Supplementary Information for:

Highly selective fluorescent OFF-ON thiol probes based on dyads of BODIPY and potent intramolecular electron sink 2,4-dinitrobenzenesulfonyl subunits

Huimin Guo,*[,†] Yingying Jing,[†] Xiaolin Yuan,[‡] Shaomin Ji,[†] Jianzhang Zhao,*[,†] Xiaohuan Li,[‡] Yanyan Kan[¶‡]

[†]State Key Laboratory of Fine Chemicals, School of Chemical Engineering, Dalian University of Technology, Dalian 116024, P. R. China; [‡]Center Laboratory, Affiliated Zhongshan Hospital of Dalian University, Dalian 116001, P. R. China [¶] Department of Immunology, Harbin Medical University, 194 Xuefu Road, Harbin 150081, P. R. China.

* E-mail: zhaojzh@dlut.edu.cn (J. Zhao); guohm@dlut.edu.cn (H. Guo)

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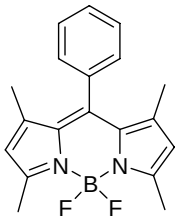
Experimental

General methods

NMR spectra were taken on a 400 MHz Varian Unity Inova spectrophotometer. Mass spectra were recorded with a Q-TOF Micro MS spectrometer. UV-Vis spectra were taken on a HP8453 UV-visible spectrophotometer. Fluorescence spectra were recorded on a JASCO FP-6500 or a Sanco 970 CRT spectrofluorometer. Luminescence quantum yields were measured with BIDIPY (see the following molecular structure) as the reference (Φ = 48 % in acetonitrile).[1] The generation of the ROS species, such as such as $O_2^{-\bullet}$ and $OH^{\bullet}$, are carried out with literature methods.[2] The detection limits of probe **1** and **2** were determined with analytes concentration for which the probes give a signal equal to the blank signal plus three times the standard deviation of the blank measurements (n= 8). The cells luminescence images were obtained using a Nikon ECLIPSE-Ti confocal laser scanning microscopy.



BODIPY

All voltammograms were obtained in a three-electrode cell under Ar atmosphere and room temperature. The working electrode was a Pt microdisk (2 mm^2). The experimental reference electrode was Ag/Ag^+ prepared by anodizing a silver wire in CH_3CN solution of 0.01 M $AgNO_3$. The counter electrode was platinum wire. All potentials are reported relative to the normal hydrogen electrode (NHE) using Fc/Fc^+ as internal reference $E_{1/2}$ (Fc/Fc^+)= 0.08 V. All reversible redox steps result from one electron processes.

The structures of the complexes were optimized using density functional theory (DFT) with B3LYP functional and 6-31G(d)/LanL2DZ basis set. The excited state related calculations were carried out with the time dependent DFT (TD-DFT) with the ground state geometry. The 6-31G(d) basis set was employed for C, H, N, O, S. There are no imaginary frequencies for all optimized structures. All these calculations were performed with Gaussian 09.[3]

References

1. Y. Gabe, Y. Urano, K. Kikuchi, H. Kojima, and T. Nagano. *J. Am. Chem. Soc.* 2004, **126**, 3357.
2. Maeda, H.; Yamamoto, K.; Nomura, Y.; Kohno, I.; Hafsi, L.; Ueda, N.; Yoshida, S.; Fukuda, M.; Fukuyasu, Y.; Yamauchi, Y.; Itoh, N. *J. Am. Chem. Soc.* **2005**, *127*, 68.
3. Frisch, M. J.; Trucks, H. W., et al. Gaussian 09, Revision A. 1; Gaussian, Inc.: Wallingford, CT, **2009**.

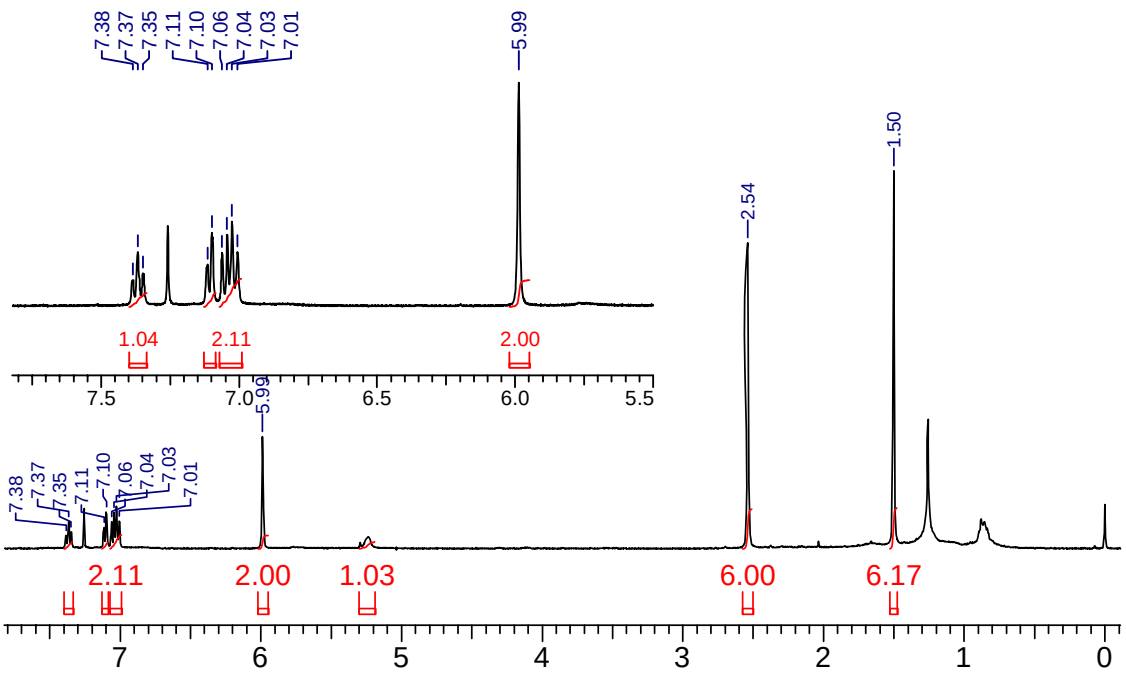


Figure S1. ^{1}H NMR of BODIPY **1** ($CDCl_3$, 400 MHz).

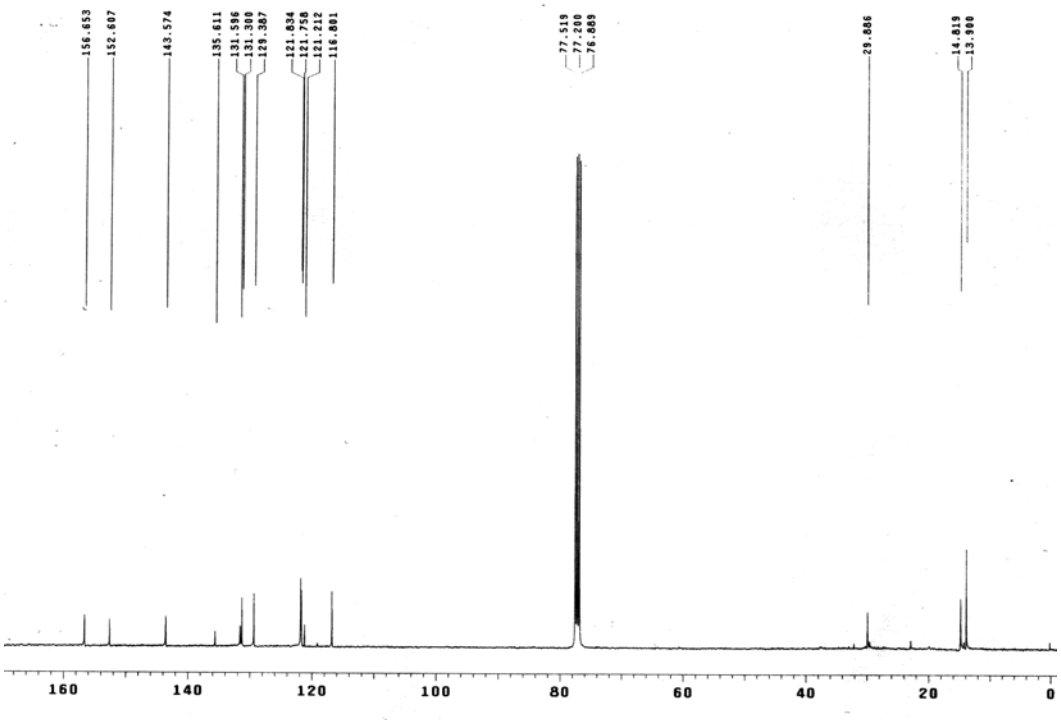


Figure S2. ^{13}C NMR of BODIPY **1** ($CDCl_3$, 100 MHz).

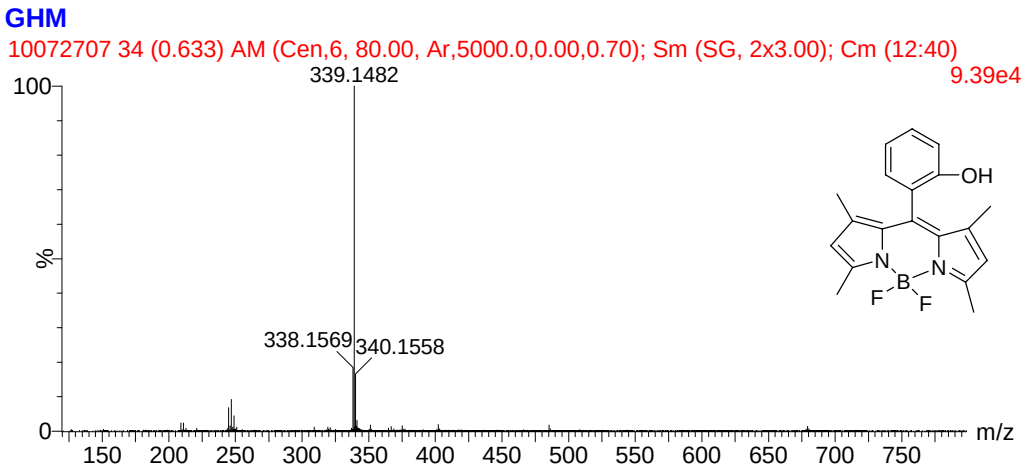
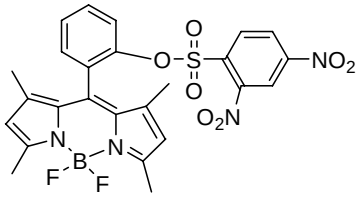


Figure S3. TOF ESI MS of BODIPY **1**.



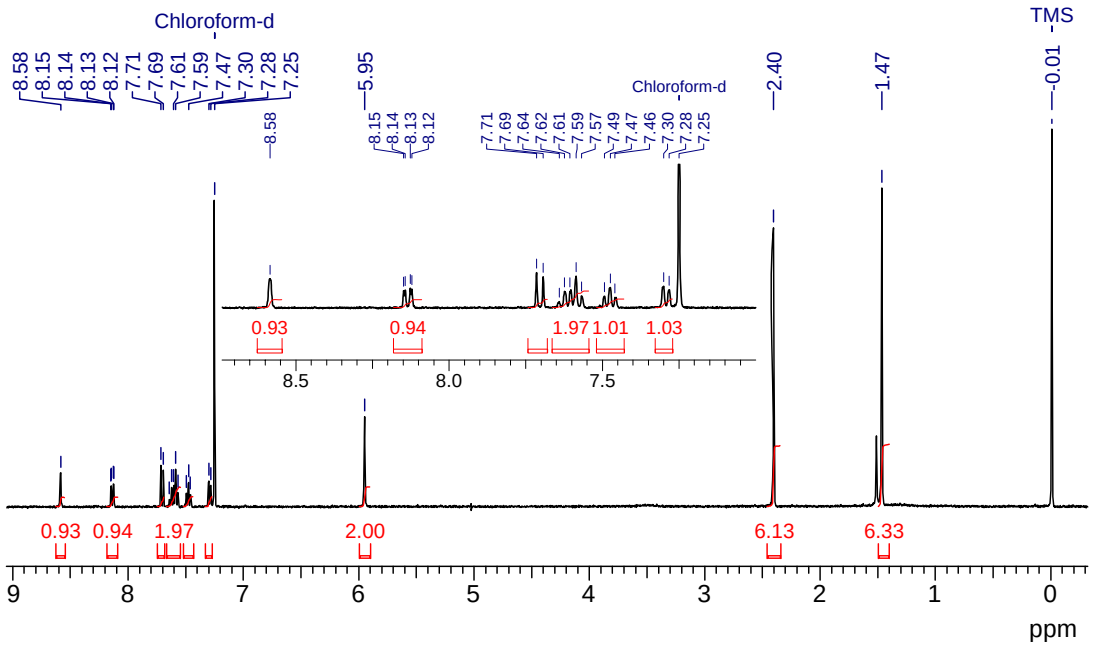


Figure S4. ^{1}H NMR of probe **1** ($CDCl_3$, 400 MHz).

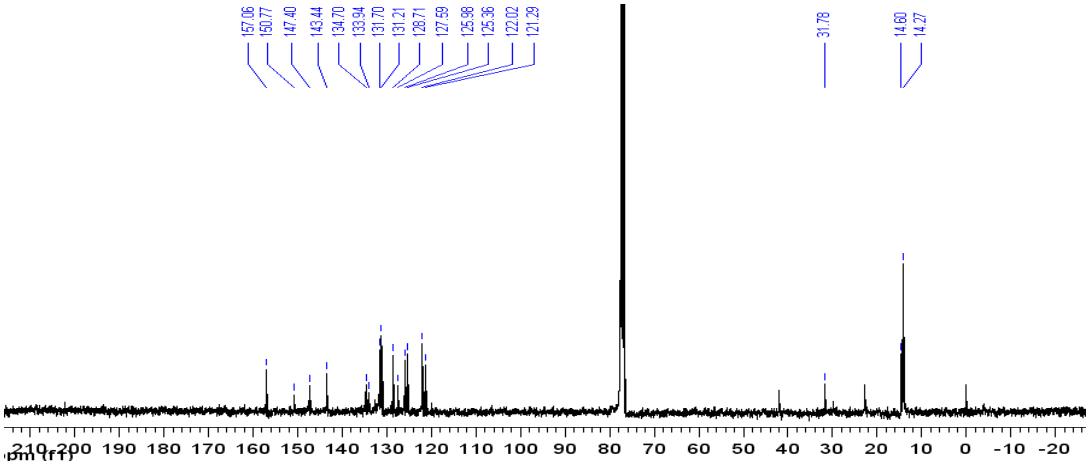


Figure S5. ^{13}C NMR of probe **1** ($CDCl_3$, 100 MHz).

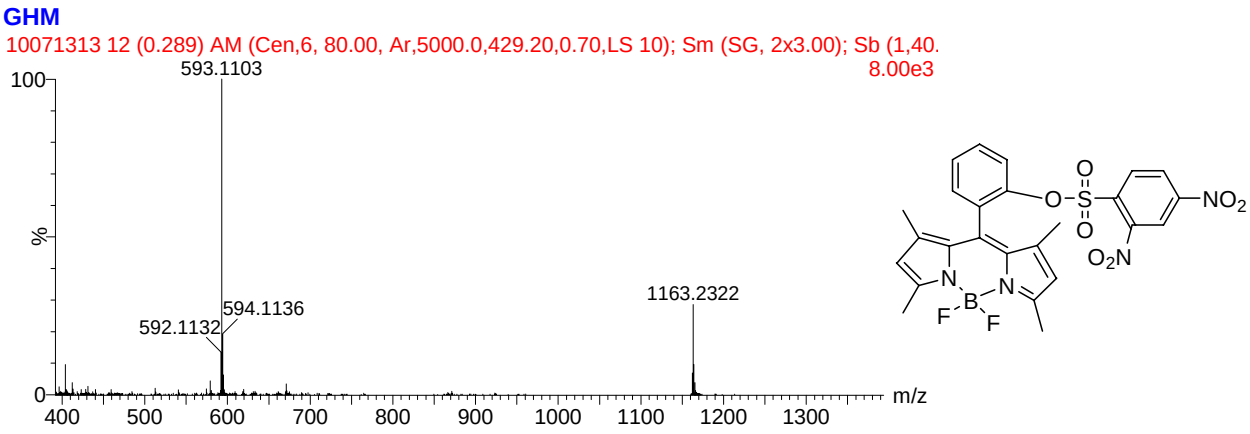


Figure S6. TOF ESI MS of probe **1**.

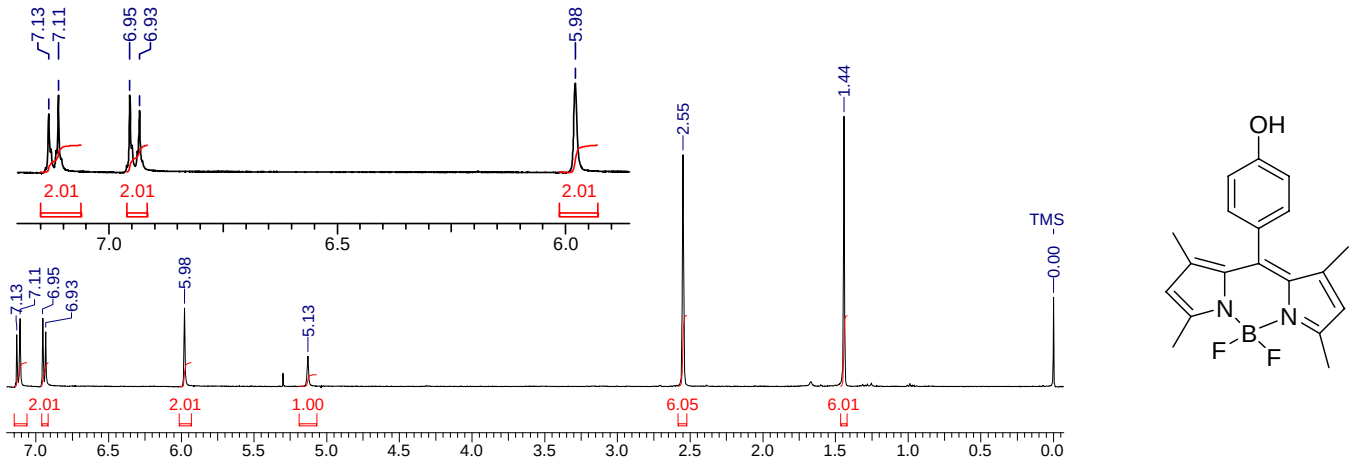


Figure S7. ^{1}H NMR of BODIPY **2** ($CDCl_3$, 400 MHz).

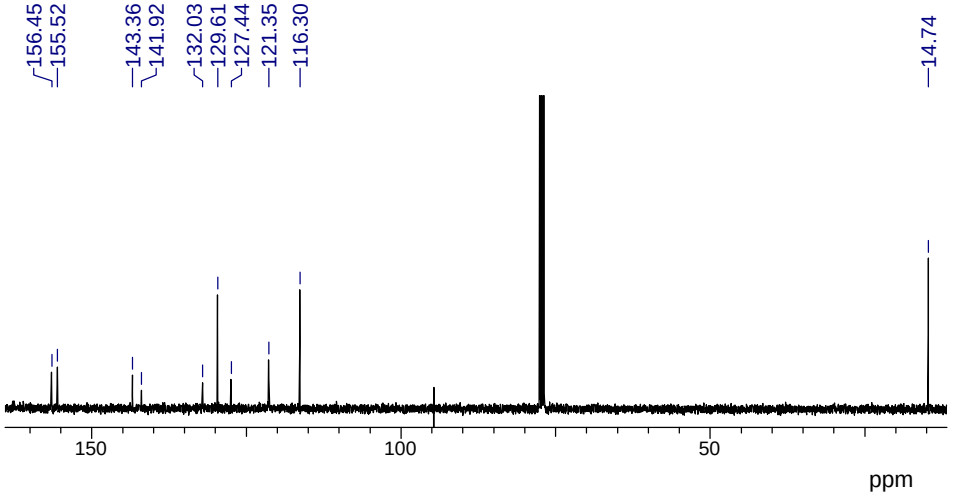


Figure S8. ^{13}C NMR of BODIPY **2** ($CDCl_3$, 100 MHz).

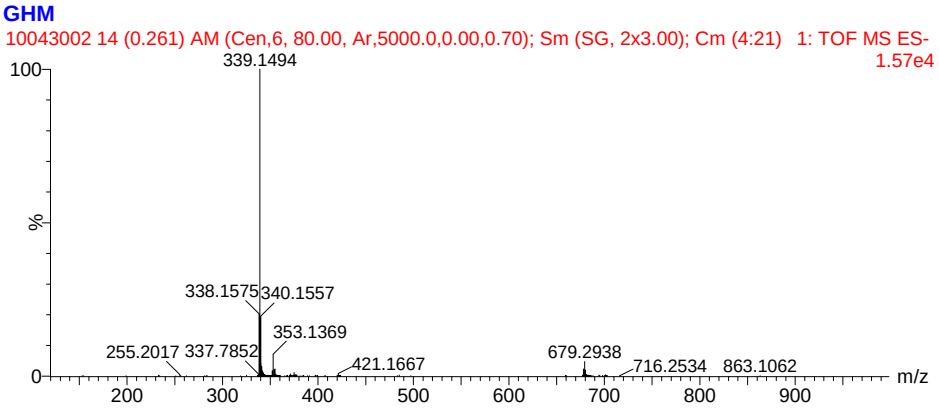


Figure S9. TOF ESI MS of BODIPY **2**.

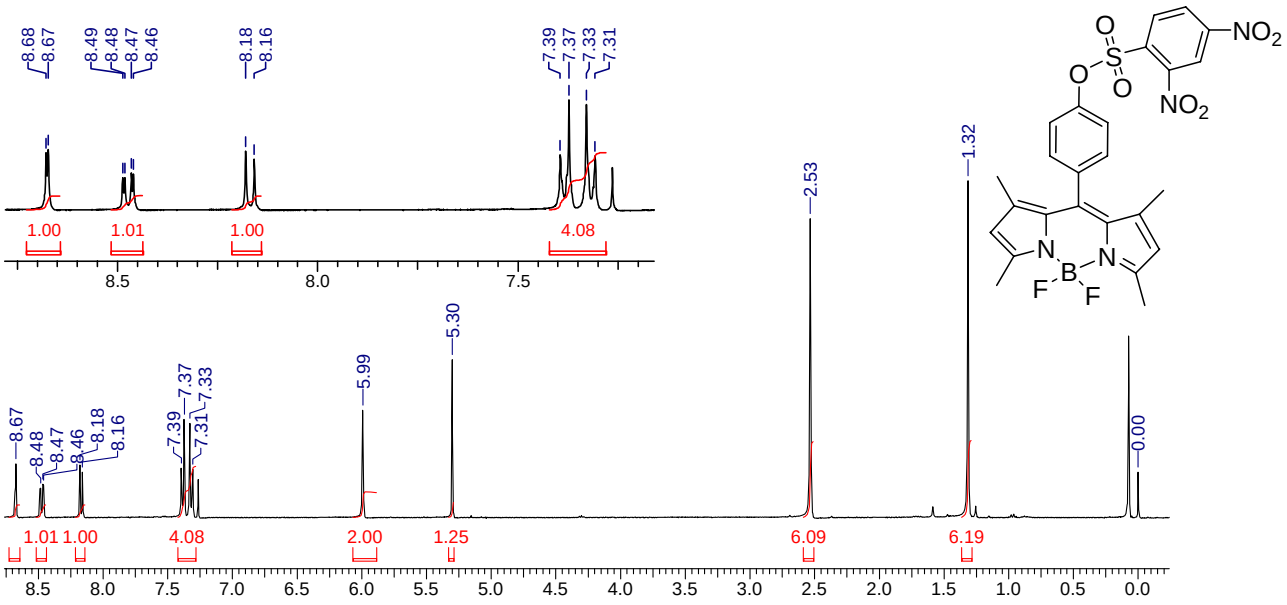


Figure S10. ^{1}H NMR of probe **2** ($CDCl_3$, 400 MHz).

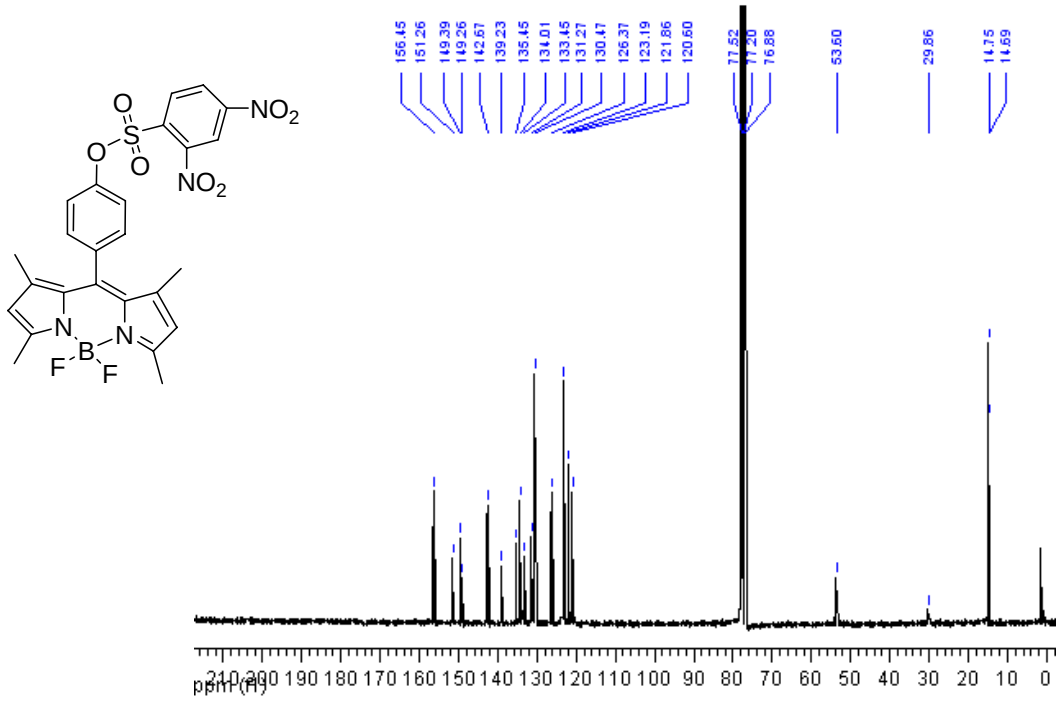


Figure S11. ^{13}C NMR of probe **2** ($CDCl_3$, 100 MHz).

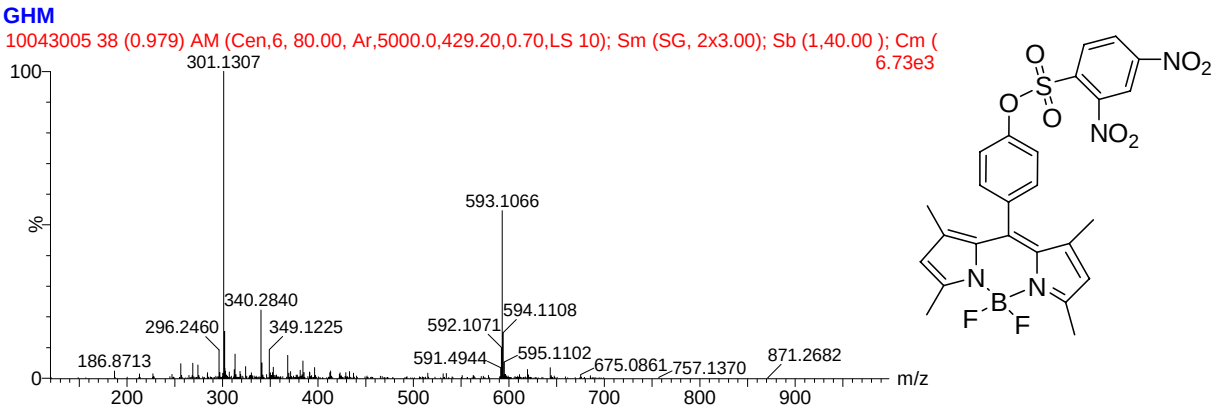
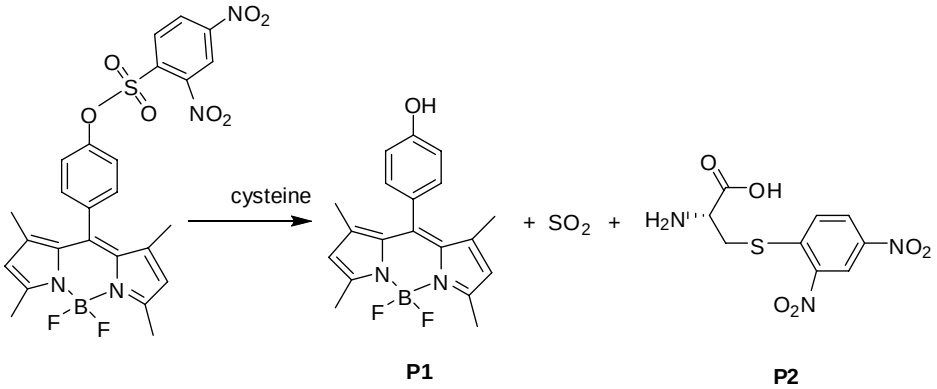


Figure S12. TOF ESI MS of probe **2**.



P1 **P2**

Scheme S1. The reaction mechanism of the probe **2** with R-SH.

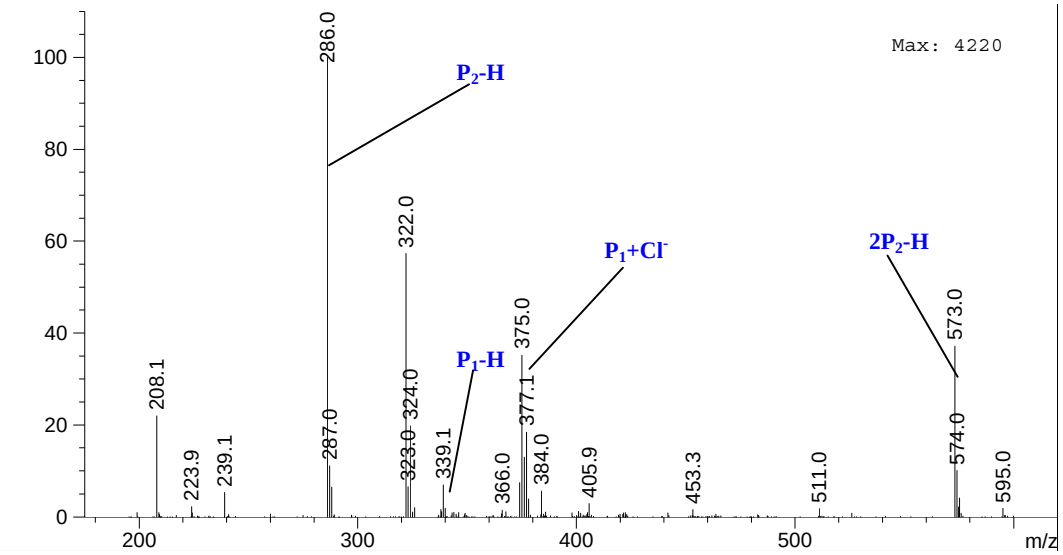


Figure S13. API-ES MS of probe **2** after adding L-Cysteine.

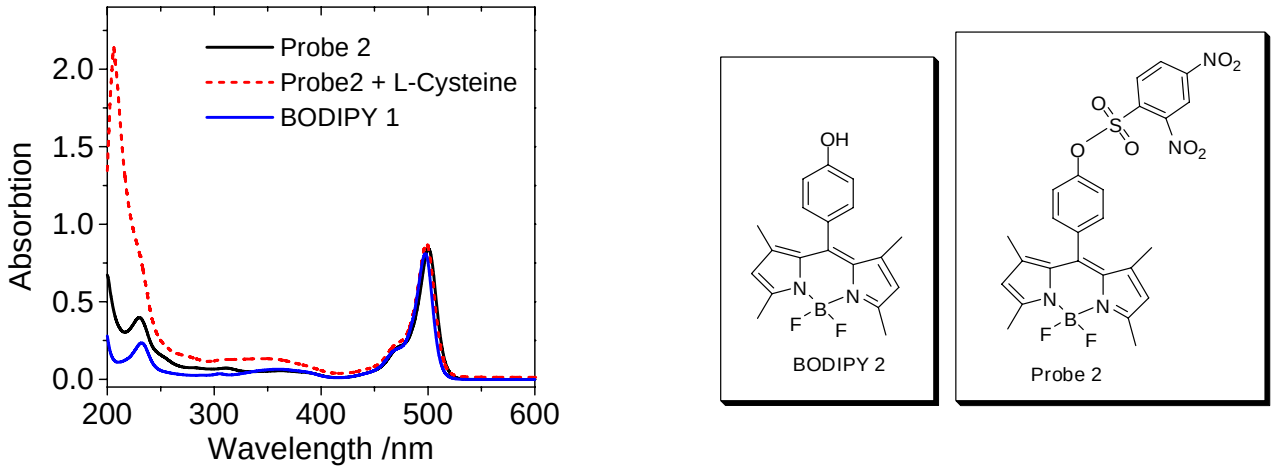


Figure S14. UV-vis absorption of BODIPY **2** and probe **2** before and after addition of L-cysteine. In MeOH/water (4:1, v/v) solution at room temperature. *c* (probe) = 1.0×10^{-5} mol dm^{-3}, *c*(L-cysteine) = 2.0×10^{-3} mol dm^{-3}. 20 °C.

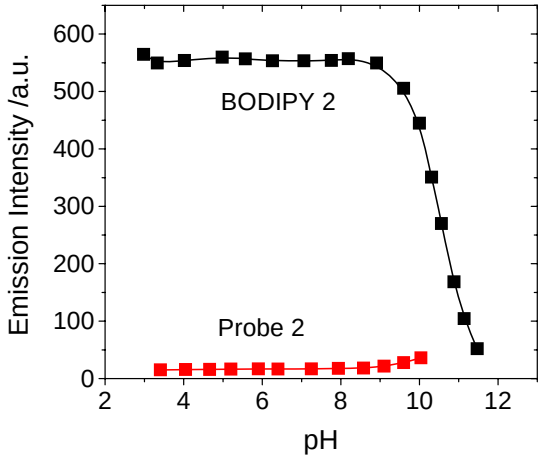


Figure S15. pH titration curve of BODIPY **2** and probe **2**. λem= 512 nm. c = 1.0 × 10^{-5} mol/L. The quench of the fluorescence of BODIPY 1 and BODIPY 2 at basic pH can be rationalized by DFT/TDDFT calculations, please refer to page S13 and S23 of the Supporting Information.

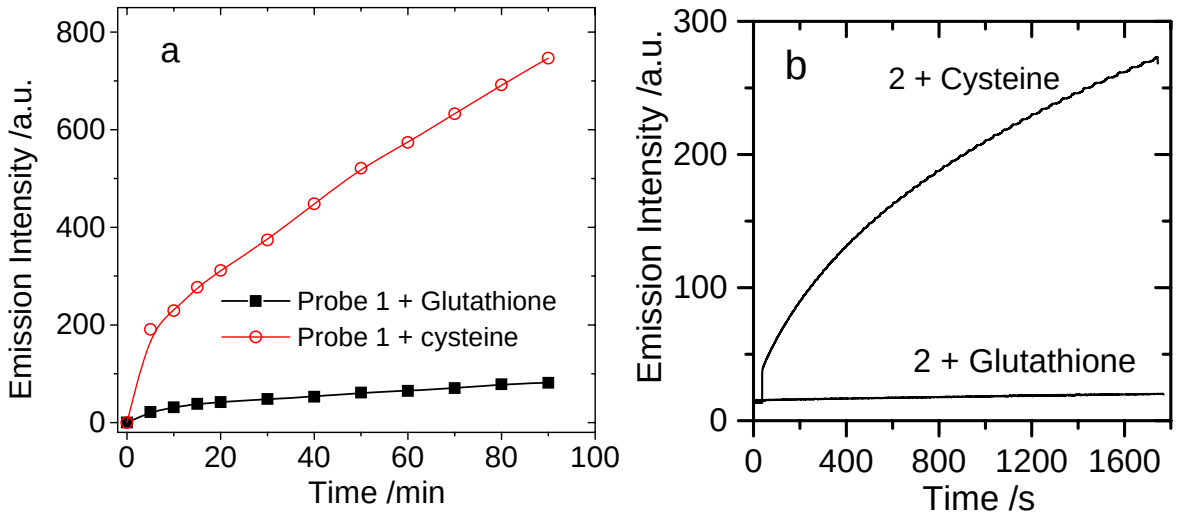


Figure S16. Reaction kinetics of Probes against cysteine and glutathione. (a) Response of Probe **1** against cysteine and glutathione. 20 μM probe **1**. 2 mM analytes. The emission intensity was measured at 514 nm (λex = 450 nm). pH 7.4, methanol/water (4/1, v/v) solution. 37 °C. (b) Response of probe **2** to cysteine and glutathione. 10 μM probe, 2 mM analytes. The emission was monitored at 512 nm (λex = 450 nm). pH 7.4, methanol/water (4:1, v/v) solution. 37 °C.

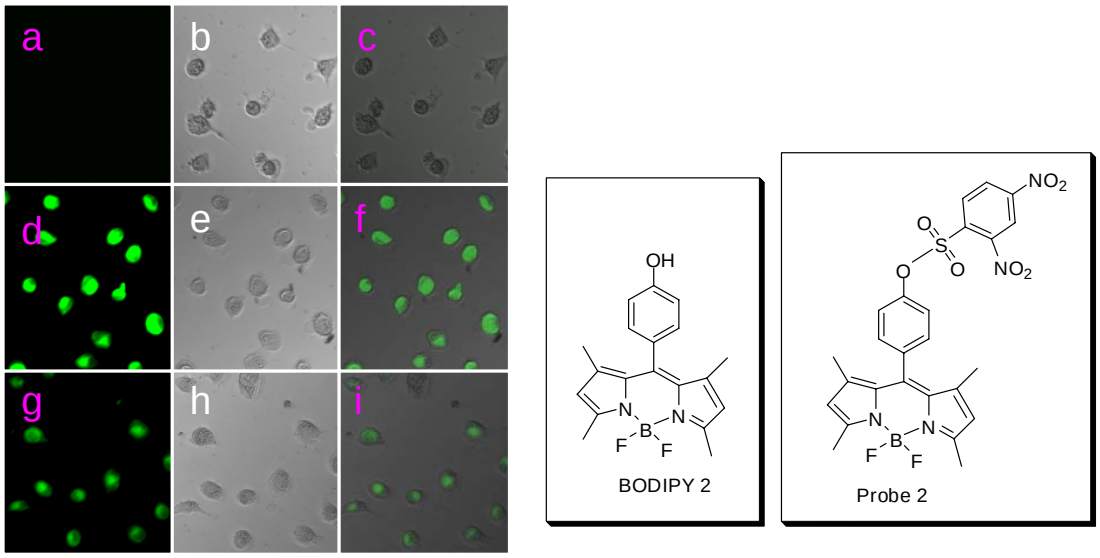


Figure S17. Fluorescence images of NCI-H446 cells. (a) Fluorescence images of cell; (d) Fluorescence images of cells incubated with probe **2** (20 μM) for 10 min. (g) Fluorescence images of cells pretreated with *N*-methylmaleimide (0.5 mM) for 1 h and then incubated with probe 2 (20 μM) for 10 min; (b, e, h) are the corresponding bright field images of (a, d, g); (c), (f) and (i) are the overlay of respective fluorescent and bright images. 37 °C.

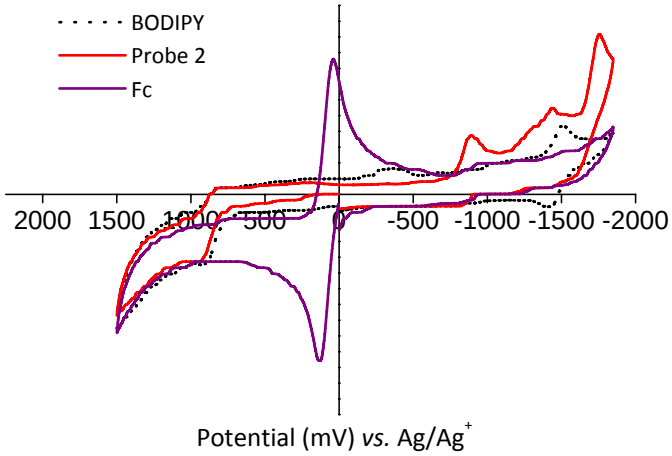


Figure S18. Cyclic voltammograms of BODIPY (black trace), Probe **2** (red trace) and Ferrocene (cyan trace) as the internal Reference in acetonitrile, containing 0.1M $TBAPF_6$, at room temperature. c= 1.0×10^{-3} mol/L. The reversible Fc/Fc^+ redox couple at 0.08 V corresponds to genuine ferrocene.

Table S1. Electrochemical properties of BODIPY and Probe 2. [a]

	E_{ox}[a] (*Ep* mV)	E_{red}[a] (*Ep* mV)	HOMO (eV)		LUMO (eV)	
			Cal.	Exp.	Cal.	Exp.
BODIPY	+922	–1500	–5.34	–5.34	–2.33	–2.92
Probe 2	+995	–890	–5.44	–5.42	–3.73	–3.53
		–1440			–3.17 (LUMO+1)	–2.98 (LUMO+1)
		–1756			–2.45 (LUMO+2)	–2.67 (LUMO+2)

[a] Potentials determined by cyclic voltammetry in CH_3CN solution, containing 0.1 M $TBAPF_6$, [electrochemical window from 1.5 to -1.9 V], at a solute concentration of 1.0 mM, using a scan rate of 200 mV/s.

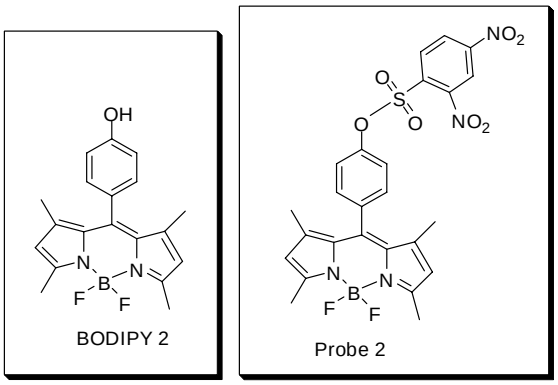
Table S2. Electronic Excitation Energies (eV) and corresponding Oscillator Strengths (*f*), main configurations and CI coefficients of the Low-lying Electronically Excited States Calculated by TDDFT//B3LYP/6-31G(d) for BODIPY **2** and thiol probe **2**, based on the DFT//B3LYP/6-31G(d) Optimized Ground State Geometries.

Sensor	Electronic transition	TDDFT//B3LYP/6-31G(d)			
		Energy (eV) [a]	*f* [b]	Main configurations [c]	CI coefficients [d]
Probe 2	$S_0 \rightarrow S_1$	1.47 eV 842 nm	0.0000	HOMO→LUMO	0.7063
	$S_0 \rightarrow S_5$	3.03 eV 410 nm	0.4610	HOMO−1→LUMO+2	0.1842
				HOMO→LUMO+2	0.5663
BODIPY 2	$S_0 \rightarrow S_1$	3.03 eV 409 nm	0.4708	HOMO→LUMO	0.5683
				HOMO−2→LUMO	0.1791
	$S_0 \rightarrow S_2$	3.33 eV 373 nm	0.0002	HOMO−1→LUMO	0.5565

[a] Only the selected low-lying excited states are presented. [b] Oscillator strength. [c] Only the main configurations are presented. [d] The CI coefficients are in absolute values.

Herein the S_1 state of probe **2** is a dark state because the oscillator strength f = 0.0000 and the HOMO→LUMO transition is an electron transfer transition (no overlap between the initial and the destination molecular orbitals). Thus the S_1 state can not be directly populated by photo-excitation, i.e. $S_0 \rightarrow S_1$ is a forbidden transition. Thus $S_1 \rightarrow S_0$ is also forbidden, and probe **2** is non-fluorescent.

For BODIPY **2**, however, the $S_0 \rightarrow S_1$ is allowed, indicated by the *f* value and the locally-excited feature of the transition (LE). Thus S_1 is probably an emissive state and BODIPY **2** is fluorescent.



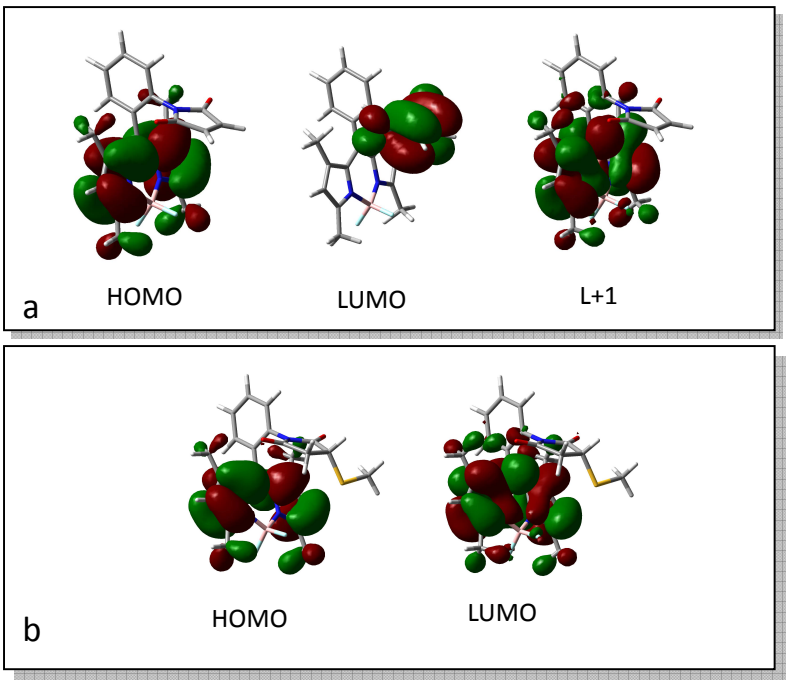
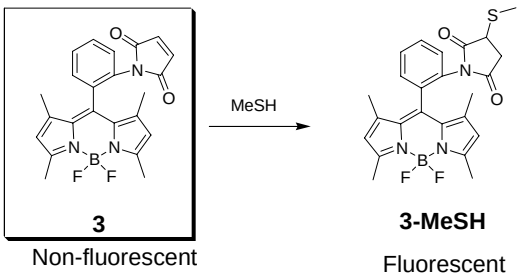


Figure S19. The frontier molecular orbitals of probe **3** before and after reaction with thiols (the thiol was simplified as MeSH). (a) HOMO and LUMO of probe 3. (b) HOMO and LUMO of probe-thiol adduct **3**-MeSH (i.e. the cleavage product of probe 3 in the presence of thiols. Calculated based on ground state geometry by DFT at the B3LYP/6-31G(d)/ LanL2DZ level using Gaussian 09.

Probe **3** was reported, please refer to: Matsumoto, T.; et al.; Nagano, T. *Org. Lett*. **2007**, *9*, 3375.



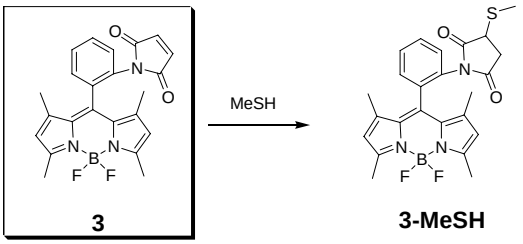
For probe **4** and **5**, similar calculation results were observed. The discrepancy between the calculation results and the experiment results (which indicated that probe **4** and **5** are fluorescent, but calculation predicts non-fluorescent) is probably due to the free energy changes of the electron transfer (ΔG°). In the DFT calculations, the distance between the electron donor and the acceptor is not considered. But this distance is important for the (ΔG°) values (Rehm-Weller equation).

Table S3. Electronic Excitation Energies (eV) and corresponding Oscillator Strengths (*f*), main configurations and CI coefficients of the Low-lying Electronically Excited States Calculated by TDDFT//B3LYP/6-31G(d) for thiol probe **3** and its thiol adduct (Probe **3** + MeSH), based on the DFT//B3LYP/6-31G(d) Optimized Ground State Geometries.

Sensor	Electronic transition	TDDFT//B3LYP/6-31G(d)			
		Energy (eV) [a]	*f* [b]	Main configurations [c]	CI coefficients [d]
Probe 3	$S_0 \rightarrow S_1$	2.00eV 619 nm	0.0004	HOMO→LUMO	0.7065
	$S_0 \rightarrow S_2$	3.00 eV 413 nm	0.4097	HOMO−1→LUMO+1	0.1806
				HOMO→LUMO+1	0.5669
Probe 3 + MeSH	$S_0 \rightarrow S_1$	2.99 eV 414 nm	0.4104	HOMO→LUMO	0.5682
				HOMO−2→LUMO	0.1758
	$S_0 \rightarrow S_2$	3.33 eV 372 nm	0.0262	HOMO−1→LUMO	0.5565
				HOMO−2→LUMO	0.3921

[a] Only the selected low-lying excited states are presented. [b] Oscillator strength. [c] Only the main configurations are presented. [d] The CI coefficients are in absolute values.

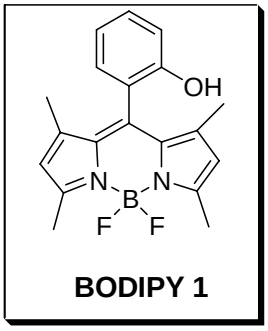
For the discussion of the property of the S_1 state, please refer to page S14.



3
Non-fluorescent

3-MeSH
Fluorescent

BODIPY 1 （DFT//B3LYP/6-31G(d)）



BODIPY 1

No imaginary frequencies.

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C						
C	1	B1				
C	2	B2	1	A1		
C	2	B3	1	A2	3	D1
C	4	B4	2	A3	1	D2
C	5	B5	4	A4	2	D3
C	6	B6	5	A5	4	D4
C	7	B7	6	A6	5	D5
C	8	B8	7	A7	6	D6
H	8	B9	7	A8	6	D7
N	1	B10	3	A9	2	D8
N	9	B11	8	A10	7	D9
B	11	B12	1	A11	3	D10
F	13	B13	11	A12	1	D11
F	13	B14	11	A13	1	D12
C	2	B15	1	A14	11	D13
H	16	B16	2	A15	1	D14
H	16	B17	2	A16	1	D15
H	16	B18	2	A17	1	D16
C	9	B19	8	A18	7	D17
H	20	B20	9	A19	8	D18
H	20	B21	9	A20	8	D19
H	20	B22	9	A21	8	D20
C	7	B23	6	A22	5	D21
H	24	B24	7	A23	6	D22
H	24	B25	7	A24	6	D23
H	24	B26	7	A25	6	D24
C	1	B27	11	A26	4	D25
H	28	B28	1	A27	11	D26
H	28	B29	1	A28	11	D27
H	28	B30	1	A29	11	D28
C	5	B31	4	A30	2	D29
C	32	B32	5	A31	4	D30
C	32	B33	5	A32	4	D31
C	33	B34	32	A33	5	D32
C	34	B35	32	A34	5	D33
H	34	B36	32	A35	5	D34
H	35	B37	33	A36	32	D35
H	36	B38	34	A37	32	D36
H	3	B39	2	A38	1	D37
C	35	B40	33	A39	32	D38
H	41	B41	35	A40	33	D39
O	33	B42	32	A41	5	D40
H	43	B43	33	A42	32	D41

B1	2.27234479
B2	1.38992145

B3	1.43457107
B4	1.40415495
B5	1.40415628
B6	1.43457257
B7	1.38992127
B8	1.40991087
B9	1.08274058
B10	1.34686125
B11	1.34686020
B12	1.55748805
B13	1.39424225
B14	1.39374381
B15	1.50025354
B16	1.09489909
B17	1.09585500
B18	1.09467644
B19	1.49397200
B20	1.09305028
B21	1.09539716
B22	1.09502999
B23	1.50025596
B24	1.09490030
B25	1.09467625
B26	1.09585358
B27	1.49397202
B28	1.09539950
B29	1.09305041
B30	1.09502788
B31	1.49587951
B32	1.40502203
B33	1.39961771
B34	1.39866272
B35	1.39597937
B36	1.08664278
B37	1.08876582
B38	1.08570737
B39	1.08274076
B40	1.39420814
B41	1.08644872
B42	1.36704159
B43	0.96998770
A1	36.04295038
A2	69.92148321
A3	131.83238132
A4	121.07332366
A5	131.83233966
A6	105.96426643
A7	108.50317227
A8	126.34012877
A9	109.00431095
A10	109.00425110
A11	125.26747791
A12	110.11776034
A13	110.01606038
A14	160.65580519

A15	112.53537269
A16	111.65377034
A17	109.73097906
A18	128.32193449
A19	110.51098098
A20	110.51269267
A21	110.59723529
A22	129.37771869
A23	112.53561589
A24	109.73061403
A25	111.65517258
A26	122.67364498
A27	110.51257851
A28	110.51100710
A29	110.59725292
A30	119.43933920
A31	121.50905606
A32	120.00111679
A33	120.36223192
A34	121.44989737
A35	118.43515283
A36	119.53392492
A37	120.12540828
A38	126.34021826
A39	120.19378463
A40	119.45691721
A41	117.34923393
A42	109.11150930
D1	179.94805026
D2	179.54943728
D3	-178.00966815
D4	178.00181605
D5	-179.57931621
D6	0.05200174
D7	179.74884135
D8	-0.17997787
D9	0.17954617
D10	179.19736557
D11	-62.80230805
D12	59.08256259
D13	176.16522817
D14	125.41433190
D15	-114.38562759
D16	5.07024206
D17	-179.67136310
D18	0.50808755
D19	121.49100490
D20	-120.62861480
D21	-1.09255917
D22	58.99529592
D23	179.33881638
D24	-61.20429648
D25	-179.51682595
D26	58.36211881
D27	179.34431975

D28	-59.51817490
D29	4.57922484
D30	-91.25134357
D31	88.74921970
D32	-180.00000000
D33	180.00000000
D34	-0.00000000
D35	180.00000000
D36	180.00000000
D37	-179.69777810
D38	-0.00000000
D39	-180.00000000
D40	0.00000000
D41	-180.00000000

1 3 1.0 11 2.0 28 1.0
2 3 2.0 4 1.0 16 1.0
3 40 1.0
4 5 2.0 11 1.0
5 6 1.0 32 1.0
6 7 2.0 12 1.0
7 8 1.0 24 1.0
8 9 2.0 10 1.0
9 12 1.0 20 1.0
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11 13 1.0
12 13 1.0
13 14 1.0 15 1.0
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16 17 1.0 18 1.0 19 1.0
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20 21 1.0 22 1.0 23 1.0
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24 25 1.0 26 1.0 27 1.0
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28 29 1.0 30 1.0 31 1.0
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32 33 1.5 34 1.5
33 35 1.5 43 1.0
34 36 1.5 37 1.0
35 38 1.0 41 1.5
36 39 1.0 41 1.5
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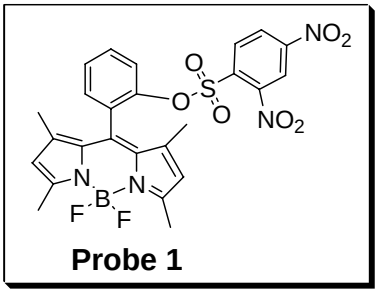
41 42 1.0
42
43 44 1.0
44

Probe 1 （DFT//B3LYP/6-31G(d)）



Probe 1

No imaginary frequencies.

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

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C	1	B1				
C	2	B2	1	A1		
C	2	B3	1	A2	3	D1
C	4	B4	2	A3	1	D2
C	5	B5	4	A4	2	D3
C	6	B6	5	A5	4	D4
C	7	B7	6	A6	5	D5
C	8	B8	7	A7	6	D6
H	8	B9	7	A8	6	D7
N	1	B10	3	A9	2	D8
N	9	B11	8	A10	7	D9
B	11	B12	1	A11	3	D10
F	13	B13	11	A12	1	D11
F	13	B14	11	A13	1	D12
C	2	B15	1	A14	11	D13
H	16	B16	2	A15	1	D14
H	16	B17	2	A16	1	D15
H	16	B18	2	A17	1	D16
C	9	B19	8	A18	7	D17
H	20	B20	9	A19	8	D18
H	20	B21	9	A20	8	D19
H	20	B22	9	A21	8	D20
C	7	B23	6	A22	5	D21
H	24	B24	7	A23	6	D22
H	24	B25	7	A24	6	D23
H	24	B26	7	A25	6	D24
C	1	B27	11	A26	4	D25
H	28	B28	1	A27	11	D26
H	28	B29	1	A28	11	D27
H	28	B30	1	A29	11	D28
C	5	B31	4	A30	2	D29
C	32	B32	5	A31	4	D30
C	32	B33	5	A32	4	D31
C	33	B34	32	A33	5	D32
C	34	B35	32	A34	5	D33
H	34	B36	32	A35	5	D34
H	35	B37	33	A36	32	D35

H	36	B38	34	A37	32	D36	
H	3	B39	2	A38	1	D37	
S	33	B40	32	A39	5	D38	
O	41	B41	33	A40	32	D39	
O	41	B42	33	A41	32	D40	
C	41	B43	33	A42	32	D41	
C	44	B44	41	A43	33	D42	
C	44	B45	41	A44	33	D43	
C	45	B46	44	A45	41	D44	
C	46	B47	44	A46	41	D45	
H	46	B48	44	A47	41	D46	
C	48	B49	46	A48	44	D47	
H	47	B50	45	A49	44	D48	
H	48	B51	46	A50	44	D49	
N	45	B52	44	A51	41	D50	
O	53	B53	45	A52	44	D51	
O	53	B54	45	A53	44	D52	
N	50	B55	48	A54	46	D53	
O	56	B56	50	A55	48	D54	
O	56	B57	50	A56	48	D55	
C	35	B58	33	A57	32	D56	
H	59	B59	35	A58	33	D57	
O	33	B60	32	A59	5	D58	

B1	2.27360981
B2	1.39076711
B3	1.43450047
B4	1.40690323
B5	1.40613619
B6	1.43782862
B7	1.38948961
B8	1.40839693
B9	1.08249774
B10	1.34902506
B11	1.34838270
B12	1.55100262
B13	1.38636556
B14	1.41206131
B15	1.50027580
B16	1.09448353
B17	1.09617763
B18	1.09439200
B19	1.49383817
B20	1.09290673
B21	1.09469053
B22	1.09560866
B23	1.49985766
B24	1.09508013
B25	1.09439233
B26	1.09382095
B27	1.49414015
B28	1.09488225
B29	1.09297222
B30	1.09544108
B31	1.49398728

B32	1.40198817
B33	1.40203472
B34	1.39271915
B35	1.39484015
B36	1.08613950
B37	1.08494441
B38	1.08605362
B39	1.08259722
B40	2.64737786
B41	1.45474435
B42	1.45910707
B43	1.80916731
B44	1.40305381
B45	1.39467267
B46	1.38823369
B47	1.39499290
B48	1.08235491
B49	1.38849449
B50	1.08212040
B51	1.08178920
B52	1.47871106
B53	1.22658606
B54	1.22485714
B55	1.47912704
B56	1.22715468
B57	1.22847366
B58	1.39426746
B59	1.08587543
B60	1.40461813
A1	35.94233926
A2	70.01241143
A3	132.02108965
A4	121.20683736
A5	132.55677137
A6	105.92523795
A7	108.72895817
A8	126.12422764
A9	108.90586006
A10	108.93771545
A11	125.94091257
A12	110.77028969
A13	109.77545730
A14	160.34680628
A15	112.50506863
A16	111.66985868
A17	109.67439006
A18	128.10804330
A19	110.28876631
A20	111.02944338
A21	110.65645869
A22	130.06702570
A23	112.63237911
A24	109.40204434
A25	111.48776921
A26	122.96991128

A27	110.95806164
A28	110.27132518
A29	110.87277979
A30	119.58177146
A31	121.90456470
A32	120.71504265
A33	122.25140716
A34	121.15990316
A35	118.64195000
A36	119.03964210
A37	119.71049362
A38	126.24341034
A39	120.13669541
A40	107.64392130
A41	88.29440304
A42	121.38641249
A43	124.59827689
A44	115.81813684
A45	120.73842181
A46	120.55033676
A47	119.96235993
A48	118.41447766
A49	120.78438992
A50	120.49795991
A51	123.30205297
A52	116.70439350
A53	116.89636042
A54	119.26110302
A55	117.23727241
A56	117.29274014
A57	119.18004094
A58	119.70049314
A59	118.94744345
D1	179.75327376
D2	-177.53903649
D3	173.64389125
D4	-178.59173395
D5	178.53664212
D6	1.03128896
D7	-179.83823793
D8	0.47809064
D9	-0.73033679
D10	-176.66379728
D11	-49.38942492
D12	72.39793666
D13	-179.76726849
D14	130.95631910
D15	-108.39904974
D16	10.72254749
D17	178.38006530
D18	-1.86316282
D19	119.25684117
D20	-122.45606279
D21	-3.14102264
D22	69.57066352

D23	-170.73334413
D24	-51.37246547
D25	179.52382627
D26	64.61618935
D27	-174.45442969
D28	-53.74159669
D29	-5.02159921
D30	-75.25366770
D31	104.47275524
D32	-178.50140887
D33	179.21617278
D34	-0.86593152
D35	-179.81436938
D36	179.68394725
D37	179.69757567
D38	-30.74471089
D39	-161.11044207
D40	-39.99966201
D41	70.10415243
D42	100.98000377
D43	-82.78867435
D44	173.71003992
D45	-177.22222137
D46	3.56852966
D47	2.91652710
D48	-178.10779135
D49	-176.50360713
D50	-9.66939752
D51	140.19607622
D52	-43.12758214
D53	178.76238604
D54	-0.91402821
D55	179.10831280
D56	-0.97594597
D57	-179.66244298
D58	7.53414788

1 3 1.5 11 1.5 28 1.0
2 3 1.5 4 1.5 16 1.0
3 40 1.0
4 5 1.5 11 1.0
5 6 1.5 32 1.0
6 7 1.5 12 1.0
7 8 1.5 24 1.0
8 9 1.5 10 1.0
9 12 1.5 20 1.0
10
11 13 1.0
12 13 1.0
13 14 1.0 15 1.0
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16 17 1.0 18 1.0 19 1.0
17
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19
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28 29 1.0 30 1.0 31 1.0
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35 38 1.0 59 1.5
36 39 1.0 59 1.5
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41 42 2.0 43 2.0 44 1.0 61 1.0
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46 48 1.5 49 1.0
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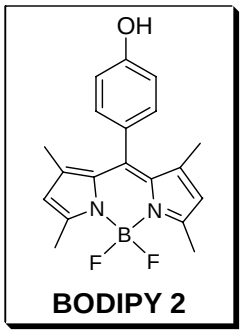

BODIPY 2

BODIPY 2 （DFT//B3LYP/6-31G(d)）

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1
No imaginary frequencies.

0 1
C
C 1 B1
C 2 B2 1 A1
C 2 B3 1 A2 3 D1

C	4	B4	2	A3	1	D2
C	5	B5	4	A4	2	D3
C	6	B6	5	A5	4	D4
C	7	B7	6	A6	5	D5
C	8	B8	7	A7	6	D6
H	8	B9	7	A8	6	D7
N	1	B10	3	A9	2	D8
N	9	B11	8	A10	7	D9
B	11	B12	1	A11	3	D10
F	13	B13	11	A12	1	D11
F	13	B14	11	A13	1	D12
C	2	B15	1	A14	11	D13
H	16	B16	2	A15	1	D14
H	16	B17	2	A16	1	D15
H	16	B18	2	A17	1	D16
C	9	B19	8	A18	7	D17
H	20	B20	9	A19	8	D18
H	20	B21	9	A20	8	D19
H	20	B22	9	A21	8	D20
C	7	B23	6	A22	5	D21
H	24	B24	7	A23	6	D22
H	24	B25	7	A24	6	D23
H	24	B26	7	A25	6	D24
C	1	B27	11	A26	4	D25
H	28	B28	1	A27	11	D26
H	28	B29	1	A28	11	D27
H	28	B30	1	A29	11	D28
C	5	B31	4	A30	2	D29
C	32	B32	5	A31	4	D30
C	32	B33	5	A32	4	D31
C	33	B34	32	A33	5	D32
H	33	B35	32	A34	5	D33
C	34	B36	32	A35	5	D34
H	34	B37	32	A36	5	D35
C	37	B38	34	A37	32	D36
H	35	B39	33	A38	32	D37
H	37	B40	34	A39	32	D38
H	3	B41	2	A40	1	D39
O	39	B42	37	A41	34	D40
H	43	B43	39	A42	37	D41

B1	2.27304878
B2	1.38991203
B3	1.43570195
B4	1.40480791
B5	1.40480452
B6	1.43570297
B7	1.38991107
B8	1.40998623
B9	1.08271887
B10	1.34666747
B11	1.34667048
B12	1.55759769
B13	1.39399900
B14	1.39381074
B15	1.50080416
B16	1.09528144
B17	1.09521044
B18	1.09461322
B19	1.49393663
B20	1.09300048

B21	1.09521404
B22	1.09520506
B23	1.50080319
B24	1.09530900
B25	1.09461265
B26	1.09518524
B27	1.49393701
B28	1.09523143
B29	1.09299983
B30	1.09518873
B31	1.49473335
B32	1.40301819
B33	1.39951979
B34	1.39171137
B35	1.08663295
B36	1.39502746
B37	1.08657977
B38	1.39888237
B39	1.08537696
B40	1.08857772
B41	1.08271821
B42	1.36548012
B43	0.96994680
A1	36.02119146
A2	69.91157699
A3	131.86969628
A4	121.07553316
A5	131.86920475
A6	105.93271672
A7	108.54879594
A8	126.30724776
A9	108.99856826
A10	108.99833203
A11	125.22084712
A12	110.04212506
A13	110.05336803
A14	160.49658094
A15	112.22493167
A16	112.25669296
A17	109.66980894
A18	128.32147375
A19	110.52212798
A20	110.53792571
A21	110.54360245
A22	129.59272814
A23	112.22078053
A24	109.66951643
A25	112.26135190
A26	122.68109318
A27	110.53708235
A28	110.52173969
A29	110.54482416
A30	119.46266861
A31	120.78782143
A32	120.73353263
A33	121.11829188
A34	119.40492185
A35	120.92474022
A36	119.58748845
A37	119.92132497
A38	121.25646090

A39	119.99718541
A40	126.30722331
A41	122.84556912
A42	109.16025439
D1	-179.99286949
D2	179.96084644
D3	-179.89347558
D4	179.86756195
D5	-179.95909312
D6	-0.00569677
D7	179.96569249
D8	-0.00977357
D9	0.01202043
D10	179.87907734
D11	-61.10749577
D12	60.79790776
D13	179.95990010
D14	119.99940522
D15	-120.01568801
D16	-0.00000000
D17	-179.99118063
D18	0.15967544
D19	121.23043021
D20	-120.91075500
D21	0.01545632
D22	60.25371930
D23	-179.75462352
D24	-59.73147155
D25	-179.97401946
D26	58.90498217
D27	179.96970070
D28	-58.95371226
D29	0.11199228
D30	-89.91628070
D31	90.08432802
D32	-180.00000000
D33	-0.00000000
D34	-180.00000000
D35	-0.00000000
D36	-0.00486912
D37	179.99629284
D38	179.99579066
D39	-179.98112875
D40	-180.00000000
D41	-0.00320408

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2 3 2.0 4 1.0 16 1.0
3 42 1.0
4 5 2.0 11 1.0
5 6 1.0 32 1.0
6 7 2.0 12 1.0
7 8 1.0 24 1.0
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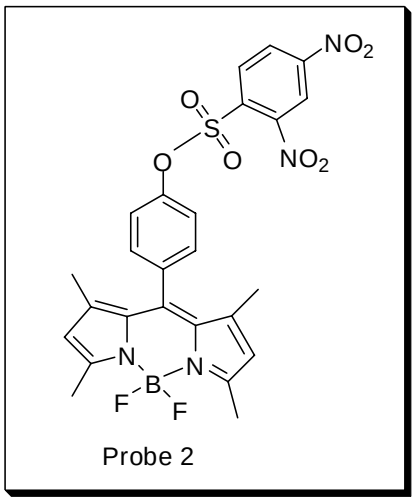

Probe 2

Probe 2 （DFT//B3LYP/6-31G(d)）

No imaginary frequencies.

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

0 1

C							
C	1	B1					
C	2	B2	1	A1			
C	2	B3	1	A2	3	D1	
C	4	B4	2	A3	1	D2	
C	5	B5	4	A4	2	D3	
C	6	B6	5	A5	4	D4	
C	7	B7	6	A6	5	D5	
C	8	B8	7	A7	6	D6	
H	8	B9	7	A8	6	D7	
N	1	B10	3	A9	2	D8	
N	9	B11	8	A10	7	D9	
B	11	B12	1	A11	3	D10	
F	13	B13	11	A12	1	D11	

F	13	B14	11	A13	1	D12	
C	2	B15	1	A14	11	D13	
H	16	B16	2	A15	1	D14	
H	16	B17	2	A16	1	D15	
H	16	B18	2	A17	1	D16	
C	9	B19	8	A18	7	D17	
H	20	B20	9	A19	8	D18	
H	20	B21	9	A20	8	D19	
H	20	B22	9	A21	8	D20	
C	7	B23	6	A22	5	D21	
H	24	B24	7	A23	6	D22	
H	24	B25	7	A24	6	D23	
H	24	B26	7	A25	6	D24	
C	1	B27	11	A26	4	D25	
H	28	B28	1	A27	11	D26	
H	28	B29	1	A28	11	D27	
H	28	B30	1	A29	11	D28	
C	5	B31	4	A30	2	D29	
C	32	B32	5	A31	4	D30	
C	32	B33	5	A32	4	D31	
C	33	B34	32	A33	5	D32	
H	33	B35	32	A34	5	D33	
C	34	B36	32	A35	5	D34	
H	34	B37	32	A36	5	D35	
C	35	B38	33	A37	32	D36	
H	35	B39	33	A38	32	D37	
H	37	B40	34	A39	32	D38	
H	3	B41	2	A40	1	D39	
O	39	B42	35	A41	33	D40	
S	43	B43	39	A42	35	D41	
O	44	B44	43	A43	39	D42	
O	44	B45	43	A44	39	D43	
C	44	B46	43	A45	39	D44	
C	47	B47	44	A46	43	D45	
C	47	B48	44	A47	43	D46	
C	48	B49	47	A48	44	D47	
C	49	B50	47	A49	44	D48	
H	49	B51	47	A50	44	D49	
C	51	B52	49	A51	47	D50	
H	50	B53	48	A52	47	D51	
H	51	B54	49	A53	47	D52	
N	48	B55	47	A54	44	D53	
O	56	B56	48	A55	47	D54	
O	56	B57	48	A56	47	D55	
N	53	B58	51	A57	49	D56	
O	59	B59	53	A58	51	D57	
O	59	B60	53	A59	51	D58	

B1	2.27351998
B2	1.38911167
B3	1.43710037
B4	1.40369603
B5	1.40480471
B6	1.43592503
B7	1.38957775
B8	1.41021274
B9	1.08266166
B10	1.34634737
B11	1.34664883
B12	1.55831109
B13	1.39315695

B14	1.39301676
B15	1.50087416
B16	1.09537599
B17	1.09516832
B18	1.09425301
B19	1.49372139
B20	1.09291740
B21	1.09522383
B22	1.09517955
B23	1.50102886
B24	1.09540260
B25	1.09440019
B26	1.09542890
B27	1.49357920
B28	1.09513892
B29	1.09288782
B30	1.09523512
B31	1.49551484
B32	1.40186496
B33	1.40142139
B34	1.39449523
B35	1.08603935
B36	1.39491583
B37	1.08608215
B38	1.39166891
B39	1.08385588
B40	1.08460920
B41	1.08260763
B42	1.41301126
B43	1.64941992
B44	1.45548208
B45	1.45959507
B46	1.81395942
B47	1.40341526
B48	1.39620594
B49	1.38920217
B50	1.39413040
B51	1.08367150
B52	1.38904745
B53	1.08221464
B54	1.08287863
B55	1.48035156
B56	1.22547050
B57	1.22486702
B58	1.47962029
B59	1.22750685
B60	1.22718719
A1	36.02233865
A2	69.85099601
A3	132.02035899
A4	121.35155372
A5	132.01481058
A6	105.91676214
A7	108.55677252
A8	126.29417466
A9	109.01447758
A10	108.98865524
A11	125.18396836
A12	110.04548840
A13	110.02802757
A14	160.45791770

A15	112.25016216
A16	112.41857723
A17	109.66839430
A18	128.32555477
A19	110.53134094
A20	110.54238451
A21	110.50930134
A22	129.66234952
A23	112.24845925
A24	109.63727384
A25	112.32734289
A26	122.65897013
A27	110.49991114
A28	110.56083128
A29	110.50544210
A30	119.28607295
A31	120.22990471
A32	120.51938806
A33	120.81841942
A34	119.49875024
A35	120.63539614
A36	119.59377521
A37	118.52294417
A38	121.69823078
A39	121.43558231
A40	126.27345452
A41	118.82811603
A42	116.51178088
A43	111.14307846
A44	108.42134516
A45	97.68995384
A46	124.91167356
A47	115.54668469
A48	120.94091023
A49	120.70274790
A50	118.75973968
A51	118.54464709
A52	120.76594763
A53	121.54723405
A54	123.46928320
A55	116.50129146
A56	117.25102345
A57	119.18204318
A58	117.10168313
A59	117.24788471
D1	179.97129110
D2	179.84664684
D3	-179.98759836
D4	-179.77507309
D5	-180.00000000
D6	0.00359836
D7	-179.99541404
D8	0.04060923
D9	-0.03543393
D10	-179.75433762
D11	-61.04321527
D12	60.97688817
D13	-179.73239550
D14	118.96297714
D15	-120.72871626
D16	-0.82815852

D17	179.96817049
D18	-0.32397557
D19	120.76236962
D20	-121.39005854
D21	0.13613776
D22	59.74972132
D23	179.59235639
D24	-60.52298397
D25	179.95616180
D26	58.70319846
D27	179.81638894
D28	-59.10029137
D29	-0.34512823
D30	-90.46600268
D31	89.40627783
D32	179.68672578
D33	-0.04766393
D34	-179.79443393
D35	0.17850756
D36	0.26966250
D37	-179.51764868
D38	179.98206365
D39	-179.98404630
D40	176.80891436
D41	95.04633629
D42	-52.68698347
D43	81.73735306
D44	-167.38911425
D45	83.68010524
D46	-103.61749537
D47	172.19829537
D48	-174.71451456
D49	4.40717352
D50	1.76718645
D51	-178.51559684
D52	-179.11060171
D53	-9.18284358
D54	141.72877894
D55	-41.11705373
D56	179.35345500
D57	-0.34640744
D58	179.58417128

1 3 1.0 11 2.0 28 1.0
2 3 2.0 4 1.0 16 1.0
3 42 1.0
4 5 2.0 11 1.0
5 6 1.0 32 1.0
6 7 2.0 12 1.0
7 8 1.0 24 1.0
8 9 2.0 10 1.0
9 12 1.0 20 1.0
10
11 13 1.0
12 13 1.0
13 14 1.0 15 1.0
14
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16 17 1.0 18 1.0 19 1.0
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19
20 21 1.0 22 1.0 23 1.0
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24 25 1.0 26 1.0 27 1.0
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26
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28 29 1.0 30 1.0 31 1.0
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32 33 1.5 34 1.5
33 35 1.5 36 1.0
34 37 1.5 38 1.0
35 39 1.5 40 1.0
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37 39 1.5 41 1.0
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39 43 1.0
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43 44 1.0
44 45 2.0 46 2.0 47 1.0
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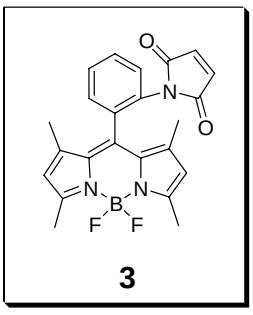
47 48 1.5 49 1.5
48 50 1.5 56 1.0
49 51 1.5 52 1.0
50 53 1.5 54 1.0
51 53 1.5 55 1.0
52
53 59 1.0
54
55
56 57 1.5 58 1.5
57
58
59 60 1.5 61 1.5
60
61
SCF Done: E(RB+HF-LYP) = -2333.52336058 Hartree
Number of Imaginary frequencies: 0

Probe 3 （DFT//B3LYP/6-31G(d)）



3

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

No imaginary frequencies.

0 1

C								
C		1	B1					
C		2	B2	1	A1			
C		3	B3	2	A2	1	D1	
N		4	B4	3	A3	2	D2	
C		1	B5	5	A4	4	D3	
C		6	B6	1	A5	5	D4	

N	7	B7	6	A6	1	D5
C	8	B8	7	A7	6	D6
C	9	B9	8	A8	7	D7
C	10	B10	9	A9	8	D8
C	6	B11	1	A10	5	D9
C	2	B12	1	A11	5	D10
C	4	B13	3	A12	2	D11
C	9	B14	8	A13	7	D12
C	11	B15	10	A14	9	D13
B	5	B16	4	A15	3	D14
F	17	B17	5	A16	4	D15
F	17	B18	5	A17	4	D16
N	12	B19	6	A18	1	D17
C	20	B20	12	A19	6	D18
C	21	B21	20	A20	12	D19
C	22	B22	21	A21	20	D20
C	20	B23	12	A22	6	D21
O	24	B24	20	A23	12	D22
O	21	B25	20	A24	12	D23
C	12	B26	6	A25	1	D24
C	27	B27	12	A26	6	D25
C	28	B28	27	A27	12	D26
C	12	B29	6	A28	1	D27
C	29	B30	28	A29	27	D28
H	3	B31	2	A30	1	D29
H	10	B32	9	A31	8	D30
H	13	B33	2	A32	1	D31
H	13	B34	2	A33	1	D32
H	13	B35	2	A34	1	D33
H	14	B36	4	A35	3	D34
H	14	B37	4	A36	3	D35
H	14	B38	4	A37	3	D36
H	15	B39	9	A38	8	D37
H	15	B40	9	A39	8	D38
H	15	B41	9	A40	8	D39
H	16	B42	11	A41	10	D40
H	16	B43	11	A42	10	D41
H	16	B44	11	A43	10	D42
H	22	B45	21	A44	20	D43
H	23	B46	22	A45	21	D44
H	27	B47	12	A46	6	D45
H	28	B48	27	A47	12	D46
H	29	B49	28	A48	27	D47
H	31	B50	29	A49	28	D48

B1	1.43820808
B2	1.38959273
B3	1.40927521
B4	1.34677232
B5	1.40573547
B6	1.40570366
B7	1.40091670
B8	1.34675773
B9	1.40928854
B10	1.38956542
B11	1.49668452
B12	1.50038765
B13	1.49393183
B14	1.49393303
B15	1.50036866
B16	1.55635699

B17	1.39356292
B18	1.39463097
B19	2.46776170
B20	1.40960563
B21	1.49899754
B22	1.33533768
B23	1.40961809
B24	1.21142699
B25	1.21144590
B26	1.40079420
B27	1.39430331
B28	1.39521960
B29	1.40672434
B30	1.39326730
B31	1.08259390
B32	1.08259168
B33	1.09463351
B34	1.09526608
B35	1.09348529
B36	1.09528481
B37	1.09493876
B38	1.09304559
B39	1.09304621
B40	1.09494099
B41	1.09528403
B42	1.09463381
B43	1.09345869
B44	1.09528727
B45	1.08236124
B46	1.08235977
B47	1.08629696
B48	1.08634401
B49	1.08597217
B50	1.08562568
A1	105.80954378
A2	108.68220304
A3	109.01037967
A4	119.96422655
A5	121.32902606
A6	119.96447066
A7	108.72854137
A8	109.01090347
A9	108.68240195
A10	119.32799931
A11	129.91902321
A12	128.28639145
A13	122.70765503
A14	124.25099924
A15	125.32220193
A16	109.91019462
A17	110.28259928
A18	91.56937492
A19	121.51532768
A20	106.05569423
A21	108.92907075
A22	121.36603140
A23	126.20674421
A24	126.20559297
A25	120.11145627
A26	121.08479824
A27	120.01529061

A28	121.51992993
A29	119.66032277
A30	126.14120171
A31	125.17534657
A32	109.40007169
A33	112.13395085
A34	111.72823250
A35	110.50336571
A36	110.74264987
A37	110.44114180
A38	110.43931813
A39	110.74359239
A40	110.50506666
A41	109.40006085
A42	111.72530060
A43	112.13638288
A44	121.47199162
A45	129.59717703
A46	118.77989040
A47	119.76072795
A48	120.44534726
A49	120.71258769
D1	0.07016934
D2	-0.53706120
D3	-178.63209658
D4	4.23296259
D5	-4.21546953
D6	178.62464379
D7	-0.78702833
D8	0.53883788
D9	-176.50534223
D10	-178.00130248
D11	179.45716436
D12	179.20684470
D13	-178.59874498
D14	178.08334980
D15	54.18621948
D16	-67.78922255
D17	90.29398051
D18	-73.75944806
D19	146.95482067
D20	2.21151793
D21	73.51673649
D22	34.41256595
D23	-34.45841081
D24	-89.69332394
D25	179.96539825
D26	0.00364516
D27	90.28506011
D28	0.00641525
D29	-179.67366022
D30	-179.21758205
D31	178.01447201
D32	58.49755416
D33	-62.57954806
D34	-125.59980573
D35	116.42129896
D36	-4.69529255
D37	-175.29728620
D38	63.58829319
D39	-54.39367963

D40	-0.03300708
D41	-119.43890364
D42	119.47963135
D43	-178.24336262
D44	179.49584508
D45	-0.02110555
D46	-179.99196432
D47	-179.99585036
D48	179.99623427

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2 3 1.5 13 1.0
3 4 1.5 32 1.0
4 5 1.5 14 1.0
5 17 1.0
6 7 1.5 12 1.0
7 8 1.0 11 1.5
8 9 1.5 17 1.0
9 10 1.5 15 1.0
10 11 1.5 33 1.0
11 16 1.0
12 27 1.5 30 1.5
13 34 1.0 35 1.0 36 1.0
14 37 1.0 38 1.0 39 1.0
15 40 1.0 41 1.0 42 1.0
16 43 1.0 44 1.0 45 1.0
17 18 1.0 19 1.0
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19
20 21 1.0 24 1.0 30 1.0
21 22 1.0 26 2.0
22 23 2.0 46 1.0
23 24 1.0 47 1.0
24 25 2.0
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27 28 1.5 48 1.0
28 29 1.5 49 1.0
29 31 1.5 50 1.0
30 31 1.5
31 51 1.0
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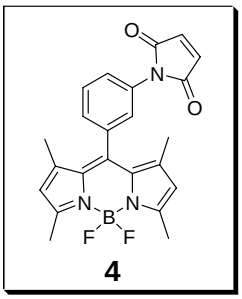

4

Probe 4 （DFT//B3LYP/6-31G(d)）

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1
No imaginary frequencies.

0 1

C						
C	1	B1				
C	2	B2	1	A1		
C	3	B3	2	A2	1	D1
N	4	B4	3	A3	2	D2
C	1	B5	5	A4	4	D3
C	6	B6	1	A5	5	D4
N	7	B7	6	A6	1	D5
C	8	B8	7	A7	6	D6
C	9	B9	8	A8	7	D7
C	10	B10	9	A9	8	D8
C	6	B11	1	A10	5	D9
C	12	B12	6	A11	1	D10
C	13	B13	12	A12	6	D11
C	14	B14	13	A13	12	D12
C	15	B15	14	A14	13	D13
C	16	B16	15	A15	14	D14
C	2	B17	1	A16	5	D15
C	4	B18	3	A17	2	D16
C	9	B19	8	A18	7	D17
C	11	B20	10	A19	9	D18
B	5	B21	4	A20	3	D19
F	22	B22	5	A21	4	D20
F	22	B23	5	A22	4	D21
N	14	B24	13	A23	12	D22
C	25	B25	14	A24	13	D23
C	26	B26	25	A25	14	D24
C	27	B27	26	A26	25	D25
C	25	B28	14	A27	13	D26
O	29	B29	25	A28	14	D27
O	26	B30	25	A29	14	D28
H	3	B31	2	A30	1	D29
H	10	B32	9	A31	8	D30
H	13	B33	12	A32	6	D31
H	15	B34	14	A33	13	D32
H	16	B35	15	A34	14	D33
H	17	B36	16	A35	15	D34
H	18	B37	2	A36	1	D35
H	18	B38	2	A37	1	D36
H	18	B39	2	A38	1	D37
H	19	B40	4	A39	3	D38
H	19	B41	4	A40	3	D39
H	19	B42	4	A41	3	D40
H	20	B43	9	A42	8	D41
H	20	B44	9	A43	8	D42
H	20	B45	9	A44	8	D43
H	21	B46	11	A45	10	D44
H	21	B47	11	A46	10	D45
H	21	B48	11	A47	10	D46
H	27	B49	26	A48	25	D47
H	28	B50	27	A49	26	D48

B1	1.43746250
B2	1.38935509
B3	1.41014099
B4	1.34639277
B5	1.40379404
B6	1.40573094
B7	1.39976904
B8	1.34694578
B9	1.40952061
B10	1.39021512
B11	1.49505642
B12	1.39800854
B13	1.39832635
B14	1.39833552
B15	1.39396700
B16	1.39486474
B17	1.50075777
B18	1.49365349
B19	1.49391377
B20	1.50102291
B21	1.55741456
B22	1.39364119
B23	1.39399638
B24	1.42516621
B25	1.41084671
B26	1.49897653
B27	1.33525977
B28	1.41266195
B29	1.21109600
B30	1.21241917
B31	1.08265732
B32	1.08271810
B33	1.08351244
B34	1.08332425
B35	1.08619497
B36	1.08608578
B37	1.09468434
B38	1.09586970
B39	1.09507410
B40	1.09521918
B41	1.09512778
B42	1.09293858
B43	1.09301557
B44	1.09523169
B45	1.09514742
B46	1.09449684
B47	1.09556179
B48	1.09494379
B49	1.08241246
B50	1.08242159
A1	105.85200595
A2	108.61001592
A3	109.03207676
A4	120.15422403
A5	121.29724075
A6	120.21714412
A7	108.75861669
A8	108.98495899
A9	108.56281335
A10	119.31069950

A11	120.24584660
A12	120.05780111
A13	120.46576969
A14	119.26905821
A15	120.60292749
A16	129.75627513
A17	128.33313434
A18	122.67926705
A19	124.34655969
A20	125.13841978
A21	110.05280962
A22	110.03214230
A23	119.45468382
A24	124.89092350
A25	106.16196756
A26	108.95951559
A27	125.29118703
A28	126.23608545
A29	126.35873866
A30	126.25057452
A31	125.16156816
A32	119.87226444
A33	120.05127387
A34	119.49281793
A35	120.36757230
A36	109.49354270
A37	112.11621301
A38	112.29289032
A39	110.43608048
A40	110.57135055
A41	110.55515617
A42	110.52462200
A43	110.56472204
A44	110.55431152
A45	109.63342912
A46	112.32347865
A47	112.31298626
A48	121.39871310
A49	129.60663374
D1	0.10623406
D2	-0.09497020
D3	179.41118092
D4	0.50822208
D5	-1.08373708
D6	179.25112659
D7	-0.24704423
D8	0.05788187
D9	-178.80247279
D10	-81.72457089
D11	178.87242480
D12	0.96763560
D13	-0.10096810
D14	-0.67688613
D15	-179.60775356
D16	179.58071193
D17	179.96524186
D18	-179.20767332
D19	178.31127002
D20	61.20414549
D21	-60.73331159
D22	-178.38249188

D23	44.52662107
D24	179.74982924
D25	-0.36341787
D26	-136.54245370
D27	0.02006456
D28	0.04498605
D29	-179.89868358
D30	-179.61566859
D31	-0.03508200
D32	179.49915041
D33	179.89702848
D34	-179.24016400
D35	-172.86440215
D36	67.60352426
D37	-52.95432001
D38	-120.81615173
D39	121.39544431
D40	0.24315511
D41	-178.11625774
D42	60.83291594
D43	-57.03260278
D44	5.51058875
D45	-114.26844978
D46	125.52973378
D47	179.85407707
D48	-179.97825755

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5 22 1.0
6 7 1.5 12 1.0
7 8 1.0 11 1.0
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9 10 1.5 20 1.0
10 11 1.5 33 1.0
11 21 1.0
12 13 1.5 17 1.5
13 14 1.5 34 1.0
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17 37 1.0
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19 41 1.0 42 1.0 43 1.0
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21 47 1.0 48 1.0 49 1.0
22 23 1.0 24 1.0
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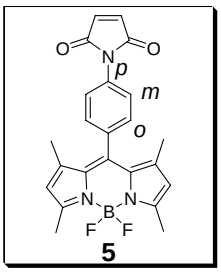

5

probe 5 （DFT//B3LYP/6-31G(d)）

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

No imaginary frequencies.

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C	1	B1					
C	2	B2	1	A1			
C	3	B3	2	A2	1	D1	
N	4	B4	3	A3	2	D2	
C	1	B5	5	A4	4	D3	
C	6	B6	1	A5	5	D4	
N	7	B7	6	A6	1	D5	
C	8	B8	7	A7	6	D6	
C	9	B9	8	A8	7	D7	
C	10	B10	9	A9	8	D8	
C	6	B11	1	A10	5	D9	
C	12	B12	6	A11	1	D10	
C	13	B13	12	A12	6	D11	
C	14	B14	13	A13	12	D12	
C	15	B15	14	A14	13	D13	
C	16	B16	15	A15	14	D14	
C	2	B17	1	A16	5	D15	
C	4	B18	3	A17	2	D16	
C	9	B19	8	A18	7	D17	
C	11	B20	10	A19	9	D18	
B	8	B21	7	A20	6	D19	
F	22	B22	8	A21	7	D20	
F	22	B23	8	A22	7	D21	
N	15	B24	14	A23	13	D22	
C	25	B25	15	A24	14	D23	
C	26	B26	25	A25	15	D24	
C	27	B27	26	A26	25	D25	
C	25	B28	15	A27	14	D26	
O	29	B29	25	A28	15	D27	
O	26	B30	25	A29	15	D28	
H	3	B31	2	A30	1	D29	
H	10	B32	9	A31	8	D30	
H	13	B33	12	A32	6	D31	

H	14	B34	13	A33	12	D32
H	16	B35	15	A34	14	D33
H	17	B36	16	A35	15	D34
H	18	B37	2	A36	1	D35
H	18	B38	2	A37	1	D36
H	18	B39	2	A38	1	D37
H	19	B40	4	A39	3	D38
H	19	B41	4	A40	3	D39
H	19	B42	4	A41	3	D40
H	20	B43	9	A42	8	D41
H	20	B44	9	A43	8	D42
H	20	B45	9	A44	8	D43
H	21	B46	11	A45	10	D44
H	21	B47	11	A46	10	D45
H	21	B48	11	A47	10	D46
H	27	B49	26	A48	25	D47
H	28	B50	27	A49	26	D48

B1	1.43603552
B2	1.38973397
B3	1.41006908
B4	1.34664885
B5	1.40453078
B6	1.40453015
B7	1.40003390
B8	1.34664914
B9	1.41006831
B10	1.38973436
B11	1.49489000
B12	1.40026088
B13	1.39336418
B14	1.39969179
B15	1.39969140
B16	1.39336410
B17	1.50088882
B18	1.49388682
B19	1.49388678
B20	1.50088758
B21	1.55791691
B22	1.39354293
B23	1.39354161
B24	1.42526200
B25	1.41339460
B26	1.49881041
B27	1.33484140
B28	1.41339572
B29	1.21147072
B30	1.21147113
B31	1.08267768
B32	1.08267731
B33	1.08629727
B34	1.08276942
B35	1.08276903
B36	1.08629730
B37	1.09447495
B38	1.09521022
B39	1.09541625
B40	1.09508467
B41	1.09297414
B42	1.09528789
B43	1.09297348

B44	1.09528770
B45	1.09508529
B46	1.09447454
B47	1.09521042
B48	1.09541746
B49	1.08241949
B50	1.08241927
A1	105.90751005
A2	108.56413629
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A5	121.23799645
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A7	108.73851377
A8	109.00269777
A9	108.56418311
A10	119.38109855
A11	120.66254452
A12	120.95181907
A13	119.75483255
A14	119.90282308
A15	119.75489002
A16	129.66304345
A17	128.33771400
A18	122.65956281
A19	124.42946575
A20	126.06174612
A21	110.03675492
A22	110.03634861
A23	120.04853128
A24	125.19562737
A25	106.21059758
A26	108.98476043
A27	125.19547855
A28	126.38750181
A29	126.38747660
A30	126.28109130
A31	125.15479919
A32	119.57245133
A33	120.13427895
A34	120.10449620
A35	119.47409038
A36	109.63399002
A37	112.23633807
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A39	110.51792924
A40	110.54107707
A41	110.52107580
A42	110.54109053
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A44	110.51798066
A45	109.63406175
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A47	112.33458865
A48	121.34109414
A49	129.67414844
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D2	-0.01842460
D3	-179.94512889
D4	0.10309607
D5	0.10286592

D6	-179.94147634
D7	0.05446660
D8	-0.02062617
D9	-179.89874565
D10	-91.27734755
D11	179.55240287
D12	0.89015165
D13	-0.43970704
D14	-0.43969779
D15	-179.83681252
D16	179.91106794
D17	-179.87993297
D18	179.88183417
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D20	119.12606113
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D24	-179.93642919
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D31	0.02822785
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D34	-179.58538122
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D41	-179.20399921
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D46	118.59826678
D47	179.82333558
D48	-179.78528780

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7 8 1.0 11 1.5
8 9 1.5 22 1.0
9 10 1.5 20 1.0
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11 21 1.0
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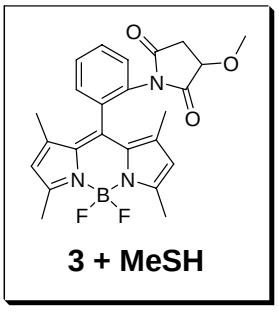

3 + MeSH

Probe 3 + MeSH

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

No imaginary frequencies.

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C								
C		1	B1					
C		2	B2	1	A1			
C		3	B3	2	A2	1	D1	
N		4	B4	3	A3	2	D2	
C		1	B5	5	A4	4	D3	
C		6	B6	1	A5	5	D4	
N		7	B7	6	A6	1	D5	
C		8	B8	7	A7	6	D6	
C		9	B9	8	A8	7	D7	
C		10	B10	9	A9	8	D8	
C		6	B11	1	A10	5	D9	
C		2	B12	1	A11	5	D10	

C	4	B13	3	A12	2	D11
C	9	B14	8	A13	7	D12
C	11	B15	10	A14	9	D13
B	8	B16	7	A15	6	D14
F	17	B17	8	A16	7	D15
F	17	B18	8	A17	7	D16
N	12	B19	6	A18	1	D17
C	20	B20	12	A19	6	D18
C	21	B21	20	A20	12	D19
C	22	B22	21	A21	20	D20
C	20	B23	12	A22	6	D21
O	24	B24	20	A23	12	D22
O	21	B25	20	A24	12	D23
C	12	B26	6	A25	1	D24
C	12	B27	6	A26	1	D25
C	28	B28	12	A27	6	D26
C	27	B29	12	A28	6	D27
C	30	B30	27	A29	12	D28
S	23	B31	22	A30	21	D29
C	32	B32	23	A31	22	D30
H	3	B33	2	A32	1	D31
H	10	B34	9	A33	8	D32
H	13	B35	2	A34	1	D33
H	13	B36	2	A35	1	D34
H	13	B37	2	A36	1	D35
H	14	B38	4	A37	3	D36
H	14	B39	4	A38	3	D37
H	14	B40	4	A39	3	D38
H	15	B41	9	A40	8	D39
H	15	B42	9	A41	8	D40
H	15	B43	9	A42	8	D41
H	16	B44	11	A43	10	D42
H	16	B45	11	A44	10	D43
H	16	B46	11	A45	10	D44
H	22	B47	21	A46	20	D45
H	22	B48	21	A47	20	D46
H	23	B49	22	A48	21	D47
H	28	B50	12	A49	6	D48
H	29	B51	28	A50	12	D49
H	30	B52	27	A51	12	D50
H	31	B53	30	A52	27	D51
H	33	B54	32	A53	23	D52
H	33	B55	32	A54	23	D53
H	33	B56	32	A55	23	D54

B1	1.43830155
B2	1.38932883
B3	1.40957805
B4	1.34660238
B5	1.40557493
B6	1.40585832
B7	1.40010191
B8	1.34614965
B9	1.40968484
B10	1.38967544

B11	1.49687321
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B13	1.49390468
B14	1.49383731
B15	1.50068191
B16	1.55643848
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B19	2.46736749
B20	1.40612777
B21	1.52238146
B22	1.53705213
B23	1.40268027
B24	1.21286431
B25	1.20939506
B26	1.40585839
B27	1.40059013
B28	1.39437752
B29	1.39585967
B30	1.39333789
B31	1.84194992
B32	1.82785871
B33	1.08260817
B34	1.08271645
B35	1.09461666
B36	1.09367353
B37	1.09521570
B38	1.09491434
B39	1.09306582
B40	1.09536866
B41	1.09318418
B42	1.09491937
B43	1.09527753
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A3	109.00270286
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A6	119.99428356
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A11	129.92334191
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D24	92.05339701
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End of Supplementary Information.