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Supplementary material

Assessment of *in silico* and chromatographic lipophilicity measures for pharmaceutically important compounds

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Content

Table S1 Summary of chromatographically determined lipophilicity indices with short description, chromatographic technique and chromatographic modality used for its derivation.

Lipophilicity index	Description	Modality	Ref.
logk_m	log$k$ value at zero micellar concentration Derived from equation $1/k = 1/k_m + K_{AM} \times [M]/k_m$ Where the [M] is the total concentration of surfactant in the mobile phase, and K_{AM} is the binding constant between micelle and solute molecule	HPLC, TLC, and OPLC derived property Micellar chromatography	[1]
R_M	Common retention parameter in TLC, A logarithmic function of the R_F value (retardation factor): $R_M = \log\left(\frac{1-R_F}{R_F}\right)$	TLC derived property	[2-4]
mR_M	Arithmetic mean of R_M values	TLC derived property	[2-4]
R_M^0	R_M value extrapolated to the zero content of organic mobile phase modifier	TLC derived property Typical reversed-phase modality	[2-4]
$PC1/R_M$	Scores corresponding to the first principal component of R_M	TLC derived property	[2-4]

Table S2 Summary of computationally estimated log*P* scales accompanied with short description.

log *P* scale	Description	Ref.
Alog*P*s	Property based, self-learning method based on the use of associative neural networks to predict the log*P* value from the molecular structure.	[5,6]
AClog*P*	Subgroup, atom-based method relying on 369 atom-type contribution values, obtained from 5000 molecules.	[5,6]
miLog*P*	Subgroup method, based on fragment contribution. It was developed using 35 small basic fragments and 185 larger fragments. Accounts for hydrogen bond contribution and charge interaction.	[5,6]
KOWWIN	Subgroup method; mixed both atom-based as well as fragment contribution method. Predicted log*P* values are obtained starting from the measured log*P* of structural analogues.	[5,6]
ABlog*P*	Subgroup method based on fragment contributions. It applies averaged correction factors, obtained from both simple and complex compounds.	[5,6]
Xlog*P*2	Subgroup, atom-based method, which uses 90 basic atom types and small number of correction factors.	[5,6]
Xlog*P*3	Subgroup, atom-based approach. The main difference compared to XlogP2 method is that it starts from the known log*P* value of a similar reference compound.	[5,6]
Mlog*P*	Property based, Moriguchi octanol-water partition coefficient - based on topological indices and quantitative structure-log*P* relationships	[5,6]
Alog*P*	Subgroup method, classical atomic contribution approach, which can be applied on neutral organic compounds containing C, H, O, N, S, Se, P, B, Si and halogen atoms.	[5,6]
Clog*P*	Subgroup, fragmental based method. Basic fragmental values were derived from measured log*P* data of simple molecules, and then the remaining fragment set was constructed.	[5,6]
logP^{C}	Subgroup, atomic based method. Calculated by the ChemOffice software based on Crippen's algorithm	[7]
logP^{V}	Subgroup, atomic based method calculated by the ChemOffice software based on Viswandahan's algorithm.	[7]
log*D*	Logarithm of a computationally estimated octanol-water distribution coefficient that takes into account the influence of pH.	[7]
Hy	Hydrophobicity index calculated by Dragon Plus software.	[7]

Table S3a Assessment of lipophilicity measures obtained by typical reversed phase TLC experiments and *in silico* approaches – Computationally estimated log*P* values of the studied compounds.

Comp. [a]	log*D*	*Hy*[b]	Mlog*P*	Alog*P*	logP_C	log*P*	Clog*P*	Alog*P*s	AClog*P*	ABlog*P*	miLog*P*	KOWWIN	Xlog*P*2	Xlog*P*3
1	1.37	0.7	1.93	1.25	1.51	1.45	1.08	1.81	0.97	0.1	1.52	0.50	1.41	1.77
2	-0.91	-0.95	3.21	3.35	4.22	0.92	4.61	3.18	2.56	3.58	1.74	4.41	3.67	4.74
3	1.18	-0.28	2.80	3.24	1.92	1.44	4.24	3.16	1.47	2.97	3.55	4.86	3.51	3.92
4	0.92	0.83	2.90	1.15	2.24	3.10	0.93	1.68	1.48	2.62	1.84	1.85	0.57	1.93
5	0.61	0.78	2.31	1.11	1.56	2.84	0.61	1.85	1.27	2.31	1.46	1.49	0.13	0.98
6	2.51	0.38	2.19	2.73	2.13	2.72	2.51	2.82	2.84	2.29	3.06	3.29	2.60	2.88
7	2.67	0.4	2.50	2.75	2.70	3.05	2.67	3.20	2.94	2.28	3.03	3.21	2.69	2.68
8	2.81	0.38	2.28	3.12	2.13	2.79	2.82	3.36	3.13	2.52	3.30	3.43	2.97	3.69
9	5.92	0.81	4.20	5.83	3.46	4.18	5.92	5.83	5.71	5.29	6.54	6.54	6.05	5.94
10	6.41	0.85	4.24	6.51	3.70	4.38	6.42	6.79	6.99	7.37	7.70	8.32	7.84	7.38
11	7.91	0.82	5.42	9.13	-2.52	3.18	7.91	6.41	8.24	8.33	8.73	10.89	9.07	8.62
12	7.88	0.84	3.72	9.74	1.20	2.45	7.88	6.99	9.59	9.07	9.43	11.63	9.88	9.89
13	-0.76	-0.8	0.13	0.91	-0.10	2.45	1.16	1.43	0.69	0.63	0.69	0.56	1.18	0.70
14	0.73	0.33	2.15	1.75	2.32	1.80	1.22	1.91	1.48	1.23	2.03	-0.15	1.44	0.99

[a]Derivatives of natural toxins and their identification numbers are given in the reference [7] (refrence [32] in the manuscript)

[b]Variables multiplied by -1

Table S3b Assessment of lipophilicity measures obtained by typical reversed phase TLC experiments and *in silico* approaches – Chromatographically estimated lipophilicity measures of the studied compounds under different chromatographic conditions.

Comp.[a]	RP-C18			RP-C18W			RP-C8			RP-C2		
	R_M^0(C18)	mR_M(C18)	PC1/R_M(C18)[b]	R_M^0(C18W)	mR_M(C18W)	$PC1/R_M$(C18W)[b]	R_M^0(C8)	mR_M(C8)	$PC1/R_M$(C8)[b]	R_M^0(C2)	mR_M(C2)	$PC1/R_M$(C2)[b]
1	3.41	-0.64	-1.92	0.85	-0.36	-1.43	2.81	-0.73	-1.55	3.84	-0.83	-0.79
2	0.33	-0.88	-2.46	0.36	-0.79	-2.38	0.82	-1.13	-2.45	5.04	-0.88	-0.93
3	1.09	-0.44	-1.47	0.60	-0.40	-1.52	1.55	-0.82	-1.76	3.56	-1.10	-1.37
4	1.34	0.44	0.5	1.83	0.70	0.94	2.54	0.04	0.17	1.93	-0.27	0.48
5	0.70	0.41	0.41	1.73	0.91	1.39	2.18	0.03	0.13	1.82	-0.32	0.37
6	2.37	0.38	0.36	2.46	0.42	0.32	3.52	0.07	0.23	1.91	-0.37	0.26
7	3.07	0.41	0.42	2.13	0.45	0.39	3.23	-0.01	0.05	1.81	-0.38	0.24
8	2.72	0.57	0.78	2.73	0.66	0.86	4.26	0.23	0.59	4.77	-0.40	0.14
9	5.44	0.68	1.05	3.83	0.33	0.14	6.22	0.44	1.08	3.18	-0.29	0.41
10	5.77	0.91	1.55	4.46	0.49	0.51	7.13	0.65	1.56	3.45	-0.18	0.67
11	7.68	1.06	1.89	5.75	0.85	1.32	8.56	0.84	1.98	4.14	-0.09	0.86
12	5.56	1.52	2.92	5.00	1.65	3.09	8.10	1.29	2.98	4.41	0.87	2.97
13	0.47	-0.89	-2.49	0.81	-0.72	-2.22	1.41	-0.88	-1.88	1.64	-1.54	-2.59
14	2.40	-0.30	-1.54	1.07	-0.36	-1.43	2.25	-0.54	-1.12	-0.17	-0.83	-0.72

[a]Derivatives of natural toxins and their identification numbers are given in the reference [7] (refrence [32] in the manuscript)

[b]Variables multiplied by -1

Table S3b Continues

Comp.[a]	RP-CN			RP-diol			RP-NH_2		
	R_M^0(CN)	mR_M(CN)	$PC1/R_M$(CN) [b]	R_M^0(Diol)	mR_M(Diol)	$PC1/R_M$(Diol) [b]	R_M^0 (NH_2)	mR_M (NH_2)	$PC1/R_M$ (NH_2) [b]
1	0.92	-0.04	-0.07	-0.16	-0.46	-0.62	-0.57	-0.84	-0.91
2	0.76	-1.01	-2.17	-0.47	-0.92	-1.66	-0.18	-0.45	-0.04
3	0.28	-0.62	-1.34	-0.38	-0.71	-1.2	-0.74	-0.81	-0.86
4	1.18	-0.08	-0.14	0.52	0.32	1.11	-0.36	-0.53	-0.22
5	0.78	-0.18	-0.36	0.63	0.42	1.35	-0.49	-0.60	-0.38
6	1.49	-0.15	-0.29	0.57	-0.07	0.25	-0.60	-0.70	-0.6
7	1.58	-0.16	-0.29	0.48	0.01	0.43	-0.60	-0.70	-0.61
8	2.07	0.04	0.16	1.06	0.16	0.77	-0.36	-0.53	-0.22
9	3.73	0.34	0.85	0.15	-0.48	-0.66	-0.02	-0.43	0.00
10	3.88	0.33	0.83	0.71	-0.37	-0.42	0.10	-0.20	0.51
11	4.67	0.43	1.09	0.67	-0.35	-0.38	0.56	0.34	1.72
12	4.72	1.29	2.96	2.36	1.17	3.03	1.11	0.76	2.67
13	0.83	-0.32	-0.67	-0.61	-0.64	-1.03	-0.51	-0.77	-0.77
14	0.90	-0.27	-0.56	-0.51	-0.61	-0.97	-0.08	-0.56	-0.30

[a]Derivatives of natural toxins and their identification numbers are given in the reference [7] (refrence [32] in the manuscript)

[b]Variables multiplied by -1

Table S4 Assessment of lipophilicity measures obtained by micellar chromatography and typical reversed phase TLC experiments combined with *in silico* approaches – Chromatographic lipophilicity indeces and computationally estimated log*P* values.

Comp.[a]	logk_m(TLC)	logk_m(OPLC)	R_M^0(1)	logk_m(HPLC)	R_M^0(2)	AClog*P*	Alog*P*s	Alog*P*	Xlog*P*3	Xlog*P*2	KOWWIN	Mlog*P*
1	0.78	0.73	1.60	1.00	2.66	2.11	2.46	2.68	2.67	2.56	2.58	2.80
2	0.88	0.82	1.82	1.23	2.80	2.52	3.02	3.05	3.10	3.02	3.00	3.05
3	0.93	0.88	1.90	1.31	3.00	2.58	2.79	3.13	3.02	3.13	3.07	3.06
4	1.02	0.93	2.11	1.46	3.10	2.58	2.64	3.39	3.27	3.49	3.30	3.55
5	1.09	0.97	2.06	1.48	3.13	2.79	3.26	3.38	3.33	3.35	3.39	3.57
6	1.02	0.93	2.10	1.50	3.10	2.69	2.96	3.36	3.30	3.26	3.47	3.31
7	1.11	1.02	2.25	1.68	3.13	2.80	3.27	3.66	3.58	3.61	3.86	3.57
8	1.16	1.05	1.90	1.80	2.96	2.92	3.00	3.71	3.73	3.65	3.79	3.79
9	1.22	1.21	2.44	1.88	3.32	3.41	3.94	4.04	3.96	3.97	3.47	4.09
10	1.36	1.23	2.55	2.22	3.6	3.49	3.87	4.13	4.02	4.15	4.28	4.20
11	0.65	0.85	1.40	2.13	2.52	1.84	1.64	1.91	2.15	2.14	2.25	2.97
12	0.75	1.12	1.65	2.57	2.66	2.24	2.37	2.28	2.58	2.60	2.67	3.22
13	0.83	1.20	1.70	2.55	2.72	2.30	2.01	2.36	2.51	2.71	2.74	3.22
14	0.86	1.33	1.91	2.80	2.81	2.31	2.15	2.62	2.75	3.07	2.98	3.71
15	0.92	1.32	1.8	2.91	3.04	2.52	2.68	2.61	2.81	2.93	3.07	3.74
16	0.81	1.27	1.95	2.86	3.00	2.41	2.78	2.59	2.79	2.84	3.15	3.47
17	0.95	1.57	2.00	3.03	3.10	2.52	2.30	2.89	3.07	3.19	3.54	3.72
18	1.01	1.68	1.86	3.12	2.89	2.65	2.40	2.94	3.21	3.23	3.47	3.94
19	1.07	1.79	2.1	3.44	3.19	3.13	3.27	3.28	3.44	3.55	3.15	4.24
20	1.14	2.00	2.3	3.67	3.41	3.21	3.58	3.36	3.51	3.73	3.96	4.36
21	0.98	1.66	1.91	3.29	3.18	2.83	2.95	3.10	3.18	3.37	3.61	3.97

[a]Derivatives of natural toxins and their identification numbers are given in the reference [1] (refrence [33] in the manuscript)

Table S5 Assessment of lipophilicity measures obtained by typical reversed phase TLC experiments and *in silico* approaches – Scaled rank values obtained by the SRD-CRRN and GPCM aproach in the case of three different pretereatment data methods: autoscaling (AS), interval scaling (IS) and ranking. (Rnk).

SRD scores						**GPCM scores**					
AS		**IS**		**Rnk**		**AS**		**IS**		**Rnk**	
mR_M(C18)	8.16	*PC*1/R_M (C18)	8.16	mR_M(C18)	8.16	*PC*1/RM(C18)	8.16	*PC*1/R_M(C18)	8.16	mR_M(C18)	8.16
*PC*1/R_M(C18)	8.16	mR_M(C18)	10.20	*PC*1/R_M (C18)	8.16	mR_M(C18)	10.54	mR_M(C18)	9.76	*PC*1/R_M(C18)	9.76
mR_M(C8)	12.24	R_M^0(C18W)	12.24	AClog*P*	12.24	mR_M(C8)	12.16	mR_M(C8)	12.98	AClog*P*	12.10
*PC*1/R_M(C8)	12.24	mR_M (C8)	12.24	mR_M(C8)	14.29	*PC*1/R_M(C8)	12.16	*PC*1/R_M(C8)	12.98	mR_M(C8)	16.16
R_M^0(C18W)	14.29	*PC*1/R_M (C8)	12.24	*PC*1/R_M (C8)	14.29	R_M^0(C18w)	12.95	R_M^0(C18W)	14.53	*PC*1/R_M(C8)	16.16
R_M^0(CN)	14.29	log*D*	14.29	R_M^0(C18w)	16.33	R_M^0(C8)	13.06	R_M^0(C8)	15.34	*PC*1/R_M(C2)	20.91
log*D*	16.33	AClog*P*	14.29	m R_M(C2)	18.37	log*D*	14.58	log*D*	15.36	R_M^0(C18W)	20.91
AClogP	16.33	R_M ^{0}(CN)	14.29	*PC*1/R_M(C2)	18.37	R_M^0(CN)	14.60	R_M^0(CN)	16.12	mR_M (C2)	20.92
R_M^0(C8)	16.33	R_M ^{0}(C8)	16.33	R_M^0(C8)	20.41	AClog*P*	17.73	AClog*P*	16.12	R_M^0(CN)	22.48
mR_M(CN)	16.33	miLog*P*	20.41	R_M^0(CN)	20.41	*PC*1/*R* (CN)	17.73	miLog*P*	21.67	mR_M(NH_2)	24.04
*PC*1/R_M(CN)	16.33	mR_M(C2)	20.41	mR_M(CN)	20.41	mR_M(CN)	17.75	*PC*1/R_M(CN)	23.22	*PC*1/R_M(CN)	25.58
mR_M (C2)	18.37	*PC*1/R_M(C2)	20.41	*PC*1/R_M(CN)	20.41	mR_M(C2)	19.40	mR_M(CN)	24.02	*PC*1/R_M(NH_2)	25.59
*PC*1/R_M(C2)	20.41	mR_M(CN)	20.41	mR_M(NH_2)	20.41	*PC*1/R_M(C2)	19.40	KOWWIN	25.66	R_M^0(C8)	26.41
R_M^0(Diol)	20.41	*PC*1/R_M(CN)	20.41	*PC*1/R_M(NH_2)	20.41	miLog*P*	24.10	ALOGPs	25.67	Alog*P*s	27.20
ALOGPs	24.49	Alog*P*s	22.45	Alog*P*s	22.45	R_M^0(Diol)	27.98	mR_M(C2)	27.18	mR_M(CN)	27.18
miLogP	24.49	R_M ^{0}(Diol)	22.45	miLog*P*	22.45	*Hy*	28.00	*PC*1/R_M(C2)	27.19	miLog*P*	28.00
R_M^0(C18)	24.49	Xlog*P*3	24.49	log*D*	24.49	*PC*1/R_M (C18W)	30.34	R_M^0(Diol)	27.96	ABlog*P*	28.00
mR_M(C18W)	24.49	R_M ^{0}(C18)	26.53	ABlog*P*	24.49	mR_M(C18W)	30.34	R_M^0(C18)	28.75	Mlog*P*	28.04
*PC*1/R_M(C18W)	24.49	Alog*P*	28.57	Mlog*P*	26.53	R_M^0(C18)	30.33	Xlog*P*3	29.51	Alog*P*	28.05
Xlog*P*3	26.53	ABlog*P*	28.57	KOWWIN	26.53	KOWWIN	31.15	*Hy*	31.90	log*D*	29.51
Hy	28.57	KOWWIN	28.57	Xlog*P*3	26.53	Alog*P*s	31.94	*PC*1/R_M(C18W)	32.74	R_M^0(Diol)	29.60
ABlog*P*	28.57	mR_M(C18W)	28.57	mR_M(C18W)	26.53	Xlog*P*3	33.51	mR_M(C18W)	32.74	Xlog*P*3	29.57
mR_M(NH_2)	28.57	*PC*1/R_M(C18W)	28.57	PC1/R_M(C18W)	26.53	Alog*P*	35.15	Alogi	34.31	*Hy*	31.18
*PC*1/R_M(NH_2)	28.57	mR_M(NH_2)	30.61	R_M^0(Diol)	26.53	mR_M(NH_2)	36.69	mR_M(NH_2)	34.35	KOWWIN	31.17
Alog*P*	30.61	PC1/R_M(NH_2)	30.61	Alog*P*	28.57	PC1/R_M(NH_2)	36.71	*PC*1/R_M(NH_2)	34.36	XLOG*P*2	31.16
KOWWIN	30.61	*Hy*	32.65	*Hy*	30.61	ABlog*P*	36.69	Xlog*P*2	35.15	*PC*1/R_M(C18w)	32.70
Mlog*P*	32.65	Mlog*P*	32.65	log*P*	32.65	Mlog*P*	36.77	ABlog*P*	35.14	mR_M(C18W)	32.70
log*P*	32.65	Xlog*P*2	32.65	Xlog*P*2	32.65	log*P*	36.72	Mlog*P*	36.72	R_M^0(C18)	34.35
Xlog*P*2	34.69	log*P*	34.69	R_M^0(C18)	32.65	Xlog*P*2	37.54	Clog*P*	38.24	R_M^0(NH_2)	35.16
R_M^0(NH_2)	36.73	Clog*P*	36.73	R_M^0(NH_2)	32.65	R_M^0(NH_2)	38.36	log*P*	38.29	Clog*P*	35.84
Clog*P*	38.78	RM0(NH2)	36.73	Clog*P*	34.69	Clog*P*	39.88	R_M^0(NH_2)	43.06	log*P*	35.93
mR_M(Diol)	38.78	mRM(Diol)	40.82	mR_M(Diol)	42.86	*PC*1/R_M Diol)	41.52	*PC*1/R_M(Diol)	45.45	*PC*1/R_M(Diol)	47.79
*PC*1/R_M(Diol)	38.78	PC1/RM(Diol)	40.82	*PC*1/R_M(Diol)	42.86	mR_M(Diol)	41.52	mR_M(Diol)	45.45	mR_M(Diol)	47.79

SRD scores						**GPCM scores**					
AS		**IS**		**Rnk**		**AS**		**IS**		**Rnk**	
R_M^0(C2)	53.06	R_M^0(C2)	53.06	logP_C	53.06	R_M^0(C2)	50.27	R_M^0(C2)	52.66	R_M^0(C2)	52.56
logP_C	55.10	logP_C	55.10	RM0(C2)	55.10	logP_C	55.10	logP_C	55.10	logP_C	55.10

Table S6 Assessment of lipophilicity measures obtained by micellar chromatography and typical reversed phase TLC experiments combined with *in silico* approaches – Scaled rank values obtained by the SRD-CRRN and GPCM aproach in the case of three different pretereatment data methods: autoscaling (AS), interval scaling (IS) and ranking (Rnk).

SRD scores						**GPCM scores**					
AS		**IS**		**Rnk**		**AS**		**IS**		**Rnk**	
AClog*P*	11.82	AClog*P*	12.73	AClog*P*	10.00	AClog*P*	11.82	AClog*P*	12.73	AClog*P*	10.00
Xlog*P*2	14.55	R_M^0(2)	14.55	R_M^0(2)	13.64	Xlog*P*2	16.60	Xlog*P*2	19.45	R_M^0(2)	19.73
R_M^0(2)	14.55	Xlog*P*2	15.45	Xlog*P*2	13.64	logk_m(TLC)	23.87	R_M^0(2)	21.91	Xlog*P*2	19.79
KOWWIN	17.27	KOWWIN	16.36	KOWWIN	15.45	R_M^0(2)	23.97	logk_m(TLC)	24.04	logk_m(TLC)	24.63
logk_m(TLC)	18.18	Mlog*P*	19.09	logk_m(TLC)	17.27	Xlog*P*3	28.70	Xlog*P*3	28.63	Xlog*P*3	24.63
Xlog*P*3	20.00	logk_m(TLC)	20.00	Xlog*P*3	19.09	R_M^0(1)	28.67	Mlog*P*	28.61	KOWWIN	24.60
Mlog*P*	20.91	Xlog*P*3	21.82	R_M^0(1)	21.82	KOWWIN	28.74	R_M^0(1)	28.57	Mlog*P*	29.54
R_M^0(1)	23.18	R_M^0(1)	25.00	Mlog*P*	21.82	Mlog*P*	31.16	KOWWIN	28.61	R_M^0(1)	32.02
Alog*P*s	27.73	Alog*P*s	29.55	Alog*P*s	26.36	Alog*P*s	33.69	Alog*P*s	35.53	Alog*P*	41.84
Alog*P*	31.36	Alog*P*	33.18	Alog*P*	30.00	Alog*P*	36.26	Alog*P*	40.18	Alog*P*s	44.26
logk_m(OPLC)	48.18	logk_m(OPLC)	46.36	logk_m(OPLC)	49.09	logk_m(OPLC)	53.09	logk_m(OPLC)	47.13	logk_m(OPLC)	54.17
logk_m(HPLC)	58.18	logk_m(HPLC)	56.36	logk_m(HPLC)	59.09	logk_m(HPLC)	58.18	logk_m(HPLC)	56.36	logk_m(HPLC)	59.09

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