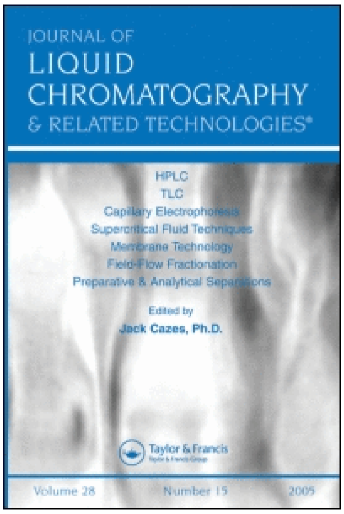

Journal of Liquid Chromatography & Related Technologies
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713597273

AUTOMATIC SELECTION OF MOBILE PHASES. TLC ON SILICA OF 2-BENZYL-3- (1-METHYLPYRROL-2-YL)-4-SUBSTITUTEDTETRAHYDROISOQUINOLINES AND CORRESPONDING 1-ONES

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To cite this Article Palamareva, M. D. , Koleva, R. I. and Kozekov, I. D.(2001) 'AUTOMATIC SELECTION OF MOBILE PHASES. TLC ON SILICA OF 2-BENZYL-3- (1-METHYLPYRROL-2-YL)-4-SUBSTITUTEDTETRAHYDROISOQUINOLINES AND CORRESPONDING 1-ONES', Journal of Liquid Chromatography & Related Technologies, 24: 10, 1411 — 1424

To link to this Article: DOI: 10.1081/JLC-100103919

URL: http://dx.doi.org/10.1081/JLC-100103919

J. LIQ. CHROM. & REL. TECHNOL., 24(10), 1411–1424 (2001)

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ABSTRACT

The automatic selection of mobile phases for thin-layer chromatography (TLC) on silica of the two groups of compounds mentioned in the title of this paper was done by the LSChrom software, which is based on the Snyder theory and chromatographic properties of the compositional functional groups of each compound. Thus, the recommended mobile phase strength ε was 0.344 for the tetrahydroisoquinolines and 0.331 for the tetrahydroisoquinolinones, and narrow ranges around these values. The software enabled selection of 14 mobile phases having such values of ε. The experimental R_F values found on two silicas with all mobile phases recommended by the software were in the range 0.01-0.88, showing the correctness of the automatic predictions for the polyfunctional compounds studied.

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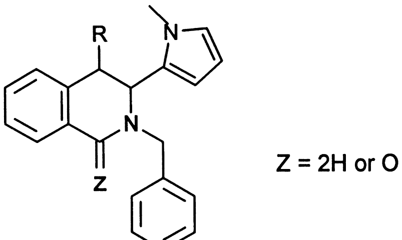
INTRODUCTION

In the last ten years,[1-9] we have tried to make use of the Snyder theory,[10-12] incorporating it into a computer program[13] called LSChrom. Concerning normal-phase liquid chromatography, the first version of the software enabled the characterisation of two to multi-component mobile phases by strength**,** ε, localization, m, and polarity, P'. This version of LSChrom has permitted us[1-9] to select mobile phases for a given set of compounds by the following procedure: a) chromatography of the compounds studied with an arbitrarily selected mobile phase having some value of ε; b) adjustment of retention by the criterion: reduce ε if retention is rather small, and vice versa, and c) adjustment of separation by using mobile phases with the settled value of and different values of m and P'. This procedure for selection of mobile phases is easier than the trial and error approach.

Recently, the LSChrom software has been developed[14] by incorporating into it of that part of the Snyder theory that permits prediction of retention on the basis of the adsorption properties of the individual functional groups participating in the sample structure. The corresponding modes give possibility for a direct selection of mobile phases without preliminary experiments, as already shown[15] for HPLC of compounds having relatively simpler structures. A further wide use of LSChrom in this respect is important.

The present paper reports the application of LSChrom[14] for a fully automatic selection of mobile phases for TLC on silica of polyfuncional compounds **1-23** which we have synthesised[16] by the important reaction between homophthalic anhydride and imines,[17,18] and following transformations[19] of the parent compound **1**.



1-23

THEORY

According to the Snyder theory,[10-12] mobile phases are characterised by strength, ε, proportional to the dimensionless Gibbs energy $\Delta G^\circ / RT \ln 10$ of adsorption of the mobile phase per unit of its area under adsorpton, localization,

m, measuring the specific interactions adsorbent-composing solvents and polarity, P', measuring the interactions sample-composing solvents. The greater the ε value, the weaker is the sample retention; m and P' tune (see ref. 6 for instance) sample retention and mobile phase selectivity.

The Snyder theory describes the adsorption properties of individual functional groups i by their adsorption energy, Q_i^0, relative to pentane (ε=0) and area under adsorption, a_i. The values of Q_i^0 and a_i for the functional groups encountered most often in the structure of organic compounds are established.[10]

A given compound X is characterised according to an adsorbent with activity $\alpha' = 1$ by its adsorption energy, S_X, and its molecular area under adsorption, A_x. The ratio $\varepsilon_X = S_X / A_X$ is the *adsorption strength of compound X* (see ref. 15) and is a measure for the adsorption energy of X per unit of its molecular area under adsorption. In a first approximation, S_X and A_X are expressed by the following sums:

$$S_X = \sum_{i=1}^{ng} w_i \cdot Q_i^o \tag{1}$$

$$A_X = \sum_{i=1}^{ng} w_i \cdot a_i \tag{2}$$

where w_i shows how many times a given group i is available in the structure of compound X containing totally ng groups.

The thermodynamic description of the Snyder's displacement model allows us to express[10-12] the retention, R_M, of compound X as a function of mobile-phase strength, ε, taking into account the adsorption properties of X and the adsorbent.

$$R_M(\varepsilon) = R_{M\,(shift)} + \alpha'(S_X - \varepsilon \cdot A_X) \tag{3}$$

or

$$R_M(\varepsilon) = R_{M\,(shift)} + \alpha' \cdot A_X(\varepsilon_X - \varepsilon) \tag{3a}$$

where α' and $R_{M(shift)} = \log \frac{V_a}{V^o / W}$ (see ref. 15) characterise the adsorption properties of the stationary phase (adsorbent).

The LSChrom software uses Eq. 3 to select the range of suitable mobile phase strength, $\varepsilon_{recommended}$, for a given separation ensuring retention in the favorable range ($0 < R_F < 1$) and maximum separation.

The conversion between the calculated values of R_M and R_F was done by the following well known equation

$$R_M = \log\left(\frac{1}{\xi \cdot R_F} - 1\right) \quad (4)$$

where ξ was assumed 1.1.[10]

EXPERIMENTAL

Compounds **1-23** were synthesised[16] by analogy to refs. 17 and 19. Their structures and trans configuration were proved by their ^{1}H-NMR spectra.

TLC was performed on two adsorbents: adsorbent 1 was TLC silica 60 GF_{254} (Merck, Germany) and adsorbent 2 was TLC plates silica 60 F_{254} (Mecrk, Germany). The thin-layers of adsorbent 1 were prepared as described in ref. 20. On a given TLC plate, the samples applied were up to 13 at a 1.2 cm distance between them. The travelling distance was 18 cm for adsorbent 1 and 10 cm for adsrobent 2. The solvents were of analytical reagent grade. The R_F values were arithmetic means of two measurements.

The computer program used was LSChrom, Ver. 2, for Windows.[14]

RESULTS AND DISCUSSION

The procedure for automatic selection of mobile phases by the Snyder theory and LSChrom includes five steps, which will be discussed in detail for compounds **1-23**. They were studied in two groups to ensure TLC of all compounds of any group to be done on individual plates. The first group included the parent compound **1** (a tetrahydroisoquinolinone) and the tetrahydroisoquinolines **2-12**. The second group consisted of parent compound **1** and the remaining tetrahydroisoquinolinones **13-23**.

Step 1: Characterisation of the Adsorbent That Will Be Used

Any type of adsorbent can be characterised, approximately, by a definite value[13] of selectivity α'. The two adsorbents used in this study are of the same type, but differ in the way of preparation of the thin layers. This and the similar retention of any compound and a given mobile phase on the two adsorbents (see below) led us to assume, for the two adsorbents, equal values of α' and $R_{M(shift)}$, namely 0.57 and –1.76, respectively. These values were input into the LSChrom software for use in the calculations. We have derived them earlier by constructing the linear plot of Eq. 3 using experimental R_F values for a given TLC silica of the compounds of refs. 1-3 and calculated values of the expression ($S_X - \varepsilon \cdot A_X$).

In contrast to ref. 15, preliminary experimental characterisation of the two adsorbents used was not done, enabling us to use a fully automatic selection of the mobile phases.

Step 2: Calculation of the Adsorption Properties of the Compounds Studied on the Basis of Their Functional Groups and Corresponding Literature Data

In this step, the structure of any compound X studied was described by the corresponding functional groups. The user selects the relevant groups from a list included in LSChrom and specifies their number. The computer calculates the values of adsorption energy, S_X and area under adsorption, A_X, by Eq. 3 and Eq. 4, respectively, using the information entered by the user and the data for Q_i^0 and a_i of Snyder (ref. 10, Table 8-4 and Table 10-2) incorporated in a corresponding file to LSChrom.

Table 1 and Table 2 show the values of S_X, A_X, and ε_X obtained for compounds **1-12** and **1**,**13-23**, respectively. The values of ε_X vary in the ranges 0.362-0.485 and 0.385-0.454, showing that the compounds of the two groups are expected to have similar adsorption properties. Table 1 and Table 2 include, also, the calculated retention, R_M, of all compounds studied and the corresponding R_F values (see the following step).

Step 3: Selection of a Range of Suitable Mobile-Phase Strength $\varepsilon_{recommended}$ for a Given Separation on the Basis of an Analysis of the Calculated Retention of the Compounds Studied as a Function of Mobile-Phase Strength

Using the data for α', $R_{M(shift)}$, S_X, and A_X, obtained in Steps 1 and 2, LSChrom predicts, by Eq. 3 retention, R_M, (and R_F by Eq. 4) of the compounds studied as a function of the mobile-phase strength. The software selects a range of suitable strength, $\varepsilon_{recommended}$, of the mobile phases for a given separation, making a visualised analysis of the calculated retention, R_M, and resolution, R_S. LSChrom selects as $\varepsilon_{recommended}$ those ranges of ε for which R_S has greater values, including the maximum value, and the retention is more or less in the favourable range (see ref. 15 for details). The predicted range of $\varepsilon_{recommended}$ was $0.320 \leq \varepsilon \leq 0.393$ for all compounds, and the most recommended value of ε was 0.344 for compounds **1-12**

Table 1. Structure Description by Functional Groups and Adsorption Properties of Compounds 1-12

			Number of Relevant Functional Groups in Compound											
Group i*	Q_i^o	a_i	1	2	3	4	5	6	7	8	9	10	11	12
C=	0.25	1.00	16	16	16	16	22	22	22	22	22	16	16	16
Ar-Me	0.11	0.80	1	1	1	1	1	1	1	1	1	1	1	1
Al-CH_2-Al	−0.05	0.90	3	5	10	9	9	9	9	9	9	9	9	9
Al-CH_3	5.80	10.50				1							2	
Al-N (tert)	9.60	10.30	1	2	4	4	4	4	4	4	4	3	3	3
Al-$CONH_2$	3.61	9.00	1											
Al-O-Me	0.07	1.60										1	1	
Al-S-Me	2.94	7.40												1
Al-CO_2-Me	5.27	10.50	1											
Al-OH	5.60	8.50		1										
Al-F	1.54	1.20							3					
Ar-F	−0.15	0.40									1			
Ar-Cl	−0.20	0.70								1				
Ar-O-Me	1.83	4.60						1						
$\sum Q_i^0$			24.63	21.06	26.81	26.93	28.36	30.19	32.98	28.16	28.21	24.76	24.81	24.00
$\sum a_i$			50.80	50.80	67.80	68.50	72.90	77.50	76.50	73.60	73.30	65.40	68.60	63.80
ε_x			0.485	0.415	0.395	0.393	0.389	0.390	0.431	0.383	0.385	0.377	0.362	0.376
R_M calc. ($\varepsilon = 0.344$)			2.31	0.28	0.22	0.15	0.10	0.24	2.03	−0.15	−0.07	−0.53	−1.08	−0.60
R_F calc. ($\varepsilon = 0.344$)			0.01	0.35	0.38	0.42	0.44	0.37	0.01	0.59	0.54	0.77	0.92	0.80

*Ar and Al denote an aryl and alkyl group, respectively.

Table 2. Structure Description by Functional Groups and Adsorption Properties of Compounds 1, 13-23

			Number of Relevant Functional Groups in Compound											
Group i*	Q_i^o	a_i	1	13	14	15	16	17	18	19	20	21	22	23
C=	0.25	1.00	16	16	16	22	16	22	22	22	22	16	16	16
Ar-Me	0.11	0.80	1	1	1	1	1	1	1		1		1	1
Al-CH_2-Al	−0.05	0.90	3	4	9	8	8	8	8	8	8	8	8	8
Al-CH_3	5.80	10.50				1							2	
Al-N (tert)	9.60	10.30	1	1	2	3	3	3	3	3	3	2	2	2
Al-$CONH_2$	3.61	9.00	1	1	1	1	1	1	1	1	1	1	1	1
Al-O-Me	0.07	1.60										1	1	
Al-S-Me	2.94	7.40												1
Al-CO_2-Me	5.27	10.50	1											
Al-OH	5.60	8.50		1										
Al-F	1.54	1.20							3					
Ar-F	−0.15	0.40									1			
Ar-Cl	−0.20	0.70								1				
Ar-O-Me	1.83	4.60						1						
$\sum Q_i^o$			21.63	21.58	21.86	27.71	29.21	31.04	33.83	29.01	29.06	25.52	25.66	24.85
$\sum a_i$			49.90	50.80	55.30	64.90	70.90	75.50	74.50	71.60	71.30	63.40	66.60	61.80
ε_X			0.433	0.425	0.395	0.427	0.412	0.411	0.454	0.405	0.408	0.403	0.385	0.402
R_M calc. ($\varepsilon = 0.331$)			1.14	0.94	0.25	1.77	1.50	1.67	3.45	1.25	1.34	0.81	0.28	0.73
R_F calc. ($\varepsilon = 0.331$)			0.07	0.10	0.36	0.02	0.03	0.02	0.00	0.05	0.04	0.13	0.34	0.16

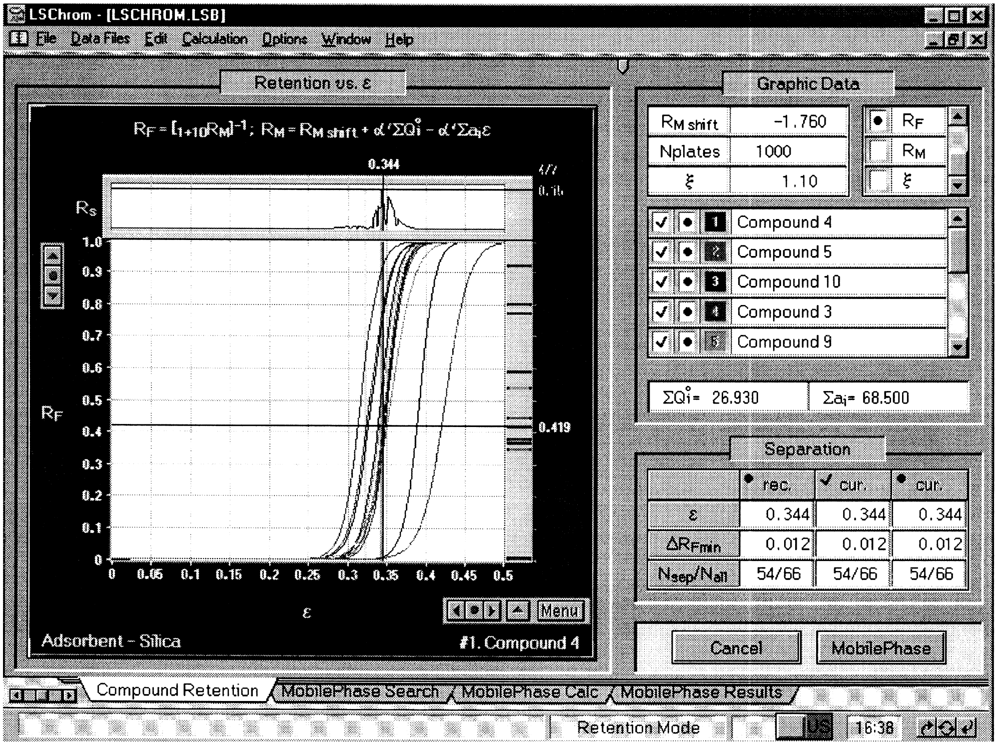
*Ar and Al denote an aryl and alkyl group, respectively.

and 0.331 for compounds **1,13-23**. Figure 1 illustrates the selection of $\varepsilon_{recommended}$ for compounds **1-12**. The most recommended value, ε=0.344, has maximum value of RS.

Any of the two values of $\varepsilon_{recommended}$ proved to be up to 0.14 units less than the corresponding values of the sample adsorption strength, ε_X, shown in Table 1 and Table 2. If a given difference is kept, in general, it will permit one to deduce, approximately, $\varepsilon_{recommended}$ on the basis of ε_X without the necessity to calculate retention. A similar difference was found, also, in Ref. 15.

Step 4: Selection of Concrete Mobile Phases Having ε in the Desired Range $\varepsilon_{recommended}$

Plenty of mobile phases have in the recommended range, $0.320 \leq \varepsilon \leq 0.393$, for the compounds studied. We selected, arbitrarily, discrete values of ε from this



$R_{M\,shift}$	-1.760	● R_F
Nplates	1000	☐ R_M
ξ	1.10	☐ ξ

☑ ● 1 Compound 4
☑ ● 2 Compound 5
☑ ● 3 Compound 10
☑ ● 4 Compound 3
☑ ● 5 Compound 9

ΣQ_i°= 26.930
Σa_i= 68.500

	● rec.	✓ cur.	● cur.
ε	0.344	0.344	0.344
$\Delta R_{F\,min}$	0.012	0.012	0.012
N_{sep}/N_{all}	54/66	54/66	54/66

Figure 1. Illustration of the prediction of $\varepsilon_{recommended}$ for compounds **1-12**.

range. Concrete mobile phases with such values of ε were found from a list available in LSChrom comprising about 200 multi-component mobile phases which differ in composition. The user inputs a given value of ε and the computer program calculates, by an iterative procedure,[13] the amounts of the solvents of any mobile phase that will ensure the desired value of ε. We selected from this list 14 mobile phases having $0.320 \leq \varepsilon \leq 0.393$ and they are given in Table 3.

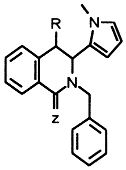
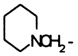
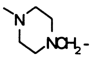
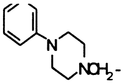
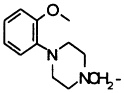
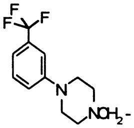
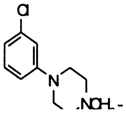
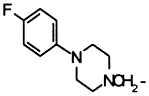
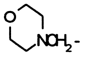
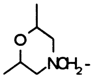
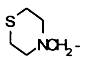
Step 5: Chromatography of the Compounds Studied with the Selected Mobile Phase

We performed TLC on two silicas of the compounds studied with the 14 selected mobile phases having ε in the predicted by LSChrom range $0.320 \leq \varepsilon \leq 0.393$ of $\varepsilon_{\text{recommended}}$. Table 4 and Table 5 show the values of ε, m, and P' of these mobile phases and the corresponding experimental values of R_F for compounds **1-12** and **1,13-23**, respectively. The most important fact is the variation of R_F within 0.04-0.81 and 0.01-0.54 for compounds **1-12** and **1,13-23**, respec-

Table 3. Mobile Phases Recommended by LSChrom for TLC on Silica of all Compounds Studied

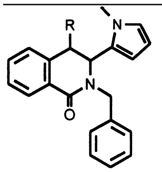
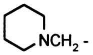
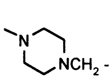
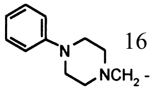
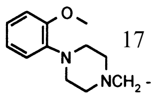
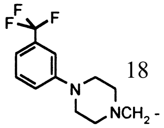
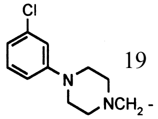
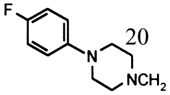
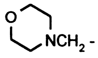
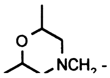
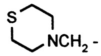
Mobile Phase No.	Composition	ε	m	P'
1 Hexane-dichloromethane-tetrahydrofuran	77.477 : 10.000 : 12.523	0.344	0.92	0.89
2 Cyclohexane-isopropanol	94.671 : 5.329	0.331	—	0.02
3 Hexane-ethyl acetate	73.425 : 26.575	0.336	0.59	1.24
4 Hexane-dioxane	83.728 : 16.272	0.336	—	0.87
5 Tetrachloromethane-acetone	90.392 : 9.608	0.336	0.83	1.94
6 Heptane-diisopropyl ether-ethyl acetate	86.931 : 10.00 : 3.069	0.336	0.51	0.55
7 Hexane-acetone	77.290 : 22.710	0.370	0.93	1.24
8 Cyclohexane-acetone	85.234 : 14.766	0.331	0.90	0.58
9 Tetrachloromethane-chloroform-acetonitrile	83.900 : 10.000 : 6.100	0.331	1.08	2.11
10 Hexane-ethyl acetate	74.799 : 25.201	0.331	0.59	1.18
11 Hexane-ethyl acetate-amonium hydroxide	74.800 : 24.600 : 0.600	~0.331	—	—
12 Hexane-ethyl acetate	62.770 : 37.230	0.370	0.59	1.70
13 Toluene-ethyl acetate	80.762 : 19.238	0.370	0.51	2.79
14 Hexane-isopropanol	84.565 : 15.435	0.370	—	0.69

Table 4. Experimental R_F Values of Compounds 1-12 on Silicas 1,2 and the Computer Selected Mobile Phases 1-7

Compound				R_F for a Given Adsorbent and Mobile Phase*							
R	Z	No.		1-1	1-2	1-3	1-4	1-5	1-6	1-7	2-7
			*ε*	0.344	0.331	0.336	0.336	0.336	0.336	0.370	0.370
			m	0.92	-	0.59	-	0.83	0.51	0.93	0.93
			P'	0.89	0.02	1.24	0.87	1.94	0.55	1.24	1.24
CH_3OOC-	O	1		0.30	0.24	0.33	0.20	0.50	0.02	0.28	0.18
HO-CH_2-	2H	2		0.24	0.23	0.33	0.08	0.36	0.02	0.35	0.10
		3		0.62	0.43	0.65	0.28	0.74	0.17	0.69	0.50
		4		0.04	0.06	0.03	0.06	0.09	0.01	0.15	0.07
		5		0.72	0.71	0.87	0.78	0.88	0.21	0.77	0.66
		6		0.58	0.51	0.69	0.58	0.83	0.09	0.63	0.51
		7		0.74	0.71	0.87	0.63	0.86	0.22	0.75	0.67
		8		0.76	0.75	0.88	0.61	0.87	0.26	0.78	0.69
		9		0.70	0.65	0.82	0.56	0.87	0.17	0.69	0.62
		10		0.53	0.46	0.55	0.51	0.77	0.06	0.58	0.51
		11		0.68	0.58	0.73	0.66	0.84	0.14	0.78	0.75
		12		0.81	0.86	0.88	0.67	0.88	0.27	0.85	0.81

*The notation "1-6" for instance denotes that TLC was done with silica 1 and mobile phase 6.

Table 5. Experimental R_F Values of Compounds 1,13-23 on Silicas 1,2 and the Computer Selected Mobile Phases 7-14

Compound			R_F for a Given Adsorbent and Mobile Phase*								
R	No.		1-8	1-9	1-10	1-11	1-12	1-13	1-14	1-7	2-7
		ε	0.331	0.331	0.331	~0.331	0.370	0.370	0.370	0.370	0.370
		m	0.90	1.08	0.59	-	0.59	0.51	-	0.93	0.93
		P'	0.58	2.11	1.18	-	1.70	2.79	0.69	1.24	1.24
CH_3OOC-	1		0.18	0.32	0.27	0.28	0.67	0.50	0.59	0.26	0.18
HO-CH_2-	13		0.08	0.18	0.10	0.10	0.28	0.20	0.48	0.17	0.10
	14		0.44	0.53	0.54	0.6	0.87	0.61	0.78	0.58	0.39
	15		0.02	0.02	0.01	0.02	0.01	0.01	0.03	0.03	0.02
	16		0.31	0.46	0.43	0.43	0.83	0.60	0.77	0.36	0.27
	17		0.26	0.4	0.31	0.32	0.68	0.50	0.70	0.31	0.24
	18		0.28	0.5	0.43	0.43	0.84	0.63	0.76	0.35	0.26
	19		0.31	0.51	0.45	0.44	0.84	0.64	0.77	0.35	0.27
	20		0.26	0.42	0.38	0.37	0.78	0.57	0.77	0.33	0.24
	21		0.22	0.31	0.22	0.22	0.49	0.38	0.62	0.29	0.22
	22		0.32	0.43	0.39	0.38	0.77	0.51	0.78	0.39	0.29
	23		0.34	0.53	0.46	0.43	0.85	0.65	0.81	0.39	0.29

*The notation “2-7” for instance denotes that TLC was done with silica 2 and mobile phase 7.

tively, with mobile phases 1 and 8-10 having the most recommended values of ε. The zones are spread over the entire ranges. The use of mobile phases 2-7 and 11-14 results in R_F values within 0.01-0.88. Hence, computer selection of the range of $\varepsilon_{recommended}$ and specific mobile phases is adequate, since the R_F values established are in the favorable range where the zones are above the start line and below the front line.

The parent compound **1** was studied with all 14 computer-selected mobile phases showing, also, R_F in the favorable range (0.02-0.67).

By contrast to ref. 15, the trans configuration of compounds **1-23** was not taken into account in the predictions, since a mobile phase, suitable for a given structure is applicable to both diastereoisomers.[2-4,6-9]

In general, a good agreement between the predicted and experimental R_F was not established; this is due to the approximate prediction of retention. However, the Snyder theory gives a proper selection of ε and the corresponding specific mobile phases for TLC of the compounds studied. This is the most important use that is expected in future applications of the Snyder theory and LSChrom.

We would like to point out other features of the data obtained. Compound **4** and compound **15**, containing 4-methyl-piperazin-1-yl group, are strong bases and show the greatest retention and smallest R_F. The presence of a small amount (0.6 %) of ammonium hydroxide in mobile phase 11 increases, slightly, RF of compound **14** relative to that of the parent mobile phase 10. A further increase of the amount of ammonium hydroxide is expected to increase R_F of compound **14**. It is worth noting that ε of mobile phases containing ammonium hydroxide cannot be calculated by LSChrom because of a lack of relevant data. It was assumed that ε of mobile phase 11 is similar to that of mobile phase 10.

TLC of compounds **1-23** with mobile phase 7 was done on both silicas used. The data obtained show that adsorbent 1 is somehow less active than adsorbent 2. Moreover, any tetrahydroisoquinoline from the set **2-12** has a weaker retention than the corresponding tetrahydroisoquinolinone (**13-23**).

CONCLUSIONS

The present study is a successful application of the Snyder theory and software LSChrom[14] to an automatic selection of mobile phases for TLC, on two silicas, of compounds **1-23** having complex structures.

The procedure used involves several steps.

1. Characterisation of the two silicas used by available values of α' and $R_{M(shift)}$, namely 0.57 and –1.76, respectively. The values were input into the software for use in the calculations.

2. Automatic and rough selection of suitable range of $\varepsilon_{recommended}$ by Eqs. 1-3 on the basis of the sample structure, using the necessary values of Q_i^0 and a_i from ref. 10, Table 8-4 and Table 10-2.

3. Selection, by an iterative procedure,[13] of 14 concrete mobile phases having some values of ε from the recommended range $0.320 \leq \varepsilon \leq 0.393$.

4. TLC on silica of compounds **1-23** with the automatically selected mobile phases. The experimentally found R_F values were in the favorable range of 0.01-0.88, proving the correctness of the predictions.

The software LSChrom[14] enables any user, even not familiar with the Snyder theory, to apply this theory for an automatic selection of mobile phases for normal-phase TLC and HPLC of non-ionic compounds whose structures can be expressed by the functional groups available in the software

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Received November 9, 2000 Manuscript 5425
Accepted January 20, 2001