Supplementary data for article:

Aleksić, I.; Šegan, S.; Andrić, F.; Zlatović, M.; Moric, I.; Opsenica, D. M.; Senerovic, L. Long-Chain 4-Aminoquinolines as Quorum Sensing Inhibitors in Serratia Marcescens and Pseudomonas Aeruginosa. *ACS Chemical Biology* **2017**, *12* (5), 1425–1434. https://doi.org/10.1021/acschembio.6b01149

List of molecular descriptors

No.	Descriptor designation
1	mol_MW
2	dipole
3	SASA
4	FOSA
5	FISA
6	PISA
7	WPSA
8	volume
9	donorHB
10	accptHB
11	dip^2/V
12	ACxDN^.5/SA
13	glob
14	QPpolrz
15	QPlogPC16
16	QPlogPoct
17	QPlogPw
18	QPlogPo/w
19	QPlogS
20	CIQPlogS
21	QPlogHERG
22	QPPCaco
23	QPlogBB
24	QPPMDCK
25	QPlogKp
26	IPeV
27	EAeV
28	#metab
29	QPlogKhsa
30	PercentHumanOralAbsorption
31	PSA
32	NO
33	#nonHatm
34	FH1
35	FH2
36	TE
37	EE
38	CCR
39	GN
40	IP
41	NOFL
42	Dipole(PC)_X
43	Dipole(PC)_Y
44	Dipole(PC)_Z
45	Dipole(PC)_Total
46	Dipole(Hyb)_X
47	Dipole(Hyb)_Y

48 Dipole(Hyb)_Z
49 Dipole(Hyb)_ Total
50 Dipole(S)_ X
51 Dipole(S)_Y
52 Dipole(S)_ Z
53 Dipole(S)_Total
54 ZM1
55 ZM1V
56 ZM2
57 ZM2V
58 Pol
59 NST
60 NHT
61 NGT
62 TSC
63 W
64 MW
65 Xu
66 Qindex
67 RC
68 MSDB
69 SP
70 Har
71 LPRS
72 Pog
73 SMT
74 SMTV
75 MDDD
76 Ram
77 GMT
78 GMTV
79 AVDD
80 UP
81 CENT
82 VAR
83 MEV
84 MEPV
85 MENV
86 ECCc
87 ECC
88 AECC
89 DECC
90 vX0
91 vX1
92 vX2
93 vX3
94 vX4
95 vX5
96 AvX0
97 AvX1

98 AvX2
99 AvX3
100 AvX4
101 AvX5
102 QW
103 FM
104 SM
105 STN
106 KBLI
107 TCI1
108 TCI2
109 TCI3
110 TCI4
111 TCI5
112 TCI6
113 TCI7
114 TCI8
115 TCI9
116 TCI10
117 MTCI1
118 MTCI2
119 MTCI3
120 MTCI4
121 MTCI5
122 MTCI6
123 MTCI7
124 MTCI8
125 MTCI9
126 MTCI10
127 GTC
128 HDPI
129 RHDPI
130 SRDS
131 MRC
132 BC
133 LC
134 KHE
135 STD(N,N)
136 WhetZ
137 Whete
138 Whetm
139 Whetv
140 Whetp
141 JhetZ
142 Jhete
143 Jhetm
144 Jhetv
145 Jhetp
146 TD
147 TR

148 PJ2DS
149 J
150 SCIX0
151 SCIX1
152 SCIX2
153 SCIX3
154 SCIX4
155 SCIX5
156 CIX0
157 CIX1
158 CIX2
159 CIX3
160 CIX4
161 CIX5
162 ACIX0
163 ACIX1
164 ACIX2
165 ACIX3
166 ACIX4
167 ACIX5
168 RDR
169 RDSR
170 KAMS1
171 KAMS2
172 KAMS3
173 KF
174 RSIpw2
175 RSIpw3
176 RSIpw4
177 RSIpw5
178 ETP
179 ATMCNT
180 BNDCNT

Description/explanation/full name

Molecular weight of the molecule

Mulican molecular dipole

Total solvent accessible surface area (SASA) in square angstroms using a probe with a 1.4 Å radius

Hydrophobic component of the SASA (saturated carbon and attached hydrogen)

Hydrophilic component of the SASA (SASA on N, O, H on heteroatoms, and carbonyl C)

π (carbon and attached hydrogen) component of the SASA

Weakly polar component of the SASA (halogens, P, and S)

Total solvent-accessible volume in cubic angstroms using a probe with a 1.4 Å radius

Estimated number of hydrogen bonds that would be donated by the solute to water molecules in an aqueous soluti

Estimated number of hydrogen bonds that would be accepted by the solute from water molecules in an aqueous sol

Square of the dipole moment divided by the molecular volume

Index of cohesive interaction in solids

Globularity descriptor. Globularity is 1.0 for a spherical molecule

Predicted polarizability in cubic angstroms

Predicted hexadecane/gas partition coefficient

Predicted octanol/gas partition coefficient

Predicted water/gas partition coefficient

Predicted octanol/water partition coefficient

Predicted aqueous solubility, log S

Conformation-independent predicted aqueous solubility, log S

Predicted IC50 value for blockage of HERG K$^+$ channels

Predicted apparent Caco-2 cell permeability in nm/sec

Predicted brain/blood partition coefficient

Predicted apparent MDCK cell permeability in nm/sec

Predicted skin permeability, log K p

PM3 calculated ionization potential (negative of HOMO energy)

PM3 calculated electron affinity (negative of LUMO energy)

Number of likely metabolic reactions

Prediction of binding to human serum albumin

PHOA

Van der Waals surface area of polar nitrogen and oxygen atoms and carbonyl carbon atoms

Number of nitrogen and oxygen atoms

Number of heavy atoms (nonhydrogen atoms)

Final heat (KCal)

Final heat (KJ)

Total energy (Ev)

Electronic energy (Ev)

Core-core repulsion (Ev)

Gradient norm

Ionization potential

No of filled levels

Point Charges componet of the dipole moment, molecular dipole along X direction

Point Charges componet of the dipole moment, molecular dipole along Y direction

Point Charges componet of the dipole moment, molecular dipole along Z direction

Point Charges componet of the dipole moment, molecular dipole total

Hybrid componet of the dipole moment, molecular dipole along X direction

Hybrid componet of the dipole moment, molecular dipole along Y direction

Hybrid componet of the dipole moment, molecular dipole along Z direction
Hybrid componet of the dipole moment, molecular dipole along total
Sum of hybrid and point-charges dipole contributions, molecular dipole along X direction
Sum of hybrid and point-charges dipole contributions, molecular dipole along Y direction
Sum of hybrid and point-charges dipole contributions, molecular dipole along Z direction
Sum of hybrid and point-charges dipole contributions, molecular dipole total
First Zagreb index
First Zagreb index by valence vertex degrees
Second Zagreb index
Second Zagreb index by valence vertex degrees
Polarity
Narumi Simple Topological index
Narumi Harmonic Topological index
Narumi Geometric Topological index
Total structure connectivity index
Wiener index
Mean Wiener index
Xu index
Quadratic index
Radial centric index
Mean Square Distance Balaban index
Superpendentic index
Harary index
Log of product of row sums (LPRS)
Pogliani index
Schultz Molecular Topological index
Schultz Molecular Topological by valence vertex degrees index
Mean Distance Degree Deviation
Ramification index
Gutman Molecular Topological index
Gutman MTI by valence vertex degrees
Average vertex distance degree
Unipolarity
Centralization
Variation
Molecular electrotopological variation
Maximal electrotopological positive variation
Maximal electrotopological negative variation
Eccentric connectivity index
Eccentricity
Average eccentricity (AECC)
Eccentric
Valence connectivity index chi-0
Valence connectivity index chi-1
Valence connectivity index chi-2
Valence connectivity index chi-3
Valence connectivity index chi-4
Valence connectivity index chi-5
Average valence connectivity index chi-0
Average valence connectivity index chi-1

Average valence connectivity index chi-2
Average valence connectivity index chi-3
Average valence connectivity index chi-4
Average valence connectivity index chi-5
Quasi Wiener index (Kirchhoff number)
First Mohar index
Second Mohar index
Spanning tree number
Kier benzene-likeliness index
Topological charge index of order 1
Topological charge index of order 2
Topological charge index of order 3
Topological charge index of order 4
Topological charge index of order 5
Topological charge index of order 6
Topological charge index of order 7
Topological charge index of order 8
Topological charge index of order 9
Topological charge index of order 10
Mean topological charge index of order 1
Mean topological charge index of order 2
Mean topological charge index of order 3
Mean topological charge index of order 4
Mean topological charge index of order 5
Mean topological charge index of order 6
Mean topological charge index of order 7
Mean topological charge index of order 8
Mean topological charge index of order 9
Mean topological charge index of order 10
Global topological charge index
Hyper-distance-path index
Reciprocal hyper-distance-path index
Square reciprocal distance sum
Modified Randic connectivity index
Balaban centric index
Lopping centric index
Kier Hall electronegativity index
Sum of topological distances between N..N
Wiener-type index from Z weighted distance matrix - Barysz matrix
Wiener-type index from electronegativity weighted distance matrix
Wiener-type index from mass weighted distance matrix
Wiener-type index from van der waals weighted distance matrix
Wiener-type index from polarizability weighted distance matrix
Balaban-type index from Z weighted distance matrix - Barysz matrix
Balaban-type index from electronegativity weighted distance matrix
Balaban-type index from mass weighted distance matrix
Balaban-type index from van der waals weighted distance matrix
Balaban-type index from polarizability weighted distance matrix
Topological diameter
Topological radius

Petitjean 2D shape index
Balaban distance connectivity index
Solvation connectivity index chi-0
Solvation connectivity index chi-1
Solvation connectivity index chi-2
Solvation connectivity index chi-3
Solvation connectivity index chi-4
Solvation connectivity index chi-5
Connectivity index chi-0 index
Connectivity chi-1 index (Randic connectivity index)
Connectivity index chi-2
Connectivity index chi-3
Connectivity index chi-4
Connectivity index chi-5
Average connectivity index chi-0
Average connectivity index chi-1
Average connectivity index chi-2
Average connectivity index chi-3
Average connectivity index chi-4
Average connectivity index chi-5
Reciprocal distance Randic-type index
reciprocal distance square Randic-type index
1-path Kier alpha-modified shape index
2-path Kier alpha-modified shape index
3-path Kier alpha-modified shape index
Kier flexibility
Path/walk 2 - Randic shape index
Path/walk 3 - Randic shape index
Path/walk 4 - Randic shape index
Path/walk 5 - Randic shape index
E-state topological parameter
Atom Count
Bond Count

Descriptor type

Electrostatic
Geometrical
Geometrical
Geometrical
Geometrical
Geometrical
Geometrical
Constitutional
Constitutional

Physico-chemical property
Physico-chemical property
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Physico-chemical property
Quantno-mechanical
Quantno-mechanical

Physico-chemical property
Physico-chemical property

Constitutional
Constitutional
Thermodynamic
Thermodynamic

Electrostatic

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Electrotopological state index

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Electrotopological state index
Constitutional
Constitutional

Compunds molecular descriptors data matrix

No.	Compound	Molecular descriptors						
		mol_MW	dipole	SASA	FOSA	FISA	PISA	WPSA
1	**23**	60.099	2.733	233.199	115.244	117.955	0	0
2	**24**	88.152	0.001	302.994	173.18	129.814	0	0
3	**25**	116.206	0	369.007	239.227	129.781	0	0
4	**26**	144.259	0.001	434.984	305.207	129.777	0	0
5	**27**	200.367	0	566.97	437.193	129.777	0	0
6	**16**	198.051	1.833	372.932	0	21.602	216.368	134.961
7	**14**	163.606	0.588	348.689	0	21.691	263.726	63.272
8	**22**	220.676	0.343	407.146	0	40.08	211.406	155.66
9	**18**	179.605	6.073	363.266	0	78.636	213.007	71.624
10	**17**	231.604	3.138	400.677	0.728	21.531	197.609	180.809
11	**8**	255.242	7.156	474.499	84.769	96.739	175.807	117.184
12	**9**	339.403	6.721	673.147	283.413	94.91	177.962	116.862
13	**10**	395.51	6.759	805.535	415.381	94.921	178.046	117.187
14	**14**	163.606	3.559	353.209	0	21.797	259.822	71.59
15	**1**	221.689	4.998	455.258	86.644	92.035	204.933	71.647
16	**2**	249.742	5.672	514.415	150.73	94.841	197.198	71.646
17	**3**	249.742	5.635	514.445	150.757	94.821	197.222	71.646
18	**4**	305.85	5.806	646.315	282.688	94.962	197.02	71.645
19	**5**	361.957	5.793	778.372	414.715	94.908	197.102	71.646
20	**20**	285.57	3.927	466.872	84.627	28.934	202.32	150.992
21	**21**	222.674	7.567	446.062	96.331	77.317	200.987	71.427
22	**11**	319.876	6.273	637.115	353.207	26.012	186.483	71.414
23	**6**	187.244	3.176	431.151	86.595	92.073	252.484	0
24	**7**	215.297	4.363	490.346	150.77	94.819	244.756	0
25	**12**	178.621	6.286	365.931	0	75.178	219.14	71.613
26	**19**	145.16	2.685	340.419	0	67.375	273.044	0
27	**13**	129.161	2.089	329.937	0	21.883	308.054	0

volume	donorHB	accptHB	dip^2/V	ACxDN^.5	glob	QPpolrz	QPlogPC16	QPlogPoct
315.238	4	2	0.023696	0.017153	0.960575	4.536	2.935	7.804
441.365	4	2	0	0.013202	0.925259	8.299	4.083	8.714
562.54	4	2	0	0.01084	0.893098	11.864	5.114	9.829
683.658	4	2	0	0.009196	0.862816	15.427	6.182	10.943
925.939	4	2	0	0.007055	0.810327	22.555	8.481	13.172
589.005	0	1	0.005702	0	0.911203	19.484	6.382	6.975
544.734	0	1	0.000634	0	0.925088	18.165	5.874	6.19
657.778	0	3.5	0.000179	0	0.898396	20.905	7.236	8.844
570.458	1	2.5	0.064653	0.006882	0.915705	18.71	6.386	9.747
642.793	0	1	0.015321	0	0.898984	21.458	5.443	7.973
781.362	3	3	0.06554	0.010951	0.864633	24.227	7.242	14.893
1146.026	3	3	0.039419	0.007719	0.786776	34.989	10.729	17.896
1388.719	3	3	0.032892	0.006451	0.747292	42.133	13.299	20.042
549.897	0	1	0.02303	0	0.91901	18.334	5.899	6.58
737.232	3	3	0.033878	0.011414	0.866916	22.739	8.236	13.737
850.903	3	3	0.037814	0.010101	0.844186	25.93	9.248	14.794
850.944	3	3	0.037321	0.010101	0.844163	25.932	9.248	14.788
1093.104	3	3	0.030835	0.00804	0.794015	33.053	11.591	16.926
1335.471	3	3	0.025126	0.006676	0.753473	40.184	14.132	19.078
757.946	1	2	0.020347	0.004284	0.861111	24.185	8.056	10.706
723.292	2	3.7	0.079156	0.011731	0.8736	22.143	7.776	13.008
1108.451	1	4	0.035501	0.006278	0.813001	34.85	10.722	15.036
693.021	3	3	0.014552	0.012052	0.878414	21.424	7.685	12.757
806.696	3	3	0.023594	0.010597	0.854677	24.615	8.677	13.884
575.883	1.5	2	0.068616	0.006694	0.914791	18.344	6.568	10.088
527.066	1	1.75	0.013682	0.005141	0.92696	16.905	5.871	7.684
506.497	0	1	0.008612	0	0.931362	17.058	5.392	5.681

QPlogPw	QPlogPo/w	QPlogS	CIQPlogS	QPlogHERG	QPPCaco	QPlogBB	QPPMDCK	QPlogKp
8.249	-1.931	2	1.866	-3.622	46.896	0.327	22.17	-7.531
8.057	-1.366	2	1.79	-4.194	36.197	0.048	16.758	-7.557
7.774	-0.68	1.939	1.463	-4.714	36.224	-0.146	16.771	-7.364
7.492	0.037	1.178	1.031	-5.204	36.227	-0.344	16.772	-7.172
6.927	1.523	-0.457	0.03	-6.053	36.226	-0.741	16.772	-6.788
3.268	3.242	-2.905	-3.414	-4.001	6180.788	0.721	10000	-1.155
3.507	2.326	-1.832	-2.683	-4.002	6168.824	0.55	7853.569	-0.99
5.47	2.437	-2.453	-2.735	-4.184	4128.776	0.494	10000	-1.321
6.529	1.606	-2.269	-2.462	-3.912	1779.08	0.114	2275.809	-2.218
3.222	3.774	-4.087	-4.127	-4.109	6190.501	0.83	10000	-1.22
9.222	1.974	-2.168	-2.534	-5.287	298.829	0.146	650.369	-4.362
8.379	4.224	-4.631	-4.198	-6.557	311.003	-0.376	676.298	-3.744
7.816	5.752	-6.363	-5.336	-7.196	310.929	-0.727	678.907	-3.36
3.495	2.36	-1.908	-2.683	-4.082	6154.527	0.567	8700.564	-1.006
9.326	1.6	-1.651	-1.897	-5.389	331.154	0.08	409.186	-4.172
8.994	2.255	-2.357	-2.429	-5.72	311.475	-0.111	382.965	-4.059
8.994	2.255	-2.357	-2.429	-5.72	311.611	-0.111	383.143	-4.059
8.429	3.742	-3.958	-3.526	-6.531	310.656	-0.469	381.87	-3.678
7.864	5.263	-5.673	-4.653	-7.187	311.016	-0.82	382.351	-3.293
5.241	3.769	-4.214	-4.775	-4.744	5266.42	0.493	10000	-1.052
8.402	2.105	-2.762	-2.849	-4.536	1831.073	-0.178	2341.97	-1.852
6.363	4.315	-4.212	-3.663	-6.173	1400.014	0.393	1938.161	-2.636
9.567	1.122	-0.946	-1.272	-5.43	330.883	-0.075	165.598	-4.006
9.234	1.771	-1.597	-1.779	-5.777	311.621	-0.265	155.203	-3.891
6.573	2.062	-2.32	-2.565	-3.956	1918.599	0.08	2468.975	-2.037
5.822	2.143	-1.886	-2.033	-4.016	2275.013	-0.02	1202.839	-1.703
3.742	2.091	-1.345	-1.951	-4.112	6143.002	0.395	3519.623	-0.838

IPeV	EAeV	#metab	QPlogKhsa	PercentHu	PSA	NO	#nonHatm	FH1
9.423	-2.641	4	-1.125	45.547	52.105	2	4	149.0623
9.481	-2.782	4	-1.015	46.845	54.996	2	6	337.1198
9.514	-2.766	4	-0.85	50.868	54.984	2	8	310.4847
9.519	-2.76	4	-0.655	55.068	54.983	2	10	291.2182
9.515	-2.762	4	-0.214	63.767	54.983	2	14	262.2149
9.095	1.271	1	0.06	100	12.244	1	12	36.69796
8.99	1.105	1	-0.068	100	12.247	1	11	43.65359
9.169	1.77	1	-0.494	100	24.745	2	14	94.59187
8.631	0.629	2	-0.281	94.523	42.463	2	12	-9.60144
9.367	1.517	1	0.217	100	12.23	1	15	-115.139
8.531	1.123	5	-0.166	82.81	51.098	3	18	42.95221
8.45	1.066	5	0.498	96.293	50.591	3	24	169.5796
8.44	1.058	5	0.978	92.281	50.592	3	28	143.0174
9.051	1.088	1	-0.053	100	12.292	1	11	43.79006
8.307	0.84	5	-0.274	81.416	50.536	3	15	380.7786
8.307	0.835	5	-0.086	84.774	50.582	3	17	353.6745
8.309	0.837	5	-0.085	84.78	50.584	3	17	353.7422
8.275	0.81	5	0.358	93.464	50.598	3	21	317.6285
8.267	0.803	5	0.833	89.422	50.592	3	25	291.3262
8.532	0.962	3	0.157	100	23.823	2	15	176.7153
8.271	0.768	4	-0.303	100	45.212	3	15	131.0262
8.334	0.809	4	0.514	100	25.462	3	22	359.1455
8.173	0.656	5	-0.374	78.611	50.527	3	14	383.8124
8.172	0.649	5	-0.192	81.945	50.563	3	16	357.0246
8.319	0.792	2	-0.275	100	37.017	2	12	168.2211
8.651	0.827	2	-0.324	100	33.347	2	11	7.5331
8.952	0.908	1	-0.179	100	12.295	1	10	51.13395

FH2	TE	EE	CCR	GN	IP	NOFL	Dipole(PC)	Dipole(PC)
623.6765	-792.048	-2848.15	2056.101	0	14.18818	13	-4.735	-0.163
1410.509	-1105.55	-4904.1	3798.555	0	19.79071	19	0	0
1299.068	-1414.14	-7101.39	5687.248	0	17.90899	25	-0.001	0
1218.457	-1722.41	-9483.33	7760.92	0	16.61201	31	0	-0.001
1097.107	-2338.54	-14675.3	12336.76	0	14.98382	43	0	0
153.5443	-2174.45	-9807.77	7633.316	0	9.21089	30	1.227	0.409
182.6466	-1804.64	-8389.43	6584.788	0	8.94825	27	-0.697	-0.651
395.7724	-2311.75	-11585.8	9274.019	0	9.20035	34	0.416	1.361
-40.1724	-2121.58	-9890.84	7769.261	0	8.78938	30	1.486	-3.152
-481.742	-3378.83	-15557.9	12179.08	0	9.38791	39	1.59	1.873
179.712	-3772.54	-20861.9	17089.39	0	11.26994	48	28.542	1.88
709.5211	-4703.58	-30694.5	25990.94	0	14.12694	66	43.984	2.423
598.3849	-5319.6	-37184	31864.45	0	13.76873	78	43.652	23.704
183.2176	-1804.64	-8301.59	6496.952	0	9.05487	27	1.696	2.157
1593.178	-2574.32	-14753.4	12179.11	0	15.33263	39	-2.503	25.452
1479.774	-2882.93	-17798.7	14915.8	0	14.7686	45	27.291	3.167
1480.057	-2882.92	-17795.7	14912.73	0	14.76782	45	26.646	12.232
1328.957	-3499.36	-23791.6	20292.28	0	14.01179	57	35.176	3.715
1218.909	-4115.37	-29981.7	25866.35	0	13.65583	69	40.405	0.335
739.3769	-2688.79	-14424.3	11735.54	0	13.05185	39	-4.132	6.488
548.2136	-2661.34	-14729.2	12067.87	0	12.85088	39	5.06	3.364
1502.665	-3651.28	-28004.1	24352.87	0	14.96413	60	-9.454	0.45
1605.871	-2204.68	-13152.2	10947.54	0	15.19939	36	-1.708	-6.247
1493.791	-2513.27	-16115.7	13602.38	0	14.58644	42	2.296	18.097
703.8372	-2037.67	-10101.5	8063.828	0	13.12308	30	7.279	2.283
31.51848	-1751.33	-8495.05	6743.726	0	8.5201	27	1.409	0.399
213.9444	-1434.81	-6953.78	5518.971	0	8.78618	24	-0.277	-1.129

Dipole(PC)	Dipole(PC)	Dipole(Hyk	Dipole(Hyk	Dipole(Hyk	Dipole(Hyk	Dipole(S)_	Dipole(S)_'	Dipole (S)_
-1.914	5.11	-0.976	-0.281	0.817	1.304	-5.711	-0.444	-1.096
-0.001	0.001	0	0	0	0	0	0	-0.001
0.011	0.011	0	0	0.001	0.001	-0.001	0	0.012
0.006	0.006	0	0	0	0	0	-0.001	0.006
0.014	0.014	0	0	0.001	0.001	0	0	0.015
-0.013	1.293	-0.131	1.103	-0.014	1.111	1.096	1.512	-0.027
-0.01	0.953	0.096	1.253	0.004	1.257	-0.6	0.602	-0.007
0	1.423	0.468	-0.811	0	0.937	0.885	0.549	0
0.014	3.485	-0.192	-1.165	0.014	1.181	1.293	-4.318	0.028
-0.053	2.457	1.025	-0.41	0.266	1.136	2.616	1.463	0.212
-8.663	29.887	1.451	-0.932	-0.388	1.767	29.993	0.948	-9.051
-9.278	45.018	0.451	-0.127	-0.212	0.514	44.435	2.296	-9.49
4.112	49.842	0.342	0.333	-0.089	0.486	43.994	24.037	4.023
-0.034	2.744	-0.173	0.855	-0.011	0.873	1.523	3.012	-0.045
2.564	25.703	-0.041	0.338	0.044	0.343	-2.544	25.789	2.608
11.641	29.838	0.31	0.222	0.172	0.419	27.601	3.389	11.813
-5.708	29.87	0.254	0.324	-0.088	0.421	26.9	12.555	-5.796
7.655	36.191	0.272	0.155	0.213	0.378	35.448	3.87	7.869
2.106	40.461	0.301	0.159	0.116	0.359	40.706	0.494	2.222
0	7.691	-0.397	0.196	0	0.442	-4.528	6.683	0
1.209	6.196	-0.178	-0.234	0.247	0.384	4.883	3.13	1.456
-9.225	13.217	0.327	0.259	0.691	0.807	-9.127	0.709	-8.534
15.293	16.608	0.022	-0.146	0.565	0.584	-1.686	-6.393	15.858
8.494	20.122	0.053	0.638	0.098	0.647	2.348	18.734	8.592
-0.051	7.629	0.031	-0.178	0.002	0.181	7.31	2.105	-0.048
0	1.465	0.89	0.653	0	1.103	2.299	1.052	0
0.002	1.162	0.037	-1.004	-0.003	1.005	-0.24	-2.132	-0.002

Dipole (S)_ ZM1		ZM1V	ZM2		ZM2V	Pol		NST	NHT	NGT
5.833	10	21	8		14	1	1.386294	1.333333	1.414214
0.001	18	24	16		20	3	2.772589	1.5	1.587401
0.012	26	32	24		28	5	4.158883	1.6	1.681793
0.006	34	40	32		36	7	5.545177	1.666667	1.741101
0.015	50	56	48		52	11	8.317766	1.75	1.811447
1.867	62	135.2099	72	151.2222		17	8.553332	1.894737	2.039649
0.85	56	127.6049	65	142.1111		15	8.147867	2	2.097435
1.041	70	176.0494	81	190.7778		20	9.939627	1.909091	2.033937
4.507	62	161.6049	72	165.1111		17	8.553332	1.894737	2.039649
3.004	80	297.6049	93	248.1111		23	9.939627	1.747573	1.93991
31.343	92	325	106		277	27	12.01907	1.785124	1.949798
45.495	116	340	130		294	33	16.17795	1.834395	1.962229
50.294	132	356	146		310	37	18.95054	1.856354	1.967581
3.376	56	127.6049	64	141.1111		14	8.147867	2	2.097435
26.045	74	153.6049	85	173.1111		21	10.63277	1.914894	2.031657
30.213	82	161.6049	93	181.1111		23	12.01907	1.924528	2.027907
30.246	82	161.6049	93	181.1111		23	12.01907	1.924528	2.027907
36.517	98	177.6049	109	197.1111		27	14.79166	1.938462	2.022561
40.769	114	193.6049	125	213.1111		31	17.56425	1.948052	2.018934
8.073	74	149.6722	85	169.6296		21	10.63277	1.914894	2.031657
5.98	74	174.6049	85	179.1111		21	10.63277	1.914894	2.031657
12.516	106	189.6049	120	214.1111		31	14.90944	1.833333	1.969347
17.181	68	146	78		164	19	10.22731	2	2.076164
20.744	76	154	86		172	21	11.6136	2	2.066487
7.607	62	134.6049	72	153.1111		17	8.553332	1.894737	2.039649
2.528	56	152	65		159	15	8.147867	2	2.097435
2.146	50	120	57		132	12	7.742402	2.142857	2.168944

TSC	W	MW	Xu	Qindex	RC	MSDB	SP	Har
0.849322	10	1.666667	3.160901	0	1	0.527046	3.162278	4.333333
0.600561	35	2.333333	5.968912	0	1.584963	0.483046	5.477226	8.7
0.490356	84	3	8.584143	0	2	0.46291	8.3666	13.74286
0.424661	165	3.666667	11.05289	0	2.321928	0.451335	11.74734	19.28968
0.346734	455	5	15.65731	0	2.807355	0.438529	19.74842	31.52187
0.341926	181	2.742424	11.73091	10	1.855389	0.264827	10.34408	31.75
0.350331	140	2.545455	10.69955	9	1.494919	0.266598	5.656854	27.85
0.317187	292	3.208791	13.89952	10	2.120952	0.267374	14.14214	39.27738
0.341926	181	2.742424	11.73091	10	1.855389	0.264827	10.34408	31.75
0.317187	346	3.295238	14.73538	13	1.965596	0.25626	58.07753	44.30714
0.288446	614	4.013072	17.84691	13	2.413834	0.262904	102.45	56.49087
0.248621	1663	6.025362	24.21402	13	3.053509	0.304337	255.9004	79.86566
0.229715	2829	7.484127	28.18219	13	3.351823	0.326433	424.0083	95.75204
0.350331	144	2.618182	10.79748	9	1.823068	0.277533	6	27.63333
0.306674	368	3.504762	15.04104	10	2.199581	0.274709	16.06238	42.9254
0.288446	566	4.161765	17.31721	10	2.513646	0.292089	20.04994	50.1917
0.288446	566	4.161765	17.31721	10	2.513646	0.292089	20.04994	50.1917
0.260011	1174	5.590476	21.67536	10	2.927799	0.323073	28.80972	64.9449
0.238608	2118	7.06	25.75512	10	3.253661	0.344996	38.704	80.18025
0.306674	368	3.504762	15.04104	10	2.199581	0.274709	16.06238	42.9254
0.306674	368	3.504762	15.04104	10	2.199581	0.274709	16.06238	42.9254
0.258982	1212	5.246753	22.04651	12	2.776725	0.283806	147.2141	71.85893
0.312694	303	3.32967	14.08432	9	2.182006	0.278978	8.246211	38.64643
0.293438	480	4	16.3999	9	2.45282	0.298142	9.848858	45.72183
0.341926	181	2.742424	11.73091	10	1.855389	0.264827	10.34408	31.75
0.350331	140	2.545455	10.69955	9	1.494919	0.266598	5.656854	27.85
0.359387	109	2.422222	9.750789	8	1.521928	0.28153	0	23.9

LPRS	Pog	SMT	SMTV	MDDD	Ram	GMT	GMTV	AVDD
6.356108	9	36	60	1	0	19	52	5
14.60634	13	126	160	2.222222	0	85	140	11.66667
24.17241	17	304	364	4	0	231	336	21
34.73256	21	602	696	6.4	0	489	660	33
58.11253	29	1686	1872	12.57143	0	1469	1820	65
40.71127	25.16667	822	1225.889	4.166667	4	771	1566.741	30.16667
35.47754	22.83333	655	1024.222	3.22314	3	618	1371.222	25.45455
51.94445	29.33333	1269	2021.667	6.530612	4	1197	2829.259	41.71429
40.71127	25.83333	822	1404	4.166667	4	771	2076.889	30.16667
57.22526	35.33333	1491	3166.222	7.626667	6	1398	5882.111	46.13333
75.58315	42	2552	5165	12.74074	6	2413	9288	68.22222
117.7029	54	6778	11620	28.01389	6	6603	17847	138.5833
147.9356	62	11502	18516	39.15816	6	11343	26943	202.0714
35.77524	22.83333	672	1044.333	3.322314	3	638	1396.111	26.18182
58.05256	31.83333	1577	2296.667	8.355556	4	1498	3020.889	49.06667
70.94332	35.83333	2383	3316	12.17301	4	2296	4251.556	66.58824
70.94332	35.83333	2383	3316	12.17301	4	2296	4251.556	66.58824
98.53451	43.83333	4867	6392	20.3356	4	4788	7939.556	111.8095
127.7458	51.83333	8727	11064.44	29.6128	4	8688	13476.44	169.44
58.05256	31.08333	1577	2160.889	8.355556	4	1498	2606.593	49.06667
58.05256	32.33333	1577	2530.667	8.355556	4	1498	3734.889	49.06667
102.9935	45.83333	4996	6472.111	18.57851	6	4869	7829.889	110.1818
52.44563	29.5	1320	1992	6.938776	3	1261	2721	43.28571
65.12441	33.5	2046	2934	10.25	3	1983	3881	60
40.71127	25.33333	822	1281	4.166667	4	771	1738.889	30.16667
35.47754	23.5	655	1170	3.22314	3	618	1811	25.45455
30.72002	20.5	527	862	2.56	2	505	1216	21.8

UP	CENT	VAR	MEV	MEPV	MENV	ECCc	ECC	AECC
4	4	2	2.888889	0.965278	0.791667	14	10	2.5
9	16	6	2.781667	0.695417	0.435	38	24	4
16	40	12	3.070782	0.767696	0.405612	74	44	5.5
25	80	20	3.238606	0.809652	0.393519	122	70	7
49	224	42	3.425363	0.856341	0.383876	254	140	10
23	86	18	9.25197	1.815185	0.988642	119	57	4.75
19	71	12	5.927037	1.805926	0.906852	99	47	4.272727
30	164	32	9.496057	1.730155	1.006035	173	84	6
23	86	18	12.62558	4.22692	1.652392	119	57	4.75
35	167	23	31.17948	4.355566	5.59902	174	85	5.666667
50	328	56	31.96504	4.567309	5.590633	279	138	7.666667
99	950	130	32.81312	4.781939	5.570137	615	301	12.54167
149	1486	182	33.40523	4.852785	5.570982	903	441	15.75
20	68	15	5.675427	1.667559	0.934074	108	51	4.636364
35	211	41	8.300292	1.813844	0.923094	210	102	6.8
47	333	60	8.892673	1.858139	0.913928	295	143	8.411765
47	333	60	8.892673	1.858139	0.913928	295	143	8.411765
81	647	100	9.421209	1.913274	0.904464	507	245	11.66667
127	1061	144	9.679214	1.946238	0.899748	767	371	14.84
35	211	41	8.043642	1.816344	0.920008	210	102	6.8
35	211	41	11.60277	2.75234	1.381258	210	102	6.8
80	664	76	9.625934	1.948509	0.906346	458	224	10.18182
31	172	36	5.384571	0.854815	0.604231	181	87	6.214286
42	288	54	5.993241	0.974676	0.495687	263	126	7.875
23	86	18	8.020581	1.743195	0.954306	119	57	4.75
19	71	12	8.678889	3.308704	1.427685	99	47	4.272727
17	48	8	2.648148	1.181204	0.606481	90	42	4.2

DECC	vX0	vX1	vX2	vX3	vX4	vX5	AvX0	AvX1
0.5	2.698671	1.408248	0.642229	0.204124	0	0	0.674668	0.469416
0.666667	4.242641	2.5	1.414214	0.75	0.353553	0.125	0.707107	0.5
1	5.656854	3.5	2.12132	1.25	0.707107	0.375	0.707107	0.5
1.2	7.071068	4.5	2.828427	1.75	1.06066	0.625	0.707107	0.5
1.714286	9.899495	6.5	4.242641	2.75	1.767767	1.125	0.707107	0.5
0.791667	6.089894	3.469813	2.454246	1.651565	1.086351	0.484195	0.507491	0.266909
0.661157	5.78928	3.370147	2.309924	1.595836	1.060962	0.44425	0.526298	0.280846
0.857143	7.067391	3.932168	2.694639	1.847853	1.25282	0.598135	0.504814	0.262145
0.791667	6.172964	3.541824	2.531827	1.720618	1.147666	0.515846	0.514414	0.272448
1.022222	7.345823	4.097777	3.022462	2.016845	1.289528	0.633159	0.489722	0.256111
1.407407	9.589179	5.512348	3.86853	2.562281	1.701631	0.956455	0.532732	0.290124
1.958333	13.88461	8.569218	6.051119	4.118129	2.765512	1.645587	0.578525	0.342769
2.428571	16.71303	10.56922	7.465332	5.118129	3.472619	2.145587	0.596894	0.364456
0.760331	5.78928	3.364164	2.340425	1.567954	1.039599	0.464517	0.526298	0.280347
1.013333	8.386036	4.941253	3.361582	2.252849	1.552522	0.840878	0.559069	0.308828
1.259516	9.80025	5.941253	4.068689	2.752849	1.854299	0.991767	0.576485	0.33007
1.259516	9.80025	5.941253	4.068689	2.752849	1.854299	0.991767	0.576485	0.33007
1.714286	12.62868	7.941253	5.482902	3.752849	2.561406	1.491767	0.601366	0.360966
2.272	15.4571	9.941253	6.897116	4.752849	3.268512	1.991767	0.618284	0.382356
1.013333	8.056894	4.708514	3.197011	2.170563	1.511379	0.796553	0.537126	0.294282
1.013333	8.126143	4.757481	3.231635	2.187876	1.520035	0.805879	0.541743	0.297343
1.561983	13.8776	8.336847	5.975972	4.32999	2.900607	1.508177	0.6308	0.362472
0.959184	8.085422	4.841587	3.21726	2.198299	1.525614	0.802257	0.57753	0.322772
1.15625	9.499636	5.841587	3.924367	2.698299	1.827391	0.953146	0.593727	0.343623
0.791667	6.342066	3.626375	2.622918	1.794347	1.198623	0.542142	0.528506	0.278952
0.661157	5.858529	3.404771	2.35226	1.611419	1.088109	0.460582	0.532594	0.283731
0.64	5.488665	3.264498	2.196103	1.512225	1.01607	0.417628	0.548867	0.296773

AvX2	AvX3	AvX4	AvX5	QW	FM	SM	STN	KBLI
0.321114	0.204124	0	0	10	-2.49877	1.707107	1	1.408248
0.353553	0.25	0.176777	0.125	35	-5.54269	2.488034	1	1.5
0.353553	0.25	0.176777	0.125	84	-9.74265	3.284268	1	1.5
0.353553	0.25	0.176777	0.125	165	-15.1	4.086346	1	1.5
0.353553	0.25	0.176777	0.125	455	-29.2881	5.697856	1	1.5
0.136347	0.071807	0.03746	0.019368	118.5429	8.241599	1.238552	35	0.800726
0.14437	0.075992	0.040806	0.022213	89.71429	6.780347	1.074945	35	0.842537
0.134732	0.071071	0.036848	0.018692	210.3429	12.6051	1.839086	35	0.786434
0.140657	0.074809	0.039575	0.020634	118.5429	8.241599	1.238552	35	0.817344
0.125936	0.069546	0.036844	0.018622	247.0286	13.84779	1.93655	35	0.768333
0.143279	0.077645	0.041503	0.022243	469.2571	22.03734	2.57674	35	0.870371
0.183367	0.105593	0.058841	0.033583	1426.714	50.58777	5.722519	35	1.028306
0.201766	0.119026	0.068091	0.040483	2531.686	77.16561	7.929655	35	1.093367
0.146277	0.078398	0.041584	0.02212	91.14286	6.888315	1.207208	35	0.841041
0.160075	0.083439	0.044358	0.024732	276.7429	15.5135	2.346421	35	0.926485
0.1769	0.094926	0.050116	0.027549	455.5429	22.61641	3.457275	35	0.990209
0.1769	0.094926	0.050116	0.027549	455.5429	22.61641	3.457275	35	0.990209
0.20307	0.113723	0.062473	0.037294	1025.143	41.42271	5.707713	35	1.082898
0.222488	0.128455	0.072634	0.045267	1930.743	65.774	7.853376	35	1.147068
0.152239	0.080391	0.043182	0.023428	276.7429	15.5135	2.346421	35	0.882846
0.153887	0.081032	0.04343	0.023702	276.7429	15.5135	2.346421	35	0.892028
0.199199	0.117027	0.064458	0.034277	1053.543	40.67762	5.024895	35	1.087415
0.169329	0.087932	0.047675	0.027664	229.5714	13.7574	2.347082	35	0.968317
0.186875	0.099937	0.053747	0.030747	391.1429	20.59675	3.47932	35	1.030868
0.145718	0.078015	0.041332	0.021686	118.5429	8.241599	1.238552	35	0.836856
0.147016	0.076734	0.04185	0.023029	89.71429	6.780347	1.074945	35	0.851193
0.156865	0.084013	0.046185	0.026102	66.42857	5.499314	1.047214	35	0.890318

TCI1	TCI2	TCI3	TCI4	TCI5	TCI6	TCI7	TCI8	TCI9
0.5	0.222222	0	0	0	0	0	0	0
0.5	0.222222	0.125	0.08	0	0	0	0	0
0.5	0.222222	0.125	0.08	0.055556	0.040816	0	0	0
0.5	0.222222	0.125	0.08	0.055556	0.040816	0.03125	0.024691	0
0.5	0.222222	0.125	0.08	0.055556	0.040816	0.03125	0.024691	0.02
2.5	1.555556	0.875	0.706667	0.201389	0.04	0	0	0
1.5	1.333333	0.6875	0.435556	0.0625	0	0	0	0
2.5	1.555556	0.875	0.746667	0.319444	0.181224	0.059028	0	0
2.5	1.555556	0.875	0.706667	0.201389	0.04	0	0	0
4.5	2.444444	1.25	0.986667	0.555556	0.266122	0.083333	0	0
4.5	2.444444	1.25	1.026667	0.673611	0.386939	0.248264	0.094482	0.06
4.5	2.444444	1.25	1.026667	0.673611	0.386939	0.263889	0.139582	0.11125
4.5	2.444444	1.25	1.026667	0.673611	0.386939	0.263889	0.139582	0.11125
2	1.111111	0.4375	0.555556	0.083333	0.04	0	0	0
2.5	1.555556	0.875	0.746667	0.319444	0.201633	0.102431	0.0451	0
2.5	1.555556	0.875	0.746667	0.319444	0.201633	0.118056	0.090199	0.06125
2.5	1.555556	0.875	0.746667	0.319444	0.201633	0.118056	0.090199	0.06125
2.5	1.555556	0.875	0.746667	0.319444	0.201633	0.118056	0.090199	0.07125
2.5	1.555556	0.875	0.746667	0.319444	0.201633	0.118056	0.090199	0.07125
2.5	1.555556	0.875	0.746667	0.319444	0.201633	0.102431	0.0451	0
2.5	1.555556	0.875	0.746667	0.319444	0.201633	0.102431	0.0451	0
4.5	2.222222	1.375	0.986667	0.625	0.343673	0.208333	0.139582	0.13
1.5	1.333333	0.6875	0.475556	0.180556	0.120816	0.071181	0.020408	0
1.5	1.333333	0.6875	0.475556	0.180556	0.120816	0.086806	0.065508	0.04125
2.5	1.555556	0.875	0.706667	0.201389	0.04	0	0	0
1.5	1.333333	0.6875	0.435556	0.0625	0	0	0	0
1	0.888889	0.25	0.284444	0	0	0	0	0

TCI10	MTCI1	MTCI2	MTCI3	MTCI4	MTCI5	MTCI6	MTCI7	MTCI8
0	0.166667	0.111111	0	0	0	0	0	0
0	0.1	0.055556	0.041667	0.04	0	0	0	0
0	0.071429	0.037037	0.025	0.02	0.018519	0.020408	0	0
0	0.055556	0.027778	0.017857	0.013333	0.011111	0.010204	0.010417	0.012346
0.016529	0.038462	0.018519	0.011364	0.008	0.006173	0.005102	0.004464	0.004115
0	0.192308	0.08642	0.051471	0.064242	0.040278	0.02	0	0
0	0.125	0.083333	0.045833	0.048395	0.020833	0	0	0
0	0.166667	0.077778	0.04375	0.046667	0.02904	0.030204	0.029514	0
0	0.192308	0.08642	0.051471	0.064242	0.040278	0.02	0	0
0	0.28125	0.101852	0.054348	0.058039	0.050505	0.033265	0.013889	0
0	0.236842	0.090535	0.046296	0.044638	0.035453	0.025796	0.022569	0.018896
0.090807	0.18	0.074074	0.037879	0.035402	0.026944	0.017588	0.013194	0.008724
0.090807	0.155172	0.066066	0.033784	0.031111	0.023228	0.014882	0.010995	0.006979
0	0.166667	0.069444	0.03125	0.069444	0.020833	0.04	0	0
0	0.15625	0.074074	0.041667	0.043922	0.024573	0.022404	0.020486	0.02255
0.028875	0.138889	0.067633	0.038043	0.039298	0.021296	0.016803	0.011806	0.011275
0.028875	0.138889	0.067633	0.038043	0.039298	0.021296	0.016803	0.011806	0.011275
0.057749	0.113636	0.057613	0.032407	0.032464	0.016813	0.012602	0.008433	0.006938
0.057749	0.096154	0.050179	0.028226	0.027654	0.013889	0.010082	0.006559	0.005306
0	0.15625	0.074074	0.041667	0.043922	0.024573	0.022404	0.020486	0.02255
0	0.15625	0.074074	0.041667	0.043922	0.024573	0.022404	0.020486	0.02255
0.086624	0.195652	0.074074	0.044355	0.036543	0.027174	0.016365	0.012255	0.009305
0	0.1	0.070175	0.036184	0.031704	0.016414	0.017259	0.017795	0.020408
0.012346	0.088235	0.063492	0.032738	0.027974	0.013889	0.012082	0.009645	0.009358
0	0.192308	0.08642	0.051471	0.064242	0.040278	0.02	0	0
0	0.125	0.083333	0.045833	0.048395	0.020833	0	0	0
0	0.090909	0.063492	0.020833	0.047407	0	0	0	0

MTCI9	MTCI10	GTC	HDPI	RHDPI	SRDS	MRC	BC	LC	
0	0	0.277778	15	3.833333	4.333333	12.19239	8	1	
0	0	0.237222	70	7.1	8.7	18.19239	12	1.584963	
0	0	0.192392	210	10.56429	13.74286	24.19239	16	2	
0	0	0.158601	495	14.14206	19.28968	30.19239	20	2.321928	
0.004	0.004132	0.100198	1820	21.49688	31.52187	42.19239	28	2.807355	
0	0	0.454718	396	23.3619	31.75	41.43012	0	0	
0	0	0.323395	285	20.93333	27.85	35.89161	0	0	
0	0	0.423619	738	27.71825	39.27738	48.47238	0	0	
0	0	0.454718	396	23.3619	31.75	38.83204	0	0	
0	0	0.593148	897	30.8619	44.30714	47.77264	0	0	
0.015	0	0.536026	1925	37.45613	56.49087	54.63292	0	0	
0.007417	0.006486	0.401223	7887	49.38981	79.86566	72.63292	0	0	
0.005855	0.005045	0.348073	16640	57.20058	95.75204	84.63292	0	0	
0	0	0.397639	305	20.78095	27.63333	35.79059	0	0	
0	0	0.405924	1016	29.75159	42.9254	48.2904	0	0	
0.01225	0.014437	0.357293	1861	33.71342	50.1917	54.2904	0	0	
0.01225	0.014437	0.357293	1861	33.71342	50.1917	54.2904	0	0	
0.005938	0.00525	0.286844	5190	41.49275	64.9449	66.2904	0	0	
0.004453	0.00385	0.242501	11771	49.23629	80.18025	78.2904	0	0	
0	0	0.405924	1016	29.75159	42.9254	58.18989	0	0	
0	0	0.405924	1016	29.75159	42.9254	48.64395	0	0	
0.008667	0.006187	0.424391	4904	45.22131	71.85893	68.45753	0	0	
0	0	0.30994	796	27.2373	38.64643	42.75189	0	0	
0.010313	0.012346	0.267726	1520	31.1658	45.72183	48.75189	0	0	
0	0	0.454718	396	23.3619	31.75	38.54337	0	0	
0	0	0.323395	285	20.93333	27.85	33.29354	0	0	
0	0	0.222642	215	18.4	23.9	30.25208	0	0	

KHE	STD(N,N)	WhetZ	Whete	Whetm	Whetv	Whetp	JhetZ	Jhete
3	3	9.142857	9.158422	9.145173	12.63478	13.6	2.14389	2.140557
4	5	33.57143	33.59737	33.57529	39.39131	41	2.421043	2.4195
5	7	82	82.03632	82.0054	90.14783	92.4	2.578122	2.577231
6	9	162.4286	162.4753	162.4355	172.9044	175.8	2.679151	2.67857
8	13	451.2857	451.3532	451.2958	466.4174	470.6	2.801341	2.801037
5.583333	0	111.7647	121.4211	111.4588	133.41	132.1615	3.175175	2.988134
5.166667	0	88.48179	92.88567	88.34492	101.6009	101.9401	3.125764	3.013224
6.722222	4	182.74	192.1798	182.5768	229.3647	234.9736	3.062028	2.953066
6.166667	0	112.0074	116.862	111.8611	133.521	135.3506	3.169966	3.075446
9.416667	0	236.7507	243.7816	235.1171	336.8628	369.6137	2.913164	2.850094
11.5	14	457.0476	458.4396	455.3474	632.8108	693.149	2.637143	2.630732
14.5	26	1399.571	1401.801	1397.323	1715.104	1818.225	1.974238	1.971445
16.5	34	2494.905	2497.687	2492.29	2902.324	3033.609	1.707687	1.705964
5.166667	0	91.14846	95.55234	91.01159	104.2675	104.6067	3.024533	2.922982
7.666667	14	265.2269	271.6341	265.0712	337.8349	353.3028	2.657272	2.609277
8.666667	18	438.409	445.8152	438.2436	540.1794	563.0508	2.312829	2.282731
8.666667	18	438.409	445.8152	438.2436	540.1794	563.0508	2.312829	2.282731
10.66667	26	996.2017	1005.616	996.0183	1158.625	1196.947	1.847408	1.833735
12.66667	34	1890.375	1901.792	1890.173	2111.9	2165.243	1.591248	1.58376
7.041667	4	255.6269	271.5406	255.1702	327.806	338.9814	2.725305	2.609895
7.916667	4	263.7269	270.1188	263.576	345.0305	361.6259	2.66758	2.619345
11.16667	18	1000.745	1011.042	1000.614	1263.496	1329.221	2.094089	2.077563
7.25	14	223.4286	223.7053	223.4697	285.5073	302.6667	2.586119	2.583093
8.25	18	380.5238	380.9077	380.5809	466.658	490.4667	2.22898	2.226715
5.916667	4	117.5014	122.3728	117.3549	138.0239	140.0807	3.059596	2.970585
5.75	0	91.69048	91.75049	91.70442	113.8093	119.0118	3.050478	3.048589
4.75	0	70.47619	70.51597	70.48211	79.4	81.86667	2.974773	2.973134

Jhetm	Jhetv	Jhetp	TD	TR	PJ2DS	J	SCIX0	SCIX1
2.143394	1.590379	1.484764	3	2	0.5	1.974745	3.414214	1.914214
2.420813	2.120272	2.050474	5	3	0.666667	2.339092	4.828427	2.914214
2.577989	2.394089	2.34822	7	4	0.75	2.53006	6.242641	3.914214
2.679065	2.555884	2.524101	9	5	0.8	2.647605	7.656854	4.914214
2.801295	2.735376	2.71784	13	7	0.857143	2.784766	10.48528	6.914214
3.181586	2.746356	2.756679	6	3	1	1.992425	9.552042	6.348207
3.129478	2.776989	2.762061	5	3	0.666667	1.993176	8.181798	5.665685
3.063945	2.515213	2.452754	8	4	1	1.951026	10.96626	7.45109
3.172916	2.744644	2.707669	6	3	1	1.992425	9.052042	6.059532
2.92789	2.208247	2.053447	7	4	0.75	1.998182	11.55204	7.270857
2.644539	2.002636	1.854466	10	5	1	1.934863	13.17336	8.520187
1.976648	1.626807	1.541932	16	8	1	1.637448	17.416	11.52019
1.709022	1.474051	1.414479	20	10	1	1.492353	20.24443	13.52019
3.027831	2.696781	2.680014	6	3	1	1.932319	8.181798	5.648848
2.658407	2.13719	2.049218	9	5	0.8	1.894129	11.17336	7.597537
2.313443	1.889413	1.811977	11	6	0.833333	1.766167	12.58758	8.597537
2.313443	1.889413	1.811977	11	6	0.833333	1.766167	12.58758	8.597537
1.847619	1.579191	1.524807	15	8	0.875	1.552044	15.416	10.59754
1.591342	1.415941	1.378003	19	10	0.9	1.413156	18.24443	12.59754
2.728711	2.182386	2.108991	9	5	0.8	1.894129	12.17336	8.304644
2.66869	2.106234	2.01644	9	5	0.8	1.894129	11.17336	7.597537
2.094212	1.662847	1.579665	13	7	0.857143	1.720021	16.44938	10.92324
2.585668	2.051376	1.941284	8	4	1	1.875551	9.803119	6.915015
2.228642	1.816875	1.72902	10	5	1	1.73713	11.21733	7.915015
3.062374	2.678964	2.641166	6	3	1	1.992425	9.052042	6.059532
3.050073	2.540745	2.446014	5	3	0.666667	1.993176	7.681798	5.37701
2.974529	2.659299	2.587003	5	3	0.666667	1.925368	6.811555	4.966326

SCIX2	SCIX3	SCIX4	SCIX5	CIX0	CIX1	CIX2	CIX3	CIX4
1	0.5	0	0	3.414214	1.914214	1	0.5	0
1.707107	0.957107	0.5	0.25	4.828427	2.914214	1.707107	0.957107	0.5
2.414214	1.457107	0.853553	0.478553	6.242641	3.914214	2.414214	1.457107	0.853553
3.12132	1.957107	1.207107	0.728553	7.656854	4.914214	3.12132	1.957107	1.207107
4.535534	2.957107	1.914214	1.228553	10.48528	6.914214	4.535534	2.957107	1.914214
6.029385	4.889302	4.075478	2.49697	8.552042	5.770857	5.250346	4.268699	3.519291
4.98737	4.291568	3.581461	1.97058	7.681798	5.37701	4.616579	3.933154	3.259983
6.480065	5.124737	4.480282	3.047737	9.966255	6.808862	5.821817	4.718211	4.060178
5.658594	4.530888	3.753999	2.302535	8.552042	5.770857	5.250346	4.268699	3.519291
7.578914	5.589669	4.392628	2.716	11.05204	6.982182	7.208123	5.231255	4.071149
8.133147	5.94977	4.707558	3.244772	13.17336	8.520187	8.133147	5.94977	4.707558
10.25447	7.44977	5.781655	3.946818	17.416	11.52019	10.25447	7.44977	5.781655
11.66868	8.44977	6.488762	4.446818	20.24443	13.52019	11.66868	8.44977	6.488762
5.131089	4.06406	3.342777	2.114918	7.681798	5.360173	4.722841	3.801872	3.108069
6.583619	5.249402	4.390408	3.025742	10.67336	7.308862	6.17537	4.987214	4.1557
7.290725	5.749402	4.757399	3.227787	12.08758	8.308862	6.882477	5.487214	4.52269
7.290725	5.749402	4.757399	3.227787	12.08758	8.308862	6.882477	5.487214	4.52269
8.704939	6.749402	5.464505	3.727787	14.916	10.30886	8.296691	6.487214	5.229797
10.11915	7.749402	6.171612	4.227787	17.74443	12.30886	9.710904	7.487214	5.936904
7.083619	5.602956	4.594533	3.287931	10.67336	7.308862	6.17537	4.987214	4.1557
6.583619	5.249402	4.390408	3.025742	10.67336	7.308862	6.17537	4.987214	4.1557
9.39569	7.490049	5.944914	3.841932	15.94938	10.63456	8.987441	7.22786	5.710206
5.541603	4.651668	3.896392	2.468205	9.803119	6.915015	5.541603	4.651668	3.896392
6.24871	5.151668	4.263382	2.67025	11.21733	7.915015	6.24871	5.151668	4.263382
5.658594	4.530888	3.753999	2.302535	8.552042	5.770857	5.250346	4.268699	3.519291
4.616579	3.933154	3.259983	1.756504	7.681798	5.37701	4.616579	3.933154	3.259983
4.089073	3.466326	2.857589	1.483163	6.811555	4.966326	4.089073	3.466326	2.857589

CIX5	ACIX0	ACIX1	ACIX2	ACIX3	ACIX4	ACIX5	RDR	RDSR
0	0.853553	0.638071	0.5	0.5	0	0	1.334199	6.781744
0.25	0.804738	0.582843	0.426777	0.319036	0.25	0.25	1.677614	15.05183
0.478553	0.78033	0.559173	0.402369	0.291421	0.213388	0.159518	1.997161	24.82292
0.728553	0.765685	0.546024	0.390165	0.279587	0.201184	0.145711	2.298526	35.6782
1.228553	0.748949	0.531863	0.377961	0.268828	0.191421	0.136506	2.862716	59.78999
2.059988	0.71267	0.443912	0.291686	0.185596	0.121355	0.0824	2.387163	71.37151
1.756504	0.698345	0.448084	0.288536	0.187293	0.125384	0.087825	2.323821	62.49115
2.625983	0.711875	0.453924	0.291091	0.18147	0.119417	0.082062	2.609225	87.58052
2.059988	0.71267	0.443912	0.291686	0.185596	0.121355	0.0824	2.387163	71.37151
2.521566	0.736803	0.436386	0.300338	0.180388	0.116319	0.074164	2.593747	99.51374
3.244772	0.731853	0.448431	0.301228	0.180296	0.114818	0.07546	2.928056	125.5193
3.946818	0.725667	0.460807	0.310741	0.19102	0.123014	0.080547	3.691997	173.5084
4.446818	0.723015	0.466213	0.31537	0.196506	0.127231	0.083902	4.187489	205.7234
1.852729	0.698345	0.446681	0.295178	0.190094	0.124323	0.088225	2.344393	61.87787
2.783195	0.711557	0.456804	0.294065	0.184712	0.118734	0.081859	2.737815	95.22144
2.985241	0.711034	0.461603	0.299238	0.189214	0.122235	0.082923	3.001796	110.2487
2.985241	0.711034	0.461603	0.299238	0.189214	0.122235	0.082923	3.001796	110.2487
3.485241	0.710286	0.468585	0.307285	0.196582	0.127556	0.087131	3.524552	140.3745
3.985241	0.709777	0.473418	0.313255	0.202357	0.131931	0.090574	4.028471	171.2441
2.783195	0.711557	0.456804	0.294065	0.184712	0.118734	0.081859	2.737815	95.22144
2.783195	0.711557	0.456804	0.294065	0.184712	0.118734	0.081859	2.737815	95.22144
3.599385	0.724972	0.462372	0.299581	0.195348	0.126893	0.081804	3.438287	156.3937
2.468205	0.700223	0.461001	0.291663	0.186067	0.121762	0.085111	2.679468	85.5219
2.67025	0.701083	0.465589	0.297558	0.190803	0.125394	0.086137	2.946428	100.1449
2.059988	0.71267	0.443912	0.291686	0.185596	0.121355	0.0824	2.387163	71.37151
1.756504	0.698345	0.448084	0.288536	0.187293	0.125384	0.087825	2.323821	62.49115
1.483163	0.681155	0.451484	0.292077	0.192574	0.12989	0.092698	2.283767	53.36972

KAMS1	KAMS2	KAMS3	KF	RSIpw2	RSIpw3	RSIpw4	RSIpw5	ETP
4	3	4	3	0.416667	0.166667	0	0	10
6	5	5.333333	5	0.444444	0.214286	0.088889	0.033333	12
8	7	7.2	7	0.458333	0.223214	0.10119	0.0475	15
10	9	9.142857	9	0.466667	0.228571	0.105952	0.051118	18
14	13	13.09091	13	0.47619	0.234694	0.111395	0.05437	24
9.46615	3.965537	3.678445	3.128197	0.583036	0.3384	0.181505	0.098326	27.88889
8.072368	3.452411	3.129615	2.533557	0.569372	0.341873	0.188031	0.094232	24.11111
11.44155	5.334324	4.569869	4.359497	0.559609	0.329443	0.193539	0.111281	32.94444
9.028326	3.676887	3.392656	2.766345	0.583036	0.3384	0.181505	0.098326	30.27778
11.75574	4.271611	3.973026	3.347729	0.609206	0.334524	0.15854	0.087184	49.02778
14.23724	5.854529	5.158536	4.630686	0.582011	0.320214	0.162538	0.097286	53.41667
20.13931	10.08933	9.205211	8.466339	0.561508	0.301668	0.149951	0.082957	61.91667
24.09627	13.19156	12.20798	11.35241	0.552721	0.294287	0.146387	0.080034	67.91667
8.072368	3.452411	3.57758	2.533557	0.570563	0.324663	0.1773	0.101298	24.11111
11.92726	5.685599	4.871928	4.520907	0.555635	0.320453	0.182254	0.109221	31.77778
13.87761	7.145049	6.250386	5.832716	0.54909	0.310764	0.171401	0.09718	34.77778
13.87761	7.145049	6.250386	5.832716	0.54909	0.310764	0.171401	0.09718	34.77778
17.8042	10.27186	9.243087	8.708684	0.539739	0.29919	0.162236	0.089435	40.77778
21.75256	13.59825	12.46349	11.83187	0.533381	0.291319	0.156278	0.085125	46.77778
12.68599	6.244504	5.397993	5.281182	0.555635	0.320453	0.182254	0.109221	31.52778
11.92726	5.685599	4.871928	4.520907	0.555635	0.320453	0.182254	0.109221	34.77778
18.78968	9.679222	8.227798	8.266794	0.56066	0.32627	0.167425	0.085643	42.27778
10.51556	5.185596	4.387812	3.894958	0.542942	0.321899	0.187689	0.107496	28
12.45675	6.666667	5.777778	5.190311	0.537574	0.311424	0.175478	0.09494	31
9.028326	3.676887	3.392656	2.766345	0.583036	0.3384	0.181505	0.098326	27.27778
7.638889	3.164063	2.844444	2.197266	0.569372	0.341873	0.188031	0.094232	26
6.694215	2.938776	3.111111	1.967279	0.554286	0.325847	0.182051	0.094863	20.33333

ATMCNT	BNDCNT
4	3
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15	16
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24	25
28	29
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17	18
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15	16
22	23
14	15
16	17
12	13
11	12
10	11

Computational details of PLS modeling (logBI$_{50}$)

Model summary

Num. LVs: 4

Cross validation: venetian blinds w/ 5 splits

RMSEC: 0.0373966	**RMSEPred**	0.100065591
RMSECV: 0.0804531	**R^2 Pred**	0.645263467

Bias: 0

CV Bias: 0.0211036

R^2 Cal: 0.949725

R^2 CV: 0.784348

Percent Variance Captured by Regression Model

```
      -----X-Block-----   -----Y-Block-----
 Comp   This    Total    This    Total
 ----  -------  -------  -------  -------
   1    56.10    56.10    62.20    62.20
   2    11.71    67.81    19.34    81.54
   3     6.60    74.41    11.67    93.21
   4     6.12    80.53     1.76    94.97
```
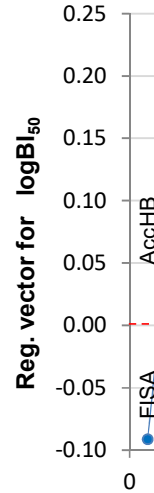
Variable loadings section

Variable no.	Variable	LV 1 (56.10%)	LV 2 (11.71%)	LV 3 (6.60%)	LV 4 (6.12%)
1	FISA	-9.30E-02	1.45E-01	-3.19E-01	-3.38E-02
2	AccHB	-8.55E-02	2.52E-01	-1.22E-01	-1.58E-01
3	QPlogS	1.54E-01	7.09E-02	-1.49E-01	4.93E-02
4	**QPlogBB**	1.36E-01	-7.54E-02	3.13E-01	-9.55E-02
5	QPPMDCK	8.60E-02	-1.60E-01	3.17E-01	-6.02E-02
6	PHAO	3.57E-02	-2.33E-01	2.58E-01	1.08E-01
7	PSA	-9.78E-02	1.85E-01	-2.99E-01	-6.94E-02
8	FH1	-4.60E-02	3.48E-01	-1.89E-01	4.83E-02
9	FH2	-4.60E-02	3.48E-01	-1.89E-01	4.83E-02
10	IP	-8.60E-02	3.16E-01	-1.28E-01	-6.14E-02

|					
11	Dipole(PC)_X	-1.53E-01	-5.07E-03	-7.37E-02	8.08E-02
12	Dipole (Hyb)_	-5.31E-02	-7.16E-02	9.85E-02	-1.98E-01
13	Dipole (Hyb)_	1.45E-03	7.36E-02	8.97E-02	2.67E-01
14	Dipole (Hyb)_	2.01E-02	1.64E-01	1.11E-02	-5.67E-02
15	Dipole (S)_X	-1.53E-01	-6.74E-03	-7.06E-02	7.50E-02
16	ZMV1	-1.37E-01	-7.50E-02	1.59E-01	-2.23E-01
17	**W**	-1.83E-01	1.34E-03	-3.94E-03	1.85E-02
18	SP	-1.56E-01	-4.26E-02	1.46E-01	-3.74E-02
19	**SMT**	-1.83E-01	1.68E-03	-5.37E-03	1.91E-02
20	**SMTV**	-1.83E-01	-2.12E-02	2.21E-02	-8.60E-03
21	**MDDD**	-1.84E-01	3.56E-02	2.03E-03	-1.52E-04
22	**GMT**	-1.82E-01	3.19E-04	-8.29E-03	2.19E-02
23	**GMTV**	-1.80E-01	-4.05E-02	4.37E-02	-3.79E-02
24	**AVDD**	-1.82E-01	3.45E-02	-4.42E-03	5.14E-03
25	**UP**	-1.82E-01	2.38E-02	-5.91E-03	5.04E-03
26	**CENT**	-1.83E-01	1.85E-02	2.82E-03	2.12E-02
27	**VAR**	-1.82E-01	5.00E-02	-3.23E-02	1.32E-02
28	MEV	-1.16E-01	-1.14E-01	1.91E-01	-2.34E-01
29	MEPV	-9.37E-02	-1.87E-01	1.33E-01	-1.77E-01
30	**MENV**	-1.03E-01	-1.44E-01	1.92E-01	-2.26E-01
31	**ECCc**	-1.82E-01	3.53E-02	-1.85E-02	1.66E-02
32	**ECC**	-1.82E-01	3.54E-02	-1.58E-02	1.33E-02
33	**QW**	-1.82E-01	-1.41E-03	-1.02E-02	2.56E-02
34	**FM**	-1.82E-01	3.34E-02	-1.15E-02	1.44E-02
35	**TCI8**	-1.54E-01	1.89E-01	5.35E-02	-2.20E-03
36	**TCI9**	-1.56E-01	1.45E-01	1.20E-01	8.12E-02
37	**TCI10**	-1.63E-01	8.43E-02	9.97E-02	1.18E-01
38	MTCI6	2.09E-02	4.36E-02	2.44E-01	-2.85E-01
39	MTCI7	-2.55E-02	1.63E-01	6.60E-03	-4.29E-01
40	MTCI8	-1.82E-02	2.31E-01	-1.64E-01	-3.00E-01
41	**MTCI9**	-8.72E-02	2.29E-01	7.07E-02	4.94E-02
42	**MTCI10**	-6.79E-02	2.69E-01	4.15E-02	2.23E-01
43	**HDPI**	-1.80E-01	-3.45E-02	-2.31E-02	3.48E-02
44	**WhetZ**	-1.82E-01	-4.56E-03	-1.30E-02	2.80E-02
45	**Whete**	-1.82E-01	-4.08E-03	-1.21E-02	2.73E-02
46	**Whetm**	-1.82E-01	-4.42E-03	-1.33E-02	2.82E-02
47	**Whetv**	-1.83E-01	3.39E-03	1.79E-03	1.53E-02
48	**Whetp**	-1.83E-01	4.10E-03	5.95E-03	1.15E-02
49	PJ2DS	-5.27E-02	8.17E-02	6.24E-02	-1.15E-02
50	ACIX5	8.57E-03	-5.22E-02	-2.63E-01	3.84E-01
51	RSIpw5	1.33E-01	8.58E-02	-1.44E-01	-1.86E-01
52	**logD(o/w)$_{exp}$**	-1.17E-01	-1.89E-01	1.81E-01	-3.65E-02

Variables with VIP scores > 1 are marked in bold
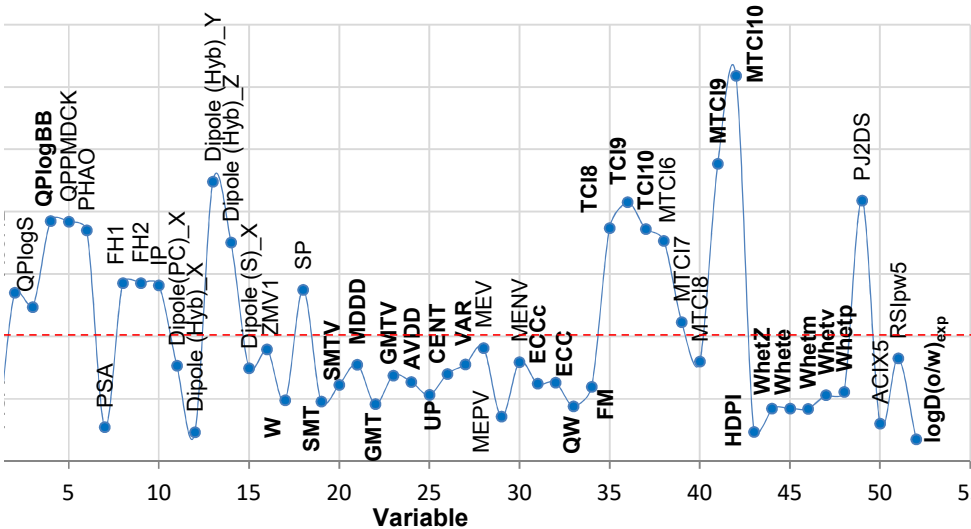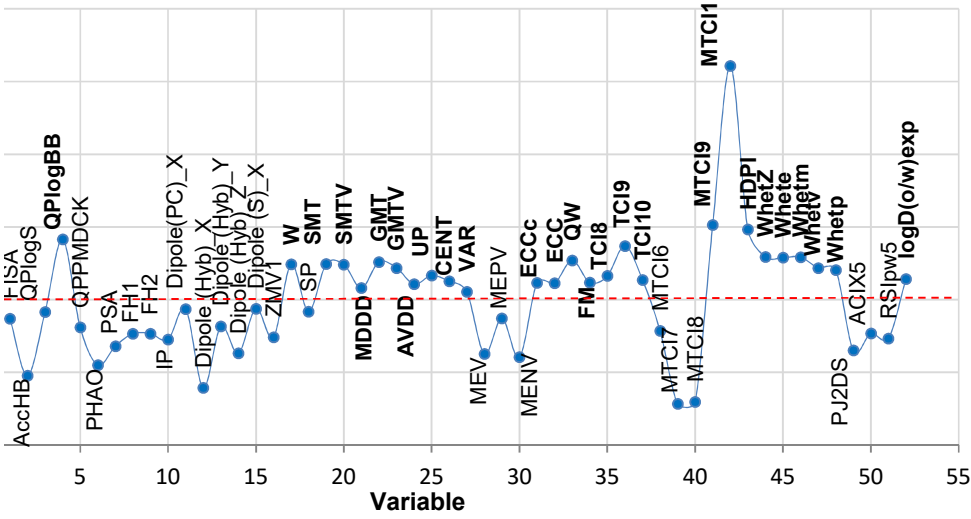
Variable diagnostics section

Variable	Reg Vector for Y logBI50	VIP Scores for Y logBI50	Selectivity Ratio for Y logBI50
FISA	-9.12E-02	0.869	2.68E-01
AccHB	3.51E-02	0.477	4.67E-02
QPlogS	2.37E-02	0.914	7.94E-01
QPlogBB	9.26E-02	**1.413**	9.11E-01
QPPMDCK	9.20E-02	0.808	1.79E-01
PHAO	8.50E-02	0.550	8.33E-03
PSA	-7.27E-02	0.679	2.30E-01
FH1	4.29E-02	0.765	5.72E-03
FH2	4.29E-02	0.765	5.72E-03
IP	4.11E-02	0.726	1.52E-02

Dipole(PC)_X	-2.35E-02	0.934	9.75E-01
Dipole (Hyb)_	-7.68E-02	0.393	9.60E-02
Dipole (Hyb)_	1.24E-01	0.815	4.68E-02
Dipole (Hyb)_	7.54E-02	0.630	7.50E-02
Dipole (S)_X	-2.54E-02	0.937	9.80E-01
ZMV1	-1.03E-02	0.741	6.76E-01
W	-5.11E-02	**1.241**	1.71E+00
SP	3.75E-02	0.918	7.05E-01
SMT	-5.21E-02	**1.245**	1.71E+00
SMTV	-3.87E-02	**1.241**	1.94E+00
MDDD	-2.25E-02	**1.079**	1.38E+00
GMT	-5.43E-02	**1.259**	1.73E+00
GMTV	-3.14E-02	**1.217**	1.95E+00
AVDD	-3.66E-02	**1.106**	1.37E+00
UP	-4.68E-02	**1.165**	1.49E+00
CENT	-3.01E-02	**1.126**	1.48E+00
VAR	-2.24E-02	**1.053**	1.33E+00
MEV	-9.21E-03	0.627	4.68E-01
MEPV	-6.43E-02	0.870	4.92E-01
MENV	-2.07E-02	0.604	4.09E-01
ECCc	-3.77E-02	**1.115**	1.41E+00
ECC	-3.70E-02	**1.112**	1.40E+00
QW	-5.60E-02	**1.269**	1.74E+00
FM	-4.03E-02	**1.118**	1.38E+00
TCI8	8.70E-02	**1.162**	2.23E-01
TCI9	1.08E-01	**1.368**	2.17E-01
TCI10	8.61E-02	**1.136**	3.83E-01
MTCI6	7.67E-02	0.784	5.55E-02
MTCI7	1.14E-02	0.282	8.81E-04
MTCI8	-2.00E-02	0.297	1.47E-06
MTCI9	1.38E-01	**1.513**	4.77E-03
MTCI10	2.09E-01	**2.606**	7.01E-03
HDPI	-7.66E-02	**1.483**	2.21E+00
WhetZ	-5.79E-02	**1.292**	1.81E+00
Whete	-5.77E-02	**1.288**	1.79E+00
Whetm	-5.79E-02	**1.292**	1.80E+00
Whetv	-4.71E-02	**1.217**	1.67E+00
Whetp	-4.44E-02	**1.204**	1.65E+00
PJ2DS	1.09E-01	0.651	1.04E-02
ACIX5	-6.98E-02	0.768	9.83E-03
RSIpw5	-1.76E-02	0.733	4.09E-01
logD(o/w)$_{exp}$	-8.23E-02	1.142	5.98E-01

Variables with VIP scores > 1 are marked in bold

Calibration
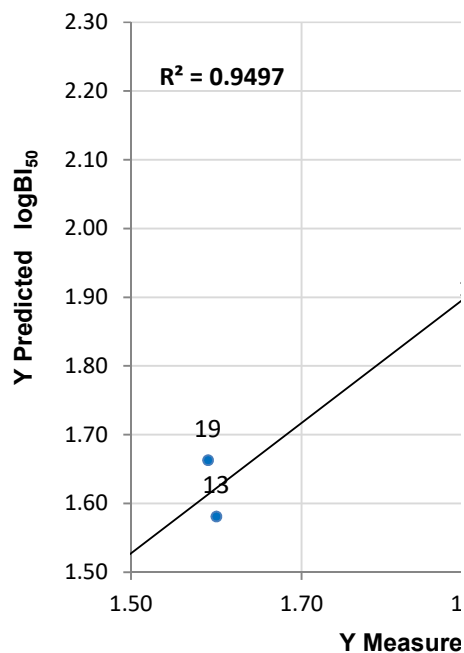
Compounds score section

Compound No.	Scores on LV 1 (56.10%)	Scores on LV 2 (11.71%)	Scores on LV 3 (6.60%)	Scores on LV 4 (6.12%)
6	4.18E+00	-1.187809138	2.406587731	1.62E+00
7	4.46E+00	-2.24189409	0.463661577	2.03E+00
8	3.29E+00	-0.428817782	0.962932082	-1.70E+00
9	2.90E+00	-2.554095263	-1.020190943	2.74E-01
10	1.41E+00	-3.217244233	3.486443391	-3.52E+00
11	-1.91E+00	-0.259723314	0.214755875	-3.24E+00
12	-9.18E+00	-0.169010949	1.563050181	9.04E-01
13	-1.58E+01	-2.500737704	0.286250282	7.90E-02
14	4.71E+00	-0.891170394	2.080114335	1.86E+00
15	2.47E+00	1.988083915	-2.571695844	-2.90E+00

Model predic

Comp. no.
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16	-4.49E-02	3.934376273	0.199359372	1.24E+00	16
17	-1.40E-01	3.638824706	0.105033387	1.27E+00	17
18	-4.19E+00	0.92157936	-1.203042164	1.26E+00	18
19	-9.73E+00	-1.561786383	-2.897283976	2.72E-01	19
20	2.94E+00	0.469425158	0.82276437	-1.69E+00	20
21	1.96E+00	0.243581649	-1.382149057	-1.56E+00	21
22	-2.98E+00	4.274881493	3.511023165	-1.32E-01	22
23	3.17E+00	2.653457157	-2.82751861	-1.68E+00	23
24	1.28E+00	3.891964094	-0.45205654	1.93E+00	24
25	3.31E+00	-0.661535468	-0.541603603	8.57E-01	25
26	3.34E+00	-3.247111277	-1.72427853	1.13E+00	26
27	4.56E+00	-3.095237808	-1.482156481	1.70E+00	27

Cross-validation
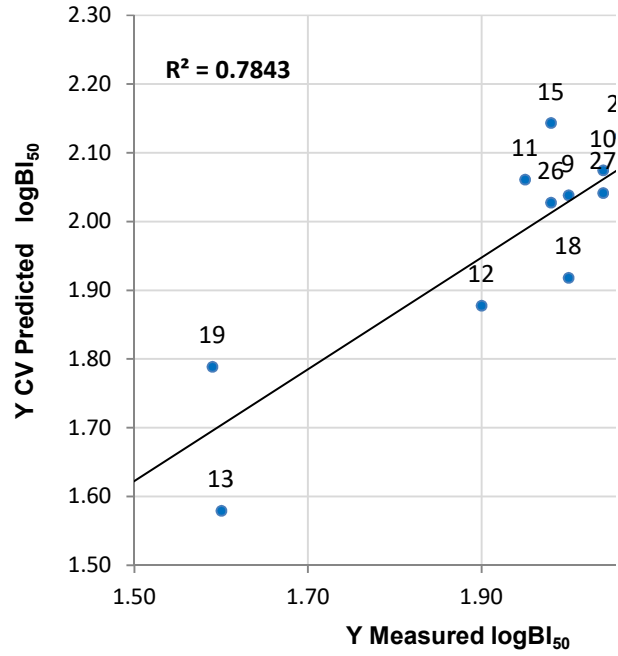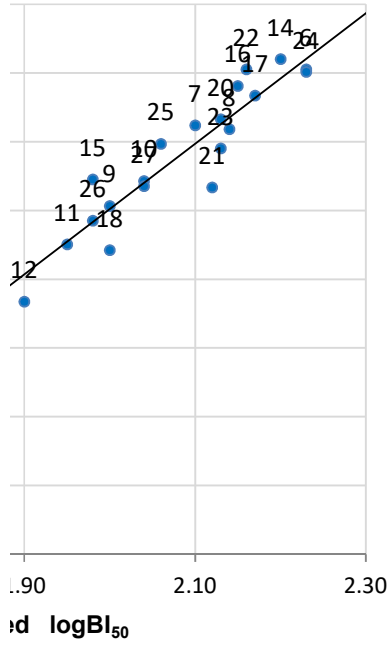
ition performance and object diagnostics section

Y Measured logBI50	Y Predicted logBI50	Y Residual logBI50	Y Stdnt Residual logBI50	Y CV Predicted logBI50	Y CV Residual logBI50	Y double CV Predicted logBI50
2.23	2.21	-2.47E-02	-5.64E-01	2.17	-6.06E-02	2.05
2.10	2.12	2.42E-02	5.46E-01	2.14	4.05E-02	2.12
2.14	2.12	-2.15E-02	-4.67E-01	2.09	-4.68E-02	2.13
2.00	2.01	6.78E-03	1.48E-01	2.04	3.85E-02	2.06
2.04	2.04	3.11E-03	8.71E-02	2.07	3.48E-02	1.97
1.95	1.95	9.55E-04	2.19E-02	2.06	1.11E-01	1.98
1.90	1.87	-3.25E-02	-7.54E-01	1.88	-2.22E-02	1.87
1.60	1.58	-1.89E-02	-5.38E-01	1.58	-2.08E-02	1.58
2.20	2.22	2.02E-02	4.60E-01	2.18	-1.60E-02	2.07
1.98	2.05	6.52E-02	1.59E+00	2.14	1.63E-01	2.18

2.15	2.18	3.15E-02	7.13E-01	2.21	5.89E-02	2.21
2.17	2.17	-2.49E-03	-5.57E-02	2.16	-1.15E-02	2.16
2.00	1.94	-5.74E-02	-1.25E+00	1.92	-8.19E-02	1.93
1.59	1.66	7.32E-02	1.82E+00	1.79	1.99E-01	1.82
2.13	2.13	2.96E-03	6.43E-02	2.20	6.85E-02	2.15
2.12	2.03	-8.62E-02	-1.87E+00	2.02	-1.01E-01	2.02
2.16	2.21	4.56E-02	1.16E+00	2.28	1.16E-01	1.98
2.13	2.09	-3.96E-02	-9.43E-01	2.08	-4.67E-02	2.22
2.23	2.20	-2.85E-02	-6.58E-01	2.16	-7.23E-02	2.20
2.06	2.10	3.72E-02	7.94E-01	2.12	6.44E-02	2.13
1.98	1.99	5.35E-03	1.22E-01	2.03	4.79E-02	2.04
2.04	2.04	-4.53E-03	-1.05E-01	2.04	1.52E-03	2.07

Double cross-validation
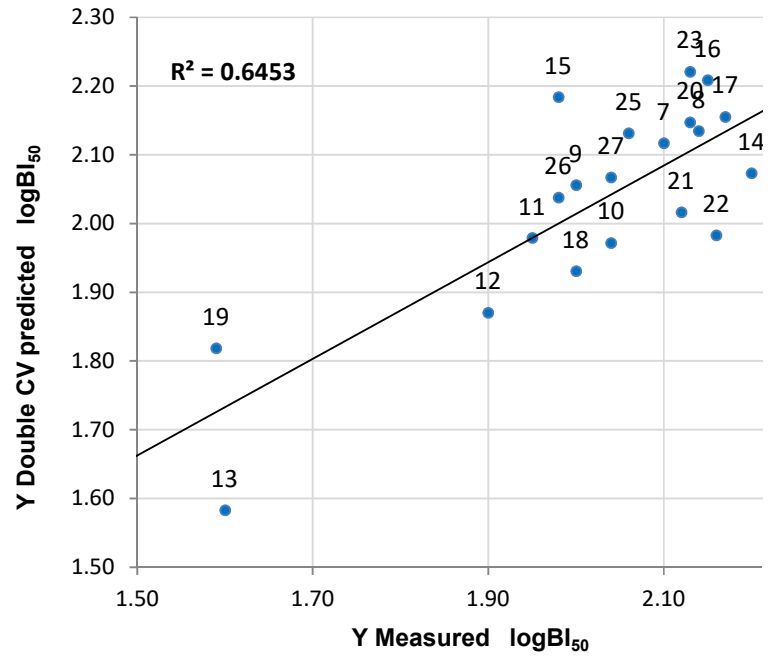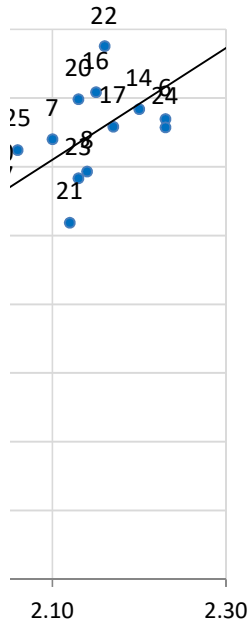
Y double CV
Residual
logBI50

-0.18
0.02
-0.01
0.06
-0.07
0.03
-0.03
-0.02
-0.13
0.20

0.06
-0.01
-0.07
0.23
0.02
-0.10
-0.18
0.09
-0.03
0.07
0.06
0.03

24

6

2.30
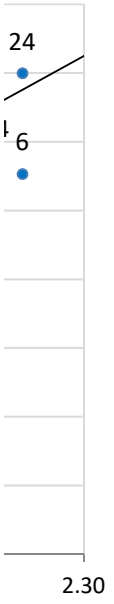
Comutational details of PLS modeling (logBI$_{25}$)

Model summary

Num. LVs: 2

Cross validation: venetian blinds w/ 5 splits

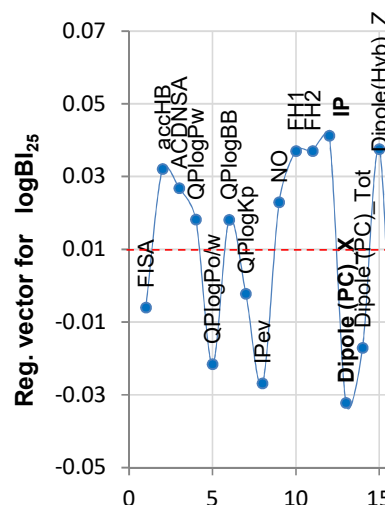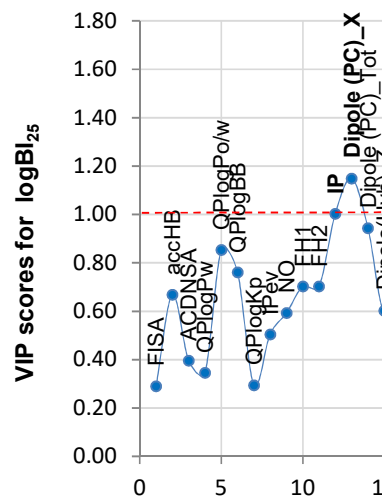|		
RMSEC: 0.0644409	**RMSEPred**	**0.0841**
RMSECV: 0.0807239	**R^2Pred**	**0.6902**

Bias: 0

CV Bias: -0.000838556

R^2 Cal: 0.816618

R^2 CV: 0.719867

Percent Variance Captured by Regression Model

```
      -----X-Block-----   -----Y-Block-----
 Comp   This    Total     This    Total
 ----  -------  -------  -------  -------
   1    63.47    63.47    67.53    67.53
   2    14.26    77.72    14.13    81.66
```


Variable loadings section

Variable no.	Variable	LV 1 (63.47%)	LV 2 (14.26%)
1	FISA	-8.38E-02	1.78E-01
2	accHB	-7.70E-02	2.46E-01
3	ACDNSA	-4.80E-02	2.76E-01
4	QPlogPw	-7.23E-02	2.63E-01
5	QPlogPo/w	-1.29E-01	-1.08E-01
6	QPlogBB	1.26E-01	-9.30E-02
7	QPlogKp	8.64E-02	-2.18E-01
8	IPev	7.13E-02	-2.47E-01
9	NO	-9.70E-02	2.54E-01
10	FH1	-5.56E-02	2.70E-01

Variable diagnostics section

Variable	Reg Vector for Y logBI25
FISA	-6.01E-03
accHB	3.21E-02
ACDNSA	2.69E-02
QPlogPw	1.82E-02
QPlogPo/w	-2.16E-02
QPlogBB	1.82E-02
QPlogKp	-2.18E-03
IPev	-2.68E-02
NO	2.30E-02
FH1	3.70E-02

11	FH2	-5.56E-02	2.70E-01	FH2	3.70E-02	
12	**IP**	-8.47E-02	2.74E-01	**IP**	4.13E-02	
13	**Dipole (PC)_X**	-1.35E-01	-1.65E-02	**Dipole (PC)_X**	-3.22E-02	
14	Dipole (PC)_Tot	-1.45E-01	9.62E-02	Dipole (PC)_Tot	-1.71E-02	
15	Dipole(Hyb)_Z	9.01E-03	1.30E-01	Dipole(Hyb)_Z	3.76E-02	
16	Dipole(Hyb)_Tot	6.06E-02	-1.76E-01	Dipole(Hyb)_Tot	-4.26E-02	
17	**Dipole(S)_X**	-1.34E-01	-1.76E-02	**Dipole(S)_X**	-3.22E-02	
18	Dipole(S)_Tot	-1.44E-01	9.29E-02	Dipole(S)_Tot	-1.87E-02	
19	**W**	-1.62E-01	-1.80E-02	**W**	-2.98E-02	
20	**MW**	-1.61E-01	3.95E-02	**MW**	-1.76E-02	
21	**MSDB**	-1.43E-01	2.14E-02	**MSDB**	-2.44E-02	
22	SP	-1.28E-01	-5.35E-02	SP	-2.46E-02	
23	**SMT**	-1.62E-01	-1.78E-02	**SMT**	-2.98E-02	
24	**SMTV**	-1.59E-01	-3.01E-02	**SMTV**	-3.18E-02	
25	**MDDD**	-1.62E-01	1.25E-02	**MDDD**	-2.32E-02	
26	**GMT**	-1.62E-01	-1.91E-02	**GMT**	-3.02E-02	
27	**GMTV**	-1.53E-01	-3.93E-02	**GMTV**	-3.29E-02	
28	**AVDD**	-1.62E-01	9.17E-03	**AVDD**	-2.38E-02	
29	**UP**	-1.62E-01	9.19E-04	**UP**	-2.58E-02	
30	**CENT**	-1.62E-01	-5.75E-03	**CENT**	-2.64E-02	
31	**VAR**	-1.62E-01	2.75E-02	**VAR**	-2.28E-02	
32	MEPV	-6.44E-02	-1.13E-01	MEPV	-3.38E-02	
33	**ECCc**	-1.63E-01	1.02E-02	**ECCc**	-2.44E-02	
34	**ECC**	-1.63E-01	1.06E-02	**ECC**	-2.42E-02	
35	**AECC**	-1.61E-01	4.77E-02	**AECC**	-1.65E-02	
36	**DECC**	-1.61E-01	3.27E-02	**DECC**	-2.08E-02	
37	**AvX5**	-1.47E-01	3.88E-02	**AvX5**	-1.98E-02	
38	**QW**	-1.61E-01	-2.10E-02	**QW**	-3.06E-02	
39	**FM**	-1.62E-01	6.95E-03	**FM**	-2.45E-02	
40	**SM**	-1.60E-01	4.38E-02	**SM**	-1.67E-02	
41	TCI6	-1.12E-01	1.13E-01	TCI6	1.48E-02	
42	MTCI6	2.52E-02	6.69E-02	MTCI6	3.04E-02	
43	MTCI7	-1.75E-02	2.20E-01	MTCI7	4.33E-02	
44	MTCI8	-1.79E-02	2.81E-01	MTCI8	4.34E-02	
45	**HDPI**	-1.59E-01	-4.45E-02	**HDPI**	-3.66E-02	
46	**WhetZ**	-1.61E-01	-2.33E-02	**WhetZ**	-3.14E-02	
47	**Whetv**	-1.61E-01	-2.29E-02	**Whetv**	-3.12E-02	
48	**Whetm**	-1.61E-01	-2.32E-02	**Whetm**	-3.14E-02	
49	**Whetv**	-1.62E-01	-1.69E-02	**Whetv**	-2.92E-02	
50	**Whetp**	-1.62E-01	-1.61E-02	**Whetp**	-2.88E-02	
51	Jhetp	1.35E-01	-1.56E-01	Jhetp	-1.16E-02	
52	**ACIX2**	-1.56E-01	-4.41E-03	**ACIX2**	-2.35E-02	
53	ACIX3	-1.18E-01	-4.41E-02	ACIX3	-2.62E-02	
54	ACIX4	-7.49E-02	-1.14E-01	ACIX4	-3.57E-02	
55	ACIX5	-8.21E-03	-9.25E-02	ACIX5	-2.90E-02	
56	**KAMS3**	-1.59E-01	3.70E-02	**KAMS3**	-1.74E-02	
57	RSIpw4	1.41E-01	3.60E-02	RSIpw4	2.22E-02	
58	**RSIpw5**	1.16E-01	1.56E-01	**RSIpw5**	4.02E-02	
59	$logD(o/w)_{exp}$	-9.84E-02	-1.68E-01	$logD(o/w)_{exp}$	-3.17E-02	

**Variables with VIP scores > 1 are marked in bold**   **Variables with VIP scores > 1 are r**

Variable (x-axis, first plot)

Labels: Dipole(Hyb)_Z, Dipole(Hyb)_Tot, Dipole(S)_X, Dipole(S)_Tot, W, MW, MSDB, SP, SMT, SMTv, MDDD, GMT, GMTv, AVDD, UP, CENT, VAR, MEPV, ECCc, ECC, AECC, DECC, AvX5, QW, FM, SM, TCl6, MTCl6, MTCl7, MTCl8, HDPI, WhetZ, Whetv, Whetm, Whetv, Whetp, Jhetp, ACIX2, ACIX3, ACIX4, ACIX5, KAMS3, RSIpw4, RSIpw5, logD(o/w)_exp

x-axis ticks: 15 20 25 30 35 40 45 50 55 60

Variable (x-axis, second plot)

Labels: Dipole(Hyb)_Tot, Dipole(S)_X, Dipole(S)_Tot, W, MW, MSDB, SP, SMT, SMTv, MDDD, GMT, GMTv, AVDD, UP, CENT, VAR, MEPV, ECCc, ECC, AECC, DECC, AvX5, QW, FM, SM, TCl6, MTCl6, MTCl7, MTCl8, HDPI, WhetZ, Whetv, Whetm, Whetv, Whetp, Jhetp, ACIX2, ACIX3, ACIX4, ACIX5, KAMS3, RSIpw4, RSIpw5, logD(o/w)_exp

x-axis ticks: 5 20 25 30 35 40 45 50 55 60

Compounds score section

VIP Scores for Y logBI25	Selectivity Ratio for Y logBI25		Comp. no.	Scores on LV 1 (63.47%)
0.290	6.74E-02		6	4.757439527
0.669	1.76E-02		7	5.001440854
0.396	4.45E-03		8	4.34979007
0.345	7.22E-03		9	4.137922775
0.854	2.62E+00		10	2.892620354
0.761	5.30E-01		11	-0.48906746
0.294	5.00E-02		12	-9.4615523
0.505	9.82E-03		13	-16.8440214
0.593	5.79E-02		14	4.741447651
0.703	2.61E-04		15	2.425574881

0.703	2.61E-04	16	-0.63549096
1.003	2.04E-02	17	-0.72553894
1.149	1.45E+00	18	-6.10276183
0.944	9.06E-01	19	-12.5853327
0.603	4.49E-02	20	3.058249631
0.912	1.58E-02	21	2.575744058
1.147	1.45E+00	22	-3.63704159
0.961	9.05E-01	23	3.107588251
1.399	5.62E+00	24	0.390183613
1.148	2.58E+00	25	4.067986112
1.049	1.44E+00	26	4.352215184
0.898	1.52E+00	27	4.622604223
1.399	5.62E+00		
1.418	5.57E+00		
1.260	3.76E+00		
1.409	5.72E+00		
1.381	4.33E+00		
1.274	3.93E+00		
1.314	4.37E+00		
1.324	4.73E+00		
1.248	3.07E+00		
0.647	3.24E-01		
1.288	3.94E+00		
1.283	3.91E+00		
1.127	2.33E+00		
1.200	2.77E+00		
1.011	1.47E+00		
1.418	5.83E+00		
1.287	4.03E+00		
1.117	2.32E+00		
0.586	3.13E-01		
0.416	5.14E-02		
0.805	2.92E-02		
0.809	6.09E-02		
1.555	7.24E+00		
1.438	6.08E+00		
1.432	6.03E+00		
1.438	6.07E+00		
1.383	5.49E+00		
1.374	5.39E+00		
0.770	4.63E-01		
1.187	3.21E+00		
0.832	1.00E+00		
0.759	4.45E-01		
0.359	2.54E-02		
1.119	2.40E+00		
0.989	2.20E+00		
1.212	2.28E+00		
0.805	1.28E+00		

marked in bold

Calibration

R² = 0.8166

Y Predicted logBI$_{25}$ (y-axis, Calibration)
Y Measured logBI$_{50}$ (x-axis)
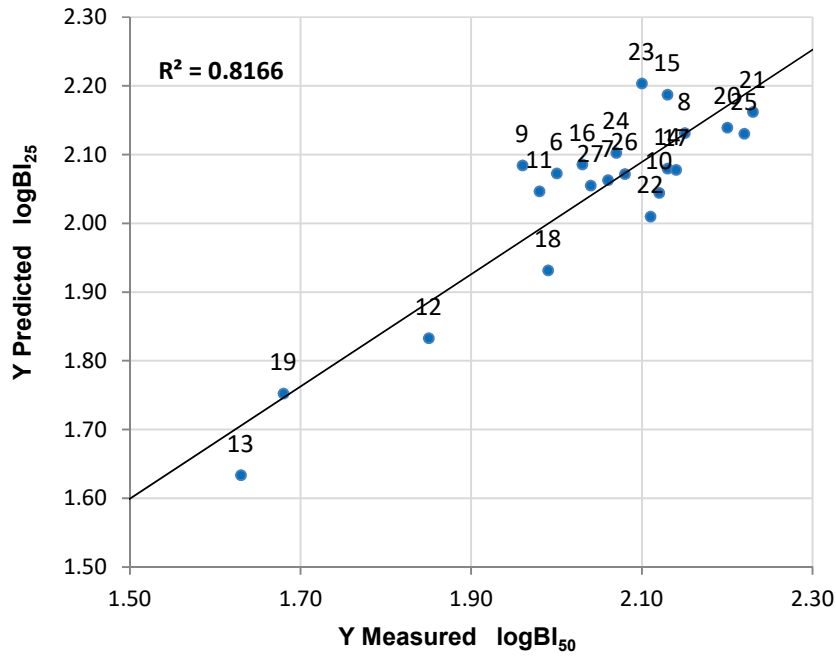
Y CV Predicted logBI$_{25}$ (y-axis, Cross-validation)
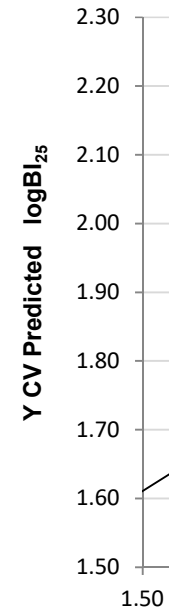
Model predicition performance and object diagnostics section

Scores on LV 2 (14.26%)	Comp. no.	Y Measured 2 logBI25	Y Predicted 2 logBI25	Y Residual 2 logBI25	Y Stdnt Residual 2 logBI25
-3.34E+00	6	2.00	2.07	7.27E-02	1.07E+00
-4.08E+00	7	2.06	2.06	2.81E-03	4.20E-02
2.05E-02	8	2.15	2.13	-1.87E-02	-2.65E-01
-2.11E+00	9	1.96	2.08	1.24E-01	1.78E+00
-2.82E+00	10	2.12	2.04	-7.56E-02	-1.09E+00
7.88E-01	11	1.98	2.05	6.65E-02	9.32E-01
-6.05E-01	12	1.85	1.83	-1.69E-02	-2.51E-01
-2.95E+00	13	1.63	1.63	3.70E-03	6.74E-02
-2.96E+00	14	2.13	2.08	-5.00E-02	-7.29E-01
4.82E+00	15	2.13	2.19	5.74E-02	8.65E-01

2.91E+00	16	2.03	2.09	5.58E-02	8.00E-01
2.61E+00	17	2.14	2.08	-6.21E-02	-8.86E-01
8.63E-01	18	1.99	1.93	-5.81E-02	-8.34E-01
-1.40E+00	19	1.68	1.75	7.27E-02	1.14E+00
1.77E+00	20	2.20	2.14	-6.05E-02	-8.59E-01
3.41E+00	21	2.23	2.16	-6.77E-02	-9.85E-01
2.22E+00	22	2.11	2.01	-1.00E-01	-1.43E+00
4.94E+00	23	2.10	2.20	1.04E-01	1.57E+00
2.68E+00	24	2.07	2.10	3.25E-02	4.64E-01
2.72E-01	25	2.22	2.13	-8.95E-02	-1.27E+00
-2.96E+00	26	2.08	2.07	-8.06E-03	-1.17E-01
-4.09E+00	27	2.04	2.05	1.49E-02	2.23E-01
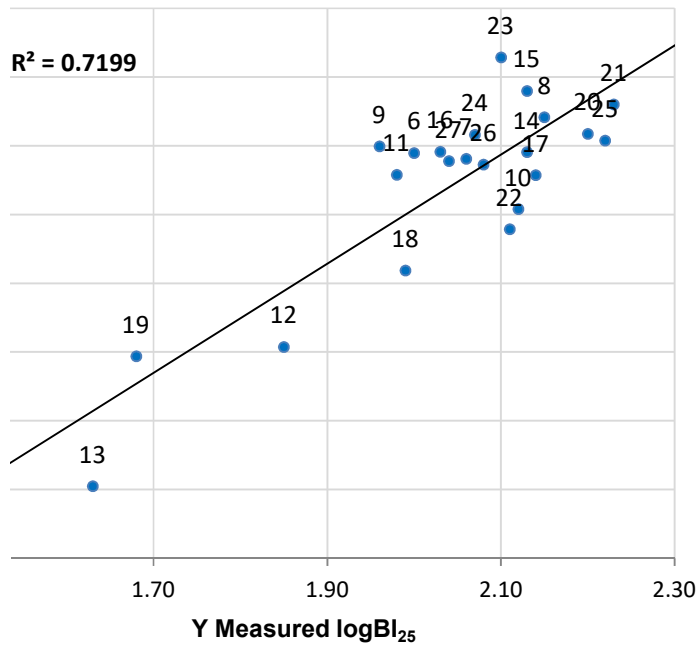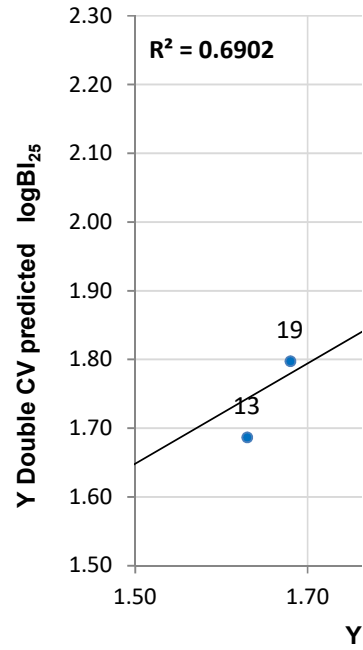
Y CV Predicted 2 logBI25	Y CV Residual 2 logBI25	Y double CV Predicted logBI25	Y double CV Residual logBI25
2.09	8.97E-02	2.10	0.10
2.08	2.11E-02	2.07	0.01
2.14	-8.47E-03	2.12	-0.03
2.10	1.39E-01	2.06	0.10
2.01	-1.12E-01	2.09	-0.03
2.06	7.79E-02	2.04	0.06
1.81	-4.27E-02	1.83	-0.02
1.60	-2.51E-02	1.69	0.06
2.09	-3.92E-02	2.11	-0.02
2.18	5.00E-02	2.23	0.10

2.09	6.15E-02	2.09	0.06
2.06	-8.25E-02	2.02	-0.12
1.92	-7.12E-02	1.89	-0.10
1.79	1.14E-01	1.80	0.12
2.12	-8.24E-02	2.13	-0.07
2.16	-6.96E-02	2.14	-0.09
1.98	-1.31E-01	2.00	-0.11
2.23	1.29E-01	2.26	0.16
2.12	4.62E-02	2.11	0.04
2.11	-1.12E-01	2.09	-0.13
2.07	-7.27E-03	2.00	-0.08
2.08	3.77E-02	2.08	0.04

Measured logBI$_{25}$