SUPPORTING INFORMATION

Predicting Absorption and Emission Maxima of Polycyclic Aromatic Azaborines: Reliable Transition Energies and Character

Robert W. Lamb,[1] Alan K. Schrock,[2] Michael T. Huggins,[3] and Charles Edwin Webster[1]

[1] *Department of Chemistry, Mississippi State University, Mississippi State, MS, 39762, United States*
[2] *Department of Chemistry, University of West Florida, Pensacola, FL, 32514, United States*
[3] *College of Science and Technology, Tarleton State University, Stephenville, TX 76402, United States*

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Solvation Schemes with B3LYP and ωB97xD

With a TD-DFT computation that incorporates an implicit solvation model, there are various schemes available in Gaussian that can be applied to obtain the absorption and emission wavelengths without changing the solvation model or its parameters. The simplest scheme is to use a linear response (LR) solvation model and simply take the excitation energy directly from the final geometry. The drawback of this method is that when the geometry relaxes in the ES, the solvation shell also relaxes, a phenomenon that is not accounted for in LR solvation. The next scheme is to optimize the ES geometry with LR solvation and perform single-point computations with external iteration (EI) state specific solvation. This method variationally relaxes the SCRF such that the compound's electrostatic potential becomes self-consistent with the solvent field. A final ΔSCRF scheme employs the previous EI single-points on the LR optimized geometries, followed by a non-equilibrium single-point computation to obtain the energy of the GS at the ES geometry. Subtraction of the ES and GS energies produces an energy gap that can be converted to a wavelength. Since the discrepancy of the computed data from experiment is specifically due to the emission from the nitro compounds, analyses in this section will focus only on the differences in λ_{em} from these schemes. Additionally, solvation models are not available for CIS(D) in Gaussian, therefore only the B3LYP and ωB97xD methods will be compared. Figure S1 are the plots of the obtained λ_{em} with each solvation scheme vs experimental values in both $CHCl_3$ and acetonitrile (ACN) (compound **8** had very weak emission in ACN, thus its experimental value is not available).

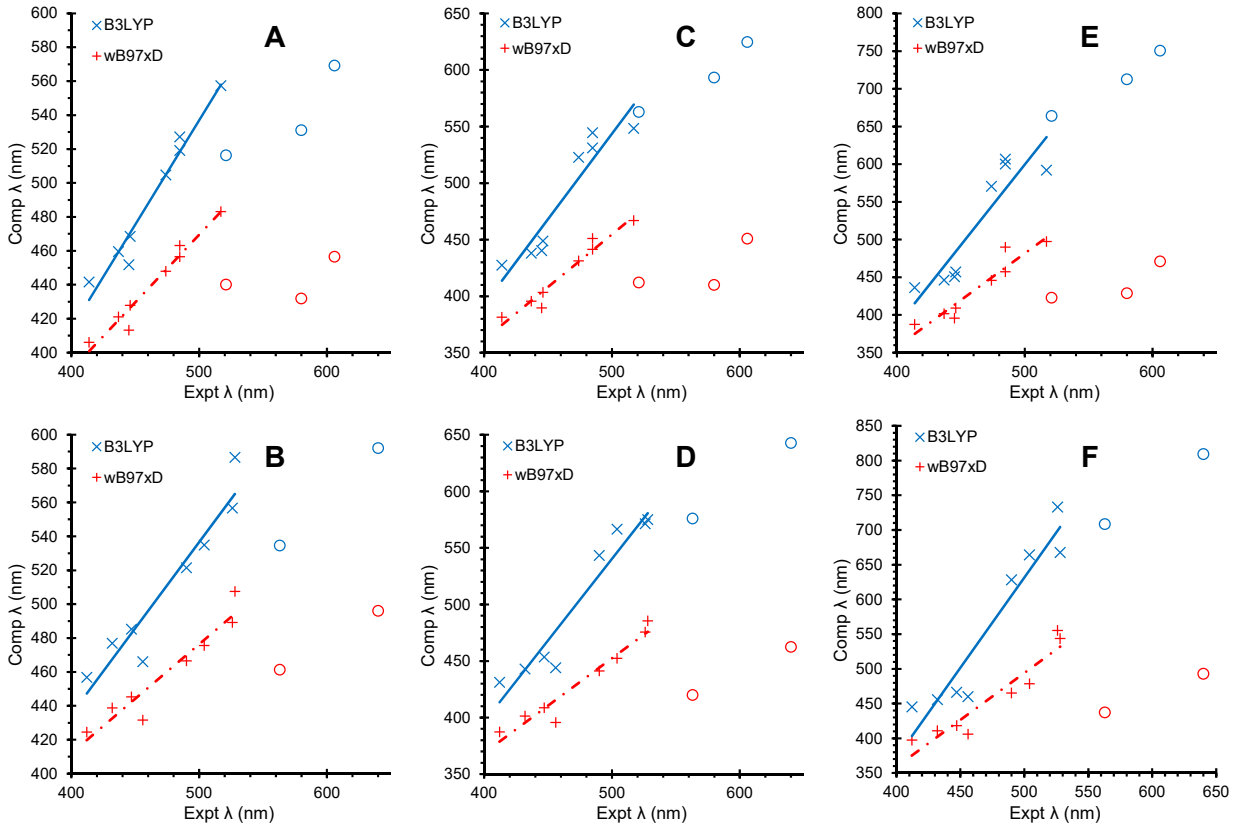


Figure S1: Computed vs experimental λ_{em} from LR (A/B), EI (C/D) and ΔSCRF (E/F) solvation schemes of $CHCl_3$ (top) and ACN (bottom) solvent. Colored circles correspond to the computed emission of the nitro compounds from the corresponding method.

Using the LR solvation scheme, both functionals place the nitro compounds as outliers to the emission of the other compounds. With the EI scheme, the nitro compounds are significantly closer to the regression line in both $CHCl_3$ and ACN (see Table S1 for trendline equations and R^2 values). However, minimal change in the position of the λ_{em} of the nitro compounds is observed with ωB97xD between LR and nLR solvation schemes. In fact, the linear regressions are generally slightly worse for ωB97xD with nLR solvation compared to LR solvation (Table S1 in the SI). The more cumbersome ΔSCRF scheme produces quite reasonable results with B3LYP in $CHCl_3$, although the values for ACN still fall somewhat off the regression line. As before, for ωB97xD, there is minimal change in the position of the λ_{em} of the nitro compounds. Examining the linear

regressions (Table S1 in the SI) indicates that with B3LYP, the best correlation to the experimental data in $CHCl_3$ (including the λ_{em} from the nitro compounds) is obtained with the ΔSCRF solvation scheme.. However, it should also be noted that if the nitro compound's λ_{em} are excluded, the best correlation to experimental data is found from LR solvation ($R^2_{LR-nitro} = 0.96$ vs $R^2_{\Delta SCRF} = 0.91$). This difference indicates that while nLR and ΔSCRF solvation schemes produce a better trendline with the nitro compounds included, the quality of the correlation for the remaining compounds worsens. Conversely with B3LYP computations compared to experimental data in ACN, nLR solvation produces the best correlation to experiment, both with and without the nitro compound's λ_{em}, compared to LR and ΔSCRF solvation. Interestingly, results from ωB97xD have a trend that is generally opposite thatn of B3LYP. With ωB97xD data, the best correlation to the experimental data in $CHCl_3$ comes from LR solvation. Using nLR and ΔSCRF solvation makes the R^2 value progressively worse, both with and without the λ_{em} for the nitro compounds. However, compared to the experimental data in ACN, the best correlation including the λ_{em} of the nitro compounds comes from LR solvation, while the best correlation excluding the λ_{em} of the nitro compounds comes from nLR solvation.

Linear Regressions

Table S1: Linear regressions, and their R^2 values, of the computed vs experimental λ_{em} with and without the nitro compounds using chloroform or acetonitrile with B3LYP/BS1 or ωB97xD/BS1. Gas-phase computations also include CIS(D)/BS2//B3LYP/BS1.

B3LYP $CHCl_3$	**Gas**		**LR**		**nLR**		**ES–GS**	
	w/out nitro	**w/ nitro**	**w/out nitro**	**w/ nitro**	**w/out nitro**	**w/ nitro**	**w/out nitro**	**w/ nitro**
Trendline Equation	0.88x + 49.68	0.42x + 257.94	1.23x – 78.519	0.63x + 195.62	1.51x – 211.87	1.08x – 12.40	2.14x – 469.61	1.77x – 300.91
R^2	0.93	0.71	0.96	0.76	0.88	0.90	0.82	0.91
B3LYP ACN	**Gas**		**LR**		**nLR**		**ES–GS**	
	w/out nitro	**w/ nitro**	**w/out nitro**	**w/ nitro**	**w/out nitro**	**w/ nitro**	**w/out nitro**	**w/ nitro**
Trendline Equation	0.64x + 153.53	0.38x + 271	1.02x + 28.87	0.63x + 206.5	1.44x – 180.05	1.02x + 10.53	2.59x – 664.87	1.85x – 320.18
R^2	0.85	0.72	0.91	0.78	0.92	0.89	0.91	0.88
ωB97xD $CHCl_3$	**Gas**		**LR**		**nLR**		**ES–GS**	
	w/out nitro	**w/ nitro**	**w/out nitro**	**w/ nitro**	**w/out nitro**	**w/ nitro**	**w/out nitro**	**w/ nitro**
Trendline Equation	0.63x + 104.24	0.16x + 316.23	0.70x + 70.93	0.25x + 317.80	0.93x – 10.95	0.27x + 290.84	1.24x – 138.03	0.35x + 264.74
R^2	0.96	0.25	0.96	0.37	0.95	0.31	0.90	0.30
ωB97xD ACN	**Gas**		**LR**		**nLR**		**ES–GS**	
	w/out nitro	**w/ nitro**	**w/out nitro**	**w/ nitro**	**w/out nitro**	**w/ nitro**	**w/out nitro**	**w/ nitro**
Trendline Equation	0.46x + 179.72	0.21x + 293.41	0.64x + 154.3	0.33x + 300.17	0.84x + 33.61	0.35x + 255.94	1.35x – 182.53	0.51x + 206.44
R^2	0.87	0.51	0.91	0.62	0.94	0.48	0.89	0.38
CIS(D)//B3LYP $CHCl_3$	**Gas**							
	w/out nitro	**w/ nitro**						
Trendline Equation	0.55x + 92.00	0.21x + 247.65						
R^2	0.93	0.47						
CIS(D)//B3LYP ACN	**Gas**							
	w/out nitro	**w/ nitro**						
Trendline Equation	0.40x + 160.05	0.23x + 236.85						
R^2	0.83	0.66						

Transition Characterization Data

Table S2: Gas-phase Φ_s for the absorption [DFT/BS1 or CIS(D)/BS2//B3LYP/BS1] and emission [TD-DFT/BS1 or CIS(D)/BS2//TD-B3LYP/BS1] maxima.

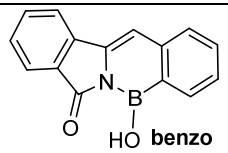
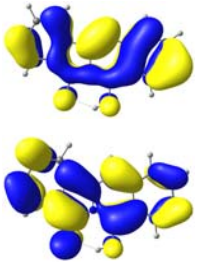
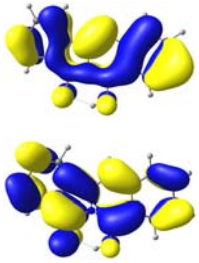
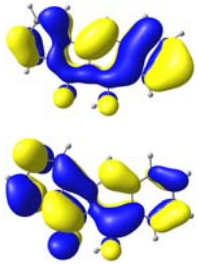
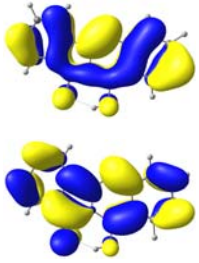
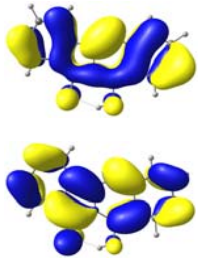
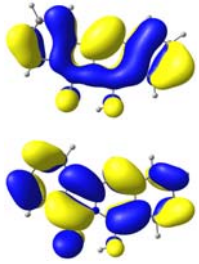
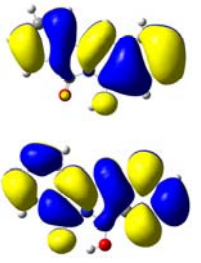
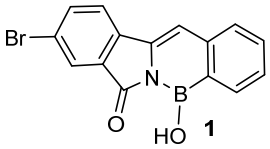
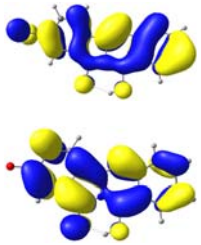
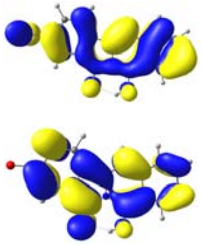
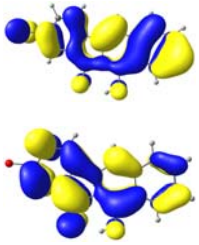
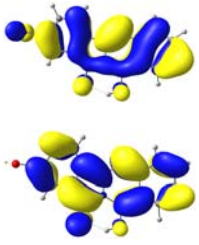
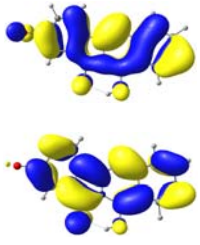
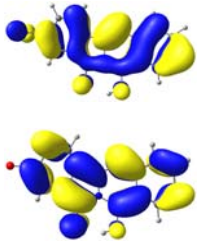
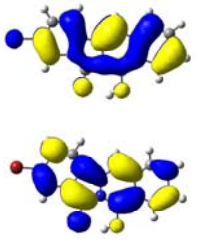
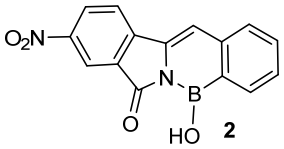
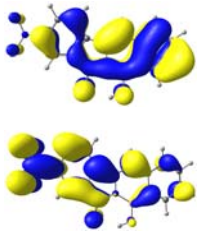
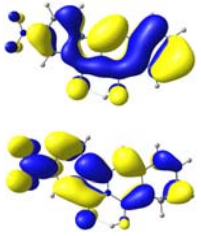
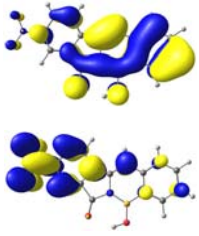
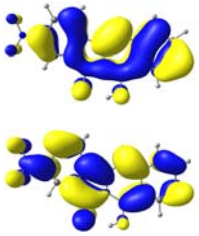
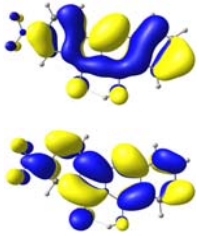
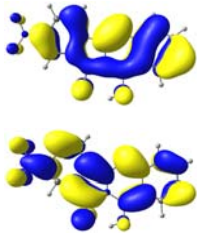
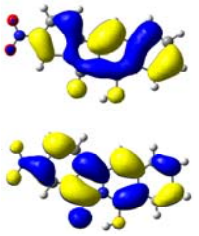
	Absorption						**Emission**					
	B3LYP	**PBE0**	**B97D**	**cam-QTP01**	**LC-ωHPBE**	**ωB97xD**	**B3LYP**	**PBE0**	**B97D**	**cam-QTP01**	**LC-ωHPBE**	**ωB97xD**
benzo	0.74	0.75	0.71	0.82	0.82	0.8	0.74	0.75	0.66	0.84	0.84	0.82
1	0.74	0.75	0.71	0.82	0.82	0.8	0.73	0.75	0.65	0.84	0.84	0.81
2	***0.63***	***0.68***	***0.44***	***0.81***	***0.81***	***0.78***	***0.52***	***0.66***	***0.37***	***0.83***	***0.83***	***0.81***
3	0.75	0.76	0.72	0.81	0.82	0.79	0.76	0.77	0.73	0.83	0.83	0.80
dioxo	0.66	0.69	0.55	0.82	0.82	0.79	0.66	0.68	0.50	0.83	0.83	0.80
4	0.65	0.68	0.55	0.81	0.82	0.78	0.63	0.67	0.48	0.82	0.83	0.79
5	***0.58***	***0.62***	***0.45***	***0.80***	***0.8***	***0.77***	***0.54***	***0.63***	***0.37***	***0.82***	***0.82***	***0.79***
6	0.72	0.73	0.64	0.81	0.82	0.79	0.72	0.74	0.60	0.83	0.83	0.80
thieno	0.70	0.71	0.65	0.82	0.82	0.79	0.67	0.70	0.60	0.83	0.83	0.80
7	0.70	0.71	0.64	0.81	0.81	0.78	0.66	0.69	0.58	0.82	0.83	0.80
8	***0.56***	***0.62***	***0.41***	***0.79***	***0.79***	***0.76***	***0.47***	***0.56***	***0.37***	***0.81***	***0.5***	***0.79***
9	0.72	0.73	0.68	0.81	0.81	0.78	0.73	0.75	0.69	0.83	0.83	0.80

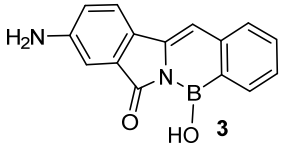
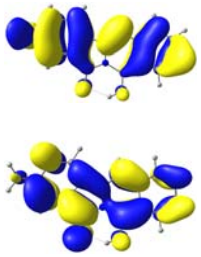
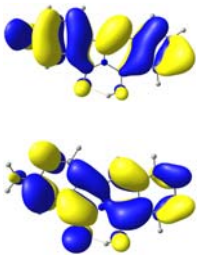
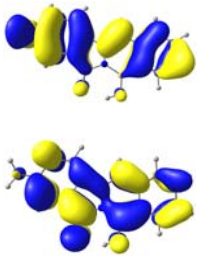
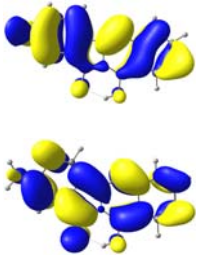
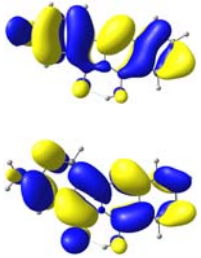
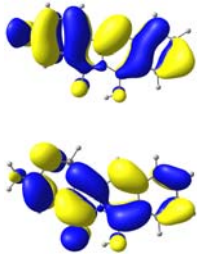
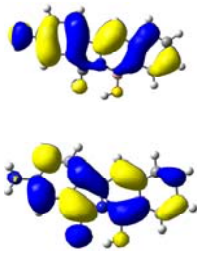
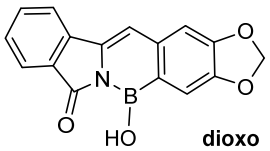
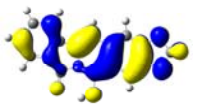
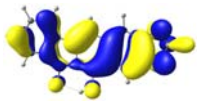
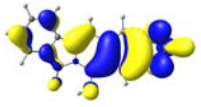
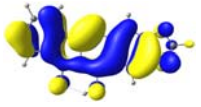
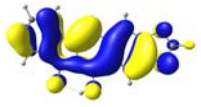
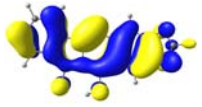
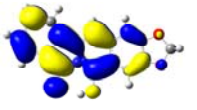
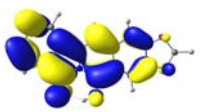
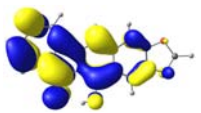
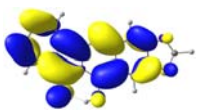
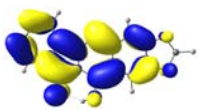
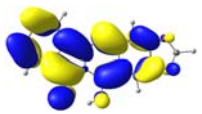
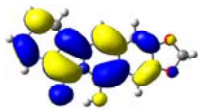
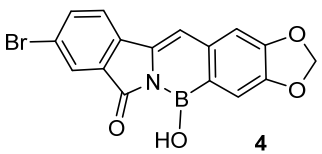
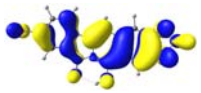
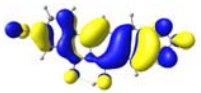
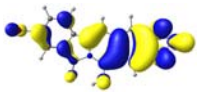
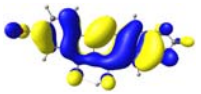
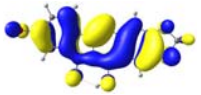
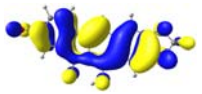
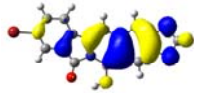
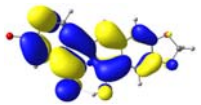
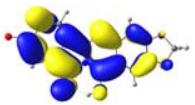
Table S3: Φ_S for λ_{em} computed with LR-SMD-TD-DFT/BS1 (acetonitrile solvent). The Φ_S values for the corresponding anions (**2**$^-$, **5**$^-$, and **8**$^-$) are shown in parenthesis.

	B3LYP	**PBE0**	**B97D**	**cam-QTP01**	**LC-ωHPBE**	**ωB97xD**
benzo	0.78	0.78	0.76	0.85	0.85	0.83
1	0.77	0.77	0.75	0.84	0.85	0.82
2	***0.56(0.40)***	***0.7(0.16)***	***0.42***	***0.84(0.81)***	***0.84(0.81)***	***0.82(0.72)***
3	0.74	0.77	0.70	0.82	0.83	0.79
dioxo	0.70	0.71	0.59	0.84	0.84	0.82
4	0.68	0.70	0.56	0.84	0.84	0.81
5	***0.53(0.44)***	***0.65(0.17)***	***0.40***	***0.82(0.80)***	***0.83(0.81)***	***0.80(0.73)***
6	0.75	0.76	0.73	0.83	0.83	0.80
thieno	0.74	0.74	0.70	0.84	0.84	0.82
7	0.73	0.74	0.69	0.84	0.84	0.81
8	***0.50(0.37)***	***0.61(0.10)***	***0.41***	***0.82(0.79)***	***0.82(0.80)***	***0.80(0.70)***
9	0.74	0.76	0.71	0.83	0.84	0.80

Natural Transition Orbitals

Table S4: Absorption Natural Transition Orbitals for the hole (top) and particle (bottom) of the azaborines from TD-DFT/BS1//DFT/BS1 and EOM-CCSD/BS2//B3LYP/BS1 (isovalue of 0.02).

Structure	B3LYP/BS1	PBE0/BS1	B97D/BS1	cam-QTP01/BS1	LC-ωHPBE/BS1	ωB97xD/BS1	EOM-CCSD/BS2//B3LYP/BS1
 benzo							
 1							
 2							

Structure	B3LYP/BS1	PBE0/BS1	B97D/BS1	cam-QTP01/BS1	LC-ωHPBE/BS1	ωB97xD/BS1	EOM-CCSD/BS2//B3LYP/BS1
 **3**							
 **dioxo**							
							
 **4**							
							
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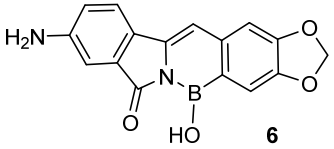
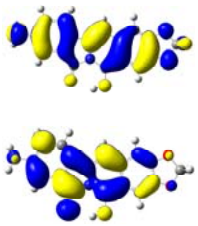
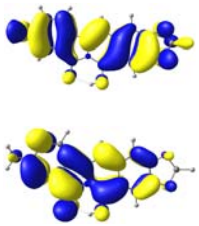
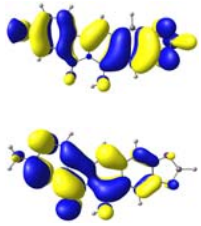
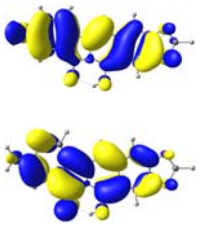
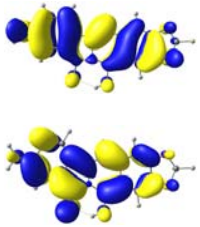
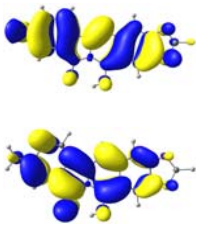
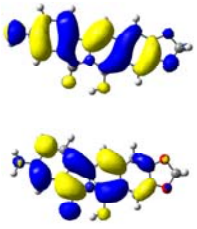
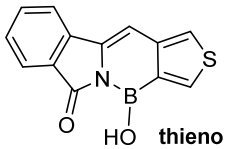
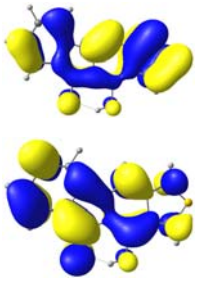
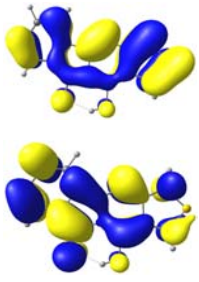
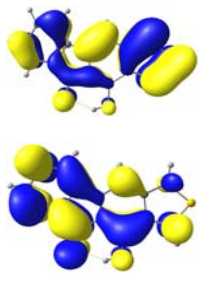
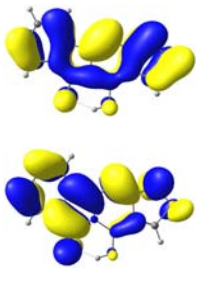
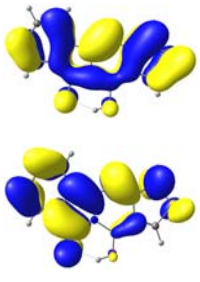
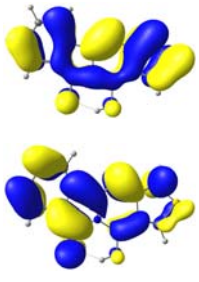
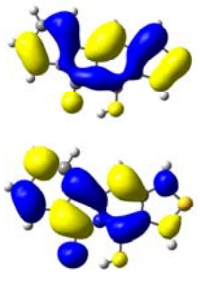
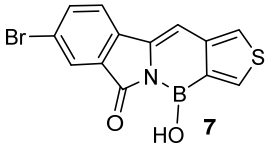
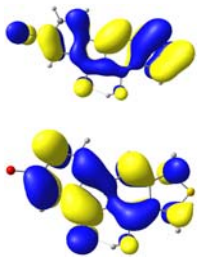
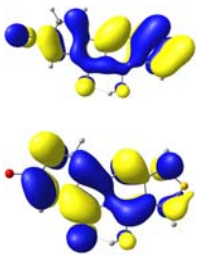
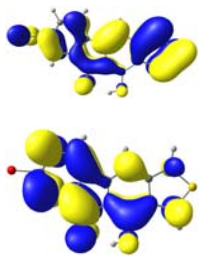
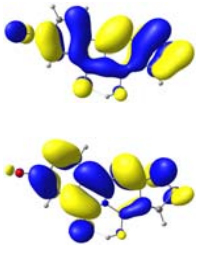
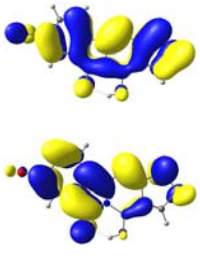
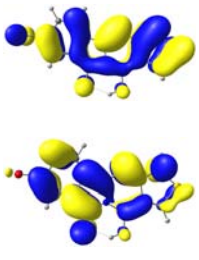
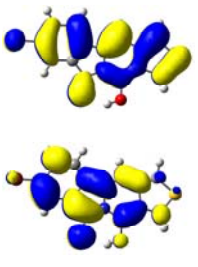
Structure	B3LYP/BS1	PBE0/BS1	B97D/BS1	cam-QTP01/BS1	LC-ωHPBE/BS1	ωB97xD/BS1	EOM-CCSD/BS2//B3LYP/BS1
 6							
 thieno							
 7							

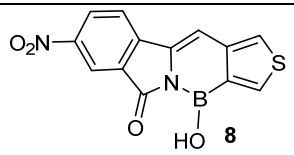
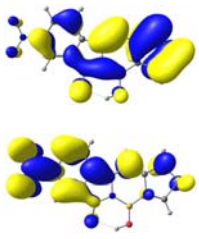
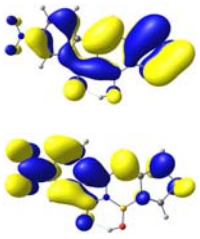
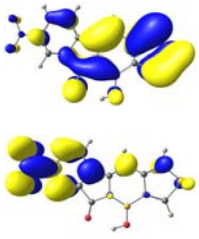
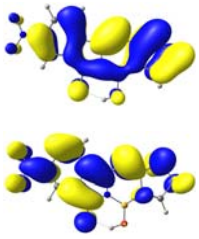
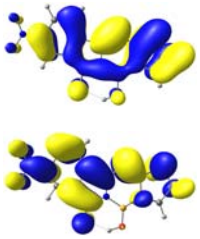
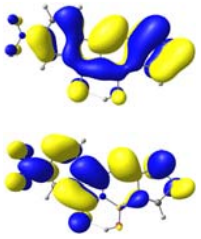
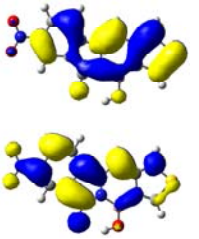
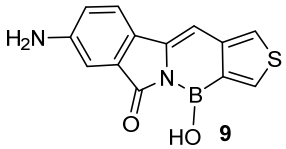
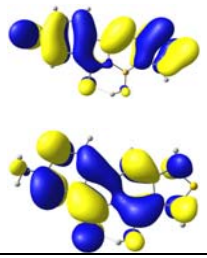
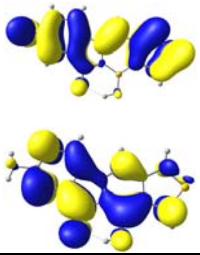
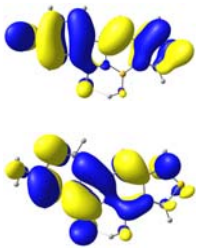
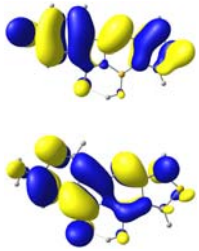
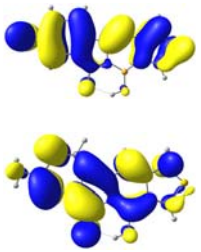
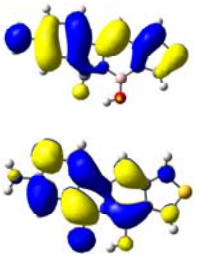
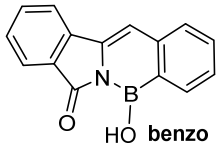
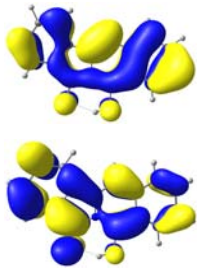
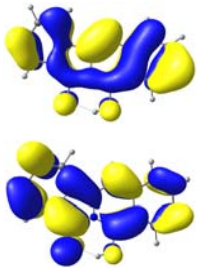
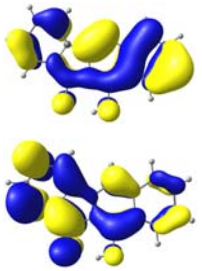
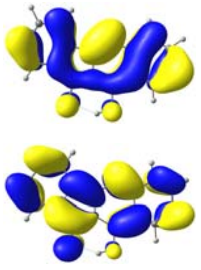
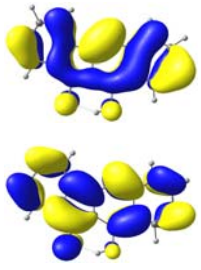
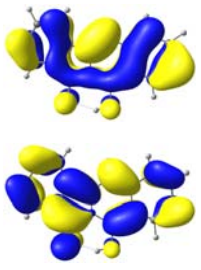
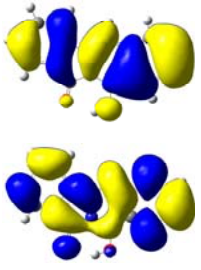
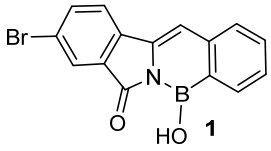
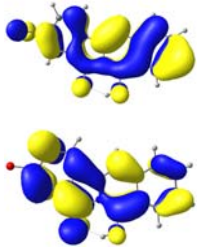
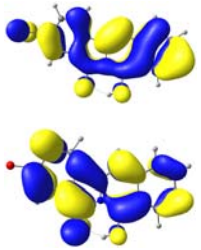
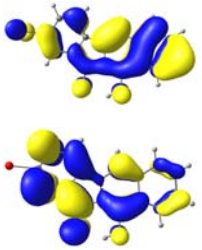
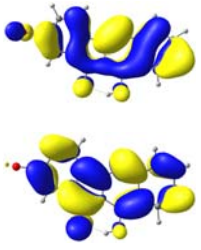
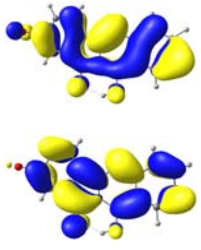
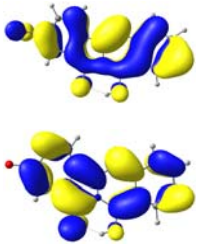
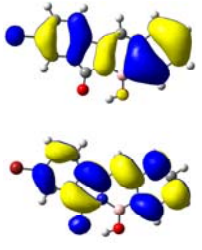
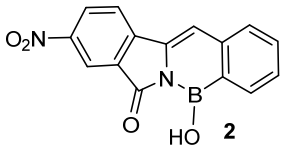
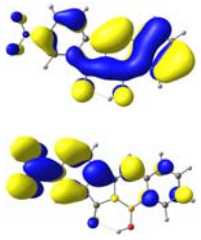
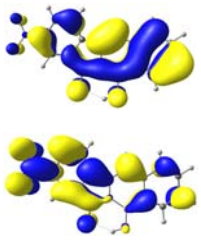
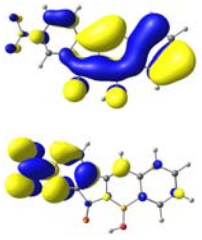
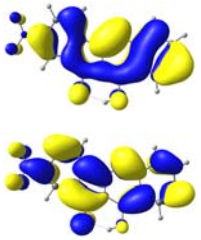
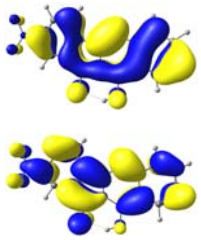
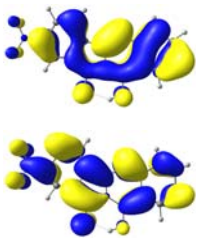
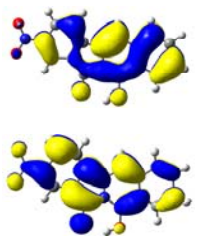
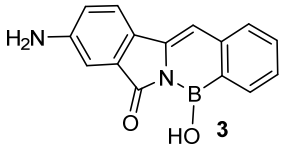
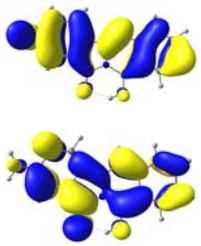
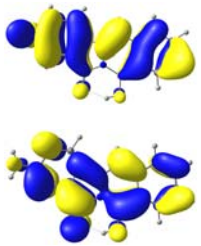
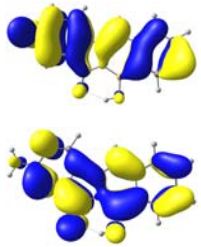
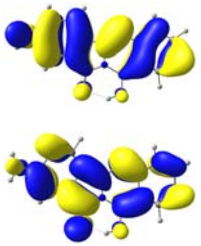
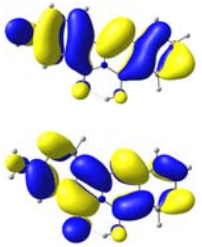
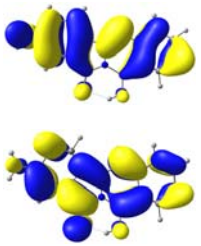
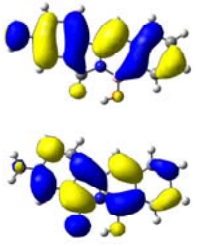
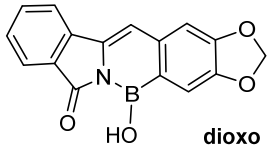
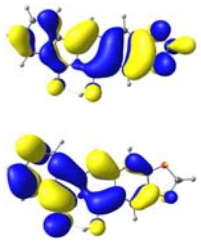
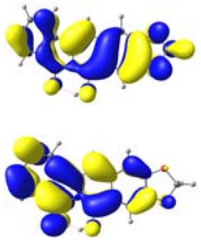
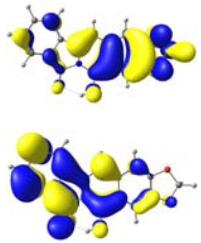
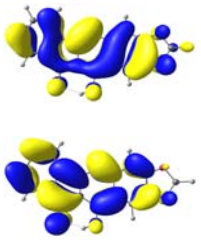
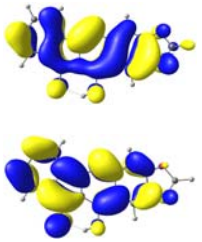
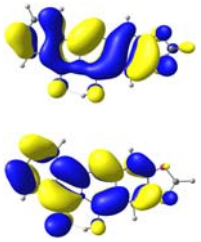
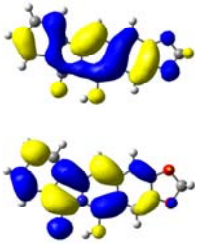
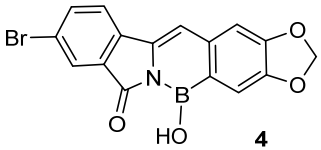
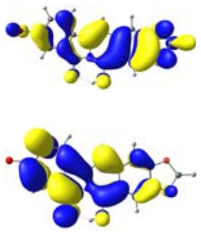
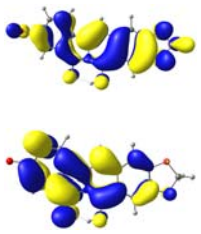
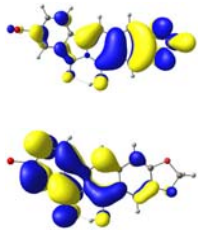
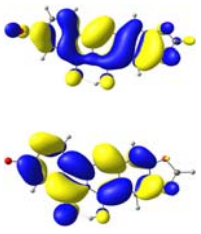
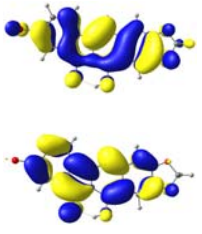
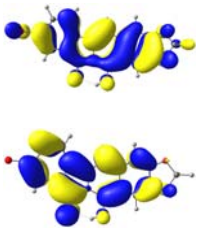
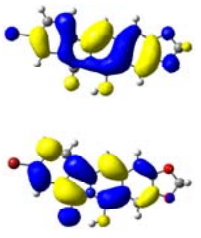
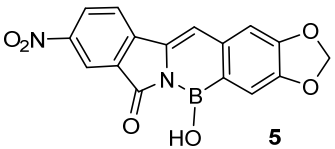
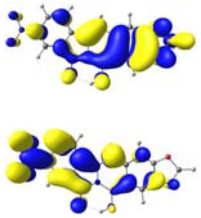
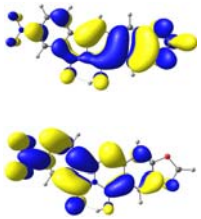
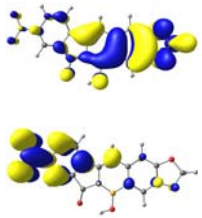
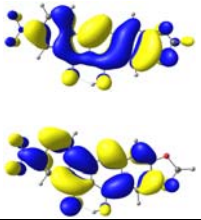
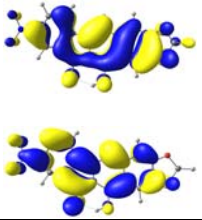
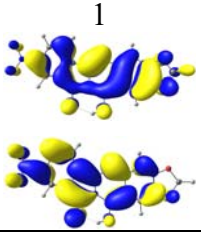
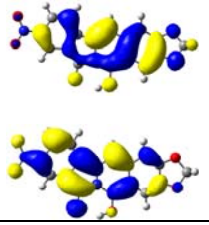
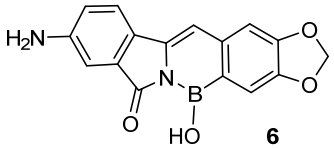
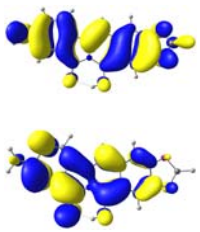
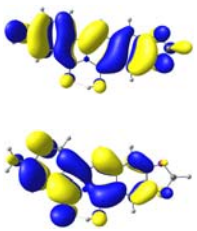
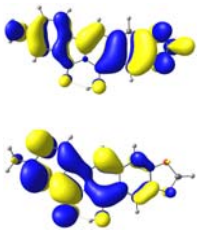
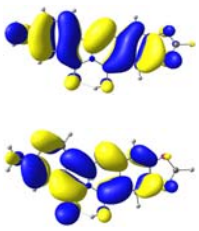
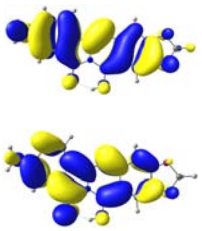
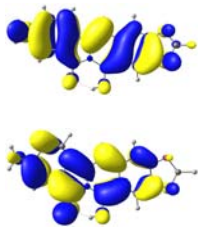
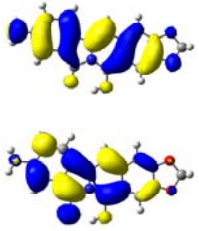
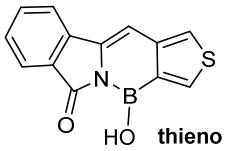
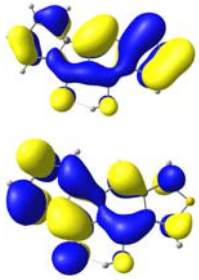
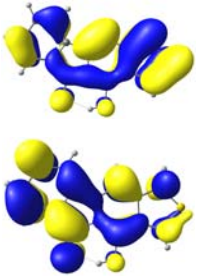
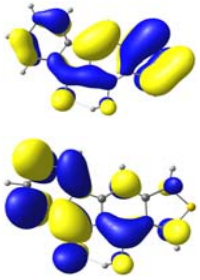
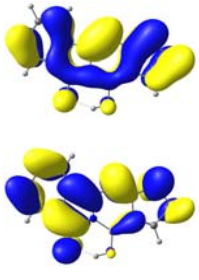
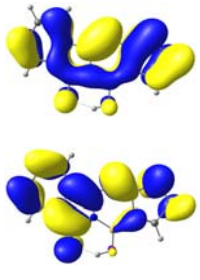
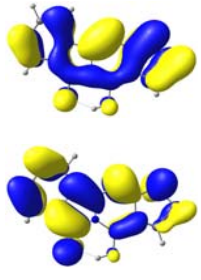
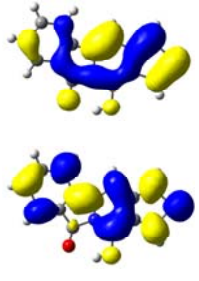
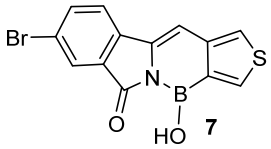
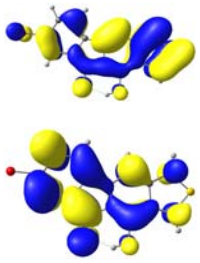
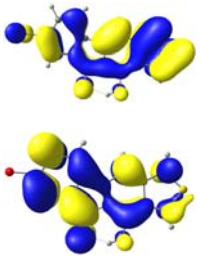
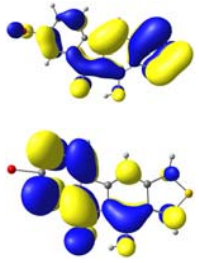
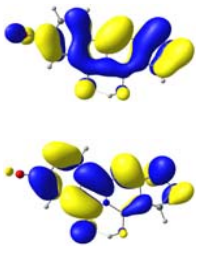
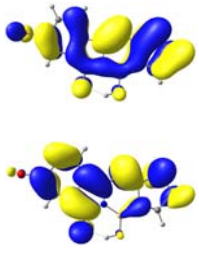
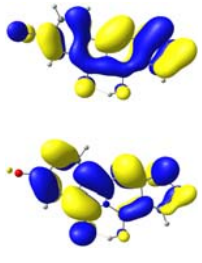
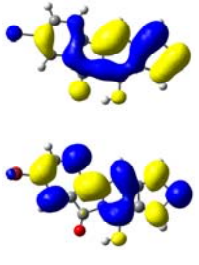
Structure	B3LYP/BS1	PBE0/BS1	B97D/BS1	cam-QTP01/BS1	LC-ωHPBE/BS1	ωB97xD/BS1	EOM-CCSD/BS2//B3LYP/BS1
 **8**							
 **9**							

Table S5: Emission Natural Transition Orbitals for the particle (top) and hole (bottom) of the azaborines from TD-DFT/BS1 and EOM-CCSD/BS2//TD-B3LYP/BS1 (isovalue of 0.02).

Structure	B3LYP/BS1	PBE0/BS1	B97D/BS1	cam-QTP01/BS1	LC-ωHPBE/BS1	ωB97xD/BS1	EOM-CCSD/BS2// B3LYP/BS1
 benzo							
 1							
 2							

Structure	B3LYP/BS1	PBE0/BS1	B97D/BS1	cam-QTP01/BS1	LC-ωHPBE/BS1	ωB97xD/BS1	EOM-CCSD/BS2// B3LYP/BS1
 3							
 dioxo							
 4							
 5						 1	

Structure	B3LYP/BS1	PBE0/BS1	B97D/BS1	cam-QTP01/BS1	LC-ωHPBE/BS1	ωB97xD/BS1	EOM-CCSD/BS2// B3LYP/BS1
 **6**							
 **thieno**							
 **7**							

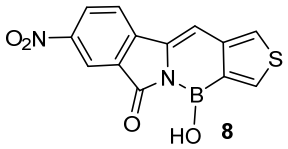
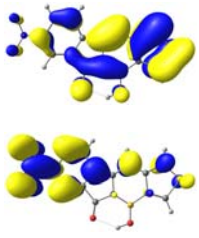
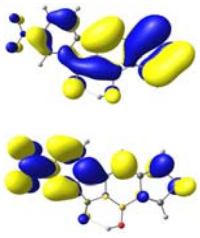
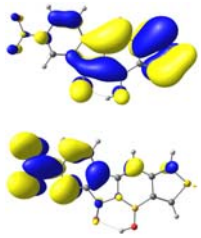
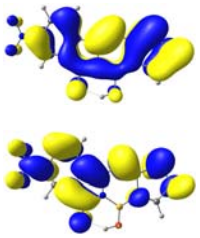
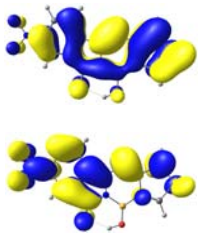
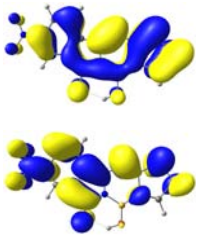
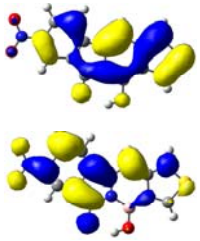
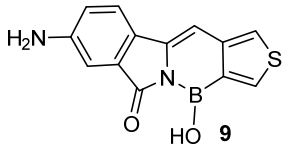
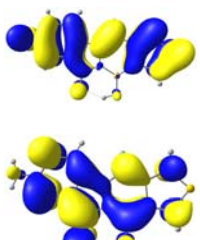
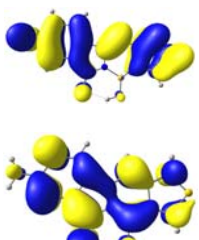
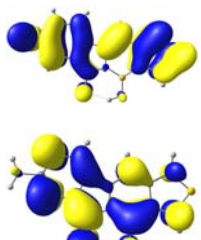
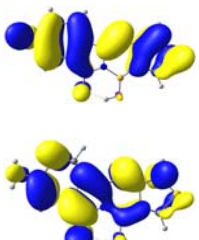
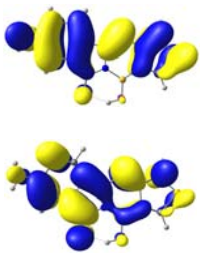
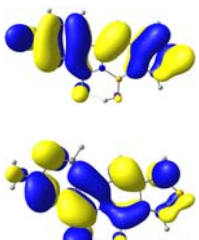
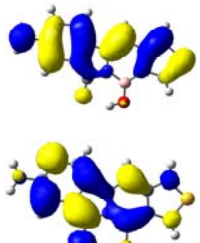
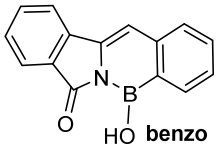
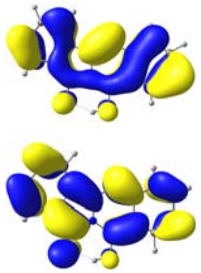
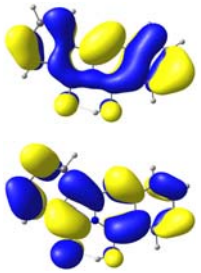
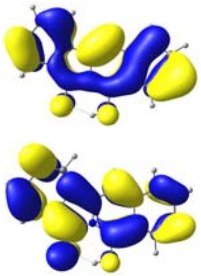
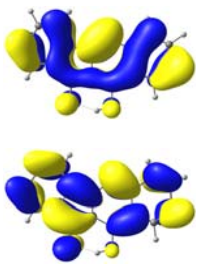
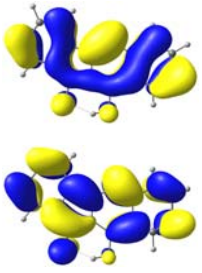
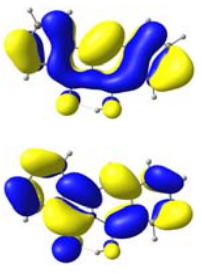
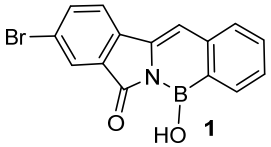
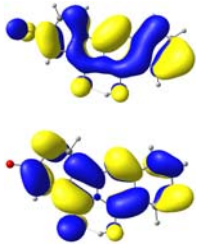
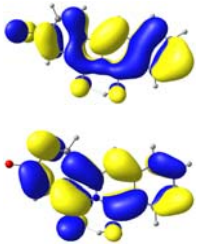
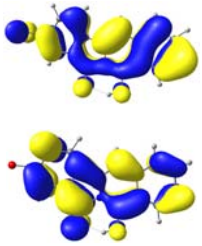
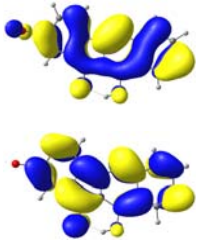
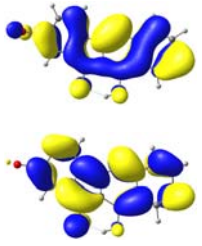
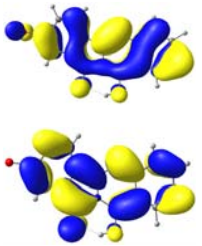
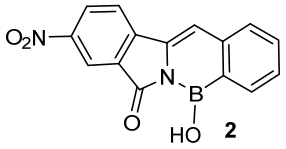
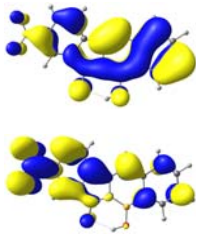
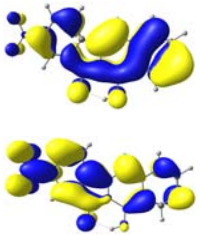
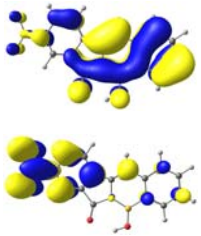
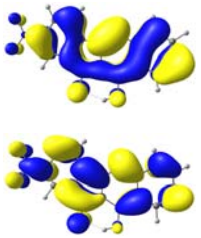
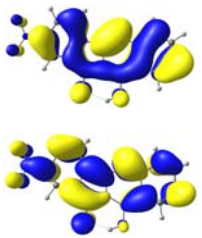
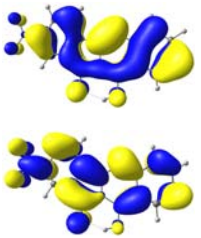
Structure	B3LYP/BS1	PBE0/BS1	B97D/BS1	cam-QTP01/BS1	LC-ωHPBE/BS1	ωB97xD/BS1	EOM-CCSD/BS2// B3LYP/BS1
 **8**							
 **9**							

Table S6: Emission Natural Transition Orbitals for the particle (top) and hole (bottom) of the azaborines from LR-SMD-TD-DFT/BS1 with acetonitrile solvent (isovalue of 0.02).

Structure	B3LYP/BS1	PBE0/BS1	B97D/BS1	cam-QTP01/BS1	LC-ωHPBE/BS1	ωB97xD/BS1
 benzo						
 1						
 2						

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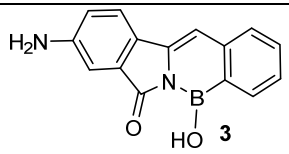
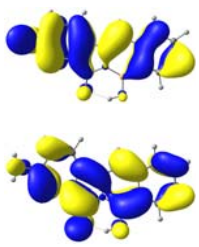
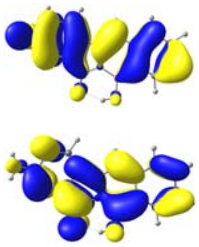
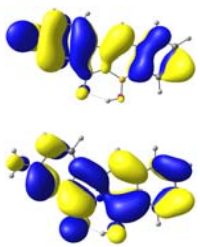
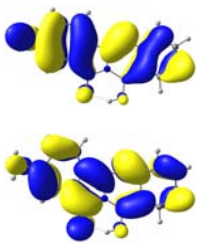
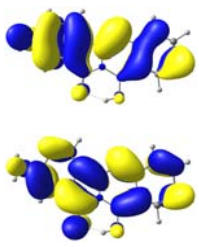
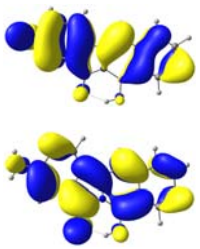
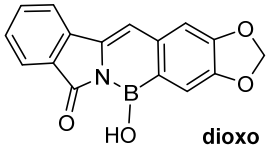
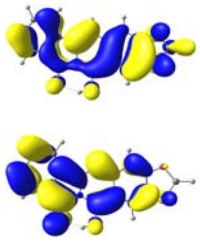
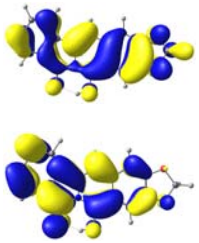
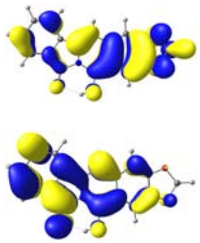
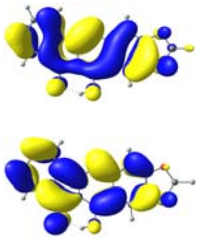
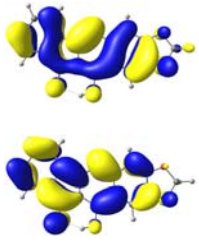
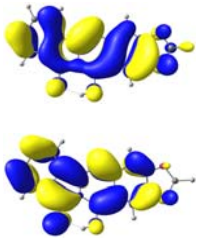
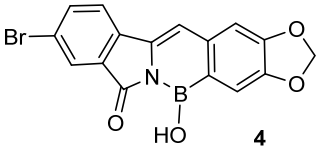
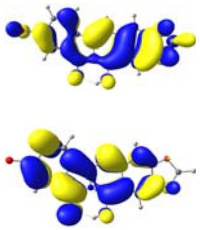
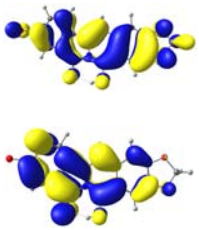
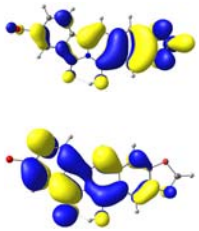
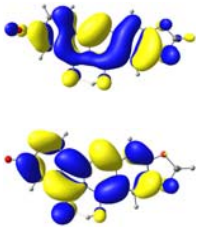
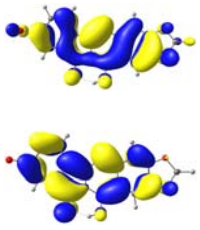
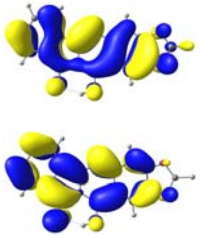
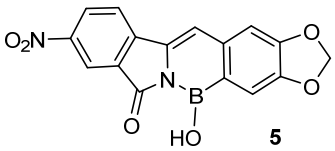
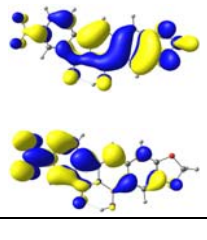
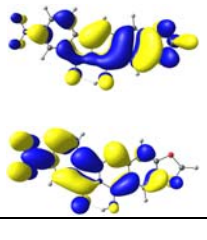
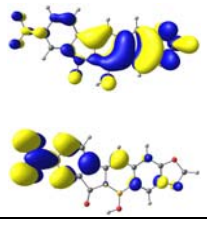
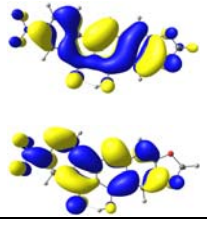
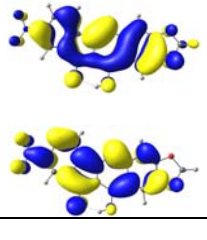
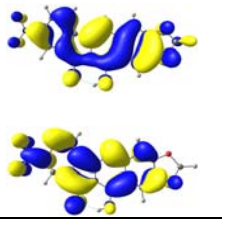
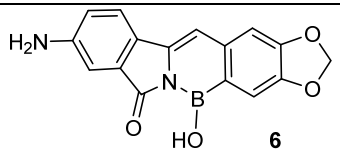
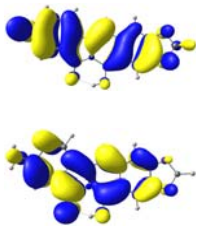
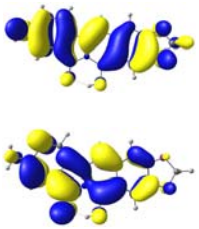
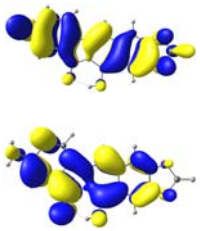
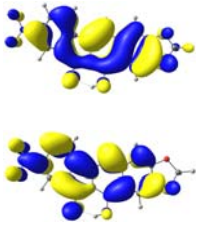
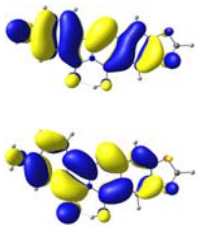
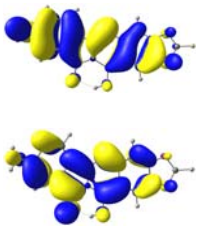
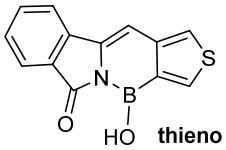
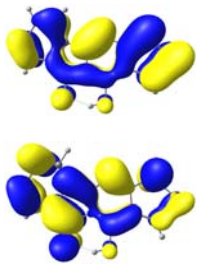
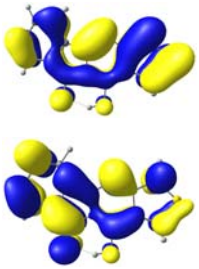
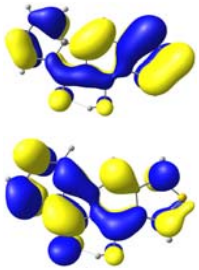
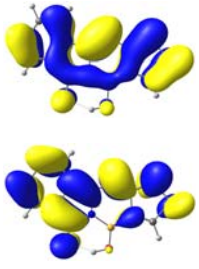
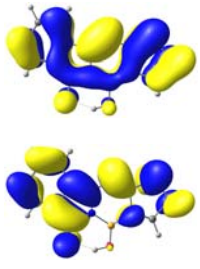
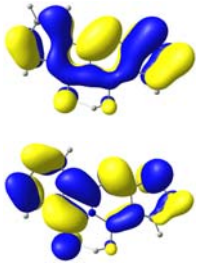
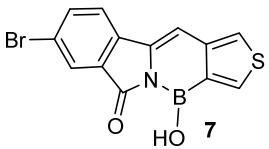
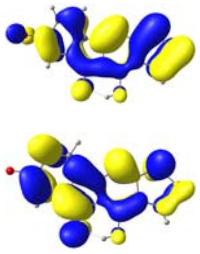
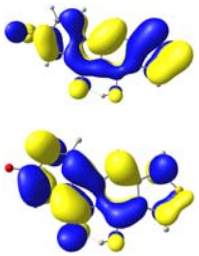
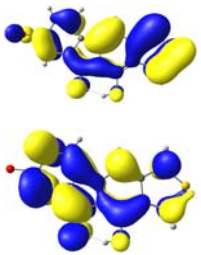
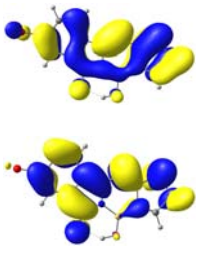
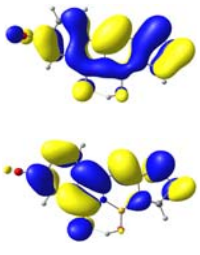
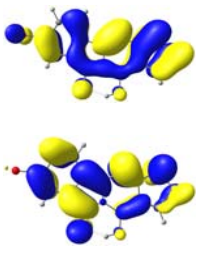
 3						
 dioxo						
 4						
 5						

Structure	B3LYP/BS1	PBE0/BS1	B97D/BS1	cam-QTP01/BS1	LC-ωHPBE/BS1	ωB97xD/BS1
 **6**						
 **thieno**						
 **7**						

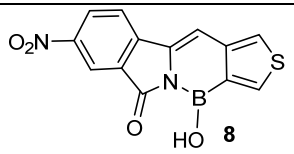
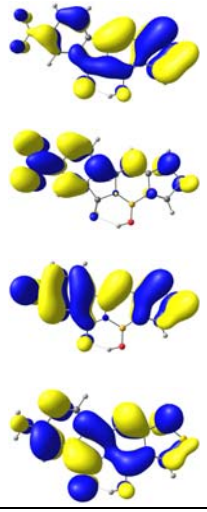
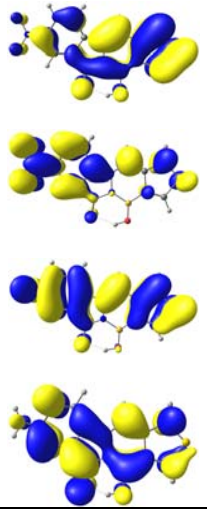
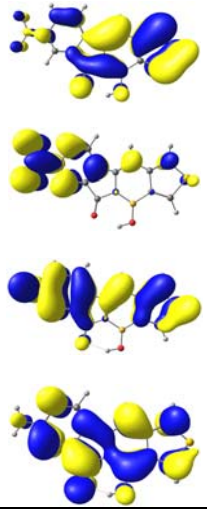
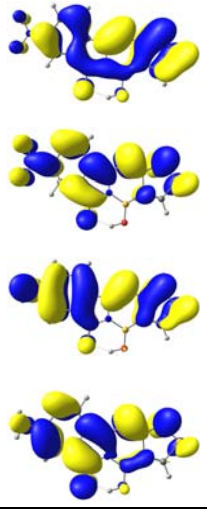
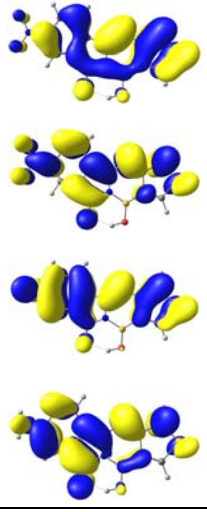
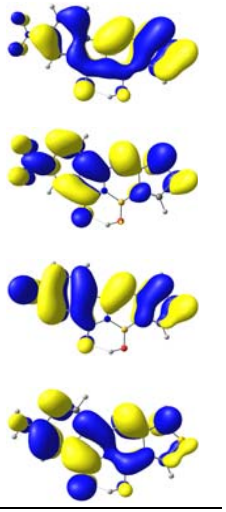
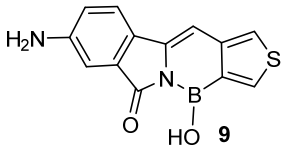
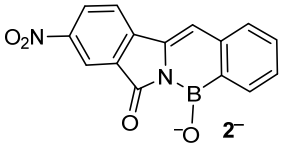
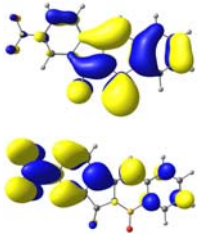
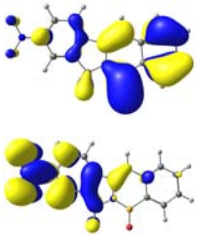
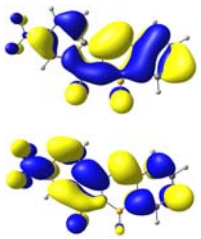
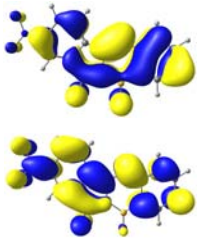
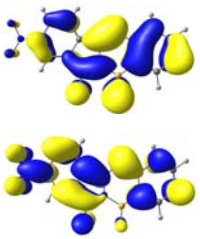
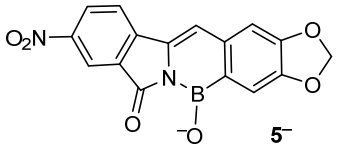
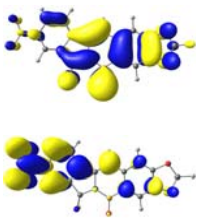
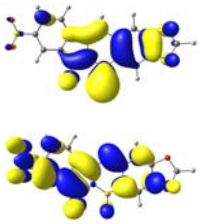
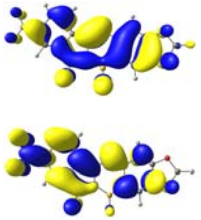
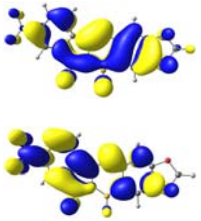
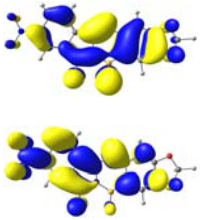
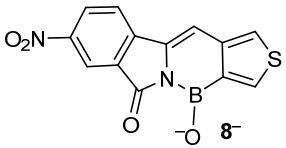
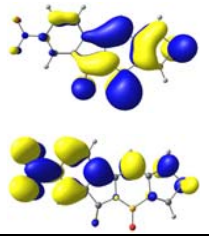
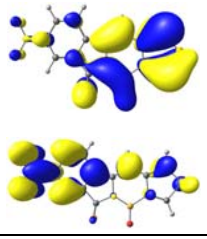
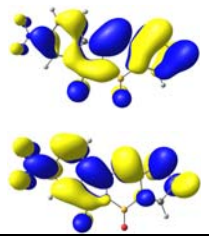
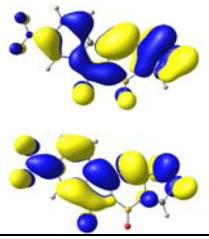
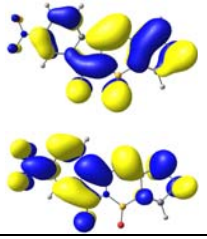
Structure	B3LYP/BS1	PBE0/BS1	B97D/BS1	cam-QTP01/BS1	LC-ωHPBE/BS1	ωB97xD/BS1
 **8**						
 **9**						

Table S7: Emission Natural Transition Orbitals for the particle (top) and hole (bottom) of the anionic nitro-azaborines (**2**$^{-}$, **5**$^{-}$, and **8**$^{-}$) from LR-SMD-TD-DFT/BS1 with acetonitrile solvent (isovalue of 0.02).

Structure	B3LYP/BS1	PBE0/BS1	cam-QTP01/BS1	LC-ωHPBE/BS1	ωB97xD/BS1
 **2**$^{-}$					
 **5**$^{-}$					
 **8**$^{-}$					

pK_a Data

Table S8: Computed GS and ES pK_as and ΔpK_as (ES–GS) from LR-SMD-DFT/BS1 and LR-SMD-TD-DFT/BS1.

	B3LYP/BS3//B3LYP/BS1			B3LYP			ωB97xD			cam-qtp01		
	GS	**ES**	**ΔpK_a**	**GS**	**ES**	**ΔpK_a**	**GS**	**ES**	**ΔpK_a**	**GS**	**ES**	**ΔpK_a**
benzo	38.4	31.8	–6.6	42.6	29.7	–12.8	49.9	39.1	–10.8	42.1	40.9	–1.3
1	38.2	31.0	–7.2	42.0	28.5	–13.5	41.6	38.1	–3.5	41.3	39.7	–1.6
2	36.6	26.1	–10.4	40.4	23.3	–17.1	39.9	37.4	–2.5	40.7	37.0	–3.7
3	39.3	40.0	0.8	43.4	37.7	–5.7	42.3	45.3	3.0	42.8	50.7	7.9
dioxo	39.2	37.6	–1.5	43.2	35.3	–7.9	42.6	42.9	0.3	42.6	41.9	–0.6
4	37.9	36.9	–1.0	42.4	34.2	–8.2	41.7	41.9	0.2	41.3	41.0	–0.3
5	37.5	32.2	–5.4	41.0	29.3	–11.7	41.0	41.6	0.6	40.9	37.6	–3.3
6	39.9	43.6	3.8	44.0	41.5	–2.5	42.1	48.1	6.0	43.0	45.8	2.8
thieno	37.8	32.6	–5.1	41.7	29.6	–12.1	41.7	40.3	–1.4	41.3	40.4	–1.0
7	37.5	31.8	–5.8	41.1	28.3	–12.8	41.2	39.1	–2.1	41.0	39.6	–1.3
8	36.8	27.5	–9.3	40.4	23.9	–16.4	39.9	39.5	–0.3	40.4	37.3	–3.1
9	38.7	39.9	1.2	42.6	36.8	–5.8	41.4	46.0	4.6	42.1	44.7	2.6

cam-QTP(01) with aug-cc-pVTZ vs BS1

We also compared BS1 and aug-cc-PVTZ with the cam-QTP(01) functional. In the seminal publication, cam-QTP(01) was tested and developed with the aug-cc-pVTZ basis set. However, due to the size of compounds studied, TD-DFT optimizations with aug-cc-pVTZ were not desirable. Therefore, cam-QTP(01)/BS1 for all computations. For justification, below is a comparison of the absorption and emission maxima computed by cam-QTP(01)/BS1 and cam-QTP(01)/aug-cc-pVTZ//cam-QTP(01)/BS1 relative to the EOM-CCSD/BS2//B3LYP/BS1 data. Figure S2 shows that the data from the two basis sets with cam-QTP(01) are comparable.

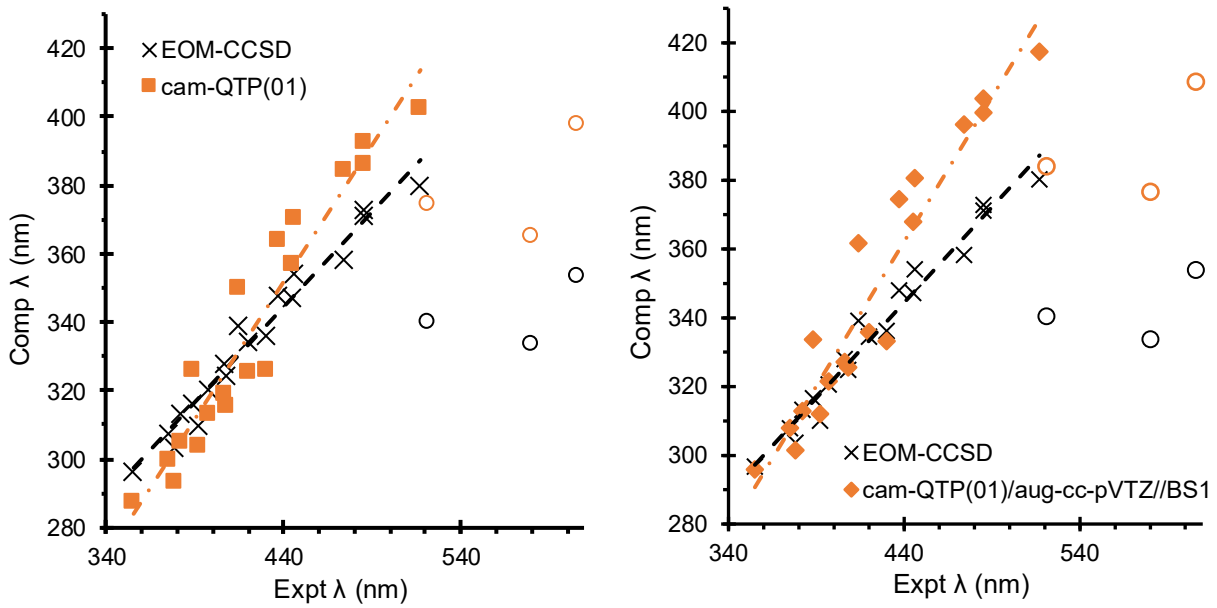


Figure S2: Absorption and emission λ_{max} computed with cam-QTP(01)/BS1 (left) and cam-QTP(01)/aug-ccpVTZ//cam-QTP(01)/BS1 (right). Both have the EOM-CCSD/BS2//B3LYP/BS1 data as a reference.

0-0 Emission Energies from B3LYP/BS1 and cam-QTP(01)/BS1

We did attempt FCHT computations using the S_0 and S_1 frequencies (for these purposes, both Hessians were obtained from G16) to simulate the 0-0 energies for the emission process with B3LYP/BS1 and cam-QTP(01)/BS1 in both the gas-phase and LR-SMD solvation and the results provided below. The data show that the computed 0-0 emission energies show the same trends as the computed λ_{em} from TD-DFT in the gas-phase; i.e. the nitro compounds do not correlate with the remainder of the data with either method.

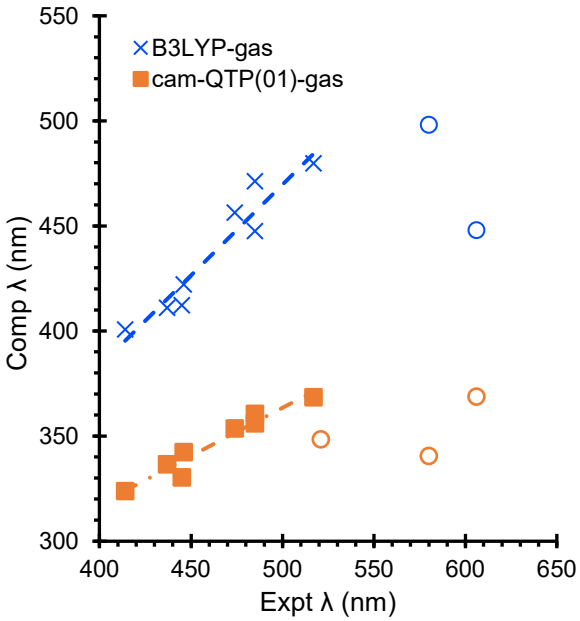


Figure S3: Computed gas-phase 0-0 emission energies from B3LYP/BS1 and cam-QTP(01)/BS1 vs experimental λ_{em}.

Unfortunately, only the cam-QTP(01)/BS1 data are available with a solvation model because multiple compounds, including each of the anions from B3LYP/BS1, failed to complete due to "poor progression" which would result in an "unreliable spectrum." Regardless, the available data from cam-QTP(01)/BS1 with LR-SMD solvation demonstrate similar trends to the λ_{em} from TD-DFT. The protonated nitro compounds are still somewhat off the line even after a solvation model is applied, while the deprotonated nitro compounds is much better aligned with the rest of the dataset.

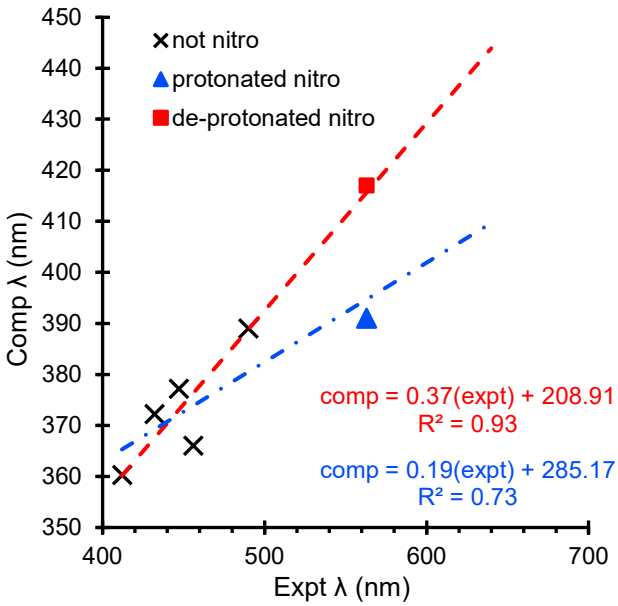


Figure S4: Computed LR-SMD 0-0 emission energies from cam-QTP(01)/BS1 vs experimental λ_{em} in acetonitrile.

Tabulated absorption and emission maxima (in nm)

Table S9: Gas-Phase computations vs experimental data in $CHCl_3$. Unless otherwise noted, each method used the BS1 basis set.

		expt ($CHCl_3$)	B3LYP	PBE0	B97D	cam-QTP(01)	ωB97xD	cam-QTP(01)/aug-cc-pVTZ// cam-QTP01	EOM-CCSD/BS2// B3LYP/BS1
abs	**benzo**	375	373	360	425	300	323	308	308
	1	382	383	370	439	305	329	313	313
	2	388	410	388	508	326	337	334	317
	3	408	404	389	473	316	342	326	325
	dioxo	397	417	399	510	313	341	321	321
	4	406	430	412	531	319	348	327	328
	5	430	463	441	597	326	359	333	336
	6	420	434	416	531	326	355	336	334
	thieno	355	362	349	418	288	310	296	297
	7	378	372	359	431	294	317	301	304
	8	392	413	388	523	304	329	312	310
	9	–	387	373	454	303	328	313	314
emission	**benzo**	437	426	411	425	364	382	374	348
	1	446	437	421	439	371	389	381	354
	2	521	468	429	508	375	392	384	340
	3	485	467	451	473	386	410	400	371
	dioxo	474	472	452	510	385	405	396	358
	4	485	488	467	531	393	414	404	373
	5	606	503	471	597	398	418	409	354
	6	517	499	482	531	403	429	417	380
	thieno	414	420	402	418	350	367	362	339
	7	445	432	413	431	357	375	368	347
	8	580	483	440	523	365	382	377	334
	9	–	441	428	454	366	389	380	356

Table S10: Linear response (LR) solvation computations vs experimental data in $CHCl_3$. Unless otherwise noted, each method used the BS1 basis set.

		expt ($CHCl_3$)	B3LYP	ωB97xD
abs	**benzo**	375	385	334
	1	382	394	339
	2	388	435	350
	3	408	428	359
	dioxo	397	428	350
	4	406	444	358
	5	430	496	372
	6	420	453	370
	thieno	355	371	319
	7	378	381	326
	8	392	441	343
	9	–	405	343
emission	**benzo**	437	460	421
	1	446	469	428
	2	521	516	440
	3	485	527	463
	dioxo	474	505	448
	4	485	519	457
	5	606	569	472
	6	517	557	483
	thieno	414	442	406
	7	445	452	413
	8	580	531	432
	9	–	491	436

Table S11: Non-linear response (LR) solvation computations vs experimental data in $CHCl_3$. Unless otherwise noted, each method used the BS1 basis set.

		expt ($CHCl_3$)	B3LYP	ωB97xD
abs	**benzo**	375	385	334
	1	382	394	339
	2	388	435	350
	3	408	428	359
	dioxo	397	428	350
	4	406	444	358
	5	430	496	372
	6	420	453	370
	thieno	355	371	319
	7	378	381	326
	8	392	441	343
	9	–	405	343
emission	**benzo**	437	438	396
	1	446	449	403
	2	521	563	412
	3	485	531	451
	dioxo	474	523	431
	4	485	545	441
	5	606	625	451
	6	517	548	467
	thieno	414	427	381
	7	445	440	390
	8	580	593	410
	9	–	489	423

Table S12: ΔSCF solvation computations vs experimental data in $CHCl_3$. Unless otherwise noted, each method used the BS1 basis set.

		expt ($CHCl_3$)	B3LYP	ωB97xD
abs	**benzo**	375	385	334
	1	382	394	339
	2	388	435	350
	3	408	428	359
	dioxo	397	428	350
	4	406	444	358
	5	430	496	372
	6	420	453	370
	thieno	355	371	319
	7	378	381	326
	8	392	441	343
	9	–	405	343
emission	**benzo**	437	446	402
	1	446	457	409
	2	521	664	423
	3	485	607	490
	dioxo	474	571	446
	4	485	600	458
	5	606	751	471
	6	517	592	497
	thieno	414	436	387
	7	445	451	396
	8	580	713	429
	9	–	544	454

Table S13: Gas-Phase computations vs experimental data in MeCN. Unless otherwise noted, each method used the BS1 basis set.

		expt (MeCN)	B3LYP	ωB97xD	EOM-CCSD/BS2// B3LYP/BS1
abs	**benzo**	371	373	323	308
	1	378	383	329	313
	2	382	410	337	317
	3	410	404	342	325
	dioxo	392	417	341	321
	4	398	430	348	328
	5	422	463	359	336
	6	424	434	355	334
	thieno	350	362	310	297
	7	372	372	317	304
	8	388	413	329	310
	9	–	387	328	314
emission	**benzo**	432	426	382	348
	1	447	437	389	354
	2	563	468	392	340
	3	526	467	410	371
	dioxo	490	472	405	358
	4	504	488	414	373
	5	640	503	418	354
	6	528	499	429	380
	thieno	412	420	367	339
	7	456	432	375	347
	8	–	483	382	334
	9	–	441	389	356

Table S14: Linear response solvation computations vs experimental data in MeCN. Unless otherwise noted, each method used the BS1 basis set.

		expt (MeCN)	B3LYP	PBE0	B97D	cam-QTP(01)	LC-ωHPBE	cam-QTP(01)/aug-cc-pVTZ// cam-QTP01
abs	**benzo**	371	383	368	433	309	303	318
	1	378	392	377	446	313	307	322
	2	382	435	404	553	321	314	330
	3	410	432	412	512	330	324	342
	dioxo	392	427	407	526	321	315	330
	4	398	442	420	550	326	321	335
	5	422	496	463	672	336	329	345
	6	424	455	433	554	339	332	351
	thieno	350	369	356	423	294	290	304
	7	372	379	365	436	300	296	309
	8	388	442	409	575	313	306	323
	9	–	408	390	480	316	311	327
emission	**benzo**	432	477	465	455	420	415	402
	1	447	485	473	468	426	421	408
	2	563	535	507	576	443	437	419
	3	526	557	539	532	461	454	447
	dioxo	490	521	505	542	445	442	429
	4	504	535	517	566	454	451	438
	5	640	592	557	703	477	474	453
	6	528	587	567	574	476	469	463
	thieno	412	457	446	441	409	406	389
	7	456	466	455	454	416	414	396
	8	–	549	517	596	439	435	416
	9	–	515	500	497	434	429	420

Table S15: Non-linear response solvation computations vs experimental data in MeCN. Unless otherwise noted, each method used the BS1 basis set.

		expt (MeCN)	B3LYP	ωB97xD
abs	**benzo**	371	383.34	331
	1	378	392	337
	2	382	435	346
	3	410	432	358
	dioxo	392	427	348
	4	398	442	355
	5	422	496	367
	6	424	455	369
	thieno	350	369	317
	7	372	379	324
	8	388	442	339
	9	–	408	342
emission	**benzo**	432	443	401
	1	447	454	409
	2	563	576	420
	3	526	571	475
	dioxo	490	543	441
	4	504	566	452
	5	640	643	462
	6	528	575	485
	thieno	412	431	387
	7	456	444	396
	8	–	610	422
	9	–	521	441

Table S16: ΔSCF solvation computations vs experimental data in MeCN. Unless otherwise noted, each method used the BS1 basis set.

		expt (MeCN)	B3LYP	ωB97xD
abs	**benzo**	371	383	331
	1	378	392	337
	2	382	435	346
	3	410	432	358
	dioxo	392	427	348
	4	398	442	355
	5	422	496	367
	6	424	455	369
	thieno	350	369	317
	7	372	379	324
	8	388	442	339
	9	–	408	342
emission	**benzo**	432	456	411
	1	447	466	418
	2	563	709	437
	3	526	733	556
	dioxo	490	628	466
	4	504	664	479
	5	640	809	493
	6	528	668	544
	thieno	412	445	397
	7	456	460	406
	8	–	767	455
	9	–	641	501

Tabulated absorption and emission maxima (in eV)

Table S17: Gas-Phase computations vs experimental data in $CHCl_3$. Unless otherwise noted, each method used the BS1 basis set.

		expt ($CHCl_3$)	B3LYP	PBE0	B97D	cam-QTP(01)	ωB97xD	cam-QTP(01)/aug-cc-pVTZ// cam-QTP01	EOM-CCSD/BS2// B3LYP/BS1
abs	**benzo**	3.31	3.32	3.84	4.13	4.03	4.11	4.03	3.31
	1	3.25	3.24	3.77	4.06	3.96	4.02	3.96	3.25
	2	3.20	3.03	3.68	3.80	3.72	3.89	3.92	3.20
	3	3.04	3.07	3.62	3.93	3.81	3.88	3.82	3.04
	dioxo	3.12	2.98	3.64	3.96	3.86	4.17	3.87	3.12
	4	3.05	2.88	3.56	3.88	3.79	3.80	3.78	3.05
	5	2.88	2.68	3.46	3.80	3.72	3.63	3.69	2.88
	6	2.95	2.85	3.49	3.81	3.69	3.73	3.71	2.95
	thieno	3.49	3.43	4.00	4.31	4.19	4.30	4.18	3.49
	7	3.28	3.33	3.91	4.22	4.11	4.17	4.08	3.28
	8	3.16	3.00	3.76	4.08	3.97	3.94	4.00	3.16
	9	–	3.20	3.78	4.10	3.96	4.07	3.94	–
emission	**benzo**	2.84	2.91	3.25	3.40	3.31	3.69	3.56	2.84
	1	2.78	2.84	3.19	3.34	3.26	3.62	3.50	2.78
	2	2.38	2.65	3.16	3.31	3.23	3.54	3.64	2.38
	3	2.56	2.66	3.02	3.21	3.10	3.47	3.34	2.56
	dioxo	2.62	2.63	3.06	3.22	3.13	3.47	3.46	2.62
	4	2.56	2.54	3.00	3.16	3.07	3.38	3.33	2.56
	5	2.05	2.47	2.97	3.11	3.03	3.27	3.50	2.05
	6	2.40	2.48	2.89	3.08	2.97	3.30	3.26	2.40
	thieno	3.00	2.95	3.38	3.54	3.43	3.86	3.66	3.00
	7	2.79	2.87	3.31	3.47	3.37	3.77	3.57	2.79
	8	2.14	2.57	3.25	3.39	3.29	3.58	3.72	2.14
	9	–	2.81	3.19	3.39	3.26	3.69	3.48	–

Table S18: Linear response (LR) solvation computations vs experimental data in $CHCl_3$. Unless otherwise noted, each method used the BS1 basis set.

		expt ($CHCl_3$)	B3LYP	ωB97xD
abs	**benzo**	3.31	3.22	3.72
	1	3.25	3.15	3.66
	2	3.20	2.85	3.55
	3	3.04	2.90	3.46
	dioxo	3.12	2.90	3.54
	4	3.05	2.80	3.46
	5	2.88	2.50	3.34
	6	2.95	2.74	3.35
	thieno	3.49	3.34	3.88
	7	3.28	3.25	3.80
	8	3.16	2.81	3.62
	9	–	3.06	3.62
emission	**benzo**	2.84	2.70	2.94
	1	2.78	2.65	2.90
	2	2.38	2.40	2.82
	3	2.56	2.35	2.68
	dioxo	2.62	2.46	2.77
	4	2.56	2.39	2.72
	5	2.05	2.18	2.63
	6	2.40	2.22	2.57
	thieno	3.00	2.81	3.05
	7	2.79	2.74	3.00
	8	2.14	2.33	2.87
	9	–	2.53	2.84

Table S19: Non-linear response (LR) solvation computations vs experimental data in $CHCl_3$. Unless otherwise noted, each method used the BS1 basis set.

		expt ($CHCl_3$)	B3LYP	ωB97xD
abs	**benzo**	3.31	3.22	3.72
	1	3.25	3.15	3.66
	2	3.20	2.85	3.55
	3	3.04	2.90	3.46
	dioxo	3.12	2.90	3.54
	4	3.05	2.80	3.46
	5	2.88	2.50	3.34
	6	2.95	2.74	3.35
	thieno	3.49	3.34	3.88
	7	3.28	3.25	3.80
	8	3.16	2.81	3.62
	9	–	3.06	3.62
emission	**benzo**	2.84	2.83	3.13
	1	2.78	2.76	3.08
	2	2.38	2.20	3.01
	3	2.56	2.33	2.75
	dioxo	2.62	2.37	2.88
	4	2.56	2.28	2.81
	5	2.05	1.98	2.75
	6	2.40	2.26	2.66
	thieno	3.00	2.90	3.25
	7	2.79	2.82	3.18
	8	2.14	2.09	3.02
	9	–	2.54	2.93

Table S20: ΔSCF solvation computations vs experimental data in $CHCl_3$. Unless otherwise noted, each method used the BS1 basis set.

		expt ($CHCl_3$)	B3LYP	ωB97xD
abs	**benzo**	3.31	3.22	3.72
	1	3.25	3.15	3.66
	2	3.20	2.85	3.55
	3	3.04	2.90	3.46
	dioxo	3.12	2.90	3.54
	4	3.05	2.80	3.46
	5	2.88	2.50	3.34
	6	2.95	2.74	3.35
	thieno	3.49	3.34	3.88
	7	3.28	3.25	3.80
	8	3.16	2.81	3.62
	9	–	3.06	3.62
emission	**benzo**	2.84	2.78	3.09
	1	2.78	2.71	3.03
	2	2.38	1.87	2.93
	3	2.56	2.04	2.53
	dioxo	2.62	2.17	2.78
	4	2.56	2.07	2.71
	5	2.05	1.65	2.63
	6	2.40	2.09	2.49
	thieno	3.00	2.84	3.20
	7	2.79	2.75	3.13
	8	2.14	1.74	2.89
	9	–	2.28	2.73

Table S21: Gas-Phase computations vs experimental data in MeCN. Unless otherwise noted, each method used the BS1 basis set.

		expt (MeCN)	B3LYP	ωB97xD	EOM-CCSD/BS2// B3LYP/BS1
abs	**benzo**	3.34	3.32	3.84	4.03
	1	3.28	3.24	3.77	3.96
	2	3.25	3.03	3.68	3.92
	3	3.02	3.07	3.62	3.82
	dioxo	3.16	2.98	3.64	3.87
	4	3.12	2.88	3.56	3.78
	5	2.94	2.68	3.46	3.69
	6	2.92	2.85	3.49	3.71
	thieno	3.54	3.43	4.00	4.18
	7	3.33	3.33	3.91	4.08
	8	3.20	3.00	3.76	4.00
	9	–	387	328	3.94
emission	**benzo**	2.87	2.91	3.25	3.56
	1	2.77	2.84	3.19	3.50
	2	2.20	2.65	3.16	3.64
	3	2.36	2.66	3.02	3.34
	dioxo	2.53	2.63	3.06	3.46
	4	2.46	2.54	3.00	3.33
	5	1.94	2.47	2.97	3.50
	6	2.35	2.48	2.89	3.26
	thieno	3.01	2.95	3.38	3.66
	7	2.72	2.87	3.31	3.57
	8	–	2.57	3.25	3.72
	9	–	2.81	3.19	3.48

Table S22: Linear response solvation computations vs experimental data in MeCN. Unless otherwise noted, each method used the BS1 basis set.

		expt (MeCN)	B3LYP	PBE0	B97D	cam-QTP(01)	LC-ωHPBE	cam-QTP(01)/aug-cc-pVTZ// cam-QTP01
abs	**benzo**	3.34	3.24	3.37	2.86	4.01	4.09	3.90
	1	3.28	3.16	3.29	2.78	3.96	4.04	3.85
	2	3.25	2.85	3.07	2.24	3.86	3.95	3.76
	3	3.02	2.87	3.01	2.42	3.76	3.83	3.63
	dioxo	3.16	2.90	3.05	2.36	3.86	3.94	3.76
	4	3.12	2.81	2.95	2.25	3.80	3.86	3.70
	5	2.94	2.50	2.68	1.85	3.69	3.77	3.59
	6	2.92	2.73	2.86	2.24	3.66	3.73	3.53
	thieno	3.54	3.36	3.48	2.93	4.22	4.28	4.08
	7	3.33	3.27	3.40	2.84	4.13	4.19	4.01
	8	3.20	2.81	3.03	2.16	3.96	4.05	3.84
	9	–	3.04	3.18	2.58	3.92	3.99	3.79
emission	**benzo**	2.87	2.60	2.67	2.73	2.95	2.99	3.08
	1	2.77	2.56	2.62	2.65	2.91	2.95	3.04
	2	2.20	2.32	2.45	2.15	2.80	2.84	2.96
	3	2.36	2.23	2.30	2.33	2.69	2.73	2.77
	dioxo	2.53	2.38	2.46	2.29	2.79	2.81	2.89
	4	2.46	2.32	2.40	2.19	2.73	2.75	2.83
	5	1.94	2.09	2.23	1.76	2.60	2.62	2.74
	6	2.35	2.11	2.19	2.16	2.61	2.64	2.68
	thieno	3.01	2.71	2.78	2.81	3.03	3.05	3.19
	7	2.72	2.66	2.73	2.73	2.98	3.00	3.13
	8	–	2.26	2.40	2.08	2.82	2.85	2.98
	9	–	2.41	2.48	2.49	2.86	2.89	2.95

Table S23: Non-linear response solvation computations vs experimental data in MeCN. Unless otherwise noted, each method used the BS1 basis set.

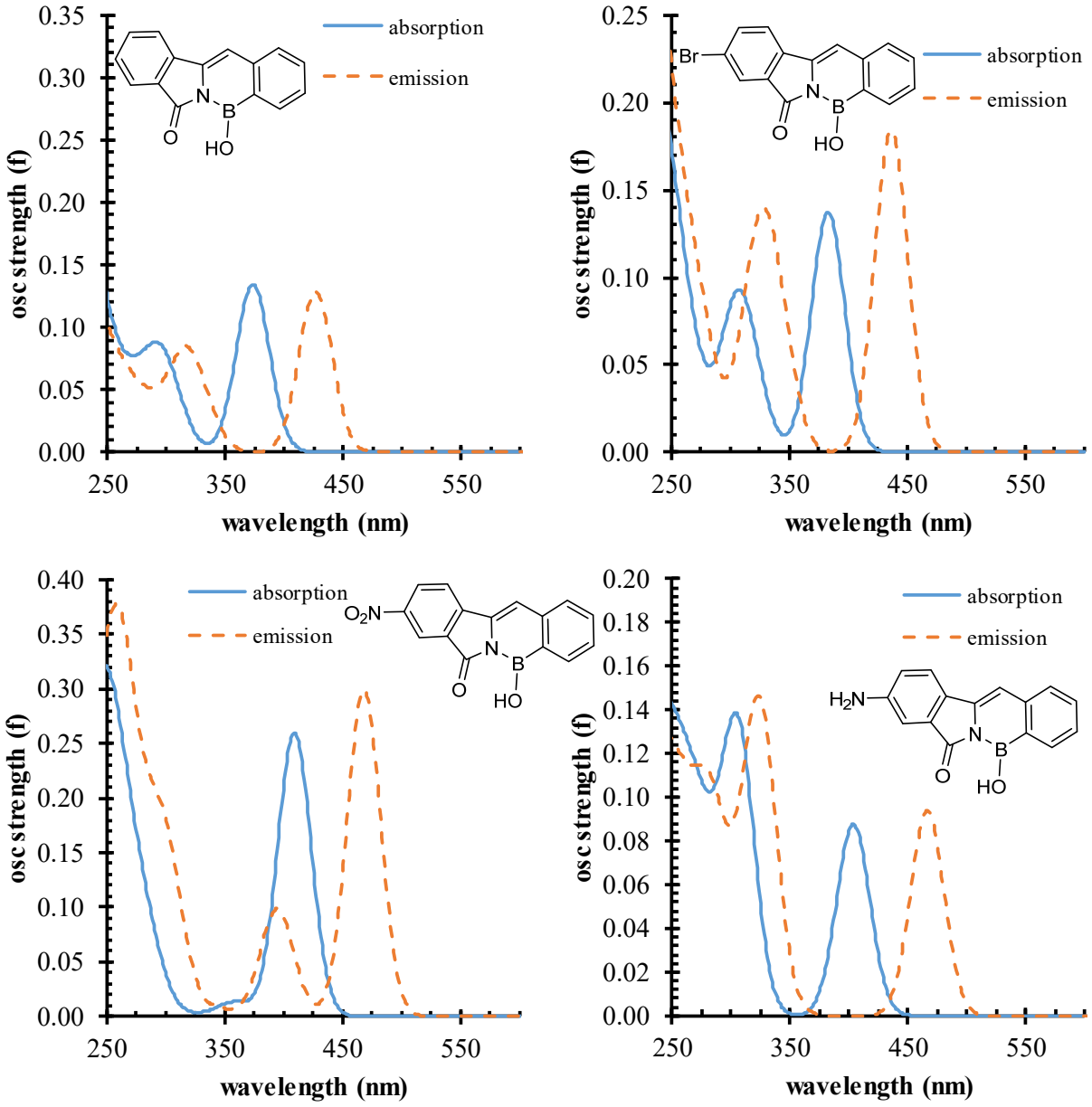
		expt (MeCN)	B3LYP	ωB97xD
abs	**benzo**	3.31	3.22	3.72
	1	3.25	3.15	3.66
	2	3.20	2.85	3.55
	3	3.04	2.90	3.46
	dioxo	3.12	2.90	3.54
	4	3.05	2.80	3.46
	5	2.88	2.50	3.34
	6	2.95	2.74	3.35
	thieno	3.49	3.34	3.88
	7	3.28	3.25	3.80
	8	3.16	2.81	3.62
	9	–	3.06	3.62
emission	**benzo**	2.84	2.83	3.13
	1	2.78	2.76	3.08
	2	2.38	2.20	3.01
	3	2.56	2.33	2.75
	dioxo	2.62	2.37	2.88
	4	2.56	2.28	2.81
	5	2.05	1.98	2.75
	6	2.40	2.26	2.66
	thieno	3.00	2.90	3.25
	7	2.79	2.82	3.18
	8	2.14	2.09	3.02
	9	–	2.54	2.93

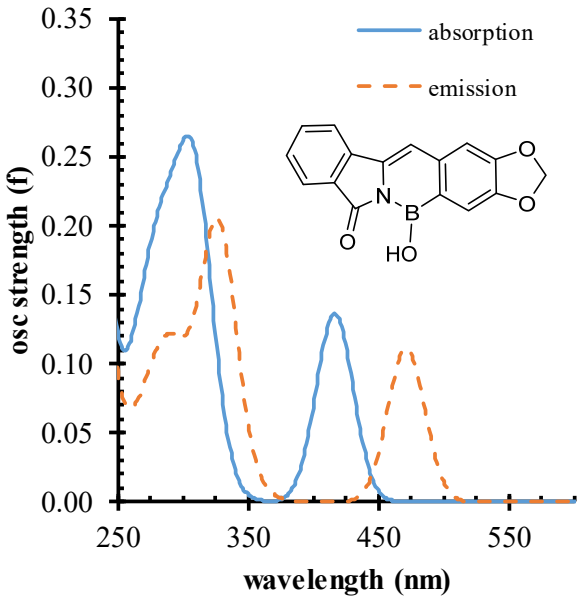
Table S24: ΔSCF solvation computations vs experimental data in MeCN. Unless otherwise noted, each method used the BS1 basis set.

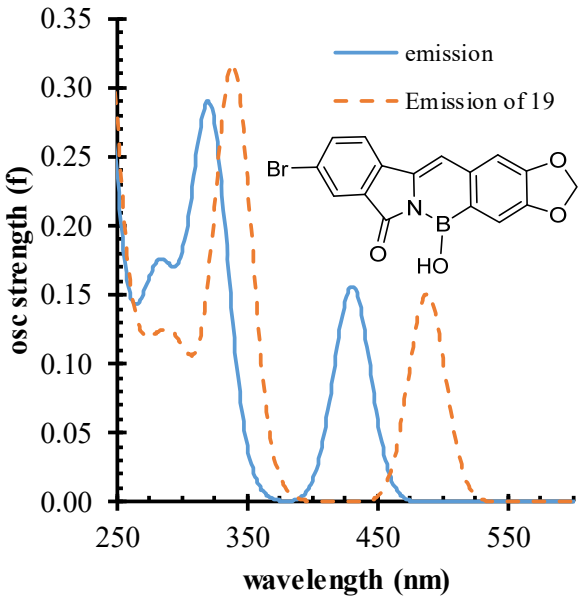
		expt (MeCN)	B3LYP	ωB97xD
abs	**benzo**	3.31	3.22	3.72
	1	3.25	3.15	3.66
	2	3.20	2.85	3.55
	3	3.04	2.90	3.46
	dioxo	3.12	2.90	3.54
	4	3.05	2.80	3.46
	5	2.88	2.50	3.34
	6	2.95	2.74	3.35
	thieno	3.49	3.34	3.88
	7	3.28	3.25	3.80
	8	3.16	2.81	3.62
	9	–	3.06	3.62
emission	**benzo**	2.84	2.78	3.09
	1	2.78	2.71	3.03
	2	2.38	1.87	2.93
	3	2.56	2.04	2.53
	dioxo	2.62	2.17	2.78
	4	2.56	2.07	2.71
	5	2.05	1.65	2.63
	6	2.40	2.09	2.49
	thieno	3.00	2.84	3.20
	7	2.79	2.75	3.13
	8	2.14	1.74	2.89
	9	–	2.28	2.73

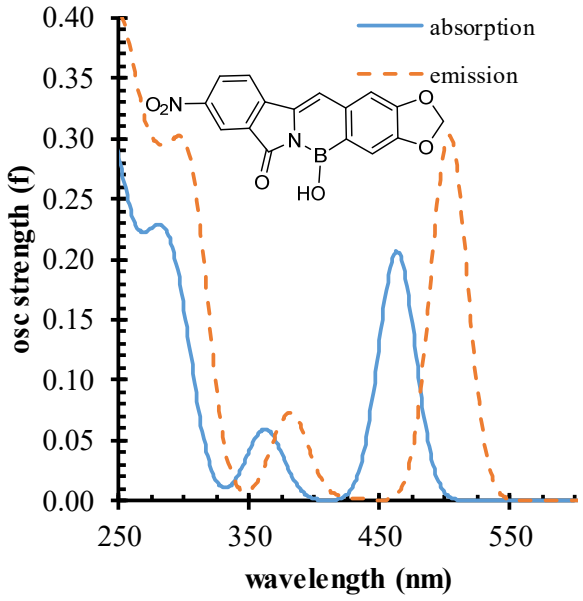
Simulated Spectra

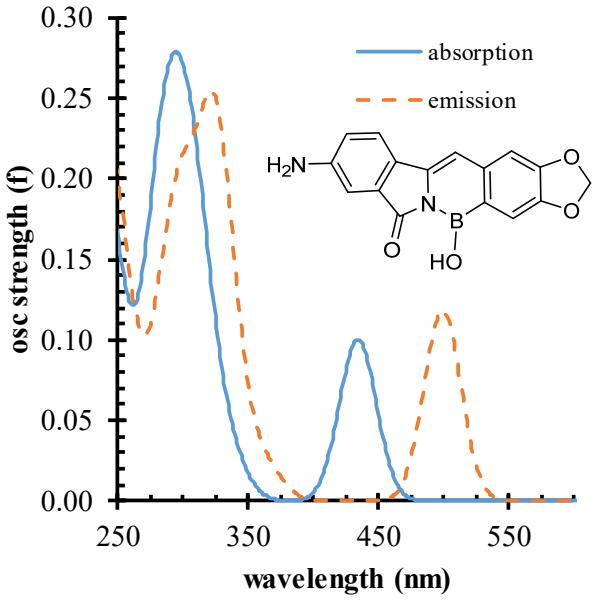
Simulated spectra from TD-B3LYP/BS1//B3LYP/BS1

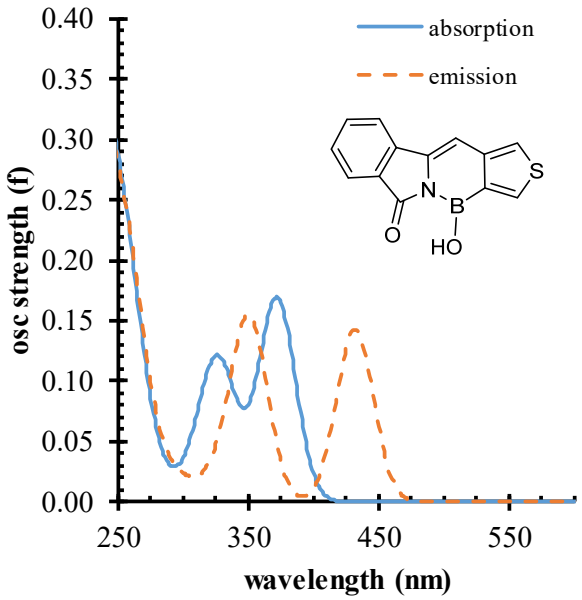


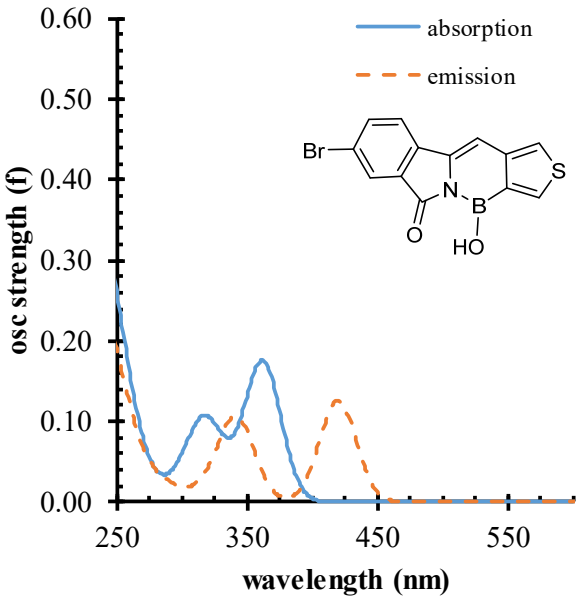

absorption
emission
osc strength (f)
wavelength (nm)
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
250
350
450
550
O
N
B
HO
O
O

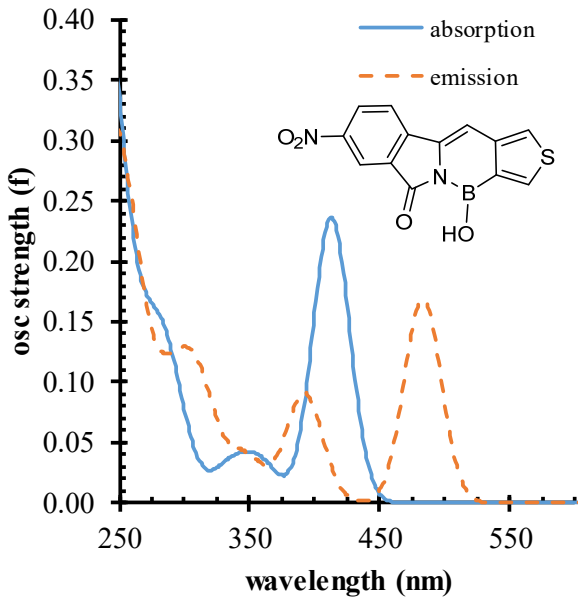

emission
Emission of 19
osc strength (f)
wavelength (nm)
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
250
350
450
550
Br
O
N
B
HO
O
O

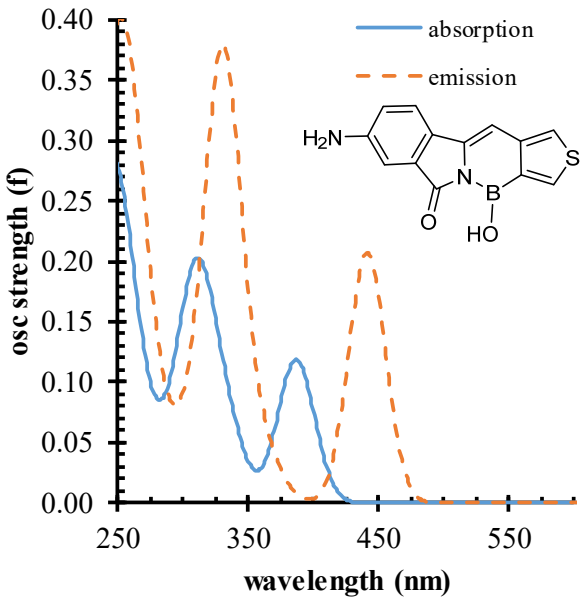

absorption
emission
osc strength (f)
wavelength (nm)
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
250
350
450
550
O2N
O
N
B
HO
O
O


absorption
emission
osc strength (f)
wavelength (nm)
0.30
0.25
0.20
0.15
0.10
0.05
0.00
250
350
450
550
H2N
O
N
B
HO
O
O


absorption
emission
osc strength (f)
wavelength (nm)
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
250
350
450
550
N
B
S
O
HO


absorption
emission
osc strength (f)
wavelength (nm)
0.60
0.50
0.40
0.30
0.20
0.10
0.00
250
350
450
550
Br
N
B
S
O
HO

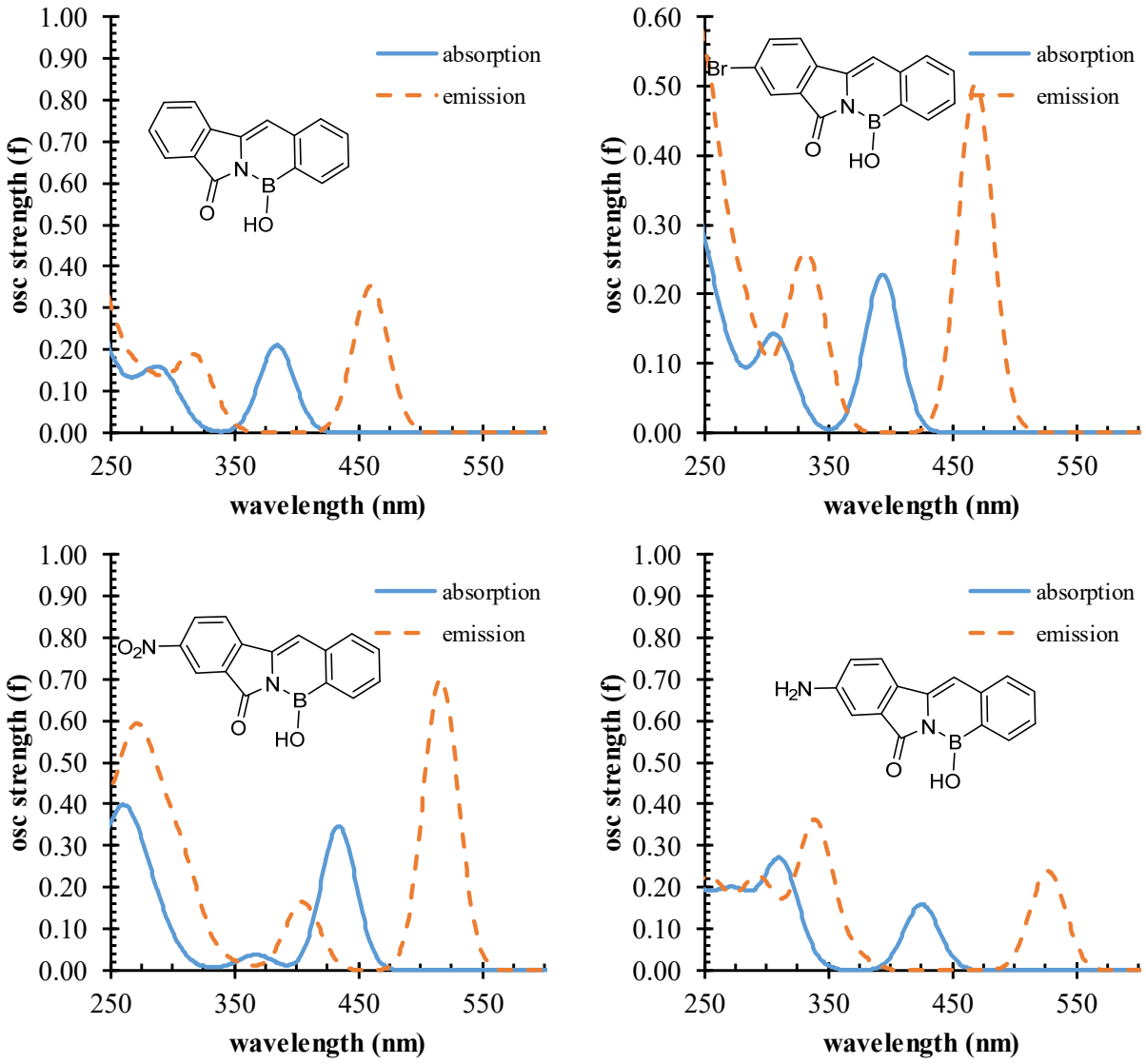

absorption
emission
osc strength (f)
wavelength (nm)
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
250
350
450
550
O2N
N
B
S
O
HO

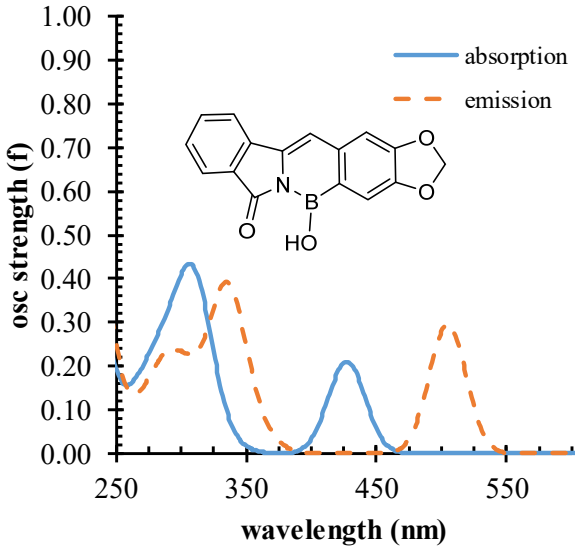

absorption
emission
osc strength (f)
wavelength (nm)
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
250
350
450
550
H2N
N
B
S
O
HO

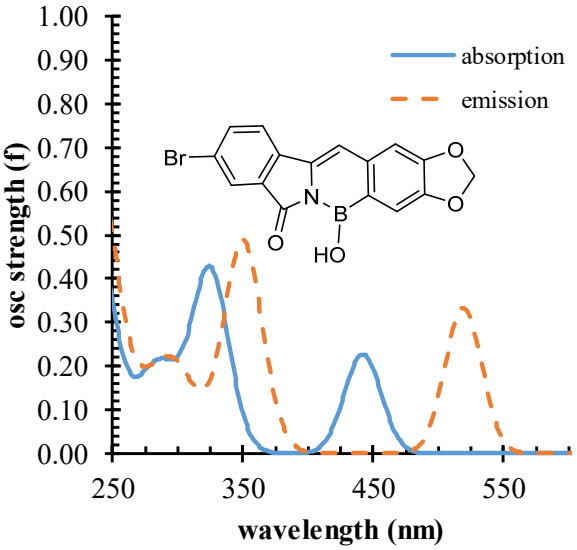
Simulated spectra for chloroform solvent

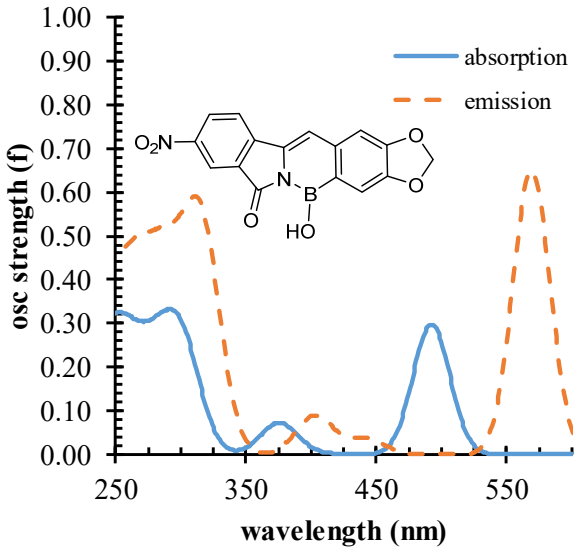
Absorption spectra obtained from LR-SMD-TD-B3LYP/BS1//B3LYP/BS1

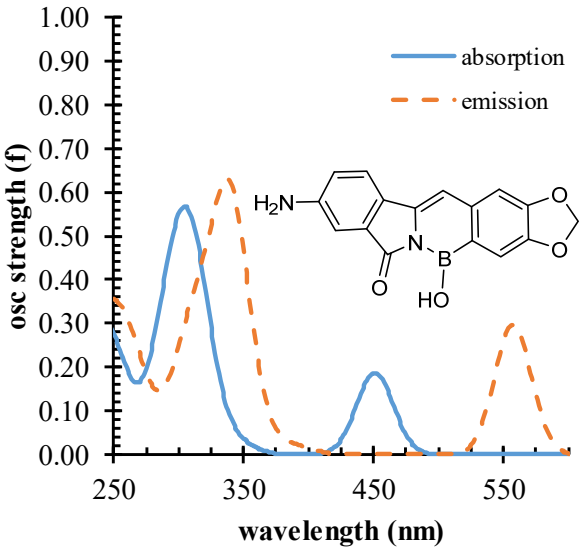
Emission spectra obtained from LR-SMD-TD-B3LYP/BS1

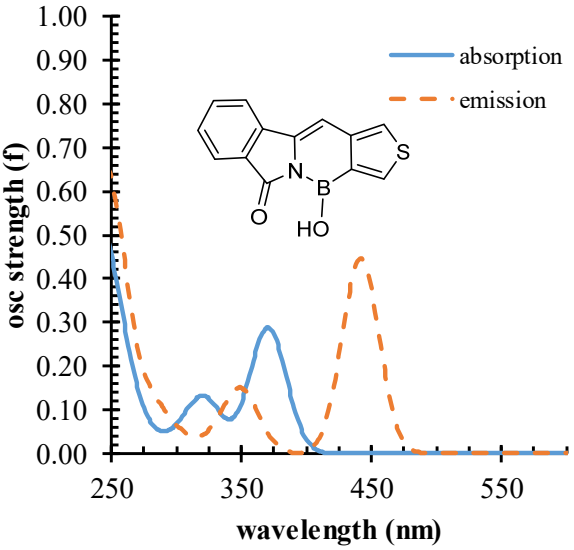


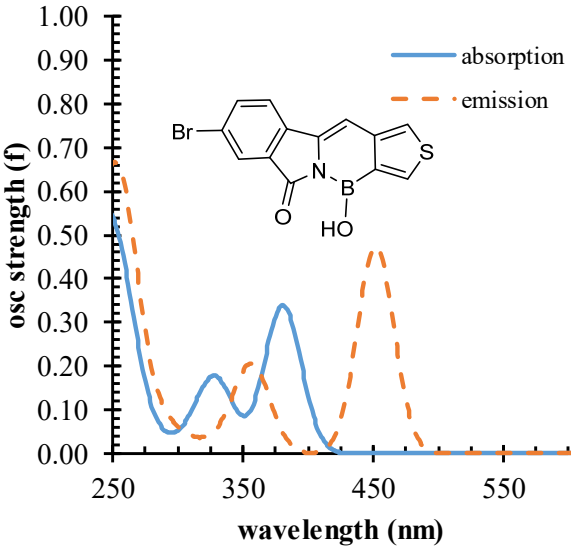

1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
osc strength (f)
absorption
emission
250
350
450
550
wavelength (nm)
O
N
B
HO
O
O

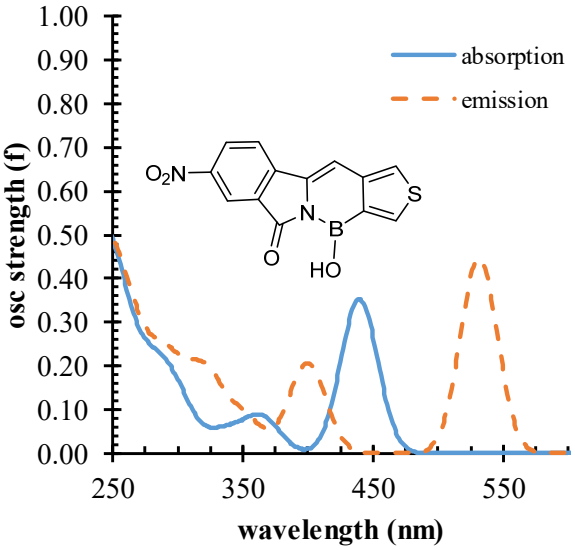

1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
osc strength (f)
absorption
emission
250
350
450
550
wavelength (nm)
Br
O
N
B
HO
O
O

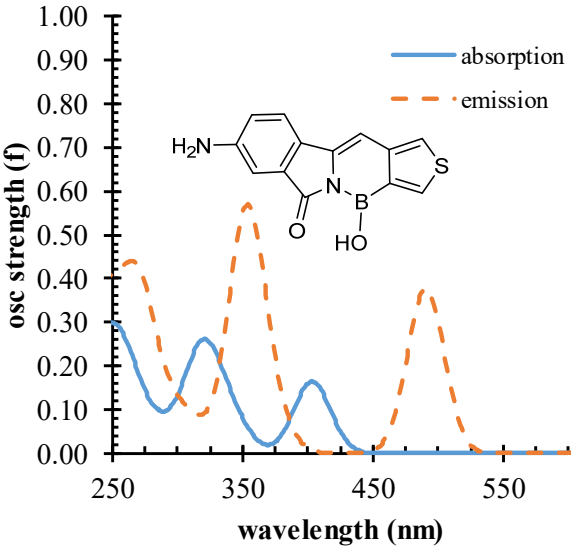

1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
osc strength (f)
absorption
emission
250
350
450
550
wavelength (nm)
O2N
O
N
B
HO
O
O


1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
osc strength (f)
absorption
emission
250
350
450
550
wavelength (nm)
H2N
O
N
B
HO
O
O


1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
osc strength (f)
absorption
emission
250
350
450
550
wavelength (nm)
N
B
S
O
HO


1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
osc strength (f)
absorption
emission
250
350
450
550
wavelength (nm)
Br
N
B
S
O
HO

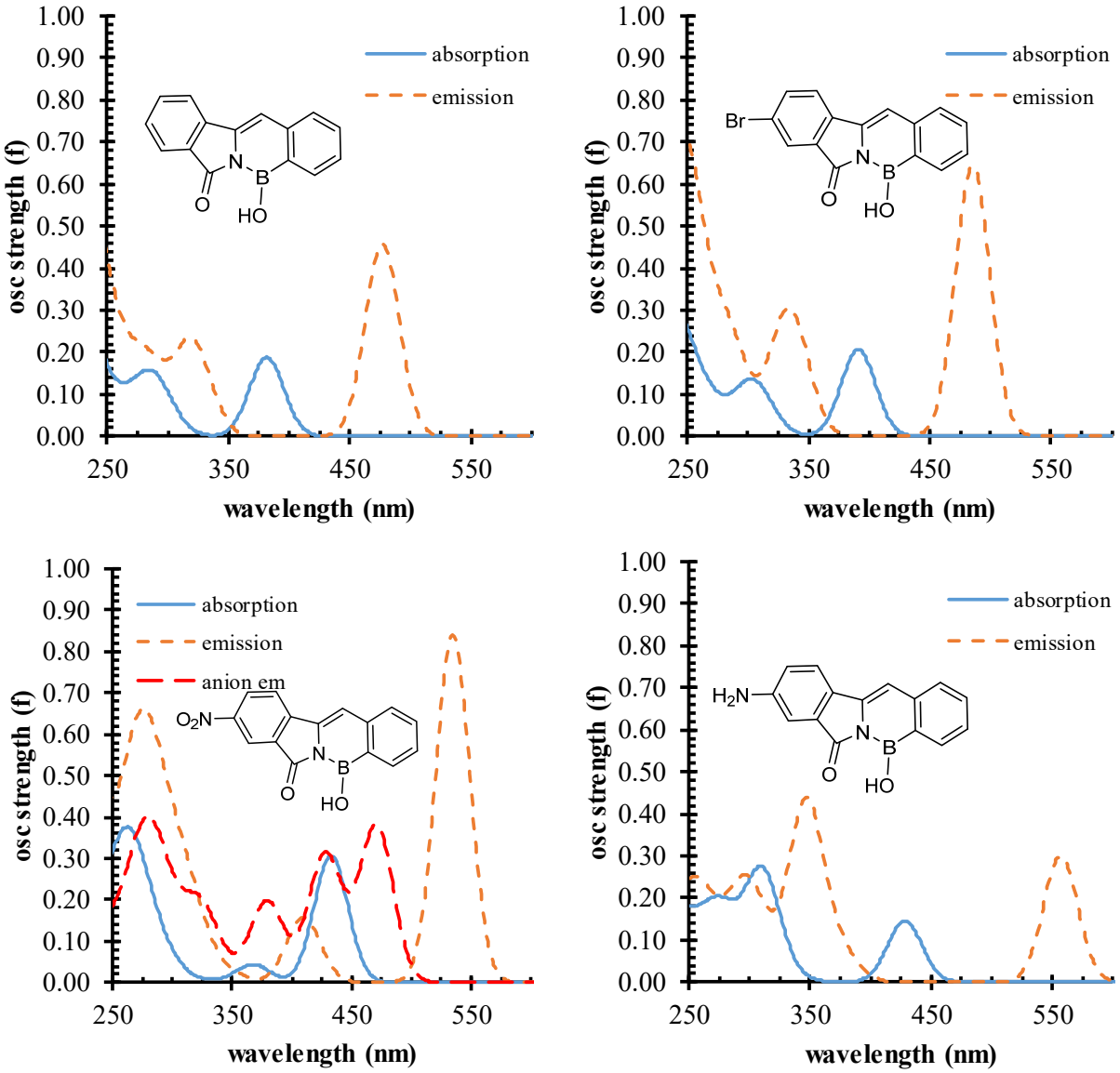

1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
osc strength (f)
absorption
emission
250
350
450
550
wavelength (nm)
O2N
N
B
S
O
HO

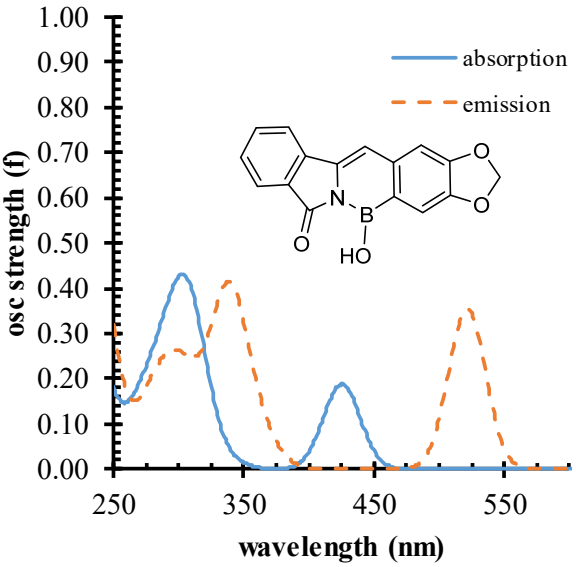

1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
osc strength (f)
absorption
emission
250
350
450
550
wavelength (nm)
H2N
N
B
S
O
HO

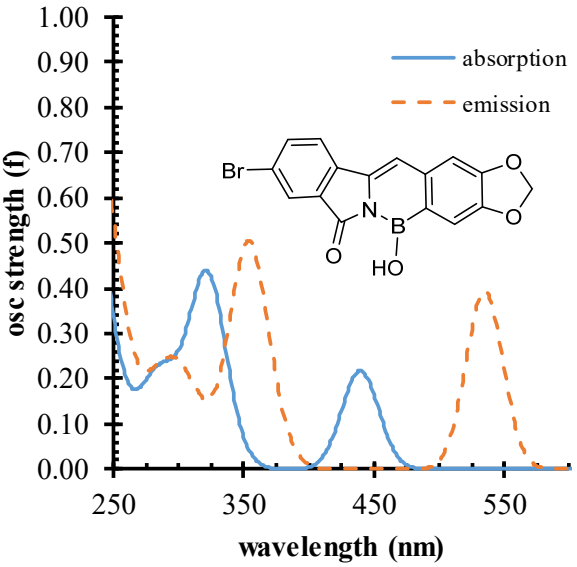
Simulated spectra for acetonitrile solvent

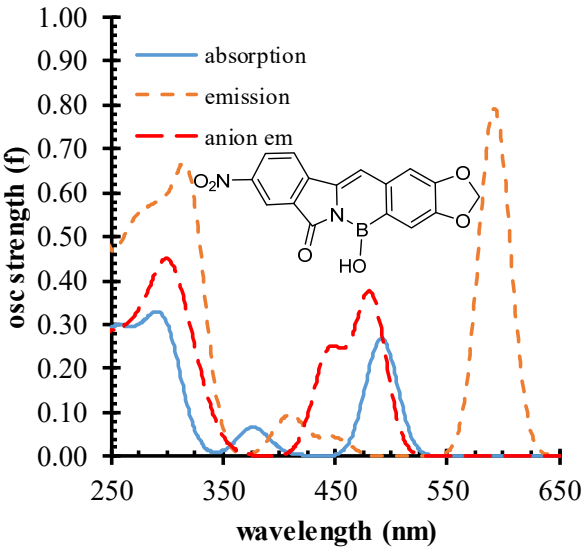
Absorption spectra obtained from LR-SMD-TD-B3LYP/BS1//B3LYP/BS1

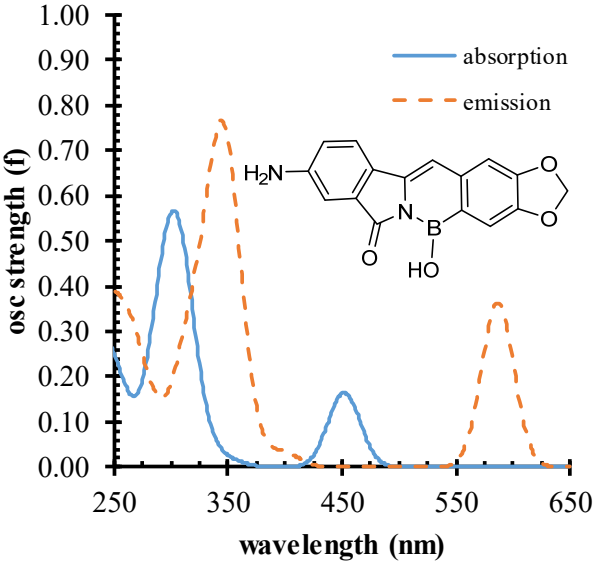
Emission spectra obtained from LR-SMD-TD-B3LYP/BS1

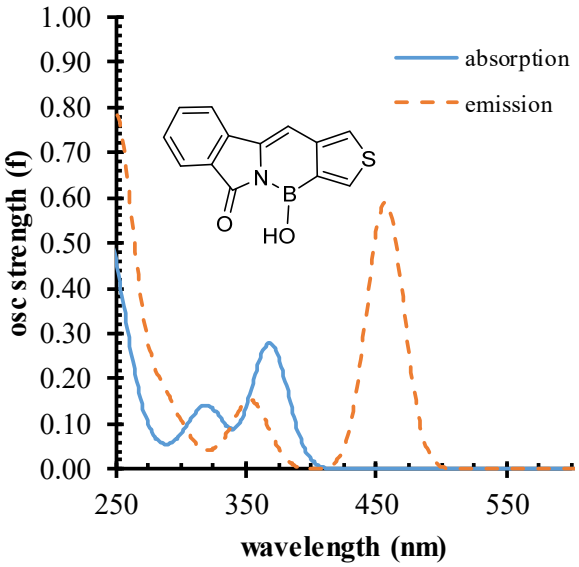



absorption
emission
osc strength (f)
wavelength (nm)
1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
250
350
450
550
O
N
B
HO


absorption
emission
osc strength (f)
wavelength (nm)
1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
250
350
450
550
Br
O
N
B
HO


absorption
emission
anion em
osc strength (f)
wavelength (nm)
1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
250
350
450
550
650
O2N
O
N
B
HO


absorption
emission
osc strength (f)
wavelength (nm)
1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
250
350
450
550
650
H2N
O
N
B
HO


absorption
emission
osc strength (f)
wavelength (nm)
1.00
0.90
0.80
0.70
0.60
0.50
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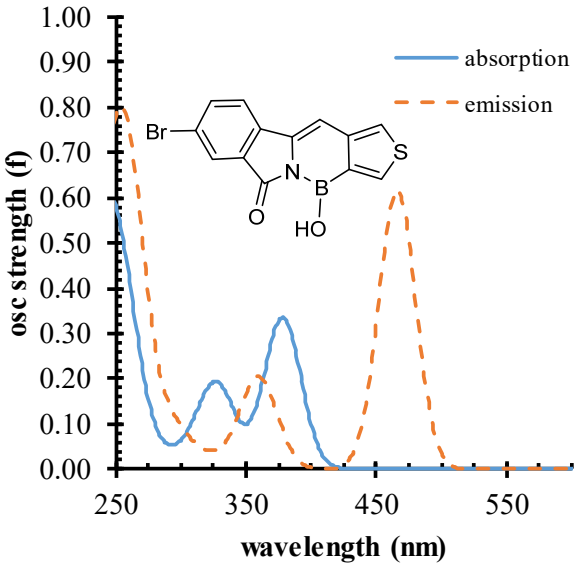
0.30
0.20
0.10
0.00
250
350
450
550
S
N
B
O
HO


absorption
emission
osc strength (f)
wavelength (nm)
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0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
250
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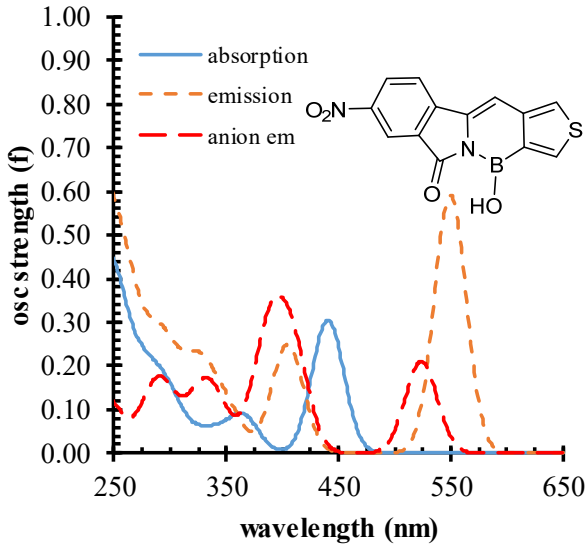
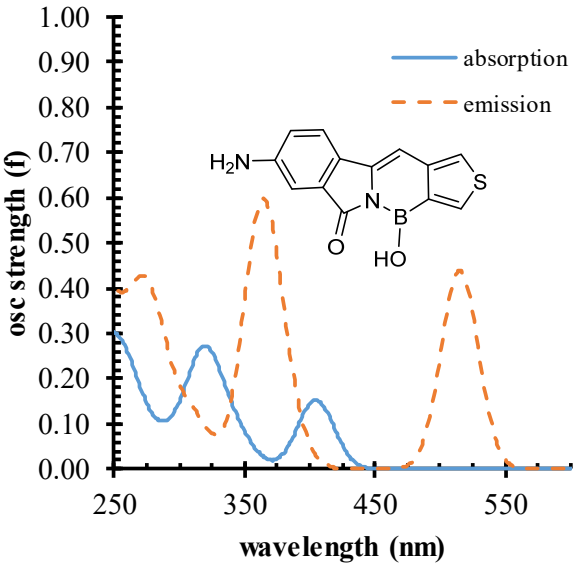
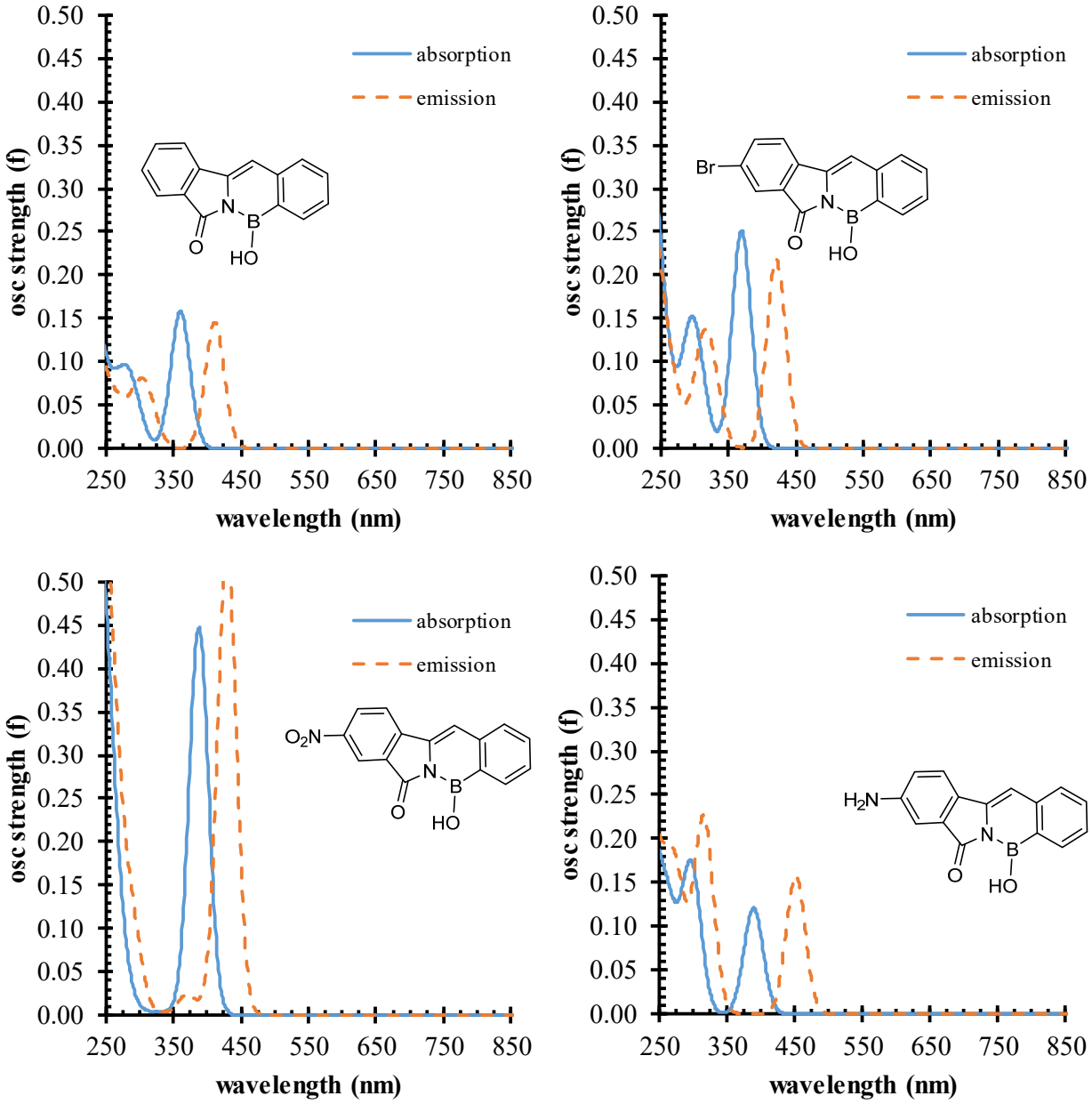
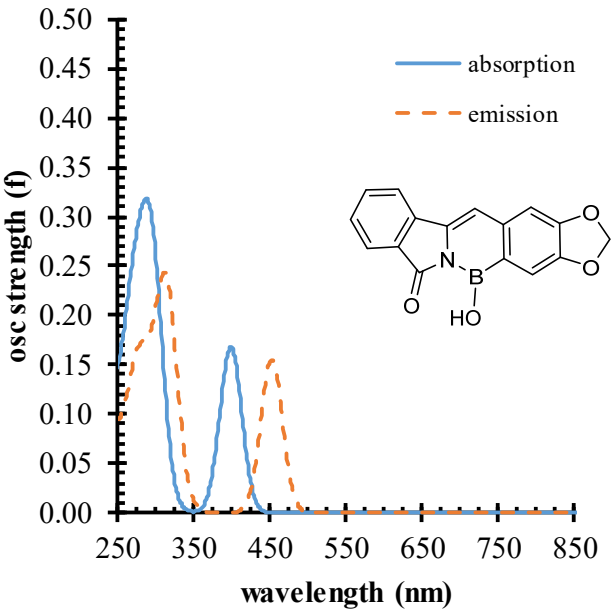
450
550
Br
S
N
B
O
HO

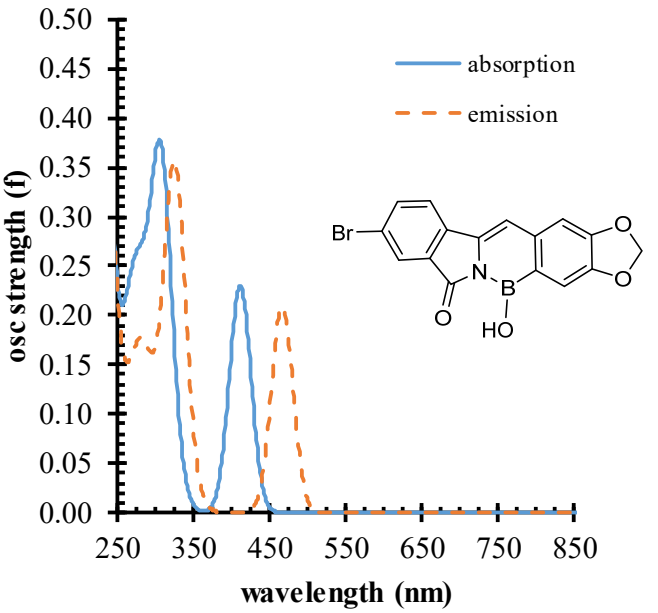

absorption
emission
anion em
osc strength (f)
wavelength (nm)
1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
250
350
450
550
650
O2N
S
N
B
O
HO

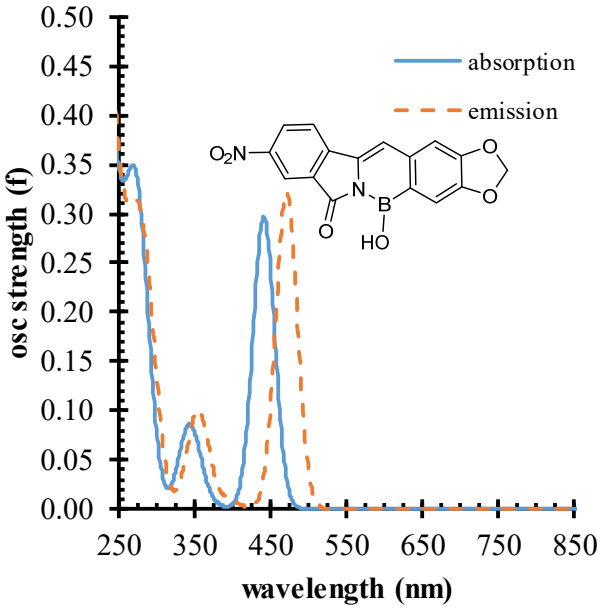

absorption
emission
osc strength (f)
wavelength (nm)
1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
250
350
450
550
H2N
S
N
B
O
HO

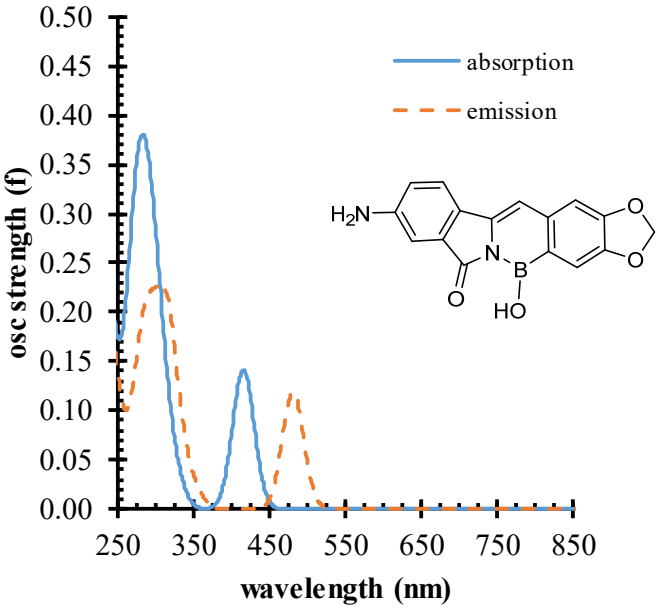
Simulated spectra from TD-PBE0/BS1//PBE0/BS1

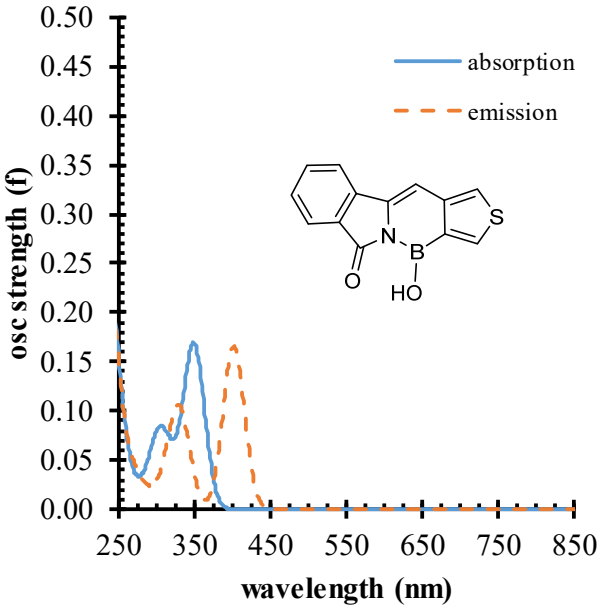


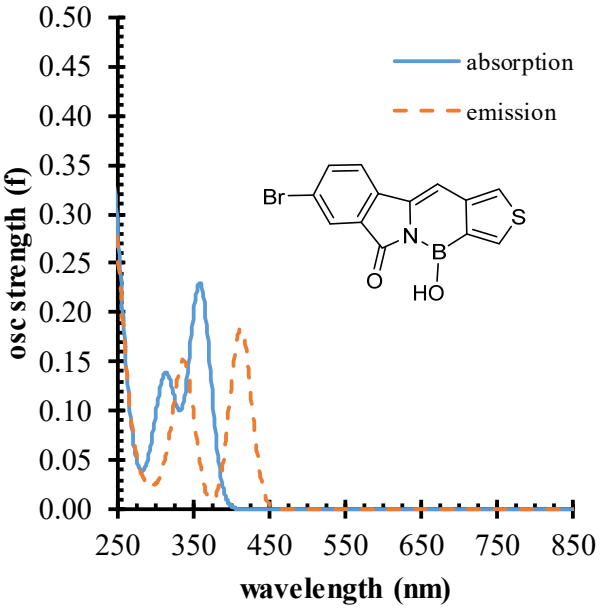

0.50
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
osc strength (f)
250 350 450 550 650 750 850
wavelength (nm)
absorption
emission
O
N
B
O
HO
O
O

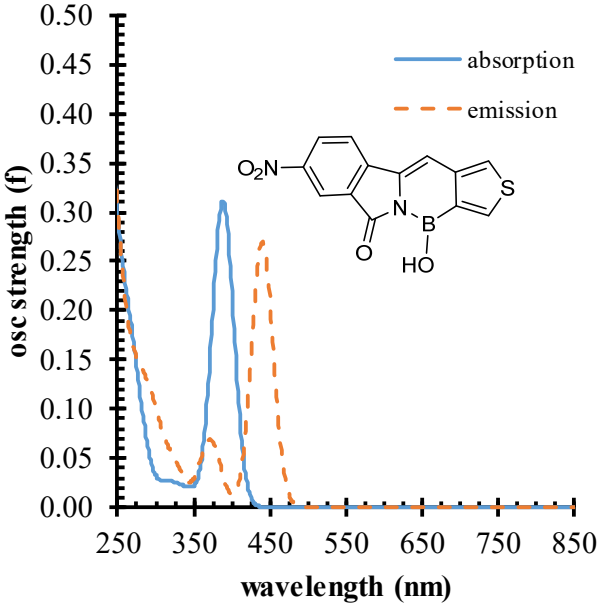

0.50
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
osc strength (f)
250 350 450 550 650 750 850
wavelength (nm)
absorption
emission
Br
O
N
B
O
HO
O
O

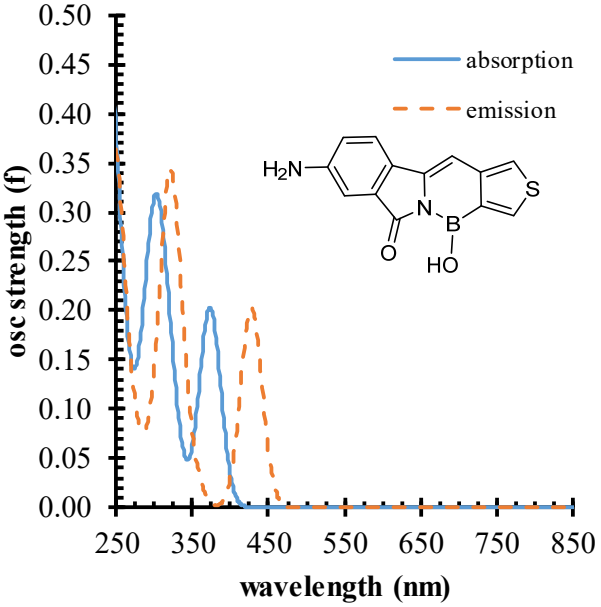

0.50
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
osc strength (f)
250 350 450 550 650 750 850
wavelength (nm)
absorption
emission
O2N
O
N
B
O
HO
O
O


0.50
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
osc strength (f)
250 350 450 550 650 750 850
wavelength (nm)
absorption
emission
H2N
O
N
B
O
HO
O
O


0.50
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
osc strength (f)
absorption
emission
250 350 450 550 650 750 850
wavelength (nm)
S
N
B
O
HO


0.50
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
osc strength (f)
absorption
emission
250 350 450 550 650 750 850
wavelength (nm)
Br
S
N
B
O
HO

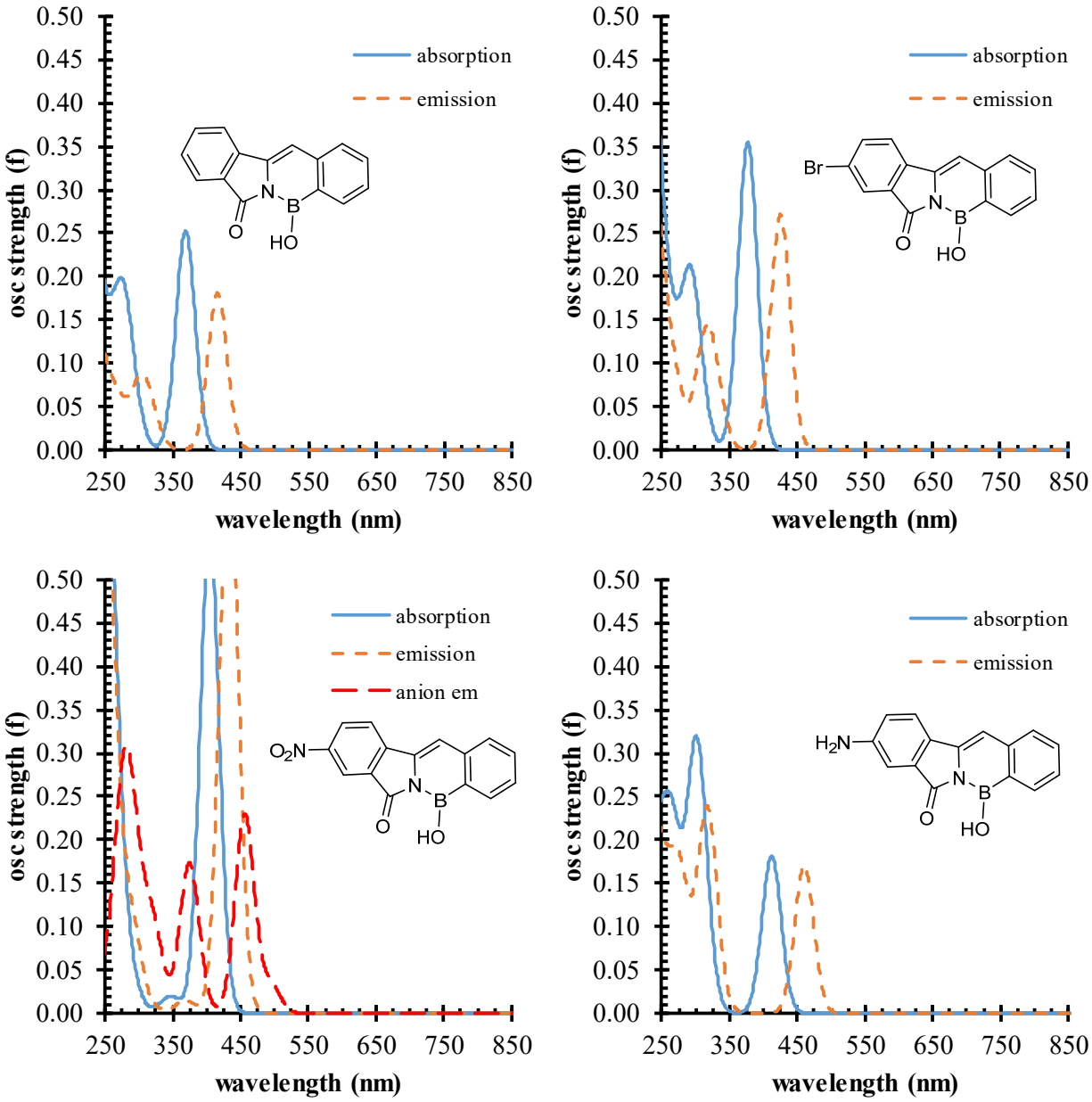

0.50
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
osc strength (f)
absorption
emission
250 350 450 550 650 750 850
wavelength (nm)
O2N
S
N
B
O
HO

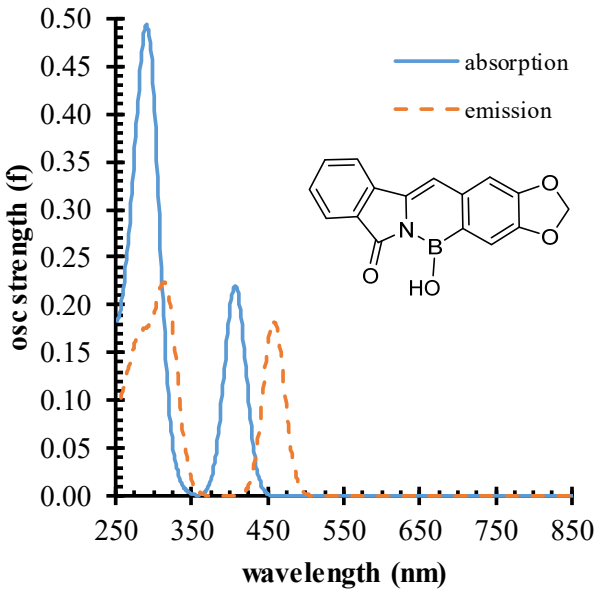

0.50
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
osc strength (f)
absorption
emission
250 350 450 550 650 750 850
wavelength (nm)
H2N
S
N
B
O
HO

Simulated spectra for acetonitrile solvent

Absorption spectra obtained from LR-SMD-TD-PBE0/BS1//PBE0/BS1

Emission spectra obtained from LR-SMD-TD-PBE0/BS1




absorption
emission
osc strength (f)
wavelength (nm)
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0.45
0.40
0.35
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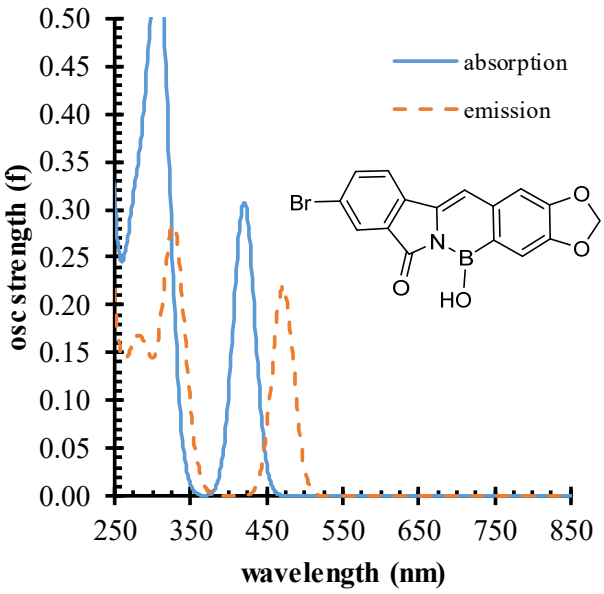
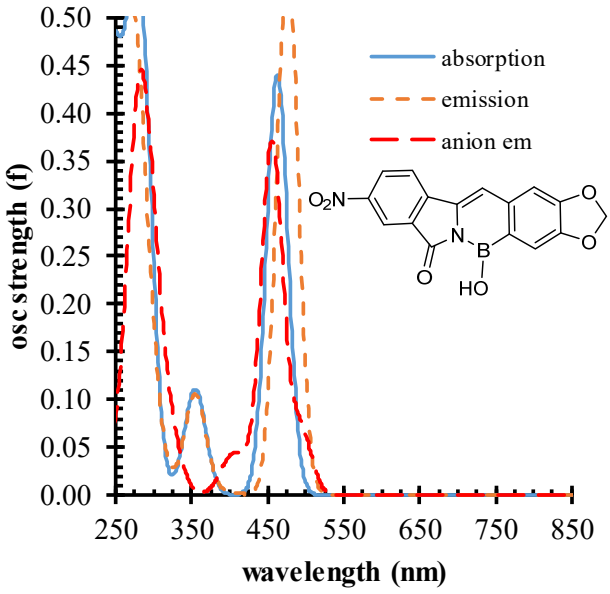
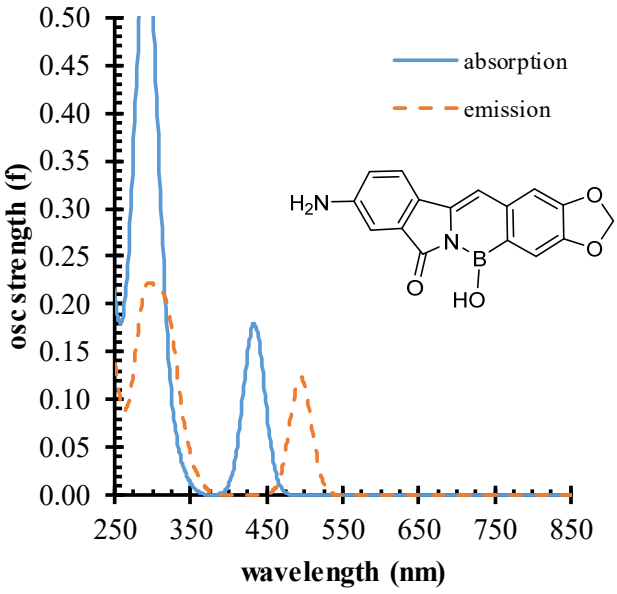
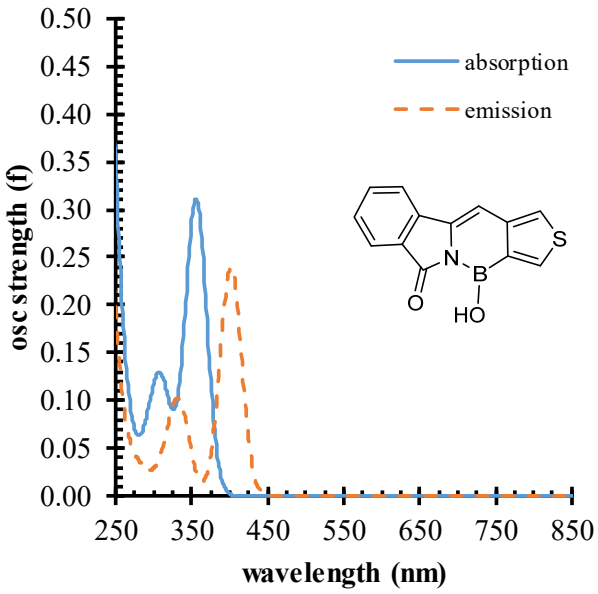
0.10
0.05
0.00
250
350
450
550
650
750
850
O
N
B
HO


absorption
emission
osc strength (f)
wavelength (nm)
Br
O
N
B
HO


absorption
emission
anion em
osc strength (f)
wavelength (nm)
O2N
O
N
B
HO


absorption
emission
osc strength (f)
wavelength (nm)
H2N
O
N
B
HO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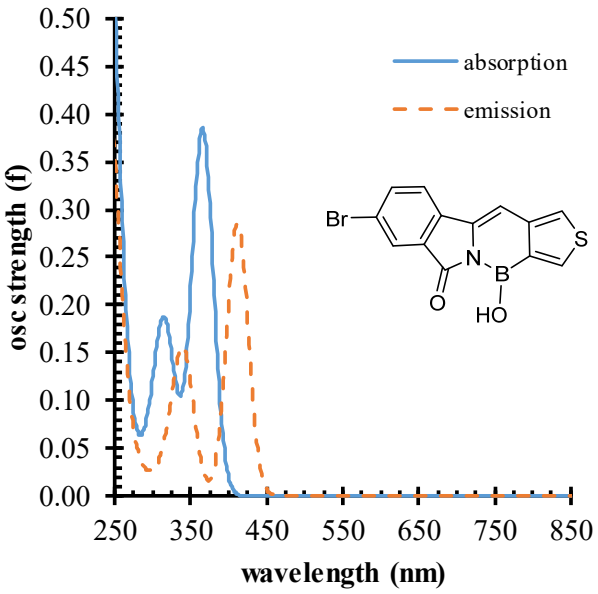
osc strength (f)
250 350 450 550 650 750 850
wavelength (nm)
absorption
emission
S
N
B
O
HO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osc strength (f)
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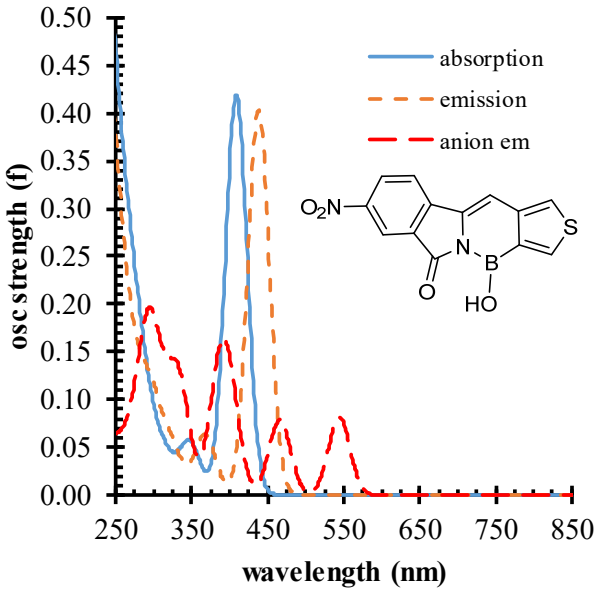
wavelength (nm)
absorption
emission
Br
S
N
B
O
HO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osc strength (f)
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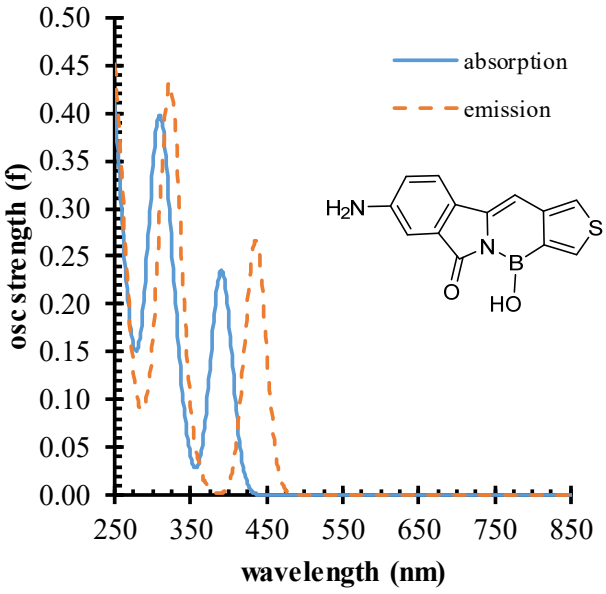
wavelength (nm)
absorption
emission
anion em
O2N
S
N
B
O
HO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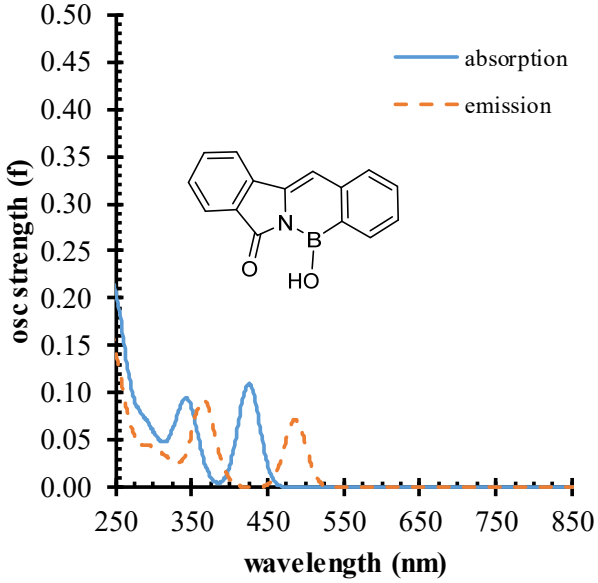
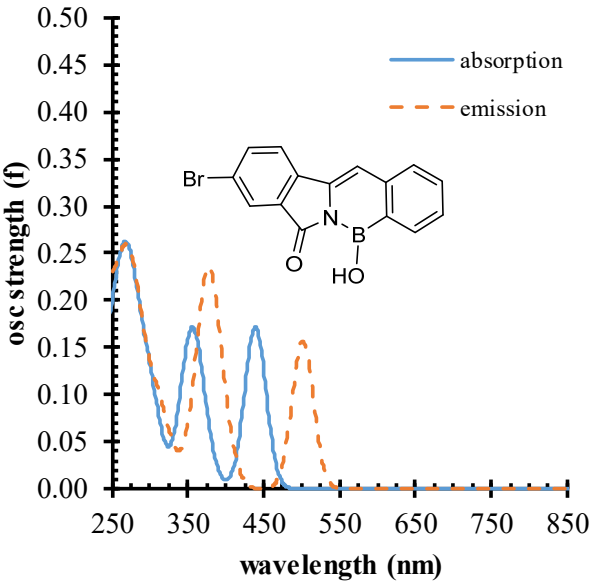
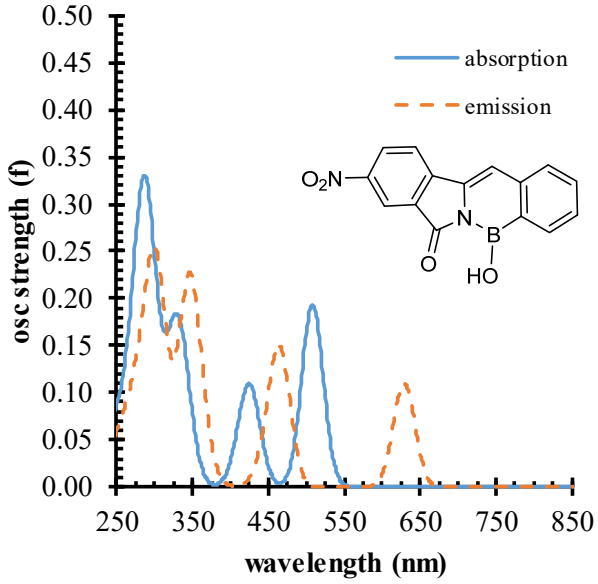
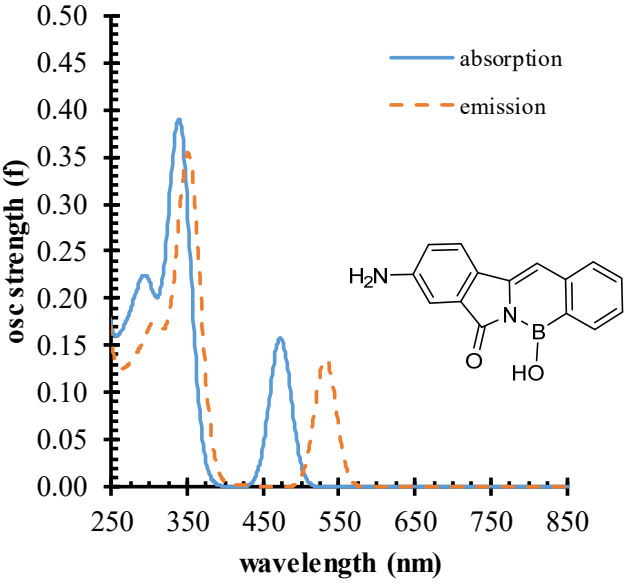
0.05
0.00
osc strength (f)
250 350 450 550 650 750 850
wavelength (nm)
absorption
emission
H2N
S
N
B
O
HO

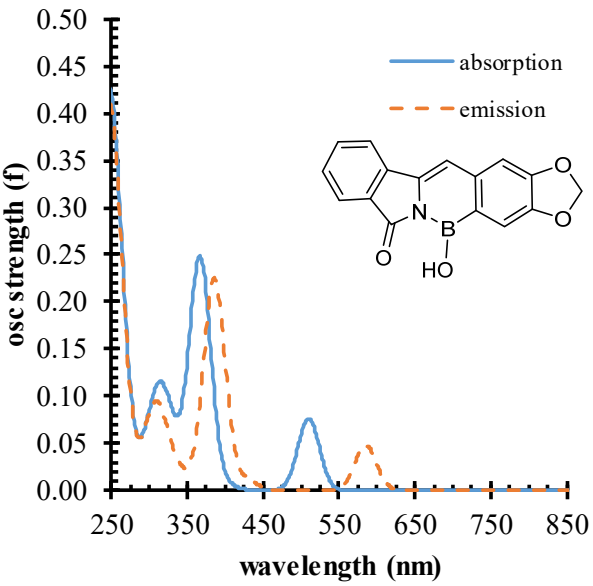
Simulated spectra from TD-B97D/BS1//B97D/BS1







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0.20
0.15
0.10
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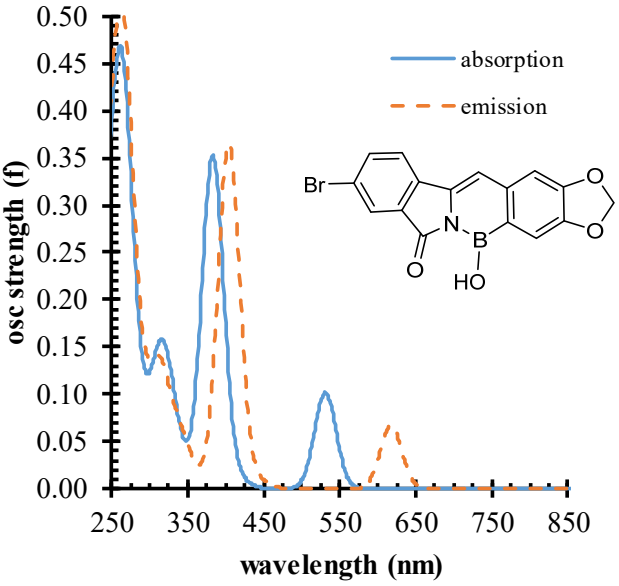
0.00
osc strength (f)
absorption
emission
250 350 450 550 650 750 850
wavelength (nm)
O
N
B
HO
O
O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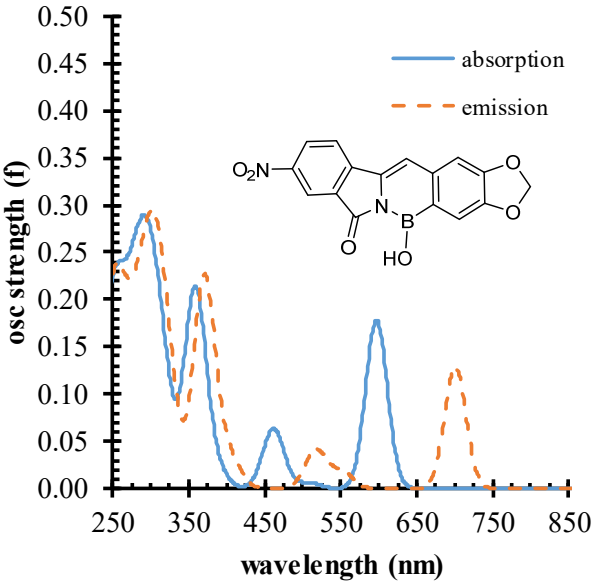
osc strength (f)
absorption
emission
250 350 450 550 650 750 850
wavelength (nm)
Br
O
N
B
HO
O
O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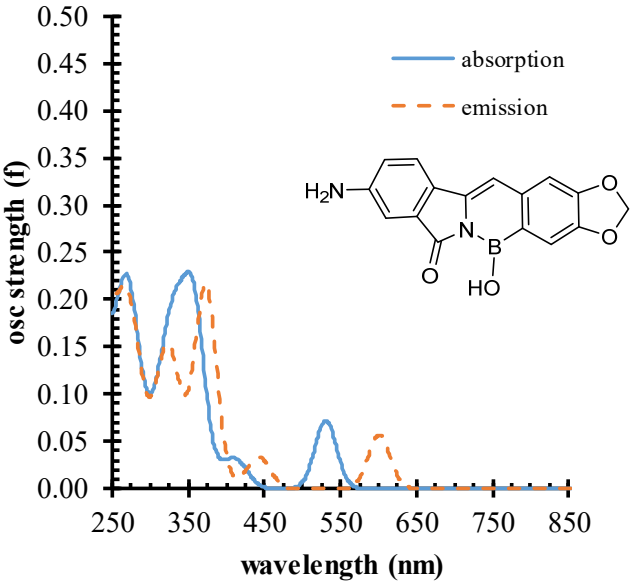
osc strength (f)
absorption
emission
250 350 450 550 650 750 850
wavelength (nm)
O2N
O
N
B
HO
O
O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absorption
emission
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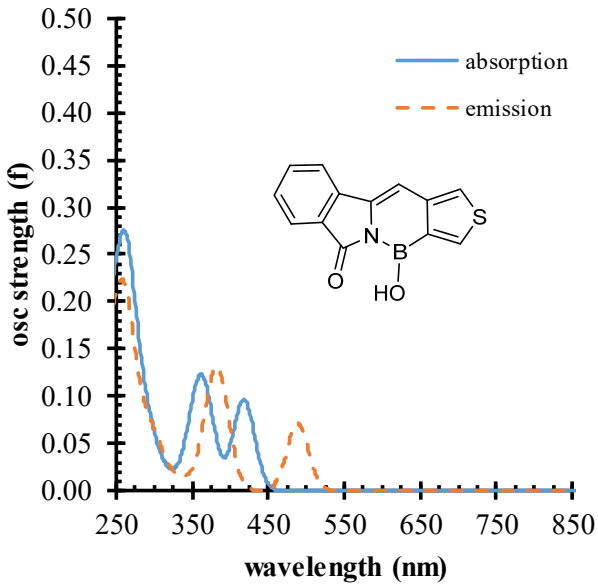
wavelength (nm)
H2N
O
N
B
HO
O
O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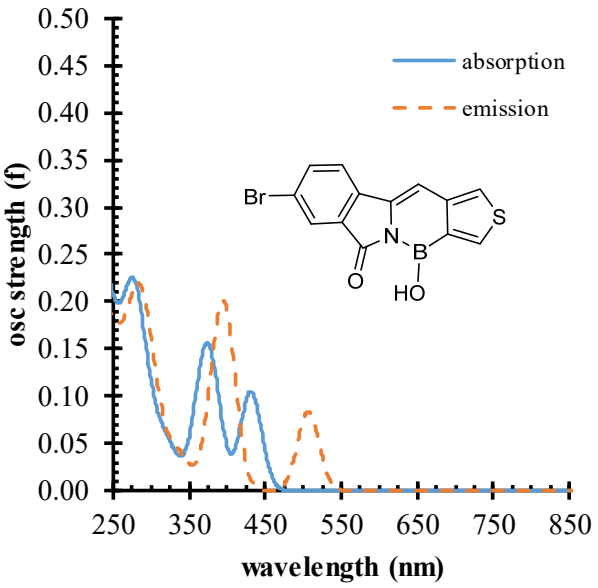
osc strength (f)
absorption
emission
250 350 450 550 650 750 850
wavelength (nm)
N
B
S
O
HO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osc strength (f)
absorption
emission
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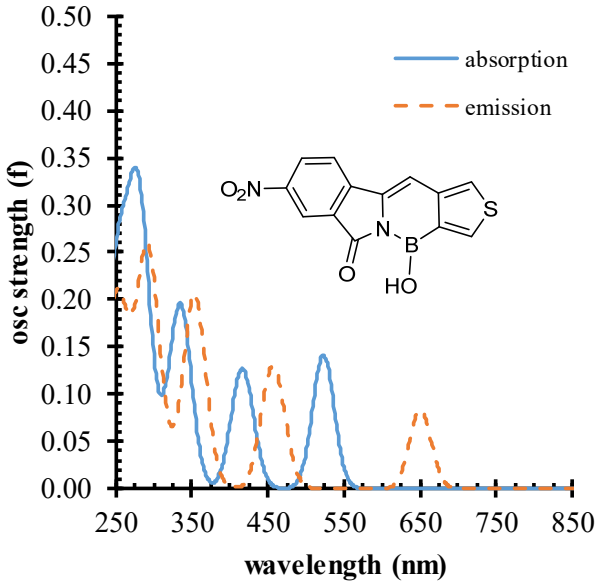
wavelength (nm)
Br
N
B
S
O
HO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absorption
emission
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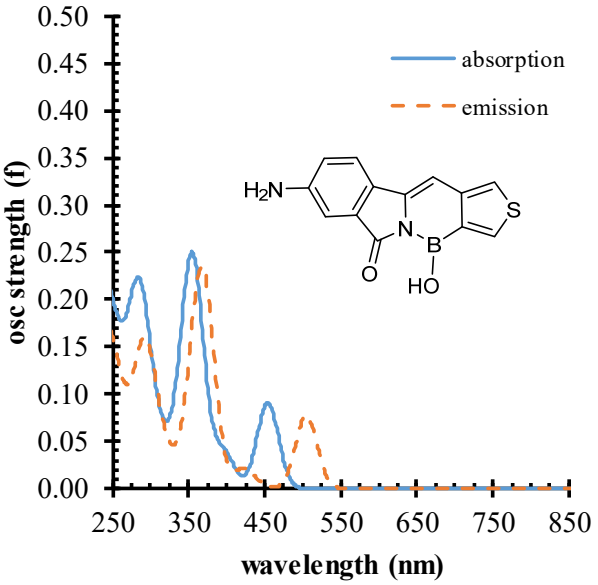
wavelength (nm)
O2N
N
B
S
O
HO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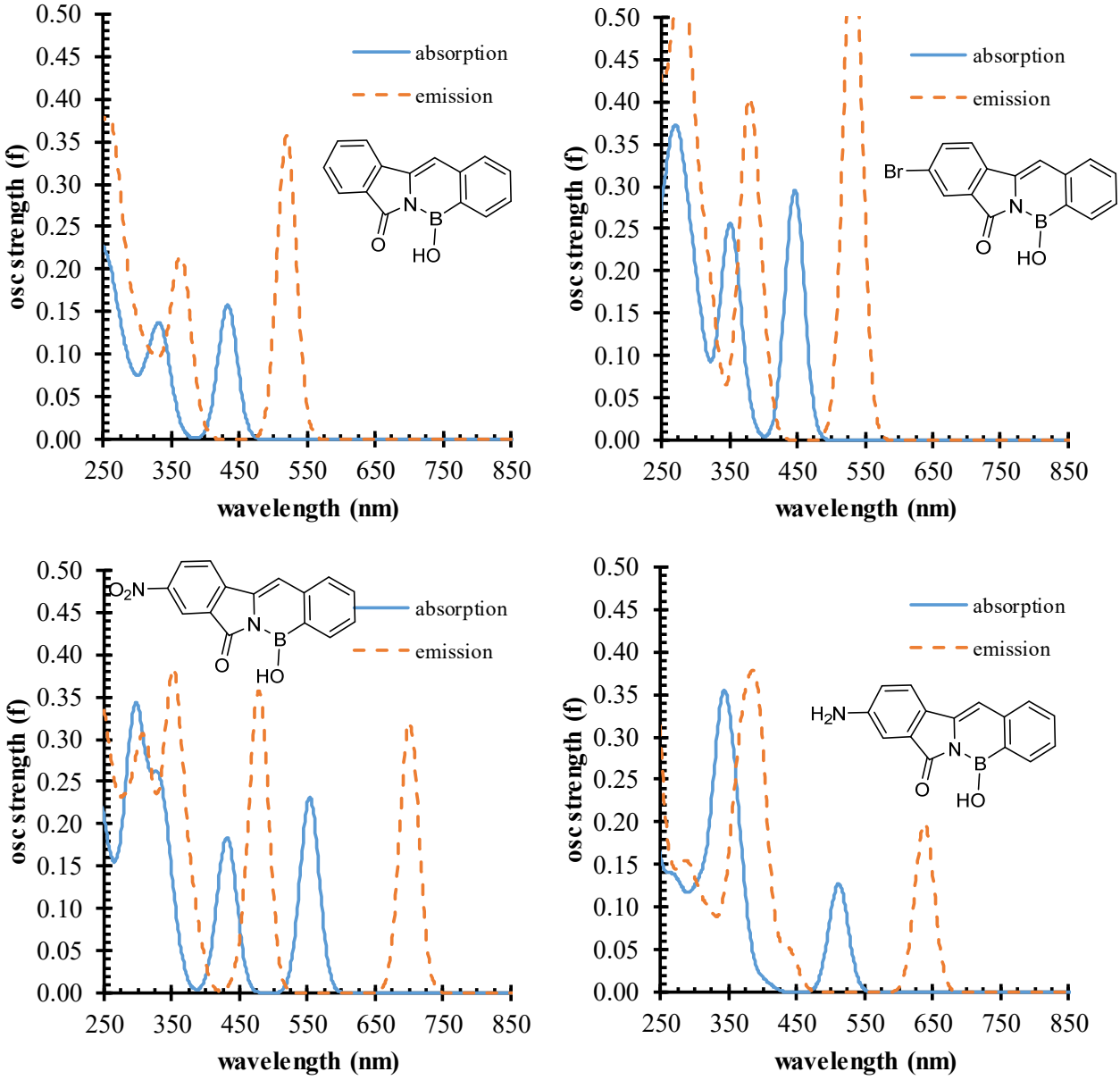
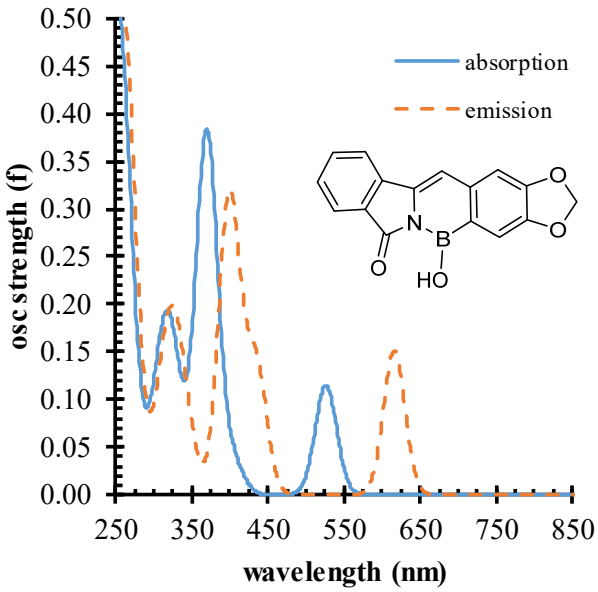
0.05
0.00
osc strength (f)
absorption
emission
250 350 450 550 650 750 850
wavelength (nm)
H2N
N
B
S
O
HO

Simulated spectra for acetonitrile solvent

Absorption spectra obtained from LR-SMD-TD-B97D/BS1//B97D/BS1

Emission spectra obtained from LR-SMD-TD-B97D/BS1

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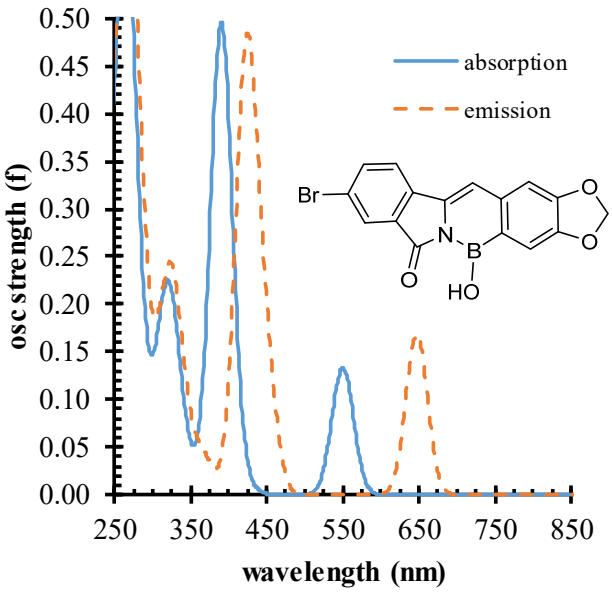
0.25
0.20
0.15
0.10
0.05
0.00
osc strength (f)
250 350 450 550 650 750 850
wavelength (nm)
absorption
emission
O
N
B
O
HO
O
O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0.15
0.10
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osc strength (f)
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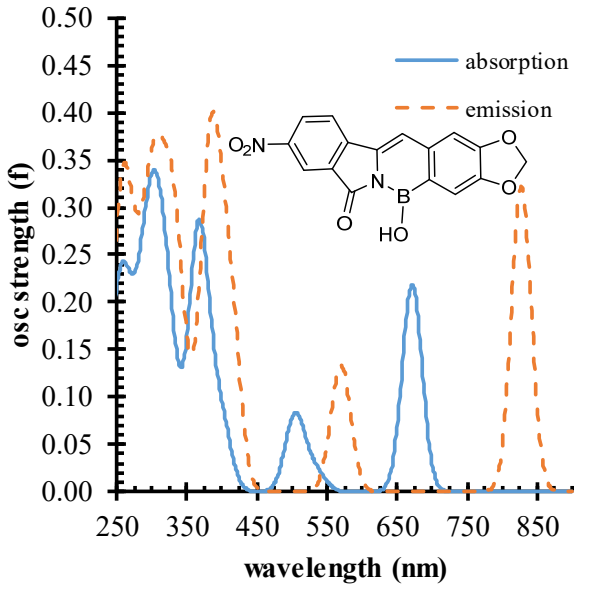
wavelength (nm)
absorption
emission
Br
O
N
B
O
HO
O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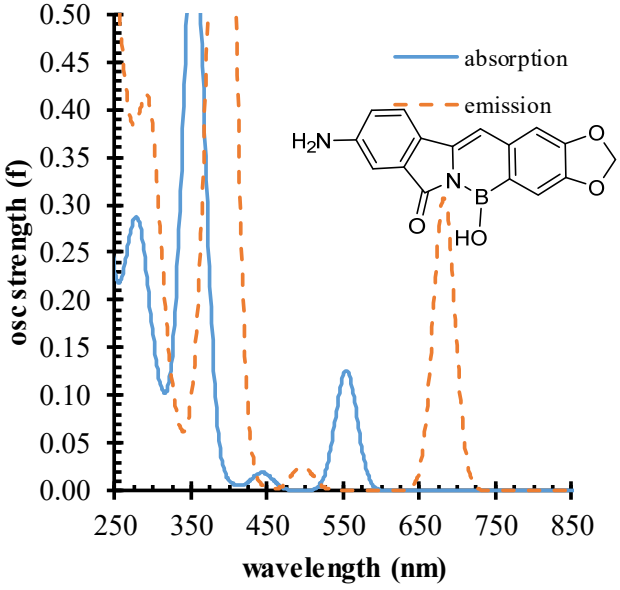
250 350 450 550 650 750 850
wavelength (nm)
absorption
emission
O2N
O
N
B
O
HO
O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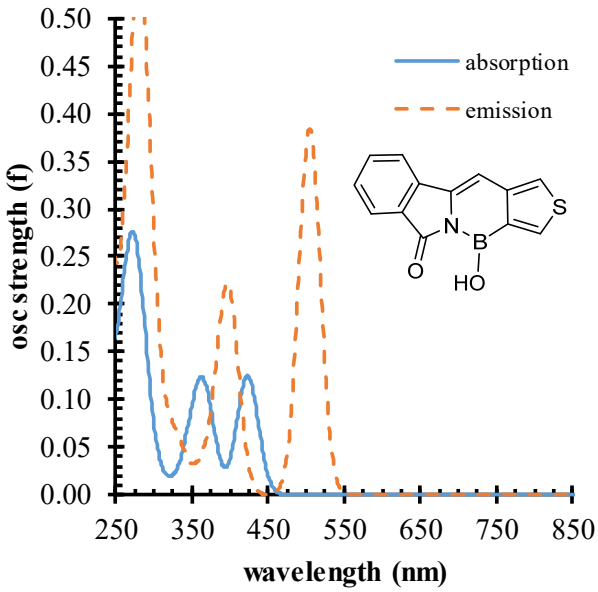
wavelength (nm)
absorption
emission
H2N
O
N
B
O
HO
O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osc strength (f)
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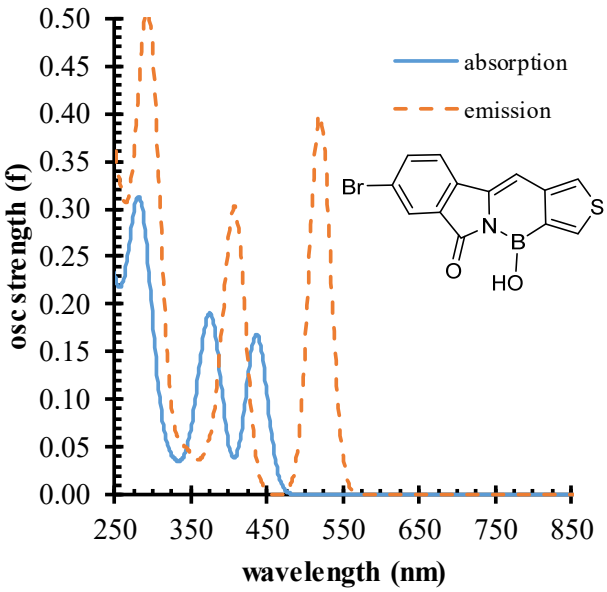
wavelength (nm)
absorption
emission
S
N
B
O
HO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osc strength (f)
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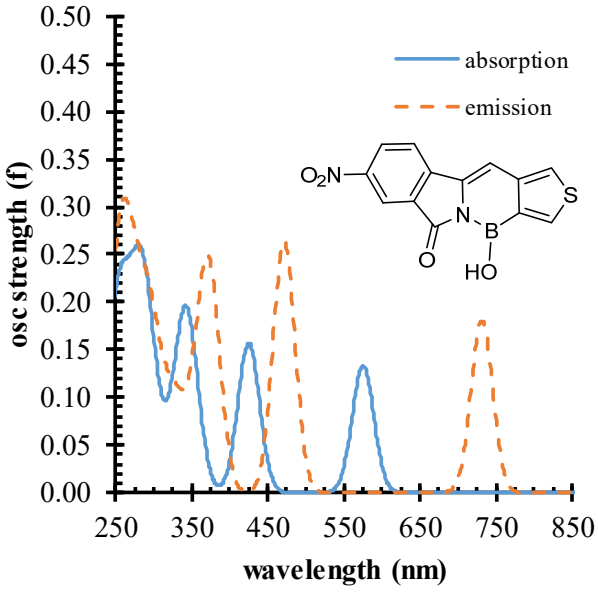
wavelength (nm)
absorption
emission
Br
S
N
B
O
HO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0.25
0.20
0.15
0.10
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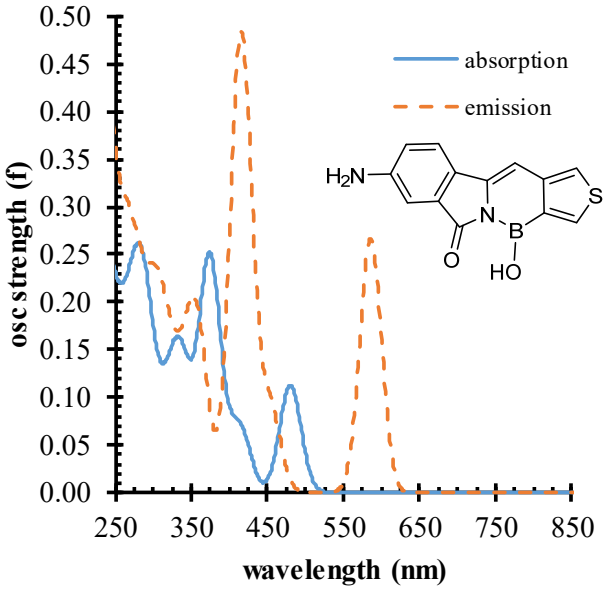
osc strength (f)
250 350 450 550 650 750 850
wavelength (nm)
absorption
emission
O2N
S
N
B
O
HO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0.30
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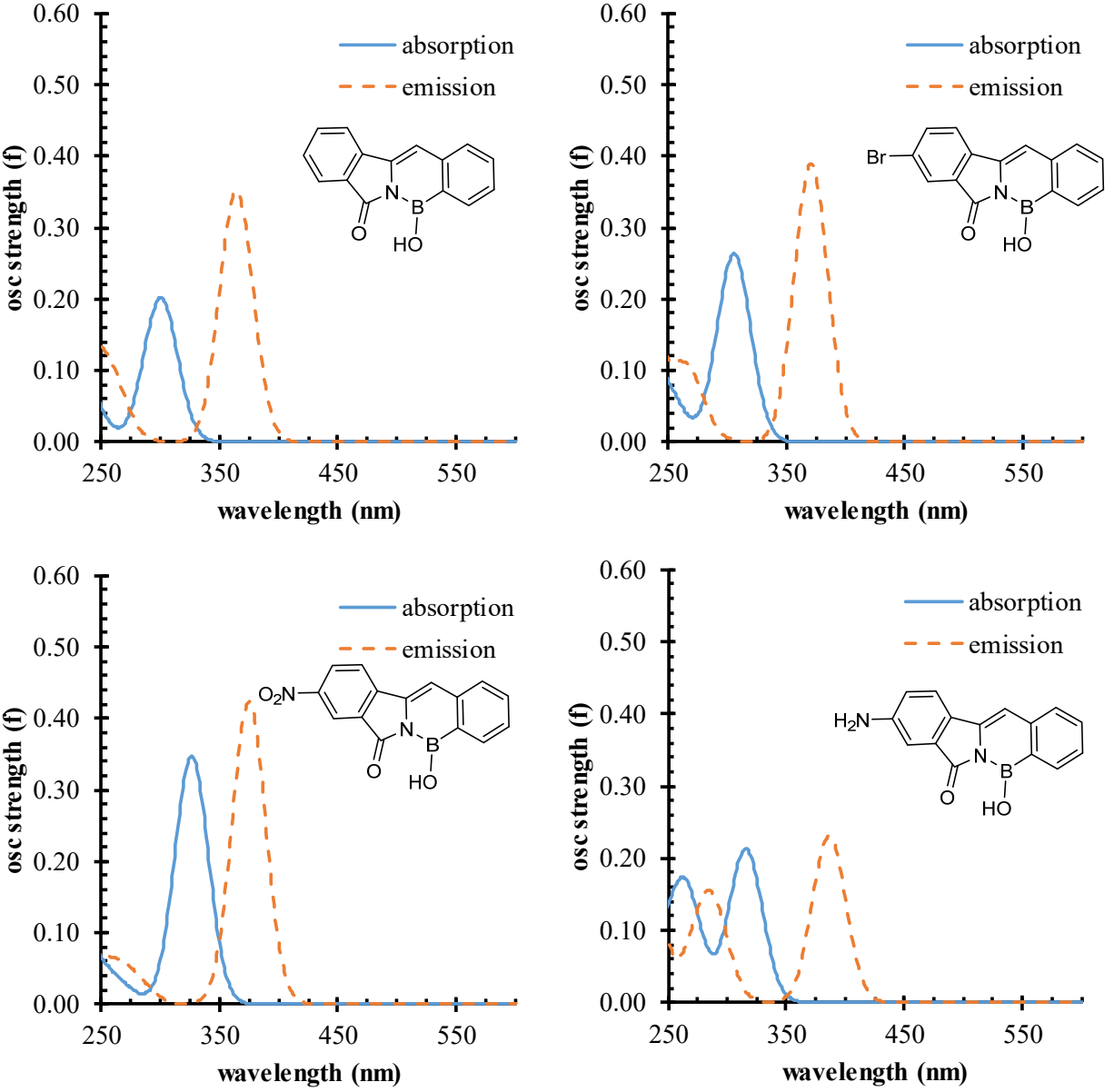
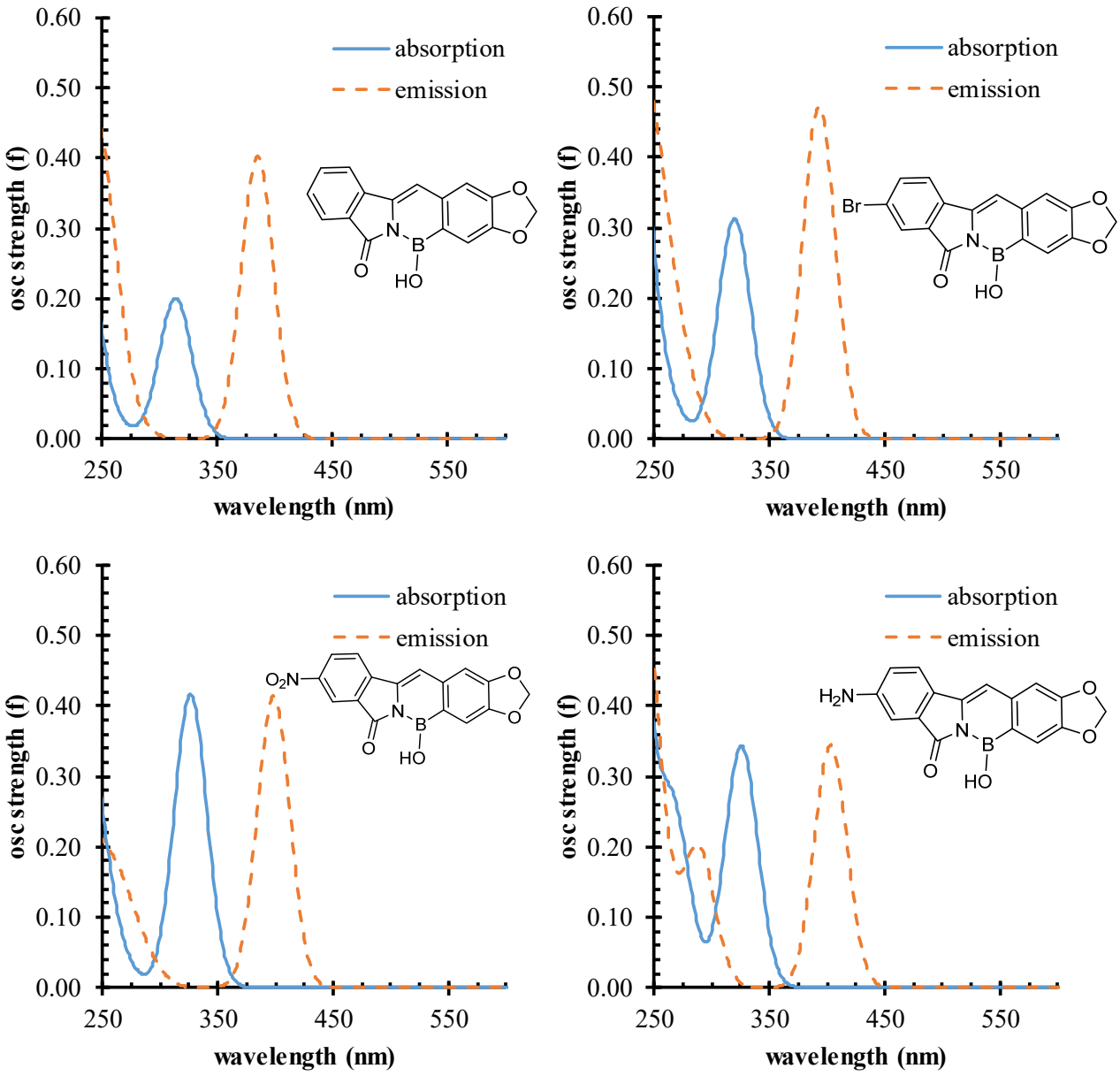
0.20
0.15
0.10
0.05
0.00
osc strength (f)
250 350 450 550 650 750 850
wavelength (nm)
absorption
emission
H2N
S
N
B
O
HO

Simulated spectra from TD-cam-QTP(01)/BS1//cam-QTP(01)/BS1

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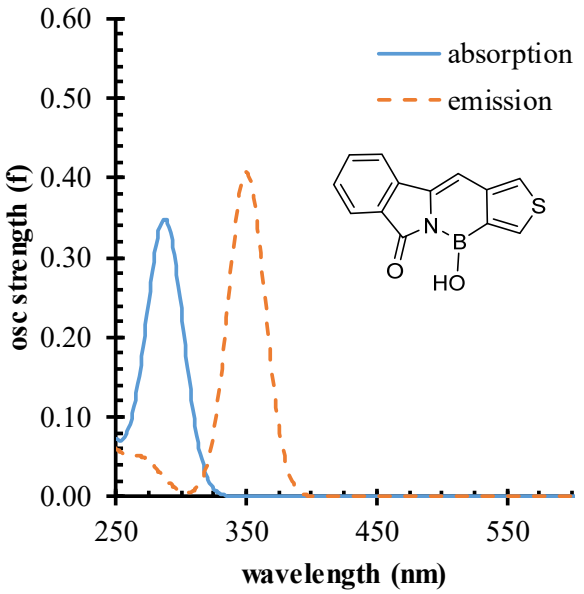
0.40
0.30
0.20
0.10
0.00
osc strength (f)
250
350
450
550
wavelength (nm)
absorption
emission
O
O
N
B
O
HO
Br
O2N
H2N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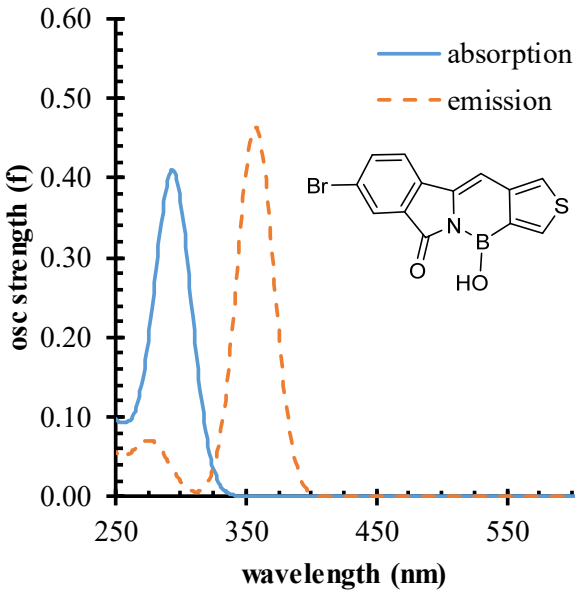
0.40
0.30
0.20
0.10
0.00
osc strength (f)
absorption
emission
250
350
450
550
wavelength (nm)
O
N
B
HO
S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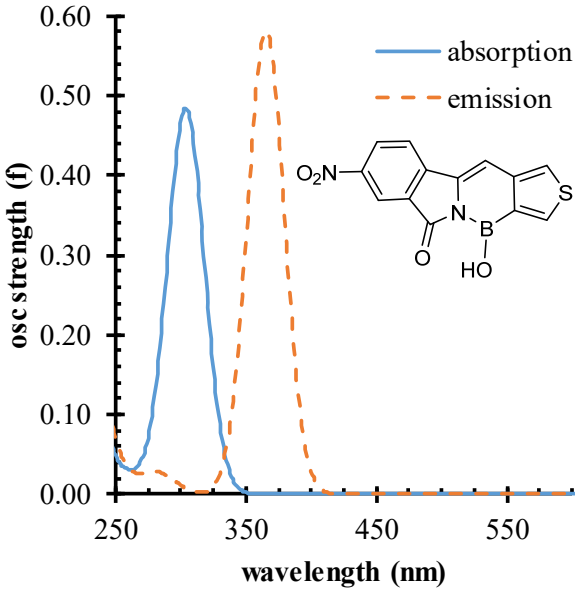
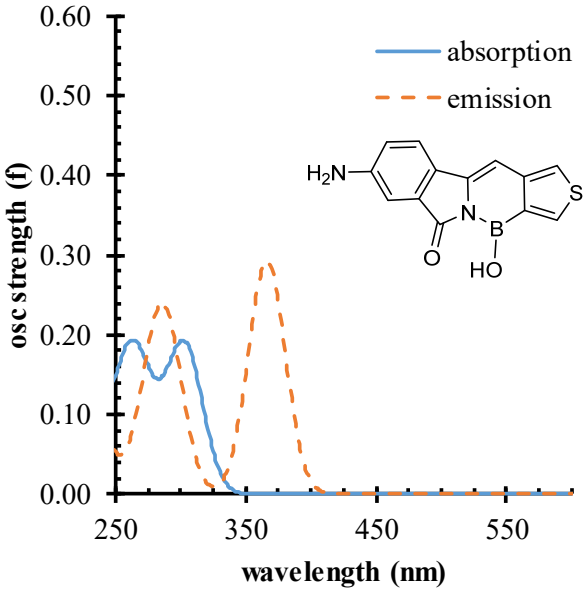
osc strength (f)
absorption
emission
250
350
450
550
wavelength (nm)
Br
O
N
B
HO
S


0.60
0.50
0.40
0.30
0.20
0.10
0.00
osc strength (f)
absorption
emission
250
350
450
550
wavelength (nm)
O2N
O
N
B
HO
S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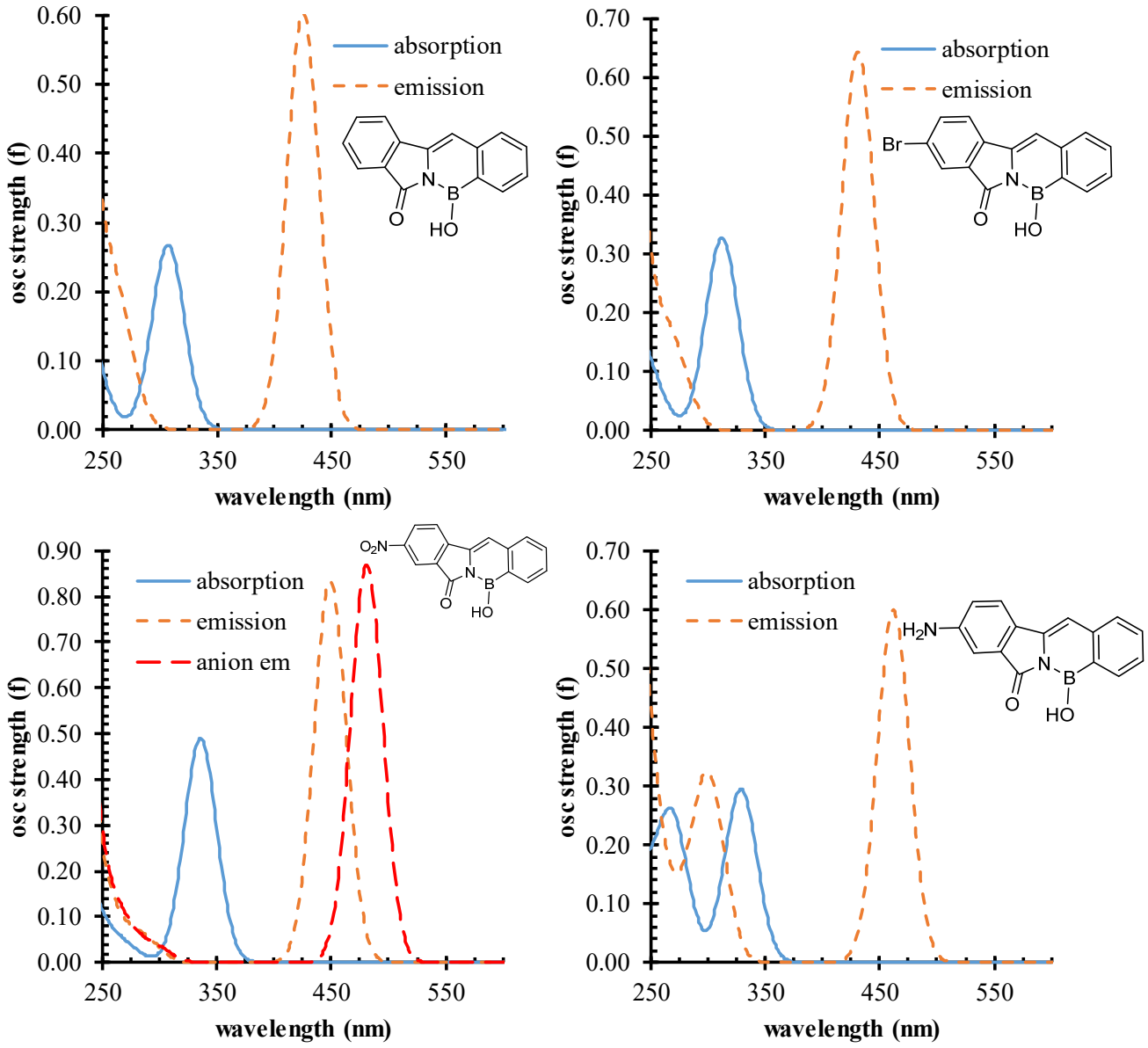
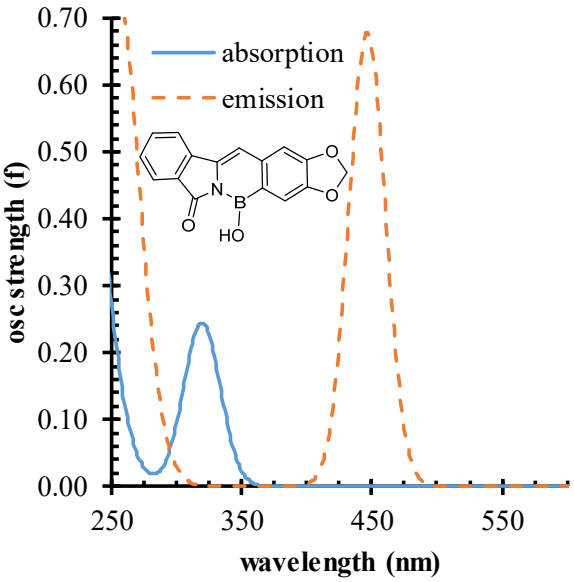
0.20
0.10
0.00
osc strength (f)
absorption
emission
250
350
450
550
wavelength (nm)
H2N
O
N
B
HO
S

Simulated spectra for acetonitrile solvent

Absorption spectra obtained from LR-SMD-TD-cam-QTP(01)/BS1//cam-QTP(01)/BS1

Emission spectra obtained from LR-SMD-TD-cam-QTP(01)/BS1




absorption
emission
osc strength (f)
wavelength (nm)
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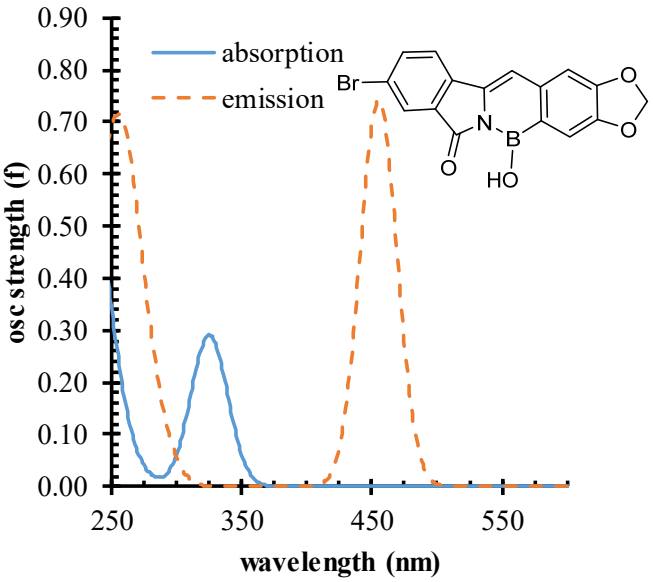
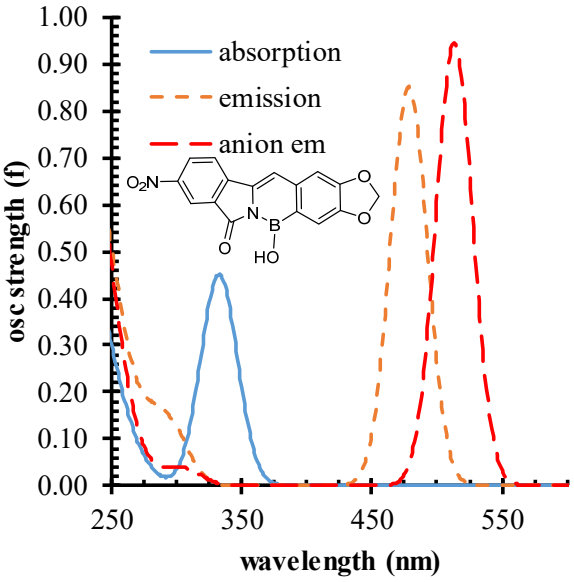
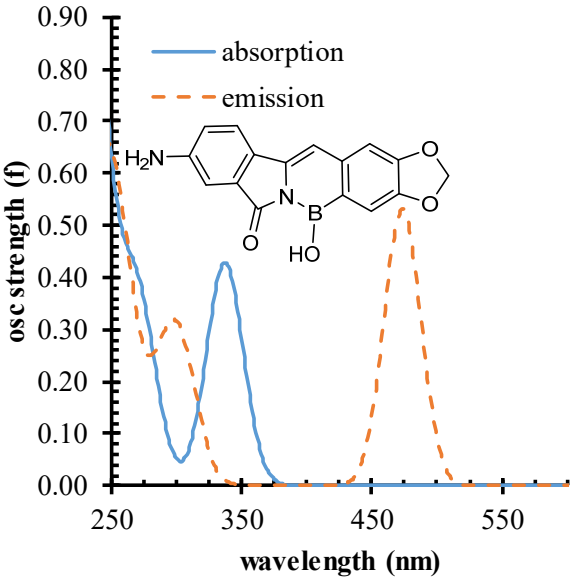
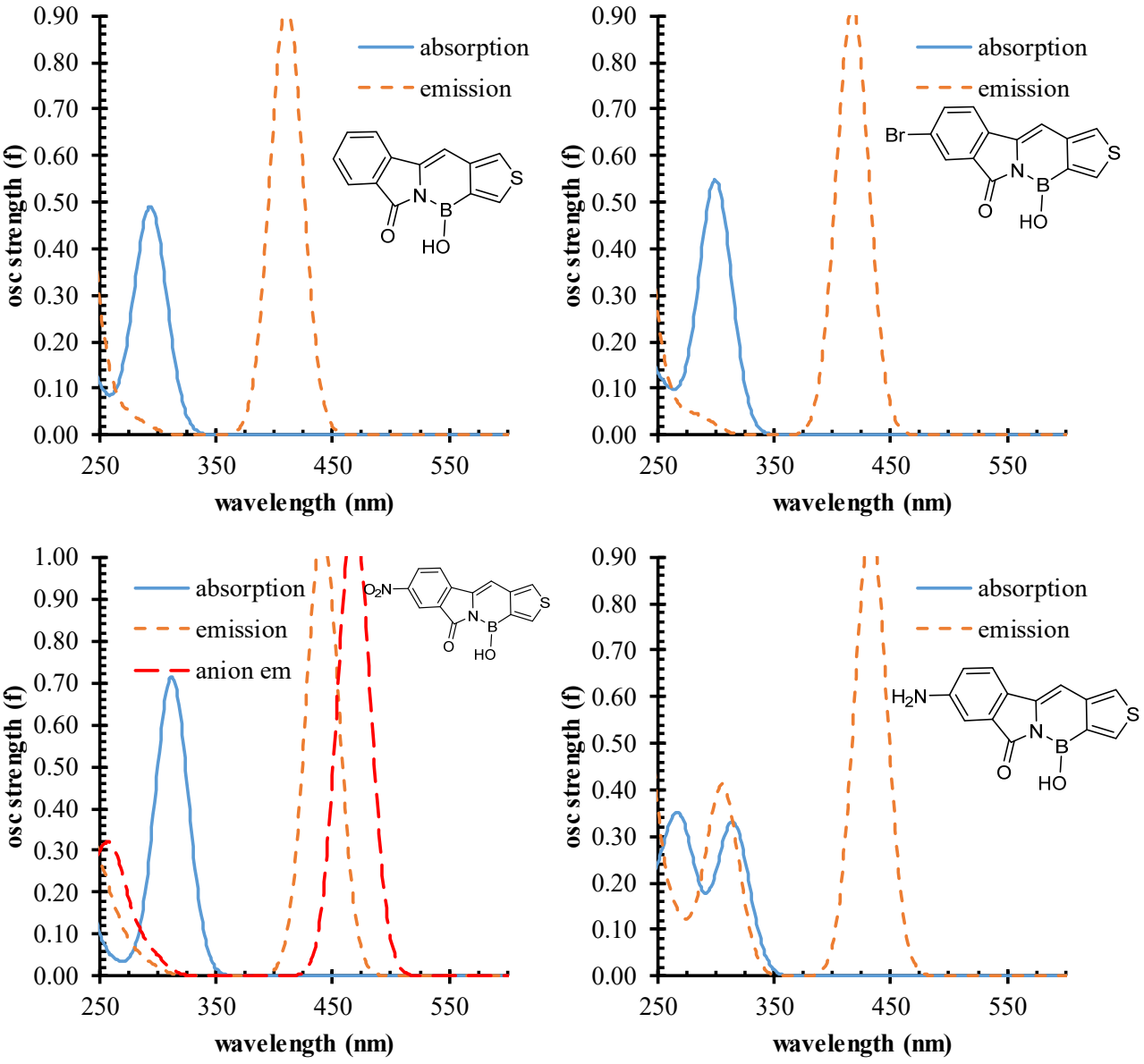
0.10
0.20
0.30
0.40
0.50
0.60
0.70
250
350
450
550
O
N
B
HO

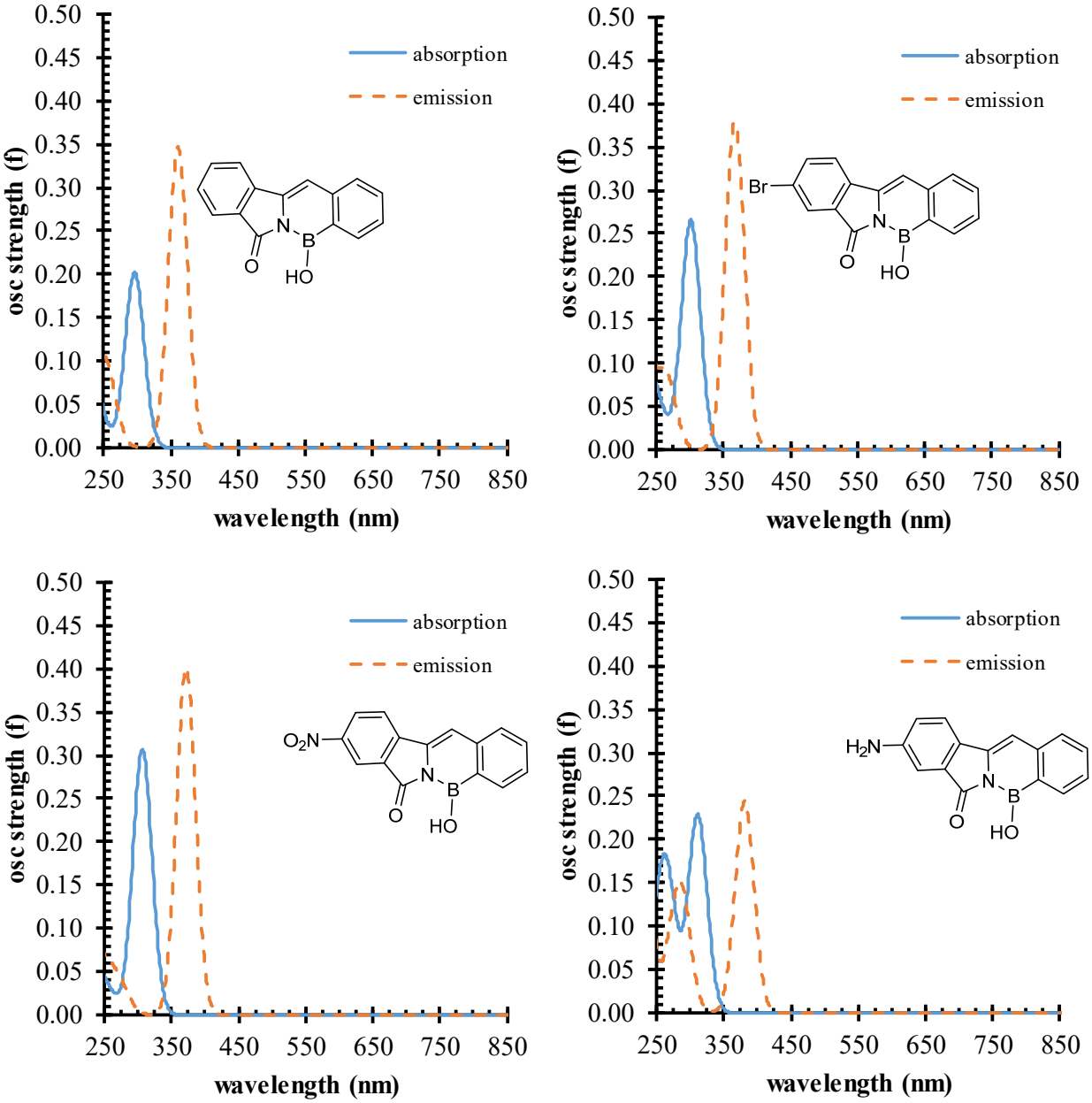

absorption
emission
osc strength (f)
wavelength (nm)
0.00
0.10
0.20
0.30
0.40
0.50
0.60
0.70
0.80
0.90
250
350
450
550
Br
O
N
B
HO

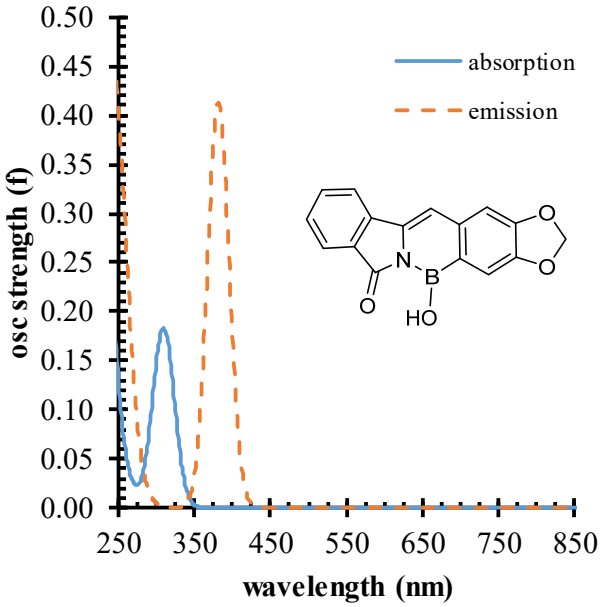

absorption
emission
anion em
osc strength (f)
wavelength (nm)
0.00
0.10
0.20
0.30
0.40
0.50
0.60
0.70
0.80
0.90
1.00
250
350
450
550
O2N
O
N
B
HO

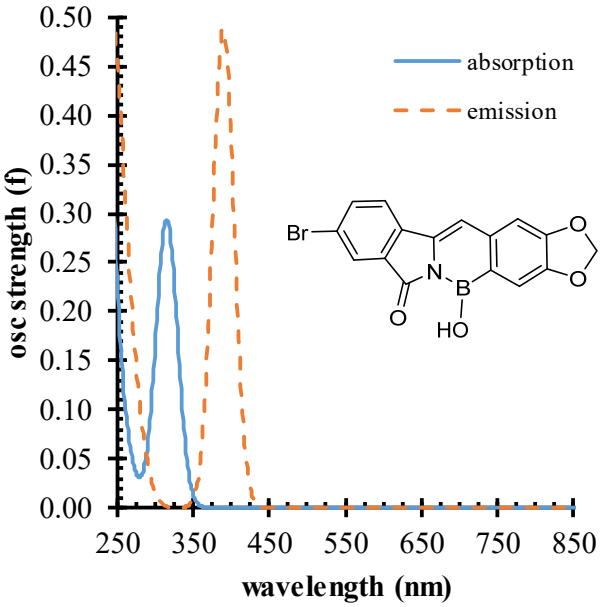

absorption
emission
osc strength (f)
wavelength (nm)
0.00
0.10
0.20
0.30
0.40
0.50
0.60
0.70
0.80
0.90
250
350
450
550
H2N
O
N
B
HO

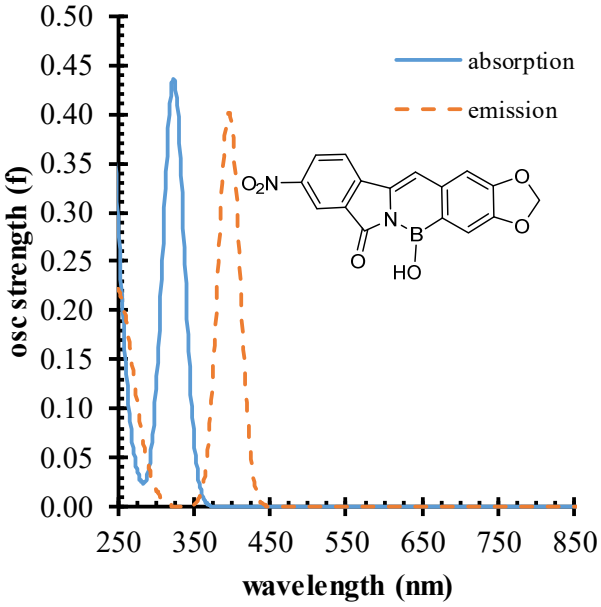

absorption
emission
anion em
osc strength (f)
wavelength (nm)
0.00
0.10
0.20
0.30
0.40
0.50
0.60
0.70
0.80
0.90
1.00
250
350
450
550
Br
O2N
H2N
S
N
B
HO
O

Simulated spectra from TD-LC-ωHPBE/BS1//LC-ωHPBE/BS1




0.50
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
osc strength (f)
absorption
emission
250 350 450 550 650 750 850
wavelength (nm)
O
N
B
O
O
HO


0.50
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
osc strength (f)
absorption
emission
250 350 450 550 650 750 850
wavelength (nm)
Br
O
N
B
O
O
HO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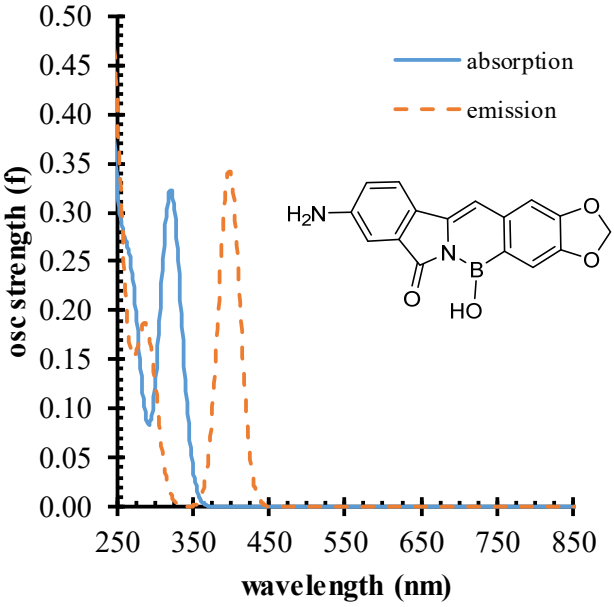
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
osc strength (f)
absorption
emission
250 350 450 550 650 750 850
wavelength (nm)
O2N
O
N
B
O
O
HO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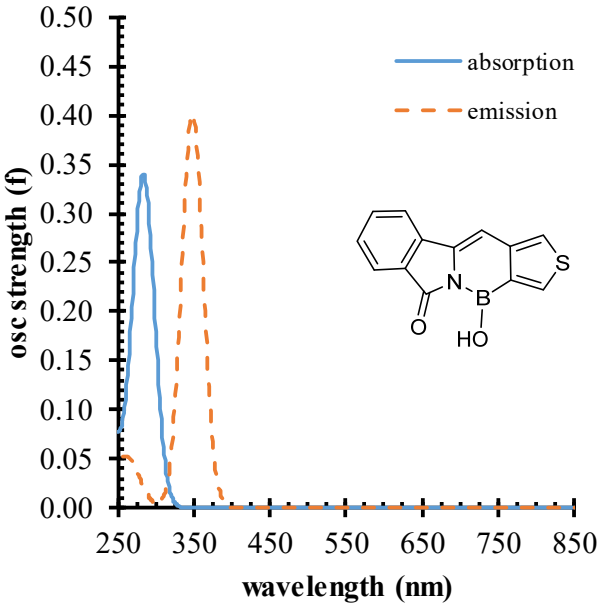
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
osc strength (f)
absorption
emission
250 350 450 550 650 750 850
wavelength (nm)
H2N
O
N
B
O
O
HO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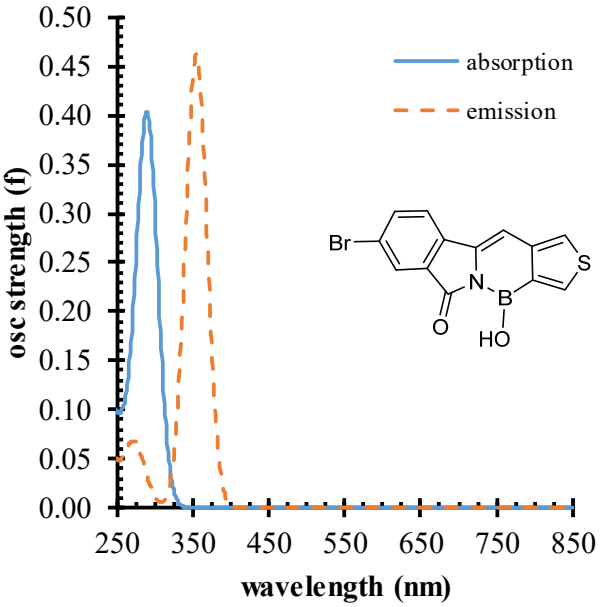
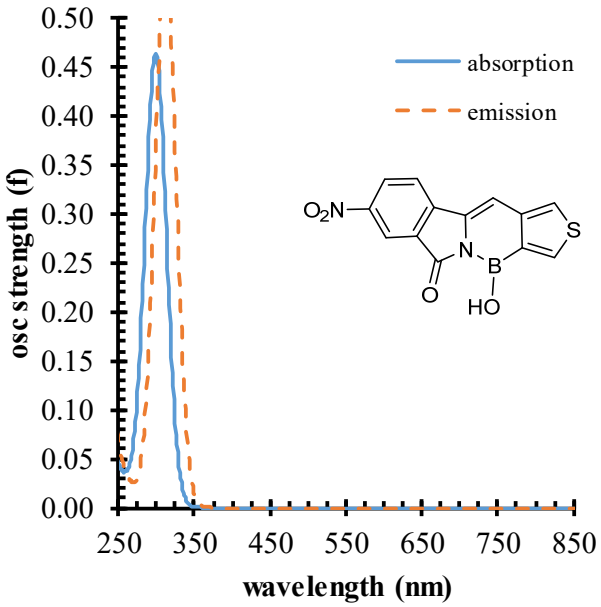
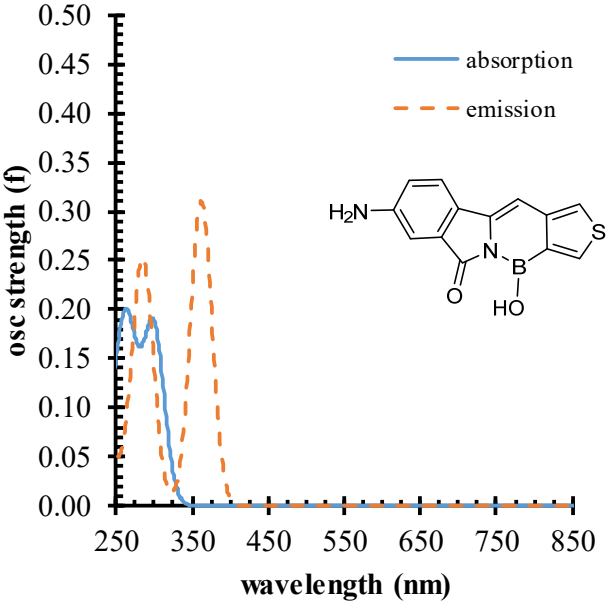
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
osc strength (f)
absorption
emission
250 350 450 550 650 750 850
wavelength (nm)
S
N
B
O
HO


0.50
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
osc strength (f)
absorption
emission
250 350 450 550 650 750 850
wavelength (nm)
Br
S
N
B
O
HO

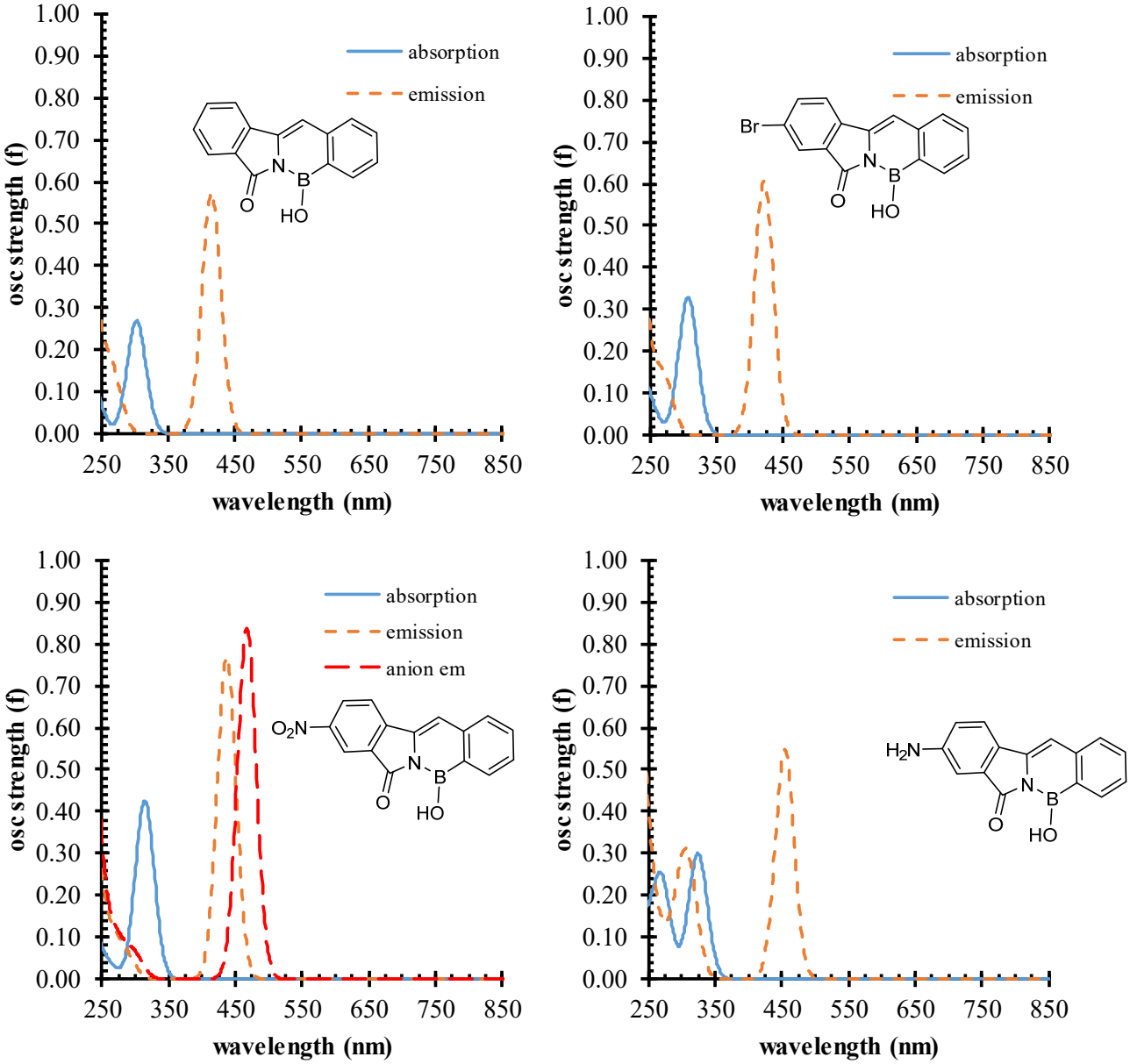

0.50
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
osc strength (f)
absorption
emission
250 350 450 550 650 750 850
wavelength (nm)
O2N
S
N
B
O
HO

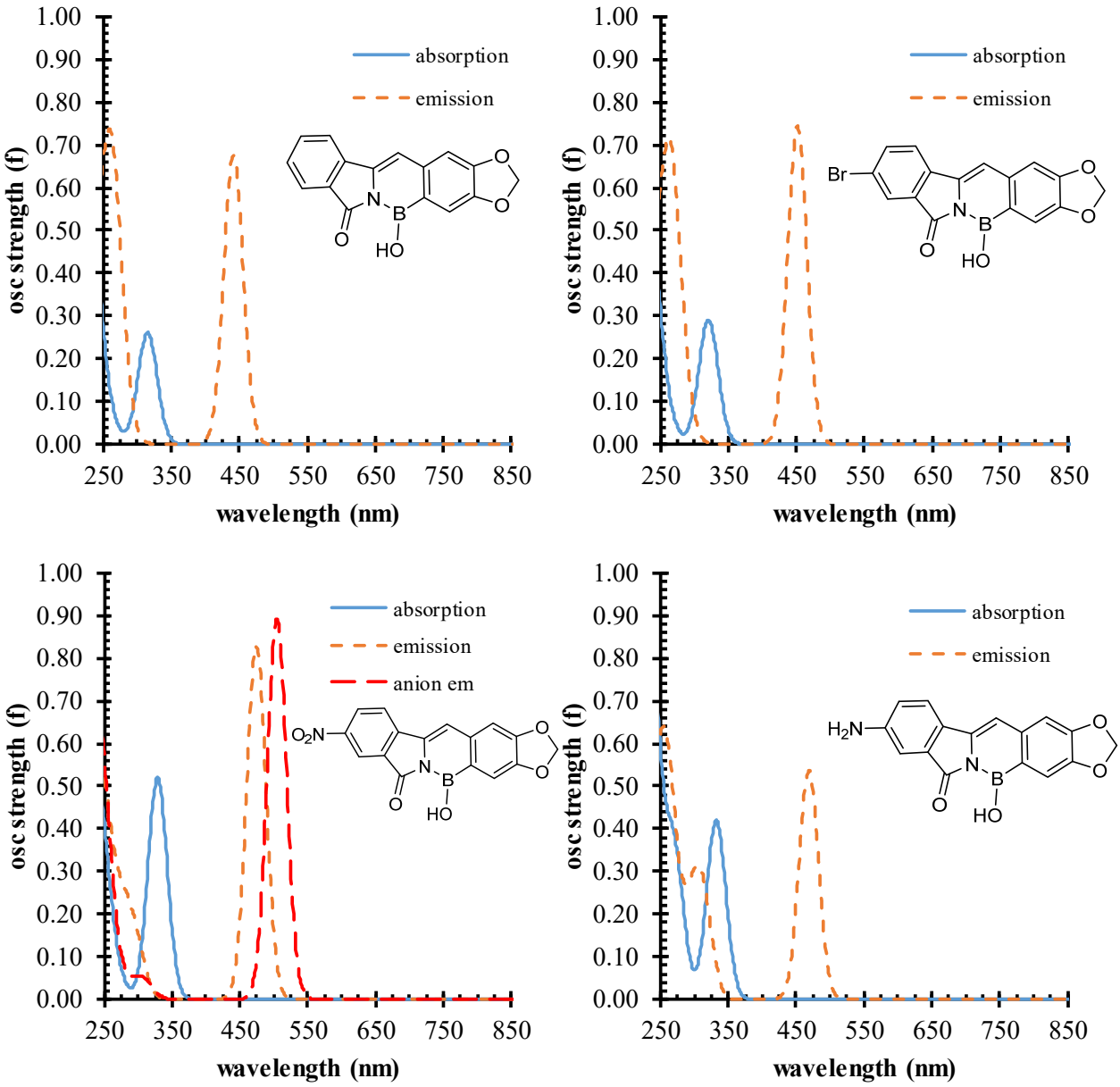

0.50
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
osc strength (f)
absorption
emission
250 350 450 550 650 750 850
wavelength (nm)
H2N
S
N
B
O
HO

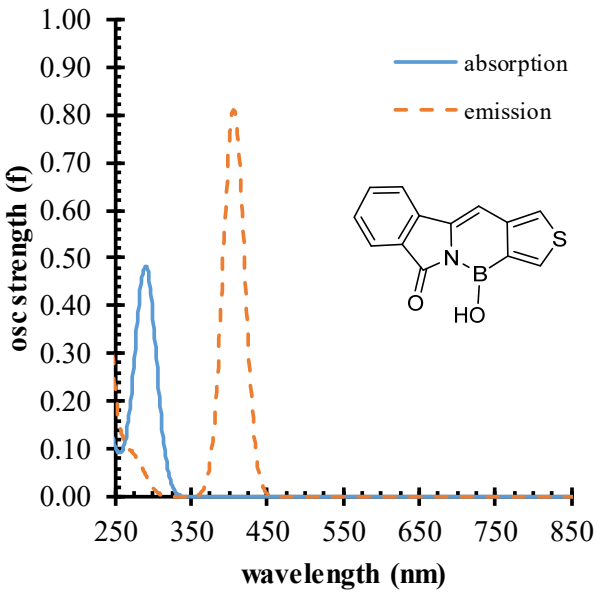
Simulated spectra for acetonitrile solvent

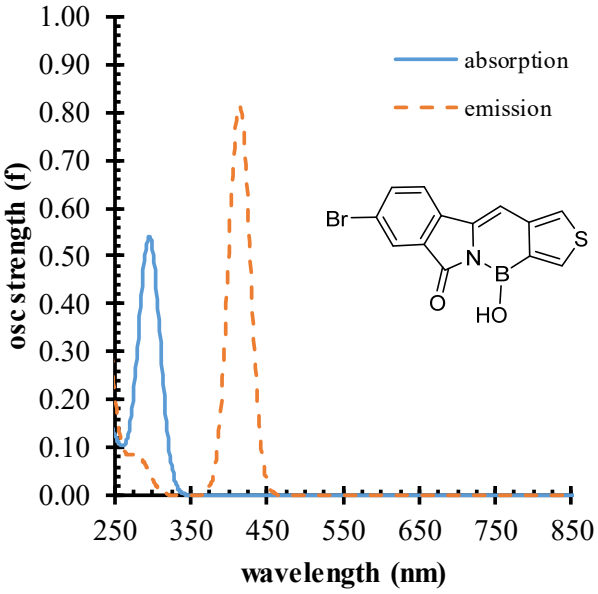
Absorption spectra obtained from LR-SMD-TD-LC-ωHPBE/BS1//LC-ωHPBE/BS1

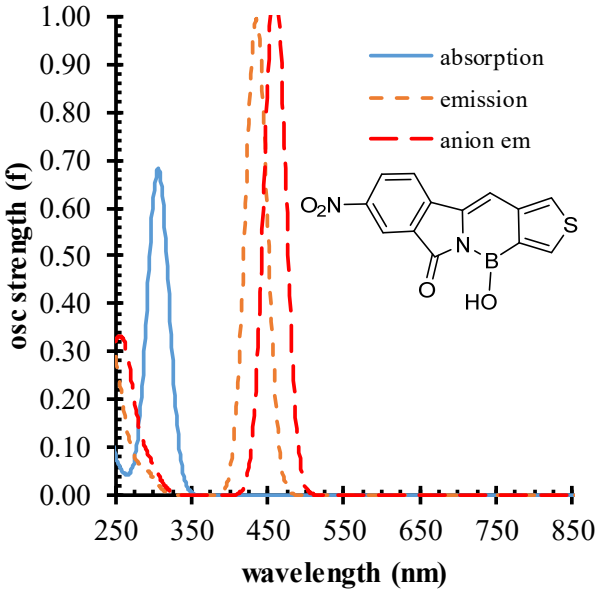
Emission spectra obtained from LR-SMD-TD-LC-ωHPBE/BS1

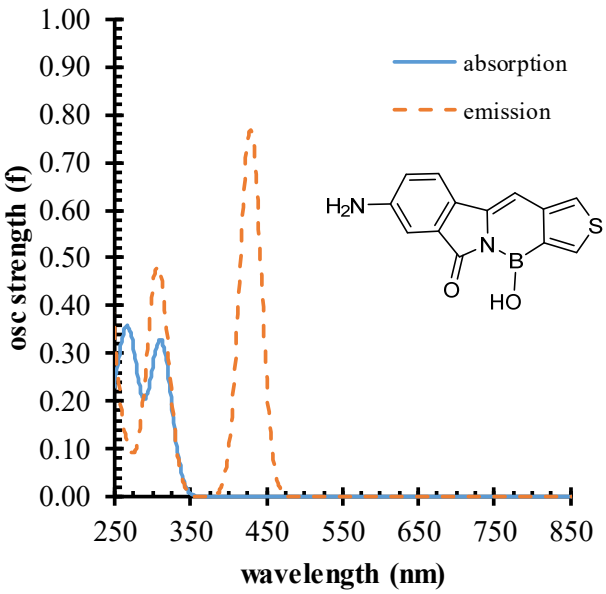



1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
osc strength (f)
250
350
450
550
650
750
850
wavelength (nm)
absorption
emission
anion em
Br
O2N
H2N
N
B
O
HO

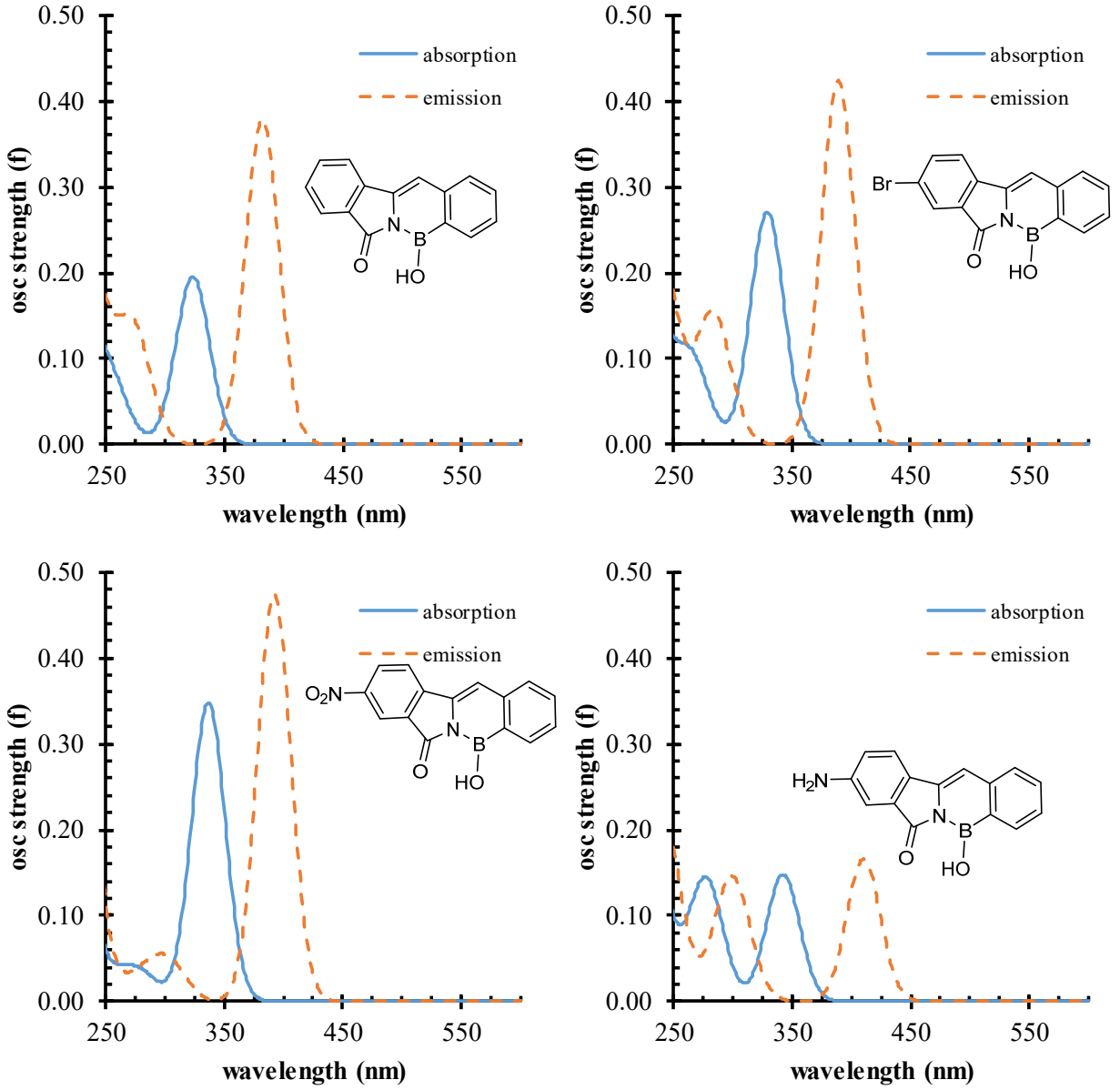

1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
osc strength (f)
250 350 450 550 650 750 850
wavelength (nm)
absorption
emission
S
N
B
O
HO

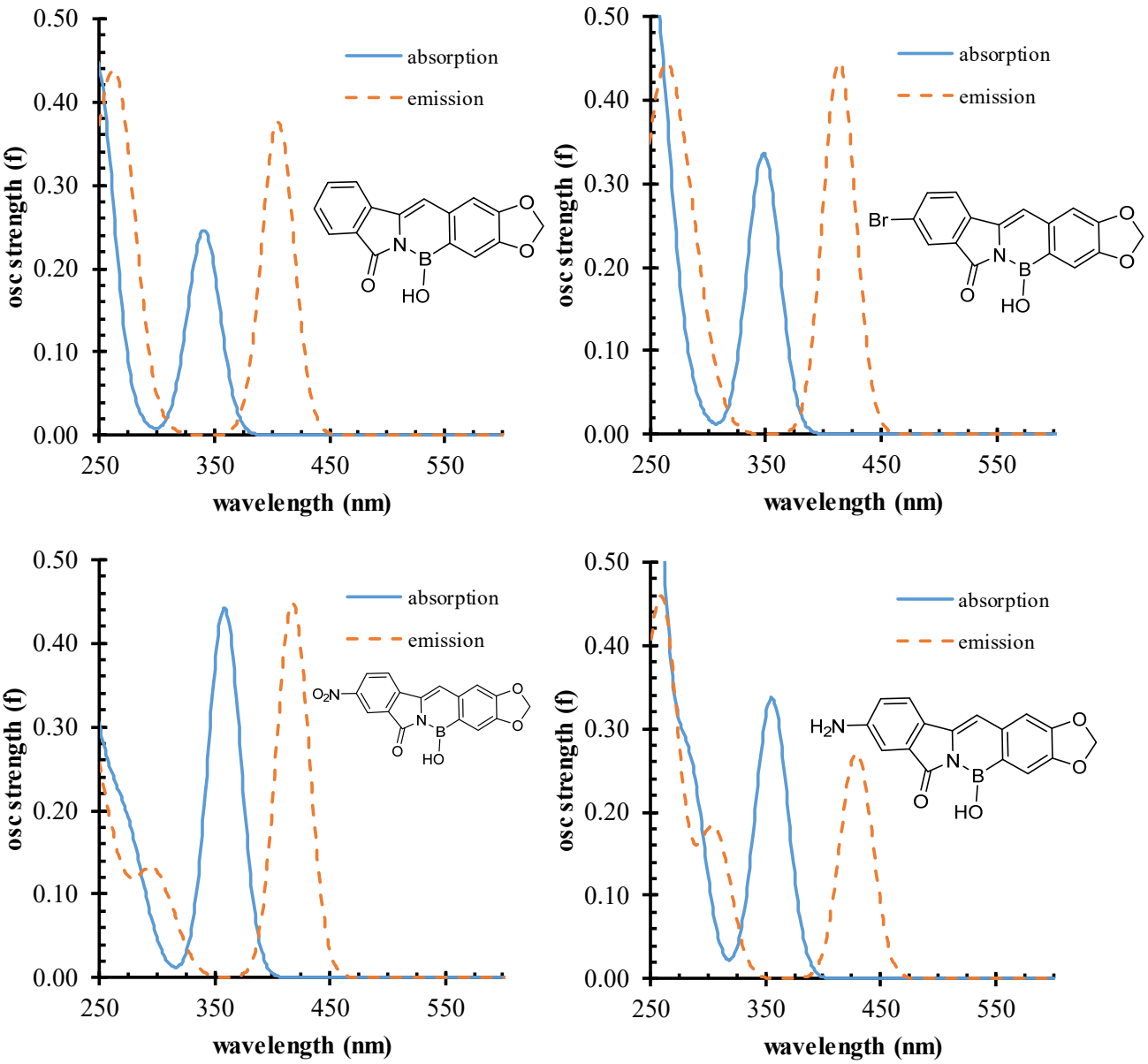

1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
osc strength (f)
250 350 450 550 650 750 850
wavelength (nm)
absorption
emission
Br
S
N
B
O
HO

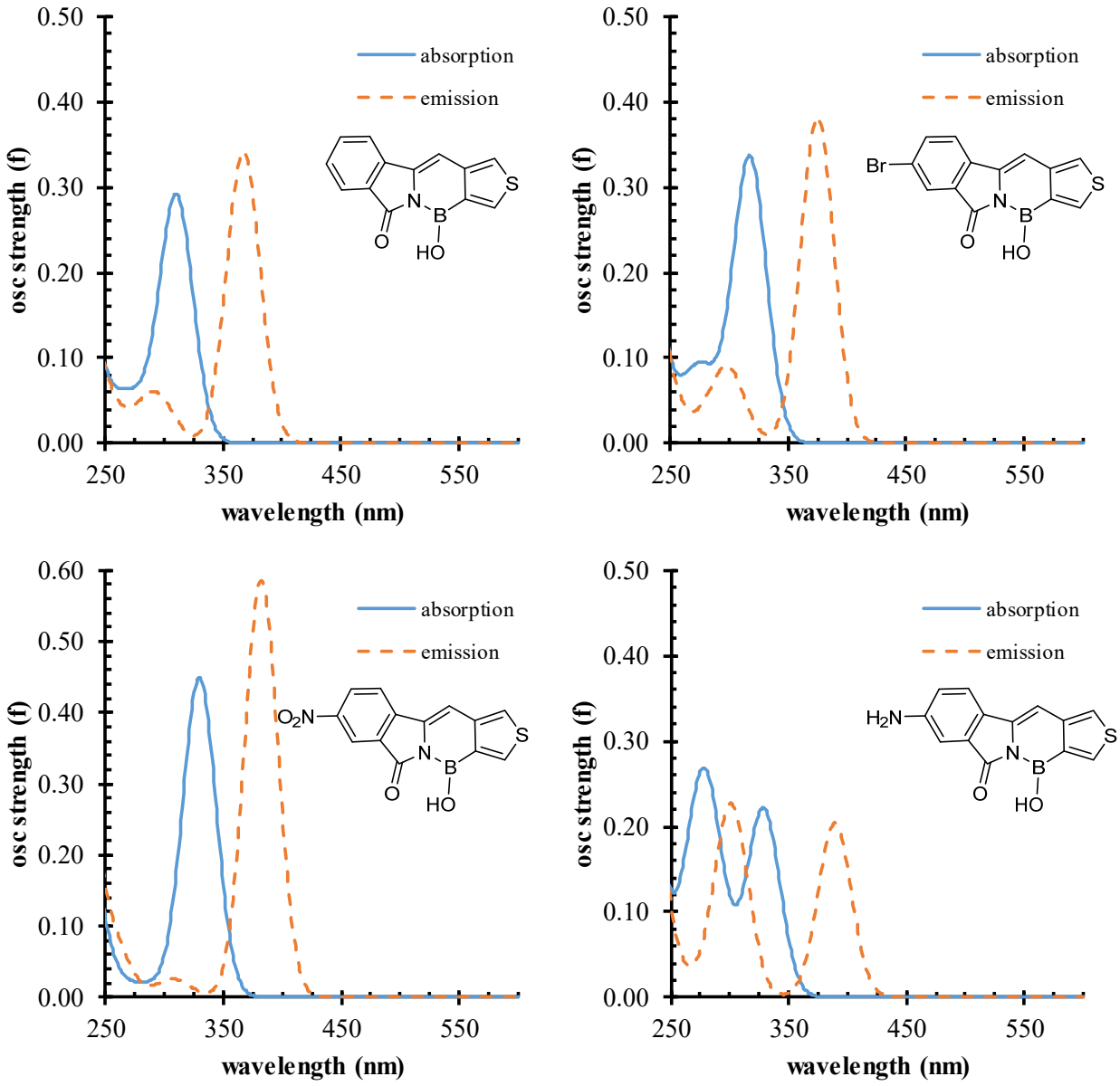

1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
osc strength (f)
250 350 450 550 650 750 850
wavelength (nm)
absorption
emission
anion em
O2N
S
N
B
O
HO


1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
osc strength (f)
250 350 450 550 650 750 850
wavelength (nm)
absorption
emission
H2N
S
N
B
O
HO

Simulated spectra from TD-ωB97xD/BS1//ωB97xD/BS1



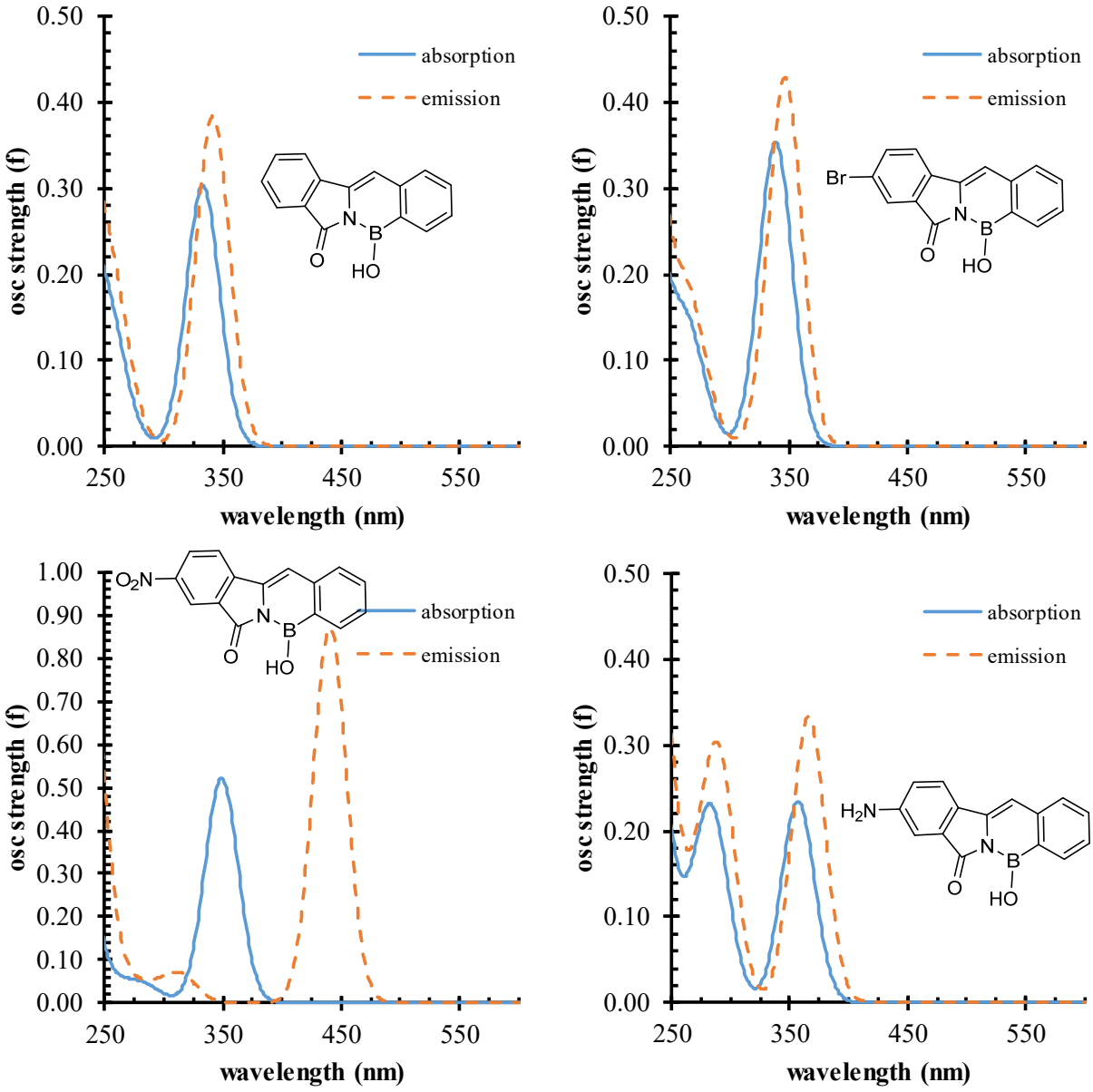

0.50
0.40
0.30
0.20
0.10
0.00
osc strength (f)
250
350
450
550
wavelength (nm)
absorption
emission
O
N
B
HO
Br
O2N
H2N

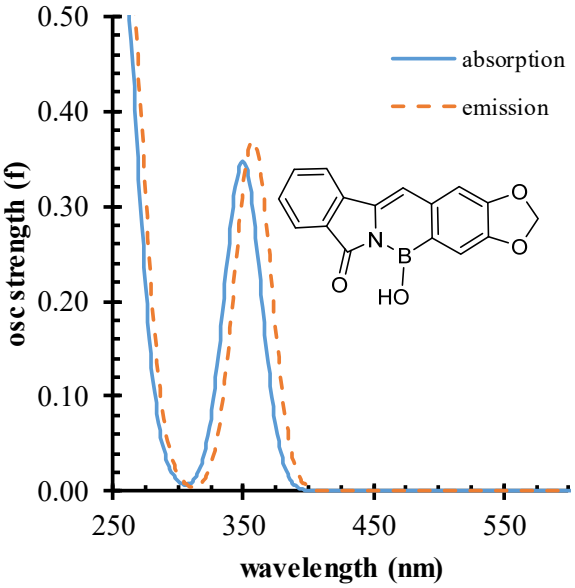

0.50
0.40
0.30
0.20
0.10
0.00
osc strength (f)
250
350
450
550
wavelength (nm)
absorption
emission
O
N
B
HO
S
Br
O2N
H2N
0.60

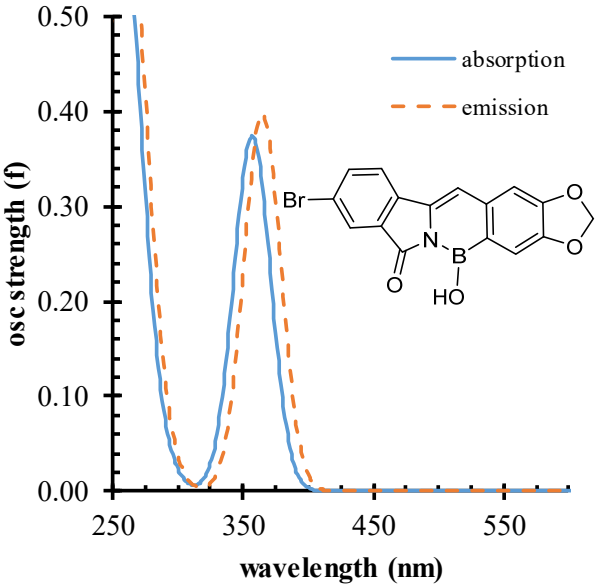
Simulated spectra for chloroform solvent

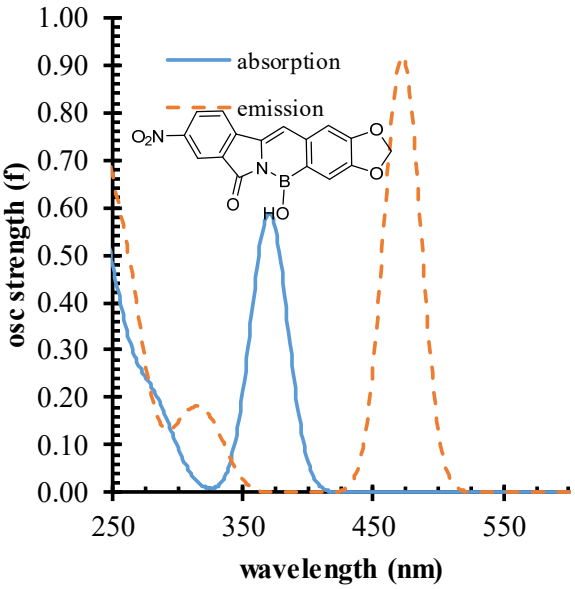
Absorption spectra obtained from LR-SMD-TD-ωB97xD/BS1//ωB97xD/BS1

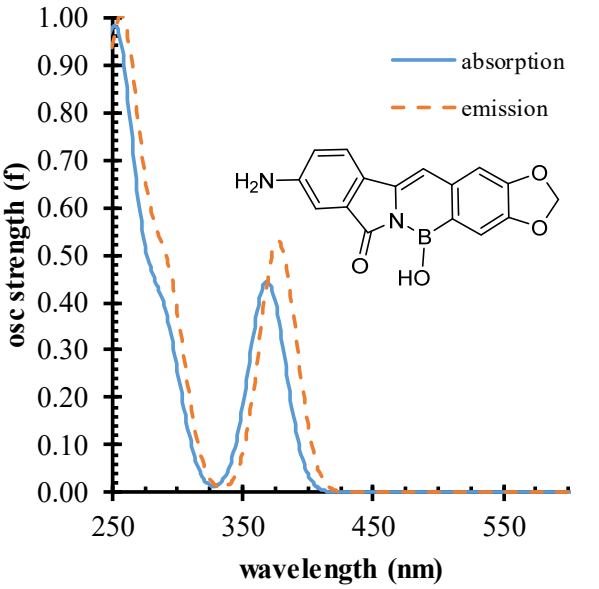
Emission spectra obtained from LR-SMD-TD-ωB97xD/BS1

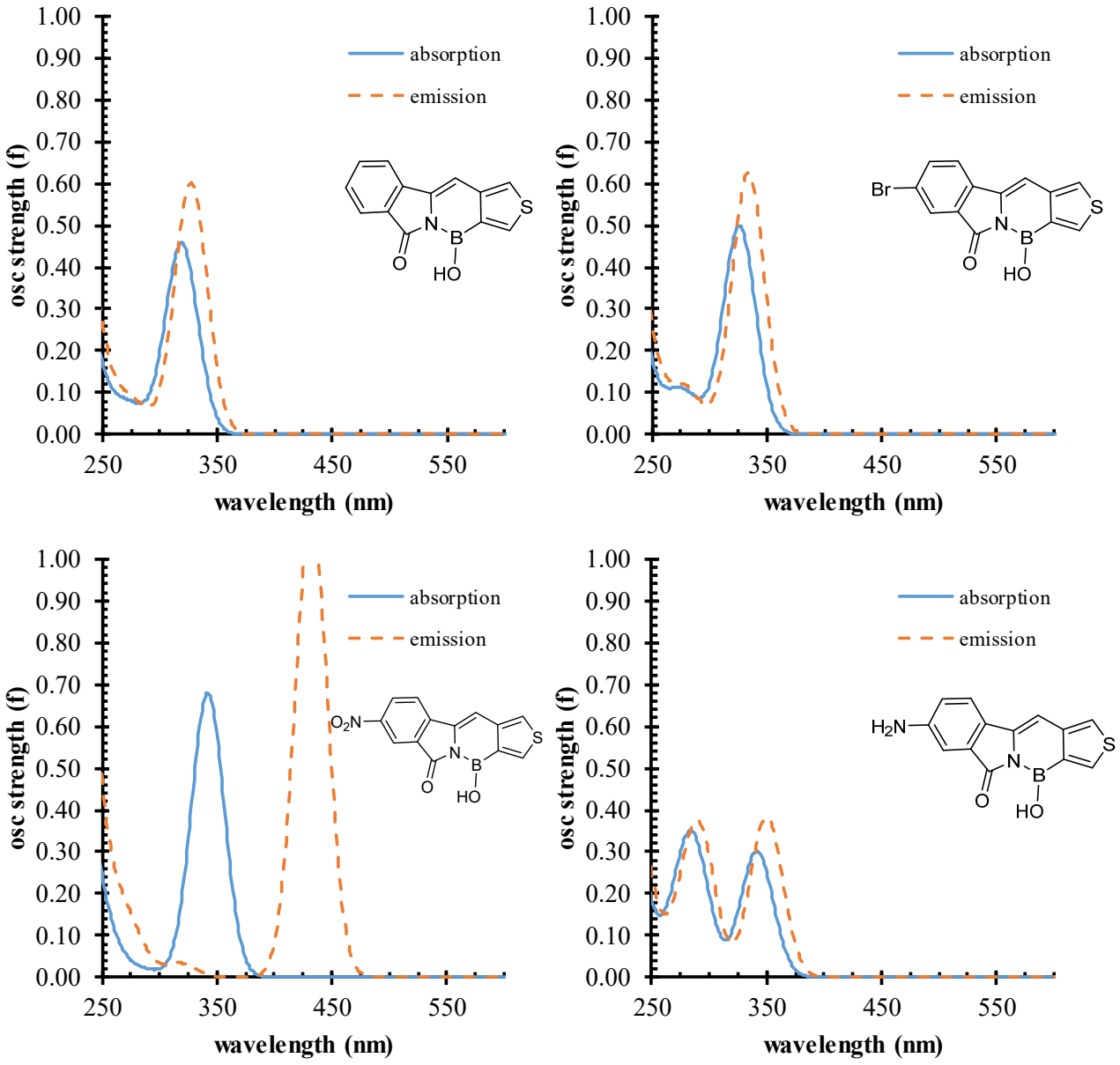



0.50
0.40
0.30
0.20
0.10
0.00
osc strength (f)
absorption
emission
250
350
450
550
wavelength (nm)
O
N
B
HO
O
O


0.50
0.40
0.30
0.20
0.10
0.00
osc strength (f)
absorption
emission
250
350
450
550
wavelength (nm)
Br
O
N
B
HO
O
O


1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
osc strength (f)
absorption
emission
250
350
450
550
wavelength (nm)
O2N
O
N
B
HO
O
O

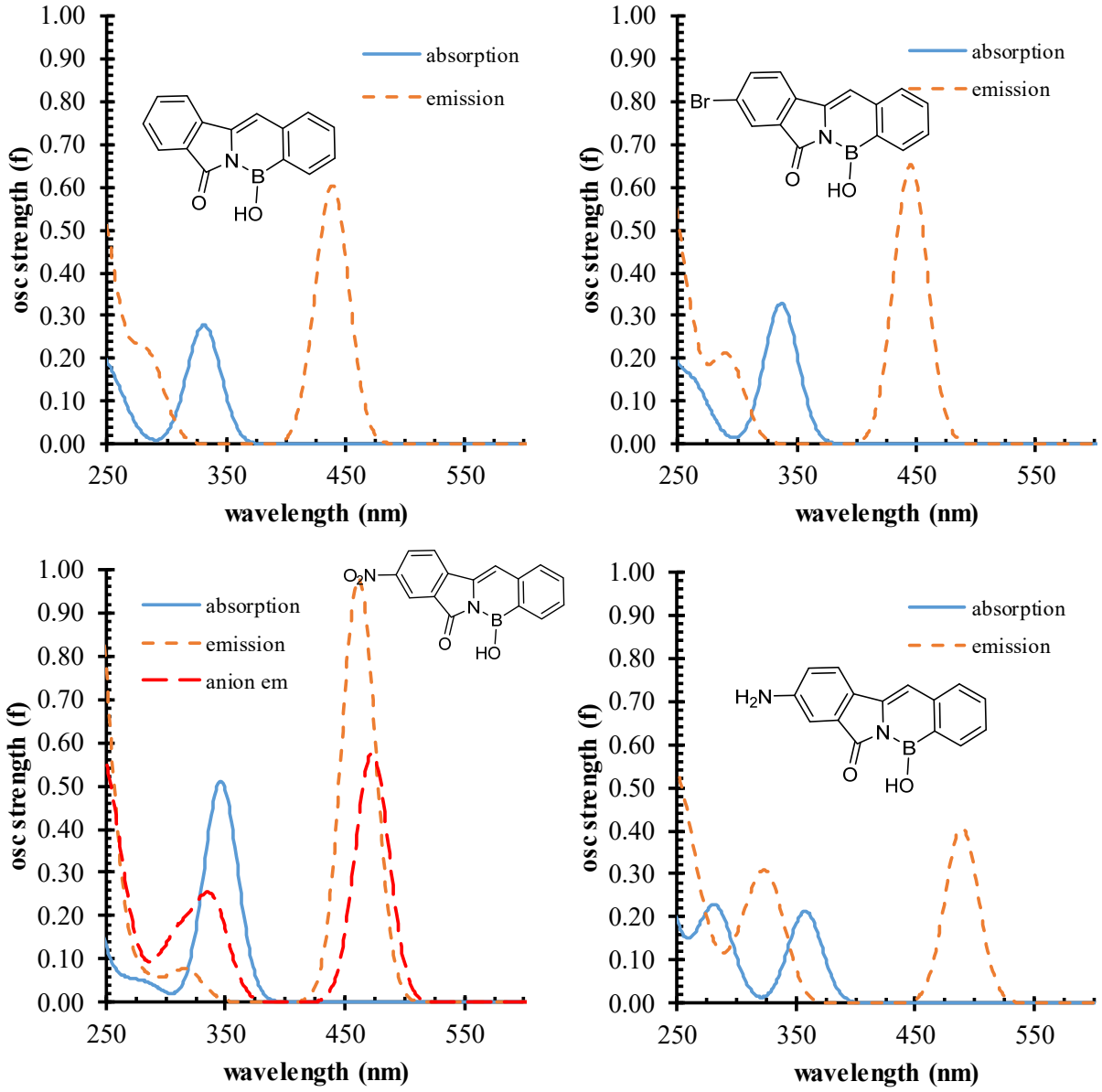

1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
osc strength (f)
absorption
emission
250
350
450
550
wavelength (nm)
H2N
O
N
B
HO
O
O

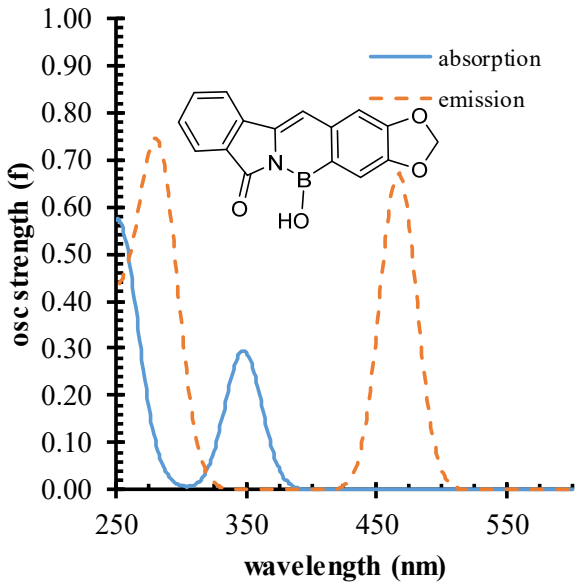

1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
osc strength (f)
250
350
450
550
wavelength (nm)
absorption
emission
O
N
B
HO
S
Br
O2N
H2N

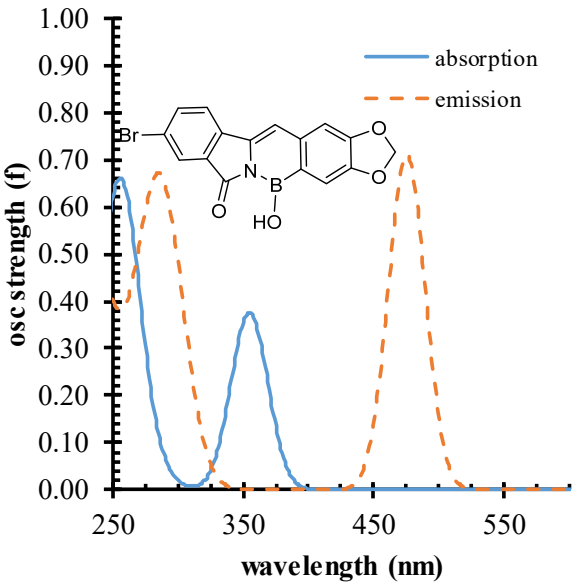
Simulated spectra for acetonitrile solvent

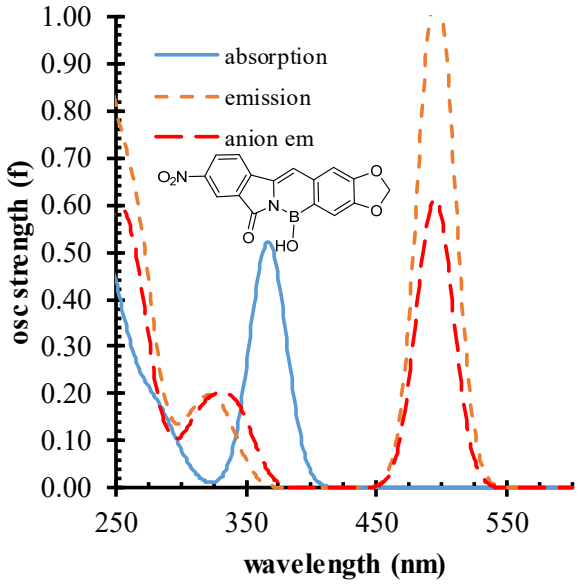
Absorption spectra obtained from LR-SMD-TD-ωB97xD/BS1//ωB97xD/BS1

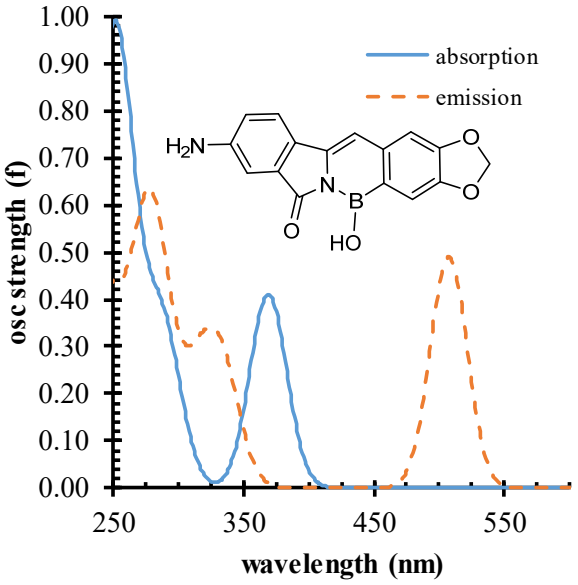
Emission spectra obtained from LR-SMD-TD-ωB97xD/BS1

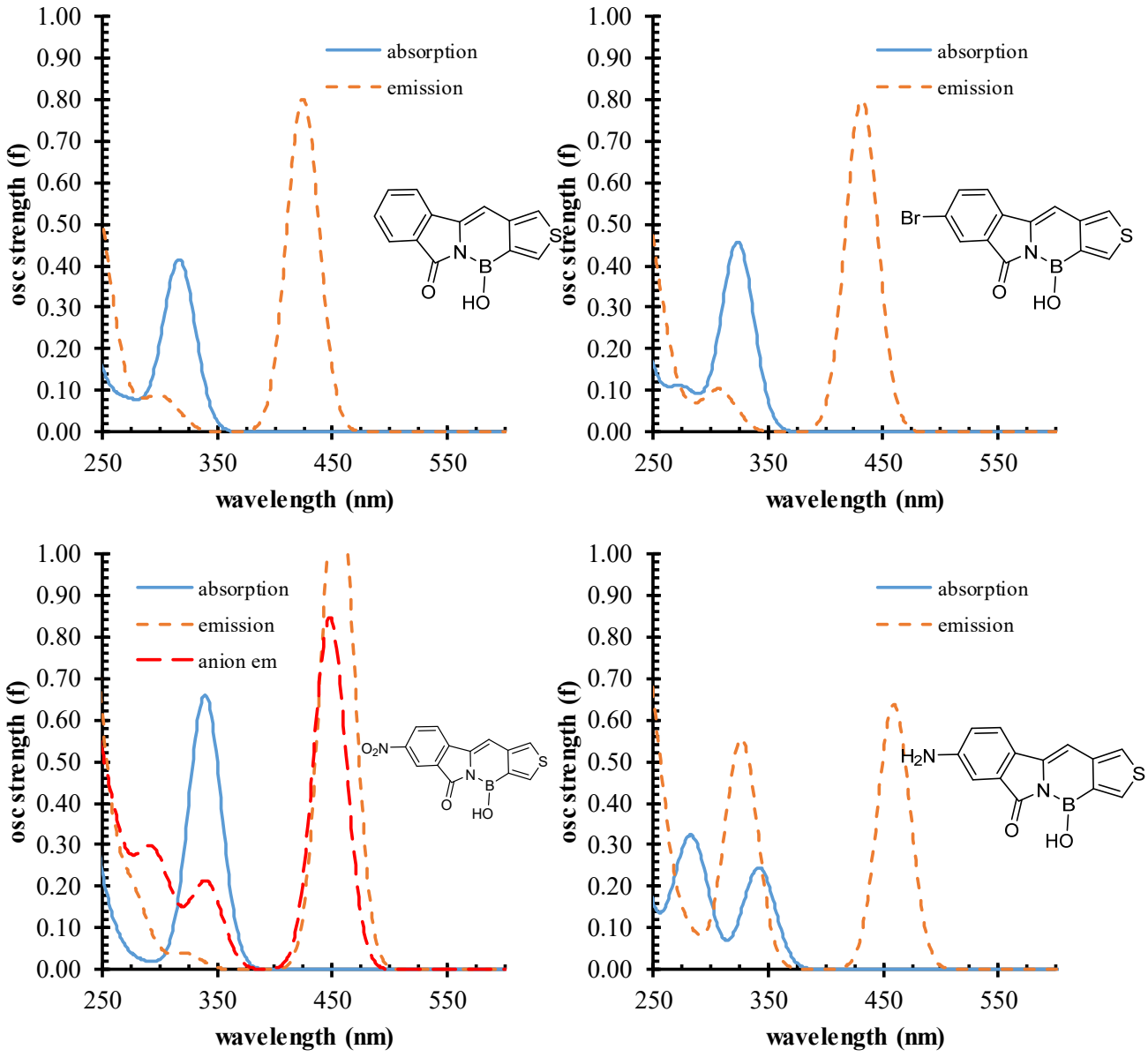



absorption
emission
osc strength (f)
wavelength (nm)
1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
250
350
450
550
O
N
B
HO
O
O

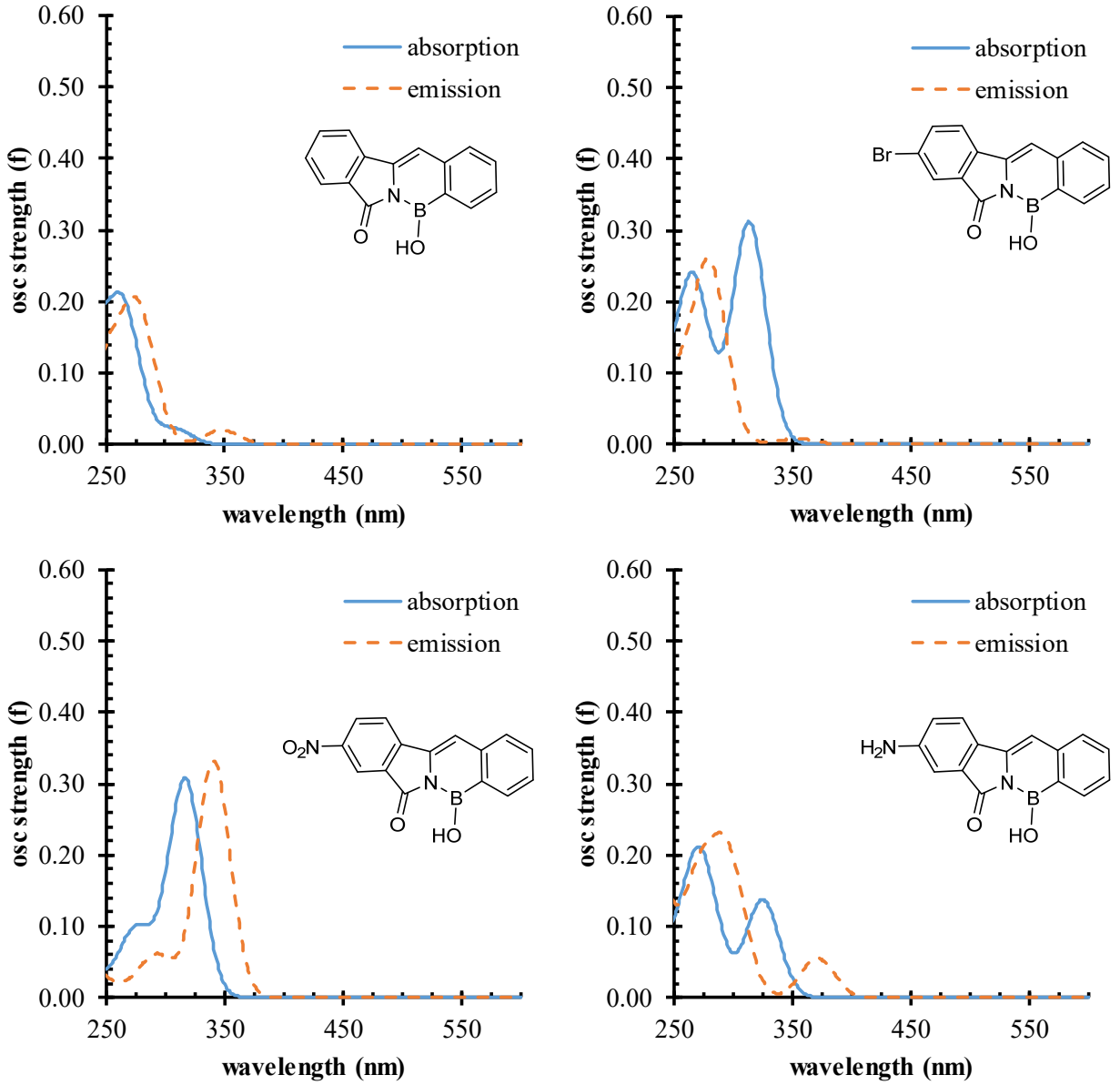

absorption
emission
osc strength (f)
wavelength (nm)
1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
250
350
450
550
Br
O
N
B
HO
O
O

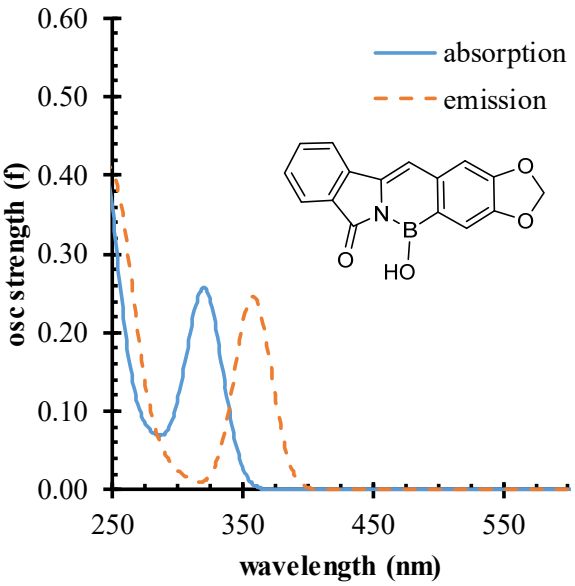

absorption
emission
anion em
osc strength (f)
wavelength (nm)
1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
250
350
450
550
O2N
O
N
B
HO
O
O

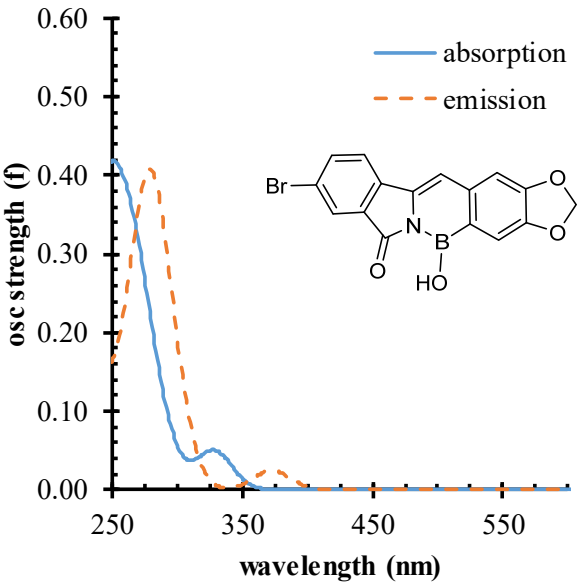

absorption
emission
osc strength (f)
wavelength (nm)
1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
250
350
450
550
H2N
O
N
B
HO
O
O


1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
osc strength (f)
250
350
450
550
wavelength (nm)
absorption
emission
anion em
Br
O2N
H2N
N
B
HO
O
S

Simulated spectra from EOM-CCSD/BS2//B3LYP/BS1




0.60
0.50
0.40
0.30
0.20
0.10
0.00
osc strength (f)
absorption
emission
250
350
450
550
wavelength (nm)
O
N
B
HO
O
O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0.40
0.30
0.20
0.10
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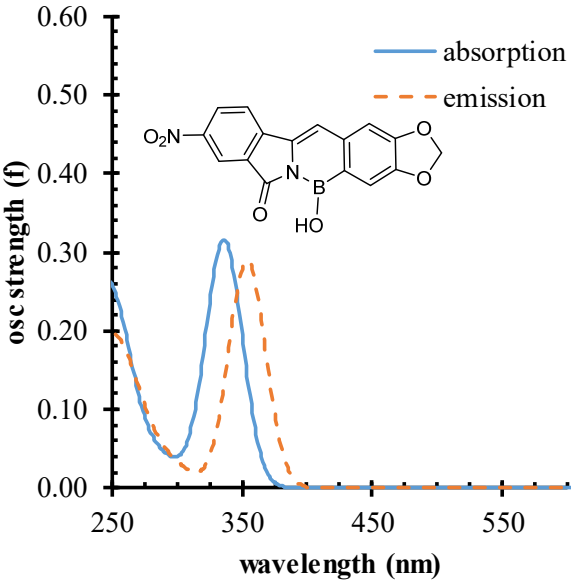
osc strength (f)
absorption
emission
250
350
450
550
wavelength (nm)
Br
O
N
B
HO
O
O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0.40
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absorption
emission
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450
550
wavelength (nm)
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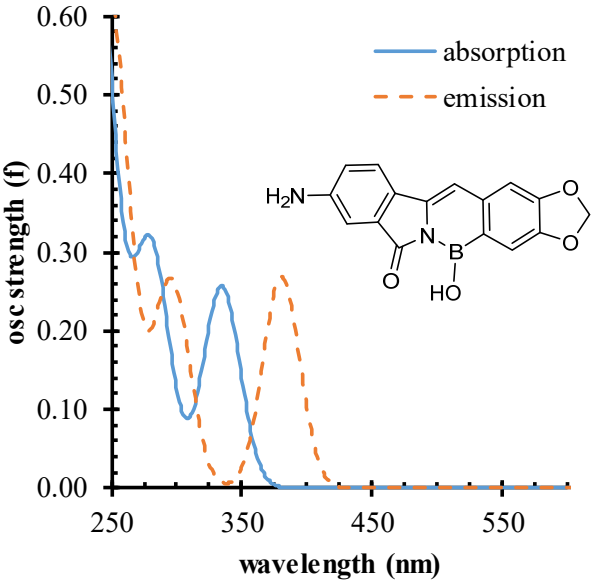
O
N
B
HO
O
O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osc strength (f)
absorption
emission
250
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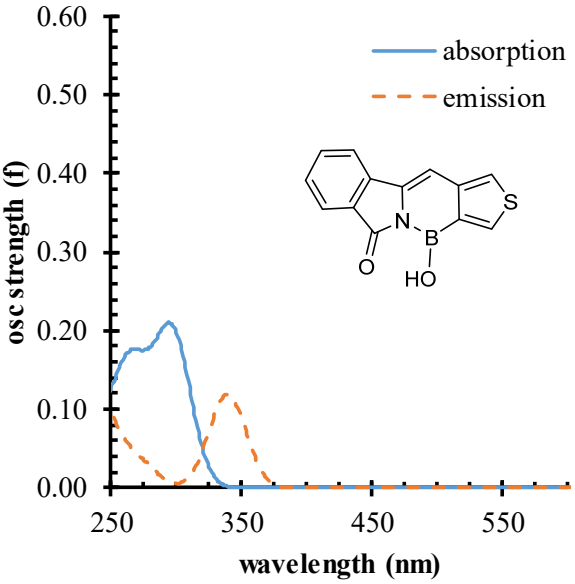
450
550
wavelength (nm)
H2N
O
N
B
HO
O
O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osc strength (f)
absorption
emission
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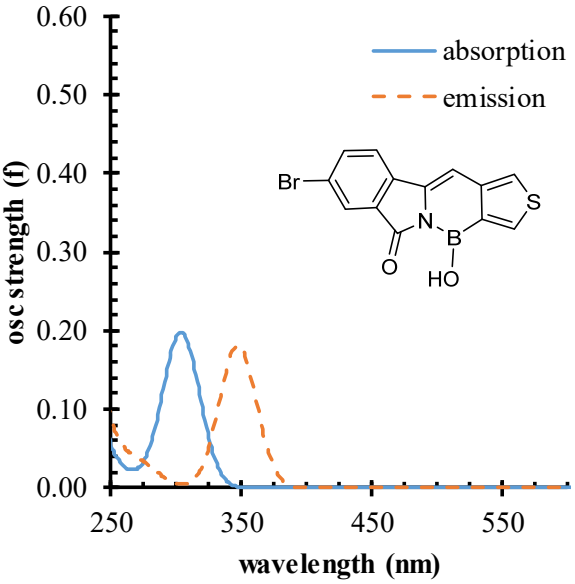
350
450
550
wavelength (nm)
O
N
B
HO
S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absorption
emission
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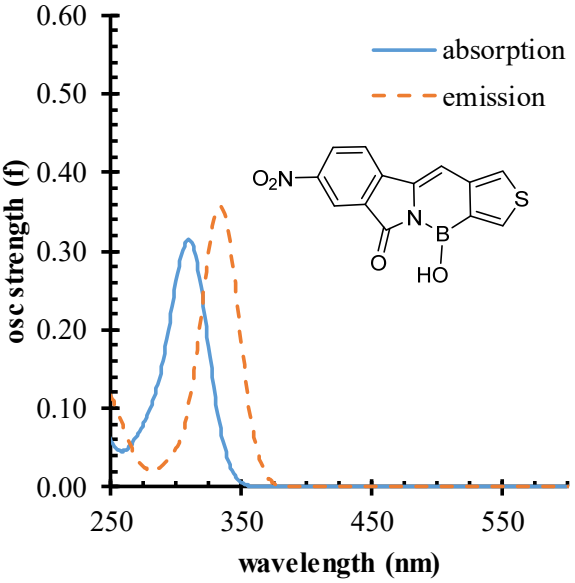
450
550
wavelength (nm)
Br
O
N
B
HO
S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osc strength (f)
absorption
emission
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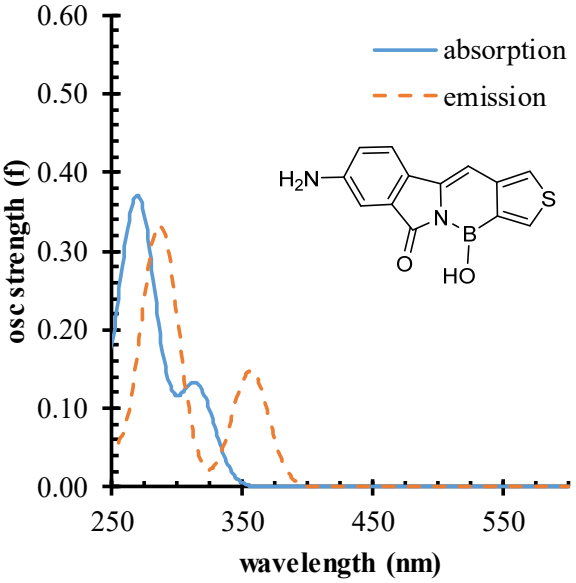
350
450
550
wavelength (nm)
O2N
O
N
B
HO
S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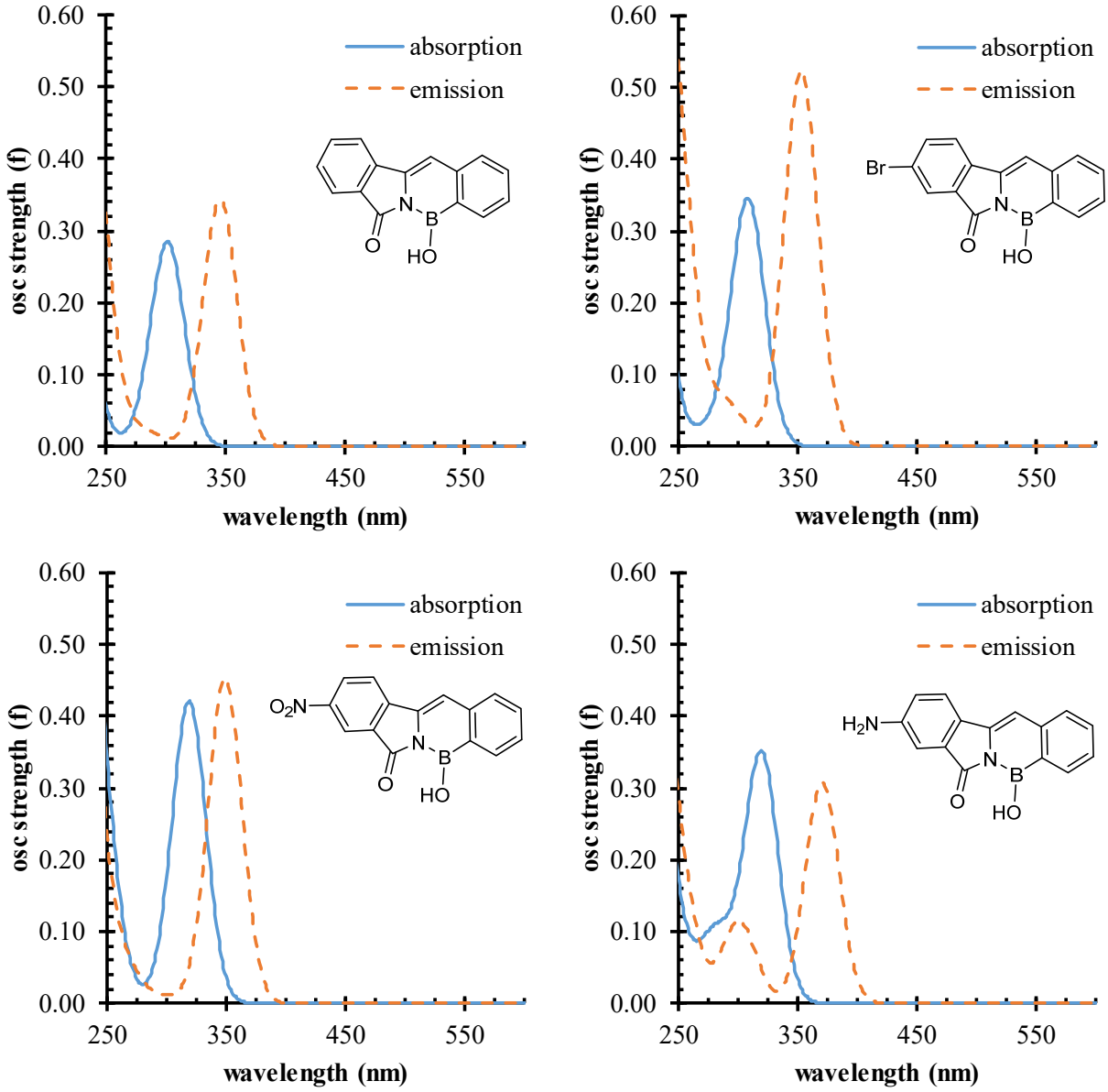
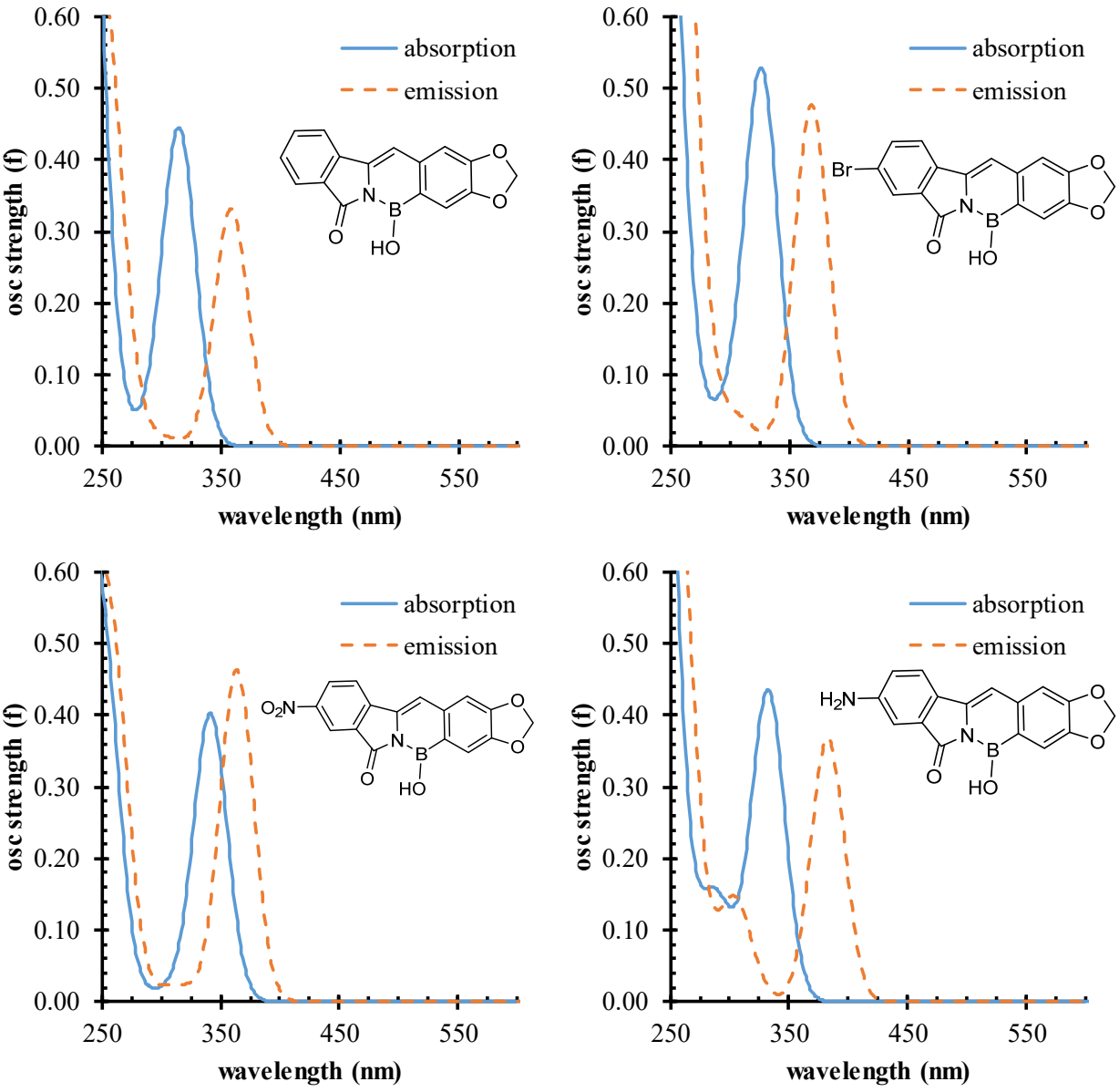
0.20
0.10
0.00
osc strength (f)
absorption
emission
250
350
450
550
wavelength (nm)
H2N
O
N
B
HO
S

Simulated spectra from CIS(D)/BS2//B3LYP/BS1

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0.50
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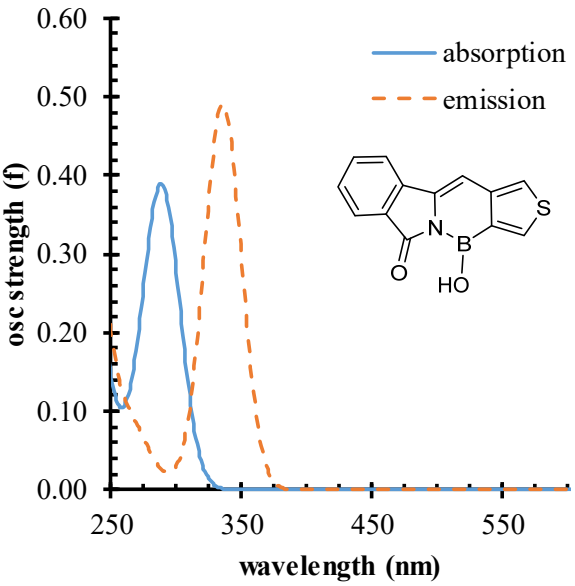
0.20
0.10
0.00
osc strength (f)
250
350
450
550
wavelength (nm)
absorption
emission
O
N
B
HO
O
O
Br
O2N
H2N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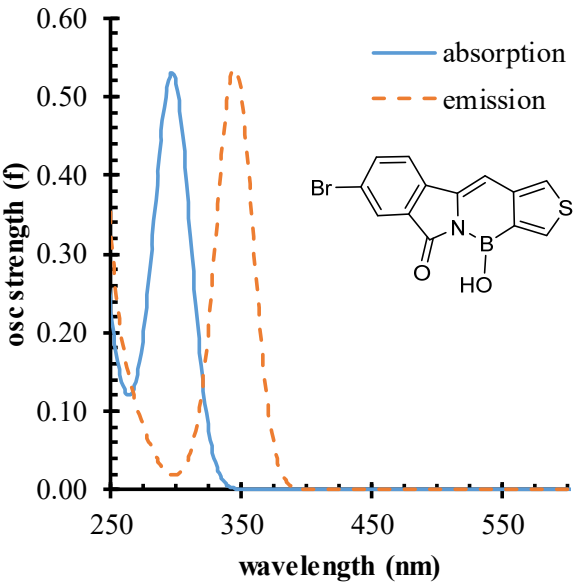
0.50
0.40
0.30
0.20
0.10
0.00
osc strength (f)
absorption
emission
250
350
450
550
wavelength (nm)
S
N
B
O
HO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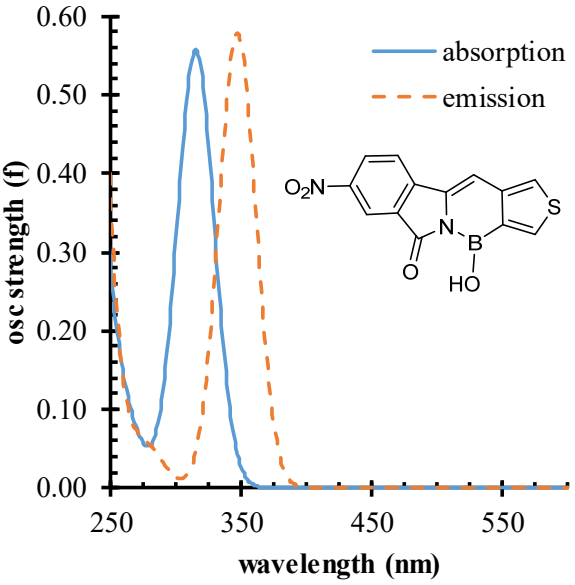
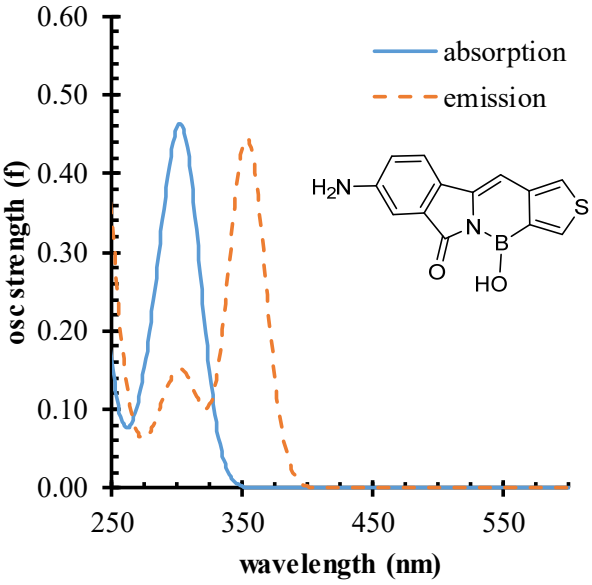
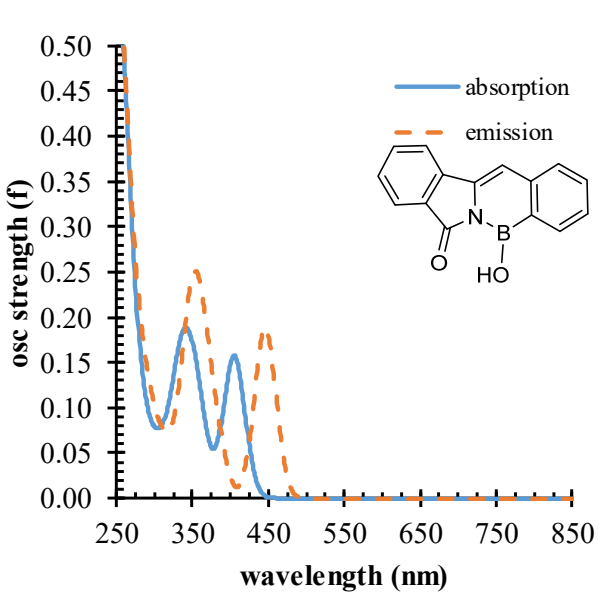
0.50
0.40
0.30
0.20
0.10
0.00
osc strength (f)
absorption
emission
250
350
450
550
wavelength (nm)
Br
S
N
B
O
HO

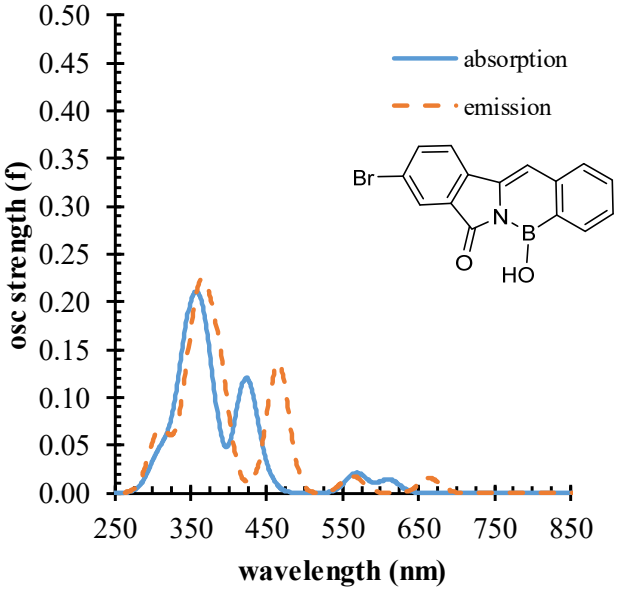

0.60
0.50
0.40
0.30
0.20
0.10
0.00
osc strength (f)
absorption
emission
250
350
450
550
wavelength (nm)
O2N
S
N
B
O
HO

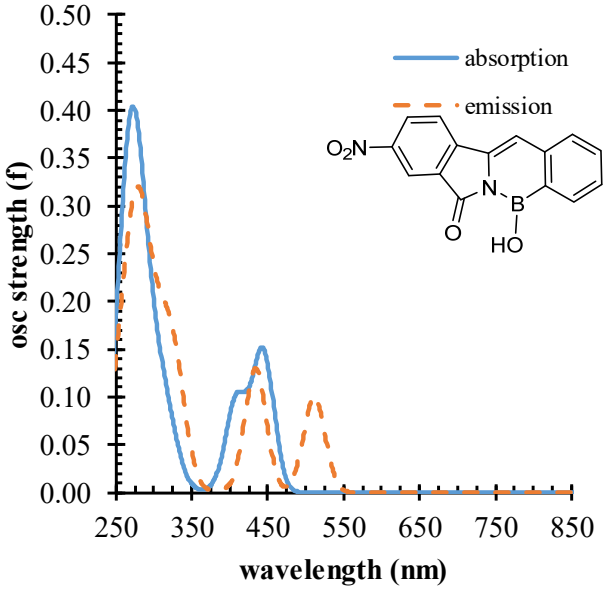

0.60
0.50
0.40
0.30
0.20
0.10
0.00
osc strength (f)
absorption
emission
250
350
450
550
wavelength (nm)
H2N
S
N
B
O
HO

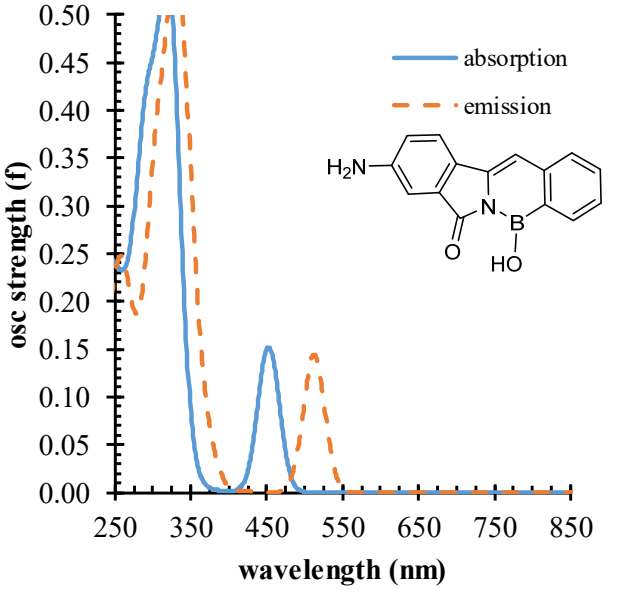
Simulated spectra from BNLLYP/BS1//B3LYP/BS1

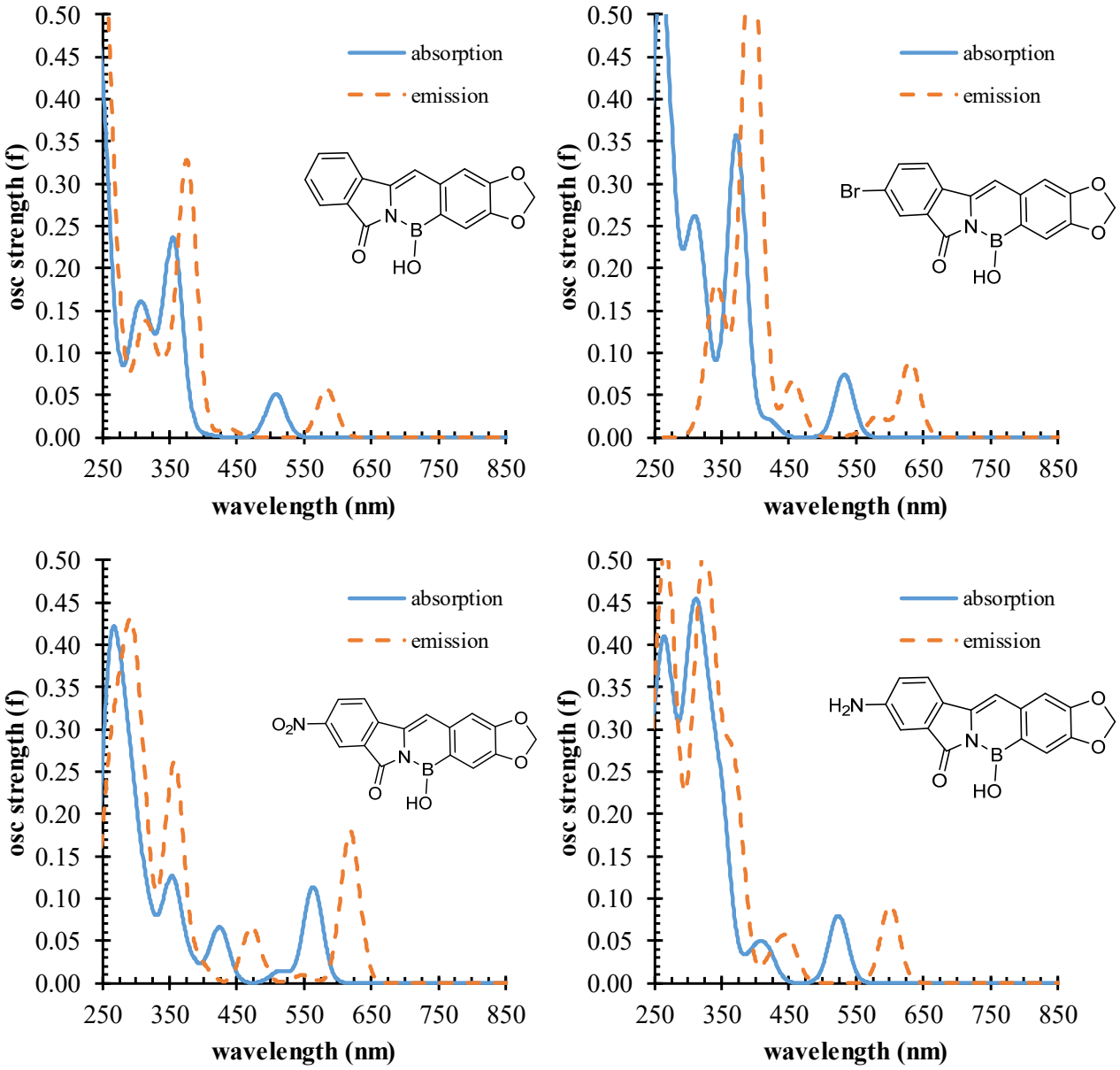
Another methodology that has been previously shown to provide "better" performance for CT excitations is the BNL functional.[1] For the sake of curiosity, we attempted BNLLYP/BS1//B3LYP/BS1 single-point computations to test for agreement with previous data. These single-point computations were carried out in QChem-5.2.2[2] using the SG2 integration grid, the SR_LDA (BNL) exchange functional and the LYP[3] correlation functional [BNLLYP] with the BS1 basis set previously described. The first 30 singlet excited states were solved iteratively and the spectra simulated using the previously described methodology. The simulated absorption and emission spectrum from this methodology are shown below.

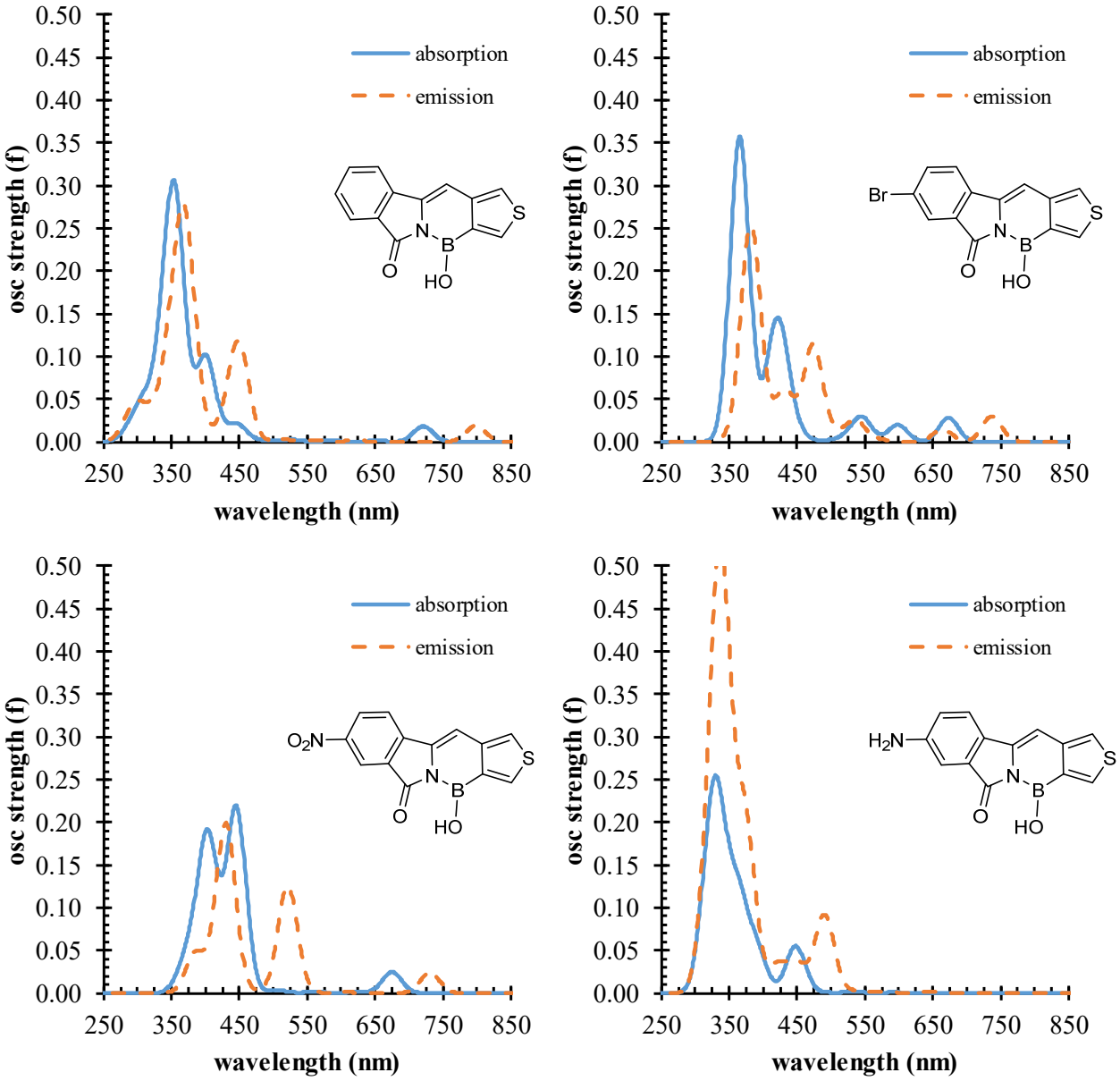

absorption
emission
osc strength (f)
wavelength (nm)
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35
0.40
0.45
0.50
250
350
450
550
650
750
850
N
B
O
HO


absorption
emission
osc strength (f)
wavelength (nm)
Br
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35
0.40
0.45
0.50
250
350
450
550
650
750
850
N
B
O
HO

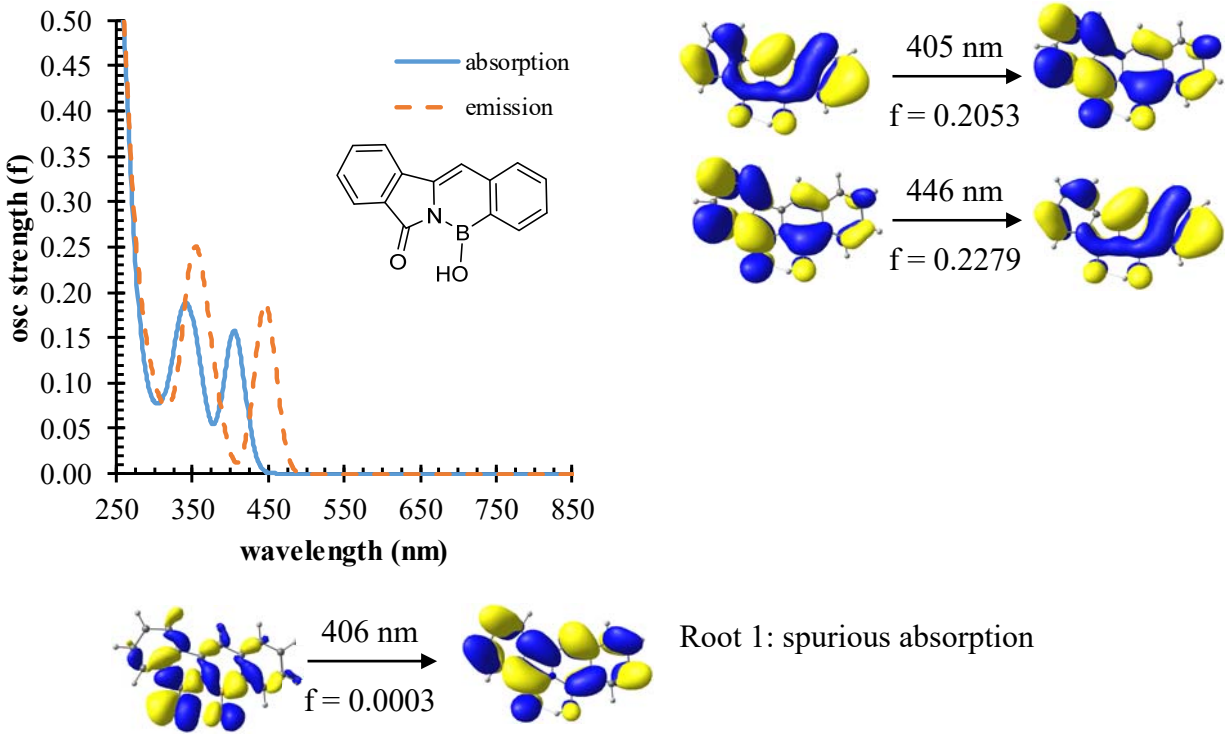

absorption
emission
osc strength (f)
wavelength (nm)
O2N
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35
0.40
0.45
0.50
250
350
450
550
650
750
850
N
B
O
HO


absorption
emission
osc strength (f)
wavelength (nm)
H2N
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35
0.40
0.45
0.50
250
350
450
550
650
750
850
N
B
O
HO


absorption
emission
osc strength (f)
wavelength (nm)
0.50
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
250
350
450
550
650
750
850
Br
O2N
H2N
N
B
HO
O

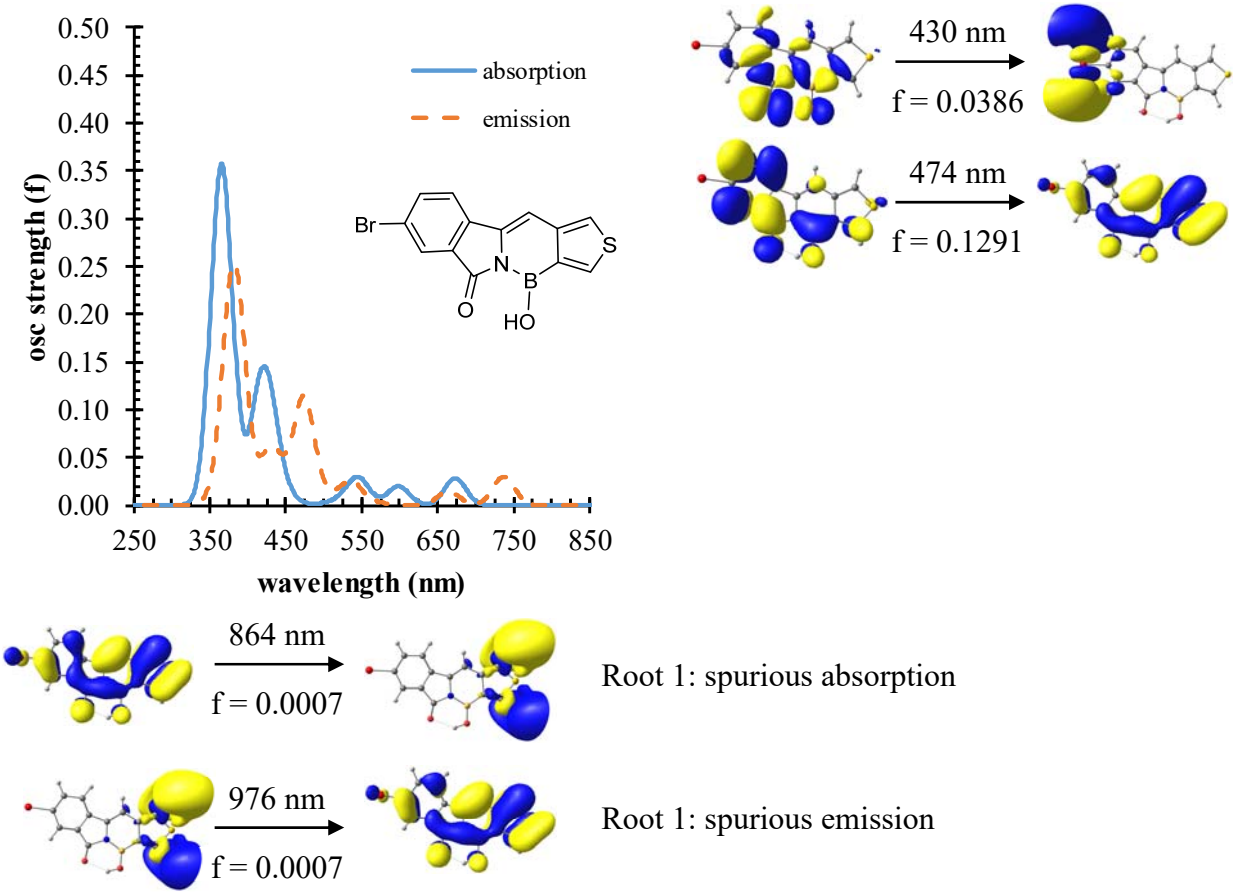

absorption
emission
osc strength (f)
wavelength (nm)
0.50
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
250
350
450
550
650
750
850
Br
O2N
H2N
N
B
O
HO
S

After running BNLLYP/BS1//B3LYP/BS1 single-point computations, the absorption and emission spectra shown above for some of the compounds started showing what appeared to be spurious excitations. Not only does this make the spectra look quite different than experiment, it also makes them rather difficult to properly analyze. Furthermore, there does not appear to be a clear pattern to which compounds are producing spurious excitations.



Root 1: spurious absorption

The absorption and emission maxima of compound **benzo** appear "normal." Checking the NTOs of the absorption and emission maxima show the expected LE character. However, in the case of the absorption, there is a spurious excitation with a low oscillator strength corresponding to root 1 as shown above. The spurious excitation represents absorption from what appears to be a σ* into the π*.



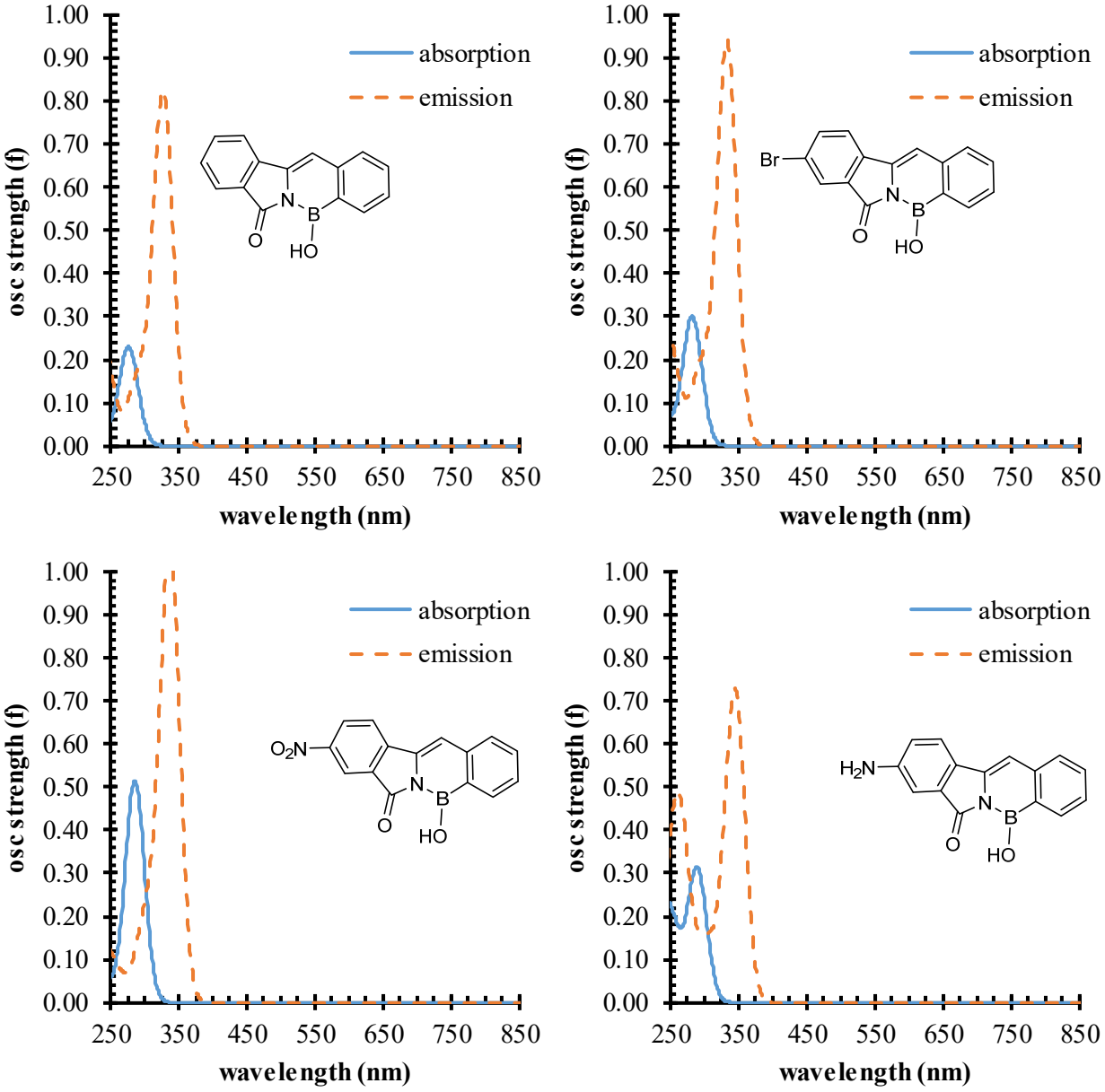
Root 1: spurious absorption

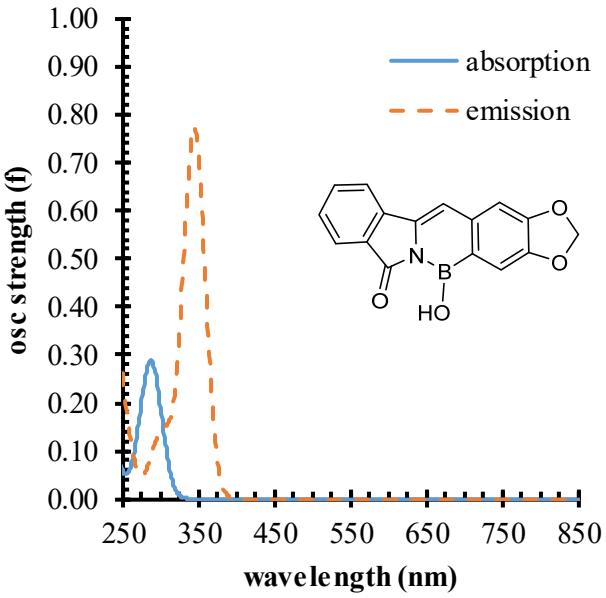
Root 1: spurious emission

The spectrum above for compound **7** represents one of the worst offenders of spurious excitations in both the absorption and emission maxima. Checking the NTOs of the first excitation with high oscillator strength (above) indicate the character of the "real" maxima. The absorption maximum is predicted to be Rydberg in character, a stark contrast from the consistent local excitation (LE) character predicted by every other method. The emission maximum appears to be consistent with the expected LE character, albeit with significant leaning towards the left-most phenyl ring. However, among the spurious excitations, the lowest singlet excitation represents what BNLLYP/BS1 predicts as the nature of the ES (*i.e.* is it a CT state, a LE state, etc.) The NTOs for Root 1 of the absorption and emission maxima are shown below the spectrum. These orbitals clearly demonstrates that BNL predicts the excited state to be Rydberg in character assuming Kasha's rule is followed. This prediction is not consistent with experimental observations, nor with EOM-CCSD computations.

Overall, it appears that BNLLYP/BS1//B3LYP/BS1 significantly overestimates the Rydberg character of the transitions. Additionally, for several of the spectra, there are numerous spurious excitations that are significantly red-shifted compared to experimental spectra.

Simulated spectra from TD-LRC-BOP/BS1//LRC-BOP/BS1

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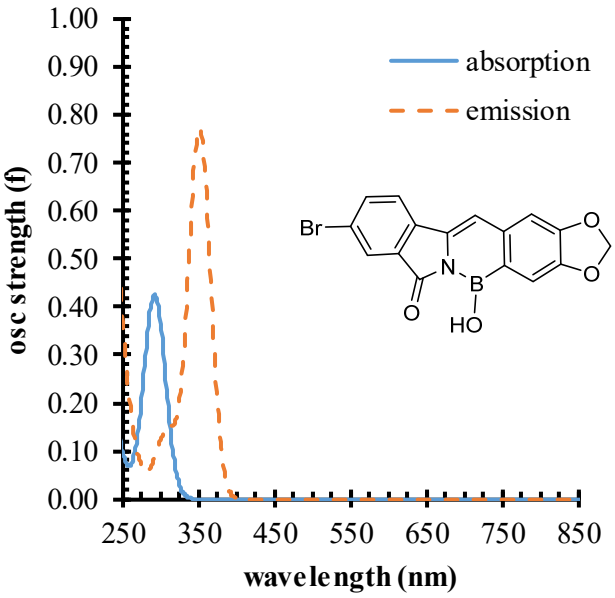
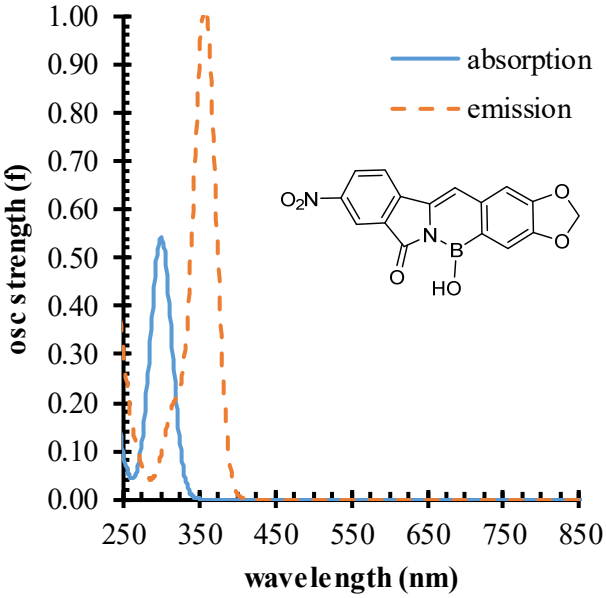
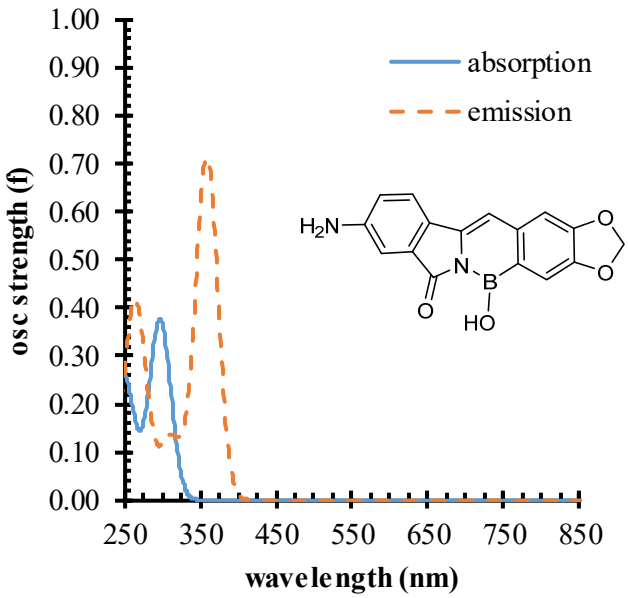
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
osc strength (f)
absorption
emission
250 350 450 550 650 750 850
wavelength (nm)
O
N
B
HO
O
O


1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
osc strength (f)
absorption
emission
250 350 450 550 650 750 850
wavelength (nm)
Br
O
N
B
HO
O
O


1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
osc strength (f)
absorption
emission
250 350 450 550 650 750 850
wavelength (nm)
O2N
O
N
B
HO
O
O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0.70
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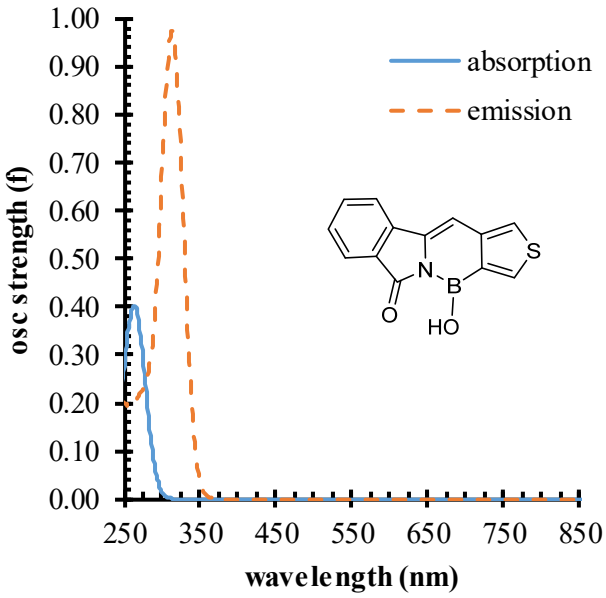
0.50
0.40
0.30
0.20
0.10
0.00
osc strength (f)
absorption
emission
250 350 450 550 650 750 850
wavelength (nm)
H2N
O
N
B
HO
O
O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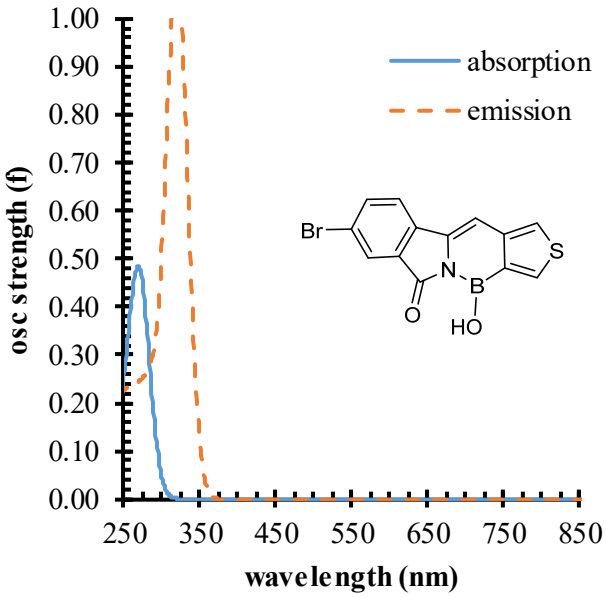
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
osc strength (f)
250 350 450 550 650 750 850
wavelength (nm)
absorption
emission
S
N
B
O
HO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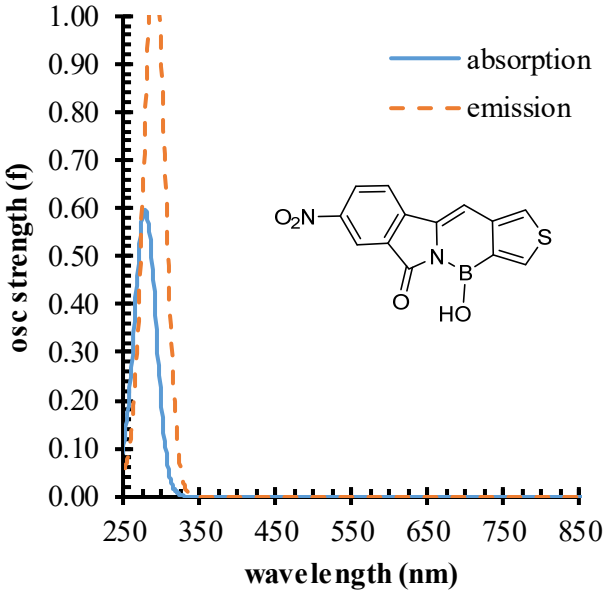
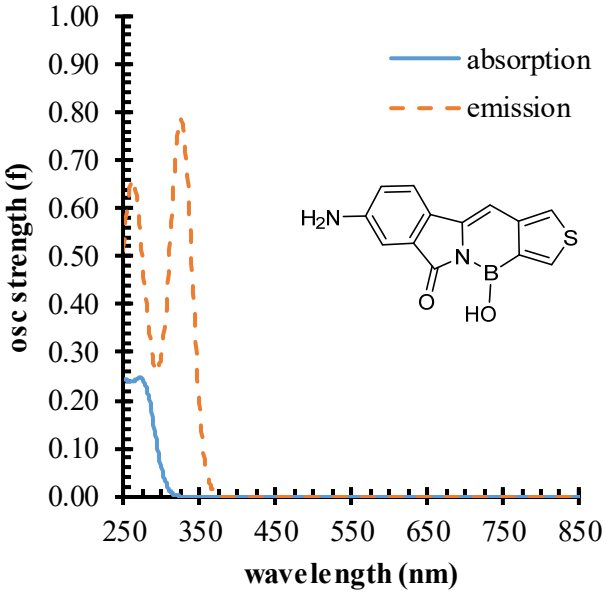
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
osc strength (f)
250 350 450 550 650 750 850
wavelength (nm)
absorption
emission
Br
S
N
B
O
HO

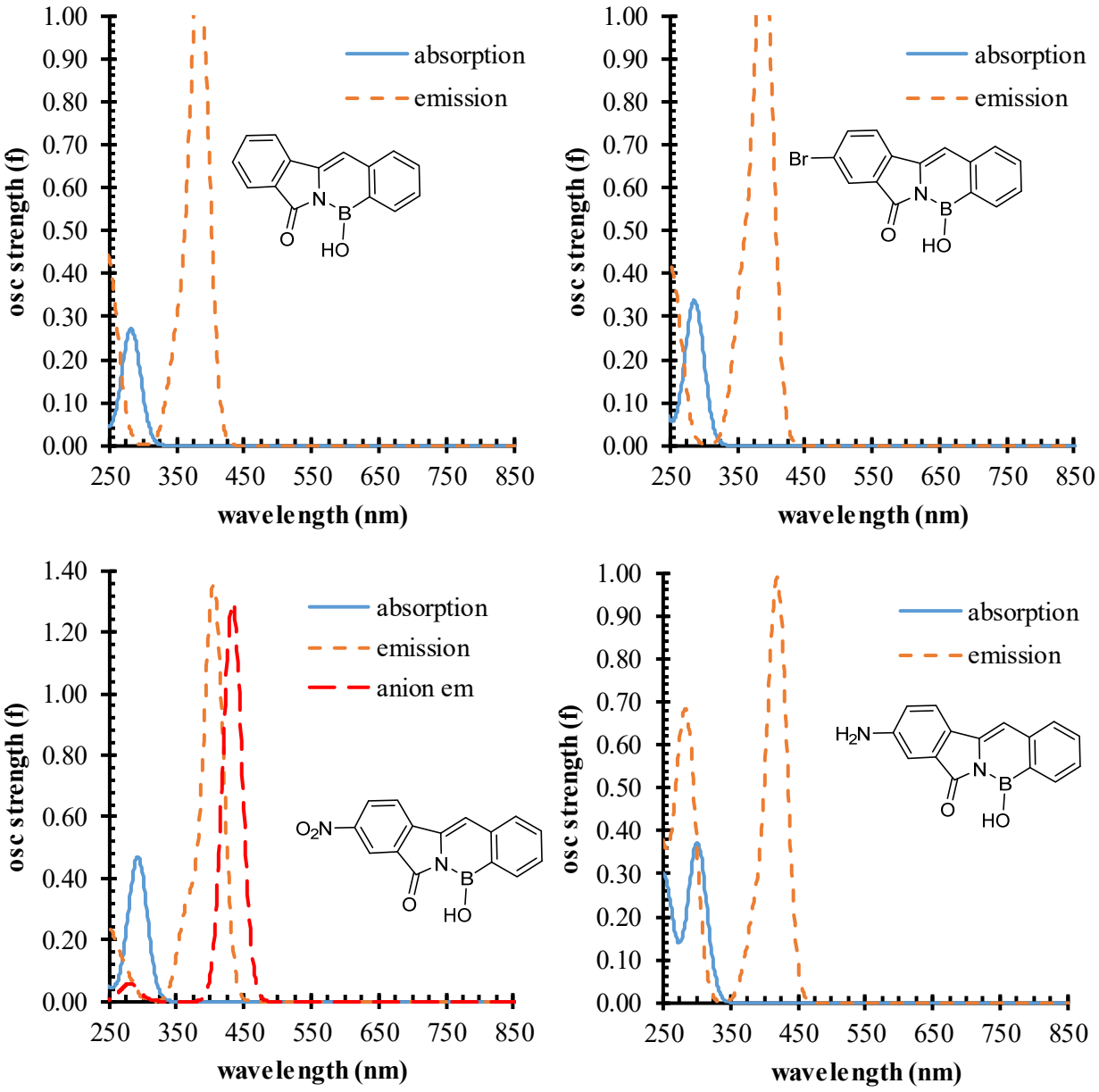

1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
osc strength (f)
250 350 450 550 650 750 850
wavelength (nm)
absorption
emission
O2N
S
N
B
O
HO

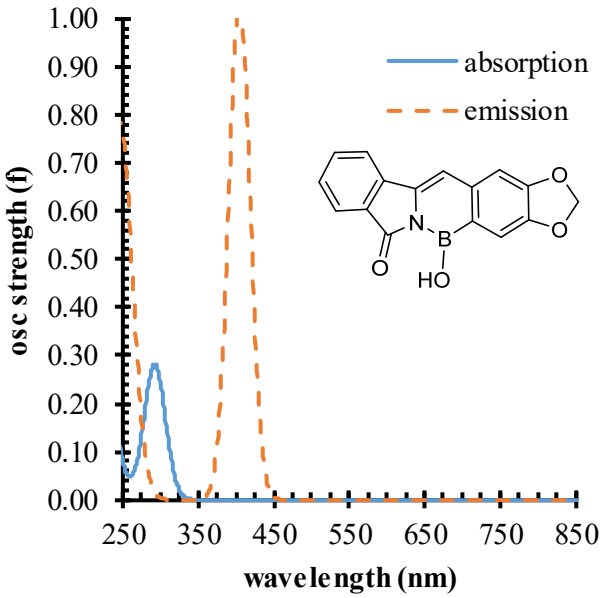

1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
osc strength (f)
250 350 450 550 650 750 850
wavelength (nm)
absorption
emission
H2N
S
N
B
O
HO

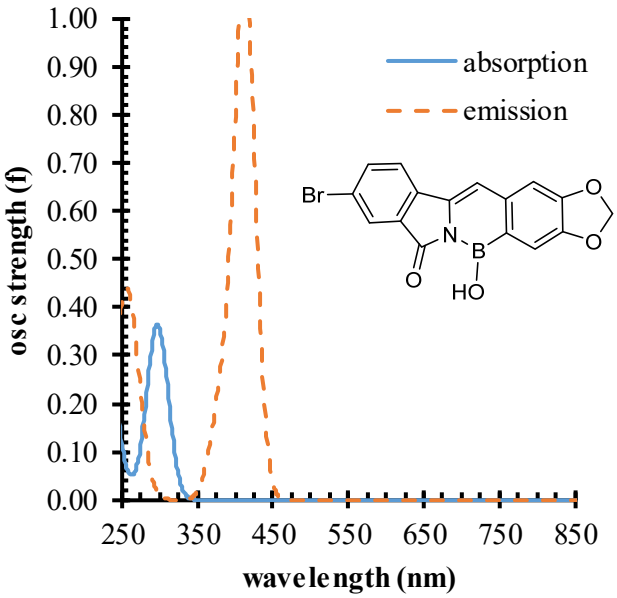
Simulated spectra for acetonitrile solvent

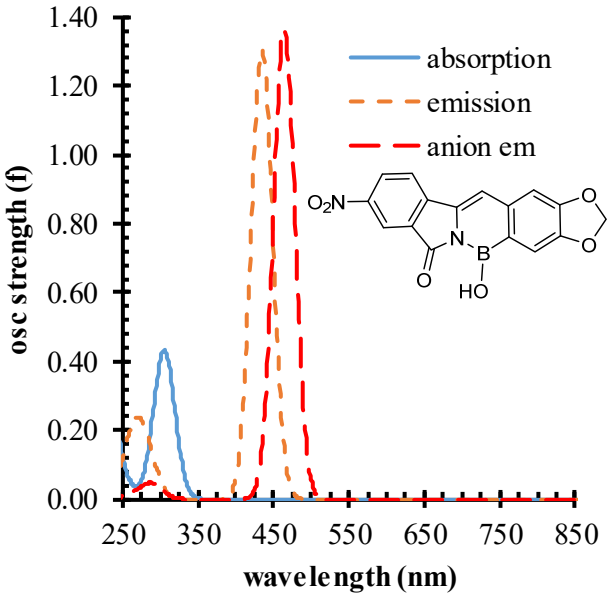
Absorption spectra obtained from LR-SMD-TD-LRC-BOP/BS1//LRC-BOP/BS1

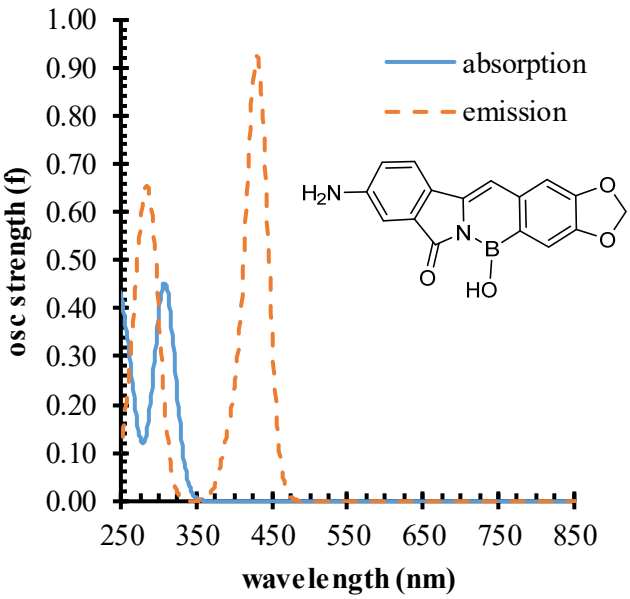
Emission spectra obtained from LR-SMD-TD-LRC-BOP/BS1




absorption
emission
osc strength (f)
wavelength (nm)
1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
250
350
450
550
650
750
850
O
N
B
HO


absorption
emission
osc strength (f)
wavelength (nm)
1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
250
350
450
550
650
750
850
Br
O
N
B
HO


absorption
emission
anion em
osc strength (f)
wavelength (nm)
1.40
1.20
1.00
0.80
0.60
0.40
0.20
0.00
250
350
450
550
650
750
850
O2N
O
N
B
HO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wavelength (nm)
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0.80
0.70
0.60
0.50
0.40
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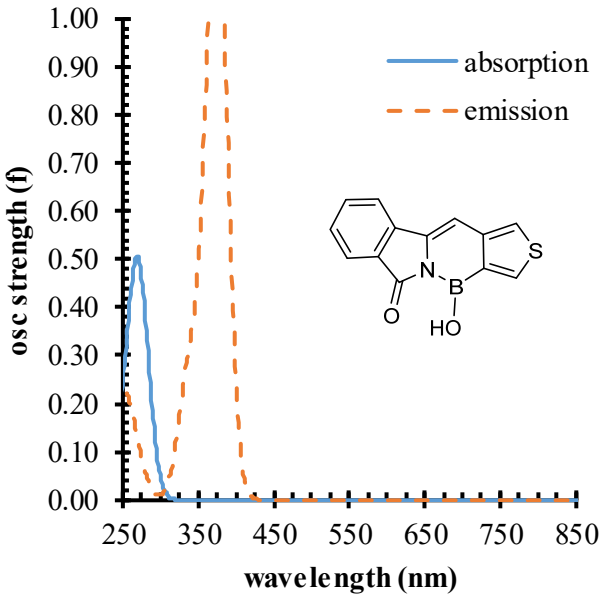
0.10
0.00
250
350
450
550
650
750
850
H2N
O
N
B
HO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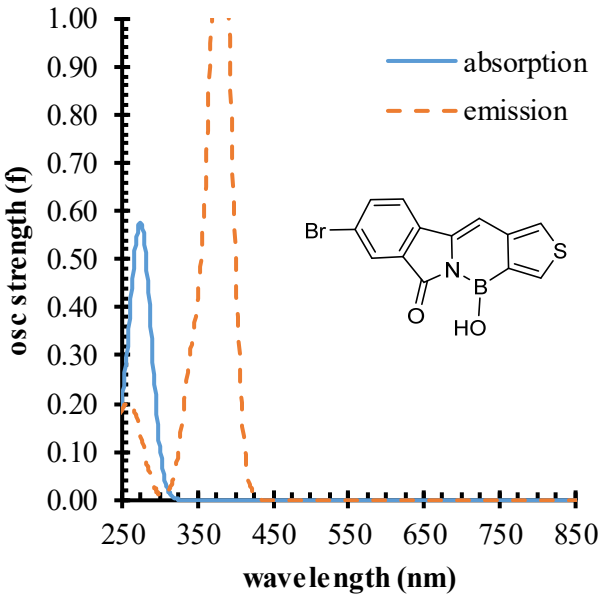
0.10
0.00
250 350 450 550 650 750 850
N
B
O
HO
S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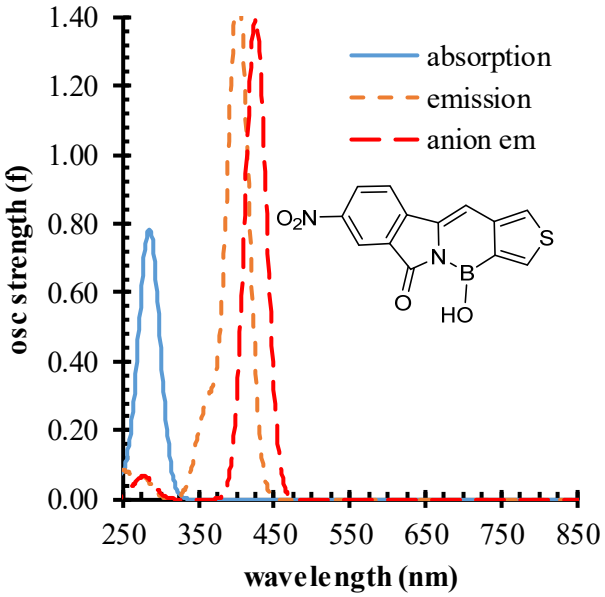
Br
N
B
O
HO
S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osc strength (f)
wavelength (nm)
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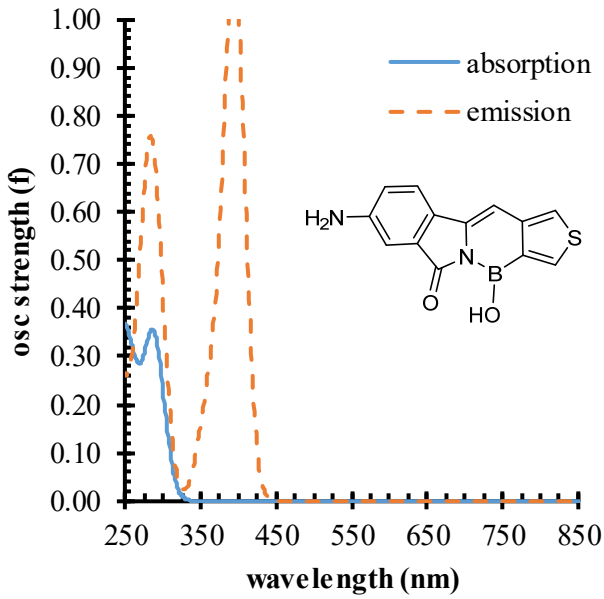
O2N
N
B
O
HO
S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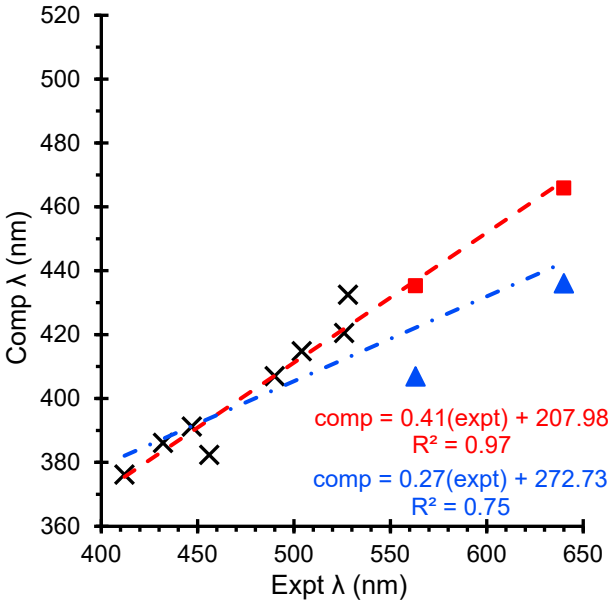
H2N
N
B
O
HO
S



The data from optimizations with LRC-BOP/BS1 also demonstrate that there is a better correlation to the experimental data when the nitro compounds are deprotonated.

Results from Additional Functionals Available in Q-Chem

Additional functionals available in Q-Chem were also tested as single-point computations on the B3LYP/BS1 geometries (DFT//B3LYP/BS1). The data overall are consistent with the discussion in the main text.

Functionals tested:

ωB97X-V[4]
ωB97X-D3[5]
HSE-HJS[6-7]
LC-rVV10[8]
ωB97M-V[9]
M11[10]
MN12-SX[11]
ωM06-D3[5]

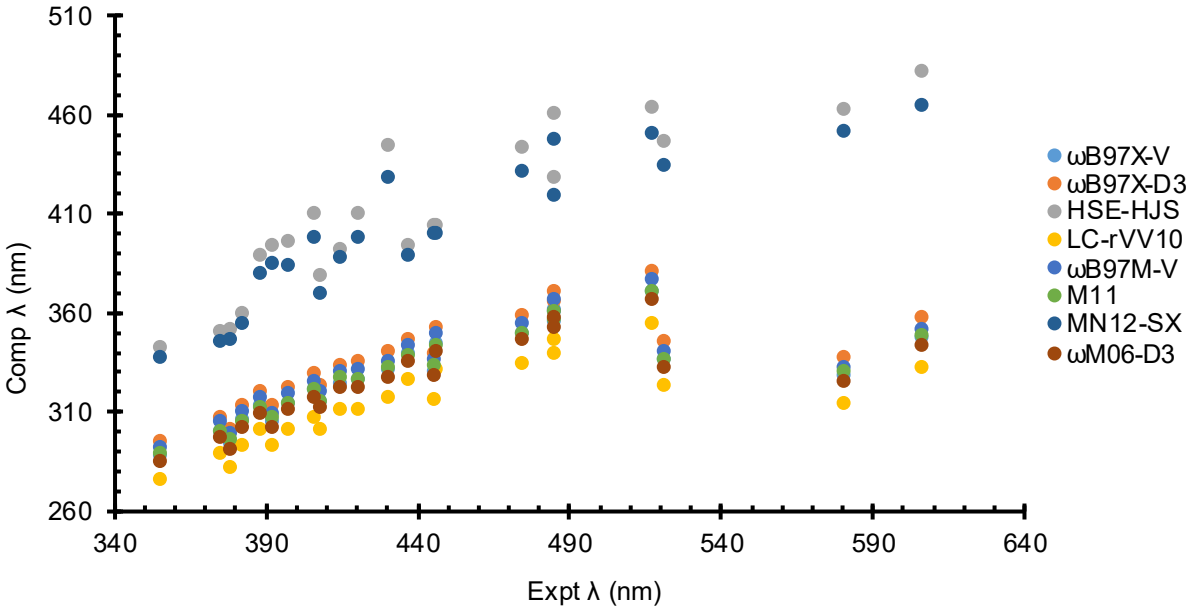


Figure S5: Computed λ_{max} (TD-DFT//DFT/BS1) and λ_{em} (TD-DFT/BS1) vs. experimental data in $CHCl_3$.

The data show that the absorption and emission maxima are in reasonable agreement, except for the three right-most points corresponding to the λ_{em} of the nitro compounds.

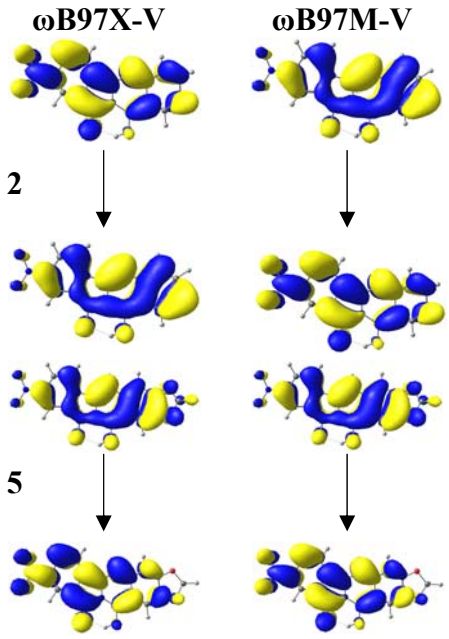


Figure S6: NTOs of λ_{em} for nitro compounds **2** and **5** at the TD-ωB97X-V//TD-B3LYP/BS1 and TD-ωB97M-V//TD-B3LYP/BS1, levels of theory. The emission process is depicted as the particle residing in the upper orbital undergoing vertical de-excitation to the lower orbital.

A full character analysis was not performed for these additional functionals, but the nitro emission character was spot-checked for two of the functionals that are recommended as part of their general class of density functional: ωB97X-V as a range-separated GGA and ωB97M-V as a range-separated meta-GGA. The data in Figure S6 show that these functionals also predict LE character for the emission of the nitro compounds, consistent with cam-QTP(01) and EOM-CCSD computations. However, as demonstrated in Figure S5, the emission wavelengths are still off the trendline compared to the other compounds.

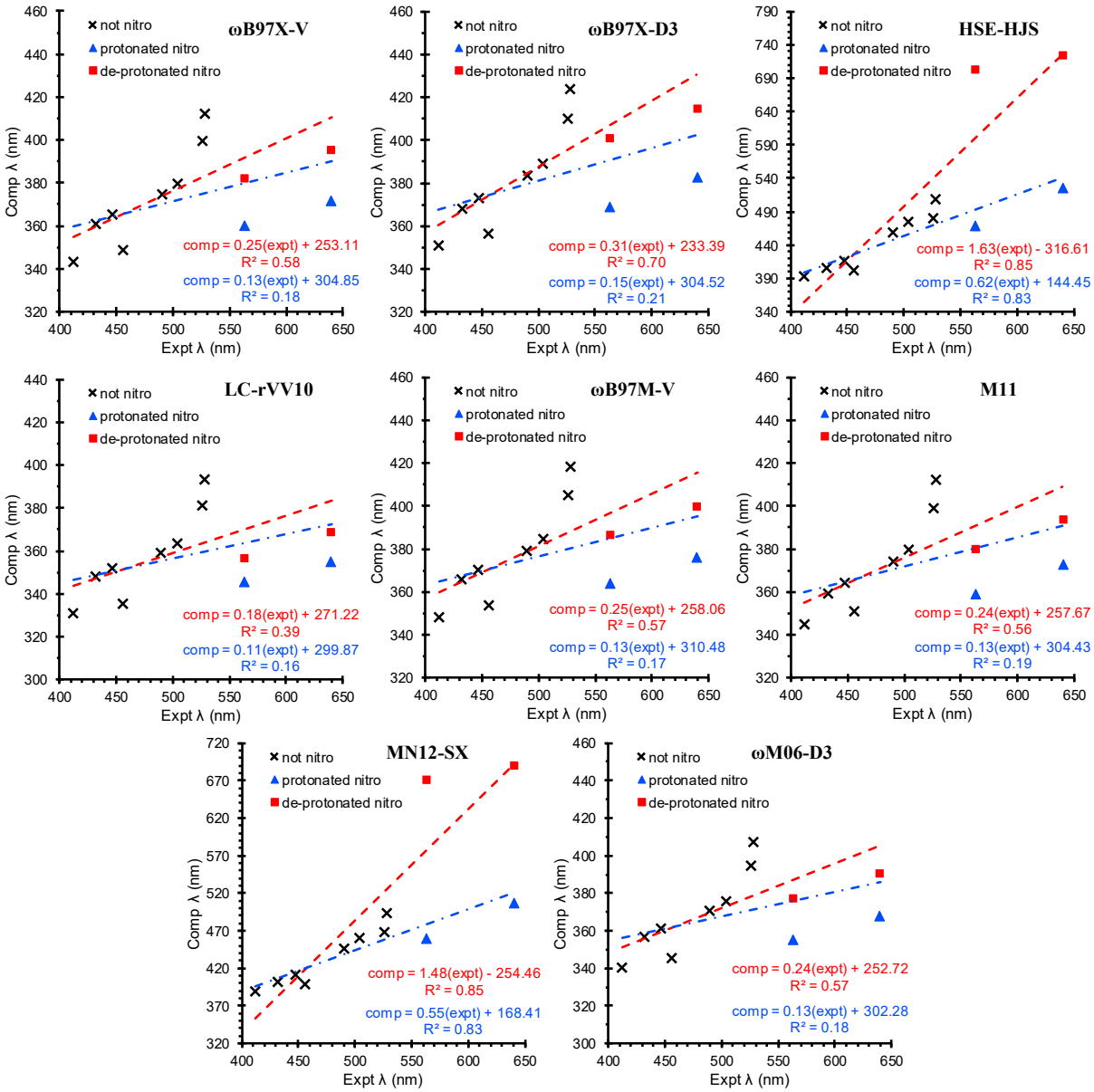


Figure S7: Computed λ_{em} from LR-SMD-TD-DFT/BS1 vs. experimental data in ACN. The blue triangles denote the λ_{em} for the protonated nitro compounds and the red squares denote the λ_{em} for the de-protonated nitro compounds. The other analogues are shown as black ×s.

These data demonstrate that with a variety of other range-corrected functionals, there is consistently a better correlation to experimental data when the nitro compounds are deprotonated.

Singles and Doubles Contributions to EOM-CCSD R Amplitudes

Table S25: Contribution from single ($R1^2$) and double ($R2^2$) excitations to the gas-phase absorption [EOM-CCSD/BS2//B3LYP/BS1] and emission [EOM-CCSD/BS2//TD-B3LYP/BS1] maxima. Values for the corresponding anions of **2** and **5** are shown in parenthesis.

		$R1^2$	$R2^2$
abs	**benzo**	0.91	0.09
	1	0.90	0.10
	2 (2^-)	***0.91 (0.90)***	***0.09 (0.10)***
	3	0.90	0.10
	dioxo	0.91	0.09
	4	0.91	0.09
	5 (5^-)	***0.90 (0.90)***	***0.10 (0.10)***
	6	0.90	0.10
	thieno	0.90	0.10
	7	0.91	0.09
	8	0.90	0.10
	9	0.91	0.09
emission	**benzo**	0.89	0.11
	1	0.90	0.10
	2 (2^-)	***0.91 (0.89)***	***0.09 (0.11)***
	3	0.90	0.10
	dioxo	0.91	0.09
	4	0.91	0.09
	5 (5^-)	***0.89 (0.91)***	***0.11 (0.09)***
	6	0.91	0.09
	thieno	0.90	0.10
	7	0.90	0.10
	8	0.89	0.11
	9	0.91	0.09

The data in Table S25 show that both the computed absorption and emission maxima are dominated by single excitations. Upon deprotonation, compounds **2** and **5** show minimal change in the nature of the excited state (in terms of contribution from single- and double-excitations).

References

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10. Peverati, R., *et al.*, *The Journal of Physical Chemistry Letters* **2011,** *2*, 2810-2817.
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Molecular Coordinates:

b3lyp--benzo

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N    -0.798374  0.918339  0.000589
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C    -4.440159  0.503412  0.010348
H    -4.941984  1.469165  0.015602
C    -5.170433 -0.699310  0.009007
C    -4.466719 -1.928571  0.003556
H    -5.037156 -2.856491  0.006271
C    -3.074904 -1.983202  0.001275
H    -2.572698 -2.948304 -0.004871
C    -2.352387 -0.786527  0.004027
C    -0.921649 -0.483646 -0.000368
C     0.179579 -1.277292 -0.004964
H     0.053222 -2.357508 -0.005391
C     1.527112 -0.734671 -0.009501
C     2.634887 -1.623320 -0.013155
H     2.497302 -2.701333 -0.015356
C     3.893659 -1.065230 -0.014201
C     4.096645  0.319577 -0.013606
C     3.042095  1.206250 -0.012058
H     3.202937  2.280583 -0.014252
C     1.730035  0.676487 -0.008787
O     5.102784 -1.707828 -0.032658
O     5.444465  0.584296 -0.034266
N    -6.561451 -0.689439  0.067448
H    -7.010057  0.163740 -0.236151
H    -7.027325 -1.517862 -0.275827
C     6.096962 -0.681442  0.078566
H     6.589716 -0.757092  1.059886
H     6.824602 -0.792203 -0.734574
    el energy= -1051.67048842
          zpe= -1051.417952
    th energy= -1051.400681
  th enthalpy= -1051.399736
  free energy= -1051.463109

b3lyp--thieno
B    -1.043360  1.443539 -0.000005
O    -1.156710  2.792228  0.000002
H    -0.266483  3.195412  0.000016
N     0.273155  0.802294  0.000009
```

```
C     1.505367  1.475976  0.000030
O     1.622717  2.696052  0.000036
C     2.549661  0.429248  0.000038
C     3.936812  0.555450  0.000057
H     4.399265  1.539561  0.000068
C     4.698202 -0.615031  0.000062
C     4.071349 -1.873680  0.000048
H     4.684108 -2.772900  0.000052
C     2.679487 -1.995957  0.000028
H     2.212260 -2.978225  0.000018
C     1.914525 -0.826279  0.000024
C     0.468028 -0.598329  0.000005
C    -0.573438 -1.467916 -0.000014
H    -0.379316 -2.537322 -0.000016
C    -1.938879 -0.983903 -0.000030
C    -3.083470 -1.754547 -0.000050
H    -3.165747 -2.835042 -0.000058
S    -4.514349 -0.769848 -0.000078
C    -3.571417  0.691676 -0.000038
H    -4.068392  1.654656 -0.000035
C    -2.221836  0.441362 -0.000027
H     5.784206 -0.556998  0.000077
    el energy= -740.481726729
          zpe= -740.294994
    th energy= -740.281985
  th enthalpy= -740.281041
  free energy= -740.334697

b3lyp--7
B    -2.485581  1.436901 -0.000023
O    -2.661063  2.778168 -0.000016
H    -1.793158  3.226400 -0.000001
N    -1.139714  0.855798 -0.000009
C     0.058379  1.585147  0.000012
O     0.125365  2.807902  0.000017
C     1.149293  0.583617  0.000020
C     2.526898  0.784346  0.000038
H     2.946736  1.785622  0.000049
C     3.329545 -0.356205  0.000042
C     2.777038 -1.648935  0.000029
H     3.436851 -2.511501  0.000033
C     1.392816 -1.828896  0.000010
H     0.978490 -2.834327 -0.000001
C     0.571068 -0.697943  0.000006
C    -0.882606 -0.535218 -0.000013
C    -1.884062 -1.451080 -0.000031
H    -1.642112 -2.510717 -0.000033
C    -3.269357 -1.029033 -0.000048
C    -4.377911 -1.850975 -0.000067
H    -4.411008 -2.934094 -0.000074
S    -5.851206 -0.932222 -0.000096
C    -4.975728  0.570557 -0.000056
H    -5.516001  1.509930 -0.000053
C    -3.616153  0.381731 -0.000045
Br    5.243305 -0.163488  0.000068
    el energy= -753.051456390
          zpe= -752.875144
    th energy= -752.860544
  th enthalpy= -752.859600
  free energy= -752.918072

b3lyp--8
B     2.055122  1.439837  0.000036
O     2.229223  2.780289 -0.000001
H     1.363040  3.231180 -0.000102
N     0.710004  0.855139 -0.000011
C    -0.490629  1.580508  0.000026
O    -0.563296  2.801726  0.000129
C    -1.577359  0.573143 -0.000037
C    -2.953634  0.760301 -0.000041
H    -3.405600  1.746459  0.000005
C    -3.736884 -0.393037 -0.000039
C    -3.183765 -1.683498 -0.000108
H    -3.855171 -2.535277 -0.000084
C    -1.801287 -1.851186 -0.000157
H    -1.374354 -2.850805 -0.000199
C    -0.991577 -0.708726 -0.000102
C     0.458362 -0.536264 -0.000082
C     1.462785 -1.450997 -0.000115
H     1.223194 -2.511137 -0.000159
C     2.844914 -1.025058 -0.000046
C     3.955779 -1.845493 -0.000036
H     3.990881 -2.928524 -0.000079
S     5.424907 -0.923921  0.000060
C     4.546749  0.577849  0.000094
H     5.085977  1.517779  0.000159
C     3.187696  0.386418  0.000035
N    -5.205046 -0.255484  0.000050
O    -5.665619  0.878994 -0.000401
O    -5.870769 -1.284442  0.000608
    el energy= -944.977288386
          zpe= -944.788119
    th energy= -944.772498
  th enthalpy= -944.771554
  free energy= -944.831923

b3lyp--9
B     1.438087  1.436864 -0.000057
O     1.577924  2.783890  0.002112
H     0.694956  3.202777  0.000312
N     0.109026  0.822865 -0.001852
C    -1.107325  1.521595 -0.002541
O    -1.201110  2.744551 -0.000023
C    -2.175546  0.497631 -0.005877
C    -3.552985  0.670876 -0.004818
H    -3.982042  1.670972 -0.007776
```

```
C    -4.368943 -0.474907 -0.003877
C    -3.757009 -1.753188 -0.001537
H    -4.394119 -2.636610 -0.004699
C    -2.373714 -1.909539 -0.002051
H    -1.943770 -2.908866  0.001601
C    -1.565092 -0.768462 -0.004535
C    -0.116216 -0.575621 -0.002731
C     0.910244 -1.463369 -0.002025
H     0.696673 -2.529126 -0.003084
C     2.285855 -1.006310 -0.000023
C     3.415502 -1.798046  0.000942
H     3.477940 -2.879829  0.000103
S     4.866643 -0.840353  0.003118
C     3.950926  0.638439  0.003129
H     4.465521  1.592115  0.004205
C     2.596995  0.412793  0.001224
N    -5.754826 -0.364403 -0.059633
H    -6.141504  0.519283  0.241329
H    -6.280428 -1.157501  0.280408
    el energy= -795.834953925
          zpe= -795.631653
    th energy= -795.617104
  th enthalpy= -795.616160
  free energy= -795.672913

b3lyp.tddft--benzo
B    -1.116634  1.407244  0.000000
O    -1.263113  2.758842 -0.000001
H    -0.372022  3.168679 -0.000003
N     0.203156  0.801040 -0.000001
C     1.473005  1.507085 -0.000002
O     1.520952  2.743503  0.000001
C     2.490165  0.480732 -0.000001
C     3.890620  0.561457  0.000001
H     4.386760  1.528717  0.000001
C     4.625301 -0.629700  0.000001
C     3.997540 -1.890222  0.000000
H     4.596692 -2.796594  0.000000
C     2.590824 -1.976309 -0.000001
H     2.100581 -2.948518 -0.000002
C     1.853668 -0.800026 -0.000001
C     0.414016 -0.559129 -0.000002
C    -0.657840 -1.469573 -0.000001
H    -0.437244 -2.533515 -0.000001
C    -1.995487 -1.021751  0.000000
C    -3.080603 -1.960825  0.000001
H    -2.852769 -3.025352  0.000000
C    -4.385500 -1.523827  0.000002
C    -4.670816 -0.133844  0.000002
C    -3.633065  0.799036  0.000002
H    -3.860019  1.863200  0.000002
C    -2.289794  0.400606  0.000001
H    -5.202636 -2.241940  0.000002
H    -5.705989  0.201388  0.000003
H     5.712814 -0.580566  0.000001
 total energy= -807.676702722

b3lyp.tddft--1
B     1.188186 -2.664206  0.000000
O     0.545366 -3.861533  0.000000
H    -0.421255 -3.700273  0.000000
N     0.447144 -1.416293  0.000000
C    -0.996470 -1.277183  0.000000
O    -1.741324 -2.263054  0.000000
C    -1.250525  0.146178  0.000000
C    -2.456125  0.862418  0.000000
H    -3.413403  0.351133  0.000000
C    -2.371331  2.257618  0.000000
C    -1.149808  2.959132  0.000000
H    -1.140968  4.043126  0.000000
C     0.054214  2.226683  0.000000
H     1.004851  2.756747  0.000000
C     0.000000  0.840892  0.000000
C     1.047564 -0.174603  0.000000
C     2.443826 -0.034188  0.000000
H     2.867600  0.966297  0.000000
C     3.291367 -1.164036  0.000000
C     4.717054 -1.006578  0.000000
H     5.134022 -0.001068  0.000000
C     5.542655 -2.107741  0.000000
C     4.988108 -3.413534  0.000000
C     3.604258 -3.592244  0.000000
H     3.186256 -4.596735  0.000000
C     2.726058 -2.500710  0.000000
H     6.623044 -1.981053  0.000000
H     5.649881 -4.277209  0.000000
Br   -4.003954  3.272520  0.000000
 total energy= -820.249212018

b3lyp.tddft--2
B    -2.496744  0.555659  0.000000
O    -3.585592 -0.239097  0.000000
H    -3.331311 -1.181881  0.000000
N    -1.140341 -0.018496  0.000000
C    -0.812212 -1.426256  0.000000
O    -1.676617 -2.280369  0.000000
C     0.655248 -1.505582  0.000000
C     1.481563 -2.622624  0.000000
H     1.111089 -3.640918  0.000000
C     2.868993 -2.382691  0.000000
C     3.386219 -1.071511  0.000000
H     4.464688 -0.960624  0.000000
C     2.531789  0.036660  0.000000
H     2.945604  1.042740  0.000000
C     1.157078 -0.192132  0.000000
C     0.000000  0.738196  0.000000
```

```
C    -0.061195  2.126792  0.000000
H     0.870215  2.686301  0.000000
C    -1.303878  2.827294  0.000000
C    -1.326993  4.253458  0.000000
H    -0.384852  4.797948  0.000000
C    -2.531686  4.937631  0.000000
C    -3.745689  4.228605  0.000000
C    -3.741042  2.823678  0.000000
H    -4.683740  2.280607  0.000000
C    -2.545490  2.104811  0.000000
H    -2.538689  6.025077  0.000000
H    -4.689552  4.768775  0.000000
N     3.777898 -3.494911  0.000000
O     3.273943 -4.648228  0.000000
O     5.010909 -3.239862  0.000000
 total energy= -1012.18168544

b3lyp.tddft--3
B    -1.509978  1.400244  0.000134
O    -1.691105  2.753368  0.000988
H    -0.809355  3.180490  0.000662
N    -0.172228  0.837138 -0.001051
C     1.047645  1.568032 -0.001729
O     1.102585  2.813037 -0.000707
C     2.100303  0.563690 -0.002727
C     3.482229  0.694318 -0.002387
H     3.946932  1.678421 -0.003429
C     4.273065 -0.480164 -0.000837
C     3.665756 -1.774837 -0.001226
H     4.300610 -2.658085 -0.003677
C     2.285317 -1.898313 -0.001799
H     1.829485 -2.886315 -0.001067
C     1.489737 -0.739367 -0.002202
C     0.071927 -0.542478 -0.001556
C    -0.973796 -1.469187 -0.001057
H    -0.733802 -2.529741 -0.001745
C    -2.325793 -1.051455 -0.000112
C    -3.384895 -2.010462  0.000313
H    -3.134549 -3.070604 -0.000282
C    -4.701745 -1.604557  0.001464
C    -5.020382 -0.222204  0.002248
C    -4.007303  0.729329  0.001842
H    -4.255812  1.788909  0.002396
C    -2.648793  0.361829  0.000574
H    -5.500819 -2.343343  0.001766
H    -6.063528  0.088539  0.003095
N     5.637532 -0.384633 -0.015560
H     6.089171  0.511942  0.078362
H     6.212959 -1.205249  0.092412
 total energy= -863.039057582

b3lyp.tddft--dioxo
B    -0.076087  1.570952 -0.000056
O    -0.116699  2.931336 -0.000130
H     0.810977  3.256167 -0.000230
N     1.172151  0.854068 -0.000063
C     2.486756  1.450173 -0.000032
O     2.638210  2.683974  0.000153
C     3.415486  0.345399  0.000018
C     4.820130  0.317597  0.000119
H     5.386708  1.245469  0.000178
C     5.459652 -0.922503  0.000120
C     4.733651 -2.132300  0.000030
H     5.261682 -3.082204  0.000038
C     3.328009 -2.109918 -0.000055
H     2.764381 -3.041723 -0.000106
C     2.680921 -0.881186 -0.000057
C     1.260374 -0.532368 -0.000085
C     0.132734 -1.340122 -0.000093
H     0.253364 -2.419092 -0.000098
C    -1.176976 -0.777246 -0.000069
C    -2.320272 -1.629040 -0.000054
H    -2.220180 -2.710137 -0.000061
C    -3.548921 -1.022967 -0.000022
C    -3.708477  0.391341 -0.000003
C    -2.626701  1.248378 -0.000016
H    -2.750761  2.327319  0.000006
C    -1.342034  0.677408 -0.000040
O    -4.776371 -1.605674 -0.000076
O    -5.033219  0.689974 -0.000051
H     6.547858 -0.959410  0.000188
C    -5.738571 -0.550775  0.000310
H    -6.354700 -0.618902 -0.905257
H    -6.353878 -0.618832  0.906459
 total energy= -996.214882732

b3lyp.tddft--4
B    -1.558770  1.649307 -0.000088
O    -1.696835  3.002604 -0.000171
H    -0.797844  3.397648 -0.000334
N    -0.265265  1.018873 -0.000123
C     1.004939  1.703426 -0.000097
O     1.075155  2.942345  0.000159
C     2.006747  0.664177 -0.000073
C     3.409829  0.745700  0.000024
H     3.914462  1.706489  0.000096
C     4.117609 -0.453733  0.000008
C     3.497795 -1.720211 -0.000094
H     4.097965 -2.623152 -0.000097
C     2.092342 -1.787191 -0.000177
H     1.601556 -2.758902 -0.000235
C     1.359855 -0.610315 -0.000162
C    -0.082534 -0.359832 -0.000168
C    -1.148833 -1.241152 -0.000172
H    -0.955957 -2.309505 -0.000194
C    -2.497068 -0.768263 -0.000106
```

```
C    -3.576712 -1.696345 -0.000075
H    -3.402876 -2.767999 -0.000122
C    -4.845260 -1.175910  0.000017
C    -5.101612  0.224003  0.000072
C    -4.081063  1.153174  0.000033
H    -4.277823  2.221166  0.000065
C    -2.760990  0.670154 -0.000046
O    -6.028216 -1.841371  0.000045
O    -6.442948  0.430654  0.000137
Br    6.044448 -0.386832  0.000125
C    -7.061762 -0.855468  0.000273
H    -7.670889 -0.966204 -0.905646
H    -7.670483 -0.966200  0.906468
 total energy= -1008.78799718

b3lyp.tddft--5
B     0.187370 -1.964531  0.000000
O     0.960623 -3.075203  0.000000
H     1.904733 -2.817567  0.000000
N     0.763977 -0.631485  0.000000
C     2.159939 -0.328282  0.000000
O     3.017543 -1.199973  0.000000
C     2.255149  1.136312  0.000000
C     3.381887  1.947576  0.000000
H     4.392284  1.553885  0.000000
C     3.169656  3.332403  0.000000
C     1.867093  3.886048  0.000000
H     1.773600  4.965401  0.000000
C     0.748183  3.048773  0.000000
H    -0.250822  3.480196  0.000000
C     0.944339  1.669595  0.000000
C     0.000000  0.532330  0.000000
C    -1.370068  0.493820  0.000000
H    -1.926500  1.426067  0.000000
C    -2.094288 -0.756023  0.000000
C    -3.510176 -0.748991  0.000000
H    -4.076442  0.177289  0.000000
C    -4.140722 -1.973642  0.000000
C    -3.430159 -3.199993  0.000000
C    -2.046782 -3.239259  0.000000
H    -1.501269 -4.178347  0.000000
C    -1.365947 -2.011977  0.000000
O    -5.470901 -2.230912  0.000000
O    -4.313127 -4.229531  0.000000
N     4.311371  4.214739  0.000000
O     5.448593  3.697550  0.000000
O     4.087045  5.443879  0.000000
C    -5.619496 -3.653319  0.000000
H    -6.154870 -3.962870  0.906301
H    -6.154870 -3.962870 -0.906301
 total energy= -1200.71907408

b3lyp.tddft--6
B     0.476588  1.609991 -0.000075
O     0.554213  2.972697 -0.001507
H    -0.362435  3.323304 -0.000755
N    -0.796176  0.934448  0.001546
C    -2.081831  1.562815  0.002445
O    -2.220674  2.801176  0.000338
C    -3.044592  0.479328  0.005366
C    -4.437594  0.499663  0.004856
H    -4.977013  1.444943  0.007205
C    -5.133585 -0.727961  0.003116
C    -4.424883 -1.964750  0.001850
H    -4.984611 -2.897512  0.007896
C    -3.032559 -1.978081  0.002691
H    -2.502148 -2.928870  0.000419
C    -2.334028 -0.767209  0.003839
C    -0.926969 -0.458511  0.002378
C     0.187294 -1.293143  0.001676
H     0.037655 -2.369170  0.003078
C     1.504735 -0.767289  0.000532
C     2.628900 -1.653213  0.000436
H     2.495509 -2.731100  0.001463
C     3.872674 -1.086056 -0.000835
C     4.070171  0.319987 -0.002106
C     3.015294  1.207047 -0.002059
H     3.172734  2.281740 -0.002835
C     1.708977  0.678577 -0.000552
O     5.087526 -1.706255 -0.001318
O     5.405709  0.584340 -0.003297
N    -6.512566 -0.740259  0.041703
H    -7.001572  0.113356 -0.184606
H    -6.990677 -1.588584 -0.223849
C     6.076717 -0.676579 -0.000992
H     6.690847 -0.759433  0.905338
H     6.693445 -0.761366 -0.905303
 total energy= -1051.57280792

b3lyp.tddft--thieno
B    -1.031985  1.455212 -0.000005
O    -1.149661  2.805214  0.000021
H    -0.248038  3.192884  0.000052
N     0.264719  0.804803  0.000012
C     1.563982  1.495064  0.000037
O     1.614823  2.729519  0.000027
C     2.562915  0.462249  0.000046
C     3.970772  0.527083  0.000062
H     4.478971  1.487570  0.000071
C     4.688770 -0.674658  0.000070
C     4.050824 -1.925656  0.000061
H     4.637068 -2.839999  0.000067
C     2.631799 -1.992256  0.000043
H     2.129583 -2.958301  0.000035
C     1.916744 -0.812264  0.000035
C     0.465795 -0.557245  0.000013
```

```
C    -0.598039 -1.465566 -0.000006
H    -0.390045 -2.530836 -0.000001
C    -1.927960 -0.978612 -0.000031
C    -3.106565 -1.757895 -0.000032
H    -3.180969 -2.838843 -0.000021
S    -4.511557 -0.783806 -0.000143
C    -3.563085  0.696823 -0.000011
H    -4.071443  1.653756  0.000014
C    -2.216233  0.453602 -0.000031
H     5.777071 -0.636880  0.000084
 total energy= -740.364383216

b3lyp.tddft--7
B     2.486255  1.447998  0.000025
O     2.680586  2.788506 -0.000011
H     1.805971  3.231481 -0.000049
N     1.156656  0.868263  0.000007
C    -0.100921  1.624790 -0.000019
O    -0.091836  2.857812  0.000000
C    -1.155147  0.645857 -0.000028
C    -2.556233  0.801235 -0.000044
H    -3.014273  1.784322 -0.000052
C    -3.323980 -0.367340 -0.000053
C    -2.776724 -1.658900 -0.000046
H    -3.419602 -2.531147 -0.000053
C    -1.360899 -1.796851 -0.000029
H    -0.920280 -2.791828 -0.000022
C    -0.580409 -0.661075 -0.000019
C     0.882208 -0.483162  0.000004
C     1.893674 -1.445596  0.000021
H     1.629721 -2.498414  0.000013
C     3.249086 -1.030675  0.000051
C     4.382526 -1.873333  0.000042
H     4.397461 -2.956756  0.000023
S     5.838194 -0.977730  0.000194
C     4.971790  0.552727  0.000017
H     5.531587  1.480519 -0.000018
C     3.614144  0.382864  0.000052
Br   -5.242693 -0.191603 -0.000078
 total energy= -752.937233452

b3lyp.tddft--8
B    -2.064868  1.441542 -0.000014
O    -2.239970  2.775162  0.000069
H    -1.380091  3.238652  0.000339
N    -0.718842  0.839357  0.000284
C     0.523980  1.580746  0.000668
O     0.535873  2.795885 -0.000071
C     1.603834  0.585841  0.000301
C     2.983254  0.774942 -0.000016
H     3.454020  1.750361 -0.000128
C     3.777936 -0.388632 -0.000062
C     3.195093 -1.669683  0.000156
H     3.867868 -2.520266  0.000079
C     1.805282 -1.831226  0.000391
H     1.373044 -2.829373  0.000469
C     1.012505 -0.684434  0.000421
C    -0.466040 -0.510860  0.000397
C    -1.488092 -1.444602  0.000328
H    -1.240660 -2.501536  0.000390
C    -2.849962 -1.016443  0.000082
C    -3.983974 -1.844624 -0.000044
H    -4.008665 -2.928179  0.000035
S    -5.446508 -0.938534 -0.000397
C    -4.556421  0.576430 -0.000312
H    -5.099500  1.514726 -0.000454
C    -3.199146  0.388685 -0.000117
N     5.208338 -0.272689 -0.000317
O     5.685161  0.894696 -0.000545
O     5.884745 -1.338126 -0.000355
 total energy= -944.874462195

b3lyp.tddft--9
B     1.426673  1.451737  0.000116
O     1.581982  2.803163  0.000900
H     0.688710  3.209192  0.000082
N     0.110602  0.848010 -0.001068
C    -1.135715  1.565361 -0.001416
O    -1.190345  2.808730 -0.000008
C    -2.171656  0.554298 -0.003401
C    -3.560244  0.668221 -0.003892
H    -4.038178  1.645792 -0.006667
C    -4.337103 -0.516607 -0.002207
C    -3.721284 -1.802115 -0.001733
H    -4.343603 -2.693624 -0.005905
C    -2.329988 -1.905251 -0.002208
H    -1.862804 -2.888295 -0.000778
C    -1.553162 -0.743048 -0.002409
C    -0.129162 -0.533018 -0.001505
C     0.911437 -1.462462 -0.001015
H     0.679334 -2.523441 -0.001950
C     2.255586 -1.012317  0.000030
C     3.406149 -1.818054  0.000689
H     3.458892 -2.900135  0.000301
S     4.836582 -0.872922  0.001985
C     3.933871  0.625976  0.001947
H     4.465922  1.569651  0.002562
C     2.578714  0.417654  0.000719
N    -5.705628 -0.427206 -0.026614
H    -6.152482  0.464388  0.124065
H    -6.267035 -1.248047  0.141000
 total energy= -795.724717438

b3lyp.tddft-mecn--benzo
B    -1.111854  1.406747  0.000000
O    -1.234252  2.764886  0.000000
```

```
H    -0.329639  3.148117  0.000000
N     0.216801  0.803830  0.000000
C     1.464487  1.503752  0.000000
O     1.524363  2.749035  0.000000
C     2.486363  0.478051 -0.000001
C     3.883254  0.557920 -0.000001
H     4.386648  1.522665 -0.000001
C     4.620910 -0.631509 -0.000001
C     3.983977 -1.895262 -0.000001
H     4.586892 -2.800033 -0.000001
C     2.590938 -1.989689 -0.000001
H     2.100644 -2.961078 -0.000001
C     1.838079 -0.803781  0.000000
C     0.424442 -0.565730  0.000000
C    -0.668834 -1.471117  0.000000
H    -0.452623 -2.536264  0.000000
C    -1.994308 -1.017676  0.000000
C    -3.084133 -1.957489  0.000001
H    -2.854226 -3.021491  0.000000
C    -4.389460 -1.519286  0.000001
C    -4.673893 -0.130127  0.000001
C    -3.631976  0.803942  0.000001
H    -3.872251  1.866008  0.000001
C    -2.289475  0.408702  0.000001
H    -5.206921 -2.237156  0.000001
H    -5.708088  0.207811  0.000001
H     5.708114 -0.584702 -0.000001
 total energy= -807.706308075

b3lyp.tddft-mecn--1
B     1.220555 -2.645960  0.000000
O     0.571303 -3.844375  0.000000
H    -0.394303 -3.668235  0.000000
N     0.453072 -1.405249  0.000000
C    -0.973726 -1.293728  0.000000
O    -1.717130 -2.291493  0.000000
C    -1.250479  0.127439  0.000000
C    -2.462428  0.825705  0.000000
H    -3.413226  0.300138  0.000000
C    -2.396940  2.220279  0.000000
C    -1.176975  2.937723  0.000000
H    -1.178210  4.022784  0.000000
C     0.028968  2.234463  0.000000
H     0.971576  2.777327  0.000000
C     0.000000  0.833753  0.000000
C     1.043724 -0.151912  0.000000
C     2.452904 -0.005775  0.000000
H     2.865560  0.999503  0.000000
C     3.302194 -1.121861  0.000000
C     4.730032 -0.946856  0.000000
H     5.131675  0.064632  0.000000
C     5.570479 -2.038010  0.000000
C     5.033718 -3.349618  0.000000
C     3.648103 -3.546130  0.000000
H     3.255546 -4.561500  0.000000
C     2.754250 -2.469766  0.000000
H     6.648985 -1.896679  0.000000
H     5.704687 -4.206096  0.000000
Br   -4.043511  3.222497  0.000000
 total energy= -820.279721322

b3lyp.tddft-mecn--2
B    -2.498229  0.538452  0.000000
O    -3.588517 -0.261374  0.000000
H    -3.326090 -1.201923  0.000000
N    -1.145933 -0.040992  0.000000
C    -0.820412 -1.429202  0.000000
O    -1.669741 -2.307341  0.000000
C     0.650549 -1.500246  0.000000
C     1.482648 -2.604513  0.000000
H     1.105894 -3.621128  0.000000
C     2.871654 -2.359328  0.000000
C     3.385824 -1.038917  0.000000
H     4.461161 -0.903817  0.000000
C     2.528078  0.059339  0.000000
H     2.931525  1.068938  0.000000
C     1.145838 -0.173136  0.000000
C     0.000000  0.723881  0.000000
C    -0.068602  2.123525  0.000000
H     0.862490  2.683479  0.000000
C    -1.303974  2.813487  0.000000
C    -1.321650  4.243281  0.000000
H    -0.376006  4.781031  0.000000
C    -2.524750  4.928254  0.000000
C    -3.739360  4.218263  0.000000
C    -3.740892  2.811317  0.000000
H    -4.691676  2.282397  0.000000
C    -2.550244  2.088267  0.000000
H    -2.532635  6.015659  0.000000
H    -4.682788  4.759283  0.000000
N     3.773468 -3.464983  0.000000
O     3.292916 -4.631892  0.000000
O     5.012627 -3.229390  0.000000
 total energy= -1012.21704174

b3lyp.tddft-mecn--2-
B    -2.503110  0.442904  0.000000
O    -3.542772 -0.380343  0.000000
N    -1.142988 -0.062628  0.000000
C    -0.792596 -1.423247  0.000000
O    -1.600139 -2.338167  0.000000
C     0.689423 -1.453342  0.000000
C     1.535300 -2.546829  0.000000
H     1.166335 -3.566610  0.000000
C     2.923790 -2.296862  0.000000
C     3.409604 -0.958403  0.000000
```

```
H     4.483673 -0.809232  0.000000
C     2.541307  0.122726  0.000000
H     2.936045  1.136760  0.000000
C     1.153393 -0.115558  0.000000
C     0.000000  0.766913  0.000000
C    -0.127490  2.123263  0.000000
H     0.766002  2.742523  0.000000
C    -1.427158  2.769611  0.000000
C    -1.523346  4.180154  0.000000
H    -0.608699  4.771212  0.000000
C    -2.762777  4.813939  0.000000
C    -3.947009  4.063630  0.000000
C    -3.870392  2.668104  0.000000
H    -4.790323  2.086522  0.000000
C    -2.632562  2.009300  0.000000
H    -2.809215  5.901870  0.000000
H    -4.914244  4.561511  0.000000
N     3.830979 -3.377597  0.000000
O     3.370810 -4.563644  0.000000
O     5.078741 -3.130084  0.000000
 total energy= -1011.74986245

b3lyp.tddft-mecn--3
B    -1.507197  1.394468 -0.000162
O    -1.664248  2.757270 -0.000341
H    -0.764428  3.151752 -0.000507
N    -0.165869  0.833763  0.000077
C     1.043366  1.563336  0.000427
O     1.089283  2.818281  0.000414
C     2.101160  0.566231  0.000154
C     3.482003  0.700848 -0.000022
H     3.963017  1.676937 -0.000025
C     4.277521 -0.477011 -0.000157
C     3.661623 -1.779090 -0.000109
H     4.304570 -2.656071 -0.000215
C     2.291512 -1.905886  0.000047
H     1.833306 -2.892267  0.000032
C     1.487535 -0.739433  0.000175
C     0.079227 -0.551202  0.000203
C    -0.976874 -1.472720  0.000166
H    -0.741056 -2.534289  0.000226
C    -2.324705 -1.048689  0.000072
C    -3.388261 -2.006175  0.000089
H    -3.137934 -3.066329  0.000194
C    -4.706710 -1.599955 -0.000019
C    -5.028775 -0.218521 -0.000162
C    -4.011635  0.731176 -0.000187
H    -4.270180  1.789564 -0.000310
C    -2.651003  0.365610 -0.000071
H    -5.504575 -2.340527 -0.000001
H    -6.071602  0.093144 -0.000257
N     5.625101 -0.386428 -0.000233
H     6.087850  0.513930 -0.000626
H     6.206215 -1.215057 -0.000822
 total energy= -863.078733959

b3lyp.tddft-mecn--dioxo
B    -0.073866  1.575762 -0.000082
O    -0.084061  2.941421 -0.000030
H     0.853878  3.238246 -0.000088
N     1.187090  0.861232 -0.000231
C     2.486499  1.448368 -0.000120
O     2.653964  2.688822 -0.000011
C     3.415292  0.340892 -0.000036
C     4.817689  0.304554  0.000155
H     5.397023  1.225793  0.000210
C     5.453567 -0.938093  0.000254
C     4.713517 -2.145917  0.000183
H     5.239398 -3.097717  0.000267
C     3.316908 -2.123673  0.000012
H     2.748849 -3.052216 -0.000037
C     2.664697 -0.883002 -0.000088
C     1.268048 -0.529802 -0.000193
C     0.116140 -1.329842 -0.000211
H     0.234149 -2.409672 -0.000250
C    -1.177211 -0.766844 -0.000142
C    -2.326339 -1.625671 -0.000153
H    -2.215280 -2.706106 -0.000259
C    -3.553349 -1.026589 -0.000025
C    -3.711744  0.388613  0.000127
C    -2.627607  1.251616  0.000122
H    -2.773298  2.328431  0.000204
C    -1.341033  0.690459 -0.000023
O    -4.778817 -1.606099 -0.000027
O    -5.022911  0.693706  0.000239
H     6.541176 -0.982188  0.000394
C    -5.747706 -0.550700  0.000124
H    -6.357937 -0.610401 -0.907896
H    -6.357874 -0.610611  0.908171
 total energy= -996.243977517

b3lyp.tddft-mecn--4
B    -1.558919  1.655896 -0.000072
O    -1.666973  3.016604 -0.000035
H    -0.754889  3.383226 -0.000035
N    -0.252074  1.029851 -0.000096
C     1.002233  1.707365 -0.000061
O     1.085806  2.954312 -0.000027
C     2.005685  0.667359 -0.000061
C     3.406409  0.744495  0.000001
H     3.915284  1.704229  0.000064
C     4.110709 -0.455952 -0.000003
C     3.482474 -1.724233 -0.000075
H     4.077085 -2.631970 -0.000074
C     2.086635 -1.792924 -0.000136
H     1.594316 -2.763204 -0.000183
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C     1.346019 -0.607162 -0.000123
C    -0.074794 -0.353179 -0.000136
C    -1.163965 -1.229772 -0.000157
H    -0.972240 -2.298973 -0.000181
C    -2.496517 -0.757716 -0.000110
C    -3.579376 -1.695179 -0.000083
H    -3.391969 -2.764933 -0.000118
C    -4.846503 -1.183999  0.000008
C    -5.104194  0.216744  0.000064
C    -4.083611  1.154218  0.000028
H    -4.304606  2.218035  0.000079
C    -2.761759  0.683464 -0.000057
O    -6.026624 -1.847880  0.000062
O    -6.432585  0.428365  0.000157
Br    6.042701 -0.396383  0.000115
C    -7.068012 -0.863590  0.000186
H    -7.672085 -0.966121 -0.907958
H    -7.671907 -0.966164  0.908445
 total energy= -1008.81825030

b3lyp.tddft-mecn--5
B     0.265398 -1.971516  0.000000
O     1.086586 -3.049400  0.000000
H     2.018925 -2.755609  0.000000
N     0.807093 -0.616626  0.000000
C     2.177030 -0.263129  0.000000
O     3.082348 -1.089388  0.000000
C     2.216461  1.209700  0.000000
C     3.307626  2.062655  0.000000
H     4.329964  1.701308  0.000000
C     3.040842  3.444354  0.000000
C     1.710968  3.936904  0.000000
H     1.558059  5.009885  0.000000
C     0.628626  3.059837  0.000000
H    -0.387546  3.447068  0.000000
C     0.881705  1.682107  0.000000
C     0.000000  0.517890  0.000000
C    -1.378297  0.421167  0.000000
H    -1.963619  1.336128  0.000000
C    -2.053555 -0.837780  0.000000
C    -3.477258 -0.865925  0.000000
H    -4.057435  0.051910  0.000000
C    -4.075121 -2.100398  0.000000
C    -3.325418 -3.304187  0.000000
C    -1.934018 -3.309438  0.000000
H    -1.380595 -4.244052  0.000000
C    -1.285542 -2.071112  0.000000
O    -5.393606 -2.401027  0.000000
O    -4.158471 -4.355436  0.000000
N     4.132862  4.365244  0.000000
O     5.307738  3.906655  0.000000
O     3.876207  5.599581  0.000000
C    -5.500928 -3.830989  0.000000
H    -6.014787 -4.163605  0.908254
H    -6.014787 -4.163605 -0.908254
 total energy= -1200.75569447

b3lyp.tddft-mecn--5-
B     1.099803  1.643255 -0.007795
O     1.186890  2.969086 -0.001830
N    -0.191465  0.981061 -0.005696
C    -1.430775  1.640772  0.001350
O    -1.560018  2.854363  0.006287
C    -2.454196  0.568263  0.001310
C    -3.832338  0.683758  0.007722
H    -4.334217  1.644941  0.013840
C    -4.585871 -0.508466  0.006039
C    -3.928123 -1.770173 -0.001980
H    -4.543428 -2.663165 -0.003294
C    -2.543568 -1.860697 -0.007862
H    -2.064519 -2.837610 -0.013784
C    -1.781341 -0.676945 -0.006096
C    -0.349530 -0.421455 -0.010287
C     0.740052 -1.237631 -0.017028
H     0.599474 -2.315418 -0.020558
C     2.096018 -0.711677 -0.020603
C     3.191229 -1.620295 -0.025095
H     3.024949 -2.694488 -0.030485
C     4.464235 -1.091868 -0.022384
C     4.702553  0.286323 -0.020059
C     3.663993  1.194630 -0.018584
H     3.863086  2.262786 -0.021302
C     2.342022  0.690004 -0.016842
O     5.655761 -1.762448 -0.050328
O     6.056079  0.519439 -0.056341
N    -5.996492 -0.446186  0.012502
O    -6.557661  0.695146  0.022590
O    -6.658170 -1.532201  0.008383
C     6.667861 -0.760025  0.153912
H     7.040473 -0.826952  1.186833
H     7.474506 -0.904694 -0.571089
 total energy= -1200.27604607

b3lyp.tddft-mecn--6
B    -0.475105  1.611576  0.000013
O    -0.522340  2.983486  0.000015
H     0.408067  3.300558 -0.000008
N     0.809449  0.941375 -0.000067
C     2.079904  1.565679 -0.000097
O     2.226126  2.813790 -0.000046
C     3.047224  0.483612 -0.000078
C     4.437661  0.501783 -0.000025
H     4.995610  1.436383  0.000002
C     5.133470 -0.734322  0.000042
C     4.409527 -1.976704  0.000080
H     4.975231 -2.905667  0.000149
```

```
C     3.030757 -1.989366  0.000030
H     2.494379 -2.936122  0.000059
C     2.325590 -0.764299 -0.000063
C     0.937381 -0.458461 -0.000116
C    -0.194314 -1.285783 -0.000136
H    -0.048650 -2.363002 -0.000162
C    -1.501526 -0.755687 -0.000101
C    -2.630565 -1.646367 -0.000112
H    -2.487867 -2.723733 -0.000174
C    -3.875700 -1.086298 -0.000020
C    -4.076040  0.317627  0.000084
C    -3.021477  1.206836  0.000083
H    -3.197275  2.279658  0.000169
C    -1.706615  0.688455 -0.000010
O    -5.086541 -1.711038  0.000036
O    -5.407711  0.584211  0.000215
N     6.488494 -0.760638 -0.000074
H     7.028518  0.094287  0.000823
H     6.993032 -1.636866  0.001201
C    -6.087152 -0.683252 -0.000007
H    -6.697951 -0.766325 -0.906766
H    -6.698208 -0.766504  0.906557
 total energy= -1051.61058500
```

b3lyp.tddft-mecn--thieno

```
B    -1.025047  1.449130  0.000005
O    -1.118036  2.804369  0.000052
H    -0.201820  3.163642  0.000107
N     0.281349  0.802306  0.000021
C     1.551525  1.492194  0.000041
O     1.613137  2.738031 -0.000004
C     2.555573  0.461726  0.000050
C     3.958483  0.525574  0.000057
H     4.471306  1.485424  0.000056
C     4.683302 -0.669178  0.000073
C     4.034796 -1.927821  0.000080
H     4.627013 -2.839491  0.000090
C     2.636651 -2.005210  0.000066
H     2.137210 -2.972275  0.000063
C     1.897361 -0.816805  0.000050
C     0.477402 -0.570559  0.000022
C    -0.611642 -1.474293  0.000004
H    -0.412219 -2.541654  0.000014
C    -1.927037 -0.979625 -0.000028
C    -3.112059 -1.755848 -0.000022
H    -3.192309 -2.837505 -0.000011
S    -4.509974 -0.772160 -0.000203
C    -3.559051  0.706959  0.000010
H    -4.075994  1.660667  0.000056
C    -2.213594  0.457389 -0.000032
H     5.771121 -0.632258  0.000082
 total energy= -740.391634642
```

b3lyp.tddft-mecn--7

```
B    -2.478358  1.441414 -0.000011
O    -2.649113  2.788584  0.000010
H    -1.758566  3.204728  0.000045
N    -1.138536  0.866236  0.000006
C     0.090958  1.623118  0.000026
O     0.089847  2.867924  0.000003
C     1.149754  0.647245  0.000031
C     2.545094  0.800641  0.000037
H     3.002022  1.786218  0.000039
C     3.315373 -0.360856  0.000044
C     2.759817 -1.662480  0.000044
H     3.403208 -2.535861  0.000048
C     1.366239 -1.806927  0.000034
H     0.927758 -2.802617  0.000029
C     0.563822 -0.665424  0.000027
C    -0.869826 -0.495099  0.000005
C    -1.903952 -1.455813 -0.000017
H    -1.646430 -2.510577 -0.000017
C    -3.246006 -1.033008 -0.000044
C    -4.386451 -1.872634 -0.000063
H    -4.406783 -2.957362 -0.000064
S    -5.835438 -0.966587 -0.000136
C    -4.965976  0.561924 -0.000047
H    -5.532174  1.487063 -0.000034
C    -3.609256  0.385102 -0.000043
Br    5.238746 -0.192106  0.000053
 total energy= -752.965587856
```

b3lyp.tddft-mecn--8

```
B    -2.060658  1.448912  0.000023
O    -2.230482  2.787081  0.000025
H    -1.366471  3.243080  0.000045
N    -0.710174  0.853790  0.000020
C     0.514759  1.585320  0.000000
O     0.553680  2.806009 -0.000018
C     1.594274  0.584865  0.000011
C     2.967777  0.766036  0.000002
H     3.428664  1.746851 -0.000010
C     3.764803 -0.397695 -0.000001
C     3.177496 -1.684872  0.000013
H     3.833699 -2.547734  0.000008
C     1.791401 -1.841528  0.000024
H     1.353197 -2.836352  0.000030
C     0.993550 -0.690994  0.000020
C    -0.458046 -0.505055  0.000016
C    -1.491062 -1.441055  0.000011
H    -1.245606 -2.498751  0.000005
C    -2.840373 -1.010660 -0.000004
C    -3.969908 -1.849093 -0.000040
H    -3.984882 -2.934040 -0.000050
S    -5.429166 -0.947839  0.000008
C    -4.550467  0.579940 -0.000051
```

```
H    -5.111458  1.508363 -0.000071
C    -3.196233  0.397927 -0.000003
N     5.185512 -0.274322 -0.000023
O     5.684911  0.889785 -0.000023
O     5.885344 -1.329831 -0.000004
 total energy= -944.908358737

b3lyp.tddft-mecn--8-
B    -2.030937  1.451240  0.000153
O    -2.205856  2.764710 -0.000014
N    -0.710996  0.847363  0.000049
C     0.485360  1.577676 -0.000095
O     0.539701  2.798290  0.000057
C     1.571646  0.570510  0.000015
C     2.940823  0.770513  0.000031
H     3.382301  1.760827  0.000005
C     3.766718 -0.372795  0.000024
C     3.186165 -1.673012  0.000040
H     3.856166 -2.525578  0.000042
C     1.810991 -1.848664  0.000044
H     1.392284 -2.852954  0.000071
C     0.976577 -0.713502  0.000030
C    -0.466652 -0.552237  0.000035
C    -1.490531 -1.449420  0.000049
H    -1.272646 -2.513953  0.000043
C    -2.869101 -0.999572  0.000026
C    -3.996927 -1.794731 -0.000033
H    -4.054448 -2.877483 -0.000057
S    -5.460070 -0.844704 -0.000063
C    -4.554256  0.642510 -0.000052
H    -5.082903  1.589346 -0.000076
C    -3.203349  0.414379  0.000043
N     5.169177 -0.226443 -0.000063
O     5.663322  0.948188 -0.000113
O     5.895704 -1.273376 -0.000010
 total energy= -944.439426983

b3lyp.tddft-mecn--9
B     1.420604  1.440488 -0.000004
O     1.551575  2.800048  0.000052
H     0.638771  3.171516  0.000031
N     0.099793  0.841441 -0.000085
C    -1.127321  1.561597 -0.000154
O    -1.175274  2.819295 -0.000079
C    -2.168848  0.559698 -0.000066
C    -3.556349  0.676806  0.000038
H    -4.048899  1.647322  0.000082
C    -4.338975 -0.507818  0.000064
C    -3.714059 -1.805148  0.000006
H    -4.347891 -2.688570  0.000055
C    -2.339951 -1.914957 -0.000078
H    -1.871652 -2.896978 -0.000098
C    -1.546845 -0.744144 -0.000112
C    -0.136639 -0.549387 -0.000111
C     0.915397 -1.473449 -0.000063
H     0.688914 -2.536088 -0.000049
C     2.256510 -1.017371  0.000003
C     3.410331 -1.816259  0.000113
H     3.472581 -2.898901  0.000142
S     4.840399 -0.858820 -0.000052
C     3.934188  0.632383  0.000244
H     4.470273  1.575325  0.000399
C     2.577386  0.415299  0.000032
N    -5.689458 -0.427401  0.000259
H    -6.159378  0.469051 -0.000061
H    -6.263834 -1.260514 -0.000157
 total energy= -795.761821972

pbe0--benzo
B    -1.122604  1.391204  0.000001
O    -1.265611  2.736400  0.000001
H    -0.386846  3.155915  0.000003
N     0.203650  0.787890  0.000002
C     1.418921  1.477720  0.000003
O     1.516294  2.693286 -0.000002
C     2.474899  0.447244  0.000000
C     3.856329  0.590444 -0.000003
H     4.307352  1.579975 -0.000004
C     4.628049 -0.569144 -0.000004
C     4.017002 -1.830811 -0.000002
H     4.640325 -2.722723 -0.000003
C     2.630097 -1.969490  0.000001
H     2.173400 -2.956724  0.000001
C     1.856220 -0.811039  0.000001
C     0.411054 -0.594775  0.000002
C    -0.627764 -1.461805  0.000002
H    -0.427956 -2.531038  0.000002
C    -2.003332 -1.006304  0.000001
C    -3.058136 -1.935428  0.000000
H    -2.833172 -3.001174  0.000001
C    -4.376636 -1.502882 -0.000001
C    -4.671266 -0.135391 -0.000001
C    -3.635403  0.792386 -0.000001
H    -3.855219  1.858521 -0.000001
C    -2.296395  0.383050  0.000000
H    -5.184154 -2.232650 -0.000001
H    -5.706923  0.198161 -0.000002
H     5.713364 -0.499642 -0.000005
    el energy= -806.874752484
          zpe= -806.652423
    th energy= -806.639124
  th enthalpy= -806.638179
  free energy= -806.692279

pbe0--1
B     1.247719 -2.620417  0.000000
```

```
O     0.619735 -3.817872  0.000000
H    -0.344206 -3.682426  0.000000
N     0.480367 -1.380521  0.000000
C    -0.911773 -1.278583  0.000000
O    -1.672720 -2.230155  0.000000
C    -1.213813  0.167420  0.000000
C    -2.446007  0.806122  0.000000
H    -3.372887  0.239902  0.000000
C    -2.429651  2.197613  0.000000
C    -1.229095  2.921154  0.000000
H    -1.262251  4.006933  0.000000
C    -0.003532  2.260371  0.000000
H     0.921034  2.833033  0.000000
C     0.000000  0.866937  0.000000
C     1.078846 -0.116065  0.000000
C     2.424623  0.025466  0.000000
H     2.853869  1.024957  0.000000
C     3.313901 -1.118405  0.000000
C     4.707009 -0.933273  0.000000
H     5.113340  0.077250  0.000000
C     5.561210 -2.026970  0.000000
C     5.044155 -3.326460  0.000000
C     3.667163 -3.520683  0.000000
H     3.256460 -4.528717  0.000000
C     2.783327 -2.435171  0.000000
H     6.638262 -1.870710  0.000000
H     5.718578 -4.180197  0.000000
Br   -4.079362  3.151231  0.000000
    el energy= -819.449578721
          zpe= -819.237655
    th energy= -819.222784
  th enthalpy= -819.221840
  free energy= -819.280718

pbe0--2
B    -2.493044  0.467247  0.000000
O    -3.559835 -0.361712  0.000000
H    -3.261140 -1.287862  0.000000
N    -1.135642 -0.067042  0.000000
C    -0.786384 -1.418361  0.000000
O    -1.584192 -2.337778  0.000000
C     0.691620 -1.454283  0.000000
C     1.546227 -2.544302  0.000000
H     1.185874 -3.568345  0.000000
C     2.907056 -2.259535  0.000000
C     3.406625 -0.952415  0.000000
H     4.482706 -0.810605  0.000000
C     2.533401  0.128220  0.000000
H     2.921036  1.143824  0.000000
C     1.161908 -0.131038  0.000000
C     0.000000  0.748769  0.000000
C    -0.099254  2.099561  0.000000
H     0.808380  2.699098  0.000000
C    -1.382233  2.770090  0.000000
C    -1.447367  4.174308  0.000000
H    -0.525494  4.754207  0.000000
C    -2.675808  4.819558  0.000000
C    -3.861964  4.078117  0.000000
C    -3.808617  2.688198  0.000000
H    -4.727690  2.105151  0.000000
C    -2.582976  2.012048  0.000000
H    -2.714727  5.907065  0.000000
H    -4.822212  4.589538  0.000000
N     3.860835 -3.372786  0.000000
O     3.403784 -4.497375  0.000000
O     5.043834 -3.096023  0.000000
    el energy= -1011.16946194
          zpe= -1010.944295
    th energy= -1010.928410
  th enthalpy= -1010.927466
  free energy= -1010.988216

pbe0--3
B    -1.514669  1.383373  0.000575
O    -1.679464  2.726681  0.002052
H    -0.806771  3.158760  0.000430
N    -0.177553  0.803589 -0.002044
C     1.023054  1.515647 -0.003430
O     1.099697  2.733423 -0.000554
C     2.100782  0.505704 -0.006258
C     3.472059  0.693469 -0.005054
H     3.890262  1.698416 -0.008628
C     4.296995 -0.441940 -0.003681
C     3.697533 -1.721668 -0.001724
H     4.342911 -2.599217 -0.005299
C     2.319479 -1.891760 -0.002519
H     1.899066 -2.895158  0.000597
C     1.503847 -0.761215 -0.004881
C     0.057115 -0.576490 -0.002899
C    -0.968567 -1.459765 -0.001771
H    -0.751430 -2.525598 -0.002828
C    -2.351906 -1.027753  0.000255
C    -3.391616 -1.973980  0.000870
H    -3.148655 -3.035844 -0.000349
C    -4.717537 -1.564463  0.002754
C    -5.036989 -0.202624  0.004117
C    -4.016598  0.742123  0.003524
H    -4.254148  1.804544  0.004446
C    -2.670703  0.355868  0.001617
H    -5.511876 -2.308747  0.003069
H    -6.078333  0.112791  0.005514
N     5.672822 -0.319684 -0.055790
H     6.054084  0.567046  0.235763
H     6.207796 -1.108957  0.271746
    el energy= -862.170039972
          zpe= -861.930892
```

```
    th energy= -861.916068
  th enthalpy= -861.915124
  free energy= -861.972275

pbe0--dioxo
B     0.090207  1.567952 -0.004391
O     0.114884  2.921805 -0.001340
H    -0.797731  3.261153  0.002508
N    -1.177303  0.851351 -0.000880
C    -2.448923  1.431094  0.004772
O    -2.653274  2.633527  0.007956
C    -3.408739  0.310715  0.005860
C    -4.797402  0.330387  0.010632
H    -5.334246  1.276134  0.014373
C    -5.463348 -0.892945  0.010383
C    -4.742173 -2.095040  0.005463
H    -5.283746 -3.038847  0.005316
C    -3.348431 -2.110186  0.000678
H    -2.806089 -3.053142 -0.003191
C    -2.679894 -0.887738  0.000909
C    -1.260924 -0.542684 -0.003308
C    -0.145758 -1.310652 -0.008912
H    -0.248746 -2.393396 -0.010721
C     1.183160 -0.736348 -0.013773
C     2.308207 -1.595838 -0.018690
H     2.197777 -2.677048 -0.023003
C     3.548411 -1.006399 -0.018995
C     3.715148  0.381186 -0.017708
C     2.641090  1.238690 -0.015761
H     2.771804  2.317379 -0.018597
C     1.348971  0.673698 -0.011856
O     4.766357 -1.609062 -0.044034
O     5.045369  0.674398 -0.045147
H    -6.550519 -0.920236  0.013991
C     5.718204 -0.564052  0.111652
H     6.158527 -0.619789  1.119452
H     6.490744 -0.660104 -0.659578
    el energy= -995.214818940
          zpe= -994.976350
    th energy= -994.960739
  th enthalpy= -994.959795
  free energy= -995.019640

pbe0--4
B    -1.563589  1.642859 -0.005350
O    -1.677866  2.991318 -0.001470
H    -0.792377  3.395121  0.001389
N    -0.250751  1.009830 -0.003935
C     0.978246  1.671630  0.000890
O     1.108963  2.883181  0.004720
C     2.008892  0.612820  0.000346
C     3.391400  0.733902  0.004119
H     3.870442  1.708870  0.008062
C     4.124104 -0.449249  0.002651
C     3.498156 -1.703769 -0.002437
H     4.108427 -2.602679 -0.003424
C     2.109653 -1.803395 -0.006208
H     1.636902 -2.782822 -0.010157
C     1.358725 -0.629071 -0.004777
C    -0.077724 -0.376527 -0.007475
C    -1.141141 -1.214976 -0.012544
H    -0.968575 -2.288822 -0.015284
C    -2.504095 -0.728413 -0.015134
C    -3.570448 -1.659613 -0.019226
H    -3.389975 -2.731302 -0.024770
C    -4.846330 -1.152091 -0.016912
C    -5.102638  0.222002 -0.013566
C    -4.086733  1.147952 -0.012613
H    -4.287493  2.215766 -0.013798
C    -2.761016  0.668098 -0.011619
O    -6.022008 -1.832097 -0.039432
O    -6.447940  0.428880 -0.036269
Br    6.027561 -0.370346  0.007723
C    -7.041251 -0.851386  0.110523
H    -7.798835 -0.994168 -0.668334
H    -7.485949 -0.938676  1.113821
    el energy= -1007.78979580
          zpe= -1007.561797
    th energy= -1007.544596
  th enthalpy= -1007.543652
  free energy= -1007.608312

pbe0--5
B    -1.115602  1.636058 -0.004511
O    -1.220025  2.984336 -0.001549
H    -0.333294  3.384899  0.000869
N     0.191377  0.990988 -0.003154
C     1.427069  1.640463  0.000864
O     1.571176  2.849388  0.003713
C     2.445584  0.569212  0.000902
C     3.826939  0.667110  0.004305
H     4.344264  1.621537  0.007454
C     4.529971 -0.532411  0.003550
C     3.896027 -1.780113 -0.000450
H     4.513021 -2.673110 -0.000789
C     2.509285 -1.858516 -0.003871
H     2.017413 -2.827991 -0.006988
C     1.779461 -0.668166 -0.003151
C     0.349584 -0.396762 -0.005698
C    -0.722361 -1.226700 -0.009786
H    -0.558501 -2.301918 -0.011770
C    -2.079001 -0.728607 -0.012142
C    -3.153849 -1.650668 -0.015510
H    -2.983230 -2.723917 -0.020099
C    -4.424481 -1.131103 -0.013804
C    -4.666822  0.246162 -0.011153
```

```
C    -3.642166  1.163263 -0.010518
H    -3.833576  2.232732 -0.011600
C    -2.321763  0.671002 -0.009528
O    -5.605798 -1.798861 -0.032742
O    -6.007504  0.467314 -0.029327
N     5.994602 -0.492071  0.007180
O     6.522277  0.601486  0.010681
O     6.584434 -1.554529  0.006481
C    -6.619517 -0.808232  0.089192
H    -7.352007 -0.937725 -0.715891
H    -7.098179 -0.895896  1.075919
    el energy= -1199.51005756
          zpe= -1199.268821
    th energy= -1199.250578
  th enthalpy= -1199.249634
  free energy= -1199.316412

pbe0--6
B     0.490019  1.595017 -0.005086
O     0.547054  2.948715 -0.003228
H    -0.357738  3.308405  0.001748
N    -0.795334  0.910615  0.000382
C    -2.049673  1.523539  0.007130
O    -2.224251  2.731281  0.008629
C    -3.041329  0.429469  0.010481
C    -4.423381  0.505443  0.013701
H    -4.921522  1.473292  0.021006
C    -5.154081 -0.692589  0.011451
C    -4.453242 -1.919373  0.004486
H    -5.025388 -2.846350  0.007379
C    -3.065656 -1.977628  0.000941
H    -2.565762 -2.943972 -0.006175
C    -2.343476 -0.785156  0.003997
C    -0.917214 -0.482730 -0.001702
C     0.180329 -1.275987 -0.008477
H     0.052422 -2.356079 -0.009726
C     1.523649 -0.734033 -0.014925
C     2.627468 -1.620408 -0.020345
H     2.490503 -2.698631 -0.023968
C     3.882383 -1.062048 -0.021577
C     4.084708  0.320216 -0.021139
C     3.032314  1.203806 -0.018954
H     3.189443  2.279018 -0.022728
C     1.726310  0.671264 -0.013704
O     5.085434 -1.695888 -0.048850
O     5.423894  0.578885 -0.052756
N    -6.535886 -0.681372  0.067793
H    -6.986183  0.172155 -0.224575
H    -7.005161 -1.509924 -0.263587
C     6.060370 -0.675153  0.123295
H     6.477407 -0.738564  1.141022
H     6.846496 -0.794876 -0.630488
    el energy= -1050.50983361
          zpe= -1050.254563
    th energy= -1050.237433
  th enthalpy= -1050.236489
  free energy= -1050.299317

pbe0--thieno
B    -1.038788  1.439499 -0.000008
O    -1.146673  2.784670 -0.000014
H    -0.253943  3.177277 -0.000008
N     0.273197  0.796595  0.000002
C     1.496259  1.468961  0.000017
O     1.611273  2.684414  0.000041
C     2.539789  0.427566  0.000030
C     3.923061  0.556444  0.000054
H     4.383792  1.541482  0.000069
C     4.682481 -0.610629  0.000056
C     4.058093 -1.866338  0.000035
H     4.672253 -2.764593  0.000037
C     2.670364 -1.990636  0.000012
H     2.203919 -2.973360 -0.000002
C     1.907731 -0.823881  0.000010
C     0.465604 -0.594981 -0.000004
C    -0.572076 -1.464049 -0.000023
H    -0.376568 -2.533191 -0.000032
C    -1.932952 -0.979356 -0.000034
C    -3.076872 -1.747179 -0.000067
H    -3.161587 -2.827761 -0.000087
S    -4.494524 -0.765827 -0.000007
C    -3.562857  0.687270 -0.000067
H    -4.060836  1.650112 -0.000087
C    -2.215017  0.438389 -0.000026
H     5.768481 -0.552557  0.000073
    el energy= -739.665089085
          zpe= -739.476476
    th energy= -739.463536
  th enthalpy= -739.462591
  free energy= -739.516141

pbe0--7
B     2.473673  1.433039  0.000027
O     2.643765  2.771068  0.000034
H     1.772903  3.208924  0.000031
N     1.132229  0.850388  0.000019
C    -0.057005  1.577948  0.000007
O    -0.121616  2.796035 -0.000024
C    -1.146878  0.581817 -0.000009
C    -2.520346  0.784415 -0.000036
H    -2.940383  1.786103 -0.000051
C    -3.321018 -0.353315 -0.000038
C    -2.769626 -1.642980 -0.000015
H    -3.431931 -2.504124 -0.000018
C    -1.389867 -1.824093  0.000009
H    -0.975686 -2.829665  0.000024
```

```
C    -0.571268 -0.695500  0.000012
C     0.878043 -0.531672  0.000026
C     1.875515 -1.447005  0.000043
H     1.632034 -2.506285  0.000052
C     3.256349 -1.024384  0.000052
C     4.364197 -1.843552  0.000083
H     4.399679 -2.926876  0.000102
S     5.824369 -0.927580  0.000023
C     4.959678  0.566362  0.000081
H     5.501045  1.505497  0.000099
C     3.601968  0.378908  0.000044
Br   -5.216491 -0.163106 -0.000072
    el energy= -752.239966267
          zpe= -752.061785
    th energy= -752.047273
  th enthalpy= -752.046329
  free energy= -752.104649

pbe0--8
B    -2.045799  1.436192  0.000012
O    -2.213831  2.773479  0.000116
H    -1.344394  3.213472  0.000234
N    -0.705184  0.849485  0.000028
C     0.486613  1.573112  0.000098
O     0.557116  2.789697 -0.000211
C     1.572070  0.571125 -0.000034
C     2.944589  0.759975 -0.000097
H     3.397495  1.746636 -0.000091
C     3.724061 -0.390602 -0.000088
C     3.173652 -1.677602 -0.000057
H     3.848149 -2.527969 -0.000063
C     1.795290 -1.846687 -0.000018
H     1.368333 -2.846384 -0.000016
C     0.989323 -0.706448  0.000007
C    -0.456486 -0.532888  0.000021
C    -1.456684 -1.447059  0.000024
H    -1.215424 -2.506827  0.000019
C    -2.834358 -1.020385  0.000007
C    -3.944487 -1.837886  0.000005
H    -3.981588 -2.921166  0.000014
S    -5.400647 -0.919038 -0.000012
C    -4.533207  0.573560 -0.000002
H    -5.072963  1.513606  0.000008
C    -3.175956  0.383836 -0.000013
N     5.183814 -0.254135  0.000011
O     5.638044  0.871581  0.000110
O     5.841523 -1.275689  0.000064
    el energy= -943.959891879
          zpe= -943.768447
    th energy= -943.752923
  th enthalpy= -943.751979
  free energy= -943.812204

pbe0--9
B     1.431984  1.433037  0.000713
O     1.564753  2.776731  0.002286
H     0.678421  3.183771  0.000924
N     0.107589  0.816332 -0.001705
C    -1.100031  1.513301 -0.002982
O    -1.191741  2.731545 -0.000537
C    -2.167098  0.494488 -0.006088
C    -3.540273  0.670773 -0.005130
H    -3.966413  1.672333 -0.008625
C    -4.355265 -0.471067 -0.003948
C    -3.744883 -1.746139 -0.001789
H    -4.382901 -2.629030 -0.005566
C    -2.365925 -1.904578 -0.002230
H    -1.937531 -2.904631  0.001007
C    -1.559082 -0.766959 -0.004571
C    -0.114744 -0.572943 -0.002608
C     0.908130 -1.459797 -0.001676
H     0.693404 -2.525245 -0.002808
C     2.278796 -1.001435  0.000175
C     3.408059 -1.789914  0.000874
H     3.472287 -2.871884 -0.000094
S     4.845830 -0.835234  0.002879
C     3.940879  0.634533  0.003141
H     4.455511  1.588573  0.004246
C     2.588722  0.410407  0.001530
N    -5.732228 -0.361158 -0.056428
H    -6.121104  0.522758  0.233557
H    -6.260218 -1.154520  0.272483
    el energy= -794.960366930
          zpe= -794.754941
    th energy= -794.740466
  th enthalpy= -794.739521
  free energy= -794.796151

pbe0.tddft--benzo
B     1.110717  1.403438  0.000001
O     1.250043  2.751137  0.000006
H     0.355027  3.148754  0.000013
N    -0.207811  0.796625  0.000003
C    -1.460248  1.500173  0.000004
O    -1.507449  2.732265 -0.000007
C    -2.479315  0.479044  0.000001
C    -3.874522  0.562397 -0.000004
H    -4.368661  1.530931 -0.000007
C    -4.608258 -0.623512 -0.000004
C    -3.982227 -1.883297  0.000000
H    -4.584489 -2.787749  0.000000
C    -2.584263 -1.972996  0.000004
H    -2.095099 -2.945879  0.000006
C    -1.845195 -0.797908  0.000004
C    -0.415560 -0.557752  0.000005
C     0.656218 -1.466932  0.000004
```

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H     0.434216 -2.530890  0.000004
C     1.987907 -1.018992  0.000001
C     3.070503 -1.954797 -0.000001
H     2.843272 -3.019627  0.000000
C     4.371689 -1.517471 -0.000004
C     4.654993 -0.130767 -0.000005
C     3.619357  0.798519 -0.000004
H     3.843160  1.863670 -0.000005
C     2.280452  0.398229 -0.000001
H     5.189434 -2.234827 -0.000005
H     5.689913  0.205318 -0.000008
H    -5.695615 -0.574117 -0.000007
 total energy= -806.756323930

pbe0.tddft--1
B     1.179757 -2.651901  0.000000
O     0.533850 -3.842549  0.000000
H    -0.429210 -3.669597  0.000000
N     0.439717 -1.404693  0.000000
C    -0.988115 -1.274296  0.000000
O    -1.730092 -2.257185  0.000000
C    -1.247009  0.145863  0.000000
C    -2.448856  0.856829  0.000000
H    -3.406367  0.344538  0.000000
C    -2.366965  2.247951  0.000000
C    -1.145880  2.949698  0.000000
H    -1.142592  4.034276  0.000000
C     0.051726  2.225600  0.000000
H     1.002125  2.756414  0.000000
C     0.000000  0.839068  0.000000
C     1.039315 -0.169023  0.000000
C     2.434956 -0.029223  0.000000
H     2.857399  0.972161  0.000000
C     3.277636 -1.155640  0.000000
C     4.699454 -0.999954  0.000000
H     5.117515  0.005314  0.000000
C     5.521456 -2.099603  0.000000
C     4.966885 -3.401473  0.000000
C     3.586943 -3.577913  0.000000
H     3.165281 -4.581224  0.000000
C     2.713662 -2.486958  0.000000
H     6.601970 -1.974069  0.000000
H     5.627878 -4.265789  0.000000
Br   -3.982061  3.252647  0.000000
 total energy= -819.334086323

pbe0.tddft--2
B    -2.488137  0.509762  0.000000
O    -3.562612 -0.301799  0.000000
H    -3.279127 -1.234788  0.000000
N    -1.130143 -0.041923  0.000000
C    -0.792904 -1.430753  0.000000
O    -1.641994 -2.299547  0.000000
C     0.668842 -1.489221  0.000000
C     1.509461 -2.584256  0.000000
H     1.151950 -3.608910  0.000000
C     2.886544 -2.323544  0.000000
C     3.396986 -1.006523  0.000000
H     4.474147 -0.881602  0.000000
C     2.530201  0.081449  0.000000
H     2.929114  1.093880  0.000000
C     1.157371 -0.162317  0.000000
C     0.000000  0.731149  0.000000
C    -0.082825  2.122703  0.000000
H     0.841123  2.695091  0.000000
C    -1.329708  2.795776  0.000000
C    -1.379628  4.220496  0.000000
H    -0.446900  4.781560  0.000000
C    -2.591536  4.878625  0.000000
C    -3.793118  4.148548  0.000000
C    -3.764386  2.750249  0.000000
H    -4.696237  2.187986  0.000000
C    -2.558696  2.053772  0.000000
H    -2.619337  5.965912  0.000000
H    -4.745526  4.673940  0.000000
N     3.799786 -3.426608  0.000000
O     3.322651 -4.566675  0.000000
O     5.007499 -3.164363  0.000000
 total energy= -1011.05769453

pbe0.tddft--3
B    -1.502931  1.396680 -0.000018
O    -1.677749  2.746005  0.000007
H    -0.792277  3.161542 -0.000006
N    -0.168409  0.831886 -0.000062
C     1.040517  1.561001 -0.000057
O     1.091706  2.800803 -0.000032
C     2.092169  0.562357 -0.000069
C     3.470479  0.694570 -0.000004
H     3.933648  1.679578  0.000043
C     4.258958 -0.476149  0.000039
C     3.653122 -1.768884 -0.000018
H     4.288951 -2.651564 -0.000046
C     2.278043 -1.893449 -0.000073
H     1.822227 -2.881586 -0.000107
C     1.484398 -0.736576 -0.000086
C     0.072484 -0.539322 -0.000082
C    -0.970538 -1.465615 -0.000071
H    -0.729130 -2.526009 -0.000092
C    -2.317625 -1.047927 -0.000025
C    -3.373770 -2.004227  0.000002
H    -3.123799 -3.064516 -0.000027
C    -4.687058 -1.598336  0.000067
C    -5.004181 -0.219659  0.000105
C    -3.992974  0.728734  0.000073
H    -4.238621  1.789244  0.000100
```

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C    -2.639191  0.359355  0.000006
H    -5.486367 -2.336745  0.000091
H    -6.047050  0.091804  0.000158
N     5.614319 -0.383481  0.000038
H     6.072045  0.512660  0.000643
H     6.193009 -1.206350  0.000864
 total energy= -862.061096853

pbe0.tddft--dioxo
B     0.075729  1.566041  0.000039
O     0.111033  2.922026  0.000027
H    -0.818918  3.235910  0.000032
N    -1.172204  0.849724  0.000008
C    -2.470967  1.445023 -0.000029
O    -2.620712  2.674078 -0.000016
C    -3.401380  0.344779 -0.000020
C    -4.801179  0.318982 -0.000028
H    -5.366636  1.247715 -0.000049
C    -5.439067 -0.916960 -0.000023
C    -4.714216 -2.124937  0.000001
H    -5.244277 -3.073775  0.000001
C    -3.315794 -2.105423  0.000018
H    -2.752541 -3.037470  0.000030
C    -2.668673 -0.877468  0.000004
C    -1.257975 -0.529107  0.000007
C    -0.129363 -1.336759  0.000020
H    -0.252737 -2.415665  0.000018
C     1.172612 -0.776225  0.000028
C     2.314164 -1.626933  0.000023
H     2.213936 -2.708182  0.000018
C     3.537520 -1.021085  0.000006
C     3.695186  0.390284 -0.000003
C     2.615875  1.245120  0.000019
H     2.737058  2.324804  0.000016
C     1.336638  0.672400  0.000024
O     4.759430 -1.595471  0.000002
O     5.010285  0.685830 -0.000009
H    -6.527088 -0.954318 -0.000040
C     5.710340 -0.545838 -0.000065
H     6.327746 -0.612060  0.905110
H     6.327630 -0.612053 -0.905322
 total energy= -995.107836504

pbe0.tddft--4
B    -1.550192  1.643860  0.000075
O    -1.682222  2.993249  0.000249
H    -0.779990  3.376995  0.000490
N    -0.257009  1.013781  0.000093
C     0.997180  1.696847  0.000071
O     1.066301  2.931076 -0.000267
C     2.000232  0.662029  0.000044
C     3.397489  0.745416 -0.000045
H     3.902223  1.706814 -0.000111
C     4.104787 -0.449955 -0.000007
C     3.484780 -1.715117  0.000098
H     4.088670 -2.616220  0.000112
C     2.087796 -1.784613  0.000163
H     1.597353 -2.756563  0.000217
C     1.354501 -0.608282  0.000135
C    -0.077174 -0.357573  0.000122
C    -1.145218 -1.238612  0.000104
H    -0.950106 -2.306804  0.000119
C    -2.484923 -0.767272  0.000050
C    -3.563340 -1.694143  0.000035
H    -3.389487 -2.765960  0.000054
C    -4.826298 -1.173375  0.000008
C    -5.080272  0.223689 -0.000032
C    -4.062115  1.150518 -0.000019
H    -4.256219  2.219419 -0.000035
C    -2.747386  0.665368  0.000013
O    -6.004736 -1.829921  0.000138
O    -6.411766  0.428429  0.000058
Br    6.011101 -0.385217 -0.000092
C    -7.026276 -0.848210 -0.000456
H    -7.636475 -0.956817 -0.906283
H    -7.637681 -0.956983  0.904505
 total energy= -1007.68608818

pbe0.tddft--5
B     0.205930 -1.951544  0.000000
O     0.990202 -3.051746  0.000000
H     1.926210 -2.768309  0.000000
N     0.769953 -0.618881  0.000000
C     2.154156 -0.315444  0.000000
O     3.016565 -1.183994  0.000000
C     2.238294  1.139416  0.000000
C     3.351209  1.963248  0.000000
H     4.366099  1.578046  0.000000
C     3.121575  3.337340  0.000000
C     1.819071  3.889090  0.000000
H     1.717670  4.968202  0.000000
C     0.713923  3.045147  0.000000
H    -0.289419  3.466678  0.000000
C     0.920386  1.667969  0.000000
C     0.000000  0.535527  0.000000
C    -1.375269  0.487539  0.000000
H    -1.936453  1.417057  0.000000
C    -2.080134 -0.759268  0.000000
C    -3.495236 -0.767430  0.000000
H    -4.070994  0.153148  0.000000
C    -4.107603 -1.994737  0.000000
C    -3.385295 -3.213259  0.000000
C    -2.006765 -3.239588  0.000000
H    -1.448667 -4.171740  0.000000
C    -1.341563 -2.007538  0.000000
O    -5.425535 -2.268521  0.000000
```

```
O    -4.255367 -4.241863  0.000000
N     4.257345  4.226805  0.000000
O     5.379938  3.729000  0.000000
O     4.027326  5.433256  0.000000
C    -5.555397 -3.680742  0.000000
H    -6.089167 -3.996756  0.905528
H    -6.089167 -3.996756 -0.905528
 total energy= -1199.40986002

pbe0.tddft--6
B     0.474480  1.604096  0.000251
O     0.546678  2.962706 -0.001301
H    -0.372566  3.302024 -0.000611
N    -0.796586  0.928519  0.002084
C    -2.068518  1.556523  0.002886
O    -2.204556  2.790175  0.000679
C    -3.031879  0.478402  0.005288
C    -4.420680  0.501406  0.004058
H    -4.957962  1.448084  0.005844
C    -5.115500 -0.722009  0.002041
C    -4.408572 -1.957556  0.001959
H    -4.970073 -2.889388  0.008122
C    -3.022617 -1.973581  0.003285
H    -2.493046 -2.924858  0.002026
C    -2.324151 -0.764476  0.004244
C    -0.924810 -0.456382  0.003067
C     0.188455 -1.290931  0.002449
H     0.036876 -2.366892  0.003887
C     1.499743 -0.766462  0.001074
C     2.621272 -1.650762  0.000846
H     2.488209 -2.728835  0.002030
C     3.860455 -1.083416 -0.000847
C     4.055956  0.319624 -0.002368
C     3.003409  1.203911 -0.002170
H     3.157507  2.279451 -0.003174
C     1.702484  0.672862 -0.000253
O     5.069372 -1.695386 -0.001665
O     5.382067  0.581013 -0.004018
N    -6.484497 -0.735856  0.034643
H    -6.980339  0.117615 -0.165757
H    -6.967397 -1.586974 -0.202966
C     6.047695 -0.670631 -0.001574
H     6.663312 -0.752158  0.904118
H     6.665730 -0.754385 -0.905338
 total energy= -1050.40817278

pbe0.tddft--thieno
B     1.026339  1.450167  0.000025
O     1.136298  2.796043  0.000083
H     0.229745  3.169641  0.000137
N    -0.268870  0.798776  0.000013
C    -1.548703  1.488330 -0.000023
O    -1.597206  2.719550 -0.000102
C    -2.550163  0.462092 -0.000024
C    -3.952423  0.529114 -0.000062
H    -4.458442  1.491120 -0.000096
C    -4.670195 -0.666018 -0.000050
C    -4.034158 -1.917953 -0.000002
H    -4.624160 -2.829979  0.000005
C    -2.625809 -1.988128  0.000032
H    -2.125013 -2.955172  0.000064
C    -1.906840 -0.809934  0.000019
C    -0.467127 -0.557745  0.000031
C     0.597217 -1.465301  0.000053
H     0.388333 -2.530556  0.000071
C     1.920489 -0.977501  0.000037
C     3.099191 -1.751747  0.000078
H     3.178756 -2.832641  0.000114
S     4.489475 -0.776606 -0.000107
C     3.551414  0.692414  0.000100
H     4.058156  1.650706  0.000150
C     2.206598  0.449523  0.000024
H    -5.758265 -0.627320 -0.000077
 total energy= -739.543260592

pbe0.tddft--7
B     2.471396  1.443205  0.000051
O     2.657815  2.780251  0.000133
H     1.777426  3.209262  0.000214
N     1.143366  0.862562  0.000049
C    -0.095014  1.617374  0.000018
O    -0.084256  2.847348 -0.000099
C    -1.151019  0.644760  0.000012
C    -2.545629  0.800259 -0.000038
H    -3.003897  1.784141 -0.000079
C    -3.313034 -0.362320 -0.000024
C    -2.765572 -1.655330  0.000035
H    -3.413168 -2.524698  0.000041
C    -1.361828 -1.794350  0.000079
H    -0.921253 -2.789702  0.000117
C    -0.578003 -0.660083  0.000065
C     0.872423 -0.483850  0.000074
C     1.884381 -1.445523  0.000094
H     1.619615 -2.498316  0.000118
C     3.233132 -1.029302  0.000062
C     4.366847 -1.866698  0.000110
H     4.387263 -2.950354  0.000160
S     5.807761 -0.968749 -0.000163
C     4.951050  0.549253  0.000136
H     5.509200  1.478551  0.000200
C     3.595397  0.379409  0.000042
Br   -5.211062 -0.189864 -0.000086
 total energy= -752.121342387

pbe0.tddft--8
B    -2.050651  1.437912  0.000029
```

```
O    -2.221575  2.768851  0.000031
H    -1.357689  3.220704  0.000195
N    -0.709654  0.836056  0.000239
C     0.518383  1.574274  0.000443
O     0.531932  2.786119  0.000023
C     1.597691  0.583969  0.000243
C     2.967548  0.773043 -0.000002
H     3.438364  1.749844 -0.000138
C     3.760732 -0.388932 -0.000048
C     3.181400 -1.673281  0.000157
H     3.856486 -2.522730  0.000092
C     1.799628 -1.834045  0.000346
H     1.367443 -2.832441  0.000420
C     1.004315 -0.687998  0.000354
C    -0.456447 -0.510895  0.000334
C    -1.481533 -1.443722  0.000277
H    -1.233858 -2.500792  0.000320
C    -2.835804 -1.013616  0.000075
C    -3.971418 -1.837033 -0.000054
H    -4.000475 -2.920889 -0.000007
S    -5.418594 -0.930185 -0.000329
C    -4.537369  0.574826 -0.000273
H    -5.079967  1.513949 -0.000408
C    -3.183304  0.387182 -0.000070
N     5.179081 -0.267317 -0.000356
O     5.651491  0.883493 -0.000414
O     5.849594 -1.315718 -0.000293
 total energy= -943.849267251

pbe0.tddft--9
B     1.419878  1.446896  0.000272
O     1.567657  2.794554  0.001224
H     0.669503  3.186851  0.000952
N     0.106699  0.841563 -0.001034
C    -1.125366  1.558069 -0.001866
O    -1.176623  2.797534 -0.000782
C    -2.161539  0.554042 -0.002644
C    -3.546056  0.669819 -0.002439
H    -4.022090  1.648562 -0.004070
C    -4.321097 -0.510397 -0.000975
C    -3.707368 -1.795776 -0.001168
H    -4.332081 -2.685778 -0.004032
C    -2.323442 -1.901005 -0.001809
H    -1.856637 -2.884339 -0.001196
C    -1.546231 -0.740715 -0.002066
C    -0.129493 -0.532198 -0.001539
C     0.908500 -1.461074 -0.001070
H     0.675103 -2.521833 -0.001756
C     2.247452 -1.010270 -0.000127
C     3.397718 -1.811308  0.000476
H     3.455016 -2.893433  0.000138
S     4.814295 -0.865559  0.001518
C     3.921574  0.621381  0.001846
H     4.451735  1.566586  0.002640
C     2.568106  0.413218  0.000599
N    -5.679594 -0.424497 -0.015076
H    -6.136063  0.467625  0.077722
H    -6.247156 -1.248660  0.089880
 total energy= -794.846248570

pbe0.tddft-mecn--benzo
B    -1.106289  1.403707  0.000000
O    -1.223138  2.757091  0.000000
H    -0.316182  3.130425  0.000000
N     0.219327  0.798977  0.000000
C     1.455816  1.497662  0.000000
O     1.511625  2.737282  0.000000
C     2.477096  0.476451  0.000000
C     3.870395  0.558670 -0.000001
H     4.372991  1.524057 -0.000001
C     4.605947 -0.627196 -0.000001
C     3.970907 -1.888698 -0.000001
H     4.575116 -2.792868 -0.000001
C     2.582971 -1.985414  0.000000
H     2.093083 -2.957322  0.000000
C     1.831769 -0.800998  0.000000
C     0.424346 -0.562671  0.000000
C    -0.667189 -1.467156  0.000000
H    -0.451200 -2.532877  0.000000
C    -1.987992 -1.013703  0.000000
C    -3.073769 -1.951731  0.000001
H    -2.843686 -3.015983  0.000001
C    -4.376300 -1.514114  0.000001
C    -4.659699 -0.128641  0.000001
C    -3.620213  0.803381  0.000001
H    -3.859015  1.866104  0.000000
C    -2.282144  0.406668  0.000000
H    -5.193772 -2.232141  0.000001
H    -5.694018  0.209608  0.000001
H     5.693316 -0.580409 -0.000002
 total energy= -806.788057787

pbe0.tddft-mecn--1
B     1.205498 -2.637947  0.000000
O     0.552127 -3.828383  0.000000
H    -0.409583 -3.640789  0.000000
N     0.444075 -1.396416  0.000000
C    -0.971451 -1.287370  0.000000
O    -1.711397 -2.280944  0.000000
C    -1.247584  0.130566  0.000000
C    -2.455464  0.827511  0.000000
H    -3.407907  0.303792  0.000000
C    -2.387597  2.218655  0.000000
C    -1.167523  2.931906  0.000000
H    -1.168901  4.017600  0.000000
C     0.033004  2.231185  0.000000
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H     0.977046  2.772149  0.000000
C     0.000000  0.831997  0.000000
C     1.035587 -0.151709  0.000000
C     2.443410 -0.008366  0.000000
H     2.858286  0.996610  0.000000
C     3.286365 -1.123716  0.000000
C     4.710391 -0.952204  0.000000
H     5.114866  0.058521  0.000000
C     5.545643 -2.043711  0.000000
C     5.006403 -3.350325  0.000000
C     3.623654 -3.542421  0.000000
H     3.226354 -4.556300  0.000000
C     2.737318 -2.464767  0.000000
H     6.624683 -1.905409  0.000000
H     5.675110 -4.208837  0.000000
Br   -4.014421  3.214815  0.000000
 total energy= -819.366342045

pbe0.tddft-mecn--2
B    -2.489756  0.502087  0.000000
O    -3.565535 -0.312728  0.000000
H    -3.275719 -1.243836  0.000000
N    -1.135983 -0.058773  0.000000
C    -0.804794 -1.433830  0.000000
O    -1.646078 -2.317856  0.000000
C     0.659677 -1.489876  0.000000
C     1.502553 -2.578068  0.000000
H     1.138431 -3.600703  0.000000
C     2.883413 -2.314157  0.000000
C     3.389581 -0.990485  0.000000
H     4.464604 -0.846580  0.000000
C     2.525152  0.092466  0.000000
H     2.917251  1.106913  0.000000
C     1.143640 -0.153843  0.000000
C     0.000000  0.716161  0.000000
C    -0.085966  2.119995  0.000000
H     0.839461  2.690407  0.000000
C    -1.323075  2.787217  0.000000
C    -1.361654  4.215900  0.000000
H    -0.423104  4.766920  0.000000
C    -2.570028  4.880823  0.000000
C    -3.774079  4.155214  0.000000
C    -3.756694  2.753061  0.000000
H    -4.699887  2.209689  0.000000
C    -2.558984  2.047909  0.000000
H    -2.593536  5.968265  0.000000
H    -4.724491  4.684561  0.000000
N     3.791247 -3.408396  0.000000
O     3.330817 -4.560619  0.000000
O     5.006603 -3.162148  0.000000
 total energy= -1011.09441633

pbe0.tddft-mecn--2-
B    -2.492182  0.402044  0.000000
O    -3.509496 -0.438368  0.000000
N    -1.125287 -0.074355  0.000000
C    -0.768858 -1.423796  0.000000
O    -1.570363 -2.340189  0.000000
C     0.706017 -1.437878  0.000000
C     1.560851 -2.517342  0.000000
H     1.203367 -3.542359  0.000000
C     2.941882 -2.249627  0.000000
C     3.416690 -0.907281  0.000000
H     4.490166 -0.748477  0.000000
C     2.541390  0.159585  0.000000
H     2.925412  1.177938  0.000000
C     1.155676 -0.092860  0.000000
C     0.000000  0.765106  0.000000
C    -0.151218  2.122681  0.000000
H     0.732097  2.756823  0.000000
C    -1.454498  2.739321  0.000000
C    -1.578606  4.146742  0.000000
H    -0.674753  4.754754  0.000000
C    -2.825297  4.754783  0.000000
C    -3.995538  3.985612  0.000000
C    -3.893807  2.596115  0.000000
H    -4.801300  1.994723  0.000000
C    -2.646584  1.962999  0.000000
H    -2.891243  5.841875  0.000000
H    -4.971187  4.466957  0.000000
N     3.853555 -3.315791  0.000000
O     3.413177 -4.488868  0.000000
O     5.079418 -3.058374  0.000000
 total energy= -1010.62338577

pbe0.tddft-mecn--3
B     1.500247  1.391553 -0.000144
O     1.651529  2.749651 -0.000407
H     0.748732  3.133595 -0.000693
N     0.162626  0.828548 -0.000061
C    -1.036975  1.556963  0.000131
O    -1.078381  2.805913  0.000436
C    -2.093502  0.565334  0.000047
C    -3.470941  0.701506  0.000110
H    -3.952170  1.677885  0.000227
C    -4.263767 -0.473489  0.000000
C    -3.649426 -1.773280 -0.000144
H    -4.293755 -2.649663 -0.000220
C    -2.283922 -1.901089 -0.000164
H    -1.825351 -2.887660 -0.000253
C    -1.482508 -0.736362 -0.000075
C    -0.079994 -0.547654 -0.000036
C     0.973509 -1.469317 -0.000013
H     0.736484 -2.531001  0.000012
C     2.316430 -1.045001  0.000033
C     3.376961 -2.000298  0.000131
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H     3.126642 -3.060681  0.000189
C     4.692007 -1.594166  0.000154
C     5.013296 -0.216386  0.000063
C     3.997999  0.730685 -0.000029
H     4.254510  1.789854 -0.000105
C     2.642213  0.363352 -0.000024
H     5.489961 -2.334786  0.000231
H     6.056091  0.095661  0.000066
N    -5.603582 -0.385551  0.000007
H    -6.066890  0.513102  0.000229
H    -6.182262 -1.214348  0.000069
 total energy= -862.103276174

pbe0.tddft-mecn--dioxo
B    -0.072945  1.571166  0.000038
O    -0.079037  2.931723  0.000121
H     0.860339  3.219148  0.000213
N     1.185990  0.856521  0.000008
C     2.473065  1.443752 -0.000009
O     2.636090  2.678884 -0.000140
C     3.402371  0.340761 -0.000018
C     4.801089  0.306207 -0.000061
H     5.380312  1.227781 -0.000103
C     5.434717 -0.933062 -0.000031
C     4.696051 -2.138642  0.000032
H     5.223319 -3.089925  0.000049
C     3.304831 -2.118781  0.000059
H     2.736528 -3.047451  0.000089
C     2.654197 -0.879023  0.000034
C     1.265142 -0.526152  0.000021
C     0.113453 -1.326409  0.000019
H     0.233346 -2.406538  0.000014
C    -1.173826 -0.765312  0.000007
C    -2.319963 -1.623688 -0.000014
H    -2.208116 -2.704410 -0.000027
C    -3.542887 -1.024863 -0.000018
C    -3.699641  0.387288  0.000003
C    -2.618153  1.248996  0.000021
H    -2.762381  2.326477  0.000033
C    -1.337147  0.685842  0.000016
O    -4.762304 -1.596021 -0.000035
O    -5.001633  0.688590  0.000002
H     6.522412 -0.977658 -0.000054
C    -5.720561 -0.546040 -0.000047
H    -6.332136 -0.604759 -0.907564
H    -6.332198 -0.604796  0.907425
 total energy= -995.139063885

pbe0.tddft-mecn--4
B    -1.549977  1.650895  0.000013
O    -1.652716  3.006973  0.000017
H    -0.738218  3.363626  0.000033
N    -0.245241  1.024147  0.000020
C     0.996446  1.701117  0.000022
O     1.075974  2.942652 -0.000009
C     1.999989  0.665499  0.000014
C     3.396166  0.744362 -0.000003
H     3.905727  1.704371 -0.000016
C     4.099606 -0.452790 -0.000001
C     3.471388 -1.719032  0.000017
H     4.068610 -2.625848  0.000016
C     2.081992 -1.790113  0.000031
H     1.589466 -2.760597  0.000039
C     1.342168 -0.604847  0.000029
C    -0.070277 -0.350607  0.000028
C    -1.160209 -1.227078  0.000029
H    -0.967006 -2.296549  0.000034
C    -2.485824 -0.756163  0.000017
C    -3.566282 -1.692875  0.000012
H    -3.378212 -2.762896  0.000020
C    -4.829010 -1.181501 -0.000004
C    -5.084604  0.216266 -0.000015
C    -4.066555  1.152219 -0.000009
H    -4.286238  2.216795 -0.000017
C    -2.750081  0.679135  0.000006
O    -6.004067 -1.836438 -0.000016
O    -6.403534  0.425221 -0.000034
Br    6.010920 -0.394738 -0.000023
C    -7.034142 -0.856594 -0.000027
H    -7.639810 -0.957922 -0.907642
H    -7.639817 -0.957909  0.907585
 total energy= -1007.71811287

pbe0.tddft-mecn--5
B     0.285122 -1.957146  0.000000
O     1.118527 -3.021839  0.000000
H     2.041596 -2.703708  0.000000
N     0.812467 -0.601359  0.000000
C     2.172095 -0.245924  0.000000
O     3.079240 -1.068271  0.000000
C     2.199901  1.218947  0.000000
C     3.276914  2.080005  0.000000
H     4.304144  1.728899  0.000000
C     2.995176  3.453944  0.000000
C     1.662785  3.940936  0.000000
H     1.503084  5.013740  0.000000
C     0.593903  3.059691  0.000000
H    -0.425967  3.438100  0.000000
C     0.857340  1.682547  0.000000
C     0.000000  0.522996  0.000000
C    -1.384083  0.412101  0.000000
H    -1.976350  1.323112  0.000000
C    -2.039144 -0.844405  0.000000
C    -3.462251 -0.888831  0.000000
H    -4.052681  0.022941  0.000000
C    -4.041848 -2.126022  0.000000
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C    -3.279959 -3.320327  0.000000
C    -1.892521 -3.311535  0.000000
H    -1.327121 -4.239637  0.000000
C    -1.260821 -2.068710  0.000000
O    -5.347366 -2.444044  0.000000
O    -4.098950 -4.370971  0.000000
N     4.076726  4.377547  0.000000
O     5.236337  3.935904  0.000000
O     3.812680  5.589314  0.000000
C    -5.435244 -3.863035  0.000000
H    -5.946937 -4.203016  0.907337
H    -5.946937 -4.203016 -0.907337
 total energy= -1199.44665688

pbe0.tddft-mecn--5-
B     1.089265  1.632439 -0.007275
O     1.164570  2.953095 -0.001574
N    -0.194826  0.963550 -0.003474
C    -1.420397  1.628974  0.003737
O    -1.537453  2.841114  0.009370
C    -2.442480  0.565546  0.003369
C    -3.814437  0.684719  0.009086
H    -4.314297  1.648332  0.015593
C    -4.567889 -0.503075  0.005853
C    -3.917429 -1.769055 -0.002963
H    -4.538329 -2.659102 -0.005804
C    -2.540156 -1.864565 -0.007868
H    -2.064469 -2.843455 -0.014595
C    -1.772136 -0.684159 -0.004558
C    -0.353897 -0.430458 -0.008187
C     0.741856 -1.244897 -0.014910
H     0.603807 -2.323318 -0.018354
C     2.085221 -0.715497 -0.019747
C     3.183173 -1.618589 -0.024223
H     3.020271 -2.693699 -0.028348
C     4.449211 -1.086277 -0.023927
C     4.684251  0.291882 -0.025443
C     3.646383  1.194277 -0.023106
H     3.838910  2.264050 -0.028887
C     2.330579  0.684213 -0.017730
O     5.636635 -1.744337 -0.055161
O     6.028018  0.521676 -0.070969
N    -5.969053 -0.433762  0.011085
O    -6.518851  0.692647  0.021391
O    -6.624188 -1.502019  0.005477
C     6.630551 -0.744257  0.168912
H     6.970752 -0.800021  1.214030
H     7.459896 -0.893602 -0.528562
 total energy= -1198.96303380

pbe0.tddft-mecn--6
B     0.472710  1.606158  0.000030
O     0.515037  2.973098  0.000004
H    -0.417397  3.279844 -0.000002
N    -0.808357  0.934835  0.000044
C    -2.068072  1.559267  0.000012
O    -2.208792  2.802034  0.000017
C    -3.035260  0.483112  0.000032
C    -4.422648  0.503907  0.000000
H    -4.979944  1.439238 -0.000032
C    -5.116772 -0.728573 -0.000021
C    -4.395046 -1.969200  0.000001
H    -4.962453 -2.897507 -0.000014
C    -3.020807 -1.984207  0.000030
H    -2.484834 -2.931519  0.000031
C    -2.317190 -0.761346  0.000044
C    -0.934569 -0.456215  0.000050
C     0.194959 -1.283623  0.000057
H     0.048111 -2.361099  0.000069
C     1.497472 -0.754330  0.000038
C     2.622542 -1.643769  0.000029
H     2.479508 -2.721407  0.000044
C     3.864117 -1.083593 -0.000011
C     4.063395  0.317467 -0.000041
C     3.011137  1.204672 -0.000025
H     3.184676  2.278278 -0.000048
C     1.701998  0.683598  0.000018
O     5.067968 -1.700297 -0.000062
O     5.385629  0.579797 -0.000113
N    -6.464001 -0.756179  0.000096
H    -7.003774  0.097381 -0.000791
H    -6.966383 -1.632166 -0.000881
C     6.058925 -0.678354  0.000033
H     6.670681 -0.761144  0.906367
H     6.670930 -0.761220 -0.906122
 total energy= -1050.44851970

pbe0.tddft-mecn--thieno
B    -1.020318  1.445495 -0.000063
O    -1.106407  2.796041 -0.000235
H    -0.186748  3.143196 -0.000404
N     0.283680  0.796914 -0.000055
C     1.539019  1.485556 -0.000013
O     1.597877  2.726552  0.000197
C     2.544693  0.460592 -0.000009
C     3.943087  0.527772  0.000071
H     4.454470  1.488672  0.000145
C     4.667100 -0.662513  0.000026
C     4.020817 -1.919906 -0.000085
H     4.615788 -2.830101 -0.000111
C     2.629503 -2.001387 -0.000141
H     2.131226 -2.969354 -0.000201
C     1.889210 -0.814175 -0.000098
C     0.477763 -0.569002 -0.000087
C    -0.611122 -1.472139 -0.000118
H    -0.411231 -2.539824 -0.000178
```

```
C    -1.920333 -0.976581 -0.000056
C    -3.104791 -1.749435 -0.000162
H    -3.187785 -2.831486 -0.000241
S    -4.489868 -0.766865  0.000482
C    -3.549474  0.702093 -0.000217
H    -4.066239  1.656667 -0.000383
C    -2.205889  0.454208 -0.000011
H     5.754971 -0.625039  0.000073
 total energy= -739.572840737

pbe0.tddft-mecn--7
B    -2.465479  1.438015  0.000001
O    -2.630310  2.780863  0.000055
H    -1.736040  3.185805  0.000125
N    -1.127801  0.861837  0.000026
C     0.087047  1.617012  0.000049
O     0.083354  2.856977 -0.000014
C     1.147078  0.646298  0.000047
C     2.537244  0.801241  0.000036
H     2.994668  1.787402  0.000026
C     3.306860 -0.356651  0.000047
C     2.750977 -1.656892  0.000065
H     3.397414 -2.528881  0.000071
C     1.365494 -1.803800  0.000068
H     0.926964 -2.799805  0.000071
C     0.562781 -0.662405  0.000057
C    -0.861378 -0.492687  0.000032
C    -1.895052 -1.453622  0.000009
H    -1.636189 -2.508497  0.000021
C    -3.231052 -1.030295 -0.000035
C    -4.371163 -1.866502 -0.000039
H    -4.394628 -2.951801 -0.000026
S    -5.807164 -0.960626 -0.000237
C    -4.947923  0.556973 -0.000024
H    -5.514217  1.482824  0.000011
C    -3.593099  0.381849 -0.000046
Br    5.209355 -0.191594  0.000040
 total energy= -752.151661470

pbe0.tddft-mecn--8
B     2.046075  1.445137  0.000006
O     2.211764  2.780474  0.000033
H     1.343295  3.224152  0.000039
N     0.701364  0.850950  0.000013
C    -0.511097  1.582035  0.000016
O    -0.547641  2.799665 -0.000030
C    -1.588504  0.586423 -0.000005
C    -2.954202  0.765850 -0.000043
H    -3.417153  1.747196 -0.000069
C    -3.748174 -0.397559 -0.000052
C    -3.163856 -1.687341 -0.000014
H    -3.822631 -2.549205 -0.000023
C    -1.785922 -1.843273  0.000022
H    -1.346792 -2.838165  0.000040
C    -0.985553 -0.692270  0.000022
C     0.447672 -0.503894  0.000034
C     1.485175 -1.441318  0.000055
H     1.239062 -2.499357  0.000082
C     2.825635 -1.008983  0.000050
C     3.958404 -1.843018  0.000131
H     3.977978 -2.928613  0.000176
S     5.401717 -0.940067 -0.000160
C     4.531825  0.577031  0.000124
H     5.092691  1.506314  0.000177
C     3.180263  0.395639  0.000025
N    -5.158041 -0.271199 -0.000103
O    -5.650921  0.875843  0.000023
O    -5.847898 -1.311123  0.000043
 total energy= -943.884336470

pbe0.tddft-mecn--8-
B    -2.015155  1.445570 -0.000577
O    -2.173063  2.754474  0.000188
N    -0.703096  0.831710 -0.000099
C     0.479704  1.565993  0.000434
O     0.522409  2.783687 -0.000115
C     1.565321  0.567313  0.000067
C     2.928078  0.770582 -0.000106
H     3.368050  1.762804 -0.000079
C     3.753351 -0.369590 -0.000160
C     3.178216 -1.672060 -0.000111
H     3.852482 -2.522256 -0.000164
C     1.810079 -1.851249 -0.000022
H     1.393835 -2.856854 -0.000048
C     0.971920 -0.718978  0.000062
C    -0.459953 -0.558463  0.000014
C    -1.488954 -1.452966 -0.000052
H    -1.274593 -2.518385  0.000026
C    -2.857536 -0.996149 -0.000057
C    -3.991022 -1.783264  0.000123
H    -4.054453 -2.866288  0.000275
S    -5.436550 -0.831076  0.000067
C    -4.536966  0.644207  0.000044
H    -5.062055  1.593620  0.000037
C    -3.188483  0.412763 -0.000197
N     5.145645 -0.218826 -0.000161
O     5.630315  0.940878  0.000187
O     5.864957 -1.249326  0.000159
 total energy= -943.411453974

pbe0.tddft-mecn--9
B     1.414560  1.437039 -0.000020
O     1.538448  2.792047 -0.000094
H     0.621995  3.151256 -0.000135
N     0.097262  0.835203  0.000003
C    -1.119205  1.554487  0.000039
```

```
O    -1.162387  2.806417  0.000089
C    -2.160150  0.558858  0.000030
C    -3.544241  0.678056  0.000044
H    -4.036416  1.649159  0.000066
C    -4.324644 -0.503059  0.000015
C    -3.701604 -1.798567 -0.000022
H    -4.337250 -2.681100 -0.000041
C    -2.332303 -1.910135 -0.000032
H    -1.864136 -2.892575 -0.000061
C    -1.540979 -0.741360 -0.000007
C    -0.136623 -0.546561 -0.000007
C     0.913162 -1.470575 -0.000039
H     0.685589 -2.533264 -0.000074
C     2.248869 -1.013274 -0.000040
C     3.402468 -1.809071 -0.000142
H     3.466844 -2.892158 -0.000209
S     4.819339 -0.853650  0.000190
C     3.923554  0.627943 -0.000196
H     4.459730  1.571528 -0.000323
C     2.568525  0.412244 -0.000024
N    -5.667404 -0.425442  0.000050
H    -6.137935  0.469222 -0.000068
H    -6.239117 -1.258801 -0.000141
 total energy= -794.885772874

b97d--benzo
B     1.135883  1.410931  0.000000
O     1.293519  2.768312  0.000003
H     0.412969  3.199171  0.000009
N    -0.208599  0.805596  0.000005
C    -1.444792  1.497599  0.000010
O    -1.549801  2.725195 -0.000005
C    -2.496434  0.453414  0.000002
C    -3.890185  0.583774 -0.000005
H    -4.351323  1.573996 -0.000007
C    -4.658494 -0.592082 -0.000006
C    -4.032298 -1.859969 -0.000002
H    -4.650924 -2.761151 -0.000003
C    -2.632692 -1.986625  0.000004
H    -2.161779 -2.972697  0.000006
C    -1.863272 -0.812303  0.000006
C    -0.417201 -0.588603  0.000006
C     0.631629 -1.466109  0.000004
H     0.424742 -2.538812  0.000005
C     2.012856 -1.014110  0.000001
C     3.072656 -1.955246 -0.000001
H     2.839201 -3.024303  0.000001
C     4.403671 -1.524870 -0.000005
C     4.705471 -0.147120 -0.000007
C     3.665058  0.793752 -0.000005
H     3.890921  1.863258 -0.000007
C     2.313525  0.389751 -0.000002
H     5.212169 -2.261193 -0.000006
H     5.747490  0.183547 -0.000010
H    -5.749424 -0.531210 -0.000010
    el energy= -807.203094374
          zpe= -806.988936
    th energy= -806.975168
  th enthalpy= -806.974224
  free energy= -807.029198

b97d--1
B     1.255802 -2.656128  0.000000
O     0.633862 -3.871855  0.000000
H    -0.337900 -3.745954  0.000000
N     0.473056 -1.404655  0.000000
C    -0.937417 -1.294870  0.000000
O    -1.710323 -2.252953  0.000000
C    -1.229432  0.160586  0.000000
C    -2.465763  0.814431  0.000000
H    -3.399946  0.251716  0.000000
C    -2.437294  2.217460  0.000000
C    -1.222012  2.941014  0.000000
H    -1.245778  4.031606  0.000000
C     0.007344  2.263658  0.000000
H     0.941773  2.829542  0.000000
C     0.000000  0.859393  0.000000
C     1.075960 -0.129595  0.000000
C     2.435766  0.016583  0.000000
H     2.859945  1.023336  0.000000
C     3.332584 -1.126672  0.000000
C     4.736379 -0.932202  0.000000
H     5.135872  0.086435  0.000000
C     5.603894 -2.029681  0.000000
C     5.089045 -3.342617  0.000000
C     3.701157 -3.547475  0.000000
H     3.295142 -4.562301  0.000000
C     2.802127 -2.460613  0.000000
H     6.685150 -1.867053  0.000000
H     5.771626 -4.196477  0.000000
Br   -4.103961  3.194412  0.000000
    el energy= -819.802609087
          zpe= -819.598536
    th energy= -819.583164
  th enthalpy= -819.582220
  free energy= -819.642105

b97d--2
B    -2.520228  0.504145  0.000000
O    -3.618286 -0.306061  0.000000
H    -3.340631 -1.245611  0.000000
N    -1.156872 -0.062515  0.000000
C    -0.814224 -1.435908  0.000000
O    -1.628944 -2.356967  0.000000
C     0.670290 -1.480341  0.000000
C     1.526024 -2.582240  0.000000
```

```
H     1.152790 -3.605874  0.000000
C     2.902196 -2.307908  0.000000
C     3.412568 -0.990414  0.000000
H     4.492707 -0.848247  0.000000
C     2.538167  0.103190  0.000000
H     2.931224  1.121965  0.000000
C     1.154300 -0.148129  0.000000
C     0.000000  0.743234  0.000000
C    -0.078452  2.110258  0.000000
H     0.845519  2.693051  0.000000
C    -1.351938  2.805932  0.000000
C    -1.389920  4.223068  0.000000
H    -0.450816  4.784340  0.000000
C    -2.614848  4.898005  0.000000
C    -3.824828  4.173225  0.000000
C    -3.799687  2.770301  0.000000
H    -4.734555  2.204189  0.000000
C    -2.580272  2.062018  0.000000
H    -2.632890  5.991086  0.000000
H    -4.779311  4.705918  0.000000
N     3.862420 -3.447148  0.000000
O     3.392341 -4.584986  0.000000
O     5.065140 -3.179442  0.000000
    el energy= -1011.59251428
          zpe= -1011.376038
    th energy= -1011.359616
  th enthalpy= -1011.358671
  free energy= -1011.420520

b97d--3
B    -1.532416  1.402630  0.000761
O    -1.714417  2.758159  0.002677
H    -0.840347  3.202769  0.001537
N    -0.176460  0.823537 -0.001689
C     1.044100  1.540245 -0.002637
O     1.126047  2.770599 -0.000211
C     2.118613  0.518973 -0.006214
C     3.501992  0.695667 -0.004785
H     3.933870  1.699909 -0.007308
C     4.323201 -0.456887 -0.003424
C     3.712636 -1.744880  0.000189
H     4.357652 -2.628668 -0.000641
C     2.322311 -1.904427 -0.001020
H     1.888085 -2.907262  0.004109
C     1.510194 -0.757764 -0.004675
C     0.062642 -0.568112 -0.002632
C    -0.972027 -1.463480 -0.001686
H    -0.746621 -2.532537 -0.002855
C    -2.361538 -1.037189  0.000093
C    -3.404546 -1.997170  0.000417
H    -3.151211 -3.061814 -0.000799
C    -4.743799 -1.592417  0.002008
C    -5.072817 -0.221066  0.003355
C    -4.049557  0.738565  0.003049
H    -4.295417  1.803817  0.003973
C    -2.690582  0.360532  0.001436
H    -5.537682 -2.344728  0.002103
H    -6.120909  0.089985  0.004523
N     5.711447 -0.342580 -0.063174
H     6.094153  0.544509  0.246084
H     6.237612 -1.139418  0.278947
    el energy= -862.522185586
          zpe= -862.291614
    th energy= -862.276324
  th enthalpy= -862.275380
  free energy= -862.333412

b97d--dioxo
B     0.091655  1.592738 -0.003250
O     0.125987  2.960399 -0.000888
H    -0.791046  3.307327  0.002082
N    -1.192055  0.869497 -0.000490
C    -2.486296  1.447609  0.003822
O    -2.701165  2.661306  0.006219
C    -3.437790  0.312733  0.004546
C    -4.837623  0.316008  0.008071
H    -5.385940  1.260760  0.010896
C    -5.496982 -0.924116  0.007817
C    -4.758183 -2.130137  0.004109
H    -5.292770 -3.083701  0.003938
C    -3.353053 -2.130077  0.000566
H    -2.795228 -3.069804 -0.002370
C    -2.691632 -0.891086  0.000804
C    -1.273578 -0.536130 -0.002313
C    -0.145642 -1.311678 -0.006584
H    -0.253398 -2.398746 -0.007862
C     1.187495 -0.738255 -0.010582
C     2.319705 -1.607413 -0.014301
H     2.202052 -2.692639 -0.017880
C     3.571872 -1.016863 -0.014136
C     3.742406  0.381120 -0.013188
C     2.661626  1.250371 -0.012319
H     2.797286  2.332816 -0.014827
C     1.357667  0.688481 -0.009232
O     4.798014 -1.635983 -0.036976
O     5.084989  0.683695 -0.037307
H    -6.588936 -0.962195  0.010483
C     5.769124 -0.576141  0.089301
H     6.243752 -0.636528  1.087397
H     6.513037 -0.669344 -0.718844
    el energy= -995.614714978
          zpe= -995.385638
    th energy= -995.369426
  th enthalpy= -995.368481
  free energy= -995.429568
```

```
b97d--4
B    -1.583237  1.671713 -0.004180
O    -1.713488  3.032707 -0.000926
H    -0.825964  3.448128  0.001116
N    -0.251460  1.037861 -0.003638
C     0.998070  1.703315 -0.000090
O     1.134832  2.926993  0.002652
C     2.024562  0.632017 -0.000331
C     3.419047  0.742272  0.002776
H     3.906442  1.718043  0.005669
C     4.146992 -0.457306  0.002071
C     3.509081 -1.719983 -0.001615
H     4.113833 -2.628007 -0.001963
C     2.108502 -1.807237 -0.004781
H     1.623140 -2.786020 -0.007610
C     1.360843 -0.617904 -0.004122
C    -0.075557 -0.359765 -0.006304
C    -1.148327 -1.210531 -0.010177
H    -0.966505 -2.287650 -0.012315
C    -2.516934 -0.729971 -0.012018
C    -3.586864 -1.674630 -0.015286
H    -3.395511 -2.749221 -0.020394
C    -4.876425 -1.170890 -0.012381
C    -5.141553  0.212456 -0.008548
C    -4.122410  1.153755 -0.008485
H    -4.331667  2.224317 -0.008837
C    -2.783626  0.682025 -0.008724
O    -6.056842 -1.871675 -0.032220
O    -6.500281  0.423661 -0.026447
Br    6.078610 -0.389695  0.006376
C    -7.099710 -0.880879  0.084955
H    -7.824203 -1.019741 -0.734309
H    -7.582440 -0.978075  1.075733
    el energy= -1008.21445177
          zpe= -1007.995530
    th energy= -1007.977687
  th enthalpy= -1007.976743
  free energy= -1008.042819

b97d--5
B    -1.131140  1.664228 -0.000607
O    -1.250760  3.025125 -0.000181
H    -0.361483  3.436321  0.000121
N     0.193737  1.017135 -0.000451
C     1.451205  1.668850  0.000078
O     1.601627  2.889685  0.000445
C     2.464560  0.584197  0.000099
C     3.856835  0.669027  0.000574
H     4.379251  1.625253  0.000969
C     4.561293 -0.545065  0.000540
C     3.907926 -1.798751  0.000042
H     4.514876 -2.703486  0.000058
C     2.509988 -1.865039 -0.000457
H     2.005502 -2.833667 -0.000843
C     1.782613 -0.660196 -0.000426
C     0.353862 -0.382043 -0.000802
C    -0.728785 -1.223636 -0.001430
H    -0.556188 -2.302213 -0.001724
C    -2.090122 -0.730604 -0.001835
C    -3.169675 -1.665336 -0.002467
H    -2.988865 -2.741650 -0.003353
C    -4.453355 -1.148405 -0.002136
C    -4.703161  0.238581 -0.001508
C    -3.674381  1.170363 -0.001436
H    -3.873506  2.242759 -0.001552
C    -2.341534  0.685186 -0.001354
O    -5.639885 -1.835875 -0.005873
O    -6.056228  0.466078 -0.004686
N     6.048413 -0.513478  0.001069
O     6.593593  0.591059  0.001429
O     6.642758 -1.593546  0.001118
C    -6.678801 -0.833920  0.014129
H    -7.309822 -0.948005 -0.884253
H    -7.268761 -0.941523  0.941598
    el energy= -1200.00495688
          zpe= -1199.773700
    th energy= -1199.754711
  th enthalpy= -1199.753767
  free energy= -1199.823276

b97d--6
B     0.496479  1.622859 -0.003953
O     0.565609  2.990142 -0.002785
H    -0.343010  3.358742  0.001484
N    -0.806705  0.934633  0.001100
C    -2.082571  1.547969  0.006263
O    -2.265631  2.767725  0.006478
C    -3.067848  0.440595  0.010030
C    -4.461458  0.500021  0.011385
H    -4.976060  1.464559  0.016249
C    -5.183297 -0.716856  0.009333
C    -4.467192 -1.949032  0.002335
H    -5.035968 -2.883806  0.002873
C    -3.068249 -1.991742  0.000402
H    -2.551748 -2.954932 -0.007657
C    -2.354480 -0.781224  0.004722
C    -0.928829 -0.470423 -0.000198
C     0.179760 -1.273545 -0.005871
H     0.045033 -2.357631 -0.006430
C     1.528181 -0.734809 -0.011998
C     2.637336 -1.633008 -0.016589
H     2.491037 -2.714823 -0.019678
C     3.905158 -1.076068 -0.017526
C     4.114074  0.316102 -0.017406
C     3.056900  1.213379 -0.016219
H     3.220610  2.292007 -0.020011
```

```
C     1.737933  0.686481 -0.011392
O     5.115031 -1.728800 -0.044928
O     5.466930  0.580975 -0.048226
N    -6.577421 -0.719331  0.072577
H    -7.030632  0.133469 -0.238445
H    -7.033066 -1.554832 -0.278935
C     6.110631 -0.695478  0.106958
H     6.551341 -0.763945  1.120787
H     6.877149 -0.814728 -0.675887
    el energy= -1050.93344702
          zpe= -1050.687942
    th energy= -1050.670225
  th enthalpy= -1050.669281
  free energy= -1050.733284

b97d--thieno
B     1.049666  1.458423  0.000006
O     1.174366  2.816103 -0.000030
H     0.279804  3.220947 -0.000069
N    -0.280238  0.814312 -0.000023
C    -1.524421  1.488946 -0.000061
O    -1.646207  2.716497 -0.000022
C    -2.563048  0.433592 -0.000054
C    -3.958595  0.548537 -0.000058
H    -4.430107  1.533836 -0.000063
C    -4.713809 -0.635192 -0.000067
C    -4.073697 -1.896749 -0.000066
H    -4.682636 -2.804511 -0.000071
C    -2.673419 -2.008131 -0.000055
H    -2.192117 -2.989237 -0.000049
C    -1.915998 -0.825203 -0.000048
C    -0.473488 -0.588745 -0.000021
C     0.575319 -1.467413  0.000001
H     0.373076 -2.540085 -0.000007
C     1.941116 -0.984742  0.000028
C     3.090512 -1.765954  0.000024
H     3.167962 -2.852095  0.000006
S     4.532143 -0.781666  0.000184
C     3.588102  0.692207  0.000004
H     4.090652  1.658135 -0.000030
C     2.230179  0.444325  0.000033
H    -5.805361 -0.586306 -0.000075
    el energy= -739.979500341
          zpe= -739.798207
    th energy= -739.784766
  th enthalpy= -739.783821
  free energy= -739.838314

b97d--7
B     2.501673  1.450879  0.000021
O     2.693225  2.799950 -0.000018
H     1.822669  3.252886 -0.000063
N     1.140539  0.871434 -0.000014
C    -0.067210  1.605843 -0.000060
O    -0.134951  2.836338 -0.000003
C    -1.155597  0.598429 -0.000043
C    -2.540907  0.794160 -0.000040
H    -2.967053  1.798025 -0.000043
C    -3.340257 -0.358568 -0.000047
C    -2.780145 -1.657907 -0.000051
H    -3.439287 -2.527079 -0.000054
C    -1.387868 -1.830507 -0.000046
H    -0.963507 -2.837108 -0.000041
C    -0.569377 -0.688626 -0.000041
C     0.880937 -0.521443 -0.000014
C     1.886856 -1.449532  0.000011
H     1.633866 -2.511385  0.000002
C     3.273555 -1.032685  0.000042
C     4.383988 -1.868556  0.000039
H     4.408879 -2.957174  0.000021
S     5.870718 -0.955119  0.000209
C     4.998949  0.562582  0.000023
H     5.547548  1.503084 -0.000010
C     3.630645  0.380500  0.000050
Br   -5.263267 -0.173892 -0.000055
    el energy= -752.579052865
          zpe= -752.407888
    th energy= -752.392837
  th enthalpy= -752.391893
  free energy= -752.451293

b97d--8
B    -2.070676  1.454735 -0.000022
O    -2.259919  2.803098 -0.000141
H    -1.390598  3.258152 -0.000421
N    -0.711122  0.870227 -0.000286
C     0.500758  1.599517 -0.000566
O     0.575052  2.828278  0.000164
C     1.583711  0.585359 -0.000239
C     2.967765  0.764698  0.000060
H     3.424281  1.754074  0.000177
C     3.751040 -0.398996  0.000062
C     3.184830 -1.694051 -0.000161
H     3.851321 -2.555770 -0.000117
C     1.794544 -1.854420 -0.000369
H     1.356759 -2.854817 -0.000446
C     0.988332 -0.701157 -0.000401
C    -0.457731 -0.523031 -0.000359
C    -1.467335 -1.449695 -0.000276
H    -1.216995 -2.512106 -0.000327
C    -2.850219 -1.028045 -0.000060
C    -3.963447 -1.861713  0.000059
H    -3.990850 -2.950247  0.000002
S    -5.445687 -0.944961  0.000378
C    -4.569986  0.571780  0.000252
H    -5.117793  1.512707  0.000349
```

```
C    -3.202722  0.386672  0.000091
N     5.234956 -0.266931  0.000291
O     5.703126  0.871664  0.000464
O     5.899764 -1.304399  0.000295
    el energy= -944.368978710
          zpe= -944.185425
    th energy= -944.169316
  th enthalpy= -944.168372
  free energy= -944.229829

b97d--9
B     1.447243  1.451854  0.000736
O     1.599928  2.807668  0.002661
H     0.712557  3.229021  0.001584
N     0.104423  0.836549 -0.001700
C    -1.123049  1.538382 -0.002637
O    -1.219471  2.769203 -0.000005
C    -2.186706  0.507975 -0.006214
C    -3.572006  0.672224 -0.004569
H    -4.012358  1.672720 -0.006780
C    -4.382599 -0.487042 -0.003365
C    -3.760521 -1.770161  0.000045
H    -4.397841 -2.659505 -0.001005
C    -2.369492 -1.917447 -0.001148
H    -1.926734 -2.916588  0.003891
C    -1.566756 -0.763318 -0.004786
C    -0.121938 -0.564121 -0.002797
C     0.910791 -1.462522 -0.002027
H     0.687991 -2.531193 -0.003366
C     2.287204 -1.008580 -0.000168
C     3.420158 -1.812227  0.000342
H     3.476669 -2.899673 -0.000823
S     4.884282 -0.857487  0.002784
C     3.968920  0.635353  0.002859
H     4.491440  1.590625  0.003999
C     2.606843  0.414258  0.001328
N    -5.771819 -0.386125 -0.063004
H    -6.162931  0.497879  0.244494
H    -6.290496 -1.187338  0.280275
    el energy= -795.298613048
          zpe= -795.100909
    th energy= -795.085935
  th enthalpy= -795.084991
  free energy= -795.142573

b97d.tddft--benzo
B    -1.129948  1.425392 -0.000001
O    -1.296211  2.786464 -0.000152
H    -0.406963  3.206384 -0.000321
N     0.194152  0.815900 -0.000041
C     1.497789  1.518260 -0.000061
O     1.549416  2.756811  0.000190
C     2.507862  0.482513 -0.000018
C     3.921605  0.558050  0.000072
H     4.426095  1.525831  0.000114
C     4.650000 -0.652328  0.000070
C     4.016091 -1.907344 -0.000002
H     4.608282 -2.824032  0.000006
C     2.582729 -1.981146 -0.000059
H     2.076290 -2.950156 -0.000096
C     1.867523 -0.795303 -0.000061
C     0.408627 -0.545654 -0.000067
C    -0.651333 -1.466126 -0.000065
H    -0.421535 -2.532658 -0.000077
C    -2.002727 -1.022951 -0.000017
C    -3.082221 -1.975383 -0.000003
H    -2.842284 -3.042220 -0.000031
C    -4.399488 -1.546191  0.000040
C    -4.696621 -0.152470  0.000075
C    -3.657898  0.795163  0.000071
H    -3.891910  1.862546  0.000097
C    -2.307397  0.403680  0.000031
H    -5.214503 -2.274199  0.000043
H    -5.738932  0.176885  0.000108
H     5.743259 -0.609458  0.000121
 total energy= -807.102387337

b97d.tddft--1
B     1.156361 -2.710946  0.000000
O     0.509009 -3.918613  0.000000
H    -0.459741 -3.754623  0.000000
N     0.429530 -1.448035  0.000000
C    -1.034210 -1.267578  0.000000
O    -1.797831 -2.241684  0.000000
C    -1.259156  0.163647  0.000000
C    -2.465697  0.904002  0.000000
H    -3.436301  0.409606  0.000000
C    -2.343657  2.310124  0.000000
C    -1.114384  2.990772  0.000000
H    -1.080702  4.079040  0.000000
C     0.095523  2.218023  0.000000
H     1.063119  2.725699  0.000000
C     0.000000  0.836778  0.000000
C     1.044010 -0.210466  0.000000
C     2.438315 -0.073885  0.000000
H     2.869214  0.928387  0.000000
C     3.285205 -1.218580  0.000000
C     4.715853 -1.065002  0.000000
H     5.137036 -0.055990  0.000000
C     5.541942 -2.177323  0.000000
C     4.978131 -3.485978  0.000000
C     3.582718 -3.658690  0.000000
H     3.155887 -4.664516  0.000000
C     2.708624 -2.557708  0.000000
H     6.627818 -2.055322  0.000000
H     5.638045 -4.357313  0.000000
```

```
Br   -3.972332  3.356273  0.000000
 total energy= -819.704964378

b97d.tddft--2
B    -2.510590  0.626945  0.000000
O    -3.626129 -0.146562  0.000000
H    -3.386490 -1.098018  0.000000
N    -1.153489  0.011609  0.000000
C    -0.846991 -1.421185  0.000000
O    -1.737923 -2.258347  0.000000
C     0.615711 -1.529877  0.000000
C     1.433479 -2.680815  0.000000
H     1.037331 -3.693992  0.000000
C     2.823722 -2.464667  0.000000
C     3.360530 -1.165019  0.000000
H     4.446869 -1.073172  0.000000
C     2.524024 -0.024609  0.000000
H     2.956888  0.978399  0.000000
C     1.146696 -0.234241  0.000000
C     0.000000  0.745067  0.000000
C    -0.017694  2.132586  0.000000
H     0.933293  2.667982  0.000000
C    -1.249511  2.874681  0.000000
C    -1.228257  4.303499  0.000000
H    -0.265101  4.820669  0.000000
C    -2.420534  5.029908  0.000000
C    -3.659445  4.355066  0.000000
C    -3.695556  2.942214  0.000000
H    -4.656804  2.422616  0.000000
C    -2.514181  2.185029  0.000000
H    -2.393149  6.121919  0.000000
H    -4.591671  4.924543  0.000000
N     3.747670 -3.614707  0.000000
O     3.206004 -4.761618  0.000000
O     4.993119 -3.367200  0.000000
 total energy= -1011.51089502

b97d.tddft--3
B    -1.524519  1.416322  0.000063
O    -1.719040  2.779500  0.000745
H    -0.836141  3.212466  0.000317
N    -0.170427  0.854208 -0.000969
C     1.056065  1.586059 -0.001424
O     1.126090  2.838480 -0.000523
C     2.111158  0.569686 -0.002777
C     3.499775  0.694448 -0.002771
H     3.974605  1.679218 -0.003690
C     4.283403 -0.494255 -0.000954
C     3.673387 -1.790151 -0.001612
H     4.309281 -2.678886 -0.003231
C     2.281806 -1.905446 -0.002021
H     1.811827 -2.891844 -0.001165
C     1.497370 -0.733499 -0.002283
C     0.070935 -0.532152 -0.001445
C    -0.966533 -1.467514 -0.000957
H    -0.716272 -2.530874 -0.001632
C    -2.330692 -1.056574 -0.000033
C    -3.382662 -2.026283  0.000412
H    -3.120706 -3.089096 -0.000117
C    -4.713010 -1.628347  0.001482
C    -5.041754 -0.241770  0.002179
C    -4.029928  0.722939  0.001800
H    -4.285794  1.785737  0.002293
C    -2.661172  0.363562  0.000566
H    -5.509935 -2.376916  0.001787
H    -6.091996  0.063605  0.002940
N     5.656232 -0.401747 -0.012808
H     6.110528  0.498875  0.073202
H     6.231277 -1.229172  0.082669
 total energy= -862.431231928

b97d.tddft--dioxo
B     0.080397  1.583061 -0.000147
O     0.138045  2.954104 -0.000060
H    -0.793082  3.281717  0.000028
N    -1.166791  0.859400  0.000029
C    -2.505829  1.456312  0.000377
O    -2.657534  2.696405  0.000060
C    -3.430437  0.348337  0.000109
C    -4.847163  0.320492 -0.000093
H    -5.415576  1.252683 -0.000073
C    -5.487218 -0.929344 -0.000242
C    -4.760640 -2.141839 -0.000183
H    -5.288186 -3.097722 -0.000309
C    -3.337146 -2.113632 -0.000002
H    -2.763740 -3.045405  0.000005
C    -2.698598 -0.882216  0.000116
C    -1.259333 -0.534874  0.000140
C    -0.150433 -1.349543  0.000129
H    -0.272352 -2.432641  0.000188
C     1.183821 -0.779205  0.000065
C     2.314471 -1.633730  0.000115
H     2.214651 -2.719610  0.000171
C     3.561338 -1.020256  0.000052
C     3.732187  0.395842 -0.000073
C     2.647808  1.258385 -0.000121
H     2.764577  2.342581 -0.000256
C     1.358508  0.678669 -0.000037
O     4.781186 -1.624064  0.000134
O     5.073799  0.687185 -0.000021
H    -6.580953 -0.966532 -0.000354
C     5.757857 -0.565515 -0.000190
H     6.370819 -0.651219  0.913016
H     6.370266 -0.651310 -0.913772
 total energy= -995.531059011
```

```
b97d.tddft--4
B    -1.571644  1.662825 -0.000100
O    -1.727964  3.025266 -0.000173
H    -0.826430  3.424324 -0.000194
N    -0.277946  1.026262  0.000095
C     1.015730  1.711667  0.000452
O     1.087800  2.956105  0.000241
C     2.014181  0.668140  0.000222
C     3.429677  0.752690  0.000080
H     3.936622  1.717178  0.000103
C     4.134882 -0.458922 -0.000048
C     3.518315 -1.728282  0.000026
H     4.118358 -2.637005 -0.000057
C     2.093432 -1.789652  0.000177
H     1.593663 -2.762256  0.000194
C     1.370462 -0.608631  0.000231
C    -0.090027 -0.360025  0.000225
C    -1.137320 -1.247174  0.000212
H    -0.941974 -2.319413  0.000266
C    -2.510745 -0.769274  0.000116
C    -3.577163 -1.700185  0.000121
H    -3.402506 -2.776521  0.000197
C    -4.864672 -1.174364 -0.000001
C    -5.132786  0.226296 -0.000139
C    -4.110460  1.161637 -0.000148
H    -4.301023  2.235209 -0.000287
C    -2.784718  0.671242 -0.000011
O    -6.038366 -1.861112 -0.000005
O    -6.490549  0.424061 -0.000224
Br    6.076347 -0.389315 -0.000193
C    -7.086992 -0.872780 -0.000172
H    -7.691512 -1.001236 -0.913815
H    -7.691649 -1.001072  0.913406
 total energy= -1008.13445961

b97d.tddft--5
B    -1.135095  1.645774 -0.000094
O    -1.257120  3.002449 -0.000134
H    -0.362409  3.409246 -0.000186
N     0.174657  0.984727 -0.000132
C     1.454567  1.643161 -0.000034
O     1.563319  2.865255  0.000055
C     2.470107  0.573909 -0.000079
C     3.874237  0.676512  0.000020
H     4.398252  1.630611  0.000135
C     4.596979 -0.528133 -0.000008
C     3.942657 -1.776965 -0.000123
H     4.563791 -2.672194 -0.000109
C     2.532321 -1.855826 -0.000228
H     2.035283 -2.829206 -0.000310
C     1.809833 -0.664545 -0.000198
C     0.328645 -0.399843 -0.000189
C    -0.732864 -1.251417 -0.000198
H    -0.559252 -2.327993 -0.000230
C    -2.111592 -0.753245 -0.000141
C    -3.183063 -1.675508 -0.000109
H    -3.016562 -2.753240 -0.000133
C    -4.469291 -1.140132 -0.000006
C    -4.719814  0.256268  0.000047
C    -3.683556  1.182604 -0.000010
H    -3.867597  2.257417  0.000042
C    -2.364986  0.675651 -0.000089
O    -5.649747 -1.817113  0.000012
O    -6.071873  0.476506  0.000066
N     6.072429 -0.492478  0.000164
O     6.611860  0.650687  0.000331
O     6.679699 -1.602404  0.000237
C    -6.688409 -0.816493  0.000478
H    -7.295182 -0.934206 -0.913052
H    -7.294168 -0.934079  0.914748
 total energy= -1199.93380790

b97d.tddft--6
B     0.482937  1.624517 -0.000633
O     0.577971  2.996371 -0.002217
H    -0.342010  3.350642 -0.001331
N    -0.788975  0.940920  0.001145
C    -2.101031  1.569451  0.002541
O    -2.235858  2.813202  0.000000
C    -3.058796  0.481002  0.006190
C    -4.463327  0.500295  0.006238
H    -5.008609  1.447585  0.010690
C    -5.157965 -0.736889  0.004582
C    -4.449262 -1.973276  0.000157
H    -5.009218 -2.911704  0.004576
C    -3.037698 -1.979675  0.001633
H    -2.497753 -2.930976 -0.002889
C    -2.350543 -0.766317  0.003979
C    -0.923736 -0.456755  0.002043
C     0.174773 -1.299270  0.001260
H     0.021652 -2.378941  0.002965
C     1.513554 -0.770510  0.000246
C     2.626434 -1.660299  0.000432
H     2.491083 -2.742535  0.001620
C     3.886049 -1.087712 -0.000600
C     4.094749  0.322509 -0.002018
C     3.036462  1.218027 -0.002261
H     3.189444  2.297848 -0.003083
C     1.727997  0.682877 -0.000957
O     5.093982 -1.724667 -0.000522
O     5.442331  0.580627 -0.002815
N    -6.548363 -0.744407  0.055260
H    -7.015191  0.108811 -0.232426
H    -7.009558 -1.590029 -0.262143
C     6.096162 -0.692682 -0.000904
H     6.707524 -0.787890  0.912862
```

```
H     6.708988 -0.789909 -0.913444
 total energy= -1050.85281632

b97d.tddft--thieno
B    -1.042717  1.475197  0.000032
O    -1.181655  2.835318  0.000029
H    -0.283281  3.235291  0.000051
N     0.260201  0.823148  0.000017
C     1.584271  1.503069 -0.000003
O     1.649387  2.738041  0.000008
C     2.580664  0.457905  0.000017
C     3.999953  0.524990  0.000027
H     4.512320  1.487940  0.000018
C     4.714073 -0.696405  0.000046
C     4.069742 -1.941143  0.000052
H     4.652282 -2.864023  0.000074
C     2.626243 -2.002964  0.000034
H     2.110807 -2.966725  0.000040
C     1.929053 -0.809693  0.000013
C     0.464663 -0.543752  0.000000
C    -0.590392 -1.458276 -0.000022
H    -0.374804 -2.526535 -0.000040
C    -1.932875 -0.972801 -0.000033
C    -3.110423 -1.768722 -0.000090
H    -3.172484 -2.855776 -0.000125
S    -4.538154 -0.804733 -0.000012
C    -3.586526  0.692885 -0.000084
H    -4.103429  1.651314 -0.000108
C    -2.229882  0.457390 -0.000014
H     5.807980 -0.665557  0.000056
 total energy= -739.877922692

b97d.tddft--7
B    -2.508354  1.467385  0.000000
O    -2.727938  2.815552  0.000110
H    -1.858936  3.273436  0.000243
N    -1.170419  0.889183  0.000102
C     0.108672  1.637734  0.000233
O     0.113684  2.871649  0.000075
C     1.163985  0.647434  0.000138
C     2.575794  0.812762  0.000082
H     3.036087  1.799014  0.000073
C     3.340819 -0.376493  0.000044
C     2.792455 -1.663394  0.000095
H     3.434139 -2.542910  0.000070
C     1.352453 -1.802338  0.000167
H     0.902522 -2.797352  0.000203
C     0.586203 -0.651692  0.000200
C    -0.889544 -0.466637  0.000154
C    -1.891047 -1.436440  0.000129
H    -1.617404 -2.491311  0.000199
C    -3.259565 -1.026557 -0.000002
C    -4.389751 -1.887620  0.000067
H    -4.389801 -2.976461  0.000195
S    -5.869214 -1.006350 -0.000632
C    -5.003126  0.542688  0.000075
H    -5.573015  1.470567  0.000176
C    -3.636011  0.383478 -0.000063
Br    5.271844 -0.199136 -0.000033
 total energy= -752.480785965

b97d.tddft--8
B     2.087431  1.452176 -0.000019
O     2.270326  2.794877 -0.000026
H     1.403602  3.255608  0.000037
N     0.727397  0.847023  0.000111
C    -0.532207  1.591849  0.000267
O    -0.545822  2.815192  0.000027
C    -1.606610  0.594188  0.000133
C    -3.006920  0.779024  0.000012
H    -3.478096  1.759431 -0.000021
C    -3.794336 -0.387031 -0.000024
C    -3.205836 -1.664543  0.000050
H    -3.876881 -2.523723  0.000010
C    -1.802460 -1.827598  0.000148
H    -1.362398 -2.827502  0.000173
C    -1.017706 -0.675067  0.000166
C     0.479380 -0.506350  0.000155
C     1.492439 -1.446030  0.000115
H     1.238978 -2.506249  0.000134
C     2.866658 -1.018928  0.000027
C     3.999266 -1.856759 -0.000034
H     4.018782 -2.945726 -0.000015
S     5.481577 -0.952975 -0.000126
C     4.590969  0.568803 -0.000140
H     5.137470  1.511191 -0.000211
C     3.220760  0.385133 -0.000044
N    -5.265428 -0.284013 -0.000131
O    -5.737857  0.892381 -0.000226
O    -5.931397 -1.364640 -0.000130
 total energy= -944.289999444

b97d.tddft--9
B     1.441178  1.471458  0.000154
O     1.613431  2.833626  0.001298
H     0.721615  3.249252  0.000465
N     0.110936  0.867899 -0.001408
C    -1.148097  1.580281 -0.001726
O    -1.219166  2.827215  0.000001
C    -2.185210  0.554675 -0.004189
C    -3.580111  0.665531 -0.005285
H    -4.067055  1.644068 -0.009671
C    -4.352103 -0.534594 -0.002453
C    -3.732422 -1.818105 -0.001503
H    -4.354173 -2.716103 -0.003437
C    -2.325881 -1.912903 -0.002640
```

```
H    -1.845305 -2.894623 -0.000098
C    -1.561929 -0.738490 -0.003180
C    -0.130414 -0.518221 -0.002058
C     0.906414 -1.455353 -0.001651
H     0.664928 -2.519016 -0.002903
C     2.259390 -1.008599 -0.000260
C     3.405761 -1.832090  0.000383
H     3.444490 -2.920153 -0.000374
S     4.857757 -0.898679  0.002736
C     3.957041  0.621258  0.002341
H     4.501441  1.563820  0.003220
C     2.592156  0.423216  0.000785
N    -5.728460 -0.441963 -0.029956
H    -6.168254  0.452521  0.149707
H    -6.286718 -1.266128  0.156313
 total energy= -795.203437937

b97d.tddft-mecn--benzo
B    -1.123624  1.423399 -0.000065
O    -1.263136  2.791993 -0.000067
H    -0.359221  3.185451 -0.000036
N     0.213920  0.817382  0.000061
C     1.485778  1.518386  0.000270
O     1.549778  2.768171  0.000047
C     2.501831  0.482927  0.000093
C     3.908870  0.550988 -0.000061
H     4.423008  1.515518 -0.000075
C     4.640525 -0.654520 -0.000141
C     3.994367 -1.916449 -0.000096
H     4.589133 -2.832113 -0.000176
C     2.582990 -1.993528  0.000024
H     2.074607 -2.961142  0.000015
C     1.848907 -0.799131  0.000103
C     0.420279 -0.554710  0.000126
C    -0.660967 -1.470464  0.000082
H    -0.435703 -2.538176  0.000082
C    -1.999680 -1.020317  0.000013
C    -3.084572 -1.972150 -0.000003
H    -2.843402 -3.038592  0.000033
C    -4.401651 -1.540645 -0.000049
C    -4.696264 -0.146305 -0.000091
C    -3.654545  0.800627 -0.000098
H    -3.900748  1.866122 -0.000136
C    -2.302229  0.411537 -0.000044
H    -5.217786 -2.267342 -0.000058
H    -5.737307  0.186432 -0.000131
H     5.733136 -0.613617 -0.000232
 total energy= -807.128750352

b97d.tddft-mecn--1
B     1.191857 -2.688016  0.000000
O     0.539005 -3.898276  0.000000
H    -0.429813 -3.721699  0.000000
N     0.432871 -1.431944  0.000000
C    -1.010382 -1.291135  0.000000
O    -1.773157 -2.280111  0.000000
C    -1.261402  0.138256  0.000000
C    -2.468935  0.862364  0.000000
H    -3.433769  0.353094  0.000000
C    -2.371485  2.266152  0.000000
C    -1.139271  2.967017  0.000000
H    -1.117076  4.056398  0.000000
C     0.064202  2.225554  0.000000
H     1.024372  2.746663  0.000000
C     0.000000  0.828832  0.000000
C     1.040922 -0.182136  0.000000
C     2.446445 -0.036703  0.000000
H     2.864630  0.971038  0.000000
C     3.296518 -1.167277  0.000000
C     4.728709 -0.995478  0.000000
H     5.133825  0.019845  0.000000
C     5.570062 -2.097066  0.000000
C     5.024030 -3.412969  0.000000
C     3.629470 -3.604711  0.000000
H     3.228003 -4.621616  0.000000
C     2.736252 -2.517720  0.000000
H     6.654018 -1.960263  0.000000
H     5.694184 -4.276299  0.000000
Br   -4.012724  3.297878  0.000000
 total energy= -819.732253917

b97d.tddft-mecn--2
B    -2.511971  0.616858  0.000000
O    -3.630573 -0.156805  0.000000
H    -3.394471 -1.108725  0.000000
N    -1.155956 -0.004634  0.000000
C    -0.852672 -1.416057  0.000000
O    -1.727678 -2.276347  0.000000
C     0.615269 -1.521388  0.000000
C     1.431835 -2.664172  0.000000
H     1.023232 -3.672995  0.000000
C     2.823645 -2.449829  0.000000
C     3.362312 -1.143815  0.000000
H     4.445783 -1.029937  0.000000
C     2.523572 -0.008783  0.000000
H     2.950375  0.995933  0.000000
C     1.142776 -0.218495  0.000000
C     0.000000  0.737143  0.000000
C    -0.020838  2.128703  0.000000
H     0.930158  2.663208  0.000000
C    -1.249184  2.865370  0.000000
C    -1.219048  4.295411  0.000000
H    -0.252131  4.804212  0.000000
C    -2.409508  5.024638  0.000000
C    -3.649839  4.351266  0.000000
C    -3.693804  2.936913  0.000000
```

```
H    -4.662371  2.431236  0.000000
C    -2.516764  2.175470  0.000000
H    -2.381218  6.116448  0.000000
H    -4.580657  4.922753  0.000000
N     3.732908 -3.597242  0.000000
O     3.209514 -4.759548  0.000000
O     4.988233 -3.375746  0.000000
 total energy= -1011.54233725

b97d.tddft-mecn--3
B    -1.521971  1.409980 -0.000160
O    -1.694124  2.783265  0.000000
H    -0.793352  3.185920  0.000037
N    -0.164826  0.849515 -0.000061
C     1.052516  1.581574  0.000188
O     1.108486  2.844182 -0.000006
C     2.113366  0.573269  0.000056
C     3.502212  0.700556 -0.000012
H     3.995328  1.675805 -0.000021
C     4.288161 -0.490784 -0.000029
C     3.670044 -1.792916  0.000020
H     4.312987 -2.675702  0.000033
C     2.287206 -1.910172  0.000050
H     1.813899 -2.894388  0.000036
C     1.498357 -0.732147  0.000066
C     0.076223 -0.540206  0.000019
C    -0.967968 -1.471034 -0.000053
H    -0.720837 -2.534962 -0.000076
C    -2.329716 -1.054279 -0.000029
C    -3.385674 -2.022620 -0.000017
H    -3.123500 -3.085276 -0.000035
C    -4.717841 -1.625070  0.000026
C    -5.050306 -0.238836  0.000039
C    -4.035406  0.724165  0.000008
H    -4.301519  1.785775  0.000003
C    -2.663279  0.366999 -0.000049
H    -5.513247 -2.375595  0.000035
H    -6.100252  0.067252  0.000072
N     5.645414 -0.404854 -0.000010
H     6.110617  0.498932 -0.000245
H     6.223339 -1.240865 -0.000210
 total energy= -862.470314200

b97d.tddft-mecn--dioxo
B     0.079865  1.588909  0.000052
O     0.106709  2.966556  0.000110
H    -0.834271  3.268415  0.000224
N    -1.181934  0.868018  0.000376
C    -2.502643  1.455276  0.000164
O    -2.673480  2.703293  0.000131
C    -3.428271  0.344272  0.000109
C    -4.842314  0.305094 -0.000183
H    -5.424499  1.230294 -0.000239
C    -5.478274 -0.946655 -0.000409
C    -4.736465 -2.157890 -0.000372
H    -5.260425 -3.116353 -0.000580
C    -3.323405 -2.126576 -0.000067
H    -2.744558 -3.054547 -0.000017
C    -2.680890 -0.884535  0.000150
C    -1.263315 -0.532265  0.000296
C    -0.133847 -1.338419  0.000312
H    -0.252169 -2.422408  0.000403
C     1.186089 -0.768947  0.000155
C     2.318574 -1.631494  0.000329
H     2.207308 -2.716295  0.000594
C     3.563225 -1.026466  0.000090
C     3.733557  0.393065 -0.000305
C     2.648220  1.263092 -0.000320
H     2.789002  2.344801 -0.000541
C     1.356647  0.693382 -0.000011
O     4.778055 -1.624064  0.000148
O     5.057023  0.689939 -0.000593
H    -6.571335 -0.991229 -0.000649
C     5.763213 -0.568103 -0.000047
H     6.368876 -0.642760  0.916289
H     6.369222 -0.643377 -0.916093
 total energy= -995.557110124

b97d.tddft-mecn--4
B    -1.573528  1.669046  0.000205
O    -1.701472  3.040209  0.000360
H    -0.788055  3.414389  0.000502
N    -0.265505  1.037639  0.000303
C     1.010012  1.716073 -0.000152
O     1.097178  2.970039 -0.000185
C     2.010852  0.672808  0.000111
C     3.424273  0.751013 -0.000029
H     3.936073  1.714362 -0.000245
C     4.125625 -0.460738  0.000015
C     3.501541 -1.733066  0.000209
H     4.095416 -2.646733  0.000215
C     2.086544 -1.793321  0.000351
H     1.584883 -2.764414  0.000508
C     1.356305 -0.606025  0.000340
C    -0.086063 -0.354917  0.000436
C    -1.150836 -1.236420  0.000491
H    -0.958102 -2.309675  0.000515
C    -2.512145 -0.760133  0.000409
C    -3.576993 -1.700605  0.000314
H    -3.389198 -2.774728  0.000341
C    -4.863168 -1.184699 -0.000086
C    -5.133273  0.219000 -0.000199
C    -4.112462  1.163431  0.000055
H    -4.328673  2.232468 -0.000218
C    -2.784782  0.684493  0.000297
O    -6.030885 -1.866747 -0.000618
```

```
O    -6.473906  0.420930 -0.000780
Br    6.073822 -0.398599 -0.000288
C    -7.089114 -0.882950 -0.000151
H    -7.688252 -1.001479 -0.915972
H    -7.686914 -1.001037  0.916625
 total energy= -1008.16198115

b97d.tddft-mecn--5
B    -1.135392  1.657743  0.000549
O    -1.246040  3.018814  0.000701
H    -0.348846  3.418935  0.000953
N     0.182846  1.000250  0.001239
C     1.449315  1.647280  0.001370
O     1.584383  2.872686  0.000247
C     2.463390  0.573320  0.000843
C     3.864532  0.669941 -0.000110
H     4.380895  1.628523 -0.000567
C     4.586167 -0.537441 -0.000272
C     3.924563 -1.788130  0.000395
H     4.527574 -2.695458  0.000213
C     2.517493 -1.861685  0.001170
H     2.015991 -2.831674  0.001535
C     1.794327 -0.664953  0.001331
C     0.330684 -0.390985  0.001483
C    -0.738417 -1.238270  0.001442
H    -0.566460 -2.315352  0.001671
C    -2.110123 -0.741912  0.000816
C    -3.174656 -1.674035  0.000565
H    -2.993895 -2.749376  0.001005
C    -4.462186 -1.148305 -0.000251
C    -4.717445  0.250210 -0.000848
C    -3.684215  1.185886 -0.000494
H    -3.890004  2.256833 -0.000854
C    -2.364497  0.689112  0.000360
O    -5.634239 -1.824380 -0.001255
O    -6.055891  0.469815 -0.002456
N     6.050640 -0.501599 -0.001196
O     6.612570  0.637671 -0.003236
O     6.679763 -1.605383 -0.000537
C    -6.685124 -0.830062 -0.000469
H    -7.286452 -0.943382 -0.915744
H    -7.283461 -0.941921  0.917038
 total energy= -1199.96876044

b97d.tddft-mecn--6
B     0.482250  1.631842  0.000592
O     0.544258  3.014920  0.000062
H    -0.388049  3.339295  0.000040
N    -0.810866  0.956891  0.001015
C    -2.096899  1.580386  0.000823
O    -2.251342  2.834536  0.000175
C    -3.061872  0.487287  0.001383
C    -4.460489  0.496692  0.000156
H    -5.029346  1.430321 -0.001400
C    -5.148426 -0.751941 -0.000219
C    -4.420035 -1.992898  0.001249
H    -4.983630 -2.928768  0.000728
C    -3.027713 -1.993156  0.001980
H    -2.477166 -2.937428  0.001501
C    -2.336941 -0.760091  0.002029
C    -0.936576 -0.448917  0.001637
C     0.185446 -1.284411  0.001452
H     0.033141 -2.365281  0.001822
C     1.507326 -0.755699  0.000837
C     2.628773 -1.654300  0.000320
H     2.479233 -2.735437  0.000525
C     3.887023 -1.094653 -0.000448
C     4.095860  0.314801 -0.000753
C     3.039721  1.215255 -0.000357
H     3.217814  2.292291 -0.000659
C     1.718409  0.697037  0.000427
O     5.093794 -1.733053 -0.000990
O     5.433935  0.579327 -0.001343
N    -6.512469 -0.781566  0.008977
H    -7.051103  0.076281 -0.053472
H    -7.012101 -1.662527 -0.054473
C     6.105003 -0.702200 -0.001644
H     6.713769 -0.790061  0.912721
H     6.712729 -0.790155 -0.916697
 total energy= -1050.88785416

b97d.tddft-mecn--thieno
B    -1.037336  1.469491 -0.000089
O    -1.150302  2.836579  0.000166
H    -0.236628  3.208724  0.000329
N     0.276510  0.819553 -0.000018
C     1.575103  1.505035  0.000069
O     1.645777  2.753552 -0.000119
C     2.572914  0.463171  0.000105
C     3.987307  0.516658  0.000132
H     4.510617  1.476050  0.000140
C     4.704204 -0.696361  0.000204
C     4.048009 -1.950341  0.000225
H     4.630759 -2.873551  0.000273
C     2.626070 -2.009152  0.000168
H     2.107276 -2.971429  0.000170
C     1.911284 -0.813264  0.000114
C     0.470681 -0.556168  0.000030
C    -0.601725 -1.467565  0.000005
H    -0.394086 -2.537588  0.000075
C    -1.931651 -0.973583 -0.000065
C    -3.111277 -1.767788  0.000126
H    -3.176429 -2.855530  0.000275
S    -4.530150 -0.796241 -0.000647
C    -3.583838  0.702774  0.000357
H    -4.112896  1.655631  0.000663
```

```
C    -2.226496  0.462946 -0.000076
H     5.797587 -0.666011  0.000250
 total energy= -739.900907589

b97d.tddft-mecn--7
B    -2.502498  1.460890 -0.000103
O    -2.699388  2.817526  0.000112
H    -1.814339  3.250379  0.000193
N    -1.154110  0.887177 -0.000084
C     0.100638  1.642490 -0.000005
O     0.106986  2.889839 -0.000158
C     1.157508  0.657860  0.000034
C     2.565067  0.809487  0.000037
H     3.029711  1.796139  0.000013
C     3.328856 -0.371034  0.000130
C     2.773994 -1.670123  0.000162
H     3.411747 -2.553151  0.000228
C     1.354199 -1.801935  0.000111
H     0.900649 -2.795805  0.000127
C     0.572976 -0.653411  0.000047
C    -0.882456 -0.476989 -0.000039
C    -1.896464 -1.446936 -0.000075
H    -1.627298 -2.503068 -0.000037
C    -3.254741 -1.029763 -0.000128
C    -4.386494 -1.890218  0.000007
H    -4.388546 -2.980146  0.000094
S    -5.858524 -1.001285 -0.000556
C    -4.998139  0.548965  0.000265
H    -5.577962  1.471650  0.000527
C    -3.630092  0.385882 -0.000096
Br    5.265822 -0.201849  0.000187
 total energy= -752.504971037

b97d.tddft-mecn--8
B     2.086047  1.459008  0.000005
O     2.263365  2.805408  0.000019
H     1.395187  3.263236  0.000018
N     0.718912  0.858095 -0.000030
C    -0.522332  1.591745 -0.000068
O    -0.561895  2.819900 -0.000027
C    -1.598793  0.590194 -0.000027
C    -2.993680  0.770617 -0.000007
H    -3.454517  1.756581  0.000003
C    -3.782479 -0.394777  0.000009
C    -3.192112 -1.677751 -0.000006
H    -3.846904 -2.548595  0.000008
C    -1.790576 -1.836664 -0.000038
H    -1.345675 -2.833357 -0.000052
C    -1.004330 -0.681737 -0.000043
C     0.475748 -0.501680 -0.000046
C     1.494434 -1.441279 -0.000028
H     1.242592 -2.501831 -0.000025
C     2.860283 -1.011921 -0.000013
C     3.985667 -1.860098 -0.000007
H     3.994618 -2.950057 -0.000014
S     5.466199 -0.961565  0.000059
C     4.587058  0.573318 -0.000005
H     5.150788  1.506083 -0.000002
C     3.219846  0.394393  0.000000
N    -5.243953 -0.283574  0.000051
O    -5.739176  0.890677  0.000089
O    -5.935122 -1.354720 -0.000004
 total energy= -944.320402906

b97d.tddft-mecn--9
B     1.435023  1.458105  0.000088
O     1.581748  2.829691  0.000351
H     0.667982  3.209462  0.000488
N     0.098788  0.859953 -0.000365
C    -1.136911  1.580922 -0.000407
O    -1.197884  2.845756 -0.000413
C    -2.181059  0.564916 -0.000208
C    -3.575439  0.673755  0.000234
H    -4.081012  1.642887  0.000307
C    -4.348884 -0.525637  0.000343
C    -3.721707 -1.821648  0.000284
H    -4.354672 -2.711474  0.000318
C    -2.334523 -1.919990 -0.000124
H    -1.849862 -2.899150 -0.000305
C    -1.557081 -0.737047 -0.000337
C    -0.135219 -0.536175 -0.000417
C     0.906855 -1.469228 -0.000400
H     0.669308 -2.534125 -0.000547
C     2.258872 -1.017719 -0.000187
C     3.406765 -1.832380 -0.000077
H     3.457413 -2.920878 -0.000205
S     4.856110 -0.883764  0.000231
C     3.957867  0.625742  0.000352
H     4.506220  1.567497  0.000608
C     2.588791  0.418865  0.000051
N    -5.708595 -0.446257  0.000693
H    -6.178432  0.454939 -0.000915
H    -6.282046 -1.285153 -0.000337
 total energy= -795.239140957

cam-qtp01--benzo
B    -1.118762  1.381696 -0.000001
O    -1.260626  2.718893 -0.000002
H    -0.389467  3.148884 -0.000005
N     0.198214  0.782835 -0.000003
C     1.403872  1.468627 -0.000004
O     1.502214  2.676281  0.000002
C     2.464212  0.441635 -0.000001
C     3.836399  0.594161  0.000002
H     4.278999  1.585283  0.000004
C     4.610468 -0.555664  0.000003
```

```
C     4.008785 -1.813162  0.000001
H     4.635310 -2.700178  0.000002
C     2.628900 -1.957619 -0.000002
H     2.175190 -2.943936 -0.000003
C     1.856595 -0.808911 -0.000003
C     0.405275 -0.601425 -0.000003
C    -0.618343 -1.461440 -0.000003
H    -0.421542 -2.529124 -0.000003
C    -1.999487 -1.001810 -0.000001
C    -3.047433 -1.924577  0.000001
H    -2.823356 -2.988264  0.000000
C    -4.358601 -1.492252  0.000003
C    -4.650334 -0.131272  0.000005
C    -3.618580  0.788397  0.000003
H    -3.831772  1.853894  0.000004
C    -2.287420  0.375468  0.000001
H    -5.165472 -2.219545  0.000005
H    -5.683365  0.203155  0.000007
H     5.693238 -0.480827  0.000006
    el energy= -806.886970906
          zpe= -806.660589
    th energy= -806.647596
  th enthalpy= -806.646652
  free energy= -806.700189

cam-qtp01--1
B     1.238751 -2.608770  0.000000
O     0.608874 -3.796094  0.000000
H    -0.354123 -3.670288  0.000000
N     0.481311 -1.374909  0.000000
C    -0.900246 -1.270345  0.000000
O    -1.660404 -2.212563  0.000000
C    -1.202972  0.176501  0.000000
C    -2.429338  0.809028  0.000000
H    -3.353197  0.241114  0.000000
C    -2.417500  2.193479  0.000000
C    -1.223187  2.911885  0.000000
H    -1.257775  3.995809  0.000000
C    -0.001974  2.256597  0.000000
H     0.922028  2.826193  0.000000
C     0.000000  0.871894  0.000000
C     1.085458 -0.111785  0.000000
C     2.415173  0.028422  0.000000
H     2.849355  1.023540  0.000000
C     3.302730 -1.125218  0.000000
C     4.687420 -0.946322  0.000000
H     5.096898  0.060616  0.000000
C     5.532192 -2.038610  0.000000
C     5.012063 -3.329620  0.000000
C     3.642152 -3.514904  0.000000
H     3.223045 -4.517417  0.000000
C     2.770148 -2.427784  0.000000
H     6.607856 -1.887503  0.000000
H     5.680961 -4.184907  0.000000
Br   -4.062813  3.141457  0.000000
    el energy= -819.427279846
          zpe= -819.211366
    th energy= -819.196830
  th enthalpy= -819.195886
  free energy= -819.254109

cam-qtp01--2
B    -2.482232  0.452342  0.000000
O    -3.535731 -0.380767  0.000000
H    -3.242200 -1.306243  0.000000
N    -1.130484 -0.068568  0.000000
C    -0.775511 -1.407397  0.000000
O    -1.560264 -2.327939  0.000000
C     0.703130 -1.438776  0.000000
C     1.553793 -2.522729  0.000000
H     1.197856 -3.546264  0.000000
C     2.904539 -2.232249  0.000000
C     3.400801 -0.934190  0.000000
H     4.474818 -0.792928  0.000000
C     2.527845  0.139277  0.000000
H     2.908380  1.155326  0.000000
C     1.166945 -0.126021  0.000000
C     0.000000  0.756879  0.000000
C    -0.102996  2.090253  0.000000
H     0.796827  2.697804  0.000000
C    -1.398180  2.752985  0.000000
C    -1.472823  4.146972  0.000000
H    -0.557147  4.732619  0.000000
C    -2.700495  4.778759  0.000000
C    -3.874861  4.031887  0.000000
C    -3.808819  2.651043  0.000000
H    -4.718599  2.057107  0.000000
C    -2.581399  1.991451  0.000000
H    -2.748071  5.863818  0.000000
H    -4.837450  4.534131  0.000000
N     3.859367 -3.340620  0.000000
O     3.409036 -4.459986  0.000000
O     5.034803 -3.064012  0.000000
    el energy= -1011.22075226
          zpe= -1010.991228
    th energy= -1010.975684
  th enthalpy= -1010.974740
  free energy= -1011.034832

cam-qtp01--3
B    -1.507958  1.373967  0.000160
O    -1.670558  2.709487  0.001738
H    -0.805465  3.151589  0.000259
N    -0.180987  0.797189 -0.002626
C     1.010882  1.503967 -0.003693
O     1.089534  2.713632 -0.001301
```

```
C     2.092048  0.496678 -0.006664
C     3.454799  0.691940 -0.006092
H     3.867848  1.696725 -0.009383
C     4.277916 -0.434027 -0.005400
C     3.689564 -1.708446 -0.003948
H     4.339405 -2.579918 -0.008152
C     2.317932 -1.883324 -0.004129
H     1.899044 -2.885204 -0.002048
C     1.505157 -0.761573 -0.005565
C     0.051988 -0.584821 -0.003585
C    -0.959628 -1.459467 -0.002216
H    -0.746993 -2.524114 -0.003213
C    -2.348153 -1.022083  0.000265
C    -3.381727 -1.961214  0.001475
H    -3.140445 -3.021165  0.000312
C    -4.699901 -1.550580  0.003959
C    -5.014933 -0.194799  0.005293
C    -3.997923  0.741072  0.004079
H    -4.228106  1.803103  0.004992
C    -2.660120  0.349936  0.001579
H    -5.494451 -2.291468  0.004804
H    -6.053398  0.122404  0.007187
N     5.652617 -0.305206 -0.048461
H     6.030172  0.583328  0.236682
H     6.191536 -1.093512  0.269730
    el energy= -862.188900057
          zpe= -861.945685
    th energy= -861.931157
  th enthalpy= -861.930213
  free energy= -861.986818

cam-qtp01--dioxo
B     0.091244  1.557573 -0.006362
O     0.116974  2.903256 -0.002258
H    -0.787917  3.256182  0.003184
N    -1.167832  0.846761 -0.001669
C    -2.429522  1.423644  0.006317
O    -2.633873  2.617829  0.010851
C    -3.394540  0.306508  0.007944
C    -4.774776  0.336533  0.014862
H    -5.303546  1.284495  0.020221
C    -5.443906 -0.877418  0.014602
C    -4.732827 -2.076351  0.007549
H    -5.278094 -3.015518  0.007423
C    -3.345499 -2.097862  0.000627
H    -2.806259 -3.040152 -0.004904
C    -2.677961 -0.885262  0.000894
C    -1.251443 -0.548691 -0.005206
C    -0.152727 -1.311339 -0.012948
H    -0.252572 -2.392317 -0.015638
C     1.181578 -0.732043 -0.018994
C     2.300135 -1.587124 -0.025487
H     2.191192 -2.666396 -0.030334
C     3.532372 -1.000483 -0.026541
C     3.698138  0.380265 -0.024726
C     2.631254  1.230360 -0.020993
H     2.757974  2.307667 -0.023646
C     1.344426  0.664294 -0.016173
O     4.749612 -1.597857 -0.052603
O     5.027797  0.668333 -0.055149
H    -6.529021 -0.899023  0.019866
C     5.692376 -0.560198  0.143830
H     6.079251 -0.609878  1.171319
H     6.501041 -0.661736 -0.584074
    el energy= -995.268890570
          zpe= -995.025925
    th energy= -995.010693
  th enthalpy= -995.009749
  free energy= -995.068754

cam-qtp01--4
B    -1.556934  1.630625 -0.007059
O    -1.669001  2.971156 -0.001792
H    -0.791085  3.385812  0.002491
N    -0.253883  1.000985 -0.005090
C     0.966712  1.657006  0.001539
O     1.100126  2.860166  0.006801
C     2.000629  0.600346  0.000707
C     3.374593  0.726779  0.005740
H     3.848040  1.702479  0.011217
C     4.109445 -0.446552  0.003447
C     3.489220 -1.694480 -0.003689
H     4.101535 -2.589647 -0.005371
C     2.107271 -1.799034 -0.008646
H     1.635035 -2.776332 -0.014238
C     1.360480 -0.633030 -0.006346
C    -0.083064 -0.387014 -0.009969
C    -1.131285 -1.217640 -0.016568
H    -0.963425 -2.290179 -0.020324
C    -2.499442 -0.724299 -0.019847
C    -3.560947 -1.649021 -0.025233
H    -3.383831 -2.719193 -0.031252
C    -4.827972 -1.141776 -0.023744
C    -5.080882  0.225853 -0.020318
C    -4.070187  1.142285 -0.017593
H    -4.265317  2.209289 -0.018927
C    -2.750241  0.658963 -0.015515
O    -6.004197 -1.814933 -0.047865
O    -6.425185  0.429372 -0.047243
Br    6.006439 -0.360437  0.010172
C    -7.012403 -0.839542  0.144671
H    -7.808137 -0.990036 -0.588988
H    -7.401864 -0.916063  1.169282
    el energy= -1007.80924496
          zpe= -1007.576771
    th energy= -1007.559972
```

```
  th enthalpy= -1007.559028
  free energy= -1007.622790

cam-qtp01--5
B    -1.110867  1.623856 -0.006867
O    -1.212549  2.964359 -0.002372
H    -0.333250  3.375619  0.001658
N     0.187040  0.982513 -0.004653
C     1.413440  1.626877  0.001658
O     1.560513  2.827498  0.006249
C     2.436088  0.558520  0.001533
C     3.809757  0.664262  0.006791
H     4.323555  1.618333  0.011958
C     4.509078 -0.527368  0.005214
C     3.888049 -1.770508 -0.001348
H     4.509955 -2.657489 -0.002222
C     2.506894 -1.852939 -0.006521
H     2.015723 -2.820359 -0.011679
C     1.781806 -0.670926 -0.004943
C     0.343351 -0.406840 -0.008782
C    -0.712272 -1.229048 -0.014836
H    -0.553254 -2.302970 -0.017976
C    -2.075052 -0.724098 -0.018176
C    -3.144460 -1.639859 -0.023090
H    -2.977029 -2.711567 -0.028623
C    -4.406625 -1.121087 -0.021989
C    -4.646418  0.249303 -0.019114
C    -3.627485  1.156990 -0.016778
H    -3.813399  2.225590 -0.018350
C    -2.312351  0.661694 -0.014593
O    -5.588246 -1.782819 -0.045108
O    -5.986976  0.466091 -0.044402
N     5.970932 -0.481086  0.010902
O     6.490618  0.607933  0.017031
O     6.562583 -1.533818  0.009224
C    -6.590297 -0.798100  0.133851
H    -7.375001 -0.938308 -0.613669
H    -6.997326 -0.873290  1.151280
    el energy= -1199.60284590
          zpe= -1199.356778
    th energy= -1199.338968
  th enthalpy= -1199.338023
  free energy= -1199.403684

cam-qtp01--6
B     0.488686  1.584122 -0.006954
O     0.545894  2.929495 -0.003549
H    -0.350940  3.302337  0.003012
N    -0.787726  0.904398 -0.000798
C    -2.032765  1.513445  0.007974
O    -2.208132  2.712722  0.010714
C    -3.028997  0.421917  0.011627
C    -4.403033  0.506375  0.017719
H    -4.895891  1.474518  0.026698
C    -5.132727 -0.682278  0.016250
C    -4.443454 -1.904784  0.007392
H    -5.020645 -2.825991  0.011008
C    -3.061990 -1.968426  0.001000
H    -2.563901 -2.933377 -0.006778
C    -2.342227 -0.784950  0.003223
C    -0.908390 -0.490142 -0.004063
C     0.173248 -1.277208 -0.012777
H     0.048875 -2.355618 -0.015039
C     1.521507 -0.729810 -0.019975
C     2.619400 -1.611211 -0.026836
H     2.484305 -2.687543 -0.031093
C     3.865811 -1.054827 -0.028477
C     4.066152  0.320994 -0.027142
C     3.020249  1.196492 -0.023206
H     3.172777  2.270491 -0.026301
C     1.719825  0.661974 -0.017571
O     5.068498 -1.682511 -0.055341
O     5.404027  0.575433 -0.059724
N    -6.513459 -0.664634  0.065942
H    -6.961830  0.191235 -0.216686
H    -6.987986 -1.492611 -0.254167
C     6.034320 -0.668461  0.150588
H     6.406720 -0.725580  1.183359
H     6.849508 -0.792532 -0.566412
    el energy= -1050.57071458
          zpe= -1050.310908
    th energy= -1050.294147
  th enthalpy= -1050.293203
  free energy= -1050.355233

cam-qtp01--thieno
B    -1.036388  1.432403  0.000001
O    -1.140253  2.769798  0.000019
H    -0.254357  3.171741  0.000043
N     0.267132  0.792980  0.000018
C     1.481173  1.460129  0.000039
O     1.598432  2.667480  0.000030
C     2.528784  0.421730  0.000043
C     3.902955  0.559495  0.000055
H     4.355755  1.545980  0.000060
C     4.664289 -0.598205  0.000060
C     4.048763 -1.849507  0.000054
H     4.665675 -2.743232  0.000058
C     2.667917 -1.978894  0.000041
H     2.203900 -2.960441  0.000034
C     1.907556 -0.821492  0.000035
C     0.459054 -0.601101  0.000015
C    -0.561958 -1.464110 -0.000005
H    -0.366720 -2.531378 -0.000003
C    -1.930168 -0.978714 -0.000028
C    -3.062156 -1.738622 -0.000042
```

```
H    -3.139210 -2.817865 -0.000040
S    -4.477673 -0.760368 -0.000123
C    -3.546056  0.684062 -0.000031
H    -4.032438  1.650827 -0.000020
C    -2.208665  0.434301 -0.000027
H     5.747817 -0.535283  0.000069
    el energy= -739.647738769
          zpe= -739.455428
    th energy= -739.442779
  th enthalpy= -739.441835
  free energy= -739.494867

cam-qtp01--7
B     2.463640  1.426473  0.000012
O     2.626415  2.757328 -0.000006
H     1.761753  3.202200 -0.000032
N     1.131890  0.844377 -0.000006
C    -0.050002  1.564041 -0.000029
O    -0.119723  2.774051 -0.000014
C    -1.142036  0.569373 -0.000030
C    -2.506759  0.775949 -0.000039
H    -2.921724  1.777844 -0.000043
C    -3.308377 -0.352108 -0.000043
C    -2.761611 -1.634533 -0.000038
H    -3.425141 -2.492338 -0.000041
C    -1.388680 -1.819350 -0.000028
H    -0.974365 -2.822602 -0.000021
C    -0.574966 -0.698333 -0.000023
C     0.880467 -0.540597 -0.000003
C     1.862926 -1.447334  0.000016
H     1.621733 -2.505203  0.000015
C     3.250503 -1.021780  0.000042
C     4.348127 -1.830730  0.000056
H     4.377811 -2.912323  0.000055
S     5.804423 -0.915394  0.000141
C     4.937248  0.568407  0.000048
H     5.465684  1.512852  0.000040
C     3.590082  0.377553  0.000042
Br   -5.196943 -0.156329 -0.000055
    el energy= -752.188052571
          zpe= -752.006209
    th energy= -751.992013
  th enthalpy= -751.991069
  free energy= -752.048806

cam-qtp01--8
B    -2.037198  1.428938  0.000121
O    -2.197585  2.759280  0.000080
H    -1.334157  3.206052  0.000228
N    -0.705844  0.843338  0.000287
C     0.477585  1.559700  0.000340
O     0.552989  2.768393  0.000094
C     1.566001  0.560185  0.000290
C     2.930377  0.755472  0.000073
H     3.380292  1.741264 -0.000079
C     3.705244 -0.387757  0.000055
C     3.166501 -1.669155  0.000260
H     3.844960 -2.513650  0.000220
C     1.794046 -1.841092  0.000456
H     1.367064 -2.838519  0.000566
C     0.993462 -0.708304  0.000429
C    -0.459460 -0.541952  0.000383
C    -1.443828 -1.447514  0.000337
H    -1.204786 -2.505907  0.000389
C    -2.829110 -1.018379  0.000095
C    -3.928504 -1.825724 -0.000062
H    -3.960115 -2.907275 -0.000024
S    -5.381462 -0.907525 -0.000451
C    -4.511904  0.574702 -0.000335
H    -5.038623  1.520102 -0.000510
C    -3.164996  0.381596 -0.000043
N     5.161328 -0.246445 -0.000345
O     5.608898  0.874023 -0.000646
O     5.819932 -1.258606 -0.000459
    el energy= -943.981525692
          zpe= -943.786067
    th energy= -943.770877
  th enthalpy= -943.769933
  free energy= -943.829485

cam-qtp01--9
B     1.427077  1.426145  0.000135
O     1.555019  2.762101  0.001638
H     0.675769  3.178489  0.000199
N     0.111756  0.811537 -0.002508
C    -1.087400  1.502337 -0.003446
O    -1.182287  2.712257 -0.001045
C    -2.158087  0.485681 -0.006540
C    -3.522899  0.669065 -0.005947
H    -3.944237  1.670377 -0.009037
C    -4.335782 -0.463680 -0.005444
C    -3.735926 -1.733271 -0.004095
H    -4.378117 -2.610397 -0.008518
C    -2.363321 -1.895971 -0.004177
H    -1.935968 -2.894298 -0.002178
C    -1.559945 -0.766697 -0.005524
C    -0.108890 -0.580252 -0.003583
C     0.898117 -1.459970 -0.002425
H     0.684517 -2.523715 -0.003549
C     2.275653 -1.000009  0.000034
C     3.393790 -1.779680  0.001425
H     3.451497 -2.860098  0.000619
S     4.828238 -0.827040  0.004436
C     3.922434  0.633603  0.003811
H     4.425256  1.591922  0.005119
C     2.580862  0.407530  0.001425
```

```
N    -5.711576 -0.347855 -0.048597
H    -6.097436  0.537572  0.235091
H    -6.243231 -1.140701  0.270509
    el energy= -794.949693199
          zpe= -794.740544
    th energy= -794.726355
  th enthalpy= -794.725411
  free energy= -794.781519

cam-qtp01.tddft--benzo
B     1.101441  1.395120 -0.000001
O     1.230389  2.732569 -0.000005
H     0.339641  3.136354 -0.000009
N    -0.217630  0.793560 -0.000002
C    -1.439653  1.489916 -0.000002
O    -1.501267  2.715094  0.000006
C    -2.463802  0.468316  0.000000
C    -3.846733  0.563990  0.000004
H    -4.327723  1.537283  0.000006
C    -4.584675 -0.605923  0.000004
C    -3.956018 -1.867217  0.000001
H    -4.567200 -2.764227  0.000002
C    -2.583721 -1.976576 -0.000002
H    -2.104724 -2.951935 -0.000004
C    -1.824059 -0.799255 -0.000002
C    -0.424603 -0.565573 -0.000003
C     0.662389 -1.467268 -0.000003
H     0.445207 -2.530988 -0.000002
C     1.977999 -1.017636 -0.000001
C     3.065415 -1.943892  0.000000
H     2.844908 -3.008193  0.000000
C     4.354008 -1.500354  0.000001
C     4.629837 -0.116192  0.000002
C     3.596675  0.800859  0.000001
H     3.811677  1.866003  0.000002
C     2.266136  0.394889  0.000000
H     5.174474 -2.211503  0.000002
H     5.661107  0.224109  0.000003
H    -5.669318 -0.557230  0.000007
 total energy= -806.748660222

cam-qtp01.tddft--1
B     1.218567 -2.614032  0.000000
O     0.589294 -3.800601  0.000000
H    -0.376481 -3.650662  0.000000
N     0.454095 -1.383253  0.000000
C    -0.948632 -1.288404  0.000000
O    -1.679674 -2.271636  0.000000
C    -1.235483  0.129849  0.000000
C    -2.443874  0.805348  0.000000
H    -3.384962  0.266077  0.000000
C    -2.401620  2.186682  0.000000
C    -1.186675  2.905134  0.000000
H    -1.213090  3.988529  0.000000
C     0.012615  2.233966  0.000000
H     0.947263  2.787681  0.000000
C     0.000000  0.832722  0.000000
C     1.034943 -0.134931  0.000000
C     2.437586  0.013689  0.000000
H     2.847196  1.019089  0.000000
C     3.284413 -1.090546  0.000000
C     4.702105 -0.920547  0.000000
H     5.107817  0.087711  0.000000
C     5.529686 -2.003789  0.000000
C     4.993352 -3.308295  0.000000
C     3.624996 -3.500231  0.000000
H     3.214013 -4.506059  0.000000
C     2.743052 -2.424949  0.000000
H     6.606624 -1.865805  0.000000
H     5.663721 -4.162644  0.000000
Br   -4.023982  3.164363  0.000000
 total energy= -819.291371866

cam-qtp01.tddft--2
B    -2.475755  0.464896  0.000000
O    -3.535792 -0.355274  0.000000
H    -3.233744 -1.283590  0.000000
N    -1.128921 -0.074636  0.000000
C    -0.792592 -1.441616  0.000000
O    -1.630926 -2.326696  0.000000
C     0.659123 -1.478991  0.000000
C     1.526602 -2.548014  0.000000
H     1.186899 -3.577220  0.000000
C     2.879350 -2.253977  0.000000
C     3.383420 -0.939158  0.000000
H     4.456944 -0.801735  0.000000
C     2.514425  0.123523  0.000000
H     2.893908  1.141032  0.000000
C     1.135135 -0.138253  0.000000
C     0.000000  0.711871  0.000000
C    -0.099080  2.118984  0.000000
H     0.819709  2.697081  0.000000
C    -1.334424  2.762651  0.000000
C    -1.409543  4.187786  0.000000
H    -0.486357  4.760927  0.000000
C    -2.620470  4.817255  0.000000
C    -3.810881  4.065910  0.000000
C    -3.764617  2.682069  0.000000
H    -4.684900  2.104557  0.000000
C    -2.554733  2.002011  0.000000
H    -2.669478  5.901784  0.000000
H    -4.768142  4.578571  0.000000
N     3.823290 -3.351735  0.000000
O     3.379617 -4.479251  0.000000
O     5.003734 -3.075478  0.000000
 total energy= -1011.08718115
```

```
cam-qtp01.tddft--3
B    -1.492782  1.386254 -0.000021
O    -1.658950  2.724867  0.000699
H    -0.777886  3.147005  0.000232
N    -0.164903  0.821878 -0.001014
C     1.032201  1.546968 -0.001277
O     1.077036  2.778128 -0.000590
C     2.082403  0.557482 -0.002149
C     3.455002  0.696937 -0.001619
H     3.911261  1.682802 -0.001929
C     4.241008 -0.458743 -0.000881
C     3.634641 -1.754505 -0.001096
H     4.277691 -2.629605 -0.003658
C     2.276301 -1.890599 -0.001435
H     1.826206 -2.879335 -0.001313
C     1.472141 -0.736635 -0.001730
C     0.077555 -0.546302 -0.001342
C    -0.973448 -1.465798 -0.001006
H    -0.737878 -2.525617 -0.001608
C    -2.308843 -1.042985 -0.000158
C    -3.368909 -1.991641  0.000204
H    -3.124279 -3.050858 -0.000352
C    -4.669895 -1.580284  0.001248
C    -4.981464 -0.205160  0.001990
C    -3.971794  0.731496  0.001614
H    -4.207604  1.792290  0.002138
C    -2.627001  0.354829  0.000483
H    -5.471369 -2.313247  0.001514
H    -6.020878  0.109603  0.002809
N     5.594831 -0.377498 -0.011834
H     6.054256  0.513672  0.058082
H     6.160817 -1.202958  0.076172
 total energy= -862.057647648

cam-qtp01.tddft--dioxo
B     0.071786  1.561932 -0.000302
O     0.093361  2.906846 -0.000178
H    -0.830517  3.230632 -0.000025
N    -1.183436  0.851672 -0.000195
C    -2.456106  1.439329  0.000108
O    -2.622253  2.657074  0.000246
C    -3.387927  0.333526  0.000208
C    -4.775592  0.313180  0.000519
H    -5.334755  1.243770  0.000721
C    -5.412785 -0.912335  0.000569
C    -4.679472 -2.116662  0.000306
H    -5.213226 -3.061913  0.000353
C    -3.303527 -2.110821  0.000001
H    -2.745079 -3.042958 -0.000194
C    -2.643870 -0.874891 -0.000045
C    -1.267590 -0.525840 -0.000281
C    -0.111990 -1.325853 -0.000511
H    -0.235757 -2.404018 -0.000578
C     1.162372 -0.771170 -0.000586
C     2.319259 -1.621181 -0.000662
H     2.218890 -2.700799 -0.000841
C     3.525283 -1.020269 -0.000578
C     3.672877  0.387346 -0.000444
C     2.599523  1.235720 -0.000463
H     2.724490  2.313323 -0.000421
C     1.322698  0.671149 -0.000499
O     4.755204 -1.583048 -0.001203
O     4.980714  0.689902 -0.000781
H    -6.497732 -0.955298  0.000814
C     5.696169 -0.531806  0.003262
H     6.308773 -0.588086  0.909220
H     6.317896 -0.588743 -0.896265
 total energy= -995.137317022

cam-qtp01.tddft--4
B     1.540423  1.640303  0.000267
O     1.658018  2.979547  0.000127
H     0.761902  3.372158  0.000041
N     0.239943  1.017824  0.000211
C    -0.988131  1.693401  0.000029
O    -1.072224  2.918022 -0.000086
C    -1.993643  0.653863  0.000030
C    -3.377296  0.740131 -0.000137
H    -3.875276  1.703694 -0.000293
C    -4.088126 -0.442206 -0.000087
C    -3.454932 -1.703899  0.000124
H    -4.063335 -2.600870  0.000148
C    -2.083601 -1.788464  0.000279
H    -1.597858 -2.760142  0.000423
C    -1.334999 -0.604344  0.000235
C     0.060646 -0.352002  0.000317
C     1.157469 -1.228520  0.000482
H     0.961388 -2.295854  0.000559
C     2.467892 -0.761968  0.000496
C     3.562282 -1.689937  0.000534
H     3.387653 -2.760010  0.000692
C     4.807379 -1.173720  0.000396
C     5.051736  0.219911  0.000248
C     4.039075  1.140656  0.000307
H     4.237665  2.207110  0.000238
C     2.727401  0.664471  0.000398
O     5.994667 -1.819824  0.000798
O     6.376030  0.431905  0.000391
Br   -5.984001 -0.388170 -0.000300
C     7.006575 -0.836311 -0.002625
H     7.621387 -0.935449  0.897845
H     7.614512 -0.934544 -0.907963
 total energy= -1007.68032818

cam-qtp01.tddft--5
```

```
B    -1.093227  1.628963 -0.000053
O    -1.199300  2.966738  0.000033
H    -0.304380  3.359336 -0.000008
N     0.199974  0.989569 -0.000196
C     1.436464  1.650664 -0.000163
O     1.535970  2.868538 -0.000109
C     2.432700  0.595327 -0.000172
C     3.809460  0.666964 -0.000068
H     4.344397  1.609490 -0.000002
C     4.496542 -0.531991 -0.000020
C     3.857295 -1.787500 -0.000079
H     4.473967 -2.676914 -0.000035
C     2.486985 -1.853838 -0.000172
H     1.986187 -2.817426 -0.000215
C     1.755771 -0.655494 -0.000210
C     0.363453 -0.383142 -0.000221
C    -0.744850 -1.243934 -0.000181
H    -0.562809 -2.313636 -0.000219
C    -2.051491 -0.761135 -0.000048
C    -3.154865 -1.676426  0.000017
H    -2.992613 -2.748359 -0.000015
C    -4.394968 -1.145490  0.000151
C    -4.623299  0.249728  0.000234
C    -3.597776  1.160110  0.000193
H    -3.784108  2.228779  0.000270
C    -2.295549  0.666878  0.000030
O    -5.588268 -1.777295  0.000368
O    -5.942076  0.478341  0.000450
N     5.944511 -0.497767  0.000169
O     6.485340  0.586311  0.000265
O     6.530730 -1.558945  0.000257
C    -6.589596 -0.782711 -0.000478
H    -7.200419 -0.872944 -0.904390
H    -7.202301 -0.873322  0.902087
 total energy= -1199.47677239

cam-qtp01.tddft--6
B     0.470248  1.594992 -0.003565
O     0.531688  2.943073 -0.002852
H    -0.382055  3.291228  0.000400
N    -0.802906  0.924514  0.000285
C    -2.054427  1.548230  0.004524
O    -2.196421  2.772776  0.005035
C    -3.018910  0.474197  0.007067
C    -4.400098  0.503508  0.008935
H    -4.931676  1.451009  0.011881
C    -5.091282 -0.707434  0.007711
C    -4.381509 -1.945815  0.004684
H    -4.950816 -2.870873  0.010595
C    -3.015305 -1.974621  0.001982
H    -2.489823 -2.925608 -0.000919
C    -2.305773 -0.761930  0.002763
C    -0.929747 -0.458687 -0.000759
C     0.196688 -1.286218 -0.004999
H     0.047878 -2.361387 -0.004915
C     1.490341 -0.762074 -0.008556
C     2.620031 -1.643668 -0.011376
H     2.489228 -2.720226 -0.013484
C     3.845001 -1.078816 -0.013686
C     4.034039  0.320146 -0.013561
C     2.987937  1.195352 -0.011970
H     3.140949  2.269299 -0.013424
C     1.689422  0.666905 -0.008604
O     5.058388 -1.681557 -0.030714
O     5.356908  0.582842 -0.028015
N    -6.454551 -0.735569  0.036613
H    -6.966355  0.115240 -0.122824
H    -6.936125 -1.593015 -0.172195
C     6.025569 -0.658574  0.072278
H     6.528603 -0.722907  1.045018
H     6.744771 -0.750426 -0.746825
 total energy= -1050.44424287

cam-qtp01.tddft--thieno
B     1.012612  1.436404 -0.000006
O     1.111136  2.770829 -0.000039
H     0.207060  3.149632 -0.000084
N    -0.283126  0.790509 -0.000025
C    -1.522900  1.478718 -0.000040
O    -1.584137  2.704554  0.000002
C    -2.532372  0.453971 -0.000043
C    -3.918252  0.534747 -0.000044
H    -4.408674  1.503482 -0.000041
C    -4.646652 -0.640001 -0.000053
C    -4.005110 -1.897542 -0.000060
H    -4.608047 -2.800160 -0.000066
C    -2.632339 -1.994538 -0.000055
H    -2.145590 -2.966333 -0.000054
C    -1.879412 -0.811297 -0.000046
C    -0.483101 -0.573654 -0.000026
C     0.606803 -1.475513 -0.000002
H     0.401343 -2.540412 -0.000001
C     1.913412 -0.988250  0.000030
C     3.096722 -1.741756  0.000056
H     3.186728 -2.819964  0.000060
S     4.470813 -0.750591  0.000127
C     3.521725  0.697431  0.000035
H     4.006462  1.665204  0.000023
C     2.191830  0.441018  0.000030
H    -5.731574 -0.600645 -0.000056
 total energy= -739.503790247

cam-qtp01.tddft--7
B     2.447714  1.429962  0.000003
O     2.617795  2.756869 -0.000031
H     1.738187  3.187431 -0.000081
```

```
N     1.120100  0.852028 -0.000020
C    -0.080082  1.603150 -0.000039
O    -0.083117  2.828779  0.000013
C    -1.141868  0.630501 -0.000037
C    -2.518180  0.793404 -0.000033
H    -2.962501  1.782946 -0.000029
C    -3.297293 -0.346950 -0.000040
C    -2.736860 -1.645075 -0.000049
H    -3.395782 -2.505407 -0.000052
C    -1.372611 -1.807640 -0.000047
H    -0.943520 -2.805870 -0.000047
C    -0.555052 -0.668206 -0.000041
C     0.850148 -0.502557 -0.000023
C     1.889948 -1.457873  0.000002
H     1.631069 -2.511076  0.000003
C     3.220779 -1.038012  0.000038
C     4.361772 -1.852724  0.000066
H     4.394448 -2.934244  0.000068
S     5.785496 -0.935797  0.000147
C     4.914596  0.560366  0.000052
H     5.449865  1.501139  0.000043
C     3.572957  0.374159  0.000042
Br   -5.185312 -0.182761 -0.000038
 total energy= -752.047017452

cam-qtp01.tddft--8
B     2.020437  1.432961  0.000150
O     2.186802  2.758494  0.000146
H     1.314497  3.198169  0.000168
N     0.693151  0.845502  0.000148
C    -0.510636  1.587354  0.000042
O    -0.527415  2.804799  0.000129
C    -1.574109  0.601617  0.000088
C    -2.938827  0.761703 -0.000005
H    -3.414842  1.735364 -0.000114
C    -3.706111 -0.394068  0.000029
C    -3.144023 -1.687759  0.000178
H    -3.816184 -2.536104  0.000198
C    -1.781177 -1.841935  0.000238
H    -1.343097 -2.835727  0.000324
C    -0.973370 -0.690317  0.000174
C     0.430679 -0.511378  0.000139
C     1.477926 -1.456681  0.000098
H     1.226813 -2.511766  0.000098
C     2.807371 -1.028041  0.000009
C     3.951265 -1.837534 -0.000136
H     3.986861 -2.919148 -0.000197
S     5.373083 -0.916766 -0.000230
C     4.491622  0.577152 -0.000096
H     5.022393  1.520646 -0.000125
C     3.152434  0.383828  0.000035
N    -5.141683 -0.266609 -0.000166
O    -5.612546  0.852192 -0.000682
O    -5.797654 -1.288469  0.000150
 total energy= -943.844690200

cam-qtp01.tddft--9
B     1.407582  1.433645 -0.000018
O     1.543775  2.769845  0.000470
H     0.647501  3.165843  0.000126
N     0.099550  0.829219 -0.000771
C    -1.113462  1.545980 -0.000992
O    -1.158271  2.779466 -0.000327
C    -2.149859  0.555459 -0.001748
C    -3.528235  0.676820 -0.001211
H    -3.998181  1.656283 -0.001163
C    -4.300382 -0.487345 -0.000780
C    -3.685119 -1.781758 -0.001346
H    -4.320449 -2.662086 -0.004535
C    -2.323899 -1.900889 -0.001524
H    -1.862203 -2.884471 -0.001812
C    -1.530907 -0.740644 -0.001454
C    -0.135210 -0.546107 -0.001046
C     0.908276 -1.467224 -0.000717
H     0.679205 -2.527477 -0.001234
C     2.241925 -1.014486 -0.000032
C     3.389713 -1.798611  0.000361
H     3.450838 -2.878624  0.000157
S     4.797057 -0.843882  0.001360
C     3.896423  0.623883  0.000940
H     4.406248  1.578371  0.001227
C     2.555128  0.404623  0.000347
N    -5.654806 -0.420574 -0.010314
H    -6.125131  0.465732  0.049454
H    -6.212244 -1.252894  0.067791
 total energy= -794.812219643

cam-qtp01.tddft-mecn--benzo
B     1.097549  1.395996  0.000003
O     1.209040  2.738540  0.000006
H     0.307238  3.119587  0.000013
N    -0.223122  0.795079  0.000008
C    -1.439365  1.486603  0.000012
O    -1.501035  2.718964 -0.000006
C    -2.463241  0.467881  0.000003
C    -3.847235  0.560864 -0.000008
H    -4.338993  1.529559 -0.000013
C    -4.584061 -0.611288 -0.000012
C    -3.950368 -1.872500 -0.000004
H    -4.561581 -2.769965 -0.000008
C    -2.580380 -1.984129  0.000006
H    -2.098282 -2.957423  0.000008
C    -1.816056 -0.801133  0.000009
C    -0.431257 -0.566844  0.000011
C     0.672224 -1.465992  0.000009
H     0.459906 -2.531083  0.000009
```

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C     1.978846 -1.011705  0.000004
C     3.066315 -1.941155  0.000000
H     2.841187 -3.004423  0.000002
C     4.357911 -1.498683 -0.000009
C     4.635040 -0.118031 -0.000013
C     3.597808  0.803647 -0.000009
H     3.827601  1.866332 -0.000012
C     2.270241  0.401626 -0.000001
H     5.177256 -2.211474 -0.000012
H     5.666251  0.222992 -0.000019
H    -5.669036 -0.564637 -0.000020
 total energy= -806.782419447

cam-qtp01.tddft-mecn--1
B     1.231045 -2.607309  0.000000
O     0.591979 -3.792307  0.000000
H    -0.371792 -3.623557  0.000000
N     0.456419 -1.380388  0.000000
C    -0.940128 -1.293843  0.000000
O    -1.668190 -2.288122  0.000000
C    -1.236571  0.119815  0.000000
C    -2.449491  0.790559  0.000000
H    -3.389344  0.247776  0.000000
C    -2.409790  2.171175  0.000000
C    -1.197482  2.895796  0.000000
H    -1.221480  3.979932  0.000000
C     0.004875  2.234158  0.000000
H     0.937211  2.790712  0.000000
C     0.000000  0.827036  0.000000
C     1.029797 -0.127627  0.000000
C     2.444794  0.020872  0.000000
H     2.850530  1.028157  0.000000
C     3.287983 -1.076401  0.000000
C     4.706463 -0.894708  0.000000
H     5.101529  0.117576  0.000000
C     5.543981 -1.973442  0.000000
C     5.018445 -3.278842  0.000000
C     3.645348 -3.481580  0.000000
H     3.254147 -4.495752  0.000000
C     2.757154 -2.417078  0.000000
H     6.619860 -1.826919  0.000000
H     5.693734 -4.129552  0.000000
Br   -4.041347  3.147400  0.000000
 total energy= -819.325959245

cam-qtp01.tddft-mecn--2
B    -2.477117  0.443832  0.000000
O    -3.526831 -0.394933  0.000000
H    -3.200894 -1.315492  0.000000
N    -1.127617 -0.090509  0.000000
C    -0.783985 -1.446320  0.000000
O    -1.616685 -2.344605  0.000000
C     0.667635 -1.474476  0.000000
C     1.539725 -2.534361  0.000000
H     1.202443 -3.564518  0.000000
C     2.895559 -2.232423  0.000000
C     3.387049 -0.908128  0.000000
H     4.458067 -0.749940  0.000000
C     2.515900  0.147768  0.000000
H     2.885583  1.168319  0.000000
C     1.130166 -0.122519  0.000000
C     0.000000  0.704031  0.000000
C    -0.119453  2.122614  0.000000
H     0.794633  2.708720  0.000000
C    -1.353771  2.748925  0.000000
C    -1.432258  4.175508  0.000000
H    -0.508914  4.748281  0.000000
C    -2.647416  4.802506  0.000000
C    -3.830966  4.047464  0.000000
C    -3.780326  2.657283  0.000000
H    -4.706735  2.088931  0.000000
C    -2.572984  1.982618  0.000000
H    -2.700704  5.886919  0.000000
H    -4.791554  4.554297  0.000000
N     3.836017 -3.315265  0.000000
O     3.408809 -4.455450  0.000000
O     5.022907 -3.045912  0.000000
 total energy= -1011.12509384

cam-qtp01.tddft-mecn--2-
B     2.183240  1.524963  0.003558
O     2.465464  2.762401  0.009540
N     0.757217  0.955303 -0.001015
C    -0.459174  1.667152 -0.003316
O    -0.588164  2.871761 -0.007021
C    -1.516184  0.645897 -0.001562
C    -2.874208  0.785586 -0.001789
H    -3.357603  1.755967 -0.003217
C    -3.634721 -0.388274  0.000168
C    -3.035406 -1.670215  0.001954
H    -3.680189 -2.540317  0.003340
C    -1.673230 -1.799469  0.001798
H    -1.214847 -2.783835  0.003035
C    -0.886240 -0.625934  0.000189
C     0.499733 -0.391586 -0.000017
C     1.533986 -1.369140 -0.000217
H     1.229754 -2.412683 -0.000762
C     2.878173 -1.033843 -0.000546
C     3.887468 -2.043525 -0.002493
H     3.586489 -3.088221 -0.003754
C     5.209544 -1.693108 -0.002833
C     5.578618 -0.337079 -0.000926
C     4.604457  0.652873  0.001302
H     4.888663  1.702190  0.003029
C     3.253235  0.348327  0.001230
H     5.978019 -2.461086 -0.004506
```

```
H     6.631633 -0.068062 -0.001194
N    -5.048312 -0.288363  0.000498
O    -5.559904  0.823862 -0.001937
O    -5.709491 -1.318440  0.003445
 total energy= -1010.62524532

cam-qtp01.tddft-mecn--3
B    -1.490071  1.382047 -0.000162
O    -1.638694  2.728444  0.000101
H    -0.743555  3.124271  0.000013
N    -0.160650  0.820641 -0.000416
C     1.029909  1.543669 -0.000230
O     1.067017  2.782783 -0.000165
C     2.084260  0.560822 -0.000156
C     3.454036  0.704657  0.000085
H     3.928357  1.682183  0.000135
C     4.246186 -0.457774  0.000252
C     3.632097 -1.761058  0.000134
H     4.283114 -2.630135  0.000261
C     2.282056 -1.898739 -0.000131
H     1.829230 -2.886007 -0.000186
C     1.469142 -0.736829 -0.000268
C     0.087701 -0.552450 -0.000387
C    -0.976432 -1.469009 -0.000405
H    -0.745294 -2.530097 -0.000529
C    -2.307116 -1.039928 -0.000196
C    -3.370409 -1.988095 -0.000107
H    -3.124679 -3.047190 -0.000299
C    -4.673882 -1.576737  0.000257
C    -4.989929 -0.204068  0.000517
C    -3.975501  0.732348  0.000361
H    -4.222179  1.791683  0.000546
C    -2.630694  0.358104 -0.000012
H    -5.473677 -2.312299  0.000348
H    -6.029422  0.110900  0.000826
N     5.582239 -0.377878  0.000387
H     6.048476  0.517420  0.001046
H     6.153734 -1.209611  0.001082
 total energy= -862.099616915

cam-qtp01.tddft-mecn--dioxo
B     0.068279  1.563993 -0.012488
O     0.069333  2.912590 -0.009419
H    -0.863976  3.211579 -0.008327
N    -1.190418  0.854196 -0.013457
C    -2.458492  1.436168 -0.004682
O    -2.626819  2.661738 -0.003719
C    -3.388184  0.333043  0.003677
C    -4.777394  0.306154  0.017769
H    -5.349159  1.230012  0.021545
C    -5.410785 -0.922065  0.027447
C    -4.669906 -2.125377  0.023129
H    -5.202194 -3.071892  0.031967
C    -3.296334 -2.119253  0.008337
H    -2.733463 -3.048433  0.005720
C    -2.634487 -0.876119 -0.001196
C    -1.273721 -0.525069 -0.012752
C    -0.099212 -1.320558 -0.023103
H    -0.218788 -2.399676 -0.028272
C     1.163869 -0.762806 -0.025092
C     2.322597 -1.617925 -0.035902
H     2.212019 -2.697005 -0.054027
C     3.530102 -1.020706 -0.025635
C     3.677858  0.385278 -0.000323
C     2.601483  1.238598  0.000017
H     2.743691  2.314565  0.011422
C     1.326286  0.679775 -0.013546
O     4.758608 -1.581376 -0.054819
O     4.977037  0.691462  0.005817
H    -6.495727 -0.969192  0.039120
C     5.697621 -0.534266  0.102156
H     6.165637 -0.596930  1.090194
H     6.440422 -0.576915 -0.697370
 total energy= -995.171205514

cam-qtp01.tddft-mecn--4
B     1.538390  1.645153 -0.000350
O     1.633920  2.989399 -0.000264
H     0.725406  3.355872 -0.000279
N     0.233605  1.023272 -0.000577
C    -0.989814  1.693942 -0.000323
O    -1.074673  2.926876 -0.000133
C    -1.993146  0.657499 -0.000308
C    -3.379086  0.739525 -0.000010
H    -3.882245  1.701086  0.000203
C    -4.083763 -0.444971  0.000052
C    -3.447586 -1.707406 -0.000180
H    -4.049325 -2.609704 -0.000144
C    -2.078531 -1.792272 -0.000457
H    -1.590004 -2.762101 -0.000645
C    -1.326879 -0.602042 -0.000504
C     0.054817 -0.347002 -0.000685
C     1.170934 -1.220992 -0.000807
H     0.977968 -2.289531 -0.000995
C     2.469658 -0.752267 -0.000577
C     3.563911 -1.687457 -0.000530
H     3.376328 -2.755934 -0.000840
C     4.810676 -1.177441  0.000022
C     5.057392  0.214526  0.000497
C     4.043336  1.142791  0.000301
H     4.262128  2.205819  0.000612
C     2.733136  0.674880 -0.000250
O     5.994120 -1.825011  0.000435
O     6.372565  0.429704  0.001249
Br   -5.986175 -0.394636  0.000508
C     7.014596 -0.843539  0.000377
```

```
H     7.622085 -0.938563  0.904685
H     7.621249 -0.937758 -0.904593
 total energy= -1007.71528069

cam-qtp01.tddft-mecn--5
B    -1.088044  1.636677 -0.000311
O    -1.176525  2.978631  0.000592
H    -0.272726  3.351184  0.000353
N     0.208422  0.998156 -0.001406
C     1.439831  1.652395 -0.001036
O     1.546729  2.875596 -0.000413
C     2.433633  0.596285 -0.001353
C     3.806033  0.663520 -0.000589
H     4.340517  1.606555  0.000018
C     4.495668 -0.539954 -0.000155
C     3.845272 -1.796326 -0.000746
H     4.450026 -2.694395 -0.000434
C     2.479429 -1.862602 -0.001801
H     1.974687 -2.823630 -0.002396
C     1.743434 -0.656321 -0.001894
C     0.372222 -0.377246 -0.001943
C    -0.758420 -1.234679 -0.002138
H    -0.580272 -2.305733 -0.002831
C    -2.050815 -0.749874 -0.001267
C    -3.153778 -1.673353 -0.001275
H    -2.976816 -2.743533 -0.002166
C    -4.395499 -1.149526  0.000040
C    -4.625397  0.243734  0.001328
C    -3.598197  1.163261  0.001268
H    -3.805744  2.228395  0.002293
C    -2.298802  0.678913 -0.000103
O    -5.585707 -1.782575  0.000642
O    -5.933583  0.476399  0.002632
N     5.928107 -0.505996  0.001709
O     6.484346  0.577569 -0.000614
O     6.529450 -1.564723  0.005767
C    -6.594461 -0.789230  0.000858
H    -7.201189 -0.873325 -0.904822
H    -7.202568 -0.875179  0.905402
 total energy= -1199.51505019

cam-qtp01.tddft-mecn--5-
B     1.146890  1.799894  0.003118
O     1.352495  3.053378  0.006981
N    -0.223370  1.125736  0.000150
C    -1.487050  1.736802 -0.001550
O    -1.714284  2.928334 -0.003248
C    -2.460956  0.636077 -0.001166
C    -3.824727  0.672433 -0.002173
H    -4.379744  1.603717 -0.003783
C    -4.497195 -0.555033 -0.000256
C    -3.799262 -1.789132  0.002126
H    -4.376528 -2.705463  0.003638
C    -2.432731 -1.815059  0.001975
H    -1.902212 -2.762747  0.003386
C    -1.732903 -0.584723  0.000420
C    -0.372130 -0.244425  0.000567
C     0.734097 -1.135687  0.000307
H     0.510683 -2.199287 -0.000248
C     2.047007 -0.706620  0.000070
C     3.123548 -1.659053 -0.001504
H     2.924760 -2.725781 -0.002591
C     4.378292 -1.159421 -0.001415
C     4.633803  0.224752  0.000275
C     3.624275  1.159632  0.001801
H     3.827555  2.225824  0.003200
C     2.311264  0.709051  0.001514
O     5.558022 -1.821713 -0.002629
O     5.957465  0.430657  0.000070
N    -5.909926 -0.562470 -0.000644
O    -6.507587  0.508192 -0.008986
O    -6.492912 -1.640757  0.007584
C     6.584995 -0.846994 -0.002303
H     7.194120 -0.950702  0.900779
H     7.192425 -0.948229 -0.906825
 total energy= -1199.01388355

cam-qtp01.tddft-mecn--6
B     0.469209  1.594160 -0.007628
O     0.509146  2.949264 -0.003017
H    -0.416430  3.268769  0.002600
N    -0.807757  0.926823 -0.003531
C    -2.053951  1.547716  0.004173
O    -2.192107  2.781101  0.009095
C    -3.021523  0.480078  0.004959
C    -4.401284  0.510140  0.012129
H    -4.952066  1.446852  0.018294
C    -5.094656 -0.710214  0.011231
C    -4.374273 -1.955232  0.002972
H    -4.950191 -2.876071  0.002018
C    -3.016047 -1.982634 -0.003667
H    -2.485331 -2.930460 -0.009849
C    -2.301262 -0.760007 -0.002508
C    -0.938836 -0.460984 -0.007494
C     0.200229 -1.283592 -0.014777
H     0.056518 -2.359844 -0.017108
C     1.489154 -0.752458 -0.019025
C     2.618978 -1.637337 -0.023865
H     2.478814 -2.713414 -0.029466
C     3.847793 -1.076993 -0.025012
C     4.042151  0.319117 -0.023471
C     2.995752  1.195965 -0.020882
H     3.163510  2.268612 -0.022594
C     1.692543  0.673628 -0.016961
O     5.057573 -1.683422 -0.055543
O     5.365030  0.578669 -0.050560
```

```
N    -6.436456 -0.745425  0.017954
H    -6.979139  0.104900  0.024958
H    -6.931931 -1.623971  0.017796
C     6.020972 -0.664676  0.147990
H     6.400367 -0.715190  1.175771
H     6.827748 -0.770766 -0.579792
 total energy= -1050.48566632

cam-qtp01.tddft-mecn--thieno
B     1.009081  1.437790  0.000008
O     1.089691  2.777195 -0.000007
H     0.174832  3.132640 -0.000031
N    -0.289846  0.793267 -0.000015
C    -1.521417  1.475203 -0.000043
O    -1.587662  2.709117 -0.000030
C    -2.530567  0.452623 -0.000045
C    -3.917971  0.530628 -0.000056
H    -4.418336  1.495169 -0.000064
C    -4.645134 -0.645591 -0.000058
C    -3.998106 -1.903492 -0.000049
H    -4.601426 -2.806464 -0.000050
C    -2.628542 -2.003479 -0.000035
H    -2.139604 -2.973584 -0.000025
C    -1.869462 -0.814038 -0.000033
C    -0.489362 -0.574367 -0.000015
C     0.619472 -1.474331  0.000009
H     0.421803 -2.541431  0.000011
C     1.913580 -0.980889  0.000031
C     3.096013 -1.740341  0.000048
H     3.180291 -2.820593  0.000049
S     4.473239 -0.751617  0.000099
C     3.523483  0.703700  0.000035
H     4.023972  1.664925  0.000027
C     2.195414  0.449628  0.000032
H    -5.730477 -0.608623 -0.000068
 total energy= -739.537540065

cam-qtp01.tddft-mecn--7
B     2.446646  1.430962  0.000021
O     2.601038  2.763293  0.000010
H     1.709985  3.172771 -0.000014
N     1.114355  0.856318 -0.000008
C    -0.078012  1.603163 -0.000044
O    -0.082356  2.837118 -0.000026
C    -1.139641  0.633650 -0.000039
C    -2.518198  0.795092 -0.000043
H    -2.965700  1.784064 -0.000051
C    -3.291976 -0.346891 -0.000040
C    -2.729807 -1.645827 -0.000031
H    -3.383768 -2.510838 -0.000027
C    -1.368605 -1.811140 -0.000024
H    -0.937930 -2.808100 -0.000013
C    -0.546702 -0.666221 -0.000028
C     0.844098 -0.499205 -0.000011
C     1.901279 -1.457217  0.000014
H     1.646536 -2.512088  0.000015
C     3.219776 -1.032843  0.000041
C     4.360177 -1.854444  0.000060
H     4.385849 -2.938039  0.000059
S     5.786860 -0.941033  0.000119
C     4.916416  0.563191  0.000056
H     5.466583  1.496710  0.000053
C     3.576960  0.380029  0.000046
Br   -5.187688 -0.187094 -0.000045
 total energy= -752.081692007

cam-qtp01.tddft-mecn--8
B     2.016458  1.437452  0.000014
O     2.170652  2.768298 -0.000026
H     1.289542  3.191240 -0.000071
N     0.686047  0.853812 -0.000006
C    -0.508373  1.588566 -0.000046
O    -0.534948  2.812199  0.000078
C    -1.571816  0.602255 -0.000009
C    -2.932343  0.760211  0.000021
H    -3.404532  1.736018  0.000014
C    -3.703670 -0.399072 -0.000002
C    -3.133421 -1.695040 -0.000021
H    -3.795389 -2.551784 -0.000053
C    -1.775185 -1.850708 -0.000030
H    -1.333624 -2.842351 -0.000054
C    -0.961453 -0.692856 -0.000033
C     0.422397 -0.507481 -0.000025
C     1.487280 -1.454656 -0.000024
H     1.241434 -2.511697 -0.000024
C     2.802190 -1.020383 -0.000013
C     3.943801 -1.838960 -0.000014
H     3.969990 -2.922764 -0.000031
S     5.367113 -0.923911  0.000025
C     4.490200  0.580381  0.000019
H     5.038059  1.515297  0.000031
C     3.153015  0.392345  0.000011
N    -5.124324 -0.271405 -0.000038
O    -5.609902  0.848283 -0.000080
O    -5.796974 -1.289169  0.000157
 total energy= -943.882799731

cam-qtp01.tddft-mecn--8-
B    -2.106081  1.585760 -0.024931
O    -2.349009  2.826398 -0.070193
N    -0.688493  0.966949  0.008105
C     0.534642  1.667204  0.024858
O     0.675030  2.869271  0.050506
C     1.587605  0.640532  0.013068
C     2.943470  0.773855  0.013055
H     3.432133  1.741470  0.021619
```

```
C     3.701305 -0.406349 -0.000436
C     3.090948 -1.685335 -0.010752
H     3.730952 -2.558932 -0.020436
C     1.729228 -1.806931 -0.008943
H     1.265191 -2.788655 -0.016957
C     0.947366 -0.627063  0.001601
C    -0.434960 -0.385275  0.001569
C    -1.467306 -1.365703  0.000097
H    -1.172079 -2.410944  0.001199
C    -2.802029 -0.995020  0.002581
C    -3.908698 -1.853794  0.011138
H    -3.901924 -2.937637  0.018351
S    -5.363505 -0.977881  0.010300
C    -4.518952  0.551798 -0.003567
H    -5.090004  1.472603 -0.009432
C    -3.177711  0.407583 -0.005933
N     5.109118 -0.314798 -0.005487
O     5.629478  0.796479  0.005466
O     5.768051 -1.349483 -0.021132
 total energy= -943.383273191

cam-qtp01.tddft-mecn--9
B     1.403860  1.428234  0.000000
O     1.522870  2.771138  0.000063
H     0.612876  3.140934  0.000035
N     0.093847  0.827003 -0.000102
C    -1.111395  1.541121 -0.000088
O    -1.150146  2.783544 -0.000056
C    -2.151293  0.556466 -0.000053
C    -3.527798  0.683213  0.000020
H    -4.013403  1.655372  0.000082
C    -4.307052 -0.484850  0.000063
C    -3.682470 -1.785995 -0.000033
H    -4.326050 -2.660485 -0.000022
C    -2.330649 -1.909128 -0.000093
H    -1.868209 -2.892178 -0.000122
C    -1.526663 -0.741501 -0.000086
C    -0.144387 -0.552950 -0.000095
C     0.914448 -1.471682 -0.000050
H     0.690566 -2.533658 -0.000062
C     2.243271 -1.013253 -0.000009
C     3.391717 -1.796777  0.000051
H     3.453812 -2.878169  0.000062
S     4.804252 -0.838962  0.000057
C     3.899085  0.629858  0.000042
H     4.418901  1.580603  0.000047
C     2.558685  0.407471  0.000010
N    -5.645462 -0.419989  0.000097
H    -6.122288  0.469629  0.000491
H    -6.207025 -1.258336  0.000490
 total energy= -794.853210670

lc-whpbe--benzo
B    -1.123660  1.387942  0.000001
O    -1.274650  2.731487  0.000002
H    -0.404915  3.165106  0.000003
N     0.200972  0.789837  0.000002
C     1.411723  1.475499  0.000004
O     1.516067  2.685624 -0.000002
C     2.472929  0.441618  0.000000
C     3.848681  0.590915 -0.000003
H     4.295724  1.581625 -0.000004
C     4.621061 -0.563119 -0.000004
C     4.015032 -1.821510 -0.000002
H     4.640012 -2.711613 -0.000003
C     2.632331 -1.962400  0.000001
H     2.176391 -2.949220  0.000001
C     1.861525 -0.808707  0.000002
C     0.406289 -0.596944  0.000002
C    -0.618080 -1.460534  0.000002
H    -0.418518 -2.528917  0.000002
C    -2.004072 -1.002589  0.000001
C    -3.052216 -1.930386  0.000000
H    -2.826471 -2.995292  0.000001
C    -4.367011 -1.500952 -0.000001
C    -4.662561 -0.137774 -0.000002
C    -3.631099  0.786106 -0.000001
H    -3.849373  1.852071 -0.000002
C    -2.295761  0.375416  0.000000
H    -5.173158 -2.231391 -0.000001
H    -5.697798  0.195084 -0.000003
H     5.705652 -0.490743 -0.000006
    el energy= -807.201288330

lc-whpbe--1
B     1.224748 -2.626260  0.000000
O     0.593316 -3.820946  0.000000
H    -0.369884 -3.694205 -0.000000
N     0.467046 -1.384577  0.000000
C    -0.918136 -1.269290 -0.000000
O    -1.690447 -2.205568 -0.000000
C    -1.209681  0.185251 -0.000000
C    -2.433673  0.828711 -0.000000
H    -3.363744  0.268093 -0.000000
C    -2.411123  2.216143 -0.000000
C    -1.207998  2.925896 -0.000000
H    -1.233276  4.011765 -0.000000
C     0.009655  2.259432  0.000000
H     0.938876  2.823076  0.000000
C     0.000000  0.871581  0.000000
C     1.081021 -0.123596  0.000000
C     2.414079  0.011957  0.000000
H     2.851793  1.006800  0.000000
C     3.300489 -1.147840  0.000000
C     4.689137 -0.973031  0.000000
H     5.103943  0.033363  0.000000
```

```
C     5.531982 -2.070001  0.000000
C     5.006289 -3.361849  0.000000
C     3.633299 -3.542657  0.000000
H     3.212083 -4.545834  0.000000
C     2.763186 -2.449875  0.000000
H     6.609695 -1.922190  0.000000
H     5.673031 -4.220847  0.000000
Br   -4.043705  3.174584 -0.000000
    el energy= -819.791303720

lc-whpbe--2
B    -2.489599  0.469405 -0.000000
O    -3.559546 -0.354525 -0.000000
H    -3.275887 -1.283407 -0.000000
N    -1.136381 -0.066021 -0.000000
C    -0.786216 -1.410616 -0.000000
O    -1.574036 -2.332589 -0.000000
C     0.697489 -1.447134 -0.000000
C     1.544837 -2.537709 -0.000000
H     1.180541 -3.560029 -0.000000
C     2.899653 -2.254427  0.000000
C     3.401607 -0.955803  0.000000
H     4.477594 -0.815177  0.000000
C     2.532153  0.123900  0.000000
H     2.919728  1.138785  0.000000
C     1.167111 -0.135358  0.000000
C     0.000000  0.755428  0.000000
C    -0.092614  2.092392  0.000000
H     0.813353  2.692903  0.000000
C    -1.386012  2.767963  0.000000
C    -1.449280  4.166006  0.000000
H    -0.528286  4.746151  0.000000
C    -2.673824  4.809400  0.000000
C    -3.856719  4.070623 -0.000000
C    -3.801714  2.686756 -0.000000
H    -4.718695  2.101258 -0.000000
C    -2.576767  2.015727 -0.000000
H    -2.712312  5.896407  0.000000
H    -4.816753  4.581150 -0.000000
N     3.854384 -3.373986  0.000000
O     3.396402 -4.492357  0.000000
O     5.032739 -3.101518  0.000000
    el energy= -1011.57130659

lc-whpbe--3
B    -1.514621  1.380018  0.000412
O    -1.687811  2.721562  0.001801
H    -0.824515  3.167798  0.000304
N    -0.179553  0.805138 -0.002124
C     1.017308  1.512293 -0.003504
O     1.101367  2.724605 -0.001601
C     2.099890  0.498350 -0.006223
C     3.466104  0.691254 -0.006262
H     3.881078  1.696658 -0.010303
C     4.289335 -0.438728 -0.005523
C     3.695462 -1.714521 -0.004453
H     4.342052 -2.590223 -0.009522
C     2.321133 -1.885865 -0.004156
H     1.900411 -2.888466 -0.002715
C     1.509086 -0.759560 -0.004905
C     0.052145 -0.579294 -0.002894
C    -0.959614 -1.458130 -0.001580
H    -0.743520 -2.523294 -0.002504
C    -2.353175 -1.023440  0.000564
C    -3.386329 -1.968233  0.001479
H    -3.142791 -3.029232  0.000431
C    -4.708145 -1.561134  0.003466
C    -5.027695 -0.203343  0.004622
C    -4.011653  0.737245  0.003727
H    -4.247270  1.799562  0.004480
C    -2.669472  0.348941  0.001702
H    -5.501704 -2.305381  0.004031
H    -6.068596  0.111451  0.006101
N     5.665977 -0.313002 -0.046161
H     6.050345  0.576432  0.228232
H     6.207913 -1.104687  0.259443
    el energy= -862.523279485

lc-whpbe--dioxo
B     0.092832  1.565497 -0.005833
O     0.126644  2.918373 -0.002031
H    -0.777335  3.274498  0.002937
N    -1.173705  0.854378 -0.001430
C    -2.440946  1.429667  0.005972
O    -2.652835  2.625627  0.010218
C    -3.405350  0.304880  0.007411
C    -4.788945  0.330431  0.013715
H    -5.322709  1.277245  0.018644
C    -5.455068 -0.887950  0.013404
C    -4.738668 -2.086806  0.006911
H    -5.281547 -3.029206  0.006740
C    -3.348861 -2.103549  0.000597
H    -2.806727 -3.045755 -0.004494
C    -2.684140 -0.885692  0.000909
C    -1.254404 -0.543650 -0.004708
C    -0.154103 -1.309075 -0.011908
H    -0.256058 -2.391067 -0.014417
C     1.184823 -0.730208 -0.017566
C     2.304248 -1.589684 -0.023847
H     2.193744 -2.670244 -0.028845
C     3.540316 -1.004494 -0.024526
C     3.708629  0.379616 -0.022826
C     2.640528  1.232707 -0.019652
H     2.770644  2.310979 -0.022607
C     1.350049  0.666798 -0.014923
O     4.757974 -1.607466 -0.049834
```

```
O     5.040808  0.669019 -0.052250
H    -6.541758 -0.913053  0.018189
C     5.705342 -0.566276  0.134900
H     6.108063 -0.618488  1.157254
H     6.504018 -0.667750 -0.606228
    el energy= -995.619866485

lc-whpbe--4
B    -1.562032  1.639861 -0.006469
O    -1.684053  2.986909 -0.001520
H    -0.807763  3.405671  0.002444
N    -0.250849  1.011623 -0.004551
C     0.974713  1.667714  0.001588
O     1.114331  2.873268  0.006514
C     2.009505  0.604452  0.000775
C     3.386717  0.728422  0.005365
H     3.863574  1.704120  0.010416
C     4.121083 -0.448871  0.003187
C     3.496003 -1.698006 -0.003403
H     4.106771 -2.596312 -0.004991
C     2.111614 -1.799329 -0.007930
H     1.637420 -2.777190 -0.013092
C     1.365986 -0.628710 -0.005753
C    -0.081309 -0.378895 -0.009079
C    -1.130119 -1.213332 -0.015222
H    -0.959089 -2.286586 -0.018716
C    -2.503337 -0.722078 -0.018283
C    -3.564383 -1.652493 -0.023440
H    -3.384347 -2.723624 -0.029422
C    -4.835671 -1.148407 -0.021707
C    -5.092772  0.222167 -0.018621
C    -4.082236  1.142838 -0.016459
H    -4.282051  2.210353 -0.018164
C    -2.758121  0.661438 -0.014298
O    -6.011287 -1.828356 -0.044810
O    -6.439877  0.425548 -0.044474
Br    6.012801 -0.367452  0.009278
C    -7.025548 -0.850702  0.134333
H    -7.809746 -1.001140 -0.613941
H    -7.432374 -0.931319  1.152946
    el energy= -1008.20995884

lc-whpbe--5
B     1.116950  1.632087 -0.005930
O     1.227897  2.979252 -0.002235
H     0.350078  3.394310  0.001373
N    -0.188835  0.991430 -0.003556
C    -1.420447  1.635222  0.001961
O    -1.574620  2.838112  0.005744
C    -2.443354  0.559835  0.001989
C    -3.820470  0.663548  0.006330
H    -4.333724  1.619735  0.010736
C    -4.519896 -0.530789  0.004664
C    -3.894170 -1.774412 -0.001022
H    -4.512111 -2.666426 -0.002131
C    -2.510266 -1.854554 -0.005164
H    -2.018261 -2.823109 -0.009607
C    -1.785691 -0.668822 -0.003595
C    -0.343231 -0.400583 -0.006975
C     0.713324 -1.225988 -0.012347
H     0.551810 -2.300744 -0.014923
C     2.081126 -0.722357 -0.015755
C     3.150629 -1.643131 -0.020382
H     2.980989 -2.715939 -0.025392
C     4.416844 -1.126722 -0.019664
C     4.660097  0.246686 -0.017648
C     3.640734  1.158005 -0.015701
H     3.830693  2.227268 -0.017923
C     2.321689  0.663826 -0.012959
O     5.598264 -1.794763 -0.041476
O     6.003460  0.464068 -0.041905
N    -5.990634 -0.487148  0.009040
O    -6.512788  0.602858  0.015820
O    -6.580514 -1.542992  0.005724
C     6.606089 -0.807187  0.120992
H     7.033642 -0.886346  1.130747
H     7.376776 -0.946903 -0.643356
    el energy= -1199.99008966

lc-whpbe--6
B     0.491798  1.591996 -0.005938
O     0.557547  2.944374 -0.003025
H    -0.338389  3.320295  0.003056
N    -0.792106  0.912427  0.000020
C    -2.042447  1.520598  0.008048
O    -2.224583  2.721996  0.010547
C    -3.038669  0.421885  0.011217
C    -4.415903  0.503780  0.016541
H    -4.910608  1.472455  0.025352
C    -5.145505 -0.688799  0.014707
C    -4.450492 -1.912092  0.007494
H    -5.023920 -2.837359  0.011680
C    -3.066497 -1.971973  0.002058
H    -2.566614 -2.937567 -0.004220
C    -2.347611 -0.784131  0.003727
C    -0.910514 -0.484724 -0.002885
C     0.172569 -1.274848 -0.010949
H     0.045724 -2.354198 -0.012929
C     1.525535 -0.728268 -0.017973
C     2.624100 -1.614254 -0.024730
H     2.487247 -2.691816 -0.028955
C     3.874383 -1.059625 -0.026468
C     4.077598  0.319455 -0.025612
C     3.030750  1.198159 -0.022046
H     3.186852  2.273019 -0.025698
C     1.726625  0.664108 -0.016020
```

```
O     5.077258 -1.693143 -0.052900
O     5.418019  0.575014 -0.057754
N    -6.527966 -0.674149  0.060267
H    -6.982693  0.181808 -0.213130
H    -7.004990 -1.506104 -0.246691
C     6.048203 -0.675758  0.140614
H     6.437145 -0.735682  1.168191
H     6.853086 -0.799786 -0.590249
    el energy= -1050.94172665

lc-whpbe--thieno
B    -1.042040  1.437766  0.000005
O    -1.156811  2.781625  0.000029
H    -0.272572  3.187898  0.000058
N     0.269296  0.798975  0.000023
C     1.487909  1.466665  0.000047
O     1.610690  2.676484  0.000028
C     2.536920  0.421929  0.000048
C     3.914494  0.557376  0.000055
H     4.371011  1.543726  0.000058
C     4.674868 -0.603938  0.000061
C     4.055753 -1.856375  0.000060
H     4.671721 -2.752727  0.000064
C     2.672210 -1.983104  0.000051
H     2.206705 -2.965454  0.000046
C     1.912552 -0.821309  0.000043
C     0.459913 -0.597450  0.000021
C    -0.561838 -1.464147  0.000002
H    -0.365075 -2.532280  0.000007
C    -1.934694 -0.979881 -0.000026
C    -3.069546 -1.742090 -0.000033
H    -3.147733 -2.822995 -0.000025
S    -4.482636 -0.766432 -0.000164
C    -3.558357  0.678467 -0.000018
H    -4.050133  1.644373  0.000003
C    -2.216485  0.433309 -0.000027
H     5.760152 -0.542869  0.000067
    el energy= -739.975577508

lc-whpbe--7
B     2.472253  1.431676  0.000005
O     2.648031  2.768275 -0.000020
H     1.785939  3.218684 -0.000053
N     1.132015  0.852164 -0.000017
C    -0.053929  1.573552 -0.000044
O    -0.127818  2.786323 -0.000013
C    -1.148548  0.573571 -0.000039
C    -2.516495  0.778839 -0.000040
H    -2.934164  1.781236 -0.000040
C    -3.318821 -0.352627 -0.000044
C    -2.768217 -1.636918 -0.000046
H    -3.431048 -2.497403 -0.000048
C    -1.392779 -1.819688 -0.000042
H    -0.977399 -2.823954 -0.000038
C    -0.579186 -0.694685 -0.000037
C     0.880601 -0.534941 -0.000016
C     1.862500 -1.446570  0.000004
H     1.618386 -2.504927 -0.000000
C     3.255117 -1.024028  0.000037
C     4.354634 -1.836522  0.000048
H     4.384256 -2.919849  0.000040
S     5.809367 -0.925097  0.000181
C     4.950958  0.559700  0.000039
H     5.485671  1.502508  0.000024
C     3.599375  0.374965  0.000041
Br   -5.202282 -0.160084 -0.000046
    el energy= -752.565616342

lc-whpbe--8
B    -2.046936  1.433880  0.000082
O    -2.219759  2.770086  0.000044
H    -1.358856  3.222179  0.000184
N    -0.707438  0.850129  0.000272
C     0.480544  1.567465  0.000338
O     0.561146  2.778864  0.000101
C     1.570782  0.561915  0.000323
C     2.938618  0.755940  0.000125
H     3.387782  1.743896 -0.000009
C     3.714399 -0.389662  0.000112
C     3.171627 -1.672121  0.000309
H     3.846819 -2.521570  0.000282
C     1.796395 -1.842580  0.000475
H     1.369177 -2.841412  0.000584
C     0.995591 -0.706480  0.000434
C    -0.461909 -0.537504  0.000356
C    -1.446160 -1.447292  0.000277
H    -1.204839 -2.506320  0.000325
C    -2.836426 -1.020391  0.000049
C    -3.938194 -1.830517 -0.000100
H    -3.970495 -2.913777 -0.000074
S    -5.389136 -0.915229 -0.000407
C    -4.527308  0.567425 -0.000302
H    -5.059669  1.511559 -0.000437
C    -3.176105  0.379470 -0.000064
N     5.179333 -0.249267 -0.000342
O     5.628469  0.872670 -0.000659
O     5.837211 -1.264161 -0.000516
    el energy= -944.345638626

lc-whpbe--9
B     1.434188  1.431220  0.000598
O     1.573891  2.773410  0.002110
H     0.696575  3.194399  0.000888
N     0.110814  0.818071 -0.001998
C    -1.092855  1.509865 -0.003428
O    -1.192499  2.722394 -0.001727
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C    -2.165368  0.487012 -0.006278
C    -3.533452  0.668943 -0.006288
H    -3.955963  1.671176 -0.010242
C    -4.347187 -0.467218 -0.005590
C    -3.742635 -1.738426 -0.004486
H    -4.382100 -2.619345 -0.009665
C    -2.367385 -1.898538 -0.004093
H    -1.939020 -2.897911 -0.002639
C    -1.563912 -0.765354 -0.004900
C    -0.108808 -0.575941 -0.002910
C     0.898546 -1.459818 -0.001736
H     0.682809 -2.524282 -0.002791
C     2.280793 -1.001622  0.000335
C     3.401619 -1.783984  0.001267
H     3.459800 -2.866111  0.000408
S     4.833689 -0.834216  0.003902
C     3.935725  0.626948  0.003320
H     4.443745  1.584401  0.004337
C     2.589607  0.405830  0.001610
N    -5.724933 -0.353437 -0.046379
H    -6.116449  0.533075  0.227478
H    -6.259789 -1.149087  0.261449
    el energy= -795.297565856

lc-whpbe.tddft--benzo
B    -1.107746  1.401135 -0.000002
O    -1.242302  2.744679 -0.000006
H    -0.352166  3.149946 -0.000013
N     0.220585  0.798813 -0.000004
C     1.449036  1.495822 -0.000007
O     1.515662  2.722835  0.000008
C     2.472604  0.466912 -0.000001
C     3.859383  0.560062  0.000006
H     4.343486  1.533435  0.000010
C     4.596691 -0.612627  0.000006
C     3.962709 -1.874621 -0.000001
H     4.572361 -2.774776 -0.000001
C     2.588071 -1.981339 -0.000006
H     2.107730 -2.957495 -0.000008
C     1.828451 -0.798966 -0.000006
C     0.426154 -0.560270 -0.000005
C    -0.664165 -1.465000 -0.000004
H    -0.444609 -2.529545 -0.000004
C    -1.983030 -1.017282 -0.000000
C    -3.070781 -1.949088  0.000002
H    -2.848556 -3.014512  0.000001
C    -4.363331 -1.508575  0.000005
C    -4.643206 -0.122405  0.000006
C    -3.610245  0.799180  0.000004
H    -3.830574  1.864664  0.000004
C    -2.275562  0.395577  0.000001
H    -5.182842 -2.223177  0.000007
H    -5.676768  0.216095  0.000009
H     5.683007 -0.566390  0.000010
 total energy= -807.061227441

lc-whpbe.tddft--1
B     1.208061 -2.630495  0.000000
O     0.574950 -3.822756  0.000000
H    -0.390528 -3.670236  0.000000
N     0.442177 -1.391060  0.000000
C    -0.965447 -1.286801  0.000000
O    -1.705951 -2.265691  0.000000
C    -1.241429  0.138279  0.000000
C    -2.448468  0.823059  0.000000
H    -3.394269  0.289018  0.000000
C    -2.398238  2.207003  0.000000
C    -1.174396  2.917268  0.000000
H    -1.192382  4.002636  0.000000
C     0.022069  2.237232  0.000000
H     0.960729  2.786631  0.000000
C     0.000000  0.831802  0.000000
C     1.030025 -0.145785  0.000000
C     2.437686 -0.002675  0.000000
H     2.850316  1.002872  0.000000
C     3.283389 -1.111000  0.000000
C     4.705253 -0.943459  0.000000
H     5.114940  0.064757  0.000000
C     5.532516 -2.030420  0.000000
C     4.991953 -3.336246  0.000000
C     3.620410 -3.525345  0.000000
H     3.208706 -4.532384  0.000000
C     2.738953 -2.445443  0.000000
H     6.611268 -1.894392  0.000000
H     5.661185 -4.193524  0.000000
Br   -4.009233  3.193637  0.000000
 total energy= -819.653639230

lc-whpbe.tddft--2
B    -2.482869  0.484953  0.000000
O    -3.558097 -0.326942  0.000000
H    -3.264087 -1.258131  0.000000
N    -1.134205 -0.070445  0.000000
C    -0.803895 -1.444702  0.000000
O    -1.647330 -2.329178  0.000000
C     0.651431 -1.487243 -0.000000
C     1.515569 -2.564070 -0.000000
H     1.165495 -3.591538 -0.000000
C     2.871928 -2.279009 -0.000000
C     3.382431 -0.963745 -0.000000
H     4.458124 -0.827501 -0.000000
C     2.518626  0.105986 -0.000000
H     2.906656  1.121698 -0.000000
C     1.133667 -0.147684 -0.000000
C     0.000000  0.709293  0.000000
C    -0.088849  2.121983  0.000000
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H     0.836511  2.692090 -0.000000
C    -1.320066  2.778218  0.000000
C    -1.381886  4.207924  0.000000
H    -0.452720  4.774222  0.000000
C    -2.588819  4.850449  0.000000
C    -3.788519  4.108498  0.000000
C    -3.755288  2.721663  0.000000
H    -4.683458  2.154210  0.000000
C    -2.549074  2.028608  0.000000
H    -2.627483  5.936940  0.000000
H    -4.742505  4.630571  0.000000
N     3.815738 -3.388913 -0.000000
O     3.364197 -4.514841 -0.000000
O     4.999173 -3.118893 -0.000000
 total energy= -1011.43590146

lc-whpbe.tddft--3
B    -1.499825  1.391902 -0.000318
O    -1.673482  2.736808 -0.000593
H    -0.793064  3.160590 -0.001134
N    -0.163273  0.828544 -0.000279
C     1.038530  1.554323  0.000150
O     1.089138  2.787681  0.000614
C     2.089508  0.558873 -0.000123
C     3.465764  0.696600  0.000084
H     3.923074  1.683412  0.000283
C     4.252337 -0.462319  0.000096
C     3.640636 -1.760678 -0.000211
H     4.280831 -2.639790 -0.000415
C     2.280197 -1.893934 -0.000340
H     1.828800 -2.883507 -0.000548
C     1.475300 -0.734966 -0.000283
C     0.078296 -0.541256 -0.000237
C    -0.974319 -1.464221 -0.000212
H    -0.735911 -2.524773 -0.000239
C    -2.313817 -1.043550 -0.000038
C    -3.373941 -1.997852  0.000147
H    -3.127179 -3.058156  0.000128
C    -4.678769 -1.589940  0.000369
C    -4.995046 -0.212831  0.000386
C    -3.985815  0.728192  0.000178
H    -4.226978  1.789287  0.000170
C    -2.636630  0.354362 -0.000023
H    -5.479097 -2.326527  0.000523
H    -6.036804  0.099813  0.000552
N     5.608280 -0.384697 -0.000088
H     6.074838  0.506311  0.002208
H     6.176933 -1.213821  0.002791
 total energy= -862.390123653

lc-whpbe.tddft--dioxo
B    -0.073486  1.569556  0.000144
O    -0.099928  2.921423  0.000154
H     0.824119  3.245414  0.000131
N     1.189537  0.857891  0.000142
C     2.467866  1.444189 -0.000012
O     2.640823  2.663580 -0.000155
C     3.398177  0.330946 -0.000020
C     4.789462  0.306885 -0.000219
H     5.352109  1.237102 -0.000377
C     5.424894 -0.921797 -0.000237
C     4.685539 -2.126104 -0.000044
H     5.217087 -3.074577 -0.000052
C     3.307664 -2.116794  0.000131
H     2.747452 -3.049414  0.000260
C     2.649022 -0.875377  0.000127
C     1.270963 -0.520938  0.000187
C     0.111258 -1.322640  0.000199
H     0.236628 -2.401992  0.000206
C    -1.165930 -0.769149  0.000130
C    -2.324184 -1.623878  0.000041
H    -2.221756 -2.704693  0.000029
C    -3.534048 -1.024554 -0.000064
C    -3.683769  0.386734 -0.000062
C    -2.608744  1.238781  0.000031
H    -2.737693  2.317241  0.000019
C    -1.329034  0.674505  0.000118
O    -4.765455 -1.591925 -0.000243
O    -4.993877  0.690699 -0.000216
H     6.511318 -0.968051 -0.000407
C    -5.707631 -0.536985 -0.000002
H    -6.325308 -0.593621 -0.903866
H    -6.324823 -0.593587  0.904206
 total energy= -995.486782665

lc-whpbe.tddft--4
B    -1.545309  1.648915  0.000086
O    -1.669662  2.994611 -0.000050
H    -0.773788  3.388339 -0.000089
N    -0.236632  1.026576  0.000073
C     0.996431  1.702312  0.000055
O     1.086375  2.929161  0.000175
C     2.001770  0.656038  0.000054
C     3.388812  0.740808  0.000036
H     3.888596  1.705154 -0.000044
C     4.100501 -0.444193  0.000032
C     3.461746 -1.707248  0.000102
H     4.068922 -2.607330  0.000079
C     2.088649 -1.790178  0.000167
H     1.602326 -2.763020  0.000204
C     1.338941 -0.601183  0.000119
C    -0.058709 -0.344804  0.000128
C    -1.159008 -1.224033  0.000175
H    -0.960498 -2.292303  0.000182
C    -2.472441 -0.759926  0.000137
C    -3.567165 -1.693560  0.000089
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H    -3.389596 -2.764542  0.000109
C    -4.816352 -1.180162 -0.000023
C    -5.064118  0.216744 -0.000091
C    -4.050856  1.142157 -0.000052
H    -4.254408  2.209014 -0.000134
C    -2.736054  0.667562  0.000063
O    -6.004393 -1.831800 -0.000119
O    -6.390865  0.429131 -0.000212
Br    5.991085 -0.394151 -0.000140
C    -7.018495 -0.845412 -0.000095
H    -7.630125 -0.944547 -0.904236
H    -7.629980 -0.944446  0.904160
 total energy= -1008.07953488

lc-whpbe.tddft--5
B     0.350585 -1.940920  0.000000
O     1.204709 -2.985341  0.000000
H     2.121326 -2.645578  0.000000
N     0.840214 -0.576637  0.000000
C     2.192154 -0.186538  0.000000
O     3.117290 -0.989635  0.000000
C     2.167411  1.268636  0.000000
C     3.206565  2.180508  0.000000
H     4.247731  1.873640  0.000000
C     2.863958  3.521190  0.000000
C     1.526622  3.973691  0.000000
H     1.343460  5.042376  0.000000
C     0.496504  3.064688  0.000000
H    -0.535016  3.408475  0.000000
C     0.808296  1.691482  0.000000
C     0.000000  0.522752  0.000000
C    -1.399613  0.369537  0.000000
H    -2.011653  1.267211  0.000000
C    -2.005729 -0.886539  0.000000
C    -3.439276 -0.993228  0.000000
H    -4.067025 -0.107607  0.000000
C    -3.965316 -2.238235  0.000000
C    -3.158301 -3.403765  0.000000
C    -1.784559 -3.346873  0.000000
H    -1.178113 -4.247911  0.000000
C    -1.189137 -2.085380  0.000000
O    -5.266404 -2.611661  0.000000
O    -3.947812 -4.487657  0.000000
N     3.931312  4.513090  0.000000
O     5.076466  4.112784  0.000000
O     3.610197  5.683865  0.000000
C    -5.292756 -4.026262  0.000000
H    -5.795407 -4.387003  0.904495
H    -5.795407 -4.387003 -0.904495
 total energy= -1199.86251977

lc-whpbe.tddft--6
B    -0.473424  1.602663 -0.002734
O    -0.540514  2.957808 -0.000392
H     0.373338  3.306309  0.000653
N     0.807608  0.931578 -0.002683
C     2.064097  1.554590 -0.000668
O     2.212970  2.780960  0.002154
C     3.028006  0.473841 -0.001953
C     4.412780  0.501072  0.000929
H     4.945236  1.449562  0.001845
C     5.104241 -0.713063  0.001692
C     4.388232 -1.953025 -0.001303
H     4.953979 -2.882089 -0.006596
C     3.020166 -1.978679 -0.003553
H     2.493460 -2.930483 -0.005504
C     2.310298 -0.760961 -0.003490
C     0.932425 -0.453513 -0.004461
C    -0.197187 -1.283226 -0.006378
H    -0.046571 -2.359510 -0.008077
C    -1.494219 -0.760150 -0.006759
C    -2.624947 -1.646482 -0.008240
H    -2.492184 -2.724216 -0.011236
C    -3.853908 -1.083461 -0.007370
C    -4.045694  0.318849 -0.005408
C    -2.998329  1.197540 -0.004957
H    -3.155273  2.272270 -0.004755
C    -1.696375  0.669732 -0.005154
O    -5.067868 -1.691969 -0.017522
O    -5.371116  0.582898 -0.012637
N     6.468935 -0.744983 -0.016661
H     6.990593  0.104649  0.117567
H     6.955140 -1.609086  0.151655
C    -6.040303 -0.665555  0.048407
H    -6.722586 -0.752250 -0.804646
H    -6.587289 -0.737265  0.997358
 total energy= -1050.81341065

lc-whpbe.tddft--thieno
B    -1.018073  1.441547 -0.000072
O    -1.124481  2.782021 -0.000060
H    -0.220695  3.161958 -0.000081
N     0.285577  0.794818 -0.000056
C     1.530856  1.484401 -0.000004
O     1.596302  2.712570  0.000071
C     2.540078  0.453190  0.000035
C     3.929846  0.532113  0.000132
H     4.422519  1.501393  0.000202
C     4.658539 -0.644453  0.000147
C     4.012359 -1.903672  0.000055
H     4.614788 -2.808758  0.000072
C     2.637894 -1.999421 -0.000034
H     2.150676 -2.972464 -0.000081
C     1.883075 -0.811364 -0.000035
C     0.484687 -0.570144 -0.000062
C    -0.609086 -1.475088 -0.000065
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H    -0.402692 -2.541162 -0.000046
C    -1.918574 -0.989225 -0.000041
C    -3.104674 -1.744776  0.000037
H    -3.195980 -2.824578  0.000068
S    -4.476986 -0.755491 -0.000064
C    -3.534593  0.692629  0.000072
H    -4.024523  1.659672  0.000142
C    -2.200512  0.440861 -0.000040
H     5.745078 -0.606720  0.000229
 total energy= -739.830145701

lc-whpbe.tddft--7
B    -2.455672  1.435015  0.000113
O    -2.635776  2.767547  0.000144
H    -1.757284  3.200740  0.000256
N    -1.119775  0.858409  0.000145
C     0.084889  1.611498  0.000158
O     0.091061  2.839782 -0.000005
C     1.147765  0.633291  0.000109
C     2.527473  0.795500  0.000011
H     2.973056  1.786139 -0.000051
C     3.308207 -0.347096 -0.000001
C     2.743115 -1.647340  0.000082
H     3.401536 -2.510394  0.000057
C     1.377266 -1.809217  0.000161
H     0.948391 -2.808932  0.000185
C     0.557580 -0.665306  0.000165
C    -0.849630 -0.497344  0.000153
C    -1.891913 -1.456873  0.000108
H    -1.631141 -2.510975  0.000097
C    -3.225988 -1.039862  0.000020
C    -4.368809 -1.857868 -0.000108
H    -4.401600 -2.941072 -0.000136
S    -5.791580 -0.944030 -0.000114
C    -4.928462  0.552854 -0.000174
H    -5.469851  1.492049 -0.000257
C    -3.582891  0.372523  0.000004
Br    5.191002 -0.186120 -0.000147
 total energy= -752.423122625

lc-whpbe.tddft--8
B    -2.055604  1.432064 -0.000464
O    -2.225503  2.768974 -0.000306
H    -1.363334  3.218608 -0.000459
N    -0.716931  0.846289 -0.000712
C     0.470543  1.562276 -0.000332
O     0.553698  2.773875 -0.000176
C     1.561915  0.556572 -0.000589
C     2.926142  0.759740 -0.000205
H     3.359636  1.755372  0.000227
C     3.714645 -0.388665 -0.000132
C     3.163981 -1.678458 -0.000596
H     3.829731 -2.536520 -0.000497
C     1.791100 -1.844388 -0.001026
H     1.365832 -2.844230 -0.001283
C     0.984495 -0.710512 -0.000947
C    -0.471972 -0.542559 -0.000947
C    -1.459198 -1.449370 -0.000871
H    -1.220600 -2.509008 -0.000941
C    -2.849106 -1.020124 -0.000313
C    -3.952445 -1.827758  0.000220
H    -3.987044 -2.910944  0.000244
S    -5.402424 -0.909586  0.001139
C    -4.537531  0.571255  0.000727
H    -5.067701  1.516629  0.001151
C    -3.186770  0.380329 -0.000063
N     5.092305 -0.258626  0.000589
O     5.752876  0.828805  0.001567
O     5.948662 -1.199219  0.001036
 total energy= -944.225029410

lc-whpbe.tddft--9
B     1.414041  1.438289  0.000070
O     1.559173  2.780743  0.000277
H     0.663257  3.178163  0.000421
N     0.098282  0.834400 -0.000026
C    -1.118524  1.552396 -0.000018
O    -1.167997  2.788411 -0.000318
C    -2.155941  0.557101 -0.000200
C    -3.538048  0.677527 -0.000091
H    -4.008269  1.658280  0.000029
C    -4.311379 -0.489372  0.000026
C    -3.691820 -1.787187  0.000064
H    -4.324910 -2.671048  0.000032
C    -2.328554 -1.904360 -0.000008
H    -1.866433 -2.889142 -0.000057
C    -1.533877 -0.739699 -0.000111
C    -0.135485 -0.543126 -0.000029
C     0.909090 -1.467163 -0.000027
H     0.678950 -2.528482 -0.000068
C     2.247364 -1.015922 -0.000014
C     3.397004 -1.802258 -0.000058
H     3.459171 -2.883968 -0.000114
S     4.803376 -0.849750 -0.000005
C     3.909378  0.618006  0.000083
H     4.424371  1.571655  0.000156
C     2.563948  0.403170  0.000038
N    -5.667873 -0.425595  0.000075
H    -6.144003  0.460495  0.000123
H    -6.227556 -1.260935  0.001267
 total energy= -795.158465062

lc-whpbe.tddft-mecn--benzo
B    -1.103675  1.402020  0.000000
O    -1.223822  2.750031  0.000000
H    -0.324414  3.136577 -0.000000
```

```
N     0.226253  0.800890 -0.000000
C     1.448241  1.493052 -0.000001
O     1.516098  2.726713  0.000000
C     2.472075  0.466880 -0.000001
C     3.859965  0.557558 -0.000000
H     4.354651  1.526446 -0.000000
C     4.595946 -0.617647 -0.000001
C     3.957250 -1.879771 -0.000001
H     4.567111 -2.780317 -0.000001
C     2.584751 -1.988891 -0.000001
H     2.101020 -2.962973 -0.000001
C     1.820787 -0.800789 -0.000001
C     0.433007 -0.561505 -0.000000
C    -0.673181 -1.464417  0.000000
H    -0.457922 -2.530284  0.000000
C    -1.983584 -1.012533  0.000001
C    -3.071681 -1.947175  0.000001
H    -2.845476 -3.011790  0.000001
C    -4.367048 -1.506842  0.000001
C    -4.647966 -0.123948  0.000001
C    -3.610724  0.802114  0.000001
H    -3.844560  1.865425  0.000001
C    -2.279377  0.401688  0.000001
H    -5.186104 -2.222431  0.000001
H    -5.681356  0.215759  0.000001
H     5.682669 -0.573337 -0.000000
 total energy= -807.095227709

lc-whpbe.tddft-mecn--1
B     1.219311 -2.625105  0.000000
O     0.578983 -3.816531  0.000000
H    -0.385021 -3.649409 -0.000000
N     0.442919 -1.389332  0.000000
C    -0.958412 -1.292739 -0.000000
O    -1.697732 -2.280811 -0.000000
C    -1.243198  0.128761 -0.000000
C    -2.454147  0.809832 -0.000000
H    -3.399253  0.273068 -0.000000
C    -2.405829  2.193140 -0.000000
C    -1.183804  2.908738 -0.000000
H    -1.198892  3.994863 -0.000000
C     0.015376  2.237515  0.000000
H     0.952387  2.788860  0.000000
C    -0.000000  0.825918  0.000000
C     1.023935 -0.139531  0.000000
C     2.444051  0.003590  0.000000
H     2.852735  1.011125  0.000000
C     3.286539 -1.097539  0.000000
C     4.709070 -0.918372  0.000000
H     5.107928  0.094131  0.000000
C     5.546170 -2.001071  0.000000
C     5.016415 -3.307877  0.000000
C     3.639958 -3.508028  0.000000
H     3.248301 -4.523635  0.000000
C     2.752372 -2.438834  0.000000
H     6.624004 -1.856469  0.000000
H     5.690307 -4.161868  0.000000
Br   -4.024870  3.178226 -0.000000
 total energy= -819.688353129

lc-whpbe.tddft-mecn--2
B    -2.484440  0.465703  0.000000
O    -3.551557 -0.361660  0.000000
H    -3.237974 -1.286817  0.000000
N    -1.133799 -0.086323  0.000000
C    -0.797645 -1.449696  0.000000
O    -1.636348 -2.346395  0.000000
C     0.657764 -1.484422  0.000000
C     1.527374 -2.552527  0.000000
H     1.180164 -3.581195  0.000000
C     2.886208 -2.259411 -0.000000
C     3.385250 -0.935176 -0.000000
H     4.458540 -0.778331 -0.000000
C     2.519190  0.128107 -0.000000
H     2.896929  1.147217 -0.000000
C     1.127826 -0.133915 -0.000000
C     0.000000  0.700665 -0.000000
C    -0.106806  2.125006 -0.000000
H     0.814994  2.701561 -0.000000
C    -1.336270  2.765975 -0.000000
C    -1.399917  4.197166 -0.000000
H    -0.470050  4.762294 -0.000000
C    -2.610733  4.838230 -0.000000
C    -3.804512  4.093673  0.000000
C    -3.768396  2.700323  0.000000
H    -4.702714  2.142320  0.000000
C    -2.565145  2.011722  0.000000
H    -2.652735  5.924738 -0.000000
H    -4.761264  4.611126  0.000000
N     3.827246 -3.355805 -0.000000
O     3.391251 -4.493310 -0.000000
O     5.016286 -3.092491 -0.000000
 total energy= -1011.47313552

lc-whpbe.tddft-mecn--2-
B    -2.555643  0.786005 -0.000000
O    -3.706973  0.236798 -0.000000
N    -1.218735  0.009862 -0.000000
C    -1.031173 -1.392581 -0.000000
O    -1.907131 -2.235502 -0.000000
C     0.426904 -1.594435 -0.000000
C     1.157757 -2.754921 -0.000000
H     0.687012 -3.733596 -0.000000
C     2.549983 -2.631910 -0.000000
C     3.192078 -1.369080  0.000000
H     4.276622 -1.336546  0.000000
```

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C     2.454287 -0.212760  0.000000
H     2.952094  0.753928  0.000000
C     1.041932 -0.313421  0.000000
C    -0.000000  0.636988  0.000000
C     0.132226  2.059217  0.000000
H     1.142913  2.462667  0.000000
C    -0.961868  2.913933  0.000000
C    -0.787852  4.335217  0.000000
H     0.221555  4.743393  0.000000
C    -1.879888  5.163125  0.000000
C    -3.179343  4.618844  0.000000
C    -3.359728  3.239060  0.000000
H    -4.364060  2.817748 -0.000000
C    -2.285221  2.359119  0.000000
H    -1.746526  6.243018  0.000000
H    -4.040674  5.284444  0.000000
N     3.349410 -3.818476 -0.000000
O     2.786488 -4.904484 -0.000000
O     4.566865 -3.702206 -0.000000
 total energy= -1010.97225749

lc-whpbe.tddft-mecn--3
B     1.496939  1.387312 -0.000150
O     1.655108  2.739499 -0.000197
H     0.762311  3.140456 -0.000310
N     0.158938  0.827009 -0.000073
C    -1.035972  1.551158  0.000059
O    -1.079398  2.791457  0.000153
C    -2.091765  0.561948  0.000012
C    -3.464399  0.705426  0.000045
H    -3.939195  1.684250  0.000131
C    -4.257987 -0.460412  0.000038
C    -3.638949 -1.767040 -0.000035
H    -4.288214 -2.639400 -0.000023
C    -2.287095 -1.902719 -0.000102
H    -1.833270 -2.891059 -0.000142
C    -1.472703 -0.735745 -0.000066
C    -0.089187 -0.548074 -0.000095
C     0.976972 -1.468569 -0.000133
H     0.742808 -2.530409 -0.000124
C     2.311808 -1.041439 -0.000082
C     3.376137 -1.994550  0.000004
H     3.129438 -3.055061 -0.000006
C     4.683231 -1.585470  0.000145
C     5.003825 -0.210601  0.000192
C     3.989161  0.729583  0.000082
H     4.239536  1.789649  0.000125
C     2.640203  0.357052 -0.000052
H     5.482439 -2.324135  0.000240
H     6.045562  0.102784  0.000319
N    -5.595954 -0.383817  0.000112
H    -6.065961  0.510676  0.000283
H    -6.166384 -1.217595  0.000250
 total energy= -862.432935937

lc-whpbe.tddft-mecn--dioxo
B    -0.069495  1.572785  0.000017
O    -0.077002  2.927843 -0.000010
H     0.855418  3.230066 -0.000037
N     1.196997  0.861252 -0.000005
C     2.470818  1.441712 -0.000018
O     2.646494  2.668354  0.000014
C     3.399124  0.330685 -0.000010
C     4.792411  0.299115 -0.000009
H     5.368387  1.222186 -0.000016
C     5.423297 -0.932688 -0.000010
C     4.675721 -2.135913 -0.000002
H     5.205500 -3.085895 -0.000001
C     3.300110 -2.125368  0.000005
H     2.734287 -3.054392  0.000013
C     2.640001 -0.876213 -0.000002
C     1.277488 -0.519590  0.000003
C     0.099045 -1.316740  0.000014
H     0.219862 -2.397137  0.000010
C    -1.166908 -0.760447  0.000019
C    -2.326472 -1.620768  0.000011
H    -2.213408 -2.701180  0.000004
C    -3.538155 -1.025624  0.000004
C    -3.688772  0.384303  0.000008
C    -2.610772  1.242087  0.000015
H    -2.757314  2.318941  0.000012
C    -1.332529  0.683735  0.000020
O    -4.765927 -1.593164 -0.000006
O    -4.989013  0.692206  0.000003
H     6.509795 -0.983915 -0.000018
C    -5.716273 -0.538581 -0.000034
H    -6.329591 -0.590746 -0.905487
H    -6.329658 -0.590759  0.905373
 total energy= -995.520701176

lc-whpbe.tddft-mecn--4
B    -1.543331  1.653272 -0.000044
O    -1.648527  3.003344 -0.000037
H    -0.741857  3.374691 -0.000028
N    -0.230405  1.031916 -0.000060
C     0.997698  1.703285 -0.000023
O     1.088134  2.937907  0.000013
C     2.001140  0.660159 -0.000034
C     3.390828  0.740774  0.000009
H     3.895895  1.703163  0.000043
C     4.096781 -0.446199  0.000007
C     3.454817 -1.710258 -0.000038
H     4.055694 -2.615340 -0.000042
C     2.083997 -1.793777 -0.000073
H     1.594661 -2.764780 -0.000104
C     1.330953 -0.598698 -0.000069
```

```
C    -0.052777 -0.340106 -0.000080
C    -1.172063 -1.217571 -0.000088
H    -0.975991 -2.286944 -0.000104
C    -2.474104 -0.752022 -0.000061
C    -3.569183 -1.692725 -0.000045
H    -3.379238 -2.762252 -0.000064
C    -4.820002 -1.184870  0.000004
C    -5.068887  0.210891  0.000031
C    -4.053956  1.143813  0.000004
H    -4.276686  2.207393  0.000022
C    -2.741394  0.676456 -0.000041
O    -6.004868 -1.836172  0.000036
O    -6.385221  0.427768  0.000090
Br    5.993345 -0.400319  0.000060
C    -7.026695 -0.850665  0.000113
H    -7.634615 -0.944108 -0.905507
H    -7.634499 -0.944132  0.905809
 total energy= -1008.11436135

lc-whpbe.tddft-mecn--5
B     0.392263 -1.934495  0.000000
O     1.276620 -2.956659  0.000000
H     2.181041 -2.584794  0.000000
N     0.861127 -0.560983  0.000000
C     2.197787 -0.146923  0.000000
O     3.145173 -0.933071  0.000000
C     2.145707  1.305931  0.000000
C     3.163498  2.236341  0.000000
H     4.209814  1.946199  0.000000
C     2.796692  3.575084  0.000000
C     1.443496  3.998086  0.000000
H     1.227062  5.061037  0.000000
C     0.431806  3.074781  0.000000
H    -0.606533  3.396379  0.000000
C     0.768739  1.697852  0.000000
C     0.000000  0.525895  0.000000
C    -1.410915  0.330711  0.000000
H    -2.041543  1.216278  0.000000
C    -1.984046 -0.926683  0.000000
C    -3.421342 -1.054238  0.000000
H    -4.054514 -0.171724  0.000000
C    -3.929751 -2.305317  0.000000
C    -3.102696 -3.455169  0.000000
C    -1.722404 -3.378188  0.000000
H    -1.115098 -4.279071  0.000000
C    -1.147674 -2.113964  0.000000
O    -5.221680 -2.701353  0.000000
O    -3.859886 -4.548496  0.000000
N     3.836881  4.575130  0.000000
O     4.998212  4.205373  0.000000
O     3.507603  5.748296  0.000000
C    -5.226586 -4.120445  0.000000
H    -5.714906 -4.493052  0.905847
H    -5.714906 -4.493052 -0.905847
 total energy= -1199.89995597

lc-whpbe.tddft-mecn--5-
B     1.153235  1.807238  0.001435
O     1.358787  3.067256  0.003148
N    -0.225608  1.128829  0.000155
C    -1.493690  1.741668 -0.000695
O    -1.721344  2.937894 -0.001693
C    -2.466422  0.636754 -0.000392
C    -3.835944  0.670487 -0.000933
H    -4.389178  1.605048 -0.001752
C    -4.508116 -0.556695 -0.000147
C    -3.808228 -1.792058  0.000980
H    -4.382252 -2.712886  0.001607
C    -2.438805 -1.818347  0.001143
H    -1.909896 -2.768596  0.001894
C    -1.735776 -0.585329  0.000485
C    -0.372522 -0.242374  0.000548
C     0.739175 -1.136365  0.000585
H     0.515105 -2.201248  0.000541
C     2.054325 -0.708133  0.000322
C     3.133678 -1.664354 -0.000288
H     2.934389 -2.732522 -0.000587
C     4.391552 -1.165020 -0.000507
C     4.647827  0.223405 -0.000049
C     3.636408  1.161156  0.000620
H     3.843556  2.228291  0.001039
C     2.320651  0.710223  0.000704
O     5.573416 -1.829739 -0.001059
O     5.972877  0.432321 -0.000329
N    -5.933534 -0.565180 -0.000462
O    -6.529431  0.505400 -0.003220
O    -6.513518 -1.644197  0.002015
C     6.600833 -0.849923 -0.001473
H     7.210833 -0.951368  0.902741
H     7.209296 -0.950499 -0.906823
 total energy= -1199.39738085

lc-whpbe.tddft-mecn--6
B     0.472352  1.602051 -0.008642
O     0.519804  2.963820 -0.004198
H    -0.404564  3.287030  0.000586
N    -0.812574  0.934018 -0.005985
C    -2.063558  1.554618  0.002114
O    -2.208616  2.788898  0.006875
C    -3.031340  0.480117  0.003541
C    -4.414515  0.508237  0.011924
H    -4.966684  1.445704  0.018262
C    -5.107912 -0.715772  0.012323
C    -4.381568 -1.962739  0.003664
H    -4.954632 -2.887191  0.003770
C    -3.021405 -1.987017 -0.004355
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```
H    -2.488824 -2.935378 -0.010612
C    -2.306548 -0.758924 -0.004278
C    -0.942238 -0.455934 -0.009824
C     0.200066 -1.281096 -0.016887
H     0.054574 -2.358521 -0.019686
C     1.492599 -0.750865 -0.019381
C     2.623698 -1.640432 -0.023509
H     2.481845 -2.717807 -0.030468
C     3.856646 -1.081696 -0.021167
C     4.053873  0.317937 -0.016572
C     3.006136  1.198267 -0.015957
H     3.177249  2.271844 -0.015873
C     1.699367  0.676184 -0.015827
O     5.066085 -1.694011 -0.046600
O     5.378531  0.579299 -0.035721
N    -6.451899 -0.754954  0.020865
H    -6.998280  0.094186  0.027357
H    -6.946168 -1.635304  0.021253
C     6.038733 -0.672162  0.127076
H     6.459683 -0.731304  1.138931
H     6.816715 -0.773346 -0.634618
 total energy= -1050.85525654

lc-whpbe.tddft-mecn--thieno
B    -1.014601  1.443227  0.000151
O    -1.104643  2.788452  0.000223
H    -0.191320  3.148233  0.000365
N     0.292265  0.797909  0.000182
C     1.528323  1.480836  0.000144
O     1.599403  2.716683 -0.000053
C     2.537876  0.452004  0.000086
C     3.929305  0.528833 -0.000086
H     4.431340  1.494217 -0.000214
C     4.656758 -0.649493 -0.000094
C     4.005637 -1.909291  0.000081
H     4.608715 -2.814576  0.000066
C     2.634032 -2.008251  0.000227
H     2.144556 -2.979710  0.000312
C     1.873338 -0.814228  0.000210
C     0.490881 -0.571087  0.000204
C    -0.621101 -1.474347  0.000162
H    -0.422159 -2.542527  0.000158
C    -1.918388 -0.982218  0.000017
C    -3.103721 -1.743956 -0.000142
H    -3.188149 -2.825929 -0.000179
S    -4.478704 -0.756730 -0.000461
C    -3.535765  0.698767 -0.000150
H    -4.039888  1.660052 -0.000186
C    -2.203609  0.449019 -0.000010
H     5.743836 -0.614190 -0.000234
 total energy= -739.863950614

lc-whpbe.tddft-mecn--7
B    -2.455045  1.436515  0.000007
O    -2.621542  2.773691  0.000044
H    -1.733079  3.188948  0.000101
N    -1.114106  0.863306  0.000035
C     0.082658  1.612487  0.000063
O     0.091080  2.848690  0.000003
C     1.145450  0.637114  0.000051
C     2.527854  0.797584  0.000033
H     2.976485  1.787887  0.000023
C     3.303564 -0.346346  0.000039
C     2.736238 -1.647861  0.000057
H     3.389628 -2.515723  0.000058
C     1.373547 -1.812439  0.000065
H     0.942451 -2.810733  0.000066
C     0.549238 -0.662912  0.000060
C    -0.843559 -0.493276  0.000040
C    -1.902796 -1.456518  0.000015
H    -1.645446 -2.512142  0.000020
C    -3.224709 -1.035249 -0.000028
C    -4.367061 -1.860437 -0.000049
H    -4.391852 -2.945706 -0.000048
S    -5.792356 -0.949797 -0.000203
C    -4.930175  0.554953 -0.000043
H    -5.485389  1.487464 -0.000029
C    -3.586619  0.377979 -0.000039
Br    5.193165 -0.190813  0.000024
 total energy= -752.457694471

lc-whpbe.tddft-mecn--8
B     2.025116  1.442388 -0.000133
O     2.190833  2.778525 -0.000068
H     1.311534  3.206237 -0.000089
N     0.687007  0.859453 -0.000202
C    -0.512644  1.595856 -0.000103
O    -0.542752  2.823035 -0.000124
C    -1.575017  0.604096 -0.000135
C    -2.941042  0.759867 -0.000015
H    -3.411467  1.738470  0.000122
C    -3.712395 -0.399904  0.000047
C    -3.138325 -1.697496 -0.000099
H    -3.796815 -2.559534 -0.000020
C    -1.777800 -1.852798 -0.000262
H    -1.337094 -2.846410 -0.000325
C    -0.961421 -0.691523 -0.000252
C     0.424364 -0.503172 -0.000281
C     1.492530 -1.455122 -0.000295
H     1.245058 -2.513110 -0.000338
C     2.809905 -1.022837 -0.000136
C     3.954698 -1.844074  0.000026
H     3.981032 -2.929475  0.000012
S     5.375147 -0.930217  0.000335
C     4.505170  0.573917  0.000233
H     5.057495  1.508148  0.000396
```

```
C     3.164134  0.390780 -0.000031
N    -5.144062 -0.273990  0.000231
O    -5.630688  0.845501  0.000449
O    -5.813796 -1.294133  0.000139
 total energy= -944.244400730

lc-whpbe.tddft-mecn--8-
B    -2.116811  1.592200 -0.026957
O    -2.361235  2.838939 -0.074662
N    -0.689153  0.968904  0.007087
C     0.538819  1.671813  0.024732
O     0.678440  2.878585  0.050375
C     1.590663  0.641261  0.013079
C     2.952564  0.772399  0.014190
H     3.439550  1.743008  0.024831
C     3.710144 -0.407017 -0.000586
C     3.098324 -1.687708 -0.013970
H     3.735502 -2.566012 -0.024863
C     1.733739 -1.810109 -0.013449
H     1.271756 -2.794440 -0.023975
C     0.948337 -0.628156 -0.000903
C    -0.436784 -0.384007 -0.001072
C    -1.474298 -1.367676 -0.003358
H    -1.180025 -2.414614 -0.003733
C    -2.811522 -0.997044  0.001261
C    -3.921975 -1.857461  0.010944
H    -3.916766 -2.942980  0.017207
S    -5.373939 -0.981896  0.014064
C    -4.535943  0.546282  0.000548
H    -5.111842  1.466328 -0.002862
C    -3.190285  0.407260 -0.005140
N     5.130839 -0.315724 -0.003115
O     5.649973  0.794848  0.008721
O     5.786124 -1.351524 -0.017222
 total energy= -943.743495840

lc-whpbe.tddft-mecn--9
B     1.410424  1.432346  0.000057
O     1.540548  2.781124  0.000067
H     0.632744  3.155973  0.000149
N     0.092542  0.831872  0.000079
C    -1.116238  1.547584  0.000054
O    -1.160036  2.791511 -0.000057
C    -2.157814  0.557639  0.000028
C    -3.537507  0.684776 -0.000061
H    -4.022689  1.658702 -0.000125
C    -4.318756 -0.485767 -0.000057
C    -3.690196 -1.790953  0.000036
H    -4.332647 -2.668257  0.000032
C    -2.336562 -1.913043  0.000106
H    -1.873954 -2.897544  0.000152
C    -1.530108 -0.741044  0.000097
C    -0.145224 -0.550395  0.000088
C     0.915236 -1.472678  0.000073
H     0.689575 -2.535636  0.000068
C     2.248885 -1.015851  0.000020
C     3.400287 -1.800890 -0.000044
H     3.463751 -2.884024 -0.000061
S     4.810958 -0.843680 -0.000085
C     3.911636  0.624230 -0.000059
H     4.434091  1.575554 -0.000091
C     2.567125  0.405163 -0.000001
N    -5.659301 -0.423703 -0.000114
H    -6.139495  0.465254 -0.000299
H    -6.220212 -1.263754 -0.000255
 total energy= -795.199977943

wb97xd--benzo
B    -1.125119  1.394808  0.000001
O    -1.282602  2.739368  0.000002
H    -0.418121  3.179171  0.000005
N     0.202439  0.796253  0.000004
C     1.421136  1.482563  0.000007
O     1.527537  2.694630 -0.000003
C     2.478509  0.445446  0.000001
C     3.859179  0.588410 -0.000005
H     4.311714  1.576310 -0.000007
C     4.629412 -0.572603 -0.000007
C     4.017040 -1.832716 -0.000003
H     4.638284 -2.725300 -0.000005
C     2.629302 -1.968582  0.000002
H     2.168246 -2.952948  0.000003
C     1.860621 -0.808561  0.000003
C     0.408602 -0.592640  0.000004
C    -0.620345 -1.460681  0.000004
H    -0.416743 -2.528688  0.000004
C    -2.005132 -1.005745  0.000002
C    -3.055500 -1.937482  0.000000
H    -2.829494 -3.002485  0.000001
C    -4.374901 -1.508057 -0.000002
C    -4.672087 -0.141345 -0.000004
C    -3.639083  0.787761 -0.000003
H    -3.861761  1.852706 -0.000004
C    -2.298352  0.379939  0.000000
H    -5.179867 -2.239510 -0.000003
H    -5.707679  0.190301 -0.000006
H     5.714049 -0.503599 -0.000010
    el energy= -807.525247965
          zpe= -807.302209
    th energy= -807.288911
  th enthalpy= -807.287966
  free energy= -807.342194

wb97xd--1
B     1.231512 -2.634312  0.000000
O     0.608771 -3.835398  0.000000
```

```
H    -0.353889 -3.720847  0.000000
N     0.467900 -1.393067  0.000000
C    -0.924345 -1.278135  0.000000
O    -1.696614 -2.217010  0.000000
C    -1.215079  0.176511  0.000000
C    -2.442286  0.823120  0.000000
H    -3.372201  0.262859  0.000000
C    -2.415463  2.214646  0.000000
C    -1.209457  2.927846  0.000000
H    -1.231945  4.013503  0.000000
C     0.011049  2.257168  0.000000
H     0.941226  2.819147  0.000000
C     0.000000  0.865405  0.000000
C     1.078816 -0.128104  0.000000
C     2.417867  0.012470  0.000000
H     2.849301  1.010411  0.000000
C     3.308380 -1.141589  0.000000
C     4.700690 -0.960914  0.000000
H     5.112701  0.046770  0.000000
C     5.550222 -2.058222  0.000000
C     5.027292 -3.355383  0.000000
C     3.650617 -3.543365  0.000000
H     3.236161 -4.549174  0.000000
C     2.771603 -2.452212  0.000000
H     6.627254 -1.906365  0.000000
H     5.697988 -4.211217  0.000000
Br   -4.059890  3.183478  0.000000
    el energy= -820.102312285
          zpe= -819.889508
    th energy= -819.874701
  th enthalpy= -819.873757
  free energy= -819.932501

wb97xd--2
B    -2.495110  0.474832  0.000000
O    -3.572262 -0.342133  0.000000
H    -3.299316 -1.272247  0.000000
N    -1.141261 -0.066017  0.000000
C    -0.791718 -1.417798  0.000000
O    -1.583086 -2.339377  0.000000
C     0.691604 -1.454698  0.000000
C     1.541150 -2.548035  0.000000
H     1.173210 -3.568610  0.000000
C     2.901860 -2.266400  0.000000
C     3.405776 -0.962509  0.000000
H     4.480653 -0.817967  0.000000
C     2.533914  0.120537  0.000000
H     2.922831  1.134845  0.000000
C     1.164323 -0.137221  0.000000
C     0.000000  0.752553  0.000000
C    -0.089842  2.096623  0.000000
H     0.820828  2.690762  0.000000
C    -1.378055  2.776830  0.000000
C    -1.436657  4.179679  0.000000
H    -0.513342  4.756385  0.000000
C    -2.662680  4.829278  0.000000
C    -3.851276  4.092190  0.000000
C    -3.802335  2.703384  0.000000
H    -4.723640  2.124977  0.000000
C    -2.577578  2.023566  0.000000
H    -2.697861  5.916285  0.000000
H    -4.809301  4.606147  0.000000
N     3.855094 -3.388080  0.000000
O     3.394139 -4.511868  0.000000
O     5.040427 -3.118364  0.000000
    el energy= -1011.95696422
          zpe= -1011.730833
    th energy= -1011.715007
  th enthalpy= -1011.714063
  free energy= -1011.774872

wb97xd--3
B    -1.517797  1.387057  0.000060
O    -1.698867  2.729391  0.001422
H    -0.841556  3.182909  0.000305
N    -0.179332  0.813292 -0.001885
C     1.024848  1.522469 -0.002506
O     1.109624  2.736765 -0.001059
C     2.104403  0.505949 -0.005865
C     3.475641  0.692177 -0.005465
H     3.896792  1.695061 -0.009629
C     4.296333 -0.445634 -0.004731
C     3.696784 -1.723630 -0.003953
H     4.339458 -2.602383 -0.009087
C     2.317310 -1.889738 -0.003964
H     1.890424 -2.889640 -0.002181
C     1.508637 -0.756532 -0.004797
C     0.054562 -0.573011 -0.002742
C    -0.960385 -1.457793 -0.001506
H    -0.738841 -2.522247 -0.002466
C    -2.353363 -1.027639  0.000511
C    -3.387823 -1.977243  0.001686
H    -3.143109 -3.038178  0.000933
C    -4.714840 -1.571566  0.003584
C    -5.037307 -0.210543  0.004338
C    -4.020482  0.736235  0.003178
H    -4.261641  1.797234  0.003674
C    -2.672668  0.352264  0.001291
H    -5.506403 -2.317638  0.004403
H    -6.078812  0.102109  0.005764
N     5.678227 -0.323690 -0.054940
H     6.056132  0.560217  0.249584
H     6.208318 -1.113796  0.278914
    el energy= -862.863433570
          zpe= -862.623460
    th energy= -862.608666
```

```
  th enthalpy= -862.607722
  free energy= -862.664924

wb97xd--dioxo
B     0.090790  1.573657 -0.004183
O     0.129592  2.928233 -0.001587
H    -0.770151  3.289868  0.001282
N    -1.178066  0.861069 -0.001642
C    -2.453578  1.435740  0.003585
O    -2.668231  2.633367  0.006245
C    -3.413130  0.307245  0.005125
C    -4.801067  0.325223  0.010194
H    -5.339634  1.269074  0.013433
C    -5.463551 -0.900296  0.011050
C    -4.739927 -2.100098  0.006859
H    -5.278121 -3.044981  0.007727
C    -3.345588 -2.110479  0.001629
H    -2.798788 -3.050021 -0.001584
C    -2.684338 -0.886127  0.000799
C    -1.258630 -0.539187 -0.003745
C    -0.152517 -1.307857 -0.009267
H    -0.258969 -2.389808 -0.011093
C     1.184758 -0.731647 -0.013761
C     2.306716 -1.594103 -0.019770
H     2.194671 -2.674550 -0.025320
C     3.546856 -1.007182 -0.019945
C     3.716152  0.379352 -0.016046
C     2.645737  1.237945 -0.012981
H     2.780854  2.315441 -0.014271
C     1.350379  0.674120 -0.010494
O     4.764188 -1.613346 -0.044029
O     5.049119  0.670140 -0.040174
H    -6.549983 -0.930385  0.015125
C     5.721751 -0.570877  0.107400
H     6.169130 -0.632036  1.110449
H     6.486027 -0.666161 -0.670778
    el energy= -995.997182450
          zpe= -995.757760
    th energy= -995.742217
  th enthalpy= -995.741273
  free energy= -995.800920

wb97xd--4
B    -1.567144  1.649017 -0.005341
O    -1.696725  2.997119 -0.001407
H    -0.825718  3.422615  0.000528
N    -0.252739  1.021404 -0.005126
C     0.979735  1.679439 -0.000692
O     1.119941  2.886998  0.002863
C     2.011759  0.613850 -0.000743
C     3.393747  0.734098  0.003357
H     3.872623  1.708400  0.007021
C     4.124323 -0.450557  0.002751
C     3.496505 -1.703004 -0.001884
H     4.102532 -2.604196 -0.002052
C     2.107181 -1.799597 -0.006124
H     1.629544 -2.775666 -0.009672
C     1.362841 -0.623445 -0.005508
C    -0.081204 -0.371082 -0.008528
C    -1.134010 -1.211186 -0.013536
H    -0.957193 -2.283866 -0.016403
C    -2.506488 -0.724709 -0.015656
C    -3.568930 -1.659489 -0.021030
H    -3.386969 -2.730341 -0.028064
C    -4.845048 -1.154958 -0.018374
C    -5.104115  0.217923 -0.012325
C    -4.092674  1.145105 -0.010172
H    -4.297405  2.211492 -0.009755
C    -2.763539  0.667173 -0.010566
O    -6.019922 -1.838460 -0.040610
O    -6.452148  0.421633 -0.032813
Br    6.032233 -0.374870  0.008624
C    -7.043912 -0.860456  0.110914
H    -7.798676 -1.003315 -0.669258
H    -7.488201 -0.952532  1.112807
    el energy= -1008.57438530
          zpe= -1008.345353
    th energy= -1008.328247
  th enthalpy= -1008.327303
  free energy= -1008.391724

wb97xd--5
B    -1.118634  1.640460 -0.006013
O    -1.235870  2.988736 -0.002377
H    -0.362684  3.409508 -0.000212
N     0.189776  0.999287 -0.005377
C     1.428540  1.644461 -0.000458
O     1.583467  2.849326  0.002866
C     2.448089  0.566348 -0.000031
C     3.829138  0.665467  0.004882
H     4.343149  1.620757  0.008821
C     4.529495 -0.534885  0.004731
C     3.896515 -1.781133 -0.000172
H     4.507162 -2.677441  0.000139
C     2.508441 -1.857136 -0.005184
H     2.013803 -2.824192 -0.008925
C     1.784045 -0.666230 -0.005055
C     0.345546 -0.394802 -0.008626
C    -0.716287 -1.224970 -0.013834
H    -0.549729 -2.299309 -0.016585
C    -2.082620 -0.725168 -0.015900
C    -3.154229 -1.649649 -0.020689
H    -2.983190 -2.722258 -0.027585
C    -4.424814 -1.131896 -0.017558
C    -4.669160  0.244141 -0.011500
C    -3.648176  1.161397 -0.010072
```

```
H    -3.842531  2.229667 -0.009485
C    -2.324582  0.669765 -0.011023
O    -5.606039 -1.802486 -0.037836
O    -6.013123  0.462597 -0.029041
N     6.000802 -0.493913  0.010157
O     6.529163  0.599955  0.014321
O     6.593257 -1.555517  0.010158
C    -6.621285 -0.813847  0.105093
H    -7.368921 -0.946090 -0.683698
H    -7.076709 -0.902648  1.101793
    el energy= -1200.42928036
          zpe= -1200.187076
    th energy= -1200.168939
  th enthalpy= -1200.167995
  free energy= -1200.234392

wb97xd--6
B     0.491365  1.600559 -0.003167
O     0.562816  2.954557 -0.001749
H    -0.328654  3.336329  0.002074
N    -0.795153  0.920302  0.001196
C    -2.053240  1.528960  0.005916
O    -2.237127  2.732310  0.005527
C    -3.045177  0.427417  0.009701
C    -4.426909  0.502676  0.011894
H    -4.926291  1.468973  0.017927
C    -5.153393 -0.697220  0.010778
C    -4.452329 -1.922195  0.007292
H    -5.021121 -2.850433  0.012383
C    -3.063617 -1.976747  0.004597
H    -2.558916 -2.939738  0.000534
C    -2.348351 -0.782397  0.005544
C    -0.914564 -0.479039  0.000274
C     0.173532 -1.273364 -0.005762
H     0.041533 -2.352503 -0.006508
C     1.525381 -0.730127 -0.012302
C     2.626163 -1.619511 -0.019520
H     2.487700 -2.696937 -0.024192
C     3.880764 -1.063505 -0.021959
C     4.085323  0.317793 -0.019053
C     3.036744  1.202384 -0.014892
H     3.197751  2.276353 -0.017323
C     1.727658  0.670853 -0.010150
O     5.083091 -1.700528 -0.048891
O     5.426612  0.574596 -0.047459
N    -6.540726 -0.687356  0.062937
H    -6.988580  0.164212 -0.238880
H    -7.005498 -1.516604 -0.273225
C     6.065011 -0.682351  0.110276
H     6.500462 -0.752859  1.118349
H     6.834829 -0.799457 -0.659459
    el energy= -1051.33520937
          zpe= -1051.078929
    th energy= -1051.061853
  th enthalpy= -1051.060909
  free energy= -1051.123621

wb97xd--thieno
B    -1.041823  1.442780 -0.000032
O    -1.165513  2.787577 -0.000046
H    -0.287287  3.202053 -0.000052
N     0.271841  0.804504 -0.000024
C     1.497945  1.473559 -0.000004
O     1.621343  2.685318  0.000042
C     2.543329  0.426008  0.000018
C     3.925659  0.555545  0.000063
H     4.387160  1.539272  0.000091
C     4.684253 -0.612540  0.000067
C     4.059336 -1.866968  0.000027
H     4.671840 -2.765553  0.000032
C     2.670860 -1.989205 -0.000015
H     2.200905 -2.969376 -0.000040
C     1.912877 -0.821418 -0.000017
C     0.463388 -0.594062 -0.000035
C    -0.563652 -1.464921 -0.000055
H    -0.364456 -2.532872 -0.000070
C    -1.934674 -0.982306 -0.000048
C    -3.071786 -1.751034 -0.000078
H    -3.151298 -2.831421 -0.000106
S    -4.497388 -0.770295  0.000101
C    -3.562600  0.684864 -0.000075
H    -4.056432  1.649031 -0.000101
C    -2.216960  0.435691 -0.000033
H     5.769529 -0.554295  0.000101
    el energy= -740.249766030
          zpe= -740.060351
    th energy= -740.047452
  th enthalpy= -740.046508
  free energy= -740.099987

wb97xd--7
B     2.477737  1.435626  0.000043
O     2.663986  2.772458  0.000054
H     1.808985  3.231944  0.000058
N     1.134996  0.857483  0.000038
C    -0.057399  1.581670  0.000026
O    -0.131141  2.796406 -0.000017
C    -1.149159  0.579316  0.000004
C    -2.521711  0.781965 -0.000034
H    -2.941194  1.783234 -0.000056
C    -3.321790 -0.356303 -0.000039
C    -2.769820 -1.644536 -0.000008
H    -3.429351 -2.507198 -0.000015
C    -1.389117 -1.823690  0.000027
H    -0.970525 -2.826568  0.000046
C    -0.575263 -0.693865  0.000031
```

```
C     0.881762 -0.531717  0.000048
C     1.868567 -1.448208  0.000065
H     1.621639 -2.506203  0.000077
C     3.259778 -1.028147  0.000064
C     4.361693 -1.847061  0.000093
H     4.392836 -2.929952  0.000117
S     5.828624 -0.929932 -0.000024
C     4.959723  0.565153  0.000082
H     5.495505  1.506678  0.000099
C     3.604470  0.375659  0.000049
Br   -5.221220 -0.161882 -0.000090
    el energy= -752.826806605
          zpe= -752.647896
    th energy= -752.633426
  th enthalpy= -752.632482
  free energy= -752.690736

wb97xd--8
B    -2.050254  1.438171 -0.000435
O    -2.235069  2.774392 -0.000356
H    -1.381666  3.236359 -0.000480
N    -0.707848  0.856726 -0.000663
C     0.486764  1.577139 -0.000435
O     0.566599  2.790431 -0.000383
C     1.574524  0.569299 -0.000534
C     2.946437  0.759874 -0.000083
H     3.396353  1.747019  0.000360
C     3.723706 -0.391442 -0.000054
C     3.174746 -1.677322 -0.000572
H     3.846001 -2.529329 -0.000522
C     1.795289 -1.844869 -0.000965
H     1.365061 -2.842257 -0.001246
C     0.993916 -0.703929 -0.000864
C    -0.460073 -0.532786 -0.000820
C    -1.448934 -1.448206 -0.000671
H    -1.203893 -2.506663 -0.000711
C    -2.837679 -1.024803 -0.000199
C    -3.941491 -1.841994  0.000333
H    -3.974741 -2.924821  0.000427
S    -5.404912 -0.921839  0.001038
C    -4.533324  0.571599  0.000580
H    -5.067345  1.514085  0.000877
C    -3.178403  0.379745 -0.000070
N     5.189341 -0.254161  0.000782
O     5.644933  0.871811  0.002083
O     5.849385 -1.275086  0.000176
    el energy= -944.681517172
          zpe= -944.489378
    th energy= -944.473876
  th enthalpy= -944.472931
  free energy= -944.533181

wb97xd--9
B     1.435465  1.435955  0.000578
O     1.586511  2.778757  0.001792
H     0.716086  3.209318  0.000561
N     0.109329  0.824851 -0.001491
C    -1.101487  1.518970 -0.002837
O    -1.201229  2.733510 -0.000785
C    -2.170622  0.493861 -0.005919
C    -3.543373  0.670036 -0.005724
H    -3.971189  1.670054 -0.010135
C    -4.355425 -0.473226 -0.004997
C    -3.745982 -1.746900 -0.003790
H    -4.382025 -2.630456 -0.008916
C    -2.365629 -1.902797 -0.003456
H    -1.932098 -2.899845 -0.001317
C    -1.564430 -0.763423 -0.004469
C    -0.112194 -0.571257 -0.002252
C     0.899369 -1.460412 -0.001000
H     0.679984 -2.524450 -0.002033
C     2.280544 -1.005392  0.000767
C     3.403319 -1.794527  0.001550
H     3.463203 -2.876168  0.000893
S     4.848417 -0.839907  0.003085
C     3.940198  0.631651  0.002646
H     4.450606  1.587142  0.003124
C     2.590371  0.406773  0.001530
N    -5.738074 -0.361927 -0.055641
H    -6.122812  0.519815  0.246552
H    -6.262753 -1.155426  0.278587
    el energy= -795.587944010
          zpe= -795.381620
    th energy= -795.367204
  th enthalpy= -795.366260
  free energy= -795.422764

wb97xd.tddft--benzo
B     1.108922  1.406177 -0.000002
O     1.254027  2.752420 -0.000004
H     0.370091  3.165607 -0.000007
N    -0.217639  0.804302 -0.000005
C    -1.458519  1.503580 -0.000007
O    -1.524742  2.733484  0.000002
C    -2.478962  0.473368  0.000000
C    -3.870205  0.559582  0.000006
H    -4.360531  1.529493  0.000008
C    -4.604998 -0.622383  0.000008
C    -3.970103 -1.885357  0.000004
H    -4.575402 -2.787915  0.000006
C    -2.585931 -1.983426 -0.000001
H    -2.099057 -2.956523 -0.000003
C    -1.834890 -0.798968 -0.000003
C    -0.423830 -0.558572 -0.000006
C     0.660616 -1.467881 -0.000006
H     0.437057 -2.531692 -0.000005
```

```
C     1.986575 -1.020872 -0.000003
C     3.073378 -1.955913 -0.000001
H     2.850438 -3.021334 -0.000003
C     4.371686 -1.515448  0.000003
C     4.653295 -0.127124  0.000006
C     3.618976  0.799369  0.000004
H     3.842973  1.863984  0.000006
C     2.278489  0.398149  0.000000
H     5.189817 -2.231402  0.000005
H     5.687197  0.210064  0.000010
H    -5.691463 -0.577140  0.000012
 total energy= -807.395304635

wb97xd.tddft--1
B     1.197719 -2.645609  0.000000
O     0.567733 -3.843544  0.000000
H    -0.396333 -3.698241  0.000000
N     0.437275 -1.404348  0.000000
C    -0.981750 -1.288837  0.000000
O    -1.728191 -2.266627  0.000000
C    -1.247818  0.137103  0.000000
C    -2.452568  0.835097  0.000000
H    -3.403036  0.310251  0.000000
C    -2.385576  2.224108  0.000000
C    -1.158698  2.931322  0.000000
H    -1.165120  4.016221  0.000000
C     0.037061  2.231598  0.000000
H     0.982094  2.770310  0.000000
C     0.000000  0.830272  0.000000
C     1.032177 -0.158607  0.000000
C     2.437795 -0.013484  0.000000
H     2.850309  0.992179  0.000000
C     3.285684 -1.128291  0.000000
C     4.709312 -0.962971  0.000000
H     5.122550  0.043918  0.000000
C     5.536901 -2.056419  0.000000
C     4.991355 -3.363125  0.000000
C     3.615290 -3.550100  0.000000
H     3.203046 -4.556737  0.000000
C     2.731939 -2.465343  0.000000
H     6.615878 -1.922951  0.000000
H     5.658880 -4.221585  0.000000
Br   -4.004021  3.228359  0.000000
 total energy= -819.974833988

wb97xd.tddft--2
B    -2.487292  0.496220  0.000000
O    -3.572312 -0.307147  0.000000
H    -3.292946 -1.240069  0.000000
N    -1.139820 -0.063999  0.000000
C    -0.809076 -1.448747  0.000000
O    -1.655990 -2.331518  0.000000
C     0.646797 -1.495015  0.000000
C     1.509347 -2.576836  0.000000
H     1.153256 -3.601715  0.000000
C     2.873483 -2.296767  0.000000
C     3.389817 -0.979313  0.000000
H     4.464361 -0.840733  0.000000
C     2.520690  0.096240  0.000000
H     2.910566  1.111442  0.000000
C     1.138272 -0.154543  0.000000
C     0.000000  0.714300  0.000000
C    -0.078604  2.125251  0.000000
H     0.851138  2.688368  0.000000
C    -1.312667  2.791597  0.000000
C    -1.367578  4.223431  0.000000
H    -0.435910  4.785794  0.000000
C    -2.576593  4.873741  0.000000
C    -3.781804  4.135963  0.000000
C    -3.754686  2.744293  0.000000
H    -4.686927  2.183798  0.000000
C    -2.548439  2.042183  0.000000
H    -2.610559  5.960332  0.000000
H    -4.733386  4.661884  0.000000
N     3.811102 -3.411950  0.000000
O     3.353221 -4.543342  0.000000
O     5.003099 -3.147146  0.000000
 total energy= -1011.83148488

wb97xd.tddft--3
B    -1.502730  1.398516 -0.000334
O    -1.688667  2.745235  0.000402
H    -0.815966  3.178781 -0.000046
N    -0.166068  0.837122 -0.001465
C     1.046848  1.565407 -0.001549
O     1.100748  2.801754 -0.000576
C     2.094557  0.564769 -0.002514
C     3.474054  0.695301 -0.001579
H     3.937836  1.679130 -0.001944
C     4.258651 -0.474108 -0.000490
C     3.646024 -1.770507 -0.001626
H     4.280710 -2.653471 -0.004714
C     2.276260 -1.895354 -0.002344
H     1.818117 -2.881796 -0.002580
C     1.480111 -0.733117 -0.002384
C     0.076251 -0.536238 -0.001923
C    -0.971014 -1.465170 -0.001453
H    -0.727143 -2.524689 -0.002191
C    -2.316450 -1.047879 -0.000273
C    -3.374541 -2.006316  0.000475
H    -3.126408 -3.066486 -0.000150
C    -4.685733 -1.599861  0.002000
C    -5.004436 -0.220963  0.002805
C    -3.994942  0.726592  0.002011
H    -4.241410  1.786342  0.002585
C    -2.639995  0.356754  0.000413
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H    -5.484083 -2.338311  0.002591
H    -6.046935  0.089184  0.004013
N     5.618278 -0.391162 -0.013195
H     6.076660  0.500582  0.071389
H     6.186282 -1.215339  0.087328
 total energy= -862.741334204

wb97xd.tddft--dioxo
B     0.072693  1.576150 -0.001134
O     0.108428  2.931308 -0.000622
H    -0.810014  3.263355 -0.000221
N    -1.188458  0.863906 -0.001070
C    -2.479785  1.451663  0.000027
O    -2.652753  2.673832  0.000513
C    -3.406663  0.336246  0.000476
C    -4.801595  0.303605  0.001797
H    -5.370443  1.229798  0.002517
C    -5.432775 -0.934488  0.002238
C    -4.691321 -2.138993  0.001344
H    -5.217515 -3.089902  0.001750
C    -3.304796 -2.118849  0.000010
H    -2.737788 -3.047660 -0.000634
C    -2.656239 -0.875586 -0.000405
C    -1.269622 -0.518312 -0.001339
C    -0.116830 -1.325326 -0.002131
H    -0.245775 -2.404179 -0.002473
C     1.168353 -0.769837 -0.002111
C     2.323852 -1.627101 -0.002255
H     2.219682 -2.707729 -0.002999
C     3.539929 -1.026031 -0.001367
C     3.692319  0.386209 -0.000510
C     2.616256  1.242884 -0.000780
H     2.749049  2.320700 -0.000277
C     1.330455  0.679543 -0.001513
O     4.769399 -1.598239 -0.002271
O     5.005713  0.688520 -0.000452
H    -6.519190 -0.983544  0.003347
C     5.717641 -0.543491  0.007543
H     6.323463 -0.602282  0.919552
H     6.342905 -0.602851 -0.890897
 total energy= -995.874506102

wb97xd.tddft--4
B    -1.551263  1.655542 -0.007137
O    -1.686900  3.003690 -0.003515
H    -0.797997  3.406627 -0.002167
N    -0.243809  1.033535 -0.008679
C     1.001204  1.712565 -0.003952
O     1.090193  2.942116 -0.000827
C     2.004284  0.665618 -0.003255
C     3.396009  0.746433  0.001795
H     3.898812  1.708715  0.005305
C     4.103012 -0.448115  0.002418
C     3.467555 -1.713554 -0.001826
H     4.069244 -2.616558 -0.000862
C     2.084467 -1.787648 -0.007026
H     1.592883 -2.757964 -0.010192
C     1.343307 -0.598148 -0.007832
C    -0.064665 -0.341154 -0.011303
C    -1.156093 -1.226214 -0.015508
H    -0.953677 -2.293632 -0.018669
C    -2.478726 -0.761916 -0.013704
C    -3.569885 -1.698362 -0.014658
H    -3.391124 -2.769106 -0.020781
C    -4.825672 -1.183789 -0.007036
C    -5.076822  0.213862  0.000882
C    -4.063524  1.144098 -0.001289
H    -4.269989  2.210175  0.003487
C    -2.742422  0.671111 -0.008337
O    -6.011165 -1.840431 -0.011219
O    -6.407060  0.423581  0.005034
Br    6.010326 -0.398704  0.009023
C    -7.030397 -0.855248  0.047021
H    -7.693399 -0.960606 -0.818556
H    -7.583530 -0.954341  0.988933
 total energy= -1008.45436417

wb97xd.tddft--5
B    -1.102433  1.641677 -0.004798
O    -1.223866  2.988368 -0.002199
H    -0.336119  3.391126 -0.001630
N     0.198416  1.000786 -0.006496
C     1.450861  1.663202 -0.003371
O     1.558103  2.885080 -0.001329
C     2.444607  0.599296 -0.002721
C     3.828588  0.667802  0.001504
H     4.360755  1.613247  0.004365
C     4.519257 -0.538629  0.002448
C     3.872710 -1.797575 -0.000913
H     4.479054 -2.695461  0.000161
C     2.491951 -1.857099 -0.005187
H     1.988334 -2.820799 -0.007577
C     1.764565 -0.655251 -0.005978
C     0.359398 -0.377596 -0.008271
C    -0.744722 -1.244269 -0.010701
H    -0.558164 -2.314439 -0.012838
C    -2.063924 -0.761628 -0.008727
C    -3.164960 -1.683605 -0.008754
H    -3.000082 -2.756471 -0.012554
C    -4.415389 -1.152407 -0.003057
C    -4.649085  0.247104  0.002149
C    -3.621558  1.165421  0.000397
H    -3.814453  2.234039  0.003851
C    -2.310404  0.673251 -0.004944
O    -5.607337 -1.793768 -0.003487
O    -5.973977  0.474905  0.006564
```

```
N     5.976902 -0.504772  0.007658
O     6.523163  0.586248  0.010349
O     6.566797 -1.573647  0.009213
C    -6.616233 -0.796243  0.023964
H    -7.250593 -0.889917 -0.864350
H    -7.200841 -0.889933  0.946496
 total energy= -1200.31173035

wb97xd.tddft--6
B     0.473429  1.610931 -0.006606
O     0.550697  2.968809 -0.004668
H    -0.357023  3.326067 -0.001181
N    -0.806403  0.939945 -0.003711
C    -2.074928  1.564372  0.002827
O    -2.225998  2.793407  0.004117
C    -3.035061  0.479265  0.006713
C    -4.422465  0.498448  0.011629
H    -4.960753  1.443758  0.016728
C    -5.110622 -0.725931  0.011091
C    -4.393382 -1.964175  0.007130
H    -4.952689 -2.896923  0.014968
C    -3.016468 -1.980102  0.001580
H    -2.483538 -2.928550 -0.002301
C    -2.316249 -0.759982  0.000612
C    -0.931555 -0.448778 -0.005295
C     0.193240 -1.284094 -0.011394
H     0.038167 -2.359797 -0.012359
C     1.496653 -0.761096 -0.013998
C     2.625363 -1.650666 -0.016881
H     2.490426 -2.728169 -0.021542
C     3.860225 -1.086545 -0.014404
C     4.054338  0.316584 -0.009882
C     3.006004  1.201101 -0.010069
H     3.167543  2.274976 -0.008502
C     1.698501  0.675382 -0.011280
O     5.073134 -1.699184 -0.028709
O     5.382397  0.579124 -0.017878
N    -6.480291 -0.754744  0.046652
H    -6.990040  0.095021 -0.132489
H    -6.959937 -1.611122 -0.177358
C     6.047944 -0.673064  0.074419
H     6.553383 -0.744061  1.046977
H     6.763123 -0.763838 -0.750174
 total energy= -1051.21813610

wb97xd.tddft--thieno
B     1.020960  1.446560 -0.000119
O     1.136731  2.789863 -0.000201
H     0.239608  3.178455 -0.000336
N    -0.282450  0.800025 -0.000134
C    -1.543622  1.492148 -0.000096
O    -1.606798  2.722687  0.000071
C    -2.547727  0.458910 -0.000070
C    -3.943167  0.530512  0.000037
H    -4.442530  1.495917  0.000126
C    -4.667545 -0.656021  0.000027
C    -4.021122 -1.915385 -0.000096
H    -4.617648 -2.823667 -0.000097
C    -2.634996 -1.999875 -0.000191
H    -2.140632 -2.969524 -0.000255
C    -1.892594 -0.811379 -0.000167
C    -0.480668 -0.566802 -0.000160
C     0.604042 -1.475770 -0.000135
H     0.395496 -2.541285 -0.000137
C     1.920752 -0.989063 -0.000014
C     3.104534 -1.753444  0.000094
H     3.193434 -2.833023  0.000108
S     4.491376 -0.763270  0.000449
C     3.542644  0.697295  0.000068
H     4.037310  1.661117  0.000062
C     2.202835  0.443958  0.000006
H    -5.754358 -0.619556  0.000113
 total energy= -740.114681504

wb97xd.tddft--7
B     2.464728  1.438926 -0.000014
O     2.656390  2.773253 -0.000077
H     1.785784  3.215987 -0.000162
N     1.128667  0.863543 -0.000047
C    -0.090869  1.621375 -0.000072
O    -0.093745  2.851722  0.000017
C    -1.149419  0.641607 -0.000063
C    -2.535739  0.799003 -0.000042
H    -2.985891  1.787014 -0.000026
C    -3.311105 -0.353491 -0.000048
C    -2.750033 -1.655678 -0.000074
H    -3.402821 -2.522023 -0.000074
C    -1.371488 -1.806593 -0.000089
H    -0.935425 -2.803411 -0.000095
C    -0.562992 -0.663207 -0.000081
C     0.858636 -0.493394 -0.000063
C     1.890769 -1.457876 -0.000042
H     1.625629 -2.510737 -0.000053
C     3.232821 -1.042104  0.000022
C     4.373366 -1.868609  0.000031
H     4.403790 -2.951504  0.000006
S     5.810150 -0.953233  0.000295
C     4.941174  0.555803  0.000017
H     5.485888  1.492259 -0.000019
C     3.590013  0.373382  0.000041
Br   -5.210161 -0.188469 -0.000019
 total energy= -752.694596068

wb97xd.tddft--8
B     2.036051  1.440401 -0.000277
O     2.223601  2.772672 -0.000222
```

```
H     1.362555  3.227963 -0.000361
N     0.698363  0.853732 -0.000557
C    -0.522187  1.599264 -0.000418
O    -0.543115  2.820030 -0.000227
C    -1.584435  0.604931 -0.000448
C    -2.956311  0.764510 -0.000013
H    -3.429385  1.740967  0.000330
C    -3.728928 -0.397712  0.000003
C    -3.159178 -1.695856 -0.000417
H    -3.824677 -2.551100 -0.000400
C    -1.785870 -1.844853 -0.000744
H    -1.345010 -2.838943 -0.000994
C    -0.981202 -0.690091 -0.000735
C     0.437960 -0.507414 -0.000719
C     1.481083 -1.458188 -0.000650
H     1.226416 -2.513639 -0.000746
C     2.821897 -1.031768 -0.000231
C     3.967230 -1.850097  0.000171
H     4.003855 -2.932965  0.000155
S     5.402015 -0.927549  0.000860
C     4.517319  0.576498  0.000527
H     5.054349  1.517625  0.000832
C     3.169297  0.383106 -0.000027
N    -5.172151 -0.270115  0.000612
O    -5.648812  0.856610  0.001325
O    -5.832188 -1.300616  0.000453
 total energy= -944.553182034

wb97xd.tddft--9
B     1.417215  1.444226 -0.000182
O     1.574861  2.788963  0.000487
H     0.687317  3.197347 -0.000020
N     0.100943  0.842573 -0.001283
C    -1.128202  1.562111 -0.001418
O    -1.181930  2.800408 -0.000445
C    -2.161811  0.559587 -0.002596
C    -3.546890  0.674719 -0.001725
H    -4.021874  1.653196 -0.001867
C    -4.319211 -0.502279 -0.000672
C    -3.699721 -1.796323 -0.001990
H    -4.326865 -2.684242 -0.006002
C    -2.325935 -1.905571 -0.002533
H    -1.858276 -2.887747 -0.003008
C    -1.540322 -0.738989 -0.002323
C    -0.133675 -0.537322 -0.001636
C     0.907083 -1.467592 -0.001030
H     0.672750 -2.528048 -0.001695
C     2.248668 -1.018154  0.000014
C     3.398162 -1.812947  0.000770
H     3.459327 -2.894311  0.000572
S     4.817393 -0.858003  0.001955
C     3.916395  0.622180  0.001568
H     4.435401  1.572859  0.002063
C     2.566013  0.405923  0.000472
N    -5.679868 -0.429638 -0.013159
H    -6.145272  0.458696  0.070518
H    -6.241171 -1.258390  0.088411
 total energy= -795.460180235

wb97xd.tddft-mecn--benzo
B     1.105064  1.407102  0.000871
O     1.232504  2.758286  0.000120
H     0.338228  3.150547  0.000286
N    -0.224489  0.806047  0.002254
C    -1.457643  1.500457  0.001062
O    -1.526018  2.737069  0.000678
C    -2.478125  0.472191  0.000039
C    -3.869995  0.556621 -0.001680
H    -4.370129  1.522373 -0.002450
C    -4.604269 -0.627392 -0.002461
C    -3.963562 -1.890199 -0.001458
H    -4.569125 -2.793090 -0.001988
C    -2.582688 -1.992138  0.000203
H    -2.093643 -2.963353  0.001011
C    -1.825701 -0.801047  0.000795
C    -0.430638 -0.560606  0.002184
C     0.670380 -1.466934  0.002593
H     0.451881 -2.531972  0.003822
C     1.987029 -1.015267  0.001225
C     3.075001 -1.953552  0.000759
H     2.848505 -3.017984  0.001752
C     4.375699 -1.513547 -0.001158
C     4.658403 -0.127833 -0.002651
C     3.620022  0.802858 -0.002032
H     3.858299  1.865087 -0.003116
C     2.282122  0.405118 -0.000093
H     5.192875 -2.230786 -0.001640
H     5.692015  0.210443 -0.004217
H    -5.690913 -0.584322 -0.003945
 total energy= -807.428820702

wb97xd.tddft-mecn--1
B    -2.547439  1.394613 -0.000444
O    -2.750093  2.735801  0.000034
H    -1.882389  3.182030 -0.000114
N    -1.188113  0.863749 -0.001080
C     0.007674  1.621464 -0.000797
O     0.015397  2.858147 -0.000610
C     1.078382  0.644431 -0.000627
C     2.461772  0.809261 -0.000159
H     2.910140  1.798891  0.000122
C     3.238334 -0.343735 -0.000003
C     2.680867 -1.646698 -0.000401
H     3.332304 -2.515127 -0.000347
C     1.307719 -1.808710 -0.000932
H     0.873833 -2.805378 -0.001199
```

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C     0.491480 -0.660263 -0.000965
C    -0.913777 -0.490520 -0.001178
C    -1.963524 -1.453438 -0.001207
H    -1.689491 -2.505431 -0.001708
C    -3.302260 -1.070891 -0.000467
C    -4.338484 -2.065147 -0.000123
H    -4.056308 -3.116094 -0.000671
C    -5.660697 -1.693449  0.000977
C    -6.014308 -0.324819  0.001754
C    -5.026035  0.659537  0.001291
H    -5.319522  1.707607  0.001825
C    -3.670090  0.331108  0.000145
H    -6.439981 -2.451497  0.001296
H    -7.064219 -0.041332  0.002648
Br    5.142997 -0.173524  0.000820
 total energy= -820.009136694

wb97xd.tddft-mecn--2
B    -2.489497  0.479808  0.000000
O    -3.568623 -0.336084  0.000000
H    -3.274871 -1.264476  0.000000
N    -1.140477 -0.080652  0.000000
C    -0.805797 -1.453625  0.000000
O    -1.646109 -2.348876  0.000000
C     0.651957 -1.493253  0.000000
C     1.516241 -2.567327  0.000000
H     1.161285 -3.592858  0.000000
C     2.885010 -2.281025  0.000000
C     3.390086 -0.954409  0.000000
H     4.462724 -0.798198  0.000000
C     2.521389  0.115599  0.000000
H     2.902831  1.133164  0.000000
C     1.131095 -0.142355  0.000000
C     0.000000  0.703799  0.000000
C    -0.094159  2.125924  0.000000
H     0.832529  2.694000  0.000000
C    -1.324702  2.779215  0.000000
C    -1.377752  4.213446  0.000000
H    -0.444331  4.772354  0.000000
C    -2.588856  4.864897  0.000000
C    -3.790296  4.126916  0.000000
C    -3.763643  2.728928  0.000000
H    -4.703501  2.180598  0.000000
C    -2.561745  2.028085  0.000000
H    -2.623625  5.951445  0.000000
H    -4.743437  4.650142  0.000000
N     3.817058 -3.380289  0.000000
O     3.374134 -4.524973  0.000000
O     5.016703 -3.123506  0.000000
 total energy= -1011.86911816

wb97xd.tddft-mecn--2-
B    -2.486519  0.373748  0.000000
O    -3.470386 -0.500839  0.000000
N    -1.110601 -0.083380  0.000000
C    -0.757942 -1.436080  0.000000
O    -1.582879 -2.359856  0.000000
C     0.693020 -1.433890  0.000000
C     1.587528 -2.501726  0.000000
H     1.244363 -3.531394  0.000000
C     2.938828 -2.199073  0.000000
C     3.423700 -0.861351  0.000000
H     4.493893 -0.688004  0.000000
C     2.535870  0.189383  0.000000
H     2.903952  1.212762  0.000000
C     1.149326 -0.078965  0.000000
C     0.000000  0.767407  0.000000
C    -0.166539  2.140276  0.000000
H     0.712868  2.779825  0.000000
C    -1.464054  2.726306  0.000000
C    -1.621679  4.143370  0.000000
H    -0.728572  4.767496  0.000000
C    -2.870073  4.725059  0.000000
C    -4.037717  3.928994  0.000000
C    -3.913264  2.550517  0.000000
H    -4.810563  1.933664  0.000000
C    -2.650927  1.925961  0.000000
H    -2.958481  5.810166  0.000000
H    -5.019175  4.397224  0.000000
N     3.892252 -3.286511  0.000000
O     3.473101 -4.437820  0.000000
O     5.085950 -3.011280  0.000000
 total energy= -1011.36993428

wb97xd.tddft-mecn--3
B    -1.499752  1.393791  0.000271
O    -1.665874  2.748846 -0.000039
H    -0.778097  3.155245 -0.000256
N    -0.161195  0.834666  0.000165
C     1.043990  1.561135  0.000066
O     1.089514  2.805722 -0.000283
C     2.095962  0.567223 -0.000077
C     3.473371  0.702831 -0.000206
H     3.953913  1.678676 -0.000450
C     4.264198 -0.472221 -0.000104
C     3.643507 -1.776095  0.000256
H     4.286437 -2.652821  0.000361
C     2.282543 -1.903743  0.000381
H     1.822242 -2.888769  0.000597
C     1.477177 -0.733772  0.000166
C     0.085413 -0.543710  0.000274
C    -0.974520 -1.469207  0.000000
H    -0.735260 -2.529899 -0.000183
C    -2.315053 -1.045157 -0.000097
C    -3.377506 -2.002742 -0.000481
H    -3.129232 -3.062888 -0.000856
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C    -4.690654 -1.595441 -0.000351
C    -5.013080 -0.218072  0.000086
C    -3.998687  0.728725  0.000308
H    -4.255220  1.787211  0.000662
C    -2.643405  0.360363  0.000201
H    -5.487844 -2.335758 -0.000607
H    -6.055438  0.092803  0.000303
N     5.606171 -0.390888 -0.000370
H     6.073020  0.505135  0.000044
H     6.180735 -1.221587  0.000518
 total energy= -862.783503122

wb97xd.tddft-mecn--dioxo
B     0.069557  1.578721 -0.017189
O     0.085662  2.937704 -0.012313
H    -0.840561  3.249186 -0.011533
N    -1.197021  0.867601 -0.020883
C    -2.482361  1.449110 -0.008433
O    -2.660118  2.678094 -0.006437
C    -3.407323  0.335103  0.002905
C    -4.803319  0.295640  0.024334
H    -5.384885  1.214936  0.030536
C    -5.430425 -0.945528  0.038771
C    -4.680065 -2.148272  0.031791
H    -5.204337 -3.100625  0.044978
C    -3.296586 -2.128125  0.009285
H    -2.725083 -3.053677  0.005067
C    -2.645998 -0.876515 -0.004644
C    -1.275854 -0.517038 -0.020713
C    -0.104258 -1.319312 -0.034111
H    -0.230193 -2.398850 -0.041888
C     1.169461 -0.761637 -0.034100
C     2.327768 -1.624199 -0.045768
H     2.214086 -2.704092 -0.069520
C     3.544795 -1.026929 -0.026536
C     3.697154  0.384409  0.008022
C     2.617798  1.246062  0.006381
H     2.767060  2.322212  0.024467
C     1.333428  0.688610 -0.016467
O     4.772071 -1.596606 -0.049768
O     5.000721  0.690431  0.025811
H    -6.516521 -0.999482  0.057031
C     5.721117 -0.546285  0.098296
H     6.205689 -0.619687  1.078445
H     6.447433 -0.584273 -0.717877
 total energy= -995.908277492

wb97xd.tddft-mecn--4
B    -1.549922  1.660432 -0.000143
O    -1.663329  3.013824 -0.000046
H    -0.763015  3.393116 -0.000053
N    -0.236350  1.039700 -0.000251
C     1.002408  1.713575 -0.000148
O     1.094383  2.950558 -0.000081
C     2.004094  0.668680 -0.000135
C     3.397397  0.745931  0.000007
H     3.904820  1.706588  0.000119
C     4.098813 -0.450880  0.000015
C     3.459569 -1.716713 -0.000123
H     4.054374 -2.625118 -0.000116
C     2.079350 -1.791991 -0.000257
H     1.585570 -2.760505 -0.000357
C     1.334489 -0.595817 -0.000250
C    -0.058899 -0.336225 -0.000304
C    -1.169413 -1.218436 -0.000331
H    -0.969086 -2.286720 -0.000406
C    -2.480279 -0.752654 -0.000209
C    -3.572120 -1.696685 -0.000144
H    -3.381203 -2.765818 -0.000231
C    -4.829220 -1.188235  0.000053
C    -5.082573  0.208647  0.000190
C    -4.067708  1.146350  0.000115
H    -4.293731  2.209093  0.000224
C    -2.747778  0.681611 -0.000088
O    -6.010233 -1.845607  0.000217
O    -6.402825  0.421845  0.000430
Br    6.012675 -0.405300  0.000226
C    -7.040242 -0.862241  0.000143
H    -7.644129 -0.959718 -0.907354
H    -7.644476 -0.959952  0.907370
 total energy= -1008.48904895

wb97xd.tddft-mecn--5
B    -1.098380  1.651080  0.000810
O    -1.204729  3.001525  0.002281
H    -0.311068  3.390553  0.001992
N     0.207937  1.012084 -0.000796
C     1.454230  1.666738 -0.000788
O     1.572243  2.892045 -0.000188
C     2.446612  0.600083 -0.001435
C     3.825230  0.664795 -0.001392
H     4.357473  1.610522 -0.001429
C     4.518764 -0.547256 -0.000449
C     3.859235 -1.806117 -0.000079
H     4.453264 -2.712811  0.000599
C     2.483369 -1.865386 -0.001113
H     1.975513 -2.826131 -0.001336
C     1.751864 -0.654452 -0.001542
C     0.368504 -0.369319 -0.001424
C    -0.757105 -1.232585 -0.001868
H    -0.572608 -2.303641 -0.002977
C    -2.062412 -0.749587 -0.001070
C    -3.163140 -1.681094 -0.001917
H    -2.983671 -2.752063 -0.003471
C    -4.415190 -1.157841 -0.000732
C    -4.651171  0.240192  0.001361
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C    -3.622267  1.168257  0.002088
H    -3.836333  2.233276  0.003637
C    -2.313411  0.685835  0.000723
O    -5.603108 -1.800521 -0.001088
O    -5.964818  0.471547  0.002357
N     5.958658 -0.514778  0.001048
O     6.521908  0.576063 -0.007213
O     6.563909 -1.582380  0.010704
C    -6.621198 -0.804988  0.000113
H    -7.225452 -0.891650 -0.908033
H    -7.226093 -0.894494  0.907526
 total energy= -1200.34975593

wb97xd.tddft-mecn--5-
B     1.079902  1.626497 -0.006264
O     1.128994  2.946114 -0.003078
N    -0.203990  0.953983 -0.000951
C    -1.424205  1.635203  0.005691
O    -1.521198  2.870389  0.010530
C    -2.426329  0.586818  0.004928
C    -3.815685  0.681396  0.008978
H    -4.321964  1.641488  0.014518
C    -4.534375 -0.502975  0.005207
C    -3.904777 -1.779112 -0.002226
H    -4.520070 -2.671693 -0.005344
C    -2.532065 -1.867132 -0.005291
H    -2.049973 -2.841845 -0.011061
C    -1.763700 -0.681381 -0.001748
C    -0.358605 -0.436538 -0.004855
C     0.751636 -1.262640 -0.011214
H     0.607631 -2.340208 -0.013614
C     2.072672 -0.732117 -0.016983
C     3.192794 -1.629883 -0.021767
H     3.039600 -2.706269 -0.024085
C     4.444548 -1.089522 -0.026244
C     4.672037  0.300594 -0.028949
C     3.637619  1.193063 -0.023990
H     3.824564  2.263651 -0.030719
C     2.311427  0.679314 -0.016238
O     5.643358 -1.735050 -0.059622
O     6.018972  0.532705 -0.076147
N    -5.977595 -0.435475  0.008541
O    -6.516337  0.665267  0.019939
O    -6.608369 -1.486103 -0.000066
C     6.627903 -0.728521  0.171079
H     6.960982 -0.780123  1.218008
H     7.462071 -0.873011 -0.520224
 total energy= -1199.84217366

wb97xd.tddft-mecn--6
B     0.472046  1.609899 -0.009271
O     0.527993  2.975201 -0.005436
H    -0.390855  3.306058 -0.004419
N    -0.812840  0.942529 -0.010693
C    -2.074960  1.564052 -0.004286
O    -2.223499  2.801817 -0.002124
C    -3.038098  0.484433  0.000062
C    -4.424742  0.504461  0.009776
H    -4.981359  1.439340  0.013416
C    -5.114655 -0.728886  0.015301
C    -4.385775 -1.972956  0.010620
H    -4.951448 -2.901598  0.015626
C    -3.017361 -1.988131  0.000302
H    -2.479382 -2.933317 -0.002727
C    -2.311863 -0.757756 -0.004928
C    -0.940412 -0.450953 -0.012215
C     0.196981 -1.281442 -0.020518
H     0.045749 -2.358009 -0.025204
C     1.495096 -0.752373 -0.021927
C     2.625417 -1.644901 -0.030888
H     2.482281 -2.721891 -0.045743
C     3.863536 -1.084895 -0.023565
C     4.062082  0.316070 -0.005106
C     3.012839  1.202029 -0.003288
H     3.188317  2.274698  0.004585
C     1.700699  0.682105 -0.012106
O     5.071753 -1.700871 -0.053851
O     5.387939  0.577972 -0.013673
N    -6.462581 -0.765971  0.025484
H    -7.007872  0.083667  0.029532
H    -6.959029 -1.644968  0.030417
C     6.051819 -0.680412  0.115477
H     6.492504 -0.756797  1.117535
H     6.811697 -0.768204 -0.665791
 total energy= -1051.25970792

wb97xd.tddft-mecn--thieno
B     1.016883  1.446955 -0.000002
O     1.117101  2.795018 -0.000177
H     0.211208  3.164853 -0.000064
N    -0.291067  0.802989  0.000311
C    -1.539845  1.488734  0.000174
O    -1.611330  2.726751  0.000153
C    -2.545599  0.457099  0.000003
C    -3.941120  0.527735 -0.000047
H    -4.448877  1.489785 -0.000011
C    -4.666207 -0.659698 -0.000158
C    -4.013628 -1.919560 -0.000197
H    -4.611799 -2.827511 -0.000260
C    -2.632627 -2.010243 -0.000114
H    -2.137431 -2.978631 -0.000101
C    -1.880961 -0.814253 -0.000026
C    -0.488193 -0.569353  0.000197
C     0.616399 -1.476147  0.000261
H     0.414761 -2.543488  0.000507
C     1.920287 -0.983537  0.000085
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C     3.105406 -1.752394  0.000122
H     3.190439 -2.833667  0.000228
S     4.493599 -0.762419 -0.000072
C     3.542979  0.704033 -0.000279
H     4.051374  1.662198 -0.000382
C     2.205251  0.451033 -0.000100
H    -5.753226 -0.625359 -0.000247
 total energy= -740.147594884

wb97xd.tddft-mecn--7
B    -2.463271  1.439238 -0.000073
O    -2.641203  2.778636  0.000328
H    -1.761266  3.204430  0.000334
N    -1.120991  0.868305 -0.000463
C     0.087453  1.621525 -0.000375
O     0.094841  2.859587 -0.000346
C     1.147541  0.643868 -0.000269
C     2.534347  0.800855 -0.000090
H     2.986952  1.788714  0.000000
C     3.305662 -0.353239 -0.000018
C     2.741580 -1.656241 -0.000171
H     3.389771 -2.527132 -0.000202
C     1.368122 -1.811930 -0.000354
H     0.931538 -2.807647 -0.000501
C     0.553000 -0.661528 -0.000347
C    -0.851500 -0.491601 -0.000429
C    -1.901430 -1.458147 -0.000319
H    -1.640263 -2.512427 -0.000520
C    -3.231240 -1.038261 -0.000026
C    -4.372893 -1.870489  0.000081
H    -4.398154 -2.955156  0.000003
S    -5.811602 -0.956523  0.000339
C    -4.941877  0.559162  0.000324
H    -5.499554  1.489356  0.000320
C    -3.592908  0.378099  0.000068
Br    5.212447 -0.192238  0.000298
 total energy= -752.728335849

wb97xd.tddft-mecn--8
B    -2.032877  1.446037  0.000155
O    -2.212895  2.782588  0.000300
H    -1.346843  3.228413  0.000343
N    -0.690888  0.864909  0.000004
C     0.518056  1.602668 -0.000009
O     0.552604  2.828245 -0.000027
C     1.582388  0.606190 -0.000161
C     2.948917  0.764232 -0.000187
H     3.418043  1.742817 -0.000221
C     3.726284 -0.403012 -0.000075
C     3.147061 -1.702478  0.000004
H     3.801500 -2.566732  0.000005
C     1.778788 -1.853007 -0.000021
H     1.334155 -2.844532 -0.000035
C     0.968555 -0.690523 -0.000068
C    -0.428833 -0.501275 -0.000032
C    -1.487655 -1.454627 -0.000024
H    -1.236383 -2.511348 -0.000105
C    -2.814756 -1.024748 -0.000003
C    -3.957201 -1.853390 -0.000088
H    -3.982858 -2.938220 -0.000186
S    -5.393850 -0.937399 -0.000083
C    -4.515366  0.577869  0.000076
H    -5.069750  1.510058  0.000111
C    -3.169320  0.390728  0.000082
N     5.152974 -0.276191  0.000024
O     5.646003  0.851919 -0.000546
O     5.830789 -1.303383  0.000706
 total energy= -944.590606801

wb97xd.tddft-mecn--8-
B    -1.992571  1.441415  0.000311
O    -2.082770  2.747627 -0.000125
N    -0.692449  0.800280 -0.000081
C     0.479661  1.558501 -0.000353
O     0.475317  2.801598 -0.000082
C     1.546665  0.584218 -0.000275
C     2.929348  0.765186 -0.000163
H     3.376216  1.754316 -0.000085
C     3.720368 -0.370580 -0.000081
C     3.173524 -1.687773 -0.000189
H     3.846946 -2.537187 -0.000108
C     1.809695 -1.860674 -0.000309
H     1.388753 -2.863592 -0.000308
C     0.965877 -0.727497 -0.000306
C    -0.455421 -0.581927 -0.000200
C    -1.502273 -1.483529 -0.000087
H    -1.294765 -2.549764 -0.000148
C    -2.857810 -1.011344  0.000036
C    -4.011301 -1.777795  0.000034
H    -4.095046 -2.858877 -0.000043
S    -5.442144 -0.799153  0.000182
C    -4.517166  0.661184  0.000155
H    -5.022864  1.620338  0.000229
C    -3.171673  0.409949  0.000163
N     5.154722 -0.210371  0.000228
O     5.624422  0.922631  0.000422
O     5.851162 -1.219700  0.000339
 total energy= -944.086475697

wb97xd.tddft-mecn--9
B     1.413067  1.437670  0.000145
O     1.553569  2.789382  0.000515
H     0.652738  3.173043  0.000316
N     0.094360  0.839405 -0.000303
C    -1.125680  1.557362 -0.000291
O    -1.172971  2.804964 -0.000368
```

```
C    -2.162793  0.561166 -0.000167
C    -3.546676  0.681538 -0.000168
H    -4.036773  1.652824 -0.000389
C    -4.325860 -0.498405  0.000102
C    -3.696673 -1.799946  0.000406
H    -4.332542 -2.681696  0.000706
C    -2.333343 -1.914032  0.000320
H    -1.864900 -2.895497  0.000523
C    -1.536019 -0.739929 -0.000025
C    -0.142068 -0.546046 -0.000181
C     0.912872 -1.473367 -0.000273
H     0.683533 -2.535365 -0.000418
C     2.250017 -1.017909 -0.000119
C     3.401390 -1.811089 -0.000335
H     3.465035 -2.893618 -0.000579
S     4.824359 -0.851497 -0.000013
C     3.918987  0.628584  0.000364
H     4.446656  1.576164  0.000686
C     2.568962  0.407772  0.000240
N    -5.670093 -0.428976 -0.000067
H    -6.145219  0.462632  0.000160
H    -6.236954 -1.264840  0.000651
 total energy= -795.500811821
```