Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

SUPPLEMENTARY INFORMATION

Site Specificity of Halogen Bonding involving Aromatic Acceptors

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Table S1: Summary of CSD search results for Cl···π-type XB

No. of Hits	*No. of Contacts*	*Parameter*	*Minimum*	*Maximum*	*Mean*	*Std Dev.*
C≡C						
16	18	α	165.8	176.4	172.2	2.7
		R_1	3.117	3.445	3.328	0.108
		R_2	3.148	3.435	3.32	0.099
C=C						
91	96	α	165.0	180.0	172.2	4.5
		R_1	3.017	3.447	3.319	0.097
		R_2	2.980	3.448	3.331	0.092
AR η_1						
2506	2688	α	165.0	179.7	170.4	3.6
		R	2.954	3.45	3.363	0.069
AR η_2						
973	1015	α	165.0	179.8	170.6	3.6
		R_1	2.005	3.45	3.331	0.122
		R_2	2.193	3.449	3.325	0.117
AR η_6						
36	58	α	175.1	179.9	177.2	1.4
		θ	85.0	89.8	87.5	1.3
		R	3.262	3.449	3.383	0.052

Table S2: Summary of CSD search results for Br···π-type XB

No. of Hits	*No. of Contacts*	*Parameter*	*Minimum*	*Maximum*	*Mean*	*Std Dev.*
C≡C						
6	7	α	165.6	175.3	170.7	3.7
		R_1	3.203	3.521	3.371	0.100
		R_2	3.208	3.514	3.362	0.120
C=C						
35	37	α	165.0	180.0	171.3	4.4
		R_1	3.164	3.547	3.419	0.099
		R_2	3.219	3.547	3.402	0.090
AR η_1						
696	733	α	165.0	179.5	170.4	3.5
		R	3.174	3.550	3.452	0.075
AR η_2						
456	500	α	165.0	178.0	170.8	3.8
		R_1	2.813	3.55	3.428	0.091
		R_2	2.677	3.55	3.42	0.101
AR η_6						
21	25	α	175.1	179.5	176.6	1.2
		θ	85.4	89.9	87.7	1.3
		R	3.334	3.542	3.434	0.058

Table S3: Summary of CSD search results for I···π-type XB

No. of Hits	*No. of Contacts*	*Parameter*	*Minimum*	*Maximum*	*Mean*	*Std Dev.*
C≡C						
10	15	α	166.0	177.5	171.7	4.1
		R_1	3.402	3.641	3.477	0.061
		R_2	3.285	3.593	3.427	0.098
C=C						
20	20	α	165.4	178.4	171.1	3.6
		R_1	3.285	3.645	3.526	0.105
		R_2	3.196	3.667	3.514	0.133
AR η_1						
66	67	α	165.2	179.6	169.7	3.6
		R	3.404	3.678	3.59	0.062
AR η_2						
199	227	α	165.0	179.5	170.6	3.3
		R_1	3.2	3.678	3.534	0.102
		R_2	3.173	3.679	3.524	0.094
AR η_6						
5	7	α	175.3	180.0	178.8	1.7
		θ	85.9	90.0	88.9	1.6
		R	3.218	3.678	3.426	0.211

Table S4: Summary of CSD search results for Cl···LP-type XB and additional search criteria unique to each XB acceptor

No. of Hits	*No. of Contacts*	*Parameter*	*Minimum*	*Maximum*	*Mean*	*Std Dev.*
C=O	β=100˚≤X···C=O≤140˚					
572	624	α	165.0	179.3	170.5	3.6
		β	100.1	134.0	123.3	10.8
		R	2.327	3.27	3.083	0.119
C=S	β=100˚≤X···C=S≤140˚					
26	37	α	165.1	179.0	171.9	3.8
		β	100.5	133.5	117.6	10.3
		R	3.099	3.611	3.382	0.141
C-O-C	β=100˚≤X···C-O≤140˚					
304	319	α	165.0	180.0	170.9	3.8
		β	100.0	139.1	115.3	10.2
		R	2.674	3.27	3.105	0.104
C-S-C	β=100˚≤X···C-S≤140˚					
82	83	α	165.1	180.0	170.4	4.0
		β	100.3	139.3	119.2	11.5
		R	3.219	3.549	3.434	0.082
C-O-H	β=100˚≤X···C-O≤140˚	γ=90˚≤X···O-H≤160˚				
66	67	α	165.1	178.0	170.4	3.6
		β	100.5	139.9	120.3	11.2
		γ	91.5	143.8	113.4	12.8
		R	2.78	3.269	3.101	0.121
C-S-H	β=100˚≤X···C-S≤140˚	γ=90˚≤X···S-H≤160˚				
1	1	α	165.6	165.6	165.6	-
		β	115.0	115.0	115.0	-
		γ	114.9	114.9	114.9	-
		R	3.412	3.412	3.412	-

Amines	β_i=90˚≤X···N-R_i≤180˚					
11	11	α	167.8	178.9	170.9	3.1
		β_1	92.0	137.3	111.2	13.5
		β_2	92.4	115.9	103.2	8.7
		β_3	91.0	138.2	107.4	13.3
		R	2.979	3.252	3.114	0.091
Imines						
83	87	α	165.2	180.0	171.0	3.8
		R	2.685	3.299	3.161	0.115
Phosphines	β_i=90˚≤X···P-R_i≤180˚					
		No Entries				

Table S5: Summary of CSD search results for Br···LP-type XB and additional search criteria unique to each XB acceptor

No. of Hits	*No. of Contacts*	*Parameter*	*Minimum*	*Maximum*	*Mean*	*Std Dev.*
C=O	β=100˚≤X···C=O≤140˚					
462	501	α	165.0	179.2	171.0	3.7
		β	100.1	140.0	122.4	11.0
		R	2.727	3.368	3.115	0.131
C=S	β=100˚≤X···C=S≤140˚					
26	37	α	165.1	179.0	171.9	3.8
		β	100.5	133.5	117.6	10.3
		R	3.099	3.611	3.382	0.141
C-O-C	β=100˚≤X···C-O≤140˚					
211	229	α	165.1	179.7	171.0	3.5
		β	100.1	139.5	115.3	10.3
		R	2.723	3.368	3.143	0.126
C-S-C	β=100˚≤X···C-S≤140˚					
45	47	α	165.9	178.5	170.1	3.4
		β	100.1	139.1	117.2	12.4
		R	3.251	3.649	3.527	0.096
C-O-H	β=100˚≤X···C-O≤140˚	γ=90˚≤X···O-H≤160˚				
74	77	α	165.0	178.5	170.6	3.4
		β	100.3	139.9	119.1	11.5
		γ	90.5	147.3	113.9	15.0
		R	2.919	3.360	3.124	0.123
C-S-H	β=100˚≤X···C-S≤140˚	γ=90˚≤X···S-H≤160˚				
		No Entries				
Amines	β_i=90˚≤X···N-R_i≤180˚					
20	26	α	166.5	180.0	172.3	4.0
		β_1	93.1	136.4	105.7	9.5
		β_2	93.3	136.6	109.3	11.4
		β_3	90.3	132.2	109.2	11.0
		R	2.347	3.379	2.863	0.294
Imines						
49	54	α	165.3	178.3	171.4	3.6
		R	2.822	3.387	3.150	0.126
Phosphines	β_i=90˚≤X···P-R_i≤180˚					
		No Entries				

Table S6: Summary of CSD search results for I···LP-type XB and additional search criteria unique to each XB acceptor

No. of Hits	*No. of Contacts*	*Parameter*	*Minimum*	*Maximum*	*Mean*	*Std Dev.*
C=O	β=100˚≤X···C=O≤140˚					
276	329	α	165.0	179.6	172.1	3.7
		β	100.1	134.0	122.4	10.0
		R	2.534	3.499	3.058	0.185
C=S	β=100˚≤X···C=S≤140˚					
45	60	α	165.6	179.1	172.5	3.7
		β	100.2	139.7	110.3	8.9
		R	2.487	3.649	3.168	0.271
C-O-C	β=100˚≤X···C-O≤140˚					
99	116	α	165.3	179.0	171.7	3.7
		β	100.8	137.6	117.3	9.6
		R	2.598	3.493	3.139	0.188
C-S-C	β=100˚≤X···C-S≤140˚					
51	59	α	165.0	179.3	172.2	20.6
		β	100.5	135.1	111.2	90.9
		R	2.717	3.774	3.355	0.100
C-O-H	β=100˚≤X···C-O≤140˚	γ=90˚≤X···O-H≤160˚				
39	45	α	165.0	179.2	172.7	3.8
		β	100.1	134.5	118.3	10.0
		γ	90.7	143.8	116.0	13.3
		R	2.752	3.478	3.07	0.146
C-S-H	β=100˚≤X···C-S≤140˚	γ=90˚≤X···S-H≤160˚				
		No Entries				
Amines	β_i=90˚≤X···N-R_i≤180˚					
106	162	α	166.1	179.5	174.3	3.4
		β_1	94.8	122.8	108.1	5.6
		β_2	93.2	135.8	110.1	7.9
		β_3	90.6	124.1	107.7	6.6
		R	2.279	3.376	2.786	0.210
Imines						
90	117	α	165.3	180.0	173.2	3.5
		R	2.717	3.461	2.999	0.184
Phosphines	β_i=90˚≤X···P-R_i≤180˚					
2	2	α	170.7	173.8	172.3	2.2
		β_1	108.3	101.0	109.1	1.2
		β_2	108.3	117.7	113.0	6.6
		β_3	123.4	125.6	124.5	1.6
		R	3.334	3.491	3.413	0.111

Table S7: ωB97X-D/aug-cc-pVTZ HOMO, HOMO-1 and HOMO-2 energies (eV) for XB acceptors

Species	HOMO	Description	HOMO-1	Description	HOMO-2	Description
benzene	-9.07	π	-9.07	π	-11.60	σ
toluene	-8.70	π	-8.99	π	-11.40	σ
styrene	-8.33	π	-9.14	π	-10.61	π
napthalene	-8.00	π	-8.78	π	-10.14	π
anthracene	-7.32	π	-8.61	π	-9.29	π
phenanthrene	-7.90	π	-8.21	π	-9.42	π
pyrrole	-7.95	π	-8.86	π	-12.43	σ
imidazole	-8.56	π	-9.75	π	-10.07	π
pyridine	-9.35	n	-9.44	π	-10.18	π
indole	-7.66	π	-8.15	π	-9.91	π
quinoline	-8.52	π	-9.01	π	-9.34	n

Table S8: Geometrical Parameters and interaction energies (I.E.) for ωB97X-D/aug-cc-pVTZ optimized 1···XY complexes

Species	α	R_1	R_2	I.E.
1···Cl_2	179.28	3.324	3.324	-2.18
1···ClF	178.48	3.038	3.049	-3.49
1···BrF	178.27	3.052	3.053	-5.38
1···BrCl	178.52	3.268	3.269	-3.63
1···Br_2	178.62	3.329	3.329	-3.19
1···$ClCF_3$	178.32	3.628	3.647	-1.79

Table S9: sSAPT0/jun-cc-pVDZ energy components for 1···XY complexes

Species	Elec	Exch	Ind	Disp	I.E.	%Elec	%Ind	%Disp
1···Cl_2	-2.56	4.30	-1.11	-2.91	-2.28	39	17	44
1···ClF	-5.50	9.02	-3.01	-3.69	-3.18	45	25	30
1···BrF	-7.87	12.44	-4.52	-4.96	-4.90	45	26	29
1···BrCl	-4.65	7.24	-2.11	-4.12	-3.64	43	19	38
1···Br_2	-3.99	6.31	-1.64	-3.99	-3.31	41	17	41
1···$ClCF_3$	-1.52	2.23	-0.39	-2.32	-2.01	36	9	55

Figure S1: Examples of η_6 contacts found in CSD

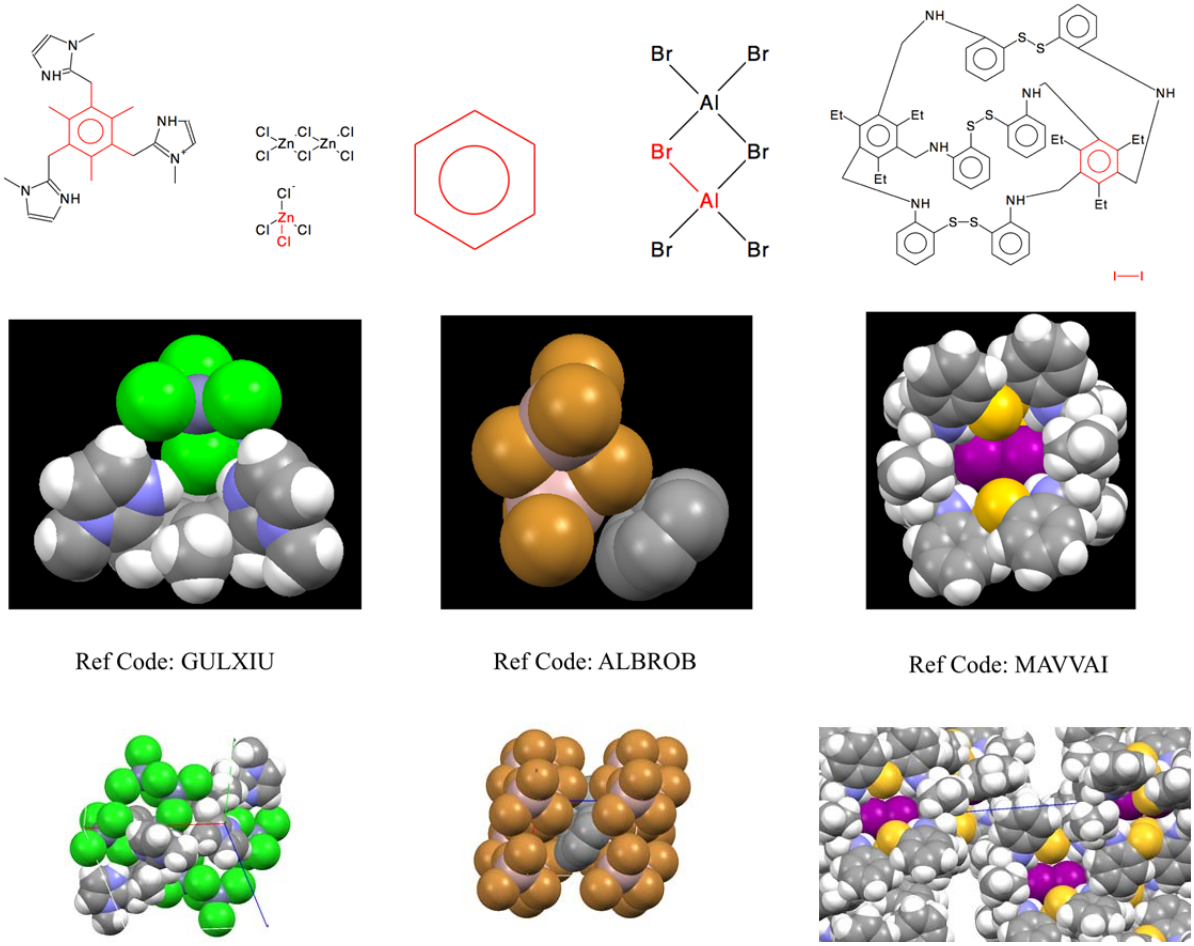


Figure S2: Counterpoise-corrected ωB97X-D/aug-cc-pVTZ Interaction Energies (kcal/mol)

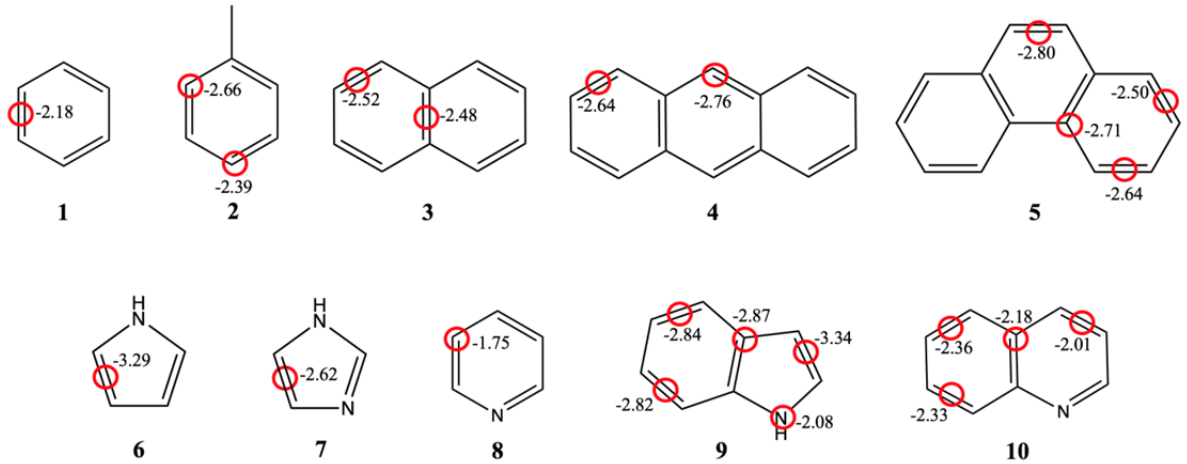


Figure S3: Counterpoise-corrected ωB97X-D/aug-cc-pVTZ Interaction Energies for amino acid···Cl_2 complexes (kcal/mol)

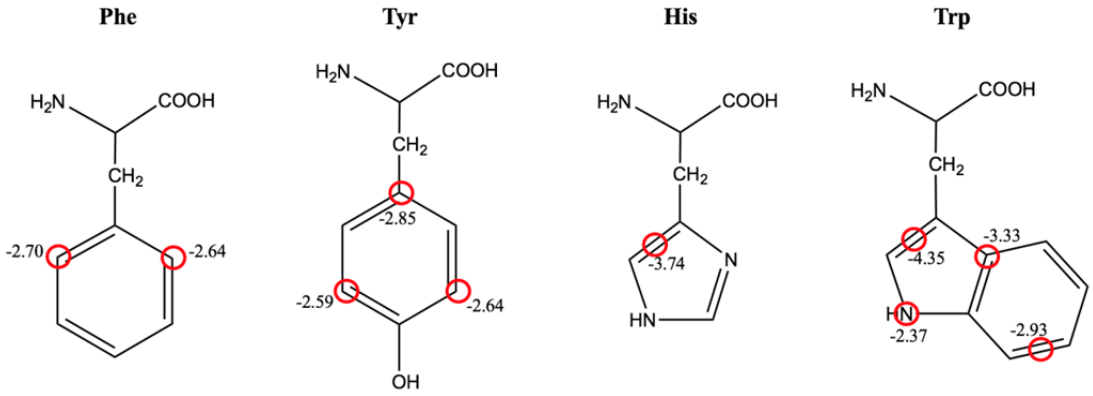


Table S10: Geometric Parameters of biological XB close contacts: d_1 is the shortest X···C contact; d_2 is the second shortest X···C contact and d_C is the X···centroid distance

PDB ID	AA residue	d_1 (Å)	d_2 (Å)	d_C (Å)
3TMZ	Phe	3.485	3.752	3.827
1P5E	Phe	3.261	3.354	3.409
1PBQ	Trp	3.152	3.275	3.740
1S9G	Phe	3.752	3.919	4.188
1WBG	Tyr	3.727	3.972	4.085
1ZOE	Phe	3.490	3.739	3.929
2BQW	Tyr	3.292	3.557	3.497
2PIT	Tyr	3.347	3.670	3.927

Figure S4: CHelpG atomic charges for N-heteroaromatic compounds

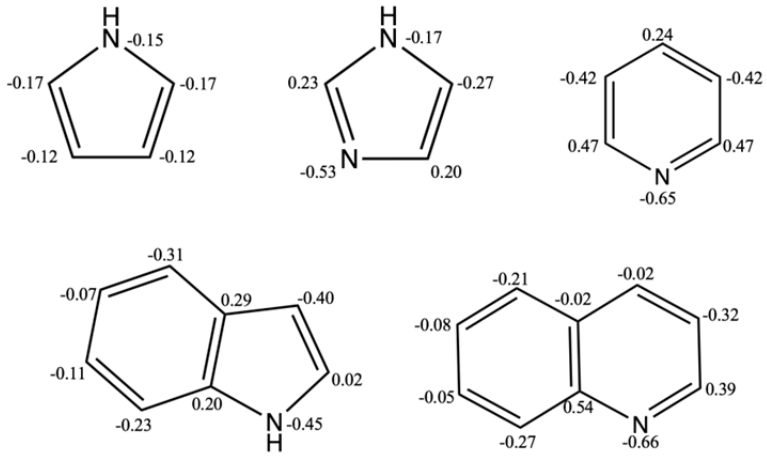


Figure S5: CHelpG atomic charges for toluene and PAHs

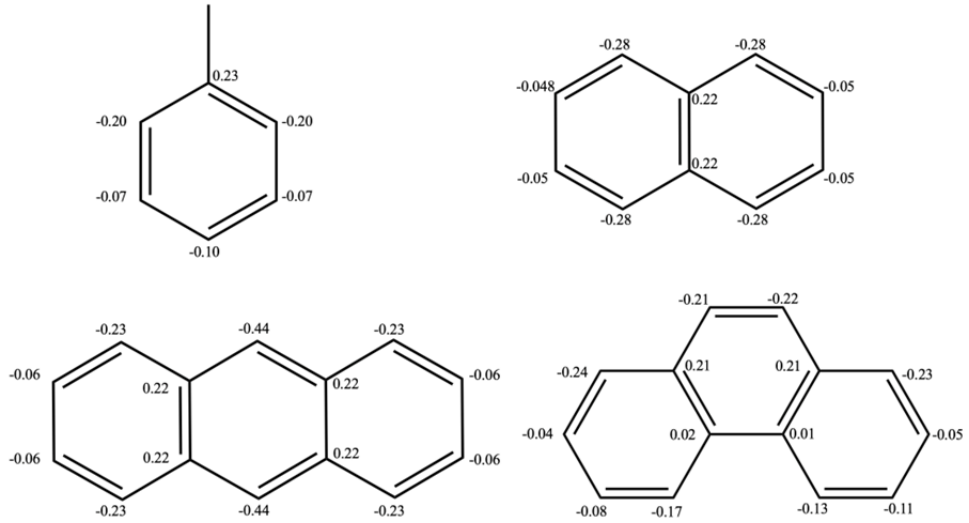


Figure S6: CHelpG atomic charges for 4 aromatic amino acid side chains

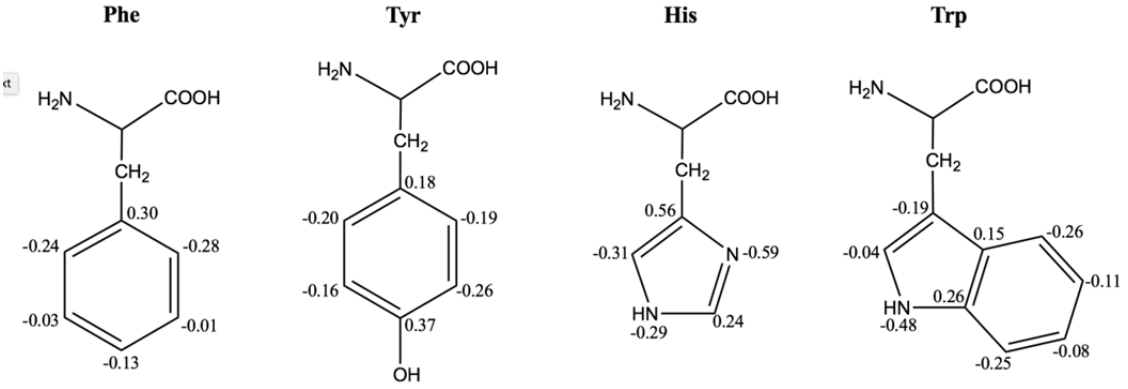


Figure S7: Electrostatic Potential(top), HOMO(middle) and HOMO-1 plots(bottom) of selected neutral amino acids at 0.001 a.u. and 0.06 a.u. respectively

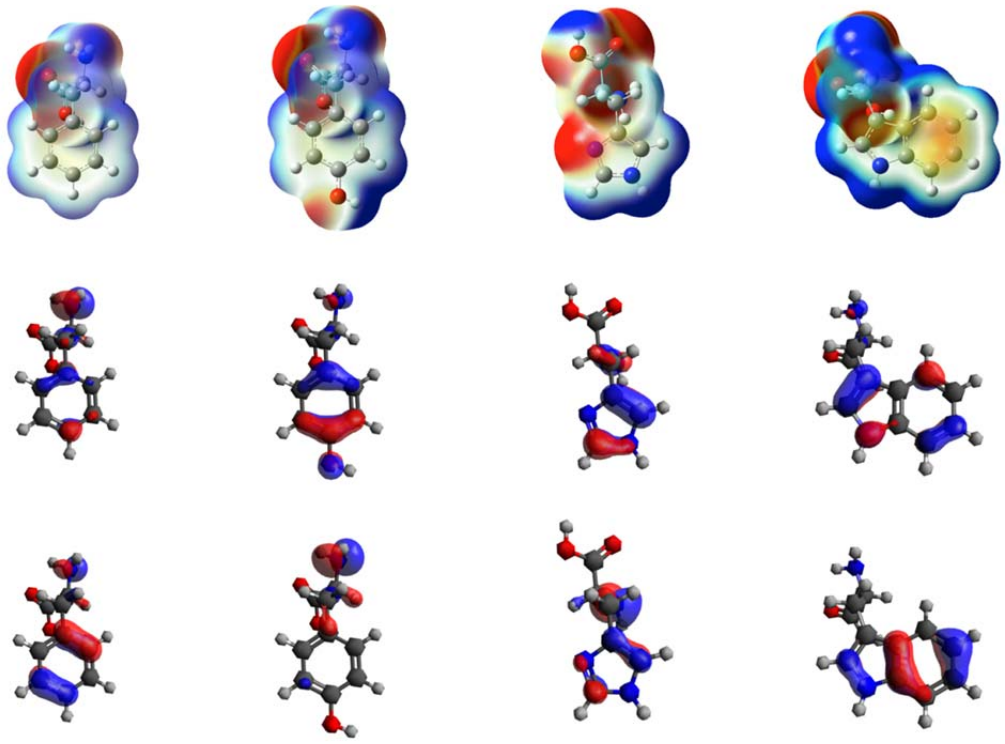


Figure S8: Illustration of lone-pair π repulsion between benzene and Cl_2 at AR and AC positions: Overlay of HOMO and HOMO-1 (Degenerate HOMO for AC position), NCIPLOT and Reduced Density Gradient(s) v.s. (λ_2 sign) ρ Plots

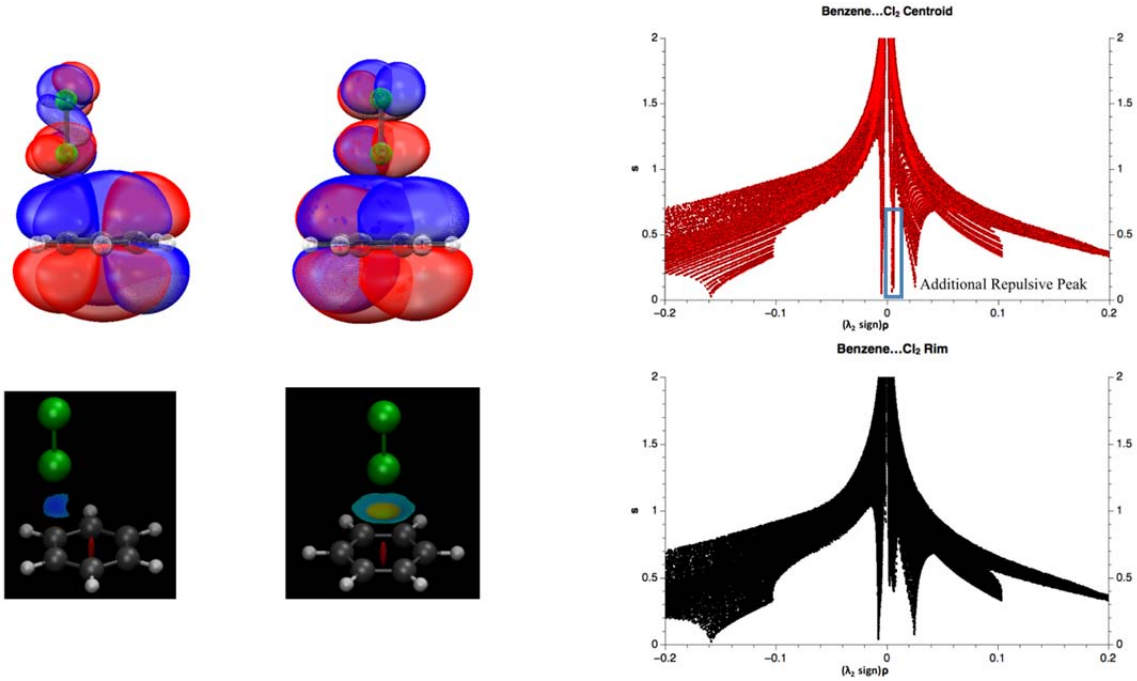


Figure S9: QTAIM critical points for various binding modes in benzene···Cl_2 (green circles: BCPs, red circles: RCPs, blue circle: CCP)

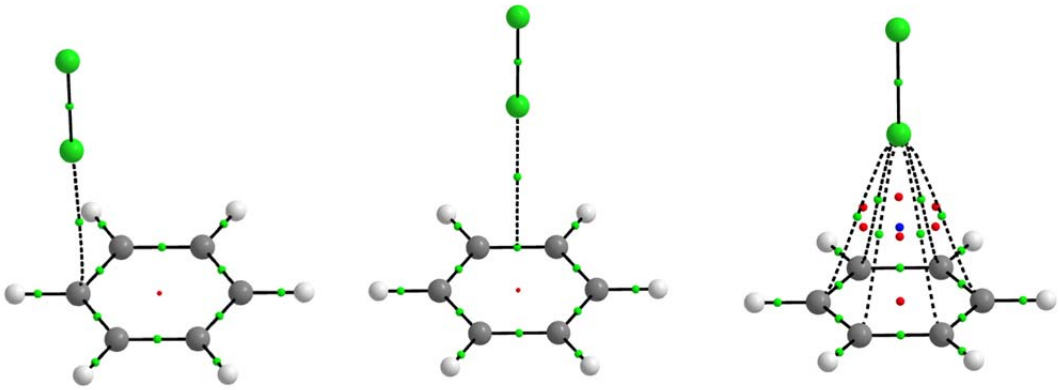


Table S11: Interaction Energies for selected aromatic-type XB evaluated using ωB97X-D and CCSD(T) with aug-cc-pVTZ basis set

Species	ωB97X-D	CCSD(T)	Error
Benzene···Cl_2	-2.18	-2.60	0.42
Naphthalene···Cl_2 (a)	-2.52	-3.03	0.51
Naphthalene···Cl_2 (b)	-2.48	-3.13	0.65
Benzene···Br_2	-3.19	-3.30	0.11
Naphthalene···Br_2 (a)	-3.68	-3.86	0.16
Naphthalene···Br_2 (b)	-3.60	-3.88	0.28

Figure S10: CCSD(T) and ωB97X-D with aug-cc-pVTZ/aug-cc-pVDZ scan A for benzene···Cl_2 (top) and naphthalene···Cl_2 (bottom) at 3.2 Å respectively

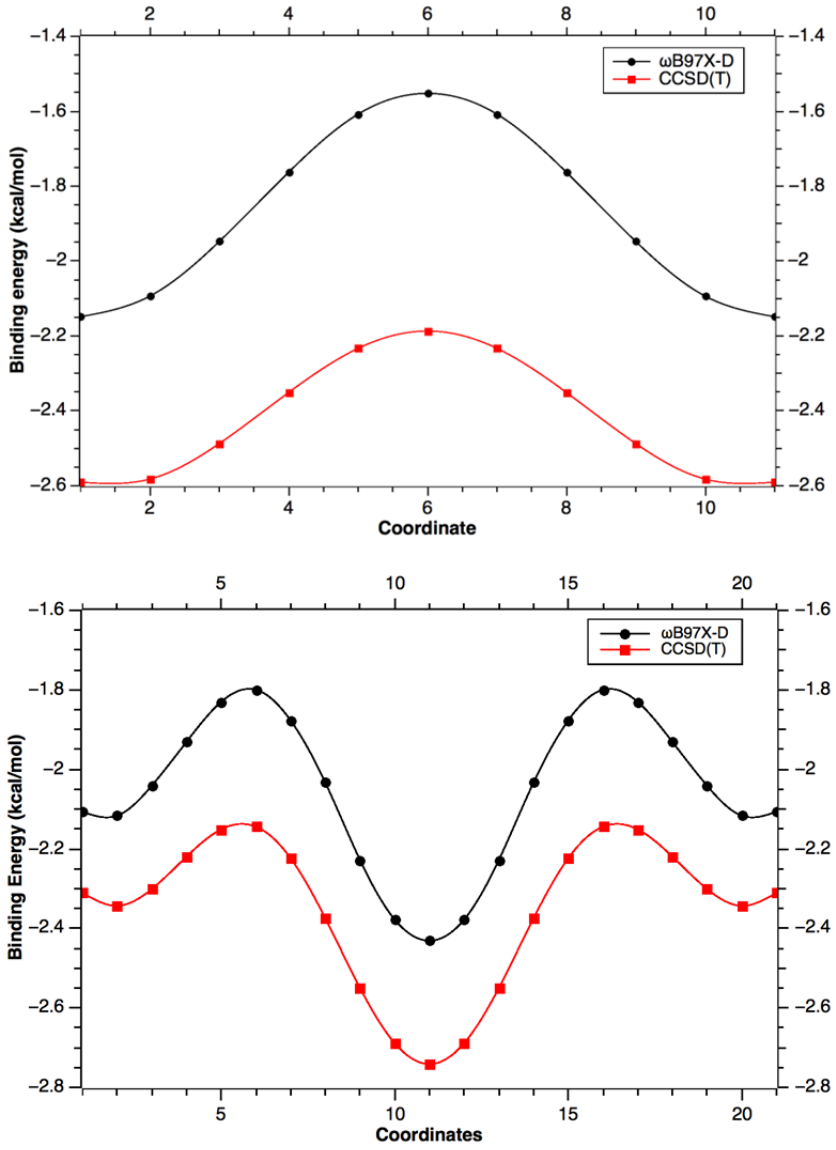


Figure S11: ωB97X-D/aug-cc-pVTZ scans 3.0-3.4 Å for benzene···Cl_2

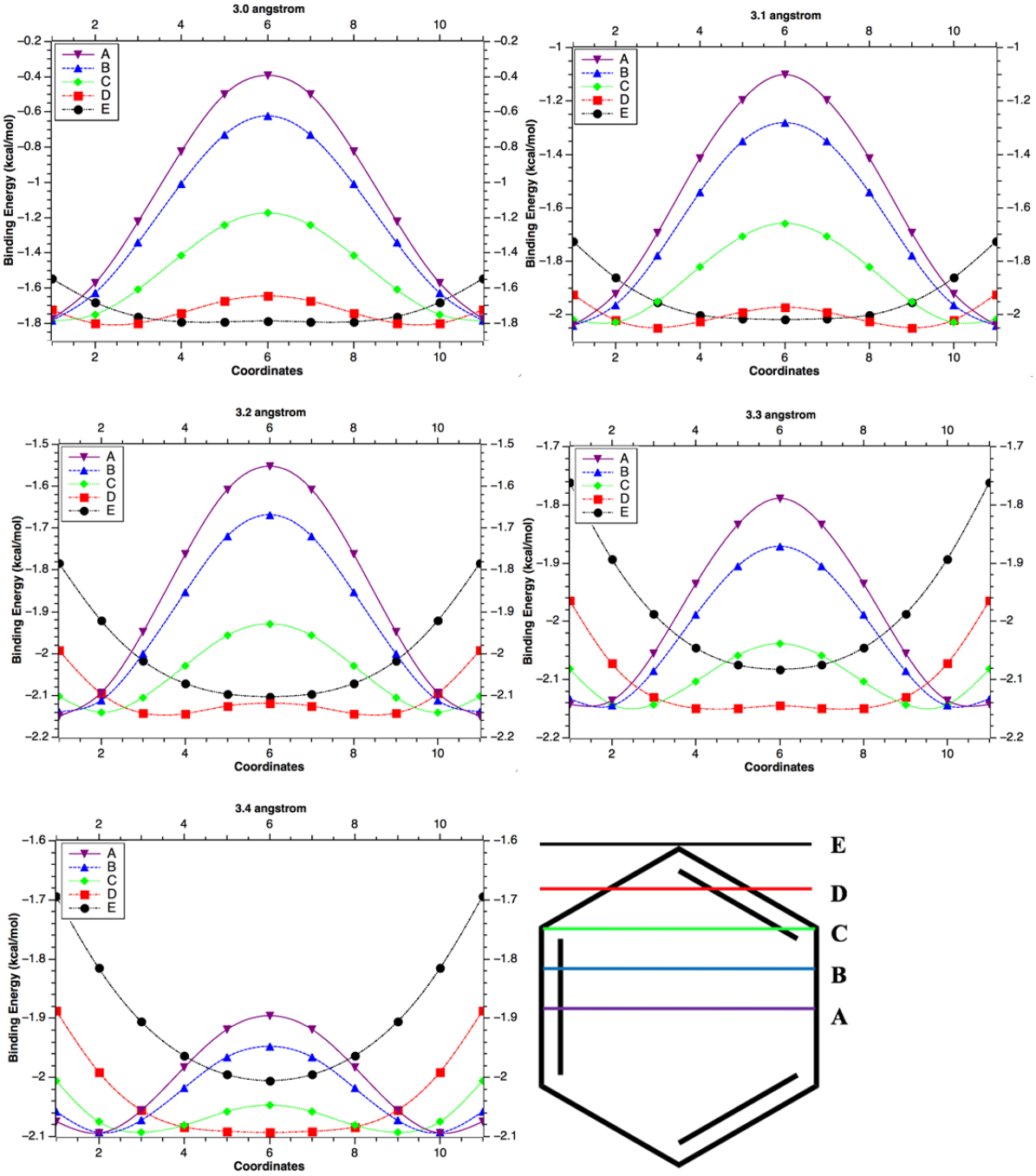


Figure S12: ωB97X-D/aug-cc-pVTZ scans 3.0-3.4 Å for benzene···Br_2

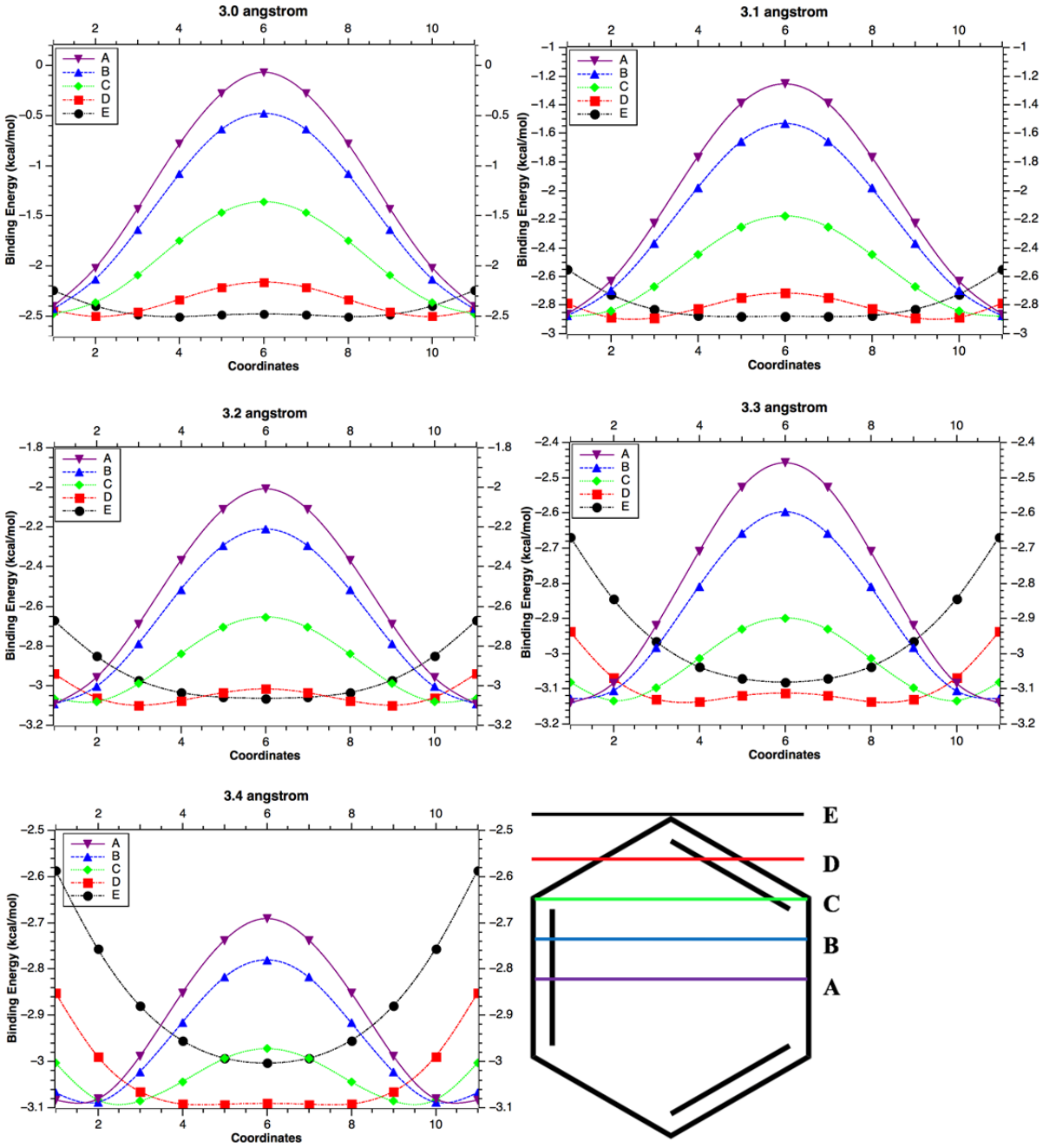


Figure S13: ωB97X-D/aug-cc-pVTZ scans 3.0-3.4 Å for naphthalene···Cl_2

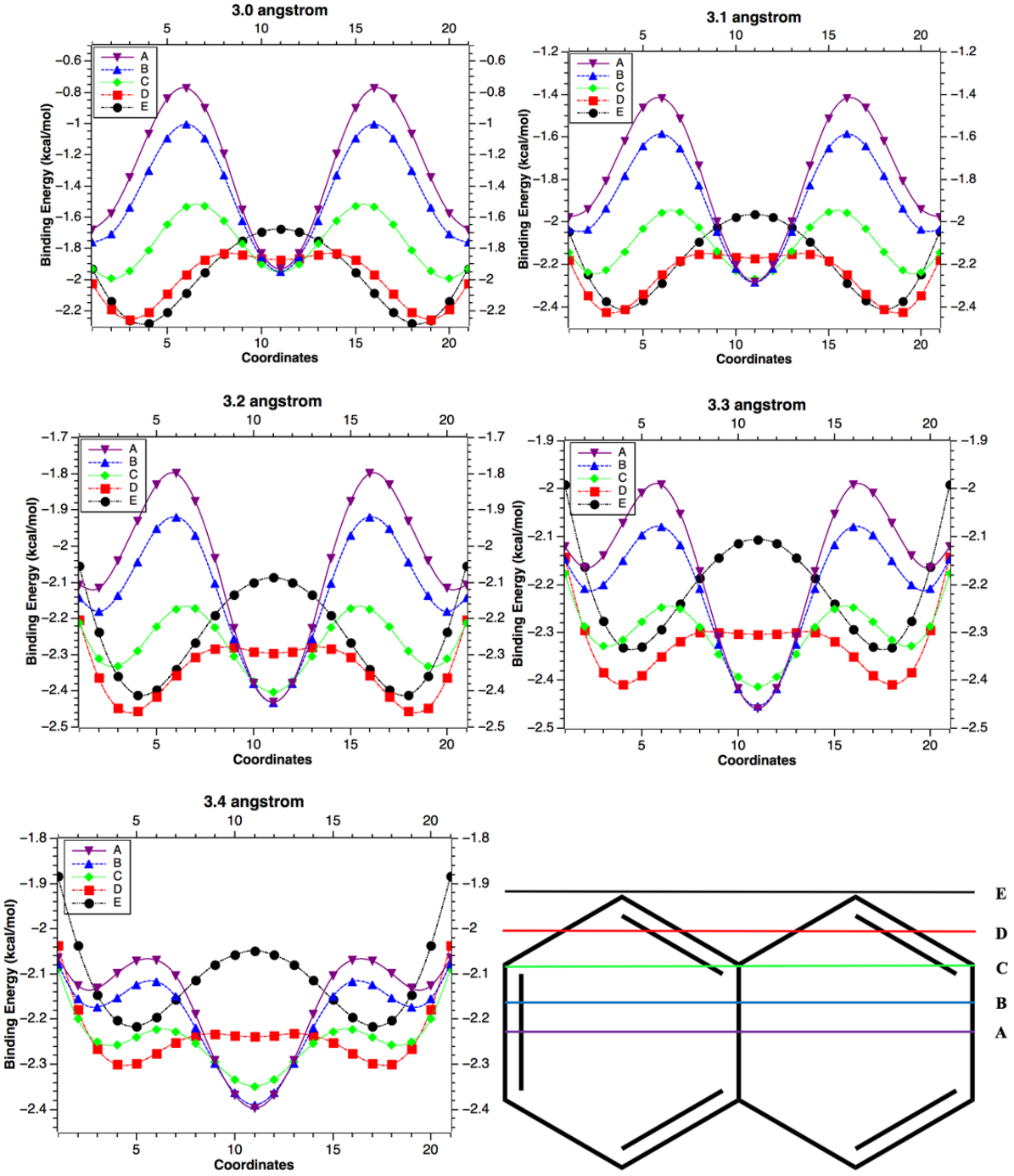


Figure S14: ωB97X-D/aug-cc-pVTZ scans 3.0-3.4 Å for naphthalene··Br_2

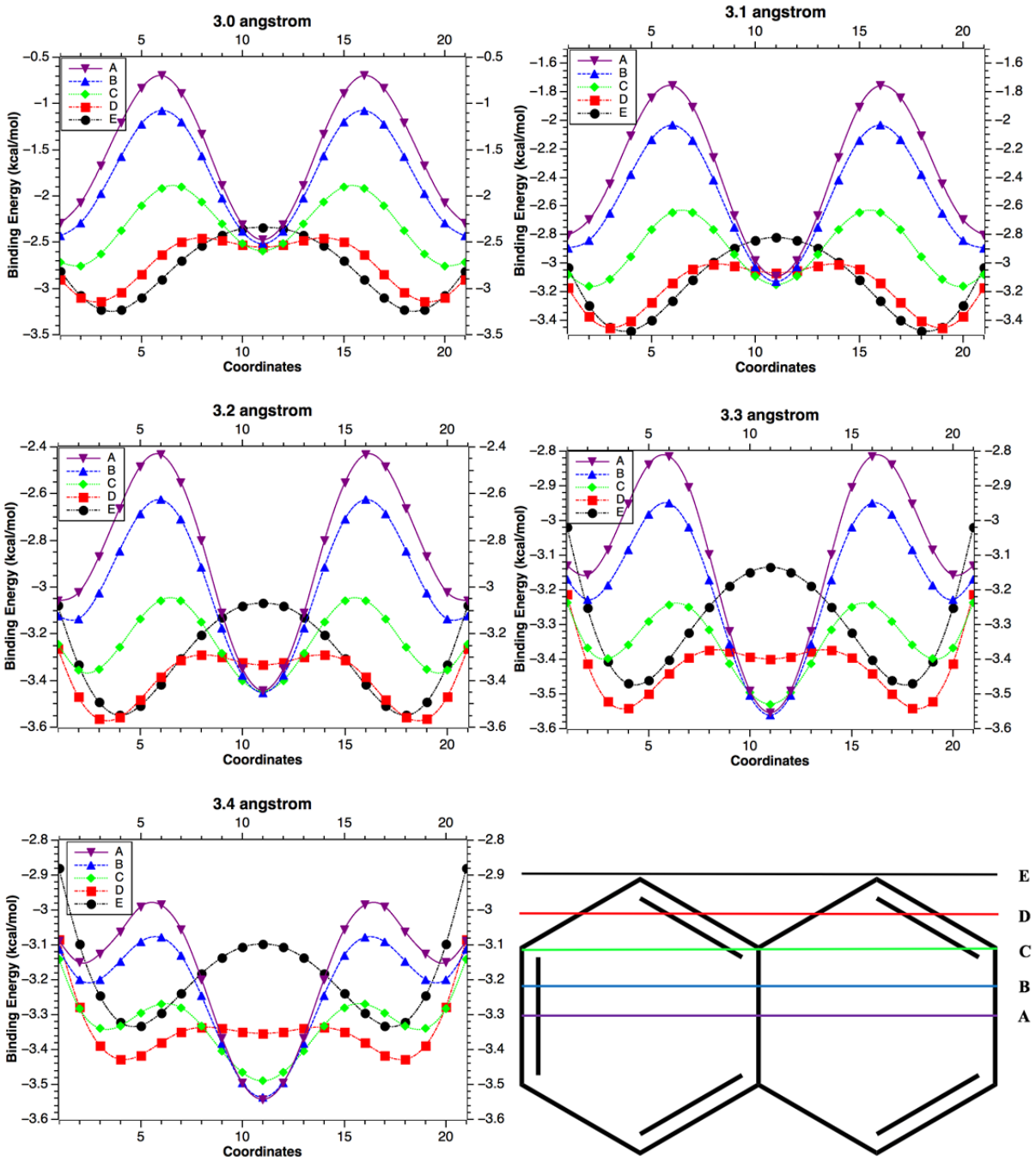


Figure S15: ωB97X-D/aug-cc-pVTZ scans 3.0-3.4 Å for anthracene···Cl_2

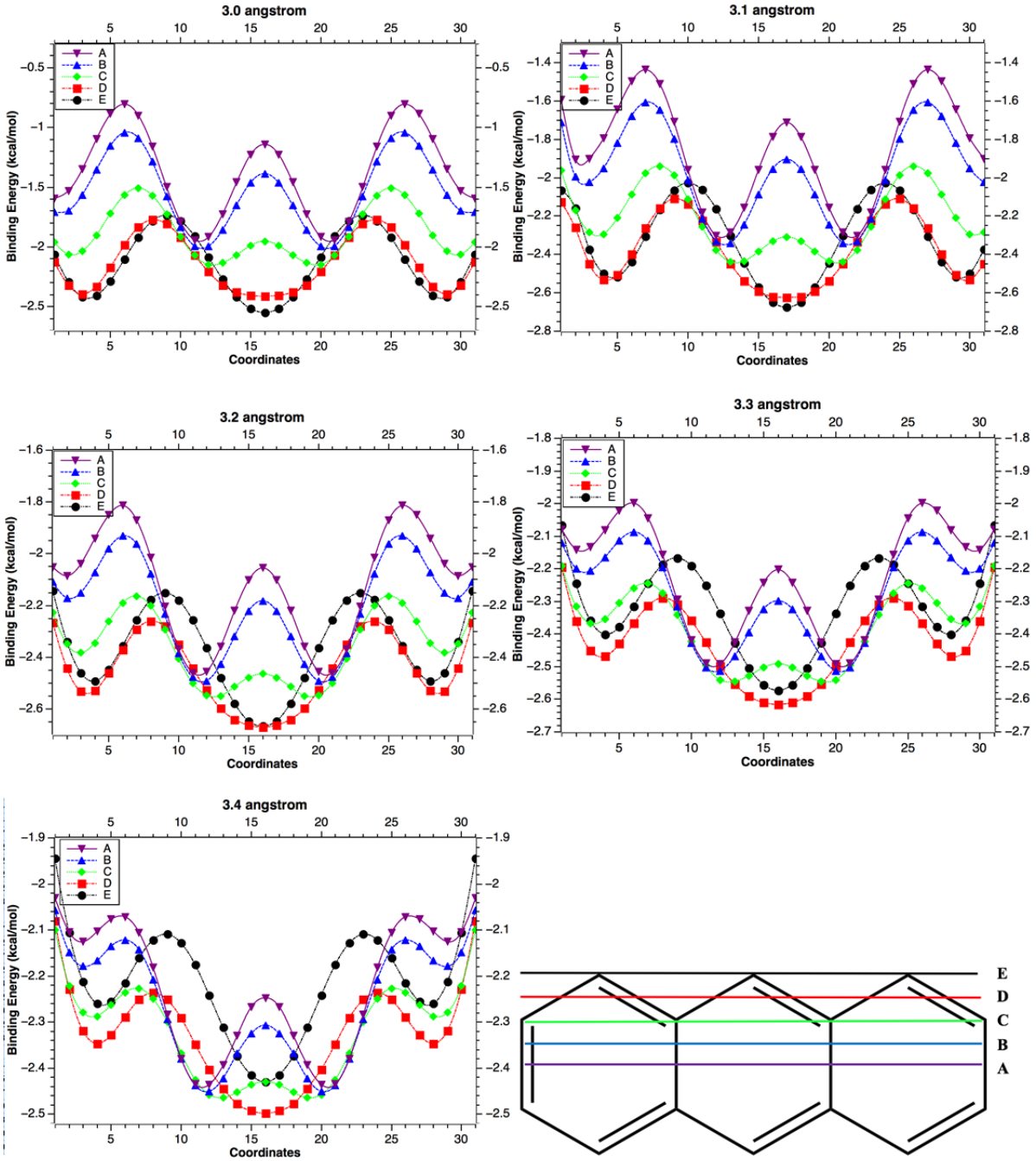


Figure S16: ωB97X-D/aug-cc-pVTZ scans 3.0-3.4 Å for phenanthrene···Cl_2

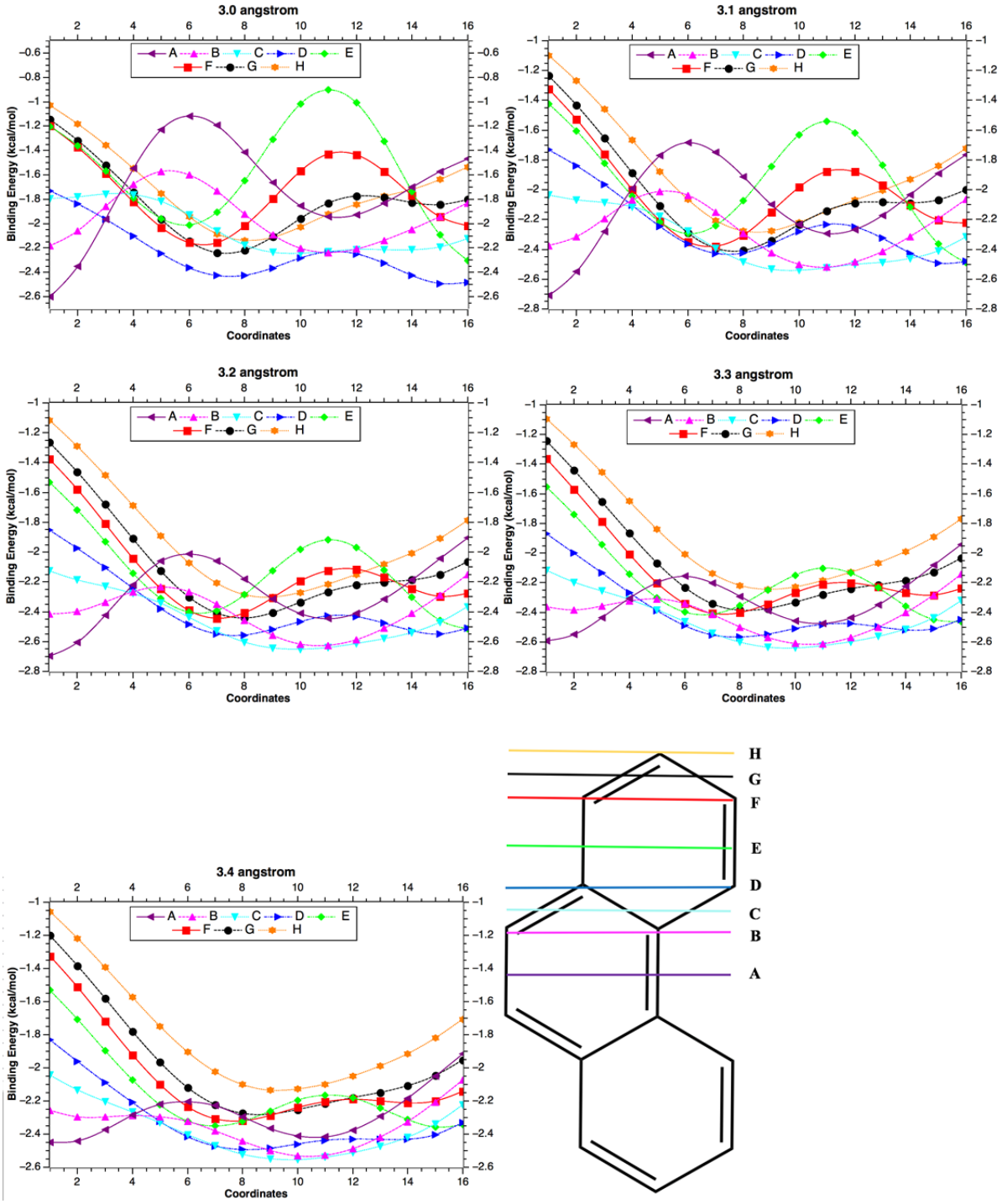


Figure S17: ωB97X-D/aug-cc-pVTZ scans 3.0-3.4 Å for toluene···Cl_2

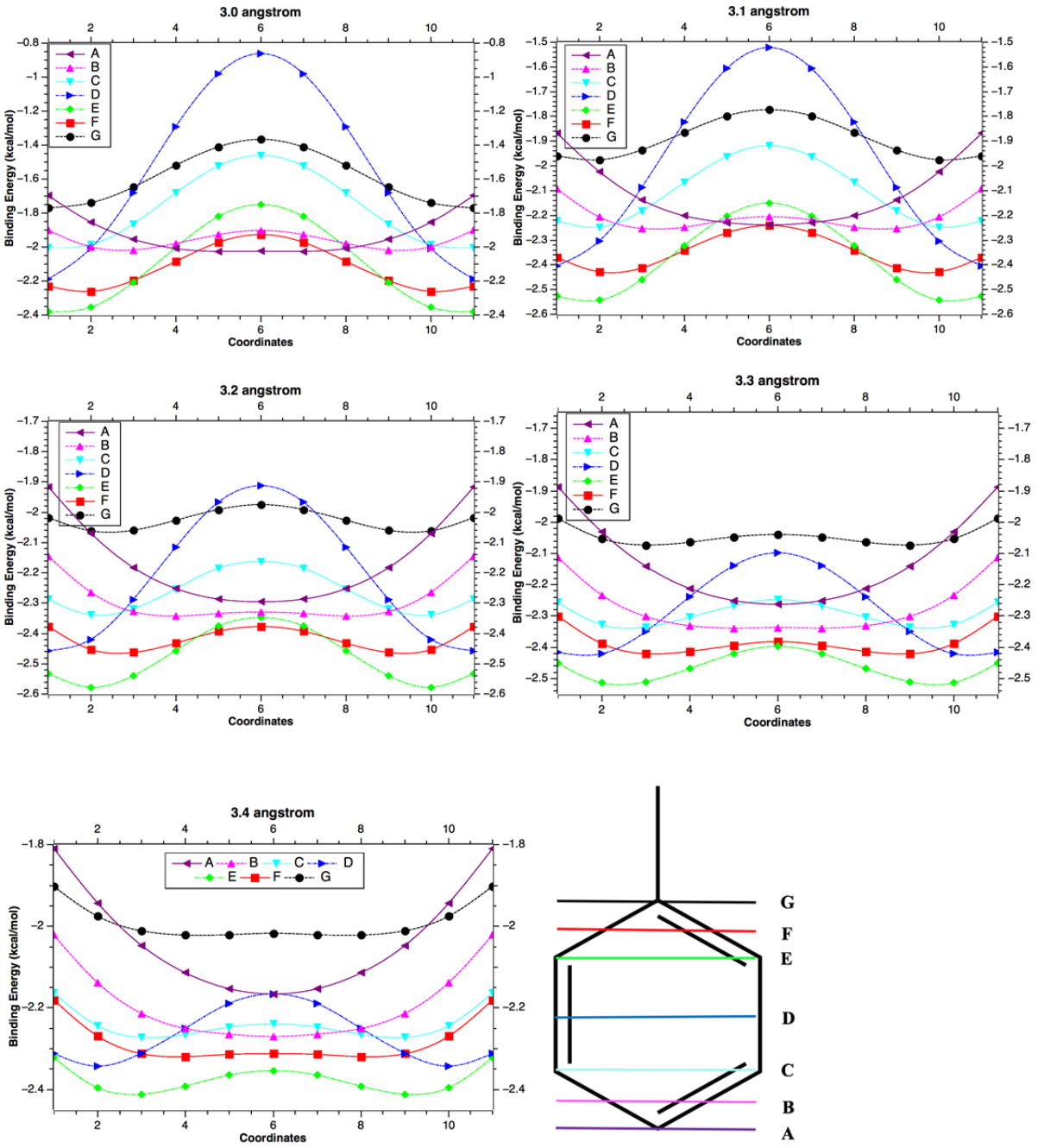


Figure S18: ωB97X-D/aug-cc-pVTZ scans 3.0 -3.4 Å for pyrrole···Cl_2

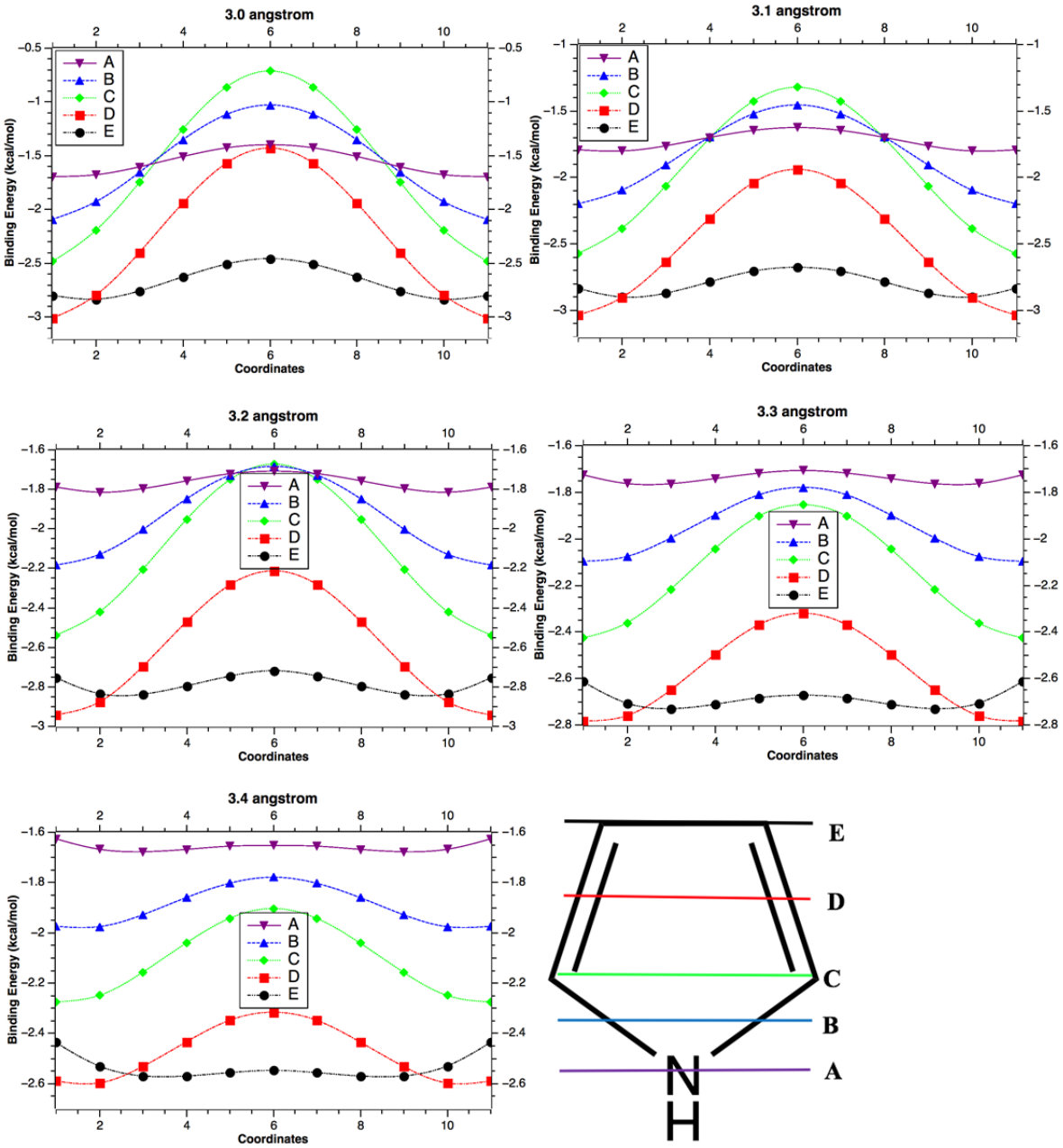


Figure S19: ωB97X-D/aug-cc-pVTZ scans 3.0-3.4 Å for imidazole···Cl_2

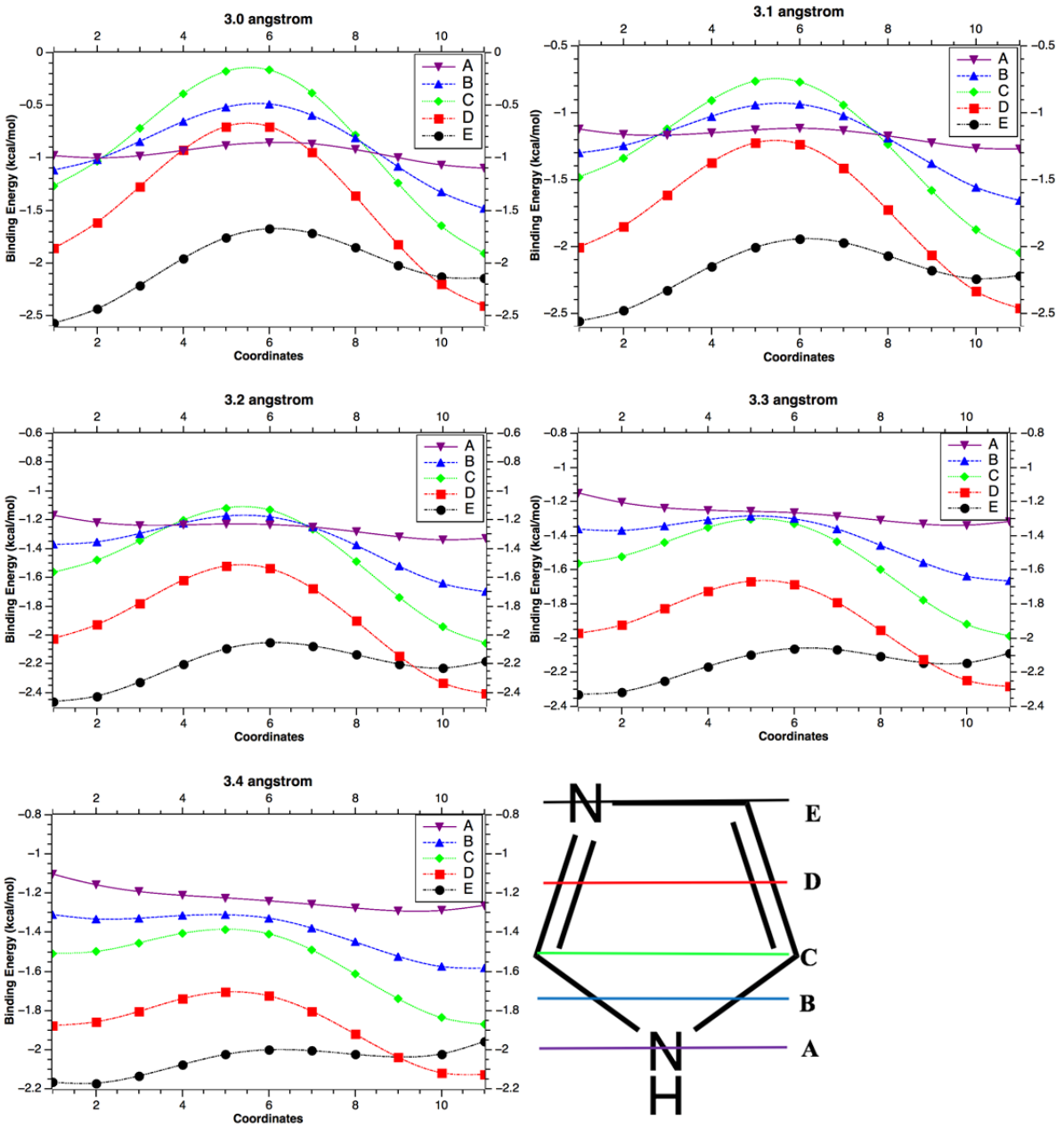


Figure S20: ωB97X-D/aug-cc-pVTZ scans 3.0-3.4 Å for pyridine···Cl_2

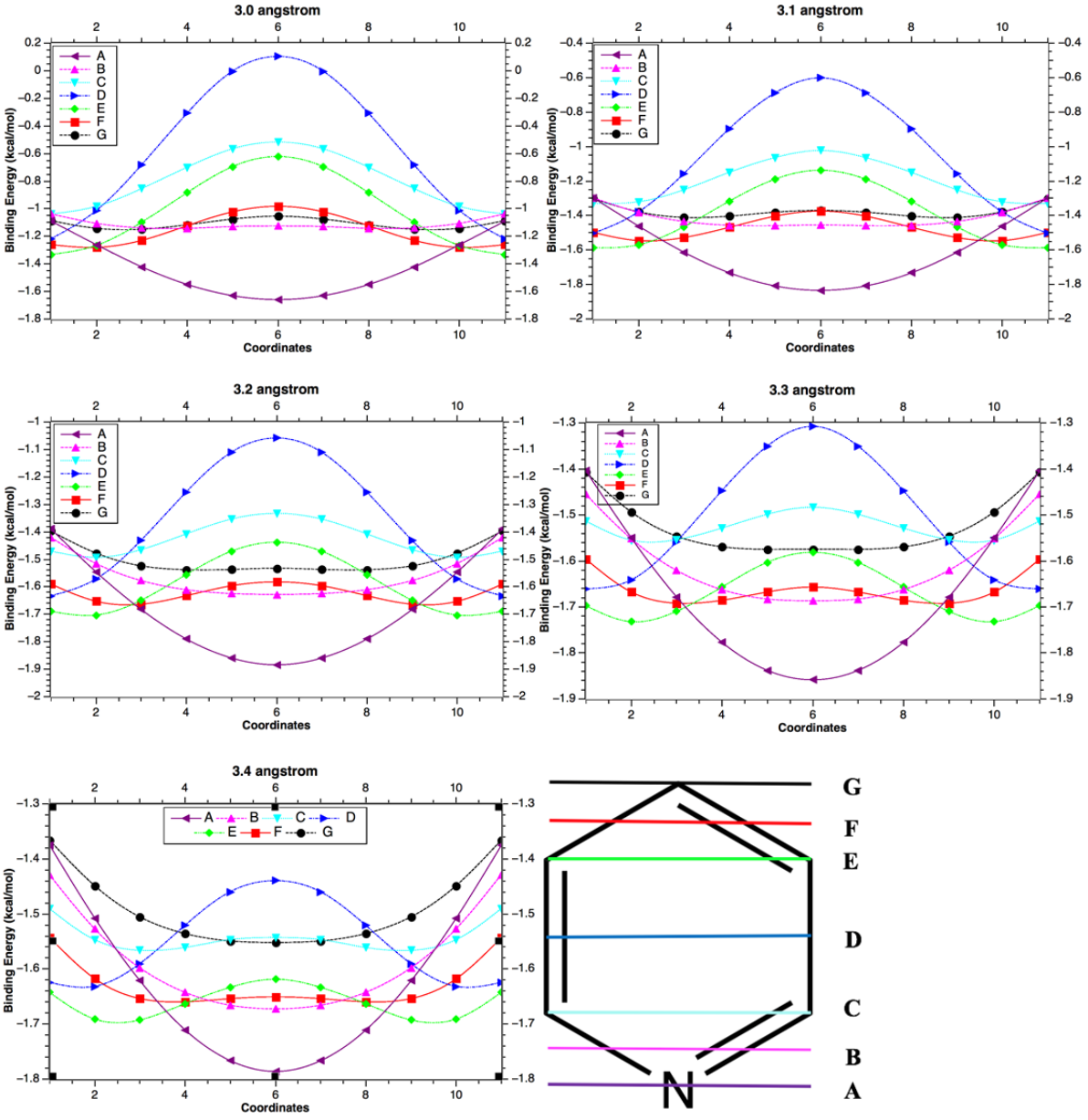


Figure S21: ωB97X-D/aug-cc-pVTZ scans 3.0-3.4 Å for indole···Cl_2

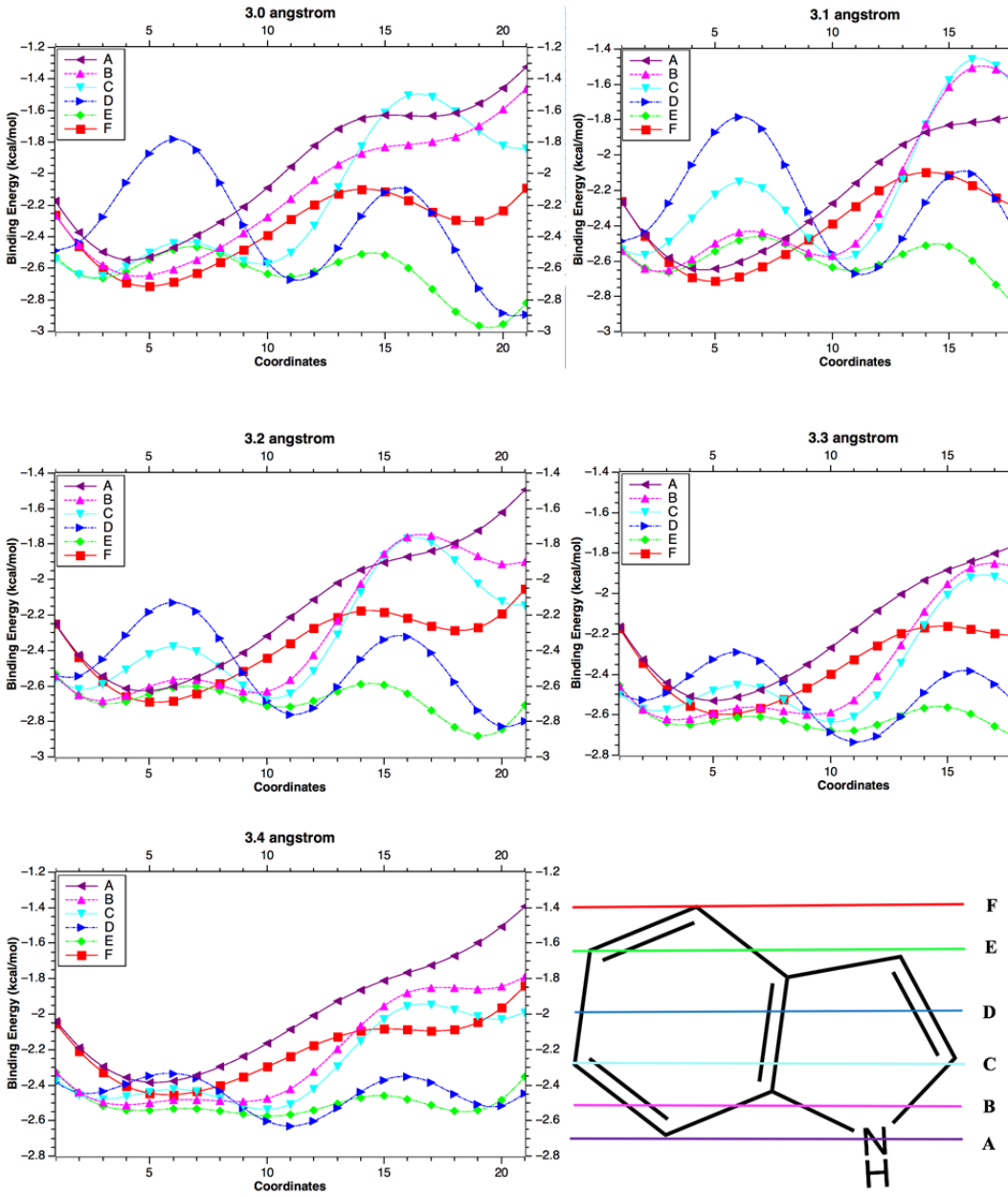


Figure S22: ωB97X-D/aug-cc-pVTZ scans 3.0-3.4 Å for quinoline···Cl_2

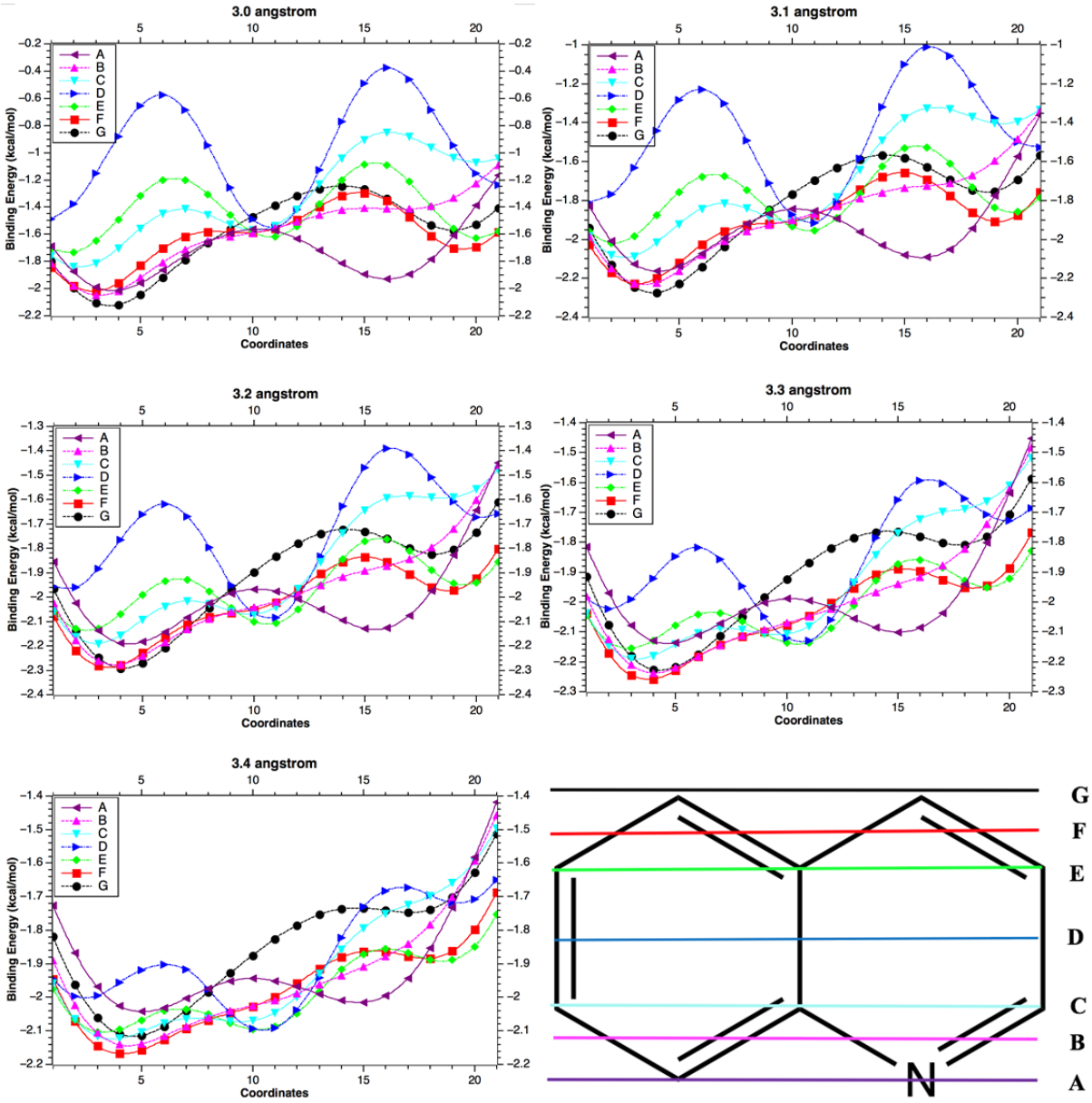


Figure S23: sSAPT0/jun-cc-pVDZ scans at with Cl_2 at 3.2 Å above aromatic plane for benzene···Cl_2

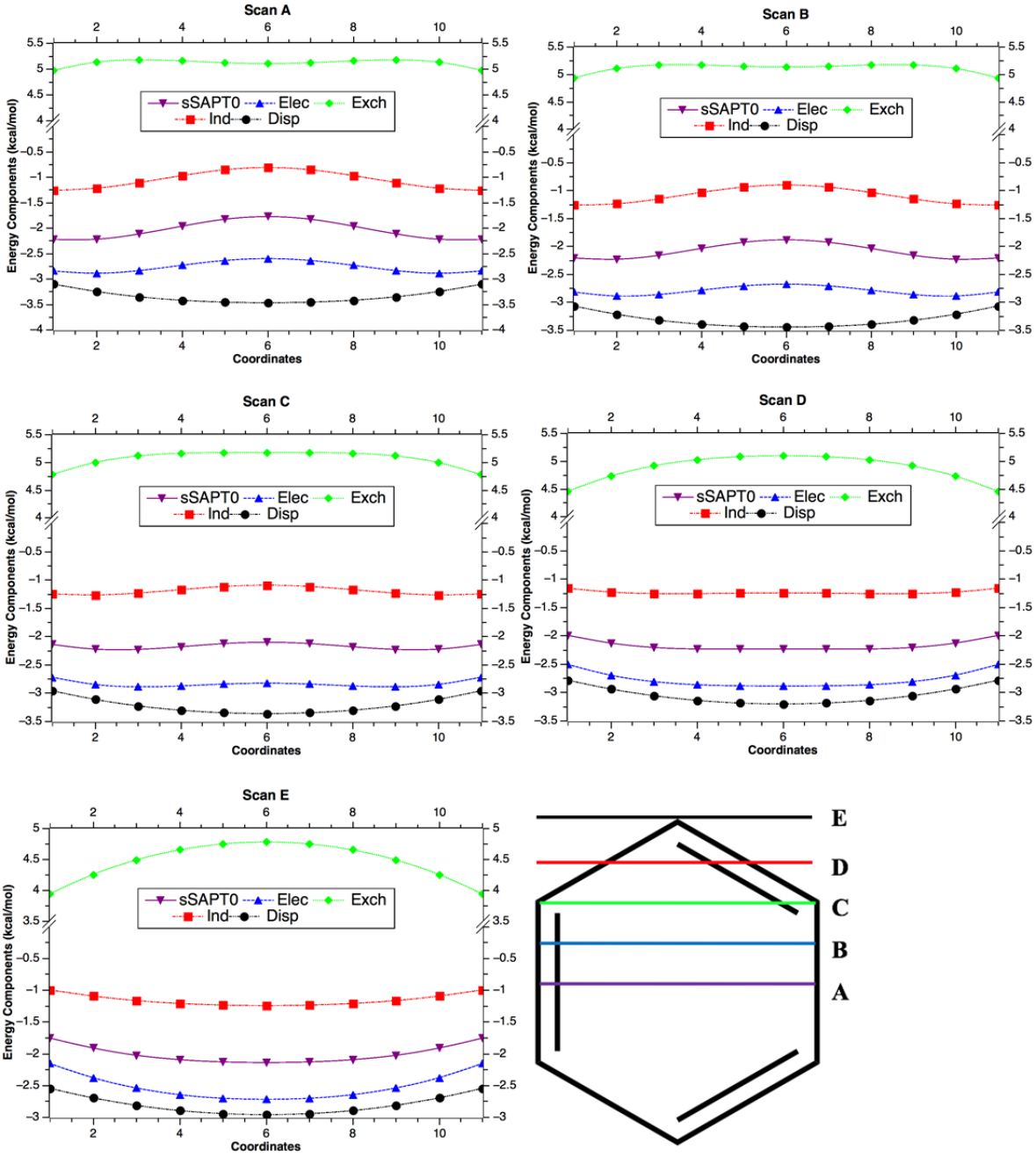


Figure S24: sSAPT0/jun-cc-pVDZ scans at with Br_2 at 3.2 Å above aromatic plane for benzene···Br_2

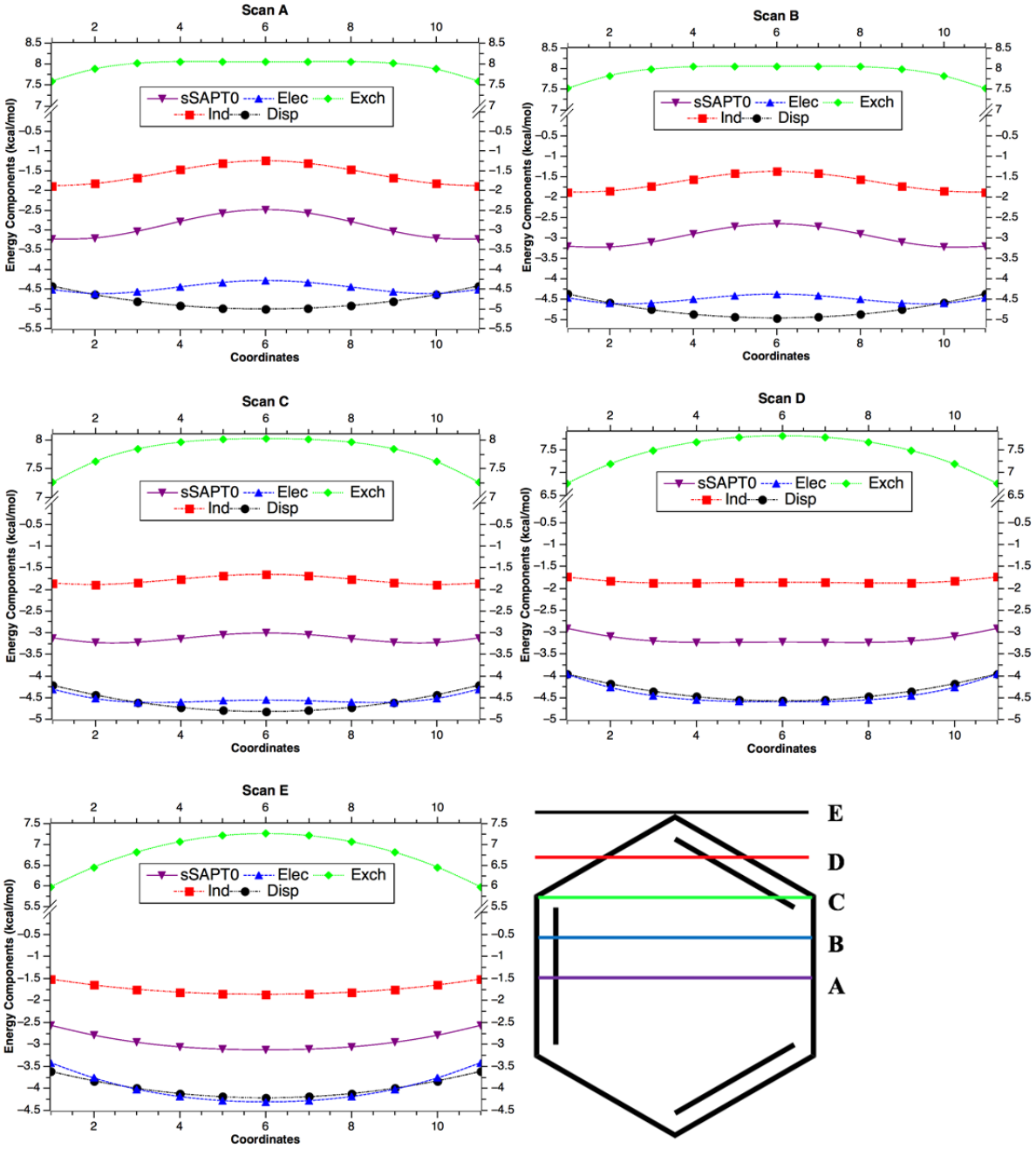


Figure S25: sSAPT0/jun-cc-pVDZ scans at with Cl_2 at 3.2 Å above aromatic plane for naphthalene···Cl_2

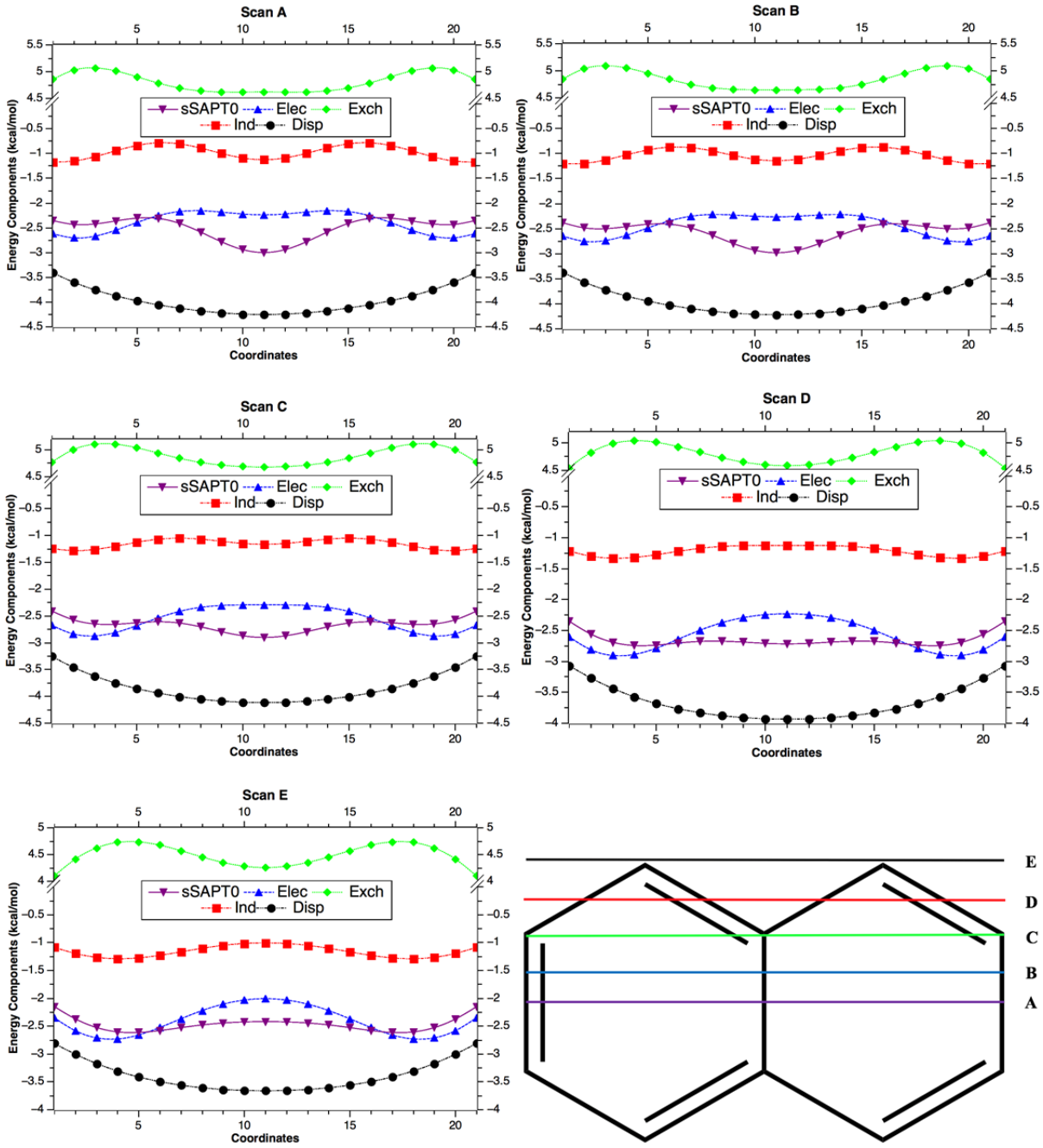


Figure S26: sSAPT0/jun-cc-pVDZ scans at with Cl_2 at 3.2 Å above aromatic plane for naphthalene···Br_2

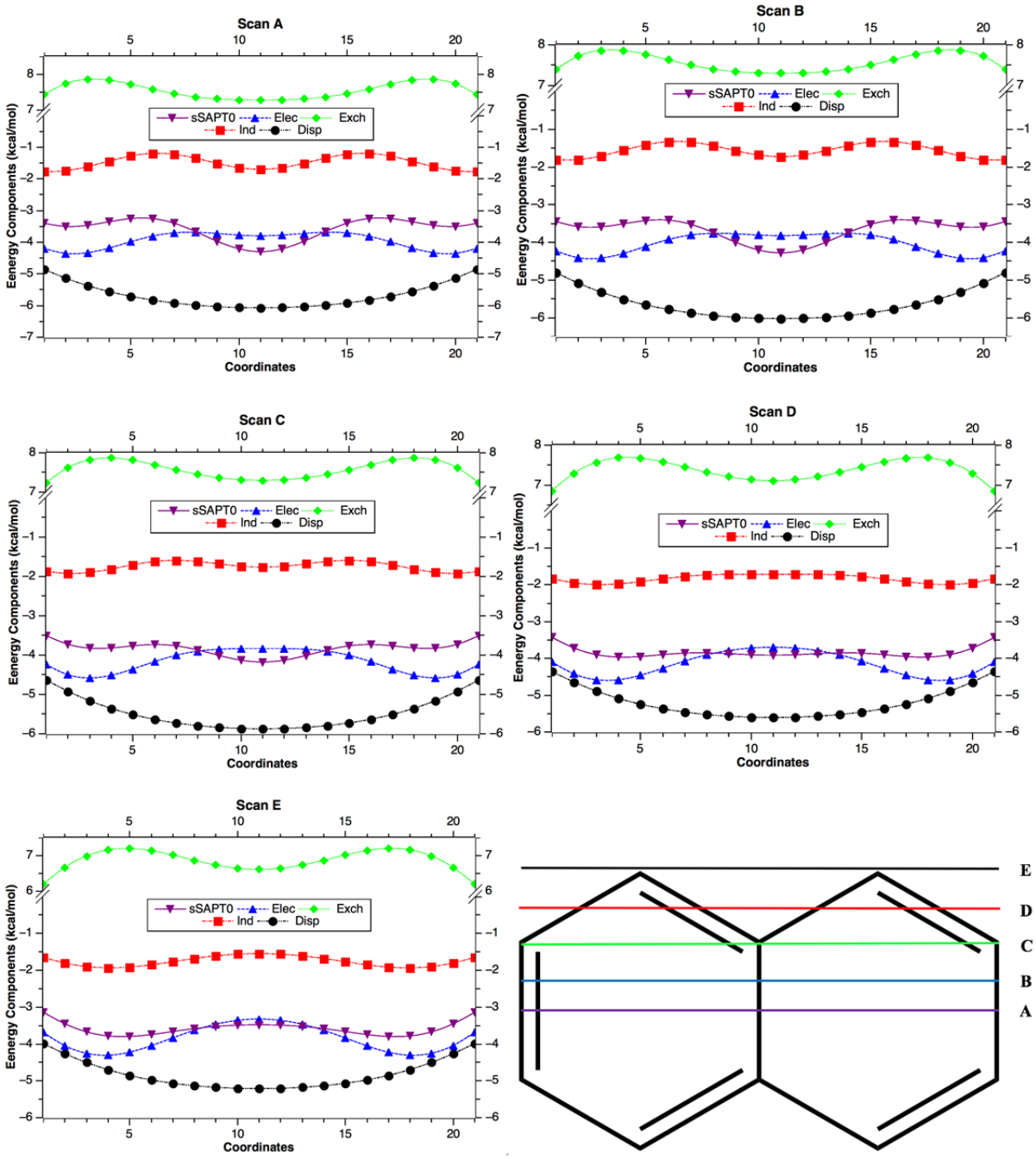


Figure S27: sSAPT0/jun-cc-pVDZ scans at with Cl_2 at 3.2 Å above aromatic plane for toluene···Cl_2

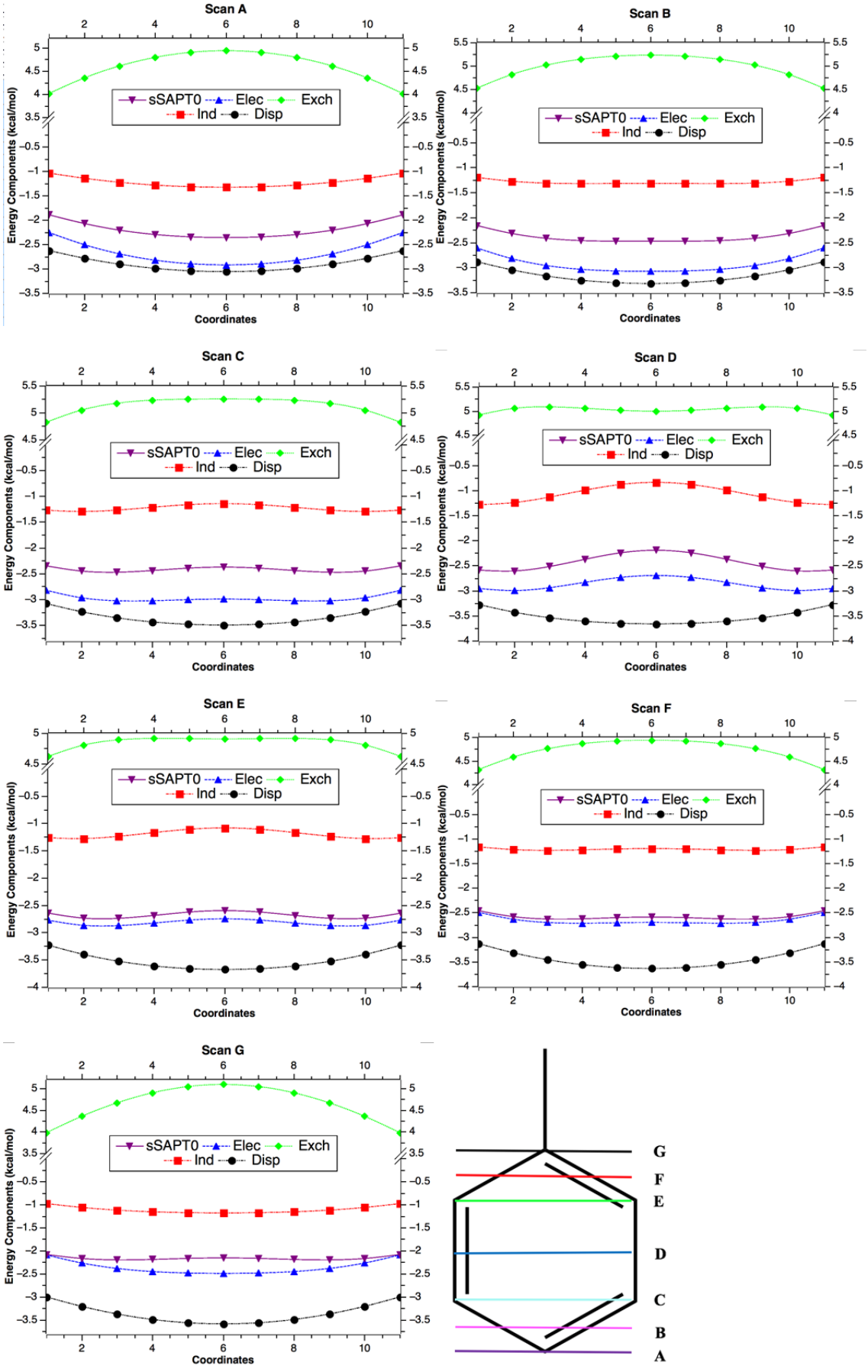


Figure S28: sSAPT0/jun-cc-pVDZ scans at with Cl_2 at 3.2 Å above aromatic plane for anthracene···Cl_2

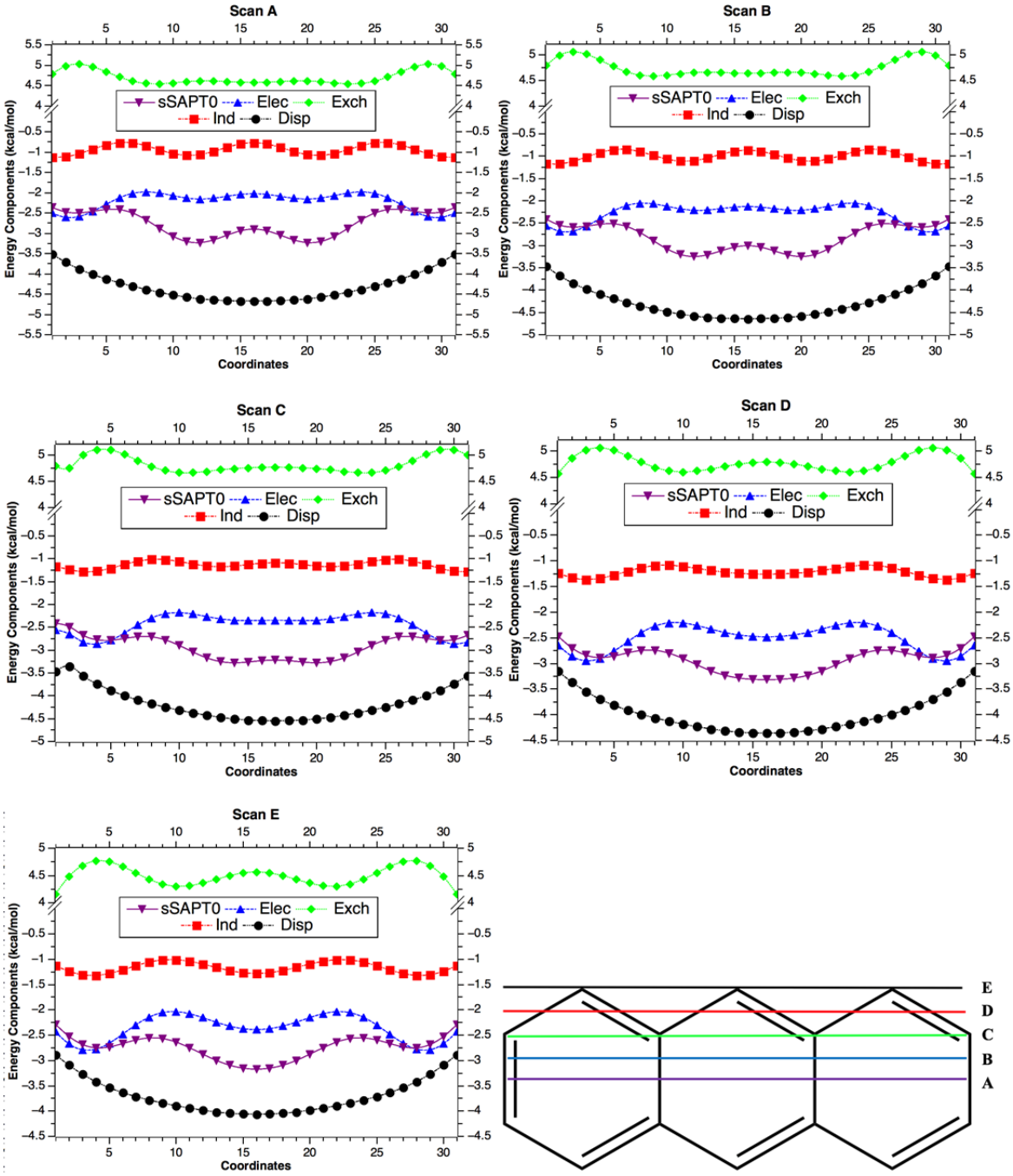
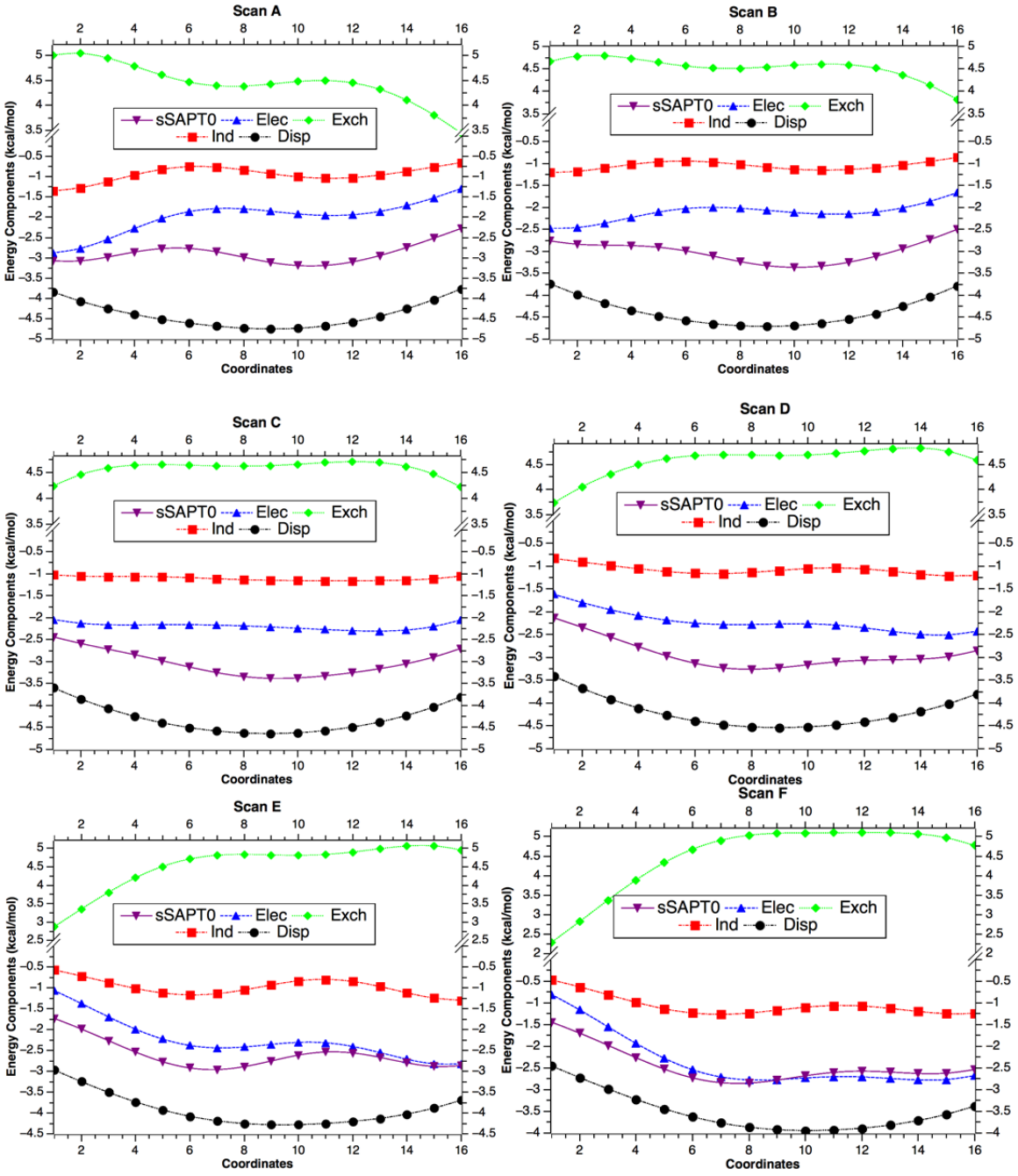
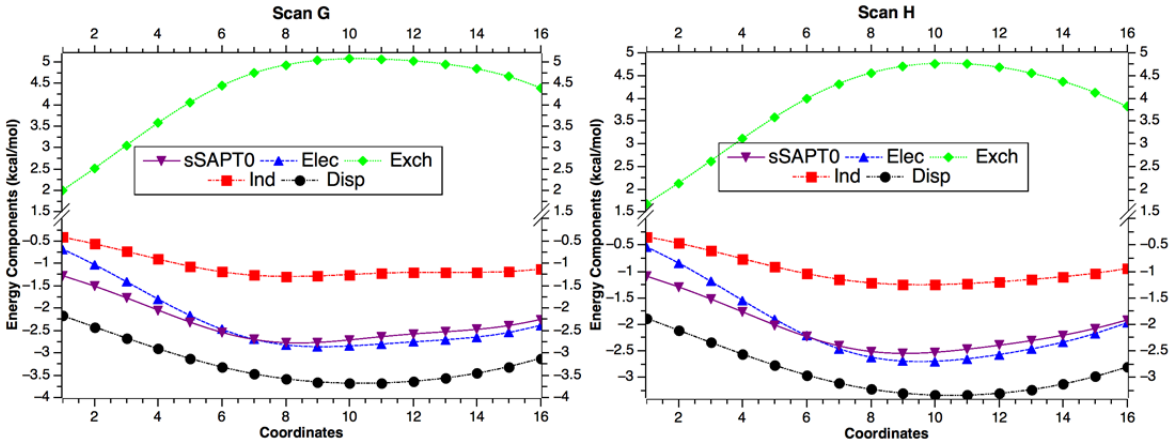


Figure S29: sSAPT0/jun-cc-pVDZ scans at with Cl_2 at 3.2 Å above aromatic plane for phenanthrene···Cl_2




Scan G
Scan H
sSAPT0
Elec
Exch
Ind
Disp
Energy Components (kcal/mol)
Coordinates

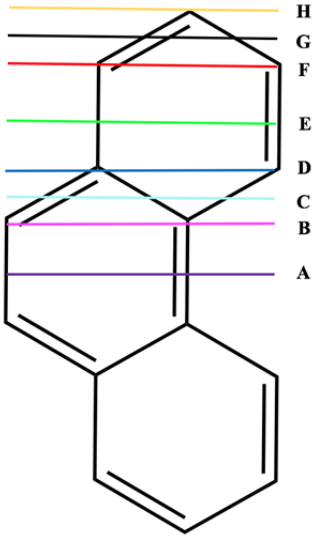

H
G
F
E
D
C
B
A

Figure S30: sSAPT0/jun-cc-pVDZ scans at with Cl_2 at 3.2 Å above aromatic plane for pyrrole···Cl_2

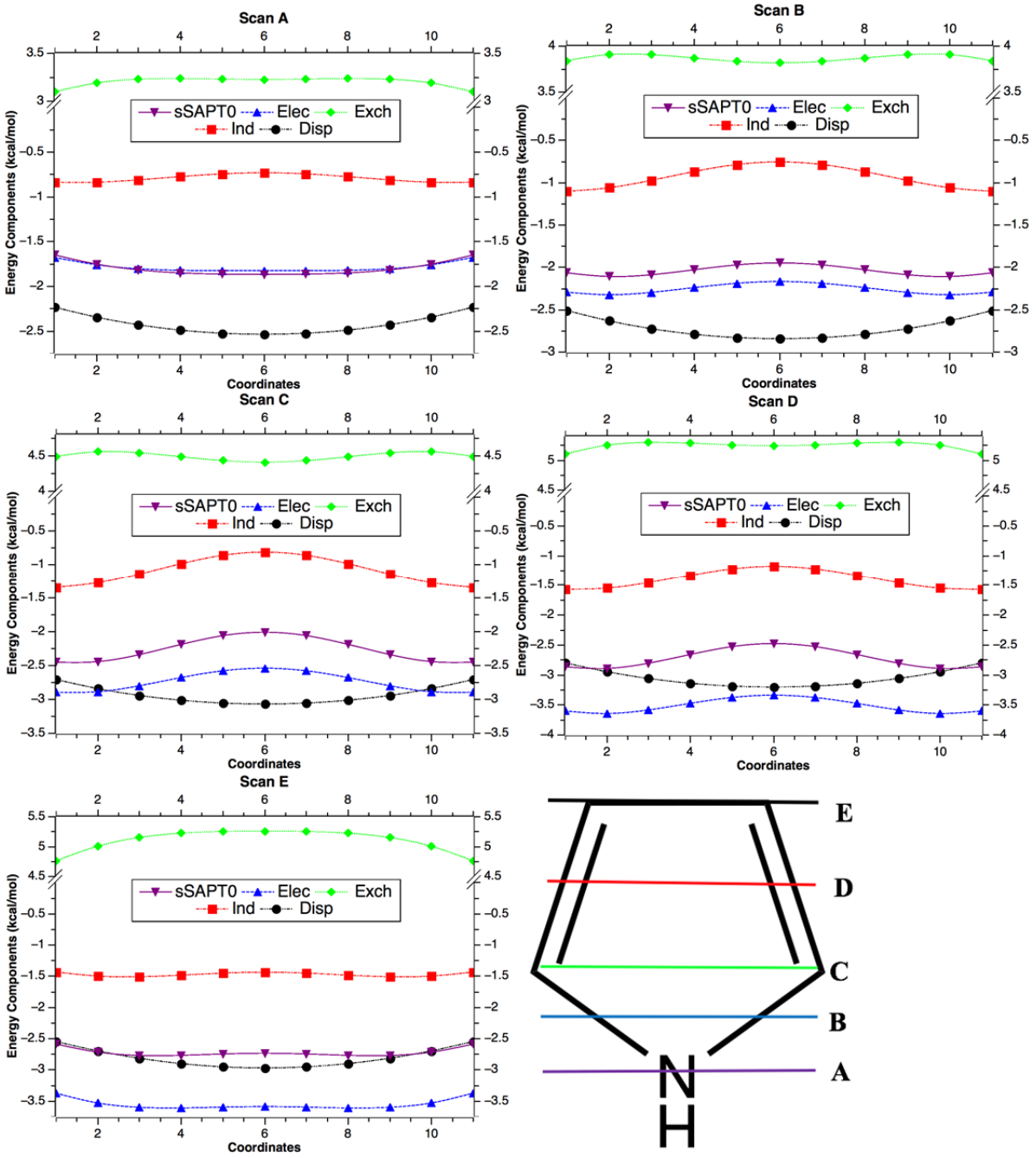


Figure S31: sSAPT0/jun-cc-pVDZ scans at with Cl_2 at 3.2 Å above aromatic plane for imidazole···Cl_2

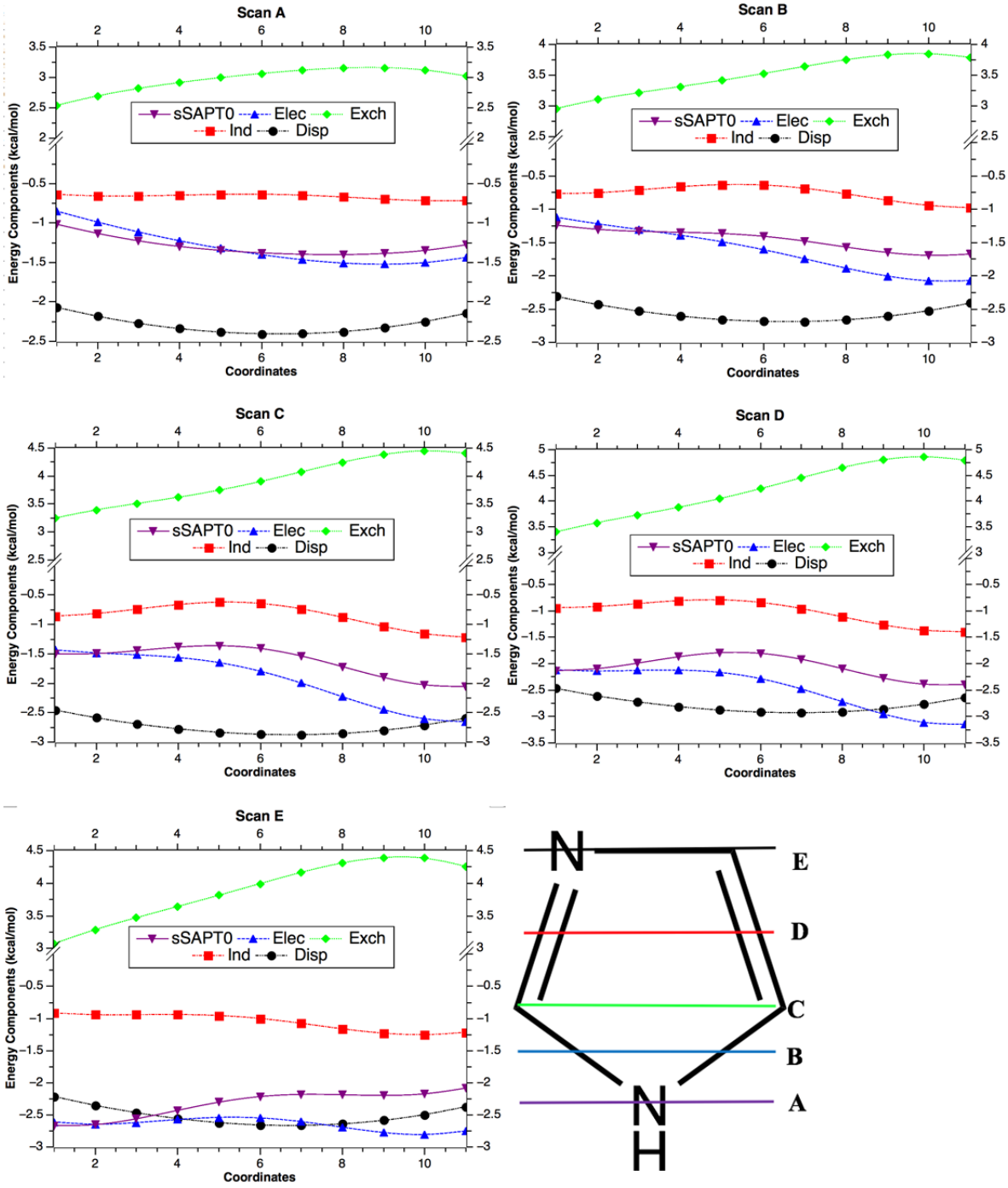


Figure S32: sSAPT0/jun-cc-pVDZ scans at with Cl_2 at 3.2 Å above aromatic plane for pyridine···Cl_2

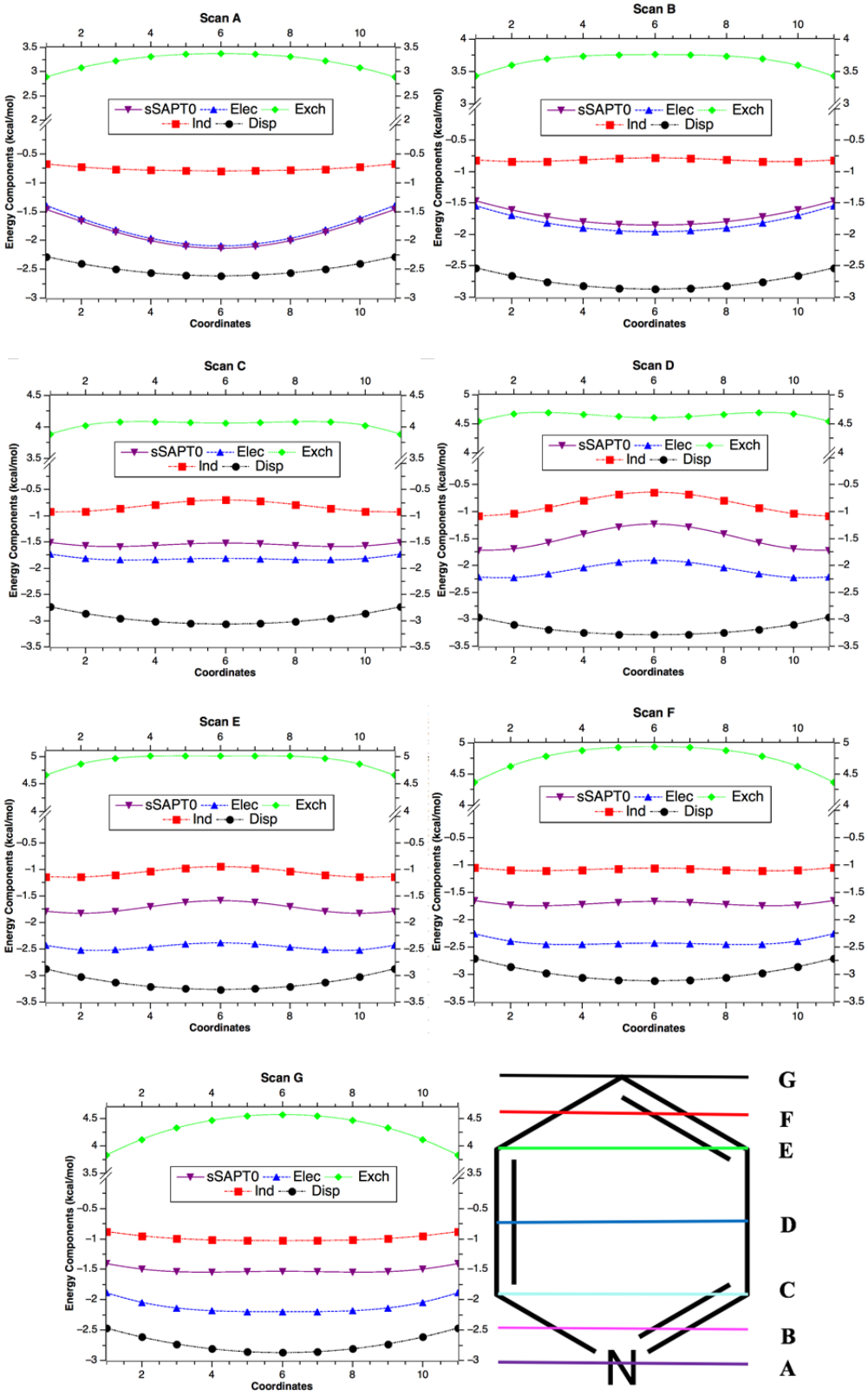


Figure S33: sSAPT0/jun-cc-pVDZ scans at with Cl_2 at 3.2 Å above aromatic plane for indole···Cl_2

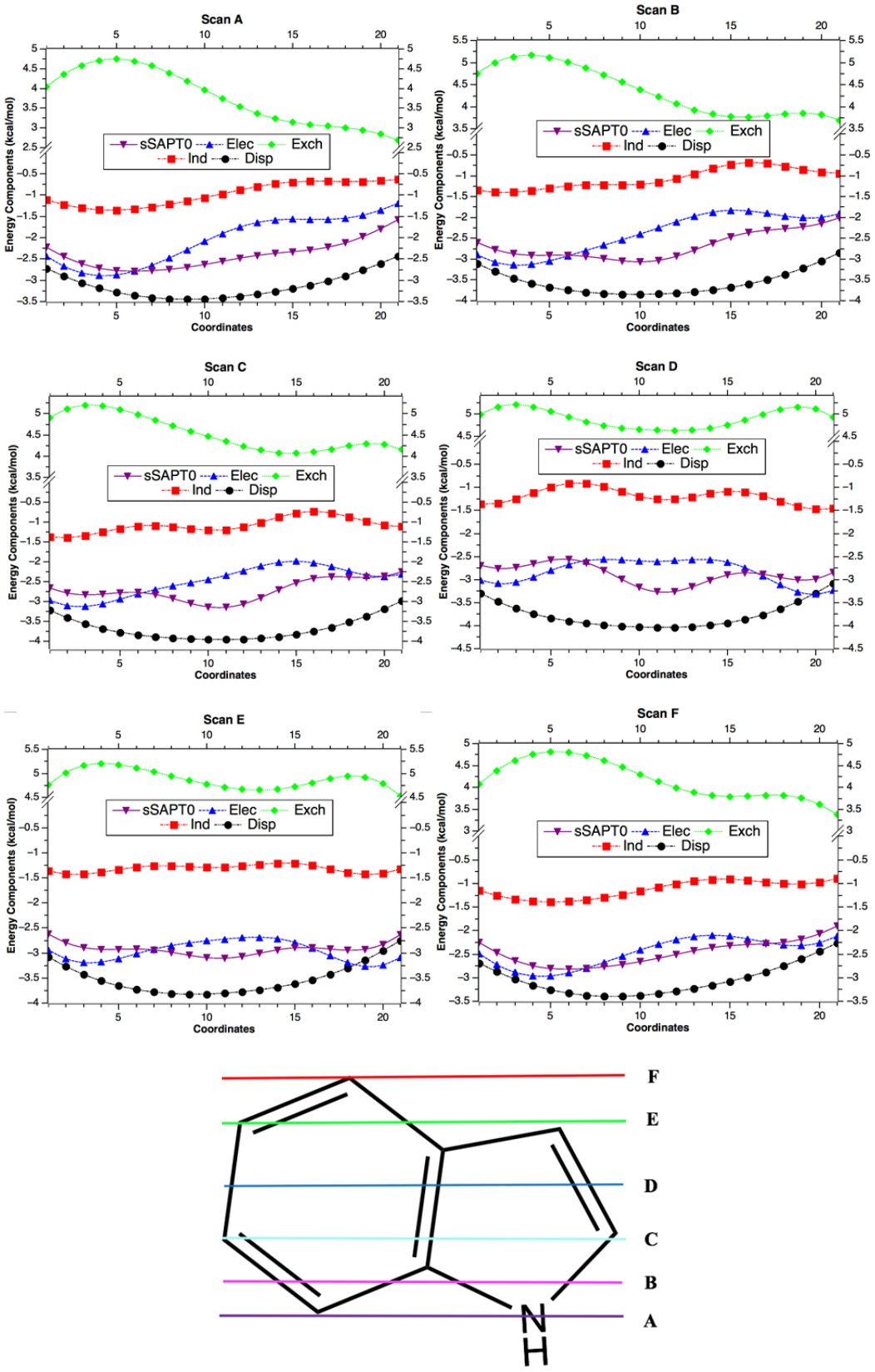


Figure S34: sSAPT0/jun-cc-pVDZ scans at with Cl_2 at 3.2 Å above aromatic plane for quinoline···Cl_2

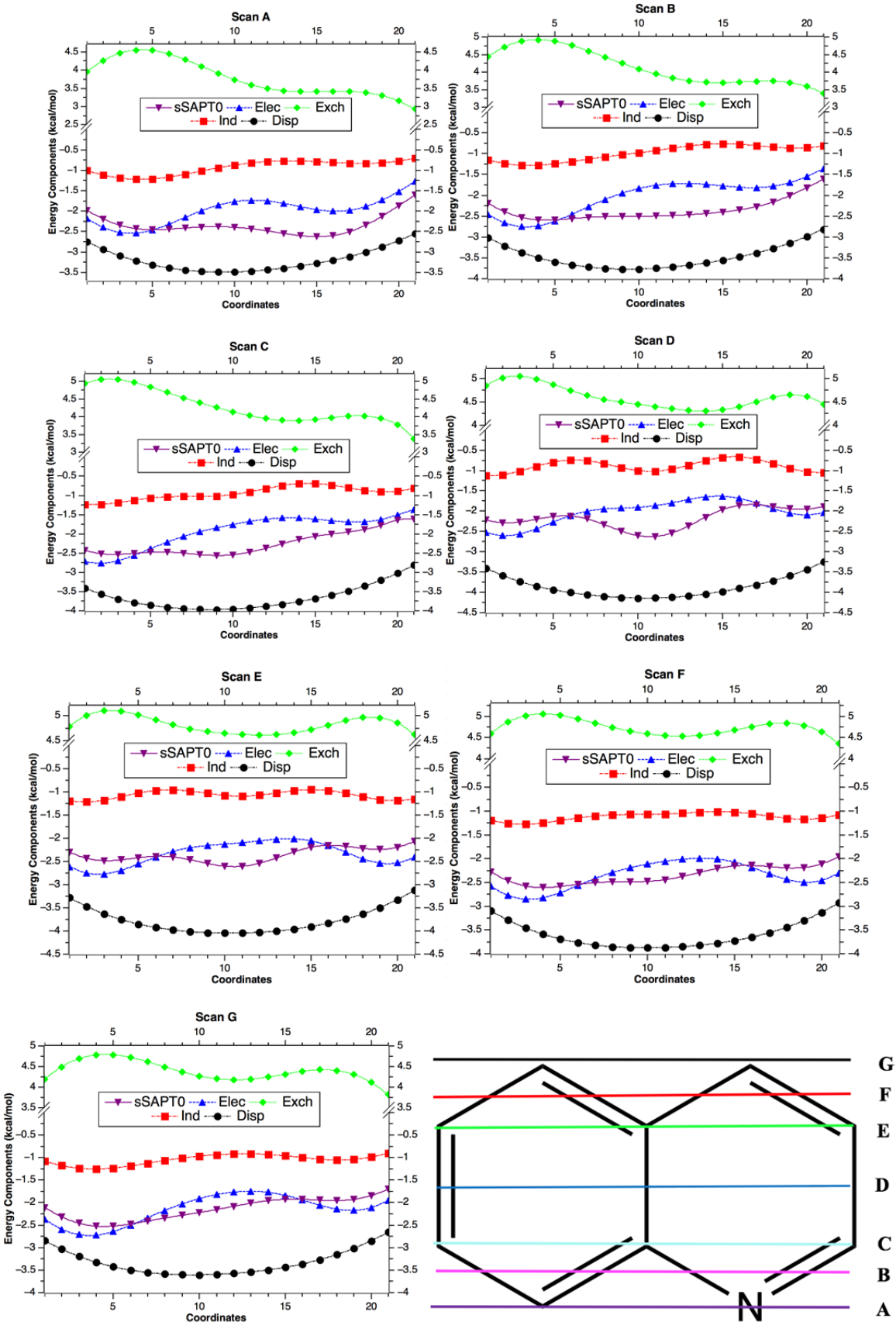
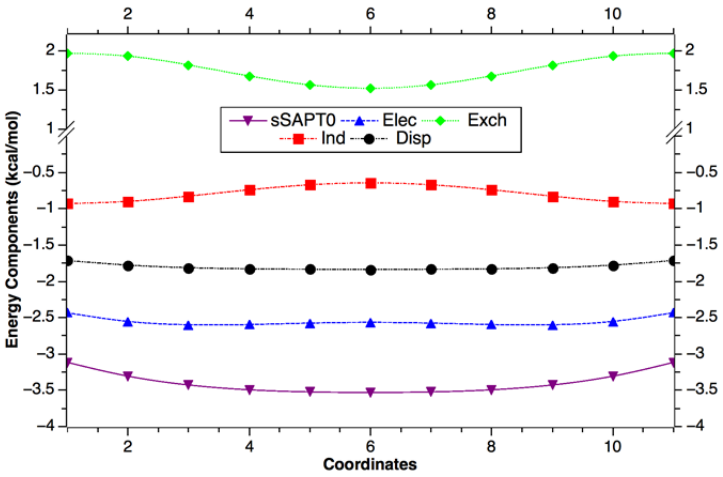
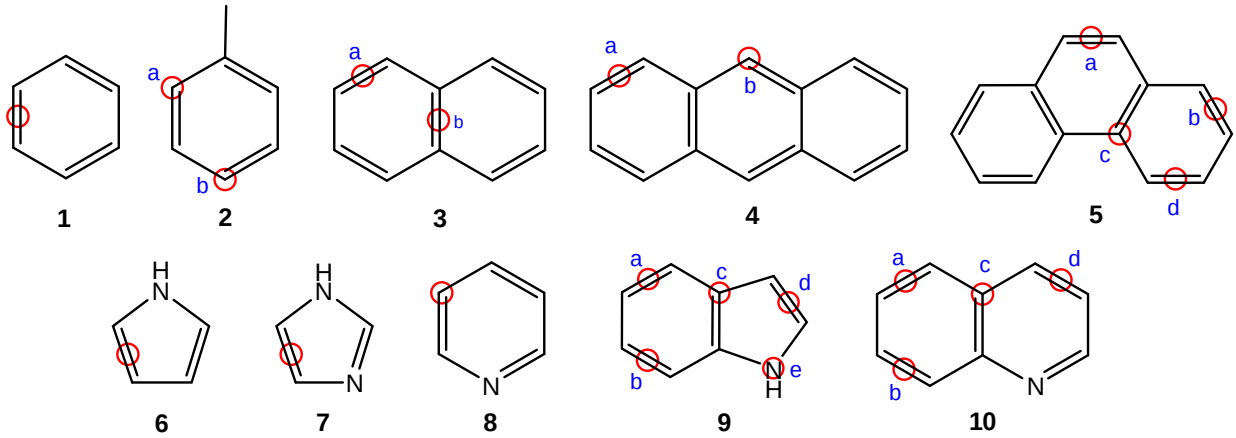


Figure S35: sSAPT0/jun-cc-pVDZ scan A at with HCl at 2.7 Å above aromatic plane for benzene···HCl



Optimized Coordinates of aromatic···Cl_2 complexes (ωB97X-D/aug-cc-pVTZ)



Benzene···Cl_2

C 1.6462000000 0.6941100000 1.1827500000
C 1.9675900000 1.3878600000 0.0242500000
C 2.2885300000 0.6939800000 -1.1323400000
H 1.9648000000 2.4692700000 0.0239000000
C 1.6462300000 -0.6943500000 1.1826100000
H 1.3959700000 1.2346400000 2.0855000000
C 1.9676400000 -1.3878600000 0.0239700000
H 1.3960100000 -1.2350700000 2.0852500000
C 2.2885500000 -0.6937400000 -1.1324800000
H 2.5367300000 1.2345000000 -2.0355800000
H 1.9648800000 -2.4692700000 0.0234100000
H 2.5367700000 -1.2340700000 -2.0358300000
Cl -1.4671100000 -0.0000200000 0.2459600000
Cl -3.3931000000 0.0000200000 -0.3070800000

Benzene···ClF

C	0.9055742466	0.7144661524	1.1528930361
C	1.4793766672	1.3886631258	0.0817772508
C	2.0390915915	0.6747635793	-0.9645021611
H	1.4856108193	2.4697522335	0.0657528399
C	0.8949756103	-0.6749433302	1.1731271586
H	0.4746786224	1.2702384419	1.9744969565
C	1.4580931176	-1.3887533399	0.1220331247
H	0.4566097349	-1.2000564258	2.0108075936
C	2.0283990686	-0.7142721984	-0.9444386030
H	2.4836364994	1.1988986866	-1.7994383360
H	1.4477344579	-2.4698207831	0.1374389100
H	2.4645718903	-1.2691020815	-1.7637998756
Cl	-1.8399024534	0.0002644934	0.0353368081
F	-3.3741735723	-0.0004389305	-0.5501469612

Benzene···BrF

C	-1.4443844328	-0.6955505596	1.0982106998
C	-1.9305552241	-1.3897879978	-0.0047597866
C	-2.4127976209	-0.6952336777	-1.1000676567
H	-1.9285957180	-2.4708596638	-0.0044861739
C	-1.4440425790	0.6952825367	1.0980449562
H	-1.0831139461	-1.2361785859	1.9623816771
C	-1.9298880534	1.3895070047	-0.0050950332
H	-1.0824620580	1.2359207390	1.9620822052
C	-2.4124038760	0.6949359838	-1.1002654103
H	-2.7886409175	-1.2343406900	-1.9587626765
H	-1.9274479591	2.4705779987	-0.0050568964
H	-2.7880038146	1.2340238398	-1.9590779180
Br	1.4077754984	0.0008534257	0.2601931937
F	3.1238191313	0.0008209792	-0.1881437324

Benzene···BrCl

C	1.8698530102	0.6943417019	1.1446400413
C	2.2908609890	1.3885583540	0.0176915885
C	2.7107673636	0.6945711743	-1.1057898192
H	2.2877377798	2.4698175816	0.0174756223
C	1.8700395822	-0.6951202380	1.1442305005
H	1.5467338772	1.2345798410	2.0241464895
C	2.2912358634	-1.3885605501	0.0168775473
H	1.5470550190	-1.2359623059	2.0234148120
C	2.7109559835	-0.6938005653	-1.1061963226
H	3.0360097143	1.2348697561	-1.9842618953
H	2.2884048870	-2.4698202328	0.0160252755
H	3.0363460011	-1.2334948002	-1.9849851958
Br	-1.1747141610	0.0000218073	0.1798901803
Cl	-3.2405628467	-0.0000407261	-0.4162760354

Benzene···Br_2

C	2.53643	-1.12042	0.69325
C	2.87480	0.03302	1.38829
C	3.21244	1.18499	0.69537
H	2.87148	0.03227	2.46960
C	2.53646	-1.11882	-0.69588
H	2.27520	-2.02068	1.23274

C	2.87486	0.03621	-1.38825
H	2.27525	-2.01783	-1.23746
C	3.21247	1.18659	-0.69267
H	3.47331	2.08414	1.23661
H	2.87159	0.03796	-2.46955
H	3.47337	2.08699	-1.23182
Br	-0.61078	-0.28648	-0.00026
Br	-2.83851	0.24613	0.00023

Benzene···$ClCF_3$

(MAX Force and RMS Force have converged while Displacement is not converging due to flat Potential Energy Surface)

C	2.64362	-1.10141	0.79362
C	2.63780	0.15575	1.38028
C	2.62487	1.29254	0.58527
H	2.64216	0.25021	2.45782
C	2.63608	-1.22131	-0.58878
H	2.65374	-1.98870	1.41196
C	2.62293	-0.08392	-1.38363
H	2.64057	-2.20030	-1.04831
C	2.61729	1.17278	-0.79668
H	2.61851	2.27149	1.04472
H	2.61536	-0.17827	-2.46118
H	2.60522	2.06009	-1.41487
Cl	-0.83470	-0.34469	0.00118
C	-2.55313	0.04780	0.00153
F	-3.09223	-0.24407	-1.17174
F	-2.72967	1.33812	0.23749
F	-3.18313	-0.64256	0.93903

Toluene···Cl_2 (a)

C 1.4096100000 0.1949300000 1.1825200000
C 1.6150900000 0.9725900000 0.0444900000
C 2.0138400000 0.3339500000 -1.1247600000
C 1.3772000000 2.4559500000 0.0764500000
C 1.5920400000 -1.1801500000 1.1505600000
H 1.1091600000 0.6740900000 2.1062300000
C 1.9856600000 -1.8031100000 -0.0235700000
H 1.4262900000 -1.7641800000 2.0457300000
C 2.1974500000 -1.0398800000 -1.1611100000
H 2.1817400000 0.9202900000 -2.0194400000
H 2.1280000000 -2.8745000000 -0.0509500000
H 2.5072700000 -1.5154800000 -2.0818800000
H 1.9273300000 2.9631000000 -0.7148100000
H 1.6785300000 2.8846400000 1.0317400000
H 0.3167000000 2.6761700000 -0.0627200000
Cl -1.5718100000 -0.0969100000 0.2223700000
Cl -3.5117400000 -0.1130800000 -0.2883400000

Toluene···Cl_2 (b)

C 1.8399200000 0.0715100000 1.1974800000
C 2.1837000000 0.6962800000 0.0035600000
C 1.9530800000 0.0149100000 -1.1882600000
C 2.7606600000 2.0842200000 -0.0039400000
C 1.2745700000 -1.1946000000 1.2035200000

H 2.0152500000 0.5833200000 2.1354600000
C 1.0448100000 -1.8611000000 0.0084300000
H 1.0135800000 -1.6626600000 2.1430500000
C 1.3890300000 -1.2502200000 -1.1894800000
H 2.2183400000 0.4834500000 -2.1278500000
H 0.6082500000 -2.8503800000 0.0106900000
H 1.2166300000 -1.7617800000 -2.1267000000
H 3.4613600000 2.2172200000 -0.8275200000
H 3.2826700000 2.3018000000 0.9269200000
H 1.9702600000 2.8281400000 -0.1211700000
Cl -1.7648700000 -0.2553900000 0.0509600000
Cl -3.5563600000 0.6374400000 -0.0627700000

Naphthalene···Cl_2 (a)
C 2.5047220000 -1.9864050000 0.6211240000
C 2.8838640000 -1.7026780000 -0.7070190000
C 2.4904730000 -0.5391350000 -1.3017070000
H 3.4882040000 -2.4138360000 -1.2533750000
C 1.6986290000 0.3997180000 -0.6001570000
H 2.7790130000 -0.3197650000 -2.3217940000
C 1.7414470000 -1.0996260000 1.3234430000
H 2.8214710000 -2.9126410000 1.0806830000
C 1.3188700000 0.1144610000 0.7343960000
H 1.4466620000 -1.3160970000 2.3423230000
C 1.2710500000 1.6132940000 -1.1901860000
C 0.5206800000 1.0519770000 1.4336290000
C 0.5030440000 2.4984780000 -0.4923500000
H 1.5624840000 1.8273490000 -2.2105830000
C 0.1217780000 2.2142380000 0.8359340000
H 0.2324360000 0.8340920000 2.4541940000
H 0.1795940000 3.4206800000 -0.9548710000
H -0.4876310000 2.9222780000 1.3806900000
Cl -2.2142180000 -0.0004940000 0.2009770000
Cl -3.8063450000 -1.0246810000 -0.4633240000

Naphthalene···Cl_2 (b)
C -1.4405000000 -2.4165200000 -0.7024100000
C -1.3910500000 -2.4167700000 0.7072800000
C -1.3708000000 -1.2390900000 1.3955000000
H -1.3668500000 -3.3571200000 1.2406500000
C -1.3977500000 0.0000300000 0.7113500000
H -1.3298000000 -1.2364300000 2.4772200000
C -1.4686500000 -1.2387000000 -1.3902100000
H -1.4538300000 -3.3567900000 -1.2363200000
C -1.4476300000 0.0000300000 -0.7061300000
H -1.5037400000 -1.2361000000 -2.4721300000
C -1.3707100000 1.2391400000 1.3955000000
C -1.4685600000 1.2387700000 -1.3902100000
C -1.3908700000 2.4168300000 0.7072800000
H -1.3297100000 1.2364800000 2.4772200000
C -1.4403300000 2.4165800000 -0.7024100000
H -1.5036500000 1.2361700000 -2.4721300000
H -1.3666100000 3.3571700000 1.2406500000
H -1.4535800000 3.3568600000 -1.2363200000
Cl 1.8379200000 -0.0000500000 0.0718500000

Cl 3.8343600000 -0.0000600000 -0.0819700000

Anthracene···Cl_2 (a)

C 2.1673480000 -0.3549230000 0.6801840000
C 2.4157640000 0.2008220000 -0.6129180000
C 1.5004710000 1.0978280000 -1.1539690000
C 0.3500460000 1.4665850000 -0.4662710000
H 1.6879630000 1.5178500000 -2.1350730000
C 1.0162610000 0.0145680000 1.3682720000
C 0.1029140000 0.9113720000 0.8270560000
H 0.8260250000 -0.4086960000 2.3474080000
C -0.5984430000 2.3828090000 -1.0108520000
C -1.0851890000 1.2938480000 1.5186890000
C -1.7160420000 2.7226840000 -0.3223940000
H -0.4084200000 2.8012420000 -1.9909360000
C -1.9648500000 2.1679940000 0.9634270000
H -1.2711320000 0.8755320000 2.4996530000
H -2.4286980000 3.4155320000 -0.7477890000
H -2.8606650000 2.4501820000 1.4994570000
Cl -2.9892550000 -0.7655590000 0.0872090000
Cl -3.8862080000 -2.3704860000 -0.7195600000
C 3.1125360000 -1.2745410000 1.2225730000
C 4.2268720000 -1.6175030000 0.5292870000
C 3.5992570000 -0.1864340000 -1.3077860000
C 4.4743040000 -1.0643260000 -0.7567680000
H 2.9221970000 -1.6951150000 2.2016940000
H 4.9360530000 -2.3162670000 0.9514810000
H 3.7857200000 0.2353590000 -2.2871410000
H 5.3682090000 -1.3501420000 -1.2940900000

Anthracene···Cl_2 (b)

C 1.2154170000 0.8860620000 0.7548730000
C 1.2143870000 1.4031500000 -0.5772830000
C -0.0001860000 1.6490070000 -1.2085590000
C -1.2147130000 1.4029060000 -0.5772880000
H -0.0002240000 2.0384900000 -2.2197680000
C -0.0000900000 0.6376620000 1.3876250000
C -1.2156450000 0.8858170000 0.7548670000
H -0.0000530000 0.2501200000 2.3996490000
C -2.4653800000 1.6452710000 -1.2179770000
C -2.4665770000 0.6334390000 1.3902060000
C -3.6347660000 1.3913620000 -0.5796210000
H -2.4624650000 2.0355130000 -2.2276560000
C -3.6349650000 0.8771860000 0.7458890000
H -2.4651070000 0.2389160000 2.3981560000
H -4.5770410000 1.5777560000 -1.0763370000
H -4.5775980000 0.6800110000 1.2378420000
Cl 0.0002710000 -2.2168040000 0.1282930000
Cl 0.0004910000 -4.0846800000 -0.6054450000
C 2.4663980000 0.6339360000 1.3902160000
C 3.6347400000 0.8779160000 0.7459030000
C 2.4650080000 1.6457640000 -1.2179680000
C 3.6344430000 1.3920890000 -0.5796080000
H 2.4650030000 0.2394140000 2.3981670000
H 4.5774100000 0.6809290000 1.2378590000

H 2.4620190000 2.0360040000 -2.2276480000
H 4.5766820000 1.5786690000 -1.0763220000

Phenanthrene···Cl_2 (a)

C 3.7380660000 -2.1903930000 0.6880100000
C 4.0649000000 -2.2490210000 -0.6709250000
C 3.8741410000 -1.1564400000 -1.4792060000
H 4.4694070000 -3.1607070000 -1.0888700000
C 3.3497040000 0.0457110000 -0.9722080000
H 4.1354460000 -1.2354620000 -2.5239200000
C 3.2251080000 -1.0318270000 1.2093090000
H 3.8888290000 -3.0544400000 1.3202230000
C 3.0232120000 0.0984260000 0.3985990000
H 2.9652290000 -0.9723210000 2.2585060000
C 3.1310850000 1.2217180000 -1.7983210000
C 2.4816640000 1.3026710000 0.9542440000
C 2.5977930000 2.3863940000 -1.2086790000
C 2.2787100000 2.3935570000 0.1878730000
H 2.2401860000 1.3196860000 2.0093060000
H 1.8719500000 3.2996280000 0.6183880000
Cl -0.4931160000 0.8902820000 -0.0491180000
Cl -2.3182630000 0.2153730000 -0.5449410000
C 2.3768110000 3.5299060000 -1.9954820000
C 3.4260950000 1.2543510000 -3.1727990000
C 3.2041190000 2.3813010000 -3.9238830000
C 2.6738150000 3.5330820000 -3.3330050000
H 1.9635720000 4.4129470000 -1.5249930000
H 2.4991100000 4.4177840000 -3.9294860000
H 3.8350020000 0.3817580000 -3.6599490000
H 3.4399780000 2.3769910000 -4.9792570000

Phenanthrene···Cl_2 (b)

C 3.8651380000 -2.2533020000 0.6127440000
C 4.2704780000 -2.2604180000 -0.7264470000
C 4.0580170000 -1.1616700000 -1.5201310000
H 4.7500210000 -3.1369120000 -1.1397490000
C 3.4326680000 -0.0047390000 -1.0204820000
H 4.3791370000 -1.2006790000 -2.5503040000
C 3.2552030000 -1.1380580000 1.1284060000
H 4.0317590000 -3.1212700000 1.2354920000
C 3.0284000000 -0.0011190000 0.3304220000
H 2.9397850000 -1.1177240000 2.1639010000
C 3.1849310000 1.1721590000 -1.8353490000
C 2.3817370000 1.1527090000 0.8781260000
C 2.5437050000 2.2857340000 -1.2538730000
C 2.1500620000 2.2419910000 0.1223420000
H 2.0785970000 1.1279190000 1.9168930000
H 1.6584610000 3.1093910000 0.5438500000
Cl 0.5328500000 -2.4016080000 0.0194050000
Cl -1.2905060000 -2.9487710000 -0.6090910000
C 2.2955170000 3.4312060000 -2.0307920000
C 3.5557560000 1.2555790000 -3.1895410000
C 3.3046110000 2.3830410000 -3.9301720000
C 2.6676720000 3.4845670000 -3.3481800000
H 1.8018430000 4.2761180000 -1.5677270000

H 2.4713330000 4.3706350000 -3.9359460000
H 4.0487210000 0.4228030000 -3.6686820000
H 3.6009010000 2.4188720000 -4.9695920000

Phenanthrene···Cl_2 (c)
C 3.7497760000 -2.1942470000 0.6736260000
C 4.0848320000 -2.2537770000 -0.6837090000
C 3.9014960000 -1.1606510000 -1.4920340000
H 4.4882440000 -3.1666400000 -1.0998320000
C 3.3752890000 0.0436570000 -0.9873420000
H 4.1670000000 -1.2393560000 -2.5356410000
C 3.2361720000 -1.0354660000 1.1929840000
H 3.8940730000 -3.0592090000 1.3060840000
C 3.0393180000 0.0971650000 0.3829120000
H 2.9701060000 -0.9769140000 2.2406200000
C 3.1624560000 1.2200730000 -1.8143480000
C 2.4954530000 1.3013120000 0.9353240000
C 2.6216640000 2.3821910000 -1.2264100000
C 2.2957950000 2.3889310000 0.1682130000
H 2.2435830000 1.3156030000 1.9878390000
H 1.8807590000 3.2934150000 0.5940320000
Cl 0.3299460000 -0.9313050000 -1.3995690000
Cl -1.5781000000 -1.3928110000 -1.7973610000
C 2.4040170000 3.5252350000 -2.0156760000
C 3.4657170000 1.2525070000 -3.1870810000
C 3.2456100000 2.3785450000 -3.9396370000
C 2.7091850000 3.5290080000 -3.3512590000
H 1.9872180000 4.4080690000 -1.5478530000
H 2.5364870000 4.4135860000 -3.9485870000
H 3.8790620000 0.3805000000 -3.6715720000
H 3.4875760000 2.3748660000 -4.9936050000

Phenanthrene···Cl_2 (d)
C 3.8185320000 -2.2160290000 0.6988960000
C 4.1733050000 -2.2717270000 -0.6529950000
C 3.9703270000 -1.1855480000 -1.4695040000
H 4.6092420000 -3.1735880000 -1.0602340000
C 3.4012710000 0.0046860000 -0.9777010000
H 4.2605550000 -1.2589560000 -2.5070620000
C 3.2670490000 -1.0682450000 1.2045910000
H 3.9781270000 -3.0736350000 1.3374650000
C 3.0478940000 0.0543420000 0.3866450000
H 2.9871810000 -1.0117860000 2.2488430000
C 3.1574020000 1.1657870000 -1.8152120000
C 2.4648630000 1.2453650000 0.9273540000
C 2.5804850000 2.3166500000 -1.2393400000
C 2.2436950000 2.3234650000 0.1527020000
H 2.2036320000 1.2587090000 1.9776850000
H 1.8018980000 3.2193090000 0.5698510000
Cl 1.0529640000 -2.1711000000 -2.1434000000
Cl -0.7981630000 -2.6434160000 -2.7522560000
C 2.3370170000 3.4477230000 -2.0383340000
C 3.4648990000 1.1954110000 -3.1872720000
C 3.2179420000 2.3091350000 -3.9496940000
C 2.6491840000 3.4496520000 -3.3723370000

H 1.8941630000 4.3225700000 -1.5795030000
H 2.4562780000 4.3249130000 -3.9771790000
H 3.9018550000 0.3306020000 -3.6639450000
H 3.4634940000 2.3033620000 -5.0028120000

Pyrrole···Cl_2
C 0.1275050000 1.6639660000 -0.1616960000
C -1.0185670000 0.8281360000 -0.1280900000
C 1.2246070000 0.8479910000 -0.1932710000
C -0.5763420000 -0.4713660000 -0.1422150000
N 0.7863410000 -0.4454010000 -0.1845900000
H -2.0482520000 1.1409660000 -0.1110760000
H -1.1191500000 -1.3998340000 -0.1385350000
Cl -1.0812810000 0.0252300000 2.8656560000
Cl -1.1384810000 -0.1526100000 4.8725880000
H 0.1424090000 2.7398080000 -0.1576940000
H 2.2745600000 1.0800450000 -0.2157800000
H 1.3771310000 -1.2540700000 -0.1828290000

Imidazole···Cl_2
N 0.1043940000 1.6025830000 -0.1009670000
C -1.0094590000 0.8052850000 -0.1086470000
C 1.1842050000 0.7853000000 -0.1766690000
C -0.5334800000 -0.4718890000 -0.1950060000
N 0.8366170000 -0.4714530000 -0.2373770000
H -2.0057570000 1.2057550000 -0.0670750000
H -1.0993530000 -1.3866630000 -0.2365900000
H 2.1934360000 1.1620780000 -0.1820920000
H 0.1185980000 2.6023470000 -0.0277370000
Cl -1.0804300000 0.0122700000 2.8838900000
Cl -1.1589970000 0.0248960000 4.8939170000

Pyridine···Cl_2
C 1.7788940000 0.7318060000 1.1512030000
N 2.1265750000 1.4061370000 0.0598630000
C 2.3340600000 0.7054570000 -1.0509900000
C 1.6263700000 -0.6472540000 1.1846580000
H 1.6120650000 1.3216850000 2.0448930000
C 1.8465320000 -1.3646370000 0.0195750000
H 1.3444950000 -1.1415130000 2.1035170000
C 2.2076510000 -0.6735260000 -1.1240840000
H 2.6151180000 1.2756960000 -1.9286800000
H 1.7360840000 -2.4403270000 0.0044590000
H 2.3871220000 -1.1876730000 -2.0573770000
Cl -1.4557720000 -0.3193360000 0.1554280000
Cl -3.3843050000 -0.1357850000 -0.3520750000

Indole···Cl_2 (a)
C -0.8982370000 -1.3753230000 0.0863040000
C -2.0796610000 -0.6673160000 0.1007660000
C -2.0875350000 0.7347900000 0.0270020000
C -0.9112080000 1.4501660000 -0.0665870000
C 0.3041420000 0.7577050000 -0.0851180000
C 1.6773630000 1.1539970000 -0.1618280000
C 2.4186920000 0.0153710000 -0.1275240000

N 1.5893650000 -1.0752730000 -0.0345030000
C 0.2865290000 -0.6487690000 -0.0055590000
H -0.8935570000 -2.4552870000 0.1477430000
H -3.0181870000 -1.1987040000 0.1749380000
H -3.0333240000 1.2586060000 0.0403180000
H -0.9280190000 2.5301370000 -0.1266980000
H 1.8903110000 -2.0288600000 0.0127820000
H 2.0619040000 2.1565750000 -0.2309630000
H 3.4870210000 -0.1130720000 -0.1614640000
Cl -1.3150830000 1.3186030000 3.0875550000
Cl -1.1444150000 1.4278120000 5.0856160000

Indole···Cl_2 (b)
C -1.0264440000 -1.3786850000 -0.0651880000
C -2.2010040000 -0.6614600000 -0.1781310000
C -2.1961070000 0.7409770000 -0.2137900000
C -1.0174050000 1.4496480000 -0.1356630000
C 0.1890120000 0.7526440000 -0.0184740000
C 1.5617570000 1.1444400000 0.0944750000
C 2.2918370000 0.0022110000 0.1880800000
N 1.4569660000 -1.0874030000 0.1368410000
C 0.1622200000 -0.6557040000 0.0122840000
H -1.0320100000 -2.4602160000 -0.0441410000
H -3.1416160000 -1.1910210000 -0.2403060000
H -3.1354760000 1.2689150000 -0.3006850000
H -1.0239530000 2.5311070000 -0.1605230000
H 1.7474820000 -2.0431230000 0.2028420000
H 1.9528550000 2.1468240000 0.1061170000
H 3.3555120000 -0.1301670000 0.2881560000
Cl -1.4978810000 -1.1745670000 3.0162560000
Cl -1.4919810000 -1.2197200000 5.0238620000

Indole···Cl_2 (c)
C -0.9230290000 -1.4215580000 -0.0493160000
C -2.1113360000 -0.7249900000 -0.0213930000
C -2.1336780000 0.6783980000 -0.0015180000
C -0.9663720000 1.4086930000 -0.0086100000
C 0.2582230000 0.7304480000 -0.0348950000
C 1.6303290000 1.1439400000 -0.0488630000
C 2.3829090000 0.0129800000 -0.0730960000
N 1.5639930000 -1.0895630000 -0.0799530000
C 0.2557490000 -0.6798950000 -0.0555510000
H -0.9086500000 -2.5030150000 -0.0617150000
H -3.0455510000 -1.2692960000 -0.0122690000
H -3.0858360000 1.1899730000 0.0223710000
H -0.9925000000 2.4899160000 0.0089870000
H 1.8748650000 -2.0411270000 -0.0781570000
H 2.0051390000 2.1524560000 -0.0375450000
H 3.4531200000 -0.1025420000 -0.0841920000
Cl 0.1585680000 0.3743390000 3.1533540000
Cl 0.2310940000 0.0902520000 5.1365670000

Indole···Cl_2 (d)
C -0.9540640000 -1.4033850000 0.0094660000
C -2.1521470000 -0.7256800000 -0.0595890000

C -2.1941920000 0.6755730000 -0.1185380000
C -1.0374920000 1.4233350000 -0.1079940000
C 0.1927260000 0.7636270000 -0.0386070000
C 1.5578880000 1.1993080000 0.0019900000
C 2.3287740000 0.0768020000 0.0728010000
N 1.5273420000 -1.0337180000 0.0785380000
C 0.2115610000 -0.6427980000 0.0176260000
H -0.9238020000 -2.4835960000 0.0563930000
H -3.0781280000 -1.2839830000 -0.0675750000
H -3.1532070000 1.1721110000 -0.1710660000
H -1.0786130000 2.5033780000 -0.1499740000
H 1.8499510000 -1.9778260000 0.1620980000
H 1.9205460000 2.2115810000 -0.0423390000
H 3.4000740000 -0.0201110000 0.1151750000
Cl 1.9432010000 1.1236400000 3.0101170000
Cl 1.9625580000 1.2178170000 5.0239610000

Indole···Cl_2 (e)

C	-0.95230	-1.35639	0.11176
C	-2.15546	-0.69816	-0.02586
C	-2.20743	0.69171	-0.20998
C	-1.05624	1.44668	-0.26199
C	0.17956	0.80662	-0.12998
C	1.54185	1.25331	-0.13771
C	2.32082	0.15607	0.04068
N	1.52579	-0.95959	0.17949
C	0.20671	-0.58810	0.05796
H	-0.91323	-2.42705	0.26068
H	-3.07696	-1.26266	0.01128
H	-3.16987	1.17395	-0.31157
H	-1.10609	2.51798	-0.40349
H	1.85987	-1.90286	0.22537
H	1.89302	2.26379	-0.25451
H	3.39252	0.07060	0.09482
Cl	1.40220	-1.05094	3.24098
Cl	1.37551	-1.26936	5.23207

Quinoline···Cl_2 (a)

C -2.3587610000 1.7763710000 -0.1962150000
C -3.4863610000 1.0056580000 -0.2221290000
C -1.0823740000 1.1743540000 -0.0984000000
C -3.3888880000 -0.4009670000 -0.1537430000
C -2.1709110000 -1.0076130000 -0.0596420000
C -0.9860950000 -0.2356560000 -0.0284660000
H -2.4269790000 2.8554540000 -0.2518030000
H -4.4595130000 1.4709890000 -0.2967780000
H -4.2907140000 -0.9971430000 -0.1734500000
H -2.0732770000 -2.0825910000 -0.0035520000
C 0.1173800000 1.9156360000 -0.0581500000
C 1.3037920000 1.2543630000 0.0432630000
C 1.2909020000 -0.1556910000 0.1040480000
N 0.2059390000 -0.8811840000 0.0708170000
H 2.2289770000 -0.6947000000 0.1843360000
H 0.0792540000 2.9966350000 -0.1056220000
H 2.2447200000 1.7844730000 0.0784960000

Cl -2.8958150000 1.6818500000 2.9529790000
Cl -2.8484020000 1.7947210000 4.9544310000

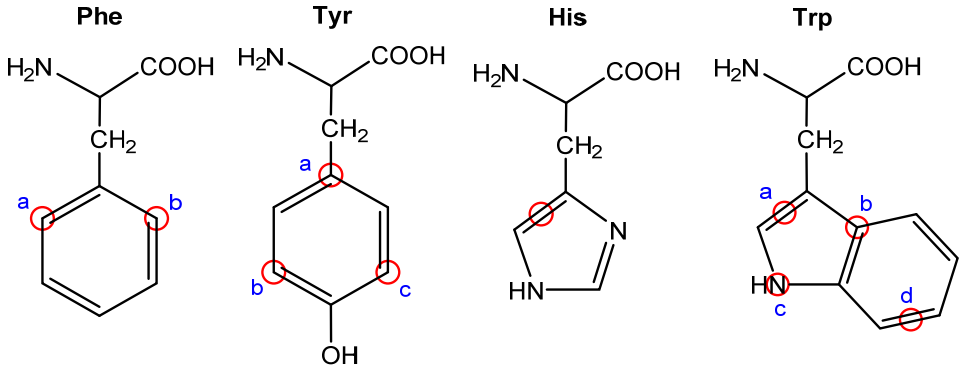
Quinoline···Cl_2 (b)
C -2.3777784724 1.7654643761 -0.1878263324
C -3.5031215535 0.9974648687 -0.2503224565
C -1.1029082694 1.1628975758 -0.0821168476
C -3.4058241533 -0.4099683796 -0.2092141072
C -2.1876520178 -1.0205401859 -0.1099846688
C -1.0038795865 -0.2482692156 -0.0451728739
H -2.4454640104 2.8456030234 -0.2147251396
H -4.4757514267 1.4630090045 -0.3274592836
H -4.3063284165 -1.0068658076 -0.2572024159
H -2.0906460937 -2.0967707113 -0.0805298859
C 0.0957022146 1.9038782686 -0.0059494637
C 1.2814223800 1.2418018134 0.0982190878
C 1.2700364126 -0.1693357944 0.1249106898
N 0.1868600675 -0.8950224689 0.0569113963
H 2.2075451967 -0.7090220461 0.2069448361
H 0.0571282209 2.9856821572 -0.0295666115
H 2.2208763824 1.7720421070 0.1605661474
Cl -2.6777273856 -0.5858009582 3.0508430330
Cl -2.6424527027 -0.3340824237 5.0391161180

Quinoline···Cl_2 (c)
C -2.3318320000 1.7717410000 -0.0520650000
C -3.4624370000 1.0085780000 -0.0667750000
C -1.0562060000 1.1610950000 -0.0779340000
C -3.3707140000 -0.3988290000 -0.1093880000
C -2.1541270000 -1.0160220000 -0.1365860000
C -0.9647760000 -0.2521350000 -0.1209270000
H -2.3947660000 2.8518720000 -0.0165240000
H -4.4353180000 1.4796570000 -0.0435390000
H -4.2763260000 -0.9897760000 -0.1183700000
H -2.0616910000 -2.0924360000 -0.1667000000
C 0.1509890000 1.8941890000 -0.0575880000
C 1.3362010000 1.2243560000 -0.0771320000
C 1.3171520000 -0.1868630000 -0.1202720000
N 0.2277380000 -0.9052620000 -0.1428490000
H 2.2547320000 -0.7324090000 -0.1362660000
H 0.1177060000 2.9758110000 -0.0224940000
H 2.2811990000 1.7479390000 -0.0590540000
Cl -1.0732040000 0.7506770000 3.1811450000
Cl -0.9810060000 0.5554020000 5.1709920000

Quinoline···Cl_2 (d)
C -2.3414250000 1.7874540000 -0.1024500000
C -3.4697610000 1.0236410000 -0.0343510000
C -1.0662580000 1.1784340000 -0.1082800000
C -3.3743320000 -0.3825820000 0.0308840000
C -2.1563060000 -0.9977780000 0.0273300000
C -0.9702610000 -0.2323450000 -0.0414970000
H -2.4070930000 2.8669610000 -0.1505850000

H -4.4436570000 1.4933250000 -0.0289050000
H -4.2780600000 -0.9741130000 0.0849110000
H -2.0608220000 -2.0732030000 0.0780700000
C 0.1378180000 1.9128170000 -0.1715610000
C 1.3268990000 1.2453100000 -0.1632570000
C 1.3118930000 -0.1657650000 -0.0965320000
N 0.2239650000 -0.8836410000 -0.0388810000
H 2.2507360000 -0.7091170000 -0.0901120000
H 0.1023170000 2.9937940000 -0.2234960000
H 2.2698530000 1.7710560000 -0.2095270000
Cl 0.7053340000 1.6977490000 3.0523550000
Cl 0.5820700000 1.7763110000 5.0501630000

Optimized Coordinates of amino acid···Cl_2 complexes (ωB97X-D/aug-cc-pVTZ)



Phenylalanine···Cl_2 (a)

N 3.1238940000 0.9941230000 -0.8579400000
C 2.5971360000 0.0906920000 0.1429950000
C 3.3743490000 -1.2040620000 0.3424720000
O 3.5214470000 -1.7603440000 1.3961190000
H 4.0213350000 1.3673490000 -0.5849590000
H 3.2434240000 0.5223160000 -1.7440100000
H 2.6151410000 0.5925030000 1.1101480000
C 1.1353050000 -0.2812020000 -0.1767370000
C 0.2007170000 0.8868520000 -0.0254650000
H 0.8261860000 -1.0857400000 0.4920460000
H 1.0929070000 -0.6733200000 -1.1951230000
C -1.5049600000 3.0753950000 0.3006290000
C -0.3627490000 1.1718170000 1.2156460000
C -0.1020380000 1.7158640000 -1.0997360000
C -0.9485040000 2.8005670000 -0.9398310000
C -1.2095230000 2.2583030000 1.3799080000
H -0.1358770000 0.5344400000 2.0619100000
H 0.3338290000 1.5099860000 -2.0679900000
H -1.1756800000 3.4336320000 -1.7867750000
H -1.6427360000 2.4605070000 2.3499130000
H -2.1688670000 3.9199440000 0.4237460000

O 3.8585810000 -1.7015300000 -0.8111800000
H 4.2947450000 -2.5343090000 -0.5985460000
Cl -2.5729480000 -0.8563150000 0.0979060000
Cl -3.9735400000 -2.2258340000 -0.3316470000

Phenylalanine···Cl_2 (b)
N 2.8280150000 0.6694530000 -1.3748830000
C 2.6001500000 0.1368410000 -0.0483900000
C 3.4766400000 -1.0423800000 0.3536250000
O 3.8882460000 -1.2435700000 1.4633450000
H 3.7414860000 1.0921180000 -1.4530190000
H 2.7651500000 -0.0588740000 -2.0731470000
H 2.8105080000 0.9176310000 0.6821420000
C 1.1283750000 -0.2912820000 0.1184850000
C 0.1872120000 0.8811680000 0.1112720000
H 1.0275280000 -0.8349150000 1.0587210000
H 0.8770020000 -0.9865130000 -0.6855380000
C -1.5239560000 3.0896150000 0.1209040000
C -0.0803000000 1.5682080000 1.2915660000
C -0.4136640000 1.3186550000 -1.0645640000
C -1.2649150000 2.4143800000 -1.0606440000
C -0.9276280000 2.6636240000 1.2988510000
H 0.3765040000 1.2353590000 2.2157090000
H -0.2046380000 0.8017770000 -1.9916850000
H -1.7258990000 2.7388800000 -1.9835170000
H -1.1288090000 3.1820310000 2.2264810000
H -2.1899720000 3.9414020000 0.1258990000
O 3.7182830000 -1.8825490000 -0.6701980000
H 4.2387990000 -2.6136960000 -0.3188260000
Cl -2.5597920000 -0.8568890000 -0.1856590000
Cl -3.9300600000 -2.2916630000 0.1120800000

Tyrosine···Cl_2 (a)
N -2.8741250000 -1.0337390000 -1.3035510000
C -2.6946480000 -0.3977290000 -0.0149480000
C -3.7617050000 0.6153920000 0.3772080000
O -4.1612220000 0.7935200000 1.4952740000
H -3.6878040000 -1.6313720000 -1.3113200000
H -2.9934510000 -0.3433790000 -2.0324940000
H -2.7212140000 -1.1638790000 0.7594120000
C -1.3245830000 0.3072550000 0.0553890000
C -0.1768020000 -0.6635940000 0.0665410000
H -1.2937150000 0.9206440000 0.9569810000
H -1.2435610000 0.9861050000 -0.7966830000
C 1.9021460000 -2.5355900000 0.1191390000
C 0.3009910000 -1.1772000000 1.2706830000
C 0.4105630000 -1.1121490000 -1.1103390000
C 1.4416290000 -2.0375020000 -1.0914830000
C 1.3271610000 -2.1015790000 1.3068210000
H -0.1377980000 -0.8411150000 2.2022680000
H 0.0525930000 -0.7382260000 -2.0598550000
H 1.8875650000 -2.3704810000 -2.0210660000
H 1.6977810000 -2.4900710000 2.2446090000
O 2.9110620000 -3.4416370000 0.2030570000
H 3.2273690000 -3.6558570000 -0.6752240000

O -4.1961640000 1.3431120000 -0.6693330000
H -4.8303000000 1.9820250000 -0.3249360000
Cl 2.0318630000 1.5911920000 -0.0921220000
Cl 3.2142250000 3.2110440000 -0.0209890000

Tyrosine···Cl_2 (b)
N 3.3770860000 1.1541770000 -0.8650560000
C 3.0241790000 0.1641790000 0.1311450000
C 4.0441100000 -0.9446990000 0.3523070000
O 4.2772030000 -1.4618620000 1.4104710000
H 4.1702110000 1.7065720000 -0.5733640000
H 3.6164480000 0.7131420000 -1.7427140000
H 2.9200160000 0.6609490000 1.0953650000
C 1.6736540000 -0.4963500000 -0.2146780000
C 0.5152000000 0.4514140000 -0.0797610000
H 1.5255030000 -1.3513550000 0.4463890000
H 1.7332640000 -0.8847720000 -1.2339100000
C -1.6168340000 2.2411300000 0.2180740000
C -0.1505300000 0.5804190000 1.1349050000
C 0.0912260000 1.2401820000 -1.1402360000
C -0.9636120000 2.1272150000 -1.0011150000
C -1.2080590000 1.4607980000 1.2925610000
H 0.1576340000 -0.0253020000 1.9784920000
H 0.5958760000 1.1660780000 -2.0938980000
H -1.2790720000 2.7305830000 -1.8439580000
H -1.7224420000 1.5542960000 2.2384710000
O -2.6589020000 3.0894420000 0.4172170000
H -2.8582870000 3.5536000000 -0.3964700000
O 4.6460190000 -1.3322870000 -0.7884880000
H 5.2369500000 -2.0593880000 -0.5625040000
Cl -2.9105090000 -1.0340920000 0.2270930000
Cl -4.1663310000 -2.4454200000 -0.4464640000

Tyrosine···Cl_2 (c)
N -3.0830900000 0.5134220000 1.5396380000
C -3.0551280000 0.1699710000 0.1330480000
C -4.1855440000 -0.7276010000 -0.3520220000
O -4.6945930000 -0.6639780000 -1.4375440000
H -3.8727800000 1.1021490000 1.7612070000
H -3.1499130000 -0.3173180000 2.1119960000
H -3.1382830000 1.0856290000 -0.4517780000
C -1.7199130000 -0.5108000000 -0.2329330000
C -0.5517670000 0.4320440000 -0.1617800000
H -1.8019250000 -0.9160910000 -1.2423090000
H -1.5703250000 -1.3566510000 0.4420040000
C 1.5891610000 2.2330450000 -0.0521820000
C -0.1679230000 1.1656210000 -1.2801910000
C 0.1577640000 0.6228750000 1.0153960000
C 1.2224950000 1.5104610000 1.0770390000
C 0.8877910000 2.0579770000 -1.2366980000
H -0.7041110000 1.0327490000 -2.2120640000
H -0.1237890000 0.0745300000 1.9039040000
H 1.7609360000 1.6468470000 2.0074600000
H 1.1837620000 2.6178810000 -2.1122770000

O 2.6231680000 3.1136260000 -0.0538920000
H 3.0377100000 3.1286390000 0.8094170000
O -4.5407960000 -1.6542360000 0.5584250000
H -5.2245000000 -2.1997400000 0.1535380000
Cl 2.9591690000 -0.9763670000 0.2425380000
Cl 4.2773600000 -2.4105410000 -0.2391580000

Histidine···Cl_2
N -1.4303340000 -0.7632110000 1.3491550000
C -2.1082380000 0.0408000000 0.3329160000
C -3.2708740000 -0.7398890000 -0.2667910000
O -3.2749830000 -1.3114410000 -1.3217970000
H -2.0775130000 -1.0742940000 2.0602240000
H -1.0053900000 -1.5806090000 0.9295690000
H -2.5214270000 0.9181260000 0.8334790000
C -1.1440020000 0.4828520000 -0.7571130000
C -0.0783230000 1.4240280000 -0.2973380000
H -1.7014230000 0.9740410000 -1.5536980000
H -0.6950300000 -0.4022450000 -1.2160900000
C 0.4867500000 1.5847730000 0.9402500000
N 0.4872700000 2.3077830000 -1.1844680000
H 0.3008720000 1.0883130000 1.8740930000
H 2.0088190000 2.9535170000 1.5086780000
C 1.3691520000 2.9853660000 -0.5006180000
N 1.4058380000 2.5934880000 0.7934440000
H 2.0021880000 3.7663270000 -0.8880580000
O -4.3202250000 -0.7770430000 0.5787780000
H -4.9936520000 -1.3337280000 0.1713600000
Cl 2.1412480000 -0.7794760000 0.1341740000
Cl 3.4280460000 -2.2932060000 -0.2041830000

Tryptophan···Cl_2 (a)
N 2.5960630000 0.5413580000 1.1059030000
C 2.4714410000 -0.7515590000 0.4388100000
C 3.7012800000 -1.0605220000 -0.4092650000
O 3.7401580000 -1.1666680000 -1.6037680000
H 3.4705380000 0.6109630000 1.6069000000
H 2.5553610000 1.2961920000 0.4330680000
H 2.4239840000 -1.5171460000 1.2174960000
C 1.2114750000 -0.8236180000 -0.4104070000
C -0.0730170000 -0.7599870000 0.3535320000
H 1.2376830000 -1.7560300000 -0.9761020000
H 1.2484270000 -0.0313990000 -1.1647540000
C -0.3073530000 -0.3093630000 1.6226680000
C -1.3381640000 -1.2273660000 -0.1440850000
H 0.3857070000 0.1244720000 2.3219850000
N -1.6311090000 -0.4826690000 1.9443330000
C -2.2888550000 -1.0329150000 0.8743710000
H -2.0571660000 -0.1832770000 2.7991360000
C -1.7445620000 -1.7873390000 -1.3578030000
C -3.6279160000 -1.3755620000 0.7134650000
H -4.3498560000 -1.2178590000 1.5034120000
C -4.0017020000 -1.9249510000 -0.4947880000
H -5.0346730000 -2.2022610000 -0.6543740000
C -3.0691160000 -2.1308620000 -1.5220160000

H -1.0325200000 -1.9441610000 -2.1574570000
H -3.3999410000 -2.5634130000 -2.4560620000
O 4.8023160000 -1.1759380000 0.3601160000
H 5.5476780000 -1.3309570000 -0.2308720000
Cl -0.5016950000 2.2466290000 0.0140740000
Cl -0.7742320000 4.1150860000 -0.6982920000

Tryptophan···Cl_2 (b)
N -2.8740980000 -0.8576130000 1.3887290000
C -2.9373830000 0.1589550000 0.3404900000
C -4.0972150000 -0.1150940000 -0.6104910000
O -4.0170330000 -0.4818140000 -1.7503310000
H -3.7634030000 -0.9510080000 1.8593580000
H -2.6305090000 -1.7574820000 0.9950790000
H -3.1381970000 1.1164400000 0.8264860000
C -1.6280950000 0.2503090000 -0.4280590000
C -0.4643710000 0.7543690000 0.3633880000
H -1.7848650000 0.9058240000 -1.2864080000
H -1.4010630000 -0.7313210000 -0.8565360000
C -0.2930410000 0.8032790000 1.7126160000
C 0.7434640000 1.2790300000 -0.2137250000
H -0.9574310000 0.4698220000 2.4902170000
N 0.9394330000 1.3366100000 2.0118880000
C 1.5988040000 1.6319340000 0.8495720000
H 1.3081540000 1.4495370000 2.9354350000
C 1.1738150000 1.4846620000 -1.5295170000
C 2.8623910000 2.1752770000 0.6344780000
H 3.5105950000 2.4385070000 1.4594760000
C 3.2604280000 2.3623440000 -0.6720120000
H 4.2376900000 2.7787320000 -0.8741350000
C 2.4240000000 2.0215960000 -1.7458620000
H 0.5373600000 1.2192150000 -2.3635000000
H 2.7718850000 2.1813400000 -2.7569590000
O -5.2825880000 0.0625820000 0.0069930000
H -5.9708120000 -0.1718860000 -0.6257630000
Cl 1.9857910000 -1.5849960000 -0.1842970000
Cl 2.6826470000 -3.4612870000 -0.0430930000

Tryptophan···Cl_2 (c)
N -2.9341470000 -0.8341030000 1.3851770000
C -2.9497880000 0.1746160000 0.3270810000
C -4.1170590000 -0.0650720000 -0.6234850000
O -4.0503560000 -0.4905910000 -1.7437790000
H -3.8215430000 -0.8694590000 1.8673860000
H -2.7507190000 -1.7508840000 0.9977620000
H -3.1105090000 1.1439260000 0.8033780000
C -1.6346340000 0.2017960000 -0.4376130000
C -0.4567620000 0.6801670000 0.3501050000
H -1.7633560000 0.8482020000 -1.3072320000
H -1.4449910000 -0.7947380000 -0.8482830000
C -0.2625180000 0.6711920000 1.6959370000
C 0.7351750000 1.2419090000 -0.2271740000
H -0.9136930000 0.3068660000 2.4708570000
N 0.9857380000 1.1774330000 1.9950380000
C 1.6076670000 1.5563010000 0.8300370000

H 1.3146210000 1.3793320000 2.9193000000
C 1.1373380000 1.5051090000 -1.5390890000
C 2.8568020000 2.1302060000 0.6181920000
H 3.5174410000 2.3636970000 1.4423200000
C 3.2253970000 2.3847730000 -0.6862790000
H 4.1901330000 2.8295420000 -0.8881850000
C 2.3743820000 2.0737510000 -1.7563640000
H 0.4899780000 1.2651660000 -2.3724800000
H 2.6985140000 2.2834040000 -2.7663920000
O -5.2936540000 0.2153470000 -0.0282780000
H -5.9902910000 -0.0062450000 -0.6565610000
Cl 2.3603920000 -1.5192620000 2.1445530000
Cl 3.3164970000 -3.2733130000 2.3071660000

Tryptophan···Cl_2 (d)
N -3.3047180000 -1.5338600000 1.1021890000
C -3.4189870000 -0.3135840000 0.3048060000
C -4.6054280000 -0.4071700000 -0.6474260000
O -4.5565420000 -0.5698500000 -1.8356150000
H -4.1680780000 -1.7324060000 1.5885510000
H -3.0905070000 -2.3250520000 0.5085360000
H -3.6176700000 0.5089530000 0.9947640000
C -2.1370000000 -0.0276380000 -0.4632720000
C -0.9631900000 0.3425000000 0.3868980000
H -2.3372280000 0.7858980000 -1.1624370000
H -1.9027990000 -0.8926440000 -1.0914850000
C -0.7212410000 0.0503470000 1.6944440000
C 0.1664200000 1.1036830000 -0.0696080000
H -1.3200170000 -0.5236660000 2.3796450000
N 0.4824100000 0.5920790000 2.0828760000
C 1.0495680000 1.2385630000 1.0189160000
H 0.8918120000 0.4936660000 2.9908120000
C 0.5103830000 1.6757560000 -1.2971740000
C 2.2602230000 1.9191730000 0.9114800000
H 2.9291300000 2.0179970000 1.7559610000
C 2.5741840000 2.4715890000 -0.3154400000
H 3.5073690000 3.0049180000 -0.4331810000
C 1.7063060000 2.3524030000 -1.4100410000
H -0.1485650000 1.5832200000 -2.1507080000
H 1.9862210000 2.7949560000 -2.3558320000
O -5.7731540000 -0.3376830000 0.0226160000
H -6.4790570000 -0.4568880000 -0.6228700000
Cl 3.6420780000 -0.6857480000 -0.1258320000
Cl 4.4529620000 -2.4813080000 -0.5138570000

Exchange-Scaled sSAPT0 energy partitioning scheme in Psi4

- Note that the numbers in the parenthesis (nm) correspond to:
  1. n = Order of intermolecular perturbation
  2. m = Order of intramolecular perturbation
- As m is 0 for sSAPT0, the intermolecular perturbations are built upon HF monomeric wavefunctions.
- $E^{(20)}_{exch-ind,r}$ and $E^{(20)}_{exch-disp}$ are calculated based on an approximation which utilises the square of orbital overlap (S^2), and hence a scaling factor of $p_{EX}(3.0)$ is multiplied to both terms to correct the error as a result of the approximation.

$$E_{elec} = E^{(10)}_{elec}$$

$$E_{exch} = E^{(10)}_{exch}$$

$$E_{ind} = E^{(20)}_{ind,r} + p_{EX}(3.0)E^{(20)}_{exch-ind,r} + \delta E^{(2)}_{HF}$$

$$E_{disp} = E^{(20)}_{disp} + p_{EX}(3.0)E^{(20)}_{exch-disp}$$

$$p_{EX}(\alpha) = \left(\frac{E^{(10)}_{exch}}{E^{(10)}_{exch}(S^2)}\right)^{\alpha}$$

Reference:

T. M. Parker, L. a Burns, R. M. Parrish, A. G. Ryno and C. D. Sherrill, Levels of symmetry adapted perturbation theory (SAPT). I. Efficiency and performance for interaction energies, *J. Chem. Phys.*, 2014, **140**, 94106.