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2 Károly Héberger, Quantitative structure - (chromatographic) retention relationships: QSRR

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8 Quantitative structure - (chromatographic) retention relationships: QSRR

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26

## Abstract

Since the pioneering works of Kaliszan (R. Kaliszan, Quantitative Structure-Chromatographic Retention Relationships, Wiley, New York, 1987. and R. Kaliszan, Structure and Retention in Chromatography. A Chemometric Approach, Harwood Academic, Amsterdam, 1997) no comprehensive summary is available in the field. Present review covers the period 1996 - August 2006. The sources are grouped according to the special properties of kinds of chromatography: Quantitative structure - retention relationship in gas chromatography, in planar chromatography, in column liquid chromatography, in micellar liquid chromatography, affinity chromatography and quantitative structure enantioselective retention relationships. General tendencies, misleading practice and conclusions, validation of the models, suggestions for future works are summarized for each sub-field. Some straightforward applications are emphasized but standard ones. The sources are gathered in tables and the model compounds, descriptors, predicted retention data, modeling methods and indicators of their performance, validation of models, and stationary phases are collected in the tables. Some important conclusions are: Not all physicochemical descriptors correlate the retention data strongly; the heat of formation is not related to the chromatographic retention. It is not appropriate to give the errors of Kovats indices in percentages. The apparently low values (1-3 %) can disorient the reviewers and readers. Contemporary mean interlaboratory reproducibility of Kovats indices are about 5-10 i.u. for standard non-polar phases and 10-25 i.u. for standard polar phases. The predictive performance of QSRR models deteriorates as the polarity of GC stationary phase increases. The correlation coefficient alone is not a particularly good indicator for the model performance. Residuals are more useful than plots of measured and calculated values. There is no need to give the retention data in a form of an equation if the numbers of compounds are small. The domain of model applicability of models should be given in all cases.

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## 1. Introduction

Quantitative structure-retention relationships, QSRRs, represent a powerful tool in chromatography. What are QSRRs? The terminology is still used confusedly. Firstly 'R' may mean 'reactivity' and not retention; secondly Quantitative structure-property relationships (QSPRs) or Quantitative structure-activity relationships (QSAR) is often used instead: generally if the retention data are used as independent variables to predict properties of the molecules. Quantitative retention-activity relationship (QRAR) is also used instead of QSRR. The principal aim of QSRR is to predict retention data from the molecular structure. However, the same methodology can be used for prediction of physical properties e.g. for octanol/water partition coefficients ( $\log P$ -s) from retention data. The relationships are empirical, but a firm theoretical basis can be rendered to them using linear free energy relationships (LFERs), in these special cases linear solvation energy relationships (LSERs).

QSRR is a technique for relating the variations in one (or rarely several) response variables ( $Y$ -variables) to the variations of several descriptors ( $X$ -variables), with predictive or at least explanatory purposes.  $Y$ -variables are often called dependent and  $X$ -variables as independent variables. One of the  $Y$ - or  $X$ -variables should be related to (chromatographic) retention, the others should encode the molecular structure.

QSRRs allow the prediction of retention data of novel, not yet synthesized compounds, solely from their structural descriptors.

In many cases the precision and accuracy of the QSRR models are not sufficient for identification purposes; still the models are useful to elucidate retention mechanisms, to optimize the separation of complex mixtures or to prepare experimental designs.

One of the crucial problems is how to represent molecular structure for QSRR. Generally the descriptors encoding the molecular structure are classified as physicochemical, quantumchemical, topological, etc. descriptors. The advantage of physicochemical

descriptors is that they are generally strongly related to the retention; i.e. they correlate the retention data strongly. However, they are often not available or with relatively large errors only. The advantage of quantumchemical descriptors is that they provide insights into the mechanism of chromatographic retention on a molecular level. Their correlation is, however, weak only and their calculation is tedious and time consuming. Topological descriptors are easy to calculate with present computing facilities, but they are not necessarily related to the retention phenomena.

The second crucial problem is to select the most informative descriptors from among a large number of correlated descriptors. A lot of variable selection method has been elaborated and the proper feature selection is a key to build successful QSRR models.

Since the pioneering reviews [1,2] a lot of interesting paper appeared; new tendencies can be observed in the field. QSRR models can be used for successful classification of drugs of various compound classes and/or chromatographic columns (systems). Another interesting and increasing application of QSRRs is to test (compare) various chemometric methods. As the descriptors are highly correlated and numerous, to select the proper model building technique is not a trivial task. Moreover, many laboratories use QSRR models to demonstrate the usefulness and advantages of recently developed chemometric techniques. Similarly, QSRR models demonstrate the applicability of novel topological descriptors many times.

Although the basic book of chromatography devotes only several pages to QSRR [3], the field achieved its 'ripened' phase. Figure 1 shows the steady and 'noisy' increase of papers dealing with QSRRs.

Figure 1

The search covers the period of 1996-2006 Aug with extensive usage of 'Web of Science' and 'Scopus' data bases. The increase is not continuous; random factors also influence the number of papers dealing with structure and retention correlations.

Figure 2 illustrates the dispersion law of spreading scientific information on this special example (QSRR). The distribution is much more peaked than the normal distribution. The core journals (disseminating 50% of scientific information) can be seen from the figure 2: J. Chromatogr. A, Chromatographia, J. Liq. Chromatogr. Rel. Technol., Anal. Chim. Acta, Anal. Chem. Chemometrics Intell. Lab. Syst., J. Chem. Inf. Modeling (earlier J. Chem. Inf. Comput. Sci.).

Figure 2

The review is divided into seven parts: QSRR in Gas chromatography, Quantitative Structure Enantiomer Retention Relationships, (QSERR), QSRR in Planar Chromatography, QSRR in column liquid chromatography, QSRR in micellar chromatography, QSRR in affinity chromatography and QSRR in remaining fields.

## **2. Quantitative structure - retention relationships in gas chromatography**

### *2.1 General tendencies*

Alkanes, alkenes, alkylbenzenes, alcohols, ketones, aldehydes, VOCs and compounds of environmental relevance (PCBs, PCDFs, PBDEs, etc.) have been often used as model compounds (explanations for abbreviations can be found in the footnotes of tables). The Kovats retention index ( $I$ ) is the most popular dependent variable in QSRR studies because of its reproducibility and accuracy. Relative retention times (RRTs) are also applied many times. In some cases response factors are also predicted from molecular structure.

Best models can be built using physical properties. There is a common statement in gas chromatography that boiling point governs the retention. In fact, the volatility governs, but the vapor pressure is of exponential function of the column temperature. Hence, normal

boiling points are used as a well-defined and in many cases known quantity instead of vapor pressure. The retention index depends from the boiling points in a complicated nonlinear manner, which can be written in an exponential [4] or in a logarithmic form [5].

Multiple linear regression (MLR) is without doubt the most frequently applied technique in building QSRR models. The features and advantages of artificial neural networks (ANNs) fascinated numerous scientists. A lot of ANN study is fairly a description how to apply ANN for model building than an elaboration of a predictive model.

## *2.2 Validation of the models*

Perhaps the most sensitive problem is the validation. Validation was not required in the first, exploratory phase of QSRR investigations, when the most important approach was to unravel the potential usefulness of the method. Later, the validation became crucial. As the physical background is not unambiguous, chance correlations have to be avoided. Therefore, efforts should be done to prove that the found QSRR relationships are not fortuitous but applicable for future predictions. If sufficient data are available to split the data into three sets is recommended: one is used for model selection, the second one for parameter estimation (calibration) and the third one for external validation (cross-validation is a poor alternative instead) [6].

The general practice is to split the data into training and testing sets. However, one single training set is not appropriate to make variable selection and parameter estimation (calibration) without bias. It is not (absolute) necessary to split the training set into two; resampling methods, cross-validation (CV) would also do. The cross-validation almost unbiasedly estimates the prediction error when no feature selection has been made [7], but it is heavily biased when a large amount of model selection is applied (i.e. sifting through



thousands of models). In the latter case, the indicators of the fit are deceptively overoptimistic (inflation of the cross-validated correlation coefficient) [8].

Independently from the fact, whether the training set is split into two sets or a CV has been made, the test set should be independent from the model building and parameter estimation. The process is called then as external validation [9].

An instinctive (naïve) way is to estimate the performance of a model using randomly generated variables. The same number of variables should be simulated as was calculated for prediction of retention data. The same steps should be carried out as in the real case: variable selection, parameter estimation, prediction for ‘unknown’ compounds. The performance indicators (correlation coefficient, prediction errors) should be compared with the same values of the real case. If the variables consisted of solely random numbers indicate approximately the same fit and prediction, the models are of little value even if physical significance can be found for its parameters.

Unfortunately, there is no agreed method how to split data set into training, calibration and test sets. Of course a lot of empirical experience was accumulated, but they are also contradictory. Some algorithms ensure that no outliers or extrapolated values are placed in the test set. However, it provides an overoptimistic performance for prediction if future samples will not be gathered according to such algorithm.

Examination of the residua is often missing from QSRR studies, i.e. nonlinear relationships are overlooked in many cases.

### *2.3 Misleading practice and conclusions*

The role of temperature is sometimes described with descriptors from the molecular structure. However, the temperature dependence of retention data is determined by thermodynamic relationships and cannot be derived from structural descriptors. Similarly, the

polarity of stationary phases is related to the structure of stationary phase and not to that of solute molecules. The more polar a stationary phase the more difficult its characterization. As the polarity of stationary phase increases, the goodness of fit (the correlation) deteriorates.

The fact that ANN (or support vector machine, SVM) provides less residual error leads to the conclusion that ANN (or SVM) is better than MLR. However, less residual error can simply be the consequence of overfit. It is true; there are no accepted, correct, fair ways to compare various methods. The conclusions “Root mean square errors (RMSEs) shows the superiority of ANN over that of the MLR”, or conversely “the results of MLR equation are better than the neural network ones” say not much about the power and usefulness of the methods. If the relation is nonlinear, ANN cannot be worse than MLR provided its proper usage. Even in the case of linear relationships ANN is at least as good as MLR. However, according to the principle of parsimony MLR models are recommended because of their simplicity and their physical relevance.

Considering variable selection an error is committed often in the literature. Namely, the variable selection is made linearly and then the linearly selected descriptors are used in a nonlinear model, i.e. for ANN. This is not simply an inconsequent but a malpractice. It has already been shown that it is expedient to use the same method (linear or nonlinear) for variable selection as for parameter estimation [10].

Some authors give errors in percentage for Kovats retention indices. The apparently low values (1-3%) can disorient the reviewers and readers. The interlaboratory reproducibility for Kovats indices is about 5-10 i.u. for standard non-polar phases and 10-25 i.u. for standard polar phases i.e. 0.1-0.5% error should be achieved for a successful identification.

The domain of model applicability is rarely given for QSRR investigations though it would be essential, e.g. which boiling point range is covered, what is the retention time

domain, how far the models can be used for extrapolation, which compounds can be included and which ones should be excluded, etc.

Quantumchemical packages provide the calculations of standard heat of formation values. As a consequence many authors try to find correlations between retention and heat of formation. However, contrary to the heat of solution (heat of vaporization), the heat of formation is not related to (chromatographic) retention; at least not better than molecular mass, carbon atom numbers, chain lengths and alike. Another problem with quantumchemical packages is that they are steadily corrected and updated, reparameterized, i.e. without giving the exact version numbers the results are not reproducible.

Many authors discover fortuitous relationships again and again, e.g. slope-intercept relations or the notorious compensation effect. It is easy to prove that such a relation is a consequence of random errors unavoidably present in the measurement process. However, such a relation can be useful that a certain phenomenon belongs to the same process. Just the physical significance is questionable.

#### *2.4 Suggestions for future works*

Apolar or medium polar phases are recommended for further studies. Use the most persistent ones methyl- and phenylsilicones (OV-1, DB-5, etc.).

Alcohols are particularly recommended as model compounds because all major interactions can take place between alcohol molecules and molecules of the stationary phases. A possible association is concentration dependent. The alcohols participate in dispersive and polar (dipole) interactions and they exert to hydrogen bond donating and accepting abilities.

The correlation coefficient is not a particularly good indicator for the model performance. It should be emphasized that its value says nothing without the degrees of freedom ( $r=0.997$  is not significant at the 5% level if  $n=3$ ! On the other hand  $r=0.300$  is significant, i.e. the

correlation is not due to random effects, if  $n=100$ .) Therefore, phrases as ‘satisfactory’ or even ‘excellent’ correlation should be avoided. The readers should evaluate the performance and not the authors themselves.

Generally, simpler models are better according to the principle of parsimony.

Way of giving correlation equations should contain the predictive equation and indicators for the model performance ( $n$ ,  $R$ ,  $F$ ,  $S$ ) both for training and external test sets. The indicators are  $n$  - number of solutes involved,  $R$  - multiple correlation coefficient,  $F$  - overall Fisher statistics, and  $S$  - the residual error.  $R$  and  $F$  are indeed linear indicators, but they can be calculated for the  $Y(\text{measured})$  vs.  $Y(\text{calculated})$  linear relationship even if the calculated  $Y$  was derived from a nonlinear model (ANN, SVM, etc.) ( $Y$  can be any form of retention data, response factor, etc.) Residual analysis, too, is strongly recommended; residual plots are more useful than plots of measured and calculated values. If curvature, trend can be seen in the residua (against  $Y(\text{calculated})$ ) the model is not adequate. Either further, nonlinear descriptors should be involved or a nonlinear relationship.

The domain of application should be given within the models are able to predict properly (compound classes, congener series, limits, polarity of columns, etc.).

## *2.5 Summary of QSRR papers in gas chromatography*

The QSRR papers in gas chromatography are gathered in table 1 covering the period of 1996-2006.

Table 1

“Isomer cluster[ing] phenomena” have been observed for a variety of monofunctional and some multi-functional compounds, i.e. isomers containing the same carbon numbers are always located on parallel lines (different numbers of methylene groups are found on

different lines) if the Kovats indices of homologous compounds are plotted on two stationary phases of different polarity [15].

Deviations from the linear boiling point correlations indicate host-guest interactions on cyclodextrin stationary phases [24,72]; e.g. bicyclic camphene is retained behind myrcene though its boiling point is appreciably smaller.

The elution orders and coelutions of all 209 PCB congeners can be predicted using a data base and structure retention correlations and congener substitution patterns [28].

Prediction of the retention indices of any organic compounds with known boiling points became possible using a three-parameter non-linear equation:

$$\log I = a \log T_b + b(n_1 + \sum k_i n_i) + c \quad (1)$$

where  $n_1$  is the serial number of homologue within corresponding series and  $n_i$  is the number of other structural fragments in the molecules. The coefficients  $k_i$  in this equation reflect the relative alterations of molecular polarizabilities and may be estimated as ratios of refractions  $k_i = R(D)(X)/R(D)(CH_2)$ , (X are variable structural fragments within a group of congeners,  $R(D)(CH_2) = 4.647 \text{ cm}^3 \text{ mol}^{-1}$ ) [5].

Factor analysis (FA) was performed to interpret the meaning of the descriptors included in the models [26]. Hydrocarbons were successfully classified into paraffins (P), olefins (O), naphthenes (N) and aromatics (A) using FA [48]. Differentiation of ketones and aldehydes has been carried out by principal component analysis (PCA) [49]. PCA, a factorial design was applied for selecting 21 representative congeners, PBDEs. The spacing of these congeners in the physicochemical domain maximizes the coverage of key factors such as molecular size and substitution pattern [94].

Using the same QSRR methodology response factors can also be predicted [39].

Theoretical prediction of gas-chromatographic retention indices could be used as an additional method for the identification of organic substances during gas-chromatographic separation [40].

The thermodynamic interpretation were given to retention time- boiling point correlations using the Trouton's rule, i.e. physical significance can be attributed to empirical QSRR equations [32]. Later the physical significance could be extended using the Trouton-Hildebrand-Everett's (THE) rule [43]. Heats of vaporization, Gibbs free energies [33] and Gibbs free energy of vaporization of one methylene group ( $\text{CH}_2$ ) of n-alkanes [46] can be calculated from QSRR equations (boiling point correlations of retention indices). A sophisticated relationship was elaborated between retention time and carbon atom number; the related thermodynamic quantities of solvation can be calculated [41].

The semiempirical topological index can help in the elucidation of the molecular structure [47,113].

Some data sets became standards for further QSRR investigations: for apolar interactions, methyl-alkanes [59], for polar interactions, oxo compounds [49].

Partition coefficients ( $K_p$ ) in a heterogeneous system consisting of two immiscible organic solvents can be successfully used for a supplementary identification parameter in qualitative GC and GC-MS analysis of organic compounds including alkyl aromatic hydrocarbons and esters, group identification of components [72].

The correlations serve as a basis for physicochemical interpretation of the topological parameters of molecules as quantities proportional to the intramolecular vibrational and rotation energies [87].

If GC-MS library search "hit list" matches the retention index of the unknown, there is a strong presumption that a correct identification can be made [119].

Quantitative prediction of normal boiling points for organic compounds using chromatographic retention times on two columns of different polarity. Only hydrocarbons on nonpolar columns gave good results with a simple linear model [126].

The only review found concerning gas chromatography was in Chinese language [146].

### **3. Quantitative structure - enantioselective retention relationships, QSERR**

Enantiomer separations are difficult to predict. Present status of solution theories does not make possible an unambiguous prediction. Nevertheless, enormous amount of empirical knowledge was gathered. Commercial data bases (CHIRBASE and CHIRSOURCE) contain more than 61 000 separation [3]. As large number of chiral stationary phases is available, the success rate in enantiomer separations is quite high. The efforts to rationalize chiral separation using QSRR methodology have achieved limited success only. QSERR models provide some insights into the role of various interactions, but they are not able to recognize chiral selectors for a particular separation. One of the crucial problems is the selection of suitable molecular descriptors. The other problem is that the available congener series are small, the small number of compounds involved exclude the proper validation of models. Even the elution order (whether R or S enantiomer elutes first) is uncertain. A QSERR can be used as an alternative method to confirm the elution order of enantiomers. The prediction of elution order can be considered as a classification study from a chemometric point of view.

#### *3.1 General tendencies*

Only one review is available in Chinese [172]. A common feature of QSERR investigations is that the authors attempt to use quantumchemical and 3D descriptors in linear

355 regression. Chiral descriptors are rarely applied. The elution order of the enantiomers can be  
356 predicted from the interaction energy calculated by molecular mechanics.

### 358 3.2 Misleading practice and suggestions for future works

359 The prediction performance of models is questionable. There is no need to give the  
360 retention data in a form of an equation, if the numbers of compounds are small. The retention  
361 data, the selectivity for enantiomeric separation ( $\alpha$ ) can be used directly for identification, for  
362 determination of absolute conformation. The conclusion that e.g. ‘molecular mechanics is  
363 suitable to study chiral separation’ is either trivial or not true. The small number of  
364 compounds involved in the studies cannot make proper validations feasible. Hence,  
365 validation is missing from the contributions with several exceptions.

366 Any model providing elution order of enantiomers has an *a priori* success rate of 50%.  
367 Sign test and other test based on binomial distribution could show whether the predicted  
368 elution order is accidental or bear definite physiochemical relevance. As the number of  
369 compounds is generally small, careful internal validation (leave-one-out, leave-multiple-out)  
370 is recommended.

### 372 3.3 Summary of QSERR papers

373 Table 2 gathers the QSERR examinations covering the period of 1996-2006.

374 Table 2

375 One example is emphasized, where hundreds of descriptors have encoded resolution for  
376 chiral separation successfully [195].



## **4. Quantitative structure - retention relationships in planar chromatography**

### *4.1 General tendencies*

Wang and Zhang have summarized the developments till 1999 [1] Moreover, Cserhati and Forgacs have critically evaluated how to calculate quantitative relationships between molecular structure and retention data, and how to determine physicochemical parameters by TLC [2]. Only the sources not covered in these reviews are enumerated here.

Physicochemical parameters, topological indices, non-specific parameters, and their combinations are used generally as descriptors. QSRRs in TLC are used for prediction of retention and determination of lipophilicity (and other physicochemical constants).

As TLC is a rapid, low-cost, simple method, the best TLC systems are routinely selected for determination of the octanol/water partition coefficient and thus the lipophilicity of the molecules.

### *4.2 Misleading practice and conclusions*

The prediction performance of models has not been examined. Correlations can be found frequently by chance, especially if the number of descriptors is large. As the number of substances is limited on a plate the validation of models is often missing from the contributions. The conclusions such as ‘correlations can be found between lipophilicity (hydrophobicity) and retention data’ are trivial or at least well-known for a long time.

### *4.3 Suggestions for future works*

The plates are of limited magnitudes; hence, QSRRs can be developed for a limited number of solutes. The mobile phases can be varied more extensively than in the case of

HPLC. As the number of compounds is necessarily small careful internal validation (leave-one-out, leave-multiple-out) is recommended.

#### 4.4 Summary of QSRR papers in planar chromatography

Table 3 summarizes the solutes, methods and techniques for QSRR models in TLC.

Table 3

### 5. Quantitative structure - retention relationships in column liquid chromatography

Despite the ever increasing usage of HPLC for the separation and analysis of various compounds, drugs, metabolites, etc., the selection of chromatographic conditions is still a tedious, time-consuming procedure mainly governed by trial and error approaches. A priori knowledge of the retention time of a given solute simplifies the selection of conditions. No wonder that the mainstream is to rationalize and to predict retention data using available and interpretable descriptors.

Although linear solvation energy relationships have similarly been defined for gas and liquid chromatography data, LSER has not gained general usage in gas chromatography, but in liquid chromatography, where LSER is used to predict retention data, to predict physical properties of solutes and classify chromatographic columns. The LSER equation for liquid chromatography is as follows [221]:

$$\text{Solute Property} = c + eE + sS + aA + bB + vV \quad (2)$$

where solute property can be of any kind, e.g.  $\log k'$ ,  $\log P$ , etc.;  $E$  is the excess molar refraction ( $R_2$ );  $S$  is the dipolarity/polarizability ( $\pi_2^H$ );  $A$  is the overall hydrogen bond acidity ( $\Sigma\alpha_2^H$ );  $B$  is the overall hydrogen bond basicity ( $\Sigma\beta_2^H$ );  $V$  is the McGowan volume ( $V_x$  in

[cc mol<sup>-3</sup>]);  $c$  is a constant (intercept, off-set, e.g.  $\log k_{\text{ref}}$ );  $e$ ,  $s$ ,  $a$ ,  $b$ ,  $v$  are regression coefficients of the multilinear model. Eq. (1) has been designed to deal with transfers from one condensed phase to another. In gas chromatography instead of the McGowan volume the gas-hexadecane partition coefficient is used:  $\log(L_{16})$ , which accounts for the transfers from the gas phase to a condensed phase.

LSER includes cavity formation/dispersive interactions ( $V$ ), dipolarity/polarizability interactions ( $S$ ), and hydrogen bonding interactions ( $A$  and  $B$ ). The outcome of a LSER analysis is a set of regression coefficients which provide us with information about which solute-solvent interactions significantly affect the retention process. The coefficients ( $e$ ,  $s$ ,  $a$ ,  $b$ ,  $v$ ) are related to the chemical nature of the mobile and stationary phases, and their values can be determined easily. It should be mentioned that the regression coefficients are interrelated (coupled) similarly to the Abraham descriptors ( $E$ ,  $S$ ,  $A$ ,  $B$ ,  $V$  or  $L$ ) i.e. they do not carry independent information. Recent (unpublished) examinations on the data of ref. [221] show that two to four (on average three) independent (orthogonal) coefficient would be sufficient to represent the retention phenomenon properly (depending on the method used for determination of independent parameters). This finding has been supported by separate examinations [222].

LSER models can be applied with very large variations in chromatographic conditions. Using a relatively small set of model compounds predictions can be made well outside of the model domain. This implies that LSER models are general and indeed the LSER explanation for partitioning is generally accepted. On the other hand LSER models are typically not accurate enough for prediction purposes. LSER models contribute mainly to the general understanding of partition processes and less to optimize separations.

Linear relationships were established for a set of compounds between logarithm of retention factor ( $k$ ) and volume fraction of organic modifier ( $\phi$ ):

$$\log k = \log k_w - S\phi \quad (3)$$

where  $S$  is the slope, and  $\log k_w$  is the intercept.  $S$  versus  $\log k_w$  correlations are chemically meaningful for a non-homologous series of compounds.

The hydrophobic-subtraction model assumes that first the major contribution of hydrophobicity is subtracted from the retention in reversed-phase liquid chromatography (RP-HPLC). Such a way the remaining contributions to retention from other solute-column interactions can be established. The general formula for retention ( $k$ ) and column selectivity ( $\alpha$ ) is given by Snyder et al.:

$$\log \alpha \equiv \log k/k_{\text{ref}} = \eta' H - \sigma' S^* + \beta' A + \alpha' B + \kappa' C \quad (4)$$

where  $k_{\text{ref}}$  - non-polar reference solute. The coefficients denote properties of the solute:  $\eta'$  - hydrophobicity;  $\sigma'$  - molecular “bulkiness” or resistance to insertion of the solute into the stationary phase;  $\beta'$  - hydrogen-bond basicity;  $\alpha'$  - hydrogen-bond acidity  $\kappa'$ , approximate charge (either positive or negative) on the solute molecule whereas parameters denoted by capital letters are complementary properties of columns:  $H$  - hydrophobicity;  $S^*$  - steric resistance to insertion of bulky solute molecules into the stationary phase;  $A$  - column hydrogen-bond acidity,  $B$  - column hydrogen-bond basicity,  $C$  - column cation-exchange activity, (hence  $C$  is pH dependent).

Snyder’s parameters are tabulated for more than 300 columns [223]. Eq. (4) is suitable for prediction and optimization of RP-HPLC separations.

### 5.1 General tendencies

Linear solvation energy relationships (LSERs) are abundantly used for characterization of stationary phases (polymers). Another important aspect is to determine lipophilicity (hydrophobicity) parameters from retention data. The reference scale for lipophilicity (logarithm of partition coefficient denoted by  $\log P$  and determined in the 1-octanol-water

partition system) is accepted broadly. As the conventional determination of  $\log P$  is tedious and lacks the acceptable interlaboratory reproducibility, alternative scales based on chromatographic retention have been defined to measure lipophilicity. The reversed-phase high - performance liquid chromatography, i.e. the partition of a solute between a polar, aqueous mobile phase and a nonpolar stationary phase appeared to be especially suitable for lipophilicity determinations. Rational drug design have profited a lot using fast screening HPLC methods.

Fundamental relationships between chromatographic parameters are reviewed from the point of view of convenient and reliable lipophilicity measurements [298].

As theoretical basis exists to rationalize the main effects of retention many colleagues do not feel to be bounded to validate QSRR models for liquid chromatography. Since the millennium the number of validated models is increasing.

## *5.2 Misleading practice and conclusions*

Statements as “the model describes the retention of ... compounds under .... conditions very well” says not much about the achievements. The description is not inevitably necessary as the retention data for *these* compounds under *these* conditions are available in tabular form. A prediction of retention data for not yet measured compounds would be a real gain. However, this should be checked and proved by cross-validation or external validation. Other valuable aims could be the rationalization of measured data and classification of column/system properties, but we should not forget that such rationalizations for the same/similar compounds are available from renowned authors abundantly. Similarly, numerous classification schemes are available, but none of them achieved general usage.

The correlation coefficients are often given without the degrees of freedom; cross-validated correlation coefficients are also missing in many cases.

Concluding remarks as “The predicted values are in very good agreement with the experimental values” say very little about the real prediction performance, they should be avoided.

There is some ambiguity in the usage of ‘test analytes’ and ‘test sets’. Test analytes form the training set whereas a new independent series of compound serve for testing the prediction performance. The prediction set is often called as test set in chemometrics.

The statements as “ANN predicts the retention data better than MLR method” has little relevance (see the text in gas chromatography part).

### *5.3 Suggestions for future works*

The domain of model applicability is rarely given for QSRR investigations in liquid chromatography, neither. Although mobile phase concentrations are provided, which compounds can be included and which ones should be excluded from the investigations are missing.

Properly validated models should be recommended for prediction purposes. The same performance indicators (adjusted correlation coefficients, cross-validated correlation coefficients, F values, standard errors, etc) should be used for comparison.

Standardization of optimization strategies for chromatographic separation conditions would provide great benefit if using QSRR equations.

### *5.4 Summary of QSRR papers in column liquid chromatography*

Table 4 summarizes the solutes, methods and techniques for QSRR models in column LC (correlation coefficients are in brackets).

Table 4

The basicity of solutes has a larger effect on the retention of the PBD-zirconia phase than of conventional bonded phases. Strong hydrogen bases and highly dipolar solutes, when compared to nonpolar ones, are less strongly retained on PBD-zirconia than on conventional phases [224].

A (good) linear correlation was obtained between the gradient retention time values and the isocratically determined  $\phi_0$  values for 76 structurally unrelated compounds. The constants of this linear correlation can be used to calculate chromatographic hydrophobicity index, CHI [238].

The assignment of HPLC peaks to their corresponding compounds in libraries of single compounds can be made on the basis of the correlation of the retention times with the different substituents in the variable positions of the molecule. The correlation is performed automatically by a new algorithm which is part of the computer program LIBFINDER [244].

Lipophilicity parameters, CHI and  $\log k_{50}$  are moderately correlated with  $\log P$  (water/octanol), and both can be used as alternative measures of lipophilicity. Analysis using the general salvation equation of Abraham shows that the solute factors that influence CHI and  $\log k_{50}$  are not entirely the same as those that influence  $\log P$ , so that neither CHI nor  $\log k_{50}$  can be used as a direct measure of  $\log P$  and *vice versa*. However, the factors that influence CHI are qualitatively and quantitatively the same as those that influence  $\log k_{50}$  [251].

Using 3D descriptors variable-reduced models resulted in considerably better predictions, although these were not as good as for those models obtained by means of classical physical-chemical descriptors [257].

QSRR investigations may reveal non-congeneric behavior of similar compounds [266], but the problem remains whether an extraordinary high lipophilicity will cause outlying biological activity or not.

Properly designed test series of analytes can be recommended for comparative studies of analytical columns. QSRRs once derived on a given column for model analytes can be used to predict the retention of other analytes of a defined structure. That in turn can facilitate the procedure of the rational optimization of chromatographic separations and can characterize modern stationary phases (systems) in an objective, quantitative manner [274].

The linear solvent strength (LSS) model + QSRR approach has been demonstrated to provide approximate, yet otherwise unattainable, a priori predictions of gradient retention of analytes based solely on their chemical formulae [302].

Solute polarity descriptor ( $p$ ) is useful to transfer retention data between solvents and/or columns. The retention for any chromatographic systems (mobile phase composition) can be predicted using the five solvation descriptors (Eq. (1)), if the polarity of the column has been characterized using a small training set. Alternatively,  $\log P$  and hydrogen-bond acidity data can be used for these predictions [313].

Numerous correlations of retention data with an octanol-water partition coefficient have been reported. K. Valko has reviewed lipophilicity correlations and alternative lipophilicity measures [315].

A comparison of chemometric methods based on predictive performance indicated the most important variables and that, individually, genetic algorithm selected descriptors with multiple linear regression modeling outperformed all other models [335].

## **6. Quantitative structure - retention relationships in micellar chromatography**

Micellar liquid chromatography, micellar electrokinetic chromatography, micellar electrokinetic capillary chromatography, biopartitioning micellar chromatography, liposome



electrokinetic chromatography, and microemulsion electrokinetic chromatography are indexed under this heading. Although physicochemical principles of separation are different in case of electrokinetic and non-electrokinetic methods, the two types were merged here. There is no use to fragment the review further.

The separation system in micellar electrokinetic chromatography (MEKC) consists of a homogeneous distribution of charged surfactant micelles in an electrolyte solution. Provided that the velocity of the micelles in a defined direction is different to the velocity of the bulk electrolyte solution in an electric field a separation of neutral solutes is possible.

#### *6.1 General tendencies*

Generally correlations are searched between retention data in micellar liquid chromatography (MLC) and different measures for hydrophobicity ( $\log P$ ). Diverse chemical compounds, substituted benzenes, drugs, pesticides, etc. are frequently used as model compounds.

Pharmacodynamic quantities, toxicity values, bioconcentration factors can preferably be predicted with micellar chromatography. The retention often serves as independent ( $X$ ) variable; the method sometimes called QRAR, i.e. quantitative retention- activity relationships.

#### *6.2 Misleading practice and suggestions for future works*

In this first phase of the research the potential of the new method is used to be revealed. Hence, chemometric methods, encoding the molecular structure and cross-validation, are rarely used. After the rationalization of measured data multivariate methods will be applied with proper validation in the near future.

### 6.3 Summary of QSRR papers in micellar chromatography

Table 5 summarizes the solutes, methods and techniques for QSRR models in micellar chromatography (correlation coefficients are in brackets).

Table 5

A migration index (MI) concept, a novel scale for measuring the hydrophobicity of neutral solutes, was extended to anionic solutes. The MI values of anionic solutes correlated very well with  $\log P$ , whereas the RP-HPLC retention parameter ( $\log k'w$ ), which is also used as a hydrophobicity scale, correlated very little with  $\log P$  for the examined anionic solutes [341].

A measure of the hydrophobic character of such amphoteric compounds (as the studied sulfonamides), could be the values of the retention coefficient determined at pH of the isoelectric point [351].

Biopartitioning micellar chromatography (BMC) based models may be a useful to screening new chemicals in the early stage of development and to select safer chemicals [356].

The retention of compounds in MLC using Brij 35 surfactant is able to describe and predict pharmacokinetic and pharmacodynamic parameters of non-steroidal anti-inflammatory drugs. QRAR model is a model which can estimate the pharmacokinetic and pharmacodynamic parameters of new compounds in vitro [359].

The chromatographic retention of any molecule in BMC, independently of its family, can be adequately described by its hydrophobicity (expressed as  $\log P$ ) and its anionic and cationic total molar charge [363].

## 7. Quantitative structure - retention relationships in affinity chromatography

Affinity chromatography (AC) and immobilized artificial membrane (IAM) chromatography are indexed under this heading. Affinity chromatography where biomacromolecules form the stationary phase became an important tool in rational drug design. AC models the drug-receptor interactions. Structural requirements of specific binding sites on biomacromolecules are also revealed. Protein based stationary phases can be used for enantiomer separations (c.f. QSERR, see there) as all proteins are in fact chiral, AC can be applied to elucidate the molecular mechanism of enantioseparation on natural biopolymer stationary phases, hence rational selection of chiral columns for specific analytical separations is enhanced.

Affinity chromatography plays an important role in rational drug design because the efficiency of finding new drugs is enhanced. Moreover, it can reduce the tedious experiments of in vivo screenings. Strictly speaking refs. [377,385] do not belong to artificial membrane chromatography as no biomacromolecules form the stationary phases. However, receptor binding, affinity is modeled; hence these references are also included.

### 7.1 General tendencies

AC followed by chemometric data evaluation (searching QSRRs) provides information on both the solute molecules and the macromolecules forming the stationary phases. QSRR equations derived for selected solutes (often drugs) can be interpreted in terms of structural requirements of the specific binding sites on macromolecules. Multiple linear regression of affinity-chromatographic data increases the speed of search for new drugs. Specific high-performance affinity-chromatographic separations can be optimized by rational selection of chiral columns, the characteristics of which are provided by QSRR.

The main efforts concern to find lipophilicity measures from IAM chromatography, i.e. a lot of work is devoted to relate hydrophobicity parameters ( $\log P$ ) and retention date on AIM phases.

## *7.2 Misleading practice and suggestions for future works*

Chemometric analysis is over and over again limited to linear regression, to search correlations. Although the way of giving correlation equations is appropriate, considerably more information could be extracted if using multivariate methods.

Calculation of descriptors encoding of the molecular structure and cross-validation are rarely used. It is easy to foreseen that multivariate methods will be applied with proper validation in the near future.

## *7.3 Summary of QSRR papers in affinity chromatography*

Table 6 summarizes the solutes, methods and techniques for QSRR models in affinity chromatography.

Table 6

Detailed reviews are available abundantly [370,374-376,383,384].

A good chromatographic model of skin permeability has been determined solely by a lipophilic property,  $\log k$ , which was measured on an immobilized artificial membrane column [369].

Immobilized human serum albumin (HSA) could be used to estimate plasma protein binding [372].

The IAM-retention is governed by hydrophobicity factors for carboxylic compounds, followed by electronic effects due to polarizability in second place. Moreover, it can be

concluded that the ratio of polarizability and hydrophobic effects is not the same toward IAM phases and biological membranes [381].

Negatively charged compounds bind more strongly to human serum albumin than it could be expected from the lipophilicity of the ionized species at a certain pH values. Several compounds showed stronger HSA binding than could be expected solely from their lipophilicity [382].

It is possible to classify potential drug molecules on the basis of QSRR analysis of retention data. Artificial neural network models utilize structural descriptors and predict pharmacological properties. Such a way diminishing the number of biological assays in the search for new drugs becomes possible [385].

## **8. Remaining quantitative structure - (chromatographic) retention relationship studies**

Mainly ion exchange systems are gathered under this heading. Other studies cannot be easily classified into the preceding groups: supercritical chromatography, fragmental approach, etc. Therefore, general tendencies, etc. have no relevance here. In ion exchange chromatography protein retention data are predicted in several cases with advanced chemometric methods e.g. with support vector machines. Whether simpler tools would do - remains unknown.

Table 7 summarizes the solutes, methods and techniques for QSRR studies, which cannot easily be categorized in the former groups.

Table 7

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1907     Standard English transliteration was applied for names, e.g. á → a, ñ → n, etc.

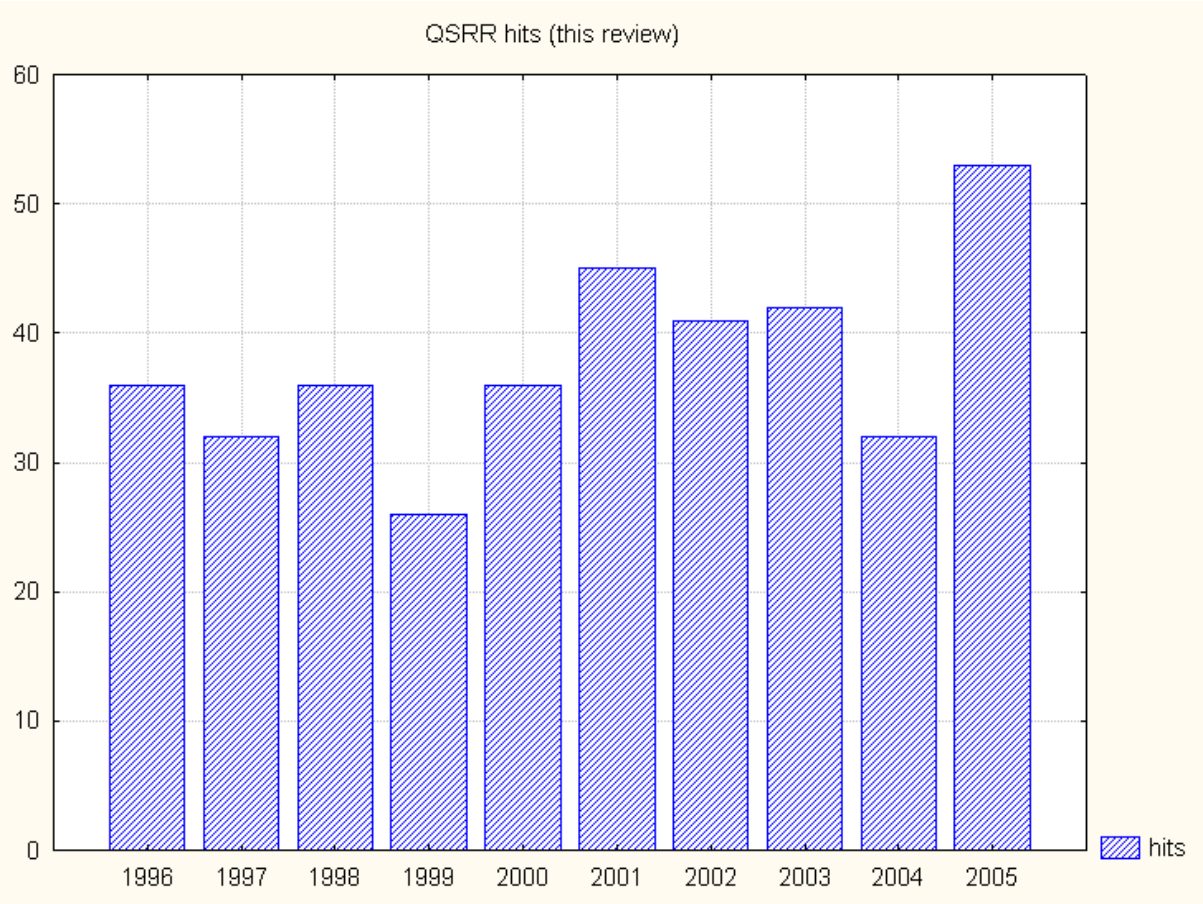
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1910     **Captions to figures**

1911     Figure 1

1912     Number of scientific papers dealing with QSRR within 1996 - 2006.



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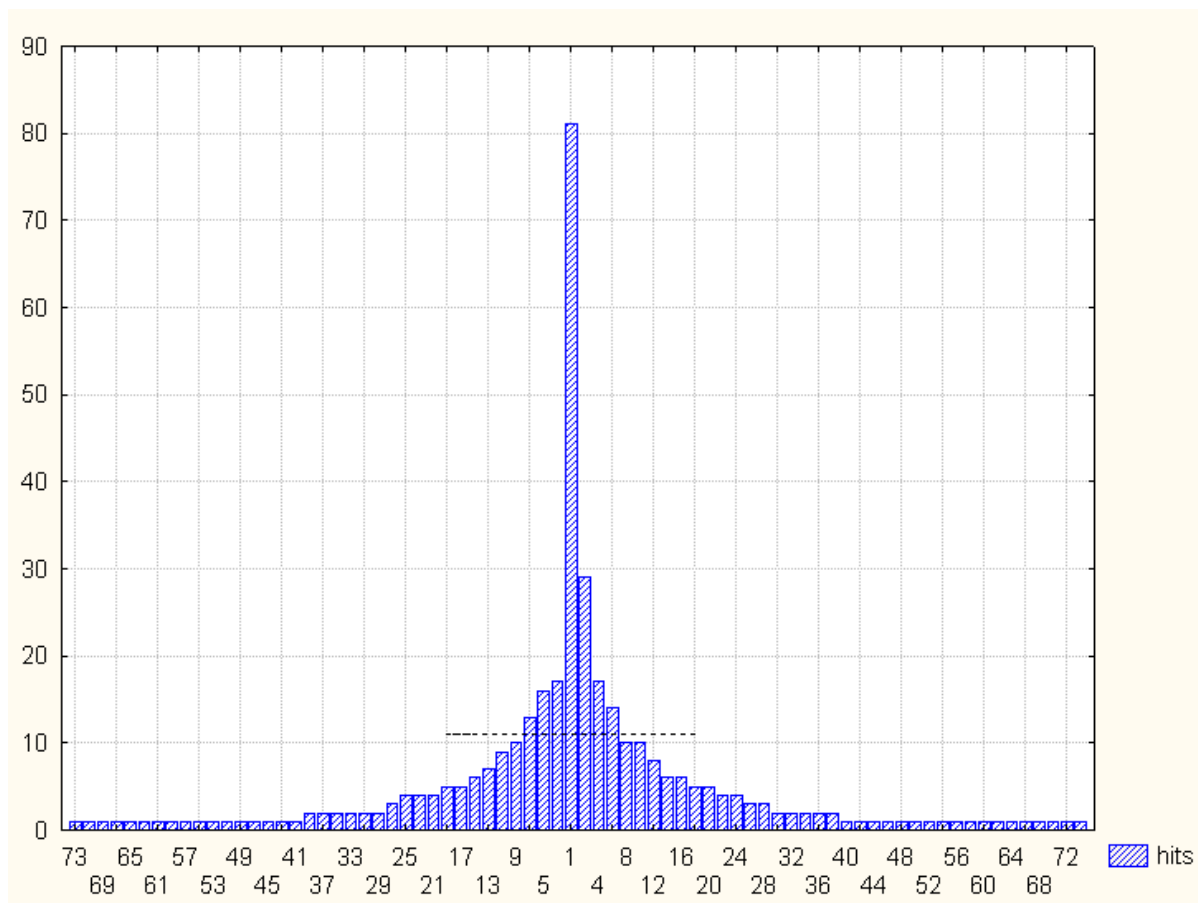
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1915 Figure 2

1916 Occurrence (frequency) of QSRR papers versus rank ordering of scientific journals within

1917 1996 - 2006.



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Table 1 QSRR in gas chromatography 1996-2006

Solutes	Descriptors	Model building	Stationary phase (SP)	Validation	Source
Linear alkylbenzene isomers with C <sub>10</sub> -C <sub>14</sub> linear alkyl chains	Balaban, Wiener, Electrototopological state and molecular shape indices	<i>I</i> , MLR		No	[11]
37 organosulfur compounds (vesicants)	Quantumchemical MNDO, PM3, AM1	MLR	three	No	[12]
Various examples	Homomorphic factors, topochemically equivalent increments	<i>I</i> , Additive schemes		No	[13]
Alkyl groups	Internal molecular energies of reactants and products	<i>I</i> , increments			[14]
Homologous series and their branched-chain isomers (1000)	Retention data on other SPs	<i>I</i>	Two various	'Relative higher accuracy'	[15]
Congener series of substituted benzenes, benzaldehydes and acetophenones	Different set of topological parameters	<i>I</i> , Correspondence factor analysis CFA	Six OV (Ohio Valley) i.e. (methyl-phenyl-siloxanes)		[16]
Polychlorinated biphenyls (PCBs)	Physicochemical descriptors (52): ultraviolet (UV) absorption spectra, semiempirical parameters (AM1): heat of formation, dipole moments, ionization potential and the barrier of internal rotation, GC retention times	PCA		No	[17]
N,N-Dialkylhydrazones	<i>T<sub>b</sub></i> , homomorphic factors, bond angle and electron density { <i>I</i> (oxo)}, volumes, van der Waals' surface.	<i>I</i> , Simple linear	HP-1, HP-5	Visual	[18, 19]
38 isoalkanes and 24 alkenes	substantial, important, likely and	<i>I</i> , MLR	Squalane,	1.6 < SD < 9.7	[20]

Aromatic analytes, positional isomers of xylenes, ethyltoluenes and diethylbenzenes	specific parameters, (quantumchemical)	RRT	citroflex, carbon black		[21]
PAHs (70)	$T_b$ , vaporization enthalpy, molecular total energy	$I$ , linear, nonlinear (Etot)	Fused-silica with calixarene oligomers	No	[22]
Anabolic steroids, stimulants and narcotics	Molecular characteristics		Methylsilicone, Carbopack		[23]
Low-polarity solutes (9) e.g. camphene, $\alpha$ -terpinene, myrcene	$T_b$	RRT, linear (0.994)	Six different modified $\alpha$ -, $\beta$ - and $\gamma$ -cyclodextrin	No	[24]
Cyclic alkanes, alkenes, alcohols, esters, ketones (C4-C10, O1-O2)	Topological (8), chemical (4)	$I$ , CP-ANN (0.892 – 0.928), SOM	Squalane, OV-1	Training and test set, 35<RMS<43	[25]
Alkylbenzenes (150)	Topological, geometric, electronic, no physical descriptor	$I$ , BP-ANN	Carbowax 20M	Training and test set, RMS(MLR)=22, RMS(ANN)=19	[26]
Compounds from Ylang-Ylang essential oil (48)	Topological, geometric, electronic	$I$ , MLR, PCA	DB-1, DB-wax		[27]
Flavonoids (49: flavones, Flavonols, flavanones, a chalcone)	Topological, geometric, electronic	Reciprocal RRT, MLR (0.975),	Apolar column	SD=0.12	[28]
Alkenes	Conformational E, no of quaternary C atoms	$I$ , MLR (0.9957-0.9987)	Graphitized carbon black	7<SD<14	[29]
All PCB congeners (209)	Congener substitution pattern				[30]
Monoterpenes, monoterpenoids homologues and isomers	$T_b$	$I$ , biparameter linear		Error< interlaboratory scatter	[31]
Allylic alcohols and unsaturated esters	Fragments increments n- $\pi$ orbital overlap of lone pairs	$I$ , Additive schemes	Polar and non-polar	Deviation<3.00%	[32]

Alkylbenzenes (18)	C=C bonds $T_b$ , reciprocal $T_b$	RRT, exponential (0.9585-0.9967)	Silicon oil 550, dinonylphthalate, PEG4000, Bentone 34	0.047<SD<0.42	[33]
Alkylbenzenes (18)	$T_b$ ,	$I$	- “ -	Theoretical derivation	[34]
Aliphatic alcohols, aldehydes, acids and amines	Orthogonalized descriptors	PCA		No	[35]
Organic compounds, homologues, congeners	$T_b$ , structural fragments, molecular polarizabilities	$I$ , linear- logarithmic	Dimethylpoly- siloxane	$I \sim 5/10$ i.u.	[5]
Acyclic and cyclic alkanes, alkenes, alcohols, esters, ketones and ethers (184)	Molar volume, $T_b$	$I$ , BP-ANN	Not given	Cross-validation and leave-20%-out	[36]
PAHs (100)	Pseudo-conjugated $\pi$ -system surface ( $S(\pi)$ ) and quasi-length of carbon chain ( $N'$ )	$I$ , bilinear (0.9968)	SE-52	7.1< $S$ <10.3	[37]
PCBs	3D WHIM,	RRT, solubility, logKow, MLR, GA	Not given	Leave-one-out, leave-multiple-out, SEC= SEP=0.023	[38]
Various organic compounds	Total energy,relative effective mass and number of carbon atoms, minimum valency on H atoms, etc	RF (0.956), MLR, BP-ANN		Two prediction sets, 5.0<SEP<7.1	[39]
Acyclic, cyclic alkanes, alkenes, dienes, ketones aldehydes ethers, aromatic hydrocarbons C3-C11 O1-O2 (381)	Informational and topological structural descriptors (16)	$I$ , MLR (0.987), BP-ANN (0.990), CP-ANN (0.969)	Squalene	LOO, 10 fold CV, average RMS: 19 (BP-ANN), 22.5 (MLR), 36.1 (CP- ANN)	[40]
n-Alkanes	Backbone carbon atom number	$k$ , exponential		Theoretical derivation	[41]
Alkylbenzenes (18)	$T_b$ , $1/T_b$ , $T/T_b$ , $(T_b-T)$ , $(1-T_b/T)$ , $T_b^2$ , $(T_b-T)^2$ , $(1-T_b/T)^2$	$I$ , linear (0.9692-0.9992)	Silicon oil 550, dinonylphthalate,	4.3<SD<47.9	[42]

Alkylbenzenes (18)	$T_b$ , reciprocal $T_b$	RRT, exponential (0.9455-0.9977)	PEG4000, Bentone 34 Silicon oil 550, dinonylphtalate, PEG4000, Bentone 34	0.028<SD<0.079	[43]
Polysubstituted alkylbenzene isomers	Indices of benzene, monsubstituted alkylbenzenes and disubstituted alkylbenzenes	$I$			[44]
Polychlorinated naphthalenes (62)	Number of chlorine substitutions, heat of formation, maximum value for atomic valence, the minimum value for electronic orbital population	RRT, MLR (0.9975)	DB-5	SE=16.7	[45]
Aldehydes, ketones	$T_b$ , $\ln T_b$ , $T_b^* \ln T_b$	$I$ , linear, (0.9976-0.99994)	DB-210	11.5<SD<12.1	[46]
Alkanes (157), cis- and trans-n-alkene isomers (79)	Semiempirical topological index, increments	$I$ , linear (0.9901), (0.99996)	Squalane	2.35<SD<26.2 Cross-validation Comparison with prediction by Wiener, Randic indices	[47]
Hydrocarbons (191)	Oblique factors	FA, varimax, promax rotations	DB-1, DB-5, SE-54, OV-1	GC/MS identification	[48]
Aldehydes, ketones	$T_b$ , $M_w$ , $V_m$ , $R_m$ , $\log P$ , Ind,	$I$ , scores, PCA, MLR (0.99901)	HP-1, HP-50, DB-210, HP-Innowax	SD=0.0491	[49]
Alkanes (156) oxygen-containing organic molecules (81)	Weighted fragments, spectral moments	Additive schemes	Squalane, OV-1		[50]
Coumarins	Total surface area (AT), electrotopological state index,, oxygen in position 1, HOMO,	MLR	Low polarity phases	Cross-validation	[51]

Alkylbenzenes (32)	Boiling point, molar volume, stationary phase	<i>I</i> , BP-ANN	Squalane, SE- 30, PEG,	Training and test sets, Relative error 3%	[52]
isoalkanes, dialkyl sulfates, and aliphatic amines and Diverse chemical compounds (152)	$T_b$ , NC, $V_m$ , $R_m$ , sum of internal rotational and vibrational energies CODESSA descriptors (296), linear selection	<i>I</i> , structural fragments Retention time, RF, MLR, nonlinear models		Molecular dynamic caculations Comparison with earlier results	[53]
Halocarbons C1-C4, hydrocarbons C4-C6 (17)	Retention time, $R_m$	Virial coefficients Interaction energies (0.973, 0.982)	Carbopack C		[55]
Trimethylsilyl ether derivatives of natural sterols (16)	Conventional, topological, quantum-chemical (60)	<i>I</i> , MLR (>0.9880)	SE-54, SE-52	Relative mean errors 2.88%, 3.24%.	[56]
Aldehydes, ketones	$T_b$ , $M_w$ , $V_m$ , $R_m$ , log $P$ , Ind,	<i>I</i> , scores, PLS, (0.990-0.995)	HP-1, HP-50, DB-210, HP-Innowax various	Cross-validation 0.975<Q <sup>2</sup> <0.990	[57]
Polychlorinated biphenyl (PCB) congeners,	New QSRR descriptors for selectivity correction	Retention time		SDs are ‘within a chromatographic peak width’	[58]
Methylalkanes produced by insects (178)	Mainly topological descriptors	<i>I</i> , MLR	DB-1	Internal (LOO, leave-33%-out) and external (30) cross-validation, SD=4.6 (overall) SD= 4.3 (truncated)	[59]
Polychlorinated dibenzofurans (PCDFs), Alkylbenzenes (129)	Substitution pattern, positions	<i>I</i> , MLR (>0.9995)	DB-5	SD<7 i.u.	[60]
	molecular graph descriptors, sequential orthogonalization	<i>I</i> , MLR		calibration and prediction sets	[61]
Diverse sets	Abraham type solvatochromic	gas-liquid	EGAD, THPED,	Residual analysis,	[62]

	parameters (6),	partition coefficient, K(L), MLR, BP-ANN, nonlinear function	Ucon 50 HB 660 DEHPA,QBES	training, prediction sets	
Alkylphenols	Wiener, hyper-Wiener, minimum and maximum eigenvalue, Ivanciuc-Balaban, and information on distance operators	<i>I</i> , MLR	Not given	S=37-38 i.u. (biparametric); S=15-19 (5-4 parametric)	[63]
Alkanes (64)	Novel molecular distance-edge vector (10 elements)	<i>I</i> , MLR (0.9988 - 0.9992)		Cross validation RMS(training) = 5.9, RMS(test) = 7.1	[64]
Alkanes, alcohols and polycyclic aromatic hydrocarbons.	Electronegativity-distance vector (MEDV),	<i>I</i> , MLR			[65]
Amines	Topological indices Aml, Am2, Am3, gravitational index G1.	<i>I</i> , MLR	Phase of various polarity (3)		[66]
Saturated and monounsaturated six- carbon aldehydes, alcohols and esters	$T_b$	<i>I</i>	DB-5, DB- 1701, DB-Wax		[67]
Hydrocarbons and derivatives containing oxygen, nitrogen and halogens	Valence connectivity indices, $1(\chi)(v)$ Wiener, W, and Balaban, J, indices	$\log V(g)$ , <i>I</i> , linear, non-linear (0.9597-0.99999)	Various, PDMS, PEA, PBD, TFPS15, XF-1150	No	[68]
Alkanes, diverse compounds	LSER	Specific retention volumes, MLR	18 polymers	No	[69]
Polychlorodibenzothiophenes PCDTs (19)	Structural features	MLR	DB-5 and DB-5ms		[70]
Hydrocarbons, benzene derivatives, esters, alcohols, aldehydes, ketones and heterocyclics (110)	Molecular mass, number of vibrational modes of the molecule, molecular surface area and Balaban index	RF, MLR, BP-ANN		Mean absolute error = 0.02	[71]
Diverse C10 polar solutes from	$T_b$	RRT, linear	12 modified	SD<5.5	[72]

volatile oils PAHs (unsubstituted six-membered fused aromatic rings, 48)	Electronic, geometric, topological (e.g. electron affinity, the difference between electron affinity and ionization potential (GAP), Wiener, and connectivity indexes, volume, surface area, length-to-breadth ratio, enthalpy of formation	(>0.990) <i>I</i>	cyclodextrin		[73]
Aldehydes, ketones	Quantum-chemical method PM3. HOMO, LUMO, polarizability, dipole moment, solvent accessible surface area	<i>I</i> , MLR, (0.9930-0.9975) PCA, CA	OV-1, HP-50, DB-210 and HP-Innowax	12<SD<19	[74]
100 polycyclic aromatic hydrocarbons (PAH)s	Novel molecular distance-edge vector (6 parameters)	<i>I</i> , linear (0.988), to the gas		Comparison with results of molecular polarizability index	[75]
Alkylbenzenes (129)	Molecular graph descriptors (5)	<i>I</i> , MLR		Calibration and prediction sets	[76]
46 alkylbenzenes them.	Simple set of six numeric codes McReynolds' constant of the different stationary phases, temperature	<i>I</i> , MLR, BP-ANN	Cit.A-4, SE-30 and Carbowax 20M		[77]
Hydrocarbons	Molecular structure	<i>I</i> , BP-ANN (0.9934)		Leave-10%-out, SD=16.5	[78]
Polychlorinated dibenzofurans PCDFs	Molecular distance-edge vector	MLR, (>0.98)	DB-5, SE-54, OV-101	Cross-validation (0.97)	[79]
Hydrocarbons (150)	Numeric structural codes	<i>I</i> , MLR (0.9874 - 0.9901)		20.2<SD<22.9	[80]
Noncyclic and monocyclic terpenes (53)	One electronic, two geometric, two topological and one physicochemical descriptors	<i>I</i> , MLR, BP-ANN	Carbowax 20 M	leave-one-out cross-validation Training and prediction (1.88%) sets, SD=38	[81]



Alkyl aromatic hydrocarbons and esters (252)	Partition coefficients ( $K_p$ ), group identification	$I$ , linear	HP-5	Visual	[82]
207 halogenated hydrocarbons	CODESSA descriptors: Kier-Hall connectivity index, number of F atoms, gravitation index	$I$ , MLR (0.994 - 0.993)	Methylsilicone	Leave-one-out cross-validation	[83]
22 amines	Novel connectivity index, mQ	$I$ , MLR (0.9734 - 0.9733)	OV-101, OV-225 and NGA	Modified Jackknife's test	[84]
Malodorous organic sulfur compounds, thiols and thioethers	Molar refractivity and connectivity index values	Second gas-solid virial coefficient	Carbopack C	Visual	[85]
373 organic compounds		$I$ , (0.975 - 0.994)			
Linear, branched alcohols with hydroxyl group on a primary, secondary, or tertiary carbon atom.	Molecular connectivity indices	$I$ , MLR, BP-ANN	OV series columns	Cross-validation	[86]
Several groups of isomeric organic compounds	Topological (Wiener and Hosoya indices) and dynamic parameters	$I$ , MLR			[87]
Chlorinated alkylarenes	Molecular dynamic parameters,	$I$ , additivity schemes	Nonpolar		[88]
Various	topological	Retention times, PCA	Various		[89]
Polycyclic aromatic hydrocarbons PAHs (94)	Molecular distance-edge vector (VMDE)	$I$ , MLR (0.9928 - 0.9946)		Leave-one-out cross validation	[90]
Alkanes (48), alcohols (31)	Variable connectivity index $1\chi^f$	$I$ , MLR (0.9933)		SD=14.2	[91]
Alkanes	Molecular distance edge vector (MDEV)-consisting of ten elements	$I$ , Wavelet NN (0.9996) BP-ANN		SD=5.06	[92]
Polychlorinated dibenzo-p-dioxins	Molecular descriptors: Randic index (order 3), the Kier shape index (order 3)	Retention time (0.9950)	DB-5	SD=0.2550.	[93]
Polybrominated diphenyl ethers PDBEs	Physicochemical descriptors (40) AM1 quantumchemical, molecular	RRT, PCA, PLS	Four capillary columns	CPSil-8, HP-1701, SP-2380, SB-	[94]

	mechanics, heats of formation, frontier molecular orbital energies, atomic charges, dipole moments, log <i>P</i> values, and molecular surface areas,			Smectic	
Organic compounds with various functional groups	<i>T<sub>b</sub></i> , $\alpha$ , heat of formation, density, various indices, inertia, HOMO. Etc.	RF, MLR, BP-ANN	Not given	Training, prediction sets; residual analysis	[95]
Methylalkanes produced by insects (178)	Semi-empirical topological index	<i>I</i> , MLR (0.99999)	DB-1	SD=3.20	[96]
Branched alkenes	Semi-empirical topological index	<i>I</i> , MLR	Squalane, 1-octadecene, Apiezon-L, OV-1, DB-1	External SD=4.6 Cross-validation (0.9985)	[97]
polychlorinated dibenzodioxins PCDDs	molecular distance edge vector (VMDE)	MLR	DB-5, SP-2100, SE-54, OV-1701	leave-one-out	[98]
13 different classes of organic compounds	molecular density, Wiener number, boiling point, polarizability and square of polarizability	RRT, MLR, BP-ANN	Rtx-5	Training, prediction sets;	[99]
Polycyclic aromatic hydrocarbons PAHs (209)	Molecular electronegativity-distance vector (MEDV)	<i>I</i> , MLR (0.9812)	SE-52	RMS=15.5	[100]
Esters, alcohols, aldehydes ketones	HOMO, molecular values, number of atoms, molecular shadow area on the xy plane,	<i>I</i> , BP-ANN	OV-1, SE-54	Training, prediction sets; average percentage deviation 2.5 - 3.0%	[101]
Alkanes, alkenes, alcohols, esthers, ketones, ethers	<i>T<sub>b</sub></i> , <i>V<sub>m</sub></i>	<i>I</i> , RBF-NN (0.9910)	Not given, as in ref. [36]	Test set, RMS=14.1	[102]
Saturated esters (98)	PM3 descriptors (Hyperchem 4.0), topological, degree of branching	<i>I</i> , MLR, PCA	SE-30, OV-7, DC-710, OV-25, 100% phenyl,	SE=13.1-23.0	[103]

Oxo compounds (54)	Semiempirical topological index	$I$ , linear (0.999)	DC-230 and DC-530 HP-1, HP-50, DB-210, HP-Innowax	SD=5.0	[104]
Chlorinated phenols		RRT, MLR (0.985)	DB-5	SD=0.0472	[105]
Polychlorinated naphthalenes (62)	Molecular electronegativity distance vector	$I$ , MLR (0.9912),		RMS=31.4, leave-one-out (0.9898) RMS=33.8	[106]
Alkenes	Class distance variable (information about the branch, position of the double bonds, the number of double bonds)	$I$ , projection pursuit	Squalane	Training and prediction sets	[107]
226 series of compounds		$\Delta I$ , additivity scheme		theoretical	[108]
Polychlorinated biphenyls, PCBs (30)	Topological parameters (Balaban index and electrotopological index	RRT, $RI$ , linear (0.78-0.99) nonlinear	PE-5MS	Relative error=2.8%-24.4%	[109]
Disulfides (50)	Semi-empirical quantum chemical (AM1) HYPERCHEM 4.0	$I$ , MLR (0.976-0.995), RBF-NN	Apiezon M, OV-17, Triton X-305 and PEG-1000	Training and validation sets	[110]
Benzene and 12 chlorobenzenes	Mosaic and bond increments	$k$ , $I$ , additivity schemes	Agilent 6850, HP-5, HP-5890, HP-5840, SE-30, SPB-1, Wax-10	Training (6) test (8) absolute deviation=1.7 i.u. relative errors=0.9% 3.5%	[111]
Benzene and 12 chlorobenzenes	topological indices (first-order connectivity index, Wiener's index and Balaban index) physico-chemical properties (freezing point, boiling point, refraction	$I$ , MLR (0.9976-0.9998), PCA	Various (7)		[112]

Aldehydes, ketones	index, dipole moment, density, molecular mass and vapor pressure Xu index, atom-type-based AI topological indices (fragments)	<i>I</i> , MLR ( $r>0.995$ )	HP-1, HP-50, DB-210, HP-Innowax	Theoretical considerations	[113]
Alkanes, alkenes, esters, ketones, aldehydes, and alcohols (548)	Semi-empirical topological index, IET	<i>I</i> , MLR (1.0000)		Test set (182), SD=7.7	[114]
Alkoxyl silicon chlorides	molecular topological index mXY	<i>I</i> ,			[115]
Alcohols (25)	hydrogen connectivity index	<i>I</i> , MLR			[116]
homologues	number of carbon atoms nC, reciprocal $T_b$	nonlinear			[117]
branched alkanes	class distance variable	projection pursuit (PP)			[118]
Various (20 chemical classes)	$T_b$	Lee's <i>I</i>	Not given		[119]
Saturated alcohols	Semi-empirical topological index	<i>I</i> , linear (0.9978)	OV-1, SE-30, OV-3, OV-7, OV-11, OV-17, OV-25	SD=9.54	[120]
Chlorinated polycyclic aromatic hydrocarbons, Cl-PAHs (18)	MNDO quantumchemical: total energy, dipole moment, net atomic charge on Cl	RRT (0.9968), Cl-atom position	HP-5ms		[121]
Polychlorinated naphthalenes (62)	Structural parameters	<i>I</i> , MLR (0.9839-0.9880)		Leave-one-out cross-validation	[122]
Trimethyl silyl derivatives of natural phenols and sterols	Descriptors generated with the HYPERCHEM 4.0, AMPAC 6.7 and CODESSA 2.3	RRT, MLR( $>0.99$ )	SE-54 and SE-52	Relative errors: 0.01% 0.37%.	[123]
Aldehydes, ketones	Semi-empirical topological index, IET	<i>I</i> , MLR ( $>0.9995$ )	HP-1, HP-50, DB-210, HP-Innowax	SD=5.5	[124]
n-alkanes, 1-alkenes, and 2-alkenes homologous series	Hyperchem, MOPAC,	$\Delta H$ , RT, MLR	DB-1	S( $\Delta H$ )=161 cal/mol; cross-	[125]

271 organic compounds of diverse structures $\alpha$ -, $\beta$ 1-, and $\beta$ 2-agonists	Retention data on two phases of different polarity Diverse connectivity and electrotopological indices	$T_b$ , bilinear(0.9724) RRT, MLR, PCA, PLS	DB1-60W, DBWAX-30N Crosslinked methylsilicone gum, DB-5, DB-17	validation SD=16.1 K  Training and prediction set	[126] [127]
CNS agents (benzodiazepines, barbiturates, phenytoin)	Calculated descriptors	$I$ , MLR (0.983-0.988)		Leave-one-out cross validation (0.967) and external prediction set (0.954)	[128]
O-, N-, and S-heterocyclic compounds	$T_b$ , WHIM, GETAWAY, connectivity indices, 0D constitutive descriptors	$I$ , MLR, PLS	Nonpolar dimethyl polysiloxane	Cross validation	[129]
Polycyclic aromatic hydrocarbons, PAHs	$T_b$ , molecular mass and connectivity index	$I$ (Lee's scale), linear, quadratic exponential	DB-5	SD=1.9, external SD=2.4; 3.3	[130]
Sulfides	Atomic structure parameters molecular connectivity index topological index	$I$ , MLR (>0.97)	Different polarity		[131]
Mercaptans, sulfides, thiophenes (34)	Molecular descriptors (7,8)	RT, $I$ , MLR		S = 0.61 and 1.63,	[132]
Methane, ethane, propane, chloromethane, chlorodifluoromethane, dimethyl ether, and sulfur hexafluoride, (65)	$R_m$ , connectivity index, surface area, surface energy contribution ( $r^2=0.952$ ) of the 65 different lnB2s values. T	Second gas-solid virial coefficient, B2s (0.9757)	Carboxen-1000 carbon molecular sieve		[133]
Polychlorinated hydroxybiphenyls (839)	Simpler structural analogues of target compounds	Additivity scheme arithmetical operations of $I_s$ PCA, MLR for variable selection	HP-5		[134]
149 C3 - C12 volatile organic compounds	Total information index of atomic composition IAC, Wiener number, W, solvation connectivity index,	BP-ANN	DB-1		[135]

118 polychlorinated biphenyls, PCBs	Xlsol, number of substituted aromatic C(sp <sup>2</sup> ), nCaR, Ionization potential (molecules and molecular ions), topological indices, inertia	RF (ECD), MLR for variable selection BP-ANN	DB-5	Training and prediction sets	[136]
Methylbenzenes, chlorobenzenes	Methyl/chlorine substitution pattern, number of substituents	<i>I</i> ,	HP-5, ZB-WAX		[137]
846 diverse organic compounds	Dragon descriptors (529)	MLR, PLS	Apolar phases, HP1, OV-101	Training and prediction (SD=80) sets.	[138]
Polychlorinated dibenzofurans, PCDFs	Modified molecular distance-edge (MDE) vector	MLR (0.958-0.995)	DB-5, SE-54, OV-101, OV-1701, SP-2300	Leave-one out (0.834-0.992)	[139]
22 alkoxyl silicon chlorides, 61 sulfides and 74 alkanes	Molecular structure information connectivity index mY	<i>I</i> , MLR		‘Clear physical significance’	[140]
Saturated hydrocarbons, olefines and dienes	Quantum chemistry parameters HOMO, LUMO, ElcE, <i>R<sub>m</sub></i>	<i>I</i> , MLR	Various	‘Good stability and prediction’	[141]
126 polybrominated diphenyl ethers, PBDEs	Congener substitution patterns	Elution order, nonlinear	DB-1, DB-5, HT-5, DB-17, DB-XLB, HT-8, CP-Sil19		[142]
Aliphatic alcohols	Hyperchem 4.0, Dragon descriptors (109)	<i>I</i> , PCA, MLR, RR, PLS (0.9712 – 0.9950)	OV-1	Leave-33%-out cross validation (0.9052-0.9900)	[143]
142 molecules (10 series of compounds)	Modified Topological Index mT	<i>I</i> , RRT, MLR			[144]
Alcohols	Quantum chemical descriptors AM1, Hartree-Fock (HF) Gaussian 98	<i>I</i> , MLR	Superox 20M-diglycerol		[145]
Polyaromatics, polychlorobiphenyls		<i>I</i>			[146]

Aliphatic alcohols	Semi-empirical topological index (IET),	Linear (>0.98)		Cross-validation leave-one-out	[147]
Polycyclic aromatic sulfur heterocyclic compounds, PASHs	$\mu$ , Constitutional, geometric, topological, molecular walks	<i>I</i> , nonlinear	BPX5	Cross-validation	[148]
136 polychlorinated dibenzofurans, PCDFs	Number and position of chlorine substitutions, quantumchemical	<i>I</i> , (0.993-0.998)	DB-5	Cross-validation	[149]
Polychlorinated dibenzo-p-dioxins, PCDDs .dibenzofurans, PCDFs	<i>I</i>	Subcooled liquid vapor pressures (PL)			[150]
Methyl-substituted alkanes produced by insects	Total number of carbons in the backbone, the number of the multiple methyl groups attached to the carbon chain, their relative positions	<i>I</i> , BP-ANN	DB-1	Average relative error=3.3%.	[151]
Polychlorinated dibenzofurans, PCDFs	Molecular structure index, group modify index	<i>I</i> , RRT, MLR,	DB-5, SE-54 and OV-101	Relative deviation=1.09%	[152]
Organic sulfur compounds	Topological descriptors, temperature	<i>I</i> , MLR		Leave-one-out (0.978) leave-two-out (0.976)	[153]
Polychlorinated dibenzofurans, PCDFs (135) PCDFs.	Molecular hologram	<i>I</i> , PLS (0.999)		Training and prediction set	[154]
Nitrogen-containing polycyclic aromatic compounds, N-PACs	Codessa descriptors (3)	<i>I</i> , MLR (0.9923)	SE-52	Cross-validation	[155]
Sulfides and mercaptans	Molecular polarizability effect index (MPEI), the effective topological steric effect index (ETSEI), the number of carbon (N), Wiener three-walk path (P3)	<i>I</i> , MLR (>0.98)	Various		[156]
Polycyclic aromatic hydrocarbons, PAHs	$T_b$ , connectivity indices and molecular weights	<i>I</i> , BP-ANN		Test sets	[157]
149 volatile organic compounds (VOCs).	Five molecular descriptors (CODESSA )	RT, SVM	DB-1	Training and prediction set	[158]

Alkanes, organic compounds	Topological index based on distance matrix and branch vertex of the atoms	<i>I</i> , MLR (0.9919 - 0.9922)	Squalane, SE-30	SD=13.7, 12.0	[159]
Polychlorinated naphthalenes PCNs	Quantumchemical (HF/6-31G* and B3LYP/6-31G* levels), relative position of chlorine substitution	<i>I</i> , MLR (0.9907 - 0.9978), 0.9983		Cross-validation (0.9885-0.9974) 0.9979	[160]
Aromatic imines	Topologic, topographic and quantum-chemical	<i>I</i> , MLR (0.987), BP-ANN (0.940)	DB-1	external set (0.911-0.985), leave-one-out (LOO) and the leave.multiple-out (LMO)	[161]
Organophosphates (35)	Electrotopological state index for atom types, ETSI	<i>I</i> , MLR (>0.99)		Calibration, validation (0.98) sets	[162]
Polybrominated diphenyl ethers (209)	Wiener index, Randic index, polarity parameter,	RRT, MLR (0.983-0.996)	DB-1 DB-5MS, HT-5, DB-17, DB-XLB, HT-8, CP-Sil 19	Cross-validation (0.979-0.995)	[163]
Aliphatic alcohols (35)	Electrotopological state index (En) the molecule connectivity index (MCI)	<i>I</i> , MLR (0.994), PLS		Leave-one-out	[164]
Saturated esters (90)	Lu index, distance-based atom-type DAI topological indices	<i>I</i> , MLR	SE-30, OV-7, DC-710, OV-25, XE-60, OV-225, Silar-5CP	SD=10-19.3 i.u- (cross validated)	[165]
Aliphatic carbonyl compounds, esters and alcohols	<i>T<sub>b</sub></i> , linear temperature programmed retention index	<i>K<sub>fg</sub></i> , bilinear	Carboxen/polydimethylsiloxane	No	[166]
PAHs	<i>T<sub>b</sub></i> , molecular mass, connectivity index, Schabron molecular size	<i>I</i> (Lee scale), BP-ANN (0.9381)	SE-52, DB-5	validation and two testing sets (0.8939-0.9460)	[167]
177 methylalkanes (insects)	Molecular tightness index, MTI,	<i>I</i> , MLR (0.99999)	DB-1	Leave-one-out	[168]



	polarizability effect index, PEI, number of carbon atoms in backbone, NC, number of the 2-methyl groups (N2-CH3) number of methyl groups attached to the carbon backbone (NCH3)			cross validation, external data set. 3.7>SD>4.6	
Fatty acid methyl esters (FAME)	Two-dimensional fatty acid retention index system, 2D-FAI	Equivalent chain lengths, ECL, MLR	BPX-70	Test sets 0.002<RMS<0.012 ECL units	[169]
Methylene-interrupted polyunsaturated fatty acids	Chain length, number of double bonds, position of the double bond system	Retention indices as equivalent chain lengths (ECL)	Cyanopropyl column	RMS=0.03 ECL units	[170]
Polycyclic aromatic sulfur heterocycles, PASH alkylated dibenzothiophenes (43)	Substitution pattern	<i>I</i>	Methylphenylsiloxane (5% and 50% phenyl groups): DB5ms, DB17ms	New synthesized compounds	[171]

## Notations

ANN - artificial neural network

$\alpha$  - polarizability

BP - back-propagation

CFA - correspondence factor analysis

CP - counter-propagation

DB-1 - 100% dimethylpolysiloxane

DB-5 - 5% diphenyl and 95% dimethylpolysiloxane

DB-210 - trifluoropropylmethyl polysiloxane

DB-wax - polyethyleneglycol

DEHPA - di(2-ethylhexyl)phosphoric acid

EGAD - polyethylene glycol adipate,

ECL - equivalent chain length

FA - factor analysis

GA - genetic algorithm

HP-1 - 100% dimethylpolysiloxane,

HP-5 - 5% diphenyl and 95% dimethylpolysiloxane

HP-50 - 50% diphenyl and 50% dimethylpolysiloxane

HP-Innowax - polyethyleneglycol

$I$  - Kovats retention index

$k$  - retention coefficient, (capacity factor)

$K_{fg}$ , distribution coefficients between fiber coating and gas phase

LOO - leave-one-out (internal) cross-validation

LMO - leave-multiple-out (internal) cross-validation

PAH - polycyclic aromatic hydrocarbon

PCA - principal component analysis

PCB - polychlorinated biphenyls

PCDF - polychlorinated dibenzofuran

PDMS - dimethylpolysiloxane

PP - projection pursuit

PPEG - poly(ethylene glycol) (Ucon 50 HB 660) (U50HB),

QBES - tetra-*n*-butylammonium *N,N*-(bis-2-hydroxyethyl)-2-aminoethanesulfonate

RBF-NN - radial basis function neural network

RF - response factors

$R_m$  - molar refraction

RR - ridge regression

RRT - relative retention time

SD - standard deviation

SE, SEC, SEP, standard error, calibration, prediction

SOM - self-organizing map, (Kohonen network)

$T_b$  - boiling point

THPED - *N,N,N',N'*-tetrakis(2-hydroxypropyl) ethylenediamine

$V_m$  - molar volume

Table 2 QSERR examinations between 1996-2006.

Solutes	Descriptors	Model building	Stationary phase (SP)	Source
Chiral $\alpha$ -alkyl arylcarboxylic acids (28)	Hydrogen bonding ability and aromaticity	Retention data	AD-CSP	[173]
Mexiletine and a series of structurally related compounds	Presence or absence of secondary hydrogen-bonding group, nonempirical descriptors	Retention data, MLR	AD-CSP	[174]
Racemic 3-phenyl-4-(1-adamantyl)-5-X-phenyl-2-1,2,4-oxadiazolines	Aromatic ring substituents, electronic and bulk parameters or CoMFA descriptors	MLR, CoMFA	Pirkle-type N,N'-(S,S-dinitrobenzoyl)-1(R),2(R)-diaminocyclohexane	[175]
12 chiral arylcarboxylic acids	Hydrophobicity and steric volume	MLR	Immobilized human serum albumin chiral stationary phase (HSA-CSP).	[176]
29 aromatic acids	Charge transfer, electrostatic, lipophilic, and dipole interactions	MLR, BP-ANN	Amylosic CSP	[177]
Enantiomeric amides	Chirality of the amylose backbone	Elution order	Amylosic CSP	[178]
Homologous series of 1,4-disubstituted piperazine	Carbon number of the alkyl substituent (max. C4-C5)	Nonlinear	Chiral cellulose tris(4-methylbenzoate)	[179]
Nonlinear data set for chiral separation	Mass (m/z)	PLS, ANN	Pirkle-type CSP	[180]
14 O-ethyl O-(substituted) phenyl N-isopropyl-phosphoro-amidothioates	Molecular descriptors (7) significant descriptors (4)	MLR		[181]
Chiral sulfoxides	Molecular connectivity indices, similarity and holistic descriptors (3D-WHIM)	RRT, MLR	Cellulose and amylose tris-phenylcarbamates coated onto 3-aminopropyl mesoporous silica	[182]
O-ethyl O-(substituted) phenyl N-isopropyl phosphoroamidothioate	LUMO, interaction of hydrogen bond, $\pi$ - $\pi$ interaction, log <i>P</i> and	MLR	Pirkle-type CSPs, Sumichiral OA4700	[183]
42 chiral arylalkylcarbinols	2D and 3D molecular descriptors	log $\alpha$ , MLR, ANN, CoMFA	Pirkle-type CSP	[184]

$\alpha$ -aminophosphonates	quantum chemical (LUMO) hydrophobicity. Molecular parameters (4)	$k$ , MLR, FA	Phenyl carbamate derivative $\beta$ -cyclodextrin bonded	[185]
Diphenyl 1-(N-benzyloxycarbonyl)-aminoalkanephosphonates	$\log P$ , Angle, HOMO and LUMO	$k$ , MLR, FA		[186]
Diphenyl 1-(N-benzyloxycarbonyl)-aminoalkanephosphonates	$\log P$ , Angle, locD and TE	MLR	Pirkle-type	[187]
Various drugs, phenoxy propionic acid derivatives	Molecular descriptors (4)	MLR	Riboflavin Binding Protein (RfBP)	[188]
Diastereomers and enantiomers	Molecular dynamics	Addition of chiral substituents	Cyclodextrin derivatives	[189]
Aryl- and hetaryl-carbinols (22)	3D descriptors descriptor based on normal mode eigenvalues (EVA)	$\log \alpha$ , CoMFA, CoMSIA, PLS, (0.97-0.99) validation (0.85-0.91)	(SS)-3,5-dinitrobenzoylated 1,2-diphenylethane-1,2-diamine	[190]
5-arylhydantoins (50)	2D and 3D molecular descriptors quantum chemical	MLR	Pirkle-type	[191]
Organophosphonates	$V_m$ , $M_w$ , H-bond acceptor, dipole-Z	Elution order	N-(3,5-dinitrobenzoyl)-S-leucine	[192]
Hydroxy acids (8 )amino acids (10)	Chiral topological indices	$I$ (HP-TLC)		[193]
2-aryloxy-2-arylacetic acids (1-3, 5-16), thioisostere derivative (4)	Polar, charge-transfer interactions, steric effects	$k$ , Elution order, enantioseparation factors ( $\alpha > 2$ )	Penicillin G Acylase chiral stationary phase (PGA-CSP)	[194]
5-arylhydantoins (50)	Dragon descriptors (557)	Selectivity, resolution, PCA, PP, UVE-PLS MLR, CART	3R,4S-Welk-O-1	[195]

## Notations

AD-CSP - amylose tris(3,5-dimethylphenylcarbamate)  
AR-CSP - amylose tris(R-phenylethyl-carbamate)  
AS- CSP - amylose tris(S-phenylethylcarbamate)  
ANN - artificial neural network  
 $\alpha$  - chiral separation factor  
BP - back-propagation  
CART - classification and regression trees  
CoMFA - comparative molecular field analysis  
CoMSIA - comparative molecular similarity indices analysis  
CSP - chiral stationary phase.  
FA- factor analysis  
HSA-CSP - immobilized human serum albumin CSP  
 $k$  - retention coefficient, (capacity factor)  
LOO - leave-one-out (internal) cross-validation  
LUMO - energy of lowest unoccupied molecular orbital  
 $M_w$  - molecular mass  
MLR - multiple linear regression

PCA - principal component analysis  
PGA-CSP - Penicillin G Acylase CSP  
PLS - partial least squares  
PP - projection pursuit  
RfBP - riboflavin binding protein  
UVE-PLS - uninformative variable elimination-PLS  
 $V_m$  - molar volume

Table 3 QSRR examinations in TLC between 1996-2006.

Solutes	descriptors	model building	Method	source
29 antibiotics	Hydrophobicity parameters, surface areas	Weak or no correlations	Impregnated silica and alumina supports	[198]
Estrone, equilin, equilenin, their 17 $\alpha$ -diols, 17 $\alpha$ -estradiol, 17 $\alpha$ -dihydroequilin (DHEQ), 17 $\alpha$ -dihydroequilenin	Dipole moments, Randic's connectivity indices, number of H atoms	PCA, NLM	TLC, RP-HPLC, capillary GC	[199]
18 nonsteroidal anti-inflammatory drugs	Lipophilicity and specific hydrophobic surface area	NLM	RP-TLC, methanol (acetic acid, sodium acetate, or sodium chloride)	[200]
7 monotetrazolium and 9 ditetrazolium salts	Physicochemical parameters (hydrophobic, electronic, steric)	PLS, CCA	Alumina and reversed-phase (RP) alumina layers using n-hexane-1-propanol and water-1-propanol	[201]
15 amino acids	Topological indexes, physicochemical properties (15)	$R_f$ , MLR	Silica gel layers	[202]
Aryloxyaminopropanol derivatives of 1,4-piperazine	Lipophilic Hansch's constants $\pi$ , the number of carbon atoms in R1 substituent	$R_m$ , linear, $\beta$ -adrenolytic activity vs. $\log k$ is parabolic	TLC, HPLC	[203]
7 mono- and 9 ditetrazolium salts	Steric and electronic parameters	PCA, NLM	TLC, HPLC	[204]
Dihydroxythiobenzanilides	Hydrophobicity, antimycotic activity, lipophilicity Hansch parameter	$\log k$ , limited linear	RPTLC, acetone-water methanol-water	[205]
18 flavonoids	Number of hydroxyl groups	Selectivities, sequences	Silica-diluent + polar modifier	[206]
O-alkyl, O-(1-methylthioethylideneamino) phosphoramidates	17 structural parameters: topologic indices, physicochemical	MLR	RPTLC,	[207]
10 ginsenosides	Topologic indices, physicochemical properties, novel	MLR	Silica gel layers (chloroform-ethyl acetate,	[208]

Homologous series of higher fatty acids, their methyl esters, higher alcohols	parameter "E" Topological indexes based on adjacency matrix, distance matrix	$R_M$ , $\log P$ (Rekker), simple linear	methanol-water)	[209]
Estradiol derivatives	$\log P$	Various chromatographically obtained hydrophobicity parameters ( $R_{M0}$ , $\log k_w$ and $\phi_0$ )	HPTLC, HPLC, methanol-water and acetonitrile-water	[210]
Methyl laurate, -myristate, -palmitate, -isostearate, -stearate, -arachidate	Dipole moments of the mobile phases, percentage impregnation of SP, topological index	$R_M$ , $\log P$ for methyl isostearate	Kieselguhr F254 impregnated with different amounts of paraffin oil	[211]
Biogenic amine neurotransmitters, their metabolites	Semi-empirical quantumchemical	Retention data, linear, CA	RP-18 plates	[212]
Meta- and para-alkoxyphenols	Topological indexes based on adjacency matrix, distance matrix, electrotopological states	$R_M$	Cellulose impregnated with ethyl oleate	[213]
13 barbiturates	Partition coefficients, dipole moments, permittivities, topological indices	$R_M$ , bilinear	13 mobile phases	[214]
Thiazole and benzothiazole derivatives,	H -antihistamine 1 activity	Retention data, $\log P$	Silica gel RP2 60F silanised precoated impregnated with amino acid mixtures	[215]
1,3-oxazolidine derivatives	PC, Theoretical molecular descriptors (ALCHEMY 2000 ), lipophilicity	$R_{M0}$ , PCA	C18 silica gel bonded, methanol	[216]
s-triazines	partition coefficients, Alog P, IAllog P, Clog P, Xlog P, log PKowin, and ACDlog P	Retention factors $R_{M0}$ ,	methanol-water, acetone-water, acetonitrile-water, 2-propanol-water, tetrahydrofuran-water	[217]

Nicotinic acid, its derivatives Alkyl nicotines (MN), nicotinamide, N-methylnicotin- amide	Measured and calculated partition coefficients, $\log P_{\text{exp}}$ , $\text{Alog}P_{\text{s}}$ , $\text{IAlog}P$ , $\text{Clog}P$ , $\log PK_{\text{ow}}$ , $\text{xlog}P$ , topological indices	$R_{M0}$ ,	RP18WF254, methanol- water	[218]
Benzimidazole and benzotriazole derivatives	Molecular descriptors, scores	$R_f$ and $R_{M0}$ , PCA	paraffin oil-impregnated silica gel plates, methanol- water	[219]
2,4-Dihydroxyphenylthioamide derivatives	Antifungal activity	$R_{Mw}$ and $\log k_w$ , linear dependence, parabolic	RPLC, TLC, Methanol- water	[220]

#### Notations

CA - cluster analysis  
FA- factor analysis  
HPTLC - high-pressure TLC  
 $k$  - retention coefficient, (capacity factor)  
MLR - multiple linear regression  
NLM - non-linear mapping  
PAH - polycyclic aromatic hydrocarbons  
PC - principal components  
PCA - principal component analysis  
PLS - partial least squares

$R_m$ ,  $R_M$  - TLC retention parameter,  $R_m = \log(1/R_f - 1)$   
RPTLC - reversed phase TLC  
TLC – thin layer chromatography



Table 4 QSRR examinations in column liquid chromatography between 1996-2006.

Solutes	Descriptors	Models	Column, mobile phase	Source
Substituted aromatic hydrocarbons	S, A, B, V	LSER	Polybutadiene (PBD)-coated zirconia	224
25 structurally diverse solutes	E, S, A, B, V; and water accessible $V_w$ , $\mu$ , atomic electron excess charge	LSER, $\log k'$	Polyethylene-coated silica (PECSiO(2)) polyethylene-coated zirconia (PECZrO(2)),	225
Substituted benzenes	Substituent constant ( $\pi$ ) and the total solubility parameter ( $\delta T$ )	MLR,	Various columns in several different eluents	226
Quinolones	$S_w$ , y-component of $\mu$ , MM+ and AM1	MLR, CA of solutes	PRP-1 column and aqueous organic solvent system	227
31 unsubstituted 3-6-ring PAHs	Moment of inertia,	CoMFA (0.973), cross-validated (0.930)	Polymeric C18 reversed-phase column	228
Small peptides	Sum of the hydrophobic contributions of respective amino acid residues	MLR, PLS, retention times	Ultrasphere Octyl, Ultrasphere ODS, Polymeric reversed phase PLRP-S, Nova-pak C-18	229
28 alkyl (1-phenylsulfonyl) cycloalkane-carboxylates	Octanol/water partition coefficients	LSER	RP-HPLC	230
Carboxamides and oxadiazoles	MM+ and AM1 descriptors for intermolecular interaction, isomeric effect and substituent effect: $S_w$ , x component of $\mu$ , $\log P$ and $\mu$	MLR, Bilinear,	RP-HPLC	231
LSER solutes (nitroalkanes, substituted benzenes)	LSER descriptors: E, S, A, B, V;	$\log k'$ or $\log k(w)$ , $\log P$ (octanole or alkane)	Poly(styrene-divinylbenzene) and immobilized artificial membrane, PRP-1	232
25 substituted biphenyls	Solute volume (V) and hydrogen bond basicity (B)	$S$ , $\log k_w$ (>0.99)	C18 column, methanol/water	233

Pesticides; triazines,	MM+ and AM1 descriptors solvation energy of specific site of solute solvation energy and polarizability, $S_w$	$t_R$	RP, methanol-water acetonitrile-water.	234
Series of xenobiotics, 83 drugs	Physicochemical parameters	LSER, classification, PCA, similarity analysis	8 systems	235
PCBs and Chlorobenzenes, non- ortho-substituted chlorobiphenyls	Polarizability, LUMO, third order valence path molecular connectivity index	$\log k$ , linear, bilinear (values are 0.994 and 0.992	PGC: porous graphitic carbon PYE: 2-(1- pyrenyl)ethyldimethyl silica)	236
Substituted benzenes	$S$ , $\delta T$ , $\log P$ molecular structure parameters	$\log k_w$ , linear, nonlinear, $\log P$	RP-HPLC	237
76 structurally unrelated compounds	CHI,	$\log k_c$ , $t_R$ , $\log P$	Fast gradient RP-HPLC, acetonitrile-water	238
Test series of structurally diverse solutes	Structurally specific dipole- dipole and charge transfer interactions	MLR	C18 and AP (N- acylaminopropylsilica)	239
42 barbituric acid derivatives	Hydrophobicity parameters (e.g. hydrophobicity)	$\log k$ , PCA, NLM	PGC porous graphitized carbon, water-acetonitrile.	240
Heteroatom containing compounds	Quantumchemical, AM1 Hamiltonian, average molecular polarizability, net atomic charges on oxygen atoms that connect with the sulfur atoms, $\mu$	$\log k$ , LSER	Not given	241
Hydroxy compounds, glucuronides	Physico-chemical constants, Parent compound	$\log k$ ,	Not given	242
Phenolic and nitrogen- containing aromatics	Quantumchemical, Hammett's constants	$pK_a$	Acetonitrile, water, sodium phosphate buffer	243
Library	Different substituents in various positions	RT	HPLC	244
Finasteride, N-methylfinasteride	Polar functionalities on the surface of adsorbent, $\log P$	$\log k_w$	Chemically-bonded-silica (SG-MIX), with hydroxyl (-	245

			OH), amino (-NH <sub>2</sub> ), cyano (-CN), phenyl (-Ph), octyl (-C <sub>8</sub> ) and octadecyl (-C <sub>18</sub> ) groups	
20 nonsteroidal anti-inflammatory drugs	Physicochemical. parameters	PCA, NLM, CA	RP-HPLC	246
72 substituted N-benzylidene anilines	Solute polarity, Hammett's constants	CA, CFA	NP: heptane and three modifiers, tetrahydrofuran, 1-octanol and ethyl acetate	247
Disubstituted N-benzylidene anilines	$\mu$ , Hammett's constants, $\sigma_X$ , $\sigma_Y$ LSER descriptors	$\log k$ ,	NP-HPLC	248
Selected phospholipid classes	Configurational + conformational descriptors	Nonlinear, ANN-PLS	RP-HPLC	249
Natural phenols in olive oils	62 molecular descriptors: conventional, topological, and quantum-chemical	MLR (0.9825 -0.9974)	RMSE 6.8% - 2.6 %	250
Very diverse set of 55 compounds	CHI, $\log P$	$\log k_{50}$	ODS column and acetonitrile mobile phase	251
29 compounds were examined under conditions using automated fast gradient methods.	CHI, LSER descriptors: E, S, A, B, V	$\log k_c$ , $t_R$ , $\log P$	20 different RP-HPLC, fast gradient	252
Homologous series	LSER descriptors	Hydrophobic selectivity and polar selectivities	Widely different RP-HPLC	253
34 solutes of widely different type	LSER descriptors	PCA	Nine prepacked narrow-pore and six wide-pore RP-HPLC various ligands (C <sub>18</sub> , C <sub>8</sub> , C <sub>4</sub> , CN)	254
Quinolones studied. At pH 3, was mainly affected by two descriptors,	HOMO $\mu$ , MM+, AM1 semiempirical	$\log k'$	PRP-1 columns, MeOH, THF	255
2-cyano-3-methylthio-3-	10 structural parameters	$\log k'$ , PCA, MLR	Not given	256

substituted amino-acrylates (25)				
Steroids	3D field descriptors	RT, SOM, PLS calibration set, test set (0.65-0.89)	NP, RP	257
2,4-dihydroxythiobenzanilides (fungicides)	$\phi$	$\log k'$ , $\log k_w$ , linear, parabolic	RP, methanol-water or acetonitrile-water	258
58 diverse analytes	LSER descriptors, $\log P$	$\log k'$ , $\log k_w$ ,	Inertsil ODS3, symmetry C8, IAM.PC.C10/C3, methanol	259
18 substituted indoles	Molecular connectivity indices and quantum chemical descriptors	$k'$	RP-HPLC, C18 column	260
O-alkyl, O-(1- methylthio-ethyl- ideneamino) phosphoramidate	Solute-related structural parameters	$k'$ , FA, CA, MLR	Not given	261
25 structurally diverse analytes	$\log P$ , LSER descriptors, simple structural descriptors	$\log k_w$ , column classification	18 RP-HPLC	262
Perhydrogenated and Perfluorinated polyoxyethylene surfactants	Length of alkyl chain, the number of oxyethylene residues, the presence of an oxygen or sulfur atom in the molecule, Molecular electrostatic potential, molecular lipophilic potential, $\log P_{\text{calc}}$ , $V_m$	$\log k$ , $\log k_w$	RP-HPLC, methanol - water	263
Iridoid glucosides	Free rotation around $\sigma$ -bonds		C18, normal diol SPs	264
Benzene and phenol derivatives, indazol, tiophene, caffeine, etc.	$\log P$ , structural- and LSER descriptors	$\log k'$ , chromatographic indices	SG-AP, Supelcosil ABZ + Plus Waters Symmetry- Shield(TM) RP8. C18 Symmetry(TM)	265
2,4-dihydroxythiobenzanilides	$\log P$ ,	Outlier detection	RP-HPLC	266
17 chalcones	Molecular descriptors, LSER	PLS (0.976) test set (0.933)	RP-HPLC, methanol-water	267
Antimicrobial hydrazides	3D-fields	$\log k$ , CoMFA	C-8, methanol-water	268

O-aryl,O-(1-methylthioethylidene-amino)phosphates (13) 233 very different compounds	8 solute-related structural parameters 4 structural descriptors, $\log P$	$k'$ , FA, MLR Solute polarity parameter (p), MLR (0.977) RT (0.967-0.984)	RP-HPLC RP-HPLC C18, RP-HPLC, water/acetonitrile	269 270 271
12 ethynyl-substituted PAHs and unsubstituted counterparts 25 substances	Polarizability and subpolarity, AM1; PM3 Structural descriptors	$\log k'$ , ANN (MLP), PLS	Polyethylene-silica and polyethylene-alumina	272
25 substances	Structural descriptors	ANN (RBF), GRNN, PCR, polynomial PLS RT	Polyethylene-silica and polyethylene-alumina RP-HPLC	273 274
Three test series of analytes 14 substituted benzaldehydes	Reduced LSER, $\log P$ Molecular connectivity indices, LSER and quantum chemical parameters LSER, structural	$\log k$	C18, RP-HPLC, methanol-water	275
Alkylbenzenes, halobenzenes, xylenes, alkanes, isoalkanes 24 steroids	3D image	$\alpha$ , $\log k$ Pulse-coupled neural network: PCNN, PLS	C8, C18, PBB, PYE RP-HPLC, cross-validation	276 277
162 drugs pyrethroid pesticides 86 diverse compounds:	Molecular similarity $\log k'$ , CHI(ACN, MeOH), hydrogen bond acidity	$\log k$ , ANN (0.992-0.996) $\log k$ , $\log P$ $\log P$ (0.943-0.970)	RP-HPLC, cross-validation RP-HPLC, LOO Fast gradient RP-HPLC	278 279 280
Hydantoin derivatives	CODESSA descriptors, AM1 main structural factors, LFER descriptors	Lipophilicity (S)	RP-HPLC RP-HPLC	281 282
Xanthines and derivatives	Semiempirical quantumchemical	$\log k'$ , MLR	Chromolith RP-18e	283
45 barbituric acid derivatives	$\phi$ , substituents steric parameters	$\log k$ , MLR, PCA, NLM	Amide embedded RP silica column (Discovery RP-AmideC16), water-acetonitrile	284
45 barbituric acid derivatives	$\phi$ , $-\phi_0$ , conventional and	$\log k$ , MLR, asymmetry	Amide embedded RP silica	285

45 barbituric acid derivatives	quantum chemical structural $\phi$ , $-\phi_0$ , conventional and quantum chemical structural	factor (AF5) theoretical plate (N) $\log k$ , MLR, 6 retention related parameters, PCA, NLM	column (Discovery RP- AmideC16), methanol-water Amide embedded RP silica column (Discovery RP- AmideC16), tetrahydrofuran- water	286
45 barbituric acid derivatives	$\phi$ , $-\phi_0$ , conventional and quantum chemical structural	$\log k$ , MLR, 6 retention related parameters, PCA, NLM	Amide embedded RP silica column (Discovery RP- AmideC16), dioxan-water	287
20 new $\alpha$ -branched phenylsulfonyl acetates	Geometric and electronic descriptors, surface area (S), ovality (O), the charge of carboxyl group (Qoc), surface area	$\log k_w$ (0.981 adjusted)	Li Chrosorb RP-18 column	288
18 selected amino acids, phenylthiocarbamyl (PTC) amino acid derivatives	36 molecular descriptors, $\log P$ , molecular size, shape (topological indices)	RT, GA-ANN	ODS column	289
Basic compounds related to caproctamine, dibenzylamine- diamide (reversible inhibitor of acetylcholinesterase)	Hammett $\sigma$ (electronic properties of the ortho- substituents)	$pK_a$ ,	C18, C4, RP-HPLC, acetonitrile	290
Drugs and model compounds	Lipophilicity and acidity	RT, $pK_a$ , $\log k_w$	Inertsil ODS3, XTerra RP- 18, Aluspher 100 RP-select B	291
67 neutral, acidic and basic solutes	LSER descriptors, and variants	$k$ ,	10 different C18 (alkylsilica) columns	292
Aromatic acids	$\log P$ , $pK_a$ (partial charges of atoms)	$k$ ,	RP-HPLC	293
Model series, 15 analytes	Total $\mu$ , electron excess charge of the most negatively charged atom water-accessible surface area	Rt, $\log k_w$ , S	Gradient RP-HPLC	294

54 disubstituted benzenes	8 molecular descriptors, PM3 semiempirical	$\log k_w$ , MLR, RBF-ANN	RP-HPLC	295
25, mainly substituted benzenes	LSE descriptors, $S_w$ ,	$\log k_w$ , MLR, PCA	8 RP-HPLC, CE	296
PAHs	Molecular connectivity, $\mu$	RT, bilinear, MLR,	Training, test sets, HPLC	297
Xenobiotics	Chromatographic parameters	$\log P$ , PCA	RP-HPLC	298
phenols	$pK_a$ , atomic partial charges by AM1 and PM3	RT	RP-HPLC	299
15 diverse aromatics (training)	$\log P$ , $\mu$ , $S_w$ , electron excess	RT, MLR (0.8953-	Supelcosil LP18	300
47 diverse compounds (test)	charge on the most negatively charged atom	0.9870)		
83 structurally diverse drugs	266 descriptors, hydrophobicity ( $\log P$ and Hy), the size (TPC) of the molecules	$\log k_w$ , CART	Unisphere PBD column isocratic elution	301
15 diverse aromatics (training)	$\log P$ , $\mu$ , $S_w$ , electron excess	RT, MLR, ANN,	RP-HPLC, methanol-water	302
	charge on the most negatively charged atom			
233 very different compounds	4 descriptors, $\log P$ , hydrogen bond acidity	Solute polarity parameter p, MLR, (0.977)	RP-HPLC,	303
Para substituted anilides of 2,2-dimethylpropanoic, benzoic and $\alpha$ -phenylacetic acid	Physicochemical parameters, $\mu$ , $\epsilon$ , topological indexes $\log P$ , $\log S$ , hydrogen-bond acceptor indicator (HA) and molecular mass	RT, MLR	RP-18 HPLC, methanol-water	304
Test solutes	LSE descriptors	MLR	C18, C8 columns methanol, acetonitrile, and tetrahydrofuran	305
PAHs	AM1: HOMO, LUMO, GAP hardness, polarizability, atomic charges, connectivity index, volume and surface area	$T_b$ , $\log P$ , $I$ , PCR, PLS (0.898-0.995)	RP-HPLC	306
18 L-amino acids	Binding energy (Eb), $\log P$ , molecular refractivity (MR),	$k$ , MLR (>0.9)	RP-HPLC	307

	polarizability ( $\alpha$ ), total energy (Et), water solubility (logS), connectivity index ( $\chi$ ) of different orders and Wiener index (W)			
16 phenols	As above + hydrophilic-lipophilic balance (HLB),	$k$ , MLR		308
PAHs, methyl substituted PAHs	Spatial and topological descriptors	PLS, structural differences, nonplanarity	Monomeric and polymeric C18 stationary phases	309
2-(2,4-dihydroxyphenyl) benzothiazoles	Specific hydrophobic surface area (S), and isocratic CHI ( $\phi_0$ )	$\log k$ , $\log k_w$ , $\log P$	RP-18, methanol-water	310
60 solutes (neutral, acidic and basic)	Retention from neutral components,	RT, MLR	C18, RP-HPLC, RP-IPC, Acetonitrile-water	311
60 solutes (neutral, acidic and basic)	LSER descriptors extended by ionization and ion-pair terms	RT, MLR	C18, RP-HPLC, RP-IPC, Acetonitrile-water	312
200 different compounds	LSER descriptors, acidity	$p$ , $\log k$ , $\log P$	RP-HPLC, Acetonitrile-water, methanol-water	313
19 Acidic drugs	Molecular mechanics, interaction energies	RT (0.878)	Pentyl bonded phase	314
Diverse	$\log P$ , various types of lipophilicity	Retention data	RP-HPLC, biomimetic stationary phases	315
75 peptides	CODESSA, seven molecular descriptors	$\log k$ , linear, nonlinear, SVM, prediction set (0.9801)	Carbonex microspherical carbon	316
Structurally diverse solutes	1000 molecular descriptors	RT, MLR (0.927), GA, prediction (0.79-0.87)	15 HPLC columns, 5 gradients	317
Aromatic compounds	9 structural descriptors, $\log P$	$\log k$ , PCA, CA, MLR	Polybutadiene coated titania SP (PBD-TiO <sub>2</sub> ), HPLC, methanol-water	318
Xanthenes, aglycones, glucosides	$S$	$\log k_w$ ,	Gradient HPLC,	319
Benzoylphenylureas,	$\mu$ , MR, $\log P$	$k$ , MLR	polystyrene-octadecene-	320



18 Dihalogeno benzoylphenylureas 101 peptides	Sum of RTs of amino acids, $\log V_w$ , $\log P$	RT, MLR	encapsulated zirconia, Kromasil-C18-SiO2 Gradient HPLC,	321
98 peptides	Sum of RTs of amino acids, $\log V_w$ , $\log P$	RT, MLR	Gradient HPLC,	322
Series of test analytes	$\log P$ , $\mu$ , $\delta$ , $S_w$ , hydrophobic subtraction LSER model	RT, classification	9 representative RP-HPLC column	323
Steroid analogues		De novo mathematical model	RP-HPLC, methanol, acetonitrile, tetrahydrofuran	324
Triazine herbicides, metabolites	4descriptors	$k$ , MLR, ANN	Methanol – water, Spherisorb ODS2, precolumn LC 8	325
Unsaturated alkenes, phenols, acidic and basic drugs	Alkyl-chain length, atomic partial charge, $pK_a$	$k$ ,	Graphitic carbon	326
28 alkyl(1-phenylsulfonyl) cycloalkane carboxylates	Ab initio quantum chemical, B3LYP/6-31G*, AM1	$\log k$ , bilinear, (0.9747, 0.9741)	LOO	327
Ricobendazole and albendazole sulfone	$\log P$	$\log k_w$ , $\log k$ , Internal standard selection by QSRR	C-18 column, rapid HPLC	328
Aromatic acid derivatives	Interaction energies, MM, $pK_a$	$\log k$ ,	RP-HPLC,	329
benzoic acid derivatives	Interaction energies, MM, $pK_a$	$\log k$ ,	RP-HPLC,	330
Model series of test analytes	Structural parameters of stationary phases	Retention data	NP, RP, CE	331
33 purine nucleobases	3D field descriptors	CoMFA (0.969) validation (0.832)	C18 column	332
Neutral and basic compounds	$\log P$ ,	$\log k_w$ , $\log k$ ,	Supelcosil ABZ+Plus, Discovery RP Amide C16, and Zorbax Extend C18	333
Antiprotozoal meso-ionic 1,3,4- thiadiazolium-3-aminides	VolSurf descriptors, hydropho- bic (DRY), amide N-atom (N(1)) and carbonyl O-atom	RT,	Supelcosil ABZ+ Plus column methanol-water acetonitrile-water	334

83 basic drugs	(O) probes 1272 molecular descriptors.	CART, stochastic gradient boosting random forest, GA-MLR (0.964), UVE-PLS	Unisphere PBD column	335
16 indole derivatives	Ab initio B3LYP/6-311G**	$\log k$ , $\log k_w$ (0.9796), S (0.9874)		336
29 nitrogen containing heterocycles	Molecular connectivity, Wiener, Kier flexibility, Harary, Balaban, Zagreb indices	$\log k$ , simple linear (0.9- 1.0)	LC	337
24 nitrogen-containing heterocycles	$\alpha$ , MR, $\log P$ , $\mu$ , Etot, $\Delta H_f$ , molecular surface area (SM), binding energy (Eb)	$\log k$ , simple linear (0.8- 1.0), multilinear (1.000)		338
Single- and multi-ring aromatic hydrocarbons (AH)	Substituent effect, electronic and geometric descriptors, IP, EA	RT, PLS, GA,	[3-(2,4- dinitroanilino)]propyl-silica column	339

#### Notations

ANN - artificial neural network

$\alpha$  - polarizability

CA - cluster analysis

CART - classification and regression tree

CE capillary electrophoresis

CFA - correspondence factor analysis

CHI - chromatographic hydrophobicity index

CoMFA - comparative molecular field analysis

$\delta$  - electron excess charge of the most negatively charged atom

$\Delta H_f$  - heat of formation

$\delta T$  - total solubility parameter

EA - electron affinity

Etot total energy

$\epsilon$  - permittivity

FA - factor analysis

$\phi$  - volume fraction of mobile phase

GA - genetic algorithm

GRNN - generalized regression neural networks

HOMO - energy of highest occupied molecular orbital

index of hydrophobicity  $\phi_0 = -\log k_w / S$

IP - ionization potential

IPC - ion pair chromatography

$k$ ,  $k'$  - retention coefficient, (capacity factor)

$\log k_w$  - intercept of the plot for  $\log k'$  vs.  $\phi$  (extrapolated to mobile phase without water)  
 $\log P$ ,  $\log k_{o/w}$  - octanol/water partition coefficient  
 LOO - leave-one-out cross validation  
 LUMO - energy of the lowest unoccupied molecular orbital  
 MLR - multiple linear regression  
 MLP - multilayer perceptron neural networks  
 MR - molar refraction  
 $\mu$  – dipole moment  
 NLM - non-linear mapping  
 NP - normal phase  
 ODS - octadecyl silica  
 $p$  - solute polarity parameter (eq(1))  
 PAH - polycyclic aromatic hydrocarbons  
 PCA - principal component analysis  
 PCR - principal components regression  
 $pK_a$  – dissociation constant  
 PLS - partial least squares  
 RBF - radial basis function  
 RP - reversed phase

RT - retention time  
 $S$  - slope of the plot for  $\log k'$  vs. volume fraction of mobile phase ( $\phi$ )  
 SOM - self-organizing map, Kohonen network  
 SP - stationary phase  
 $S_w$  - solvent-accessible surface area  
 $T_b$  - boiling point  
 UVE-PLS - uninformative variable elimination-PLS  
 $V_m$  - molar volume  
 $V_w$  - van der Waals volume

Table 5 QSRR examinations in micellar liquid chromatography between 1996-2006.

Solutes	Descriptors	Models	Column, mobile phase, surfactant	Source
Congener series of steroid hormones	Topological i.e., connectivity indices, X, steric factors	RT, linear, multilinear	ODS column (RP-HPLC,) sodium dodecyl sulfate (SDS)-borate system and with a mixed micellar solution of SDS and sodium cholate	340
Anionic solutes	Migration index, $\log k_w$	$\log P$	Sodium dodecyl sulfate/1-butanol/heptane/buffer, CE	341
	$\log P$ , $\log k_w$ , LSER descriptors	$I$ , linear	SDS surfactant no such a linear relationship with CTAB, DTAB	342
Catecholamines	Physico-chemical parameters	$\log k$ , $\log P$ , MLR, PLS		343
Local Anesthetics	molar fraction of the charged form, $\log P$ ,	$\log k$ , MLR,	Nonionic surfactant solution	344
14 flavonoids	183 structural descriptors, electrotopological state indices (Si) of skeletal carbons	Mobility, effective mobility CA, FA, $\log k$ , migration	38 buffer conditions, CZE, MEKC	345
Barbiturates	Hydrophobic and electrostatic ( $\log P$ , $\delta'$ ) PC	$\log k$ , $\log k = a \log P + b \delta' + c$	C18, surfactant: Brij 35, SDS and CTAB	346
Catecholamines, local anesthetics, diuretics and o-phthalaldehyde-N-acetyl-l-cysteine amino acid derivatives	Hydrophobic and electrostatic forces	$\log k = a \log P + b \alpha' + c$	Brij35, SDS	347
	$\log P$ , molecular structure parameters	$\log k'$ , ANN, MLR (>0.998)	MECC	348
21 basic pharmaceutical substances	$-0.026 < \log P < 6.45$ )	PCA, drug classification	MLC, MEKC, IMC, HPLC	349
Non-steroidal anti-inflammatory drugs	Retention data	Biological activity, pharmacokinetic	MLC, RP-HPLC, Brij35	350

10 amphoteric sulfonamides	$\log P$ ,	parameters $\log k$	MLC, SDS	351
60 aromatic compounds and 9 corticosteroids	$\log P$ , LSER descriptors	$\log k'$	MEKC, SDS, SC, LiPFOS, C14TAB	352
16 $\beta$ -blocking agents	$\log P$ ,	$\log k$	MLC, SDS, n-propanol (organic modifier)	353
Phenoxy acid herbicides	Migration parameters	Toxicity	MLC, MEKC, Brij35	354
Antihistamine drugs	Hydrophobic, electronic and steric, $k$ in BMC	Pharmacokinetic parameters	BMC, Brij35	355
66 organic pollutants	$\log k$ , structural parameters	ecotoxicity parameters, $\log P$ , PCA	BMC, Cross-validation, calibration set	356
Neutral aromatic compounds, $\beta$ -blockers, and other drugs	$\log P$ , LSER descriptors	$\log k$ , $K_{lw}$ ,	LEKC, CE, liposomes are in a buffer solution (pseudostationary phase)	357
Basic pharmaceutical substances	$pK_a$ , $\log D$	Fast $\log P$ , PCA	MLC, monolithic silica	358
Non-steroidal anti-inflammatory drugs	$\log P$ , IC50 (concentration required to 50% inhibition), $t_{1/2}$ (half-life time)	$V_d$ (volume of distribution), CL (clearance), $\log k$	MLC, Brij 35	359
85 pesticides	$\log k$ ,	Acute toxicity pLC50	BMC,	360
85 pesticides	$\log k$ , $\log P$ ,	BCF, $\log k$ ,	BMC,	361
10 $\beta$ -blockers, 7 tricyclic antidepressants (TA), 8 steroids 12 sulfonamides	$\log P$ , $\log P_{\text{apparent}}$	$\log k$ ,	RPLC acetonitrile, MLC	362
151 structurally unrelated solutes	$\log P$ , molecular size, hydrogen bonding properties, ionization degrees	$\log k$ , MLR	BMC, Brij35	363
Benzene derivatives, heterocyclic compounds	Molecular surface area, maximum value of electron density, path four connectivity index, Mw, sum of atomic	$\log k$ , MLR, ANN	MEKC, Training set	364

Substituted benzenes	polarizability LSER, hydrophobic, H-bond, polar interactions	$\log K_{mw}$ (0.979) MLR,	MEKC	365
79 heterogeneous pesticides	LSER descriptors	$\log k$ , MLR, SVM (09755)	BMC	366

#### Notations

ANN - artificial neural network

$\alpha$  - polarizability

$\alpha'$  - molar total charge of compound at a given pH value

BMC - biopartitioning micellar chromatography

C14TAB - cationic surfactant

CA - cluster analysis

CART - classification and regression tree

CE capillary electrophoresis

CHI - chromatographic hydrophobicity index

CoMFA - comparative molecular field analysis

$\delta$  - electron excess charge of the most negatively charged atom

$\delta'$  - molar fraction of the charged form of the compound

$\delta T$  - total solubility parameter

EA - electron affinity

$E_{tot}$  total energy

$\epsilon$  - permittivity

FA - factor analysis

$\phi$  - volume fraction of mobile phase

GA - genetic algorithm

GRNN - generalized regression neural networks

index of hydrophobicity  $\phi_0 = -\log k_w / S$

IPC - ion pair chromatography

$k, k'$  - retention coefficient, (capacity factor)

$K_{mw}$  - micelle-water partition coefficient

$K_{lw}$  - liposome-water partition coefficients

LiPFOS - lithium perfluorooctane sulfonate

LEKC - liposome electrokinetic chromatography

$\log k_w$  - intercept of the plot for  $\log k'$  vs.  $\phi$  (extrapolated to mobile phase without water)

$\log P, \log k_{o/w}$  - octanol/water partition coefficient

MLC - micellar liquid chromatography

MECC - micellar electrokinetic capillary chromatography

MEKC - micellar electrokinetic chromatography

MI - migration index, a general hydrophobicity scale

MLR - multiple linear regression

MLP - multilayer perceptron neural networks

MR - molar refraction

$\mu$  - dipole moment

NP - normal phase

ODS - octadecyl silica

$p$  - solute polarity parameter (eq(1))

PAH - polycyclic aromatic hydrocarbons

PCA - principal component analysis

$pK_a$  - dissociation constant

PLS - partial least squares

RP - reversed phase

RT - retention time

$S$  - slope of the plot for  $\log k'$  vs. volume fraction of mobile phase ( $\phi$ )

SC - sodium cholate

SDS - sodium dodecyl sulfate

Table 6 QSRR examinations in affinity chromatography between 1996-2006.

Solutes	Descriptors	Models	Column, protein	Source
Antihistamine drugs	$\log k(\text{IAM})$ , electron excess charge on the aliphatic N	$\log k(\text{AGP})$	$\alpha 1$ -acid glycoprotein (AGP), IAM	367
56 acidic, basic and neutral drugs	$\log k(\text{IAM})$ , $\log P$ , ionization of acidic groups	Brain/blood concentration,	Commercial IAM.PC.DD	368
Xenobiotics	$M_w$ , $\mu$ , $\log P$ , $\log k(\text{IAM})$	$\log k(\text{keratin})$ , $\log K_p$	IAM, physical immobilization of keratin on silica support	369
Test series of drug analytes	$\log P$ , structural descriptors from molecular modeling	Drug-macromolecule binding	AGP, keratin, collagen, melanin,	370
24 test analytes	$\log P$ , LSER descriptors	$\log k$ , $\log k_w$ , MLR	Immobilized cholesterol on spherical silica gel, RP-HPLC, C18, IAM	371
40 structurally unrelated drug	Percentage of binding	Retention	Immobilized human serum albumin (HSA)	372
Set of standards	LSER descriptors	$\log k(\text{IAM})$ , CHI, CHI(IAM)	Fast gradient, IAM	373
drugs	$\log P$ , $\log k$ ,	$\log k(\dots)$ ,	HPLC, CE, biomacromolecules	374
Drugs, standards	QSRR descriptors	Retention	Macromolecules as SP	375
Appropriately designed sets	$\log k(\text{AGP})$ , $\log k_w$	$\log K_p$ , $\log k(\text{KER})$ , $\log k(\text{COLL})$ , $\log k(\text{MEL})$ , etc.)	HAS, AGP, keratin, collagen, melanin, amylose tris(3,5-dimethylphenylcarbamate) basic fatty acid binding protein	376
Series of analytes, 65 new buspirones		Diverse and mutually interrelated retention parameters, PCA	9 carefully designed HPLC systems, 5-HT1A serotonin receptors	377
	$\log P$ , molecular structural parameters	$\log k$	C18, C8, IAM, AGP, PBCA, PGC	378
Antihelmintic 6,7-diaryl-pteridine derivatives	$\log P$ , $\log k(\text{IAM})$ ,	$\log k(\text{IAM})$ , IC50	ODS, IAM.PC.DD2	379
11 arylpropionic acid derivatives	$\log P$ , $\log D$	$\log k_w(\text{IAM})$ , $\log k_w(\text{ODS})$	ODS, IAM.PC.MG	380

32 structurally diverse drugs	$\log P$ , $\log D$ , $\log P_{app}$	$\log k(\text{IAM})$ , MLR, PLS	Phospholipids, IAM	381
68 drug molecules.	CHI (IAM), $\log P$ , LSER,	$\log K(\text{HAS})$	Fast gradient HPLC, HSA	382
Long fatty acids	$\log P$ , total lipole	$\log k$ ,	Immobilized liver basic FABP	383
			“Embedded” phases: aminopropylated silica gel, e.g. phospholipids and cholesterol, IAM's	384
Azapirone derivatives	Molecular structural	Retention parameters, BP-ANN	Rat brain serotonin 5-HT1A receptors, 14 HPLC systems	385

## Notations

BP-ANN - back propagation artificial neural network

C18 - bonded octadecyl silica

C8 - bonded octyl silica

CHI - chromatographic hydrophobicity index

$\phi$  - volume fraction of mobile phase

FABP - fatty acid binding protein

HSA - human serum albumin

index of hydrophobicity  $\phi_0 = -\log k_w/S$

IAM - immobilized artificial membrane

$k$ ,  $k'$  - retention coefficient, (capacity factor)

$K_p$  - human skin permeation coefficient

$\log D$  -  $\log P$  for ionisable compounds

$\log k_w$  - intercept of the plot for  $\log k'$  vs.  $\phi$  (extrapolated to mobile phase without water)

$\log P$ ,  $\log k_{o/w}$  - octanol/water partition coefficient

$\log P_{app}$  - apparent  $\log P$

LSER - linear solvation energy relationships

MLR - multiple linear regression

$\mu$  – dipole moment

NP - normal phase

ODS - octadecyl silica, C18

PCA - principal component analysis

$pK_a$  – dissociation constant

PBCA - polybutadiene-coated alumina

PGC - porous graphitic carbon

RP - reversed phase

$S$  - slope of the plot for  $\log k'$  vs. volume fraction of mobile phase ( $\phi$ )



Table 7 remaining QSRR examinations between 1996-2006.

Solutes	descriptors	models	Column, method	Source
Series of sulfonamides		Electrophoretic mobility, MLR, BP-ANN	CZE, cross-validation	386
20 beta-diketones	6 descriptors	<i>I</i> , MLR, polynoms		387
Proteins	Descriptors, from protein structure	RT (0.969-0.952)	Ion exchange systems, cross and external validation	388
Probe molecules	Traditional and novel molecular property descriptors	GA, PLS	Ion-exchange chromatography (IEC)	389
19 solutes (Ala, Gly, Lys, Phe, homopeptides)	log <i>P</i> and specific hydrophobic surface area	PCA, NLM	TLC, impregnated alumina layers	390
o-Acetylphenyl esters	Topological	RT	Not given	391
1-bromo-2-aryloxyetanes and 3- aryloxypropionitrile derivatives	5 quantumchemical	RT, polynoms	Not given	392
	Set of fragmental descriptors	<i>I</i> , <i>T<sub>b</sub></i>	GC	393
Proteins	Topological, subdivided surface area, TAE, electron-density-based descriptors	RT, SVM	Anion exchange chromatography, training and validation sets	394
Proteins	Molecular descriptors	RT, SVM (0.943 - 0.994) cross-validated	Anion exchange chromatography salt-in	395
Proteins		RT, SVM (0.919 - 0.980)	Cation-exchange systems, counterions,	396
	Number of single bonds, of double bonds, hydrophilic factor	Retention factors, BP-ANN, MLR	Supercritical fluid chromatography, cross-validation	397
Basic compounds (drugs)	Molecular interaction energies	Elution order	Ion-exchange chromatography	398
Proteins, human lactoferrin	New protein descriptors, ASP 1	RT	Ion-exchange chromatography	399
Set of model proteins	New hydrophobicity descriptors,	RT, SVM	Hydrophobic interaction	400

$S_w$

chromatography, 4 resins

## Notations

ASP - average surface potential

BP-ANN - back propagation artificial neural network

CHI - chromatographic hydrophobicity index

CZE - capillary zone electrophoresis

FABP - fatty acid binding protein

GA - genetic algorithm

HSA - human serum albumin

$I$  - Kovats retention index

IAM - immobilized artificial membrane

IEC - ion-exchange chromatography

LSER - linear solvation energy relationships

MLR - multiple linear regression

NLM – nonlinear mapping

ODS - octadecyl silica, C18

PCA - Principal Component Analysis

PLS - partial least squares

RT - retention time

SFC - supercritical fluid chromatography

SVM - support vector machines

$S_w$  - solvent accessible surface area

TAE - transferable atom equivalent