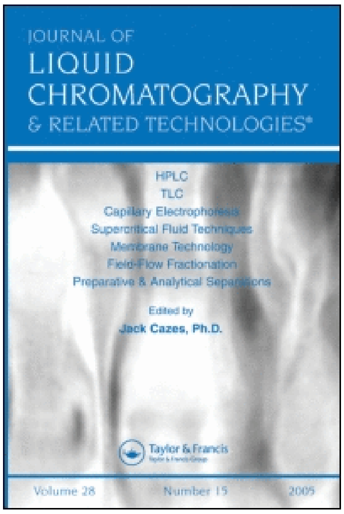

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LIPOPHILICITY OF NATURAL SWEETENERS ESTIMATED ON VARIOUS OILS AND FATS IMPREGNATED THIN-LAYER CHROMATOGRAPHY PLATES

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□ *A variety of oils (paraffin, olive, sunflower, corn, castor, cod liver) and fats (margarine, butter, pig, sheep, pullet, human) impregnated TLC-plates were indirectly evaluated and characterized from the lipophilicity point of view by employing a series of experimental lipophilicity parameters estimated for a representative group of natural sweeteners from retention data. The relevance of the results was evaluated by a critical comparison of the lipophilicity parameters with a series of theoretical lipophilicity and solubility indices. The ALOGPs descriptor offers the best correlation coefficients, higher than 0.9. The principal component analysis applied to the retention data and the matrices formed by each distinct group of experimental lipophilicity indices allowed a realistic classification of the fats and oils, through the 3D graphs ("lipophilicity spaces") and gave new insights into the retention mechanism involved in the chromatographic process.*

Keywords animal and human fats, lipophilicity, natural sweeteners, oils, PCA, TLC

INTRODUCTION

In the last decades, many predicting statistical models based on more or less complex equations were produced in order to determine with an adequate statistical degree of confidence, the physicochemical properties of new molecules, even before they are actually synthesized. This is, in fact, the main advantage of the quantitative structure property relationships (QSPR), quantitative structure retention relationships (QSRR), or quantitative structure activity relationship (QSAR) experiments. On the basis of these concepts, a large number of scientific papers have invaded the literature presenting correlations of biological activity or toxicity of compounds with their physicochemical and pharmaceutical properties, such

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as lipophilicity, solubility, stability, reactivity, retention (partition), permeability, transportability, pharmacokinetics, toxicity, and mutagenicity.[1] The lipophilicity is the major property involved in the QSAR/QSPR/QSRR experiments, and as a direct consequence many software were developed for generating theoretical values on the basis of molecular, atomistic or properties particularities of a large number of compounds.

The lipophilicity is defined as the tendency of a compound to partition to non-polar versus aqueous environments, such so, there may be considered that the environmental circumstances play a decisive role over the chemical and biological behavior.[2,3] The possibilities of lipophilicity experimental determination are divided in two major groups such as direct and indirect techniques. The most known, and in the same time the most used direct method, describes the shake flask technique, but it has been almost totally replaced by the indirect techniques, such as the chromatographic ones,[4,5] which are more flexible and presents some significant advantages: dynamic process, the consumption of the investigated compounds is minimal, high purity chemicals and additional analytical quantification is not required. These methods require only the determination of some retention parameters.[6,7]

The lipophilicity is usually expressed by the partition coefficient, denoted in few different ways, frequently depending on the determination method (Log P, Log k_w, Log K_{ow}, R_M). Considering that the lipophilicity experiments are performed mainly to evidence the *in vivo* behavior of a specific compound, it may be appreciated that the actual stationary phase's materials are too simple and does not offer a realistic alternative of biological membranes. Moreover, the large number of software are able to offer different log P values, which are often very different and until now there are not rationale and objective evidences to differentiate and choose the best ones.

Concerning the experimental estimation of lipophilicity, the chromatographic procedures offer large possibilities because the combinations between both stationary and mobile phases are practically unlimited. Reverse phase thin-layer chromatography using impregnated layers with different materials appears to be one of the most suited solutions. In this order, for example, any oil or fat, which may be homogeneously dissolved in a solvent may be used for impregnation. In addition, the vegetable oils or animal fats may satisfy the complexity requirements, and may be involved in the obtaining of new realistic models for the mimesis of biological membranes. The chemical composition of vegetable oils and related products are rich in triglycerides, free fatty acids (especially oleic and linoleic acid), phytosterols, lipophilic vitamins, and traces of minerals.[8,9] On the other hand, the animal fats present a high concentration of saturated fatty acids and cholesterol.[10]

Over years, the paraffin oil,[11–15] near by silicon oil,[16,17] and ethyl oleate,[18] were successfully used for the impregnation of TLC-plates in order to change the stationary phase characteristics and improve the chromatographic performances.

The goal of this paper was to investigate the chromatographic behavior of a representative class of natural sweeteners (arabitol, xylitol, adonitol, mannitol, sorbitol, galactose, fructose, glucose, xylose, mannose, galactosamine, sucrose, maltose), which were characterized and compared with the contribution of various experimental lipophilicity indices (R_{M0}, b, mean of R_F (mR_F), mean of R_M (mR_M), scores corresponding to the first principal components of R_F ($PC1/R_F$) and R_M ($PC1/R_M$)) on oils and fats impregnated TLC-silica gel plates (paraffin – Pa, olive – Ol, sunflower – SF, corn – Co, castor – Ca, margarine – Ma, butter – Bu, cod, pig, sheep – Sh, pullet – Pu, and human – Hu). Furthermore, the obtained lipophilicity indices of the investigated natural sweeteners were compared between them and with computed log P values. We also have to mention the lack of information concerning the lipophilicity of sweeteners; the literature and data bases offer only few data.[19] The principal components analysis (PCA), through "lipophilicity space" option, offers once more the possibility to analyze and compare the lipophilicity of the vegetal and animal fats in the context of human fat. In addition, PCA loadings are used to investigate and to compare the retention mechanism involved in the chromatographic process.

THEORY

Methods

The retention factor (R_F) is the basis of lipophilicity estimation by TLC, since all the lipophilicity indices are directly derived from retention data. The most popular descriptor in TLC is considered the retardation factor (R_M) obtained, as was described by Bate-Smith and Westall[20] through the following formula:

$$R_M = \log(1/R_F - 1) \qquad (1)$$

The direct influence of the organic modifier concentration from the mobile phase over the R_M value is recovered into the linear relationship described by a TLC adapted Soczewiński-Wachtmeister[21] Eq.:

$$R_M = R_{M0} + bC \qquad (2)$$

where R_{M0} represents the extrapolated value to pure water, b is the regression slope and in the same time it is considered to be the specific surface area of the stationary phase and also an alternative descriptor of lipophilicity; *C* represents the volume fraction of the organic solvent in the mobile phase. The R_{M0} is usually expressed directly from regression equation of five R_M values obtained for mobile phases containing different fractions of organic modifier.

More recently the PCA has been successfully applied for the lipophilicity estimation from retention data. The methodology based on PCA is not only more robust to different errors but it is also more informative, because the results (scores and loadings) offer new scales of lipophilicity and more efficient alternatives for characterization and ranking of investigated compounds and stationary phases, including new insights into the chromatographic mechanism. Much more, the mean of R_F and R_M values can be also an illuminating alternative for the lipophilicity estimation.[22–25]

Log P

A large number of software and internet module are now available to compute theoretical log P values applying different algorithms based on structural, atomistic, topological, electrotopological, or other considerations. In the present study, the structure of the compounds were first preoptimized with the Molecular Mechanics Force Field procedure included in Hyperchem version 7.5 (HyperChem, release 7.5 for Windows, Molecular Modeling System; Hypercube), and the resulting geometries were further refined by means of the semi empirical method Parametric Method-3 using the Fletcher-Reeves algorithm and a gradient norm limit of 0.009 kcal $Å^{-1}$. The optimized geometries were loaded by software like Chem3D Ultra 8.0 and Dragon Plus version 5.4 in order to calculate various lipophilicity descriptors. Three of the log P values were calculated by Chem3D Ultra 8.0 (CLogP, $Log(p)^C$-Crippen method, $Log(p)^V$-Viswanadhan method) and four are given by the Dragon 5.4 (MLOGP-Moriguchi method, $MLOGP^2$-Squared Moriguchi method, ALOGP-Ghose-Crippen method, $ALOGP^2$- Squared Ghose-Crippen method). Another six were offered by the internet module ALOGPS 2.1-vcclab (ALOGPs, AC logP, miLogP, KOWWIN, XLOGP2, XLOGP3).[26] Moreover, the ALOGPS 2.1 offered a series of solubility computed indices (ALOGpS, AC logs, AB/LogS). All the computed lipophilicity indices are listed in Table 1, while the solubility values are presented in Table 2.

TABLE 1 The Computed Lipophilicity Descriptors of Some Natural Sweeteners

No.	Compound	$LogP^C$	$LogP^V$	CLogP	MLOGP	$MLOGP^2$	ALOGP	$ALOGP^2$	ALOGPs	AC logP	miLogP	KOWWIN	XLOGP2	XLOGP3
1	Arabitol	−2.40	−1.83	−1.88	−2.10	4.42	−2.43	5.90	−2.41	−2.18	−2.67	−2.56	−3.22	−2.48
2	Xylitol	−2.40	−1.83	−1.88	−2.10	4.42	−2.43	5.90	−2.41	−2.18	−2.67	−2.56	−3.22	−2.48
3	Adonitol	−2.40	−1.83	−1.88	−2.10	4.42	−2.43	5.90	−2.41	−2.18	−2.67	−2.56	−3.22	−2.48
4	Mannitol	−2.94	−2.20	−2.05	−2.50	6.24	−2.94	8.64	−2.57	−2.73	−3.10	−3.01	−3.90	−3.10
5	Sorbitol	−2.94	−2.20	−2.05	−2.50	6.24	−2.94	8.64	−2.57	−2.73	−3.10	−3.01	−3.90	−3.10
6	Galactose	−2.38	−1.76	−2.21	−2.48	6.17	−2.51	6.32	−2.47	−2.32	−2.64	−2.89	−2.34	−2.59
7	Fructose	−2.08	−1.25	−2.18	−2.48	6.17	−2.48	6.57	−2.35	−1.98	−2.78	−1.55	−2.38	2.84
8	Glucose	−2.38	−1.76	−2.21	−2.48	6.17	−2.51	6.32	−2.47	−2.32	−2.64	−2.89	−2.34	−2.59
9	Xylose	−1.84	−1.39	−2.18	−2.09	4.36	−2.00	4.01	−2.32	−1.65	−2.22	−2.91	−1.88	−2.52
10	Mannose	−2.38	−1.76	−2.21	−2.48	6.17	−2.51	6.32	−2.47	−2.32	−2.64	−2.89	−2.34	−2.59
11	Galactosamine	−2.76	−2.11	−2.18	−2.48	6.17	−2.80	7.86	−2.61	−2.86	−3.35	−2.20	−2.41	−2.84
12	Sucrose	−3.82	−2.47	−3.09	−3.90	15.19	−4.31	18.58	−2.68	−3.99	−3.74	−4.27	−4.13	−3.70
13	Maltose	−4.71		−4.40	−3.90	15.19	−4.26	18.15	−2.73	−4.17	−4.45	−5.12	−4.31	−4.73

TABLE 2 The Solubility Values of Natural Sweeteners

No	Compound	ALOGpS	ALOGpS (g/L)	AC logS	AC logS (g/L)	AB/logS	AB/logS (g/L)	S_{exp}*
1	Arabitol	0.26	2800	0.42	400	1.12	2010	729[27]
2	Xylitol	0.26	2800	0.42	400	1.12	2010	627[28]
3	Adonitol	0.26	2800	0.42	400	1.12	2010	936[27]
4	Mannitol	0.17	270	0.55	640	1.03	1950	145[28]
5	Sorbitol	0.17	270	0.55	640	1.03	1950	687[28]
6	Galactose	0.35	400	0.25	320	0.77	1060	683[29]
7	Fructose	0.29	350	0.38	430	0.93	1530	778[27]
8	Glucose	0.35	400	0.25	320	0.77	1060	1200[27]
9	Xylose	0.45	430	0.12	200	1.08	1810	555[27]
10	Mannose	0.35	400	0.25	320	0.77	1060	713[27]
11	Galactosamine	0.29	350	0.17	270	0.76	1030	500[30]
12	Sucrose	0.06	390	0.64	1640	0.10	430	2100[27]
13	Maltose	0.04	380	0.55	1210	0.12	450	780[27]

*S_{exp} – Experimental determined solubility.

EXPERIMENTAL

All the compounds and solvents were obtained from commercial sources (Merck, Fluka, and Sigma) in analytical degree purity. The oils (paraffin, olive, sunflower, corn, castor, cod liver) and fats (margarine, butter, pig, sheep, pullet) used for the impregnation were from local markets, while the female fat was obtained from liposuction surgery. The standard solutions of natural sweeteners were prepared in water (1 mg mL^{-1}). The spots (1 μL) were applied at 1.5 cm from the bottom edge and at 0.7 cm from lateral edges using a Hamilton microsyringe of 10 μL. The distance between the spots was by 0.7 cm. The elution was performed by ascendant development into a chromatographic chamber previously saturated for 10 minutes.

The silica gel 60 F_{254} plates (10 × 20 cm) were impregnated with 10% diethyl ether solution of fats, except for pig, sheep, and pullet fats, which were prepared as 5% solutions. The water presence in the margarine and butter lead to the necessity of its elimination from the etheric solution by using a separation funnel previously of impregnation. The pig, pullet, and sheep fats used as raw material were extracted from the natural membranes by heating to melting point followed by a filtration. The obtained fats were used for the impregnation as 5% diethyl ether solution. The human fat was simply dissolved in the diethyl ether by using a porcelain mortar. The impregnation was performed by ascendant development.

In order to select the most exclusive organic modifier for the mobile phase, five organic solvents were tested. The investigated solvents were:

methanol, ethanol, isopropanol, acetone, and acetonitrile (ACN). The best results were obtained when ACN was used. The mobile phases containing different mixtures of ACN and water were optimized in order to obtain a significant increase of migration of the compounds while the elution step was changed. In each case, 5 steps were performed at different fractions of ACN between 70% and 90% for all the stationary phases, in 5% increments. The sugars were visualized by reducing directly on the plate with silver nitrate and sodium hydroxide (Tollens reaction). The sugars spots appeared as brown spots on a white background, after heating at 105°C for 5 min.

RESULTS AND DISCUSSION

The experimental lipophilicity indices obtained on the investigated plates are listed in Tables 3 and 4. All the results, including the computed lipophilicity indices, show the disaccharides as the most hydrophilic compounds, followed by the monosaccharide. The alcohols are more lipophilic. Observing the galactosamine versus galactose it is easy to conclude that the amino group leads to an increased lipophilic character. If the classical R_{M0} values are considered to be the experimental reference values, there is a need to show the degree of confidence, described through the regression correlation coefficients obtained for the R_M values and the ACN fraction in the mobile phase, which were higher than 0.99 except for xylitol ($r_{Ma} = 0.98$), mannitol ($r_{Ma} = 0.98$), sorbitol ($r_{Ma} = 0.97$, $r_{Pig} = 0.98$), galactose ($r_{Ca} = 0.98$, $r_{Cod} = 0.98$), galactosamine ($r_{SF} = 0.98$, $r_{Ca} = 0.97$, $r_{Ma} = 0.96$, $r_{Bu} = 0.98$, $r_{Cod} = 0.98$, $r_{Hu} = 0.98$), sucrose ($r_{SF} = 0.95$, $r_{Ca} = 0.98$, $r_{Pig} = 0.97$, $r_{Pu} = 0.98$), and maltose ($r_{SF} = 0.97$, $r_{Ma} = 0.98$, $r_{Bu} = 0.98$, $r_{Cod} = 0.98$, $r_{Sh} = 0.98$). Concerning the computed log P values, as it was expected they are strongly correlated. This expectation is clearly illustrated in Figure 1 (obtained by applying PCA to the theoretical log P values) where all the values form a compact group, except for XLOGP3. Moreover, the log S values are identified as a distinct correlated group.

The correlation matrix of the experimental values versus theoretical ones is characterized by fair correlation coefficients (Tables 5 and 6), except for the solubilities expressed as gL^{-1}, including the experimental determined values ($r \leq 0.60$). Considering the theoretical descriptors, it may be observed that the ALOGPs values offer the best correlation, followed by the AC logP, $LogP^C$ and miLogP, which may indicate that the lipophilicity of natural sweeteners is better estimated by the newly developed methods based on topological descriptors, rather than those obtained on the basis of atomistic or molecular approaches (XLOGP2, XLOGP3, CLOGP). The newly ALOGPS 2.1. version of log P computing module,

TABLE 3 The Lipophilicity Indices of Natural Sweeteners Obtained on Paraffin, Olive, Sunflower, Corn, Castor Oil and Margarine-Impregnated TLC-Plates

		Paraffin						Olive						Sunflower					
No.	Compound	mR_F	mR_M	R_{M0}	b	$PC1/R_F$	$PC1/R_M$	mR_F	mR_M	R_{M0}	b	$PC1/R_F$	$PC1/R_M$	mR_F	mR_M	R_{M0}	b	$PC1/R_F$	$PC1/R_M$
1	Arabitol	0.351	0.290	−2.61	0.036	−0.109	0.399	0.338	0.322	−2.96	0.041	−0.089	0.340	0.316	0.366	−2.62	0.037	−0.069	0.288
2	Xylitol	0.344	0.312	−2.93	0.040	−0.099	0.348	0.334	0.332	−2.97	0.041	−0.080	0.319	0.310	0.379	−2.62	0.037	−0.057	0.261
3	Adonitol	0.390	0.211	−2.63	0.036	−0.197	0.576	0.387	0.218	−2.89	0.039	−0.196	0.573	0.366	0.265	−2.95	0.040	−0.189	0.515
4	Manitol	0.284	0.460	−3.34	0.047	0.029	0.013	0.271	0.505	−3.75	0.053	0.052	−0.072	0.253	0.542	−3.50	0.050	0.057	−0.110
5	Sorbitol	0.274	0.489	−3.52	0.050	0.049	−0.055	0.261	0.520	−3.49	0.050	0.078	−0.105	0.255	0.535	−3.40	0.049	0.056	−0.094
6	Galactose	0.298	0.419	−3.18	0.045	−0.002	0.104	0.303	0.411	−3.34	0.047	−0.017	0.140	0.275	0.470	−3.00	0.043	0.015	0.056
7	Fructose	0.346	0.304	−2.78	0.039	−0.102	0.367	0.354	0.291	−3.03	0.042	−0.125	0.408	0.313	0.371	−2.63	0.038	−0.066	0.282
8	Glucose	0.315	0.378	−3.01	0.042	−0.035	0.199	0.326	0.356	−3.27	0.045	−0.067	0.261	0.300	0.407	−2.89	0.041	−0.041	0.198
9	Xylose	0.463	0.068	−2.36	0.030	−0.349	0.900	0.468	0.060	−2.46	0.031	−0.359	0.925	0.429	0.130	−1.90	0.025	−0.302	0.825
10	Mannose	0.347	0.310	−3.18	0.044	−0.112	0.351	0.350	0.303	−3.19	0.044	−0.119	0.380	0.318	0.365	−2.79	0.039	−0.078	0.292
11	Galactosamine	0.031	1.572	−1.47	0.038	0.644	−2.466	0.028	1.588	−0.94	0.032	0.654	−2.492	0.032	1.547	−1.26	0.035	0.605	−2.350
12	Sucrose	0.247	0.581	−4.06	0.058	0.105	−0.264	0.246	0.578	−3.96	0.057	0.107	−0.235	0.308	0.394	−2.95	0.042	−0.062	0.231
13	Maltose	0.217	0.672	−4.13	0.060	0.177	−0.470	0.222	0.670	−4.47	0.064	0.160	−0.443	0.220	0.665	−4.16	0.060	0.132	−0.394

		Corn						Castor						Margarine					
		mR_F	mR_M	R_{M0}	b	$PC1/R_F$	$PC1/R_M$	mR_F	mR_M	R_{M0}	b	$PC1/R_F$	$PC1/R_M$	mR_F	mR_M	R_{M0}	b	$PC1/R_F$	$PC1/R_M$
1	Arabitol	0.314	0.374	−2.84	0.040	−0.061	0.265	0.327	0.351	−3.08	0.043	−0.071	0.289	0.391	0.216	−3.08	0.041	−0.203	0.501
2	Xylitol	0.306	0.390	−2.79	0.040	−0.044	0.230	0.325	0.355	−3.07	0.043	−0.066	0.278	0.391	0.219	−3.14	0.042	−0.203	0.492
3	Adonitol	0.350	0.292	−2.76	0.038	−0.141	0.448	0.370	0.258	−3.06	0.041	−0.165	0.497	0.372	0.243	−2.28	0.032	−0.146	0.465
4	Manitol	0.256	0.538	−3.66	0.053	0.054	−0.102	0.251	0.542	−3.37	0.049	0.097	−0.144	0.258	0.506	−2.73	0.040	0.104	−0.141
5	Sorbitol	0.254	0.542	−3.59	0.052	0.059	−0.111	0.251	0.547	−3.53	0.051	0.094	−0.158	0.259	0.507	−2.80	0.041	0.101	−0.146
6	Galactose	0.283	0.460	−3.36	0.048	−0.004	0.074	0.292	0.445	−3.46	0.049	0.003	0.068	0.265	0.483	−2.59	0.038	0.089	−0.081
7	Fructose	0.329	0.344	−3.04	0.042	−0.100	0.332	0.329	0.345	−3.08	0.043	−0.076	0.303	0.355	0.281	−2.52	0.035	−0.113	0.371
8	Glucose	0.308	0.398	−3.34	0.047	−0.061	0.212	0.317	0.381	−3.33	0.046	−0.052	0.212	0.332	0.338	−2.90	0.040	−0.066	0.233
9	Xylose	0.435	0.121	−2.60	0.034	−0.319	0.831	0.443	0.109	−2.53	0.033	−0.308	0.834	0.462	0.069	−1.99	0.026	−0.340	0.860
10	Mannose	0.327	0.351	−3.19	0.044	−0.101	0.318	0.381	0.256	−4.27	0.057	−0.218	0.487	0.358	0.280	−2.77	0.038	−0.123	0.368
11	Galactosamine	0.039	1.459	−1.31	0.035	0.602	−2.161	0.046	1.415	−2.17	0.045	0.607	−2.093	0.055	1.339	−2.43	0.047	0.584	−2.005
12	Sucrose	0.259	0.539	−3.90	0.055	0.039	−0.102	0.279	0.529	−4.81	0.067	0.011	−0.139	0.239	0.583	−3.55	0.052	0.138	−0.330
13	Maltose	0.241	0.598	−4.09	0.059	0.077	−0.233	0.227	0.662	−4.51	0.065	0.144	−0.436	0.219	0.685	−4.45	0.064	0.179	−0.586

TABLE 4 The Lipophilicity Indices of Natural Sweeteners Obtained on Butter, Cod, Human, Pig, Sheep and Pullet Fat-Impregnated TLC Plates

		Butter						Cod						Human					
No.	Compound	mR_F	mR_M	R_{M0}	b	$PC1/R_F$	$PC1/R_M$	mR_F	mR_M	R_{M0}	b	$PC1/R_F$	$PC1/R_M$	mR_F	mR_M	R_{M0}	b	$PC1/R_F$	$PC1/R_M$
1	Arabitol	0.353	0.290	−2.91	0.040	−0.089	0.284	0.393	0.205	−2.75	0.037	−0.083	0.231	0.279	0.437	−2.14	0.032	−0.022	0.197
2	Xylitol	0.354	0.290	−2.97	0.041	−0.091	0.284	0.396	0.201	−2.78	0.037	−0.088	0.240	0.297	0.401	−2.30	0.034	−0.064	0.274
3	Adonitol	0.428	0.141	−3.15	0.041	−0.259	0.618	0.443	0.109	−2.83	0.037	−0.193	0.422	0.367	0.252	−2.16	0.030	−0.217	0.608
4	Manitol	0.280	0.464	−3.21	0.046	0.072	−0.105	0.333	0.334	−2.87	0.040	0.050	−0.034	0.230	0.573	−2.54	0.039	0.087	−0.117
5	Sorbitol	0.279	0.471	−3.28	0.047	0.075	−0.119	0.350	0.311	−3.86	0.052	−0.006	0.054	0.226	0.587	−2.67	0.041	0.094	−0.154
6	Galactose	0.314	0.380	−3.06	0.043	−0.003	0.083	0.393	0.208	−3.54	0.047	−0.098	0.244	0.249	0.514	−2.30	0.035	0.046	0.015
7	Fructose	0.363	0.266	−2.69	0.037	−0.106	0.335	0.417	0.160	−2.69	0.036	−0.133	0.326	0.311	0.370	−2.36	0.034	−0.096	0.341
8	Glucose	0.339	0.324	−3.01	0.042	−0.057	0.207	0.385	0.223	−2.84	0.038	−0.067	0.203	0.305	0.392	−2.81	0.040	−0.089	0.279
9	Xylose	0.477	0.044	−2.25	0.029	−0.343	0.830	0.522	−0.039	−2.18	0.027	−0.349	0.717	0.427	0.132	−1.73	0.023	−0.343	0.890
10	Mannose	0.365	0.264	−2.78	0.033	−0.112	0.340	0.403	0.184	−2.55	0.032	−0.101	0.269	0.305	0.388	−2.60	0.037	−0.086	0.295
11	Galactosamine	0.046	1.350	−0.71	0.026	0.642	−2.091	0.049	1.151	−0.69	0.025	0.727	−2.052	0.048	1.398	−2.23	0.045	0.516	−1.964
12	Sucrose	0.267	0.517	−3.77	0.054	0.097	−0.221	0.304	0.403	−3.14	0.044	0.109	−0.168	0.238	0.597	−3.85	0.056	0.056	−0.215
13	Maltose	0.233	0.619	−4.00	0.058	0.174	−0.447	0.251	0.531	−2.99	0.044	0.232	−0.452	0.211	0.695	−4.24	0.062	0.118	−0.448

		Pig						Sheep						Pullet					
		mR_F	mR_M	R_{M0}	b	$PC1/R_F$	$PC1/R_M$	mR_F	mR_M	R_{M0}	b	$PC1/R_F$	$PC1/R_M$	mR_F	mR_M	R_{M0}	b	$PC1/R_F$	$PC1/R_M$
1	Arabitol	0.352	0.279	−1.87	0.027	−0.102	0.415	0.208	0.608	−1.72	0.029	−0.036	0.258	0.340	0.313	−2.55	0.036	−0.080	0.274
2	Xylitol	0.341	0.305	−2.21	0.031	−0.084	0.353	0.212	0.602	−1.90	0.031	−0.047	0.272	0.344	0.302	−2.40	0.034	−0.086	0.299
3	Adonitol	0.383	0.225	−2.44	0.033	−0.180	0.530	0.231	0.544	−1.52	0.026	−0.084	0.403	0.392	0.202	−2.26	0.031	−0.191	0.521
4	Manitol	0.267	0.487	−2.85	0.042	0.077	−0.063	0.144	0.825	−2.03	0.036	0.108	−0.226	0.275	0.462	−2.69	0.039	0.066	−0.061
5	Sorbitol	0.258	0.523	−3.27	0.047	0.093	−0.149	0.143	0.833	−2.17	0.037	0.109	−0.243	0.264	0.498	−3.02	0.044	0.086	−0.142
6	Galactose	0.299	0.408	−2.83	0.040	0.002	0.114	0.174	0.714	−1.82	0.032	0.042	0.023	0.303	0.402	−2.87	0.041	−0.000	0.073
7	Fructose	0.357	0.274	−2.28	0.032	−0.119	0.421	0.213	0.592	−1.57	0.027	−0.044	0.295	0.358	0.272	−2.31	0.032	−0.115	0.364
8	Glucose	0.332	0.331	−2.59	0.037	−0.068	0.290	0.228	0.577	−2.55	0.039	−0.095	0.328	0.329	0.343	−2.89	0.040	−0.061	0.206
9	Xylose	0.475	0.045	−1.82	0.023	−0.373	0.940	0.346	0.290	−1.80	0.026	−0.344	0.970	0.465	0.065	−2.08	0.027	−0.345	0.829
10	Mannose	0.356	0.279	−2.50	0.035	−0.121	0.408	0.241	0.541	−2.44	0.037	−0.122	0.411	0.364	0.259	−2.30	0.032	−0.128	0.393
11	Galactosamine	0.026	1.634	−1.00	0.033	0.647	−2.616	0.024	1.637	−0.17	0.023	0.400	−2.044	0.039	1.428	−0.70	0.027	0.628	−2.220
12	Sucrose	0.257	0.570	−4.39	0.062	0.086	−0.269	0.176	0.766	−3.35	0.051	0.018	−0.093	0.267	0.505	−3.43	0.049	0.075	−0.158
13	Maltose	0.234	0.620	−4.09	0.059	0.142	−0.375	0.145	0.883	−3.42	0.054	0.094	−0.354	0.232	0.604	−3.63	0.053	0.152	−0.379

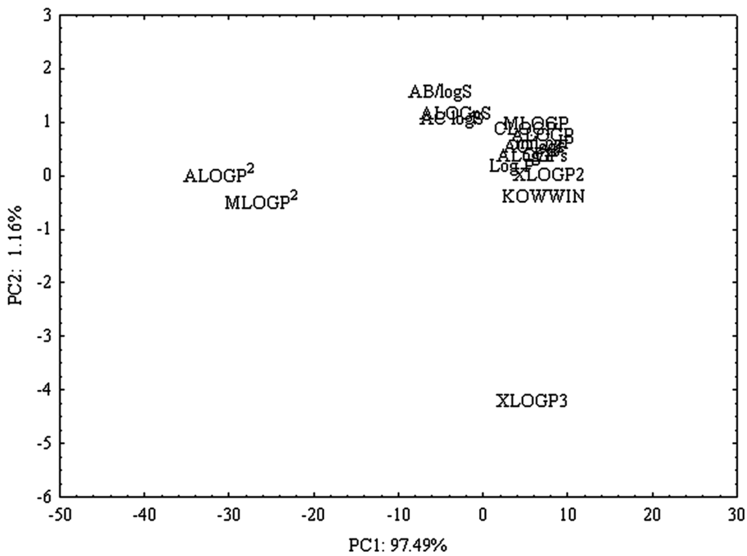


FIGURE 1 Loadings scatterplot corresponding to PC1 and PC2 obtained for the calculated log P and log S values.

based on associative neural networks method,[31] seems to cover, in the most efficient way, the lipophilic character of the studied compounds.

The higher correlations were obtained for the lipophilicity indices estimated on paraffin oil impregnated plates. The vegetable oils are highly similar, except for sunflower oil, which had a relative level of failure in terms of lipophilicity descriptors, while the olive oil lead to a high association level. Moreover, the pig and human fats seem to present higher similarities than the rest of animal fats. The Ghose-Crippen (ALOGP) and Moriguchi (MLOGP) algorithms and their squared values ($ALOGP^2$, $MLOGP^2$) near by the ALOGPs and AC logP offered a fair description of the lipophilicity in the context of human fat. In addition, the log S values presented some significant correlations, especially for the $R_{M0,Bu}$ vs. ALOGpS and $R_{M0,Hu}$ vs. AB/LogS ($r = 0.88$); lower correlations were obtained for experimental solubility and the TLC lipophilicity indices. On the other hand, comparing the experimental indices, it may be appreciated that the best correlations were obtained for the classical R_{M0} value, and b (regression parameters).

Concerning the similarities and differences of TLC-layers, it is easy to observe (Figure 2) that all the impregnation fats are highly associated, except for the sheep fat, which seems to be the most lipophilic layer. At the other pole is found the code liver oil. Moreover, the mR_F, mR_M, $PC1/R_F$ and $PC1/R_M$ patterns illustrate high regularities and show also the extreme behavior of sheep fat and code liver oil.

TABLE 5 The Correlations between the Theoretical and Experimental Lipophilicity Indices of Natural Sweeteners (Plates Impregnated with Paraffin Oil, Vegetable Oils and Margarine)

Stationary Phase	Index	Log P^C	Log P^V	CLOGP	MLOGP	$MLOGP^2$	ALOGP	$ALOGP^2$	ALOGPs	AC logP	miLogP	KOWWIN	XLOGP2	XLOGP3	S_{Exp}	ALOGpS	AC logS	AB/logS
Paraffin oil	mR_F	**0.81**	0.75	0.45	0.68	−0.64	0.77	−0.70	**0.87**	**0.81**	**0.83**	0.46	0.66	0.23	−0.36	0.75	−0.70	0.57
	mR_M	**-0.86**	−0.79	−0.53	−0.74	0.70	**-0.82**	0.77	**−0.91**	**−0.86**	**−0.87**	−0.54	−0.68	−0.28	0.41	−0.78	0.72	−0.63
	R_{M0}	**0.91**	**0.82**	0.70	**0.86**	**−0.83**	**0.90**	**−0.86**	**0.95**	**0.93**	**0.89**	0.71	0.65	0.38	−0.51	0.75	−0.66	0.76
	b	**−0.91**	**−0.82**	−0.66	**−0.84**	**0.81**	**−0.89**	**0.85**	**−0.96**	**−0.92**	**−0.90**	−0.68	−0.66	−0.36	0.49	−0.77	0.68	−0.74
	$PC1/R_F$	**−0.81**	−0.75	−0.44	−0.68	0.63	−0.76	0.70	**−0.87**	**−0.80**	**−0.83**	−0.46	−0.66	−0.23	0.35	−0.75	0.70	−0.56
	$PC1/R_M$	**0.86**	0.79	0.53	0.74	−0.71	**0.82**	−0.77	**0.91**	**0.86**	**0.87**	0.54	0.68	0.28	−0.41	0.78	−0.72	0.63
Olive oil	mR_F	**0.83**	**0.80**	0.38	0.63	−0.59	0.76	−0.69	**0.88**	**0.80**	**0.84**	0.46	0.74	0.28	−0.29	**0.80**	−0.76	0.49
	mR_M	**−0.86**	**−0.83**	−0.44	−0.68	0.64	**−0.80**	0.74	**−0.91**	**−0.84**	**−0.87**	−0.52	−0.75	−0.31	0.32	**−0.82**	0.78	−0.53
	R_{M0}	**0.89**	**0.82**	0.58	0.78	−0.75	**0.86**	**−0.81**	**0.95**	**0.89**	**0.89**	0.61	0.69	0.32	−0.39	0.78	−0.72	0.66
	b	**−0.89**	**−0.83**	−0.55	−0.76	0.73	**−0.85**	0.79	**−0.95**	**−0.89**	**−0.89**	−0.59	−0.71	−0.32	0.37	**−0.80**	0.74	−0.63
	$PC1/R_F$	**−0.83**	**−0.80**	−0.38	−0.63	0.60	−0.76	0.69	**−0.88**	**−0.80**	**−0.84**	−0.47	−0.74	−0.28	0.29	**−0.80**	0.77	−0.49
	$PC1/R_M$	**0.87**	**0.83**	0.44	0.68	−0.65	**0.80**	−0.74	**0.91**	**0.84**	**0.87**	0.52	0.75	0.31	−0.32	**0.82**	−0.77	0.53
	mR_F	0.51	0.54	0.04	0.29	−0.23	0.41	−0.32	0.63	0.47	0.55	0.12	0.52	0.09	0.07	0.55	−0.55	0.18
Sunflower oil	mR_M	−0.53	−0.57	−0.03	−0.29	0.23	−0.42	0.33	−0.66	−0.48	−0.56	−0.15	−0.55	−0.14	−0.10	−0.56	0.57	−0.16
	R_{M0}	0.62	0.70	0.03	0.31	−0.26	0.48	−0.39	0.73	0.56	0.62	0.25	0.67	0.27	0.02	0.66	−0.66	0.16
	b	−0.61	−0.69	−0.03	−0.31	0.26	−0.48	0.38	−0.73	−0.55	−0.62	−0.23	−0.66	−0.24	−0.04	−0.65	0.66	−0.16
	$PC1/R_F$	−0.49	−0.52	−0.03	−0.28	0.22	−0.39	0.30	−0.62	−0.45	−0.53	−0.10	−0.50	−0.09	−0.09	−0.53	0.53	−0.17
	$PC1/R_M$	0.53	0.57	0.03	0.29	−0.22	0.42	−0.32	0.66	0.48	0.56	0.15	0.55	0.14	0.11	0.56	−0.57	0.16
Corn oil	mR_F	0.76	0.76	0.25	0.52	−0.48	0.67	−0.59	**0.82**	0.72	0.77	0.36	0.72	0.25	−0.19	0.77	−0.75	0.38
	mR_M	**−0.80**	−0.79	−0.31	−0.57	0.53	−0.71	0.64	**−0.86**	−0.76	**−0.81**	−0.43	−0.74	−0.28	0.21	−0.79	0.76	−0.42
	R_{M0}	**0.83**	0.75	0.63	0.79	−0.75	**0.82**	−0.77	**0.93**	**0.85**	**0.83**	0.62	0.57	0.30	−0.38	0.68	−0.60	0.69
	b	**−0.84**	−0.77	−0.57	−0.76	0.71	**−0.81**	0.76	**−0.93**	**−0.85**	**−0.85**	−0.59	−0.62	−0.31	0.35	−0.72	0.65	−0.64
	$PC1/R_F$	−0.75	−0.75	−0.22	−0.49	0.45	−0.65	0.57	**−0.80**	−0.70	−0.76	−0.34	−0.73	−0.25	0.17	−0.77	0.75	−0.35
	$PC1/R_M$	**0.80**	0.79	0.31	0.57	−0.53	0.71	−0.64	**0.86**	0.76	**0.81**	0.43	0.74	0.28	−0.21	0.79	−0.76	0.42
Castor oil	mR_F	0.69	0.69	0.18	0.45	−0.41	0.61	−0.53	0.75	0.64	0.73	0.28	0.72	0.17	−0.11	0.75	−0.75	0.27
	mR_M	−0.78	−0.76	−0.31	−0.56	0.52	−0.70	0.63	**−0.83**	−0.74	**−0.80**	−0.39	−0.75	−0.23	0.20	−0.79	0.77	−0.38
	R_{M0}	0.78	0.66	0.75	**0.85**	**−0.83**	**0.82**	**−0.80**	**0.81**	**0.84**	0.75	0.68	0.42	0.33	−0.64	0.57	−0.46	**0.85**

(*Continued*)

TABLE 5 Continued

Stationary Phase	Index	Log P^C	Log P^V	CLOGP	MLOGP	$MLOGP^2$	ALOGP	$ALOGP^2$	ALOGPs	AC logP	miLogP	KOWWIN	XLOGP2	XLOGP3	S_{Exp}	ALOGpS	AC logS	AB/logS
	b	**−0.85**	−0.73	−0.73	**−0.86**	**0.84**	**−0.86**	**0.84**	**−0.88**	**−0.89**	**−0.83**	−0.68	−0.52	−0.34	0.61	−0.66	0.56	**−0.83**
	$PC1/R_F$	−0.65	−0.66	−0.13	−0.39	0.35	−0.56	0.48	−0.70	−0.59	−0.69	−0.24	−0.70	−0.15	0.05	−0.72	0.73	−0.21
	$PC1/R_M$	0.79	0.76	0.33	0.58	−0.54	0.72	−0.65	**0.84**	0.75	**0.81**	0.41	0.75	0.24	−0.21	0.79	−0.77	0.41
Margarine	mR_F	0.78	0.73	0.47	0.68	−0.63	0.74	−0.68	**0.88**	0.78	**0.80**	0.50	0.61	0.26	−0.29	0.69	−0.64	0.56
	mR_M	**−0.82**	−0.76	−0.52	−0.72	0.68	−0.79	0.73	**−0.90**	**−0.82**	**−0.83**	−0.55	−0.64	−0.29	0.33	−0.72	0.66	−0.60
	R_{M0}	0.73	0.66	0.45	0.62	−0.63	0.71	−0.69	0.66	0.74	0.71	0.49	0.60	0.30	−0.55	0.69	−0.63	0.57
	b	**−0.84**	−0.77	−0.52	−0.72	0.71	**−0.81**	0.78	**−0.81**	**−0.84**	**−0.82**	−0.56	−0.68	−0.33	0.55	−0.77	0.71	−0.64
	$PC1/R_F$	−0.77	−0.72	−0.47	−0.67	0.62	−0.73	0.67	**−0.87**	−0.77	−0.79	−0.50	−0.60	−0.26	0.28	−0.68	0.63	−0.55
	$PC1/R_M$	**0.83**	0.77	0.53	0.73	−0.68	**0.80**	−0.74	**0.91**	0.83	**0.84**	0.56	0.65	0.30	−0.34	0.73	−0.67	0.60

TABLE 6 The Correlations between the Theoretical and Experimental Lipophilicity Indices of Natural Sweeteners (Plates Impregnated with Butter, Animal and Human Fat)

Stationary Phase	Index	Log P^C	Log P^V	CLOGP	MLOGP	MLOGP^2	ALOGP	ALOGP^2	ALOGPs	AC logP	miLogP	KOWWIN	XLOGP2	XLOGP3	S_{Exp}	ALOGpS	AC logS	AB/LogS
Butter	mR_F	0.78	0.74	0.39	0.62	−0.58	0.73	−0.66	**0.85**	0.77	**0.80**	0.44	0.67	0.24	−0.24	0.74	−0.70	0.49
	mR_M	**−0.83**	−0.78	−0.44	−0.67	0.63	−0.77	0.71	**−0.89**	**−0.81**	**−0.84**	−0.50	−0.70	−0.28	0.28	−0.77	0.73	−0.53
	R_{M0}	**0.93**	**0.89**	0.49	0.71	−0.71	**0.87**	**−0.82**	**0.89**	**0.91**	**0.89**	0.63	**0.83**	0.43	−0.57	**0.88**	**−0.83**	0.59
	b	0.08	0.06	−0.06	−0.02	−0.01	0.08	−0.09	−0.03	0.03	0.12	−0.05	0.26	−0.07	−0.07	0.23	−0.27	−0.15
	$PC1/R_F$	−0.78	−0.73	−0.40	−0.62	0.58	−0.72	0.66	**−0.85**	−0.76	**−0.80**	−0.44	−0.66	−0.23	0.23	−0.73	0.69	−0.49
	$PC1/R_M$	**0.83**	0.78	0.44	0.67	−0.63	0.77	−0.71	**0.88**	**0.81**	**0.84**	0.50	0.70	0.28	−0.28	0.77	−0.73	0.53
Cod liver oil	mR_F	**0.87**	**0.82**	0.42	0.67	−0.64	**0.81**	−0.74	**0.89**	**0.84**	**0.88**	0.49	0.77	0.29	−0.36	**0.84**	**−0.80**	0.53
	mR_M	**−0.89**	**−0.84**	−0.45	−0.70	0.67	**−0.83**	0.77	**−0.91**	**−0.87**	**−0.90**	−0.53	−0.78	−0.31	0.37	**−0.86**	**0.81**	−0.55
	R_{M0}	0.53	0.57	0.13	0.32	−0.29	0.44	−0.37	0.61	0.49	0.52	0.28	0.51	0.25	−0.15	0.51	−0.50	0.22
	b	0.09	0.06	−0.05	−0.02	−0.01	0.08	−0.10	−0.03	0.04	0.13	−0.04	0.27	−0.07	−0.08	0.23	−0.27	−0.15
	$PC1/R_F$	**−0.86**	**−0.82**	−0.42	−0.67	0.64	**−0.80**	0.74	**−0.89**	**−0.84**	**−0.87**	−0.49	−0.77	−0.29	0.35	**−0.84**	**0.80**	−0.53
	$PC1/R_M$	**0.89**	**0.84**	0.46	0.70	−0.67	**0.83**	−0.77	**0.91**	**0.87**	**0.90**	0.53	0.78	0.30	−0.38	**0.86**	**−0.81**	0.55
Pig fat	mR_F	**0.80**	0.79	0.34	0.60	−0.55	0.73	−0.66	**0.87**	0.77	**0.82**	0.43	0.73	0.27	−0.24	0.79	−0.75	0.45
	mR_M	**−0.87**	**−0.83**	−0.45	−0.69	0.65	**−0.81**	0.75	**−0.92**	**−0.85**	**−0.88**	−0.53	−0.76	−0.32	0.33	**−0.82**	0.78	−0.54
	R_{M0}	**0.92**	0.79	0.78	**0.91**	**−0.90**	**0.94**	**−0.92**	**0.92**	**0.95**	**0.91**	0.76	0.64	0.37	−0.66	0.76	−0.67	**0.81**
	b	**−0.93**	**−0.82**	−0.74	**−0.89**	**0.87**	**−0.94**	**0.91**	**−0.94**	**−0.95**	**−0.92**	−0.73	−0.67	−0.36	0.62	−0.79	0.70	−0.78
	$PC1/R_F$	**−0.80**	−0.78	−0.32	−0.58	0.54	−0.72	0.64	**−0.86**	−0.76	**−0.81**	−0.42	−0.73	−0.27	0.22	−0.78	0.76	−0.43
	$PC1/R_M$	**0.88**	**0.83**	0.46	0.70	−0.66	**0.82**	−0.76	**0.92**	**0.85**	**0.88**	0.54	0.76	0.32	−0.34	**0.83**	−0.78	0.55
Sheep fat	mR_F	0.67	0.68	0.10	0.39	−0.35	0.57	−0.49	0.72	0.61	0.71	0.20	0.73	0.14	−0.06	0.76	−0.77	0.22
	mR_M	−0.75	−0.76	−0.21	−0.49	0.45	−0.66	0.58	**−0.80**	−0.70	−0.78	−0.33	−0.77	−0.22	0.11	**−0.80**	0.79	−0.31
	R_{M0}	0.76	0.65	**0.83**	**0.86**	**−0.85**	**0.80**	**−0.80**	0.78	**0.82**	0.69	**0.83**	0.36	0.47	−0.73	0.48	−0.35	**0.87**
	b	**−0.86**	−0.77	−0.79	**−0.88**	**0.87**	**−0.88**	**0.86**	**−0.90**	**−0.91**	**−0.81**	**−0.81**	−0.52	−0.47	0.67	−0.63	0.51	**−0.84**
	$PC1/R_F$	−0.64	−0.65	−0.06	−0.35	0.31	−0.53	0.45	−0.68	−0.57	−0.68	−0.16	−0.72	−0.11	0.01	−0.74	0.76	−0.18
	$PC1/R_M$	0.75	0.75	0.21	0.48	−0.44	0.65	−0.58	**0.80**	0.70	0.78	0.33	0.77	0.22	−0.11	**0.80**	−0.79	0.30
Pullet fat	mR_F	0.79	0.77	0.33	0.58	−0.54	0.71	−0.64	**0.85**	0.76	**0.80**	0.42	0.72	0.27	−0.23	0.77	−0.74	0.44
	mR_M	**−0.82**	**−0.80**	−0.38	−0.62	0.58	−0.75	0.68	**−0.88**	−0.79	**−0.83**	−0.48	−0.73	−0.30	0.27	−0.78	0.75	−0.48
	R_{M0}	**0.85**	0.78	0.64	0.78	−0.77	**0.83**	**−0.80**	**0.88**	**0.86**	**0.81**	0.70	0.60	0.42	−0.60	0.68	−0.60	0.71
	b	**−0.86**	**−0.80**	−0.59	−0.76	0.74	**−0.83**	0.79	**−0.90**	**−0.86**	**−0.83**	−0.66	−0.64	−0.40	0.53	−0.72	0.65	−0.67
	$PC1/R_F$	−0.78	−0.77	−0.32	−0.57	0.53	−0.71	0.63	**−0.85**	−0.75	**−0.80**	−0.41	−0.72	−0.26	0.22	−0.77	0.74	−0.43
	$PC1/R_M$	**0.82**	**0.80**	0.38	0.62	−0.59	0.75	−0.68	**0.88**	0.79	**0.83**	0.48	0.73	0.30	−0.28	0.78	−0.75	0.48

(*Continued*)

TABLE 6 Continued

Stationary Phase	Index	Log P^C	Log P^V	CLOGP	MLOGP	$MLOGP^2$	ALOGP	$ALOGP^2$	ALOGPs	AC logP	miLogP	KOWWIN	XLOGP2	XLOGP3	S_{Exp}	ALOGpS	AC logS	AB/LogS
Human fat	mR_F	0.71	0.71	0.25	0.50	−0.46	0.63	−0.56	0.78	0.68	0.73	0.34	0.66	0.22	−0.12	0.71	−0.69	0.37
	mR_M	−0.78	−0.76	−0.35	−0.59	0.55	−0.71	0.65	**−0.84**	−0.76	−0.79	−0.44	−0.70	−0.27	0.20	−0.76	0.72	−0.45
	R_{M0}	**0.88**	0.71	**0.81**	**0.93**	**−0.92**	**0.93**	**−0.92**	**0.86**	**0.93**	**0.89**	0.69	0.56	0.27	−0.78	0.72	−0.62	**0.88**
	b	**−0.91**	−0.77	−0.76	**−0.91**	**0.89**	**−0.94**	**0.91**	**−0.91**	**−0.95**	**−0.92**	−0.67	−0.62	−0.28	0.70	−0.77	0.68	**−0.83**
	$PC1/R_F$	−0.70	−0.70	−0.23	−0.48	0.44	−0.61	0.54	−0.77	−0.66	−0.71	−0.33	−0.66	−0.22	0.09	−0.70	0.68	−0.35
	$PC1/R_M$	**0.80**	0.77	0.38	0.62	−0.58	0.74	−0.67	**0.86**	0.78	**0.81**	0.46	0.70	0.28	−0.23	0.77	−0.73	0.48

In order to get more information concerning the similarities and differences between the oil and fat layers, PCA was applied to the matrices resulted by considering each of the six experimental lipophilicity indices (Figure 3). According to the 3D representations, the human fat

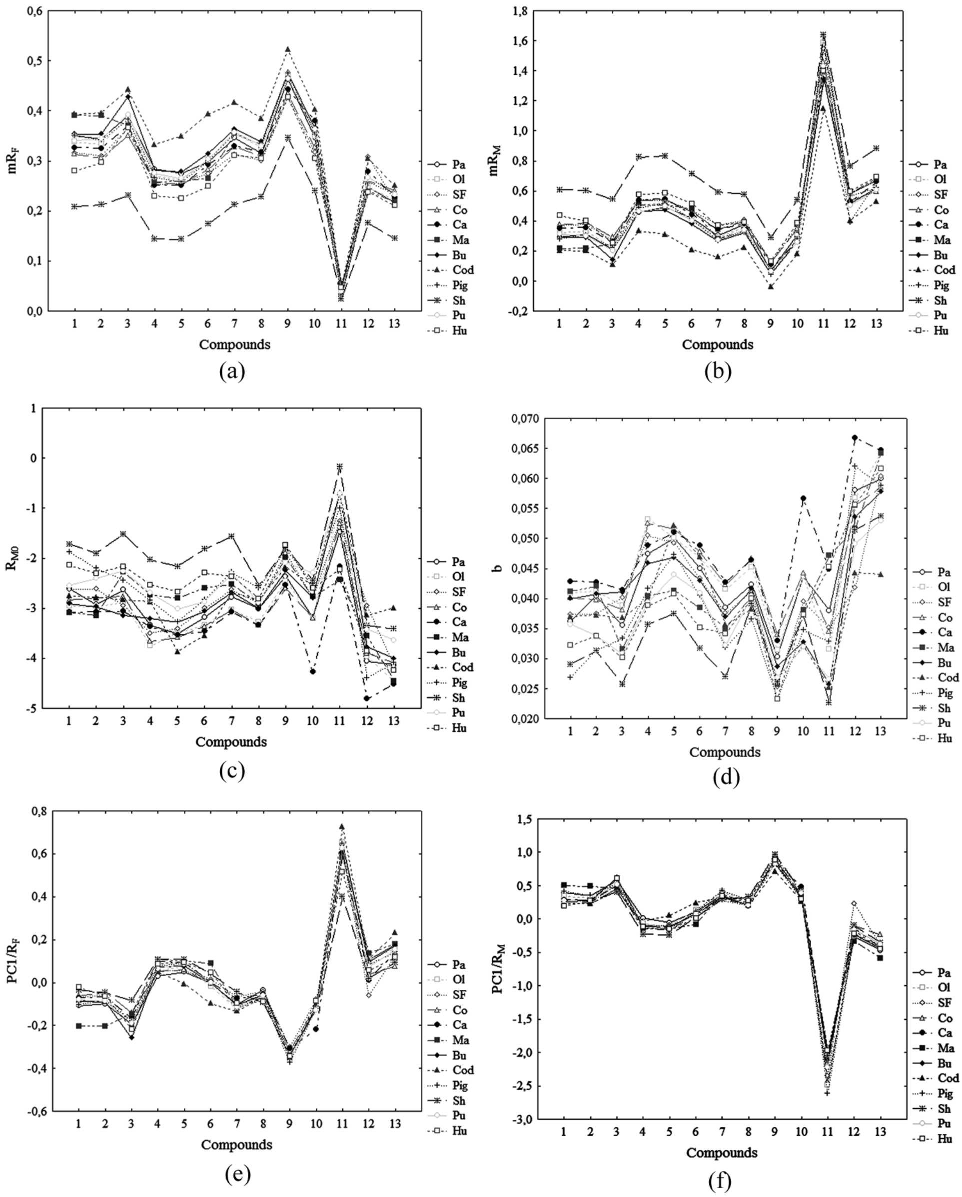


FIGURE 2 The correlation patterns of mR_F (a), mR_M (b), R_{M0} (c), b (d), $PC1/R_F$ (e), and $PC1/R_M$ (f) corresponding to the investigated reverse stationary phases.

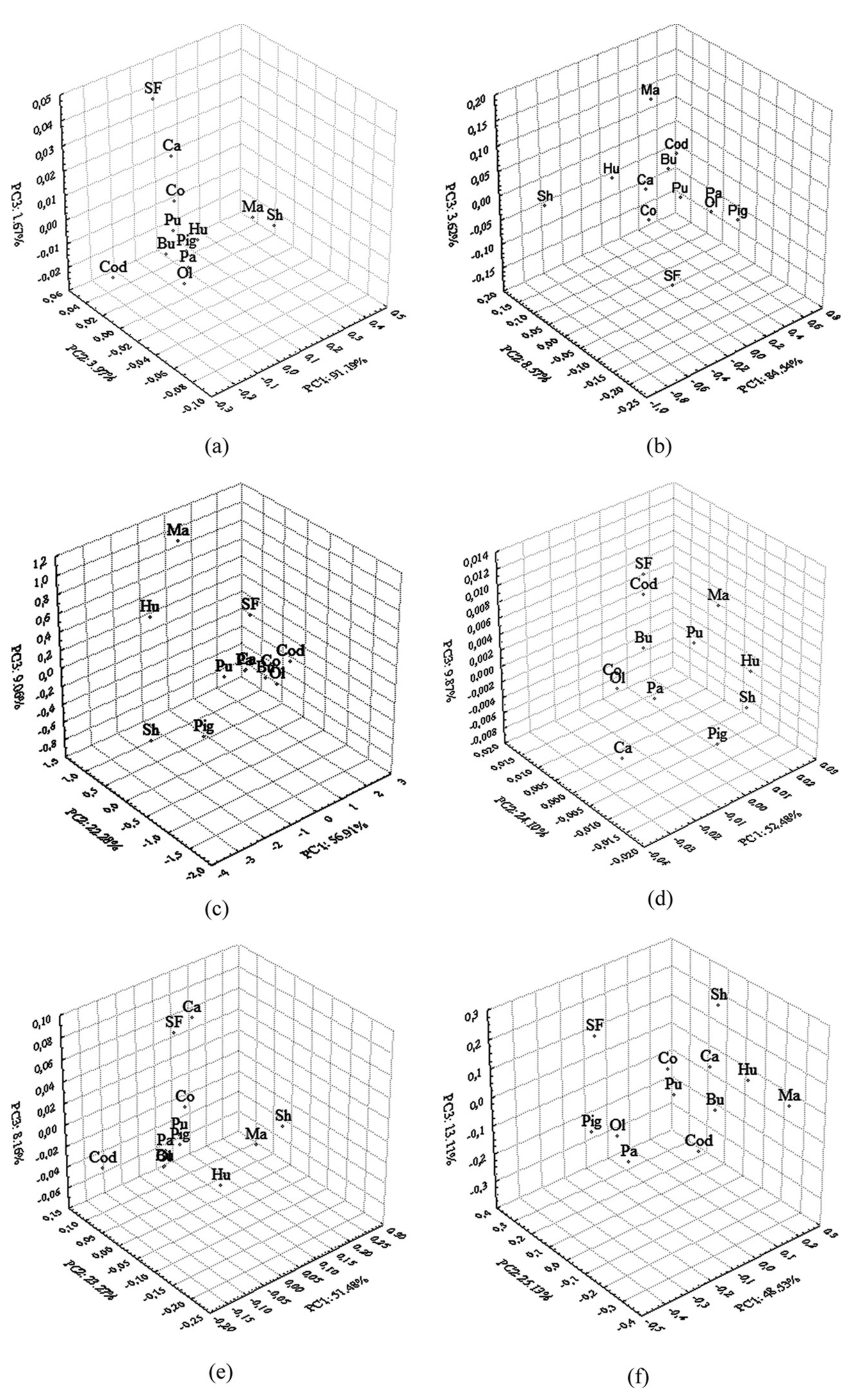
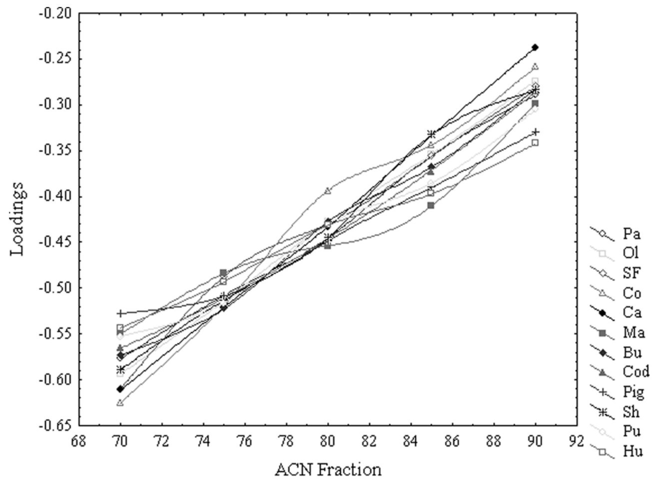


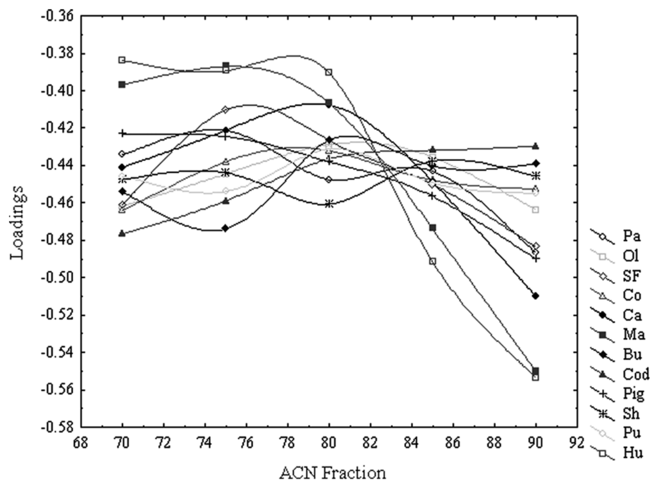
FIGURE 3 The "lipophilicity spaces" obtained by PC1-PC2-PC3 score plot obtained on the matrices formed by the TLC lipophilicity indices estimated on all investigated reverse stationary phases: mR_F (a); mR_M (b); R_{M0} (c); b (d); $PC1/R_F$ (e); $PC1/R_M$ (f).

lipophilicity appears in the group of outliers including sheep and pig fat, margarine, and sunflower oil. The sunflower and castor plant oil are the less lipophilic oils, closely followed by the corn and olive, while the cod liver oil is confirmed as the less lipophilic animal fat.

Moreover, the PCA might be used for investigating the retention mechanism involved in the chromatographic process by examination of the profile of loadings/eigenvectors corresponding to the first principal component. The profiles of loadings presented in Figure 4 illustrate once again the similarity and differences between the investigated reversed



(a)



(b)

FIGURE 4 Profiles of loadings corresponding to the first principal component obtained by applying PCA to R_F values (a) and R_M values (b) obtained using spline function.

phases, and confirm the above statements. The profiles are more or less similar and one may conclude that the main retention mechanism (lipophilic interactions) is more or less the same; a highest similarity may be easily observed in the case of human fat and margarine.

CONCLUSIONS

The results obtained and discussed in this paper indicate no significant differences between oil and fat impregnated TLC-silica gel plates and recommend them as an alternative in the field of lipophilicity estimation. This conclusion is more evident illustrated by the correlation between the theoretical lipophilicity descriptors and the lipophilicity indices estimated from retention data. However, the chromatographic behavior is weakly corelated with the theoretical and experimental solubility. From the tested lipophilicity indices, the mean of R_M values showed, in all cases, the best regularities and significant correlations and might be one of the most attractive alternative. In addition, the PCA offered a realistic characterization and ranking of impregnation materials, both from the lipophilicity and retention mechanism point of view.

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