Supporting Information: Spin-scaled double hybrids with long-range correction solve the TD-DFT overestimation problem in BODIPY dyes: benchmarking and experimental validation

Shebual Sebastian,[†] Vaughan Riley,[†] Binuki Wanniarachchi,[‡] Chris Ritchie,[*,‡] and Lars Goerigk[*,†]

[†]*School of Chemistry, The University of Melbourne, Victoria 3010, Australia; Ph: +61-(0)3-83446784*

[‡]*School of Chemistry, Monash University, Victoria 3800, Australia; Ph: +61-(0)3-99029916*

E-mail: chris.ritchie@monash.edu.au; lars.goerigk@unimelb.edu.au

Contents

SI.1 The SBYD31 set

Table S1: Experimental Reference Values

Compound	Solvent	λ_{max} **abs** (eV)	Reference
B1	Et_2O	2.087	S1
B1	MeCN	2.077	S1
B2	Et_2O	2.191	S2
B2	MeCN	2.198	S2
B2	MeOH	2.187	S2
B3	Et_2O	2.066	S3
B3	MeCN	2.060	S3
B3	MeOH	2.060	S3
B4	Et_2O	2.214	S3
B4	MeCN	2.226	S3
B4	MeOH	2.218	S3
B5	$CHCl_3$	2.322	S4
B6	$CHCl_3$	2.238	S5
B7	$CHCl_3$	2.242	S6
B8	$CHCl_3$	2.275	S7
B9	$CHCl_3$	2.331	S8
B10	THF	4.161	S9
B11	THF	2.480	S10
B11	$CHCl_3$	2.455	S10
B12	$CHCl_3$	2.292	S7
B13	$CHCl_3$	1.712	S11
B14	MeOH	2.520	S12
B15	DCM	1.864	S13
B16	DCM	1.922	S14
B17	THF	3.123	S15
B18	DCM	2.389	S16
B19	DCM	1.527	S17
B20	THF	1.916	S18
B21	THF	2.119	S19
B22	MeOH	3.139	S20
B23	MeOH	2.353	S21

SI.2 DSD functionals - sample input

Correct inputs for TD-DSD-BLYP and TD-DSD-PBEP86 in ORCA5 and above. Note the necessity of the 'scspar' line and specifying the scaling parameters in the %cis block.

DSD-BLYP input:

```
! RI-DSD-BLYP nopop PAL16 DEFGRID2 SCFCONV7 def2-TZVP def2-TZVP/C RIJCOSX DEF2/J USESYM CPCM(THF)
*xyzfile 0 1 B1.xyz
%TDDFT
NROOTS 5
TRIPLETS FALSE
TDA FALSE
doscs true
scspar 0.60, 0.46, 0.60, 0.46
END
```

DSD-PBEP86 input:

```
! RI-DSD-PBEP86 nopop PAL16 DEFGRID2 SCFCONV7 def2-TZVP def2-TZVP/C RIJCOSX DEF2/J USESYM CPCM(THF)
*xyzfile 0 1 B1.xyz
%TDDFT
NROOTS 5
TRIPLETS FALSE
TDA FALSE
doscs true
scspar 0.36, 0.51, 0.36, 0.51
END
```

SI.3 TD-DFT figures and tables

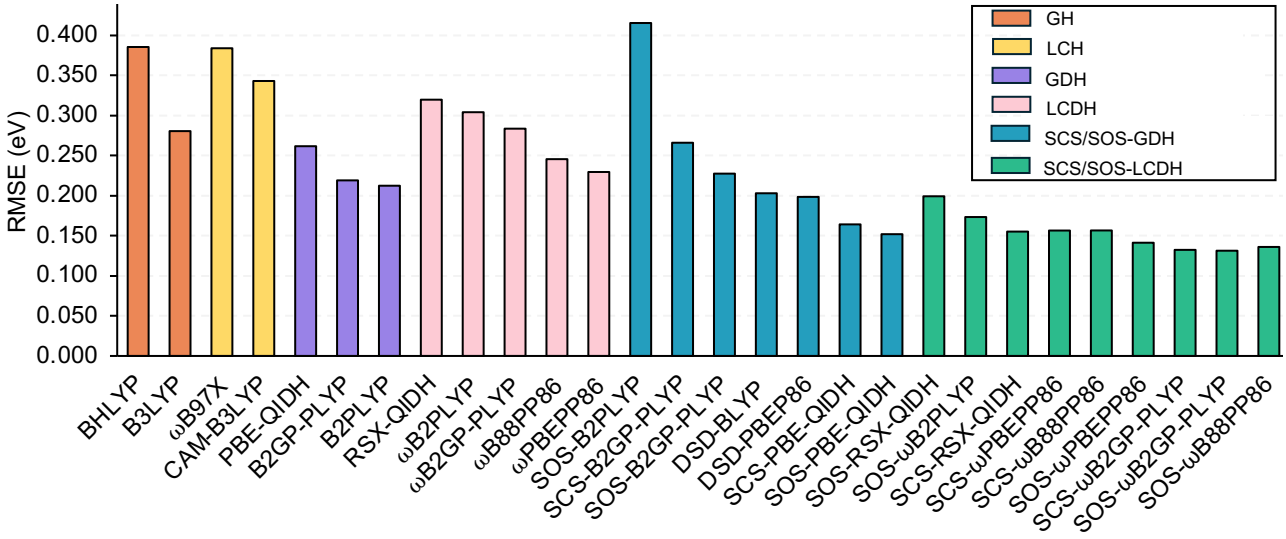

Figure S1: RMSEs (in eV) for TD-DFT methods

Table S2: Rankings for all functionals within the TD-DFT regime for the five quantities. Wherever numerical values were identical up to three decimal places, the next decimal place was used to determine the ranking.

Ranking	MAE	MSE	RMSE	Δ_{err}	R^2
1	SOS-ωB88PP86	SCS-ωB2GP-PLYP	SOS-ωB2GP-PLYP	SOS-RSX-QIDH	SOS-RSX-QIDH
2	SOS-ωB2GP-PLYP	SOS-ωB88PP86	SCS-ωB2GP-PLYP	SOS-ωB2GP-PLYP	SOS-ωB2GP-PLYP
3	SCS-ωB2GP-PLYP	SOS-ωB2GP-PLYP	SOS-ωB88PP86	SOS-ωB2PLYP	SOS-ωB2PLYP
4	SOS-PBE-QIDH	SOS-PBE-QIDH	SOS-ωPBEPP86	SCS-ωB2GP-PLYP	SCS-ωB2GP-PLYP
5	SOS-ωPBEPP86	SOS-ωPBEPP86	SOS-PBE-QIDH	RSX-QIDH	SOS-ωPBEPP86
6	SCS-PBE-QIDH	SCS-RSX-QIDH	SCS-RSX-QIDH	ωB2GP-PLYP	SOS-ωB88PP86
7	SCS-ωB88PP86	SCS-ωPBEPP86	SCS-ωPBEPP86	SCS-RSX-QIDH	SCS-ωB88PP86
8	SCS-ωPBEPP86	SCS-PBE-QIDH	SCS-ωB88PP86	ωB2PLYP	ωB2GP-PLYP
9	SCS-RSX-QIDH	SCS-ωB88PP86	SCS-PBE-QIDH	SOS-ωPBEPP86	ωPBEPP86
10	SOS-ωB2PLYP	B2PLYP	SOS-ωB2PLYP	SOS-ωB88PP86	ωB2PLYP
11	B2PLYP	B3LYP	DSD-PBEP86	SCS-ωB88PP86	RSX-QIDH
12	DSD-PBEP86	SOS-ωB2PLYP	SOS-RSX-QIDH	ωB97X	ωB88PP86
13	SOS-RSX-QIDH	DSD-PBEP86	DSD-BLYP	SCS-ωPBEPP86	SCS-RSX-QIDH
14	DSD-BLYP	DSD-BLYP	B2PLYP	ωB88PP86	SCS-ωPBEPP86
15	B2GP-PLYP	B2GP-PLYP	B2GP-PLYP	ωPBEPP86	SOS-PBE-QIDH
16	SOS-B2GP-PLYP	SOS-RSX-QIDH	SOS-B2GP-PLYP	SOS-PBE-QIDH	DSD-PBEP86
17	ωPBEPP86	SOS-B2GP-PLYP	ωPBEPP86	SCS-PBE-QIDH	DSD-BLYP
18	B3LYP	ωPBEPP86	ωB88PP86	DSD-PBEP86	ωB97X
19	ωB88PP86	ωB88PP86	PBE-QIDH	DSD-BLYP	SCS-PBE-QIDH
20	PBE-QIDH	PBE-QIDH	SCS-B2GP-PLYP	SCS-B2GP-PLYP	SCS-B2GP-PLYP
21	SCS-B2GP-PLYP	SCS-B2GP-PLYP	B3LYP	SOS-B2GP-PLYP	SOS-B2GP-PLYP
22	ωB2GP-PLYP	ωB2GP-PLYP	ωB2GP-PLYP	PBE-QIDH	PBE-QIDH
23	ωB2PLYP	ωB2PLYP	ωB2PLYP	B2GP-PLYP	B2GP-PLYP
24	RSX-QIDH	RSX-QIDH	RSX-QIDH	CAM-B3LYP	SOS-B2PYLP
25	CAM-B3LYP	CAM-B3LYP	CAM-B3LYP	BHLYP	CAM-B3LYP
26	BHLYP	BHLYP	ωB97X	SOS-B2PLYP	BHLYP
27	ωB97X	ωB97X	BHLYP	B2PLYP	B2PLYP
28	SOS-B2PLYP	SOS-B2PLYP	SOS-B2PLYP	B3LYP	B3LYP

SI.4 TDA-DFT figures and tables

Table S3: Performance of every functional in terms of MAE, MSE, RMSE, Δ_{err} (all in eV) and R^2 for TDA-DFT (same as Table 1 in main paper).

	MAE	MSE	RMSE	Δ_{err}	R^2
GH					
BHLYP	0.511	0.498	0.538	1.060	0.864
B3LYP	0.319	0.238	0.384	1.470	0.725
LCH					
ωB97X	0.524	0.524	0.546	0.816	0.920
CAM-B3LYP	0.473	0.457	0.493	1.031	0.880
DH					
PBE-QIDH	0.342	0.320	0.361	0.931	0.903
B2GP-PLYP	0.274	0.241	0.297	0.988	0.893
B2PLYP	0.223	0.179	0.277	1.123	0.846
LCDH					
RSX-QIDH	0.439	0.439	0.462	0.729	0.931
ωB2PLYP	0.424	0.421	0.443	0.755	0.932
ωB2GP-PLYP	0.397	0.392	0.416	0.750	0.933
ωB88PP86	0.340	0.324	0.354	0.824	0.927
ωPBEPP86	0.317	0.299	0.331	0.822	0.928
SCS/SOS-GDH					
SOS-B2PLYP	0.518	0.501	0.535	1.054	0.875
SCS-B2GP-PLYP	0.357	0.332	0.369	0.920	0.911
SOS-B2GP-PLYP	0.310	0.281	0.323	0.921	0.911
DSD-BLYP	0.256	0.227	0.276	0.905	0.913
DSD-PBEP86	0.257	0.226	0.275	0.904	0.914
SCS-PBE-QIDH	0.212	0.177	0.236	0.894	0.914
SOS-PBE-QIDH	0.188	0.151	0.214	0.877	0.918
SCS/SOS-LCDH					
SOS-RSX-QIDH	**0.075**	**0.022**	**0.126**	**0.681**	**0.945**
SOS-ωB2PLYP	0.291	0.276	0.305	0.716	**0.941**
SCS-RSX-QIDH	**0.130**	**0.098**	0.177	0.752	0.928
SCS-ωPBEPP86	**0.113**	**0.073**	**0.162**	0.794	0.927
SCS-ωB88PP86	0.242	0.219	0.258	0.777	0.934
SOS-ωPBEPP86	0.132	0.099	**0.165**	0.756	0.938
SCS-ωB2GP-PLYP	0.187	0.163	0.209	**0.715**	0.940
SOS-ωB2GP-PLYP	0.214	0.193	0.230	**0.700**	**0.944**
SOS-ωB88PP86	0.200	0.172	0.218	0.765	0.937

Table S4: Rankings for all TDA-DFT methods for the five quantities. Wherever numerical values were identical up to three decimal places, the next decimal place was used to determine the ranking.

Ranking	MAE	MSE	RMSE	Δ_{err}	R^2
1	SOS-RSX-QIDH	SOS-RSX-QIDH	SOS-RSX-QIDH	SOS-RSX-QIDH	SOS-RSX-QIDH
2	SCS-ωPBEPP86	SCS-ωPBEPP86	SCS-ωPBEPP86	SOS-ωB2GP-PLYP	SOS-ωB2GP-PLYP
3	SCS-RSX-QIDH	SCS-RSX-QIDH	SOS-ωPBEPP86	SCS-ωB2GP-PLYP	SOS-ωB2PLYP
4	SOS-ωPBEPP86	SOS-ωPBEPP86	SCS-RSX-QIDH	SOS-ωB2PLYP	SCS-ωB2GP-PLYP
5	SCS-ωB2GP-PLYP	SOS-PBE-QIDH	SCS-ωB2GP-PLYP	RSX-QIDH	SOS-ωPBEPP86
6	SOS-PBE-QIDH	SCS-ωB2GP-PLYP	SOS-PBE-QIDH	ωB2GP-PLYP	SOS-ωB88PP86
7	SOS-ωB88PP86	SOS-ωB88PP86	SOS-ωB88PP86	SCS-RSX-QIDH	SCS-ωB88PP86
8	SCS-PBE-QIDH	SCS-PBE-QIDH	SOS-ωB2GP-PLYP	ωB2PLYP	ωB2GP-PLYP
9	SOS-ωB2GP-PLYP	B2PLYP	SCS-PBE-QIDH	SOS-ωPBEPP86	ωB2PLYP
10	B2PLYP	SOS-ωB2GP-PLYP	SCS-ωB88PP86	SOS-ωB88PP86	RSX-QIDH
11	SCS-ωB88PP86	SCS-ωB88PP86	DSD-PBEP86	SCS-ωB88PP86	ωPBEPP86
12	DSD-BLYP	DSD-PBEP86	DSD-BLYP	SCS-ωPBEPP86	SCS-RSX-QIDH
13	DSD-PBEP86	DSD-BLYP	B2PLYP	ωB97X	ωB88PP86
14	B2GP-PLYP	B3LYP	B2GP-PLYP	ωPBEPP86	SCS-ωPBEPP86
15	SOS-ωB2PLYP	B2GP-PLYP	SOS-ωB2PLYP	ωB88PP86	ωB97X
16	SOS-B2GP-PLYP	SOS-ωB2PLYP	SOS-B2GP-PLYP	SOS-PBE-QIDH	SOS-PBE-QIDH
17	ωPBEPP86	SOS-B2GP-PLYP	ωPBEPP86	SCS-PBE-QIDH	SCS-PBE-QIDH
18	B3LYP	ωPBEPP86	ωB88PP86	DSD-PBEP86	DSD-PBEP86
19	ωB88PP86	PBE-QIDH	PBE-QIDH	DSD-BLYP	DSD-BLYP
20	PBE-QIDH	ωB88PP86	SCS-B2GP-PLYP	SCS-B2GP-PLYP	SCS-B2GP-PLYP
21	SCS-B2GP-PLYP	SCS-B2GP-PLYP	B3LYP	SOS-B2GP-PLYP	SOS-B2GP-PLYP
22	ωB2GP-PLYP	ωB2GP-PLYP	ωB2GP-PLYP	PBE-QIDH	PBE-QIDH
23	ωB2PLYP	ωB2PLYP	ωB2PLYP	B2GP-PLYP	B2GP-PLYP
24	RSX-QIDH	RSX-QIDH	RSX-QIDH	CAM-B3LYP	CAM-B3LYP
25	CAM-B3LYP	CAM-B3LYP	CAM-B3LYP	SOS-B2PLYP	SOS-B2PLYP
26	BHLYP	BHLYP	SOS-B2PLYP	BHLYP	BHLYP
27	SOS-B2PLYP	SOS-B2PLYP	BHLYP	B2PLYP	B2PLYP
28	ωB97X	ωB97X	ωB97X	B3LYP	B3LYP

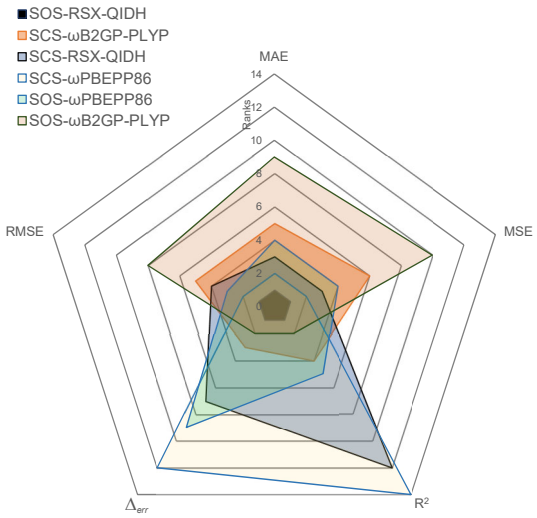

Figure S2: Radar chart showing the overall performance of select TDA-DFT methods.

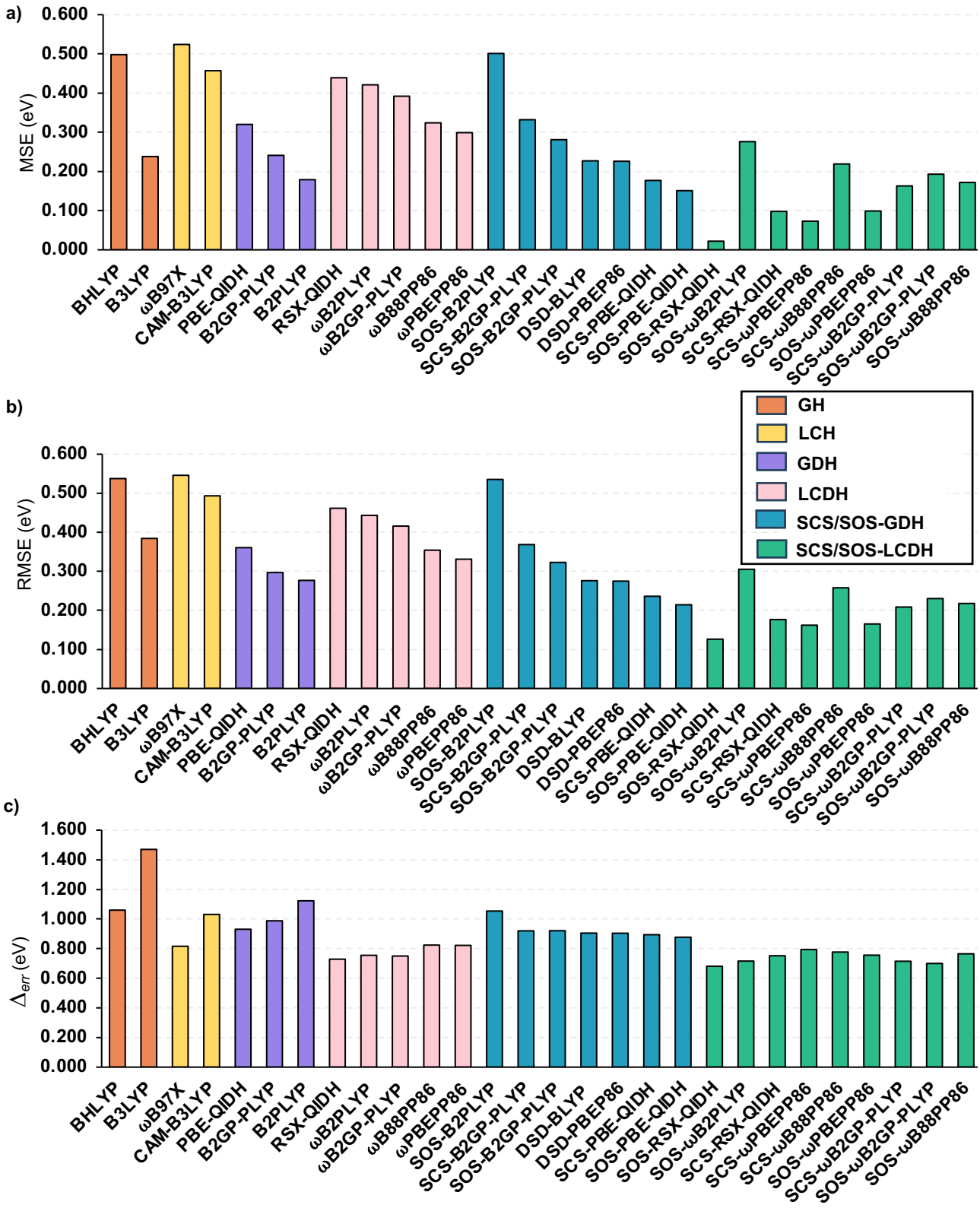

Figure S3: TDA-DFT metrics: a) MSE, b) RMSE and c)Δ_{err} (all in eV)

SI.5 Experimental cross-validation results

Table S5: Predicted (Pred) and experimentally measured (Exp.) values for the three synthesised compounds; see Section SI.8.2 for experimental details. H: HOMO, L: LUMO.

Compound	Solvent[a]	Pred. (eV)	Pred. (nm)	Exp. λ_{max} (nm)	Exp. λ_{max} (eV)	Pred.−Exp. (eV)	Transition details State, Osc. Str., MOs
TD-SOS-ωB2GP-PLYP							
1	DCM	2.424	511	503	2.465	-0.041	$S_0 \rightarrow S_1$, 0.649, H → L
	Tol	2.392	518	505	2.455	-0.063	$S_0 \rightarrow S_1$, 0.668, H → L
2	Tol	2.022	613	613	2.023	-0.001	$S_0 \rightarrow S_1$, 1.184, H → L
	DCM	2.027	611	612	2.026	0.001	$S_0 \rightarrow S_1$, 1.197, H → L
	Acet	2.045	606	599	2.070	-0.025	$S_0 \rightarrow S_1$, 1.192, H → L
	MeOH	2.054	603	599	2.070	-0.016	$S_0 \rightarrow S_1$, 1.184, H → L
	MeCN	2.049	605	596	2.080	-0.031	$S_0 \rightarrow S_1$, 1.197, H → L
3	Tol	2.016	615	617	2.009	0.007	$S_0 \rightarrow S_1$, 1.190, H → L
	DCM	2.021	613	615	2.016	0.005	$S_0 \rightarrow S_1$, 1.207, H → L
	Acet	2.038	608	607	2.043	-0.005	$S_0 \rightarrow S_1$, 1.201, H → L
	MeOH	2.048	605	604	2.053	-0.005	$S_0 \rightarrow S_1$, 1.200, H → L
	MeCN	2.042	607	605	2.049	-0.007	$S_0 \rightarrow S_1$, 1.203, H → L
TD-SCS-ωB2GP-PLYP							
1	DCM	2.414	513	503	2.465	-0.051	$S_0 \rightarrow S_1$, 0.646, H → L
	Tol	2.381	520	505	2.455	-0.074	$S_0 \rightarrow S_1$, 0.665, H → L
2	Tol	1.992	622	613	2.023	-0.031	$S_0 \rightarrow S_1$, 1.166, H → L
	DCM	1.996	621	612	2.026	-0.03	$S_0 \rightarrow S_1$, 1.178, H → L
	Acet	2.014	615	599	2.070	-0.056	$S_0 \rightarrow S_1$, 1.174, H → L
	MeOH	2.023	613	599	2.070	-0.047	$S_0 \rightarrow S_1$, 1.166, H → L
	MeCN	2.018	614	596	2.080	-0.062	$S_0 \rightarrow S_1$, 1.176, H → L
3	Tol	1.986	624	617	2.009	-0.023	$S_0 \rightarrow S_1$, 1.172, H → L
	DCM	1.990	623	615	2.016	-0.026	$S_0 \rightarrow S_1$, 1.189, H → L
	Acet	2.007	618	607	2.043	-0.036	$S_0 \rightarrow S_1$, 1.183, H → L
	MeOH	2.017	615	604	2.053	-0.036	$S_0 \rightarrow S_1$, 1.182, H → L
	MeCN	2.011	617	605	2.049	-0.038	$S_0 \rightarrow S_1$, 1.185, H → L
TD-SOS-ωB88PP86							
1	DCM	2.448	506	503	2.465	-0.017	$S_0 \rightarrow S_1$, 0.649, H → L
	Tol	2.417	513	505	2.455	-0.038	$S_0 \rightarrow S_1$, 0.669, H → L
2	Tol	2.020	613	613	2.023	-0.003	$S_0 \rightarrow S_1$, 1.196, H → L
	DCM	2.022	613	612	2.026	-0.004	$S_0 \rightarrow S_1$, 1.208, H → L
	Acet	2.038	608	599	2.070	-0.032	$S_0 \rightarrow S_1$, 1.203, H → L
	MeOH	2.047	513	599	2.070	-0.023	$S_0 \rightarrow S_1$, 1.196, H → L
	MeCN	2.042	606	596	2.080	-0.038	$S_0 \rightarrow S_1$, 1.205, H → L
3	Tol	2.015	615	617	2.009	0.006	$S_0 \rightarrow S_1$, 1.203, H → L
	DCM	2.015	615	615	2.016	-0.001	$S_0 \rightarrow S_1$, 1.219, H → L
	Acet	2.031	610	607	2.043	-0.012	$S_0 \rightarrow S_1$, 1.213, H → L
	MeOH	2.041	607	604	2.053	-0.012	$S_0 \rightarrow S_1$, 1.212, H → L
	MeCN	2.035	609	605	2.049	-0.014	$S_0 \rightarrow S_1$, 1.215, H → L

[a] Tol—Toluene, DCM—Dichloromethane, Acet—Acetone
MeOH—Methanol, MeCN—Acetonitrile

SI.6 TD-DFT: all calculated values for SBYD31

Table S6: TD-DFT details: solvent, transition, excitation energy, oscillator strength, and MO designation. For the DSD functionals, results for the correct and wrong implementations are shown. H: HOMO, L: LUMO.

Compound	Method	Solvent	Transition	Excitation energy (eV)	Oscillator strength	MO designation
B1	B2GP-PLYP	Et_2O	$S_0 \rightarrow S_1$	2.197	1.288	H $\rightarrow$ L
B1	B2PLYP	Et_2O	$S_0 \rightarrow S_1$	2.152	1.291	H $\rightarrow$ L
B1	B3LYP	Et_2O	$S_0 \rightarrow S_1$	2.129	1.316	H $\rightarrow$ L
B1	BHLYP	Et_2O	$S_0 \rightarrow S_1$	2.359	1.423	H $\rightarrow$ L
B1	CAM-B3LYP	Et_2O	$S_0 \rightarrow S_1$	2.322	1.356	H $\rightarrow$ L
B1	DSD-BLYP(CORRECT)	Et_2O	$S_0 \rightarrow S_1$	2.176	1.287	H $\rightarrow$ L
B1	DSD-BLYP(WRONG)	Et_2O	$S_0 \rightarrow S_1$	1.900	1.123	H $\rightarrow$ L
B1	DSD-PBEP86(CORRECT)	Et_2O	$S_0 \rightarrow S_1$	2.175	1.295	H $\rightarrow$ L
B1	DSD-PBEP86(WRONG)	Et_2O	$S_0 \rightarrow S_1$	1.866	1.111	H $\rightarrow$ L
B1	PBE-QIDH	Et_2O	$S_0 \rightarrow S_1$	2.247	1.312	H $\rightarrow$ L
B1	RSX-QIDH	Et_2O	$S_0 \rightarrow S_1$	2.315	1.297	H $\rightarrow$ L
B1	SCS-B2GP-PLYP	Et_2O	$S_0 \rightarrow S_1$	2.281	1.338	H $\rightarrow$ L
B1	SCS-PBE-QIDH	Et_2O	$S_0 \rightarrow S_1$	2.125	1.241	H $\rightarrow$ L
B1	SCS-RSX-QIDH	Et_2O	$S_0 \rightarrow S_1$	1.980	1.109	H $\rightarrow$ L
B1	SOS-B2PLYP	Et_2O	$S_0 \rightarrow S_1$	2.433	1.459	H $\rightarrow$ L
B1	SOS-ωB2PLYP	Et_2O	$S_0 \rightarrow S_1$	2.164	1.200	H $\rightarrow$ L
B1	SCS-ωB2GP-PLYP	Et_2O	$S_0 \rightarrow S_1$	2.056	1.149	H $\rightarrow$ L
B1	SCS-ωB88PP86	Et_2O	$S_0 \rightarrow S_1$	2.130	1.204	H $\rightarrow$ L
B1	SCS-ωPBEPP86	Et_2O	$S_0 \rightarrow S_1$	1.982	1.124	H $\rightarrow$ L
B1	SOS-B2GP-PLYP	Et_2O	$S_0 \rightarrow S_1$	2.233	1.310	H $\rightarrow$ L
B1	SOS-PBE-QIDH	Et_2O	$S_0 \rightarrow S_1$	2.101	1.227	H $\rightarrow$ L
B1	SOS-RSX-QIDH	Et_2O	$S_0 \rightarrow S_1$	1.902	1.066	H $\rightarrow$ L
B1	SOS-ωB2GP-PLYP	Et_2O	$S_0 \rightarrow S_1$	2.086	1.166	H $\rightarrow$ L
B1	SOS-ωB88PP86	Et_2O	$S_0 \rightarrow S_1$	2.083	1.178	H $\rightarrow$ L
B1	SOS-ωPBEPP86	Et_2O	$S_0 \rightarrow S_1$	2.009	1.140	H $\rightarrow$ L
B1	ωB2GP-PLYP	Et_2O	$S_0 \rightarrow S_1$	2.286	1.277	H $\rightarrow$ L
B1	ωB2PLYP	Et_2O	$S_0 \rightarrow S_1$	2.305	1.278	H $\rightarrow$ L
B1	ωB88PP86	Et_2O	$S_0 \rightarrow S_1$	2.244	1.269	H $\rightarrow$ L
B1	ωB97X	Et_2O	$S_0 \rightarrow S_1$	2.376	1.301	H $\rightarrow$ L
B1	ωPBEPP86	Et_2O	$S_0 \rightarrow S_1$	2.228	1.263	H $\rightarrow$ L
B1	B2GP-PLYP	MeCN	$S_0 \rightarrow S_1$	2.172	1.316	H $\rightarrow$ L
B1	B2PLYP	MeCN	$S_0 \rightarrow S_1$	2.123	1.317	H $\rightarrow$ L
B1	B3LYP	MeCN	$S_0 \rightarrow S_1$	2.101	1.338	H $\rightarrow$ L
B1	BHLYP	MeCN	$S_0 \rightarrow S_1$	2.342	1.463	H $\rightarrow$ L
B1	CAM-B3LYP	MeCN	$S_0 \rightarrow S_1$	2.303	1.395	H $\rightarrow$ L
B1	DSD-BLYP(CORRECT)	MeCN	$S_0 \rightarrow S_1$	2.167	1.292	H $\rightarrow$ L
B1	DSD-BLYP(WRONG)	MeCN	$S_0 \rightarrow S_1$	1.880	1.120	H $\rightarrow$ L
B1	DSD-PBEP86(CORRECT)	MeCN	$S_0 \rightarrow S_1$	2.165	1.300	H $\rightarrow$ L
B1	DSD-PBEP86(WRONG)	MeCN	$S_0 \rightarrow S_1$	1.843	1.106	H $\rightarrow$ L
B1	PBE-QIDH	MeCN	$S_0 \rightarrow S_1$	2.224	1.343	H $\rightarrow$ L
B1	RSX-QIDH	MeCN	$S_0 \rightarrow S_1$	2.302	1.331	H $\rightarrow$ L
B1	SCS-B2GP-PLYP	MeCN	$S_0 \rightarrow S_1$	2.258	1.368	H $\rightarrow$ L
B1	SCS-PBE-QIDH	MeCN	$S_0 \rightarrow S_1$	2.101	1.268	H $\rightarrow$ L
B1	SCS-RSX-QIDH	MeCN	$S_0 \rightarrow S_1$	1.962	1.134	H $\rightarrow$ L
B1	SOS-B2PLYP	MeCN	$S_0 \rightarrow S_1$	2.407	1.494	H $\rightarrow$ L
B1	SOS-ωB2PLYP	MeCN	$S_0 \rightarrow S_1$	2.150	1.231	H $\rightarrow$ L
B1	SCS-ωB2GP-PLYP	MeCN	$S_0 \rightarrow S_1$	2.041	1.176	H $\rightarrow$ L
B1	SCS-ωB88PP86	MeCN	$S_0 \rightarrow S_1$	2.112	1.233	H $\rightarrow$ L
B1	SCS-ωPBEPP86	MeCN	$S_0 \rightarrow S_1$	1.961	1.148	H $\rightarrow$ L
B1	SOS-B2GP-PLYP	MeCN	$S_0 \rightarrow S_1$	2.210	1.339	H $\rightarrow$ L
B1	SOS-PBE-QIDH	MeCN	$S_0 \rightarrow S_1$	2.076	1.253	H $\rightarrow$ L
B1	SOS-RSX-QIDH	MeCN	$S_0 \rightarrow S_1$	1.886	1.090	H $\rightarrow$ L
B1	SOS-ωB2GP-PLYP	MeCN	$S_0 \rightarrow S_1$	2.072	1.194	H $\rightarrow$ L
B1	SOS-ωB88PP86	MeCN	$S_0 \rightarrow S_1$	2.065	1.206	H $\rightarrow$ L
B1	SOS-ωPBEPP86	MeCN	$S_0 \rightarrow S_1$	1.991	1.166	H $\rightarrow$ L

B1	ωB2GP-PLYP	MeCN	$S_0 \rightarrow S_1$	2.272	1.309	H $\rightarrow$ L
B1	ωB2PLYP	MeCN	$S_0 \rightarrow S_1$	2.291	1.312	H $\rightarrow$ L
B1	ωB88PP86	MeCN	$S_0 \rightarrow S_1$	2.225	1.299	H $\rightarrow$ L
B1	ωB97X	MeCN	$S_0 \rightarrow S_1$	2.364	1.341	H $\rightarrow$ L
B1	ωPBEPP86	MeCN	$S_0 \rightarrow S_1$	2.207	1.292	H $\rightarrow$ L
B2	B2GP-PLYP	Et_2O	$S_0 \rightarrow S_1$	2.339	1.143	H $\rightarrow$ L
B2	B2PLYP	Et_2O	$S_0 \rightarrow S_1$	2.326	1.145	H $\rightarrow$ L
B2	B3LYP	Et_2O	$S_0 \rightarrow S_1$	2.342	1.203	H $\rightarrow$ L
B2	BHLYP	Et_2O	$S_0 \rightarrow S_1$	2.478	1.223	H $\rightarrow$ L
B2	CAM-B3LYP	Et_2O	$S_0 \rightarrow S_1$	2.443	1.158	H $\rightarrow$ L
B2	DSD-BLYP(CORRECT)	Et_2O	$S_0 \rightarrow S_1$	2.319	1.135	H $\rightarrow$ L
B2	DSD-BLYP(WRONG)	Et_2O	$S_0 \rightarrow S_1$	2.095	1.026	H $\rightarrow$ L
B2	DSD-PBEP86(CORRECT)	Et_2O	$S_0 \rightarrow S_1$	2.319	1.136	H $\rightarrow$ L
B2	DSD-PBEP86(WRONG)	Et_2O	$S_0 \rightarrow S_1$	2.080	1.019	H $\rightarrow$ L
B2	PBE-QIDH	Et_2O	$S_0 \rightarrow S_1$	2.378	1.159	H $\rightarrow$ L
B2	RSX-QIDH	Et_2O	$S_0 \rightarrow S_1$	2.405	1.144	H $\rightarrow$ L
B2	SCS-B2GP-PLYP	Et_2O	$S_0 \rightarrow S_1$	2.407	1.177	H $\rightarrow$ L
B2	SCS-PBE-QIDH	Et_2O	$S_0 \rightarrow S_1$	2.256	1.100	H $\rightarrow$ L
B2	SCS-RSX-QIDH	Et_2O	$S_0 \rightarrow S_1$	2.087	0.993	H $\rightarrow$ L
B2	SOS-B2PLYP	Et_2O	$S_0 \rightarrow S_1$	2.579	1.270	H $\rightarrow$ L
B2	SOS-ωB2PLYP	Et_2O	$S_0 \rightarrow S_1$	2.251	1.055	H $\rightarrow$ L
B2	SCS-ωB2GP-PLYP	Et_2O	$S_0 \rightarrow S_1$	2.149	1.020	H $\rightarrow$ L
B2	SCS-ωB88PP86	Et_2O	$S_0 \rightarrow S_1$	2.231	1.066	H $\rightarrow$ L
B2	SCS-ωPBEPP86	Et_2O	$S_0 \rightarrow S_1$	2.092	1.004	H $\rightarrow$ L
B2	SOS-B2GP-PLYP	Et_2O	$S_0 \rightarrow S_1$	2.361	1.154	H $\rightarrow$ L
B2	SOS-PBE-QIDH	Et_2O	$S_0 \rightarrow S_1$	2.229	1.087	H $\rightarrow$ L
B2	SOS-RSX-QIDH	Et_2O	$S_0 \rightarrow S_1$	1.995	0.949	H $\rightarrow$ L
B2	SOS-ωB2GP-PLYP	Et_2O	$S_0 \rightarrow S_1$	2.174	1.032	H $\rightarrow$ L
B2	SOS-ωB88PP86	Et_2O	$S_0 \rightarrow S_1$	2.183	1.042	H $\rightarrow$ L
B2	SOS-ωPBEPP86	Et_2O	$S_0 \rightarrow S_1$	2.111	1.013	H $\rightarrow$ L
B2	ωB2GP-PLYP	Et_2O	$S_0 \rightarrow S_1$	2.378	1.129	H $\rightarrow$ L
B2	ωB2PLYP	Et_2O	$S_0 \rightarrow S_1$	2.396	1.123	H $\rightarrow$ L
B2	ωB88PP86	Et_2O	$S_0 \rightarrow S_1$	2.353	1.124	H $\rightarrow$ L
B2	ωB97X	Et_2O	$S_0 \rightarrow S_1$	2.464	1.121	H $\rightarrow$ L
B2	ωPBEPP86	Et_2O	$S_0 \rightarrow S_1$	2.339	1.122	H $\rightarrow$ L
B2	B2GP-PLYP	MeCN	$S_0 \rightarrow S_1$	2.341	1.143	H $\rightarrow$ L
B2	B2PLYP	MeCN	$S_0 \rightarrow S_1$	2.327	1.145	H $\rightarrow$ L
B2	B3LYP	MeCN	$S_0 \rightarrow S_1$	2.342	1.204	H $\rightarrow$ L
B2	BHLYP	MeCN	$S_0 \rightarrow S_1$	2.481	1.224	H $\rightarrow$ L
B2	CAM-B3LYP	MeCN	$S_0 \rightarrow S_1$	2.445	1.158	H $\rightarrow$ L
B2	DSD-BLYP(CORRECT)	MeCN	$S_0 \rightarrow S_1$	2.323	1.131	H $\rightarrow$ L
B2	DSD-BLYP(WRONG)	MeCN	$S_0 \rightarrow S_1$	2.096	1.021	H $\rightarrow$ L
B2	DSD-PBEP86(CORRECT)	MeCN	$S_0 \rightarrow S_1$	2.323	1.133	H $\rightarrow$ L
B2	DSD-PBEP86(WRONG)	MeCN	$S_0 \rightarrow S_1$	2.080	1.014	H $\rightarrow$ L
B2	PBE-QIDH	MeCN	$S_0 \rightarrow S_1$	2.380	1.159	H $\rightarrow$ L
B2	RSX-QIDH	MeCN	$S_0 \rightarrow S_1$	2.409	1.144	H $\rightarrow$ L
B2	SCS-B2GP-PLYP	MeCN	$S_0 \rightarrow S_1$	2.409	1.176	H $\rightarrow$ L
B2	SCS-PBE-QIDH	MeCN	$S_0 \rightarrow S_1$	2.257	1.099	H $\rightarrow$ L
B2	SCS-RSX-QIDH	MeCN	$S_0 \rightarrow S_1$	2.091	0.993	H $\rightarrow$ L
B2	SOS-B2PLYP	MeCN	$S_0 \rightarrow S_1$	2.580	1.270	H $\rightarrow$ L
B2	SOS-ωB2PLYP	MeCN	$S_0 \rightarrow S_1$	2.255	1.055	H $\rightarrow$ L
B2	SCS-ωB2GP-PLYP	MeCN	$S_0 \rightarrow S_1$	2.152	1.020	H $\rightarrow$ L
B2	SCS-ωB88PP86	MeCN	$S_0 \rightarrow S_1$	2.234	1.065	H $\rightarrow$ L
B2	SCS-ωPBEPP86	MeCN	$S_0 \rightarrow S_1$	2.095	1.004	H $\rightarrow$ L
B2	SOS-B2GP-PLYP	MeCN	$S_0 \rightarrow S_1$	2.363	1.154	H $\rightarrow$ L
B2	SOS-PBE-QIDH	MeCN	$S_0 \rightarrow S_1$	2.230	1.086	H $\rightarrow$ L
B2	SOS-RSX-QIDH	MeCN	$S_0 \rightarrow S_1$	1.999	0.950	H $\rightarrow$ L
B2	SOS-ωB2GP-PLYP	MeCN	$S_0 \rightarrow S_1$	2.178	1.032	H $\rightarrow$ L
B2	SOS-ωB88PP86	MeCN	$S_0 \rightarrow S_1$	2.186	1.042	H $\rightarrow$ L
B2	SOS-ωPBEPP86	MeCN	$S_0 \rightarrow S_1$	2.114	1.013	H $\rightarrow$ L
B2	ωB2GP-PLYP	MeCN	$S_0 \rightarrow S_1$	2.382	1.129	H $\rightarrow$ L
B2	ωB2PLYP	MeCN	$S_0 \rightarrow S_1$	2.399	1.123	H $\rightarrow$ L

B2	ωB88PP86	MeCN	$S_0 \rightarrow S_1$	2.356	1.123	H $\rightarrow$ L
B2	ωB97X	MeCN	$S_0 \rightarrow S_1$	2.468	1.121	H $\rightarrow$ L
B2	ωPBEPP86	MeCN	$S_0 \rightarrow S_1$	2.342	1.122	H $\rightarrow$ L
B2	B2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.346	1.139	H $\rightarrow$ L
B2	B2PLYP	MeOH	$S_0 \rightarrow S_1$	2.332	1.141	H $\rightarrow$ L
B2	B3LYP	MeOH	$S_0 \rightarrow S_1$	2.347	1.200	H $\rightarrow$ L
B2	BHLYP	MeOH	$S_0 \rightarrow S_1$	2.486	1.220	H $\rightarrow$ L
B2	CAM-B3LYP	MeOH	$S_0 \rightarrow S_1$	2.450	1.154	H $\rightarrow$ L
B2	DSD-BLYP(CORRECT)	MeOH	$S_0 \rightarrow S_1$	2.328	1.128	H $\rightarrow$ L
B2	DSD-BLYP(WRONG)	MeOH	$S_0 \rightarrow S_1$	2.102	1.018	H $\rightarrow$ L
B2	DSD-PBEP86(CORRECT)	MeOH	$S_0 \rightarrow S_1$	2.329	1.129	H $\rightarrow$ L
B2	DSD-PBEP86(WRONG)	MeOH	$S_0 \rightarrow S_1$	2.086	1.011	H $\rightarrow$ L
B2	PBE-QIDH	MeOH	$S_0 \rightarrow S_1$	2.385	1.155	H $\rightarrow$ L
B2	RSX-QIDH	MeOH	$S_0 \rightarrow S_1$	2.414	1.140	H $\rightarrow$ L
B2	SCS-B2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.414	1.172	H $\rightarrow$ L
B2	SCS-PBE-QIDH	MeOH	$S_0 \rightarrow S_1$	2.263	1.096	H $\rightarrow$ L
B2	SCS-RSX-QIDH	MeOH	$S_0 \rightarrow S_1$	2.097	0.990	H $\rightarrow$ L
B2	SOS-B2PLYP	MeOH	$S_0 \rightarrow S_1$	2.585	1.265	H $\rightarrow$ L
B2	SOS-ωB2PLYP	MeOH	$S_0 \rightarrow S_1$	2.260	1.052	H $\rightarrow$ L
B2	SCS-ωB2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.158	1.017	H $\rightarrow$ L
B2	SCS-ωB88PP86	MeOH	$S_0 \rightarrow S_1$	2.240	1.062	H $\rightarrow$ L
B2	SCS-ωPBEPP86	MeOH	$S_0 \rightarrow S_1$	2.101	1.001	H $\rightarrow$ L
B2	SOS-B2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.368	1.150	H $\rightarrow$ L
B2	SOS-PBE-QIDH	MeOH	$S_0 \rightarrow S_1$	2.236	1.083	H $\rightarrow$ L
B2	SOS-RSX-QIDH	MeOH	$S_0 \rightarrow S_1$	2.005	0.947	H $\rightarrow$ L
B2	SOS-ωB2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.184	1.029	H $\rightarrow$ L
B2	SOS-ωB88PP86	MeOH	$S_0 \rightarrow S_1$	2.191	1.039	H $\rightarrow$ L
B2	SOS-ωPBEPP86	MeOH	$S_0 \rightarrow S_1$	2.120	1.010	H $\rightarrow$ L
B2	ωB2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.387	1.125	H $\rightarrow$ L
B2	ωB2PLYP	MeOH	$S_0 \rightarrow S_1$	2.405	1.119	H $\rightarrow$ L
B2	ωB88PP86	MeOH	$S_0 \rightarrow S_1$	2.361	1.120	H $\rightarrow$ L
B2	ωB97X	MeOH	$S_0 \rightarrow S_1$	2.472	1.117	H $\rightarrow$ L
B2	ωPBEPP86	MeOH	$S_0 \rightarrow S_1$	2.347	1.118	H $\rightarrow$ L
B3	B2GP-PLYP	Et_2O	$S_0 \rightarrow S_1$	2.181	1.306	H $\rightarrow$ L
B3	B2PLYP	Et_2O	$S_0 \rightarrow S_1$	2.135	1.309	H $\rightarrow$ L
B3	B3LYP	Et_2O	$S_0 \rightarrow S_1$	2.114	1.338	H $\rightarrow$ L
B3	BHLYP	Et_2O	$S_0 \rightarrow S_1$	2.344	1.447	H $\rightarrow$ L
B3	CAM-B3LYP	Et_2O	$S_0 \rightarrow S_1$	2.307	1.379	H $\rightarrow$ L
B3	DSD-BLYP(CORRECT)	Et_2O	$S_0 \rightarrow S_1$	2.160	1.305	H $\rightarrow$ L
B3	DSD-BLYP(WRONG)	Et_2O	$S_0 \rightarrow S_1$	1.883	1.137	H $\rightarrow$ L
B3	DSD-PBEP86(CORRECT)	Et_2O	$S_0 \rightarrow S_1$	2.159	1.313	H $\rightarrow$ L
B3	DSD-PBEP86(WRONG)	Et_2O	$S_0 \rightarrow S_1$	1.849	1.124	H $\rightarrow$ L
B3	PBE-QIDH	Et_2O	$S_0 \rightarrow S_1$	2.231	1.331	H $\rightarrow$ L
B3	RSX-QIDH	Et_2O	$S_0 \rightarrow S_1$	2.300	1.314	H $\rightarrow$ L
B3	SCS-B2GP-PLYP	Et_2O	$S_0 \rightarrow S_1$	2.266	1.357	H $\rightarrow$ L
B3	SCS-PBE-QIDH	Et_2O	$S_0 \rightarrow S_1$	2.109	1.258	H $\rightarrow$ L
B3	SCS-RSX-QIDH	Et_2O	$S_0 \rightarrow S_1$	1.964	1.122	H $\rightarrow$ L
B3	SOS-B2PLYP	Et_2O	$S_0 \rightarrow S_1$	2.417	1.482	H $\rightarrow$ L
B3	SOS-ωB2PLYP	Et_2O	$S_0 \rightarrow S_1$	2.148	1.216	H $\rightarrow$ L
B3	SCS-ωB2GP-PLYP	Et_2O	$S_0 \rightarrow S_1$	2.041	1.163	H $\rightarrow$ L
B3	SCS-ωB88PP86	Et_2O	$S_0 \rightarrow S_1$	2.114	1.220	H $\rightarrow$ L
B3	SCS-ωPBEPP86	Et_2O	$S_0 \rightarrow S_1$	1.965	1.137	H $\rightarrow$ L
B3	SOS-B2GP-PLYP	Et_2O	$S_0 \rightarrow S_1$	2.218	1.328	H $\rightarrow$ L
B3	SOS-PBE-QIDH	Et_2O	$S_0 \rightarrow S_1$	2.085	1.243	H $\rightarrow$ L
B3	SOS-RSX-QIDH	Et_2O	$S_0 \rightarrow S_1$	1.886	1.077	H $\rightarrow$ L
B3	SOS-ωB2GP-PLYP	Et_2O	$S_0 \rightarrow S_1$	2.071	1.180	H $\rightarrow$ L
B3	SOS-ωB88PP86	Et_2O	$S_0 \rightarrow S_1$	2.067	1.193	H $\rightarrow$ L
B3	SOS-ωPBEPP86	Et_2O	$S_0 \rightarrow S_1$	1.993	1.153	H $\rightarrow$ L
B3	ωB2GP-PLYP	Et_2O	$S_0 \rightarrow S_1$	2.271	1.294	H $\rightarrow$ L
B3	ωB2PLYP	Et_2O	$S_0 \rightarrow S_1$	2.290	1.296	H $\rightarrow$ L
B3	ωB88PP86	Et_2O	$S_0 \rightarrow S_1$	2.229	1.286	H $\rightarrow$ L
B3	ωB97X	Et_2O	$S_0 \rightarrow S_1$	2.362	1.321	H $\rightarrow$ L

B3	ωPBEPP86	Et_2O	$S_0 \rightarrow S_1$	2.212	1.280	H $\rightarrow$ L
B3	B2GP-PLYP	MeCN	$S_0 \rightarrow S_1$	2.156	1.336	H $\rightarrow$ L
B3	B2PLYP	MeCN	$S_0 \rightarrow S_1$	2.107	1.338	H $\rightarrow$ L
B3	B3LYP	MeCN	$S_0 \rightarrow S_1$	2.088	1.366	H $\rightarrow$ L
B3	BHLYP	MeCN	$S_0 \rightarrow S_1$	2.327	1.489	H $\rightarrow$ L
B3	CAM-B3LYP	MeCN	$S_0 \rightarrow S_1$	2.289	1.420	H $\rightarrow$ L
B3	DSD-BLYP(CORRECT)	MeCN	$S_0 \rightarrow S_1$	2.150	1.310	H $\rightarrow$ L
B3	DSD-BLYP(WRONG)	MeCN	$S_0 \rightarrow S_1$	1.862	1.134	H $\rightarrow$ L
B3	DSD-PBEP86(CORRECT)	MeCN	$S_0 \rightarrow S_1$	2.149	1.319	H $\rightarrow$ L
B3	DSD-PBEP86(WRONG)	MeCN	$S_0 \rightarrow S_1$	1.826	1.121	H $\rightarrow$ L
B3	PBE-QIDH	MeCN	$S_0 \rightarrow S_1$	2.208	1.363	H $\rightarrow$ L
B3	RSX-QIDH	MeCN	$S_0 \rightarrow S_1$	2.286	1.350	H $\rightarrow$ L
B3	SCS-B2GP-PLYP	MeCN	$S_0 \rightarrow S_1$	2.243	1.390	H $\rightarrow$ L
B3	SCS-PBE-QIDH	MeCN	$S_0 \rightarrow S_1$	2.085	1.287	H $\rightarrow$ L
B3	SCS-RSX-QIDH	MeCN	$S_0 \rightarrow S_1$	1.945	1.149	H $\rightarrow$ L
B3	SOS-B2PLYP	MeCN	$S_0 \rightarrow S_1$	2.392	1.519	H $\rightarrow$ L
B3	SOS-ωB2PLYP	MeCN	$S_0 \rightarrow S_1$	2.135	1.250	H $\rightarrow$ L
B3	SCS-ωB2GP-PLYP	MeCN	$S_0 \rightarrow S_1$	2.025	1.193	H $\rightarrow$ L
B3	SCS-ωB88PP86	MeCN	$S_0 \rightarrow S_1$	2.096	1.251	H $\rightarrow$ L
B3	SCS-ωPBEPP86	MeCN	$S_0 \rightarrow S_1$	1.945	1.164	H $\rightarrow$ L
B3	SOS-B2GP-PLYP	MeCN	$S_0 \rightarrow S_1$	2.194	1.360	H $\rightarrow$ L
B3	SOS-PBE-QIDH	MeCN	$S_0 \rightarrow S_1$	2.060	1.272	H $\rightarrow$ L
B3	SOS-RSX-QIDH	MeCN	$S_0 \rightarrow S_1$	1.870	1.104	H $\rightarrow$ L
B3	SOS-ωB2GP-PLYP	MeCN	$S_0 \rightarrow S_1$	2.056	1.211	H $\rightarrow$ L
B3	SOS-ωB88PP86	MeCN	$S_0 \rightarrow S_1$	2.049	1.223	H $\rightarrow$ L
B3	SOS-ωPBEPP86	MeCN	$S_0 \rightarrow S_1$	1.975	1.182	H $\rightarrow$ L
B3	ωB2GP-PLYP	MeCN	$S_0 \rightarrow S_1$	2.256	1.329	H $\rightarrow$ L
B3	ωB2PLYP	MeCN	$S_0 \rightarrow S_1$	2.276	1.332	H $\rightarrow$ L
B3	ωB88PP86	MeCN	$S_0 \rightarrow S_1$	2.210	1.318	H $\rightarrow$ L
B3	ωB97X	MeCN	$S_0 \rightarrow S_1$	2.350	1.362	H $\rightarrow$ L
B3	ωPBEPP86	MeCN	$S_0 \rightarrow S_1$	2.191	1.311	H $\rightarrow$ L
B3	B2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.162	1.331	H $\rightarrow$ L
B3	B2PLYP	MeOH	$S_0 \rightarrow S_1$	2.112	1.333	H $\rightarrow$ L
B3	B3LYP	MeOH	$S_0 \rightarrow S_1$	2.093	1.359	H $\rightarrow$ L
B3	BHLYP	MeOH	$S_0 \rightarrow S_1$	2.332	1.482	H $\rightarrow$ L
B3	CAM-B3LYP	MeOH	$S_0 \rightarrow S_1$	2.294	1.414	H $\rightarrow$ L
B3	DSD-BLYP(CORRECT)	MeOH	$S_0 \rightarrow S_1$	2.156	1.306	H $\rightarrow$ L
B3	DSD-BLYP(WRONG)	MeOH	$S_0 \rightarrow S_1$	1.867	1.132	H $\rightarrow$ L
B3	DSD-PBEP86(CORRECT)	MeOH	$S_0 \rightarrow S_1$	2.155	1.316	H $\rightarrow$ L
B3	DSD-PBEP86(WRONG)	MeOH	$S_0 \rightarrow S_1$	1.831	1.118	H $\rightarrow$ L
B3	PBE-QIDH	MeOH	$S_0 \rightarrow S_1$	2.214	1.358	H $\rightarrow$ L
B3	RSX-QIDH	MeOH	$S_0 \rightarrow S_1$	2.292	1.345	H $\rightarrow$ L
B3	SCS-B2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.248	1.386	H $\rightarrow$ L
B3	SCS-PBE-QIDH	MeOH	$S_0 \rightarrow S_1$	2.091	1.283	H $\rightarrow$ L
B3	SCS-RSX-QIDH	MeOH	$S_0 \rightarrow S_1$	1.951	1.146	H $\rightarrow$ L
B3	SOS-B2PLYP	MeOH	$S_0 \rightarrow S_1$	2.397	1.514	H $\rightarrow$ L
B3	SOS-ωB2PLYP	MeOH	$S_0 \rightarrow S_1$	2.140	1.246	H $\rightarrow$ L
B3	SCS-ωB2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.031	1.190	H $\rightarrow$ L
B3	SCS-ωB88PP86	MeOH	$S_0 \rightarrow S_1$	2.102	1.248	H $\rightarrow$ L
B3	SCS-ωPBEPP86	MeOH	$S_0 \rightarrow S_1$	1.951	1.162	H $\rightarrow$ L
B3	SOS-B2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.200	1.356	H $\rightarrow$ L
B3	SOS-PBE-QIDH	MeOH	$S_0 \rightarrow S_1$	2.066	1.268	H $\rightarrow$ L
B3	SOS-RSX-QIDH	MeOH	$S_0 \rightarrow S_1$	1.876	1.102	H $\rightarrow$ L
B3	SOS-ωB2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.062	1.208	H $\rightarrow$ L
B3	SOS-ωB88PP86	MeOH	$S_0 \rightarrow S_1$	2.055	1.220	H $\rightarrow$ L
B3	SOS-ωPBEPP86	MeOH	$S_0 \rightarrow S_1$	1.981	1.179	H $\rightarrow$ L
B3	ωB2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.262	1.323	H $\rightarrow$ L
B3	ωB2PLYP	MeOH	$S_0 \rightarrow S_1$	2.281	1.329	H $\rightarrow$ L
B3	ωB88PP86	MeOH	$S_0 \rightarrow S_1$	2.215	1.313	H $\rightarrow$ L
B3	ωB97X	MeOH	$S_0 \rightarrow S_1$	2.355	1.356	H $\rightarrow$ L
B3	ωPBEPP86	MeOH	$S_0 \rightarrow S_1$	2.197	1.306	H $\rightarrow$ L
B4	B2GP-PLYP	Et_2O	$S_0 \rightarrow S_1$	2.367	1.074	H $\rightarrow$ L

B4	B2PLYP	Et_2O	$S_0 \rightarrow S_1$	2.358	1.072	H $\rightarrow$ L
B4	B3LYP	Et_2O	$S_0 \rightarrow S_1$	2.379	1.109	H $\rightarrow$ L
B4	BHLYP	Et_2O	$S_0 \rightarrow S_1$	2.503	1.139	H $\rightarrow$ L
B4	CAM-B3LYP	Et_2O	$S_0 \rightarrow S_1$	2.468	1.078	H $\rightarrow$ L
B4	DSD-BLYP(CORRECT)	Et_2O	$S_0 \rightarrow S_1$	2.347	1.069	H $\rightarrow$ L
B4	DSD-BLYP(WRONG)	Et_2O	$S_0 \rightarrow S_1$	2.132	0.971	H $\rightarrow$ L
B4	DSD-PBEP86(CORRECT)	Et_2O	$S_0 \rightarrow S_1$	2.347	1.068	H $\rightarrow$ L
B4	DSD-PBEP86(WRONG)	Et_2O	$S_0 \rightarrow S_1$	2.118	0.964	H $\rightarrow$ L
B4	PBE-QIDH	Et_2O	$S_0 \rightarrow S_1$	2.404	1.089	H $\rightarrow$ L
B4	RSX-QIDH	Et_2O	$S_0 \rightarrow S_1$	2.425	1.079	H $\rightarrow$ L
B4	SCS-B2GP-PLYP	Et_2O	$S_0 \rightarrow S_1$	2.432	1.103	H $\rightarrow$ L
B4	SCS-PBE-QIDH	Et_2O	$S_0 \rightarrow S_1$	2.282	1.034	H $\rightarrow$ L
B4	SCS-RSX-QIDH	Et_2O	$S_0 \rightarrow S_1$	2.113	0.940	H $\rightarrow$ L
B4	SOS-B2PLYP	Et_2O	$S_0 \rightarrow S_1$	2.605	1.185	H $\rightarrow$ L
B4	SOS-ωB2PLYP	Et_2O	$S_0 \rightarrow S_1$	2.271	0.994	H $\rightarrow$ L
B4	SCS-ωB2GP-PLYP	Et_2O	$S_0 \rightarrow S_1$	2.170	0.963	H $\rightarrow$ L
B4	SCS-ωB88PP86	Et_2O	$S_0 \rightarrow S_1$	2.254	1.004	H $\rightarrow$ L
B4	SCS-ωPBEPP86	Et_2O	$S_0 \rightarrow S_1$	2.118	0.948	H $\rightarrow$ L
B4	SOS-B2GP-PLYP	Et_2O	$S_0 \rightarrow S_1$	2.386	1.083	H $\rightarrow$ L
B4	SOS-PBE-QIDH	Et_2O	$S_0 \rightarrow S_1$	2.254	1.021	H $\rightarrow$ L
B4	SOS-RSX-QIDH	Et_2O	$S_0 \rightarrow S_1$	2.017	0.897	H $\rightarrow$ L
B4	SOS-ωB2GP-PLYP	Et_2O	$S_0 \rightarrow S_1$	2.195	0.974	H $\rightarrow$ L
B4	SOS-ωB88PP86	Et_2O	$S_0 \rightarrow S_1$	2.204	0.982	H $\rightarrow$ L
B4	SOS-ωPBEPP86	Et_2O	$S_0 \rightarrow S_1$	2.133	0.955	H $\rightarrow$ L
B4	ωB2GP-PLYP	Et_2O	$S_0 \rightarrow S_1$	2.399	1.064	H $\rightarrow$ L
B4	ωB2PLYP	Et_2O	$S_0 \rightarrow S_1$	2.416	1.057	H $\rightarrow$ L
B4	ωB88PP86	Et_2O	$S_0 \rightarrow S_1$	2.376	1.059	H $\rightarrow$ L
B4	ωB97X	Et_2O	$S_0 \rightarrow S_1$	2.483	1.052	H $\rightarrow$ L
B4	ωPBEPP86	Et_2O	$S_0 \rightarrow S_1$	2.363	1.058	H $\rightarrow$ L
B4	B2GP-PLYP	MeCN	$S_0 \rightarrow S_1$	2.371	1.071	H $\rightarrow$ L
B4	B2PLYP	MeCN	$S_0 \rightarrow S_1$	2.361	1.070	H $\rightarrow$ L
B4	B3LYP	MeCN	$S_0 \rightarrow S_1$	2.382	1.106	H $\rightarrow$ L
B4	BHLYP	MeCN	$S_0 \rightarrow S_1$	2.508	1.137	H $\rightarrow$ L
B4	CAM-B3LYP	MeCN	$S_0 \rightarrow S_1$	2.472	1.076	H $\rightarrow$ L
B4	DSD-BLYP(CORRECT)	MeCN	$S_0 \rightarrow S_1$	2.352	1.064	H $\rightarrow$ L
B4	DSD-BLYP(WRONG)	MeCN	$S_0 \rightarrow S_1$	2.135	0.966	H $\rightarrow$ L
B4	DSD-PBEP86(CORRECT)	MeCN	$S_0 \rightarrow S_1$	2.352	1.064	H $\rightarrow$ L
B4	DSD-PBEP86(WRONG)	MeCN	$S_0 \rightarrow S_1$	2.121	0.959	H $\rightarrow$ L
B4	PBE-QIDH	MeCN	$S_0 \rightarrow S_1$	2.408	1.086	H $\rightarrow$ L
B4	RSX-QIDH	MeCN	$S_0 \rightarrow S_1$	2.431	1.076	H $\rightarrow$ L
B4	SCS-B2GP-PLYP	MeCN	$S_0 \rightarrow S_1$	2.435	1.100	H $\rightarrow$ L
B4	SCS-PBE-QIDH	MeCN	$S_0 \rightarrow S_1$	2.286	1.031	H $\rightarrow$ L
B4	SCS-RSX-QIDH	MeCN	$S_0 \rightarrow S_1$	2.119	0.938	H $\rightarrow$ L
B4	SOS-B2PLYP	MeCN	$S_0 \rightarrow S_1$	2.608	1.182	H $\rightarrow$ L
B4	SOS-ωB2PLYP	MeCN	$S_0 \rightarrow S_1$	2.277	0.992	H $\rightarrow$ L
B4	SCS-ωB2GP-PLYP	MeCN	$S_0 \rightarrow S_1$	2.176	0.961	H $\rightarrow$ L
B4	SCS-ωB88PP86	MeCN	$S_0 \rightarrow S_1$	2.259	1.002	H $\rightarrow$ L
B4	SCS-ωPBEPP86	MeCN	$S_0 \rightarrow S_1$	2.123	0.946	H $\rightarrow$ L
B4	SOS-B2GP-PLYP	MeCN	$S_0 \rightarrow S_1$	2.390	1.080	H $\rightarrow$ L
B4	SOS-PBE-QIDH	MeCN	$S_0 \rightarrow S_1$	2.258	1.019	H $\rightarrow$ L
B4	SOS-RSX-QIDH	MeCN	$S_0 \rightarrow S_1$	2.023	0.895	H $\rightarrow$ L
B4	SOS-ωB2GP-PLYP	MeCN	$S_0 \rightarrow S_1$	2.200	0.971	H $\rightarrow$ L
B4	SOS-ωB88PP86	MeCN	$S_0 \rightarrow S_1$	2.210	0.980	H $\rightarrow$ L
B4	SOS-ωPBEPP86	MeCN	$S_0 \rightarrow S_1$	2.139	0.953	H $\rightarrow$ L
B4	ωB2GP-PLYP	MeCN	$S_0 \rightarrow S_1$	2.405	1.061	H $\rightarrow$ L
B4	ωB2PLYP	MeCN	$S_0 \rightarrow S_1$	2.422	1.055	H $\rightarrow$ L
B4	ωB88PP86	MeCN	$S_0 \rightarrow S_1$	2.381	1.056	H $\rightarrow$ L
B4	ωB97X	MeCN	$S_0 \rightarrow S_1$	2.489	1.049	H $\rightarrow$ L
B4	ωPBEPP86	MeCN	$S_0 \rightarrow S_1$	2.368	1.055	H $\rightarrow$ L
B4	B2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.377	1.068	H $\rightarrow$ L
B4	B2PLYP	MeOH	$S_0 \rightarrow S_1$	2.366	1.066	H $\rightarrow$ L
B4	B3LYP	MeOH	$S_0 \rightarrow S_1$	2.386	1.103	H $\rightarrow$ L

B4	BHLYP	MeOH	$S_0 \rightarrow S_1$	2.512	1.133	H $\rightarrow$ L
B4	CAM-B3LYP	MeOH	$S_0 \rightarrow S_1$	2.477	1.072	H $\rightarrow$ L
B4	DSD-BLYP(CORRECT)	MeOH	$S_0 \rightarrow S_1$	2.358	1.060	H $\rightarrow$ L
B4	DSD-BLYP(WRONG)	MeOH	$S_0 \rightarrow S_1$	2.141	0.963	H $\rightarrow$ L
B4	DSD-PBEP86(CORRECT)	MeOH	$S_0 \rightarrow S_1$	2.358	1.060	H $\rightarrow$ L
B4	DSD-PBEP86(WRONG)	MeOH	$S_0 \rightarrow S_1$	2.126	0.956	H $\rightarrow$ L
B4	PBE-QIDH	MeOH	$S_0 \rightarrow S_1$	2.413	1.083	H $\rightarrow$ L
B4	RSX-QIDH	MeOH	$S_0 \rightarrow S_1$	2.437	1.072	H $\rightarrow$ L
B4	SCS-B2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.441	1.096	H $\rightarrow$ L
B4	SCS-PBE-QIDH	MeOH	$S_0 \rightarrow S_1$	2.291	1.028	H $\rightarrow$ L
B4	SCS-RSX-QIDH	MeOH	$S_0 \rightarrow S_1$	2.125	0.935	H $\rightarrow$ L
B4	SOS-B2PLYP	MeOH	$S_0 \rightarrow S_1$	2.613	1.177	H $\rightarrow$ L
B4	SOS-ωB2PLYP	MeOH	$S_0 \rightarrow S_1$	2.282	0.988	H $\rightarrow$ L
B4	SCS-ωB2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.182	0.957	H $\rightarrow$ L
B4	SCS-ωB88PP86	MeOH	$S_0 \rightarrow S_1$	2.264	0.998	H $\rightarrow$ L
B4	SCS-ωPBEPP86	MeOH	$S_0 \rightarrow S_1$	2.129	0.943	H $\rightarrow$ L
B4	SOS-B2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.395	1.076	H $\rightarrow$ L
B4	SOS-PBE-QIDH	MeOH	$S_0 \rightarrow S_1$	2.264	1.016	H $\rightarrow$ L
B4	SOS-RSX-QIDH	MeOH	$S_0 \rightarrow S_1$	2.029	0.893	H $\rightarrow$ L
B4	SOS-ωB2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.206	0.968	H $\rightarrow$ L
B4	SOS-ωB88PP86	MeOH	$S_0 \rightarrow S_1$	2.215	0.977	H $\rightarrow$ L
B4	SOS-ωPBEPP86	MeOH	$S_0 \rightarrow S_1$	2.145	0.950	H $\rightarrow$ L
B4	ωB2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.410	1.058	H $\rightarrow$ L
B4	ωB2PLYP	MeOH	$S_0 \rightarrow S_1$	2.427	1.051	H $\rightarrow$ L
B4	ωB88PP86	MeOH	$S_0 \rightarrow S_1$	2.386	1.052	H $\rightarrow$ L
B4	ωB97X	MeOH	$S_0 \rightarrow S_1$	2.494	1.045	H $\rightarrow$ L
B4	ωPBEPP86	MeOH	$S_0 \rightarrow S_1$	2.373	1.051	H $\rightarrow$ L
B5	B2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.485	1.288	H-1 $\rightarrow$ L
B5	B2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.412	1.229	H-1 $\rightarrow$ L
B5	B3LYP	$CHCl_3$	$S_0 \rightarrow S_2$	2.633	1.088	H-1 $\rightarrow$ L
B5	BHLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.713	1.358	H-1 $\rightarrow$ L
B5	CAM-B3LYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.662	1.340	H-1 $\rightarrow$ L
B5	DSD-BLYP(CORRECT)	$CHCl_3$	$S_0 \rightarrow S_1$	2.475	1.281	H-1 $\rightarrow$ L
B5	DSD-BLYP(WRONG)	$CHCl_3$	$S_0 \rightarrow S_1$	2.083	1.078	H-1 $\rightarrow$ L
B5	DSD-PBEP86(CORRECT)	$CHCl_3$	$S_0 \rightarrow S_1$	2.465	1.279	H-1 $\rightarrow$ L
B5	DSD-PBEP86(WRONG)	$CHCl_3$	$S_0 \rightarrow S_1$	2.044	1.061	H-1 $\rightarrow$ L
B5	PBE-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.557	1.327	H-1 $\rightarrow$ L
B5	RSX-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.642	1.349	H-1 $\rightarrow$ L
B5	SCS-B2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.555	1.324	H-1 $\rightarrow$ L
B5	SCS-PBE-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.402	1.246	H-1 $\rightarrow$ L
B5	SCS-RSX-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.295	1.172	H-1 $\rightarrow$ L
B5	SOS-B2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.711	1.382	H-1 $\rightarrow$ L
B5	SOS-ωB2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.458	1.247	H-1 $\rightarrow$ L
B5	SCS-ωB2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.346	1.195	H-1 $\rightarrow$ L
B5	SCS-ωB88PP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.417	1.241	H-1 $\rightarrow$ L
B5	SCS-ωPBEPP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.278	1.171	H-1 $\rightarrow$ L
B5	SOS-B2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.504	1.298	H-1 $\rightarrow$ L
B5	SOS-PBE-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.370	1.230	H-1 $\rightarrow$ L
B5	SOS-RSX-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.183	1.114	H-1 $\rightarrow$ L
B5	SOS-ωB2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.369	1.207	H-1 $\rightarrow$ L
B5	SOS-ωB88PP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.364	1.214	H-1 $\rightarrow$ L
B5	SOS-ωPBEPP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.288	1.177	H-1 $\rightarrow$ L
B5	ωB2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.599	1.324	H-1 $\rightarrow$ L
B5	ωB2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.624	1.331	H-1 $\rightarrow$ L
B5	ωB88PP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.543	1.306	H-1 $\rightarrow$ L
B5	ωB97X	$CHCl_3$	$S_0 \rightarrow S_1$	2.715	1.366	H-1 $\rightarrow$ L
B5	ωPBEPP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.521	1.296	H-1 $\rightarrow$ L
B6	B2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.424	1.708	H-1 $\rightarrow$ L
B6	B2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.367	1.659	H-1 $\rightarrow$ L
B6	B3LYP	$CHCl_3$	$S_0 \rightarrow S_3$	2.438	1.164	H-1 $\rightarrow$ L
B6	BHLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.640	1.835	H-1 $\rightarrow$ L
B6	CAM-B3LYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.600	1.756	H-1 $\rightarrow$ L

B6	DSD-BLYP(CORRECT)	$CHCl_3$	$S_0 \rightarrow S_1$	2.416	1.695	H-1 $\rightarrow$ L
B6	DSD-BLYP(WRONG)	$CHCl_3$	$S_0 \rightarrow S_1$	2.042	1.432	H-1 $\rightarrow$ L
B6	DSD-PBEP86(CORRECT)	$CHCl_3$	$S_0 \rightarrow S_1$	2.406	1.691	H-1 $\rightarrow$ L
B6	DSD-PBEP86(WRONG)	$CHCl_3$	$S_0 \rightarrow S_1$	2.005	1.409	H-1 $\rightarrow$ L
B6	PBE-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.494	1.752	H-1 $\rightarrow$ L
B6	RSX-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.585	1.746	H-1 $\rightarrow$ L
B6	SCS-B2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.495	1.758	H-1 $\rightarrow$ L
B6	SCS-PBE-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.339	1.643	H-1 $\rightarrow$ L
B6	SCS-RSX-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.231	1.507	H-1 $\rightarrow$ L
B6	SOS-B2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.663	1.866	H-1 $\rightarrow$ L
B6	SOS-ωB2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.400	1.600	H-1 $\rightarrow$ L
B6	SCS-ωB2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.284	1.542	H-1 $\rightarrow$ L
B6	SCS-ωB88PP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.359	1.613	H-1 $\rightarrow$ L
B6	SCS-ωPBEPP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.213	1.519	H-1 $\rightarrow$ L
B6	SOS-B2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.444	1.722	H-1 $\rightarrow$ L
B6	SOS-PBE-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.307	1.620	H-1 $\rightarrow$ L
B6	SOS-RSX-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.119	1.431	H-1 $\rightarrow$ L
B6	SOS-ωB2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.309	1.558	H-1 $\rightarrow$ L
B6	SOS-ωB88PP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.306	1.576	H-1 $\rightarrow$ L
B6	SOS-ωPBEPP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.227	1.528	H-1 $\rightarrow$ L
B6	ωB2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.543	1.717	H-1 $\rightarrow$ L
B6	ωB2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.569	1.712	H-1 $\rightarrow$ L
B6	ωB88PP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.491	1.703	H-1 $\rightarrow$ L
B6	ωB97X	$CHCl_3$	$S_0 \rightarrow S_1$	2.661	1.727	H-1 $\rightarrow$ L
B6	ωPBEPP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.469	1.695	H-1 $\rightarrow$ L
B7	B2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.421	1.711	H $\rightarrow$ L
B7	B2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.369	1.665	H-1 $\rightarrow$ L
B7	B3LYP	$CHCl_3$	$S_0 \rightarrow S_2$	2.416	1.077	H-1 $\rightarrow$ L
B7	BHLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.639	1.842	H-1 $\rightarrow$ L
B7	CAM-B3LYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.597	1.758	H-1 $\rightarrow$ L
B7	DSD-BLYP(CORRECT)	$CHCl_3$	$S_0 \rightarrow S_1$	2.411	1.699	H $\rightarrow$ L
B7	DSD-BLYP(WRONG)	$CHCl_3$	$S_0 \rightarrow S_1$	2.035	1.434	H $\rightarrow$ L
B7	DSD-PBEP86(CORRECT)	$CHCl_3$	$S_0 \rightarrow S_1$	2.401	1.694	H $\rightarrow$ L
B7	DSD-PBEP86(WRONG)	$CHCl_3$	$S_0 \rightarrow S_1$	1.999	1.410	H $\rightarrow$ L
B7	PBE-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.490	1.755	H $\rightarrow$ L
B7	RSX-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.581	1.755	H $\rightarrow$ L
B7	SCS-B2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.491	1.761	H $\rightarrow$ L
B7	SCS-PBE-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.334	1.645	H $\rightarrow$ L
B7	SCS-RSX-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.225	1.513	H $\rightarrow$ L
B7	SOS-B2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.662	1.871	H-1 $\rightarrow$ L
B7	SOS-ωB2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.394	1.606	H $\rightarrow$ L
B7	SCS-ωB2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.279	1.548	H $\rightarrow$ L
B7	SCS-ωB88PP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.353	1.618	H $\rightarrow$ L
B7	SCS-ωPBEPP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.208	1.524	H $\rightarrow$ L
B7	SOS-B2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.439	1.724	H $\rightarrow$ L
B7	SOS-PBE-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.302	1.623	H $\rightarrow$ L
B7	SOS-RSX-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.113	1.437	H $\rightarrow$ L
B7	SOS-ωB2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.303	1.565	H $\rightarrow$ L
B7	SOS-ωB88PP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.300	1.581	H $\rightarrow$ L
B7	SOS-ωPBEPP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.221	1.533	H $\rightarrow$ L
B7	ωB2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.538	1.725	H $\rightarrow$ L
B7	ωB2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.564	1.720	H $\rightarrow$ L
B7	ωB88PP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.486	1.709	H $\rightarrow$ L
B7	ωB97X	$CHCl_3$	$S_0 \rightarrow S_1$	2.656	1.729	H-1 $\rightarrow$ L
B7	ωPBEPP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.464	1.700	H $\rightarrow$ L
B8	B2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.377	1.663	H-1 $\rightarrow$ L
B8	B2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.276	1.559	H-1 $\rightarrow$ L
B8	B3LYP	$CHCl_3$	$S_0 \rightarrow S_3$	2.405	1.200	H-1 $\rightarrow$ L
B8	BHLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.587	1.727	H-1 $\rightarrow$ L
B8	CAM-B3LYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.558	1.705	H-1 $\rightarrow$ L
B8	DSD-BLYP(CORRECT)	$CHCl_3$	$S_0 \rightarrow S_1$	2.381	1.652	H-1 $\rightarrow$ L
B8	DSD-BLYP(WRONG)	$CHCl_3$	$S_0 \rightarrow S_1$	2.006	1.392	H-1 $\rightarrow$ L

B8	DSD-PBEP86(CORRECT)	$CHCl_3$	$S_0 \rightarrow S_1$	2.370	1.650	H-1 $\rightarrow$ L
B8	DSD-PBEP86(WRONG)	$CHCl_3$	$S_0 \rightarrow S_1$	1.962	1.366	H-1 $\rightarrow$ L
B8	PBE-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.456	1.710	H-1 $\rightarrow$ L
B8	RSX-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.559	1.704	H-1 $\rightarrow$ L
B8	SCS-B2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.453	1.716	H-1 $\rightarrow$ L
B8	SCS-PBE-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.302	1.603	H-1 $\rightarrow$ L
B8	SCS-RSX-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.208	1.470	H-1 $\rightarrow$ L
B8	SOS-B2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.594	1.777	H-1 $\rightarrow$ L
B8	SOS-ωB2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.373	1.568	H-1 $\rightarrow$ L
B8	SCS-ωB2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.258	1.505	H-1 $\rightarrow$ L
B8	SCS-ωB88PP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.333	1.576	H-1 $\rightarrow$ L
B8	SCS-ωPBEPP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.189	1.482	H-1 $\rightarrow$ L
B8	SOS-B2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.401	1.680	H-1 $\rightarrow$ L
B8	SOS-PBE-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.271	1.581	H-1 $\rightarrow$ L
B8	SOS-RSX-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.095	1.395	H-1 $\rightarrow$ L
B8	SOS-ωB2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.282	1.521	H-1 $\rightarrow$ L
B8	SOS-ωB88PP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.280	1.541	H-1 $\rightarrow$ L
B8	SOS-ωPBEPP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.202	1.491	H-1 $\rightarrow$ L
B8	ωB2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.516	1.677	H-1 $\rightarrow$ L
B8	ωB2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.542	1.680	H-1 $\rightarrow$ L
B8	ωB88PP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.465	1.666	H-1 $\rightarrow$ L
B8	ωB97X	$CHCl_3$	$S_0 \rightarrow S_1$	2.635	1.717	H-1 $\rightarrow$ L
B8	ωPBEPP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.443	1.655	H-1 $\rightarrow$ L
B9	B2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.455	1.376	H-1 $\rightarrow$ L
B9	B2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.357	1.280	H-1 $\rightarrow$ L
B9	B3LYP	$CHCl_3$	$S_0 \rightarrow S_2$	2.563	1.124	H-1 $\rightarrow$ L
B9	BHLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.679	1.402	H-1 $\rightarrow$ L
B9	CAM-B3LYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.642	1.415	H-1 $\rightarrow$ L
B9	DSD-BLYP(CORRECT)	$CHCl_3$	$S_0 \rightarrow S_1$	2.446	1.364	H-1 $\rightarrow$ L
B9	DSD-BLYP(WRONG)	$CHCl_3$	$S_0 \rightarrow S_1$	2.040	1.137	H-1 $\rightarrow$ L
B9	DSD-PBEP86(CORRECT)	$CHCl_3$	$S_0 \rightarrow S_1$	2.437	1.363	H-1 $\rightarrow$ L
B9	DSD-PBEP86(WRONG)	$CHCl_3$	$S_0 \rightarrow S_1$	1.998	1.117	H-1 $\rightarrow$ L
B9	PBE-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.531	1.416	H-1 $\rightarrow$ L
B9	RSX-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.622	1.415	H-1 $\rightarrow$ L
B9	SCS-B2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.533	1.420	H-1 $\rightarrow$ L
B9	SCS-PBE-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.375	1.328	H-1 $\rightarrow$ L
B9	SCS-RSX-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.262	1.220	H-1 $\rightarrow$ L
B9	SOS-B2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.682	1.457	H-1 $\rightarrow$ L
B9	SOS-ωB2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.435	1.302	H-1 $\rightarrow$ L
B9	SCS-ωB2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.318	1.250	H-1 $\rightarrow$ L
B9	SCS-ωB88PP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.391	1.304	H-1 $\rightarrow$ L
B9	SCS-ωPBEPP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.245	1.228	H-1 $\rightarrow$ L
B9	SOS-B2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.481	1.391	H-1 $\rightarrow$ L
B9	SOS-PBE-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.345	1.311	H-1 $\rightarrow$ L
B9	SOS-RSX-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.153	1.162	H-1 $\rightarrow$ L
B9	SOS-ωB2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.343	1.264	H-1 $\rightarrow$ L
B9	SOS-ωB88PP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.338	1.275	H-1 $\rightarrow$ L
B9	SOS-ωPBEPP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.260	1.236	H-1 $\rightarrow$ L
B9	ωB2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.578	1.390	H-1 $\rightarrow$ L
B9	ωB2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.604	1.392	H-1 $\rightarrow$ L
B9	ωB88PP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.519	1.374	H-1 $\rightarrow$ L
B9	ωB97X	$CHCl_3$	$S_0 \rightarrow S_1$	2.701	1.421	H-1 $\rightarrow$ L
B9	ωPBEPP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.496	1.365	H-1 $\rightarrow$ L
B10	B2GP-PLYP	THF	$S_0 \rightarrow S_1$	3.678	0.392	H $\rightarrow$ L
B10	B2PLYP	THF	$S_0 \rightarrow S_1$	3.558	0.356	H $\rightarrow$ L
B10	B3LYP	THF	$S_0 \rightarrow S_1$	3.418	0.221	H $\rightarrow$ L
B10	BHLYP	THF	$S_0 \rightarrow S_1$	3.877	0.379	H $\rightarrow$ L
B10	CAM-B3LYP	THF	$S_0 \rightarrow S_1$	3.844	0.360	H $\rightarrow$ L
B10	DSD-BLYP(CORRECT)	THF	$S_0 \rightarrow S_1$	3.726	0.410	H $\rightarrow$ L
B10	DSD-BLYP(WRONG)	THF	$S_0 \rightarrow S_1$	3.305	0.364	H $\rightarrow$ L
B10	DSD-PBEP86(CORRECT)	THF	$S_0 \rightarrow S_1$	3.706	0.404	H $\rightarrow$ L
B10	DSD-PBEP86(WRONG)	THF	$S_0 \rightarrow S_1$	3.229	0.352	H $\rightarrow$ L

B10	PBE-QIDH	THF	$S_0 \rightarrow S_1$	3.790	0.408	H $\rightarrow$ L
B10	RSX-QIDH	THF	$S_0 \rightarrow S_1$	4.024	0.440	H $\rightarrow$ L
B10	SCS-B2GP-PLYP	THF	$S_0 \rightarrow S_1$	3.757	0.400	H $\rightarrow$ L
B10	SCS-PBE-QIDH	THF	$S_0 \rightarrow S_1$	3.644	0.392	H $\rightarrow$ L
B10	SCS-RSX-QIDH	THF	$S_0 \rightarrow S_1$	3.717	0.406	H $\rightarrow$ L
B10	SOS-B2PLYP	THF	$S_0 \rightarrow S_1$	3.850	0.385	H $\rightarrow$ L
B10	SOS-ωB2PLYP	THF	$S_0 \rightarrow S_1$	3.839	0.409	H $\rightarrow$ L
B10	SCS-ωB2GP-PLYP	THF	$S_0 \rightarrow S_1$	3.741	0.407	H $\rightarrow$ L
B10	SCS-ωB88PP86	THF	$S_0 \rightarrow S_1$	3.756	0.408	H $\rightarrow$ L
B10	SCS-ωPBEPP86	THF	$S_0 \rightarrow S_1$	3.635	0.398	H $\rightarrow$ L
B10	SOS-B2GP-PLYP	THF	$S_0 \rightarrow S_1$	3.709	0.395	H $\rightarrow$ L
B10	SOS-PBE-QIDH	THF	$S_0 \rightarrow S_1$	3.614	0.389	H $\rightarrow$ L
B10	SOS-RSX-QIDH	THF	$S_0 \rightarrow S_1$	3.604	0.394	H $\rightarrow$ L
B10	SOS-ωB2GP-PLYP	THF	$S_0 \rightarrow S_1$	3.758	0.409	H $\rightarrow$ L
B10	SOS-ωB88PP86	THF	$S_0 \rightarrow S_1$	3.703	0.402	H $\rightarrow$ L
B10	SOS-ωPBEPP86	THF	$S_0 \rightarrow S_1$	3.635	0.398	H $\rightarrow$ L
B10	ωB2GP-PLYP	THF	$S_0 \rightarrow S_1$	3.961	0.431	H $\rightarrow$ L
B10	ωB2PLYP	THF	$S_0 \rightarrow S_1$	3.985	0.425	H $\rightarrow$ L
B10	ωB88PP86	THF	$S_0 \rightarrow S_1$	3.854	0.419	H $\rightarrow$ L
B10	ωB97X	THF	$S_0 \rightarrow S_1$	4.042	0.407	H $\rightarrow$ L
B10	ωPBEPP86	THF	$S_0 \rightarrow S_1$	3.834	0.420	H $\rightarrow$ L
B11	B2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.756	0.678	H $\rightarrow$ L
B11	B2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.781	0.655	H $\rightarrow$ L
B11	B3LYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.934	0.567	H $\rightarrow$ L
B11	BHLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.958	0.686	H $\rightarrow$ L
B11	CAM-B3LYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.900	0.649	H $\rightarrow$ L
B11	DSD-BLYP(CORRECT)	$CHCl_3$	$S_0 \rightarrow S_1$	2.720	0.691	H $\rightarrow$ L
B11	DSD-BLYP(WRONG)	$CHCl_3$	$S_0 \rightarrow S_1$	2.458	0.625	H $\rightarrow$ L
B11	DSD-PBEP86(CORRECT)	$CHCl_3$	$S_0 \rightarrow S_1$	2.703	0.681	H $\rightarrow$ L
B11	DSD-PBEP86(WRONG)	$CHCl_3$	$S_0 \rightarrow S_1$	2.452	0.618	H $\rightarrow$ L
B11	PBE-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.791	0.694	H $\rightarrow$ L
B11	RSX-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.774	0.713	H $\rightarrow$ L
B11	SCS-B2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.763	0.680	H $\rightarrow$ L
B11	SCS-PBE-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.630	0.654	H $\rightarrow$ L
B11	SCS-RSX-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.527	0.650	H $\rightarrow$ L
B11	SOS-B2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.976	0.701	H $\rightarrow$ L
B11	SOS-ωB2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.587	0.650	H $\rightarrow$ L
B11	SCS-ωB2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.506	0.640	H $\rightarrow$ L
B11	SCS-ωB88PP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.594	0.655	H $\rightarrow$ L
B11	SCS-ωPBEPP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.505	0.636	H $\rightarrow$ L
B11	SOS-B2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.721	0.669	H $\rightarrow$ L
B11	SOS-PBE-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.587	0.643	H $\rightarrow$ L
B11	SOS-RSX-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.330	0.599	H $\rightarrow$ L
B11	SOS-ωB2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.501	0.639	H $\rightarrow$ L
B11	SOS-ωB88PP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.528	0.638	H $\rightarrow$ L
B11	SOS-ωPBEPP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.456	0.624	H $\rightarrow$ L
B11	ωB2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.743	0.701	H $\rightarrow$ L
B11	ωB2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.763	0.694	H $\rightarrow$ L
B11	ωB88PP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.735	0.690	H $\rightarrow$ L
B11	ωB97X	$CHCl_3$	$S_0 \rightarrow S_1$	2.859	0.678	H $\rightarrow$ L
B11	ωPBEPP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.7190	0.691	H $\rightarrow$ L
B11	B2GP-PLYP	THF	$S_0 \rightarrow S_1$	2.773	0.666	H $\rightarrow$ L
B11	B2PLYP	THF	$S_0 \rightarrow S_1$	2.797	0.643	H $\rightarrow$ L
B11	B3LYP	THF	$S_0 \rightarrow S_1$	2.947	0.552	H $\rightarrow$ L
B11	BHLYP	THF	$S_0 \rightarrow S_1$	2.975	0.674	H $\rightarrow$ L
B11	CAM-B3LYP	THF	$S_0 \rightarrow S_1$	2.916	0.636	H $\rightarrow$ L
B11	DSD-BLYP(CORRECT)	THF	$S_0 \rightarrow S_1$	2.738	0.680	H $\rightarrow$ L
B11	DSD-BLYP(WRONG)	THF	$S_0 \rightarrow S_1$	2.474	0.614	H $\rightarrow$ L
B11	DSD-PBEP86(CORRECT)	THF	$S_0 \rightarrow S_1$	2.720	0.669	H $\rightarrow$ L
B11	DSD-PBEP86(WRONG)	THF	$S_0 \rightarrow S_1$	2.467	0.607	H $\rightarrow$ L
B11	PBE-QIDH	THF	$S_0 \rightarrow S_1$	2.809	0.682	H $\rightarrow$ L
B11	RSX-QIDH	THF	$S_0 \rightarrow S_1$	2.793	0.701	H $\rightarrow$ L

B11	SCS-B2GP-PLYP	THF	$S_0 \rightarrow S_1$	2.781	0.668	H $\rightarrow$ L
B11	SCS-PBE-QIDH	THF	$S_0 \rightarrow S_1$	2.649	0.643	H $\rightarrow$ L
B11	SCS-RSX-QIDH	THF	$S_0 \rightarrow S_1$	2.547	0.639	H $\rightarrow$ L
B11	SOS-B2PLYP	THF	$S_0 \rightarrow S_1$	2.992	0.688	H $\rightarrow$ L
B11	SOS-ωB2PLYP	THF	$S_0 \rightarrow S_1$	2.607	0.639	H $\rightarrow$ L
B11	SCS-ωB2GP-PLYP	THF	$S_0 \rightarrow S_1$	2.506	0.640	H $\rightarrow$ L
B11	SCS-ωB88PP86	THF	$S_0 \rightarrow S_1$	2.613	0.644	H $\rightarrow$ L
B11	SCS-ωPBEPP86	THF	$S_0 \rightarrow S_1$	2.525	0.626	H $\rightarrow$ L
B11	SOS-B2GP-PLYP	THF	$S_0 \rightarrow S_1$	2.738	0.658	H $\rightarrow$ L
B11	SOS-PBE-QIDH	THF	$S_0 \rightarrow S_1$	2.605	0.632	H $\rightarrow$ L
B11	SOS-RSX-QIDH	THF	$S_0 \rightarrow S_1$	2.351	0.590	H $\rightarrow$ L
B11	SOS-ωB2GP-PLYP	THF	$S_0 \rightarrow S_1$	2.521	0.629	H $\rightarrow$ L
B11	SOS-ωB88PP86	THF	$S_0 \rightarrow S_1$	2.547	0.628	H $\rightarrow$ L
B11	SOS-ωPBEPP86	THF	$S_0 \rightarrow S_1$	2.476	0.614	H $\rightarrow$ L
B11	ωB2GP-PLYP	THF	$S_0 \rightarrow S_1$	2.762	0.689	H $\rightarrow$ L
B11	ωB2PLYP	THF	$S_0 \rightarrow S_1$	2.782	0.682	H $\rightarrow$ L
B11	ωB88PP86	THF	$S_0 \rightarrow S_1$	2.753	0.678	H $\rightarrow$ L
B11	ωB97X	THF	$S_0 \rightarrow S_1$	2.877	0.666	H $\rightarrow$ L
B11	ωPBEPP86	THF	$S_0 \rightarrow S_1$	2.738	0.679	H $\rightarrow$ L
B12	B2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.405	1.900	H-1 $\rightarrow$ L
B12	B2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.327	1.838	H-1 $\rightarrow$ L
B12	B3LYP	$CHCl_3$	$S_0 \rightarrow S_3$	2.416	1.348	H-1 $\rightarrow$ L
B12	BHLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.609	2.036	H-1 $\rightarrow$ L
B12	CAM-B3LYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.577	1.950	H-1 $\rightarrow$ L
B12	DSD-BLYP(CORRECT)	$CHCl_3$	$S_0 \rightarrow S_1$	2.404	1.872	H-1 $\rightarrow$ L
B12	DSD-BLYP(WRONG)	$CHCl_3$	$S_0 \rightarrow S_1$	2.048	1.595	H-1 $\rightarrow$ L
B12	DSD-PBEP86(CORRECT)	$CHCl_3$	$S_0 \rightarrow S_1$	2.393	1.871	H-1 $\rightarrow$ L
B12	DSD-PBEP86(WRONG)	$CHCl_3$	$S_0 \rightarrow S_1$	2.009	1.571	H-1 $\rightarrow$ L
B12	PBE-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.477	1.938	H-1 $\rightarrow$ L
B12	RSX-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.567	1.889	H-1 $\rightarrow$ L
B12	SCS-B2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.477	1.957	H-1 $\rightarrow$ L
B12	SCS-PBE-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.324	1.818	H-1 $\rightarrow$ L
B12	SCS-RSX-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.218	1.632	H-1 $\rightarrow$ L
B12	SOS-B2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.632	2.080	H-1 $\rightarrow$ L
B12	SOS-ωB2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.381	1.736	H-1 $\rightarrow$ L
B12	SCS-ωB2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.267	1.673	H-1 $\rightarrow$ L
B12	SCS-ωB88PP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.345	1.759	H-1 $\rightarrow$ L
B12	SCS-ωPBEPP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.202	1.656	H-1 $\rightarrow$ L
B12	SOS-B2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.425	1.916	H-1 $\rightarrow$ L
B12	SOS-PBE-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.292	1.793	H-1 $\rightarrow$ L
B12	SOS-RSX-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.104	1.548	H-1 $\rightarrow$ L
B12	SOS-ωB2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.291	1.691	H-1 $\rightarrow$ L
B12	SOS-ωB88PP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.292	1.719	H-1 $\rightarrow$ L
B12	SOS-ωPBEPP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.215	1.666	H-1 $\rightarrow$ L
B12	ωB2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.526	1.864	H-1 $\rightarrow$ L
B12	ωB2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.550	1.859	H-1 $\rightarrow$ L
B12	ωB88PP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.480	1.860	H-1 $\rightarrow$ L
B12	ωB97X	$CHCl_3$	$S_0 \rightarrow S_1$	2.644	1.889	H-1 $\rightarrow$ L
B12	ωPBEPP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.460	1.850	H-1 $\rightarrow$ L
B13	B2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	1.782	1.208	H $\rightarrow$ L
B13	B2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	1.705	1.154	H $\rightarrow$ L
B13	B3LYP	$CHCl_3$	$S_0 \rightarrow S_1$	1.589	1.012	H $\rightarrow$ L
B13	BHLYP	$CHCl_3$	$S_0 \rightarrow S_1$	1.900	1.285	H $\rightarrow$ L
B13	CAM-B3LYP	$CHCl_3$	$S_0 \rightarrow S_1$	1.897	1.241	H $\rightarrow$ L
B13	DSD-BLYP(CORRECT)	$CHCl_3$	$S_0 \rightarrow S_1$	1.800	1.223	H $\rightarrow$ L
B13	DSD-BLYP(WRONG)	$CHCl_3$	$S_0 \rightarrow S_1$	1.587	1.078	H $\rightarrow$ L
B13	DSD-PBEP86(CORRECT)	$CHCl_3$	$S_0 \rightarrow S_1$	1.800	1.223	H $\rightarrow$ L
B13	DSD-PBEP86(WRONG)	$CHCl_3$	$S_0 \rightarrow S_1$	1.542	1.048	H $\rightarrow$ L
B13	PBE-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	1.837	1.246	H $\rightarrow$ L
B13	RSX-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	1.937	1.291	H $\rightarrow$ L
B13	SCS-B2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	1.893	1.283	H $\rightarrow$ L
B13	SCS-PBE-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	1.730	1.174	H $\rightarrow$ L

B13	SCS-RSX-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	1.579	1.052	H $\rightarrow$ L
B13	SOS-B2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.023	1.369	H $\rightarrow$ L
B13	SOS-ωB2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	1.793	1.176	H $\rightarrow$ L
B13	SCS-ωB2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	1.678	1.114	H $\rightarrow$ L
B13	SCS-ωB88PP86	$CHCl_3$	$S_0 \rightarrow S_1$	1.753	1.167	H $\rightarrow$ L
B13	SCS-ωPBEPP86	$CHCl_3$	$S_0 \rightarrow S_1$	1.584	1.061	H $\rightarrow$ L
B13	SOS-B2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	1.842	1.249	H $\rightarrow$ L
B13	SOS-PBE-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	1.711	1.161	H $\rightarrow$ L
B13	SOS-RSX-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	1.528	1.018	H $\rightarrow$ L
B13	SOS-ωB2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	1.718	1.140	H $\rightarrow$ L
B13	SOS-ωB88PP86	$CHCl_3$	$S_0 \rightarrow S_1$	1.709	1.138	H $\rightarrow$ L
B13	SOS-ωPBEPP86	$CHCl_3$	$S_0 \rightarrow S_1$	1.634	1.094	H $\rightarrow$ L
B13	ωB2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	1.911	1.269	H $\rightarrow$ L
B13	ωB2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	1.928	1.264	H $\rightarrow$ L
B13	ωB88PP86	$CHCl_3$	$S_0 \rightarrow S_1$	1.870	1.245	H $\rightarrow$ L
B13	ωB97X	$CHCl_3$	$S_0 \rightarrow S_1$	1.996	1.266	H $\rightarrow$ L
B13	ωPBEPP86	$CHCl_3$	$S_0 \rightarrow S_1$	1.857	1.243	H $\rightarrow$ L
B14	B2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.729	0.811	H $\rightarrow$ L
B14	B2PLYP	MeOH	$S_0 \rightarrow S_1$	2.713	0.791	H $\rightarrow$ L
B14	B3LYP	MeOH	$S_0 \rightarrow S_1$	2.776	0.736	H $\rightarrow$ L
B14	BHLYP	MeOH	$S_0 \rightarrow S_1$	2.965	0.858	H $\rightarrow$ L
B14	CAM-B3LYP	MeOH	$S_0 \rightarrow S_1$	2.884	0.820	H $\rightarrow$ L
B14	DSD-BLYP(CORRECT)	MeOH	$S_0 \rightarrow S_1$	2.695	0.812	H $\rightarrow$ L
B14	DSD-BLYP(WRONG)	MeOH	$S_0 \rightarrow S_1$	2.307	0.695	H $\rightarrow$ L
B14	DSD-PBEP86(CORRECT)	MeOH	$S_0 \rightarrow S_1$	2.700	0.811	H $\rightarrow$ L
B14	DSD-PBEP86(WRONG)	MeOH	$S_0 \rightarrow S_1$	2.276	0.684	H $\rightarrow$ L
B14	PBE-QIDH	MeOH	$S_0 \rightarrow S_1$	2.790	0.834	H $\rightarrow$ L
B14	RSX-QIDH	MeOH	$S_0 \rightarrow S_1$	2.851	0.863	H $\rightarrow$ L
B14	SCS-B2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.809	0.835	H $\rightarrow$ L
B14	SCS-PBE-QIDH	MeOH	$S_0 \rightarrow S_1$	2.658	0.795	H $\rightarrow$ L
B14	SCS-RSX-QIDH	MeOH	$S_0 \rightarrow S_1$	2.531	0.766	H $\rightarrow$ L
B14	SOS-B2PLYP	MeOH	$S_0 \rightarrow S_1$	2.983	0.870	H $\rightarrow$ L
B14	SOS-ωB2PLYP	MeOH	$S_0 \rightarrow S_1$	2.688	0.804	H $\rightarrow$ L
B14	SCS-ωB2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.587	0.780	H $\rightarrow$ L
B14	SCS-ωB88PP86	MeOH	$S_0 \rightarrow S_1$	2.651	0.797	H $\rightarrow$ L
B14	SCS-ωPBEPP86	MeOH	$S_0 \rightarrow S_1$	2.521	0.761	H $\rightarrow$ L
B14	SOS-B2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.762	0.821	H $\rightarrow$ L
B14	SOS-PBE-QIDH	MeOH	$S_0 \rightarrow S_1$	2.631	0.787	H $\rightarrow$ L
B14	SOS-RSX-QIDH	MeOH	$S_0 \rightarrow S_1$	2.434	0.737	H $\rightarrow$ L
B14	SOS-ωB2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.609	0.786	H $\rightarrow$ L
B14	SOS-ωB88PP86	MeOH	$S_0 \rightarrow S_1$	2.601	0.782	H $\rightarrow$ L
B14	SOS-ωPBEPP86	MeOH	$S_0 \rightarrow S_1$	2.531	0.763	H $\rightarrow$ L
B14	ωB2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.806	0.846	H $\rightarrow$ L
B14	ωB2PLYP	MeOH	$S_0 \rightarrow S_1$	2.829	0.846	H $\rightarrow$ L
B14	ωB88PP86	MeOH	$S_0 \rightarrow S_1$	2.747	0.826	H $\rightarrow$ L
B14	ωB97X	MeOH	$S_0 \rightarrow S_1$	2.913	0.846	H $\rightarrow$ L
B14	ωPBEPP86	MeOH	$S_0 \rightarrow S_1$	2.725	0.822	H $\rightarrow$ L
B15	B2GP-PLYP	DCM	$S_0 \rightarrow S_1$	1.967	1.392	H $\rightarrow$ L
B15	B2PLYP	DCM	$S_0 \rightarrow S_1$	1.858	1.374	H $\rightarrow$ L
B15	B3LYP	DCM	$S_0 \rightarrow S_1$	1.674	1.152	H $\rightarrow$ L
B15	BHLYP	DCM	$S_0 \rightarrow S_1$	2.119	1.580	H $\rightarrow$ L
B15	CAM-B3LYP	DCM	$S_0 \rightarrow S_1$	2.111	1.517	H $\rightarrow$ L
B15	DSD-BLYP(CORRECT)	DCM	$S_0 \rightarrow S_1$	1.990	1.363	H $\rightarrow$ L
B15	DSD-BLYP(WRONG)	DCM	$S_0 \rightarrow S_1$	1.721	1.179	H $\rightarrow$ L
B15	DSD-PBEP86(CORRECT)	DCM	$S_0 \rightarrow S_1$	1.988	1.375	H $\rightarrow$ L
B15	DSD-PBEP86(WRONG)	DCM	$S_0 \rightarrow S_1$	1.669	1.155	H $\rightarrow$ L
B15	PBE-QIDH	DCM	$S_0 \rightarrow S_1$	2.037	1.419	H $\rightarrow$ L
B15	RSX-QIDH	DCM	$S_0 \rightarrow S_1$	2.149	1.388	H $\rightarrow$ L
B15	SCS-B2GP-PLYP	DCM	$S_0 \rightarrow S_1$	2.076	1.468	H $\rightarrow$ L
B15	SCS-PBE-QIDH	DCM	$S_0 \rightarrow S_1$	1.924	1.341	H $\rightarrow$ L
B15	SCS-RSX-QIDH	DCM	$S_0 \rightarrow S_1$	1.809	1.168	H $\rightarrow$ L
B15	SOS-B2PLYP	DCM	$S_0 \rightarrow S_1$	2.189	1.618	H $\rightarrow$ L

B15	SOS-ωB2PLYP	DCM	$S_0 \rightarrow S_1$	2.001	1.286	H $\rightarrow$ L
B15	SCS-ωB2GP-PLYP	DCM	$S_0 \rightarrow S_1$	1.891	1.224	H $\rightarrow$ L
B15	SCS-ωB88PP86	DCM	$S_0 \rightarrow S_1$	1.962	1.292	H $\rightarrow$ L
B15	SCS-ωPBEPP86	DCM	$S_0 \rightarrow S_1$	1.807	1.192	H $\rightarrow$ L
B15	SOS-B2GP-PLYP	DCM	$S_0 \rightarrow S_1$	2.027	1.433	H $\rightarrow$ L
B15	SOS-PBE-QIDH	DCM	$S_0 \rightarrow S_1$	1.904	1.327	H $\rightarrow$ L
B15	SOS-RSX-QIDH	DCM	$S_0 \rightarrow S_1$	1.741	1.124	H $\rightarrow$ L
B15	SOS-ωB2GP-PLYP	DCM	$S_0 \rightarrow S_1$	1.925	1.246	H $\rightarrow$ L
B15	SOS-ωB88PP86	DCM	$S_0 \rightarrow S_1$	1.917	1.262	H $\rightarrow$ L
B15	SOS-ωPBEPP86	DCM	$S_0 \rightarrow S_1$	1.843	1.216	H $\rightarrow$ L
B15	ωB2GP-PLYP	DCM	$S_0 \rightarrow S_1$	2.119	1.372	H $\rightarrow$ L
B15	ωB2PLYP	DCM	$S_0 \rightarrow S_1$	2.138	1.374	H $\rightarrow$ L
B15	ωB88PP86	DCM	$S_0 \rightarrow S_1$	2.073	1.365	H $\rightarrow$ L
B15	ωB97X	DCM	$S_0 \rightarrow S_1$	2.213	1.413	H $\rightarrow$ L
B15	ωPBEPP86	DCM	$S_0 \rightarrow S_1$	2.057	1.358	H $\rightarrow$ L
B16	B2GP-PLYP	DCM	$S_0 \rightarrow S_1$	2.002	1.192	H $\rightarrow$ L
B16	B2PLYP	DCM	$S_0 \rightarrow S_1$	1.961	1.161	H $\rightarrow$ L
B16	B3LYP	DCM	$S_0 \rightarrow S_1$	1.881	1.041	H $\rightarrow$ L
B16	BHLYP	DCM	$S_0 \rightarrow S_1$	2.101	1.242	H $\rightarrow$ L
B16	CAM-B3LYP	DCM	$S_0 \rightarrow S_1$	2.092	1.192	H $\rightarrow$ L
B16	DSD-BLYP(CORRECT)	DCM	$S_0 \rightarrow S_1$	2.001	1.200	H $\rightarrow$ L
B16	DSD-BLYP(WRONG)	DCM	$S_0 \rightarrow S_1$	1.824	1.094	H $\rightarrow$ L
B16	DSD-PBEP86(CORRECT)	DCM	$S_0 \rightarrow S_1$	2.008	1.202	H $\rightarrow$ L
B16	DSD-PBEP86(WRONG)	DCM	$S_0 \rightarrow S_1$	1.800	1.078	H $\rightarrow$ L
B16	PBE-QIDH	DCM	$S_0 \rightarrow S_1$	2.043	1.219	H $\rightarrow$ L
B16	RSX-QIDH	DCM	$S_0 \rightarrow S_1$	2.101	1.242	H $\rightarrow$ L
B16	SCS-B2GP-PLYP	DCM	$S_0 \rightarrow S_1$	2.097	1.249	H $\rightarrow$ L
B16	SCS-PBE-QIDH	DCM	$S_0 \rightarrow S_1$	1.939	1.157	H $\rightarrow$ L
B16	SCS-RSX-QIDH	DCM	$S_0 \rightarrow S_1$	1.757	1.038	H $\rightarrow$ L
B16	SOS-B2PLYP	DCM	$S_0 \rightarrow S_1$	2.247	1.331	H $\rightarrow$ L
B16	SOS-ωB2PLYP	DCM	$S_0 \rightarrow S_1$	1.960	1.138	H $\rightarrow$ L
B16	SCS-ωB2GP-PLYP	DCM	$S_0 \rightarrow S_1$	1.850	1.089	H $\rightarrow$ L
B16	SCS-ωB88PP86	DCM	$S_0 \rightarrow S_1$	1.930	1.137	H $\rightarrow$ L
B16	SCS-ωPBEPP86	DCM	$S_0 \rightarrow S_1$	1.769	1.048	H $\rightarrow$ L
B16	SOS-B2GP-PLYP	DCM	$S_0 \rightarrow S_1$	2.049	1.221	H $\rightarrow$ L
B16	SOS-PBE-QIDH	DCM	$S_0 \rightarrow S_1$	1.919	1.145	H $\rightarrow$ L
B16	SOS-RSX-QIDH	DCM	$S_0 \rightarrow S_1$	1.704	1.007	H $\rightarrow$ L
B16	SOS-ωB2GP-PLYP	DCM	$S_0 \rightarrow S_1$	1.887	1.111	H $\rightarrow$ L
B16	SOS-ωB88PP86	DCM	$S_0 \rightarrow S_1$	1.887	1.112	H $\rightarrow$ L
B16	SOS-ωPBEPP86	DCM	$S_0 \rightarrow S_1$	1.814	1.075	H $\rightarrow$ L
B16	ωB2GP-PLYP	DCM	$S_0 \rightarrow S_1$	2.077	1.223	H $\rightarrow$ L
B16	ωB2PLYP	DCM	$S_0 \rightarrow S_1$	2.092	1.215	H $\rightarrow$ L
B16	ωB88PP86	DCM	$S_0 \rightarrow S_1$	2.048	1.206	H $\rightarrow$ L
B16	ωB97X	DCM	$S_0 \rightarrow S_1$	2.152	1.200	H $\rightarrow$ L
B16	ωPBEPP86	DCM	$S_0 \rightarrow S_1$	2.037	1.207	H $\rightarrow$ L
B17	B2GP-PLYP	THF	$S_0 \rightarrow S_1$	3.458	0.506	H $\rightarrow$ L
B17	B2PLYP	THF	$S_0 \rightarrow S_1$	3.421	0.503	H $\rightarrow$ L
B17	B3LYP	THF	$S_0 \rightarrow S_1$	3.492	0.461	H $\rightarrow$ L
B17	BHLYP	THF	$S_0 \rightarrow S_1$	3.793	0.557	H $\rightarrow$ L
B17	CAM-B3LYP	THF	$S_0 \rightarrow S_1$	3.683	0.545	H $\rightarrow$ L
B17	DSD-BLYP(CORRECT)	THF	$S_0 \rightarrow S_1$	3.425	0.493	H $\rightarrow$ L
B17	DSD-BLYP(WRONG)	THF	$S_0 \rightarrow S_1$	2.824	0.407	H $\rightarrow$ L
B17	DSD-PBEP86(CORRECT)	THF	$S_0 \rightarrow S_1$	3.420	0.497	H $\rightarrow$ L
B17	DSD-PBEP86(WRONG)	THF	$S_0 \rightarrow S_1$	2.779	0.404	H $\rightarrow$ L
B17	PBE-QIDH	THF	$S_0 \rightarrow S_1$	3.563	0.522	H $\rightarrow$ L
B17	RSX-QIDH	THF	$S_0 \rightarrow S_1$	3.692	0.535	H $\rightarrow$ L
B17	SCS-B2GP-PLYP	THF	$S_0 \rightarrow S_1$	3.526	0.515	H $\rightarrow$ L
B17	SCS-PBE-QIDH	THF	$S_0 \rightarrow S_1$	3.378	0.495	H $\rightarrow$ L
B17	SCS-RSX-QIDH	THF	$S_0 \rightarrow S_1$	3.326	0.482	H $\rightarrow$ L
B17	SOS-B2PLYP	THF	$S_0 \rightarrow S_1$	3.711	0.545	H $\rightarrow$ L
B17	SOS-ωB2PLYP	THF	$S_0 \rightarrow S_1$	3.461	0.507	H $\rightarrow$ L
B17	SCS-ωB2GP-PLYP	THF	$S_0 \rightarrow S_1$	3.348	0.484	H $\rightarrow$ L

B17	SCS-ωB88PP86	THF	$S_0 \rightarrow S_1$	3.407	0.498	H $\rightarrow$ L
B17	SCS-ωPBEPP86	THF	$S_0 \rightarrow S_1$	3.278	0.478	H $\rightarrow$ L
B17	SOS-B2GP-PLYP	THF	$S_0 \rightarrow S_1$	3.473	0.508	H $\rightarrow$ L
B17	SOS-PBE-QIDH	THF	$S_0 \rightarrow S_1$	3.341	0.490	H $\rightarrow$ L
B17	SOS-RSX-QIDH	THF	$S_0 \rightarrow S_1$	3.180	0.461	H $\rightarrow$ L
B17	SOS-ωB2GP-PLYP	THF	$S_0 \rightarrow S_1$	3.363	0.486	H $\rightarrow$ L
B17	SOS-ωB88PP86	THF	$S_0 \rightarrow S_1$	3.346	0.489	H $\rightarrow$ L
B17	SOS-ωPBEPP86	THF	$S_0 \rightarrow S_1$	3.268	0.476	H $\rightarrow$ L
B17	ωB2GP-PLYP	THF	$S_0 \rightarrow S_1$	3.613	0.522	H $\rightarrow$ L
B17	ωB2PLYP	THF	$S_0 \rightarrow S_1$	3.646	0.534	H $\rightarrow$ L
B17	ωB88PP86	THF	$S_0 \rightarrow S_1$	3.522	0.515	H $\rightarrow$ L
B17	ωB97X	THF	$S_0 \rightarrow S_1$	3.766	0.565	H $\rightarrow$ L
B17	ωPBEPP86	THF	$S_0 \rightarrow S_1$	3.489	0.508	H $\rightarrow$ L
B18	B2GP-PLYP	DCM	$S_0 \rightarrow S_1$	2.594	0.659	H $\rightarrow$ L
B18	B2PLYP	DCM	$S_0 \rightarrow S_1$	2.620	0.641	H $\rightarrow$ L
B18	B3LYP	DCM	$S_0 \rightarrow S_1$	2.420	0.037	H-1 $\rightarrow$ L
B18	BHLYP	DCM	$S_0 \rightarrow S_1$	2.784	0.673	H $\rightarrow$ L
B18	CAM-B3LYP	DCM	$S_0 \rightarrow S_1$	2.724	0.641	H $\rightarrow$ L
B18	DSD-BLYP(CORRECT)	DCM	$S_0 \rightarrow S_1$	2.549	0.667	H $\rightarrow$ L+1
B18	DSD-BLYP(WRONG)	DCM	$S_0 \rightarrow S_1$	2.287	0.598	H $\rightarrow$ L+1
B18	DSD-PBEP86(CORRECT)	DCM	$S_0 \rightarrow S_1$	2.543	0.660	H $\rightarrow$ L+1
B18	DSD-PBEP86(WRONG)	DCM	$S_0 \rightarrow S_1$	2.285	0.593	H $\rightarrow$ L+1
B18	PBE-QIDH	DCM	$S_0 \rightarrow S_1$	2.623	0.674	H $\rightarrow$ L+1
B18	RSX-QIDH	DCM	$S_0 \rightarrow S_1$	2.600	0.691	H $\rightarrow$ L
B18	SCS-B2GP-PLYP	DCM	$S_0 \rightarrow S_1$	2.626	0.667	H $\rightarrow$ L
B18	SCS-PBE-QIDH	DCM	$S_0 \rightarrow S_1$	2.475	0.636	H $\rightarrow$ L+1
B18	SCS-RSX-QIDH	DCM	$S_0 \rightarrow S_1$	2.304	0.612	H $\rightarrow$ L
B18	SOS-B2PLYP	DCM	$S_0 \rightarrow S_1$	2.837	0.695	H $\rightarrow$ L
B18	SOS-ωB2PLYP	DCM	$S_0 \rightarrow S_1$	2.430	0.631	H $\rightarrow$ L
B18	SCS-ωB2GP-PLYP	DCM	$S_0 \rightarrow S_1$	2.332	0.615	H $\rightarrow$ L
B18	SCS-ωB88PP86	DCM	$S_0 \rightarrow S_1$	2.425	0.632	H $\rightarrow$ L+1
B18	SCS-ωPBEPP86	DCM	$S_0 \rightarrow S_1$	2.306	0.605	H $\rightarrow$ L+1
B18	SOS-B2GP-PLYP	DCM	$S_0 \rightarrow S_1$	2.581	0.656	H $\rightarrow$ L
B18	SOS-PBE-QIDH	DCM	$S_0 \rightarrow S_1$	2.439	0.627	H $\rightarrow$ L+1
B18	SOS-RSX-QIDH	DCM	$S_0 \rightarrow S_1$	2.163	0.575	H $\rightarrow$ L
B18	SOS-ωB2GP-PLYP	DCM	$S_0 \rightarrow S_1$	2.344	0.618	H $\rightarrow$ L
B18	SOS-ωB88PP86	DCM	$S_0 \rightarrow S_1$	2.369	0.618	H $\rightarrow$ L+1
B18	SOS-ωPBEPP86	DCM	$S_0 \rightarrow S_1$	2.295	0.602	H $\rightarrow$ L+1
B18	ωB2GP-PLYP	DCM	$S_0 \rightarrow S_1$	2.573	0.679	H $\rightarrow$ L
B18	ωB2PLYP	DCM	$S_0 \rightarrow S_1$	2.595	0.674	H $\rightarrow$ L
B18	ωB88PP86	DCM	$S_0 \rightarrow S_1$	2.561	0.668	H $\rightarrow$ L+1
B18	ωB97X	DCM	$S_0 \rightarrow S_1$	2.686	0.662	H $\rightarrow$ L
B18	ωPBEPP86	DCM	$S_0 \rightarrow S_1$	2.543	0.668	H $\rightarrow$ L+1
B19	B2GP-PLYP	DCM	$S_0 \rightarrow S_1$	1.614	1.818	H $\rightarrow$ L
B19	B2PLYP	DCM	$S_0 \rightarrow S_1$	1.557	1.762	H $\rightarrow$ L
B19	B3LYP	DCM	$S_0 \rightarrow S_1$	1.552	1.734	H $\rightarrow$ L
B19	BHLYP	DCM	$S_0 \rightarrow S_1$	1.766	2.003	H $\rightarrow$ L
B19	CAM-B3LYP	DCM	$S_0 \rightarrow S_1$	1.756	1.932	H $\rightarrow$ L
B19	DSD-BLYP(CORRECT)	DCM	$S_0 \rightarrow S_1$	1.625	1.825	H $\rightarrow$ L
B19	DSD-BLYP(WRONG)	DCM	$S_0 \rightarrow S_1$	1.393	1.564	H $\rightarrow$ L
B19	DSD-PBEP86(CORRECT)	DCM	$S_0 \rightarrow S_1$	1.615	1.822	H $\rightarrow$ L
B19	DSD-PBEP86(WRONG)	DCM	$S_0 \rightarrow S_1$	1.346	1.518	H $\rightarrow$ L
B19	PBE-QIDH	DCM	$S_0 \rightarrow S_1$	1.660	1.879	H $\rightarrow$ L
B19	RSX-QIDH	DCM	$S_0 \rightarrow S_1$	1.745	1.930	H $\rightarrow$ L
B19	SCS-B2GP-PLYP	DCM	$S_0 \rightarrow S_1$	1.707	1.923	H $\rightarrow$ L
B19	SCS-PBE-QIDH	DCM	$S_0 \rightarrow S_1$	1.527	1.728	H $\rightarrow$ L
B19	SCS-RSX-QIDH	DCM	$S_0 \rightarrow S_1$	1.338	1.480	H $\rightarrow$ L
B19	SOS-B2PLYP	DCM	$S_0 \rightarrow S_1$	1.865	2.111	H $\rightarrow$ L
B19	SOS-ωB2PLYP	DCM	$S_0 \rightarrow S_1$	1.584	1.723	H $\rightarrow$ L
B19	SCS-ωB2GP-PLYP	DCM	$S_0 \rightarrow S_1$	1.451	1.592	H $\rightarrow$ L
B19	SCS-ωB88PP86	DCM	$S_0 \rightarrow S_1$	1.538	1.698	H $\rightarrow$ L
B19	SCS-ωPBEPP86	DCM	$S_0 \rightarrow S_1$	1.349	1.497	H $\rightarrow$ L

B19	SOS-B2GP-PLYP	DCM	$S_0 \rightarrow S_1$	1.652	1.861	H $\rightarrow$ L
B19	SOS-PBE-QIDH	DCM	$S_0 \rightarrow S_1$	1.502	1.700	H $\rightarrow$ L
B19	SOS-RSX-QIDH	DCM	$S_0 \rightarrow S_1$	1.286	1.422	H $\rightarrow$ L
B19	SOS-ωB2GP-PLYP	DCM	$S_0 \rightarrow S_1$	1.498	1.643	H $\rightarrow$ L
B19	SOS-ωB88PP86	DCM	$S_0 \rightarrow S_1$	1.493	1.648	H $\rightarrow$ L
B19	SOS-ωPBEPP86	DCM	$S_0 \rightarrow S_1$	1.408	1.563	H $\rightarrow$ L
B19	ωB2GP-PLYP	DCM	$S_0 \rightarrow S_1$	1.724	1.892	H $\rightarrow$ L
B19	ωB2PLYP	DCM	$S_0 \rightarrow S_1$	1.743	1.896	H $\rightarrow$ L
B19	ωB88PP86	DCM	$S_0 \rightarrow S_1$	1.685	1.860	H $\rightarrow$ L
B19	ωB97X	DCM	$S_0 \rightarrow S_1$	1.829	1.936	H $\rightarrow$ L
B19	ωPBEPP86	DCM	$S_0 \rightarrow S_1$	1.669	1.852	H $\rightarrow$ L
B20	B2GP-PLYP	THF	$S_0 \rightarrow S_1$	2.058	1.664	H $\rightarrow$ L
B20	B2PLYP	THF	$S_0 \rightarrow S_1$	2.045	1.662	H $\rightarrow$ L
B20	B3LYP	THF	$S_0 \rightarrow S_1$	2.008	1.666	H $\rightarrow$ L
B20	BHLYP	THF	$S_0 \rightarrow S_1$	2.183	1.776	H $\rightarrow$ L
B20	CAM-B3LYP	THF	$S_0 \rightarrow S_1$	2.148	1.676	H $\rightarrow$ L
B20	DSD-BLYP(CORRECT)	THF	$S_0 \rightarrow S_1$	2.037	1.651	H $\rightarrow$ L
B20	DSD-BLYP(WRONG)	THF	$S_0 \rightarrow S_1$	1.835	1.487	H $\rightarrow$ L
B20	DSD-PBEP86(CORRECT)	THF	$S_0 \rightarrow S_1$	2.045	1.654	H $\rightarrow$ L
B20	DSD-PBEP86(WRONG)	THF	$S_0 \rightarrow S_1$	1.823	1.475	H $\rightarrow$ L
B20	PBE-QIDH	THF	$S_0 \rightarrow S_1$	2.096	1.692	H $\rightarrow$ L
B20	RSX-QIDH	THF	$S_0 \rightarrow S_1$	2.118	1.685	H $\rightarrow$ L
B20	SCS-B2GP-PLYP	THF	$S_0 \rightarrow S_1$	2.142	1.733	H $\rightarrow$ L
B20	SCS-PBE-QIDH	THF	$S_0 \rightarrow S_1$	1.977	1.595	H $\rightarrow$ L
B20	SCS-RSX-QIDH	THF	$S_0 \rightarrow S_1$	1.743	1.386	H $\rightarrow$ L
B20	SOS-B2PLYP	THF	$S_0 \rightarrow S_1$	2.322	1.887	H $\rightarrow$ L
B20	SOS-ωB2PLYP	THF	$S_0 \rightarrow S_1$	1.961	1.537	H $\rightarrow$ L
B20	SCS-ωB2GP-PLYP	THF	$S_0 \rightarrow S_1$	1.842	1.461	H $\rightarrow$ L
B20	SCS-ωB88PP86	THF	$S_0 \rightarrow S_1$	1.938	1.536	H $\rightarrow$ L
B20	SCS-ωPBEPP86	THF	$S_0 \rightarrow S_1$	1.767	1.406	H $\rightarrow$ L
B20	SOS-B2GP-PLYP	THF	$S_0 \rightarrow S_1$	2.092	1.692	H $\rightarrow$ L
B20	SOS-PBE-QIDH	THF	$S_0 \rightarrow S_1$	1.954	1.577	H $\rightarrow$ L
B20	SOS-RSX-QIDH	THF	$S_0 \rightarrow S_1$	1.700	1.352	H $\rightarrow$ L
B20	SOS-ωB2GP-PLYP	THF	$S_0 \rightarrow S_1$	1.886	1.496	H $\rightarrow$ L
B20	SOS-ωB88PP86	THF	$S_0 \rightarrow S_1$	1.897	1.503	H $\rightarrow$ L
B20	SOS-ωPBEPP86	THF	$S_0 \rightarrow S_1$	1.823	1.450	H $\rightarrow$ L
B20	ωB2GP-PLYP	THF	$S_0 \rightarrow S_1$	2.089	1.657	H $\rightarrow$ L
B20	ωB2PLYP	THF	$S_0 \rightarrow S_1$	2.103	1.649	H $\rightarrow$ L
B20	ωB88PP86	THF	$S_0 \rightarrow S_1$	2.070	1.641	H $\rightarrow$ L
B20	ωB97X	THF	$S_0 \rightarrow S_1$	2.161	1.647	H $\rightarrow$ L
B20	ωPBEPP86	THF	$S_0 \rightarrow S_1$	2.058	1.638	H $\rightarrow$ L
B21	B2GP-PLYP	THF	$S_0 \rightarrow S_1$	2.288	1.505	H $\rightarrow$ L
B21	B2PLYP	THF	$S_0 \rightarrow S_1$	2.190	1.423	H $\rightarrow$ L
B21	B3LYP	THF	$S_0 \rightarrow S_1$	1.915	0.581	H $\rightarrow$ L
B21	BHLYP	THF	$S_0 \rightarrow S_1$	2.525	1.616	H $\rightarrow$ L
B21	CAM-B3LYP	THF	$S_0 \rightarrow S_1$	2.488	1.573	H $\rightarrow$ L
B21	DSD-BLYP(CORRECT)	THF	$S_0 \rightarrow S_1$	2.290	1.494	H $\rightarrow$ L
B21	DSD-BLYP(WRONG)	THF	$S_0 \rightarrow S_1$	1.869	1.219	H $\rightarrow$ L
B21	DSD-PBEP86(CORRECT)	THF	$S_0 \rightarrow S_1$	2.281	1.499	H $\rightarrow$ L
B21	DSD-PBEP86(WRONG)	THF	$S_0 \rightarrow S_1$	1.818	1.195	H $\rightarrow$ L
B21	PBE-QIDH	THF	$S_0 \rightarrow S_1$	2.373	1.563	H $\rightarrow$ L
B21	RSX-QIDH	THF	$S_0 \rightarrow S_1$	2.489	1.573	H $\rightarrow$ L
B21	SCS-B2GP-PLYP	THF	$S_0 \rightarrow S_1$	2.379	1.565	H $\rightarrow$ L
B21	SCS-PBE-QIDH	THF	$S_0 \rightarrow S_1$	2.221	1.462	H $\rightarrow$ L
B21	SCS-RSX-QIDH	THF	$S_0 \rightarrow S_1$	2.119	1.339	H $\rightarrow$ L
B21	SOS-B2PLYP	THF	$S_0 \rightarrow S_1$	2.522	1.639	H $\rightarrow$ L
B21	SOS-ωB2PLYP	THF	$S_0 \rightarrow S_1$	2.304	1.442	H $\rightarrow$ L
B21	SCS-ωB2GP-PLYP	THF	$S_0 \rightarrow S_1$	2.182	1.375	H $\rightarrow$ L
B21	SCS-ωB88PP86	THF	$S_0 \rightarrow S_1$	2.255	1.445	H $\rightarrow$ L
B21	SCS-ωPBEPP86	THF	$S_0 \rightarrow S_1$	2.102	1.349	H $\rightarrow$ L
B21	SOS-B2GP-PLYP	THF	$S_0 \rightarrow S_1$	2.325	1.530	H $\rightarrow$ L
B21	SOS-PBE-QIDH	THF	$S_0 \rightarrow S_1$	2.192	1.443	H $\rightarrow$ L

B21	SOS-RSX-QIDH	THF	$S_0 \rightarrow S_1$	2.017	1.275	H $\rightarrow$ L
B21	SOS-ωB2GP-PLYP	THF	$S_0 \rightarrow S_1$	2.210	1.392	H $\rightarrow$ L
B21	SOS-ωB88PP86	THF	$S_0 \rightarrow S_1$	2.204	1.412	H $\rightarrow$ L
B21	SOS-ωPBEPP86	THF	$S_0 \rightarrow S_1$	2.124	1.364	H $\rightarrow$ L
B21	ωB2GP-PLYP	THF	$S_0 \rightarrow S_1$	2.445	1.540	H $\rightarrow$ L
B21	ωB2PLYP	THF	$S_0 \rightarrow S_1$	2.473	1.548	H-1 $\rightarrow$ L
B21	ωB88PP86	THF	$S_0 \rightarrow S_1$	2.383	1.527	H $\rightarrow$ L
B21	ωB97X	THF	$S_0 \rightarrow S_1$	2.575	1.604	H-1 $\rightarrow$ L
B21	ωPBEPP86	THF	$S_0 \rightarrow S_1$	2.358	1.514	H $\rightarrow$ L
B22	B2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	3.421	0.502	H $\rightarrow$ L
B22	B2PLYP	MeOH	$S_0 \rightarrow S_1$	3.366	0.482	H $\rightarrow$ L
B22	B3LYP	MeOH	$S_0 \rightarrow S_1$	3.390	0.436	H $\rightarrow$ L
B22	BHLYP	MeOH	$S_0 \rightarrow S_1$	3.641	0.517	H $\rightarrow$ L
B22	CAM-B3LYP	MeOH	$S_0 \rightarrow S_1$	3.578	0.488	H $\rightarrow$ L
B22	DSD-BLYP(CORRECT)	MeOH	$S_0 \rightarrow S_1$	3.431	0.511	H $\rightarrow$ L
B22	DSD-BLYP(WRONG)	MeOH	$S_0 \rightarrow S_1$	3.031	0.451	H $\rightarrow$ L
B22	DSD-PBEP86(CORRECT)	MeOH	$S_0 \rightarrow S_1$	3.415	0.506	H $\rightarrow$ L
B22	DSD-PBEP86(WRONG)	MeOH	$S_0 \rightarrow S_1$	2.985	0.442	H $\rightarrow$ L
B22	PBE-QIDH	MeOH	$S_0 \rightarrow S_1$	3.509	0.516	H $\rightarrow$ L
B22	RSX-QIDH	MeOH	$S_0 \rightarrow S_1$	3.649	0.536	H $\rightarrow$ L
B22	SCS-B2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	3.470	0.509	H $\rightarrow$ L
B22	SCS-PBE-QIDH	MeOH	$S_0 \rightarrow S_1$	3.350	0.493	H $\rightarrow$ L
B22	SCS-RSX-QIDH	MeOH	$S_0 \rightarrow S_1$	3.352	0.493	H $\rightarrow$ L
B22	SOS-B2PLYP	MeOH	$S_0 \rightarrow S_1$	3.617	0.518	H $\rightarrow$ L
B22	SOS-ωB2PLYP	MeOH	$S_0 \rightarrow S_1$	3.454	0.498	H $\rightarrow$ L
B22	SCS-ωB2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	3.361	0.492	H $\rightarrow$ L
B22	SCS-ωB88PP86	MeOH	$S_0 \rightarrow S_1$	3.405	0.499	H $\rightarrow$ L
B22	SCS-ωPBEPP86	MeOH	$S_0 \rightarrow S_1$	3.294	0.485	H $\rightarrow$ L
B22	SOS-B2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	3.423	0.502	H $\rightarrow$ L
B22	SOS-PBE-QIDH	MeOH	$S_0 \rightarrow S_1$	3.314	0.487	H $\rightarrow$ L
B22	SOS-RSX-QIDH	MeOH	$S_0 \rightarrow S_1$	3.215	0.473	H $\rightarrow$ L
B22	SOS-ωB2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	3.373	0.494	H $\rightarrow$ L
B22	SOS-ωB88PP86	MeOH	$S_0 \rightarrow S_1$	3.348	0.490	H $\rightarrow$ L
B22	SOS-ωPBEPP86	MeOH	$S_0 \rightarrow S_1$	3.280	0.483	H $\rightarrow$ L
B22	ωB2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	3.590	0.526	H $\rightarrow$ L
B22	ωB2PLYP	MeOH	$S_0 \rightarrow S_1$	3.612	0.521	H $\rightarrow$ L
B22	ωB88PP86	MeOH	$S_0 \rightarrow S_1$	3.517	0.515	H $\rightarrow$ L
B22	ωB97X	MeOH	$S_0 \rightarrow S_1$	3.683	0.509	H $\rightarrow$ L
B22	ωPBEPP86	MeOH	$S_0 \rightarrow S_1$	3.498	0.515	H $\rightarrow$ L
B23	B2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.829	0.528	H $\rightarrow$ L
B23	B2PLYP	MeOH	$S_0 \rightarrow S_1$	2.830	0.506	H $\rightarrow$ L
B23	B3LYP	MeOH	$S_0 \rightarrow S_1$	2.955	0.443	H $\rightarrow$ L
B23	BHLYP	MeOH	$S_0 \rightarrow S_1$	3.062	0.539	H $\rightarrow$ L
B23	CAM-B3LYP	MeOH	$S_0 \rightarrow S_1$	3.006	0.507	H $\rightarrow$ L
B23	DSD-BLYP(CORRECT)	MeOH	$S_0 \rightarrow S_1$	2.805	0.540	H $\rightarrow$ L
B23	DSD-BLYP(WRONG)	MeOH	$S_0 \rightarrow S_1$	2.460	0.473	H $\rightarrow$ L
B23	DSD-PBEP86(CORRECT)	MeOH	$S_0 \rightarrow S_1$	2.783	0.530	H $\rightarrow$ L
B23	DSD-PBEP86(WRONG)	MeOH	$S_0 \rightarrow S_1$	2.439	0.465	H $\rightarrow$ L
B23	PBE-QIDH	MeOH	$S_0 \rightarrow S_1$	2.885	0.543	H $\rightarrow$ L
B23	RSX-QIDH	MeOH	$S_0 \rightarrow S_1$	2.929	0.565	H $\rightarrow$ L
B23	SCS-B2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.845	0.531	H $\rightarrow$ L
B23	SCS-PBE-QIDH	MeOH	$S_0 \rightarrow S_1$	2.712	0.510	H $\rightarrow$ L
B23	SCS-RSX-QIDH	MeOH	$S_0 \rightarrow S_1$	2.646	0.510	H $\rightarrow$ L
B23	SOS-B2PLYP	MeOH	$S_0 \rightarrow S_1$	3.043	0.544	H $\rightarrow$ L
B23	SOS-ωB2PLYP	MeOH	$S_0 \rightarrow S_1$	2.735	0.514	H $\rightarrow$ L
B23	SCS-ωB2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.639	0.506	H $\rightarrow$ L
B23	SCS-ωB88PP86	MeOH	$S_0 \rightarrow S_1$	2.712	0.514	H $\rightarrow$ L
B23	SCS-ωPBEPP86	MeOH	$S_0 \rightarrow S_1$	2.609	0.498	H $\rightarrow$ L
B23	SOS-B2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.799	0.522	H $\rightarrow$ L
B23	SOS-PBE-QIDH	MeOH	$S_0 \rightarrow S_1$	2.669	0.502	H $\rightarrow$ L
B23	SOS-RSX-QIDH	MeOH	$S_0 \rightarrow S_1$	2.470	0.476	H $\rightarrow$ L
B23	SOS-ωB2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.642	0.506	H $\rightarrow$ L

B23	SOS-ωB88PP86	MeOH	$S_0 \rightarrow S_1$	2.650	0.502	H $\rightarrow$ L
B23	SOS-ωPBEPP86	MeOH	$S_0 \rightarrow S_1$	2.575	0.492	H $\rightarrow$ L
B23	ωB2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.887	0.554	H $\rightarrow$ L
B23	ωB2PLYP	MeOH	$S_0 \rightarrow S_1$	2.914	0.548	H $\rightarrow$ L
B23	ωB88PP86	MeOH	$S_0 \rightarrow S_1$	2.852	0.541	H $\rightarrow$ L
B23	ωB97X	MeOH	$S_0 \rightarrow S_1$	3.015	0.533	H $\rightarrow$ L
B23	ωPBEPP86	MeOH	$S_0 \rightarrow S_1$	2.832	0.541	H $\rightarrow$ L

SI.7 TDA-DFT: all calculated values for SBYD31

Table S7: TDA-DFT details: solvent, transition, excitation energy, oscillator strength, and MO designation. For the DSD functionals, results for the correct and wrong implementations are shown. H: HOMO, L: LUMO.

Compound	Method	Solvent	Transition	Excitation energy (eV)	Oscillator strength	MO designation
B1	B2GP-PLYP	Et_2O	$S_0 \rightarrow S_1$	2.283	1.499	H $\rightarrow$ L
B1	B2PLYP	Et_2O	$S_0 \rightarrow S_1$	2.233	1.571	H $\rightarrow$ L
B1	B3LYP	Et_2O	$S_0 \rightarrow S_1$	2.299	1.790	H $\rightarrow$ L
B1	BHLYP	Et_2O	$S_0 \rightarrow S_1$	2.526	1.809	H $\rightarrow$ L
B1	CAM-B3LYP	Et_2O	$S_0 \rightarrow S_1$	2.484	1.704	H $\rightarrow$ L
B1	DSD-BLYP(CORRECT)	Et_2O	$S_0 \rightarrow S_1$	2.252	1.429	H $\rightarrow$ L
B1	DSD-BLYP(WRONG)	Et_2O	$S_0 \rightarrow S_1$	1.876	1.190	H $\rightarrow$ L
B1	DSD-PBEP86(CORRECT)	Et_2O	$S_0 \rightarrow S_1$	2.258	1.463	H $\rightarrow$ L
B1	DSD-PBEP86(WRONG)	Et_2O	$S_0 \rightarrow S_1$	1.828	1.184	H $\rightarrow$ L
B1	PBE-QIDH	Et_2O	$S_0 \rightarrow S_1$	2.350	1.517	H $\rightarrow$ L
B1	RSX-QIDH	Et_2O	$S_0 \rightarrow S_1$	2.463	1.416	H $\rightarrow$ L
B1	SCS-B2GP-PLYP	Et_2O	$S_0 \rightarrow S_1$	2.390	1.570	H $\rightarrow$ L
B1	SCS-PBE-QIDH	Et_2O	$S_0 \rightarrow S_1$	2.226	1.438	H $\rightarrow$ L
B1	SCS-RSX-QIDH	Et_2O	$S_0 \rightarrow S_1$	2.120	1.220	H $\rightarrow$ L
B1	SOS-B2PLYP	Et_2O	$S_0 \rightarrow S_1$	2.559	1.800	H $\rightarrow$ L
B1	SOS-ωB2PLYP	Et_2O	$S_0 \rightarrow S_1$	2.324	1.342	H $\rightarrow$ L
B1	SCS-ωB2GP-PLYP	Et_2O	$S_0 \rightarrow S_1$	2.211	1.273	H $\rightarrow$ L
B1	SCS-ωB88PP86	Et_2O	$S_0 \rightarrow S_1$	2.265	1.350	H $\rightarrow$ L
B1	SCS-ωPBEPP86	Et_2O	$S_0 \rightarrow S_1$	2.111	1.258	H $\rightarrow$ L
B1	SOS-B2GP-PLYP	Et_2O	$S_0 \rightarrow S_1$	2.339	1.536	H $\rightarrow$ L
B1	SOS-PBE-QIDH	Et_2O	$S_0 \rightarrow S_1$	2.205	1.424	H $\rightarrow$ L
B1	SOS-RSX-QIDH	Et_2O	$S_0 \rightarrow S_1$	2.073	1.192	H $\rightarrow$ L
B1	SOS-ωB2GP-PLYP	Et_2O	$S_0 \rightarrow S_1$	2.246	1.293	H $\rightarrow$ L
B1	SOS-ωB88PP86	Et_2O	$S_0 \rightarrow S_1$	2.224	1.326	H $\rightarrow$ L
B1	SOS-ωPBEPP86	Et_2O	$S_0 \rightarrow S_1$	2.151	1.282	H $\rightarrow$ L
B1	ωB2GP-PLYP	Et_2O	$S_0 \rightarrow S_1$	2.425	1.396	H $\rightarrow$ L
B1	ωB2PLYP	Et_2O	$S_0 \rightarrow S_1$	2.452	1.415	H $\rightarrow$ L
B1	ωB88PP86	Et_2O	$S_0 \rightarrow S_1$	2.360	1.406	H $\rightarrow$ L
B1	ωB97X	Et_2O	$S_0 \rightarrow S_1$	2.547	1.514	H $\rightarrow$ L
B1	ωPBEPP86	Et_2O	$S_0 \rightarrow S_1$	2.335	1.392	H $\rightarrow$ L
B1	B2GP-PLYP	MeCN	$S_0 \rightarrow S_1$	2.253	1.524	H $\rightarrow$ L
B1	B2PLYP	MeCN	$S_0 \rightarrow S_1$	2.198	1.595	H $\rightarrow$ L
B1	B3LYP	MeCN	$S_0 \rightarrow S_1$	2.271	1.825	H $\rightarrow$ L
B1	BHLYP	MeCN	$S_0 \rightarrow S_1$	2.505	1.852	H $\rightarrow$ L
B1	CAM-B3LYP	MeCN	$S_0 \rightarrow S_1$	2.462	1.745	H $\rightarrow$ L
B1	DSD-BLYP(CORRECT)	MeCN	$S_0 \rightarrow S_1$	2.241	1.432	H $\rightarrow$ L
B1	DSD-BLYP(WRONG)	MeCN	$S_0 \rightarrow S_1$	1.853	1.184	H $\rightarrow$ L
B1	DSD-PBEP86(CORRECT)	MeCN	$S_0 \rightarrow S_1$	2.246	1.466	H $\rightarrow$ L
B1	DSD-PBEP86(WRONG)	MeCN	$S_0 \rightarrow S_1$	1.801	1.175	H $\rightarrow$ L
B1	PBE-QIDH	MeCN	$S_0 \rightarrow S_1$	2.323	1.546	H $\rightarrow$ L
B1	RSX-QIDH	MeCN	$S_0 \rightarrow S_1$	2.446	1.447	H $\rightarrow$ L
B1	SCS-B2GP-PLYP	MeCN	$S_0 \rightarrow S_1$	2.362	1.598	H $\rightarrow$ L
B1	SCS-PBE-QIDH	MeCN	$S_0 \rightarrow S_1$	2.197	1.462	H $\rightarrow$ L
B1	SCS-RSX-QIDH	MeCN	$S_0 \rightarrow S_1$	2.099	1.242	H $\rightarrow$ L
B1	SOS-B2PLYP	MeCN	$S_0 \rightarrow S_1$	2.528	1.834	H $\rightarrow$ L
B1	SOS-ωB2PLYP	MeCN	$S_0 \rightarrow S_1$	2.307	1.370	H $\rightarrow$ L
B1	SCS-ωB2GP-PLYP	MeCN	$S_0 \rightarrow S_1$	2.193	1.298	H $\rightarrow$ L
B1	SCS-ωB88PP86	MeCN	$S_0 \rightarrow S_1$	2.244	1.376	H $\rightarrow$ L
B1	SCS-ωPBEPP86	MeCN	$S_0 \rightarrow S_1$	2.088	1.280	H $\rightarrow$ L
B1	SOS-B2GP-PLYP	MeCN	$S_0 \rightarrow S_1$	2.311	1.563	H $\rightarrow$ L
B1	SOS-PBE-QIDH	MeCN	$S_0 \rightarrow S_1$	2.176	1.448	H $\rightarrow$ L
B1	SOS-RSX-QIDH	MeCN	$S_0 \rightarrow S_1$	2.054	1.215	H $\rightarrow$ L
B1	SOS-ωB2GP-PLYP	MeCN	$S_0 \rightarrow S_1$	2.229	1.319	H $\rightarrow$ L
B1	SOS-ωB88PP86	MeCN	$S_0 \rightarrow S_1$	2.203	1.351	H $\rightarrow$ L
B1	SOS-ωPBEPP86	MeCN	$S_0 \rightarrow S_1$	2.129	1.306	H $\rightarrow$ L

B1	ωB2GP-PLYP	MeCN	$S_0 \rightarrow S_1$	2.408	1.425	H $\rightarrow$ L
B1	ωB2PLYP	MeCN	$S_0 \rightarrow S_1$	2.435	1.447	H $\rightarrow$ L
B1	ωB88PP86	MeCN	$S_0 \rightarrow S_1$	2.337	1.433	H $\rightarrow$ L
B1	ωB97X	MeCN	$S_0 \rightarrow S_1$	2.531	1.553	H $\rightarrow$ L
B1	ωPBEPP86	MeCN	$S_0 \rightarrow S_1$	2.312	1.417	H $\rightarrow$ L
B2	B2GP-PLYP	Et_2O	$S_0 \rightarrow S_1$	2.451	1.373	H $\rightarrow$ L
B2	B2PLYP	Et_2O	$S_0 \rightarrow S_1$	2.442	1.447	H $\rightarrow$ L
B2	B3LYP	Et_2O	$S_0 \rightarrow S_1$	2.561	1.765	H $\rightarrow$ L
B2	BHLYP	Et_2O	$S_0 \rightarrow S_1$	2.672	1.608	H $\rightarrow$ L
B2	CAM-B3LYP	Et_2O	$S_0 \rightarrow S_1$	2.631	1.508	H $\rightarrow$ L
B2	DSD-BLYP(CORRECT)	Et_2O	$S_0 \rightarrow S_1$	2.415	1.300	H $\rightarrow$ L
B2	DSD-BLYP(WRONG)	Et_2O	$S_0 \rightarrow S_1$	2.094	1.127	H $\rightarrow$ L
B2	DSD-PBEP86(CORRECT)	Et_2O	$S_0 \rightarrow S_1$	2.424	1.325	H $\rightarrow$ L
B2	DSD-PBEP86(WRONG)	Et_2O	$S_0 \rightarrow S_1$	2.068	1.130	H $\rightarrow$ L
B2	PBE-QIDH	Et_2O	$S_0 \rightarrow S_1$	2.503	1.381	H $\rightarrow$ L
B2	RSX-QIDH	Et_2O	$S_0 \rightarrow S_1$	2.564	1.282	H $\rightarrow$ L
B2	SCS-B2GP-PLYP	Et_2O	$S_0 \rightarrow S_1$	2.539	1.423	H $\rightarrow$ L
B2	SCS-PBE-QIDH	Et_2O	$S_0 \rightarrow S_1$	2.377	1.312	H $\rightarrow$ L
B2	SCS-RSX-QIDH	Et_2O	$S_0 \rightarrow S_1$	2.237	1.118	H $\rightarrow$ L
B2	SOS-B2PLYP	Et_2O	$S_0 \rightarrow S_1$	2.739	1.624	H $\rightarrow$ L
B2	SOS-ωB2PLYP	Et_2O	$S_0 \rightarrow S_1$	2.422	1.210	H $\rightarrow$ L
B2	SCS-ωB2GP-PLYP	Et_2O	$S_0 \rightarrow S_1$	2.312	1.157	H $\rightarrow$ L
B2	SCS-ωB88PP86	Et_2O	$S_0 \rightarrow S_1$	2.378	1.226	H $\rightarrow$ L
B2	SCS-ωPBEPP86	Et_2O	$S_0 \rightarrow S_1$	2.232	1.152	H $\rightarrow$ L
B2	SOS-B2GP-PLYP	Et_2O	$S_0 \rightarrow S_1$	2.490	1.396	H $\rightarrow$ L
B2	SOS-PBE-QIDH	Et_2O	$S_0 \rightarrow S_1$	2.353	1.299	H $\rightarrow$ L
B2	SOS-RSX-QIDH	Et_2O	$S_0 \rightarrow S_1$	2.172	1.086	H $\rightarrow$ L
B2	SOS-ωB2GP-PLYP	Et_2O	$S_0 \rightarrow S_1$	2.343	1.173	H $\rightarrow$ L
B2	SOS-ωB88PP86	Et_2O	$S_0 \rightarrow S_1$	2.334	1.204	H $\rightarrow$ L
B2	SOS-ωPBEPP86	Et_2O	$S_0 \rightarrow S_1$	2.263	1.168	H $\rightarrow$ L
B2	ωB2GP-PLYP	Et_2O	$S_0 \rightarrow S_1$	2.529	1.266	H $\rightarrow$ L
B2	ωB2PLYP	Et_2O	$S_0 \rightarrow S_1$	2.556	1.277	H $\rightarrow$ L
B2	ωB88PP86	Et_2O	$S_0 \rightarrow S_1$	2.482	1.280	H $\rightarrow$ L
B2	ωB97X	Et_2O	$S_0 \rightarrow S_1$	2.651	1.344	H $\rightarrow$ L
B2	ωPBEPP86	Et_2O	$S_0 \rightarrow S_1$	2.461	1.270	H $\rightarrow$ L
B2	B2GP-PLYP	MeCN	$S_0 \rightarrow S_1$	2.451	1.373	H $\rightarrow$ L
B2	B2PLYP	MeCN	$S_0 \rightarrow S_1$	2.442	1.448	H $\rightarrow$ L
B2	B3LYP	MeCN	$S_0 \rightarrow S_1$	2.562	1.769	H $\rightarrow$ L
B2	BHLYP	MeCN	$S_0 \rightarrow S_1$	2.675	1.610	H $\rightarrow$ L
B2	CAM-B3LYP	MeCN	$S_0 \rightarrow S_1$	2.634	1.510	H $\rightarrow$ L
B2	DSD-BLYP(CORRECT)	MeCN	$S_0 \rightarrow S_1$	2.419	1.296	H $\rightarrow$ L
B2	DSD-BLYP(WRONG)	MeCN	$S_0 \rightarrow S_1$	2.094	1.122	H $\rightarrow$ L
B2	DSD-PBEP86(CORRECT)	MeCN	$S_0 \rightarrow S_1$	2.428	1.322	H $\rightarrow$ L
B2	DSD-PBEP86(WRONG)	MeCN	$S_0 \rightarrow S_1$	2.068	1.126	H $\rightarrow$ L
B2	PBE-QIDH	MeCN	$S_0 \rightarrow S_1$	2.504	1.382	H $\rightarrow$ L
B2	RSX-QIDH	MeCN	$S_0 \rightarrow S_1$	2.567	1.283	H $\rightarrow$ L
B2	SCS-B2GP-PLYP	MeCN	$S_0 \rightarrow S_1$	2.540	1.423	H $\rightarrow$ L
B2	SCS-PBE-QIDH	MeCN	$S_0 \rightarrow S_1$	2.378	1.312	H $\rightarrow$ L
B2	SCS-RSX-QIDH	MeCN	$S_0 \rightarrow S_1$	2.239	1.118	H $\rightarrow$ L
B2	SOS-B2PLYP	MeCN	$S_0 \rightarrow S_1$	2.739	1.624	H $\rightarrow$ L
B2	SOS-ωB2PLYP	MeCN	$S_0 \rightarrow S_1$	2.424	1.210	H $\rightarrow$ L
B2	SCS-ωB2GP-PLYP	MeCN	$S_0 \rightarrow S_1$	2.315	1.158	H $\rightarrow$ L
B2	SCS-ωB88PP86	MeCN	$S_0 \rightarrow S_1$	2.380	1.227	H $\rightarrow$ L
B2	SCS-ωPBEPP86	MeCN	$S_0 \rightarrow S_1$	2.234	1.152	H $\rightarrow$ L
B2	SOS-B2GP-PLYP	MeCN	$S_0 \rightarrow S_1$	2.491	1.395	H $\rightarrow$ L
B2	SOS-PBE-QIDH	MeCN	$S_0 \rightarrow S_1$	2.354	1.299	H $\rightarrow$ L
B2	SOS-RSX-QIDH	MeCN	$S_0 \rightarrow S_1$	2.175	1.087	H $\rightarrow$ L
B2	SOS-ωB2GP-PLYP	MeCN	$S_0 \rightarrow S_1$	2.345	1.173	H $\rightarrow$ L
B2	SOS-ωB88PP86	MeCN	$S_0 \rightarrow S_1$	2.336	1.204	H $\rightarrow$ L
B2	SOS-ωPBEPP86	MeCN	$S_0 \rightarrow S_1$	2.265	1.168	H $\rightarrow$ L
B2	ωB2GP-PLYP	MeCN	$S_0 \rightarrow S_1$	2.532	1.266	H $\rightarrow$ L
B2	ωB2PLYP	MeCN	$S_0 \rightarrow S_1$	2.558	1.277	H $\rightarrow$ L

B2	ωB88PP86	MeCN	$S_0 \rightarrow S_1$	2.484	1.280	H $\rightarrow$ L
B2	ωB97X	MeCN	$S_0 \rightarrow S_1$	2.654	1.345	H $\rightarrow$ L
B2	ωPBEPP86	MeCN	$S_0 \rightarrow S_1$	2.462	1.270	H $\rightarrow$ L
B2	B2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.457	1.373	H $\rightarrow$ L
B2	B2PLYP	MeOH	$S_0 \rightarrow S_1$	2.448	1.448	H $\rightarrow$ L
B2	B3LYP	MeOH	$S_0 \rightarrow S_1$	2.569	1.768	H $\rightarrow$ L
B2	BHLYP	MeOH	$S_0 \rightarrow S_1$	2.681	1.610	H $\rightarrow$ L
B2	CAM-B3LYP	MeOH	$S_0 \rightarrow S_1$	2.640	1.510	H $\rightarrow$ L
B2	DSD-BLYP(CORRECT)	MeOH	$S_0 \rightarrow S_1$	2.425	1.296	H $\rightarrow$ L
B2	DSD-BLYP(WRONG)	MeOH	$S_0 \rightarrow S_1$	2.100	1.123	H $\rightarrow$ L
B2	DSD-PBEP86(CORRECT)	MeOH	$S_0 \rightarrow S_1$	2.434	1.322	H $\rightarrow$ L
B2	DSD-PBEP86(WRONG)	MeOH	$S_0 \rightarrow S_1$	2.073	1.126	H $\rightarrow$ L
B2	PBE-QIDH	MeOH	$S_0 \rightarrow S_1$	2.510	1.382	H $\rightarrow$ L
B2	RSX-QIDH	MeOH	$S_0 \rightarrow S_1$	2.573	1.282	H $\rightarrow$ L
B2	SCS-B2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.546	1.423	H $\rightarrow$ L
B2	SCS-PBE-QIDH	MeOH	$S_0 \rightarrow S_1$	2.384	1.312	H $\rightarrow$ L
B2	SCS-RSX-QIDH	MeOH	$S_0 \rightarrow S_1$	2.244	1.119	H $\rightarrow$ L
B2	SOS-B2PLYP	MeOH	$S_0 \rightarrow S_1$	2.745	1.624	H $\rightarrow$ L
B2	SOS-ωB2PLYP	MeOH	$S_0 \rightarrow S_1$	2.430	1.210	H $\rightarrow$ L
B2	SCS-ωB2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.321	1.158	H $\rightarrow$ L
B2	SCS-ωB88PP86	MeOH	$S_0 \rightarrow S_1$	2.386	1.227	H $\rightarrow$ L
B2	SCS-ωPBEPP86	MeOH	$S_0 \rightarrow S_1$	2.239	1.152	H $\rightarrow$ L
B2	SOS-B2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.497	1.395	H $\rightarrow$ L
B2	SOS-PBE-QIDH	MeOH	$S_0 \rightarrow S_1$	2.360	1.299	H $\rightarrow$ L
B2	SOS-RSX-QIDH	MeOH	$S_0 \rightarrow S_1$	2.181	1.087	H $\rightarrow$ L
B2	SOS-ωB2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.351	1.173	H $\rightarrow$ L
B2	SOS-ωB88PP86	MeOH	$S_0 \rightarrow S_1$	2.342	1.204	H $\rightarrow$ L
B2	SOS-ωPBEPP86	MeOH	$S_0 \rightarrow S_1$	2.270	1.168	H $\rightarrow$ L
B2	ωB2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.538	1.266	H $\rightarrow$ L
B2	ωB2PLYP	MeOH	$S_0 \rightarrow S_1$	2.564	1.277	H $\rightarrow$ L
B2	ωB88PP86	MeOH	$S_0 \rightarrow S_1$	2.490	1.280	H $\rightarrow$ L
B2	ωB97X	MeOH	$S_0 \rightarrow S_1$	2.660	1.345	H $\rightarrow$ L
B2	ωPBEPP86	MeOH	$S_0 \rightarrow S_1$	2.468	1.270	H $\rightarrow$ L
B3	B2GP-PLYP	Et_2O	$S_0 \rightarrow S_1$	2.266	1.517	H $\rightarrow$ L
B3	B2PLYP	Et_2O	$S_0 \rightarrow S_1$	2.215	1.590	H $\rightarrow$ L
B3	B3LYP	Et_2O	$S_0 \rightarrow S_1$	2.284	1.817	H $\rightarrow$ L
B3	BHLYP	Et_2O	$S_0 \rightarrow S_1$	2.511	1.836	H $\rightarrow$ L
B3	CAM-B3LYP	Et_2O	$S_0 \rightarrow S_1$	2.469	1.730	H $\rightarrow$ L
B3	DSD-BLYP(CORRECT)	Et_2O	$S_0 \rightarrow S_1$	2.236	1.445	H $\rightarrow$ L
B3	DSD-BLYP(WRONG)	Et_2O	$S_0 \rightarrow S_1$	1.857	1.201	H $\rightarrow$ L
B3	DSD-PBEP86(CORRECT)	Et_2O	$S_0 \rightarrow S_1$	2.242	1.480	H $\rightarrow$ L
B3	DSD-PBEP86(WRONG)	Et_2O	$S_0 \rightarrow S_1$	1.809	1.194	H $\rightarrow$ L
B3	PBE-QIDH	Et_2O	$S_0 \rightarrow S_1$	2.334	1.536	H $\rightarrow$ L
B3	RSX-QIDH	Et_2O	$S_0 \rightarrow S_1$	2.448	1.432	H $\rightarrow$ L
B3	SCS-B2GP-PLYP	Et_2O	$S_0 \rightarrow S_1$	2.374	1.589	H $\rightarrow$ L
B3	SCS-PBE-QIDH	Et_2O	$S_0 \rightarrow S_1$	2.209	1.454	H $\rightarrow$ L
B3	SCS-RSX-QIDH	Et_2O	$S_0 \rightarrow S_1$	2.104	1.231	H $\rightarrow$ L
B3	SOS-B2PLYP	Et_2O	$S_0 \rightarrow S_1$	2.543	1.825	H $\rightarrow$ L
B3	SOS-ωB2PLYP	Et_2O	$S_0 \rightarrow S_1$	2.309	1.356	H $\rightarrow$ L
B3	SCS-ωB2GP-PLYP	Et_2O	$S_0 \rightarrow S_1$	2.196	1.285	H $\rightarrow$ L
B3	SCS-ωB88PP86	Et_2O	$S_0 \rightarrow S_1$	2.250	1.365	H $\rightarrow$ L
B3	SCS-ωPBEPP86	Et_2O	$S_0 \rightarrow S_1$	2.094	1.270	H $\rightarrow$ L
B3	SOS-B2GP-PLYP	Et_2O	$S_0 \rightarrow S_1$	2.323	1.555	H $\rightarrow$ L
B3	SOS-PBE-QIDH	Et_2O	$S_0 \rightarrow S_1$	2.188	1.440	H $\rightarrow$ L
B3	SOS-RSX-QIDH	Et_2O	$S_0 \rightarrow S_1$	2.057	1.203	H $\rightarrow$ L
B3	SOS-ωB2GP-PLYP	Et_2O	$S_0 \rightarrow S_1$	2.231	1.306	H $\rightarrow$ L
B3	SOS-ωB88PP86	Et_2O	$S_0 \rightarrow S_1$	2.208	1.340	H $\rightarrow$ L
B3	SOS-ωPBEPP86	Et_2O	$S_0 \rightarrow S_1$	2.135	1.295	H $\rightarrow$ L
B3	ωB2GP-PLYP	Et_2O	$S_0 \rightarrow S_1$	2.410	1.411	H $\rightarrow$ L
B3	ωB2PLYP	Et_2O	$S_0 \rightarrow S_1$	2.437	1.432	H $\rightarrow$ L
B3	ωB88PP86	Et_2O	$S_0 \rightarrow S_1$	2.344	1.422	H $\rightarrow$ L
B3	ωB97X	Et_2O	$S_0 \rightarrow S_1$	2.533	1.534	H $\rightarrow$ L

B3	ωPBEPP86	Et_2O	$S_0 \rightarrow S_1$	2.320	1.407	H $\rightarrow$ L
B3	B2GP-PLYP	MeCN	$S_0 \rightarrow S_1$	2.237	1.544	H $\rightarrow$ L
B3	B2PLYP	MeCN	$S_0 \rightarrow S_1$	2.181	1.616	H $\rightarrow$ L
B3	B3LYP	MeCN	$S_0 \rightarrow S_1$	2.259	1.863	H $\rightarrow$ L
B3	BHLYP	MeCN	$S_0 \rightarrow S_1$	2.491	1.881	H $\rightarrow$ L
B3	CAM-B3LYP	MeCN	$S_0 \rightarrow S_1$	2.447	1.773	H $\rightarrow$ L
B3	DSD-BLYP(CORRECT)	MeCN	$S_0 \rightarrow S_1$	2.223	1.448	H $\rightarrow$ L
B3	DSD-BLYP(WRONG)	MeCN	$S_0 \rightarrow S_1$	1.834	1.195	H $\rightarrow$ L
B3	DSD-PBEP86(CORRECT)	MeCN	$S_0 \rightarrow S_1$	2.230	1.484	H $\rightarrow$ L
B3	DSD-PBEP86(WRONG)	MeCN	$S_0 \rightarrow S_1$	1.783	1.187	H $\rightarrow$ L
B3	PBE-QIDH	MeCN	$S_0 \rightarrow S_1$	2.306	1.566	H $\rightarrow$ L
B3	RSX-QIDH	MeCN	$S_0 \rightarrow S_1$	2.431	1.465	H $\rightarrow$ L
B3	SCS-B2GP-PLYP	MeCN	$S_0 \rightarrow S_1$	2.346	1.619	H $\rightarrow$ L
B3	SCS-PBE-QIDH	MeCN	$S_0 \rightarrow S_1$	2.180	1.480	H $\rightarrow$ L
B3	SCS-RSX-QIDH	MeCN	$S_0 \rightarrow S_1$	2.083	1.255	H $\rightarrow$ L
B3	SOS-B2PLYP	MeCN	$S_0 \rightarrow S_1$	2.513	1.862	H $\rightarrow$ L
B3	SOS-ωB2PLYP	MeCN	$S_0 \rightarrow S_1$	2.292	1.387	H $\rightarrow$ L
B3	SCS-ωB2GP-PLYP	MeCN	$S_0 \rightarrow S_1$	2.178	1.313	H $\rightarrow$ L
B3	SCS-ωB88PP86	MeCN	$S_0 \rightarrow S_1$	2.229	1.393	H $\rightarrow$ L
B3	SCS-ωPBEPP86	MeCN	$S_0 \rightarrow S_1$	2.071	1.294	H $\rightarrow$ L
B3	SOS-B2GP-PLYP	MeCN	$S_0 \rightarrow S_1$	2.295	1.584	H $\rightarrow$ L
B3	SOS-PBE-QIDH	MeCN	$S_0 \rightarrow S_1$	2.160	1.466	H $\rightarrow$ L
B3	SOS-RSX-QIDH	MeCN	$S_0 \rightarrow S_1$	2.038	1.228	H $\rightarrow$ L
B3	SOS-ωB2GP-PLYP	MeCN	$S_0 \rightarrow S_1$	2.214	1.334	H $\rightarrow$ L
B3	SOS-ωB88PP86	MeCN	$S_0 \rightarrow S_1$	2.187	1.367	H $\rightarrow$ L
B3	SOS-ωPBEPP86	MeCN	$S_0 \rightarrow S_1$	2.114	1.321	H $\rightarrow$ L
B3	ωB2GP-PLYP	MeCN	$S_0 \rightarrow S_1$	2.392	1.442	H $\rightarrow$ L
B3	ωB2PLYP	MeCN	$S_0 \rightarrow S_1$	2.420	1.465	H $\rightarrow$ L
B3	ωB88PP86	MeCN	$S_0 \rightarrow S_1$	2.322	1.451	H $\rightarrow$ L
B3	ωB97X	MeCN	$S_0 \rightarrow S_1$	2.517	1.574	H $\rightarrow$ L
B3	ωPBEPP86	MeCN	$S_0 \rightarrow S_1$	2.296	1.434	H $\rightarrow$ L
B3	B2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.243	1.545	H $\rightarrow$ L
B3	B2PLYP	MeOH	$S_0 \rightarrow S_1$	2.187	1.617	H $\rightarrow$ L
B3	B3LYP	MeOH	$S_0 \rightarrow S_1$	2.266	1.857	H $\rightarrow$ L
B3	BHLYP	MeOH	$S_0 \rightarrow S_1$	2.497	1.882	H $\rightarrow$ L
B3	CAM-B3LYP	MeOH	$S_0 \rightarrow S_1$	2.453	1.774	H $\rightarrow$ L
B3	DSD-BLYP(CORRECT)	MeOH	$S_0 \rightarrow S_1$	2.229	1.449	H $\rightarrow$ L
B3	DSD-BLYP(WRONG)	MeOH	$S_0 \rightarrow S_1$	1.839	1.195	H $\rightarrow$ L
B3	DSD-PBEP86(CORRECT)	MeOH	$S_0 \rightarrow S_1$	2.235	1.485	H $\rightarrow$ L
B3	DSD-PBEP86(WRONG)	MeOH	$S_0 \rightarrow S_1$	1.788	1.188	H $\rightarrow$ L
B3	PBE-QIDH	MeOH	$S_0 \rightarrow S_1$	2.312	1.567	H $\rightarrow$ L
B3	RSX-QIDH	MeOH	$S_0 \rightarrow S_1$	2.436	1.465	H $\rightarrow$ L
B3	SCS-B2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.352	1.620	H $\rightarrow$ L
B3	SCS-PBE-QIDH	MeOH	$S_0 \rightarrow S_1$	2.186	1.481	H $\rightarrow$ L
B3	SCS-RSX-QIDH	MeOH	$S_0 \rightarrow S_1$	2.088	1.256	H $\rightarrow$ L
B3	SOS-B2PLYP	MeOH	$S_0 \rightarrow S_1$	2.519	1.862	H $\rightarrow$ L
B3	SOS-ωB2PLYP	MeOH	$S_0 \rightarrow S_1$	2.298	1.388	H $\rightarrow$ L
B3	SCS-ωB2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.183	1.313	H $\rightarrow$ L
B3	SCS-ωB88PP86	MeOH	$S_0 \rightarrow S_1$	2.234	1.394	H $\rightarrow$ L
B3	SCS-ωPBEPP86	MeOH	$S_0 \rightarrow S_1$	2.077	1.295	H $\rightarrow$ L
B3	SOS-B2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.301	1.585	H $\rightarrow$ L
B3	SOS-PBE-QIDH	MeOH	$S_0 \rightarrow S_1$	2.165	1.467	H $\rightarrow$ L
B3	SOS-RSX-QIDH	MeOH	$S_0 \rightarrow S_1$	2.044	1.229	H $\rightarrow$ L
B3	SOS-ωB2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.219	1.335	H $\rightarrow$ L
B3	SOS-ωB88PP86	MeOH	$S_0 \rightarrow S_1$	2.193	1.368	H $\rightarrow$ L
B3	SOS-ωPBEPP86	MeOH	$S_0 \rightarrow S_1$	2.119	1.322	H $\rightarrow$ L
B3	ωB2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.398	1.443	H $\rightarrow$ L
B3	ωB2PLYP	MeOH	$S_0 \rightarrow S_1$	2.426	1.465	H $\rightarrow$ L
B3	ωB88PP86	MeOH	$S_0 \rightarrow S_1$	2.327	1.452	H $\rightarrow$ L
B3	ωB97X	MeOH	$S_0 \rightarrow S_1$	2.523	1.575	H $\rightarrow$ L
B3	ωPBEPP86	MeOH	$S_0 \rightarrow S_1$	2.301	1.435	H $\rightarrow$ L
B4	B2GP-PLYP	Et_2O	$S_0 \rightarrow S_1$	2.483	1.303	H $\rightarrow$ L

B4	B2PLYP	Et_2O	$S_0 \rightarrow S_1$	2.480	1.369	H $\rightarrow$ L
B4	B3LYP	Et_2O	$S_0 \rightarrow S_1$	2.608	1.636	H $\rightarrow$ L
B4	BHLYP	Et_2O	$S_0 \rightarrow S_1$	2.703	1.511	H $\rightarrow$ L
B4	CAM-B3LYP	Et_2O	$S_0 \rightarrow S_1$	2.662	1.418	H $\rightarrow$ L
B4	DSD-BLYP(CORRECT)	Et_2O	$S_0 \rightarrow S_1$	2.448	1.236	H $\rightarrow$ L
B4	DSD-BLYP(WRONG)	Et_2O	$S_0 \rightarrow S_1$	2.135	1.078	H $\rightarrow$ L
B4	DSD-PBEP86(CORRECT)	Et_2O	$S_0 \rightarrow S_1$	2.456	1.257	H $\rightarrow$ L
B4	DSD-PBEP86(WRONG)	Et_2O	$S_0 \rightarrow S_1$	2.111	1.081	H $\rightarrow$ L
B4	PBE-QIDH	Et_2O	$S_0 \rightarrow S_1$	2.533	1.310	H $\rightarrow$ L
B4	RSX-QIDH	Et_2O	$S_0 \rightarrow S_1$	2.587	1.219	H $\rightarrow$ L
B4	SCS-B2GP-PLYP	Et_2O	$S_0 \rightarrow S_1$	2.568	1.347	H $\rightarrow$ L
B4	SCS-PBE-QIDH	Et_2O	$S_0 \rightarrow S_1$	2.407	1.245	H $\rightarrow$ L
B4	SCS-RSX-QIDH	Et_2O	$S_0 \rightarrow S_1$	2.264	1.067	H $\rightarrow$ L
B4	SOS-B2PLYP	Et_2O	$S_0 \rightarrow S_1$	2.771	1.529	H $\rightarrow$ L
B4	SOS-ωB2PLYP	Et_2O	$S_0 \rightarrow S_1$	2.443	1.150	H $\rightarrow$ L
B4	SCS-ωB2GP-PLYP	Et_2O	$S_0 \rightarrow S_1$	2.335	1.102	H $\rightarrow$ L
B4	SCS-ωB88PP86	Et_2O	$S_0 \rightarrow S_1$	2.403	1.166	H $\rightarrow$ L
B4	SCS-ωPBEPP86	Et_2O	$S_0 \rightarrow S_1$	2.259	1.097	H $\rightarrow$ L
B4	SOS-B2GP-PLYP	Et_2O	$S_0 \rightarrow S_1$	2.519	1.321	H $\rightarrow$ L
B4	SOS-PBE-QIDH	Et_2O	$S_0 \rightarrow S_1$	2.382	1.232	H $\rightarrow$ L
B4	SOS-RSX-QIDH	Et_2O	$S_0 \rightarrow S_1$	2.195	1.035	H $\rightarrow$ L
B4	SOS-ωB2GP-PLYP	Et_2O	$S_0 \rightarrow S_1$	2.364	1.116	H $\rightarrow$ L
B4	SOS-ωB88PP86	Et_2O	$S_0 \rightarrow S_1$	2.358	1.144	H $\rightarrow$ L
B4	SOS-ωPBEPP86	Et_2O	$S_0 \rightarrow S_1$	2.287	1.111	H $\rightarrow$ L
B4	ωB2GP-PLYP	Et_2O	$S_0 \rightarrow S_1$	2.552	1.204	H $\rightarrow$ L
B4	ωB2PLYP	Et_2O	$S_0 \rightarrow S_1$	2.578	1.213	H $\rightarrow$ L
B4	ωB88PP86	Et_2O	$S_0 \rightarrow S_1$	2.508	1.217	H $\rightarrow$ L
B4	ωB97X	Et_2O	$S_0 \rightarrow S_1$	2.674	1.272	H $\rightarrow$ L
B4	ωPBEPP86	Et_2O	$S_0 \rightarrow S_1$	2.488	1.208	H $\rightarrow$ L
B4	B2GP-PLYP	MeCN	$S_0 \rightarrow S_1$	2.487	1.300	H $\rightarrow$ L
B4	B2PLYP	MeCN	$S_0 \rightarrow S_1$	2.483	1.366	H $\rightarrow$ L
B4	B3LYP	MeCN	$S_0 \rightarrow S_1$	2.611	1.635	H $\rightarrow$ L
B4	BHLYP	MeCN	$S_0 \rightarrow S_1$	2.707	1.510	H $\rightarrow$ L
B4	CAM-B3LYP	MeCN	$S_0 \rightarrow S_1$	2.666	1.416	H $\rightarrow$ L
B4	DSD-BLYP(CORRECT)	MeCN	$S_0 \rightarrow S_1$	2.452	1.232	H $\rightarrow$ L
B4	DSD-BLYP(WRONG)	MeCN	$S_0 \rightarrow S_1$	2.138	1.073	H $\rightarrow$ L
B4	DSD-PBEP86(CORRECT)	MeCN	$S_0 \rightarrow S_1$	2.461	1.253	H $\rightarrow$ L
B4	DSD-PBEP86(WRONG)	MeCN	$S_0 \rightarrow S_1$	2.114	1.076	H $\rightarrow$ L
B4	PBE-QIDH	MeCN	$S_0 \rightarrow S_1$	2.537	1.308	H $\rightarrow$ L
B4	RSX-QIDH	MeCN	$S_0 \rightarrow S_1$	2.592	1.218	H $\rightarrow$ L
B4	SCS-B2GP-PLYP	MeCN	$S_0 \rightarrow S_1$	2.571	1.344	H $\rightarrow$ L
B4	SCS-PBE-QIDH	MeCN	$S_0 \rightarrow S_1$	2.410	1.242	H $\rightarrow$ L
B4	SCS-RSX-QIDH	MeCN	$S_0 \rightarrow S_1$	2.268	1.065	H $\rightarrow$ L
B4	SOS-B2PLYP	MeCN	$S_0 \rightarrow S_1$	2.774	1.526	H $\rightarrow$ L
B4	SOS-ωB2PLYP	MeCN	$S_0 \rightarrow S_1$	2.448	1.148	H $\rightarrow$ L
B4	SCS-ωB2GP-PLYP	MeCN	$S_0 \rightarrow S_1$	2.340	1.100	H $\rightarrow$ L
B4	SCS-ωB88PP86	MeCN	$S_0 \rightarrow S_1$	2.407	1.164	H $\rightarrow$ L
B4	SCS-ωPBEPP86	MeCN	$S_0 \rightarrow S_1$	2.263	1.096	H $\rightarrow$ L
B4	SOS-B2GP-PLYP	MeCN	$S_0 \rightarrow S_1$	2.522	1.319	H $\rightarrow$ L
B4	SOS-PBE-QIDH	MeCN	$S_0 \rightarrow S_1$	2.385	1.230	H $\rightarrow$ L
B4	SOS-RSX-QIDH	MeCN	$S_0 \rightarrow S_1$	2.200	1.033	H $\rightarrow$ L
B4	SOS-ωB2GP-PLYP	MeCN	$S_0 \rightarrow S_1$	2.369	1.114	H $\rightarrow$ L
B4	SOS-ωB88PP86	MeCN	$S_0 \rightarrow S_1$	2.362	1.142	H $\rightarrow$ L
B4	SOS-ωPBEPP86	MeCN	$S_0 \rightarrow S_1$	2.291	1.109	H $\rightarrow$ L
B4	ωB2GP-PLYP	MeCN	$S_0 \rightarrow S_1$	2.557	1.202	H $\rightarrow$ L
B4	ωB2PLYP	MeCN	$S_0 \rightarrow S_1$	2.583	1.212	H $\rightarrow$ L
B4	ωB88PP86	MeCN	$S_0 \rightarrow S_1$	2.512	1.215	H $\rightarrow$ L
B4	ωB97X	MeCN	$S_0 \rightarrow S_1$	2.679	1.271	H $\rightarrow$ L
B4	ωPBEPP86	MeCN	$S_0 \rightarrow S_1$	2.491	1.206	H $\rightarrow$ L
B4	B2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.493	1.300	H $\rightarrow$ L
B4	B2PLYP	MeOH	$S_0 \rightarrow S_1$	2.489	1.366	H $\rightarrow$ L
B4	B3LYP	MeOH	$S_0 \rightarrow S_1$	2.617	1.633	H $\rightarrow$ L

B4	BHLYP	MeOH	$S_0 \rightarrow S_1$	2.713	1.509	H $\rightarrow$ L
B4	CAM-B3LYP	MeOH	$S_0 \rightarrow S_1$	2.672	1.416	H $\rightarrow$ L
B4	DSD-BLYP(CORRECT)	MeOH	$S_0 \rightarrow S_1$	2.458	1.231	H $\rightarrow$ L
B4	DSD-BLYP(WRONG)	MeOH	$S_0 \rightarrow S_1$	2.143	1.073	H $\rightarrow$ L
B4	DSD-PBEP86(CORRECT)	MeOH	$S_0 \rightarrow S_1$	2.467	1.253	H $\rightarrow$ L
B4	DSD-PBEP86(WRONG)	MeOH	$S_0 \rightarrow S_1$	2.119	1.076	H $\rightarrow$ L
B4	PBE-QIDH	MeOH	$S_0 \rightarrow S_1$	2.543	1.308	H $\rightarrow$ L
B4	RSX-QIDH	MeOH	$S_0 \rightarrow S_1$	2.598	1.217	H $\rightarrow$ L
B4	SCS-B2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.577	1.344	H $\rightarrow$ L
B4	SCS-PBE-QIDH	MeOH	$S_0 \rightarrow S_1$	2.416	1.242	H $\rightarrow$ L
B4	SCS-RSX-QIDH	MeOH	$S_0 \rightarrow S_1$	2.274	1.065	H $\rightarrow$ L
B4	SOS-B2PLYP	MeOH	$S_0 \rightarrow S_1$	2.780	1.526	H $\rightarrow$ L
B4	SOS-ωB2PLYP	MeOH	$S_0 \rightarrow S_1$	2.454	1.148	H $\rightarrow$ L
B4	SCS-ωB2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.346	1.100	H $\rightarrow$ L
B4	SCS-ωB88PP86	MeOH	$S_0 \rightarrow S_1$	2.413	1.164	H $\rightarrow$ L
B4	SCS-ωPBEPP86	MeOH	$S_0 \rightarrow S_1$	2.269	1.096	H $\rightarrow$ L
B4	SOS-B2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.528	1.318	H $\rightarrow$ L
B4	SOS-PBE-QIDH	MeOH	$S_0 \rightarrow S_1$	2.391	1.229	H $\rightarrow$ L
B4	SOS-RSX-QIDH	MeOH	$S_0 \rightarrow S_1$	2.206	1.033	H $\rightarrow$ L
B4	SOS-ωB2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.375	1.114	H $\rightarrow$ L
B4	SOS-ωB88PP86	MeOH	$S_0 \rightarrow S_1$	2.368	1.142	H $\rightarrow$ L
B4	SOS-ωPBEPP86	MeOH	$S_0 \rightarrow S_1$	2.297	1.109	H $\rightarrow$ L
B4	ωB2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.563	1.202	H $\rightarrow$ L
B4	ωB2PLYP	MeOH	$S_0 \rightarrow S_1$	2.589	1.211	H $\rightarrow$ L
B4	ωB88PP86	MeOH	$S_0 \rightarrow S_1$	2.518	1.215	H $\rightarrow$ L
B4	ωB97X	MeOH	$S_0 \rightarrow S_1$	2.685	1.270	H $\rightarrow$ L
B4	ωPBEPP86	MeOH	$S_0 \rightarrow S_1$	2.497	1.206	H $\rightarrow$ L
B5	B2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.565	1.445	H-1 $\rightarrow$ L
B5	B2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.453	1.362	H-1 $\rightarrow$ L
B5	B3LYP	$CHCl_3$	$S_0 \rightarrow S_2$	2.769	0.768	H-1 $\rightarrow$ L
B5	BHLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.850	1.526	H-1 $\rightarrow$ L
B5	CAM-B3LYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.803	1.554	H-1 $\rightarrow$ L
B5	DSD-BLYP(CORRECT)	$CHCl_3$	$S_0 \rightarrow S_1$	2.557	1.403	H-1 $\rightarrow$ L
B5	DSD-BLYP(WRONG)	$CHCl_3$	$S_0 \rightarrow S_1$	2.077	1.140	H-1 $\rightarrow$ L
B5	DSD-PBEP86(CORRECT)	$CHCl_3$	$S_0 \rightarrow S_1$	2.551	1.418	H-1 $\rightarrow$ L
B5	DSD-PBEP86(WRONG)	$CHCl_3$	$S_0 \rightarrow S_1$	2.020	1.123	H-1 $\rightarrow$ L
B5	PBE-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.657	1.489	H-1 $\rightarrow$ L
B5	RSX-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.787	1.460	H-1 $\rightarrow$ L
B5	SCS-B2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.657	1.497	H-1 $\rightarrow$ L
B5	SCS-PBE-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.501	1.402	H-1 $\rightarrow$ L
B5	SCS-RSX-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.435	1.275	H-1 $\rightarrow$ L
B5	SOS-B2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.804	1.557	H-1 $\rightarrow$ L
B5	SOS-ωB2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.613	1.372	H-1 $\rightarrow$ L
B5	SCS-ωB2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.498	1.309	H-1 $\rightarrow$ L
B5	SCS-ωB88PP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.550	1.371	H-1 $\rightarrow$ L
B5	SCS-ωPBEPP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.406	1.293	H-1 $\rightarrow$ L
B5	SOS-B2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.604	1.468	H-1 $\rightarrow$ L
B5	SOS-PBE-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.473	1.386	H-1 $\rightarrow$ L
B5	SOS-RSX-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.349	1.230	H-1 $\rightarrow$ L
B5	SOS-ωB2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.525	1.324	H-1 $\rightarrow$ L
B5	SOS-ωB88PP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.501	1.345	H-1 $\rightarrow$ L
B5	SOS-ωPBEPP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.427	1.304	H-1 $\rightarrow$ L
B5	ωB2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.736	1.434	H-1 $\rightarrow$ L
B5	ωB2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.767	1.453	H-1 $\rightarrow$ L
B5	ωB88PP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.658	1.429	H-1 $\rightarrow$ L
B5	ωB97X	$CHCl_3$	$S_0 \rightarrow S_1$	2.875	1.541	H-1 $\rightarrow$ L
B5	ωPBEPP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.630	1.414	H-1 $\rightarrow$ L
B6	B2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.503	1.882	H-1 $\rightarrow$ L
B6	B2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.425	1.849	H-1 $\rightarrow$ L
B6	B3LYP	$CHCl_3$	$S_0 \rightarrow S_3$	2.527	1.411	H-1 $\rightarrow$ L
B6	BHLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.767	2.094	H-1 $\rightarrow$ L
B6	CAM-B3LYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.731	2.026	H-1 $\rightarrow$ L

B6	DSD-BLYP(CORRECT)	$CHCl_3$	$S_0 \rightarrow S_1$	2.498	1.822	H-1 → L
B6	DSD-BLYP(WRONG)	$CHCl_3$	$S_0 \rightarrow S_1$	2.049	1.495	H-1 → L
B6	DSD-PBEP86(CORRECT)	$CHCl_3$	$S_0 \rightarrow S_1$	2.493	1.840	H-1 → L
B6	DSD-PBEP86(WRONG)	$CHCl_3$	$S_0 \rightarrow S_1$	1.997	1.474	H-1 → L
B6	PBE-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.591	1.929	H-1 → L
B6	RSX-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.730	1.865	H-1 → L
B6	SCS-B2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.595	1.951	H-1 → L
B6	SCS-PBE-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.440	1.816	H-1 → L
B6	SCS-RSX-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.376	1.624	H-1 → L
B6	SOS-B2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.757	2.102	H-1 → L
B6	SOS-ωB2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.557	1.743	H-1 → L
B6	SCS-ωB2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.441	1.672	H-1 → L
B6	SCS-ωB88PP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.495	1.760	H-1 → L
B6	SCS-ωPBEPP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.347	1.658	H-1 → L
B6	SOS-B2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.542	1.912	H-1 → L
B6	SOS-PBE-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.412	1.796	H-1 → L
B6	SOS-RSX-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.295	1.568	H-1 → L
B6	SOS-ωB2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.470	1.691	H-1 → L
B6	SOS-ωB88PP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.447	1.727	H-1 → L
B6	SOS-ωPBEPP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.372	1.676	H-1 → L
B6	ωB2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.680	1.835	H-1 → L
B6	ωB2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.710	1.848	H-1 → L
B6	ωB88PP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.606	1.839	H-1 → L
B6	ωB97X	$CHCl_3$	$S_0 \rightarrow S_1$	2.815	1.930	H-1 → L
B6	ωPBEPP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.579	1.822	H-1 → L
B7	B2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.500	1.877	H → L
B7	B2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.431	1.856	H-1 → L
B7	B3LYP	$CHCl_3$	$S_0 \rightarrow S_3$	2.516	1.350	H-1 → L
B7	BHLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.767	2.105	H-1 → L
B7	CAM-B3LYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.728	2.020	H-1 → L
B7	DSD-BLYP(CORRECT)	$CHCl_3$	$S_0 \rightarrow S_1$	2.492	1.818	H → L
B7	DSD-BLYP(WRONG)	$CHCl_3$	$S_0 \rightarrow S_1$	2.044	1.491	H → L
B7	DSD-PBEP86(CORRECT)	$CHCl_3$	$S_0 \rightarrow S_1$	2.487	1.834	H → L
B7	DSD-PBEP86(WRONG)	$CHCl_3$	$S_0 \rightarrow S_1$	1.992	1.469	H → L
B7	PBE-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.586	1.923	H → L
B7	RSX-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.724	1.866	H → L
B7	SCS-B2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.590	1.944	H → L
B7	SCS-PBE-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.434	1.810	H → L
B7	SCS-RSX-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.370	1.623	H → L
B7	SOS-B2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.758	2.105	H-1 → L
B7	SOS-ωB2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.551	1.742	H → L
B7	SCS-ωB2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.435	1.670	H → L
B7	SCS-ωB88PP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.488	1.757	H → L
B7	SCS-ωPBEPP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.340	1.655	H → L
B7	SOS-B2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.537	1.905	H → L
B7	SOS-PBE-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.406	1.790	H → L
B7	SOS-RSX-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.288	1.567	H → L
B7	SOS-ωB2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.464	1.690	H → L
B7	SOS-ωB88PP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.441	1.724	H → L
B7	SOS-ωPBEPP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.365	1.672	H → L
B7	ωB2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.674	1.835	H → L
B7	ωB2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.704	1.847	H → L
B7	ωB88PP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.600	1.836	H → L
B7	ωB97X	$CHCl_3$	$S_0 \rightarrow S_1$	2.808	1.924	H-1 → L
B7	ωPBEPP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.573	1.819	H → L
B8	B2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.447	1.828	H-1 → L
B8	B2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.302	1.674	H-1 → L
B8	B3LYP	$CHCl_3$	$S_0 \rightarrow S_3$	2.477	1.265	H-1 → L
B8	BHLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.702	1.881	H-1 → L
B8	CAM-B3LYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.683	1.921	H-1 → L
B8	DSD-BLYP(CORRECT)	$CHCl_3$	$S_0 \rightarrow S_1$	2.458	1.781	H-1 → L
B8	DSD-BLYP(WRONG)	$CHCl_3$	$S_0 \rightarrow S_1$	2.002	1.450	H-1 → L

B8	DSD-PBEP86(CORRECT)	$CHCl_3$	$S_0 \rightarrow S_1$	2.451	1.798	H-1 $\rightarrow$ L
B8	DSD-PBEP86(WRONG)	$CHCl_3$	$S_0 \rightarrow S_1$	1.939	1.423	H-1 $\rightarrow$ L
B8	PBE-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.547	1.884	H-1 $\rightarrow$ L
B8	RSX-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.703	1.825	H-1 $\rightarrow$ L
B8	SCS-B2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.548	1.903	H-1 $\rightarrow$ L
B8	SCS-PBE-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.397	1.774	H-1 $\rightarrow$ L
B8	SCS-RSX-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.350	1.586	H-1 $\rightarrow$ L
B8	SOS-B2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.670	1.942	H-1 $\rightarrow$ L
B8	SOS-ωB2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.530	1.711	H-1 $\rightarrow$ L
B8	SCS-ωB2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.414	1.635	H-1 $\rightarrow$ L
B8	SCS-ωB88PP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.467	1.725	H-1 $\rightarrow$ L
B8	SCS-ωPBEPP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.320	1.622	H-1 $\rightarrow$ L
B8	SOS-B2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.494	1.863	H-1 $\rightarrow$ L
B8	SOS-PBE-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.371	1.754	H-1 $\rightarrow$ L
B8	SOS-RSX-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.269	1.531	H-1 $\rightarrow$ L
B8	SOS-ωB2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.442	1.654	H-1 $\rightarrow$ L
B8	SOS-ωB88PP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.420	1.693	H-1 $\rightarrow$ L
B8	SOS-ωPBEPP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.345	1.640	H-1 $\rightarrow$ L
B8	ωB2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.653	1.797	H-1 $\rightarrow$ L
B8	ωB2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.683	1.815	H-1 $\rightarrow$ L
B8	ωB88PP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.578	1.803	H-1 $\rightarrow$ L
B8	ωB97X	$CHCl_3$	$S_0 \rightarrow S_1$	2.790	1.921	H-1 $\rightarrow$ L
B8	ωPBEPP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.552	1.784	H-1 $\rightarrow$ L
B9	B2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.526	1.537	H-1 $\rightarrow$ L
B9	B2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.370	1.355	H-1 $\rightarrow$ L
B9	B3LYP	$CHCl_3$	$S_0 \rightarrow S_3$	2.675	1.275	H-1 $\rightarrow$ L
B9	BHLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.794	1.475	H-1 $\rightarrow$ L
B9	CAM-B3LYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.775	1.628	H-1 $\rightarrow$ L
B9	DSD-BLYP(CORRECT)	$CHCl_3$	$S_0 \rightarrow S_1$	2.525	1.496	H-1 $\rightarrow$ L
B9	DSD-BLYP(WRONG)	$CHCl_3$	$S_0 \rightarrow S_1$	2.035	1.206	H-1 $\rightarrow$ L
B9	DSD-PBEP86(CORRECT)	$CHCl_3$	$S_0 \rightarrow S_1$	2.520	1.512	H-1 $\rightarrow$ L
B9	DSD-PBEP86(WRONG)	$CHCl_3$	$S_0 \rightarrow S_1$	1.975	1.184	H-1 $\rightarrow$ L
B9	PBE-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.625	1.588	H-1 $\rightarrow$ L
B9	RSX-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.766	1.534	H-1 $\rightarrow$ L
B9	SCS-B2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.630	1.601	H-1 $\rightarrow$ L
B9	SCS-PBE-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.472	1.496	H-1 $\rightarrow$ L
B9	SCS-RSX-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.403	1.333	H-1 $\rightarrow$ L
B9	SOS-B2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.758	1.576	H-1 $\rightarrow$ L
B9	SOS-ωB2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.590	1.435	H-1 $\rightarrow$ L
B9	SCS-ωB2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.471	1.373	H-1 $\rightarrow$ L
B9	SCS-ωB88PP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.524	1.445	H-1 $\rightarrow$ L
B9	SCS-ωPBEPP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.374	1.360	H-1 $\rightarrow$ L
B9	SOS-B2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.576	1.568	H-1 $\rightarrow$ L
B9	SOS-PBE-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.446	1.480	H-1 $\rightarrow$ L
B9	SOS-RSX-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.323	1.288	H-1 $\rightarrow$ L
B9	SOS-ωB2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.501	1.389	H-1 $\rightarrow$ L
B9	SOS-ωB88PP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.477	1.418	H-1 $\rightarrow$ L
B9	SOS-ωPBEPP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.401	1.376	H-1 $\rightarrow$ L
B9	ωB2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.714	1.507	H-1 $\rightarrow$ L
B9	ωB2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.745	1.521	H-1 $\rightarrow$ L
B9	ωB88PP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.633	1.507	H-1 $\rightarrow$ L
B9	ωB97X	$CHCl_3$	$S_0 \rightarrow S_1$	2.857	1.604	H-1 $\rightarrow$ L
B9	ωPBEPP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.604	1.492	H-1 $\rightarrow$ L
B10	B2GP-PLYP	THF	$S_0 \rightarrow S_1$	3.779	0.473	H $\rightarrow$ L
B10	B2PLYP	THF	$S_0 \rightarrow S_1$	3.648	0.429	H $\rightarrow$ L
B10	B3LYP	THF	$S_0 \rightarrow S_1$	3.527	0.254	H $\rightarrow$ L
B10	BHLYP	THF	$S_0 \rightarrow S_1$	4.018	0.461	H $\rightarrow$ L
B10	CAM-B3LYP	THF	$S_0 \rightarrow S_1$	3.981	0.438	H $\rightarrow$ L
B10	DSD-BLYP(CORRECT)	THF	$S_0 \rightarrow S_1$	3.827	0.494	H $\rightarrow$ L
B10	DSD-BLYP(WRONG)	THF	$S_0 \rightarrow S_1$	3.337	0.431	H $\rightarrow$ L
B10	DSD-PBEP86(CORRECT)	THF	$S_0 \rightarrow S_1$	3.810	0.487	H $\rightarrow$ L
B10	DSD-PBEP86(WRONG)	THF	$S_0 \rightarrow S_1$	3.252	0.416	H $\rightarrow$ L

B10	PBE-QIDH	THF	$S_0 \rightarrow S_1$	3.905	0.493	H $\rightarrow$ L
B10	RSX-QIDH	THF	$S_0 \rightarrow S_1$	4.173	0.531	H $\rightarrow$ L
B10	SCS-B2GP-PLYP	THF	$S_0 \rightarrow S_1$	3.873	0.485	H $\rightarrow$ L
B10	SCS-PBE-QIDH	THF	$S_0 \rightarrow S_1$	3.758	0.474	H $\rightarrow$ L
B10	SCS-RSX-QIDH	THF	$S_0 \rightarrow S_1$	3.851	0.490	H $\rightarrow$ L
B10	SOS-B2PLYP	THF	$S_0 \rightarrow S_1$	3.963	0.466	H $\rightarrow$ L
B10	SOS-ωB2PLYP	THF	$S_0 \rightarrow S_1$	3.991	0.499	H $\rightarrow$ L
B10	SCS-ωB2GP-PLYP	THF	$S_0 \rightarrow S_1$	3.889	0.495	H $\rightarrow$ L
B10	SCS-ωB88PP86	THF	$S_0 \rightarrow S_1$	3.890	0.494	H $\rightarrow$ L
B10	SCS-ωPBEPP86	THF	$S_0 \rightarrow S_1$	3.763	0.481	H $\rightarrow$ L
B10	SOS-B2GP-PLYP	THF	$S_0 \rightarrow S_1$	3.823	0.479	H $\rightarrow$ L
B10	SOS-PBE-QIDH	THF	$S_0 \rightarrow S_1$	3.732	0.471	H $\rightarrow$ L
B10	SOS-RSX-QIDH	THF	$S_0 \rightarrow S_1$	3.763	0.479	H $\rightarrow$ L
B10	SOS-ωB2GP-PLYP	THF	$S_0 \rightarrow S_1$	3.911	0.498	H $\rightarrow$ L
B10	SOS-ωB88PP86	THF	$S_0 \rightarrow S_1$	3.841	0.488	H $\rightarrow$ L
B10	SOS-ωPBEPP86	THF	$S_0 \rightarrow S_1$	3.775	0.482	H $\rightarrow$ L
B10	ωB2GP-PLYP	THF	$S_0 \rightarrow S_1$	4.101	0.522	H $\rightarrow$ L
B10	ωB2PLYP	THF	$S_0 \rightarrow S_1$	4.129	0.516	H $\rightarrow$ L
B10	ωB88PP86	THF	$S_0 \rightarrow S_1$	3.975	0.505	H $\rightarrow$ L
B10	ωB97X	THF	$S_0 \rightarrow S_1$	4.195	0.494	H $\rightarrow$ L
B10	ωPBEPP86	THF	$S_0 \rightarrow S_1$	3.952	0.505	H $\rightarrow$ L
B11	B2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.911	0.860	H $\rightarrow$ L
B11	B2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.945	0.863	H $\rightarrow$ L
B11	B3LYP	$CHCl_3$	$S_0 \rightarrow S_1$	3.215	0.729	H $\rightarrow$ L
B11	BHLYP	$CHCl_3$	$S_0 \rightarrow S_1$	3.203	0.932	H $\rightarrow$ L
B11	CAM-B3LYP	$CHCl_3$	$S_0 \rightarrow S_1$	3.137	0.872	H $\rightarrow$ L
B11	DSD-BLYP(CORRECT)	$CHCl_3$	$S_0 \rightarrow S_1$	2.862	0.846	H $\rightarrow$ L
B11	DSD-BLYP(WRONG)	$CHCl_3$	$S_0 \rightarrow S_1$	2.511	0.742	H $\rightarrow$ L
B11	DSD-PBEP86(CORRECT)	$CHCl_3$	$S_0 \rightarrow S_1$	2.849	0.842	H $\rightarrow$ L
B11	DSD-PBEP86(WRONG)	$CHCl_3$	$S_0 \rightarrow S_1$	2.494	0.737	H $\rightarrow$ L
B11	PBE-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.959	0.872	H $\rightarrow$ L
B11	RSX-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.963	0.849	H $\rightarrow$ L
B11	SCS-B2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.929	0.866	H $\rightarrow$ L
B11	SCS-PBE-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.787	0.821	H $\rightarrow$ L
B11	SCS-RSX-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.702	0.774	H $\rightarrow$ L
B11	SOS-B2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	3.174	0.930	H $\rightarrow$ L
B11	SOS-ωB2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.777	0.790	H $\rightarrow$ L
B11	SCS-ωB2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.690	0.772	H $\rightarrow$ L
B11	SCS-ωB88PP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.766	0.799	H $\rightarrow$ L
B11	SCS-ωPBEPP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.671	0.774	H $\rightarrow$ L
B11	SOS-B2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.882	0.852	H $\rightarrow$ L
B11	SOS-PBE-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.743	0.808	H $\rightarrow$ L
B11	SOS-RSX-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.524	0.723	H $\rightarrow$ L
B11	SOS-ωB2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.688	0.771	H $\rightarrow$ L
B11	SOS-ωB88PP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.701	0.780	H $\rightarrow$ L
B11	SOS-ωPBEPP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.629	0.761	H $\rightarrow$ L
B11	ωB2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.922	0.839	H $\rightarrow$ L
B11	ωB2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.950	0.839	H $\rightarrow$ L
B11	ωB88PP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.897	0.837	H $\rightarrow$ L
B11	ωB97X	$CHCl_3$	$S_0 \rightarrow S_1$	3.080	0.852	H $\rightarrow$ L
B11	ωPBEPP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.876	0.833	H $\rightarrow$ L
B11	B2GP-PLYP	THF	$S_0 \rightarrow S_1$	2.929	0.852	H $\rightarrow$ L
B11	B2PLYP	THF	$S_0 \rightarrow S_1$	2.962	0.852	H $\rightarrow$ L
B11	B3LYP	THF	$S_0 \rightarrow S_1$	3.229	0.703	H $\rightarrow$ L
B11	BHLYP	THF	$S_0 \rightarrow S_1$	3.223	0.920	H $\rightarrow$ L
B11	CAM-B3LYP	THF	$S_0 \rightarrow S_1$	3.156	0.860	H $\rightarrow$ L
B11	DSD-BLYP(CORRECT)	THF	$S_0 \rightarrow S_1$	2.881	0.838	H $\rightarrow$ L
B11	DSD-BLYP(WRONG)	THF	$S_0 \rightarrow S_1$	2.526	0.735	H $\rightarrow$ L
B11	DSD-PBEP86(CORRECT)	THF	$S_0 \rightarrow S_1$	2.868	0.834	H $\rightarrow$ L
B11	DSD-PBEP86(WRONG)	THF	$S_0 \rightarrow S_1$	2.509	0.730	H $\rightarrow$ L
B11	PBE-QIDH	THF	$S_0 \rightarrow S_1$	2.979	0.864	H $\rightarrow$ L
B11	RSX-QIDH	THF	$S_0 \rightarrow S_1$	2.984	0.842	H $\rightarrow$ L

B11	SCS-B2GP-PLYP	THF	$S_0 \rightarrow S_1$	2.948	0.857	H $\rightarrow$ L
B11	SCS-PBE-QIDH	THF	$S_0 \rightarrow S_1$	2.806	0.813	H $\rightarrow$ L
B11	SCS-RSX-QIDH	THF	$S_0 \rightarrow S_1$	2.722	0.768	H $\rightarrow$ L
B11	SOS-B2PLYP	THF	$S_0 \rightarrow S_1$	3.193	0.918	H $\rightarrow$ L
B11	SOS-ωB2PLYP	THF	$S_0 \rightarrow S_1$	2.797	0.783	H $\rightarrow$ L
B11	SCS-ωB2GP-PLYP	THF	$S_0 \rightarrow S_1$	2.689	0.771	H $\rightarrow$ L
B11	SCS-ωB88PP86	THF	$S_0 \rightarrow S_1$	2.785	0.792	H $\rightarrow$ L
B11	SCS-ωPBEPP86	THF	$S_0 \rightarrow S_1$	2.690	0.767	H $\rightarrow$ L
B11	SOS-B2GP-PLYP	THF	$S_0 \rightarrow S_1$	2.901	0.844	H $\rightarrow$ L
B11	SOS-PBE-QIDH	THF	$S_0 \rightarrow S_1$	2.762	0.801	H $\rightarrow$ L
B11	SOS-RSX-QIDH	THF	$S_0 \rightarrow S_1$	2.544	0.718	H $\rightarrow$ L
B11	SOS-ωB2GP-PLYP	THF	$S_0 \rightarrow S_1$	2.708	0.765	H $\rightarrow$ L
B11	SOS-ωB88PP86	THF	$S_0 \rightarrow S_1$	2.721	0.774	H $\rightarrow$ L
B11	SOS-ωPBEPP86	THF	$S_0 \rightarrow S_1$	2.895	0.843	H $\rightarrow$ L
B11	ωB2GP-PLYP	THF	$S_0 \rightarrow S_1$	2.942	0.832	H $\rightarrow$ L
B11	ωB2PLYP	THF	$S_0 \rightarrow S_1$	2.970	0.832	H $\rightarrow$ L
B11	ωB88PP86	THF	$S_0 \rightarrow S_1$	2.917	0.829	H $\rightarrow$ L
B11	ωB97X	THF	$S_0 \rightarrow S_1$	3.100	0.843	H $\rightarrow$ L
B11	ωPBEPP86	THF	$S_0 \rightarrow S_1$	2.895	0.826	H $\rightarrow$ L
B12	B2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.483	2.110	H-1 $\rightarrow$ L
B12	B2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.373	2.034	H-1 $\rightarrow$ L
B12	B3LYP	$CHCl_3$	$S_0 \rightarrow S_3$	2.480	1.392	H-1 $\rightarrow$ L
B12	BHLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.733	2.299	H-1 $\rightarrow$ L
B12	CAM-B3LYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.709	2.248	H-1 $\rightarrow$ L
B12	DSD-BLYP(CORRECT)	$CHCl_3$	$S_0 \rightarrow S_1$	2.487	2.029	H-1 $\rightarrow$ L
B12	DSD-BLYP(WRONG)	$CHCl_3$	$S_0 \rightarrow S_1$	2.052	1.674	H-1 $\rightarrow$ L
B12	DSD-PBEP86(CORRECT)	$CHCl_3$	$S_0 \rightarrow S_1$	2.481	2.054	H-1 $\rightarrow$ L
B12	DSD-PBEP86(WRONG)	$CHCl_3$	$S_0 \rightarrow S_1$	1.996	1.653	H-1 $\rightarrow$ L
B12	PBE-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.575	2.154	H-1 $\rightarrow$ L
B12	RSX-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.717	2.027	H-1 $\rightarrow$ L
B12	SCS-B2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.579	2.191	H-1 $\rightarrow$ L
B12	SCS-PBE-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.427	2.030	H-1 $\rightarrow$ L
B12	SCS-RSX-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.366	1.766	H-1 $\rightarrow$ L
B12	SOS-B2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.721	2.333	H-1 $\rightarrow$ L
B12	SOS-ωB2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.544	1.901	H-1 $\rightarrow$ L
B12	SCS-ωB2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.429	1.822	H-1 $\rightarrow$ L
B12	SCS-ωB88PP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.486	1.934	H-1 $\rightarrow$ L
B12	SCS-ωPBEPP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.339	1.821	H-1 $\rightarrow$ L
B12	SOS-B2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.526	2.147	H-1 $\rightarrow$ L
B12	SOS-PBE-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.400	2.008	H-1 $\rightarrow$ L
B12	SOS-RSX-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.284	1.704	H-1 $\rightarrow$ L
B12	SOS-ωB2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.457	1.843	H-1 $\rightarrow$ L
B12	SOS-ωB88PP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.439	1.898	H-1 $\rightarrow$ L
B12	SOS-ωPBEPP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.365	1.841	H-1 $\rightarrow$ L
B12	ωB2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.668	2.001	H-1 $\rightarrow$ L
B12	ωB2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.697	2.015	H-1 $\rightarrow$ L
B12	ωB88PP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.599	2.022	H-1 $\rightarrow$ L
B12	ωB97X	$CHCl_3$	$S_0 \rightarrow S_1$	2.804	2.129	H-1 $\rightarrow$ L
B12	ωPBEPP86	$CHCl_3$	$S_0 \rightarrow S_1$	2.573	2.003	H-1 $\rightarrow$ L
B13	B2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	1.845	1.307	H $\rightarrow$ L
B13	B2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	1.756	1.303	H $\rightarrow$ L
B13	B3LYP	$CHCl_3$	$S_0 \rightarrow S_1$	1.684	1.262	H $\rightarrow$ L
B13	BHLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.027	1.521	H $\rightarrow$ L
B13	CAM-B3LYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.023	1.450	H $\rightarrow$ L
B13	DSD-BLYP(CORRECT)	$CHCl_3$	$S_0 \rightarrow S_1$	1.857	1.260	H $\rightarrow$ L
B13	DSD-BLYP(WRONG)	$CHCl_3$	$S_0 \rightarrow S_1$	1.541	1.046	H $\rightarrow$ L
B13	DSD-PBEP86(CORRECT)	$CHCl_3$	$S_0 \rightarrow S_1$	1.865	1.286	H $\rightarrow$ L
B13	DSD-PBEP86(WRONG)	$CHCl_3$	$S_0 \rightarrow S_1$	1.483	1.023	H $\rightarrow$ L
B13	PBE-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	1.917	1.340	H $\rightarrow$ L
B13	RSX-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	2.075	1.310	H $\rightarrow$ L
B13	SCS-B2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	1.979	1.402	H $\rightarrow$ L
B13	SCS-PBE-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	1.816	1.269	H $\rightarrow$ L

B13	SCS-RSX-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	1.724	1.088	H $\rightarrow$ L
B13	SOS-B2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.113	1.569	H $\rightarrow$ L
B13	SOS-ωB2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	1.951	1.231	H $\rightarrow$ L
B13	SCS-ωB2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	1.835	1.158	H $\rightarrow$ L
B13	SCS-ωB88PP86	$CHCl_3$	$S_0 \rightarrow S_1$	1.884	1.224	H $\rightarrow$ L
B13	SCS-ωPBEPP86	$CHCl_3$	$S_0 \rightarrow S_1$	1.715	1.116	H $\rightarrow$ L
B13	SOS-B2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	1.927	1.365	H $\rightarrow$ L
B13	SOS-PBE-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	1.802	1.260	H $\rightarrow$ L
B13	SOS-RSX-QIDH	$CHCl_3$	$S_0 \rightarrow S_1$	1.710	1.079	H $\rightarrow$ L
B13	SOS-ωB2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	1.879	1.186	H $\rightarrow$ L
B13	SOS-ωB88PP86	$CHCl_3$	$S_0 \rightarrow S_1$	1.849	1.201	H $\rightarrow$ L
B13	SOS-ωPBEPP86	$CHCl_3$	$S_0 \rightarrow S_1$	1.778	1.157	H $\rightarrow$ L
B13	ωB2GP-PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.040	1.288	H $\rightarrow$ L
B13	ωB2PLYP	$CHCl_3$	$S_0 \rightarrow S_1$	2.064	1.303	H $\rightarrow$ L
B13	ωB88PP86	$CHCl_3$	$S_0 \rightarrow S_1$	1.972	1.281	H $\rightarrow$ L
B13	ωB97X	$CHCl_3$	$S_0 \rightarrow S_1$	2.148	1.374	H $\rightarrow$ L
B13	ωPBEPP86	$CHCl_3$	$S_0 \rightarrow S_1$	1.951	1.269	H $\rightarrow$ L
B14	B2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.855	0.992	H $\rightarrow$ L
B14	B2PLYP	MeOH	$S_0 \rightarrow S_1$	2.847	1.008	H $\rightarrow$ L
B14	B3LYP	MeOH	$S_0 \rightarrow S_1$	3.025	1.022	H $\rightarrow$ L
B14	BHLYP	MeOH	$S_0 \rightarrow S_1$	3.193	1.133	H $\rightarrow$ L
B14	CAM-B3LYP	MeOH	$S_0 \rightarrow S_1$	3.114	1.092	H $\rightarrow$ L
B14	DSD-BLYP(CORRECT)	MeOH	$S_0 \rightarrow S_1$	2.805	0.956	H $\rightarrow$ L
B14	DSD-BLYP(WRONG)	MeOH	$S_0 \rightarrow S_1$	2.308	0.787	H $\rightarrow$ L
B14	DSD-PBEP86(CORRECT)	MeOH	$S_0 \rightarrow S_1$	2.816	0.968	H $\rightarrow$ L
B14	DSD-PBEP86(WRONG)	MeOH	$S_0 \rightarrow S_1$	2.265	0.779	H $\rightarrow$ L
B14	PBE-QIDH	MeOH	$S_0 \rightarrow S_1$	2.931	1.014	H $\rightarrow$ L
B14	RSX-QIDH	MeOH	$S_0 \rightarrow S_1$	3.019	1.002	H $\rightarrow$ L
B14	SCS-B2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.954	1.027	H $\rightarrow$ L
B14	SCS-PBE-QIDH	MeOH	$S_0 \rightarrow S_1$	2.788	0.965	H $\rightarrow$ L
B14	SCS-RSX-QIDH	MeOH	$S_0 \rightarrow S_1$	2.676	0.889	H $\rightarrow$ L
B14	SOS-B2PLYP	MeOH	$S_0 \rightarrow S_1$	3.164	1.120	H $\rightarrow$ L
B14	SOS-ωB2PLYP	MeOH	$S_0 \rightarrow S_1$	2.859	0.952	H $\rightarrow$ L
B14	SCS-ωB2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.745	0.912	H $\rightarrow$ L
B14	SCS-ωB88PP86	MeOH	$S_0 \rightarrow S_1$	2.801	0.946	H $\rightarrow$ L
B14	SCS-ωPBEPP86	MeOH	$S_0 \rightarrow S_1$	2.659	0.897	H $\rightarrow$ L
B14	SOS-B2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.903	1.009	H $\rightarrow$ L
B14	SOS-PBE-QIDH	MeOH	$S_0 \rightarrow S_1$	2.762	0.956	H $\rightarrow$ L
B14	SOS-RSX-QIDH	MeOH	$S_0 \rightarrow S_1$	2.596	0.862	H $\rightarrow$ L
B14	SOS-ωB2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.771	0.920	H $\rightarrow$ L
B14	SOS-ωB88PP86	MeOH	$S_0 \rightarrow S_1$	2.752	0.929	H $\rightarrow$ L
B14	SOS-ωPBEPP86	MeOH	$S_0 \rightarrow S_1$	2.678	0.903	H $\rightarrow$ L
B14	ωB2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.965	0.985	H $\rightarrow$ L
B14	ωB2PLYP	MeOH	$S_0 \rightarrow S_1$	2.999	0.999	H $\rightarrow$ L
B14	ωB88PP86	MeOH	$S_0 \rightarrow S_1$	2.887	0.975	H $\rightarrow$ L
B14	ωB97X	MeOH	$S_0 \rightarrow S_1$	3.130	1.057	H $\rightarrow$ L
B14	ωPBEPP86	MeOH	$S_0 \rightarrow S_1$	2.856	0.964	H $\rightarrow$ L
B15	B2GP-PLYP	DCM	$S_0 \rightarrow S_1$	2.028	1.562	H $\rightarrow$ L
B15	B2PLYP	DCM	$S_0 \rightarrow S_1$	1.893	1.573	H $\rightarrow$ L
B15	B3LYP	DCM	$S_0 \rightarrow S_1$	1.752	1.336	H $\rightarrow$ L
B15	BHLYP	DCM	$S_0 \rightarrow S_1$	2.252	1.897	H $\rightarrow$ L
B15	CAM-B3LYP	DCM	$S_0 \rightarrow S_1$	2.247	1.820	H $\rightarrow$ L
B15	DSD-BLYP(CORRECT)	DCM	$S_0 \rightarrow S_1$	2.051	1.473	H $\rightarrow$ L
B15	DSD-BLYP(WRONG)	DCM	$S_0 \rightarrow S_1$	1.675	1.203	H $\rightarrow$ L
B15	DSD-PBEP86(CORRECT)	DCM	$S_0 \rightarrow S_1$	2.055	1.513	H $\rightarrow$ L
B15	DSD-PBEP86(WRONG)	DCM	$S_0 \rightarrow S_1$	1.603	1.180	H $\rightarrow$ L
B15	PBE-QIDH	DCM	$S_0 \rightarrow S_1$	2.120	1.593	H $\rightarrow$ L
B15	RSX-QIDH	DCM	$S_0 \rightarrow S_1$	2.292	1.482	H $\rightarrow$ L
B15	SCS-B2GP-PLYP	DCM	$S_0 \rightarrow S_1$	2.165	1.668	H $\rightarrow$ L
B15	SCS-PBE-QIDH	DCM	$S_0 \rightarrow S_1$	2.009	1.510	H $\rightarrow$ L
B15	SCS-RSX-QIDH	DCM	$S_0 \rightarrow S_1$	1.947	1.258	H $\rightarrow$ L
B15	SOS-B2PLYP	DCM	$S_0 \rightarrow S_1$	2.278	1.893	H $\rightarrow$ L

B15	SOS-ωB2PLYP	DCM	$S_0 \rightarrow S_1$	2.159	1.408	H $\rightarrow$ L
B15	SCS-ωB2GP-PLYP	DCM	$S_0 \rightarrow S_1$	2.044	1.328	H $\rightarrow$ L
B15	SCS-ωB88PP86	DCM	$S_0 \rightarrow S_1$	2.093	1.417	H $\rightarrow$ L
B15	SCS-ωPBEPP86	DCM	$S_0 \rightarrow S_1$	1.933	1.307	H $\rightarrow$ L
B15	SOS-B2GP-PLYP	DCM	$S_0 \rightarrow S_1$	2.113	1.628	H $\rightarrow$ L
B15	SOS-PBE-QIDH	DCM	$S_0 \rightarrow S_1$	1.994	1.498	H $\rightarrow$ L
B15	SOS-RSX-QIDH	DCM	$S_0 \rightarrow S_1$	1.913	1.237	H $\rightarrow$ L
B15	SOS-ωB2GP-PLYP	DCM	$S_0 \rightarrow S_1$	2.083	1.353	H $\rightarrow$ L
B15	SOS-ωB88PP86	DCM	$S_0 \rightarrow S_1$	2.054	1.391	H $\rightarrow$ L
B15	SOS-ωPBEPP86	DCM	$S_0 \rightarrow S_1$	1.982	1.341	H $\rightarrow$ L
B15	ωB2GP-PLYP	DCM	$S_0 \rightarrow S_1$	2.253	1.464	H $\rightarrow$ L
B15	ωB2PLYP	DCM	$S_0 \rightarrow S_1$	2.280	1.487	H $\rightarrow$ L
B15	ωB88PP86	DCM	$S_0 \rightarrow S_1$	2.181	1.477	H $\rightarrow$ L
B15	ωB97X	DCM	$S_0 \rightarrow S_1$	2.376	1.608	H $\rightarrow$ L
B15	ωPBEPP86	DCM	$S_0 \rightarrow S_1$	2.158	1.459	H $\rightarrow$ L
B16	B2GP-PLYP	DCM	$S_0 \rightarrow S_1$	2.081	1.322	H $\rightarrow$ L
B16	B2PLYP	DCM	$S_0 \rightarrow S_1$	2.038	1.355	H $\rightarrow$ L
B16	B3LYP	DCM	$S_0 \rightarrow S_1$	2.001	1.270	H $\rightarrow$ L
B16	BHLYP	DCM	$S_0 \rightarrow S_1$	2.250	1.513	H $\rightarrow$ L
B16	CAM-B3LYP	DCM	$S_0 \rightarrow S_1$	2.240	1.441	H $\rightarrow$ L
B16	DSD-BLYP(CORRECT)	DCM	$S_0 \rightarrow S_1$	2.069	1.265	H $\rightarrow$ L
B16	DSD-BLYP(WRONG)	DCM	$S_0 \rightarrow S_1$	1.789	1.094	H $\rightarrow$ L
B16	DSD-PBEP86(CORRECT)	DCM	$S_0 \rightarrow S_1$	2.084	1.292	H $\rightarrow$ L
B16	DSD-PBEP86(WRONG)	DCM	$S_0 \rightarrow S_1$	1.756	1.089	H $\rightarrow$ L
B16	PBE-QIDH	DCM	$S_0 \rightarrow S_1$	2.138	1.343	H $\rightarrow$ L
B16	RSX-QIDH	DCM	$S_0 \rightarrow S_1$	2.242	1.286	H $\rightarrow$ L
B16	SCS-B2GP-PLYP	DCM	$S_0 \rightarrow S_1$	2.198	1.397	H $\rightarrow$ L
B16	SCS-PBE-QIDH	DCM	$S_0 \rightarrow S_1$	2.036	1.279	H $\rightarrow$ L
B16	SCS-RSX-QIDH	DCM	$S_0 \rightarrow S_1$	1.899	1.089	H $\rightarrow$ L
B16	SOS-B2PLYP	DCM	$S_0 \rightarrow S_1$	2.363	1.571	H $\rightarrow$ L
B16	SOS-ωB2PLYP	DCM	$S_0 \rightarrow S_1$	2.119	1.214	H $\rightarrow$ L
B16	SCS-ωB2GP-PLYP	DCM	$S_0 \rightarrow S_1$	2.005	1.150	H $\rightarrow$ L
B16	SCS-ωB88PP86	DCM	$S_0 \rightarrow S_1$	2.063	1.215	H $\rightarrow$ L
B16	SCS-ωPBEPP86	DCM	$S_0 \rightarrow S_1$	1.899	1.120	H $\rightarrow$ L
B16	SOS-B2GP-PLYP	DCM	$S_0 \rightarrow S_1$	2.148	1.366	H $\rightarrow$ L
B16	SOS-PBE-QIDH	DCM	$S_0 \rightarrow S_1$	2.020	1.269	H $\rightarrow$ L
B16	SOS-RSX-QIDH	DCM	$S_0 \rightarrow S_1$	1.880	1.078	H $\rightarrow$ L
B16	SOS-ωB2GP-PLYP	DCM	$S_0 \rightarrow S_1$	2.047	1.174	H $\rightarrow$ L
B16	SOS-ωB88PP86	DCM	$S_0 \rightarrow S_1$	2.027	1.194	H $\rightarrow$ L
B16	SOS-ωPBEPP86	DCM	$S_0 \rightarrow S_1$	1.957	1.154	H $\rightarrow$ L
B16	ωB2GP-PLYP	DCM	$S_0 \rightarrow S_1$	2.210	1.267	H $\rightarrow$ L
B16	ωB2PLYP	DCM	$S_0 \rightarrow S_1$	2.234	1.280	H $\rightarrow$ L
B16	ωB88PP86	DCM	$S_0 \rightarrow S_1$	2.156	1.269	H $\rightarrow$ L
B16	ωB97X	DCM	$S_0 \rightarrow S_1$	2.314	1.340	H $\rightarrow$ L
B16	ωPBEPP86	DCM	$S_0 \rightarrow S_1$	2.136	1.260	H $\rightarrow$ L
B17	B2GP-PLYP	THF	$S_0 \rightarrow S_1$	3.566	0.619	H $\rightarrow$ L
B17	B2PLYP	THF	$S_0 \rightarrow S_1$	3.521	0.623	H $\rightarrow$ L
B17	B3LYP	THF	$S_0 \rightarrow S_1$	3.640	0.593	H $\rightarrow$ L
B17	BHLYP	THF	$S_0 \rightarrow S_1$	3.936	0.699	H $\rightarrow$ L
B17	CAM-B3LYP	THF	$S_0 \rightarrow S_1$	3.826	0.685	H $\rightarrow$ L
B17	DSD-BLYP(CORRECT)	THF	$S_0 \rightarrow S_1$	3.539	0.598	H $\rightarrow$ L
B17	DSD-BLYP(WRONG)	THF	$S_0 \rightarrow S_1$	2.896	0.489	H $\rightarrow$ L
B17	DSD-PBEP86(CORRECT)	THF	$S_0 \rightarrow S_1$	3.535	0.604	H $\rightarrow$ L
B17	DSD-PBEP86(WRONG)	THF	$S_0 \rightarrow S_1$	2.838	0.485	H $\rightarrow$ L
B17	PBE-QIDH	THF	$S_0 \rightarrow S_1$	3.683	0.636	H $\rightarrow$ L
B17	RSX-QIDH	THF	$S_0 \rightarrow S_1$	3.842	0.642	H $\rightarrow$ L
B17	SCS-B2GP-PLYP	THF	$S_0 \rightarrow S_1$	3.647	0.633	H $\rightarrow$ L
B17	SCS-PBE-QIDH	THF	$S_0 \rightarrow S_1$	3.502	0.605	H $\rightarrow$ L
B17	SCS-RSX-QIDH	THF	$S_0 \rightarrow S_1$	3.475	0.581	H $\rightarrow$ L
B17	SOS-B2PLYP	THF	$S_0 \rightarrow S_1$	3.829	0.677	H $\rightarrow$ L
B17	SOS-ωB2PLYP	THF	$S_0 \rightarrow S_1$	3.617	0.615	H $\rightarrow$ L
B17	SCS-ωB2GP-PLYP	THF	$S_0 \rightarrow S_1$	3.506	0.587	H $\rightarrow$ L

B17	SCS-ωB88PP86	THF	$S_0 \rightarrow S_1$	3.548	0.603	H $\rightarrow$ L
B17	SCS-ωPBEPP86	THF	$S_0 \rightarrow S_1$	3.419	0.578	H $\rightarrow$ L
B17	SOS-B2GP-PLYP	THF	$S_0 \rightarrow S_1$	3.593	0.623	H $\rightarrow$ L
B17	SOS-PBE-QIDH	THF	$S_0 \rightarrow S_1$	3.468	0.599	H $\rightarrow$ L
B17	SOS-RSX-QIDH	THF	$S_0 \rightarrow S_1$	3.355	0.561	H $\rightarrow$ L
B17	SOS-ωB2GP-PLYP	THF	$S_0 \rightarrow S_1$	3.525	0.590	H $\rightarrow$ L
B17	SOS-ωB88PP86	THF	$S_0 \rightarrow S_1$	3.492	0.593	H $\rightarrow$ L
B17	SOS-ωPBEPP86	THF	$S_0 \rightarrow S_1$	3.419	0.578	H $\rightarrow$ L
B17	ωB2GP-PLYP	THF	$S_0 \rightarrow S_1$	3.757	0.629	H $\rightarrow$ L
B17	ωB2PLYP	THF	$S_0 \rightarrow S_1$	3.789	0.644	H $\rightarrow$ L
B17	ωB88PP86	THF	$S_0 \rightarrow S_1$	3.649	0.620	H $\rightarrow$ L
B17	ωB97X	THF	$S_0 \rightarrow S_1$	3.916	0.687	H $\rightarrow$ L
B17	ωPBEPP86	THF	$S_0 \rightarrow S_1$	3.616	0.612	H $\rightarrow$ L
B18	B2GP-PLYP	DCM	$S_0 \rightarrow S_1$	2.750	0.849	H $\rightarrow$ L
B18	B2PLYP	DCM	$S_0 \rightarrow S_1$	2.789	0.862	H $\rightarrow$ L
B18	B3LYP	DCM	$S_0 \rightarrow S_1$	2.424	0.022	H-1 $\rightarrow$ L
B18	BHLYP	DCM	$S_0 \rightarrow S_1$	3.040	0.938	H $\rightarrow$ L
B18	CAM-B3LYP	DCM	$S_0 \rightarrow S_1$	2.972	0.887	H $\rightarrow$ L
B18	DSD-BLYP(CORRECT)	DCM	$S_0 \rightarrow S_1$	2.688	0.823	H $\rightarrow$ L+1
B18	DSD-BLYP(WRONG)	DCM	$S_0 \rightarrow S_1$	2.324	0.712	H $\rightarrow$ L+1
B18	DSD-PBEP86(CORRECT)	DCM	$S_0 \rightarrow S_1$	2.689	0.827	H $\rightarrow$ L+1
B18	DSD-PBEP86(WRONG)	DCM	$S_0 \rightarrow S_1$	2.311	0.711	H $\rightarrow$ L+1
B18	PBE-QIDH	DCM	$S_0 \rightarrow S_1$	2.793	0.861	H $\rightarrow$ L+1
B18	RSX-QIDH	DCM	$S_0 \rightarrow S_1$	2.793	0.832	H $\rightarrow$ L
B18	SCS-B2GP-PLYP	DCM	$S_0 \rightarrow S_1$	2.797	0.863	H $\rightarrow$ L
B18	SCS-PBE-QIDH	DCM	$S_0 \rightarrow S_1$	2.634	0.812	H $\rightarrow$ L+1
B18	SCS-RSX-QIDH	DCM	$S_0 \rightarrow S_1$	2.483	0.740	H $\rightarrow$ L
B18	SOS-B2PLYP	DCM	$S_0 \rightarrow S_1$	3.045	0.942	H $\rightarrow$ L
B18	SOS-ωB2PLYP	DCM	$S_0 \rightarrow S_1$	2.627	0.777	H $\rightarrow$ L
B18	SCS-ωB2GP-PLYP	DCM	$S_0 \rightarrow S_1$	2.520	0.749	H $\rightarrow$ L
B18	SCS-ωB88PP86	DCM	$S_0 \rightarrow S_1$	2.601	0.782	H $\rightarrow$ L+1
B18	SCS-ωPBEPP86	DCM	$S_0 \rightarrow S_1$	2.474	0.746	H $\rightarrow$ L+1
B18	SOS-B2GP-PLYP	DCM	$S_0 \rightarrow S_1$	2.748	0.848	H $\rightarrow$ L
B18	SOS-PBE-QIDH	DCM	$S_0 \rightarrow S_1$	2.598	0.801	H $\rightarrow$ L+1
B18	SOS-RSX-QIDH	DCM	$S_0 \rightarrow S_1$	2.361	0.704	H $\rightarrow$ L
B18	SOS-ωB2GP-PLYP	DCM	$S_0 \rightarrow S_1$	2.536	0.754	H $\rightarrow$ L
B18	SOS-ωB88PP86	DCM	$S_0 \rightarrow S_1$	2.547	0.766	H $\rightarrow$ L+1
B18	SOS-ωPBEPP86	DCM	$S_0 \rightarrow S_1$	2.471	0.745	H $\rightarrow$ L+1
B18	ωB2GP-PLYP	DCM	$S_0 \rightarrow S_1$	2.757	0.820	H $\rightarrow$ L
B18	ωB2PLYP	DCM	$S_0 \rightarrow S_1$	2.788	0.824	H $\rightarrow$ L
B18	ωB88PP86	DCM	$S_0 \rightarrow S_1$	2.725	0.820	H $\rightarrow$ L+1
B18	ωB97X	DCM	$S_0 \rightarrow S_1$	2.916	0.850	H $\rightarrow$ L
B18	ωPBEPP86	DCM	$S_0 \rightarrow S_1$	2.700	0.814	H $\rightarrow$ L+1
B19	B2GP-PLYP	DCM	$S_0 \rightarrow S_1$	1.676	1.971	H $\rightarrow$ L
B19	B2PLYP	DCM	$S_0 \rightarrow S_1$	1.611	2.030	H $\rightarrow$ L
B19	B3LYP	DCM	$S_0 \rightarrow S_1$	1.707	2.489	H $\rightarrow$ L
B19	BHLYP	DCM	$S_0 \rightarrow S_1$	1.910	2.452	H $\rightarrow$ L
B19	CAM-B3LYP	DCM	$S_0 \rightarrow S_1$	1.893	2.298	H $\rightarrow$ L
B19	DSD-BLYP(CORRECT)	DCM	$S_0 \rightarrow S_1$	1.679	1.863	H $\rightarrow$ L
B19	DSD-BLYP(WRONG)	DCM	$S_0 \rightarrow S_1$	1.334	1.480	H $\rightarrow$ L
B19	DSD-PBEP86(CORRECT)	DCM	$S_0 \rightarrow S_1$	1.677	1.905	H $\rightarrow$ L
B19	DSD-PBEP86(WRONG)	DCM	$S_0 \rightarrow S_1$	1.272	1.445	H $\rightarrow$ L
B19	PBE-QIDH	DCM	$S_0 \rightarrow S_1$	1.741	2.020	H $\rightarrow$ L
B19	RSX-QIDH	DCM	$S_0 \rightarrow S_1$	1.888	1.920	H $\rightarrow$ L
B19	SCS-B2GP-PLYP	DCM	$S_0 \rightarrow S_1$	1.793	2.109	H $\rightarrow$ L
B19	SCS-PBE-QIDH	DCM	$S_0 \rightarrow S_1$	1.610	1.869	H $\rightarrow$ L
B19	SCS-RSX-QIDH	DCM	$S_0 \rightarrow S_1$	1.497	1.522	H $\rightarrow$ L
B19	SOS-B2PLYP	DCM	$S_0 \rightarrow S_1$	1.964	2.475	H $\rightarrow$ L
B19	SOS-ωB2PLYP	DCM	$S_0 \rightarrow S_1$	1.752	1.780	H $\rightarrow$ L
B19	SCS-ωB2GP-PLYP	DCM	$S_0 \rightarrow S_1$	1.621	1.643	H $\rightarrow$ L
B19	SCS-ωB88PP86	DCM	$S_0 \rightarrow S_1$	1.677	1.761	H $\rightarrow$ L
B19	SCS-ωPBEPP86	DCM	$S_0 \rightarrow S_1$	1.492	1.570	H $\rightarrow$ L

B19	SOS-B2GP-PLYP	DCM	$S_0 \rightarrow S_1$	1.736	2.042	H $\rightarrow$ L
B19	SOS-PBE-QIDH	DCM	$S_0 \rightarrow S_1$	1.591	1.846	H $\rightarrow$ L
B19	SOS-RSX-QIDH	DCM	$S_0 \rightarrow S_1$	1.483	1.509	H $\rightarrow$ L
B19	SOS-ωB2GP-PLYP	DCM	$S_0 \rightarrow S_1$	1.670	1.692	H $\rightarrow$ L
B19	SOS-ωB88PP86	DCM	$S_0 \rightarrow S_1$	1.641	1.724	H $\rightarrow$ L
B19	SOS-ωPBEPP86	DCM	$S_0 \rightarrow S_1$	1.562	1.644	H $\rightarrow$ L
B19	ωB2GP-PLYP	DCM	$S_0 \rightarrow S_1$	1.858	1.883	H $\rightarrow$ L
B19	ωB2PLYP	DCM	$S_0 \rightarrow S_1$	1.885	1.916	H $\rightarrow$ L
B19	ωB88PP86	DCM	$S_0 \rightarrow S_1$	1.790	1.880	H $\rightarrow$ L
B19	ωB97X	DCM	$S_0 \rightarrow S_1$	1.987	2.068	H $\rightarrow$ L
B19	ωPBEPP86	DCM	$S_0 \rightarrow S_1$	1.765	1.858	H $\rightarrow$ L
B20	B2GP-PLYP	THF	$S_0 \rightarrow S_1$	2.165	1.951	H $\rightarrow$ L
B20	B2PLYP	THF	$S_0 \rightarrow S_1$	2.151	2.068	H $\rightarrow$ L
B20	B3LYP	THF	$S_0 \rightarrow S_1$	2.075	1.392	H $\rightarrow$ L
B20	BHLYP	THF	$S_0 \rightarrow S_1$	2.354	2.303	H $\rightarrow$ L
B20	CAM-B3LYP	THF	$S_0 \rightarrow S_1$	2.320	2.141	H $\rightarrow$ L
B20	DSD-BLYP(CORRECT)	THF	$S_0 \rightarrow S_1$	2.135	1.836	H $\rightarrow$ L
B20	DSD-BLYP(WRONG)	THF	$S_0 \rightarrow S_1$	1.846	1.587	H $\rightarrow$ L
B20	DSD-PBEP86(CORRECT)	THF	$S_0 \rightarrow S_1$	2.150	1.876	H $\rightarrow$ L
B20	DSD-PBEP86(WRONG)	THF	$S_0 \rightarrow S_1$	1.824	1.591	H $\rightarrow$ L
B20	PBE-QIDH	THF	$S_0 \rightarrow S_1$	2.216	1.960	H $\rightarrow$ L
B20	RSX-QIDH	THF	$S_0 \rightarrow S_1$	2.278	1.815	H $\rightarrow$ L
B20	SCS-B2GP-PLYP	THF	$S_0 \rightarrow S_1$	2.268	2.044	H $\rightarrow$ L
B20	SCS-PBE-QIDH	THF	$S_0 \rightarrow S_1$	2.098	1.856	H $\rightarrow$ L
B20	SCS-RSX-QIDH	THF	$S_0 \rightarrow S_1$	1.907	1.520	H $\rightarrow$ L
B20	SOS-B2PLYP	THF	$S_0 \rightarrow S_1$	2.464	2.369	H $\rightarrow$ L
B20	SOS-ωB2PLYP	THF	$S_0 \rightarrow S_1$	2.137	1.702	H $\rightarrow$ L
B20	SCS-ωB2GP-PLYP	THF	$S_0 \rightarrow S_1$	2.017	1.609	H $\rightarrow$ L
B20	SCS-ωB88PP86	THF	$S_0 \rightarrow S_1$	2.090	1.711	H $\rightarrow$ L
B20	SCS-ωPBEPP86	THF	$S_0 \rightarrow S_1$	1.919	1.571	H $\rightarrow$ L
B20	SOS-B2GP-PLYP	THF	$S_0 \rightarrow S_1$	2.216	1.997	H $\rightarrow$ L
B20	SOS-PBE-QIDH	THF	$S_0 \rightarrow S_1$	2.079	1.839	H $\rightarrow$ L
B20	SOS-RSX-QIDH	THF	$S_0 \rightarrow S_1$	1.893	1.508	H $\rightarrow$ L
B20	SOS-ωB2GP-PLYP	THF	$S_0 \rightarrow S_1$	2.064	1.646	H $\rightarrow$ L
B20	SOS-ωB88PP86	THF	$S_0 \rightarrow S_1$	2.055	1.682	H $\rightarrow$ L
B20	SOS-ωPBEPP86	THF	$S_0 \rightarrow S_1$	1.984	1.625	H $\rightarrow$ L
B20	ωB2GP-PLYP	THF	$S_0 \rightarrow S_1$	2.242	1.788	H $\rightarrow$ L
B20	ωB2PLYP	THF	$S_0 \rightarrow S_1$	2.264	1.804	H $\rightarrow$ L
B20	ωB88PP86	THF	$S_0 \rightarrow S_1$	2.200	1.801	H $\rightarrow$ L
B20	ωB97X	THF	$S_0 \rightarrow S_1$	2.342	1.902	H $\rightarrow$ L
B20	ωPBEPP86	THF	$S_0 \rightarrow S_1$	2.182	1.787	H $\rightarrow$ L
B21	B2GP-PLYP	THF	$S_0 \rightarrow S_1$	2.354	1.684	H $\rightarrow$ L
B21	B2PLYP	THF	$S_0 \rightarrow S_1$	2.226	1.588	H $\rightarrow$ L
B21	B3LYP	THF	$S_0 \rightarrow S_1$	1.958	0.598	H $\rightarrow$ L
B21	BHLYP	THF	$S_0 \rightarrow S_1$	2.653	1.856	H $\rightarrow$ L
B21	CAM-B3LYP	THF	$S_0 \rightarrow S_1$	2.622	1.826	H $\rightarrow$ L
B21	DSD-BLYP(CORRECT)	THF	$S_0 \rightarrow S_1$	2.360	1.635	H $\rightarrow$ L
B21	DSD-BLYP(WRONG)	THF	$S_0 \rightarrow S_1$	1.845	1.278	H $\rightarrow$ L
B21	DSD-PBEP86(CORRECT)	THF	$S_0 \rightarrow S_1$	2.356	1.660	H $\rightarrow$ L
B21	DSD-PBEP86(WRONG)	THF	$S_0 \rightarrow S_1$	1.774	1.249	H $\rightarrow$ L
B21	PBE-QIDH	THF	$S_0 \rightarrow S_1$	2.461	1.752	H $\rightarrow$ L
B21	RSX-QIDH	THF	$S_0 \rightarrow S_1$	2.634	1.708	H $\rightarrow$ L
B21	SCS-B2GP-PLYP	THF	$S_0 \rightarrow S_1$	2.472	1.768	H $\rightarrow$ L
B21	SCS-PBE-QIDH	THF	$S_0 \rightarrow S_1$	2.311	1.645	H $\rightarrow$ L
B21	SCS-RSX-QIDH	THF	$S_0 \rightarrow S_1$	2.258	1.464	H $\rightarrow$ L
B21	SOS-B2PLYP	THF	$S_0 \rightarrow S_1$	2.608	1.860	H $\rightarrow$ L
B21	SOS-ωB2PLYP	THF	$S_0 \rightarrow S_1$	2.462	1.593	H $\rightarrow$ L
B21	SCS-ωB2GP-PLYP	THF	$S_0 \rightarrow S_1$	2.336	1.512	H $\rightarrow$ L
B21	SCS-ωB88PP86	THF	$S_0 \rightarrow S_1$	2.388	1.602	H $\rightarrow$ L
B21	SCS-ωPBEPP86	THF	$S_0 \rightarrow S_1$	2.229	1.496	H $\rightarrow$ L
B21	SOS-B2GP-PLYP	THF	$S_0 \rightarrow S_1$	2.417	1.728	H $\rightarrow$ L
B21	SOS-PBE-QIDH	THF	$S_0 \rightarrow S_1$	2.288	1.629	H $\rightarrow$ L

B21	SOS-RSX-QIDH	THF	$S_0 \rightarrow S_1$	2.188	1.419	H $\rightarrow$ L
B21	SOS-ωB2GP-PLYP	THF	$S_0 \rightarrow S_1$	2.369	1.534	H $\rightarrow$ L
B21	SOS-ωB88PP86	THF	$S_0 \rightarrow S_1$	2.343	1.572	H $\rightarrow$ L
B21	SOS-ωPBEPP86	THF	$S_0 \rightarrow S_1$	2.264	1.520	H $\rightarrow$ L
B21	ωB2GP-PLYP	THF	$S_0 \rightarrow S_1$	2.581	1.671	H $\rightarrow$ L
B21	ωB2PLYP	THF	$S_0 \rightarrow S_1$	2.615	1.693	H-1 $\rightarrow$ L
B21	ωB88PP86	THF	$S_0 \rightarrow S_1$	2.494	1.674	H $\rightarrow$ L
B21	ωB97X	THF	$S_0 \rightarrow S_1$	2.736	1.811	H-1 $\rightarrow$ L
B21	ωPBEPP86	THF	$S_0 \rightarrow S_1$	2.463	1.653	H $\rightarrow$ L
B22	B2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	3.521	0.616	H $\rightarrow$ L
B22	B2PLYP	MeOH	$S_0 \rightarrow S_1$	3.464	0.603	H $\rightarrow$ L
B22	B3LYP	MeOH	$S_0 \rightarrow S_1$	3.550	0.572	H $\rightarrow$ L
B22	BHLYP	MeOH	$S_0 \rightarrow S_1$	3.793	0.658	H $\rightarrow$ L
B22	CAM-B3LYP	MeOH	$S_0 \rightarrow S_1$	3.722	0.615	H $\rightarrow$ L
B22	DSD-BLYP(CORRECT)	MeOH	$S_0 \rightarrow S_1$	3.525	0.618	H $\rightarrow$ L
B22	DSD-BLYP(WRONG)	MeOH	$S_0 \rightarrow S_1$	3.059	0.536	H $\rightarrow$ L
B22	DSD-PBEP86(CORRECT)	MeOH	$S_0 \rightarrow S_1$	3.513	0.615	H $\rightarrow$ L
B22	DSD-PBEP86(WRONG)	MeOH	$S_0 \rightarrow S_1$	3.005	0.526	H $\rightarrow$ L
B22	PBE-QIDH	MeOH	$S_0 \rightarrow S_1$	3.621	0.631	H $\rightarrow$ L
B22	RSX-QIDH	MeOH	$S_0 \rightarrow S_1$	3.782	0.642	H $\rightarrow$ L
B22	SCS-B2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	3.581	0.627	H $\rightarrow$ L
B22	SCS-PBE-QIDH	MeOH	$S_0 \rightarrow S_1$	3.457	0.603	H $\rightarrow$ L
B22	SCS-RSX-QIDH	MeOH	$S_0 \rightarrow S_1$	3.471	0.589	H $\rightarrow$ L
B22	SOS-B2PLYP	MeOH	$S_0 \rightarrow S_1$	3.740	0.651	H $\rightarrow$ L
B22	SOS-ωB2PLYP	MeOH	$S_0 \rightarrow S_1$	3.587	0.602	H $\rightarrow$ L
B22	SCS-ωB2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	3.490	0.593	H $\rightarrow$ L
B22	SCS-ωB88PP86	MeOH	$S_0 \rightarrow S_1$	3.524	0.602	H $\rightarrow$ L
B22	SCS-ωPBEPP86	MeOH	$S_0 \rightarrow S_1$	3.408	0.585	H $\rightarrow$ L
B22	SOS-B2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	3.532	0.618	H $\rightarrow$ L
B22	SOS-PBE-QIDH	MeOH	$S_0 \rightarrow S_1$	3.422	0.597	H $\rightarrow$ L
B22	SOS-RSX-QIDH	MeOH	$S_0 \rightarrow S_1$	3.352	0.569	H $\rightarrow$ L
B22	SOS-ωB2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	3.505	0.596	H $\rightarrow$ L
B22	SOS-ωB88PP86	MeOH	$S_0 \rightarrow S_1$	3.470	0.593	H $\rightarrow$ L
B22	SOS-ωPBEPP86	MeOH	$S_0 \rightarrow S_1$	3.402	0.584	H $\rightarrow$ L
B22	ωB2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	3.715	0.631	H $\rightarrow$ L
B22	ωB2PLYP	MeOH	$S_0 \rightarrow S_1$	3.741	0.627	H $\rightarrow$ L
B22	ωB88PP86	MeOH	$S_0 \rightarrow S_1$	3.628	0.620	H $\rightarrow$ L
B22	ωB97X	MeOH	$S_0 \rightarrow S_1$	3.826	0.619	H $\rightarrow$ L
B22	ωPBEPP86	MeOH	$S_0 \rightarrow S_1$	3.605	0.619	H $\rightarrow$ L
B23	B2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.959	0.678	H $\rightarrow$ L
B23	B2PLYP	MeOH	$S_0 \rightarrow S_1$	2.963	0.669	H $\rightarrow$ L
B23	B3LYP	MeOH	$S_0 \rightarrow S_1$	3.189	0.608	H $\rightarrow$ L
B23	BHLYP	MeOH	$S_0 \rightarrow S_1$	3.270	0.733	H $\rightarrow$ L
B23	CAM-B3LYP	MeOH	$S_0 \rightarrow S_1$	3.204	0.682	H $\rightarrow$ L
B23	DSD-BLYP(CORRECT)	MeOH	$S_0 \rightarrow S_1$	2.924	0.674	H $\rightarrow$ L
B23	DSD-BLYP(WRONG)	MeOH	$S_0 \rightarrow S_1$	2.495	0.575	H $\rightarrow$ L
B23	DSD-PBEP86(CORRECT)	MeOH	$S_0 \rightarrow S_1$	2.906	0.668	H $\rightarrow$ L
B23	DSD-PBEP86(WRONG)	MeOH	$S_0 \rightarrow S_1$	2.463	0.566	H $\rightarrow$ L
B23	PBE-QIDH	MeOH	$S_0 \rightarrow S_1$	3.028	0.693	H $\rightarrow$ L
B23	RSX-QIDH	MeOH	$S_0 \rightarrow S_1$	3.094	0.692	H $\rightarrow$ L
B23	SCS-B2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.985	0.684	H $\rightarrow$ L
B23	SCS-PBE-QIDH	MeOH	$S_0 \rightarrow S_1$	2.844	0.651	H $\rightarrow$ L
B23	SCS-RSX-QIDH	MeOH	$S_0 \rightarrow S_1$	2.795	0.625	H $\rightarrow$ L
B23	SOS-B2PLYP	MeOH	$S_0 \rightarrow S_1$	3.209	0.725	H $\rightarrow$ L
B23	SOS-ωB2PLYP	MeOH	$S_0 \rightarrow S_1$	2.899	0.639	H $\rightarrow$ L
B23	SCS-ωB2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.796	0.625	H $\rightarrow$ L
B23	SCS-ωB88PP86	MeOH	$S_0 \rightarrow S_1$	2.859	0.641	H $\rightarrow$ L
B23	SCS-ωPBEPP86	MeOH	$S_0 \rightarrow S_1$	2.749	0.619	H $\rightarrow$ L
B23	SOS-B2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.936	0.673	H $\rightarrow$ L
B23	SOS-PBE-QIDH	MeOH	$S_0 \rightarrow S_1$	2.801	0.641	H $\rightarrow$ L
B23	SOS-RSX-QIDH	MeOH	$S_0 \rightarrow S_1$	2.636	0.590	H $\rightarrow$ L
B23	SOS-ωB2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	2.803	0.627	H $\rightarrow$ L

B23	SOS-ωB88PP86	MeOH	$S_0 \rightarrow S_1$	2.798	0.627	H $\rightarrow$ L
B23	SOS-ωPBEPP86	MeOH	$S_0 \rightarrow S_1$	2.723	0.613	H $\rightarrow$ L
B23	ωB2GP-PLYP	MeOH	$S_0 \rightarrow S_1$	3.043	0.680	H $\rightarrow$ L
B23	ωB2PLYP	MeOH	$S_0 \rightarrow S_1$	3.076	0.678	H $\rightarrow$ L
B23	ωB88PP86	MeOH	$S_0 \rightarrow S_1$	2.991	0.671	H $\rightarrow$ L
B23	ωB97X	MeOH	$S_0 \rightarrow S_1$	3.203	0.678	H $\rightarrow$ L
B23	ωPBEPP86	MeOH	$S_0 \rightarrow S_1$	2.966	0.668	H $\rightarrow$ L

SI.8 Experimental details

SI.8.1 Synthesis of BODIPYs

Synthesis of 1

Methyl-4-formylbenzoate (0.82 g, 4.99 mmol) and 2,4-dimethylpyrrole (1.34 mL, 13.01 mmol) were dissolved in 300.0 mL of dry DCM. 2 drops of trifluoroacetic acid (TFA) were added to the solution and the reaction mixture was stirred for three hours in the dark under N_2 atmosphere at room temperature. 2,3-Dichloro-5,6-dicyano-1,4-benzoquinone (DDQ) (2.95 g, 13.01 mmol) was then added as a solid to the reaction and stirred for a further two hours. Triethylamine (TEA) (10.00 mL, 71.00 mmol) was added to the reaction and after two minutes the temperature was lowered to 0 °C followed by the drop-wise addition of $BF_3.OEt_2$ (10.00 mL, 81.00 mmol). Following the addition, the reaction mixture was warmed to room temperature and stirred overnight. Distilled water (100.0 mL) was then added to the mixture and the biphasic mixture was filtered through celite. The organic layer was separated and washed with distilled water (3 x 100 mL) followed by saturated Na_2CO_3 solution (3 x 100 mL) to remove H-DDQ. The organic layer was then dried with anhydrous $MgSO_4$. Removal of solvents under reduced pressure afforded a crude product that was purified using silica gel column chromatography in EtOAc: n-hexane, 1:9 (R_f: 0.67 in DCM). The collected yellow fraction which was green emissive was concentrated under reduced pressure to yield the product as a red solid (840.0 mg, 44%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (d, J = 8.6 Hz, 2H), 7.39 (d, J =8.6Hz, 2H), 5.98 (s, 2H), 3.96 (s, 3H), 2.55 (s, 6H), 1.35 (s, 6H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 166.58, 156.11, 142.99, 140.33, 139.95, 131.03, 130.92, 130.48, 128.50, 121.59, 52.50, 14.71, 14.60. ^{19}F NMR (376 MHz, $CDCl_3$) δ 146.18 (q, J = 32.6 Hz, 2F). ^{11}B NMR (128 MHz, $CDCl_3$) δ 0.74 (t, J = 32.9 Hz, 1B). HRMS (ESI) calcd. For $C_{21}H_{21}BF_2N_2O_2$ [M+Na]+ : 405.156, found: 405.1567.

Synthesis of B3

Compound 1 (840.0 mg, 2.20 mmol), p-N,N-dimethylaminobenzaldehyde (4.26 g, 28.56 mmol), piperidine (144.32 μL, 1.46 mmol) and acetic acid (100.37 μ L, 1.75 mmol) were dissolved in 22.0 mL of dry toluene in a glass tube sealed with a teflon cap. The sample was irradiated at 200 W (CEM-Discover monomode microwave) and 190 °C for 20 min. On cooling, the mixture was concentrated in vacuo, dissolved in DCM, and washed with distilled water. The organic layer was dried with anhydrous MgSO4, filtered, and the solvents removed under reduced pressure to afford the crude product that was purified using silica gel column chromatography in DCM: n-hexane, 2:3 (R_f: 0.3 in DCM: n-hexane, 4:1).The resulting blue fraction was concentrated to yield a deep green solid that was washed with acetonitrile through centrifugation to afford (382.0 mg, 34%) of the target compound. ^{1}H NMR (400 MHz, CD_2Cl_2) δ 8.16 (d, J = 8.6 Hz, 2H), 7.49 (d, J = 8.9 Hz, 2H), 7.45 (d, J = 8.6 Hz, 2H), 7.41 (d, J = 16.6 Hz, 1H), 7.26 (d, J = 16.6 Hz, 1H), 6.71 (d, J = 8.9 Hz, 2H), 6.64 (s, 1H), 6.01 (s, 1H), 3.94 (s, 3H), 3.03 (s, 6H), 2.55 (s, 3H), 1.43 (s, 3H), 1.38 (s, 3H). ^{13}C{^{1}H} NMR (101 MHz, CD_2Cl_2) δ 166.36, 155.02, 153.00, 151.36, 142.93, 140.66, 139.98, 138.33, 137.54, 130.78, 130.58, 130.12, 129.15, 128.86, 124.10, 120.51, 117.78, 113.51, 111.91, 52.14, 39.93, 29.65, 14.58, 14.28, 14.11. ^{19}F NMR (376 MHz, CD_2Cl_2) δ -142.38 (q, J = 33.3 Hz, 2F). ^{11}B NMR (128 MHz, CD_2Cl_2) δ 0.96 (t, J = 33.6 Hz, 1B). HRMS (ESI) calcd. For $C_{30}H_{30}BF_2N_3O_2$ [M+Na]+ : 536.2297, found: 536.2303.

Synthesis of 2

To a solution of the methyl ester, compound B3 (285.0 mg, 0.56 mmol) in 50.0 mL of DCM:MeOH (9:1, v/v) mixture, an aqueous solution of NaOH (11.2 mmol, 20 Eq) was added. The reaction mixture was stirred at room temperature for 24 hrs. Then the reaction mixture was filtered and the precipitate on the filter paper was dissolved with distilled water and acidified by HCl (1M) until pH 3 and extracted with DCM (3 x 20 mL). The organic layers were collected, dried with anhydrous $MgSO_4$ and concentrated in vacuo to yield the product as a dark green film (266.0 mg, 95%). R_f: 0.67 in EtOAc:MeOH, 4:1. ^{1}H NMR (400 MHz, 1 drop of DMSO-d_6 in CD_2Cl_2) δ 8.14 (d, J = 8.4 Hz, 2H), 7.47 (d, J = 8.9 Hz, 2H), 7.42 (d, J = 8.4 Hz, 2H), 7.36 (d, J = 16.1 Hz, 1H), 7.24 (d, J = 16.1 Hz, 1H), 6.69 (d, J = 8.9 Hz, 2H), 6.62 (s, 1H), 5.99 (s, 1H), 3.01 (s, 6H), 2.51 (s, 3H), 1.41 (s, 3H), 1.36 (s, 3H). ^{19}F NMR (376 MHz, 1 drop of DMSO-d_6 in CD_2Cl_2) δ -142.20 (q, J = 33.5 Hz, 2F). ^{11}B NMR (128 MHz, 1 drop of DMSO-d_6 in CD_2Cl_2) δ 0.94 (t, J = 33.6 Hz, 1B). HRMS (ESI) calcd. For $C_{29}H_{28}BF_2N_3O_2$ [M-H] : 498.2175, found: 498.2182.

Synthesis of 3

Under N_2 atmosphere and at room temperature, a 4 mL dry DMF solution of compound 2 (24.0 mg, 0.05 mmol), N-hydroxysuccinimide (11.06 mg, 0.10 mmol) and 1-Ethyl-3-(3-dimethylaminopropyl) carbodiimide (EDC.HCl) (18.42 mg, 0.10 mmol) were stirred overnight until thin-layer chromatography (TLC) confirmed the complete consumption of starting material. The reaction was then quenched by washing with a saturated aqueous solution of ammonium chloride (3 x 20 mL) and distilled water (3 x 20 mL). The organic layers were collected, dried with anhydrous $MgSO_4$ and solvents were removed under reduced pressure to afford the product as a dark green solid. (28.0 mg, 100 %). R_f: 0.8 in EtOAc. ^{1}H NMR (400 MHz, CD_2Cl_2) δ 8.28 (d, J = 8.4 Hz, 2H), 7.57 (d, J = 8.4 Hz, 2H), 7.50 (d, J = 8.9 Hz, 2H), 7.41 (d, J = 16.1 Hz, 1H), 7.27 (d, J = 16.1 Hz, 1H), 6.71 (d, J = 8.9 Hz, 2H), 6.66 (s, 1H), 6.02 (s, 1H), 3.03 (s, 6H), 2.91 (s, 4H), 2.55 (s, 3H), 1.45 (s, 3H), 1.40 (s, 3H). ^{13}C{^{1}H} NMR (101 MHz, CD_2Cl_2) δ 169.43, 161.68, 155.52, 153.36, 151.59, 143.06, 142.52, 140.70, 138.84, 136.67, 132.62, 131.25, 129.79, 129.41, 125.83, 124.23, 120.82, 118.19, 113.60, 112.10, 40.11, 29.83, 25.89, 15.04, 14.56, 14.48. ^{19}F NMR (376 MHz, CD_2Cl_2) δ -142.34 (q, J = 34.0 Hz, 2F). ^{11}B NMR (128 MHz, CD_2Cl_2) δ 0.96 (t, J = 33.4 Hz, 1B). HRMS (ESI) calcd. For $C_{33}H_{31}BF_2N_4O_4$ [M+H+] : 597.2485, found: 597.2477.

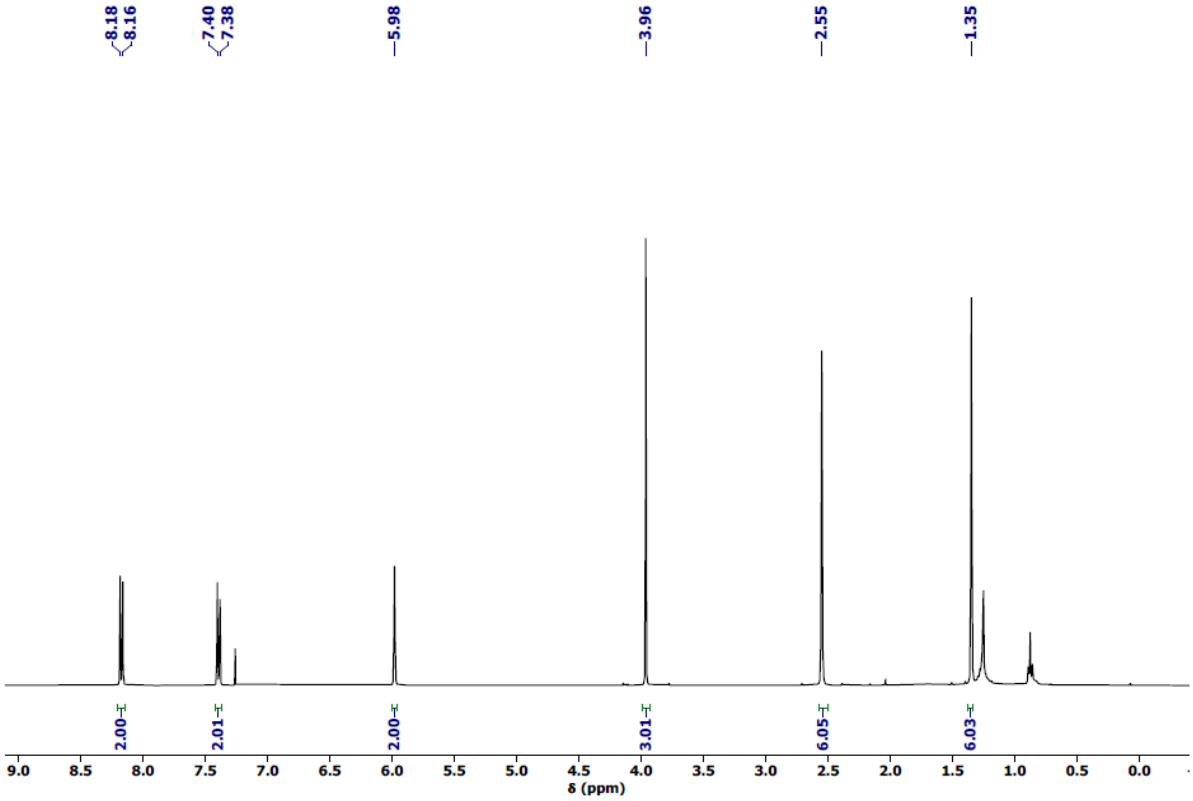

Figure S4: ^{1}H NMR spectrum of **1**, $CDCl_3$

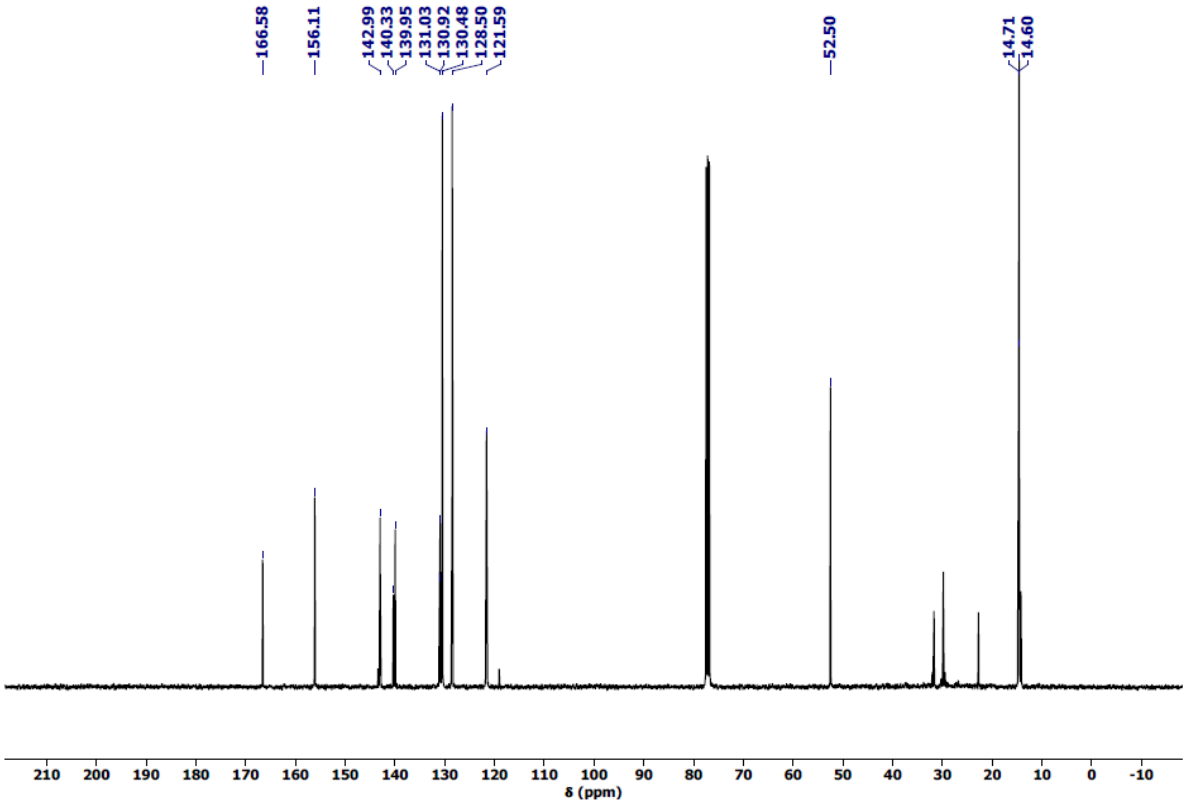

Figure S5: $^{13}C\{^{1}H\}$ NMR spectrum of **1**, $CDCl_3$

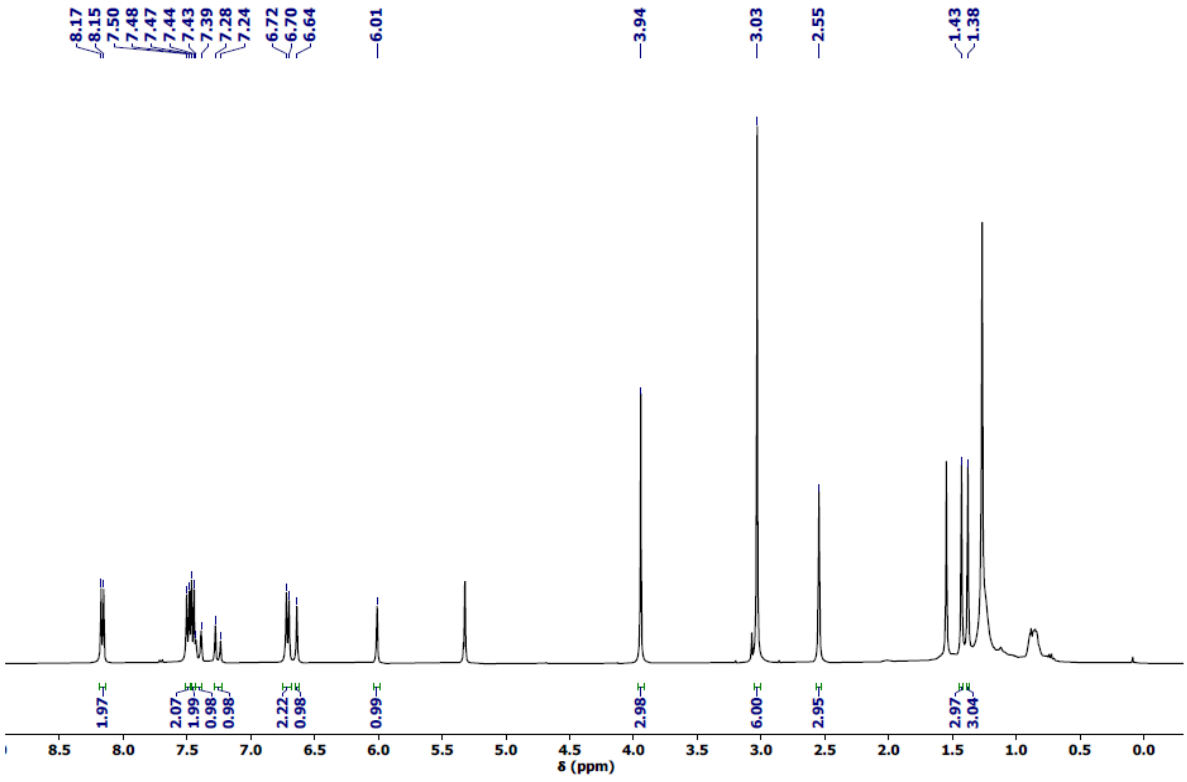

Figure S6: ^{1}H NMR spectrum of **B3**, CD_2Cl_2

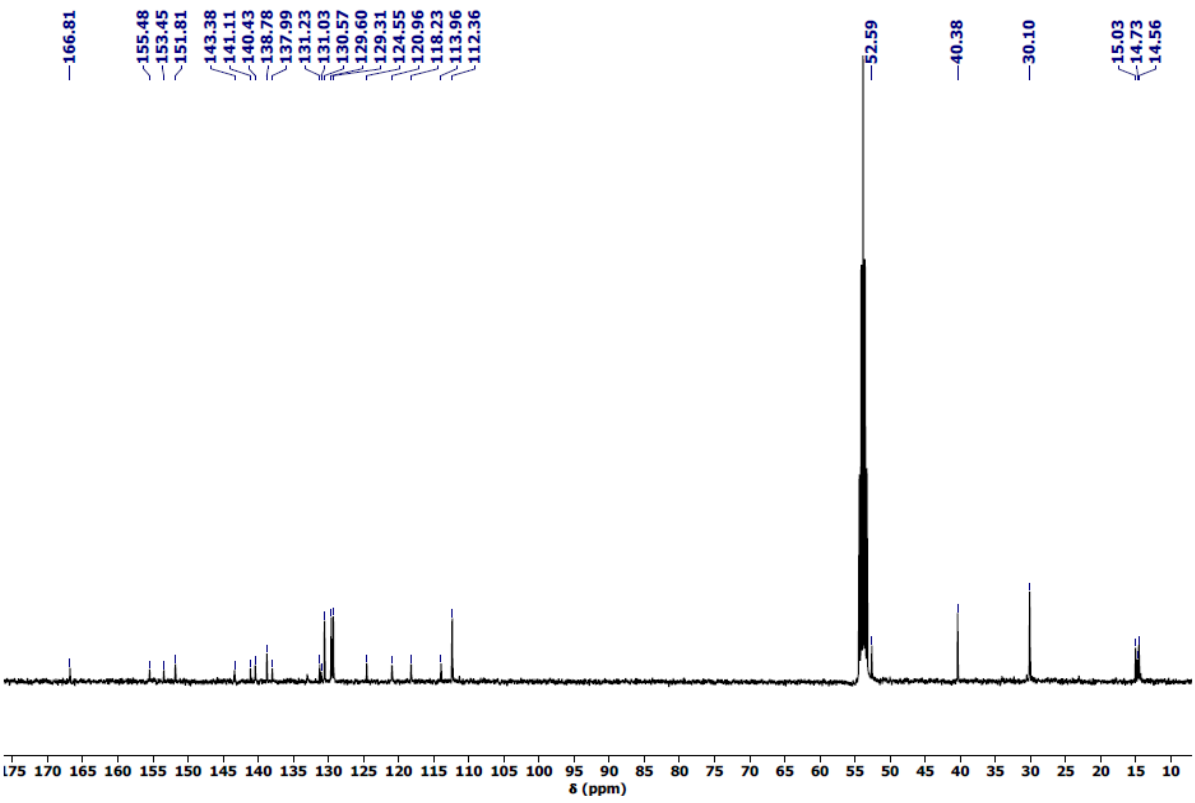

Figure S7: $^{13}C\{^{1}H\}$ NMR spectrum of **B3**, CD_2Cl_2

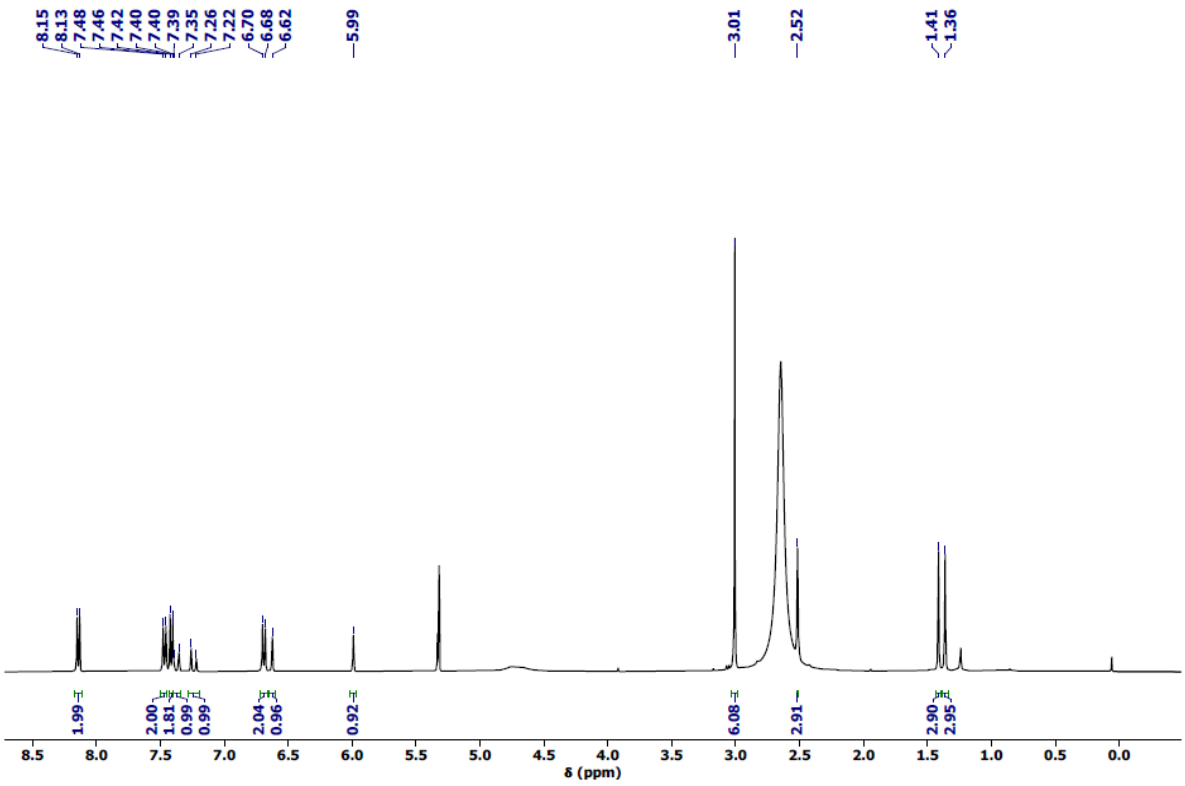

Figure S8: ^{1}H NMR spectrum of **2**, 1 drop of DMSO-d_6 in CD_2Cl_2

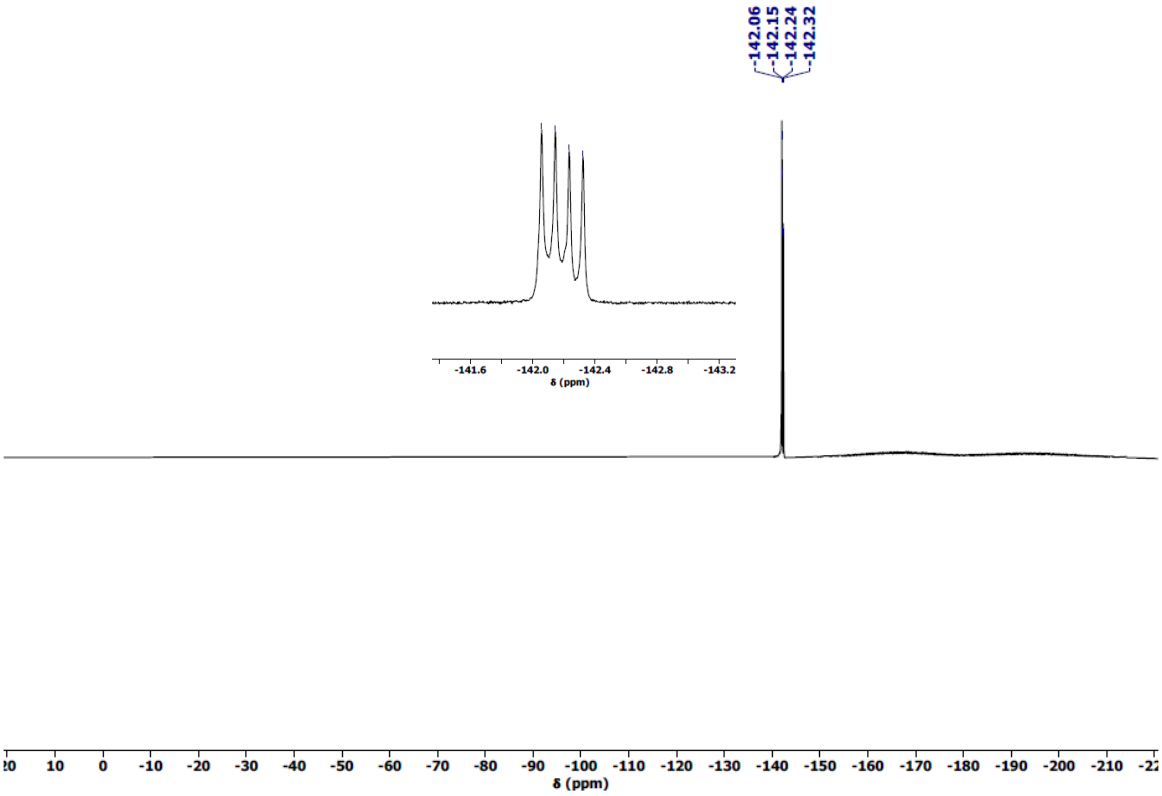

Figure S9: ^{19}F NMR spectrum of **2**, 1 drop of DMSO-d_6 in CD_2Cl_2

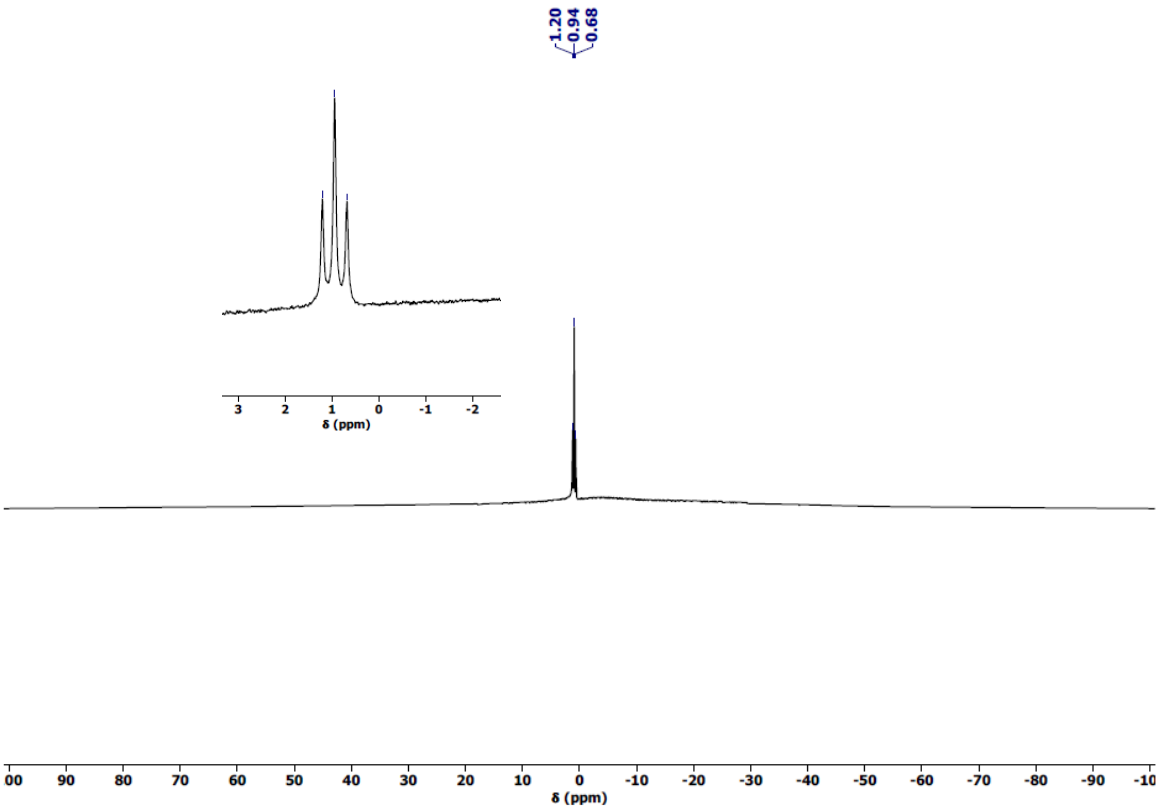

Figure S10: ^{11}B NMR spectrum of **2**, 1 drop of DMSO-d_6 in CD_2Cl_2

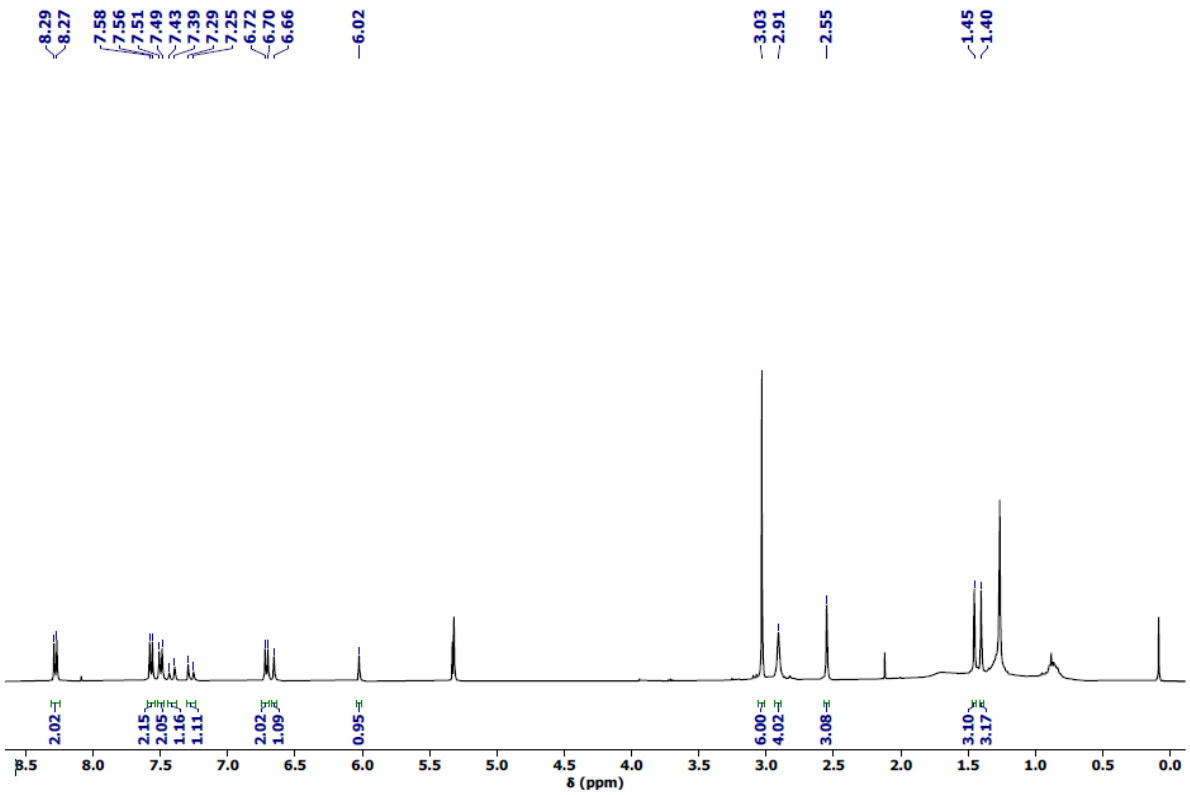

Figure S11: ^{1}H NMR spectrum of **3**, CD_2Cl_2

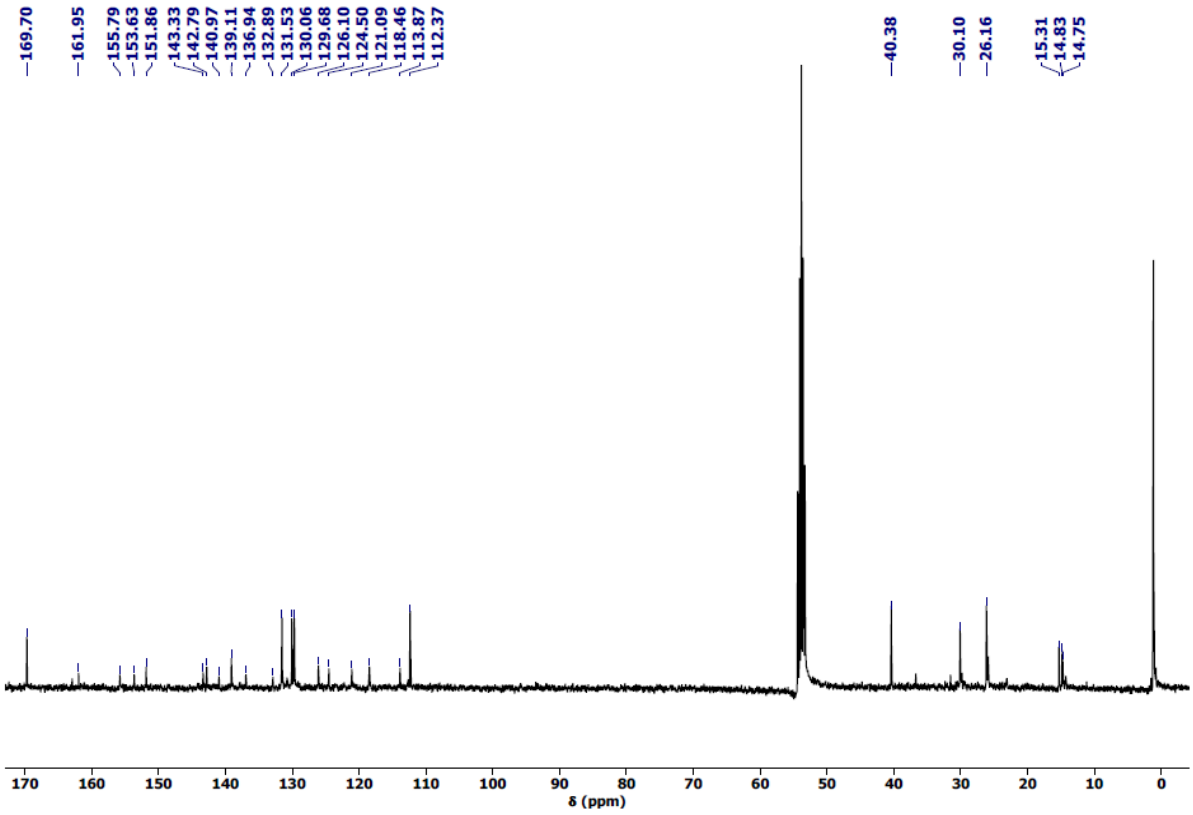

Figure S12: $^{13}C\{^{1}H\}$ NMR spectrum of **3**, CD_2Cl_2

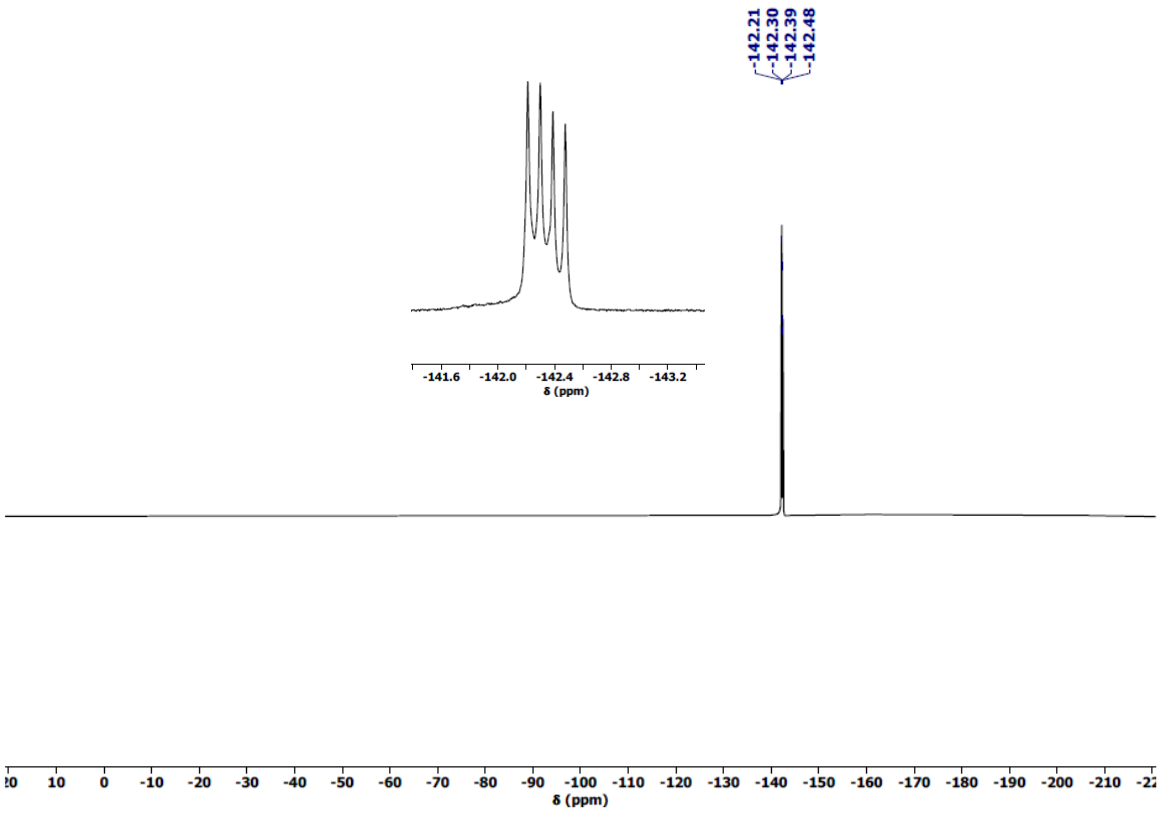

Figure S13: ^{19}F NMR spectrum of **3**, CD_2Cl_2

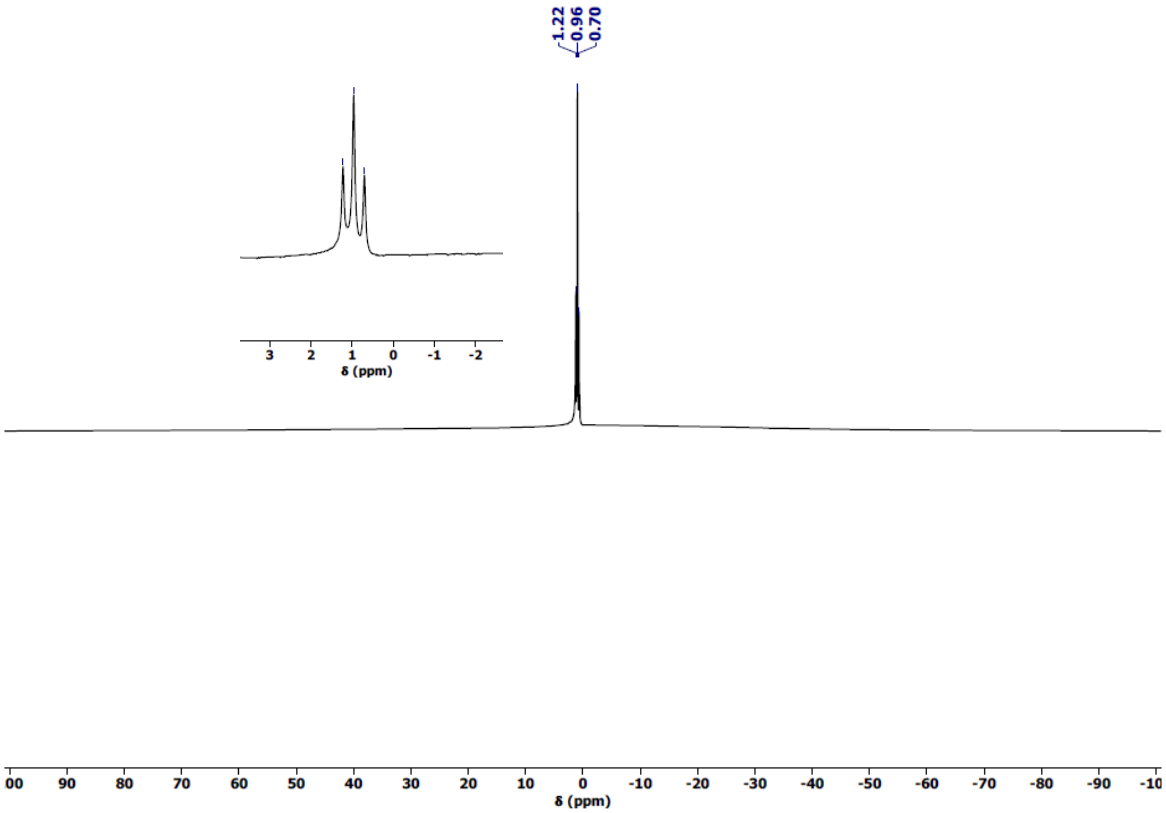

Figure S14: ^{11}B NMR spectrum of **3**, CD_2Cl_2

SI.8.2 UV-Vis Spectroscopy

Table S8: Spectral Measurements

Compound	Solvent	λ_{max} (nm)	ϵ_{max} ($M^{-1}cm^{-1}$)
1	Dichloromethane	503	54150
	Toluene	505	75140
2	Toluene	613	2250
	Dichloromethane	612	6114
	Acetone	599	5990
	Methanol	599	12356
	Acetonitrile	596	3052
3	Toluene	617	23650
	Dichloromethane	615	22082
	Acetone	607	21573
	Methanol	604	20559
	Acetonitrile	605	18284

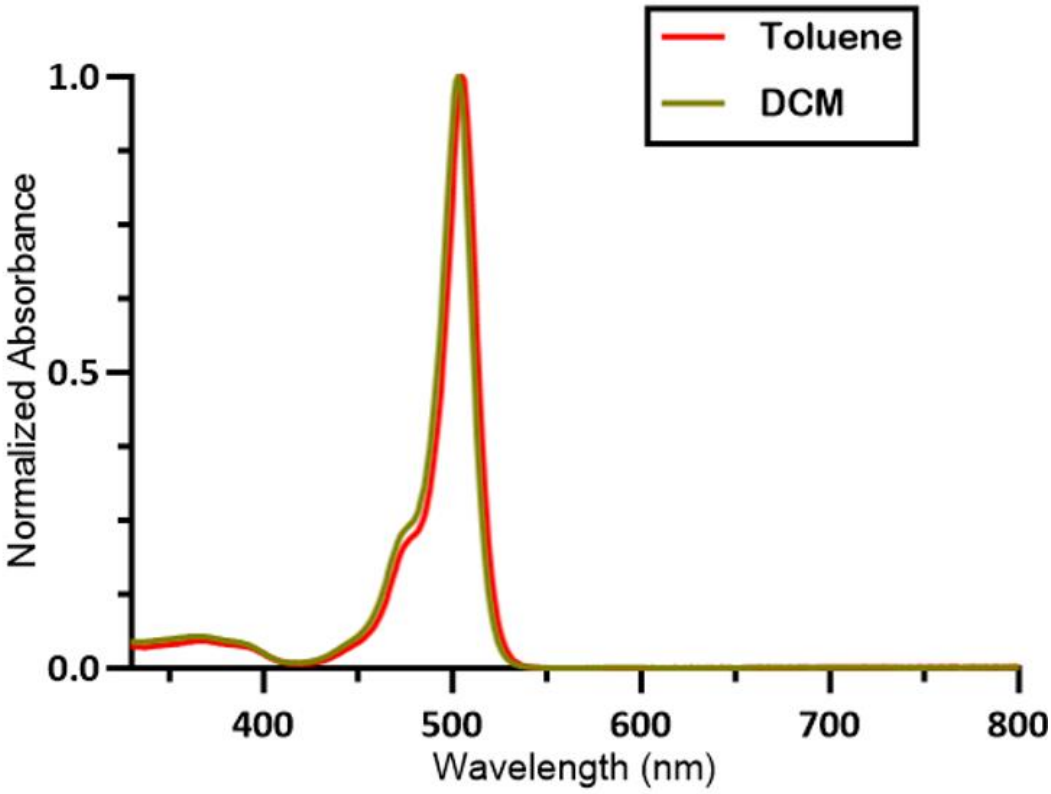

Figure S15: UV-Vis Spectra of **1**

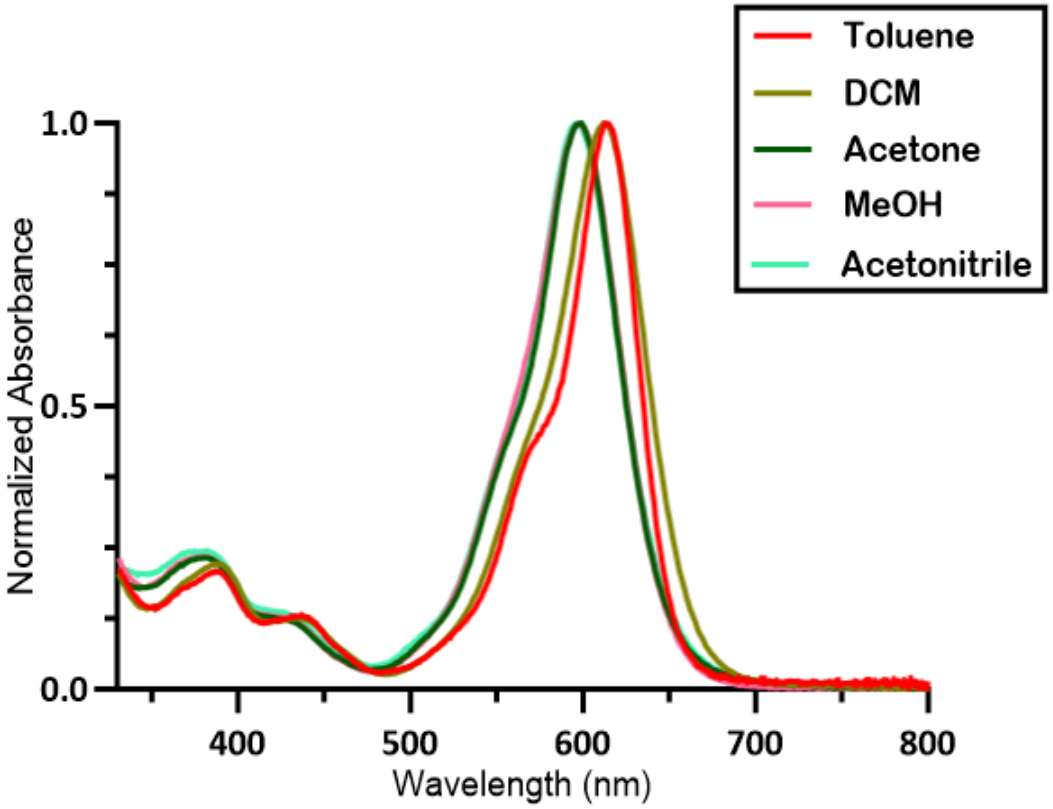

Figure S16: UV-Vis Spectra of **2**

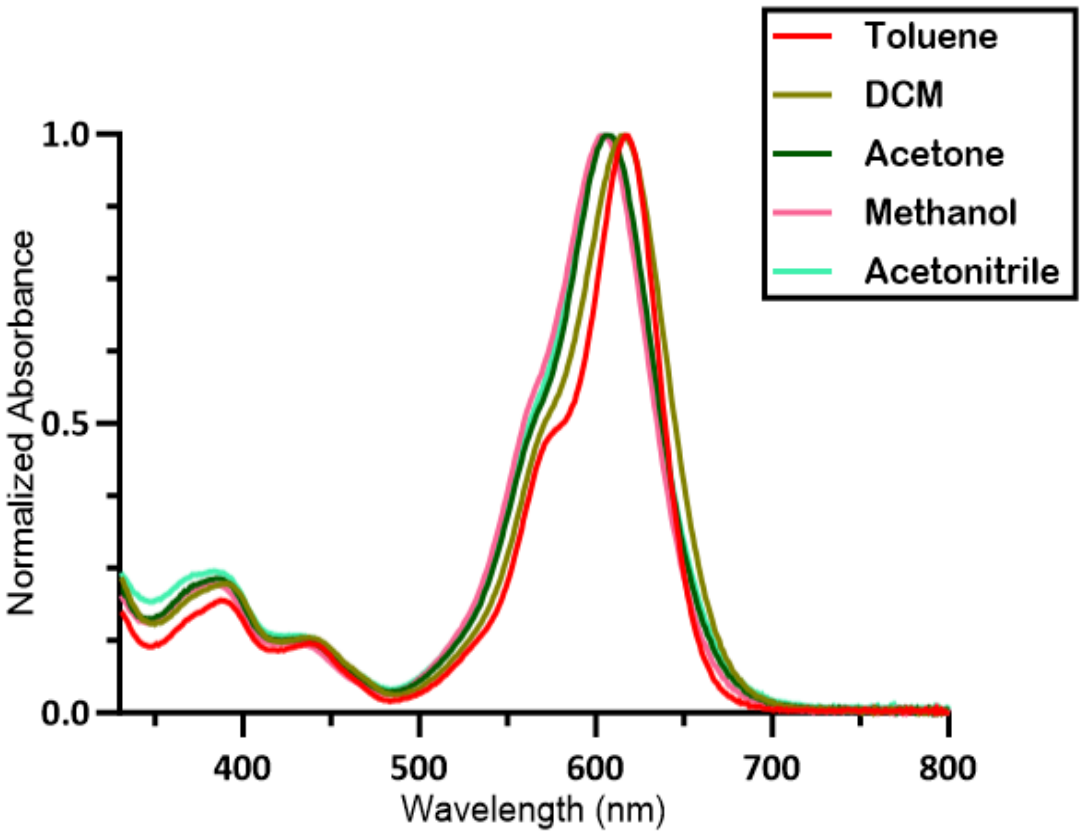

Figure S17: UV-Vis Spectra of **3**

SI.9 Errors versus Charge Transfer Diagnostic

Table S9: Calculated Λ for our **SBYD31** set

Molecule	Solvent	Λ
B1	Et_2O	0.680
B1	MeCN	0.672
B2	Et_2O	0.736
B2	MeCN	0.735
B2	MeOH	0.735
B3	Et_2O	0.679
B3	MeCN	0.671
B3	MeOH	0.671
B4	Et_2O	0.741
B4	MeCN	0.741
B4	MeOH	0.741
B5	$CHCl_3$	0.563
B6	$CHCl_3$	0.545
B7	$CHCl_3$	0.527
B8	$CHCl_3$	0.507
B9	$CHCl_3$	0.572
B10	THF	0.600
B11	$CHCl_3$	0.716
B11	THF	0.715
B12	$CHCl_3$	0.504
B13	$CHCl_3$	0.641
B14	MeOH	0.747
B15	DCM	0.554
B16	DCM	0.702
B17	THF	0.675
B18	DCM	0.593
B19	DCM	0.660
B20	THF	0.688
B21	THF	0.515
B22	MeOH	0.628
B23	MeOH	0.681

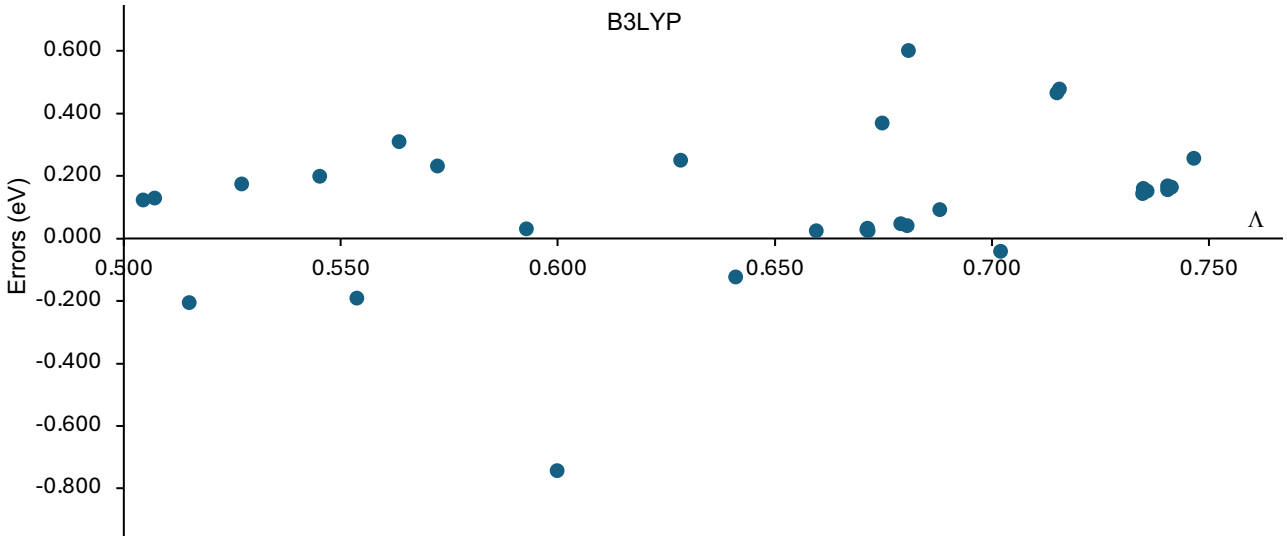

Figure S18: Λ and Errors plot - B3LYP

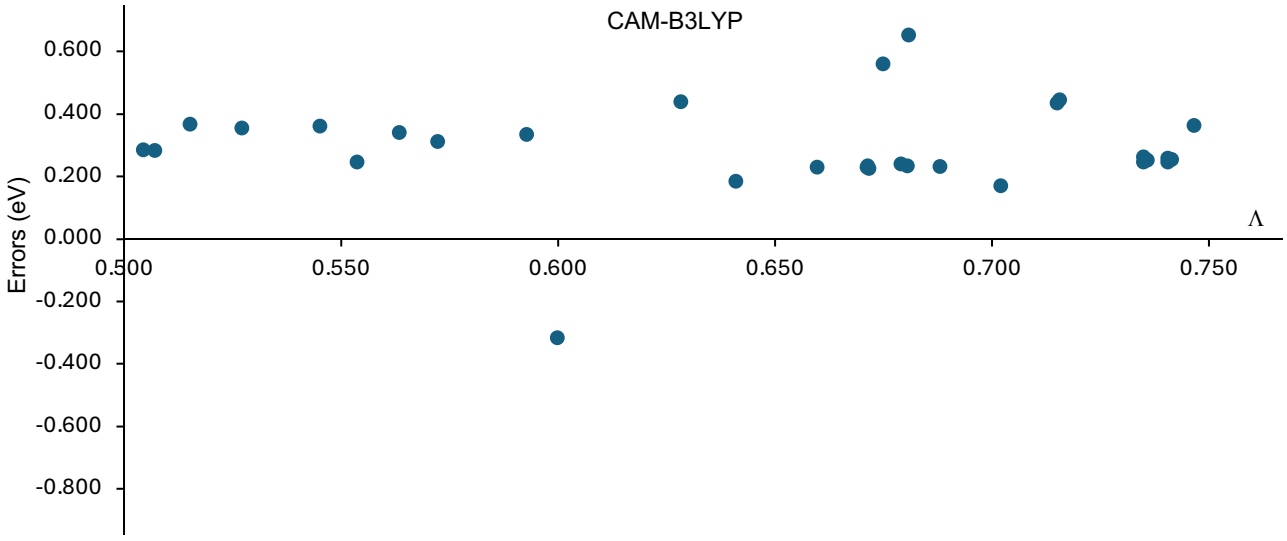

Figure S19: Λ and Errors plot - CAM-B3LYP

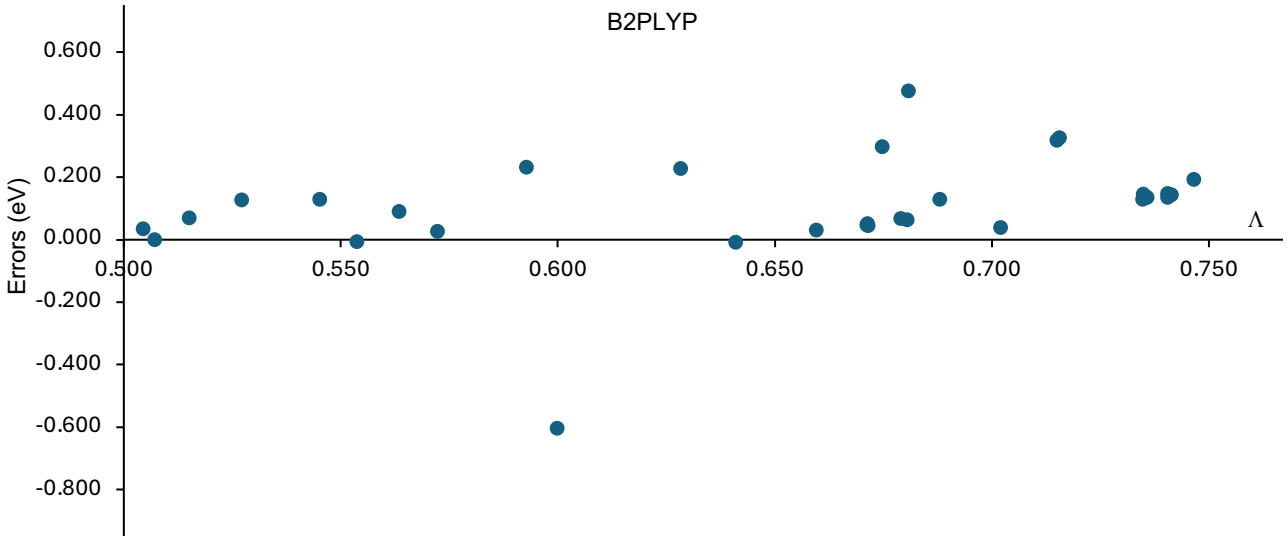

Figure S20: Λ and Errors plot - B2PLYP

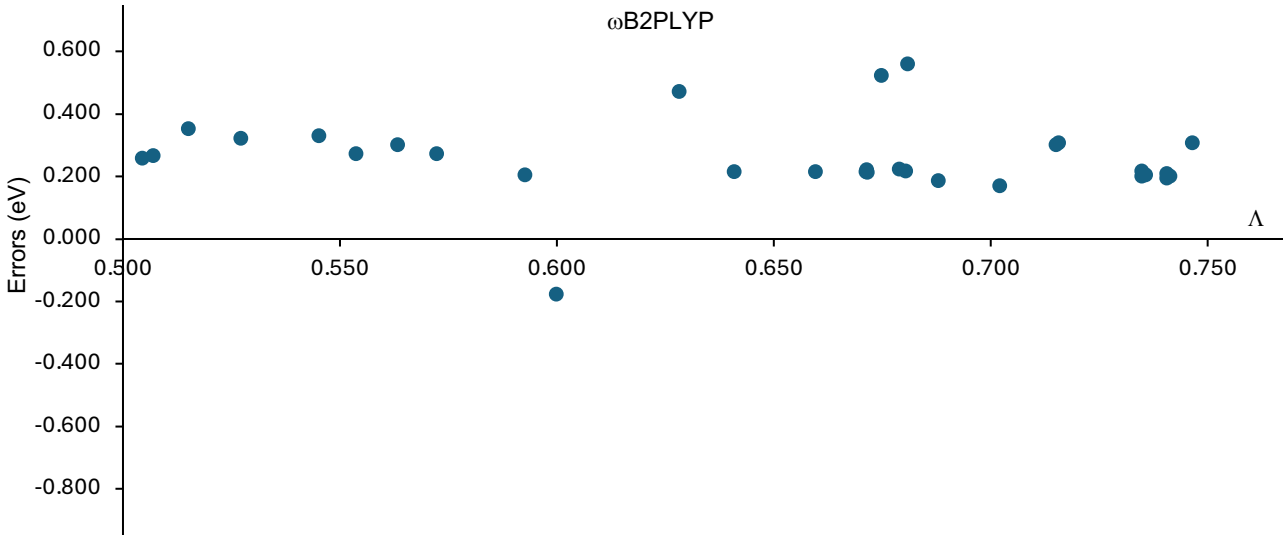

Figure S21: Λ and Errors plot - ωB2PLYP

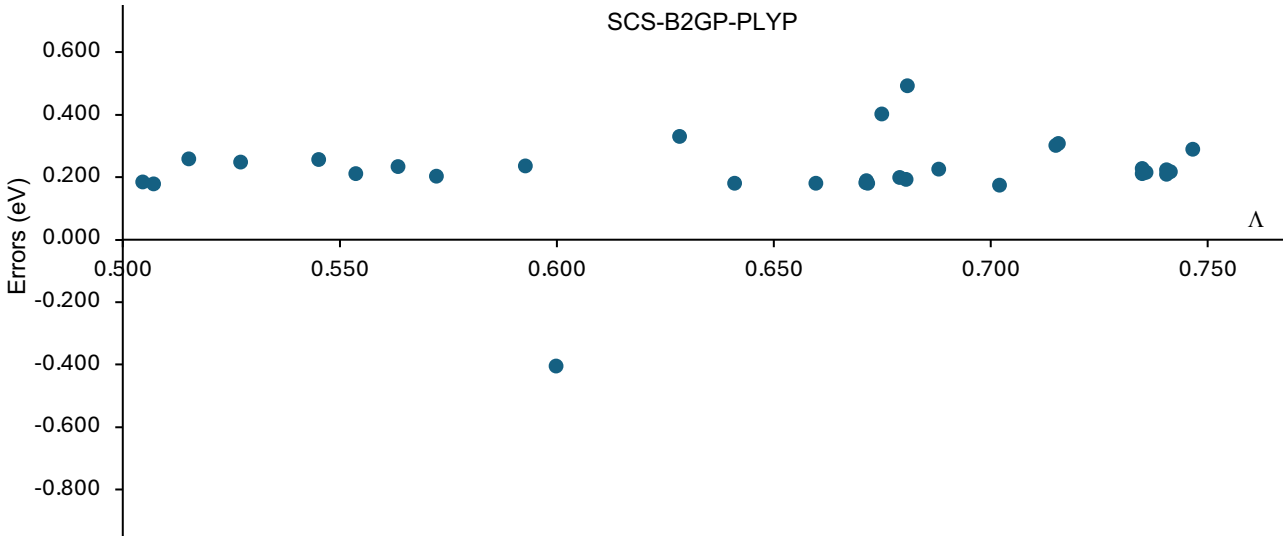

Figure S22: Λ and Errors plot - SCS-B2GP-PLYP

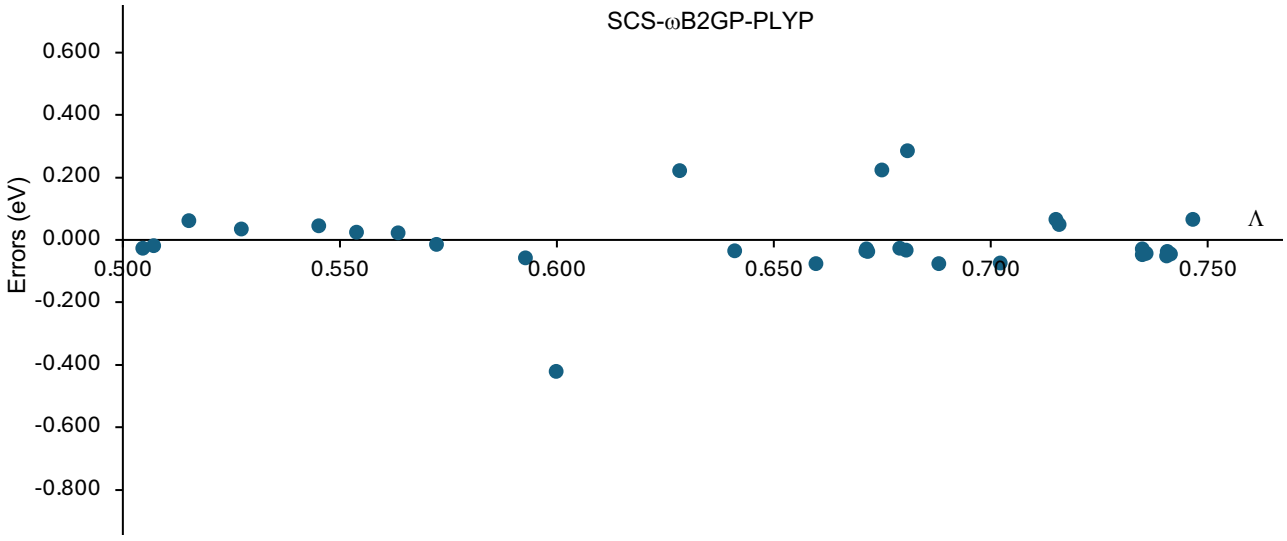

Figure S23: Λ and Errors plot - SCS-ωB2GP-PLYP

SI.10 CIS(D) results

Table S10: Performance of CIS(D) methods in terms of MAE, MSE, RMSE, Δ_{err} (all in eV) and R^2 for the **SBYD31** set.

	MAE	MSE	RMSE	Δ_{err}	R^2
CIS(D)	0.169	0.144	0.189	0.641	0.946
SCS-CIS(D)[a]	0.147	-0.126	0.167	0.582	0.957

[a] We used the SCS-CIS(D)$^{\lambda=1}$ variant, with the following parameters: $\lambda = 1$, $c_T^{SS} = 0.333$, $c_T^{OS} = 1.2$, $c_U^{SS} = 0.43$, $c_U^{OS} = 1.24$. See e.g. Refs S22 or S23 for detailed explanations of these parameters.

Table S11: CIS(D) details: solvent, transition, excitation energy, oscillator strength, and MO designation. H: HOMO, L: LUMO.

Compound	Method	Solvent	Transition	Excitation energy (eV)	Oscillator strength	MO designation
B1	CIS(D)	Et_2O	$S_0 \rightarrow S_1$	2.202	1.207	H → L
B1	SCS-CIS(D)	Et_2O	$S_0 \rightarrow S_1$	1.939	1.062	H → L
B1	CIS(D)	MeCN	$S_0 \rightarrow S_1$	2.180	1.224	H → L
B1	SCS-CIS(D)	MeCN	$S_0 \rightarrow S_1$	1.920	1.078	H → L
B2	CIS(D)	Et_2O	$S_0 \rightarrow S_1$	2.307	1.121	H → L
B2	SCS-CIS(D)	Et_2O	$S_0 \rightarrow S_1$	2.032	0.987	H → L
B2	CIS(D)	MeCN	$S_0 \rightarrow S_1$	2.308	1.120	H → L
B2	SCS-CIS(D)	MeCN	$S_0 \rightarrow S_1$	2.033	0.986	H → L
B2	CIS(D)	MeOH	$S_0 \rightarrow S_1$	2.313	1.120	H → L
B2	SCS-CIS(D)	MeOH	$S_0 \rightarrow S_1$	2.039	0.987	H → L
B3	CIS(D)	Et_2O	$S_0 \rightarrow S_1$	2.186	1.217	H → L
B3	SCS-CIS(D)	Et_2O	$S_0 \rightarrow S_1$	1.923	1.071	H → L
B3	CIS(D)	MeCN	$S_0 \rightarrow S_1$	2.164	1.236	H → L
B3	SCS-CIS(D)	MeCN	$S_0 \rightarrow S_1$	1.905	1.088	H → L
B3	CIS(D)	MeOH	$S_0 \rightarrow S_1$	2.169	1.237	H → L
B3	SCS-CIS(D)	MeOH	$S_0 \rightarrow S_1$	1.910	1.089	H → L
B4	CIS(D)	Et_2O	$S_0 \rightarrow S_1$	2.334	1.073	H → L
B4	SCS-CIS(D)	Et_2O	$S_0 \rightarrow S_1$	2.057	0.946	H → L
B4	CIS(D)	MeCN	$S_0 \rightarrow S_1$	2.338	1.071	H → L
B4	SCS-CIS(D)	MeCN	$S_0 \rightarrow S_1$	2.061	0.944	H → L
B4	CIS(D)	MeOH	$S_0 \rightarrow S_1$	2.343	1.070	H → L
B4	SCS-CIS(D)	MeOH	$S_0 \rightarrow S_1$	2.067	0.944	H → L
B5	CIS(D)	$CHCl_3$	$S_0 \rightarrow S_1$	2.459	1.243	H → L
B5	SCS-CIS(D)	$CHCl_3$	$S_0 \rightarrow S_1$	2.180	1.102	H → L
B6	CIS(D)	$CHCl_3$	$S_0 \rightarrow S_1$	2.419	1.615	H → L
B6	SCS-CIS(D)	$CHCl_3$	$S_0 \rightarrow S_1$	2.133	1.424	H → L
B7	CIS(D)	$CHCl_3$	$S_0 \rightarrow S_1$	2.411	1.615	H → L
B7	SCS-CIS(D)	$CHCl_3$	$S_0 \rightarrow S_1$	2.125	1.423	H → L
B8	CIS(D)	$CHCl_3$	$S_0 \rightarrow S_1$	2.393	1.565	H → L
B8	SCS-CIS(D)	$CHCl_3$	$S_0 \rightarrow S_1$	2.106	1.377	H → L
B9	CIS(D)	$CHCl_3$	$S_0 \rightarrow S_1$	2.428	1.310	H → L
B9	SCS-CIS(D)	$CHCl_3$	$S_0 \rightarrow S_1$	2.146	1.158	H → L
B10	CIS(D)	THF	$S_0 \rightarrow S_1$	3.937	0.521	H → L
B10	SCS-CIS(D)	THF	$S_0 \rightarrow S_1$	3.686	0.488	H → L
B11	CIS(D)	$CHCl_3$	$S_0 \rightarrow S_1$	2.680	0.780	H → L
B11	SCS-CIS(D)	$CHCl_3$	$S_0 \rightarrow S_1$	2.372	0.690	H → L
B11	CIS(D)	THF	$S_0 \rightarrow S_1$	2.699	0.774	H → L
B11	SCS-CIS(D)	THF	$S_0 \rightarrow S_1$	2.392	0.686	H → L
B12	CIS(D)	$CHCl_3$	$S_0 \rightarrow S_1$	2.415	1.753	H → L
B12	SCS-CIS(D)	$CHCl_3$	$S_0 \rightarrow S_1$	2.125	1.542	H → L
B13	CIS(D)	$CHCl_3$	$S_0 \rightarrow S_1$	1.872	1.142	H → L

B13	SCS-CIS(D)	$CHCl_3$	$S_0 \rightarrow S_1$	1.611	0.983	H $\rightarrow$ L
B14	CIS(D)	MeOH	$S_0 \rightarrow S_1$	2.663	0.857	H $\rightarrow$ L
B14	SCS-CIS(D)	MeOH	$S_0 \rightarrow S_1$	2.416	0.778	H $\rightarrow$ L
B15	CIS(D)	DCM	$S_0 \rightarrow S_1$	2.053	1.264	H $\rightarrow$ L
B15	SCS-CIS(D)	DCM	$S_0 \rightarrow S_1$	1.794	1.104	H $\rightarrow$ L
B16	CIS(D)	DCM	$S_0 \rightarrow S_1$	2.031	1.130	H $\rightarrow$ L
B16	SCS-CIS(D)	DCM	$S_0 \rightarrow S_1$	1.770	0.985	H $\rightarrow$ L
B17	CIS(D)	THF	$S_0 \rightarrow S_1$	3.421	0.525	H $\rightarrow$ L
B17	SCS-CIS(D)	THF	$S_0 \rightarrow S_1$	3.162	0.485	H $\rightarrow$ L
B18	CIS(D)	DCM	$S_0 \rightarrow S_1$	2.474	0.736	H $\rightarrow$ L +1
B18	SCS-CIS(D)	DCM	$S_0 \rightarrow S_1$	2.173	0.646	H $\rightarrow$ L +1
B19	CIS(D)	DCM	$S_0 \rightarrow S_1$	1.666	1.606	H $\rightarrow$ L
B19	SCS-CIS(D)	DCM	$S_0 \rightarrow S_1$	1.367	1.318	H $\rightarrow$ L
B20	CIS(D)	THF	$S_0 \rightarrow S_1$	2.039	1.589	H $\rightarrow$ L
B20	SCS-CIS(D)	THF	$S_0 \rightarrow S_1$	1.757	1.370	H $\rightarrow$ L
B21	CIS(D)	THF	$S_0 \rightarrow S_1$	2.284	1.424	H $\rightarrow$ L
B21	SCS-CIS(D)	THF	$S_0 \rightarrow S_1$	1.998	1.246	H $\rightarrow$ L
B22	CIS(D)	MeOH	$S_0 \rightarrow S_1$	3.509	0.613	H $\rightarrow$ L
B22	SCS-CIS(D)	MeOH	$S_0 \rightarrow S_1$	3.240	0.566	H $\rightarrow$ L
B23	CIS(D)	MeOH	$S_0 \rightarrow S_1$	2.770	0.640	H $\rightarrow$ L
B23	SCS-CIS(D)	MeOH	$S_0 \rightarrow S_1$	2.460	0.568	H $\rightarrow$ L

References

(S1) Rurack, K.; Kollmannsberger, M.; Daub, J. *Angew. Chem., Int. Ed.* **2001**, *40*, 385–387.

(S2) Qin, W.; Baruah, M.; De Borggraeve, W. M.; Boens, N. *J. Photochem. Photobiol., A* **2006**, *183*, 190–197.

(S3) Filarowski, A.; Kluba, M.; Cieślik-Boczula, K.; Koll, A.; Kochel, A.; Pandey, L.; De Borggraeve, W. M.; Van der Auweraer, M.; Catalán, J.; Boens, N. *Photochem. Photobiol. Sci.* **2010**, *9*, 996–1008.

(S4) Wang, J.-B.; Fang, X.-Q.; Pan, X.; Dai, S.-Y.; Song, Q.-H. *Chem. - Asian J.* **2012**, *7*, 696–700.

(S5) Mao, M.; Li, Q.-S.; Zhang, X.-L.; Wu, G.-H.; Dai, C.-G.; Ding, Y.; Dai, S.-Y.; Song, Q.-H. *Dyes Pigm.* **2017**, *141*, 148–160.

(S6) Mao, M.; Zhang, X.-L.; Fang, X.-Q.; Wu, G.-H.; Ding, Y.; Liu, X.-L.; Dai, S.-Y.; Song, Q.-H. *Org. Electron.* **2014**, *15*, 2079–2090.

(S7) Yeh, S.-C.; Wang, L.-J.; Yang, H.-M.; Dai, Y.-H.; Lin, C.-W.; Chen, C.-T.; Jeng, R.-J. *Chem. - Eur. J.* **2017**, *23*, 14747–14759.

(S8) Mao, M.; Wang, J.-B.; Xiao, Z.-F.; Dai, S.-Y.; Song, Q.-H. *Dyes Pigm.* **2012**, *94*, 224–232.

(S9) Mao, M.; Xiao, S.; Yi, T.; Zou, K. *J. Fluorine Chem.* **2011**, *132*, 612–616.

(S10) Arroyo, I. J.; Hu, R.; Merino, G.; Tang, B. Z.; Pena-Cabrera, E. *J. Org. Chem.* **2009**, *74*, 5719–5722.

(S11) Kolemen, S.; Bozdemir, O. A.; Cakmak, Y.; Barin, G.; Erten-Ela, S.; Marszalek, M.; Yum, J.-H.; Zakeeruddin, S. M.; Nazeeruddin, M. K.; Grätzel, M. et al. *Chem. Sci.* **2011**, *2*, 949–954.

(S12) Wu, L.; Burgess, K. *J. Am. Chem. Soc.* **2008**, *130*, 4089–4096.

(S13) Çakmak, Y.; Kolemen, S.; Buyuktemiz, M.; Dede, Y.; Erten-Ela, S. *New J. Chem.* **2015**, *39*, 4086–4092.

(S14) Zhang, J.; Lu, F.; Qi, S.; Zhao, Y.; Wang, K.; Zhang, B.; Feng, Y. *Dyes Pigm.* **2016**, *128*, 296–303.

(S15) Banuelos, J.; Arbeloa, F. L.; Martinez, V.; Liras, M.; Costela, A.; Moreno, I. G.; Arbeloa, I. L. *Phys. Chem. Chem. Phys.* **2011**, *13*, 3437–3445.

(S16) Lu, Z.; Liang, M.; Dai, P.; Miao, K.; Zhang, C.; Sun, Z.; Xue, S. *J. Phys. Chem. C* **2016**, *120*, 25657–25667.

(S17) Kubota, Y.; Kimura, K.; Jin, J.; Manseki, K.; Funabiki, K.; Matsui, M. *New J. Chem.* **2019**, *43*, 1156–1165.

(S18) Kubo, Y.; Eguchi, D.; Matsumoto, A.; Nishiyabu, R.; Yakushiji, H.; Shigaki, K.; Kaneko, M. *J. Mater. Chem. A* **2014**, *2*, 5204–5211.

(S19) Shi, W.-J.; Kinoshita, T.; Ng, D. K. *Asian J. Org. Chem.* **2017**, *6*, 758–767.

(S20) Bañuelos, J.; Martín, V.; Gómez-Durán, C. A.; Córdoba, I. J. A.; Peña-Cabrera, E.; García-Moreno, I.; Costela, Á.; Pérez-Ojeda, M. E.; Arbeloa, T.; Arbeloa, Í. L. *Chem. - Eur. J.* **2011**, *17*, 7261–7270.

(S21) Goud, T. V.; Tutar, A.; Biellmann, J.-F. *Tetrahedron* **2006**, *62*, 5084–5091.

(S22) Rhee, Y. M.; Head-Gordon, M. *J. Phys. Chem. A* **2007**, *111*, 5314–5326.

(S23) Goerigk, L.; Grimme, S. *J. Chem. Phys.* **2010**, *132*, 184103.