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Evaluation of PCB's chromatographic retention indices using multilinear regression method

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The multilinear regression method for polychlorinated biphenyls (PCBs) chromatographic retention indices evaluation was applied. Nine reference PCB's chromatographic retention indices (R) were evaluated using 8 calculated molecular properties (descriptors): molecular volume, molecular weight, partition coefficient (logP), van der Waals and solvent accessible surface, dipole moment, and frontier orbital energies. The best equations were selected via the highest value of the F quality index and the most efficient combinations of descriptors. As expected, the van der Waals surface descriptor appears frequently in the best quality equations. In the discussed equations, the logP descriptor, correlated with the lipophilicity and the reactivity indices of ε_{HOMO} and ε_{LUMO}, has the biggest weight.

Keywords: PCBs; chromatographic retention indices; multilinear regression method; molecular descriptors

INTRODUCTION

Although the production of polychlorobiphenils (PCBs) is forbidden now, the problems of their recurrence in the environmental components are an issue due to the partitioning, biotransformation and bioaccumulation [1–11] of these hazardous chemicals. In these processes, the PCB adsorption in different phases [1–3] is very important.

There are 209 PCB's congeners and their identification is a very difficult task. Such identification is possible trough determination of their retention times using the high resolution gas-chromotography [12–14].

The content of PCBs in transformers oil have been evaluated by GC–MS hyphenated method [15]. Now the chromatographic retention indices were evaluated using the multiple linear regression method (MLR).

We adhered to the following equation:

$$R = a_0 + \sum_{i=1}^{k} a_i x_i \qquad (1)$$

MLR attempts to model the correlation between the chromatographic retention index R and the independent variables x_i (descriptors), mediated by a_0 - a_i which are estimated regression parameters. Recently, B. Tiperciuc and C. Sarbu predicted the chromatographic retention indices (lipophilicity) of some new methyl thiazolil oxadiazoline derivatives using the MLR [16].

CALCULATION DETAILS

Chromatographic retention index values of the PCBs are taken from two literature sources [17, 18]. The molecular weight is considered as a descriptor of a special type because the toxicity and the irreversible absorption increase with the complexity of its structure [12–14]. The molecular properties of the PCBs, the grid (solvent accessible) surface (Sg), the approximate (van der Waals) surface (Sa), the molecular volume (V), the dipole moment (μ), the partition coefficient (logP), the and frontier orbital energies ($\varepsilon_{HOMO,}$ ε_{LUMO}) were calculated for structures, optimized with the AM1 method in the Restricted Hartree Fock (RHF) approximation *in vacuo,* using the HYPERCHEM software [19]. Minimum energy structures were obtained using the Root Mean Square (RMS) gradient of 0.01 kcal/mol·Å. Multilinear regression equations were derived trough the MATHCAD 7 software [20].

RESULTS and DISCUSSION

In our study, we considered as descriptors the properties on molecular level such as the molecular volume and weight. We also took into

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consideration the properties significant for the energy of the molecular interaction: the partition coefficient, van der Waals and solvent accessible surface, and some properties, related to the nuclear-electronic level such as the dipole moment and frontier orbital energies.

These descriptors can serve as a basis for the development of predictive models with improved accuracy and precision [21].

A set of 9 PCBs are included in this study: **1**(1), **8**(2), **31**(3), **44**(4), **101**(5), **138**(6), **180**(7), **203**(8) and **206**(9). The bold characters indicate the compound in accordance with IUPAC Convention and the number of the chlorine atoms is given in the brackets [13, 14, 17, 22]. In this series, the **PCB1** elutes first, and the **PCB206** elutes last on almost every stationary phase, tested as showed in a 2008 research report of the LECO Corporation [18]. We assumed that these nine PCBs are representative for the multilinear regression study for two reasons: (i) it is considered one PCB of each of the nine classes and (ii) these nine PCB's were proposed as reference compounds because they exhibit linear retention behavior on stationary phases [18]. For example, the regression of the PCB reference series (the retention time versus the chlorine atom number) demonstrates that the behavior is linear for the DB-XLB phase [12–14].

The CAS registry numbers, the retention indices (**RT1** and **RT2**), and the descriptor values, calculated as described in the calculation detail paragraph, are listed in Table 1. This table shows an increase in the property values and the number of the chlorine atoms in the PCB molecules.

Table 1. PCB CAS numbers, calculated molecular properties and chromatographic retention indices.

No.	**PCB** (Cl position)	CAS number	M (g/mol)	logP	ε_{HOMO} (eV)	ε_{LUMO} (eV)	Sg(Å^2)	Sa(Å^2)	V(Å^3)	μ(D)	RT 1	RT 2
	1 (2)	2051-60-7	188.66	4.25	9.5023	0.1206	377.27	302.9	589.26	1.160	364.49	2.036
	8 (2,4')	34883-43-7	223.1	4.77	-9.5698	-0.2036	401.05	339.32	631.79	1.402	568.09	2.885
	31 (25,4')	16606-02-3	257.55	5.29	-9.5645	-0.3201	425.68	376.22	675.33	1.043	767.41	4.04
	44 (23,2'5')	41464-39-5	326.44	5.8	-9.5582	-0.3265	438.46	390.02	706.13	1.880	874.29	4.655
	101 (245,2'5')	37680-73-2	291.99	6.32	-9.6378	-0.5953	465.35	428.94	749.93	1.102	1026.68	5.396
	138 (234,2'4'5')	35065-28-2	360.88	6.84	-9.7085	-0.6671	480	458.46	783.3	1.643	1270.29	6.677
	180 (2345,2'4'5')	35065-29-3	395.33	7.36	-9.7703	-0.8302	501.61	492.81	821.63	0.845	1414.49	7.412
	203 (23456,2'4'5')	52663-76-0	429.77	7.88	-9.7548	-0.9909	511.93	510.52	851.71	0.03	1494.29	7.763
	206 (23456,2'3'4'5'	40186-72-9	464.22	8.39	-9.8484	-1.0539	527.61	540.27	884.83	0.820	1669.89	8.642

Taking into account only the combinations with Sa or Sg, 183 equations were derived for each of the retention index series: 27 equations with 2 descriptors, 50 with 3 descriptors, 55 with 4 descriptors, 36 with 5 descriptors, 13 with 6 descriptors, and 2 with 7 descriptors. In tables 2 and 3, according to then F values, the best 10 equations with 2-6 descriptors were selected for each of the index series, and the best 2 equations with 7 descriptors were selected for each of the retention index series.

In practical terms, the MLR equations of Tables 2 and 3, were evaluated by values of correlation coefficient r^2, F factor, and p value(the equation significance level. The correlation coefficient r^2 is 0.999 for all equations. The F factor which is the measure of the regression relationship, was calculated with the formula: $F = \frac{MSR}{MSE}$, where MSR is mean square regression, and MSE is mean square error [24]. An examination of Tables 2 and 3 shows that the same combinations of 6 descriptors (M, logP, $E_{LUMO,}$ Sa, V, μ), 5 descriptors (M, logP, $E_{LUMO,}$ Sa, μ) and 3 descriptors ($E_{LUMO,}$ Sa, μ) give the biggest F value (see lines 12, 22 and 42 in the tables 2 and 3). The quality of the obtained equations was good, taking into consideration the r^2 and F values. Additionally, the calculated p values (data not shown) are very small for the high quality obtained equations. As expected, M, μ, Sa, and logP descriptors are the most frequently used descriptors in the best equations, with highest F factor. Even equations with 2 descriptors have highest F values when Sa and μ are used as descriptors.

Surely, the weight of a descriptor is determined by the value of the a_i coefficients. Thus, in Table 2, in the equations with 5, 6 and 7 descriptors, logP has the biggest weight almost always and the ε_{HOMO} descriptor has the second biggest weight. LogP has the biggest weight 4 times and ε_{LUMO} 5 times in the case of 4 descriptor equations. The biggest weight for the equations with 3 descriptors corresponds to ε_{LUMO} for half of the equations, and for 3 equations to μ, logP, and ε_{HOMO}. The biggest weight varies for the equations with 2 descriptors. We have similar comments about Table 3, and one may see that the M descriptor is never of the biggest weight.

Table 2. Multilinear regression equations, obtained using RT1 (r^2=0.999).

No.	Descriptors (X_i)	F	Coefficients (a_i)
	7 descriptors		
1	M, logP, E_{HOMO}, E_{LUMO}, Sg, V, μ	6.247E+4	-2.475E+4; -123.183; 7.236E+3; -894.756; 368.737; -23.36; 30.238; 39.314
2	M, logP, E_{HOMO}, E_{LUMO}, Sa, V, μ	1.265E+5	-1.207E+4; -124.437; 8.464E+3; 77.901; 146.13; 5.715; -1.952; 72.107
	6 descriptors		
3	logP, E_{HOMO}, E_{LUMO}, Sg, V, μ	1.919E+3	-1.986E+4; -1.932E+3; -1.38E+3; 445.058; -43.617; 53.861; -11.478
4	M, logP, E_{LUMO}, Sg, V, μ	2.057E+3	-1.86E+4; -185.356; 1.29E+4; 84.216; 10.622; -8.514; 85.615
5	M, logP, E_{HOMO}, Sg, V, μ	2.648E+3	-1.853E+4; -141.438; 9.493E+3; -363.543; -0.93; 3.453; 73.595
6	M, E_{HOMO}, E_{LUMO}, Sg, V, μ	3.101E+3	-2.222E+4; -28.453; -1.352E+3; 466.216; -43.289; 53.27; -3.421
7	M, logP, E_{HOMO}, E_{LUMO}, Sg, μ	4.219E+3	-2.09E+4; -165.311; 1.121E+4; -355.324; 169.036; 3.517; 73.036
8	M, logP, E_{HOMO}, E_{LUMO}, Sa, μ	4.372E+4	-1.464E+4; -131.66; 8.889E+3; -74.275; 176.453; 4.164; 69.082
9	M, logP, E_{HOMO}, E_{LUMO}, Sg, V	5.293E+3	-2.524E+4; -68.681; 2.798E+3; -1.283E+3; 522.517; -40.684; 50.528
10	M, logP, E_{HOMO}, E_{LUMO}, V, μ	5.51E+3	-2.143E+4; -158.192; 1.057E+4; -436.346; 206.675; 4.192; 67.217
11	M, logP, E_{HOMO}, Sa, V, μ	1.026E+4	-8.177E+3; -107.624; 7.423E+3; 244.702; 6.936; -4.376; 77.831
12	M, logP, E_{LUMO}, Sa, V, μ	9.087E+4	-1.328E+4; -127.564; 8.65E+3; 156.964; 5.041; -1.163; 71.097
	5 Descriptors		
13	M, logP, E_{LUMO}, Sg, μ	1.775E+3	-1.877E+4; -179.604; 1.221E+4; 119.102; 2.709; 78.422
14	logP, E_{HOMO}, E_{LUMO}, Sg, V	1.8E+3	-1.805E+4; -1.672E+3; -1.262E+3; 363.264; -37.918; 47.156
15	logP, E_{HOMO}, Sa, V, μ	1.844E+3	4.146E+3; 211.043; 439.95; 10.58; -6.387; 50.514
16	M, logP, Sg, V, μ	1.92E+3	-1.752E+4; -177.493; 1.244E+4; 11.573; -10.107; 88.477
17	M, logP, E_{HOMO}, Sg, μ	2.61E+3	-1.843E+4; -148.515; 1.01E+4; -308.293; 2.303; 76.921
18	M, logP, E_{HOMO}, V, μ	2.645E+3	-1.849E+4; -143.297; 9.654E+3; -348.053; 2.47; 74.479
19	M, E_{HOMO}, E_{LUMO}, Sg, V	3.063E+3	-2.169E+4; -27.514; -1.324E+3; 441.677; -41.958; 51.661
20	M, logP, E_{HOMO}, Sa, μ	5.033E+3	-1.349E+4; -118.896; 8.054E+3; -110.175; 3.019; 72.287
21	M, logP, Sa, V, μ	7.475E+3	-1.159E+4; -114.647; 7.832E+3; 4.759; -2.097; 75.648
22	M, logP, E_{LUMO}, Sa, μ	2.754E+4	-1.389E+4; -130.726; 8.822E+3; 182.972; 4.374; 68.106
	4 descriptors		
23	M, E_{LUMO}, Sa, μ	1.423E+3	-1.559E+3; -0.036; 117.365; 6.207; 32.731
24	logP, E_{LUMO}, Sa, μ	1.423E+3	-1.549E+3; 0.402; 115.411; 6.149; 32.804
25	E_{HOMO}, E_{LUMO}, Sa, μ	1.434E+3	-1.968E+3; -46.539; 112.788; 6.078; 33.181
26	M, logP, V, μ	1.458E+3	-1.743E+4; -168.106; 1.139E+4; 1.702; 81.196
27	E_{LUMO}, Sa, V, μ	1.472E+3	-1.417E+3; 117.902; 7.008; -0.668; 34.308
28	M, Sa, V, μ	1.473E+3	-714.62; 1.296; 6.894; -2.213; 42.352
29	logP, Sa, V, μ	1.5E+3	-808.741; 93.232; 6.9; -2.315; 42.992
30	M, logP, E_{HOMO}, μ	1.526E+3	-2.096E+4; -186.295; 1.27E+4; -250.549; 92.171
31	M, logP, Sg, μ	1.565E+3	-1.716E+4; -165.901; 1.129E+4; 1.898; 80.748
32	M, logP, Sa, μ	4.37E+3	-1.23E+4; -116.773; 7.907E+3; 3.273; 70.992
	3 descriptors		
33	E_{HOMO}, E_{LUMO}, Sa	765.695	-1.487E+3; 14.667; 218.625; 6.557
35	E_{LUMO}, Sa, V	765.812	-1.642E+3; 216.891; 6.383; 0.116
35	logP, E_{LUMO}, Sa	771.36	-1.659E+3; -19.33; 229.507; 6.927
36	M, E_{LUMO}, Sa	771.432	-1.686E+3; -0.289; 229.992; 6.927
37	M, logP μ	1.205E+3	-1.952E+4; -195.322; 1.332E+4; 93.133
38	M, Sa, μ	1.274E+3	-1.348E+3; 0.233; 5.347; 37.097
39	logP, Sa, μ	1.278E+3	-1.367E+3; 18.117; 5.301; 37.173
40	E_{HOMO}, Sa, μ	1.279E+3	-1.978E+3; -65.106; 5.527; 37.5
41	Sa, V, μ	1.295E+3	-1.262E+3; 6.396; -0.618; 38.587
42	E_{LUMO}, Sa, μ	1.423E+3	-1.55E+3; 115.684; 6.157; 32.792
	2 descriptors		
43	M, V	396.399	-2.466E+3; -0.699; 5.034
44	E_{HOMO}, Sg	417.698	-7.811E+3; -570.231; 7.312

45	V, μ	467.245	-2.289E+3; 4.451; 25.281
46	$E_{HOMO,}$ V	502.724	-5.92E+3; -420.719; 3.909
47	$E_{HOMO,}$ Sa	599.557	-1.371E+3; -8.739; 5.477
48	logP, Sa	601.981	-1.274E+3; 15.222; 5.223
49	M, Sa	602.332	-1.251E+3; 0.241; 5.209
50	Sa, V	603.079	-1.38E+3; 4.967; 0.418
51	$E_{LUMO,}$ Sa	765.373	-1.619E+3; 218.096; 6.533
52	Sa, μ	1.262E+3	-1.388E+3; 5.618; 37.107

Table 3. Multilinear regression equations, obtained using RT2 (r^2=0.999).

No.	Descriptors (X_i)	F	Coefficients (a_i)
	7 descriptors		
1	M, logP, $E_{HOMO,}$ $E_{LUMO,}$ Sa, V, μ	4.288E+4	-80.928; -0.727; 48.587; 1.601E-3; 2.202; 0.023; 0.01; 0.327
2	M, logP, $E_{HOMO,}$ $E_{LUMO,}$ Sg, V, μ	1.628E+6	-133.123; -0.704; 41.968; -4.11; 3.173; -0.105; 0.152; 0.182
	6 descriptors		
3	M, $E_{HOMO,}$ $E_{LUMO,}$ Sa, V, μ	1.401E+3	9.29; 2.74E- 3; 1.763; 1.564; 0.049; -0.011; 0.181
4	logP, $E_{HOMO,}$ $E_{LUMO,}$ Sa, V, μ	1.414E+3	11.499; 0.283; 1.957; 1.519; 0.05; -0.013; 0.189
5	logP, $E_{HOMO,}$ $E_{LUMO,}$ Sg, V, μ	1.604E+3	-105.191; -10.407;-6.882; 3.609; -0.221; 0.287; -0.108
6	M, $E_{HOMO,}$ $E_{LUMO,}$ Sg, V, μ	2.563E+3	-118.467; -0.154; -6.759; 3.738; -0.221; 0.286; -0.066
7	M, logP, $E_{LUMO,}$ Sg, V, μ	2.665E+3	-104.887; -0.989; 67.99; 1.866; 0.051; -0.026; 0.395
8	M, logP, $E_{HOMO,}$ $E_{LUMO,}$ Sg, μ	4.725E+3	-113.808; -0.915; 61.954; -1.398; 2.169; 0.03; 0.351
9	M, logP, $E_{HOMO,}$ $E_{LUMO,}$ Sg, V	7.122E+3	-135.402; -0.452; 21.434; -5.904; 3.884; -0.185; 0.246
10	M, logP, $E_{HOMO,}$ $E_{LUMO,}$ V, μ	7.856E+3	-118.196; -0.861; 56.976; -2.046; 2.443; 0.035; 0.307
11	M, logP, $E_{HOMO,}$ $E_{LUMO,}$ Sa, μ	2.562E+4	-67.387; -0.689; 46.348; 0.804; 2.042; 0.031; 0.343
12	M, logP, $E_{LUMO,}$ Sa, V, μ	4.288E+4	-80.952; -0.727; 48.591; 2.202; 0.023; 0.01; 0.327
	5 descriptors		
13	logP, $E_{LUMO,}$ Sa, V, μ	1.265E+3	-11.204; -0.317; 1.742; 0.035; 6.255E-3; 0.144
14	M, $E_{LUMO,}$ Sa, V, μ	1.283E+3	-11.962; -5.351E-3; 1.772; 0.035; 7.057E-3; 0.142
15	logP, $E_{HOMO,}$ $E_{LUMO,}$ Sg, V	1.353E+3	-88.117; -7.953; -5.769; 2.837; -0.167; 0.224
16	logP, $E_{HOMO,}$ $E_{LUMO,}$ Sa, μ	1.358E+3	-1.124; -0.138; 0.942; 1.699; 0.041; 0.156
17	M, $E_{HOMO,}$ $E_{LUMO,}$ Sa, μ	1.366E+3	-1.307; -2.274E-3; 0.949; 1.711; 0.041; 0.156
18	$E_{HOMO,}$ $E_{LUMO,}$ Sa, V, μ	1.392E+3	4.331; 1.393; 1.652; 0.046; -5.583E-3; 0.168
19	M, logP, $E_{LUMO,}$ V, μ	2.033E+3	-106.309; -0.962; 64.299; 2.005; 0.027; 0.359
20	M, $E_{HOMO,}$ $E_{LUMO,}$ Sg, V	2.245E+3	-108.184; -0.136; -6.218; 3.265; -0.195; 0.255
21	M, logP, $E_{LUMO,}$ Sg, μ	2.485E+3	-105.401; -0.972; 65.873; 1.972; 0.027; 0.373
22	M, logP, $E_{LUMO,}$ Sa, μ	1.016E+4	-75.479; -0.699; 47.067; 1.972; 0.029; 0.353
	4 descriptors		
23	logP, $E_{HOMO,}$ $E_{LUMO,}$ Sa	812.951	1.334; -0.246; 1.276; 2.26; 0.045
24	M, $E_{HOMO,}$ $E_{LUMO,}$ Sa	813.658	1; -3.679E-3; 1.278; 2.267; 0.045
25	M, logP, Sg, μ	843.345	-78.743; -0.745; 50.74; 0.013; 0.411
26	logP, $E_{LUMO,}$ Sa, V	893.939	-14.44; -0.756; 2.342; 0.032; 0.017
27	M, $E_{LUMO,}$ Sa, V	902.636	-15.695; -0.012; 2.367; 0.031; 0.017
28	M, logP, Sa, μ	1.059E+3	-58.29; -0.549; 37.212; 0.017; 0.385
29	$E_{LUMO,}$ Sa, V, μ	1.21E+3	-9.405; 1.545; 0.035; 5.677E-4; 0.166
30	logP, $E_{LUMO,}$ Sa, μ	1.222E+3	-9.489; -0.094; 1.61; 0.038; 0.165
31	M, $E_{LUMO,}$ Sa, μ	1.227E+3	-9.673; -1.616E-3; 1.622; 0.038; 0.165
32	$E_{HOMO,}$ $E_{LUMO,}$ Sa, μ	1.324E+3	-1.454; 0.873; 1.601; 0.038; 0.16
	3 descriptors		
33	M, logP, μ	647.926	-95.341; -0.951; 64.991; 0.498
35	Sa, V, μ	699.133	-7.368; 0.027; 1.217E-3; 0.222
35	M, Sa, μ	708.933	-6.76; 2.104E-3; 0.027; 0.225

36	logP, Sa, μ	710.797	-6.944; 0.153; 0.026; 0.226
37	$E_{HOMO,}$ Sa, μ	715.451	-1.595; 0.609; 0.03; 0.221
38	logP, $E_{LUMO,}$ Sa	722.501	-10.037; -0.193; 2.183; 0.042
39	M, $E_{LUMO,}$ Sa	722.804	-10.316; -2.888E-3; 2.188; 0.042
40	$E_{LUMO,}$ Sa, V	723.541	-10.493; 2.024; 0.032; 4.362E-3
41	$E_{HOMO,}$ $E_{LUMO,}$ Sa	774.729	0.867; 1.168; 2.112; 0.04
42	$E_{LUMO,}$ Sa, μ	1.209E+3	-9.291; 1.546; 0.036; 0.167
	2 descriptors		
43	Sg, V	337.821	-12.167; 0.011; 0.017
44	$E_{HOMO,}$ V	349.881	-22.437; -1.267; 0.021
45	logP, Sa	379.717	-6.382; 0.136; 0.026
46	M, Sa	380.153	-6.172; 2.149E-3; 0.026
47	$E_{LUMO,}$ V	387.726	-13.962; 1.174; 0.027
48	$E_{HOMO,}$ Sa	389.388	1.989; 0.942; 0.03
49	Sa, V	393.198	-8.049; 0.019; 7.185E-3
50	V, μ	419.303	-11.779; 0.023; 0.165
51	Sa, μ	697.685	-7.12; 0.029; 0.225
52	$E_{LUMO,}$ Sa	703.095	-9.644; 2.069; 0.038

CONCLUSIONS

Good correlations of chromatographic retention indices for the 9 PCBs with molecular properties using multilinear regression were obtained. The best 10 combinations of 2, 3, 4, 5 and 6 descriptors from the group of 8 considered were determined for each retention index series according the values of the regression quality indices [23, 24].

In the majority of best equations with the biggest F value, the presence of Sa descriptor shows the importance of the molecular surface and stationary phase interaction.

The descriptors with the biggest weight are the logP, correlated with the lipophilicity, and the reactivity indices, ε_{HOMO} and ε_{LUMO}.

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ОПРЕДЕЛЯНЕ НА ИНДЕКСИТЕ НА ЗАДЪРЖАНЕ ПРИ ХРОМАТОГРАФСКИЯ АНАЛИЗ НА ПОЛИ-ХЛОРИРАНИ БИФЕНИЛИ (PCB) С ПОМОЩТА НА МНОЖЕСТВЕНА ЛИНЕЙНА РЕГРЕСИЯ

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(Резюме)

Приложен е методът на множествената линейна регресия за определяне на времената на задържане при хроматографията на поли-хлорирани бифенили (PCB). Определени са девет референтни хроматографски индекса (R) използвайки 8 изчислени молекулни свойства (дескриптори): моларен обем, молекулна маса, коефициент на разпределение (logP), ван-дер-Ваалс'ова и достъпна повърхност по разтворител, диполен момент, and гранични орбитални енергии. Подбрани са най-подходящите уравнения според най-високия качетсвен индекс F и най-ефективната комбинация от дескриптори. Както се очаква, дескрипторът "ван-дер-Ваалс'ова повърхност" се явява често в най-добрите уравнения. В обсъжданите уравнения дескрипторът logP, корелиран с липофилността и индекса на реактовпспособност (ε_{HOMO} and ε_{LUMO}) има най-голямо тегло.