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Quantitative structure - (chromatographic) retention relationships: QSRR

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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.

Contents

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

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

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

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

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

132 Figure 1

133 The search covers the period of 1996-2006 Aug with extensive usage of 'Web of Science'
134 and 'Scopus' data bases. The increase is not continuous; random factors also influence the
135 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 reverence (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***(measured) vs. ***Y***(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***(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

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

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

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

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

292 $$\log I = a\log T_b + b(n_1 + \Sigma k_i n_i) + c \quad (1)$$

293 where n_1 is the serial number of homologue within corresponding series and n_1 is the number
294 of other structural fragments in the molecules. The coefficients k_i in this equation reflect the
295 relative alterations of molecular polarizabilities and may be estimated as ratios of refractions
296 $k_i = R(D)(X)/R(D)(CH_2)$, (X are variable structural fragments within a group of congeners,
297 $R(D)(CH_2) = 4.647\ cm^3mol^{-1}$) [5].

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

305 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 (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 (Kp) 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.
357
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 enatiomeric separation (α) 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.
371
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].
377
378

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 (π_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^{-3}]); *c* is a constant (intercept, off-set, e.g. $\log k_{ref}$); *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 (φ):

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

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 (α) is given by Snyder at al.:

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

where k_{ref} - non-polar reference solute. The coefficients denote properties of the solute: η' - hydrophobicity; σ' - molecular "bulkiness" or resistance to insertion of the solute into the stationary phase; β' - hydrogen-bond basicity; α' - hydrogen-bond acidity κ', 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 l-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.

503 Concluding remarks as “The predicted values are in very good agreement with the
504 experimental values” say very little about the real prediction performance, they should be
505 avoided.
506 There is some ambiguity in the usage of ‘test analytes’ and ‘test sets’. Test analytes form
507 the training set whereas a new independent series of compound serve for testing the
508 prediction performance. The prediction set is often called as test set in chemometrics.
509 The statements as “ANN predicts the retention data better than MLR method” has little
510 relevance (see the text in gas chromatography part).
511
512 *5.3 Suggestions for future works*
513 The domain of model applicability is rarely given for QSRR investigations in liquid
514 chromatography, neither. Although mobile phase concentrations are provided, which
515 compounds can be included and which ones should be excluded from the investigations are
516 missing.
517 Properly validated models should be recommended for prediction purposes. The same
518 performance indicators (adjusted correlation coefficients, cross-validated correlation
519 coefficients, F values, standard errors, etc) should be used for comparison.
520 Standardization of optimization strategies for chromatographic separation conditions
521 would provide great benefit if using QSRR equations.
522
523 *5.4 Summary of QSRR papers in column liquid chromatography*
524 Table 4 summarizes the solutes, methods and techniques for QSRR models in column LC
525 (correlation coefficients are in brackets).
526 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 φ_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].

Lipopholicity 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.

552 Properly designed test series of analytes can be recommended for comparative studies of
553 analytical columns. QSRRs once derived on a given column for model analytes can be used
554 to predict the retention of other analytes of a defined structure. That in turn can facilitate the
555 procedure of the rational optimization of chromatographic separations and can characterize
556 modern stationary phases (systems) in an objective, quantitative manner [274].
557 The linear solvent strength (LSS) model + QSRR approach has been demonstrated to
558 provide approximate, yet otherwise unattainable, a priori predictions of gradient retention of
559 analytes based solely on their chemical formulae [302].
560 Solute polarity descriptor (p) is useful to transfer retention data between solvents and/or
561 columns. The retention for any chromatographic systems (mobile phase composition) can be
562 predicted using the five solvation descriptors (Eq. (1)), if the polarity of the column has been
563 characterized using a small training set. Alternatively, log*P* and hydrogen-bond acidity data
564 can be used for these predictions [313].
565 Numerous correlations of retention data with an octanol-water partition coefficient
566 have been reported. K. Valko has reviewed lipophilicity correlations and alternative
567 lipophilicity measures [315].
568 A comparison of chemometric methods based on predictive performance indicated the
569 most important variables and that, individually, genetic algorithm selected descriptors with
570 multiple linear regression modeling outperformed all other models [335].
571
572
573 **6. Quantitative structure - retention relationships in micellar chromatography**
574
575 Micellar liquid chromatography, micellar electrokinetic chromatography, micellar
576 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 chromatoghraphy (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 multivarate 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 lipohilicity 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 multivarate 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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Standard English transliteration was applied for names, e.g. á → a, ñ → n, etc.

Captions to figures

Figure 1

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

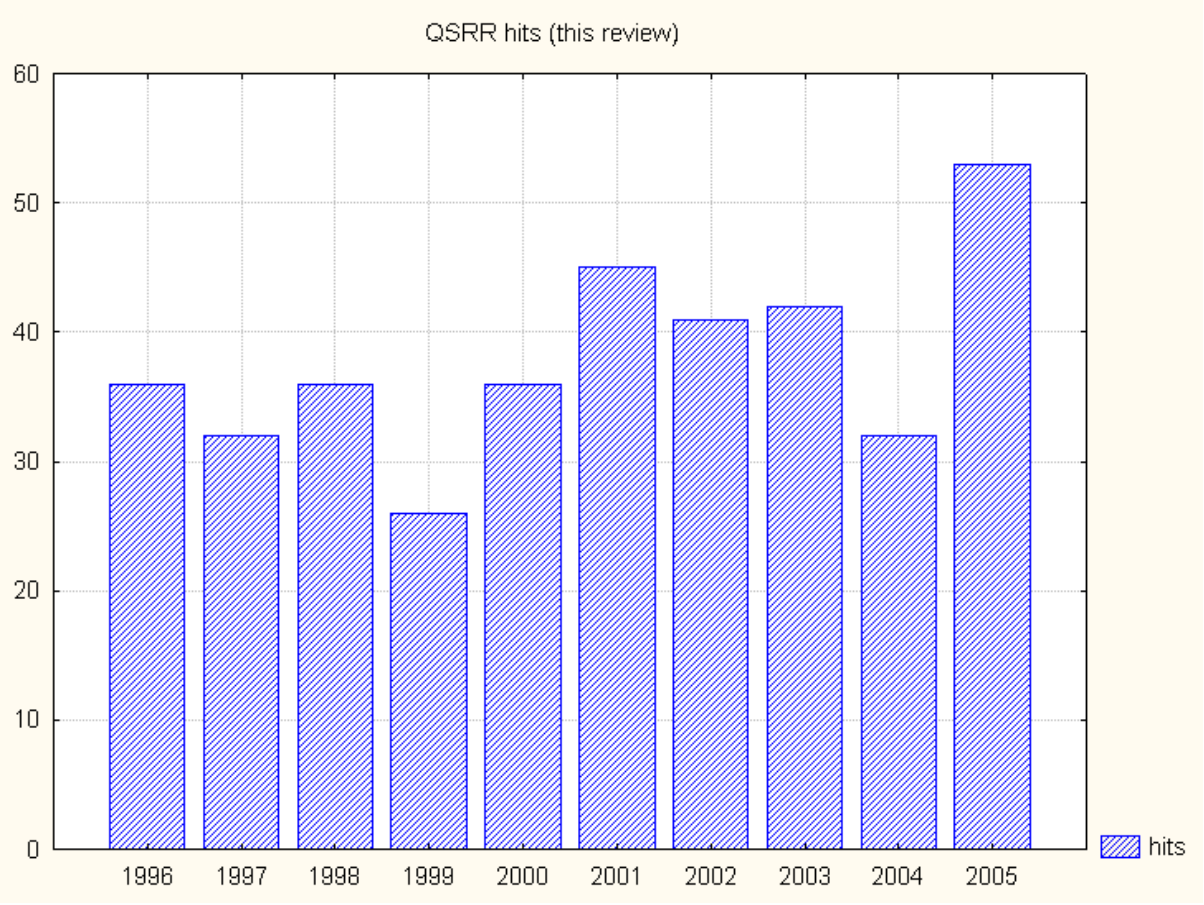

Figure 2

Occurrence (frequency) of QSRR papers versus rank ordering of scientific journals within 1996 - 2006.

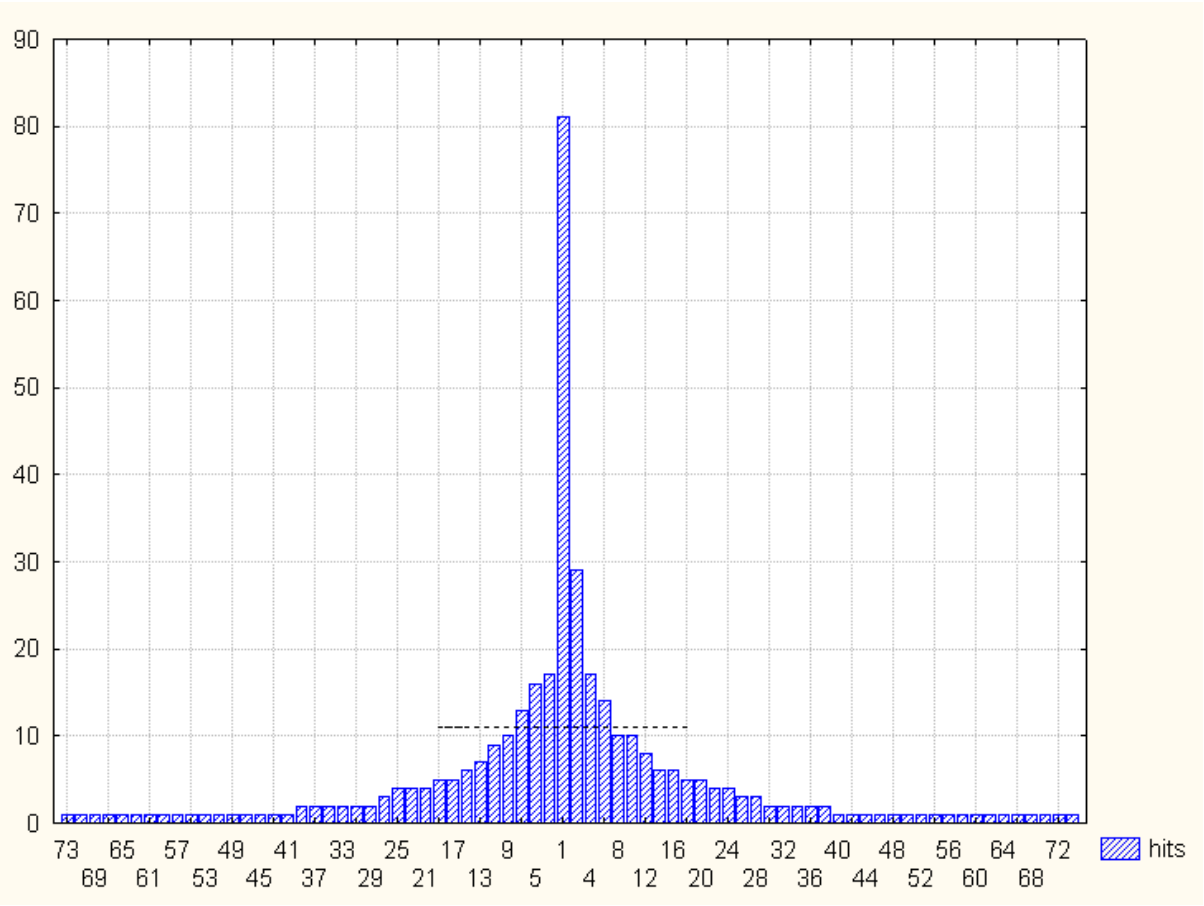

Table 1 QSRR in gas chromatography 1996-2006

Solutes	Descriptors	Model building	Stationary phase (SP)	Validation	Source
Linear alkylbenzene isomers with C_{10}-C_{14} linear alkyl chains	Balaban, Wiener, Electrotopological state and molecular shape indices	*I*, MLR		No	[11]
37 organosulfur compounds (vesicants)	Quantumchemical MNDO, PM3, AM1	MLR	three	No	[12]
Various examples	Homomorphic factors, topochemically equivalent increments	*I*, Additive schemes		No	[13]
Alkyl groups	Internal molecular energies of reactants and products	*I*, increments			[14]
Homologous series and their branched-chain isomers (1000)	Retention data on other SPs	*I*	Two various	'Relative higher accuracy'	[15]
Congener series of substituted benzenes, benzaldehydes and acetophenones	Different set of topological parameters	*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	T_b, homomorphic factors, bond angle and electron density {I(oxo)}, volumes, van der Waals' surface.	*I*, Simple linear	HP-1, HP-5	Visual	[18, 19]
38 isoalkanes and 24 alkenes	substantial, important, likely and	*I*, MLR	Squalane,	1.6 < SD < 9.7	[20]

	specific parameters, (quantumchemical)		citroflex, carbon black		
Aromatic analytes, positional isomers of xylenes, ethyltoluenes and diethylbenzenes		RRT	Fused-silica with calixarene oligomers		[21]
PAHs (70)	T_b, vaporization enthalpy, molecular total energy	*I*, linear, nonlinear (Etot)	Methylsilicone, Carbopack	No	[22]
Anabolic steroids, stimulants and narcotics	Molecular characteristics				[23]
Low-polarity solutes (9) e.g. camphene, α-terpinene, myrcene	T_b	RRT, linear (0.994)	Six different modified α-, β- and γ-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-π orbital overlap of lone pairs	*I*, Additive schemes	Polar and non-polar	Deviation<3.00%	[32]

	C=C bonds				
Alkylbenzenes (18)	T_b, reciprocal T_b	RRT, exponential (0.9585-0.9967)	Silicon oil 550, dinonylphtalate, PEG4000, Bentone 34	0.047<SD<0.42	[33]
Alkylbenzenes (18)	T_b ,	*I*	- " -	Theoretical derivation	[34]
Aliphatic alcohols, aldehydes, acids and amines	Ortogonalized descriptors	PCA		No	[35]
Organic compounds, homologues, congeners	T_b, structural fragments, molecular polarizabilities	*I*, linear-logarithmic	Dimethylpoly-siloxane	*I* ~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 π-system surface (S(π)) 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, dinonylphtalate,	4.3<SD<47.9	[42]

			PEG4000, Bentone 34		
Alkylbenzenes (18)	T_b, reciprocal T_b	RRT, exponential (0.9455-0.9977)	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*, BP-ANN	Squalane, SE- 30, PEG,	Training and test sets, Relative error 3%	[52]
isoalkanes, dialkyl sulfates, and aliphatic amines and	T_b, NC, V_m, R_m, sum of internal rotational and vibrational energies	*I*, structural fragments		Molecular dynamic caculations	[53]
Diverse chemical compounds (152)	CODESSA descriptors (296), linear selection	Retention time, RF, MLR, nonlinear models		Comparison with earlier results	[54]
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*, 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*, scores, PLS, (0.990-0.995)	HP-1, HP-50, DB-210, HP-Innowax	Cross-validation 0.975<Q^2<0.990	[57]
Polychlorinated biphenyl (PCB) congeners,	New QSRR descriptors for selectivity correction	Retention time	various	SDs are ‘within a chromatographic peak width’	[58]
Methylalkanes produced by insects (178)	Mainly topological descriptors	*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),	Substitution pattern, positions	*I*, MLR (>0.9995)	DB-5	SD<7 i.u.	[60]
Alkylbenzenes (129)	molecular graph descriptors, sequential orthogonalization	*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*, 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*, 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*, MLR			[65]
Amines	Topological indices Aml, Am2, Am3, gravitational index G1.	*I*, MLR	Phase of various polarity (3)		[66]
Saturated and monounsaturated six- carbon aldehydes, alcohols and esters	T_b	*I*	DB-5, DB- 1701, DB-Wax		[67]
Hydrocarbons and derivatives containing oxygen, nitrogen and halogens	Valence connectivity indices, 1(χ)(ν) Wiener, W, and Balaban, J, indices	logV(g), *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		(>0.990)	cyclodextrin		
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	*I*			[73]
Aldehydes, ketones	Quantum-chemical method PM3. HOMO, LUMO, polarizability, dipole moment, solvent accessible surface area	*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*, linear (0.988), to the gas		Comparison with results of molecular polarizability index	[75]
Alkylbenzenes (129)	Molecular graph descriptors (5)	*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*, MLR, BP-ANN	Cit.A-4, SE-30 and Carbowax 20M		[77]
Hydrocarbons	Molecular structure	*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*, MLR (0.9874 - 0.9901)		20.2<SD<22.9 leave-one-out cross-validation	[80]
Noncyclic and monocyclic terpenes (53)	One electronic, two geometric, two topological and one physicochemical descriptors	*I*, MLR, BP-ANN	Carbowax 20 M	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 0.991<q<0.992	[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 8.15<RMS<9.35	[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*P* values, and molecular surface areas,			Smectic	
Organic compounds with various functional groups	T_b, α, 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*, MLR (0.99999)	DB-1	SD=3.20 External SD=4.6	[96]
Branched alkenes	Semi-empirical topological index	*I*, MLR	Squalane, 1-octadecene, Apiezon-L, OV-1, DB-1	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*, 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*, BP-ANN	OV-1, SE-54	Training, prediction sets; average percentage deviation 2.5 - 3.0%	[101]
Alkanes, alkenes, alcohols, esthers, ketones, ethers	T_b, V_m	*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*, MLR, PCA	SE-30, OV-7, DC-710, OV-25, 100% phenyl,	SE=13.1-23.0	[103]

			DC-230 and DC-530		
Oxo compounds (54)	Semiempirical topological index	*I*, linear (0.999)	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		Δ*I*, additivity scheme		theoretical	[108]
Polychlorinated biphenyls, PCBs (30)	Topological parameters (Balaban index and electrotopological index	RRT, R*I*, 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]

	index, dipole moment, density, molecular mass and vapor pressure				
Aldehydes, ketones	Xu index, atom-type-based AI topological indices (fragments)	*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*, MLR (1.0000)		Test set (182), SD=7.7	[114]
Alkoxyl silicon chlorides	molecular topological index mXY	*I*,			[115]
Alcohols (25)	hydrogen connectivity index	*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*	Not given		[119]
Saturated alcohols	Semi-empirical topological index	*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*, 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	Relatieve errors: 0.01% 0.37%.	[123]
Aldehydes, ketones	Semi-empirical topological index, IET	*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,	ΔH, RT, MLR	DB-1	S(ΔH)=161 cal/mol; cross-	[125]

				validation	
271 organic compounds of diverse structures	Retention data on two phases of different polarity	T_b, bilinear(0.9724)	DB1-60W, DBWAX-30N	SD=16.1 K	[126]
α-, β1-, and β2-agonists	Diverse connectivity and electrotopological indices	RRT, MLR, PCA, PLS	Crosslinked methylsilicone gum,	Training and prediction set	[127]
CNS agents (benzodiazepines, barbiturates, phenytoin)	Calculated descriptors	*I*, MLR (0.983-0.988)	DB-5, DB-17	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, chlorodifluoro-methane, dimethyl ether, and sulfur hexafluoride, (65)	R_m, connectivity index, surface area, surface energy contribution (r2=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	HP-5		[134]
149 C3 - C12 volatile organic compounds	Total information index of atomic composition IAC, Wiener number, W, solvation connectivity index,	PCA, MLR for variable selection BP-ANN	DB-1		[135]

	Xlsol, number of substituted aromatic C(sp2), nCaR,				
118 polychlorinated biphenyls, PCBs	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*,	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*, MLR		'Clear physical significance'	[140]
Saturated hydrocarbons, olefines and dienes	Quantum chemistry parameters HOMO, LUMO, ElcE, R_m	*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*, 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*, RRT, MLR			[144]
Alcohols	Quantum chemical descriptors AM1, Hartree-Fock (HF) Gaussian 98	*I*, MLR	Superox 20M-diglycerol		[145]
Polyaromatics, polychlorobiphenyls		*I*			[146]

Aliphatic alcohols	Semi-empirical topological index (IET),	Linear (>0.98)		Cross-validation leave-one-out	[147]
Polycyclic aromatic sulfur heterocyclic compounds, PASHs	μ, Constitutional, geometric, topological, molecular walks	*I*, nonlinear	BPX5	Cross-validation	[148]
136 polychlorinated dibenzofurans, PCDFs	Number and position of chlorine substitutions, quantumchemical	*I*, (0.993-0.998)	DB-5	Cross-validation	[149]
Polychlorinated dibenzo-p-dioxins, PCDDs .dibenzofurans, PCDFs	*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*, BP-ANN	DB-1	Average relative error=3.3%.	[151]
Polychlorinated dibenzofurans, PCDFs	Molecular structure index, group modify index	*I*, RRT, MLR,	DB-5, SE-54 and OV-101	Relative deviation=1.09%	[152]
Organic sulfur compounds	Topological descriptors, temperature	*I*, MLR		Leave-one-out (0.978) leave-two-out (0.976)	[153]
Polychlorinated dibenzofurans, PCDFs (135) PCDFs.	Molecular hologram	*I*, PLS (0.999)		Training and prediction set	[154]
Nitrogen-containing polycyclic aromatic compounds, N-PACs	Codessa descriptors (3)	*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*, MLR (>0.98)	Various		[156]
Polycyclic aromatic hydrocarbons, PAHs	T_b , connectivity indices and molecular weights	*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*, 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*, MLR (0.9907 - 0.9978), 0.9983		Cross-validation (0.9885-0.9974) 0.9979	[160]
Aromatic imines	Topologic, topographic and quantum-chemical	*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*, 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*, MLR (0.994), PLS		Leave-one-out	[164]
Saturated esters (90)	Lu index, distance-based atom-type DAI topological indices	*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	T_b, linear temperature programmed retention index	K_{fg}, bilinear	Carboxen/polydimethylsiloxane	No	[166]
PAHs	T_b, molecular mass, connectivity index, Schabron molecular size	*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*, 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-FA*I*	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*	Methylphenylsiloxane (5% and 50% phenyl groups): DB5ms, DB17ms	New synthesized compounds	[171]

Notations
ANN - artificial neural network
α - 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 - eqivalent 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-hydroxylethyl)-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 α-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 sulphoxides	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, π-π interaction, log*P* and	MLR	Pirkle-type CSPs, Sumichiral OA4700	[183]
42 chiral arylalkylcarbinols	2D and 3D molecular descriptors	logα, MLR, ANN, CoMFA	Pirkle-type CSP	[184]

	quantum chemical (LUMO) hydrophobicity.			
α-aminophosphonates	Molecular parameters (4)	*k*, MLR, FA	Phenyl carbamate derivative β-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, loc*D* 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)	logα, 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]
Organophosponates	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
α - 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 17α-diols, 17α-estradiol, 17α-dihydroequilin (DHEQ), 17α-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	Ttopological indexes, physicochemical properties (15)	R_f, MLR	Silica gel layers	[202]
Aryloxyaminopropanol derivatives of 1,4-piperazine	Lipophilic Hansch's constants π, the number of carbon atoms in R1 substituent	R_m, linear, β-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-methylthioethyl-ideneamino) 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]

	parameter "E"		methanol-water)	
Homologous series of higher fatty acids, their methyl esters, higher alcohols	Topological indexes based on adjacency matrix, distance matrix	R_M, log*P*(Rekker), simple linear		[209]
Estradiol derivates	log*P*	Various chromatographically obtained hydrophobicity parameters (R_{M0}, logk_w and φ_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, IAlog 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 nicotinates (MN), nicotinamide, N-methylnicotinamide	Measured and calculated partition coefficients, log*P*exp, Alog*P*s, IAlog*P*, Clog*P*, log*PK*owin, xlog*P*, topological indices	R_{M0},	RP18WF254, methanol-water	[218]
Benzimidazole and benztriazole 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 logk_w, linear dependence, parabolic	RPLC, TLC, Methanol-water	[220]

Notations

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

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

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, μ, atomic electron excess charge	LSER, log*k*'	Polyethylene-coated silica (PECSiO(2)) polyethylene-coated zirconia (PECZrO(2)),	225
Substituted benzenes	Substituent constant (π) and the total solubility parameter (δT)	MLR,	Various columns in several different eluents	226
Quinolones	S_w, y-component of μ, 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 μ, logP and μ	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*, logk_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*, δT, log*P* molecular structure parameters	logk_w, linear, nonlinear, log*P*	RP-HPLC	237
76 structurally unrelated compounds	CHI,	logk_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, μ	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*	logk_w	Chemically-bonded-silica (SG-MIX), with hydroxyl (-	245

			OH), amino (-NH2), cyano (-CN), phenyl (-Ph), octyl (-C8) and octadecyl (- C18) 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	μ, Hammett's constants, σ_X, σ_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*	logk_{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	logk_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 (C18, C8, C4, CN)	254
Quinolones studied. At pH 3, was mainly affected by two descriptors,	HOMO μ, MM+, AM1 semiempirical	logk'	PRP-1 columns, MeOH, THF	255
2-cyano-3-methylthio-3-	10 structural parameters	logk', 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)	φ	logk', logk_w, linear, parabolic	RP, methanol-water or acetonitrile-water	258
58 diverse analytes	LSER descriptors, log$P$	logk', logk_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	logk_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$P$calc, V_m	logk, logk_w	RP-HPLC, methanol - water	263
Iridoid glucosides	Free rotation around σ-bonds		C18, normal diol SPs	264
Benzene and phenol derivatives, indazol, tiophene, caffeine, etc.	log$P$, structural- and LSER descriptors	logk', 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)	8 solute-related structural parameters	*k*', FA, MLR	RP-HPLC	269
233 very different compounds	4 structural descriptors, log*P*	Solute polarity parameter (p), MLR (0.977)	RP-HPLC	270
12 ethynyl-substituted PAHs and unsubstituted counterparts	Polarizability and subpolarity, AM1; PM3	RT (0.967-0.984)	C18, RP-HPLC, water/acetonitrile	271
25 substances	Structural descriptors	log*k*', ANN (MLP), PLS	Polyethylene-silica and polyethylene-alumina	272
25 substances	Structural descriptors	ANN (RBF), GRNN, PCR, polynomial PLS	Polyethylene-silica and polyethylene-alumina	273
Three test series of analytes	Reduced LSER, log*P*	RT	RP-HPLC	274
14 substituted benzaldehydes	Molecular connectivity indices, LSER and quantum chemical parameters	log*k*	C18, RP-HPLC, methanol-water	275
Alkylbenzenes, halobenzenes, xylenes, alkanes, isoalkanes	LSER, structural	α, log*k*	C8, C18, PBB, PYE	276
24 steroids	3D image	Pulse-coupled neural network: PCNN, PLS	RP-HPLC, cross-validation	277
162 drugs	Molecular similarity	log*k*, ANN (0.992-0.996)	RP-HPLC, cross-validation	278
pyrethroid pesticides	log*k*',	log*k*, log*P*	RP-HPLC, LOO	279
86 diverse compounds:	CHI(ACN, MeOH), hydrogen bond acidity	log*P* (0.943-0.970)	Fast gradient RP-HPLC	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	φ, substituents steric parameters	log*k*, MLR, PCA, NLM	Amide embedded RP silica column (Discovery RP-AmideC16), water-acetonitrile	284
45 barbituric acid derivatives	φ, -φ_0, conventional and	log*k*, MLR, asymmetry	Amide embedded RP silica	285

	quantum chemical structural	factor (AF5) theoretical plate (N)	column (Discovery RP-AmideC16), methanol-water	
45 barbituric acid derivatives	φ, -φ_0, conventional and quantum chemical structural	log*k*, MLR, 6 retention related parameters, PCA, NLM	Amide embedded RP silica column (Discovery RP-AmideC16), tetrahydrofuran-water	286
45 barbituric acid derivatives	φ, -φ_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 α-branched phenylsulfonyl acetates	Geometric and electronic descriptors, surface area (S), ovality (O), the charge of carboxyl group (Qoc), surface area	logk_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 σ (electronic properties of the ortho-substituents)	pK_a,	C18, C4, RP-HPLC, acetonitrile	290
Drugs and model compounds	Lipophilicity and acidity	RT, pK_a, logk_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 μ, electron excess charge of the most negatively charged atom water-accessible surface area	Rt, logk_w, S	Gradient RP-HPLC	294

54 disubstituted benzenes	8 molecular descriptors, PM3 semiempirical	logk_w, MLR, RBF-ANN	RP-HPLC	295
25, mainly substituted benzenes	LSER descriptors, S_w,	logk_w, MLR, PCA	8 RP-HPLC, CE	296
PAHs	Molecular connectivity, μ	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) 47 diverse compounds (test)	log*P*, μ, S_w, electron excess charge on the most negatively charged atom	RT, MLR (0.8953-0.9870)	Supelcosil LP18	300
83 structurally diverse drugs	266 descriptors, hydrophobicity (log*P* and Hy), the size (TPC) of the molecules	logk_w, CART	Unisphere PBD column isocratic elution	301
15 diverse aromatics (training)	log*P*, μ, S_w, electron excess charge on the most negatively charged atom	RT, MLR, ANN,	RP-HPLC, methanol-water	302
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 α-phenylacetic acid	Physicochemical parameters, μ, ε, topological indexes log*P*, logS, hydrogen-bond acceptor indicator (HA) and molecular mass	RT, MLR	RP-18 HPLC, methanol-water	304
Test solutes	LSER 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 (α), total energy (Et), water solubility (logS), connectivity index (χ) 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 (φ_0)	log*k*, logk_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-TiO2), HPLC, methanol-water	318
Xanthones, aglycones, glucosides	*S*	logk_w,	Gradient HPLC,	319
Benzoylphenylureas,	μ, MR, log*P*	k, MLR	polystyrene-octadecene-	320

18 Dihalogeno benzoylphenylureas			encapsulated zirconia, Kromasil-C18-SiO2	
101 peptides	Sum of RTs of amino acids, logV_w, log$P$	RT, MLR	Gradient HPLC,	321
98 peptides	Sum of RTs of amino acids, logV_w, log$P$	RT, MLR	Gradient HPLC,	322
Series of test analytes	log$P$, μ, δ, 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$P$	logk_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$P$,	logk_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, hydrophobic (DRY), amide N-atom (N(1)) and carbonyl O-atom	RT,	Supelcosil ABZ+ Plus column methanol-water acetonitrile-water	334

	(O) probes			
83 basic drugs	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*, logk_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	α, MR, log*P*, μ, Etot, ΔHf, 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
α - 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
δ - electron excess charge of the most negatively charged atom
ΔH_f - heat of formation
δT - total solubility parameter
EA - electron affinity
Etot total energy
ε - permittivity
FA - factor analysis
φ - volume fraction of mobile phase
GA - genetic algorithm
GRNN - generalized regression neural networks
HOMO - energy of highest occupied molecular orbital
index of hydrophobicity φ_0=-logk_w/S
IP - ionization potential
IPC - ion pair chromatography
k, *k*' - retention coefficient, (capacity factor)

logk_w - intercept of the plot for log$k$' vs. φ (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
μ – dipole moment
NLM - non-linear mapping
NP - normal phase
ODS - octadecil 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 (φ)
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, logk_w	log$P$	Sodium dodecyl sulfate/1-butanol/heptane/buffer, CE	341
	log$P$, logk_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$P$, δ') PC	log$k$, log$k$=a log$P$ + bδ' + 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$P$ + bα' + c	Brij35, SDS	347
	log$P$, molecular structure parameters	logk', 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

		parameters		
10 amphoteric sulfonamides	log*P*,	log*k*	MLC, SDS	351
60 aromatic compounds and 9 corticosteroids	log*P*, LSER descriptors	log*k*′	MEKC, SDS, SC, LiPFOS, C14TAB	352
16 β-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, β-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 β-blockers, 7 tricyclic antidepressants (TA), 8 steroids 12 sulfonamides	log*P*, log$P_{apparent}$	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

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

Notations
ANN - artificial neural network
α - polarizability
α’ - 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
δ - electron excess charge of the most negatively charged atom
δ’ - molar fraction of the charged form of the compound
δT - total solubility parameter
EA - electron affinity
Etot total energy
ε - permittivity
FA - factor analysis
φ - volume fraction of mobile phase
GA - genetic algorithm
GRNN - generalized regression neural networks
index of hydrophobicity φ_0=-logk_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
logk_w - intercept of the plot for log$k$' vs. φ (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
μ – dipole moment
NP - normal phase
ODS - octadecil 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 (φ)
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*(IAM), electron excess charge on thealiphatic N	log*k*(AGP)	α1-acid glycoprotein (AGP), IAM	367
56 acidic, basic and neutral drugs	log*k*(IAM), log*P*, ionization of acidic groups	Brain/blood concentration,	Commercial IAM.PC.DD	368
Xenobiotics	M_w, μ, log*P*, log*k*(IAM)	log*k*(keratin), logK_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*, logk_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*(IAM), CHI, CHI(IAM)	Fast gradient, IAM	373
drugs	log*P*, log*k*,	log*k* (…),	HPLC, CE, biomacromolecules	374
Drugs, standards	QSRR descriptors	Retention	Macromolecules as SP	375
Appropriately designed sets	log*k*(AGP), logk_w	logK_p, log*k*(KER, COLL, 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*(IAM),	log*k*(IAM), IC50	ODS, IAM.PC.DD2	379
11 arylpropionic acid derivatives	log*P*, log*D*	logk_w(IAM), logk_w(ODS)	ODS, IAM.PC.MG	380

32 structurally diverse drugs	log*P*, log*D*, log*P*app	log*k*(IAM), MLR, PLS	Phospholipids, IAM	381
68 drug molecules.	CHI (IAM), log*P*, LSER,	log*K*(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 octadecil silica
C8 - bonded octyl silica
CHI - chromatographic hydrophobicity index
φ - volume fraction of mobile phase
FABP - fatty acid binding protein
HSA - human serum albumin
index of hydrophobicity φ_0=-logk_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
logk_w - intercept of the plot for log*k*' vs. φ (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
μ – dipole moment
NP - normal phase
ODS - octadecil 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 (φ)

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*, 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*P* and specific hydrophobic surface area	PCA, NLM	TLC, impregnated alumina layers	390
o-Acetylphenyl esters	Topological	RT	Not given	391
1-bromo-2-aryiloxyetanes and 3- aryloxypropiononitrile derivatives	5 quantumchemical	RT, polynoms	Not given	392
	Set of fragmental descriptors	*I*, T_b	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 l	RT	Ion-exchange chromatography	399
Set of model proteins	New hydrophobicity descriptors,	RT, SVM	Hydrophobic interaction	400

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 - octadecil 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