, d_6-DMSO): δ= 158.0, 139.4, 125.3, 122.1, 50.4, 37.1, 30.9, 30.2, 22.4, 17.6 ppm.

1-Butyl-3-methylimidazolium acetate. (IM14 1COO). Pale yellow oil. Yield: 99%. ^{1}H NMR (300 MHz, d_6-DMSO): δ=9.73 (s, 1 H), 7.88 (d, *J*=21 Hz, 2 H), 4.24 (t, *J*= 7.6 Hz, 2 H), 3.92 (s, 3 H), 1.82 (quint, *J*=7.5 Hz, 2 H), 1.64 (s, 3 H), 1.29 (quint, *J*=7 Hz, 2 H), 0.95 (t, *J*=7 Hz, 3 H) ppm. ^{13}C NMR (300 MHz, d_6-DMSO) δ= 172.9, 137.4, 123.7, 122.4, 59.2, 48.5, 35.7, 25.9, 18.9, 13.4 ppm.

1-butyl-4-methylpyridinium tetrafluoroborate (Py4-4Me BF4) requested a different synthetic procedure. 2 g (10.7 mmol) of 1-butyl-4-methylpyridinium chloride were dissolved in 30 mL of anhydrous CH_2Cl_2

under Argon athmosphere, and 1.17 g (10.7 mmol) of $NaBF_4$ were added. The solution was stirred for 24h. The suspension was filtered and washed with anhydrous dichloromethane to remove the precipitated sodium chloride salt, then the organic phase was filtered on alumina and charcoal (to remove residual impurities) and washed with small volumes of water. The absence of residual halides was verified by silver nitrate test. The solvent was removed *in vacuo* and no further treatments were needed. The organic salt was recovered as a pale yellow oil with 80.8 % of yield, and the structure confirmed by the NMR spectra in agreement with literature data.[68]

^{1}H NMR (500 MHz, DMSO): δ=8.87 (d, *J*=6.5 Hz, 2 H), 7.95 (d, *J*=6.5 Hz, 2 H), 4.50 (t, *J*=7.5 Hz, 3 H), 2.59 (s, 3 H), 1.86 (m, *J*=7.5 Hz, 2 H), 1.26(m, *J*=7.5 Hz, 2 H), 0.90 (t, *J*=7.5 Hz, 3 H) ppm. ^{13}C NMR (500 MHz, DMSO): δ=159.3, 144.1, 128.8, 60.2, 32.9, 21.8, 19.2, 13.7 ppm.

2.2.2 E_{NR} measurements

The determination of the polarity parameter E_{NR}[73] was carried out by mixing into a quartz cuvette (optical path 0.2 cm), 500 µL of IL and 75 µL of a concentrated solution of the solvatochromic probe (Nile Red, NR) in 1,4-dioxane. The concentration of the probe was equal to 2.0 10^{-4} M. The obtained solution was thermostated at 298 K.

2.2.3 Heat capacity measurements

The heat capacities (C_p) were measured by means of DSC analysis carrying out experiments on a Linseis STA PT 1600 instrument at atmospheric pressure over the temperature ranging from 303 to 353 K. Samples (20.0 ± 0.1 mg) were heated in a platinum sample boat up. In accordance with Chiu[74] a method was created to hold isothermally at the desired starting temperature (298 K) for 10 min, then heating at 5 K/min up to 353 K, then holding at this temperature for 10 min. The purge gas used was nitrogen with a flow rate of 50 cc/min. Water was used as standard to check the heat capacity measurements according to the method reported by Chiu.[74]

3. Results and Discussion

3.1 ILs *in silico* descriptors

3.1.1 ILs VolSurf+ descriptors

128 cationic *in silico* descriptors (Table C1)[75] were calculated by importing the corresponding SMILES codes in VolSurf+ and using the aforementioned steps. Derivation of the anions descriptors required a slightly different procedure as compared to that adopted for organic ILs cations.

It is well known that small negative ions like halides do not exist in solution as free compounds. Rather they are complexed by water molecules producing hydrated complexes.[76] Therefore halides ($Cl^-/Br^-/I^-$) were initially imported in Sybyl[77] where a solvation shell was created within 3 Å sphere by using three water molecules selected around the ions. Next, the hydrated ions have been processed (as .kout files) using the GRID force field to produce the corresponding MIFs. All the other ions, including ions containing metals or phosphorus, were directly imported by means of their SMILES codes in GRID force fields without hydration shell. Finally VolSurf+ was used to convert the MIFs into molecular descriptors. It is noteworthy that, due to the different information embedded in the file format, a large number of VolSurf+ anionic descriptors results not to be generated. Thus, only 48 non-zero variables (see Table C2) were extracted as anions descriptors.[75]

3.1.2 ILs Principal properties

VolSurf+ allowed to derive reliable descriptors for a large number of compounds, either when physico-chemical characteristics are scattered in literature and can be hard collected or organic structures result not synthesized and therefore their properties are not available. Nevertehless, handling hundreds descriptors, especially for very big data matrices, could be very difficult. Reducing ILs descriptors was a prerogative in our studies. Furthermore, it was necessary to make simpler our QSPR studies limiting ILs descriptors but not losing relevant information. A solution could be the parameterization of variables into few intrinsic properties (the so-called Principal Properties, or PPs) by means of the PCA algorithm summarizing many parameters into few ones, more easy to use and to interpret. VolSurf+ *in silico* descriptors are related to molecular properties such as hydrophobic/hydrophilic balance, solubility, organic solvent/water partition coefficients, H-bonding ability both as donor and acceptor, as well as flexibility and skin permeability. Consequently PPs were expected to have a great potential for modelling biological activities and physico-chemical properties for a large number of ILs.

I. Principal properties for cations (PP+)

PPs depend on the number of objects selected as learning set and on their "structural" features. The Principal Component Analysis approach is an “open” statistical procedure leaving the choice of the data matrix to the user, who has to decide which is an optimal balance between model (and therefore PPs) generality and prediction ability. In our case the generality of cationic structures was privileged by including as objects 218 different heterocyclic aromatic and non-aromatic cationic cores (imidazolium, pyridinium, quinolinium, piperidinium, pyrrolidinium, morpholinium) for the derivation of cationic PPs. Cation structures were imported in VolSurf+ by using their SMILES codes (Table B1[78] in Appendix section). Then, a PCA model was carried out on a data matrix containing 218 cations. A 5 PCs (Principal Components) model explains 77.5 % of variance (see Table A1[78] in Appendix section). All 5 PCs can be considered significant for the above PLS model. Therefore, the scores for the 218 cations can be selected as cationic PPs (Table B1).[78]

In the above model, the 1st and the 2nd PC explain 54.3% of total variance. In the corresponding loadings plot (Fig. 3)[78] variables referring to hydrophobic interactions ( and  on the plot, or 13-20 and 49-56 in Table C1)[78] are located in the bottom left quadrant, whereas those related to hydrophilic interactions ( ,  and  or 5-12, 21-32 and 37-44 respectively) are in the upper right one. In the same upper right quadrant but closer to zero for p[2] (*i.e.* providing lower information) we find descriptors related to the unbalance of hydrophilic and hydrophobic regions with respect to the molecular barycenter ( and  , and 33-36 and 45-48 variables). In the bottom right quadrant there are solubility in water descriptors ( and  , or 98-108), while on the opposite quadrant (upper left) organic solvent/water partition coefficients ( and  or 67;68 and 73-79) together with molecular weight ( , 62), flexibility ( , 63-64), molecular volume and surface (,  , 1-2), and skin permeability ( , 112). Descriptors related to H-bonding ability ( and 21-26 as donor;  and 27-32 as acceptor) are in the upper right quadrant. Comparison of the loadings plot with the scores plot, reported in Fig. 4[78] (see Fig. A1[78] for a simplified plot in Appendix section), evidences the descriptors influence on the structural features of cations. In the bottom left quadrant are present cations characterized by long alkyl chains increasing hydrophobic interactions, while, on decreasing the alkyl chain length, cations move towards the right part of the scores plot driven by an increasing importance of solubility descriptors (see above). Finally, cations having oxygenated chains (such as *O*-ether) and poly-oxygenated ones (such as *O*-ester or carboxylic) move upward along the 2ndPC (t[2]) due to their increasing ability to give H-bonds (Fig. A1).[78] Moreover the 1st PC (t[1]) discriminates morpholinium and piperidinium cations, exhibiting positive t[1] score values, from quinoliniums with negative t[2] score values.

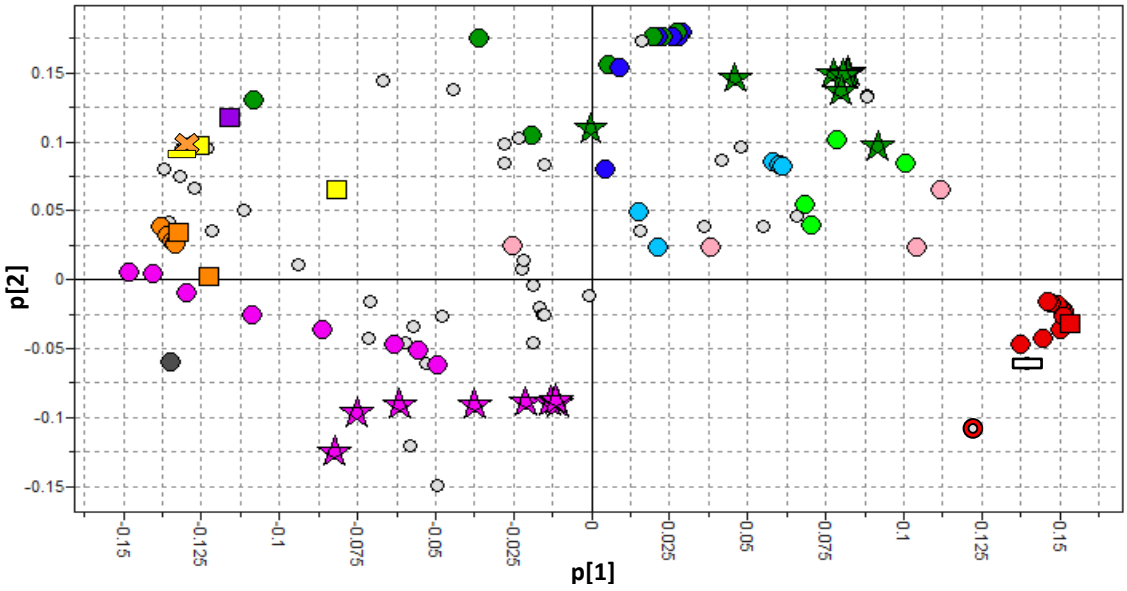


Fig. 3 p[1]-p[2] loadings plot reporting cations model descriptors. W1-W8; D1-D8; WO1-WO6; WN1-WN6; IW1-IW4; CW1-CW8; ID-ID4; CD1-CD8; HL1, HL2; MW; Flex, Flex_RB; LogP org. solv./water; LgD5-LgD10; S; V; %FU4-%FU10; SOLY; LgS3-LgS11; DIFF; CACO2; SKIN; lgBB; MetStab; *others*. See Table C1 for descriptors code explanation.

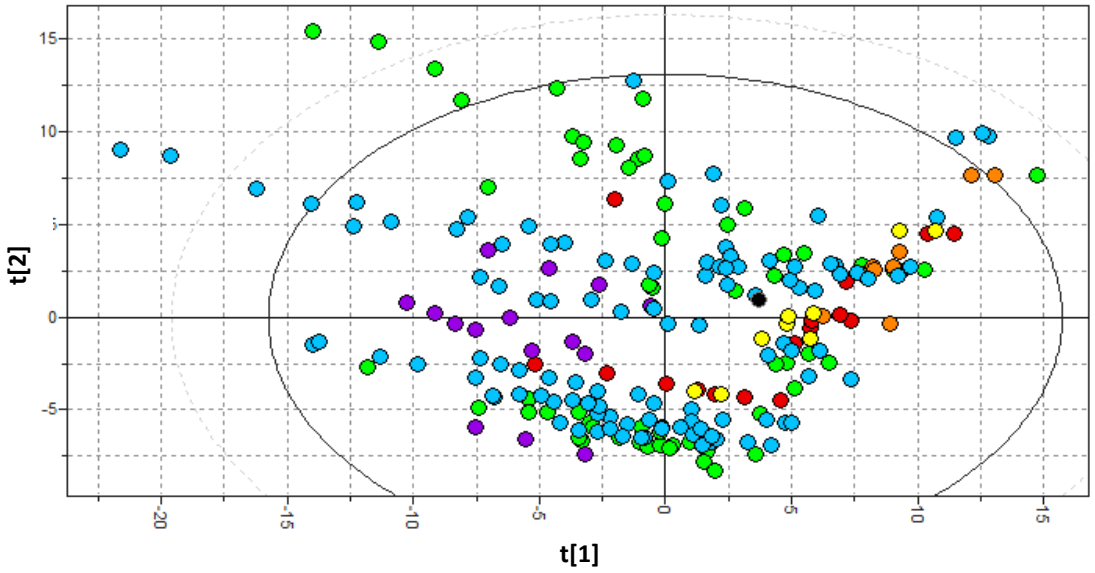


Fig. 4 t[1]-t[2] scores plot reporting the 218 cations coloured on the basis of their scaffolds: imidazoliums; pyridiniums; quinoliniums; pyrrolidiniums; morpholiniums; piperidiniums; diaza bicyclooctanium. See Fig. A1 for a more simplified scores plot.

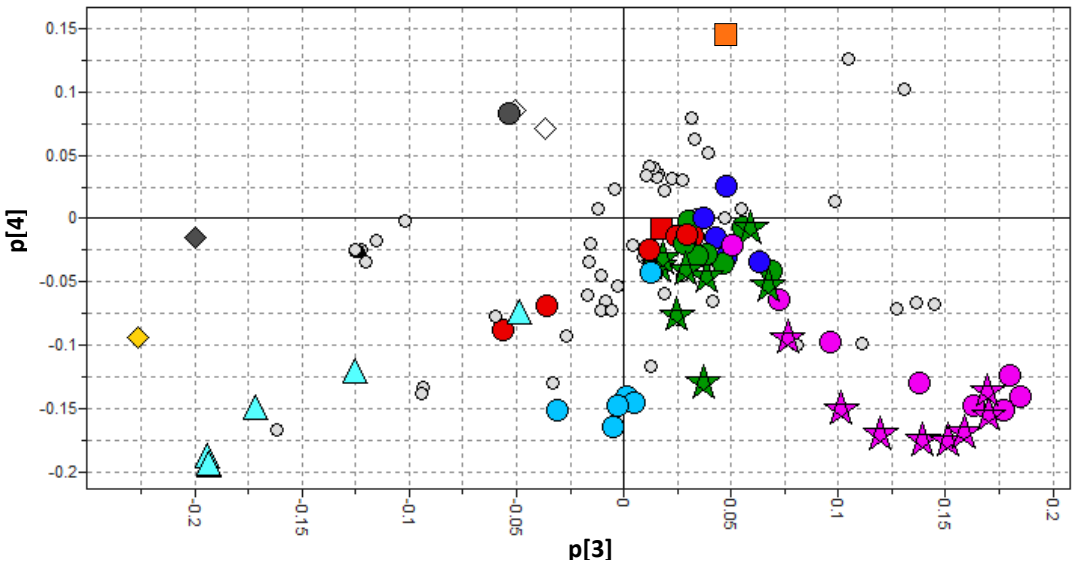


Fig. 5 p[3]-p[4] loadings plot reporting cations model descriptors. ● W1-W8; ● D1-D8; ● WO1-WO6; ● WN1-WN6; ● IW1-IW4; ★ CW1-CW8; ● ID-ID4; ★ CD1-CD8; ◇ HL1, HL2; ▲ %FU4-%FU10; ■ SOLY; ● LgS3-LgS11; ■ LogP org. solv./water ; ◆ CACO2; ● SKIN; ◆ lgBB; ● *others.* See Table C1 for descriptors code explanation.

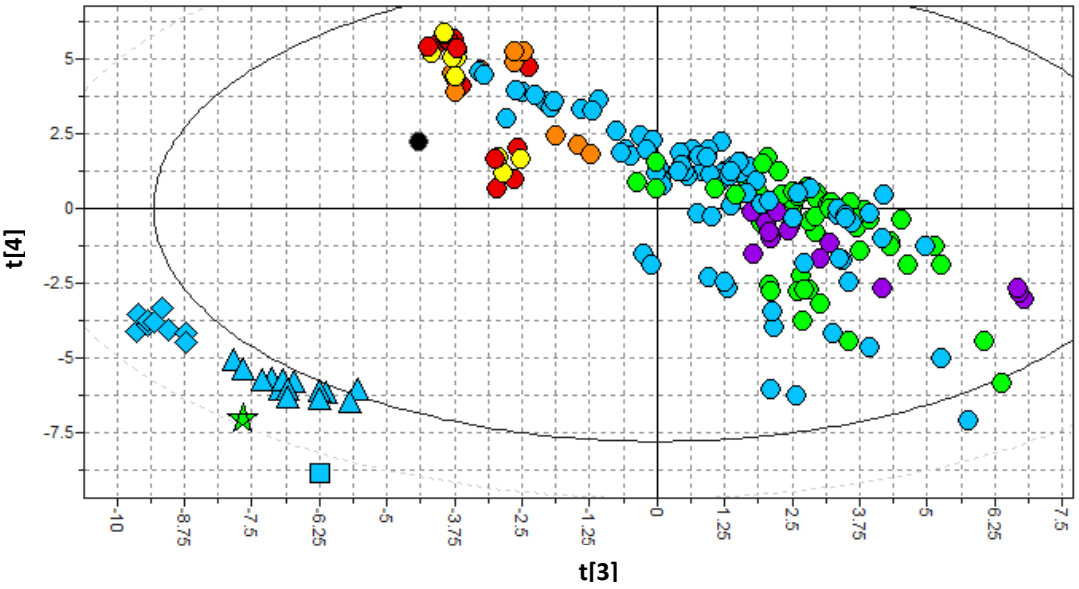


Fig. 6 t[3]-t[4] scores plot reporting the 218 cations coloured on the basis of their scaffolds: ● *N*,*N*-substituted imidazoliums; ◆ *N*-alkyloxymethyl substituted imidazoliums; ▲ *N*-alkyl substituted imidazoliums; ■ cat. 144 in Table B1; ● *N*-substituted pyridiniums; ★ unsubstituted pyridinium; ● quinoliniums; ● pyrrolidiniums; ● morpholiniums; ● piperidiniums; ● diaza bicyclooctanium.

The 3rd PC evidences the difference between more amphiphilic ILs from those with a higher hydrophobic character. On the upper left quadrant of the p[3]-p[4] loadings plot (Fig. 5)[78] we find few descriptors such as skin permeability (●, 112), and hydrophilic/hydrophobic ratio (◇, 57-58) . On the bottom left quadrant there are variables describing permeability into CACO2 cells (◆, 111), blood-brain barrier permeation (◆, 113), ability to form H-bonds as donor (●, 21-26) and, moving from zero to highly negative p[3] and p[4], loading values descriptors related to percentage of unionized species at different pH in the range 4-10 (▲, 81-87). In the corresponding bottom left scores plot quadrant (Fig. 6)[78] a clear clustering of imidazolium scaffolds with endocyclic NH groups (▲ *N*-alkylimidazoliums and ◆ *N*-alkyloxymethyl-imidazoliums) capable of H-bonding donation can be observed, together with other H-bond donors such as unsubstituted pyridinium (★) and imidazolium with an ethanol substituent (■). Furthermore mono alkyloxy substituted imidazoliums (◆) appear to be superimposable to the blood-brain barrier permeation descriptor in the corresponding loadings plot, suggesting that these cations possess a high ability to cross the blood brain membrane. It is worth mentioning that all the above cations exhibit pK_a values below 7, and consequently lose their cationic character on increasing pH; this finding is in agreement with the position of the descriptors related to the percentage of unionized species (▲ in Fig. 5,[78] %FU4 - %FU10 from the right to the left in the bottom left quadrant) in the lower left region of the loadings plot. In Fig. 6[78] cations with morpholinium, pyrrolidinium, and piperidinium scaffolds are all in the upper left quadrant, while pyridinium and quinolinium cations exhibit positive t[3] score values. Moving on the diagonal from the upper left to the bottom right of the loadings plot (Fig. 5),[78] we find solubility (■ and ●, 98-108) interaction with water (● and ★, 5-12 and 37-44) and H-bond acceptor descriptors (●, 27-32), and then hydrophobic interaction ones (● and ★, 13-20 and 49-56). Moving along the same direction in the corresponding scores plot (Fig. 6)[78] we find imidazolium and pyridinium cations bearing substituents which increase hydrophobic interactions capability.

The 5th PC is mainly required to discriminate H-bond donor descriptors (●, 21-24) exhibiting high p[5] loading values from H-bond acceptor descriptors (●,●, ★ and ▲, ▼ or 32, 12, 44 and 91, 94) having highly negative p[5] loading values (Fig. 7).[78] Consequently in the corresponding scores plot (Fig. 8)[78] cations with H-bond donor OH groups are in the upper part of the plot and cations with strong H-bond acceptor capability exhibiting t[5] score values below -7.5 due to the presence of six carbonyl or ether oxygen atoms (see cations evidenced in Fig. 8).[78]

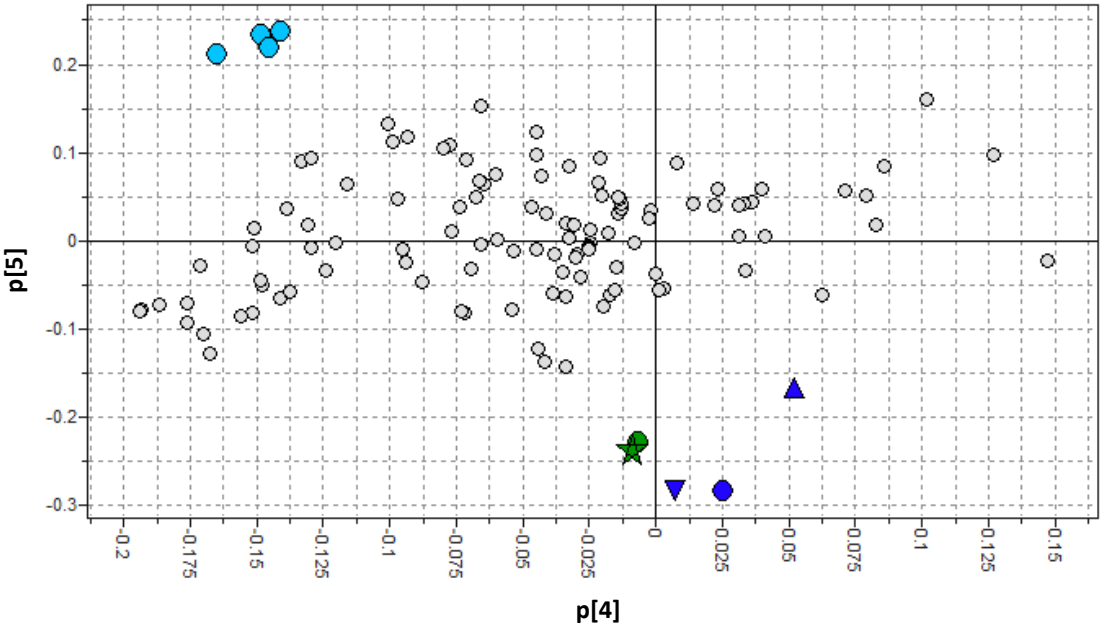


Fig. 7 p[4]-p[5] loadings plot reporting cations model descriptors. ● WO1-WO4; ● WN6; ▲ DRACAC; ▼ ACACAC; ● W8; ★ CW8; ● *others.* See Table C1 for descriptors code explanation.

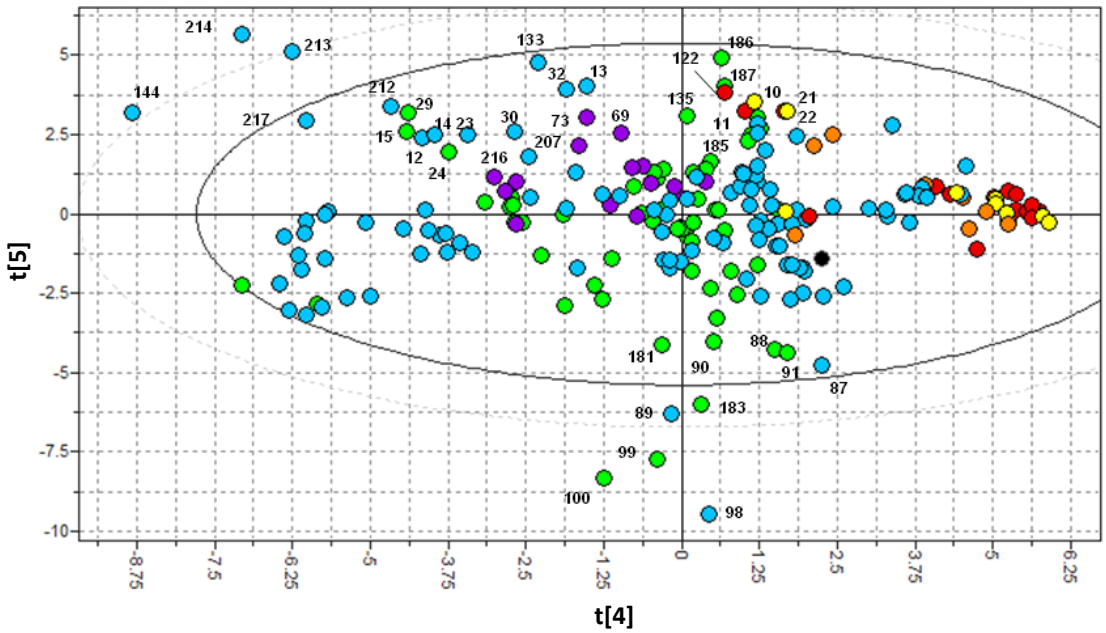


Fig. 8 t[4]-t[5] scores plot reporting cations. ● imidazoliums; ● pyridiniums; ● quinoliniums; ● pyrrolidiniums; ● morpholiniums; ● piperidiniums; ● diaza bicyclooctanium. See Table B1 for evidenced cations labels.

II. Principal properties for anions (PP-).

VolSurf+ was also used to derive a PCA model on a data matrix containign 38 ILs anions as objects (anions list and corresponding SMILES codes in Table B2)[78] and 48 variables (reported in Table C2).[75] This model gave four significant principal components that altogether explained 73.5% of the variance, with the 1st PC describing alone the 27.5% of the variance (Table A2).[78]

Looking at the p[1]-p[2] loadings plot (Fig. 9),[78] the 1st component discriminates anions according to their hydrophobicity/hydrophilicity. Indeed, the main hydrophobic descriptors D1-D8 and CD1-CD8 (and on the plot, or 13-20 and 49-56 in Table C1[75] respectively) are all located on the left, while the corresponding hydrophilic descriptors W1-W8 and CW1-CW8 (and on the plot or 5-12 and 37-44 respectively) are found in the opposite region of the plot. Also HL1 and HL2 (, or 57,58) variables are located on the right in the plot, in agreement with the high hydrophilicity explained. The analysis of the corresponding t[1]-t[2] scores plot (Fig. 10)[78] indicates that the 1st component mainly distinguish two anions (tetracyanoborate and tricyanomethanide, 4 and 7 in Table B2[78] respectively) among the other objects in the matrix. Tetracyanoborate and tricyanomethanide are hydrophobic anions, used to generate hydrophobic ILs[79] and also used to prepare dye-sensitive solar cells. The two anions also seem to share similar behavior when used to prepare ionic liquids. Moreover, a low viscosity is associated to the use of these anions.[80,81]

In the p[3]-p[4] loadings plot (Fig. 11),[78] the PC [3] has high positive loadings for four VolSurf+ descriptors related to the size/shape of the anions: V, S, R and G (, , , , 1-4). Furthermore, among the W1-W8 (, 5-12) descriptors, only W1-W5 rely in the right region of the plot, while W6-W8 are oppositely located on the left side. In VolSurf+, the W1-W4 descriptors are related to hydrophilicity due to polarizability, while W5-W8 are related to hydrophilicity due to the ability of an object to form H-bonds as donor or acceptor. The variables IW1-IW4 (, 33-36) are also located in the upper-left region of the plot. Based on these considerations, in the corresponding scores plot (Fig. 12)[78] highly polarizable anions having large and globular size should be situated on the right along the t[3], while small hydrophilic anions more suitable to give H-bond interactions and with the polar features well localized in a portion of the anions should rely in the upper-left side of the t[3]-t[4] scores plot.

Indeed, large and bulky anions such as tris(trifluoromethylsulfonyl)methide, tris(pentafluoroethyl)trifluorophosphate and tris(heptafluoropropyl)trifluorophosphate (8, 32, 33 in Table B2)[78] are disposed on the right region of the plot, while acetate, 2-(S)-hydroxypropanoate and, 2-(R)-hydroxypropanoate (15-17 in Table B2),[78] all bearing a carboxylate moiety able to give H-bonds as acceptors and responsible for a localization of the charge in a portion of the anions, are located in the upper left region.

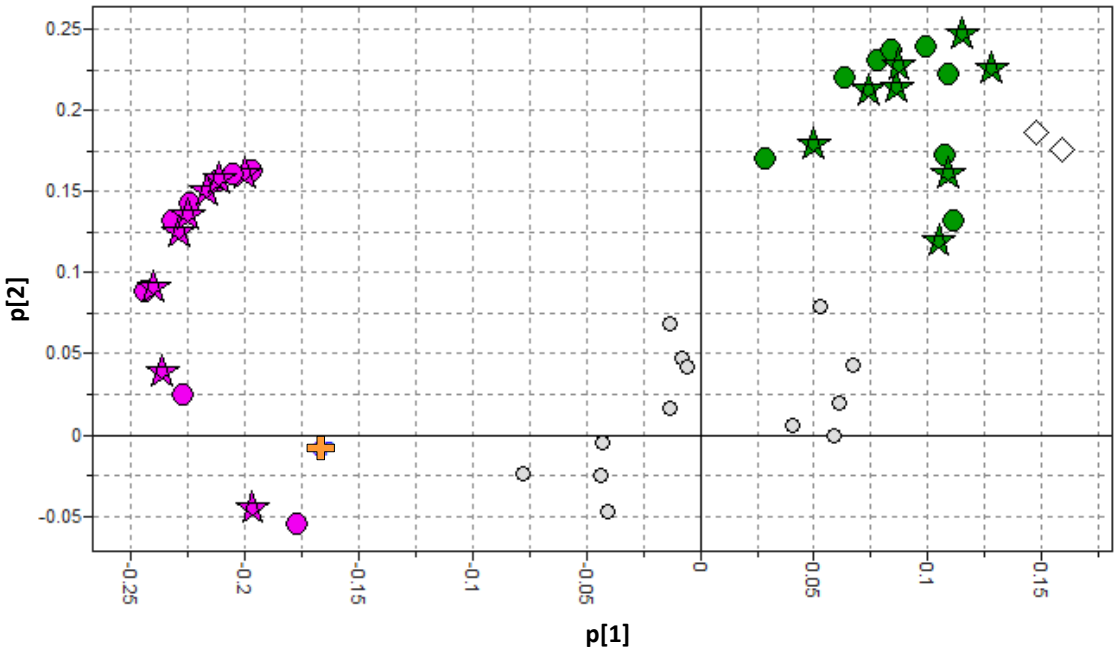


Fig. 9 p[1]-p[2] loadings plot reporting anions model descriptors. ● W1-W8; ● D1-D8; ● IW1-IW4; ★ CW1-CW8; ★ CD1-CD8; ✚ CP; ◇ HL1, HL2; ● *others.* See Table C1 for descriptors code explanation.

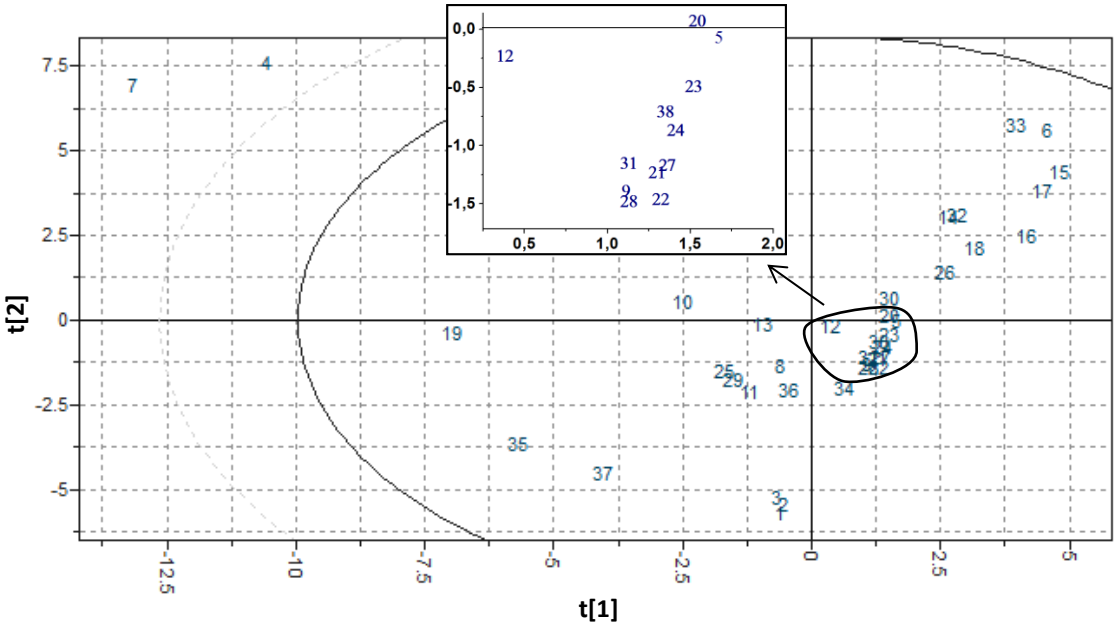


Fig. 10 t[1]-t[2] scores plot reporting anions. Object labels reported in Table B2.

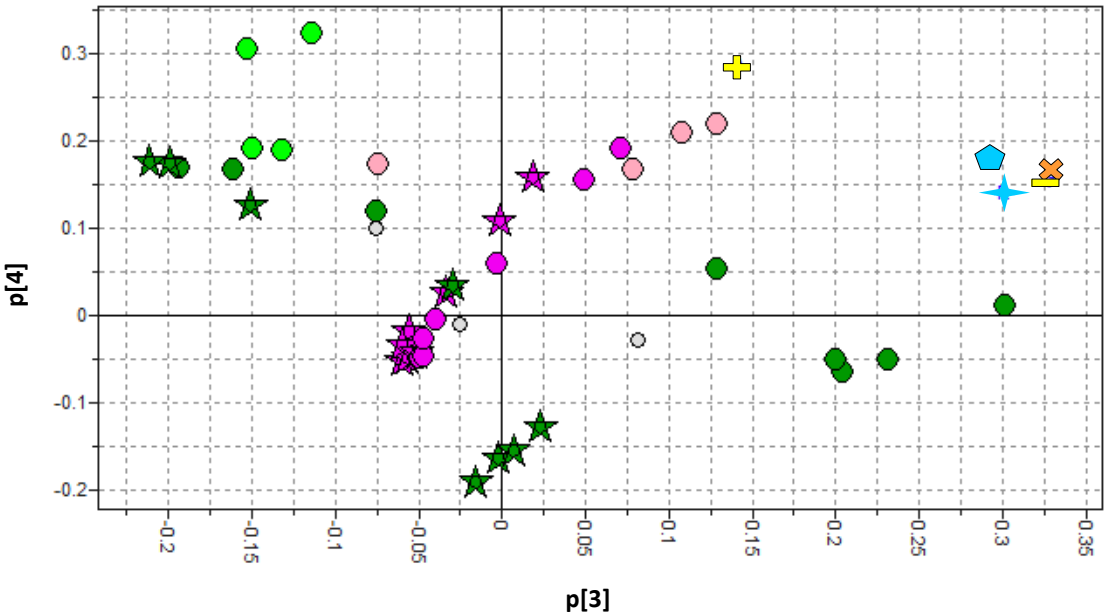


Figure 11 p[3]-p[4] loadings plot reporting anions model descriptors. W1-W8; D1-D8; IW1-IW4; CW1-CW8; ID-ID4; CD1-CD8; A; G; R; S; V; *others*. See Table C1 for descriptors code explanation.

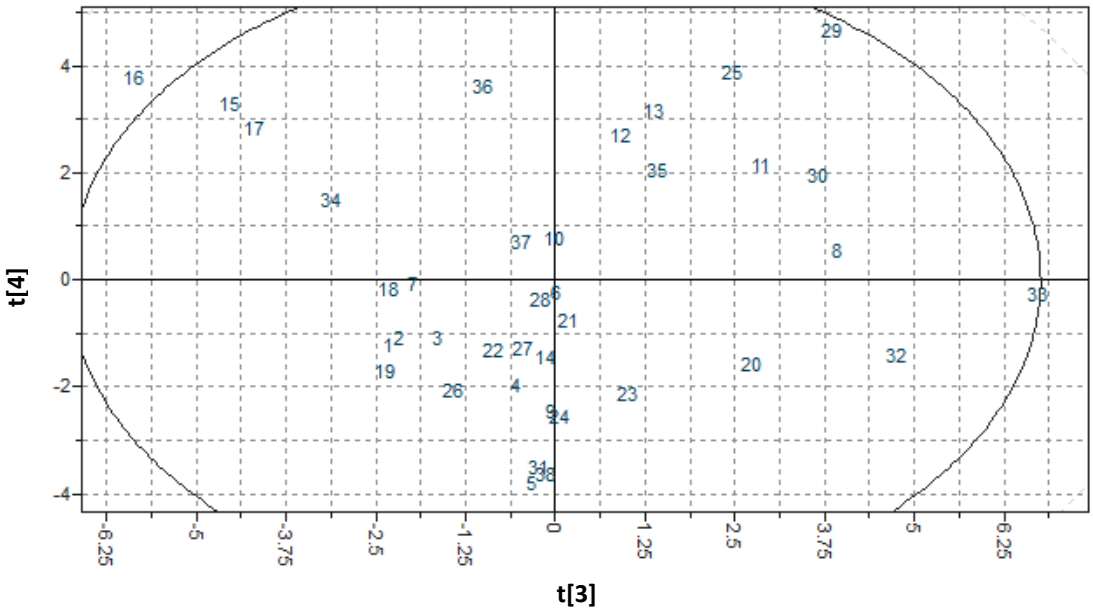


Figure 12 t[3]-t[4] scores plot reporting the 38 anions. Object labels reported in Table B2.

Tables C1, C2 were derived from an article published in SAR and QSAR in Environmental Research on 04 January 2016, available online: http//dx.doi.org/10.1080/1062936X.2015.1120778 (ref. 75).
Figures 3-12, A1 and Tables B1, B2, A1, A2 were derived from an article published in SAR and QSAR in Environmental Research on 08 March 2016, available online: http://dx.doi.org/10.1080/1062936X.2016.1156571 (ref. 78).

3.2 A glance at ILs structures influence on their *toxicity*

Ionic liquids toxicological data were collected by consulting the UFT-Merck Ionic Liquids Biological Effects Database[41] (nowadays no longer available) where data were taken from different scientific works, or performed by Merck laboratories. The UFT data can be summarized in a Table including 592 structures and 288 measurements (258 biological and 30 degradation tests). In the case of data from different literature sources, values deriving from a higher number of replicates were selected. The present investigation was limited to structures having an organic heterocyclic cationic scaffold (based on imidazolium, pyridinium, quinolinium, piperidinium, pyrroldinium and morpholinium cation). The resulting multivariate data matrix included 451 ILs and 258 biological plus 30 degradation tests. However a high number of missing data were here present, therefore the corresponding rows and columns were excluded from the matrix. The remaining data matrix contained 403 ILs and 35 variables which included biological tests defined as ecotoxicity in the UFT-Merck database herein sub-classified into: aquatic ecotoxicity (*e.g.* sensitivity to: *Scenedesmus vacuolatus, Vibrio fischeri*, *Lemna minor*), toxicity towards fungi and bacteria (*e.g.* sensitivity to Gram-positive and Gram-negative bacteria and fungi) and toxicity tests at a higher level of biological complexity: IPC-81 rat cell line cytotoxicity and acetylcholinesterase (AChE) enzyme inhibition. The biological data originally reported as EC_{50} or IC_{50} (the concentration at which half of the test organisms or test systems show a specific effect), MIC (Minimum Inhibitory Concentration) and MBC (Minimum Bactericidal Concentration) were converted into a positive log scale. These data were analysed by using PCA as discussed below.

3.2.1 Overall toxicity model

A PCA model from a 403x35 data matrix (ILs in Table B3 and variables in Table B4)[82] provided a 3 PCs model explaining 85.5% of total variance, with a predictability of 0.668, where 2 PCs already explaining 77% of variance (Q^2 = 0.587).[82] The scores plot showed in Fig. 13,[82] represents the projection of the 403 ILs from 35 down to 2 dimensions, *i.e.* a plane maintaining the most relevant information (in the present case 77%) of the dataset. In this plot no clustering according to the cation can be evidenced. In the corresponding loadings plot (Fig. 14)[82] all toxicity variables are in the right part of the plot, indicating that the 1st PC is an index of overall toxicity. As shown in Fig. 13,[82] one can note that non aromatic rings such as pyrrolidinium, piperidinium and morpholinium appear to be less toxic than aromatic ones (imidazolium, pyridinium, quinolinium). In agreement with several previous studies,[40] a toxicity increase can be observed on increasing alkyl side chain length (*i.e.* hydrophobicity), while the presence of oxygen in the side chain results in lower toxicity for long side chains. No clear cut anion effect can be evidenced in this plot.

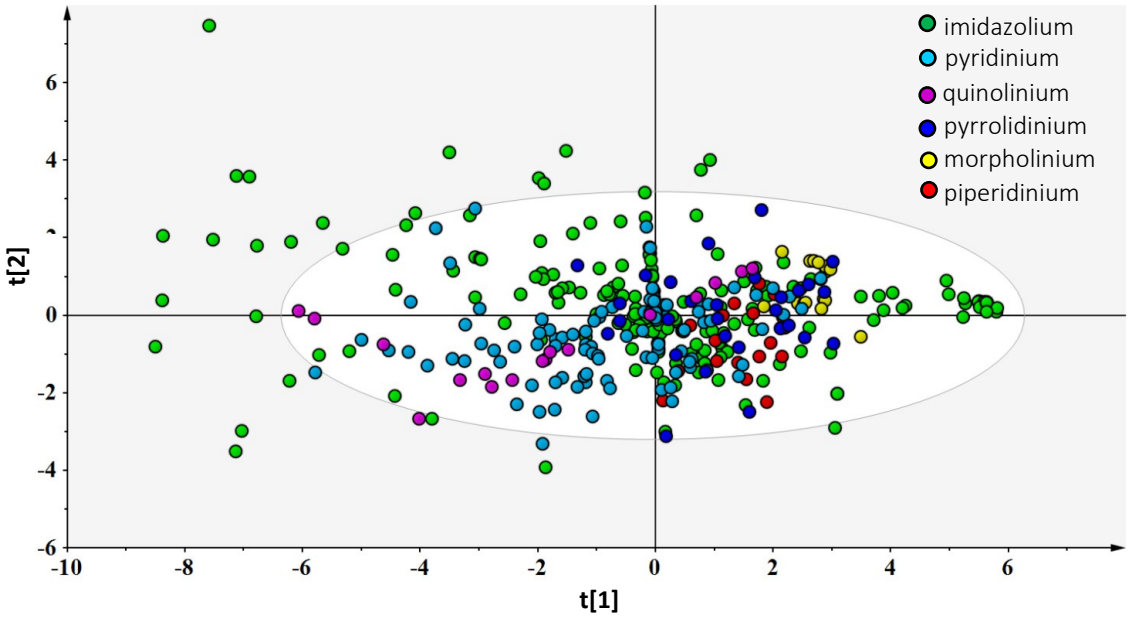


Fig. 13 t[1]-t[2] scores plot in the overall toxicity model.

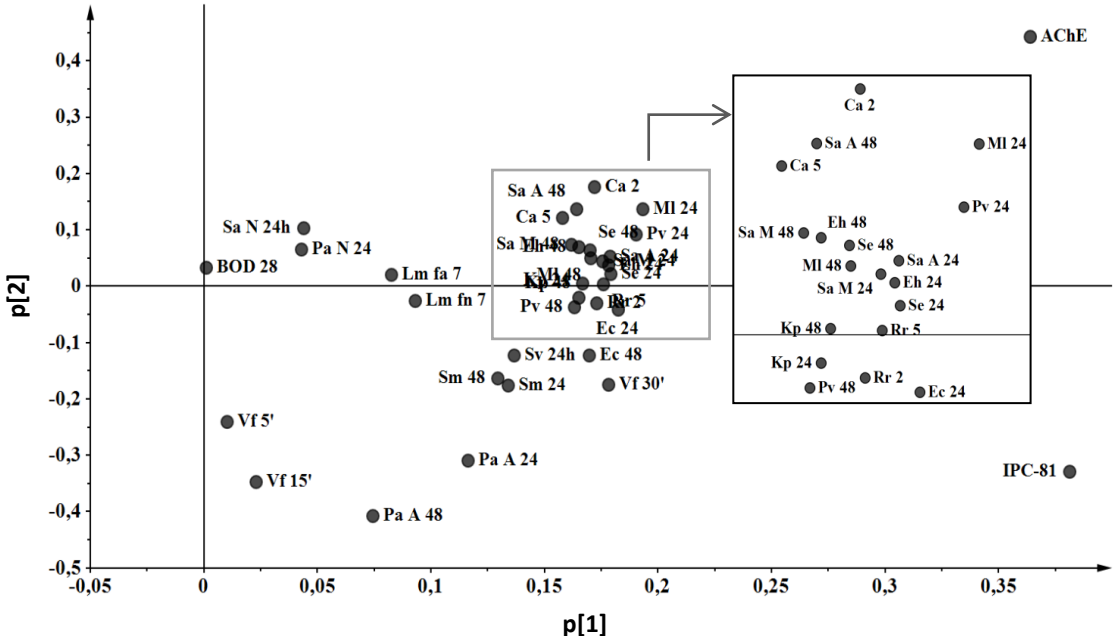


Fig. 14 p[1]-p[2] loadings plot in the overall toxicity model.

Ca 2: *Candida albicans* ATCC 10231 (growth inhib.) 48h;
Ca 5:*Candida albicans* ATCC 10231 (death) 5d;
Eh 24: *Enterococcus hirae* ATCC 10541 (growth inhib.)24h;
Eh 48: *Enterococcus hirae* ATCC 10541 (death) 48h;
Ec 24: *Escherichia coli* ATCC 25922 (growth inhib.) 24h;
Ec 48: *Escherichia coli* ATCC 25922 (death) 48h;
Kp 24: *Klebsiella pneumoniae* ATCC 4352 (growth inhib.) 24h;
Kp 48: *Klebsiella pneumoniae* ATCC 4352 (death) 48h;
Lm fa 7: *Lemna minor* (frond area) 7d;
Lm fn 7: *Lemna minor* (frond number) 7d;
Ml 24: *Micrococcus luteus* ATCC 9341 (growth inhib.) 24h;
Ml 48: *Micrococcus luteus* ATCC 9341 (death) 48h;
Pv 24: *Proteus vulgaris* NCTC 4635 (growth inhib.) 24h;
Pv 48: *Proteus vulgaris* NCTC 4635 (death) 48h;
Pa A 24: *Pseudomonas aeruginosa* ATCC 27853 (growth inhib.) 24h;
Pa A 48: *Pseudomonas aeruginosa* ATCC 27853 (death) 48h;
Pa N 24: *Pseudomonas aeruginosa* NCTC 6749 (growth inhib.)24h;
Rr 2: *Rhodotorul arubra* PhB (growth inhib.) 48h;
Rr 5: *Rhodotorula rubra*PhB (death) 5d;
Sv 24: *Scenedesmus vacuolatus* (cell count) 24h;
Sm 24: *Serratia marcescens* ATCC 8100 (growth inhib.) 24h;
Sm 48: *Serratia marcescens* ATCC 8100 (death) 48h;
Sa A 24: *Staphylococcus aureus* ATCC 6538 (growth inhib.) 24h;
Sa A 48: *Staphylococcus aureus* ATCC 6538 (death) 48h;
Sa M 24: *Staphylococcus aureus* (MRSA) (growth inhib.) 24h;
Sa M 48: *Staphylococcus aureus* (MRSA) (death) 48h;
Sa N 24: *Staphylococcus aureus* NCTC 4163 (growth inhib.) 24h;
Se 24: *Staphylococcus epidermidis* ATCC 12228 (growth inhib.) 24h;
Se 48: *Staphylococcus epidermidis* ATCC 12228 (death) 48h;
Vf 5': *Vibrio fischeri* 5min;
Vf 15': *Vibrio fischeri* 15min;
Vf 30': *Vibrio fischeri* 30min;
AChE:Acetylcholinesterase inhibition;
IPC-81: IPC-81 leukemia cells cytotoxicity;
BOD 28: BOD 28d.

The loadings plot in the above overall model (Fig. 14)[82] shows also that the 1st PC separates AChE and IPC-81 variables from all other biological tests, whereas the 2nd PC is required to discriminate the above two variables. This bio-informatics finding has a rational biological explanation as AChE and ICP-81, biological tests aimed at evaluating toxicity towards more complex living organisms, are expected to have a different information content with respect to the other examined variables (*i.e.* they are not representative of ecotoxicity). Moreover the model is somewhat "driven" by the great information content provided by a large number of data (*e.g.* ILs) available for these two variables (232 for AChE and 245 for IPC-81) as compared to that of all other variables. Consequently, in order to have a better insight on the influence of the latter variables on ILs ecotoxicity, AChE and IPC-81 were excluded in further PCA analysis and considered separately. PCA could not be carried out on a reduced data matrix including both aquatic eco-toxicities and toxicity towards fungi and bacteria as both toxicological data are not available for most ILs, probably due to different hydrophilic/hydrophobic properties which prevent their determination in both systems. Therefore, aquatic ecotoxicity and toxicity towards fungi and bacteria were separately analyzed. The above toxicities, which appear to be independent to each other, are both extremely important to assess overall ILs eco-sustainability in relation to the new EU chemical legislation for the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) adopted in June 2007.

3.2.2 Aquatic ecotoxicity

A further PCA was carried out on a 104x6 data matrix (ILs in Table B5 and variables in Table B6),[82] where the variables are toxicological data derived from different aquatic organisms: *Scenedesmus vacuolatus* (a green alga), *Vibrio fischeri* (a Gram-negative rod-shaped bacterium found in symbiosis with various marine animals), *Lemna minor* (a floating freshwater aquatic plant). PCA provided a 2PCs model explaining 94.9% of total variance (Q^2 = 0.756), with the 1st PC already explaining 81.1% of variance (Q^2 = 0.544).[82] The resulting loadings plot (Fig. 15)[82] shows that the 2nd PC is required to discriminate *Lemna minor* from *Vibrio fischeri* and *Scenedesmus vacuolatus*. The corresponding scores plot (Fig. 16)[82] opens a two dimensional window into ILs aquatic toxicity. This plot shows that the different nature of aromatic cations has not a significant effect on toxicity (although non aromatic heterocycles such as pirrolidinium, piperidinium and morpholinium cations appear to be less toxic) and no significant anion effect can be evidenced. The 1st PC scores can be assumed as an estimate of aquatic toxicity, according to the corresponding loadings plot (Fig 15)[82] with less toxic ILs in the right part of the plot and more toxic ones on the left. These scores, considered as a unique "aquatic ecotoxicity scores" for all the examined 104 ILs, are reported in Table B5[82]in order of decreasing t[1] values corresponding to increasing toxicity, together with the rank of the same ILs for logICP-81 rat cell line growth inhibition and logAChE enzyme inhibition toxicity values (Table B9-B10[82] respectively).

It is worth mentioning here that no single aquatic toxicity test is available for such a high number of ILs (104) and this result was achieved by applying multivariate data analysis to six different tests, each available for a lower number of ILs.

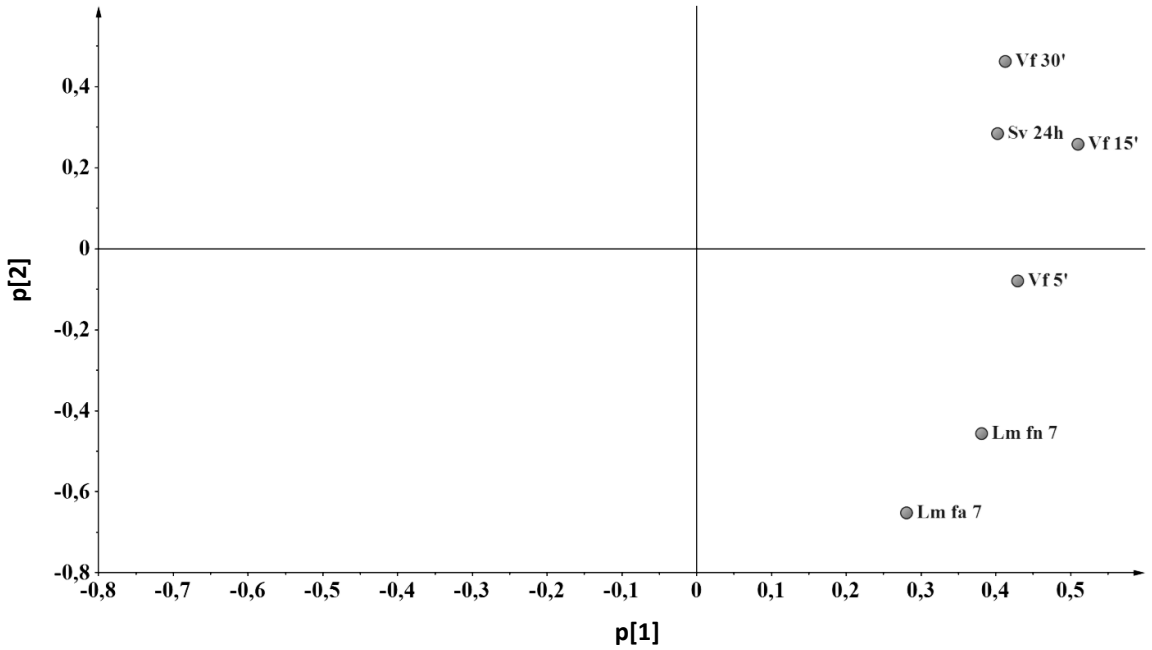


Fig. 15 p[1]-p[2] loadings plot in the aquatic toxicity model.
Lm fa 7: *Lemna minor* (frond area) 7d;
Lm fn 7: *Lemna minor* (frond number) 7d;
Sv 24: *Scenedesmus vacuolatus* (cell count) 24h;
Vf 5': *Vibrio fischeri* 5min;
Vf 15': *Vibrio fischeri* 15min;
Vf 30': *Vibrio fischeri* 30min

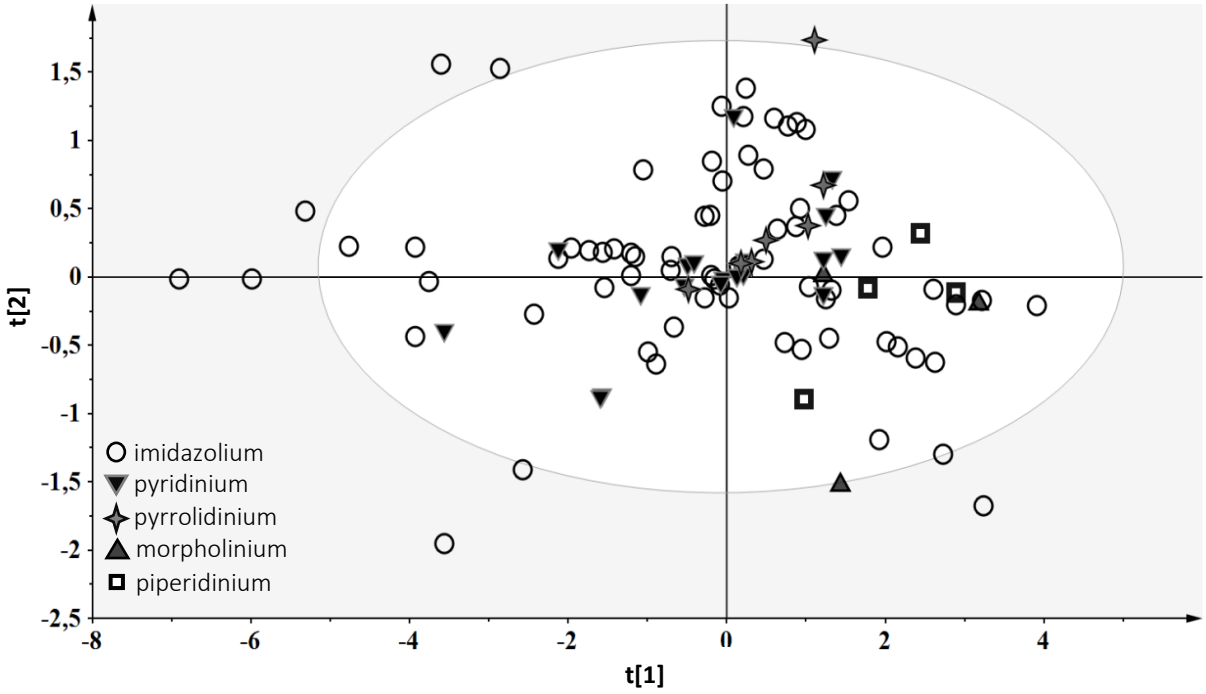


Fig. 16 t[1]-t[2] scores plot in the aquatic toxicity model.

3.2.3 Toxicity towards fungi and bacteria

A PCA model was carried out on an 87x26 data matrix: ILs are reported in Table B7 and variables in Table B8.[82] PCA provided a 7 PCs model explaining 96.2% of total variance (Q^2 = 0.756), where the 1st PC already explained 70.4% of variance (Q^2 = 0.660) and 3 PCs 86.7% of variance (Q^2 = 0.728).[82] The p[2]-p[3] loadings plot (Fig. 17b)[82] shows that the 2nd and 3rd components (both of which are statistically significant) are required to discriminate the variables into Gram-positive bacteria (in the lower left quadrant) from Gram-negative bacteria (in the two right quadrants). This finding points out the potentialities of PCA, a totally independent data analysis, in recognizing different groups according to a well known microbiological classification. However, the most relevant information provided in all 26 tests is summarized by the 1st PC explaining above 70% of variance. Therefore the 1st PC scores can be again used as an estimate of ILs toxicity towards fungi and bacteria (according to the loadings plot, Fig. 17a)[82] for all the examined 87 ILs. These ILs are reported in Table B7[82] in order of decreasing t[1] values, *i.e.* of increasing toxicity. It is worth mentioning that none of the 26 fungi and bacteria toxicities in the matrix was available for 87 ILs and that the above scores are affected by lower errors as compared to single toxicity determinations.

In the t[1]-t[2] scores plot (Fig.18)[82] only 3 cations (imidazolium, pyridinium and quinolinium) are present (due to the lack of experimental data for the others) and exhibit t[1] values distributed all over the 1st PC.

3.2.4 Imidazolium cations toxicity model

In previous sections no clear cut anion effects could be evidenced. The selection of the datamatrices for PCA is limited by the data structure, therefore decisions on how to improve the model quality for specific purposes, at the expense of generality, are subjective choices guided by the information provided by PCA as the investigation goes along.

In order to achieve a deeper insight into the effect of anions, PCA was limited to imidazolium-based ionic liquids (a data matrix with 218 ILs and 43 biological and degradation tests). In this case PCA provided a 3PCs model explaining 85% of total variance (Q^2 = 0.706) with the 1st PC explaining already 66% of variance (Q^2 = 0.594).[82] In the t[1]-t[2] scores plot reported in Fig. 19,[82] where ILs were coloured according to their anion, no anion clustering was evident, pointing out that the anion seems not to have a key role in addressing the ILs toxicity, which indeed appears more significantly affected by the chemical structure of the imidazolium substituents. These effects could be better proved by carrying out a PCA on a data matrix including only ILs with the same cation scaffold (imidazolium) and the same anion (chloride).[82] This data matrix contained 37 ILs and 24 biological and degradation tests.

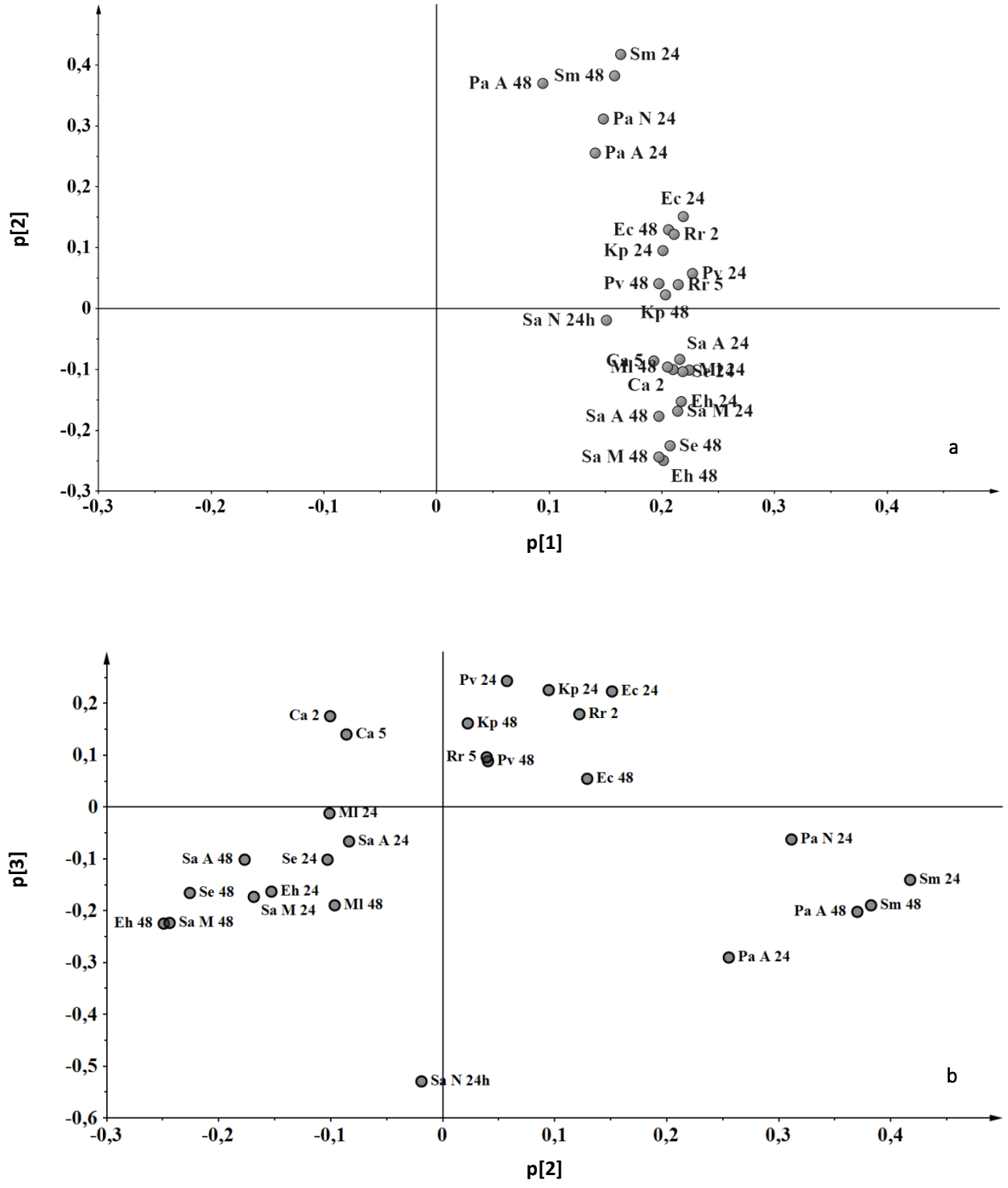


Fig. 17 p[1]-p[2] (a) and p[2]-p[3] (b) loadings plots in the bacteria and fungi toxicity model.

Ca 2: *Candida albicans* ATCC 10231 (growth inhib.) 48h;
Ca 5: *Candida albicans* ATCC 10231 (death) 5d;
Eh 24: *Enterococcus hirae* ATCC 10541 (growth inhib.)24h;
Eh 48: *Enterococcus hirae* ATCC 10541 (death) 48h;
Ec 24: *Escherichia coli* ATCC 25922 (growth inhib.)24h;
Ec 48: *Escherichia coli* ATCC 25922 (death) 48h;
Kp 24: *Klebsiella pneumoniae* ATCC 4352 (growth inhib.)24h;
Kp 48: *Klebsiella pneumoniae* ATCC 4352 (death) 48h;
Ml 24: *Micrococcus luteus* ATCC 9341 (growth inhib.) 24h;
Ml 48: *Micrococcus luteus* ATCC 9341 (death) 48h;
Pv 24: *Proteus vulgaris* NCTC 4635 (growth inhib.) 24h;
Pv 48: *Proteus vulgaris* NCTC 4635 (death) 48h;
PaA 24: *Pseudomonas aeruginosa* ATCC 27853 (growth inhib.) 24h;
Pa A 48: *Pseudomonas aeruginosa* ATCC 27853 (death) 48h;
Pa N 24: *Pseudomonas aeruginosa* NCTC 6749 (growth inhib.)24h;
Rr 2: *Rhodotorula rubra* PhB (growth inhib.) 48h;
Rr 5: *Rhodotorula rubra* PhB (death) 5d;
Sm 24: *Serratia marcescens* ATCC 8100 (growth inhib.)24h;
Sm 48: *Serratia marcescens* ATCC 8100 (death) 48h;
Sa A 24: *Staphylococcus aureus* ATCC 6538 (growth inhib.)24h;
Sa A 48: *Staphylococcus aureus* ATCC 6538 (death) 48h;
Sa M 24: *Staphylococcus aureus* (MRSA) (growth inhib.)24h;
Sa M 48: *Staphylococcus aureus* (MRSA) (death) 48h;
Sa N 24: *Staphylococcus aureus* NCTC 4163 (growth inhib.)24h;
Se 24: *Staphylococcus epidermidis* ATCC 12228 (growth inhib.)24h;
Se 48: *Staphylococcus epidermidis* ATCC 12228 (death) 48h.

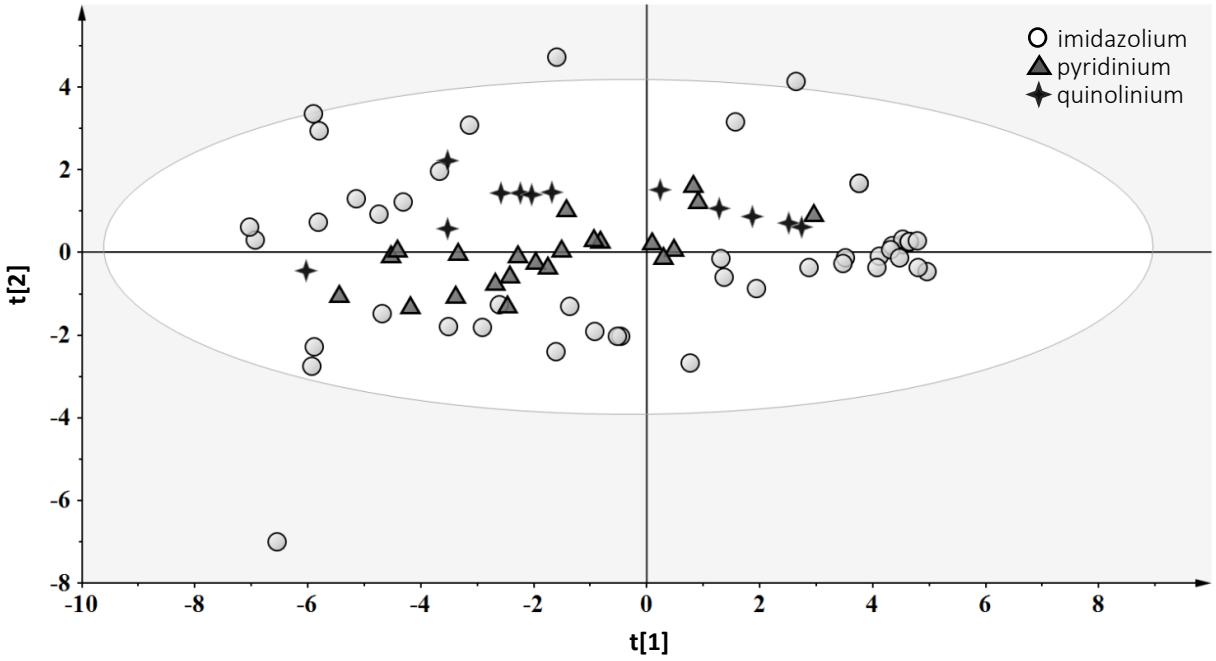


Fig. 18 t[1]-t[2] scores plot in the bacteria and fungi toxicity model.

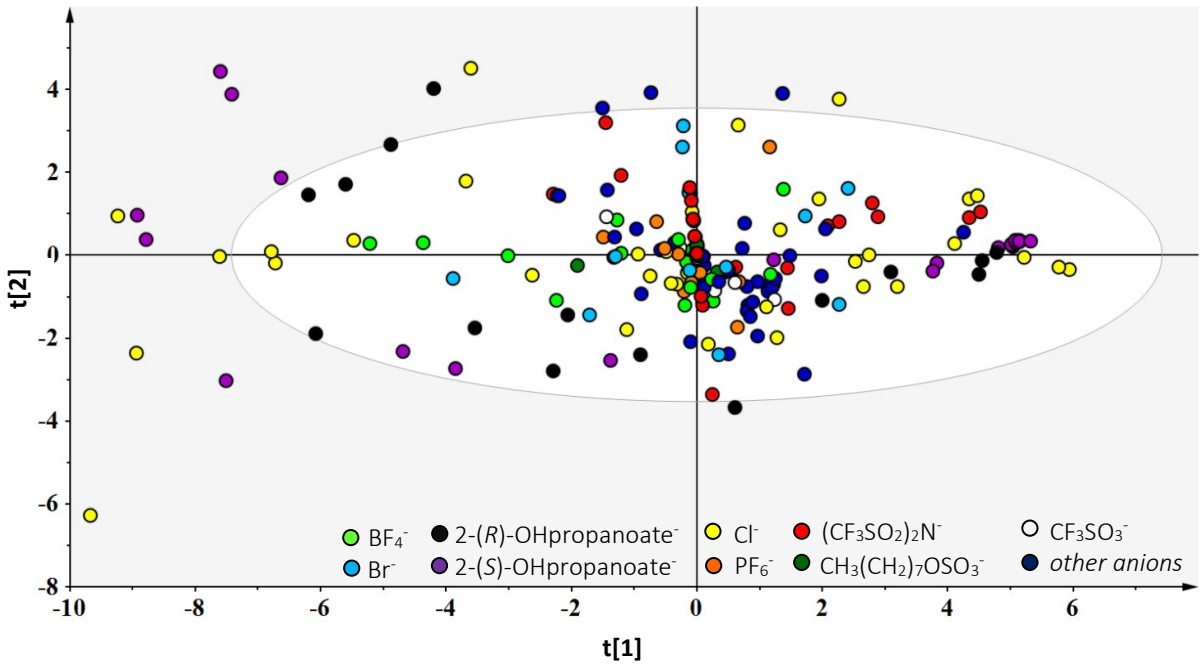


Fig. 19 t[1]-t[2] scores plot in the overall toxicity model for imidazolium-based ILs.

Taking into account the superimposition with the p[1]-p[2] loadings reported in Fig. 20,[82] in the right part of the t[1]-t[2] scores plot (Fig. 21)[82] in which the least toxic ILs should be present, one could find ILs with short alkyl side chains and di-alkyloxy methyl ethers with short (2-5) and long (11-14) carbon alkyl chains, whereas ILs with long alkyl side chains and di-alkyloxy methyl ethers with medium length (7-10 carbon atoms) are in the left part of the plot (more toxic compounds). The higher toxicity of alkyl imidazolium with longer side chains is well known and has been reported in the literature also for pyrrolidinium, piperidinium and pyridinium ILs:[40] It was related to the higher hydrophobicity of long side chains. However, the toxicity "levelled off on reaching a threshold side chain length"[40] which depends on the IL class. It has also been noted that "the presence of oxygen in the side chain seems to decrease the toxicity".[40] Moreover Pernak *et al.*[83] reported that mono-alkyloxy ether imidazoliums exhibit a maximum of (microbial) toxicity for dodecyloxymethyl imidazolium (12 carbon atom side chain), while toxicity decreasing was observed up to 16 carbon atoms side chains. Garcia *et al.*[84] reported an analogous behaviour for mono-alkyl esters imidazolium and pyridinium ILs. They noted that an increase of the number of carbon atoms in the ester side chain resulted in a higher tendency to form micellar aggregates. In this perspective, our findings (see Fig. 21)[82] evidenced the highest toxicity of di-alkyloxy methyl ether imidazoliums for ILs having 7-9 carbon atoms in each side chain. The decrease of toxicity observed for di-alkyloxy ethers ILs with more than 12 carbon atoms in each side chain may be ascribed to the formation of micellar aggregates, which avoid the interaction of the ILs with the cell membrane.[84] Therefore toxicity might be due to a balance of hydrophobicity and hydrophilicity. The above toxicity trend found for the overall imidazolium model has been confirmed in the case of more specific models which consider separately toxicity of imidazolium based ILs towards aquatic organisms and towards fungi and bacteria (Fig. 22-23 respectively).[82]

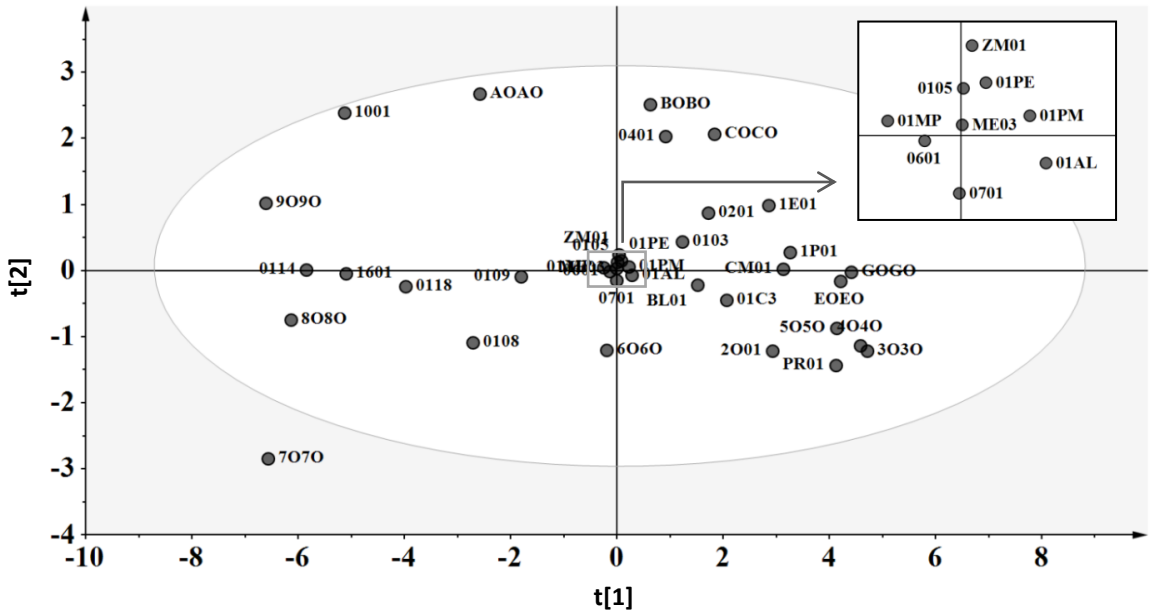


Fig. 20 t[1]-t[2] scores plot in the overall toxicity model for imidazolium chloride-based ILs. Side chains labels as in Table C3.

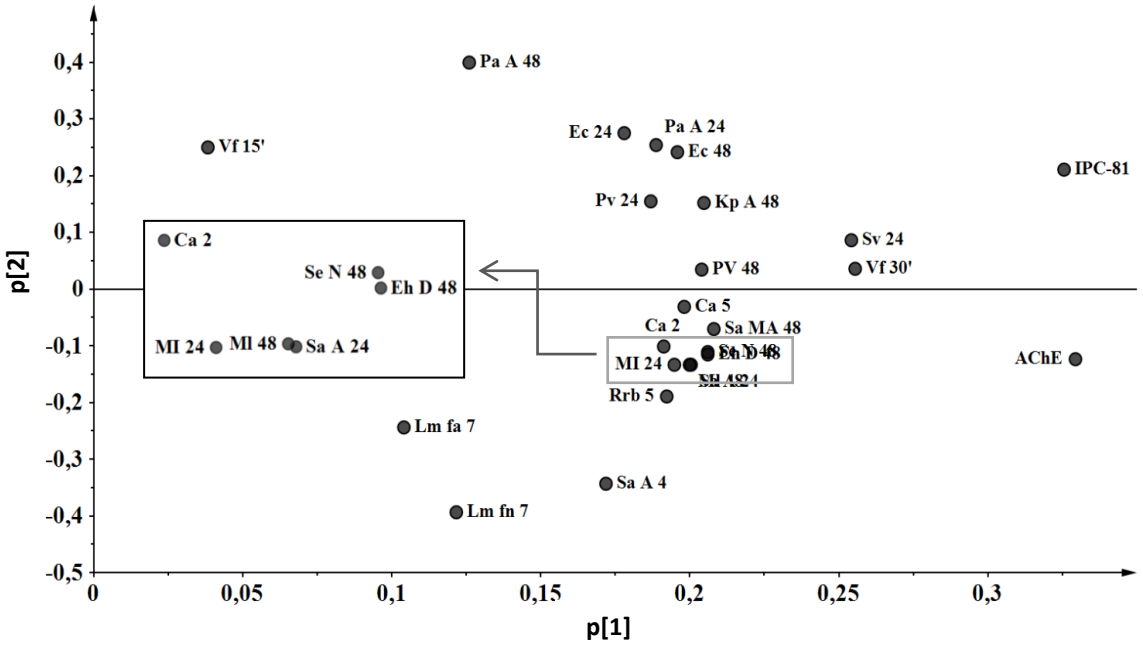


Fig. 21 p[1]-p[2] loadings plot in the overall toxicity model for imidazolium chloride-based ILs.

Ca 2: *Candida albicans* ATCC 10231 (growth inhib.) 48h;
Ca 5: *Candida albicans* ATCC 10231 (death) 5d;
Eh 24: *Enterococcus hirae* ATCC 10541 (growth inhib.) 24h;
Eh 48: *Enterococcus hirae* ATCC 10541 (death) 48h;
Eh D 48: *Enterococcus hirae* DSM 20160 (death) 48h;
Ec 24: *Escherichia coli* ATCC 25922 (growth inhib.) 24h;
Ec 48: *Escherichia coli* ATCC 25922 (death) 48h;
Kp 24: *Klebsiella pneumoniae* ATCC 4352 (growth inhib.) 24h;
Kp 48: *Klebsiella pneumoniae* ATCC 4352 (death) 48h;
Kp A 48h: *Klebsiella pneumoniae* ATCC 13886 (death) 48h;
Lm fa 7: *Lemna minor* (frond area) 7d;
Lm fn 7: *Lemna minor* (frond number) 7d;
Ml 24: *Micrococcus luteus* ATCC 9341 (growth inhib.) 24h;
Ml 48: *Micrococcus luteus* ATCC 9341 (death) 48h;
Pv 24: *Proteus vulgaris* NCTC 4635 (growth inhib.) 24h;
Pv 48: *Proteus vulgaris* NCTC 4635 (death) 48h;
Pa A 24: *Pseudomonas aeruginosa* ATCC 27853 (growth inhib.) 24h;
Pa A 48: *Pseudomonas aeruginosa* ATCC 27853 (death) 48h;
Rrb 5: *Rhodotorula rubra* (death) 5d;
Rr 2: *Rhodotorula rubra* PhB (growth inhib.) 48h;
Rr 5: *Rhodotorula rubra* PhB (death) 5d;
Sv 24: *Scenedesmus vacuolatus* (cell count) 24h;
Sm 24h: *Serratia marcescens* ATCC 8100 (growth inhib.) 24h;
Sm 48: *Serratia marcescens* ATCC 8100 (death) 48h;
Sa A 24: *Staphylococcus aureus* ATCC 6538 (growth inhib.) 24h;
Sa A 48: *Staphylococcus aureus* ATCC 6538 (death) 48h;
Sa M 24: *Staphylococcus aureus* (MRSA) (growth inhib.) 24h;
Sa M 48: *Staphylococcus aureus* (MRSA) (death) 48h;
Sa MA 48: *Staphylococcus aureus* (MRSA) ATCC 43300 (death) 48h;
Se 24: *Staphylococcus epidermidis* ATCC 12228 (growth inhib.) 24h;
Se 48: *Staphylococcus epidermidis* ATCC 12228 (death) 48h;
Se N 48: *Staphylococcus epidermidis* NCTC 11047 (death) 48h;
Vf 15': *Vibrio fischeri* 15min;
Vf 30': *Vibrio fischeri* 30min;
AChE: Acetylcholinesterase inhibition;
IPC-81: IPC-81 leukemia cells cytotoxicity.

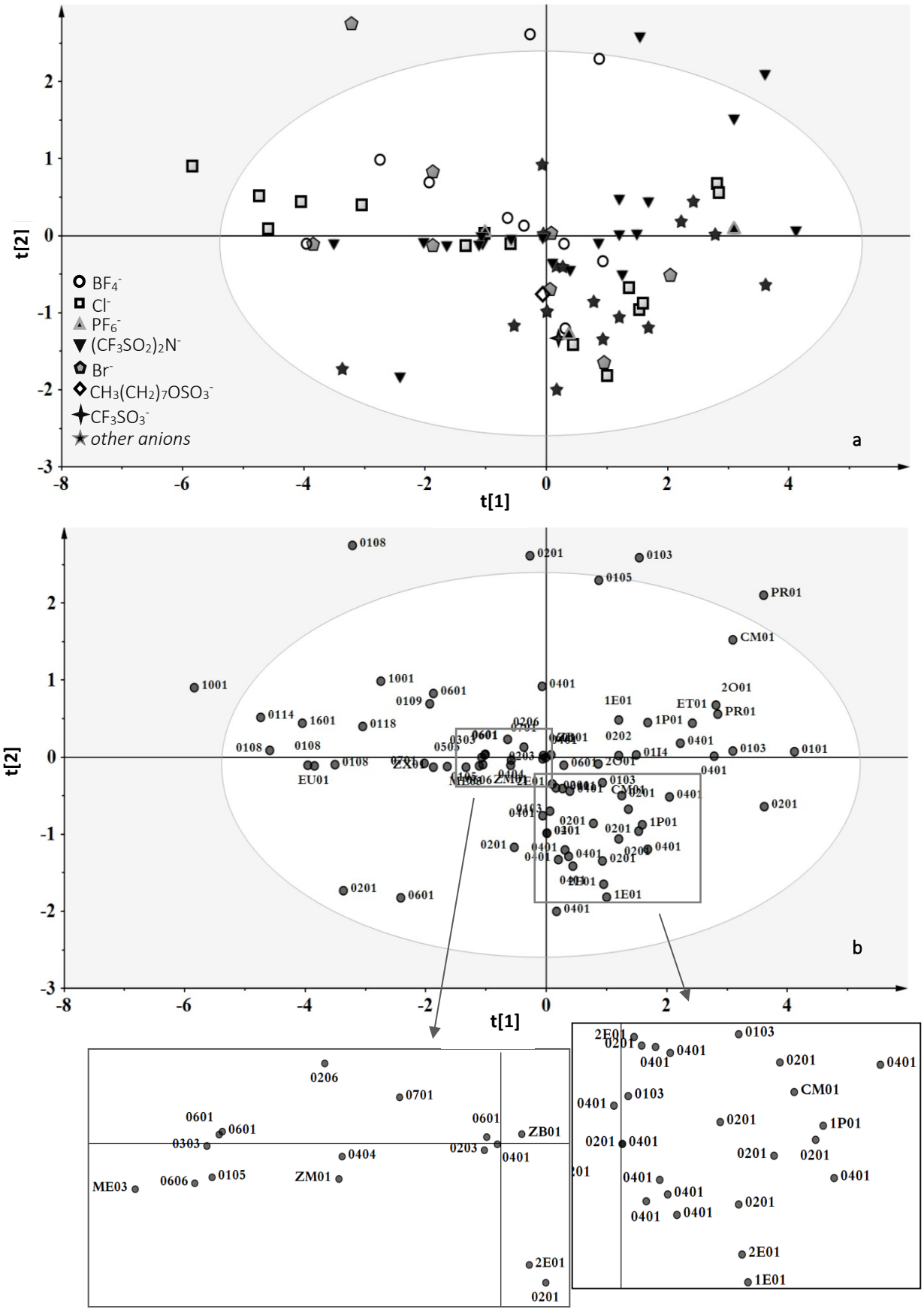


Fig. 22 t[1]-t[2] scores plots in the aquatic toxicity model for imidazolium-based ILs. Fig. 22a: anions distribution. Fig. 22b: side chains distribution. Side chains labels as in Table C3.

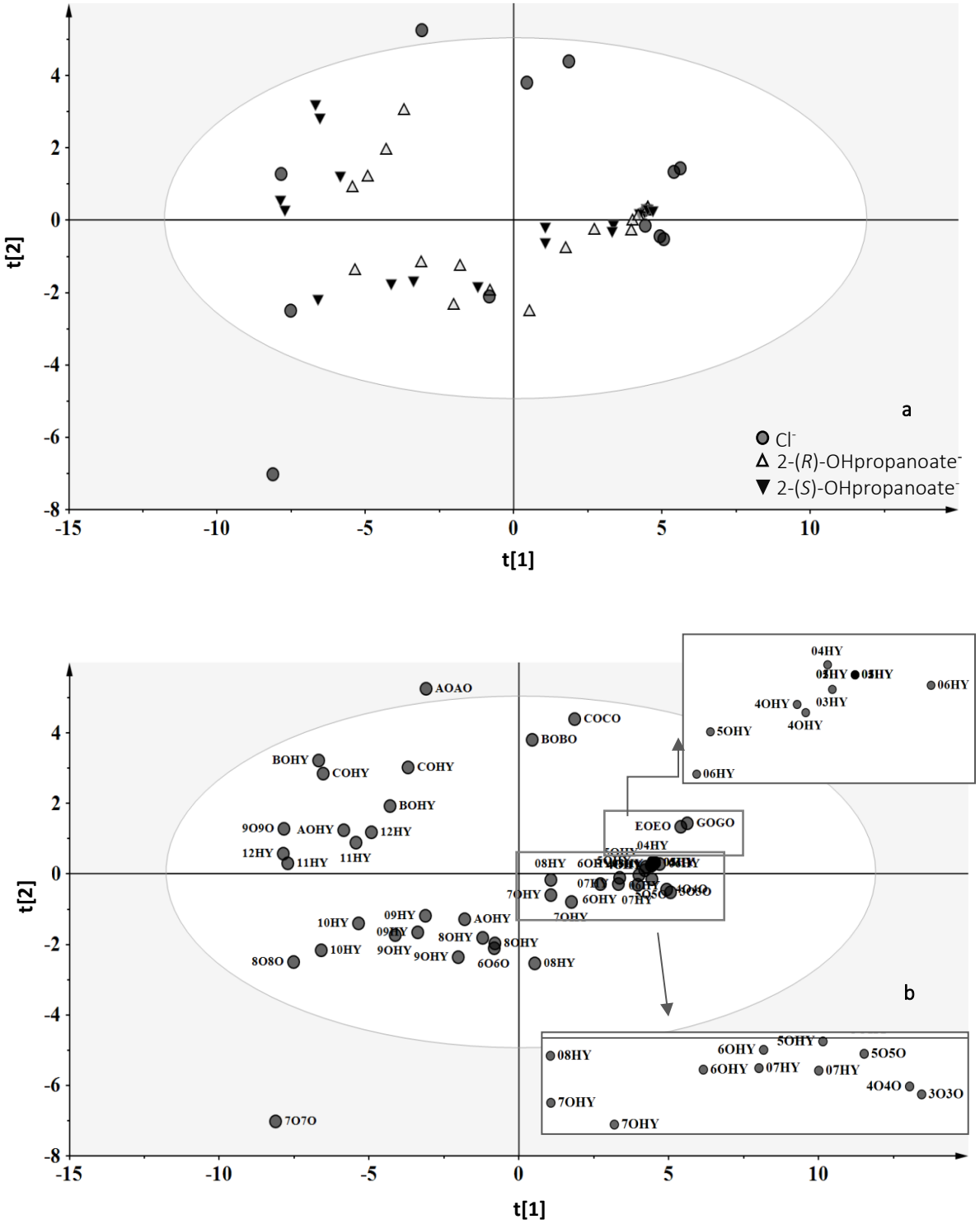


Fig. 23 t[1]-t[2] scores plots in the bacteria and fungi toxicity model for imidazolium-based ILs. Fig. 23a: anions distribution; Fig. 23b: side chains distribution. Side chains labels as in Table C3.

3.2.5 Relationships between different toxicities

One of the aims of the present study was to assess whether negative impact on aquatic organisms can be ascribed to the same structures resulting harsher to mammalian targets such as growth inhibition of IPC-81 rat cell line and AChE inhibition. Estimation of the latter toxicities by PCA, Neural Network (NN) and multilayer perceptron has been already reported.[85]

In Tables B9-B10[82] we reported respectively the log of ICP-81 rat cell line growth inhibition, and AChE enzyme inhibition ordered according to decreasing log values, *i.e.* of increasing toxicity. Fig. 24a[82] shows no correlation between toxicity towards AChE and IPC-81, as expected on the basis of the biological differences in these toxicity "sensors". It is worth to comment also correlations plots between the t[1] scores of the aquatic ecotoxicity model and AChE or IPC-81 values plotted in Fig. 24b[82] and 24c[82] respectively. No correlation can be observed with the enzymatic activity (Fig. 24b),[82] while a correlation with IPC-81 can be envisaged (Fig. 24c).[82] The latter correlation provides an answer to the question whether "a negative impact on water" may be "caused by the same structures as the ones that were showed to be harsher to rat cell lines".[38] In fact the impact of aquatic ecotoxicity is found to be paralleled by an effect on the cellular response in living organisms such as IPC-81 rat cell line. IPC-81 and AChE toxicity values are not available for most ILs tested with fungi and bacteria, therefore no correlation can be attempted with t[1] scores of this model.

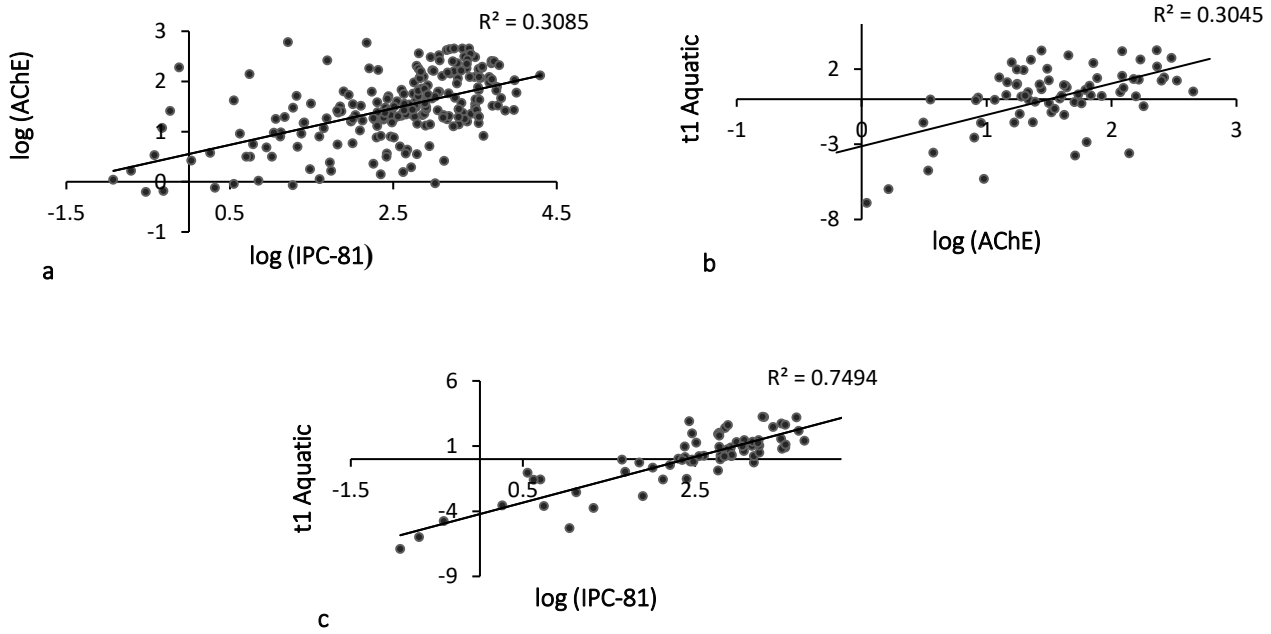


Fig. 24 Correlations among different toxicities.

Table B5 reports the ILs according to the aquatic toxicity t[1] scores together with the rank of the same ILs in Table B9 (logICP-81 rat cell line growth inhibition)[82] and Table B10 (logAChE enzyme inhibition)[82] respectively. According to three out of the four toxicities considered in the present section, compounds n. *2*, *4*, *7*, *8*, *12*, *17* and *20* (Table B5, Chart 1)[82] can be recommended as safe ILs, while the use of *86*, *87*, *93*, *96*, *101*, *103* and *104* (Table B5, Chart 2)[82] should be discouraged or limited. The latter ILs should be foremost assigned in more extensive (and likely expensive) toxicological studies. Guidance on the choice of less toxic ILs according to fungi and bacteria ecotoxicity can be obtained from Table B7.[82] Inspection of both Tables B5 and B7[82] is necessary to obtain information about ILs toxicity, as it was not possible to summarize available toxicity information using a unique toxicity score. This is due to the lack of data which can be ascribed to different ILs hydrophilic/hydrophobic properties, preventing their determination in different biological "sensors". However, the above tables provide a simplified picture of scattered toxicity data available in the literature, resulting very useful for the new EU chemical legislation.

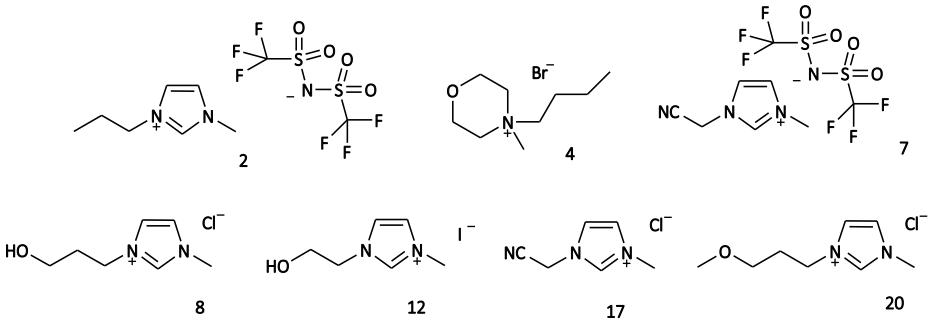


Chart 1 Eco and bio-sustainable ILs

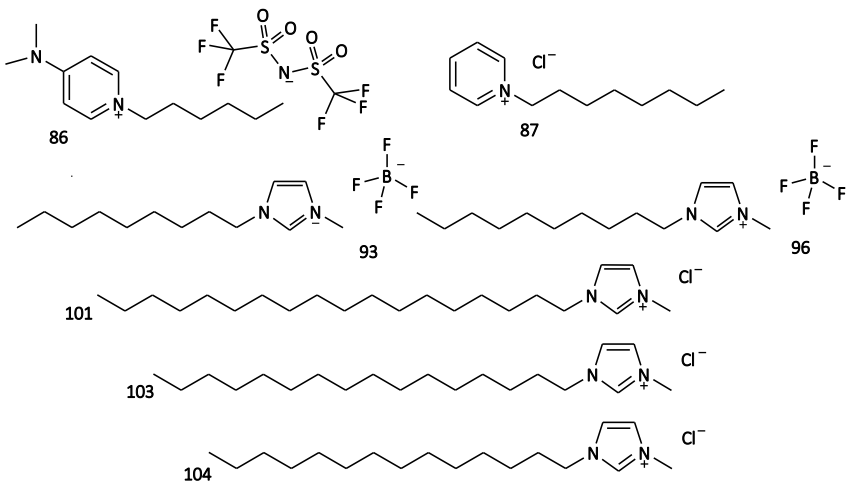


Chart 2 Potentially toxic ILs

Figures 13-24, Charts 1, 2 and Tables B3-B10, C3 were reproduced from ref. 82 with permission from the Royal Society of Chemistry.

3.3 *QSPR* models analyzing ILs structures influence on their *toxicity*

3.3.1 A*quatic toxicity* PLS model

The descriptors calculated by means of VolSurf+ (see section 3.1.1) allowed to recover the link between the characteristics of the positive-negative ions and the specific property under study, which is at least partially lost when the relationship is studied by describing only one of the two ion player. A more general alternative, by considering simultaneously both ILs cationic and anionic counterparts including both sets of descriptors for a given IL in the same QSPR model, is herein presented.

PLS approach was adopted to relate both cation and anion VolSurf+ *in silico* physico-chemical properties (the descriptor matrix) to the *aquatic toxicity scores* (the response) derived as discussed in section 3.2.2, and summarizing toxicities towards aquatic living organisms chosen among the most commonly used as targets in biological essays. The data matrix undergoing PLS modelling is reported in Table B11.[75] The resulting model provides four significant PLS components (Table A3)[75] explaining an overall 75.5 % of Y variance, with the 1st PC already containing 59.1% Y of variance. The cumulative Q^2 value (*i.e.* the fraction of the total variation of the Y which can be predicted by the four extracted components) is 0.620 (Q^2 = 0.570 for the 1st PLS component) indicating a satisfactory model predicting ability.

Table 1[75] shows the VIP values for the top 100 descriptors, indicating their relevance in this model, together with coefficients values referring to the contribution of each descriptor to aquatic toxicity scores along the 1st PC (the most informative one). Cations influence on aquatic toxicity is mainly expressed by size-describing variables (molecular volume V, surface S, globularity G, weight MW, and polarizability POL) as well as by molecular hydrophobic volume and surface (HSA, DD and D descriptors), LogP and LogD, molecular flexibility (FLEX) and protein binding (PB). All these variables give a negative contribution to the 1st PLS component, *i.e.* increase aquatic toxicity. Conversely, a strong but positive contribution to PC[1] is given by molecular diffusivity (DIFF), water thermodynamic solubility (SOLY and LgS), molecular bio-metabolic stability (MetStab) which decrease toxicity. The anions play a minor role. Big anions (exhibiting high S, V and G values) with wide both hydrophilic and hydrophobic areas distant from the molecular barycenter (IW and ID respectively) influence positively the aquatic toxicity scores increasing ILs sustainability. In a previous section we noted a structural influence on aquatic toxicity scores by means of a qualitative analysis. The derived PLS model reported here allows to evaluate *quantitatively* structural features contributing to toxicity of ILs. On the basis of the c-weights plot (Fig. A2) in which the toxicity variable lies on the upper right quadrant, compounds in the right part of the scores plot (Fig. 25 and Fig. A3)[75] can be considered less toxic than those situated on the left. Among the cationic scaffolds, non aromatic ones (piperidinium, pyrrolidinium and morpholinium-based cations)

contribute to decrease aquatic toxicity. Pyridiniums and imidazoliums ILs exhibit higher structural variations and allow to evaluate also the side chain effects on toxicity (Fig. A3):[75] it is evident that longer side chains determine a higher toxicity. In fact very short alkylic side chains (ethyl or methyl substituents) or the presence of heteroatoms such as *O*-ether or nitrile groups cause high positive t[1] scores for ILs, whereas longer side chains (for instance, more than four carbon atoms in one side chain at least, and also ILs 350, 369 and 418 having eight, ten and twelve carbon atoms in total) or bulky substituted ILs (for example, ILs 372 and 376) are on the opposite region. However very long side chain compounds (ILs 227, 229 and 231 in Figure 25,[75] with 14, 16 and 18 carbon atoms respectively) behave as outliers: as already noted from a qualitatively point of view in the previous section, these compounds do not apparently follow the trend described above due to possible molecular aggregation phenomenon which prevent them from interacting as surfactants (hence as toxicants). All the above considerations are based on the descriptors coefficients aforementioned and reported in Table 1.[75] Therefore the PLS model can provide a clear interpretation of the structural features (and descriptors) related to ILs aquatic toxicities allowing a useful insight on this relationships.

In Table B11[75] aquatic toxicity scores are reported, among the others, for eleven 1-butyl-3-methylimidazoliums with different anions (compounds 160-171) spanning over 3 orders of magnitude (ranging from -0.887 for the octylsulfate to 2.609 for methanesulfonate). The present approach accounts for a non-negligible role of the anions in determining aquatic toxicity, an effect previously reported to be insignificant in papers considering only few halogen anions (chloride, bromide and iodide).[86,87]

Another potentiality of the PLS approach is the possibility, once a reliable model has been built, to predict the “response” for the same set of ILs (Table B11)[75] and plot modelled *vs.* experimental data. The correlation plot in Fig. 26[75] can be considered as very satisfactory taking into account the wide range of aquatic toxicity scores spanning eleven units. Deviation from linearity can be envisaged in the lower left part of the correlation plot for long alkyl chain (14 and 18 C atoms, entry 227 and 231 in Table B11 respectively)[75] imidazolium substituents. This might be due to a higher percentage of errors in the experimental quantitative determination of ILs at very low concentrations and/or to the molecular aggregation in the reaction media for very long alkyl side chain ILs.

Table 1. Top 100 VIP values and 1st PLS coefficients values (scaled and centered) for VolSurf+ descriptors in the aquatic toxicity PLS model.[a]

	Var. ID	VIP values	Coeff. Values		Var. ID	VIP values	Coeff. Values		Var. ID	VIP values	Coeff. Values
1	G_Cat	1.902	-0.018	34	D2_Cat	1.560	-0.016	67	CD2_An	0.818	0.004
2	HSA_Cat	1.873	-0.019	35	DRDRDR_Cat	1.557	-0.015	68	D7_Cat	0.795	-0.007
3	DD1_Cat	1.866	-0.019	36	W1_Cat	1.506	-0.014	69	R_An	0.791	0.003
4	S_Cat	1.796	-0.018	37	D3_Cat	1.459	-0.015	70	W1_An	0.784	0.003
5	FLEX_Cat	1.780	-0.018	38	PB_Cat	1.457	-0.014	71	CD1_Cat	0.779	-0.006
6	LgS10_Cat	1.771	0.018	39	MW_Cat	1.454	-0.014	72	ID2_An	0.776	0.004
7	LgS11_Cat	1.771	0.018	40	ID4_Cat	1.336	-0.011	73	CD1_An	0.776	0.004
8	LgS7,5_Cat	1.771	0.018	41	LOGPc-Hex_Cat	1.327	-0.013	74	IW2_Cat	0.774	0.006
9	LgS8_Cat	1.771	0.018	42	SKIN_Cat	1.324	-0.013	75	D3_An	0.763	0.003
10	LgS9_Cat	1.771	0.018	43	CP_Cat	1.319	-0.013	76	HL2_Cat	0.754	0.003
11	SOLY_Cat	1.771	0.018	44	D4_Cat	1.246	-0.012	77	W2_An	0.743	0.002
12	LgS7_Cat	1.771	0.018	45	FLEX_RB_Cat	1.183	-0.012	78	CW6_Cat	0.740	0.005
13	LgS6_Cat	1.771	0.018	46	R_Cat	1.167	-0.011	79	PSAR_Cat	0.740	0.005
14	LgS5_Cat	1.770	0.018	47	VD_Cat	1.111	-0.010	80	DD5_Cat	0.736	-0.007
15	L0LgS_Cat	1.770	0.018	48	DD4_Cat	1.100	-0.011	81	A_Cat	0.733	0.004
16	LgS4_Cat	1.764	0.018	49	ID1_An	1.062	0.005	82	D8_Cat	0.733	-0.007
17	V_Cat	1.756	-0.017	50	ID2_Cat	1.045	0.006	83	CW5_Cat	0.731	0.005
18	LgS3_Cat	1.748	0.018	51	ID1_Cat	1.008	0.008	84	ID3_An	0.730	0.004
19	MetStab_Cat	1.741	0.017	52	ID3_Cat	1.005	-0.005	85	W2_Cat	0.729	-0.005
20	LgD10_Cat	1.714	-0.017	53	D5_Cat	0.953	-0.010	86	W3_An	0.722	0.002
21	LgD9_Cat	1.714	-0.017	54	IW1_An	0.930	0.005	87	CD2_Cat	0.721	-0.006
22	LOGPn-Oct_Cat	1.714	-0.017	55	IW3_Cat	0.911	0.008	88	D1_An	0.717	0.004
23	LgD7,5_Cat	1.714	-0.017	56	IW1_Cat	0.897	0.008	89	PHSAR_Cat	0.715	0.005
24	LgD8_Cat	1.714	-0.017	57	V_An	0.866	0.003	90	CD3_An	0.713	0.003
25	LgD7_Cat	1.714	-0.017	58	IW2_An	0.864	0.005	91	CW4_Cat	0.705	0.004
26	LgD6_Cat	1.714	-0.017	59	G_An	0.862	0.003	92	HL1_Cat	0.702	0.003
27	LgD5_Cat	1.711	-0.017	60	DD8_Cat	0.862	-0.005	93	W5_An	0.702	-0.001
28	DD2_Cat	1.702	-0.017	61	S_An	0.860	0.003	94	IW3_An	0.701	0.004
29	D1_Cat	1.680	-0.017	62	HL1_An	0.851	-0.004	95	W4_An	0.698	0.001
30	DIFF_Cat	1.660	0.016	63	ID4_An	0.849	0.004	96	CW3_Cat	0.696	0.004
31	POL_Cat	1.652	-0.016	64	IW4_Cat	0.841	0.007	97	LgBB_Cat	0.688	-0.006
32	DD3_Cat	1.641	-0.016	65	D6_Cat	0.822	-0.008	98	DRDRDO_Cat	0.673	0.006
33	HL2_An	1.589	-0.003	66	D2_An	0.820	0.004	99	WO4_Cat	0.668	0.006
								100	CW1_Cat	0.664	0.005

[a] VolSurf+ variables codes as in Table C1.

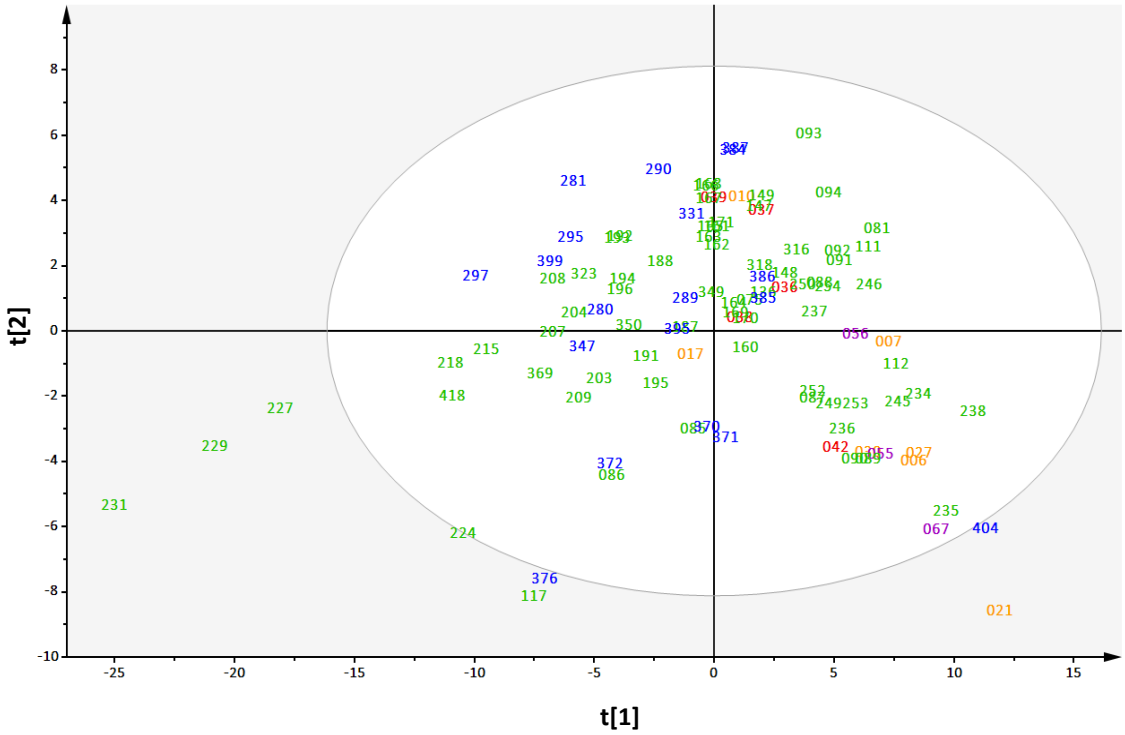


Fig. 25 t[1]-t[2] scores plot for the aquatic toxicity PLS model. The objects are labelled as in Table B11, and coloured as follows: imidazoliums, pyridiniums, pyrrolidiniums, piperidiniums, morpholiniums based ILs. See also Fig. A3 which highlights the side chain effects for the imidazoliums-based ILs.

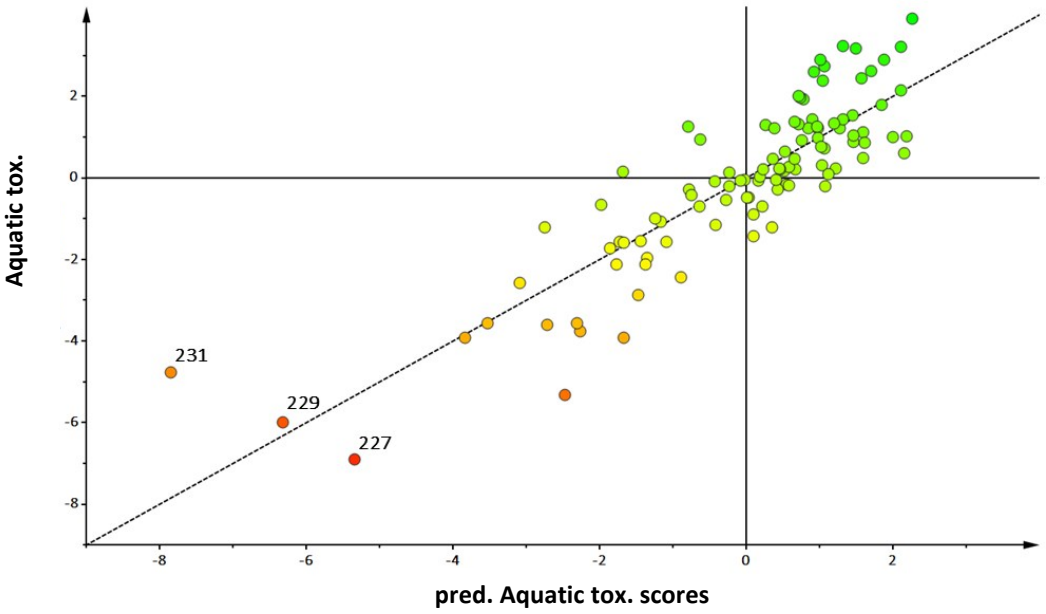


Fig. 26 Calculated vs. predicted values for the PLS aquatic model. ILs are coloured on the basis of their toxicity scores: red for the most toxic compounds, green for the least toxic ones (negative and positive aquatic toxicity scores respectively). Evidenced labels as in Table B11.

Figures 25, 26, A3 and Tables 1, A3, B11, C1, C2 were derived from an article published in SAR and QSAR in Environmental Research on 04 January 2016, available online: http//dx.doi.org/10.1080/1062936X.2015.1120778. Ref. 75

3.3.2 *IPC-81* cytotoxicity PLS model

The leukemia rat cell line IPC-81 has been frequently used in cytotoxicity assays of chemicals. IPC-81 cytotoxicity data, expressed as log EC_{50} (mg/L) and spanning 5 log units, were available for 243 heterocyclic ILs (Table B9).[82] Howevere the whole dataset was divided into a learning set including 207 ILs (L in Table B12)[78] and a randomly selected test set of 36 ILs (15% of the data; T in Table B12)[78] used as an external model validation set. Next thePLS method was applied on a matrix including 207 ILs and 9 variables, *i.e.* 5 cationic and 4 anionic PPs (section 3.1.2), and IPC-81 cytotoxicities as the responses. The analysis provided a 2 PLS components model explaining 67.8% of Y variance (Q^2 = 0.655) whith the 1st PLS component explaining already 46.1% of Y variance (Q^2 = 0.446) (see paramters in Table A4).[78]

The resulting coefficients plots in Fig. 27[78] (the size of the coefficient represents the change in the Y-variable when the X-variable varies) shows that the cytotoxicity response along the 1st component is mainly influenced by cationic PPs_{1-3}, with PP_1+ and PP_2+ having a positive contribution (the higher the descriptor values, the higher the response) while cationic PP_3+ provides a negative contribution (the higher the descriptor values, the lower the response). Less contribution, but different from zero, is also given by anionic 4th and 1st-2nd anionic PPs (positive and negative contribution respectively) (Fig. 27a).[78] Cationic PP_1 and PP_5, and anionic PP_3-, the latter ones providing a negative contribution, have a major effect on the 2nd PC (Fig. 27b).[78] The anionic PPs provide a lower contribution in both plots. The overall descriptor variables contributions can be evidenced from the VIP (expressed as absolute values) plot, reported in Fig. 28.[78] Among the anionic PPs, PP_4- related to the distance of hydrophilic or hydrophobic areas from anion molecular barycentre and to the amphiphilicity, exhibits the highest VIP value.

The lower effect of anions on ILs toxicity was pointed out[88] and a more detailed study simplified the complexity of the problem addressing three elements such as headgroup, side chain and anion.[89] In these papers the effect of each IL structural element on IPC-81 toxicity was evaluated by changing only one parameter at the time (*e.g.* side chain or anion). whereas the QSPR approach here discussed dealt with simultaneous variations in both the cation (heterocyclic core, side chain length, presence of hetero-atoms in the side chain) and the anion structural features by means of 9 descriptors (PPs) whose physico-chemical interpretation has previously been commented (section 3.1.2).

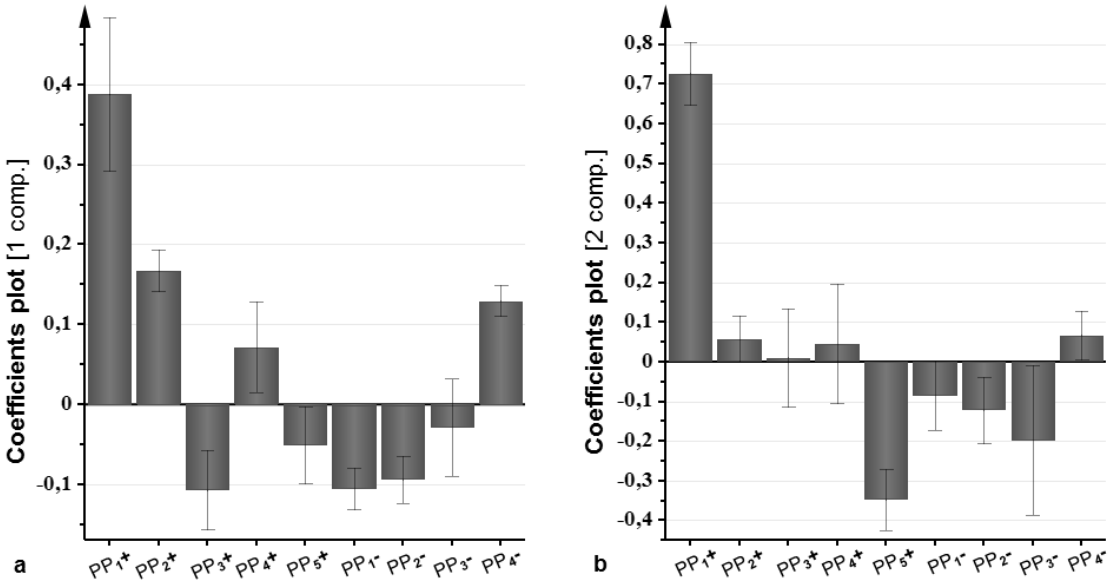


Fig.27 Coefficients plots along the 1st component (a) and the 2nd component (b) into IPC-81 cytotoxicity PLS model.

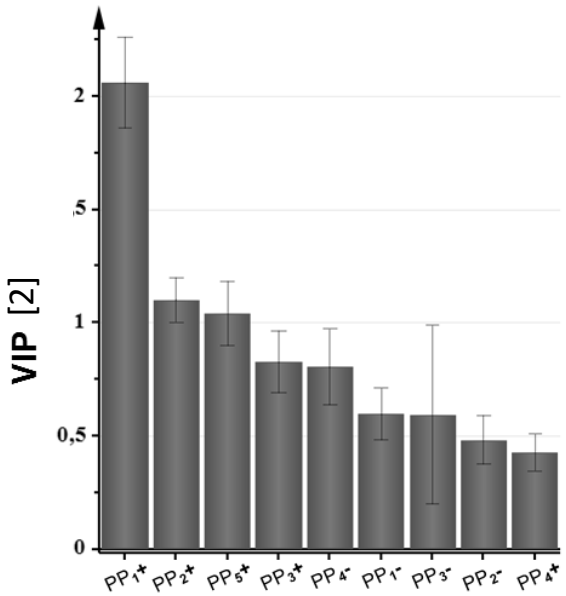


Fig. 28 VIP bars plot for the IPC-81 cytotoxicity PLS model.

The 1st and 2nd PP+ are mainly related to hydrophobicity/hydrophylicity ratio in cations. High values of PP_1+ indicate high solubility in water, while low values are related to molecular size and shape and to solubility in organic solvents. The 2nd PP+ is defined by descriptors referring to interactions with water (positive values indicate high interactions). Finally, the 5th PC+ indicates strong H-bonding acceptor ability. Hence, for a good interaction between ionic liquids and IPC-81 cells, the structure of the cations is clearly highly relevant as compared to the anionic counterpart (Fig. 28),[78] and high hydrophobicity is expected to be a very important property to make ILs behave as a toxicants. On the contrary, non aromatic cations, especially morpholiniums, are positively related to log(EC_{50}) value resulting in lower toxicity and also a side chain effect is evident: the less the carbon atoms number (shorter alkyl side chains, or hetero atoms like *O*-ether or *O*-carboxilic present into substituents) the lower toxicity, *i.e.* the closer to the Y variable located on the second quadrant in the weights plot, and *vice versa* (see the scores plot in Fig. 29 and A5,[78] and weights plot in Fig. A4). Very long side chain cations (IL 227, 229, 231, 315 in Table B12)[78] lie outside the confidence ellipse (and on the opposite quadrant with respect to the Y variable), indicating that their X-properties are not well explained into the PLS model due to their strange behaviour as already observed in aquatic toxicity model (see section 3.3.1).

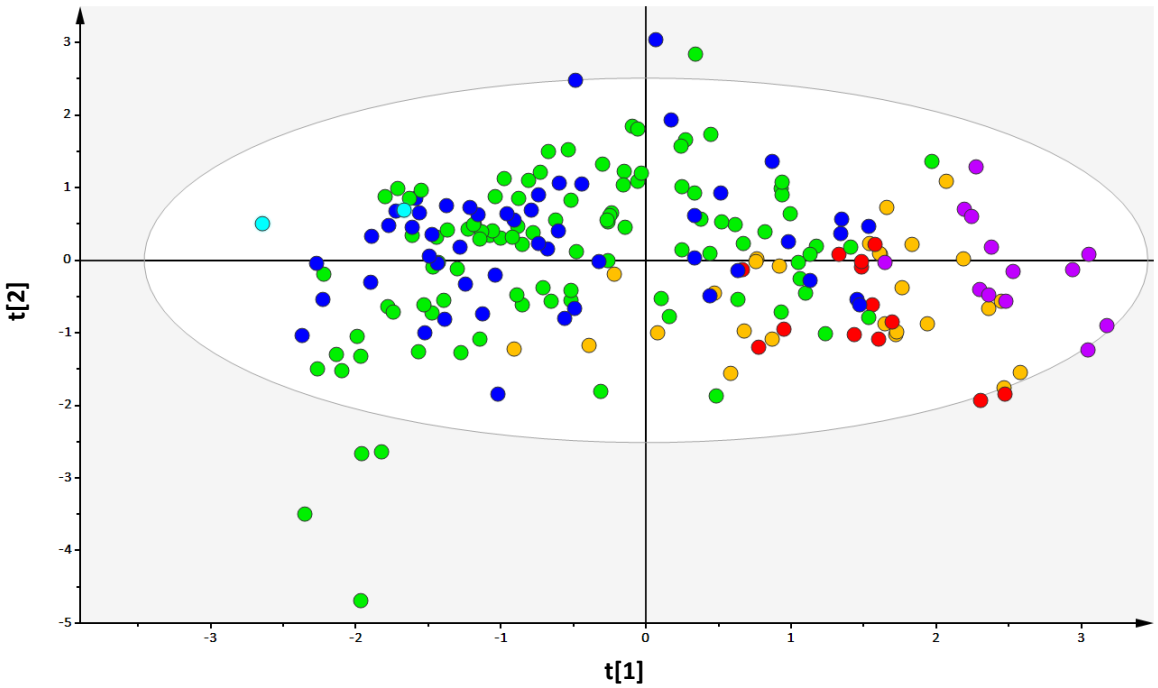


Fig. 29 t[1]-t[2] scores plot for IPC-81 toxicity PLS model. The objects are coloured as follows: imidazoliums, pyridiniums, quinoliniums, pyrrolidiniums, piperidiniums, morpholiniums based ILs. See also Fig. A5 which highlights the side chain effects for the imidazoliums-based ILs.

Predicting responses is one of the aim of QSPR studies, once a reliable correlation model is achieved. Predictions of IPC-81 values are displayed in Fig. 30[78] and their numerical values are reported in Table B12.[78] The correlation plot (Fig. 30)[78] shows the relationships between predicted and experimental values over 5 log units. Such a correlation might not appear very significant from a strictly statistical point of view as in many cases prediction errors are about one log unit. However, in our opinion this correlation can be regarded as satisfactory, taking into account some important aspects: i) the high experimental errors in some biological determinations (especially for the lowest EC_{50} values); ii) the significant effect of ILs impurities on analytical determinations;[2] iii) the high number of ILs (207) used to derive the model exhibit significant structural variations either in the anionic or cationic counterparts (cations include aromatic and non-aromatic cores, different alkyl chain length and the presence of oxygen atoms in the substituents)

In addition to cross validation, which assesses the predictive power of the model, another validation tool was adopted, the response permutation test, assessing the statistical significance of the estimated predictive power. The resulting permutation plot (Fig. A6)[78] clearly exclude fitting of random response data.

The predicting ability of the PLS model was additionally confirmed by an external validation by predicting IPC-81 values for 36 ILs. The prediction errors for these ILs, plotted in Fig. 30[78] and reported in Table B12[78] together with the confidence intervals for each predicted value, are not significantly different from those of ILs in the learning set.

The reliability of the PLS model suggested that predictions could be reasonably extended to a higher number of commonly used ILs (as many as 520 arbitrarily chosen) also reported in Table B12[78] and indicated as “U”. However, the prediction affordability for such a high unprecedented number of ILs cannot be the same for each single ionic compound. Guidance on the “goodness” of the prediction can be evaluated not only from the confidence intervals reported in Table B12,[78] but also by DModX values, the model residuals in the X matrix, which give an estimate of the similarity of a new observation to the training set observations. Predictions for ILs exhibiting DModX values higher than 1.50 in Table B12[78] should be considered with caution.[61] It is noteworthy that higher confidence intervals values are found for ILs 438, 439, 443-448 and 452-485 with hydroxypropanoate anions not present in the learning set. This finding indicates the capability of the PLS model to indicate molecular structures not considered in its derivation which lie outside the model chemical space and therefore cannot be predicted with satisfactory confidence.

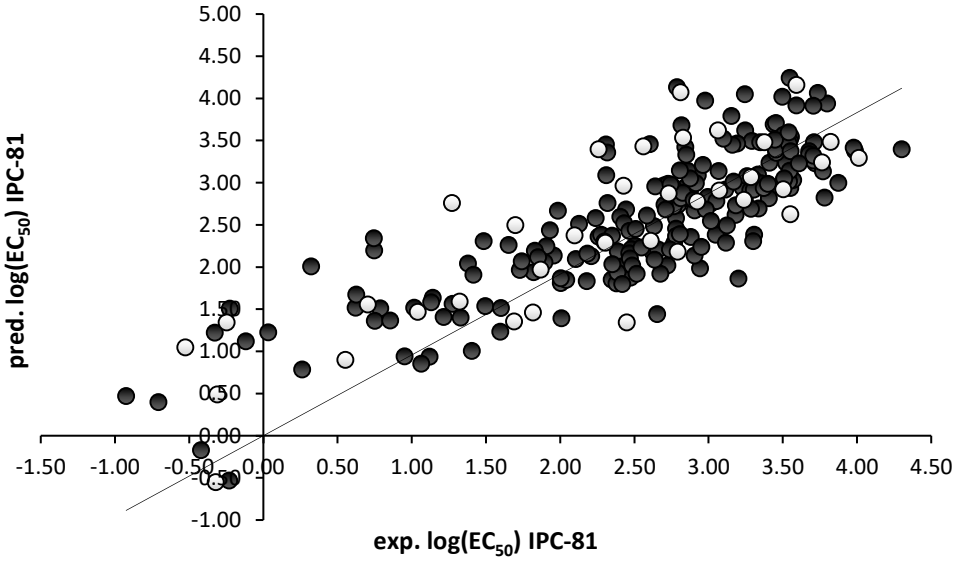


Fig. 30 Experimental vs. predicted log(EC_{50}) correlation plot for cytotoxicity (IPC-81) PLS model. ● ILs in Learning set (L in Table B12); ○ ILs in Test set (T in Table B12).

Figures 27- 30, A5,A6, and Tables A4, B12 were derived from an article published in SAR and QSAR in Environmental Research on 08 March 2016, available online: http://dx.doi.org/10.1080/1062936X.2016.1156571 (ref. 78).

3.3.3 *AChE* inhibition PLS model

AChE (acethylcholinesterase) inhibition data, expressed as log EC_{50} (mg/L), spanning 3 log units were collected for 230 heterocyclic ILs (Table B10).[82] This data set was divided into a learning set including 196 ILs (L in Table B13),[78] while 15% of the data (T in Table B13)[78] was included into a randomly selected test set of 34 ILs used as a model validation set by predicting their toxicity values.

A PLS analysis was carried out on the learning set data matrix including 5 cationic and 4 anionic PPs as variables (section 3.1.2) and AChE inhibition as the responses. The resulting model had a 2 significant components explaining 70.1% of Y variance (Q^2 = 0.671) where the 1st PC explains already 60.6% of Y variance (Q^2 = 0.592) (see parameters in Table A5).[78]

As showed in the coefficients plot (Fig. 31a),[78] cationic PP_1+, PP_2+ and PP_3+ contribute significantly to the 1st PLS component: positively PP_1+ and PP_2+, negatively PP_3+.

The overwhelming importance of cationic descriptors is consistent with available knowledge on the inhibition of AChE, an enzyme present in the brain, which hydrolyzes the neurotransmitter acetylcholine. In fact the AChE active site consists of the entrance site (a peripheral anionic site, PAS) and the catalytic site (CAS): basic or permanently charged nitrogens and aromatic systems can form interactions to one, or both, of the subsites, interacting with AChE.[90,91]

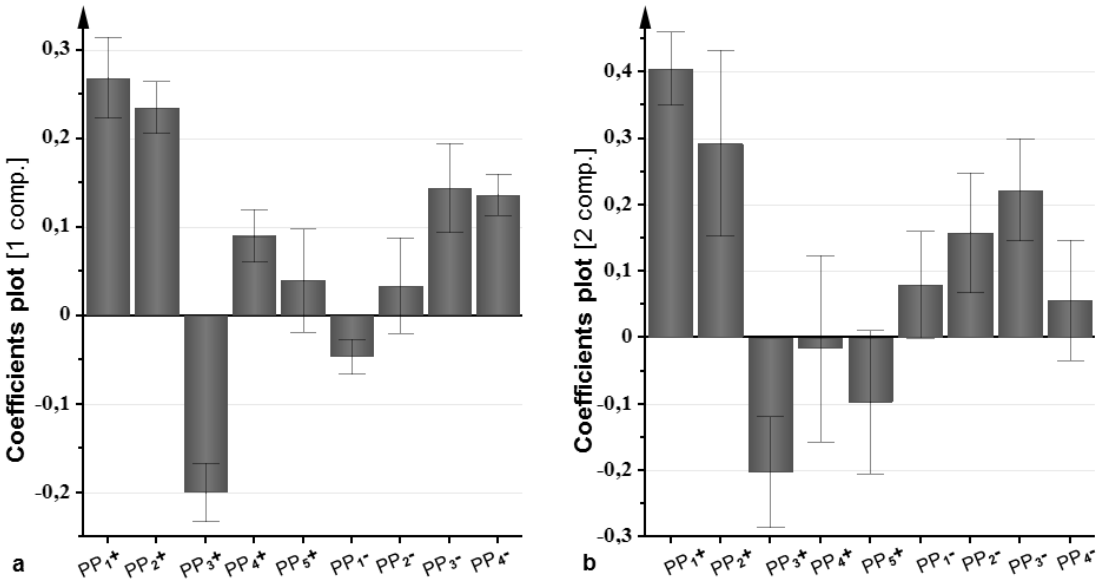


Fig. 31 Coefficients plot for the 1st component (a) and the 2nd component (b) in the AChE PLS model. The size of the coefficient represents the change in the Y-variable when the X-variable varies.

Considering the cationic counterpart, the decrease of the enzymatic inhibition activity is related to high water solubility at different pH (PP_1+), acceptor H-bonding ability and, in general, to a wide polar surface area (PP_2+), moreover to a low ability to give attractively hydrophobic interactions, to a high percentage of unionized species above pH = 5 (unsubstituted heterocyclic nitrogen into the scaffold), and to CACO2 and blood brain barrier permeability (related to PP_3+). PP_3- and PP_4- have the strongest influence among the anionic PPs, the former being positively related to the shape of anions (large surface, volume, rugosity and globularity) and to their amphiphilic moment. With the 2nd PLS component (Fig. 31b)[78] the above trend does not change. These results can be rationalized as follows (see Fig. 32[78] and the corresponding c-weights plot in Fig. A7). Low toxic ILs towards AChE have non aromatic cationic scaffolds (fused aromatic cycles result the strongest interactive compounds, hence the most toxic ones) and oxygen atoms in the side chain. In particular, moving from the right to the left part of the scores plot (Fig. 32 and also Fig. A8)[78] oxygenated ILs give place to the aliphatic ones, and the increase of carbon atoms number in the side chains is associated to an increase of toxicity (*i.e.* the decrease of EC_{50} values). The overall descriptor variables contributions can be evidenced from the VIP (expressed as absolute values) reported in Fig. 33,[78] which highlights the high importance of cationic $PP_{1\text{-}3,}$ then anionic PP_4- and PP_3- for the model explanation.

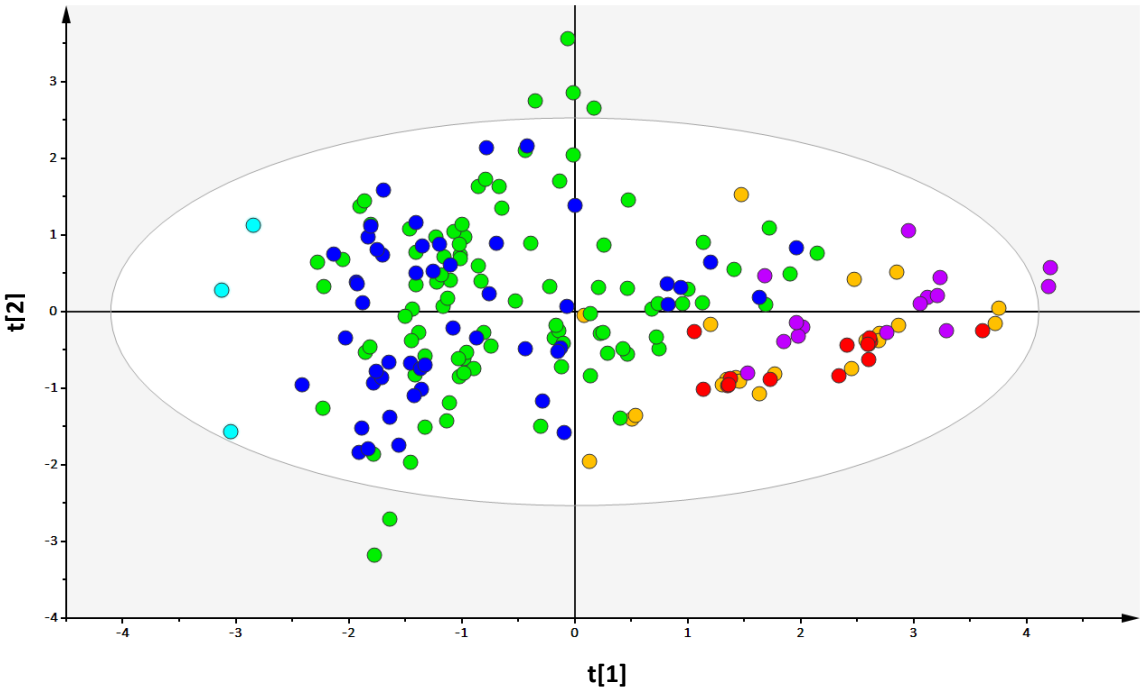


Fig. 32 t[1]-t[2] scores plot for AChE toxicity PLS model. The objects are coloured as follows: imidazoliums, pyridiniums, quinoliniums, pyrrolidiniums, piperidiniums, morpholiniums based ILs. See also Fig. A8 which highlights the side chain effects for imidazoliums based ILs.

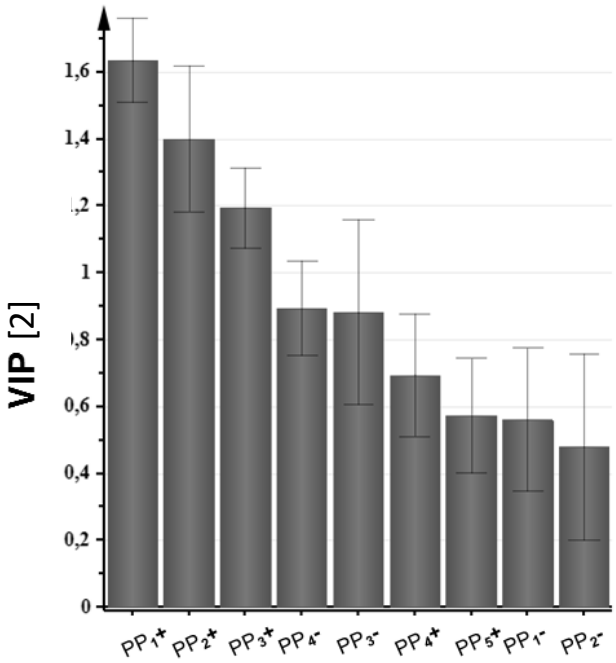


Fig. 33 VIP bars plot for the AChE PLS model.

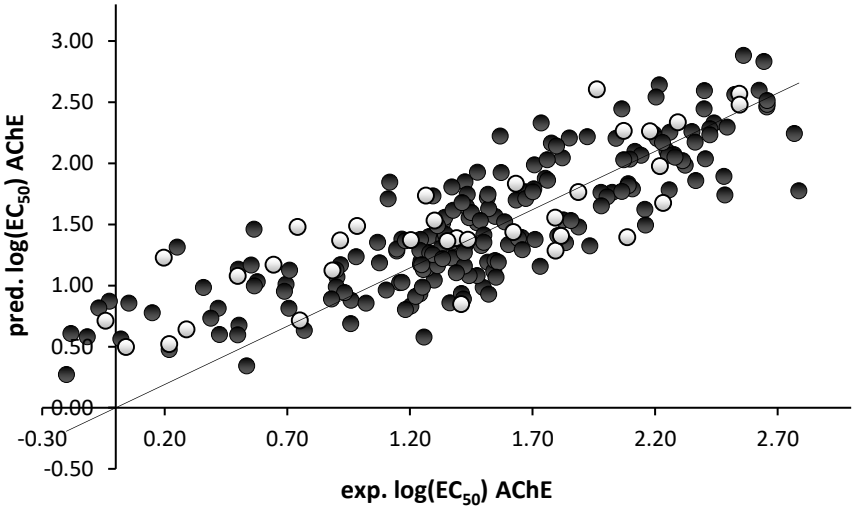


Fig.34 Experimental vs. predicted log(EC_{50}) correlation plot for AChE inhibition PLS model. ●ILs in Learning set (L in Table B13); ○ ILs in Test set (T in Table B13).

The PLS correlation plot (Fig. 34)[78] shows again a satisfactory correlation between predicted and experimental values taking into account the order of magnitude of experimental errors in biological tests and the effect of ILs impurities on analytical determinations.[2] Also for this model, the response permutation plot (Fig. A9)[78] supported the significance of the correlation and the predicting ability of the PLS model which was also tested by predicting AChE inhibition values for an external validation set of 34 ILs, whose confidence intervals (Table B13)[78] are comparable with those of ILs in the learning set. A single parameter QSAR analysis between AChE inhibition values and experimental HPLC-derived imidazolium cation lipophilicity was carried out for 22 ILs, while it was reported that the vast majority of anions, with the exception of fluoride containing ones, has no effect.[92] The correlation here reported and displayed in Fig. 34[78] included 196 ILs spanning significant cation structural variations (aromatic and non-aromatic cores, different alkyl chain length and the presence of oxygen atoms in the substituents) but was also able to evaluate the much lower effect of the anionic counterpart. The latter contribution, although less important than that of the cations (Fig. 33),[78] can be estimated quantitatively by the PLS model. The observed correlation with experimental imidazolium cation lipophilicity[92] was confirmed by the high negative values of the in silico PP_3+, and positive values of PP_1+ and PP_2+ (Fig. 31),[78] which are all descriptors derived from the interactions with OH2 and DRY probes (see section 3.1.2).

Also in the case of AChE inhibition, predictions were extended to 520 arbitrarily chosen ILs reported in Table B13[78] together with the confidence intervals for each predicted value. However predictions for ILs exhibiting DModX values lower than 1.50 in Table B13[78] can be considered as more reliable. Table B13[78] confirms that also in the AChE model higher confidence intervals values are found for ILs with hydroxypropanoate anions which lie outside the model chemical space being not present in the learning set. Furthermore it is worth evidencing that in Table B13[78] PLS predictions for 1-butyl-3-methylimidazolium, 1-methyl-3-octylimidazolium, and 1-butylpyridinium chlorides (1.02, 0.88 and 0.94 respectively) are in very good agreement with recently reported experimental values (1.16, 0.96 and 0.93 respectively)[93] and can be considered a further external validation set.

Figures. 31- 34, A8. A9 and Tables A5, B13 were derived from an article published in SAR and QSAR in Environmental Research on 08 March 2016, available online: http://dx.doi.org/10.1080/1062936X.2016.1156571 (ref. 78).

3.3.4 *Vibrio fischeri* PLS model

Vibrio fischeri is a marine luminescent bacterium which emits light as a result of normal metabolic processes. A reduction in luminescence during exposure to contaminants or pollutants is taken as a measure of eco-toxicity. These measurements in bioluminescent bacterium *Vibrio fischeri* are international standard ecotoxicological bioassays (DIN EN ISO11348)[88] widely applied for toxicity determination,[94,95] adopted in environmental toxicity studies[88,96] and for toxicity testing of chemicals.[95,97] Such an extensive use can be ascribed to its low cost, to the simplicity and to the speed of this bioluminescence test as compared to other experimental procedures. Furthermore *Vibrio fischeri,* being a Gram negative bacterium used for aquatic toxicity evaluation, exhibits an optimum hydrophilic/lipophilic balance allowing measurements for a significantly high number of ILs.

The chronic bioluminescence inhibition of *Vibrio fischeri* values reported here are log EC_{50} for 65 ionic liquids including 35 different heterocyclic cations and 18 organic and inorganic anions (see Chart 3, or Table B14).[98] These homogeneous toxicity values, spanning almost 5 log units, were taken from a literature database[41] last accessed in August 2014 and unfortunately no longer open access since September 2014.

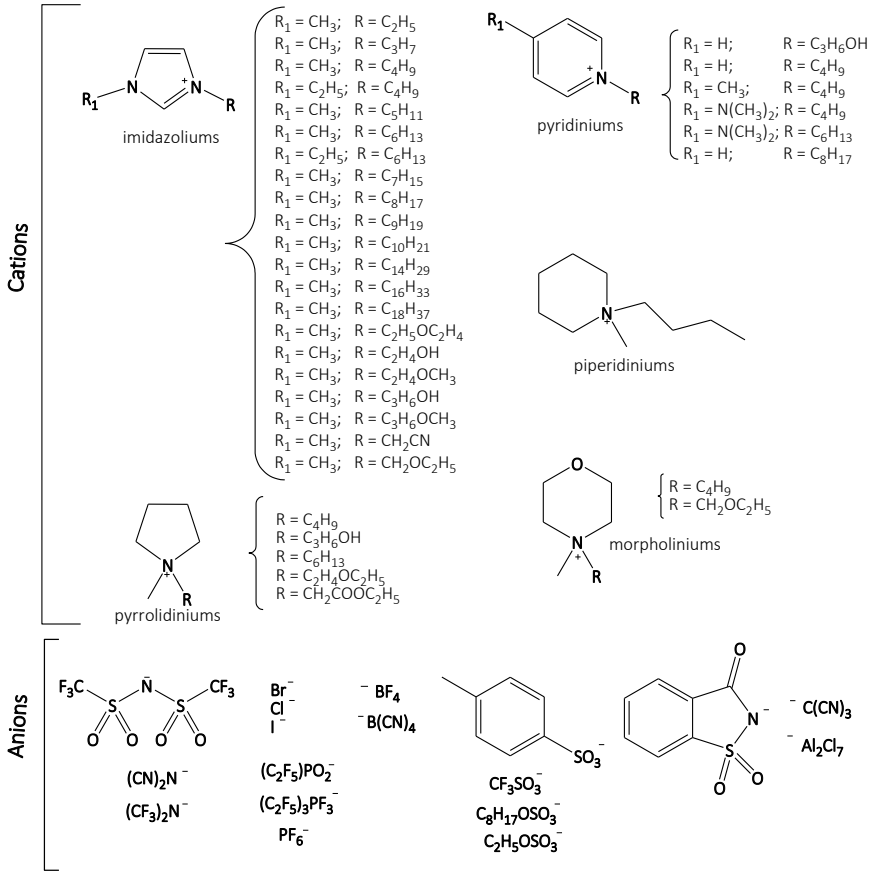


Chart 3 Cations and anions structures used *in Vibrio fischeri* PLS correlation model as learning and test sets (L and T respectively in Table B14).

In order to verify the statistical significance of the resulting model by means of a validation set, the dataset was randomly divided into a learning set (L) and test set (T) containing 55 and 10 (15% of the total dataset) ILs respectively. The 9 PPs (derived as in section 3.1.2) were used as descriptors. In such a model, 2 significant PLS components describe 76.9% of the total Y variance, with a predictive ability of 0.681 (Table A6).[98] In the VIP plot, which shows the importance of each X-variable in explaining X-variation and correlation to Y (Fig. A10),[98] PP_1+ resulted as the most important descriptor, followed by PP_2+, PP_5+ (with a high error which affects its significance)[61] and PP_3-, while all other descriptors appear to be less important. Hence, in order to simplify the model removing less important information and limiting its dimensionality, a new PLS correlation model was built maintaining only three relevant X descriptors: PP_1+ and PP_2+ for cations and PP_3- for the anions. The new simplified 55x3 matrix provided a 2 PLS components model explaining 78.9% of the total variance, and with a cumulative Q^2 of 0.770 (see Table A7 for model details, and Table B14 for the data matrix)[98] showing that the exclusion of low relevance six descriptors does not affect the "goodness" of fit. It is worth highlighting that the QSPR approach presented here considered simultaneous variations in both the cation (heterocyclic core, side chain length, presence of oxygen atoms in the side chain) and the anion structural features by means of 3 descriptors (PPs) whose physico-chemical interpretation was commented above (see section 3.1.2). In particular, PP_1+ embodies information related to cation solubility, size, flexibility and molecular weight, PP_2+ describes the interaction with water and the hydrophobic volume of the cation, while PP_3- is related to anionic size/shape and to the anion ability to form H-bonds as donor or acceptor.

EC_{50} values represent the concentration of a compound at which 50% of its maximal effect is observed, therefore the higher this value, the less toxic the IL. The correlation between X descriptors and the Y response can be displayed by means of the loadings plot for both PLS model components (Fig.35).[98] PP_1+ shows a high positive influence on *Vibrio fischeri* toxicity, being very close to log EC_{50}, whereas PP_3- has a negative contribution being on the opposite quadrant. The projection of PP_2+ on the dotted line shows a slighter positive contribution towards log EC_{50}: this variable can be considered less important for the correlation with Y, but still useful in explaining X and modelling Y variance as Fig. 36 (the VIP plot)[98] points out.

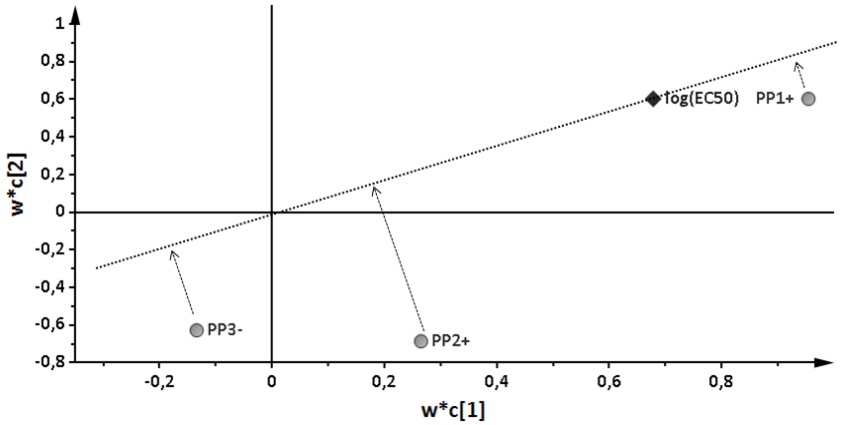


Fig. 35 w*c[1]-w*c[2] loadings plot for *Vibrio fischeri* ecotoxicity PLS model, showing the descriptors (w*) and response (c) loadings superimposition. The correlation between each descriptor (●) and the dependent variable (log EC_{50}, ◆) is elucidated by the PPs projections on the dotted line.

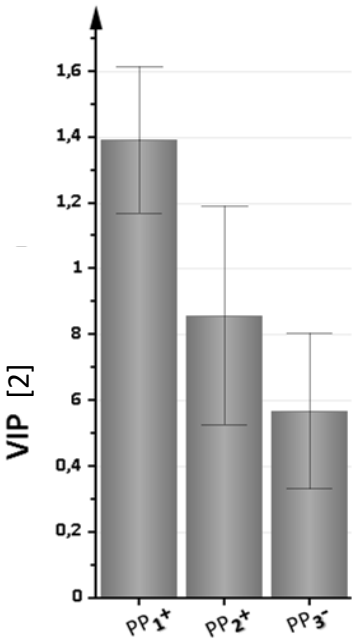


Fig. 36 VIP bars plot for the *Vibrio fischeri* ecotoxicity PLS model.

The model interpretation allowed to furtherly confirm the results on toxicity towards aquatic biological targets discussed above. In fact the influence of PPs on the response evidenced that: less toxic ILs have small cations bearing a non-aromatic cationic scaffold and short alkyl side chains highly soluble in water in the pH range 3-10 also showing a great dispersion in it (PP_1+); are able to interact with water and as H-bonding acceptors (PP_2+) having oxygen atoms in the scaffold and/or in the side chain. These considerations emerged also from the interpretation of the corresponding scores plot (Fig. A11),[98] which, when superimposed to the loadings plot in Fig. 35,[98] can evidence the ILs cationic structures influence on toxicity. Similar features such as small dimensions and wide hydrophilic regions with H-

bonding ability (PP_3-) are important for the anions. However the VIP plot (Fig. 36)[98] stresses the relevance of PP_1+: for a good interaction between ionic liquids and the *Vibrio fischeri* bacterial membrane, the structure of the cations is more relevant as compared to that of the anionic counterpart. Evidently a very soluble and highly dispersed in physiological media IL is not able to interact with bacterial membranes not penetrating them and resulting less toxic. This finding is consistent with literature[96] and our previous studies.[82] Nevertheless, the anions cannot be considered as "silent audience" in the interaction. In fact, in Table B14,[98] ILs containing the same cation (1-butyl-3-methylimidazolium ILs 160-164, 166-168, 170) exhibit different log EC_{50} values, ranging from 1.83 for octylsulfate, to 2.47 for bis(trifluormethylsulfonyl)imide (also known as 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl] methanesulfonamide), to 3.07 for bromide, and up to 3.60 for iodide and trifluormethylsulfate. Such a variation is appreciated by our QSPR approach (by means of PP_3-) allowing to evaluate anions effect, which cannot be evidenced when similar anions such as halogens are considered.[86,87]

Fig. 37[98] shows the correlation plot between experimental and predicted log EC_{50} values for both learning (L) and test (T) set ILs. Only in few cases the difference between experimental and predicted values is over one log unit, and could be considered less significant from a strictly statistical point of view. In particular, IL 231 (Table B14, Fig. 37)[98] with a cationic side chain formed of 18 carbon atoms, exhibited a high discrepancy between experimental and predicted toxicity value, being predicted as more toxic than it is: the longest cationic side chain ILs may form intermolecular aggregates[99] which prevent them from interacting as surfactants with the biological target (*i.e.* resulting less toxic with respect to its prediction).

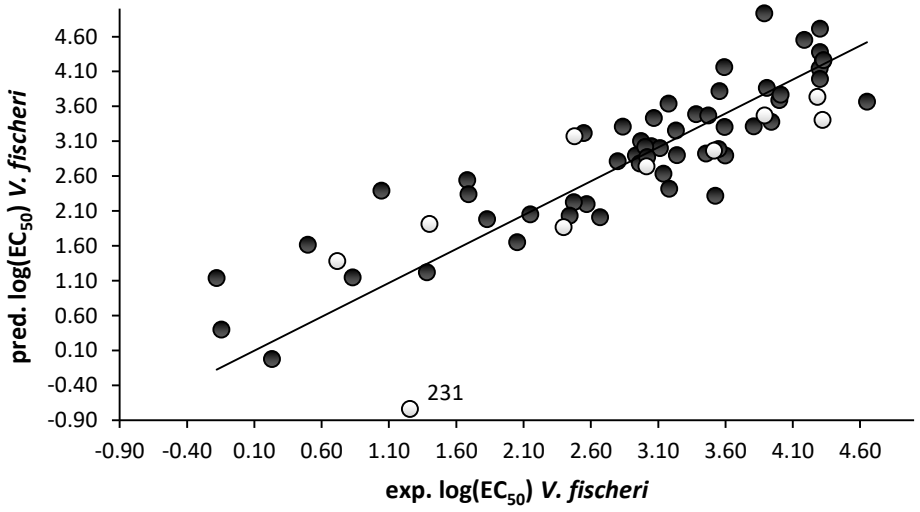


Figure 37 Experimental vs. predicted log(EC_{50}) correlation plot for *Vibrio fischeri* ecotoxicity PLS model. ● ILs in Learning set (L in Table B14); ○ ILs in Test set (T in Table B14).

The reliability of a PLS model may be evaluated by using different statistical tools. Internal cross validation gives a first important assessment about the goodness of fit and predictions by means of R^2 and Q^2 parameters, eventually supported by a test set used for external validation. Furthermore, a permutation plot can give information about the statistical significance of a correlation model (section 2). The permutation plot for this correlation model, reported in Fig. A12,[98] fulfilled the validation criteria and excludeed chance correlation.[61] On the basis of the above considerations, predictions could be extended to a higher number of commonly used ILs (the same as the 520 arbitrarily chosen in previous sections) also reported in Table B14[98] together with DModX values. However, as before commented, predictions reliability for such a wide set cannot be the same for each single IL. Some guidance on the "goodness" of the prediction can be evaluated by DModX values, reported in Table B14,[98] which give an estimate of the similarity of a new observation to the training set observation.[61] Predictions for ILs exhibiting DModX values higher than 2.33 in Table B14[98] should be considered with great caution. Among the 520 ILs not belonging neither to learning nor test set some compounds should be carefully considered in their predictions, due to their high DModX value (for instance, see ILs 85,86, 117 bulky side chain imidazoliums; 255-264, 268-271, 328-330 long amido-side chain pyridiniums; 424-436 long bis ethers imidazoliums). DModX value represents only one parameter indicating prediction reliability, which in specific cases of interest might be supported by experimental validation. Nevertheless, PLS predictions provided approximate toxicity estimates useful to orient the selection among several efficient ILs for specific applications. When considering the utility of the predictions, one should also take into account the generality of a data matrix containing five different cationic scaffolds and side chains and different anionic structures, as well as experimental errors in biological determinations and the effects of ILs impurities influencing analytical determinations[2] which can strongly affect the significance of any model. Therefore this QSPR correlation, spanning 5 log units, can be considered as satisfactory, since it tried to rationalize and quantitatively explain in a simple way the complex interactions between ionic liquids and living organisms.

The attempt to study and predict *Vibrio fischeri* and other biological toxicities in ILs using QSPR approaches is not new. An interesting work[100] reports *Vibrio fischeri* standardized toxicity values and applies PLS-DA for discriminating ILs on the basis of their toxicity. In this approach the input variable for each IL was equal to 1 if the anion/cation was in the molecule, and 0 if not, and ILs expected toxicity was assessed with respect to toluene, an organic solvent traditionally used in industrial applications. However, this binary classification cannot be considered a proper QSPR study. In general, several papers[101] denote the growing interest in QSPR studies for ILs toxicity prediction, aimed at limiting time and costly consuming tests and reducing the number of *in vitro* and *in vivo* experiments for the REACH

regulation.[102] However these papers usually have some relevant limitations, adopting a somewhat "univariate" approach by considering the cation effect for a fixed anion and the anion effect keeping the cation as constant (assuming that toxicity does not vary on varying the cationic/anionic IL counterpart) or use less informative structural descriptors and very often do not give the possibility to reproduce their results.

Couling *et al.*[103] carried out a QSPR study considering 25 ILs (including 10 pyridinium and 6 imidazolium cationic scaffolds) and using a multiple linear regression approach. They reported an interpretation based on electrostatic and topological descriptors. However, descriptor values are not published and the results cannot be reproduced. Furthermore the model is not validated by an external validation set as recommended by the OECD principles for QSAR studies.[104] Another paper[105] reported a MLR correlation model in which ILs structures for 9 cations and 17 anions were described by three main groups of descriptors: anions (A), cations (C) and substitutions (S) describing ecotoxicity as the summation of the contributions of each group. Descriptors are based on the Boolean approach: their numerical value is 1 if a specific group is present, 0 if not. Each descriptor is multiplied for a parameter (a, c and s) indicating the descriptors contribution to the model. This approach is very simple although the specific information depending on the chemical features of cations and anions is limited due to the 0/1 variation in the descriptors. A four-parameter correlation was found[87] for ionic liquids with halide (Cl^- or Br^-) anions. Descriptors were based on ILs cations structures and the corresponding model was used to predict ILs toxicity in water or in the gas phase. A heuristic procedure was used to select the most influent descriptors to obtain a reliable correlation model. Estimation of the descriptors collinearity and reproducibility of the results by using different QSPR approaches are not possible due to the lack of descriptors numerical values. The paper conclusion asserted that the model could be applied to a broader range of ILs with different anions as, according to the literature,[96] ILs with the same cation and different anions do not show any statistical difference in toxicity. Actually the effect of anions was pointed out both by the results of our statistical approach and by experimental data reported in Table B14[98] showing two orders of magnitude difference in *Vibrio fischeri* toxicity for 1-butyl-3-methylimidazoliums.

Das and Roy[106] published an interesting paper using linear discriminant analysis with respect to toluene, and MLR and PLS approaches to derive QSPR models whose predictions are comparable with those reported in Fig. 37[98] Rigorous validation was performed either for the classification or the regression models by applying multiple strategies and in both the cases encouraging results were obtained for external and internal validation. The influence of ILs features on toxicity is discussed, but unfortunately no descriptor values are reported and this represents a limitation to the QSPR model reproducibility.

A more recent study,[107] reported a five parameter MLR approach for a large dataset by using topological descriptors regarding the position and the features of non-hydrogen atoms, used to mathematically derive cationic and anionic descriptors whose numerical values are not reported.

In my opinion, correlation models should not only be just reliable (*i.e.* have a good predictability), but also provide either the possibility to easily interpret the results and the correlation itself or to employ general, useful, reusable "building blocks" as descriptors whose numerical values are reported allowing the readers to reproduce the work or to apply alternative statistical models. In the present section a QSPR approach able to include all the above aspects was discussed

Commercial softwares and tools such as VolSurf+ and PLS are not available to everybody. For this reason we provide equation (5) in which the three descriptors for both cations and anions, adopted to predict *Vibrio fischeri* toxicity values reported in Fig. 37,[98] can be easily used to extend predictions to any combination of ILs cations and anions for which PPs are available (Table B1-2):[78]

$$\log(EC_{50}) \text{ pred.} = 0.264\ (PP_1+) - 0.091\ (PP_2+) - 0.240\ (PP_3-) + 2.219 \qquad \text{(eq. 5)}$$

Many potential users can benefit from the application of this simple equation allowing to predict *Vibrio fischeri* toxicity for thousands (in principle 218x38 = 8284) ILs, well above the 520 reported in Table B14.[98]

Tables B1, B2 were derived from an article published in SAR and QSAR in Environmental Research on 08 March 2016, available online: http://dx.doi.org/10.1080/1062936X.2016.1156571 (ref. 78).
Figures 35-37, A10-A12, Chart 3 and Tables A6, A7, B14 were reproduced from ref. 98 with permission from the Royal Society of Chemistry.

3.4 *QSPR* models analyzing ILs structures influence on their *physico-chemical properties*

3.4.1 E_{NR} PLS model

Among solvent properties, polarity is one of the most widely used and different empirical scales are known. In the case of UV-Vis active probes, both charged and neutral "sensors" have been used.In fact the polarity of ILs has been evaluated using pyridinium betaine dyes (Kosower[108] and Reichardt[109,110] scales), transition-metal complexes such as $[Cu(acac)(tmen)]^+$, merocyanine probes and Nile Red (NR). Interesting experimental studies on the determination of ILs dielectric constants have been carried out by Weingaertner and coworkers.[111-114] The use of empirical scales to evaluate their polarity has been the object of an intense debate. Indeed, the response of the probe to the solvent is determined by all possible solvent-solute interactions, and in the case of ionic solvents media, some can play a more significant role than others. Also in the case of ILs, their polarity has been determined using single-molecules as spectroscopic probes, taking advantage of the effects they are able to exert on electronic absorption, fluorescence and vibrational spectra, as well as on paramagnetic resonance signals.[115]

NR has been used to evaluate the polarity of ILs by means of the E_{NR} parameter but also to have information about their 3-D organization as neat solvents or in combination with other ILs or conventional organic solvents to give binary mixtures.[73,116] Carmichael *et al.* showed in a study on NR polarity of 1-alkyl-3-methylimidazolium ILs[117] that their polarity is comparable with that of the lower alcohols. Furthermore that paper points out "a paucity of good reproducible data" and the need "to create a reliable database". Other studies relating different ILs structures to ILs polarity[118,119] using the empirical Kamlet–Taft solvent parameters have been reported.

In this context, the polarity of 18 ILs, having different aromatic and non-aromatic cationic scaffolds, different alkyl chain length and different anions, were here reported to carry out a quantitative structure-property relationships model based on VolSurf+ descriptors with the aim to predict E_{NR} values for a large number of commonly used ILs.

Literature[120-122] and experimental E_{NR} values for 18 ILs were collected in Table 2[123] (see also Chart 4)[123] with different cationic and anionic structural features: mainly imidazolium cationic scaffolds (plus one piperidinium and one pyrrolidinium), different length alkyl side chains (up to 8 carbon atoms), and 8 anions ranging from tetrafluoroborate to oxygenated anions.

PLS analysis was carried out using a data matrix including 18 ILs (Table 2)[123] and 176 variables, *i.e.* 128 cation and 48 anion VolSurf+ descriptors (section 3.1.1). E_{NR} polarity values were used as the responses

Table 2 Experimental E_{NR} values for ILs used as learning and test set and PLS predictions.

	Ionic Liquids	ENR (kcal/mol)	ENR[a] (kcal/mol)	PLS pred.	DModX[b]	Name
1	IM1-(1Ph) (CF3SO2)2N	216.2[c]		216.3	1.54	1-Benzyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
2	IM12 (CF3SO2)2N	217.9[d]		217.8	1.07	1-Ethyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
3	IM14 (1O)2PO2	218.0[e]		217.8	0.63	1-Butyl-3-methylimidazolium dimethyl phosphate
4	IM14 N(CN)2	215.7[f]		215.6	0.74	1-Butyl-3-methylimidazolium N-cyanocyanamide
5	IM14 PF6	217.7[f]	218.5	217.5	0.79	1-Butyl-3-methylimidazolium hexafluorophosphate
6	IM14 (CF3SO2)2N	218.2[f]	218.0	217.8	0.85	1-Butyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
7	IM14 BF4	217.3[d]	217.2	217.2	0.86	1-Butyl-3-methylimidazolium tetrafluoroborate
8	IM14 CF3COO	216.6[e]		216.9	1.01	1-Butyl-3-Methylimidazolium trifluoroacetate
9	IM14 1COO	217.2[e]		217.3	1.57	1-Butyl-3-methylimidazolium acetate
10	IM14-2Me (CF3SO2)2N	217.7[d]		218.0	0.92	1-Butyl-2,3-dimethylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
11	IM16 N(CN)2	215.3[f]		215.1	0.70	1-Hexyl-3-methylimidazolium dicyanamide
12	IM16 (CF3SO2)2N	217.9[d]		217.3	0.84	1-Hexyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
13	IM16 SbF6	216.1[d]		216.8	1.03	1-Hexyl-3-methylimidazolium hexafluoridoantimonate
14	IM18 (CF3SO2)2N	217.9[d]		217.7	0.61	1-Methyl-3-octylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
15	IM18 N(CN)2	215.7[f]		215.5	1.07	1-Methyl-3-octylimidazolium dicyanamide
16	IM4-(1Ph) (CF3SO2)2N	216.1[c]		216.4	1.41	1-Benzyl-3-butylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
17	Pip14 (CF3SO2)2N	219.0[d]		219.5	0.87	1-Butyl-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
18	Pyr14 (CF3SO2)2N	219.9[d]		219.6	0.77	1-Butyl-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
19	IM1-10 BF4		219.2	216.9	1.40	1-Decyl-3-methylimidazolium tetrafluoroborate
20	IM16 PF6		216.8	217.0	0.87	1-Hexyl-3-methylimidazolium hexafluorophosphate
21	IM16 BF4		216.8	216.7	0.96	1-Hexyl-3-methylimidazolium tetrafluoroborate
22	IM18 PF6		217.6	217.4	0.86	1-Methyl-3-octylimidazolium hexafluorophosphate
23	IM18 BF4		217.7	217.1	1.01	1-Methyl-3-octylimidazolium tetrafluoroborate
N_1	IM14 NO3		215.3	212.3	35.32	1-Butyl-3-methylimidazolium nitrate
N_2	IM16 NO3		216.3	211.8	35.28	1-Hexyl-3-methylimidazolium nitrate
N_3	IM18 NO3		217.4	212.2	35.29	1-Methyl-3-octylimidazolium nitrate

[a]Ref. 117; [b]DModX values indicate the distance of the observations to the X-model hyperplane.[61] Predictions for ILs with DModX > 1.32 should be considered with caution; [c]Ref. 120; [d]Ref. 121; [e]This work; [f]Ref. 122.

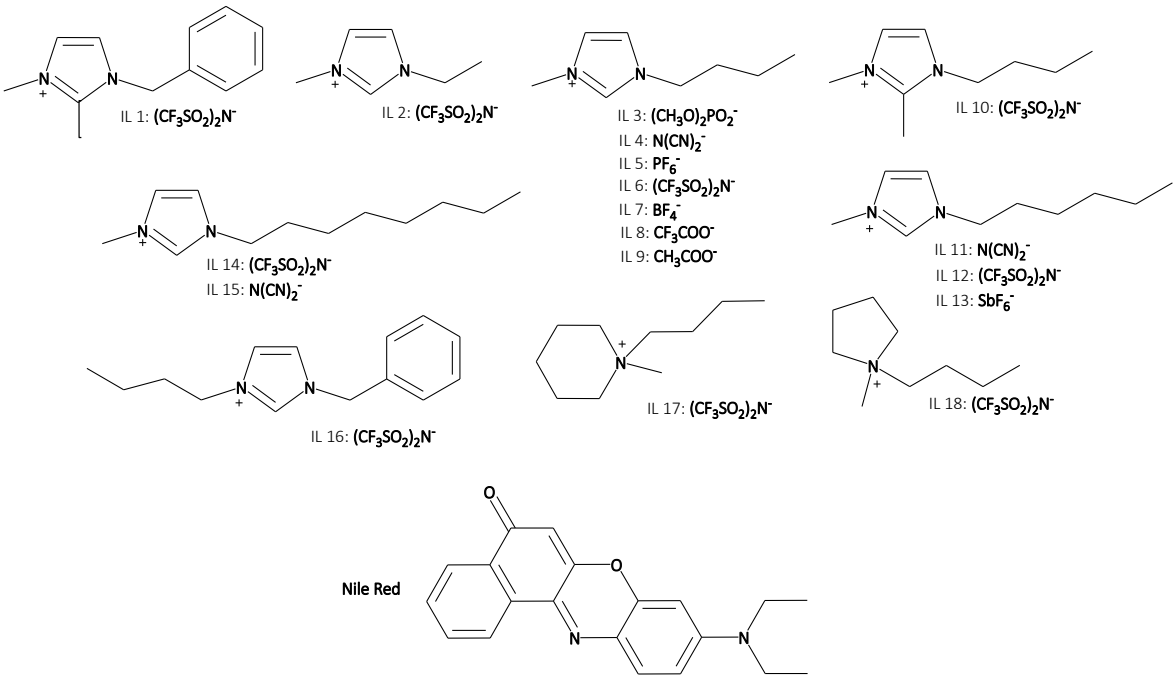


Chart 4 Structure of ILs and of the solvatochromic probe used.

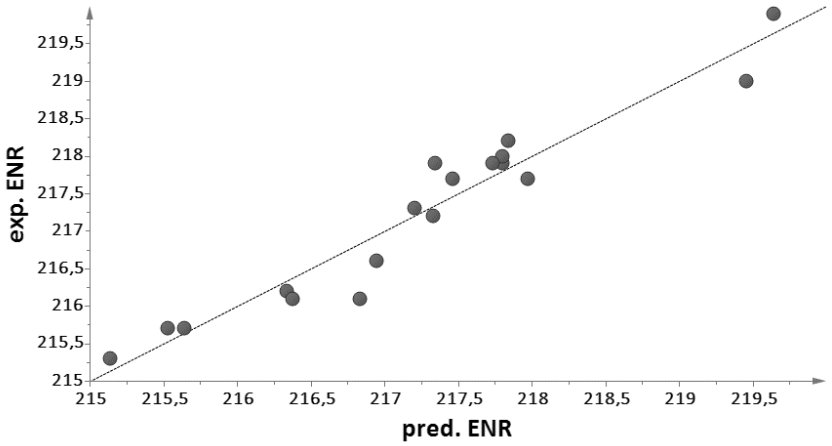


Fig. 38 Experimental *vs.* predicted correlation plot in the E_{NR} PLS model reporting the ILs 1-18 in Table 2.

The analysis provided a 3 PLS components model explaining 93.2% of Y variance (Q^2 = 0.770) with 88.1% of Y variance (Q^2 = 0.728) already in the 1st and the 2nd PC (see Table A8).[123] The plot of predicted *vs.* experimental data (Fig. 38)[123] showed a good agreement between experimental and predicted E_{NR} values. Moreover, in Fig. A13 the E_{NR} permutation plot was reported to prove the PLS correlation significance.

SIMCA[61] models are soft models applicable within the experimental space covered by the observations considered in the analyzed data matrix. Therefore the prediction reliability for each single IL depends on its structural similarity with the structures used in the learning set. The PLS model predictions are reported in Table 2[123] together with DModX values, the model residuals in the X matrix, providing an estimate of the similarity of a new observation to the training set. Predictions for ILs exhibiting DModX values higher than 1.32 should be considered with some caution:[61] the higher the DModX value is, the lower the prediction reliability could be.

In order to check the experimental reliability of the model predictions, the E_{NR} values reported by Carmichael and co.[117] were also reported as an external test set in Table 2.[123] Although the Kamlet–Taft parameters are well established for traditional solvents, for ILs they are very sensitive to impurities.[2,124] Moreover, in the present case, the E_{NR} values used as a test set were determined in the presence of 1,4-dioxane. However, as previously reported, in comparison with literature values the co-solvent had a negligible effect.[121] This statement was furtherly supported by the agreement between the E_{NR} values measured for this thesis with literature ones[117] for three ILs (Table 2),[123] indicating also a good inter-laboratory reproducibility.

The PLS model predictions for the test set were likewise in agreement with the experimental data in Table 2.[123] Predictions for objects with very high DModX values, such as ILs with nitrate anions absent in the learning set, are definitely unreliable. A possible interpretation of this result might rely on both anion geometry and size. Anions used in this study exhibit different geometries, as well as different ionic radii, comparable for [BF_4^-] and [PF_6^-] anions (232 and 240 pm, respectively) but significantly lower for [NO_3^-] (179 pm) which determines a different charge distribution. Anyway, a specific effect which renders nitrate modelling more difficult might be responsible for their peculiar behaviour.

As concerns 1-decyl-3-methylimidazolium tetrafluoroborate, the poor agreement between experimental and predicted values could be ascribed to segregation effects, which heavily depend on the alkyl chain length.[69,125] On the grounds of the above effects, the fluorescent probe could feel different polar and apolar microenvironments, more evident for decylimidazolium, than for octylimidazolium tetrafluoroborate.

The E_{NR} predictions were extended to a higher number of ILs (up to 116) which show structural similarity to those used in the model derivation, exhibiting DModX values lower than 2.00 (Table B15).[123]

The analysis of VIP values for the descriptors allowed to evaluate quantitatively their importance in influencing the E_{NR} parameters. Table 3[123] reports the VIP values for the top 75 descriptors, together with the coefficients along the 1st PLS component (the most relevant one) providing information on the sign of the descriptor contribution. Table 3[123] showed that the major influence on the response is provided by cation descriptors, especially by those related to cations hydrophobic character (hydrophobic volumes D_n and hydrophobic capacity factors CD_n at different energy levels). A lower contribution is given by cationic descriptors referring to a general hydrophilic character (hydrophilic volumes indicating polarizability W1-W4 and hydrophilic capacity factors CW1-CW3) and water solubility (intrinsic solubility SOLY and solubility at various pH LgSs). The former descriptors are inversely correlated to the responses, whereas the latter have a positive contribution to the E_{NR} values (as expressed by the relative coefficients), indicating that molecular polarizability (expressed by W1-W3) in ILs contribute to decrease the response, whereas ILs able to be dissolved in water have higher E_{NR} values. Similar considerations can be made for the anionic hydrophobic character (D4-D8 and CD4-CD8) and hydrophilic (W1,W5 and CW1-CW5) character descriptors. In particular, a positive contribution is found for anionic size descriptors (molecular globularity G, volume V, surface S and volume/surface ratio R), in agreement with the considerations made to rationalize the peculiarity of [NO_3^-]-based ionic liquids.

Table 3 VIP values for the top 75 descriptors[a] in E_{NR} PLS model together with the coefficients (scaled and centerd) of the 1st PLS component. The coefficients values express the sign and the magnitude of the contribution between the Xs and the Y.

	Var. ID	VIP values	Coeff. Values
1	D3_Cat	1.80	-0.022
2	CP_Cat	1.80	-0.022
3	D5_Cat	1.78	-0.022
4	VD_Cat	1.78	-0.022
5	D4_Cat	1.78	-0.022
6	D6_Cat	1.77	-0.022
7	CD1_Cat	1.77	-0.022
8	CD2_Cat	1.77	-0.022
9	CD3_Cat	1.74	-0.021
10	CACO2_Cat	1.73	0.021
11	CD4_Cat	1.71	-0.021
12	D7_Cat	1.70	-0.021
13	D2_Cat	1.69	-0.021
14	CD7_Cat	1.66	-0.021
15	CD8_Cat	1.64	-0.021
16	CW2_Cat	1.62	-0.020
17	CD6_Cat	1.62	-0.020
18	CD5_Cat	1.61	-0.020
19	PSA_Cat	1.60	-0.019
20	D8_Cat	1.60	-0.020
21	D1_Cat	1.58	-0.019
22	D8_An	1.58	-0.019
23	CD8_An	1.58	-0.019
24	CD6_An	1.55	-0.018
25	CD7_An	1.55	-0.018
26	W2_Cat	1.54	-0.019
27	D6_An	1.53	-0.018
28	D7_An	1.52	-0.018
29	CD5_An	1.51	-0.018
30	CW1_Cat	1.48	-0.018
31	CD4_An	1.47	-0.017
32	D5_An	1.45	-0.017
33	W3_Cat	1.39	-0.018
34	D4_An	1.35	-0.016
35	CW3_An	1.35	-0.016
36	S_An	1.35	0.016
37	V_An	1.34	0.016
38	G_An	1.33	0.015
39	CW3_Cat	1.32	-0.016
40	W1_Cat	1.32	-0.015
41	CW2_An	1.32	-0.015
42	IW4_An	1.32	-0.015
43	CW5_An	1.30	-0.015
44	ID4_Cat	1.29	-0.014
45	W5_An	1.26	-0.015
46	R_An	1.25	0.014
47	DD1_Cat	1.24	-0.012
48	FLEX_Cat	1.24	-0.013
49	W1_An	1.21	0.014
50	SOLY_Cat	1.20	0.013
51	LgS3_Cat	1.20	0.013
52	LgS4_Cat	1.20	0.013
53	LgS5_Cat	1.20	0.013
54	LgS6_Cat	1.20	0.013
55	LgS7_Cat	1.20	0.013
56	LgS7,5_Cat	1.20	0.013
57	LgS8_Cat	1.20	0.013
58	LgS9_Cat	1.20	0.013
59	LgS10_Cat	1.20	0.013
60	LgS11_Cat	1.20	0.013
61	L0LgS_Cat	1.20	0.013
62	LgBB_Cat	1.19	0.012
63	G_Cat	1.18	-0.013
64	DRDRDR_Cat	1.16	-0.013
65	DD2_Cat	1.15	-0.011
66	FLEX_RB_Cat	1.11	-0.013
67	CW4_An	1.11	-0.013
68	DD3_Cat	1.10	-0.009
69	A_An	1.10	0.013
70	S_Cat	1.10	-0.011
71	HSA_Cat	1.09	-0.011
72	MW_Cat	1.09	-0.012
73	CW1_An	1.06	-0.012
74	V_Cat	1.05	-0.010
75	DIFF_Cat	1.01	0.009

[a] VolSurf+ variables codes as in Table C1.

In Fig. 39[123] the t*c[1]-t*c[2] biplot (reporting t-scores and c-loadings together) displays the 18 learning set ILs and E_{NR} (the Y response) in the same chemical space. In the upper right quadrant ILs with a non-aromatic heterocyclic scaffold are located very close to E_{NR} showing that they positively influence the response (*i.e.* exhibit higher E_{NR} values). Moreover the shorter the side chain (*i.e.* more water soluble ILs located in the lower right part of the plot) the higher the E_{NR} values. When considering different ILs with the same cation (IM14) the anions size plays a relevant role evidenced by the second component, in agreement with the positive contribution of the anionic size descriptors: the higher the t*c[2] score, the higher the E_{NR} value.

The above considerations can prove that the present QSPR approach, considering simultaneous variations in both the cation (heterocyclic core and side chain length) and the anion structural features by means of 176 ILs descriptors, was suitable to provide an estimate of descriptors importance and an effort to interpret their physico-chemical significance in relation to the polarity of ILs. It is perhaps worth mentioning here that attempted correlations with Kosower and Reichardt empirical solvent parameters were not satisfactory probably due to the ionic structure of the solvatochromic dyes which in solution with ILs implies the presence of two cations and two anions: a condition quite difficult to be modelled. A neutral "sensor" such as Nile Red simplifies the above picture rendering possible *in silico* modelling.

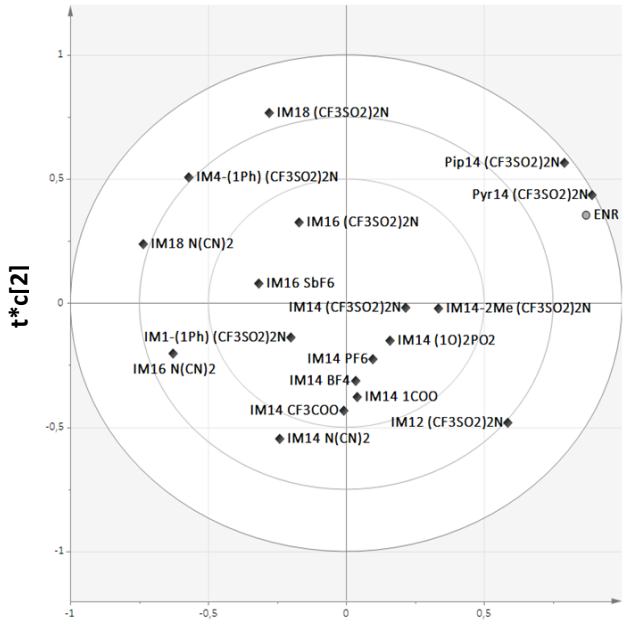


Fig. 39 t*c[1]-t*c[2] plot reporting t**t*c[1]** s for ILs 1-18 (Table 2) together with c-loadings for Y-response: this plot can show similarities and dissimilarities among the objects (ILs) and allows to interpret how they are related to the response (E_{NR} variable) along the 1st and the 2nd PLS components.

Tables C1 was derived from an article published in SAR and QSAR in Environmental Research on 04 January 2016, available online: http//dx.doi.org/10.1080/1062936X.2015.1120778 (ref. 75).
Figures 38, 39, Chart 4 and Tables 2, 3, A8, B15 from http://dx.doi.org/10.1016/j.tet.2016.04.056 (ref. 123).

3.4.2 C_p PLS model

Heat-transfer fluids have a large number of industrial and consumer applications ranging from refrigeration at low temperatures to solar energy collection and storage at high temperatures. Hence heat capacity is a fundamental thermodynamic property of liquids needed to estimate heating and cooling requirements as well as heat-storage capacity of a material, being therefore an important parameter to verify its applicability in heat-exchanger equipments. Heat capacities are also involved in the estimation of the temperature dependence of some thermodynamic properties of chemical compounds, such as entropy, enthalpy and Gibbs energy.

Probably the most exhaustive collection of ILs heat capacities can be found in the IL Thermo database,[126] containing lots of available literature data. However for most ILs these values are still lacking. Moreover heat capacity data show a high degree of uncertainty, depending on the analytical method used, on the experimental apparatus precision as well as on the presence of impurities. Paulechka collected and critically reviewed experimental data on heat capacity of many room-temperature ionic liquids (102 aprotic ILs from 63 literature references),[127] pointing out once again that the purity of ILs can dramatically affect their properties, as specifically demonstrated for ILs containing water or halide impurities.[2]

The present study was aimed at testing the potentialities of the *in silico* ILs PPs to develop a PLS model able to quantitatively correlate the above descriptors to heat capacity. The final purpose was to predict C_p values for a large number of commonly used ILs with the aim to fulfill the REACH requirements by establishing priorities in planning the synthesis of new ILs for industrial applications.

Heat capacity data[126,127] expressed as J/(K*mol) were available for 65 heterocyclic ILs. These ILs (Table B16)[128] exhibited different structural features such as aromatic and non-aromatic heterocyclic cationic scaffolds (imidazoliums, pyridinium, piperidinium and pyrrolidinium), different side chain lengths and presence of heteroatoms in cationic structures as well as wide range of anions (halides, fluoborates, sulphonates and organic anions). PLS approach was applied on a matrix including 65 ILs and 9 variables (5 cation and 4 anion PPs, as in section 3.1.2) and the heat capacities as the responses. It resulted in an excellent 2 PLS components model (see Table A9)[128] explaining 91.9% of Y variance (Q^2 = 0.807) with already 77.9% of Y variance (Q^2 = 0.709) along the 1st PC.[128]

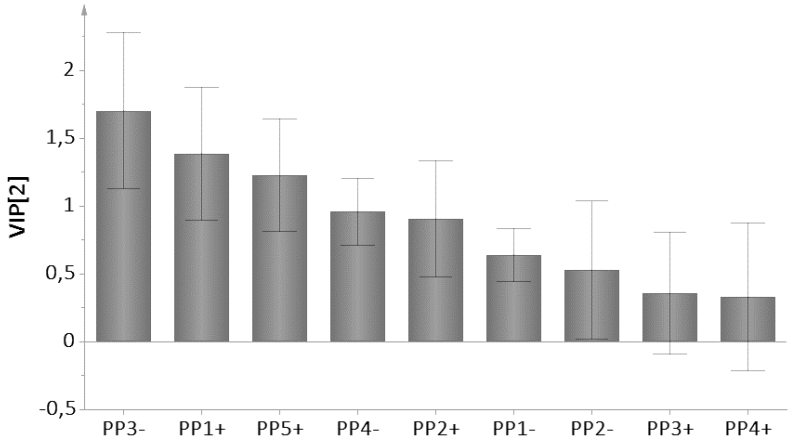


Fig. 40 VIP bars plot for the C_p PLS model.

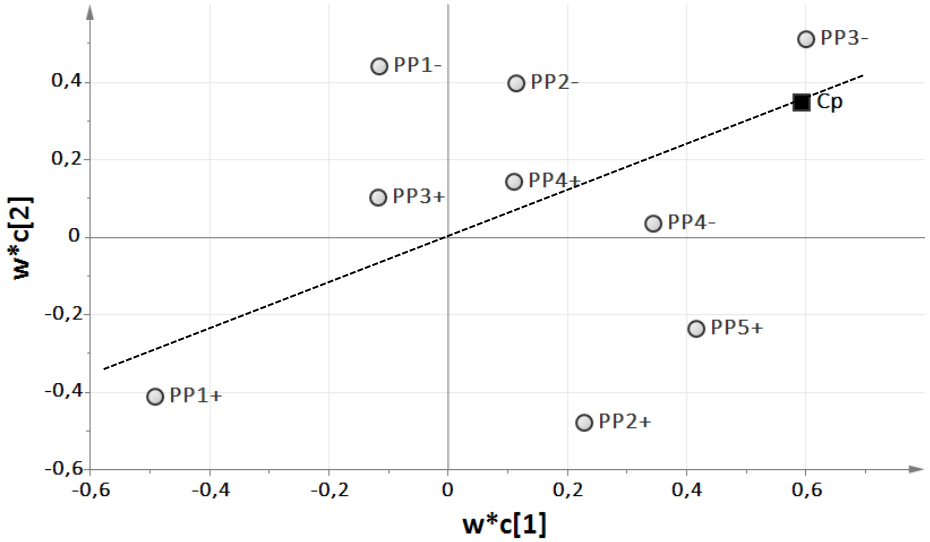


Fig. 41 w*c[1]-w*c[2] plot for the C_p PLS model showing descriptors (w*) and response (c) loadings superimposition. The correlation between each descriptor (○) and the dependent variable (C_p■) is elucidated by the PPs projections on the dotted line.

On the basis of the VIP bars plot (Fig. 40),[128] the response is affected by both cationic and anionic principal properties. In detail, the PLS loadings plot (Fig. 41)[128] showed that the anionic PP_3-, lying in the same quadrant of the Y, contributes positively to C_p (*i.e.* the higher PP_3- values, the higher C_p) whereas cationic PP_1+, being in the opposite quadrant, provides a negative contribution. PP_5+ and PP_4- follow in order of importance. The physico-chemical meaning of each single ILs PP has been above widely commented (section 3.1.2). In the present case the PP_1+ negative contribution means that a large cationic structure (wide surface, large volume and flexibility) together with hydrophobic surface and high molecular weight determine an increase in C_p values. On the other hand, a more water soluble cation is responsible for the decrease of C_p. The cationic PP_5+ refers to the H-bonding ability: a cation

able to interact as H-bonds donor contributes to increase the C_p value, and *vice versa*. Anion PPs have a high effect on the response, in particular anionic PP_3- and PP_4-, both positively contributing to the C_p value. Consequently large anions surface and volume, high hydrophilicity and polarizability (related to high positive PP_3- values) and the unbalance between anions hydrophobic areas and their barycentre (referring to positive PP_4-), contribute to the increase of C_p. On the other hand, anions with strong H-bonding ability (high negative PP_3-) result in lower C_p values. I want to stress that the present QSPR approach, considering simultaneous variations in both the cation and the anion structural features by means of 9 descriptors (PPs), was also able to provide an estimate of the importance and an interpretation of physico-chemical parameters in relation to C_p.

A good agreement between experimental and predicted values can be be observed in Fig. 42,[128] which reports the plot of predicted *vs.* experimental literature data (see also Table B16[128] for corresponding numerical values). This correlation can be considered as very good, taking into account the intrinsic variability of heat capacity data reported in the literature, strongly affected by errors due to different apparatus and analytical methods used in the C_p determination and to the presence of impurities in the ILs. Modelling of a series of ILs derivative thermodynamic properties including heat capacity, by means of ePC-SAFT theoretical model, has been recently reported[129] and percentage prediction errors lower than 20% were claimed to be much better than those previously reported in the literature. The correlation reported in Fig. 42,[128] including a much higher number of ILs with structurally different characteristics in both cations and anions, pointed out a significant improvement of the PLS model prediction ability.

In order to validate the above model, an external set (Chart 5)[128] was used and their C_p values were determined experimentally by DSC. These measurements gave C_p values in excellent agreement with those reported in literature (see Table 4),[128] with differences of 6%, 5% and 2% for ILs IM14 1COO, IM16 BF4 and Py4-4Me BF4 respectively (ILs 511, 196 and 331 in Table 4).[128] FurthermoreTable 4[128] points out a good agreement between experimental and predicted C_p values for the test set of the 8 ILs, thus confirming that the PLS approach represents a valid tool to predict ILs heat capacity by a QSPR model using PPs *in silico* structural descriptors.

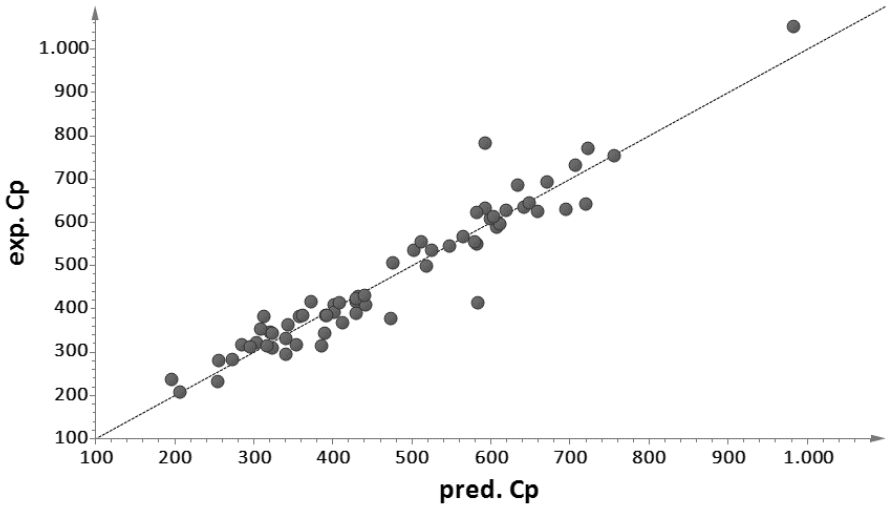


Fig. 42 PLS predictions *vs*. experimental literature data in C_p PLS model.

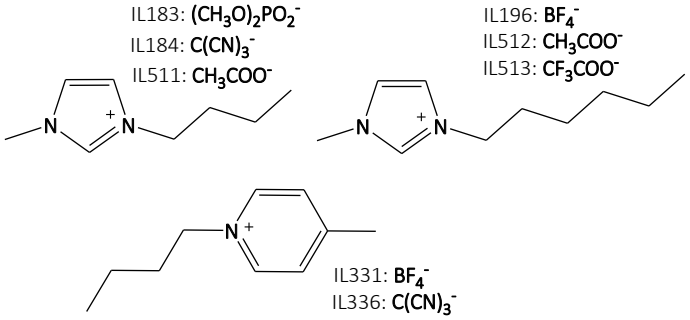


Chart 5 ILs structures used as validation set in the C_p PLS model.

Table 4 Experimental and predicted C_p values for test set

IL	C_p (liter.)[a] J/(K*mol)	C_p (exp.)[b] J/(K*mol)	C_p (*pred.*) J/(K*mol)
183		437.4	459.1
184		370.5	413.0
196[C]	429.8	452.0	440.8
331[C]	414.0	424.1	409.0
336		407.6	409.2
511[C]	383.2	360.0	392.3
512		400.1	420.3
513		481.0	470.6

[a]from Ref. 127; [b]this work; [c]the C_p values for these learning set ILs was measured to test the reliability of the adopted experimental procedure.

In PLS Q^2 estimates the predictive power of the model, however the so-called response permutation testing[61] may represent a further internal validation tool to confirm the model statistical significance. The resulting permutation plot on C_p PLS model (Fig. A14)[128] clearly excludes fitting of random response data.[61]

The reliability of the PLS model suggested that predictions could be extended to a higher number of commonly used ILs (the same set of 520 arbitrarily chosen in previous sections) also reported in Table B16.[128] However, the prediction ability for a high number of ILs is different for each single IL. Guidance on the "goodness" of predictions can be evaluated not only from the confidence intervals reported in Table B16,[128] but also by DModX values, the model residuals in the X matrix, which give an estimate of the similarity of a new observation to the training set observations. Predictions for ILs exhibiting DModX values higher than 1.60 in Table B16[128] should be regarded with caution:[61] the higher DModX is, the lower the prediction reliability could result.

In Fig. 42[128] one can see that a single ionic liquid (IL 517, 1-methyl-3-octadecylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide) exhibits an extraordinary high experimental C_p value in agreement with its PLS model prediction, while very few ILs can be found in the range 700-1000 J/(K*mol). Predictions in Table B16[128] for 16 ILs lie in the above range, in particular IL 419 (1,3-didecyl-2-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide) exhibits a predicted C_p value comparable with that of IL 517. It is worth mentioning that this set includes ILs with different aromatic (imidazolium, pyridinium) and non-aromatic (pyrrolidinium) cationic scaffolds, side chains containing oxygen atoms, chlorides, sulfonates and sulfates, fluorine organic anions *etc*. (Chart 6).[128] Table B16[128] and Chart 6[128] provide *in silico* opportunities for the selection of a limited number of ILs with comparable heat capacity efficiency and, therefore, as alternative candidates for experimental C_p measurements when a high C_p value is desired. Those in Table B16[128] exhibiting DModX values lower than 1.60 should be preferred to those with a lower prediction reliability (labelled with * in both Table B16 and Chart 6).[128]

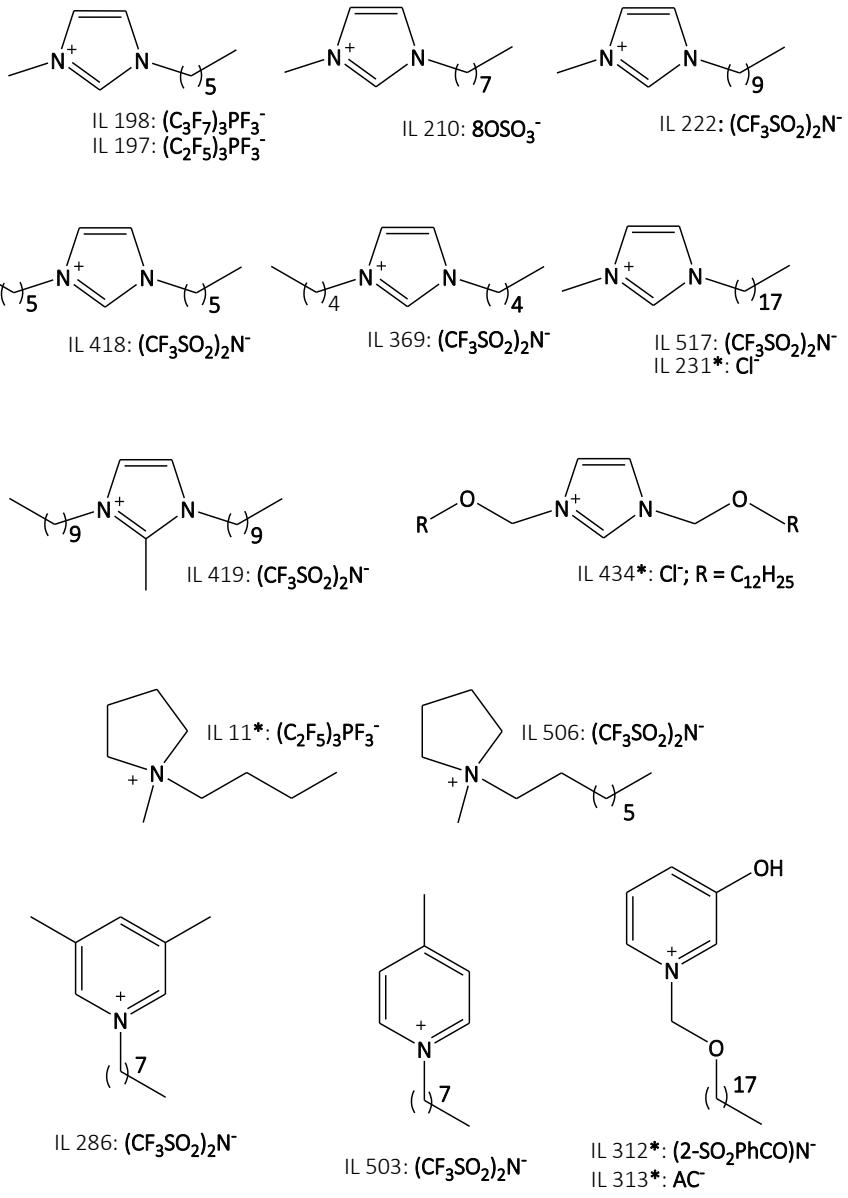


Chart 6 Ionic liquids having a predicted C_p > 700 J/(K*mol). *ILs with DModX higher than 1.60.

Figures 40-42, A14, Charts 5,6 and Tables 4,A9, B16 were reproduced from ref. 128 with permission from the Royal Society of Chemistry.

3.4.3 Other ILs physico-chemical properties PLS models

Last PLS correlation models hereafter presented dealt with other relevant physico-chemical properties of ILs (whose structures were reported in Chart 7): these properties may have a key role in using ILs for industrial or "every-day" applications. The analysis shortly presented is mainly aimed at highlighting the design potentialities of PLS approach, applied for “data collection”, providing new opportunities to complement available theory-driven models in the field and embodies an encouraging starting point for future and more detailed investigations about ILs potentialities. Having this in mind, for the interpretation of PLS models, the cheminformatics tools were adopted from a slightly different point of view: as an example, data sets were not divided into learning and test sets, considering the internal validation (expressed by Q^2 parameter) enough to assess the reliability of correlations, having already widely proved the validity of the approach and the reliability of descriptors in the above applications. Interestingly, when PPs were used, the experimental space explored by existing data was also analyzed (which is one of the advange in using PPs), evidencing the possible steps in future works.

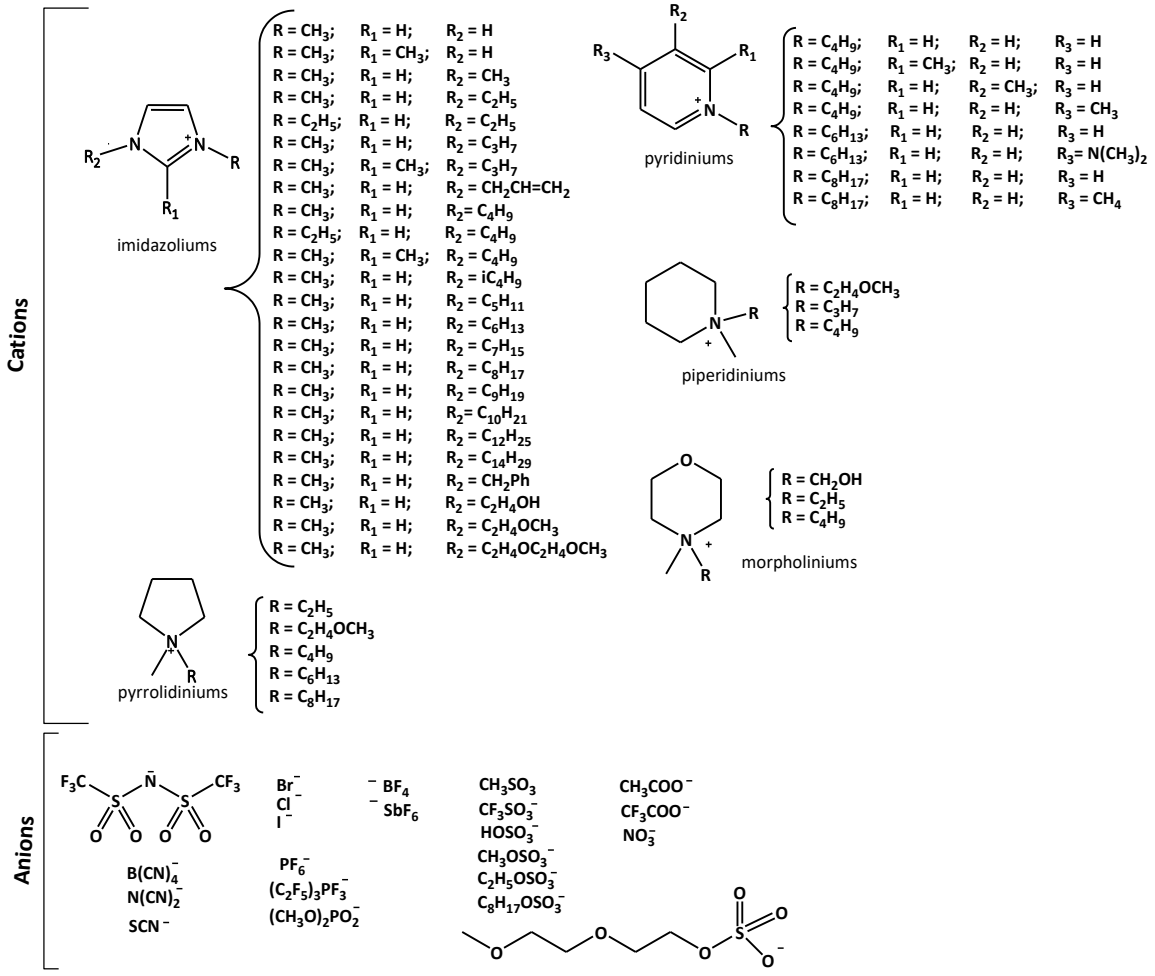


Chart 7 ILs cations and anions structures used in PLS models presented in this section.

I. Viscosity

Viscosity is a very relevant property required for process design in the industrial field, such as in heat exchangers, pipelines or distillation columns. High viscosities may be favorable when ILs are used as lubricants or in membranes whereas a low viscosity is generally desired in applications as solvent, to minimize pumping costs and increase mass transfer rates.[130] Therefore it is not surprising that several viscosity QSPR modelling studies using different approaches have been reported.

QSPR models for ionic conductivity and viscosity of ILs with group descriptors exhibited relatively good correlation using the polynomial expansion by a genetic algorithm model based on the type of cation, length of side chain and type of anion, also allowing design of ILs by means of a software matching structures and a desired property.[131] The group contribution method was also applied in QSPR modelling to estimate the viscosity of imidazolium-, pyridinium-, and pyrrolidinium-based ILs containing several anions covering wide ranges of temperature.[130] A similar approach was adopted to derive a relationship between viscosities of imidazolium-based ILs and descriptive parameters of anions and cations considering temperature, molecular weight, and the number of the branched-chain carbon atoms in the imidazole ring.[132] A group contribution model based on a Feed-Forward Artificial Neural Network was applied to over 13,000 data points of temperature- and pressure-dependent viscosity of 1484 ILs published in the open literature in the last three decades. The data were critically revised and divided into training, validation, and testing sets, to develop a new model allowing *in silico* predictions on the basis of the chemical structures of ILs cations and anions described by 242 building blocks.[133]

Many theory-driven QSPR models using *ab initio* calculations based on CODESSA or COSMOS-RS methods have been reported. CODESSA (Comprehensive Descriptors for Structural and Statistical Analysis) derives descriptors using quantum mechanical methods to develop QSAR/QSPR models. This approach was adopted to establish QSPR correlations for conductivities and viscosities of low-temperature melting ILs with the bis(trifluoromethylsulphonyl) imide anion. The authors concluded that the models were highly temperature dependent, stressing that experimental properties of ILs depend heavily on the degree of purity which cannot always be easily controlled.[134]

A QSPR study addressing the viscosity of imidazolium-based ionic liquids[135] pointed out the predominant effects of cation–anion electrostatic interaction while other interactions (*e.g.* interionic hydrogen-bond, van der Waals) or micro-characteristics (*e.g*. molecular orbital, electronic population, dipole moment, volume, shape, branching degree, symmetry) provide a minor contribution. However, it is worth mentioning that this work considered only one heterocyclic scaffold, and divided the original dataset into four different sets each modelled by multiparameter equations involving up to 25 “independent” variables with a clear danger of collinearity providing overoptimistic correlations. The same research group developed other QSPR models concluding that besides temperature, pressure, and impurity, the

ionic structural characteristics of ILs cation or anion have also significant effects on the viscosity.[136] These results were confirmed in more recent work,[137] deriving QSPR models at eight different temperatures on ILs containing the bis(trifluoromethylsulphonyl) imide: the authors concluded that interionic electrostatic interaction are the most important factors affecting viscosity and this effect changes with temperature.

Dynamic viscosity for 27 ILs was reported as a function of temperature and the data systematically analyzed to study anion and cation effects.[138] The COSMO-RS method established relationships between molecular level features and viscosity data. The QSPR approach used a Genetic Function approximation considering six molecular parameters from selected molecular descriptors.

The most abundant viscosity data set, analyzed using COSMO-RS molecular descriptors, included 1502 experimental data points for 89 ILs under a wide range of temperatures and pressures.[139] QSPR linear and non-linear models were developed and the second one provided better viscosity predictions. An advantage of COSMO-RS approach is that a unique model can take into account temperature and pressure variation. However, a careful insight into the data shows that, in analyzing all available literature data, very similar or even identical values reported in different papers are all included in the analysis. For instance, ten values are provided for 1-methyl-3-octylimidazolium hexafluorophosphate at 101.325 kPa and 343.15 K, some of which in the training set, others in the test set. Inclusion of identical values under the same pressure and temperature conditions either in the training or in the test set is common in this theoretical approach. Such a situation obviously improves the model performance and the correlation, but it would not be tolerated in QSPR studies.

In order to compare the advantages and drawbacks of our modelling approach the same abundant literature database was selected.[139] PLS procedure should be applied to data obtained under the same experimental conditions. In case of multiple literature values only one was considered, either the most reproducible one or an average value.

In a preliminary investigation aimed at obtaining information on the data structure, log viscosity values at fixed temperature and pressure (283.15 K and 101 kPa respectively) for 23 ILs were used as dependent variables and the correspondent 9 PPs (5 for cations and 4 for anions, as in section 3.1.2) as the descriptor variables. In such a model, 3 significant PLS components described 94.9% of the total Y variance with a predictive ability of 0.872 (Table A10).[140] In the VIP plot (Fig. A15)[140] PP_2-, and PP_3- are the most important descriptors, followed by PP_1+ and PP_5+, while all other descriptors appear to be less relevant. In order to limit the number of descriptors and simplify the model, a new PLS correlation model was built maintaining only four relevant X descriptors: PP_1+ and PP_5+,PP_2- and PP_3- for the cationic and anionic counterpart respectively. The new simplified 23x4 matrix provided a 2 PLS components model explaining 92.6% of the total variance, with a cumulative Q^2 of 0.903 (see Table A11 for model details)[140]

showing that the exclusion of five low relevance descriptors improved the "goodness" of this model. The correlation between predicted and experimental values is reported in Fig. A16 (dataset and predictions in Table B17).[140]

Theory-driven approaches aim at the best fit of all available data by a unique often non linear model, while the SIMCA approach[61] aims at raw data reduction by compacting them into data of higher relevance, eventually adopting different soft models of local validity but providing more easily interpretable results. In this context, different PLS models at 9 different temperatures were carried out, and their statistical parameters were reported together in Table A11.[140] The correlation plots at 293.15 K is displayed in Fig. 43[140] and those at other temperatures in Fig. A16 (dataset and predictions in Table B17). [140]

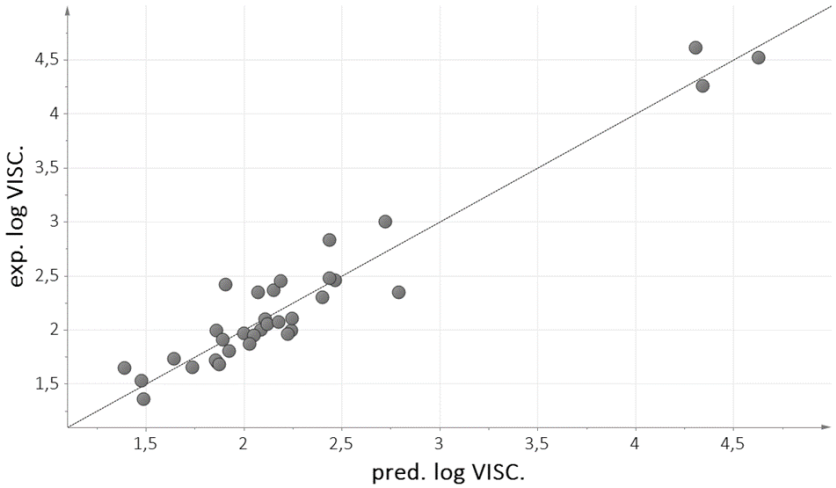


Fig. 43 Predicted *vs.* experimental PLS correlation plot for log viscosities (mPa*s) at 293.15 K.

One advantage of this approach is that log viscosity values at different temperatures can be easily calculated by four parameters equations (6)-(14) derived from the correspondent PLS models:

$\log\eta_{283.15}$ = 2.43378 -0.0467197(PP_1 +) +0.246482(PP_5+) -0.321282(PP_2 -) -0.299658(PP_3-) (eq. 6)

$\log\eta_{293.15}$ = 2.12028 -0.05129(PP_1+) +0.200276(PP_5+) -0.29018(PP_2 -) -0.2723(PP_3 -) (eq. 7)

$\log\eta_{298.15}$ = 1.94932 -0.0719465(PP_1+) +0.11487(PP_5+) -0.259657(PP_2 -) -0.197003(PP_3 -) (eq. 8)

$\log\eta_{303.15}$ = 1.962 -0.0450731(PP_1+) +0.165658(PP_5+) -0.207737(PP_2 -) -0.214209(PP_3 -) (eq. 9)

$\log\eta_{313.15}$= 1.74491 -0.0563375(PP_1+) +0.148687(PP_5+) -0.173187(PP_2 -) -0.176367(PP_3 -) (eq. 10)

$\log\eta_{323.15}$ = 1.55596 -0.047622(PP_1+) +0.0926056(PP_5+) -0.145431(PP_2 -) -0.154512(PP_3 -) (eq. 11)

$\log\eta_{333.15}$ = 1.48278 -0.0501674(PP_1+) +0.124556(PP_5+) -0.126096(PP_2 -) -0.136255(PP_3 -) (eq. 12)

$\log\eta_{343.15}$ = 1.32238 -0.0423298(PP_1+) 0.0930893(PP_5+) -0.116262(PP_2 -) -0.134434(PP_3 -) (eq. 13)

$\log\eta_{353.15}$ = 1.22789 -0.041984(PP_1+) +0.106297(PP_5+) -0.0979848(PP_2 -) -0.11833(PP_3 -) (eq. 14)

The coefficients of equations (6)-(14) indicate, together with the sign and the order of magnitude of correlation to Y, that the importance of both anionic descriptors decreases on increasing temperature, and only the cationic descriptor PP_1+ exhibits the same trend (Fig. A17).[140] At 353.15 K PP_5+ appears to have the same importance as PP_2- and PP_3-. This can be interpreted considering that the directional polar interactions, such as the H-bond interactions (expressed by PP_5+), are less efficient when the temperature increases. PP_1+, being a contribute of molecular descriptors that are positively and negatively influenced by temperature, is not affected by temperature variation and anyway provides a lower contribution.

The physico-chemical interpretation of cations and anions PPs has been previously commented (section 3.1.2). In particular PP_2- is related to both hydrophilic and hydrophobic character, while PP_3- is related to anionic size/shape and to the capability to form H-bonds as donor or acceptor. PP_1+ embodies information related to cation solubility, size, flexibility and molecular weight. High values of PP_1+ indicate high solubility in water, while low values are related to molecular size and shape and to solubility in organic solvents, while PP_5+ discriminates the H-bond donor/acceptor ability.

Another advantage of the adopted approach is that the results can be summarized into plots allowing, in addition to data prediction, also interpretation and design. Fig. 44 and 45[140] show respectively the cations and anions experimental space explored by data analysis as compared to the potential experimental space which could be covered by cations and anions PPs. ILs with high viscosity possess cations with negative PP_1+ and positive PP_5+ values and anions located in the lower left quadrant of Fig. 45b.[140]

Complementary considerations can be drawn from inspection of Fig. 46,[140] where the VIP for cations and anions descriptors are reported. The latter have a higher effect on the Y-variable, in particular PP_2- is the most important descriptor in determining viscosity, the lower the PP_2- value (such as chlorides and iodides), the higher the viscosity. Accordingly, anions with high PP_2- values are expected to contribute in decreasing viscosity. Tetracyanoborate and tricyanomethanide, which exhibit the highest PP_2- values in Fig. 45b[140] (7.57 and 6.89 respectively, as in Table B2),[78] are hydrophobic anions used to generate hydrophobic ILs[79] with interesting applications in dye-sensitized solar cells. It has been reported[80,81] that a low viscosity seems to be associated to the use of these anions. This is in qualitative agreement with the trend suggested by the present analysis, although a quantitative estimate would be less reliable as tetracyanoborate and tricyanomethanide anions (Fig. 45b)[140] are both outside the experimental space explored by anions PPs in our model (Fig. 45a).[140]

The above consideration indicated that Fig. 44 and 45[140] provide *in silico* design opportunities which can be handled directly by an experimentalist, able to evaluate the synthetic affordability and identifying

potential ILs candidates for specific applications. The simplicity and the practical utility of this approach in R&D studies on ILs result evident.

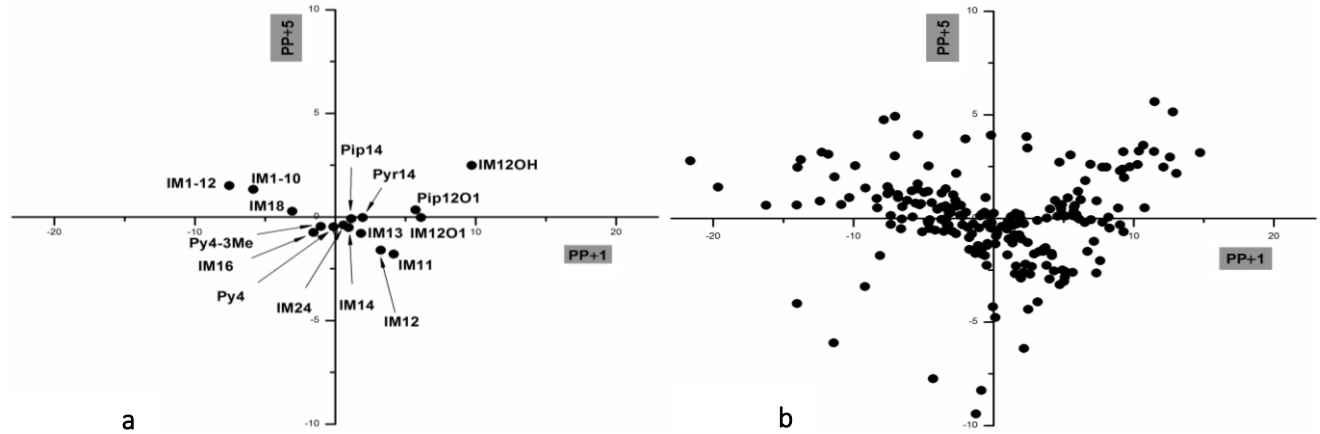


Fig. 44 Cations PP_1+/PP_5+ descriptors space explored by the viscosity PLS model (a) as compared with the PP_1+/PP_5+ available descriptors space (b).

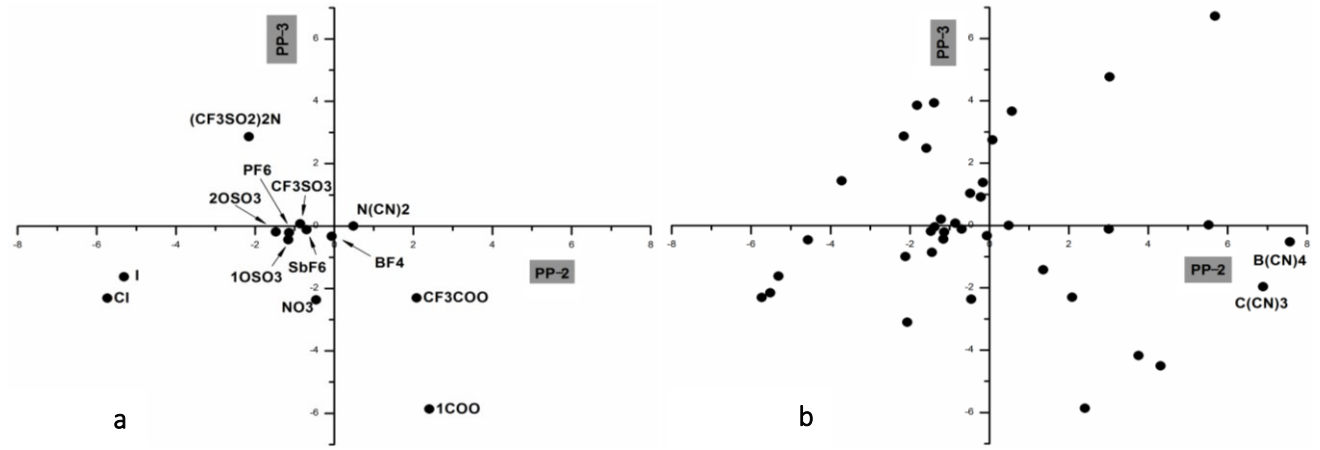


Fig. 45 Anions PP_2-/PP_3- descriptors space explored by the viscosity PLS model (a) as compared with the PP_2-/PP_3- available descriptors space (b).

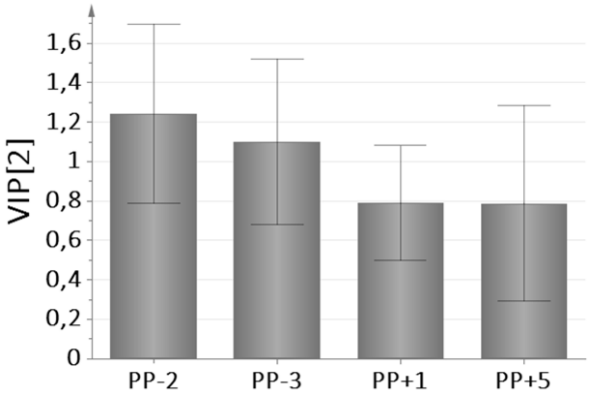


Fig. 46 VIP bars plot for the viscosity (T = 283.15 K) PLS model displaying the importance of each PP to explain the X-matrix and to correlate to Y.

II. Density

Density is a crucial physical property of a liquid required in the industrial process design of equipments such as condensers, reboilers, liquid/liquid two phase mixer–settler units, in liquid metering calculations and in material and energy balances involving liquids, vapor–liquid, and liquid–liquid separation processes.[132,141] Hence the longstanding interest in predicting densities of ILs with several approaches from studies using a surface tension weighted molar volume, the parachor,[142] to QSPR modelling based on semiempirical calculations with 11 molecular descriptors,[141] to COSMOS-RS based on quantum chemistry calculations,[143] to a group contribution method using the Patel-Teja equation.[144] Recent studies[145] suggested that the use of semiempirical methods - faster and less expensive as compared to *ab initio* ones - for geometry optimization, provide comparable QSPR models in predicting the density of 66 ionic liquids.

The approach herein presented, based on reliable and easily accessible sources,[126,146-150] considered density values for 109 ILs (see Table B18).[140] A preliminary PLS analysis using 9 PPs as descriptors (section 3.1.2), whose statistical parameters were reported in Table A12,[140] gave model D1[140] in which anions such as long chain sulfates, SbF_6, bromides, iodides and nitrates deviate from the linear correlation (Fig. A18a).[140]

Deviation from linear behaviour may be ascribed to size differences between ions and packing effects.[150] Exclusion of the above anions led to the soft model D2[140] whose statistical parameters are reported in Table A12,[140] using 98 ILs as objects and 9 PPs as the descriptors. The correlation plot and VIP plot were displayed in Fig. A18b and A19[140] respectively. Nevertheless, in analogy with the procedure adopted for viscosity, a further simplified PLS correlation model was derived including just four relevant X descriptors: PP_1+ and PP_2+ for cations, PP_1- and PP_3- for the anions (model D3).[140] This model, explaining 80.2% of the total variance (Table A12),[140] provided the correlation plot in Fig. 47,[140] and corresponding predicted numerical were made available in Table B18.[140]

Fig. 48 and 49[140] show respectively the cations and anions PPs experimental spaces explored by the present data analysis as compared to those spanned by all PPs. It is worth mentioning that the cations experimental space included many heterocyclic scaffolds but no cations are present in the upper left quadrant of Fig. 48a[140] as those in the same quadrant of Fig. 48b,[140] characterized by long alkyl chains, not liquid at 298.15 K.

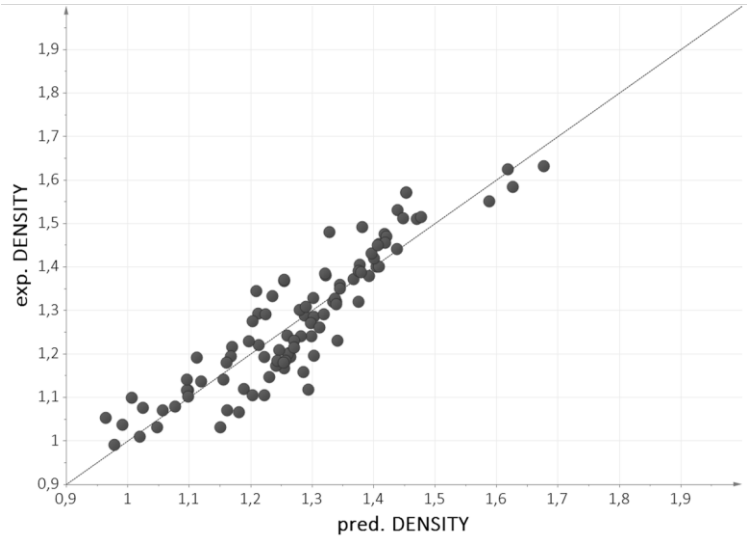


Fig. 47 Predicted vs. experimental PLS correlation plot for densities (g/cm^3) from model D3.

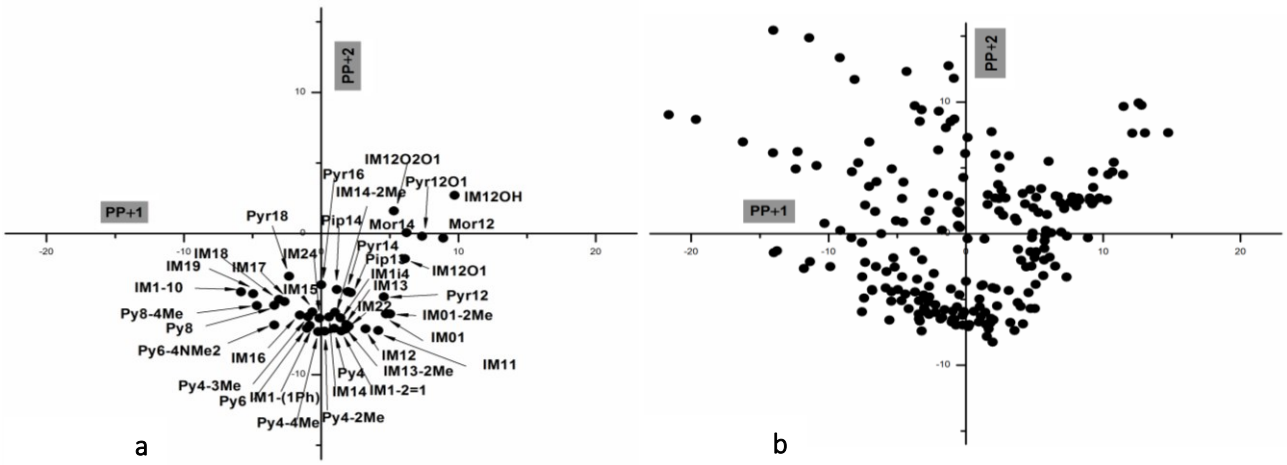


Fig. 48 Cations PP_1+/PP_2+ descriptors space explored by the density PLS model (a) as compared with the PP_1+/PP_2+ available descriptors space (b).

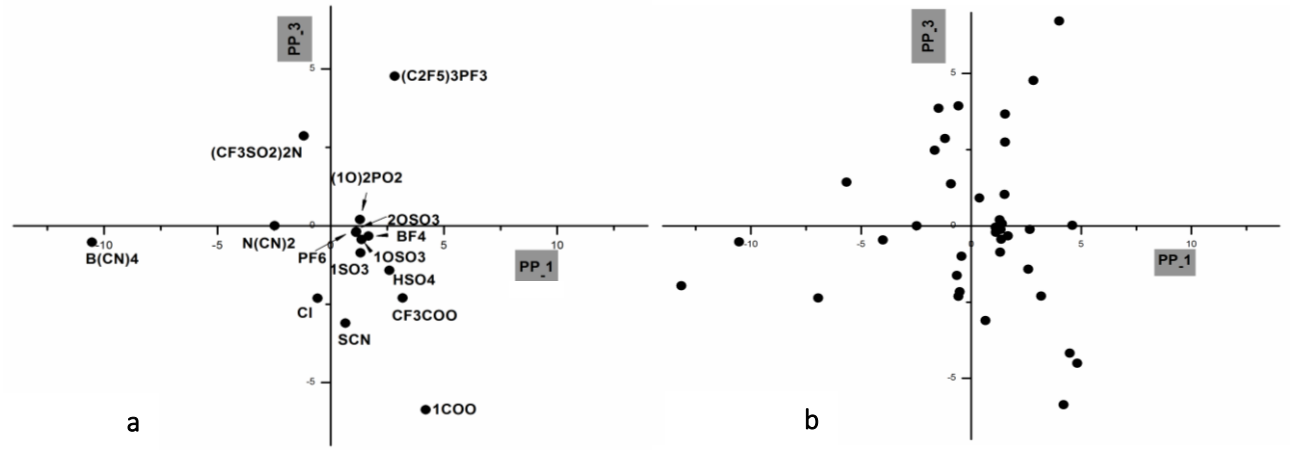


Fig. 49 Anions PP_1-/PP_3 - descriptors space explored by the density PLS model (a) as compared with the PP_1-/PP_3 - available descriptors space (b).

Predicted density values at 298.15 K can be easily calculated by the following four parameters equation, derived from the correspondent PLS model, using the PPs values reported in Table B18[140] (or Table B1-2):[78]

$D_{298.15\,K}$ = 1.1968 + 0.0138095(PP_1+) -0.0061904(PP_2+) +0.0244469(PP_1-) + 0.0646624(PP_3-) (eq. 15)

From equation (15) it is evident that anions have a higher effect on density, in particular PP_3-. ILs with high density exhibit high PP_3- values (*e.g.* 4.77 for tris(pentafluoroethyl)trifluorophosphate and 2.86 for 1,1,1-trifluoro-N-(trifluoromethylsulfonyl) methanesulfonamide)[78] while low density ILs have low PP_3- values (*e.g.*, chlorides, thiocyanates and acetates having PP_3- values from -2.30 to -5.87).[78] High PP_3- values are related to high anionic size, surface and polarizability resulting in higher densities, while low PP_3- values indicate a high anion capability to form H-bonds resulting in lower densities (section 3.1.2). Inspection of the above plots may provide insights for experimental design, although great caution should be adopted as the developed model has local validity and cannot be applied with the same reliability to anions not included for the model derivation.

III. Decomposition temperature

Decomposition temperature of ILs represents an essential physico-chemical property to evaluate their thermal stability and therefore the industrial applicability temperature range. Decomposition temperatures for 35 ILs are available in the literature[147,150,151] (see Table B19).[140]

A preliminary PLS analysis using PPs as descriptors provided a statistically unreliable model (M1)[140] as evidenced by the parameters reported in Table A13.[140] Therefore, in order to improve the modelling ability and achieve more accurate predictions, a new PLS analysis was performed using all the original VolSurf+ descriptors (see section 3.1.1) and their product terms (taking into account also cation-anion interactions). The resulting PLS model (M2)[140] including 35 objects (ILs) and 244 variables (128 cation descriptors, 48 anion descriptors, plus 48 cross terms) had just the 2nd PC as significant PLS component while the 1st and 3rd PCs turned out to be non significant (negative Q^2 values, Table A13).[140] This situation is encountered for particular data structures where the orthogonal information in the X-block is strong. This is the case of the present data structure needing a different chemometric approach: the OPLS algorithm[64-66] is able to discriminate between the orthogonal and predictive X-variation, resulting in a higher Q^2 value. The OPLS model (M3)[140] provided, in addition to the predictive component, seven statistically significant orthogonal components (Table A14).[140] The correlation plot in Fig. 50[140] can be considered as satisfactory taking into account that it refers to an OPLS model with an optimum Q^2 value (see Table B19[140] for predictions values). This analysis was also exploited to show how a QSPR study

could be excessively improved to give very excellent fitting of the data but resulting to detriment of predictability, falling into an overfitting case. Fig. A20-A21[140] clearly show the risk due to an exaggerate increase of R^2 by increasing the dimensionality of the above model.

Table 5[140] reports the OPLS coefficients higher than 0.03 and lower than -0.03 for cation and anion VolSurf+ descriptors as well as for their interactions. Interestingly, Table 5[140] reports that the decomposition temperature decreases on increasing hydrophobic cations-anions interactions (D3_CatxAn, D4_CatxAn, D5_CatxAn, D7_CatxAn) while it increases with the increase of H-bond-derived polar interactions (W5_CatxAn, W6_CatxAn, CW5_CatxAn, CW6_CatxAn). Therefore, not surprisingly, the thermal stability data of ionic liquids are influenced by both anionic and cationic components, and this finding may allow to modulate the degradation processes. Such an easy computational approach, leading to the prediction of thermal degradation of ionic liquids, may allow selective and application-driven design.

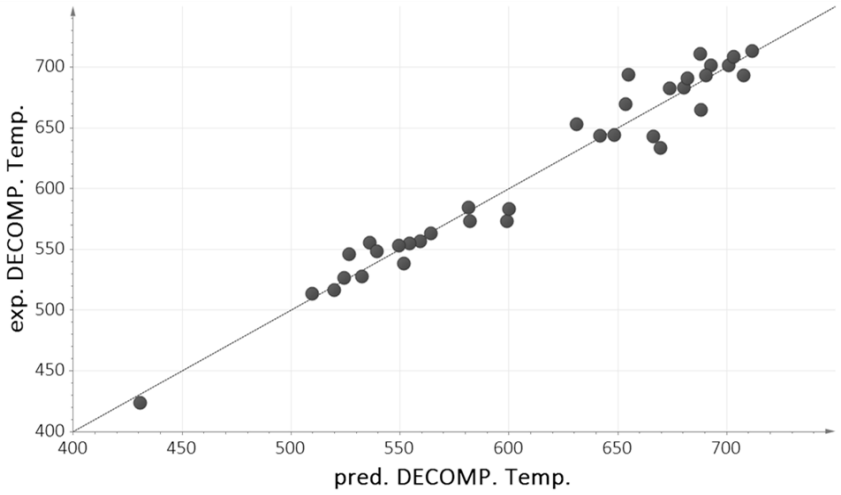


Fig. 50 Predicted *vs.* experimental OPLS correlation plot for decomposition temperatures (K) from model M3.

Table 5 Coefficients (scaled and centered) for the VolSurf+ descriptors[a] in the decomposition temperature OPLS model.

Var ID	Coeff (+)
CW1_An	0.1236
CW2_An	0.1093
CW3_An	0.1013
CW4_An	0.0943
CW1_CatxAn	0.0886
W1_An	0.0824
A_An	0.0752
W2_An	0.0737
ID1_An	0.0713
ID1_CatxAn	0.0711
ID2_CatxAn	0.0706
W3_An	0.0632
DD7_Cat	0.0602
CP_An	0.0582
D2_An	0.0576
D3_An	0.0545
ID3_An	0.0513
ID4_An	0.0496
D1_An	0.0488
W4_An	0.0487
W5_CatxAn	0.0483
ID2_An	0.0471
HL2_CatxAn	0.0464
CW5_CatxAn	0.0463
W6_CatxAn	0.0430
CW6_CatxAn	0.0429
A_CatxAn	0.0415
CD2_An	0.0399
CD3_An	0.0355
CW5_An	0.0331
…	…

Var ID	Coeff (-)
…	…
IW3_An	-0.0306
D5_CatxAn	-0.0312
D7_CatxAn	-0.0320
R_CatxAn	-0.0325
HL1_An	-0.0357
D4_CatxAn	-0.0386
CW8_An	-0.0413
W8_An	-0.0413
D3_CatxAn	-0.0450
R_Cat	-0.0465
CP_CatxAn	-0.0481
S_CatxAn	-0.0493
CW7_An	-0.0503
V_CatxAn	-0.0512
IW1_An	-0.0530
W7_An	-0.0550
ID4_CatxAn	-0.0592
IW4_An	-0.0778
CW6_An	-0.1085
HL2_An	-0.1253
W6_An	-0.1280

[a] VolSurf+ variables codes as in Table C1.

IV. Conductivity

Among the common properties of ILs, conductivity is of crucial importance for their potential application as electrolytes in electrochemical devices. For instance, in the application to electrolysis solutions for batteries larger ionic conductivities are required.[131,152,153]

Conductivity data for 43 ILs are available in the literature[126,147] (see Table B20).[140] In such a dataset conductivity values for 1-hexyl- and 1-octyl-3-xmethylimidazolium bromides (12.06 e 10.55 S/m respectively) are signicantly different from all others (in the range 0.007-2.93 S/m). These values, measured in the same work,[154] were considered as outliers with respect to the others, therefore excluded from the dataset.

Recent studies[155] adopted the logarithm of conductivity in QSPR modelling. Accordingly, a preliminary PLS analysis using 9 PPs as descriptors and log conductivity as the dependent variable provided a statistically unreliable model (Table A15)[140], probably because two ILs (IM01 1COO and IM01 CF3COO, 440 and 441 respectively in Table B20),[140] resulting to be far from the confidence ellipse of the scores plot (Fig. A22),[140] biased the model. This could be due to the fact that in the above ILs only one imidazolium ring nitrogen bears an alkyl substituent while all other imidazoliums have two *N*-alkyl substituents. Therefore the above two ILs, behaving as outliers with respect to all other imidazoliums in the dataset, were excluded and the correspondent new PLS model derived (C2 in Table A15).[140] However the statistical parameters of such a model were not satisfactory again, probably because of the limited ability of compacted PPs in describing conductivity. These findings suggested to carry out a new OPLS analysis using all the original VolSurf+ descriptors (section 3.1.1) and their product terms which take into account also cation-anion interactions (C3 in Table A16).[140] It is perhaps worth mentioning here that exclusion of four ILs was not arbitrary but suggested by the adopted data-driven approach by means of data examination and structural features inspection.

The statistical parameters for the soft C3 OPLS model provided a good predictive ability (Q^2=0.833) and a very satisfactory correlation plot displayed in Fig. 51[140] (predictions values are available in Table B20).[140]

Table 6[140] reports the OPLS coefficients higher than 0.03 and lower than -0.03 for cation and anion VolSurf+ descriptors as well as for their interactions. Table 6[140] shows that also experimental conductivity data are influenced by cations-anions interactions as demonstrated by the coefficients of the descriptors ID2, ID3, ID4, D1, D2, D3, D4, CP, A for both cations and anions moieties. The interpretation is that hydrophobic spots on cations and anions partners (Dn) and their locations at the molecular surface (IDn), plus amphiphilic moment and critical packing (A and CP), influence the ILs packing and viscosity of the mixture, thus having an effect on the overall conductivity.

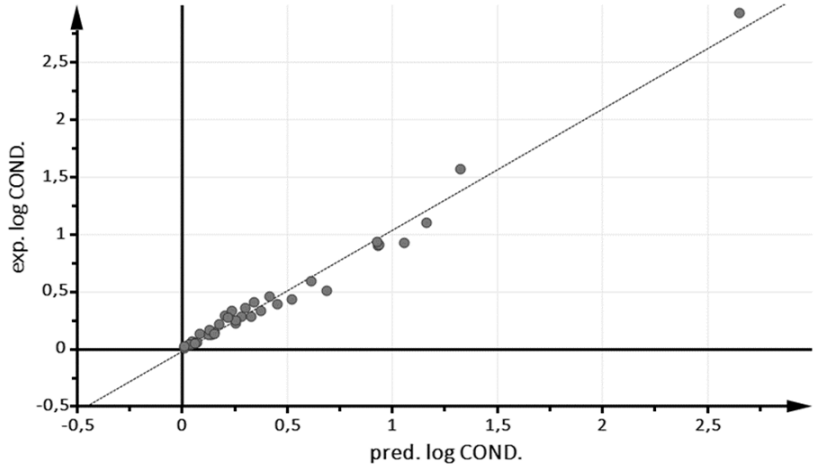


Fig. 51 Predicted vs. experimental OPLS correlation plot for log conductivities (S/m) from model C3.

Table 6 Coefficients (scaled and centered) for the VolSurf+ descriptors[a] in the conductivity OPLS model.

Var ID	Coeff (+)
ID3_CatxAn	0.1144
CW2_An	0.1062
ID4_CatxAn	0.1050
CW3_An	0.1013
CW1_An	0.0965
CW4_An	0.0912
D3_CatxAn	0.0869
CP_CatxAn	0.0863
CW5_An	0.0857
IW3_An	0.0811
CW1_CatxAn	0.0742
D2_CatxAn	0.0696
D1_Cat*An	0.0695
W2_An	0.0627
ID1_An	0.0601
DD2_Cat	0.0568
W3_An	0.0562
DD5_Cat	0.0539
A_CatxAn	0.0498
ID2_Cat	0.0491
ID2_CatxAn	0.0474
G_CatxAn	0.0441
DD1_Cat	0.0429
W1_An	0.0401
W4_An	0.0374
DIFF_Cat	0.0373
CD5_Cat	0.0349
CW2_CatxAn	0.0340
D4_CatxAn	0.0331
G_Cat	0.0304
…	…

Var ID	Coeff (-)
…	…
V_An	-0.0320
W1_Cat	-0.0324
IW2_Cat	-0.0325
CD1_Cat	-0.0329
IW2_An	-0.0353
D2_Cat	-0.0373
D3_Cat	-0.0386
DD6_Cat	-0.0433
A_Cat	-0.0486
CW1_Cat	-0.0500
PB_Cat	-0.0514
R_An	-0.0524
CD3_Cat	-0.0540
IW1_An	-0.0546
CD2_Cat	-0.0582
W8_An	-0.0693
CW8_An	-0.0727
DD3_Cat	-0.0737
R_CatxAn	-0.0810
FLEX_RB_Cat	-0.1110
R_Cat	-0.1167

[a] VolSurf+ variables codes as in Table C1.

V. Glass transition temperature and Melting point

The use of ILs at an industrial scale requires the knowledge of their melting and glass transition temperatures, which are needed to set a feasible temperature operation range. However experimental determination of solid–liquid phase transitions cannot be clearly distinguished into melting points and glass transition temperatures for ILs as many samples after glass transition start melting and no distinct peaks can be observed.[156] As expected, no significant PLS or OPLS models were obtained using PPs or VolSurf+ descriptors, also because their derivation, and consequently their use, is relative to the liquid phase.

Tables C1 was derived from an article published in SAR and QSAR in Environmental Research on 04 January 2016, available online: http//dx.doi.org/10.1080/1062936X.2015.1120778 (ref. 75).
Tables B1, B2 were derived from an article published in SAR and QSAR in Environmental Research on 08 March 2016, available online: http://dx.doi.org/10.1080/1062936X.2016.1156571 (ref. 78).
Figures 43-51, A15- A22 and Tables 5, 6, A10- A16, B17-B20 were reproduced from ref. 140.

4. Conclusions

Theory-driven approaches aim at the best fit of all available data by means of a unique often non linear model and many authors, in order to demonstrate the superiority of such models, report plots of predicted *vs.* experimental data providing a better correlation as compared with that of other models. However, a good correlation using many theoretical descriptors by means of the MRA approach, or others (as above discussed), has a high risk of descriptors collinearity and therefore may not be statistically significant. Unfortunately in many cases the numerical values of the descriptors are not reported preventing other researchers to replicate their results and apply other approaches to the same data set, a desirable condition which often produces further achievements in scientific knowledge. Moreover, the model interpretation may result unclear and the model findings are not always usable in practice by experimentalists for the design of specific properties.

On the other hand, the *data-driven* approach presented here starts with an overlook at the raw data and then compacts them into data of higher relevance eventually modelled by different soft models of local validity. Descriptors availability allows the readers to reproduce the results, and a simple evaluation of their relevance. This approach is more flexible as it may adopt different data modelling techniques depending on the purpose of the investigation and on the data structure. Data-driven chemometrics and cheminformatic methodologies are often an unexploited opportunity for experimentalists to model, design and predict physicochemical properties of ionic liquids. Modelling from data complements theory-driven approaches for interpretation and correlation purposes and may represent an alternative for experimental design in industrial applications.

Having in mind the above considerations, in relation to the aims of my research project, new cations and anions *in silico* VolSurf+ descriptors were derived[75] and eventually compacted into the so-called "principal properties"[78] easier to use and more suitable for experimental design. Such descriptors turned out to be functional for molecular modelling of ILs structures exploring the huge ILs chemical space. The availability of these *in silico* descriptors opens a new scenario for conjugating efficiency and sustainability of ILs, and represents the main final outcome of my Ph.D work.

Throughout my work the objective was also to analyze the influence of ILs structures on their properties from a quantitative point of view. At first, the focus was on the most representative and widely used toxicological essays (on aquatic[75,98] and cyto-toxicity,[78] as well as enzymatic inhibition[78]), having in mind the rapid diffusion of ILs in industrial applications and their possible hazard effects towards living organisms and taking into account that, for many ILs structures, these effects result still unmeasured. The affordability and reliability of the developed correlation models and of the resulting predictions may

represent a useful indication for the synthesis and a responsible use of these salts. Nowadays shortcuts are needed for the fulfillment of the REACH requirements and priorities have to be established in selecting ILs for experimental hazards assessment to focus more expensive *in vivo* studies on more potentially toxic compounds thus reducing the number of tests on animals.

Then, relationships between cations/anions structures and several physico-chemical properties of ILs were succesfully investigated,[123,128,140] in addition to experimental validation, in order to simplify the modelling of results and to let also non statisticians to extract important structural information leading to a rational design of both synthesis and experiments.

QSPR studies on ILs are not new, as often here stressed. However, in my opinion, the simplicity and clarity of the presented approaches, the non-expensive tools adopted to derive the models, together with the possibility to reproduce these results, represent an achievement in a literature scenario in which very often QSPR models seem to be prerogative of few people.

During these three years I have had the opportunity to appreciate the potentialities of multivariate approaches, unfortunately not widely applied in the field of Organic Chemistry. In particular they may represent a crucial resource in the field of ionic liquids whose properties cannot be totally experimentally investigated due to the (in theory) infinite combinations of very structurally different cations and anions. With my work, and the precious collaborations with other research groups, I intended to contribute to make simpler and more affordable the study of such an open field.

5. References

1 H. Martens, *J. Chemom.*, 2015, **29**, 563–581.

2 K. R. Seddon, A. Stark and M-J. Torres, *Pure Appl. Chem.*, 2000, **72**, 2275–2287.

3 R. Carlson and J.E. Carlson, in *Design and optimisation in organic synthesis*, sec. rev. enl. ed., Elsevier, Amsterdam, 2005.

4 F. P. Ballistreri, C. G. Fortuna, G. Musumarra, D. Pavone and S. Scirè, *Arkivoc*, 2002, part. 11, 54-64.

5 R. Carlson, M. P. Prochazka and T. Lundstedt, *Acta Chem. Scand. B*, 1988, **42**, 145-156.

6 R. Carlson, M. P. Prochazka and T. Lundstedt, *Acta Chem. Scand. B*, 1988, **42**, 157-165.

7 R. Carlson, T. Lundstedt, A. Nordahl and M. P. Prochazka, *Acta Chem. Scand. B*, 1986, **40**, 522-533.

8 C. G. Fortuna, G. Musumarra, M. Nardi, A. Procopio, G. Sindona and S. Scire, *J Chemom.*, 2006, **20**, 418–424.

9 M. Skagerberg, D. Bonelli, S. Clementi, G. Cruciani and C. Ebert, *Quant. Struct.-Act. Relat.*, 1989, **8**, 32-38.

10 S. Hellberg, M. Sjöström and S. Wold, *Acta Chem. Scand. B*, 1986, **40**, 135-140.

11 S. Hellberg, M. Sjöström, B. Skagerberg and S. Wold, *J. Med. Chem.*, 1987, **30**, 1126-1135.

12 M. Skagerberg, M. Sjöström and S. Wold, *J. Chemom.*, 1990, **4**, 241-253.

13 G. Cruciani, M. Baroni, E. Carosati, M. Clementi, R.Valigi and S. Clementi, *J Chemom.*, 2004, **18**, 146-155.

14 L. Caruso, G. Musumarra and A. R. Katritzky, *Quant. Struct.-Act. Relat.*, 1993, **12**, 146-151.

15 S. Clementi, G. Cruciani, P. Fifi, D. Riganelli, R. Valigi and G. Musumarra, *Quant. Struct.-Act. Relat.*, 1996, **15**, 108-120.

16 M. P. Prochazka and R. Carlson, *Acta Chem. Scand.*, 1989, **43**, 651-659.

17 M. P. Prochazka and R. Carlson, *Acta Chem. Scand.*, 1990, **44**, 614-616.

18 E. Fischer and V.F. Hess, *Ber Dtsch. Chem. Ges.*, 1884, **17,** 559-568.

19 B. Robinson, in *The Fischer Indole Synthesis*, Wiley, Chichester, 1982.

20 M. Sandberg, L. Eriksson, J. Jonsson, M. Sjostrom and S. Wold, *J Med. Chem.*, 1998, **41**, 2481-2491.

21 A. Duran, I. Zamora and M. Pastor, *J Chem. Inf. Model.*, 2009, **49**, 2129-2138.

22 R. Mancuso, C. S. Pomelli, C. Chiappe, R. C. Larock and B. Gabriele, *Org. Biomol. Chem.*, 2014, **12**, 651-659.

23 N. Szesni, K. Meyer and P. Wasserscheid, *ChemCatChem*, 2014, **6**, 162-169.

24 F. D'Anna, S. Marullo, P. Vitale and R. Noto, *Ultrason. Sonochem*., 2012, **19**, 136-142.

25 E. E. L. Tanner, R. R. Hawker, H. M. Yau, A. K. Croft and J. B. Harper, *Org. Biomol. Chem*., 2013, **11**, 7516-7521.

26 A. E. Somers, B. Khemchandani, P. C. Howlett, J. Sun, D. R. MacFarlane and M. Forsyth, *ACS Appl. Mater. Interfaces*, 2013, **5**, 11544-11553.

27 Z. Liu, P. Hu, X. Meng, R. Zhang, H. Yue, C. Xu and Y. Hu, *Chem. Eng. Sci.*, 2014, **108**, 176-182.

28 P. K. Khatri, G. D. Thakre and S. L. Jain, *Ind. Eng. Chem. Res.*, 2013, **52**, 15829-15837.

29 Q. Zhang, Q. Wang, S. Zhang and X. Lu, *J. Solid State Electrochem.*, 2014, **18**, 257-267.

30 S. Rodríguez-Sánchez, P. Galindo-Iranzo, A. C. Soria, M. L. Sanz, J. E. Quintanilla-López and R. Lebrón-Aguilar, *J. Chromatogr. A*, 2014, **1326**, 96-102.

31 S. Hyvärinen, J. P. Mikkola, D. Y. Murzin, M. Vaher, M. Kaljurand and M. Koel, *Catal. Today*, 2014, **223**, 18-24.

32 M. D. Joshi and J. L. Anderson, *RSC Adv.*, 2012, **2**, 5470-5484.

33 L. Vidal, M. L. Riekkola and A. Canals, *Anal. Chim. Acta*, 2012, **715**, 19-41.

34 T. D. Ho, C. Zhang, L.W. Hantao and J. L. Anderson, *Anal. Chem.*, 2014, **86**, 262-285.

35 S. Kitagaki, F. Inagaki and C. Mukai, *Chem. Soc. Rev.,* 2014, **43**, 2956-2978.

36 H-P. Steinruck and P. Wasserscheid, *Catal. Lett.*, 2015, **145**, 380-397.

37 M. Smiglak, J.M. Pringle, X. Lu, L. Han, S. Zhang, H. Gao, D.R. MacFarlane and R.D. Rogers*, Chem. Comm.*, 2014, **50**, 9228-9250.

38 R. F. M. Frade and C. A. M. Afonso, *Hum. Exp. Toxicol.*, 2010, **29,** 1038-1054.

39 REACH regulation available at: http://echa.europa.eu/regulations/reach/

40 K.S. Egorova and V.P. Ananikov, *ChemSusChem*, 2014, **7**, 336–360.

41 UFT-Merck Ionic Liquids Biological Effects Database available at: http://www.il-eco.uft.unibremen.de/?page=home&chent_id=&view=intro&lang=en (last access in September 2014).

42 N. Wood and G. Stephens, *Phys. Chem. Chem. Phys.*, 2010,**12**, 1670-1674.

43 P. Walden, *Bull. Acad. Imper. Sci. St. Pétersbourg*, 1914, **8**, 405-422

44 G. Cruciani, P. Crivori, P.A. Carrupt and B. Testa, J. Mol. Struct. Theochem., 2000, **503**, 17–30.

45 VolSurf+, available at: http://www.moldiscovery.com/docs/vsplus/

46 GRID v. 20, Software from Molecular Discovery Ltd., Perugia, Italy

47 P.J. Goodford, *J Med. Chem.*, 1985, **28**, 849-857.

48 D.N.A. Boobbyer, P.J. Goodford, P.M. Mcwhinnie and R.C. Wade, *J. Med. Chem.*, 1989, **32**, 1083-1094.

49 R. Wade, K.J. Clerk and P.J. Goodford, *J. Med. Chem.*, 1993, **36**, 140-147.

50 V. Barresi, C. Bonaccorso, G. Consiglio, L. Goracci, N. Musso, G. Musumarra, C. Satriano, C. G. Fortuna, *Mol. Biosyst.*, 2013, **9**, 2426-2429.

51 C. G. Fortuna, V. Barresi, C. Bonaccorso, G. Consiglio, S. Failla, N. Musso and G. Musumarra**,** *Eur. J. Med. Chem.*, 2012, **47,** 221-227.

52 C. G. Fortuna, V. Barresi and G. Musumarra, *Bioorg. Med. Chem.*, 2010, **18**, 4516-4523.

53 C. G. Fortuna, V. Barresi, G. Berellini and G. Musumarra, *Bioorg. Med. Chem.*, 2008, **16**, 4150-4159.

54 G. Forte, C. G. Fortuna, L. Salerno, M. N. Modica, M. A. Siracusa, V. Cardile, G. Romeo, A. Bulbarelli, E. Lonati and V. Pittala, *Bioorg. Med. Chem.*, 2013, **21**, 5233-5245

55 M. Barone, A. C. E. Graziano, C. G. Fortuna, G. Ronsisvalle and V. Cardile, *Med. Chem.*, 2014, **10**, 700-710.

56 L. Goracci, M. Ceccarelli, D. Bonelli and G. Cruciani, *J. Chem. Inf. Model.*, 2013, **53**, 1436-46.

57 L. Goracci, S. Buratta, L. Urbanelli, G. Ferrara, R. Di Guida, C. Emiliani and S. Cross, *Eur. J. Med. Chem.*, 2015, **92**, 49-63.

58 P. Crivori, G. Cruciani, P.A. Carrupt and B. Testa, *J. Med. Chem.*, 2000, **43**, 2204-2216.

59 G. Cruciani, M. Meniconi, E. Carosati, I. Zamora and R. Mannhold, in *Drug Bioavailability: Estimation of Solubility, Permeability, Absorption and Bioavailability*, H. van de Waterbeemd, H. Lennernäs, P. Artursson, Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, 2003, pp. 406-419.

60 G. Berellini, G. Cruciani and R. Mannhold, *J. Med. Chem.,* 2005, **48**, 4389-4399.

61 *SIMCA* v.13.0.3, MKS *Umetrics AB*, Malmo, Sweden, 2013.

62 S. Wold and M. Sjöström, in *Chemometrics: Theory and Application*, B.R. Kowalski, ACS Symposium Series, Washington, 1977, pp. 243-282.

63 S. Wold, M. Sjöström, and L. Eriksson, in *The Encyclopedia of Computational Chemistry*, Schleyer P.v.R., John Wiley & Sons, Chichester, 1998, pp. 2006-2020.

64 J. Trygg, and S. Wold, *J. Chemom.*, 2002, **16**, 119-128.

65 J. Trygg, *J. Chemom.*, 2002, **16**, 283-293.

66 J. Trygg, and S. Wold, *J. Chemom.*, 2003, **17**, 53-64.

67 S. Wold, A. Ruhe, H. Wold, and W. J. Dunn, *SIAM J. Sci. Stat. Comp.*, 1984, **5**, 735-743.

68 K. L. dos Santos Castro, P. G. de Lima, L. S. M. e Miranda, R. O. M. A. de Souza, *Tetrahedron Lett.,* 2011, **52**, 4168-4171.

69 J. D. Holbrey and K. R. Seddon, *J. Chem. Soc., Dalton Trans*., 1999, 2133-2140.

70 W. Guan, X.-X. Ma, L. Li, J. Tong, D.-W. Fang , J.-Z. Yang, *J. Phys. Chem. B*, 2011, **115**, 12915-12920.

71 L. P. Jameson and S. V. Dzyuba, *RSC Adv*., 2013, **3**, 4582-4587.

72 B. Lu, A. Xu and J. Wang, *Green Chem.,* 2014, **16**, 1326-1335.

73 F. D'Anna, S. Marullo, P. Vitale and R. Noto, *ChemPhysChem*, 2012, **13**, 1877 – 1884.

74 L-F. Chiu, H-F. Liu and M-H. Li, *J. Chem. Eng. Data*, 1999, **44**, 631-636.

75 A. Paternò, G. Bocci, L. Goracci, S. Scirè and G. Musumarra, *SAR QSAR Environ. Res.*, 2016, **27**, 1-15.

76 M. Arshadi and P. Kebarle, *J. Phys. Chem.*, 1970, **74**, 1483–1485.

77 SYBYL-X 1.3, Tripos, available at: http://www.tripos.com

78 A. Paternò, G. Bocci, G. Cruciani, C. G. Fortuna, L. Goracci, S. Scirè and G. Musumarra, *SAR QSAR Environ. Res.* 2016, **27**, 221-244.

79 M. Marszalek, Z. Fei, D-R. Zhu, R. Scopelliti, P.J. Dyson, S.M. Zakeeruddin and M. Gratzel, *Inorg. Chem.*, 2011, **50**, 11561−11567.

80 Y. Yoshida, K. Muroi, A. Otsuka, G. Saito, M. Takahashi and T. Yoko, *Inorg. Chem.*, 2004, **43**, 1458-1462.

81 D. Kuang, P. Wang, S. Ito, S. M. Zakeeruddin and M. Gratzel, *J. Am. Chem. Soc.*, 2006, **128**, 7732-7733.

82 A. Paternò, F. D'Anna, G. Musumarra, R. Noto and S. Scirè, *RSC Adv.,* 2014, **4**, 23985-24000.

83 J. Pernak, K. Sobaszkiewicz and I. Mirska*, Green Chem.*, 2003, **5**, 52-56.

84 M. T. Garcia, I. Ribosa, L. Perez, A. Manresa and F. Comelles, *Langmuir*, 2013, **29**, 2536-2545.

85 J. S. Torrecilla, J. Garcìa, E. Rojo and F. Rodrìguez, *J.Hazard. Mater.*, 2009, **164**, 182-194.

86 S. Stolte, J. Arning, U. Bottin-Weber, A. Muller, W-R. Pitner, U. Welz-Biermann, B. Jastorff and J. Ranke, *Green Chem.*, 2007, **9**, 760–767

87 S. Bruzzone, C. Chiappe, S. E. Focardi, C. Pretti and M. Renzi, *Chem. Eng. J.*, 2011, **175**, 17– 23.

88 A. Romero, A. Santos, J. Tojo and A. Rodríguez, *J Hazard. Mater.*, 2008, **151**, 268-273.

89 S. Stolte, J. Arning, U. Bottin-Weber, M. Matzke, F. Stock, K. Thiele, M. Uerdingen, U. Welz-Biermann, B. Jastorff and J. Ranke, *Green Chem.*, 2006, **8**, 621-629.

90 L. Berg, C. D. Andersson, E. Artursson, A. Hornberg, A. K. Tunemalm, A. Linusson and F. Ekstrom, *PLoS ONE*, 2011, **6**, e26039.

91 C. D. Andersson, J. M. Hillgren, C. Lindgren, W. Qian, C. Akfur, L. Berg, F. Ekstrom and A. Linusson, *J Comput. Aided Mol. Des.*, 2015, **29**, 199–215.

92 J. Arning, S. Stolte, A. Böschen, F. Stock, W.R. Pitner, U. Welz-Biermann, B. Jastorff and J. Ranke, *Green Chem.*, 2008, **10**, 47-58.

93 B. Peric, J. Sierra, E. Martí, R. Cruanas, M. A. Garaua, J. Arning, U. Bottin-Weber and S. Stolte, *J Hazard. Mater.*, 2013, **261**, 99-105.

94 S. P. M. Ventura, A. M. M. Goncalves, F. Goncalves and J. A. P. Coutinho, *Aquat. Toxicol.*, 2010, **96**, 290–297.

95 B. T. Johnson, in *Small-scale Freshwater Toxicity Investigations*, *Volume 1- Toxicity Test Methods*, C. Blaise and J-F. Férard, Springer, Dordrecht, The Netherlands, 2005, pp. 69-105.

96 J. Ranke, K. Molter, F. Stock, U. Bottin-Weber, J. Poczobutt, J. Hoffmann, B. Ondruschka, J. Filser and B. Jastorff, *Ecotoxicol. Environ. Saf.*, 2004, **58**, 396–404.

97 S. M. Steinberg, E. J. Poziomek, W. H. Engelmann and K. R. Rogers, *Chemosphere*, 1995, **30**, 2155–2197.

98 A. Paternò, S. Scirè and G. Musumarra, *Toxicol. Res.*, 2016, **5**, 1090-1096.

99 R. Hayes, G. G. Warr and R. Atkin, *Chem. Rev.*, 2015, **115**, 6357−6426.

100 M. Alvarez-Guerra and A. Irabien, *Green Chem.*, 2011, **13**, 1507-1516.

101 Y. Zhao, J. Zhao, Y. Huang, Q. Zhou, X. Zhang and S. Zhang, *J. Hazard. Mater.,* 2014, **278**, 320–329 and refs. therein.

102 B. Peric, J. Sierra, E. Martí, R. Cruanas and M. A. Garau, *Ecotoxicol. Environ. Saf.,* 2015, **115**, 257–262.

103 D. J. Couling, R. J. Bernot, K. M. Docherty, J. N. K. Dixona and E. J. Maginn, *Green Chem.,* 2006, **8**, 82–90.

104 *Guidance document on the validation of (quantitative) structures-activity [(Q)SAR] models* available at : http://www.oecd.org/officialdocuments/publicdisplaydocumentpdf/?doclanguage=en&cote=env/jm/mono(2007)2 (accessed in December 2015).

105 P. Luis , A. Garea and A. Irabien, *J. Mol. Liq.*, 2010, **152**, 28–33.

106 R. N. Das and K. Roy, *Toxicol. Res.*, 2012, **1**, 186-195.

107 F. Yan, Q. Shang, S. Xia, Q. Wang and P. Ma, *J. Hazard. Mater.*, 2015, **286**, 410–415.

108 E. M. Kosower, *J. Am. Chem. Soc.*, 1958, **80**, 3253-3260.

109 C. Reichardt, in *Solvents and Solvent Effects in Organic Chemistry-2, rev. and enl. ed.*; Wiley-VCH, Weinheim, Germany, 1988.

110 C. Reichardt, *Chem. Rev.,* 1994, **94**, 2319e2358.

111 C. Wakai, A. Oleinikova, M. Ott and H. J. Weingartner, *Phys. Chem. B*, 2005, **109**, 17028-17030.

112 H. Weingartner, P. Sasisanker, C. Daguenet, P. J. Dyson, I. Krossing, J. M. Slattery and T. J. Schubert, *Phys. Chem. B*, 2007, **111**, 4775-4780.

113 M. M. Huang,; Y. Jiang, P. Sasisanker, G. W. Driver and H. Weingartner, *J. Chem.Eng. Data*, 2011, *56*, 1494-1499.

114 H. Weingartner, J. *Mol. Liq.*, 2014, **192**, 185-190.

115 J. P. Hallett and T. Welton, *Chem. Rev.*, 2011, **111**, 3508-3576.

116 R. Vanyur, L. Biczok and Z. Miskolczy*, Colloids Surf. A*, 2007, **299**, 256-261.

117 A. J. Carmichael and K. R. Seddon, *J. Phys. Org. Chem.*, 2000, **13**, 591-595.

118 S. Spange, R. Lungwitz and A. Schade, *J. Mol. Liq.*, 2014, **192**, 137-143.

119 C. Chiappe, C. S. Pomelli and S. Rajamani, *J. Phys. Chem. B* 2011, **115**, 9653-9661.

120 F. D'Anna, S. Marullo, P. Vitale and R. Noto, *Eur. J. Org. Chem.*, 2011, **2011**, 5681-5689.

121 F. D'Anna, S. La Marca, P. Lo Meo and R. Noto, *Chem. Eur. J.*, 2009, **15**, 7896-7902.

122 F. D'Anna, D. Millan and R. Noto, *Tetrahedron*, 2015, **71**, 7361-7366.

123 A. Paternò, F. D'Anna, C. G. Fortuna and G. Musumarra, *Tetrahedron* 2016, **72**, 3282-3287.

124 A. F. M. Claudio, L. Swift, J. P. Hallett, T. Welton, J. A. P. Coutinho and M. G.Freire, *Phys. Chem. Chem. Phys.*, 2014, **16**, 6593-6601.

125 A. Triolo, O. Russina, H.-J. Bleif and E. Di Cola, *J. Phys. Chem. B*, 2007, **111**, 4641-4644.

126 IL Thermo Database, available at: http://ilthermo.boulder.nist.gov/ (accessed 1 October 2015).

127 Y. U. Paulechka, *J. Phys. Chem. Ref. Data*, 2010, **39**, 033108-1/23.

128 A. Paternò, R. Fiorenza, S. Marullo, G. Musumarra and S. Scirè, *RSC Adv.* 2016, **6**, 36085-36089.

129 G. Shen, C. Held, X. Lu and X. Ji, *Fluid Phase Equilib.*, 2015, **405**, 73-82.

130 R. L. Gardas, J. A. P. Coutinho, *Fluid Phase Equilib.*, 2008, **266**, 195-201.

131 H. Matsuda, H. Yamamoto, K. Kurihama and K. Tokigi, *Fluid Phase Equilib.*, 2007, **261**, 434-443.

132 B.-K. Chen, M.-J- Liang, T.-Y- Wu and H. P. Wang, *Fluid Phase Equilib.,* 2013, **350**, 37-42.

133 K. Paduszynski and U. Domanska, *J. Chem. Inf. Model.* 2014, **54**, 1311-1324.

134 R. Bini, M. Malvaldi, W. R. Pitner and C. Chiappe, *J. Phys. Org. Chem.* 2008, **21**, 622-629.

135 C. Han, G. Yu, L. Wen, D. Zhao, C. Asumana and X. Chen, *Fluid Phase Equilib.*, 2011, **300**, 95-104.

136 G. Yu, D. Zhao, L. Wen, S. Yang and X. Chen, *AlChE J.*, 2012, **58**, 2885-2899.

137 G. Yu, L. Wen, D. Zhao, C. Asumana and X. Chen, *J. Mol. Liq.*, 2013, **184**, 51-59.

138 R. Alcalde, G. Garcia, M. Atilhan and S. Aparicio, *Ind. Eng. Chem. Res.*, 2015, **54**, 10918-10924.

139 Y. Zhao, Y Huang, X. Zhang and S. Zhang, *Phys. Chem. Chem. Phys.*, 2015, **17**, 3761-3767

140 A. Paternò, L. Goracci, S. Scire and G. Musumarra, *ChemistryOpen*, 2017, doi:10.1002/open.201600119.

141 J. A. Lazzus, *J. Phys Org. Chem.*, 2009, **22**, 1193–1197.

142 M. Deetlefs, K. R. Seddon and M. Shara, *Phys. Chem. Chem. Phys.*, 2006, **8**, 642-649.

143 J. Palomar, V. R. Ferro, J. S. Torrecilla and F. Rodriguez, *Ind. Eng. Chem. Res.*, 2007, **46**, 6041-6048.

144 C. Shen, C. Li, X. Li, Y. Lu and Y. Muhammad, *Chem. Eng. Sci*., 2011, **66**, 2690-2698.

145 A. Rybinska, A. Sosnowska, M. Barycki and T. Puzyn, *J. Comput. Aided Mol. Des.*, 2016, **30**, 165-176.

146 N. Papaiconomou, J. Salminen, J.-M, Lee and J. M. Prausnitz, *J. Chem. Eng. Data*, 2007, **52**, 833-840.

147 S. Zhang, X. Lu, Q. Zhou, X. Li, X. Zhang, S. Li, in *Ionic Liquids-Physicochemical Properties*, Elsevier, Oxford, **2009**.

148 B. Gonzalez, E. Gomez, A. Domınguez, M. Vilas, E. Tojo, *J. Chem. Engin. Data* 2011, **56**, 14-20.

149 A. Bhattacharjee, P. J. Carvalho and J. A.P. Coutinho, *Fluid Phase Equilib.*, 2014, **375**, 80–88.

150 M. T. Clough, C. R. Crick, J. Grasvik, P. A. Hunt, H. Niedermeyer, T. Welton and O. P. Whitaker, *Chem. Sci.*, 2015, **6**, 1101–1114.

151 S.-H. Yeon, K.-S. Kim, S. Choi, H. Lee, H. S. Kim and H. Kim, *Electrochim. Acta*, 2005, **50**, 5399–5407.

152 I. Bandres, R. Alcalde, C. Lafuente, M. Atilhan and S. Aparicio, *J. Phys. Chem. B*, 2011, **115**, 12499-12513.

153 M. A. Taige, D. Hilbert and T. J. S. Schubert, *Z. Phys. Chem.*, 2012, **226**, 129-139.

154 J.-G- Li, Y.-F. Hu, C.-W. Jin, H.-D. Chu, X.-M. Peng and Y.-G. Liang, *J. Solution Chem.* 2010, **39**, 1877-1887.

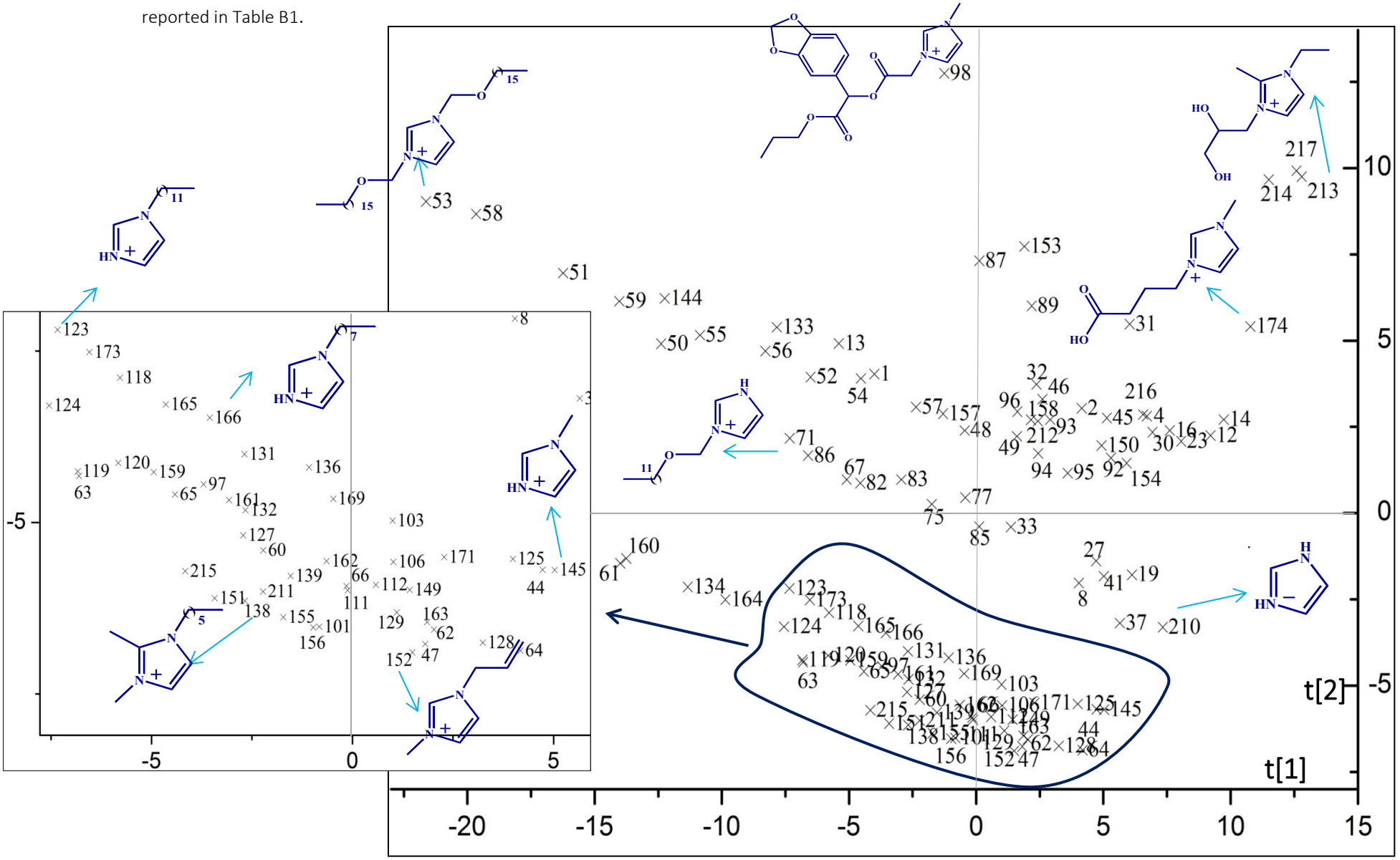
155 P. Eiden, S. Bulut, T. Kochner, C. Friedrich, T. Schubert, and I. Krossing, J. *Phys. Chem. B*, 2011, **115**, 300-309.

156 E. S. Sashina, D. A. Kashirskii, G. Janowska and M. Zaborski, *Thermochim. Acta*, 2013, **568**, 185-188.

6 Appendix

6.1 A-Figures

Fig. A1 Simplified t[1]-t[2] cations scores plot for cations PCA model, containing only imidazolium-based structures for simplicity. Labels as numeration reported in Table B1.



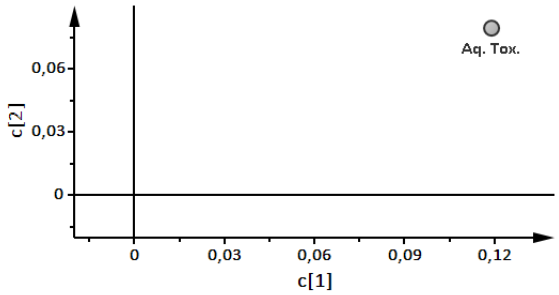


Fig. A2 c[1]-c[2] loadings plot for the aquatic toxicity PLS model. Such a plot reports the position of Y in the statistical space. Loadings and scores plot are superimposable to each other, hence a specific trend onto the scores plot (showing the objects) can be interpreted looking along the same direction on the loadings plot (reporting the variables). The increasing of aquatic toxicity scores (along both positive axes) indicates the decreasing of toxicity towards the selected biological targets.

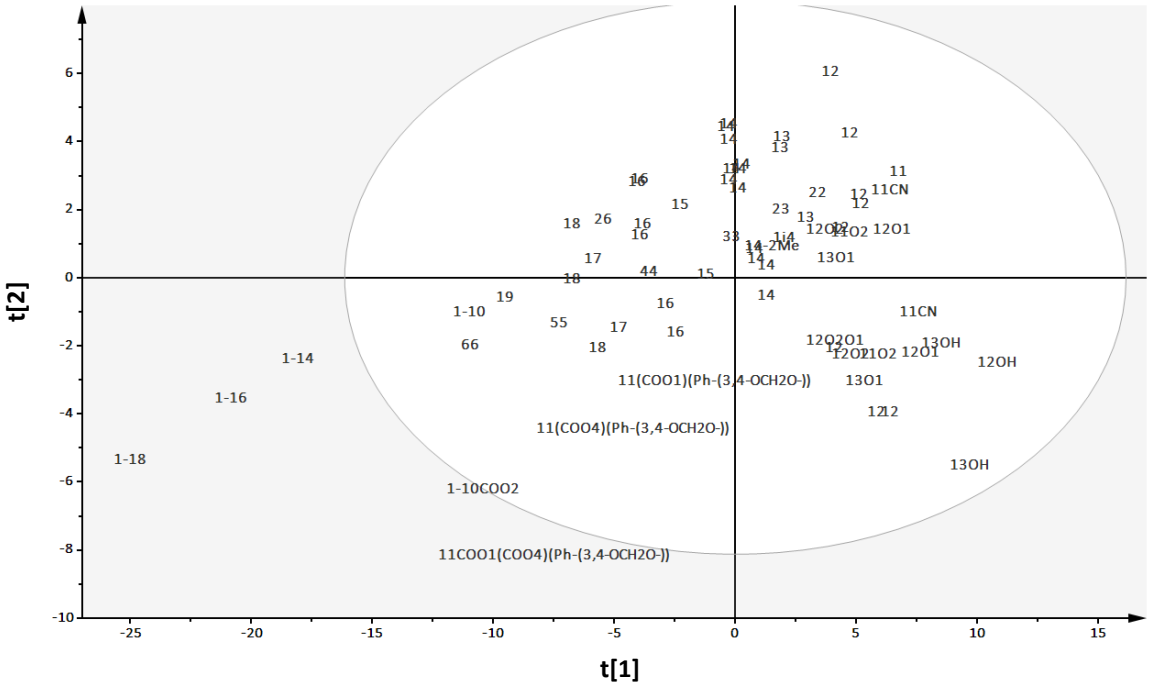


Fig. A3 t[1]-t[2] scores plot for aquatic toxicity PLS model. In the plot above only the imidazoliums based ionic liquids (the most populated ILs groups) are displayed for simplicity (see Figure 25 for the whole plot), and labels refer to their cationic *N*-side chain (objects are reported in Table B11): first values refers to the first *N*-substituents; second values (and the following molecular group) refers to the second one (for instance: "12" means "*N*-methyl-*N*-ethyl"; "1-18" means "*N*-methyl-*N*-octadecyl"; "1-10COO2" means "*N*-methyl-*N*-(11-ethyl-11-oxoundecyl)) and so on.

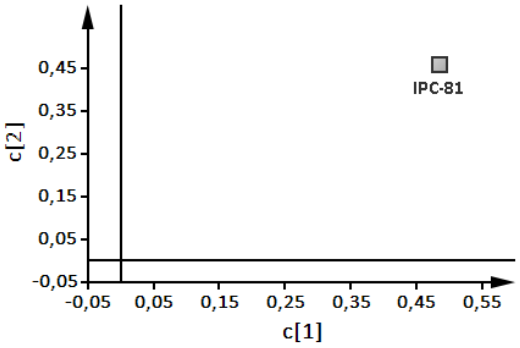


Fig. A4 c[1]-c[2] loadings plot for the IPC-81 PLS model. Such a plot reports the position of Y in the statistical space. Loadings and scores plot are superimposable to each other, hence a specific trend onto the loadings plot (showing the objects) can be interpreted looking along the same direction on the loadings plot (reporting the variables). The increasing of cytotoxicity values (along both positive axes) indicates the decreasing of toxicity towards the selected biological targets.

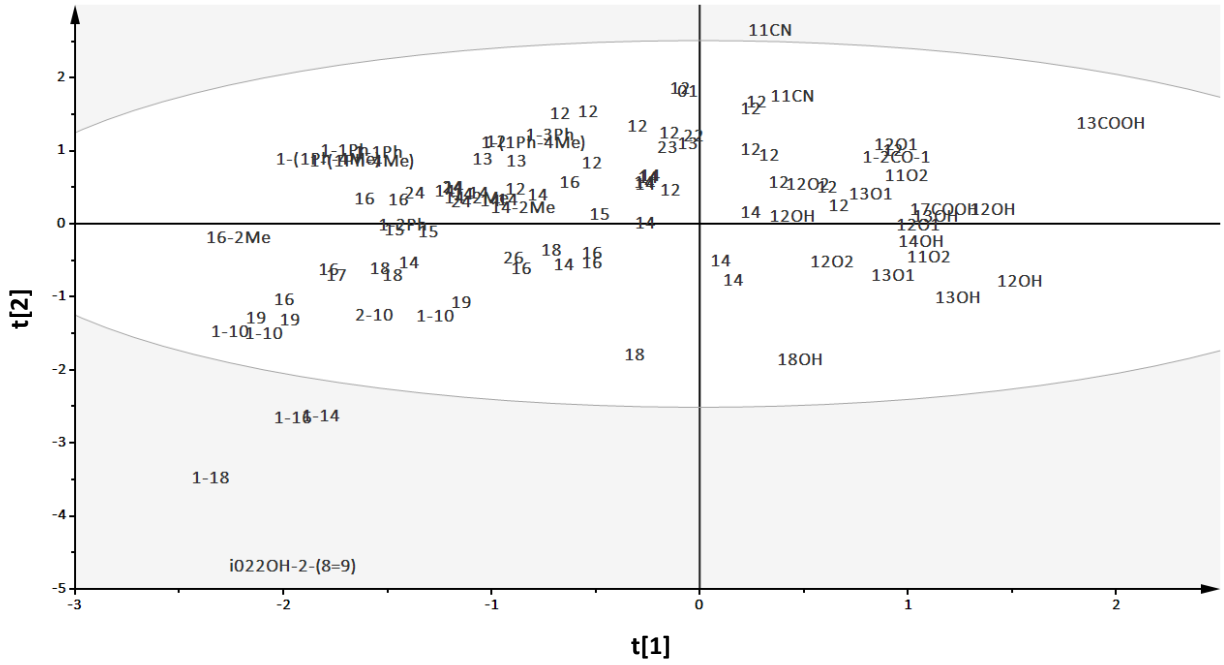


Fig. A5 t[1]-t[2] scores plot for the IPC-81 PLS model. In the plot above only the imidazoliums based ionic liquids (the most populated ILs groups) are displayed for simplicity (see Fig. 29 for the whole plot), and labels refer to their cationic *N*-side chain (objects are reported in Table B12): the first values refers to the first *N*-substituents; the second values (and the following molecular group) refers to the second one (for instance: "12" means "*N*-methyl-*N*-ethyl"; "1-18" means "*N*-methyl-*N*-octadecyl"; "13O1" means "*N*-methyl-*N*-(methoxypropyl)).

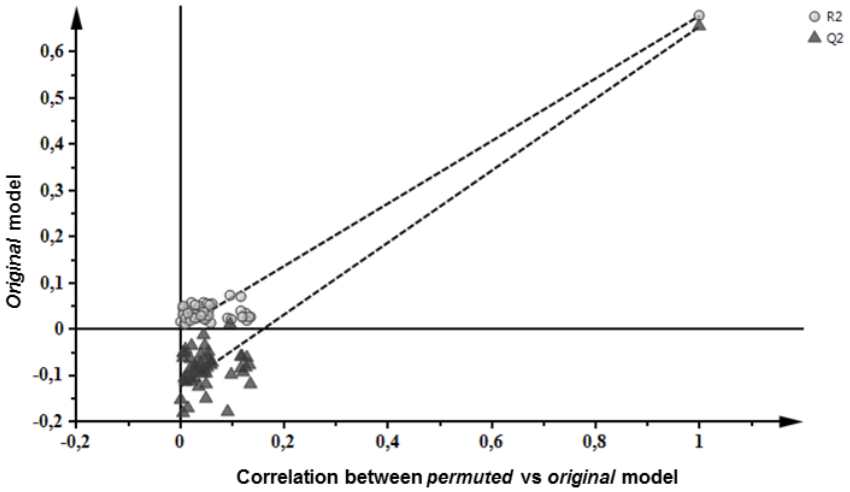


Fig. A6 Permutation plot for IPC-81 PLS correlation model. The plot above strongly indicates that the corresponding PLS model is valid (see section 2).

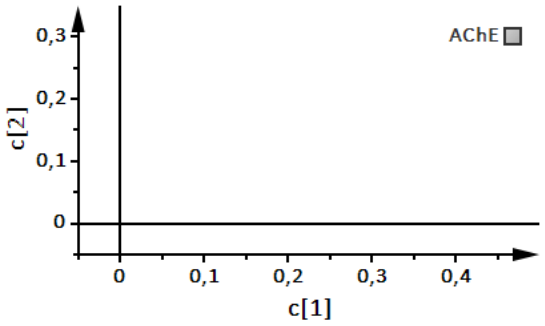


Fig. A7 c[1]-c[2] loadings plot for the AChE toxicity PLS model. Such a plot reports the position of Y in the statistical space. Loadings and scores plot are superimposable to each other, hence a specific trend onto the scores plot (showing the objects) can be interpreted looking along the same direction on the loadings plot (reporting the variables). The increasing of inhibitory activity values (along both positive axes) indicates the decreasing of toxicity towards the selected biological targets.

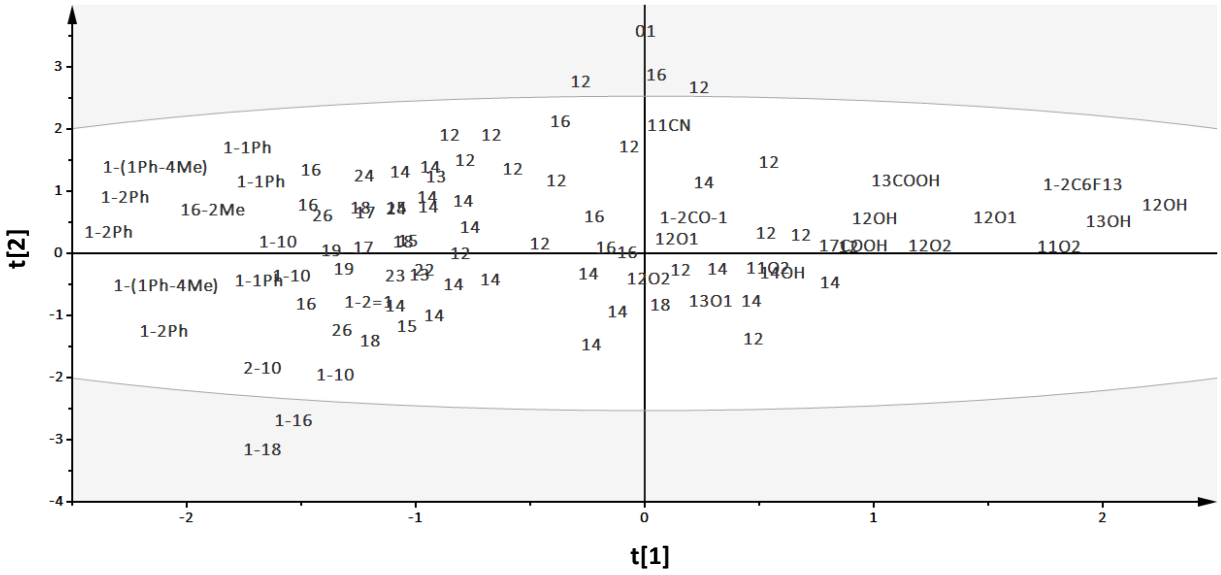


Fig. A8 t[1]-t[2] scores plot for the AChE PLS model. In the plot above only the imidazoliums based ionic liquids (the most populated ILs groups) are displayed for simplicity (see Fig. 32 for the whole plot), and labels refer to their cationic *N*-side chain (objects are reported in Table B13 for labels significance): the first values refers to the first *N*-substituents; the second values (and the following molecular group) refers to the second one (for instance: "12" means "*N*-methyl-*N*-ethyl"; "1-18" means "*N*-methyl-*N*-octadecyl"; "1-2Ph" means "*N*-methyl-*N*-(phenylethyl)).

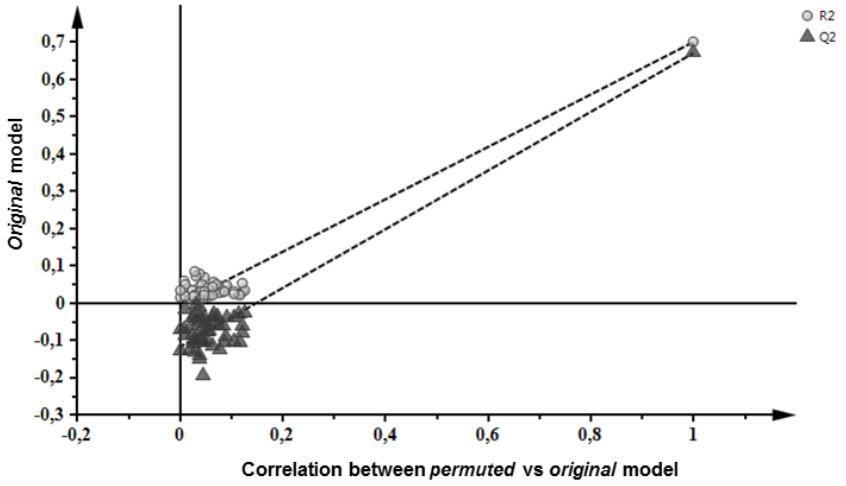


Fig. A9 Permutation plot for AChE PLS correlation model. The permutation plot above fulfills all the three internal validation criteria, indicating the validity of the AChE PLS model (see section 2).

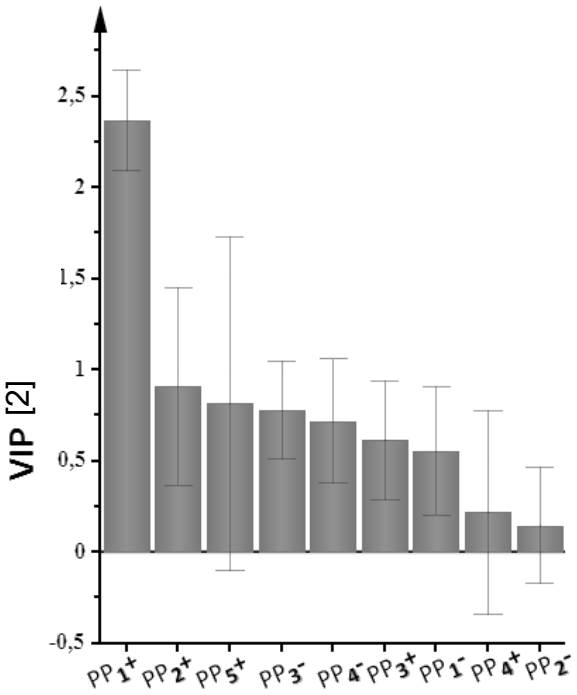


Fig. A10 VIP bars plot for the *Vibrio fischeri* correlation resulting from the 55x9 matrix correlation model.

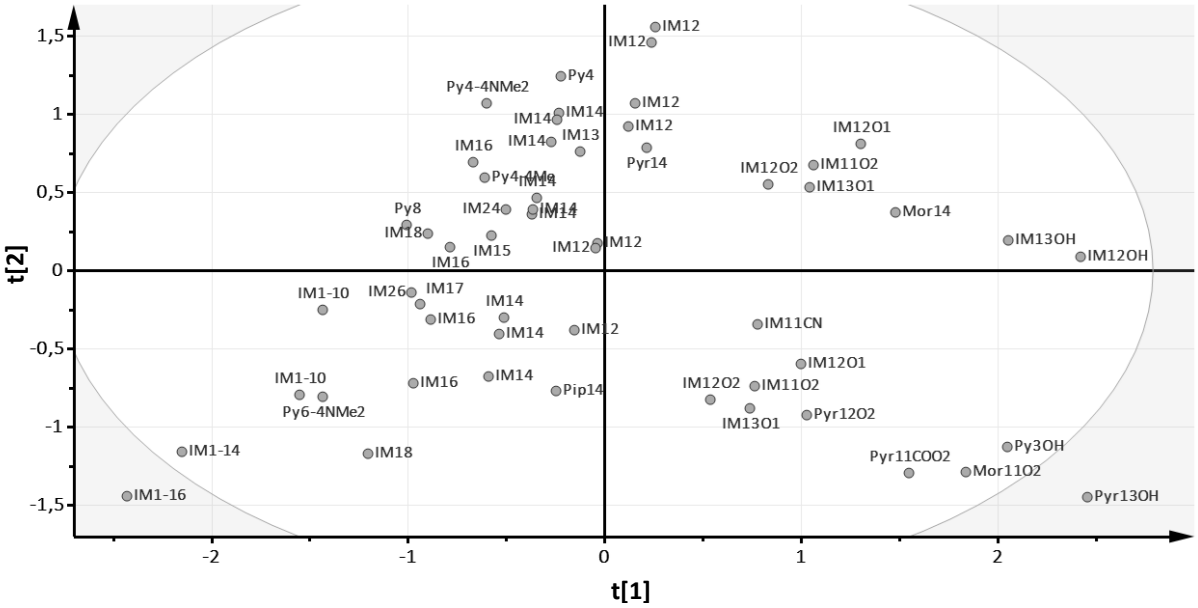


Fig. A11 t[1]-t[2] scores plot for *Vibrio fischeri* toxicity PLS model. Log(EC_{50}) increases from the bottom left to the upper right (as Fig. 35 displays). In this plot labels refer to their cationic substituents:
-for imidazolium-based ILs (IM): the first value refers to the first *N*-substituent; the second values (and the following molecular group) refers to the second one (*i. e.*: "12" means "*N*-methyl-*N*-ethyl"; "1-16" means "*N*-methyl-*N*-hexadecyl"; "12O1" means "*N*-methyl-*N*-(methoxyethyl)).
-for pyrrolidinium, piperidinium and morpholinium-based ILs (PYR, PIP, MOR): the first value refers to the first *N*-substituent; the second values (and the following molecular group) refers to the second one in the same nitrogen atom (*i. e.*: 14 means "N-butyl-N-methyl");
-for pyridinium-based ILs (PY): the first value refers to the *N*-substituent; if present, the second values (and the following molecular group) refers to the second one and its C-position (*i. e.*: Py4-4NMe2 means "1-methyl-4-dimethylaminopyridinium").

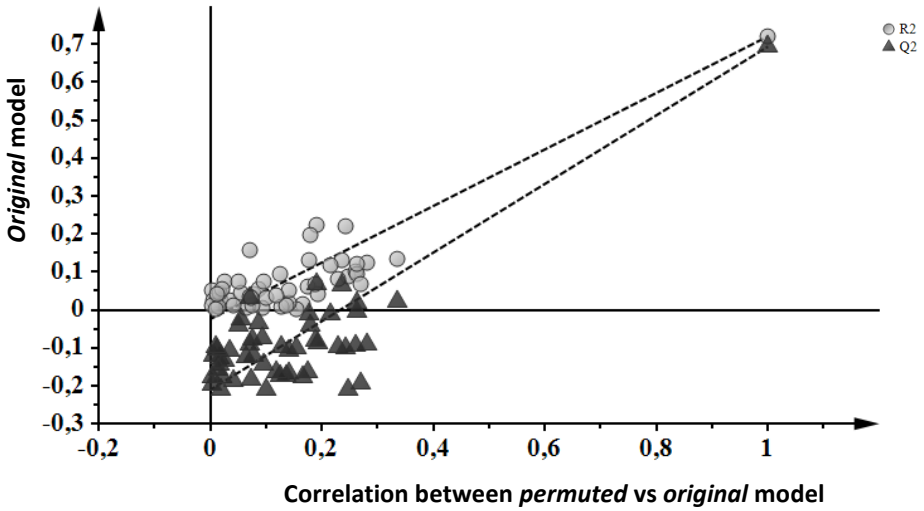


Fig. A12 Permutation plot confirming the validity of the *Vibrio fischeri* PLS model, as reported in section 2.

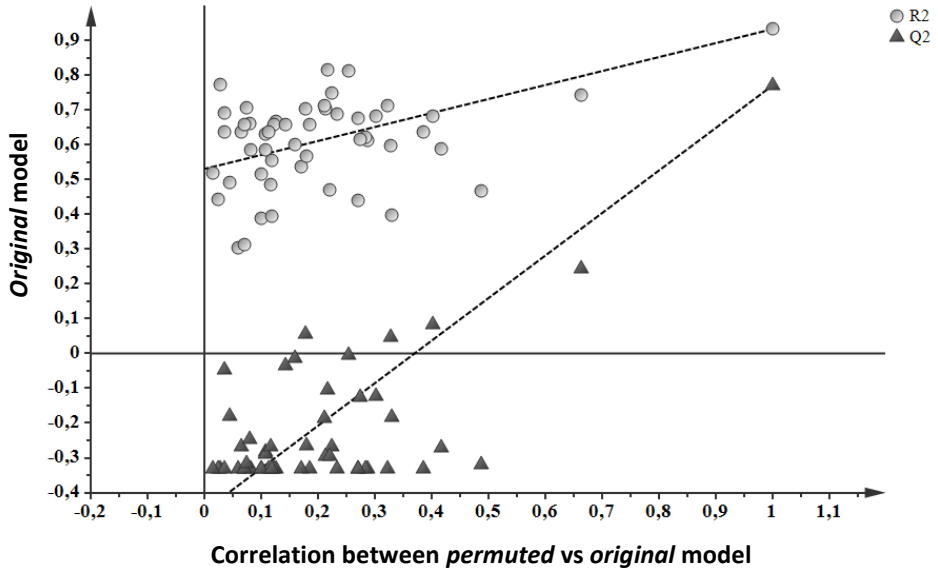


Fig. A13 Permutation plot confirming the validity of the E_{NR} PLS model, as reported in section 2.

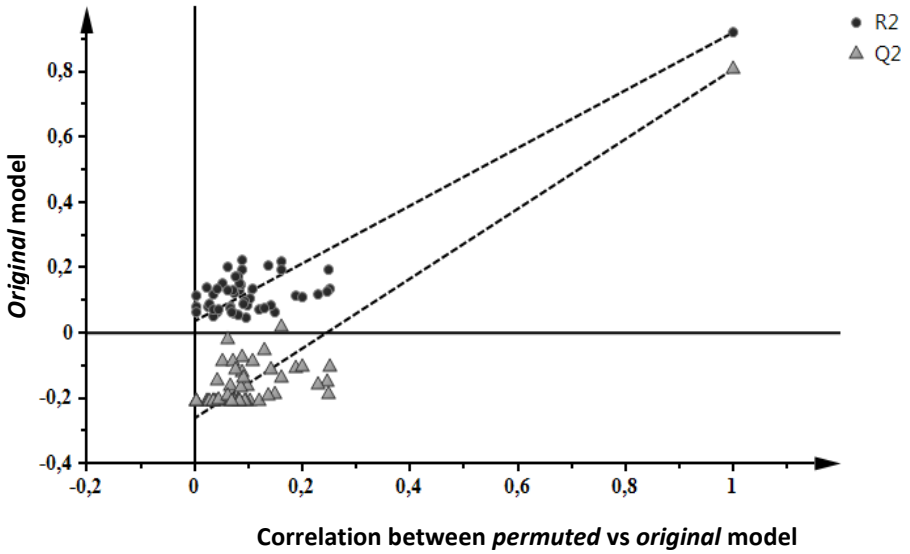


Fig. A14 Permutation plot confirming the validity of the C_p PLSmodel, as reported in section 2.

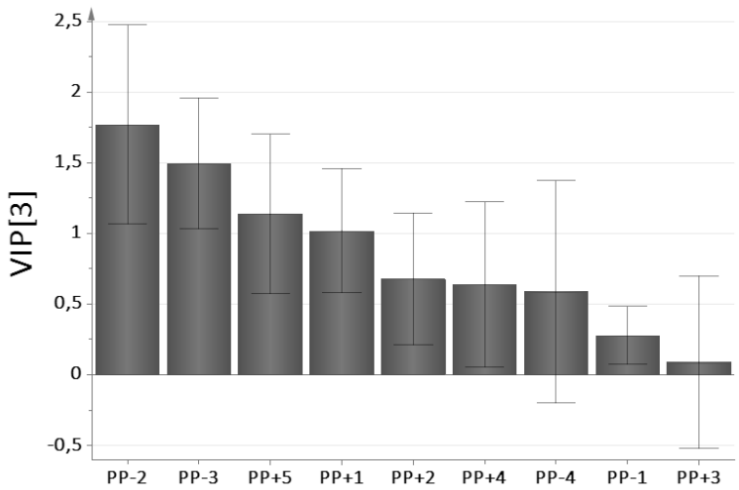


Figure A15. VIP bars plot for the viscosity (T = 283.15 K) PLS model derived using 23 ILs as objects and 9 PPs as descriptors.

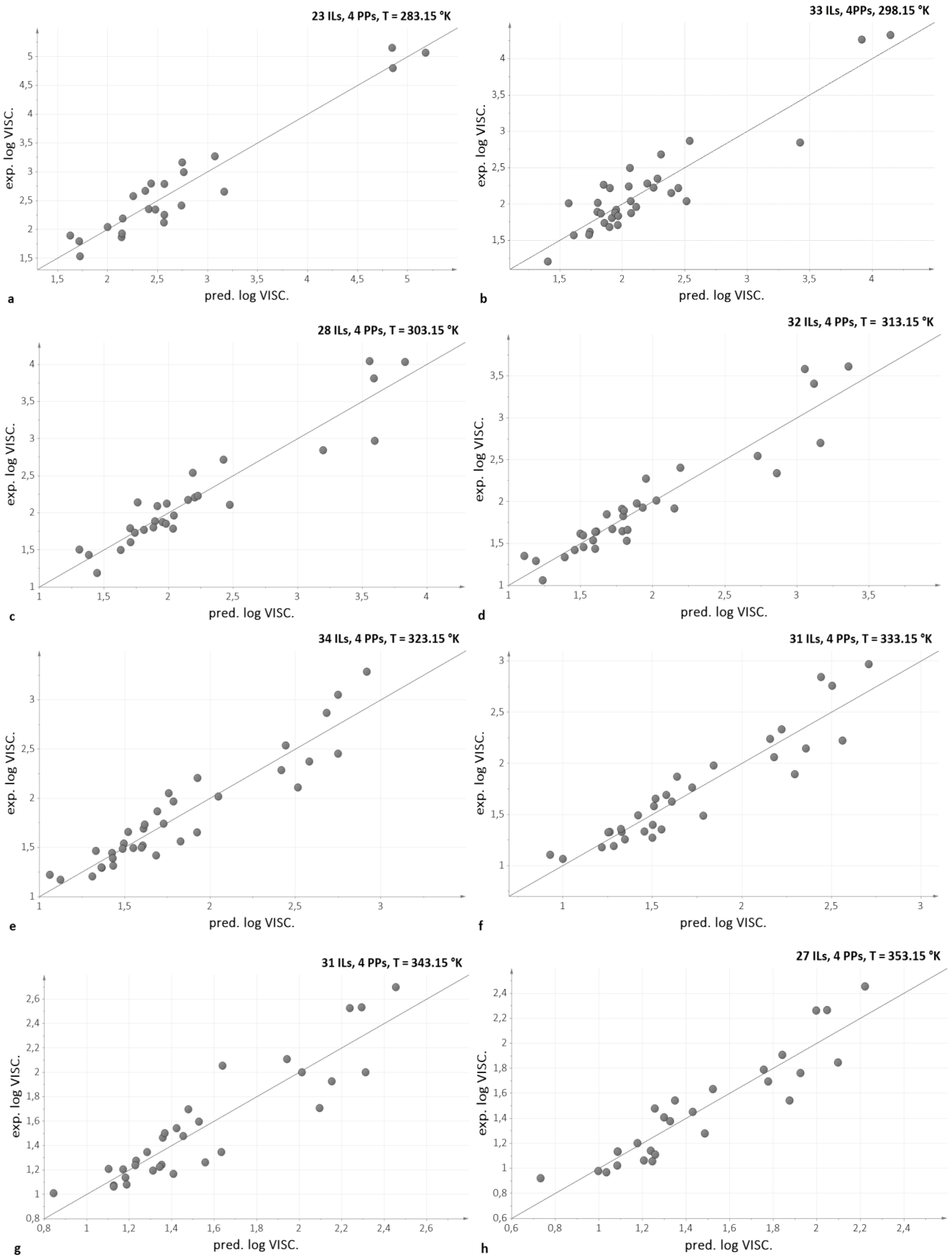


Figure A16 Predicted *vs.* experimental plots for log viscosity at T = 283.15/353.15 K.

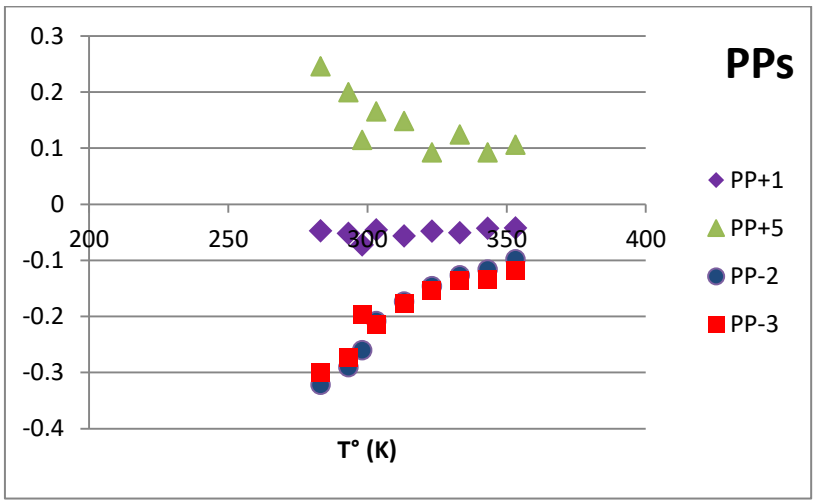


Figure A17 This plot displays the variation of the PPs coefficients in viscosity equations on increasing the temperature.

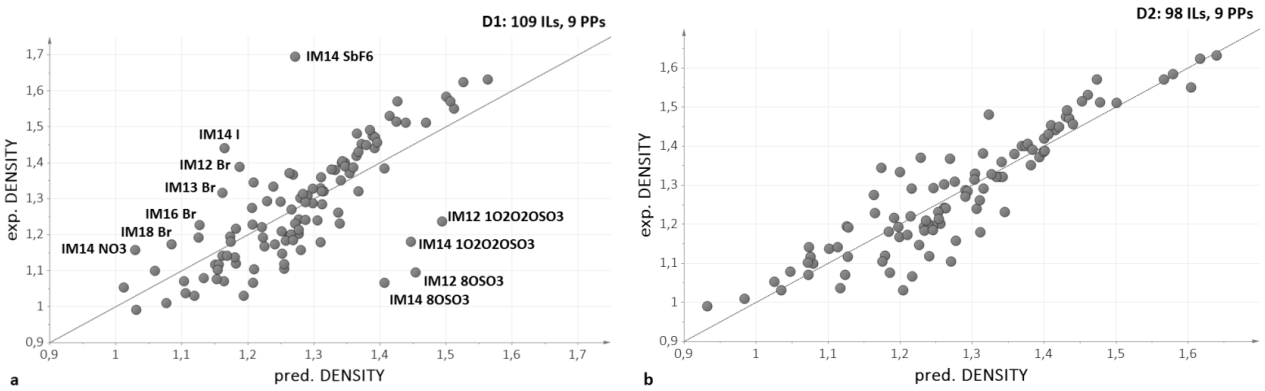


Figure A18 Predicted *vs.* experimental plots for density (a:D1; b: D2) at T = 298.15 K.

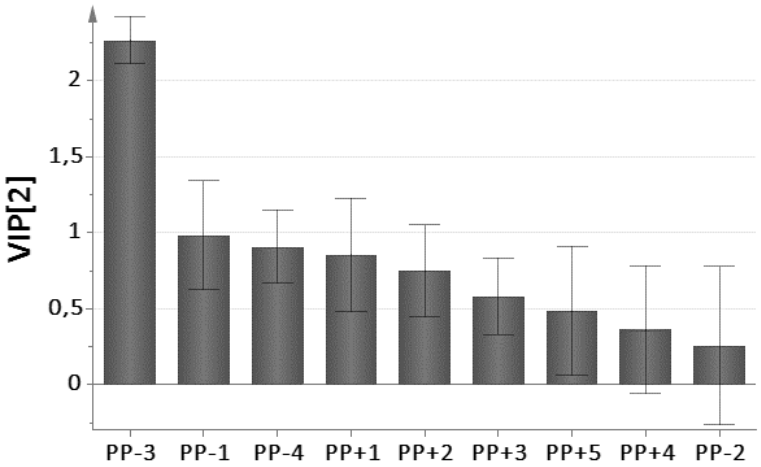


Figure A19 VIP bars plot for the density PLS model D2.

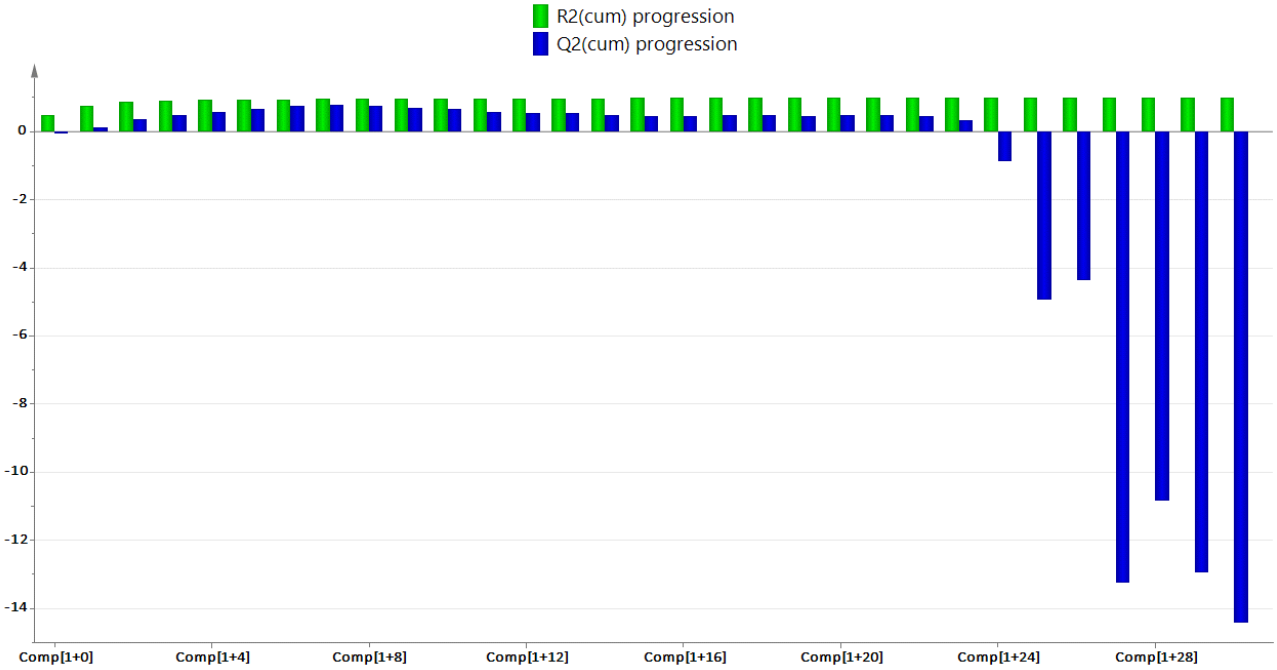


Figure A20. Summary of fit for the overfitted decomposition temperature OPLS model (M3). Note that the R^2 value, related to the model fitting capability, increases on increasing the number of components, while the Q^2 value, indicating the model predicting ability, reaches a maximum (corresponding to maximum predicting ability) and then decreases. On increasing the number of orthogonal components up to 30 an extremely good correlation (Fig. A21) can be obtained. However such a model is not statistically meaningful, as elucidated by the Q^2 trend in the above figure.

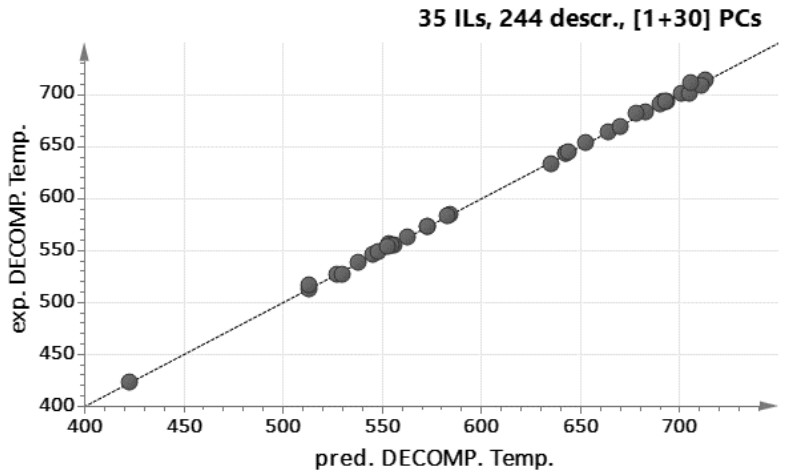


Figure A21 Predicted *vs.* experimental plots for the *overfitted* decomposition temperature OPLS model (M3).

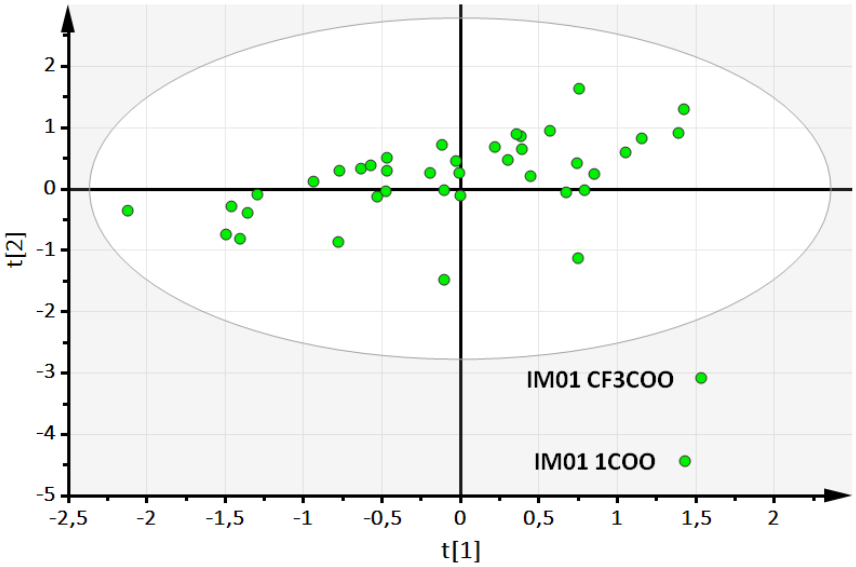


Figure A22 Scores plot for the conductivity C1 PLS model.

6.2 A-Tables: models statistical parameters

Table A1 Cations PCA summary (218 objects).

PC	R^2	R^2 (cum.)
1	0.319	0.319
2	0.224	0.543
3	0.114	0.657
4	0.080	0.737
5	0.038	0.775

Table A2 Anions PCA summary (38 objects).

PC	R^2	R^2 (cum.)
1	0.275	0.275
2	0.206	0.480
3	0.138	0.619
4	0.117	0.735

Table A3 Aquatic toxicity scores PLS model parameters.

PC	R^2X	R^2X(cum.)	R^2Y	R^2Y(cum.)	Q^2	Q^2(cum.)
1	0.274	0.274	0.591	0.591	0.570	0.570
2	0.123	0.397	0.067	0.658	0.008	0.576
3	0.159	0.556	0.039	0.697	0.040	0.593
4	0.057	0.613	0.058	0.755	0.066	0.620

Table A4. IPC-81 PLS model parameters.

PC	R^2X	R^2X(cum.)	R^2Y	R^2Y(cum.)	Q^2	Q^2(cum.)
1	0.272	0.272	0.461	0.461	0.446	0.446
2	0.12	0.391	0.218	0.678	0.378	0.655

Table A5. AChE PLS model parameters.

PC	R^2X	R^2X(cum.)	R^2Y	R2Y(cum.)	Q^2	Q^2(cum.)
1	0.325	0.325	0.606	0.606	0.592	0.592
2	0.136	0.46	0.0949	0.701	0.196	0.671

Table A6 *Vibrio fischeri* PLS model parameters derived by using 55x9 matrix correlation model (model not used for predictions).

PC	R^2X	R^2X(cum.)	R^2Y	R^2Y(cum.)	Q^2	Q^2(cum.)
1	0.187	0.187	0.602	0.602	0.527	0.527
2	0.176	0.364	0.167	0.769	0.326	0.681

Table A7 *Vibrio fischeri* PLS model parameters derived by using 55x3 matrix correlation model.

PC	R^2X	R^2X(cum.)	R^2Y	R^2Y(cum.)	Q^2	Q^2(cum.)
1	0.493	0.493	0.554	0.554	0.537	0.537
2	0.239	0.732	0.236	0.789	0.502	0.77

Table A8 E_{NR} PLS model parameters.

PC	R^2X	R^2X(cum.)	R^2Y	R^2Y(cum.)	Q^2	Q^2(cum.)
1	0.295	0.295	0.756	0.756	0.603	0.603
2	0.234	0.529	0.126	0.881	0.315	0.728
3	0.128	0.657	0.051	0.932	0.153	0.770

Table A9 C_p PLS model parameters.

PC	R^2X	R^2X(cum.)	R^2Y	R^2Y(cum.)	Q^2	Q^2(cum.)
1	0.27	0.27	0.779	0.779	0.709	0.709
2	0.135	0.405	0.141	0.919	0.338	0.807

Table A10 Viscosity (T = 283.15 K) PLS model derived using 23 ILs as objects and 9 PPs as descriptors (this model was not used for predictions).

PC	R^2X	R^2X(cum.)	R^2Y	R^2Y(cum.)	Q^2	Q^2(cum.)
1	0.244	0.244	0.828	0.828	0.727	0.727
2	0.224	0.468	0.101	0.929	0.485	0.859
3	0.144	0.612	0.021	0.949	0.093	0.872

Table A11 Viscosity (T° = 283.15/353.15 K) PLS model parameters.

Model	*PC*	R^2X	R^2X(cum.)	R^2Y	R^2Y(cum.)	Q^2	Q^2(cum.)
23 ILs, X = 4PPs, Y = log (Viscosity at 283.15 K)	*1*	0.437	0.437	0.873	0.873	0.845	0.845
	2	0.248	0.684	0.053	0.926	0.37	0.903
34 ILs, X = 4PPs, Y = log (Viscosity at 293.15 K)	*1*	0.298	0.298	0.904	0.904	0.879	0.879
	2	0.22	0.518	0.025	0.928	0.147	0.897
33 ILs, X = 4PPs, Y = log (Viscosity at 298.15 K)	*1*	0.352	0.352	0.737	0.737	0.628	0.628
	2	0.313	0.665	0.108	0.845	0.292	0.736
28 ILs, X = 4PPs, Y = log (Viscosity at 303.15 K)	*1*	0.466	0.466	0.839	0.839	0.821	0.821
	2	0.276	0.742	0.053	0.893	0.265	0.868
32 ILs, X = 4PPs, Y = log (Viscosity at 313.15 K)	*1*	0.475	0.475	0.823	0.823	0.794	0.794
	2	0.308	0.783	0.06	0.882	0.266	0.849
34 ILs, X = 4PPs, Y = log (Viscosity at 323.15 K)	*1*	0.358	0.358	0.825	0.825	0.78	0.78
	2	0.393	0.751	0.055	0.88	0.244	0.834
31 ILs, X = 4PPs, Y = log (Viscosity at 333.15 K)	*1*	0.424	0.424	0.846	0.846	0.8	0.8
	2	0.386	0.811	0.026	0.872	0.102	0.82
31 ILs, X = 4PPs, Y = log (Viscosity at 343.15 K)	*1*	0.367	0.367	0.811	0.811	0.754	0.754
	2	0.441	0.808	0.018	0.829	-0.074	0.736
27 ILs, X = 4PPs, Y = log (Viscosity at 353.15 K)	*1*	0.403	0.403	0.839	0.839	0.795	0.795
	2	0.423	0.826	0.019	0.857	0.026	0.8

Table A12 Density (T = 298.15 K) PLS models parameters.

Model	*PC*	R^2X	R^2X(cum.)	R^2Y	R^2Y(cum.)	Q^2	Q^2(cum.)
D1: 109 ILs. 9 PPs	*1*	0.182	0.182	0.408	0.408	0.304	0.304
	2	0.113	0.295	0.13	0.538	0.075	0.357
D2: 98 ILs. 9 PPs	*1*	0.19	0.19	0.614	0.614	0.556	0.556
	2	0.119	0.309	0.214	0.828	0.444	0.753
D3: 98 ILs. 4 PPs	*1*	0.337	0.337	0.654	0.654	0.629	0.629
	2	0.194	0.531	0.169	0.823	0.465	0.802

Table A13 Decomposition temperature (M1-2) PLS models parameters (not used for predictions).

Model	*PC*	R^2X	R^2X(cum.)	R^2Y	R^2Y(cum.)	Q^2	Q^2(cum.)
M1: 35 ILs, X = 9 PPs	*1*	0.204	0.204	0.233	0.233	-0.225	-0.1
	2	0.182	0.385	0.128	0.361	-0.428	-0.21
M2: 35 ILs, X = VolSurf+ descriptors	*1*	0.196	0.196	0.478	0.478	-0.043	-0.0432
	2	0.224	0.42	0.294	0.772	0.483	0.461
	3	0.067	0.487	0.109	0.881	-0.169	0.407

Table A14 Decomposition temperature OPLS model (M3)parameters.

	PC	R^2X	R^2X(cum.)	R^2	R^2(cum.)	Q^2	Q^2(cum.)	R^2Y	R^2Y(cum.)
OPLS, M3: 35 ILS, X = VolSurf+ descriptors	Model		0,865		0,96		0,795		1
	Predictive		0,0345		0,96		0,795		1
	P1	0,0345	0,0345	0,96	0,96	0,795	0,795	1	1
	Orthogonal in X(OPLS)		0,83		0				
	O1	0,371	0,371	0	0				
	O2	0,0763	0,447	0	0				
	O3	0,147	0,594	0	0				
	O4	0,0317	0,626	0	0				
	O5	0,101	0,727	0	0				
	O6	0,0809	0,808	0	0				
	O7	0,0224	0,83	0	0				

Table A15 Conductivity (C1 and C2) PLS models parameters (not used for predictions).

Model	PC	R^2X	R^2X(cum.)	R^2Y	R^2Y(cum.)	Q^2	Q^2(cum.)
C1: 41 ILs. 9 PPs. log Conductivity (298.15 K)	1	0.136	0.136	0.52	0.517	0.213	0.213
	2	0.168	0.304	0.17	0.688	-0.115	0.135
C2: 39 ILs. 9 PPs. log Conductivity (298.15 K)	1	0.12	0.12	0.62	0.616	0.312	0.312
	2	0.231	0.35	0.09	0.708	-0.011	0.304

Table A16 Conductivity OPLS model (C3) parameters.

	PC	R^2X	R^2X(cum.)	R^2	R^2(cum.)	Q^2	Q^2(cum.)	R^2Y	R^2Y(cum.)
	Model		0.878		0.968		0.833		1
OPLS, C3: 39 ILS, X = VolSurf+ descriptors, log Conductivity (298.15 K)									
	Predictive		0.1		0.968		0.833		1
	P1	0.1	0.1	0.968	0.968	0.833	0.833	1	1
	Orthogonal in X(OPLS)		0.778		0				
	O1	0.299	0.299	0	0				
	O2	0.131	0.431	0	0				
	O3	0.109	0.54	0	0				
	O4	0.111	0.651	0	0				
	O5	0.0624	0.714	0	0				
	O6	0.052	0.766	0	0				
	O7	0.0128	0.778	0	0				

6.3 B-Tables: objects, descriptors, properties and predictions

Table B1 List of the 218 cations with their SMILES codes and PPs+ values.

entry	SMILES codes	Cations	PP1+	PP2+	PP3+	PP4+	PP5+
1	[N+]1(C)=CN(C=C1)CCCCCCCCCCC(=O)OCC	1-(11-Ethoxy-11-oxoundecyl)-3-methylimidazolium	-4.00	4.03	0.76	-0.19	0.44
2	[N+]1(C)=CN(C=C1)CC(=O)OCCCC	1-(2-Butoxy-2-oxoethyl)-3-methylimidazolium	4.15	3.03	-0.57	1.95	-1.69
3	[N+]1(C)(CCCC1)CC(=O)OCC	1-(2-Ethoxy-2-oxoethyl)-1-methylpyrrolidinium	7.17	1.90	-2.39	4.75	-1.11
4	[N+]1(C)=CN(C=C1)CC(=O)OCC	1-(2-Ethoxy-2-oxoethyl)-3-methylimidazolium	6.71	2.81	-0.50	1.76	-1.59
5	[n+]1(ccccc1)CC(=O)OCC	1-(2-Ethoxy-2-oxoethyl)pyridinium	4.31	2.25	-0.36	0.90	-2.53
6	[N+]1(C)(CCCCC1)CCOCC	1-(2-Ethoxyethyl)-1-methylpiperidinium	4.83	-0.32	-3.71	5.03	0.45
7	[N+]1(C)(CCCC1)CCOCC	1-(2-Ethoxyethyl)-1-methylpyrrolidinium	5.75	-0.56	-3.73	5.02	0.54
8	[N+]1(C)=CN(C=C1)CCOCC	1-(2-Ethoxyethyl)-3-methylimidazolium	4.04	-2.03	1.37	0.09	0.45
9	[n+]1(ccccc1)CCOCC	1-(2-Ethoxyethyl)pyridinium	4.79	-2.48	2.51	-0.28	0.17
10	[N+]1(C)(CCCCC1)CCO	1-(2-Hydroxyethyl)-1-methylpiperidinium	10.68	4.70	-2.87	1.16	3.53
11	[N+]1(C)(CCCC1)CCO	1-(2-Hydroxyethyl)-1-methylpyrrolidinium	11.45	4.49	-2.64	1.01	3.23
12	[N+]1(C)=C(C)N(C=C1)CCO	1-(2-hydroxyethyl)-2,3-dimethylimidazolium	9.21	2.25	3.25	-4.16	2.37
13	[N+]1(CCCCCCCCCCCCCC)=C(C)N(C=C1)CCO	1-(2-Hydroxyethyl)-2-methyl-3-tetradecylimidazolium	-5.40	4.92	-0.25	-1.53	4.03
14	[N+]1(C)=CN(C=C1)CCO	1-(2-Hydroxyethyl)-3-methylimidazolium	9.73	2.71	2.15	-3.96	2.49
15	[n+]1(ccccc1)CCO	1-(2-Hydroxyethyl)pyridinium	10.28	2.57	3.54	-4.42	2.59
16	[N+]1(C)=CN(C=C1)CC(=O)OC	1-(2-Methoxy-2-oxoethyl)-3-methylimidazolium	7.61	2.40	0.08	1.03	-2.04
17	[N+]1(C)(CCCCC1)CCOC	1-(2-Methoxyethyl)-1-methylpiperidinium	5.73	-1.14	-3.80	5.03	0.34
18	[N+]1(C)(CCCC1)CCOC	1-(2-Methoxyethyl)-1-methylpyrrolidinium	7.36	-0.19	-3.63	4.10	0.85
19	[N+]1(C)=CN(C=C1)CCOC	1-(2-Methoxyethyl)-3-methylimidazolium	6.12	-1.79	1.00	-0.25	-0.03
20	[n+]1(ccccc1)CCOC	1-(2-Methoxyethyl)pyridinium	6.51	-2.48	1.93	-0.46	-0.20
21	[N+]1(C)(CCCCC1)CCCO	1-(3-Hydroxypropyl)-1-methylpiperidinium	9.27	4.69	-2.96	1.70	3.21
22	[N+]1(C)(CCCC1)CCCO	1-(3-Hydroxypropyl)-1-methylpyrrolidinium	10.38	4.48	-2.99	1.65	3.25
23	[N+]1(C)=CN(C=C1)CCCO	1-(3-Hydroxypropyl)-3-methylimidazolium	8.05	2.08	2.12	-3.44	2.47
24	[n+]1(ccccc1)CCCO	1-(3-Hydroxypropyl)pyridinium	9.31	2.44	2.69	-3.75	1.97
25	[N+]1(C)(CCCCC1)CCCOC	1-(3-Methoxypropyl)-1-methylpiperidinium	4.88	0.03	-3.74	4.40	0.67

26	[N+]1(C)(CCCC1)CCCOC	1-(3-Methoxypropyl)-1-methylpyrrolidinium	5.81	-0.16	-3.72	4.31	0.62
27	[N+]1(C)=CN(C=C1)CCCOC	1-(3-Methoxypropyl)-3-methylimidazolium	4.71	-1.38	0.08	0.80	0.67
28	[n+]1(ccccc1)CCCOC	1-(3-Methoxypropyl)pyridinium	4.39	-2.54	2.94	-0.77	0.87
29	[n+]1(ccccc1)CCCS(=O)(=O)O	1-(3-Sulfopropyl)pyridinium	14.74	7.66	6.06	-4.40	3.17
30	[N+]1(C)=CN(C=C1)CCCCO	1-(4-Hydroxybutyl)-3-methylimidazolium	6.92	2.34	1.31	-2.68	2.61
31	[N+]1(C)=CN(C=C1)CCCCCCCC(=O)O	1-(7-Carboxyheptyl)-3-methylimidazolium	6.03	5.48	3.42	-1.70	1.31
32	[N+]1(C)=CN(C=C1)CCCCCCCCO	1-(8-Hydroxyoctyl)-3-methylimidazolium	2.36	3.73	-0.11	-1.86	3.95
33	[NH+]1=CN(C=C1)COCCCC	1-(Butoxymethyl)imidazolium	1.36	-0.40	-9.16	-3.36	-1.19
34	[n+]1(cc(O)ccc1)COCCCC	1-(Butoxymethyl)-3-hydroxypyridinium	7.76	2.79	1.60	1.11	2.48
35	[N+]1(C)(CCCCC1)CC#N	1-(Cyanomethyl)-1-methylpiperidinium	5.85	0.24	-2.52	1.66	0.09
36	[N+]1(C)(CCCC1)CC#N	1-(Cyanomethyl)-1-methylpyrrolidinium	6.95	0.11	-2.58	2.04	-0.06
37	[N+]1(C)=CN(C=C1)CC#N	1-(Cyanomethyl)-3-methylimidazolium	5.65	-3.19	5.25	-4.99	-2.61
38	[n+]1(ccccc1)CC#N	1-(Cyanomethyl)pyridinium	5.10	-3.86	6.39	-5.86	-2.84
39	[N+]1(C)(CCCCC1)COCC	1-(Ethoxymethyl)-1-methylpiperidinium	3.80	-1.20	-4.17	5.21	0.01
40	[N+]1(C)(CCCC1)COCC	1-(Ethoxymethyl)-1-methylpyrrolidinium	5.12	-1.38	-4.24	5.38	0.11
41	[N+]1(C)=CN(C=C1)COCC	1-(Ethoxymethyl)-3-methylimidazolium	5.01	-1.83	-0.67	1.85	0.11
42	[n+]1(ccccc1)COCC	1-(Ethoxymethyl)pyridinium	5.70	-2.01	-0.01	1.57	0.11
43	[N+]1(CCCCCC)(CCCC1)CCCCCC	1,1-Dihexylpyrrolidinium	-5.18	-2.55	-3.71	5.26	0.71
44	Cc1[nH]cc[n+]1C	1,2-dimethylimidazolium	4.73	-5.69	-5.54	-6.03	-3.20
45	[N+]1(C)=C(C)N(C=C1)CC(=O)OCCC	1,2-Dimethyl-3-(2-oxo-2-propoxyethyl)imidazolium	5.13	2.76	0.82	1.26	-2.57
46	[N+]1(C)=C(C)N(C=C1)CC(=O)OCCCCC	1,2-Dimethyl-3-[2-oxo-2-(pentyloxy)ethyl]imidazolium	2.60	3.30	0.45	1.76	-2.70
47	CCCn1cc[n+](c1C)C	1,2-dimethyl-3-propylimidazolium	1.81	-6.77	2.84	0.66	-0.92
48	[N+]1(COCCCC)=CN(C=C1)COCCCC	1,3-Bis(butoxymethyl)imidazolium	-0.46	2.39	-1.08	3.65	-0.28
49	[N+]1(COCCC)=CN(C=C1)COCCC	1,3-Bis(propoxymethyl)imidazolium	1.60	2.22	-0.33	2.43	0.25
50	[N+]1(COCCCCCCCCCC)=CN(C=C1)COCCCCCCCCCC	1,3-Bis[(decyloxy)methyl]imidazolium	-12.39	4.91	-2.50	3.87	0.83
51	[N+]1(COCCCCCCCCCCCC)=CN(C=C1)COCCCCCCCCCCCC	1,3-Bis[(dodecyloxy)methyl]imidazolium	-16.24	6.96	-2.08	3.57	0.63
52	[N+]1(COCCCCCCC)=CN(C=C1)COCCCCCCC	1,3-Bis[(heptyloxy)methyl]imidazolium	-6.51	3.95	-2.25	3.80	0.56
53	[N+]1(COCCCCCCCCCCCCCCCC)=CN(C=C1)COCCCCCCCCCCCCCCCC	1,3-Bis[(hexadecyloxy)methyl]imidazolium	-21.63	9.04	-1.98	3.39	2.77
54	[N+]1(COCCCCCC)=CN(C=C1)COCCCCCC	1,3-Bis[(hexyloxy)methyl]imidazolium	-4.54	3.90	-1.41	3.31	-0.06
55	[N+]1(COCCCCCCCCC)=CN(C=C1)COCCCCCCCCC	1,3-Bis[(nonyloxy)methyl]imidazolium	-10.86	5.16	-1.92	3.61	0.67

56	[N+]1(COCCCCCCCCC)=CN(C=C1)COCCCCCCCC	1,3-Bis[(octyloxy)methyl]imidazolium	-8.29	4.70	-2.62	3.95	0.51
57	[N+]1(COCCCCC)=CN(C=C1)COCCCCC	1,3-Bis[(pentyloxy)methyl]imidazolium	-2.37	3.08	-1.21	3.28	0.15
58	[N+]1(COCCCCCCCCCCCCCCC)=CN(C=C1)COCCCCCCCCCCCCCCC	1,3-Bis[(tetradecyloxy)methyl]imidazolium	-19.66	8.67	-3.30	4.57	1.51
59	[N+]1(COCCCCCCCCCCC)=CN(C=C1)COCCCCCCCCCC	1,3-Bis[(undecyloxy)methyl]imidazolium	-14.03	6.14	-3.22	4.48	0.64
60	[N+]1(CCCC)=CN(C=C1)CCCC	1,3-Dibutylimidazolium	-2.22	-5.41	1.53	1.53	-0.31
61	[N+]1(CCCCCCCCCC)=C(C)N(C=C1)CCCCCCCCC	1,3-Didecyl-2-methylimidazolium	-13.99	-1.46	0.53	1.86	2.47
62	[N+]1(CC)=CN(C=C1)CC	1,3-Diethylimidazolium	2.03	-6.56	1.57	1.51	-0.99
63	[N+]1(CCCCCC)=CN(C=C1)CCCCCC	1,3-Dihexylimidazolium	-6.81	-4.32	1.77	1.22	1.01
64	[N+]1(C)=CN(C)C=C1	1,3-Dimethylimidazolium	4.18	-6.87	0.65	1.98	-1.80
65	[N+]1(CCCCC)=CN(C=C1)CCCCC	1,3-Dipentylimidazolium	-4.42	-4.59	1.39	1.41	0.75
66	[N+]1(CCC)=CN(C=C1)CCC	1,3-Dipropylimidazolium	-0.15	-5.93	1.74	1.28	-0.21
67	[NH+]1=CN(C=C1)COCCCCCCCCCC	1-[(Decyloxy)methyl]imidazolium	-5.09	0.97	-9.44	-3.89	-0.65
68	[n+]1(cccc2cc(C)ccc12)COCCCCCCCCCC	1-[(Decyloxy)methyl]-6-methylquinolinium	-8.33	-0.33	2.01	-0.49	0.96
69	[n+]1(cccc2cccc(O)c12)COCCCCCCCCCC	1-[(Decyloxy)methyl]-8-hydroxyquinolinium	-4.64	2.67	2.11	-0.97	2.53
70	[n+]1(cccc2ccccc12)COCCCCCCCCCC	1-[(Decyloxy)methyl]quinolinium	-7.56	-0.68	2.47	-0.62	1.53
71	[NH+]1=CN(C=C1)COCCCCCCCCCCCC	1-[(Dodecyloxy)methyl]imidazolium	-7.33	2.17	-9.65	-4.12	0.13
72	[n+]1(cccc2cc(C)ccc12)COCCCCCCCCCCCC	1-[(Dodecyloxy)methyl]-6-methylquinolinium	-10.30	0.77	1.45	0.40	1.01
73	[n+]1(cccc2cccc(O)c12)COCCCCCCCCCCCC	1-[(Dodecyloxy)methyl]-8-hydroxyquinolinium	-7.05	3.58	1.77	-1.52	3.02
74	[n+]1(cccc2ccccc12)COCCCCCCCCCCCC	1-[(Dodecyloxy)methyl]quinolinium	-9.13	0.23	2.06	-0.80	1.46
75	[NH+]1=CN(C=C1)COCCCCCCC	1-[(Heptyloxy)methyl]imidazolium	-1.75	0.26	-9.61	-3.55	-0.93
76	[n+]1(cc(O)ccc1)COCCCCCCC	1-[(Heptyloxy)methyl]-3-hydroxypyridinium	4.71	3.35	1.30	1.26	2.71
77	[NH+]1=CN(C=C1)COCCCCCC	1-[(Hexyloxy)methyl]imidazolium	-0.43	0.45	-9.42	-3.76	-1.21
78	[n+]1(cc(O)ccc1)COCCCCCC	1-[(Hexyloxy)methyl]-3-hydroxypyridinium	5.49	3.42	1.24	1.23	3.06
79	[n+]1(cccc2cc(C)ccc12)COCCCCCC	1-[(Hexyloxy)methyl]-6-methylquinolinium	-3.71	-1.36	2.43	-0.72	-0.06
80	[n+]1(cccc2cccc(O)c12)COCCCCCC	1-[(Hexyloxy)methyl]-8-hydroxyquinolinium	-0.56	0.61	4.16	-2.65	1.01
81	[n+]1(cccc2ccccc12)COCCCCCC	1-[(Hexyloxy)methyl]quinolinium	-3.19	-1.99	3.20	-1.15	0.26
82	[NH+]1=CN(C=C1)COCCCCCCCCC	1-[(Nonyloxy)methyl]imidazolium	-4.56	0.87	-8.72	-4.46	-0.49
83	[NH+]1=CN(C=C1)COCCCCCCCC	1-[(Octyloxy)methyl]imidazolium	-2.94	0.97	-9.30	-3.78	-0.63
84	[n+]1(cccc2ccccc12)COCCCCCCCC	1-[(Octyloxy)methyl]quinolinium	-5.27	-1.84	2.22	-0.10	0.66
85	[NH+]1=CN(C=C1)COCCCCC	1-[(Pentyloxy)methyl]imidazolium	0.12	-0.39	-8.73	-4.18	-1.24

86	[NH+]1=CN(C=C1)COCCCCCCCCCCC	1-[(Undecyloxy)methyl]imidazolium	-6.60	1.67	-9.05	-4.06	-0.50
87	[N+]1(C)=CN(C=C1)C(C(=O)OCCCC)c1ccc2OCOc2c1	1-[1-(1,3-Benzodioxol-5-yl)-2-butoxy-2-oxoethyl]-3-methylimidazolium	0.12	7.31	1.19	2.24	-4.78
88	[n+]1(ccccc1)C(C(=O)OCCCC)c1ccc2OCOc2c1	1-[1-(1,3-Benzodioxol-5-yl)-2-butoxy-2-oxoethyl]pyridinium	-0.04	6.08	1.97	1.50	-4.27
89	[N+]1(C)=CN(C=C1)C(C(=O)OC)c1ccc2OCOc2c1	1-[1-(1,3-Benzodioxol-5-yl)-2-methoxy-2-oxoethyl]-3-methylimidazolium	2.18	6.00	3.93	-0.16	-6.28
90	[n+]1(ccccc1)C(C(=O)OC)c1ccc2OCOc2c1	1-[1-(1,3-Benzodioxol-5-yl)-2-methoxy-2-oxoethyl]pyridinium	3.15	5.90	2.96	0.51	-4.03
91	[n+]1(ccccc1)C(C(=O)OC)c1cc(OC)c(OC)cc1	1-[1-(3,4-Dimethoxyphenyl)-2-methoxy-2-oxoethyl]pyridinium	2.48	4.98	2.05	1.69	-4.39
92	[N+]1(C)=CN(C=C1)CCOCCOC	1-[2-(2-Methoxyethoxy)ethyl]-3-methylimidazolium	5.30	1.60	0.58	1.08	0.99
93	[N+]1(C)=CN(C=C1)CC(=O)NCCCC	1-[2-(Butylamino)-2-oxoethyl]-3-methylimidazolium	2.91	2.71	3.36	-1.67	-1.72
94	[N+]1(C)=CN(C=C1)CC(=O)N(C)CCCC	1-[2-(Butylmethylamino)-2-oxoethyl]-3-methylimidazolium	2.43	1.73	1.93	0.17	-1.17
95	[N+]1(C)=CN(C=C1)CC(=O)N(CC)CC	1-[2-(Diethylamino)-2-oxoethyl]-3-methylimidazolium	3.60	1.16	2.52	-0.30	-1.47
96	[N+]1(C)=CN(C=C1)CC(=O)OCCCCCC	1-[2-(Hexyloxy)-2-oxoethyl]-3-methylimidazolium	1.62	2.95	-0.77	2.59	-2.31
97	[N+]1(C)=CN(C=C1)CCC1=CC[C@@H]2C(C)(C)[C@H]1C2	1-[2-[(1R,5S)-6,6-Dimethylbicyclo[3.1.1]hept-2-en-2-yl]ethyl]-3-methylimidazolium	-3.71	-4.44	1.54	1.20	1.21
98	[N+]1(C)=CN(C=C1)CC(=O)OC(C(=O)OCCCC)c1ccc2OCOc2c1	1-[2-[1-(1,3-Benzodioxol-5-yl)-2-butoxy-2-oxoethoxy]-2-oxoethyl]-3-methylimidazolium	-1.26	12.75	4.21	0.45	-9.43
99	[n+]1(ccccc1)CC(=O)OC(C(=O)OCCCC)c1ccc2OCOc2c1	1-[2-[1-(1,3-Benzodioxol-5-yl)-2-butoxy-2-oxoethoxy]-2-oxoethyl]pyridinium	-4.31	12.32	4.51	-0.39	-7.74
100	[n+]1(ccccc1)CC(=O)OC(C(=O)OC)c1ccc2OCOc2c1	1-[2-[1-(1,3-Benzodioxol-5-yl)-2-methoxy-2-oxoethoxy]-2-oxoethyl]pyridinium	-0.87	11.80	5.15	-1.25	-8.30
101	CN1C=C[N+](=C1)CC2=CC=CC=C2	1-Benzyl-3-methylimidazolium	-0.83	-6.52	3.35	-0.20	-1.72
102	[N+]1(CC)(CCCC1)CCCC	1-Butyl-1-ethylpyrrolidinium	1.25	-3.90	-3.89	5.76	0.08
103	[NH+]1=CN(C=C1)CCCC	1-Butylimidazolium	1.00	-4.97	-6.24	-6.11	-1.76
104	[N+]1(C)(CCCCC1)CCCC	1-Butyl-1-methylpiperidinium	1.15	-3.97	-3.95	5.81	-0.09
105	[N+]1(C)(CCCC1)CCCC	1-Butyl-1-methylpyrrolidinium	1.96	-4.12	-3.78	5.67	-0.03
106	[N+]1(C)=C(C)N(C=C1)CCCC	1-Butyl-2,3-dimethylimidazolium	1.01	-5.58	0.95	1.99	-0.19
107	[n+]1(c(C)cccc1)CCCC	1-Butyl-2-methylpyridinium	0.27	-6.91	3.51	0.08	-0.72
108	[n+]1(cc(C)c(C)cc1)CCCC	1-Butyl-3,4-dimethylpyridinium	-1.83	-6.48	3.18	-0.01	-0.44
109	[n+]1(cc(C)cc(C)c1)CCCC	1-Butyl-3,5-dimethylpyridinium	-3.35	-6.65	3.68	-0.65	0.01
110	[n+]1(cc(C(=O)NCCCC)ccc1)CCCC	1-Butyl-3-[(butylamino)carbonyl]pyridinium	-0.50	1.56	3.74	-1.41	-2.27
111	[N+]1(CC)=CN(C=C1)CCCC	1-Butyl-3-ethylimidazolium	-0.12	-5.99	1.68	1.39	-0.48
112	[N+]1(C)=CN(C=C1)CCCC	1-Butyl-3-methylimidazolium	0.58	-5.91	1.21	1.20	-0.39
113	[n+]1(cc(C)ccc1)CCCC	1-Butyl-3-methylpyridinium	-1.02	-6.72	3.14	0.02	-0.45
114	[n+]1(ccc(N(C)C)cc1)CCCC	1-Butyl-4-(dimethylamino)pyridinium	-0.73	-6.95	4.30	-1.12	-1.38

115	[n+]1(ccc(C)cc1)CCCC	1-Butyl-4-methylpyridinium	-0.22	-6.95	3.85	-0.06	-0.45
116	[n+]1(ccccc1)CCCC	1-Butylpyridinium	0.96	-6.71	2.76	0.70	-0.52
117	[n+]1(cccc2ccccc12)CCCC	1-Butylquinolinium	-3.22	-7.41	6.68	-2.67	-0.32
118	[NH+]1=CN(C=C1)CCCCCCCCCC	1-Decylimidazolium	-5.78	-2.89	-7.12	-5.67	0.06
119	[N+]1(CC)=CN(C=C1)CCCCCCCCCC	1-Decyl-3-ethylimidazolium	-6.83	-4.25	2.07	0.24	1.15
120	[N+]1(C)=CN(C=C1)CCCCCCCCCC	1-Decyl-3-methylimidazolium	-5.83	-4.13	1.06	0.96	1.33
121	[n+]1(ccccc1)CCCCCCCCCC	1-Decylpyridinium	-5.41	-4.43	2.31	0.46	1.66
122	[N+]1(CCCCCCCCCCCC)(CCCC1)CCO	1-Dodecyl-1-(2-hydroxyethyl)pyrrolidinium	-2.02	6.35	-2.97	0.68	3.83
123	[NH+]1=CN(C=C1)CCCCCCCCCCCC	1-Dodecylimidazolium	-7.34	-2.19	-7.84	-5.07	-0.29
124	[N+]1(C)=CN(C=C1)CCCCCCCCCCCC	1-Dodecyl-3-methylimidazolium	-7.55	-3.29	0.51	1.23	1.51
125	[NH+]1=CN(C=C1)CC	1-Ethylimidazolium	3.99	-5.53	-6.71	-5.77	-2.93
126	[N+]1(C)(CCCC1)CC	1-Ethyl-1-methylpyrrolidinium	4.57	-4.49	-4.03	5.55	0.10
127	[N+]1(CC)=CN(C=C1)CCCCCC	1-Ethyl-3-hexylimidazolium	-2.72	-5.19	1.84	0.95	0.87
128	[N+]1(C)=CN(C=C1)CC	1-Ethyl-3-methylimidazolium	3.24	-6.75	0.93	1.70	-1.60
129	[N+]1(CC)=CN(C=C1)CCC	1-Ethyl-3-propylimidazolium	1.10	-6.31	1.51	1.58	-0.99
130	[n+]1(ccccc1)CC	1-Ethylpyridinium	3.56	-7.36	2.26	1.22	-1.59
131	[NH+]1=CN(C=C1)CCCCCCC	1-Heptylimidazolium	-2.69	-4.01	-6.24	-6.38	-0.74
132	[N+]1(C)=CN(C=C1)CCCCCCC	1-Heptyl-3-methylimidazolium	-2.66	-4.82	0.99	1.12	0.77
133	[N+]1(CCCCCCCCCCCCCCCC)=C(C)N(C=C1)CCO	1-Hexadecyl-3-(2-hydroxyethyl)-2-methylimidazolium	-7.84	5.39	0.95	-2.31	4.75
134	[N+]1(C)=CN(C=C1)CCCCCCCCCCCCCCCC	1-Hexadecyl-3-methylimidazolium	-11.34	-2.14	0.02	1.34	2.01
135	[n+]1(ccccc1)CCCCCCCCCCCCCCCC	1-Hexadecylpyridinium	-11.79	-2.66	2.50	0.08	3.09
136	[NH+]1=CN(C=C1)CCCCCC	1-Hexylimidazolium	-1.08	-4.19	-6.92	-5.73	-1.42
137	[N+]1(C)(CCCC1)CCCCCC	1-Hexyl-1-methylpyrrolidinium	0.02	-3.63	-3.89	5.63	0.25
138	[N+]1(C)=C(C)N(C=C1)CCCCCC	1-Hexyl-2,3-dimethylimidazolium	-2.67	-6.14	4.17	-0.99	0.57
139	[N+]1(C)=CN(C=C1)CCCCCC	1-Hexyl-3-methylimidazolium	-1.54	-5.78	1.66	0.51	-0.75
140	[n+]1(cc(C)ccc1)CCCCCC	1-Hexyl-3-methylpyridinium	-3.03	-5.66	2.50	0.25	0.50
141	[n+]1(ccc(C)cc1)CCCCCC	1-Hexyl-4-methylpyridinium	-2.88	-5.97	3.94	-0.40	1.13
142	[n+]1(ccccc1)CCCCCC	1-Hexylpyridinium	-0.95	-5.90	2.50	0.55	0.12
143	[n+]1(cccc2ccccc12)CCCCCC	1-Hexylquinolinium	-5.56	-6.58	6.69	-2.83	0.73
144	[N+]1(CC)=C(CCCCCCCC=CCCCCCCCC)N(CC1)CCO	1-Ethyl-2-(8-heptadecenyl)-4,5-dihydro-3-(2-hydroxyethyl)imidazolium	-12.25	6.23	-6.24	-8.83	3.20

145	[NH+]1=CN(C=C1)C	1-Methylimidazolium	5.03	-5.69	-6.83	-6.30	-3.04
146	[N+]1(C)(CCCC1)CCCCCCCC	1-Methyl-1-octylpyrrolidinium	-2.33	-3.03	-3.71	5.36	0.63
147	[N+]1(C)(CCCCC1)CCC	1-Methyl-1-propylpiperidinium	2.18	-4.18	-3.94	5.90	-0.26
148	[N+]1(C)(CCCC1)CCC	1-Methyl-1-propylpyrrolidinium	3.13	-4.34	-3.85	5.63	-0.10
149	[N+]1(C)=CN(C=C1)CC(C)C	1-Methyl-3-(2-methylpropyl)imidazolium	1.42	-5.98	0.77	1.78	-0.34
150	[N+]1(C)=CN(C=C1)CC(=O)OCCC	1-Methyl-3-(2-oxo-2-propoxyethyl)imidazolium	4.93	1.96	-0.19	1.96	-2.50
151	[N+]1(C)=CN(C=C1)CCc1ccccc1	1-Methyl-3-(2-phenylethyl)imidazolium	-3.43	-6.10	4.96	-1.28	0.61
152	[N+]1(C)=CN(C=C1)CC=C	1-Methyl-3-(2-propenyl)imidazolium	1.49	-6.89	2.60	0.50	-0.78
153	[N+]1(C)=CN(C=C1)CCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	1-Methyl-3-(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)imidazolium	1.89	7.73	-2.78	3.01	0.18
154	[N+]1(C)=CN(C=C1)CCC(=O)C	1-Methyl-3-(3-oxobutyl)imidazolium	5.91	1.45	2.73	-1.85	0.18
155	[N+]1(C)=CN(C=C1)Cc1ccc(cc1)C	1-Methyl-3-(4-methylphenylmethyl)imidazolium	-1.72	-6.38	3.34	-0.01	-1.50
156	[N+]1(C)=CN(C=C1)Cc1ccccc1	1-Methyl-3-(phenylmethyl)imidazolium	-0.98	-6.53	3.48	-0.20	-1.45
157	[N+]1(C)=CN(C=C1)CC(=O)OCCCCCCCC	1-Methyl-3-[2-(octyloxy)-2-oxoethyl]imidazolium	-1.30	2.89	0.41	1.89	-1.69
158	[N+]1(C)=CN(C=C1)CC(=O)OCCCCC	1-Methyl-3-[2-oxo-2-(pentyloxy)ethyl]imidazolium	2.15	2.70	-0.08	2.28	-2.61
159	[N+]1(C)=CN(C=C1)CCCCCCCCC	1-Methyl-3-nonylimidazolium	-4.95	-4.26	1.20	0.99	1.25
160	[N+]1(C)=CN(C=C1)CCCCCCCCCCCCCCCCCC	1-Methyl-3-octadecylimidazolium	-13.76	-1.31	-0.02	1.21	2.84
161	[N+]1(C)=CN(C=C1)CCCCCCCC	1-Methyl-3-octylimidazolium	-3.07	-4.67	0.46	1.44	0.28
162	[N+]1(C)=CN(C=C1)CCCCC	1-Methyl-3-pentylimidazolium	-0.64	-5.56	1.33	1.08	0.30
163	[N+]1(C)=CN(C=C1)CCC	1-Methyl-3-propylimidazolium	1.85	-6.45	1.37	1.24	-0.80
164	[N+]1(C)=CN(C=C1)CCCCCCCCCCCCCC	1-Methyl-3-tetradecylimidazolium	-9.86	-2.51	0.38	1.23	2.54
165	[NH+]1=CN(C=C1)CCCCCCCCC	1-Nonylimidazolium	-4.64	-3.28	-6.83	-6.04	-0.24
166	[NH+]1=CN(C=C1)CCCCCCCC	1-Octylimidazolium	-3.55	-3.47	-6.97	-6.04	-0.63
167	[n+]1(ccccc1)CCCCCCCC	1-Octylpyridinium	-3.41	-5.10	2.61	0.39	1.43
168	[n+]1(cccc2ccccc12)CCCCCCCC	1-Octylquinolinium	-7.55	-5.95	6.77	-3.00	1.19
169	[NH+]1=CN(C=C1)CCCCC	1-Pentylimidazolium	-0.48	-4.65	-6.13	-6.17	-1.31
170	[n+]1(ccccc1)CCCCC	1-Pentylpyridinium	-0.24	-6.22	2.71	0.59	0.14
171	[NH+]1=CN(C=C1)CCC	1-Propylimidazolium	2.28	-5.50	-5.68	-6.45	-2.21
172	[n+]1(ccccc1)CCC	1-Propylpyridinium	1.68	-7.24	3.58	0.18	-0.27
173	[NH+]1=CN(C=C1)CCCCCCCCCCC	1-Undecylimidazolium	-6.55	-2.51	-7.31	-5.72	-0.03
174	[N+]1(C)=CN(C=C1)CCCC(=O)O	3-(3-Carboxypropyl)-1-methylimidazolium	10.77	5.41	3.56	-2.44	0.51

175	[n+]1(cc(C(=O)N)ccc1)COC1CCCCCCCCCCC1	3-(Aminocarbonyl)-1-[(cyclododecyloxy)methyl]pyridinium	-1.11	8.51	2.67	-2.27	-1.31
176	[n+]1(cc(C(=O)N)ccc1)COCCCCCCCCCC	3-(Aminocarbonyl)-1-[(decyloxy)methyl]pyridinium	-1.45	8.05	2.07	-2.56	-0.26
177	[n+]1(cc(C(=O)N)ccc1)COCCCCCCCCCCCC	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium	-3.72	9.72	2.10	-2.74	0.54
178	[n+]1(cc(C(=O)N)ccc1)COCCCCCCCCCCC	3-(Aminocarbonyl)-1-[(undecyloxy)methyl]pyridinium	-3.36	8.53	2.80	-2.69	-0.26
179	[n+]1(cc(C(=O)OCCCC)ccc1)CCCC	3-(Butoxycarbonyl)-1-butylpyridinium	-0.63	1.72	1.77	0.78	-1.80
180	[n+]1(cc(C(=O)OCCCC)ccc1)C	3-(Butoxycarbonyl)-1-methylpyridinium	2.74	1.39	1.45	0.46	-2.32
181	[n+]1(cc(C(=O)NCOCOCCCCCCCCCC)ccc1)COCCCCCCCCCC	3-[[[[(Decyloxy)methoxy]methyl]amino]carbonyl]-1-[(decyloxy)methyl]pyridinium	-14.01	15.45	3.67	-0.31	-4.11
182	[n+]1(cc(C(=O)NCOCOCCCCCCC)ccc1)COCCCCCCC	3-[[[[(Heptyloxy)methoxy]methyl]amino]carbonyl]-1-[(heptyloxy)methyl]pyridinium	-8.10	11.70	3.19	0.15	-1.79
183	[n+]1(cc(C(=O)NCOCOCCCCCCCCC)ccc1)COCCCCCCCCC	3-[[[[(Nonyloxy)methoxy]methyl]amino]carbonyl]-1-[(nonyloxy)methyl]pyridinium	-11.41	14.87	2.97	0.32	-6.01
184	[n+]1(cc(C(=O)NCOCOCCCCCCCC)ccc1)COCCCCCCCC	3-[[[[(Octyloxy)methoxy]methyl]amino]carbonyl]-1-[(octyloxy)methyl]pyridinium	-9.18	13.37	1.88	0.56	-3.29
185	[n+]1(cc(O)ccc1)COCCC	3-Hydroxy-1-(propoxymethyl)pyridinium	9.04	2.53	1.71	1.07	2.30
186	[n+]1(cc(O)ccc1)COCCCCCCCCCCCCCCCCCC	3-Hydroxy-1-[(octadecyloxy)methyl]pyridinium	-7.03	6.97	-0.02	0.65	4.92
187	[n+]1(cc(O)ccc1)COCCCCCCCCCCC	3-Hydroxy-1-[(undecyloxy)methyl]pyridinium	-0.18	4.26	1.07	0.69	4.01
188	[n+]1(cc(C)ccc1)CCCCCCCC	3-Methyl-1-octylpyridinium	-5.44	-5.13	2.92	-0.28	1.42
189	[n+]1(cc(C)ccc1)CCC	3-Methyl-1-propylpyridinium	0.18	-7.09	3.15	0.16	-0.85
190	[N+]1(C)(CCOCC1)CCOCC	4-(2-Ethoxyethyl)-4-methylmorpholinium	8.20	2.70	-2.65	4.89	0.06
191	[N+]1(C)(CCOCC1)CCO	4-(2-Hydroxyethyl)-4-methylmorpholinium	13.05	7.64	-1.48	2.13	2.17
192	[N+]1(C)(CCOCC1)CCOC	4-(2-Methoxyethyl)-4-methylmorpholinium	9.02	2.70	-2.46	5.23	-0.32
193	[N+]1(C)(CCOCC1)CCCO	4-(3-Hydroxypropyl)-4-methylmorpholinium	12.12	7.62	-1.88	2.42	2.48
194	[N+]1(C)(CCOCC1)CCCOC	4-(3-Methoxypropyl)-4-methylmorpholinium	7.79	2.32	-2.66	5.24	-0.19
195	[n+]1(ccc(C(=O)N)cc1)COCCCCCCCCCC	4-(Aminocarbonyl)-1-[(decyloxy)methyl]pyridinium	-0.84	8.71	2.60	-2.76	0.20
196	[n+]1(ccc(C(=O)N)cc1)COCCCCCCCCCCCC	4-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium	-3.23	9.40	3.02	-3.16	0.39
197	[n+]1(ccc(C(=O)N)cc1)COCCCCCCCCCC	4-(Aminocarbonyl)-1-[(undecyloxy)methyl]pyridinium	-1.97	9.29	2.71	-2.72	0.30
198	[N+]1(C)(CCOCC1)CC#N	4-(Cyanomethyl)-4-methylmorpholinium	9.29	3.51	-1.23	1.82	-0.65
199	[n+]1(ccc(N(C)C)cc1)CC	4-(Dimethylamino)-1-ethylpyridinium	1.55	-7.82	4.30	-1.27	-2.67
200	[n+]1(ccc(N(C)C)cc1)CCCCCC	4-(Dimethylamino)-1-hexylpyridinium	-3.42	-6.49	5.27	-1.90	-0.04
201	[n+]1(ccc(N(C)C)cc1)C	4-(Dimethylamino)-1-methylpyridinium	1.97	-8.24	4.64	-1.89	-2.88
202	[N+]1(C)(CCOCC1)COCC	4-(Ethoxymethyl)-4-methylmorpholinium	8.27	2.53	-3.27	4.62	-0.47

203	[N+]1(C)(CCOCC1)CCCC	4-Butyl-4-methylmorpholinium	6.23	0.06	-3.73	3.90	0.91
204	[N+]1(C)(CCOCC1)CC	4-Ethyl-4-methylmorpholinium	8.90	-0.32	-3.78	4.51	0.50
205	[n+]1(ccc(C)cc1)CCCCCCCC	4-Methyl-1-octylpyridinium	-4.69	-5.10	3.21	0.18	1.30
206	[n+]1(cccc2cc(C)ccc12)COCCCCCCCC	6-Methyl-1-[(octyloxy)methyl]quinolinium	-6.17	-0.01	1.74	-0.12	0.87
207	[n+]1(cccc2cccc(O)c12)COCCCCCCCC	8-Hydroxy-1-[(octyloxy)methyl]quinolinium	-2.66	1.72	3.00	-1.66	2.18
208	[nH+]1ccccc1	Pyridinium	3.78	-5.25	-7.66	-7.06	-2.26
209	[n+]1(cc(C)cc(C)c1)CCCCCCCC	1-Octyl-3,5-dimethylpyridinium	-7.40	-4.91	2.82	-0.43	1.31
210	c1c[nH+]c[nH]1	Imidazolium	7.34	-3.31	-7.65	-5.38	-2.63
211	CCCCCCn1cc[n+](c1C)C	1-Hexyl-2,3-dimethyl imidazolium	-2.23	-6.01	3.61	-0.45	0.11
212	[N+]1(CCO)=CN(C=C1)CCc2=cc=cc=c2	1-(2-Hydroxyethyl)-3-(2-phenylethyl)imidazolium	2.41	2.66	3.93	-4.66	3.40
213	[N+]1(C)=C(C)N(C=C1)CC(CO)O	1,2-Dimethyl-3-glycerylimidazolium	12.79	9.75	2.58	-6.27	5.14
214	[N+]1(CCO)=CN(C=C1)CCO	1,3-Di-(2-hydroxyethyl)imidazolium	11.50	9.67	5.76	-7.07	5.63
215	[N+]1(Cc2=cc=cc=c2)=CN(C=C1)CCCC	1-Benzyl-3-butylimidazolium	-4.16	-5.71	3.48	-0.32	-0.57
216	[N+]1(CCCC)=CN(C=C1)CCO	1-Butyl-3-(2-hydroxyethyl)imidazolium	6.56	2.86	1.24	-2.46	1.82
217	[N+]1(C)=CN(C=C1)CC(CO)O	1-Methyl-3-glycerylimidazolium	12.59	9.92	2.10	-6.03	2.96
218	C1C[N+]2(CCCCCC)CCN1CC2	1-Hexyl-1,4-diaza[2.2.2]bicyclooctanium	3.71	0.96	-4.42	2.25	-1.41

Table B2 List of the 38 anions with their SMILES codes and PPs- values.

entry	SMILES codes	Anions	PP1-	PP2-	PP3-	PP4-	PP4-
1	[Cl-]	Cl^-	-0.57	-5.73	-2.31	-1.25	-2.00
2	[Br-]	Br^-	-0.52	-5.52	-2.16	-1.13	-1.78
3	[I-]	I^-	-0.65	-5.31	-1.63	-1.12	-1.96
4	[B-](C#N)(C#N)(C#N)C#N	$B(CN)_4^-$	-10.53	7.57	-0.53	-2.02	-0.65
5	[B-](F)(F)(F)F	BF_4^-	1.67	-0.06	-0.33	-3.83	1.25
6	[B-]12(OC(=O)C(=O)O1)OC(=O)C(=O)O2	bis(ethanedioato-O1,O2)borate	4.60	5.52	0.02	-0.26	-2.85
7	[C-](C#N)(C#N)C#N	$C(CN)_3^-$	-13.16	6.89	-1.96	-0.13	0.76
8	[C-](S(=O)(=O)C(F)(F)F)(S(=O)(=O)C(F)(F)F)S(=O)(=O)C(F)(F)F	tris[(trifluoromethyl)sulfonyl]methide	-0.58	-1.39	3.93	0.50	-1.52
9	[N-](C(F)(F)F)C(F)(F)F	$N(CF3)_2^-$	1.11	-1.38	-0.04	-2.50	0.94

10	[N-](C#N)C#N	$N(CN)_2^-$	-2.48	0.49	0.00	0.73	2.81
11	[N-](S(=O)(=O)C(F)(F)F)S(=O)(=O)C(F)(F)F	1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	-1.19	-2.15	2.86	2.10	0.77
12	[N-]1C(=O)C=C(C)OS1(=O)=O	6-methyl-2,2-dioxo-1,2,3-oxathiazin-4(3H)-onate	0.38	-0.22	0.92	2.67	2.80
13	[N-]1C(=O)c2ccccc2S1(=O)=O	1,2-benzisothiazol-3(2H)-one	-0.91	-0.17	1.38	3.13	1.57
14	[O-][Cl](=O)(=O)=O	ClO_4^-	2.67	3.01	-0.12	-1.50	1.98
15	[O-]C(=O)[C@H](C)O	2-(*S*)-hydroxypropanoate	4.81	4.31	-4.51	3.25	-1.97
16	[O-]C(=O)C	CH_3COO^-	4.20	2.41	-5.87	3.73	-0.53
17	[O-]C(=O)C(C)O	2-(*R*)-hydroxypropanoate	4.48	3.75	-4.18	2.80	-1.68
18	[O-]C(=O)C(F)(F)F	CF_3COO-	3.18	2.08	-2.30	-0.22	0.57
19	[O-]N(=O)=O	NO_3^-	-6.94	-0.46	-2.37	-1.73	-0.41
20	[O-]P(=O)(C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)F	bis(pentafluoroethyl)phosphinate	1.54	0.08	2.75	-1.62	-0.42
21	COP(=O)([O-])OC	dimethylphosphate	1.30	-1.22	0.20	-0.78	-0.66
22	[O-]S(=O)(=O)C	methanesulfonate	1.32	-1.45	-0.86	-1.35	1.00
23	[O-]S(=O)(=O)C(F)(F)C(F)(F)F	perfluoro ethanesulfonate	1.52	-0.48	1.03	-2.17	0.81
24	[O-]S(=O)(=O)C(F)(F)F	trifluoromethanesulfonate	1.41	-0.86	0.07	-2.60	1.12
25	[O-]S(=O)(=O)c1ccc(C)cc1	4-methylbenzenesulfonate	-1.66	-1.59	2.48	3.83	2.16
26	[O-]S(=O)(=O)O	HSO_4^-	2.60	1.36	-1.42	-2.11	0.90
27	[O-]S(=O)(=O)OC	methylsulfate	1.36	-1.16	-0.44	-1.31	0.92
28	[O-]S(=O)(=O)OCC	ethyl sulfate	1.13	-1.47	-0.18	-0.39	0.43
29	[O-]S(=O)(=O)OCCCCCCCC	octyl sulfate	-1.48	-1.82	3.86	4.62	0.92
30	[O-]S(=O)(=O)OCCOCCOC	2-(2-methoxyethoxy)ethylsulfate	1.54	0.57	3.67	1.93	1.19
31	[P-](F)(F)(F)(F)(F)F	PF_6^-	1.13	-1.14	-0.21	-3.53	0.83
32	[P-](F)(F)(F)(C(F)(F)C(F)(F)F)(C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)F	$(C_2F_5)_3\ PF_3^-$	2.83	3.03	4.77	-1.46	-1.31
33	[P-](F)(F)(F)(C(F)(F)C(F)(F)C(F)(F)F)(C(F)(F)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)F	$(C_3F_7)_3PF_3^-$	4.00	5.68	6.72	-0.31	-2.96
34	[S-]C#N	SCN^-	0.65	-2.07	-3.10	1.46	2.84
35	[Cl-]([Al](Cl)(Cl)Cl)[Al](Cl)(Cl)Cl	$[Al_2Cl_7]^-$	-5.66	-3.72	1.43	2.02	-3.96
36	[Co-@TH1](C#[O])(C#[O])(C#[O])C#[O]	$[Co(CO)_4]^-$	-0.43	-2.12	-1.00	3.57	0.29
37	[Fe-](Cl)(Cl)(Cl)Cl	$[FeCl_4]^-$	-4.01	-4.57	-0.46	0.67	-3.04
38	[Sb-@OH1](F)(F)(F)(F)(F)F	SbF_6^-	1.35	-0.70	-0.12	-3.68	0.86

Table B3 The 403 heterocyclic ILs used in PCA on overall toxicity.

	Name
1	1-Methylimidazoliumhydrogen tetrafluoroborate
2	1-Methylimidazolium 2-hydroxypropanoate
3	1-Methylimidazolium (2S)-2-hydroxypropanoate
4	1-Decylimidazolium 2-hydroxypropanoate
5	1-Decylimidazolium (2S)-2-hydroxypropanoate
6	1-Undecylimidazolium 2-hydroxypropanoate
7	1-Undecylimidazolium (2S)-2-hydroxypropanoate
8	1-Dodecylimidazolium 2-hydroxypropanoate
9	1-Dodecylimidazolium (2S)-2-hydroxypropanoate
10	1-[(Decyloxy)methyl]imidazolium 2-hydroxypropanoate
11	1-[(Decyloxy)methyl]imidazolium (2S)-2-hydroxypropanoate
12	1-[(Undecyloxy)methyl]imidazolium 2-hydroxypropanoate
13	1-[(Undecyloxy)methyl]imidazolium (2S)-2-hydroxypropanoate
14	1-[(Dodecyloxy)methyl]imidazolium 2-hydroxypropanoate
15	1-[(Dodecyloxy)methyl]imidazolium (2S)-2-hydroxypropanoate
16	1-(Butoxymethyl)imidazolium 2-hydroxypropanoate
17	1-(Butoxymethyl)imidazolium (2S)-2-hydroxypropanoate
18	1-[(Pentyloxy)methyl]imidazolium 2-hydroxypropanoate
19	1-[(Pentyloxy)methyl]imidazolium (2S)-2-hydroxypropanoate
20	1-[(Hexyloxy)methyl]imidazolium 2-hydroxypropanoate
21	1-[(Hexyloxy)methyl]imidazolium (2S)-2-hydroxypropanoate
22	1-[(Heptyloxy)methyl]imidazolium 2-hydroxypropanoate
23	1-[(Heptyloxy)methyl]imidazolium (2S)-2-hydroxypropanoate
24	1-[(Octyloxy)methyl]imidazolium 2-hydroxypropanoate
25	1-[(Octyloxy)methyl]imidazolium (2S)-2-hydroxypropanoate
26	1-[(Nonyloxy)methyl]imidazolium 2-hydroxypropanoate
27	1-[(Nonyloxy)methyl]imidazolium (2S)-2-hydroxypropanoate
28	1-Ethylimidazolium 2-hydroxypropanoate
29	1-Ethylimidazolium (2S)-2-hydroxypropanoate
30	1-Propylimidazolium 2-hydroxypropanoate
31	1-Propylimidazolium (2S)-2-hydroxypropanoate
32	1-Butylimidazolium (2S)-2-hydroxypropanoate
33	1-Pentylimidazolium 2-hydroxypropanoate
34	1-Pentylimidazolium (2S)-2-hydroxypropanoate
35	1-Hexylimidazolium 2-hydroxypropanoate
36	1-Hexylimidazolium (2S)-2-hydroxypropanoate
37	1-Heptylimidazolium 2-hydroxypropanoate
38	1-Heptylimidazolium (2S)-2-hydroxypropanoate
39	1-Octylimidazolium 2-hydroxypropanoate
40	1-Octylimidazolium (2S)-2-hydroxypropanoate
41	1-Nonylimidazolium 2-hydroxypropanoate
42	1-Nonylimidazolium (2S)-2-hydroxypropanoate
43	1-Methyl-3-(phenylmethyl)imidazoliumtetrafluoroborate
44	1-Methyl-3-[(4-methylphenyl)methyl]imidazolium chloride
45	1-Methyl-3-[(4-methylphenyl)methyl]imidazoliumhexafluorophosphate
46	1,3-Didecyl-2-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
47	1,3-Dimethylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
48	1-[1-(1,3-Benzodioxol-5-yl)-2-methoxy-2-oxoethyl]-3-methylimidazolium chloride
49	1-[1-(1,3-Benzodioxol-5-yl)-2-butoxy-2-oxoethyl]-3-methylimidazolium bromide
50	1-Decyl-3-methylimidazolium tetrafluoroborate
51	1-Decyl-3-methylimidazolium bromide
52	1-Decyl-3-methylimidazolium chloride
53	1-Decyl-3-methylimidazolium hexafluorophosphate
54	1-(11-Ethoxy-11-oxoundecyl)-3-methylimidazolium bromide
55	1-Methyl-3-tetradecylimidazolium chloride

56 1-Hexadecyl-3-methylimidazolium chloride
57 1-Methyl-3-octadecylimidazolium chloride
58 1-(Cyanomethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
59 1-(Cyanomethyl)-3-methylimidazolium chloride
60 1-[2-(Butylamino)-2-oxoethyl]-3-methylimidazolium bromide
61 1-[2-(Butylmethylamino)-2-oxoethyl]-3-methylimidazolium bromide
62 1-(2-Methoxy-2-oxoethyl)-3-methylimidazolium bromide
63 1-[2-[1-(1,3-Benzodioxol-5-yl)-2-butoxy-2-oxoethoxy]-2-oxoethyl]-3-methylimidazolium bromide
64 1-(2-Ethoxy-2-oxoethyl)-3-methylimidazolium tetrafluoroborate
65 1-(2-Ethoxy-2-oxoethyl)-3-methylimidazolium bromide
66 1-Methyl-3-(2-oxo-2-propoxyethyl)imidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
67 1-Methyl-3-(2-oxo-2-propoxyethyl)imidazoliumoctylsulfate
68 1-Methyl-3-(2-oxo-2-propoxyethyl)imidazoliumtetrafluoroborate
69 1-Methyl-3-(2-oxo-2-propoxyethyl)imidazolium bromide
70 1-Methyl-3-(2-oxo-2-propoxyethyl)imidazolium N-cyanocyanamide
71 1-Methyl-3-(2-oxo-2-propoxyethyl)imidazoliumhexafluorophosphate
72 1,2-Dimethyl-3-(2-oxo-2-propoxyethyl)imidazoliumoctylsulfate
73 1,2-Dimethyl-3-(2-oxo-2-propoxyethyl)imidazolium bromide
74 1-(2-Butoxy-2-oxoethyl)-3-methylimidazolium bromide
75 1-Methyl-3-[2-oxo-2-(pentyloxy)ethyl]imidazoliumoctylsulfate
76 1-Methyl-3-[2-oxo-2-(pentyloxy)ethyl]imidazolium bromide
77 1,2-Dimethyl-3-[2-oxo-2-(pentyloxy)ethyl]imidazoliumoctylsulfate
78 1,2-Dimethyl-3-[2-oxo-2-(pentyloxy)ethyl]imidazolium bromide
79 1-[2-(Hexyloxy)-2-oxoethyl]-3-methylimidazolium bromide
80 1-Methyl-3-[2-(octyloxy)-2-oxoethyl]imidazoliumbromide
81 1-(Ethoxymethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
82 1-(Ethoxymethyl)-3-methylimidazolium chloride
83 1-Methyl-3-(phenylmethyl)imidazoliumtetrafluoroborate
84 1-Methyl-3-(phenylmethyl)imidazolium chloride
85 1-Methyl-3-(phenylmethyl)imidazoliumhexafluorophosphate
86 1-Ethyl-3-methylimidazolium bis[1,2-benzenediolato-O1,O2]borate
87 1-Ethyl-3-methylimidazolium bis(pentafluoroethyl)phosphinate
88 1-Ethyl-3-methylimidazolium trifluorotris(pentafluoroethyl)phosphate
89 1-Ethyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
90 1-Ethyl-3-methylimidazolium bis[ethanedioato-O1,O2]borate
91 1-Ethyl-3-methylimidazolium acetate
92 1-Ethyl-3-methylimidazolium 2-(2-methoxyethoxy)ethyl sulfate
93 1-Ethyl-3-methylimidazolium methyl sulfate
94 1-Ethyl-3-methylimidazolium methanesulfonate
95 1-Ethyl-3-methylimidazolium ethyl sulfate
96 1-Ethyl-3-methylimidazolium 4-methylbenzenesulfonate
97 1-Ethyl-3-methylimidazolium octylsulfate
98 1-Ethyl-3-methylimidazolium tetracyanoborate
99 1-Ethyl-3-methylimidazolium tetrafluoroborate
100 1-Ethyl-3-methylimidazolium, salt with methanetricarbonitrile
101 1-Ethyl-3-methylimidazolium trifluoroacetate
102 1-Ethyl-3-methylimidazolium trifluoromethanesulfonate
103 1-Ethyl-3-methylimidazolium chloride
104 1-Ethyl-3-methylimidazolium hydrogen sulfate
105 1-Ethyl-3-methylimidazolium N-cyanocyanamide
106 1-Ethyl-3-methylimidazolium thiocyanate
107 1-Methyl-3-(2-propenyl)imidazolium chloride
108 1-Methyl-3-(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)imidazolium hexafluorophosphate
109 1-Methyl-3-(3-oxobutyl)imidazolium bromide
110 1,2-Dimethylimidazolium
111 1-(2-Methoxyethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
112 1-(2-Methoxyethyl)-3-methylimidazolium chloride
113 1-(2-Ethoxyethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
114 1-(2-Ethoxyethyl)-3-methylimidazolium bromide

115 1-[2-(2-Methoxyethoxy)ethyl]-3-methylimidazolium chloride
116 1-(2-Hydroxyethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
117 1-(2-Hydroxyethyl)-3-methylimidazolium tetrafluoroborate
118 1-(2-Hydroxyethyl)-3-methylimidazolium iodide
119 1-Methyl-3-(2-phenylethyl)imidazoliumtetrafluoroborate
120 1-Methyl-3-(2-phenylethyl)imidazolium chloride
121 1-Methyl-3-(2-phenylethyl)imidazoliumhexafluorophosphate
122 1-Methyl-3-propylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
123 1-Methyl-3-propylimidazolium tetrafluoroborate
124 1-Methyl-3-propylimidazolium chloride
125 1-Methyl-3-propylimidazolium hexafluorophosphate
126 3-(3-Carboxypropyl)-1-methylimidazolium chloride
127 1-(3-Methoxypropyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
128 1-(3-Methoxypropyl)-3-methylimidazolium chloride
129 1-(3-Hydroxypropyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
130 1-(3-Hydroxypropyl)-3-methylimidazolium chloride
131 1-Butyl-3-methylimidazolium trifluorotris(pentafluoroethyl)phosphate
132 1-Butyl-3-methylimidazolium 1,1,1-trifluoro-N-(trifluoromethyl)methanaminate
133 1-Butyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
134 1-Butyl-3-methylimidazolium 2-(2-methoxyethoxy)ethyl sulfate
135 1-Butyl-3-methylimidazolium methyl sulfate
136 1-Butyl-3-methylimidazolium methanesulfonate
137 1-Butyl-3-methylimidazolium 4-methylbenzenesulfonate
138 1-Butyl-3-methylimidazolium octylsulfate
139 1-Butyl-3-methylimidazolium tetrafluoroborate
140 1-Butyl-3-methylimidazolium bromide
141 1-Butyl-3-methylimidazolium trifluoromethanesulfonate
142 1-Butyl-3-methylimidazolium chloride
143 1-Butyl-3-methylimidazolium (T-4)-tetracarbonylcobaltate
144 1-Butyl-3-methylimidazolium tetrachloroferrate
145 1-Butyl-3-methylimidazolium hydrogen sulfate
146 1-Butyl-3-methylimidazolium iodide
147 1-Butyl-3-methylimidazolium N-cyanocyanamide
148 1-Butyl-3-methylimidazolium hexafluorophosphate
149 1-Butyl-3-methylimidazolium (OC-6-11)-hexafluoroantimonate
150 1-Butyl-3-methylimidazolium thiocyanate
151 1-Butyl-2,3-dimethylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
152 1-Butyl-2,3-dimethylimidazolium tetrafluoroborate
153 1-Butyl-2,3-dimethylimidazolium trifluoromethanesulfonate
154 1-(4-Hydroxybutyl)-3-methylimidazolium chloride
155 1-Methyl-3-pentylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
156 1-Methyl-3-pentylimidazolium tetrafluoroborate
157 1-Methyl-3-pentylimidazolium chloride
158 1-Methyl-3-pentylimidazolium hexafluorophosphate
159 1-Hexyl-3-methylimidazolium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide
160 1-Hexyl-3-methylimidazolium trifluorotris(pentafluoroethyl)phosphate
161 1-Hexyl-3-methylimidazolium trifluorotris(heptafluoropropyl)phosphate
162 1-Hexyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
163 1-Hexyl-3-methylimidazolium tris[(trifluoromethyl)sulfonyl]methide
164 1-Hexyl-3-methylimidazolium tetrafluoroborate
165 1-Hexyl-3-methylimidazolium bromide
166 1-Hexyl-3-methylimidazolium chloride
167 1-Hexyl-3-methylimidazolium hexafluorophosphate
168 1-Hexyl-2,3-dimethylimidazolium tetrafluoroborate
169 1-Heptyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
170 1-Heptyl-3-methylimidazolium tetrafluoroborate
171 1-Heptyl-3-methylimidazolium chloride
172 1-Heptyl-3-methylimidazolium hexafluorophosphate
173 1-(7-Carboxyheptyl)-3-methylimidazolium bromide

174 1-Methyl-3-octylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
175 3-Methyl-1-octylimidazolium octylsulfate
176 1-Methyl-3-octylimidazolium tetrafluoroborate
177 1-Methyl-3-octylimidazolium bromide
178 1-Methyl-3-octylimidazolium trifluormethanesulfonate
179 1-Methyl-3-octylimidazolium chloride
180 1-Methyl-3-octylimidazolium hexafluorophosphate
181 1-(8-Hydroxyoctyl)-3-methylimidazolium bromide
182 1-Methyl-3-nonylimidazolium tetrafluoroborate
183 1-Methyl-3-nonylimidazolium chloride
184 1-Methyl-3-nonylimidazolium hexafluorophosphate
185 1-Methyl-3-(2-methylpropyl)imidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
186 1,3-Bis[(decyloxy)methyl]imidazolium chloride
187 1,3-Bis[(undecyloxy)methyl]imidazolium chloride
188 1,3-Bis[(dodecyloxy)methyl]imidazolium chloride
189 1,3-Bis[(tetradecyloxy)methyl]imidazolium chloride
190 1,3-Bis[(hexadecyloxy)methyl]imidazolium chloride
191 1,3-Bis(propoxymethyl)imidazolium chloride
192 1,3-Bis(butoxymethyl)imidazolium chloride
193 1,3-Bis[(pentyloxy)methyl]imidazolium chloride
194 1,3-Bis[(hexyloxy)methyl]imidazolium chloride
195 1,3-Bis[(heptyloxy)methyl]imidazolium chloride
196 1,3-Bis[(octyloxy)methyl]imidazolium chloride
197 1,3-Bis[(nonyloxy)methyl]imidazolium chloride
198 1-Decyl-3-ethylimidazolium bromide
199 1,3-Diethylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
200 1,3-Diethylimidazolium bromide
201 1-Ethyl-3-propylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
202 1-Ethyl-3-propylimidazolium bromide
203 1-Butyl-3-ethylimidazolium tetrafluoroborate
204 1-Butyl-3-ethylimidazolium trifluoroacetate
205 1-Butyl-3-ethylimidazolium trifluoromethanesulfonate
206 1-Ethyl-3-hexylimidazolium tetrafluoroborate
207 1-Ethyl-3-hexylimidazolium bromide
208 1,3-Dipropylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
209 1,3-Dibutylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
210 1,3-Dipentylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
211 1,3-Dihexylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
212 1H-Imidazolium, 1-ethyl-2-(8-heptadecenyl)-4,5-dihydro-3-(2-hydroxyethyl)-, ethylsulfate
213 4-(Cyanomethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
214 4-(Cyanomethyl)-4-methylmorpholinium chloride
215 4-(Ethoxymethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
216 4-(Ethoxymethyl)-4-methylmorpholinium chloride
217 4-Ethyl-4-methylmorpholinium 4-methylbenzenesulfonate
218 4-(2-Methoxyethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
219 4-(2-Methoxyethyl)-4-methylmorpholinium chloride
220 4-(2-Ethoxyethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
221 4-(2-Ethoxyethyl)-4-methylmorpholinium bromide
222 4-(2-Hydroxyethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
223 4-(2-Hydroxyethyl)-4-methylmorpholinium iodide
224 4-(3-Methoxypropyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
225 4-(3-Methoxypropyl)-4-methylmorpholinium chloride
226 4-(3-Hydroxypropyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
227 4-(3-Hydroxypropyl)-4-methylmorpholinium chloride
228 4-Butyl-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
229 4-Butyl-4-methylmorpholinium bromide
230 1-(Cyanomethyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
231 1-(Cyanomethyl)-1-methylpiperidinium chloride
232 1-(Ethoxymethyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide

233 1-(Ethoxymethyl)-1-methylpiperidinium chloride
234 1-(2-Methoxyethyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
235 1-(2-Methoxyethyl)-1-methylpiperidinium bromide
236 1-(2-Ethoxyethyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
237 1-(2-Ethoxyethyl)-1-methylpiperidinium bromide
238 1-(2-Hydroxyethyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
239 1-(2-Hydroxyethyl)-1-methylpiperidinium iodide
240 1-Methyl-1-propylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
241 1-Methyl-1-propylpiperidinium hexafluorophosphate
242 1-(3-Methoxypropyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
243 1-(3-Methoxypropyl)-1-methylpiperidinium chloride
244 1-(3-Hydroxypropyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
245 1-(3-Hydroxypropyl)-1-methylpiperidinium chloride
246 1-Butyl-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
247 1-Butyl-1-methylpiperidinium bromide
248 Pyridinehydrochloride
249 1-[1-(1,3-Benzodioxol-5-yl)-2-methoxy-2-oxoethyl]pyridiniumbromide
250 1-[1-(3,4-Dimethoxyphenyl)-2-methoxy-2-oxoethyl]pyridinium chloride
251 1-[1-(1,3-Benzodioxol-5-yl)-2-butoxy-2-oxoethyl]pyridiniumbromide
252 4-(Dimethylamino)-1-methylpyridinium iodide
253 1-(Cyanomethyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
254 1-(Cyanomethyl)pyridiniumchloride
255 1-[2-[1-(1,3-Benzodioxol-5-yl)-2-methoxy-2-oxoethoxy]-2-oxoethyl]pyridinium bromide
256 1-[2-[1-(1,3-Benzodioxol-5-yl)-2-butoxy-2-oxoethoxy]-2-oxoethyl]pyridinium bromide
257 3-(Aminocarbonyl)-1-[(cyclododecyloxy)methyl]pyridiniumchloride
258 3-[[[[(Decyloxy)methoxy]methyl]amino]carbonyl]-1-[(decyloxy)methyl]pyridinium chloride
259 3-(Aminocarbonyl)-1-[(decyloxy)methyl]pyridiniumchloride
260 3-(Aminocarbonyl)-1-[(decyloxy)methyl]pyridinium (T-4)-tetrachloroferrate
261 Bis[3-(aminocarbonyl)-1-[(decyloxy)methyl]pyridinium] (T-4)-tetrachlorocobaltate
262 Bis[3-(aminocarbonyl)-1-[(decyloxy)methyl]pyridinium] (T-4)-tetrachlorocuprate
263 Bis[3-(aminocarbonyl)-1-[(decyloxy)methyl]pyridinium] (T-4)-tetrachloromagnesate
264 Bis[3-(aminocarbonyl)-1-[(decyloxy)methyl]pyridinium] (T-4)-tetrachlorozincate
265 4-(Aminocarbonyl)-1-[(decyloxy)methyl]pyridiniumchloride
266 3-(Aminocarbonyl)-1-[(undecyloxy)methyl]pyridinium chloride
267 3-Hydroxy-1-[(undecyloxy)methyl]pyridinium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide
268 3-Hydroxy-1-[(undecyloxy)methyl]pyridinium 6-methyl-2,2-dioxo-1,2,3-oxathiazin-4(3H)-onate
269 3-Hydroxy-1-[(undecyloxy)methyl]pyridinium chloride
270 4-(Aminocarbonyl)-1-[(undecyloxy)methyl]pyridinium chloride
271 3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium acetate
272 3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridiniumtetrafluoroborate
273 3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium bromide
274 3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridiniumchloride
275 3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridiniumperchlorate
276 3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridiniumiodide
277 3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium nitrate
278 4-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridiniumchloride
279 3-Hydroxy-1-[(octadecyloxy)methyl]pyridinium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide
280 3-Hydroxy-1-[(octadecyloxy)methyl]pyridinium 6-methyl-2,2-dioxo-1,2,3-oxathiazin-4(3H)-onate
281 1-(Ethoxymethyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
282 1-(Ethoxymethyl)pyridiniumchloride
283 3-Hydroxy-1-(propoxymethyl)pyridinium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide
284 3-Hydroxy-1-(propoxymethyl)pyridinium 6-methyl-2,2-dioxo-1,2,3-oxathiazin-4(3H)-onate
285 3-Hydroxy-1-(propoxymethyl)pyridiniumchloride
286 1-(Butoxymethyl)-3-hydroxypyridinium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide
287 1-(Butoxymethyl)-3-hydroxypyridinium 6-methyl-2,2-dioxo-1,2,3-oxathiazin-4(3H)-onate
288 1-[(Hexyloxy)methyl]-3-hydroxypyridinium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide
289 1-[(Hexyloxy)methyl]-3-hydroxypyridinium 6-methyl-2,2-dioxo-1,2,3-oxathiazin-4(3H)-onate
290 3-[[[[(Heptyloxy)methoxy]methyl]amino]carbonyl]-1-[(heptyloxy)methyl]pyridinium chloride
291 1-[(Heptyloxy)methyl]-3-hydroxypyridinium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide

292 1-[(Heptyloxy)methyl]-3-hydroxypyridinium 6-methyl-2,2-dioxo-1,2,3-oxathiazin-4(3H)-onate
293 1-[(Heptyloxy)methyl]-3-hydroxypyridinium chloride
294 3-[[[[(Octyloxy)methoxy]methyl]amino]carbonyl]-1-[(octyloxy)methyl]pyridinium chloride
295 3-[[[[(Nonyloxy)methoxy]methyl]amino]carbonyl]-1-[(nonyloxy)methyl]pyridinium chloride
296 1-Ethylpyridinium chloride
297 4-(Dimethylamino)-1-ethylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
298 4-(Dimethylamino)-1-ethylpyridinium bromide
299 1-(2-Methoxyethyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
300 1-(2-Methoxyethyl)pyridiniumchloride
301 1-(2-Ethoxyethyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
302 1-(2-Ethoxyethyl)pyridiniumbromide
303 1-(2-Hydroxyethyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
304 1-(2-Hydroxyethyl)pyridiniumiodide
305 1-Propylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
306 1-Propylpyridinium bromide
307 1-(3-Methoxypropyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
308 1-(3-Methoxypropyl)pyridiniumchloride
309 1-(3-Hydroxypropyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
310 1-(3-Hydroxypropyl)pyridiniumchloride
311 1-(3-Sulfopropyl)pyridiniumtrifluoromethanesulfonate
312 1-Butylpyridinium methylsulfate
313 1-Butylpyridinium μ-chlorohexachlorodialuminate
314 1-Butylpyridinium tetrafluoroborate
315 1-Butylpyridinium bromide
316 1-Butylpyridinium trifluoromethanesulfonate
317 1-Butylpyridinium chloride
318 1-Butylpyridinium N-cyanocyanamide
319 1-Butylpyridinium hexafluorophosphate
320 1-Butyl-2-methylpyridinium tetrafluoroborate
321 1-Butyl-2-methylpyridinium chloride
322 1-Butyl-3-methylpyridinium tetrafluoroborate
323 1-Butyl-3-methylpyridinium bromide
324 1-Butyl-3-methylpyridinium chloride
325 1-Butyl-3-methylpyridinium N-cyanocyanamide
326 1-Butyl-3-methylpyridinium hexafluorophosphate
327 1-Butyl-3,4-dimethylpyridinium tetrafluoroborate
328 1-Butyl-3,4-dimethylpyridinium chloride
329 1-Butyl-3,5-dimethylpyridinium tetrafluoroborate
330 1-Butyl-3,5-dimethylpyridinium bromide
331 1-Butyl-3,5-dimethylpyridinium chloride
332 1-Butyl-3,5-dimethylpyridinium N-cyanocyanamide
333 1-Butyl-4-methylpyridinium trifluorotris(pentafluoroethyl)phosphate
334 1-Butyl-4-methylpyridinium tetracyanoborate
335 1-Butyl-4-methylpyridinium tetrafluoroborate
336 1-Butyl-4-methylpyridinium chloride
337 1-Butyl-4-methylpyridinium hexafluorophosphate
338 1-Butyl-4-(dimethylamino)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
339 1-Butyl-4-(dimethylamino)pyridiniumchloride
340 1-Pentylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
341 1-Pentylpyridinium bromide
342 1-Hexylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
343 1-Hexylpyridinium trifluoromethanesulfonate
344 1-Hexylpyridinium chloride
345 1-Hexylpyridinium hexafluorophosphate
346 1-Hexyl-3-methylpyridinium bromide
347 1-Hexyl-3-methylpyridinium chloride
348 1-Hexyl-4-methylpyridinium tetrafluoroborate
349 1-Hexyl-4-methylpyridinium chloride
350 4-(Dimethylamino)-1-hexylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide

351 4-(Dimethylamino)-1-hexylpyridinium chloride
352 1-Octylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
353 1-Octylpyridinium chloride
354 3-Methyl-1-octylpyridinium bromide
355 3-Methyl-1-octylpyridinium chloride
356 4-Methyl-1-octylpyridinium tetrafluoroborate
357 4-Methyl-1-octylpyridinium chloride
358 1-(Cyanomethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
359 1-(Cyanomethyl)-1-methylpyrrolidinium chloride
360 1-(2-Ethoxy-2-oxoethyl)-1-methylpyrrolidinium tris(pentafluoroethyl)trifluorophosphate
361 1-(2-Ethoxy-2-oxoethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
362 1-(2-Ethoxy-2-oxoethyl)-1-methylpyrrolidinium bromide
363 1-(Ethoxymethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
364 1-(Ethoxymethyl)-1-methylpyrrolidinium chloride
365 1-(2-Methoxyethyl)-1-methylpyrrolidinium tris(pentafluoroethyl)trifluorophosphate
366 1-(2-Methoxyethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
367 1-(2-Methoxyethyl)-1-methylpyrrolidinium chloride
368 1-(2-Ethoxyethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
369 1-(2-Ethoxyethyl)-1-methylpyrrolidinium bromide
370 1-(2-Hydroxyethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
371 1-(2-Hydroxyethyl)-1-methylpyrrolidinium iodide
372 1-Methyl-1-propylpyrrolidinium hexafluorophosphate
373 1-(3-Methoxypropyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
374 1-(3-Methoxypropyl)-1-methylpyrrolidinium chloride
375 1-(3-Hydroxypropyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
376 1-(3-Hydroxypropyl)-1-methylpyrrolidinium chloride
377 1-Butyl-1-methylpyrrolidinium trifluorotris(pentafluoroethyl)phosphate
378 1-Butyl-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
379 1-Butyl-1-methylpyrrolidinium tetrafluoroborate
380 1-Butyl-1-methylpyrrolidinium bromide
381 1-Butyl-1-methylpyrrolidinium chloride
382 1-Butyl-1-methylpyrrolidinium N-cyanocyanamide
383 1-Hexyl-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
384 1-Hexyl-1-methylpyrrolidinium chloride
385 1-Methyl-1-octylpyrrolidinium tetrafluoroborate
386 1-Methyl-1-octylpyrrolidinium chloride
387 1-[(Decyloxy)methyl]quinoliniumchloride
388 1-[(Decyloxy)methyl]-6-methylquinolinium chloride
389 1-[(Decyloxy)methyl]-8-hydroxyquinolinium chloride
390 1-[(Dodecyloxy)methyl]quinoliniumchloride
391 1-[(Dodecyloxy)methyl]-6-methylquinolinium chloride
392 1-[(Dodecyloxy)methyl]-8-hydroxyquinolinium chloride
393 1-[(Hexyloxy)methyl]quinoliniumchloride
394 1-[(Hexyloxy)methyl]-6-methylquinolinium chloride
395 1-[(Hexyloxy)methyl]-8-hydroxyquinolinium chloride
396 1-[(Octyloxy)methyl]quinoliniumchloride
397 6-Methyl-1-[(octyloxy)methyl]quinolinium chloride
398 8-Hydroxy-1-[(octyloxy)methyl]quinoliniumchloride
399 1-Butylquinolinium tetrafluoroborate
400 1-Butylquinolinium bromide
401 1-Hexylquinolinium tetrafluoroborate
402 1-Octylquinolinium tetrafluoroborate
403 1-Octylquinolinium bromide

Table B4 The 35 variables use in PCA on overall toxicity.

	Variables	unit
1	*Candida albicans* ATCC 10231 (growth inhibition) 48h	**log(MIC)**
2	*Candida albicans* ATCC 10231 (death) 5d	**log(MBC)**
3	*Enterococcus hirae* ATCC 10541 (growth inhibition) 24h	**log(MIC)**
4	*Enterococcus hirae* ATCC 10541 (death) 48h	**log(MBC)**
5	*Escherichia coli*ATCC 25922 (growth inhibition) 24h	**log(MIC)**
6	*Escherichia coli* ATCC 25922 (death) 48h	**log(MBC)**
7	*Klebsiella pneumoniae* ATCC 4352 (growth inhibition) 24h	**log(MIC)**
8	*Klebsiella pneumoniae* ATCC 4352 (death) 48h	**log(MBC)**
9	*Lemna minor* (frond area) 7d	**log(EC50)**
10	*Lemna minor* (frond number) 7d	**log(EC50)**
11	*Micrococcus luteus* ATCC 9341 (growth inhibition) 24h	**log(MIC)**
12	*Micrococcus luteus* ATCC 9341 (death) 48h	**log(MBC)**
13	*Proteus vulgaris* NCTC 4635 (growth inhibition) 24h	**log(MIC)**
14	*Proteus vulgaris* NCTC 4635 (death) 48h	**log(MBC)**
15	*Pseudomonas aeruginosa* ATCC 27853 (growth inhibition) 24h	**log(MIC)**
16	*Pseudomonas aeruginosa* ATCC 27853 (death) 48h	**log(MBC)**
17	*Pseudomonas aeruginosa* NCTC 6749 (growth inhibition) 24h	**log(MIC)**
18	*Rhodotorula rubra* PhB (growth inhibition) 48h	**log(MIC)**
19	*Rhodotorula rubra* PhB (death) 5d	**log(MBC)**
20	*Scenedesmus vacuolatus* (cell count) 24h	**log(EC50)**
21	*Serratia marcescens* ATCC 8100 (growth inhibition) 24h	**log(MIC)**
22	*Serratia marcescens* ATCC 8100 (death) 48h	**log(MBC)**
23	*Staphylococcus aureus* ATCC 6538 (growth inhibition) 24h	**log(MIC)**
24	*Staphylococcus aureus* ATCC 6538 (death) 48h	**log(MBC)**
25	*Staphylococcus aureus* (MRSA) (growth inhibition) 24h	**log(MIC)**
26	*Staphylococcus aureus* (MRSA) (death) 48h	**log(MBC)**
27	*Staphylococcus aureus* NCTC 4163 (growth inhibition) 24h	**log(MIC)**
28	*Staphylococcus epidermidis* ATCC 12228 (growth inhibition) 24h	**log(MIC)**
29	*Staphylococcus epidermidis* ATCC 12228 (death) 48h	**log(MBC)**
30	*Vibrio fischeri* 5'	**log(EC50)**
31	*Vibrio fischeri* 15'	**log(EC50)**
32	*Vibrio fischeri* 30'	**log(EC50)**
33	Acetylcholinesterase inhibition	**log(EC50)**
34	IPC-81 leukemia cells cytotoxicity	**log(EC50)**
35	BOD 28 d	**%**

Table B5 Ranking of ILs according to aquatic toxicity PCA model together with IPC-81 toxicity rank and AChE toxicity rank.

	Name	t[1] Aquatictoxicity model	IPC-81Rank[a]	AChERank[b]
1	1,3-Dimethylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3.91		
2	1-(3-Hydroxypropyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3.24	**61**	**22**
3	1-Ethyl-3-methylimidazolium ethyl sulfate	3.21	**57**	**117**
4	4-Butyl-4-methylmorpholinium bromide	3.18	**17**	**50**
5	1-Methyl-1-propylpiperidinium hexafluorophosphate	2.90		
6	1-Methyl-3-propylimidazolium hexafluorophosphate	2.89	**155**	**88**
7	1-(Cyanomethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.73	**36**	**14**
8	1-(3-Hydroxypropyl)-3-methylimidazolium chloride	2.62	**28**	**33**
9	1-Butyl-3-methylimidazolium methanesulfonate	2.61	**101**	**138**
10	1-Butyl-1-methylpiperidinium bromide	2.44	**46**	**171**
11	1-(Ethoxymethyl)-3-methylimidazolium chloride	2.38	**104**	**65**
12	1-(2-Hydroxyethyl)-3-methylimidazolium iodide	2.15	**15**	**21**
13	1-Butyl-3-methylimidazolium 4-methylbenzenesulfonate	2.01	**118**	**112**
14	1-Butyl-3-methylimidazolium N-cyanocyanamide	1.97	**152**	**166**
15	1-Butyl-3-methylimidazolium bromide	1.92	**121**	**152**
16	1-Methyl-1-propylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.78	**119**	
17	1-(Cyanomethyl)-3-methylimidazolium chloride	1.54	**38**	**49**
18	1-Butylpyridinium bromide	1.44	**67**	**181**
19	4-Butyl-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.44	**80**	**17**
20	1-(3-Methoxypropyl)-3-methylimidazolium chloride	1.38	**9**	**63**
21	1-(3-Hydroxypropyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.33	**73**	**40**
22	1-Methyl-3-(2-methylpropyl)imidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.32		
23	1-(3-Methoxypropyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.29	**88**	**35**
24	1-Methyl-3-propylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.25		
25	1-Hexylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.25	**144**	**109**
26	1-(3-Hydroxypropyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.22	**68**	**19**
27	1-[1-(1,3-Benzodioxol-5-yl)-2-methoxy-2-oxoethyl]pyridiniumbromide	1.22		
28	4-(Ethoxymethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.22	**82**	**11**
29	1-Butylpyridinium N-cyanocyanamide	1.21		
30	1-Butyl-1-methylpyrrolidinium chloride	1.11	**26**	**175**
31	1,3-Diethylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.04		
32	1-(2-Ethoxy-2-oxoethyl)-1-methylpyrrolidinium bromide	1.03	**66**	

33	1-Ethyl-3-methylimidazolium chloride	1.00	**74**	**164**
34	1-Butyl-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	0.97	**84**	**122**
35	1-Methyl-3-pentylimidazolium tetrafluoroborate	0.94	**162**	**167**
36	1-Methyl-3-propylimidazolium tetrafluoroborate	0.92	**117**	**93**
37	1-(2-Methoxyethyl)-3-methylimidazolium chloride	0.88	**27**	**68**
38	1-Ethyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	0.87	**95**	**90**
39	1-(2-Ethoxyethyl)-3-methylimidazolium bromide	0.77	**34**	**89**
40	1-(2-Methoxyethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	0.73	**102**	**46**
41	1-Butyl-3-methylimidazolium iodide	0.64	**97**	**118**
42	1-Ethyl-3-methylimidazolium N-cyanocyanamide	0.60	**81**	**74**
43	1-(2-Ethoxy-2-oxoethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	0.49	**64**	**5**
44	1-Ethyl-3-methylimidazolium tetracyanoborate	0.46	**103**	**144**
45	1-(Ethoxymethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	0.46	**108**	**51**
46	1-(2-Methoxyethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	0.31	**93**	**79**
47	1-Butyl-3-methylimidazolium chloride	0.27	**114**	**176**
48	1-Ethyl-3-methylimidazolium, salt with methanetricarbonitrile	0.24	**140**	**67**
49	1-Butylpyridinium μ-chlorohexachlorodialuminate	0.23	**71**	**150**
50	1-Butyl-3-methylimidazolium hexafluorophosphate	0.21	**143**	**94**
51	1-Butyl-3-methylpyridinium bromide	0.21		
52	1-(3-Methoxypropyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	0.21	**94**	**62**
53	1-(2-Ethoxyethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	0.18	**106**	**39**
54	1-Hexyl-3-methylimidazolium tetrafluoroborate	0.15	**161**	**156**
55	1-Butyl-3,5-dimethylpyridinium bromide	0.13		
56	1-Butylpyridinium chloride	0.09		**189**
57	1-Butyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	0.02	**170**	**95**
58	1-Butyl-3-methylpyridinium N-cyanocyanamide	-0.04	**115**	**208**
59	1-Butyl-3-methylimidazolium tetrafluoroborate	-0.06	**151**	**143**
60	1-Butyl-3-methylimidazolium 1,1,1-trifluoro-N-(trifluoromethyl)methanaminate	-0.06	**201**	**183**
61	1-Butyl-4-methylpyridinium tetrafluoroborate	-0.07	**163**	**190**
62	1-[1-(1,3-Benzodioxol-5-yl)-2-butoxy-2-oxoethyl]-3-methylimidazolium bromide	-0.08		
63	1-Butyl-2,3-dimethylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	-0.16		
64	1-Butyl-3-methylimidazolium trifluoromethanesulfonate	-0.19	**148**	**131**
65	1-Ethyl-3-propylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	-0.20		
66	1-Ethyl-3-methylimidazolium bis(pentafluoroethyl)phosphinate	-0.21	**154**	**83**
67	1-Hexyl-3-methylimidazolium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide	-0.28	**193**	**108**
68	1-(2-Ethoxyethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	-0.28	**72**	**76**
69	1-[1-(1,3-Benzodioxol-5-yl)-2-butoxy-2-oxoethyl]pyridiniumbromide	-0.41		

70	1-Hexyl-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	-0.48	**177**	**30**
71	1-[1-(3,4-Dimethoxyphenyl)-2-methoxy-2-oxoethyl]pyridinium chloride	-0.49		
72	1-Butyl-3,5-dimethylpyridinium N-cyanocyanamide	-0.54		
73	1-Heptyl-3-methylimidazolium tetrafluoroborate	-0.66	**184**	**101**
74	1-[1-(1,3-Benzodioxol-5-yl)-2-methoxy-2-oxoethyl]-3-methylimidazolium chloride	-0.69		
75	1,3-Dibutylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	-0.71		
76	1-Butyl-3-methylimidazolium octylsulfate	-0.89	**120**	**103**
77	1-Ethyl-3-hexylimidazolium tetrafluoroborate	-1.00	**200**	**158**
78	1-Ethyl-3-methylimidazolium bis[1,2-benzenediolato(2-)-O1,O2]borate	-1.06	**231**	**92**
79	1-Hexyl-3-methylpyridinium bromide	-1.08		
80	1-Methyl-3-pentylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	-1.16		
81	1,3-Dipropylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	-1.21		
82	1,3-Dihexylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	-1.21		
83	1-[2-(2-Methoxyethoxy)ethyl]-3-methylimidazolium chloride	-1.42		
84	1-Hexyl-3-methylimidazolium hexafluorophosphate	-1.54	**159**	**136**
85	1-Hexyl-3-methylimidazolium chloride	-1.57	**180**	**169**
86	4-(Dimethylamino)-1-hexylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	-1.57	**227**	**212**
87	1-Octylpyridinium chloride	-1.59	**228**	**188**
88	1,3-Dipentylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	-1.74		
89	1-[2-[1-(1,3-Benzodioxol-5-yl)-2-butoxy-2-oxoethoxy]-2-oxoethyl]-3-methylimidazolium bromide	-1.96		
90	1-[2-[1-(1,3-Benzodioxol-5-yl)-2-methoxy-2-oxoethoxy]-2-oxoethyl]pyridinium bromide	-2.13		
91	1-Heptyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	-2.13		
92	1-Hexyl-3-methylimidazolium bromide	-2.43		
93	1-Methyl-3-nonylimidazolium tetrafluoroborate	-2.57	**217**	**192**
94	1-Hexyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	-2.86	**191**	**71**
95	3-Methyl-1-octylpyridinium bromide	-3.56		
96	1-Decyl-3-methylimidazolium tetrafluoroborate	-3.56	**233**	**205**
97	1-Ethyl-3-methylimidazolium trifluorotris(pentafluoroethyl)phosphate	-3.60	**226**	**43**
98	1-Methyl-3-octylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	-3.75	**210**	**81**
99	1-Methyl-3-octylimidazolium bromide	-3.93		
100	1-(11-Ethoxy-11-oxoundecyl)-3-methylimidazolium bromide	-3.93		
101	1-Methyl-3-octadecylimidazolium chloride	-4.76	**242**	**209**
102	1-Methyl-3-octylimidazolium tetrafluoroborate	-5.32	**219**	**186**
103	1-Hexadecyl-3-methylimidazolium chloride	-5.99	**244**	**220**
104	1-Methyl-3-tetradecylimidazolium chloride	-6.90	**245**	**225**

[a]In a list for 245 ILs ordered according to decreasing logIPC-81 values (Table B9). [b]In a list for 232 ILs ordered according to decreasing logAChE values (Table B10).

Table B6 The 6 variables used in aquatic toxicity model.

	Variables	unit
1	*Lemna minor* (frond area) 7d	log(EC50)
2	*Lemna minor* (frond number) 7d	log(EC50)
3	*Scenedesmus vacuolatus* (cell count) 24h	log(EC50)
4	*Vibrio fischeri* 5'	log(EC50)
5	*Vibrio fischeri* 15'	log(EC50)
6	*Vibrio fischeri* 30'	log(EC50)

Table B7 Ranking of ILs according to Bacteria and Fungi toxicity model.

	Name	t[1] Bacteria and Fungi toxicity model
1	1,3-Bis(propoxymethyl)imidazolium chloride	4.96
2	1,3-Bis(butoxymethyl)imidazolium chloride	4.81
3	1-Hexylimidazolium (2S)-2-hydroxypropanoate	4.78
4	1-Methylimidazolium 2-hydroxypropanoate	4.64
5	1-Methylimidazolium (2S)-2-hydroxypropanoate	4.64
6	1-Ethylimidazolium 2-hydroxypropanoate	4.64
7	1-Ethylimidazolium (2S)-2-hydroxypropanoate	4.64
8	1-Propylimidazolium 2-hydroxypropanoate	4.64
9	1-Pentylimidazolium 2-hydroxypropanoate	4.64
10	1-Pentylimidazolium (2S)-2-hydroxypropanoate	4.64
11	1-Propylimidazolium (2S)-2-hydroxypropanoate	4.62
12	1-Butylimidazolium (2S)-2-hydroxypropanoate	4.54
13	1-(Butoxymethyl)imidazolium 2-hydroxypropanoate	4.53
14	1-(Butoxymethyl)imidazolium (2S)-2-hydroxypropanoate	4.53
15	1,3-Bis[(pentyloxy)methyl]imidazolium chloride	4.47
16	1-[(Pentyloxy)methyl]imidazolium (2S)-2-hydroxypropanoate	4.34
17	1-Hexylimidazolium 2-hydroxypropanoate	4.32
18	1-[(Pentyloxy)methyl]imidazolium 2-hydroxypropanoate	4.11
19	1-Heptylimidazolium 2-hydroxypropanoate	4.08
20	1,3-Bis[(tetradecyloxy)methyl]imidazolium chloride	3.76
21	1,3-Bis[(hexadecyloxy)methyl]imidazolium chloride	3.76
22	1-[(Hexyloxy)methyl]imidazolium (2S)-2-hydroxypropanoate	3.51
23	1-Heptylimidazolium (2S)-2-hydroxypropanoate	3.47
24	3-(Aminocarbonyl)-1-[(cyclododecyloxy)methyl]pyridinium chloride	2.97
25	1-[(Hexyloxy)methyl]imidazolium 2-hydroxypropanoate	2.87
26	1-[(Octyloxy)methyl]quinolinium chloride	2.74
27	1,3-Bis[(dodecyloxy)methyl]imidazolium chloride	2.64
28	1-[(Hexyloxy)methyl]quinolinium chloride	2.52
29	1-[(Heptyloxy)methyl]imidazolium 2-hydroxypropanoate	1.94
30	1-[(Decyloxy)methyl]quinolinium chloride	1.87
31	1,3-Bis[(undecyloxy)methyl]imidazolium chloride	1.57
32	1-[(Heptyloxy)methyl]imidazolium (2S)-2-hydroxypropanoate	1.36
33	1-Octylimidazolium (2S)-2-hydroxypropanoate	1.31
34	1-[(Dodecyloxy)methyl]quinolinium chloride	1.28
35	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium iodide	0.91
36	3-[[[[(Decyloxy)methoxy]methyl]amino]carbonyl]-1-[(decyloxy)methyl]pyridinium chloride	0.82
37	1-Octylimidazolium 2-hydroxypropanoate	0.76
38	4-(Aminocarbonyl)-1-[(decyloxy)methyl]pyridinium chloride	0.48

39	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium tetrafluoroborate	0.29
40	1-[(Hexyloxy)methyl]-6-methylquinolinium chloride	0.25
41	3-(Aminocarbonyl)-1-[(decyloxy)methyl]pyridinium chloride	0.10
42	1-[(Octyloxy)methyl]imidazolium 2-hydroxypropanoate	-0.47
43	1,3-Bis[(hexyloxy)methyl]imidazolium chloride	-0.52
44	4-(Aminocarbonyl)-1-[(undecyloxy)methyl]pyridinium chloride	-0.81
45	1-[(Octyloxy)methyl]imidazolium (2S)-2-hydroxypropanoate	-0.92
46	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium perchlorate	-0.94
47	1-[(Decyloxy)methyl]imidazolium 2-hydroxypropanoate	-1.36
48	3-(Aminocarbonyl)-1-[(undecyloxy)methyl]pyridinium chloride	-1.42
49	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium chloride	-1.51
50	1,3-Bis[(decyloxy)methyl]imidazolium chloride	-1.59
51	1-[(Nonyloxy)methyl]imidazolium 2-hydroxypropanoate	-1.60
52	1-[(Dodecyloxy)methyl]-8-hydroxyquinolinium chloride	-1.67
53	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium nitrate	-1.75
54	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium bromide	-1.97
55	8-Hydroxy-1-[(octyloxy)methyl]quinolinium chloride	-2.03
56	1-[(Hexyloxy)methyl]-8-hydroxyquinolinium chloride	-2.24
57	Bis[3-(aminocarbonyl)-1-[(decyloxy)methyl]pyridinium] (T-4)-tetrachlorocuprate	-2.28
58	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium acetate	-2.43
59	Bis[3-(aminocarbonyl)-1-[(decyloxy)methyl]pyridinium] (T-4)-tetrachlorozincate	-2.47
60	6-Methyl-1-[(octyloxy)methyl]quinolinium chloride	-2.58
61	1-Nonylimidazolium 2-hydroxypropanoate	-2.61
62	3-(Aminocarbonyl)-1-[(decyloxy)methyl]pyridinium (T-4)-tetrachloroferrate	-2.69
63	1-Nonylimidazolium (2S)-2-hydroxypropanoate	-2.91
64	1-[(Dodecyloxy)methyl]imidazolium 2-hydroxypropanoate	-3.14
65	4-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium chloride	-3.34
66	Bis[3-(aminocarbonyl)-1-[(decyloxy)methyl]pyridinium] (T-4)-tetrachlorocobaltate	-3.38
67	1-[(Nonyloxy)methyl]imidazolium (2S)-2-hydroxypropanoate	-3.51
68	1-[(Decyloxy)methyl]-8-hydroxyquinolinium chloride	-3.52
69	1-[(Dodecyloxy)methyl]-6-methylquinolinium chloride	-3.52
70	1-[(Undecyloxy)methyl]imidazolium 2-hydroxypropanoate	-3.66
71	Bis[3-(aminocarbonyl)-1-[(decyloxy)methyl]pyridinium] (T-4)-tetrachloromagnesate	-4.18
72	1-Dodecylimidazolium 2-hydroxypropanoate	-4.31
73	3-[[[[(Nonyloxy)methoxy]methyl]amino]carbonyl]-1-[(nonyloxy)methyl]pyridinium chloride	-4.41
74	3-[[[[(Heptyloxy)methoxy]methyl]amino]carbonyl]-1-[(heptyloxy)methyl]pyridinium chloride	-4.53
75	1-Decylimidazolium 2-hydroxypropanoate	-4.69
76	1-Undecylimidazolium 2-hydroxypropanoate	-4.74
77	1-[(Decyloxy)methyl]imidazolium (2S)-2-hydroxypropanoate	-5.14
78	3-[[[[(Octyloxy)methoxy]methyl]amino]carbonyl]-1-[(octyloxy)methyl]pyridinium chloride	-5.44
79	1-[(Dodecyloxy)methyl]imidazolium (2S)-2-hydroxypropanoate	-5.81
80	1,3-Bis[(nonyloxy)methyl]imidazolium chloride	-5.82
81	1-Decylimidazolium (2S)-2-hydroxypropanoate	-5.89
82	1-[(Undecyloxy)methyl]imidazolium (2S)-2-hydroxypropanoate	-5.90
83	1,3-Bis[(octyloxy)methyl]imidazolium chloride	-5.92
84	1-[(Decyloxy)methyl]-6-methylquinolinium chloride	-6.04
85	1,3-Bis[(heptyloxy)methyl]imidazolium chloride	-6.54
86	1-Undecylimidazolium (2S)-2-hydroxypropanoate	-6.93
87	1-Dodecylimidazolium (2S)-2-hydroxypropanoate	-7.03

Table B8 The 26 variables used in Bacteria and Fungi toxicity model

	Variables	unit
1	*Candida albicans* ATCC 10231 (growth inhibition) 48h	log(MIC)
2	*Candida albicans* ATCC 10231 (death) 5d	log(MBC)
3	*Enterococcus hirae* ATCC 10541 (growth inhibition) 24h	log(MIC)
4	*Enterococcus hirae* ATCC 10541 (death) 48h	log(MBC)
5	*Escherichia coli* ATCC 25922 (growth inhibition) 24h	log(MIC)
6	*Escherichia coli* ATCC 25922 (death) 48h	log(MBC)
7	*Klebsiella pneumoniae* ATCC 4352 (growth inhibition) 24h	log(MIC)
8	*Klebsiella pneumoniae* ATCC 4352 (death) 48h	log(MBC)
9	*Micrococcus luteus* ATCC 9341 (growth inhibition) 24h	log(MIC)
10	*Micrococcus luteus* ATCC 9341 (death) 48h	log(MBC)
11	*Proteus vulgaris* NCTC 4635 (growth inhibition) 24h	log(MIC)
12	*Proteus vulgaris* NCTC 4635 (death) 48h	log(MBC)
13	*Pseudomonas aeruginosa* ATCC 27853 (growth inhibition) 24h	log(MIC)
14	*Pseudomonas aeruginosa* ATCC 27853 (death) 48h	log(MBC)
15	*Pseudomonas aeruginosa* NCTC 6749 (growth inhibition) 24h	log(MIC)
16	*Rhodotorula rubra* PhB (growth inhibition) 48h	log(MIC)
17	*Rhodotorula rubra* PhB (death) 5d	log(MBC)
18	*Serratia marcescens* ATCC 8100 (growth inhibition) 24h	log(MIC)
19	*Serratia marcescens* ATCC 8100 (death) 48h	log(MBC)
20	*Staphylococcus aureus* ATCC 6538 (growth inhibition) 24h	log(MBC)
21	*Staphylococcus aureus* ATCC 6538 (death) 48h	log(MIC)
22	*Staphylococcus aureus* (MRSA) (growth inhibition) 24h	log(MIC)
23	*Staphylococcus aureus* (MRSA) (death) 48h	log(MBC)
24	*Staphylococcus aureus* NCTC 4163 (growth inhibition) 24h	log(MIC)
25	*Staphylococcus epidermidis* ATCC 12228 (growth inhibition) 24h	log(MIC)
26	*Staphylococcus epidermidis* ATCC 12228 (death) 48h	log(MBC)

Table B9 Ranking of the 245 IPC-81 variables according to decreasing values.

	Name	IPC-81, log (EC_{50})
1	1-(3-Hydroxypropyl)-1-methylpyrrolidinium chloride	4.30
2	1-(2-Hydroxyethyl)-1-methylpiperidinium iodide	4.01
3	1-(3-Methoxypropyl)-1-methylpyrrolidinium chloride	3.99
4	1-(2-Methoxyethyl)-1-methylpiperidinium bromide	3.98
5	1-(3-Methoxypropyl)pyridinium chloride	3.88
6	1-(Cyanomethyl)-1-methylpiperidinium chloride	3.82
7	4-(3-Methoxypropyl)-4-methylmorpholinium chloride	3.80
8	1-Propylpyridinium bromide	3.78
9	1-(3-Methoxypropyl)-3-methylimidazolium chloride	3.77
10	1-(3-Hydroxypropyl)-1-methylpiperidinium chloride	3.76
11	4-(2-Hydroxyethyl)-4-methylmorpholinium iodide	3.74
12	1-(3-Methoxypropyl)-1-methylpiperidinium chloride	3.72
13	1-(2-Hydroxyethyl)-1-methylpyrrolidinium iodide	3.71
14	1-(2-Ethoxyethyl)-1-methylpiperidinium bromide	3.71
15	1-(2-Hydroxyethyl)-3-methylimidazolium iodide	3.71
16	4-(2-Ethoxyethyl)-4-methylmorpholinium bromide	3.71
17	4-Butyl-4-methylmorpholinium bromide	3.68
18	1-(2-Ethoxyethyl)-1-methylpyrrolidinium bromide	3.68
19	1-(2-Ethoxyethyl)pyridinium bromide	3.61
20	4-(2-Methoxyethyl)-4-methylmorpholinium chloride	3.59
21	4-(3-Hydroxypropyl)-4-methylmorpholinium chloride	3.59
22	1-(Cyanomethyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3.57
23	1-(2-Methoxyethyl)-1-methylpyrrolidinium chloride	3.56
24	1-(2-Hydroxyethyl)pyridinium iodide	3.55
25	1-Butyl-1-methylpyrrolidinium N-cyanocyanamide	3.55
26	1-Butyl-1-methylpyrrolidinium chloride	3.55
27	1-(2-Methoxyethyl)-3-methylimidazolium chloride	3.55
28	1-(3-Hydroxypropyl)-3-methylimidazolium chloride	3.55
29	4-(Cyanomethyl)-4-methylmorpholinium chloride	3.55
30	1-Ethyl-3-methylimidazolium methyl sulfate	3.54
31	1-(2-Methoxyethyl)pyridinium chloride	3.54
32	1-(3-Hydroxypropyl)pyridinium chloride	3.54
33	1-(Ethoxymethyl)-1-methylpiperidinium chloride	3.52
34	1-(2-Ethoxyethyl)-3-methylimidazolium bromide	3.51
35	1-Methyl-3-propylimidazolium chloride	3.51
36	1-(Cyanomethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3.51
37	1-Ethyl-3-methylimidazolium trifluoromethanesulfonate	3.50
38	1-(Cyanomethyl)-3-methylimidazolium chloride	3.50
39	1-Ethyl-3-methylimidazolium acetate	3.46
40	1-Ethyl-3-methylimidazolium thiocyanate	3.45
41	4-(2-Methoxyethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3.45
42	1-(3-Sulfopropyl)pyridinium trifluoromethanesulfonate	3.45
43	1-(Cyanomethyl)-1-methylpyrrolidinium chloride	3.44
44	4-(3-Methoxypropyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3.43
45	1-(Cyanomethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3.41
46	1-Butyl-1-methylpiperidinium bromide	3.41
47	1-(3-Methoxypropyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3.40
48	1-(2-Hydroxyethyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3.40
49	1-Ethylpyridinium chloride	3.38

50	1-(2-Hydroxyethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3.37
51	1-Ethyl-3-methylimidazolium trifluoroacetate	3.35
52	4-(2-Ethoxyethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3.35
53	1-Ethyl-3-methylimidazolium 2-(2-methoxyethoxy)ethyl sulfate	3.34
54	1-(2-Hydroxyethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3.33
55	1-Butylpyridinium methyl sulfate	3.31
56	1-Ethyl-3-methylimidazolium hydrogen sulfate	3.31
57	1-Ethyl-3-methylimidazolium ethyl sulfate	3.30
58	1-Butylpyridinium hexafluorophosphate	3.30
59	4-Ethyl-4-methylmorpholinium 4-methylbenzenesulfonate	3.29
60	1-Ethyl-3-methylimidazolium methanesulfonate	3.29
61	1-(3-Hydroxypropyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3.29
62	1-(2-Hydroxyethyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3.28
63	1-Ethyl-3-methylimidazolium 4-methylbenzenesulfonate	3.26
64	1-(2-Ethoxy-2-oxoethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3.25
65	1-(3-Hydroxypropyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3.25
66	1-(2-Ethoxy-2-oxoethyl)-1-methylpyrrolidinium bromide	3.25
67	1-Butylpyridinium bromide	3.24
68	1-(3-Hydroxypropyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3.23
69	1-Hexyl-3-methylimidazolium tris[(trifluoromethyl)sulfonyl]methide	3.20
70	4-(3-Hydroxypropyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3.19
71	1-Butylpyridinium μ-chlorohexachlorodialuminate	3.18
72	1-(2-Ethoxyethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3.18
73	1-(3-Hydroxypropyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3.17
74	1-Ethyl-3-methylimidazolium chloride	3.16
75	4-(Cyanomethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3.16
76	1-Butyl-3-methylpyridinium chloride	3.12
77	1-Butylpyridinium trifluoromethanesulfonate	3.12
78	1-Butyl-1-methylpyrrolidinium bromide	3.11
79	1-(Cyanomethyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3.10
80	4-Butyl-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3.07
81	1-Ethyl-3-methylimidazolium N-cyanocyanamide	3.07
82	4-(Ethoxymethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3.06
83	1-(Ethoxymethyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3.05
84	1-Butyl-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3.05
85	1-(3-Methoxypropyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3.02
86	1-Butyl-2-methylpyridinium chloride	3.02
87	1-(2-Ethoxyethyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3.00
88	1-(3-Methoxypropyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.98
89	1-(Cyanomethyl)pyridinium chloride	2.98
90	1-(7-Carboxyheptyl)-3-methylimidazolium bromide	2.96
91	1-Butylpyridinium tetrafluoroborate	2.95
92	1-Butyl-3-methylpyridinium hexafluorophosphate	2.94
93	1-(2-Methoxyethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.93
94	1-(3-Methoxypropyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.92
95	1-Ethyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.91
96	1-Butyl-3-ethylimidazolium trifluoromethanesulfonate	2.91
97	1-Butyl-3-methylimidazolium iodide	2.91
98	1-(2-Ethoxyethyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.90
99	1-(2-Methoxyethyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.89
100	1-(Ethoxymethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.89

101	1-Butyl-3-methylimidazolium methanesulfonate	2.88
102	1-(2-Methoxyethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.88
103	1-Ethyl-3-methylimidazolium tetracyanoborate	2.86
104	1-(Ethoxymethyl)-3-methylimidazolium chloride	2.85
105	1-Methyl-3-(3-oxobutyl)imidazolium bromide	2.84
106	1-(2-Ethoxyethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.84
107	Pyridine hydrochloride	2.83
108	1-(Ethoxymethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.83
109	4-(2-Hydroxyethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.82
110	1-(2-Hydroxyethyl)-3-methylimidazolium tetrafluoroborate	2.81
111	4-(Ethoxymethyl)-4-methylmorpholinium chloride	2.81
112	1-(2-Methoxyethyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.81
113	1-Propylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.81
114	1-Butyl-3-methylimidazolium chloride	2.80
115	1-Butyl-3-methylpyridinium N-cyanocyanamide	2.79
116	3-(3-Carboxypropyl)-1-methylimidazolium chloride	2.79
117	1-Methyl-3-propylimidazolium tetrafluoroborate	2.78
118	1-Butyl-3-methylimidazolium 4-methylbenzenesulfonate	2.78
119	1-Methyl-1-propylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.78
120	1-Butyl-3-methylimidazolium octylsulfate	2.77
121	1-Butyl-3-methylimidazolium bromide	2.77
122	1-(4-Hydroxybutyl)-3-methylimidazolium chloride	2.76
123	1-(Ethoxymethyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.74
124	1-Butyl-3-ethylimidazolium trifluoroacetate	2.74
125	1-Ethyl-3-methylimidazolium tetrafluoroborate	2.73
126	1-Ethyl-3-methylimidazolium octylsulfate	2.73
127	1-Butyl-3,5-dimethylpyridinium chloride	2.72
128	1-Butyl-3-methylimidazolium tetrachloroferrate	2.70
129	1-(2-Ethoxy-2-oxoethyl)-1-methylpyrrolidinium tris(pentafluoroethyl)trifluorophosphate	2.70
130	1-Butyl-3-methylimidazolium-2-(2-methoxyethoxy)ethyl sulfate	2.69
131	1-Butyl-3-methylpyridinium tetrafluoroborate	2.68
132	1-Butyl-3-methylimidazolium hydrogen sulfate	2.66
133	1-Butyl-3,5-dimethylpyridinium tetrafluoroborate	2.65
134	1-Ethyl-3-propylimidazolium bromide	2.64
135	1-Butyl-3-ethylimidazolium tetrafluoroborate	2.64
136	1-Butyl-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.63
137	1-Butyl-2-methylpyridinium tetrafluoroborate	2.62
138	1-Butyl-3-methylimidazolium methyl sulfate	2.61
139	1,2-Dimethylimidazolium	2.61
140	1-Ethyl-3-methylimidazolium, salt with methanetricarbonitrile	2.60
141	1-Butyl-4-methylpyridinium chloride	2.59
142	1-(Ethoxymethyl)pyridinium chloride	2.56
143	1-Butyl-3-methylimidazolium hexafluorophosphate	2.55
144	1-Hexylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.52
145	1-Pentylpyridinium bromide	2.51
146	1-Methyl-3-(phenylmethyl)imidazolium hexafluorophosphate	2.50
147	1-Pentylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.49
148	1-Butyl-3-methylimidazolium trifluoromethanesulfonate	2.48
149	1-Methyl-3-pentylimidazolium hexafluorophosphate	2.47
150	1-Butyl-4-methylpyridinium hexafluorophosphate	2.47
151	1-Butyl-3-methylimidazolium tetrafluoroborate	2.47
152	1-Butyl-3-methylimidazolium N-cyanocyanamide	2.47
153	1-Methyl-3-(2-phenylethyl)imidazolium hexafluorophosphate	2.45
154	1-Ethyl-3-methylimidazolium bis(pentafluoroethyl)phosphinate	2.45
155	1-Methyl-3-propylimidazolium hexafluorophosphate	2.43

156	4-(Dimethylamino)-1-ethylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.43
157	1-Butyl-3,4-dimethylpyridinium tetrafluoroborate	2.42
158	1-Ethyl-3-methylimidazolium bis[ethanedioato-O1,O2]borate	2.41
159	1-Hexyl-3-methylimidazolium hexafluorophosphate	2.40
160	1-Methyl-3-(phenylmethyl)imidazolium tetrafluoroborate	2.39
161	1-Hexyl-3-methylimidazolium tetrafluoroborate	2.39
162	1-Methyl-3-pentylimidazolium tetrafluoroborate	2.38
163	1-Butyl-4-methylpyridinium tetrafluoroborate	2.35
164	1-Butyl-3,4-dimethylpyridinium chloride	2.35
165	1-Methyl-3-(2-phenylethyl)imidazolium chloride	2.35
166	1-Methyl-3-(phenylmethyl)imidazolium chloride	2.32
167	1-Methylimidazolium hydrogen tetrafluoroborate	2.32
168	1,3-Diethylimidazolium bromide	2.31
169	4-(Dimethylamino)-1-methylpyridinium iodide	2.31
170	1-Butyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.31
171	1-(Ethoxymethyl)-1-methylpyrrolidinium chloride	2.31
172	1-Butyl-4-methylpyridinium tetracyanoborate	2.30
173	1-Methyl-3-pentylimidazolium chloride	2.28
174	4-(Dimethylamino)-1-ethylpyridinium bromide	2.26
175	1-Butyl-1-methylpyrrolidinium tetrafluoroborate	2.26
176	1-Hexyl-1-methylpyrrolidinium chloride	2.24
177	1-Hexyl-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.21
178	1-Methyl-3-[(4-methylphenyl)methyl]imidazolium hexafluorophosphate	2.18
179	1-Butyl-1-methylpyrrolidinium trifluorotris(pentafluoroethyl)phosphate	2.18
180	1-Hexyl-3-methylimidazolium chloride	2.13
181	1-Methyl-3-(phenylmethyl)imidazolium tetrafluoroborate	2.11
182	1-Hexylpyridinium chloride	2.10
183	1-Hexylpyridinium trifluoromethanesulfonate	2.04
184	1-Heptyl-3-methylimidazolium tetrafluoroborate	2.01
185	1-Hexylpyridinium hexafluorophosphate	2.00
186	1-Hexyl-4-methylpyridinium chloride	2.00
187	1-Methyl-3-[(4-methylphenyl)methyl]imidazolium chloride	1.99
188	1-Methyl-1-octylpyrrolidinium chloride	1.96
189	1-(2-Methoxyethyl)-1-methylpyrrolidinium tris(pentafluoroethyl)trifluorophosphate	1.93
190	1-Butyl-2,3-dimethylimidazolium trifluoromethanesulfonate	1.91
191	1-Hexyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.89
192	1-Heptyl-3-methylimidazolium chloride	1.87
193	1-Hexyl-3-methylimidazolium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide	1.85
194	1-Butyl-3-methylimidazolium (OC-6-11)-hexafluoroantimonate	1.83
195	1-(8-Hydroxyoctyl)-3-methylimidazolium bromide	1.82
196	1-Heptyl-3-methylimidazolium hexafluorophosphate	1.82
197	1-Butylquinolinium bromide	1.74
198	1-Hexyl-3-methylpyridinium chloride	1.73
199	1-Methyl-3-(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)imidazolium hexafluorophosphate	1.70
200	1-Ethyl-3-hexylimidazolium tetrafluoroborate	1.69
201	1-Butyl-3-methylimidazolium 1,1,1-trifluoro-N-(trifluoromethyl)methanaminate	1.65
202	1-Butylquinolinium tetrafluoroborate	1.60
203	1-Hexyl-4-methylpyridinium tetrafluoroborate	1.60
204	1-Methyl-3-octylimidazolium hexafluorophosphate	1.50
205	1-Butyl-4-(dimethylamino)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.49
206	1-Ethyl-3-hexylimidazolium bromide	1.41
207	1-Methyl-3-nonylimidazolium hexafluorophosphate	1.40
208	1-Methyl-3-octylimidazolium chloride	1.38
209	1-Hexyl-2,3-dimethylimidazolium tetrafluoroborate	1.33
210	1-Methyl-3-octylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.32

211	1-Methyl-1-octylpyrrolidinium tetrafluoroborate	1.28
212	1-Butyl-4-(dimethylamino)pyridinium chloride	1.27
213	1-Hexyl-3-methylimidazolium trifluorotris(pentafluoroethyl)phosphate	1.21
214	1-Butyl-3-methylimidazolium thiocyanate	1.18
215	1-Butyl-3-methylimidazolium trifluorotris(pentafluoroethyl)phosphate	1.14
216	3-Methyl-1-octylimidazolium octylsulfate	1.13
217	1-Methyl-3-nonylimidazolium tetrafluoroborate	1.12
218	1-Decyl-3-methylimidazolium hexafluorophosphate	1.06
219	1-Methyl-3-octylimidazolium tetrafluoroborate	1.04
220	4-Methyl-1-octylpyridinium chloride	1.02
221	4-Methyl-1-octylpyridinium tetrafluoroborate	0.95
222	3-Methyl-1-octylpyridinium chloride	0.85
223	1-Methyl-3-nonylimidazolium chloride	0.79
224	1-Decyl-3-methylimidazolium chloride	0.75
225	1-Butyl-2,3-dimethylimidazolium tetrafluoroborate	0.75
226	1-Ethyl-3-methylimidazolium trifluorotris(pentafluoroethyl)phosphate	0.75
227	4-(Dimethylamino)-1-hexylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	0.70
228	1-Octylpyridinium chloride	0.63
229	1-Methyl-3-octylimidazolium trifluormethanesulfonate	0.62
230	1-Hexylquinolinium tetrafluoroborate	0.55
231	1-Ethyl-3-methylimidazolium bis[1,2-benzenediolato-O1,O2]borate	0.55
232	4-(Dimethylamino)-1-hexylpyridinium chloride	0.32
233	1-Decyl-3-methylimidazolium tetrafluoroborate	0.26
234	1-Decyl-3-ethylimidazolium bromide	0.03
235	1-Hexyl-3-methylimidazolium trifluorotris(heptafluoropropyl)phosphate	-0.12
236	1-Butyl-4-methylpyridinium trifluorotris(pentafluoroethyl)phosphate	-0.23
237	1H-Imidazolium, 1-ethyl-2-(8-heptadecenyl)-4,5-dihydro-3-(2-hydroxyethyl)imidazolium ethyl sulfate	-0.23
238	1-Decyl-3-methylimidazolium bromide	-0.25
239	1-Octylquinolinium tetrafluoroborate	-0.31
240	1,3-Didecyl-2-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	-0.32
241	1-Octylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	-0.33
242	1-Methyl-3-octadecylimidazolium chloride	-0.42
243	1-Octylquinolinium bromide	-0.52
244	1-Hexadecyl-3-methylimidazolium chloride	-0.71
245	1-Methyl-3-tetradecylimidazolium chloride	-0.92

Table B10 Ranking of the 232 AChE variables according to decreasing values.

	Name	**AChE. log(EC_{50})**
1	1-Hexyl-3-methylimidazolium trifluorotris(pentafluoroethyl)phosphate	2.79
2	1-Butyl-1-methylpyrrolidinium trifluorotris(pentafluoroethyl)phosphate	2.77
3	4-(2-Ethoxyethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.66
4	4-(3-Methoxypropyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.66
5	1-(2-Ethoxy-2-oxoethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.66
6	4-(3-Hydroxypropyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.64
7	4-(Cyanomethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.62
8	4-(2-Hydroxyethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.56
9	1-(3-Sulfopropyl)pyridinium trifluoromethanesulfonate	2.55
10	4-(2-Methoxyethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.54
11	4-(Ethoxymethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.53
12	1-(2-Hydroxyethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.49
13	1-(7-Carboxyheptyl)-3-methylimidazolium bromide	2.48
14	1-(Cyanomethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.48
15	1-(Cyanomethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.44

16	1-Methyl-3-(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)imidazolium hexafluorophosphate	2.42
17	4-Butyl-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.42
18	4-(2-Ethoxyethyl)-4-methylmorpholinium bromide	2.40
19	1-(3-Hydroxypropyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.40
20	4-(2-Hydroxyethyl)-4-methylmorpholinium iodide	2.40
21	1-(2-Hydroxyethyl)-3-methylimidazolium iodide	2.37
22	1-(3-Hydroxypropyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.36
23	1-(3-Methoxypropyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.35
24	4-(3-Methoxypropyl)-4-methylmorpholinium chloride	2.32
25	3-(3-Carboxypropyl)-1-methylimidazolium chloride	2.31
26	4-(3-Hydroxypropyl)-4-methylmorpholinium chloride	2.29
27	1-Hexyl-3-methylimidazolium trifluorotris(heptafluoropropyl)phosphate	2.28
28	4-(2-Methoxyethyl)-4-methylmorpholinium chloride	2.28
29	1-(2-Hydroxyethyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.26
30	1-Hexyl-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.26
31	4-(Ethoxymethyl)-4-methylmorpholinium chloride	2.26
32	4-(Cyanomethyl)-4-methylmorpholinium chloride	2.25
33	1-(3-Hydroxypropyl)-3-methylimidazolium chloride	2.23
34	1-Methylimidazolium hydrogen tetrafluoroborate	2.23
35	1-(3-Methoxypropyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.22
36	1-(2-Hydroxyethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.22
37	1-(2-Ethoxyethyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.21
38	1-(3-Hydroxypropyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.20
39	1-(2-Ethoxyethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.20
40	1-(3-Hydroxypropyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.18
41	1-Hexyl-3-methylimidazolium tris[(trifluoromethyl)sulfonyl]methide	2.16
42	1-Methyl-3-(3-oxobutyl)imidazolium bromide	2.16
43	1-Ethyl-3-methylimidazolium trifluorotris(pentafluoroethyl)phosphate	2.14
44	1-(3-Hydroxypropyl)-1-methylpyrrolidinium chloride	2.12
45	1-(Cyanomethyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.11
46	1-(2-Methoxyethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.10
47	1-(2-Hydroxyethyl)pyridinium iodide	2.09
48	1-(Cyanomethyl)-1-methylpyrrolidinium chloride	2.09
49	1-(Cyanomethyl)-3-methylimidazolium chloride	2.09
50	4-Butyl-4-methylmorpholinium bromide	2.09
51	1-(Ethoxymethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.07
52	1-(Cyanomethyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.07
53	4-Ethyl-4-methylmorpholinium 4-methylbenzenesulfonate	2.06
54	Pyridine hydrochloride	2.06
55	1-(2-Hydroxyethyl)-1-methylpyrrolidinium iodide	2.04
56	1-(3-Methoxypropyl)-1-methylpyrrolidinium chloride	2.03
57	1-(2-Ethoxyethyl)-1-methylpiperidinium bromide	2.00
58	1-(4-Hydroxybutyl)-3-methylimidazolium chloride	1.98
59	1-(2-Ethoxyethyl)-1-methylpyrrolidinium bromide	1.98
60	1-(2-Hydroxyethyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.96
61	1-Butyl-3-methylimidazolium (T-4)-tetracarbonylcobaltate	1.93
62	1-(3-Methoxypropyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.92
63	1-(3-Methoxypropyl)-3-methylimidazolium chloride	1.89
64	1-(3-Hydroxypropyl)pyridinium chloride	1.89
65	1-(Ethoxymethyl)-3-methylimidazolium chloride	1.86
66	1-(Ethoxymethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.85
67	1-Ethyl-3-methylimidazolium, salt with methanetricarbonitrile	1.84
68	1-(2-Methoxyethyl)-3-methylimidazolium chloride	1.83
69	1-(3-Hydroxypropyl)-1-methylpiperidinium chloride	1.82
70	1-Propylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.82

71	1-Hexyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.80
72	1-(Ethoxymethyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.80
73	1-Hexyl-1-methylpyrrolidinium chloride	1.79
74	1-Ethyl-3-methylimidazolium N-cyanocyanamide	1.79
75	1-(2-Hydroxyethyl)-1-methylpiperidinium iodide	1.78
76	1-(2-Ethoxyethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.76
77	1-(Ethoxymethyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.76
78	1-Butyl-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.75
79	1-(2-Methoxyethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.73
80	1-Methyl-1-octylpyrrolidinium chloride	1.73
81	1-Methyl-3-octylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.71
82	1-(2-Methoxyethyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.71
83	1-Ethyl-3-methylimidazolium bis(pentafluoroethyl)phosphinate	1.71
84	1-(3-Methoxypropyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.70
85	1-Ethyl-3-methylimidazolium 4-methylbenzenesulfonate	1.67
86	1-(Cyanomethyl)-1-methylpiperidinium chloride	1.67
87	1-(Cyanomethyl)pyridinium chloride	1.66
88	1-Methyl-3-propylimidazolium hexafluorophosphate	1.66
89	1-(2-Ethoxyethyl)-3-methylimidazolium bromide	1.64
90	1-Ethyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.63
91	1-(2-Methoxyethyl)-1-methylpyrrolidinium chloride	1.63
92	1-Ethyl-3-methylimidazolium bis[1,2-benzenediolato-O1,O2]borate	1.62
93	1-Methyl-3-propylimidazolium tetrafluoroborate	1.62
94	1-Butyl-3-methylimidazolium hexafluorophosphate	1.60
95	1-Butyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.59
96	1-Ethyl-3-methylimidazolium 2-(2-methoxyethoxy)ethyl sulfate	1.57
97	1-(2-Methoxyethyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.57
98	1-Methyl-3-octylimidazolium hexafluorophosphate	1.56
99	1-Ethyl-3-propylimidazolium bromide	1.55
100	1-Ethyl-3-methylimidazolium trifluoromethanesulfonate	1.55
101	1-Heptyl-3-methylimidazolium tetrafluoroborate	1.55
102	1-Butyl-3-methylimidazolium tetrachloroferrate	1.54
103	1-Butyl-3-methylimidazolium octylsulfate	1.52
104	1-Propylpyridinium bromide	1.52
105	1-Butyl-3-methylimidazolium 2-(2-methoxyethoxy)ethyl sulfate	1.52
106	1-Methyl-3-(phenylmethyl)imidazolium tetrafluoroborate	1.52
107	1-(3-Methoxypropyl)-1-methylpiperidinium chloride	1.52
108	1-Hexyl-3-methylimidazolium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide	1.50
109	1-Hexylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.50
110	1-Methyl-3-(2-propenyl)imidazolium chloride	1.50
111	1-Butyl-3-ethylimidazolium trifluoromethanesulfonate	1.49
112	1-Butyl-3-methylimidazolium 4-methylbenzenesulfonate	1.49
113	1-Ethyl-3-methylimidazolium bis[ethanedioato-O1,O2]borate	1.48
114	1-Methyl-3-propylimidazolium chloride	1.47
115	1-Methyl-1-octylpyrrolidinium tetrafluoroborate	1.47
116	1-Ethyl-3-methylimidazolium hydrogen sulfate	1.45
117	1-Ethyl-3-methylimidazolium ethyl sulfate	1.44
118	1-Butyl-3-methylimidazolium iodide	1.44
119	1-Butyl-3-ethylimidazolium trifluoroacetate	1.44
120	1-(2-Methoxyethyl)-1-methylpiperidinium bromide	1.43
121	1-(Ethoxymethyl)-1-methylpiperidinium chloride	1.43
122	1-Butyl-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.42
123	1-Butyl-3-ethylimidazolium tetrafluoroborate	1.42
124	1-Heptyl-3-methylimidazolium hexafluorophosphate	1.42
125	1-(3-Methoxypropyl)pyridinium chloride	1.42

126	1-Methyl-3-(2-phenylethyl)imidazolium hexafluorophosphate	1.42
127	1-Butyl-4-methylpyridinium trifluorotris(pentafluoroethyl)phosphate	1.41
128	1-Methyl-3-(2-phenylethyl)imidazolium tetrafluoroborate	1.41
129	1-Heptyl-3-methylimidazolium chloride	1.41
130	1-Methyl-3-(phenylmethyl)imidazolium tetrafluoroborate	1.40
131	1-Butyl-3-methylimidazolium trifluoromethanesulfonate	1.39
132	1,3-Diethylimidazolium bromide	1.39
133	1-Butyl-3-methylimidazolium (OC-6-11)-hexafluoroantimonate	1.38
134	1-Ethyl-3-methylimidazolium trifluoroacetate	1.38
135	1-Ethyl-3-methylimidazolium octylsulfate	1.37
136	1-Hexyl-3-methylimidazolium hexafluorophosphate	1.37
137	1-Methyl-3-(phenylmethyl)imidazolium chloride	1.36
138	1-Butyl-3-methylimidazolium methanesulfonate	1.36
139	1-Ethyl-3-methylimidazolium thiocyanate	1.35
140	1-Butyl-3-methylimidazolium methyl sulfate	1.35
141	1-Butyl-3-methylimidazolium hydrogen sulfate	1.34
142	1-Ethyl-3-methylimidazolium tetrafluoroborate	1.34
143	1-Butyl-3-methylimidazolium tetrafluoroborate	1.34
144	1-Ethyl-3-methylimidazolium tetracyanoborate	1.33
145	1-Hexylpyridinium trifluoromethanesulfonate	1.33
146	1-Butylpyridinium trifluoromethanesulfonate	1.33
147	1-Methyl-3-pentylimidazolium hexafluorophosphate	1.32
148	1,2-Dimethylimidazolium	1.32
149	1-(2-Methoxyethyl)pyridinium chloride	1.31
150	1-Butylpyridinium μ-chlorohexachlorodialuminate	1.31
151	1-(Ethoxymethyl)pyridinium chloride	1.30
152	1-Butyl-3-methylimidazolium bromide	1.30
153	1-Butyl-1-methylpyrrolidinium N-cyanocyanamide	1.29
154	1-Butyl-3-methylimidazolium thiocyanate	1.29
155	1-Butylpyridinium hexafluorophosphate	1.29
156	1-Hexyl-3-methylimidazolium tetrafluoroborate	1.28
157	1-Butyl-1-methylpyrrolidinium bromide	1.28
158	1-Ethyl-3-hexylimidazolium tetrafluoroborate	1.27
159	1-Butyl-1-methylpyrrolidinium tetrafluoroborate	1.26
160	1-Methyl-3-(2-phenylethyl)imidazolium chloride	1.26
161	1-Ethylpyridinium chloride	1.26
162	1-Decyl-3-methylimidazolium hexafluorophosphate	1.25
163	1-Hexylpyridinium hexafluorophosphate	1.25
164	1-Ethyl-3-methylimidazolium chloride	1.25
165	1-Methyl-3-(phenylmethyl)imidazolium hexafluorophosphate	1.24
166	1-Butyl-3-methylimidazolium N-cyanocyanamide	1.24
167	1-Methyl-3-pentylimidazolium tetrafluoroborate	1.24
168	1-Methyl-3-pentylimidazolium chloride	1.24
169	1-Hexyl-3-methylimidazolium chloride	1.22
170	1-Methyl-3-[(4-methylphenyl)methyl]imidazolium chloride	1.20
171	1-Butyl-1-methylpiperidinium bromide	1.20
172	1-Ethyl-3-hexylimidazolium bromide	1.18
173	1-Pentylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.18
174	1-Methyl-3-nonylimidazolium hexafluorophosphate	1.17
175	1-Butyl-1-methylpyrrolidinium chloride	1.17
176	1-Butyl-3-methylimidazolium chloride	1.16
177	1-Butylpyridinium methyl sulfate	1.15
178	1-Butylpyridinium tetrafluoroborate	1.15
179	1-(2-Ethoxyethyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.12
180	1-(Ethoxymethyl)-1-methylpyrrolidinium chloride	1.11

181	1-Butylpyridinium bromide	1.10
182	1-Octylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.08
183	1-Butyl-3-methylimidazolium 1,1,1-trifluoro-N-(trifluoromethyl)methanaminate	1.07
184	1-Hexylpyridinium chloride	1.02
185	3-Methyl-1-octylimidazolium octylsulfate	0.98
186	1-Methyl-3-octylimidazolium tetrafluoroborate	0.98
187	1-Methyl-3-octylimidazolium chloride	0.96
188	1-Octylpyridinium chloride	0.96
189	1-Butylpyridinium chloride	0.93
190	1-Butyl-4-methylpyridinium tetrafluoroborate	0.92
191	1-(2-Ethoxyethyl)pyridinium bromide	0.92
192	1-Methyl-3-nonylimidazolium tetrafluoroborate	0.90
193	1-Hexyl-4-methylpyridinium tetrafluoroborate	0.90
194	1-Butyl-4-methylpyridinium hexafluorophosphate	0.90
195	1-Butyl-4-methylpyridinium tetracyanoborate	0.88
196	1-Pentylpyridinium bromide	0.88
197	1-Hexyl-4-methylpyridinium chloride	0.77
198	1-Methyl-3-nonylimidazolium chloride	0.75
199	1-(8-Hydroxyoctyl)-3-methylimidazolium bromide	0.74
200	1-Butyl-3-methylpyridinium hexafluorophosphate	0.71
201	1-Butyl-4-methylpyridinium chloride	0.71
202	1-Hexyl-2,3-dimethylimidazolium tetrafluoroborate	0.69
203	4-Methyl-1-octylpyridinium tetrafluoroborate	0.69
204	1-Butyl-3-methylpyridinium tetrafluoroborate	0.64
205	1-Decyl-3-methylimidazolium tetrafluoroborate	0.58
206	1-Butyl-3,5-dimethylpyridinium tetrafluoroborate	0.56
207	4-(Dimethylamino)-1-ethylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	0.56
208	1-Butyl-3-methylpyridinium N-cyanocyanamide	0.55
209	1-Methyl-3-octadecylimidazolium chloride	0.53
210	1-Decyl-3-methylimidazolium chloride	0.50
211	1-Butyl-3,4-dimethylpyridinium tetrafluoroborate	0.50
212	4-(Dimethylamino)-1-hexylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	0.50
213	4-Methyl-1-octylpyridinium chloride	0.50
214	1-Decyl-3-ethylimidazolium bromide	0.42
215	1-Butyl-3-methylpyridinium chloride	0.42
216	1-Hexyl-3-methylpyridinium chloride	0.39
217	4-(Dimethylamino)-1-ethylpyridinium bromide	0.36
218	1-Butyl-3,5-dimethylpyridinium chloride	0.29
219	1-Butyl-4-(dimethylamino)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	0.25
220	1-Hexadecyl-3-methylimidazolium chloride	0.22
221	1-Butylquinolinium bromide	0.22
222	1-Butyl-2-methylpyridinium tetrafluoroborate	0.20
223	1-Butyl-3,4-dimethylpyridinium chloride	0.15
224	1-Butylquinolinium tetrafluoroborate	0.05
225	1-Methyl-3-tetradecylimidazolium chloride	0.04
226	3-Methyl-1-octylpyridinium chloride	0.02
227	1-Butyl-2-methylpyridinium chloride	-0.03
228	1-Hexylquinolinium tetrafluoroborate	-0.04
229	1-Butyl-4-(dimethylamino)pyridinium chloride	-0.07
230	4-(Dimethylamino)-1-hexylpyridinium chloride	-0.12
231	1-Octylquinolinium tetrafluoroborate	-0.18
232	1-Octylquinolinium bromide	-0.20

Table B11 List of the 103 ionic liquids used in the aquatic toxicity PLS model, with their t[1] scores and the corresponding PLS scores predictions[a].

IL	IL code	IL name	Aq. Tox. scores	*Pred.* Aq. Tox. Scores
6	Pyr11COO2 (CF3SO2)2N	1-(2-Ethoxy-2-oxoethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	0.491	1.598
7	Pyr11COO2 Br	1-(2-Ethoxy-2-oxoethyl)-1-methylpyrrolidinium bromide	1.025	2.189
10	Pyr14 Cl	1-Butyl-1-methylpyrrolidinium chloride	1.109	1.589
17	Pyr16 (CF3SO2)2N	1-Hexyl-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	-0.484	0.029
21	Pyr13OH (CF3SO2)2N	1-(3-Hydroxypropyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.224	0.979
27	Pyr12O1 (CF3SO2)2N	1-(2-Methoxyethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	0.31	1.037
30	Pyr12O2 (CF3SO2)2N	1-(2-Ethoxyethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	0.179	0.521
36	Pip13 (CF3SO2)2N	1-Methyl-1-propylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.781	1.845
37	Pip13 PF6	1-Methyl-1-propylpiperidinium hexafluorophosphate	2.895	1.883
38	Pip14 (CF3SO2)2N	1-Butyl-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	0.973	0.982
39	Pip14 Br	1-Butyl-1-methylpiperidinium bromide	2.444	1.573
42	Pip13O1 (CF3SO2)2N	1-(3-Methoxypropyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	0.207	0.673
55	Mor14 (CF3SO2)2N	4-Butyl-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.437	0.901
56	Mor14 Br	4-Butyl-4-methylmorpholinium bromide	3.176	1.493
67	Mor11O2 (CF3SO2)2N	4-(Ethoxymethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.218	0.842
75	IM14-2Me (CF3SO2)2N	1-Butyl-2,3-dimethylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	-0.159	0.546
81	IM11 (CF3SO2)2N	1,3-Dimethylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3.911	2.269
85	IM11(COO1)(Ph-(3,4-OCH2O-)) Cl	1-[1-(1,3-Benzodioxol-5-yl)-2-methoxy-2-oxoethyl]-3-methylimidazolium chloride	-0.695	0.216
86	IM11(COO4)(Ph-(3,4-OCH2O-)) Br	1-[1-(1,3-Benzodioxol-5-yl)-2-butoxy-2-oxoethyl]-3-methylimidazolium bromide	-0.082	-0.434
87	IM12 (C2F5)3PF3	1-Ethyl-3-methylimidazolium trifluorotris(pentafluoroethyl)phosphate	-3.604	-2.713
88	IM12 (C2F5)2PO2	1-Ethyl-3-methylimidazolium bis(pentafluoroethyl)phosphinate	-0.209	-0.232
89	IM12 C(CN)3	1-Ethyl-3-methylimidazolium, salt with methanetricarbonitrile	0.237	1.215
90	IM12 B(CN)4	1-Ethyl-3-methylimidazolium tetracyanoborate	0.462	0.367
91	IM12 N(CN)2	1-Ethyl-3-methylimidazolium N-cyanocyanamide	0.599	2.151
92	IM12 (CF3SO2)2N	1-Ethyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	0.871	1.61

93	IM12 Cl	1-Ethyl-3-methylimidazolium chloride	1	2.001
94	IM12 2OSO3	1-Ethyl-3-methylimidazolium ethyl sulfate	3.214	2.114
111	IM11CN Cl	1-(Cyanomethyl)-3-methylimidazolium chloride	1.535	1.455
112	IM11CN (CF3SO2)2N	1-(Cyanomethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.73	1.064
117	IM11COO1(COO4)(Ph-(3,4-OCH2O-)) Br	1-[2-[1-(1,3-Benzodioxol-5-yl)-2-butoxy-2-oxoethoxy]-2-oxoethyl]-3-methylimidazolium bromide	-1.959	-1.352
136	IM1i4 (CF3SO2)2N	1-Methyl-3-(2-methylpropyl)imidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.317	0.709
147	IM13 BF4	1-Methyl-3-propylimidazolium tetrafluoroborate	0.92	0.762
148	IM13 (CF3SO2)2N	1-Methyl-3-propylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.252	0.971
149	IM13 PF6	1-Methyl-3-propylimidazolium hexafluorophosphate	2.895	1.01
160	IM14 8OSO3	1-Butyl-3-methylimidazolium octylsulfate	-0.887	0.094
161	IM14 CF3SO3	1-Butyl-3-methylimidazolium trifluoromethanesulfonate	-0.192	0.581
162	IM14 (CF3)2N	1-Butyl-3-methylimidazolium 1,1,1-trifluoro-N-(trifluoromethyl)methanaminate	-0.061	0.164
163	IM14 BF4	1-Butyl-3-methylimidazolium tetrafluoroborate	-0.055	-0.018
164	IM14 (CF3SO2)2N	1-Butyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	0.022	0.191
165	IM14 PF6	1-Butyl-3-methylimidazolium hexafluorophosphate	0.214	0.229
166	IM14 Cl	1-Butyl-3-methylimidazolium chloride	0.272	0.582
167	IM14 I	1-Butyl-3-methylimidazolium iodide	0.637	0.523
168	IM14 Br	1-Butyl-3-methylimidazolium bromide	1.92	0.782
169	IM14 N(CN)2	1-Butyl-3-methylimidazolium N-cyanocyanamide	1.967	0.732
170	IM14 4MePhSO3	1-Butyl-3-methylimidazolium 4-methylbenzenesulfonate	2.013	0.711
171	IM14 1SO3	1-Butyl-3-methylimidazolium methanesulfonate	2.609	0.919
187	IM15 (CF3SO2)2N	1-Methyl-3-pentylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	-1.155	-0.423
188	IM15 BF4	1-Methyl-3-pentylimidazolium tetrafluoroborate	0.944	-0.632
191	IM16 (CF3SO2)2N	1-Hexyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	-2.863	-1.478
192	IM16 Br	1-Hexyl-3-methylimidazolium bromide	-2.429	-0.887
193	IM16 Cl	1-Hexyl-3-methylimidazolium chloride	-1.566	-1.086
194	IM16 PF6	1-Hexyl-3-methylimidazolium hexafluorophosphate	-1.539	-1.44
195	IM16 (2-SO2PhCO)N	1-Hexyl-3-methylimidazolium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide	-0.276	-0.784
196	IM16 BF4	1-Hexyl-3-methylimidazolium tetrafluoroborate	0.147	-1.687
203	IM17 (CF3SO2)2N	1-Heptyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	-2.128	-1.766

204	IM17 BF4	1-Heptyl-3-methylimidazolium tetrafluoroborate	-0.663	-1.975
207	IM18 BF4	1-Methyl-3-octylimidazolium tetrafluoroborate	-5.319	-2.477
208	IM18 Br	1-Methyl-3-octylimidazolium bromide	-3.926	-1.677
209	IM18 (CF3SO2)2N	1-Methyl-3-octylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	-3.754	-2.268
215	IM19 BF4	1-Methyl-3-nonylimidazolium tetrafluoroborate	-2.571	-3.09
218	IM1-10 BF4	1-Decyl-3-methylimidazolium tetrafluoroborate	-3.564	-3.524
224	IM1-10COO2 Br	1-(11-Ethoxy-11-oxoundecyl)-3-methylimidazolium bromide	-3.926	-3.835
227	IM1-14 Cl	1-Methyl-3-tetradecylimidazolium chloride	-6.903	-5.346
229	IM1-16 Cl	1-Hexadecyl-3-methylimidazolium chloride	-5.987	-6.318
231	IM1-18 Cl	1-Methyl-3-octadecylimidazolium chloride	-4.759	-7.846
234	IM13OH Cl	1-(3-Hydroxypropyl)-3-methylimidazolium chloride	2.623	1.708
235	IM13OH (CF3SO2)2N	1-(3-Hydroxypropyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3.236	1.316
236	IM13O1 (CF3SO2)2N	1-(3-Methoxypropyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.288	0.264
237	IM13O1 Cl	1-(3-Methoxypropyl)-3-methylimidazolium chloride	1.383	0.655
238	IM12OH I	1-(2-Hydroxyethyl)-3-methylimidazolium iodide	2.155	2.108
245	IM12O1 (CF3SO2)2N	1-(2-Methoxyethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	0.732	1.069
246	IM12O1 Cl	1-(2-Methoxyethyl)-3-methylimidazolium chloride	0.878	1.461
249	IM12O2 (CF3SO2)2N	1-(2-Ethoxyethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	-0.28	0.428
250	IM12O2 Br	1-(2-Ethoxyethyl)-3-methylimidazolium bromide	0.769	1.02
252	IM12O2O1 Cl	1-[2-(2-Methoxyethoxy)ethyl]-3-methylimidazolium chloride	-1.421	0.095
253	IM11O2 (CF3SO2)2N	1-(Ethoxymethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	0.462	0.654
254	IM11O2 Cl	1-(Ethoxymethyl)-3-methylimidazolium chloride	2.382	1.046
280	Py4-3Me-5Me N(CN)2	1-Butyl-3,5-dimethylpyridinium N-cyanocyanamide	-0.537	-0.279
281	Py4-3Me-5Me Br	1-Butyl-3,5-dimethylpyridinium bromide	0.13	-0.23
289	Py4-3Me N(CN)2	1-Butyl-3-methylpyridinium N-cyanocyanamide	-0.041	0.407
290	Py4-3Me Br	1-Butyl-3-methylpyridinium bromide	0.207	0.456
295	Py6-3Me Br	1-Hexyl-3-methylpyridinium bromide	-1.079	-1.171
297	Py8-3Me Br	3-Methyl-1-octylpyridinium bromide	-3.563	-2.312
316	IM22 (CF3SO2)2N	1,3-Diethylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.039	1.464
318	IM23 (CF3SO2)2N	1-Ethyl-3-propylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	-0.199	1.072

323	IM26 BF4	1-Ethyl-3-hexylimidazolium tetrafluoroborate	-0.996	-1.243
331	Py4-4Me BF4	1-Butyl-4-methylpyridinium tetrafluoroborate	-0.073	-0.082
347	Py6-4NMe2 (CF3SO2)2N	4-(Dimethylamino)-1-hexylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	-1.573	-1.724
349	IM33 (CF3SO2)2N	1,3-Dipropylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	-1.205	0.352
350	IM44 (CF3SO2)2N	1,3-Dibutylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	-0.707	-0.644
369	IM55 (CF3SO2)2N	1,3-Dipentylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	-1.736	-1.862
370	Py1(COO1)(Ph-3-OMe-4-OMe) Cl	1-[1-(3,4-Dimethoxyphenyl)-2-methoxy-2-oxoethyl]pyridinium chloride	-0.49	0.007
371	Py1(COO1)(Ph-(3,4-OCH2O-)) Br	1-[1-(1,3-Benzodioxol-5-yl)-2-methoxy-2-oxoethyl]pyridinium bromide	1.22	0.383
372	Py1(COO4)(Ph-(3,4-OCH2O-)) Br	1-[1-(1,3-Benzodioxol-5-yl)-2-butoxy-2-oxoethyl]pyridinium bromide	-0.414	-0.75
376	Py1COO1(COO1)(Ph-(3,4-OCH2O-)) Br	1-[2-[1-(1,3-Benzodioxol-5-yl)-2-methoxy-2-oxoethoxy]-2-oxoethyl]pyridinium bromide	-2.128	-1.379
384	Py4 Cl	1-Butylpyridinium chloride	0.086	1.121
385	Py4 Al2Cl7	1-Butylpyridinium μ-chlorohexachlorodialuminate	0.226	0.447
386	Py4 N(CN)2	1-Butylpyridinium N-cyanocyanamide	1.215	1.271
387	Py4 Br	1-Butylpyridinium bromide	1.443	1.32
395	Py6 (CF3SO2)2N	1-Hexylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.25	-0.792
399	Py8 Cl	1-Octylpyridinium chloride	-1.594	-1.669
404	Py3OH (CF3SO2)2N	1-(3-Hydroxypropyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.331	1.193
418	IM66 (CF3SO2)2N	1,3-Dihexylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	-1.212	-2.749

[a] Y_predictions according to PLS correlation model, as reported in the section 3.3.1. ILs numeration as in the other PLS datamatrices.

Table B12 Experimental and predicted[a] IPC-81 cytotoxicity values. The (*) indicates a DModX value higher than 1.50, corresponding to 95% C.I. L: learning set; T: test set; U: unknown log(EC_{50}).

IL	Il code	IL name	Set	Y = log (EC_{50}) *IPC-81 mg/L*	Ý = log (EC_{50}) *IPC-81 pred.*	Y-Ý	Confidence Interval (C.I.) for prediction	DModX
1	Py4-2Me BF4	1-Butyl-2-methylpyridinium tetrafluoroborate	L	2.62	2.18	0.45		0.47
2	Py4-2Me Cl	1-Butyl-2-methylpyridinium chloride	L	3.02	2.75	0.26		0.65
3	Pyr12 2OSO3	1-Ethyl-1-methylpyrrolidinium ethyl sulfate	U		2.88		2.56 - 3.21	1.04
4	Pyr11CN (CF3SO2)2N	1-(Cyanomethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	3.41	3.24	0.17		0.60
5	Pyr11CN Cl	1-(Cyanomethyl)-1-methylpyrrolidinium chloride	L	3.44	3.69	-0.25		0.71
6	Pyr11COO2 (CF3SO2)2N	1-(2-Ethoxy-2-oxoethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	3.25	3.62	-0.37		0.89
7	Pyr11COO2 Br	1-(2-Ethoxy-2-oxoethyl)-1-methylpyrrolidinium bromide	L	3.25	4.05	-0.80		0.91
8	Pyr11COO2 (C2F5)3PF3	1-(2-Ethoxy-2-oxoethyl)-1-methylpyrrolidinium tris(pentafluoroethyl)trifluorophosphate	L	2.70	2.97	-0.27		1.70*
9	Pyr13 PF6	1-Methyl-1-propylpyrrolidinium hexafluorophosphate	U		2.62		2.26 - 2.98	1.22
10	Pyr14 Cl	1-Butyl-1-methylpyrrolidinium chloride	L	3.55	2.94	0.61		1.17
11	Pyr14 (C2F5)3PF3	1-Butyl-1-methylpyrrolidinium trifluorotris(pentafluoroethyl)phosphate	L	2.18	1.83	0.35		1.58*
12	Pyr14 (CF3SO2)2N	1-Butyl-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	2.63	2.48	0.15		1.05
13	Pyr14 1OSO3	1-Butyl-1-methylpyrrolidinium methyl sulfate	U		2.51		2.18 - 2.83	1.07
14	Pyr14 BF4	1-Butyl-1-methylpyrrolidinium tetrafluoroborate	L	2.26	2.36	-0.10		1.30
15	Pyr14 Br	1-Butyl-1-methylpyrrolidinium bromide	L	3.11	2.92	0.20		1.14
16	Pyr14 N(CN)2	1-Butyl-1-methylpyrrolidinium N-cyanocyanamide	T	3.55	2.62	0.93	2.37 - 2.88	1.12
17	Pyr16 (CF3SO2)2N	1-Hexyl-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	2.21	2.13	0.08		1.01
18	Pyr16 Cl	1-Hexyl-1-methylpyrrolidinium chloride	L	2.24	2.58	-0.34		1.18
19	Pyr18 BF4	1-Methyl-1-octylpyrrolidinium tetrafluoroborate	L	1.28	1.56	-0.29		1.19
20	Pyr18 Cl	1-Methyl-1-octylpyrrolidinium chloride	L	1.96	2.14	-0.18		1.18
21	Pyr13OH (CF3SO2)2N	1-(3-Hydroxypropyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	3.23	2.94	0.29		0.58
22	Pyr13OH Cl	1-(3-Hydroxypropyl)-1-methylpyrrolidinium chloride	L	4.30	3.39	0.91		1.16
23	Pyr13O1 (CF3SO2)2N	1-(3-Methoxypropyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	3.40	2.92	0.48		0.63

24	Pyr13O1 Cl	1-(3-Methoxypropyl)-1-methylpyrrolidinium chloride	L	3.99	3.38	0.61			0.92
25	Pyr12OH (CF3SO2)2N	1-(2-Hydroxyethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	3.33	3.09	0.24			0.70
26	Pyr12OH I	1-(2-Hydroxyethyl)-1-methylpyrrolidinium iodide	L	3.71	3.48	0.23			1.10
27	Pyr12O1 (CF3SO2)2N	1-(2-Methoxyethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	2.93	3.09	-0.16			0.58
28	Pyr12O1 (C2F5)3PF3	1-(2-Methoxyethyl)-1-methylpyrrolidinium tris(pentafluoroethyl)trifluorophosphate	L	1.93	2.44	-0.50			1.53*
29	Pyr12O1 Cl	1-(2-Methoxyethyl)-1-methylpyrrolidinium chloride	L	3.56	3.54	0.01			0.90
30	Pyr12O2 (CF3SO2)2N	1-(2-Ethoxyethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	2.84	2.94	-0.10			0.72
31	Pyr12O2 Br	1-(2-Ethoxyethyl)-1-methylpyrrolidinium bromide	L	3.68	3.37	0.30			0.95
32	Pyr11O2 (CF3SO2)2N	1-(Ethoxymethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	2.89	2.95	-0.07			0.88
33	Pyr11O2 Cl	1-(Ethoxymethyl)-1-methylpyrrolidinium chloride	L	2.31	3.40	-1.10			1.07
34	Pip11CN (CF3SO2)2N	1-(Cyanomethyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	3.57	3.03	0.54			0.58
35	Pip11CN Cl	1-(Cyanomethyl)-1-methylpiperidinium chloride	T	3.82	3.48	0.34	3.1	- 3.87	0.72
36	Pip13 (CF3SO2)2N	1-Methyl-1-propylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	2.78	2.58	0.20			1.11
37	Pip13 PF6	1-Methyl-1-propylpiperidinium hexafluorophosphate	U		2.52		2.16	- 2.89	1.25
38	Pip14 (CF3SO2)2N	1-Butyl-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	3.05	2.38	0.67			1.08
39	Pip14 Br	1-Butyl-1-methylpiperidinium bromide	L	3.41	2.81	0.59			1.18
40	Pip13OH (CF3SO2)2N	1-(3-Hydroxypropyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	3.25	2.79	0.46			0.53
41	Pip13OH Cl	1-(3-Hydroxypropyl)-1-methylpiperidinium chloride	T	3.76	3.24	0.52	2.92	- 3.56	1.13
42	Pip13O1 (CF3SO2)2N	1-(3-Methoxypropyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	T	2.92	2.78	0.15	2.53	- 3.02	0.62
43	Pip13O1 Cl	1-(3-Methoxypropyl)-1-methylpiperidinium chloride	L	3.72	3.23	0.49			0.94
44	Pip12OH (CF3SO2)2N	1-(2-Hydroxyethyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	3.28	2.91	0.37			0.68
45	Pip12OH I	1-(2-Hydroxyethyl)-1-methylpiperidinium iodide	T	4.01	3.29	0.72	3.03	- 3.56	1.13
46	Pip12O1 (CF3SO2)2N	1-(2-Methoxyethyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	2.89	2.98	-0.09			0.77
47	Pip12O1 Br	1-(2-Methoxyethyl)-1-methylpiperidinium bromide	L	3.98	3.42	0.56			0.96
48	Pip12O2 (CF3SO2)2N	1-(2-Ethoxyethyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	3.00	2.83	0.16			0.73
49	Pip12O2 Br	1-(2-Ethoxyethyl)-1-methylpiperidinium bromide	L	3.71	3.26	0.44			0.96

50	Pip11O2 (CF3SO2)2N	1-(Ethoxymethyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	3.05	2.78	0.27			0.88
51	Pip11O2 Cl	1-(Ethoxymethyl)-1-methylpiperidinium chloride	L	3.52	3.23	0.29			1.07
52	Mor12 4MePhSO3	4-Ethyl-4-methylmorpholinium 4-methylbenzenesulfonate	L	3.29	3.49	-0.20			0.80
53	Mor11CN (CF3SO2)2N	4-(Cyanomethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	3.16	3.79	-0.63			0.70
54	Mor11CN Cl	4-(Cyanomethyl)-4-methylmorpholinium chloride	L	3.55	4.24	-0.69			0.73
55	Mor14 (CF3SO2)2N	4-Butyl-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	T	3.07	2.91	0.17	2.66	- 3.15	0.55
56	Mor14 Br	4-Butyl-4-methylmorpholinium bromide	L	3.68	3.34	0.34			0.86
57	Mor13OH (CF3SO2)2N	4-(3-Hydroxypropyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	3.19	3.46	-0.27			0.68
58	Mor13OH Cl	4-(3-Hydroxypropyl)-4-methylmorpholinium chloride	L	3.59	3.92	-0.32			1.16
59	Mor13O1 (CF3SO2)2N	4-(3-Methoxypropyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	3.43	3.48	-0.05			0.76
60	Mor13O1 Cl	4-(3-Methoxypropyl)-4-methylmorpholinium chloride	L	3.80	3.94	-0.14			0.94
61	Mor12OH (CF3SO2)2N	4-(2-Hydroxyethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	2.82	3.68	-0.86			0.73
62	Mor12OH I	4-(2-Hydroxyethyl)-4-methylmorpholinium iodide	L	3.74	4.06	-0.33			1.06
63	Mor12O1 (CF3SO2)2N	4-(2-Methoxyethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	3.45	3.71	-0.25			0.77
64	Mor12O1 Cl	4-(2-Methoxyethyl)-4-methylmorpholinium chloride	T	3.59	4.16	-0.57	3.64	- 4.68	0.92
65	Mor12O2 (CF3SO2)2N	4-(2-Ethoxyethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	3.35	3.48	-0.13			0.68
66	Mor12O2 Br	4-(2-Ethoxyethyl)-4-methylmorpholinium bromide	L	3.71	3.91	-0.21			0.88
67	Mor11O2 (CF3SO2)2N	4-(Ethoxymethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	T	3.06	3.62	-0.55	3.41	- 3.83	0.76
68	Mor11O2 Cl	4-(Ethoxymethyl)-4-methylmorpholinium chloride	T	2.81	4.07	-1.26	3.56	- 4.59	0.92
69	IM11COO3-2Me 8OSO3	1,2-Dimethyl-3-(2-oxo-2-propoxyethyl)imidazolium octylsulfate	U		3.65		3.33	- 3.97	1.46
70	IM11COO3-2Me Br	1,2-Dimethyl-3-(2-oxo-2-propoxyethyl)imidazolium bromide	U		4.09		3.67	- 4.51	0.88
71	IM11COO5-2Me 8OSO3	1,2-Dimethyl-3-[2-oxo-2-(pentyloxy)ethyl]imidazolium octylsulfate	U		3.32		2.99	- 3.66	1.55*
72	IM11COO5-2Me Br	1,2-Dimethyl-3-[2-oxo-2-(pentyloxy)ethyl]imidazolium bromide	U		3.76		3.36	- 4.17	1.06
73	IM1gly-2Me N(NC)2	1,2-dimethyl-3-glycerylimidazolium dicyanamide	U		2.91		2.31	- 3.50	2.33*
74	IM1gly-2Me (CF3SO2)2N	1,2-dimethyl-3-glycerylimidazolium bis(trifluoromethylsulphonyl)imide	U		2.77		2.05	- 3.48	2.21*
75	IM14-2Me (CF3SO2)2N	1-Butyl-2,3-dimethylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		2.32		1.98	- 2.65	0.82
76	IM14-2Me BF4	1-Butyl-2,3-dimethylimidazolium tetrafluoroborate	L	0.75	2.19	-1.45			0.66

77	IM14-2Me CF3SO3	1-Butyl-2,3-dimethylimidazolium trifluoromethanesulfonate	L	1.91	2.24	-0.34			0.47
78	IM16-2Me BF4	1-Hexyl-2,3-dimethylimidazolium tetrafluoroborate	L	1.33	1.40	-0.07			0.55
79	IM16-2Me (CF3SO2)2N	1-hexyl-2,3-dimethylimidazolium bis(trifluoromethylsulphonyl)imide	U		1.52		0.99	2.05	1.05
80	IM12OH-2Me Cl	1-(2-hydroxyethyl)-2,3-dimethylimidazolium chloride	U		3.34		2.99	3.68	1.51*
81	IM11 (CF3SO2)2N	1,3-Dimethylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		3.19		2.96	3.41	1.03
82	IM11 1OSO3	1,3-dimethylimidazolium methylsulfate	U		3.21		2.98	3.43	0.60
83	IM11 4MePhSO3	1,3-dimethylimidazolium p-toluenesulfonate	U		3.27		3	3.53	1.23
84	IM11 N(CN)2	1-methyl-3-methylimidaziolium N-cyanocyanamide	U		3.33		3.21	3.45	0.92
85	IM11(COO1)(Ph-(3,4-OCH2O-)) Cl	1-[1-(1,3-Benzodioxol-5-yl)-2-methoxy-2-oxoethyl]-3-methylimidazolium chloride	U		4.67		4.14	5.20	1.84*
86	IM11(COO4)(Ph-(3,4-OCH2O-)) Br	1-[1-(1,3-Benzodioxol-5-yl)-2-butoxy-2-oxoethyl]-3-methylimidazolium bromide	U		4.01		3.53	4.49	1.80*
87	IM12 (C2F5)3PF3	1-Ethyl-3-methylimidazolium trifluorotris(pentafluoroethyl)phosphate	L	0.75	2.34	-1.60			1.44
88	IM12 (C2F5)2PO2	1-Ethyl-3-methylimidazolium bis(pentafluoroethyl)phosphinate	L	2.45	2.68	-0.24			0.90
89	IM12 C(CN)3	1-Ethyl-3-methylimidazolium, salt with methanetricarbonitrile	L	2.60	3.46	-0.85			3.15*
90	IM12 B(CN)4	1-Ethyl-3-methylimidazolium tetracyanoborate	L	2.86	3.14	-0.28			2.73*
91	IM12 N(CN)2	1-Ethyl-3-methylimidazolium N-cyanocyanamide	L	3.07	3.14	-0.07			0.90
92	IM12 (CF3SO2)2N	1-Ethyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	2.91	2.99	-0.08			1.01
93	IM12 Cl	1-Ethyl-3-methylimidazolium chloride	L	3.16	3.45	-0.29			0.63
94	IM12 2OSO3	1-Ethyl-3-methylimidazolium ethyl sulfate	L	3.30	3.05	0.25			0.54
95	IM12 (OOCCOO)2B	1-Ethyl-3-methylimidazolium bis[ethanedioato-O1,O2]borate	L	2.41	2.60	-0.19			1.56*
96	IM12 1COO	1-Ethyl-3-methylimidazolium acetate	L	3.46	3.35	0.10			1.80*
97	IM12 1O2O2OSO3	1-Ethyl-3-methylimidazolium 2-(2-methoxyethoxy)ethyl sulfate	L	3.34	2.69	0.64			1.22
98	IM12 1OSO3	1-Ethyl-3-methylimidazolium methylsulfate	L	3.54	3.02	0.53			0.53
99	IM12 1SO3	1-Ethyl-3-methylimidazolium methanesulfonate	T	3.29	3.06	0.22	2.85	3.28	0.49
100	IM12 4MePhSO3	1-Ethyl-3-methylimidazolium 4-methylbenzenesulfonate	L	3.26	3.08	0.18			1.22
101	IM12 8OSO3	1-Ethyl-3-methylimidazolium octylsulfate	L	2.73	2.99	-0.26			1.43
102	IM12 BF4	1-Ethyl-3-methylimidazolium tetrafluoroborate	T	2.73	2.87	-0.14	2.63	3.11	0.73
103	IM12 CF3COO	1-Ethyl-3-methylimidazolium trifluoroacetate	L	3.35	2.99	0.36			1.06
104	IM12 CF3SO3	1-Ethyl-3-methylimidazolium trifluoromethanesulfonate	T	3.50	2.92	0.58	2.73	3.11	0.59
105	IM12 HSO4	1-Ethyl-3-methylimidazolium hydrogen sulfate	L	3.31	2.92	0.39			0.84

106	IM12 PF6	1-Ethyl-3-methylimidazolium hexafluorophosphate	U		2.94		2.72 - 3.15		0.61
107	IM12 SCN	1-Ethyl-3-methylimidazolium thiocyanate	L	3.45	3.39	0.06			0.78
108	IM12 Br	1-Ethyl-3-methylimidazolium bromide	U		3.43		3.08 - 3.77		0.59
109	IM12 NO3	1-Ethyl-3-methylimidazolium nitrate	U		3.49		3.24 - 3.74		1.55*
110	IM12 FeCl4	1-ethyl-3-methylimidazolium tetrachloroferrate	U		3.45		3.24 - 3.65		0.99
111	IM11CN Cl	1-(Cyanomethyl)-3-methylimidazolium chloride	L	3.50	4.02	-0.52			1.01
112	IM11CN (CF3SO2)2N	1-(Cyanomethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	3.51	3.56	-0.06			1.50
113	IM11CONMeBu Br	1-[2-(Butylmethylamino)-2-oxoethyl]-3-methylimidazolium bromide	U		3.29		3 - 3.58		0.80
114	IM11CONEt2 Br	1-[2-(Diethylamino)-2-oxoethyl]-3-methylimidazolium bromide	U		3.53		3.22 - 3.84		0.76
115	IM11CONHBu Br	1-[2-(Butylamino)-2-oxoethyl]-3-methylimidazolium bromide	U		3.50		3.17 - 3.82		1.01
116	IM11COO1 Br	1-(2-Methoxy-2-oxoethyl)-3-methylimidazolium bromide	U		4.31		3.87 - 4.75		0.71
117	IM11COO1(COO4)(Ph-(3,4-OCH2O-)) Br	1-[2-[1-(1,3-Benzodioxol-5-yl)-2-butoxy-2-oxoethoxy]-2-oxoethyl]-3-methylimidazolium bromide	U		5.07		4.41 - 5.74		3.05*
118	IM11COO2 BF4	1-(2-Ethoxy-2-oxoethyl)-3-methylimidazolium tetrafluoroborate	U		3.52		3.12 - 3.92		1.17
119	IM11COO2 Br	1-(2-Ethoxy-2-oxoethyl)-3-methylimidazolium bromide	U		4.07		3.65 - 4.50		0.75
120	IM11COO3 (CF3SO2)2N	1-Methyl-3-(2-oxo-2-propoxyethyl)imidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		3.61		3.42 - 3.79		1.10
121	IM11COO3 8OSO3	1-Methyl-3-(2-oxo-2-propoxyethyl)imidazolium octylsulfate	U		3.60		3.29 - 3.90		1.41
122	IM11COO3 BF4	1-Methyl-3-(2-oxo-2-propoxyethyl)imidazolium tetrafluoroborate	U		3.48		3.08 - 3.88		1.20
123	IM11COO3 Br	1-Methyl-3-(2-oxo-2-propoxyethyl)imidazolium bromide	U		4.04		3.6 - 4.48		0.87
124	IM11COO3 N(CN)2	1-Methyl-3-(2-oxo-2-propoxyethyl)imidazolium N-cyanocyanamide	U		3.75		3.62 - 3.88		1.06
125	IM11COO3 PF6	1-Methyl-3-(2-oxo-2-propoxyethyl)imidazolium hexafluorophosphate	U		3.55		3.18 - 3.92		1.09
126	IM11COO4 (CF3SO2)2N	3-(2-Butoxy-2-oxoethyl)-1-methylimidazolium N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		3.29		3.08 - 3.51		0.99
127	IM11COO4 8OSO3	1-(2-Butoxy-2-oxoethyl)-3-methylimidazolium octylsulfate	U		3.29		2.95 - 3.63		1.30
128	IM11COO4 BF4	1-(2-Butoxy-2-oxoethyl)-3-methylimidazolium tetrafluoroborate	U		3.17		2.8 - 3.54		1.20
129	IM11COO4 Br	1-(2-Butoxy-2-oxoethyl)-3-methylimidazolium bromide	U		3.73		3.33 - 4.13		0.87
130	IM11COO4 N(CN)2	1-(2-Butoxy-2-oxoethyl)-3-methylimidazolium N-cyanocyanamide	U		3.44		3.32 - 3.55		1.00
131	IM11COO4 PF6	1-(2-Butoxy-2-oxoethyl)-3-methylimidazolium hexafluorophosphate	U		3.24		2.9 - 3.58		1.08
132	IM11COO5 8OSO3	1-Methyl-3-[2-oxo-2-(pentyloxy)ethyl]imidazolium octylsulfate	U		3.23		2.9 - 3.56		1.53*
133	IM11COO5 Br	1-Methyl-3-[2-oxo-2-(pentyloxy)ethyl]imidazolium bromide	U		3.67		3.26 - 4.08		1.06
134	IM11COO6 Br	1-[2-(Hexyloxy)-2-oxoethyl]-3-methylimidazolium bromide	U		3.52		3.11 - 3.93		1.08

135	IM11COO8 Br	1-Methyl-3-[2-(octyloxy)-2-oxoethyl]imidazolium bromide	U		2.92		2.61 - 3.22	1.08
136	IM1i4 (CF3SO2)2N	1-Methyl-3-(2-methylpropyl)imidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		2.41		2.09 - 2.73	0.84
137	IM1gly Cl	1-methyl-3-glycerylrylimidazolium chloride	U		3.76		3.24 - 4.28	2.07*
138	IM1gly N(CN)2	1-methyl-3-glycerylimidazolium dicyanamide	U		3.45		2.91 - 3.99	2.02*
139	IM1gly (CF3SO2)2N	1-methyl-3-glycerylimidazolium bis(trifluoromethylsulphonyl)imide	U		3.31		2.66 - 3.95	1.93*
140	IM1-2=1 Cl	1-Methyl-3-(2-propenyl)imidazolium chloride	U		2.96		2.67 - 3.24	0.60
141	IM1-(1Ph-4Me) BF4	1-Methyl-3-(phenylmethyl)imidazolium tetrafluoroborate	L	2.11	2.09	0.02		0.45
142	IM1-(1Ph-4Me) Cl	1-Methyl-3-[(4-methylphenyl)methyl]imidazolium chloride	L	1.99	2.67	-0.68		0.70
143	IM1-(1Ph-4Me) PF6	1-Methyl-3-[(4-methylphenyl)methyl]imidazolium hexafluorophosphate	L	2.18	2.16	0.02		0.34
144	IM1-1Ph BF4	1-Methyl-3-(phenylmethyl)imidazolium tetrafluoroborate	L	2.39	2.18	0.21		0.44
145	IM1-1Ph Cl	1-Methyl-3-(phenylmethyl)imidazolium chloride	L	2.32	2.76	-0.44		0.67
146	IM1-1Ph PF6	1-Methyl-3-(phenylmethyl)imidazolium hexafluorophosphate	L	2.50	2.25	0.25		0.33
147	IM13 BF4	1-Methyl-3-propylimidazolium tetrafluoroborate	L	2.78	2.45	0.33		0.62
148	IM13 (CF3SO2)2N	1-Methyl-3-propylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		2.58		2.27 - 2.88	0.91
149	IM13 PF6	1-Methyl-3-propylimidazolium hexafluorophosphate	L	2.43	2.52	-0.09		0.49
150	IM13 Br	1-Methyl-3-propylimidazolium bromide	U		3.01		2.72 - 3.29	0.57
151	IM13 Cl	1-Methyl-3-propylimidazolium chloride	L	3.51	3.03	0.48		0.61
152	IM13 I	1-Methyl-3-propylimidazolium iodide	U		2.96		2.72 - 3.20	0.52
153	IM1-2CO-1 Br	1-Methyl-3-(3-oxobutyl)imidazolium bromide	L	2.84	3.42	-0.58		0.90
154	IM1-2C6F13 PF6	1-Methyl-3-(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)imidazolium hexafluorophosphate	T	1.70	2.50	-0.80	2.16 - 2.83	1.36
155	IM12(2Pin_1R) Cl	1-[2-[(1R,5S)-6,6-Dimethylbicyclo[3.1.1]hept-2-en-2-yl]ethyl]-3-methylimidazolium chloride	U		1.71		1.48 - 1.94	0.83
156	IM12(2Pin_1R) NO3	1-[2-[(1R,5S)-6,6-Dimethylbicyclo[3.1.1]hept-2-en-2-yl]ethyl]-3-methylimidazolium nitrate	U		1.75		1.39 - 2.10	1.67*
157	IM1-2Ph BF4	1-Methyl-3-(2-phenylethyl)imidazolium tetrafluoroborate	U		1.28		1.09 - 1.46	0.59
158	IM1-2Ph Cl	1-Methyl-3-(2-phenylethyl)imidazolium chloride	L	2.35	1.85	0.50		0.95
159	IM1-2Ph PF6	1-Methyl-3-(2-phenylethyl)imidazolium hexafluorophosphate	T	2.45	1.34	1.11	1.15 - 1.54	0.54
160	IM14 8OSO3	1-Butyl-3-methylimidazolium octylsulfate	L	2.77	2.28	0.49		1.30
161	IM14 CF3SO3	1-Butyl-3-methylimidazolium trifluoromethanesulfonate	L	2.48	2.21	0.27		0.39
162	IM14 (CF3)2N	1-Butyl-3-methylimidazolium 1,1,1-trifluoro-N-(trifluoromethyl)methanaminate	L	1.65	2.26	-0.61		0.32
163	IM14 BF4	1-Butyl-3-methylimidazolium tetrafluoroborate	L	2.47	2.16	0.30		0.59

164	IM14 (CF3SO2)2N	1-Butyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	T	2.31	2.29	0.02	1.95 - 2.63	0.86
165	IM14 PF6	1-Butyl-3-methylimidazolium hexafluorophosphate	L	2.55	2.23	0.32		0.46
166	IM14 Cl	1-Butyl-3-methylimidazolium chloride	L	2.80	2.74	0.06		0.64
167	IM14 I	1-Butyl-3-methylimidazolium iodide	L	2.91	2.67	0.24		0.55
168	IM14 Br	1-Butyl-3-methylimidazolium bromide	L	2.77	2.72	0.05		0.61
169	IM14 N(CN)2	1-Butyl-3-methylimidazolium N-cyanocyanamide	L	2.47	2.43	0.04		0.80
170	IM14 4MePhSO3	1-Butyl-3-methylimidazolium 4-methylbenzenesulfonate	L	2.78	2.37	0.41		1.10
171	IM14 1SO3	1-Butyl-3-methylimidazolium methanesulfonate	L	2.88	2.36	0.52		0.30
172	IM14 (2-SO2PhCO)N	1-Butyl-3-methylimidazolium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide	U		2.35		2.06 - 2.63	0.94
173	IM14 (C2F5)3PF3	1-Butyl-3-methylimidazolium trifluorotris(pentafluoroethyl)phosphate	L	1.14	1.63	-0.49		1.25
174	IM14 1O2O2OSO3	1-Butyl-3-methylimidazolium 2-(2-methoxyethoxy)ethyl sulfate	L	2.69	1.99	0.70		1.03
175	IM14 1OSO3	1-Butyl-3-methylimidazolium methyl sulfate	T	2.61	2.31	0.30	2.23 - 2.39	0.31
176	IM14 AC	3-Butyl-1-methylimidazolium 6-methyl-2,2-dioxo-1,2,3-oxathiazin-4(3H)-onate	U		2.32		2.11 - 2.53	0.83
177	IM14 Co(CO)4	1-Butyl-3-methylimidazolium (T-4)-tetracarbonylcobaltate	U		2.62		2.48 - 2.76	0.92
178	IM14 FeCl4	1-Butyl-3-methylimidazolium tetrachloroferrate	L	2.70	2.74	-0.04		0.98
179	IM14 HSO4	1-Butyl-3-methylimidazolium hydrogen sulfate	L	2.66	2.21	0.45		0.72
180	IM14 NO3	1-Butyl-3-methylimidazolium nitrate	U		2.78		2.52 - 3.04	1.57*
181	IM14 SbF6	1-Butyl-3-methylimidazolium (OC-6-11)-hexafluoroantimonate	L	1.83	2.19	-0.36		0.51
182	IM14 SCN	1-Butyl-3-methylimidazolium thiocyanate	L	2.71	2.68	0.03		0.75
183	IM14 (CH3O)2PO2	1-butyl-3-methylimidazolium dimethyl phosphate	U		2.28		2.21 - 2.34	0.34
184	IM14 C(CN)3	1-butyl-3-methylimidazolium tricyanomethanide	U		2.75		2.21 - 3.29	3.13*
185	IM14 CF3COO	1-Butyl-3-Methylimidazolium trifluoroacetate	U		2.28		2.07 - 2.49	0.96
186	IM13COOH Cl	3-(3-Carboxypropyl)-1-methylimidazolium chloride	L	2.79	4.13	-1.34		1.27
187	IM15 (CF3SO2)2N	1-Methyl-3-pentylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		1.93		1.53 - 2.32	0.80
188	IM15 BF4	1-Methyl-3-pentylimidazolium tetrafluoroborate	L	2.38	1.81	0.57		0.56
189	IM15 Cl	1-Methyl-3-pentylimidazolium chloride	L	2.28	2.38	-0.10		0.70
190	IM15 PF6	1-Methyl-3-pentylimidazolium hexafluorophosphate	L	2.47	1.87	0.60		0.44
191	IM16 (CF3SO2)2N	1-Hexyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	1.89	2.06	-0.16		0.94
192	IM16 Br	1-Hexyl-3-methylimidazolium bromide	U		2.49		2.26 - 2.72	0.64
193	IM16 Cl	1-Hexyl-3-methylimidazolium chloride	L	2.13	2.51	-0.38		0.68

194	IM16 PF6	1-Hexyl-3-methylimidazolium hexafluorophosphate	L	2.40	2.00	0.40			0.37
195	IM16 (2-SO2PhCO)N	1-Hexyl-3-methylimidazolium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide	L	1.85	2.12	-0.27			1.01
196	IM16 BF4	1-Hexyl-3-methylimidazolium tetrafluoroborate	L	2.39	1.93	0.45			0.50
197	IM16 (C2F5)3PF3	1-Hexyl-3-methylimidazolium trifluorotris(pentafluoroethyl)phosphate	L	1.21	1.41	-0.19			1.22
198	IM16 (C3F7)3PF3	1-Hexyl-3-methylimidazolium trifluorotris(heptafluoropropyl)phosphate	L	-0.12	1.12	-1.24			1.78*
199	IM16 (CF3SO2)3C	1-Hexyl-3-methylimidazolium tris[(trifluoromethyl)sulfonyl]methide	L	3.20	1.86	1.34			0.88
200	IM16 N(CN)2	1-hexyl-3-methylimidazolium dicyanamide	U		2.20		1.99	- 2.41	0.85
201	IM16 NO3	1-hexyl-3-methylimidazolium nitrate	U		2.55		2.29	- 2.81	1.61*
202	IM16 SbF6	1-hexyl-3-methylimidazolium hexafluoridoantimonate	U		1.96		1.87	- 2.06	0.42
203	IM17 (CF3SO2)2N	1-Heptyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		1.52		1.08	- 1.95	0.75
204	IM17 BF4	1-Heptyl-3-methylimidazolium tetrafluoroborate	L	2.01	1.39	0.62			0.56
205	IM17 Cl	1-Heptyl-3-methylimidazolium chloride	T	1.87	1.97	-0.10	1.74	- 2.19	0.77
206	IM17 PF6	1-Heptyl-3-methylimidazolium hexafluorophosphate	T	1.82	1.46	0.36	1.42	- 1.50	0.44
207	IM18 BF4	1-Methyl-3-octylimidazolium tetrafluoroborate	T	1.04	1.47	-0.43	1.37	- 1.56	0.57
208	IM18 Br	1-Methyl-3-octylimidazolium bromide	U		2.02		1.81	- 2.24	0.73
209	IM18 (CF3SO2)2N	1-Methyl-3-octylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	T	1.32	1.59	-0.27	1.19	- 1.99	0.78
210	IM18 8OSO3	3-Methyl-1-octylimidazolium octylsulfate	L	1.13	1.58	-0.45			1.23
211	IM18 CF3SO3	1-Methyl-3-octylimidazolium trifluormethanesulfonate	L	0.62	1.52	-0.89			0.36
212	IM18 Cl	1-Methyl-3-octylimidazolium chloride	L	1.38	2.04	-0.66			0.78
213	IM18 PF6	1-Methyl-3-octylimidazolium hexafluorophosphate	L	1.50	1.53	-0.04			0.46
214	IM17COOH Br	1-(7-Carboxyheptyl)-3-methylimidazolium bromide	L	2.96	3.21	-0.25			1.28
215	IM19 BF4	1-Methyl-3-nonylimidazolium tetrafluoroborate	L	1.12	0.94	0.19			0.54
216	IM19 Cl	1-Methyl-3-nonylimidazolium chloride	L	0.79	1.51	-0.72			0.86
217	IM19 PF6	1-Methyl-3-nonylimidazolium hexafluorophosphate	L	1.40	1.00	0.40			0.44
218	IM1-10 BF4	1-Decyl-3-methylimidazolium tetrafluoroborate	L	0.26	0.79	-0.52			0.54
219	IM1-10 Br	1-Decyl-3-methylimidazolium bromide	T	-0.25	1.34	-1.59	1.14	- 1.54	0.85
220	IM1-10 Cl	1-Decyl-3-methylimidazolium chloride	L	0.75	1.36	-0.61			0.89
221	IM1-10 PF6	1-Decyl-3-methylimidazolium hexafluorophosphate	L	1.06	0.85	0.21			0.45
222	IM1-10 (CF3SO2)2N	1-decyl-3-methylimidazolium bis(trifluoromethylsulphonyl)imide	U		0.91		0.4	- 1.42	0.76
223	IM1-10 FeCl4	1-decyl-3-methylimidazolium tetrachloroferrate	U		1.36		1	- 1.72	1.12

224	IM1-10COO2 Br	1-(11-Ethoxy-11-oxoundecyl)-3-methylimidazolium bromide	U		1.94		1.72 - 2.16	1.14
225	IM1-12 Br	1-Dodecyl-3-methylimidazolium bromide	U		1.05		0.86 - 1.24	0.91
226	IM1-12 Cl	1-dodecyl-3-methylimidazolium chloride	U		1.07		0.87 - 1.28	0.95
227	IM1-14 Cl	1-Methyl-3-tetradecylimidazolium chloride	L	-0.92	0.47	-1.40		1.10
228	IM1-14 Br	1-Methyl-3-tetradecylimidazolium bromide	U		0.45		0.22 - 0.68	1.05
229	IM1-16 Cl	1-Hexadecyl-3-methylimidazolium chloride	L	-0.71	0.40	-1.10		1.13
230	IM1-16 Br	1-Hexadecyl-3-methylimidazolium bromide	U		0.38		0.16 - 0.59	1.08
231	IM1-18 Cl	1-Methyl-3-octadecylimidazolium chloride	L	-0.42	-0.17	-0.25		1.26
232	IM18OH Br	1-(8-Hydroxyoctyl)-3-methylimidazolium bromide	L	1.82	1.94	-0.12		1.38
233	IM14OH Cl	1-(4-Hydroxybutyl)-3-methylimidazolium chloride	L	2.76	2.95	-0.20		1.30
234	IM13OH Cl	1-(3-Hydroxypropyl)-3-methylimidazolium chloride	L	3.55	3.14	0.41		1.39
235	IM13OH (CF3SO2)2N	1-(3-Hydroxypropyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	3.29	2.69	0.60		1.28
236	IM13O1 (CF3SO2)2N	1-(3-Methoxypropyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	2.98	2.68	0.30		0.60
237	IM13O1 Cl	1-(3-Methoxypropyl)-3-methylimidazolium chloride	L	3.77	3.13	0.64		0.65
238	IM12OH I	1-(2-Hydroxyethyl)-3-methylimidazolium iodide	L	3.71	3.32	0.39		1.43
239	IM12OH (2-SO2PhCO)N	1-(2-Hydroxyethyl)-3-methylimidazolium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide	U		3.00		2.54 - 3.45	1.45
240	IM12OH (CF3SO2)2N	1-(2-Hydroxyethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	3.37	2.94	0.44		1.39
241	IM12OH AC	1-(2-Hydroxyethyl)-3-methylimidazolium 6-methyl-2,2-dioxo-1,2,3-oxathiazin-4(3H)-onate	U		2.97		2.56 - 3.37	1.46
242	IM12OH BF4	1-(2-Hydroxyethyl)-3-methylimidazolium tetrafluoroborate	L	2.81	2.81	0.00		1.68*
243	IM12OH PF6	1-(2-Hydroxyethyl)-3-methylimidazolium hexafluorophosphate	U		2.88		2.52 - 3.24	1.58*
244	IM12OH Cl	1-(2-hydroxyethyl)-3-methylimidazolium chloride	U		3.39		3.04 - 3.73	1.47
245	IM12O1 (CF3SO2)2N	1-(2-Methoxyethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	2.88	3.05	-0.17		0.75
246	IM12O1 Cl	1-(2-Methoxyethyl)-3-methylimidazolium chloride	L	3.55	3.50	0.04		0.59
247	IM12O1 BF4	1-(2-Methoxyethyl)-3-methylimidazolium tetrafluoroborate	U		2.93		2.68 - 3.17	0.87
248	IM12O1 N(CN)2	1-(2-Methoxyethyl)-3-methylimidazolium dicyanamide	U		3.19		3.06 - 3.32	0.74
249	IM12O2 (CF3SO2)2N	1-(2-Ethoxyethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	3.18	2.62	0.56		0.72
250	IM12O2 Br	1-(2-Ethoxyethyl)-3-methylimidazolium bromide	L	3.51	3.05	0.46		0.61
251	IM12O2 Cl	1-(2-Ethoxyethyl)-3-methylimidazolium chloride	U		3.07		2.81 - 3.33	0.65

252	IM12O2O1 Cl	1-[2-(2-Methoxyethoxy)ethyl]-3-methylimidazolium chloride	U		3.19		2.9 - 3.47		0.77
253	IM11O2 (CF3SO2)2N	1-(Ethoxymethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	2.83	2.88	-0.05			0.60
254	IM11O2 Cl	1-(Ethoxymethyl)-3-methylimidazolium chloride	L	2.85	3.33	-0.48			0.61
255	Py1O(Cdd)-3CONH2 Cl	3-(Aminocarbonyl)-1-[(cyclododecyloxy)methyl]pyridinium chloride	U		2.88		2.51 - 3.25		1.63*
256	Py1O-10-3CONH2 Cl	3-(Aminocarbonyl)-1-[(decyloxy)methyl]pyridinium chloride	U		2.54		2.19 - 2.90		1.56*
257	Py1O-10-3CONH2 FeCl4	3-(Aminocarbonyl)-1-[(decyloxy)methyl]pyridinium (T-4)-tetrachloroferrate	U		2.55		2.2 - 2.89		1.63*
258	Py1O-11-3CONH2 Cl	3-(Aminocarbonyl)-1-[(undecyloxy)methyl]pyridinium chloride	U		2.27		1.92 - 2.62		1.69*
259	Py1O-12-3CONH2 1COO	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium acetate	U		1.93		1.5 - 2.35		2.42*
260	Py1O-12-3CONH2 BF4	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium tetrafluoroborate	U		1.44		1.02 - 1.86		1.78*
261	Py1O-12-3CONH2 Br	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium bromide	U		2.00		1.64 - 2.36		1.74*
262	Py1O-12-3CONH2 Cl	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium chloride	U		2.02		1.66 - 2.38		1.76*
263	Py1O-12-3CONH2 ClO4	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium perchlorate	U		1.33		0.85 - 1.80		1.85*
264	Py1O-12-3CONH2 I	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium iodide	U		1.95		1.6 - 2.30		1.71*
265	Py1O-12-3CONH2 NO3	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium nitrate	U		2.06		1.67 - 2.45		2.24*
266	Py4-3CONHBu 8OSO3	1-Butyl-3-[(butylamino)carbonyl]pyridinium octyl sulfate	U		2.68		2.18 - 3.18		1.70*
267	Py4-3CONHBu I	1-Butyl-3-[(butylamino)carbonyl]pyridinium iodide	U		3.07		2.82 - 3.33		1.07
268	Py1O7-3CONH(MeO-MeO-Hp) Cl	3-[[[[(Heptyloxy)methoxy]methyl]amino]carbonyl]-1-[(heptyloxy)methyl]pyridinium chloride	U		2.06		1.77 - 2.35		2.13*
269	Py1O8-3CONH(MeO-MeO-Oc) Cl	3-[[[[(Octyloxy)methoxy]methyl]amino]carbonyl]-1-[(octyloxy)methyl]pyridinium chloride	U		2.32		1.95 - 2.68		2.46*
270	Py1O9-3CONH(MeO-MeO-No) Cl	3-[[[[(Nonyloxy)methoxy]methyl]amino]carbonyl]-1-[(nonyloxy)methyl]pyridinium chloride	U		2.71		2.26 - 3.17		3.07*
271	Py1O-10-3CONH(MeO-MeO-De) Cl	3-[[[[(Decyloxy)methoxy]methyl]amino]carbonyl]-1-[(decyloxy)methyl]pyridinium chloride	U		1.83		1.46 - 2.20		2.98*
272	Py1-3COOBu (CF3SO2)2N	3-(Butoxycarbonyl)-1-methylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		3.21		2.96 - 3.45		1.13
273	Py1-3COOBu 8OSO3	3-(Butoxycarbonyl)-1-methylpyridinium octyl sulfate	U		3.20		2.82 - 3.58		1.48
274	Py1-3COOBu I	3-(Butoxycarbonyl)-1-methylpyridinium iodide	U		3.59		3.28 - 3.90		0.83
275	Py1-3COOBu PF6	3-(Butoxycarbonyl)-1-methylpyridinium hexafluorophosphate	U		3.15		2.86 - 3.44		0.98
276	Py4-3COOBu 8OSO3	3-(Butoxycarbonyl)-1-butylpyridinium octyl sulfate	U		2.57		2.13 - 3.01		1.49
277	Py4-3COOBu I	3-(Butoxycarbonyl)-1-butylpyridinium iodide	U		2.96		2.73 - 3.20		0.94
278	Py4-3Me-4Me BF4	1-Butyl-3,4-dimethylpyridinium tetrafluoroborate	L	2.42	1.80	0.62			0.41
279	Py4-3Me-4Me Cl	1-Butyl-3,4-dimethylpyridinium chloride	L	2.35	2.37	-0.02			0.71

280	Py4-3Me-5Me N(CN)2	1-Butyl-3,5-dimethylpyridinium N-cyanocyanamide	U		1.71		1.36 - 2.06	0.94
281	Py4-3Me-5Me Br	1-Butyl-3,5-dimethylpyridinium bromide	U		2.00		1.76 - 2.23	0.77
282	Py4-3Me-5Me BF4	1-Butyl-3,5-dimethylpyridinium tetrafluoroborate	L	2.65	1.44	1.21		0.40
283	Py4-3Me-5Me Cl	1-Butyl-3,5-dimethylpyridinium chloride	L	2.72	2.02	0.71		0.81
284	Py4-3Me-5Me (CF3SO2)2N	1-butyl-3,5-dimethil pyridinium bistrifluoromethanesulfonamide	U		1.57		1.07 - 2.06	1.03
285	Py8-3Me-5Me Br	1-octyl-3,5-dimethylpyridinium bromide	U		1.08		0.84 - 1.33	0.94
286	Py8-3Me-5Me (CF3SO2)2N	1-octyl-3,5-dimethylpyridinium bromide 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		0.65		0.05 - 1.24	0.95
287	Py3-3Me Br	3-Methyl-1-propylpyridinium bromide	U		2.75		2.5 - 3.01	0.60
288	Py3-3Me PF6	3-Methyl-1-propylpyridinium hexafluorophosphate	U		2.26		2.18 - 2.35	0.32
289	Py4-3Me N(CN)2	1-Butyl-3-methylpyridinium N-cyanocyanamide	T	2.79	2.18	0.61	1.91 - 2.45	0.88
290	Py4-3Me Br	1-Butyl-3-methylpyridinium bromide	U		2.47		2.23 - 2.71	0.65
291	Py4-3Me 8OSO3	1-Butyl-3-methylpyridinium octyl sulfate	U		2.03		1.46 - 2.60	1.43
292	Py4-3Me BF4	1-Butyl-3-methylpyridinium tetrafluoroborate	L	2.68	1.92	0.76		0.43
293	Py4-3Me Cl	1-Butyl-3-methylpyridinium chloride	L	3.12	2.49	0.63		0.69
294	Py4-3Me PF6	1-Butyl-3-methylpyridinium hexafluorophosphate	L	2.94	1.98	0.96		0.30
295	Py6-3Me Br	1-Hexyl-3-methylpyridinium bromide	U		1.94		1.72 - 2.16	0.74
296	Py6-3Me Cl	1-Hexyl-3-methylpyridinium chloride	L	1.73	1.96	-0.23		0.78
297	Py8-3Me Br	3-Methyl-1-octylpyridinium bromide	U		1.35		1.1 - 1.59	0.90
298	Py8-3Me Cl	3-Methyl-1-octylpyridinium chloride	L	0.85	1.37	-0.51		0.94
299	Py1O3-3OH (2-SO2PhCO)N	3-Hydroxy-1-(propoxymethyl)pyridinium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide	U		3.03		2.74 - 3.32	0.97
300	Py1O3-3OH AC	3-Hydroxy-1-(propoxymethyl)pyridinium 6-methyl-2,2-dioxo-1,2,3-oxathiazin-4(3H)-onate	U		3.00		2.79 - 3.21	0.99
301	Py1O3-3OH Cl	3-Hydroxy-1-(propoxymethyl)pyridinium chloride	U		3.42		3.13 - 3.71	1.06
302	Py1O4-3OH (2-SO2PhCO)N	1-(Butoxymethyl)-3-hydroxypyridinium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide	U		2.80		2.49 - 3.10	0.95
303	Py1O4-3OH AC	1-(Butoxymethyl)-3-hydroxypyridinium 6-methyl-2,2-dioxo-1,2,3-oxathiazin-4(3H)-onate	U		2.77		2.54 - 3.00	0.97
304	Py1O6-3OH (2-SO2PhCO)N	1-[(Hexyloxy)methyl]-3-hydroxypyridinium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide	U		2.31		1.96 - 2.67	0.94
305	Py1O6-3OH AC	1-[(Hexyloxy)methyl]-3-hydroxypyridinium 6-methyl-2,2-dioxo-1,2,3-oxathiazin-4(3H)-onate	U		2.29		2.01 - 2.56	0.96
306	Py1O7-3OH (2-SO2PhCO)N	1-[(Heptyloxy)methyl]-3-hydroxypyridinium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide	U		2.29		1.94 - 2.64	0.90
307	Py1O7-3OH AC	1-[(Heptyloxy)methyl]-3-hydroxypyridinium 6-methyl-2,2-dioxo-1,2,3-oxathiazin-4(3H)-onate	U		2.26		1.99 - 2.53	0.91
308	Py1O7-3OH Cl	1-[(Heptyloxy)methyl]-3-hydroxypyridinium chloride	U		2.68		2.44 - 2.92	1.10

309	Py1O-11-3OH (2-SO2PhCO)N	3-Hydroxy-1-[(undecyloxy)methyl]pyridinium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide	U		1.23		0.74	-	1.72	1.01
310	Py1O-11-3OH AC	3-Hydroxy-1-[(undecyloxy)methyl]pyridinium 6-methyl-2,2-dioxo-1,2,3-oxathiazin-4(3H)-onate	U		1.20		0.79	-	1.61	1.02
311	Py1O-11-3OH Cl	3-Hydroxy-1-[(undecyloxy)methyl]pyridinium chloride	U		1.62		1.4	-	1.84	1.33
312	Py1O-18-3OH (2-SO2PhCO)N	3-Hydroxy-1-[(octadecyloxy)methyl]pyridinium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide	U		0.01		-0.61	-	0.62	1.14
313	Py1O-18-3OH AC	3-Hydroxy-1-[(octadecyloxy)methyl]pyridinium 6-methyl-2,2-dioxo-1,2,3-oxathiazin-4(3H)-onate	U		-0.02		-0.55	-	0.51	1.15
314	Pyr24 2OSO3	1-Butyl-1-ethylpyrrolidinium ethyl sulfate	U		2.41		2.11	-	2.70	1.02
315	IMi022OH-2-(8=9) 2OSO3	1-ethyl-2-(8-heptadecenyl)-4,5-dihydro-3-(2-hydroxyethyl)imidazolium ethyl sulfate	L	-0.23	-0.53	0.30				2.23*
316	IM22 (CF3SO2)2N	1,3-Diethylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		2.66		2.36	-	2.96	0.94
317	IM22 Br	1,3-Diethylimidazolium bromide	L	2.31	3.09	-0.78				0.58
318	IM23 (CF3SO2)2N	1-Ethyl-3-propylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		2.52		2.21	-	2.83	0.94
319	IM23 Br	1-Ethyl-3-propylimidazolium bromide	L	2.64	2.95	-0.31				0.60
320	IM24 BF4	1-Butyl-3-ethylimidazolium tetrafluoroborate	L	2.64	2.09	0.55				0.56
321	IM24 CF3COO	1-Butyl-3-ethylimidazolium trifluoroacetate	L	2.74	2.21	0.53				0.95
322	IM24 CF3SO3	1-Butyl-3-ethylimidazolium trifluoromethanesulfonate	L	2.91	2.14	0.77				0.37
323	IM26 BF4	1-Ethyl-3-hexylimidazolium tetrafluoroborate	T	1.69	1.35	0.34	1.28	-	1.43	0.53
324	IM26 Br	1-Ethyl-3-hexylimidazolium bromide	L	1.41	1.91	-0.49				0.75
325	IM2-10 Br	1-Decyl-3-ethylimidazolium bromide	L	0.03	1.23	-1.19				0.89
326	IM1-(1Ph) (CF3SO2)2N	1-benzyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		2.40		2.04	-	2.76	1.11
327	IM4-(1Ph) (CF3SO2)2N	1-benzyl-3-butylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		1.61		1.15	-	2.08	1.05
328	Py1O-10-4CONH2 Cl	4-(Aminocarbonyl)-1-[(decyloxy)methyl]pyridinium chloride	U		2.52		2.17	-	2.88	1.62*
329	Py1O-11-4CONH2 Cl	4-(Aminocarbonyl)-1-[(undecyloxy)methyl]pyridinium chloride	U		2.34		1.98	-	2.70	1.70*
330	Py1O-12-4CONH2 Cl	4-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium chloride	U		2.12		1.75	-	2.49	1.78*
331	Py4-4Me BF4	1-Butyl-4-methylpyridinium tetrafluoroborate	L	2.35	2.03	0.32				0.47
332	Py4-4Me (C2F5)3PF3	1-Butyl-4-methylpyridinium trifluorotris(pentafluoroethyl)phosphate	L	-0.23	1.50	-1.73				1.26
333	Py4-4Me B(CN)4	1-Butyl-4-methylpyridinium tetracyanoborate	L	2.30	2.30	0.00				2.75*
334	Py4-4Me Cl	1-Butyl-4-methylpyridinium chloride	L	2.59	2.61	-0.02				0.70
335	Py4-4Me PF6	1-Butyl-4-methylpyridinium hexafluorophosphate	L	2.47	2.10	0.37				0.35
336	Py4-4Me C(CN)3	1-butyl-4-methylpyridinium tricyanomethanide	U		2.62		1.98	-	3.25	3.19*
337	Py6-4Me BF4	1-Hexyl-4-methylpyridinium tetrafluoroborate	L	1.60	1.23	0.36				0.60

338	Py6-4Me Cl	1-Hexyl-4-methylpyridinium chloride	L	2.00	1.81	0.20			0.92
339	Py8-4Me BF4	4-Methyl-1-octylpyridinium tetrafluoroborate	L	0.95	0.94	0.01			0.54
340	Py8-4Me Cl	4-Methyl-1-octylpyridinium chloride	L	1.02	1.52	-0.50			0.92
341	Py1-4NMe2 I	4-(Dimethylamino)-1-methylpyridinium iodide	L	2.31	3.45	-1.14			0.66
342	Py2-4NMe2 (CF3SO2)2N	4-(Dimethylamino)-1-ethylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	T	2.43	2.96	-0.54	2.64	3.28	1.26
343	Py2-4NMe2 Br	4-(Dimethylamino)-1-ethylpyridinium bromide	T	2.26	3.40	-1.14	3.1	3.69	0.62
344	Py4-4NMe2 (CF3SO2)2N	1-Butyl-4-(dimethylamino)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	1.49	2.31	-0.82			1.15
345	Py4-4NMe2 Br	1-Butyl-4-(dimethylamino)pyridinium bromide	U		2.74		2.49	2.99	0.67
346	Py4-4NMe2 Cl	1-Butyl-4-(dimethylamino)pyridinium chloride	T	1.27	2.76	-1.49	2.49	3.02	0.70
347	Py6-4NMe2 (CF3SO2)2N	4-(Dimethylamino)-1-hexylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	T	0.70	1.55	-0.85	1	2.11	1.20
348	Py6-4NMe2 Cl	4-(Dimethylamino)-1-hexylpyridinium chloride	L	0.32	2.01	-1.68			0.94
349	IM33 (CF3SO2)2N	1,3-Dipropylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		2.14		1.76	2.51	0.86
350	IM44 (CF3SO2)2N	1,3-Dibutylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		1.86		1.48	2.25	0.88
351	IM42OH Cl	1-butyl-3-(2-hydroxyethyl)imidazolium chloride	U		3.12		2.81	3.42	1.17
352	Quin1O6-6Me Cl	1-[(Hexyloxy)methyl]-6-methylquinolinium chloride	U		2.05		1.83	2.27	0.90
353	Quin1O8-6Me Cl	6-Methyl-1-[(octyloxy)methyl]quinolinium chloride	U		1.47		1.27	1.67	1.02
354	Quin1O-10-6Me Cl	1-[(Decyloxy)methyl]-6-methylquinolinium chloride	U		1.12		0.9	1.33	1.11
355	Quin1O-12-6Me Cl	1-[(Dodecyloxy)methyl]-6-methylquinolinium chloride	U		0.84		0.64	1.05	1.21
356	Quin1O6-8OH Cl	1-[(Hexyloxy)methyl]-8-hydroxyquinolinium chloride	U		2.24		1.97	2.52	1.17
357	Quin1O8-8OH Cl	8-Hydroxy-1-[(octyloxy)methyl]quinolinium chloride	U		1.66		1.4	1.91	1.23
358	Quin1O-10-8OH Cl	1-[(Decyloxy)methyl]-8-hydroxyquinolinium chloride	U		1.29		1.05	1.53	1.26
359	Quin1O-12-8OH Cl	1-[(Dodecyloxy)methyl]-8-hydroxyquinolinium chloride	U		0.81		0.53	1.09	1.41
360	Quin4 BF4	1-Butylquinolinium tetrafluoroborate	L	1.60	1.51	0.09			0.66
361	Quin4 Br	1-Butylquinolinium bromide	L	1.74	2.07	-0.32			1.02
362	Quin6 BF4	1-Hexylquinolinium tetrafluoroborate	T	0.55	0.90	-0.34	0.6	1.20	0.78
363	Quin8 BF4	1-Octylquinolinium tetrafluoroborate	T	-0.31	0.49	-0.80	0.14	0.84	0.86
364	Quin8 Br	1-Octylquinolinium bromide	T	-0.52	1.04	-1.57	0.66	1.43	1.27
365	Quin1O6 Cl	1-[(Hexyloxy)methyl]quinolinium chloride	U		2.03		1.8	2.26	0.91
366	Quin1O8 Cl	1-[(Octyloxy)methyl]quinolinium chloride	U		1.64		1.43	1.84	0.92

367	Quin1O-10 Cl	1-[(Decyloxy)methyl]quinolinium chloride	U		1.08		0.84 - 1.31		1.10
368	Quin1O-12 Cl	1-[(Dodecyloxy)methyl]quinolinium chloride	U		0.87		0.63 - 1.11		1.19
369	IM55 (CF3SO2)2N	1,3-Dipentylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		1.27		0.8 - 1.74		0.79
370	Py1(COO1)(Ph-3-OMe-4-OMe) Cl	1-[1-(3,4-Dimethoxyphenyl)-2-methoxy-2-oxoethyl]pyridinium chloride	U		4.24		3.76 - 4.71		1.45
371	Py1(COO1)(Ph-(3,4-OCH2O-)) Br	1-[1-(1,3-Benzodioxol-5-yl)-2-methoxy-2-oxoethyl]pyridinium bromide	U		4.22		3.78 - 4.65		1.42
372	Py1(COO4)(Ph-(3,4-OCH2O-)) Br	1-[1-(1,3-Benzodioxol-5-yl)-2-butoxy-2-oxoethyl]pyridinium bromide	U		3.82		3.4 - 4.25		1.61*
373	Py2 Cl	1-Ethylpyridinium chloride	T	3.38	3.48	-0.10	3.13 - 3.83		0.56
374	Py1CN (CF3SO2)2N	1-(Cyanomethyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	3.10	3.52	-0.42			1.65*
375	Py1CN Cl	1-(Cyanomethyl)pyridinium chloride	L	2.98	3.97	-1.00			1.15
376	Py1COO1(COO1)(Ph-(3,4-OCH2O-)) Br	1-[2-[1-(1,3-Benzodioxol-5-yl)-2-methoxy-2-oxoethoxy]-2-oxoethyl]pyridinium bromide	U		4.80		4.19 - 5.40		2.77*
377	Py1COO1(COO4)(Ph-(3,4-OCH2O-)) Br	1-[2-[1-(1,3-Benzodioxol-5-yl)-2-butoxy-2-oxoethoxy]-2-oxoethyl]pyridinium bromide	U		4.16		3.61 - 4.70		2.85*
378	Py1COO2 (CF3SO2)2N	1-(2-Ethoxy-2-oxoethyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		3.51		3.27 - 3.74		1.13
379	Py1COO2 8OSO3	1-(2-Ethoxy-2-oxoethyl)pyridinium octyl sulfate	U		3.50		3.16 - 3.84		1.45
380	Py1COO2 Br	1-(2-Ethoxy-2-oxoethyl)pyridinium bromide	U		3.94		3.51 - 4.37		0.91
381	Py1COO2 PF6	1-(2-Ethoxy-2-oxoethyl)pyridinium hexafluorophosphate	U		3.45		3.07 - 3.84		1.11
382	Py3 (CF3SO2)2N	1-Propylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	2.81	2.39	0.42			1.01
383	Py3 Br	1-Propylpyridinium bromide	L	3.78	2.82	0.96			0.65
384	Py4 Cl	1-Butylpyridinium chloride	U		2.81		2.53 - 3.10		0.63
385	Py4 Al2Cl7	1-Butylpyridinium μ-chlorohexachlorodialuminate	L	3.18	2.73	0.45			1.43
386	Py4 N(CN)2	1-Butylpyridinium N-cyanocyanamide	U		2.50		2.27 - 2.73		0.85
387	Py4 Br	1-Butylpyridinium bromide	T	3.24	2.79	0.44	2.53 - 3.06		0.59
388	Py4 1OSO3	1-Butylpyridinium methyl sulfate	L	3.31	2.38	0.92			0.30
389	Py4 8OSO3	1-Butylpyridinium octyl sulfate	U		2.35		1.83 - 2.88		1.39
390	Py4 BF4	1-Butylpyridinium tetrafluoroborate	L	2.95	2.24	0.71			0.52
391	Py4 CF3SO3	1-Butylpyridinium trifluoromethanesulfonate	L	3.12	2.29	0.83			0.35
392	Py4 PF6	1-Butylpyridinium hexafluorophosphate	L	3.30	2.31	0.99			0.39
393	Py5 (CF3SO2)2N	1-Pentylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	2.49	2.02	0.47			0.91
394	Py5 Br	1-Pentylpyridinium bromide	L	2.51	2.45	0.06			0.67

395	Py6 (CF3SO2)2N	1-Hexylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	2.52	1.92	0.60			0.89
396	Py6 CF3SO3	1-Hexylpyridinium trifluoromethanesulfonate	L	2.04	1.85	0.19			0.30
397	Py6 Cl	1-Hexylpyridinium chloride	T	2.10	2.37	-0.28	2.12 -	2.62	0.70
398	Py6 PF6	1-Hexylpyridinium hexafluorophosphate	L	2.00	1.87	0.14			0.37
399	Py8 Cl	1-Octylpyridinium chloride	L	0.63	1.67	-1.05			0.88
400	Py8 (CF3SO2)2N	1-Octylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	-0.33	1.22	-1.55			0.86
401	Py-10 Br	1-Decylpyridinium bromide	U		1.31		1.07 -	1.54	0.89
402	Py-16 Br	1-Hexadecylpyridinium bromide	U		0.00		-0.33 -	0.34	1.21
403	Py-16 Cl	1-Hexadecylpyridinium chloride	U		0.02		-0.31 -	0.36	1.25
404	Py3OH (CF3SO2)2N	1-(3-Hydroxypropyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	3.17	3.01	0.16			1.35
405	Py3OH Cl	1-(3-Hydroxypropyl)pyridinium chloride	L	3.54	3.46	0.08			1.39
406	Py3O1 (CF3SO2)2N	1-(3-Methoxypropyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	3.02	2.55	0.47			0.90
407	Py3O1 Cl	1-(3-Methoxypropyl)pyridinium chloride	L	3.88	3.00	0.88			0.81
408	Py3SO3H CF3SO3	1-(3-Sulfopropyl)pyridinium trifluoromethanesulfonate	L	3.45	3.51	-0.06			2.24*
409	Py2OH (CF3SO2)2N	1-(2-Hydroxyethyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	3.40	2.99	0.41			1.57*
410	Py2OH I	1-(2-Hydroxyethyl)pyridinium iodide	L	3.55	3.37	0.18			1.58*
411	Py2O1 (CF3SO2)2N	1-(2-Methoxyethyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	2.81	3.14	-0.33			0.83
412	Py2O1 Cl	1-(2-Methoxyethyl)pyridinium chloride	L	3.54	3.60	-0.06			0.58
413	Py2O2 (CF3SO2)2N	1-(2-Ethoxyethyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	2.90	2.80	0.10			0.84
414	Py2O2 Br	1-(2-Ethoxyethyl)pyridinium bromide	L	3.61	3.23	0.38			0.62
415	Py1O2 (CF3SO2)2N	1-(Ethoxymethyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	2.74	2.98	-0.23			0.63
416	Py1O2 Cl	1-(Ethoxymethyl)pyridinium chloride	T	2.56	3.43	-0.87	3.1 -	3.76	0.58
417	Pyr66 BF4	1,1-Dihexylpyrrolidinium tetrafluoroborate	U		1.12		0.88 -	1.37	1.17
418	IM66 (CF3SO2)2N	1,3-Dihexylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		0.85		0.32 -	1.38	0.84
419	IM-10-10-2Me (CF3SO2)2N	1,3-Didecyl-2-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	T	-0.32	-0.55	0.23	-1.21 -	0.11	0.90
420	Pyr-12-2OH Cl	1-Dodecyl-1-(2-hydroxyethyl)pyrrolidinium chloride	U		1.41		1.19 -	1.62	1.31
421	IM-14-2OH-2Me Cl	1-(2-Hydroxyethyl)-2-methyl-3-tetradecylimidazolium chloride	U		0.80		0.53 -	1.08	1.47
422	IM-16-2OH-2Me Cl	1-Hexadecyl-3-(2-hydroxyethyl)-2-methylimidazolium chloride	U		0.25		-0.11 -	0.61	1.69*

423	IM2OH-(2Ph) Cl	1-(2-hydroxyethyl)-3-(2-phenylethyl)immidazolium chloride	U		2.06		1.69	-	2.43	1.71*
424	IM2OH-(2OH) Cl	1,3-di-(2-hydroxyethyl)imidazolium chloride	U		2.89		2.35	-	3.44	2.74*
425	IM1O3-1O3 Cl	1,3-Bis(propoxymethyl)imidazolium chloride	U		2.86		2.57	-	3.15	0.83
426	IM1O4-1O4 Cl	1,3-Bis(butoxymethyl)imidazolium chloride	U		2.71		2.39	-	3.04	1.00
427	IM1O5-1O5 Cl	1,3-Bis[(pentyloxy)methyl]imidazolium chloride	U		2.32		2.04	-	2.60	1.07
428	IM1O6-1O6 Cl	1,3-Bis[(hexyloxy)methyl]imidazolium chloride	U		2.06		1.8	-	2.33	1.22
429	IM1O7-1O7 Cl	1,3-Bis[(heptyloxy)methyl]imidazolium chloride	U		1.61		1.37	-	1.86	1.29
430	IM1O8-1O8 Cl	1,3-Bis[(octyloxy)methyl]imidazolium chloride	U		1.38		1.14	-	1.61	1.43
431	IM1O9-1O9 Cl	1,3-Bis[(nonyloxy)methyl]imidazolium chloride	U		0.95		0.75	-	1.15	1.52*
432	IM1O-10-1O-10 Cl	1,3-Bis[(decyloxy)methyl]imidazolium chloride	U		0.68		0.48	-	0.88	1.58*
433	IM1O-11-1O-11 Cl	1,3-Bis[(undecyloxy)methyl]imidazolium chloride	U		0.52		0.3	-	0.73	1.78*
434	IM1O-12-1O-12 Cl	1,3-Bis[(dodecyloxy)methyl]imidazolium chloride	U		0.19		0	-	0.38	1.88*
435	IM1O-14-1O-14 Cl	1,3-Bis[(tetradecyloxy)methyl]imidazolium chloride	U		-0.51		-0.71	-	-0.31	2.10*
436	IM1O-16-1O-16 Cl	1,3-Bis[(hexadecyloxy)methyl]imidazolium chloride	U		-1.14		-1.4	-	-0.89	2.08*
437	IM01 BF4	1-Methylimidazole hydrogen tetrafluoroborate	L	2.32	3.36	-1.04				2.00*
438	IM01 HO1(1)COO	1-Methylimidazole 2-hydroxypropanoate	U		3.60		2.68	-	4.53	2.49*
439	IM01 HO1(1)COO_S	1-Methylimidazole (2S)-2-hydroxypropanoate	U		3.61		2.66	-	4.55	2.59*
440	IM01 1COO	1-methylimidazolium acetate	U		3.84		2.88	-	4.80	2.54*
441	IM01 CF3COO	1-methylimidazolium trifluoroacetate	U		3.48		2.6	-	4.35	2.12*
442	IM01 CF3SO3	1-methylimidazolium 1,1,1-trifluoromethanesulfonate	U		3.40		2.61	-	4.19	1.93*
443	IM02 HO1(1)COO	1-Ethylimidazole 2-hydroxypropanoate	U		3.43		2.54	-	4.33	2.44*
444	IM02 HO1(1)COO_S	1-Ethylimidazole (2S)-2-hydroxypropanoate	U		3.44		2.53	-	4.35	2.54*
445	IM03 HO1(1)COO	1-Propylimidazole 2-hydroxypropanoate	U		2.98		2.15	-	3.81	2.36*
446	IM03 HO1(1)COO_S	1-Propylimidazole (2S)-2-hydroxypropanoate	U		2.99		2.14	-	3.83	2.46*
447	IM04 HO1(1)COO	1-Butylimidazole 2-hydroxypropanoate	U		2.69		1.87	-	3.50	2.36*
448	IM04 HO1(1)COO_S	1-Butylimidazole (2S)-2-hydroxypropanoate	U		2.69		1.86	-	3.52	2.46*
449	IM04 1COO	1-butylimidazolium acetate	U		2.92		2.08	-	3.76	2.44*
450	IM04 CF3COO	1-butylimidazolium trifluoroacetate	U		2.56		1.79	-	3.33	1.95*
451	IM04 CF3SO3	1-butylimidazolium 1,1,1-trifluoromethanesulfonate	U		2.49		1.79	-	3.19	1.74*

452	IM05 HO1(1)COO	1-Pentylimidazole 2-hydroxypropanoate	U	2.35	1.57 - 3.14	2.33*
453	IM05 HO1(1)COO_S	1-Pentylimidazole (2S)-2-hydroxypropanoate	U	2.36	1.56 - 3.16	2.44*
454	IM06 HO1(1)COO	1-Hexylimidazole 2-hydroxypropanoate	U	2.30	1.49 - 3.11	2.37*
455	IM06 HO1(1)COO_S	1-Hexylimidazole (2S)-2-hydroxypropanoate	U	2.31	1.48 - 3.13	2.48*
456	IM07 HO1(1)COO	1-Heptylimidazole 2-hydroxypropanoate	U	1.88	1.11 - 2.65	2.34*
457	IM07 HO1(1)COO_S	1-Heptylimidazole (2S)-2-hydroxypropanoate	U	1.88	1.1 - 2.67	2.45*
458	IM08 HO1(1)COO	1-Octylimidazole 2-hydroxypropanoate	U	1.73	0.95 - 2.52	2.37*
459	IM08 HO1(1)COO_S	1-Octylimidazole (2S)-2-hydroxypropanoate	U	1.74	0.94 - 2.54	2.48*
460	IM09 HO1(1)COO	1-Nonylimidazole 2-hydroxypropanoate	U	1.47	0.71 - 2.24	2.35*
461	IM09 HO1(1)COO_S	1-Nonylimidazole (2S)-2-hydroxypropanoate	U	1.48	0.7 - 2.25	2.46*
462	IM0-10 HO1(1)COO	1-Decylimidazole 2-hydroxypropanoate	U	1.24	0.49 - 1.99	2.34*
463	IM0-10 HO1(1)COO_S	1-Decylimidazole (2S)-2-hydroxypropanoate	U	1.24	0.48 - 2.00	2.45*
464	IM0-11 HO1(1)COO	1-Undecylimidazole 2-hydroxypropanoate	U	1.15	0.39 - 1.91	2.37*
465	IM0-11 HO1(1)COO_S	1-Undecylimidazole (2S)-2-hydroxypropanoate	U	1.15	0.38 - 1.93	2.48*
466	IM0-12 HO1(1)COO	1-Dodecylimidazole 2-hydroxypropanoate	U	1.12	0.35 - 1.89	2.40*
467	IM0-12 HO1(1)COO_S	1-Dodecylimidazole (2S)-2-hydroxypropanoate	U	1.12	0.34 - 1.90	2.50*
468	IM01O4 HO1(1)COO	1-(Butoxymethyl)imidazole 2-hydroxypropanoate	U	2.70	1.82 - 3.57	2.42*
469	IM01O4 HO1(1)COO_S	1-(Butoxymethyl)imidazole (2S)-2-hydroxypropanoate	U	2.70	1.81 - 3.59	2.53*
470	IM01O5 HO1(1)COO	1-[(Pentyloxy)methyl]imidazole 2-hydroxypropanoate	U	2.51	1.64 - 3.38	2.44*
471	IM01O5 HO1(1)COO_S	1-[(Pentyloxy)methyl]imidazole (2S)-2-hydroxypropanoate	U	2.51	1.62 - 3.40	2.54*
472	IM01O6 HO1(1)COO	1-[(Hexyloxy)methyl]imidazole 2-hydroxypropanoate	U	2.44	1.54 - 3.33	2.49*
473	IM01O6 HO1(1)COO_S	1-[(Hexyloxy)methyl]imidazole (2S)-2-hydroxypropanoate	U	2.44	1.53 - 3.35	2.59*
474	IM01O7 HO1(1)COO	1-[(Heptyloxy)methyl]imidazole 2-hydroxypropanoate	U	2.17	1.3 - 3.04	2.48*
475	IM01O7 HO1(1)COO_S	1-[(Heptyloxy)methyl]imidazole (2S)-2-hydroxypropanoate	U	2.17	1.29 - 3.06	2.58*
476	IM01O8 HO1(1)COO	1-[(Octyloxy)methyl]imidazole 2-hydroxypropanoate	U	1.92	1.07 - 2.77	2.46*
477	IM01O8 HO1(1)COO_S	1-[(Octyloxy)methyl]imidazole (2S)-2-hydroxypropanoate	U	1.93	1.06 - 2.79	2.57*
478	IM01O9 HO1(1)COO	1-[(Nonyloxy)methyl]imidazole 2-hydroxypropanoate	U	1.63	0.8 - 2.47	2.46*
479	IM01O9 HO1(1)COO_S	1-[(Nonyloxy)methyl]imidazole (2S)-2-hydroxypropanoate	U	1.64	0.79 - 2.49	2.56*
480	IM01O-10 HO1(1)COO	1-[(Decyloxy)methyl]imidazole 2-hydroxypropanoate	U	1.60	0.75 - 2.46	2.51*
481	IM01O-10 HO1(1)COO_S	1-[(Decyloxy)methyl]imidazole (2S)-2-hydroxypropanoate	U	1.61	0.74 - 2.47	2.61*

482	IM01O-11 HO1(1)COO	1-[(Undecyloxy)methyl]imidazole 2-hydroxypropanoate	U		1.35		0.51 - 2.18	2.50*
483	IM01O-11 HO1(1)COO_S	1-[(Undecyloxy)methyl]imidazole (2S)-2-hydroxypropanoate	U		1.35		0.5 - 2.20	2.60*
484	IM01O-12 HO1(1)COO	1-[(Dodecyloxy)methyl]imidazole 2-hydroxypropanoate	U		1.08		0.24 - 1.92	2.53*
485	IM01O-12 HO1(1)COO_S	1-[(Dodecyloxy)methyl]imidazole (2S)-2-hydroxypropanoate	U		1.08		0.23 - 1.94	2.63*
486	Py0 Cl	Pyridine hydrochloride	T	2.83	3.53	-0.70	2.74 - 4.32	2.01*
487	0600NN (CF3SO2)2N	1-hexyl-1,4-diaza[2.2.2]bicyclooctanium bis(trifluoromethylsulfonyl)imide	U		3.12		2.83 - 3.40	1.02
488	IM00 1COO	1H-Imidazol-1-ium acetate	U		4.12		3.13 - 5.12	2.51*
489	IM00 CF3COO	1H-Imidazol-1-ium trifluoroacetate	U		3.76		2.86 - 4.66	2.11*
490	IM00 CFSO3	1H-Imidazol-1-ium 1,1,1-trifluoromethanesulfonate	U		3.69		2.88 - 4.50	1.91*
491	IM01-2Me (CF3SO2)2N	1,2-dimethylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		3.49		2.85 - 4.12	1.94*
492	IM16-2Me Cl	1-hexyl-2,3-dimethyl imidazolium chloride	U		2.17		1.92 - 2.42	0.77
493	IM13-2Me (CF3SO2)2N	1,2-dimethyl-3-propylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		2.59		2.25 - 2.93	0.98
494	IM18 N(CN)2	1-Methyl-3-octylimidazolium dicyanamide	U		1.73		1.48 - 1.98	0.79
495	Py4-3Me (CF3SO2)2N	1-buthyl-3-methylpyridinium1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		2.04		1.62 - 2.46	0.99
496	IM18 SbF6	1-methyl-3-octylimidazolium hexafluoroantimonate	U		1.49		1.42 - 1.56	0.50
497	IM11 (1O)2PO2	1,3-dimethyl imidazolium dimethyl phopsphate	U		3.18		3 - 3.36	0.64
498	IM18 CF3COO	1-methyl-3-octylimidazolium trifluoroacetate	U		1.59		1.42 - 1.75	0.96
499	IM12OH 1COO	1-(2-hydroxyethyl)-3-methylimidazolium acetate	U		3.30		2.89 - 3.70	2.29*
500	IM12OH N(CN2)	1-(2-hydroxyethyl)-3-methylimidazolium dicyanamide	U		3.08		2.7 - 3.45	1.45
501	IM12OH NO3	1-(2-hydroxyethyl)-3-methylimidazolium nitrate	U		3.43		3.08 - 3.78	1.98*
502	Py6-4NMe2 Br	4-(Dimethylamino)-1-hexylpyridinium bromide	U		1.99		1.72 - 2.25	0.90
503	Py8-4Me (CF3SO2)2N	1-octyl-4-methylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		1.06		0.51 - 1.62	0.92
504	Py4 (CF3SO2)2N	1-butylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		2.36		1.99 - 2.73	0.95
505	Pip12OH N(CN)2	1-(2-hydroxyethyl)-1-methylpiperidinium N-cyanocyanamide	U		3.05		2.85 - 3.24	1.01
506	Pyr18 (CF3SO2)2N	1-methyl-1-octylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		1.68		1.34 - 2.03	0.93
507	Mor14 N(CN)2	4-butyl-4-methylmorpholinium dicyanamide	U		3.05		2.88 - 3.21	0.78
508	Mor12OH N(CN)2	4-(2-hydroxyethyl)-4-methylmorpholinium dicyanamide	U		3.82		3.65 - 3.99	1.00
509	Mor12 N(CN)2	1-ethyl-1-methylmorpholinium dicyanamide	U		3.55		3.35 - 3.76	0.86
510	Mor12 (CF3SO2)2N	1-ethyl-1-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		3.41		3.19 - 3.64	0.68
511	IM14 1COO	1-butyl-3-methylimidazolium acetate	U		2.65		2.26 - 3.04	1.77*

512	IM16 1COO	1-hexyl-3-methylimidazolium acetate	U	2.42	2.06 - 2.78	1.76*
513	IM16 CF3COO	1-hexyl-3-methylimidazolium trifluoroacetate	U	2.06	1.87 - 2.25	0.92
514	Pyr14 1COO	1-butyl-1-methylpyrroldinium acetate	U	2.84	2.23 - 3.46	2.07*
515	IM18 NO3	1-methyl-3-octylimidazolium nitrate	U	2.08	1.8 - 2.36	1.63*
516	IM14 (CF3SO2)3C	1-butyl-3-methylimidazolium tris[(trifluoromethyl)sulfonyl]methide	U	2.09	1.71 - 2.47	0.82
517	IM1-18 (CF3SO2)2N	1-methyl-3-octadecylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	-0.62	-1.3 - 0.05	0.85
518	Py4-3Me (CF3SO2)2N	1-butyl-3-methylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	2.04	1.62 - 2.46	0.99
519	Py6-3Me (CF3SO2)2N	1-hexyl-3-methylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	1.51	1.04 - 1.99	0.88
520	Pyr13 (CF3SO2)2N	1-methyl-1-propylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	2.67	2.38 - 2.96	1.05

[a] Y_predictions according to IPC-81 PLS correlation model, as reported in the section 3.3.2. Note: ILs numeration as in the other PLS datamatrices.

Table B13 Experimental and predicted[a] acethylcholinesterase inhibition values. The (*)indicates a DModX value higher than 1.50 corresponding to 95% C. I. L: learning set; T: test set; U: unknown log(EC_{50}).

IL	IL code	Systematic name	Set	Y = log (EC_{50}) *AChE mg/L*	Ý = log (EC_{50}) *AChE pred.*	Y-Ý	Confidence Interval (C.I.) for prediction	DModX
1	Py4-2Me BF4	1-Butyl-2-methylpyridinium tetrafluoroborate	T	0.20	1.23	-1.03	1.18 - 1.28	0.37
2	Py4-2Me Cl	1-Butyl-2-methylpyridinium chloride	L	-0.03	0.87	-0.90		0.57
3	Pyr12 2OSO3	1-Ethyl-1-methylpyrrolidinium ethyl sulfate	U		1.87		1.65 - 2.08	1.07
4	Pyr11CN (CF3SO2)2N	1-(Cyanomethyl)-1-methylpyrrolidinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	2.44	2.33	0.11		0.40
5	Pyr11CN Cl	1-(Cyanomethyl)-1-methylpyrrolidinium chloride	L	2.09	1.83	0.26		0.90
6	Pyr11COO2 (CF3SO2)2N	1-(2-Ethoxy-2-oxoethyl)-1-methylpyrrolidinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	2.66	2.46	0.19		0.75
7	Pyr11COO2 Br	1-(2-Ethoxy-2-oxoethyl)-1-methylpyrrolidinium bromide	U		1.98		1.83 - 2.14	1.16
8	Pyr11COO2 (C2F5)3PF3	1-(2-Ethoxy-2-oxoethyl)-1-methylpyrrolidinium tris(pentafluoroethyl)trifluorophosphate	U		2.83		2.68 - 2.98	1.02
9	Pyr13 PF6	1-Methyl-1-propylpyrrolidinium hexafluorophosphate	U		1.75		1.56 - 1.95	1.29
10	Pyr14 Cl	1-Butyl-1-methylpyrrolidinium chloride	L	1.17	1.38	-0.21		1.02

11	Pyr14 (C2F5)3PF3	1-Butyl-1-methylpyrrolidinium trifluorotris(pentafluoroethyl)phosphate	L	2.77	2.24	0.53				1.53*
12	Pyr14 (CF3SO2)2N	1-Butyl-1-methylpyrrolidinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	1.75	1.88	-0.12				1.12
13	Pyr14 1OSO3	1-Butyl-1-methylpyrrolidinium methyl sulfate	U		1.72		1.51	-	1.93	1.16
14	Pyr14 BF4	1-Butyl-1-methylpyrrolidinium tetrafluoroborate	T	1.26	1.73	-0.47	1.54	-	1.93	1.40
15	Pyr14 Br	1-Butyl-1-methylpyrrolidinium bromide	L	1.28	1.40	-0.12				1.01
16	Pyr14 N(CN)2	1-Butyl-1-methylpyrrolidinium N-cyanocyanamide	L	1.29	1.73	-0.44				1.19
17	Pyr16 (CF3SO2)2N	1-Hexyl-1-methylpyrrolidinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	2.26	1.78	0.48				1.17
18	Pyr16 Cl	1-Hexyl-1-methylpyrrolidinium chloride	T	1.79	1.29	0.51	1.10	-	1.47	0.98
19	Pyr18 BF4	1-Methyl-1-octylpyrrolidinium tetrafluoroborate	L	1.47	1.51	-0.04				1.48
20	Pyr18 Cl	1-Methyl-1-octylpyrrolidinium chloride	L	1.73	1.16	0.57				0.94
21	Pyr13OH (CF3SO2)2N	1-(3-Hydroxypropyl)-1-methylpyrrolidinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	2.40	2.59	-0.19				0.96
22	Pyr13OH Cl	1-(3-Hydroxypropyl)-1-methylpyrrolidinium chloride	L	2.12	2.10	0.02				1.37
23	Pyr13O1 (CF3SO2)2N	1-(3-Methoxypropyl)-1-methylpyrrolidinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	2.35	2.26	0.09				0.55
24	Pyr13O1 Cl	1-(3-Methoxypropyl)-1-methylpyrrolidinium chloride	L	2.03	1.76	0.26				0.87
25	Pyr12OH (CF3SO2)2N	1-(2-Hydroxyethyl)-1-methylpyrrolidinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	2.22	2.64	-0.42				1.02
26	Pyr12OH I	1-(2-Hydroxyethyl)-1-methylpyrrolidinium iodide	L	2.04	2.20	-0.16				1.38
27	Pyr12O1 (CF3SO2)2N	1-(2-Methoxyethyl)-1-methylpyrrolidinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	1.73	2.33	-0.60				0.47
28	Pyr12O1 (C2F5)3PF3	1-(2-Methoxyethyl)-1-methylpyrrolidinium tris(pentafluoroethyl)trifluorophosphate	U		2.70		2.54	-	2.85	1.14
29	Pyr12O1 Cl	1-(2-Methoxyethyl)-1-methylpyrrolidinium chloride	T	1.63	1.83	-0.20	1.67	-	2.00	0.89
30	Pyr12O2 (CF3SO2)2N	1-(2-Ethoxyethyl)-1-methylpyrrolidinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	2.20	2.24	-0.04				0.65
31	Pyr12O2 Br	1-(2-Ethoxyethyl)-1-methylpyrrolidinium bromide	L	1.98	1.76	0.22				0.89
32	Pyr11O2 (CF3SO2)2N	1-(Ethoxymethyl)-1-methylpyrrolidinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	1.85	2.20	-0.35				0.81
33	Pyr11O2 Cl	1-(Ethoxymethyl)-1-methylpyrrolidinium chloride	L	1.11	1.71	-0.60				1.01

34	Pip11CN (CF3SO2)2N	1-(Cyanomethyl)-1-methylpiperidinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	T	2.07	2.26	-0.19	2.16	-	2.36	0.44
35	Pip11CN Cl	1-(Cyanomethyl)-1-methylpiperidinium chloride	L	1.67	1.77	-0.10				0.85
36	Pip13 (CF3SO2)2N	1-Methyl-1-propylpiperidinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		1.90		1.54	-	2.26	1.15
37	Pip13 PF6	1-Methyl-1-propylpiperidinium hexafluorophosphate	U		1.72		1.51	-	1.93	1.34
38	Pip14 (CF3SO2)2N	1-Butyl-1-methylpiperidinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	1.42	1.85	-0.42				1.17
39	Pip14 Br	1-Butyl-1-methylpiperidinium bromide	T	1.20	1.37	-0.17	1.17	-	1.57	1.03
40	Pip13OH (CF3SO2)2N	1-(3-Hydroxypropyl)-1-methylpiperidinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	2.20	2.54	-0.34				0.96
41	Pip13OH Cl	1-(3-Hydroxypropyl)-1-methylpiperidinium chloride	L	1.82	2.04	-0.22				1.34
42	Pip13O1 (CF3SO2)2N	1-(3-Methoxypropyl)-1-methylpiperidinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	1.92	2.22	-0.29				0.60
43	Pip13O1 Cl	1-(3-Methoxypropyl)-1-methylpiperidinium chloride	L	1.52	1.72	-0.20				0.85
44	Pip12OH (CF3SO2)2N	1-(2-Hydroxyethyl)-1-methylpiperidinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	T	1.96	2.60	-0.64	2.35	-	2.85	1.08
45	Pip12OH I	1-(2-Hydroxyethyl)-1-methylpiperidinium iodide	L	1.78	2.17	-0.39				1.40
46	Pip12O1 (CF3SO2)2N	1-(2-Methoxyethyl)-1-methylpiperidinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	1.57	2.22	-0.65				0.70
47	Pip12O1 Br	1-(2-Methoxyethyl)-1-methylpiperidinium bromide	L	1.43	1.74	-0.31				0.91
48	Pip12O2 (CF3SO2)2N	1-(2-Ethoxyethyl)-1-methylpiperidinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	2.21	2.20	0.01				0.69
49	Pip12O2 Br	1-(2-Ethoxyethyl)-1-methylpiperidinium bromide	L	2.00	1.72	0.28				0.88
50	Pip11O2 (CF3SO2)2N	1-(Ethoxymethyl)-1-methylpiperidinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	1.80	2.14	-0.34				0.84
51	Pip11O2 Cl	1-(Ethoxymethyl)-1-methylpiperidinium chloride	L	1.43	1.64	-0.21				0.98
52	Mor12 4MePhSO3	4-Ethyl-4-methylmorpholinium 4-methylbenzenesulfonate	L	2.06	2.44	-0.38				0.65
53	Mor11CN (CF3SO2)2N	4-(Cyanomethyl)-4-methylmorpholinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	2.62	2.60	0.03				0.56
54	Mor11CN Cl	4-(Cyanomethyl)-4-methylmorpholinium chloride	L	2.25	2.10	0.15				1.21
55	Mor14 (CF3SO2)2N	4-Butyl-4-methylmorpholinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	2.42	2.28	0.14				0.49
56	Mor14 Br	4-Butyl-4-methylmorpholinium bromide	L	2.09	1.81	0.28				0.83

57	Mor13OH (CF3SO2)2N	4-(3-Hydroxypropyl)-4-methylmorpholinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	2.64	2.83	-0.19				0.87
58	Mor13OH Cl	4-(3-Hydroxypropyl)-4-methylmorpholinium chloride	T	2.29	2.33	-0.04	1.89	-	2.78	1.46
59	Mor13O1 (CF3SO2)2N	4-(3-Methoxypropyl)-4-methylmorpholinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	2.66	2.48	0.18				0.57
60	Mor13O1 Cl	4-(3-Methoxypropyl)-4-methylmorpholinium chloride	L	2.32	1.98	0.34				1.09
61	Mor12OH (CF3SO2)2N	4-(2-Hydroxyethyl)-4-methylmorpholinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	2.56	2.88	-0.32				0.86
62	Mor12OH I	4-(2-Hydroxyethyl)-4-methylmorpholinium iodide	L	2.40	2.44	-0.04				1.41
63	Mor12O1 (CF3SO2)2N	4-(2-Methoxyethyl)-4-methylmorpholinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	T	2.54	2.57	-0.02	2.41	-	2.72	0.56
64	Mor12O1 Cl	4-(2-Methoxyethyl)-4-methylmorpholinium chloride	L	2.28	2.07	0.21				1.16
65	Mor12O2 (CF3SO2)2N	4-(2-Ethoxyethyl)-4-methylmorpholinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	2.66	2.51	0.15				0.47
66	Mor12O2 Br	4-(2-Ethoxyethyl)-4-methylmorpholinium bromide	L	2.40	2.04	0.37				1.03
67	Mor11O2 (CF3SO2)2N	4-(Ethoxymethyl)-4-methylmorpholinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	2.53	2.56	-0.04				0.53
68	Mor11O2 Cl	4-(Ethoxymethyl)-4-methylmorpholinium chloride	L	2.26	2.07	0.19				1.15
69	IM11COO3-2Me 8OSO3	1.2-Dimethyl-3-(2-oxo-2-propoxyethyl)imidazolium octylsulfate	U		2.44		2.18	-	2.70	1.44
70	IM11COO3-2Me Br	1.2-Dimethyl-3-(2-oxo-2-propoxyethyl)imidazolium bromide	U		1.85		1.63	-	2.07	1.44
71	IM11COO5-2Me 8OSO3	1.2-Dimethyl-3-[2-oxo-2-(pentyloxy)ethyl]imidazolium octylsulfate	U		2.35		2.07	-	2.62	1.55*
72	IM11COO5-2Me Br	1.2-Dimethyl-3-[2-oxo-2-(pentyloxy)ethyl]imidazolium bromide	U		1.76		1.56	-	1.96	1.47
73	IM1gly-2Me N(NC)2	1.2-dimethyl-3-glycerylimidazolium dicyanamide	U		2.53		1.78	-	3.29	2.81*
74	IM1gly-2Me (CF3SO2)2N	1.2-dimethyl-3-glycerylimidazolium bis(trifluoromethylsulphonyl)imide	U		2.68		1.93	-	3.43	2.71*
75	IM14-2Me (CF3SO2)2N	1-Butyl-2.3-dimethylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		1.56		1.32	-	1.80	0.92
76	IM14-2Me BF4	1-Butyl-2.3-dimethylimidazolium tetrafluoroborate	U		1.42		1.34	-	1.50	0.70
77	IM14-2Me CF3SO3	1-Butyl-2.3-dimethylimidazolium trifluoromethanesulfonate	U		1.43		1.35	-	1.50	0.50
78	IM16-2Me BF4	1-Hexyl-2.3-dimethylimidazolium tetrafluoroborate	L	0.69	1.01	-0.32				0.65
79	IM16-2Me (CF3SO2)2N	1-hexyl-2.3-dimethylimidazolium bis(trifluoromethylsulphonyl)imide	U		1.15		0.97	-	1.33	1.25

80	IM12OH-2Me Cl	1-(2-hydroxyethyl)-2.3-dimethylimidazolium chloride	U		1.70		1.14	-	2.27	1.80*
81	IM11 (CF3SO2)2N	1.3-Dimethylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		1.77		1.45	-	2.08	1.10
82	IM11 1OSO3	1.3-dimethylimidazolium methylsulfate	U		1.61		1.46	-	1.76	0.71
83	IM11 4MePhSO3	1.3-dimethylimidazolium p-toluenesulfonate	U		1.78		1.41	-	2.14	1.32
84	IM11 N(CN)2	1-methyl-3-methylimidaziolium N-cyanocyanamide	U		1.62		1.32	-	1.93	1.12
85	IM11(COO1)(Ph-(3,4-OCH2O-)) Cl	1-[1-(1.3-Benzodioxol-5-yl)-2-methoxy-2-oxoethyl]-3-methylimidazolium chloride	U		1.88		1.54	-	2.21	2.71*
86	IM11(COO4)(Ph-(3,4-OCH2O-)) Br	1-[1-(1.3-Benzodioxol-5-yl)-2-butoxy-2-oxoethyl]-3-methylimidazolium bromide	U		1.89		1.62	-	2.15	2.31*
87	IM12 (C2F5)3PF3	1-Ethyl-3-methylimidazolium trifluorotris(pentafluoroethyl)phosphate	L	2.14	2.07	0.08				0.81
88	IM12 (C2F5)2PO2	1-Ethyl-3-methylimidazolium bis(pentafluoroethyl)phosphinate	L	1.71	1.79	-0.08				0.60
89	IM12 C(CN)3	1-Ethyl-3-methylimidazolium. salt with methanetricarbonitrile	L	1.84	1.35	0.49				3.66*
90	IM12 B(CN)4	1-Ethyl-3-methylimidazolium tetracyanoborate	L	1.33	1.51	-0.18				3.18*
91	IM12 N(CN)2	1-Ethyl-3-methylimidazolium N-cyanocyanamide	T	1.79	1.56	0.24	1.27	-	1.85	1.07
92	IM12 (CF3SO2)2N	1-Ethyl-3-methylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	1.63	1.70	-0.06				1.07
93	IM12 Cl	1-Ethyl-3-methylimidazolium chloride	L	1.25	1.20	0.05				0.91
94	IM12 2OSO3	1-Ethyl-3-methylimidazolium ethyl sulfate	L	1.44	1.55	-0.11				0.63
95	IM12 (OOCCOO)2B	1-Ethyl-3-methylimidazolium bis[ethanedioato-O1.O2]borate	L	1.48	1.93	-0.45				1.17
96	IM12 1COO	1-Ethyl-3-methylimidazolium acetate	U		1.49		1.33	-	1.65	2.02*
97	IM12 1O2O2OSO3	1-Ethyl-3-methylimidazolium 2-(2-methoxyethoxy)ethyl sulfate	L	1.57	1.92	-0.35				0.98
98	IM12 1OSO3	1-Ethyl-3-methylimidazolium methylsulfate	U		1.54		1.41	-	1.67	0.61
99	IM12 1SO3	1-Ethyl-3-methylimidazolium methanesulfonate	U		1.50		1.38	-	1.63	0.64
100	IM12 4MePhSO3	1-Ethyl-3-methylimidazolium 4-methylbenzenesulfonate	L	1.67	1.71	-0.04				1.31
101	IM12 8OSO3	1-Ethyl-3-methylimidazolium octylsulfate	L	1.37	1.81	-0.44				1.50
102	IM12 BF4	1-Ethyl-3-methylimidazolium tetrafluoroborate	L	1.34	1.56	-0.21				0.74
103	IM12 CF3COO	1-Ethyl-3-methylimidazolium trifluoroacetate	L	1.38	1.61	-0.24				1.08

104	IM12 CF3SO3	1-Ethyl-3-methylimidazolium trifluoromethanesulfonate	L	1.55	1.56	-0.02				0.61
105	IM12 HSO4	1-Ethyl-3-methylimidazolium hydrogen sulfate	L	1.45	1.59	-0.14				0.82
106	IM12 PF6	1-Ethyl-3-methylimidazolium hexafluorophosphate	U		1.51		1.40	-	1.62	0.70
107	IM12 SCN	1-Ethyl-3-methylimidazolium thiocyanate	L	1.35	1.37	-0.01				1.04
108	IM12 Br	1-Ethyl-3-methylimidazolium bromide	U		1.22		1.09	-	1.35	0.87
109	IM12 NO3	1-Ethyl-3-methylimidazolium nitrate	U		1.20		0.89	-	1.51	1.86*
110	IM12 FeCl4	1-ethyl-3-methylimidazolium tetrachloroferrate	U		1.29		1.05	-	1.54	1.18
111	IM11CN Cl	1-(Cyanomethyl)-3-methylimidazolium chloride	T	2.09	1.39	0.69	1.09	-	1.70	1.70*
112	IM11CN (CF3SO2)2N	1-(Cyanomethyl)-3-methylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	2.48	1.89	0.59				1.66*
113	IM11CONMeBu Br	1-[2-(Butylmethylamino)-2-oxoethyl]-3-methylimidazolium bromide	U		1.54		1.31	-	1.76	1.04
114	IM11CONEt2 Br	1-[2-(Diethylamino)-2-oxoethyl]-3-methylimidazolium bromide	U		1.56		1.33	-	1.80	1.13
115	IM11CONHBu Br	1-[2-(Butylamino)-2-oxoethyl]-3-methylimidazolium bromide	U		1.58		1.27	-	1.89	1.39
116	IM11COO1 Br	1-(2-Methoxy-2-oxoethyl)-3-methylimidazolium bromide	U		1.98		1.75	-	2.22	1.35
117	IM11COO1(COO4)(Ph-(3,4-OCH2O-)) Br	1-[2-[1-(1.3-Benzodioxol-5-yl)-2-butoxy-2-oxoethoxy]-2-oxoethyl]-3-methylimidazolium bromide	U		2.18		1.72	-	2.64	4.01*
118	IM11COO2 BF4	1-(2-Ethoxy-2-oxoethyl)-3-methylimidazolium tetrafluoroborate	U		2.29		2.12	-	2.45	1.17
119	IM11COO2 Br	1-(2-Ethoxy-2-oxoethyl)-3-methylimidazolium bromide	U		1.95		1.73	-	2.17	1.22
120	IM11COO3 (CF3SO2)2N	1-Methyl-3-(2-oxo-2-propoxyethyl)imidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		2.32		2.12	-	2.52	1.10
121	IM11COO3 8OSO3	1-Methyl-3-(2-oxo-2-propoxyethyl)imidazolium octylsulfate	U		2.43		2.15	-	2.71	1.38
122	IM11COO3 BF4	1-Methyl-3-(2-oxo-2-propoxyethyl)imidazolium tetrafluoroborate	U		2.18		2.06	-	2.30	1.24
123	IM11COO3 Br	1-Methyl-3-(2-oxo-2-propoxyethyl)imidazolium bromide	U		1.84		1.65	-	2.04	1.36
124	IM11COO3 N(CN)2	1-Methyl-3-(2-oxo-2-propoxyethyl)imidazolium N-cyanocyanamide	U		2.18		1.98	-	2.38	1.24
125	IM11COO3 PF6	1-Methyl-3-(2-oxo-2-propoxyethyl)imidazolium hexafluorophosphate	U		2.13		2.01	-	2.26	1.22
126	IM11COO4 (CF3SO2)2N	3-(2-Butoxy-2-oxoethyl)-1-methylimidazolium N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		2.31		2.15	-	2.46	0.93
127	IM11COO4 8OSO3	1-(2-Butoxy-2-oxoethyl)-3-methylimidazolium octylsulfate	U		2.41		2.18	-	2.65	1.24

128	IM11COO4 BF4	1-(2-Butoxy-2-oxoethyl)-3-methylimidazolium tetrafluoroborate	U		2.16		2.02	-	2.31	1.20
129	IM11COO4 Br	1-(2-Butoxy-2-oxoethyl)-3-methylimidazolium bromide	U		1.83		1.63	-	2.03	1.21
130	IM11COO4 N(CN)2	1-(2-Butoxy-2-oxoethyl)-3-methylimidazolium N-cyanocyanamide	U		2.16		2.01	-	2.32	1.10
131	IM11COO4 PF6	1-(2-Butoxy-2-oxoethyl)-3-methylimidazolium hexafluorophosphate	U		2.12		1.97	-	2.27	1.15
132	IM11COO5 8OSO3	1-Methyl-3-[2-oxo-2-(pentyloxy)ethyl]imidazolium octylsulfate	U		2.31		2.01	-	2.60	1.52*
133	IM11COO5 Br	1-Methyl-3-[2-oxo-2-(pentyloxy)ethyl]imidazolium bromide	U		1.72		1.54	-	1.90	1.41
134	IM11COO6 Br	1-[2-(Hexyloxy)-2-oxoethyl]-3-methylimidazolium bromide	U		1.72		1.55	-	1.89	1.35
135	IM11COO8 Br	1-Methyl-3-[2-(octyloxy)-2-oxoethyl]imidazolium bromide	U		1.47		1.31	-	1.63	1.19
136	IM1i4 (CF3SO2)2N	1-Methyl-3-(2-methylpropyl)imidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		1.58		1.33	-	1.82	0.92
137	IM1gly Cl	1-methyl-3-glycerylrylimidazolium chloride	U		2.31		1.46	-	3.15	2.57*
138	IM1gly N(CN)2	1-methyl-3-glycerylimidazolium dicyanamide	U		2.66		2.00	-	3.32	2.40*
139	IM1gly (CF3SO2)2N	1-methyl-3-glycerylimidazolium bis(trifluoromethylsulphonyl)imide	U		2.80		2.15	-	3.45	2.27*
140	IM1-2=1 Cl	1-Methyl-3-(2-propenyl)imidazolium chloride	L	1.50	0.98	0.52				0.61
141	IM1-(1Ph-4Me) BF4	1-Methyl-3-(phenylmethyl)imidazolium tetrafluoroborate	L	1.52	1.19	0.33				0.38
142	IM1-(1Ph-4Me) Cl	1-Methyl-3-[(4-methylphenyl)methyl]imidazolium chloride	L	1.20	0.83	0.37				0.68
143	IM1-(1Ph-4Me) PF6	1-Methyl-3-[(4-methylphenyl)methyl]imidazolium hexafluorophosphate	U		1.15		1.10	-	1.19	0.35
144	IM1-1Ph BF4	1-Methyl-3-(phenylmethyl)imidazolium tetrafluoroborate	L	1.40	1.21	0.18				0.34
145	IM1-1Ph Cl	1-Methyl-3-(phenylmethyl)imidazolium chloride	L	1.36	0.86	0.51				0.69
146	IM1-1Ph PF6	1-Methyl-3-(phenylmethyl)imidazolium hexafluorophosphate	L	1.24	1.17	0.07				0.32
147	IM13 BF4	1-Methyl-3-propylimidazolium tetrafluoroborate	T	1.62	1.44	0.19	1.37	-	1.51	0.58
148	IM13 (CF3SO2)2N	1-Methyl-3-propylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		1.58		1.33	-	1.83	0.97
149	IM13 PF6	1-Methyl-3-propylimidazolium hexafluorophosphate	L	1.66	1.39	0.26				0.51
150	IM13 Br	1-Methyl-3-propylimidazolium bromide	U		1.10		1.01	-	1.19	0.59
151	IM13 Cl	1-Methyl-3-propylimidazolium chloride	L	1.47	1.08	0.40				0.62

152	IM13 I	1-Methyl-3-propylimidazolium iodide	U		1.14		1.06	-	1.22	0.55
153	IM1-2CO-1 Br	1-Methyl-3-(3-oxobutyl)imidazolium bromide	L	2.16	1.62	0.54				1.18
154	IM1-2C6F13 PF6	1-Methyl-3-(3.3.4.4.5.5.6.6.7.7.8.8.8-tridecafluorooctyl)imidazolium hexafluorophosphate	L	2.42	2.23	0.19				1.52*
155	IM12(2Pin_1R) Cl	1-[2-[(1R.5S)-6.6-Dimethylbicyclo[3.1.1]hept-2-en-2-yl]ethyl]-3-methylimidazolium chloride	U		0.76		0.65	-	0.87	0.32
156	IM12(2Pin_1R) NO3	1-[2-[(1R.5S)-6.6-Dimethylbicyclo[3.1.1]hept-2-en-2-yl]ethyl]-3-methylimidazolium nitrate	U		0.76		0.60	-	0.93	1.62*
157	IM1-2Ph BF4	1-Methyl-3-(2-phenylethyl)imidazolium tetrafluoroborate	L	1.41	0.93	0.48				0.70
158	IM1-2Ph Cl	1-Methyl-3-(2-phenylethyl)imidazolium chloride	L	1.26	0.58	0.68				0.56
159	IM1-2Ph PF6	1-Methyl-3-(2-phenylethyl)imidazolium hexafluorophosphate	L	1.42	0.89	0.53				0.63
160	IM14 8OSO3	1-Butyl-3-methylimidazolium octylsulfate	L	1.52	1.63	-0.11				1.43
161	IM14 CF3SO3	1-Butyl-3-methylimidazolium trifluoromethanesulfonate	T	1.39	1.39	0.00	1.32	-	1.45	0.39
162	IM14 (CF3)2N	1-Butyl-3-methylimidazolium 1.1.1-trifluoro-N-(trifluoromethyl)methanaminate	L	1.07	1.35	-0.29				0.34
163	IM14 BF4	1-Butyl-3-methylimidazolium tetrafluoroborate	L	1.34	1.38	-0.04				0.59
164	IM14 (CF3SO2)2N	1-Butyl-3-methylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	1.59	1.52	0.07				0.95
165	IM14 PF6	1-Butyl-3-methylimidazolium hexafluorophosphate	L	1.60	1.34	0.27				0.49
166	IM14 Cl	1-Butyl-3-methylimidazolium chloride	L	1.16	1.02	0.14				0.45
167	IM14 I	1-Butyl-3-methylimidazolium iodide	L	1.44	1.08	0.36				0.38
168	IM14 Br	1-Butyl-3-methylimidazolium bromide	L	1.30	1.04	0.26				0.42
169	IM14 N(CN)2	1-Butyl-3-methylimidazolium N-cyanocyanamide	L	1.24	1.38	-0.13				0.92
170	IM14 4MePhSO3	1-Butyl-3-methylimidazolium 4-methylbenzenesulfonate	L	1.49	1.53	-0.04				1.21
171	IM14 1SO3	1-Butyl-3-methylimidazolium methanesulfonate	L	1.36	1.32	0.03				0.36
172	IM14 (2-SO2PhCO)N	1-Butyl-3-methylimidazolium. salt with 1.2-benzisothiazol-3(2H)-one 1.1-dioxide	U		1.52		1.27	-	1.78	1.03
173	IM14 (C2F5)3PF3	1-Butyl-3-methylimidazolium trifluorotris(pentafluoroethyl)phosphate	U		1.89		1.67	-	2.10	0.93
174	IM14 1O2O2OSO3	1-Butyl-3-methylimidazolium 2-(2-methoxyethoxy)ethyl sulfate	L	1.52	1.75	-0.23				0.99
175	IM14 1OSO3	1-Butyl-3-methylimidazolium methyl sulfate	T	1.35	1.36	-0.01	1.30	-	1.43	0.34

176	IM14 AC	3-Butyl-1-methylimidazolium 6-methyl-2.2-dioxo-1.2.3-oxathiazin-4(3H)-onate	U		1.52		1.31	-	1.73	0.90
177	IM14 Co(CO)4	1-Butyl-3-methylimidazolium (T-4)-tetracarbonylcobaltate	L	1.93	1.32	0.61				0.99
178	IM14 FeCl4	1-Butyl-3-methylimidazolium tetrachloroferrate	L	1.54	1.12	0.43				0.89
179	IM14 HSO4	1-Butyl-3-methylimidazolium hydrogen sulfate	L	1.34	1.42	-0.07				0.73
180	IM14 NO3	1-Butyl-3-methylimidazolium nitrate	U		1.02		0.79	-	1.26	1.67*
181	IM14 SbF6	1-Butyl-3-methylimidazolium (OC-6-11)-hexafluoroantimonate	L	1.38	1.36	0.02				0.53
182	IM14 SCN	1-Butyl-3-methylimidazolium thiocyanate	L	1.29	1.19	0.11				0.81
183	IM14 (CH3O)2PO2	1-butyl-3-methylimidazolium dimethyl phosphate	U		1.41		1.33	-	1.49	0.35
184	IM14 C(CN)3	1-butyl-3-methylimidazolium tricyanomethanide	U		1.17		0.61	-	1.74	3.55*
185	IM14 CF3COO	1-Butyl-3-Methylimidazolium trifluoroacetate	U		1.44		1.34	-	1.53	1.01
186	IM13COOH Cl	3-(3-Carboxypropyl)-1-methylimidazolium chloride	L	2.31	2.02	0.29				1.76*
187	IM15 (CF3SO2)2N	1-Methyl-3-pentylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		1.43		1.22	-	1.63	0.98
188	IM15 BF4	1-Methyl-3-pentylimidazolium tetrafluoroborate	L	1.24	1.29	-0.05				0.68
189	IM15 Cl	1-Methyl-3-pentylimidazolium chloride	L	1.24	0.93	0.31				0.27
190	IM15 PF6	1-Methyl-3-pentylimidazolium hexafluorophosphate	L	1.32	1.24	0.08				0.56
191	IM16 (CF3SO2)2N	1-Hexyl-3-methylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	1.80	1.41	0.40				1.05
192	IM16 Br	1-Hexyl-3-methylimidazolium bromide	U		0.93		0.86	-	1.00	0.44
193	IM16 Cl	1-Hexyl-3-methylimidazolium chloride	L	1.22	0.91	0.31				0.46
194	IM16 PF6	1-Hexyl-3-methylimidazolium hexafluorophosphate	L	1.37	1.22	0.15				0.41
195	IM16 (2-SO2PhCO)N	1-Hexyl-3-methylimidazolium. salt with 1.2-benzisothiazol-3(2H)-one 1.1-dioxide	L	1.50	1.41	0.09				1.12
196	IM16 BF4	1-Hexyl-3-methylimidazolium tetrafluoroborate	L	1.28	1.27	0.02				0.50
197	IM16 (C2F5)3PF3	1-Hexyl-3-methylimidazolium trifluorotris(pentafluoroethyl)phosphate	L	2.79	1.77	1.01				0.95
198	IM16 (C3F7)3PF3	1-Hexyl-3-methylimidazolium trifluorotris(heptafluoropropyl)phosphate	L	2.28	2.05	0.23				1.37
199	IM16 (CF3SO2)3C	1-Hexyl-3-methylimidazolium tris[(trifluoromethyl)sulfonyl]methide	L	2.16	1.49	0.67				0.96

200	IM16 N(CN)2	1-hexyl-3-methylimidazolium dicyanamide	U		1.26		1.04	-	1.49	0.98
201	IM16 NO3	1-hexyl-3-methylimidazolium nitrate	U		0.91		0.67	-	1.15	1.71*
202	IM16 SbF6	1-hexyl-3-methylimidazolium hexafluoridoantimonate	U		1.25		1.20	-	1.30	0.44
203	IM17 (CF3SO2)2N	1-Heptyl-3-methylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		1.34		1.15	-	1.54	1.06
204	IM17 BF4	1-Heptyl-3-methylimidazolium tetrafluoroborate	L	1.55	1.20	0.34				0.84
205	IM17 Cl	1-Heptyl-3-methylimidazolium chloride	T	1.41	0.85	0.56	0.75	-	0.94	0.23
206	IM17 PF6	1-Heptyl-3-methylimidazolium hexafluorophosphate	L	1.42	1.16	0.26				0.72
207	IM18 BF4	1-Methyl-3-octylimidazolium tetrafluoroborate	L	0.98	1.23	-0.25				0.82
208	IM18 Br	1-Methyl-3-octylimidazolium bromide	U		0.90		0.83	-	0.97	0.28
209	IM18 (CF3SO2)2N	1-Methyl-3-octylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	1.71	1.38	0.33				1.05
210	IM18 8OSO3	3-Methyl-1-octylimidazolium octylsulfate	T	0.98	1.48	-0.50	1.18	-	1.79	1.50
211	IM18 CF3SO3	1-Methyl-3-octylimidazolium trifluormethanesulfonate	U		1.24		1.16	-	1.32	0.65
212	IM18 Cl	1-Methyl-3-octylimidazolium chloride	L	0.96	0.88	0.08				0.29
213	IM18 PF6	1-Methyl-3-octylimidazolium hexafluorophosphate	L	1.56	1.19	0.37				0.70
214	IM17COOH Br	1-(7-Carboxyheptyl)-3-methylimidazolium bromide	L	2.48	1.74	0.74				1.52*
215	IM19 BF4	1-Methyl-3-nonylimidazolium tetrafluoroborate	L	0.90	1.07	-0.17				1.02
216	IM19 Cl	1-Methyl-3-nonylimidazolium chloride	T	0.75	0.71	0.04	0.60	-	0.83	0.39
217	IM19 PF6	1-Methyl-3-nonylimidazolium hexafluorophosphate	L	1.17	1.03	0.14				0.90
218	IM1-10 BF4	1-Decyl-3-methylimidazolium tetrafluoroborate	L	0.58	1.03	-0.45				1.08
219	IM1-10 Br	1-Decyl-3-methylimidazolium bromide	U		0.69		0.58	-	0.80	0.47
220	IM1-10 Cl	1-Decyl-3-methylimidazolium chloride	L	0.50	0.67	-0.17				0.46
221	IM1-10 PF6	1-Decyl-3-methylimidazolium hexafluorophosphate	L	1.25	0.99	0.26				0.96
222	IM1-10 (CF3SO2)2N	1-decyl-3-methylimidazolium bis(trifluoromethylsulphonyl)imide	U		1.17		0.98	-	1.36	1.27
223	IM1-10 FeCl4	1-decyl-3-methylimidazolium tetrachloroferrate	U		0.77		0.68	-	0.86	0.90

224	IM1-10COO2 Br	1-(11-Ethoxy-11-oxoundecyl)-3-methylimidazolium bromide	U		1.26		0.98	-	1.55	1.12
225	IM1-12 Br	1-Dodecyl-3-methylimidazolium bromide	U		0.65		0.54	-	0.77	0.65
226	IM1-12 Cl	1-dodecyl-3-methylimidazolium chloride	U		0.63		0.51	-	0.76	0.64
227	IM1-14 Cl	1-Methyl-3-tetradecylimidazolium chloride	T	0.04	0.50	-0.46	0.32	-	0.67	0.99
228	IM1-14 Br	1-Methyl-3-tetradecylimidazolium bromide	U		0.52		0.34	-	0.69	1.01
229	IM1-16 Cl	1-Hexadecyl-3-methylimidazolium chloride	L	0.22	0.47	-0.26				1.03
230	IM1-16 Br	1-Hexadecyl-3-methylimidazolium bromide	U		0.50		0.35	-	0.64	1.04
231	IM1-18 Cl	1-Methyl-3-octadecylimidazolium chloride	L	0.53	0.34	0.19				1.35
232	IM18OH Br	1-(8-Hydroxyoctyl)-3-methylimidazolium bromide	T	0.74	1.48	-0.74	0.97	-	1.99	1.60*
233	IM14OH Cl	1-(4-Hydroxybutyl)-3-methylimidazolium chloride	L	1.98	1.65	0.33				1.51*
234	IM13OH Cl	1-(3-Hydroxypropyl)-3-methylimidazolium chloride	T	2.23	1.67	0.56	1.15	-	2.20	1.63*
235	IM13OH (CF3SO2)2N	1-(3-Hydroxypropyl)-3-methylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	2.36	2.17	0.19				1.52*
236	IM13O1 (CF3SO2)2N	1-(3-Methoxypropyl)-3-methylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	T	2.22	1.98	0.24	1.88	-	2.07	0.64
237	IM13O1 Cl	1-(3-Methoxypropyl)-3-methylimidazolium chloride	L	1.89	1.48	0.41				0.67
238	IM12OH I	1-(2-Hydroxyethyl)-3-methylimidazolium iodide	L	2.37	1.86	0.51				1.75*
239	IM12OH (2-SO2PhCO)N	1-(2-Hydroxyethyl)-3-methylimidazolium. salt with 1.2-benzisothiazol-3(2H)-one 1.1-dioxide	U		2.30		1.93	-	2.67	1.66*
240	IM12OH (CF3SO2)2N	1-(2-Hydroxyethyl)-3-methylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	2.49	2.30	0.20				1.62*
241	IM12OH AC	1-(2-Hydroxyethyl)-3-methylimidazolium 6-methyl-2.2-dioxo-1.2.3-oxathiazin-4(3H)-onate	U		2.30		1.90	-	2.70	1.63*
242	IM12OH BF4	1-(2-Hydroxyethyl)-3-methylimidazolium tetrafluoroborate	U		2.16		1.60	-	2.71	1.81*
243	IM12OH PF6	1-(2-Hydroxyethyl)-3-methylimidazolium hexafluorophosphate	U		2.11		1.56	-	2.66	1.77*
244	IM12OH Cl	1-(2-hydroxyethyl)-3-methylimidazolium chloride	U		1.80		1.23	-	2.37	1.79*
245	IM12O1 (CF3SO2)2N	1-(2-Methoxyethyl)-3-methylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	2.10	2.03	0.06				0.73
246	IM12O1 Cl	1-(2-Methoxyethyl)-3-methylimidazolium chloride	L	1.83	1.53	0.29				0.86

247	IM12O1 BF4	1-(2-Methoxyethyl)-3-methylimidazolium tetrafluoroborate	U		1.89		1.71	-	2.08	0.80
248	IM12O1 N(CN)2	1-(2-Methoxyethyl)-3-methylimidazolium dicyanamide	U		1.89		1.78	-	2.00	0.85
249	IM12O2 (CF3SO2)2N	1-(2-Ethoxyethyl)-3-methylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	1.76	1.86	-0.10				0.77
250	IM12O2 Br	1-(2-Ethoxyethyl)-3-methylimidazolium bromide	L	1.64	1.38	0.26				0.65
251	IM12O2 Cl	1-(2-Ethoxyethyl)-3-methylimidazolium chloride	U		1.36		1.16	-	1.57	0.68
252	IM12O2O1 Cl	1-[2-(2-Methoxyethoxy)ethyl]-3-methylimidazolium chloride	U		1.62		1.35	-	1.89	0.85
253	IM11O2 (CF3SO2)2N	1-(Ethoxymethyl)-3-methylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	2.07	2.03	0.04				0.55
254	IM11O2 Cl	1-(Ethoxymethyl)-3-methylimidazolium chloride	L	1.86	1.53	0.33				0.67
255	Py1O(Cdd)-3CONH2 Cl	3-(Aminocarbonyl)-1-[(cyclododecyloxy)methyl]pyridinium chloride	U		1.64		1.19	-	2.08	1.87*
256	Py1O-10-3CONH2 Cl	3-(Aminocarbonyl)-1-[(decyloxy)methyl]pyridinium chloride	U		1.57		1.10	-	2.04	1.74*
257	Py1O-10-3CONH2 FeCl4	3-(Aminocarbonyl)-1-[(decyloxy)methyl]pyridinium (T-4)-tetrachloroferrate	U		1.66		1.32	-	2.01	1.78*
258	Py1O-11-3CONH2 Cl	3-(Aminocarbonyl)-1-[(undecyloxy)methyl]pyridinium chloride	U		1.45		0.98	-	1.93	1.84*
259	Py1O-12-3CONH2 1COO	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium acetate	U		1.78		1.31	-	2.24	2.71*
260	Py1O-12-3CONH2 BF4	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium tetrafluoroborate	U		1.84		1.34	-	2.34	2.02*
261	Py1O-12-3CONH2 Br	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium bromide	U		1.51		0.99	-	2.03	1.91*
262	Py1O-12-3CONH2 Cl	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium chloride	U		1.49		0.96	-	2.01	1.92*
263	Py1O-12-3CONH2 ClO4	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium perchlorate	U		2.04		1.60	-	2.47	2.03*
264	Py1O-12-3CONH2 I	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium iodide	U		1.54		1.04	-	2.05	1.89*
265	Py1O-12-3CONH2 NO3	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium nitrate	U		1.49		1.10	-	1.88	2.44*
266	Py4-3CONHBu 8OSO3	1-Butyl-3-[(butylamino)carbonyl]pyridinium octyl sulfate	U		1.93		1.67	-	2.18	1.75*
267	Py4-3CONHBu I	1-Butyl-3-[(butylamino)carbonyl]pyridinium iodide	U		1.38		1.15	-	1.61	1.34
268	Py1O7-3CONH(MeO-MeO-Hp) Cl	3-[[[[(Heptyloxy)methoxy]methyl]amino]carbonyl]-1-[(heptyloxy)methyl]pyridinium chloride	U		1.39		1.01	-	1.77	2.28*
269	Py1O8-3CONH(MeO-MeO-Oc) Cl	3-[[[[(Octyloxy)methoxy]methyl]amino]carbonyl]-1-[(octyloxy)methyl]pyridinium chloride	U		1.55		1.19	-	1.90	2.68*

270	Py1O9-3CONH(MeO-MeO-No) Cl	3-[[[[(Nonyloxy)methoxy]methyl]amino]carbonyl]-1-[(nonyloxy)methyl]pyridinium chloride	U		1.58		1.21	-	1.95	3.46*
271	Py1O-10-3CONH(MeO-MeO-De) Cl	3-[[[[(Decyloxy)methoxy]methyl]amino]carbonyl]-1-[(decyloxy)methyl]pyridinium chloride	U		1.34		0.94	-	1.74	3.22*
272	Py1-3COOBu (CF3SO2)2N	3-(Butoxycarbonyl)-1-methylpyridinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		2.09		1.91	-	2.27	1.15
273	Py1-3COOBu 8OSO3	3-(Butoxycarbonyl)-1-methylpyridinium octyl sulfate	U		2.20		1.94	-	2.46	1.48
274	Py1-3COOBu I	3-(Butoxycarbonyl)-1-methylpyridinium iodide	U		1.65		1.47	-	1.84	1.23
275	Py1-3COOBu PF6	3-(Butoxycarbonyl)-1-methylpyridinium hexafluorophosphate	U		1.91		1.76	-	2.05	1.08
276	Py4-3COOBu 8OSO3	3-(Butoxycarbonyl)-1-butylpyridinium octyl sulfate	U		1.98		1.73	-	2.24	1.53*
277	Py4-3COOBu I	3-(Butoxycarbonyl)-1-butylpyridinium iodide	U		1.44		1.28	-	1.60	1.10
278	Py4-3Me-4Me BF4	1-Butyl-3.4-dimethylpyridinium tetrafluoroborate	L	0.50	1.13	-0.63				0.41
279	Py4-3Me-4Me Cl	1-Butyl-3.4-dimethylpyridinium chloride	L	0.15	0.78	-0.63				0.40
280	Py4-3Me-5Me N(CN)2	1-Butyl-3.5-dimethylpyridinium N-cyanocyanamide	U		0.99		0.80	-	1.19	1.10
281	Py4-3Me-5Me Br	1-Butyl-3.5-dimethylpyridinium bromide	U		0.66		0.58	-	0.74	0.36
282	Py4-3Me-5Me BF4	1-Butyl-3.5-dimethylpyridinium tetrafluoroborate	L	0.56	1.00	-0.43				0.49
283	Py4-3Me-5Me Cl	1-Butyl-3.5-dimethylpyridinium chloride	T	0.29	0.64	-0.35	0.56	-	0.72	0.36
284	Py4-3Me-5Me (CF3SO2)2N	1-butyl-3.5-dimethil pyridinium bistrifluoromethanesulfonamide	U		1.14		0.93	-	1.35	1.21
285	Py8-3Me-5Me Br	1-octyl-3.5-dimethylpyridinium bromide	U		0.49		0.36	-	0.63	0.58
286	Py8-3Me-5Me (CF3SO2)2N	1-octyl-3.5-dimethylpyridinium bromide 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		0.97		0.78	-	1.16	1.43
287	Py3-3Me Br	3-Methyl-1-propylpyridinium bromide	U		0.90		0.83	-	0.97	0.55
288	Py3-3Me PF6	3-Methyl-1-propylpyridinium hexafluorophosphate	U		1.19		1.15	-	1.23	0.30
289	Py4-3Me N(CN)2	1-Butyl-3-methylpyridinium N-cyanocyanamide	L	0.55	1.17	-0.61				1.02
290	Py4-3Me Br	1-Butyl-3-methylpyridinium bromide	U		0.83		0.77	-	0.90	0.41
291	Py4-3Me 8OSO3	1-Butyl-3-methylpyridinium octyl sulfate	U		1.42		1.10	-	1.74	1.58*
292	Py4-3Me BF4	1-Butyl-3-methylpyridinium tetrafluoroborate	T	0.64	1.17	-0.53	1.11	-	1.23	0.39

293	Py4-3Me Cl	1-Butyl-3-methylpyridinium chloride	L	0.42	0.81	-0.39				0.43
294	Py4-3Me PF6	1-Butyl-3-methylpyridinium hexafluorophosphate	L	0.71	1.13	-0.42				0.30
295	Py6-3Me Br	1-Hexyl-3-methylpyridinium bromide	U		0.75		0.67	-	0.84	0.22
296	Py6-3Me Cl	1-Hexyl-3-methylpyridinium chloride	L	0.39	0.73	-0.35				0.23
297	Py8-3Me Br	3-Methyl-1-octylpyridinium bromide	U		0.58		0.44	-	0.72	0.51
298	Py8-3Me Cl	3-Methyl-1-octylpyridinium chloride	L	0.02	0.56	-0.54				0.50
299	Py1O3-3OH (2-SO2PhCO)N	3-Hydroxy-1-(propoxymethyl)pyridinium. salt with 1.2-benzisothiazol-3(2H)-one 1.1-dioxide	U		2.26		2.07	-	2.45	1.12
300	Py1O3-3OH AC	3-Hydroxy-1-(propoxymethyl)pyridinium 6-methyl-2.2-dioxo-1.2.3-oxathiazin-4(3H)-onate	U		2.26		2.05	-	2.47	1.12
301	Py1O3-3OH Cl	3-Hydroxy-1-(propoxymethyl)pyridinium chloride	U		1.76		1.39	-	2.13	1.23
302	Py1O4-3OH (2-SO2PhCO)N	1-(Butoxymethyl)-3-hydroxypyridinium. salt with 1.2-benzisothiazol-3(2H)-one 1.1-dioxide	U		2.20		2.00	-	2.40	1.15
303	Py1O4-3OH AC	1-(Butoxymethyl)-3-hydroxypyridinium 6-methyl-2.2-dioxo-1.2.3-oxathiazin-4(3H)-onate	U		2.20		1.98	-	2.42	1.16
304	Py1O6-3OH (2-SO2PhCO)N	1-[(Hexyloxy)methyl]-3-hydroxypyridinium. salt with 1.2-benzisothiazol-3(2H)-one 1.1-dioxide	U		2.09		1.87	-	2.31	1.29
305	Py1O6-3OH AC	1-[(Hexyloxy)methyl]-3-hydroxypyridinium 6-methyl-2.2-dioxo-1.2.3-oxathiazin-4(3H)-onate	U		2.09		1.84	-	2.33	1.31
306	Py1O7-3OH (2-SO2PhCO)N	1-[(Heptyloxy)methyl]-3-hydroxypyridinium. salt with 1.2-benzisothiazol-3(2H)-one 1.1-dioxide	U		2.06		1.85	-	2.26	1.22
307	Py1O7-3OH AC	1-[(Heptyloxy)methyl]-3-hydroxypyridinium 6-methyl-2.2-dioxo-1.2.3-oxathiazin-4(3H)-onate	U		2.05		1.83	-	2.28	1.23
308	Py1O7-3OH Cl	1-[(Heptyloxy)methyl]-3-hydroxypyridinium chloride	U		1.55		1.18	-	1.93	1.15
309	Py1O-11-3OH (2-SO2PhCO)N	3-Hydroxy-1-[(undecyloxy)methyl]pyridinium. salt with 1.2-benzisothiazol-3(2H)-one 1.1-dioxide	U		1.78		1.50	-	2.05	1.71*
310	Py1O-11-3OH AC	3-Hydroxy-1-[(undecyloxy)methyl]pyridinium 6-methyl-2.2-dioxo-1.2.3-oxathiazin-4(3H)-onate	U		1.77		1.47	-	2.07	1.72*
311	Py1O-11-3OH Cl	3-Hydroxy-1-[(undecyloxy)methyl]pyridinium chloride	U		1.27		0.83	-	1.71	1.46
312	Py1O-18-3OH (2-SO2PhCO)N	3-Hydroxy-1-[(octadecyloxy)methyl]pyridinium. salt with 1.2-benzisothiazol-3(2H)-one 1.1-dioxide	U		1.53		1.20	-	1.86	2.28*
313	Py1O-18-3OH AC	3-Hydroxy-1-[(octadecyloxy)methyl]pyridinium 6-methyl-2.2-dioxo-1.2.3-oxathiazin-4(3H)-onate	U		1.53		1.16	-	1.89	2.30*
314	Pyr24 2OSO3	1-Butyl-1-ethylpyrrolidinium ethyl sulfate	U		1.70		1.48	-	1.93	1.12
315	IMi022OH-2-(8=9) 2OSO3	1-ethyl-2-(8-heptadecenyl)-4.5-dihydro-3-(2-hydroxyethyl)imidazolium ethyl sulfate	U		1.46		0.87	-	2.06	3.04*
316	IM22 (CF3SO2)2N	1.3-Diethylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		1.58		1.31	-	1.85	1.00

317	IM22 Br	1.3-Diethylimidazolium bromide	L	1.39	1.10	0.29				0.65
318	IM23 (CF3SO2)2N	1-Ethyl-3-propylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		1.54		1.27	-	1.81	1.01
319	IM23 Br	1-Ethyl-3-propylimidazolium bromide	L	1.55	1.07	0.49				0.60
320	IM24 BF4	1-Butyl-3-ethylimidazolium tetrafluoroborate	L	1.42	1.32	0.11				0.58
321	IM24 CF3COO	1-Butyl-3-ethylimidazolium trifluoroacetate	T	1.44	1.37	0.06	1.27	-	1.48	1.02
322	IM24 CF3SO3	1-Butyl-3-ethylimidazolium trifluoromethanesulfonate	L	1.49	1.33	0.17				0.39
323	IM26 BF4	1-Ethyl-3-hexylimidazolium tetrafluoroborate	L	1.27	1.14	0.13				0.82
324	IM26 Br	1-Ethyl-3-hexylimidazolium bromide	L	1.18	0.80	0.38				0.22
325	IM2-10 Br	1-Decyl-3-ethylimidazolium bromide	L	0.42	0.60	-0.17				0.51
326	IM1-(1Ph) (CF3SO2)2N	1-benzyl-3-methylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		1.38		1.13	-	1.64	1.19
327	IM4-(1Ph) (CF3SO2)2N	1-benzyl-3-butylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		1.18		0.95	-	1.40	1.20
328	Py1O-10-4CONH2 Cl	4-(Aminocarbonyl)-1-[(decyloxy)methyl]pyridinium chloride	U		1.59		1.08	-	2.11	1.81*
329	Py1O-11-4CONH2 Cl	4-(Aminocarbonyl)-1-[(undecyloxy)methyl]pyridinium chloride	U		1.55		1.02	-	2.07	1.87*
330	Py1O-12-4CONH2 Cl	4-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium chloride	U		1.46		0.93	-	2.00	1.95*
331	Py4-4Me BF4	1-Butyl-4-methylpyridinium tetrafluoroborate	L	0.92	1.17	-0.25				0.40
332	Py4-4Me (C2F5)3PF3	1-Butyl-4-methylpyridinium trifluorotris(pentafluoroethyl)phosphate	L	1.41	1.68	-0.26				0.93
333	Py4-4Me B(CN)4	1-Butyl-4-methylpyridinium tetracyanoborate	T	0.88	1.12	-0.24	0.63	-	1.61	3.16*
334	Py4-4Me Cl	1-Butyl-4-methylpyridinium chloride	L	0.71	0.81	-0.11				0.52
335	Py4-4Me PF6	1-Butyl-4-methylpyridinium hexafluorophosphate	L	0.90	1.13	-0.23				0.32
336	Py4-4Me C(CN)3	1-butyl-4-methylpyridinium tricyanomethanide	U		0.96		0.41	-	1.52	3.63*
337	Py6-4Me BF4	1-Hexyl-4-methylpyridinium tetrafluoroborate	L	0.90	0.99	-0.09				0.82
338	Py6-4Me Cl	1-Hexyl-4-methylpyridinium chloride	L	0.77	0.63	0.14				0.48
339	Py8-4Me BF4	4-Methyl-1-octylpyridinium tetrafluoroborate	L	0.69	0.95	-0.26				0.94
340	Py8-4Me Cl	4-Methyl-1-octylpyridinium chloride	L	0.50	0.60	-0.10				0.43

341	Py1-4NMe2 I	4-(Dimethylamino)-1-methylpyridinium iodide	U		1.02		0.89	-	1.15	1.22
342	Py2-4NMe2 (CF3SO2)2N	4-(Dimethylamino)-1-ethylpyridinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	0.56	1.46	-0.90				1.41
343	Py2-4NMe2 Br	4-(Dimethylamino)-1-ethylpyridinium bromide	L	0.36	0.98	-0.63				1.14
344	Py4-4NMe2 (CF3SO2)2N	1-Butyl-4-(dimethylamino)pyridinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	0.25	1.31	-1.06				1.24
345	Py4-4NMe2 Br	1-Butyl-4-(dimethylamino)pyridinium bromide	U		0.84		0.75	-	0.92	0.73
346	Py4-4NMe2 Cl	1-Butyl-4-(dimethylamino)pyridinium chloride	L	-0.07	0.82	-0.88				0.75
347	Py6-4NMe2 (CF3SO2)2N	4-(Dimethylamino)-1-hexylpyridinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	T	0.50	1.08	-0.58	0.89	-	1.27	1.34
348	Py6-4NMe2 Cl	4-(Dimethylamino)-1-hexylpyridinium chloride	L	-0.12	0.58	-0.70				0.62
349	IM33 (CF3SO2)2N	1.3-Dipropylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		1.44		1.21	-	1.68	0.98
350	IM44 (CF3SO2)2N	1.3-Dibutylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		1.37		1.12	-	1.61	1.04
351	IM42OH Cl	1-butyl-3-(2-hydroxyethyl)imidazolium chloride	U		1.70		1.23	-	2.16	1.39
352	Quin1O6-6Me Cl	1-[(Hexyloxy)methyl]-6-methylquinolinium chloride	U		0.94		0.76	-	1.12	0.68
353	Quin1O8-6Me Cl	6-Methyl-1-[(octyloxy)methyl]quinolinium chloride	U		0.85		0.65	-	1.06	0.80
354	Quin1O-10-6Me Cl	1-[(Decyloxy)methyl]-6-methylquinolinium chloride	U		0.70		0.50	-	0.91	0.90
355	Quin1O-12-6Me Cl	1-[(Dodecyloxy)methyl]-6-methylquinolinium chloride	U		0.67		0.48	-	0.85	1.05
356	Quin1O6-8OH Cl	1-[(Hexyloxy)methyl]-8-hydroxyquinolinium chloride	U		1.09		0.73	-	1.46	1.14
357	Quin1O8-8OH Cl	8-Hydroxy-1-[(octyloxy)methyl]quinolinium chloride	U		1.02		0.64	-	1.40	1.19
358	Quin1O-10-8OH Cl	1-[(Decyloxy)methyl]-8-hydroxyquinolinium chloride	U		0.98		0.60	-	1.35	1.25
359	Quin1O-12-8OH Cl	1-[(Dodecyloxy)methyl]-8-hydroxyquinolinium chloride	U		0.88		0.46	-	1.30	1.50
360	Quin4 BF4	1-Butylquinolinium tetrafluoroborate	L	0.05	0.85	-0.80				0.55
361	Quin4 Br	1-Butylquinolinium bromide	T	0.22	0.52	-0.30	0.38	-	0.66	0.80
362	Quin6 BF4	1-Hexylquinolinium tetrafluoroborate	T	-0.04	0.71	-0.75	0.51	-	0.91	0.88
363	Quin8 BF4	1-Octylquinolinium tetrafluoroborate	L	-0.18	0.61	-0.79				1.09
364	Quin8 Br	1-Octylquinolinium bromide	L	-0.20	0.27	-0.47				0.97

365	Quin1O6 Cl	1-[(Hexyloxy)methyl]quinolinium chloride	U		0.89		0.69	-	1.09	0.67
366	Quin1O8 Cl	1-[(Octyloxy)methyl]quinolinium chloride	U		0.80		0.64	-	0.97	0.59
367	Quin1O-10 Cl	1-[(Decyloxy)methyl]quinolinium chloride	U		0.68		0.44	-	0.91	0.90
368	Quin1O-12 Cl	1-[(Dodecyloxy)methyl]quinolinium chloride	U		0.66		0.41	-	0.90	1.04
369	IM55 (CF3SO2)2N	1.3-Dipentylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		1.24		1.03	-	1.45	1.15
370	Py1(COO1)(Ph-3-OMe-4-OMe) Cl	1-[1-(3.4-Dimethoxyphenyl)-2-methoxy-2-oxoethyl]pyridinium chloride	U		1.83		1.57	-	2.08	2.07*
371	Py1(COO1)(Ph-(3,4-OCH2O-)) Br	1-[1-(1.3-Benzodioxol-5-yl)-2-methoxy-2-oxoethyl]pyridinium bromide	U		1.88		1.59	-	2.16	2.04*
372	Py1(COO4)(Ph-(3,4-OCH2O-)) Br	1-[1-(1.3-Benzodioxol-5-yl)-2-butoxy-2-oxoethyl]pyridinium bromide	U		1.76		1.51	-	2.01	2.09*
373	Py2 Cl	1-Ethylpyridinium chloride	L	1.26	1.13	0.13				0.91
374	Py1CN (CF3SO2)2N	1-(Cyanomethyl)pyridinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	2.11	1.79	0.32				1.83*
375	Py1CN Cl	1-(Cyanomethyl)pyridinium chloride	L	1.66	1.29	0.37				1.84*
376	Py1COO1(COO1)(Ph-(3,4-OCH2O-)) Br	1-[2-[1-(1.3-Benzodioxol-5-yl)-2-methoxy-2-oxoethoxy]-2-oxoethyl]pyridinium bromide	U		2.06		1.61	-	2.51	3.66*
377	Py1COO1(COO4)(Ph-(3,4-OCH2O-)) Br	1-[2-[1-(1.3-Benzodioxol-5-yl)-2-butoxy-2-oxoethoxy]-2-oxoethyl]pyridinium bromide	U		1.89		1.48	-	2.30	3.56*
378	Py1COO2 (CF3SO2)2N	1-(2-Ethoxy-2-oxoethyl)pyridinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		2.31		2.13	-	2.50	1.13
379	Py1COO2 8OSO3	1-(2-Ethoxy-2-oxoethyl)pyridinium octyl sulfate	U		2.42		2.16	-	2.68	1.41
380	Py1COO2 Br	1-(2-Ethoxy-2-oxoethyl)pyridinium bromide	U		1.84		1.62	-	2.05	1.39
381	Py1COO2 PF6	1-(2-Ethoxy-2-oxoethyl)pyridinium hexafluorophosphate	U		2.13		1.97	-	2.29	1.22
382	Py3 (CF3SO2)2N	1-Propylpyridinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	T	1.82	1.40	0.41	1.19	-	1.62	1.09
383	Py3 Br	1-Propylpyridinium bromide	L	1.52	0.93	0.59				0.58
384	Py4 Cl	1-Butylpyridinium chloride	L	0.93	0.94	-0.01				0.52
385	Py4 Al2Cl7	1-Butylpyridinium µ-chlorohexachlorodialuminate	L	1.31	1.16	0.15				1.53*
386	Py4 N(CN)2	1-Butylpyridinium N-cyanocyanamide	U		1.30		1.07	-	1.52	0.98
387	Py4 Br	1-Butylpyridinium bromide	L	1.10	0.96	0.14				0.50

388	Py4 1OSO3	1-Butylpyridinium methyl sulfate	L	1.15	1.28	-0.14				0.30
389	Py4 8OSO3	1-Butylpyridinium octyl sulfate	U		1.55		1.22	-	1.88	1.51*
390	Py4 BF4	1-Butylpyridinium tetrafluoroborate	L	1.15	1.30	-0.15				0.48
391	Py4 CF3SO3	1-Butylpyridinium trifluoromethanesulfonate	L	1.33	1.31	0.02				0.29
392	Py4 PF6	1-Butylpyridinium hexafluorophosphate	L	1.29	1.25	0.04				0.39
393	Py5 (CF3SO2)2N	1-Pentylpyridinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	1.18	1.37	-0.18				1.05
394	Py5 Br	1-Pentylpyridinium bromide	L	0.88	0.89	-0.01				0.33
395	Py6 (CF3SO2)2N	1-Hexylpyridinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	1.50	1.35	0.15				1.05
396	Py6 CF3SO3	1-Hexylpyridinium trifluoromethanesulfonate	L	1.33	1.22	0.11				0.39
397	Py6 Cl	1-Hexylpyridinium chloride	L	1.02	0.86	0.17				0.30
398	Py6 PF6	1-Hexylpyridinium hexafluorophosphate	L	1.25	1.17	0.08				0.45
399	Py8 Cl	1-Octylpyridinium chloride	L	0.96	0.69	0.27				0.42
400	Py8 (CF3SO2)2N	1-Octylpyridinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	1.08	1.18	-0.11				1.24
401	Py-10 Br	1-Decylpyridinium bromide	U		0.63		0.49	-	0.77	0.53
402	Py-16 Br	1-Hexadecylpyridinium bromide	U		0.28		0.05	-	0.52	1.24
403	Py-16 Cl	1-Hexadecylpyridinium chloride	U		0.26		0.02	-	0.50	1.22
404	Py3OH (CF3SO2)2N	1-(3-Hydroxypropyl)pyridinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	T	2.18	2.26	-0.08	1.91	-	2.61	1.52*
405	Py3OH Cl	1-(3-Hydroxypropyl)pyridinium chloride	T	1.89	1.76	0.12	1.23	-	2.30	1.69*
406	Py3O1 (CF3SO2)2N	1-(3-Methoxypropyl)pyridinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	1.70	1.77	-0.07				0.99
407	Py3O1 Cl	1-(3-Methoxypropyl)pyridinium chloride	L	1.42	1.27	0.15				0.84
408	Py3SO3H CF3SO3	1-(3-Sulfopropyl)pyridinium trifluoromethanesulfonate	T	2.55	2.48	0.07	1.74	-	3.22	2.47*
409	Py2OH (CF3SO2)2N	1-(2-Hydroxyethyl)pyridinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	2.26	2.25	0.01				1.80*
410	Py2OH I	1-(2-Hydroxyethyl)pyridinium iodide	L	2.09	1.82	0.27				1.90*
411	Py2O1 (CF3SO2)2N	1-(2-Methoxyethyl)pyridinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	1.71	1.99	-0.28				0.83

412	Py2O1 Cl	1-(2-Methoxyethyl)pyridinium chloride	L	1.31	1.49	-0.18				0.91
413	Py2O2 (CF3SO2)2N	1-(2-Ethoxyethyl)pyridinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	1.12	1.84	-0.73				0.87
414	Py2O2 Br	1-(2-Ethoxyethyl)pyridinium bromide	T	0.92	1.37	-0.45	1.17	-	1.57	0.75
415	Py1O2 (CF3SO2)2N	1-(Ethoxymethyl)pyridinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	1.76	2.03	-0.27				0.58
416	Py1O2 Cl	1-(Ethoxymethyl)pyridinium chloride	T	1.30	1.53	-0.23	1.38	-	1.69	0.69
417	Pyr66 BF4	1.1-Dihexylpyrrolidinium tetrafluoroborate	U		1.37		1.19	-	1.56	1.57*
418	IM66 (CF3SO2)2N	1.3-Dihexylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		1.09		0.88	-	1.30	1.31
419	IM-10-10-2Me (CF3SO2)2N	1.3-Didecyl-2-methylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		0.81		0.59	-	1.03	1.95*
420	Pyr-12-2OH Cl	1-Dodecyl-1-(2-hydroxyethyl)pyrrolidinium chloride	U		1.47		1.02	-	1.91	1.57*
421	IM-14-2OH-2Me Cl	1-(2-Hydroxyethyl)-2-methyl-3-tetradecylimidazolium chloride	U		1.08		0.59	-	1.58	1.73*
422	IM-16-2OH-2Me Cl	1-Hexadecyl-3-(2-hydroxyethyl)-2-methylimidazolium chloride	U		0.88		0.32	-	1.44	2.05*
423	IM2OH-(2Ph) Cl	1-(2-hydroxyethyl)-3-(2-phenylethyl)immidazolium chloride	U		1.26		0.67	-	1.86	1.88*
424	IM2OH-(2OH) Cl	1.3-di-(2-hydroxyethyl)imidazolium chloride	U		1.94		0.93	-	2.94	3.20*
425	IM1O3-1O3 Cl	1.3-Bis(propoxymethyl)imidazolium chloride	U		1.52		1.33	-	1.71	0.78
426	IM1O4-1O4 Cl	1.3-Bis(butoxymethyl)imidazolium chloride	U		1.46		1.33	-	1.60	0.92
427	IM1O5-1O5 Cl	1.3-Bis[(pentyloxy)methyl]imidazolium chloride	U		1.38		1.22	-	1.53	0.95
428	IM1O6-1O6 Cl	1.3-Bis[(hexyloxy)methyl]imidazolium chloride	U		1.32		1.17	-	1.46	1.13
429	IM1O7-1O7 Cl	1.3-Bis[(heptyloxy)methyl]imidazolium chloride	U		1.21		1.07	-	1.35	1.21
430	IM1O8-1O8 Cl	1.3-Bis[(octyloxy)methyl]imidazolium chloride	U		1.17		1.03	-	1.31	1.38
431	IM1O9-1O9 Cl	1.3-Bis[(nonyloxy)methyl]imidazolium chloride	U		1.01		0.86	-	1.16	1.52*
432	IM1O-10-1O-10 Cl	1.3-Bis[(decyloxy)methyl]imidazolium chloride	U		0.93		0.79	-	1.06	1.62*
433	IM1O-11-1O-11 Cl	1.3-Bis[(undecyloxy)methyl]imidazolium chloride	U		0.94		0.81	-	1.06	1.86*
434	IM1O-12-1O-12 Cl	1.3-Bis[(dodecyloxy)methyl]imidazolium chloride	U		0.81		0.65	-	0.96	2.00*
435	IM1O-14-1O-14 Cl	1.3-Bis[(tetradecyloxy)methyl]imidazolium chloride	U		0.71		0.53	-	0.88	2.39*

436	IM1O-16-1O-16 Cl	1.3-Bis[(hexadecyloxy)methyl]imidazolium chloride	U		0.50		0.22	-	0.77	2.53*
437	IM01 BF4	1-Methylimidazole hydrogen tetrafluoroborate	L	2.23	2.17	0.06				2.03*
438	IM01 HO1(1)COO	1-Methylimidazole 2-hydroxypropanoate	U		2.26		2.07	-	2.44	2.51*
439	IM01 HO1(1)COO_S	1-Methylimidazole (2S)-2-hydroxypropanoate	U		2.27		2.09	-	2.45	2.60*
440	IM01 1COO	1-methylimidazolium acetate	U		2.11		1.90	-	2.31	2.74*
441	IM01 CF3COO	1-methylimidazolium trifluoroacetate	U		2.23		2.00	-	2.45	2.10*
442	IM01 CF3SO3	1-methylimidazolium 1.1.1-trifluoromethanesulfonate	U		2.18		1.92	-	2.44	1.97*
443	IM02 HO1(1)COO	1-Ethylimidazole 2-hydroxypropanoate	U		2.19		2.02	-	2.37	2.45*
444	IM02 HO1(1)COO_S	1-Ethylimidazole (2S)-2-hydroxypropanoate	U		2.21		2.04	-	2.38	2.55*
445	IM03 HO1(1)COO	1-Propylimidazole 2-hydroxypropanoate	U		2.02		1.86	-	2.18	2.37*
446	IM03 HO1(1)COO_S	1-Propylimidazole (2S)-2-hydroxypropanoate	U		2.04		1.88	-	2.19	2.48*
447	IM04 HO1(1)COO	1-Butylimidazole 2-hydroxypropanoate	U		1.98		1.81	-	2.14	2.39*
448	IM04 HO1(1)COO_S	1-Butylimidazole (2S)-2-hydroxypropanoate	U		1.99		1.83	-	2.15	2.50*
449	IM04 1COO	1-butylimidazolium acetate	U		1.83		1.64	-	2.01	2.60*
450	IM04 CF3COO	1-butylimidazolium trifluoroacetate	U		1.95		1.74	-	2.15	1.94*
451	IM04 CF3SO3	1-butylimidazolium 1.1.1-trifluoromethanesulfonate	U		1.90		1.66	-	2.14	1.76*
452	IM05 HO1(1)COO	1-Pentylimidazole 2-hydroxypropanoate	U		1.88		1.71	-	2.05	2.40*
453	IM05 HO1(1)COO_S	1-Pentylimidazole (2S)-2-hydroxypropanoate	U		1.90		1.73	-	2.06	2.51*
454	IM06 HO1(1)COO	1-Hexylimidazole 2-hydroxypropanoate	U		1.91		1.74	-	2.08	2.44*
455	IM06 HO1(1)COO_S	1-Hexylimidazole (2S)-2-hydroxypropanoate	U		1.93		1.76	-	2.09	2.55*
456	IM07 HO1(1)COO	1-Heptylimidazole 2-hydroxypropanoate	U		1.77		1.57	-	1.96	2.47*
457	IM07 HO1(1)COO_S	1-Heptylimidazole (2S)-2-hydroxypropanoate	U		1.78		1.59	-	1.97	2.58*
458	IM08 HO1(1)COO	1-Octylimidazole 2-hydroxypropanoate	U		1.77		1.58	-	1.97	2.53*
459	IM08 HO1(1)COO_S	1-Octylimidazole (2S)-2-hydroxypropanoate	U		1.79		1.60	-	1.98	2.64*

460	IM09 HO1(1)COO	1-Nonylimidazole 2-hydroxypropanoate	U	1.69	1.49	-	1.90	2.56*
461	IM09 HO1(1)COO_S	1-Nonylimidazole (2S)-2-hydroxypropanoate	U	1.71	1.51	-	1.91	2.67*
462	IM0-10 HO1(1)COO	1-Decylimidazole 2-hydroxypropanoate	U	1.65	1.44	-	1.85	2.60*
463	IM0-10 HO1(1)COO_S	1-Decylimidazole (2S)-2-hydroxypropanoate	U	1.66	1.46	-	1.87	2.71*
464	IM0-11 HO1(1)COO	1-Undecylimidazole 2-hydroxypropanoate	U	1.64	1.43	-	1.84	2.65*
465	IM0-11 HO1(1)COO_S	1-Undecylimidazole (2S)-2-hydroxypropanoate	U	1.65	1.45	-	1.86	2.75*
466	IM0-12 HO1(1)COO	1-Dodecylimidazole 2-hydroxypropanoate	U	1.64	1.45	-	1.83	2.67*
467	IM0-12 HO1(1)COO_S	1-Dodecylimidazole (2S)-2-hydroxypropanoate	U	1.66	1.47	-	1.84	2.78*
468	IM01O4 HO1(1)COO	1-(Butoxymethyl)imidazole 2-hydroxypropanoate	U	2.32	2.12	-	2.51	2.48*
469	IM01O4 HO1(1)COO_S	1-(Butoxymethyl)imidazole (2S)-2-hydroxypropanoate	U	2.33	2.14	-	2.52	2.58*
470	IM01O5 HO1(1)COO	1-[(Pentyloxy)methyl]imidazole 2-hydroxypropanoate	U	2.23	2.03	-	2.44	2.51*
471	IM01O5 HO1(1)COO_S	1-[(Pentyloxy)methyl]imidazole (2S)-2-hydroxypropanoate	U	2.25	2.05	-	2.45	2.62*
472	IM01O6 HO1(1)COO	1-[(Hexyloxy)methyl]imidazole 2-hydroxypropanoate	U	2.27	2.06	-	2.48	2.57*
473	IM01O6 HO1(1)COO_S	1-[(Hexyloxy)methyl]imidazole (2S)-2-hydroxypropanoate	U	2.29	2.09	-	2.49	2.68*
474	IM01O7 HO1(1)COO	1-[(Heptyloxy)methyl]imidazole 2-hydroxypropanoate	U	2.18	1.98	-	2.38	2.60*
475	IM01O7 HO1(1)COO_S	1-[(Heptyloxy)methyl]imidazole (2S)-2-hydroxypropanoate	U	2.20	2.00	-	2.39	2.71*
476	IM01O8 HO1(1)COO	1-[(Octyloxy)methyl]imidazole 2-hydroxypropanoate	U	2.12	1.91	-	2.34	2.63*
477	IM01O8 HO1(1)COO_S	1-[(Octyloxy)methyl]imidazole (2S)-2-hydroxypropanoate	U	2.14	1.93	-	2.35	2.74*
478	IM01O9 HO1(1)COO	1-[(Nonyloxy)methyl]imidazole 2-hydroxypropanoate	U	2.00	1.77	-	2.22	2.67*
479	IM01O9 HO1(1)COO_S	1-[(Nonyloxy)methyl]imidazole (2S)-2-hydroxypropanoate	U	2.01	1.79	-	2.23	2.77*
480	IM01O-10 HO1(1)COO	1-[(Decyloxy)methyl]imidazole 2-hydroxypropanoate	U	2.01	1.80	-	2.22	2.72*
481	IM01O-10 HO1(1)COO_S	1-[(Decyloxy)methyl]imidazole (2S)-2-hydroxypropanoate	U	2.03	1.82	-	2.23	2.82*
482	IM01O-11 HO1(1)COO	1-[(Undecyloxy)methyl]imidazole 2-hydroxypropanoate	U	1.93	1.72	-	2.15	2.76*
483	IM01O-11 HO1(1)COO_S	1-[(Undecyloxy)methyl]imidazole (2S)-2-hydroxypropanoate	U	1.95	1.74	-	2.16	2.87*

484	IM01O-12 HO1(1)COO	1-[(Dodecyloxy)methyl]imidazole 2-hydroxypropanoate	U		1.92		1.67	-	2.16	2.87*
485	IM01O-12 HO1(1)COO_S	1-[(Dodecyloxy)methyl]imidazole (2S)-2-hydroxypropanoate	U		1.93		1.69	-	2.17	2.97*
486	Py0 Cl	Pyridine hydrochloride	L	2.06	1.77	0.30				2.37*
487	0600NN (CF3SO2)2N	1-hexyl-1.4-diaza[2.2.2]bicyclooctanium bis(trifluoromethylsulfonyl)imide	U		2.34		2.15	-	2.53	0.90
488	IM00 1COO	1H-Imidazol-1-ium acetate	U		2.37		2.14	-	2.60	2.71*
489	IM00 CF3COO	1H-Imidazol-1-ium trifluoroacetate	U		2.49		2.24	-	2.74	2.07*
490	IM00 CFSO3	1H-Imidazol-1-ium 1.1.1-trifluoromethanesulfonate	U		2.44		2.15	-	2.73	1.94*
491	IM01-2Me (CF3SO2)2N	1.2-dimethylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		2.24		2.01	-	2.48	2.02*
492	IM16-2Me Cl	1-hexyl-2.3-dimethyl imidazolium chloride	U		0.73		0.63	-	0.83	0.38
493	IM13-2Me (CF3SO2)2N	1.2-dimethyl-3-propylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		1.50		1.26	-	1.74	1.05
494	IM18 N(CN)2	1-Methyl-3-octylimidazolium dicyanamide	U		1.23		1.03	-	1.44	0.99
495	Py4-3Me (CF3SO2)2N	1-buthyl-3-methylpyridinium1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		1.31		1.09	-	1.53	1.10
496	IM18 SbF6	1-methyl-3-octylimidazolium hexafluoroantimonate	U		1.22		1.13	-	1.30	0.74
497	IM11 (1O)2PO2	1.3-dimethyl imidazolium dimethyl phopsphate	U		1.65		1.49	-	1.82	0.69
498	IM18 CF3COO	1-methyl-3-octylimidazolium trifluoroacetate	U		1.29		1.18	-	1.40	1.18
499	IM12OH 1COO	1-(2-hydroxyethyl)-3-methylimidazolium acetate	U		2.09		1.59	-	2.60	2.55*
500	IM12OH N(CN2)	1-(2-hydroxyethyl)-3-methylimidazolium dicyanamide	U		2.15		1.76	-	2.54	1.71*
501	IM12OH NO3	1-(2-hydroxyethyl)-3-methylimidazolium nitrate	U		1.80		1.38	-	2.22	2.32*
502	Py6-4NMe2 Br	4-(Dimethylamino)-1-hexylpyridinium bromide	U		0.60		0.47	-	0.73	0.61
503	Py8-4Me (CF3SO2)2N	1-octyl-4-methylpyridinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		1.09		0.90	-	1.28	1.30
504	Py4 (CF3SO2)2N	1-butylpyridinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		1.44		1.20	-	1.67	1.03
505	Pip12OH N(CN)2	1-(2-hydroxyethyl)-1-methylpiperidinium N-cyanocyanamide	U		2.46		2.20	-	2.72	1.32
506	Pyr18 (CF3SO2)2N	1-methyl-1-octylpyrrolidinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		1.65		1.34	-	1.96	1.23
507	Mor14 N(CN)2	4-butyl-4-methylmorpholinium dicyanamide	U		2.14		2.02	-	2.26	0.79

508	Mor12OH N(CN)2	4-(2-hydroxyethyl)-4-methylmorpholinium dicyanamide	U	2.74	2.48	-	3.00	1.19
509	Mor12 N(CN)2	1-ethyl-1-methylmorpholinium dicyanamide	U	2.29	2.14	-	2.44	0.82
510	Mor12 (CF3SO2)2N	1-ethyl-1-methylmorpholinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	2.43	2.27	-	2.59	0.47
511	IM14 1COO	1-butyl-3-methylimidazolium acetate	U	1.32	1.19	-	1.44	1.96*
512	IM16 1COO	1-hexyl-3-methylimidazolium acetate	U	1.20	1.08	-	1.32	1.95*
513	IM16 CF3COO	1-hexyl-3-methylimidazolium trifluoroacetate	U	1.32	1.24	-	1.41	0.98
514	Pyr14 1COO	1-butyl-1-methylpyrroldinium acetate	U	1.67	1.44	-	1.91	2.28*
515	IM18 NO3	1-methyl-3-octylimidazolium nitrate	U	0.88	0.67	-	1.09	1.62*
516	IM14 (CF3SO2)3C	1-butyl-3-methylimidazolium tris[(trifluoromethyl)sulfonyl]methide	U	1.61	1.39	-	1.82	0.88
517	IM1-18 (CF3SO2)2N	1-methyl-3-octadecylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	0.84	0.63	-	1.04	1.98*
518	Py4-3Me (CF3SO2)2N	1-butyl-3-methylpyridinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	1.31	1.09	-	1.53	1.10
519	Py6-3Me (CF3SO2)2N	1-hexyl-3-methylpyridinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	1.23	1.03	-	1.43	1.13
520	Pyr13 (CF3SO2)2N	1-methyl-1-propylpyrrolidinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	1.94	1.60	-	2.28	1.08

[a] Y_predictions according to AChE PLS correlation model, as reported in the section 3.3.3. Note: ILs numeration as in the other PLS datamatrices.

Table B14 Experimental and predicted[a] *Vibrio fischeri* ecotoxicity values. Predictions are calculated using the *Vibrio fischeri* correlation model derived by using 3 PPs as descriptors. The (*) indicates a DModX value higher than 2.33. L: learning set; T: test set; U: unknown log(EC_{50}).

IL	IL code	Systematic name	Set	PP_1+	PP_2+	PP_3-	Y = log (EC_{50}) *Vibrio f.* µg/L	Ý[a] = log (EC_{50}) *Vibrio f.*	Y-Ý	Confidence Interval (C.I.) for prediction	DModX
1	Py4-2Me BF4	1-Butyl-2-methylpyridinium tetrafluoroborate	U	0.27	-6.91	-0.33		3.00		2.7 - 3.32	0,51
2	Py4-2Me Cl	1-Butyl-2-methylpyridinium chloride	U	0.27	-6.91	-2.31		3.48		3.3 - 3,62	0,07
3	Pyr12 2OSO3	1-Ethyl-1-methylpyrrolidinium ethyl sulfate	U	4.57	-4.49	-0.18		3.88		3.6 - 4,14	0,37
4	Pyr11CN (CF3SO2)2N	1-(Cyanomethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	6.95	0.11	2.86		3.36		3.2 - 3,48	0,29
5	Pyr11CN Cl	1-(Cyanomethyl)-1-methylpyrrolidinium chloride	U	6.95	0.11	-2.31		4.60		4 - 5,17	1,21
6	Pyr11COO2 (CF3SO2)2N	1-(2-Ethoxy-2-oxoethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	7.17	1.90	2.86	3.23	3.25	-0.02		0,18
7	Pyr11COO2 Br	1-(2-Ethoxy-2-oxoethyl)-1-methylpyrrolidinium bromide	U	7.17	1.90	-2.16		4.46		3.7 - 5,26	1,63
8	Pyr11COO2 (C2F5)3PF3	1-(2-Ethoxy-2-oxoethyl)-1-methylpyrrolidinium tris(pentafluoroethyl)trifluorophosphate	U	7.17	1.90	4.77		2.79		2.6 - 2,98	0,38
9	Pyr13 PF6	1-Methyl-1-propylpyrrolidinium hexafluorophosphate	U	3.13	-4.34	-0.21		3.49		3.4 - 3,62	0,16
10	Pyr14 Cl	1-Butyl-1-methylpyrrolidinium chloride	L	1.96	-4.12	-2.31	4.65	3.67	0.99		0,65
11	Pyr14 (C2F5)3PF3	1-Butyl-1-methylpyrrolidinium trifluorotris(pentafluoroethyl)phosphate	U	1.96	-4.12	4.77		1.96		1.4 - 2,56	1,42
12	Pyr14 (CF3SO2)2N	1-Butyl-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	1.96	-4.12	2.86		2.42		2.1 - 2,79	0,87
13	Pyr14 1OSO3	1-Butyl-1-methylpyrrolidinium methyl sulfate	U	1.96	-4.12	-0.44		3.22		3.2 - 3,25	0,09
14	Pyr14 BF4	1-Butyl-1-methylpyrrolidinium tetrafluoroborate	U	1.96	-4.12	-0.33		3.19		3.2 - 3,22	0,06
15	Pyr14 Br	1-Butyl-1-methylpyrrolidinium bromide	U	1.96	-4.12	-2.16		3.63		3.4 - 3,86	0,59
16	Pyr14 N(CN)2	1-Butyl-1-methylpyrrolidinium N-cyanocyanamide	U	1.96	-4.12	0.00		3.11		3.1 - 3,15	0,04
17	Pyr16 (CF3SO2)2N	1-Hexyl-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	T	0.02	-3.63	2.86	2.40	1.87	0.53	1.7 2,06	0,52
18	Pyr16 Cl	1-Hexyl-1-methylpyrrolidinium chloride	U	0.02	-3.63	-2.31		3.11		2.7 - 3,55	0,98
19	Pyr18 BF4	1-Methyl-1-octylpyrrolidinium tetrafluoroborate	U	-2.33	-3.03	-0.33		1.96		1.5 - 2,42	0,82
20	Pyr18 Cl	1-Methyl-1-octylpyrrolidinium chloride	U	-2.33	-3.03	-2.31		2.43		1.8 - 3,12	1,40
21	Pyr13OH (CF3SO2)2N	1-(3-Hydroxypropyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	10.38	4.48	2.86	3.91	3.86	0.04		0,52
22	Pyr13OH Cl	1-(3-Hydroxypropyl)-1-methylpyrrolidinium chloride	U	10.38	4.48	-2.31		5.11		4.1 - 6,12	2,01
23	Pyr13O1 (CF3SO2)2N	1-(3-Methoxypropyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	5.81	-0.16	2.86		3.08		3 - 3,19	0,23
24	Pyr13O1 Cl	1-(3-Methoxypropyl)-1-methylpyrrolidinium chloride	U	5.81	-0.16	-2.31		4.32		3.7 - 4,92	1,27
25	Pyr12OH (CF3SO2)2N	1-(2-Hydroxyethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	11.45	4.49	2.86		4.15		3.8 - 4,53	0,39

26	Pyr12OH I	1-(2-Hydroxyethyl)-1-methylpyrrolidinium iodide	U	11.45	4.49	-1.63		5.22		4.4	-	6,1	1,69
27	Pyr12O1 (CF3SO2)2N	1-(2-Methoxyethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	7.36	-0.19	2.86		3.49		3.3	-	3,66	0,41
28	Pyr12O1 (C2F5)3PF3	1-(2-Methoxyethyl)-1-methylpyrrolidinium tris(pentafluoroethyl)trifluorophosphate	U	7.36	-0.19	4.77		3.03		2.7	-	3,4	0,96
29	Pyr12O1 Cl	1-(2-Methoxyethyl)-1-methylpyrrolidinium chloride	U	7.36	-0.19	-2.31		4.74		4.2	-	5,24	1,09
30	Pyr12O2 (CF3SO2)2N	1-(2-Ethoxyethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	5.75	-0.56	2.86	2.97	3.10	-0.13				0,34
31	Pyr12O2 Br	1-(2-Ethoxyethyl)-1-methylpyrrolidinium bromide	U	5.75	-0.56	-2.16		4.31		3.8	-	4,83	1,12
32	Pyr11O2 (CF3SO2)2N	1-(Ethoxymethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	5.12	-1.38	2.86		3.01		2.8	-	3,19	0,48
33	Pyr11O2 Cl	1-(Ethoxymethyl)-1-methylpyrrolidinium chloride	U	5.12	-1.38	-2.31		4.25		3.8	-	4,71	1,02
34	Pip11CN (CF3SO2)2N	1-(Cyanomethyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	5.85	0.24	2.86		3.05		2.9	-	3,18	0,13
35	Pip11CN Cl	1-(Cyanomethyl)-1-methylpiperidinium chloride	U	5.85	0.24	-2.31		4.30		3.6	-	4,95	1,37
36	Pip13 (CF3SO2)2N	1-Methyl-1-propylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	2.18	-4.18	2.86		2.49		2.1	-	2,88	0,91
37	Pip13 PF6	1-Methyl-1-propylpiperidinium hexafluorophosphate	U	2.18	-4.18	-0.21		3.23		3.2	-	3,27	0,02
38	Pip14 (CF3SO2)2N	1-Butyl-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	1.15	-3.97	2.86	2.57	2.20	0.37				0,76
39	Pip14 Br	1-Butyl-1-methylpiperidinium bromide	T	1.15	-3.97	-2.16	4.32	3.40	0.92	3.1		3,7	0,72
40	Pip13OH (CF3SO2)2N	1-(3-Hydroxypropyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	9.27	4.69	2.86		3.55		3	-	4,09	0,69
41	Pip13OH Cl	1-(3-Hydroxypropyl)-1-methylpiperidinium chloride	U	9.27	4.69	-2.31		4.80		3.7	-	5,91	2,19
42	Pip13O1 (CF3SO2)2N	1-(3-Methoxypropyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	4.88	0.03	2.86		2.82		2.7	-	2,96	0,08
43	Pip13O1 Cl	1-(3-Methoxypropyl)-1-methylpiperidinium chloride	U	4.88	0.03	-2.31		4.06		3.4	-	4,74	1,42
44	Pip12OH (CF3SO2)2N	1-(2-Hydroxyethyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	10.68	4.70	2.86		3.92		3.5	-	4,38	0,53
45	Pip12OH I	1-(2-Hydroxyethyl)-1-methylpiperidinium iodide	U	10.68	4.70	-1.63		5.00		4.1	-	5,95	1,84
46	Pip12O1 (CF3SO2)2N	1-(2-Methoxyethyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	5.73	-1.14	2.86		3.15		3	-	3,33	0,49
47	Pip12O1 Br	1-(2-Methoxyethyl)-1-methylpiperidinium bromide	U	5.73	-1.14	-2.16		4.36		3.9	-	4,8	0,97
48	Pip12O2 (CF3SO2)2N	1-(2-Ethoxyethyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	4.83	-0.32	2.86		2.84		2.7	-	2,95	0,17
49	Pip12O2 Br	1-(2-Ethoxyethyl)-1-methylpiperidinium bromide	U	4.83	-0.32	-2.16		4.04		3.4	-	4,66	1,29
50	Pip11O2 (CF3SO2)2N	1-(Ethoxymethyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	3.80	-1.20	2.86		2.64		2.5	-	2,75	0,29
51	Pip11O2 Cl	1-(Ethoxymethyl)-1-methylpiperidinium chloride	U	3.80	-1.20	-2.31		3.89		3.3	-	4,45	1,21
52	Mor12 4MePhSO3	4-Ethyl-4-methylmorpholinium 4-methylbenzenesulfonate	U	8.90	-0.32	2.48		4.00		3.8	-	4,23	0,50
53	Mor11CN (CF3SO2)2N	4-(Cyanomethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	9.29	3.51	2.86		3.66		3.3	-	4,03	0,37

54	Mor11CN Cl	4-(Cyanomethyl)-4-methylmorpholinium chloride	U	9.29	3.51	-2.31		4.91		4	-	5,84	1,87
55	Mor14 (CF3SO2)2N	4-Butyl-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	T	6.23	0.06	2.86	2.48	3.17	-0.69	3.1		3,29	0,22
56	Mor14 Br	4-Butyl-4-methylmorpholinium bromide	L	6.23	0.06	-2.16	4.30	4.38	-0.08				1,27
57	Mor13OH (CF3SO2)2N	4-(3-Hydroxypropyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	12.12	7.62	2.86		4.04		3.2	-	4,84	1,16
58	Mor13OH Cl	4-(3-Hydroxypropyl)-4-methylmorpholinium chloride	U	12.12	7.62	-2.31		5.28		3.9	-	6,66	2,66*
59	Mor13O1 (CF3SO2)2N	4-(3-Methoxypropyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	7.79	2.32	2.86		3.38		3.1	-	3,66	0,21
60	Mor13O1 Cl	4-(3-Methoxypropyl)-4-methylmorpholinium chloride	U	7.79	2.32	-2.31		4.62		3.8	-	5,47	1,72
61	Mor12OH (CF3SO2)2N	4-(2-Hydroxyethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	13.05	7.64	2.86		4.28		3.5	-	5,03	1,06
62	Mor12OH I	4-(2-Hydroxyethyl)-4-methylmorpholinium iodide	U	13.05	7.64	-1.63		5.36		4.1	-	6,61	2,37*
63	Mor12O1 (CF3SO2)2N	4-(2-Methoxyethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	9.02	2.70	2.86		3.67		3.4	-	3,94	0,18
64	Mor12O1 Cl	4-(2-Methoxyethyl)-4-methylmorpholinium chloride	U	9.02	2.70	-2.31		4.91		4.1	-	5,74	1,68
65	Mor12O2 (CF3SO2)2N	4-(2-Ethoxyethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	8.20	2.70	2.86		3.45		3.1	-	3,76	0,27
66	Mor12O2 Br	4-(2-Ethoxyethyl)-4-methylmorpholinium bromide	U	8.20	2.70	-2.16		4.66		3.8	-	5,52	1,73
67	Mor11O2 (CF3SO2)2N	4-(Ethoxymethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	8.27	2.53	2.86	3.38	3.49	-0.10				0,22
68	Mor11O2 Cl	4-(Ethoxymethyl)-4-methylmorpholinium chloride	U	8.27	2.53	-2.31		4.73		3.9	-	5,58	1,72
69	IM11COO3-2Me 8OSO3	1,2-Dimethyl-3-(2-oxo-2-propoxyethyl)imidazolium octylsulfate	U	5.13	2.76	3.86		2.40		2	-	2,81	0,34
70	IM11COO3-2Me Br	1,2-Dimethyl-3-(2-oxo-2-propoxyethyl)imidazolium bromide	U	5.13	2.76	-2.16		3.84		2.8	-	4,91	2,08
71	IM11COO5-2Me 8OSO3	1,2-Dimethyl-3-[2-oxo-2-(pentyloxy)ethyl]imidazolium octylsulfate	U	2.60	3.30	3.86		1.68		1	-	2,34	0,76
72	IM11COO5-2Me Br	1,2-Dimethyl-3-[2-oxo-2-(pentyloxy)ethyl]imidazolium bromide	U	2.60	3.30	-2.16		3.13		1.8	-	4,44	2,51*
73	IM1gly-2Me N(NC)2	1,2-dimethyl-3-glycerylimidazolium dicyanamide	U	12.79	9.75	0.00		4.71		3.3	-	6,11	2,49*
74	IM1gly-2Me (CF3SO2)2N	1,2-dimethyl-3-glycerylimidazolium bis(trifluoromethylsulphonyl)imide	U	12.79	9.75	2.86		4.02		2.9	-	5,1	1,66
75	IM14-2Me (CF3SO2)2N	1-Butyl-2,3-dimethylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	1.01	-5.58	2.86		2.31		1.8	-	2,83	1,16
76	IM14-2Me BF4	1-Butyl-2,3-dimethylimidazolium tetrafluoroborate	U	1.01	-5.58	-0.33		3.07		2.9	-	3,24	0,23
77	IM14-2Me CF3SO3	1-Butyl-2,3-dimethylimidazolium trifluoromethanesulfonate	U	1.01	-5.58	0.07		2.98		2.8	-	3,18	0,35
78	IM16-2Me BF4	1-Hexyl-2,3-dimethylimidazolium tetrafluoroborate	U	-2.67	-6.14	-0.33		2.15		2.1	-	2,23	0,02
79	IM16-2Me (CF3SO2)2N	1-hexyl-2,3-dimethylimidazolium bis(trifluoromethylsulphonyl)imide	U	-2.67	-6.14	2.86		1.38		1	-	1,78	0,90
80	IM12OH-2Me Cl	1-(2-hydroxyethyl)-2,3-dimethylimidazolium chloride	U	9.21	2.25	-2.31		5.00		4.3	-	5,75	1,54
81	IM11 (CF3SO2)2N	1,3-Dimethylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	4.18	-6.87	2.86		3.26		2.3	-	4,19	1,85
82	IM11 1OSO3	1,3-dimethylimidazolium methylsulfate	U	4.18	-6.87	-0.44		4.05		3.5	-	4,62	0,90
83	IM11 4MePhSO3	1,3-dimethylimidazolium p-toluenesulfonate	U	4.18	-6.87	2.48		3.35		2.5	-	4,24	1,74

84	IM11 N(CN)2	1-methyl-3-methylimidaziolium N-cyanocyanamide	U	4.18	-6.87	0.00		3.95		3.3	-	4,56	1,02
85	IM11(COO1)(Ph-(3,4-OCH2O-)) Cl	1-[1-(1,3-Benzodioxol-5-yl)-2-methoxy-2-oxoethyl]-3-methylimidazolium chloride	U	2.18	6.00	-2.31		2.80		1	-	4,58	3,32*
86	IM11(COO4)(Ph-(3,4-OCH2O-)) Br	1-[1-(1,3-Benzodioxol-5-yl)-2-butoxy-2-oxoethyl]-3-methylimidazolium bromide	U	0.12	7.31	-2.16		2.11		0	-	4,2	3,86*
87	IM12 (C2F5)3PF3	1-Ethyl-3-methylimidazolium trifluorotris(pentafluoroethyl)phosphate	L	3.24	-6.75	4.77	1.68	2.54	-0.86				2,33
88	IM12 (C2F5)2PO2	1-Ethyl-3-methylimidazolium bis(pentafluoroethyl)phosphinate	L	3.24	-6.75	2.75	3.05	3.03	0.02				1,73
89	IM12 C(CN)3	1-Ethyl-3-methylimidazolium, salt with methanetricarbonitrile	L	3.24	-6.75	-1.96	3.59	4.16	-0.57				0,33
90	IM12 B(CN)4	1-Ethyl-3-methylimidazolium tetracyanoborate	L	3.24	-6.75	-0.53	3.56	3.82	-0.26				0,76
91	IM12 N(CN)2	1-Ethyl-3-methylimidazolium N-cyanocyanamide	L	3.24	-6.75	0.00	4.00	3.69	0.31				0,91
92	IM12 (CF3SO2)2N	1-Ethyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	3.24	-6.75	2.86	3.11	3.00	0.11				1,77
93	IM12 Cl	1-Ethyl-3-methylimidazolium chloride	L	3.24	-6.75	-2.31	4.32	4.25	0.08				0,22
94	IM12 2OSO3	1-Ethyl-3-methylimidazolium ethyl sulfate	T	3.24	-6.75	-0.18	4.28	3.73	0.55	3.2		4,24	0,83
95	IM12 (OOCCOO)2B	1-Ethyl-3-methylimidazolium bis[ethanedioato-O1,O2]borate	U	3.24	-6.75	0.02		3.69		3.2	-	4,22	0,89
96	IM12 1COO	1-Ethyl-3-methylimidazolium acetate	U	3.24	-6.75	-5.87		5.10		4.8	-	5,4	0,81
97	IM12 1O2O2OSO3	1-Ethyl-3-methylimidazolium 2-(2-methoxyethoxy)ethyl sulfate	U	3.24	-6.75	3.67		2.81		1.9	-	3,75	1,95
98	IM12 1OSO3	1-Ethyl-3-methylimidazolium methylsulfate	U	3.24	-6.75	-0.44		3.79		3.3	-	4,28	0,76
99	IM12 1SO3	1-Ethyl-3-methylimidazolium methanesulfonate	U	3.24	-6.75	-0.86		3.90		3.5	-	4,33	0,64
100	IM12 4MePhSO3	1-Ethyl-3-methylimidazolium 4-methylbenzenesulfonate	U	3.24	-6.75	2.48		3.09		2.3	-	3,9	1,61
101	IM12 8OSO3	1-Ethyl-3-methylimidazolium octylsulfate	U	3.24	-6.75	3.86		2.76		1.8	-	3,73	2,01
102	IM12 BF4	1-Ethyl-3-methylimidazolium tetrafluoroborate	U	3.24	-6.75	-0.33		3.77		3.3	-	4,26	0,79
103	IM12 CF3COO	1-Ethyl-3-methylimidazolium trifluoroacetate	U	3.24	-6.75	-2.30		4.24		3.9	-	4,54	0,22
104	IM12 CF3SO3	1-Ethyl-3-methylimidazolium trifluoromethanesulfonate	U	3.24	-6.75	0.07		3.67		3.1	-	4,21	0,91
105	IM12 HSO4	1-Ethyl-3-methylimidazolium hydrogen sulfate	U	3.24	-6.75	-1.42		4.03		3.6	-	4,41	0,48
106	IM12 PF6	1-Ethyl-3-methylimidazolium hexafluorophosphate	U	3.24	-6.75	-0.21		3.74		3.2	-	4,25	0,83
107	IM12 SCN	1-Ethyl-3-methylimidazolium thiocyanate	U	3.24	-6.75	-3.10		4.44		4.2	-	4,68	0,01
108	IM12 Br	1-Ethyl-3-methylimidazolium bromide	U	3.24	-6.75	-2.16		4.21		3.9	-	4,52	0,26
109	IM12 NO3	1-Ethyl-3-methylimidazolium nitrate	U	3.24	-6.75	-2.37		4.26		4	-	4,55	0,20
110	IM12 FeCl4	1-ethyl-3-methylimidazolium tetrachloroferrate	U	3.24	-6.75	-0.46		3.80		3.3	-	4,28	0,75
111	IM11CN Cl	1-(Cyanomethyl)-3-methylimidazolium chloride	U	5.65	-3.19	-2.31		4.56		4.4	-	4,76	0,47
112	IM11CN (CF3SO2)2N	1-(Cyanomethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	5.65	-3.19	2.86	3.81	3.31	0.50				1,06
113	IM11CONMeBu Br	1-[2-(Butylmethylamino)-2-oxoethyl]-3-methylimidazolium bromide	U	2.43	1.73	-2.16		3.22		2.1	-	4,3	2,11
114	IM11CONEt2 Br	1-[2-(Diethylamino)-2-oxoethyl]-3-methylimidazolium bromide	U	3.60	1.16	-2.16		3.58		2.7	-	4,5	1,83
115	IM11CONHBu Br	1-[2-(Butylamino)-2-oxoethyl]-3-methylimidazolium bromide	U	2.91	2.71	-2.16		3.26		2.1	-	4,46	2,32

116	IM11COO1 Br	1-(2-Methoxy-2-oxoethyl)-3-methylimidazolium bromide	U	7.61	2.40	-2.16		4.53		3.7	-	5,38	1,71
117	IM11COO1(COO4)(Ph-(3,4-OCH2O-)) Br	1-[2-[1-(1,3-Benzodioxol-5-yl)-2-butoxy-2-oxoethoxy]-2-oxoethyl]-3-methylimidazolium bromide	U	-1.26	12.75	-2.16		1.24		-1.8	-	4,27	5,47*
118	IM11COO2 BF4	1-(2-Ethoxy-2-oxoethyl)-3-methylimidazolium tetrafluoroborate	U	6.71	2.81	-0.33		3.81		3.1	-	4,57	1,39
119	IM11COO2 Br	1-(2-Ethoxy-2-oxoethyl)-3-methylimidazolium bromide	U	6.71	2.81	-2.16		4.25		3.3	-	5,22	1,92
120	IM11COO3 (CF3SO2)2N	1-Methyl-3-(2-oxo-2-propoxyethyl)imidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	4.93	1.96	2.86		2.65		2.3	-	3,06	0,44
121	IM11COO3 8OSO3	1-Methyl-3-(2-oxo-2-propoxyethyl)imidazolium octylsulfate	U	4.93	1.96	3.86		2.41		2.1	-	2,73	0,15
122	IM11COO3 BF4	1-Methyl-3-(2-oxo-2-propoxyethyl)imidazolium tetrafluoroborate	U	4.93	1.96	-0.33		3.42		2.7	-	4,16	1,36
123	IM11COO3 Br	1-Methyl-3-(2-oxo-2-propoxyethyl)imidazolium bromide	U	4.93	1.96	-2.16		3.86		2.9	-	4,82	1,89
124	IM11COO3 N(CN)2	1-Methyl-3-(2-oxo-2-propoxyethyl)imidazolium N-cyanocyanamide	U	4.93	1.96	0.00		3.34		2.6	-	4,05	1,26
125	IM11COO3 PF6	1-Methyl-3-(2-oxo-2-propoxyethyl)imidazolium hexafluorophosphate	U	4.93	1.96	-0.21		3.39		2.7	-	4,12	1,33
126	IM11COO4 (CF3SO2)2N	3-(2-Butoxy-2-oxoethyl)-1-methylimidazolium N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	4.15	3.03	2.86		2.35		1.7	-	2,97	0,81
127	IM11COO4 8OSO3	1-(2-Butoxy-2-oxoethyl)-3-methylimidazolium octylsulfate	U	4.15	3.03	3.86		2.11		1.6	-	2,63	0,52
128	IM11COO4 BF4	1-(2-Butoxy-2-oxoethyl)-3-methylimidazolium tetrafluoroborate	U	4.15	3.03	-0.33		3.12		2.2	-	4,08	1,73
129	IM11COO4 Br	1-(2-Butoxy-2-oxoethyl)-3-methylimidazolium bromide	U	4.15	3.03	-2.16		3.56		2.4	-	4,73	2,27
130	IM11COO4 N(CN)2	1-(2-Butoxy-2-oxoethyl)-3-methylimidazolium N-cyanocyanamide	U	4.15	3.03	0.00		3.04		2.1	-	3,96	1,64
131	IM11COO4 PF6	1-(2-Butoxy-2-oxoethyl)-3-methylimidazolium hexafluorophosphate	U	4.15	3.03	-0.21		3.09		2.1	-	4,04	1,70
132	IM11COO5 8OSO3	1-Methyl-3-[2-oxo-2-(pentyloxy)ethyl]imidazolium octylsulfate	U	2.15	2.70	3.86		1.61		1	-	2,21	0,65
133	IM11COO5 Br	1-Methyl-3-[2-oxo-2-(pentyloxy)ethyl]imidazolium bromide	U	2.15	2.70	-2.16		3.06		1.8	-	4,31	2,40*
134	IM11COO6 Br	1-[2-(Hexyloxy)-2-oxoethyl]-3-methylimidazolium bromide	U	1.62	2.95	-2.16		2.90		1.6	-	4,22	2,52*
135	IM11COO8 Br	1-Methyl-3-[2-(octyloxy)-2-oxoethyl]imidazolium bromide	U	-1.30	2.89	-2.16		2.13		0.6	-	3,64	2,83*
136	IM1i4 (CF3SO2)2N	1-Methyl-3-(2-methylpropyl)imidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	1.42	-5.98	2.86		2.45		1.8	-	3,07	1,31
137	IM1gly Cl	1-methyl-3-glycerylrylimidazolium chloride	U	12.59	9.92	-2.31		5.20		3.5	-	6,89	3,23*
138	IM1gly N(CN)2	1-methyl-3-glycerylimidazolium dicyanamide	U	12.59	9.92	0.00		4.64		3.2	-	6,08	2,56*
139	IM1gly (CF3SO2)2N	1-methyl-3-glycerylimidazolium bis(trifluoromethylsulphonyl)imide	U	12.59	9.92	2.86		3.95		2.8	-	5,07	1,73
140	IM1-2=1 Cl	1-Methyl-3-(2-propenyl)imidazolium chloride	U	1.49	-6.89	-2.31		3.80		3.6	-	4	0,06
141	IM1-(1Ph-4Me) BF4	1-Methyl-3-(phenylmethyl)imidazolium tetrafluoroborate	U	-1.72	-6.38	-0.33		2.42		2.3	-	2,54	0,15
142	IM1-(1Ph-4Me) Cl	1-Methyl-3-[(4-methylphenyl)methyl]imidazolium chloride	U	-1.72	-6.38	-2.31		2.90		2.7	-	3,06	0,43
143	IM1-(1Ph-4Me) PF6	1-Methyl-3-[(4-methylphenyl)methyl]imidazolium hexafluorophosphate	U	-1.72	-6.38	-0.21		2.40		2.3	-	2,53	0,18
144	IM1-1Ph BF4	1-Methyl-3-(phenylmethyl)imidazolium tetrafluoroborate	U	-0.98	-6.53	-0.33		2.63		2.5	-	2,81	0,27
145	IM1-1Ph Cl	1-Methyl-3-(phenylmethyl)imidazolium chloride	U	-0.98	-6.53	-2.31		3.11		3	-	3,22	0,31
146	IM1-1Ph PF6	1-Methyl-3-(phenylmethyl)imidazolium hexafluorophosphate	U	-0.98	-6.53	-0.21		2.61		2.4	-	2,8	0,30
147	IM13 BF4	1-Methyl-3-propylimidazolium tetrafluoroborate	L	1.85	-6.45	-0.33	3.94	3.37	0.57				0,58

148	IM13 (CF3SO2)2N	1-Methyl-3-propylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	1.85	-6.45	2.86		2.61		1.9	-	3,32	1,48
149	IM13 PF6	1-Methyl-3-propylimidazolium hexafluorophosphate	U	1.85	-6.45	-0.21		3.35		3	-	3,71	0,59
150	IM13 Br	1-Methyl-3-propylimidazolium bromide	U	1.85	-6.45	-2.16		3.82		3.6	-	4	0,03
151	IM13 Cl	1-Methyl-3-propylimidazolium chloride	U	1.85	-6.45	-2.31		3.85		3.7	-	4,03	0,02
152	IM13 I	1-Methyl-3-propylimidazolium iodide	U	1.85	-6.45	-1.63		3.69		3.5	-	3,91	0,18
153	IM1-2CO-1 Br	1-Methyl-3-(3-oxobutyl)imidazolium bromide	U	5.91	1.45	-2.16		4.17		3.4	-	4,98	1,65
154	IM1-2C6F13 PF6	1-Methyl-3-(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)imidazolium hexafluorophosphate	U	1.89	7.73	-0.21		2.07		0.2	-	3,89	3,21*
155	IM12(2Pin_1R) Cl	1-[2-[(1R,5S)-6,6-Dimethylbicyclo[3.1.1]hept-2-en-2-yl]ethyl]-3-methylimidazolium chloride	U	-3.71	-4.44	-2.31		2.20		1.6	-	2,76	1,17
156	IM12(2Pin_1R) NO3	1-[2-[(1R,5S)-6,6-Dimethylbicyclo[3.1.1]hept-2-en-2-yl]ethyl]-3-methylimidazolium nitrate	U	-3.71	-4.44	-2.37		2.21		1.6	-	2,78	1,19
157	IM1-2Ph BF4	1-Methyl-3-(2-phenylethyl)imidazolium tetrafluoroborate	U	-3.43	-6.10	-0.33		1.95		1.8	-	2,05	0,12
158	IM1-2Ph Cl	1-Methyl-3-(2-phenylethyl)imidazolium chloride	U	-3.43	-6.10	-2.31		2.43		2.1	-	2,72	0,69
159	IM1-2Ph PF6	1-Methyl-3-(2-phenylethyl)imidazolium hexafluorophosphate	U	-3.43	-6.10	-0.21		1.92		1.8	-	2,02	0,08
160	IM14 8OSO3	1-Butyl-3-methylimidazolium octylsulfate	L	0.58	-5.91	3.86	1.83	1.98	-0.15				1,53
161	IM14 CF3SO3	1-Butyl-3-methylimidazolium trifluoromethanesulfonate	L	0.58	-5.91	0.07	3.60	2.89	0.70				0,40
162	IM14 (CF3)2N	1-Butyl-3-methylimidazolium 1,1,1-trifluoro-N-(trifluoromethyl)methanaminate	L	0.58	-5.91	-0.04	3.46	2.92	0.54				0,36
163	IM14 BF4	1-Butyl-3-methylimidazolium tetrafluoroborate	L	0.58	-5.91	-0.33	3.55	2.99	0.56				0,28
164	IM14 (CF3SO2)2N	1-Butyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	0.58	-5.91	2.86	2.47	2.22	0.25				1,23
165	IM14 PF6	1-Butyl-3-methylimidazolium hexafluorophosphate	T	0.58	-5.91	-0.21	3.51	2.96	0.55	2.8		3,16	0,30
166	IM14 Cl	1-Butyl-3-methylimidazolium chloride	L	0.58	-5.91	-2.31	3.47	3.47	0.01				0,31
167	IM14 I	1-Butyl-3-methylimidazolium iodide	L	0.58	-5.91	-1.63	3.59	3.30	0.29				0,11
168	IM14 Br	1-Butyl-3-methylimidazolium bromide	L	0.58	-5.91	-2.16	3.07	3.43	-0.36				0,27
169	IM14 N(CN)2	1-Butyl-3-methylimidazolium N-cyanocyanamide	U	0.58	-5.91	0.00		2.91		2.7	-	3,13	0,37
170	IM14 4MePhSO3	1-Butyl-3-methylimidazolium 4-methylbenzenesulfonate	L	0.58	-5.91	2.48	3.53	2.31	1.21				1,12
171	IM14 1SO3	1-Butyl-3-methylimidazolium methanesulfonate	U	0.58	-5.91	-0.86		3.12		3	-	3,25	0,12
172	IM14 (2-SO2PhCO)N	1-Butyl-3-methylimidazolium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide	U	0.58	-5.91	1.38		2.58		2.2	-	2,96	0,77
173	IM14 (C2F5)3PF3	1-Butyl-3-methylimidazolium trifluorotris(pentafluoroethyl)phosphate	U	0.58	-5.91	4.77		1.76		1	-	2,54	1,75
174	IM14 1O2O2OSO3	1-Butyl-3-methylimidazolium 2-(2-methoxyethoxy)ethyl sulfate	U	0.58	-5.91	3.67		2.03		1.4	-	2,67	1,43
175	IM14 1OSO3	1-Butyl-3-methylimidazolium methyl sulfate	U	0.58	-5.91	-0.44		3.02		2.8	-	3,19	0,24
176	IM14 AC	3-Butyl-1-methylimidazolium 6-methyl-2,2-dioxo-1,2,3-oxathiazin-4(3H)-onate	U	0.58	-5.91	0.92		2.69		2.4	-	3,01	0,63
177	IM14 Co(CO)4	1-Butyl-3-methylimidazolium (T-4)-tetracarbonylcobaltate	U	0.58	-5.91	-1.00		3.15		3	-	3,27	0,08
178	IM14 FeCl4	1-Butyl-3-methylimidazolium tetrachloroferrate	U	0.58	-5.91	-0.46		3.02		2.9	-	3,19	0,23
179	IM14 HSO4	1-Butyl-3-methylimidazolium hydrogen sulfate	U	0.58	-5.91	-1.42		3.25		3.2	-	3,34	0,04
180	IM14 NO3	1-Butyl-3-methylimidazolium nitrate	U	0.58	-5.91	-2.37		3.48		3.4	-	3,59	0,32

181	IM14 SbF6	1-Butyl-3-methylimidazolium (OC-6-11)-hexafluoroantimonate	U	0.58	-5.91	-0.12		2.94		2.7	-	3,15	0,33
182	IM14 SCN	1-Butyl-3-methylimidazolium thiocyanate	U	0.58	-5.91	-3.10		3.66		3.5	-	3,84	0,53
183	IM14 (CH3O)2PO2	1-butyl-3-methylimidazolium dimethyl phosphate	U	0.58	-5.91	0.20		2.86		2.6	-	3,1	0,43
184	IM14 C(CN)3	1-butyl-3-methylimidazolium tricyanomethanide	U	0.58	-5.91	-1.96		3.38		3.3	-	3,47	0,20
185	IM14 CF3COO	1-Butyl-3-Methylimidazolium trifluoroacetate	U	0.58	-5.91	-2.30		3.46		3.4	-	3,57	0,30
186	IM13COOH Cl	3-(3-Carboxypropyl)-1-methylimidazolium chloride	U	10.77	5.41	-2.31		5.13		4	-	6,26	2,22
187	IM15 (CF3SO2)2N	1-Methyl-3-pentylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	-0.64	-5.56	2.86		1.87		1.4	-	2,29	0,97
188	IM15 BF4	1-Methyl-3-pentylimidazolium tetrafluoroborate	L	-0.64	-5.56	-0.33	3.14	2.63	0.51				0,05
189	IM15 Cl	1-Methyl-3-pentylimidazolium chloride	U	-0.64	-5.56	-2.31		3.11		2.9	-	3,31	0,53
190	IM15 PF6	1-Methyl-3-pentylimidazolium hexafluorophosphate	U	-0.64	-5.56	-0.21		2.61		2.5	-	2,68	0,08
191	IM16 (CF3SO2)2N	1-Hexyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	-1.54	-5.78	2.86	2.05	1.65	0.40				0,96
192	IM16 Br	1-Hexyl-3-methylimidazolium bromide	U	-1.54	-5.78	-2.16		2.86		2.7	-	3,06	0,53
193	IM16 Cl	1-Hexyl-3-methylimidazolium chloride	L	-1.54	-5.78	-2.31	2.93	2.89	0.04				0,59
194	IM16 PF6	1-Hexyl-3-methylimidazolium hexafluorophosphate	U	-1.54	-5.78	-0.21		2.39		2.3	-	2,46	0,04
195	IM16 (2-SO2PhCO)N	1-Hexyl-3-methylimidazolium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide	L	-1.54	-5.78	1.38	2.67	2.01	0.66				0,51
196	IM16 BF4	1-Hexyl-3-methylimidazolium tetrafluoroborate	L	-1.54	-5.78	-0.33	3.18	2.42	0.76				0,00
197	IM16 (C2F5)3PF3	1-Hexyl-3-methylimidazolium trifluorotris(pentafluoroethyl)phosphate	U	-1.54	-5.78	4.77		1.19		0.6	-	1,82	1,48
198	IM16 (C3F7)3PF3	1-Hexyl-3-methylimidazolium trifluorotris(heptafluoropropyl)phosphate	U	-1.54	-5.78	6.72		0.72		-0.1	-	1,58	2,05
199	IM16 (CF3SO2)3C	1-Hexyl-3-methylimidazolium tris[(trifluoromethyl)sulfonyl]methide	U	-1.54	-5.78	3.93		1.39		0.9	-	1,92	1,24
200	IM16 N(CN)2	1-hexyl-3-methylimidazolium dicyanamide	U	-1.54	-5.78	0.00		2.34		2.3	-	2,42	0,10
201	IM16 NO3	1-hexyl-3-methylimidazolium nitrate	U	-1.54	-5.78	-2.37		2.91		2.7	-	3,14	0,59
202	IM16 SbF6	1-hexyl-3-methylimidazolium hexafluoridoantimonate	U	-1.54	-5.78	-0.12		2.37		2.3	-	2,44	0,06
203	IM17 (CF3SO2)2N	1-Heptyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	-2.66	-4.82	2.86		1.27		1	-	1,49	0,55
204	IM17 BF4	1-Heptyl-3-methylimidazolium tetrafluoroborate	L	-2.66	-4.82	-0.33	2.44	2.03	0.41				0,39
205	IM17 Cl	1-Heptyl-3-methylimidazolium chloride	U	-2.66	-4.82	-2.31		2.51		2.1	-	2,95	0,95
206	IM17 PF6	1-Heptyl-3-methylimidazolium hexafluorophosphate	U	-2.66	-4.82	-0.21		2.01		1.8	-	2,21	0,35
207	IM18 BF4	1-Methyl-3-octylimidazolium tetrafluoroborate	T	-3.07	-4.67	-0.33	1.40	1.91	-0.51	1.6		2,18	0,46
208	IM18 Br	1-Methyl-3-octylimidazolium bromide	U	-3.07	-4.67	-2.16		2.35		1.9	-	2,82	0,99
209	IM18 (CF3SO2)2N	1-Methyl-3-octylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	-3.07	-4.67	2.86	0.83	1.15	-0.32				0,48
210	IM18 8OSO3	3-Methyl-1-octylimidazolium octylsulfate	U	-3.07	-4.67	3.86		0.91		0.6	-	1,21	0,75
211	IM18 CF3SO3	1-Methyl-3-octylimidazolium trifluormethanesulfonate	U	-3.07	-4.67	0.07		1.82		1.6	-	2,04	0,35
212	IM18 Cl	1-Methyl-3-octylimidazolium chloride	L	-3.07	-4.67	-2.31	1.05	2.39	-1.34				1,07

213	IM18 PF6	1-Methyl-3-octylimidazolium hexafluorophosphate	U	-3.07	-4.67	-0.21		1.88		1.6	-	2,14	0,43
214	IM17COOH Br	1-(7-Carboxyheptyl)-3-methylimidazolium bromide	U	6.03	5.48	-2.16		3.83		2.4	-	5,25	2,72*
215	IM19 BF4	1-Methyl-3-nonylimidazolium tetrafluoroborate	T	-4.95	-4.26	-0.33	0.72	1.38	-0.66	0.9		1,84	0,78
216	IM19 Cl	1-Methyl-3-nonylimidazolium chloride	U	-4.95	-4.26	-2.31		1.86		1.2	-	2,53	1,35
217	IM19 PF6	1-Methyl-3-nonylimidazolium hexafluorophosphate	U	-4.95	-4.26	-0.21		1.35		0.9	-	1,8	0,75
218	IM1-10 BF4	1-Decyl-3-methylimidazolium tetrafluoroborate	L	-5.83	-4.13	-0.33	-0.18	1.14	-1.31				0,94
219	IM1-10 Br	1-Decyl-3-methylimidazolium bromide	U	-5.83	-4.13	-2.16		1.58		0.8	-	2,31	1,44
220	IM1-10 Cl	1-Decyl-3-methylimidazolium chloride	L	-5.83	-4.13	-2.31	0.50	1.61	-1.11				1,53
221	IM1-10 PF6	1-Decyl-3-methylimidazolium hexafluorophosphate	U	-5.83	-4.13	-0.21		1.11		0.6	-	1,64	0,88
222	IM1-10 (CF3SO2)2N	1-decyl-3-methylimidazolium bis(trifluoromethylsulphonyl)imide	U	-5.83	-4.13	2.86		0.37		0.1	-	0,65	0,01
223	IM1-10 FeCl4	1-decyl-3-methylimidazolium tetrachloroferrate	U	-5.83	-4.13	-0.46		1.17		0.6	-	1,72	0,95
224	IM1-10COO2 Br	1-(11-Ethoxy-11-oxoundecyl)-3-methylimidazolium bromide	U	-4.00	4.03	-2.16		1.31		-0.6	-	3,18	3,43*
225	IM1-12 Br	1-Dodecyl-3-methylimidazolium bromide	U	-7.55	-3.29	-2.16		1.04		0.1	-	2,03	1,86
226	IM1-12 Cl	1-dodecyl-3-methylimidazolium chloride	U	-7.55	-3.29	-2.31		1.08		0.1	-	2,08	1,90
227	IM1-14 Cl	1-Methyl-3-tetradecylimidazolium chloride	L	-9.86	-2.51	-2.31	-0.14	0.40	-0.54				2,43*
228	IM1-14 Br	1-Methyl-3-tetradecylimidazolium bromide	U	-9.86	-2.51	-2.16		0.36		-0.9	-	1,62	2,32
229	IM1-16 Cl	1-Hexadecyl-3-methylimidazolium chloride	L	-11.34	-2.14	-2.31	0.23	-0.03	0.26				2,71*
230	IM1-16 Br	1-Hexadecyl-3-methylimidazolium bromide	U	-11.34	-2.14	-2.16		-0.06		-1.5	-	1,36	2,59*
231	IM1-18 Cl	1-Methyl-3-octadecylimidazolium chloride	T	-13.76	-1.31	-2.31	1.26	-0.74	1.99	-2.5		0,99	3,12*
232	IM18OH Br	1-(8-Hydroxyoctyl)-3-methylimidazolium bromide	U	2.36	3.73	-2.16		3.02		1.6	-	4,42	2,65*
233	IM14OH Cl	1-(4-Hydroxybutyl)-3-methylimidazolium chloride	U	6.92	2.34	-2.31		4.39		3.5	-	5,29	1,82
234	IM13OH Cl	1-(3-Hydroxypropyl)-3-methylimidazolium chloride	L	8.05	2.08	-2.31	4.30	4.71	-0.41				1,67
235	IM13OH (CF3SO2)2N	1-(3-Hydroxypropyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	T	8.05	2.08	2.86	3.89	3.47	0.42	3.2		3,7	0,12
236	IM13O1 (CF3SO2)2N	1-(3-Methoxypropyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	4.71	-1.38	2.86	3.24	2.90	0.34				0,45
237	IM13O1 Cl	1-(3-Methoxypropyl)-3-methylimidazolium chloride	L	4.71	-1.38	-2.31	4.30	4.15	0.16				1,09
238	IM12OH I	1-(2-Hydroxyethyl)-3-methylimidazolium iodide	L	9.73	2.71	-1.63	3.89	4.93	-1.05				1,45
239	IM12OH (2-SO2PhCO)N	1-(2-Hydroxyethyl)-3-methylimidazolium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide	U	9.73	2.71	1.38		4.21		3.8	-	4,58	0,54
240	IM12OH (CF3SO2)2N	1-(2-Hydroxyethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	9.73	2.71	2.86		3.85		3.6	-	4,09	0,11
241	IM12OH AC	1-(2-Hydroxyethyl)-3-methylimidazolium 6-methyl-2,2-dioxo-1,2,3-oxathiazin-4(3H)-onate	U	9.73	2.71	0.92		4.32		3.9	-	4,75	0,67
242	IM12OH BF4	1-(2-Hydroxyethyl)-3-methylimidazolium tetrafluoroborate	U	9.73	2.71	-0.33		4.62		4.1	-	5,18	1,03
243	IM12OH PF6	1-(2-Hydroxyethyl)-3-methylimidazolium hexafluorophosphate	U	9.73	2.71	-0.21		4.59		4	-	5,14	1,00
244	IM12OH Cl	1-(2-hydroxyethyl)-3-methylimidazolium chloride	U	9.73	2.71	-2.31		5.10		4.3	-	5,88	1,61

245	IM12O1 (CF3SO2)2N	1-(2-Methoxyethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	6.12	-1.79	2.86	2.84	3.31	-0.47				0,72
246	IM12O1 Cl	1-(2-Methoxyethyl)-3-methylimidazolium chloride	L	6.12	-1.79	-2.31	4.18	4.55	-0.37				0,82
247	IM12O1 BF4	1-(2-Methoxyethyl)-3-methylimidazolium tetrafluoroborate	U	6.12	-1.79	-0.33		4.08		3.9	-	4,21	0,22
248	IM12O1 N(CN)2	1-(2-Methoxyethyl)-3-methylimidazolium dicyanamide	U	6.12	-1.79	0.00		4.00		3.9	-	4,1	0,13
249	IM12O2 (CF3SO2)2N	1-(2-Ethoxyethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	4.04	-2.03	2.86	2.96	2.78	0.18				0,55
250	IM12O2 Br	1-(2-Ethoxyethyl)-3-methylimidazolium bromide	L	4.04	-2.03	-2.16	4.30	3.99	0.31				0,95
251	IM12O2 Cl	1-(2-Ethoxyethyl)-3-methylimidazolium chloride	U	4.04	-2.03	-2.31		4.03		3.6	-	4,45	0,96
252	IM12O2O1 Cl	1-[2-(2-Methoxyethoxy)ethyl]-3-methylimidazolium chloride	U	5.30	1.60	-2.31		4.03		3.1	-	4,92	1,80
253	IM11O2 (CF3SO2)2N	1-(Ethoxymethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	5.01	-1.83	2.86	3.00	3.02	-0.02				0,61
254	IM11O2 Cl	1-(Ethoxymethyl)-3-methylimidazolium chloride	L	5.01	-1.83	-2.31	4.33	4.26	0.06				0,93
255	Py1O(Cdd)-3CONH2 Cl	3-(Aminocarbonyl)-1-[(cyclododecyloxy)methyl]pyridinium chloride	U	-1.11	8.51	-2.31		1.71		-0.7	-	4,08	4,36*
256	Py1O-10-3CONH2 Cl	3-(Aminocarbonyl)-1-[(decyloxy)methyl]pyridinium chloride	U	-1.45	8.05	-2.31		1.66		-0.7	-	3,99	4,27*
257	Py1O-10-3CONH2 FeCl4	3-(Aminocarbonyl)-1-[(decyloxy)methyl]pyridinium (T-4)-tetrachloroferrate	U	-1.45	8.05	-0.46		1.21		-0.9	-	3,34	3,74*
258	Py1O-11-3CONH2 Cl	3-(Aminocarbonyl)-1-[(undecyloxy)methyl]pyridinium chloride	U	-3.36	8.53	-2.31		1.11		-1.4	-	3,64	4,61*
259	Py1O-12-3CONH2 1COO	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium acetate	U	-3.72	9.72	-5.87		1.76		-1.4	-	4,9	6,00*
260	Py1O-12-3CONH2 BF4	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium tetrafluoroborate	U	-3.72	9.72	-0.33		0.43		-2.1	-	2,95	4,40*
261	Py1O-12-3CONH2 Br	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium bromide	U	-3.72	9.72	-2.16		0.87		-1.9	-	3,59	4,93*
262	Py1O-12-3CONH2 Cl	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium chloride	U	-3.72	9.72	-2.31		0.91		-1.8	-	3,65	4,97*
263	Py1O-12-3CONH2 ClO4	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium perchlorate	U	-3.72	9.72	-0.12		0.38		-2.1	-	2,88	4,34*
264	Py1O-12-3CONH2 I	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium iodide	U	-3.72	9.72	-1.63		0.74		-1.9	-	3,41	4,77*
265	Py1O-12-3CONH2 NO3	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium nitrate	U	-3.72	9.72	-2.37		0.92		-1.8	-	3,67	4,99*
266	Py4-3CONHBu 8OSO3	1-Butyl-3-[(butylamino)carbonyl]pyridinium octyl sulfate	U	-0.50	1.56	3.86		1.02		0.4	-	1,62	0,64
267	Py4-3CONHBu I	1-Butyl-3-[(butylamino)carbonyl]pyridinium iodide	U	-0.50	1.56	-1.63		2.34		1.1	-	3,53	2,23
268	Py1O7-3CONH(MeO-MeO-Hp) Cl	3-[[[[(Heptyloxy)methoxy]methyl]amino]carbonyl]-1-[(heptyloxy)methyl]pyridinium chloride	U	-8.10	11.70	-2.31		-0.43		-3.8	-	2,91	5,99*
269	Py1O8-3CONH(MeO-MeO-Oc) Cl	3-[[[[(Octyloxy)methoxy]methyl]amino]carbonyl]-1-[(octyloxy)methyl]pyridinium chloride	U	-9.18	13.37	-2.31		-0.87		-4.5	-	2,81	6,56*
270	Py1O9-3CONH(MeO-MeO-No) Cl	3-[[[[(Nonyloxy)methoxy]methyl]amino]carbonyl]-1-[(nonyloxy)methyl]pyridinium chloride	U	-11.41	14.87	-2.31		-1.59		-5.7	-	2,46	7,20*
271	Py1O-10-3CONH(MeO-MeO-De) Cl	3-[[[[(Decyloxy)methoxy]methyl]amino]carbonyl]-1-[(decyloxy)methyl]pyridinium chloride	U	-14.01	15.45	-2.31		-2.33		-6.7	-	1,99	7,65*
272	Py1-3COOBu (CF3SO2)2N	3-(Butoxycarbonyl)-1-methylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	2.74	1.39	2.86		2.13		1.7	-	2,59	0,52
273	Py1-3COOBu 8OSO3	3-(Butoxycarbonyl)-1-methylpyridinium octyl sulfate	U	2.74	1.39	3.86		1.89		1.5	-	2,26	0,24
274	Py1-3COOBu I	3-(Butoxycarbonyl)-1-methylpyridinium iodide	U	2.74	1.39	-1.63		3.21		2.3	-	4,15	1,83

275	Py1-3COOBu PF6	3-(Butoxycarbonyl)-1-methylpyridinium hexafluorophosphate	U	2.74	1.39	-0.21	2.87	2.1 -	3,65	1,42
276	Py4-3COOBu 8OSO3	3-(Butoxycarbonyl)-1-butylpyridinium octyl sulfate	U	-0.63	1.72	3.86	0.97	0.3 -	1,61	0,69
277	Py4-3COOBu I	3-(Butoxycarbonyl)-1-butylpyridinium iodide	U	-0.63	1.72	-1.63	2.29	1.1 -	3,51	2,28
278	Py4-3Me-4Me BF4	1-Butyl-3,4-dimethylpyridinium tetrafluoroborate	U	-1.83	-6.48	-0.33	2.40	2.3 -	2,53	0,16
279	Py4-3Me-4Me Cl	1-Butyl-3,4-dimethylpyridinium chloride	U	-1.83	-6.48	-2.31	2.88	2.7 -	3,03	0,42
280	Py4-3Me-5Me N(CN)2	1-Butyl-3,5-dimethylpyridinium N-cyanocyanamide	U	-3.35	-6.65	0.00	1.94	1.8 -	2,06	0,13
281	Py4-3Me-5Me Br	1-Butyl-3,5-dimethylpyridinium bromide	U	-3.35	-6.65	-2.16	2.46	2.3 -	2,66	0,49
282	Py4-3Me-5Me BF4	1-Butyl-3,5-dimethylpyridinium tetrafluoroborate	U	-3.35	-6.65	-0.33	2.02	1.9 -	2,12	0,04
283	Py4-3Me-5Me Cl	1-Butyl-3,5-dimethylpyridinium chloride	U	-3.35	-6.65	-2.31	2.50	2.3 -	2,71	0,54
284	Py4-3Me-5Me (CF3SO2)2N	1-butyl-3,5-dimethil pyridinium bistrifluoromethanesulfonamide	U	-3.35	-6.65	2.86	1.25	0.8 -	1,68	0,96
285	Py8-3Me-5Me Br	1-octyl-3,5-dimethylpyridinium bromide	U	-7.40	-4.91	-2.16	1.23	0.5 -	1,96	1,41
286	Py8-3Me-5Me (CF3SO2)2N	1-octyl-3,5-dimethylpyridinium bromide 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	-7.40	-4.91	2.86	0.02	-0.3 -	0,32	0,05
287	Py3-3Me Br	3-Methyl-1-propylpyridinium bromide	U	0.18	-7.09	-2.16	3.43	3.3 -	3,6	0,01
288	Py3-3Me PF6	3-Methyl-1-propylpyridinium hexafluorophosphate	U	0.18	-7.09	-0.21	2.96	2.6 -	3,31	0,58
289	Py4-3Me N(CN)2	1-Butyl-3-methylpyridinium N-cyanocyanamide	U	-1.02	-6.72	0.00	2.56	2.3 -	2,8	0,41
290	Py4-3Me Br	1-Butyl-3-methylpyridinium bromide	U	-1.02	-6.72	-2.16	3.08	3 -	3,18	0,22
291	Py4-3Me 8OSO3	1-Butyl-3-methylpyridinium octyl sulfate	U	-1.02	-6.72	3.86	1.63	0.9 -	2,32	1,53
292	Py4-3Me BF4	1-Butyl-3-methylpyridinium tetrafluoroborate	U	-1.02	-6.72	-0.33	2.64	2.4 -	2,85	0,31
293	Py4-3Me Cl	1-Butyl-3-methylpyridinium chloride	U	-1.02	-6.72	-2.31	3.12	3 -	3,22	0,26
294	Py4-3Me PF6	1-Butyl-3-methylpyridinium hexafluorophosphate	U	-1.02	-6.72	-0.21	2.61	2.4 -	2,83	0,35
295	Py6-3Me Br	1-Hexyl-3-methylpyridinium bromide	U	-3.03	-5.66	-2.16	2.45	2.1 -	2,77	0,73
296	Py6-3Me Cl	1-Hexyl-3-methylpyridinium chloride	U	-3.03	-5.66	-2.31	2.49	2.2 -	2,82	0,77
297	Py8-3Me Br	3-Methyl-1-octylpyridinium bromide	U	-5.44	-5.13	-2.16	1.77	1.2 -	2,33	1,13
298	Py8-3Me Cl	3-Methyl-1-octylpyridinium chloride	U	-5.44	-5.13	-2.31	1.81	1.2 -	2,38	1,18
299	Py1O3-3OH (2-SO2PhCO)N	3-Hydroxy-1-(propoxymethyl)pyridinium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide	U	9.04	2.53	1.38	4.04	3.7 -	4,43	0,56
300	Py1O3-3OH AC	3-Hydroxy-1-(propoxymethyl)pyridinium 6-methyl-2,2-dioxo-1,2,3-oxathiazin-4(3H)-onate	U	9.04	2.53	0.92	4.16	3.7 -	4,59	0,70
301	Py1O3-3OH Cl	3-Hydroxy-1-(propoxymethyl)pyridinium chloride	U	9.04	2.53	-2.31	4.93	4.1 -	5,73	1,63
302	Py1O4-3OH (2-SO2PhCO)N	1-(Butoxymethyl)-3-hydroxypyridinium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide	U	7.76	2.79	1.38	3.68	3.2 -	4,19	0,78
303	Py1O4-3OH AC	1-(Butoxymethyl)-3-hydroxypyridinium 6-methyl-2,2-dioxo-1,2,3-oxathiazin-4(3H)-onate	U	7.76	2.79	0.92	3.79	3.2 -	4,35	0,91
304	Py1O6-3OH (2-SO2PhCO)N	1-[(Hexyloxy)methyl]-3-hydroxypyridinium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide	U	5.49	3.42	1.38	3.02	2.3 -	3,77	1,19
305	Py1O6-3OH AC	1-[(Hexyloxy)methyl]-3-hydroxypyridinium 6-methyl-2,2-dioxo-1,2,3-oxathiazin-4(3H)-onate	U	5.49	3.42	0.92	3.14	2.3 -	3,93	1,33

306	Py1O7-3OH (2-SO2PhCO)N	1-[(Heptyloxy)methyl]-3-hydroxypyridinium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide	U	4.71	3.35	1.38		2.82		2 -	3,61	1,26
307	Py1O7-3OH AC	1-[(Heptyloxy)methyl]-3-hydroxypyridinium 6-methyl-2,2-dioxo-1,2,3-oxathiazin-4(3H)-onate	U	4.71	3.35	0.92		2.94		2.1 -	3,77	1,40
308	Py1O7-3OH Cl	1-[(Heptyloxy)methyl]-3-hydroxypyridinium chloride	U	4.71	3.35	-2.31		3.71		2.5 -	4,91	2,33
309	Py1O-11-3OH (2-SO2PhCO)N	3-Hydroxy-1-[(undecyloxy)methyl]pyridinium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide	U	-0.18	4.26	1.38		1.45		0.2 -	2,7	2,05
310	Py1O-11-3OH AC	3-Hydroxy-1-[(undecyloxy)methyl]pyridinium 6-methyl-2,2-dioxo-1,2,3-oxathiazin-4(3H)-onate	U	-0.18	4.26	0.92		1.56		0.3 -	2,86	2,18
311	Py1O-11-3OH Cl	3-Hydroxy-1-[(undecyloxy)methyl]pyridinium chloride	U	-0.18	4.26	-2.31		2.34		0.7 -	4	3,12*
312	Py1O-18-3OH (2-SO2PhCO)N	3-Hydroxy-1-[(octadecyloxy)methyl]pyridinium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide	U	-7.03	6.97	1.38		-0.60		-2.7 -	1,53	3,53*
313	Py1O-18-3OH AC	3-Hydroxy-1-[(octadecyloxy)methyl]pyridinium 6-methyl-2,2-dioxo-1,2,3-oxathiazin-4(3H)-onate	U	-7.03	6.97	0.92		-0.49		-2.7 -	1,69	3,66*
314	Pyr24 2OSO3	1-Butyl-1-ethylpyrrolidinium ethyl sulfate	U	1.25	-3.90	-0.18		2.95		2.9 -	3,02	0,15
315	IMi022OH-2-(8=9) 2OSO3	1-ethyl-2-(8-heptadecenyl)-4,5-dihydro-3-(2-hydroxyethyl)imidazolium ethyl sulfate	U	-12.25	6.23	-0.18		-1.54		-4.1 -	1,01	4,36*
316	IM22 (CF3SO2)2N	1,3-Diethylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	2.03	-6.56	2.86		2.66		1.9 -	3,41	1,53
317	IM22 Br	1,3-Diethylimidazolium bromide	U	2.03	-6.56	-2.16		3.87		3.7 -	4,08	0,07
318	IM23 (CF3SO2)2N	1-Ethyl-3-propylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	1.10	-6.31	2.86		2.40		1.8 -	3,04	1,36
319	IM23 Br	1-Ethyl-3-propylimidazolium bromide	U	1.10	-6.31	-2.16		3.60		3.5 -	3,73	0,09
320	IM24 BF4	1-Butyl-3-ethylimidazolium tetrafluoroborate	L	-0.12	-5.99	-0.33	2.80	2.81	-0.01			0,22
321	IM24 CF3COO	1-Butyl-3-ethylimidazolium trifluoroacetate	U	-0.12	-5.99	-2.30		3.28		3.2 -	3,41	0,36
322	IM24 CF3SO3	1-Butyl-3-ethylimidazolium trifluoromethanesulfonate	U	-0.12	-5.99	0.07		2.72		2.5 -	2,91	0,33
323	IM26 BF4	1-Ethyl-3-hexylimidazolium tetrafluoroborate	L	-2.72	-5.19	-0.33	2.15	2.05	0.10			0,29
324	IM26 Br	1-Ethyl-3-hexylimidazolium bromide	U	-2.72	-5.19	-2.16		2.49		2.1 -	2,86	0,82
325	IM2-10 Br	1-Decyl-3-ethylimidazolium bromide	U	-6.83	-4.25	-2.16		1.32		0.5 -	2,11	1,52
326	IM1-(1Ph) (CF3SO2)2N	1-benzyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	-0.83	-6.52	2.86		1.91		1.4 -	2,46	1,21
327	IM4-(1Ph) (CF3SO2)2N	1-benzyl-3-butylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	-4.16	-5.71	2.86		0.95		0.7 -	1,22	0,62
328	Py1O-10-4CONH2 Cl	4-(Aminocarbonyl)-1-[(decyloxy)methyl]pyridinium chloride	U	-0.84	8.71	-2.31		1.76		-0.6 -	4,15	4,38*
329	Py1O-11-4CONH2 Cl	4-(Aminocarbonyl)-1-[(undecyloxy)methyl]pyridinium chloride	U	-1.97	9.29	-2.31		1.41		-1.1 -	3,96	4,66*
330	Py1O-12-4CONH2 Cl	4-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium chloride	U	-3.23	9.40	-2.31		1.07		-1.6 -	3,72	4,83*
331	Py4-4Me BF4	1-Butyl-4-methylpyridinium tetrafluoroborate	L	-0.22	-6.95	-0.33	3.02	2.87	0.15			0,48
332	Py4-4Me (C2F5)3PF3	1-Butyl-4-methylpyridinium trifluorotris(pentafluoroethyl)phosphate	U	-0.22	-6.95	4.77		1.65		0.8 -	2,53	1,94
333	Py4-4Me B(CN)4	1-Butyl-4-methylpyridinium tetracyanoborate	U	-0.22	-6.95	-0.53		2.92		2.6 -	3,19	0,40
334	Py4-4Me Cl	1-Butyl-4-methylpyridinium chloride	U	-0.22	-6.95	-2.31		3.35		3.2 -	3,47	0,11

335	Py4-4Me PF6	1-Butyl-4-methylpyridinium hexafluorophosphate	U	-0.22	-6.95	-0.21		2.84		2.5	-	3,15	0,49
336	Py4-4Me C(CN)3	1-butyl-4-methylpyridinium tricyanomethanide	U	-0.22	-6.95	-1.96		3.26		3.1	-	3,4	0,01
337	Py6-4Me BF4	1-Hexyl-4-methylpyridinium tetrafluoroborate	U	-2.88	-5.97	-0.33		2.08		2	-	2,17	0,09
338	Py6-4Me Cl	1-Hexyl-4-methylpyridinium chloride	U	-2.88	-5.97	-2.31		2.56		2.3	-	2,84	0,67
339	Py8-4Me BF4	4-Methyl-1-octylpyridinium tetrafluoroborate	U	-4.69	-5.10	-0.33		1.52		1.2	-	1,84	0,52
340	Py8-4Me Cl	4-Methyl-1-octylpyridinium chloride	U	-4.69	-5.10	-2.31		2.00		1.5	-	2,53	1,10
341	Py1-4NMe2 I	4-(Dimethylamino)-1-methylpyridinium iodide	U	1.97	-8.24	-1.63		3.88		3.4	-	4,38	0,67
342	Py2-4NMe2 (CF3SO2)2N	4-(Dimethylamino)-1-ethylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	1.55	-7.82	2.86		2.65		1.7	-	3,56	1,82
343	Py2-4NMe2 Br	4-(Dimethylamino)-1-ethylpyridinium bromide	U	1.55	-7.82	-2.16		3.86		3.5	-	4,22	0,36
344	Py4-4NMe2 (CF3SO2)2N	1-Butyl-4-(dimethylamino)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	-0.73	-6.95	2.86		1.97		1.3	-	2,6	1,33
345	Py4-4NMe2 Br	1-Butyl-4-(dimethylamino)pyridinium bromide	U	-0.73	-6.95	-2.16		3.18		3.1	-	3,29	0,12
346	Py4-4NMe2 Cl	1-Butyl-4-(dimethylamino)pyridinium chloride	L	-0.73	-6.95	-2.31	2.55	3.22	-0.67				0,17
347	Py6-4NMe2 (CF3SO2)2N	4-(Dimethylamino)-1-hexylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	-3.42	-6.49	2.86	1.38	1.22	0.16				0,94
348	Py6-4NMe2 Cl	4-(Dimethylamino)-1-hexylpyridinium chloride	U	-3.42	-6.49	-2.31		2.46		2.2	-	2,71	0,59
349	IM33 (CF3SO2)2N	1,3-Dipropylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	-0.15	-5.93	2.86		2.03		1.5	-	2,54	1,12
350	IM44 (CF3SO2)2N	1,3-Dibutylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	-2.22	-5.41	2.86		1.44		1.1	-	1,75	0,75
351	IM42OH Cl	1-butyl-3-(2-hydroxyethyl)imidazolium chloride	U	6.56	2.86	-2.31		4.25		3.2	-	5,25	2,00
352	Quin1O6-6Me Cl	1-[(Hexyloxy)methyl]-6-methylquinolinium chloride	U	-3.71	-1.36	-2.31		1.92		0.9	-	2,95	2,00
353	Quin1O8-6Me Cl	6-Methyl-1-[(octyloxy)methyl]quinolinium chloride	U	-6.17	-0.01	-2.31		1.15		-0.3	-	2,55	2,63*
354	Quin1O-10-6Me Cl	1-[(Decyloxy)methyl]-6-methylquinolinium chloride	U	-8.33	-0.33	-2.31		0.60		-0.9	-	2,11	2,79*
355	Quin1O-12-6Me Cl	1-[(Dodecyloxy)methyl]-6-methylquinolinium chloride	U	-10.30	0.77	-2.31		-0.02		-1.8	-	1,79	3,30*
356	Quin1O6-8OH Cl	1-[(Hexyloxy)methyl]-8-hydroxyquinolinium chloride	U	-0.56	0.61	-2.31		2.57		1.4	-	3,7	2,18
357	Quin1O8-8OH Cl	8-Hydroxy-1-[(octyloxy)methyl]quinolinium chloride	U	-2.66	1.72	-2.31		1.91		0.5	-	3,35	2,71*
358	Quin1O-10-8OH Cl	1-[(Decyloxy)methyl]-8-hydroxyquinolinium chloride	U	-4.64	2.67	-2.31		1.31		-0.4	-	3,02	3,18*
359	Quin1O-12-8OH Cl	1-[(Dodecyloxy)methyl]-8-hydroxyquinolinium chloride	U	-7.05	3.58	-2.31		0.59		-1.4	-	2,61	3,69*
360	Quin4 BF4	1-Butylquinolinium tetrafluoroborate	U	-3.22	-7.41	-0.33		2.12		1.9	-	2,3	0,26
361	Quin4 Br	1-Butylquinolinium bromide	U	-3.22	-7.41	-2.16		2.56		2.4	-	2,68	0,28
362	Quin6 BF4	1-Hexylquinolinium tetrafluoroborate	U	-5.56	-6.58	-0.33		1.43		1.2	-	1,61	0,22
363	Quin8 BF4	1-Octylquinolinium tetrafluoroborate	U	-7.55	-5.95	-0.33		0.84		0.4	-	1,24	0,61
364	Quin8 Br	1-Octylquinolinium bromide	U	-7.55	-5.95	-2.16		1.29		0.7	-	1,87	1,15
365	Quin1O6 Cl	1-[(Hexyloxy)methyl]quinolinium chloride	U	-3.19	-1.99	-2.31		2.11		1.2	-	3,01	1,77
366	Quin1O8 Cl	1-[(Octyloxy)methyl]quinolinium chloride	U	-5.27	-1.84	-2.31		1.55		0.5	-	2,61	2,04
367	Quin1O-10 Cl	1-[(Decyloxy)methyl]quinolinium chloride	U	-7.56	-0.68	-2.31		0.84		-0.6	-	2,24	2,61*

368	Quin1O-12 Cl	1-[(Dodecyloxy)methyl]quinolinium chloride	U	-9.13	0.23	-2.31		0.34		-1.3 -	1,99	3,02*
369	IM55 (CF3SO2)2N	1,3-Dipentylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	-4.42	-4.59	2.86		0.78		0.6 -	0,98	0,29
370	Py1(COO1)(Ph-3-OMe-4-OMe) Cl	1-[1-(3,4-Dimethoxyphenyl)-2-methoxy-2-oxoethyl]pyridinium chloride	U	2.48	4.98	-2.31		2.98		1.4 -	4,57	3,02*
371	Py1(COO1)(Ph-(3,4-OCH2O-)) Br	1-[1-(1,3-Benzodioxol-5-yl)-2-methoxy-2-oxoethyl]pyridinium bromide	U	3.15	5.90	-2.16		3.03		1.4 -	4,71	3,15*
372	Py1(COO4)(Ph-(3,4-OCH2O-)) Br	1-[1-(1,3-Benzodioxol-5-yl)-2-butoxy-2-oxoethyl]pyridinium bromide	U	-0.04	6.08	-2.16		2.17		0.3 -	4,09	3,55*
373	Py2 Cl	1-Ethylpyridinium chloride	U	3.56	-7.36	-2.31		4.38		4 -	4,79	0,41
374	Py1CN (CF3SO2)2N	1-(Cyanomethyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	5.10	-3.86	2.86		3.23		2.7 -	3,76	1,14
375	Py1CN Cl	1-(Cyanomethyl)pyridinium chloride	U	5.10	-3.86	-2.31		4.47		4.3 -	4,63	0,36
376	Py1COO1(COO1)(Ph-(3,4-OCH2O-)) Br	1-[2-[1-(1,3-Benzodioxol-5-yl)-2-methoxy-2-oxoethoxy]-2-oxoethyl]pyridinium bromide	U	-0.87	11.80	-2.16		1.43		-1.4 -	4,29	5,17*
377	Py1COO1(COO4)(Ph-(3,4-OCH2O-)) Br	1-[2-[1-(1,3-Benzodioxol-5-yl)-2-butoxy-2-oxoethoxy]-2-oxoethyl]pyridinium bromide	U	-4.31	12.32	-2.16		0.48		-2.7 -	3,64	5,69*
378	Py1COO2 (CF3SO2)2N	1-(2-Ethoxy-2-oxoethyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	4.31	2.25	2.86		2.46		2 -	2,95	0,58
379	Py1COO2 8OSO3	1-(2-Ethoxy-2-oxoethyl)pyridinium octyl sulfate	U	4.31	2.25	3.86		2.23		1.8 -	2,62	0,29
380	Py1COO2 Br	1-(2-Ethoxy-2-oxoethyl)pyridinium bromide	U	4.31	2.25	-2.16		3.67		2.6 -	4,71	2,04
381	Py1COO2 PF6	1-(2-Ethoxy-2-oxoethyl)pyridinium hexafluorophosphate	U	4.31	2.25	-0.21		3.20		2.4 -	4,02	1,47
382	Py3 (CF3SO2)2N	1-Propylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	1.68	-7.24	2.86		2.63		1.8 -	3,46	1,68
383	Py3 Br	1-Propylpyridinium bromide	U	1.68	-7.24	-2.16		3.84		3.6 -	4,12	0,22
384	Py4 Cl	1-Butylpyridinium chloride	L	0.96	-6.71	-2.31	3.18	3.64	-0.46			0,05
385	Py4 Al2Cl7	1-Butylpyridinium μ-chlorohexachlorodialuminate	T	0.96	-6.71	1.43	3.01	2.74	0.27	2.2	3,27	1,04
386	Py4 N(CN)2	1-Butylpyridinium N-cyanocyanamide	U	0.96	-6.71	0.00		3.08		2.7 -	3,45	0,63
387	Py4 Br	1-Butylpyridinium bromide	U	0.96	-6.71	-2.16		3.60		3.4 -	3,77	0,00
388	Py4 1OSO3	1-Butylpyridinium methyl sulfate	U	0.96	-6.71	-0.44		3.19		2.9 -	3,51	0,50
389	Py4 8OSO3	1-Butylpyridinium octyl sulfate	U	0.96	-6.71	3.86		2.16		1.3 -	2,97	1,74
390	Py4 BF4	1-Butylpyridinium tetrafluoroborate	U	0.96	-6.71	-0.33		3.16		2.8 -	3,5	0,53
391	Py4 CF3SO3	1-Butylpyridinium trifluoromethanesulfonate	U	0.96	-6.71	0.07		3.07		2.7 -	3,44	0,65
392	Py4 PF6	1-Butylpyridinium hexafluorophosphate	U	0.96	-6.71	-0.21		3.13		2.8 -	3,48	0,56
393	Py5 (CF3SO2)2N	1-Pentylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	-0.24	-6.22	2.86		2.03		1.5 -	2,58	1,19
394	Py5 Br	1-Pentylpyridinium bromide	U	-0.24	-6.22	-2.16		3.24		3.1 -	3,34	0,27
395	Py6 (CF3SO2)2N	1-Hexylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	-0.95	-5.90	2.86		1.82		1.4 -	2,27	1,03
396	Py6 CF3SO3	1-Hexylpyridinium trifluoromethanesulfonate	U	-0.95	-5.90	0.07		2.49		2.4 -	2,62	0,22
397	Py6 Cl	1-Hexylpyridinium chloride	U	-0.95	-5.90	-2.31		3.06		2.9 -	3,23	0,47
398	Py6 PF6	1-Hexylpyridinium hexafluorophosphate	U	-0.95	-5.90	-0.21		2.56		2.5 -	2,66	0,13

399	Py8 Cl	1-Octylpyridinium chloride	L	-3.41	-5.10	-2.31	1.69	2.34	-0.65				0,99
400	Py8 (CF3SO2)2N	1-Octylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	-3.41	-5.10	2.86		1.09		0.9	-	1,32	0,54
401	Py-10 Br	1-Decylpyridinium bromide	U	-5.41	-4.43	-2.16		1.71		1	-	2,38	1,32
402	Py-16 Br	1-Hexadecylpyridinium bromide	U	-11.79	-2.66	-2.16		-0.13		-1.5	-	1,24	2,50*
403	Py-16 Cl	1-Hexadecylpyridinium chloride	U	-11.79	-2.66	-2.31		-0.10		-1.5	-	1,29	2,54*
404	Py3OH (CF3SO2)2N	1-(3-Hydroxypropyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	9.31	2.44	2.86	4.01	3.77	0.24				0,08
405	Py3OH Cl	1-(3-Hydroxypropyl)pyridinium chloride	U	9.31	2.44	-2.31		5.01		4.2	-	5,78	1,58
406	Py3O1 (CF3SO2)2N	1-(3-Methoxypropyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	4.39	-2.54	2.86		2.92		2.6	-	3,21	0,71
407	Py3O1 Cl	1-(3-Methoxypropyl)pyridinium chloride	U	4.39	-2.54	-2.31		4.17		3.8	-	4,5	0,79
408	Py3SO3H CF3SO3	1-(3-Sulfopropyl)pyridinium trifluoromethanesulfonate	U	14.74	7.66	0.07		5.40		4.4	-	6,35	1,69
409	Py2OH (CF3SO2)2N	1-(2-Hydroxyethyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	10.28	2.57	2.86		4.01		3.8	-	4,22	0,01
410	Py2OH I	1-(2-Hydroxyethyl)pyridinium iodide	U	10.28	2.57	-1.63		5.09		4.4	-	5,75	1,31
411	Py2O1 (CF3SO2)2N	1-(2-Methoxyethyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	6.51	-2.48	2.86		3.48		3.1	-	3,9	0,93
412	Py2O1 Cl	1-(2-Methoxyethyl)pyridinium chloride	U	6.51	-2.48	-2.31		4.72		4.5	-	4,96	0,57
413	Py2O2 (CF3SO2)2N	1-(2-Ethoxyethyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	4.79	-2.48	2.86		3.02		2.7	-	3,33	0,74
414	Py2O2 Br	1-(2-Ethoxyethyl)pyridinium bromide	U	4.79	-2.48	-2.16		4.23		3.9	-	4,53	0,72
415	Py1O2 (CF3SO2)2N	1-(Ethoxymethyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	5.70	-2.01	2.86		3.22		2.9	-	3,52	0,72
416	Py1O2 Cl	1-(Ethoxymethyl)pyridinium chloride	U	5.70	-2.01	-2.31		4.46		4.1	-	4,8	0,78
417	Pyr66 BF4	1,1-Dihexylpyrrolidinium tetrafluoroborate	U	-5.18	-2.55	-0.33		1.16		0.4	-	1,89	1,27
418	IM66 (CF3SO2)2N	1,3-Dihexylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	-6.81	-4.32	2.86		0.13		-0.2	-	0,44	0,04
419	IM-10-10-2Me (CF3SO2)2N	1,3-Didecyl-2-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	-13.99	-1.46	2.86		-2.03		-3.2	-	-0,8	1,61*
420	Pyr-12-2OH Cl	1-Dodecyl-1-(2-hydroxyethyl)pyrrolidinium chloride	U	-2.02	6.35	-2.31		1.66		-0.4	-	3,77	3,88*
421	IM-14-2OH-2Me Cl	1-(2-Hydroxyethyl)-2-methyl-3-tetradecylimidazolium chloride	U	-5.40	4.92	-2.31		0.90		-1.2	-	3,01	3,87*
422	IM-16-2OH-2Me Cl	1-Hexadecyl-3-(2-hydroxyethyl)-2-methylimidazolium chloride	U	-7.84	5.39	-2.31		0.21		-2.1	-	2,57	4,26*
423	IM2OH-(2Ph) Cl	1-(2-hydroxyethyl)-3-(2-phenylethyl)immidazolium chloride	U	2.41	2.66	-2.31		3.17		1.9	-	4,41	2,40*
424	IM2OH-(2OH) Cl	1,3-di-(2-hydroxyethyl)imidazolium chloride	U	11.50	9.67	-2.31		4.93		3.2	-	6,66	3,28*
425	IM1O3-1O3 Cl	1,3-Bis(propoxymethyl)imidazolium chloride	U	1.60	2.22	-2.31		2.99		1.8	-	4,22	2,37*
426	IM1O4-1O4 Cl	1,3-Bis(butoxymethyl)imidazolium chloride	U	-0.46	2.39	-2.31		2.44		1	-	3,83	2,65*
427	IM1O5-1O5 Cl	1,3-Bis[(pentyloxy)methyl]imidazolium chloride	U	-2.37	3.08	-2.31		1.87		0.2	-	3,49	3,04*
428	IM1O6-1O6 Cl	1,3-Bis[(hexyloxy)methyl]imidazolium chloride	U	-4.54	3.90	-2.31		1.22		-0.7	-	3,12	3,50*
429	IM1O7-1O7 Cl	1,3-Bis[(heptyloxy)methyl]imidazolium chloride	U	-6.51	3.95	-2.31		0.70		-1.3	-	2,73	3,73*

430	IM1O8-1O8 Cl	1,3-Bis[(octyloxy)methyl]imidazolium chloride	U	-8.29	4.70	-2.31	0.16	-2.1	-	2,43	4,13*
431	IM1O9-1O9 Cl	1,3-Bis[(nonyloxy)methyl]imidazolium chloride	U	-10.86	5.16	-2.31	-0.56	-3.1	-	1,96	4,54*
432	IM1O-10-1O-10 Cl	1,3-Bis[(decyloxy)methyl]imidazolium chloride	U	-12.39	4.91	-2.31	-0.94	-3.5	-	1,65	4,64*
433	IM1O-11-1O-11 Cl	1,3-Bis[(undecyloxy)methyl]imidazolium chloride	U	-14.03	6.14	-2.31	-1.49	-4.4	-	1,4	5,15*
434	IM1O-12-1O-12 Cl	1,3-Bis[(dodecyloxy)methyl]imidazolium chloride	U	-16.24	6.96	-2.31	-2.15	-5.3	-	1,02	5,61*
435	IM1O-14-1O-14 Cl	1,3-Bis[(tetradecyloxy)methyl]imidazolium chloride	U	-19.66	8.67	-2.31	-3.21	-6.9	-	0,46	6,45*
436	IM1O-16-1O-16 Cl	1,3-Bis[(hexadecyloxy)methyl]imidazolium chloride	U	-21.63	9.04	-2.31	-3.76	-7.6	-	0,1	6,77*
437	IM01 BF4	1-Methylimidazole hydrogen tetrafluoroborate	U	5.03	-5.69	-0.33	4.14	3.7	-	4,6	0,71
438	IM01 HO1(1)COO	1-Methylimidazole 2-hydroxypropanoate	U	5.03	-5.69	-4.18	5.07	4.8	-	5,3	0,41
439	IM01 HO1(1)COO_S	1-Methylimidazole (2S)-2-hydroxypropanoate	U	5.03	-5.69	-4.51	5.15	4.9	-	5,39	0,51
440	IM01 1COO	1-methylimidazolium acetate	U	5.03	-5.69	-5.87	5.48	5.1	-	5,82	0,90
441	IM01 CF3COO	1-methylimidazolium trifluoroacetate	U	5.03	-5.69	-2.30	4.62	4.3	-	4,89	0,13
442	IM01 CF3SO3	1-methylimidazolium 1,1,1-trifluoromethanesulfonate	U	5.03	-5.69	0.07	4.05	3.6	-	4,55	0,82
443	IM02 HO1(1)COO	1-Ethylimidazole 2-hydroxypropanoate	U	3.99	-5.53	-4.18	4.78	4.6	-	5,01	0,57
444	IM02 HO1(1)COO_S	1-Ethylimidazole (2S)-2-hydroxypropanoate	U	3.99	-5.53	-4.51	4.86	4.6	-	5,11	0,67
445	IM03 HO1(1)COO	1-Propylimidazole 2-hydroxypropanoate	U	2.28	-5.50	-4.18	4.33	4.1	-	4,6	0,76
446	IM03 HO1(1)COO_S	1-Propylimidazole (2S)-2-hydroxypropanoate	U	2.28	-5.50	-4.51	4.41	4.1	-	4,72	0,86
447	IM04 HO1(1)COO	1-Butylimidazole 2-hydroxypropanoate	U	1.00	-4.97	-4.18	3.94	3.5	-	4,34	1,05
448	IM04 HO1(1)COO_S	1-Butylimidazole (2S)-2-hydroxypropanoate	U	1.00	-4.97	-4.51	4.02	3.6	-	4,46	1,14
449	IM04 1COO	1-butylimidazolium acetate	U	1.00	-4.97	-5.87	4.35	3.7	-	4,95	1,54
450	IM04 CF3COO	1-butylimidazolium trifluoroacetate	U	1.00	-4.97	-2.30	3.49	3.3	-	3,67	0,50
451	IM04 CF3SO3	1-butylimidazolium 1,1,1-trifluoromethanesulfonate	U	1.00	-4.97	0.07	2.92	2.8	-	3,03	0,18
452	IM05 HO1(1)COO	1-Pentylimidazole 2-hydroxypropanoate	U	-0.48	-4.65	-4.18	3.52	3	-	4,06	1,30
453	IM05 HO1(1)COO_S	1-Pentylimidazole (2S)-2-hydroxypropanoate	U	-0.48	-4.65	-4.51	3.60	3	-	4,18	1,39
454	IM06 HO1(1)COO	1-Hexylimidazole 2-hydroxypropanoate	U	-1.08	-4.19	-4.18	3.32	2.7	-	3,96	1,49
455	IM06 HO1(1)COO_S	1-Hexylimidazole (2S)-2-hydroxypropanoate	U	-1.08	-4.19	-4.51	3.40	2.7	-	4,08	1,58
456	IM07 HO1(1)COO	1-Heptylimidazole 2-hydroxypropanoate	U	-2.69	-4.01	-4.18	2.88	2.1	-	3,65	1,72
457	IM07 HO1(1)COO_S	1-Heptylimidazole (2S)-2-hydroxypropanoate	U	-2.69	-4.01	-4.51	2.96	2.1	-	3,77	1,81
458	IM08 HO1(1)COO	1-Octylimidazole 2-hydroxypropanoate	U	-3.55	-3.47	-4.18	2.60	1.7	-	3,51	1,95
459	IM08 HO1(1)COO_S	1-Octylimidazole (2S)-2-hydroxypropanoate	U	-3.55	-3.47	-4.51	2.68	1.7	-	3,63	2,05
460	IM09 HO1(1)COO	1-Nonylimidazole 2-hydroxypropanoate	U	-4.64	-3.28	-4.18	2.30	1.3	-	3,31	2,13
461	IM09 HO1(1)COO_S	1-Nonylimidazole (2S)-2-hydroxypropanoate	U	-4.64	-3.28	-4.51	2.38	1.3	-	3,43	2,22
462	IM0-10 HO1(1)COO	1-Decylimidazole 2-hydroxypropanoate	U	-5.78	-2.89	-4.18	1.96	0.8	-	3,11	2,36*
463	IM0-10 HO1(1)COO_S	1-Decylimidazole (2S)-2-hydroxypropanoate	U	-5.78	-2.89	-4.51	2.04	0.8	-	3,23	2,45*

464	IM0-11 HO1(1)COO	1-Undecylimidazole 2-hydroxypropanoate	U	-6.55	-2.51	-4.18	1.72	0.5	- 2,98	2,54*
465	IM0-11 HO1(1)COO_S	1-Undecylimidazole (2S)-2-hydroxypropanoate	U	-6.55	-2.51	-4.51	1.80	0.5	- 3,1	2,64*
466	IM0-12 HO1(1)COO	1-Dodecylimidazole 2-hydroxypropanoate	U	-7.34	-2.19	-4.18	1.48	0.1	- 2,85	2,72*
467	IM0-12 HO1(1)COO_S	1-Dodecylimidazole (2S)-2-hydroxypropanoate	U	-7.34	-2.19	-4.51	1.56	0.2	- 2,96	2,81*
468	IM01O4 HO1(1)COO	1-(Butoxymethyl)imidazole 2-hydroxypropanoate	U	1.36	-0.40	-4.18	3.62	2.6	- 4,68	2,24
469	IM01O4 HO1(1)COO_S	1-(Butoxymethyl)imidazole (2S)-2-hydroxypropanoate	U	1.36	-0.40	-4.51	3.70	2.6	- 4,79	2,33
470	IM01O5 HO1(1)COO	1-[(Pentyloxy)methyl]imidazole 2-hydroxypropanoate	U	0.12	-0.39	-4.18	3.29	2.1	- 4,43	2,38*
471	IM01O5 HO1(1)COO_S	1-[(Pentyloxy)methyl]imidazole (2S)-2-hydroxypropanoate	U	0.12	-0.39	-4.51	3.37	2.2	- 4,55	2,47*
472	IM01O6 HO1(1)COO	1-[(Hexyloxy)methyl]imidazole 2-hydroxypropanoate	U	-0.43	0.45	-4.18	3.07	1.8	- 4,37	2,66*
473	IM01O6 HO1(1)COO_S	1-[(Hexyloxy)methyl]imidazole (2S)-2-hydroxypropanoate	U	-0.43	0.45	-4.51	3.15	1.8	- 4,49	2,76*
474	IM01O7 HO1(1)COO	1-[(Heptyloxy)methyl]imidazole 2-hydroxypropanoate	U	-1.75	0.26	-4.18	2.74	1.4	- 4,1	2,76*
475	IM01O7 HO1(1)COO_S	1-[(Heptyloxy)methyl]imidazole (2S)-2-hydroxypropanoate	U	-1.75	0.26	-4.51	2.82	1.4	- 4,22	2,85*
476	IM01O8 HO1(1)COO	1-[(Octyloxy)methyl]imidazole 2-hydroxypropanoate	U	-2.94	0.97	-4.18	2.36	0.8	- 3,91	3,08*
477	IM01O8 HO1(1)COO_S	1-[(Octyloxy)methyl]imidazole (2S)-2-hydroxypropanoate	U	-2.94	0.97	-4.51	2.44	0.9	- 4,03	3,17*
478	IM01O9 HO1(1)COO	1-[(Nonyloxy)methyl]imidazole 2-hydroxypropanoate	U	-4.56	0.87	-4.18	1.94	0.3	- 3,58	3,23*
479	IM01O9 HO1(1)COO_S	1-[(Nonyloxy)methyl]imidazole (2S)-2-hydroxypropanoate	U	-4.56	0.87	-4.51	2.02	0.3	- 3,7	3,33*
480	IM01O-10 HO1(1)COO	1-[(Decyloxy)methyl]imidazole 2-hydroxypropanoate	U	-5.09	0.97	-4.18	1.79	0.1	- 3,48	3,32*
481	IM01O-10 HO1(1)COO_S	1-[(Decyloxy)methyl]imidazole (2S)-2-hydroxypropanoate	U	-5.09	0.97	-4.51	1.87	0.1	- 3,6	3,41*
482	IM01O-11 HO1(1)COO	1-[(Undecyloxy)methyl]imidazole 2-hydroxypropanoate	U	-6.60	1.67	-4.18	1.33	-0.6	- 3,23	3,67*
483	IM01O-11 HO1(1)COO_S	1-[(Undecyloxy)methyl]imidazole (2S)-2-hydroxypropanoate	U	-6.60	1.67	-4.51	1.41	-0.5	- 3,35	3,77*
484	IM01O-12 HO1(1)COO	1-[(Dodecyloxy)methyl]imidazole 2-hydroxypropanoate	U	-7.33	2.17	-4.18	1.09	-0.9	- 3,12	3,89*
485	IM01O-12 HO1(1)COO_S	1-[(Dodecyloxy)methyl]imidazole (2S)-2-hydroxypropanoate	U	-7.33	2.17	-4.51	1.17	-0.9	- 3,24	3,98*
486	Py0 Cl	Pyridine hydrochloride	U	3.78	-5.25	-2.31	4.25	4.1	- 4,4	0,13
487	0600NN (CF3SO2)2N	1-hexyl-1,4-diaza[2.2.2]bicyclooctanium bis(trifluoromethylsulfonyl)imide	U	3.71	0.96	2.86	2.42	2.1	- 2,75	0,30
488	IM00 1COO	1H-Imidazol-1-ium acetate	U	7.34	-3.31	-5.87	5.87	5.4	- 6,37	1,29
489	IM00 CF3COO	1H-Imidazol-1-ium trifluoroacetate	U	7.34	-3.31	-2.30	5.01	4.8	- 5,2	0,25
490	IM00 CFSO3	1H-Imidazol-1-ium 1,1,1-trifluoromethanesulfonate	U	7.34	-3.31	0.07	4.44	4.1	- 4,74	0,44
491	IM01-2Me (CF3SO2)2N	1,2-dimethylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	4.73	-5.69	2.86	3.30	2.5	- 4,09	1,60
492	IM16-2Me Cl	1-hexyl-2,3-dimethyl imidazolium chloride midazolium chloride	U	-2.23	-6.01	-2.31	2.73	2.5	- 2,97	0,59
493	IM13-2Me (CF3SO2)2N	1,2-dimethyl-3-propylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	1.81	-6.77	2.86	2.62	1.9	- 3,38	1,56
494	IM18 N(CN)2	1-Methyl-3-octylimidazolium dicyanamide	U	-3.07	-4.67	0.00	1.83	1.6	- 2,07	0,37
495	Py4-3Me (CF3SO2)2N	1-buthyl-3-methylpyridinium1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	-1.02	-6.72	2.86	1.87	1.3	- 2,45	1,24

496	IM18 SbF6	1-methyl-3-octylimidazolium hexafluoroantimonate	U	-3.07	-4.67	-0.12	1.86	1.6	- 2,11	0,40
497	IM11 (1O)2PO2	1,3-dimethyl imidazolium dimethyl phopsphate	U	4.18	-6.87	0.20	3.90	3.3	- 4,53	1,08
498	IM18 CF3COO	1-methyl-3-octylimidazolium trifluoroacetate	U	-3.07	-4.67	-2.30	2.39	1.9	- 2,87	1,03
499	IM12OH 1COO	1-(2-hydroxyethyl)-3-methylimidazolium acetate	U	9.73	2.71	-5.87	5.95	4.7	- 7,15	2,64*
500	IM12OH N(CN2)	1-(2-hydroxyethyl)-3-methylimidazolium dicyanamide	U	9.73	2.71	0.00	4.54	4	- 5,07	0,94
501	IM12OH NO3	1-(2-hydroxyethyl)-3-methylimidazolium nitrate	U	9.73	2.71	-2.37	5.11	4.3	- 5,9	1,62
502	Py6-4NMe2 Br	4-(Dimethylamino)-1-hexylpyridinium bromide	U	-3.42	-6.49	-2.16	2.43	2.2	- 2,65	0,55
503	Py8-4Me (CF3SO2)2N	1-octyl-4-methylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	-4.69	-5.10	2.86	0.76	0.5	- 0,97	0,40
504	Py4 (CF3SO2)2N	1-butylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	0.96	-6.71	2.86	2.40	1.7	- 3,09	1,46
505	Pip12OH N(CN)2	1-(2-hydroxyethyl)-1-methylpiperidinium N-cyanocyanamide	U	10.68	4.70	0.00	4.61	3.8	- 5,37	1,36
506	Pyr18 (CF3SO2)2N	1-methyl-1-octylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	-2.33	-3.03	2.86	1.19	1	- 1,38	0,10
507	Mor14 N(CN)2	4-butyl-4-methylmorpholinium dicyanamide	U	6.23	0.06	0.00	3.86	3.5	- 4,2	0,61
508	Mor12OH N(CN)2	4-(2-hydroxyethyl)-4-methylmorpholinium dicyanamide	U	13.05	7.64	0.00	4.97	3.9	- 6,03	1,89
509	Mor12 N(CN)2	1-ethyl-1-methylmorpholinium dicyanamide	U	8.90	-0.32	0.00	4.60	4.4	- 4,77	0,21
510	Mor12 (CF3SO2)2N	1-ethyl-1-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	8.90	-0.32	2.86	3.91	3.6	- 4,18	0,62
511	IM14 1COO	1-butyl-3-methylimidazolium acetate	U	0.58	-5.91	-5.87	4.32	3.8	- 4,82	1,33
512	IM16 1COO	1-hexyl-3-methylimidazolium acetate	U	-1.54	-5.78	-5.87	3.75	3.1	- 4,39	1,60
513	IM16 CF3COO	1-hexyl-3-methylimidazolium trifluoroacetate	U	-1.54	-5.78	-2.30	2.89	2.7	- 3,11	0,57
514	Pyr14 1COO	1-butyl-1-methylpyrroldinium acetate	U	1.96	-4.12	-5.87	4.52	3.9	- 5,19	1,66
515	IM18 NO3	1-methyl-3-octylimidazolium nitrate	U	-3.07	-4.67	-2.37	2.40	1.9	- 2,89	1,05
516	IM14 (CF3SO2)3C	1-butyl-3-methylimidazolium tris[(trifluoromethyl)sulfonyl]methide	U	0.58	-5.91	3.93	1.97	1.3	- 2,64	1,51
517	IM1-18 (CF3SO2)2N	1-methyl-3-octadecylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	-13.76	-1.31	2.86	-1.98	-3.2	- -0,8	1,62*
518	Py4-3Me (CF3SO2)2N	1-butyl-3-methylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	-1.02	-6.72	2.86	1.87	1.3	- 2,45	1,24
519	Py6-3Me (CF3SO2)2N	1-hexyl-3-methylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	-3.03	-5.66	2.86	1.25	0.9	- 1,55	0,73
520	Pyr13 (CF3SO2)2N	1-methyl-1-propylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	3.13	-4.34	2.86	2.75	2.3	- 3,23	1,06

[a] Y_predictions according to *Vibrio fischeri* 55x3 PLS correlation model, as reported in the section 3.3.4. Note: ILs numeration as in the other PLS datamatrices.

Table B15 Experimental and predicted E_{NR} values for ILs used as learning (L) and prediction set (U).

entry	IL code	ILs name	Set	exp. ENR[a] (kcal/mol)	pred. ENR[b] (kcal/mol)	DModX	IL[c]
1	IM1-(1Ph) (CF3SO2)2N	1-benzyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	216.2	216.3	1.54	326
2	IM12 (CF3SO2)2N	1-Ethyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	217.9	217.8	1.07	92
3	IM14 (1O)2PO2	1-butyl-3-methylimidazolium dimethyl phosphate	L	218	217.8	0.63	183
4	IM14 N(CN)2	1-Butyl-3-methylimidazolium N-cyanocyanamide	L	215.7	215.6	0.74	169
5	IM14 PF6	1-Butyl-3-methylimidazolium hexafluorophosphate	L	217.7	217.5	0.79	165
6	IM14 (CF3SO2)2N	1-Butyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	218.2	217.8	0.85	164
7	IM14 BF4	1-Butyl-3-methylimidazolium tetrafluoroborate	L	217.3	217.2	0.86	163
8	IM14 CF3COO	1-Butyl-3-Methylimidazolium trifluoroacetate	L	216.6	216.9	1.01	185
9	IM14 1COO	1-butyl-3-methylimidazolium acetate	L	217.2	217.3	1.57	511
10	IM14-2Me (CF3SO2)2N	1-Butyl-2,3-dimethylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	217.7	218.0	0.92	75
11	IM16 N(CN)2	1-hexyl-3-methylimidazolium dicyanamide	L	215.3	215.1	0.70	200
12	IM16 (CF3SO2)2N	1-Hexyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	217.9	217.3	0.84	191
13	IM16 SbF6	1-hexyl-3-methylimidazolium hexafluoridoantimonate	L	216.1	216.8	1.03	202
14	IM18 (CF3SO2)2N	1-Methyl-3-octylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	217.9	217.7	0.61	209
15	IM18 N(CN)2	1-Methyl-3-octylimidazolium dicyanamide	L	215.7	215.5	1.07	494
16	IM4-(1Ph) (CF3SO2)2N	1-benzyl-3-butylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	216.1	216.4	1.41	327
17	Pip14 (CF3SO2)2N	1-Butyl-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	219	219.5	0.87	38
18	Pyr14 (CF3SO2)2N	1-Butyl-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	219.9	219.6	0.77	12
19	IM1-10 BF4	1-Decyl-3-methylimidazolium tetrafluoroborate	U		216.9	1.40	218
20	IM16 PF6	1-Hexyl-3-methylimidazolium hexafluorophosphate	U		217.0	0.87	194
21	IM16 BF4	1-Hexyl-3-methylimidazolium tetrafluoroborate	U		216.7	0.96	196
22	IM18 PF6	1-Methyl-3-octylimidazolium hexafluorophosphate	U		217.4	0.86	213
23	IM18 BF4	1-Methyl-3-octylimidazolium tetrafluoroborate	U		217.1	1.01	207
24	IM1-(1Ph-4Me) PF6	1-Methyl-3-[(4-methylphenyl)methyl]imidazolium hexafluorophosphate	U		215.9	1.61	143
25	IM1-(1Ph-4Me) BF4	1-Methyl-3-(phenylmethyl)imidazolium tetrafluoroborate	U		215.6	1.67	141
26	IM11 N(CN)2	1-methyl-3-methylimidaziolium N-cyanocyanamide	U		215.7	0.89	84
27	IM11 (CF3SO2)2N	1,3-Dimethylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		217.9	1.26	81
28	IM11 (1O)2PO2	1,3-dimethyl imidazolium dimethyl phopsphate	U		217.8	1.28	497
29	IM11 1OSO3	1,3-dimethylimidazolium methylsulfate	U		217.6	1.29	82
30	IM11 4MePhSO3	1,3-dimethylimidazolium p-toluenesulfonate	U		217.5	1.30	83
31	IM1-10 (CF3SO2)2N	1-decyl-3-methylimidazolium bis(trifluoromethylsulphonyl)imide	U		217.6	1.12	222
32	IM1-10 PF6	1-Decyl-3-methylimidazolium hexafluorophosphate	U		217.2	1.28	221
33	IM1-1Ph PF6	1-Methyl-3-(phenylmethyl)imidazolium hexafluorophosphate	U		215.9	1.54	146
34	IM1-1Ph BF4	1-Methyl-3-(phenylmethyl)imidazolium tetrafluoroborate	U		215.7	1.58	144

35	IM12 N(CN)2	1-Ethyl-3-methylimidazolium N-cyanocyanamide	U	215.6	0.56	91
36	IM12 1OSO3	1-Ethyl-3-methylimidazolium methylsulfate	U	217.6	1.00	98
37	IM12 4MePhSO3	1-Ethyl-3-methylimidazolium 4-methylbenzenesulfonate	U	217.5	1.01	100
38	IM12 2OSO3	1-Ethyl-3-methylimidazolium ethyl sulfate	U	217.7	1.01	94
39	IM12 1SO3	1-Ethyl-3-methylimidazolium methanesulfonate	U	217.6	1.03	99
40	IM12 PF6	1-Ethyl-3-methylimidazolium hexafluorophosphate	U	217.4	1.11	106
41	IM12 BF4	1-Ethyl-3-methylimidazolium tetrafluoroborate	U	217.2	1.16	102
42	IM12 HSO4	1-Ethyl-3-methylimidazolium hydrogen sulfate	U	216.9	1.17	105
43	IM12 CF3SO3	1-Ethyl-3-methylimidazolium trifluoromethanesulfonate	U	217.4	1.18	104
44	IM12 CF3COO	1-Ethyl-3-methylimidazolium trifluoroacetate	U	216.9	1.27	103
45	IM12 8OSO3	1-Ethyl-3-methylimidazolium octylsulfate	U	217.9	1.27	101
46	IM12 1COO	1-Ethyl-3-methylimidazolium acetate	U	217.3	1.63	96
47	IM12 SCN	1-Ethyl-3-methylimidazolium thiocyanate	U	217.7	1.74	107
48	IM12 1O2O2OSO3	1-Ethyl-3-methylimidazolium 2-(2-methoxyethoxy)ethyl sulfate	U	217.4	1.93	97
49	IM12 (C2F5)2PO2	1-Ethyl-3-methylimidazolium bis(pentafluoroethyl)phosphinate	U	217.4	1.95	88
50	IM1-2Ph PF6	1-Methyl-3-(2-phenylethyl)imidazolium hexafluorophosphate	U	216.0	1.94	159
51	IM1-2Ph BF4	1-Methyl-3-(2-phenylethyl)imidazolium tetrafluoroborate	U	215.8	1.95	157
52	IM13 (CF3SO2)2N	1-Methyl-3-propylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	217.8	0.83	148
53	IM13 PF6	1-Methyl-3-propylimidazolium hexafluorophosphate	U	217.4	0.90	149
54	IM13 BF4	1-Methyl-3-propylimidazolium tetrafluoroborate	U	217.2	0.96	147
55	IM13-2Me (CF3SO2)2N	1,2-dimethyl-3-propylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	217.5	1.17	493
56	IM14 1OSO3	1-Butyl-3-methylimidazolium methyl sulfate	U	217.6	0.56	175
57	IM14 1SO3	1-Butyl-3-methylimidazolium methanesulfonate	U	217.7	0.62	171
58	IM14 (CF3)2N	1-Butyl-3-methylimidazolium 1,1,1-trifluoro-N-(trifluoromethyl)methanaminate	U	217.6	0.72	162
59	IM14 SbF6	1-Butyl-3-methylimidazolium (OC-6-11)-hexafluoroantimonate	U	217.3	0.73	181
60	IM14 HSO4	1-Butyl-3-methylimidazolium hydrogen sulfate	U	216.9	0.75	179
61	IM14 (2-SO2PhCO)N	1-Butyl-3-methylimidazolium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide	U	217.0	0.80	172
62	IM14 CF3SO3	1-Butyl-3-methylimidazolium trifluoromethanesulfonate	U	217.4	0.80	161
63	IM14 AC	3-Butyl-1-methylimidazolium 6-methyl-2,2-dioxo-1,2,3-oxathiazin-4(3H)-onate	U	217.2	0.83	176
64	IM14 4MePhSO3	1-Butyl-3-methylimidazolium 4-methylbenzenesulfonate	U	217.5	0.90	170
65	IM14 (CF3SO2)3C	1-butyl-3-methylimidazolium tris[(trifluoromethyl)sulfonyl]methide	U	217.9	1.09	516
66	IM14 8OSO3	1-Butyl-3-methylimidazolium octylsulfate	U	218.0	1.15	160
67	IM14 SCN	1-Butyl-3-methylimidazolium thiocyanate	U	217.7	1.59	182
68	IM14 1O2O2OSO3	1-Butyl-3-methylimidazolium 2-(2-methoxyethoxy)ethyl sulfate	U	217.4	1.75	174
69	IM14 Co(CO)4	1-Butyl-3-methylimidazolium (T-4)-tetracarbonylcobaltate	U	218.0	1.80	177
70	IM14-2Me CF3SO3	1-Butyl-2,3-dimethylimidazolium trifluoromethanesulfonate	U	217.6	1.05	77
71	IM14-2Me BF4	1-Butyl-2,3-dimethylimidazolium tetrafluoroborate	U	217.3	1.06	76

72	IM15 PF6	1-Methyl-3-pentylimidazolium hexafluorophosphate	U	217.5	0.91	190
73	IM15 (CF3SO2)2N	1-Methyl-3-pentylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	217.8	0.92	187
74	IM15 BF4	1-Methyl-3-pentylimidazolium tetrafluoroborate	U	217.2	0.98	188
75	IM16 (2-SO2PhCO)N	1-Hexyl-3-methylimidazolium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide	U	216.5	0.86	195
76	IM16 (CF3SO2)3C	1-Hexyl-3-methylimidazolium tris[(trifluoromethyl)sulfonyl]methide	U	217.4	1.11	199
77	IM16 CF3COO	1-hexyl-3-methylimidazolium trifluoroacetate	U	216.4	1.15	513
78	IM16 1COO	1-hexyl-3-methylimidazolium acetate	U	216.8	1.59	512
79	IM16-2Me BF4	1-Hexyl-2,3-dimethylimidazolium tetrafluoroborate	U	216.5	1.40	78
80	IM16-2Me (CF3SO2)2N	1-hexyl-2,3-dimethylimidazolium bis(trifluoromethylsulphonyl)imide	U	217.2	1.52	79
81	IM17 (CF3SO2)2N	1-Heptyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	217.8	0.88	203
82	IM17 PF6	1-Heptyl-3-methylimidazolium hexafluorophosphate	U	217.4	0.94	206
83	IM17 BF4	1-Heptyl-3-methylimidazolium tetrafluoroborate	U	217.2	1.05	204
84	IM18 SbF6	1-methyl-3-octylimidazolium hexafluoroantimonate	U	217.2	0.93	496
85	IM18 CF3SO3	1-Methyl-3-octylimidazolium trifluormethanesulfonate	U	217.3	0.96	211
86	IM18 8OSO3	3-Methyl-1-octylimidazolium octylsulfate	U	217.9	1.01	210
87	IM18 CF3COO	1-methyl-3-octylimidazolium trifluoroacetate	U	216.8	1.27	498
88	IM19 PF6	1-Methyl-3-nonylimidazolium hexafluorophosphate	U	217.2	1.27	217
89	IM19 BF4	1-Methyl-3-nonylimidazolium tetrafluoroborate	U	217.0	1.37	215
90	IM1i4 (CF3SO2)2N	1-Methyl-3-(2-methylpropyl)imidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	218.0	0.85	136
91	IM22 (CF3SO2)2N	1,3-Diethylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	217.7	1.01	316
92	IM23 (CF3SO2)2N	1-Ethyl-3-propylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	217.6	0.88	318
93	IM24 CF3SO3	1-Butyl-3-ethylimidazolium trifluoromethanesulfonate	U	217.1	1.24	322
94	IM24 BF4	1-Butyl-3-ethylimidazolium tetrafluoroborate	U	216.9	1.27	320
95	IM24 CF3COO	1-Butyl-3-ethylimidazolium trifluoroacetate	U	216.6	1.45	321
96	IM26 BF4	1-Ethyl-3-hexylimidazolium tetrafluoroborate	U	217.0	1.44	323
97	IM33 (CF3SO2)2N	1,3-Dipropylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	217.7	0.89	349
98	IM44 (CF3SO2)2N	1,3-Dibutylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	217.3	0.98	350
99	IM55 (CF3SO2)2N	1,3-Dipentylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	217.4	1.10	369
100	IM66 (CF3SO2)2N	1,3-Dihexylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	217.0	1.57	418
101	Pip13 (CF3SO2)2N	1-Methyl-1-propylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	219.6	0.90	36
102	Pip13 PF6	1-Methyl-1-propylpiperidinium hexafluorophosphate	U	219.2	1.63	37
103	Pip14 N(CN)2	1-butyl-1-methylpiperidinium N-cyanocyanamide	U	217.3	1.60	524
104	Py2-4NMe2 (CF3SO2)2N	4-(Dimethylamino)-1-ethylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	216.2	1.94	342
105	Py4-4NMe2 (CF3SO2)2N	1-Butyl-4-(dimethylamino)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	216.4	1.59	344
106	Py6-4NMe2 (CF3SO2)2N	4-(Dimethylamino)-1-hexylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	216.3	1.82	347

107	Pyr12 2OSO3	1-Ethyl-1-methylpyrrolidinium ethyl sulfate	U	220.3	1.86	3
108	Pyr13 (CF3SO2)2N	1-methyl-1-propylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	219.9	0.79	520
109	Pyr13 PF6	1-Methyl-1-propylpyrrolidinium hexafluorophosphate	U	219.5	1.43	9
110	Pyr14 (1O)2PO2	1-butyl-1-methylpyrrolidinium dimethylphosphate	U	219.6	1.25	521
111	Pyr14 1OSO3	1-Butyl-1-methylpyrrolidinium methyl sulfate	U	219.4	1.32	13
112	Pyr14 N(CN)2	1-Butyl-1-methylpyrrolidinium N-cyanocyanamide	U	217.4	1.51	16
113	Pyr14 BF4	1-Butyl-1-methylpyrrolidinium tetrafluoroborate	U	219.0	1.64	14
114	Pyr16 (CF3SO2)2N	1-Hexyl-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	219.4	0.88	17
115	Pyr18 (CF3SO2)2N	1-methyl-1-octylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	219.2	1.19	506
116	Pyr24 2OSO3	1-Butyl-1-ethylpyrrolidinium ethyl sulfate	U	219.5	1.34	314

[a]Y_experimental E_{NR} values as reported in Table 2; [b]Y_predictions according to the E_{NR} PLS models; [c]ILs numeration as in the other PLS datamatrices.

Table B16 Experimental and predicted C_p values. The (*) indicates DModX values higher than 1.60 corresponding to 95% C.I.

IL	IL code	Systematic name	Y: exp.Cp J/(K*mol)	Ý[c]: Cp *pred.* J/(K*mol)	Y-Ý	Confidence Interval (C.I.) for predictions	DMod X
1	Py4-2Me BF4	1-Butyl-2-methylpyridinium tetrafluoroborate		392		341.9 - 442,7	0.83
2	Py4-2Me Cl	1-Butyl-2-methylpyridinium chloride		265		175.4 - 354.7	0.93
3	Pyr12 2OSO3	1-Ethyl-1-methylpyrrolidinium ethyl sulfate		434		259.7 - 607.9	1.90*
4	Pyr11CN (CF3SO2)2N	1-(Cyanomethyl)-1-methylpyrrolidinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide		430		92.7 - 767.4	1.79*
5	Pyr11CN Cl	1-(Cyanomethyl)-1-methylpyrrolidinium chloride		151		-234.3 - 535.3	1.61*
6	Pyr11COO2 (CF3SO2)2N	1-(2-Ethoxy-2-oxoethyl)-1-methylpyrrolidinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide		420		71.5 - 767.9	2.48*
7	Pyr11COO2 Br	1-(2-Ethoxy-2-oxoethyl)-1-methylpyrrolidinium bromide		151		-244.0 - 545.4	2.35*
8	Pyr11COO2 (C2F5)3PF3	1-(2-Ethoxy-2-oxoethyl)-1-methylpyrrolidinium tris(pentafluoroethyl)trifluorophosphate		534		139.6 - 928.6	3.00*
9	Pyr13 PF6	1-Methyl-1-propylpyrrolidinium hexafluorophosphate		416		233.5 - 599.0	1.96*
10	Pyr14 Cl	1-Butyl-1-methylpyrrolidinium chloride		329		160.4 - 497.5	1.85*
11	Pyr14 (C2F5)3PF3	1-Butyl-1-methylpyrrolidinium trifluorotris(pentafluoroethyl)phosphate	769[a]	723	46		2.04*
12	Pyr14 (CF3SO2)2N	1-Butyl-1-methylpyrrolidinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	588[a]	608	-20		1.75*
13	Pyr14 1OSO3	1-Butyl-1-methylpyrrolidinium methyl sulfate		474		306.1 - 640.9	1.84*
14	Pyr14 BF4	1-Butyl-1-methylpyrrolidinium tetrafluoroborate		456		267.6 - 644.6	2.00*
15	Pyr14 Br	1-Butyl-1-methylpyrrolidinium bromide		339		172.8 - 506.0	1.84*
16	Pyr14 N(CN)2	1-Butyl-1-methylpyrrolidinium N-cyanocyanamide		518		363.2 - 672.6	1.82*

17	Pyr16 (CF3SO2)2N	1-Hexyl-1-methylpyrrolidinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide		660		534.4	-	785.7	1.64*
18	Pyr16 Cl	1-Hexyl-1-methylpyrrolidinium chloride		381		202.4	-	558.7	1.87*
19	Pyr18 BF4	1-Methyl-1-octylpyrrolidinium tetrafluoroborate		568		382.1	-	753.5	2.03*
20	Pyr18 Cl	1-Methyl-1-octylpyrrolidinium chloride		441		252.4	-	628.9	1.85*
21	Pyr13OH (CF3SO2)2N	1-(3-Hydroxypropyl)-1-methylpyrrolidinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide		432		-265.4	-	1129.7	2.69*
22	Pyr13OH Cl	1-(3-Hydroxypropyl)-1-methylpyrrolidinium chloride		153		-592.8	-	898.0	2.59*
23	Pyr13O1 (CF3SO2)2N	1-(3-Methoxypropyl)-1-methylpyrrolidinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide		509		203.5	-	814.4	1.95*
24	Pyr13O1 Cl	1-(3-Methoxypropyl)-1-methylpyrrolidinium chloride		229		-128.5	-	587.3	1.92*
25	Pyr12OH (CF3SO2)2N	1-(2-Hydroxyethyl)-1-methylpyrrolidinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide		398		-324.8	-	1120.9	2.74*
26	Pyr12OH I	1-(2-Hydroxyethyl)-1-methylpyrrolidinium iodide		150		-613.9	-	913.6	2.61*
27	Pyr12O1 (CF3SO2)2N	1-(2-Methoxyethyl)-1-methylpyrrolidinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide		477		141.7	-	812.6	2.01*
28	Pyr12O1 (C2F5)3PF3	1-(2-Methoxyethyl)-1-methylpyrrolidinium tris(pentafluoroethyl)trifluorophosphate		592		211.2	-	971.8	2.64*
29	Pyr12O1 Cl	1-(2-Methoxyethyl)-1-methylpyrrolidinium chloride		198		-187.8	-	583.0	1.94*
30	Pyr12O2 (CF3SO2)2N	1-(2-Ethoxyethyl)-1-methylpyrrolidinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide		518		239.6	-	796.2	2.00*
31	Pyr12O2 Br	1-(2-Ethoxyethyl)-1-methylpyrrolidinium bromide		249		-80.6	-	578.4	2.00*
32	Pyr11O2 (CF3SO2)2N	1-(Ethoxymethyl)-1-methylpyrrolidinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide		528		300.1	-	756.2	2.04*
33	Pyr11O2 Cl	1-(Ethoxymethyl)-1-methylpyrrolidinium chloride		249		-31.8	-	529.0	2.05*
34	Pip11CN (CF3SO2)2N	1-(Cyanomethyl)-1-methylpiperidinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide		455		117.9	-	792.1	1.69*
35	Pip11CN Cl	1-(Cyanomethyl)-1-methylpiperidinium chloride		175		-210.8	-	561.8	1.54
36	Pip13 (CF3SO2)2N	1-Methyl-1-propylpiperidinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	607[a]	600	7				1.84*
37	Pip13 PF6	1-Methyl-1-propylpiperidinium hexafluorophosphate		436		254.1	-	618.8	2.00*
38	Pip14 (CF3SO2)2N	1-Butyl-1-methylpiperidinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide		627		497.9	-	756.3	1.73*
39	Pip14 Br	1-Butyl-1-methylpiperidinium bromide		358		187.7	-	528.5	1.90*
40	Pip13OH (CF3SO2)2N	1-(3-Hydroxypropyl)-1-methylpiperidinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide		457		-232.0	-	1145.6	2.63*
41	Pip13OH Cl	1-(3-Hydroxypropyl)-1-methylpiperidinium chloride		177		-560.3	-	914.8	2.55*
42	Pip13O1 (CF3SO2)2N	1-(3-Methoxypropyl)-1-methylpiperidinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide		532		231.2	-	833.6	1.92*
43	Pip13O1 Cl	1-(3-Methoxypropyl)-1-methylpiperidinium chloride		253		-102.7	-	608.4	1.93*
44	Pip12OH (CF3SO2)2N	1-(2-Hydroxyethyl)-1-methylpiperidinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide		427		-302.0	-	1155.4	2.74*
45	Pip12OH I	1-(2-Hydroxyethyl)-1-methylpiperidinium iodide		179		-592.0	-	949.0	2.65*
46	Pip12O1 (CF3SO2)2N	1-(2-Methoxyethyl)-1-methylpiperidinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide		514		264.4	-	764.2	1.97*

47	Pip12O1 Br	1-(2-Methoxyethyl)-1-methylpiperidinium bromide	245	-55.2	-	545.7	1.95*
48	Pip12O2 (CF3SO2)2N	1-(2-Ethoxyethyl)-1-methylpiperidinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	536	263.1	-	808.4	1.97*
49	Pip12O2 Br	1-(2-Ethoxyethyl)-1-methylpiperidinium bromide	267	-58.7	-	592.2	1.99*
50	Pip11O2 (CF3SO2)2N	1-(Ethoxymethyl)-1-methylpiperidinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	553	337.6	-	768.4	1.95*
51	Pip11O2 Cl	1-(Ethoxymethyl)-1-methylpiperidinium chloride	273	2.7	-	544.2	2.00*
52	Mor12 4MePhSO3	4-Ethyl-4-methylmorpholinium 4-methylbenzenesulfonate	456	117.3	-	794.4	2.23*
53	Mor11CN (CF3SO2)2N	4-(Cyanomethyl)-4-methylmorpholinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	340	-164.2	-	844.7	2.54*
54	Mor11CN Cl	4-(Cyanomethyl)-4-methylmorpholinium chloride	61	-487.9	-	609.3	2.29*
55	Mor14 (CF3SO2)2N	4-Butyl-4-methylmorpholinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	502	167.8	-	836.5	1.94*
56	Mor14 Br	4-Butyl-4-methylmorpholinium bromide	233	-151.7	-	618.0	1.91*
57	Mor13OH (CF3SO2)2N	4-(3-Hydroxypropyl)-4-methylmorpholinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	364	-458.9	-	1187.5	3.32*
58	Mor13OH Cl	4-(3-Hydroxypropyl)-4-methylmorpholinium chloride	85	-784.8	-	954.3	3.17*
59	Mor13O1 (CF3SO2)2N	4-(3-Methoxypropyl)-4-methylmorpholinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	438	40.2	-	836.5	2.53*
60	Mor13O1 Cl	4-(3-Methoxypropyl)-4-methylmorpholinium chloride	159	-288.0	-	605.7	2.43*
61	Mor12OH (CF3SO2)2N	4-(2-Hydroxyethyl)-4-methylmorpholinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	329	-502.7	-	1160.2	3.38*
62	Mor12OH I	4-(2-Hydroxyethyl)-4-methylmorpholinium iodide	81	-790.8	-	951.9	3.21*
63	Mor12O1 (CF3SO2)2N	4-(2-Methoxyethyl)-4-methylmorpholinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	404	-24.2	-	832.3	2.67*
64	Mor12O1 Cl	4-(2-Methoxyethyl)-4-methylmorpholinium chloride	125	-350.6	-	599.7	2.54*
65	Mor12O2 (CF3SO2)2N	4-(2-Ethoxyethyl)-4-methylmorpholinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	431	-2.1	-	863.9	2.54*
66	Mor12O2 Br	4-(2-Ethoxyethyl)-4-methylmorpholinium bromide	162	-318.3	-	642.1	2.44*
67	Mor11O2 (CF3SO2)2N	4-(Ethoxymethyl)-4-methylmorpholinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	413	-4.9	-	830.1	2.61*
68	Mor11O2 Cl	4-(Ethoxymethyl)-4-methylmorpholinium chloride	133	-332.0	-	598.2	2.47*
69	IM11COO3-2Me 8OSO3	1.2-Dimethyl-3-(2-oxo-2-propoxyethyl)imidazolium octylsulfate	445	106.8	-	782.3	2.68*
70	IM11COO3-2Me Br	1.2-Dimethyl-3-(2-oxo-2-propoxyethyl)imidazolium bromide	99	-296.7	-	494.2	2.34*
71	IM11COO5-2Me 8OSO3	1.2-Dimethyl-3-[2-oxo-2-(pentyloxy)ethyl]imidazolium octylsulfate	505	193.1	-	816.6	2.75*
72	IM11COO5-2Me Br	1.2-Dimethyl-3-[2-oxo-2-(pentyloxy)ethyl]imidazolium bromide	159	-216.1	-	534.2	2.52*
73	IM1gly-2Me N(NC)2	1.2-dimethyl-3-glycerylimidazolium dicyanamide	212	-1010.6	-	1434.1	4.31*
74	IM1gly-2Me (CF3SO2)2N	1.2-dimethyl-3-glycerylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	302	-872.5	-	1477.1	4.24*
75	IM14-2Me (CF3SO2)2N	1-Butyl-2.3-dimethylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	570	546.7	-	593.7	0.51
76	IM14-2Me BF4	1-Butyl-2.3-dimethylimidazolium tetrafluoroborate	418	351.6	-	484.2	0.81
77	IM14-2Me CF3SO3	1-Butyl-2.3-dimethylimidazolium trifluoromethanesulfonate	437	388.1	-	486.4	0.60

78	IM16-2Me BF4	1-Hexyl-2.3-dimethylimidazolium tetrafluoroborate		482		414.4	-	549.3	1.41
79	IM16-2Me (CF3SO2)2N	1-hexyl-2.3-dimethylimidazolium bis(trifluoromethylsulphonyl)imide	686[a]	634	52				1.21
80	IM12OH-2Me Cl	1-(2-hydroxyethyl)-2.3-dimethylimidazolium chloride		71		-627.7	-	768.7	2.31*
81	IM11 (CF3SO2)2N	1.3-Dimethylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide		454		351.6	-	556.0	1.10
82	IM11 1OSO3	1.3-dimethylimidazolium methylsulfate		319		236.7	-	401.1	0.52
83	IM11 4MePhSO3	1.3-dimethylimidazolium 4-methylbenzenesulfonate		473		370.4	-	575.0	1.26
84	IM11 N(CN)2	1.3-dimethylimidaziolium N-cyanocyanamide		363		287.8	-	438.7	1.04
85	IM11(COO1)(Ph-(3.4-OCH2O-)) Cl	1-[1-(1.3-Benzodioxol-5-yl)-2-methoxy-2-oxoethyl]-3-methylimidazolium chloride		8		-395.7	-	411.2	4.19*
86	IM11(COO4)(Ph-(3.4-OCH2O-)) Br	1-[1-(1.3-Benzodioxol-5-yl)-2-butoxy-2-oxoethyl]-3-methylimidazolium bromide		144		-301.3	-	590.1	4.03*
87	IM12 (C2F5)3PF3	1-Ethyl-3-methylimidazolium trifluorotris(pentafluoroethyl)phosphate		591		424.6	-	757.4	0.93
88	IM12 (C2F5)2PO2	1-Ethyl-3-methylimidazolium bis(pentafluoroethyl)phosphinate		466		354.2	-	578.7	0.65
89	IM12 C(CN)3	1-Ethyl-3-methylimidazolium. salt with methanetricarbonitrile		324		175.2	-	473.7	3.30*
90	IM12 B(CN)4	1-Ethyl-3-methylimidazolium tetracyanoborate		373		236.5	-	509.2	2.95*
91	IM12 N(CN)2	1-Ethyl-3-methylimidazolium N-cyanocyanamide	314.6[b]	386	-71				0.96
92	IM12 (CF3SO2)2N	1-Ethyl-3-methylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	506.5[a]	477	30				1.00
93	IM12 Cl	1-Ethyl-3-methylimidazolium chloride	235[b]	197	38				0.73
94	IM12 2OSO3	1-Ethyl-3-methylimidazolium ethyl sulfate	382.8[a]	358	24				0.43
95	IM12 (OOCCOO)2B	1-Ethyl-3-methylimidazolium bis[ethanedioato-O1.O2]borate		494		333.7	-	654.2	1.10
96	IM12 1COO	1-Ethyl-3-methylimidazolium acetate	321.9[b]	304	18				1.54
97	IM12 1O2O2OSO3	1-Ethyl-3-methylimidazolium 2-(2-methoxyethoxy)ethyl sulfate		561		431.6	-	690.0	0.84
98	IM12 1OSO3	1-Ethyl-3-methylimidazolium methylsulfate	331[b]	342	-11				0.37
99	IM12 1SO3	1-Ethyl-3-methylimidazolium methanesulfonate	345.5[b]	322	24				0.35
100	IM12 4MePhSO3	1-Ethyl-3-methylimidazolium 4-methylbenzenesulfonate		496		400.0	-	591.1	1.15
101	IM12 8OSO3	1-Ethyl-3-methylimidazolium octylsulfate		553		438.2	-	668.7	1.30
102	IM12 BF4	1-Ethyl-3-methylimidazolium tetrafluoroborate	308.1[a]	324	-16				0.60
103	IM12 CF3COO	1-Ethyl-3-methylimidazolium trifluoroacetate	316.5[b]	354	-38				0.74
104	IM12 CF3SO3	1-Ethyl-3-methylimidazolium trifluoromethanesulfonate	363[a]	344	19				0.47
105	IM12 HSO4	1-Ethyl-3-methylimidazolium hydrogen sulfate	295.5[b]	341	-45				0.55
106	IM12 PF6	1-Ethyl-3-methylimidazolium hexafluorophosphate		313		241.8	-	384.9	0.54
107	IM12 SCN	1-Ethyl-3-methylimidazolium thiocyanate	281.4[b]	274	7				0.67
108	IM12 Br	1-Ethyl-3-methylimidazolium bromide	207.5[b]	208	0				0.71
109	IM12 NO3	1-Ethyl-3-methylimidazolium nitrate		221		147.6	-	294.0	1.56
110	[C2MIM][FeCl4] 1.51	1-ethyl-3-methylimidazolium tetrachloroferrate		284		214.0	-	354.8	1.08
111	IM11CN Cl	1-(Cyanomethyl)-3-methylimidazolium chloride		5		-279.2	-	288.7	2.05*

112	IM11CN (CF3SO2)2N	1-(Cyanomethyl)-3-methylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	284	15.3	-	553.3	2.45*
113	IM11CONMeBu Br	1-[2-(Butylmethylamino)-2-oxoethyl]-3-methylimidazolium bromide	190	-188.8	-	569.2	1.79*
114	IM11CONEt2 Br	1-[2-(Diethylamino)-2-oxoethyl]-3-methylimidazolium bromide	149	-217.9	-	515.0	1.75*
115	IM11CONHBu Br	1-[2-(Butylamino)-2-oxoethyl]-3-methylimidazolium bromide	133	-313.3	-	578.5	2.26*
116	IM11COO1 Br	1-(2-Methoxy-2-oxoethyl)-3-methylimidazolium bromide	58	-378.9	-	494.8	2.17*
117	IM11COO1(COO4)(Ph-(3.4-OCH2O-)) Br	1-[2-[1-(1.3-Benzodioxol-5-yl)-2-butoxy-2-oxoethoxy]-2-oxoethyl]-3-methylimidazolium bromide	-12	-559.5	-	535.2	6.63*
118	IM11COO2 BF4	1-(2-Ethoxy-2-oxoethyl)-3-methylimidazolium tetrafluoroborate	219	-248.7	-	686.0	2.68*
119	IM11COO2 Br	1-(2-Ethoxy-2-oxoethyl)-3-methylimidazolium bromide	102	-345.3	-	549.3	2.19*
120	IM11COO3 (CF3SO2)2N	1-Methyl-3-(2-oxo-2-propoxyethyl)imidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	389	83.2	-	695.3	2.40*
121	IM11COO3 8OSO3	1-Methyl-3-(2-oxo-2-propoxyethyl)imidazolium octylsulfate	466	175.6	-	756.4	2.52*
122	IM11COO3 BF4	1-Methyl-3-(2-oxo-2-propoxyethyl)imidazolium tetrafluoroborate	237	-134.9	-	608.6	2.58*
123	IM11COO3 Br	1-Methyl-3-(2-oxo-2-propoxyethyl)imidazolium bromide	120	-230.3	-	470.7	2.20*
124	IM11COO3 N(CN)2	1-Methyl-3-(2-oxo-2-propoxyethyl)imidazolium N-cyanocyanamide	299	-59.8	-	657.0	2.41*
125	IM11COO3 PF6	1-Methyl-3-(2-oxo-2-propoxyethyl)imidazolium hexafluorophosphate	226	-136.3	-	588.0	2.49*
126	IM11COO4 (CF3SO2)2N	3-(2-Butoxy-2-oxoethyl)-1-methylimidazolium N-[(trifluoromethyl)sulfonyl]methanesulfonamide	429	59.4	-	798.6	2.39*
127	IM11COO4 8OSO3	1-(2-Butoxy-2-oxoethyl)-3-methylimidazolium octylsulfate	506	152.7	-	858.9	2.48*
128	IM11COO4 BF4	1-(2-Butoxy-2-oxoethyl)-3-methylimidazolium tetrafluoroborate	277	-157.1	-	710.4	2.69*
129	IM11COO4 Br	1-(2-Butoxy-2-oxoethyl)-3-methylimidazolium bromide	160	-257.0	-	577.0	2.24*
130	IM11COO4 N(CN)2	1-(2-Butoxy-2-oxoethyl)-3-methylimidazolium N-cyanocyanamide	338	-83.3	-	760.2	2.44*
131	IM11COO4 PF6	1-(2-Butoxy-2-oxoethyl)-3-methylimidazolium hexafluorophosphate	266	-159.5	-	690.8	2.59*
132	IM11COO5 8OSO3	1-Methyl-3-[2-oxo-2-(pentyloxy)ethyl]imidazolium octylsulfate	528	255.4	-	800.8	2.61*
133	IM11COO5 Br	1-Methyl-3-[2-oxo-2-(pentyloxy)ethyl]imidazolium bromide	182	-156.6	-	521.1	2.40*
134	IM11COO6 Br	1-[2-(Hexyloxy)-2-oxoethyl]-3-methylimidazolium bromide	209	-142.4	-	560.2	2.42*
135	IM11COO8 Br	1-Methyl-3-[2-(octyloxy)-2-oxoethyl]imidazolium bromide	283	-58.8	-	624.7	2.25*
136	IM1i4 (CF3SO2)2N	1-Methyl-3-(2-methylpropyl)imidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	556	517.9	-	593.7	0.58
137	IM1gly Cl	1-methyl-3-glycerylrylimidazolium chloride	-34	-1179.8	-	1111.6	3.88*
138	IM1gly N(CN)2	1-methyl-3-glycerylimidazolium dicyanamide	155	-996.4	-	1306.2	4.17*
139	IM1gly (CF3SO2)2N	1-methyl-3-glycerylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	245	-858.1	-	1349.0	4.12*
140	IM1-2=1 Cl	1-Methyl-3-(2-propenyl)imidazolium chloride	243	175.2	-	310.8	0.73
141	IM1-(1Ph-4Me) BF4	1-Methyl-3-(phenylmethyl)imidazolium tetrafluoroborate	413	347.3	-	478.2	0.90
142	IM1-(1Ph-4Me) Cl	1-Methyl-3-[(4-methylphenyl)methyl]imidazolium chloride	286	175.8	-	395.3	1.07
143	IM1-(1Ph-4Me) PF6	1-Methyl-3-[(4-methylphenyl)methyl]imidazolium hexafluorophosphate	402	333.3	-	470.2	0.88
144	IM1-1Ph BF4	1-Methyl-3-(phenylmethyl)imidazolium tetrafluoroborate	395	332.3	-	457.4	0.88
145	IM1-3Ph Cl	1-Methyl-3-(phenylmethyl)imidazolium chloride	268	164.3	-	371.0	1.03
146	IM1-1Ph PF6	1-Methyl-3-(phenylmethyl)imidazolium hexafluorophosphate	384	319.9	-	447.8	0.86

147	IM13 BF4	1-Methyl-3-propylimidazolium tetrafluoroborate		373		318.0	-	427.7	0.60
148	IM13 (CF3SO2)2N	1-Methyl-3-propylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	535[b]	525	10				0.73
149	IM13 PF6	1-Methyl-3-propylimidazolium hexafluorophosphate		362		322.6	-	401.1	0.51
150	IM13 Br	1-Methyl-3-propylimidazolium bromide	281[b]	256	25				0.58
151	IM13 Cl	1-Methyl-3-propylimidazolium chloride		246		191.6	-	299.7	0.59
152	IM13 I	1-Methyl-3-propylimidazolium iodide		277		230.1	-	323.9	0.55
153	IM1-2CO-1 Br	1-Methyl-3-(3-oxobutyl)imidazolium bromide		124		-372.2	-	620.2	1.71*
154	IM1-2C6F13 PF6	1-Methyl-3-(3.3.4.4.5.5.6.6.7.7.8.8.8-tridecafluorooctyl)imidazolium hexafluorophosphate		379		-278.2	-	1035.9	3.54*
155	IM12(2Pin-1R) Cl	1-[2-[(1R.5S)-6.6-Dimethylbicyclo[3.1.1]hept-2-en-2-yl]ethyl]-3-methylimidazolium chloride		427		288.0	-	566.4	1.05
156	IM12(2Pin-1R) NO3	1-[2-[(1R.5S)-6.6-Dimethylbicyclo[3.1.1]hept-2-en-2-yl]ethyl]-3-methylimidazolium nitrate		451		285.7	-	616.1	1.48
157	IM1-2Ph BF4	1-Methyl-3-(2-phenylethyl)imidazolium tetrafluoroborate		494		412.9	-	575.5	1.59*
158	IM1-2Ph Cl	1-Methyl-3-(2-phenylethyl)imidazolium chloride		367		219.7	-	514.2	1.55
159	IM1-2Ph PF6	1-Methyl-3-(2-phenylethyl)imidazolium hexafluorophosphate		483		395.7	-	570.7	1.54
160	IM14 8OSO3	1-Butyl-3-methylimidazolium octylsulfate	635[a]	642	-7				0.90
161	IM14 CF3SO3	1-Butyl-3-methylimidazolium trifluoromethanesulfonate	427.7[a]	432	-4				0.50
162	IM14 (CF3)2N	1-Butyl-3-methylimidazolium 1.1.1-trifluoro-N-(trifluoromethyl)methanaminate		420		395.6	-	444.7	0.45
163	IM14 BF4	1-Butyl-3-methylimidazolium tetrafluoroborate	367.1[a]	413	-46				0.73
164	IM14 (CF3SO2)2N	1-Butyl-3-methylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	565.1[a]	565	0				0.54
165	IM14 PF6	1-Butyl-3-methylimidazolium hexafluorophosphate	408.7[a]	402	7				0.63
166	IM14 Cl	1-Butyl-3-methylimidazolium chloride	317[a]	286	31				0.62
167	IM14 I	1-Butyl-3-methylimidazolium iodide	314[a]	317	-3				0.55
168	IM14 Br	1-Butyl-3-methylimidazolium bromide	311.4[a]	296	15				0.58
169	IM14 N(CN)2	1-Butyl-3-methylimidazolium N-cyanocyanamide	375.7[a]	475	-99				0.67
170	IM14 4MePhSO3	1-Butyl-3-methylimidazolium 4-methylbenzenesulfonate	412.7[b]	584	-171				0.75
171	IM14 1SO3	1-Butyl-3-methylimidazolium methanesulfonate		410		389.6	-	430.9	0.33
172	IM14 (2-SO2PhCO)N	1-Butyl-3-methylimidazolium. salt with 1.2-benzisothiazol-3(2H)-one 1.1-dioxide		561		527.9	-	593.9	0.60
173	IM14 (C2F5)3PF3	1-Butyl-3-methylimidazolium trifluorotris(pentafluoroethyl)phosphate		680		563.5	-	795.5	0.84
174	IM14 1O2O2OSO3	1-Butyl-3-methylimidazolium 2-(2-methoxyethoxy)ethyl sulfate	643[a]	649	-6				0.52
175	IM14 1OSO3	1-Butyl-3-methylimidazolium methyl sulfate	416[a]	430	-14				0.33
176	IM14 AC	3-Butyl-1-methylimidazolium 6-methyl-2.2-dioxo-1.2.3-oxathiazin-4(3H)-onate		546		515.9	-	576.1	0.49
177	IM14 Co(CO)4	1-Butyl-3-methylimidazolium (T-4)-tetracarbonylcobaltate		460		429.1	-	491.1	0.69
178	IM14 FeCl4	1-Butyl-3-methylimidazolium tetrachloroferrate	415[a]	373	42				0.76
179	IM14 HSO4	1-Butyl-3-methylimidazolium hydrogen sulfate		429		366.7	-	491.5	0.72

180	IM14 NO3	1-Butyl-3-methylimidazolium nitrate	353.5[a]	309	44		1.43
181	IM14 SbF6	1-Butyl-3-methylimidazolium (OC-6-11)-hexafluoroantimonate		411		371.7 - 450.0	0.66
182	IM14 SCN	1-Butyl-3-methylimidazolium thiocyanate	385[b]	363	22		0.59
183	IM14 (1O)2PO2	1-butyl-3-methylimidazolium dimethyl phosphate		459		438.4 - 479.7	0.26
184	IM14 C(CN)3	1-butyl-3-methylimidazolium tricyanomethanide		413		247.1 - 578.8	3.15*
185	IM14 CF3COO	1-Butyl-3-Methylimidazolium trifluoroacetate	408.2[a]	443	-34		0.89
186	IM13COOH Cl	3-(3-Carboxypropyl)-1-methylimidazolium chloride		-12		-776.4 - 752.0	2.74*
187	IM15 (CF3SO2)2N	1-Methyl-3-pentylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	596[b]	611	-15		0.39
188	IM15 BF4	1-Methyl-3-pentylimidazolium tetrafluoroborate		459		404.4 - 513.3	0.91
189	IM15 Cl	1-Methyl-3-pentylimidazolium chloride		332		241.3 - 422.1	0.72
190	IM15 PF6	1-Methyl-3-pentylimidazolium hexafluorophosphate		448		403.3 - 492.5	0.80
191	IM16 (CF3SO2)2N	1-Hexyl-3-methylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	631.6[a]	593	38		0.64
192	IM16 Br	1-Hexyl-3-methylimidazolium bromide	344[a]	324	20		0.77
193	IM16 Cl	1-Hexyl-3-methylimidazolium chloride	381[b]	314	67		0.80
194	IM16 PF6	1-Hexyl-3-methylimidazolium hexafluorophosphate	424[b]	430	-6		0.73
195	IM16 (2-SO2PhCO)N	1-Hexyl-3-methylimidazolium. salt with 1.2-benzisothiazol-3(2H)-one 1.1-dioxide		589		533.2 - 644.7	0.67
196	IM16 BF4	1-Hexyl-3-methylimidazolium tetrafluoroborate	429.8[a]	441	-11		0.80
197	IM16 (C2F5)3PF3	1-Hexyl-3-methylimidazolium trifluorotris(pentafluoroethyl)phosphate	730[b]	708	22		0.83
198	IM16 (C3F7)3PF3	1-Hexyl-3-methylimidazolium trifluorotris(heptafluoropropyl)phosphate		840		674.6 - 1005.5	1.08
199	IM16 (CF3SO2)3C	1-Hexyl-3-methylimidazolium tris[(trifluoromethyl)sulfonyl]methide		621		547.7 - 693.6	0.57
200	IM16 N(CN)2	1-hexyl-3-methylimidazolium dicyanamide	534[b]	503	31		0.77
201	IM16 NO	1-hexyl-3-methylimidazolium nitrate		337		238.7 - 435.9	1.49
202	IM16 SbF6	1-hexyl-3-methylimidazolium hexafluoridoantimonate		439		413.7 - 464.0	0.74
203	IM17 (CF3SO2)2N	1-Heptyl-3-methylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide		671		626.5 - 716.3	0.24
204	IM17 BF4	1-Heptyl-3-methylimidazolium tetrafluoroborate		519		443.5 - 594.6	1.12
205	IM17 Cl	1-Heptyl-3-methylimidazolium chloride		392		272.1 - 511.7	0.89
206	IM17 PF6	1-Heptyl-3-methylimidazolium hexafluorophosphate		508		436.7 - 579.5	1.01
207	IM18 BF4	1-Methyl-3-octylimidazolium tetrafluoroborate	497.8[a]	519	-21		1.09
208	IM18 Br	1-Methyl-3-octylimidazolium bromide	392[a]	402	-10		0.88
209	IM18 (CF3SO2)2N	1-Methyl-3-octylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	692.7[a]	671	22		0.23
210	IM18 8OSO3	3-Methyl-1-octylimidazolium octylsulfate		748		699.1 - 796.7	0.53
211	IM18 CF3SO3	1-Methyl-3-octylimidazolium trifluormethanesulfonate		538		483.2 - 593.0	0.86
212	IM18 Cl	1-Methyl-3-octylimidazolium chloride		392		279.2 - 503.9	0.89
213	IM18 PF6	1-Methyl-3-octylimidazolium hexafluorophosphate	851[a,c]	508	343	445.0 - 570.6	0.97

214	IM17COOH Br	1-(7-Carboxyheptyl)-3-methylimidazolium bromide		141		-572.2	-	855.0	2.55*
215	IM19 BF4	1-Methyl-3-nonylimidazolium tetrafluoroborate		582		489.6	-	674.7	1.36
216	IM19 Cl	1-Methyl-3-nonylimidazolium chloride		455		307.3	-	602.7	1.15
217	IM19 PF6	1-Methyl-3-nonylimidazolium hexafluorophosphate		571		478.3	-	664.2	1.26
218	IM1-10 BF4	1-Decyl-3-methylimidazolium tetrafluoroborate		605		509.3	-	699.8	1.43
219	IM1-10 Br	1-Decyl-3-methylimidazolium bromide		488		337.4	-	638.3	1.20
220	IM1-10 Cl	1-Decyl-3-methylimidazolium chloride		477		323.1	-	631.6	1.23
221	IM1-10 PF6	1-Decyl-3-methylimidazolium hexafluorophosphate		594		496.6	-	690.6	1.34
222	IM1-10 (CF3SO2)2N	1-decyl-3-methylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	754[b]	757	-3				0.53
223	IM1-10 FeCl4	1-decyl-3-methylimidazolium tetrachloroferrate		565		411.8	-	717.6	0.90
224	IM1-10COO2 Br	1-(11-Ethoxy-11-oxoundecyl)-3-methylimidazolium bromide		380		-90.4	-	849.6	2.20*
225	IM1-12 Br	1-Dodecyl-3-methylimidazolium bromide		536		361.0	-	710.7	1.38
226	1201IMCL	1-dodecyl-3-methylimidazolium chloride		525		346.7	-	703.9	1.41
227	IM1-14 Cl	1-Methyl-3-tetradecylimidazolium chloride		607		383.3	-	831.6	1.76*
228	IM1-14 Br	1-Methyl-3-tetradecylimidazolium bromide		618		397.5	-	838.4	1.73*
229	IM1-16 Cl	1-Hexadecyl-3-methylimidazolium chloride		627		404.2	-	850.1	1.84*
230	IM1-16 Br	1-Hexadecyl-3-methylimidazolium bromide		638		418.4	-	856.9	1.82*
231	IM1-18 Cl	1-Methyl-3-octadecylimidazolium chloride		704		438.2	-	969.8	2.18*
232	IM18OH Br	1-(8-Hydroxyoctyl)-3-methylimidazolium bromide		321		-361.9	-	1003.6	2.19*
233	IM14OH Cl	1-(4-Hydroxybutyl)-3-methylimidazolium chloride		154		-495.2	-	804.1	1.99*
234	IM13OH Cl	1-(3-Hydroxypropyl)-3-methylimidazolium chloride		113		-549.9	-	776.8	2.09*
235	IM13OH (CF3SO2)2N	1-(3-Hydroxypropyl)-3-methylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide		393		-227.7	-	1013.6	2.31*
236	IM13O1 (CF3SO2)2N	1-(3-Methoxypropyl)-3-methylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide		485		210.9	-	759.2	1.09
237	IM13O1 Cl	1-(3-Methoxypropyl)-3-methylimidazolium chloride		205		-117.8	-	528.7	0.92
238	IM12OH I	1-(2-Hydroxyethyl)-3-methylimidazolium iodide		98		-622.0	-	817.8	2.34*
239	IM12OH (2-SO2PhCO)N	1-(2-Hydroxyethyl)-3-methylimidazolium. salt with 1.2-benzisothiazol-3(2H)-one 1.1-dioxide		342		-362.5	-	1046.3	2.70*
240	IM12OH (CF3SO2)2N	1-(2-Hydroxyethyl)-3-methylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide		346		-337.7	-	1029.9	2.57*
241	IM12OH AC	1-(2-Hydroxyethyl)-3-methylimidazolium 6-methyl-2.2-dioxo-1.2.3-oxathiazin-4(3H)-onate		327		-379.6	-	1033.5	2.79*
242	IM12OH BF4	1-(2-Hydroxyethyl)-3-methylimidazolium tetrafluoroborate		194		-540.6	-	928.1	3.03*
243	IM12OH PF6	1-(2-Hydroxyethyl)-3-methylimidazolium hexafluorophosphate		183		-544.9	-	910.4	2.89*
244	IM12OH Cl	1-(2-hydroxyethyl)-3-methylimidazolium chloride		67		-658.7	-	791.8	2.32*
245	IM12O1 (CF3SO2)2N	1-(2-Methoxyethyl)-3-methylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide		417		142.3	-	692.2	1.25
246	IM12O1 Cl	1-(2-Methoxyethyl)-3-methylimidazolium chloride		138		-179.3	-	454.8	0.88
247	IM12O1 BF4	1-(2-Methoxyethyl)-3-methylimidazolium tetrafluoroborate		265		-66.7	-	596.6	1.57

248	IM12O1 N(CN)2	1-(2-Methoxyethyl)-3-methylimidazolium dicyanamide	327	3.0	650.4	1.30
249	IM12O2 (CF3SO2)2N	1-(2-Ethoxyethyl)-3-methylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	484	241.8	725.7	1.00
250	IM12O2 Br	1-(2-Ethoxyethyl)-3-methylimidazolium bromide	215	-72.7	502.1	0.78
251	IM12O2 Cl	1-(2-Ethoxyethyl)-3-methylimidazolium chloride	204	-84.9	493.3	0.77
252	IM12O2O1 Cl	1-[2-(2-Methoxyethoxy)ethyl]-3-methylimidazolium chloride	194	-276.5	663.9	1.53
253	IM11O2 (CF3SO2)2N	1-(Ethoxymethyl)-3-methylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	478	254.3	701.8	1.15
254	IM11O2 Cl	1-(Ethoxymethyl)-3-methylimidazolium chloride	199	-75.0	472.0	0.98
255	Py1O(Cdd)-3CONH2 Cl	3-(Aminocarbonyl)-1-[(cyclododecyloxy)methyl]pyridinium chloride	204	-480.2	887.7	3.52*
256	Py1O-10-3CONH2 Cl	3-(Aminocarbonyl)-1-[(decyloxy)methyl]pyridinium chloride	243	-457.0	942.9	3.24*
257	Py1O-10-3CONH2 FeCl4	3-(Aminocarbonyl)-1-[(decyloxy)methyl]pyridinium (T-4)-tetrachloroferrate	330	-361.0	1021.6	3.00*
258	Py1O-11-3CONH2 Cl	3-(Aminocarbonyl)-1-[(undecyloxy)methyl]pyridinium chloride	282	-419.8	983.0	3.44*
259	Py1O-12-3CONH2 1COO	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium acetate	419	-393.3	1230.6	4.46*
260	Py1O-12-3CONH2 BF4	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium tetrafluoroborate	439	-336.8	1215.0	4.11*
261	Py1O-12-3CONH2 Br	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium bromide	322	-454.5	1099.3	3.58*
262	Py1O-12-3CONH2 Cl	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium chloride	312	-466.6	1090.4	3.57*
263	Py1O-12-3CONH2 ClO4	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium perchlorate	535	-242.1	1311.5	4.26*
264	Py1O-12-3CONH2 I	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium iodide	343	-428.8	1115.3	3.57*
265	Py1O-12-3CONH2 NO3	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium nitrate	336	-485.0	1156.1	3.54*
266	Py4-3CONHBu 8OSO3	1-Butyl-3-[(butylamino)carbonyl]pyridinium octyl sulfate	546	269.1	823.9	2.47*
267	Py4-3CONHBu I	1-Butyl-3-[(butylamino)carbonyl]pyridinium iodide	222	-104.8	547.9	2.23*
268	Py1O7-3CONH(MeO-MeO-Hp) Cl	3-[[[[(Heptyloxy)methoxy]methyl]amino]carbonyl]-1-[(heptyloxy)methyl]pyridinium chloride	368	-314.7	1051.1	4.52*
269	Py1O8-3CONH(MeO-MeO-Oc) Cl	3-[[[[(Octyloxy)methoxy]methyl]amino]carbonyl]-1-[(octyloxy)methyl]pyridinium chloride	352	-337.7	1042.2	5.21*
270	Py1O9-3CONH(MeO-MeO-No) Cl	3-[[[[(Nonyloxy)methoxy]methyl]amino]carbonyl]-1-[(nonyloxy)methyl]pyridinium chloride	311	-333.6	955.7	6.34*
271	Py1O-10-3CONH(MeO-MeO-De) Cl	3-[[[[(Decyloxy)methoxy]methyl]amino]carbonyl]-1-[(decyloxy)methyl]pyridinium chloride	417	-300.8	1134.0	6.12*
272	Py1-3COOBu (CF3SO2)2N	3-(Butoxycarbonyl)-1-methylpyridinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	424	145.0	702.3	2.16*
273	Py1-3COOBu 8OSO3	3-(Butoxycarbonyl)-1-methylpyridinium octyl sulfate	500	235.1	765.7	2.28*
274	Py1-3COOBu I	3-(Butoxycarbonyl)-1-methylpyridinium iodide	175	-143.2	494.2	1.97*
275	Py1-3COOBu PF6	3-(Butoxycarbonyl)-1-methylpyridinium hexafluorophosphate	260	-68.1	588.7	2.26*
276	Py4-3COOBu 8OSO3	3-(Butoxycarbonyl)-1-butylpyridinium octyl sulfate	596	352.7	839.4	2.13*
277	Py4-3COOBu I	3-(Butoxycarbonyl)-1-butylpyridinium iodide	271	-33.1	575.3	1.98*
278	Py4-3Me-4Me BF4	1-Butyl-3.4-dimethylpyridinium tetrafluoroborate	448	407.7	488.6	0.94
279	Py4-3Me-4Me Cl	1-Butyl-3.4-dimethylpyridinium chloride	321	217.3	424.7	1.01
280	Py4-3Me-5Me N(CN)2	1-Butyl-3.5-dimethylpyridinium N-cyanocyanamide	550	459.2	640.1	1.19
281	Py4-3Me-5Me Br	1-Butyl-3.5-dimethylpyridinium bromide	371	245.8	496.6	1.26
282	Py4-3Me-5Me BF4	1-Butyl-3.5-dimethylpyridinium tetrafluoroborate	488	431.5	544.2	1.23

283	Py4-3Me-5Me Cl	1-Butyl-3.5-dimethylpyridinium chloride		361		232.7	-	488.6	1.29
284	Py4-3Me-5Me (CF3SO2)2N	1-butyl-3.5-dimethil pyridinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide		640		512.8	-	767.6	1.09
285	Py8-3Me-5Me Br	1-octyl-3.5-dimethylpyridinium bromide		504		342.7	-	665.2	1.54
286	Py8-3Me-5Me (CF3SO2)2N	1-octyl-3.5-dimethylpyridinium bromide 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide		773		655.4	-	890.5	1.07
287	Py3-3Me Br	3-Methyl-1-propylpyridinium bromide		277		186.4	-	366.7	0.88
288	Py3-3Me PF6	3-Methyl-1-propylpyridinium hexafluorophosphate		382		326.9	-	437.7	0.72
289	Py4-3Me N(CN)2	1-Butyl-3-methylpyridinium N-cyanocyanamide		492		424.6	-	559.0	0.96
290	Py4-3Me Br	1-Butyl-3-methylpyridinium bromide		313		218.8	-	407.9	0.94
291	Py4-3Me 8OSO3	1-Butyl-3-methylpyridinium octyl sulfate		659		530.8	-	787.6	1.15
292	Py4-3Me BF4	1-Butyl-3-methylpyridinium tetrafluoroborate	388[a]	430	-42				0.91
293	Py4-3Me Cl	1-Butyl-3-methylpyridinium chloride		303		205.7	-	400.0	0.96
294	Py4-3Me PF6	1-Butyl-3-methylpyridinium hexafluorophosphate		419		376.1	-	462.0	0.84
295	Py6-3Me Br	1-Hexyl-3-methylpyridinium bromide	343[a]	390	-47				1.03
296	Py6-3Me Cl	1-Hexyl-3-methylpyridinium chloride		379		266.8	-	492.1	1.03
297	Py8-3Me Br	3-Methyl-1-octylpyridinium bromide		464		314.8	-	612.9	1.39
298	Py8-3Me Cl	3-Methyl-1-octylpyridinium chloride		453		300.7	-	605.9	1.41
299	Py1O3-3OH (2-SO2PhCO)N	3-Hydroxy-1-(propoxymethyl)pyridinium. salt with 1.2-benzisothiazol-3(2H)-one 1.1-dioxide		415		-165.5	-	995.2	2.30*
300	Py1O3-3OH AC	3-Hydroxy-1-(propoxymethyl)pyridinium 6-methyl-2.2-dioxo-1.2.3-oxathiazin-4(3H)-onate		400		-183.5	-	983.2	2.40*
301	Py1O3-3OH Cl	3-Hydroxy-1-(propoxymethyl)pyridinium chloride		139		-464.9	-	743.8	1.98*
302	Py1O4-3OH (2-SO2PhCO)N	1-(Butoxymethyl)-3-hydroxypyridinium. salt with 1.2-benzisothiazol-3(2H)-one 1.1-dioxide		450		-129.2	-	1028.7	2.25*
303	Py1O4-3OH AC	1-(Butoxymethyl)-3-hydroxypyridinium 6-methyl-2.2-dioxo-1.2.3-oxathiazin-4(3H)-onate		435		-147.1	-	1016.7	2.36*
304	Py1O6-3OH (2-SO2PhCO)N	1-[(Hexyloxy)methyl]-3-hydroxypyridinium. salt with 1.2-benzisothiazol-3(2H)-one 1.1-dioxide		521		-71.2	-	1112.3	2.24*
305	Py1O6-3OH AC	1-[(Hexyloxy)methyl]-3-hydroxypyridinium 6-methyl-2.2-dioxo-1.2.3-oxathiazin-4(3H)-onate		506		-88.9	-	1100.2	2.37*
306	Py1O7-3OH (2-SO2PhCO)N	1-[(Heptyloxy)methyl]-3-hydroxypyridinium. salt with 1.2-benzisothiazol-3(2H)-one 1.1-dioxide		529		-36.6	-	1093.7	2.15*
307	Py1O7-3OH AC	1-[(Heptyloxy)methyl]-3-hydroxypyridinium 6-methyl-2.2-dioxo-1.2.3-oxathiazin-4(3H)-onate		514		-54.3	-	1081.5	2.28*
308	Py1O7-3OH Cl	1-[(Heptyloxy)methyl]-3-hydroxypyridinium chloride		253		-342.2	-	848.6	1.98*
309	Py1O-11-3OH (2-SO2PhCO)N	3-Hydroxy-1-[(undecyloxy)methyl]pyridinium. salt with 1.2-benzisothiazol-3(2H)-one 1.1-dioxide		672		77.7	-	1265.7	2.21*
310	Py1O-11-3OH AC	3-Hydroxy-1-[(undecyloxy)methyl]pyridinium 6-methyl-2.2-dioxo-1.2.3-oxathiazin-4(3H)-onate		657		60.5	-	1253.0	2.38*
311	Py1O-11-3OH Cl	3-Hydroxy-1-[(undecyloxy)methyl]pyridinium chloride		396		-234.6	-	1027.3	2.23*
312	Py1O-18-3OH (2-SO2PhCO)N	3-Hydroxy-1-[(octadecyloxy)methyl]pyridinium. salt with 1.2-benzisothiazol-3(2H)-one 1.1-dioxide		852		188.4	-	1516.0	2.70*
313	Py1O-18-3OH AC	3-Hydroxy-1-[(octadecyloxy)methyl]pyridinium 6-methyl-2.2-dioxo-1.2.3-oxathiazin-4(3H)-onate		837		171.5	-	1503.0	2.88*
314	Pyr24 2OSO3	1-Butyl-1-ethylpyrrolidinium ethyl sulfate		511		348.9	-	672.4	1.83*
315	IMi022OH-2-(8=9) 2OSO3	1-ethyl-2-(8-heptadecenyl)-4.5-dihydro-3-(2-hydroxyethyl)imidazolium ethyl sulfate		716		1.4	-	1430.0	4.27*
316	IM22 (CF3SO2)2N	1.3-Diethylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide		518		440.0	-	596.4	0.77
317	IM22 Br	1.3-Diethylimidazolium bromide		249		196.1	-	302.3	0.60
318	IM23 (CF3SO2)2N	1-Ethyl-3-propylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide		540		462.5	-	617.6	0.70

319	IM23 Br	1-Ethyl-3-propylimidazolium bromide		271		210.6	-	331.4	0.62
320	IM24 BF4	1-Butyl-3-ethylimidazolium tetrafluoroborate		427		388.9	-	466.0	0.71
321	IM24 CF3COO	1-Butyl-3-ethylimidazolium trifluoroacetate		457		404.3	-	510.3	0.84
322	IM24 CF3SO3	1-Butyl-3-ethylimidazolium trifluoromethanesulfonate		447		418.6	-	475.0	0.49
323	IM26 BF4	1-Ethyl-3-hexylimidazolium tetrafluoroborate		520		459.7	-	579.6	1.14
324	IM26 Br	1-Ethyl-3-hexylimidazolium bromide		403		290.7	-	515.2	0.94
325	IM2-10 Br	1-Decyl-3-ethylimidazolium bromide		494		338.9	-	649.9	1.35
326	IM1-(1Ph) (CF3SO2)2N	1-benzyl-3-methylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide		536		405.8	-	666.1	1.12
327	IM4-(1Ph) (CF3SO2)2N	1-benzyl-3-butylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide		643		525.0	-	761.6	1.02
328	Py1O-10-4CONH2 Cl	4-(Aminocarbonyl)-1-[(decyloxy)methyl]pyridinium chloride		236		-520.1	-	992.9	3.35*
329	Py1O-11-4CONH2 Cl	4-(Aminocarbonyl)-1-[(undecyloxy)methyl]pyridinium chloride		264		-507.6	-	1035.1	3.49*
330	Py1O-12-4CONH2 Cl	4-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium chloride		289		-484.2	-	1062.1	3.58*
331	Py4-4Me BF4	1-Butyl-4-methylpyridinium tetrafluoroborate	414[a]	409	5				0.98
332	Py4-4Me (C2F5)3PF3	1-Butyl-4-methylpyridinium trifluorotris(pentafluoroethyl)phosphate		676		538.5	-	813.0	1.04
333	Py4-4Me B(CN)4	1-Butyl-4-methylpyridinium tetracyanoborate		458		325.3	-	589.9	2.97*
334	Py4-4Me Cl	1-Butyl-4-methylpyridinium chloride		282		183.9	-	379.8	1.04
335	Py4-4Me PF6	1-Butyl-4-methylpyridinium hexafluorophosphate		398		347.4	-	448.7	0.92
336	Py4-4Me C(CN)3	1-butyl-4-methylpyridinium tricyanomethanide		409		247.8	-	570.6	3.31*
337	Py6-4Me BF4	1-Hexyl-4-methylpyridinium tetrafluoroborate		511		444.4	-	577.3	1.45
338	Py6-4Me Cl	1-Hexyl-4-methylpyridinium chloride		384		250.3	-	516.9	1.36
339	Py8-4Me BF4	4-Methyl-1-octylpyridinium tetrafluoroborate		564		490.9	-	637.6	1.47
340	Py8-4Me Cl	4-Methyl-1-octylpyridinium chloride		437		292.8	-	581.3	1.34
341	Py1-4NMe2 I	4-(Dimethylamino)-1-methylpyridinium iodide		169		16.1	-	322.2	1.49
342	Py2-4NMe2 (CF3SO2)2N	4-(Dimethylamino)-1-ethylpyridinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide		441		257.4	-	624.3	1.60*
343	Py2-4NMe2 Br	4-(Dimethylamino)-1-ethylpyridinium bromide		172		37.7	-	306.0	1.32
344	Py4-4NMe2 (CF3SO2)2N	1-Butyl-4-(dimethylamino)pyridinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide		531		387.2	-	674.8	1.32
345	Py4-4NMe2 Br	1-Butyl-4-(dimethylamino)pyridinium bromide		262		145.4	-	378.5	1.22
346	Py4-4NMe2 Cl	1-Butyl-4-(dimethylamino)pyridinium chloride		251		133.5	-	369.4	1.23
347	Py6-4NMe2 (CF3SO2)2N	4-(Dimethylamino)-1-hexylpyridinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	628[a]	619	9				1.58
348	Py6-4NMe2 Cl	4-(Dimethylamino)-1-hexylpyridinium chloride		340		187.7	-	492.1	1.64*
349	IM33 (CF3SO2)2N	1.3-Dipropylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide		587		534.3	-	638.9	0.50
350	IM44 (CF3SO2)2N	1.3-Dibutylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide		634		569.0	-	698.4	0.43
351	IM42OH Cl	1-butyl-3-(2-hydroxyethyl)imidazolium chloride		140		-496.9	-	777.6	1.96*
352	Quin1O6-6Me Cl	1-[(Hexyloxy)methyl]-6-methylquinolinium chloride		353		116.0	-	590.3	1.33
353	Quin1O8-6Me Cl	6-Methyl-1-[(octyloxy)methyl]quinolinium chloride		443		151.1	-	734.8	1.58*

354	Quin1O-10-6Me Cl	1-[(Decyloxy)methyl]-6-methylquinolinium chloride	492	215.4	-	767.7	1.76*
355	Quin1O-12-6Me Cl	1-[(Dodecyloxy)methyl]-6-methylquinolinium chloride	547	253.5	-	841.5	2.01*
356	Quin1O6-8OH Cl	1-[(Hexyloxy)methyl]-8-hydroxyquinolinium chloride	277	-150.4	-	703.7	1.81*
357	Quin1O8-8OH Cl	8-Hydroxy-1-[(octyloxy)methyl]quinolinium chloride	373	-97.2	-	842.6	1.86*
358	Quin1O-10-8OH Cl	1-[(Decyloxy)methyl]-8-hydroxyquinolinium chloride	437	-52.5	-	926.8	2.00*
359	Quin1O-12-8OH Cl	1-[(Dodecyloxy)methyl]-8-hydroxyquinolinium chloride	499	-32.4	-	1030.7	2.30*
360	Quin4 BF4	1-Butylquinolinium tetrafluoroborate	443	316.2	-	570.5	1.91*
361	Quin4 Br	1-Butylquinolinium bromide	327	147.5	-	505.9	1.98*
362	Quin6 BF4	1-Hexylquinolinium tetrafluoroborate	525	393.2	-	656.0	2.18*
363	Quin8 BF4	1-Octylquinolinium tetrafluoroborate	580	433.6	-	726.6	2.39*
364	Quin8 Br	1-Octylquinolinium bromide	463	249.3	-	677.5	2.36*
365	Quin1O6 Cl	1-[(Hexyloxy)methyl]quinolinium chloride	345	108.5	-	581.5	1.31
366	Quin1O8 Cl	1-[(Octyloxy)methyl]quinolinium chloride	421	200.1	-	641.0	1.32
367	Quin1O-10 Cl	1-[(Decyloxy)methyl]quinolinium chloride	489	201.6	-	776.3	1.70*
368	Quin1O-12 Cl	1-[(Dodecyloxy)methyl]quinolinium chloride	520	206.5	-	832.5	1.91*
369	IM55 (CF3SO2)2N	1.3-Dipentylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	713	652.1	-	773.7	0.36
370	Py1(COO1)(Ph-3-OMe-4-OMe) Cl	1-[1-(3.4-Dimethoxyphenyl)-2-methoxy-2-oxoethyl]pyridinium chloride	89	-302.1	-	480.5	3.36*
371	Py1(COO1)(Ph-(3.4-OCH2O-)) Br	1-[1-(1.3-Benzodioxol-5-yl)-2-methoxy-2-oxoethyl]pyridinium bromide	75	-397.7	-	547.5	3.46*
372	Py1(COO4)(Ph-(3.4-OCH2O-)) Br	1-[1-(1.3-Benzodioxol-5-yl)-2-butoxy-2-oxoethyl]pyridinium bromide	156	-259.4	-	572.0	3.60*
373	Py2 Cl	1-Ethylpyridinium chloride	182	115.0	-	249.4	0.74
374	Py1CN (CF3SO2)2N	1-(Cyanomethyl)pyridinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	278	8.1	-	548.4	2.71*
375	Py1CN Cl	1-(Cyanomethyl)pyridinium chloride	-1	-278.8	-	276.2	2.34*
376	Py1COO1(COO1)(Ph-(3.4-OCH2O-)) Br	1-[2-[1-(1.3-Benzodioxol-5-yl)-2-methoxy-2-oxoethoxy]-2-oxoethyl]pyridinium bromide	-8	-586.9	-	571.5	6.12*
377	Py1COO1(COO4)(Ph-(3.4-OCH2O-)) Br	1-[2-[1-(1.3-Benzodioxol-5-yl)-2-butoxy-2-oxoethoxy]-2-oxoethyl]pyridinium bromide	100	-462.8	-	662.1	6.11*
378	Py1COO2 (CF3SO2)2N	1-(2-Ethoxy-2-oxoethyl)pyridinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	389	61.3	-	717.0	2.43*
379	Py1COO2 8OSO3	1-(2-Ethoxy-2-oxoethyl)pyridinium octyl sulfate	466	153.2	-	778.6	2.55*
380	Py1COO2 Br	1-(2-Ethoxy-2-oxoethyl)pyridinium bromide	120	-252.3	-	492.5	2.23*
381	Py1COO2 PF6	1-(2-Ethoxy-2-oxoethyl)pyridinium hexafluorophosphate	226	-156.2	-	607.7	2.54*
382	Py3 (CF3SO2)2N	1-Propylpyridinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	528	429.0	-	626.5	1.04
383	Py3 Br	1-Propylpyridinium bromide	259	181.7	-	335.8	0.93
384	Py4 Cl	1-Butylpyridinium chloride	265	193.1	-	336.0	0.76
385	Py4 Al2Cl7	1-Butylpyridinium µ-chlorohexachlorodialuminate	439	336.0	-	543.0	1.31
386	Py4 N(CN)2	1-Butylpyridinium N-cyanocyanamide	453	403.0	-	504.0	0.85
387	Py4 Br	1-Butylpyridinium bromide	275	206.4	-	343.6	0.73
388	Py4 1OSO3	1-Butylpyridinium methyl sulfate	409	373.5	-	444.8	0.45
389	Py4 8OSO3	1-Butylpyridinium octyl sulfate	621	512.7	-	729.0	1.11

390	Py4 BF4	1-Butylpyridinium tetrafluoroborate	383[a]	392	-9		-		0.74
391	Py4 CF3SO3	1-Butylpyridinium trifluoromethanesulfonate		411		372.3	-	449.8	0.56
392	Py4 PF6	1-Butylpyridinium hexafluorophosphate		381		350.6	-	410.8	0.66
393	Py5 (CF3SO2)2N	1-Pentylpyridinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide		589		522.8	-	654.8	0.70
394	Py5 Br	1-Pentylpyridinium bromide		320		238.1	-	401.5	0.81
395	Py6 (CF3SO2)2N	1-Hexylpyridinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	612[a]	604	8				0.64
396	Py6 CF3SO3	1-Hexylpyridinium trifluoromethanesulfonate		471		444.4	-	497.1	0.74
397	Py6 Cl	1-Hexylpyridinium chloride		324		233.4	-	415.0	0.83
398	Py6 PF6	1-Hexylpyridinium hexafluorophosphate		440		412.4	-	468.5	0.84
399	Py8 Cl	1-Octylpyridinium chloride		416		276.6	-	555.1	1.19
400	Py8 (CF3SO2)2N	1-Octylpyridinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	629[b]	695	-66				0.77
401	Py-10 Br	1-Decylpyridinium bromide		479		322.4	-	636.2	1.31
402	Py-16 Br	1-Hexadecylpyridinium bromide		659		415.2	-	903.3	2.11*
403	Py-16 Cl	1-Hexadecylpyridinium chloride		649		401.1	-	896.4	2.13*
404	Py3OH (CF3SO2)2N	1-(3-Hydroxypropyl)pyridinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide		342		-303.3	-	986.7	2.49*
405	Py3OH Cl	1-(3-Hydroxypropyl)pyridinium chloride		62		-623.7	-	748.0	2.21*
406	Py3O1 (CF3SO2)2N	1-(3-Methoxypropyl)pyridinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide		474		215.1	-	733.4	1.19
407	Py3O1 Cl	1-(3-Methoxypropyl)pyridinium chloride		195		-107.4	-	496.7	0.96
408	Py3SO3H CF3SO3	1-(3-Sulfopropyl)pyridinium trifluoromethanesulfonate		83		-963.7	-	1130.0	4.28*
409	Py2OH (CF3SO2)2N	1-(2-Hydroxyethyl)pyridinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide		327		-373.0	-	1026.3	2.75*
410	Py2OH I	1-(2-Hydroxyethyl)pyridinium iodide		79		-656.0	-	813.0	2.51*
411	Py2O1 (CF3SO2)2N	1-(2-Methoxyethyl)pyridinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide		400		149.3	-	650.3	1.27
412	Py2O1 Cl	1-(2-Methoxyethyl)pyridinium chloride		120		-168.4	-	409.0	0.83
413	Py2O2 (CF3SO2)2N	1-(2-Ethoxyethyl)pyridinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide		451		217.3	-	684.7	1.13
414	Py2O2 Br	1-(2-Ethoxyethyl)pyridinium bromide		182		-92.1	-	456.1	0.82
415	Py1O2 (CF3SO2)2N	1-(Ethoxymethyl)pyridinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide		457		227.8	-	686.6	1.15
416	Py1O2 Cl	1-(Ethoxymethyl)pyridinium chloride		178		-98.7	-	454.1	0.90
417	Pyr66 BF4	1.1-Dihexylpyrrolidinium tetrafluoroborate		633		449.9	-	816.6	2.11*
418	IM66 (CF3SO2)2N	1.3-Dihexylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide		771		681.9	-	861.0	0.65
419	IM-10-10-2Me (CF3SO2)2N	1.3-Didecyl-2-methylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide		984		810.8	-	1157.9	1.45
420	Pyr-12-2OH Cl	1-Dodecyl-1-(2-hydroxyethyl)pyrrolidinium chloride		440		-266.3	-	1145.9	2.61*
421	IM-14-2OH-2Me Cl	1-(2-Hydroxyethyl)-2-methyl-3-tetradecylimidazolium chloride		493		-150.0	-	1137.0	2.45*
422	IM-16-2OH-2Me Cl	1-Hexadecyl-3-(2-hydroxyethyl)-2-methylimidazolium chloride		557		-119.0	-	1232.7	2.78*
423	IM2OH-(2Ph) Cl	1-(2-hydroxyethyl)-3-(2-phenylethyl)imidazolium chloride		249		-424.5	-	923.0	2.49*
424	IM2OH-(2OH) Cl	1.3-di-(2-hydroxyethyl)imidazolium chloride		48		-1181.4	-	1277.4	4.36*
425	IM1O3-1O3 Cl	1.3-Bis(propoxymethyl)imidazolium chloride		274		-132.4	-	681.2	1.76*

426	IM1O4-1O4 Cl	1.3-Bis(butoxymethyl)imidazolium chloride	323	-35.8	681.6	2.03*
427	IM1O5-1O5 Cl	1.3-Bis[(pentyloxy)methyl]imidazolium chloride	374	-13.8	761.3	2.12*
428	IM1O6-1O6 Cl	1.3-Bis[(hexyloxy)methyl]imidazolium chloride	416	21.2	811.0	2.40*
429	IM1O7-1O7 Cl	1.3-Bis[(heptyloxy)methyl]imidazolium chloride	489	92.4	885.7	2.49*
430	IM1O8-1O8 Cl	1.3-Bis[(octyloxy)methyl]imidazolium chloride	529	117.9	940.6	2.75*
431	IM1O9-1O9 Cl	1.3-Bis[(nonyloxy)methyl]imidazolium chloride	586	169.9	1001.6	2.90*
432	IM1O-10-1O-10 Cl	1.3-Bis[(decyloxy)methyl]imidazolium chloride	632	230.9	1033.0	2.97*
433	IM1O-11-1O-11 Cl	1.3-Bis[(undecyloxy)methyl]imidazolium chloride	670	240.5	1099.4	3.38*
434	IM1O-12-1O-12 Cl	1.3-Bis[(dodecyloxy)methyl]imidazolium chloride	704	252.2	1155.0	3.57*
435	IM1O-14-1O-14 Cl	1.3-Bis[(tetradecyloxy)methyl]imidazolium chloride	820	301.8	1337.3	4.09*
436	IM1O-16-1O-16 Cl	1.3-Bis[(hexadecyloxy)methyl]imidazolium chloride	884	317.6	1449.5	4.09*
437	IM01 BF4	1-Methylimidazolium hydrogen tetrafluoroborate	165	-22.1	352.3	3.09*
438	IM01 HO1(1)COO	1-Methylimidazolium 2-hydroxypropanoate	211	-18.5	439.5	3.40*
439	IM01 HO1(1)COO-S	1-Methylimidazolium (2S)-2-hydroxypropanoate	216	-19.3	452.3	3.47*
440	IM01 1COO	1-methylimidazolium acetate	145	-76.4	365.7	3.41*
441	IM01 CF3COO	1-methylimidazolium trifluoroacetate	195	-14.6	404.4	3.16*
442	IM01 CF3SO3	1-methylimidazolium 1.1.1-trifluoromethanesulfonate	184	12.6	356.4	3.06*
443	IM02 HO1(1)COO	1-Ethylimidazolium 2-hydroxypropanoate	243	30.9	455.6	3.28*
444	IM02 HO1(1)COO-S	1-Ethylimidazolium (2S)-2-hydroxypropanoate	249	30.0	468.4	3.36*
445	IM03 HO1(1)COO	1-Propylimidazolium 2-hydroxypropanoate	293	81.8	504.0	3.18*
446	IM03 HO1(1)COO-S	1-Propylimidazolium (2S)-2-hydroxypropanoate	299	81.4	516.3	3.26*
447	IM04 HO1(1)COO	1-Butylimidazolium 2-hydroxypropanoate	340	121.6	559.0	3.21*
448	IM04 HO1(1)COO-S	1-Butylimidazolium (2S)-2-hydroxypropanoate	346	121.5	570.9	3.28*
449	IM04 1COO	1-butylimidazolium acetate	274	57.2	491.6	3.23*
450	IM04 CF3COO	1-butylimidazolium trifluoroacetate	325	124.0	525.4	2.95*
451	IM04 CF3SO3	1-butylimidazolium 1.1.1-trifluoromethanesulfonate	314	146.5	482.0	2.82*
452	IM05 HO1(1)COO	1-Pentylimidazolium 2-hydroxypropanoate	386	163.9	607.9	3.21*
453	IM05 HO1(1)COO-S	1-Pentylimidazolium (2S)-2-hydroxypropanoate	392	164.3	619.5	3.28*
454	IM06 HO1(1)COO	1-Hexylimidazolium 2-hydroxypropanoate	403	179.0	627.0	3.29*
455	IM06 HO1(1)COO-S	1-Hexylimidazolium (2S)-2-hydroxypropanoate	409	179.5	638.5	3.36*
456	IM07 HO1(1)COO	1-Heptylimidazolium 2-hydroxypropanoate	450	212.2	688.1	3.30*
457	IM07 HO1(1)COO-S	1-Heptylimidazolium (2S)-2-hydroxypropanoate	456	213.3	698.9	3.38*
458	IM08 HO1(1)COO	1-Octylimidazolium 2-hydroxypropanoate	478	229.8	726.2	3.39*
459	IM08 HO1(1)COO-S	1-Octylimidazolium (2S)-2-hydroxypropanoate	484	231.1	736.8	3.47*
460	IM09 HO1(1)COO	1-Nonylimidazolium 2-hydroxypropanoate	514	260.7	767.5	3.40*
461	IM09 HO1(1)COO-S	1-Nonylimidazolium (2S)-2-hydroxypropanoate	520	262.3	777.8	3.47*
462	IM0-10 HO1(1)COO	1-Decylimidazolium 2-hydroxypropanoate	554	294.1	813.1	3.43*

463	IM0-10 HO1(1)COO-S	1-Decylimidazolium (2S)-2-hydroxypropanoate		560		296.1	-	823.1	3.50*
464	IM0-11 HO1(1)COO	1-Undecylimidazolium 2-hydroxypropanoate		567		302.5	-	832.2	3.50*
465	IM0-11 HO1(1)COO-S	1-Undecylimidazolium (2S)-2-hydroxypropanoate		573		304.7	-	842.0	3.58*
466	IM0-12 HO1(1)COO	1-Dodecylimidazolium 2-hydroxypropanoate		586		333.7	-	838.9	3.54*
467	IM0-12 HO1(1)COO-S	1-Dodecylimidazolium (2S)-2-hydroxypropanoate		592		336.0	-	848.6	3.61*
468	IM01O4 HO1(1)COO	1-(Butoxymethyl)imidazolium 2-hydroxypropanoate		377		-28.7	-	782.1	3.66*
469	IM01O4 HO1(1)COO-S	1-(Butoxymethyl)imidazolium (2S)-2-hydroxypropanoate		383		-27.7	-	793.0	3.74*
470	IM01O5 HO1(1)COO	1-[(Pentyloxy)methyl]imidazolium 2-hydroxypropanoate		393		-3.0	-	788.6	3.67*
471	IM01O5 HO1(1)COO-S	1-[(Pentyloxy)methyl]imidazolium (2S)-2-hydroxypropanoate		399		-1.9	-	799.4	3.75*
472	IM01O6 HO1(1)COO	1-[(Hexyloxy)methyl]imidazolium 2-hydroxypropanoate		411		-12.0	-	834.0	3.83*
473	IM01O6 HO1(1)COO-S	1-[(Hexyloxy)methyl]imidazolium (2S)-2-hydroxypropanoate		417		-10.7	-	844.6	3.91*
474	IM01O7 HO1(1)COO	1-[(Heptyloxy)methyl]imidazolium 2-hydroxypropanoate		453		51.1	-	855.9	3.80*
475	IM01O7 HO1(1)COO-S	1-[(Heptyloxy)methyl]imidazolium (2S)-2-hydroxypropanoate		459		52.5	-	866.4	3.88*
476	IM01O8 HO1(1)COO	1-[(Octyloxy)methyl]imidazolium 2-hydroxypropanoate		484		56.1	-	912.1	3.84*
477	IM01O8 HO1(1)COO-S	1-[(Octyloxy)methyl]imidazolium (2S)-2-hydroxypropanoate		490		57.8	-	922.4	3.92*
478	IM01O9 HO1(1)COO	1-[(Nonyloxy)methyl]imidazolium 2-hydroxypropanoate		516		103.2	-	929.5	3.82*
479	IM01O9 HO1(1)COO-S	1-[(Nonyloxy)methyl]imidazolium (2S)-2-hydroxypropanoate		522		105.1	-	939.5	3.90*
480	IM01O-10 HO1(1)COO	1-[(Decyloxy)methyl]imidazolium 2-hydroxypropanoate		533		132.0	-	933.2	3.90*
481	IM01O-10 HO1(1)COO-S	1-[(Decyloxy)methyl]imidazolium (2S)-2-hydroxypropanoate		539		133.9	-	943.2	3.98*
482	IM01O-11 HO1(1)COO	1-[(Undecyloxy)methyl]imidazolium 2-hydroxypropanoate		567		149.7	-	983.5	3.96*
483	IM01O-11 HO1(1)COO-S	1-[(Undecyloxy)methyl]imidazolium (2S)-2-hydroxypropanoate		573		151.9	-	993.2	4.04*
484	IM01O-12 HO1(1)COO	1-[(Dodecyloxy)methyl]imidazolium 2-hydroxypropanoate		602		148.4	-	1055.7	4.09*
485	IM01O-12 HO1(1)COO-S	1-[(Dodecyloxy)methyl]imidazolium (2S)-2-hydroxypropanoate		608		150.8	-	1065.3	4.17*
486	Py0 Cl	pyridinium hydrochloride		82		-111.4	-	275.5	3.14*
487	0600NN (CF3SO2)2N	1-hexyl-1.4-diaza[2.2.2]bicyclooctanium bis(trifluoromethylsulfonyl)imide		470		178.7	-	762.0	2.23*
488	IM00 1COO	1H-Imidazol-1-ium acetate		109		-245.4	-	463.9	3.53*
489	IM00 CF3COO	1H-Imidazol-1-ium trifluoroacetate		160		-179.9	-	499.1	3.30*
490	IM00 CFSO3	1H-Imidazol-1-ium 1.1.1-trifluoromethanesulfonate		149		-155.4	-	453.6	3.15*
491	IM01-2Me (CF3SO2)2N	1.2-dimethylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide		319		198.8	-	438.2	2.99*
492	IM16-2Me Cl	1-hexyl-2.3-dimethyl imidazolium chloride		338		224.1	-	452.3	1.13
493	IM13-2Me (CF3SO2)2N	1.2-dimethyl-3-propylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	555[a]	512	43				0.91
494	IM18 N(CN)2	1-Methyl-3-octylimidazolium dicyanamide		581		522.4	-	638.7	0.68
495	Py4-3Me (CF3SO2)2N	1-buthyl-3-methylpyridinium1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	548[b]	582	-34				0.91
496	IM18 SbF6	1-methyl-3-octylimidazolium hexafluoroantimonate		517		454.0	-	579.7	1.00
497	IM11 (1O)2PO2	1.3-dimethyl imidazolium dimethyl phopsphate		348		260.4	-	435.1	0.57
498	IM18 CF3COO	1-methyl-3-octylimidazolium trifluoroacetate	544[b]	549	-5				1.21

499	IM12OH 1COO	1-(2-hydroxyethyl)-3-methylimidazolium acetate		173		-599.5	-	946.0	3.47*
500	IM12OH N(CN2)	1-(2-hydroxyethyl)-3-methylimidazolium dicyanamide	231.8[b]	256	-24				2.69*
501	IM12OH NO3	1-(2-hydroxyethyl)-3-methylimidazolium nitrate		90		-680.0	-	860.4	2.41*
502	Py6-4NMe2 Br	4-(Dimethylamino)-1-hexylpyridinium bromide		350		200.5	-	500.4	1.62*
503	Py8-4Me (CF3SO2)2N	1-octyl-4-methylpyridinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide		717		623.0	-	810.1	0.91
504	Py4 (CF3SO2)2N	1-butylpyridinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide		544		459.3	-	628.8	0.80
505	Pip12OH N(CN)2	1-(2-hydroxyethyl)-1-methylpiperidinium N-cyanocyanamide		336		-443.8	-	1116.0	2.85*
506	Pyr18 (CF3SO2)2N	1-methyl-1-octylpyrrolidinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	642[b]	720	-78				1.53
507	Mor14 N(CN)2	4-butyl-4-methylmorpholinium dicyanamide		412		23.8	-	799.4	2.05*
508	Mor12OH N(CN)2	4-(2-hydroxyethyl)-4-methylmorpholinium dicyanamide		238		-644.5	-	1120.8	3.45*
509	Mor12 N(CN)2	1-ethyl-1-methylmorpholinium dicyanamide		346		-45.4	-	738.2	2.27*
510	Mor12 (CF3SO2)2N	1-ethyl-1-methylmorpholinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide		437		98.3	-	775.5	2.20*
511	IM14 1COO	1-butyl-3-methylimidazolium acetate	383.2[a]	392	-9				1.64*
512	IM16 1COO	1-hexyl-3-methylimidazolium acetate		420		375.6	-	465.1	1.62*
513	IM16 CF3COO	1-hexyl-3-methylimidazolium trifluoroacetate		471		429.0	-	512.2	0.90
514	Pyr14 1COO	1-butyl-1-methylpyrroldinium acetate		436		239.3	-	632.0	2.50*
515	IM18 NO3	1-methyl-3-octylimidazolium nitrate		415		280.6	-	549.9	1.43
516	IM14 (CF3SO2)3C	1-butyl-3-methylimidazolium tris[(trifluoromethyl)sulfonyl]methide	783[a]	593	190				0.50
517	IM1-18 (CF3SO2)2N	1-methyl-3-octadecylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1052[a]	984	68				1.49
518	Py4-3Me (CF3SO2)2N	1-butyl-3-methylpyridinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	622[a]	582	40				0.91
519	Py6-3Me (CF3SO2)2N	1-hexyl-3-methylpyridinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	624[a]	659	-35				0.69
520	Pyr13 (CF3SO2)2N	1-methyl-1-propylpyrrolidinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	554[a]	580	-26				1.81*

[a]Ref. 127; [b]Ref. 126; [c]Y_predictions according to the C_p PLS models. Note: ILs numeration as in the other PLS datamatrices.

Table B17 Experimental and predicted viscosity values. Predictions are calculated using the correlation models derived by using 4 PPs as descriptors.

IL	IL Code	Systematic name	PP+1	PP+5	PP-2	PP-3	logη (283.15 K) (mPa*s)[a]	pred. logη (283.15 K) (mPa*s)	logη (293.15 K) (mPa*s)[a]	pred. logη (293.15 K) (mPa*s)	logη (298.15 K) (mPa*s)[a]	pred. logη (298.15 K) (mPa*s)
12	Pyr14 (CF3SO2)2N	1-Butyl-1-methylpyrrolidinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.96	-0.03	-2.15	2.86			1.99	1.86	1.89	1.80
38	Pip14 (CF3SO2)2N	1-Butyl-1-methylpiperidinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.15	-0.09	-2.15	2.86					2.26	1.85
46	Pip12O1 (CF3SO2)2N	1-(2-Methoxyethyl)-1-methylpiperidinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	5.73	0.34	-2.15	2.86					2.01	1.57
81	IM11 (CF3SO2)2N	1.3-Dimethylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	4.18	-1.80	-2.15	2.86	1.89	1.63	1.64	1.39		
82	IM11 1OSO3	1.3-dimethylimidazolium methylsulfate	4.18	-1.80	-1.16	-0.44			1.97	2.00	1.86	1.83
91	IM12 N(CN)2	1-Ethyl-3-methylimidazolium N-cyanocyanamide	3.24	-1.60	0.49	0.00	1.53	1.73	1.36	1.49	1.21	1.40
92	IM12 (CF3SO2)2N	1-Ethyl-3-methylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3.24	-1.60	-2.15	2.86	1.79	1.72	1.53	1.48		
93	IM12 Cl	1-Ethyl-3-methylimidazolium chloride	3.24	-1.60	-5.73	-2.31						
94	IM12 2OSO3	1-Ethyl-3-methylimidazolium ethyl sulfate	3.24	-1.60	-1.47	-0.18	2.35	2.42	2.10	2.11	1.92	1.95
98	IM12 1OSO3	1-Ethyl-3-methylimidazolium methylsulfate	3.24	-1.60	-1.16	-0.44			2.00	2.09	1.80	1.92
102	IM12 BF4	1-Ethyl-3-methylimidazolium tetrafluoroborate	3.24	-1.60	-0.06	-0.33	2.04	2.00	1.66	1.74	1.57	1.61
104	IM12 CF3SO3	1-Ethyl-3-methylimidazolium trifluoromethanesulfonate	3.24	-1.60	-0.86	0.07	1.86	2.14	1.70	1.86	1.61	1.74
109	IM12 NO3	1-Ethyl-3-methylimidazolium nitrate	3.24	-1.60	-0.46	-2.37						
147	IM13 BF4	1-Methyl-3-propylimidazolium tetrafluoroborate	1.85	-0.80	-0.06	-0.33					2.01	1.80
149	IM13 PF6	1-Methyl-3-propylimidazolium hexafluorophosphate	1.85	-0.80	-1.14	-0.21					2.49	2.06
152	IM13 I	1-Methyl-3-propylimidazolium iodide	1.85	-0.80	-5.31	-1.63					2.84	3.42
161	IM14 CF3SO3	1-Butyl-3-methylimidazolium trifluoromethanesulfonate	0.58	-0.39	-0.86	0.07	2.12	2.57	2.00	2.24	1.87	2.07
163	IM14 BF4	1-Butyl-3-methylimidazolium tetrafluoroborate	0.58	-0.39	-0.06	-0.33			2.05	2.12	1.88	1.94
164	IM14 (CF3SO2)2N	1-Butyl-3-methylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	0.58	-0.39	-2.15	2.86	1.92	2.15	1.72	1.86	1.74	1.86
165	IM14 PF6	1-Butyl-3-methylimidazolium hexafluorophosphate	0.58	-0.39	-1.14	-0.21	2.41	2.74	2.30	2.40	2.28	2.20
166	IM14 Cl	1-Butyl-3-methylimidazolium chloride	0.58	-0.39	-5.73	-2.31	5.15	4.85	4.61	4.31		
167	IM14 I	1-Butyl-3-methylimidazolium iodide	0.58	-0.39	-5.31	-1.63						
169	IM14 N(CN)2	1-Butyl-3-methylimidazolium N-cyanocyanamide	0.58	-0.39	0.49	0.00					1.57	1.74
175	IM14 1OSO3	1-Butyl-3-methylimidazolium methyl sulfate	0.58	-0.39	-1.16	-0.44			2.46	2.47	2.22	2.25
180	IM14 NO3	1-Butyl-3-methylimidazolium nitrate	0.58	-0.39	-0.46	-2.37	2.65	3.17	2.35	2.79	2.22	2.45
181	IM14 SbF6	1-Butyl-3-methylimidazolium (OC-6-11)-hexafluoroantimonate	0.58	-0.39	-0.70	-0.12	2.25	2.57	2.10	2.25	2.03	2.07

191	IM16 (CF3SO2)2N	1-Hexyl-3-methylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	-1.54	-0.75	-2.15	2.86	2.19	2.15	1.91	1.89	1.83	1.97
193	IM16 Cl	1-Hexyl-3-methylimidazolium chloride	-1.54	-0.75	-5.73	-2.31	4.80	4.86	4.26	4.34	4.26	3.92
194	IM16 PF6	1-Hexyl-3-methylimidazolium hexafluorophosphate	-1.54	-0.75	-1.14	-0.21	3.16	2.75	2.83	2.44	2.68	2.31
196	IM16 BF4	1-Hexyl-3-methylimidazolium tetrafluoroborate	-1.54	-0.75	-0.06	-0.33	2.79	2.44	2.37	2.15	2.24	2.05
207	IM18 BF4	1-Methyl-3-octylimidazolium tetrafluoroborate	-3.07	0.28	-0.06	-0.33	2.99	2.76	2.48	2.44	2.35	2.28
209	IM18 (CF3SO2)2N	1-Methyl-3-octylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	-3.07	0.28	-2.15	2.86	2.34	2.48	2.08	2.18		
212	IM18 Cl	1-Methyl-3-octylimidazolium chloride	-3.07	0.28	-5.73	-2.31	5.07	5.18	4.52	4.63	4.32	4.15
213	IM18 PF6	1-Methyl-3-octylimidazolium hexafluorophosphate	-3.07	0.28	-1.14	-0.21	3.27	3.08	3.00	2.72	2.86	2.54
222	IM1-10 (CF3SO2)2N	1-decyl-3-methylimidazolium bis(trifluoromethylsulphonyl)imide	-5.83	1.33	-2.15	2.86					2.03	2.52
242	IM12OH BF4	1-(2-Hydroxyethyl)-3-methylimidazolium tetrafluoroborate	9.73	2.49	-0.06	-0.33			1.96	2.23		
245	IM12O1 (CF3SO2)2N	1-(2-Methoxyethyl)-3-methylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	6.12	-0.03	-2.15	2.86			1.73	1.65		
247	IM12O1 BF4	1-(2-Methoxyethyl)-3-methylimidazolium tetrafluoroborate	6.12	-0.03	-0.06	-0.33	2.57	2.26	2.42	1.91		
292	PY4-3Me BF4	1-Butyl-3-methylpyridinium tetrafluoroborate	-1.02	-0.45	-0.06	-0.33						
321	IM24 CF3COO	1-Butyl-3-ethylimidazolium trifluoroacetate	-0.12	-0.48	2.08	-2.30			1.95	2.05		
322	IM24 CF3SO3	1-Butyl-3-ethylimidazolium trifluoromethanesulfonate	-0.12	-0.48	-0.86	0.07					1.95	2.11
390	Py4 BF4	1-Butylpyridinium tetrafluoroborate	0.96	-0.52	-0.06	-0.33	2.67	2.38	2.35	2.07	2.21	1.90
495	PY4-3Me (CF3SO2)2N	1-buthyl-3-methylpyridinium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	-1.02	-0.45	-2.15	2.86			1.80	1.93	1.71	1.97
511	IM14 1COO	1-butyl-3-methylimidazolium acetate	0.58	-0.39	2.41	-5.87					2.15	2.39
531	IM12O1 PF6	1-(2-Methoxyethyl)-3-methylimidazolium hexaphluorophosphate	6.12	-0.03	-1.14	-0.21	2.78	2.57	2.45	2.19		
532	IM12O1 CF3SO3	1-(2-Methoxyethyl)-3-methylimidazolium trifluoromethanesulfonate	6.12	-0.03	-0.86	0.07			1.87	2.03		
534	IM24 (CF3SO2)2N	1-butyl-3-ethylimidazolium 1.1.1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	-0.12	-0.48	-2.15	2.86			1.68	1.88	1.68	1.90
535	IM1-12 PF6	1-dodecyl-3-methylimidazolium hexafluorophosphate	-7.55	1.51	-1.14	-0.21						
536	IM16 I	1-hexyl-3-methylimidazolium iodide	-1.54	-0.75	-5.31	-1.63						
537	IM18 I	1-methyl-3-octylimidazolium iodide	-3.07	0.28	-5.31	-1.63						

Table B17 (continued)

IL	IL Code	PP+1	PP+5	PP-2	PP-3	logη (303.15 K) (mPa*s)[a]	pred. logη (303.15 K) (mPa*s)	logη (313.15 K) (mPa*s)[a]	pred. logη (313.15 K) (mPa*s)	logη (323.15 K) (mPa*s)[a]	pred. logη (323.15 K) (lmPa*s)	logη (333.15 K) (mPa*s)[a]	pred. logη (333.15 K) (mPa*s)	logη (343.15 K) (mPa*s)[a]	pred. logη (343.15 K) (mPa*s)	logη (353.15 K) (mPa*s)[a]	pred. logη (353.15 K) (mPa*s)
12	Pyr14 (CF3SO2)2N	1.96	-0.03	-2.15	2.86	1.79	1.70	1.62	1.50	1.46	1.33	1.33	1.26	1.21	1.10		
38	Pip14 (CF3SO2)2N	1.15	-0.09	-2.15	2.86												
46	Pip12O1 (CF3SO2)2N	5.73	0.34	-2.15	2.86												
81	IM11 (CF3SO2)2N	4.18	-1.80	-2.15	2.86	1.50	1.31	1.35	1.11	1.22	1.06	1.11	0.93	1.01	0.84	0.92	0.73
82	IM11 1OSO3	4.18	-1.80	-1.16	-0.44	1.77	1.81	1.59	1.52	1.44	1.43	1.32	1.25	1.20	1.17		
91	IM12 N(CN)2	3.24	-1.60	0.49	0.00	1.19	1.45	1.06	1.24								
92	IM12 (CF3SO2)2N	3.24	-1.60	-2.15	2.86	1.43	1.38	1.29	1.19	1.17	1.12	1.06	1.00				
93	IM12 Cl	3.24	-1.60	-5.73	-2.31					2.53	2.44	2.24	2.16	2.00	2.01	1.79	1.76
94	IM12 2OSO3	3.24	-1.60	-1.47	-0.18	1.88	1.90	1.64	1.61	1.54	1.50	1.33	1.33	1.27	1.23	1.13	1.09
98	IM12 1OSO3	3.24	-1.60	-1.16	-0.44	1.80	1.88	1.63	1.60	1.48	1.49	1.35	1.33	1.24	1.23	1.13	1.09
102	IM12 BF4	3.24	-1.60	-0.06	-0.33	1.50	1.63	1.33	1.39	1.20	1.31						
104	IM12 CF3SO3	3.24	-1.60	-0.86	0.07			1.42	1.46	1.29	1.37	1.18	1.22	1.07	1.13	0.98	1.00
109	IM12 NO3	3.24	-1.60	-0.46	-2.37			1.53	1.82	1.42	1.69	1.27	1.50	1.17	1.41	1.05	1.25
147	IM13 BF4	1.85	-0.80	-0.06	-0.33												
149	IM13 PF6	1.85	-0.80	-1.14	-0.21												
152	IM13 I	1.85	-0.80	-5.31	-1.63	2.84	3.20	2.54	2.73	2.29	2.42	2.06	2.18			1.69	1.78
161	IM14 CF3SO3	0.58	-0.39	-0.86	0.07	1.79	2.04	1.64	1.79	1.52	1.61	1.40	1.50	1.24	1.35	1.14	1.24
163	IM14 BF4	0.58	-0.39	-0.06	-0.33	1.87	1.95	1.67	1.72	1.49	1.55	1.33	1.46	1.19	1.31	1.06	1.21
164	IM14 (CF3SO2)2N	0.58	-0.39	-2.15	2.86	1.60	1.71	1.45	1.52	1.29	1.36	1.19	1.29	1.06	1.13	0.97	1.03
165	IM14 PF6	0.58	-0.39	-1.14	-0.21	2.17	2.15	1.98	1.89	1.87	1.69	1.69	1.58	1.54	1.42	1.41	1.30
166	IM14 Cl	0.58	-0.39	-5.73	-2.31	4.04	3.56	3.58	3.06	2.86	2.68	2.84	2.44	2.52	2.24	2.26	2.00
167	IM14 I	0.58	-0.39	-5.31	-1.63			2.34	2.86	2.11	2.52	1.89	2.30	1.71	2.10	1.54	1.88
169	IM14 N(CN)2	0.58	-0.39	0.49	0.00												
175	IM14 1OSO3	0.58	-0.39	-1.16	-0.44	2.21	2.21	1.93	1.93	1.74	1.73	1.63	1.61	1.48	1.45	1.37	1.33
180	IM14 NO3	0.58	-0.39	-0.46	-2.37	2.10	2.47	1.92	2.15	1.65	1.93	1.49	1.79	1.35	1.63	1.28	1.49
181	IM14 SbF6	0.58	-0.39	-0.70	-0.12	1.96	2.04	1.83	1.80	1.69	1.61	1.58	1.51	1.46	1.36		
191	IM16 (CF3SO2)2N	-1.54	-0.75	-2.15	2.86	1.73	1.74	1.53	1.59	1.39	1.43	1.25	1.35	1.14	1.18	1.02	1.08
193	IM16 Cl	-1.54	-0.75	-5.73	-2.31	3.81	3.59	3.41	3.12	3.05	2.75	2.76	2.50	2.53	2.29	2.26	2.05
194	IM16 PF6	-1.54	-0.75	-1.14	-0.21	2.53	2.19	2.27	1.95	2.05	1.76	1.87	1.64	1.70	1.48	1.54	1.35
196	IM16 BF4	-1.54	-0.75	-0.06	-0.33	2.12	1.99	1.91	1.79	1.73	1.62	1.65	1.52	1.50	1.37	1.48	1.26

207	IM18 BF4	-3.07	0.28	-0.06	-0.33	2.23	2.23	2.01	2.03	1.96	1.79	1.76	1.72	1.60	1.53	1.45	1.43
209	IM18 (CF3SO2)2N	-3.07	0.28	-2.15	2.86	1.85	1.98	1.66	1.83	1.50	1.60	1.35	1.55	1.22	1.34	1.11	1.26
212	IM18 Cl	-3.07	0.28	-5.73	-2.31	4.03	3.83	3.61	3.36	3.29	2.92	2.97	2.71	2.70	2.46	2.45	2.22
213	IM18 PF6	-3.07	0.28	-1.14	-0.21	2.72	2.43	2.40	2.19	2.20	1.93	1.98	1.84	2.05	1.64	1.63	1.52
222	IM1-10 (CF3SO2)2N	-5.83	1.33	-2.15	2.86					1.56	1.83			1.26	1.56		
242	IM12OH BF4	9.73	2.49	-0.06	-0.33												
245	IM12O1 (CF3SO2)2N	6.12	-0.03	-2.15	2.86												
247	IM12O1 BF4	6.12	-0.03	-0.06	-0.33	2.14	1.76										
292	PY4-3Me BF4	-1.02	-0.45	-0.06	-0.33			1.89	1.80								
321	IM24 CF3COO	-0.12	-0.48	2.08	-2.30												
322	IM24 CF3SO3	-0.12	-0.48	-0.86	0.07												
390	Py4 BF4	0.96	-0.52	-0.06	-0.33	2.09	1.92	1.85	1.68	1.65	1.52	1.49	1.42	1.35	1.28	1.20	1.18
495	PY4-3Me (CF3SO2)2N	-1.02	-0.45	-2.15	2.86			1.44	1.60	1.31	1.43			1.08	1.19		
511	IM14 1COO	0.58	-0.39	2.41	-5.87					2.02	2.05						
531	IM12O1 PF6	6.12	-0.03	-1.14	-0.21												
532	IM12O1 CF3SO3	6.12	-0.03	-0.86	0.07												
534	IM24 (CF3SO2)2N	-0.12	-0.48	-2.15	2.86												
535	IM1-12 PF6	-7.55	1.51	-1.14	-0.21							2.33	2.22	2.11	1.94	1.91	1.84
536	IM16 I	-1.54	-0.75	-5.31	-1.63					2.37	2.58	2.14	2.36	1.92	2.15	1.76	1.93
537	IM18 I	-3.07	0.28	-5.31	-1.63	2.97	3.60	2.70	3.17	2.45	2.75	2.22	2.56	2.00	2.31	1.84	2.10

[a]Ref. 139. Note: ILs numeration as in the other PLS datamatrices.

Table B18 Experimental and predicted density values. Predictions are calculated using the PLS correlation model D3.

IL	IL Codes	Systematic name	PP+1	PP+2	PP-1	PP-3	d (g cm^{-3}) (273.15 K)	pred. d (g cm^{-3}) (273.15 K)	Ref.
1	Py4-2Me BF4	1-Butyl-2-methylpyridinium tetrafluoroborate	0.27	-6.91	1.67	-0.33	1.20	1.26	a
3	Pyr12 2OSO3	1-Ethyl-1-methylpyrrolidinium ethyl sulfate	4.57	-4.49	1.13	-0.18	1.20	1.30	b
11	Pyr14 (C2F5)3PF3	1-Butyl-1-methylpyrrolidinium trifluorotris(pentafluoroethyl)phosphate	1.96	-4.12	2.83	4.77	1.58	1.63	a
12	Pyr14 (CF3SO2)2N	1-Butyl-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.96	-4.12	-1.19	2.86	1.40	1.41	a
13	Pyr14 1OSO3	1-Butyl-1-methylpyrrolidinium methyl sulfate	1.96	-4.12	1.36	-0.44	1.17	1.25	a
16	Pyr14 N(CN)2	1-Butyl-1-methylpyrrolidinium N-cyanocyanamide	1.96	-4.12	-2.48	0.00	1.12	1.19	a
17	Pyr16 (CF3SO2)2N	1-Hexyl-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	0.02	-3.63	-1.19	2.86	1.32	1.38	a
28	Pyr12O1 (C2F5)3PF3	1-(2-Methoxyethyl)-1-methylpyrrolidinium tris(pentafluoroethyl)trifluorophosphate	7.36	-0.19	2.83	4.77	1.63	1.68	a
36	Pip13 (CF3SO2)2N	1-Methyl-1-propylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.18	-4.18	-1.19	2.86	1.40	1.41	a
38	Pip14 (CF3SO2)2N	1-Butyl-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.15	-3.97	-1.19	2.86	1.38	1.39	c
55	Mor14 (CF3SO2)2N	4-Butyl-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	6.23	0.06	-1.19	2.86	1.44	1.44	c
75	IM14-2Me (CF3SO2)2N	1-Butyl-2,3-dimethylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.01	-5.58	-1.19	2.86	1.42	1.40	a
76	IM14-2Me BF4	1-Butyl-2,3-dimethylimidazolium tetrafluoroborate	1.01	-5.58	1.67	-0.33	1.19	1.27	a
81	IM11 (CF3SO2)2N	1,3-Dimethylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	4.18	-6.87	-1.19	2.86	1.57	1.45	a
82	IM11 1OSO3	1,3-dimethylimidazolium methylsulfate	4.18	-6.87	1.36	-0.44	1.33	1.30	a
90	IM12 B(CN)4	1-Ethyl-3-methylimidazolium tetracyanoborate	3.24	-6.75	-10.53	-0.53	1.04	0.99	a
91	IM12 N(CN)2	1-Ethyl-3-methylimidazolium N-cyanocyanamide	3.24	-6.75	-2.48	0.00	1.10	1.22	a
92	IM12 (CF3SO2)2N	1-Ethyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3.24	-6.75	-1.19	2.86	1.53	1.44	c
93	IM12 Cl	1-Ethyl-3-methylimidazolium chloride	3.24	-6.75	-0.57	-2.31	1.14	1.12	c
94	IM12 2OSO3	1-Ethyl-3-methylimidazolium ethyl sulfate	3.24	-6.75	1.13	-0.18	1.24	1.30	c
96	IM12 1COO	1-Ethyl-3-methylimidazolium acetate	3.24	-6.75	4.20	-5.87	1.10	1.01	a
97	IM12 1O2O2OSO3	1-Ethyl-3-methylimidazolium 2-(2-methoxyethoxy)ethyl sulfate	3.24	-6.75	1.54	3.67	1.24		a
98	IM12 1OSO3	1-Ethyl-3-methylimidazolium methylsulfate	3.24	-6.75	1.36	-0.44	1.29	1.29	a
99	IM12 1SO3	1-Ethyl-3-methylimidazolium methanesulfonate	3.24	-6.75	1.32	-0.86	1.24	1.26	a
101	IM12 8OSO3	1-Ethyl-3-methylimidazolium octylsulfate	3.24	-6.75	-1.48	3.86	1.09		a
102	IM12 BF4	1-Ethyl-3-methylimidazolium tetrafluoroborate	3.24	-6.75	1.67	-0.33	1.28	1.30	a
103	IM12 CF3COO	1-Ethyl-3-methylimidazolium trifluoroacetate	3.24	-6.75	3.18	-2.30	1.29	1.21	a
104	IM12 CF3SO3	1-Ethyl-3-methylimidazolium trifluoromethanesulfonate	3.24	-6.75	1.41	0.07	1.38	1.32	c
105	IM12 HSO4	1-Ethyl-3-methylimidazolium hydrogen sulfate	3.24	-6.75	2.60	-1.42	1.37	1.26	a
107	IM12 SCN	1-Ethyl-3-methylimidazolium thiocyanate	3.24	-6.75	0.65	-3.10	1.12	1.10	a
108	IM12 Br	1-Ethyl-3-methylimidazolium bromide	3.24	-6.75	-0.52	-2.16	1.39		a
136	IM1i4 (CF3SO2)2N	1-Methyl-3-(2-methylpropyl)imidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.42	-5.98	-1.19	2.86	1.45	1.41	c
140	IM1-2=1 Cl	1-Methyl-3-(2-propenyl)imidazolium chloride	1.49	-6.89	-0.57	-2.31	1.12	1.10	a

147	IM13 BF4	1-Methyl-3-propylimidazolium tetrafluoroborate	1.85	-6.45	1.67	-0.33	1.24	1.28	a
148	IM13 (CF3SO2)2N	1-Methyl-3-propylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.85	-6.45	-1.19	2.86	1.47	1.42	a
150	IM13 Br	1-Methyl-3-propylimidazolium bromide	1.85	-6.45	-0.52	-2.16	1.32		a
151	IM13 Cl	1-Methyl-3-propylimidazolium chloride	1.85	-6.45	-0.57	-2.31	1.10	1.10	c
160	IM12 8OSO3	1-Butyl-3-methylimidazolium octylsulfate	0.58	-5.91	-1.48	3.86	1.07		a
161	IM14 CF3SO3	1-Butyl-3-methylimidazolium trifluoromethanesulfonate	0.58	-5.91	1.41	0.07	1.30	1.28	a
163	IM14 BF4	1-Butyl-3-methylimidazolium tetrafluoroborate	0.58	-5.91	1.67	-0.33	1.20	1.26	a
164	IM14 (CF3SO2)2N	1-Butyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	0.58	-5.91	-1.19	2.86	1.43	1.40	c
165	IM14 PF6	1-Butyl-3-methylimidazolium hexafluorophosphate	0.58	-5.91	1.13	-0.21	1.37	1.26	c
166	IM14 Cl	1-Butyl-3-methylimidazolium chloride	0.58	-5.91	-0.57	-2.31	1.08	1.08	a
167	IM14 I	1-Butyl-3-methylimidazolium iodide	0.58	-5.91	-0.65	-1.63	1.44		c
169	IM14 N(CN)2	1-Butyl-3-methylimidazolium N-cyanocyanamide	0.58	-5.91	-2.48	0.00	1.07	1.18	a
173	IM14 (C2F5)3PF3	1-Butyl-3-methylimidazolium trifluorotris(pentafluoroethyl)phosphate	0.58	-5.91	2.83	4.77	1.62	1.62	a
174	IM14 1O2O2OSO3	1-Butyl-3-methylimidazolium 2-(2-methoxyethoxy)ethyl sulfate	0.58	-5.91	1.54	3.67	1.18		a
175	IM14 1OSO3	1-Butyl-3-methylimidazolium methyl sulfate	0.58	-5.91	1.36	-0.44	1.21	1.25	a
179	IM14 HSO4	1-Butyl-3-methylimidazolium hydrogen sulfate	0.58	-5.91	2.60	-1.42	1.22	1.21	a
180	IM14 NO3	1-Butyl-3-methylimidazolium nitrate	0.58	-5.91	-6.94	-2.37	1.16		a
181	IM14 SbF4	1-Butyl-3-methylimidazolium (OC-6-11)-hexafluoroantimonate	0.58	-5.91	1.35	-0.12	1.69		a
182	IM14 SCN	1-Butyl-3-methylimidazolium thiocyanate	0.58	-5.91	0.65	-3.10	1.07	1.06	a
183	IM14 (1O)2PO2	1-butyl-3-methylimidazolium dimethyl phosphate	0.58	-5.91	1.30	0.20	1.16	1.29	d
185	IM14 CF3COO	1-Butyl-3-Methylimidazolium trifluoroacetate	0.58	-5.91	3.18	-2.30	1.22	1.17	a
187	IM15 (CF3SO2)2N	1-Methyl-3-pentylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	-0.64	-5.56	-1.19	2.86	1.40	1.38	a
188	IM15 BF4	1-Methyl-3-pentylimidazolium tetrafluoroborate	-0.64	-5.56	1.67	-0.33	1.17	1.24	a
190	IM15 PF6	1-Methyl-3-pentylimidazolium hexafluorophosphate	-0.64	-5.56	1.13	-0.21	1.33	1.24	a
191	IM16 (CF3SO2)2N	1-Hexyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	-1.54	-5.78	-1.19	2.86	1.37	1.37	a
192	IM16 Br	1-Hexyl-3-methylimidazolium bromide	-1.54	-5.78	-0.52	-2.16	1.23		a
193	IM16 Cl	1-Hexyl-3-methylimidazolium chloride	-1.54	-5.78	-0.57	-2.31	1.03	1.05	c
194	IM16 PF6	1-Hexyl-3-methylimidazolium hexafluorophosphate	-1.54	-5.78	1.13	-0.21	1.29	1.23	a
196	IM16 BF4	1-Hexyl-3-methylimidazolium tetrafluoroborate	-1.54	-5.78	1.67	-0.33	1.15	1.23	a
197	IM16 (C2F5)3PF3	1-Hexyl-3-methylimidazolium trifluorotris(pentafluoroethyl)phosphate	-1.54	-5.78	2.83	4.77	1.55	1.59	a
200	IM16 N(CN)2	1-hexyl-3-methylimidazolium dicyanamide	-1.54	-5.78	-2.48	0.00	1.03	1.15	a
203	IM17 (CF3SO2)2N	1-Heptyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	-2.66	-4.82	-1.19	2.86	1.36	1.35	a
204	IM17 BF4	1-Heptyl-3-methylimidazolium tetrafluoroborate	-2.66	-4.82	1.67	-0.33	1.34	1.21	a
206	IM17 PF6	1-Heptyl-3-methylimidazolium hexafluorophosphate	-2.66	-4.82	1.13	-0.21	1.27	1.20	a
207	IM18 BF4	1-Methyl-3-octylimidazolium tetrafluoroborate	-3.07	-4.67	1.67	-0.33	1.10	1.20	a
208	IM18 Br	1-Methyl-3-octylimidazolium bromide	-3.07	-4.67	-0.52	-2.16	1.17		a
209	IM18 (CF3SO2)2N	1-Methyl-3-octylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	-3.07	-4.67	-1.19	2.86	1.32	1.34	a

211	IM18 CF3SO3	1-Methyl-3-octylimidazolium trifluormethanesulfonate	-3.07	-4.67	1.41	0.07	1.19	1.22	a
212	IM18 Cl	1-Methyl-3-octylimidazolium chloride	-3.07	-4.67	-0.57	-2.31	1.01	1.02	a
213	IM18 PF6	1-Methyl-3-octylimidazolium hexafluorophosphate	-3.07	-4.67	1.13	-0.21	1.23	1.20	c
217	IM19 PF6	1-Methyl-3-nonylimidazolium hexafluorophosphate	-4.95	-4.26	1.13	-0.21	1.19	1.17	a
218	IM1-10 BF4	1-Decyl-3-methylimidazolium tetrafluoroborate	-5.83	-4.13	1.67	-0.33	1.07	1.16	c
220	IM1-10 Cl	1-Decyl-3-methylimidazolium chloride	-5.83	-4.13	-0.57	-2.31	0.99	0.98	a
221	IM1-10 PF6	1-Decyl-3-methylimidazolium hexafluorophosphate	-5.83	-4.13	1.13	-0.21	1.14	1.16	c
222	IM1-10 (CF3SO2)2N	1-decyl-3-methylimidazolium bis(trifluoromethylsulphonyl)imide	-5.83	-4.13	-1.19	2.86	1.27	1.30	c
240	IM12OH (CF3SO2)2N	1-(2-Hydroxyethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	9.73	2.71	-1.19	2.86	1.51	1.47	a
242	IM12OH BF4	1-(2-Hydroxyethyl)-3-methylimidazolium tetrafluoroborate	9.73	2.71	1.67	-0.33	1.32	1.33	c
243	IM12OH PF6	1-(2-Hydroxyethyl)-3-methylimidazolium hexafluorophosphate	9.73	2.71	1.13	-0.21	1.48	1.33	c
245	IM12O1 (CF3SO2)2N	1-(2-Methoxyethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	6.12	-1.79	-1.19	2.86	1.51	1.45	c
247	IM12O1 BF4	1-(2-Methoxyethyl)-3-methylimidazolium tetrafluoroborate	6.12	-1.79	1.67	-0.33	1.26	1.31	c
252	IM12O2O1 Cl	1-[2-(2-Methoxyethoxy)ethyl]-3-methylimidazolium chloride	5.30	1.60	-0.57	-2.31	1.14	1.10	c
292	Py4-3Me BF4	1-Butyl-3-methylpyridinium tetrafluoroborate	-1.02	-6.72	1.67	-0.33	1.18	1.24	a
316	IM22 (CF3SO2)2N	1,3-Diethylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2.03	-6.56	-1.19	2.86	1.47	1.42	a
321	IM24 CF3COO	1-Butyl-3-ethylimidazolium trifluoroacetate	-0.12	-5.99	3.18	-2.30	1.18	1.16	a
322	IM24 CF3SO3	1-Butyl-3-ethylimidazolium trifluoromethanesulfonate	-0.12	-5.99	1.41	0.07	1.23	1.27	c
326	IM1-(1Ph) (CF3SO2)2N	1-benzyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	-0.83	-6.52	-1.19	2.86	1.49	1.38	c
331	Py4-4Me BF4	1-Butyl-4-methylpyridinium tetrafluoroborate	-0.22	-6.95	1.67	-0.33	1.18	1.26	a
347	Py6-4NMe2 (CF3SO2)2N	4-(Dimethylamino)-1-hexylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	-3.42	-6.49	-1.19	2.86	1.35	1.35	a
390	Py4 BF4	1-Butylpyridinium tetrafluoroborate	0.96	-6.71	1.67	-0.33	1.21	1.27	a
391	Py4 CF3SO3	1-Butylpyridinium trifluoromethanesulfonate	0.96	-6.71	1.41	0.07	1.31	1.29	a
395	Py6 (CF3SO2)2N	1-Hexylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	-0.95	-5.90	-1.19	2.86	1.39	1.38	a
400	Py8 (CF3SO2)2N	1-Octylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	-3.41	-5.10	-1.19	2.86	1.33	1.34	a
437	IM01 BF4	1-Methylimidazole hydrogen tetrafluoroborate	5.03	-5.69	1.67	-0.33	1.38	1.32	a
440	IM01 1COO	1-methylimidazolium acetate	5.03	-5.69	4.20	-5.87	1.08	1.02	a
491	IM01-2Me (CF3SO2)2N	1,2-dimethylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	4.73	-5.69	-1.19	2.86	1.57	1.45	a
493	IM13-2Me (CF3SO2)2N	1,2-dimethyl-3-propylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1.81	-6.77	-1.19	2.86	1.46	1.42	c
495	Py4-3Me (CF3SO2)2N	1-butyl-3-methylpyridinium1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	-1.02	-6.72	-1.19	2.86	1.41	1.38	e
497	IM11 (1O)2PO2	1,3-dimethyl imidazolium dimethyl phopsphate	4.18	-6.87	1.30	0.20	1.24	1.34	a
498	IM18 CF3COO	1-methyl-3-octylimidazolium trifluoroacetate	-3.07	-4.67	3.18	-2.30	1.19	1.11	a
500	IM12OH N(CN)2	1-(2-hydroxyethyl)-3-methylimidazolium dicyanamide	9.73	2.71	-2.48	0.00	1.20	1.25	a
503	Py8-4Me (CF3SO2)2N	1-octyl-4-methylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	-4.69	-5.10	-1.19	2.86	1.29	1.32	f
504	Py4 (CF3SO2)2N	1-butylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	0.96	-6.71	-1.19	2.86	1.45	1.41	a
506	Pyr18 (CF3SO2)2N	1-methyl-1-octylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	-2.33	-3.03	-1.19	2.86	1.31	1.34	a
510	Mor12 (CF3SO2)2N	1-ethyl-1-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	8.90	-0.32	-1.19	2.86	1.51	1.48	a

511	IM14 1COO	1-butyl-3-methylimidazolium acetate	0.58	-5.91	4.20	-5.87	1.05	0.96	a
521	Pyr14 (1O)2PO2	1-butyl-1-methylpyrrolidinium dimethyl phosphate	1.96	-4.12	1.30	0.20	1.12	1.29	d

[a]Ref. 126; [b]Ref. 148; [c]Ref. 147; [d]Ref. 150; [e]Ref. 149; [f] Ref. 146. Note: ILs numeration as in the other PLS datamatrices.

Table B19 Experimental and predicted decomposition temperature values. Predictions are calculated using the OPLS correlation model M3.

IL	IL code	Systematic name	Decomp. Temp. (K)	pred. Decomp. Temp. (K)	Ref.
12	Pyr14 (CF3SO2)2N	1-Butyl-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	701.00	701.07	a
61	Mor12OH (CF3SO2)2N	4-(2-Hydroxyethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	643.00	641.85	b
91	IM12 N(CN)2	1-Ethyl-3-methylimidazolium N-cyanocyanamide	513.15	509.94	c
92	IM12 (CF3SO2)2N	1-Ethyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	664.30	688.23	c
93	IM12 Cl	1-Ethyl-3-methylimidazolium chloride	556.15	559.48	c
102	IM12 BF4	1-Ethyl-3-methylimidazolium tetrafluoroborate	693.15	707.91	c
103	IM12 CF3COO	1-Ethyl-3-methylimidazolium trifluoroacetate	423.15	430.87	c
104	IM12 CF3SO3	1-Ethyl-3-methylimidazolium trifluoromethanesulfonate	713.15	711.96	c
106	IM12 PF6	1-Ethyl-3-methylimidazolium hexafluorophosphate	701.15	692.82	c
108	IM12 Br	1-Ethyl-3-methylimidazolium bromide	584.15	581.78	c
147	IM13 BF4	1-Methyl-3-propylimidazolium tetrafluoroborate	708.15	703.40	c
149	IM13 PF6	1-Methyl-3-propylimidazolium hexafluorophosphate	710.65	688.10	c
151	IM13 Cl	1-Methyl-3-propylimidazolium chloride	554.65	554.69	c
161	IM14 CF3SO3	1-Butyl-3-methylimidazolium trifluoromethanesulfonate	683.00	680.55	c
163	IM14 BF4	1-Butyl-3-methylimidazolium tetrafluoroborate	690.33	682.01	c
164	IM14 (CF3SO2)2N	1-Butyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	693.65	654.92	c
165	IM14 PF6	1-Butyl-3-methylimidazolium hexafluorophosphate	642.65	666.46	c
166	IM14 Cl	1-Butyl-3-methylimidazolium chloride	527.15	532.83	c
167	IM14 I	1-Butyl-3-methylimidazolium iodide	538.15	551.86	c
175	IM14 1OSO3	1-Butyl-3-methylimidazolium methyl sulfate	644.00	648.48	c
183	IM14 (1O)2PO2	1-butyl-3-methylimidazolium dimethyl phosphate	555.00	536.31	a
193	IM16 Cl	1-Hexyl-3-methylimidazolium chloride	526.15	524.64	c
196	IM16 BF4	1-Hexyl-3-methylimidazolium tetrafluoroborate	682.15	673.97	c
197	IM16 (C2F5)3PF3	1-Hexyl-3-methylimidazolium trifluorotris(pentafluoroethyl)phosphate	563.15	564.36	c
207	IM18 BF4	1-Methyl-3-octylimidazolium tetrafluoroborate	633.15	669.76	c
212	IM18 Cl	1-Methyl-3-octylimidazolium chloride	516.15	519.80	c
213	IM18 PF6	1-Methyl-3-octylimidazolium hexafluorophosphate	669.15	653.70	c
222	IM1-10 (CF3SO2)2N	1-decyl-3-methylimidazolium bis(trifluoromethylsulphonyl)imide	573.15	599.14	c

228	IM1-14 Br	1-Methyl-3-tetradecylimidazolium bromide	545.65	526.78	c
240	IM12OH (CF3SO2)2N	1-(2-Hydroxyethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	693.00	690.75	c
242	IM12OH BF4	1-(2-Hydroxyethyl)-3-methylimidazolium tetrafluoroborate	653.00	631.23	c
243	IM12OH PF6	1-(2-Hydroxyethyl)-3-methylimidazolium hexafluorophosphate	583.00	600.24	c
521	Pyr14 (1O)2PO2	1-butyl-3-methylpyrrolidinium dimethyl phosphate	548.00	539.57	a
538	Mor12OH PF6	4-(2-Hydroxyethyl)-4-methylmorpholinium hexafluorophosphate	553.00	549.63	a
539	Mor12OH BF4	4-(2-Hydroxyethyl)-4-methylmorpholinium tetrafluoroborate	573.00	582.34	b

[a] Ref. 150; [b]Ref. 151; [c]Ref. 147. Note: ILs numeration as in the other PLS datamatrices.

Table B20 Experimental and predicted conductivity values. Predictions are calculated using the OPLS correlation model C3.

IL	IL Code	Systematic name	Electr. Conduct. (25°C) S/m	pred. Electr. Conduct. (25°C) S/m	Ref.
12	Pyr14 (CF3SO2)2N	1-Butyl-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	0.2800	0.2175	a
36	Pip13 (CF3SO2)2N	1-Methyl-1-propylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	0.1400	0.1507	b
81	IM11 (CF3SO2)2N	1,3-Dimethylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	0.9000	0.9345	a
91	IM12 N(CN)2	1-Ethyl-3-methylimidazolium N-cyanocyanamide	2.9281	2.6535	a
92	IM12 (CF3SO2)2N	1-Ethyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	0.9100	0.9380	a
93	IM12 Cl	1-Ethyl-3-methylimidazolium chloride	0.0622	0.0481	a
94	IM12 2OSO3	1-Ethyl-3-methylimidazolium ethyl sulfate	0.3880	0.4546	a
96	IM12 1COO	1-Ethyl-3-methylimidazolium acetate	0.2770	0.2836	a
102	IM12 BF4	1-Ethyl-3-methylimidazolium tetrafluoroborate	1.5660	1.3259	a
103	IM12 CF3COO	1-Ethyl-3-methylimidazolium trifluoroacetate	0.9200	1.0566	b
104	IM12 CF3SO3	1-Ethyl-3-methylimidazolium trifluoromethanesulfonate	0.9300	0.9315	b
106	IM12 PF6	1-Ethyl-3-methylimidazolium hexafluorophosphate	0.5100	0.6905	b
140	IM1-2=1 Cl	1-Methyl-3-(2-propenyl)imidazolium chloride	0.0070	0.0107	a
147	IM13 BF4	1-Methyl-3-propylimidazolium tetrafluoroborate	0.5900	0.6140	a
161	IM14 CF3SO3	1-Butyl-3-methylimidazolium trifluoromethanesulfonate	0.2900	0.2068	a
163	IM14 BF4	1-Butyl-3-methylimidazolium tetrafluoroborate	0.3530	0.3035	a
164	IM14 (CF3SO2)2N	1-Butyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	0.4060	0.3450	a
165	IM14 PF6	1-Butyl-3-methylimidazolium hexafluorophosphate	0.1430	0.1572	a
169	IM14 N(CN)2	1-Butyl-3-methylimidazolium N-cyanocyanamide	1.0960	1.1638	a
175	IM14 1OSO3	1-Butyl-3-methylimidazolium methyl sulfate	0.1260	0.1406	a
185	IM14 CF3COO	1-Butyl-3-Methylimidazolium trifluoroacetate	0.3320	0.2386	a
191	IM16 (CF3SO2)2N	1-Hexyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	0.2200	0.2572	a

192	IM16 Br	1-Hexyl-3-methylimidazolium bromide	12.0600		a
194	IM16 PF6	1-Hexyl-3-methylimidazolium hexafluorophosphate	0.0543	0.0657	a
196	IM16 BF4	1-Hexyl-3-methylimidazolium tetrafluoroborate	0.1229	0.1267	a
197	IM16 (C2F5)3PF3	1-Hexyl-3-methylimidazolium trifluorotris(pentafluoroethyl)phosphate	0.1665	0.1304	a
207	IM18 BF4	1-Methyl-3-octylimidazolium tetrafluoroborate	0.0585	0.0743	a
208	IM18 Br	1-Methyl-3-octylimidazolium bromide	10.5500		a
209	IM18 (CF3SO2)2N	1-Methyl-3-octylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	0.1300	0.1564	a
213	IM18 PF6	1-Methyl-3-octylimidazolium hexafluorophosphate	0.0260	0.0384	a
218	IM1-10 BF4	1-Decyl-3-methylimidazolium tetrafluoroborate	0.0350	0.0366	a
222	IM1-10 (CF3SO2)2N	1-decyl-3-methylimidazolium bis(trifluoromethylsulphonyl)imide	0.1300	0.0852	a
240	IM12OH (CF3SO2)2N	1-(2-Hydroxyethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	0.2800	0.3308	b
242	IM12OH BF4	1-(2-Hydroxyethyl)-3-methylimidazolium tetrafluoroborate	0.4600	0.4166	b
243	IM12OH PF6	1-(2-Hydroxyethyl)-3-methylimidazolium hexafluorophosphate	0.2100	0.1763	b
245	IM12O1 (CF3SO2)2N	1-(2-Methoxyethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	0.4300	0.5235	b
321	IM24 CF3COO	1-Butyl-3-ethylimidazolium trifluoroacetate	0.2500	0.2577	b
322	IM24 CF3SO3	1-Butyl-3-ethylimidazolium trifluoromethanesulfonate	0.2700	0.2175	b
387	Py4 Br	1-Butylpyridinium bromide	0.0253	0.0144	a
440	IM01 1COO	1-methylimidazolium acetate	0.3710		a
441	IM01 CF3COO	1-methylimidazolium trifluoroacetate	0.1000		b
504	Py4 (CF3SO2)2N	1-butylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	0.3300	0.3742	a
511	IM14 1COO	1-butyl-3-methylimidazolium acetate	0.049	0.0611	a

[a]Ref. 126; [b]Ref. 147. Note: ILs numeration as in the other PLS datamatrices.

6.4 C-Tables: others

Table C1. List of the 128 VolSurf+ descriptors.[a]

code		name
1	V	Molecular volume
2	S	Molecular surface
3	R	Volume/surface ratio
4	G	Molecular globularity = S/S_{eq}, with S_{eq} = surface area of a sphere of volume V
5-12	W1-W8	Hydrophilic regions
13-20	D1-D8	Hydrophobic regions
21-26	WO1-WO6	H-bond donor volumes
27-32	WN1-WN6	H-bond acceptor volumes
33-36	IW1-IW4	Hydrophilic interaction energy: distance between hydrophilic areas and molecular barycenter
37-44	CW1-CW8	Capacity factor for OH2: hydrophilic regions/total molecular surface
45-48	ID1-ID4	Hydrophobic integy moment: distance between hydrophobic areas and molecular barycenter
49-56	CD1-CD8	Capacity Factor for DRY: hydrophobic regions/total molecular surface
57-58	HL1-HL2	Hydrophilic-Lipophilic balance
59	A	Amphiphilic moment
60	CP	Critical Packing, predicting molecular packing such as in micelle formation
61	POL	Polarizability
62	MW	Molecular weight
63-64	FLEX, FLEX_RB	Flexibility parameters
65	NCC	Number of charged centers
66	DIFF	Diffusivity: dispersion of chemicals in water fluid at 25°C.
67	LOGP N-oCT	LogP octanol/water
68	LOGP c-Hex	LogP cyclohexane/water
69-72	PSA	Polar and hydrophobic surface areas
	HSA	
	PSAR	
	PHSAR	
73-79	LgD5 - LgD10	LogD: logP oct/water at different pH
80	AUS7.4	Available uncharged species
81-87	%FU4 - %FU10	Percentage of unionized species at different pH
88-97	DRDRDR	Dry, H-bond donor, H-bond acceptor and mixed Dry, H-bond donor and acceptor 3D triplets pharmacophoric areas
	DRDRAC	
	DRDRDO	
	DRACAC	
	DRACDO	
	DRDODO	
	ACACAC	
	ACACDO	
	ACDODO	
98	SOLY	Intrinsic water solubility in mol/L at 25 °C
99-108	LgS3 - LgS11	Solubility in water at various pH
109	PB	Precentage of protein binding
110	VD	Volume of distribution
111	CACO2	CACO2 cells permeability

112	SKIN	Skin permeability
113	LgBB	Log blood-brain barrier distribution
114	MetStab	Metabolic Stability
115	HTSFlag	High throughput screening flag
116-120	L0lgS - L4lgS	Solubility profiling coefficients
121-128	DD1 - DD8	Differences of the hydrophobic volumes

[a] See also Table C2 for the reduced list of the 48 non-zero VolSurf+ descriptors used to describe anions structures.

Table C2 List of the 48 variables used to model ILs anions.

Variable	description	Variable	description
V	volume	CW1	Capacity factor at W1 volume
S	surface	CW2	Capacity factor at W2 volume
R	rugosity	CW3	Capacity factor at W3 volume
G	globularity	CW4	Capacity factor at W4 volume
W1	Hydrophilic region volume at -0.2 kcal/mol	CW5	Capacity factor at W5 volume
W2	Hydrophilic region volume at -0.5 kcal/mol	CW6	Capacity factor at W6 volume
W3	Hydrophilic region volume at -1.0 kcal/mol	CW7	Capacity factor at W7 volume
W4	Hydrophilic region volume at -2.0 kcal/mol	CW8	Capacity factor at W8 volume
W5	Hydrophilic region volume at -3.0 kcal/mol	ID1	Interaction energy moment at D1
W6	Hydrophilic region volume at -4.0 kcal/mol	ID2	Interaction energy moment at D2
W7	Hydrophilic region volume at -5.0 kcal/mol	ID3	Interaction energy moment at D3
W8	Hydrophilic region volume at -6.0 kcal/mol	ID4	Interaction energy moment at D4
D1	Hydrophobic region volume at -0.2 kcal/mol	CD1	Capacity factor at D1 volume
D2	Hydrophobic region volume at -0.5 kcal/mol	CD2	Capacity factor at D2 volume
D3	Hydrophobic region volume at -1.0 kcal/mol	CD3	Capacity factor at D3 volume
D4	Hydrophobic region volume at -2.0 kcal/mol	CD4	Capacity factor at D4 volume
D5	Hydrophobic region volume at -3.0 kcal/mol	CD5	Capacity factor at D5 volume
D6	Hydrophobic region volume at -4.0 kcal/mol	CD6	Capacity factor at D6 volume
D7	Hydrophobic region volume at -5.0 kcal/mol	CD7	Capacity factor at D7 volume
D8	Hydrophobic region volume at -6.0 kcal/mol	CD8	Capacity factor at D8 volume
IW1	Interaction energy moment at W1	HL1	hydrophilic/lipophilic balance (low energy)
IW2	Interaction energy moment at W2	HL2	hydrophilic/lipophilic balance (high energy)
IW3	Interaction energy moment at W3	A	amphiphilic moment
IW4	Interaction energy moment at W4	CP	critical packing

Table C3 Imidazolium side chains labels.

	Side chain	label
none	hydrogen	HY
alkylic	methyl	01
	ethyl	02
	propyl	03
	2-propenyl (*allyl*)	AL
	2-methylpropyl (*isobutyl*)	I4
	butyl	04
	pentyl	05
	hexyl	06
	heptyl	07
	octyl	08
	nonyl	09
	decyl	10
	undecyl	11
	dodecyl	12
	tridecyl	13
	tetradecyl	14
	pentadecyl	15
	hexadecyl	16
	heptadecyl	17
	octadecyl	18
	nonadecyl	19
aromatic	phenylmethyl	PM
	phenylethyl	PE
	(4-methylphenyl)methyl	MP
	(1,3-benzodioxol-5-yl)-2-methoxy-2-oxoethyl	ZM
	1-(1,3-benzodioxol-5-yl)-2-butoxy-2-oxoethyl	ZB
	2-[1-(1,3-benzodioxol-5-yl)-2-butoxy-2-oxoethoxy]-2-oxoethyl	ZX
alkyloxymethyl ether	metoxymethyl	1O
	etoxymethyl	2O
	propoxymethyl	3O
	butoxymethyl	4O
	pentoxymethyl	5O
	hexyloxymethyl	6O
	heptyloxymethyl	7O
	octyloxymethyl	8O
	nonyloxymethyl	9O
	decyloxymethyl	AO
	undecyloxymethyl	BO
	dodecyloxymethyl	CO
	tetradecyloxymethyl	EO
	hexadecyloxymethyl	GO
ether	2-metoxyethyl	1E
	2-etoxyethyl	2E
	2-(2-methoxyethoxy)ethyl	ME
	3-methoxypropyl	1P
alcoholic	2-hydroxyethyl	ET
	3-hydroxypropyl	PR
	4-hydroxypropyl	BL
carboxylic	3-carboxypropyl	C3
ester	11-ethoxy-11-oxoundecyl	EU
amidic	2-(diethylamino)-2-oxoethyl	EE
nitrile	cyanomethyl	CM