Evaluating the role of electron-correlation in the external prediction of the toxicity of Nitrobenzenes towards *Tetrahymena pyriformis*

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Supporting Information Tables S1-S7

List of Tables

Table S1	Computed values of quantum-chemical descriptors: Total energy (E), energies of HOMO and LUMO (E_{HOMO} and E_{LUMO}), dipole moment (d), absolute electronegativity (χ), chemical hardness (η), electrophilicity index (ω), and their correlation contribution (CORR), (all in a.u., 1a.u.=27.21165 eV, 627.50956 kcal/mol except dipole moment, which is in debye) calculated HF/6-311G (d,p), DFT/B3LYP/6-311G(d,p) and PM7 level of the theory for 43 alkyl- and halogen-substituted nitrobenzenes along with their inhibitory growth concentration as Log IGC_{50}^{-1}.
Table S2	Compounds in the training set (T), prediction set (P) and excluded set (E) in different types of splitting methods employed[a]. Excluded compounds are either response or structural outliers (determined from Williams plot).
Table S3	Value of internal and external validation parameters of two- and one-descriptor QSAR models, for inhibitory growth concentration (Log IGC_{50}^{-1}) of alkyl- and halogen-substituted nitrobenzenes, developed using PM7, HF, DFT and electron-correlation contribution (CORR) based descriptors through activity sampling (ordered response) splitting method.
Table S4	Value of internal and external validation parameters of two- and one-descriptor QSAR models, for inhibitory growth concentration (Log IGC_{50}^{-1}) of alkyl- and halogen-substituted nitrobenzenes, developed using PM7, HF, DFT and electron-correlation contribution (CORR) based descriptors through 30% ordered response splitting method.
Table S5	Value of internal and external validation parameters of two- and one-descriptor QSAR models, for inhibitory growth concentration (Log IGC_{50}^{-1}) of alkyl- and halogen-substituted nitrobenzenes, developed using PM7, HF, DFT and electron-correlation contribution (CORR) based descriptors through 45% ordered response splitting method.
Table S6	Value of internal validation parameters of two- and one-descriptor QSAR models, for inhibitory growth concentration (Log IGC_{50}^{-1}) of alkyl- and halogen-substituted nitrobenzenes, developed using PM7, HF, DFT and electron-correlation contribution (CORR) based descriptors, by employing complete data set comprising of 42 compounds in the training set, with no prediction set.
Table S7	Value of internal validation parameters of two- and one-descriptor QSAR models, for inhibitory growth concentration (Log IGC_{50}^{-1}) of alkyl- and halogen-substituted nitrobenzenes, developed using PM7, HF, DFT and electron-correlation contribution (CORR) based descriptors, by employing full data set comprising of 35 compounds in the training set excluding outliers as listed in Table S1, with no prediction set.

Table 1. Computed values of quantum-chemical descriptors: Total energy (E), energies of HOMO and LUMO (E_{HOMO} and E_{LUMO}), dipole moment (d), absolute electronegativity (χ), chemical hardness (η), electrophilicity index (ω), and their correlation contribution (CORR), (all in a.u., 1a.u.=27.21165 eV, 627.50956 kcal/mol except dipole moment, which is in debye) calculated HF/6-311G (d,p), DFT/B3LYP/6-311G(d,p) and PM7 level of the theory for 43 alkyl- and halogen-substituted nitrobenzenes along with their inhibitory growth concentration as Log IGC_{50}^{-1}.

Sr. No.	Name of Compounds	Log IGC_{50}^{-1}	$-E_{PM7}$	$-E_{HF}$	$-E_{DFT}$	$-E_{CORR}$	$-E_{PM7}^{HOMO}$	$-E_{HF}^{HOMO}$	$-E_{DFT}^{HOMO}$	E_{CORR}^{HOMO}	$-E_{PM7}^{LUMO}$	E_{HF}^{LUMO}	$-E_{DFT}^{LUMO}$	$-E_{CORR}^{LUMO}$	d_{PM7}	d_{HF}	d_{DFT}	$-d_{CORR}$
1	2-methylnitrobenzene	0.052	63.508	473.319	476.189	2.870	0.377	0.357	0.275	0.082	0.043	0.064	0.091	0.155	4.776	4.696	4.263	0.433
2	3methylnitrobenzene	0.054	63.509	473.323	476.193	2.870	0.378	0.356	0.274	0.082	0.045	0.057	0.093	0.150	5.505	5.311	4.866	0.445
3	nitrobenzene	0.140	57.991	434.277	436.865	2.588	0.394	0.369	0.287	0.082	0.048	0.055	0.096	0.151	5.059	5.017	4.541	0.476
4	4methylnitrobenzene	0.170	63.506	473.324	476.194	2.869	0.378	0.363	0.278	0.085	0.026	0.060	0.092	0.152	5.979	5.618	5.201	0.417
5	2,6dimethylnitrobenzene	0.300	69.024	512.362	515.514	3.152	0.367	0.347	0.265	0.082	0.034	0.082	0.084	0.166	4.106	4.134	3.650	0.484
6	4bromonitrobenzene	0.380	65.667	3006.058	3010.405	4.347	0.379	0.370	0.279	0.091	0.061	0.043	0.105	0.148	3.353	3.203	3.061	0.142
7	4chloronitrobenzene	0.430	67.307	893.197	896.485	3.288	0.390	0.376	0.285	0.091	0.061	0.044	0.105	0.149	3.146	3.082	2.863	0.219
8	3,5dinitrobenzyl alcohol	0.530	107.806	790.758	795.301	4.543	0.401	0.384	0.293	0.091	0.071	0.029	0.115	0.144	6.736	6.815	6.238	0.577
9	2,3dimethylnitrobenzene	0.560	69.024	512.361	515.514	3.153	0.367	0.347	0.265	0.082	0.039	0.072	0.086	0.158	5.208	4.938	4.541	0.397
10	2methyl3chloronitrobenzene	0.680	72.823	932.234	935.806	3.572	0.377	0.361	0.274	0.087	0.052	0.058	0.098	0.156	3.422	3.456	3.101	0.354
11	2chloronitrobenzene	0.680	67.303	893.182	896.472	3.290	0.383	0.367	0.279	0.088	0.052	0.059	0.097	0.156	5.466	5.552	4.952	0.600
12	3chloronitrobenzene	0.730	67.306	893.195	896.484	3.288	0.386	0.369	0.282	0.087	0.060	0.043	0.106	0.149	4.244	4.264	3.835	0.429
13	2bromonitrobenzene	0.750	65.662	3006.043	3010.393	4.350	0.371	0.362	0.273	0.089	0.052	0.059	0.096	0.155	5.362	5.394	4.774	0.620
14	2methyl5chloronitrobenzene	0.820	72.823	932.237	935.808	3.571	0.373	0.357	0.272	0.085	0.054	0.052	0.101	0.153	4.345	4.297	3.888	0.409
15	2,4,6trimethylnitrobenzene	0.860	74.544	551.409	554.842	3.433	0.365	0.345	0.260	0.085	0.030	0.084	0.081	0.165	5.016	4.677	4.262	0.415
16	6methyl1,3dinitrobenzene	0.870	91.449	676.837	680.741	3.904	0.407	0.393	0.304	0.089	0.071	0.031	0.115	0.146	5.490	5.385	4.854	0.531
17	1,3dinitrobenzene	0.890	85.922	637.793	641.415	3.622	0.418	0.404	0.316	0.088	0.062	0.023	0.121	0.144	4.590	4.742	4.211	0.531
18	2,4dichloronitrobenzene	0.990	76.618	1352.100	1356.091	3.991	0.390	0.378	0.286	0.092	0.065	0.047	0.105	0.152	3.642	3.679	3.315	0.363
19	3bromonitrobenzene	1.030	65.666	3006.057	3010.404	4.347	0.375	0.364	0.275	0.089	0.059	0.043	0.106	0.149	4.309	4.287	3.862	0.425
20	2,3dichloronitrobenzene	1.070	76.615	1352.094	1356.086	3.992	0.382	0.371	0.281	0.090	0.060	0.052	0.102	0.154	4.800	4.914	4.304	0.610
21	3,4dinitrobenzyl alcohol	1.090	107.795	790.739	795.285	4.546	0.398	0.385	0.286	0.099	0.066	0.040	0.109	0.149	9.500	9.542	8.684	0.858
22	2,5dichloronitrobenzene	1.130	76.617	1352.099	1356.090	3.991	0.380	0.367	0.278	0.089	0.064	0.047	0.106	0.153	4.317	4.420	3.915	0.505
23	3,5dichloronitrobenzene	1.130	76.619	1352.112	1356.101	3.989	0.390	0.375	0.287	0.088	0.071	0.032	0.115	0.147	3.022	2.951	2.643	0.309
24	3,4dichloronitrobenzene	1.160	76.618	1352.109	1356.099	3.990	0.387	0.377	0.286	0.091	0.070	0.034	0.112	0.146	2.849	2.833	2.645	0.188
25	3methyl4bromonitrobenzene	1.160	71.185	3045.104	3049.734	4.630	0.373	0.363	0.274	0.089	0.057	0.045	0.101	0.146	3.818	3.537	3.450	0.088
26	1,2dinitrobenzene	1.250	85.919	637.774	641.399	3.625	0.416	0.402	0.299	0.103	0.074	0.032	0.117	0.149	7.284	7.577	6.667	0.910
27	1,4dinitrobenzene	1.300	85.930	637.792	641.415	3.623	0.422	0.399	0.314	0.085	0.089	0.007	0.134	0.141	0.002	0.001	0.000	0.001
28	2,5dibromonitrobenzene	1.370	73.337	5577.822	5583.932	6.109	0.368	0.359	0.270	0.089	0.062	0.048	0.105	0.153	4.387	4.370	3.873	0.497
29	2,4,6trichloronitrobenzene	1.430	85.929	1811.009	1815.701	4.692	0.395	0.384	0.286	0.098	0.064	0.066	0.096	0.162	3.788	4.039	3.334	0.705
30	2,3,4trichloronitrobenzene	1.510	85.926	1811.006	1815.700	4.694	0.388	0.380	0.287	0.093	0.063	0.043	0.108	0.151	3.406	3.466	3.075	0.391
31	5methyl1,2dinitrobenzene	1.520	91.438	676.822	680.728	3.906	0.402	0.389	0.291	0.098	0.069	0.038	0.112	0.150	8.129	8.177	7.323	0.855
32	2,4,5trichloronitrobenzene	1.530	85.928	1811.012	1815.704	4.692	0.384	0.375	0.283	0.092	0.073	0.038	0.112	0.150	2.974	2.968	2.730	0.238
33	2,3,4,5tetrachloronitrobenzene	1.780	95.237	2269.916	2275.312	5.396	0.385	0.379	0.286	0.093	0.078	0.035	0.115	0.150	2.412	2.417	2.230	0.187
34	2,3,5,6tetrachloronitrobenzene	1.820	95.238	2269.915	2275.310	5.395	0.380	0.375	0.282	0.093	0.070	0.058	0.100	0.158	3.662	3.968	3.253	0.715
35	6chloro1,3dinitrobenzene	1.980	95.240	1096.697	1101.022	4.325	0.408	0.401	0.306	0.095	0.085	0.017	0.125	0.142	4.066	4.249	3.763	0.485
36	6iodo1,3dinitrobenzene	2.120	93.632	648.339	652.175	3.835	0.356	0.375	0.283	0.092	0.080	0.018	0.123	0.141	4.108	4.620	4.191	0.429
37	2,4,6trichloro1,3dinitrobenzene	2.190	113.861	2014.498	2020.230	5.732	0.410	0.406	0.299	0.107	0.085	0.043	0.111	0.154	3.609	3.920	3.207	0.714
38	1,2dichloro4,5dinitrobenzene	2.210	104.542	1555.602	1560.630	5.028	0.404	0.400	0.300	0.100	0.092	0.014	0.130	0.144	4.688	4.896	4.395	0.501
39	6bromo1,3dinitrobenzene	2.310	93.600	3209.558	3214.942	5.385	0.393	0.393	0.298	0.095	0.084	0.017	0.124	0.141	4.199	4.323	3.876	0.447
40	4,6dichloro1,2dinitrobenzene	2.420	104.543	1555.597	1560.626	5.029	0.406	0.400	0.297	0.103	0.090	0.015	0.130	0.145	5.500	5.869	4.963	0.906
41	2,4,5trichloro1,3dinitrobenzene	2.590	113.859	2014.501	2020.233	5.732	0.397	0.395	0.298	0.097	0.092	0.018	0.126	0.144	2.893	3.098	2.606	0.492
42	2,3,5,6tetrachloro1,4dinitrobenzene	2.740	123.168	2473.403	2479.838	6.435	0.393	0.394	0.297	0.097	0.093	0.036	0.112	0.148	0.004	0.001	0.001	0.001
43	pentachloronitrobenzene	NTAS*	104.547	2728.819	2734.918	6.099	0.384	0.380	0.287	0.093	0.077	0.051	0.103	0.154	2.642	2.911	2.414	0.497

***Not toxic at saturation [Ref. 17]**

Table 1 continued….

Sr. No.	Name of Compounds	Log IGC_{50}^{-1}	χ_{PM7}	χ_{HF}	χ_{DFT}	χ_{CORR}	η_{PM7}	η_{HF}	η_{DFT}	$-\eta_{CORR}$	ω_{M7}	ω_{HF}	ω_{DFT}	$-\omega_{CORR}$
1	2-methylnitrobenzene	0.052	0.210	0.147	0.183	0.037	0.334	0.421	0.184	0.237	0.066	0.025	0.091	0.003
2	3methylnitrobenzene	0.054	0.212	0.150	0.184	0.034	0.333	0.413	0.181	0.232	0.067	0.027	0.093	0.002
3	nitrobenzene	0.140	0.221	0.157	0.192	0.035	0.346	0.424	0.191	0.233	0.071	0.029	0.096	0.003
4	4methylnitrobenzene	0.170	0.202	0.152	0.185	0.034	0.351	0.423	0.186	0.237	0.058	0.027	0.092	0.002
5	2,6dimethylnitrobenzene	0.300	0.201	0.133	0.175	0.042	0.333	0.429	0.181	0.248	0.060	0.020	0.084	0.004
6	4bromonitrobenzene	0.380	0.220	0.164	0.192	0.029	0.318	0.413	0.174	0.239	0.076	0.032	0.106	0.002
7	4chloronitrobenzene	0.430	0.225	0.166	0.195	0.029	0.329	0.420	0.180	0.240	0.077	0.033	0.106	0.002
8	3,5dinitrobenzyl alcohol	0.530	0.236	0.178	0.204	0.027	0.330	0.413	0.178	0.235	0.084	0.038	0.117	0.001
9	2,3dimethylnitrobenzene	0.560	0.203	0.138	0.176	0.038	0.327	0.419	0.179	0.240	0.063	0.023	0.086	0.003
10	2methyl3chloronitrobenzene	0.680	0.215	0.152	0.186	0.035	0.325	0.419	0.176	0.243	0.071	0.027	0.098	0.002
11	2chloronitrobenzene	0.680	0.218	0.154	0.188	0.034	0.331	0.426	0.182	0.244	0.072	0.028	0.097	0.002
12	3chloronitrobenzene	0.730	0.223	0.163	0.194	0.031	0.326	0.412	0.176	0.236	0.076	0.032	0.107	0.002
13	2bromonitrobenzene	0.750	0.212	0.152	0.185	0.033	0.319	0.421	0.177	0.244	0.070	0.027	0.096	0.002
14	2methyl5chloronitrobenzene	0.820	0.214	0.153	0.187	0.034	0.320	0.409	0.171	0.238	0.071	0.028	0.102	0.002
15	2,4,6trimethylnitrobenzene	0.860	0.198	0.131	0.171	0.040	0.335	0.429	0.179	0.250	0.058	0.020	0.081	0.003
16	6methyl1,3dinitrobenzene	0.870	0.239	0.181	0.210	0.029	0.335	0.424	0.189	0.235	0.085	0.039	0.116	0.002
17	1,3dinitrobenzene	0.890	0.240	0.191	0.219	0.028	0.356	0.427	0.195	0.232	0.081	0.042	0.122	0.002
18	2,4dichloronitrobenzene	0.990	0.227	0.166	0.196	0.030	0.325	0.425	0.181	0.244	0.079	0.032	0.106	0.002
19	3bromonitrobenzene	1.030	0.217	0.161	0.191	0.030	0.316	0.407	0.169	0.238	0.075	0.032	0.107	0.002
20	2,3dichloronitrobenzene	1.070	0.221	0.160	0.192	0.032	0.321	0.423	0.179	0.244	0.076	0.030	0.102	0.002
21	3,4dinitrobenzyl alcohol	1.090	0.232	0.173	0.198	0.025	0.332	0.425	0.177	0.248	0.081	0.035	0.110	0.001
22	2,5dichloronitrobenzene	1.130	0.222	0.160	0.192	0.032	0.317	0.414	0.172	0.242	0.078	0.031	0.107	0.002
23	3,5dichloronitrobenzene	1.130	0.230	0.172	0.201	0.030	0.319	0.407	0.172	0.235	0.083	0.036	0.117	0.002
24	3,4dichloronitrobenzene	1.160	0.228	0.172	0.199	0.028	0.317	0.411	0.174	0.237	0.082	0.036	0.114	0.002
25	3methyl4bromonitrobenzene	1.160	0.215	0.159	0.188	0.029	0.316	0.408	0.173	0.235	0.073	0.031	0.102	0.002
26	1,2dinitrobenzene	1.250	0.245	0.185	0.208	0.023	0.343	0.434	0.182	0.252	0.087	0.039	0.119	0.001
27	1,4dinitrobenzene	1.300	0.256	0.196	0.224	0.028	0.333	0.406	0.180	0.226	0.098	0.047	0.139	0.002
28	2,5dibromonitrobenzene	1.370	0.215	0.156	0.188	0.032	0.306	0.407	0.165	0.242	0.075	0.030	0.107	0.002
29	2,4,6trichloronitrobenzene	1.430	0.230	0.159	0.191	0.032	0.330	0.450	0.190	0.260	0.080	0.028	0.096	0.002
30	2,3,4trichloronitrobenzene	1.510	0.226	0.169	0.198	0.029	0.325	0.423	0.179	0.244	0.078	0.034	0.109	0.002
31	5methyl1,2dinitrobenzene	1.520	0.235	0.176	0.202	0.026	0.333	0.427	0.179	0.248	0.083	0.036	0.113	0.001
32	2,4,5trichloronitrobenzene	1.530	0.228	0.169	0.198	0.029	0.310	0.413	0.171	0.242	0.084	0.034	0.114	0.002
33	2,3,4,5tetrachloronitrobenzene	1.780	0.232	0.172	0.201	0.029	0.307	0.414	0.171	0.243	0.088	0.036	0.118	0.002
34	2,3,5,6tetrachloronitrobenzene	1.820	0.225	0.159	0.191	0.033	0.310	0.433	0.182	0.251	0.082	0.029	0.100	0.002
35	6chloro1,3dinitrobenzene	1.980	0.247	0.192	0.216	0.024	0.323	0.418	0.181	0.237	0.094	0.044	0.128	0.001
36	6iodo1,3dinitrobenzene	2.120	0.218	0.179	0.203	0.025	0.276	0.393	0.160	0.233	0.086	0.041	0.129	0.001
37	2,4,6trichloro1,3dinitrobenzene	2.190	0.248	0.182	0.205	0.024	0.325	0.449	0.188	0.261	0.094	0.037	0.112	0.001
38	1,2dichloro4,5dinitrobenzene	2.210	0.248	0.193	0.215	0.022	0.312	0.414	0.170	0.244	0.098	0.045	0.136	0.001
39	6bromo1,3dinitrobenzene	2.310	0.239	0.188	0.211	0.023	0.309	0.410	0.174	0.236	0.092	0.043	0.128	0.001
40	4,6dichloro1,2dinitrobenzene	2.420	0.248	0.193	0.214	0.021	0.316	0.415	0.167	0.248	0.097	0.045	0.136	0.001
41	2,4,5trichloro1,3dinitrobenzene	2.590	0.244	0.189	0.212	0.024	0.306	0.413	0.172	0.241	0.098	0.043	0.131	0.001
42	2,3,5,6tetrachloro1,4dinitrobenzene	2.740	0.243	0.179	0.205	0.026	0.300	0.430	0.185	0.245	0.099	0.037	0.113	0.001
43	pentachloronitrobenzene	NTAS*	0.231	0.165	0.195	0.031	0.307	0.431	0.184	0.247	0.087	0.031	0.103	0.002

***Not toxic at saturation [Ref. 17]**

Table S2. Compounds in the training set (T), prediction set (P) and excluded set (E) in different types of splitting methods employed[a]. Excluded compounds are either response or structural outliers (determined from Williams plot).

ID Number of Chemicals	*Name of the Chemicals*	Log IGC_{50}^{-1}	*Complete Set*	*Full Set (excluding outliers)*	*Activity Sampling (ordered response splitting)*	*30% ordered response splitting*	*45% ordered response splitting*
1	2-methylnitrobenzene	0.052	T	T	T	T	T
2	3-methylnitrobenzene	0.054	T	T	P	P	P
3	nitrobenzene	0.140	T	T	T	P	P
4	4-methylnitrobenzene	0.170	T	T	P	T	T
5	2,6-dimethylnitrobenzene	0.300	T	E	E	E	E
6	4-bromonitrobenzene	0.380	T	T	T	T	T
7	4-chloronitrobenzene	0.430	T	T	P	T	P
8	3,5-dinitrobenzyl alcohol	0.530	T	E	E	E	E
9	2,3-dimethylnitrobenzene	0.560	T	T	T	P	T
10	2-methyl-3-chloronitrobenzene	0.680	T	T	P	P	T
11	2-chloronitrobenzene	0.680	T	T	T	T	P
12	3-chloronitrobenzene	0.730	T	T	P	T	T
13	2-bromonitrobenzene	0.750	T	T	T	T	T
14	2-methyl-5-chloronitrobenzene	0.820	T	T	P	P	P
15	2,4,6-trimethylnitrobenzene	0.860	T	T	T	T	T
16	6-methyl-1,3-dinitrobenzene	0.870	T	T	P	T	T
17	1,3-dinitrobenzene	0.890	T	T	T	T	P
18	2,4-dichloronitrobenzene	0.990	T	T	P	T	P
19	3-bromonitrobenzene	1.030	T	T	T	P	T
20	2,3-dichloronitrobenzene	1.070	T	T	P	T	T
21	3,4-dinitrobenzyl alcohol	1.090	T	T	T	T	T
22	2,5-dichloronitrobenzene	1.130	T	T	P	T	P
23	3,5-dichloronitrobenzene	1.130	T	T	T	P	T
24	3,4-dichloronitrobenzene	1.160	T	T	P	T	P
25	3-methyl-4-bromonitrobenzene	1.160	T	T	T	P	P
26	1,2-dinitrobenzene	1.250	T	E	E	E	E
27	1,4-dinitrobenzene	1.300	T	T	P	T	T
28	2,5-dibromonitrobenzene	1.370	T	E	E	E	E
29	2,4,6-trichloronitrobenzene	1.430	T	T	T	T	T
30	2,3,4-trichloronitrobenzene	1.510	T	T	P	T	P
31	5-methyl-1,2-dinitrobenzene	1.520	T	T	T	T	T
32	2,4,5-trichloronitrobenzene	1.530	T	T	P	T	T
33	2,3,4,5-tetrachloronitrobenzene	1.780	T	T	T	P	P
34	2,3,5,6-tetrachloronitrobenzene	1.820	T	T	P	P	P
35	6-chloro-1,3-dinitrobenzene	1.980	T	T	T	T	T
36	6-iodo-1,3-dinitrobenzene	2.120	T	E	E	E	E
37	2,4,6-trichloro-1,3-dinitrobenzene	2.190	T	E	E	E	E
38	1,2-dichloro-4,5-dinitrobenzene	2.210	T	T	P	T	P
39	6-bromo-1,3-dinitrobenzene	2.310	T	T	T	T	T
40	4,6-dichloro-1,2-dinitrobenzene	2.420	T	T	P	P	T
41	2,4,5-trichloro-1,3-dinitrobenzene	2.590	T	T	T	T	T
42	2,3,5,6-tetrachloro-1,4-dinitrobenzene	2.740	T	E	E	E	E
Number of compounds in Training Set			42	35	18	24	21
Number of compounds in Prediction Set			0	0	17	11	14
Number of compounds in Excluded Set			0	7	7	7	7

[a] Splitting is performed through QSARINS software. Ref. [43] Chirico, N.; Papa, E.; Kovarich, S.; Cassani, S.; Gramatica, P. QSARINS, Software for QSAR MLR model development and validation. 2012. QSAR Res. Unit in Environ Chem and Ecotox University of Insubria, Varese, Italy, (http://www.qsar.it).

Table S3. Value of internal and external validation parameters of two- and one-descriptor QSAR models, for inhibitory growth concentration (Log IGC_{50}^{-1}) of alkyl- and halogen-substituted nitrobenzenes, developed using PM7, HF, DFT and electron-correlation contribution (CORR) based descriptors through activity sampling (ordered response) splitting method.

Model	Variables	Q^2_{LOO}	R^2-Q^2_{LOO}	R^2_{adj}	R^2-R^2_{adj}	R^2	ΔK	$RMSE_{TR}$	$RMSE_{CV}$	$RMSE_{EXT}$	F	N. ExtOK	Q^2_{F1}	Q^2_{F2}	Q^2_{F3}	CCC_{TR}	CCC_{CV}	CCC_{EXT}	$\overline{r}^2_m$	Δr^2_m	MAE_{TR}	MAE_{CV}	MAE_{EXT}	RSS_{TR}	$PRESS_{CV}$	$PRESS_{EXT}$	R^2_{LMO}	Q^2_{LMO}	R^2_{Yscr}	Q^2_{Yscr}	R^2_{Xrand}	Q^2_{Xrand}	R^2_{Yrand}	Q^2_{Yrand}
1	E_{CORR}, E_{HF}	0.7138	0.0946	0.7828	0.0256	0.8084	-0.0657	0.2996	0.3661	0.2061	31.6376	5	0.8932	0.8931	0.9093	0.894	0.8421	0.939	0.7888	0.094	0.2271	0.2762	0.1642	1.6156	2.4127	0.7221	81.2052	59.8714	11.4945	-28.2559	12.1912	-27.6783	12.1708	-27.1183
2	E_{PM7}, η_{PM7}	0.7118	0.1103	0.7984	0.0237	0.8221	0.3008	0.2886	0.3674	0.1983	34.6675	5	0.9011	0.901	0.916	0.9024	0.8473	0.9427	0.748	0.0954	0.2236	0.2757	0.1523	1.4995	2.4295	0.6685	82.4457	59.5313	11.6118	-29.3432	11.7442	-28.2962	12.1306	-28.678
3	E_{CORR}, E_{PM7}	0.7011	0.1147	0.7912	0.0246	0.8158	0.092	0.2937	0.3742	0.1965	33.216	5	0.9029	0.9028	0.9175	0.8986	0.838	0.9439	0.8216	0.0766	0.2234	0.2756	0.1581	1.5529	2.5199	0.6566	82.1415	58.7959	11.534	-28.303	12.1042	-27.4905	11.6509	-27.6911
4	E_{CORR}, ω_{PM7}	0.7073	0.1	0.7816	0.0257	0.8073	0.0675	0.3005	0.3703	0.1961	31.411	5	0.9033	0.9032	0.9179	0.8933	0.8393	0.9458	0.7981	0.087	0.2335	0.2865	0.152	1.625	2.4678	0.6538	81.0642	56.353	11.7766	-28.5218	11.7746	-27.6394	11.9406	-27.8469
5	E_{CORR}, χ_{PM7}	0.6885	0.0998	0.7601	0.0282	0.7883	0.1493	0.3149	0.382	0.1894	27.9256	5	0.9098	0.9097	0.9234	0.8816	0.8264	0.9483	0.8119	0.0778	0.2521	0.3078	0.1506	1.7849	2.6262	0.6095	78.6776	55.9878	12.1393	-27.3425	12.0868	-27.9827	11.9466	-27.9717
6	E_{CORR}, ω_{HF}	0.6815	0.0944	0.7461	0.0299	0.776	0.126	0.3239	0.3862	0.1903	25.9765	5	0.9089	0.9088	0.9227	0.8738	0.8202	0.9443	0.7654	0.0798	0.2686	0.3244	0.1518	1.8888	2.6849	0.6156	77.4098	50.5623	12.4681	-27.2254	11.7398	-28.048	11.6769	-28.1056
7	E_{CORR}, ω_{CORR}	0.6721	0.0902	0.7305	0.0317	0.7622	0.0625	0.3337	0.3919	0.2634	24.0428	4	0.8256	0.8254	0.8519	0.8651	0.8127	0.8768	0.5782	0.1779	0.2596	0.3109	0.2076	2.0046	2.7647	1.1791	76.5568	49.955	11.8772	-27.6576	10.8023	-29.292	11.4777	-28.5731
8	E_{CORR}, E^{LUMO}_{PM7}	0.6716	0.1211	0.7651	0.0276	0.7927	0.0383	0.3116	0.3922	0.2043	28.6838	5	0.895	0.8949	0.9108	0.8844	0.8204	0.9408	0.7772	0.0954	0.2422	0.3001	0.1605	1.7474	2.7686	0.7099	79.341	54.0738	11.7515	-28.5538	11.3464	-28.9361	11.9632	-28.2651
9	E_{CORR}, E^{HOMO}_{PM7}	0.6687	0.1012	0.7392	0.0307	0.7699	0.3263	0.3283	0.3939	0.2025	25.0979	5	0.8969	0.8968	0.9125	0.87	0.8128	0.9399	0.8217	0.0763	0.2734	0.3316	0.1564	1.9397	2.7929	0.6969	77.5112	51.3542	11.5813	-28.3174	11.9834	-27.6685	12.1326	-27.7257
10	E_{CORR}, E^{HOMO}_{HF}	0.6686	0.104	0.7423	0.0303	0.7726	0.1686	0.3263	0.394	0.2044	25.4879	5	0.8949	0.8949	0.9108	0.8717	0.8135	0.9374	0.7963	0.0814	0.2667	0.3249	0.1636	1.9167	2.7939	0.7101	77.3354	53.2595	11.6332	-28.5408	11.3184	-28.8288	11.4892	-28.6536
11	E_{CORR}, χ_{HF}	0.658	0.1059	0.7324	0.0315	0.7639	0.1316	0.3325	0.4002	0.1925	24.2665	5	0.9068	0.9067	0.9209	0.8662	0.807	0.9424	0.7636	0.0785	0.2708	0.3294	0.1494	1.9904	2.8834	0.6301	76.5402	47.9975	10.5828	-29.9195	12.0449	-27.7737	11.9528	-28.0806
12	E_{CORR}, E^{LUMO}_{HF}	0.6438	0.1006	0.7102	0.0341	0.7443	0.1109	0.3461	0.4085	0.1949	21.8337	5	0.9045	0.9044	0.9189	0.8534	0.7957	0.9389	0.7335	0.0829	0.2885	0.3453	0.1424	2.1555	3.0032	0.6457	74.6332	44.392	11.5082	-28.7427	11.8024	-28.3623	11.8085	-28.1559
13	E_{CORR}	0.6315	0.0618	0.6741	0.0192	0.6933	0.8326	0.379	0.4155	0.2635	36.165	5	0.8253	0.8252	0.8517	0.8189	0.7788	0.8921	0.7361	0.1228	0.3017	0.3355	0.1817	2.5858	3.1071	1.1806	68.9468	39.4356	6.0239	-19.5987	5.8952	-19.3182	5.7429	-20.1775
14	E_{CORR}, χ_{CORR}	0.6245	0.1103	0.6995	0.0354	0.7348	0.0425	0.3524	0.4194	0.2137	20.7844	5	0.8852	0.8851	0.9025	0.8472	0.7843	0.9264	0.7288	0.0931	0.2791	0.3354	0.172	2.2355	3.1654	0.7761	73.4488	43.6869	11.6808	-28.0063	11.6704	-28.4265	12.3988	-26.7524
15	E_{CORR}, η_{PM7}	0.6216	0.0802	0.662	0.0398	0.7018	-0.0382	0.3737	0.421	0.2764	17.6481	5	0.8078	0.8076	0.8368	0.8248	0.7753	0.8835	0.7591	0.1213	0.3038	0.3525	0.206	2.5143	3.1903	1.2992	69.8721	40.9105	11.3215	-31.4583	11.8426	-28.2286	11.8299	-31.7658
16	$E_{CORR}, E^{HOMO}_{CORR}$	0.6156	0.11	0.689	0.0366	0.7256	0.0196	0.3585	0.4243	0.2277	19.8344	5	0.8696	0.8695	0.8893	0.841	0.777	0.923	0.7946	0.0952	0.2881	0.3465	0.1674	2.3132	3.2409	0.8815	72.3623	48.2445	11.6208	-28.7121	12.0129	-27.6709	11.7733	-28.5204
17	$E_{CORR}, E^{LUMO}_{CORR}$	0.6101	0.0984	0.6696	0.0389	0.7085	0.1457	0.3695	0.4273	0.2409	18.2275	5	0.8541	0.8539	0.8761	0.8294	0.7705	0.905	0.7072	0.1107	0.2947	0.3478	0.1705	2.4577	3.287	0.9865	71.0585	42.5941	11.3232	-29.889	12.2156	-27.4509	11.5001	-29.435
18	E_{PM7}, d_{PM7}	0.6099	0.1855	0.7681	0.0273	0.7954	0.3315	0.3096	0.4274	0.2991	29.1537	4	0.775	0.7748	0.809	0.886	0.7971	0.8672	0.5921	0.1966	0.2543	0.329	0.2182	1.725	3.2886	1.521	80.617	46.9042	11.428	-34.0182	11.726	-28.2647	12.0493	-31.5865
19	E_{CORR}, d_{CORR}	0.6093	0.1189	0.6919	0.0362	0.7282	0.3179	0.3568	0.4278	0.2878	20.0899	5	0.7916	0.7915	0.8231	0.8427	0.7748	0.8873	0.761	0.0146	0.2844	0.3414	0.2039	2.2918	3.2938	1.4083	73.133	42.5676	12.4508	-26.677	12.198	-27.6389	11.9284	-28.1375
20	E_{CORR}, η_{CORR}	0.6091	0.0843	0.6525	0.0409	0.6934	0.2648	0.3789	0.4279	0.2629	16.9615	5	0.8262	0.826	0.8524	0.8189	0.7666	0.8921	0.7323	0.1228	0.3002	0.3478	0.1811	2.5848	3.2958	1.1749	69.3829	37.4548	12.0843	-28.94	11.866	-28.0292	11.8689	-29.4584
21	E_{PM7}, E^{LUMO}_{PM7}	0.6067	0.1936	0.7736	0.0266	0.8003	0.0521	0.3059	0.4292	0.2775	30.0513	5	0.8063	0.8061	0.8356	0.8891	0.7957	0.8936	0.6889	0.1539	0.2446	0.3196	0.203	1.6838	3.3161	1.3093	81.5259	46.6206	12.0948	-29.4395	12.4124	-27.5345	11.9746	-28.8426
22	E_{PM7}, ω_{PM7}	0.5904	0.1935	0.755	0.0288	0.7838	0.035	0.3182	0.438	0.2879	27.1914	5	0.7916	0.7914	0.8231	0.8788	0.7844	0.8834	0.6668	0.1676	0.2568	0.3327	0.206	1.8226	3.4535	1.4087	79.8249	45.7273	11.7134	-29.8121	11.4157	-28.5187	11.6219	-30.5169
23	E^{LUMO}_{PM7}	0.5895	0.1299	0.7019	0.0175	0.7194	0.8482	0.3625	0.4385	0.3756	41.0188	0	0.6451	0.6448	0.6988	0.8368	0.7684	0.8116	0.5739	0.2245	0.2789	0.3256	0.2918	2.3657	3.4609	2.3986	72.3821	40.5206	6.0517	-19.595	5.4627	-20.2387	6.2545	-19.3601
24	ω_{PM7}	0.5894	0.1189	0.6901	0.0182	0.7083	0.8416	0.3696	0.4385	0.3862	38.853	0	0.6249	0.6246	0.6816	0.8293	0.7652	0.7983	0.5508	0.2298	0.2994	0.3457	0.2869	2.4591	3.4612	2.5355	71.2179	39.3552	6.3732	-19.2906	5.9687	-19.3021	5.9891	-19.574
25	E_{CORR}, η_{HF}	0.582	0.1154	0.6571	0.0403	0.6975	0.1904	0.3764	0.4424	0.2813	17.2903	5	0.801	0.8008	0.8311	0.8218	0.7602	0.8814	0.751	0.1333	0.3048	0.3687	0.1999	2.5506	3.5236	1.3451	70.263	40.1699	11.6668	-33.9668	11.9217	-28.0715	11.8199	-34.8221
26	E_{PM7}	0.5602	0.129	0.6698	0.0194	0.6892	0.8302	0.3815	0.4538	0.2713	35.4763	4	0.8148	0.8147	0.8428	0.816	0.7435	0.8773	0.583	0.192	0.2871	0.3324	0.2114	2.6204	3.7076	1.2517	69.9443	32.05	5.9702	-19.3238	6.1685	-19.1587	5.6378	-19.9816
27	E_{PM7}, E^{HOMO}_{PM7}	0.5407	0.1571	0.6575	0.0403	0.6978	0.0259	0.3762	0.4638	0.2633	17.32	4	0.8256	0.8255	0.852	0.822	0.7341	0.884	0.5962	0.1807	0.2815	0.3439	0.212	2.5475	3.8718	1.1786	70.7192	34.8851	11.6971	-28.5536	11.8368	-28.0685	12.2308	-27.8287
28	E_{PM7}, χ_{PM7}	0.5283	0.1804	0.6698	0.0389	0.7086	0.0123	0.3694	0.4701	0.2824	18.2382	4	0.7994	0.7993	0.8297	0.8295	0.7323	0.874	0.5979	0.1921	0.2835	0.3521	0.221	2.4566	3.9771	1.3556	71.6492	26.7359	11.7992	-29.4579	11.4703	-29.2113	11.558	-29.3421
29	E_{CORR}, d_{PM7}	0.4987	0.196	0.654	0.0407	0.6947	0.1758	0.3781	0.4846	0.2707	17.0666	5	0.8157	0.8155	0.8435	0.8199	0.7168	0.8876	0.7494	0.1228	0.3031	0.3837	0.187	2.5738	4.2265	1.2461	69.788	32.8385	11.5111	-31.6087	11.7916	-28.6556	11.9412	-32.3293
30	E_{CORR}, d_{HF}	0.4914	0.2051	0.6561	0.0405	0.6965	0.1953	0.377	0.4881	0.2732	17.2137	5	0.8123	0.8121	0.8407	0.8211	0.7145	0.8867	0.7584	0.1222	0.303	0.3846	0.1883	2.5585	4.2879	1.2687	70.4483	29.8495	11.5706	-33.1812	11.8542	-28.0367	11.3049	-33.0846
31	ω_{CORR}	0.4877	0.1162	0.5792	0.0248	0.6039	0.7771	0.4307	0.4898	0.4969	24.3983	0	0.379	0.3785	0.4728	0.7531	0.6829	0.4639	-0.026	0.7073	0.3619	0.411	0.4026	3.339	4.3189	4.1977	60.2548	26.2145	6.0888	-19.4284	5.6104	-19.9081	6.0537	-19.1941
32	ω_{DFT}	0.4446	0.1357	0.5541	0.0262	0.5803	0.7618	0.4433	0.51	0.4592	22.1255	0	0.4697	0.4693	0.5498	0.7344	0.6519	0.6836	0.3591	0.3089	0.3669	0.4194	0.3542	3.538	4.6825	3.5843	58.4642	14.003	5.5382	-20.0857	5.7171	-19.7536	6.4115	-18.8645
33	E^{HOMO}_{CORR}	0.4329	0.1321	0.5378	0.0272	0.565	0.7517	0.4514	0.5154	0.3279	20.7802	3	0.7296	0.7293	0.7704	0.722	0.6444	0.8295	0.5643	0.2231	0.3697	0.4206	0.2537	3.6674	4.7809	1.828	57.1429	21.836	5.3032	-20.2211	5.8124	-19.8665	5.9671	-19.4537
34	χ_{CORR}	0.4018	0.1522	0.5261	0.0279	0.554	0.7443	0.457	0.5293	0.4291	19.8763	0	0.5368	0.5365	0.6068	0.713	0.6253	0.6694	0.2958	0.3686	0.3735	0.4289	0.3353	3.7598	5.0429	3.1306	55.804	10.8584	5.6462	-20.343	6.3404	-19.0578	5.6213	-19.9662
35	E_{DFT}, ω_{DFT}	0.3997	0.1979	0.544	0.0536	0.5977	0.1985	0.4341	0.5302	0.4064	11.1419	0	0.5845	0.5842	0.6473	0.7482	0.6307	0.7423	0.4181	0.2958	0.3617	0.4392	0.3176	3.3918	5.0606	2.8082	61.9376	12.4316	11.5506	-27.966	11.4518	-28.7114	11.7239	-27.7726
36	E^{LUMO}_{DFT}	0.3928	0.1523	0.5166	0.0284	0.545	0.7383	0.4616	0.5333	0.458	19.1672	0	0.4724	0.4719	0.5521	0.7055	0.6141	0.6651	0.3159	0.3358	0.3837	0.4394	0.3661	3.8357	5.1194	3.5663	54.9329	4.4914	5.7116	-19.7251	5.3863	-20.1291	5.8459	-19.6135
37	ω_{HF}	0.3685	0.1578	0.4967	0.0296	0.5263	0.7255	0.471	0.5439	0.4842	17.7775	0	0.4103	0.4099	0.4994	0.6897	0.5946	0.616	0.2734	0.3247	0.3794	0.434	0.39	3.9935	5.3241	3.9856	52.7958	7.7089	5.9365	-19.4486	5.9491	-19.5882	5.8616	-19.6991
38	χ_{PM7}	0.3613	0.1565	0.4876	0.0301	0.5178	0.7196	0.4752	0.547	0.4569	17.1789	0	0.4749	0.4744	0.5542	0.6823	0.592	0.6766	0.3498	0.3075	0.3888	0.4432	0.3641	4.0655	5.385	3.5495	52.4839	10.543	5.8247	-19.4771	5.7086	-19.8195	5.2971	-20.6388
39	E_{DFT}, E^{LUMO}_{DFT}	0.3473	0.2198	0.5093	0.0577	0.567	0.1986	0.4503	0.5529	0.4016	9.823	0	0.5945	0.5941	0.6557	0.7237	0.5948	0.7327	0.3816	0.3223	0.3783	0.4606	0.3231	3.65	5.5027	2.7412	58.4018	11.2388	11.9577	-27.0281	11.9092	-27.6017	11.4539	-28.0469
40	E_{HF}, ω_{HF}	0.3349	0.225	0.5012	0.0587	0.5598	0.2264	0.454	0.5581	0.4193	9.5395	0	0.5578	0.5574	0.6246	0.7178	0.5869	0.7017	0.3591	0.3227	0.3723	0.4537	0.3468	3.7107	5.6074	2.9889	57.5185	3.0048	11.4627	-28.2862	11.8287	-27.8166	11.9238	-27.4915
41	χ_{HF}	0.2942	0.1854	0.4471	0.0325	0.4797	0.6926	0.4937	0.575	0.4682	14.7486	0	0.4486	0.4481	0.5319	0.6483	0.5412	0.6079	0.2322	0.3807	0.399	0.4589	0.3895	4.3868	5.9502	3.7271	48.6694	0.0144	5.7048	-19.9391	5.6591	-19.8419	5.6976	-19.9208
42	E^{LUMO}_{HF}	0.2709	0.1836	0.4204	0.0341	0.4545	0.6741	0.5055	0.5844	0.5048	13.3288	0	0.3591	0.3586	0.4559	0.6249	0.514	0.5389	0.1709	0.3796	0.4125	0.4734	0.4195	4.5992	6.1467	4.3319	45.6353	-5.568	5.4104	-20.5359	6.0589	-19.4841	5.5502	-19.8771
43	E_{HF}, E^{HOMO}_{HF}	0.2672	0.2646	0.4694	0.0624	0.5318	0.2374	0.4683	0.5859	0.3672	8.5181	1	0.6609	0.6606	0.7121	0.6943	0.5492	0.7582	0.4287	0.3026	0.3726	0.4619	0.3146	3.9474	6.178	2.2921	55.288	0.9028	11.8427	-27.5924	11.5455	-28.149	12.1336	-27.2977
44	E_{HF}, χ_{HF}	0.262	0.2637	0.4625	0.0632	0.5257	0.2394	0.4713	0.5879	0.3987	8.313	0	0.6003	0.5999	0.6606	0.6891	0.542	0.7099	0.3353	0.3624	0.3893	0.4788	0.3362	3.9986	6.222	2.702	54.5272	-0.9214	11.5932	-28.2705	11.3248	-28.8671	11.4429	-28.4827
45	E^{HOMO}_{HF}	0.2429	0.1938	0.4015	0.0352	0.4367	0.6608	0.5137	0.5955	0.4524	12.4032	0	0.4852	0.4848	0.563	0.6079	0.495	0.6193	0.2347	0.3992	0.4048	0.4639	0.3831	4.7491	6.3827	3.4796	45.1476	-17.8971	6.1656	-19.0776	5.8407	-19.6739	6.4234	-18.8235
46	E_{HF}, E^{LUMO}_{HF}	0.2151	0.2606	0.4058	0.0699	0.4757	0.1501	0.4955	0.6063	0.4523	6.8048	0	0.4855	0.4851	0.5632	0.6447	0.4891	0.6143	0.2179	0.4212	0.4188	0.5099	0.3758	4.4202	6.6168	3.4778	49.9936	-11.8605	11.634	-27.9594	11.5955	-28.2459	12.2981	-26.8489
47	E_{DFT}, χ_{DFT}	0.2019	0.2965	0.4315	0.0669	0.4984	0.2847	0.4847	0.6114	0.4083	7.4522	0	0.5808	0.5805	0.6441	0.6652	0.5022	0.6959	0.3274	0.361	0.3988	0.494	0.3383	4.2288	6.7284	2.8335	51.597	0.2764	12.0946	-27.2438	11.6047	-27.8588	11.5967	-28.0908
48	χ_{DFT}	0.2013	0.2214	0.3866	0.0361	0.4227	0.6501	0.52	0.6116	0.4978	11.7145	0	0.3768	0.3763	0.471	0.5942	0.4681	0.5538	0.1882	0.371	0.4165	0.4803	0.4103	4.8671	6.7334	4.2122	42.694	-3.6091	6.0117	-19.5233	5.8691	-19.5255	5.9166	-19.6591
49	η_{PM7}	0.1044	0.2317	0.2946	0.0415	0.3361	0.5798	0.5576	0.6477	0.4633	8.1004	0	0.4603	0.4598	0.5418	0.5031	0.3651	0.571	0.1392	0.5102	0.4846	0.5558	0.3835	5.597	7.5505	3.6482	34.0742	-25.6332	5.7218	-20.4428	5.8289	-19.7014	5.8615	-19.9828
50	E_{DFT}, E^{HOMO}_{DFT}	0.0384	0.3708	0.3304	0.0788	0.4092	0.2694	0.526	0.6711	0.4455	5.1943	0	0.5008	0.5004	0.5763	0.5807	0.3847	0.6066	0.2283	0.432	0.4323	0.5406	0.3675	4.9809	8.1068	3.374	44.4596	-24.0288	11.7676	-28.7269	11.7871	-28.0247	12.0731	-27.6981
51	E^{LUMO}_{CORR}	0.0057	0.2342	0.1924	0.0475	0.2399	0.4898	0.5967	0.6824	0.6113	5.0495	0	0.0603	0.0595	0.2022	0.3869	0.2362	0.1702	-0.015	0.1685	0.5032	0.5748	0.5027	6.4082	8.3822	6.352	26.2296	-34.7059	6.3022	-19.4988	6.1223	-19.3794	5.6883	-20.4875
52	E^{HOMO}_{DFT}	-0.0412	0.3119	0.2251	0.0456	0.2706	0.5202	0.5845	0.6983	0.552	5.9371	0	0.2338	0.2332	0.3495	0.426	0.2628	0.3721	0.0473	0.3654	0.4602	0.5347	0.4552	6.1489	8.7782	5.1791	29.5263	-31.0209	5.6908	-20.5334	6.0164	-19.4635	5.6928	-20.5248
53	E^{HOMO}_{PM7}	-0.0501	0.2293	0.1279	0.0513	0.1792	0.4233	0.62	0.7013	0.562	3.4931	0	0.2057	0.2051	0.3257	0.3039	0.158	0.3258	0.015	0.3709	0.4813	0.5442	0.4701	6.9198	8.8532	5.3686	19.5269	-31.3147	5.7671	-19.7872	6.2822	-19.1455	5.7203	-20.3121
54	η_{DFT}	-0.0761	0.2205	0.091	0.0535	0.1444	0.3801	0.633	0.7099	0.5476	2.7013	0	0.246	0.2453	0.3599	0.2524	0.09	0.3292	-0.0834	0.6362	0.5516	0.6225	0.4565	7.2128	9.0718	5.0968	15.8046	-42.0409	5.6951	-20.2155	5.6379	-20.0982	5.7883	-20.4837
55	E_{DFT}	-0.1285	0.246	0.0624	0.0552	0.1176	0.3429	0.6429	0.727	0.5536	2.1314	0	0.2293	0.2286	0.3457	0.2104	0.0091	0.2621	-0.7234	1.9498	0.5218	0.5915	0.4145	7.4395	9.5136	5.2095	13.2385	-40.2256	6.0365	-19.1972	5.8818	-19.7205	5.4938	-19.8709
56	E_{HF}	-0.1289	0.2461	0.062	0.0552	0.1172	0.3424	0.643	0.7271	0.5538	2.1246	0	0.2287	0.2281	0.3453	0.2098	0.0085	0.2614	-0.726	1.9543	0.5219	0.5916	0.4147	7.4423	9.5169	5.2131	13.9459	-35.1437	5.834	-19.4981	5.7612	-19.8148	6.2723	-19.0302
57	η_{CORR}	-0.1536	0.1731	-0.0418	0.0613	0.0195	0.1396	0.6777	0.7351	0.5889	0.3178	0	0.1279	0.1272	0.2596	0.0382	-0.1256	0.1417	-0.7205	1.7954	0.531	0.58	0.4739	8.2664	9.7254	5.895	3.3749	-38.9558	6.182	-20.9903	6.467	-18.7627	6.031	-21.1546
58	d_{CORR}	-0.1672	0.1759	-0.0532	0.062	0.0087	0.0935	0.6814	0.7394	0.6079	0.1412	0	0.0707	0.0699	0.2111	0.0173	-0.1461	0.0791	-0.5428	1.3106	0.5471	0.6033	0.4926	8.3568	9.8401	6.2814	1.7879	-39.7127	6.1939	-19.8055	6.1937	-19.318	6.0631	-19.7787
59	E_{DFT}, η_{DFT}	-0.1714	0.3355	0.0526	0.1115	0.164	-0.1601	0.6257	0.7407	0.5186	1.4717	0	0.3236	0.323	0.4258	0.2818	0.0417	0.3751	-0.211	1.0042	0.5338	0.6395	0.4224	7.0476	9.8758	4.5723	19.8427	-47.0658	12.2644	-27.5024	11.4667	-28.7041	11.6082	-28.411
60	d_{HF}	-0.2066	0.2368	-0.0303	0.0606	0.0303	0.174	0.6739	0.7517	0.637	0.4998	0	-0.0205	-0.0213	0.1337	0.0588	-0.1096	0.0122	-0.0036	0.0104	0.5547	0.6271	0.4985	8.1752	10.172	6.8976	4.7466	-53.5421	6.2452	-22.1654	5.7255	-19.7344	5.9273	-21.5997
61	d_{DFT}	-0.2176	0.2596	-0.0179	0.0599	0.042	0.2049	0.6699	0.7552	0.632	0.7009	0	-0.0045	-0.0053	0.1473	0.0806	-0.0874	0.0381	-0.0214	0.0677	0.5539	0.6313	0.4987	8.0768	10.2653	6.7895	6.3457	-53.3261	6.1046	-21.5176	5.7621	-19.5488	5.9624	-21.9935
62	d_{PM7}	-0.2177	0.2691	-0.0078	0.0593	0.0514	0.2268	0.6665	0.7552	0.63	0.8677	0	0.0017	0.0009	0.1525	0.0979	-0.0723	0.0552	-0.028	0.0974	0.5523	0.6313	0.4999	7.9969	10.2656	6.7477	7.476	-54.7553	6.198	-21.7309	5.8139	-19.7513	5.9486	-21.3766
63	E_{HF}, d_{HF}	-0.2383	0.3562	0.0003	0.1176	0.1179	-0.1155	0.6428	0.7616	0.5548	1.0023	0	0.226	0.2253	0.3429	0.2109	-0.0499	0.255	-0.7625	2.019	0.5237	0.6293	0.413	7.4367	10.4396	5.232	15.5156	-55.4203	11.6504	-29.0996	11.8369	-28.1834	12.1692	-29.0596
64	E_{DFT}, d_{DFT}	-0.2523	0.374	0.0045	0.1171	0.1216	-0.0995	0.6414	0.7659	0.5544	1.0385	0	0.227	0.2264	0.3438	0.2169	-0.045	0.254	-0.6977	1.8868	0.5245	0.6348	0.4086	7.4052	10.558	5.2247	16.8788	-66.7669	11.9714	-30.0232	11.3763	-28.7411	11.384	-30.5847
65	E_{HF}, η_{HF}	-0.2656	0.3828	-0.0004	0.1177	0.1173	-0.1422	0.643	0.7699	0.5541	0.9964	0	0.2278	0.2272	0.3445	0.2099	-0.0536	0.2589	-0.779	2.0555	0.5223	0.6397	0.415	7.4419	10.6694	5.2195	14.7951	-53.3372	11.8898	-37.2368	11.7812	-28.5091	11.9422	-37.8772
66	η_{HF}	-0.311	0.3404	-0.0313	0.0607	0.0293	0.1713	0.6743	0.7836	0.6376	0.4836	0	-0.0224	-0.0232	0.1321	0.057	-0.1307	-0.0024	-0.0003	0.0007	0.5547	0.6405	0.4975	8.1832	11.0528	6.9106	5.3125	-55.2905	5.8058	-21.6351	5.9193	-19.5396	5.8617	-23.4844

Models are arranged according to Q^2_{LOO} values.

Parameters are obtained through QSARINS software. Ref. [43] (Chirico, N.; Papa, E.; Kovarich, S.; Cassani, S.; Gramatica, P. QSARINS, Software for QSAR MLR model development and validation. 2012, QSAR Res. Unit in Environ. Chem. and Ecotox., University of Insubria, Varese, Italy (http://www.qsar.it).

R^2_{adj} adjusted R^2

N. Ext.OK Number of external validation parameters meeting threshold values

F "F-test" statistic value

Table S4. Value of internal and external validation parameters of two- and one-descriptor QSAR models, for inhibitory growth concentration (Log IGC_{50}^{-1}) of alkyl- and halogen-substituted nitrobenzenes, developed using PM7, HF, DFT and electron-correlation contribution (CORR) based descriptors through 30% ordered response splitting method.

Model	Variables	Q^2_{LOO}	R^2-Q^2_{LOO}	R^2_{adj}	R^2-R^2_{adj}	R^2	ΔK	$RMSE_{TR}$	$RMSE_{CV}$	$RMSE_{EXT}$	F	N. Ext.OK	Q^2_{F1}	Q^2_{F2}	Q^2_{F3}
1	E_{CORR}, ω_{PM7}	0.7567	0.0601	0.7994	0.0174	0.8168	0.1075	0.2741	0.3159	0.1796	46.8246	5	0.934	0.9327	0.9214
2	E_{PM7}, η_{PM7}	0.7552	0.0768	0.8159	0.016	0.8319	0.2913	0.2626	0.3169	0.2041	51.9793	5	0.9148	0.9131	0.8984
3	E_{CORR}, ω_{HF}	0.7457	0.0543	0.781	0.019	0.8	0.181	0.2864	0.323	0.1974	42.0022	5	0.9203	0.9187	0.905
4	E_{CORR}, χ_{PM7}	0.7406	0.0626	0.7845	0.0187	0.8033	0.171	0.2841	0.3262	0.1904	42.8737	5	0.9258	0.9243	0.9116
5	E_{CORR}, E^{LUMO}_{PM7}	0.7371	0.0656	0.784	0.0188	0.8028	0.0848	0.2844	0.3284	0.1872	42.7331	5	0.9283	0.9269	0.9146
6	E_{CORR}, E_{HF}	0.7297	0.0874	0.7996	0.0174	0.817	-0.0557	0.274	0.333	0.2216	46.8827	5	0.8995	0.8975	0.8803
7	E_{CORR}, E^{LUMO}_{HF}	0.7216	0.061	0.7619	0.0207	0.7826	0.1819	0.2986	0.3379	0.2201	37.793	5	0.9009	0.8989	0.8819
8	E_{CORR}, E^{HOMO}_{PM7}	0.7211	0.0637	0.7643	0.0205	0.7848	0.3115	0.2971	0.3382	0.2059	38.2972	5	0.9132	0.9115	0.8966
9	E_{CORR}, χ_{HF}	0.719	0.0696	0.7685	0.0201	0.7887	0.1714	0.2944	0.3395	0.2027	39.1824	5	0.916	0.9143	0.8999
10	E_{CORR}, E_{PM7}	0.7187	0.0938	0.7947	0.0179	0.8126	0.0667	0.2773	0.3397	0.1733	45.5209	5	0.9385	0.9373	0.9268
11	E_{CORR}, E^{HOMO}_{HF}	0.7095	0.0761	0.7652	0.0204	0.7856	0.171	0.2965	0.3452	0.2075	38.4745	5	0.9119	0.9102	0.8951
12	E_{CORR}, ω_{CORR}	0.6952	0.0717	0.7447	0.0222	0.7669	0.0883	0.3092	0.3536	0.239	34.5523	5	0.8831	0.8808	0.8608
13	$E_{CORR}, E^{LUMO}_{CORR}$	0.6794	0.0663	0.7215	0.0242	0.7457	0.2241	0.323	0.3626	0.2661	30.7874	5	0.8551	0.8522	0.8274
14	E_{CORR}	0.6754	0.0389	0.7013	0.013	0.7143	0.8452	0.3423	0.3649	0.2823	54.9992	5	0.837	0.8338	0.8058
15	E_{CORR}, χ_{CORR}	0.6751	0.0836	0.7357	0.023	0.7586	0.0745	0.3146	0.3651	0.2134	33.0034	5	0.9068	0.9049	0.8889
16	E_{CORR}, η_{HF}	0.6696	0.0525	0.6956	0.0265	0.7221	0.3165	0.3376	0.3681	0.2972	27.2825	5	0.8193	0.8157	0.7847
17	E_{CORR}, η_{CORR}	0.6688	0.0574	0.7002	0.0261	0.7262	0.2022	0.3351	0.3686	0.3049	27.8539	5	0.8098	0.806	0.7734
18	E_{CORR}, η_{PM7}	0.6632	0.0513	0.6872	0.0272	0.7144	0.0054	0.3422	0.3717	0.2804	26.269	5	0.8391	0.8359	0.8083
19	E_{PM7}, E^{LUMO}_{PM7}	0.6506	0.1237	0.7528	0.0215	0.7743	0.0524	0.3042	0.3786	0.2413	36.0294	5	0.8809	0.8785	0.8581
20	$E_{CORR}, E^{HOMO}_{CORR}$	0.6382	0.086	0.6979	0.0263	0.7241	0.0033	0.3364	0.3852	0.219	27.5618	5	0.9018	0.8999	0.883
21	E_{CORR}, d_{PM7}	0.6307	0.0895	0.6935	0.0266	0.7202	0.338	0.3388	0.3892	0.2976	27.026	5	0.8188	0.8152	0.7841
22	E_{PM7}, d_{PM7}	0.6298	0.1456	0.754	0.0214	0.7754	0.3165	0.3035	0.3897	0.2637	36.2503	5	0.8577	0.8549	0.8305
23	E_{PM7}, ω_{PM7}	0.6249	0.1363	0.7384	0.0227	0.7612	0.034	0.313	0.3922	0.2607	33.4655	5	0.8609	0.8581	0.8343
24	E_{CORR}, d_{HF}	0.6237	0.0946	0.6915	0.0268	0.7183	0.375	0.3399	0.3929	0.2973	26.7789	5	0.8191	0.8155	0.7845
25	E_{PM7}	0.6129	0.0879	0.6872	0.0136	0.7008	0.8371	0.3503	0.3985	0.2807	51.5233	5	0.8388	0.8356	0.8079
26	E_{CORR}, d_{CORR}	0.6029	0.1118	0.6875	0.0272	0.7147	0.2969	0.3421	0.4036	0.2728	26.3041	5	0.8477	0.8447	0.8185
27	E_{PM7}, E^{HOMO}_{PM7}	0.5932	0.1188	0.6846	0.0274	0.712	0.0162	0.3437	0.4085	0.2687	25.9583	5	0.8522	0.8493	0.8239
28	E_{PM7}, χ_{PM7}	0.5749	0.1368	0.6842	0.0275	0.7117	0.0139	0.3439	0.4176	0.2862	25.9169	5	0.8324	0.829	0.8003
29	E^{LUMO}_{PM7}	0.5426	0.1021	0.6286	0.0161	0.6447	0.8029	0.3817	0.4331	0.3271	39.9215	3	0.7811	0.7768	0.7392
30	ω_{PM7}	0.5374	0.103	0.6241	0.0163	0.6405	0.8003	0.384	0.4356	0.3543	39.189	2	0.7431	0.738	0.6939
31	ω_{CORR}	0.4155	0.114	0.5081	0.0214	0.5295	0.7277	0.4393	0.4896	0.5063	24.7589	0	0.4755	0.4651	0.3751
32	E^{HOMO}_{CORR}	0.415	0.1038	0.497	0.0219	0.5188	0.7203	0.4443	0.4899	0.2755	23.7217	5	0.8447	0.8417	0.815
33	χ_{CORR}	0.3869	0.1406	0.506	0.0215	0.5275	0.7263	0.4402	0.5015	0.4522	24.5605	0	0.5816	0.5733	0.5015
34	ω_{DFT}	0.3743	0.1332	0.4851	0.0224	0.5075	0.7124	0.4494	0.5066	0.4406	22.673	0	0.6027	0.5948	0.5267
35	E_{DFT}, ω_{DFT}	0.3624	0.2132	0.5352	0.0404	0.5756	0.2809	0.4172	0.5114	0.3654	14.2431	2	0.7268	0.7214	0.6745
36	χ_{PM7}	0.3457	0.1359	0.458	0.0236	0.4816	0.694	0.4611	0.5181	0.4761	20.4359	0	0.5362	0.527	0.4474
37	E^{LUMO}_{DFT}	0.3423	0.1406	0.4594	0.0235	0.4829	0.6949	0.4606	0.5194	0.4496	20.5442	0	0.5865	0.5783	0.5073
38	E_{DFT}, E^{LUMO}_{DFT}	0.3301	0.2263	0.5142	0.0422	0.5564	0.2821	0.4265	0.5242	0.3742	13.1721	2	0.7135	0.7079	0.6587
39	E_{HF}, ω_{HF}	0.3223	0.2195	0.4981	0.0436	0.5418	0.1739	0.4335	0.5272	0.3986	12.4136	0	0.6749	0.6685	0.6127
40	ω_{HF}	0.3179	0.1349	0.4279	0.0249	0.4528	0.6729	0.4738	0.5289	0.4845	18.2031	0	0.5197	0.5102	0.4278
41	E_{HF}, E^{HOMO}_{HF}	0.2954	0.2469	0.4987	0.0436	0.5423	0.06	0.4333	0.5376	0.3806	12.4404	2	0.7037	0.6978	0.6469
42	χ_{HF}	0.2861	0.1509	0.4114	0.0256	0.437	0.6611	0.4805	0.5411	0.4861	17.0788	0	0.5165	0.5069	0.4239
43	E^{HOMO}_{HF}	0.2783	0.1501	0.4024	0.026	0.4284	0.6545	0.4842	0.5441	0.4965	16.4884	0	0.4956	0.4856	0.3991
44	E_{HF}, χ_{HF}	0.2769	0.2506	0.4825	0.045	0.5275	0.2952	0.4402	0.5446	0.3949	11.7243	0	0.6808	0.6745	0.6197
45	E_{DFT}, χ_{DFT}	0.2422	0.2567	0.4512	0.0477	0.4989	0.0278	0.4534	0.5575	0.4047	10.453	0	0.6649	0.6583	0.6008
46	E^{LUMO}_{HF}	0.2422	0.1559	0.3707	0.0274	0.3981	0.6309	0.4969	0.5575	0.5193	14.5499	0	0.4481	0.4372	0.3425
47	E_{HF}, E^{LUMO}_{HF}	0.2195	0.2574	0.4271	0.0498	0.477	0.2565	0.4632	0.5658	0.4477	9.5746	0	0.5899	0.5818	0.5114
48	χ_{DFT}	0.2132	0.1635	0.3484	0.0283	0.3767	0.6138	0.5056	0.5681	0.5194	13.2961	0	0.448	0.4371	0.3423
49	η_{PM7}	0.1997	0.1567	0.3272	0.0293	0.3564	0.597	0.5138	0.573	0.5252	12.184	0	0.4355	0.4244	0.3275
50	E_{DFT}, E^{HOMO}_{DFT}	0.1209	0.2925	0.3575	0.0559	0.4134	0.2496	0.4905	0.6005	0.4554	7.3989	0	0.5757	0.5673	0.4945
51	E^{HOMO}_{DFT}	0.0599	0.1863	0.2119	0.0343	0.2462	0.4962	0.5561	0.621	0.5991	7.1853	0	0.2655	0.2509	0.1248
52	E^{HOMO}_{PM7}	0.0378	0.1563	0.1574	0.0366	0.1941	0.4405	0.575	0.6282	0.6296	5.2977	0	0.1888	0.1728	0.0336
53	E^{LUMO}_{CORR}	0.0254	0.179	0.1683	0.0362	0.2044	0.4522	0.5712	0.6323	0.6669	5.6535	0	0.09	0.072	-0.0842
54	η_{DFT}	0.0007	0.1721	0.1352	0.0376	0.1728	0.4157	0.5825	0.6402	0.6206	4.5966	0	0.2118	0.1962	0.0609
55	d_{CORR}	-0.105	0.1268	-0.0227	0.0445	0.0218	0.1476	0.6334	0.6732	0.6647	0.4897	0	0.096	0.0781	-0.0771
56	η_{CORR}	-0.1121	0.1247	-0.0323	0.0449	0.0126	0.1122	0.6364	0.6754	0.6496	0.2807	0	0.1365	0.1194	-0.0288
57	d_{PM7}	-0.1163	0.1437	-0.0168	0.0442	0.0274	0.1655	0.6316	0.6767	0.6851	0.6193	0	0.0397	0.0207	-0.1442
58	d_{DFT}	-0.1187	0.1385	-0.0248	0.0446	0.0198	0.1407	0.6341	0.6774	0.6885	0.4445	0	0.03	0.0108	-0.1557
59	d_{HF}	-0.1191	0.1313	-0.0327	0.0449	0.0122	0.1106	0.6365	0.6775	0.695	0.2726	0	0.0117	-0.0079	-0.1775
60	E_{DFT}, η_{DFT}	-0.1236	0.3346	0.1358	0.0751	0.211	-0.0524	0.5689	0.6789	0.5788	2.8077	0	0.3144	0.3009	0.1832
61	E_{DFT}	-0.1422	0.2779	0.0964	0.0393	0.1357	0.3684	0.5954	0.6845	0.5948	3.4539	0	0.2761	0.2618	0.1375
62	E_{HF}	-0.1427	0.278	0.096	0.0393	0.1353	0.3678	0.5956	0.6846	0.595	3.4424	0	0.2755	0.2612	0.1368
63	E_{DFT}, d_{DFT}	-0.2037	0.3433	0.0576	0.0819	0.1396	0.0321	0.5941	0.7027	0.5956	1.7034	0	0.2742	0.2598	0.1353
64	E_{HF}, d_{HF}	-0.2084	0.3449	0.0543	0.0822	0.1365	0.0303	0.5951	0.704	0.597	1.6603	0	0.2707	0.2562	0.131
65	E_{HF}, η_{HF}	-0.2399	0.3914	0.0706	0.0808	0.1514	0.0486	0.59	0.7132	0.6289	1.874	0	0.1908	0.1748	0.0358
66	η_{HF}	-0.251	0.2928	-0.0017	0.0436	0.0419	0.2046	0.6269	0.7163	0.7292	0.9611	0	-0.0882	-0.1097	-0.2965

Model	CCC_{TR}	CCC_{CV}	CCC_{EXT}	$\overline{r}^2_m$	Δr^2_m	MAE_{TR}	MAE_{CV}	MAE_{EXT}	RSS_{TR}	$PRESS_{CV}$	$PRESS_{EXT}$	R^2_{LMO}	Q^2_{LMO}	R^2_{Yscr}	Q^2_{Yscr}	R^2_{Xrand}	Q^2_{Xrand}	R^2_{Yrand}	Q^2_{Yrand}
1	0.8992	0.867	0.9655	0.9061	0.0297	0.2016	0.2334	0.1423	1.8031	2.3949	0.3548	81.7738	68.9792	8.8905	-20.2788	8.7518	-19.6776	8.8409	-20.0362
2	0.9083	0.869	0.9532	0.8391	0.0727	0.1882	0.2207	0.1833	1.6544	2.4102	0.4583	83.1895	72.5186	8.8207	-20.173	8.8942	-19.6423	8.6921	-20.173
3	0.8889	0.859	0.9592	0.8894	0.018	0.2065	0.2352	0.1649	1.9688	2.5038	0.4286	79.8337	66.3837	8.9593	-19.443	9.0138	-19.3324	8.4981	-20.5491
4	0.8909	0.857	0.9617	0.8976	0.0225	0.2183	0.2508	0.1459	1.9366	2.5531	0.3989	80.2773	66.967	8.6895	-20.3686	8.9727	-19.2235	8.4304	-20.8153
5	0.8906	0.856	0.9622	0.8929	0.0589	0.2046	0.2369	0.1502	1.9417	2.5879	0.3854	80.1793	69.8116	8.7403	-20.4925	8.476	-19.8646	8.4465	-20.7035
6	0.8993	0.850	0.9516	0.8697	0.0721	0.2037	0.2408	0.1816	1.8013	2.6613	0.5402	82.4472	67.1872	8.7224	-20.5937	8.7977	-19.5053	8.1568	-21.3033
7	0.878	0.844	0.949	0.8626	0.0369	0.2142	0.2455	0.1783	2.1404	2.7405	0.5328	78.7922	59.723	8.6554	-20.4881	8.9112	-19.503	8.3527	-20.8247
8	0.8794	0.843	0.9562	0.8816	0.0654	0.2363	0.2707	0.1648	2.1182	2.7454	0.4664	78.2534	64.7729	8.4676	-20.5076	8.887	-19.4629	8.7332	-20.2254
9	0.8818	0.844	0.9572	0.8853	0.04	0.2165	0.2502	0.1583	2.0805	2.766	0.4518	78.7458	65.0113	8.8034	-19.6884	8.4151	-20.4088	8.5943	-20.3775
10	0.8966	0.846	0.9685	0.9152	0.031	0.2048	0.2423	0.1453	1.8451	2.7688	0.3305	81.9208	64.9258	8.6014	-19.9982	8.6123	-19.8488	8.6899	-20.2189
11	0.8799	0.838	0.956	0.8603	0.0635	0.2363	0.2745	0.1622	2.1106	2.8594	0.4735	78.8052	63.6019	9.2367	-19.1889	8.7887	-19.7771	8.4898	-20.6491
12	0.8681	0.827	0.9382	0.8362	0.0421	0.2187	0.2525	0.1963	2.2943	3.0006	0.6282	76.7126	62.126	8.7614	-19.9467	8.8957	-19.3766	8.6047	-20.2223
13	0.8543	0.817	0.9245	0.8063	0.1053	0.2349	0.2687	0.2054	2.5035	3.156	0.7789	74.0584	59.3015	8.3256	-21.2661	8.9453	-19.5611	8.5389	-20.4274
14	0.8333	0.808	0.9188	0.7996	0.0746	0.2525	0.2734	0.2306	2.8127	3.1958	0.8763	71.2653	54.0153	4.1908	-14.5061	4.4318	-13.9036	4.2162	-14.6236
15	0.8628	0.817	0.9518	0.8699	0.0077	0.2272	0.2648	0.1826	2.376	3.1988	0.5011	76.1304	59.03	8.4955	-20.3015	8.8069	-19.5795	8.8401	-20.019
16	0.8386	0.806	0.9092	0.7789	0.1189	0.2347	0.2613	0.2407	2.7358	3.2524	0.9714	71.7753	55.5028	8.6782	-22.849	8.8525	-19.6383	8.8998	-22.7222
17	0.8414	0.807	0.9029	0.765	0.1295	0.2353	0.2648	0.2363	2.695	3.2603	1.0226	71.915	58.4205	8.4984	-21.0344	9.0543	-19.0751	8.4459	-20.721
18	0.8334	0.801	0.92	0.8011	0.0658	0.2531	0.2819	0.2304	2.8112	3.3157	0.865	71.0606	54.8055	8.7673	-20.8572	8.4274	-20.3532	8.8809	-20.3784
19	0.8728	0.810	0.9274	0.8338	0.0688	0.2429	0.2899	0.2004	2.2215	3.4393	0.6403	78.1804	59.6997	8.7717	-20.673	8.5345	-20.0751	8.1359	-21.6482
20	0.84	0.787	0.9513	0.8703	0.0108	0.2526	0.2939	0.1964	2.7157	3.562	0.5277	72.6336	53.9113	8.6913	-20.1731	8.4596	-19.9102	8.741	-20.1015
21	0.8373	0.786	0.9109	0.7832	0.0662	0.2463	0.2879	0.2393	2.7545	3.6357	0.9743	71.5608	54.9222	8.8036	-21.0156	8.6957	-19.8616	8.6383	-21.2522
22	0.8735	0.802	0.9176	0.8274	0.0896	0.2445	0.2962	0.1892	2.211	3.6442	0.7649	78.6244	58.8895	9.116	-20.5602	9.1117	-19.3621	8.4114	-21.6745
23	0.8644	0.796	0.9145	0.8208	0.0788	0.2502	0.2998	0.2214	2.351	3.6924	0.7478	77.1976	54.9827	8.3394	-20.9509	8.3745	-20.5151	8.3739	-21.2684
24	0.8361	0.782	0.9109	0.783	0.0683	0.2481	0.291	0.239	2.7727	3.7043	0.9723	72.0068	53.0841	9.0892	-20.2055	8.877	-19.4918	8.5271	-21.3489
25	0.8241	0.774	0.8991	0.7728	0.1029	0.2567	0.286	0.2314	2.9456	3.8111	0.8667	70.1705	49.7486	4.4785	-14.069	4.265	-14.0291	4.2356	-14.2322
26	0.8336	0.770	0.9241	0.812	0.074	0.2528	0.2964	0.2252	2.8085	3.9093	0.8187	72.4414	51.934	8.3013	-20.7088	8.4627	-20.0874	8.5788	-20.0617
27	0.8318	0.767	0.91	0.7673	0.1096	0.2534	0.2957	0.2153	2.8352	4.005	0.7944	72.428	47.3898	8.3813	-20.7586	8.0523	-20.4804	9.2917	-19.4799
28	0.8316	0.759	0.8946	0.7862	0.0955	0.2676	0.3152	0.238	2.8384	4.1846	0.9012	71.4738	50.8011	8.9862	-19.9594	9.1876	-19.2572	8.6883	-20.86
29	0.784	0.730	0.8444	0.5661	0.1988	0.3099	0.3459	0.272	3.4976	4.5023	1.1766	65.4187	40.9495	4.4435	-14.5029	4.2896	-14.1966	4.3619	-14.2502
30	0.7808	0.724	0.8187	0.5624	0.2085	0.3132	0.3483	0.3018	3.5394	4.5538	1.3812	64.3937	41.8011	4.3066	-14.3199	4.2834	-14.1565	4.3239	-14.2909
31	0.6924	0.625	0.6239	0.3532	0.2956	0.3684	0.407	0.3937	4.6317	5.7538	2.8197	53.1172	26.7471	4.2859	-14.4533	4.3317	-14.0288	4.4022	-14.2191
32	0.6832	0.618	0.9094	0.8835	0.0196	0.3496	0.3849	0.2409	4.7368	5.759	0.8347	51.8274	28.822	4.1757	-14.3965	4.3024	-14.0482	4.0812	-14.5313
33	0.6907	0.613	0.7164	0.494	0.2506	0.3546	0.3957	0.3411	4.6514	6.0355	2.2494	52.7509	29.1486	4.5069	-14.3531	4.6233	-13.9056	4.5839	-14.048
34	0.6733	0.595	0.7059	0.3992	0.3067	0.3769	0.4197	0.3455	4.848	6.1596	2.1357	51.1275	19.2751	4.3256	-14.1856	4.4492	-14.0657	4.6406	-13.7798
35	0.7307	0.609	0.8182	0.5517	0.222	0.3417	0.4078	0.297	4.1775	6.2766	1.4685	59.3881	28.0601	8.7957	-20.1515	8.9223	-19.2951	7.992	-21.3939
36	0.6501	0.573	0.6402	0.341	0.3457	0.3836	0.4262	0.398	5.1036	6.4412	2.4934	48.9504	23.0789	4.6183	-13.9211	4.196	-14.1851	4.4796	-14.3066
37	0.6513	0.569	0.6869	0.3717	0.3259	0.3857	0.4299	0.3589	5.0906	6.4745	2.2231	49.0779	15.4539	4.0488	-14.5457	4.2082	-14.2653	4.2989	-14.3136
38	0.715	0.587	0.8072	0.5345	0.2314	0.3473	0.4155	0.3097	4.3665	6.5945	1.54	57.5654	25.1722	8.6263	-20.3602	8.5885	-20.1495	8.9334	-20.3563
39	0.7028	0.576	0.7753	0.495	0.2527	0.3574	0.4242	0.3435	4.5111	6.6715	1.7475	56.0514	27.5484	8.315	-21.0007	8.5922	-19.4792	8.5305	-20.5894
40	0.6233	0.541	0.6198	0.295	0.3758	0.4045	0.4483	0.3635	5.387	6.7148	2.5819	45.1175	17.0746	4.0132	-14.7965	4.2632	-14.1378	4.1123	-14.4988
41	0.7032	0.566	0.8102	0.6788	0.1695	0.3411	0.4103	0.3246	4.5058	6.9362	1.593	56.5248	20.8429	8.4782	-20.6702	8.909	-19.4832	8.488	-20.7924
42	0.6082	0.521	0.6214	0.3237	0.3575	0.4088	0.4548	0.3848	5.542	7.0277	2.5992	44.8757	7.8432	4.539	-14.0167	4.4508	-13.9987	4.2591	-14.4135
43	0.5998	0.512	0.6311	0.4389	0.2822	0.4009	0.4456	0.4324	5.627	7.1047	2.7114	43.7469	11.6097	4.1015	-14.6588	4.0924	-14.4101	4.5556	-13.9288
44	0.6907	0.552	0.7804	0.5262	0.2364	0.3594	0.4302	0.3396	4.651	7.1184	1.7157	55.113	19.5284	8.7428	-20.3798	8.9047	-19.3948	8.5789	-20.4621
45	0.6657	0.521	0.7613	0.4721	0.266	0.3741	0.4478	0.3395	4.9332	7.4598	1.8013	52.3801	14.9203	9.0649	-20.0923	8.6933	-20.0999	8.5877	-20.6953
46	0.5695	0.476	0.5404	0.1666	0.454	0.4221	0.4695	0.397	5.9254	7.4604	2.9667	40.0566	9.7123	4.2833	-14.14	4.4445	-13.9796	4.3409	-14.2192
47	0.6459	0.498	0.7012	0.3541	0.3298	0.3816	0.4548	0.3753	5.149	7.6834	2.2044	50.3856	15.4288	8.8746	-20.3745	8.9453	-19.6486	8.4956	-20.5497
48	0.5473	0.451	0.5377	0.1875	0.4674	0.4228	0.4709	0.4061	6.1359	7.7452	2.9675	38.6703	4.24	4.3424	-14.1523	4.5365	-13.8007	4.2015	-14.315
49	0.5255	0.427	0.5799	0.0526	0.6816	0.4374	0.4835	0.4516	6.3355	7.8785	3.0345	36.2498	2.1342	4.5294	-14.2685	4.488	-13.85	4.315	-14.2503
50	0.5849	0.419	0.6804	0.3622	0.3274	0.4077	0.4872	0.3674	5.7749	8.6544	2.281	44.1121	6.3178	8.9472	-20.422	8.558	-19.8824	8.7729	-20.4878
51	0.3951	0.286	0.3323	-0.0298	0.6048	0.4601	0.5103	0.459	7.4207	9.255	3.9487	26.07	-5.6527	4.377	-14.3435	4.2256	-14.063	4.4508	-14.0861
52	0.3251	0.224	0.2608	-0.0132	0.4033	0.4695	0.5147	0.4924	7.9338	9.4725	4.3606	20.2749	-7.214	3.8737	-15.0684	4.3481	-14.2249	4.3963	-14.0425
53	0.3395	0.223	0.153	-0.0237	0.1957	0.4841	0.5344	0.5313	7.8317	9.5939	4.8918	21.1341	-8.9797	4.141	-14.6573	4.4163	-14.011	4.2299	-14.5749
54	0.2947	0.174	0.3868	-0.0374	0.6134	0.4878	0.536	0.5798	8.1429	9.8373	4.2372	18.4381	-16.1073	4.3311	-14.3174	4.2442	-14.1867	4.2724	-14.3729
55	0.0426	-0.072	0.1101	-0.3137	0.855	0.5128	0.5526	0.5549	9.6299	10.8779	4.8597	2.9091	-21.0595	4.6138	-14.0174	4.6235	-13.8486	4.4035	-14.1509
56	0.0249	-0.091	0.1384	-2.3898	5.1524	0.4988	0.5347	0.5329	9.7202	10.9476	4.642	2.2814	-19.8127	4.7898	-14.167	4.5955	-13.7503	4.4323	-14.8868
57	0.0533	-0.063	0.052	-0.4495	1.0524	0.5019	0.543	0.5591	9.5747	10.989	5.1625	3.748	-21.394	4.3268	-14.905	4.4598	-13.8549	4.3109	-14.9023
58	0.0388	-0.077	0.0404	-0.4939	1.1231	0.5012	0.5405	0.5619	9.6493	11.0127	5.2144	2.9992	-23.3673	4.4949	-14.6173	4.3106	-14.0623	4.4866	-15.008
59	0.0242	-0.091	0.0194	-0.2122	0.4774	0.4991	0.5354	0.5668	9.7238	11.0165	5.313	2.0985	-23.6574	4.0699	-15.6171	4.2162	-14.1948	4.2345	-15.6291
60	0.3484	0.128	0.4866	0.0399	0.5909	0.4631	0.5459	0.5409	7.7673	11.0609	3.6855	24.7551	-17.6526	8.4605	-20.938	8.3854	-20.1374	8.6257	-20.938
61	0.239	0.039	0.3893	-0.0195	0.5682	0.4488	0.5071	0.5059	8.5085	11.2442	3.8915	16.3605	-15.6656	4.3049	-14.4733	4.1322	-14.4097	4.076	-14.7416
62	0.2384	0.038	0.3885	-0.0202	0.5687	0.4489	0.5073	0.5061	8.5123	11.2494	3.8946	16.5687	-20.5539	4.2298	-15.0105	4.4411	-13.9447	4.206	-14.581
63	0.245	0.015	0.3893	-0.0208	0.5712	0.4493	0.5304	0.5072	8.4702	11.8497	3.9017	18.2381	-23.0503	8.6168	-21.3379	8.5898	-19.7012	8.4913	-21.6591
64	0.2403	0.010	0.3854	-0.0203	0.5637	0.4494	0.5303	0.5082	8.5002	11.896	3.9207	18.2916	-29.4277	8.5527	-21.6837	8.4491	-20.1652	8.3703	-22.388
65	0.2631	0.019	0.3373	-0.021	0.4836	0.4493	0.5396	0.5602	8.3534	12.2062	4.3502	19.5931	-23.1083	8.3939	-22.7221	8.5011	-20.2244	8.6029	-23.0729
66	0.0804	-0.072	-0.0187	-0.0078	0.0217	0.4964	0.5586	0.6417	9.4322	12.3148	5.8497	6.5042	-31.4806	4.1979	-15.9255	3.9933	-14.4727	4.1748	-16.1044

Models are arranged according to Q^2_{LOO} values.
Parameters are obtained through QSARINS software. Ref. [43], (Chirico, N.; Papa, E.; Kovarich, S.; Cassani, S.; Gramatica, P. QSARINS, Software for QSAR MLR model development and validation. 2012, QSAR Res. Unit in Environ. Chem. and Ecotox., University of Insubria, Varese, Italy (http://www.qsar.it).

R^2_{adj} adjusted R^2
N. Ext.OK Number of external validation parameters meeting threshold values
F "F-test" statistic value

Table S5. Value of internal and external validation parameters of two- and one-descriptor QSAR models, for inhibitory growth concentration (Log IGC_{50}^{-1}) of alkyl- and halogen-substituted nitrobenzenes, developed using PM7, HF, DFT and electron-correlation contribution (CORR) based descriptors through 45% ordered response splitting method.

Model	Variables	Q^2_{LOO}	R^2-Q^2_{LOO}	R^2_{adj}	R^2-R^2_{adj}	R^2	ΔK	$RMSE_{TR}$	$RMSE_{CV}$	$RMSE_{EXT}$	F	N. Ext.OK	Q^2_{F1}	Q^2_{F2}	Q^2_{F3}	CCC_{TR}	CCC_{CV}	CCC_{EXT}	$\bar{r}^2_m$	Δr^2_m	MAE_{TR}	MAE_{CV}	MAE_{EXT}	RSS_{TR}	$PRESS_{CV}$	$PRESS_{EXT}$	R^2_{LMO}	Q^2_{LMO}	R^2_{Yscr}	Q^2_{Yscr}	R^2_{Xrand}	Q^2_{Xrand}	R^2_{Yrand}	Q^2_{Yrand}
1	E_{CORR}, ω_{PM7}	0.7416	0.068	0.7884	0.0212	0.8096	0.0828	0.3004	0.3499	0.1426	38.2616	5	0.9464	0.9446	0.9571	0.8948	0.8581	0.9701	0.8441	0.0494	0.2316	0.2739	0.1189	1.8949	2.5711	0.2845	81.1147	63.9868	10.2631	-23.8601	10.1349	-22.5629	10.1533	-24.4337
2	E_{PM7}, η_{PM7}	0.7411	0.0922	0.8148	0.0185	0.8333	0.2883	0.281	0.3502	0.2042	44.9942	5	0.8899	0.8863	0.912	0.9091	0.864	0.9481	0.8396	0.0793	0.2311	0.2787	0.1691	1.6586	2.5758	0.584	84.07	65.776	10.1155	-23.734	10.0309	-23.1875	10.3261	-23.4322
3	E_{CORR}, ω_{HF}	0.7351	0.0606	0.773	0.0227	0.7957	0.137	0.3111	0.3543	0.1659	35.0527	5	0.9273	0.925	0.9419	0.8862	0.8521	0.9605	0.8507	0.0634	0.2401	0.2785	0.1406	2.0329	2.6361	0.3853	79.5022	62.5253	10.3293	-23.3788	9.9672	-23.6399	10.0679	-23.7012
4	E_{CORR}, E_{HF}	0.7283	0.0825	0.7898	0.021	0.8109	-0.0591	0.2994	0.3588	0.1939	38.5816	5	0.9008	0.8975	0.9207	0.8955	0.85	0.9562	0.8596	0.0561	0.2346	0.2783	0.1465	1.8821	2.7034	0.5263	81.4167	61.7714	10.0702	-23.8039	10.1931	-22.943	10.0942	-23.6889
5	E_{CORR}, χ_{PM7}	0.7279	0.0688	0.7741	0.0226	0.7967	0.1332	0.3104	0.3591	0.1535	35.2605	5	0.9378	0.9357	0.9502	0.8868	0.8486	0.9656	0.8418	0.056	0.2408	0.2834	0.1321	2.0233	2.7077	0.3301	79.8247	58.9975	9.6516	-25.2371	9.6968	-23.8247	9.8832	-24.288
6	E_{CORR}, E^{LUMO}_{PM7}	0.7246	0.0697	0.7714	0.0229	0.7943	0.0628	0.3122	0.3612	0.1463	34.7517	5	0.9435	0.9416	0.9548	0.8854	0.8476	0.9687	0.8389	0.0501	0.2418	0.2837	0.1173	2.0469	2.7403	0.2998	79.7979	58.1499	9.5861	-24.5636	9.9642	-23.4006	10.1147	-23.7938
7	E_{CORR}, E^{HOMO}_{PM7}	0.7174	0.0683	0.7618	0.0238	0.7857	0.2412	0.3187	0.3659	0.1844	32.9896	5	0.9102	0.9073	0.9282	0.88	0.8409	0.9517	0.8447	0.0759	0.2499	0.2911	0.1608	2.1328	2.812	0.4761	78.5303	62.0962	10.0088	-23.7138	9.9218	-23.1668	9.7318	-23.8901
8	E_{CORR}, E_{PM7}	0.7138	0.0967	0.7894	0.0211	0.8105	0.082	0.2997	0.3683	0.1467	38.4901	5	0.9432	0.9413	0.9546	0.8953	0.8433	0.9726	0.8965	0.0438	0.2236	0.267	0.1247	1.8857	2.848	0.3013	81.9532	61.0286	10.048	-23.4054	9.8481	-23.3314	10.2238	-23.1668
9	E_{CORR}, E^{HOMO}_{HF}	0.7119	0.075	0.7632	0.0237	0.7868	0.118	0.3178	0.3695	0.1895	33.2219	5	0.9052	0.9021	0.9242	0.8807	0.8384	0.9489	0.8341	0.0797	0.2469	0.2897	0.1515	2.121	2.8672	0.5029	78.7709	60.2773	10.3321	-22.8482	10.167	-22.8986	10.3057	-22.8707
10	E_{CORR}, χ_{HF}	0.7115	0.0726	0.7601	0.024	0.784	0.1224	0.3199	0.3697	0.1704	32.6759	5	0.9233	0.9209	0.9387	0.879	0.8388	0.9582	0.8409	0.0667	0.2396	0.2796	0.1428	2.1488	2.871	0.4065	78.6466	57.8378	10.1455	-23.3574	9.831	-23.1034	9.9848	-23.6193
11	E_{CORR}, E^{LUMO}_{HF}	0.7007	0.0678	0.7428	0.0257	0.7685	0.1374	0.3312	0.3766	0.1648	29.8785	5	0.9283	0.926	0.9427	0.8691	0.831	0.9615	0.8569	0.0605	0.2502	0.2884	0.1344	2.3034	2.978	0.3801	76.5227	58.2278	10.4093	-23.7281	10.0088	-23.2691	9.6992	-23.9987
12	E_{CORR}, χ_{CORR}	0.6679	0.0861	0.7267	0.0273	0.754	0.0408	0.3414	0.3967	0.1841	27.5914	5	0.9105	0.9076	0.9284	0.8598	0.8104	0.9493	0.7977	0.0821	0.2588	0.3054	0.1503	2.4474	3.3043	0.4747	75.2986	54.9444	9.8851	-23.595	9.6563	-24.2656	9.8155	-23.4661
13	E_{CORR}, ω_{CORR}	0.6621	0.083	0.7169	0.0283	0.7452	0.0559	0.3475	0.4001	0.1678	26.3191	5	0.9257	0.9233	0.9406	0.854	0.8055	0.9584	0.8421	0.0679	0.2685	0.3141	0.1235	2.5356	3.3619	0.3941	74.7536	51.2934	9.6108	-23.9316	9.6351	-23.6302	9.9462	-23.4459
14	E_{PM7}, E^{LUMO}_{PM7}	0.6576	0.1284	0.7622	0.0238	0.786	0.0492	0.3185	0.4028	0.228	33.0491	5	0.8627	0.8583	0.8902	0.8802	0.8147	0.9124	0.6765	0.1379	0.2525	0.3086	0.1801	2.1297	3.4075	0.7281	79.3455	59.1547	9.6563	-24.5825	10.0094	-23.045	10.1155	-23.9712
15	$E_{CORR}, E^{LUMO}_{CORR}$	0.6476	0.0773	0.6944	0.0306	0.7249	0.1701	0.361	0.4086	0.1997	23.7177	5	0.8947	0.8913	0.9158	0.8405	0.7961	0.9449	0.8425	0.0821	0.2745	0.3178	0.1547	2.7372	3.5067	0.5586	71.8959	52.168	10.14	-23.9339	10.1837	-23.6272	9.7963	-24.1982
16	E_{CORR}	0.6444	0.048	0.6762	0.0162	0.6924	0.8321	0.3818	0.4105	0.2146	42.7649	5	0.8785	0.8745	0.9028	0.8182	0.7866	0.9424	0.8601	0.045	0.2934	0.3201	0.1759	3.0609	3.5384	0.6446	68.3857	47.722	4.9347	-16.7544	4.8601	-16.7198	5.0623	-16.5232
17	E_{PM7}, ω_{PM7}	0.6367	0.1412	0.7532	0.0247	0.7779	0.0347	0.3244	0.4149	0.2529	31.5152	4	0.8312	0.8257	0.865	0.8751	0.8035	0.8909	0.6441	0.1637	0.2557	0.3151	0.2047	2.2104	3.6154	0.8955	78.4991	53.5822	9.5561	-24.3882	10.1638	-22.8789	10.266	-23.5943
18	E_{CORR}, η_{HF}	0.6321	0.0639	0.6623	0.0338	0.696	0.3313	0.3795	0.4175	0.2163	20.6087	5	0.8765	0.8725	0.9013	0.8208	0.7816	0.9411	0.8563	0.0347	0.2813	0.3177	0.1708	3.0246	3.6608	0.6549	68.9632	47.5616	9.413	-28.1056	10.288	-23.0847	9.7862	-27.0461
19	$E_{CORR}, E^{HOMO}_{CORR}$	0.6255	0.0935	0.6878	0.0312	0.719	-0.0008	0.3649	0.4212	0.1571	23.0285	5	0.9348	0.9327	0.9479	0.8365	0.7768	0.9666	0.9112	0.0414	0.2874	0.3388	0.14	2.7961	3.7264	0.3457	72.0156	47.5213	10.3097	-23.7037	10.007	-23.4334	10.2746	-23.683
20	E_{CORR}, η_{CORR}	0.6219	0.0754	0.6636	0.0336	0.6972	0.2012	0.3788	0.4233	0.2195	20.7274	5	0.8729	0.8687	0.8983	0.8216	0.7759	0.9388	0.851	0.0108	0.2829	0.3239	0.1714	3.0125	3.7628	0.6743	69.7788	45.2321	10.1777	-23.9657	10.3531	-22.9152	10.1198	-24.0807
21	E_{CORR}, η_{PM7}	0.6198	0.0741	0.66	0.034	0.694	-0.0279	0.3808	0.4244	0.2126	20.4083	5	0.8806	0.8768	0.9046	0.8193	0.7738	0.9432	0.8605	0.0451	0.2978	0.3405	0.1761	3.0452	3.7828	0.633	68.9301	46.5238	9.6506	-24.2767	9.6499	-23.8825	9.881	-23.7194
22	ω_{PM7}	0.5938	0.0969	0.6743	0.0163	0.6906	0.831	0.3829	0.4387	0.364	42.4137	1	0.6503	0.6389	0.7204	0.817	0.7634	0.7373	0.3315	0.3826	0.3031	0.3418	0.3021	3.0784	4.0424	1.8548	69.4207	44.2297	5.1697	-16.5077	4.8802	-16.4534	5.2194	-16.1498
23	E^{LUMO}_{PM7}	0.593	0.0943	0.6708	0.0165	0.6873	0.829	0.3849	0.4392	0.3385	41.759	1	0.6975	0.6876	0.7581	0.8147	0.7632	0.7746	0.3556	0.3704	0.3108	0.3507	0.2823	3.1116	4.0503	1.6045	69.0627	47.8921	4.8813	-16.6719	4.8827	-16.5216	4.8506	-16.7567
24	E_{PM7}	0.5916	0.1025	0.678	0.0161	0.6941	0.8331	0.3807	0.4399	0.229	43.1077	5	0.8616	0.8571	0.8894	0.8194	0.7612	0.9139	0.7265	0.1232	0.2815	0.319	0.1864	3.044	4.0642	0.7339	69.3018	39.048	5.0723	-16.3811	4.9341	-16.3167	5.2012	-16.1955
25	E_{CORR}, d_{PM7}	0.5903	0.1064	0.663	0.0337	0.6967	0.3488	0.3791	0.4406	0.2274	20.6707	5	0.8634	0.859	0.8908	0.8212	0.7598	0.9364	0.8516	0.0484	0.2859	0.3383	0.1843	3.0183	4.0767	0.7242	70.1392	43.455	9.6344	-25.4624	10.5117	-22.4274	9.8974	-24.1321
26	E_{PM7}, d_{PM7}	0.5889	0.1738	0.7363	0.0264	0.7627	0.2875	0.3353	0.4414	0.205	28.9279	5	0.8891	0.8855	0.9113	0.8654	0.7804	0.9378	0.803	0.0974	0.2622	0.3268	0.1577	2.3612	4.0906	0.5883	77.2271	54.0827	10.2193	-24.9576	9.4398	-23.8479	9.5466	-25.4721
27	E_{CORR}, d_{HF}	0.5817	0.1131	0.661	0.0339	0.6949	0.4043	0.3802	0.4452	0.226	20.4964	5	0.8652	0.8608	0.8922	0.82	0.7549	0.9371	0.8518	0.0519	0.2879	0.3421	0.184	3.0361	4.1618	0.7151	69.72	43.9212	9.9756	-25.1026	9.8638	-23.5555	9.6478	-24.487
28	E_{PM7}, χ_{PM7}	0.5718	0.1537	0.695	0.0305	0.7255	0.015	0.3607	0.4504	0.2791	23.7862	4	0.7944	0.7878	0.8357	0.8409	0.7606	0.8652	0.6064	0.1913	0.2779	0.3388	0.2312	2.7315	4.2604	1.0902	73.8453	46.7901	9.8172	-24.6836	10.0251	-23.4215	10.026	-24.1264
29	E_{PM7}, E^{HOMO}_{PM7}	0.5631	0.1312	0.6603	0.034	0.6942	-0.0009	0.3806	0.455	0.2226	20.4342	5	0.8692	0.8649	0.8954	0.8195	0.7459	0.9191	0.7401	0.1159	0.2809	0.3284	0.1811	3.0425	4.3477	0.6938	70.4412	38.3669	10.131	-24.1757	10.0779	-23.1059	10.3135	-24.3566
30	E_{CORR}, d_{CORR}	0.5608	0.1378	0.6651	0.0335	0.6986	0.2214	0.3779	0.4562	0.1919	20.8616	5	0.9028	0.8996	0.9223	0.8226	0.741	0.9522	0.876	0.022	0.2966	0.3546	0.1549	2.999	4.3702	0.5156	70.2783	43.7659	10.1711	-23.5298	9.7552	-23.7591	10.2287	-23.19
31	χ_{CORR}	0.5109	0.1097	0.6006	0.02	0.6206	0.7878	0.424	0.4814	0.4694	31.0798	0	0.4184	0.3995	0.535	0.7659	0.7039	0.5642	0.2004	0.3678	0.3399	0.3825	0.3732	3.7751	4.8669	3.0845	62.4223	38.4522	5.0577	-16.1734	5.1039	-16.3491	4.8788	-16.7541
32	E^{HOMO}_{CORR}	0.4865	0.0955	0.5601	0.022	0.5821	0.7629	0.445	0.4933	0.3124	26.4625	3	0.7424	0.734	0.7941	0.7358	0.6774	0.8199	0.5024	0.2536	0.3579	0.3972	0.2525	4.1586	5.1092	1.3662	58.764	31.7934	4.8489	-16.695	5.1595	-16.0648	4.7675	-16.6692
33	E^{HOMO}_{HF}	0.4582	0.115	0.5508	0.0225	0.5733	0.7571	0.4497	0.5067	0.5337	25.5229	0	0.248	0.2236	0.3988	0.7287	0.6626	0.4753	0.1292	0.2103	0.3546	0.398	0.4479	4.2463	5.3911	3.988	57.9872	28.5849	5.1124	-16.3125	4.8307	-16.5921	4.8903	-16.3688
34	ω_{DFT}	0.4566	0.1301	0.5649	0.0218	0.5867	0.7659	0.4425	0.5074	0.4506	26.9688	0	0.4641	0.4467	0.5716	0.7395	0.6655	0.5977	0.2248	0.3803	0.3719	0.4201	0.3564	4.1128	5.4071	2.842	58.7682	30.649	5.0467	-16.5954	5.5483	-15.6434	5.0476	-16.3903
35	ω_{CORR}	0.4548	0.1107	0.5426	0.0229	0.5655	0.752	0.4537	0.5083	0.4703	24.7281	0	0.4162	0.3973	0.5333	0.7225	0.6572	0.52	0.151	0.4225	0.3833	0.4284	0.3675	4.3235	5.4251	3.0959	56.646	26.044	5.0023	-16.5385	5.2657	-15.9231	4.8531	-16.6093
36	E_{HF}, E^{HOMO}_{HF}	0.4443	0.1793	0.5818	0.0418	0.6236	0.3155	0.4223	0.5131	0.4387	14.9119	0	0.4919	0.4754	0.5938	0.7682	0.6676	0.6488	0.3017	0.3309	0.3326	0.4001	0.3599	3.7452	5.5296	2.6945	63.8905	29.9942	10.1905	-23.0472	9.5371	-23.7784	9.429	-23.9898
37	χ_{PM7}	0.4384	0.1333	0.5492	0.0225	0.5717	0.7561	0.4505	0.5158	0.4849	25.3655	0	0.3793	0.3592	0.5038	0.7275	0.6537	0.502	0.1184	0.4333	0.3624	0.409	0.4089	4.2614	5.5878	3.2917	57.8493	24.682	4.9204	-16.3242	4.7489	-16.9701	4.8869	-16.4149
38	ω_{HF}	0.4336	0.1286	0.5392	0.023	0.5622	0.7498	0.4554	0.5181	0.5039	24.401	0	0.3296	0.3079	0.4641	0.7198	0.6453	0.4876	0.1428	0.3435	0.3769	0.4241	0.4004	4.3561	5.6361	3.5551	56.5259	22.2145	4.861	-16.6448	5.1463	-16.1127	4.8376	-16.5283
39	E^{LUMO}_{DFT}	0.4296	0.1356	0.5424	0.0229	0.5652	0.7518	0.4539	0.5199	0.4592	24.7025	0	0.4433	0.4252	0.5549	0.7222	0.6453	0.575	0.1976	0.3938	0.3817	0.4313	0.3676	4.326	5.6757	2.9524	56.6175	28.4869	4.9427	-16.664	5.0602	-16.2474	5.2181	-16.1371
40	χ_{HF}	0.4248	0.1327	0.5342	0.0233	0.5575	0.7466	0.4579	0.5221	0.512	23.9354	0	0.3081	0.2856	0.4468	0.7159	0.6412	0.4774	0.1374	0.3262	0.379	0.4272	0.4163	4.4033	5.724	3.6696	56.176	26.2639	4.5735	-16.98	5.085	-16.3269	4.9277	-16.5076
41	E_{DFT}, ω_{DFT}	0.414	0.1961	0.5668	0.0433	0.6101	0.2462	0.4298	0.5269	0.3857	14.0827	0	0.6072	0.5945	0.686	0.7578	0.6473	0.709	0.324	0.3712	0.3687	0.4433	0.293	3.8797	5.8305	2.0829	62.2718	29.7768	10.1666	-22.9685	9.825	-23.5332	9.5085	-24.2914
42	E_{HF}, ω_{HF}	0.4038	0.191	0.5497	0.045	0.5947	0.2644	0.4382	0.5315	0.4293	13.2069	0	0.5135	0.4978	0.6111	0.7459	0.6369	0.6328	0.2469	0.3958	0.3727	0.4456	0.3395	4.0327	5.9329	2.5799	60.6394	27.6052	9.7997	-23.6756	10.2384	-23.2381	10.1731	-22.921
43	E_{HF}, χ_{HF}	0.3889	0.2007	0.544	0.0456	0.5896	0.2614	0.441	0.5381	0.4361	12.9309	0	0.498	0.4817	0.5987	0.7418	0.6298	0.6235	0.2399	0.393	0.3718	0.4461	0.3476	4.0835	6.0806	2.6622	60.9441	22.7631	9.7871	-23.6136	10.1463	-23.3525	9.8945	-23.6388
44	E_{DFT}, E^{LUMO}_{DFT}	0.3859	0.204	0.5443	0.0456	0.5899	0.2411	0.4408	0.5394	0.3926	12.9458	0	0.5931	0.5799	0.6747	0.7421	0.6271	0.6933	0.2953	0.3948	0.3795	0.4562	0.3021	4.0807	6.1109	2.1579	60.739	24.4996	9.6374	-23.9371	10.2254	-23.1175	10.4721	-22.845
45	χ_{DFT}	0.3462	0.1589	0.4791	0.026	0.5051	0.7107	0.4843	0.5566	0.5433	19.3918	0	0.2208	0.1956	0.3771	0.6712	0.5841	0.4078	0.0841	0.2568	0.3957	0.4478	0.4373	4.9245	6.5059	4.1322	52.1375	2.6166	5.0683	-16.4061	5.1122	-16.0371	5.1814	-16.5169
46	E_{DFT}, χ_{DFT}	0.3356	0.2231	0.5097	0.049	0.5588	0.2713	0.4572	0.5611	0.4431	11.3969	0	0.4817	0.4649	0.5857	0.7169	0.5943	0.6089	0.2212	0.4032	0.3833	0.4628	0.3468	4.3906	6.6106	2.7485	57.8881	21.6488	9.8188	-23.7848	9.9369	-23.4602	10.0203	-23.315
47	E^{LUMO}_{HF}	0.3325	0.152	0.4573	0.0271	0.4845	0.696	0.4942	0.5624	0.5171	17.8542	0	0.2941	0.2712	0.4357	0.6527	0.5645	0.4254	0.0756	0.3889	0.4179	0.4707	0.4107	5.1299	6.6424	3.7437	49.0534	11.6723	4.9184	-16.5438	4.6911	-16.7154	4.6255	-16.7668
48	E_{HF}, E^{LUMO}_{HF}	0.2824	0.2279	0.456	0.0544	0.5104	0.2089	0.4817	0.5831	0.4527	9.3808	0	0.459	0.4415	0.5675	0.6758	0.5443	0.5643	0.1433	0.4879	0.4146	0.4959	0.3642	4.8722	7.1401	2.8689	52.9025	11.8464	9.5152	-24.2724	9.7231	-23.5918	9.7275	-23.7635
49	η_{PM7}	0.2538	0.1215	0.3425	0.0329	0.3754	0.6127	0.544	0.5946	0.4665	11.4183	0	0.4256	0.4069	0.5408	0.5459	0.4538	0.6728	0.3382	0.188	0.4768	0.522	0.391	6.2153	7.4245	3.0464	36.8595	0.2542	4.8763	-16.843	4.8083	-16.5657	4.9066	-16.8888
50	E_{DFT}, E^{HOMO}_{DFT}	0.2455	0.2407	0.4291	0.0571	0.4862	0.3428	0.4934	0.5979	0.4987	8.5169	0	0.3434	0.3221	0.4751	0.6543	0.521	0.5075	0.1525	0.3588	0.4012	0.4834	0.3961	5.1125	7.5078	3.4822	51.7601	-0.8423	9.9514	-23.7962	9.8184	-23.4156	10.3133	-23.0306
51	E^{HOMO}_{DFT}	0.2171	0.1753	0.3604	0.032	0.3924	0.6264	0.5366	0.6091	0.6255	12.2686	0	-0.0329	-0.0664	0.1743	0.5636	0.4676	0.2228	0.0116	0.0775	0.4237	0.477	0.5129	6.0463	7.7902	5.4777	40.5661	1.4399	5.206	-16.5675	5.0927	-16.2259	5.1671	-16.5358
52	E^{HOMO}_{PM7}	0.1778	0.1667	0.31	0.0345	0.3445	0.587	0.5573	0.6242	0.6554	9.9867	0	-0.1341	-0.1709	0.0933	0.5125	0.4182	0.0945	-0.0002	0.0176	0.436	0.487	0.5512	6.5223	8.181	6.0145	35.5314	3.7358	5.0613	-16.4534	5.1852	-15.9486	5.3973	-16.1265
53	E^{LUMO}_{CORR}	0.0875	0.1891	0.2386	0.0381	0.2767	0.526	0.5854	0.6575	0.6374	7.2675	0	-0.0725	-0.1073	0.1426	0.4334	0.3171	0.0628	-0.0034	0.0214	0.4958	0.5553	0.5272	7.1974	9.0795	5.688	29.5069	-13.8721	4.8848	-16.6836	4.9577	-16.3539	5.1455	-16.3944
54	η_{DFT}	-0.0509	0.2185	0.1238	0.0438	0.1676	0.4094	0.628	0.7057	0.5279	3.8248	0	0.2644	0.2405	0.4119	0.287	0.1244	0.4308	0.1013	0.2893	0.539	0.6031	0.4593	8.283	10.4568	3.9013	17.7501	-22.7513	4.6182	-17.1874	5.016	-16.2253	4.7934	-17.0159
55	d_{CORR}	-0.089	0.1851	0.0486	0.0476	0.0962	0.3101	0.6544	0.7183	0.6227	2.0217	0	-0.0235	-0.0567	0.1818	0.1755	0.0245	0.0189	-0.001	0.0043	0.5352	0.5916	0.524	8.9935	10.8356	5.4277	11.0308	-25.5666	4.8955	-16.8615	5.0535	-16.3718	5.0979	-16.4012
56	η_{CORR}	-0.1314	0.1538	-0.0291	0.0515	0.0223	0.1494	0.6806	0.7322	0.5628	0.434	0	0.1638	0.1367	0.3315	0.0437	-0.0934	0.17	-1.1365	2.6792	0.5432	0.5881	0.4552	9.7283	11.2584	4.4346	3.198	-25.9225	5.4912	-16.7379	5.3167	-15.8746	5.0518	-17.4894
57	d_{PM7}	-0.1375	0.155	-0.0342	0.0517	0.0175	0.1322	0.6823	0.7342	0.6013	0.3382	0	0.0456	0.0146	0.237	0.0344	-0.0998	0.0651	-1.2591	2.7811	0.5496	0.5968	0.4855	9.7765	11.3186	5.0617	3.1018	-33.5333	4.909	-17.5761	5.0147	-16.2175	4.7254	-17.8423
58	d_{DFT}	-0.1381	0.1497	-0.0404	0.052	0.0116	0.1078	0.6843	0.7343	0.6046	0.2235	0	0.0349	0.0036	0.2284	0.023	-0.1104	0.0487	-1.3823	2.9983	0.5479	0.5924	0.4859	9.8348	11.3244	5.1182	2.1814	-32.9463	4.7381	-17.8953	5.0958	-16.3012	5.0466	-17.5519
59	d_{HF}	-0.1429	0.1467	-0.0487	0.0524	0.0037	0.0611	0.6871	0.7359	0.6102	0.0711	0	0.0171	-0.0148	0.2142	0.0074	-0.1299	0.0246	-1.8471	3.8787	0.5443	0.5856	0.489	9.9133	11.3726	5.2126	1.301	-28.8858	5.214	-17.8328	5.1534	-16.1149	4.7025	-17.8497
60	E_{DFT}	-0.1542	0.2515	0.0497	0.0475	0.0973	0.3119	0.654	0.7395	0.509	2.0469	0	0.3162	0.294	0.4533	0.1773	-0.0202	0.3624	-0.2902	1.1375	0.5236	0.5903	0.406	8.9827	11.4851	3.6265	12.5404	-34.3594	5.4503	-15.9671	5.0868	-16.3522	5.1879	-16.3037
61	E_{HF}	-0.1546	0.2515	0.0494	0.0475	0.0969	0.3113	0.6541	0.7396	0.5092	2.0395	0	0.3155	0.2933	0.4527	0.1767	-0.0208	0.3616	-0.2918	1.1398	0.5237	0.5905	0.4063	8.9859	11.4887	3.6303	12.4505	-35.5692	5.2083	-16.2167	5.1212	-16.1706	5.048	-16.4961
62	E_{DFT}, η_{DFT}	-0.204	0.3879	0.0932	0.0907	0.1839	-0.0839	0.6218	0.7553	0.4893	2.0281	0	0.3679	0.3474	0.4946	0.3107	0.0472	0.5038	0.1403	0.3855	0.5285	0.6365	0.43	8.1206	11.9808	3.3524	22.5127	-36.7177	9.9432	-24.03	10.3333	-22.7809	10.3626	-23.0892
63	E_{DFT}, d_{DFT}	-0.2118	0.3112	-0.0006	0.1001	0.0994	0.0127	0.6532	0.7578	0.5083	0.9935	0	0.3179	0.2957	0.4546	0.1809	-0.0483	0.3689	-0.2761	1.1144	0.525	0.6155	0.4054	8.9612	12.0581	3.6177	13.3262	-40.3568	9.77	-25.0499	9.7752	-23.6461	10.2105	-25.038
64	E_{HF}, d_{HF}	-0.2214	0.3183	-0.0034	0.1003	0.0969	0.0085	0.6541	0.7607	0.5092	0.9661	0	0.3154	0.2932	0.4527	0.1767	-0.0559	0.3619	-0.2908	1.138	0.5239	0.6148	0.4061	8.9858	12.1532	3.6304	13.3152	-42.2351	10.061	-24.6574	10.0288	-22.9542	10.3051	-24.3268
65	E_{HF}, η_{HF}	-0.2423	0.3435	0.0013	0.0999	0.1012	-0.0215	0.6526	0.7672	0.5176	1.013	0	0.2928	0.2699	0.4346	0.1838	-0.0504	0.3412	-0.2572	1.0441	0.5283	0.6302	0.4163	8.9438	12.3615	3.7503	13.2237	-36.6344	9.722	-28.688	10.0491	-23.2641	9.9233	-26.8582
66	η_{HF}	-0.2466	0.2677	-0.0304	0.0515	0.0211	0.1453	0.681	0.7686	0.6202	0.41	0	-0.0153	-0.0483	0.1883	0.0414	-0.1103	0.0016	-0.0001	0.0003	0.5506	0.6208	0.5042	9.7403	12.4043	5.3848	3.9906	-40.4919	5.24	-18.7977	4.9954	-16.232	5.052	-19.1554

Models are arranged according to Q^2_{LOO} values.
Parameters are obtained through QSARINS software. Ref. [43] (Chirico, N.; Papa, E.; Kovarich, S.; Cassani, S.; Gramatica, P. QSARINS, Software for QSAR MLR model development and validation. 2012, QSAR Res. Unit in Environ. Chem. and Ecotox., University of Insubria, Varese, Italy (http://www.qsar.it).

R^2_{adj} adjusted R^2
N. Ext.OK Number of external validation parameters meeting threshold values
F "F-test" statistic value

Table S6. Value of internal validation parameters of two- and one-descriptor QSAR models, for inhibitory growth concentration (Log IGC_{50}^{-1}) of alkyl- and halogen-substituted nitrobenzenes, developed using PM7, HF, DFT and electron-correlation contribution (CORR) based descriptors, by employing complete data set comprising of 42 compounds in the training set, with no prediction set.

Model	Variables	Q^2_{LOO}	R^2-Q^2_{LOO}	R^2_{adj}	R^2-R^2_{adj}	R^2	ΔK	$RMSE_{TR}$	$RMSE_{CV}$	F	CCC_{TR}	CCC_{CV}	MAE_{TR}	MAE_{CV}	RSS_{TR}	$PRESS_{CV}$	R^2_{LMO}	Q^2_{LMO}	R^2_{Yscr}	Q^2_{Yscr}	R^2_{Xsand}	Q^2_{Xsand}	R^2_{Ysand}	Q^2_{Ysand}
1	E_{CORR}, ω_{PM7}	0.7744	0.0317	0.7961	0.0099	0.8061	0.1082	0.3105	0.335	81.0581	0.8926	0.8758	0.2224	0.2416	4.0499	4.7126	80.8906	75.1785	4.9306	-10.5181	4.797	-10.5496	4.8924	-10.6862
2	E_{CORR}, E^{LUMO}_{PM7}	0.7705	0.0361	0.7966	0.0099	0.8066	0.0903	0.3101	0.3378	81.3019	0.8929	0.874	0.2259	0.2466	4.0401	4.7931	80.8836	75.3285	4.8272	-10.7709	4.6753	-10.6588	4.6076	-11.0062
3	E_{PM7}, η_{PM7}	0.7544	0.0438	0.7879	0.0103	0.7983	0.2527	0.3167	0.3494	77.1563	0.8878	0.8654	0.2273	0.2483	4.2134	5.1287	80.2466	73.9012	4.7441	-10.8613	4.9644	-10.3776	4.914	-10.61
4	E_{CORR}, ω_{HF}	0.7351	0.039	0.7626	0.0116	0.7742	0.2071	0.3351	0.3629	66.8409	0.8727	0.851	0.2525	0.2742	4.7168	5.5321	77.8056	71.5374	4.9761	-10.3993	4.8008	-10.4391	4.804	-10.6845
5	E_{CORR}, χ_{HF}	0.723	0.0404	0.7513	0.0121	0.7634	0.1918	0.343	0.3711	62.9175	0.8658	0.8436	0.25	0.2715	4.9413	5.7855	76.6453	70.6075	5.0313	-10.379	5.0244	-10.2235	4.9907	-10.4761
6	E_{CORR}, E_{HF}	0.7158	0.0396	0.7429	0.0125	0.7554	-0.089	0.3487	0.3759	60.2246	0.8607	0.839	0.2437	0.2645	5.1082	5.936	75.6682	71.0968	5.1155	-10.7469	4.7688	-10.5806	4.9083	-11.165
7	E_{CORR}, E^{HOMO}_{HF}	0.7141	0.0371	0.7385	0.0128	0.7512	0.1815	0.3517	0.3771	58.8807	0.8579	0.8375	0.2546	0.2755	5.1958	5.9713	75.2042	70.0685	4.7836	-10.7455	5.1374	-10.2211	4.7337	-10.8434
8	E_{CORR}, E_{PM7}	0.7113	0.0517	0.7509	0.0122	0.763	0.0575	0.3433	0.3789	62.7936	0.8656	0.8378	0.2388	0.2612	4.9487	6.0289	76.8877	70.5231	5.008	-10.6156	4.9188	-10.3873	4.9539	-10.7269
9	E_{CORR}, χ_{CORR}	0.7108	0.0433	0.7414	0.0126	0.7541	0.1373	0.3497	0.3792	59.7865	0.8598	0.8359	0.2614	0.2842	5.1364	6.0403	75.0895	71.2462	4.8695	-10.539	4.7521	-10.5539	5.0095	-10.4154
10	E_{PM7}, E^{LUMO}_{PM7}	0.7066	0.058	0.7526	0.0121	0.7646	0.0211	0.3421	0.3819	63.3481	0.8666	0.8357	0.2592	0.2841	4.9156	6.1269	76.7431	70.4088	4.5461	-11.0478	4.7725	-10.492	4.9606	-10.5456
11	E_{CORR}, χ_{PM7}	0.7058	0.0375	0.7301	0.0132	0.7433	0.162	0.3573	0.3825	56.4536	0.8527	0.8319	0.2457	0.2656	5.3618	6.1446	74.3857	69.4339	4.9096	-10.4982	4.9487	-10.3973	4.8565	-10.6452
12	E_{CORR}, E^{LUMO}_{HF}	0.7053	0.0453	0.7378	0.0128	0.7506	0.2128	0.3522	0.3828	58.6771	0.8575	0.8322	0.2651	0.2881	5.2093	6.1557	75.2782	69.2635	5.1637	-10.2968	5.0744	-10.2183	4.907	-10.481
13	$E_{CORR}, E^{HOMO}_{CORR}$	0.6903	0.0438	0.7205	0.0136	0.7341	0.0743	0.3636	0.3924	53.8377	0.8467	0.8226	0.2679	0.2915	5.5531	6.468	73.6821	67.9733	4.8604	-10.7792	4.6964	-10.569	5.1614	-10.3026
14	E_{PM7}, ω_{PM7}	0.6799	0.0616	0.7282	0.0133	0.7414	0.0042	0.3586	0.399	55.9101	0.8515	0.8181	0.2685	0.2937	5.4005	6.6859	74.8658	65.7077	5.0432	-10.2692	4.7128	-10.6817	4.8761	-10.6236
15	E_{CORR}, ω_{CORR}	0.6764	0.0535	0.716	0.0139	0.7298	0.1255	0.3665	0.4012	52.6801	0.8438	0.8152	0.2677	0.2923	5.6421	6.7588	73.2911	66.8612	4.7707	-10.7046	5.1248	-10.2023	4.5662	-11.0536
16	E^{LUMO}_{PM7}	0.6683	0.0392	0.7002	0.0073	0.7076	0.8412	0.3813	0.4061	96.7787	0.8287	0.8074	0.3066	0.3246	6.1076	6.9266	70.7448	64.5062	2.4854	-7.5902	2.4181	-7.6383	2.5817	-7.5532
17	E_{PM7}, d_{PM7}	0.6592	0.0658	0.7109	0.0141	0.725	0.3729	0.3698	0.4117	51.4094	0.8406	0.8068	0.2854	0.3138	5.7432	7.1184	73.0336	65.7637	5.0698	-10.7055	4.6236	-10.745	4.9218	-10.8443
18	$E_{CORR}, E^{LUMO}_{CORR}$	0.6463	0.0525	0.6834	0.0154	0.6988	0.2696	0.387	0.4194	45.2503	0.8227	0.7929	0.2896	0.3137	6.2895	7.386	70.3035	62.2353	4.7286	-10.8224	4.9335	-10.3731	4.9537	-10.5049
19	ω_{PM7}	0.6418	0.0391	0.6729	0.008	0.6809	0.8252	0.3983	0.422	85.3619	0.8102	0.788	0.3234	0.3411	6.6638	7.4812	68.3094	59.9734	2.3941	-7.6771	2.3373	-7.7268	2.5416	-7.539
20	E_{PM7}, E^{HOMO}_{PM7}	0.627	0.0528	0.6634	0.0164	0.6798	0.038	0.399	0.4307	41.3948	0.8094	0.778	0.2876	0.3098	6.6878	7.7899	68.033	61.433	4.7706	-10.6857	4.6815	-10.6924	5.0332	-10.4419
21	E_{PM7}	0.6174	0.0456	0.6546	0.0084	0.663	0.8143	0.4093	0.4362	78.7004	0.7974	0.7703	0.2936	0.3102	7.0378	7.9909	66.917	56.7013	2.5073	-7.6001	2.3767	-7.6851	2.4942	-7.6083
22	E_{CORR}	0.6162	0.0374	0.645	0.0087	0.6536	0.8085	0.415	0.4368	75.4884	0.7906	0.7683	0.2945	0.3097	7.2335	8.015	65.603	57.761	2.442	-7.7076	2.5775	-7.4849	2.4304	-7.7196
23	E_{CORR}, E^{HOMO}_{PM7}	0.616	0.0702	0.67	0.0161	0.6861	0.292	0.3951	0.437	42.6246	0.8138	0.7745	0.2765	0.3019	6.5554	8.0206	69.2483	60.9631	4.8771	-10.6406	4.6776	-10.6783	4.8851	-10.6273
24	E_{PM7}, χ_{PM7}	0.6096	0.0599	0.6526	0.0169	0.6696	-0.0053	0.4053	0.4406	39.5171	0.8021	0.7664	0.2969	0.3212	6.9005	8.1524	66.9847	59.8976	4.5279	-10.8516	4.8915	-10.4001	4.7991	-10.674
25	E_{CORR}, d_{PM7}	0.6014	0.0571	0.6409	0.0175	0.6585	0.196	0.4121	0.4452	37.5929	0.7941	0.7612	0.2885	0.3128	7.1331	8.3248	66.1483	58.9004	4.8178	-10.9374	4.8783	-10.4468	4.9477	-10.6969
26	E_{CORR}, d_{CORR}	0.6013	0.0591	0.6429	0.0174	0.6603	0.3951	0.411	0.4453	37.9072	0.7954	0.7598	0.2945	0.3201	7.0941	8.3275	66.4112	59.0569	4.8138	-10.7669	4.8332	-10.4968	5.0663	-10.4755
27	E_{CORR}, η_{CORR}	0.5977	0.056	0.6359	0.0178	0.6537	0.1428	0.415	0.4473	36.8084	0.7906	0.7579	0.2946	0.3178	7.2325	8.4021	65.8141	58.2321	4.8409	-10.4992	4.8285	-10.4896	4.8498	-10.6056
28	E_{CORR}, d_{HF}	0.5952	0.0596	0.6372	0.0177	0.6549	0.2121	0.4143	0.4486	37.0013	0.7914	0.7569	0.2921	0.3177	7.2078	8.4533	65.982	57.6286	4.8396	-10.8665	5.0017	-10.3701	4.6352	-11.1763
29	E_{CORR}, η_{PM7}	0.5885	0.096	0.6683	0.0162	0.6845	0.073	0.3961	0.4523	42.3093	0.8127	0.7568	0.2929	0.3265	6.5888	8.593	68.9562	60.422	5.0371	-11.4574	4.8114	-10.4759	4.7111	-12.1894
30	E_{CORR}, η_{HF}	0.5842	0.0719	0.6384	0.0176	0.6561	0.3561	0.4135	0.4547	37.2001	0.7923	0.7507	0.2931	0.3184	7.1825	8.6838	65.9035	57.5606	4.6812	-10.9349	4.7001	-10.6951	4.8484	-10.76
31	E^{HOMO}_{CORR}	0.5164	0.0496	0.5551	0.0109	0.566	0.7523	0.4646	0.4904	52.1574	0.7228	0.6947	0.3699	0.39	9.0648	10.1005	56.7275	49.5059	2.5213	-7.5938	2.6191	-7.3801	2.3583	-7.818
32	E_{HF}, E^{HOMO}_{HF}	0.492	0.079	0.549	0.022	0.571	0.3378	0.4619	0.5026	25.9566	0.7269	0.6828	0.3667	0.3996	8.9591	10.6095	57.5935	48.4276	4.8597	-11.0412	5.1868	-10.0522	4.6143	-11.4565
33	E_{DFT}, ω_{DFT}	0.4754	0.0939	0.5472	0.0221	0.5693	0.299	0.4628	0.5107	25.7767	0.7256	0.6753	0.3649	0.4005	8.9947	10.9559	58.1132	46.6929	4.8363	-11.1325	4.9594	-10.402	4.7731	-10.9417
34	E_{HF}, χ_{HF}	0.4673	0.091	0.5357	0.0226	0.5583	0.2949	0.4686	0.5147	24.6508	0.7166	0.6676	0.389	0.4253	9.2241	11.1251	56.6839	46.1924	5.1298	-10.6276	4.9585	-10.3638	5.1635	-10.7186
35	E_{HF}, ω_{HF}	0.4643	0.0911	0.5326	0.0228	0.5554	0.1859	0.4702	0.5161	24.3593	0.7142	0.6648	0.387	0.4231	9.2854	11.1884	56.942	43.9514	4.8651	-10.8622	4.8916	-10.4087	4.9937	-10.6425
36	E_{DFT}, E^{LUMO}_{DFT}	0.4613	0.0965	0.5351	0.0227	0.5578	0.2968	0.4689	0.5175	24.5967	0.7161	0.6646	0.3736	0.4102	9.2354	11.2499	56.1793	47.7036	4.9514	-10.9542	5.0913	-10.2008	4.9208	-10.9293
37	χ_{CORR}	0.4599	0.0513	0.499	0.0122	0.5112	0.715	0.493	0.5182	41.8414	0.6766	0.6456	0.4	0.4212	10.2074	11.2797	51.1572	42.3698	2.3267	-7.9039	2.4104	-7.705	2.2787	-7.8527
38	ω_{DFT}	0.4222	0.0553	0.4645	0.0131	0.4775	0.691	0.5097	0.536	36.5576	0.6464	0.6114	0.3991	0.4199	10.9118	12.0668	47.9109	38.7978	2.3799	-7.7022	2.4634	-7.6094	2.3505	-7.7792
39	E_{DFT}, χ_{DFT}	0.4195	0.1067	0.5019	0.0243	0.5262	0.2768	0.4854	0.5373	21.6563	0.6896	0.6331	0.3959	0.4348	9.8952	12.1229	53.4773	43.3862	4.9393	-10.9975	5.047	-10.3015	4.8774	-10.9877
40	E^{LUMO}_{DFT}	0.4058	0.0586	0.4509	0.0134	0.4643	0.6814	0.5161	0.5436	34.6744	0.6342	0.5974	0.4096	0.4315	11.187	12.4102	46.5454	37.2918	2.2479	-7.92	2.3309	-7.7405	2.3531	-7.7202
41	ω_{CORR}	0.3974	0.0676	0.4516	0.0134	0.465	0.6819	0.5158	0.5474	34.7632	0.6348	0.5976	0.4258	0.4508	11.1737	12.5846	47.1878	35.5851	2.5936	-7.6065	2.3994	-7.6065	2.4484	-7.8125
42	ω_{HF}	0.3817	0.0591	0.4269	0.014	0.4409	0.664	0.5273	0.5545	31.5398	0.612	0.5737	0.4225	0.4443	11.6772	12.9121	44.3913	35.0495	2.4128	-7.7214	2.4596	-7.5418	2.4211	-7.679
43	χ_{HF}	0.3788	0.0617	0.4266	0.014	0.4406	0.6637	0.5274	0.5558	31.4998	0.6116	0.5726	0.432	0.4548	11.6837	12.9728	44.2109	34.0939	2.7336	-7.3446	2.5539	-7.5277	2.4273	-7.6066
44	χ_{PM7}	0.3778	0.0613	0.4251	0.014	0.4391	0.6626	0.5281	0.5562	31.3126	0.6102	0.5704	0.4274	0.4498	11.7144	12.9937	43.7193	35.4202	2.5219	-7.5674	2.3316	-7.7621	2.4298	-7.617
45	E^{HOMO}_{HF}	0.3656	0.0611	0.4124	0.0143	0.4267	0.6532	0.5339	0.5616	29.773	0.5982	0.5579	0.4341	0.4565	11.9729	13.2489	43.1731	31.3544	2.5074	-7.5697	2.3505	-7.7347	2.4862	-7.5978
46	E_{HF}, E^{LUMO}_{HF}	0.3652	0.1093	0.4476	0.0269	0.4745	0.0749	0.5112	0.5618	17.6104	0.6436	0.5844	0.4182	0.458	10.974	13.2568	48.1899	38.5582	4.9928	-10.8486	4.7677	-10.5956	4.9022	-10.8558
47	η_{PM7}	0.3345	0.0703	0.3899	0.0149	0.4048	0.6362	0.544	0.5753	27.2058	0.5763	0.5389	0.4682	0.4943	12.4302	13.8994	40.7587	30.8502	2.2427	-8.1394	2.4951	-7.5651	2.3329	-7.9576
48	E_{DFT}, E^{HOMO}_{DFT}	0.3251	0.121	0.4178	0.0284	0.4462	0.237	0.5248	0.5793	15.7096	0.617	0.5519	0.4223	0.4635	11.5664	14.0944	45.3626	34.2373	4.902	-11.1184	4.8179	-10.4744	5.049	-10.8955
49	E^{LUMO}_{HF}	0.3059	0.0657	0.3559	0.0157	0.3716	0.6096	0.559	0.5875	23.6578	0.5419	0.4983	0.4489	0.4723	13.123	14.4957	37.7616	26.3813	2.4365	-7.7334	2.5291	-7.4714	2.3261	-7.8174
50	χ_{DFT}	0.3046	0.0766	0.3657	0.0155	0.3812	0.6174	0.5547	0.588	24.6407	0.552	0.5043	0.4512	0.4765	12.9235	14.5231	38.4112	27.6289	2.4807	-7.6549	2.4195	-7.626	2.3185	-7.8684
51	E^{HOMO}_{DFT}	0.1566	0.093	0.2308	0.0188	0.2496	0.4996	0.6109	0.6476	13.3026	0.3994	0.3393	0.5002	0.5282	15.6725	17.614	25.5169	13.0542	2.4378	-7.7288	2.3572	-7.6372	2.4547	-7.7391
52	E^{LUMO}_{CORR}	0.0783	0.0782	0.1355	0.0211	0.1565	0.3957	0.6476	0.677	7.4242	0.2707	0.207	0.5325	0.5585	17.6151	19.2488	16.3296	4.2526	2.5	-7.6747	2.2934	-7.7316	2.4156	-7.7206
53	η_{CORR}	0.0139	0.0817	0.073	0.0226	0.0956	0.3092	0.6706	0.7002	4.2288	0.1745	0.1034	0.545	0.5715	18.8878	20.5933	9.8602	0.424	2.4081	-7.8245	2.292	-7.8032	2.3167	-7.9115
54	η_{DFT}	0.0125	0.0906	0.0807	0.0224	0.1031	0.3211	0.6678	0.7007	4.5986	0.1869	0.1061	0.55	0.5774	18.7312	20.6228	11.2936	-0.5304	2.4469	-7.7624	2.399	-7.6838	2.4887	-7.6677
55	E_{DFT}, d_{DFT}	0.0124	0.1703	0.1408	0.0419	0.1827	0.034	0.6375	0.7008	4.359	0.309	0.2117	0.5216	0.5709	17.069	20.6255	19.7482	5.1434	4.924	-11.3044	4.9917	-10.3495	5.0773	-10.9585
56	E_{DFT}	0.0114	0.1389	0.1291	0.0212	0.1504	0.3878	0.65	0.7011	7.0803	0.2615	0.1927	0.5272	0.5635	17.7438	20.6457	16.1903	2.0446	2.473	-8.3286	2.4571	-7.6268	2.2252	-8.5521
57	E_{HF}	0.0112	0.1389	0.1288	0.0212	0.15	0.3873	0.6501	0.7012	7.0606	0.2609	0.1922	0.5274	0.5637	17.7512	20.6513	16.1235	1.4825	2.4397	-8.038	2.6407	-7.4039	2.424	-8.2026
58	E^{HOMO}_{PM7}	0.0032	0.1006	0.0815	0.0224	0.1039	0.3223	0.6675	0.704	4.6369	0.1882	0.1094	0.5397	0.5684	18.7151	20.817	11.0865	-0.9266	2.3284	-7.6987	2.5079	-7.5404	2.507	-7.6171
59	E_{HF}, d_{HF}	-0.0057	0.1758	0.1275	0.0426	0.1701	0.0278	0.6424	0.7072	3.9961	0.2907	0.1902	0.5253	0.5749	17.3326	21.0036	18.9006	2.1939	4.8166	-11.3124	4.894	-10.4351	5.1317	-10.8761
60	d_{PM7}	-0.0071	0.1037	0.074	0.0226	0.0966	0.3107	0.6703	0.7077	4.2749	0.1761	0.0946	0.5616	0.5933	18.8681	21.0337	10.7779	-4.5839	2.5504	-7.6202	2.4196	-7.6459	2.4229	-7.9501
61	d_{DFT}	-0.0227	0.103	0.0573	0.023	0.0803	0.2833	0.6763	0.7131	3.4908	0.1486	0.065	0.5662	0.5976	19.2083	21.3586	8.7771	-4.898	2.3383	-8.1072	2.5744	-7.4619	2.2936	-8.0043
62	E_{DFT}, η_{DFT}	-0.0256	0.2082	0.1407	0.0419	0.1826	-0.0331	0.6375	0.7141	4.3556	0.3088	0.1875	0.5307	0.5854	17.0714	21.4194	20.9207	2.1415	4.6847	-11.3257	4.702	-10.703	5.001	-10.8807
63	d_{HF}	-0.0432	0.1024	0.0357	0.0235	0.0592	0.2434	0.684	0.7202	2.5181	0.1118	0.0236	0.5717	0.6023	19.6477	21.7864	6.8992	-6.5665	2.396	-7.8574	2.4404	-7.598	2.4358	-7.8042
64	E_{HF}, η_{HF}	-0.0521	0.2053	0.1098	0.0434	0.1533	0.0438	0.6489	0.7233	3.5296	0.2658	0.1484	0.5224	0.5747	17.6837	21.9718	18.1074	-0.8243	5.0533	-10.9242	4.7277	-10.5574	4.6454	-11.265
65	d_{CORR}	-0.1074	0.1159	-0.0164	0.0248	0.0084	0.0918	0.7022	0.7421	0.3397	0.0167	-0.0911	0.5694	0.5981	20.7087	23.1285	2.2605	-10.102	2.4852	-7.7633	2.43	-7.6267	2.294	-7.8678
66	η_{HF}	-0.1125	0.1126	-0.0249	0.025	0.0001	0.0096	0.7051	0.7438	0.0037	0.0002	-0.1052	0.5693	0.5996	20.8827	23.2351	1.2293	-12.2215	2.5293	-7.6944	2.5237	-7.5738	2.4616	-7.8679

Models are arranged according to Q^2_{LOO} values.
Parameters are obtained through QSARINS software. Ref. [43] (Chirico, N.; Papa, E.; Kovarich, S.; Cassani, S.; Gramatica, P. QSARINS, Software for QSAR MLR model development and validation. 2012, QSAR Res. Unit in Environ. Chem. and Ecotox., University of Insubria, Varese, Italy (http://www.qsar.it).

R^2_{adj} adjusted R^2
N. Ext.OK Number of external validation parameters meeting threshold values
F "F-test" statistic value

Table S7. Value of internal validation parameters of two- and one-descriptor QSAR models, for inhibitory growth concentration (Log IGC_{50}^{-1}) of alkyl- and halogen-substituted nitrobenzenes, developed using PM7, HF, DFT and electron-correlation contribution (CORR) based descriptors, by employing full data set comprising of 35 compounds in the training set excluding outliers as listed in Table S1, with no prediction set.

Model	Variables	Q^2_{LOO}	R^2-Q^2_{LOO}	R^2_{adj}	R^2-R^2_{adj}	R^2	ΔK	$RMSE_{TR}$	$RMSE_{CV}$	F	CCC_{TR}	CCC_{CV}	MAE_{TR}	MAE_{CV}	RSS_{TR}	$PRESS_{CV}$	R^2_{LMO}	Q^2_{LMO}	Q^2_{Yer}	Q^2_{Yer}	R^2_{Yrand}	Q^2_{Yrand}	R^2_{Yrand}	Q^2_{Yrand}
1	E_{CORR}, ω_{PM7}	0.8286	0.0297	0.8494	0.0089	0.8583	0.1108	0.248	0.2727	96.9148	0.9237	0.908	0.1832	0.202	2.152	2.6036	85.6795	81.6074	5.7223	-13.1896	5.6215	-13.135	5.9835	-13.053
2	E_{PM7}, η_{PM7}	0.8179	0.0434	0.8526	0.0087	0.8613	0.2583	0.2453	0.2811	99.3484	0.9255	0.9036	0.1863	0.2081	2.1066	2.7654	86.4772	80.7938	5.9378	-13.1119	5.7862	-12.7705	6.032	-12.9777
3	E_{CORR}, χ_{PM7}	0.8164	0.0305	0.8373	0.0096	0.8468	0.18	0.2578	0.2823	88.465	0.9171	0.9006	0.1963	0.2157	2.3261	2.7891	84.7297	79.681	5.6125	-13.4215	5.9665	-12.6642	6.0053	-12.775
4	E_{CORR}, ω_{HF}	0.8149	0.0279	0.833	0.0098	0.8428	0.1861	0.2612	0.2834	85.7745	0.9147	0.8993	0.1948	0.2128	2.3876	2.8116	84.1642	79.0757	6.0155	-12.8736	5.8637	-12.8258	6.1713	-12.7154
5	E_{CORR}, E^{LUMO}_{PM7}	0.814	0.0335	0.838	0.0095	0.8475	0.087	0.2572	0.2841	88.9369	0.9175	0.8999	0.1875	0.207	2.3156	2.8245	84.8945	79.8927	6.2103	-12.5515	5.8932	-12.713	5.957	-12.8841
6	E_{CORR}, E_{PM7}	0.8112	0.0462	0.8485	0.0089	0.8574	0.0707	0.2488	0.2863	96.1964	0.9232	0.8989	0.1846	0.2065	2.1658	2.8681	86.1778	79.7023	5.9639	-12.8959	5.7564	-12.906	5.6874	-12.984
7	E_{CORR}, E_{HF}	0.8063	0.0412	0.8379	0.0095	0.8475	-0.0449	0.2573	0.2899	88.8918	0.9174	0.8951	0.1961	0.2184	2.3166	2.9422	85.2673	79.4879	5.7321	-13.3025	6.0085	-12.7296	5.828	-13.1233
8	E_{CORR}, χ_{HF}	0.8006	0.0335	0.8238	0.0104	0.8341	0.1779	0.2683	0.2941	80.4652	0.9096	0.8914	0.1978	0.2174	2.519	3.028	83.6631	77.4428	5.846	-12.7349	5.6552	-13.1089	5.8157	-13.0613
9	E_{CORR}, E^{HOMO}_{PM7}	0.7984	0.0326	0.8204	0.0106	0.831	0.3301	0.2708	0.2958	78.6728	0.9077	0.8897	0.2125	0.2331	2.5667	3.0625	83.3655	77.1697	5.8143	-13.0602	5.6514	-13.1327	5.682	-13.2361
10	E_{CORR}, E^{HOMO}_{HF}	0.7966	0.0351	0.8212	0.0105	0.8318	0.1782	0.2702	0.2971	79.1007	0.9082	0.8889	0.2116	0.2333	2.5551	3.0887	83.085	77.1534	5.9825	-12.6376	6.4488	-12.123	5.7446	-13.0577
11	E_{CORR}, E^{LUMO}_{HF}	0.7922	0.0324	0.8136	0.011	0.8246	0.188	0.2759	0.3003	75.2105	0.9039	0.8861	0.2046	0.224	2.6641	3.1559	82.4311	75.9355	5.7855	-13.1565	5.8769	-12.7784	5.9325	-12.9026
12	E_{CORR}, χ_{CORR}	0.7739	0.0371	0.7991	0.0118	0.8109	0.1032	0.2864	0.3132	68.6208	0.8956	0.8749	0.2142	0.2357	2.8716	3.4343	81.8425	72.2085	5.8767	-13.0991	6.126	-12.4714	5.7948	-13.053
13	E_{CORR}, ω_{CORR}	0.7693	0.0384	0.7958	0.012	0.8078	0.1149	0.2888	0.3164	67.235	0.8937	0.8725	0.2126	0.2343	2.9194	3.5029	81.1197	72.9717	5.6912	-13.224	5.6789	-13.0259	5.9568	-12.797
14	E_{CORR}, E^{HOMO}_{CORR}	0.7541	0.0403	0.7816	0.0128	0.7944	0.0339	0.2987	0.3267	61.8277	0.8854	0.862	0.2261	0.2495	3.1222	3.7345	79.3658	72.6104	5.8074	-12.9943	5.8126	-13.0104	5.7312	-13.1559
15	E_{PM7}, E^{LUMO}_{PM7}	0.7497	0.0657	0.8038	0.0115	0.8153	0.045	0.2831	0.3296	70.648	0.8983	0.8648	0.2153	0.2427	2.8044	3.8017	82.1065	73.5693	6.0146	-12.8827	5.8443	-12.8509	5.7286	-13.3305
16	E_{CORR}, E^{LUMO}_{CORR}	0.7472	0.0375	0.7713	0.0135	0.7848	0.2572	0.3056	0.3312	58.3438	0.8794	0.8586	0.2249	0.2461	3.2685	3.8388	78.2467	72.6914	6.146	-12.6077	6.0311	-12.6198	5.5832	-13.3687
17	E_{CORR}	0.7344	0.0253	0.7524	0.0073	0.7597	0.8716	0.3229	0.3395	104.3214	0.8634	0.8484	0.2431	0.2576	3.6497	4.0338	75.7004	70.0061	2.8053	-9.4043	2.9703	-9.1854	2.9102	-9.3592
18	E_{CORR}, η_{PM7}	0.7298	0.0314	0.7463	0.0149	0.7612	-0.0004	0.3219	0.3424	51.0096	0.8644	0.8462	0.2452	0.2638	3.6263	4.1031	76.0638	68.6495	5.8314	-13.6427	6.1157	-12.4674	5.6143	-13.604
19	E_{PM7}, ω_{PM7}	0.7293	0.071	0.7879	0.0125	0.8004	0.0306	0.2943	0.3427	64.149	0.8891	0.8527	0.2236	0.252	3.0318	4.1106	80.666	71.5625	6.0053	-12.8952	5.7814	-12.9847	5.967	-13.023
20	E_{CORR}, η_{HF}	0.7274	0.0341	0.7465	0.0149	0.7614	0.3761	0.3217	0.3439	51.0646	0.8646	0.8453	0.237	0.2568	3.6233	4.1405	76.1567	69.7071	5.796	-13.528	5.8388	-12.7554	5.7923	-13.3137
21	E_{CORR}, η_{CORR}	0.7207	0.0405	0.7462	0.0149	0.7612	0.1494	0.3219	0.3481	50.995	0.8644	0.8414	0.239	0.2615	3.6271	4.2418	76.203	69.8057	5.9029	-12.9582	5.7175	-12.9642	6.0137	-12.7241
22	E_{PM7}, d_{PM7}	0.7188	0.0874	0.794	0.0121	0.8061	0.3975	0.29	0.3493	66.526	0.8927	0.8488	0.2203	0.2525	2.9445	4.2712	81.1769	72.3726	5.9771	-13.3559	5.8404	-12.6378	6.0096	-13.2708
23	E_{CORR}, d_{CORR}	0.7129	0.0583	0.7569	0.0143	0.7712	0.3266	0.3151	0.3529	53.9374	0.8708	0.8383	0.2379	0.2652	3.4745	4.3597	77.8886	67.5906	5.9435	-12.9789	6.2722	-12.2768	5.7986	-12.9654
24	E_{PM7}	0.7058	0.0471	0.7454	0.0075	0.7529	0.8677	0.3274	0.3573	100.5679	0.8591	0.8329	0.2348	0.252	3.7522	4.4675	75.537	65.5995	3.0697	-9.1406	2.7987	-9.3906	3.1177	-9.1954
25	E_{PM7}, E^{HOMO}_{PM7}	0.7051	0.058	0.7483	0.0148	0.7631	0.045	0.3206	0.3577	51.5381	0.8656	0.834	0.2292	0.2523	3.5979	4.4792	76.8309	68.2883	5.6326	-13.3518	5.8029	-12.8508	5.911	-13.0139
26	E_{CORR}, d_{PM7}	0.6981	0.0619	0.745	0.015	0.76	0.2803	0.3227	0.3619	50.6597	0.8636	0.8298	0.2428	0.2724	3.6453	4.5847	76.5783	68.2601	5.9504	-13.3794	5.7384	-12.9014	5.637	-13.8345
27	E_{CORR}, d_{HF}	0.694	0.0656	0.7447	0.015	0.7597	0.32	0.3229	0.3644	50.5811	0.8634	0.8277	0.2431	0.2735	3.6496	4.6466	76.6897	66.9832	5.6811	-13.449	5.9201	-12.8173	6.1242	-13.0357
28	E_{PM7}, χ_{PM7}	0.6917	0.0676	0.7443	0.015	0.7593	0.0207	0.3232	0.3658	50.4734	0.8632	0.8268	0.2394	0.2655	3.6555	4.6824	76.6057	64.7418	5.9102	-13.0641	6.0544	-12.6925	5.9497	-13.2578
29	E^{LUMO}_{PM7}	0.6433	0.0551	0.6893	0.0091	0.6984	0.8357	0.3618	0.3934	76.4158	0.8224	0.7927	0.2905	0.3124	4.5805	5.417	70.1242	59.8426	2.8587	-9.54	2.9905	-9.2408	2.8354	-9.4864
30	ω_{PM7}	0.6259	0.0553	0.6716	0.0097	0.6812	0.8254	0.3719	0.4029	70.5284	0.8104	0.7796	0.3022	0.3238	4.841	5.6814	68.0731	59.2356	2.9654	-9.3368	2.972	-9.2781	3.0632	-9.1607
31	E^{HOMO}_{CORR}	0.5923	0.0475	0.629	0.0109	0.6399	0.7999	0.3953	0.4206	58.6377	0.7804	0.7521	0.3084	0.3277	5.4691	6.1911	63.9071	53.8348	3.0813	-9.3218	2.9053	-9.3096	2.7713	-9.6362
32	E_{DFT}, ω_{DFT}	0.5286	0.1017	0.6072	0.0231	0.6303	0.2744	0.4005	0.4523	27.2759	0.7732	0.7148	0.323	0.3606	5.615	7.1588	64.0416	49.7898	5.4709	-13.4922	6.0789	-12.5943	5.8191	-13.0172
33	E_{DFT}, E^{LUMO}_{DFT}	0.5054	0.1078	0.589	0.0242	0.6132	0.2725	0.4097	0.4633	25.3644	0.7602	0.6985	0.331	0.3699	5.8745	7.5116	62.514	47.3856	5.9302	-12.9781	6.078	-12.6002	5.807	-13.0341
34	E_{HF}, E^{HOMO}_{HF}	0.4953	0.1099	0.5806	0.0247	0.6053	0.336	0.4139	0.468	24.5324	0.7541	0.6914	0.331	0.3695	5.9951	7.6644	61.706	45.9385	5.6268	-13.2035	5.8616	-12.7719	5.8741	-12.8461
35	χ_{CORR}	0.4846	0.0653	0.5363	0.0136	0.5499	0.7416	0.4419	0.4729	40.3196	0.7096	0.6694	0.3505	0.3742	6.8355	7.8267	54.6536	44.3245	3.0136	-9.2408	3.0337	-9.2223	2.9599	-9.4002
36	E_{HF}, ω_{HF}	0.4818	0.1085	0.5647	0.0256	0.5903	0.2892	0.4216	0.4742	23.057	0.7424	0.6791	0.3499	0.3894	6.2215	7.8699	59.9205	43.619	5.5596	-13.2817	6.26	-12.29	6.148	-12.6139
37	ω_{DFT}	0.4696	0.0743	0.5301	0.0138	0.5439	0.7375	0.4449	0.4797	39.3556	0.7046	0.6596	0.3628	0.3889	6.9266	8.0553	54.4727	41.5116	2.9931	-9.2423	2.8013	-9.418	2.8967	-9.3251
38	E_{HF}, χ_{HF}	0.4671	0.1169	0.558	0.026	0.584	0.2915	0.4248	0.4809	22.4648	0.7374	0.6707	0.3502	0.3908	6.3173	8.093	59.4013	44.9001	6.1386	-12.6232	5.8652	-12.7542	6.2381	-12.3271
39	ω_{CORR}	0.4488	0.0639	0.4979	0.0148	0.5127	0.716	0.4598	0.4891	34.717	0.6778	0.6376	0.3735	0.3975	7.401	8.3718	50.9747	38.7984	3.1333	-9.0849	2.9965	-9.2247	2.7151	-9.7362
40	E^{LUMO}_{DFT}	0.4438	0.0791	0.5085	0.0145	0.5229	0.7231	0.455	0.4913	36.173	0.6867	0.6389	0.3732	0.4006	7.2453	8.4473	52.1744	39.0714	2.8357	-9.3522	3.0749	-9.1286	3.0396	-9.2437
41	E_{DFT}, χ_{DFT}	0.4348	0.1254	0.5327	0.0275	0.5602	0.0707	0.4369	0.4952	20.3796	0.7181	0.6469	0.3591	0.4018	6.6794	8.5841	57.0689	41.7721	5.9836	-13.0113	5.8703	-12.8546	5.9711	-12.7941
42	χ_{PM7}	0.4249	0.0808	0.4908	0.015	0.5057	0.7112	0.4631	0.4995	33.7663	0.6717	0.6242	0.3825	0.4096	7.5064	8.7337	51.0062	37.2729	3.1062	-9.247	2.9827	-9.1339	3.0389	-9.2713
43	ω_{HF}	0.4006	0.0801	0.4649	0.0157	0.4806	0.6933	0.4747	0.51	30.5409	0.6492	0.5986	0.3872	0.4144	7.8875	9.1037	47.8165	35.0342	2.7374	-9.5228	3.0278	-9.1479	2.7269	-9.6238
44	E_{HF}, E^{LUMO}_{HF}	0.3873	0.1309	0.4881	0.0301	0.5182	0.2426	0.4572	0.5156	17.2079	0.6826	0.6056	0.3762	0.4199	7.3174	9.305	52.972	36.5859	5.7354	-13.2008	5.9398	-12.6776	6.0039	-12.8869
45	χ_{HF}	0.3857	0.0848	0.4545	0.016	0.4705	0.6859	0.4793	0.5163	29.3247	0.6399	0.5877	0.3967	0.4249	8.0414	9.3288	47.4212	31.4633	2.7916	-9.5565	2.6793	-9.5324	3.0943	-9.1527
46	E^{HOMO}_{HF}	0.3783	0.084	0.446	0.0163	0.4622	0.6799	0.4831	0.5194	28.3664	0.6322	0.5799	0.3947	0.4223	8.1669	9.4421	46.1949	31.5406	3.0305	-9.2386	2.9148	-9.2843	2.9813	-9.2832
47	E_{DFT}, E^{HOMO}_{DFT}	0.3292	0.1444	0.4408	0.0329	0.4737	0.2938	0.4779	0.5395	14.399	0.6428	0.5601	0.3913	0.4371	7.9935	10.1873	49.2584	28.7689	5.804	-12.9779	5.8152	-12.9486	6.0485	-12.8499
48	E^{LUMO}_{HF}	0.3245	0.094	0.4009	0.0176	0.4185	0.6469	0.5023	0.5414	23.7477	0.59	0.5307	0.4118	0.4418	8.8317	10.2588	42.1763	26.423	2.8197	-9.5341	2.8436	-9.421	2.8376	-9.4794
49	η_{PM7}	0.3081	0.0932	0.3831	0.0181	0.4013	0.6335	0.5097	0.548	22.1163	0.5727	0.5167	0.4288	0.4565	9.0931	10.5087	41.1544	22.9719	2.7182	-9.6325	2.8248	-9.3659	2.9562	-9.4927
50	χ_{DFT}	0.3047	0.1024	0.3892	0.018	0.4072	0.6381	0.5072	0.5493	22.6641	0.5787	0.5169	0.415	0.4459	9.0036	10.5591	41.381	23.8955	3.1517	-9.0444	2.8738	-9.3145	2.8773	-9.3869
51	E^{HOMO}_{DFT}	0.1331	0.123	0.2336	0.0225	0.2561	0.5061	0.5681	0.6133	11.3608	0.4078	0.3333	0.4579	0.491	11.2977	13.1662	26.5878	8.9538	2.9241	-9.5082	2.8196	-9.3756	2.7984	-9.6336
52	η_{DFT}	0.0923	0.1073	0.1753	0.0243	0.1996	0.4467	0.5893	0.6276	8.2278	0.3327	0.2528	0.5015	0.5344	12.1563	13.7856	20.5108	2.0655	2.8265	-9.5209	2.7737	-9.5122	2.7919	-9.5302
53	E^{HOMO}_{PM7}	0.0871	0.1057	0.1683	0.0245	0.1927	0.439	0.5918	0.6294	7.8792	0.3232	0.2507	0.4758	0.5065	12.2599	13.8649	19.6499	5.2332	3.0893	-9.211	2.8669	-9.3781	2.9945	-9.4015
54	E_{DFT}, η_{DFT}	0.0849	0.1774	0.2162	0.0461	0.2623	-0.0334	0.5658	0.6301	5.6886	0.4156	0.293	0.4694	0.5213	11.2038	13.8981	28.0431	6.7079	6.0157	-12.7378	5.9456	-12.7021	5.7828	-13.1019
55	E_{DFT}	0.0611	0.1307	0.1674	0.0245	0.1919	0.438	0.5922	0.6383	7.8356	0.322	0.2274	0.4556	0.4896	12.273	14.2586	20.0579	3.1683	2.7541	-9.4954	2.992	-9.2335	2.8558	-9.4112
56	E_{HF}	0.0606	0.1308	0.1669	0.0245	0.1914	0.4375	0.5923	0.6384	7.8126	0.3213	0.2267	0.4558	0.4898	12.2799	14.2665	20.3285	4.3683	3.0021	-9.1187	2.8632	-9.4005	2.7967	-9.5628
57	E^{LUMO}_{CORR}	0.0462	0.1163	0.1372	0.0254	0.1625	0.4032	0.6028	0.6433	6.4049	0.2796	0.1939	0.4965	0.5296	12.7186	14.4856	17.3847	-0.3769	2.9639	-9.4277	2.9902	-9.2479	3.2115	-9.111
58	E_{HF}, η_{HF}	0.036	0.1555	0.1409	0.0505	0.1914	0.0326	0.5923	0.6468	3.7885	0.3214	0.2077	0.4555	0.5001	12.2796	14.6405	20.3892	3.4713	6.0049	-13.3866	5.6789	-13.0373	5.8319	-13.7237
59	E_{DFT}, d_{DFT}	0.0156	0.1784	0.1437	0.0504	0.1941	0.0326	0.5914	0.6536	3.8526	0.325	0.2047	0.4536	0.504	12.2399	14.9498	21.1246	2.2158	5.5991	-13.8267	5.5613	-13.1813	5.8878	-13.4507
60	E_{HF}, d_{HF}	0.01	0.1814	0.1409	0.0505	0.1914	0.0255	0.5923	0.6554	3.788	0.3213	0.1988	0.4557	0.5061	12.2799	15.0345	21.7273	-2.1017	6.0571	-13.0075	5.8294	-12.7847	5.849	-13.4008
61	η_{CORR}	-0.0014	0.1018	0.0731	0.0273	0.1004	0.3169	0.6248	0.6592	3.6831	0.1825	0.1053	0.5058	0.5364	13.6623	15.2083	10.9407	-4.1494	2.8156	-9.741	2.8906	-9.3107	2.9498	-9.5041
62	d_{CORR}	-0.0507	0.106	0.0267	0.0286	0.0553	0.2352	0.6402	0.6752	1.932	0.1048	0.0076	0.5257	0.5568	14.3472	15.9577	6.1921	-8.7001	3.0068	-9.431	2.9515	-9.2563	2.9136	-9.4614
63	d_{PM7}	-0.0724	0.1066	0.005	0.0293	0.0343	0.1851	0.6473	0.6821	1.1707	0.0663	-0.0171	0.512	0.5428	14.6668	16.2861	4.417	-12.1472	2.8678	-10.1438	2.7394	-9.4187	3.1145	-9.7983
64	d_{DFT}	-0.0776	0.1033	-0.0039	0.0295	0.0257	0.1602	0.6502	0.6838	0.8692	0.05	-0.0333	0.5131	0.543	14.7974	16.3664	3.3543	-12.2411	2.8799	-9.5699	3.0152	-9.2118	2.8753	-9.9661
65	d_{HF}	-0.0845	0.0974	-0.017	0.0299	0.0129	0.1136	0.6545	0.686	0.4315	0.0255	-0.0605	0.5122	0.5394	14.9912	16.4702	2.1432	-12.8106	3.1015	-9.5156	2.7022	-9.4593	2.9919	-9.7417
66	η_{HF}	-0.1096	0.1197	-0.0199	0.03	0.0101	0.1006	0.6554	0.6939	0.3374	0.02	-0.0762	0.5172	0.5498	15.0334	16.8521	1.9566	-13.8978	2.9528	-9.876	2.817	-9.4118	3.0362	-9.5653

Models are arranged according to Q^2_{LOO} values.

Parameters are obtained through QSARINS software. Ref. [43] (Chirico, N.; Papa, E.; Kovarich, S.; Cassani, S.; Gramatica, P. QSARINS, Software for QSAR MLR model development and validation. 2012, QSAR Res. Unit in Environ. Chem. and Ecotox., University of Insubria, Varese, Italy (http://www.qsar.it).

R^2_{adj} adjusted R^2

N. Ext.OK Number of external validation parameters meeting threshold values

F "F-test" statistic value

Supporting Information Figures S1 and S2

Evaluating the role of electron-correlation in the external prediction of the toxicity of Nitrobenzenes towards *Tetrahymena pyriformis*

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List of Figures

Figure S1

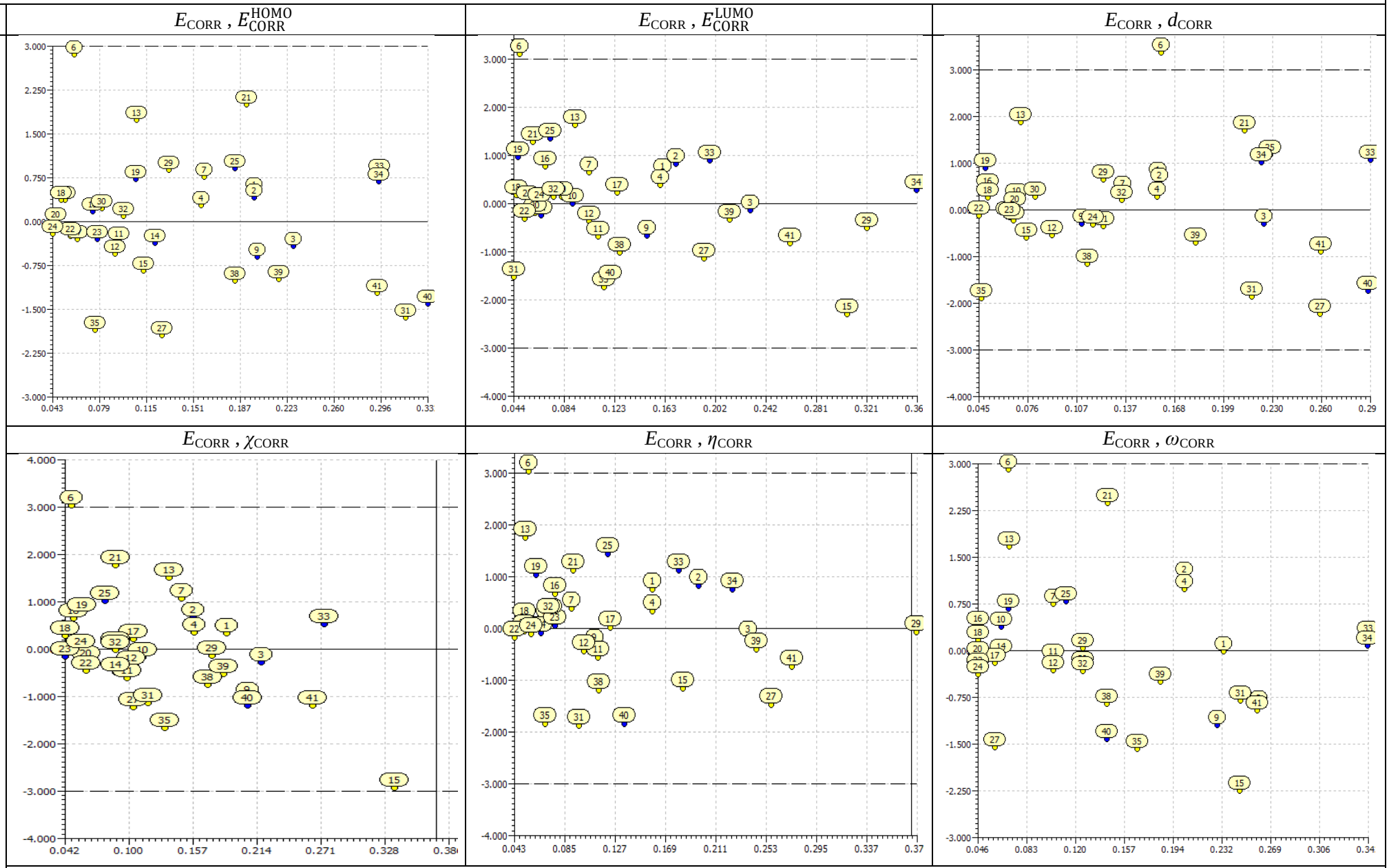
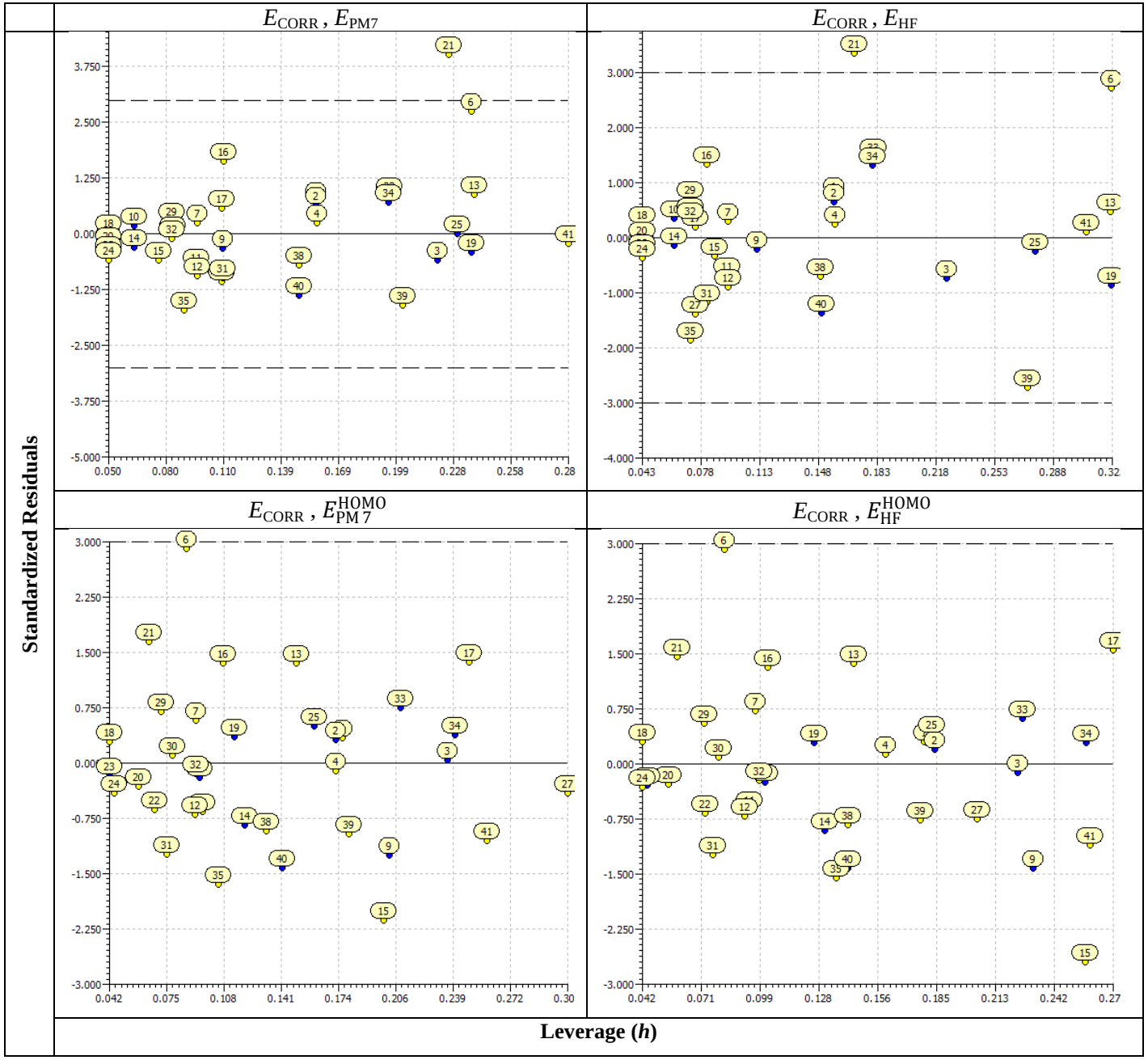


Figure S1 continued…



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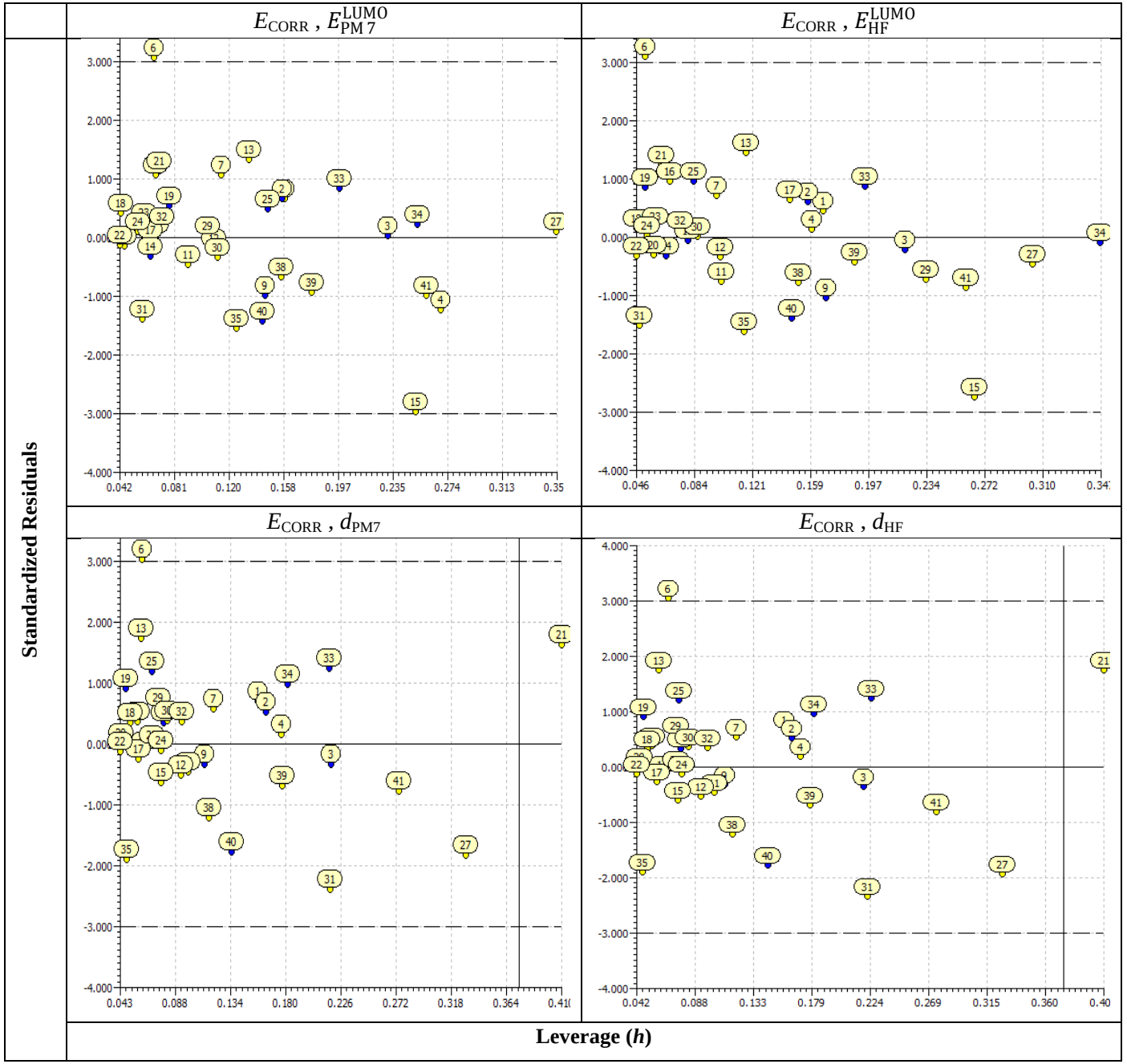
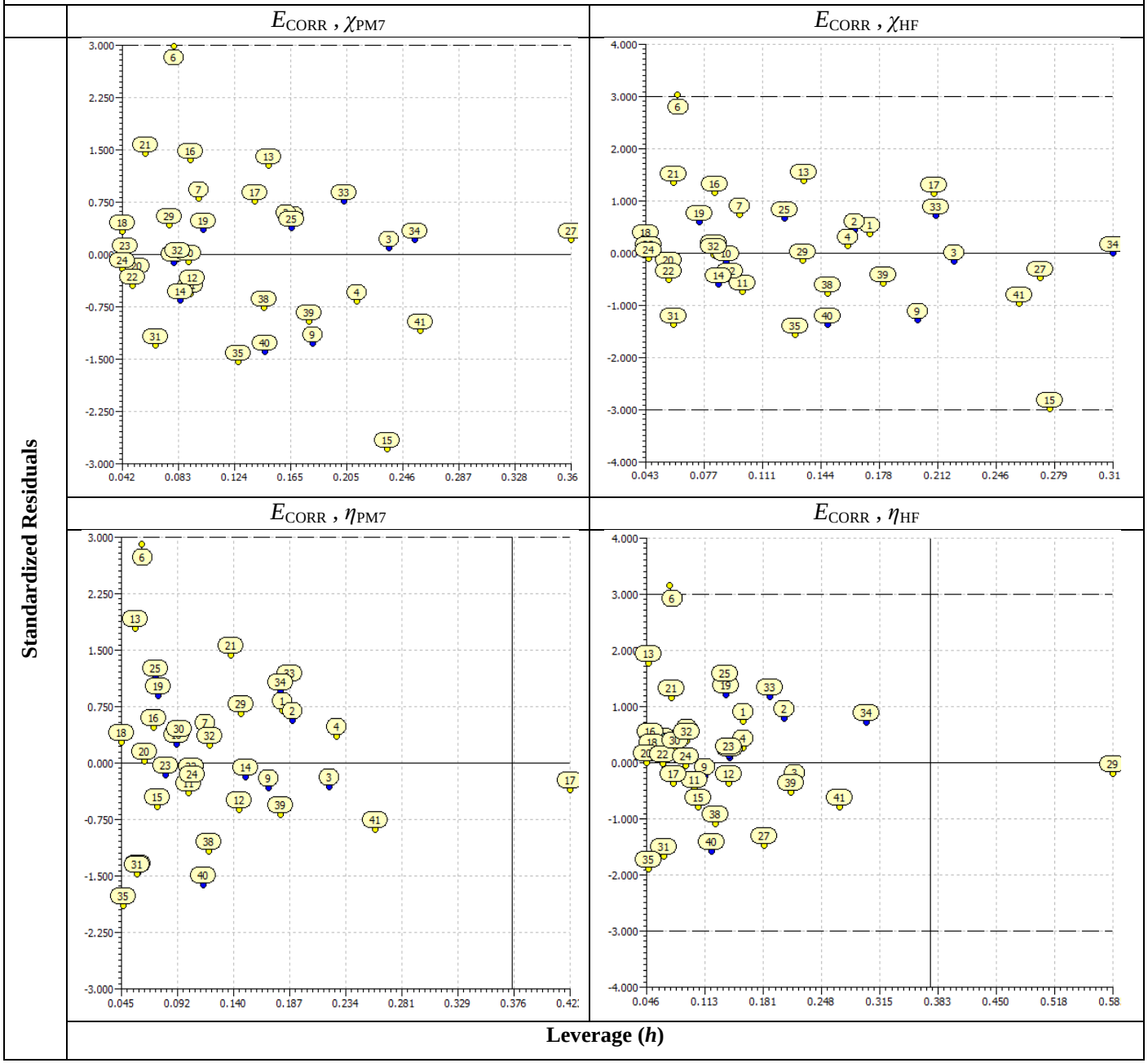


Figure S1 continued…

Figure S1



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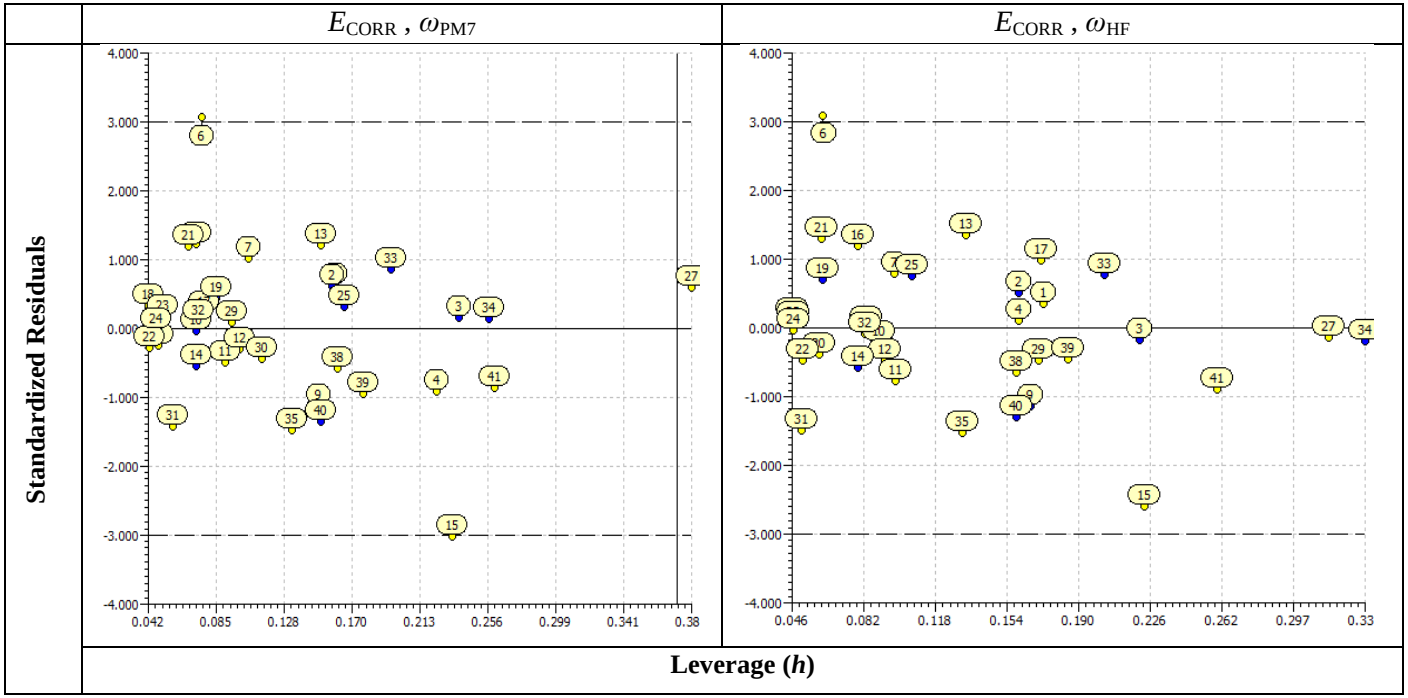

E_{CORR} , ω_{PM7}
E_{CORR} , ω_{HF}
Standardized Residuals
Leverage (h)
4.000
3.000
2.000
1.000
0.000
-1.000
-2.000
-3.000
-4.000
0.042
0.085
0.128
0.170
0.213
0.256
0.299
0.341
0.38
0.046
0.082
0.118
0.154
0.190
0.226
0.262
0.297
0.33

Figure S2

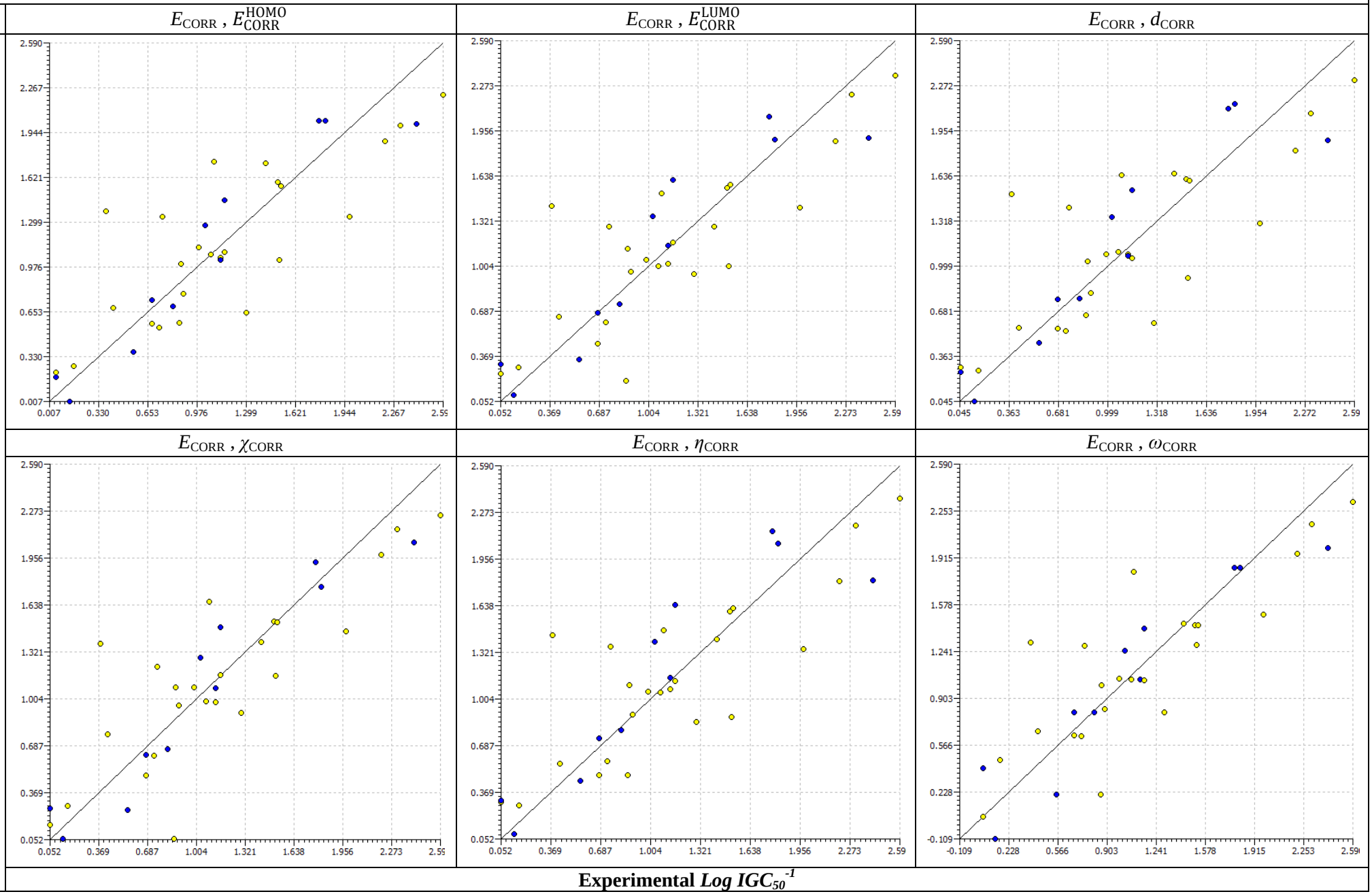


Figure S2 continued…

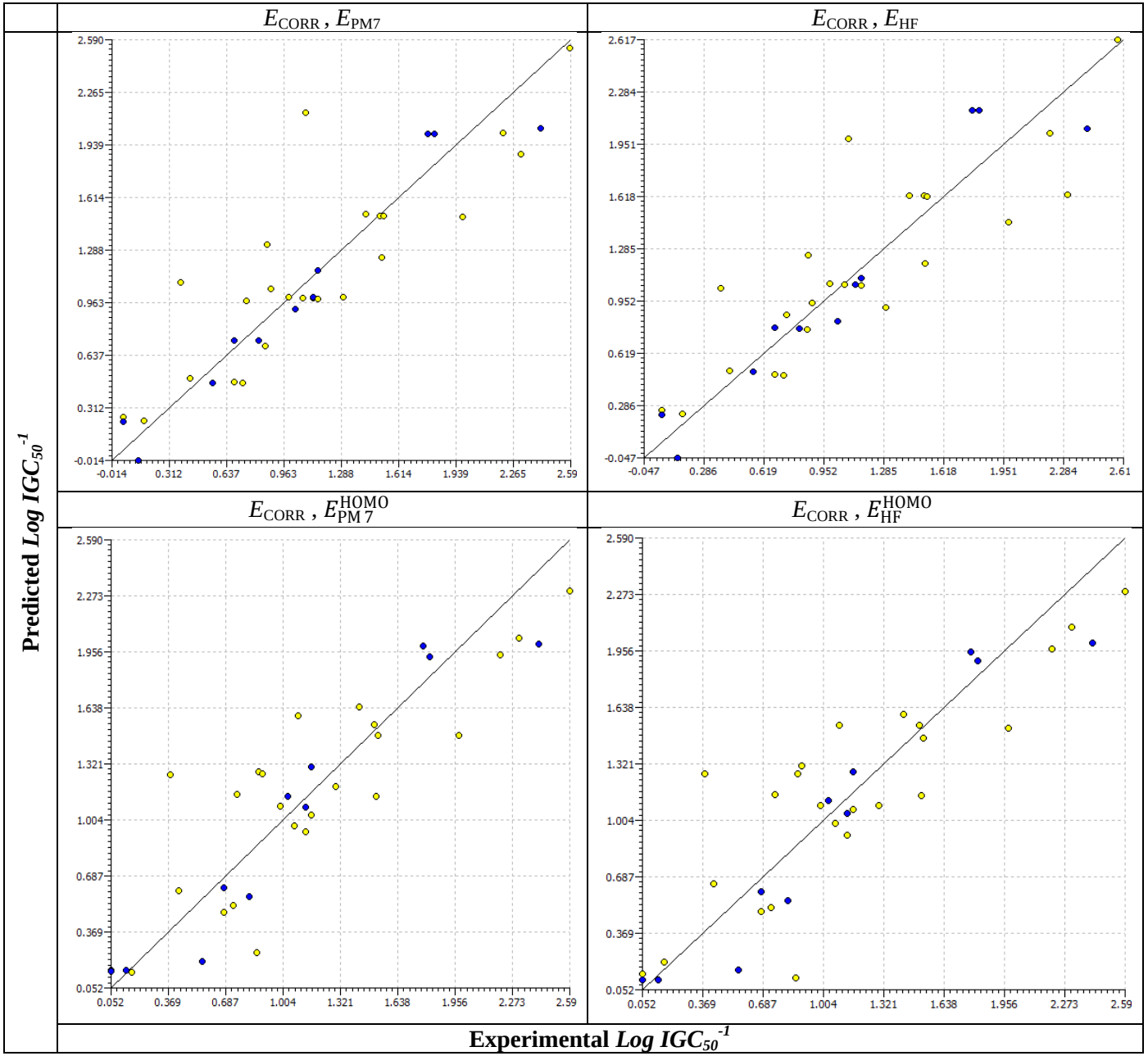
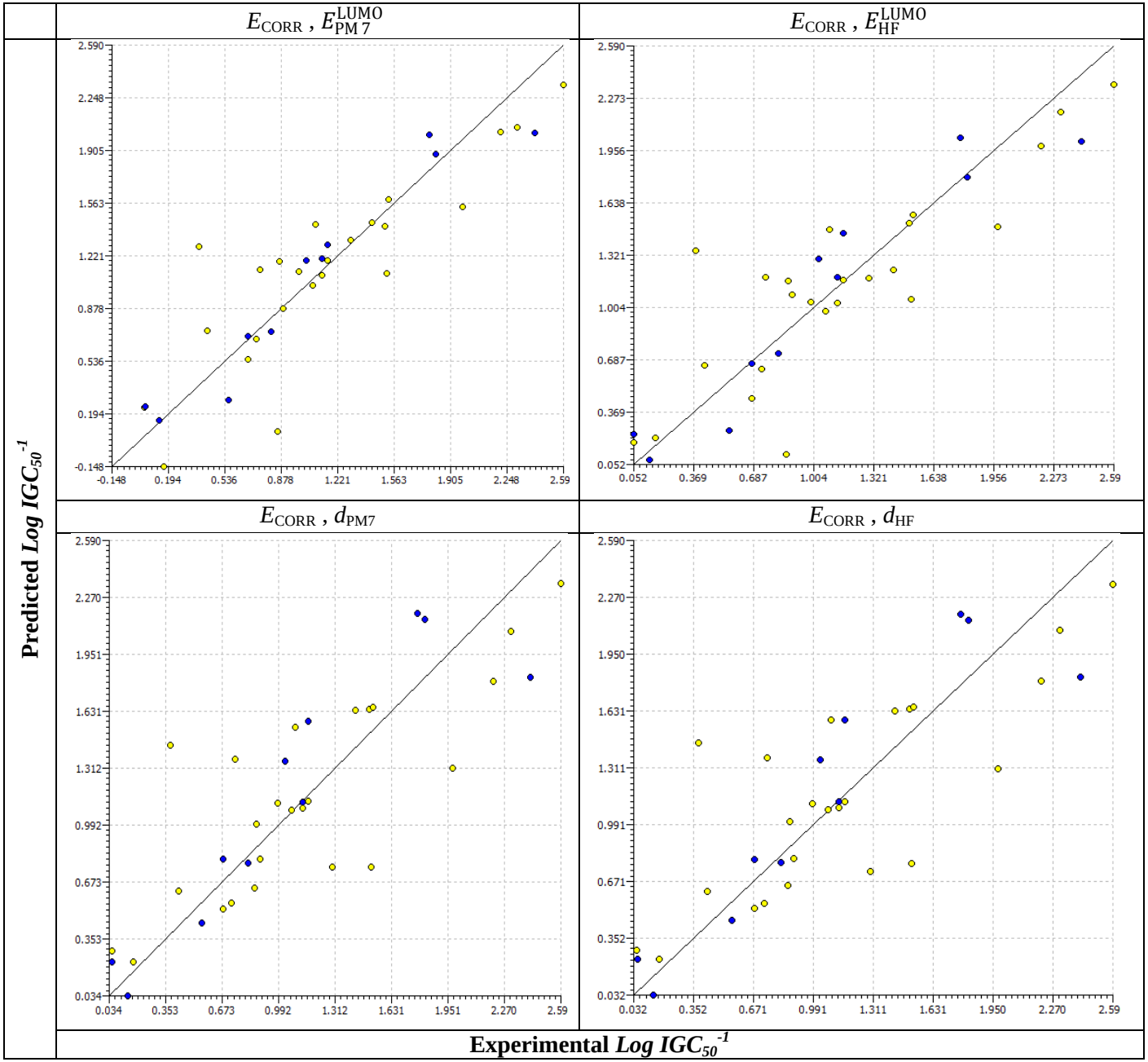


Figure S1 continued…



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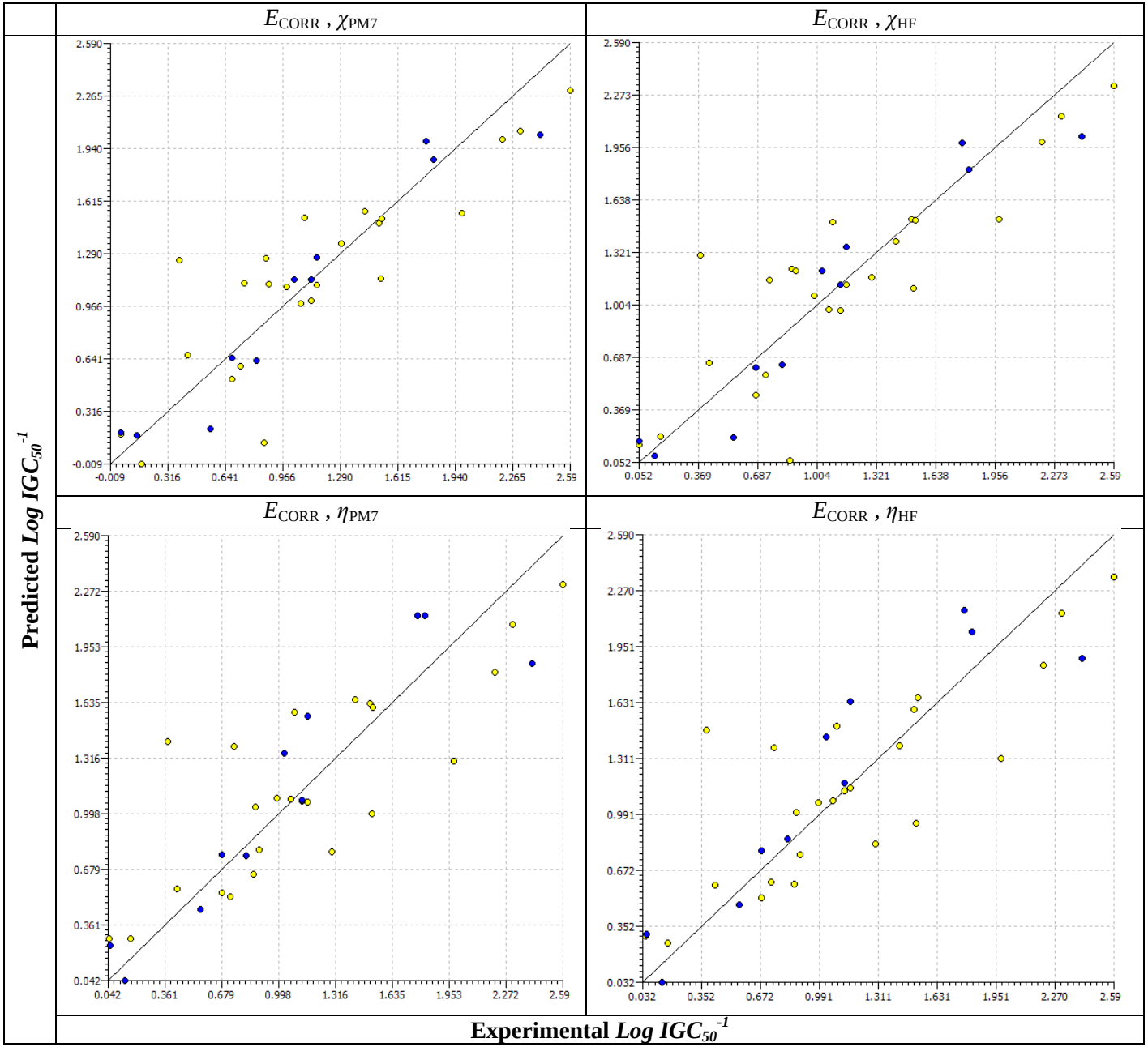

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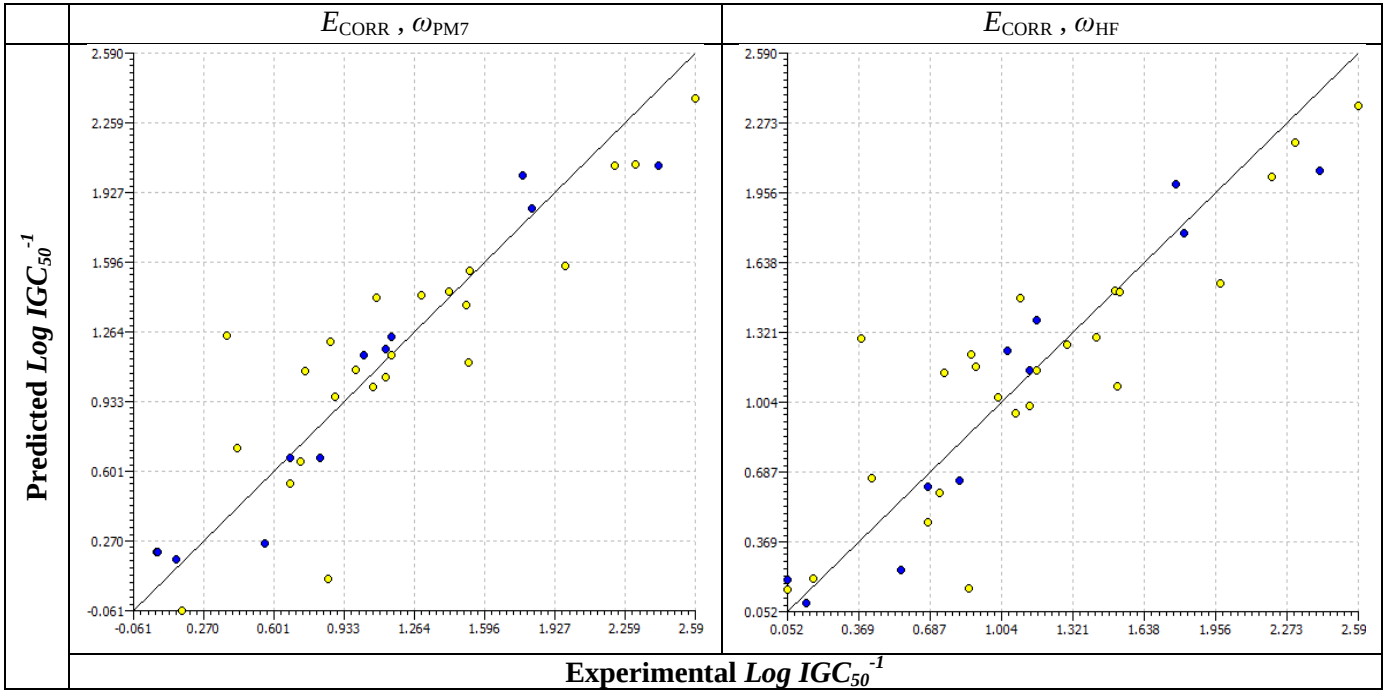
E_{CORR} , ω_{PM7}
E_{CORR} , ω_{HF}
Predicted *Log* IGC_{50}^{-1}
Experimental *Log* IGC_{50}^{-1}
2.590
2.259
1.927
1.596
1.264
0.933
0.601
0.270
-0.061
2.590
2.273
1.956
1.638
1.321
1.004
0.687
0.369
0.052