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Comparison of the octanol/water partition coefficients calculated by ClogP®, ACDlogP and KowWin® to experimentally determined values

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Abstract

The experimental octanol/water partition coefficient data, of 108 compounds from the data set [Rytting, E., Lentz, K.A., Chen, X., Qian, F., Venkatesh, S., 2004. A quantitative structure–property relationship for predicting drug solubility in PEG 400/water cosolvent systems. Pharm. Res. 21, 237–244] was compared to calculated values using the computer programs ClogP®, ACD/logPdb® and KowWin®. It was found that all the three programs have a user friendly interface but ClogP® appears to be the more accurate predictor of $\log K_{ow}$.

Keywords: Comparison; Calculated; Octanol/water partition coefficient

1. Introduction

The octanol/water partition coefficient (K_{ow}) is the ratio of a compound's concentration in octanol to its concentration in water when the phases are at equilibrium. Since partition coefficient values (K_{ow}) can range over many orders of magnitude they are normally expressed in logarithmic form ($\log K_{ow}$). The partition coefficient has been widely used in calculating numerous physical properties such as membrane transport and water solubility.

Eros et al. (2002) and Mannhold and van de Waterbeemd (2001), have looked at various predictors of $\log K_{ow}$. In this manuscript we will focus on three commonly used programs: ClogP® v4.0 (BioByte Corp. 1999), ACD/logPdb® v7.0 (Advanced Chemistry Development Inc., Toronto Ont., Canada, 2003), and KowWin® v1.67 (Syracuse Research Corporation (SRC) Syracuse NY 2000). Mannhold and van de Waterbeemd (2001) described these programs as substructure approaches where the final $\log K_{ow}$ is

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determined by summing the single-atom or fragment contributions.

Note that these programs are designed to determine the partition coefficient of the non-ionized form of a compound. Edward et al. (1997) conducted a study where they tested the accuracy of the three programs on 34 analogs of pyridoxal isonicotinoyl hydrazone. They showed that the programs are not particularly good predictors of log K_{ow} for zwitterionic, tautomeric and charged compounds as well as for strongly hydrogen bonding compounds. In this report the accuracy and ease of use of ClogP®, ACd/logP and KowWin® will be evaluated using the data set of Rytting et al. (2004).

2. Method

2.1. Acquisition of data

In order to avoid any bias the compounds selected by Rytting et al. (2004), are used as the evaluation set. Fourteen of the 122 reported compounds were omitted due to lack of experimental values of log K_{ow}. The partition coefficients of the remaining 108 compounds were determined using ClogP®, ACD/logPdb®, and KowWin®. The experimental log K_{ow} values were acquired from references listed in the ACD/logP database. If more than one reference was listed the average log K_{ow} was taken as the experimental value.

2.2. Statistical analysis

The average absolute error (AAE) was determined using the relationship below:

$$\mathrm{AAE} = \frac{\sum |\text{observed} - \text{predicted}|}{n} \quad (1)$$

where n is the number of compounds studied.

t-Tests were performed on the logarithmic data using Microsoft Excel 1997 (Los Angeles, CA). The *P*-value was determined using a paired *t*-test with a two-tailed distribution. The significance level was set at 0.05, hence, if the *P*-value is <0.05 than the two data sets are considered to be significantly different.

3. Results and discussion

The data were separated into three groups. The first group consists of all the compounds with reported experimental log K_{ow} values. The second group consists of all of the compounds which are not zwitterionic or tautomeric. The third group consisted of the zwitterionic and tautomeric compounds. The absolute errors of the data from each of the predictive tools were determined and are listed in Table 1 .

The calculation of the partition coefficient of the drug sulindac by the three methods is illustrated in Table 2. All three programs use somewhat similar molecular breakdown schemes. However, there are significant differences in the use of non-constitutive descriptors. ClogP® and ACDlogP use different interfragmental interaction parameters, while KowWin® simply adds a constant. These are discussed in more detail by Mannhold and van de Waterbeemd (2001).

A paired *t*-test was performed and the series of experimental values predicted by each program was compared to the series of experimental values to calculate a *P*-value for each program. The *P*-values as well as the average absolute errors (AAEs) for each method are listed in Table 3.

It is clear from Table 3 that all three programs are associated with low absolute errors of prediction for uncharged, non-tautomeric compounds. However, ClogP® clearly has the lowest error and the highest *P*-value for the compounds selected. Based on this data set ClogP® is significantly better than ACDlogP and KowWin®. This study confirms the conclusions of Edward et al. (1997), that the log K_{ow} values of zwitterionic and tautomeric compounds are poorly predicted by group contribution programs.

Graphs of the predicted against the experimental values from all three programs are shown in Fig. 1.

It was observed that there were five compounds whose predicted values were one log unit or more off from the experimental value in at least two of the programs. These outliers are terfenadine, 5-aminosalicylic acid, bumetanide, diatrizoic and uric acid. This large error may be due to experimental or reporting error. The AAE was recalculated after excluding these compounds and the results are shown in Table 4.

While prediction accuracy is a major basis for the selection of a particular program there are a number of

Table 1
Comparison between the three log K_{ow} prediction programs

Name	MW	mp (°C)	KowWin®	ACD	ClogP®	Experimental value	Absolute error		
							KowWin®	ACD	ClogP®
1,2,3-Trichlorobenzene	181.45	52.6	3.81	4.27	4.04	4.09	0.28	0.18	0.05
2-Naphthol	144.17	122	2.69	2.70	2.65	2.78	0.09	0.08	0.13
5,5-Diphenylhydantoin	252.27	296.5	2.16	2.52	2.08	2.38	0.22	0.14	0.30
5-Aminosalicylic acid[a]	153.14	280	0.98	0.46	1.06	−0.16	1.14	0.62	1.22
5-Fluorocytosine[b]	129.09	296	−0.72	−1.78	−1.65				
Acetazolamide[a]	222.25	258.5	−0.73	−0.26	−1.25	−0.26	0.47	0.00	0.99
Adenine[a]	135.13	110	−0.73	−0.03	−0.29	−0.11	0.62	0.08	0.18
Adenosine[a]	267.24	234.5	−1.38	−1.02	−2.27	−1.12	0.26	0.10	1.15
Allopurinol	136.11	350	−1.03	−1.33	−0.88	−0.55	0.48	0.78	0.33
Aminopyrine	231.3	108	0.60	0.76	0.57	0.90	0.30	0.14	0.33
Ampicillin[a]	349.4	200.5	−0.88	1.35	−1.20	−0.81	0.07	2.16	0.39
Aspirin	180.16	135	1.13	1.20	1.02	1.25	0.12	0.05	0.23
Atropine	289.37	115	1.91	1.50	1.32	1.82	0.09	0.32	0.50
Azathioprine[a]	277.26	243.5	−0.09	0.90	0.01	0.10	0.19	0.80	0.09
Baclofen[a]	213.66	207	−1.32	1.56	−0.62	−0.96	0.36	2.52	0.34
Benzamide	121.14	130	0.74	0.70	0.65	0.65	0.09	0.05	0.00
Benzocaine	165.19	89	1.80	1.95	1.92	1.97	0.17	0.02	0.05
Benzoic acid	122.12	122.4	1.87	1.90	1.88	1.87	0.00	0.03	0.01
Biphenyl	154.21	70	3.93	3.98	4.03	3.91	0.02	0.07	0.12
Bumetanide[a]	364.42	230.5	2.57	2.78	3.36	−0.30	2.87	3.08	3.66
Butamben	193.25	58	2.78	3.60	2.98	3.02	0.24	0.58	0.04
Butylparaben	194.23	68.5	3.47	3.50	3.57	3.57	0.10	0.07	0.00
Caffeine	194.19	238	0.16	−0.13	−0.06	−0.07	0.23	0.06	0.01
Camphor	152.24	179.8	3.04	2.10	2.18	2.38	0.66	0.28	0.20
Carbamazepine	236.27	191.5	2.25	2.70	1.98	2.32	0.07	0.38	0.34
Cephradine[b]	349.4		1.01	0.98	−1.53				
Chloramphenicol	323.13	151	0.92	1.00	1.28	1.14	0.22	0.14	0.14
Chlorthalidone[b]	338.76	225	1.59	−0.74	0.45				
Chlorzoxazone[b]	169.57	191.75	1.99	2.29	1.87				
Cimetidine	252.34	142	0.57	0.40	0.35	0.47	0.10	0.07	0.12
Clofazimine	473.4	211	7.55	7.50	6.69	7.48	0.07	0.02	0.79
Corticosterone[a]	346.47	145	1.99	1.80	2.32	1.94	0.05	0.14	0.38
Cortisone	360.45	222	1.81	1.20	1.30	1.47	0.34	0.27	0.17
Cytosine[a]	111.1		−1.47	−1.71	−1.85	−1.73	0.26	0.02	0.12
Dapsone	248.3	175.5	0.77	0.90	0.89	0.97	0.20	0.07	0.08
Deoxycorticosterone	330.47	141.5	3.12	3.40	3.25	2.88	0.24	0.52	0.37
Dexamethasone	392.47	263	1.72	2.10	1.75	1.89	0.17	0.21	0.14
Diatrizoic acid[a]	613.92		1.37	0.45	0.73	−1.05	2.42	1.50	1.78
Diflunisal	250.2	210.5	4.41	4.30	4.39	3.56	0.85	0.74	0.83
Diosgenin[b]	414.63	205.5	3.35						
Disopyramide	339.48	94.75	2.96	2.90	2.58	2.65	0.31	0.25	0.07
Diuron	233.1	158.5	2.67	2.80	2.68	2.68	0.01	0.12	0.00
Equilin[b]	268.35	239	−2.81	3.53	2.90				
Estradiol	272.39	176	3.94	4.10	3.78	3.86	0.08	0.24	0.08
Estriol	288.39	282	2.81	2.90	3.20	2.45	0.36	0.45	0.75
Estrone	270.37	255.3	3.43	3.70	3.38	2.95	0.48	0.75	0.43
Ethylparaben	166.18	116	2.49	2.40	2.51	2.47	0.02	0.07	0.04
Ethynylestradiol-17-alpha	296.41	143.5	4.12	4.52	4.61	3.67	0.45	0.85	0.94
Fenbufen	254.28	186	3.18	3.00	3.14	3.20	0.02	0.20	0.06
Flufenamic acid	281.23	125	5.15	5.60	4.88	4.32	0.83	1.28	0.56

Table 1 (*Continued*)

Name	MW	mp (°C)	KowWin®	ACD	ClogP®	Experimental value	Absolute error		
							KowWin®	ACD	ClogP®
Fluorouracil	130.08	282	−0.81	−0.78	−0.58	−0.85	0.04	0.07	0.27
Flurbiprofen	244.26	110	3.81	4.10	3.75	4.16	0.35	0.06	0.41
Folic acid[b]	441.4		3.66	−2.32	−2.17				
Glafenine[b]	372.81	169.5	0.42	3.49	3.04				
Griseofulvin	352.77	220	1.92	2.40	1.75	2.18	0.26	0.22	0.43
Guaifenesin[b]	198.22	78.75	−1.05	0.57	0.10				
Guanine[a]	151.13		−1.05	−0.98	−1.28	−0.94	0.11	0.04	0.34
Haloperidol	375.87	148.7	4.20	4.10	3.85	4.29	0.09	0.19	0.44
Hydrochlorothiazide	297.74	274	−0.07	−0.07	−0.40	−0.07	0.00	0.00	0.33
Hydrocortisone	362.47	218.5	1.62	1.40	1.70	1.65	0.03	0.25	0.05
Hydroflumethiazide	331.28	272.5	0.22	0.50	−0.25	0.36	0.14	0.14	0.61
Hyoscyamine	289.37	108.5	1.91	1.50	1.32	1.83	0.08	0.33	0.51
Ibuprofen	206.28	76	3.79	3.70	3.68	3.50	0.29	0.20	0.18
Indapamide[b]	365.83	161	5.78	2.09	2.94				
Indoprofen	281.31	213.5	2.32	2.77	2.74	2.77	0.45	0.00	0.03
Iopanoic acid[b]	570.93	156.1	3.00	4.19	4.89				
Ketoprofen	254.28	94	3.00	2.80	2.76	3.12	0.12	0.32	0.36
Khellin[b]	260.25	154.5	−0.26	1.66	2.57				
Linuron	249.1	93.5	2.91	3.20	3.00	3.16	0.25	0.04	0.16
Mefenamic acid	241.29	230.5	5.28	5.30	4.94	4.29	0.99	1.01	0.65
Methocarbamol[b]	241.24	93	0.00	0.55	0.15				
Methylparaben	152.15	131	2.00	1.86	1.99	1.96	0.04	0.10	0.03
Metronidazole	171.16	159	0.00	−0.01	−0.46	−0.02	0.02	0.01	0.44
Minoxidil	209.25	248	1.35	0.69	0.48	1.33	0.02	0.64	0.85
Nadolol	309.4	125	1.17	1.29	0.38	0.71	0.46	0.58	0.33
Nalidixic acid	232.24	229.5	1.64	1.00	1.32	1.50	0.14	0.50	0.18
Naphthalene	128.17	80.2	3.17	3.35	3.32	3.30	0.13	0.05	0.02
Naproxen	230.26	153	3.10	3.00	2.82	3.26	0.16	0.26	0.44
Nitrofurantoin[a]	238.16		−0.17	−0.99	−0.47	−0.47	0.30	0.52	0.00
Norethisterone	298.42	203.5	2.99	3.38	2.78	2.97	0.02	0.41	0.19
Norfloxacin[a]	319.33	220.5	−0.31	1.48	−0.99	−1.26	0.95	2.74	0.27
p-Aminobenzoic acid[a]	137.14	187.75	0.96	0.83	0.98	0.73	0.23	0.10	0.25
p-Aminosalicylic acid[a]	153.14	150.5	0.98	1.14	1.06	0.91	0.07	0.23	0.15
Paracetamol	151.16	169.75	0.27	0.34	0.49	0.48	0.21	0.14	0.01
Perphenazine	403.97	97	3.82	4.50	4.32	4.20	0.38	0.30	0.12
Phenacetin	179.22	134.5	1.67	1.60	1.77	1.57	0.10	0.03	0.20
Phenolphthalein	318.33	260	3.06	2.63	2.63	2.41	0.65	0.22	0.22
Phenylbutazone	308.38	105	3.52	3.16	3.38	3.23	0.29	0.07	0.15
Praziquantel[b]	312.41	137	2.42	2.44	3.36				
Prednisolone[a]	360.45		1.40	1.49	1.38	1.59	0.19	0.10	0.21
Primidone	218.25	281.5	0.73	0.40	0.88	0.91	0.18	0.51	0.03
Progesterone	314.47	126	3.67	4.00	3.77	3.87	0.20	0.13	0.10
Propylparaben	180.2	96.5	2.98	2.90	3.04	3.04	0.06	0.14	0.00
Pyrazinamide	123.11	190	−0.53	−0.37	−0.71	−0.60	0.07	0.23	0.11
Quinidine	324.42	174.5	3.29	3.40	2.79	2.36	0.93	1.04	0.43
Quinine	324.42	177	3.29	3.44	2.79	2.36	0.93	1.08	0.43
Salicylamide	137.14	140	1.03	1.40	1.28	1.28	0.25	0.12	0.00
Salicylic acid	138.12	158	2.24	2.06	2.19	2.24	0.00	0.18	0.05
Spironolactone	416.57	134	2.88	3.12	2.25	2.26	0.62	0.86	0.01
Strychnine	334.42	280	1.85	1.70	1.66	1.93	0.08	0.23	0.27
Sulfacetamide	214.24	183	−0.60	−0.96	−0.98	−0.96	0.36	0.00	0.02

Table 1 (*Continued*)

Name	MW	mp (°C)	KowWin®	ACD	ClogP®	Experimental value	Absolute error		
							KowWin®	ACD	ClogP®
Sulfadiazine	250.27	252.5	−0.34	−0.12	−0.09	−0.07	0.27	0.05	0.02
Sulfamerazine	264.3	236.5	0.21	0.30	0.57	0.14	0.07	0.16	0.43
Sulfamethazine	278.33	176	0.76	0.80	1.07	0.28	0.48	0.52	0.79
Sulfamethoxazole	253.28	171.5	0.48	0.90	0.55	0.89	0.41	0.01	0.34
Sulfanilamide	172.2	165.5	−0.55	−0.72	−0.57	−0.70	0.15	0.02	0.13
Sulfathiazole	255.31	202	0.72	0.30	0.72	0.05	0.67	0.25	0.67
Sulindac	356.41	183.5	4.28	3.59	3.16	3.24	1.04	0.35	0.08
Sulpiride[a]	341.42	179	0.65	0.45	1.11	0.42	0.23	0.03	0.69
Tenoxicam[a]	337.37	211	2.40	1.52	1.61	0.81	1.59	0.71	0.80
Terfenadine	471.68	147.5	7.62	6.90	6.09	5.69	1.93	1.21	0.40
Tetraethylthiuram disulfide	296.52	70	3.76	3.88	3.88	3.88	0.12	0.00	0.00
Theobromine	180.17	357	−0.05	−0.72	−0.69	−0.77	0.72	0.05	0.08
Theophylline[a]	180.17	272.5	−0.39	−0.17	−0.06	−0.02	0.37	0.15	0.04
Thiamphenicol	356.22	165.3	−0.33	−0.27	−0.10	−0.27	0.06	0.00	0.17
Thymine[a]	126.11		−0.32	−0.12	−0.56	−0.62	0.30	0.50	0.06
Triamcinolone	394.44	270	0.96	0.83	0.67	1.16	0.20	0.33	0.49
Triamterene	253.27	201	0.80	1.34	1.31	0.98	0.18	0.36	0.33
Trimethoprim	290.32	201	0.73	0.80	0.88	0.91	0.18	0.11	0.03
Uracil	112.09	335	−0.87	−0.71	−1.06	−1.06	0.19	0.35	0.00
Uric acid[a]	168.11		−1.46	−1.08	−1.46	−2.66	1.20	1.58	1.20
Xanthine[a]	152.11		−1.15	−0.81	−0.70	−0.73	0.42	0.08	0.03

[a] Zwitterionic and tautomeric compounds.
[b] Compounds without reported log K_o values.

other factors that should be considered. Table 5 compares the three programs on the basis of several criteria.

As can be seen from Table 5, these programs considered are similar in many respects. For example, they each accept the common name and SMILES input which can be supplied in batch mode for large data sets. Each is available on-line or as a compact disc for use offline. They all utilize similar sized databases of about thirteen thousand experimental values to generate group values and correction factors. They each show

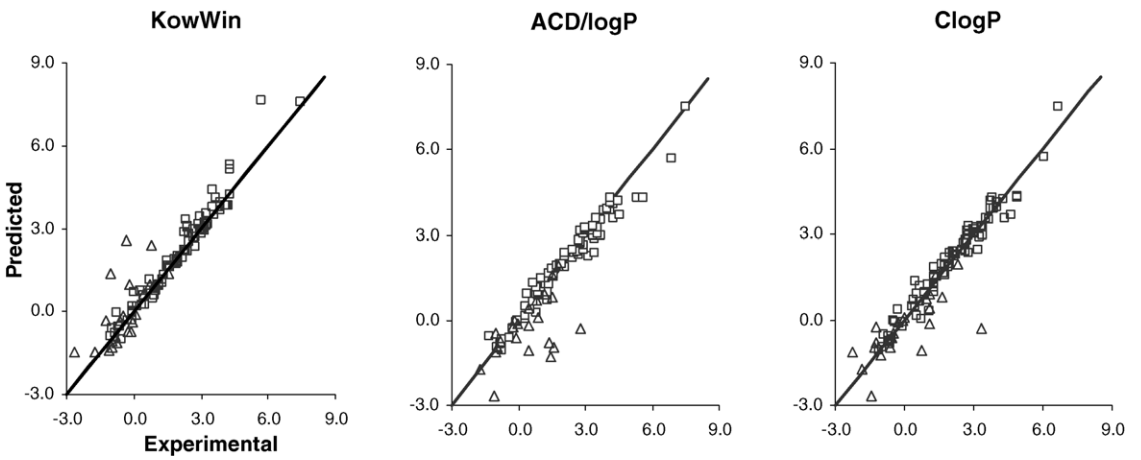
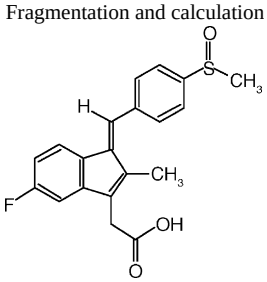


Fig. 1. Plots of experimental against predicted log K_{ow} values for the three programs (KowWin®, ACD/logP, ClogP®): (□) non-tautomers/zwitterions and (△) zwitterions and tautomers.

Table 2
Fragmentation and calculation of the log K_{ow} of sulindac using ClogP®, ACD/logP and KowWin®



	Type	KowWin®	ACd/logP	ClogP®
Flouride	Fragment	0.2004	0.5007	0.370
Sulfoxide	Fragment	−2.1103	−2.1284	−2.12
—C aromatic	Fragment	0.294		
—CH aromatic	Fragment	–	0.3697	0.130
—CR aromatic	Fragment	–	−0.0793	–
—COOH aliphatic	Fragment	−0.6895	−1.1945	−1.070
$-CH_2$ aliphatic	Fragment	0.4911	0.5314	–
$-CH_3$ aliphatic	Fragment	0.5473	0.9091	–
Aliphatic isolating C	Fragment	–	–	0.195
Connecting aromatic C	Fragment	–	0.0840	–
—H on isolating carbons	Fragment	–	–	0.227
=CH— (olefinic carbon)	Fragment	0.3836	0.2722	–
Chain and cluster branches	Branch	–	–	−0.130
Chain and alicyclic (net)	Bonds	–	–	−0.540
Allylic structure	Proximity	–	–	0.200
Phenyl-fragment pair	Proximity	–	–	0.150
Vinylic	Interaction		0.750	–
Aliphatic	Interaction	–	0.0678	–
	Interaction		0.1509	
	Interaction		0.2750	
Aromatic	Interaction		−0.0428	–
	Interaction		0.0722	
Equation constant		0.2290	–	–

ACD/logP: $0.5007 - 2.1284 + 7(0.3697) - 2(0.0793) - 1.1945 + 0.5314 + 2(0.9091) + 2(0.084) + 0.2722 + 0.75 + 0.0678 + 0.1509 + 0.2750 - 0.0428 + 0.0722 = 3.59$; KowWin®: $0.2004 - 2.1103 + 12(0.294) - 0.6895 + 0.4911 + 2(0.5473) + 4(0.3836) + 0.2290 = 4.28$; ClogP®: $0.370 - 2.12 + 12(0.130) - 1.070 + 7(0.195) + 16(0.227) + 0.200 + 0.15 - 3(0.13) - 0.54 = 3.16$.

Table 3
Average absolute errors and *P*-values

Group	n[a]	AAE (*P*-values)		
		KowWin®	ACD/logPdb®	ClogP®
All compounds	108	0.358 (0.0032)	0.386 (0.0002)	0.329 (0.3035)
w/o Tautomers and zwitterions	85	0.282 (0.0176)	0.281 (0.0086)	0.250 (0.6828)
Tautomers and zwitterions	23	0.638 (0.0658)	0.774 (0.0049)	0.623 (0.1357)

[a] n is the number of compounds.

Table 4
Average absolute errors and *P*-values without the five outliers

Group	*n*[a]	AAE (*P*-values)		
		KowWin®	ACD/logPdb®	ClogP®
All compounds	103	0.282 (0.0441)	0.327 (0.0019)	0.265 (0.5524)
w/o Tautomers and zwitterions	84	0.262 (0.0313)	0.270 (0.0153)	0.248 (0.5906)
Tautomers and zwitterions	19	0.371 (0.6921)	0.580 (0.0434)	0.341 (0.8004)

[a] *n* is the number of compounds.

the details of their calculations and provide warnings of potentially unreliable values.

In spite of their similarities there are significant differences, beside the greater accuracy of ClogP®, among the programs. Some of the differences in utility and convenience are summarized below:

- ACD/logP contains a built in structure generating program. While this program is less user friendly than Chem Draw or other commercially available packages, it is convenient for single compound evaluation, especially for compounds with complex SMILES strings.
- Both ClogP® and KowWin® accept CAS numbers as input whereas ACD/logP does not.
- Unlike other programs, ClogP® cannot account for stereochemistry. However, this does not affect the results.
- The ACD/logP output includes many experimentally determined values along with complete citations, whereas both ClogP® and KowWin® include only one literature value for each compound.
- At present both ACD/logP and ClogP® can be integrated with programs for other important molecular properties including water solubility. They both give the pH dependent distribution coefficient. The ACD suite program is the only one that can calculate pK_a values. The KowWin® suite has programs which can determine melting point, boiling point and vapor pressure.
- Interestingly ACD/logP costs nearly US$ 400.00 more for industry and US$ 500.00 less for academia than ClogP®. On the other hand KowWin® is available at no cost.

Table 5
Comparison between the three log K_{ow} prediction programs

Item	KowWin®	ACD/logP	ClogP®
Input			
SMILES	Yes	Yes	Yes
CAS no.	Yes	N/A	Yes
Structure drawing	N/A[a]	Yes	N/A[a]
Batch	Yes	Yes	Yes
Online availability	Yes	Yes	Yes
Calculations			
In database	13058	>12400	12800
Distinguish enantiomers	Yes	Yes	N/A
Output			
Details of calculation	Yes	Yes	Yes
Accuracy	See Table 3	See Table 3	See Table 3
References provided	1	Many	1
Warnings	Yes	Yes	Yes
Determine other properties	Yes[b]	Yes[c]	Yes[d]
Cost (US$)[e]	Free	2895/995	2500/1500

[a] Convert structure to smiles name from MDL MOL file type.
[b] Comes as a free suite program (EPI suite) down loaded from the EPA website.
[c] Dissociation constant (log *D* and pK_a) and water solubility along with other physical property data are available in ACD suite at a cost of US$ 9895 for industry use and US$ 2495 for academia.
[d] Biobyte corporation has suite program Bioloom that predicts log K_{ow}, log *D* and pK_a at a cost of US$ 3200 for industry and US$ 1600 for academia.
[e] Cost (US$) industry/academia.

4. Conclusion

As it has been demonstrated using an independent data set, ClogP® is a more accurate predictor of the octanol/water partition coefficient than ACD/logPdb® and KowWin®. All the three programs are similar in many respects and they all have user friendly interfaces. It is the prerogative of the individual as to which program they prefer to use.

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