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

Synthesis and Characterization of Chiral and Achiral Diamines Containing One or Two BODIPY Molecules

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Supporting Information

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1) Multinuclear NMR for Boen

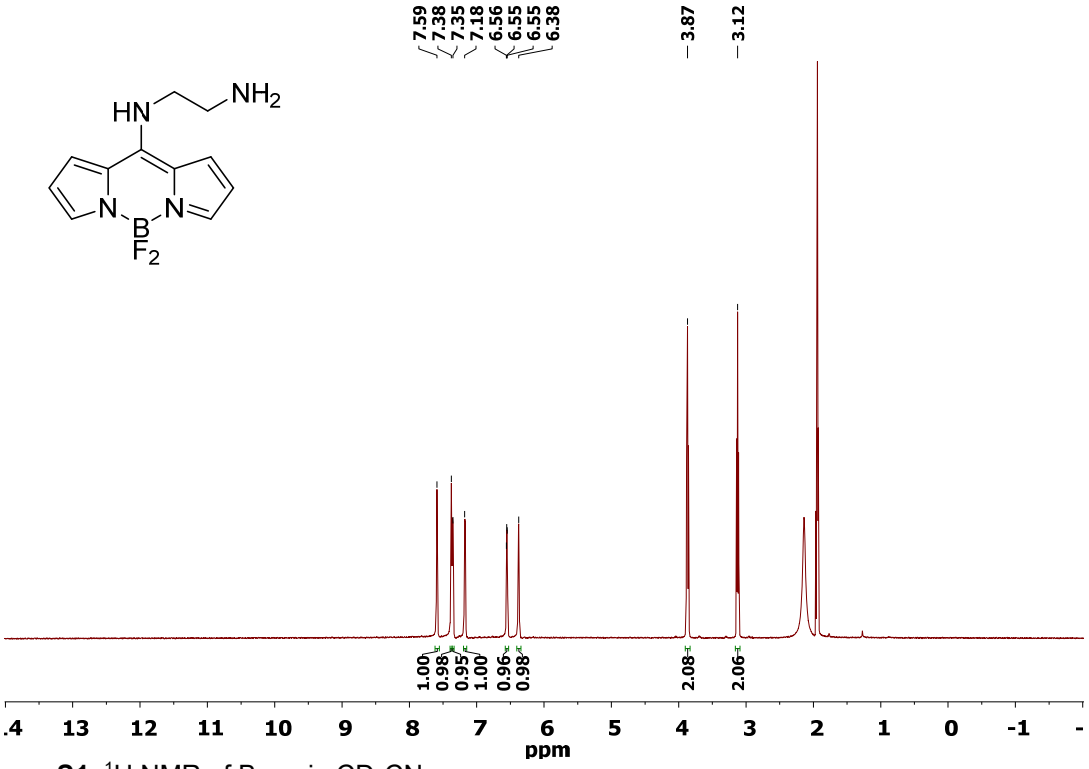

Figure S1. ^{1}H NMR of Boen in CD_3CN.

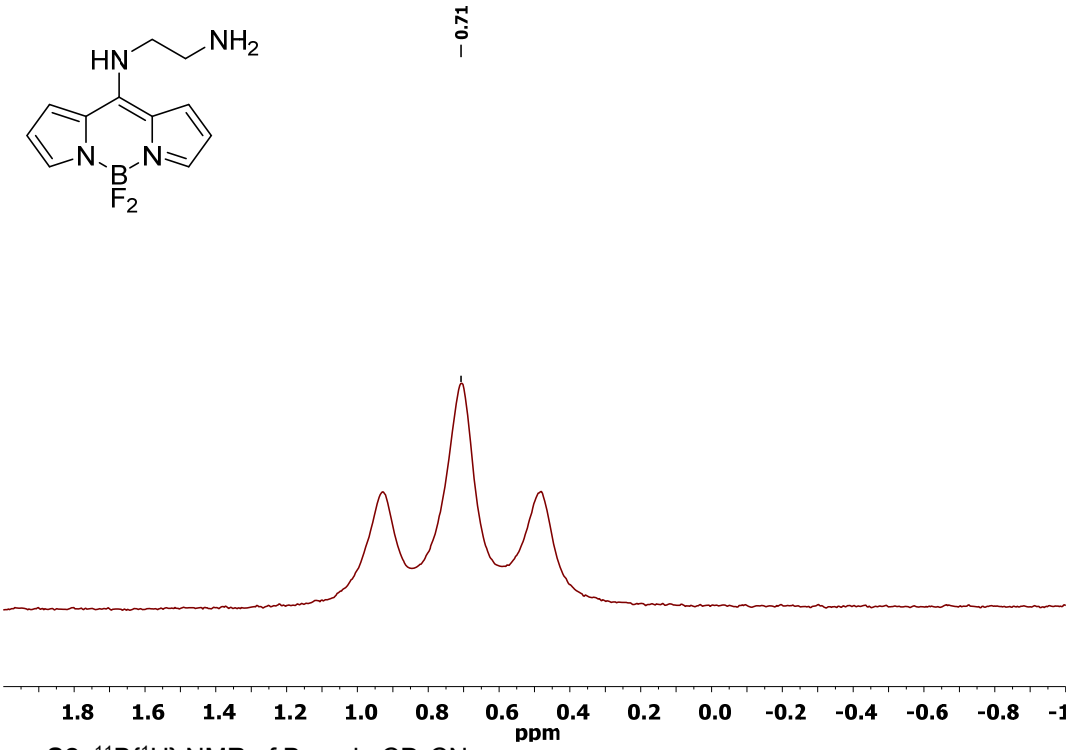

Figure S2. $^{11}B\{^{1}H\}$ NMR of Boen in CD_3CN.

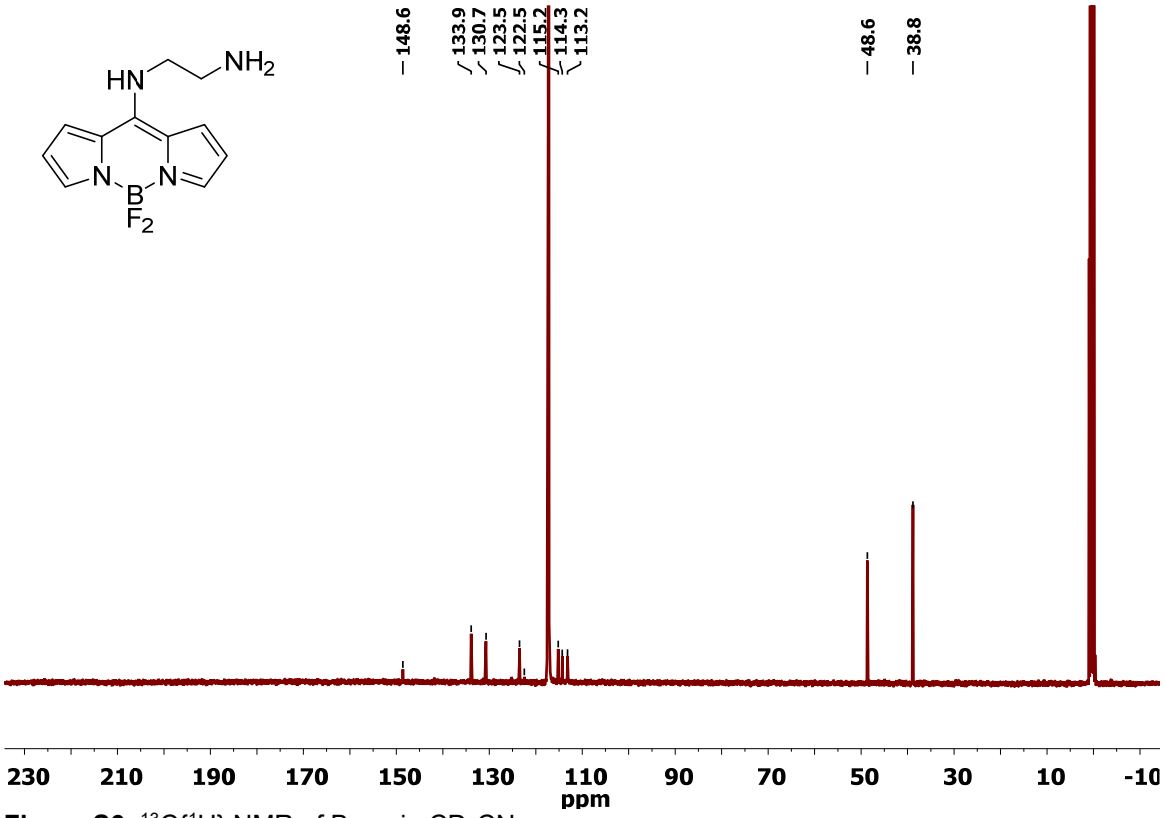

Figure S3. $^{13}C\{^{1}H\}$ NMR of Boen in CD_3CN.

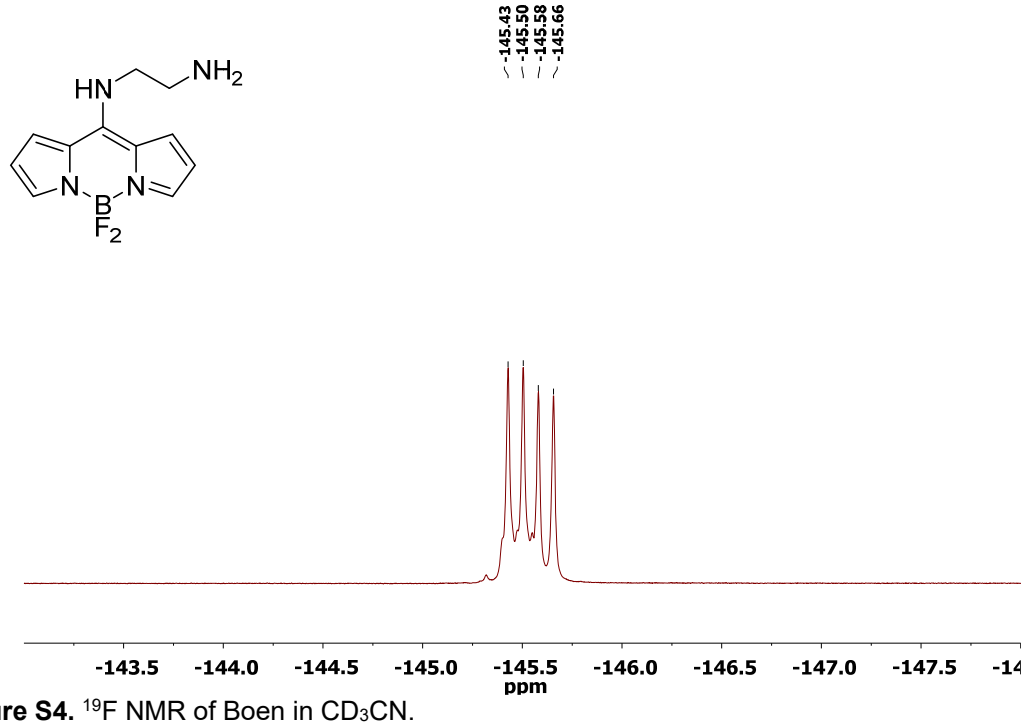

Figure S4. ^{19}F NMR of Boen in CD_3CN.

2) Multinuclear NMR for Bophen

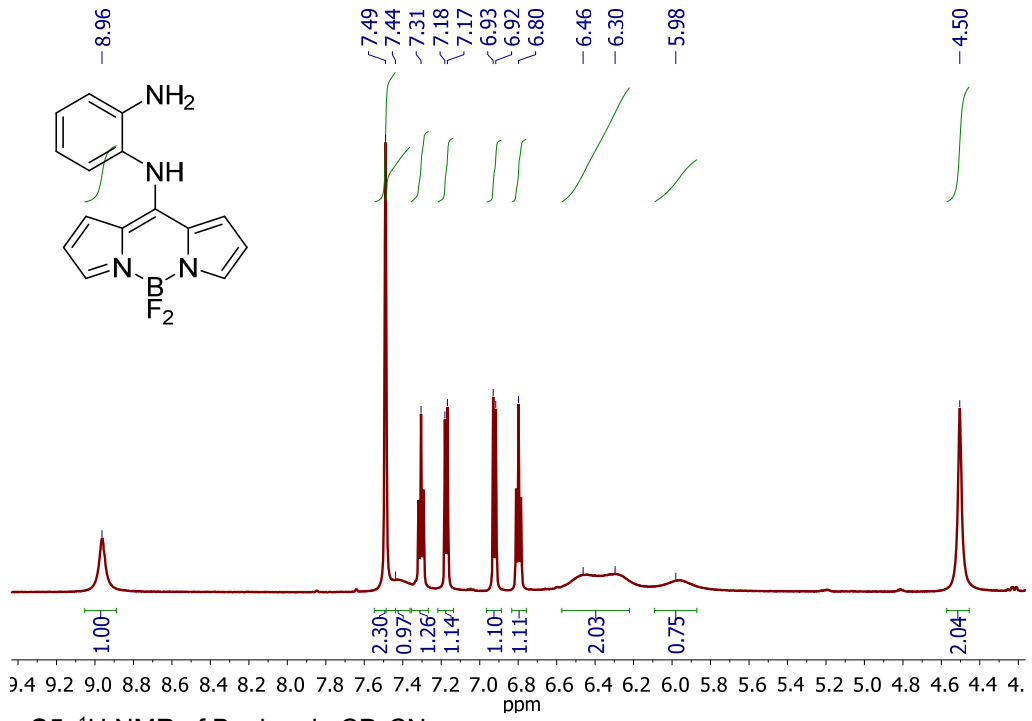

Figure S5. ^{1}H NMR of Bophen in CD_3CN.

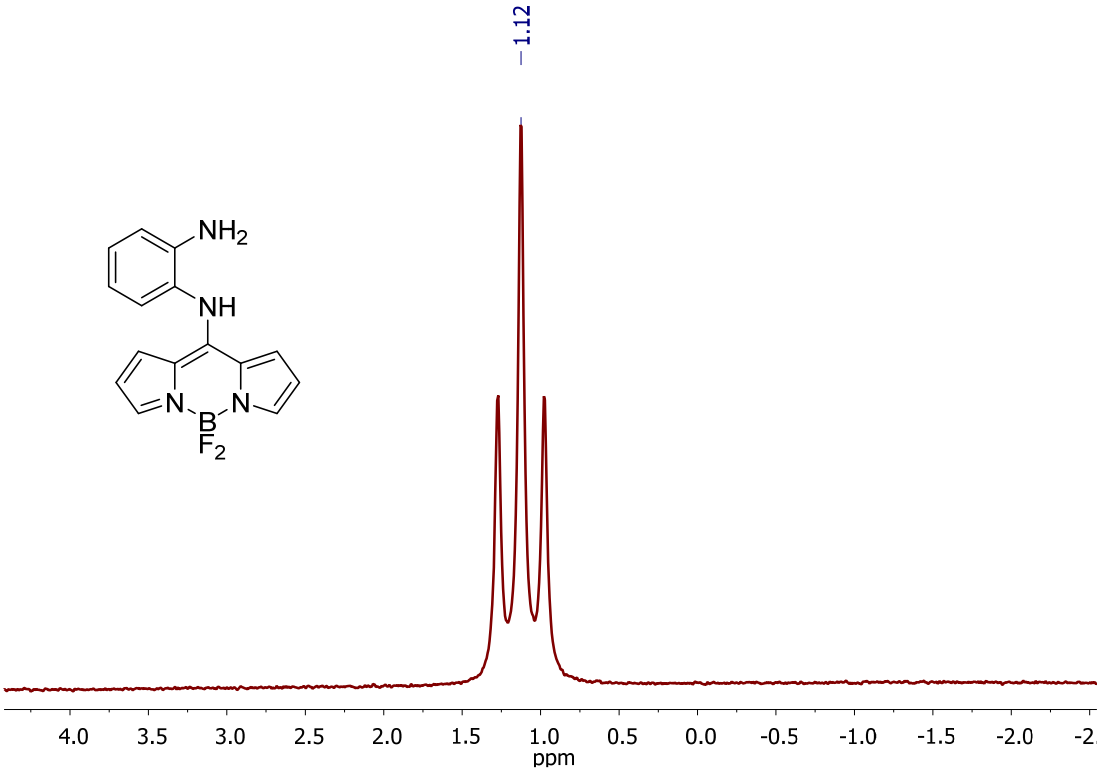

Figure S6. $^{11}B\{^{1}H\}$ NMR of Bophen in CD_3CN.

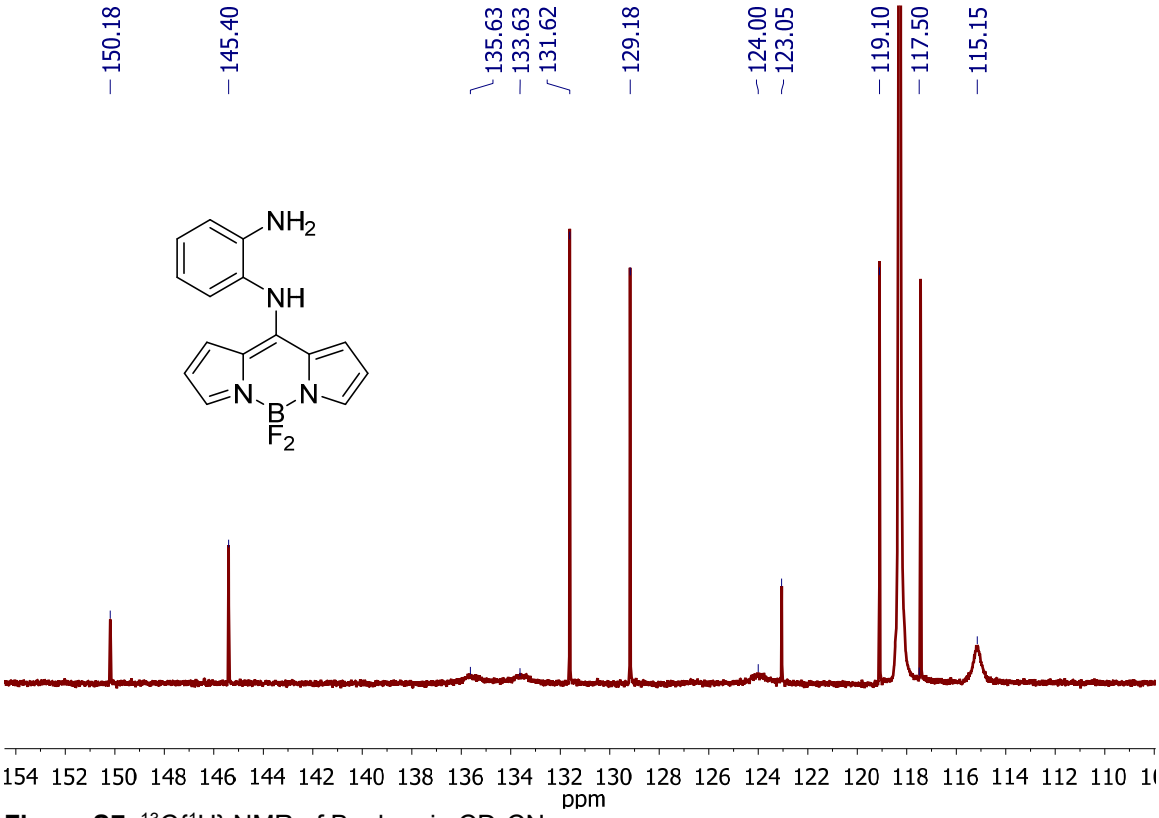

Figure S7. $^{13}C\{^{1}H\}$ NMR of Bophen in CD_3CN.

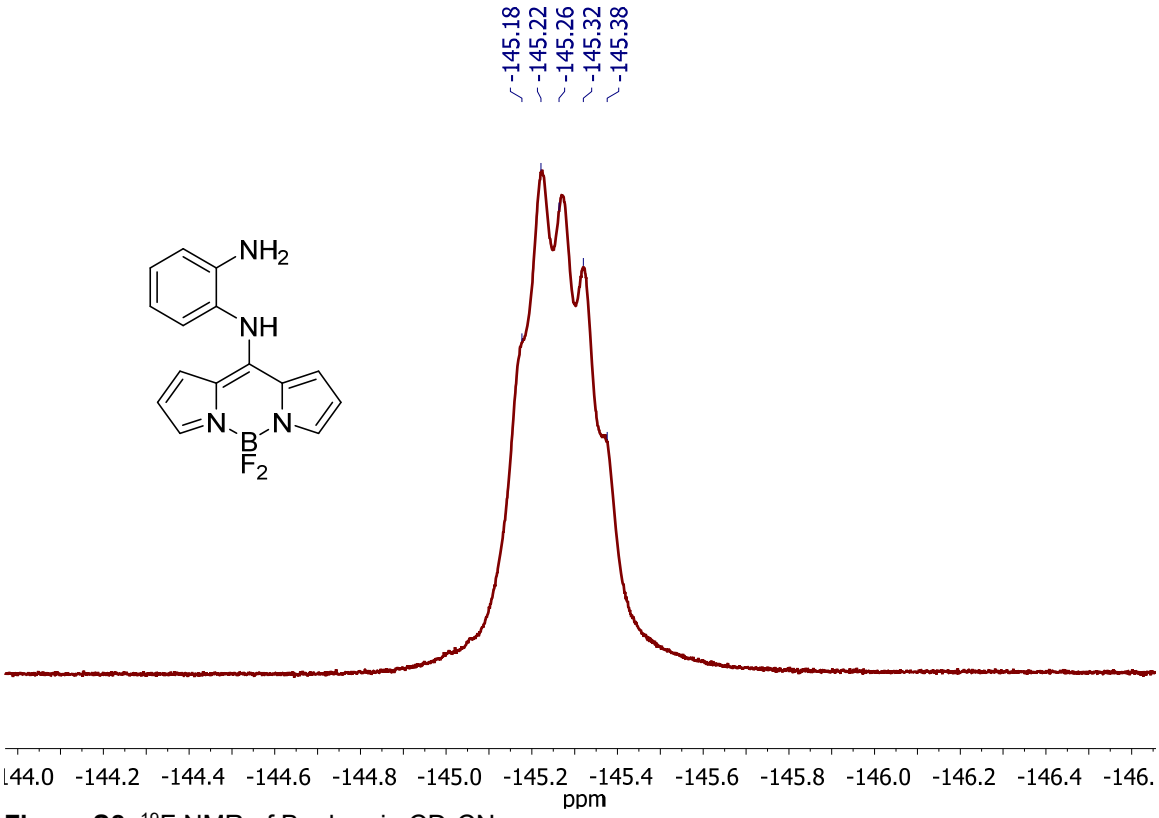

Figure S8. ^{19}F NMR of Bophen in CD_3CN.

3) Multinuclear NMR for Bodach

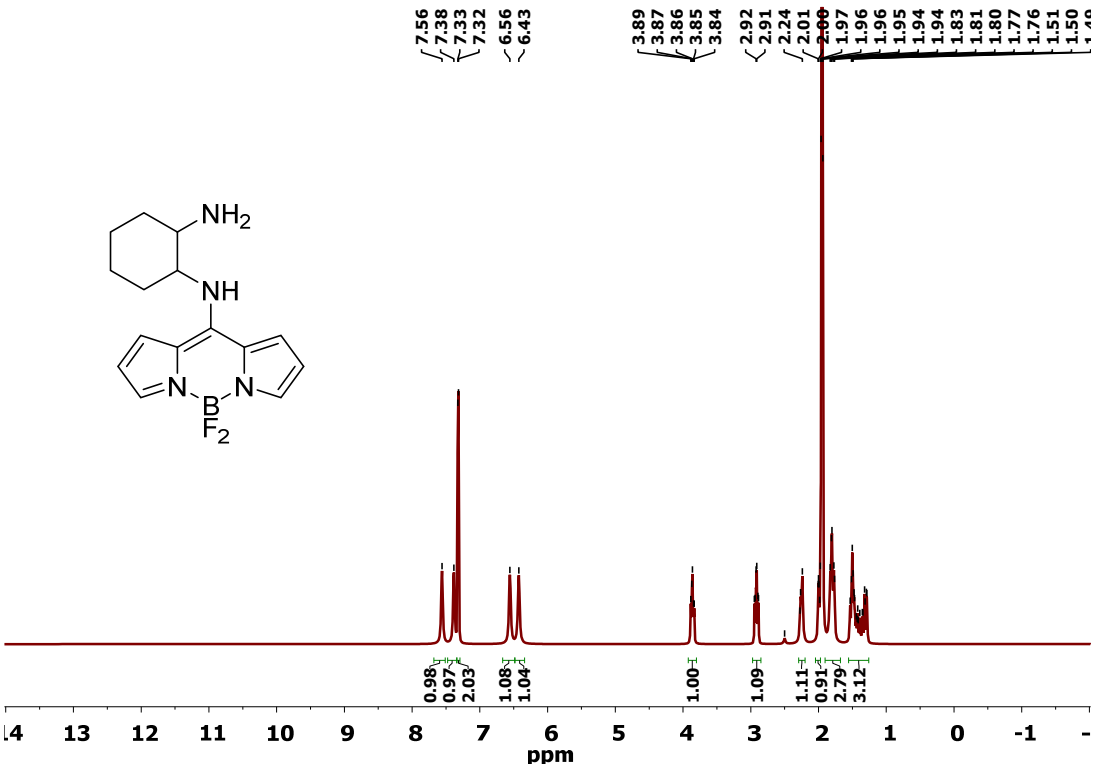

Figure S9. ^{1}H NMR of Bodach in CD_3CN.

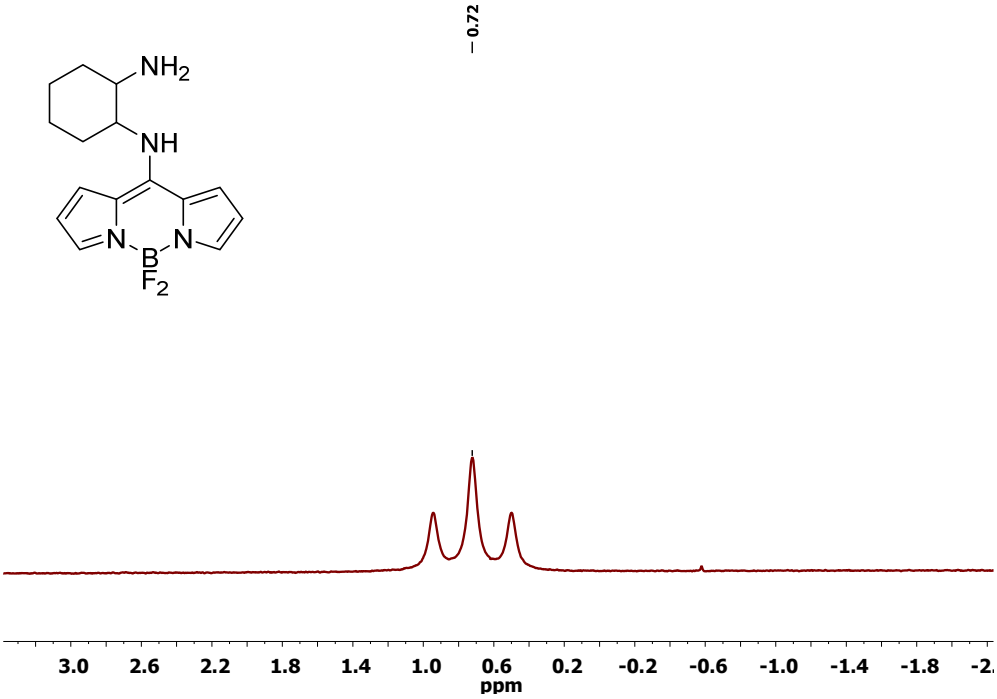

Figure S10. $^{11}B\{^{1}H\}$ NMR of Bodach in CD_3CN.

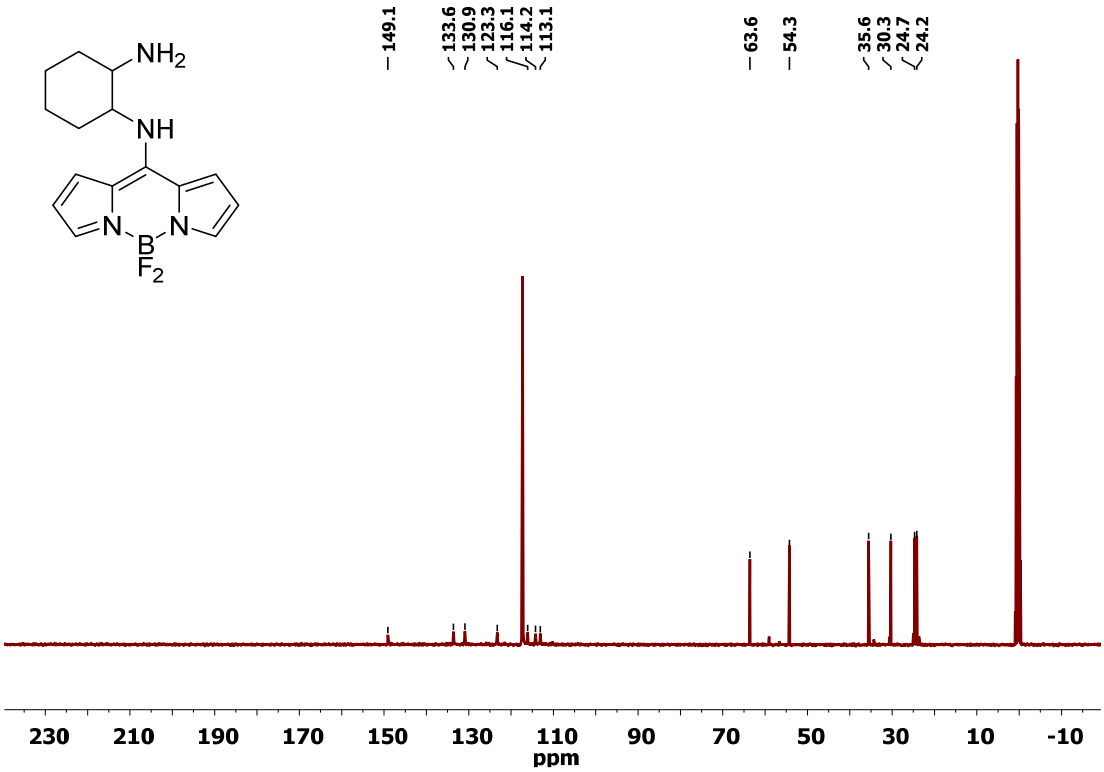

Figure S11. $^{13}C\{^{1}H\}$ NMR of Bodach in CD_3CN.

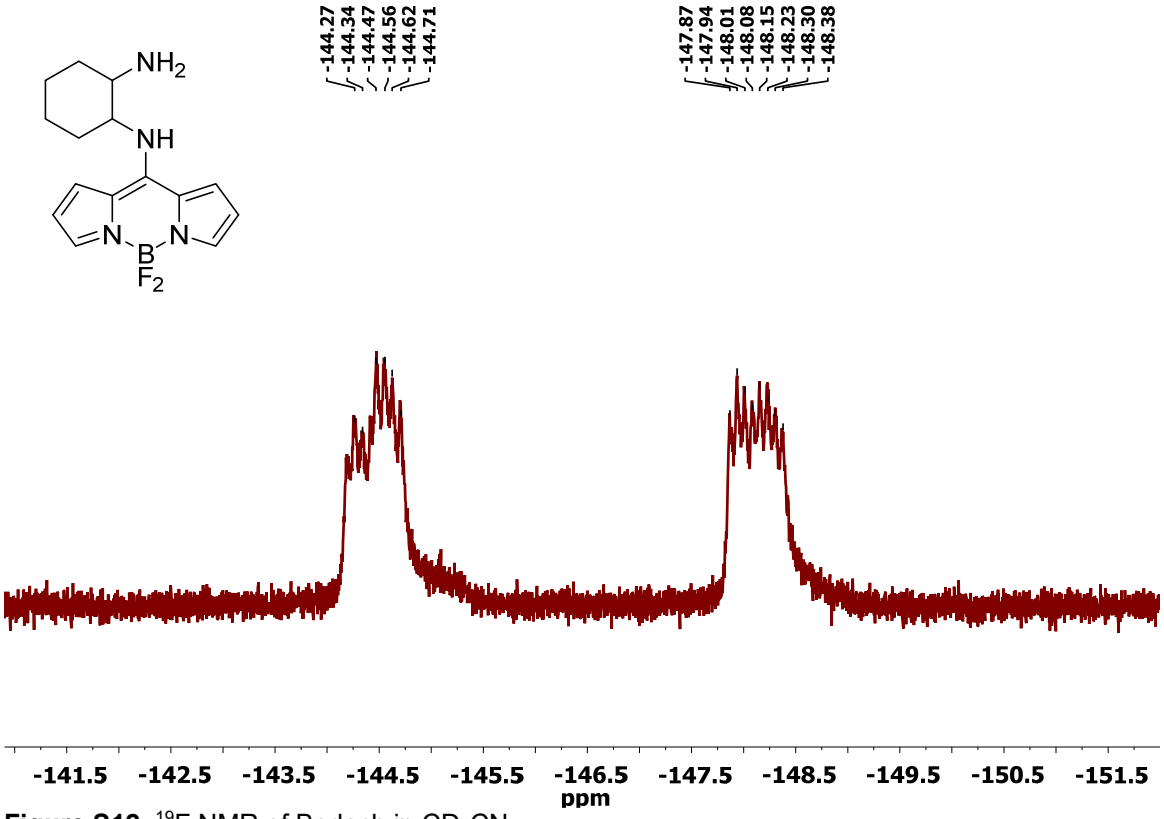

Figure S12. ^{19}F NMR of Bodach in CD_3CN.

4) Multinuclear NMR for Bodpen

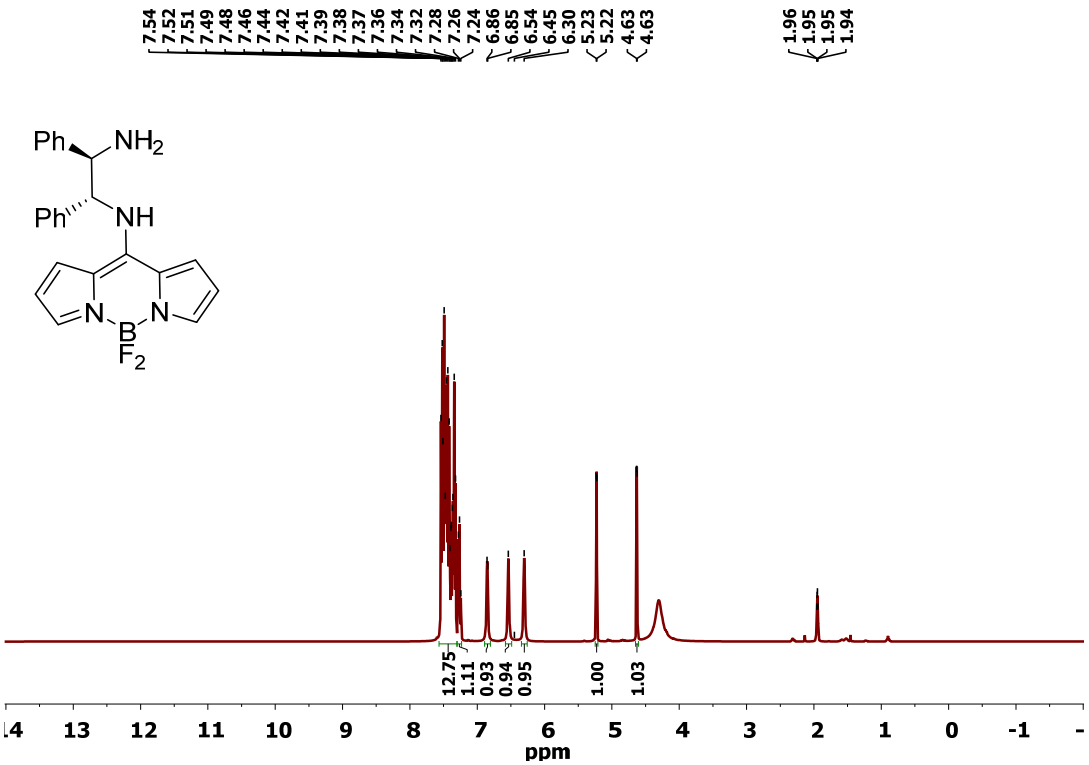

Figure S13. ^{1}H NMR of Bodpen in CD_3CN.

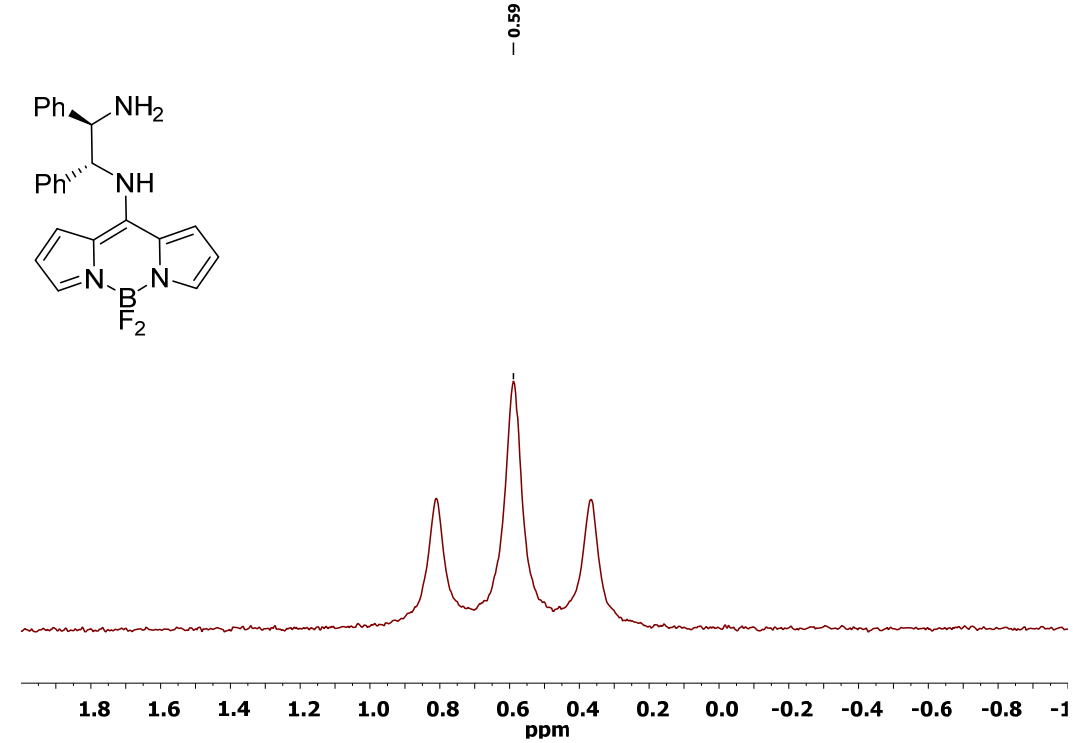

Figure S14. $^{11}B\{^{1}H\}$ NMR of Bodpen in CD_3CN.

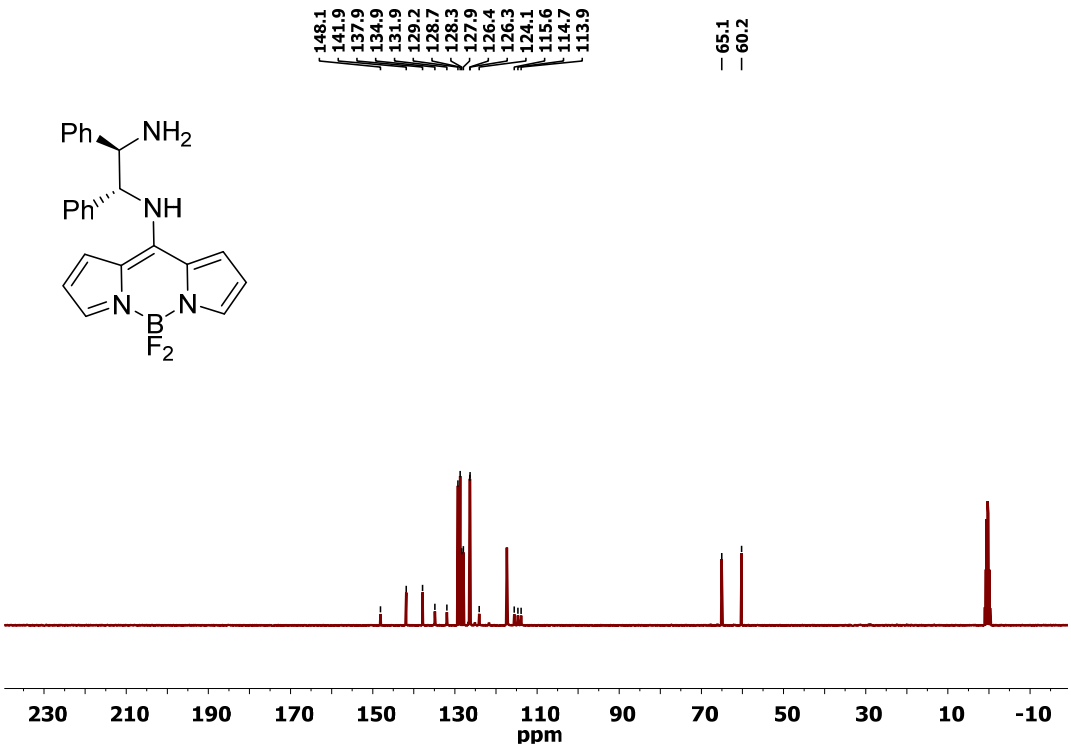

Figure S15. $^{13}C\{^{1}H\}$ NMR of Bodpen in CD_3CN.

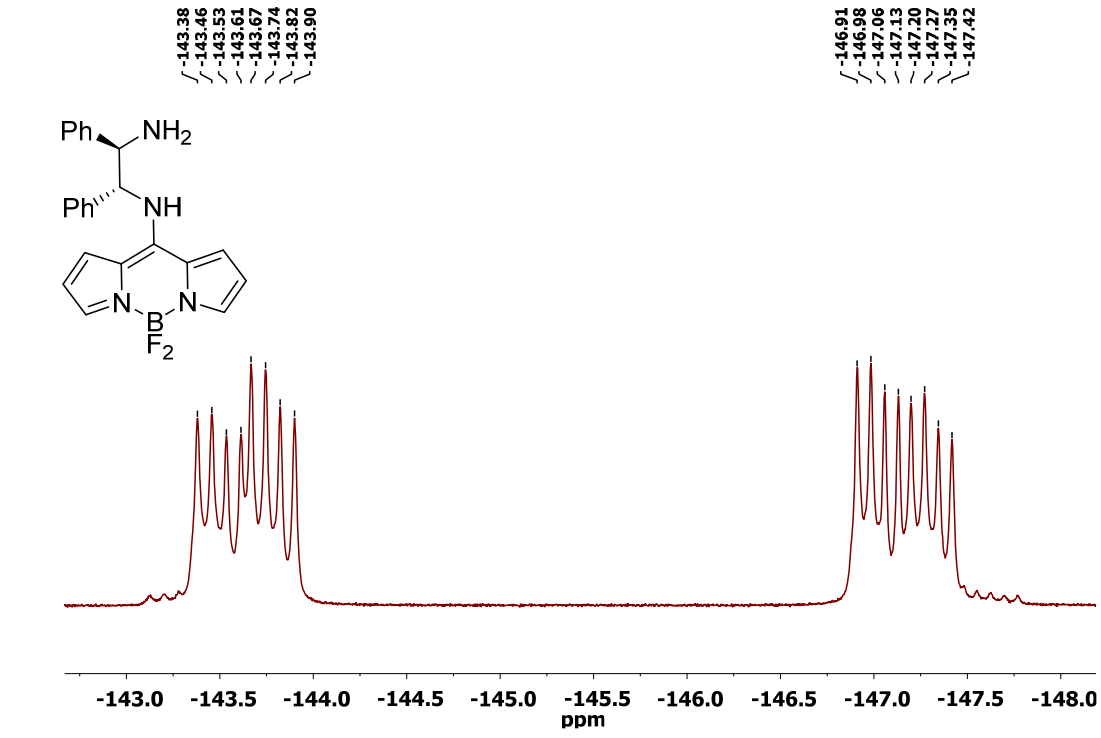

Figure S16. ^{19}F NMR of Bodpen in CD_3CN.

5) Multinuclear NMR for Bo$_2$en

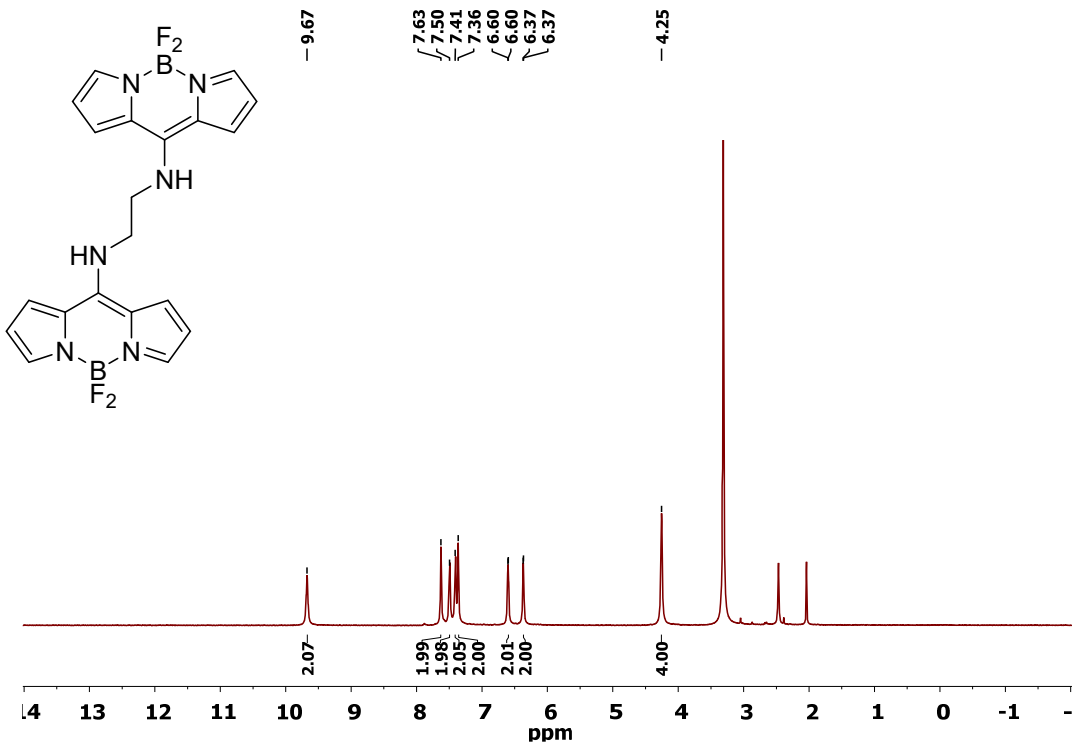

Figure S17. ^{1}H NMR of Bo$_2$en in DMSO-d_6.

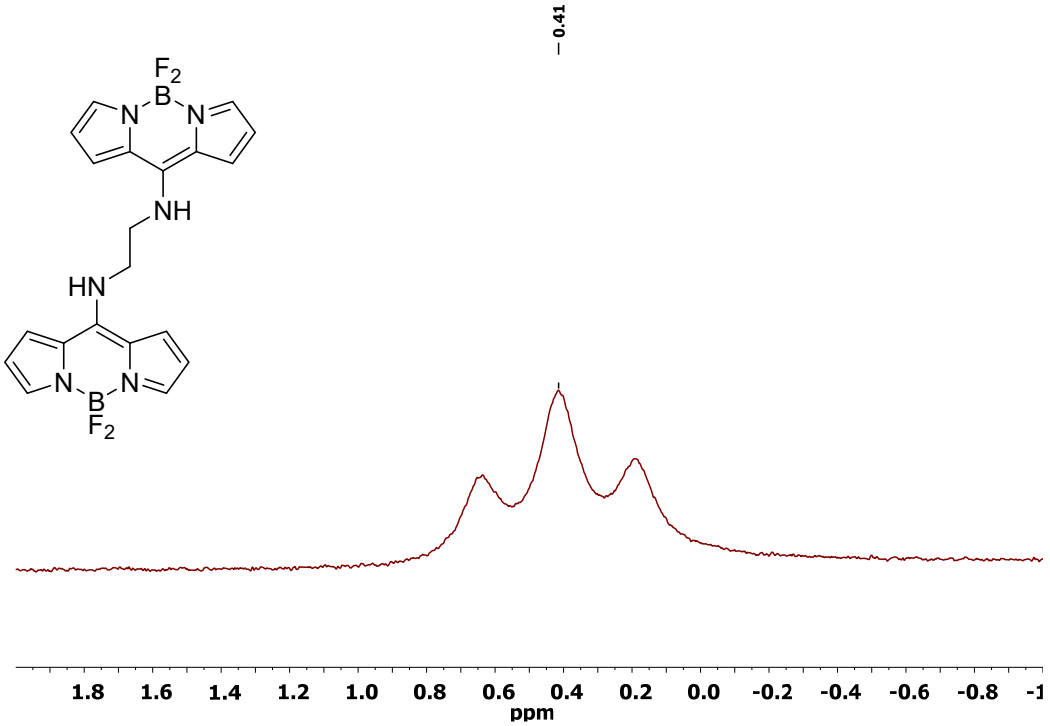

Figure S18. ^{11}B{^{1}H} NMR of Bo$_2$en in DMSO-d_6.

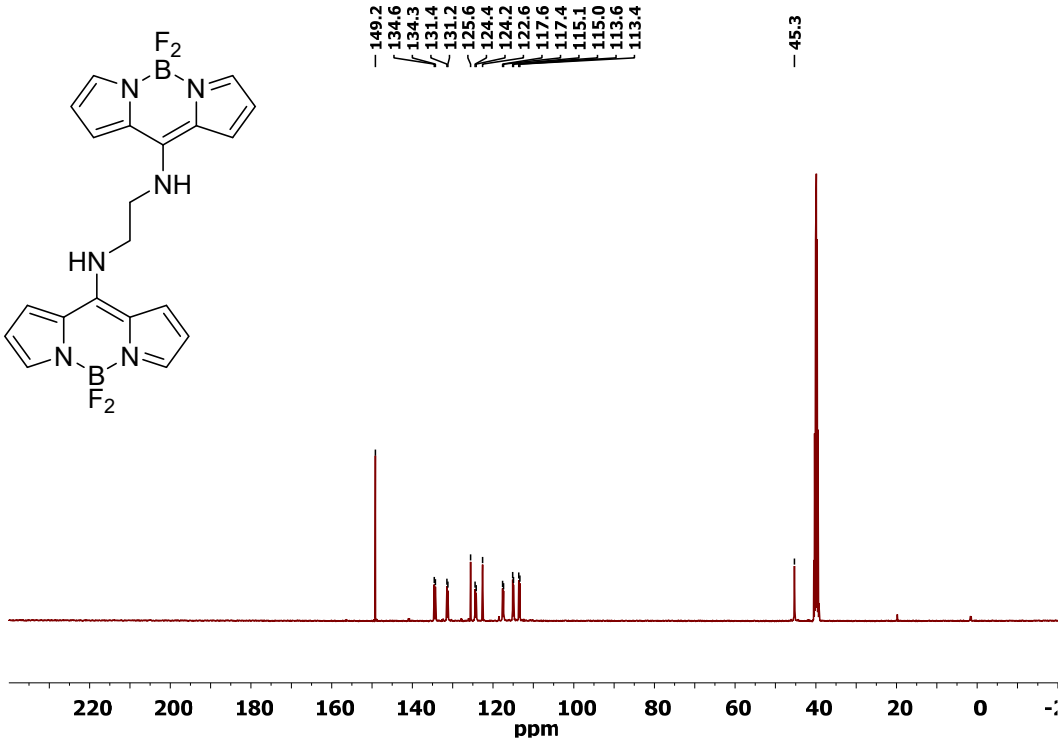

Figure S19. $^{13}C\{^{1}H\}$ NMR of Bo_2en in DMSO-d_6.

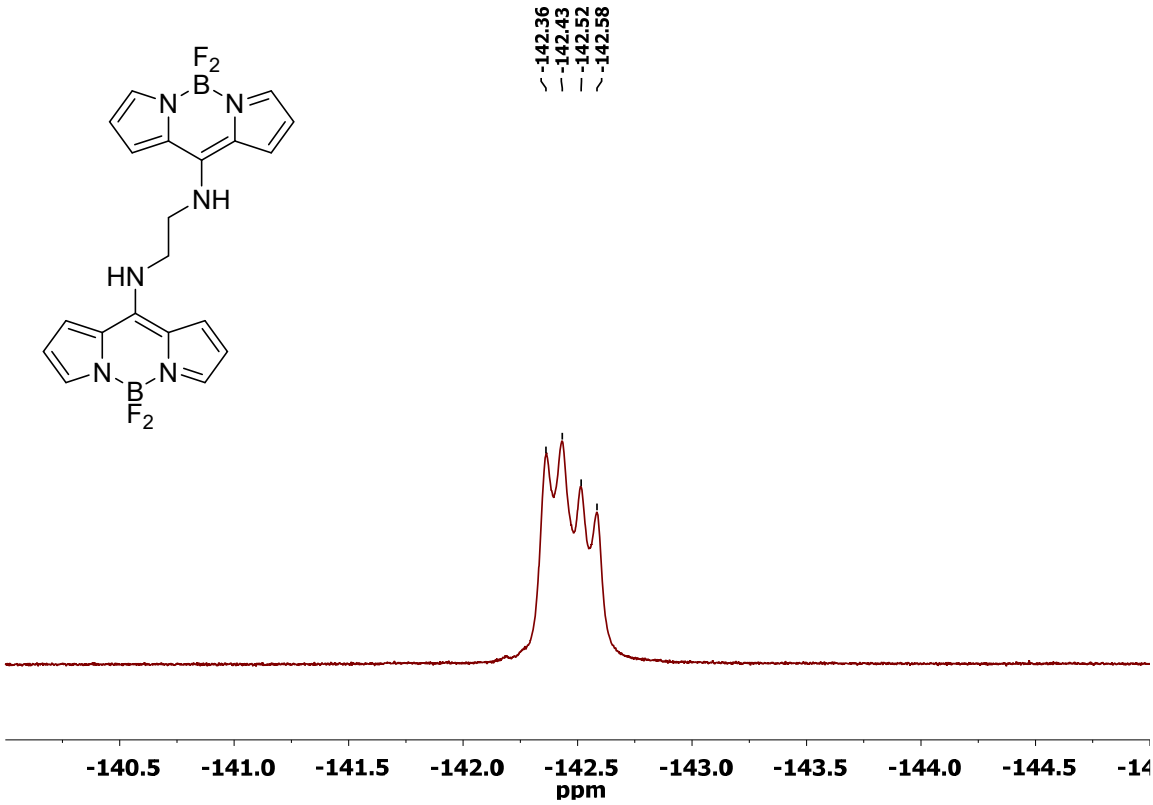

Figure S20. ^{19}F NMR of Bo_2en in DMSO-d_6.

6) Multinuclear NMR for Bo$_2$dach

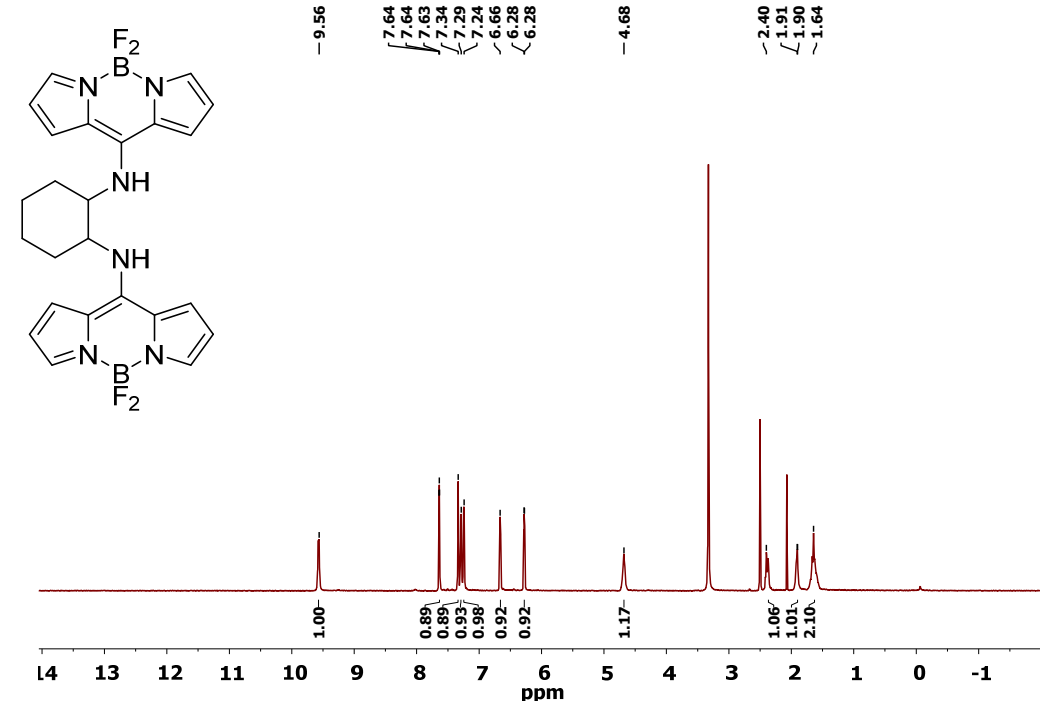

Figure S21. ^{1}H NMR of Bo$_2$dach in DMSO-d_6.

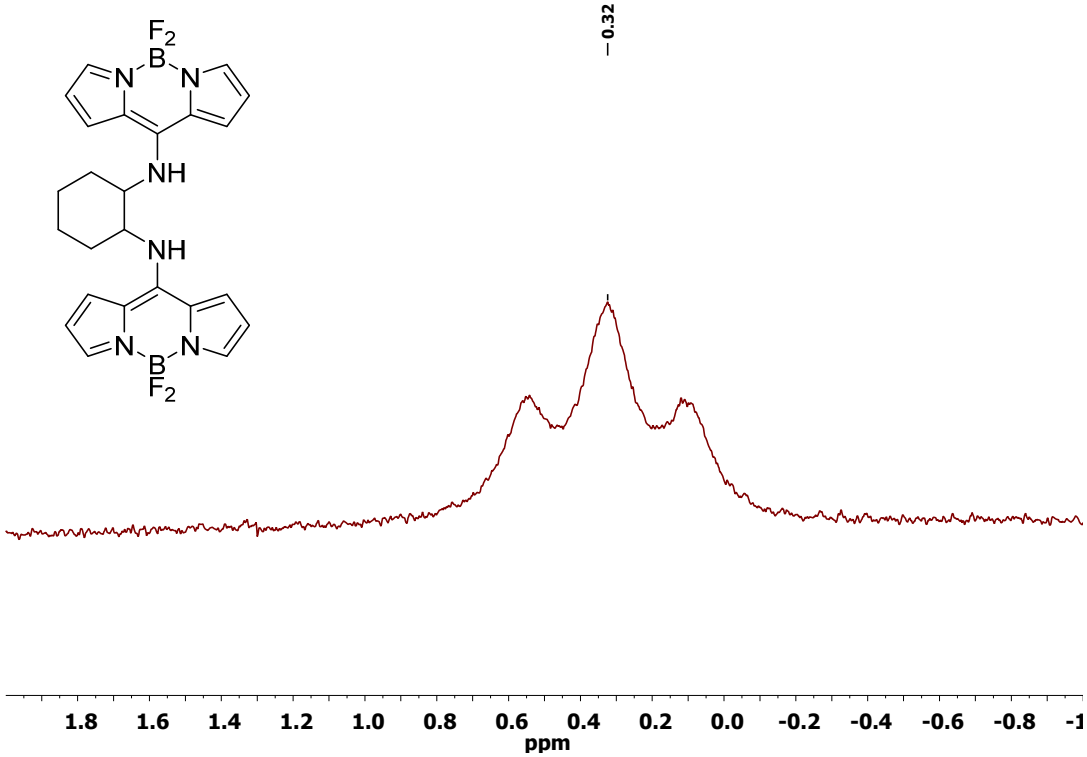

Figure S22. ^{11}B{^{1}H} NMR of Bo$_2$dach in DMSO-d_6.

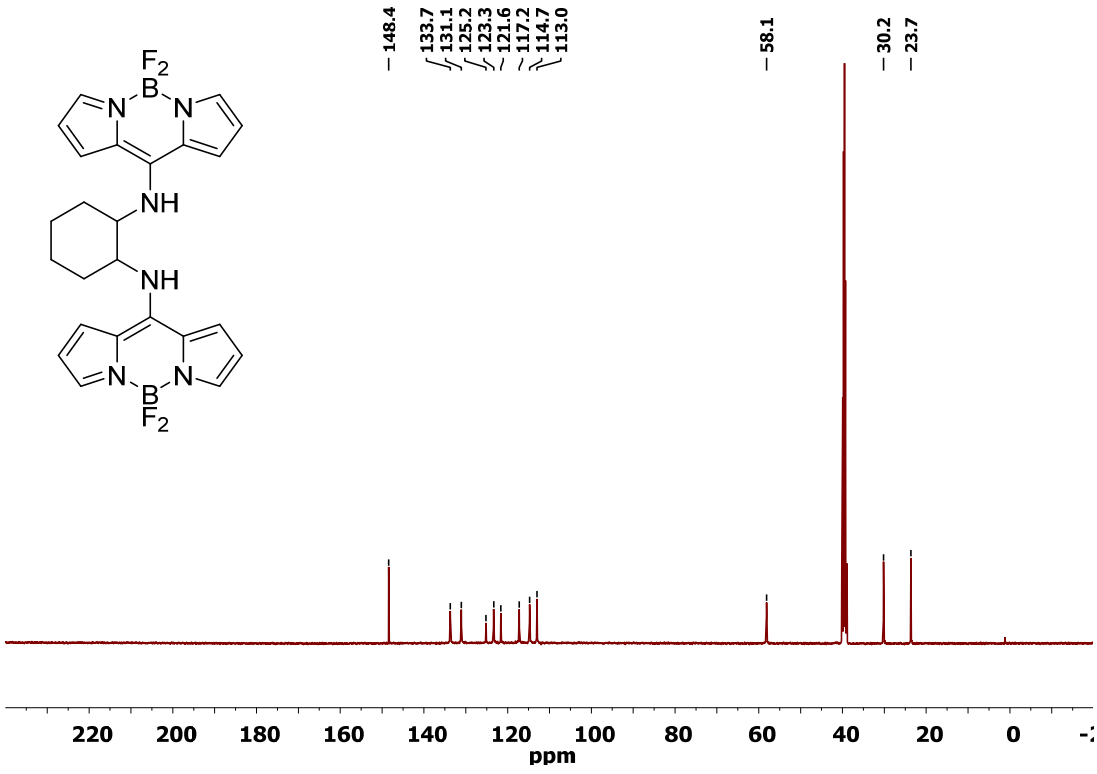

Figure S23. $^{13}C\{^{1}H\}$ NMR of Bo_2dach in DMSO-d_6.

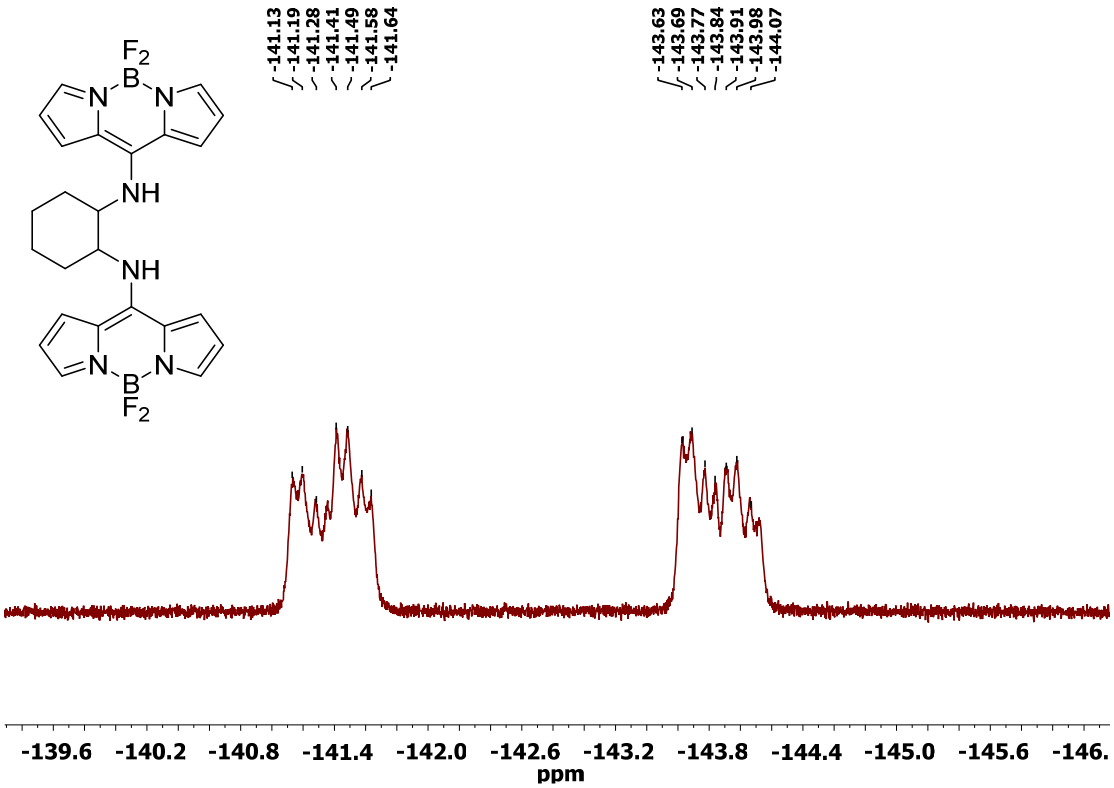

Figure S24. ^{19}F NMR of Bo_2dach in DMSO-d_6.

7) Multinuclear NMR for Bo$_2$dpen

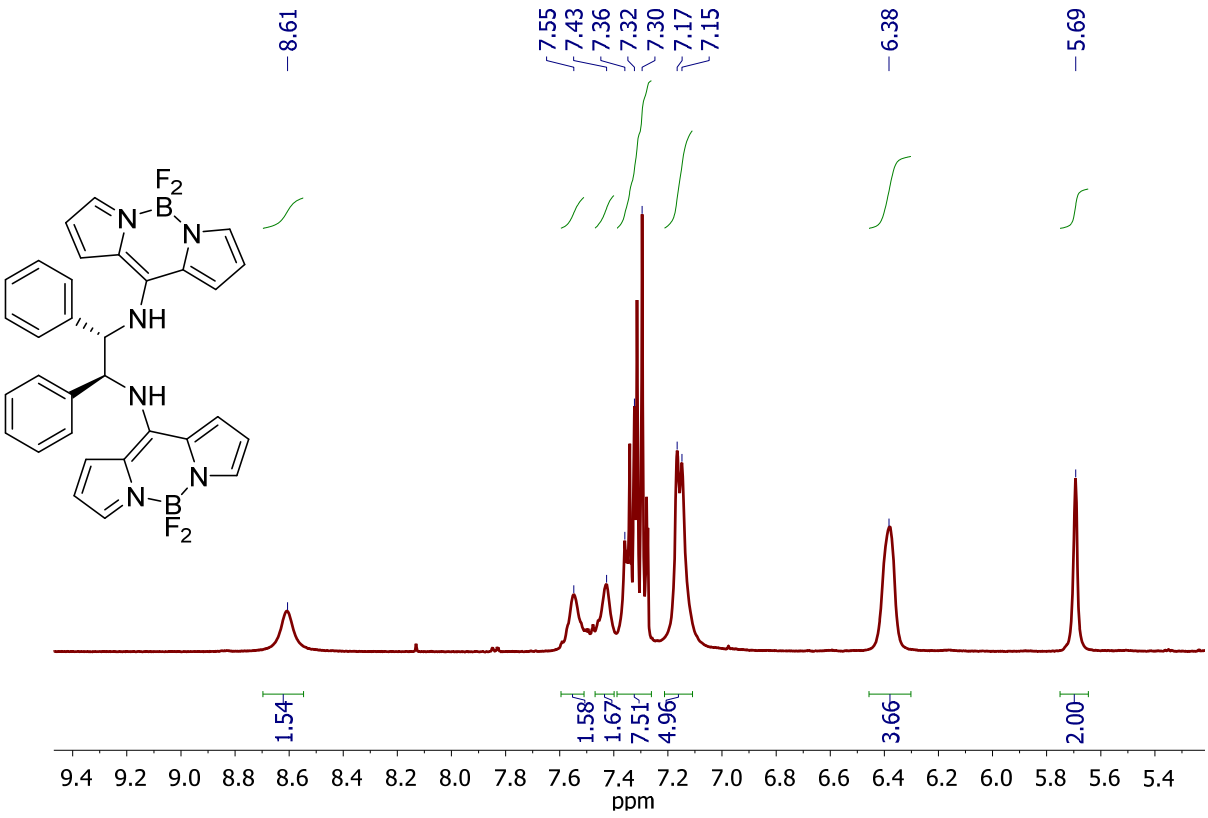

Figure S25. ^{1}H NMR of Bo$_2$dpen in CD$_3$CN.

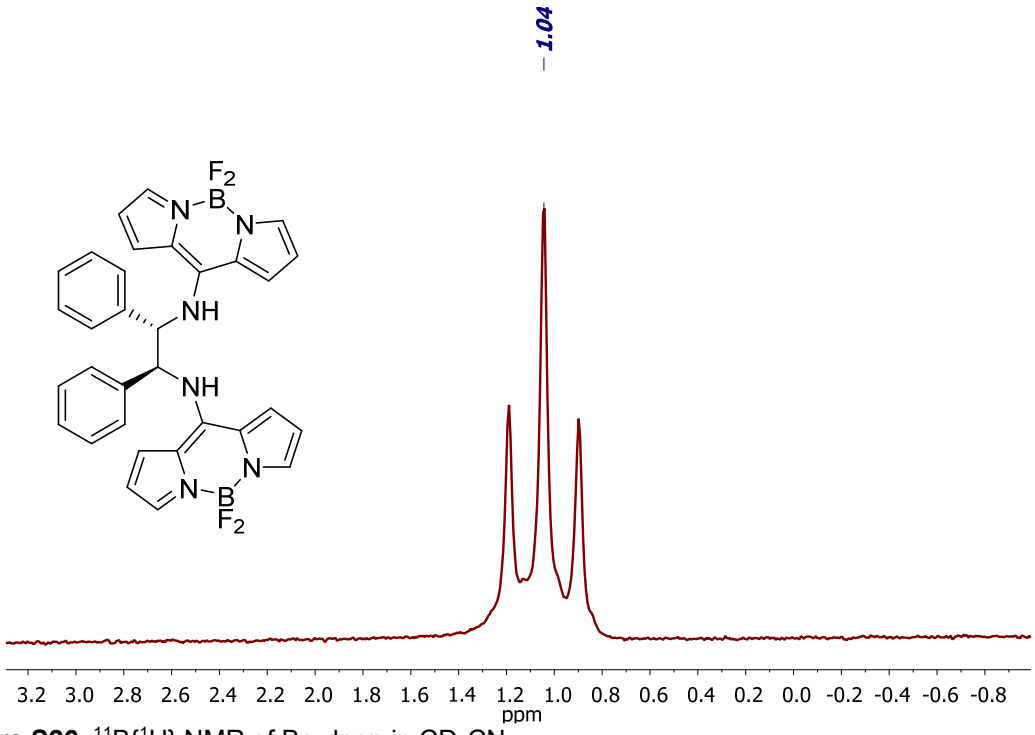

Figure S26. ^{11}B{^{1}H} NMR of Bo$_2$dpen in CD$_3$CN.

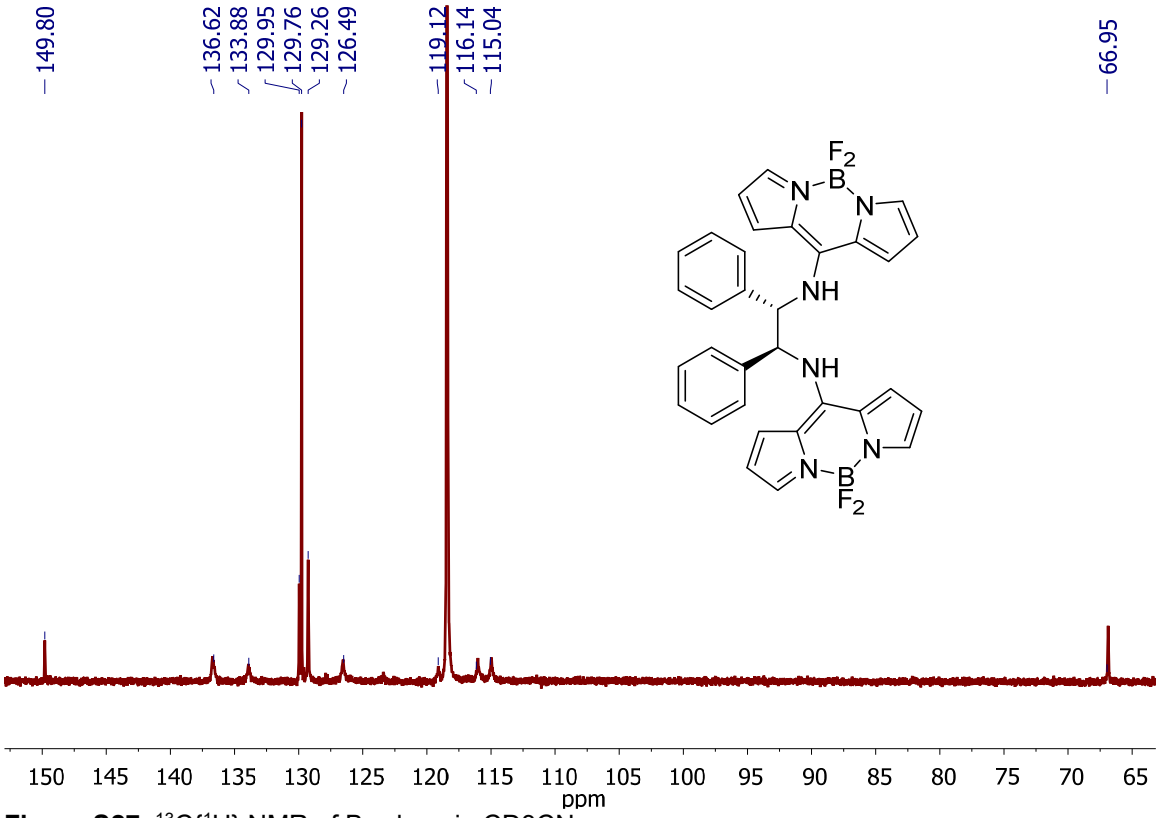

Figure S27. $^{13}C\{^{1}H\}$ NMR of Bo_2dpen in CD3CN.

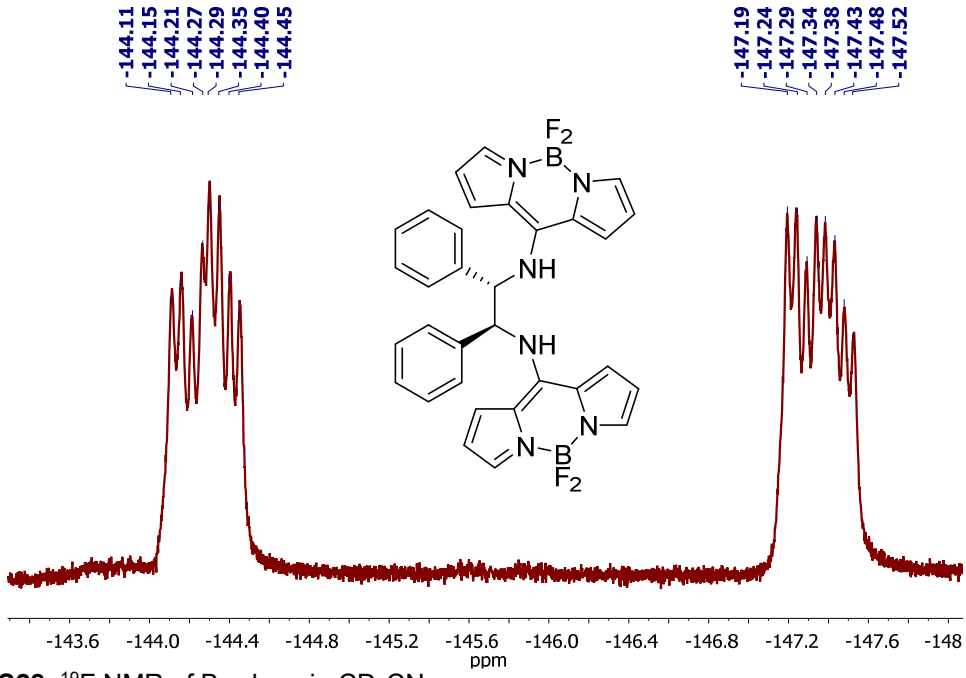

Figure S28. ^{19}F NMR of Bo_2dpen in CD_3CN.

8) Fluorescence and Emission Spectra of Diamines Containing One BODIPY Molecule

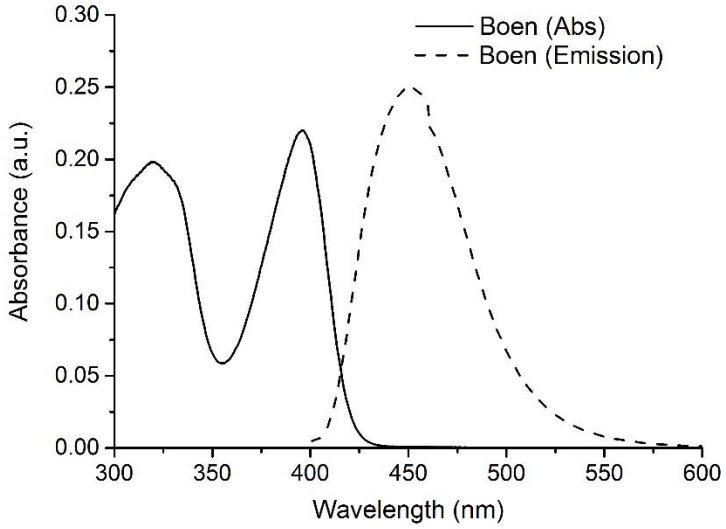

Figure S29. Normalized absorbance and emission spectra of Boen in DMSO.

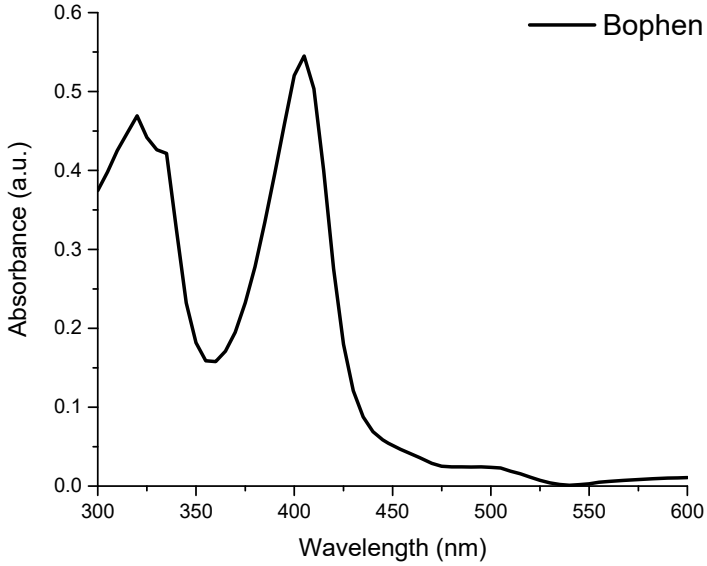

Figure S30. Normalized absorption of Bophen in DMSO. Bophen does not fluoresce.

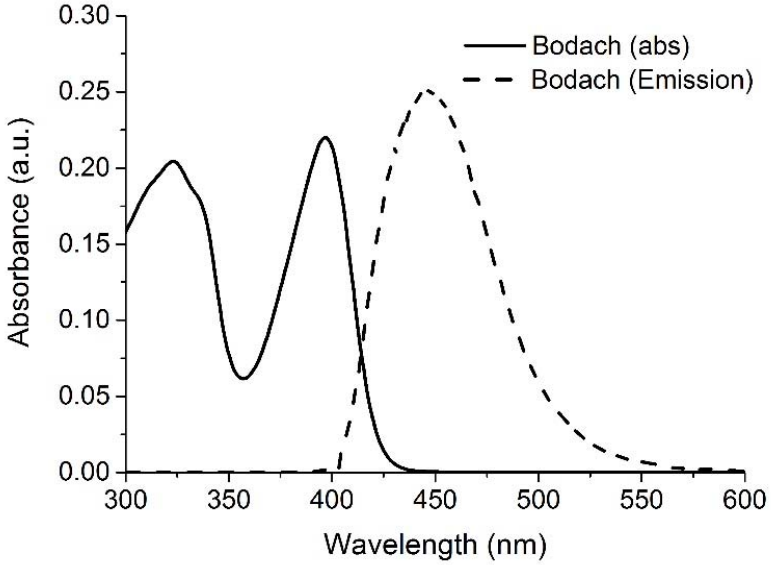

Figure S31. Normalized absorption and emission spectra of Bodach in DMSO.

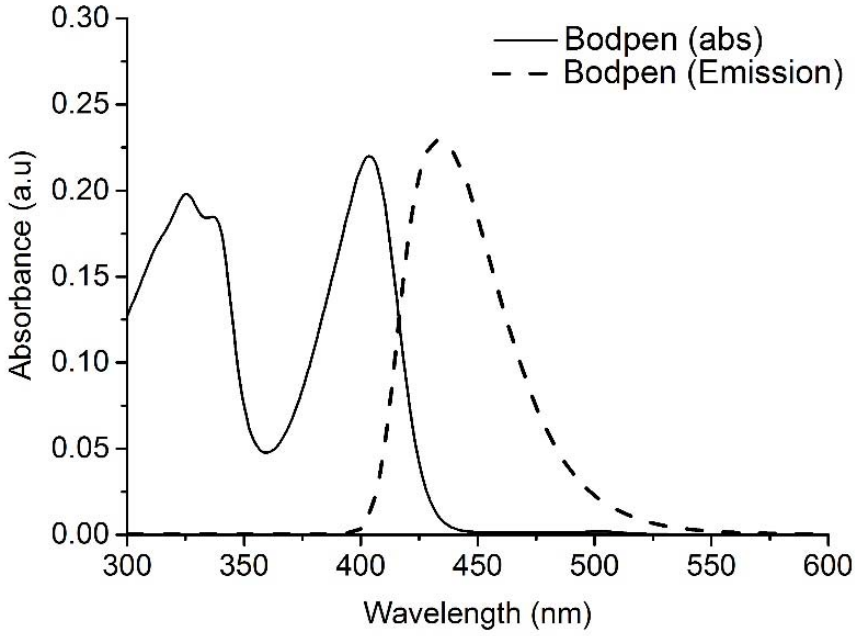

Figure S32. Normalized absorption and emission spectra of Bodpen in DMSO.

9) Fluorescence and Emission Spectra of Diamines Containing Two BODIPY Molecules

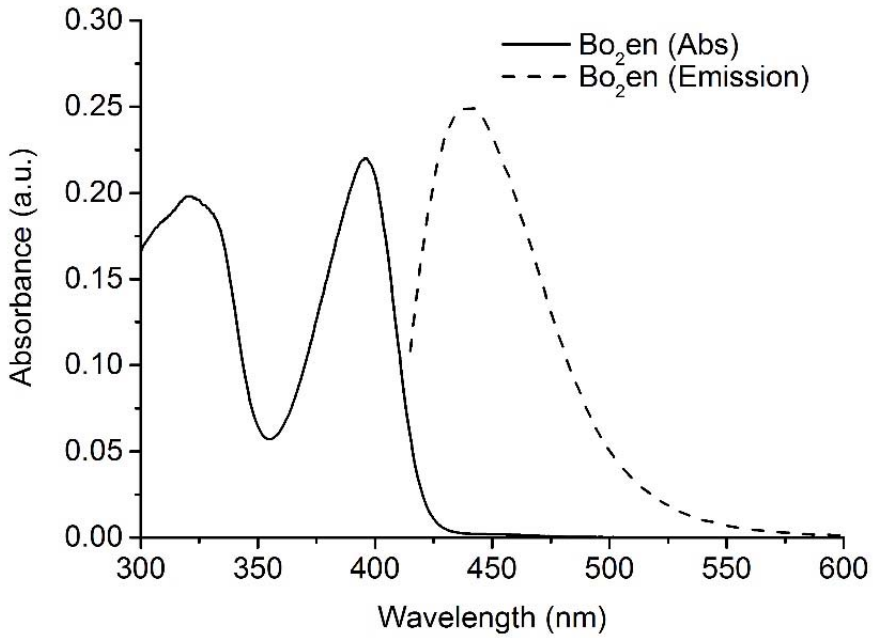

Figure S33. Normalized absorption and emission spectra of Bo_2en in DMSO.

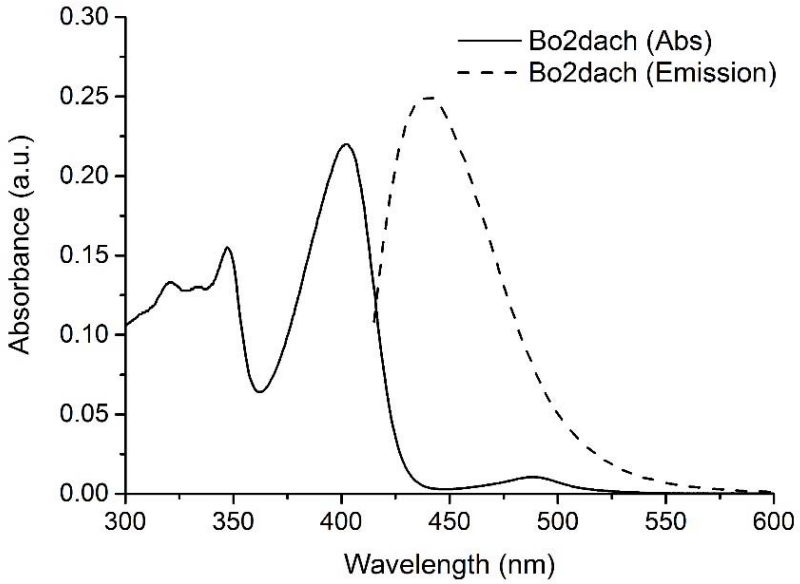

Figure S34. Normalized absorption and emission spectra of Bo_2dach in DMSO.

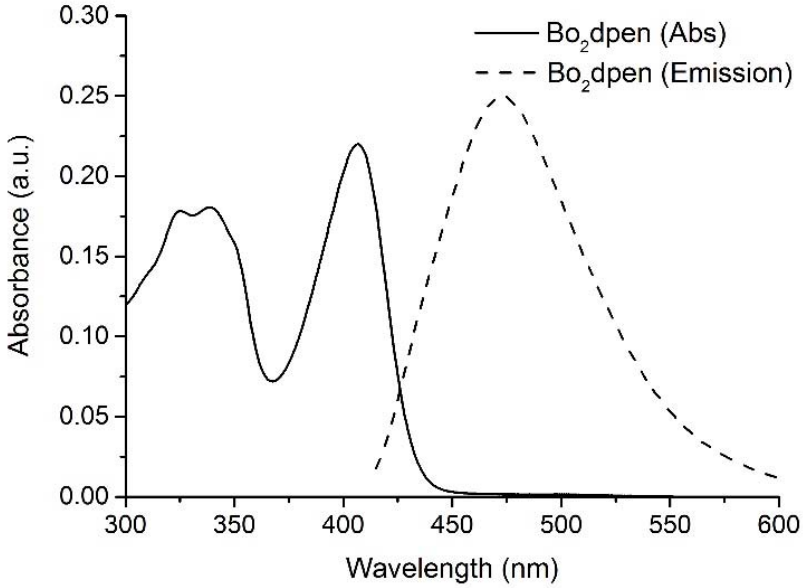

Figure S35. Normalized absorption and emission spectra of Bo_2dpen in DMSO.

10) Comparison of the Absorbance Spectra of Diamines Containing One and Two BODIPY Molecules

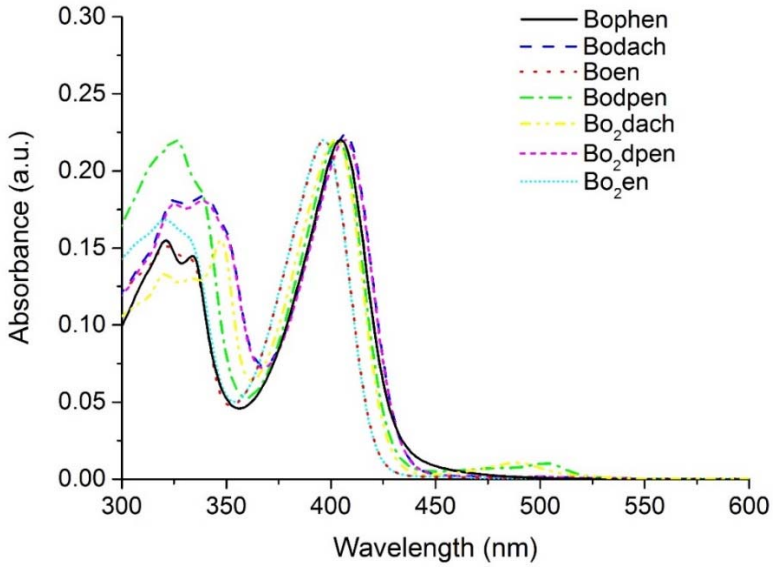

Figure S36. Normalized absorption spectra of the mono and bis-substituted BODIPY diamine ligands in DMSO.

11) Sample Quantum Yield Calculation for BoSMe

To determine the quantum yields of the BODIPY-appended diamines the following procedure was followed. Approximately 3.00 mg of the BODIPY-appended diamine was massed out and dissolved in dimethyl sulfoxide (DMSO). Due to the fact that the diamines containing two BODIPY fragments only dissolved in DMSO, DMSO was employed as the solvent for all of the quantum yield measurements. Approximately 3.00 mg of Rhodamine 6G (quantum yield = 0.98 in MeOH)[1] was also massed, dissolved in methanol, and used as the quantum yield standard for the comparative method. A series of five dilutions were performed to get absorance readings between 0.05 and 0.5 on the Cary 60 UV-Vis Spectrometer for all quantum yield samples, to determine whether the absorbances followed Beer's Law. Due to concerns of sample degradation, fluorescence experiments were undertaken within 16 hours, ideally immediately after the UV-Vis spectra are taken.

Fluorescence spectra were collected on a Horiba Scientific: Fluoromax-4 Spectrofluorometer. Excitation values were chosen based on the maximum absorbance observed in the UV-Vis spectrum. The fluorescence data was collected from the excitation wavelength to 800 nm at each nanometer. Slit widths of the fluorimeter were set to 1.5 nm. Integrated fluorescence values were obtained using the Integration Gadget in OriginPro and plotted versus the absorbance (Figures S36 and S37).

Calculation of the quantum yield employed the comparative method, utilizing Rhodamine 6G as quantum yield standard[1] and Equation S1.

$$\Phi_x = \Phi_{ref}\left(\frac{Slope_x}{Slope_{ref}}\right)\left(\frac{(\eta_x)^2}{(\eta_{ref})^2}\right) \quad \text{(S1)}$$

Φ_x and Φ_{ref} are the quantum yields of the sample and the reference, respectively. $Slope_x$ and the $Slope_{ref}$ refer to the slopes calculated from the graphs correlating absorbance intensity of the UV-Vis spectra to the integrated fluorescence for the sample and the Rhodamine 6G reference standard (Figures S37 and S37), respectively. η_x is the refractive index of the sample and η_{ref} is the refractive index of the Rhodamine 6G standard. All BODIPY-appended diamines were measured in DMSO while the Rhodamine 6G standard was measured in methanol.

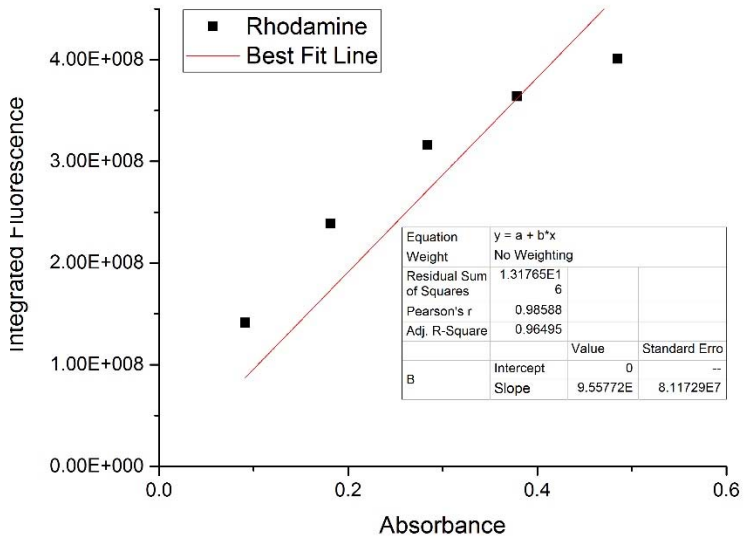

Figure S37. Correlation graph of the absorbance and integrated fluorescence values for the standard Rhodamine 6G. The slope (9.55772×10^8) was used for the quantum yield calculation.

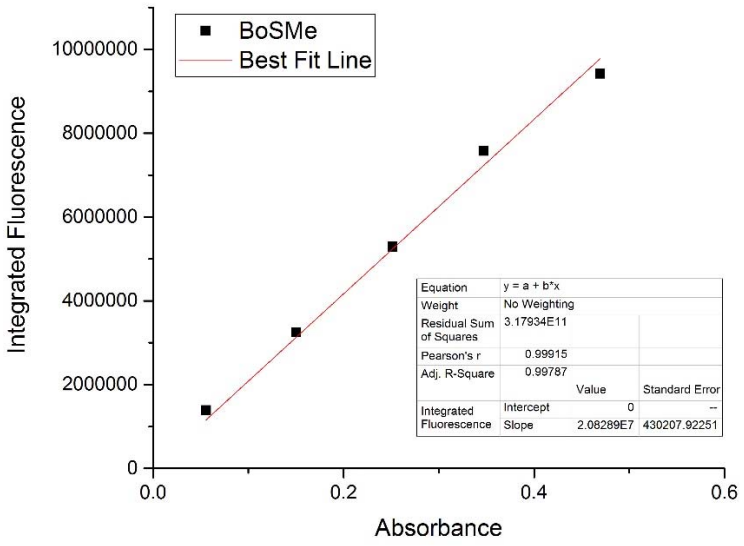

Figure S38. Correlation graph of the absorbance and integrated fluorescence values for the sample **BoSMe**. The slope of (2.08289 ×10^7) was used for the quantum yield calculation.

Insertion of the slopes for the reference and samples, the solvent refractive indeces, and the quantum yield for Rhodamine 6G, yields the following:

$$\Phi_x = \mathbf{0.98}\left(\frac{\mathbf{2.08289} \times 10^7}{\mathbf{9.55772} \times 10^8}\right)\left(\frac{(\mathbf{1.4772})^2}{(\mathbf{1.3281})^2}\right) = 0.03$$

Solving for Φ_x yields a quantum yield of 0.03 for **BoSMe** in DMSO.

12) Cyclic Voltammograms of Diamines Containing One or Two BODIPY Molecules

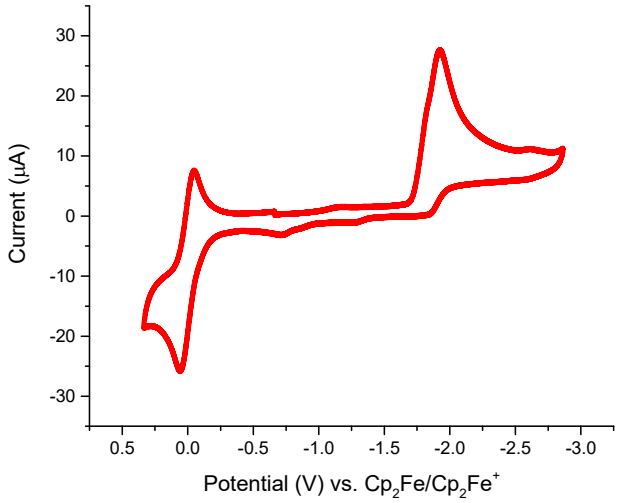

Figure S39. Cyclic Voltammogram of **Boen** in DMSO. Electrolyte = Bu_4NPF_6, scan rate = 250 mV/s.

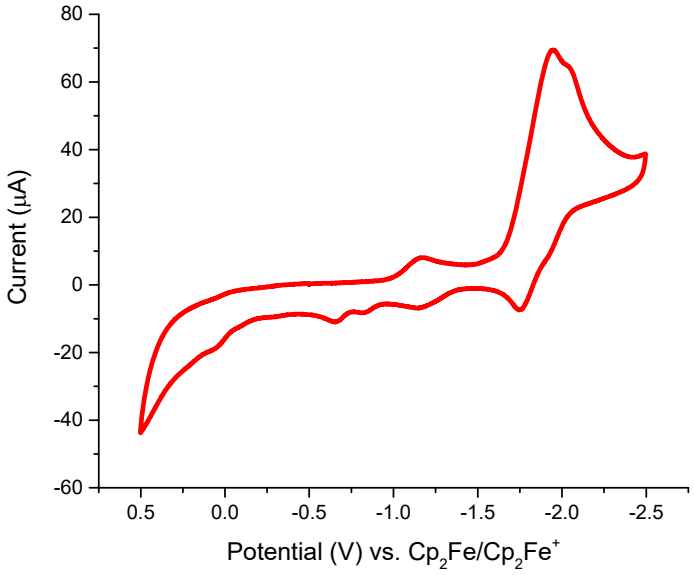

Figure S40. Cyclic Voltammogram of **Bodach** in DMSO. Electrolyte = Bu_4NPF_6, scan rate = 250 mV/s.

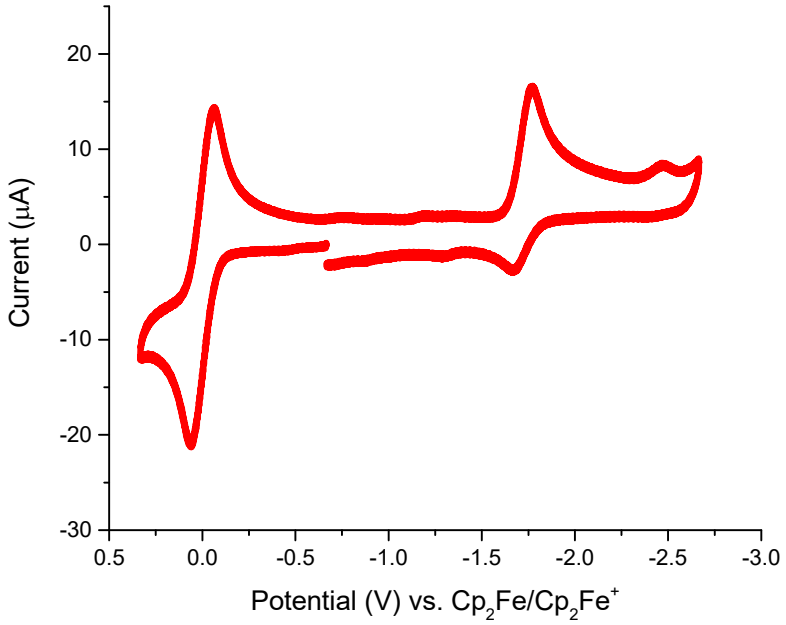

Figure S41. Cyclic Voltammogram of **Bophen** in DMSO. Electrolyte = Bu_4NPF_6, scan rate = 250 mV/s. The reversible peak at 0 V is from the presence of ferrocene (internal standard).

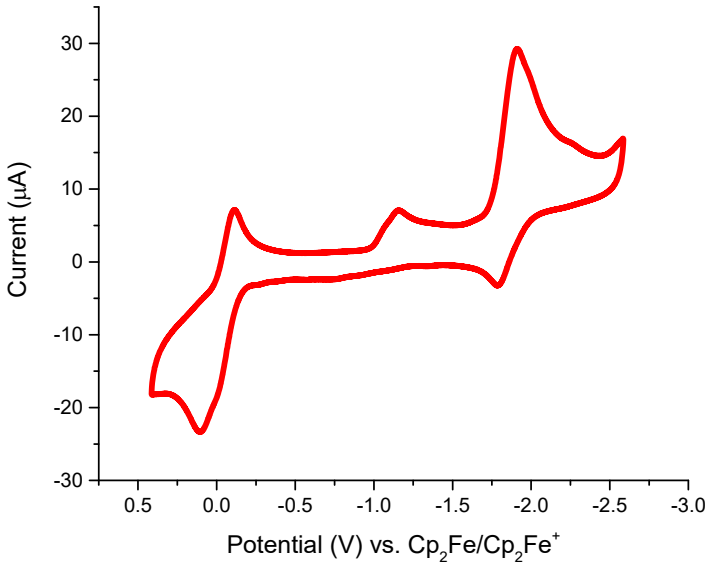

Figure S42. Cyclic Voltammogram of **Bodpen** in DMSO. Electrolyte = Bu_4NPF_6, scan rate = 250 mV/s. The reversible peak at 0 V is from the presence of ferrocene (internal standard).

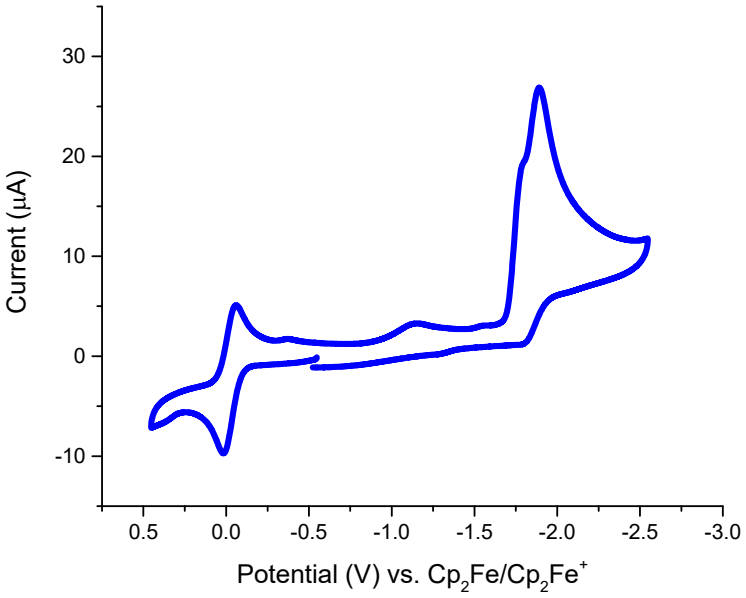

Figure S43. Cyclic Voltammogram of **Bo$_2$en** in DMSO. Electrolyte = Bu_4NPF_6, scan rate = 250 mV/s. The reversible peak at 0 V is from the presence of ferrocene (internal standard).

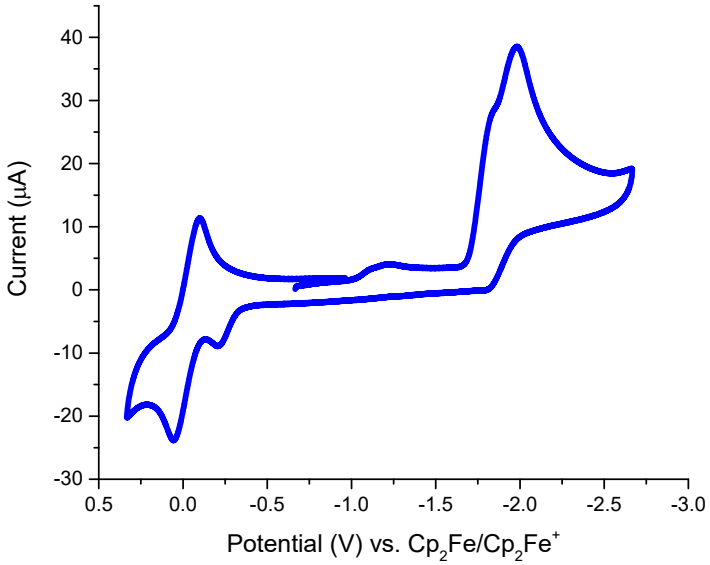

Figure S44. Cyclic Voltammogram of **Bo$_2$dach** in DMSO. Electrolyte = Bu_4NPF_6, scan rate = 250 mV/s. The reversible peak at 0 V is from the presence of ferrocene (internal standard).

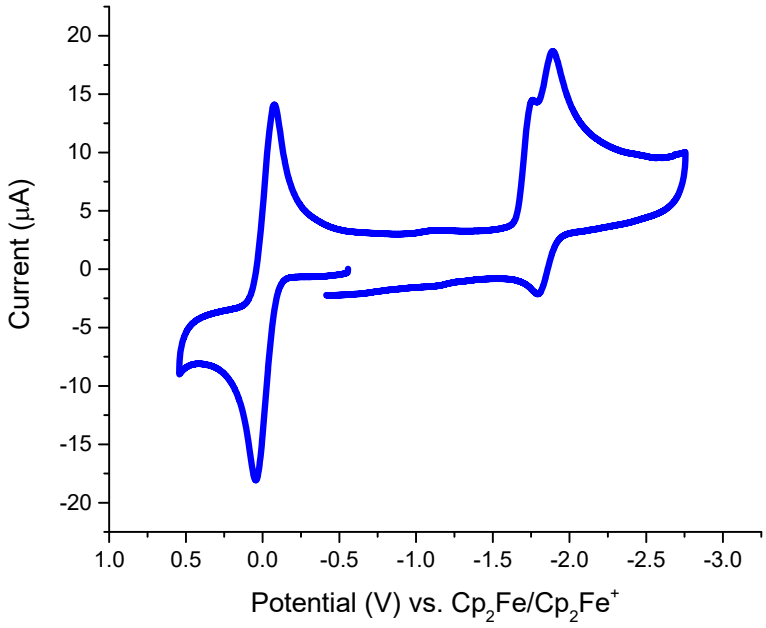

Figure S45. Cyclic Voltammogram of **Bo$_2$dpen** in DMSO. Electrolyte = Bu_4NPF_6, scan rate = 250 mV/s. The reversible peak at 0 V is from the presence of ferrocene (internal standard).

13) FT-IR spectra of Diamines Containing One and Two BODIPY Molecules

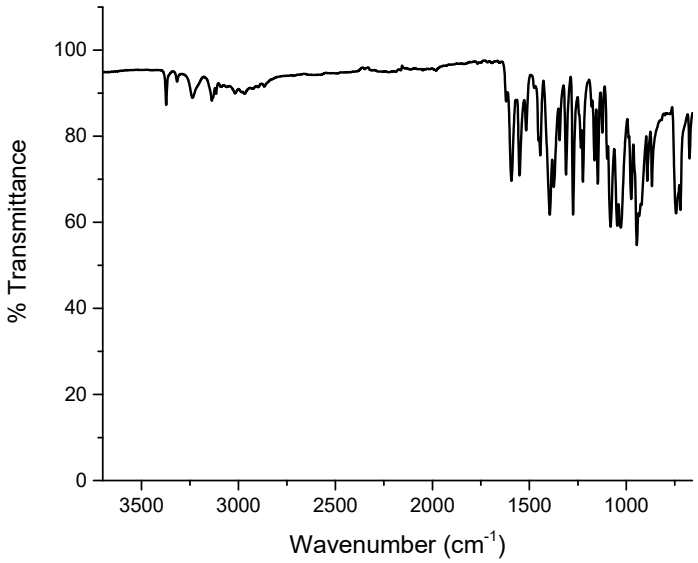

Figure S46. Infrared spectrum of Boen (FT-IR).

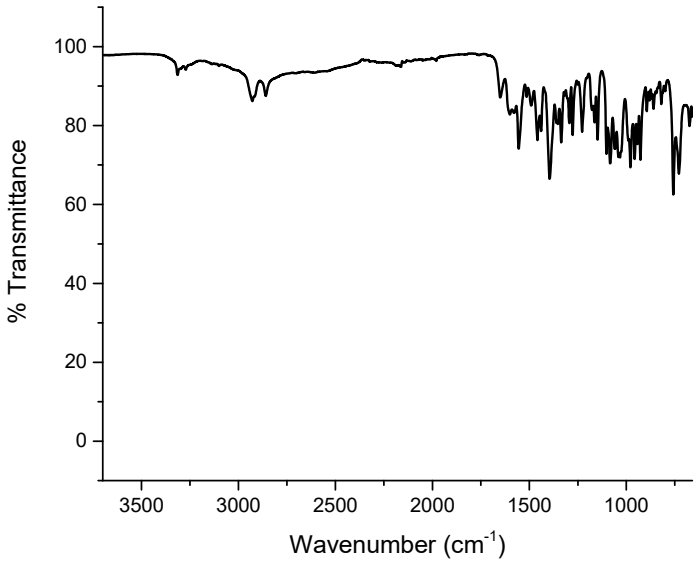

Figure S47. Infrared spectrum of Bodach (FT-IR).

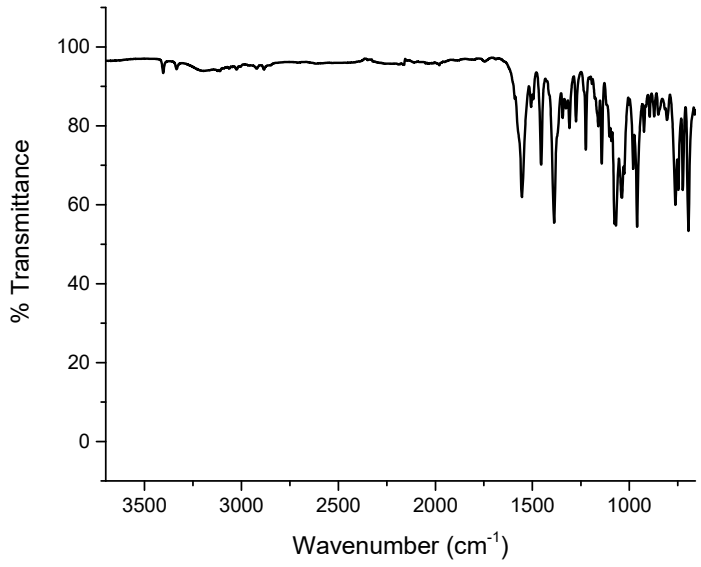

Figure S48. Infrared spectrum of Bodpen (FT-IR).

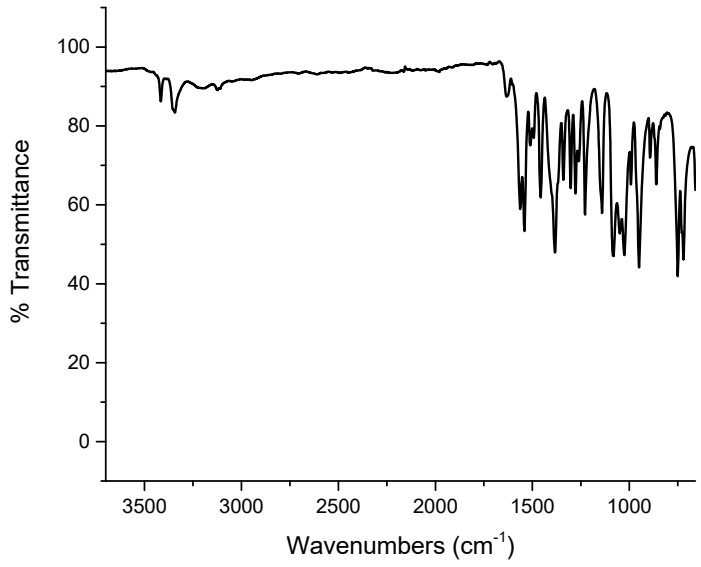

Figure S49. Infrared spectrum of Bophen (FT-IR).

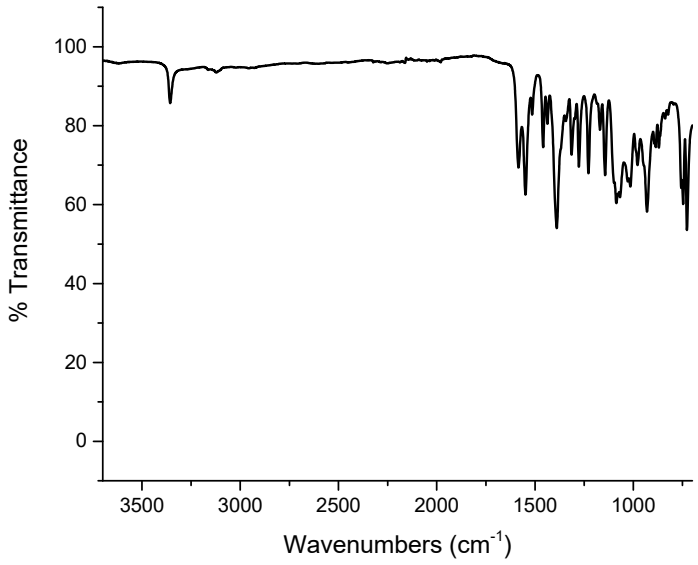

Figure S50. Infrared spectrum of Bo_2en (FT-IR).

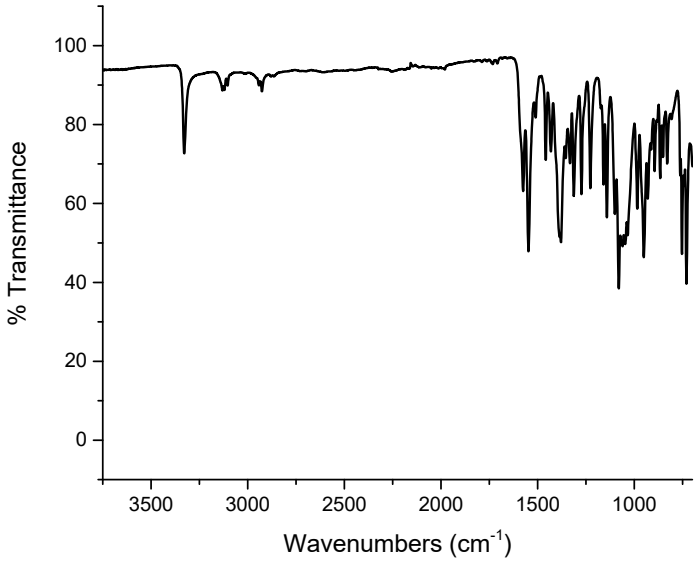

Figure S51. Infrared spectrum of Bo_2dach (FT-IR).

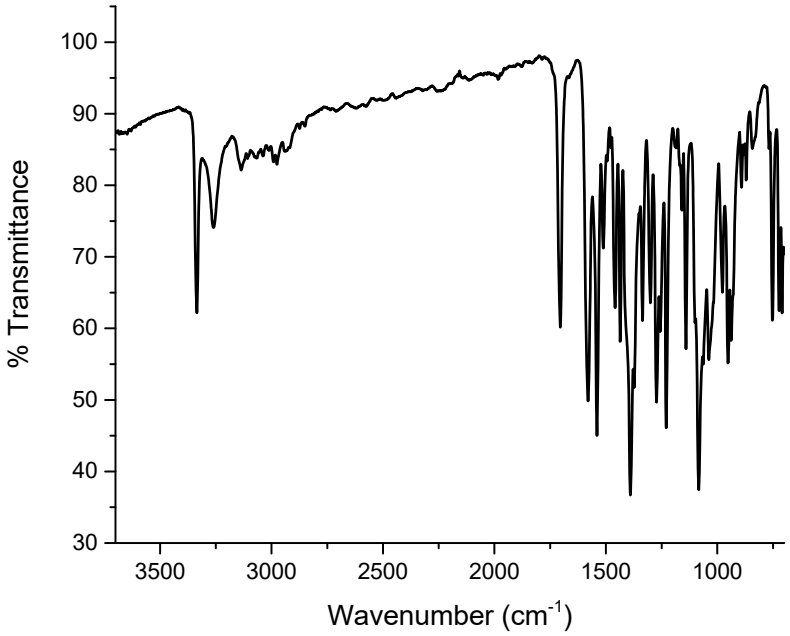

Figure S52. Infrared spectrum of Bo_2dpen (FT-IR).

14) Frontier Molecular Orbitals for Boen

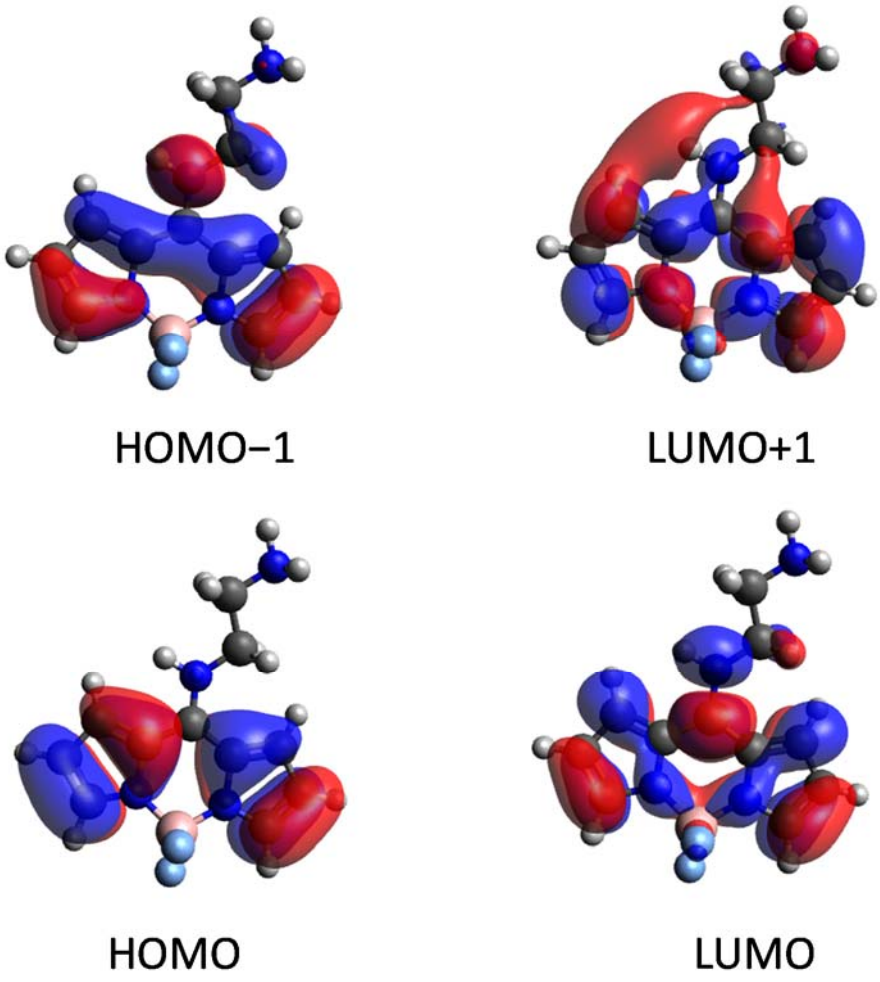

Figure S53. Frontier molecular orbitals of Boen.

15) Frontier Molecular Orbitals for Bophen

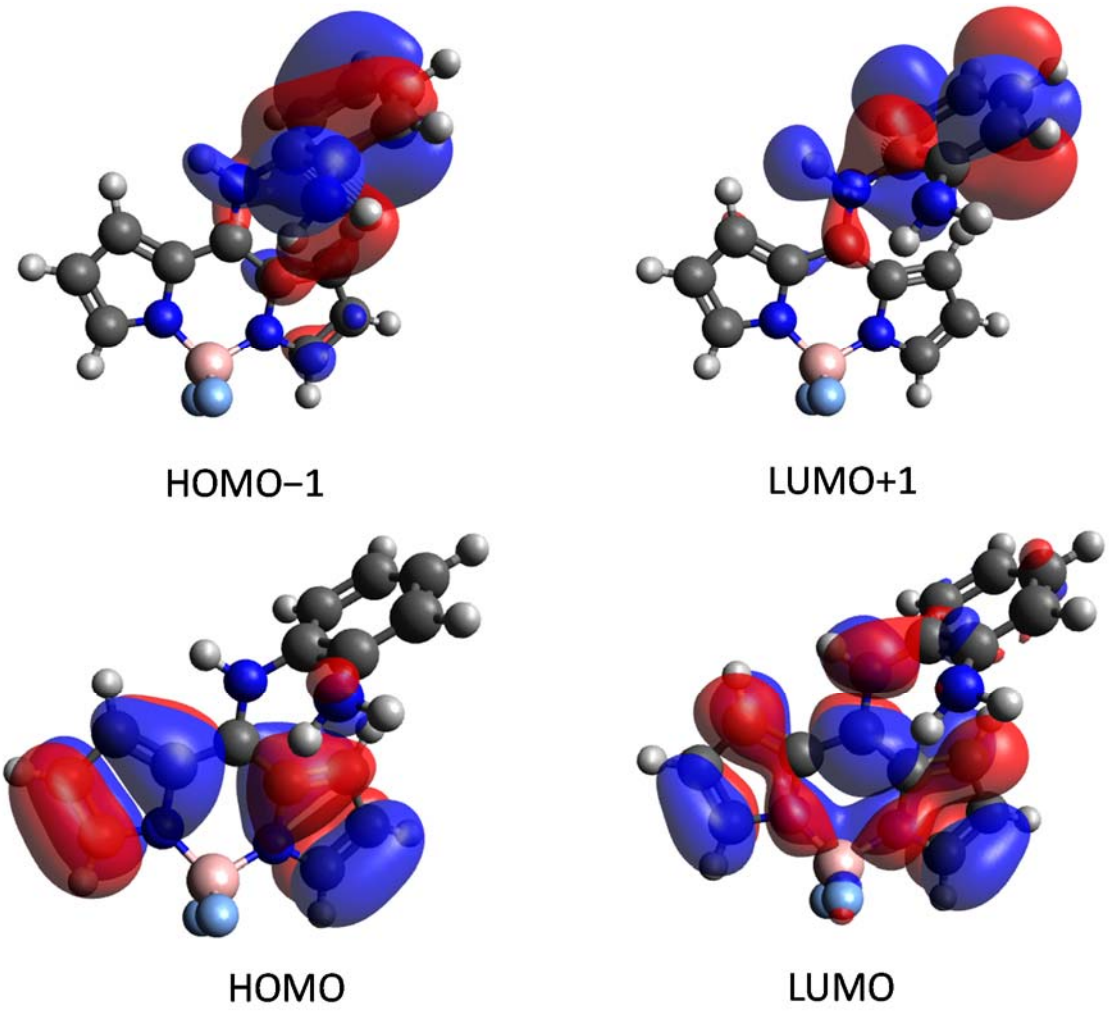

Figure S54. Frontier molecular orbitals of Bophen.

16) Frontier Molecular Orbitals for Bodach

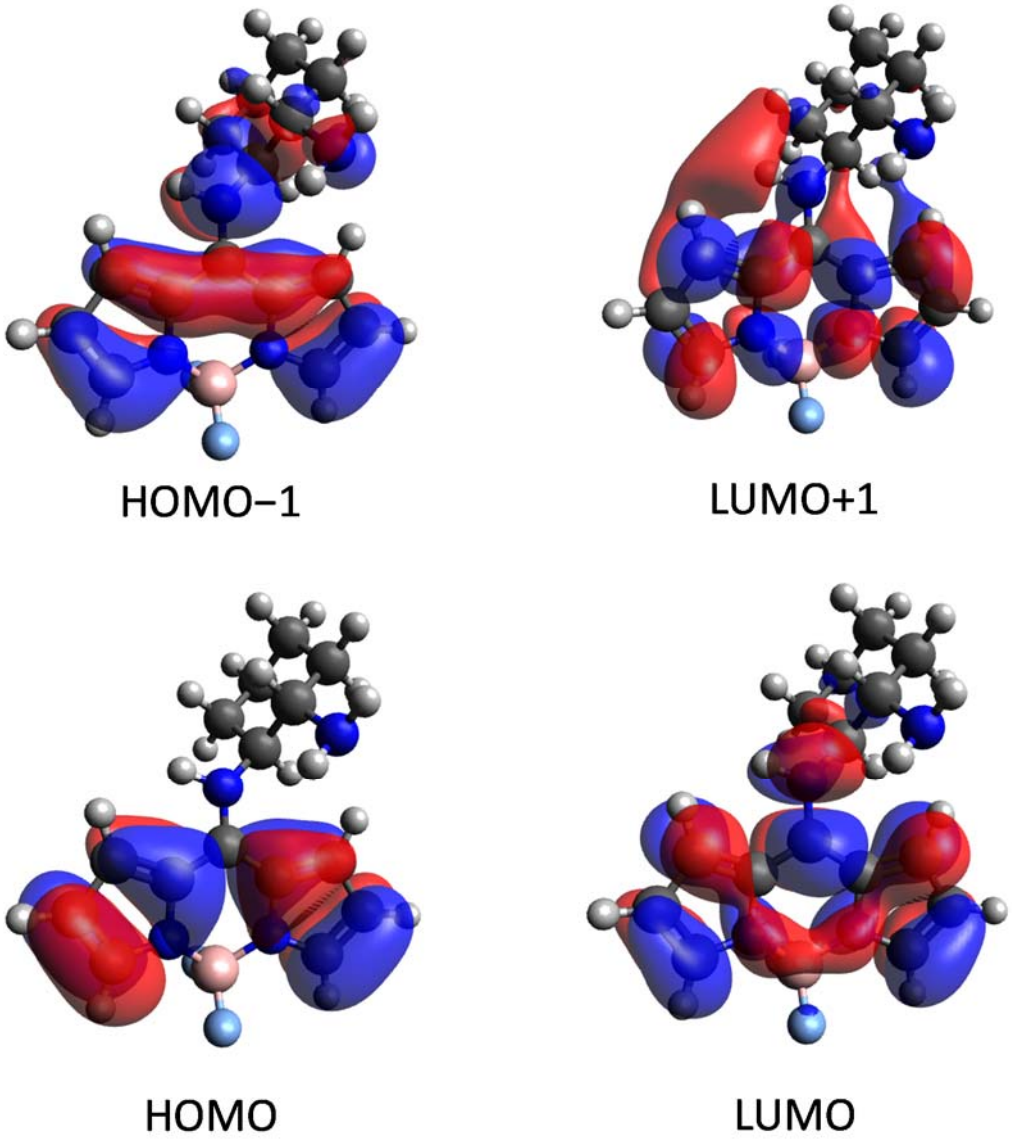

Figure S55. Frontier molecular orbitals of Bodach.

17) Frontier Molecular Orbitals for Bodpen

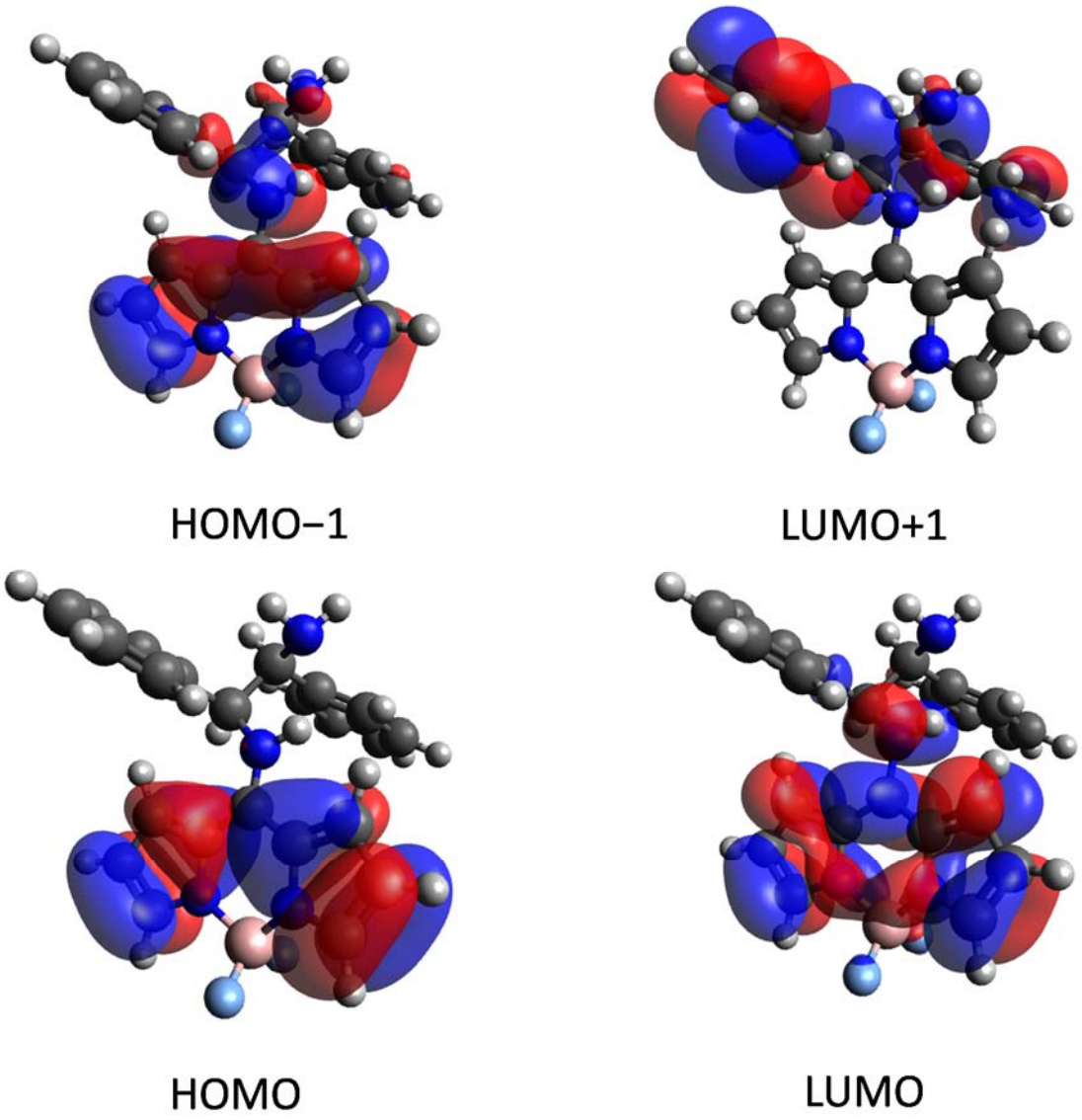

Figure S56. Frontier molecular orbitals of Bodpen.

18) Frontier Molecular Orbitals for Bo_2en

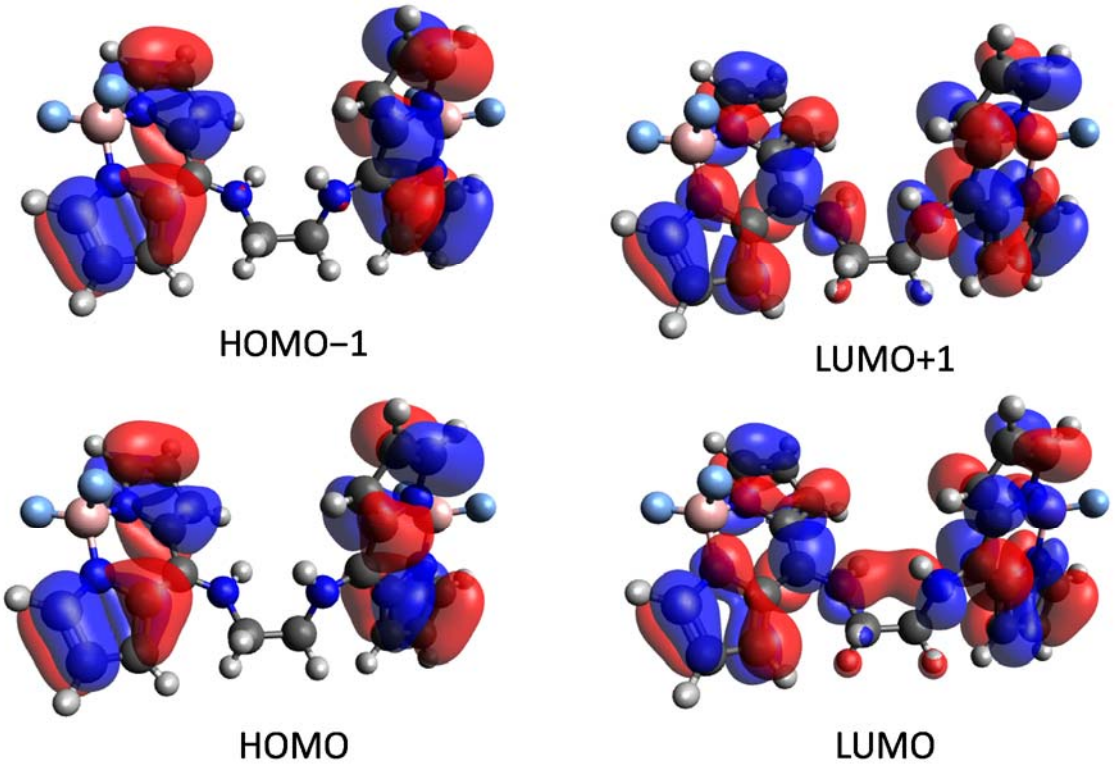

Figure S57. Frontier molecular orbitals of Bo_2en.

19) Frontier Molecular Orbitals for Bo_2phen

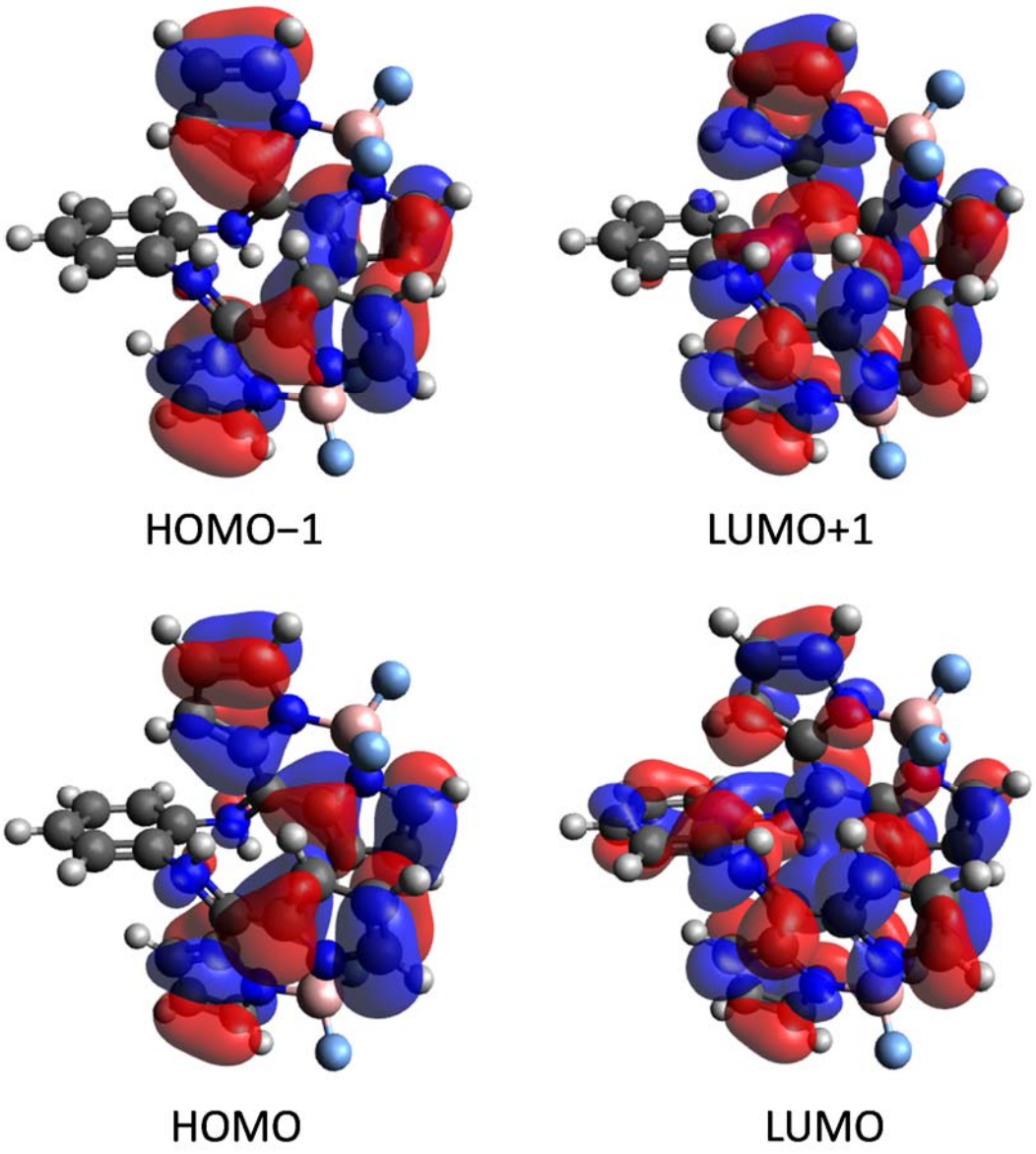

Figure S58. Frontier molecular orbitals of Bo_2phen.

20) Frontier Molecular Orbitals for Bo_2dach

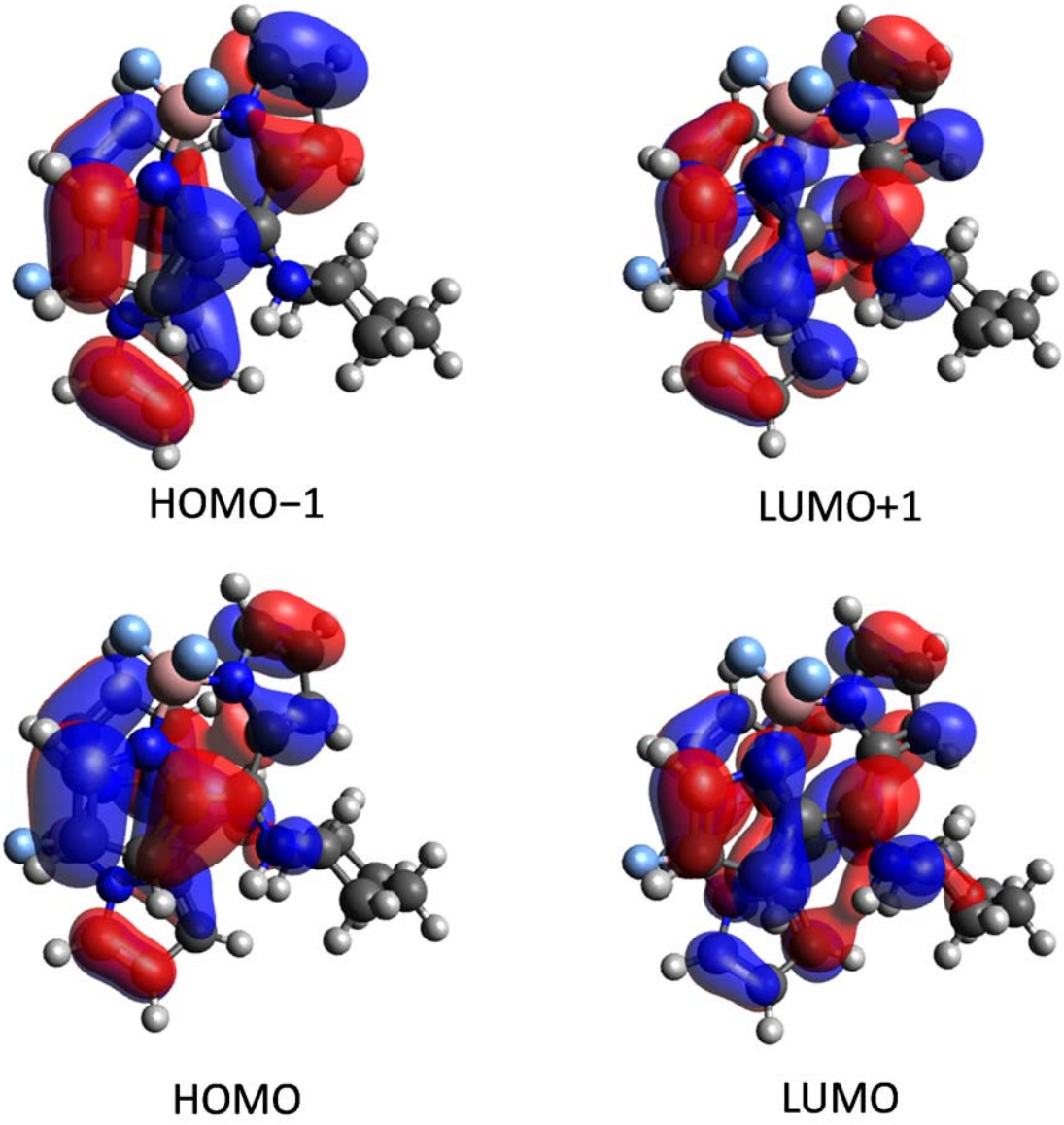

Figure S59. Frontier molecular orbitals of Bo_2dach.

21) Frontier Molecular Orbitals for Bo_2dpen

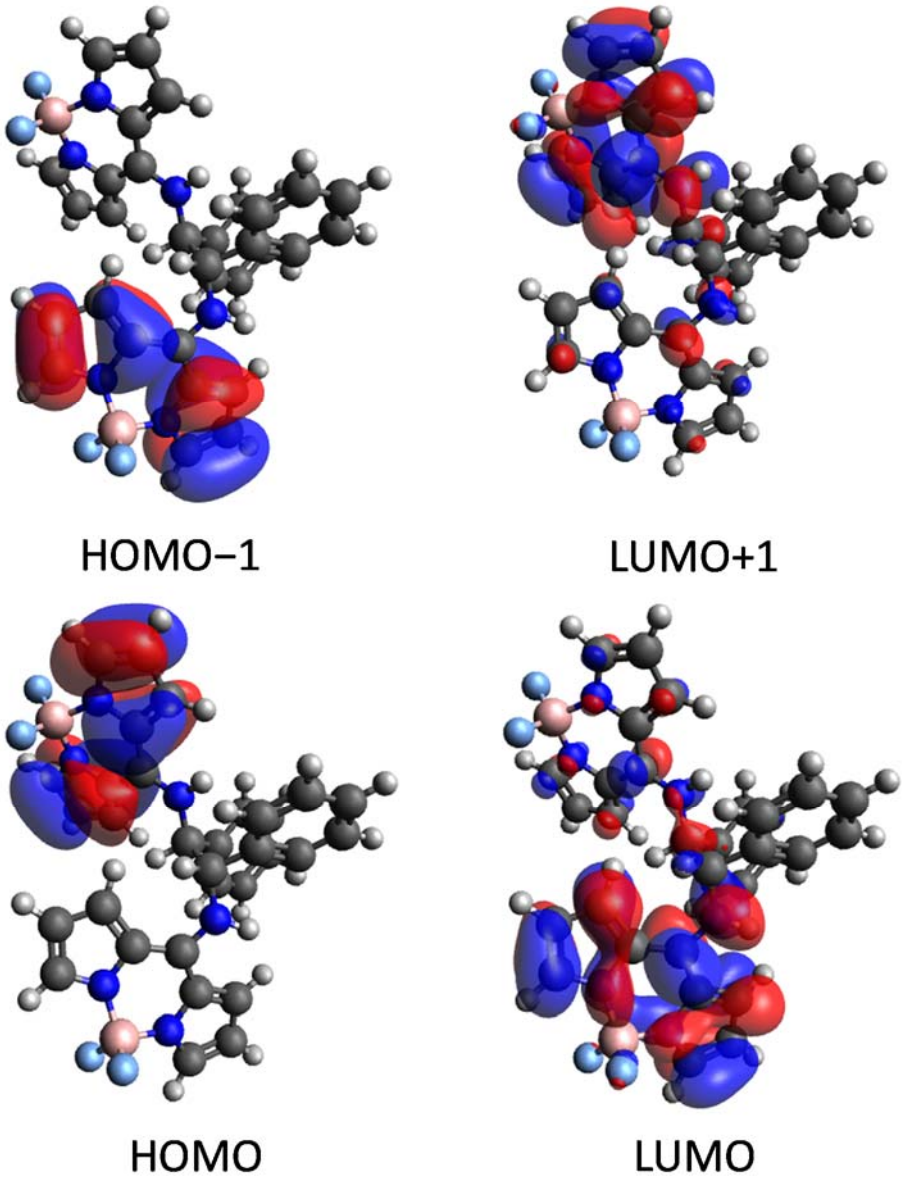

Figure S60. Frontier molecular orbitals of Bo_2dpen.

22) Computed p*K*a's of the BODIPY-Appended Diamines in MeCN

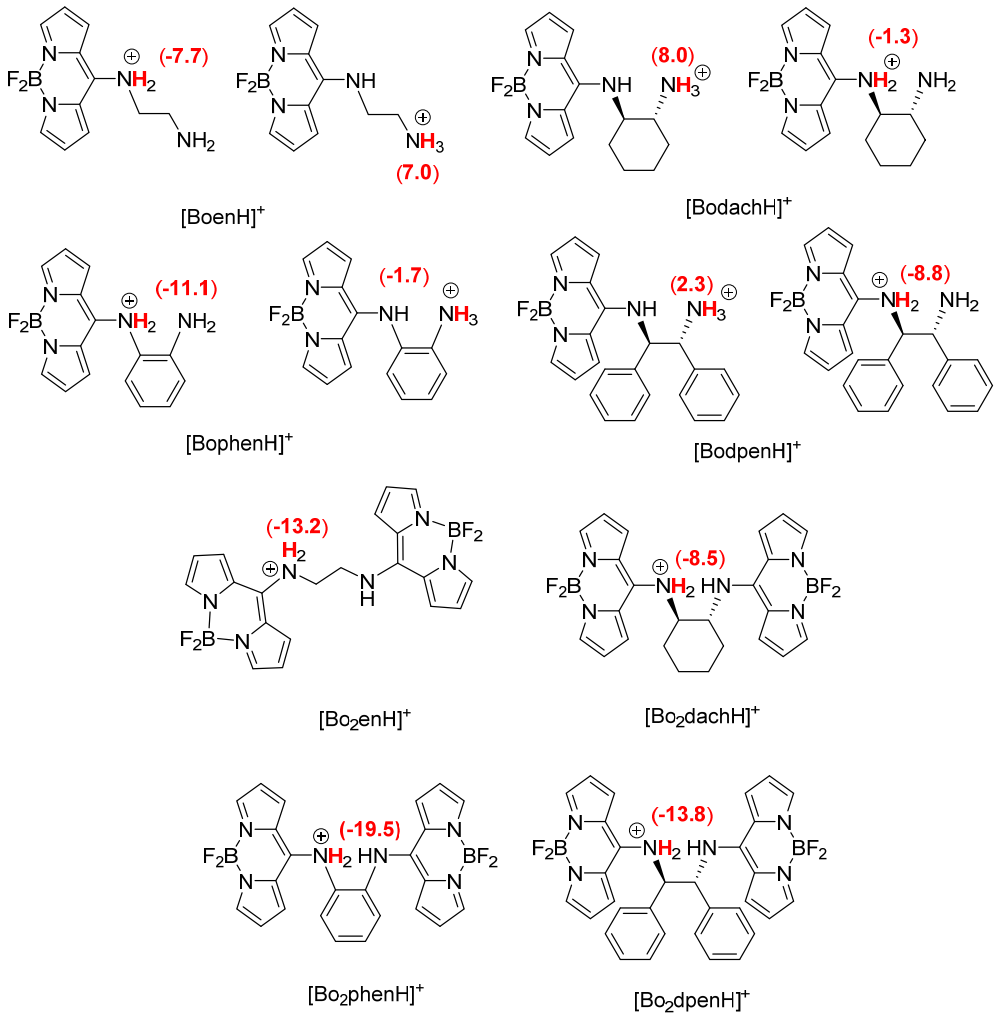

Figure S61. List of computed p*K*a's in acetonitrile for the respective ammonium BODIPY-substituted diamines. The acidic proton is highlighted in red.

23) 3D Coordinates of All Computed Structures

The coordinates listed are in xyz format for easily visualization in a program like Mercury. The first number is the number of atoms, followed by the name of the molecule and the xyz coordinates.

31
Boen

N	-0.787835	0.448911	-0.926905
C	-1.382138	1.747193	-0.671748
C	-2.639088	1.917496	-1.517157
C	0.128950	-0.187850	-0.191905
C	0.515389	-1.500198	-0.617734
N	1.340337	-2.278500	0.157622
N	-3.218064	3.221609	-1.235625
N	1.579086	-0.394890	1.725930
C	0.743589	0.392102	0.954236
C	0.242589	-2.190775	-1.807479
C	0.920547	-3.409166	-1.730515
C	1.580361	-3.422969	-0.499810
C	2.118573	0.367724	2.680809
C	1.662269	1.684482	2.556551
C	0.792962	1.706017	1.470626
B	1.758111	-1.946948	1.621163
F	0.913660	-2.575450	2.509852
F	3.074946	-2.279385	1.834600
H	-1.159683	-0.072148	-1.708924
H	-1.634387	1.815556	0.393388
H	-0.682271	2.556843	-0.906382
H	-2.357895	1.888093	-2.576244
H	-3.310649	1.062242	-1.333669
H	-3.926849	3.451508	-1.923286
H	-3.680136	3.211827	-0.331216
H	-0.337731	-1.838057	-2.650395
H	0.950266	-4.186636	-2.478777
H	2.206513	-4.183148	-0.054789
H	2.798340	-0.068026	3.399644
H	1.945607	2.520153	3.178343
H	0.297689	2.579900	1.079612

32
[BoenH]$^+$ (protonated primary amine)

N	-2.064893	-0.226116	-0.052290
C	-2.444417	1.145732	-0.376258
C	-1.615286	1.800646	-1.492065
C	-0.779291	-0.516693	0.292068
C	-0.126598	-1.643339	-0.237519
N	1.258575	-1.704085	-0.176614
N	-0.204024	2.184858	-1.094018
N	1.309161	0.367071	1.139798
C	-0.068855	0.375905	1.158088
C	-0.591218	-2.817606	-0.874640
C	0.527190	-3.579957	-1.172140
C	1.651370	-2.839100	-0.757245
C	1.759583	1.283171	2.011268
C	0.671632	1.900428	2.639759
C	-0.488005	1.333265	2.100151
B	2.068076	-0.396272	0.024278
F	3.372471	-0.599333	0.298103
F	1.870106	0.390902	-1.160432
H	-2.503091	-0.920971	-0.643782
H	-3.476072	1.118970	-0.734054
H	-2.445086	1.774549	0.513817
H	-1.526075	1.146083	-2.361363
H	-2.111855	2.723797	-1.796877
H	0.139148	2.937667	-1.697510
H	-0.164074	2.508786	-0.116588
H	0.495246	1.407000	-1.166858
H	-1.622807	-3.107068	-1.027199
H	0.547305	-4.558397	-1.627571
H	2.703834	-3.059515	-0.875644
H	2.821175	1.443674	2.138664
H	0.727366	2.637658	3.426620
H	-1.503440	1.513473	2.425363

32
[BoenH]$^+$ (protonated secondary amine)

N	-0.286419	0.856155	-1.160077
C	-1.731987	1.066081	-0.729386
C	-2.450754	2.027973	-1.672239
C	0.464648	-0.026557	-0.259351
C	0.427196	-1.386454	-0.519402
N	1.103486	-2.238671	0.339769
N	-3.803553	2.153773	-1.176635
N	1.824440	-0.253444	1.680727
C	1.137642	0.564959	0.798118
C	-0.110002	-2.160232	-1.589915
C	0.260737	-3.464621	-1.354336
C	1.009637	-3.468191	-0.146892
C	2.459528	0.522822	2.548292
C	2.208005	1.890803	2.261072
C	1.375627	1.921688	1.164653
B	1.692608	-1.833117	1.756693

F	0.777732	-2.149475	2.716967
F	2.916006	-2.396156	1.931708
H	-0.265589	0.463438	-2.108319
H	0.190451	1.763601	-1.215040
H	-2.205509	0.083615	-0.724251
H	-1.686064	1.445409	0.293784
H	-1.888553	2.974410	-1.745088
H	-2.479321	1.593561	-2.677586
H	-3.889273	2.888967	-0.484083
H	-4.461979	2.346970	-1.921100
H	-0.689591	-1.803345	-2.432397
H	0.038682	-4.329226	-1.961301
H	1.466550	-4.301268	0.371538
H	3.060691	0.088953	3.336854
H	2.606764	2.733357	2.805410
H	0.992367	2.811095	0.679633

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[BoenH$_2$]$^{2+}$

N	-0.143601	0.953351	-1.228653
C	-1.554875	1.197799	-0.757738
C	-2.308271	2.149467	-1.693653
C	0.559073	0.027530	-0.300485
C	0.444917	-1.326187	-0.567526
N	1.026326	-2.204403	0.334697
N	-3.713035	2.363828	-1.183038
N	1.815758	-0.250331	1.686183
C	1.224834	0.604333	0.767670
C	-0.037270	-2.080007	-1.683264
C	0.275806	-3.393903	-1.428761
C	0.929946	-3.427426	-0.162070
C	2.509630	0.482763	2.542317
C	2.400272	1.864788	2.208285
C	1.589383	1.946443	1.101532
B	1.446731	-1.794676	1.815688
F	0.334903	-1.887505	2.599351
F	2.520543	-2.505845	2.216708
H	-0.124590	0.537710	-2.170218
H	0.396742	1.828156	-1.277713
H	-2.020154	0.209104	-0.703784
H	-1.459356	1.597241	0.256283
H	-1.842174	3.136652	-1.745043
H	-2.403264	1.747792	-2.705609
H	-4.228296	3.002731	-1.805835
H	-4.256168	1.490212	-1.140723
H	-3.732570	2.786268	-0.244341
H	-0.515568	-1.708149	-2.582157
H	0.084885	-4.248376	-2.061115
H	1.314721	-4.279083	0.385455
H	3.050694	0.017970	3.357408
H	2.883157	2.678192	2.729479
H	1.329166	2.858116	0.575989

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Bo$_2$en

N	0.604648	-1.536662	-0.141330
C	1.811031	-1.113606	0.539799
C	2.168851	0.304384	0.121570
C	-0.213591	-2.543966	0.209442
C	-1.418719	-2.697858	-0.538103
N	-2.368372	-3.618671	-0.158934
N	1.067285	1.196716	0.419174
N	-0.870190	-4.366164	1.646383
C	0.092588	-3.451244	1.262217
C	-1.849878	-2.077737	-1.723130
C	-3.080660	-2.644953	-2.048562
C	-3.365025	-3.585819	-1.052909
C	-0.342342	-5.182079	2.561421
C	0.992973	-4.834544	2.799214
C	1.272848	-3.743596	1.984185
B	-2.374344	-4.369366	1.206850
F	-3.125038	-3.669051	2.124461
F	-2.809205	-5.662016	1.051247
C	0.846873	2.415204	-0.104202
C	1.786011	3.069262	-0.950052
N	1.414941	4.255385	-1.555877
N	-0.735594	4.249799	-0.356863
C	-0.376643	3.062916	0.239770
C	3.149680	2.844357	-1.249293
C	3.574331	3.905858	-2.040278
C	2.469571	4.749528	-2.207962
C	-1.894098	4.655163	0.178988
C	-2.313896	3.741849	1.152150
C	-1.356510	2.729714	1.190336
B	-0.030589	4.858345	-1.606498
F	0.034036	6.226276	-1.512432
F	-0.665567	4.439765	-2.754360
H	0.297049	-0.963930	-0.916123
H	1.640737	-1.159231	1.622504
H	2.656117	-1.771870	0.306453
H	3.082779	0.604988	0.647216
H	2.374505	0.342817	-0.955259
H	0.340612	0.834298	1.022119
H	-1.322261	-1.331873	-2.303735
H	-3.695513	-2.417916	-2.906122
H	-4.225073	-4.228914	-0.930751
H	-0.943530	-5.968458	2.995993
H	1.671724	-5.331592	3.475412
H	2.232546	-3.260614	1.894860
H	3.774054	2.039292	-0.896732
H	4.564834	4.063493	-2.439098
H	2.380213	5.676309	-2.757293

H	-2.360559	5.567971	-0.163607
H	-3.202410	3.820500	1.759898
H	-1.361219	1.877535	1.857842

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$[Bo_2enH]^+$

N	-0.164371	-0.920152	0.605463
C	-0.024426	-0.985844	2.117804
C	1.294441	-1.592786	2.607210
C	-1.487767	-0.421018	0.216581
C	-1.648190	0.951195	0.148294
N	-2.907020	1.456155	-0.145593
N	2.443853	-0.706119	2.437374
N	-3.762229	-0.885335	-0.322169
C	-2.494998	-1.349739	-0.011483
C	-0.732351	2.042500	0.236376
C	-1.462701	3.182214	-0.007753
C	-2.804302	2.773803	-0.239927
C	-4.530106	-1.936214	-0.585942
C	-3.783808	-3.134019	-0.457397
C	-2.504537	-2.769979	-0.091986
B	-4.247984	0.613227	-0.158324
F	-4.860939	0.744733	1.056160
F	-5.019952	0.977430	-1.216714
C	2.768135	-0.318605	1.160685
C	2.957595	-1.309531	0.166865
N	2.996647	-0.939892	-1.166947
N	2.921783	1.427839	-0.503605
C	2.849916	1.052207	0.829347
C	3.296366	-2.679047	0.250581
C	3.534034	-3.113692	-1.047027
C	3.325741	-2.010658	-1.894563
C	2.964265	2.761673	-0.560699
C	2.959587	3.297503	0.740751
C	2.865662	2.225602	1.618428
B	2.450962	0.439863	-1.612695
F	2.837448	0.801127	-2.853627
F	1.033144	0.355572	-1.467980
H	0.536478	-0.313336	0.132712
H	-0.012637	-1.849024	0.194647
H	-0.152804	0.042162	2.466816
H	-0.876122	-1.579607	2.458483
H	1.177584	-1.792991	3.674827
H	1.483701	-2.552905	2.124843
H	2.448610	0.056974	3.103989
H	0.334319	1.980290	0.416874
H	-1.099754	4.198223	-0.040174
H	-3.674049	3.377607	-0.464714
H	-5.571765	-1.803390	-0.847505
H	-4.158982	-4.132194	-0.624448
H	-1.672860	-3.442645	0.077608
H	3.437851	-3.242363	1.163178
H	3.851240	-4.097629	-1.357545
H	3.394700	-1.941993	-2.971810
H	2.972999	3.268671	-1.516454
H	3.031916	4.344054	0.995586
H	2.871392	2.284031	2.699099

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$[Bo_2enH_2]^{2+}$

N	1.613574	0.014234	-1.043774
C	0.741344	-0.003547	0.188442
C	-0.741344	-0.003547	-0.188441
C	3.050830	0.009687	-0.673632
C	3.675061	-1.222404	-0.593372
N	4.997061	-1.242152	-0.172573
N	-1.613575	0.014237	1.043775
N	4.944026	1.251847	0.027064
C	3.625994	1.240585	-0.401492
C	3.308028	-2.547722	-0.986707
C	4.421952	-3.330676	-0.801851
C	5.446240	-2.481419	-0.288769
C	5.340909	2.513081	0.103321
C	4.282851	3.385164	-0.282635
C	3.202922	2.591655	-0.592941
B	5.698276	-0.031461	0.589606
F	5.392085	-0.146164	1.913386
F	7.012561	0.020655	0.286004
C	-3.050830	0.009689	0.673632
C	-3.625995	1.240586	0.401492
N	-4.944028	1.251846	-0.027065
N	-4.997060	-1.242153	0.172573
C	-3.675060	-1.222404	0.593373
C	-3.202925	2.591656	0.592940
C	-4.282855	3.385164	0.282634
C	-5.340911	2.513079	-0.103323
C	-5.446237	-2.481421	0.288769
C	-4.421948	-3.330676	0.801851
C	-3.308025	-2.547721	0.986708
B	-5.698275	-0.031463	-0.589607
F	-7.012561	0.020651	-0.286004
F	-5.392085	-0.146167	-1.913386
H	1.429902	-0.801776	-1.642939
H	1.429725	0.848832	-1.617292
H	1.037765	-0.897763	0.744054
H	1.031567	0.879502	0.764756
H	-1.031568	0.879500	-0.764757
H	-1.037766	-0.897765	-0.744051
H	-1.429902	-0.801772	1.642943
H	-1.429726	0.848837	1.617290
H	2.360350	-2.883369	-1.391680
H	4.525610	-4.384800	-1.012214

H	6.461255	-2.730674	-0.004804
H	6.344336	2.758636	0.428485
H	4.341502	4.462313	-0.331872
H	2.243077	2.942086	-0.954638
H	-2.243081	2.942089	0.954639
H	-4.341508	4.462313	0.331870
H	-6.344339	2.758633	-0.428488
H	-6.461251	-2.730677	0.004804
H	-4.525605	-4.384800	1.012215
H	-2.360348	-2.883366	1.391682

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Bophen

C	-3.861413	2.067469	-0.824609
C	-4.189001	0.815912	-0.294390
N	-3.071363	0.115522	-0.058003
C	-1.992289	0.890154	-0.414826
C	-2.469242	2.118558	-0.898663
N	-1.540361	-1.768170	0.354251
B	-2.970833	-1.240422	0.703805
C	-0.448644	-0.992694	0.001026
C	-0.661198	0.377187	-0.322998
C	-1.131196	-3.029318	0.506202
C	0.242737	-3.121361	0.246812
C	0.680479	-1.840395	-0.069553
N	0.348113	1.229573	-0.568902
C	1.746657	0.967935	-0.444731
C	2.308336	0.820273	0.837482
N	1.535833	0.946053	1.977489
C	3.689068	0.588838	0.915497
C	4.468713	0.515681	-0.230051
C	3.900456	0.666198	-1.494003
C	2.532710	0.890957	-1.589576
F	-3.921290	-2.123434	0.254064
F	-3.061129	-1.020311	2.062382
H	-4.558612	2.833751	-1.127846
H	-5.155753	0.388177	-0.069378
H	-1.882849	2.937465	-1.294474
H	-1.838060	-3.795281	0.793383
H	0.837747	-4.021650	0.276307
H	1.682377	-1.555775	-0.351784
H	0.081555	2.183204	-0.774143
H	1.958000	0.571791	2.814670
H	0.566493	0.672631	1.890371
H	4.144786	0.470324	1.894330
H	5.534408	0.334732	-0.132885
H	4.510234	0.604113	-2.387625
H	2.047462	0.997188	-2.554977

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[BophenH]$^+$ (Protonated primary amine)

C	-3.768418	2.090003	-0.457253
C	-3.942405	0.910092	0.289711
N	-2.839379	0.160582	0.220188
C	-1.901015	0.842206	-0.539472
C	-2.474606	2.063661	-0.958602
N	-1.339237	-1.779220	0.354172
B	-2.371840	-0.970340	1.183495
C	-0.397141	-1.097827	-0.398780
C	-0.637482	0.250387	-0.753012
C	-0.966649	-3.057074	0.442124
C	0.229295	-3.253707	-0.275426
C	0.600686	-2.021113	-0.792037
N	0.408087	1.002934	-1.228451
C	1.715680	0.872217	-0.700260
C	1.923636	0.778870	0.684612
N	0.772180	0.858282	1.607777
C	3.191738	0.636414	1.222669
C	4.294027	0.625128	0.371803
C	4.110625	0.761017	-1.000672
C	2.830180	0.874646	-1.534394
F	-3.386119	-1.719000	1.664888
F	-1.602508	-0.336038	2.204142
H	-4.509796	2.859912	-0.607590
H	-4.787565	0.587049	0.882482
H	-2.021204	2.808571	-1.599481
H	-1.554887	-3.761987	1.014318
H	0.740160	-4.195749	-0.405148
H	1.451214	-1.805695	-1.423793
H	0.195169	1.849015	-1.741370
H	1.076173	1.164720	2.536720
H	0.229798	-0.022327	1.727414
H	0.064998	1.529410	1.277594
H	3.328005	0.549812	2.297285
H	5.289776	0.519101	0.785982
H	4.967884	0.761583	-1.664539
H	2.675704	0.946078	-2.606037

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[BophenH]$^+$ (protonated secondary amine)

C	-3.184488	1.998927	-1.598933
C	-3.643131	0.663527	-1.468146
N	-2.808914	-0.038042	-0.709960
C	-1.782206	0.802767	-0.314911
C	-2.015613	2.092016	-0.873917
N	-1.624719	-1.936180	0.410861
B	-3.022221	-1.531865	-0.220896
C	-0.627613	-1.053289	0.800192
C	-0.744901	0.276808	0.442472
C	-1.268299	-3.149572	0.808904
C	-0.013978	-3.103553	1.475043

C	0.389323	-1.787846	1.474352
N	0.329504	1.190719	0.840231
C	1.561923	1.130780	0.017773
C	2.740872	1.032001	0.757087
N	2.596926	1.004188	2.183829
C	3.940573	0.933854	0.057466
C	3.933659	0.945167	-1.334922
C	2.737613	1.056898	-2.043074
C	1.524976	1.149027	-1.365978
F	-3.299139	-2.330976	-1.286442
F	-3.972606	-1.549587	0.756678
H	-3.667315	2.779421	-2.167115
H	-4.527587	0.200973	-1.886479
H	-1.390541	2.971439	-0.776763
H	-1.908449	-4.001094	0.617092
H	0.508348	-3.952271	1.889851
H	1.301168	-1.379062	1.888688
H	0.697935	0.975243	1.801380
H	-0.047122	2.144671	0.872731
H	3.182686	0.286177	2.602190
H	2.868602	1.890068	2.606484
H	4.873731	0.851784	0.605992
H	4.871831	0.867972	-1.873166
H	2.746419	1.065616	-3.126886
H	0.581828	1.214336	-1.899986

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[BophenH$_2$]$^{2+}$

C	-3.388546	2.287677	0.082039
C	-3.638997	1.044921	0.716973
N	-2.650916	0.193400	0.449272
C	-1.721380	0.840812	-0.350934
C	-2.178084	2.174483	-0.575001
N	-1.411796	-1.936239	0.135885
B	-2.251067	-1.129810	1.185654
C	-0.466200	-1.267748	-0.641074
C	-0.637573	0.091789	-0.811642
C	-1.147075	-3.232201	0.083498
C	-0.017283	-3.467915	-0.758689
C	0.427450	-2.244264	-1.191357
N	0.462599	0.842244	-1.448752
C	1.724379	0.898054	-0.647919
C	1.759907	1.042491	0.747998
N	0.567316	1.142570	1.615151
C	2.992704	1.088781	1.384513
C	4.177871	1.000891	0.657173
C	4.134714	0.867516	-0.724162
C	2.903498	0.815660	-1.373851
F	-3.289073	-1.808155	1.681440
F	-1.294790	-0.719070	2.163514
H	-4.042215	3.147631	0.098785
H	-4.466639	0.752482	1.351788
H	-1.734321	2.936566	-1.205975
H	-1.738484	-3.943871	0.647482
H	0.391883	-4.438085	-1.000529
H	1.261640	-2.063309	-1.857422
H	0.137190	1.792067	-1.679952
H	0.689853	0.402167	-2.352407
H	0.860366	1.452945	2.550069
H	0.030131	0.246750	1.754814
H	-0.127142	1.824856	1.280784
H	3.036655	1.194865	2.465643
H	5.127839	1.040116	1.178639
H	5.049233	0.800412	-1.303036
H	2.871921	0.712194	-2.456321

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Bo$_2$phen

F	4.182242	-2.531976	-0.612464
F	2.819137	-2.395307	1.209393
B	3.103328	-1.894584	-0.053713
N	3.375778	-0.358956	0.047172
N	1.836227	-2.017348	-0.953408
N	0.438142	1.333045	-1.369078
C	4.490624	0.174910	0.559922
C	4.403878	1.571007	0.543395
C	3.169335	1.890409	-0.015558
C	2.529526	0.671350	-0.323548
C	1.311310	0.359060	-0.994719
C	0.986486	-0.980924	-1.293841
C	-0.202958	-1.532986	-1.811664
C	-0.051959	-2.912266	-1.785161
C	1.217801	-3.166551	-1.244942
C	0.304246	2.561593	-0.664776
C	0.471109	3.774755	-1.319257
C	0.372868	4.968628	-0.605918
F	-4.453677	-2.076529	0.583860
F	-3.059911	-2.139745	-1.218620
B	-3.295267	-1.588612	0.033423
N	-3.372777	-0.031877	-0.092935
N	-2.067790	-1.852780	0.955182
N	-0.266635	1.298580	1.346749
C	-4.408469	0.625043	-0.627447
C	-4.154703	2.000632	-0.626008
C	-2.898203	2.177128	-0.053210
C	-2.412282	0.893524	0.277613
C	-1.248659	0.441485	0.967352
C	-1.095174	-0.927726	1.283371
C	0.004802	-1.614092	1.834169
C	-0.325670	-2.963094	1.841569
C	-1.609786	-3.065137	1.287659
C	-0.014127	2.542213	0.704882

C	-0.079441	3.732174	1.417630
C	0.121066	4.946379	0.762555
H	-0.394628	1.013446	-1.851539
H	5.288093	-0.466976	0.907280
H	5.158846	2.260202	0.890315
H	2.785744	2.882414	-0.199009
H	-1.097943	-1.011162	-2.125607
H	-0.784498	-3.644047	-2.089072
H	1.698442	-4.110893	-1.028706
H	0.708411	3.768660	-2.377697
H	0.510329	5.914138	-1.118956
H	0.514375	0.886936	1.844828
H	-5.273061	0.078783	-0.977730
H	-4.816704	2.771152	-0.991193
H	-2.404096	3.119803	0.125155
H	0.957039	-1.204971	2.145972
H	0.297466	-3.776111	2.181380
H	-2.209121	-3.943587	1.091209
H	-0.321317	3.696171	2.474450
H	0.061847	5.874295	1.320683

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[Bo_2phenH]$^+$

F	4.735726	0.182340	-0.688040
F	5.149447	-1.871601	0.268593
B	4.244679	-0.895484	0.006762
N	3.597045	-0.347909	1.340443
N	3.016818	-1.463784	-0.810876
C	4.214744	-0.039174	2.474791
C	3.353532	0.714944	3.310857
C	2.166938	0.873954	2.624898
C	2.323386	0.195398	1.386216
C	1.455395	-0.088245	0.340510
C	1.748140	-0.907396	-0.733237
C	0.957116	-1.427346	-1.800197
C	1.767797	-2.296890	-2.492653
C	3.037099	-2.283597	-1.851537
H	5.237000	-0.350005	2.646551
H	3.594979	1.083193	4.296321
H	-0.083760	-1.203516	-2.003357
H	1.505331	-2.892428	-3.353683
H	3.940396	-2.820048	-2.111892
N	0.136543	0.546386	0.339689
C	0.090276	1.912631	-0.264783
C	1.206647	2.426211	-0.905064
C	1.153334	3.723134	-1.413683
F	-3.042554	-3.256998	-0.218481
F	-1.254522	-1.900245	0.379736
B	-2.622652	-1.994072	0.011532
N	-2.757973	-1.059737	-1.224656
N	-3.436174	-1.267187	1.122986
N	-2.233219	2.110334	0.503352
C	-2.710635	-1.331649	-2.531637
C	-2.485359	-0.145585	-3.253080
C	-2.369922	0.881993	-2.323337
C	-2.552962	0.297723	-1.049491
C	-2.707703	0.855321	0.252348
C	-3.280254	0.098339	1.295637
C	-3.758464	0.438868	2.580638
C	-4.216964	-0.735575	3.159637
C	-3.970335	-1.770378	2.237530
C	-1.097441	2.654308	-0.150901
C	-1.124711	3.950678	-0.654214
C	-0.000450	4.485983	-1.276484
H	-0.517413	-0.110300	-0.132842
H	-0.218717	0.584249	1.304885
H	2.119485	1.845792	-0.992245
H	2.026619	4.132354	-1.908095
H	-2.553835	2.577441	1.342092
H	-2.823421	-2.347984	-2.884486
H	-2.433535	-0.057455	-4.327810
H	-2.227125	1.933531	-2.529498
H	-3.824009	1.430447	3.009420
H	-4.680588	-0.847871	4.127946
H	-4.128356	-2.835770	2.337092
H	-2.043803	4.521292	-0.568865
H	-0.034962	5.497131	-1.666272
H	1.286188	1.397629	2.973856

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[Bo_2phenH_2]$^{2+}$

F	2.944488	3.116251	-0.830798
F	2.592880	1.304994	0.533008
B	2.131979	2.090603	-0.494855
N	0.694181	2.628081	-0.105234
N	1.861117	1.150161	-1.737175
C	0.451831	3.694200	0.657066
C	-0.932611	3.806332	0.901578
C	-1.548560	2.753201	0.239069
C	-0.508731	2.006285	-0.389450
C	-0.455480	0.893421	-1.248545
C	0.662835	0.465564	-1.920204
C	0.865714	-0.523021	-2.947984
C	2.160258	-0.392486	-3.361778
C	2.749676	0.646749	-2.567438
H	1.263662	4.330186	0.985860
H	-1.417339	4.598280	1.453494
H	0.135113	-1.216803	-3.346463
H	2.666021	-0.951900	-4.134833
H	3.768860	1.014323	-2.580504
N	-1.672123	0.085523	-1.542959
C	-2.891155	0.143040	-0.709920

C	-4.085948	0.284745	-1.401279
C	-5.308512	0.214632	-0.735653
F	2.875998	-3.152944	0.856043
F	2.497992	-1.386010	-0.560250
B	2.058005	-2.138035	0.502261
N	0.611650	-2.682900	0.158303
N	1.811420	-1.158139	1.719749
N	-1.719604	-0.082251	1.543030
C	0.342111	-3.779690	-0.548870
C	-1.046415	-3.874951	-0.780321
C	-1.636642	-2.778427	-0.168585
C	-0.577911	-2.024876	0.419752
C	-0.504215	-0.886329	1.241993
C	0.625278	-0.449189	1.889569
C	0.847134	0.558928	2.894420
C	2.139430	0.413261	3.310517
C	2.709124	-0.654657	2.539881
C	-2.915875	-0.084501	0.672892
C	-4.135266	-0.159234	1.330829
C	-5.333435	-0.020992	0.631678
H	-1.956208	0.300762	-2.508292
H	-1.360776	-0.908742	-1.533013
H	-4.074042	0.447478	-2.476368
H	-6.230600	0.334949	-1.293404
H	-2.032961	-0.343050	2.488219
H	-1.400724	0.908750	1.588929
H	1.138581	-4.446364	-0.853744
H	-1.549457	-4.680274	-1.295105
H	-2.699189	-2.598676	-0.075735
H	0.130407	1.276051	3.276945
H	2.656343	0.980581	4.070324
H	3.720939	-1.041659	2.561786
H	-4.162534	-0.319985	2.405917
H	-6.275325	-0.089505	1.164589
H	-2.615216	2.606770	0.137029

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Bodach

C	-3.675701	-0.204010	0.100357
C	-3.615219	-1.366607	0.877948
N	-2.345682	-1.758031	1.016053
C	-1.535044	-0.854110	0.350714
C	-2.366835	0.123903	-0.238762
N	-0.475931	-3.337127	1.236675
B	-1.864714	-2.985003	1.855423
C	0.344604	-2.427262	0.613749
C	-0.142092	-1.129130	0.251477
C	0.215164	-4.470766	1.422818
C	1.505852	-4.329150	0.906206
C	1.593035	-3.031409	0.398573
N	0.758947	-0.248189	-0.217364
C	0.659249	1.211248	-0.273145
C	0.794974	1.716658	-1.714670
N	-0.283597	1.165608	-2.521230
C	0.725448	3.243645	-1.735949
C	1.794354	3.873808	-0.843914
C	1.675831	3.354040	0.589695
C	1.736121	1.825760	0.626323
F	-2.742307	-4.031494	1.697798
F	-1.710196	-2.627286	3.176763
H	-4.573479	0.315506	-0.198906
H	-4.409554	-1.942252	1.332299
H	-2.048723	0.909759	-0.909974
H	-0.247235	-5.312166	1.919218
H	2.274694	-5.086836	0.892959
H	2.448638	-2.603529	-0.107962
H	1.712396	-0.589475	-0.208203
H	-0.327143	1.487704	0.108426
H	1.802238	1.413704	-2.064651
H	-0.194878	1.473156	-3.485171
H	-0.235841	0.149451	-2.525088
H	-0.276098	3.539452	-1.397245
H	0.827515	3.595137	-2.769221
H	1.706645	4.964114	-0.862285
H	2.790033	3.629211	-1.237348
H	0.720942	3.684984	1.017750
H	2.467296	3.770906	1.219466
H	1.609111	1.450120	1.646231
H	2.724793	1.492635	0.276220

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[BodachH]$^+$ (Protonated primary amine)

C	-3.521135	0.218182	1.176438
C	-3.544817	-1.082875	0.661231
N	-2.292190	-1.557123	0.591176
C	-1.421592	-0.582467	1.030382
C	-2.180127	0.543330	1.403947
N	-0.483325	-3.208592	0.676847
B	-1.747869	-2.817597	-0.131611
C	0.413988	-2.217391	1.039993
C	-0.018062	-0.873987	1.046864
C	0.152549	-4.382366	0.718018
C	1.475190	-4.194059	1.157864
C	1.652402	-2.828741	1.333839
N	0.890254	0.131882	1.018295
C	0.704178	1.370730	0.259127
C	0.558171	1.137607	-1.264373
N	-0.683999	0.334775	-1.622638
C	0.474301	2.465047	-2.020781
C	1.689633	3.349132	-1.737278
C	1.834383	3.593667	-0.237056

C	1.920548	2.268663	0.516603
F	-1.287338	-2.347971	-1.403003
F	-2.655714	-3.810508	-0.238145
H	-4.382944	0.830416	1.395895
H	-4.379826	-1.691406	0.342819
H	-1.811040	1.440187	1.881851
H	-0.350635	-5.289857	0.412678
H	2.202032	-4.973381	1.329596
H	2.544345	-2.341218	1.705408
H	1.855654	-0.176560	1.048381
H	-0.189113	1.888820	0.615283
H	1.405561	0.541480	-1.622205
H	-0.879803	0.442271	-2.623243
H	-0.644076	-0.691744	-1.444495
H	-1.503484	0.674973	-1.099861
H	-0.440141	2.990820	-1.711297
H	0.390006	2.268020	-3.095910
H	1.581572	4.292209	-2.277744
H	2.593099	2.861874	-2.124068
H	0.975957	4.170514	0.128820
H	2.726287	4.189711	-0.031066
H	1.995482	2.428056	1.595660
H	2.827276	1.730198	0.204121

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[BodachH]$^+$ (Protonated secondary amine)

C	-3.965685	-0.798713	-0.411538
C	-3.763849	-1.715711	0.652416
N	-2.466497	-1.902173	0.859001
C	-1.772912	-1.121988	-0.052614
C	-2.717265	-0.420364	-0.855521
N	-0.298775	-2.897144	1.591297
B	-1.805806	-2.712490	2.046297
C	0.361063	-2.087753	0.679654
C	-0.389982	-1.221041	-0.102004
C	0.596113	-3.703208	2.147499
C	1.885788	-3.450189	1.612643
C	1.743563	-2.433553	0.693915
N	0.310244	-0.348986	-1.035618
C	0.590680	1.061766	-0.526635
C	0.806155	1.914989	-1.782626
N	-0.317488	1.649274	-2.686409
C	1.023031	3.369311	-1.360953
C	2.189160	3.483388	-0.372959
C	1.980132	2.586631	0.850395
C	1.754804	1.122714	0.445154
F	-2.406469	-3.924816	2.179119
F	-1.829427	-1.943204	3.174900
H	-4.923201	-0.479630	-0.794212
H	-4.497038	-2.230854	1.259528
H	-2.490616	0.251079	-1.673950
H	0.296418	-4.421135	2.899929
H	2.792864	-3.970212	1.880663
H	2.532973	-1.998791	0.093712
H	-0.253085	-0.155536	-1.898725
H	1.189835	-0.787494	-1.328486
H	-0.344953	1.360405	-0.037726
H	1.719374	1.554292	-2.279354
H	-1.100768	2.261834	-2.465120
H	-0.068208	1.834325	-3.653426
H	0.099333	3.740300	-0.894572
H	1.201935	3.979044	-2.251397
H	2.306192	4.523616	-0.059796
H	3.120976	3.201075	-0.879154
H	1.112166	2.936800	1.422440
H	2.840924	2.644295	1.520322
H	1.560819	0.498620	1.322410
H	2.657859	0.736418	-0.050466

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Bo_2dach

N	-1.608187	0.409788	-1.356508
C	-2.862751	0.448490	-0.638773
C	-2.862727	-0.448543	0.638778
C	-0.489516	1.097226	-1.042398
C	0.732915	0.595150	-1.565760
N	1.933302	1.229253	-1.322036
N	-1.608154	-0.409803	1.356492
N	0.732412	2.915232	-0.014849
C	-0.465140	2.243105	-0.161930
C	1.015348	-0.654716	-2.160210
C	2.396324	-0.754279	-2.259686
C	2.923711	0.433384	-1.732625
C	0.597294	3.865630	0.916035
C	-0.702410	3.848621	1.421672
C	-1.376963	2.830117	0.747865
B	2.057494	2.689910	-0.818889
F	3.136754	2.826613	0.025029
F	2.112906	3.565553	-1.879432
C	-4.070455	0.064340	-1.492131
C	-4.070425	-0.064425	1.492159
C	-5.346406	0.344972	-0.685230
C	-0.489474	-1.097223	1.042383
C	0.732949	-0.595129	1.565746
N	1.933343	-1.229228	1.322051
N	0.732482	-2.915207	0.014832
C	-0.465082	-2.243102	0.161915
C	1.015363	0.654742	2.160194
C	2.396337	0.754313	2.259696
C	2.923740	-0.433349	1.732651
C	0.597381	-3.865602	-0.916057

C	-0.702322	-3.848614	-1.421695
C	-1.376894	-2.830125	-0.747883
B	2.057553	-2.689879	0.818889
F	3.136822	-2.826562	-0.025019
F	2.112961	-3.565533	1.879423
C	-5.346383	-0.345092	0.685283
H	-1.448208	-0.419754	-1.916963
H	-3.019256	1.484704	-0.343999
H	-3.019208	-1.484762	0.344008
H	-1.448192	0.419737	1.916954
H	0.309355	-1.435271	-2.418485
H	2.963046	-1.602847	-2.610189
H	3.952412	0.747705	-1.624251
H	1.438666	4.494653	1.169774
H	-1.104153	4.496414	2.186190
H	-2.402176	2.561758	0.942439
H	-4.066427	0.644316	-2.419355
H	-4.017434	-0.998421	-1.767385
H	-4.017427	0.998337	1.767412
H	-4.066365	-0.644401	2.419383
H	-6.225561	0.035248	-1.257130
H	-5.432059	1.430086	-0.542820
H	0.309358	1.435294	2.418449
H	2.963047	1.602887	2.610203
H	3.952445	-0.747667	1.624303
H	1.438763	-4.494612	-1.169796
H	-1.104054	-4.496409	-2.186217
H	-2.402108	-2.561775	-0.942462
H	-6.225536	-0.035392	1.257198
H	-5.432010	-1.430209	0.542874

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[Bo_2dachH]$^+$

N	2.021443	1.669324	-1.240468
C	2.845145	0.559133	-0.564391
C	2.640117	0.588874	0.959251
C	0.554420	1.613746	-1.136803
C	-0.057439	2.562543	-0.304451
N	-1.428716	2.547807	-0.175924
N	1.269129	0.339160	1.371404
N	-1.497192	0.556248	-1.687956
C	-0.109077	0.628116	-1.820786
C	0.467528	3.544281	0.571885
C	-0.619942	4.110772	1.223137
C	-1.771377	3.467338	0.728108
C	-1.916192	-0.512027	-2.332437
C	-0.809773	-1.198643	-2.932679
C	0.314394	-0.484867	-2.627454
B	-2.425633	1.663344	-1.022114
F	-3.336524	1.064399	-0.207466
F	-2.975139	2.422606	-2.013335
C	4.300660	0.785723	-0.963960
C	3.658720	-0.275428	1.728880
C	5.227387	-0.197568	-0.243213
C	0.384404	-0.662650	1.132385
C	0.659023	-1.863492	0.403128
N	-0.396869	-2.712457	0.122353
N	-1.964956	-1.301187	1.403709
C	-0.920668	-0.429975	1.640913
C	1.822585	-2.460358	-0.136563
C	1.442273	-3.651058	-0.746064
C	0.062197	-3.766828	-0.560551
C	-3.044199	-0.851103	2.045956
C	-2.734768	0.331611	2.736557
C	-1.399582	0.600211	2.482682
B	-1.911116	-2.565436	0.505772
F	-2.651595	-2.376392	-0.651973
F	-2.329679	-3.671719	1.188933
C	5.096130	-0.034005	1.269544
H	2.270338	1.658834	-2.237377
H	2.336391	2.580826	-0.886534
H	2.449649	-0.361822	-0.991719
H	2.832996	1.629121	1.264826
H	0.852651	1.118832	1.860301
H	1.505444	3.823688	0.713219
H	-0.600501	4.901486	1.957944
H	-2.810608	3.625639	0.982947
H	-2.964803	-0.772853	-2.352676
H	-0.875607	-2.115026	-3.499279
H	1.328372	-0.733504	-2.913408
H	4.406714	0.692678	-2.051359
H	4.596813	1.809737	-0.690771
H	3.394527	-1.331114	1.636352
H	3.540356	-0.026866	2.787007
H	6.255052	-0.015044	-0.566039
H	4.982515	-1.224951	-0.540258
H	2.838555	-2.110603	-0.058971
H	2.085409	-4.366156	-1.236224
H	-0.614458	-4.554361	-0.863078
H	-3.981735	-1.385966	1.981965
H	-3.413630	0.905780	3.348350
H	-0.842700	1.439749	2.882035
H	5.764612	-0.725077	1.788324
H	5.412159	0.979035	1.550446

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[Bo_2dachH_2]$^{2+}$

N	-2.509549	1.879843	0.985708
C	-1.157280	2.547043	0.633890
C	0.060169	1.612283	0.778162
C	-2.792717	0.583050	0.372238
C	-2.711061	-0.535175	1.195463

N	-2.825192	-1.786072	0.599753
N	0.136513	0.568671	-0.355081
N	-3.181765	-0.686970	-1.598747
C	-3.069545	0.557602	-0.988498
C	-2.689536	-0.720655	2.614048
C	-2.803080	-2.074959	2.833876
C	-2.869828	-2.702644	1.557981
C	-3.581783	-0.501752	-2.849934
C	-3.764015	0.887049	-3.102103
C	-3.428587	1.556041	-1.946482
B	-2.522160	-1.948921	-0.933845
F	-1.131313	-1.729450	-1.044943
F	-2.960717	-3.106415	-1.441992
C	-1.091013	3.766793	1.566966
C	1.367683	2.428506	0.741285
C	0.218910	4.540505	1.439093
C	1.426856	-0.140139	-0.386488
C	2.340342	0.204925	-1.367489
N	3.610221	-0.348168	-1.287499
N	2.911396	-1.624437	0.730353
C	1.646037	-1.074011	0.617852
C	2.259601	0.964584	-2.574982
C	3.478722	0.838307	-3.199209
C	4.294074	0.030119	-2.356221
C	2.872616	-2.565099	1.664483
C	1.556466	-2.676174	2.187886
C	0.785471	-1.735268	1.539281
B	4.168316	-0.914173	0.086481
F	5.181782	-1.781515	-0.113230
F	4.449353	0.182048	0.868830
C	1.380286	3.597733	1.721631
H	-3.250124	2.551650	0.739703
H	-2.554799	1.784580	2.008217
H	-1.266011	2.863915	-0.410212
H	0.001260	1.022250	1.701546
H	-0.587919	-0.171549	-0.302515
H	0.001008	1.029429	-1.262755
H	-2.652547	0.040186	3.384989
H	-2.855650	-2.579702	3.787546
H	-2.933481	-3.756513	1.315056
H	-3.713380	-1.341976	-3.521056
H	-4.119627	1.315908	-4.027575
H	-3.497489	2.625313	-1.786136
H	-1.950997	4.413660	1.359418
H	-1.182683	3.416283	2.605580
H	1.507231	2.809894	-0.280290
H	2.204865	1.756397	0.947085
H	0.201824	5.375280	2.142907
H	0.308814	4.970618	0.434883
H	1.398384	1.490928	-2.969084
H	3.776006	1.254356	-4.150279
H	5.328729	-0.263316	-2.483493
H	3.766096	-3.112916	1.935335
H	1.238049	-3.382933	2.939446
H	-0.278851	-1.574432	1.655771
H	2.336675	4.115273	1.623920
H	1.327814	3.228842	2.753025

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Bodpen

N	-0.457307	-0.067195	-0.646098
C	-1.685287	0.108238	0.095664
C	-2.619120	-1.068453	-0.314402
C	0.789891	0.263187	-0.309869
C	1.829245	-0.157385	-1.202246
N	3.151988	0.043577	-0.891574
N	-2.704624	-1.065919	-1.772343
N	2.451621	1.210856	1.163986
C	1.118675	1.030644	0.843515
C	1.752885	-0.741961	-2.474213
C	3.066334	-0.889951	-2.927144
C	3.896090	-0.398399	-1.917273
C	2.526547	2.038307	2.210939
C	1.242783	2.434109	2.600841
C	0.349701	1.802936	1.739652
B	3.679589	0.500381	0.502256
F	4.050282	-0.595473	1.251022
F	4.712403	1.397858	0.357659
C	-2.362420	1.444086	-0.169343
C	-2.081634	-2.389271	0.197639
C	-3.387177	1.866443	0.682554
C	-4.057265	3.061247	0.444440
C	-3.709899	3.848161	-0.652228
C	-2.688382	3.435398	-1.501026
C	-2.015201	2.239131	-1.261077
C	-1.218737	-3.180073	-0.563617
C	-0.704977	-4.364482	-0.041742
C	-1.047867	-4.771245	1.243740
C	-1.909506	-3.988615	2.008603
C	-2.422196	-2.806603	1.485695
H	-0.593723	-0.579293	-1.512623
H	-1.469175	0.006060	1.165528
H	-3.584775	-0.878444	0.178462
H	-3.200578	-0.236249	-2.088685
H	-3.218952	-1.879861	-2.094398
H	0.853945	-0.997003	-3.021500
H	3.387729	-1.291028	-3.876606
H	4.974287	-0.341822	-1.869324
H	3.490838	2.306655	2.619446
H	1.001288	3.114898	3.403023
H	-0.720329	1.942057	1.724503
H	-3.653029	1.258563	1.545386

H	-4.845714	3.382141	1.117552
H	-4.228512	4.782990	-0.837283
H	-2.406013	4.048215	-2.350854
H	-1.205840	1.929557	-1.915597
H	-0.950187	-2.872729	-1.569931
H	-0.031948	-4.967707	-0.642183
H	-0.645761	-5.694005	1.648690
H	-2.184864	-4.300152	3.010906
H	-3.097444	-2.198132	2.083674

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[BodpenH]$^+$ (Protonated primary amine)

N	-0.628156	0.263927	0.033817
C	-1.324803	-0.957634	-0.314122
C	-2.735133	-0.839727	0.333693
C	0.717529	0.545842	-0.175928
C	1.173596	1.741461	0.430113
N	2.497800	2.115288	0.350114
N	-2.502498	-0.839115	1.828002
N	2.927893	0.090898	-0.989990
C	1.582544	-0.250989	-0.939468
C	0.468654	2.759627	1.107540
C	1.390848	3.750322	1.418433
C	2.636078	3.303253	0.943819
C	3.524965	-0.669769	-1.898415
C	2.589046	-1.547615	-2.487460
C	1.372908	-1.290952	-1.887488
B	3.646175	1.130073	-0.053275
F	4.627558	1.777529	-0.748064
F	4.101344	0.485681	1.071017
C	-0.667363	-2.221312	0.223797
C	-3.525791	0.376701	-0.082469
C	-1.041805	-3.446515	-0.333061
C	-0.532399	-4.637331	0.175115
C	0.353335	-4.613345	1.250129
C	0.727900	-3.396565	1.812548
C	0.219028	-2.201426	1.306097
C	-3.518367	1.572441	0.643697
C	-4.219089	2.681943	0.174752
C	-4.924357	2.605039	-1.021208
C	-4.935030	1.415479	-1.747729
C	-4.241532	0.305647	-1.280092
H	-1.201980	1.095807	-0.071884
H	-1.499710	-1.061241	-1.395360
H	-3.291799	-1.753693	0.112663
H	-2.103745	-1.743494	2.114349
H	-3.357609	-0.638190	2.353600
H	-1.784897	-0.128872	2.037324
H	-0.593251	2.783360	1.317409
H	1.203359	4.686718	1.921477
H	3.609643	3.768380	1.015774
H	4.582982	-0.556211	-2.093163
H	2.795438	-2.267007	-3.265157
H	0.439627	-1.778421	-2.122073
H	-1.718140	-3.469099	-1.185697
H	-0.820013	-5.581716	-0.274322
H	0.758746	-5.540206	1.640889
H	1.432513	-3.369708	2.636785
H	0.557712	-1.257110	1.725901
H	-2.979406	1.667592	1.585102
H	-4.211434	3.602662	0.747520
H	-5.469484	3.468897	-1.385303
H	-5.489950	1.350102	-2.677166
H	-4.259448	-0.622245	-1.846237

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[BodpenH]$^+$ (Protonated secondary amine)

N	-0.608984	0.386218	-0.890992
C	-1.047293	1.216291	0.325702
C	-2.455244	1.756383	-0.029337
C	0.524928	-0.490958	-0.634874
C	1.785709	-0.118589	-1.068083
N	2.855298	-0.950351	-0.765597
N	-2.373475	2.477770	-1.298897
N	1.288480	-2.522024	0.367801
C	0.245293	-1.670122	0.049077
C	2.261218	0.930090	-1.909242
C	3.605467	0.705029	-2.098411
C	3.932680	-0.467769	-1.367261
C	0.770533	-3.616553	0.914929
C	-0.641191	-3.515893	0.967894
C	-0.978367	-2.290835	0.428285
B	2.816961	-2.131960	0.288543
F	3.553208	-3.182399	-0.165196
F	3.213871	-1.649443	1.504796
C	0.025230	2.211760	0.679355
C	-3.407191	0.574962	-0.110363
C	0.631294	2.103321	1.931968
C	1.634594	2.990255	2.310273
C	2.047334	3.987250	1.432491
C	1.457942	4.094215	0.174260
C	0.451210	3.212463	-0.203444
C	-3.712228	-0.049512	-1.325634
C	-4.491682	-1.208343	-1.347231
C	-4.975607	-1.746779	-0.160119
C	-4.688231	-1.119882	1.053126
C	-3.907394	0.030114	1.076836
H	-1.424695	-0.182052	-1.172866
H	-0.448335	1.044960	-1.663428
H	-1.145743	0.486493	1.133149
H	-2.752574	2.387913	0.818814

H	-2.057485	3.428995	-1.132013
H	-3.301798	2.558470	-1.706347
H	1.679664	1.737032	-2.333780
H	4.290993	1.290354	-2.692038
H	4.890011	-0.960859	-1.258511
H	1.413622	-4.420350	1.248471
H	-1.312933	-4.268213	1.352239
H	-1.979795	-1.893155	0.298882
H	0.322745	1.315902	2.614235
H	2.097792	2.893562	3.285968
H	2.832655	4.676494	1.723510
H	1.783952	4.865735	-0.515136
H	0.017115	3.303337	-1.196089
H	-3.361886	0.373761	-2.264699
H	-4.724282	-1.680901	-2.295598
H	-5.585233	-2.643533	-0.177514
H	-5.077848	-1.525120	1.980950
H	-3.687721	0.514877	2.025296

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[BodpenH$_2$]$^{2+}$

N	0.493137	-0.669671	-1.177571
C	1.287299	-0.938348	0.097030
C	0.826526	0.091236	1.175784
C	-0.963187	-0.702610	-0.950995
C	-1.661842	0.472621	-1.173875
N	-2.957308	0.550898	-0.680389
N	1.671162	-0.186524	2.413699
N	-2.804032	-1.803067	0.064683
C	-1.513080	-1.875240	-0.436320
C	-1.400892	1.657523	-1.931579
C	-2.552082	2.408046	-1.890386
C	-3.485792	1.697471	-1.081521
C	-3.197960	-3.030307	0.384968
C	-2.174390	-3.963286	0.073254
C	-1.107687	-3.243078	-0.423296
B	-3.380523	-0.407488	0.500879
F	-2.608956	-0.001709	1.596151
F	-4.709428	-0.427220	0.697405
C	2.762749	-1.039089	-0.209706
C	0.902418	1.565471	0.864960
C	3.497411	-2.006680	0.488967
C	4.863420	-2.154559	0.264198
C	5.499787	-1.355843	-0.682158
C	4.771072	-0.408901	-1.400594
C	3.409486	-0.244222	-1.163712
C	2.107212	2.207461	0.539622
C	2.121728	3.583207	0.332277
C	0.946678	4.323274	0.461553
C	-0.244672	3.691899	0.810214
C	-0.270209	2.316296	1.018015
H	0.749152	0.264038	-1.527962
H	0.792098	-1.356585	-1.884812
H	0.931569	-1.919542	0.425538
H	-0.202487	-0.153078	1.466427
H	1.496067	-1.111333	2.825229
H	1.457235	0.524515	3.124666
H	2.674799	-0.125245	2.189487
H	-0.503309	1.901742	-2.487192
H	-2.736809	3.350361	-2.384562
H	-4.485624	1.982793	-0.777917
H	-4.169610	-3.200414	0.831403
H	-2.242243	-5.034875	0.189129
H	-0.182994	-3.654255	-0.810443
H	2.996877	-2.681085	1.182787
H	5.420692	-2.910408	0.806683
H	6.560331	-1.480448	-0.872220
H	5.263337	0.202827	-2.148756
H	2.877557	0.522248	-1.723851
H	3.039775	1.655332	0.466437
H	3.053647	4.080828	0.087019
H	0.966476	5.396884	0.307021
H	-1.154797	4.269560	0.930917
H	-1.198349	1.818462	1.295421

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Bo$_2$dpen

N	-1.664536	0.773712	0.128027
C	-0.279564	0.713153	-0.287588
C	0.577416	1.166112	0.947732
C	-2.642933	-0.112263	-0.122587
C	-3.873614	0.070923	0.581491
N	-4.880268	-0.860100	0.490401
N	1.986658	1.006508	0.669271
N	-3.511392	-2.129098	-1.118160
C	-2.510812	-1.175170	-1.054013
C	-4.318705	1.132603	1.384722
C	-5.621541	0.820112	1.775709
C	-5.924040	-0.421331	1.208362
C	-3.241863	-2.956223	-2.130891
C	-2.061410	-2.559843	-2.772927
C	-1.596756	-1.436112	-2.100361
B	-4.706950	-2.286998	-0.119310
F	-4.373822	-3.179927	0.874779
F	-5.837969	-2.662542	-0.802042
C	0.035239	1.512886	-1.536076
C	0.265602	2.586078	1.368325
C	1.199197	1.221329	-2.255562
C	1.563138	1.998079	-3.352001
C	0.758257	3.063492	-3.749570
C	-0.415939	3.339352	-3.054508
C	-0.775972	2.568266	-1.952369

C	0.736291	3.689774	0.648422
C	0.392988	4.979854	1.039292
C	-0.436640	5.183786	2.139457
C	-0.916604	4.092329	2.856078
C	-0.560325	2.800496	2.475212
C	2.683718	-0.138578	0.587822
C	2.189717	-1.416070	0.973903
N	3.081516	-2.477659	0.973508
N	4.883134	-1.070118	0.062055
C	3.995373	-0.024682	0.024633
C	0.916791	-1.935879	1.322084
C	1.070707	-3.300485	1.524877
C	2.423898	-3.589009	1.307187
C	5.987370	-0.710692	-0.608538
C	5.835514	0.584898	-1.110713
C	4.570689	1.022733	-0.714055
B	4.644976	-2.389610	0.852429
F	5.198881	-2.303858	2.108674
F	5.115624	-3.467257	0.143582
H	-1.899045	1.521628	0.769658
H	-0.029389	-0.336948	-0.466600
H	0.319388	0.504877	1.780515
H	2.499563	1.845490	0.436574
H	-3.779018	2.039729	1.628702
H	-6.280168	1.419973	2.385465
H	-6.822260	-1.018075	1.280656
H	-3.906732	-3.780754	-2.347458
H	-1.615808	-3.030105	-3.636155
H	-0.741801	-0.838842	-2.380036
H	1.823537	0.378854	-1.965616
H	2.469596	1.760322	-3.899351
H	1.037791	3.666020	-4.607515
H	-1.055157	4.157685	-3.369280
H	-1.690743	2.791088	-1.411447
H	1.352952	3.549666	-0.236997
H	0.766577	5.827946	0.475134
H	-0.705687	6.191668	2.437315
H	-1.556680	4.242580	3.719188
H	-0.915824	1.948682	3.051211
H	-0.024502	-1.410857	1.381893
H	0.295132	-4.006827	1.778707
H	2.952884	-4.529499	1.375363
H	6.816396	-1.398230	-0.697409
H	6.554222	1.124410	-1.708684
H	4.103315	1.962587	-0.981378

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[Bo_2dpenH]$^+$

N	1.448826	0.535109	-1.281510
C	0.055434	0.517760	-0.642177
C	-0.756998	1.652479	-1.356118
C	2.440405	-0.377947	-0.700545
C	3.572482	0.209643	-0.150767
N	4.536268	-0.598386	0.424896
N	-2.131090	1.644804	-0.888474
N	3.131137	-2.587305	-0.157818
C	2.192816	-1.739464	-0.735394
C	3.997499	1.564696	-0.037911
C	5.212126	1.542764	0.613589
C	5.507687	0.182923	0.882100
C	2.692478	-3.830890	-0.287074
C	1.446059	-3.847590	-0.966266
C	1.128408	-2.540549	-1.252969
B	4.533910	-2.181636	0.457898
F	5.528441	-2.647165	-0.352158
F	4.621643	-2.620151	1.744015
C	0.102695	0.537402	0.858668
C	-0.126602	3.016015	-1.151514
C	-0.720939	-0.376145	1.521597
C	-0.785293	-0.383786	2.910815
C	0.001950	0.497910	3.645668
C	0.849944	1.389388	2.990246
C	0.897259	1.417736	1.600654
C	-0.331747	3.754893	0.018500
C	0.310151	4.975975	0.198524
C	1.176952	5.466320	-0.776348
C	1.389576	4.739370	-1.943787
C	0.732621	3.523766	-2.132989
C	-2.914029	0.555364	-0.684245
C	-2.740956	-0.647423	-1.436373
N	-3.374972	-1.797042	-1.019204
N	-4.642278	-0.500311	0.641487
C	-3.941495	0.635163	0.279766
C	-2.127366	-0.916341	-2.677494
C	-2.404021	-2.248894	-2.986441
C	-3.173765	-2.755107	-1.930441
C	-5.568368	-0.151503	1.536076
C	-5.517705	1.235630	1.765013
C	-4.481860	1.731435	0.987532
B	-4.111305	-1.942351	0.357010
F	-5.125848	-2.845589	0.265801
F	-3.173008	-2.266436	1.327967
H	1.340577	0.310609	-2.278806
H	1.809410	1.500195	-1.241944
H	-0.371747	-0.431600	-0.954498
H	-0.729351	1.440205	-2.433584
H	-2.400173	2.467357	-0.367424
H	3.480330	2.451209	-0.389974
H	5.831511	2.387158	0.874793
H	6.371549	-0.244952	1.373840
H	3.272057	-4.660719	0.096851
H	0.868119	-4.727444	-1.204612

H	-1.321461	-1.092066	0.966048
H	-1.447103	-1.089546	3.400851
H	-0.034683	0.486231	4.729810
H	1.477020	2.064540	3.562468
H	1.558008	2.126984	1.110740
H	-0.966850	3.369455	0.812183
H	0.136638	5.542473	1.107140
H	1.673403	6.419657	-0.631476
H	2.043040	5.126131	-2.718368
H	0.856240	2.990779	-3.074775
H	-1.632540	-0.204778	-3.324525
H	-2.125294	-2.781906	-3.883245
H	-3.595945	-3.739813	-1.786703
H	-6.209485	-0.901339	1.979174
H	-4.193026	2.771206	0.901602
H	0.241303	-2.206944	-1.778973
H	-6.173258	1.796866	2.413256

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$[Bo_2dpenH_2]^{2+}$

N	-1.494092	0.025333	1.180156
C	-0.740213	-0.281988	-0.148598
C	0.783013	-0.235058	0.154369
C	-2.934512	-0.218710	1.053824
C	-3.742722	0.861497	0.747338
N	-5.069700	0.611387	0.429874
N	1.537714	-0.046285	-1.194198
N	-4.682615	-1.816935	0.828889
C	-3.360257	-1.539125	1.137079
C	-3.536738	2.274229	0.730236
C	-4.748926	2.843203	0.416647
C	-5.669663	1.774712	0.223466
C	-4.905843	-3.100782	1.082910
C	-3.725469	-3.711400	1.582938
C	-2.749568	-2.738289	1.607761
B	-5.583705	-0.823078	-0.004608
F	-6.892676	-0.981171	0.282553
F	-5.249225	-0.983746	-1.334518
C	-1.311736	0.531906	-1.282035
C	1.308619	0.724578	1.190987
C	-2.413493	-0.019327	-1.948282
C	-3.094120	0.707944	-2.918681
C	-2.653569	1.982466	-3.264404
C	-1.538488	2.531911	-2.632581
C	-0.876237	1.819154	-1.637574
C	0.822481	2.030633	1.369495
C	1.427620	2.884052	2.286456
C	2.534381	2.453819	3.017871
C	3.024337	1.161818	2.846554
C	2.404112	0.296484	1.951016
C	2.974920	-0.294350	-1.035341
C	3.386803	-1.622383	-1.034999
N	4.699804	-1.895245	-0.685360
N	5.107752	0.545352	-0.419041
C	3.791332	0.793722	-0.781492
C	2.777030	-2.837103	-1.465219
C	3.745270	-3.814274	-1.376903
C	4.918875	-3.190452	-0.876950
C	5.719071	1.710651	-0.264887
C	4.818957	2.778014	-0.543985
C	3.605966	2.207846	-0.852001
B	5.571366	-0.865138	0.133691
F	5.149036	-0.931355	1.448430
F	6.891539	-1.061383	-0.059423
H	-1.106908	-0.556459	1.935260
H	-1.313808	0.997779	1.459598
H	-1.014775	-1.327176	-0.320775
H	1.098134	-1.242640	0.441786
H	1.147474	-0.685381	-1.899606
H	1.369898	0.901068	-1.554139
H	-2.623778	2.807280	0.966037
H	-4.981651	3.895012	0.343474
H	-6.713642	1.814540	-0.061566
H	-5.877098	-3.540666	0.894844
H	-3.632743	-4.740852	1.894989
H	-2.781451	-1.007092	-1.682071
H	-3.970202	0.272276	-3.386089
H	-3.175109	2.549777	-4.027874
H	-1.190356	3.521703	-2.907218
H	-0.036860	2.297592	-1.137872
H	-0.015899	2.410322	0.789465
H	1.039968	3.887598	2.423966
H	3.009529	3.127649	3.722880
H	3.891866	0.817369	3.398928
H	2.817065	-0.700743	1.819064
H	1.772759	-2.970632	-1.849508
H	3.651713	-4.855560	-1.646637
H	5.881665	-3.628596	-0.645842
H	6.755751	1.753281	0.045404
H	2.704513	2.737980	-1.134180
H	-1.737170	-2.862243	1.973374
H	5.065307	3.829158	-0.526820

24) Reference

1) Reisfeld, R.; Zusman, R.; Cohen, Y.; Eyal, M. *Chem. Phys. Lett.,* **1988**, *147*, 142-147.