

Supplementary Information

Table S1. Molecular descriptors of brominated diphenyl ethers (BDEs) used in the quantitative structure-property relationship (QSPR) study calculated at the PCM/B3LYP/6-311++G(d,p) level (units: hartree for total energy, eV for the others).

Congener	E _{S1}	E _{T1}	E _{LUMO}	E _{HOMO}	HOMO–LUMO Gap	Br Number
BDE-209	3.7996	3.2118	−0.08718	−0.25705	0.16987	10
BDE-208	3.8262	3.22	−0.08502	−0.2568	0.17178	9
BDE-207	3.8218	3.221	−0.08495	−0.25492	0.16997	9
BDE-206	3.8336	3.221	−0.08461	−0.25549	0.17088	9
BDE-203	3.846	3.2274	−0.08398	−0.25254	0.16856	8
BDE-196	3.8309	3.2229	−0.08489	−0.25602	0.17113	8
BDE-190	3.9397	3.2642	−0.08324	−0.24852	0.16528	7
BDE-183	4.1444	3.3164	−0.07061	−0.25178	0.18117	7
BDE-181	3.9175	3.2591	−0.0835	−0.24954	0.16604	7
BDE-155	4.3949	3.3942	−0.06106	−0.25234	0.19128	6
BDE-154	4.3799	3.4327	−0.05758	−0.24875	0.19117	6
BDE-153	4.4181	3.418	−0.05861	−0.24967	0.19106	6
BDE-139	4.1221	3.3175	−0.06979	−0.24926	0.17947	6
BDE-138	4.1844	3.3693	−0.06256	−0.24548	0.18292	6
BDE-100	4.4286	3.4028	−0.05682	−0.24819	0.19137	5
BDE-99	4.4037	3.4209	−0.05466	−0.24791	0.19325	5
BDE-85	4.1269	3.4145	−0.06185	−0.24277	0.18092	5
BDE-77	4.459	3.4481	−0.05036	−0.24066	0.1903	4
BDE-47	4.4543	3.4479	−0.05043	−0.24065	0.19022	4
BDE-28	4.4539	3.4594	−0.04691	−0.23678	0.18987	3

Table S2. Pearson correlation analysis for the descriptor variables calculated at the PCM/B3LYP/6-311++G(d,p) level.

Descriptor	E _{T1}	E _{S1}	E _{LUMO}	E _{HOMO}	HOMO–LUMO Gap	Br Number
E _{T1}	1	-	-	-	-	-
E _{S1}	0.992 **	1	-	-	-	-
E _{LUMO}	0.985 **	0.990 **	1	-	-	-
E _{HOMO}	0.766 **	0.809 **	0.802 **	1	-	-
HOMO–LUMO gap	0.954 **	0.939 **	0.956 **	0.591 *	1	-
Br number	−0.919 **	−0.927 **	−0.919 **	−0.925 **	−0.786 **	1

** Significant at 0.01 level ($n = 20$), * Significant at 0.05 level ($n = 20$)

Table S3. Principal component 1 extracted from the 6 descriptor variables of the BDE congeners calculated at PCM/B3LYP/6-311++G(d,p) level.

Congener	Value in PC1	Congener	Value in PC1
BDE-209	−1.41609	BDE-154	0.74014
BDE-208	−1.22278	BDE-153	0.69722
BDE-207	−1.20136	BDE-139	−0.02337
BDE-206	−1.18951	BDE-138	0.37348
BDE-203	−1.02516	BDE-100	0.8368

Table S3. *Cont.*

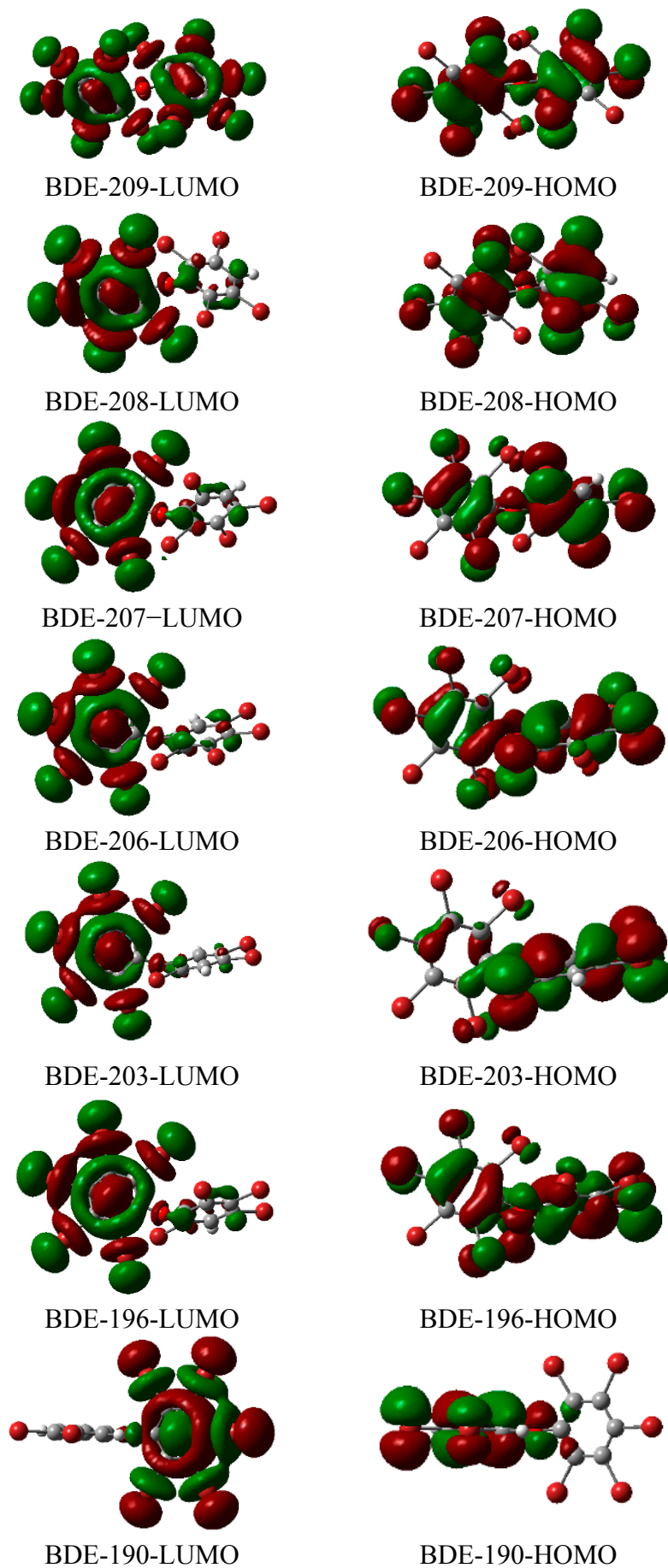
Congener	Value in PC1	Congener	Value in PC1
BDE-196	-1.10873	BDE-99	0.92171
BDE-190	-0.73204	BDE-85	0.56522
BDE-183	-0.15488	BDE-77	1.31037
BDE-181	-0.7757	BDE-47	1.30484
BDE-155	0.53417	BDE-28	1.56566

Table S4. Predicted $\log k_{UV}$ of the QSPR models by artificial neural network (ANN) using different number of neurons in hidden layer.

Neuron	1	2	3	4
<i>training set</i>				
BDE-209	-3.62	-3.58	-3.43	-3.44
BDE-208	-3.97	-3.99	-3.90	-3.91
BDE-206	-4.02	-4.05	-3.97	-3.95
BDE-203	-4.36	-4.35	-4.30	-4.33
BDE-190	-4.64	-4.63	-4.62	-4.59
BDE-155	-5.36	-5.36	-5.42	-5.31
BDE-154	-5.35	-5.35	-5.48	-5.50
BDE-139	-5.26	-5.32	-5.34	-5.31
BDE-138	-5.35	-5.33	-5.38	-5.40
BDE-99	-5.63	-5.60	-5.66	-5.67
BDE-47	-5.81	-5.79	-5.86	-5.96
<i>test set</i>				
BDE-207	-4.00	-4.02	-3.94	-3.92
BDE-183	-5.00	-5.12	-5.18	-5.06
BDE-181	-4.62	-4.61	-4.60	-4.61
BDE-77	-5.81	-5.79	-5.86	-5.96

Table S5. Predicted $\log k_{sun}$ of the QSPR models by ANN using different number of neurons in hidden layer.

Neuron	1	2	3	4
BDE-209	-3.17	-3.22	-3.27	-3.27
BDE-206	-3.44	-3.41	-3.43	-3.43
BDE-196	-3.58	-3.58	-3.49	-3.46
BDE-183	-4.12	-4.03	-4.04	-4.08
BDE-153	-4.36	-4.33	-4.38	-4.33
BDE-100	-4.79	-4.86	-4.83	-4.81
BDE-99	-4.53	-4.59	-4.57	-4.63
BDE-85	-4.20	-4.21	-4.26	-4.26
BDE-28	-5.34	-5.28	-5.24	-5.25
BDE-208	-3.33	-3.37	-3.41	-3.39
BDE-207	-3.45	-3.41	-3.41	-3.41
BDE-154	-4.14	-4.11	-4.21	-4.21
BDE-47	-5.10	-5.05	-5.14	-5.10

Figure S1. *Cont.*

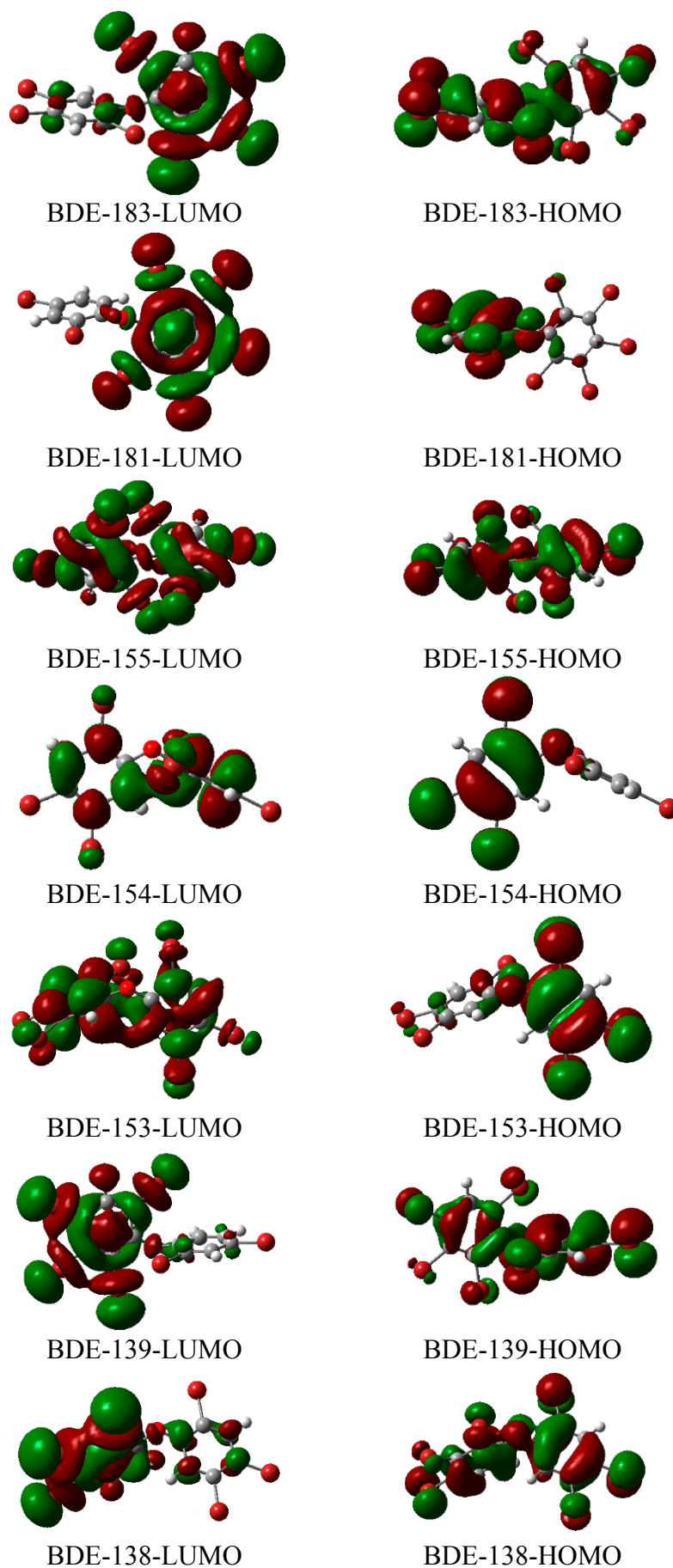


Figure S1. *Cont.*

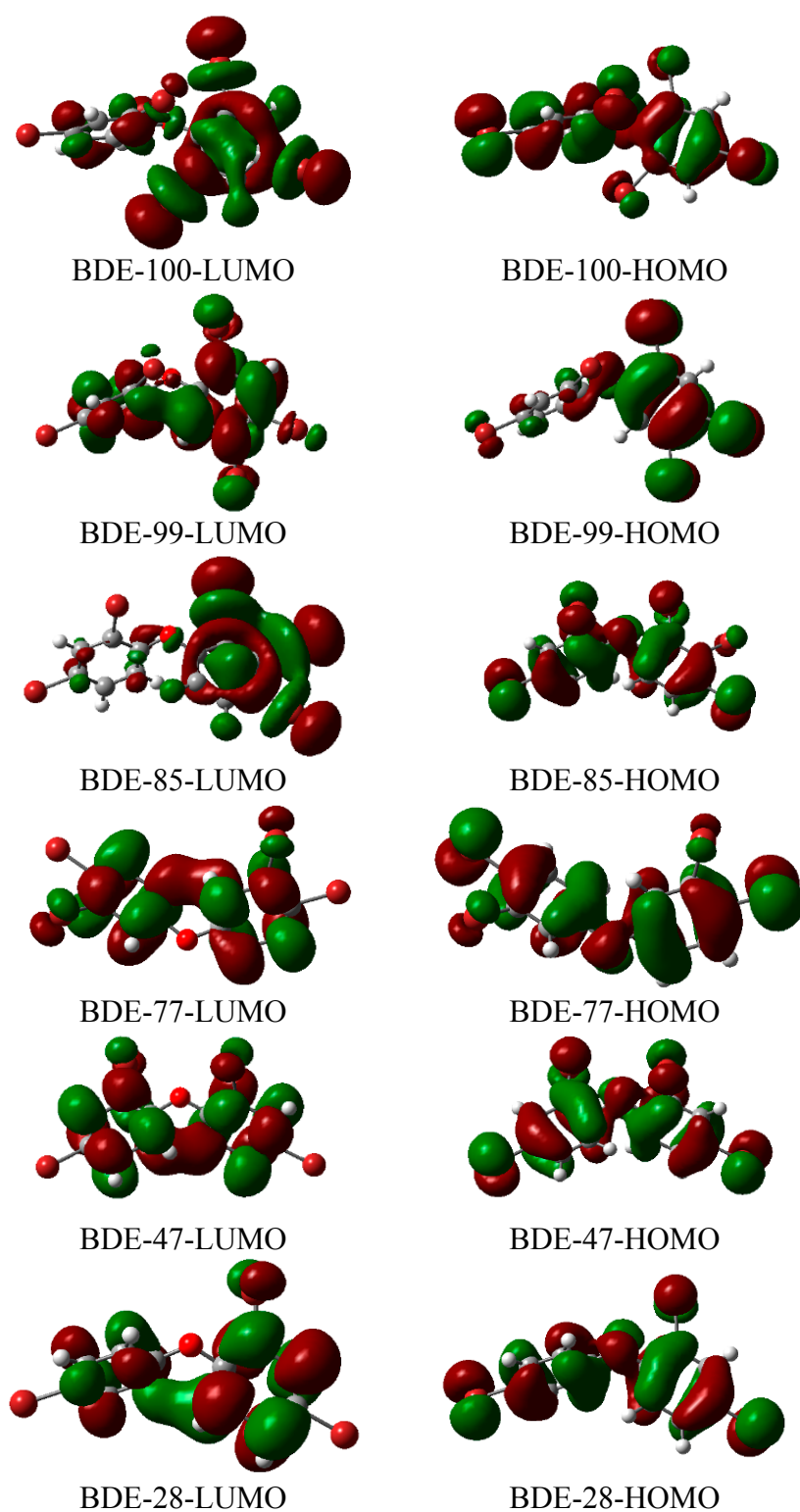
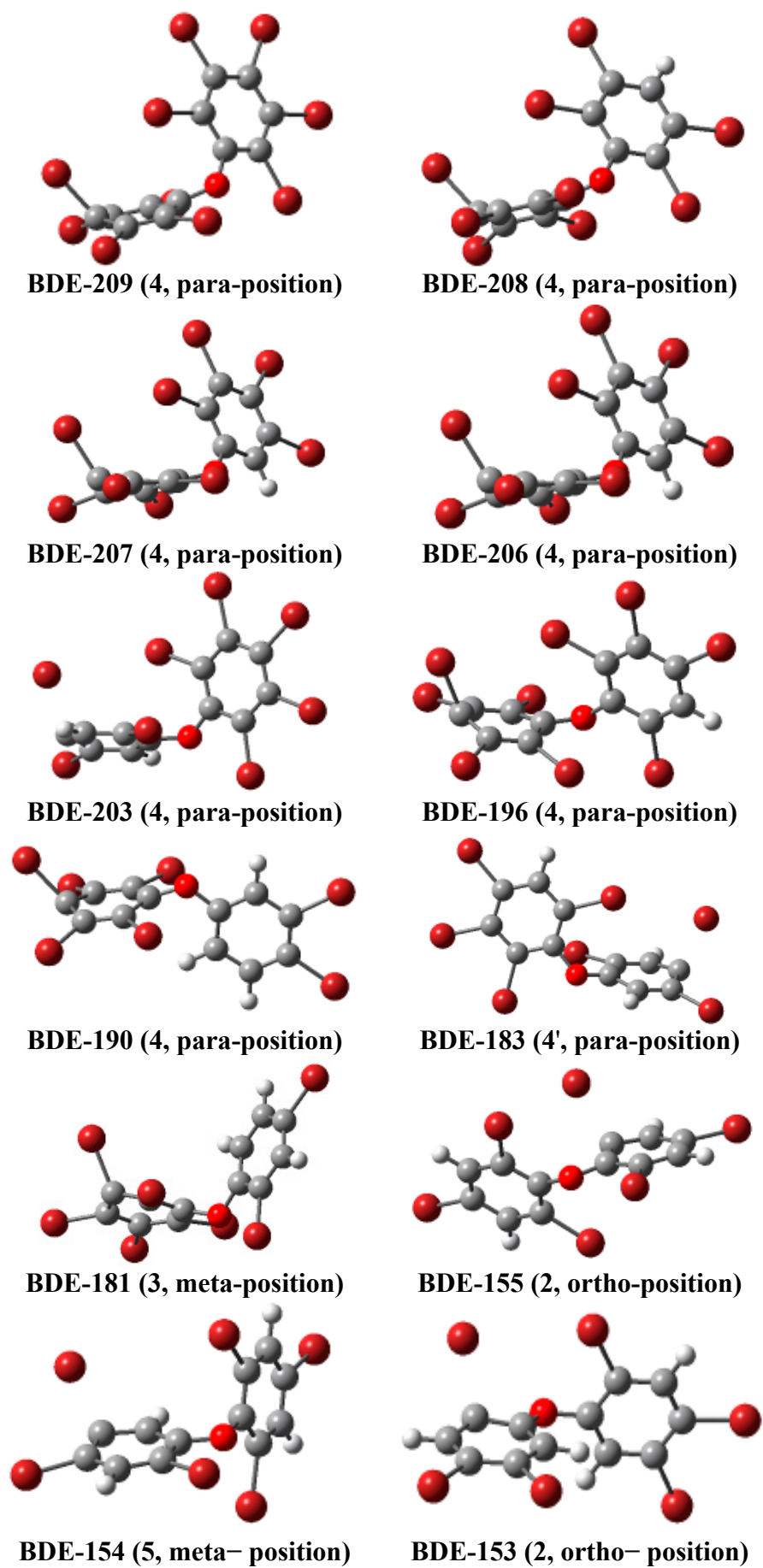


Figure S1. Surface images of HOMO and LUMO from PCM/B3LYP/6-311++G(d,p) calculation(iso-surface value = 0.02 au).

Figure S2. *Cont.*

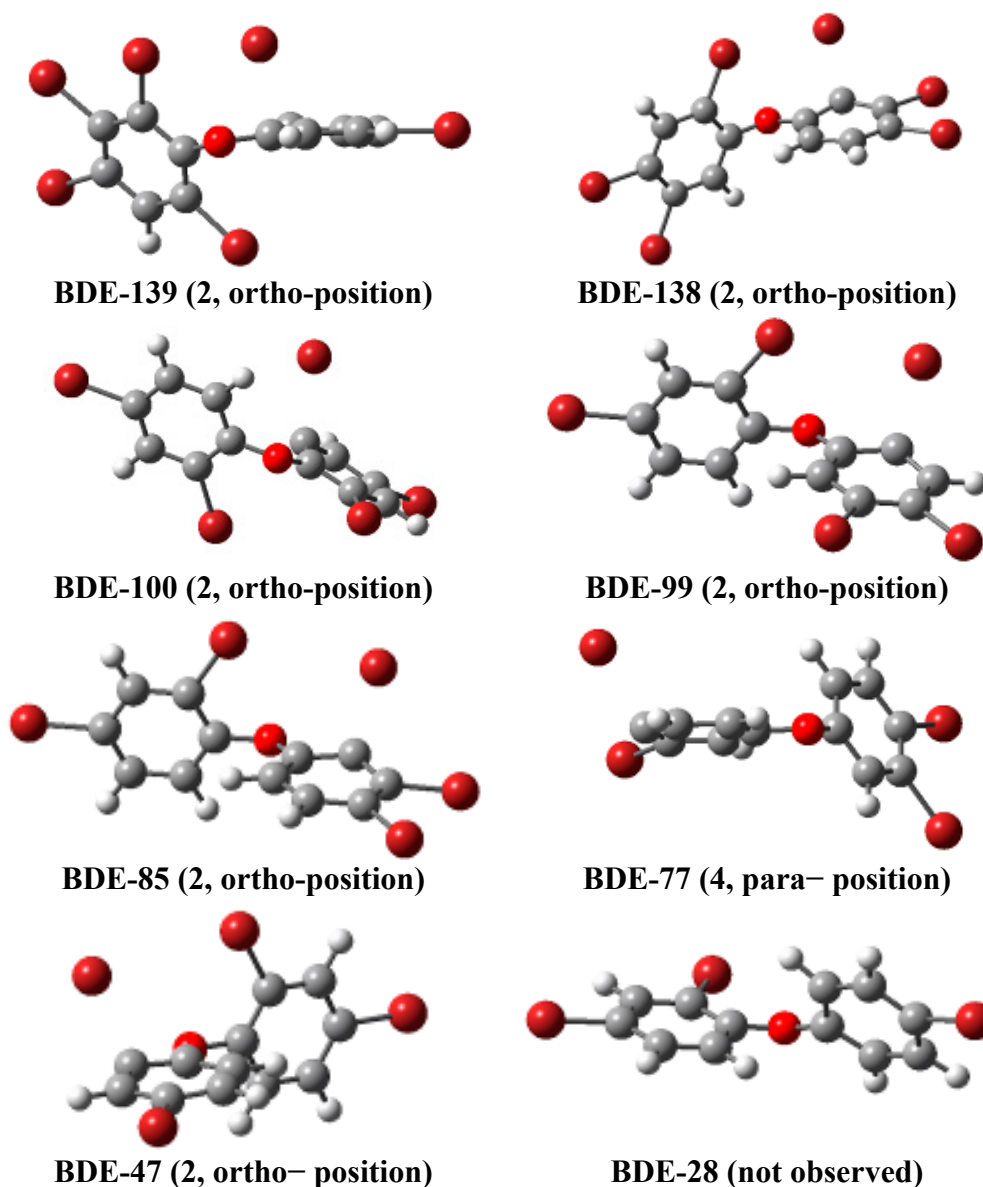


Figure S2. Visualized geometries (directly from GaussView 4.1) of the selected BDE congeners optimized at the PCM/B3LYP/6–31G(d) level (in the triplet excited states) and the positions of the bent C–Br bonds.

Molecular geometries

The Cartesian coordinates of optimized triplet excited states of the BDE congeners at PCM/B3LYP/6–31G(d) level are shown as follows:

BDE-209				Br	–5.03006243	–1.68713926	0.27928382
C	–2.40072327	1.45005484	–0.58410687	Br	–5.22372881	1.59654823	–0.10420917
C	–1.16764851	0.79751471	–0.72184355	Br	–2.49659271	3.32693259	–0.81737430
C	–1.09558574	–0.58717793	–0.53726049	Br	0.39984164	1.75999246	–1.18589014
C	–2.24768292	–1.32448909	–0.24386344	Br	2.24117006	–1.89210113	–2.69221379
C	–3.48093657	–0.67808787	–0.12361712	Br	5.21459537	–0.60333689	–1.51555776
C	–3.55742469	0.71433498	–0.28596924	Br	3.85466615	2.21932482	0.41907849
C	1.24946794	–0.97376095	–0.15992810	Br	–0.01005987	–1.08081696	2.43699152
C	2.41119384	–1.05005171	–1.00362902	Br	2.96539680	0.28547538	3.45580566
C	1.38291843	–0.63335752	1.22494709	BDE-208			
C	3.57702831	–0.49106145	–0.57233815	C	–2.77003638	1.07249356	1.00495839
C	2.55368579	–0.06550704	1.64301767	C	–3.65677836	0.00272588	0.93008628
C	3.54626703	0.27659240	0.65065260	C	–3.38009933	–1.06921536	0.08540279
O	0.06507043	–1.30720469	–0.73565236				
Br	–2.06219538	–3.18637589	0.01462428				

C	-2.21088706	-1.08681495	-0.67712218
C	-1.32263066	-0.00582037	-0.59268409
C	-1.59917132	1.08910164	0.23786518
O	-0.23300688	-0.03610456	-1.44151951
C	1.03214678	0.23193529	-1.02750124
C	1.60855844	-0.33294517	0.15567009
C	2.78104767	0.19289536	0.62129368
C	3.31397558	1.36868534	-0.02711280
C	2.99493466	1.57955320	-1.41971046
C	1.82108344	1.07011369	-1.88927890
Br	-0.41793759	2.57172524	0.28697087
Br	-3.21025480	2.50908548	2.16550336
Br	-4.62143680	-2.50244226	0.02291090
Br	-1.76196476	-2.54088476	-1.79458191
Br	1.15944314	1.45118158	-3.62309546
Br	4.19512662	2.60336983	-2.46710687
Br	3.31119844	3.00621555	1.08432035
Br	3.76705770	-0.54232251	2.05870260
Br	0.79245121	-1.84865998	0.96038479
H	-4.56420198	0.00543795	1.52756385

BDE-207

C	-2.20722657	0.35325776	1.99635817
C	-1.27977349	-0.51228808	1.52111879
C	-1.42271576	-1.00686249	0.15768416
C	-2.74349930	-1.06843486	-0.42454787
C	-3.66886693	-0.19286277	0.03356537
C	-3.30031033	0.68375415	1.12324369
O	-0.37220980	-1.19095645	-0.69816714
C	0.82559926	-0.52521546	-0.52203855
C	1.97235490	-1.29260271	-0.29915132
C	3.21896170	-0.66950194	-0.18858401
C	3.31148630	0.72810973	-0.29346620
C	2.16015877	1.49369103	-0.53261960
C	0.91498262	0.86351544	-0.66032777
Br	-0.65198044	1.84424880	-1.07348931
Br	2.27707664	3.37677420	-0.69632370
Br	4.99512219	1.57839143	-0.11696278
Br	4.76289704	-1.71747258	0.12563970
Br	1.76364430	-3.16190669	-0.12739408
Br	-3.11364118	-2.42237418	-1.73663667
Br	-5.47628628	-0.17724231	-0.59801189
Br	-4.09886564	2.38506766	1.29646287
Br	0.06929590	-1.25898511	2.67289552
H	-2.16341648	0.77274990	3.00164039

BDE-206

C	3.78100712	0.03882554	-0.32171819
C	2.67104786	-0.43271894	-1.04212109
C	1.38633282	0.07485736	-0.78957958
C	1.22620272	1.04272548	0.21002309
C	2.32090032	1.52452500	0.91792735
C	3.58969586	1.02967363	0.65107540
O	0.02000848	1.65935872	0.50119077
C	-1.14879584	0.98458835	0.63859860
C	-1.28704644	-0.19282391	1.44525680
C	-2.43278024	-0.92879887	1.33224508
C	-3.39044877	-0.56103300	0.31684139
C	-3.44039808	0.81918329	-0.10227576
C	-2.29911240	1.55907907	-0.00364975
Br	5.51527675	-0.64432483	-0.65713040
Br	2.90439887	-1.75469437	-2.38109318
Br	-0.11142373	-0.50043281	-1.80301039
Br	0.07120239	-0.62418236	2.70078973
Br	-2.84691466	-2.40769406	2.43764744
Br	-3.58704794	-1.88284813	-1.15328249
Br	-5.06582747	1.47745645	-0.81622318
Br	-2.15006660	3.31147574	-0.70952872
Br	5.03662373	1.73082389	1.66162659
H	2.16255703	2.28134914	1.68189427

BDE-203

C	3.78100712	0.03882554	-0.32171819
C	2.67104786	-0.43271894	-1.04212109
C	1.38633282	0.07485736	-0.78957958
C	1.22620272	1.04272548	0.21002309
C	2.32090032	1.52452500	0.91792735
C	3.58969586	1.02967363	0.65107540
O	0.02000848	1.65935872	0.50119077
C	-1.14879584	0.98458835	0.63859860
C	-1.28704644	-0.19282391	1.44525680

C	-2.43278024	-0.92879887	1.33224508
C	-3.39044877	-0.56103300	0.31684139
C	-3.44039808	0.81918329	-0.10227576
C	-2.29911240	1.55907907	-0.00364975
Br	5.51527675	-0.64432483	-0.65713040
Br	2.90439887	-1.75469437	-2.38109318
Br	-0.11142373	-0.50043281	-1.80301039
Br	0.07120239	-0.62418236	2.70078973
Br	-2.84691466	-2.40769406	2.43764744
Br	-3.58704794	-1.88284813	-1.15328249
Br	-5.06582747	1.47745645	-0.81622318
Br	-2.15006660	3.31147574	-0.70952872
Br	5.03662373	1.73082389	1.66162659
H	2.16255703	2.28134914	1.68189427

BDE-196

C	-3.22076104	0.50962731	-0.24336072
C	-2.49802703	0.05978716	0.86871433
C	-1.17470661	-0.37751672	0.69555596
C	-0.58316056	-0.33874728	-0.57489585
C	-1.32815704	0.10787852	-1.67004630
C	-2.64118469	0.52643186	-1.50986119
O	0.68463556	-0.82397132	-0.83183048
C	1.77171435	-0.46635350	-0.10128675
C	2.67276380	-1.52555426	0.26300470
C	3.63494812	-1.28181010	1.19742578
C	3.60607900	-0.01006910	1.88039952
C	3.03517966	1.12129246	1.18744134
C	2.07515809	0.89054297	0.24234817
Br	-0.52291805	0.18376043	-3.38262170
Br	-5.01372536	1.11796892	-0.08963797
Br	-3.29970309	0.02761412	2.58345564
Br	-0.17868102	-1.05198384	2.16506324
Br	2.43964532	-3.22139639	-0.54933023
Br	4.95971861	-2.53737356	1.70107041
Br	3.16100248	-0.11433238	3.81000754
Br	3.68268025	2.84224197	1.63236764
Br	1.22406797	2.30423940	-0.69929406
H	-3.20998102	0.87926723	-2.36586655

BDE-190

C	-1.43869454	-2.32635639	-1.35672884
C	-0.70044831	-1.53513887	-0.47823186
C	-0.82210229	-1.76545910	0.89068051
C	-1.66055633	-2.75845113	1.39069450
C	-2.39378987	-3.53847847	0.49982346
C	-2.28553671	-3.32677110	-0.87919376
O	-0.14404222	-1.02584054	1.85442138
C	0.78980151	-0.10340795	1.50476179
C	2.15424918	-0.49741516	1.31952787
C	3.12347498	0.46381174	1.21084469
C	2.76426880	1.84542453	1.44132917
C	1.38031311	2.23138856	1.27729299
C	0.41036543	1.27054394	1.39010796
Br	-1.43968279	1.67866286	1.33596288
Br	1.01318427	4.04575339	0.90418790
Br	3.65756452	2.66860993	3.03565931
Br	4.92194703	0.08676435	0.77193137
Br	2.53982448	-2.34805794	1.19090643
Br	-3.53428030	-4.88347808	1.21863888
Br	-3.26709928	-4.36845237	-2.13700181
H	-1.35543943	-2.16030771	-2.42837031
H	-0.04912684	-0.75692947	-0.86848887
H	-1.73490125	-2.91422058	2.46399156

BDE-183

C	-3.91105391	-0.34577868	0.91482379
C	-2.79994155	-0.50108929	1.79886715
C	-1.56568975	-0.74513928	1.24998715
C	-1.44440350	-0.94240930	-0.16073671
C	-2.59350668	-1.09868191	-0.96861210
C	-3.82604699	-0.87015183	-0.40955091
O	-0.25796093	-1.08966628	-0.80940791
C	0.82744431	-0.26678721	-0.58613368
C	0.74519379	1.12942567	-0.58219345
C	1.89988677	1.89491222	-0.45923947
C	3.14158916	1.27543855	-0.35007501
C	3.24583055	-0.12199670	-0.35075248
C	2.07829904	-0.88681898	-0.46171318
Br	-4.44956794	1.81047102	0.77742267
Br	-0.92574345	2.02509378	-0.73679256

Br	-0.04313846	-0.90407287	2.37602480
Br	4.67331493	2.38891021	-0.20099461
Br	4.93124001	-0.96517851	-0.18518760
Br	2.11796551	-2.77648560	-0.39720295
Br	-5.42309005	-1.11164617	-1.39704511
H	-2.92488675	-0.36766358	2.87268041
H	-2.46384161	-1.36838976	-2.01579709
H	1.83248991	2.97962902	-0.45750916

BDE-181

C	-2.74539126	-0.59898900	2.54077474
C	-3.28975796	-1.39136344	1.53237894
C	-2.95724534	-1.19673997	0.19327272
C	-2.06226348	-0.18218873	-0.14336640
C	-1.50159896	0.61673796	0.85285893
C	-1.84410130	0.40423183	2.19124091
C	1.38663660	0.66875653	-0.22962322
C	0.31057611	1.49711810	-0.40372942
O	-0.65352353	1.67196905	0.55481995
C	2.34142839	0.52772429	-1.30423532
C	2.44667419	1.60075811	-2.26909726
C	1.38444782	2.44401432	-2.44445914
C	0.24644734	2.31442930	-1.57991664
Br	-1.36759919	3.18946824	-1.94792729
Br	1.41904802	3.81760193	-3.75585345
Br	4.09187320	1.77793241	-3.19169247
Br	2.49957363	-1.29778285	-2.05221135
Br	1.69855139	-0.24856717	1.39557406
Br	-1.05285739	1.47079022	3.55196537
Br	-4.51952097	-2.77863996	2.00629169
H	-3.00521997	-0.76151228	3.58330426
H	-3.39421499	-1.81849790	-0.58418892
H	-1.81508130	-0.00231409	-1.18703389

BDE-155

C	-3.46103373	-0.88331618	0.50628251
C	-2.27774565	-1.31783924	1.05627911
C	-1.11292845	-0.57666808	0.75517112
C	-1.11192571	0.38116478	-0.30814132
C	-2.34456905	0.82844934	-0.81197739
C	-3.51615529	0.21223282	-0.40434395
O	0.02037208	0.91288486	-0.80815360
C	1.24163487	0.31529237	-0.54584804
C	1.55241728	-0.98069992	-0.97434486
C	2.81848919	-1.51891249	-0.75832321
C	3.77912684	-0.73516674	-0.12353498
C	3.50744366	0.56747247	0.28883081
C	2.23422404	1.08515915	0.06994959
Br	-2.39581533	2.19637802	-2.13335224
Br	-5.10182250	-1.73185507	0.96396739
Br	-0.36359656	0.49338294	2.65169624
Br	0.26238005	-2.02111521	-1.90728301
Br	5.51479842	-1.46305912	0.17820474
Br	1.83788386	2.85183959	0.62720189
H	-2.24275092	-2.14285012	1.76514064
H	-4.47382608	0.53839163	-0.80233486
H	3.04813890	-2.52795452	-1.08979624
H	4.26761507	1.17133434	0.77699717

BDE-154

C	-4.04333082	-0.48462832	-0.29434926
C	-3.56198289	0.54051243	-1.10549660
C	-2.30886397	1.07898715	-0.82305148
C	-1.54874724	0.60787221	0.25129311
C	-2.06010805	-0.42320535	1.04676543
C	-3.30880985	-0.97993253	0.78122161
O	-0.35674606	1.22120011	0.57973826
C	0.81967219	0.68483209	0.14569760
C	0.92389313	-0.38713399	-0.70548880
C	2.21706365	-0.90995951	-0.98472384
C	3.37306749	-0.13152207	-0.64690993
C	3.27746428	0.94225236	0.22084521
C	2.00521476	1.33815179	0.64487003
Br	-1.03065583	-1.07160132	2.50404184
Br	-5.75798918	-1.23302652	-0.66715568
Br	-1.61574730	2.47134328	-1.91264934
Br	2.44960505	-2.94441013	-0.18293081
Br	5.03019722	-0.58944178	-1.43280742
Br	1.83288593	2.77384195	1.84204080
H	-4.14542038	0.91510672	-1.94214468
H	-3.69755251	-1.78098350	1.40416328

H	0.04112460	-0.89499469	-1.08749295
H	4.15826560	1.49922116	0.53465061

BDE-153

C	-3.74667397	0.06066388	-0.36876312
C	-2.88690003	0.90583475	-1.07149178
C	-1.63297205	1.21326137	-0.55101766
C	-1.24107946	0.66981258	0.67595102
C	-2.09528408	-0.17095378	1.38109078
C	-3.35109894	-0.47969012	0.85992396
O	-0.04288609	1.03678750	1.27443270
C	1.12474373	0.46763665	0.88963107
C	1.24191351	-0.55896065	-0.04047258
C	2.49761946	-1.13771138	-0.24769740
C	3.64010150	-0.71683794	0.50701110
C	3.52541087	0.30720502	1.41827745
C	2.29944949	1.01222563	1.50822921
Br	-5.44695144	-0.31738758	-1.12706945
Br	-0.46705903	2.36904220	-1.49846456
Br	2.63053369	-2.52622820	-1.51131852
Br	5.32239640	-1.56680296	0.28190432
Br	2.56631017	3.15432847	0.80301418
Br	-4.48221015	-1.63146636	1.85989003
H	-3.19760871	1.32683396	-2.02424688
H	-1.77488766	-0.57450835	2.33923236
H	0.37592779	-0.95788189	-0.56270057
H	4.38258911	0.62434507	2.00976128

BDE-139

C	-3.25083925	0.51355766	1.30621173
C	-1.94481424	0.11055392	1.48375834
C	-1.08719295	0.18232682	0.36916784
C	-1.61592826	0.40671288	-0.93617707
C	-2.93907801	0.84778990	-1.08755898
C	-3.75226100	0.90576396	0.03068435
O	-0.88644683	0.25165696	-2.06552396
C	0.34365204	-0.37616490	-2.02732460
C	0.48248290	-1.72290793	-1.68144246
C	1.72837007	-2.33623524	-1.73690803
C	2.83947685	-1.60923985	-2.15627506
C	2.71888096	-0.26421972	-2.53249803
C	1.45969822	0.34753532	-2.46705337
Br	-4.44048012	0.57800691	2.79115077
Br	0.52124519	1.90488842	0.74780841
Br	-1.02784037	-2.75621108	-1.17408974
Br	4.50931574	-2.51172310	-2.20989747
Br	1.20946504	2.15475065	-2.95414923
Br	4.22969205	0.71629858	-3.10986936
H	-1.56133036	-0.16897997	2.46340954
H	-3.32403314	1.07343378	-2.08109688
H	-4.79049786	1.21558917	-0.06435565
H	1.83333265	-3.38268945	-1.46365764

BDE-138

C	-3.30901479	1.20745097	1.41834526
C	-2.47517652	0.38505220	2.17719626
C	-1.09884834	0.40672524	1.96941785
C	-0.56082330	1.25077741	0.99371670
C	-1.38712245	2.07353006	0.23650086
C	-2.76532136	2.05423583	0.44606265
O	0.81309667	1.36788098	0.82211547
C	1.49218448	0.44158185	0.10572987
C	0.92547199	-0.63193970	-0.57659440
C	1.74925523	-1.42378848	-1.37529567
C	3.13197960	-1.12743907	-1.54046297
C	3.69832388	-0.07134277	-0.86016769
C	2.92268539	0.61417800	0.10510243
Br	-5.17815413	1.13830048	1.75073741
Br	0.03672452	-0.69878431	3.00953443
Br	4.13018046	-2.21538942	-2.73142904
Br	3.68824307	0.29724536	2.16392811
Br	5.50182532	0.46741564	-1.09308216
Br	-3.85323057	3.19339345	-0.61442648
H	-2.90011449	-0.26930539	2.93407517
H	-0.94564950	2.73012191	-0.51006582
H	-0.14390961	-0.82754308	-0.54688767
H	1.32575882	-2.26525253	-1.91877909

BDE-100

C	-2.53828509	2.66395607	1.05403083
C	-1.58441245	1.82589798	1.62758914
C	-0.39343062	1.59453580	0.94095027

C	-0.17791353	2.19001033	-0.30598699
C	-1.13675051	3.03508616	-0.85946528
C	-2.32833476	3.27638091	-0.18173360
O	1.02921087	2.06466951	-0.99143016
C	1.43572922	0.86060783	-1.42019903
C	0.56412789	-0.26547191	-1.51802925
C	1.06702874	-1.56474159	-1.71281152
C	2.39288179	-1.67903323	-2.07001484
C	3.25056207	-0.54551668	-2.16719155
C	2.77240880	0.71014487	-1.84153666
Br	-4.16912126	2.98467892	1.99451046
Br	0.93723837	0.49502427	1.74319328
Br	-0.96089209	0.24835020	-3.25247954
Br	3.13096223	-3.38115241	-2.48809586
Br	3.93935516	2.21182833	-1.84725224
H	-1.75455963	1.36453617	2.59667387
H	-0.94213879	3.48735526	-1.82926321
H	-3.08283499	3.92857217	-0.61425629
H	0.40895737	-2.43047039	-1.67021062
H	4.28757969	-0.67621786	-2.46615054

BDE-99

C	4.25519641	-0.57854899	0.49265570
C	3.60880187	0.15160846	-0.50303957
C	2.35151989	0.68892508	-0.23077057
C	1.76047504	0.49057415	1.02076003
C	2.42196670	-0.23773666	2.00620986
C	3.67887773	-0.78170616	1.74571039
O	0.55426947	1.10529000	1.34711036
C	-0.62286143	0.57054873	0.95266622
C	-0.76185124	-0.63293699	0.26685424
C	-2.04659127	-1.12894511	0.03557095
C	-3.20554636	-0.43905149	0.51944222
C	-3.06837799	0.75867733	1.18295403
C	-1.78440851	1.34720596	1.27629853
Br	5.98035560	-1.31451787	0.12371001
Br	1.44376627	1.69593836	-1.56124631
Br	-2.20905198	-2.76351057	-0.88524395
Br	-4.94249717	-1.16268560	0.27089847
Br	-1.71075378	3.29491245	0.08298114
H	4.07087361	0.30576947	-1.47453309
H	1.94748609	-0.36969843	2.97709020
H	4.19888814	-1.35250370	2.51091024
H	0.10271470	-1.21762335	-0.03670532
H	-3.94098742	1.28526374	1.56600521

BDE-85

C	-2.78381893	2.83383813	0.96550306
C	-2.39276786	1.95855604	1.97721568
C	-1.14820199	1.33739117	1.88268493
C	-0.32257487	1.58915770	0.78300157
C	-0.72568246	2.47072754	-0.21647255
C	-1.96615464	3.10108891	-0.13133616
O	0.96134604	1.05323211	0.71106099
C	1.14621609	-0.22939812	0.33010525
C	0.14518054	-1.10115556	-0.09885673
C	0.51576945	-2.34932623	-0.59173608
C	1.88440579	-2.72832160	-0.70457368
C	2.87566883	-1.87533254	-0.26986911
C	2.50760089	-0.69129788	0.40835645
Br	-4.48788211	3.69013192	1.09636901
Br	-0.57397454	0.15725858	3.25585840
Br	2.26967773	-4.41447132	-1.48278380
Br	3.13896231	-0.73052336	2.55196823
Br	4.72616822	-2.24908022	-0.46358250
H	-3.03815262	1.76366727	2.82960800
H	-0.05937273	2.66074937	-1.05611413
H	-2.28622365	3.78970520	-0.90925260
H	-0.90087108	-0.80413228	-0.11241420
H	-0.24877448	-3.04174836	-0.93682426

BDE-77

C	-3.96819906	0.89748412	0.37641669
C	-2.89716396	0.05289023	0.74796758
C	-1.60119337	0.33109124	0.36014764
C	-1.36999602	1.55691532	-0.30182817
C	-2.41601899	2.49889750	-0.52374768
C	-3.69952473	2.19317646	-0.14160025
O	-0.15083734	1.96289279	-0.71395224
M.; Fagnoni, M.; Albini, A. Homoly	1.09951623	-0.71833522	
C	1.01003809	0.04340275	-1.62504625

C	2.16414734	-0.73530395	-1.66193816
C	3.23555144	-0.45501062	-0.81036885
C	3.15304263	0.61538767	0.08692228
C	2.00087084	1.40115965	0.13621982
Br	-5.37395626	-0.26280217	-1.14208236
Br	4.78468951	-1.55511025	-0.91270328
Br	4.58276633	1.04772998	1.26494579
Br	-3.27981211	-1.49314823	1.78103657
H	-0.78520329	-0.34740747	0.59464691
H	-2.16524233	3.44801508	-0.99489359
H	-4.51243829	2.90208605	-0.29291280
H	0.18023218	-0.16159912	-2.29886870
H	2.23729216	-1.56382122	-2.36265588
H	1.92389880	2.23851832	0.82556003

BDE-47

C	-2.51731283	-0.83958310	2.89625702
C	-2.96634273	-1.13339498	1.61016283
C	-2.39275128	-0.46344828	0.53035511
C	-1.38265774	0.47823499	0.74763289
C	-0.94724605	0.76275980	2.03910578
C	-1.51414100	0.10063103	3.12695663
O	-0.86703559	1.23080150	-0.30586867
C	0.08563391	0.72053542	-1.11449391
C	0.68273447	-0.53889785	-0.95859954
C	1.75628178	-0.86857734	-1.77312389
C	2.24515125	0.05822198	-2.74006409
C	1.65778195	1.28919884	-2.92962418
C	0.48478749	1.56658439	-2.19836813
Br	-3.30535910	-1.75283689	4.37910031
Br	-2.98764445	-0.83061861	-1.23568171
Br	3.75460913	-0.45442911	-3.78271955
Br	-1.34560240	1.74533945	-3.65457806
H	-3.75214537	-1.86550907	1.44431897
H	-0.16769250	1.50862695	2.18414447
H	-1.17771551	0.31794058	4.13752762
H	0.36684648	-1.22265037	-0.17398091
H	2.25421510	-1.82799686	-1.65218100
H	2.02980820	1.99217054	-3.67266622

BDE-28

C	-4.07773566	-0.24439363	-0.07546455
C	-3.04944086	-0.65613142	-0.94218330
C	-1.76810790	-0.19532149	-0.76174173
C	-1.50785513	0.73052820	0.39757446
C	-2.55882160	1.21796885	1.19751155
C	-3.84019419	0.76891109	1.01001998
O	-0.25480874	1.24332575	0.59556274
C	0.84705618	0.44174224	0.43428555
C	0.82251906	-0.93173628	0.70914396
C	1.97665492	-1.69853421	0.55519987
C	3.15361962	-1.07975465	0.14255616
C	3.20678968	0.29090611	-0.11710309
C	2.04636561	1.04285087	0.02866727
Br	-5.81351967	-0.96492296	-0.23007594
Br	4.74580954	-2.12207197	-0.06725938
Br	2.09074759	2.91473321	-0.33057174
H	-3.28144389	-1.32174013	-1.77215305
H	-0.98397573	-0.38083087	-1.48966398
H	-2.32646372	1.94042056	1.97943464
H	-4.67557013	1.11129744	1.61117189
H	-0.09352586	-1.38999724	1.07506057
H	1.95588624	-2.76436476	0.76976418
H	4.13215277	0.76555479	-0.43216571