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ScienceDirect
European Journal of Medicinal Chemistry 41 (2006) 1271–1278
EUROPEAN JOURNAL OF MEDICINAL CHEMISTRY
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Original article

Comparison of QSPR models of octanol/water partition coefficient for vitamins and non vitamins

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Received 17 December 2005; accepted 27 June 2006
Available online 21 August 2006

Abstract

Comparison of QSPR models for vitamins and for various substances, which are not vitamins indicates that vitamins have less number of molecular features (topologic and kinds of atomic orbitals), but, most probably, more complex mechanisms of interactions with molecules of water and octanol.

Keywords: QSPR; Octanol/water partition coefficient; Vitamins; Graph of atomic orbitals (GAO)

1. Introduction

Quantitative structure–property/activity relationships (QSPR/QSAR) are a tools of modern research in fields of chemistry, biochemistry, and ecology. There is the tendency to using in the QSAR/QSPR analysis as large as possible the number of substances [1]. However, prediction of properties/activities of chemicals of rare features, also, is an important problem, for example in drug design.

In particular, vitamins, from medical point of view, are important biologically active substances. However, in fact, QSAR/QSPR analysis of these substances is absent in literature. Number of vitamins is not large, but QSPR/QSAR models of these substances can be useful in the chemical and medical research.

Recently, so-called optimisation of correlation weights of local graph invariants (OCWLI) has been tested as a tool of the QSAR/QSPR analysis [2–12]. The OCWLI may be based on the Hydrogen-Filled Molecular Graphs (HFG) [2,3] as well as on the graph of atomic orbitals (GAO) [9–12].

Octanol/water partition coefficient is physicochemical parameter that is often correlated with different kinds of biological activity. Taking into account biochemical role of vitamins it is interesting to compare models of the parameter in case of vitamins and in case of organic compounds which are not vitamins. It is aim of the present study.

Data on octanol/water partition coefficient of vitamins taken from the United States National Library of Medicine [13]. Data on octanol/water partition coefficient of various organic compounds which are not vitamins taken from Ref. [14].

2. Methods

Descriptors which have been used in this QSAR study are defined as

$$DCW(G,x) = \prod_{k=1}^{n} CW(V_k) \cdot CW({}^{x}EC_k) \quad (1)$$

where G is type of molecular graph, i.e. the HFG or the GAO; x is order of Morgan extended connectivity (EC); V_k are atoms in case of the HFG (H, C, O, etc.) and atomic orbitals (AO) in case of the GAO ($1s^1$, $2s^2$, $2p^2$, etc); $CW(V_k)$ and $CW({}^{x}EC_k)$ are correlation weights of the V_k and the ${}^{x}EC_k$, respectively.

The GAO can be obtained from the HFG by scheme:

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doi:10.1016/j.ejmech.2006.06.006

Table 1
AO groups on the chemical elements which take place in compounds under consideration

Chemical element	Group of AOs
H	$1s^1$
C	$1s^2$, $2s^2$, $2p^2$
N	$1s^2$, $2s^2$, $2p^3$
F	$1s^2$, $2s^2$, $2p^5$
O	$1s^2$, $2s^2$, $2p^4$
P	$1s^2$, $2s^2$, $2p^6$, $3s^2$, $3p^3$
S	$1s^2$, $2s^2$, $2p^6$, $3s^2$, $3p^4$
Cl	$1s^2$, $2s^2$, $2p^6$, $3s^2$, $3p^5$
Br	$1s^2$, $2s^2$, $2p^6$, $3s^2$, $3p^6$, $3d^{10}$, $4s^2$, $4p^5$
J	$1s^2$, $2s^2$, $2p^6$, $3s^2$, $3p^6$, $3d^{10}$, $4s^2$, $4p^6$, $4d^{10}$, $5s^2$, $5p^5$

- each vertex of the HFG is replaced by a group of AOs. Such groups of AOs are listed in Table 1;
- elements of adjacency matrix of the GAO are defined as

$$a_{ij} = \begin{cases} 1, \text{ if } i\text{th and } j\text{th vertices of GAO fall in groups of different atoms from HFG and these atomshave joint edge in HFG;} \\ 0, \text{ in all other cases.} \end{cases} \quad (1)$$

The extended connectivity of xth order are calculated with values of extended connectivity of $(x-1)$th order by the recurrent formula

$${}^{x}EC_i = \sum_{(i,j)} {}^{(x-1)}EC_j \quad (2)$$

where (i, j) is an edge in molecular graph. In role of the ${}^{0}EC_i$, a vertex degree (number of neighbours) has been used.

The HFG and GAO of vitamin B11 are shown in Figs. 1 and 2, respectively.

By Monte Carlo method such values of the $CW(V_k)$ and $CW({}^{x}EC_k)$ which produce maximal value of correlation coefficient between the property/activity of interest and the $DCW(G, x)$ can be calculated. Having this numerical data, one can calculate with substance of a training set model of view

$$PA = C_0 + C_1 \cdot DCW(G, x) \quad (3)$$

Predictive ability of the model can be estimated with an external test set.

This approach has been used in QSPR modelling octanol/water partition coefficient of 24 vitamins. Separation into the training set ($N = 18$) and the test set ($N = 6$) has been done randomly, but according to principle: all local graph invariants must be present in the training set.

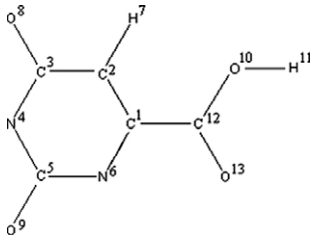

Fig. 1. HFG of vitamin B11.

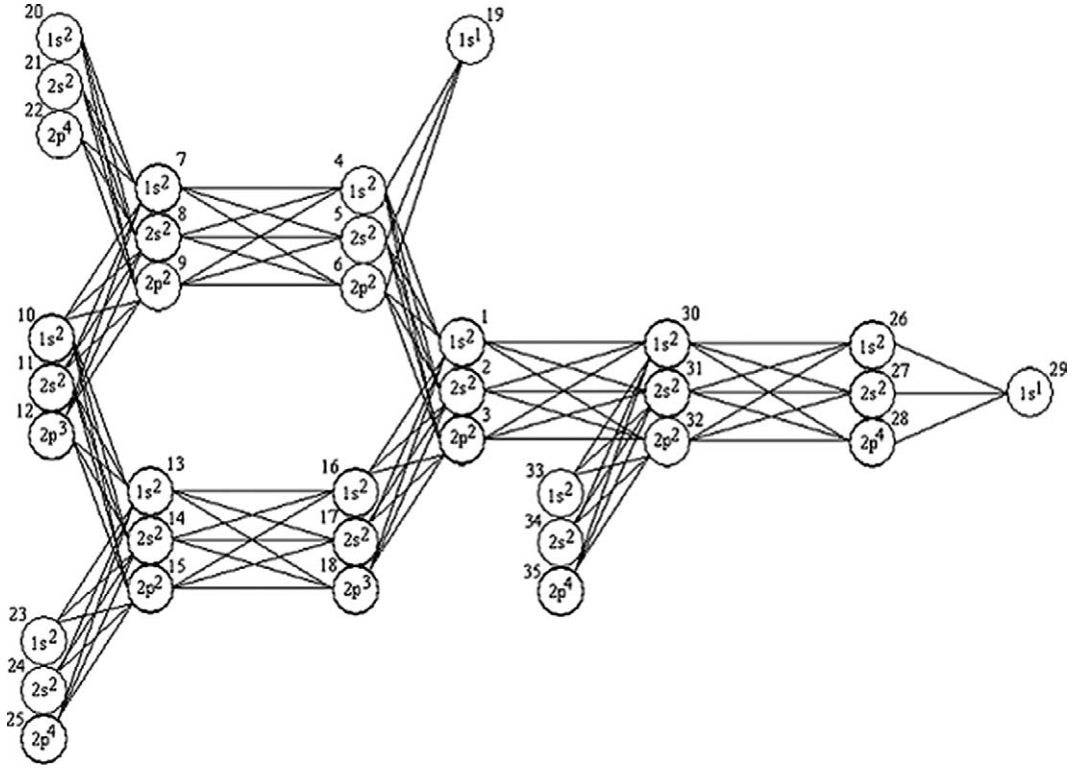

Fig. 2. GAO of vitamin B11.

3. Results and discussion

Statistical characteristics of the OCWLI models (for vitamins) based on the DCW(HFG, 0), DCW(HFG, 1), DCW (GAO, 0), and DCW(GAO, 1) are shown in Table 2. From Table 2 one can see the best OCWLI model takes place in case of the DCW(GAO, 0). Optimal values of the correlation weights are presented in Table 3. Calculation of the DCW (GAO, 0) is demonstrated in Table 4.

Table 2
The statistical characteristics of OCWLI models for vitamins

			Training set, $N = 18$			Test set, $N = 6$		
Descriptor	Probe	Number optimised parameters	R^{2a}	s	F	r^2	s	F
DCW(HFG, 0)	1	10	0.9257	1.436	199	0.6819	2.487	9
	2		0.9191	1.499	182	0.8280	1.881	19
	3		0.9302	1.392	213	0.6510	2.683	7
DCW(HFG, 1)	1	21	0.9950	0.371	3207	0.8185	1.733	18
	2		0.9829	0.689	921	0.6037	2.730	6
	3		0.9840	0.667	983	0.7508	2.199	12
DCW(GAO, 0)	*1*	*20*	*0.9804*	*0.738*	*800*	*0.9497*	*0.910*	*75*
	2		*0.9829*	*0.688*	*922*	*0.9473*	*0.911*	*72*
	3		*0.9820*	*0.707*	*874*	*0.9576*	*0.793*	*90*
DCW(GAO, 1)	1	47	0.9984	0.210	10015	0.5983	2.578	6
	2		0.9999	0.063	113452	0.8008	1.910	16
	3		0.9998	0.079	71281	0.7600	1.914	13

[a] r, s, and F are correlation coefficient, standard error, and Fischer F-ratio, respectively.

Table 3
Correlation weights of local graph invariants for calculation of DCW(GAO, 0) on three probes of the OCWLI for vitamins and compounds which are not vitamins

Vitamins	Probe 1	Probe 2	Probe 3	Non vitamins	Probe 1	Probe 2	Probe 3
AO_k				AO_k			
$1s^1$ ↑	1.0006588	1.0025450	1.0026898	$1s^1$	0.9999023	1.0007478	1.0003594
$1s^2$ ↓	0.9971412	0.9977988	0.9997013	$1s^2$	1.0000684	1.0006172	0.9999332
$2s^2$	0.9963664	1.0013899	0.9983899	$2s^2$ ↑	1.0038863	1.0036274	1.0038823
$2p^2$ ↑	1.0021693	1.0012604	1.0015810	$2p^2$	1.0001152	0.9995722	1.0002031
$2p^3$ ↓	0.9937885	0.9936475	0.9942833				
$2p^4$	0.9958719	0.9952698	0.9962488				
				$2p^5$ ↓	0.9980570	0.9975255	0.9985719
$2p^6$ ↑	1.0023927	1.0041916	1.0027279	$2p^6$	1.0007832	0.9992617	1.0001888
$3s^2$	0.9979719	0.9999691	1.0004897	$3s^2$ ↓	0.9994923	0.9992444	1.0007689
$3p^3$ ↑	1.0355017	1.0297217	1.0345681				
$3p^4$ ↓	0.9954809	0.9943753	0.9958126	$3p^4$ ↓	0.9891157	0.9887247	0.9878376
				$3p^5$	0.9997578	0.9998612	0.9994255
				$3p^6$	0.9983470	1.0000702	1.0013535
				$3d^{10}$	1.0027624	1.0001151	0.9976784
				$4s^2$	1.0015453	0.9993223	1.0026360
				$4p^5$	0.9992126	1.0021747	1.0000887
				$4p^6$	1.0024087	0.9991447	1.0031116
				$4d^{10}$	0.9994505	1.0008362	0.9982203
				$5s^2$	1.0005646	1.0052002	1.0022268
				$5p^5$	0.9988365	1.0002884	1.0000448
${}^0EC_k$				${}^0EC_k$			
0003	1.0022657	0.9994911	0.9992681	0003	1.0001816	1.0005250	1.0001152
0004	0.9989142	0.9973127	0.9975685				
0005	1.0006615	0.9989547	0.9985956	0005	0.9997012	0.9993436	0.9995468
0006 ↑	1.0020181	1.0000610	1.0003792	0006 ↑	1.0010410	1.0007932	1.0009492
0007	1.0012973	0.9996831	1.0000132	0007	0.9997539	0.9998340	0.9997676
0008	1.0005418	0.9992462	0.9998174	0008 ↑	1.0003281	1.0002246	1.0002910
0009 ↑	1.0024363	1.0015577	1.0016171	0009 ↓	0.9993240	0.9996464	0.9994357
0010 ↑	1.0012808	1.0002430	1.0002736	0010 ↓	0.9991758	0.9990641	0.9991348
0011 ↓	0.9742473	0.9757525	0.9756581	0011 ↑	1.0003321	1.0014600	1.0007910
0012	1.0000413	0.9987516	0.9979509	0012	0.9979725	0.9978364	0.9979482
				0013	1.0001479	1.0016630	1.0008021
				0014	0.9997167	1.0006874	1.0001932
				0017	0.9998632	1.0004141	1.0000371
				0018	0.9999484	1.0018419	1.0007921
				0020	1.0011803	1.0039483	1.0023873

Table 4
Calculation of DCW(GAO, 0) for vitamin B11. The numbering of vertex in HFG and GAO shown in Figs. 1 and 2. DCW(GAO, 0) = 0.97866

Atom	Atom number	^{0}EC	AO	AO number	^{0}EC	CW(AO)	CW(^{0}EC)
C	1	3	$1s^2$	1	9	0.9971412	1.0024363
			$2s^2$	2	9	0.9963664	1.0024363
			$2p^2$	3	9	1.0021693	1.0024363
C	2	3	$1s^2$	4	7	0.9971412	1.0012973
			$2s^2$	5	7	0.9963664	1.0012973
			$2p^2$	6	7	1.0021693	1.0012973
C	3	3	$1s^2$	7	9	0.9971412	1.0024363
			$2s^2$	8	9	0.9963664	1.0024363
			$2p^2$	9	9	1.0021693	1.0024363
N	4	2	$1s^2$	10	6	0.9971412	1.0020181
			$2s^2$	11	6	0.9963664	1.0020181
			$2p^3$	12	6	0.9937885	1.0020181
C	5	3	$1s^2$	13	9	0.9971412	1.0024363
			$2s^2$	14	9	0.9963664	1.0024363
			$2p^2$	15	9	1.0021693	1.0024363
N	6	2	$1s^2$	16	6	0.9971412	1.0020181
			$2s^2$	17	6	0.9963664	1.0020181
			$2p^3$	18	6	0.9937885	1.0020181
H	7	1	$1s^1$	19	3	1.0006588	1.0022657
O	8	1	$1s^2$	20	3	0.9971412	1.0022657
			$2s^2$	21	3	0.9963664	1.0022657
			$2p^4$	22	3	0.9958719	1.0022657
O	9	1	$1s^2$	23	3	0.9971412	1.0022657
			$2s^2$	24	3	0.9963664	1.0022657
			$2p^4$	25	3	0.9958719	1.0022657
O	10	2	$1s^2$	26	4	0.9971412	0.9989142
			$2s^2$	27	4	0.9963664	0.9989142
			$2p^4$	28	4	0.9958719	0.9989142
H	11	1	$1s^1$	29	3	1.0006588	1.0022657
C	12	3	$1s^2$	30	9	0.9971412	1.0024363
			$2s^2$	31	9	0.9963664	1.0024363
			$2p^2$	32	9	1.0021693	1.0024363
O	13	1	$1s^2$	33	3	0.9971412	1.0022657
			$2s^2$	34	3	0.9963664	1.0022657
			$2p^4$	35	3	0.9958719	1.0022657

Lists of the training and test sets, experimental data on octanol/water partition coefficient of vitamins and calculated by

$$\mathrm{Log}P = -88.98 + 89.41\ \mathrm{DCW(GAO,\ 0)} \quad (4)$$

$N = 18$, $R^2 = 0.9804$, $s = 0.738$, $F = 800$
$N = 6$, R^2=0.9497, $s = 0.910$, $F = 75$
are present in Table 5.

Calculated by the same manner correlation weights for octanol/water model of various organic compounds (non vitamins) are, also, listed in Table 3. Model of octanol/water partition coefficient for these compounds (Probe 1) is

$$\mathrm{Log}P = -103.8 + 103.8\ \mathrm{DCW(GAO,\ 0)} \quad (5)$$

$N = 69$, $R^2 = 0.9953$, $s = 0.096$, $F = 14136$
$N = 70$, $R^2 = 0.9930$, $s = 0.119$, $F = 9631$

Experimental and calculated with Eq. (5) octanol/water partition values are present in Table 6. It is to be noted, 1,2-dibromoethane is influential outlier, without this compounds statistical characteristics for the training set are $N = 69$, $R^2 = 0.9978$, $s = 0.066$, $F = 30968$.

Comparison of statistical characteristics of Eqs. (4) and (5) indicates that phenomenon under consideration is more complex for case of vitamins.

One can see from Eq. (1) that correlation weight more than 1.0 is a promoter increase octanol/water partition coefficient, and correlation weight less than 1.0 is a promoter of decrease of the parameter. It can be seen from Table 3, that two kinds, from statistical point of view category of invariants take place, first, invariants with stable (more or less 1) values of the correlation weights, second, invariants with unstable correlation weights. Second kind of invariants was removed from consideration. Others were marked by ↑ in case they are promoter of increase the log$P$, and ↓ in opposition case. It is to be noted, that vitamins have the number of chemical (AO kinds) and topological (numerical values of vertex degree in the GAO) features less than the number for non vitamin compounds under consideration.

Comparison of promoters increase/decrease of the log$P$ values for vitamins and compounds which are not vitamins has shown: first, there are only five invariants comparable from statistical stability (namely $3p^4$, 0006, 0009, 0010, and 0011), second, the same roles have $3p^4$ (promoter of increase

Table 5
Experimental and calculated with Eq. (4) values of octanol/water partition coefficient for series of vitamins

Number	Substances	CAS number	DCW(GAO, 0)	Experimental	Calculated	Experimental – calculated
Training set						
1	Vitamin D3	67-97-0	1.095	10.240	8.912	1.328
2	Vitamin 2′,3′-trans K1	84-80-0	1.123	11.710	11.418	0.292
3	Vitamin K3H2	481-85-6	1.016	2.760	1.846	0.914
4	Vitamin K4	573-20-6	1.037	3.590	3.773	–0.183
5	Vitamin H3	59-46-1	1.033	2.140	3.425	–1.285
6	Vitamin U	1115-84-0	1.003	0.280	0.724	–0.444
7	Vitamin P	153-18-4	0.971	–2.020	–2.184	0.164
8	Vitamin B13	65-86-1	0.979	–0.830	–1.478	0.648
9	Vitamin B8	61-19-8	0.975	–1.680	–1.771	0.091
10	Vitamin B7	58-85-5	0.995	0.390	–0.012	0.402
11	Vitamin B4	73-24-5	0.983	–0.090	–1.081	0.991
12	Vitamin B2	83-88-5	0.987	–1.460	–0.741	–0.719
13	Vitamin B1	59-43-8	0.952	–3.930	–3.846	–0.084
14	Vitamin B3	98-92-0	1.000	–0.370	0.464	–0.834
15	Vitamin E	59-02-09	1.132	12.180	12.188	–0.008
16	Vitamin A	68-26-8	1.068	5.680	6.479	–0.799
17	Vitamin D2	50-14-6	1.106	10.440	9.895	0.545
18	Vitamin D3	434-16-2	1.103	8.650	9.618	–0.968
Testset						
1	Vitamin K0	58-27-5	1.030	2.200	3.080	–0.880
2	Vitamin A2	79-80-1	1.078	7.410	7.405	0.005
3	Vitamin C	50-81-7	0.965	–1.850	–2.686	0.836
4	Vitamin H	150-13-0	0.999	0.830	0.346	0.484
5	Vitamin B9	59-30-3	0.977	–2.810	–1.660	–1.150
6	Vitamin B5	79-83-4	0.988	–1.690	–0.642	–1.048

Table 6
Experimental and calculated with Eq. (5) values of octanol/water partition coefficient for series of various compounds which are not vitamins

Number	Structures	DCW(GAO, 0)	Experimental	Calculated	Experimental – calculated
	Training set				
1	1,1,1-Trichloroethane	1.0264	2.4810	2.7351	–0.2541
2	1,1,2,2-Tetrachloroethane	1.0265	2.6440	2.7497	–0.1057
3	1,2,3,5-Tetramethylbenzene	1.0457	4.7380	4.7447	–0.0067
4	1,2,3-Trichlorobenzene	1.0409	4.2810	4.2433	0.0377
5	1,2,4,5-Tetramethylbenzene	1.0457	4.7380	4.7447	–0.0067
6	1,2-Dibromobenzene	1.0357	3.5880	3.7108	–0.1228
7	1,2-Dichlorobenzene	1.0341	3.5680	3.5385	0.0295
8	1,2-Diphenylethane	1.0498	4.8880	5.1661	–0.2781
9	1,3-Dichlorobenzene	1.0341	3.5680	3.5385	0.0295
10	1,3-Dimethylnaphthalene	1.0444	4.6140	4.6098	0.0042
11	1,4-Dibromobenzene	1.0357	3.8680	3.7108	0.1572
12	1,4-Dichlorobenzene	1.0341	3.5680	3.5385	0.0295
13	1,4-Dimethylnaphthalene	1.0444	4.6140	4.6098	0.0042
14	1-Butene	1.0214	2.2660	2.2234	0.0426
15	1-Chloroheptane	1.0410	4.1100	4.2527	–0.1427
16	1-Chloronaphthalene	1.0386	4.0290	4.0056	0.0234
17	1-Chloropropane	1.0195	1.9940	2.0220	–0.0280
18	1-Hexene	1.0321	3.3240	3.3351	–0.0111
19	1-Methylbenz(a)anthracene	1.0609	6.3130	6.3256	–0.0126
20	1-Methylnaphthalene	1.0381	3.9650	3.9548	0.0102
21	2,2′,4-Trichlorobiphenyl	1.0595	6.1690	6.1719	–0.0029
22	2,2,4-Trimethylpentane	1.0429	4.5360	4.4561	0.0799
23	2,3-Dimethylnaphthalene	1.0444	4.6140	4.6098	0.0042
24	2,4′-Dichlorobiphenyl	1.0526	5.4560	5.4557	0.0003
25	2,4,6-Tetrachlorobiphenyl	1.0595	6.1690	6.1719	–0.0029
26	2,5-Dichlorobiphenyl	1.0526	5.4560	5.4557	0.0003
27	2,6-Dichlorobiphenyl	1.0526	5.4560	5.4557	0.0003
28	2-Chloronaphthalene	1.0386	4.0290	4.0056	0.0234

(continued)

Table 6 *(continued)*

Number	Structures	DCW(GAO, 0)	Experimental	Calculated	Experimental – calculated
29	2-Chlorotoluene	1.0336	3.5040	3.4877	0.0163
30	2-Methylanthracene	1.0495	5.1390	5.1339	0.0051
31	2-Methylhexane	1.0404	4.2670	4.1956	0.0714
32	2-Methylpentane	1.0350	3.7380	3.6340	0.1040
33	4-Chlorotoluene	1.0336	3.5040	3.4877	0.0163
34	5-Methylchrysene	1.0609	6.3130	6.3256	–0.0126
35	7-Methylbenz(a)anthracene	1.0609	6.3130	6.3256	–0.0126
36	9,10-Dimethylanthracene	1.0558	5.7880	5.7962	–0.0082
37	Acenaphthene	1.0398	4.0700	4.1292	–0.0592
38	Adamantane	1.0387	3.9820	4.0181	–0.0361
39	Anthracene	1.0431	4.4900	4.4759	0.0141
40	Benz(b)anthracene	1.0509	5.6640	5.2876	0.3764
41	Benzene	1.0207	2.1420	2.1445	–0.0025
42	Benz(a)pyrene	1.0588	6.1240	6.1066	0.0174
43	Benzo(b)fluorene	1.0509	5.3990	5.2876	0.1114
44	Benzo(ghi)perylene	1.0631	6.5840	6.5539	0.0301
45	Carbontetrachloride	1.0275	2.8750	2.8566	0.0184
46	Chrysene	1.0545	5.6640	5.6602	0.0038
47	Cyclohexane	1.0318	3.3540	3.2988	0.0552
48	Cyclooctane	1.0426	4.4720	4.4219	0.0501
49	Dibenz(a,h)anthracene	1.0661	6.8380	6.8581	–0.0201
50	Diethylsulphide	1.0170	1.9000	1.7656	0.1344
51	Dimethylsulphide	1.0091	0.8420	0.9467	–0.1047
52	Ethylchloride	1.0142	1.4650	1.4719	–0.0069
53	Fluorobenzene	1.0219	2.2850	2.2691	0.0159
54	Hexamethylbenzene	1.0585	6.0360	6.0681	–0.0321
55	Iodobenzene	1.0313	3.2650	3.2489	0.0161
56	Pentachlorobenzene	1.0546	5.7070	5.6654	0.0416
57	Pentachloroethane	1.0321	3.6270	3.3372	0.2898
58	Pentamethylbenzene	1.0521	5.3870	5.4038	–0.0168
59	Phenanthrene	1.0431	4.4900	4.4759	0.0141
60	Tetrachloroethylene	1.0290	3.0200	3.0081	0.0119
61	Trichloroethylene	1.0215	2.2670	2.2338	0.0332
62	*m*-Xylene	1.0331	3.4400	3.4368	0.0032
63	*n*-Octane	1.0472	4.9260	4.9035	0.0225
64	*n*-Heptane	1.0418	4.3970	4.3378	0.0592
65	*n*-Butylbenzene	1.0431	4.7380	4.4686	0.2694
66	*n*-Pentane	1.0310	3.3390	3.2157	0.1233
67	*p*-Xylene	1.0331	3.4400	3.4368	0.0032
68	Tert-butylbenzene	1.0401	4.1180	4.1665	–0.0485
69	Trans-1,2-dichloroethylene	1.0141	1.5140	1.4646	0.0494
	Test set				
1	1,2,3,4-Tetrachlorobenzene	1.0477	4.9940	4.9513	0.0427
2	1,2,3,4-Tetramethylbenzene	1.0457	4.7380	4.7447	–0.0067
3	1,2,3,5-Tetrachlorobenzene	1.0477	4.9940	4.9513	0.0427
4	1,2,3-Trimethylbenzene	1.0394	4.0890	4.0887	0.0003
5	1,2,4,5-Tetrachlorobenzene	1.0477	4.7380	4.9513	–0.2133
6	1,2,4-Trichlorobenzene	1.0409	4.2810	4.2433	0.0377
7	1,2,4-Trimethylbenzene	1.0394	4.0890	4.0887	0.0003
8	1,2-Dibromoethane	1.0247	1.7380	2.5659	–0.8279
9	1,2-Dichloroethane	1.0134	1.4580	1.3888	0.0692
10	1,3,5-Trichlorobenzene	1.0409	4.2810	4.2433	0.0377
11	1,3,5-Trimethylbenzene	1.0394	4.0890	4.0887	0.0003
12	1,4,5-Trimethylnaphthalene	1.0508	5.2630	5.2689	–0.0059
13	1,5-Dimethylnaphthalene	1.0444	4.6140	4.6098	0.0042
14	1-Chlorobutane	1.0248	2.5230	2.5753	–0.0523
15	1-Chlorohexane	1.0356	3.5810	3.6901	–0.1091
16	1-Chloropentane	1.0302	3.0520	3.1316	–0.0796
17	1-Ethylnaphthalene	1.0435	4.4940	4.5184	–0.0244
18	1-isopropyl-4-methylbenzene	1.0426	4.3680	4.4177	–0.0497
19	1-Methylfluorene	1.0478	4.8740	4.9596	–0.0856
20	1-Penten	1.0268	2.7950	2.7777	0.0173
21	12-Methylbenz(a)anthracene	1.0609	6.3130	6.3256	–0.0126
22	2,2′,4,5-Tetrachlorobiphenyl	1.0664	6.8820	6.8934	–0.0114

(continued)

Table 6 *(continued)*

Number	Structures	DCW(GAO, 0)	Experimental	Calculated	Experimental – calculated
23	2,3,4,5-Tetrachlorobiphenyl	1.0664	6.8820	6.8934	–0.0114
24	2,4,5-Tetrachlorobiphenyl	1.0595	6.1690	6.1719	–0.0029
25	2,6-Dimethylnaphthalene	1.0444	4.6140	4.6098	0.0042
26	2-Chlorobiphenyl	1.0457	4.7430	4.7437	–0.0007
27	2-Chlorophenanthrene	1.0500	5.2030	5.1858	0.0172
28	2-Methylbutane	1.0296	3.2090	3.0746	0.1344
29	2-Methylnaphthalene	1.0381	3.9650	3.9548	0.0102
30	2-Methylphenanthrene	1.0495	5.1390	5.1339	0.0051
31	3-Chlorotoluene	1.0336	3.5040	3.4877	0.0163
32	5,6-Dimethylchrysene	1.0674	6.9620	6.9951	–0.0331
33	6-Methylbenzo(e)pyrene	1.0653	6.7730	6.7750	–0.0020
34	6-Methylchrysene	1.0609	6.3130	6.3256	–0.0126
35	7-Ethylbenz(a)anthracene	1.0665	6.8420	6.9017	–0.0597
36	9-Methylanthracene	1.0495	5.1390	5.1339	0.0051
37	Benz(a)anthracene	1.0545	5.6640	5.6602	0.0038
38	Benzo(a)fluorene	1.0509	5.3990	5.2876	0.1114
39	Benzo(b)fluoranthene	1.0588	6.1240	6.1066	0.0174
40	Benzo(e)pyrene	1.0588	6.1240	6.1066	0.0174
41	Benzo(j)fluoranthene	1.0588	6.1240	6.1066	0.0174
42	Benzo(k)fluoranthene	1.0588	6.1240	6.1066	0.0174
43	Biphenyl	1.0389	4.0300	4.0357	–0.0057
44	Bromobenzene	1.0282	3.0050	2.9251	0.0799
45	Cholanthrene	1.0627	6.4180	6.5041	–0.0861
46	Chlorobenzene	1.0274	2.8550	2.8389	0.0161
47	Cycloheptane	1.0372	3.9130	3.8582	0.0548
48	Cyclohexene	1.0281	2.8100	2.9126	–0.1026
49	Cyclopentane	1.0264	2.7950	2.7414	0.0536
50	Cyclopentene	1.0227	2.2510	2.3573	–0.1063
51	Dibenz(a,j)anthracene	1.0661	6.8380	6.8581	–0.0201
52	Ethylbenzene	1.0322	3.3200	3.3455	–0.0255
53	Fluoranthene	1.0474	4.9500	4.9170	0.0330
54	Fluorene	1.0396	4.2250	4.1074	0.1176
55	Fluorotrichloromethane	1.0213	2.4350	2.2151	0.2199
56	Hexachlorobenzene	1.0615	6.4200	6.3837	0.0363
57	Isopropylbenzene	1.0363	3.7190	3.7638	–0.0448
58	Naphthalene	1.0318	3.3160	3.3040	0.0120
59	Perylene	1.0588	6.1240	6.1066	0.0174
60	Pyrene	1.0474	4.9500	4.9170	0.0330
61	Toluene	1.0269	2.7910	2.7881	0.0029
62	Triphenylene	1.0545	5.6640	5.6602	0.0038
63	*n*-Decane	1.0582	5.9840	6.0432	–0.0592
64	*n*-Nonane	1.0527	5.4550	5.4713	–0.0163
65	*n*-Undecane	1.0637	6.5130	6.6172	–0.1042
66	*n*-Butane	1.0256	2.8100	2.6594	0.1506
67	*n*-Hexane	1.0364	3.8680	3.7752	0.0928
68	*n*-Propylbenzene	1.0376	3.8490	3.9060	–0.0570
69	*o*-Xylene	1.0331	3.4400	3.4368	0.0032
70	Tert-amylbenzene	1.0456	4.6470	4.7302	–0.0832

the log*P* for both vitamins and compounds which are not vitamins) and 0006 (promoter of decrease the log*P*), third, all others invariants have contradict roles. Thus, similar molecular fragment are effected to the log*P* in cases of two mentioned classes of substances by different (opposite) ways. In other words, mechanisms of interaction of molecules of vitamins with water and octanol are considerable different than mechanisms of interaction of non vitamins with water and octanol.

4. Conclusion

GAO is reasonable an alternative to hydrogen-filled molecular graph in QSPR analysis of octanol/water partition coefficient for two classes of substances, vitamins and various organic compounds which are not vitamins. Analysis of correlation weights of models for mentioned two kinds of substances indicates that very probably, vitamins interact with water and octanol by more complex mechanisms than various compounds under consideration, which are not vitamins.

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