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CHROMATOGRAPHIC BEHAVIOR AND LIPOPHILICITY OF s-TRIAZINE DERIVATIVES ON SILICA GEL IMPREGNATED WITH PARAFFIN OIL

Lidija R. Jevrić, Gordana B. Koprivica, Nevena M. Mišljenović, Bratislav Ž. Jovanović

The chromatographic behavior of four group of s-triazine derivatives (14 compounds) has been studied by TLC on silica gel impregnated with paraffin oil. Retention mechanism has been determined using the following mobile phases: water-acetone, water-acetonitrile, water-dioxane, water-tetrahydrofuran, water-methanol and water-ethanol, by changing the volume fraction of modifier in the mobile phase. On impregnated silica gel, a reversed-phase chromatographic process occurs. Good correlation was obtained between the retention constants, R_M^0 (determined by linear extrapolation), and slope, S, of chromatographic equations. There was also satisfactory correlation between these retention constants and logP values calculated using different theoretical methods. The study showed that the retention constants can be used as a measure of lipophilicity of investigated compounds.

KEYWORDS: s-Triazine derivatives, RP-TLC, impregnated silica gel, multiple linear regression analysis, lipophilicity

INTRODUCTION

Considerable attention has been paid to the analysis of chemical in the s-triazine group, due to their widespread use in agricultural chemistry and their subsequent degradation in biological syistems (1, 2). For initial chemical screening of the activity of newly synthesized compounds it is recommended first to determine their lipopholicity, an important physico-chemical property in relation to biological activity. Lipophilicity is difficult to quantitate, but the most widely accepted measure of lipopholicity is the octanol-water partition coefficient, defined as the ratio of the concentrations of the solute in the two phases of a saturated 1-octanol-water system. Measurement of the octanol-water partition coefficient is achieved by an alternative method, reversed-phase liquid chromatography (3). Reversed-phase thin-layer chromatography (RP TLC) has been found to offer a rapid method for the analysis of a large number of s-triazine type compounds. Certain relationships between the structure of s-triazine compounds and their mobility on silica gel impregnated with paraffin oil have recently been demonstrated (4). The reten-

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tion behavior of compounds in various chromatographic systems is believed to be different by nature, i.e. the different physico-chemical properties of an analyte can influence its retention. Most recently, much effort has been done with the major aim of finding a mathematical model relating the retention of a given analyte to physico-chemical and structural parameters (descriptors) of test molecules. These correlations are known as quantitative structure-retention relationships (QSRR) (5-7). Besides practical application in optimization strategies, QSRR studies can significantly contribute to getting some insight into the molecular mechanism of separation. The QSRR equations describing R_M^0 determined for different mobile phase organic component in terms of logarithms of *n*-octanol-water partition coefficients were derived. The partition coefficients (*A*log*P*, *IA*log*P*, *C*log*P*, logP_{Kowin}, *X*log*P*, *ACD*log*P*) were calculated by using different software packages. The purpose of the work described in this paper was, therefore, to select the logP data and TLC system that best characterize octanol/water partitioning, and thus the lipophilicity of the investigated molecules.

EXPERIMENTAL

Fourteen derivatives of s-triazine (Table 1) were investigated. The compounds were synthesized in the laboratory of the Department of Organic Chemistry, Faculty of Technology and Metallurgy, University of Belgrade (8, 9). Standard solutions (1 mg cm^{-3}) were prepared in methanol, acetone, or chloroform. Samples were spotted on the plates by means of a micro-pipette.

TLC was performed on 20 × 20 cm glass plates precoated with impregnate silica gel. The thin-layer of impregnate silica gel was prepared by suspending 25 g silica gel 60 GF_{254} (Merck) in 100 ml diethyl ether containing 2.5 % paraffin oil. To ease the visualization, fluorescent indicator F_{254} (Merck) was incorporated into the layers (10).

Impregnate silica gel layer was developed using the following mobile phases:

Aprotic solvents: Acetonitrile-water (ϕ =0.2-0.6; *v/v*), Acetone-water (ϕ =0.5-0.8; *v/v*), Tetrahydrofuran-water (ϕ=0.45-0.7; *v/v*), Dioxane-water (ϕ=0.5-0.8; *v/v*).

Protic solvents: Methanol-water (ϕ=0.5-0.8; *v/v*), Ethanol-water (ϕ=0.5-0.8; *v/v*).

The plates were developed to a distance of 15 cm by the ascending tchnique at room temperature without previous saturation of the chamber with mobile phase. Dark spots were observed under UV light (λ=254 nm). R_M values were calculated from R_M = log ((1/R_f) - 1). All calculations were performed using the computer software Origin, Version 6.1. The partition coefficients *A*log*P*, *IA*log*P*, *C*log*P*, logP_{Kowin} and *X*log*P*, were calculated for the compounds by applying different theoretical procedures (11, 12). *ACD*log*P* was calculated using commercial software and the other partition coefficients were obtained from the internet (13).

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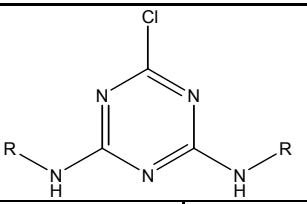
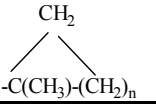
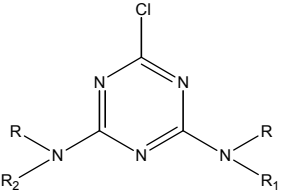
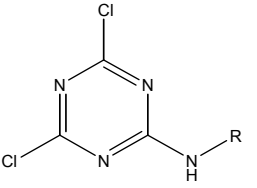
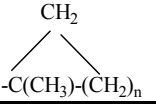
Table 1. Chemical structures of the s-triazines studied



Series I		Series II		
Compound	**R**	Compound	**R**	**n**
I.1	-CH(CH$_3$)-C$_6$H$_5$	II.1		3
I.2	-CH(CH$_3$)-C$_6$H$_4$-4-CH$_3$	II.2		4
I.3	-CH(CH$_3$)-C$_6$H$_4$-4-Cl	II.3		5
I.4	-CH(CH$_3$)-C$_6$H$_4$-4-Br			

Series III				Series IV		
						
Compound	**R**	**R**	**R**	Compound	**R**	**n**
III.1	C$_6$H$_{11}$	H	H	IV.1		3
III.2	C$_6$H$_{11}$	CH$_3$	CH$_3$	IV.2		4
III.3	C$_6$H$_{11}$	C$_6$H$_5$	H	IV.3		5
III.4	C$_6$H$_{11}$	C$_6$H$_5$	C$_6$H$_5$			

RESULTS AND DISCUSSION

Determination of Retention Constants, R_M^0, TLC Equations

When the R_M values calculated from R_f values (retention factor defined as the distance migrated by the sample from the origin compared with the distance migrated by the solvent front from the origin) were plotted against mobile phase composition for each compound there was a range in which a linear relationship was observed between the R_M values and organic modifier concentration in the mobile phase, which can be expressed by the equation $R_M = R_{M^0}{}^0 + S\phi$, indicative of the reversed-phase chromatography, were ϕ is the amount (%) of organic compounds in the mobile phase (14). The obtained slopes, S, and intercept values, $R_M{}^0$, of TLC equation for each solute are presented in Table 2. The correlation coefficients of the TLC equations were satisfactory.

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Table 2. Extrapolated $R_M{}^0$ values, slopes, S, and correlation coefficients, r, obtained on silica gel impregnated with paraffin oil

Comp.	*Acetone*			*Acetonitrile*			*Dioxane*			*Tetrahydrofuran*			*Methanol*			*Ethanol*		
	R_M^0	S	r	R_M^0	S	r	R_M^0	S	r	R_M^0	S	r	R_M^0	S	r	R_M^0	S	r
I.1	1.892	-2.753	0.997	2.905	-5.405	0.985	2.888	-4.616	0.996	1.972	-2.436	0.997	2.143	-3.119	0.993	2.933	-4.648	0.997
I.2	2.352	-3.240	0.999	3.850	-6.97	0.993	2.729	-4.955	0.993	2.576	-3.332	0.990	2.602	-3.506	0.998	2.921	-4.224	0.997
I.3	2.589	-3.526	0.999	4.578	-8.307	0.985	2.491	-5.34	0.995	2.854	-3.753	0.998	2.704	-3.700	0.996	3.847	-5.652	0.993
I.4	2.418	-3.267	0.996	5.169	-9.324	0.984	3.658	-5.598	0.997	2.857	-3.721	0.992	3.056	-4.085	0.994	3.580	-5.252	0.992
II.1	2.878	-3.976	0.999	3.246	-5.953	0.946	3.624	-5.257	0.989	2.652	-3.385	0.994	2.930	-3.878	0.997	2.929	-4.116	0.998
II.2	3.218	-4.274	0.999	4.793	-8.495	0.969	3.840	-5.423	0.995	3.257	-4.14	0.992	3.185	-4.038	0.996	2.323	-3.226	0.995
II.3	3.750	-4.914	0.998	5.320	-9.222	0.976	4.363	-5.993	0.994	3.408	-4.311	0.996	3.672	-4.538	0.994	3.215	-4.277	0.991
III.1	2.626	-3.501	0.998	5.072	-7.764	0.993	3.454	-5.078	0.991	3.031	-3.948	0.998	3.391	-4.485	0.997	2.650	-3.768	0.997
III.2	3.364	-4.187	0.999	5.497	-8.370	0.987	4.368	-6.003	0.997	3.601	-4.682	0.995	3.888	-4.956	0.998	3.798	-4.637	0.995
III.3	3.154	-4.022	0.998	5.718	-8.650	0.983	4.219	-5.942	0.998	3.495	-4.549	0.997	3.978	-4.924	0.998	3.677	-4.973	0.991
III.4	3.946	-4.889	0.999	5.880	-8.393	0.987	5.268	-7.2	0.997	4.142	-5.425	0.990	4.454	-5.280	0.993	4.436	-5.725	0.995
IV.1	1.867	-2.601	0.999	2.334	-4.304	0.996	2.342	-3.763	0.994	2.367	-3.424	0.995	2.250	-3.424	0.996	1.635	-2.694	0.996
IV.2	2.013	-2.740	0.998	2.465	-4.415	0.996	2.392	-3.856	0.998	2.653	4.821	0.998	2.625	-3.832	0.995	1.809	-2.851	0.996
IV.3	1.364	-2.102	0.999	2.257	-4.163	0.996	2.751	4.219	0.994	3.500	5.593	0.998	2.258	-3.42	0.997	2.091	-3.155	0.995

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Correlation Between Retention Constants, R_M^0, and Slope, S

A linear relationship was observed between the intercept, R_M^0, and slope, S, for protic and aprotic solvents, as shown by the equations given in Table 3. The best correlation was obtained for aceton as mobile-phase modifier (r = 0.994). There is a good correlation between R_M^0 and S, which might reflect the suitability of the systems examined for estimating the lipophilicity of the compounds. The R_M^0 values, which are chromatographic data describing the partitioning between a non-polar stationary and a polar mobile phase, may therefore be appropriate for the assessment of lipophlicity.

Table 3. Equations for the relationships between the retention constants, R_M^0, and slope, S.

Mobile phase	Equation	*r*	*sd*	*n*
Acetone-water	$R_M^0 = -0.572 - 1.121S$	0.994	0.101	14
Acetonitrile-water	$R_M^0 = -1.717 - 1.356S$	0.954	0.590	14
Dioxane-water	$R_M^0 = -1.895 - 0.965S$	0.920	0.392	14
Tetrahydrofuran-water	$R_M^0 = -0.231 - 1.231S$	0.985	0.140	14
Methanol-water	$R_M^0 = -1.278 - 1.911S$	0.987	0.110	14
Ethanol-water	$R_M^0 = -0.786 - 1.152S$	0.962	0.283	14

Based on the results obtained on silica gel impregnated paraffin oil, R_M^0 is directly dependent on the nature of mobile phase modifiers. In other words, the selectivity of separation of the tested substances are the result of specific interactions with the mobile phase.

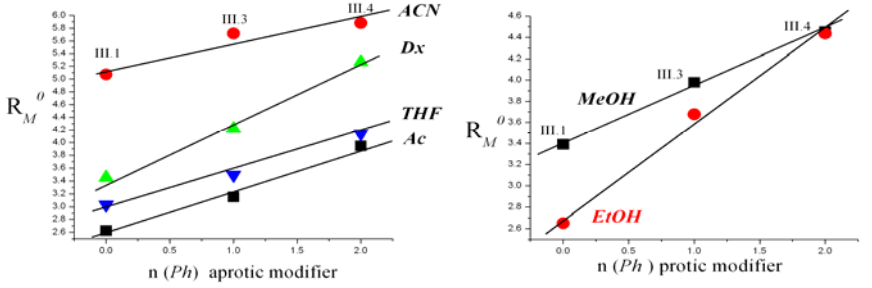

Figure 1. Relationship between the extrapolated retention constants, R_M^0, and the number of phenyl groups compounds of *series III* derivatives s-triazine molecules

As can be seen from Figure 1, of structural parameters, the most pronounced effect on R_M^0 values has phenyl group. Namely, a linear relationship was observed between the R_M^0 values and the number of phenyl groups, n(*Ph*), in the substituents at position 4 and 6 in the compounds of *series III* derivatives of s-triazine. A decrease in the polarity of the molecule (increase in the number of phenyl groups) resulted in the increased retention (Figure 1).

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Correlation of Retention Constants, R_M^0 and logP

Lipophilic character often seems to be the most important physico-chemical parameter in determining the biological activity of chemical agents. Lipophilicity can be expressed in terms of many different descriptors (log*P*, logk_w, R_M, R_M^0), obtained experimentally or calculated. The experimental parameters most frequently used are the retention constants R_M^0 (RPTLC) and logk_w (RPHPLC), whereas the calculated quantity is log*P*. The partiton coefficient, log*P*, of a given compound between a non-aqueous and an aqueous phase can be used as an expression of its lipophilic character (15).

Because the retention of a compound in reversed-phase chromatography is governed by hydrophobic interactions, linear relationships between the retention constant, R_M^0, and log*P* could be expected (16).

The partition coefficients (*A*log*P*, *IA*log*P*, *C*log*P*, logP_{Kowin}, *X*log*P*, *ACD*log*P*) of s-triazine derivatives are listed in Table 4.

Table 4. Partition coefficients calculated by different theoretical methods

Comp.	*A*log*P*	*IA*log*P*	*C*logP	logPK_{owin}	*X*logP	*ACD*log*P*
I.1	5.25	5.06	4.85	5.07	4.83	3.87
I.2	5.65	5.13	5.85	6.16	5.70	4.79
I.3	5.94	7.08	6.28	6.36	6.07	5.06
I.4	6.18	5.89	6.58	6.85	6.43	5.42
II.1	4.96	5.15	5.32	5.88	3.71	3.70
II.2	5.78	5.96	6.44	6.86	4.85	4.82
II.3	6.55	6.65	7.55	7.85	5.99	5.95
III.1	4.91	4.76	5.40	5.96	4.01	3.74
III.2	5.55	4.81	5.48	6.86	5.14	4.82
III.3	6.07	5.80	7.21	8.17	6.14	5.36
III.4	6.98	7.98	9.02	10.39	8.27	7.07
IV.1	3.83	3.63	3.12	3.81	2.37	2.85
IV.2	4.21	4.08	3.67	4.30	2.94	3.41
IV.3	4.64	4.48	4.23	4.79	3.51	3.98

Table 5. Correlation coefficients (r) for the correlation between R_M^0 and different log*P* values

R_M^0	*A*log*P*	*IA*log*P*	*C*log*P*	logP_{Kowin}	*X*log*P*	*ACD*log*P*
Acetonitrile	0.835	0.705	0.858	0.877	0.795	0.804
Acetone	0.763	0.708	0.828	0.875	0.671	0.757
Dioxane	0.747	0.624	0.815	0.900	0.681	0.770
Tetrahydrofuran	0.570	0.533	0.648	0.756	0.532	0.707
Methanol	0.702	0.604	0.794	0.895	0.665	0.750
Ethanol	0.855	0.795	0.822	0.838	0.900	0.825

By comparing the calculated values to define the lipophilicity of the investigated molecules, it is evident that ethanol as a modifier gives the highest correlation (calculated average correlation coefficient is 0.839).

Retention Constants, R_M^0 for QSRR

The ***QSRRs*** are statistical models which quantify the relationship between the structure of a molecule and its chromatographic retention parameters in different kinds of chromatography. The application of QSRR allows the prediction of the retention of a new solute, identification of the most informative structural descriptors, elucidation of the molecular mechanisms of separation in a given chromatographic system, evaluation of complex physico-chemical properties of solutes and estimation of biological activities. The relationship between the retention and the structural characteristics of a molecule explains the effect of chemical structure on the retention behavior in a more accurate way (17).

The use of multiple linear regression (MLR) analysis for fourteen s-triazine derivatives led to statistically significant equations relating lipophilicity (estimated by R_M^0 values (dependent variable) to different theoretically calculated six types of log P namely *A*log*P*, *C*log*P*, *ACD*log*P*, logP_{Kowin}, *X* log*P* and *IA*log*P* values for each compound (independent variable). The specifications for the best-selected MLR models are shown in Table 6 and Table 7.

These relationships were analyzed and the best model was selected on the basis of various statistical parameters like correlation coefficient (*r*), and standard deviation (*SD*).

In the first phase of work, the multilinear relationships between the retention constant and two variable lipophilicity descriptors was examined.

Table 6. Statistical parameters for multilinear dependence between R_M^0 and two variables descriptors lipophilicity

Modifier	Descriptors		$R_M^0 = a\ logP_1 + b logP_2 + c$				
R_M^0	logP_1	logP_2	*a*	*b*	*c*	*r*	*SD*
Acetone	logP_{Kow}	*X*log*P*	0.0993	0.648	-0.313	0.916	0.329
Dioxane	*A*og*P*	logP_{Kow}	0.312	0.813	-0.410	**0.949**	0.306
Methanol	logP_{Kow}	*X*log*P*	0.571	0.672	-0.357	**0.953**	0.234

From the data in Table 6, it is evident that the retention constant correlates best with *X*log*P* combined with logP_{kowin} (r = 0.953) - modifier methanol and logP_{kowin} with *A*log*P* (r = 0.949) - modifier dioxane.

The multilinear dependence of the retention constant, R_M^0, and the three lipophilicity descriptors is shown in Table 7. The best correlation was observed for the combined logP_{Kow}, *X*log*P* and *IA*log*P* (r = 0.964)

Table 7. Statistical parameters for multilinear dependence between R_M^0 and three variables descriptors lipophilicity

Modifier	Descriptors			$R_M^0 = a\,logP_1 + b\,logP_2 + c\,logP_3 + d$					
R_M^0	logP_1	logP_2	logP_3	*a*	*b*	*c*	*d*	*r*	*SD*
Acetone	*A*log*P*	logP_{Kow}	*X*log*P*	-1.969	0.811	0.524	-0.632	0.948	0.274
Dioxane	logP_{Kow}	*X*log*P*	*IA*log*P*	0.731	0.853	-0.292	-0.231	**0.957**	0.294
Acetonitrile	*A*og*P*	logP_{Kow}	*ACD*log*P*	-2.713	1.401	0.756	-1.203	0.901	0.659
Tetrahydrofuran	logP_{Kow}	*X*log*P*	*ACD*log*P*	0.664	0.271	-0.609	0.791	0.904	0.280
Methanol	logP_{Kow}	*X*log*P*	*IA*log*P*	0.948	0.708	-0.251	-0.208	**0.964**	0.216
Ethanol	logP_{Kow}	*X*log*P*	*C*log*P*	0.625	0.408	0.537	-0.503	0.907	0.398

The analysis of these results indicates that the proposed models can correctly represent the relationship between the retention parameters of the investigated compounds on silica gel and different log *P* values calculated for various compound solely from the molecular structure. These models are suitable for prediction of the retention of structurally similar compounds under the same chromatographic conditions.

CONCLUSION

Experimentally obtained RP R_M^0 values depend on the nature of organic modifier in the mobile phase. A linear relationship between R_M^0 and slope, *S*, values was found for all mobile phases. Satisfactory linear correlation was obtained between the retention constants and *A*log*P*, *C*log*P*, *ACD*log*P*, logP_{Kowin}, *X* log*P* and *IA*log*P*. According to the correlation coefficients, R_M^0 is a useful property for evaluation of the relative lipophilicity of the examined compounds.

The correlations between the retention constants, R_M^0, and selected lipofilicity parameter (different log*P* values) of the solutes were expressed by multiparametric equations of high statistical significance, indicate that these models can be used to predict the retention constants of these molecules.

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ХРОМАТОГРАФСКО ПОНАШАЊЕ И ЛИПОФИЛНОСТ *s*-ТРИАЗИНСКИХ ДЕРИВАТА НА ТАНКОМ СЛОЈУ СИЛИКА ГЕЛА ИМПРЕГНИРАНОГ ПАРАФИНСКИМ УЉЕМ

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Испитано је хроматографско понашање четири групе новосинтетисаних деривата *s*-триазина на танком слоју силика гела имрегнираног парафинским уљем. Ретенциони механизам је одређен употребом мобилних фаза: ацетон-вода, ацетонитрил-вода, диоксан-вода, тетрахидрофуран-вода, метанол-вода и етанол-вода, варирањем запреминског удела модификатора у покретној фази. На танком слоју сили-

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ка гела импрегнираног парафинским уљем долази до обрнуто-фазног ретенционог механизма. Добре корелације су постигнуте између ретенционе константе, R_M^0, (ретенција растворка у чистој води), и нагиба, S, хроматографске једначине. Такође су постигнуте задовољавајуће корелације између ретенционе константе и вредности log$P$, израчунатих коришћењем различитих рачунарских програма. То указује да R_M^0 може бити алтернативни дескриптор у дефинисању липофилности испитиваних деривата с-триазина.

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