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Original Article

Comparing the Correctness of Different Relations for Approximation of Retention Times in Reversed Phase HPLC with Methanol–Water Eluents

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ABSTRACT

The correctness of different relations for approximating the retention times of selected analytes of different chemical origin in reversed phase high performance liquid chromatography (isocratic conditions, methanol–water eluents) is compared. Five equations most often used in analytical practice were considered: hyperbolic (Scott-Kuchera model), logarithmic (Soczewinski–Wachtmeister and Snyder–Soczewinski models), second degree polynomial, and recently proposed recurrent relations, $t_R(C + \Delta C) = at_R(C) + b$, where t_R is net retention time, and ΔC is the constant increment of the concentration of an organic modifier in an eluent. Two criteria for comparing the approximation quality were used. The first of them (known previously) is the maximal value of the correlation coefficient for the dependence $t_R(C)$; the second one is newly proposed. It implies hypothetical exclusion of the maximal and the minimal t_R values from the total data set, followed by precalculation of these values using the remaining data and evaluation of the differences ($t_R - t_{R,calc}$) for both of them.
The results obtained show that just recurrent relations provide the maximal precision of approximations compared to all the previously known approaches. In addition, the important advantage of recurrences is their applicability to net retention times without converting them to adjusted retention times.

1. Introduction

In different chromatographic and related separation methods, the signal of every analyte should be characterized by at least two principal parameters: retention time (t_R) or any proportional variable (retention factor, migration time, scan number, etc.) and peak area (S). If the analysis conditions are fixed, the peak heights (H) can be used instead of areas. The auxiliary parameters include the asymmetry factor (A_s) and several rarely used quantities.
For all separation methods, it is important to understand how the experimental conditions influence the retention parameters. In gas chromatography, the equation relating logarithms of so-called adjusted retention time values (t'_R) to the reciprocal separation temperature ($1/T$) is one of the most general relationships [1, 2]:

$$\log t'_R = a/T + b, \qquad (1)$$

where $t'_R = t_R - t_0$, t_0 is the retention time of a nonsorbable analyte (experimentally evaluated or theoretically estimated), a and b are the coefficients calculated by the least-squares method (LSM), and T is the absolute temperature, K.

Equation (1) is an example of so-called two-parameter Antoine equation. If the precision of $t_R(T)$ approximation by this equation should be improved, it can be replaced by three-parameter Antoine equation:

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$$\log t'_R = a/(T + c) + b. \quad (2)$$

These equations permit us, for example, to convert analyte retention times measured at a certain temperature to the values at other temperatures.

The same problem exists in reversed phase high performance liquid chromatography (RP HPLC), where the equivalent of the $t_R(T)$ function is the dependence of the retention time on the organic solvent content of an eluent [2–8], $t_R(C)$. However, in this case there is no such universal equation for the dependence $t_R(C)$ as in gas chromatography. More than a dozen of different relations have been proposed for this approximation [2–8].

In this work, we discuss five most often used relations for the dependence of the retention parameters on the organic modifier content of an eluent, $t_R(C)$. To evaluate their accuracy, we have examined the data for five selected analytes of various chemical origins.

2. Materials and Methods

2.1. Selected analytes. Commercial samples of nitrobenzene, toluene ("reagent grade for chromatography", Reakhim, Moscow), and 3-nitrophenol (indicator, British Drug Houses, LTD, UK) were used in our work. *p*-Toluenesulfonamides were synthesized by PhD T. Kornilova (St. Petersburg State University) from *p*-toluenesulfonyl chloride (99%, Acros Organics, Belgium), which is the most readily available reagent among sulfonyl chlorides, and the following amines: allylamine (I, analytical grade, Merck, Germany) and *tert*-butylamine (II, 99%, Acros Organics, Belgium).

CH_3-C_6H_4-SO_2Cl + 2HNRR' → CH_3-C_6H_4-SO_2-NRR' + RR'NH·HCl,
where R = H, R' = -CH_2-CH=CH_2 (I), *tert*-C_4H_9 (II).

A 2.5-fold excess of each amine was added to a 0.06 M solution of *p*-toluenesulfonyl chloride in methylene chloride, and the mixture was allowed to stand for 10 min. Then, the reaction mixtures were analyzed directly, because excess amounts of amines and their salts do not hinder UV detection of reaction products, which (except aniline) do not absorb in the near-UV region. The presence of certain amounts of *p*-toluenesulfonic acid (in the form of the anion) follows from the appearance of peaks in the region of the retention time of the nonsorbable component [9, 10].

The molecular masses and CAS numbers of all the analytes selected are summarized in Table 1.

2.2. Conditions of reversed phase high performance liquid chromatography. The retention parameters of selected analytes under various isocratic elution conditions in RP-HPLC were determined using a Shimadzu LC-20 Prominence liquid chromatograph equipped with a diode-array detector and Phenomenex C18columns 250 mm long and 4.6 mm i.d. The sorbent particle size was5 μm. Water–methanol mobile phases were used in several isocratic modes with 5% concentration "steps" of the organic component. The flow rate was 1mLmin^{-1}, and the column temperature was 30°C. The samples were injected using a SIL-20A/AC autosampler; the sample volume was 20 μL.

To prepare eluents, we used deionized water (resistivity 18.2 MΩcm) prepared using a Milli-Q device (Millipore, USA) and methanol (analytical grade, Kriokhrom, St. Petersburg).

All the samples for analyses were prepared by dissolving individual compounds or reaction mixtures in the corresponding mobile phase. The number of replicate injections of each sample in each regime was 2–3. The inter-injection variations of the retention times of the target analytes in all the cases did not exceed 0.01–0.02 min.

The retention times of the theoretically nonsorbable component were precalculated using the well-known Peterson–Hirsch relation (3) [11] based on the retention times of three reference *n*-alkyl phenyl ketones $C_6H_5COC_nH_{2n+1}$ (n = 1 ÷ 3) added to all samples:

$$t_0 = (t_{R,1}t_{R,3} - t^2_{R,2}) / (t_{R,1} + t_{R,3} - 2t_{R,2}) \quad (3)$$

2.3. Data processing. The adjusted retention times of selected compounds, measured at different methanol concentrations, and their reciprocal values and logarithms were processed using Excel software (Microsoft Office, 2010). Origin software (versions 4.1 and 8.1) was used for calculating the regression parameter sand plotting the data.

3. Results and Discussion

As mentioned in the Introduction, in reversed-phase high-performance liquid chromatography (RP HPLC) there is no single general equation for the dependence of the retention parameters on the concentration of an organic component in an eluent, $t_R(C)$. Several approximation functions were proposed in the literature [2–8]. These approximations are used for compounds of different chemical origin under different elution conditions.

We have selected five relations for approximating the dependences $t_R(C)$ most often used in analytical practice. To compare them, we have selected five analytes listed in Table 1. To avoid the risk of nonlinearity of the dependences $t_R(C)$, caused by formation of hydrates of polar analytes, which is possible in the case of acetonitrile–water eluents [10, 12, 13], we have restricted our experimental conditions to methanol–water eluents.

Table 1. Molecular weights and CAS numbers of selected analytes

Compound	Molecular weight (Da)	CAS n^o
Toluene	92	10-88-3
Nitrobenzene	123	98-95-3
3-Nitrophenol	139	554-84-7
N-allyl-*p*-toluene-sulfonamide	211	50487-71-3
N-*tert*-butyl-*p*-toluene-sulfonamide	227	2849-81-2

In all equations considered below, the variable C means the volume fraction of the organic modifier in an eluent; coefficients a, b (and c, if necessary) are calculated by LSM. It is important that most of the models considered below imply using not the net retention parameters (t_R) but adjusted retention times (t'_R).

Let us start our discussion with the simplest model: hyperbolic correlation (4) based on the Scott–Kuchera approach and proposed by Row [14]:

$$1/t'_R = aC + b \qquad (4)$$

The second and the most important group of retention models is based on Soczewinski–Wachtmeister equation (5), which assumes linear dependence of the logarithms of the adjusted retention times on the volume fraction of the modifier [15, 16]:

$$\log t'_R = aC + b \qquad (5)$$

In the literature, this model is frequently referred to as the linear solvent strength (LSS) model [17].

The next approach is the log–log dependence, which assumes the linear relationship between $\log t'_R$ and the logarithm of the volume fraction of the modifier. This model is often named as the Snyder–Soczewinski equation (6) because it was developed by Soczewinski from earlier findings by Snyder [15, 18]:

$$\log t'_R = a\log C + b \qquad (6)$$

The reasonable extension of the last two models is the second-degree polynomial form (7) proposed by Schoenmakers [19]:

$$\log t'_R = aC^2 + bC + c \qquad (7)$$

In addition, the $t_R(C)$ dependences in RP HPLC can be approximated by so-called recurrent relations recently proposed by Zenkevich [20–24]:

$$t_R(C + \Delta C) = at_R(C) + b, \qquad (8)$$

where ΔC = const is a constant increment of the organic component concentration in an eluent (in our work, we chose ΔC = 5%).

The mathematical properties of recurrent relations (8) were considered in [20–24]. The important advantage of recurrences is their applicability directly to net retention times, without their conversion to the adjusted parameters.

Table 2 includes the net retention times of the selected analytes and the retention times of the nonsorbable component (dead time), precalculated at different methanol concentrations in an eluent ($50 \le C \le 75$ %, *v/v*).

Table 2. Average values of net retention time (min) of the selected analytes and the retention time of the nonsorbable component (dead time), measured at different methanol concentrations in the eluent

C	t_R			t_0
	Toluene	Nitro benzene	3-Nitro phenol	
75	7.262	4.121	3.604	1.548
70	9.178	4.622	3.932	1.604
65	12.223	5.329	4.440	1.620
60	16.278	6.267	5.076	1.606
55	22.618	7.626	6.050	1.543
50	30.621	9.525	7.429	1.515
C	t_R			t_0
	N-Allyl-*p*-toluene sulfonamide		N-*tert*-Butyl-*p*-toluene sulfonamide	
75	3.611		4.297	1.551
70	4.035		5.131	1.603
65	4.712		6.543	1.622
60	5.702		8.735	1.604
55	7.387		12.679	1.518
50	10.154		19.561	1.458

Table 3 contains the results of processing the retention data for various analytes using different approximation equations (4) – (8), namely, coefficients of linear

regression (*a*, *b*, and *c*, if necessary), correlation coefficients (*R*), and the estimated accuracy of the minimal and maximal t_R values ($\Delta t_{R,\,min}$ and $\Delta t_{R,\,max}$).

Table 3. Parameters of different approximations of dependence $t_R(C)$ (regression and correlation coefficients, *R*) and the differences between the precalculated and experimental minimal and maximal retention times for each analyte, $\Delta t_R = t_{R,\,cal} - t_{R,\,exp}$, min

Approximation equation	Coefficients	*R*	$\Delta t_{R,min}$	$\Delta t_{R,max}$
Toluene				
$1/t'_R = aC + b$	a = 0.006 b = -0.259	0.98	0.54	-129.1*
$\log t'_R = aC + b$	a = -0.027 b = 2.893	-0.9994	0.04	1.02
$\log t'_R = a\log C + b$	a = -4.066 b = 8.388	-0.9991	0.16	2.4
$\log t'_R = aC^2 + bC + c$	a = 9.571 ×10^{-5} b = -0.041 c = 3.260	0.9995	0.08	1.6
$t'_R(C + \Delta C) = at'_R(C) + b$	a = 0.711 b = 0.129	0.999	-0.39	1.5
$t_R(C + \Delta C) = at_R(C) + b$	a = 0.713 b = 0.545	0.9991	-0.33	1.3
Nitrobenzene				
$1/t'_R = aC + b$	a = 0.011 b = -0.421	0.997	0.29	3.4
$\log t'_R = aC + b$	a = -0.020 b = 1.879	-0.995	-0.17	-0.91
$\log t'_R = a\log C + b$	a = -2.836 b = 5.716	-0.9993	-0.11	-0.20
$\log t'_R = aC^2 + bC + c$	a = 2.5×10^{-4} b = -0.051 c = 2.838	0.9998	0.08	-0.26
$t'_R(C + \Delta C) = at'_R(C) + b$	a = 0.703 b = 0.426	0.9997	0.05	0.15
$t_R(C + \Delta C) = at_R(C) + b$	a = 0.714 b = 0.826	0.9999	0.01	0.02
3-Nitrophenol				
$1/t'_R = aC + b$	a = 0.113 b = -0.488	0.998	0.02	1.5
$\log t'_R = aC + b$	a = -0.019 b = 1.675	-0.992	-0.18	-0.59
$\log t'_R = a\log C + b$	a = -2.649 b = 5.262	-0.997	-0.16	-0.14
$\log t'_R = aC^2 + bC + c$	a = 3.171×10^{-4} b = -0.058 c= 2.891	0.9996	-0.22	0.37
$t'_R(C + \Delta C) = at'_R(C) + b$	a = 0.686 b = 0.426	0.9993	-0.06	0.16
$t_R(C + \Delta C) = at_R(C) + b$	a = 0.701 b = 0.848	0.9997	-0.00	-0.02
N-Allyl-*p*-toluenesulfonamide				
$1/t'_R = aC + b$	a = 0.015 b = -0.656	0.998	0.01	2.3
$\log t'_R = aC + b$	a = -0.025 b = 2.157	-0.98	-0.16	-1.7
$\log t'_R = a\log C + b$	a = -3.596 b = 7.028	-0.996	-0.25	-0.91
$\log t'_R = aC^2 + bC + c$	a = 4.743×10^{-4} b = -0.085 c = 3.987	0.9999	-0.16	-0.35
$t'_R(C + \Delta C) = at'_R(C) + b$	a = 0.574 b = 0.607	0.9998	0.00	0.64
$t_R(C + \Delta C) = at_R(C) + b$	a = 0.616 b = 1.152	0.9998	0.04	-0.11
N-*tert*-Butyl-*p*-toluenesulfonamide				
$1/t'_R = aC + b$	a = 0.013 b = -0.593	0.98	0.66	40.7*
$\log t'_R = aC + b$	a = -0.033 b = 2.862	-0.993	-0.70	-4.1
$\log t'_R = a\log C + b$	a = -4.694 b = 9.217	-0.998	-0.28	-1.8
$\log t'_R = aC^2 + bC + c$	a = 5.064×10^{-4} b = -0.096 c = 4.803	0.9999	0.16	1.8
$t'_R(C + \Delta C) = at'_R(C) + b$	a = 0.576 b = 0.733	0.9999	-0.01	-0.04
$t_R(C + \Delta C) = at_R(C) + b$	a = 0.579 b = 1.377	0.9998	0.09	-0.28

*) Anomalous outlier which was not used in averaging the results.

The quantities Δt_R presented in Table 3 were calculated from the results obtained using all the relations (4)–(8). This approach to the estimation of the approximation accuracy has been proposed for the first time. It implies hypothetical exclusion of the maximal and the minimal t_R values from each total data set, followed by precalculation of these values using the remaining retention data and calculation of the differences ($t_{R,cal} - t_{R,\,exp}$) for both of them. In other words, for evaluating the $\Delta t_{R,\,min}$ values we deleted the t_R-point corresponding to the highest methanol concentration in the eluent, after which we estimated the coefficients *a*, *b* (and *c*, if necessary) and then calculated $t_{R,\,cal}$ or $t'_{R,cal}$.

On the contrary, to evaluate $\Delta t_{R,\,max}$, we deleted the point corresponding to the low concentration of methanol in the eluent, after which we estimated the coefficients *a*, *b* (and *c*, if necessary) and then calculated $t_{R,\,cal}$ or $t'_{R,cal}$.

Figures 1–6 present the plots of all the relations approximating the dependences of the retention times on the methanol concentration in the eluent for N-allyl-*p*-toluenesulfonamide selected as an example. For all figures red lines correspond to the linear regressions.

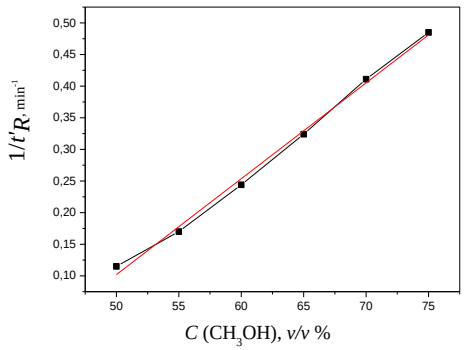

Fig. 1. Hyperbolic correlation of the adjusted retention times of N-allyl-*p*-toluenesulfonamide with the methanol concentration in the eluent. Linear regression parameters: a = 0.015 ± 0.000, b = –0.66 ± 0.03, R = 0.998, and S_0 = 0.01.

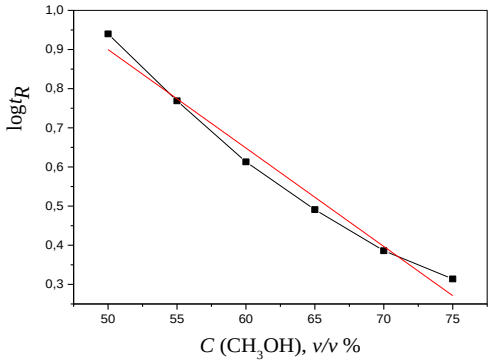

Fig. 2. Logarithm of the adjusted retention times of N-allyl-*p*-toluenesulfonamide as a function of the methanol concentration in the eluent. Linear regression parameters: a = –0.025 ± 0.002, b = 2.16 ± 0.12, R = –0.98, and S_0 = 0.04.

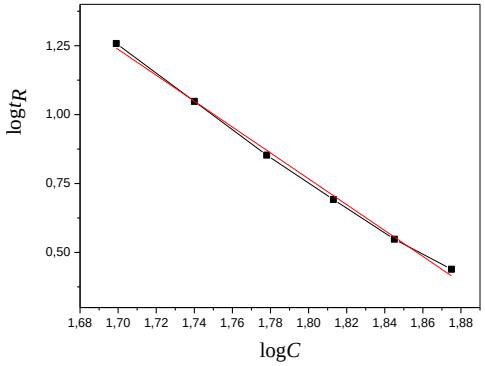

Fig. 3. The adjusted retention times of N-allyl-*p*-toluenesulfonamide as a function of the logarithm of the methanol concentration in the eluent. Linear regression parameters: a = –3.60 ± 0.16, b = 7.03 ± 0.28, R = –0.996, and S_0 = 0.02.

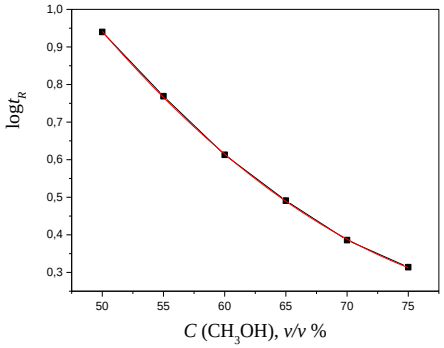

Fig. 4. Polynomial approximation of the logarithms of the adjusted retention times of N-allyl-*p*-toluenesulfonamide as a function of the methanol concentration in the eluent. Linear regression parameters: a = 4.74×10^{-4} ± 0.000, b = –0.085 ± 0.003, c = 3.99 ± 0.08, R = 0.9999, and S_0 = 0.003.

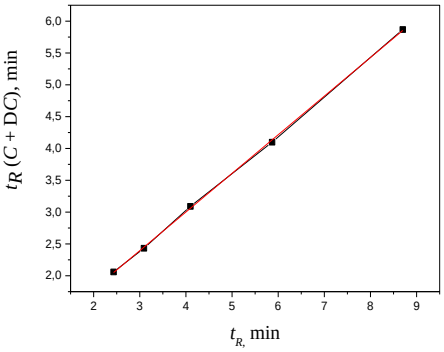

Fig. 5. Linearity of the recurrent dependence of the adjusted retention times of N-allyl-*p*-toluenesulfonamide on the methanol concentration in the eluent. Linear regression parameters: a = 0.574 ± 0.006, b = 0.61 ± 0.03, R = 0.9998, and S_0 = 0.03.

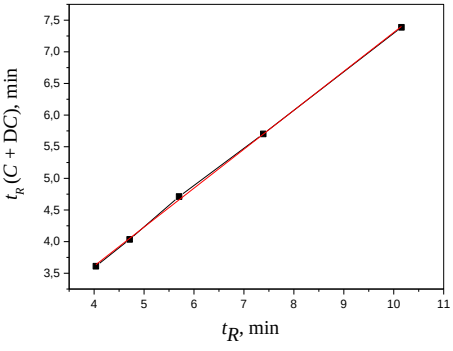

Fig. 6. Linearity of the recurrent dependence of the retention times of N-allyl-*p*-toluenesulfonamide on the methanol concentration in the eluent. Linear regression parameters: $a = 0.616 \pm 0.007$, $b = 1.15 \pm 0.05$, $R = 0.9998$, and $S_0 = 0.04$.

Comparison of the results allows the following conclusions:

The values of the correlation coefficients in Table 3 (0.99–0.9999) do not allow reliable conclusions on the preference of any approximation model. All *R*-values seem to be acceptable.

Relatively low absolute values of the correlation coefficients (Table 3) were obtained only with approximation function (1) for toluene and N-*tert*-butyl-*p*-toluenesulfonamide ($R = 0.98$) and with function (5) for N-allyl-*p*-toluenesulfonamide ($R = –0.98$).

Because comparison of the *R*-values appeared to be noninformative, we have decided to complete our characterization with comparing the values of Δt_R for all the approximation relations and all the analytes chosen. The "raw" results are presented in Table 3. It also seems reasonable to average all the $\Delta t_{R,min}$ and $\Delta t_{R,\ max}$ values estimated for different analytes. Such averages $\Sigma\Delta t_R/N$ ($N = 5$) characterize specifically the approximation abilities of different equations and are compared in Table 4.

Table 4. Averaged accuracy of the minimal and maximal t_R values ($\Delta t_{R,min}$ and $\Delta t_{R,max}$, min) for different approximation models

Approximation equation	Average value $\Delta t_{R,\ min}$	Average value $\Delta t_{R,\ max}$
$1/t'_R = aC + b$	0.30	2.4*
$\log t'_R = aC + b$	0.25	1.7
$\log t'_R = a\log C + b$	0.19	1.1
$\log t'_R = aC^2 + bC + c$	0.14	0.88
$t'_R(C + \Delta C) = at'_R(C) + b$	0.10	0.50
$t_R(C + \Delta C) = at_R(C) + b$	0.09	0.35

*) Anomalous outlier which was not used in averaging the results.

Table 4 presents the averaged accuracy $\Sigma\Delta t_R/N$ for the minimal and maximal t_R values for all the approximation functions selected in our work.

The largest $\Sigma\Delta t_R/N$ values demonstrate the minimal precision of the hyperbolic equation (Row model), because $\Delta t_{R,min} = 0.30$ min and $\Delta t_{R,\ max} = 2.4$ min. The Soczewinski–Wachtmeister and Snyder–Soczewinski models are characterized by medium precision, as well as the polynomial approach, and recurrent relations ensure the highest precision. It is important that two kinds of recurrences should be compared. The first of them implies using the adjusted retention times (t'_R) by analogy with other approximation relations. However, this is not necessary, because the unique properties of recurrences allow approximation of net retention times (t_R). The results are shown in the list line of Table 4: $\Delta t_{R,min} = 0.09$ min (5s), and $\Delta t_{R,\ max} = 0.35$ min (21 s). Such values are comparable with the widths of chromatographic peaks for standard RP HPLC columns.

The fact of better precision of $\Delta t_{R,\ min}$ and $\Delta t_{R,\ max}$ estimates appeared to be rather interesting. It can be attributed to the features of the dead time (t_0) calculation with Eq. (3). The retention times of three reference *n*-alkyl phenyl ketones contain some additional uncertainties influencing t_0 evaluation. If we use net retention times, such influence is excluded.

4. Conclusion

Comparison of the results of approximating the dependence of the retention times of five selected analytes of different chemical origin in reversed phase HPLC with methanol–water eluents on the methanol concentration (the range is 50–75 vol %) allows the following conclusions:

1. All the approximation models considered provide the correlation coefficients of the dependence $t_R(C)$ no less than 0.99; for some of them, the *R*-values are as high as 0.9999.

2. To simplify the search for the preferable approximation models, we have applied the newly proposed criterion: comparison of the minimal and maximal experimental t_R values in data sets with the values precalculated after their hypothetical exclusion from these sets (Δt_R).The next step is calculating the average values, $\Sigma\Delta t_R/N$, which characterize not the individual analytes but the overall accuracy of different approximation equations.

3. The recurrent approximation of retention times, namely $t_R(C + \Delta C) = at_R(C) + b$, ΔC = const, provides the highest precision of the approximated t_R-values compared to other models. It is applicable to both adjusted ($t_R' = t_R - t_0$) and net retention times. The accuracy of such approximations appeared to be better in the case of net retention times, which seems to be a unique feature of recurrent functions. This anomaly is attributable to the use of retention times of three consecutive *n*-alkyl phenyl ketones for evaluating t_0-values, because these data contain additional uncertainties.

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Conflict of interest

The authors declare that they have no conflict of interest.

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