

Models Report – 2 parameters

Neat

Only Boronic Acids

formula	R.sq	Q.sq	MAE
output ~ X.1.2. + dip_y	0.7502635	0.6550705	0.0979900
output ~ X.2.9. + B5	0.7523212	0.4994522	0.1156619

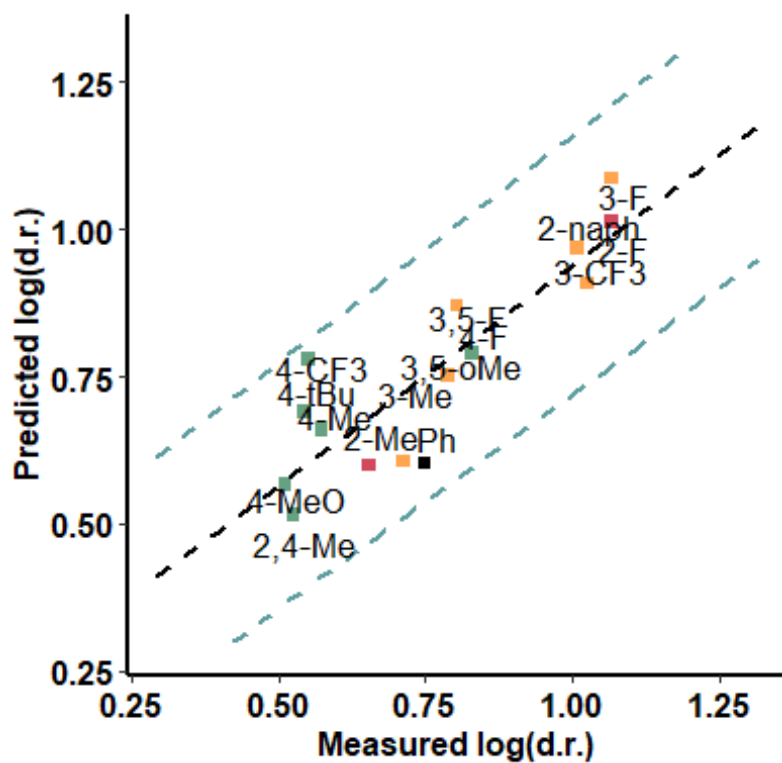
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.7602560	0.0284190	26.751640	0.0000000
X.1.2.	0.1240787	0.0294255	4.216711	0.0011959
dip_y	0.1287997	0.0294255	4.377149	0.0009008

3 & 5 fold CV

Q2	MAE
0.6138099	0.1070997

Q2	MAE
0.6366031	0.1012295

Top Ranked Full Model



With Catalyst - Close to the active site

formula	R.sq	Q.sq	MAE
output ~ NBO.N.19 + diff.B1.016	0.6684152	0.6025137	0.0923752
output ~ Dist.8..14. + Dist.16..17.	0.6849151	0.5438933	0.1078794

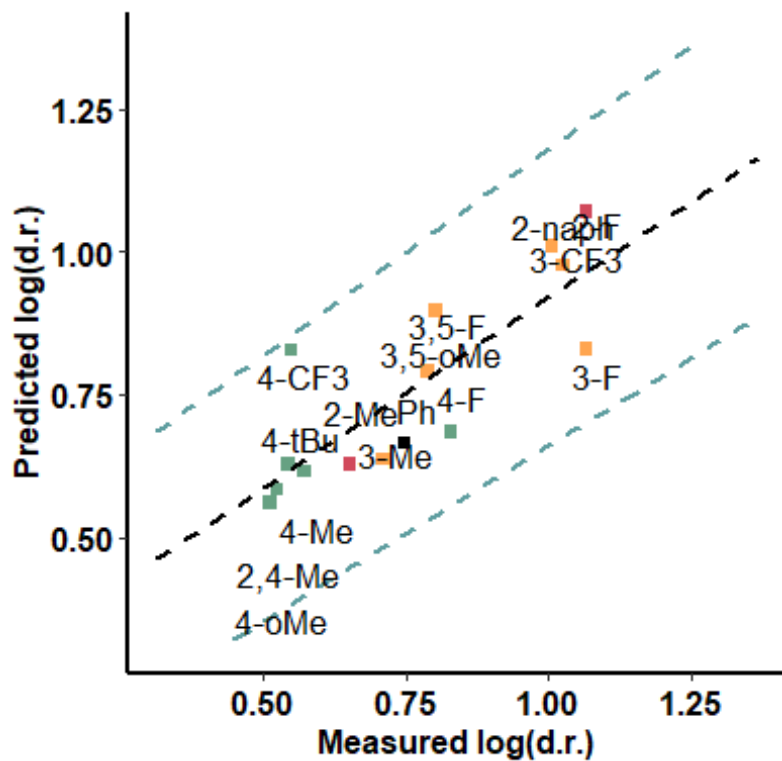
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.7602560	0.0327466	23.216357	0.0000000
NBO.N.19	0.1606125	0.0343340	4.677943	0.0005342
diff.B1.016	0.0770560	0.0343340	2.244306	0.0444510

3 & 5 fold CV

Q2	MAE
0.4914689	0.1235114

Q2	MAE
0.547022	0.110013

Top Ranked Full Model



With Catalyst - far from the active site

formula	R.sq	Q.sq	MAE
output ~ dip_y + diff.H14.018	0.7555236	0.5734527	0.1034078

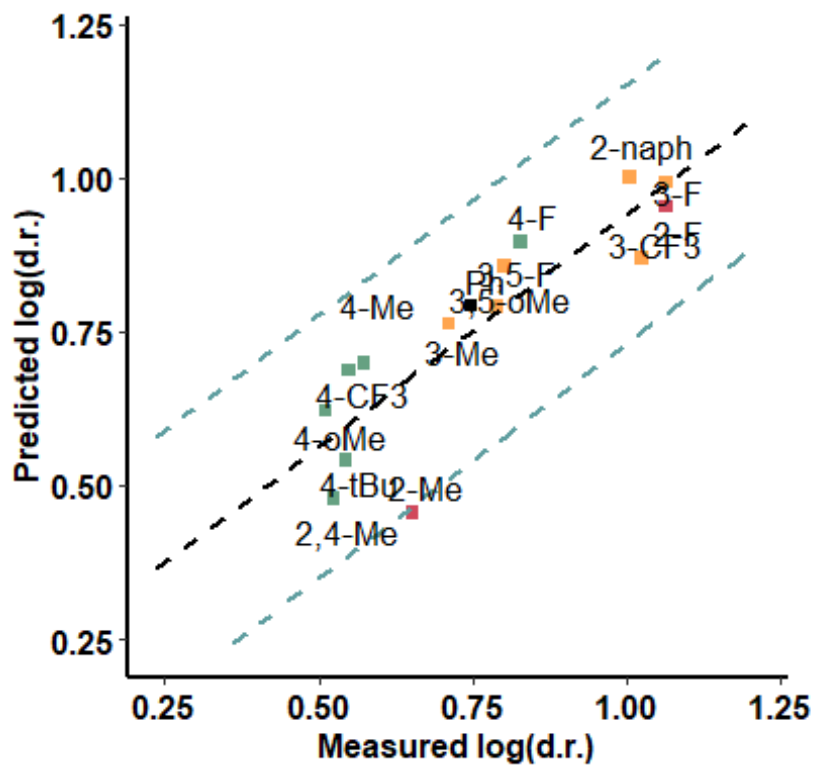
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.7602560	0.0281182	27.037899	0.0000000
dip_y	0.1068162	0.0305356	3.498088	0.0043973
diff.H14.018	-0.1773930	0.0305356	-5.809382	0.0000835

3 & 5 fold CV

Q2	MAE
0.5445424	0.1149639

Q2	MAE
0.5596977	0.1086652

Top Ranked Full Model



BA + Pentanone

formula	R.sq	Q.sq	MAE
output ~ X.2.9. + NBO.0.9	0.7416260	0.6443590	0.0948581
output ~ X.2.9. + diff.09.H16	0.6997166	0.6195804	0.0937588

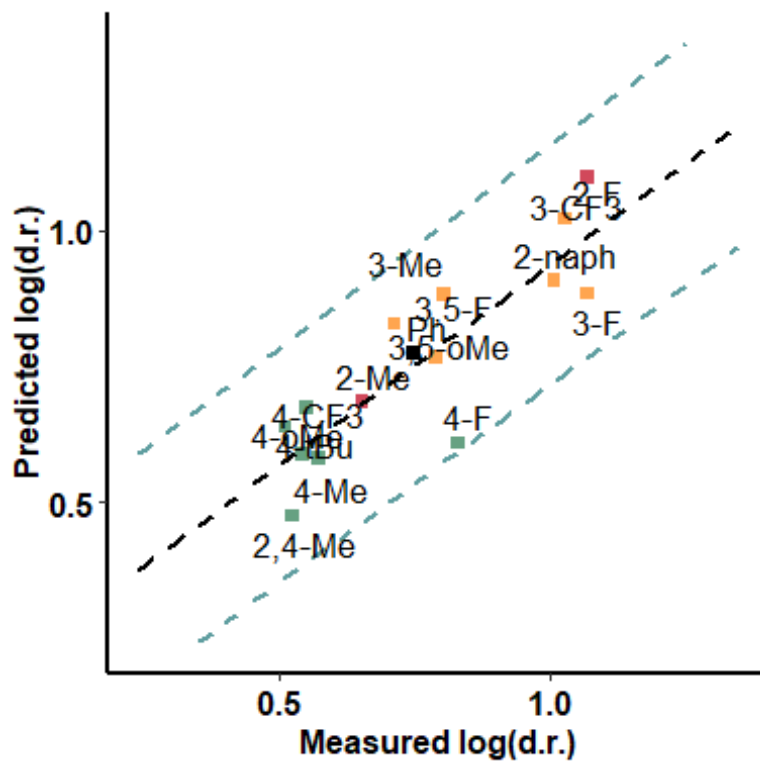
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.7602560	0.0289063	26.300683	0.0000000
X.2.9.	0.2386137	0.0441253	5.407635	0.0001581
NBO.0.9	-0.1071345	0.0441253	-2.427959	0.0318511

3 & 5 fold CV

Q2	MAE
0.6028835	0.1072041

Q2	MAE
0.6241444	0.1005212

Top Ranked Full Model



BA + Aldehyde (pi interaction) - oxygen side

formula	R.sq	Q.sq	MAE
output ~ Dist.18..20. + dip_y	0.5730471	0.4039036	0.1174817
output ~ Dist.2..9. + B1	0.5697977	0.3272534	0.1497725

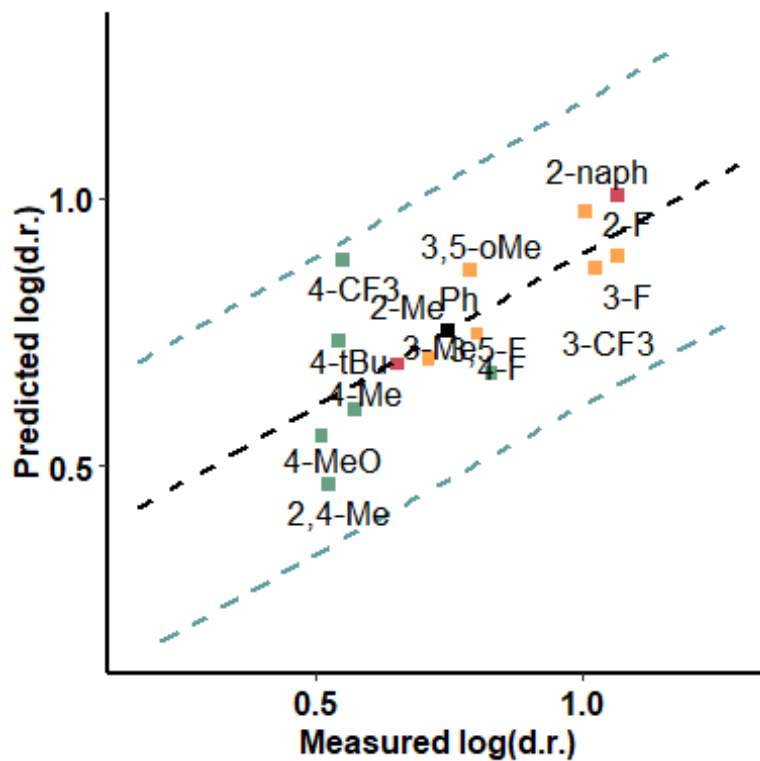
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.7602560	0.0371585	20.459802	0.0000000
Dist.18..20.	0.1510292	0.0407446	3.706729	0.0029987
dip_y	-0.1090000	0.0407446	-2.675199	0.0202156

3 & 5 fold CV

Q2	MAE
0.3743475	0.1293962

Q2	MAE
0.3844913	0.1231027

Top Ranked Full Model



BA + Aldehyde - pi interaction - hydrogen side

formula	R.sq	Q.sq	MAE
output ~ Dist.16..17. + diff.017.C18	0.7049055	0.5944731	0.1055027
output ~ Dist.18..19. + diff.C18.H19	0.7084203	0.5591932	0.1079523

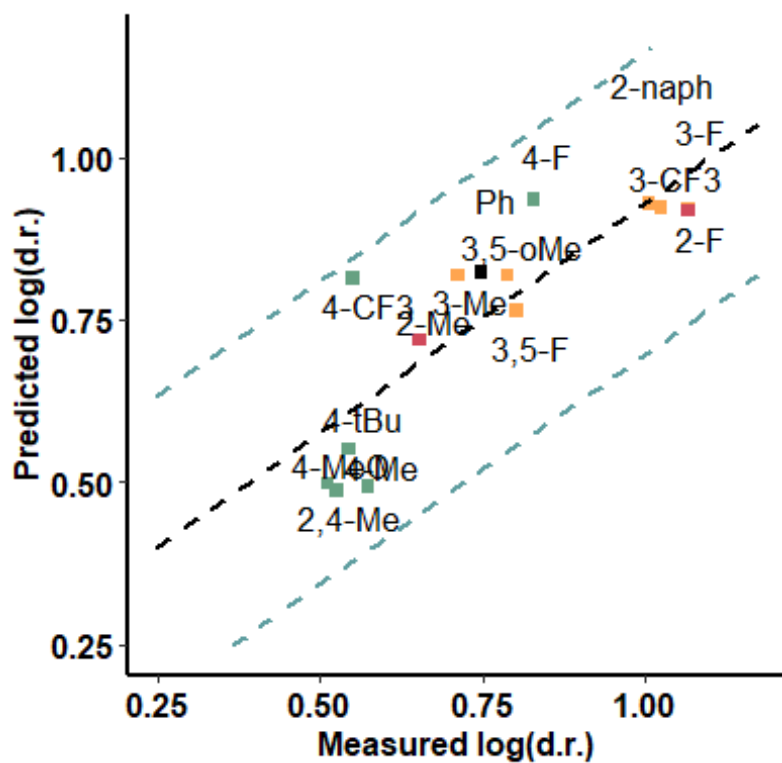
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.7602560	0.0308922	24.609956	0.0000000
Dist.16..17.	0.1308435	0.0330176	3.962841	0.0018837
diff.017.C18	0.0825206	0.0330176	2.499290	0.0279518

3 & 5 fold CV

Q2	MAE
0.5279509	0.1191171

Q2	MAE
0.560222	0.111728

Top Ranked Full Model



BA + Aldehyde - H bond - aldehyde side

formula	R.sq	Q.sq	MAE
output ~ para + Dist.16..17.	0.6512250	0.4952162	0.1185252
output ~ para + NB0.0.1	0.6511833	0.4907146	0.1242047

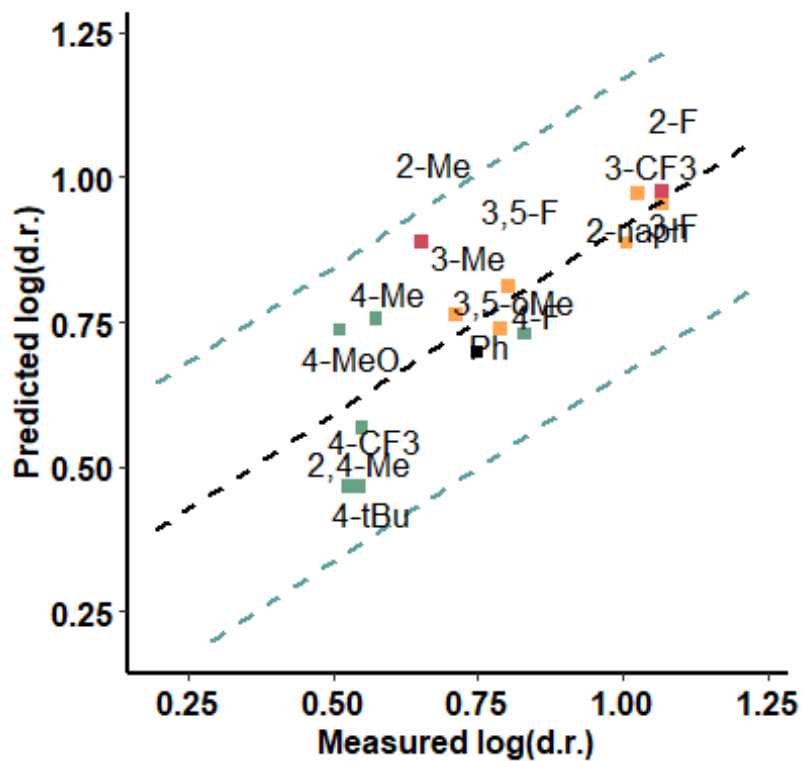
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.7602560	0.0335847	22.636993	0.0000000
para	0.1172961	0.0354264	3.310975	0.0062132
Dist.16..17.	-0.0950124	0.0354264	-2.681964	0.0199643

3 & 5 fold CV

Q2	MAE
0.4601792	0.1292474

Q2	MAE
0.4773838	0.1229769

Top Ranked Full Model



BA + Aldehyde - H bond - opposite to aldehyde

formula	R.sq	Q.sq	MAE
output ~ Dist.2..9. + B5	0.5912006	0.4547096	0.1286433
output ~ diff.B2.09 + B5	0.5512341	0.4285776	0.1308614

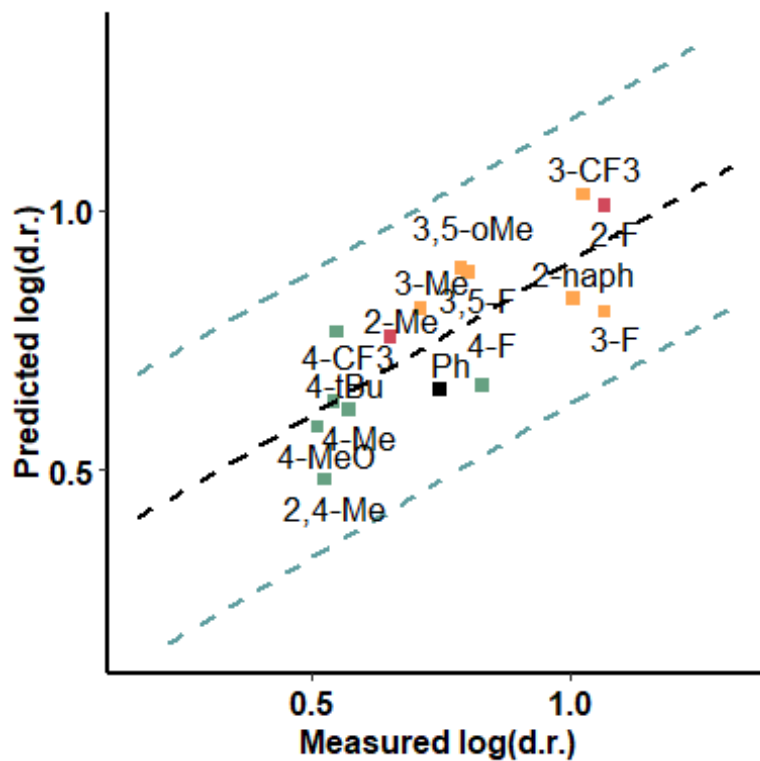
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.7602560	0.0363600	20.909145	0.0000000
Dist.2..9.	-0.1350464	0.0377053	-3.581633	0.0037709
B5	0.0882433	0.0377053	2.340343	0.0373624

3 & 5 fold CV

Q2	MAE
0.4214863	0.1398078

Q2	MAE
0.4360454	0.1335854

Top Ranked Full Model



Enamine - far from the active site

formula	R.sq	Q.sq	MAE
output ~ para + Dist.1..2.	0.7076306	0.5792479	0.0948479
output ~ para + diff.01.B2	0.6849136	0.5356607	0.1031372

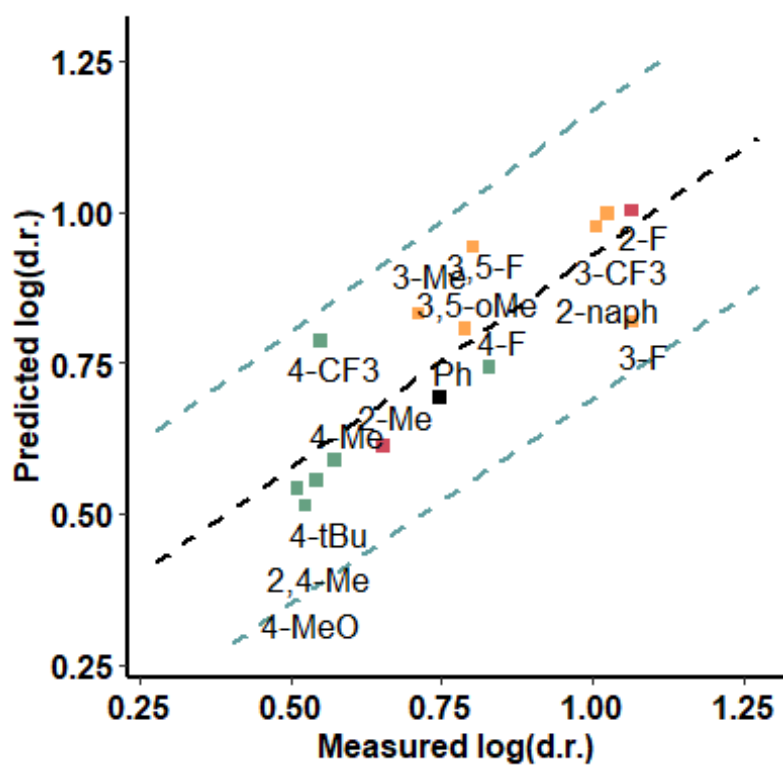
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.7602560	0.0307492	24.724384	0.0000000
para	0.1146593	0.0326403	3.512814	0.0042797
Dist.1..2.	-0.1046718	0.0326403	-3.206825	0.0075365

3 & 5 fold CV

Q2	MAE
0.5222579	0.1065229

Q2	MAE
0.5381343	0.1004736

Top Ranked Full Model



Enamine - close to the active site

formula	R.sq	Q.sq	MAE
output ~ Total + NBO.H.10	0.6745607	0.4649195	0.1246208

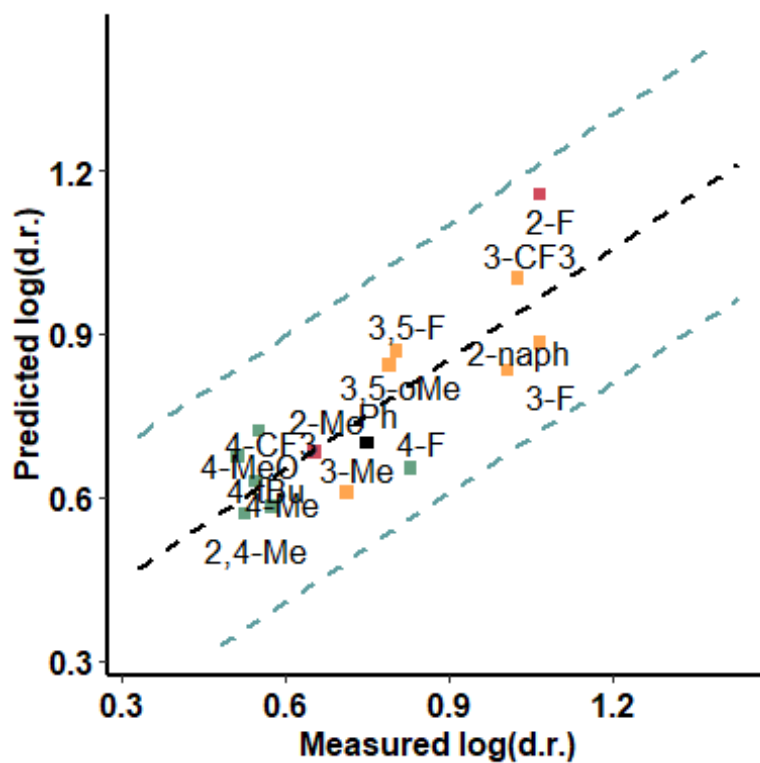
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.7602560	0.0324417	23.434538	0.0000000
Total	-0.1252952	0.0371527	-3.372443	0.0055451
NBO.H.10	0.1769896	0.0371527	4.763847	0.0004611

3 & 5 fold CV

Q2	MAE
0.4496495	0.1333502

Q2	MAE
0.4523634	0.1295369

Top Ranked Full Model



ACN

Only Boronic Acids

formula	R.sq	Q.sq	MAE
output ~ X.2.3. + Dist.2..9.	0.8549778	0.7987696	0.0465792

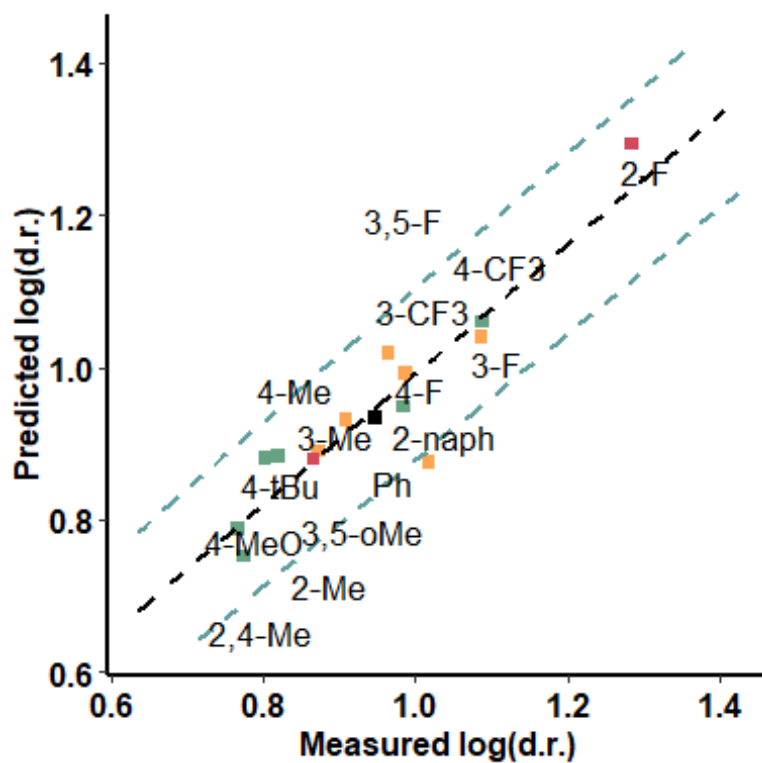
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.9445187	0.0148379	63.655912	0.0000000
X.2.3.	-0.0445812	0.0163465	-2.727256	0.0183595
Dist.2..9.	-0.1374663	0.0163465	-8.409507	0.0000022

3 & 5 fold CV

Q2	MAE
0.7596139	0.0545887

Q2	MAE
0.7792024	0.0507687

Top Ranked Full Model



With Catalyst - Close to the active site

formula	R.sq	Q.sq	MAE
output ~ X.8.14. + Dist.14..18.	0.8234273	0.7638875	0.0531336
output ~ Dist.1..16. + NBO.B.1	0.7991561	0.7319453	0.0601752

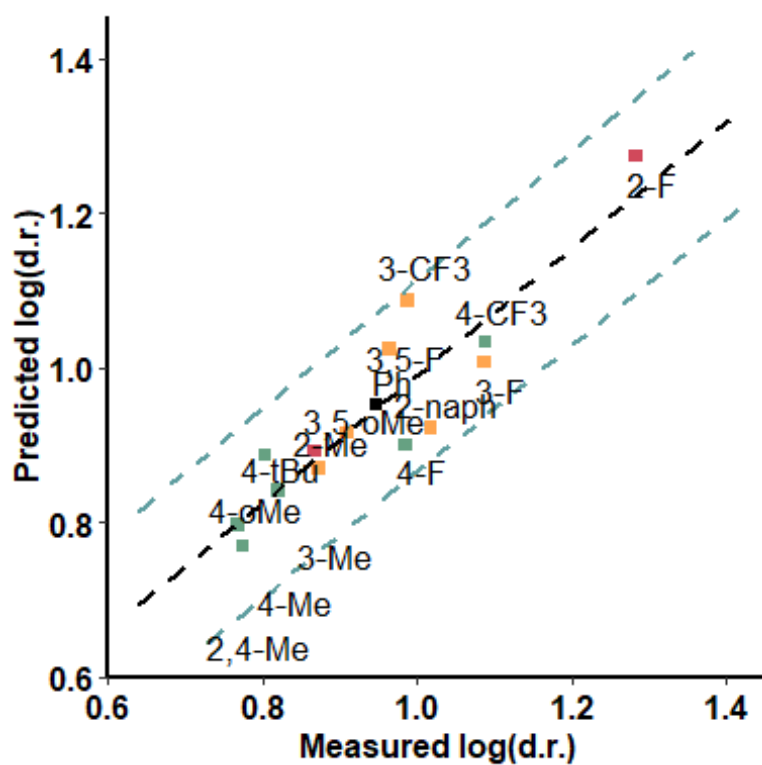
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.9445187	0.0163725	57.689166	0.00e+00
X.8.14.	-0.1047128	0.0176703	-5.925917	6.97e-05
Dist.14..18.	0.1070219	0.0176703	6.056592	5.70e-05

3 & 5 fold CV

Q2	MAE
0.6678096	0.0687734

Q2	MAE
0.7106756	0.0614302

Top Ranked Full Model



With Catalyst - far from the active site

formula	R.sq	Q.sq	MAE
output ~ Dist.19..20. + diff.C17.018	0.8684463	0.7960916	0.0509759

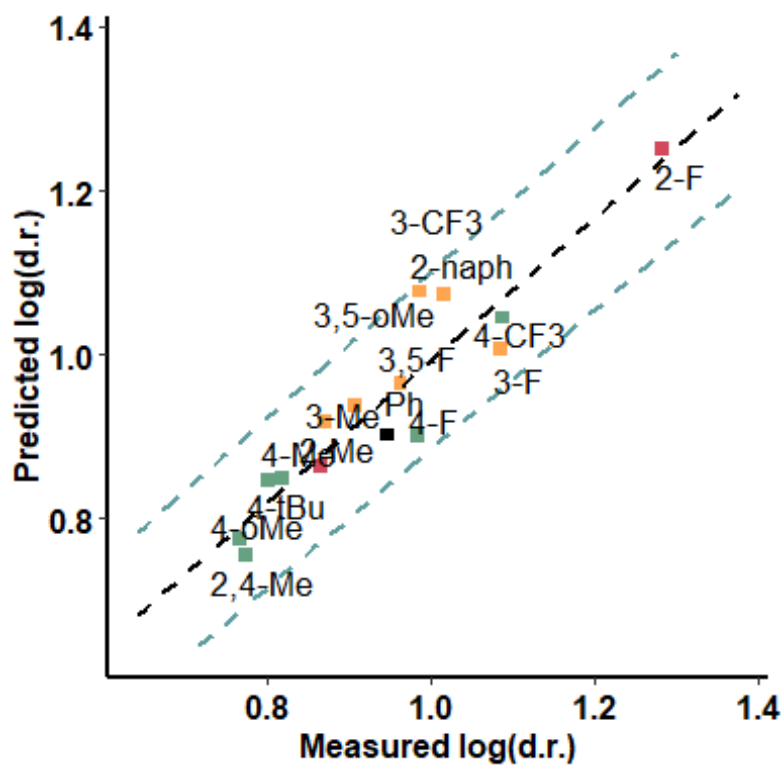
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.9445187	0.0141321	66.835076	0.0000000
Dist.19..20.	0.1003721	0.0202799	4.949344	0.0003368
diff.C17.018	-0.1777287	0.0202799	-8.763794	0.0000015

3 & 5 fold CV

Q2	MAE
0.7655674	0.056806

Q2	MAE
0.7815421	0.0538645

Top Ranked Full Model



BA + Pentanone

formula	R.sq	Q.sq	MAE
output ~ Total + diff.01.H10	0.7983838	0.7466983	0.0557884
output ~ Dist.1..2. + diff.09.H16	0.8079846	0.7417208	0.0592688

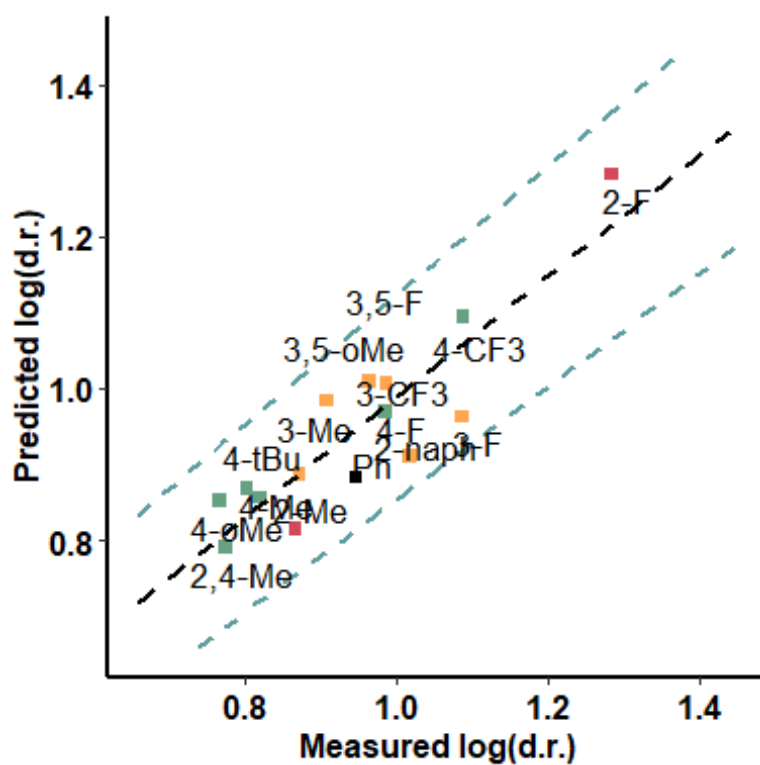
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.9445187	0.0174951	53.987515	0.00e+00
Total	0.0859449	0.0189700	4.530573	6.89e-04
diff.01.H10	-0.1196818	0.0189700	-6.309005	3.89e-05

3 & 5 fold CV

Q2	MAE
0.6509652	0.0890807

Q2	MAE
0.6937687	0.0732998

Top Ranked Full Model



BA + Aldehyde (pi interaction) - oxygen side

formula	R.sq	Q.sq	MAE
output ~ Dist.2..9. + dip_y	0.8969871	0.8489363	0.0436013
output ~ Dist.2..9. + NBO.C.20	0.8901088	0.8385889	0.0372199

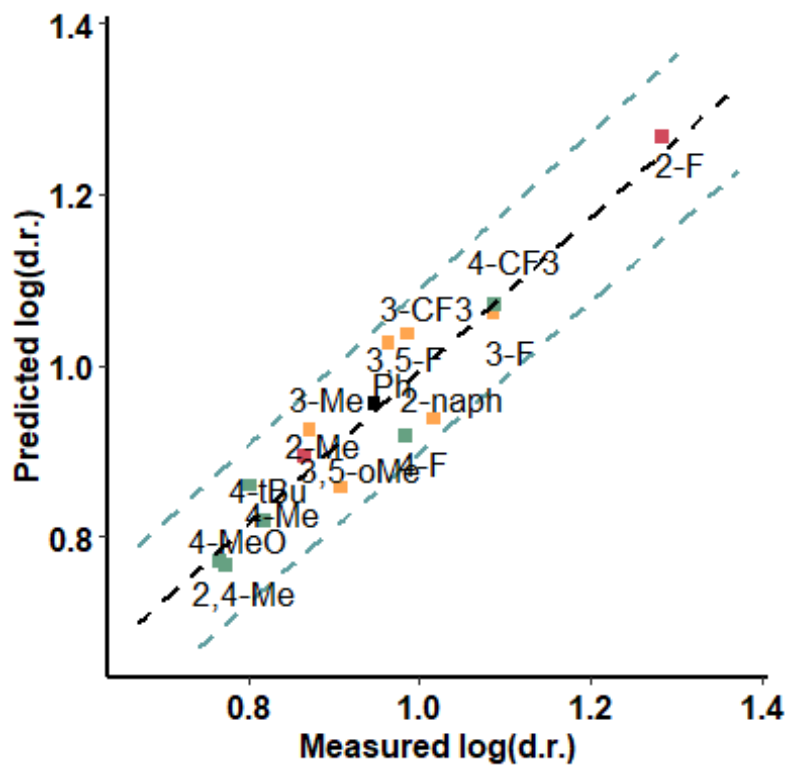
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.9445187	0.0125055	75.528377	0.0000000
Dist.2..9.	-0.1177076	0.0131926	-8.922225	0.0000012
dip_y	-0.0418457	0.0131926	-3.171897	0.0080413

3 & 5 fold CV

Q2	MAE
0.8321263	0.0482246

Q2	MAE
0.8389818	0.0461439

Top Ranked Full Model



BA + Aldehyde (pi interaction) - hydrogen side

formula	R.sq	Q.sq	MAE
output ~ X.18.19. + NBO.0.1	0.9018949	0.8684135	0.0427732
output ~ NBO.0.1 + NBO.0.17	0.9062933	0.8552073	0.0428522

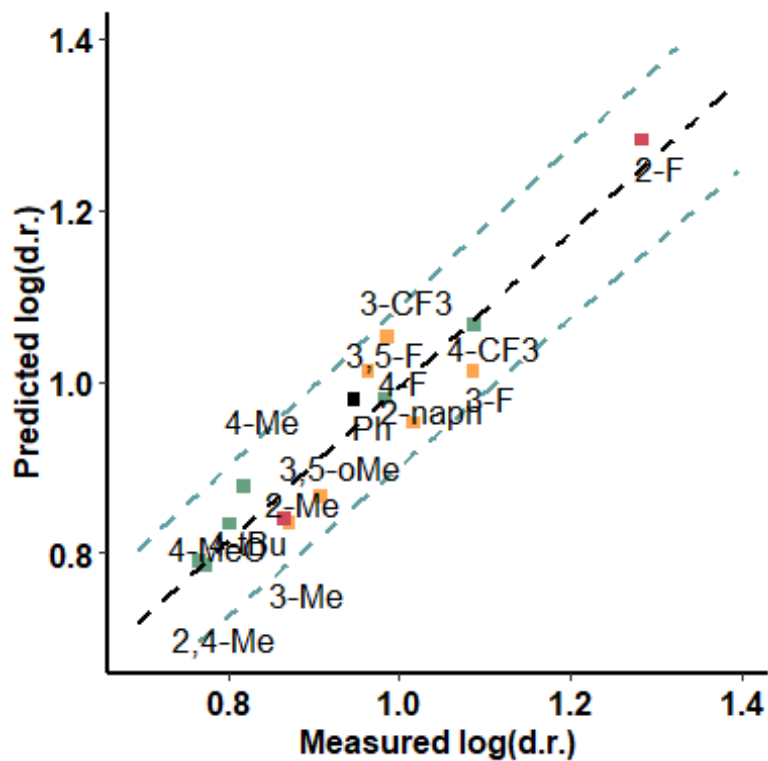
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.9445187	0.0122039	77.394515	0.00e+00
X.18.19.	-0.0729285	0.0126645	-5.758496	9.04e-05
NBO.0.1	0.1161605	0.0126645	9.172123	9.00e-07

3 & 5 fold CV

Q2	MAE
0.8356473	0.0496494

Q2	MAE
0.8527622	0.0467147

Top Ranked Full Model



BA + Aldehyde - H bond - aldehyde side

formula	R.sq	Q.sq	MAE
output ~ Dist.9..16. + NBO.0.9	0.7822189	0.6928175	0.0695343
output ~ Dist.2..9. + Dist.9..16.	0.7637982	0.6243849	0.0751802

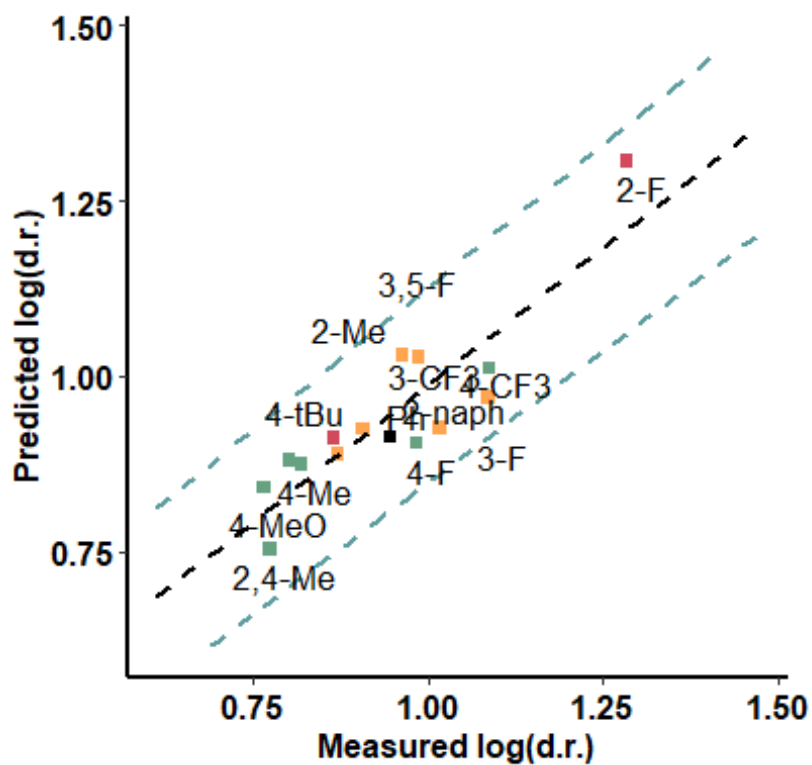
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.9445187	0.0181830	51.945259	0.0000000
Dist.9..16.	0.2120352	0.0322972	6.565129	0.0000267
NBO.0.9	0.1719997	0.0322972	5.325530	0.0001807

3 & 5 fold CV

Q2	MAE
0.6637378	0.07748

Q2	MAE
0.6799558	0.0725864

Top Ranked Full Model



BA + Aldehyde - H bond - opposite to aldehyde

formula	R.sq	Q.sq	MAE
output ~ Dist.9..16. + NBO.0.9	0.7599594	0.6901046	0.0680400
output ~ Dist.2..9. + Dist.9..16.	0.7636245	0.5847323	0.0788087

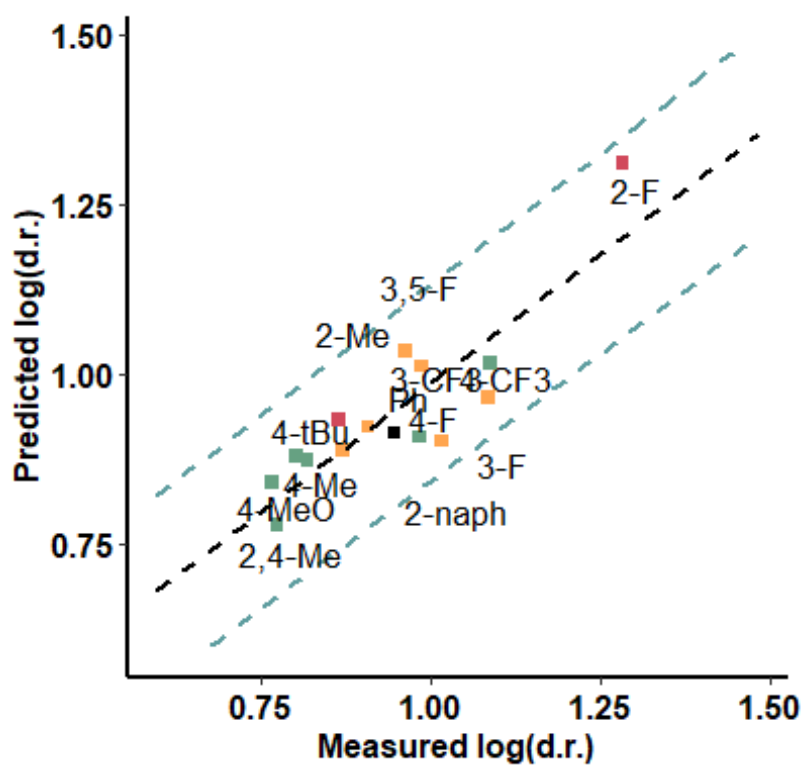
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.9445187	0.0190896	49.478182	0.0000000
Dist.9..16.	0.0828234	0.0236594	3.500661	0.0043765
NBO.0.9	0.1457957	0.0236594	6.162284	0.0000486

3 & 5 fold CV

Q2	MAE
0.5764615	0.0902935

Q2	MAE
0.6204771	0.0810264

Top Ranked Full Model



Enamine - far from the active site

formula	R.sq	Q.sq	MAE
output ~ Dist.1..2. + B1	0.8053431	0.7372605	0.0570261
output ~ X.1.2. + Dist.1..2.	0.7866995	0.7148957	0.0608419

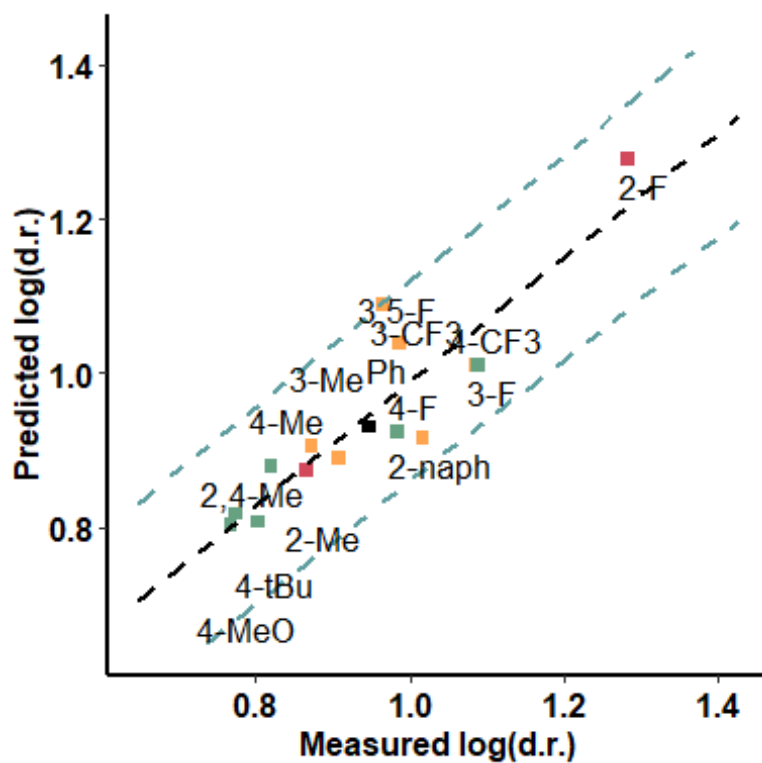
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.9445187	0.0171905	54.944117	0.0000000
Dist.1..2.	-0.1202990	0.0179879	-6.687766	0.0000224
B1	-0.0218504	0.0179879	-1.214726	0.2478327

3 & 5 fold CV

Q2	MAE
0.6115763	0.076565

Q2	MAE
0.6610066	0.0699747

Top Ranked Full Model



Enamine - close to the active site

formula	R.sq	Q.sq	MAE
output ~ Dist.2..9. + Dist.9..16.	0.7768762	0.6797322	0.067488
output ~ Dist.2..9. + Dist.16..36.	0.7704016	0.6700345	0.068579

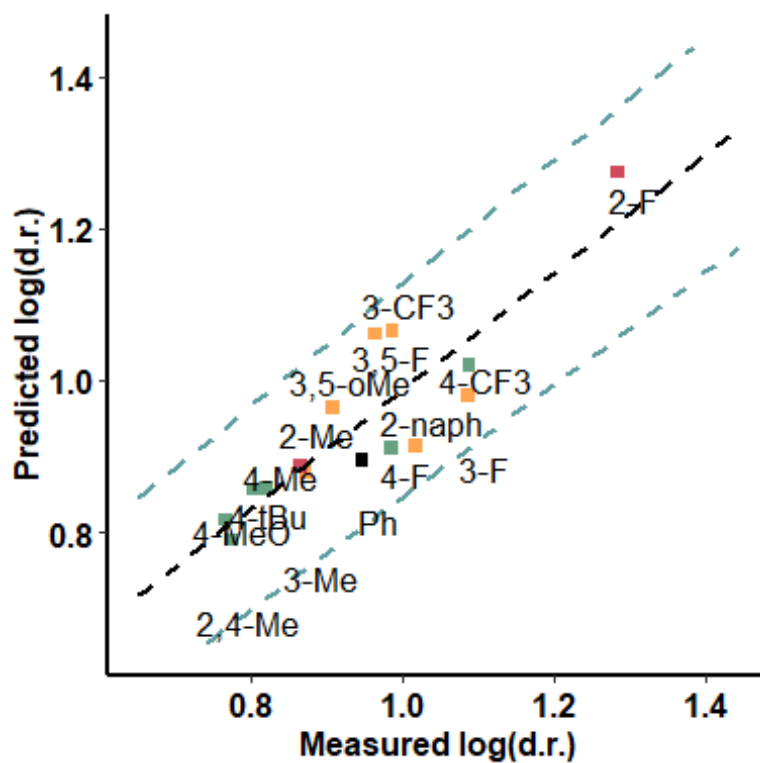
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.9445187	0.0184046	51.319587	0.0000000
Dist.2..9.	-0.1528354	0.0288622	-5.295346	0.0001898
Dist.9..16.	-0.0441940	0.0288622	-1.531205	0.1516461

3 & 5 fold CV

Q2	MAE
0.6242363	0.0764223

Q2	MAE
0.6471299	0.0723483

Top Ranked Full Model



Methanol

Only Boronic Acids

formula	R.sq	Q.sq	MAE
output ~ Dist.2..3. + L	0.4873112	0.2284430	0.1113156
output ~ X.9.16. + Dist.1..10.	0.4564576	0.1695005	0.1092643

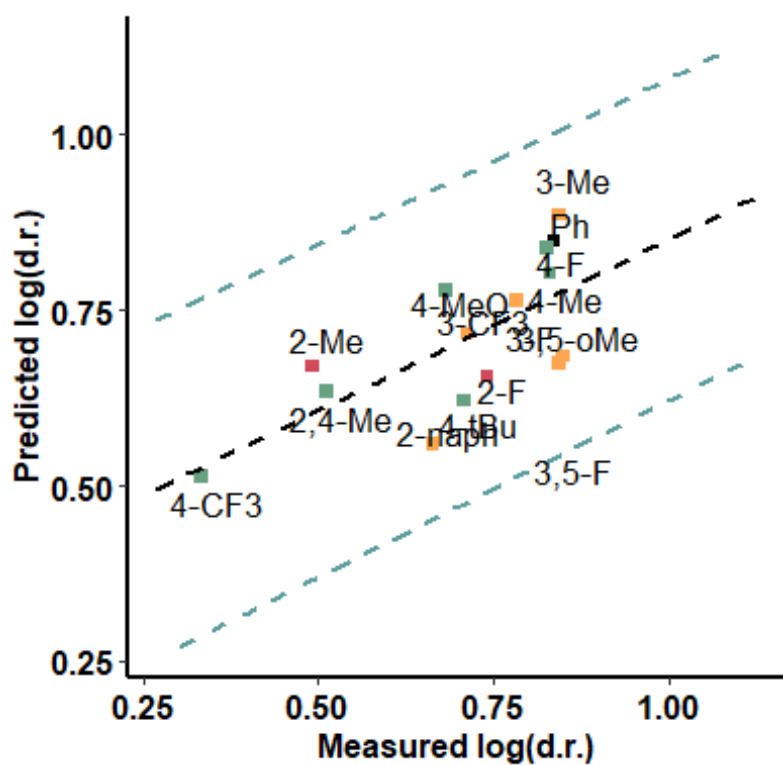
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.7096271	0.0309442	22.932499	0.0000000
Dist.2..3.	-0.1209816	0.0399098	-3.031378	0.0104398
L	-0.1198623	0.0399098	-3.003331	0.0109984

3 & 5 fold CV

Q2	MAE
0.226258	0.1182279

Q2	MAE
0.2285191	0.1142997

Top Ranked Full Model



With Catalyst - Close to the active site

formula	R.sq	Q.sq	MAE
output ~ Dist.14..18. + dip_y	0.6566038	0.383088	0.0995996

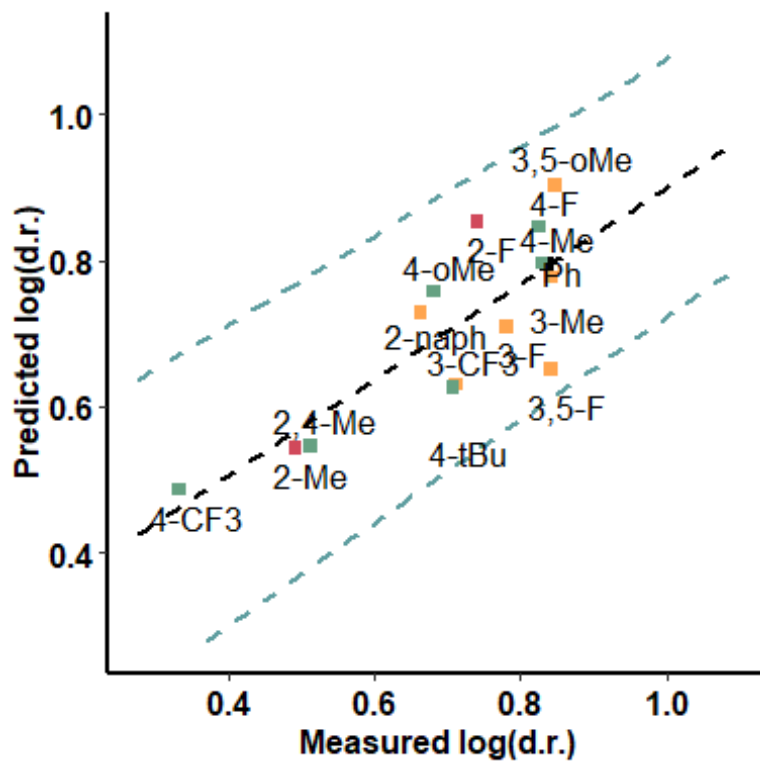
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.7096271	0.0253250	28.020802	0.0000000
Dist.14..18.	0.1154762	0.0278342	4.148713	0.0013497
dip_y	0.1015918	0.0278342	3.649887	0.0033272

3 & 5 fold CV

Q2	MAE
0.3368284	0.1074321

Q2	MAE
0.3563787	0.1021568

Top Ranked Full Model



With Catalyst - far from the active site

formula	R.sq	Q.sq	MAE
output ~ Dist.8..14. + L	0.6877579	0.5648867	0.068771
output ~ X.1.8. + dip_y	0.6851683	0.4564739	0.087374

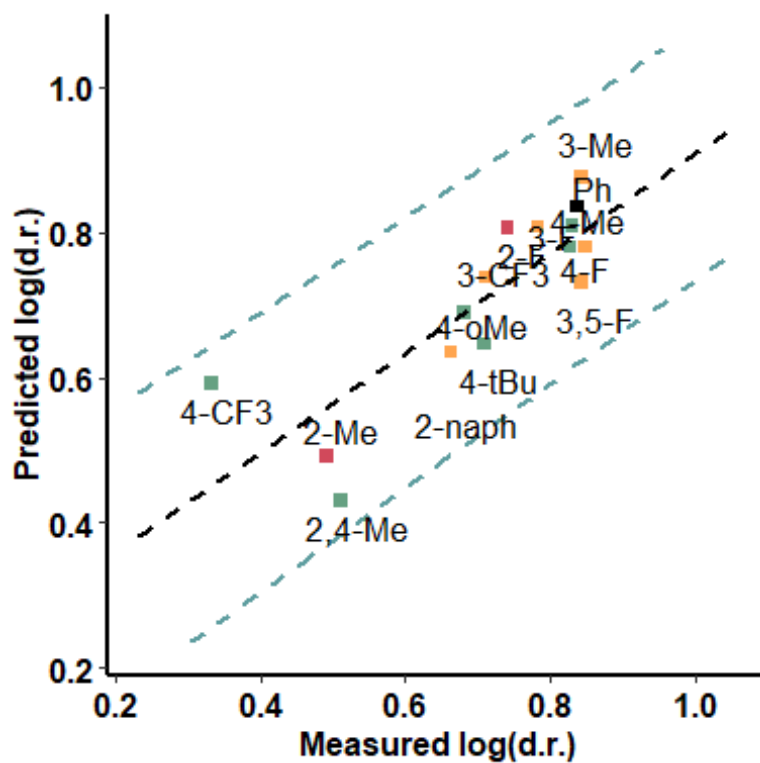
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.7096271	0.0241489	29.385465	0.0000000
Dist.8..14.	-0.1296404	0.0271915	-4.767682	0.0004581
L	-0.0991157	0.0271915	-3.645101	0.0033565

3 & 5 fold CV

Q2	MAE
0.5017991	0.0889416

Q2	MAE
0.5300659	0.0817515

Top Ranked Full Model



BA + Pentanone

formula	R.sq	Q.sq	MAE
output ~ cross + Dist.9..16.	0.5703362	0.3409087	0.1008972
output ~ Dist.2..3. + L	0.5713759	0.3257863	0.1033847

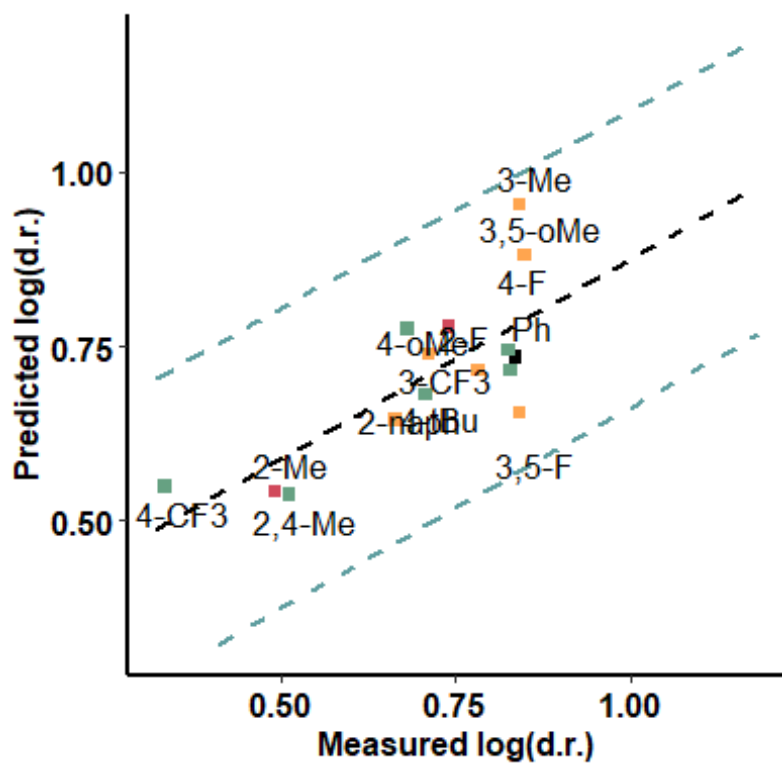
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.7096271	0.0283280	25.050356	0.0000000
cross	0.0944118	0.0304279	3.102801	0.0091423
Dist.9..16.	-0.0988260	0.0304279	-3.247869	0.0069840

3 & 5 fold CV

Q2	MAE
0.3166677	0.1113414

Q2	MAE
0.3214076	0.1058011

Top Ranked Full Model



BA + Aldehyde (pi interaction) - oxygen side

formula	R.sq	Q.sq	MAE
output ~ Dist.9..16. + L	0.6620972	0.4737708	0.0906331

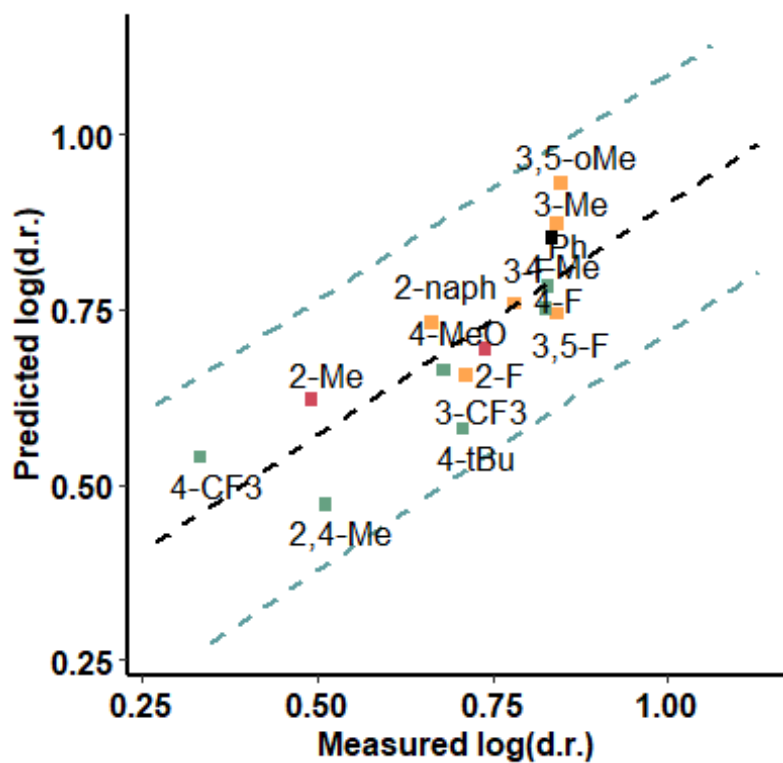
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.7096271	0.0251216	28.247655	0.0000000
Dist.9..16.	-0.1262061	0.0282996	-4.459648	0.0007796
L	-0.0993057	0.0282996	-3.509089	0.0043091

3 & 5 fold CV

Q2	MAE
0.4402504	0.0984614

Q2	MAE
0.4495994	0.0948711

Top Ranked Full Model



BA + Aldehyde (pi interaction) - hydrogen side

formula	R.sq	Q.sq	MAE
output ~ Dist.1..10. + L	0.7248318	0.568937	0.0707027
output ~ X.18.20. + L	0.6504974	0.442189	0.0874867

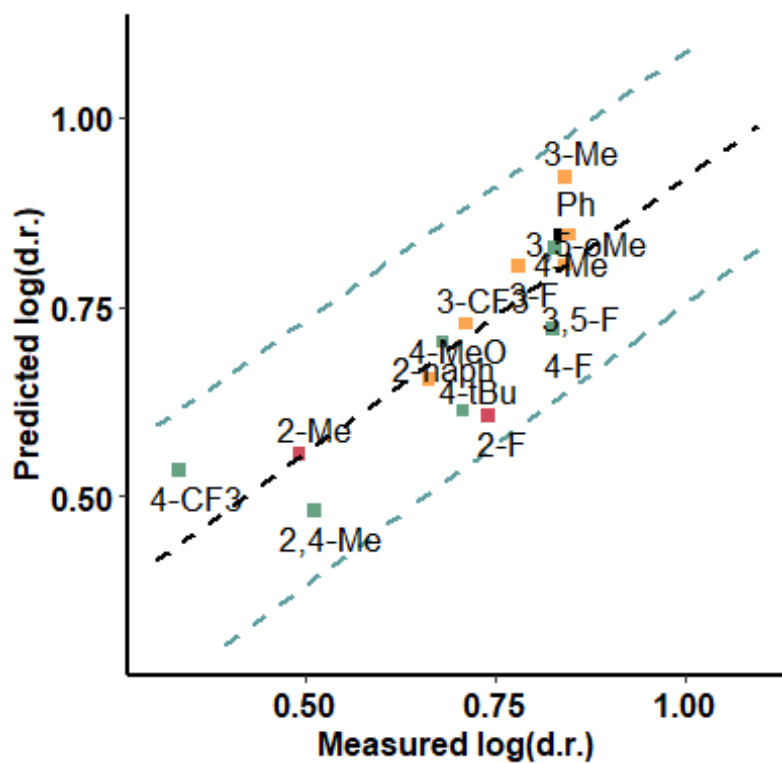
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.7096271	0.0226700	31.302511	0.0000000
Dist.1..10.	-0.1402467	0.0268696	-5.219523	0.0002149
L	-0.1173549	0.0268696	-4.367568	0.0009161

3 & 5 fold CV

Q2	MAE
0.5269259	0.0809355

Q2	MAE
0.5409732	0.0764907

Top Ranked Full Model



BA + Aldehyde - H bond - aldehyde side

formula	R.sq	Q.sq	MAE
output ~ X.18.20. + NBO.H.19	0.6990670	0.4779786	0.0789922
output ~ X.18.20. + Dist.18..19.	0.6858546	0.4635106	0.0781010

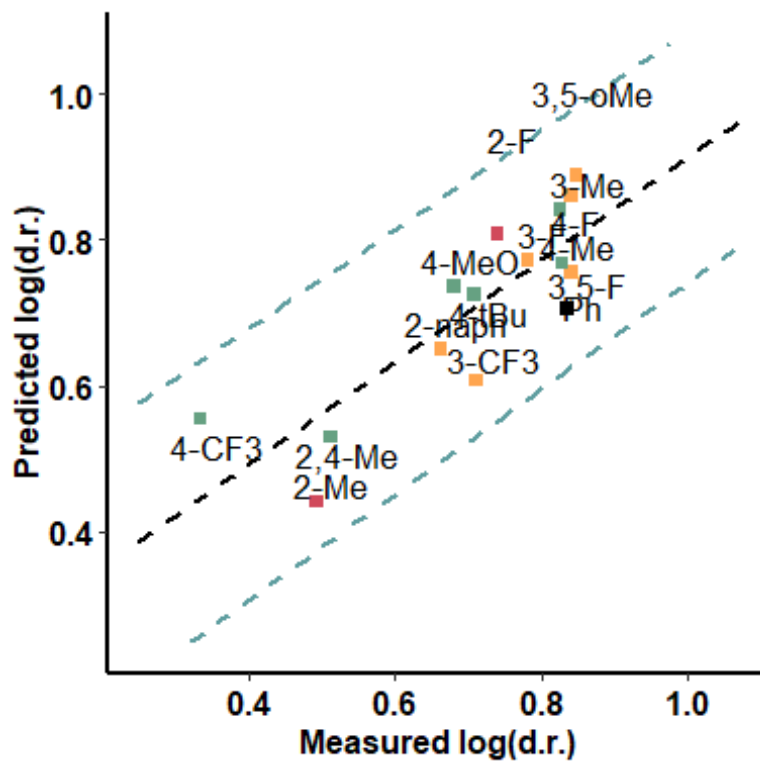
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.7096271	0.0237076	29.932524	0.0000000
X.18.20.	-0.2182619	0.0441527	-4.943340	0.0003402
NBO.H.19	-0.2269562	0.0441527	-5.140253	0.0002449

3 & 5 fold CV

Q2	MAE
0.4545821	0.0851356

Q2	MAE
0.4630493	0.0819673

Top Ranked Full Model



BA + Aldehyde - H bond - opposite to aldehyde

formula	R.sq	Q.sq	MAE
output ~ X.1.10. + dip_x	0.6561442	0.5032629	0.0819531
output ~ X.18.20. + diff.H16.017	0.6885971	0.4593459	0.0960803

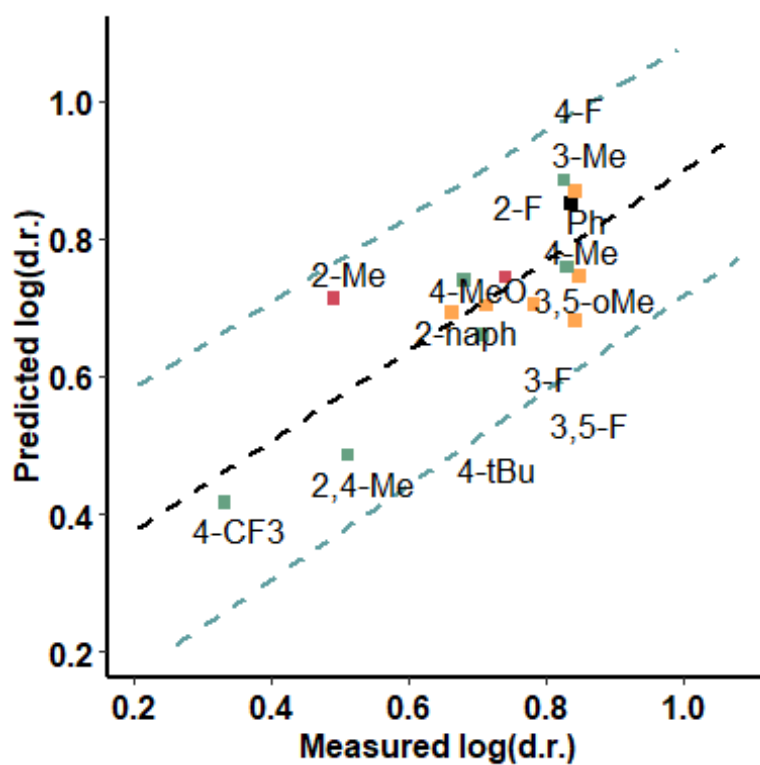
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.7096271	0.0253420	28.002068	0.0000000
X.1.10.	0.1044065	0.0265931	3.926069	0.0020129
dip_x	-0.0889245	0.0265931	-3.343888	0.0058459

3 & 5 fold CV

Q2	MAE
0.4488384	0.2491514

Q2	MAE
0.4820735	0.110239

Top Ranked Full Model



Enamine - far from the active site

formula	R.sq	Q.sq	MAE
output ~ Dist.1..10. + L	0.5981772	0.4639326	0.0785754

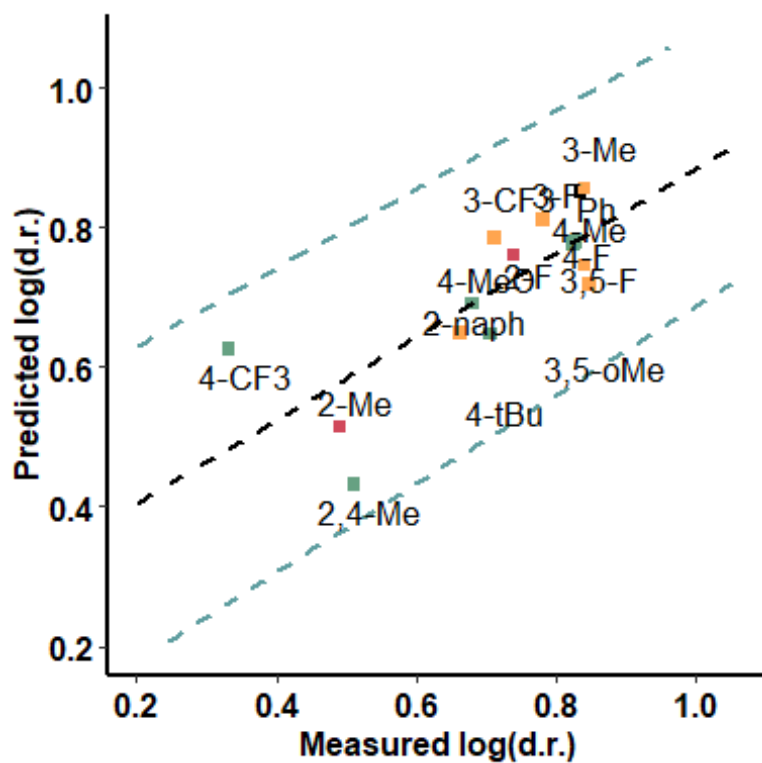
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.7096271	0.0273949	25.903652	0.0000000
Dist.1..10.	-0.1178298	0.0303279	-3.885193	0.0021674
L	-0.0889777	0.0303279	-2.933855	0.0125140

3 & 5 fold CV

Q2	MAE
0.4033939	0.1017179

Q2	MAE
0.4317359	0.0887341

Top Ranked Full Model



Enamine - close to the active site

formula	R.sq	Q.sq	MAE
output ~ X.2.9. + L	0.5227355	0.3755615	0.0842177
output ~ Dist.2..3. + L	0.4794867	0.2163765	0.1138705

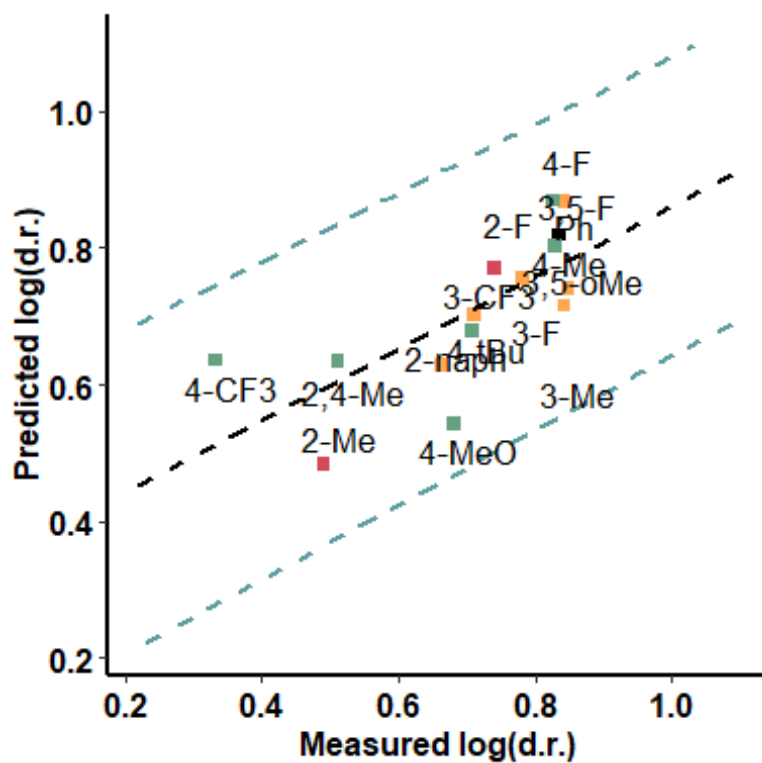
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.7096271	0.0298560	23.768334	0.0000000
X.2.9.	0.1099819	0.0334978	3.283257	0.0065405
L	-0.0899466	0.0334978	-2.685150	0.0198471

3 & 5 fold CV

Q2	MAE
0.339072	0.1005616

Q2	MAE
0.3494414	0.0923993

Top Ranked Full Model



Chloroform

Only Boronic Acids

formula	R.sq	Q.sq	MAE
output ~ X.1.2. + diff.01.H10	0.7063467	0.5249278	0.0997979
output ~ X.2.9. + Dist.2..9.	0.6799762	0.5177720	0.1004984

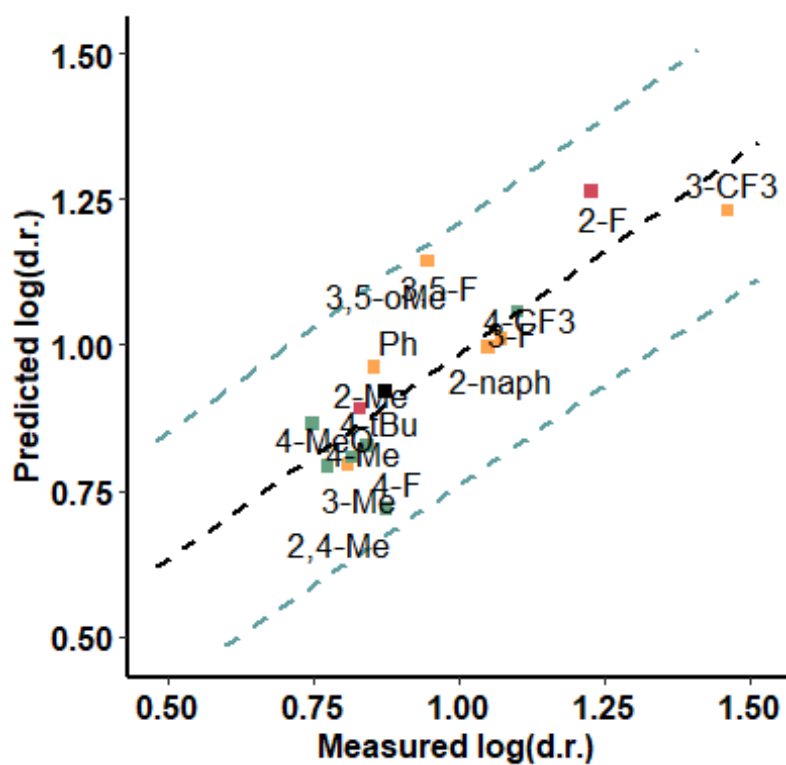
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.9516937	0.0296959	32.047999	0.0000000
X.1.2.	0.1387619	0.0308544	4.497313	0.0007301
diff.01.H10	0.0783109	0.0308544	2.538079	0.0260300

3 & 5 fold CV

Q2	MAE
0.4856652	0.1135153

Q2	MAE
0.5046355	0.1064469

Top Ranked Full Model



With Catalyst - Close

formula	R.sq	Q.sq	MAE
output ~ X.19.20. + Dist.8..14.	0.8365717	0.7100281	0.0737639
output ~ Dist.8..14. + dip_z	0.8301853	0.6769120	0.0928861

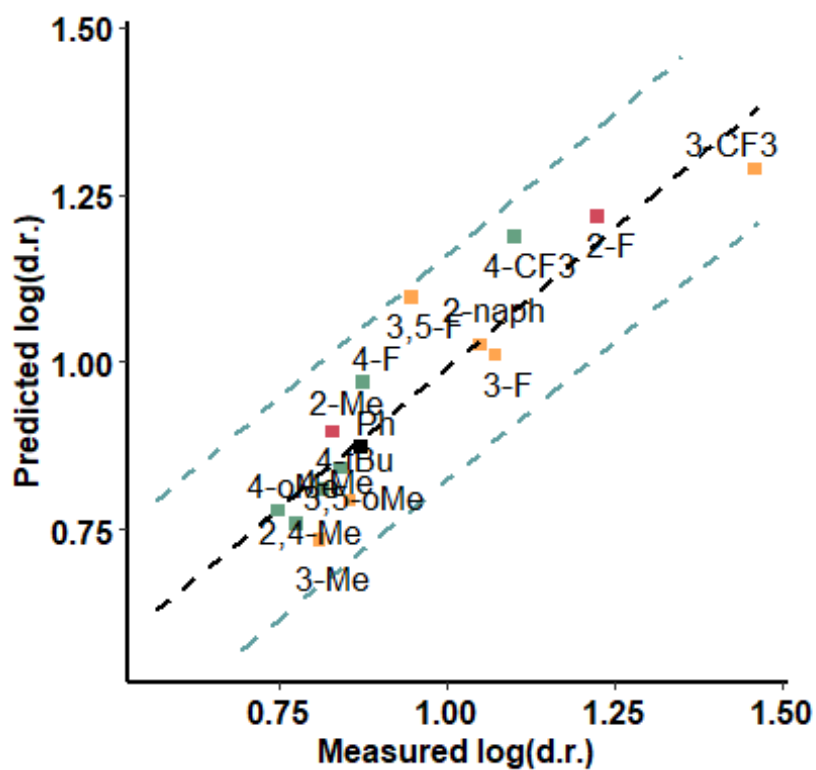
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.9516937	0.0221535	42.959056	0.0000000
X.19.20.	0.0668236	0.0229337	2.913769	0.0129898
Dist.8..14.	0.1658221	0.0229337	7.230493	0.0000104

3 & 5 fold CV

Q2	MAE
0.6881715	0.082144

Q2	MAE
0.6948214	0.0788665

Top Ranked Full Model



With Catalyst - far

formula	R.sq	Q.sq	MAE
output ~ Total + NB0.0.16	0.9105786	0.8313782	0.0600844
output ~ Total + L	0.8567410	0.7745529	0.0776621

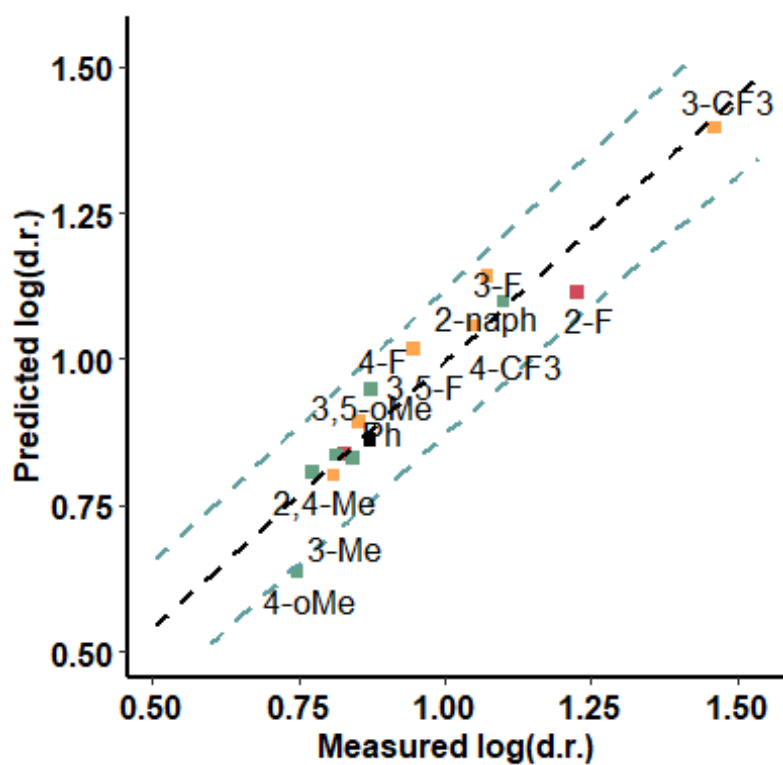
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.9516937	0.0163870	58.076115	0.0000000
Total	0.1614673	0.0177496	9.096969	0.0000010
NB0.0.16	-0.0589669	0.0177496	-3.322162	0.0060858

3 & 5 fold CV

Q2	MAE
0.7533024	0.0723211

Q2	MAE
0.7807192	0.0673714

Top Ranked Full Model



BA + Pentanone

formula	R.sq	Q.sq	MAE
output ~ NBO.H.16 + NBO.C.18	0.7881859	0.5923135	0.0992653

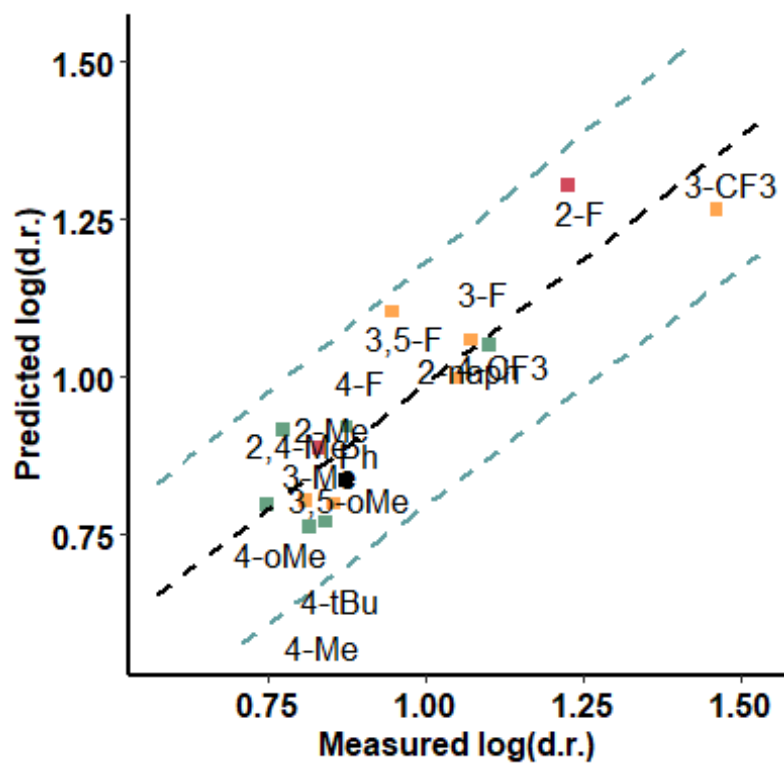
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.9516937	0.0252206	37.734700	0.0000000
NBO.H.16	0.6243529	0.1445792	4.318414	0.0009989
NBO.C.18	-0.4809641	0.1445792	-3.326647	0.0060354

3 & 5 fold CV

Q2	MAE
0.548231	0.1075869

Q2	MAE
0.5743685	0.1026113

Top Ranked Full Model



BA + Aldehyde (pi interaction) - oxygen side

formula	R.sq	Q.sq	MAE
output ~ X.18.19. + Dist.2..9.	0.8932486	0.4999122	2.042431

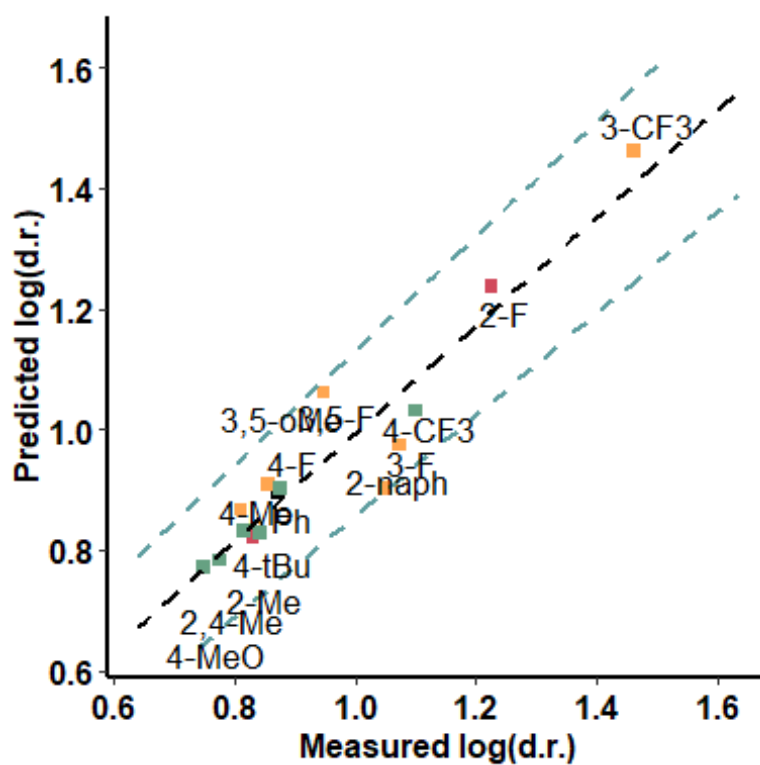
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.9516937	0.0179046	53.153471	0.0000000
X.18.19.	0.1040733	0.0193622	5.375069	0.0001667
Dist.2..9.	-0.1266026	0.0193622	-6.538638	0.0000278

3 & 5 fold CV

Q2	MAE
0.4993602	1.950007

Q2	MAE
0.4966702	1.949219

Top Ranked Full Model



BA + Aldehyde (pi interaction) - hydrogen side

formula	R.sq	Q.sq	MAE
output ~ X.18.19. + Dist.1..2.	0.6947638	0.5417311	0.0872277
output ~ Dist.1..2. + Dist.17..18.	0.6868608	0.5405861	0.0784905

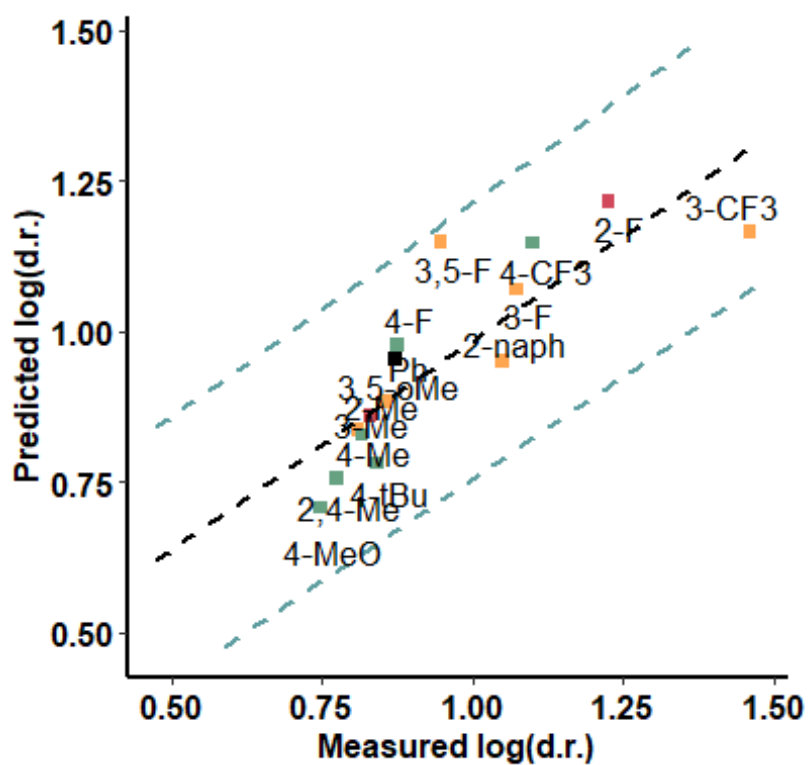
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.9516937	0.0302759	31.434051	0.0000000
X.18.19.	-0.0609723	0.0327582	-1.861283	0.0873696
Dist.1..2.	-0.1352892	0.0327582	-4.129932	0.0013957

3 & 5 fold CV

Q2	MAE
0.4853537	0.1071252

Q2	MAE
0.5054695	0.0984294

Top Ranked Full Model



BA + Aldehyde - H bond - aldehyde side

formula	R.sq	Q.sq	MAE
output ~ Dist.16..17. + NBO.H.10	0.8075570	0.6547173	0.0894582
output ~ Dist.10..17. + NBO.H.10	0.7608458	0.6280473	0.0919192

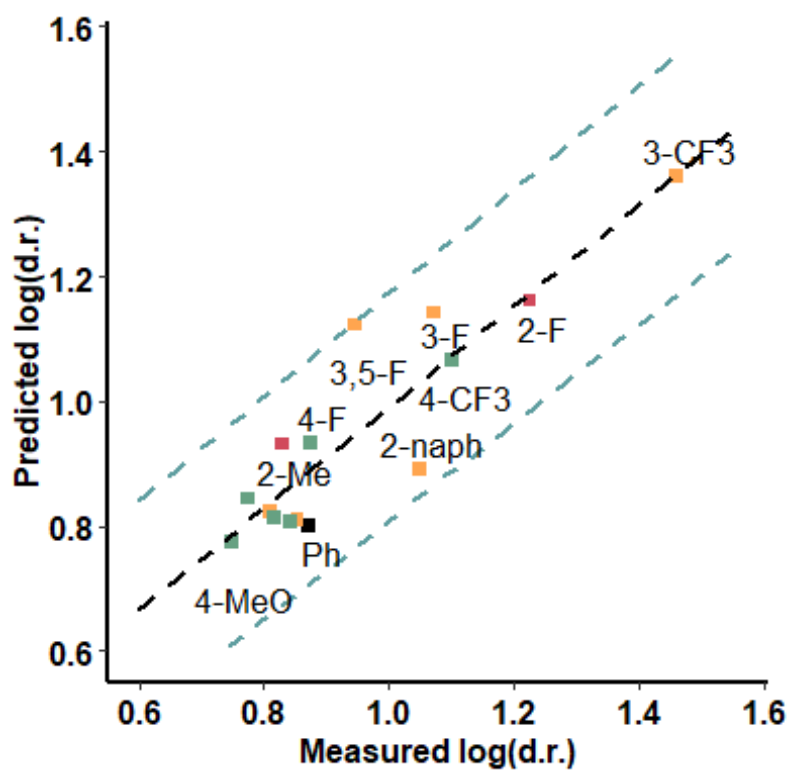
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.9516937	0.0240397	39.588343	0.0000000
Dist.16..17.	-0.2823593	0.0397995	-7.094542	0.0000126
NBO.H.10	0.2165431	0.0397995	5.440847	0.0001499

3 & 5 fold CV

Q2	MAE
0.6010178	0.1003702

Q2	MAE
0.6290117	0.0946882

Top Ranked Full Model



BA + Aldehyde - H bond - opposite to aldehyde

formula	R.sq	Q.sq	MAE
output ~ Dist.2..3. + diff.C18.H19	0.7284930	0.5572243	0.0966339
output ~ NBO.C.20 + diff.C18.C20	0.7187271	0.5269840	0.1001709

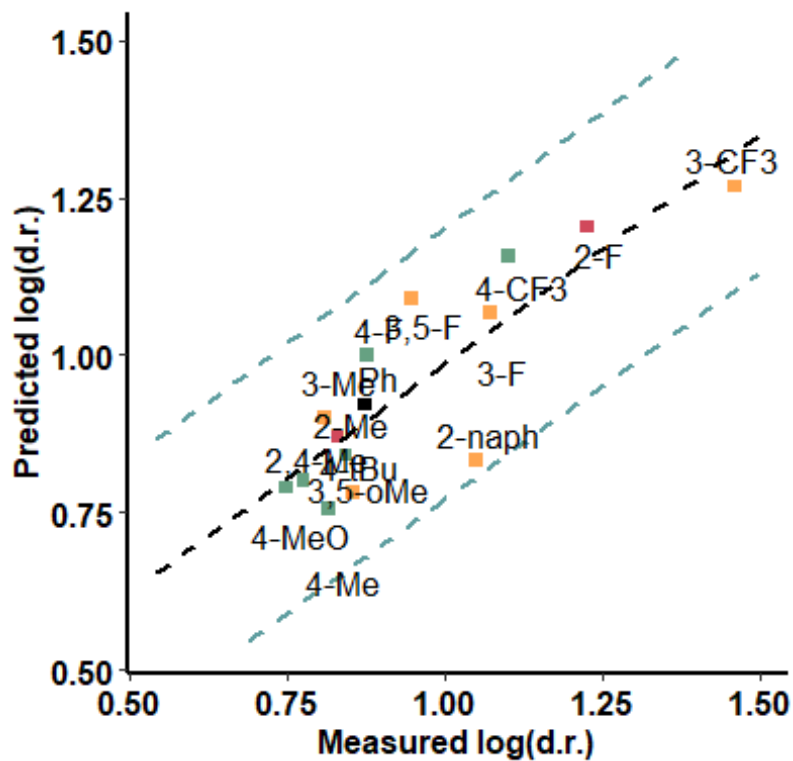
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.9516937	0.0285542	33.329428	0.0000000
Dist.2..3.	0.1311625	0.0302822	4.331339	0.0009764
diff.C18.H19	-0.1368899	0.0302822	-4.520473	0.0007012

3 & 5 fold CV

Q2	MAE
0.5049053	0.1091854

Q2	MAE
0.528301	0.1023787

Top Ranked Full Model



Enamine - far from the active site

formula	R.sq	Q.sq	MAE
output ~ Total + B5	0.8007607	0.7127119	0.0857386
output ~ para + Total	0.7954438	0.6829290	0.0834981

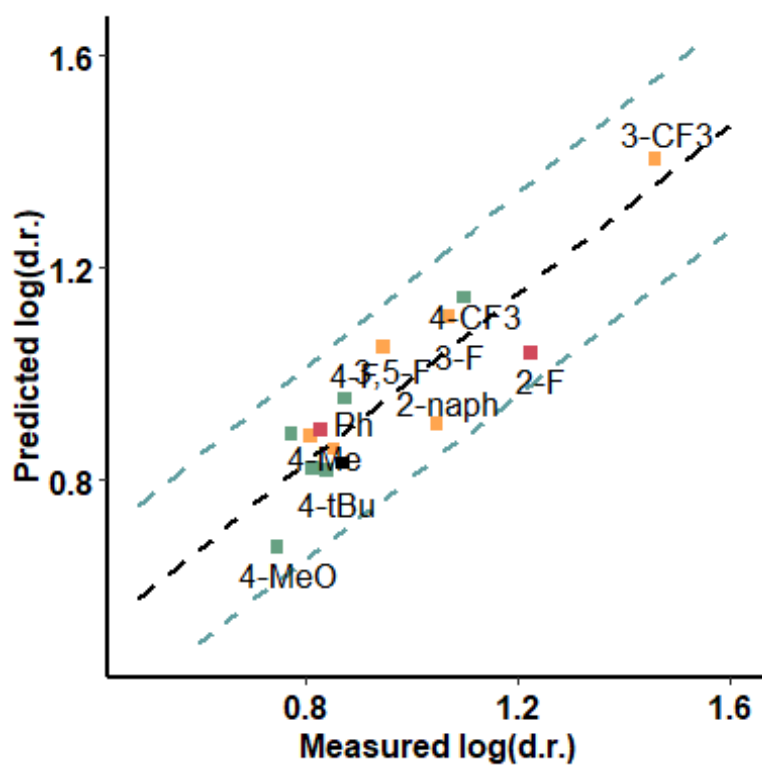
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.9516937	0.0244606	38.907275	0.0000000
Total	0.1692428	0.0253730	6.670194	0.0000229
B5	0.0599766	0.0253730	2.363797	0.0358032

3 & 5 fold CV

Q2	MAE
0.6765567	0.0938786

Q2	MAE
0.6941914	0.0893493

Top Ranked Full Model



Enamine - close to the active site

formula	R.sq	Q.sq	MAE
output ~ Total + NBO.H.10	0.759132	0.5977506	0.0830164

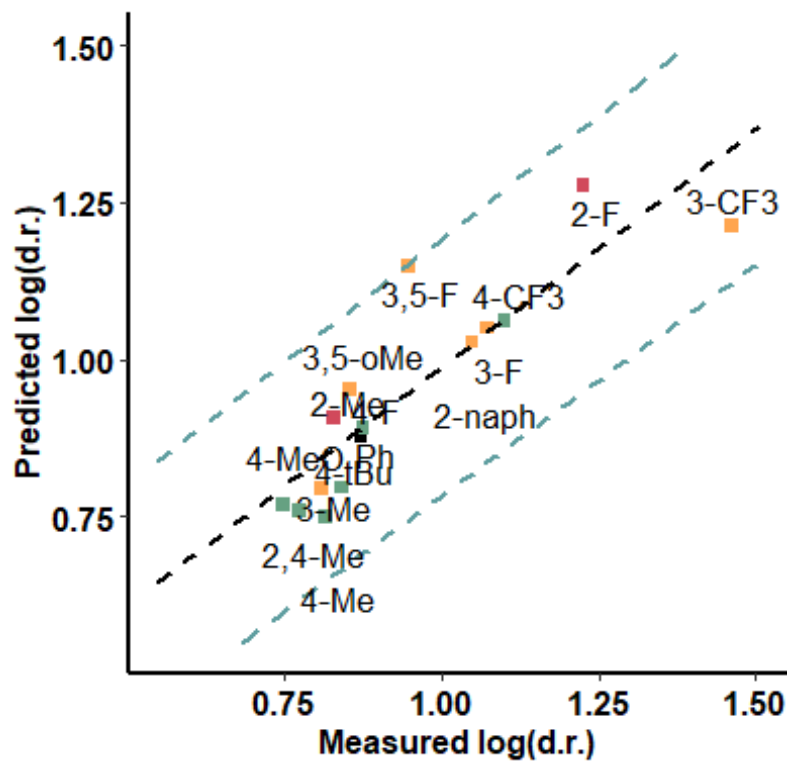
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.9516937	0.0268948	35.385782	0.0000000
Total	-0.0676258	0.0308003	-2.195621	0.0485164
NBO.H.10	0.1888533	0.0308003	6.131542	0.0000509

3 & 5 fold CV

Q2	MAE
0.5304826	0.100116

Q2	MAE
0.562416	0.0914321

Top Ranked Full Model



Hexane

Only Boronic Acids

formula	R.sq	Q.sq	MAE
output ~ X.2.9. + B5	0.7807392	0.6338624	0.0840461

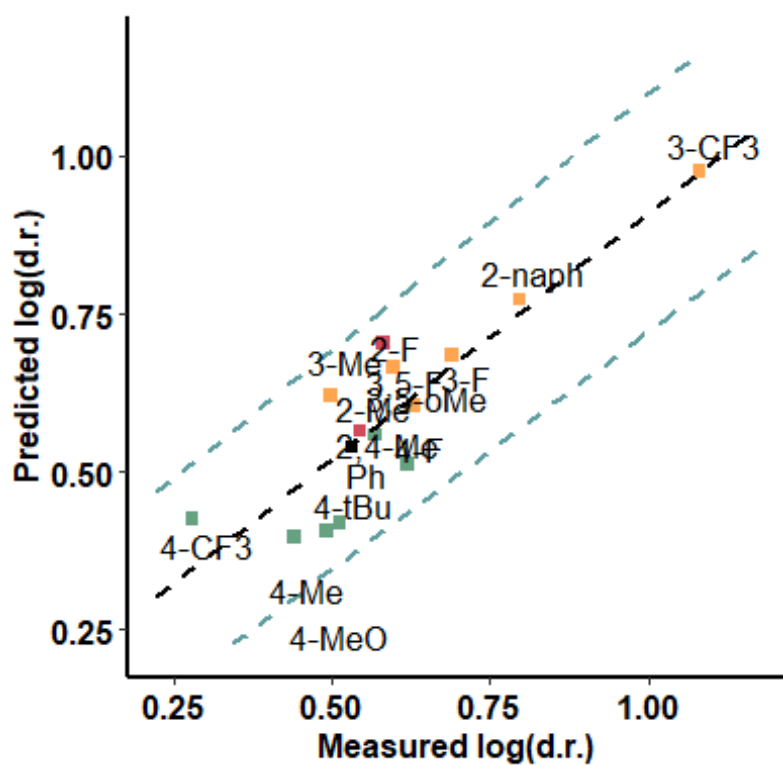
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.5902181	0.0233012	25.329975	0.0000000
X.2.9.	0.1257364	0.0251956	4.990413	0.0003143
B5	0.1381919	0.0251956	5.484766	0.0001396

3 & 5 fold CV

Q2	MAE
0.5817496	0.0922794

Q2	MAE
0.6050105	0.0888198

Top Ranked Full Model



With Catalyst - Close to the active site

formula	R.sq	Q.sq	MAE
output ~ Total + diff.B1.016	0.6696	0.332226	0.1168222

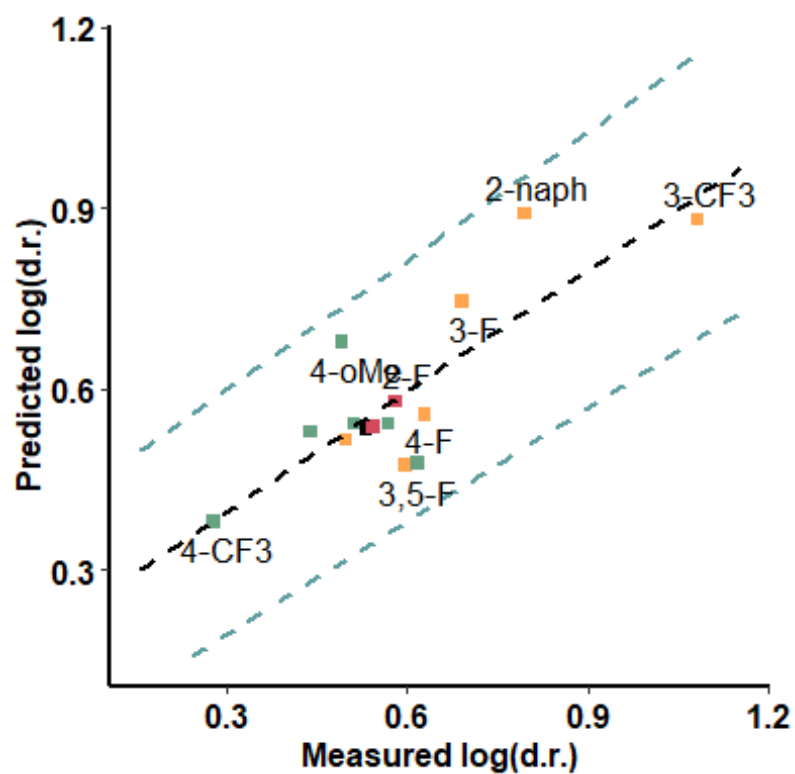
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.5902181	0.0286034	20.634563	0.0000000
Total	-0.1342640	0.0309348	-4.340225	0.0009612
diff.B1.016	0.1082315	0.0309348	3.498699	0.0043924

3 & 5 fold CV

Q2	MAE
0.3319761	0.1312353

Q2	MAE
0.3351846	0.1248125

Top Ranked Full Model



With Catalyst - far from the active site

formula	R.sq	Q.sq	MAE
output ~ Dist.19..20. + B5	0.6112505	0.3108150	0.1124397
output ~ Dist.17..18. + B5	0.5824655	0.2988876	0.1132490

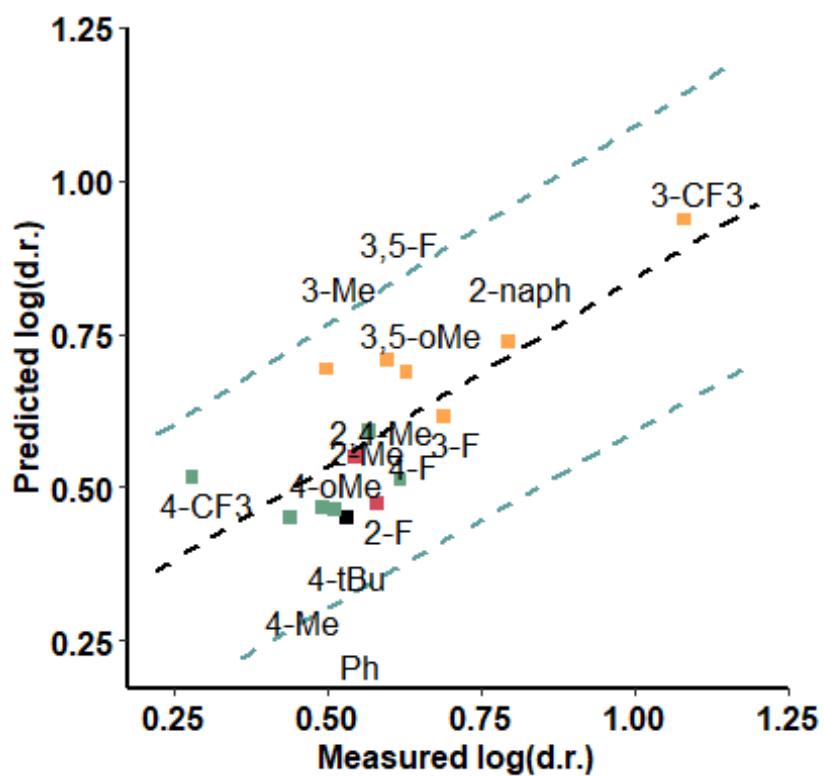
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.5902181	0.0310265	19.023059	0.0000000
Dist.19..20.	-0.0812907	0.0337947	-2.405424	0.0331887
B5	0.1414656	0.0337947	4.186025	0.0012629

3 & 5 fold CV

Q2	MAE
0.2852269	0.1274527

Q2	MAE
0.290438	0.1165023

Top Ranked Full Model



BA + Aldehyde (pi interaction) - oxygen side

formula	R.sq	Q.sq	MAE
output ~ X.18.19. + X.18.20.	0.7054320	0.5783839	3.052036
output ~ X.1.10. + X.18.19.	0.7179386	0.5745548	1.596017

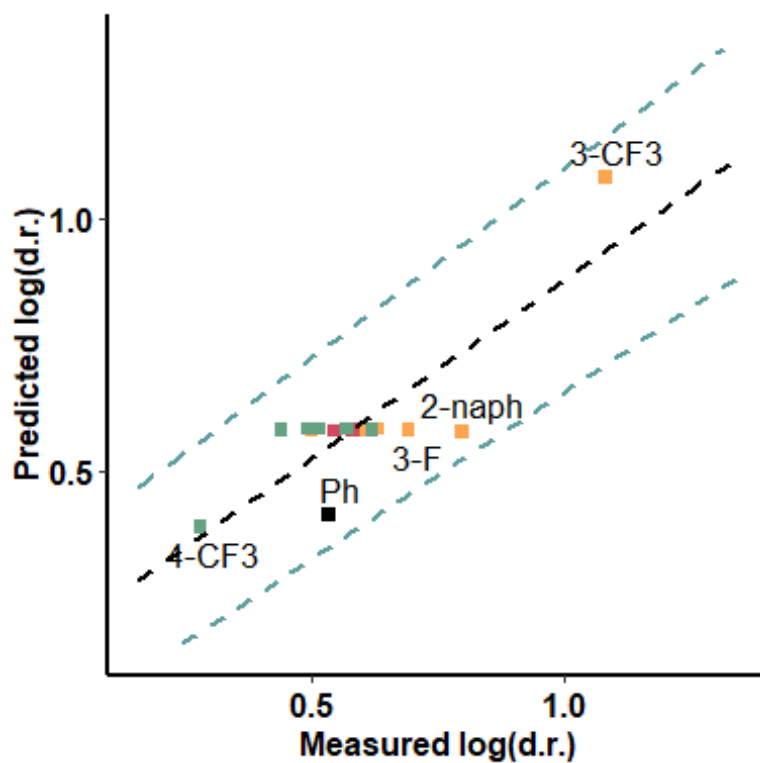
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.5902181	0.0270079	21.853575	0.0000000
X.18.19.	0.1285421	0.0281339	4.568938	0.0006447
X.18.20.	0.0639465	0.0281339	2.272932	0.0422139

3 & 5 fold CV

Q2	MAE
0.5627528	3.186934

Q2	MAE
0.5658159	2.950431

Top Ranked Full Model



BA + Aldehyde (pi interaction) - hydrogen side

formula	R.sq	Q.sq	MAE
output ~ diff.B2.09 + B5	0.5484099	0.2333914	0.1209806
output ~ dip_x + B5	0.4869764	0.2012582	0.1242570

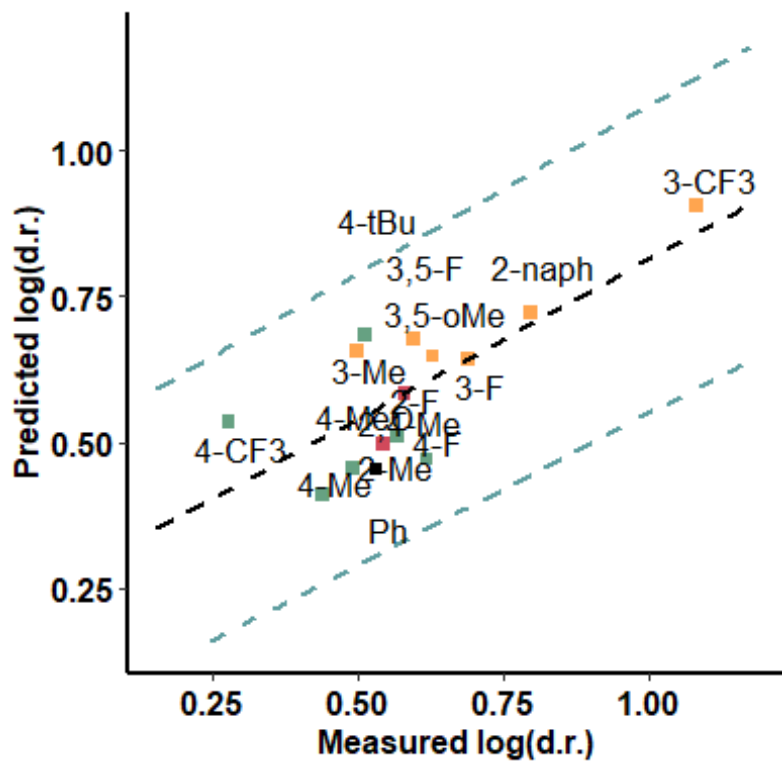
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.5902181	0.0334402	17.649933	0.0000000
diff.B2.09	-0.1433809	0.0431471	-3.323070	0.0060755
B5	0.1506338	0.0431471	3.491169	0.0044537

3 & 5 fold CV

Q2	MAE
0.2232037	0.131803

Q2	MAE
0.2235731	0.1267003

Top Ranked Full Model



BA + Aldehyde - H bond - aldehyde side

formula	R.sq	Q.sq	MAE
output ~ X.18.19. + B5	0.5642604	0.2868490	0.1194131
output ~ X.2.9. + B5	0.5633176	0.2811037	0.1177249

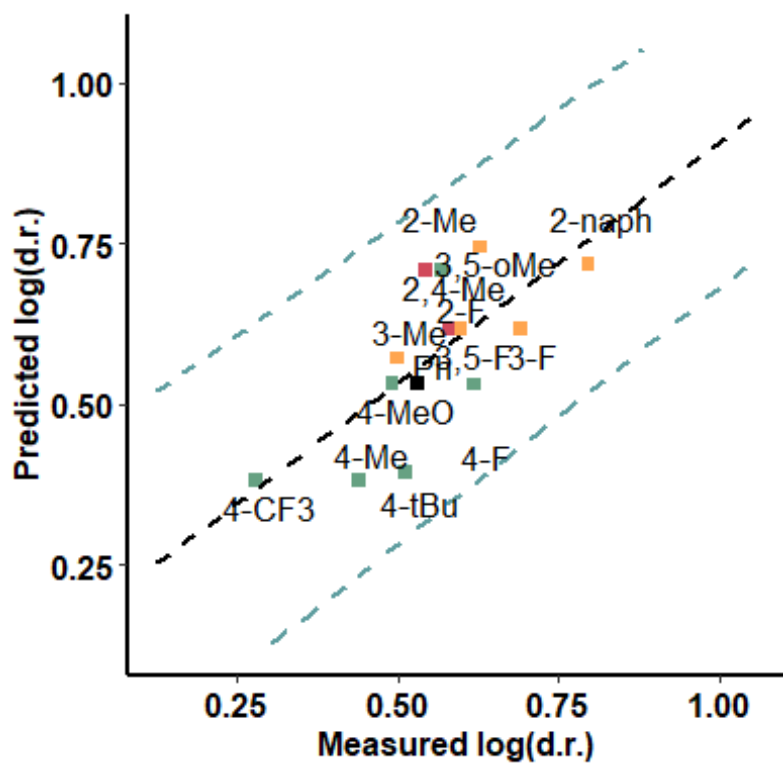
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.5902181	0.0328481	17.968084	0.0000000
X.18.19.	0.0687508	0.0358645	1.916960	0.0793580
B5	0.0952443	0.0358645	2.655673	0.0209583

3 & 5 fold CV

Q2	MAE
0.2744458	0.1700764

Q2	MAE
0.2787109	0.1400443

Top Ranked Full Model



BA + Aldehyde - H bond - opposite to aldehyde

formula	R.sq	Q.sq	MAE
output ~ diff.C18.H19 + B5	0.6759283	0.4534682	0.0958661

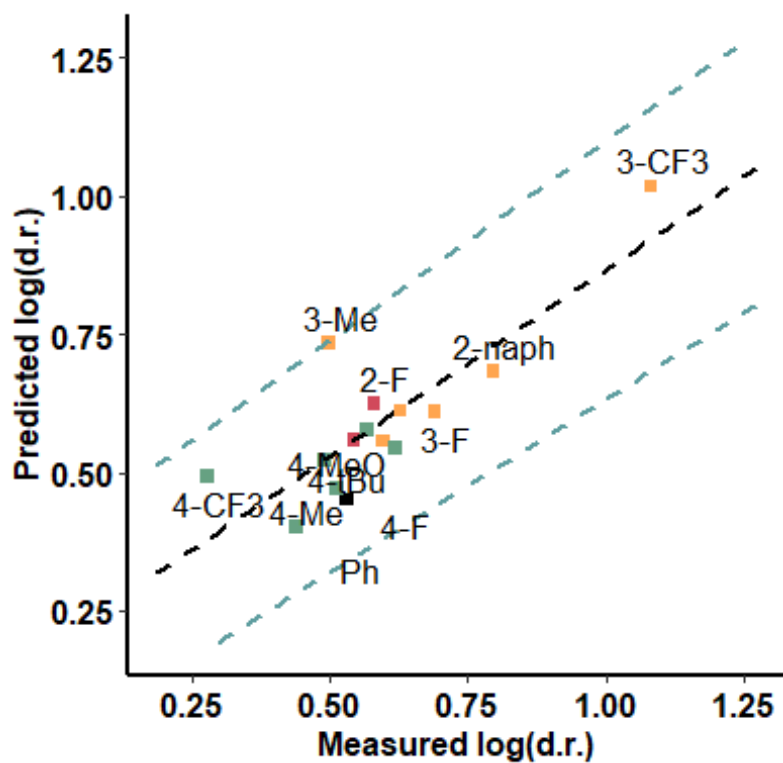
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.5902181	0.0283281	20.835060	0.0000000
diff.C18.H19	-0.0925083	0.0309449	-2.989449	0.0112858
B5	0.1471882	0.0309449	4.756455	0.0004669

3 & 5 fold CV

Q2	MAE
0.3809066	0.1061728

Q2	MAE
0.4135812	0.0999656

Top Ranked Full Model



Enamine - far from the active site

formula	R.sq	Q.sq	MAE
output ~ dip_z + B5	0.6124885	0.3204784	0.1230525
output ~ X.1.2. + B5	0.5737977	0.2919757	0.1075037

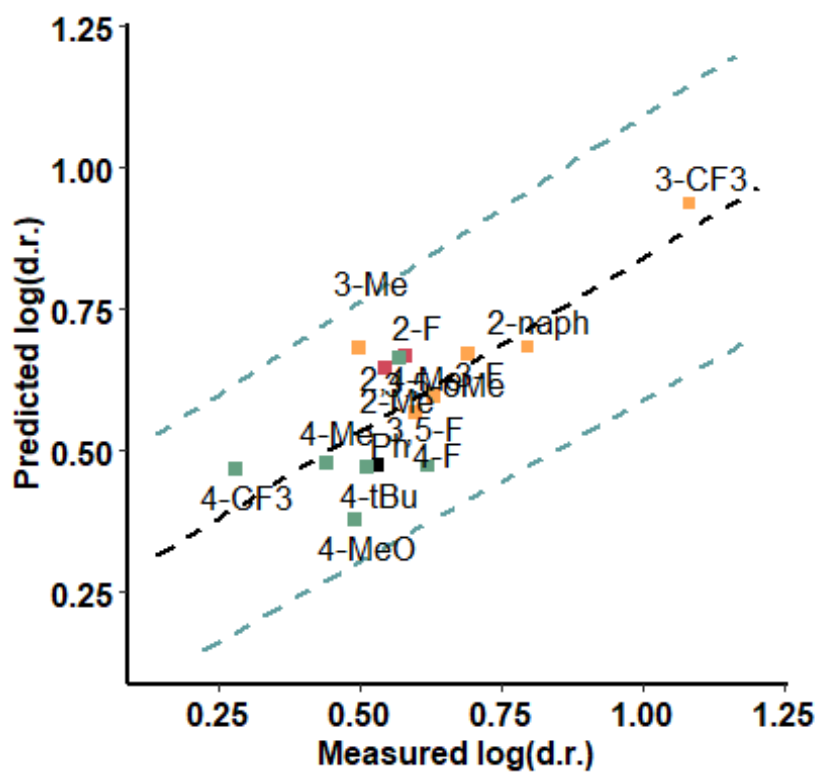
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.5902181	0.0309770	19.053423	0.0000000
dip_z	-0.0968785	0.0340775	-2.842888	0.0148171
B5	0.1385923	0.0340775	4.066974	0.0015621

3 & 5 fold CV

Q2	MAE
0.2832877	0.1351236

Q2	MAE
0.2966598	0.1266062

Top Ranked Full Model



Enamine - close to the active site

formula	R.sq	Q.sq	MAE
output ~ X.1.2. + B5	0.5322447	0.2874310	0.1168694
output ~ para + X.2.3.	0.4783236	0.2051382	0.1226364

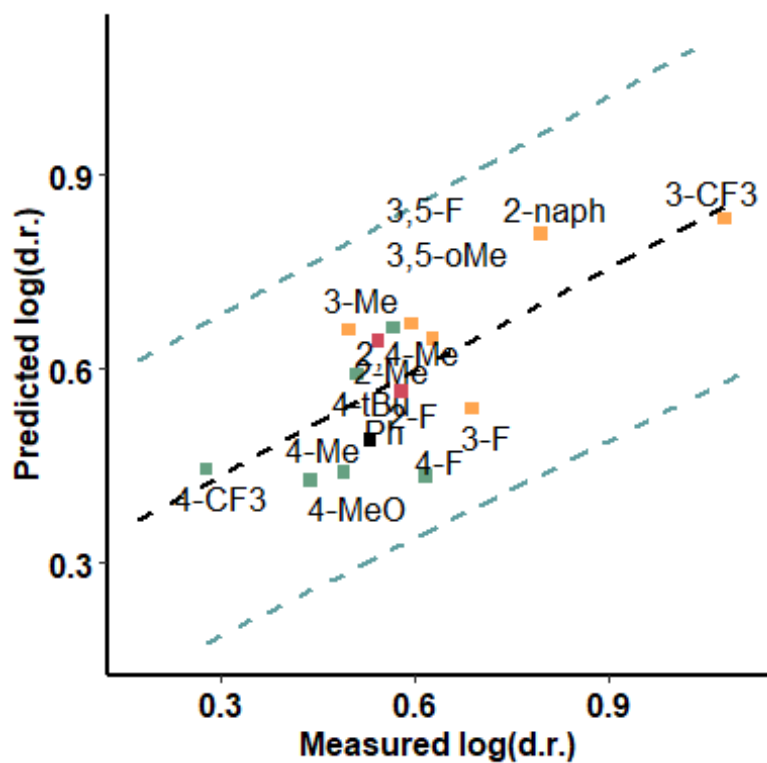
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.5902181	0.0340335	17.342271	0.0000000
X.1.2.	0.1041529	0.0453229	2.298020	0.0403419
B5	0.1674694	0.0453229	3.695031	0.0030635

3 & 5 fold CV

Q2	MAE
0.2306424	0.1382326

Q2	MAE
0.2471289	0.1261854

Top Ranked Full Model



Hexane - against ee

Only Boronic Acids

formula	R.sq	Q.sq	MAE
output ~ X.2.9. + B5	0.6619781	0.3685013	0.1744393

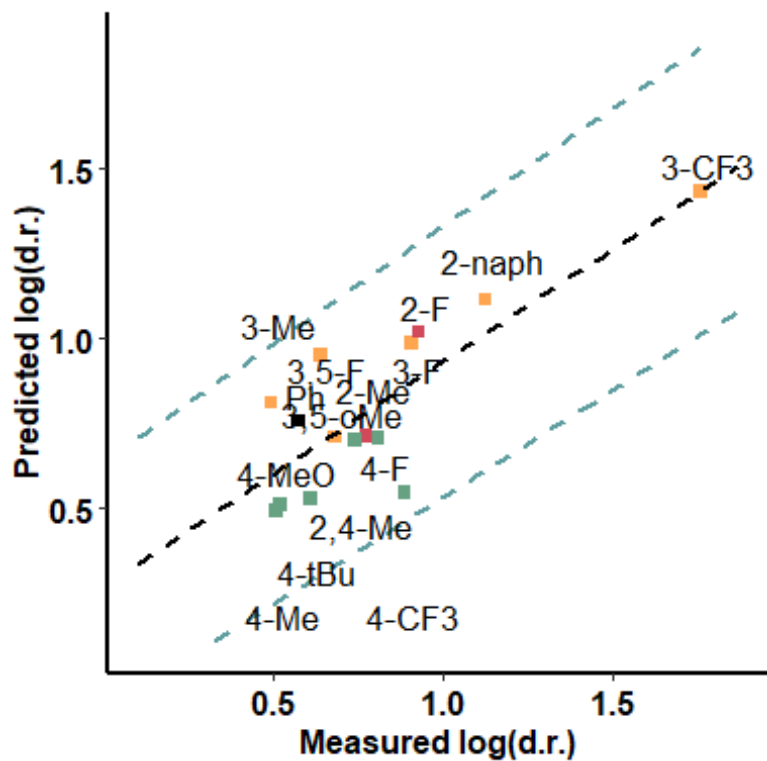
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.7999364	0.0520187	15.37785	0.0000000
X.2.9.	0.2338040	0.0562479	4.15667	0.0013307
B5	0.2019317	0.0562479	3.59003	0.0037132

3 & 5 fold CV

Q2	MAE
0.3230509	0.2046499

Q2	MAE
0.3365788	0.1887413

Top Ranked Full Model



With Catalyst - Close to the active site

formula	R.sq	Q.sq	MAE
output ~ Total + NBO.0.18	0.7249018	0.3737202	0.1771361
output ~ Total + diff.H14.018	0.6997620	0.3502341	0.1963199

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.7999364	0.0469279	17.046071	0.0000000
Total	-0.2096349	0.0504998	-4.151205	0.0013437
NBO.0.18	0.2415795	0.0504998	4.783773	0.0004457

3 & 5 fold CV

Q2	MAE
0.3665489	0.1908736

Q2	MAE
0.3675552	0.1859561

Top Ranked Full Model

With Catalyst - far

formula	R.sq	Q.sq	MAE
output ~ Total + diff.016.C17	0.7672782	0.3967453	0.1729457
output ~ Total + NB0.0.16	0.7653131	0.3063869	0.1942524

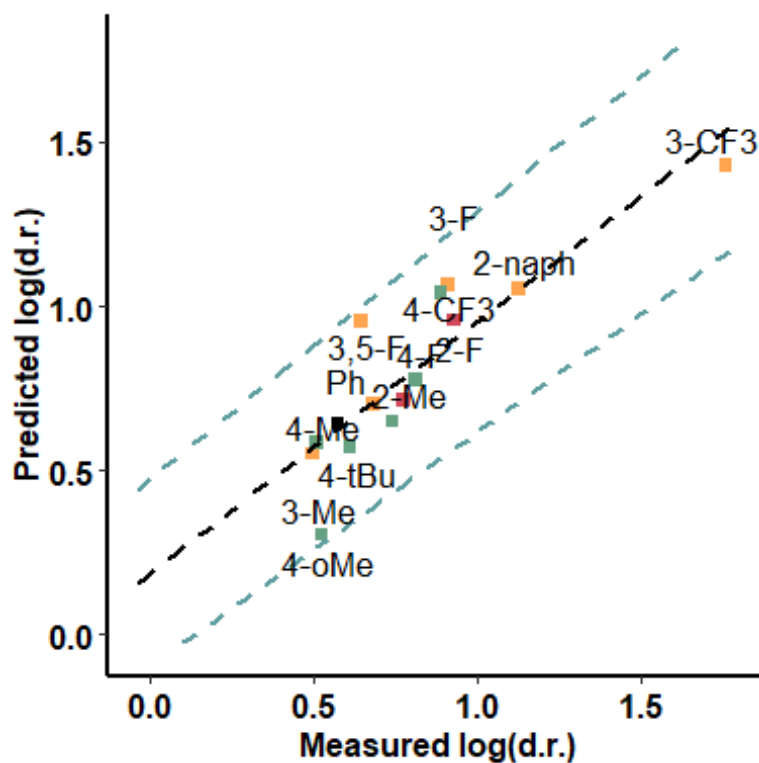
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.7999364	0.0431624	18.533167	0.0000000
Total	0.2203704	0.0463757	4.751856	0.0004706
diff.016.C17	0.1250300	0.0463757	2.696026	0.0194518

3 & 5 fold CV

Q2	MAE
0.3853301	0.181412

Q2	MAE
0.3900278	0.1766446

Top Ranked Full Model



BA + Aldehyde (pi interaction) - oxygen side

formula	R.sq	Q.sq	MAE
output ~ X.18.19. + diff.H10.017	0.8017001	0.6902510	1.671395
output ~ X.18.19. + NBO.H.19	0.7782123	0.6867141	2.019213

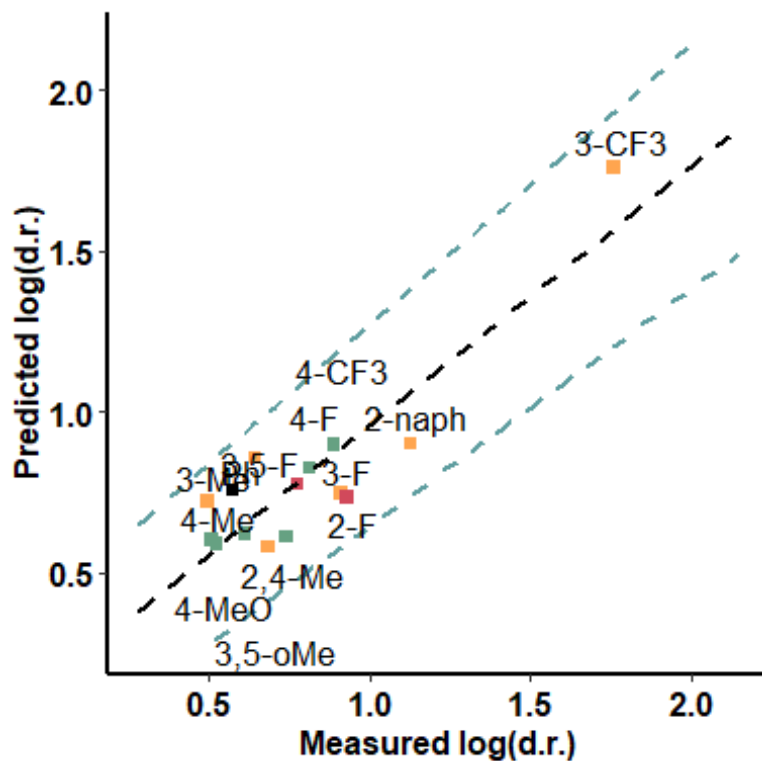
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.7999364	0.0398427	20.077373	0.0000000
X.18.19.	0.2606542	0.0412709	6.315686	0.0000386
diff.H10.017	0.1112211	0.0412709	2.694903	0.0194923

3 & 5 fold CV

Q2	MAE
0.6778579	5.92548

Q2	MAE
0.674292	4.498462

Top Ranked Full Model



BA + Aldehyde (pi interaction) - hydrogen side

formula	R.sq	Q.sq	MAE
output ~ Total + diff.H10.017	0.5156322	0.2522363	0.1940352
output ~ Dist.17..18. + B5	0.4771292	0.1989185	0.2259979

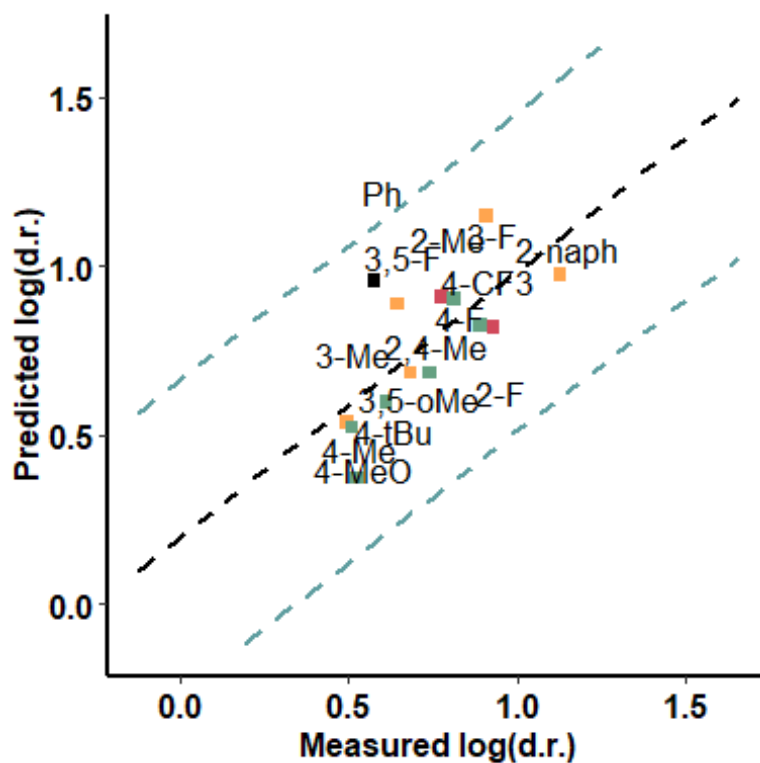
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.7999364	0.0622694	12.846372	0.0000000
Total	-0.2264213	0.1100461	-2.057513	0.0620429
diff.H10.017	0.3718911	0.1100461	3.379413	0.0054741

3 & 5 fold CV

Q2	MAE
0.2279574	0.2171824

Q2	MAE
0.2428908	0.2035005

Top Ranked Full Model



BA + Aldehyde - H bond - aldehyde side

formula	R.sq	Q.sq	MAE
output ~ Total + B5	0.6490579	0.3421465	0.1853301
output ~ Dist.1..10. + Dist.16..17.	0.6098284	0.2705932	0.1833607

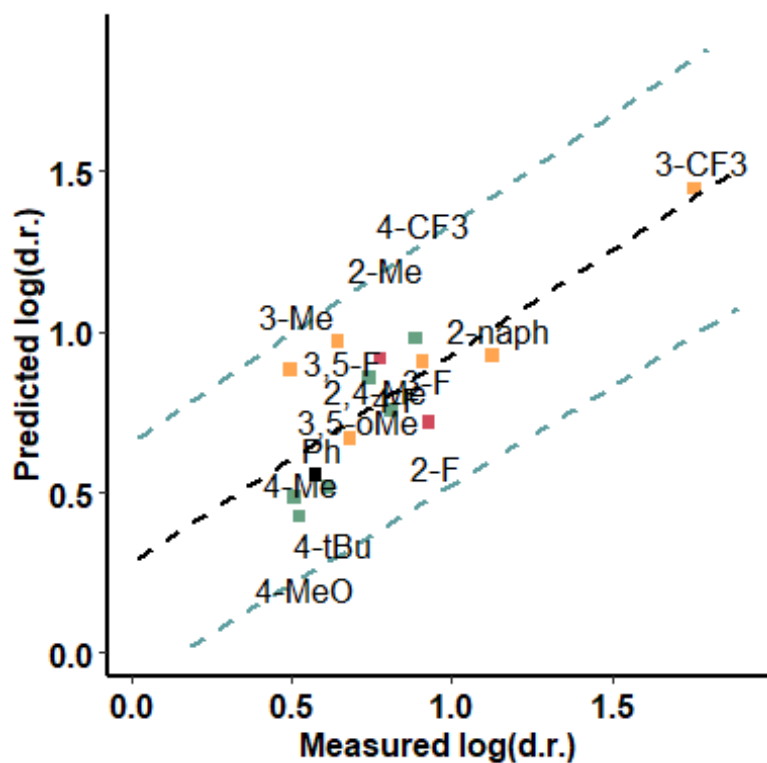
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.7999364	0.0530036	15.092126	0.0000000
Total	0.1951871	0.0550626	3.544821	0.0040349
B5	0.1868034	0.0550626	3.392564	0.0053426

3 & 5 fold CV

Q2	MAE
0.317911	0.2047416

Q2	MAE
0.3352989	0.1935397

Top Ranked Full Model



BA + Aldehyde - H bond - opposite to aldehyde

formula	R.sq	Q.sq	MAE
output ~ diff.C18.H19 + B5	0.6637662	0.3151564	0.1711994

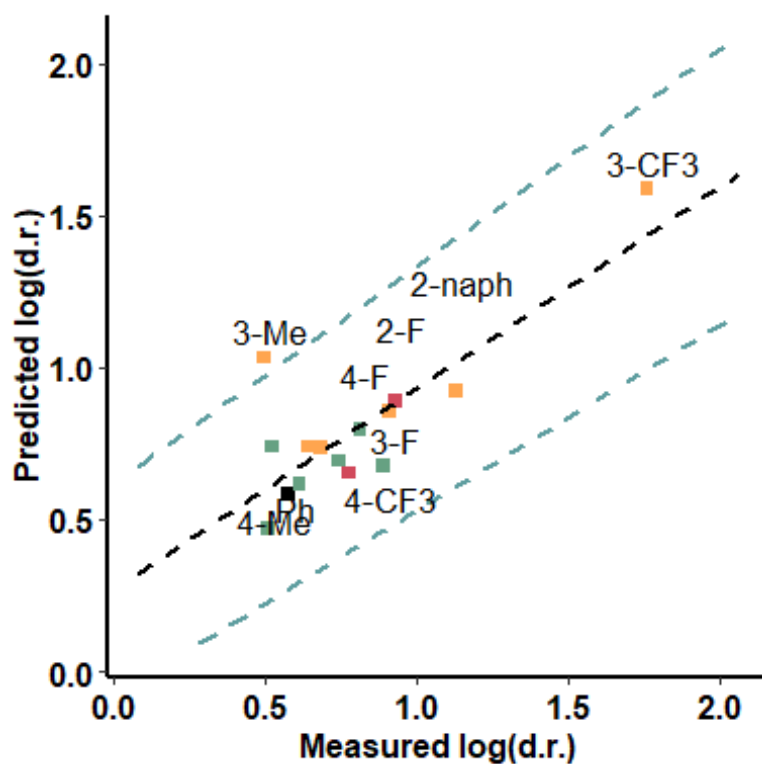
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.7999364	0.0518810	15.418689	0.0000000
diff.C18.H19	-0.2080839	0.0566735	-3.671628	0.0031974
B5	0.2380773	0.0566735	4.200859	0.0012300

3 & 5 fold CV

Q2	MAE
0.3125577	0.1907002

Q2	MAE
0.2890364	0.1823723

Top Ranked Full Model



Enamine - far from the active site

formula	R.sq	Q.sq	MAE
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output ~ Total + B5 0.7294911 0.4561942 0.1714146

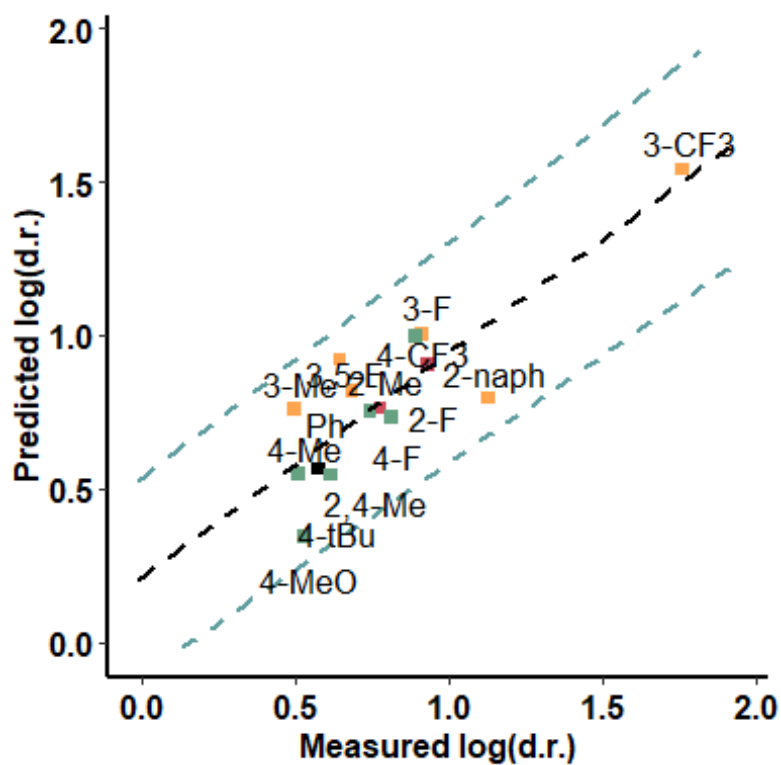
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.7999364	0.0465348	17.190058	0.0000000
Total	0.2356612	0.0482707	4.882076	0.0003772
B5	0.1560044	0.0482707	3.231865	0.0071944

3 & 5 fold CV

Q2	MAE
0.4344219	0.1819997

Q2	MAE
0.4488754	0.1761558

Top Ranked Full Model



Enamine - close to the active site

formula	R.sq	Q.sq	MAE
output ~ NB0.C.16 + diff.N24.C25	0.5837550	0.2885550	0.1949026
output ~ NB0.C.16 + NB0.C.25	0.5748357	0.1919583	0.2045477

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.7999364	0.0577247	13.857779	0.0000000
NBO.C.16	0.3436096	0.0889212	3.864204	0.0022514
diff.N24.C25	-0.3367733	0.0889212	-3.787325	0.0025888

3 & 5 fold CV

Q2	MAE
0.2489813	0.2307942

Q2	MAE
0.2694418	0.2065041

Top Ranked Full Model

