Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting information for

Halogen Bonding from the Bonding Perspective with Considerations for Mechanisms of Thyroid Hormone Activation and Inhibition

C.A. Bayse

M06-2X/aug-cc-pvtz results:
R-X molecules

bs2	E	C-X, ang	%x C-I	100-%C-I	%xp C-X	εHOMO	εϕR-X*
MeF	-139.74222	1.3797	71.80	28.20	73.14	-0.42982	0.01510
EtF	-179.05580	1.3886	72.20	27.80	72.84	-0.40573	0.01286
PhF	-331.47681	1.3430	71.95	28.05	69.67	-0.30942	0.03586
4F-Pyr	-347.51819	1.3355	71.82	28.18	69.41	-0.33703	0.01906
HCCF	-176.55288	1.2749	70.80	29.20	69.07	-0.35875	0.00732
MeCl	-500.10670	1.7825	56.02	43.98	83.27	-0.36236	0.00988
CF3Cl	-797.87613	1.7574	53.96	46.04	86.84	-0.42647	0.00858
CCl4	-1878.90543	1.7684	50.15	49.85	83.72	-0.38628	-0.02504
PhCl	-691.83541	1.7406	54.63	45.37	80.94	-0.30560	0.03134
4Cl-Pyr	-707.87586	1.7342	54.23	45.77	80.91	-0.33744	0.01675
1,3,5-Cl3Ph	-1611.05374	1.7334	53.93	46.07	81.22	-0.32195	0.01332
EtCl	-539.41735	1.7968	56.52	43.48	83.38	-0.35782	0.02675
C6F5Cl	-1188.05075	1.7120	51.69	48.31	82.20	-0.33332	-0.02461
C6Cl6	-2989.85933	1.7168	51.96	48.04	81.88	-0.31909	-0.02648
3,4,5-Cl3Pyr	-1627.08740	1.7122	52.30	47.70	81.22	-0.32660	-0.00276
HCCCl	-536.92664	1.6397	51.87	48.13	79.79	-0.34165	0.00707
MeCCCl	-576.24419	1.6446	51.87	48.13	80.02	-0.31955	0.00498
MeBr	-2614.14242	1.9394	52.41	47.59	86.62	-0.33815	0.00088
CF3Br	-2911.90695	1.9267	50.68	49.32	89.99	-0.38899	-0.01096
CCl3Br	-3992.93828	1.9443	44.95	55.05	88.25	-0.36620	-0.04189
CBr4	-10335.03876	1.9364	44.87	55.13	87.06	-0.34970	-0.06586
CHBr3	-7761.41234	1.9268	47.07	52.93	87.21	-0.34449	-0.04170
CH2Br2	-5187.77987	1.9261	49.65	50.35	87.08	-0.34476	-0.01704

PhBr	-2805.86897	1.8962	50.73	49.27	84.78	-0.30172	0.01458
C6F5Br	-3302.08596	1.8678	47.34	52.66	86.05	-0.32859	-0.02752
C6Cl5Br	-5103.89252	1.8753	47.53	52.47	85.84	-0.31654	-0.03427
C6Br6	-15674.05524	1.8791	47.53	52.47	85.81	-0.31158	-0.05367
1,3,5-Br3Ph	-7953.15440	1.8902	49.86	50.14	85.11	-0.31673	-0.01473
4ClPhBr	-3265.47889	1.8927	50.33	49.67	84.88	-0.30081	0.01089
4MePhBr	-2845.17986	1.8962	50.79	49.21	84.76	-0.29195	0.01926
4NMe2PhBr	-2939.82609	1.8961	50.88	49.12	84.74	-0.24892	0.02164
4COOHPhBr	-2994.46272	1.8909	50.37	49.63	84.70	-0.31457	0.01199
4CONH2PhBr	-2974.58399	1.8918	50.42	49.58	84.78	-0.31055	0.01302
4CONHMePhBr	-3013.88474	1.8926	50.48	49.52	84.78	-0.30742	0.01237
4Br-Pyr	-2821.90922	1.8896	50.21	49.79	84.78	-0.33026	0.00813
3,4,5-Br3Pyr	-7969.18764	1.8723	47.89	52.11	85.25	-0.31954	-0.02547
HCCBr	-2650.96174	1.7916	47.17	52.83	83.92	-0.33367	0.00391
MeCCBr	-2690.27964	1.7953	47.23	52.77	84.11	-0.31383	0.00647
Br4-ethene	-10373.13377	1.8768	46.73	53.27	85.95	-0.30832	-0.01980
cis-Br2-ethene	-5225.86160	1.8714	50.31	49.69	85.17	-0.31098	0.00066
BrCN	-2667.05901	1.7892	46.48	53.52	86.15	-0.38824	-0.02093
trans-Br2-ethene	-5225.86143	1.8822	50.66	49.34	85.53	-0.30987	-0.00384
Br-ethene	-2652.21867	1.8899	51.91	48.09	85.05	-0.31768	0.01788
EtBr	-2653.45244	1.9556	53.18	46.82	86.82	-0.33434	0.00572
C2F5Br	-3149.72256	1.9256	49.78	50.22	89.14	-0.39189	-0.01453
C2Cl5Br	-4951.45382	1.9448	45.40	54.60	86.89	-0.36050	-0.03252
MeI	-335.52522	2.1392	48.01	51.99	89.76	-0.31171	-0.01363
CF3I	-633.28595	2.1461	46.03	53.97	92.88	-0.35174	-0.04100
CCl3I	-1714.32035	2.1630	38.38	61.62	92.01	-0.33815	-0.06401
CBr3I	-8056.42047	2.1570	37.77	62.23	91.35	-0.33046	-0.07779
CI4	-1220.56809	2.1591	38.75	61.25	90.53	-0.31219	-0.09689
EtI	-374.83380	2.1568	48.89	51.11	89.99	-0.30838	-0.00821
C2F5I	-871.10171	2.1454	44.66	55.34	92.32	-0.35438	-0.04438
C2Cl5I	-2672.83568	2.1675	38.65	61.35	91.06	-0.33390	-0.05805
PhI	-527.24925	2.1003	45.74	54.26	88.62	-0.29274	-0.00791
1,3,5-I3Ph	-1117.29646	2.0965	44.72	55.28	88.97	-0.30446	-0.04208

C6F5I	-1023.46959	2.0755	41.62	58.38	89.92	-0.31880	-0.03835
C6Cl5I	-2825.27360	2.0879	41.79	58.21	89.78	-0.31030	-0.04379
C6Br5I	-13395.43528	2.0954	41.78	58.22	89.88	-0.30695	-0.06034
4ClPhI	-986.85930	2.0969	45.23	54.77	88.72	-0.29422	-0.01327
3ClPhI	-986.85922	2.0968	45.13	54.87	88.80	-0.30039	-0.01490
3,5-Cl2PhI	-1446.46795	2.0953	44.60	55.40	89.00	-0.30868	-0.02292
2,6-Cl2PhI	-1446.46304	2.0866	42.63	57.37	89.36	-0.30365	-0.02288
2,4,6-Cl3PhI	-1906.07114	2.0844	42.32	57.68	89.43	-0.30443	-0.02861
4FPhI	-626.50059	2.0978	45.28	54.72	88.74	-0.29427	-0.01149
3,5-F2PhI	-725.75098	2.0944	44.55	55.45	88.96	-0.30857	-0.01806
2,6-F2PhI	-725.74898	2.0776	42.72	57.28	89.48	-0.30352	-0.01486
2,4,6-F3PhI	-824.99847	2.0763	42.38	57.62	89.59	-0.30524	-0.01904
2,3,5,6F4PhI2	-822.27324	2.0971	45.24	54.76	88.73	-0.28924	-0.01803
1,4-I2Ph	-1219.25319	2.0745	41.74	58.26	89.84	-0.30907	-0.04077
4MePhI	-566.56022	2.0998	45.83	54.17	88.57	-0.28518	-0.00605
2,4,6-Me3PhI	-645.18419	2.1128	47.08	52.92	88.49	-0.28017	-0.00155
4-MeOPhI	-641.77502	2.0969	45.68	54.32	88.58	-0.27455	-0.00563
4NO2PHI	-731.76116	2.0931	44.69	55.31	88.79	-0.31741	-0.06861
4NMe2PhI	-661.20670	2.0978	46.00	54.00	88.51	-0.24762	-0.00629
4CNPhI	-619.49631	2.0944	44.82	55.18	88.80	-0.31111	-0.04206
4COOHPhI	-715.84289	2.0960	45.26	54.74	88.66	-0.30432	-0.03837
4CONH2PhI	-695.96427	2.0967	45.33	54.67	88.66	-0.30106	-0.02903
4CONHMePhI	-735.26500	2.0959	45.39	54.61	88.62	-0.29848	-0.02461
4I-Pyr	-543.28948	2.0955	45.07	54.93	88.69	-0.31470	-0.01730
HCCI	-372.34625	1.9925	40.99	59.01	88.06	-0.31895	-0.01251
MeCCI	-411.66435	1.9938	41.18	58.82	88.17	-0.30266	-0.00531
ICCI	-667.36791	1.9905	40.37	59.63	88.53	-0.30281	-0.02681
I4-ethene	-1258.66250	2.0956	41.01	58.99	89.75	-0.29643	-0.04502
cis-I2-ethene	-668.62434	2.0766	45.28	54.72	88.92	-0.29816	-0.02333
trans-I2-ethene	-668.62513	2.0920	45.81	54.19	89.29	-0.29655	-0.03053
I-ethene	-373.59932	2.0897	46.99	53.01	88.67	-0.30280	-0.00338
ICN	-388.44518	1.9976	40.29	59.71	89.93	-0.36227	-0.04388
ICCCN	-464.59289	1.9837	39.78	60.22	88.66	-0.34171	-0.03497
4HCCPhI	-603.39384	1.9908	40.99	59.01	88.21	-0.28426	-0.01517

RX-SeMe2 XB complexes

	E, a.u.	Se-X, ang	C-X, ang	dC-X	WBI ΔE kcal/mol		NBO ΔEd->a kcal/mol
MeCl	-2981.53567	3.5591	1.7849	0.0024	0.0139	-1.98	1.29
CF3Cl	-3279.30640	3.4356	1.7575	0.0001	0.0217	-2.80	2.47
CCl4	-4360.33632	3.3671	1.7711	0.0027	0.0290	-3.19	3.03
PhCl	-3173.26465	3.5768	1.7418	0.0012	0.0135	-2.15	1.09
4Cl-Pyr	-3189.30515	3.5187	1.7345	0.0003	0.0162	-2.18	1.53
1,3,5-Cl3Ph	-4092.48319	3.5112	1.7350	0.0016	0.0165	-2.28	1.56
EtCl	-3020.84623	3.5908	1.7980	0.0012	0.0122	-1.93	1.12
C6F5Cl	-3669.48084	3.4327	1.7155	0.0035	0.0217	-2.69	2.31
C6Cl6	-5471.28961	3.4512	1.7185	0.0017	0.0181	-2.80	1.78
3,4,5-Cl3Pyr	-4108.51755	3.449	1.7137	0.0015	0.0192	-2.72	2.08
HCCCl	-3018.35688	3.4495	1.6430	0.0033	0.0213	-2.78	1.94
MeCCCl	-3057.67416	3.4614	1.6481	0.0035	0.0193	-2.61	1.80
MeBr	-5095.57258	3.5998	1.9412	0.0018	0.0213	-2.73	2.32
Cf3Br	-5393.33905	3.4129	1.9312	0.0045	0.0383	-3.95	5.15
CCl3Br	-6474.37148	3.3351	1.9515	0.0072	0.0571	-4.64	6.93
CBr4	-12816.47157	3.3238	1.9470	0.0106	0.0597	-4.39	6.90
CH2Br2	-7669.21095	3.4934	1.9303	0.0042	0.0304	-3.31	3.48
PhBr	-5287.29930	3.5766	1.8986	0.0024	0.0226	-2.84	2.35
C6F5Br	-5783.51798	3.4046	1.8769	0.0091	0.0405	-3.90	4.69
C6Cl5Br	-7585.32457	3.4429	1.8826	0.0073	0.0347	-3.92	3.21
C6Br6	-18155.48716	3.407	1.8862	0.0071	0.0381	-3.83	4.93
1,3,5-Br3Ph	-10434.58532	3.5239	1.8940	0.0038	0.0276	-3.21	2.91
4ClPhBr	-5746.90936	3.5598	1.8961	0.0034	0.0245	-2.92	2.53
4MePhBr	-5326.61017	3.5871	1.8990	0.0028	0.0219	-2.82	2.28
4NMe2PhBr	-5421.25630	3.6162	1.8978	0.0017	0.0196	-2.76	1.95
4COOHPhBr	-5475.89323	3.5499	1.8940	0.0031	0.0250	-2.95	2.64
4CONH2PhBr	-5456.01461	3.5563	1.8949	0.0031	0.0245	-3.02	2.57
4CONHMePhBr	-5495.31530	3.5612	1.8963	0.0037	0.0240	-2.98	2.50
4Br-Pyr	-5303.33982	3.5503	1.8925	0.0029	0.0255	-3.01	2.66
3,4,5-Br3Pyr	-10450.61961	3.4299	1.8788	0.0065	0.0363	-3.87	4.15

HCCBr	-5132.39375	3.4222	1.8008	0.0092	0.0375	-3.89	4.12
MeCCBr	-5171.71132	3.4473	1.8033	0.0080	0.0335	-3.68	3.60
Br4-ethene	-12854.56565	3.3952	1.8837	0.0069	0.0427	-3.81	4.99
cis-Br2-ethene	-7707.29214	3.5521	1.8752	0.0038	0.0250	-2.97	2.62
BrCN	-5148.49300	3.331	1.8040	0.0148	0.0532	-5.13	6.29
trans-Br2-ethene	-7707.29207	3.54	1.8870	0.0048	0.0259	-3.03	2.81
Br-ethene	-5133.64885	3.6007	1.8912	0.0013	0.0212	-2.74	2.16
EtBr	-5134.88233	3.631	1.9562	0.0006	0.0192	-2.56	1.98
C2F5Br	-5631.15463	3.3966	1.9306	0.0050	0.0411	-3.93	5.56
C2Cl5Br	-7432.88667	3.34	1.9539	0.0091	0.0564	-4.42	6.87
MeI	-2816.95700	3.616	2.1442	0.0050	0.0374	-3.75	4.54
CF3I	-3114.72101	3.4131	2.1558	0.0097	0.0707	-5.80	10.14
CCl3I	-4195.75714	3.2821	2.1834	0.0204	0.1227	-6.89	15.90
CBr3I	-10537.85779	3.2545	2.1818	0.0248	0.1349	-7.22	16.90
CI4	-3702.00449	3.2692	2.1802	0.0211	0.1291	-6.65	15.37
EtI	-2856.26530	3.6549	2.1585	0.0017	0.0328	-3.57	3.83
C2F5I	-3352.53720	3.3976	2.1572	0.0118	0.0779	-6.07	10.80
C2Cl5I	-5154.27234	3.2841	2.1909	0.0234	0.1241	-6.81	15.30
PhI	-3008.68154	3.6057	2.1053	0.0050	0.0392	-4.07	4.08
1,3,5-I3Ph	-3598.72952	3.5193	2.1054	0.0089	0.0519	-4.55	5.73
C6F5I	-3504.90481	3.3989	2.0950	0.0195	0.0782	-5.90	8.83
C6Cl5I	-5306.70833	3.4303	2.1041	0.0162	0.0705	-5.60	5.52
C6Br5I	-15876.87007	3.4221	2.1107	0.0153	0.0736	-5.63	7.51
4ClPhI	-3468.29185	3.5867	2.1006	0.0037	0.0424	-4.23	4.34
3ClPhI	-3468.29211	3.5644	2.1027	0.0059	0.0449	-4.44	4.75
3,5-Cl2PhI	-3927.90122	3.5292	2.1028	0.0075	0.0507	-4.68	5.37
2,6-Cl2PhI	-3927.89684	3.4978	2.0981	0.0115	0.0569	-5.01	6.15
2,4,6-Cl3PhI	-4387.50525	3.4708	2.0976	0.0132	0.0621	-5.21	6.79
4FPhI	-3107.93311	3.5916	2.1014	0.0036	0.0416	-4.21	4.27
3,5-F2PhI	-3207.18415	3.5365	2.1018	0.0074	0.0496	-4.62	5.17
2,6-F2PhI	-3207.18277	3.4948	2.0894	0.0118	0.0566	-5.01	6.27
2,4,6-F3PhI	-3306.43259	3.4706	2.0901	0.0138	0.0614	-5.21	6.83
2,3,5,6F4PhI2	-3303.70589	3.5568	2.1035	0.0064	0.0453	-4.29	4.91

1,4-I2Ph	-3700.68825	3.4083	2.0926	0.0181	0.0755	-5.80	8.54
4MePhI	-3047.99240	3.6145	2.1021	0.0023	0.0378	-4.00	3.91
2,4,6-Me3PhI	-3126.61592	3.6235	2.1163	0.0035	0.0358	-3.71	4.09
4-MeOPhI	-3123.20730	3.6043	2.1018	0.0049	0.0386	-4.06	4.04
4NO2PHI	-3213.19439	3.5288	2.1005	0.0074	0.0509	-4.66	5.40
4NMe2PhI	-3142.63871	3.6049	2.1011	0.0033	0.0371	-3.89	4.02
4CNPhI	-3100.92933	3.5568	2.0994	0.0050	0.0474	-4.52	4.86
4COOHPhI	-3197.27557	3.567	2.1014	0.0054	0.0444	-4.31	4.66
4CONH2PhI	-3177.39699	3.5715	2.1010	0.0043	0.0437	-4.34	4.59
4CONHMePhI	-3216.69762	3.5749	2.1010	0.0051	0.0430	-4.27	4.51
4I-Pyr	-3024.72230	3.5437	2.1025	0.0070	0.0476	-4.40	5.19
HCCI	-2853.78134	3.435	2.0107	0.0182	0.0668	-5.82	7.25
MeCCI	-2893.09886	3.4746	2.0093	0.0155	0.0586	-5.46	6.00
ICCI	-3148.80337	3.4181	2.0106	0.0201	0.0711	-6.06	7.62
I4-ethene	-3740.09762	3.387	2.1150	0.0194	0.0848	-5.84	9.70
cis-I2-ethene	-3150.05693	3.5578	2.0849	0.0083	0.0455	-4.25	5.27
trans-I2-ethene	-3150.05799	3.5379	2.0996	0.0076	0.0491	-4.42	5.78
I-ethene	-2855.03137	3.6028	2.0958	0.0061	0.0382	-3.92	4.40
ICN	-2869.88357	3.2953	2.0314	0.0338	0.1069	-7.89	13.84
ICCCN	-2946.03012	3.3481	2.0098	0.0261	0.0908	-7.17	9.72
4HCCPhI	-3084.82873	3.4424	2.0081	0.0173	0.0647	-5.70	6.90

RX-Cl XB complexes						
	E, a.u.	Se-X, ang	C-X, ang	dC-X	WBI	delta E (kcal/mol)	NBO dEd->a
MeCl	-960.38017	3.3012	1.7788	-0.0037	0.0232	0.88	2.89
CF3Cl	-1258.16747	2.9914	1.7369	-0.0205	0.0528	-10.33	7.69
CCl4	-2339.19774	2.8834	1.7572	-0.0112	0.0583	-10.94	11.36
PhCl	-1152.11465	3.1306	1.7277	-0.0129	0.0330	-2.74	4.33
4Cl-Pyr	-1168.16112	3.0841	1.7190	-0.0152	0.0388	-6.52	5.03
1,3,5-Cl3Ph	-2071.34067	3.0531	1.7227	-0.0107	0.0442	-7.57	5.59
EtCl	-999.69003	3.3412	1.7852	-0.0116	0.0200	1.37	2.52
C6F5Cl	-1648.34214	2.9663	1.7169	0.0049	0.0635	-10.37	7.84
C6Cl6	-3450.15007	2.9693	1.7146	-0.0022	0.0601	-9.96	7.07

3,4,5-Cl3Pyr	-2087.37637	3.0009	1.7069	-0.0053	0.0535	-8.85	6.78
HCCCl	-997.21558	3.0313	1.6466	0.0069	0.0434	-8.83	5.94
MeCCCl	-1036.52928	3.0588	1.6510	0.0064	0.0395	-6.41	5.22
MeBr	-3074.42125	3.1677	1.9486	0.0092	0.0565	-2.48	7.54
Cf3Br	-3372.20580	2.8937	1.9304	0.0037	0.1163	-15.05	18.88
CCl3Br	-4453.24120	2.714	1.9864	0.0421	0.2333	-17.60	37.64
CBr4	-10795.34267	2.6706	1.9937	0.0573	0.2633	-18.22	43.16
CH2Br2	-5648.06861	2.995	1.9315	0.0054	0.0960	-8.70	12.83
PhBr	-3266.15363	3.0805	1.8973	0.0011	0.0672	-6.14	9.10
C6F5Br	-3762.38603	2.849	1.9099	0.0421	0.1430	-15.81	20.38
C6Cl5Br	-5564.19146	2.8567	1.9076	0.0323	0.1380	-15.10	21.71
C6Br6	-16134.35470	2.8394	1.9128	0.0337	0.1479	-15.43	23.14
1,3,5-Br3Ph	-8413.44831	2.9631	1.8997	0.0095	0.0984	-11.95	13.40
4ClPhBr	-3725.76800	3.0331	1.8972	0.0045	0.0780	-8.94	10.63
4MePhBr	-3305.46342	3.0885	1.8975	0.0013	0.0656	-5.45	8.89
4NMe2PhBr	-3400.10669	3.1093	1.8979	0.0018	0.0600	-3.60	8.28
4COOHPhBr	-3454.75344	3.0136	1.8923	0.0014	0.0818	-9.95	11.18
4CONH2PhBr	-3434.87380	3.0241	1.8937	0.0019	0.0794	-9.37	10.84
4CONHMePhBr	-3474.17369	3.0293	1.8944	0.0018	0.0781	-8.84	10.66
4Br-Pyr	-3282.20032	3.0196	1.8919	0.0023	0.0806	-10.18	11.02
3,4,5-Br3Pyr	-8429.48481	2.8904	1.8945	0.0222	0.1240	-13.99	17.95
HCCBr	-3111.25779	2.9552	1.8224	0.0308	0.0918	-13.29	13.66
MeCCBr	-3150.57149	2.9861	1.8240	0.0287	0.0836	-10.65	12.03
Br4-ethene	-10833.43331	2.8205	1.9101	0.0333	0.1606	-15.48	23.17
cis-Br2-ethene	-5686.14937	3.0366	1.8797	0.0083	0.0763	-8.09	10.42
BrCN	-3127.37161	2.7959	1.8464	0.0572	0.1491	-23.68	25.37
trans-Br2-ethene	-5686.15224	3.0044	1.8934	0.0112	0.0866	-10.00	11.67
Br-ethene	-3112.50175	3.1237	1.8878	-0.0021	0.0576	-5.15	7.84
EtBr	-3113.73011	3.1803	1.9553	-0.0003	0.0527	-1.76	7.16
C2F5Br	-3610.02350	2.8607	1.9357	0.0101	0.1335	-16.36	21.31
C2Cl5Br	-5411.75735	2.6888	2.0105	0.0657	0.2560	-17.98	41.81
MeI	-795.81398	3.0907	2.1705	0.0313	0.1173	-8.72	15.48

CF3I	-1093.59911	2.8189	2.1903	0.0442	0.2248	-24.03	40.41
CCl3I	-2174.64105	2.6882	2.2563	0.0933	0.3627	-28.76	64.76
CBr3I	-8516.74372	2.6588	2.2680	0.1110	0.3953	-30.36	69.64
CI4	-1680.89055	2.6424	2.2775	0.1184	0.4136	-29.86	71.07
EtI	-835.12107	3.102	2.1764	0.0196	0.1120	-7.78	14.67
C2F5I	-1331.41764	2.7928	2.2019	0.0565	0.2499	-25.77	43.59
C2Cl5I	-3133.15791	2.6718	2.2946	0.1271	0.3912	-29.72	69.06
PhI	-987.54461	2.9918	2.1336	0.0333	0.1460	-12.86	18.27
1,3,5-I3Ph	-1577.60282	2.868	2.1501	0.0536	0.2104	-19.76	27.92
C6F5I	-1483.78571	2.7623	2.1827	0.1072	0.2766	-25.88	41.99
C6Cl5I	-3285.58817	2.7643	2.1854	0.0975	0.2814	-24.91	62.03
C6Br5I	-13855.75064	2.7452	2.1979	0.1025	0.2964	-25.41	71.99
4ClPhI	-1447.15984	2.9428	2.1382	0.0413	0.1670	-16.11	21.51
3ClPhI	-1447.16019	2.9248	2.1393	0.0425	0.1749	-16.38	22.70
3,5-Cl2PhI	-1906.77387	2.8848	2.1465	0.0512	0.1973	-19.48	26.25
2,6-Cl2PhI	-1906.76655	2.8466	2.1599	0.0733	0.2253	-17.97	32.04
2,4,6-Cl3PhI	-2366.37944	2.816	2.1600	0.0756	0.2446	-20.98	35.79
4FPhI	-1086.79949	2.9594	2.1385	0.0407	0.1601	-15.08	20.45
3,5-F2PhI	-1186.05527	2.9066	2.1425	0.0481	0.1851	-18.46	24.11
2,6-F2PhI	-1186.05221	2.8546	2.1558	0.0782	0.2156	-17.80	30.51
2,4,6-F3PhI	-1285.30540	2.8297	2.1630	0.0867	0.2316	-20.12	33.39
2,3,5,6F4PhI2	-1282.57439	2.9353	2.1383	0.0412	0.1706	-16.49	22.04
1,4-I2Ph	-1679.56903	2.7607	2.1796	0.1051	0.2766	-25.71	42.31
4MePhI	-1026.85441	2.9983	2.1330	0.0332	0.1431	-12.12	17.91
2,4,6-Me3PhI	-1105.47772	3.0261	2.1404	0.0276	0.1252	-11.71	17.11
4-MeOPhI	-1102.06909	2.9931	2.1337	0.0368	0.1452	-12.05	18.25
4NO2PHI	-1192.07019	2.8884	2.1381	0.0450	0.1960	-21.44	25.47
4NMe2PhI	-1121.49769	3.0119	2.1305	0.0327	0.1372	-10.12	17.16
4CNPhI	-1079.80389	2.8999	2.1387	0.0443	0.1906	-20.53	24.61
4COOHPhI	-1176.14512	2.9284	2.1345	0.0385	0.1753	-17.17	22.28
4CONH2PhI	-1156.26547	2.9376	2.1349	0.0382	0.1684	-16.52	21.67
4CONHMePhI	-1195.56529	2.9429	2.1343	0.0384	0.1659	-15.95	21.30
4I-Pyr	-1003.59203	2.9361	2.1344	0.0389	0.1697	-17.37	21.77
HCCl	-832.65534	2.8654	2.0782	0.0857	0.1975	-21.47	27.37

MeCCI	-871.96869	2.8928	2.0737	0.0799	0.1829	-18.49	24.28
ICCI	-1127.68102	2.812	2.0910	0.1005	0.2313	-24.00	33.44
I4-ethene	-1718.97878	2.7132	2.2056	0.1100	0.3311	-25.98	51.71
cis-I2-ethene	-1128.92422	2.9287	2.1219	0.0453	0.1735	-15.69	24.14
trans-I2-ethene	-1128.92856	2.8885	2.1478	0.0558	0.1991	-17.92	27.70
I-ethene	-833.89245	3.0427	2.1168	0.0271	0.1251	-11.46	16.25
ICN	-848.77431	2.7204	2.1358	0.1382	0.2876	-34.05	52.73
ICCCN	-924.92180	2.74	2.0991	0.1154	0.2742	-33.91	40.98
4HCCPhI	-1063.70375	2.8407	2.0786	0.0878	0.2109	-21.99	28.94

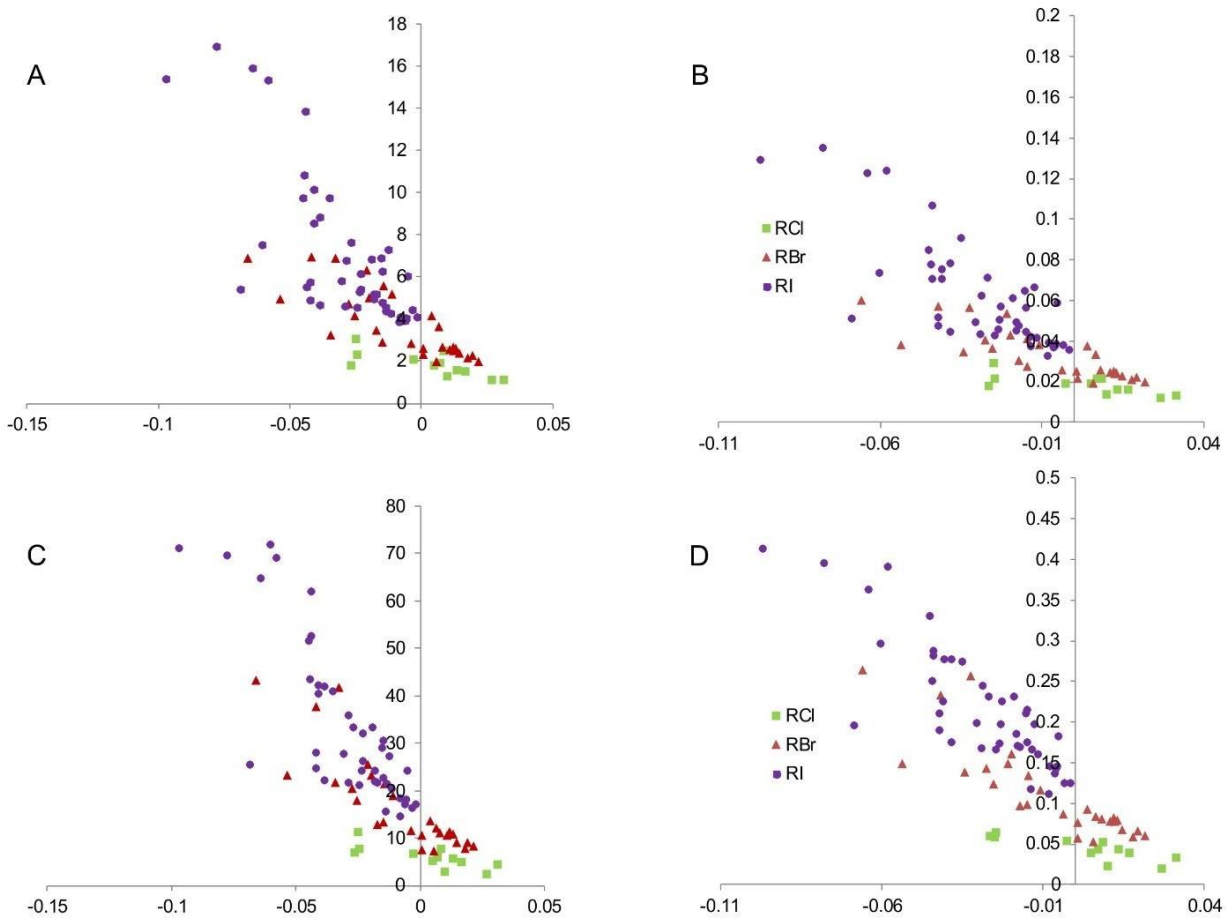

Fig. S1 Correlation of the energy of the lowest R-X* MO (ε $\phi_{R\text{-}X}$*, a.u.) with several descriptors of the strength of the $Me_2Se\cdots XR$ (A , B) and $Cl^-\cdots XR$ (C, D) XB interactions: (A, C) ε $\phi_{R\text{-}X}$* versus the NBO donor-acceptor energy of the XB complex ($\Delta E_{d\rightarrow a}$, kcal/mol); (B, D); ε $\phi_{R\text{-}X}$* versus the Se···X Wiberg bond index (WBI).