Electronic Supplementary Information for manuscript

Intrinsic Bond Strength Index as a halogen bond interaction energy predictor

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Supporting Figures and Tables

Table S1: IBSI values and X$\cdots$B interaction distances (d_{int}, Å) for **Set 1** (n = 99). X = XB donor atom; B = XB acceptor atom. Interaction energies (E_{int}, in kcal mol^{-1}) calculated at CCSD(T)/CBS level of theory[S1]. Some points were removed from the respective linear fits (see Outlier Removal Section below).

XB donor	XB acceptor	X	B	E_{int}	d_{int}	IBSI^{H}	IBSI^{PRO}	IBSI^{GBP}
chlorine	acetonitrile	Cl	N	-3.336	2.777	0.01787	0.07563	0.037
trifluorochloromethane	pyrazine	Cl	N	-2.899	2.974	0.01030	0.04674	0.026
chloromethane	pyrazine	Cl	N	-1.371	3.315	0.00523	0.02111	0.012
chlorobenzene	pyrazine	Cl	N	-1.848	3.230	0.00632	0.02573	0.015
chlorine	pyrazine	Cl	N	-5.858	2.476	0.03588	0.15346	0.087
chloromethane	trimethylamine	Cl	N	-1.692	3.096	0.00805	0.03551	0.023
chlorobenzene	trimethylamine	Cl	N	-2.258	3.028	0.00917	0.04138	0.026
chlorine	trimethylamine	Cl	N	-14.518	2.303	0.06121	0.23489	0.156
trifluorochloromethane	acetone	Cl	O	-2.873	2.946	0.00847	0.03704	0.025
chlorine	acetone	Cl	O	-4.244	2.602	0.02173	0.09500	0.054
trifluorochloromethane	furan	Cl	O	-1.927	3.028	0.00592	0.03542	0.018
chlorobenzene	furan	Cl	O	-1.467	3.292	0.00421	0.01923	0.010
chlorine	furan	Cl	O	-2.628	2.796	0.01234	0.06141	0.032
trifluorochloromethane	nitromethane	Cl	O	-2.138	3.097	0.00659	0.02934	0.015
chlorine	nitromethane	Cl	O	-2.813	2.790	0.01335	0.05916	0.032
trifluorochloromethane	pyridine-N-oxide	Cl	O	-4.074	2.844	0.01306	0.04274	0.031
chlorobenzene	pyridine-N-oxide	Cl	O	-0.910	3.121	0.00637	0.02887	0.016
chlorine	pyridine-N-oxide	Cl	O	-6.895	2.437	0.03656	0.11666	0.083
trifluorochloromethane	dimethylthioether	Cl	S	-2.944	3.298	0.00973	0.04280	0.024
chloromethane	dimethylthioether	Cl	S	-1.961	3.569	0.00590	0.02424	0.013
chlorine	dimethylthioether	Cl	S	-9.062	2.614	0.04839	0.18947	0.118
trifluorochloromethane	thioacetone	Cl	S	-2.375	3.417	0.00879	0.03040	0.022
chlorine	thioacetone	Cl	S	-7.329	2.639	0.04788	0.16351	0.115
chlorine	fluorine	Cl	F	-0.657	3.082	0.00552	0.02664	0.011
chlorine	chlorine	Cl	Cl	-1.481	3.221	0.00811	0.04452	0.020
chlorine	bromine	Cl	Br	-1.777	3.262	0.01168	0.05083	0.024
chlorine	iodine	Cl	I	-2.095	3.286	0.01611	0.06521	0.033
bromine	pyrazine	Br	N	-8.920	2.534	0.03766	0.15874	0.096
bromobenzene	pyrazine	Br	N	-2.607	3.096	0.01021	0.04444	0.025
trifluorobromomethane	pyrazine	Br	N	-4.396	2.919	0.01334	0.06536	0.036
bromomethane	pyrazine	Br	N	-2.206	3.171	0.00976	0.03741	0.021
bromine	trimethylamine	Br	N	-17.144	2.423	0.05640	0.20456	0.141
bromobenzene	trimethylamine	Br	N	-3.959	2.974	0.01252	0.05684	0.034
bromomethane	trimethylamine	Br	N	-3.272	2.994	0.01267	0.04761	0.033
bromine	acetone	Br	O	-6.133	2.634	0.02591	0.09893	0.061
bromobenzene	acetone	Br	O	-2.324	3.137	0.00914	0.03047	0.020
trifluorobromomethane	acetone	Br	O	-4.068	2.923	0.01060	0.04894	0.031

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Table S1 – continued from previous page

XB donor	XB acceptor	X	B	E_{int}	d_{int}	IBSI^{H}	IBSI^{PRO}	IBSI^{GBP}
bromomethane	acetone	Br	O	-1.771	3.190	0.00764	0.02879	0.018
bromine	furan	Br	O	-3.552	2.828	0.01365	0.06540	0.037
bromobenzene	furan	Br	O	-1.888	3.221	0.00630	0.02871	0.015
trifluorobromomethane	furan	Br	O	-2.592	3.118	0.00761	0.03530	0.019
bromomethane	furan	Br	O	-1.577	3.280	0.00547	0.02341	0.013
bromine	nitromethane	Br	O	-3.975	2.810	0.01423	0.07089	0.038
trifluorobromomethane	nitromethane	Br	O	-2.938	3.087	0.00852	0.03769	0.020
bromine	pyridine-N-oxide	Br	O	-9.950	2.483	0.03838	0.12123	0.092
bromobenzene	pyridine-N-oxide	Br	O	-2.971	3.066	0.00998	0.04071	0.025
trifluorobromomethane	pyridine-N-oxide	Br	O	-5.779	2.799	0.01805	0.06001	0.041
bromomethane	pyridine-N-oxide	Br	O	-2.821	3.114	0.00953	0.02982	0.021
bromine	dimethylthioether	Br	S	-12.078	2.723	0.04646	0.17645	0.114
trifluorobromomethane	dimethylthioether	Br	S	-4.346	3.239	0.01236	0.05968	0.032
bromine	thioacetone	Br	S	-10.662	2.729	0.04781	0.15788	0.117
trifluorobromomethane	thioacetone	Br	S	-3.652	3.335	0.01262	0.04436	0.030
bromomethane	thioacetone	Br	S	-1.904	3.589	0.00765	0.02579	0.019
bromine	fluorine	Br	F	-0.775	3.149	0.00580	0.02854	0.013
bromine	chlorine	Br	Cl	-1.976	3.255	0.00916	0.05155	0.025
trifluorobromomethane	chlorine	Br	Cl	-1.483	3.552	0.00590	0.02744	0.013
bromine	bromine	Br	Br	-2.493	3.281	0.01182	0.05840	0.030
trifluorobromomethane	bromine	Br	Br	-1.756	3.660	0.00509	0.02735	0.013
bromine	iodine	Br	I	-3.324	3.292	0.01871	0.07832	0.042
trifluorobromomethane	iodine	Br	I	-2.048	3.796	0.00603	0.02848	0.014
iodine	acetonitrile	I	N	-5.453	2.875	0.01662	0.09481	0.047
iodobenzene	acetonitrile	I	N	-2.468	3.219	0.00908	0.04523	0.022
trifluoroiodomethane	pyrazine	I	N	-6.406	2.899	0.01756	0.09019	0.046
iodomethane	pyrazine	I	N	-3.373	3.085	0.01534	0.06084	0.031
iodine	pyrazine	I	N	-9.208	2.678	0.03443	0.14597	0.083
iodobenzene	pyrazine	I	N	-3.987	3.062	0.01483	0.06358	0.032
iodine	trimethylamine	I	N	-15.618	2.613	0.04233	0.16779	0.109
iodobenzene	trimethylamine	I	N	-6.133	2.956	0.01646	0.07771	0.042
iodomethane	acetone	I	O	-2.801	3.134	0.01038	0.04211	0.025
iodine	acetone	I	O	-6.679	2.768	0.02188	0.09689	0.054
iodobenzene	acetone	I	O	-3.380	3.093	0.01160	0.04543	0.027
trifluoroiodomethane	furan	I	O	-3.439	3.041	0.01170	0.05711	0.028
iodomethane	furan	I	O	-2.092	3.220	0.00719	0.03656	0.020
iodine	furan	I	O	-3.909	2.944	0.01297	0.07042	0.035
iodobenzene	furan	I	O	-2.334	3.175	0.00792	0.04286	0.021
trifluoroiodomethane	nitromethane	I	O	-3.989	3.085	0.01090	0.05119	0.025
iodomethane	nitromethane	I	O	-2.669	3.282	0.00640	0.03063	0.017
iodine	nitromethane	I	O	-4.419	2.933	0.01339	0.06804	0.036

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Table S1 – continued from previous page

XB donor	XB acceptor	X	B	E_{int}	d_{int}	$IBSI^{H}$	$IBSI^{PRO}$	$IBSI^{GBP}$
iodobenzene	nitromethane	I	O	-2.968	3.258	0.00604	0.03349	0.018
trifluoroiodomethane	pyridine-N-oxide	I	O	-8.389	2.773	0.02342	0.08184	0.053
iodomethane	pyridine-N-oxide	I	O	-4.404	3.001	0.01453	0.05836	0.032
iodine	pyridine-N-oxide	I	O	-9.978	2.637	0.03300	0.12510	0.077
iodobenzene	pyridine-N-oxide	I	O	-4.533	2.999	0.01340	0.05671	0.033
trifluoroiodomethane	dimethylthioether	I	S	-6.344	3.207	0.01775	0.08463	0.045
iodomethane	dimethylthioether	I	S	-3.825	3.434	0.01266	0.05363	0.027
iodine	dimethylthioether	I	S	-10.823	2.934	0.03521	0.14511	0.089
trifluoroiodomethane	thioacetone	I	S	-5.332	3.285	0.01671	0.06515	0.041
iodomethane	thioacetone	I	S	-2.853	3.528	0.01108	0.04007	0.025
iodine	thioacetone	I	S	-9.468	2.938	0.03789	0.12971	0.093
trifluoroiodomethane	fluorine	I	F	-0.744	3.378	0.00387	0.02320	0.010
trifluoroiodomethane	chlorine	I	Cl	-1.837	3.591	0.00574	0.03430	0.016
iodomethane	chlorine	I	Cl	-1.419	3.712	0.00470	0.02593	0.013
iodine	chlorine	I	Cl	-2.126	3.412	0.01033	0.04994	0.023
trifluoroiodomethane	bromine	I	Br	-2.237	3.680	0.00617	0.03593	0.017
iodomethane	bromine	I	Br	-5.021	3.197	0.02281	0.08772	0.052
iodine	bromine	I	Br	-2.696	3.442	0.01328	0.05821	0.028
trifluoroiodomethane	iodine	I	I	-2.681	3.797	0.00666	0.03845	0.019
iodomethane	iodine	I	I	-2.005	3.956	0.00532	0.02756	0.014
iodine	iodine	I	I	-3.530	3.478	0.01605	0.07227	0.037

Table S2: IBSI values and X$\cdots$B interaction distances (d_{int}, Å) for **Set 2** (n = 124). X = XB donor atom; B = XB acceptor atom. Interaction energies (E_{int}, in kcal mol^{-1}) calculated at the CCSD(T)-F12b/CBS level of theory[S2]. Some points were removed from the respective linear fits (see Outlier Removal Section below)

XB donor	XB acceptor	X	B	E_{int}	d_{int}	IBSI^{H}	IBSI^{PRO}	IBSI^{GBP}
Br_2	CH_2O	Br	O	-4.441659	2.750	0.01781	0.08532	0.045
Br_2	CH_2S	Br	S	-6.419127	2.911	0.03060	0.11980	0.071
Br_2	CH_3OH	Br	O	-5.23228	2.690	0.02248	0.09792	0.052
Br_2	H_2O	Br	O	-3.992106	2.792	0.01535	0.07696	0.040
Br_2	H_2S	Br	S	-4.03399	3.114	0.01687	0.07764	0.043
Br_2	HCN	Br	N	-3.65643	2.889	0.01246	0.06998	0.035
Br_2	NH_3	Br	N	-7.81033	2.598	0.03452	0.13758	0.077
Br_2	Oxirane	Br	O	-5.88747	2.650	0.02472	0.10057	0.057
Br_2	PH_3	Br	P	-4.96557	2.993	0.02651	0.10717	0.063
Br_2	Thiirane	Br	S	-8.64385	2.825	0.03700	0.12579	0.091
BrI	CH_2O	I	O	-6.181753	2.787	0.01729	0.10125	0.051
BrI	CH_2S	I	S	-8.712724	2.979	0.03166	0.13287	0.081
BrI	CH_3OH	I	O	-7.45631	2.718	0.02311	0.11769	0.060
BrI	H_2O	I	O	-5.666235	2.827	0.01559	0.09283	0.045
BrI	H_2S	I	S	-5.675712	3.162	0.01848	0.09275	0.051
BrI	HCN	I	N	-5.350233	2.906	0.01555	0.08890	0.043
BrI	NH_3	I	N	-11.052197	2.647	0.03660	0.15602	0.086
BrI	Oxirane	I	O	-8.16424	2.682	0.02773	0.12015	0.066
BrI	PH_3	I	P	-7.87352	2.979	0.03512	0.14033	0.089
BrI	Thiirane	I	S	-11.19074	2.921	0.03770	0.13229	0.095
CF_3Br	CH_2O	Br	O	-3.152176866	2.961	0.00885	0.05162	0.028
CF_3Br	CH_2S	Br	S	-2.956610128	3.392	0.01060	0.04339	0.024
CF_3Br	H_2O	Br	O	-3.088507554	2.969	0.00926	0.04251	0.025
CF_3Br	H_2S	Br	S	-2.13846848	3.506	0.00841	0.02924	0.019
CF_3Br	HCN	Br	N	-2.903893237	3.091	0.00957	0.04494	0.022
CF_3Br	NH_3	Br	N	-4.245178573	2.976	0.01199	0.05759	0.030
CF_3Cl	CH_2O	Cl	O	-2.231514607	2.983	0.00650	0.03933	0.022
CF_3Cl	CH_2S	Cl	S	-1.99353537	3.444	0.00719	0.03143	0.018
CF_3Cl	H_2O	Cl	O	-2.130372848	2.995	0.00732	0.03219	0.019
CF_3Cl	H_2S	Cl	S	-1.330261833	3.547	0.00619	0.02149	0.014
CF_3Cl	HCN	Cl	N	-1.984478547	3.120	0.00604	0.03377	0.016
CF_3Cl	NH_3	Cl	N	-2.795788981	3.064	0.00835	0.03823	0.022
CF_3I	CH_2O	I	O	-4.153863941	3.021	0.01310	0.06086	0.030
CF_3I	CH_2S	I	S	-4.155608511	3.396	0.01305	0.05761	0.030
CF_3I	H_2O	I	O	-4.048780317	3.043	0.01206	0.04903	0.027
CF_3I	H_2S	I	S	-3.025128277	3.546	0.00969	0.03556	0.022

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Table S2 – continued from previous page

XB donor	XB acceptor	X	B	E_{int}	d_{int}	IBSI^{H}	IBSI^{PRO}	IBSI^{GBP}
CF_3I	HCN	I	N	-3.72207077	3.147	0.01184	0.05324	0.025
CF_3I	NH_3	I	N	-6.080220246	2.976	0.01671	0.07684	0.037
Cl_2	CH_2O	Cl	O	-3.30976	2.764	0.01520	0.06783	0.037
Cl_2	CH_2S	Cl	S	-4.01468	3.027	0.01778	0.07709	0.043
Cl_2	H_2O	Cl	O	-2.89013	2.813	0.01322	0.06004	0.031
Cl_2	H_2S	Cl	S	-2.59368	3.214	0.01221	0.05110	0.029
Cl_2	HCN	Cl	N	-2.61172	2.922	0.01039	0.05291	0.026
Cl_2	NH_3	Cl	N	-4.99195	2.680	0.02366	0.09536	0.051
ClBr	CH_2O	Br	O	-5.349523	2.681	0.02247	0.10052	0.053
ClBr	CH_2S	Br	S	-7.760402	2.839	0.03455	0.13826	0.085
ClBr	CH_3OH	Br	O	-6.36767	2.621	0.02570	0.11424	0.061
ClBr	H_2O	Br	O	-4.88784	2.721	0.02047	0.09179	0.047
ClBr	H_2S	Br	S	-4.915292	3.040	0.02180	0.09112	0.051
ClBr	HCN	Br	N	-4.560241	2.804	0.01710	0.08533	0.043
ClBr	NH_3	Br	N	-9.796414	2.515	0.04117	0.16578	0.095
ClBr	Oxirane	Br	O	-7.00288	2.584	0.02685	0.11707	0.067
ClBr	PH_3	Br	P	-6.78735	2.856	0.03654	0.14097	0.088
ClBr	Thiirane	Br	S	-10.29857	2.761	0.04258	0.14312	0.106
ClI	CH_2O	I	O	-7.186337	2.728	0.02144	0.11512	0.058
ClI	CH_2S	I	S	-10.144137	2.920	0.03592	0.14877	0.092
ClI	CH_3OH	I	O	-8.62254	2.666	0.02715	0.13154	0.067
ClI	H_2O	I	O	-6.643573	2.769	0.01857	0.10539	0.051
ClI	H_2S	I	S	-6.656585	3.102	0.02138	0.10425	0.058
ClI	HCN	I	N	-6.409411	2.824	0.01799	0.10552	0.052
ClI	NH_3	I	N	-12.942191	2.598	0.04075	0.17319	0.096
ClI	Oxirane	I	O	-9.3813	2.634	0.03139	0.13412	0.074
ClI	PH_3	I	P	-10.03259	2.880	0.04392	0.16973	0.111
ClI	Thiirane	I	S	-12.77416	2.872	0.04183	0.14578	0.106
FBr	CH_2O	Br	O	-8.672808	2.473	0.03339	0.16160	0.089
FBr	CH_2S	Br	S	-14.343649	2.567	0.06571	0.24189	0.165
FBr	CH_3OH	Br	O	-10.48929	2.412	0.04055	0.18385	0.104
FBr	H_2O	Br	O	-8.054001	2.510	0.03041	0.15066	0.079
FBr	H_2S	Br	S	-9.031993	2.756	0.04040	0.16503	0.103
FBr	HCN	Br	N	-7.795704	2.535	0.03189	0.15831	0.086
FBr	NH_3	Br	N	-16.674148	2.329	0.06463	0.25570	0.156
FBr	Oxirane	Br	O	-11.20104	2.389	0.04444	0.18432	0.113
FBr	PH_3	Br	P	-18.63295	2.428	0.09971	0.33100	0.240
FBr	Thiirane	Br	S	-17.15031	2.561	0.07003	0.21605	0.175
FCl	CH_2O	Cl	O	-5.850389	2.501	0.02544	0.12722	0.069

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Table S2 – continued from previous page

XB donor	XB acceptor	X	B	E_{int}	d_{int}	IBSI^{H}	IBSI^{PRO}	IBSI^{GBP}
FCl	CH_2S	Cl	S	-9.781415	2.543	0.05626	0.21894	0.143
FCl	CH_3OH	Cl	O	-7.03658	2.431	0.03290	0.14910	0.083
FCl	H_2O	Cl	O	-5.364156	2.544	0.02319	0.11647	0.061
FCl	H_2S	Cl	S	-5.368393	2.815	0.02886	0.12238	0.070
FCl	HCN	Cl	N	-4.818638	2.636	0.02068	0.10552	0.053
FCl	NH_3	Cl	N	-11.651009	2.298	0.05877	0.23775	0.143
FCl	Oxirane	Cl	O	-7.78485	2.388	0.03733	0.15650	0.094
FCl	PH_3	Cl	P	-20.50979	2.184	0.15436	0.47284	0.353
FCl	Thiirane	Cl	S	-13.15334	2.483	0.06624	0.25368	0.167
FI	CH_2O	I	O	-10.12494	2.586	0.03243	0.15807	0.082
FI	CH_2S	I	S	-14.712791	2.760	0.05194	0.20297	0.133
FI	CH_3OH	I	O	-12.06356	2.534	0.03702	0.17450	0.092
FI	H_2O	I	O	-9.448778	2.624	0.02879	0.14707	0.072
FI	H_2S	I	S	-9.958498	2.924	0.03498	0.14846	0.089
FI	HCN	I	N	-9.552144	2.620	0.03301	0.16518	0.087
FI	NH_3	I	N	-17.96776	2.491	0.05274	0.21784	0.124
FI	Oxirane	I	O	-12.7146	2.512	0.03942	0.17480	0.098
FI	PH_3	I	P	-16.47788	2.693	0.06771	0.24211	0.166
FI	Thiirane	I	S	-17.30951	2.760	0.05393	0.18099	0.137
HBr	CH_2O	Br	O	-2.109841	3.107	0.00860	0.03622	0.020
HBr	CH_2S	Br	S	-2.186941	3.562	0.00757	0.03050	0.017
HBr	CH_3OH	Br	O	-2.25889	3.080	0.00855	0.03819	0.021
HBr	H_2O	Br	O	-1.686314	3.117	0.00910	0.03649	0.019
HBr	H_2S	Br	S	-1.38504	3.650	0.00583	0.02573	0.014
HBr	HCN	Br	N	-1.435816	3.246	0.00764	0.03187	0.016
HBr	NH_3	Br	N	-2.262964	3.171	0.01020	0.03770	0.020
HBr	Oxirane	Br	O	-2.79531	3.052	0.00876	0.03864	0.023
HBr	PH_3	Br	P	-1.28236	3.735	0.00478	0.02433	0.013
HBr	Thiirane	Br	S	-2.88576	3.507	0.00882	0.03082	0.019
HI	CH_2O	I	O	-2.901197	3.155	0.00881	0.04375	0.022
HI	CH_2S	I	S	-2.978537	3.596	0.00741	0.03818	0.020
HI	CH_3OH	I	O	-3.24772	3.114	0.01115	0.04777	0.025
HI	H_2O	I	O	-2.543681	3.172	0.00839	0.04322	0.021
HI	H_2S	I	S	-1.995972	3.710	0.00541	0.03112	0.016
HI	HCN	I	N	-2.246903	3.308	0.00588	0.03705	0.018
HI	NH_3	I	N	-3.595643	3.187	0.01262	0.04875	0.025
HI	Oxirane	I	O	-3.79304	3.087	0.01109	0.04888	0.026
HI	PH_3	I	P	-1.92365	3.779	0.00504	0.03066	0.015
HI	Thiirane	I	S	-3.88741	3.538	0.00889	0.03882	0.023

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Table S2 – continued from previous page

XB donor	XB acceptor	X	B	E_{int}	d_{int}	$IBSI^{H}$	$IBSI^{PRO}$	$IBSI^{GBP}$
I_2	CH_2O	I	O	-4.758603	2.903	0.01522	0.07893	0.039
I_2	CH_2S	I	S	-6.463099	3.110	0.02228	0.10263	0.059
I_2	CH_3OH	I	O	-5.6749	2.827	0.01657	0.09249	0.046
I_2	H_2O	I	O	-4.342814	2.933	0.01501	0.07398	0.036
I_2	H_2S	I	S	-4.203034	3.302	0.01552	0.07021	0.037
I_2	HCN	I	N	-4.023849	3.036	0.01485	0.06766	0.032
I_2	NH_3	I	N	-8.177679	2.758	0.02757	0.12194	0.065
I_2	Oxirane	I	O	-6.42749	2.788	0.01852	0.09432	0.051
I_2	PH_3	I	P	-5.00193	3.207	0.01997	0.09123	0.052
I_2	Thiirane	I	S	-8.57727	3.033	0.02821	0.10648	0.073

Table S3: IBSI values and X$\cdots$B interaction distances (d_{int}, Å) for **Set 3** (n = 64). X = XB donor atom; B = XB acceptor atom. Dissociation energies ($-E_{diss}$ in kcal mol^{-1}) calculated at CCSD(T)CBS level of theory[S3] . Some points were removed from the respective linear fits (see Outlier Removal Section below).

XB donor	XB acceptor	X	B	$-E_{diss}$	d_{int}	IBSI^{H}	IBSI^{PRO}	IBSI^{GBP}
BrI	NCH	I	N	-5.31	2.900	0.01556	0.08991	0.044
BrI	OCH_2	I	O	-6.10	2.783	0.02039	0.09273	0.052
ClBr	NCH	Br	N	-4.47	2.793	0.01779	0.08764	0.044
ClBr	OCH_2	Br	O	-5.27	2.663	0.02372	0.09125	0.057
ClI	NCH	I	N	-6.31	2.816	0.01862	0.10741	0.054
ClI	OCH_2	I	O	-7.08	2.716	0.02440	0.10490	0.062
FBr	OCH_2	Br	O	-8.60	2.452	0.03671	0.15809	0.095
HBr	NCH	Br	N	-1.41	3.236	0.00788	0.03260	0.016
HBr	OCH_2	Br	O	-2.10	3.112	0.00856	0.03566	0.020
HI	NCH	I	N	-2.24	3.298	0.00616	0.03785	0.018
HI	OCH_2	I	O	-2.87	3.163	0.00871	0.04273	0.022
I_2	NCH	I	N	-4.03	3.029	0.01493	0.06866	0.033
I_2	OCH_2	I	O	-4.78	2.892	0.01464	0.07683	0.041
F_3CI	NCH	I	N	-3.61	3.105	0.01322	0.05821	0.027
FBr	NCH	Br	N	-7.53	2.529	0.03268	0.16067	0.087
FCl	NCH	Cl	N	-4.81	2.613	0.02176	0.11143	0.056
NBS	NCH	Br	N	-4.32	2.816	0.01604	0.08302	0.041
NIS	NCH	I	N	-5.91	2.862	0.01591	0.09740	0.047
PhBr	NCH	Br	N	-1.15	3.189	0.00918	0.03621	0.018
PhI	NCH	I	N	-1.87	3.259	0.00752	0.04129	0.020
F_3CI	NH_3	I	N	-5.88	2.992	0.01644	0.07419	0.036
FBr	NH_3	Br	N	-15.30	2.357	0.06034	0.23908	0.146
FCl	NH_3	Cl	N	-10.54	2.348	0.05281	0.21054	0.126
NBS	NH_3	Br	N	-8.02	2.663	0.02944	0.11877	0.063
NIS	NH_3	I	N	-10.99	2.694	0.03227	0.14072	0.074
PhBr	NH_3	Br	N	-2.02	3.138	0.01057	0.04055	0.022
PhI	NH_3	I	N	-3.33	3.177	0.01332	0.04992	0.025
F_3CI	PCH	CI	P	-0.89	3.724	0.00465	0.03399	0.015
FBr	PCH	Br	P	-2.07	3.088	0.01673	0.08834	0.049
FCl	PCH	Cl	P	-1.16	3.163	0.01179	0.06231	0.034
NBS	PCH	Br	P	-1.19	3.410	0.00842	0.04693	0.024
NIS	PCH	I	P	-1.53	3.496	0.00997	0.05241	0.026
PhBr	PCH	Br	P	-0.85	3.634	0.00570	0.03004	0.014
PhI	PCH	I	P	-0.92	3.764	0.00431	0.03158	0.015
Br_2	FCCH	Br	F	-0.74	3.191	0.00412	0.02580	0.010
Br_2	FMe	Br	F	-2.87	2.811	0.01189	0.05517	0.030

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Table S3 – continued from previous page

XB donor	XB acceptor	X	B	E_{int}	d_{int}	$IBSI^{H}$	$IBSI^{PRO}$	$IBSI^{GBP}$
Br_2	HLi	Br	H	-23.11	1.634	0.18485	0.44721	0.382
Br_2	NCH	Br	N	-3.61	2.868	0.01351	0.07340	0.037
Br_2	NH_3	Br	N	-7.29	2.670	0.03043	0.11693	0.065
Br_2	OCH_2	Br	O	-4.41	2.757	0.01817	0.07404	0.045
Br_2	OPH_3	Br	O	-5.95	2.682	0.02386	0.09809	0.054
Br_2	PCH	Br	P	-1.18	3.443	0.00883	0.04408	0.020
Br_2	$PdHP_2Cl$	Br	P	-9.00	2.967	0.02523	0.08607	0.053
Br_2	pyr	Br	N	-9.07	2.578	0.03499	0.14375	0.087
FI	FCCH	I	F	-0.29	3.028	0.00255	0.01191	0.008
FI	FMe	I	F	-5.97	2.664	0.02264	0.11104	0.050
FI	HLi	I	H	-33.79	1.849	0.12846	0.32927	0.259
FI	NCH	I	N	-9.33	2.615	0.03349	0.16708	0.088
FI	NH_3	I	N	-17.11	2.509	0.05047	0.20965	0.120
FI	OCH_2	I	O	-9.94	2.577	0.03392	0.15282	0.084
FI	OPH_3	I	O	-13.36	2.503	0.04145	0.18205	0.102
FI	PCH	I	P	-2.74	3.177	0.01642	0.09657	0.051
FI	$PdHP_2Cl$	I	Cl	-17.66	2.828	0.04340	0.14132	0.098
FI	pyr	I	N	-20.34	2.428	0.06209	0.24905	0.154
MeI	FCCH	I	F	-0.50	3.399	0.00430	0.02225	0.010
MeI	FMe	I	F	-1.70	3.188	0.00665	0.03263	0.017
MeI	HLi	I	H	-3.62	2.747	0.01964	0.06233	0.038
MeI	NCH	I	N	-1.42	3.288	0.00671	0.03865	0.019
MeI	NH_3	I	N	-2.73	3.210	0.01200	0.04615	0.024
MeI	OCH_2	I	O	-2.39	3.176	0.00944	0.03944	0.022
MeI	OPH_3	I	O	-3.34	3.145	0.01117	0.04424	0.024
MeI	PCH	I	P	-0.85	3.770	0.00425	0.03117	0.014
MeI	$PdHP_2Cl$	I	Cl	-5.05	3.515	0.00982	0.03497	0.020
MeI	pyr	I	N	-3.61	3.116	0.01468	0.05687	0.030

Table S4: Final fitted parameters for the equation $E_{int} = m \times IBSI + b$. MAE values in kcal mol^{-1}.

System	m	b	R^2	r	τ	ρ	MAE
Set 1							
IBSI$^{\mathrm{GBP}}$	-98.9	-0.3854	0.88	-0.94	-0.76	-0.91	0.62
IBSI$^{\mathrm{PRO}}$	-67.7	0.1980	0.87	-0.93	-0.69	-0.87	0.70
IBSI$^{\mathrm{H}}$	-236.5	-0.4485	0.87	-0.93	-0.73	-0.90	0.67
Set 2							
IBSI$^{\mathrm{GBP}}$	-91.2	-0.8735	0.90	-0.95	-0.85	-0.97	0.84
IBSI$^{\mathrm{PRO}}$	-58.4	-0.2346	0.91	-0.95	-0.85	-0.97	0.79
IBSI$^{\mathrm{H}}$	-227.0	-0.8814	0.90	-0.95	-0.83	-0.96	0.89
Set 3							
IBSI$^{\mathrm{GBP}}$	-122.6	0.5568	0.87	-0.93	-0.81	-0.93	1.10
IBSI$^{\mathrm{PRO}}$	-70.8	0.9987	0.88	-0.94	-0.79	-0.92	0.97
IBSI$^{\mathrm{H}}$	-301.8	0.6092	0.90	-0.95	-0.81	-0.94	0.98

Table S5: List of outliers for IBSI^{GBP} methods as identified by the minimum covariance determinant (MCD) method[S4,S5]. These points were removed from the final linear models. In bold, the common outliers with IBSI^{PRO} are given.

XB donor	XB acceptor	X	B	E_{int} (kcal mol^{-1})	d_{int} (Å)	IBSI^{GBP}
Set 1						
chlorine	**trimethylamine**	Cl	N	**-14.52**	2.303	**0.156**
chlorine	**dimethylthioether**	Cl	S	**-9.06**	2.614	**0.118**
chlorine	**thioacetone**	Cl	S	**-7.33**	2.639	**0.115**
bromine	**trimethylamine**	Br	N	**-17.14**	2.423	**0.141**
iodine	**trimethylamine**	I	N	**-15.62**	2.613	**0.109**
Set 2						
FBr	PH_3	Br	P	-18.63	2.248	0.240
FCl	**PH_3**	Cl	P	**-20.51**	2.184	**0.353**
FI	**NH_3**	I	N	**-17.97**	2.491	**0.124**
FI	**Thiirane**	I	S	**-17.31**	2.760	**0.137**
Set 3						
Br_2	**HLi**	Br	H	**-23.11**	1.634	**0.382**
FI	**HLi**	I	H	**-33.79**	1.849	**0.259**

Table S6: Final list of outliers for when using IBSI^{PRO} as identified by the minimum covariance determinant (MCD) method[S4,S5]. These points were removed from the final linear models. In bold, the common outliers with IBSI^{GBP} are given.

XB donor	XB acceptor	X	B	E_{int} (kcal mol^{-1})	d_{int} (Å)	IBSI^{PRO}
Set 1						
chlorine	pyrazine	Cl	N	-5.86	2.476	0.15346
chlorine	**trimethylamine**	Cl	N	**-14.52**	2.303	**0.23489**
chlorine	**dimethylthioether**	Cl	S	**-9.06**	2.614	**0.18947**
chlorine	**thioacetone**	Cl	S	**-7.33**	2.639	**0.16351**
bromine	**trimethylamine**	Br	N	**-17.14**	2.423	**0.20456**
iodine	**trimethylamine**	I	N	**-15.62**	2.613	**0.16779**
Set 2						
FBr	Thiirane	Br	S	-17.15	2.561	0.21605
FCl	**PH_3**	Cl	P	**-20.51**	2.184	**0.47284**
FI	**NH_3**	I	N	**-17.97**	2.491	**0.21784**
FI	**Thiirane**	I	S	**-17.31**	2.760	**0.18099**
Set 3						
Br_2	**HLi**	Br	H	**-23.11**	1.634	**0.44721**
FI	**HLi**	I	H	**-33.79**	1.849	**0.32927**
FI	$PdHP_2Cl$	I	Cl	-17.66	2.828	0.14132

Table S7: van der Waals radii (Å) used for the calculation of $V_{overlap}$.[S6]

Atom	R_{vdw}
Cl	1.75
Br	1.85
I	1.98
O	1.52
N	1.55
F	1.47
P	1.80
S	1.80
H	1.20

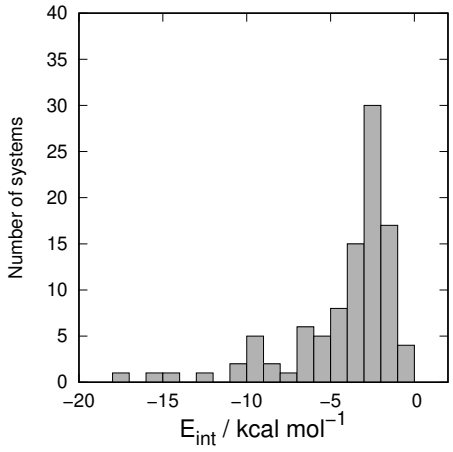

Figure S1: A histogram showing the distribution of E_{int} for systems in **Set 1**.

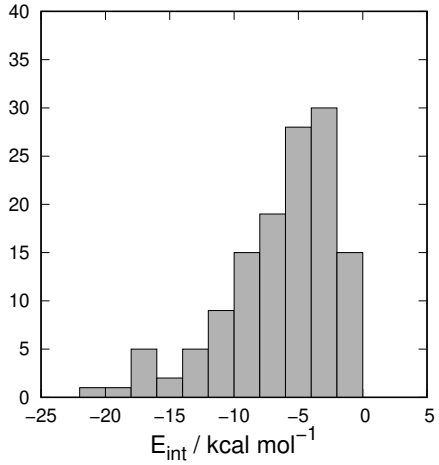

Figure S2: A histogram showing the distribution of E_{int} for systems in **Set 2**.

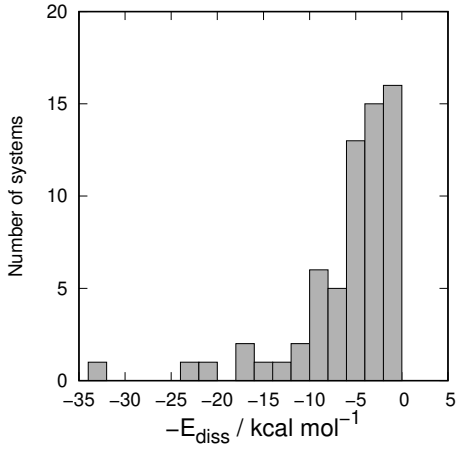

Figure S3: A histogram showing the distribution of $-E_{diss}$ for systems in **Set 3**.

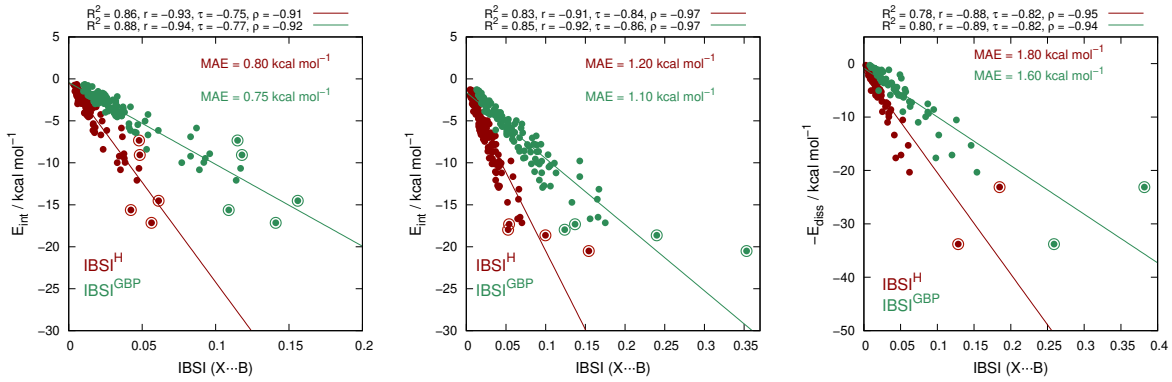

Figure S4: E_{int} as a function of IBSI (IBSI^{GBP} and IBSI^{H}) for the full **Set 1** (left, n = 99) and **Set 2** (center, n = 124). $-E_{diss}$ as a function of IBSI for the full **Set 3** (right, n = 69) is also represented. Bivariate outliers are marked with circles (Table S5).

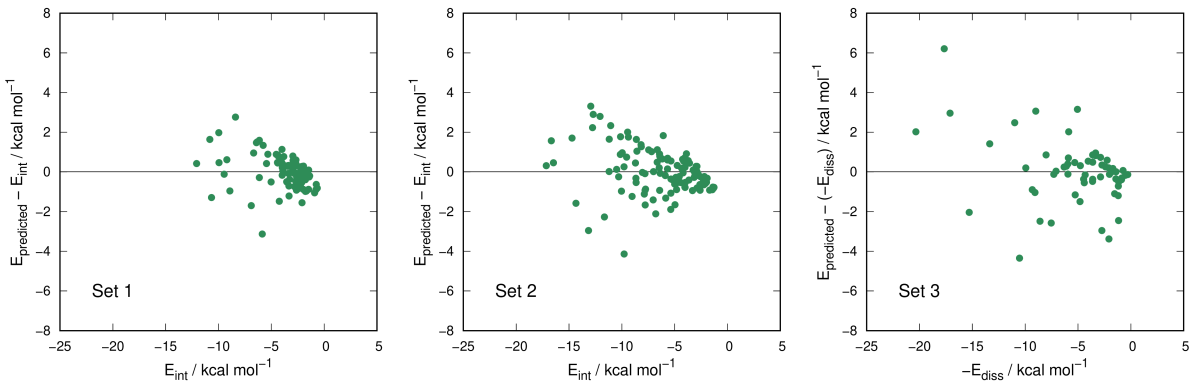

Figure S5: $E_{int}/-E_{diss}$ as a function of the difference between $E_{predicted}$ and the reference value for the final datasets calculated using IBSI^{GBP} values.

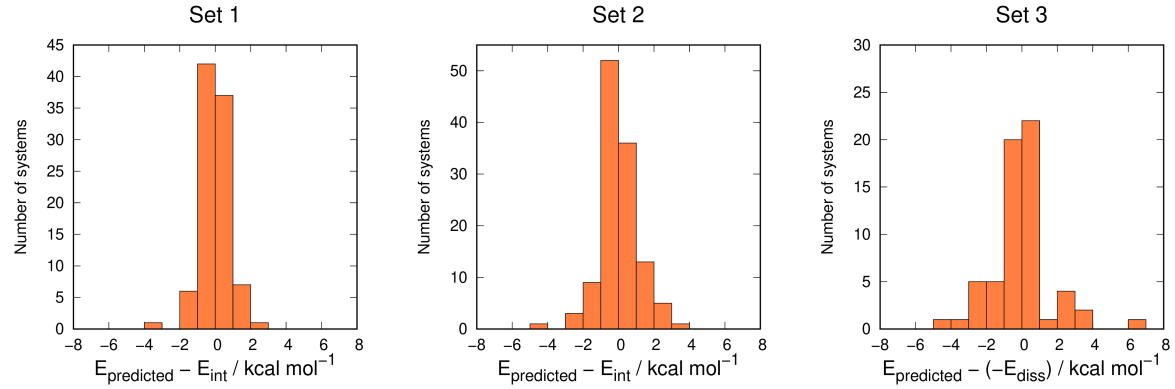

Figure S6: Histograms of the difference between $E_{predicted}$ and the reference $E_{int}/-E_{diss}$ values for the final datasets calculated using IBSI^{GBP} values.

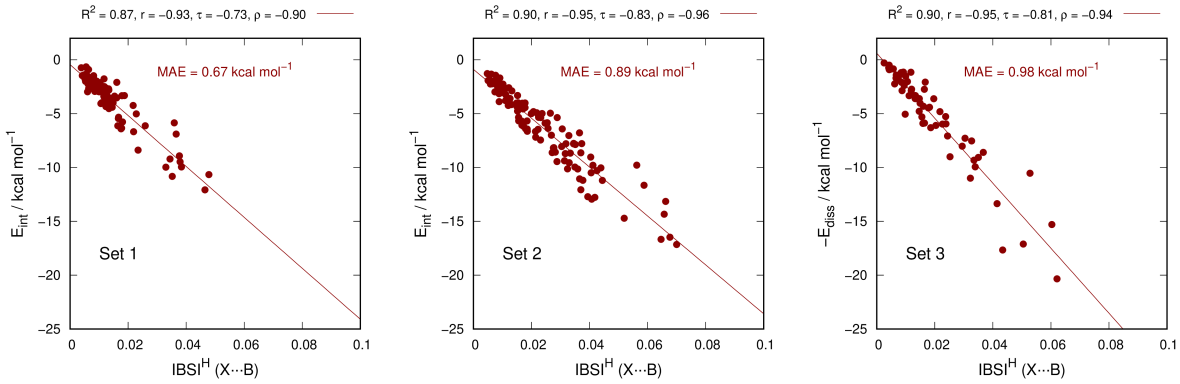

Figure S7: Interaction energies (E_{int}, **Set 1-Set 2**) or dissociation energies ($-E_{diss}$, **Set 3**) as a function of IBSI^{H}. The number of points used for the linear fit was 94, 120, and 62 respectively).

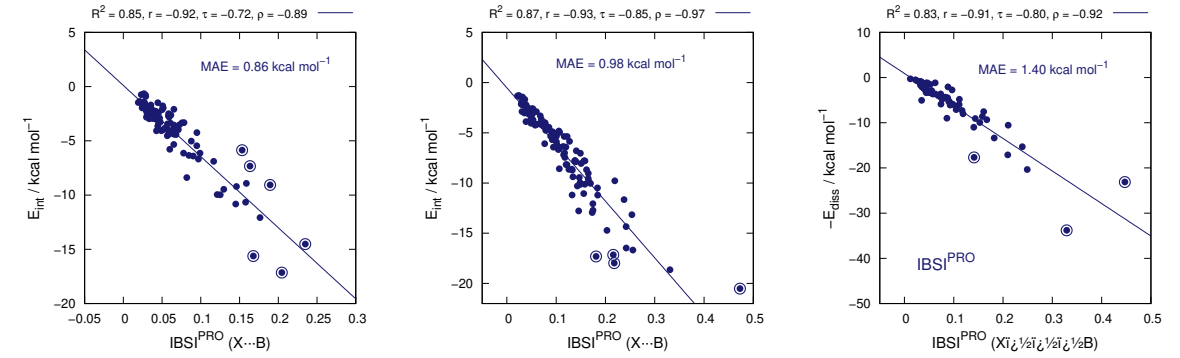

Figure S8: E_{int} as a function of IBSI^{PRO} for the full **Set 1** (left, n = 99) and **Set 2** (center, n = 124). $-E_{diss}$ as a function of IBSI^{PRO} for the full **Set 3** (right, n = 69) is also represented. Bivariate outliers are marked with circles (Table S6).

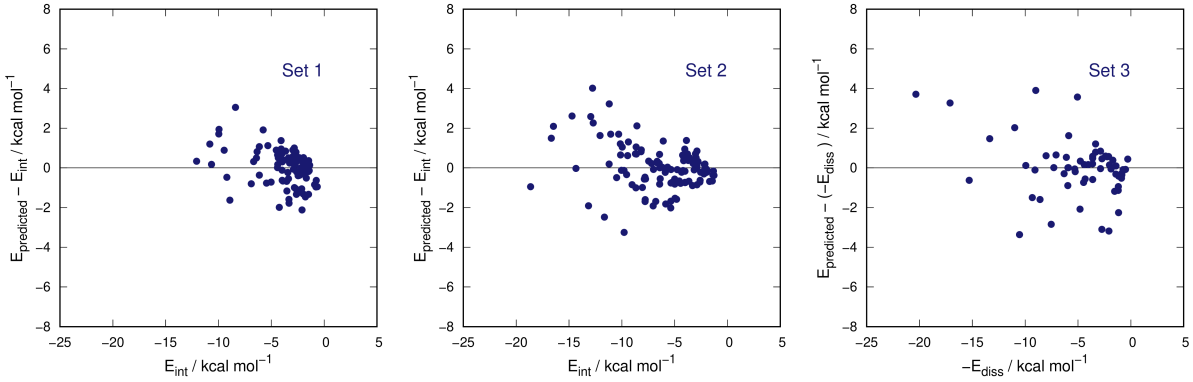

Figure S9: $E_{int}/-E_{diss}$ as a function of the difference between $E_{predicted}$ and the reference value for the final datasets calculated using IBSI^{PRO} values.

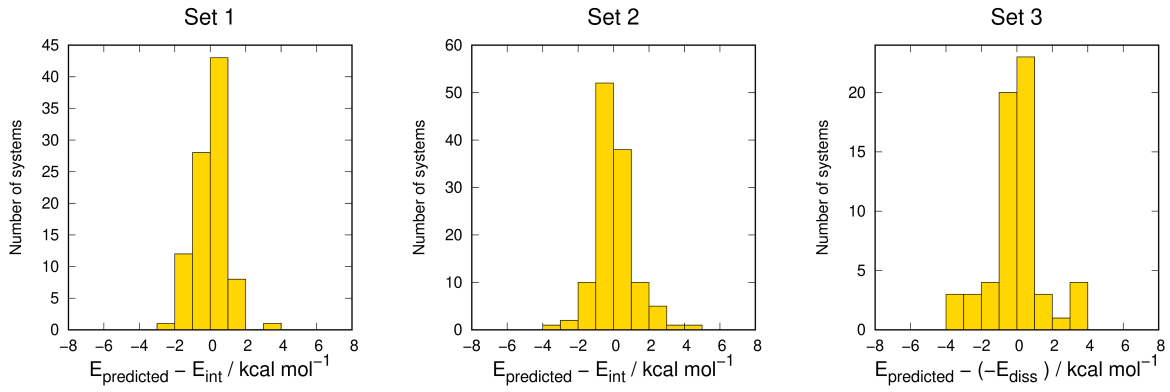

Figure S10: Histograms of the difference between $E_{predicted}$ and the reference $E_{int}/-E_{diss}$ values for the final datasets calculated using IBSI$^{\text{PRO}}$ values.

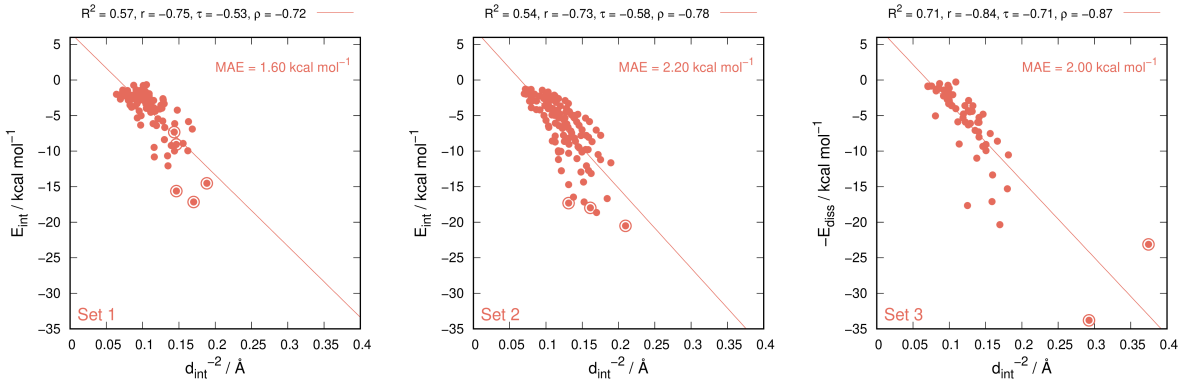

Figure S11: Interaction energies (E_{int}, **Set 1-Set 2**) or dissociation energies ($-E_{diss}$, **Set 3**) as a function of $1/d^2$ for the full sets. Common bivariate outliers (Tables S5-S6) are marked with circles.

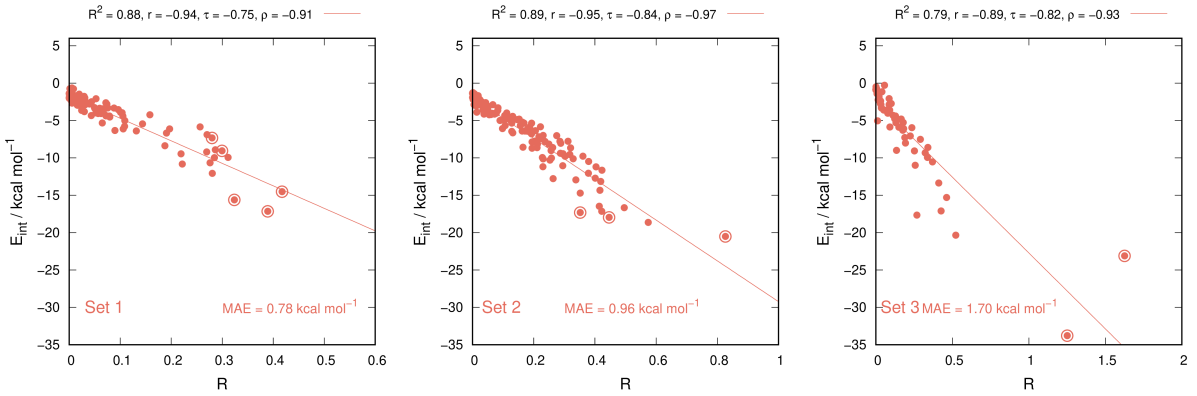

Figure S12: Interaction energies (E_{int}, **Set 1-Set 2**) or dissociation energies ($-E_{diss}$, **Set 3**) as a function of R as defined in Equations 9-10 for the full sets. Common bivariate outliers (Tables S5-S6) are marked with circles.

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