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Prediction of RO/NF membrane rejections of PhACs and organic compounds: a statistical analysis

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Rejections of pharmaceutical compounds (Ibuprofen, Diclofenac, Clofibrac acid, Naproxen, Primidone, Phenacetin) and organic compounds (Dichloroacetic acid, Trichloroacetic acid, Chloroform, Bromoform, Trichloroethene, Perchloroethene, Carbontetrachloride, Carbontetrabromide) by NF (Filmtec, Saehan) and RO (Filmtec, Saehan, Toray, Koch) membranes were studied. Chloroform presented the lowest rejection due to small molar volume, equivalent width and length. Diclofenac and Primidone showed high rejections related to high molar volume and length. Dichloroacetic acid and Trichloroacetic acid presented good rejections caused by charge exclusion instead of steric hindrance mechanism influencing rejection. Bromoform and Trichloroethene showed low rejections due to small length and equivalent width. Carbontetrabromide, Perchloroethene and Carbontetrachloride with higher equivalent width than BF and TCE presented better rejections. A qualitative analysis of variables using Principal Component Analysis was successfully implemented for reduction of physical-chemical compound properties that influence membrane rejection of PhACs and organic compounds. Properties such as dipole moment, molar volume, hydrophobicity/hydrophilicity, molecular length and equivalent width were found to be important descriptors for prediction of membrane rejection. Ionic and neutral compounds were successfully separated before analysis. For membranes used in the experiments, we may conclude that charge repulsion was an important mechanism of rejection for ionic compounds. Molecular weight was a poor variable for rejection prediction. Membrane rejection of neutral compounds was well predicted by dipole moment, molar volume, length, equivalent width and hydrophobicity/hydrophilicity of compounds after analysis with Multiple Linear Regression.

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1 Introduction

The presence of pharmaceutically activated compounds (PhACs) and endocrine disrupters compounds (EDCs) in surface waters has been reported, detailed and quantified in many studies (Ternes, 1998; Hirsch et al., 1999; Heberer, 2002; Kolpin et al., 2002). Although pharmaceuticals are generally taken up by the human organism, a significant amount of the original substance is often excreted with urine or faeces, thus entering raw sewage and eventually ending up in the aquatic environment. The fate of pharmaceuticals in the environment has raised the interest of scientists because the accumulation of them may result in environmentally significant concentrations with unknown effects. It has been studied that conventional water treatment presented limitations in removing PhACs and EDCs (Vieno et al., 2006; Adams et al., 2002). In that sense, many studies have investigated the removal of micropollutants i.e. PhACs, EDCs, by membrane treatment (NF, RO) and their separation mechanisms such as size/steric exclusion, hydrophobic adsorption, partition and electrostatic repulsion (Kiso et al., 2001a, b, 2002; Schäfer et al., 2003; Nghiem et al., 2004; Kimura et al., 2003; Kimura et al., 2004; Kim et al., 2005). Characteristics such as MWCO, porosity, membrane morphology, charge, and hydrophobicity of the membrane influence rejection of compounds (Schaep and Vandecasteele, 2001; Childress and Elimelech, 2000); compound properties such as molecular weight, molecular size, charge, dipole moment and hydrophobicity can be used as predictors of rejection in applications of membrane water treatment (Ozaki and Li, 2002; Van der Bruggen et al., 2000; Kiso et al. 2001a; Van der Bruggen et al., 1999). However, there are disagreements defining the importance of each descriptor, in that sense our objective is to investigate compound properties and membrane characteristics with a statistical approach in order to predict membrane rejection.

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2 Background of statistics

2.1 Principal component analysis

A summary of principal component analysis is presented by Landau and Everitt (2004). Principal Component Analysis (PCA) is essentially a method of data reduction that aims to produce a small number of derived variables that can be used in place of the larger number of original variables to simplify subsequent analysis of the data. The principal component variables y_1, y_2, \dots, y_q are defined to be linear combinations of the original variables x_1, x_2, \dots, x_q that are uncorrelated and account for maximal proportions of the variation in the original data, i.e., y_1 accounts for the maximum amount of the variance among all possible linear combinations of x_1, \dots, x_q , y_2 accounts for the maximum variance subject to being uncorrelated with y_1 and so on. Explicitly, the principal component variables are obtained from x_1, \dots, x_q as follows:

$$y_1 = a_{11}x_1 + a_{12}x_2 + \dots + a_{1q}x_q$$

$$y_2 = a_{21}x_1 + a_{22}x_2 + \dots + a_{2q}x_q$$

\vdots

$$y_q = a_{q1}x_1 + a_{q2}x_2 + \dots + a_{qq}x_q \quad (1)$$

Where the coefficients a_{ij} ($i=1, \dots, q, j=1, \dots, q$) are chosen so that the required maximal variance and uncorrelated conditions hold. Since the variances of the principal components variables could be increased without limit, simply by increasing the coefficients that define them, a restriction must be placed on these coefficients. The constraint usually applied is that the sum of squares of the coefficients is one in that way the total variance of all the components is equal to the total variance of all the observed variables. It is often convenient to rescale the coefficients in order that their sum of squares is equal to the variance of the component they define. In the case of components derived from the correlation matrix of the data, these rescaled coefficients give the correlations between the components and the original variables. Those values

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are often presented as the result of a principal components analysis. The coefficients defining the principal components are given by what are known as the eigenvectors of the correlation matrix, \mathbf{R} . PCA transforms the multivariate set into a set of artificial components (principal components) based on the symmetric correlation matrix. The procedure of PCA starts with assigning eigenvalues to each component for transforming a set of multi variables into a set of components.

2.2 Multiple linear regression

Multiple linear regression is a method of analysis for assessing the strength of the relationship between a set of explanatory variables known as independent variables, and a single response or dependent variable. Applying multiple regression analysis to a set of data results in what are known as regression coefficients, one for each explanatory variable (Landau and Everitt, 2004). The multiple regression model for a response variable, y , with observed values, y_1, y_2, \dots, y_n (where n is the sample size) and q explanatory variables, x_1, x_2, \dots, x_q with observed values, $x_{1i}, x_{2i}, \dots, x_{qi}$ for $i=1, \dots, n$, is:

$$y_i = \beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + \dots + \beta_q x_{qi} + \varepsilon_i \quad (2)$$

The regression coefficients, $\beta_0, \beta_1, \dots, \beta_q$, are generally estimated by least squares. The term ε_i is the residual or error for individual i and represents the deviation of the observed value of the response for this individual from that expected by the model. These error terms are assumed to have a normal distribution with variance σ^2 . The fit of a multiple regression model can be judged with calculation of the multiple correlation coefficient, R , defined as the correlation between the observed values of the response variable and the values predicted by the model. The value of R^2 gives the proportion of the variability of the response variable accounted for by the explanatory variables. Analysis of variance (ANOVA) will provide an F -test of the null hypothesis that each of $\beta_0, \beta_1, \dots, \beta_q$, is equal to zero, or in other words that R^2 is zero.

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3 Materials and methods

3.1 Compounds, membranes and properties

A list of selected compounds is presented in Table 1; it also shows physical-chemical estimations of compound properties, such as: molecular weight (MW), dipole moment, water-octanol partition coefficient ($\log K_{ow}$), acid dissociation constant (pK_a), molar volume (MV), length, width and depth. Compounds were classified in ionic and neutral considering the acid dissociation constant, compounds with a pK_a greater than 6 or not available (N/A) pK_a were selected as neutral, otherwise were ionic, this classification is related to acidity of normal waters. Compounds were classified as hydrophilic (HL) when $\log K_{ow}$ was less than 2; and as hydrophobic (HP) when $\log K_{ow} > 2$. Values of pK_a were calculated with online software Sparc (Sparc, 2006). Octanol-water partition coefficients expressed as $\log K_{ow}$ correspond to neutral molecule forms and were calculated with software Kowwin (Kowwin, 2006). However some available experimental database values of pK_a and $\log K_{ow}$ were used. Calculation of dipole moments was carried out with commercial software Chem3D Ultra 7 (Chemoffice, 2002). Molar Volume (MV) of compounds was calculated as quotient of molecular weight (g/mol) and liquid density of compound (g/cm^3), unknown liquid density values were calculated by Grain's Method (Lyman et al., 1990). Molecular size represented by length, width, depth (current, maximum and minimum calculated by geometry) was calculated with software Molecular Modeling Pro (ChemSW, 2006). Afterwards, an equivalent width was defined as $(\text{width} \times \text{depth})^{0.5}$ to represent the width of molecules.

Anhydrous sodium sulfate and sodium chloride were obtained from Fisher Scientific. Potassium hydroxide, potassium chloride, and a buffer solution based on potassium phosphate, used for water quality maintenance, were also purchased from Fisher Scientific. Sulfuric acid was purchased from Mallinckrodt Chemicals (USA). Methyl tert-Butyl Ether (MtBE), used for GC-ECD analysis, and HPLC grade methanol were obtained from Fisher Scientific. BF, PCE, CT, CTB, and DCAA were obtained from Aldrich (USA). CF, TCE, and TCAA were purchased from Fisher Scientific (USA). IBP

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and PMD were purchased from Sigma, DCF from TCI America, PAC from Fluka. CFA, CBM and NPX were ordered from Aldrich. A summary of membrane characteristics used for PCA, is shown in Table 2.

3.2 Apparatus, analysis, equipment setup and experimental conditions

5 A membrane filtration unit SEPA cell of flat-sheet type (Osmonics, USA) was used for cross-flow tests. The system was composed of a polymeric membrane, a membrane holder, pumps with a gear type pump head, needle valves (for the feed, retentate, and permeate streams), pressure sensors, flow meters and a reservoir of 120L. Either varying the pump head speed or controlling the needle valve in the
10 retentate stream controlled the feed flow rate, the corresponding cross-flow velocity, and the trans-membrane pressure. The feed water temperature was maintained in the range (20–25°C). The total membrane surface area in the test cell was approximately 135.8 cm² and the total cross flow area in the test cell was approximately 1.45 cm². All permeates and concentrates were not recirculated but wasted in these experiments.
15 Changes in pressures permitted variation of the J_0/k ratio, a hydrodynamic condition embodying initial flux (J_0) toward the membrane and back-diffusion (k , mass transfer coefficient, a function of diffusion coefficient and cross-flow velocity) away from the membrane (Cho et al., 2000). The system recovery ratio ($Q_p/Q_f=10\%$) was controlled through the use of needle valves. Feed concentrations of compounds were 0.1 mg/L.
20 Experiments were carried out at a pH of 8 and conductivity of 300 μ S/cm conditioned with KCl. The J_0/k ratio was 1 for all experiments reported in this publication.

EPA sample vials (40 mL) with a screw cap lined with Teflon were used for sample collection and extraction. Autosampler vials used were 2.0 mL amber glass vials with a crimp cap and a Teflon-faced seal. Disposable Pasteur pipettes (9 inch) were
25 used to transfer extracted samples. Micropipettes (10–100 mL, 100–1000 mL, and 1–5 mL) with disposable tips were purchased from Fisher Scientific (USA). A mini-vortexer (VWR Scientific, USA) was used as an orbital mixer. A Brinkmann bottle top dispenser was used for adding solvent. An analytical balance (Mettler Toledo AT201) was capa-

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ble of weighing to 0.01 mg. A diazomethane reaction chamber was used for a step of HAAs analysis. The GC used was an HP 6890 series GC system with a micro electron capture detector, an HP7683 autoinjector, an autosampler tray module, and an HP PC. A DB-1 capillary column coated with dimethylpolysiloxane (30 m×0.25 mm×1 mm) was employed.

3.3 Statistical analysis

Statistical analysis was used to determine which physical-chemical properties of compounds contributed most significantly to membrane rejection. The performed statistical methods included principal component analysis (PCA) and multiple linear regression (MLR). The first step for data analysis was carried out with PCA to reduce the number of variables (physical-chemical properties) that are representative for a group of compounds. The following analysis of the reduced number of variables was performed with MLR. The statistical software package SPSS 14 (SPSS, 2005) was used for analysis. The selected method of linear regression was *stepwise*. Stepwise regression is the most sophisticated of statistical methods for multiple linear regression. Each variable is entered in sequence and its value assessed. If adding the variable contributes to the model then it is retained, but all other variables in the model are then re-tested to see if they are still contributing to the success of the model. If they no longer contribute significantly they are removed. Therefore, the method should ensure that we end up with the smallest possible set of predictor variables included in the model.

4 Results and discussion

4.1 Rejection of compounds by membranes

Table 3 presents results of rejection for compounds corresponding to the membrane with which the test was carried out. All results are from samples taken after 48 h of

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experimental running. Two membrane types were selected for experiments with all compounds: LE-440 (RO) and NF-90 (NF).

4.2 PCA for compounds and membranes

Our hypothesis is that a reduced number of variables will appropriately explain rejection qualitatively based on physical-chemical properties of compounds and membrane characteristics. In order to validate it, we formulated the following questions: i) which physical-chemical properties significantly represent a compound in a smaller set of variables? ii) which compounds depending on their properties were better rejected? iii) which membrane characteristics can describe rejection much better? Variables considered for PCA were molecular weight (MW), dipole moment (dipole), molar volume (MV), water-octanol partition coefficient expressed as $\log K_{ow}$, hydrophobicity/hydrophilicity (HP) a dummy variable that takes the value of 0 when the compound is hydrophilic (HL) and 1 when the compound is hydrophobic (HP), molecular length (length), molecular width (width), molecular depth (depth) and equivalent width (eqwidth). After the first analysis considering all mentioned variables, three principal components accounted for 82.7% of the total variance. A graph (Fig. 1a) of the first and second rotated and unrotated components shows that MW and depth presented small and variable component loadings; therefore we can neglect MW and depth.

The second test of PCA considered dipole, MV, $\log K_{ow}$, HP, length, width and eqwidth. Figure 1b shows final component loadings of variables for this PCA. According to Table 4, the first and second principal components (scaled eigenvectors), explained the largest part of the total variance, they have eigenvalues of 3.2 and 2.2, respectively; this accounts to 45.6% and 31.8% of the total variance. The third principal component has a variance of 0.7 and accounts for a further 9.9% of the variance. The cumulative % column shows how much of the total variance was accounted for by the components with eigenvalues greater than 1. The first two principal components accounted for 77.4% of the total variance. Thus, we can answer question i), we can reduce our first nine variables to seven variables that can be explained by the first two

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components of Table 4. Subsequently we answer question ii) which compounds depending on their properties were better rejected? We present Fig. 2, a graph of the first and second components scores for each compound. That plot helps to visualize the rejection patterns of the fifteen compounds. Scores on the x-axis (component 1) may indicate the overall level of rejection, while scores on the y-axis indicate possibly differences between compound properties. Clustering of compounds classified according to groups is a first notice from the graph. CF (chloroform) clearly appeared outside from the other compounds, presenting the lowest rejection (see Table 3) due to small molar volume, equivalent width and length. DCF (diclofenac) and PMD (primidone) showed high rejections related to high molar volume. CBM (carbamazepine) appears outside of the clustered group of hydrophobic-neutral compounds due to his high molar volume and dipole moment when compared to the rest of the compounds in his group. Dipole moment also influenced that CFA (clofibric acid) appeared outside of its group. Also notable was the clustering of DCAA (dichloroacetic acid) and TCAA (trichloroacetic acid), both compounds presented good rejections (Table 3); however their charge prevailed the mechanism of electrostatic instead of size exclusion mechanism influencing rejection. BF (bromoform) and TCE (trichloroethene) had low rejections due to small length and equivalent width. By contrast, CTB (carbontetrabromide), PCE (perchloroethene) and CT (carbontetrachloride) with higher equivalent width and lower values of dipole moment than BF and TCE presented better rejections.

Results of PCA for membrane characteristics presented in Figure 3a suggest that no further reduction of variables is suitable. Therefore, the answer of question iii) is not possible considering only the set of variables we have. In general nanofiltration membranes (NF-90 and NE90) presented low membrane rejection when compared to reverse osmosis membranes, excluding CTA. Figure 3b present scores for each membrane. According to this, LE-440 performed better than XLE-440; NE 90 better than NF-90, and BW-400 performed better than UTC-70 and RE BLR, in this order BW-400>UTC-70>RE BLR. Although Figure 3b describes well the rejection performances of membranes, the information provided must be analyzed and disregard misleading

results, it was the case for CTA (compare rejections Table 3).

4.3 Multiple linear regression

MLR analysis of rejections was separated for ionic and neutral compounds, and for two membranes (LE-440 and NF-90). Thus, MLR was performed for these cases: 1) ionic LE440 48h; 2) ionic NF90 48h; 3) neutral LE440 48h; 4) neutral NF90 48h. Rejection can be defined as a linear function with compound properties as variables. In general, we may assume that rejection can be described by the following linear equation.

$$\text{rej} = B_0 + B_1MV + B_2HP + B_3K_{ow} + B_4\text{Dipole} + B_5\text{length} + B_6\text{eqwidth} \quad (3)$$

Inclusion of all variables will give a R^2 value approaching 1. However the optimum output implies having the less number of variables in the equation that may explain or predict rejection with appropriate fit and significance. Thus, stepwise regression will achieve this by adding and removing variables until an acceptable statistical significance would possibly be reached. The summary of results is shown in Table 5. We can notice that our R^2 values varied between 0.435 and 0.952. Ionic compounds were less favoured in prediction and significance. The rejection prediction of ionic compounds by membrane NF-90 presented the lowest confidence (85%) and R^2 value (0.435). However, R^2 value (0.628) and significance (96%) improved for ionic compounds and LE-440 membrane. Thus, we may use the models and predictors under certain restrictions when referring to ionic compounds. The effect of charge repulsion between the membrane and those charged compounds was evident. On the other hand, neutral compounds showed acceptable R^2 values and good levels of confidence (>95%). An important observation was that MW was disregarded as predictor. According to Table 5, it seems that dipole moment may predict differences in rejection prediction for ionic compounds. The influence of molar volume (MV) was more notable for neutral compounds. A combination of MV, dipole moment and length was able to predict rejection of neutral compounds by LE-440 membrane (Fig. 4). The rejection prediction of

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neutral compounds for NF-90 membrane involved variables of equivalent width and hydrophobicity/hydrophilicity (Fig. 5). It seems that equivalent width replaced predictors MV and length as we compare NF and RO membranes.

5 Conclusions

5 A qualitative analysis of variables using principal component analysis was successfully implemented for reduction of physical-chemical compound properties that influence membrane rejection of PhACs and organic compounds. Properties of dipole moment, molar volume, hydrophobicity/hydrophilicity, molecular length and equivalent width were found to be important descriptors for prediction of membrane rejection. Ionic and neutral compounds were successfully separated before analysis. For membranes used in the experiments we may conclude that charge repulsion was an important mechanism of rejection for ionic compounds. Molecular weight was a poor property for rejection prediction. We could model membrane rejection of neutral compounds with multiple linear regression; real results were well represented by dipole moment, molar volume, length, equivalent width and hydrophobicity/hydrophilicity of compounds.

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Table 1. Physical-chemical properties of compounds.

Compound	Abbr.	MW (g/mol)	Dipole (Debye)	Molar Vol. (cm ³ /mol)	Log <i>K_{ow}</i>	<i>pK_a</i>	Mole. length (nm)	Mole. width (nm)	Mole. depth (nm)	eqwidth (nm)	Class.*
Dichloro-acetic acid	DCAA	129	2.40	82	0.92	1.48	0.7	0.69	0.52	0.60	HL-ion
Trichloro-acetic acid	TCAA	163	1.50	100	1.33	0.70	0.89	0.67	0.41	0.52	HL-ion
Ibuprofen	IBP	206	1.29	130	3.97	4.91	1.31	0.77	0.64	0.70	HP-ion
Diclofenac	DCF	296	1.48	182	4.51	4.15	1.13	0.91	0.45	0.64	HP-ion
Clofibric acid	CFA	214	0.79	155	2.57	3.64	0.95	0.66	0.41	0.52	HP-ion
Naproxen	NPX	230	2.74	167	3.18	4.15	1.26	0.69	0.54	0.61	HP-ion
Chloroform	CF	119	1.12	80	1.97	N/A	0.53	0.5	0.35	0.42	HL-neu
Primidone	PMD	218	4.31	164	0.91	N/A	0.97	0.88	0.48	0.65	HL-neu
Phenacetin	PAC	179	2.40	146	1.58	N/A	1.39	0.68	0.42	0.53	HL-neu
Bromoform	BF	253	1.00	87	2.40	N/A	0.69	0.65	0.48	0.56	HP-neu
Trichloro-ethene	TCE	131	0.95	90	2.29	N/A	0.78	0.66	0.36	0.49	HP-neu
Perchloro-ethene	PCE	165	0.11	102	3.40	N/A	0.78	0.77	0.45	0.59	HP-neu
Carbontetra-chloride	CT	154	0.30	96	2.83	N/A	0.64	0.64	0.57	0.60	HP-neu
Carbontetra-bromide	CTB	332	0.01	112	3.42	N/A	0.69	0.63	0.65	0.64	HP-neu

* HL, hydrophilic; HP, hydrophobic; ion, ionic; neu, neutral.

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Table 2. Characteristics of membranes.

Membrane	BW-400	LE-440	XLE-440	NF-90	RE-BLR	NE-90	UTC-70	CTA
Company	FilmTec	FilmTec	FilmTec	FilmTec	Saehan	Saehan	Toray	Koch
Group (Type)	PA (RO)	PA (RO)	PA (LPRO)	PA (NF)	PA (RO)	PA (NF)	PA (LPRO)	CTA (RO)
MWCO	n/a	n/a	n/a	200	n/a	200	n/a	n/a
NaCl Rej. (%)	98	98	98	90	99.5	90	99.6	98
Contact Angle (°)	57	42	40	60	47	52	54	47
Zeta Potential (mV), pH8, 10mM KCl	-4.5	-23	-19	-31	-21	-24	-15	-19
J_0 (L/m ² hr)	18	18	16	26	15	22	14	18
Oper. Pressure (kPa)	620	550	410	280	480	240	340	550
PWP (L/m ² day kPa)	0.68	0.77	0.92	2.23	0.77	2.17	0.99	0.79

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Table 3. Membrane rejection results after 48 hours.

Membrane	Compounds & rejections (%)					
	CF	TCE	BF	CT	PCE	CTB
LE-440	3	2	7	69	76	89
NF-90	0	3	0	35	39	70
BW-400	4	0	16	78	71	96
XLE-440	10	3	16	69	71	83
RE_BLR	34	33	50	90	87	99
NE90	1	0	17	52	57	70
UTC-70	9	6	34	84	57	79
CTA	27	6	2	13	2	N/A

Membrane	Compounds & rejections (%)							
	DCAA	TCAA	IBP	DCF	CFA	NPX	PMD	PAC
LE-440	77	95	91	91	87	75	83	56
NF-90	89	87	86	90	86	89	82	45

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Table 4. Principal components and total variance.

Comp.	Initial Eigenvalues			Extraction Sums of Squared Loadings			Rotation Sums of Squared Loadings		
	Total	% of Variance	Cumulative %	Total	% of Variance	Cumulative %	Total	% of Variance	Cumulative %
1	3.192	45.607	45.607	3.192	45.607	45.607	3.115	44.500	44.500
2	2.228	31.827	77.434	2.228	31.827	77.434	2.305	32.934	77.434
3	0.697	9.959	87.393						
4	0.417	5.950	93.343						
5	0.215	3.075	96.417						
6	0.160	2.292	98.710						
7	0.090	1.290	100.000						

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Table 5. Results of multiple linear regressions.

Case	R^2	Std. Error of Estimate	F	Sig.	Equation for rejection
Ionic LE440 48h	0.628	5.58	6.75	0.060	$101.104 - 8.885 \text{Dipole}$
Ionic NF90 48h	0.435	1.45	3.08	0.154	$85.184 + 1.559 \text{Dipole}$
Neutr LE440 48h	0.952	10.14	33.07	0.001	$-118.889 + 2.503 \text{MV} - 29.830 \text{Dipole} - 86.339 \text{length}$
Neutr NF90 48h	0.868	12.56	19.74	0.002	$-163.619 - 30.423 \text{HP} + 386.160 \text{eqwidth}$

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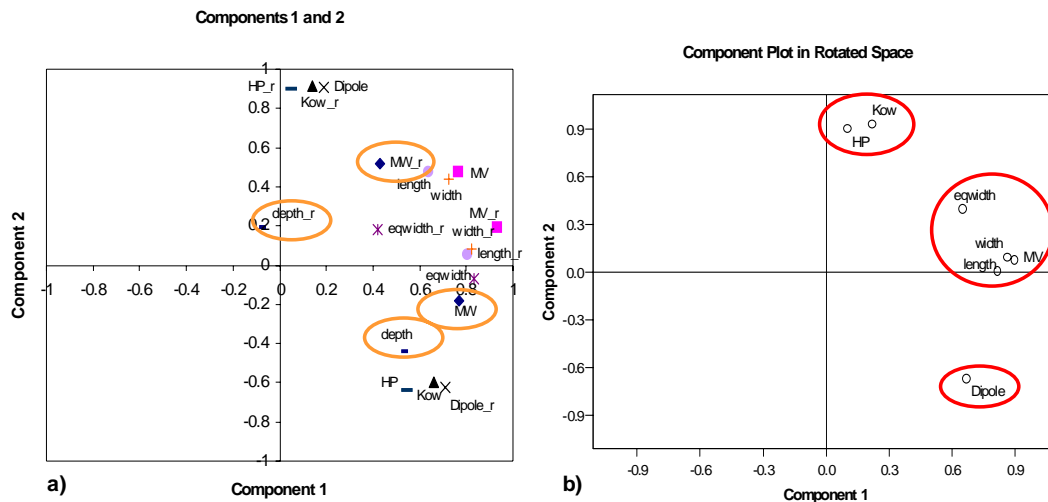


Fig. 1. (a) Component loadings for all compound variables; (b) Component loadings for reduced variables.

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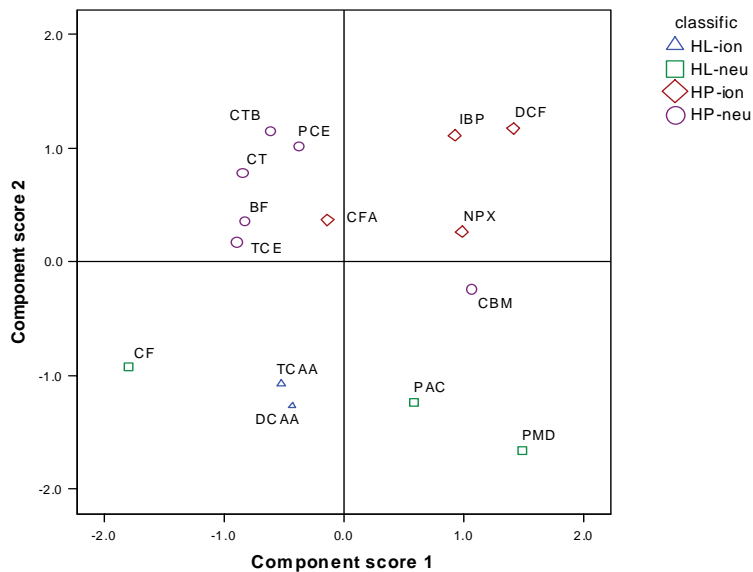


Fig. 2. Component scores for compounds.

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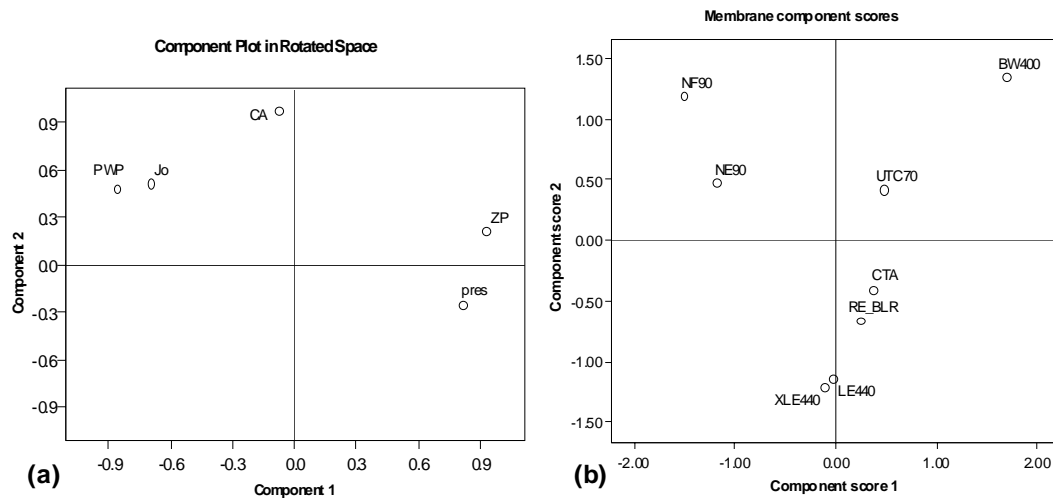


Fig. 3. (a) Component loadings for membrane variables; (b) Component scores for membranes.

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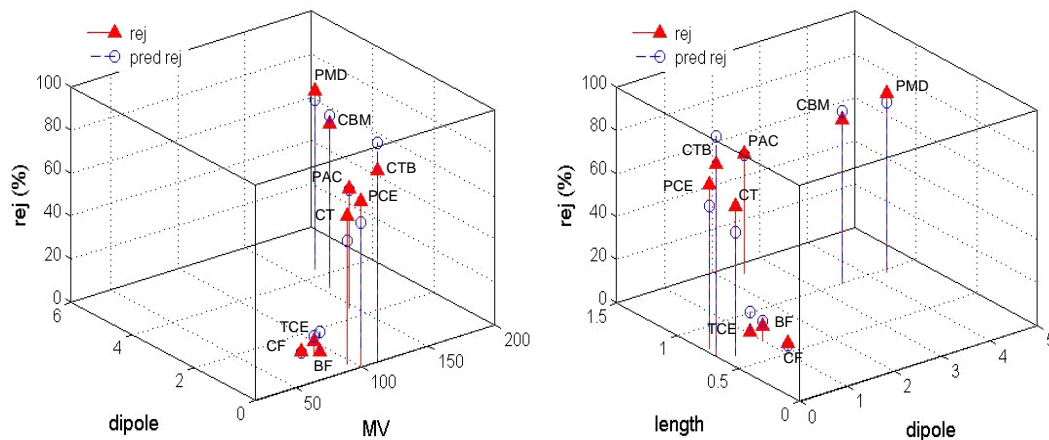


Fig. 4. LE-440 membrane rejection prediction of neutral compounds.

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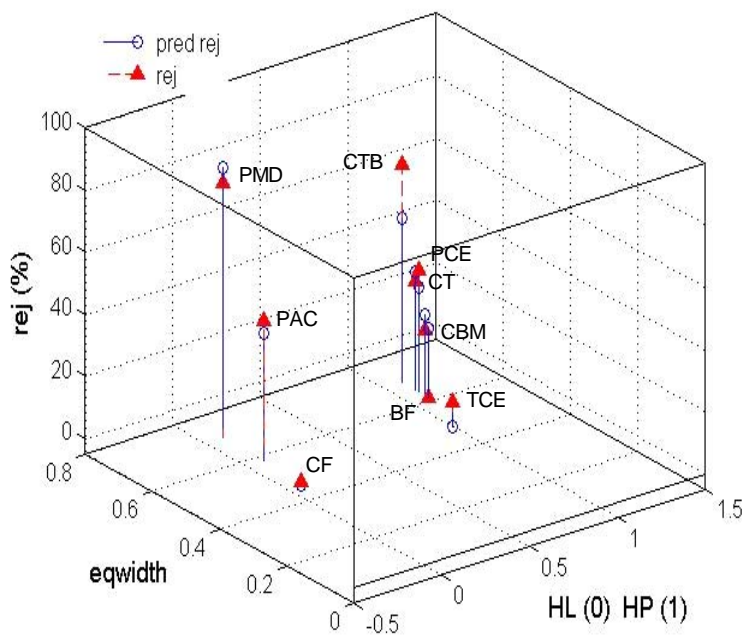


Fig. 5. NF-90 membrane rejection prediction of neutral compounds.

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