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Supplementary material

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

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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.
$\log k_m$	<p>$\log k$ value at zero micellar concentration</p> <p>Derived from equation</p> $1/k = 1/k_m + K_{AM} \times [M]/k_m$ <p>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</p>	HPLC, TLC, and OPLC derived property Micellar chromatography	[1]
R_M	<p>Common retention parameter in TLC, A logarithmic function of the R_F value (retardation factor):</p> $R_M = \log \left(\frac{1 - R_F}{R_F} \right)$	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.
AlogPs	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]
AClogP	Subgroup, atom-based method relying on 369 atom-type contribution values, obtained from 5000 molecules.	[5,6]
miLogP	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]
ABlogP	Subgroup method based on fragment contributions. It applies averaged correction factors, obtained from both simple and complex compounds.	[5,6]
XlogP2	Subgroup, atom-based method, which uses 90 basic atom types and small number of correction factors.	[5,6]
XlogP3	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]
MlogP	Property based, Moriguchi octanol-water partition coefficient - based on topological indices and quantitative structure- $\log P$ relationships	[5,6]
AlogP	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]
ClogP	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]
$\log P^C$	Subgroup, atomic based method. Calculated by the ChemOffice software based on Crippen's algorithm	[7]
$\log P^V$	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	MlogP	AlogP	$\log P_C$	$\log P$	ClogP	AlogPs	AClogP	ABlogP	miLogP	KOWWIN	XlogP2	XlogP3
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

^aDerivatives of natural toxins and their identification numbers are given in the reference [7] (reference [32] in the manuscript)

^bVariables 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		
	$R_M^0(\text{C18})$	$mR_M(\text{C18})$	$PC1/R_M(\text{C18})^b$	$R_M^0(\text{C18W})$	$mR_M(\text{C18W})$	$PC1/R_M(\text{C18W})^b$	$R_M^0(\text{C8})$	$mR_M(\text{C8})$	$PC1/R_M(\text{C8})^b$	$R_M^0(\text{C2})$	$mR_M(\text{C2})$	$PC1/R_M(\text{C2})^b$
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

^aDerivatives of natural toxins and their identification numbers are given in the reference [7] (reference [32] in the manuscript)

^bVariables multiplied by -1

Table S3b Continues

Comp. ^a	RP-CN			RP-diol			RP-NH ₂		
	$R_M^0(\text{CN})$	$mR_M(\text{CN})$	$PC1/R_M(\text{CN})^b$	$R_M^0(\text{Diol})$	$mR_M(\text{Diol})$	$PC1/R_M(\text{Diol})^b$	$R_M^0(\text{NH}_2)$	$mR_M(\text{NH}_2)$	$PC1/R_M(\text{NH}_2)^b$
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

^aDerivatives of natural toxins and their identification numbers are given in the reference [7] (reference [32] in the manuscript)

^bVariables 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 indices and computationally estimated log*P* values.

Comp. ^a	log <i>k</i> _m (TLC)	log <i>k</i> _m (OPLC)	<i>R</i> _M ⁰ (1)	log <i>k</i> _m (HPLC)	<i>R</i> _M ⁰ (2)	AClog <i>P</i>	Alog <i>P</i> _s	Alog <i>P</i>	Xlog <i>P</i> ₃	Xlog <i>P</i> ₂	KOWWIN	Mlog <i>P</i>
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

^aDerivatives of natural toxins and their identification numbers are given in the reference [1] (reference [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 approach in the case of three different pretreatment data methods: autoscaling (AS), interval scaling (IS) and ranking. (Rnk).

SRD scores				GPCM scores							
AS		IS	Rnk	AS		IS		Rnk		Rnk	
$mR_M(C18)$	8.16	$PC1/R_M(C18)$	8.16	$mR_M(C18)$	8.16	$PC1/R_M(C18)$	8.16	$PC1/R_M(C18)$	8.16	$mR_M(C18)$	8.16
$PC1/R_M(C18)$	8.16	$mR_M(C18)$	10.20	$PC1/R_M(C18)$	8.16	$mR_M(C18)$	10.54	$mR_M(C18)$	9.76	$PC1/R_M(C18)$	9.76
$mR_M(C8)$	12.24	$R_M^0(C18W)$	12.24	AClogP	12.24	$mR_M(C8)$	12.16	$mR_M(C8)$	12.98	AClogP	12.10
$PC1/R_M(C8)$	12.24	$mR_M(C8)$	12.24	$mR_M(C8)$	14.29	$PC1/R_M(C8)$	12.16	$PC1/R_M(C8)$	12.98	$mR_M(C8)$	16.16
$R_M^0(C18W)$	14.29	$PC1/R_M(C8)$	12.24	$PC1/R_M(C8)$	14.29	$R_M^0(C18w)$	12.95	$R_M^0(C18W)$	14.53	$PC1/R_M(C8)$	16.16
$R_M^0(CN)$	14.29	logD	14.29	$R_M^0(C18w)$	16.33	$R_M^0(C8)$	13.06	$R_M^0(C8)$	15.34	$PC1/R_M(C2)$	20.91
logD	16.33	AClogP	14.29	$mR_M(C2)$	18.37	logD	14.58	logD	15.36	$R_M^0(C18W)$	20.91
AClogP	16.33	$R_M^0(CN)$	14.29	$PC1/R_M(C2)$	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	AClogP	17.73	AClogP	16.12	$R_M^0(CN)$	22.48
$mR_M(CN)$	16.33	miLogP	20.41	$R_M^0(CN)$	20.41	$PC1/R(CN)$	17.73	miLogP	21.67	$mR_M(NH_2)$	24.04
$PC1/R_M(CN)$	16.33	$mR_M(C2)$	20.41	$mR_M(CN)$	20.41	$mR_M(CN)$	17.75	$PC1/R_M(CN)$	23.22	$PC1/R_M(CN)$	25.58
$mR_M(C2)$	18.37	$PC1/R_M(C2)$	20.41	$PC1/R_M(CN)$	20.41	$mR_M(C2)$	19.40	$mR_M(CN)$	24.02	$PC1/R_M(NH_2)$	25.59
$PC1/R_M(C2)$	20.41	$mR_M(CN)$	20.41	$mR_M(NH_2)$	20.41	$PC1/R_M(C2)$	19.40	KOWWIN	25.66	$R_M^0(C8)$	26.41
$R_M^0(Diol)$	20.41	$PC1/R_M(CN)$	20.41	$PC1/R_M(NH_2)$	20.41	miLogP	24.10	ALOGPs	25.67	AlogPs	27.20
ALOGPs	24.49	AlogPs	22.45	AlogPs	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	miLogP	22.45	Hy	28.00	$PC1/R_M(C2)$	27.19	miLogP	28.00
$R_M^0(C18)$	24.49	XlogP3	24.49	logD	24.49	$PC1/R_M(C18W)$	30.34	$R_M^0(Diol)$	27.96	ABlogP	28.00
$mR_M(C18W)$	24.49	$R_M^0(C18)$	26.53	ABlogP	24.49	$mR_M(C18W)$	30.34	$R_M^0(C18)$	28.75	MlogP	28.04
$PC1/R_M(C18W)$	24.49	AlogP	28.57	MlogP	26.53	$R_M^0(C18)$	30.33	XlogP3	29.51	AlogP	28.05
XlogP3	26.53	ABlogP	28.57	KOWWIN	26.53	KOWWIN	31.15	Hy	31.90	logD	29.51
Hy	28.57	KOWWIN	28.57	XlogP3	26.53	AlogPs	31.94	$PC1/R_M(C18W)$	32.74	$R_M^0(Diol)$	29.60
ABlogP	28.57	$mR_M(C18W)$	28.57	$mR_M(C18W)$	26.53	XlogP3	33.51	$mR_M(C18W)$	32.74	XlogP3	29.57
$mR_M(NH_2)$	28.57	$PC1/R_M(C18W)$	28.57	$PC1/R_M(C18W)$	26.53	AlogP	35.15	Alogi	34.31	Hy	31.18
$PC1/R_M(NH_2)$	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
AlogP	30.61	$PC1/R_M(NH_2)$	30.61	AlogP	28.57	$PC1/R_M(NH_2)$	36.71	$PC1/R_M(NH_2)$	34.36	XLOGP2	31.16
KOWWIN	30.61	Hy	32.65	Hy	30.61	ABlogP	36.69	XlogP2	35.15	$PC1/R_M(C18w)$	32.70
MlogP	32.65	MlogP	32.65	logP	32.65	MlogP	36.77	ABlogP	35.14	$mR_M(C18W)$	32.70
logP	32.65	XlogP2	32.65	XlogP2	32.65	logP	36.72	MlogP	36.72	$R_M^0(C18)$	34.35
XlogP2	34.69	logP	34.69	$R_M^0(C18)$	32.65	XlogP2	37.54	ClogP	38.24	$R_M^0(NH_2)$	35.16
$R_M^0(NH_2)$	36.73	ClogP	36.73	$R_M^0(NH_2)$	32.65	$R_M^0(NH_2)$	38.36	logP	38.29	ClogP	35.84
ClogP	38.78	$RM^0(NH_2)$	36.73	ClogP	34.69	ClogP	39.88	$R_M^0(NH_2)$	43.06	logP	35.93
$mR_M(Diol)$	38.78	$mR_M(Diol)$	40.82	$mR_M(Diol)$	42.86	$PC1/R_M(Diol)$	41.52	$PC1/R_M(Diol)$	45.45	$PC1/R_M(Diol)$	47.79
$PC1/R_M(Diol)$	38.78	$PC1/R_M(Diol)$	40.82	$PC1/R_M(Diol)$	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	$R_M^0(C2)$	50.27	$R_M^0(C2)$	52.66
$\log P_C$	55.10	$\log P_C$	55.10	$\log P_C$	55.10	$\log P_C$	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 approach in the case of three different pretreatment data methods: autoscaling (AS), interval scaling (IS) and ranking (Rnk).

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

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References are cited in the manuscript as: [33], [14], [15], [26], [29], [30], and [32] respectively.