Supporting Information

Carbazole-BODIPY conjugates: design, synthesis, structure and properties

Rajneesh Misra,* Thaksen Jadhav, Bhausaheb Dhokale, Prabhat Gautam, Rekha Sharma,

Ramesh Maragani,and Shaikh M. Mobin

Department of Chemistry,
Indian Institute of Technology Indore,
Indore- 452 017, India.

rajneeshmisra@iiti.ac.in

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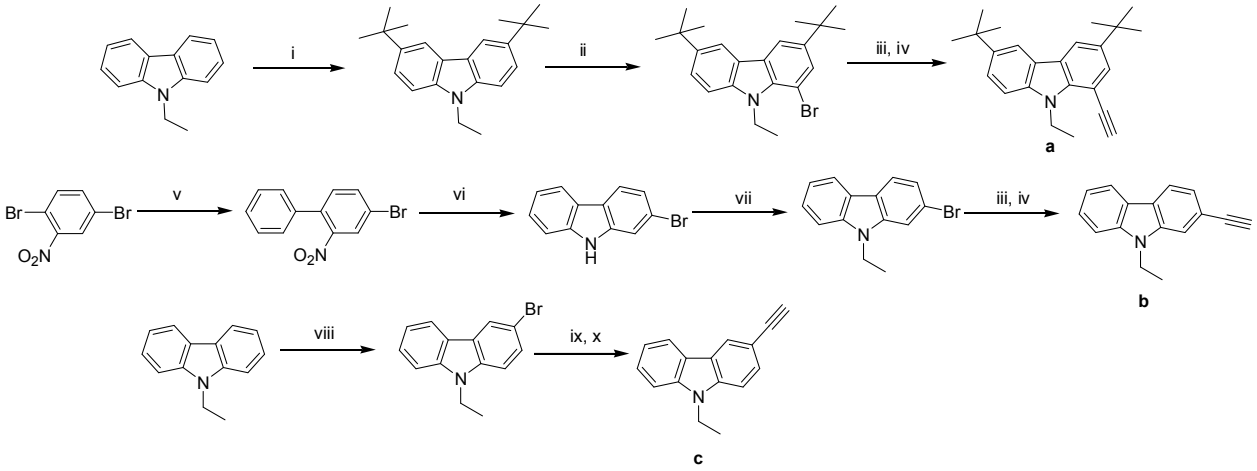
Synthesis of ethynyl-carbazoles:



i: *tert*-butyl chloride, $ZnCl_2$, Nitromethane; ii: NBS, DMF; iii: 2-methyl-3-butyn-2-ol, $PdCl_2(PPh_3)_2$, CuI, Et_3N, THF; iv: KOH, toluene; v: phenylboronic acid, $Pd(PPh_3)_4$, 2 M Na2CO3, toluene, 90 °C, 12 h; vi: $P(OEt)_3$, 190 °C, 10 h; vii: ethyl bromide, KOH, DMF; viii: NBS, $CHCl_3$; ix: 2-methyl-3-butyn-2-ol, $PdCl_2(PPh_3)_2$, PPh_3, CuI, DIPA; x: KOH, 2-propanol.

Scheme S1. Synthesis of ethynyl-carbazoles **a-c.**

Crystallographic Data

A single crystal X-ray structural study of **2a-2c** was performed on a CCD Agilent Technologies (Oxford Diffraction) SUPER NOVA diffractometer. Data were collected at 150(2) K using graphite-monochromated Mo Kα radiation (λ_α = 0.71073 Å). The strategy for the Data collection was evaluated by using the CrysAlisPro CCD software. The data were collected by the standard 'phi-omega scan techniques, and were scaled and reduced using CrysAlisPro RED software. The structures were solved by direct methods using SHELXS-97, and refined by full matrix least-squares with SHELXL-97, refining on F^2. The positions of all the atoms were obtained by direct methods. All non-hydrogen atoms were refined anisotropically. The remaining hydrogen atoms were placed in geometrically constrained positions, and refined with isotropic temperature factors, generally $1.2U_{eq}$ of their parent atoms. The crystal, and refinement data are summarized in Table 1. The CCDC number **994993**, **994994**, and **994991** contain the supplementary crystallographic data for **2a-2c** respectively. These data can be obtained free of charge via www.ccdc.cam.ac.uk (or from the Cambridge Crystallographic Data Centre, 12 union Road, Cambridge CB21 EZ, UK; Fax: (+44) 1223-336-033; or deposit@ccdc.cam.ac.uk).

Table S1. Crystal data and structure refinement for BODIPY **2a-2c.**

Parameter	2a	2b	2c
Identification code	rm124	rm126	rm116
Empirical formula	C33 H34 B F2 N3	C25 H18 B F2 N3	C25 H18 B F2 N3
Formula weight	521.44	409.23	409.23
Temperature	150(2) K	150(2) K	150(2) K
Wavelength(A)	0.71073	0.71073	0.71073
Crystal system, space group	Orthorhombic, P n a 21	Orthorhombic, P 21 21 21	Orthorhombic, P b c n
***a*/ (Å)**	17.3150(5)	5.5240(3)	30.9020(9)
***b*/ (Å)**	16.0128(6)	13.3635(8)	8.2967(2)
***c*/ (Å)**	10.1781(3)	27.7672(15)	15.5348(4)
α /(°)	90	90	90
β/ (°)	90	90	90
γ/ (°)	90	90	90
Volume	2822.00(16) Å^3	2049.8(2) Å^3	3982.88(18) Å^3

Z, Calculated density (mg m^{-3})	4, 1.227	4, 1.326	8, 1.365
Absorption coefficient /(mm^{-1})	0.081	0.091	0.094
F(000)	1104	848	1696
Crystal size	0.33 x 0.26 x 0.21 mm	0.26 x 0.21 x 0.18 mm	0.33 x 0.26 x 0.21 mm
θ range for data collection/(°)	3.09 to 25.00	2.93 to 24.99	2.94 to 32.19
Limiting indices	-20<=h<=20, -19<=k<=18, -11<=l<=12	-6<=h<=6, -15<=k<=15, -33<=l<=32	-46<=h<=45, -12<=k<=12, -22<=l<=22
Reflections collected / unique	20965 / 4886 [R(int) = 0.0458]	12564 / 3620 [R(int) = 0.0583]	52570 / 6770 [R(int) = 0.0727]
Completeness to theta	θ = 25.00; 99.7 %	θ = 24.99; 99.8 %	θ = 25.00; 99.8 %
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents
Max. and min. transmission	0.9833 and 0.9739	0.9838 and 0.9767	0.9806 and 0.9697
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	4886 / 1 / 359	3620 / 0 / 282	6770 / 0 / 281
Goodness-of-fit on F^2	1.017	1.081	1.027
Final R indices [I>2sigma(I)]	R1 = 0.0461, wR2 = 0.1099	R1 = 0.0466, wR2 = 0.1219	R1 = 0.0541, wR2 = 0.1267
R indices (all data)	R1 = 0.0609, wR2 = 0.1203	R1 = 0.0584, wR2 = 0.1333	R1 = 0.0915, wR2 = 0.1468
Largest diff. peak and hole (eÅ^{-3})	0.180 and -0.192	0.156 and -0.177	0.426 and -0.254

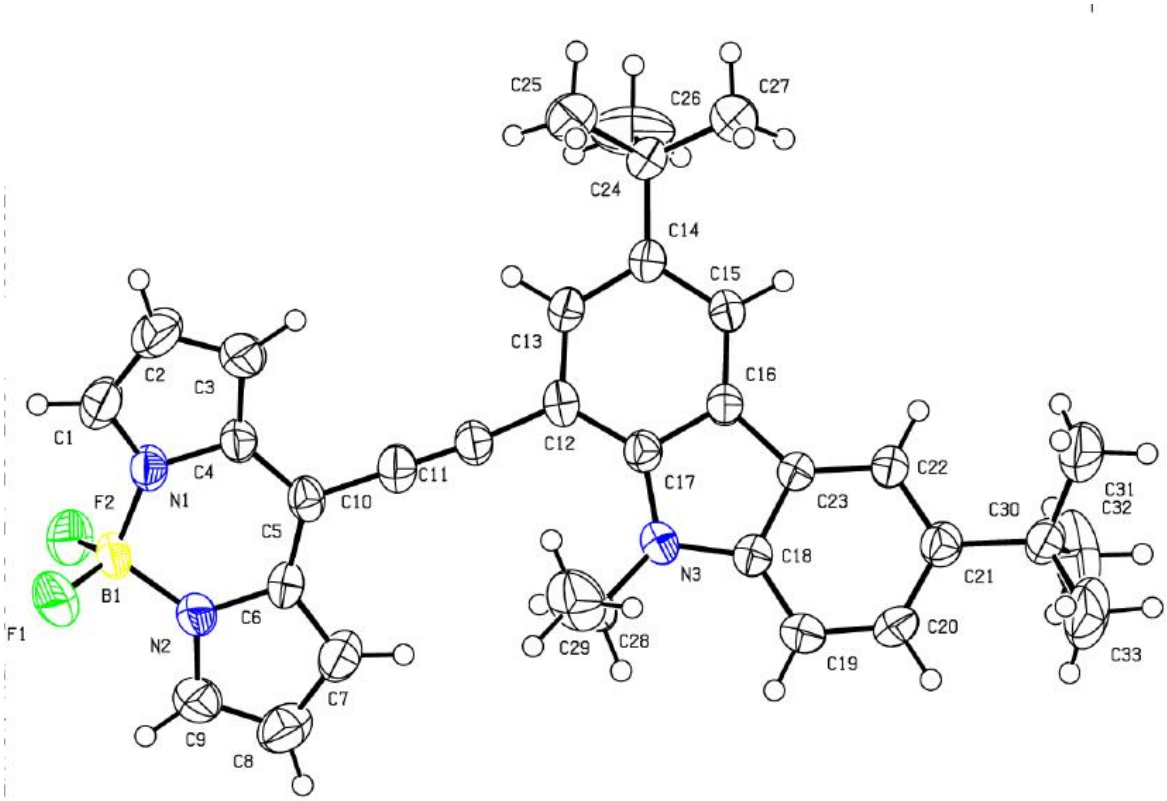


Fig. S1 Crystal structure of BODIPY **2a**.

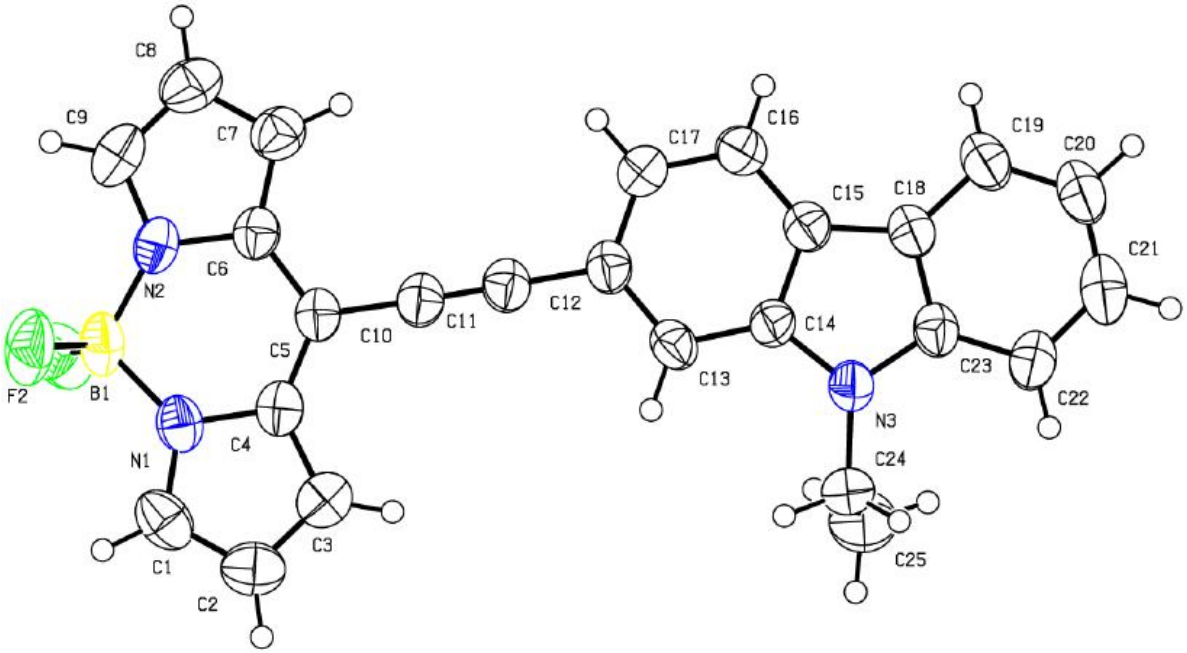


Fig. S2 Crystal structure of BODIPY **2b**.

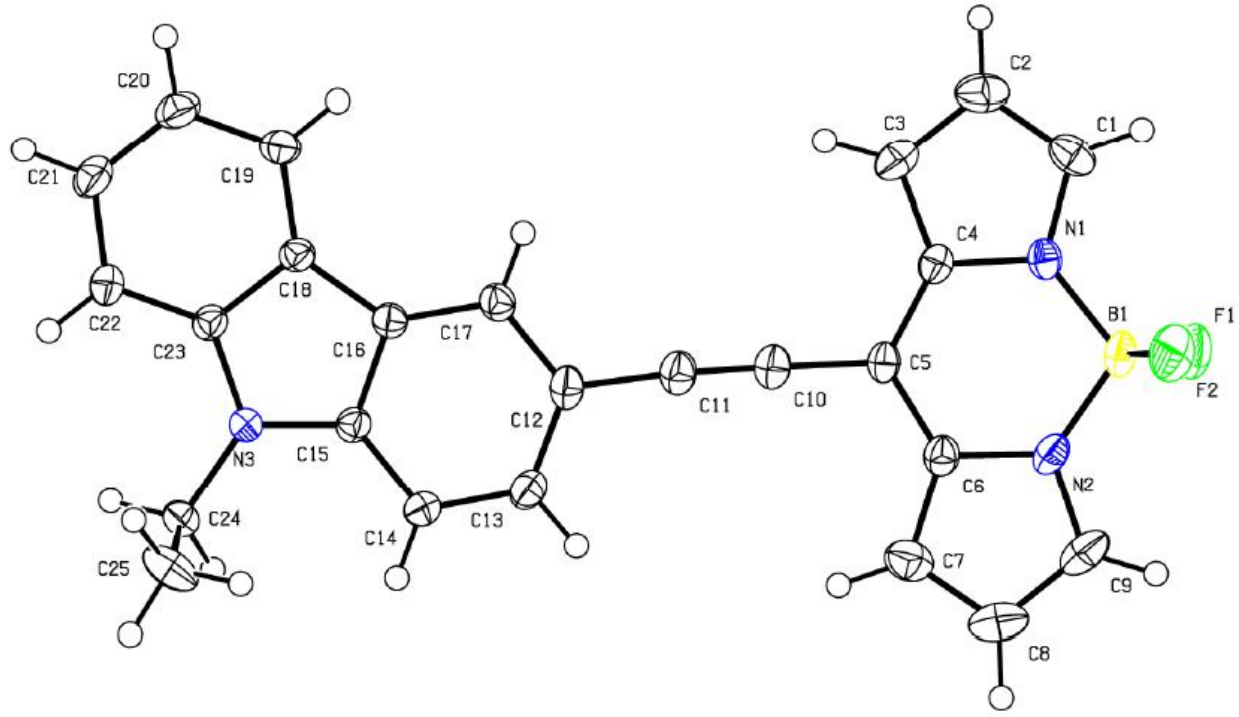


Fig. S3 Crystal structure of BODIPY **2c**.

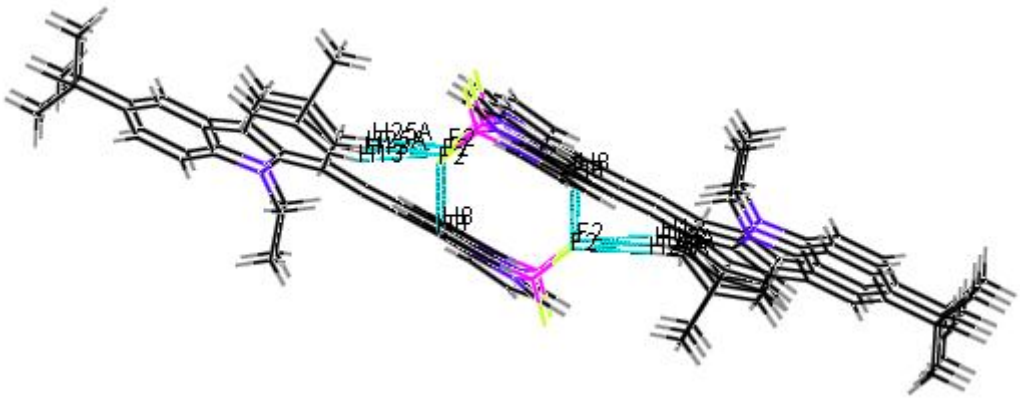


Fig. S4 Packing diagram of BODIPY **2a.**

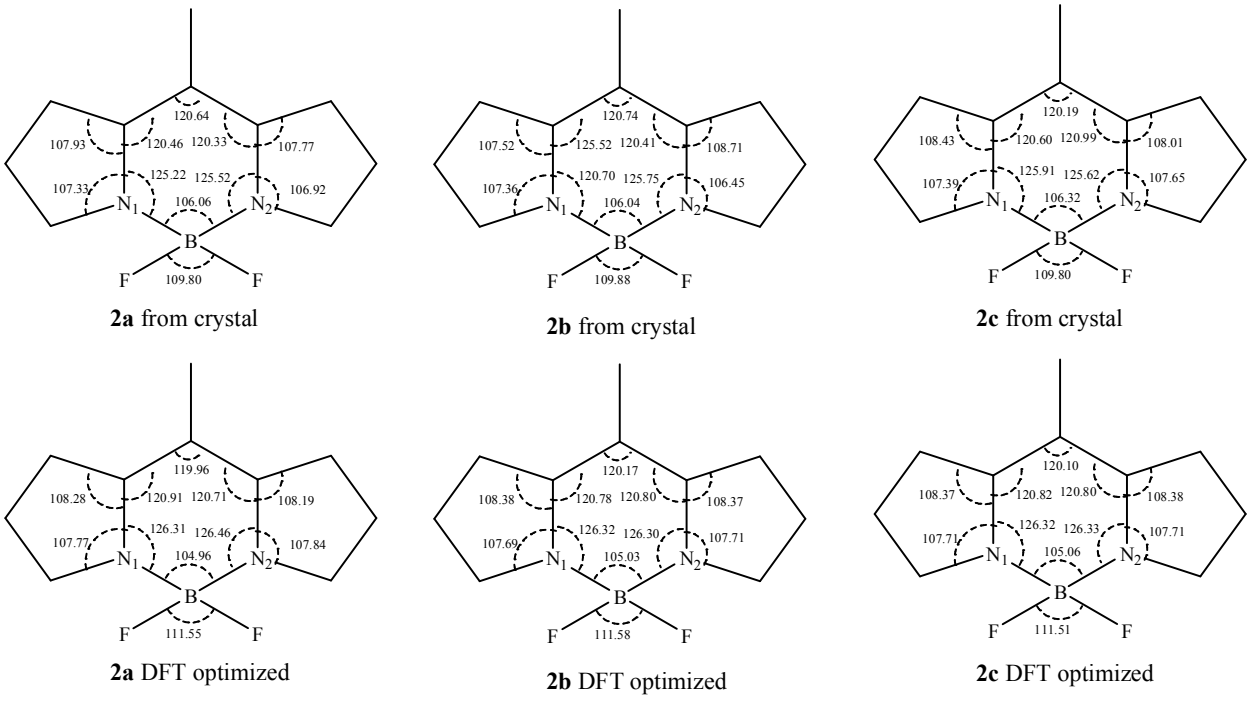
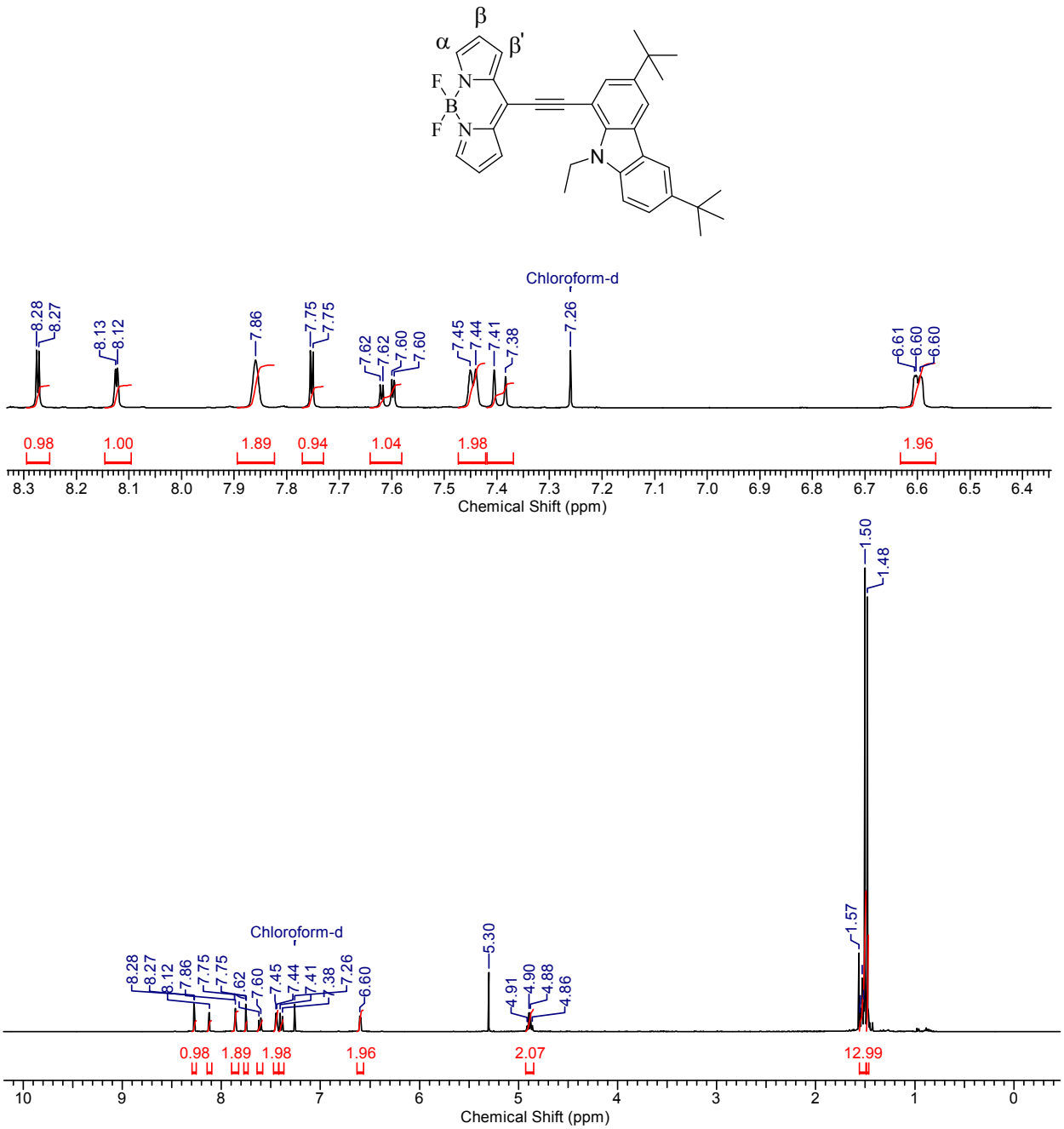


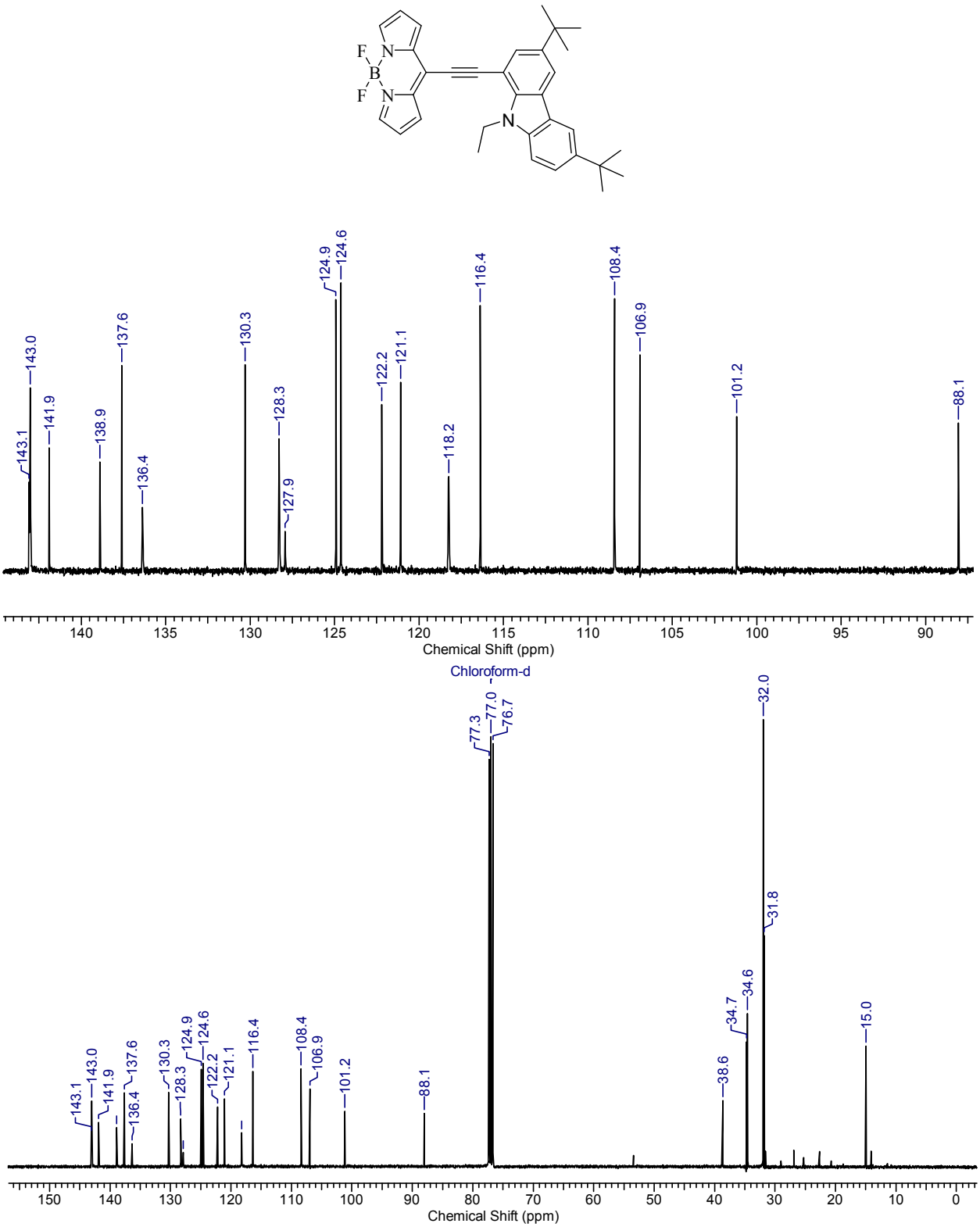
Fig. S5 Comparison of selected bond angles of the crystal structures and DFT optimized structures of BODIPYs **2a-2c.**

Copies of NMR and HRMS Spectra of the New Compounds:

^{1}H NMR of **2a**



^{13}C NMR of **2b**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141.9
138.9
137.6
136.4
130.3
128.3
127.9
124.9
124.6
122.2
121.1
118.2
116.4
108.4
106.9
101.2
88.1
Chemical Shift (ppm)
Chloroform-d
77.3
77.0
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32.0
31.8
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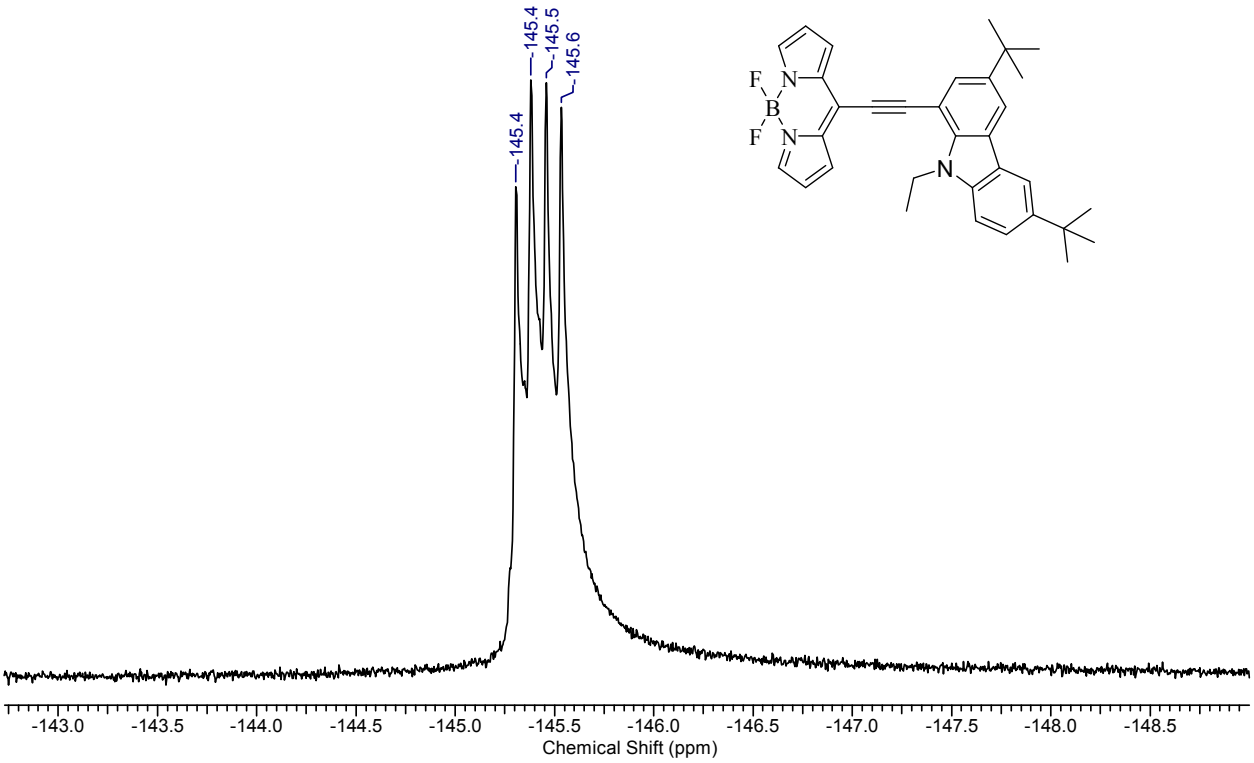
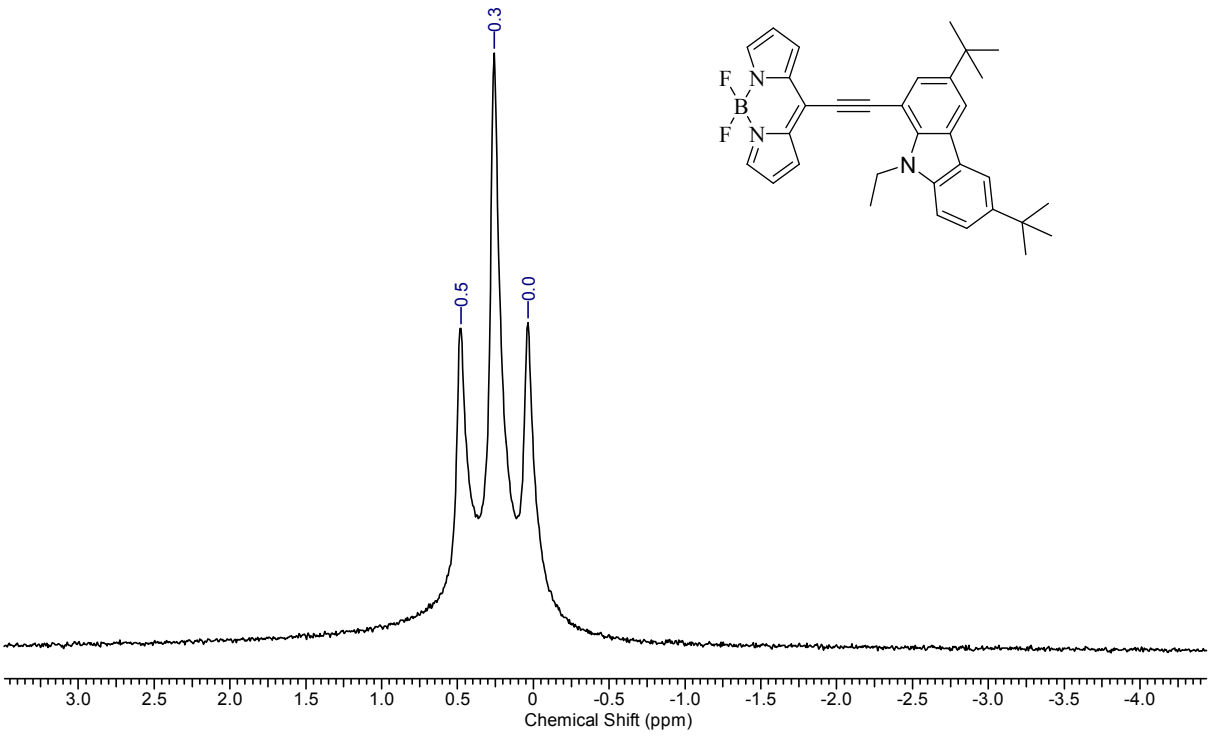
15.0
Chemical Shift (ppm)

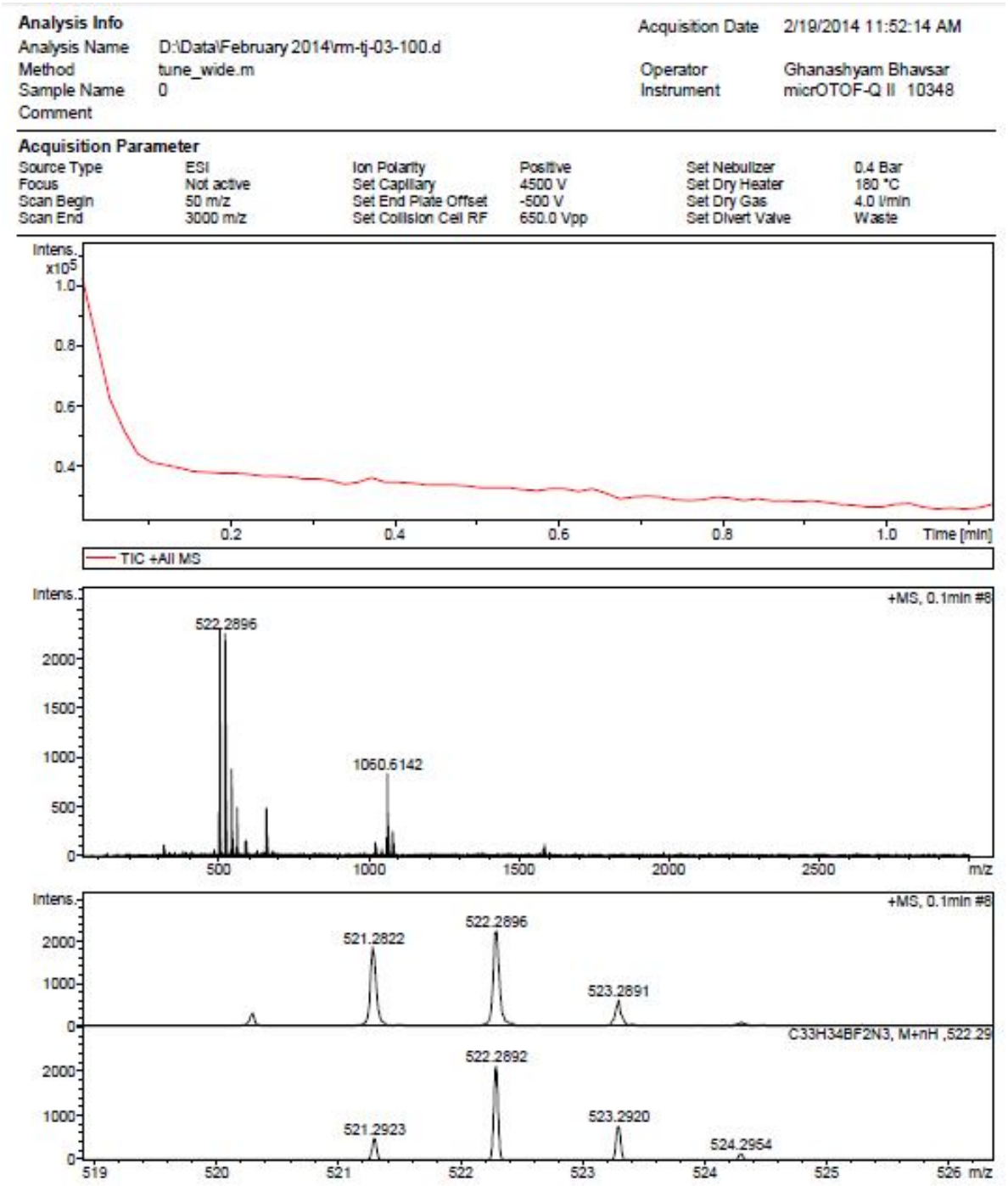
^{9}F NMR of **2a**



^{11}B NMR of **2a**



HRMS of **2a**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0.6
0.4
0.2
0.4
0.6
0.8
1.0
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1060.6142
2000
1500
1000
500
0
500
1000
1500
2000
2500
m/z
Intens.
+MS, 0.1min #8
522.2896
521.2822
523.2891
2000
1000
0
C33H34BF2N3, M+nH ,522.29
522.2892
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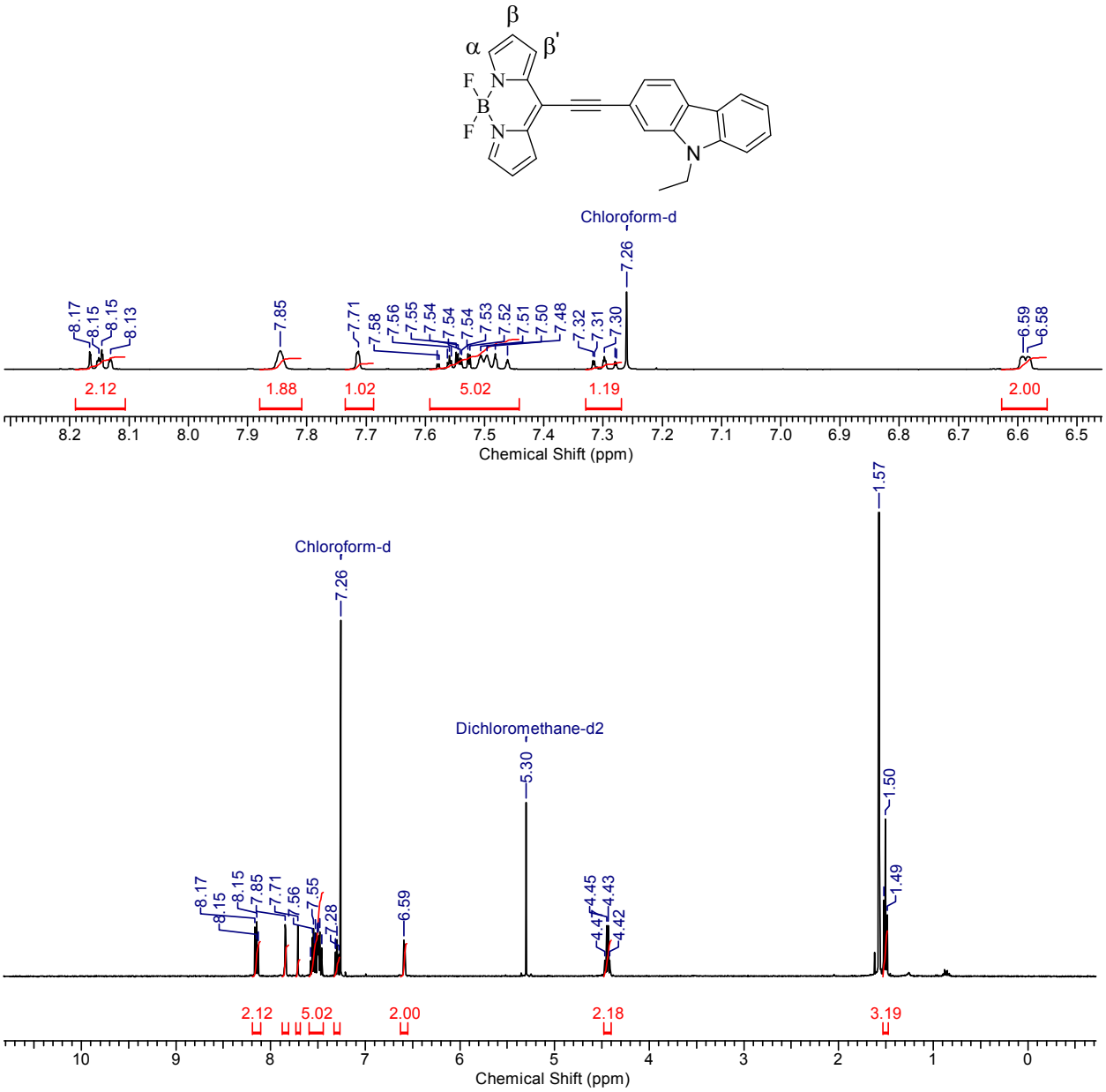
524.2954
519
520
521
522
523
524
525
526 m/z

^{1}H NMR of **2b**


β
α
β'
F
N
B
F
N
N
Chloroform-d
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8.15
8.15
8.13
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7.71
7.58
7.56
7.55
7.54
7.54
7.54
7.53
7.52
7.51
7.50
7.48
7.32
7.31
7.30
6.59
6.58
2.12
1.88
1.02
5.02
1.19
2.00
Chemical Shift (ppm)
1.57
Chloroform-d
7.26
Dichloromethane-d2
5.30
1.50
1.49
8.17
8.15
8.15
7.85
7.71
7.56
7.55
7.28
6.59
4.45
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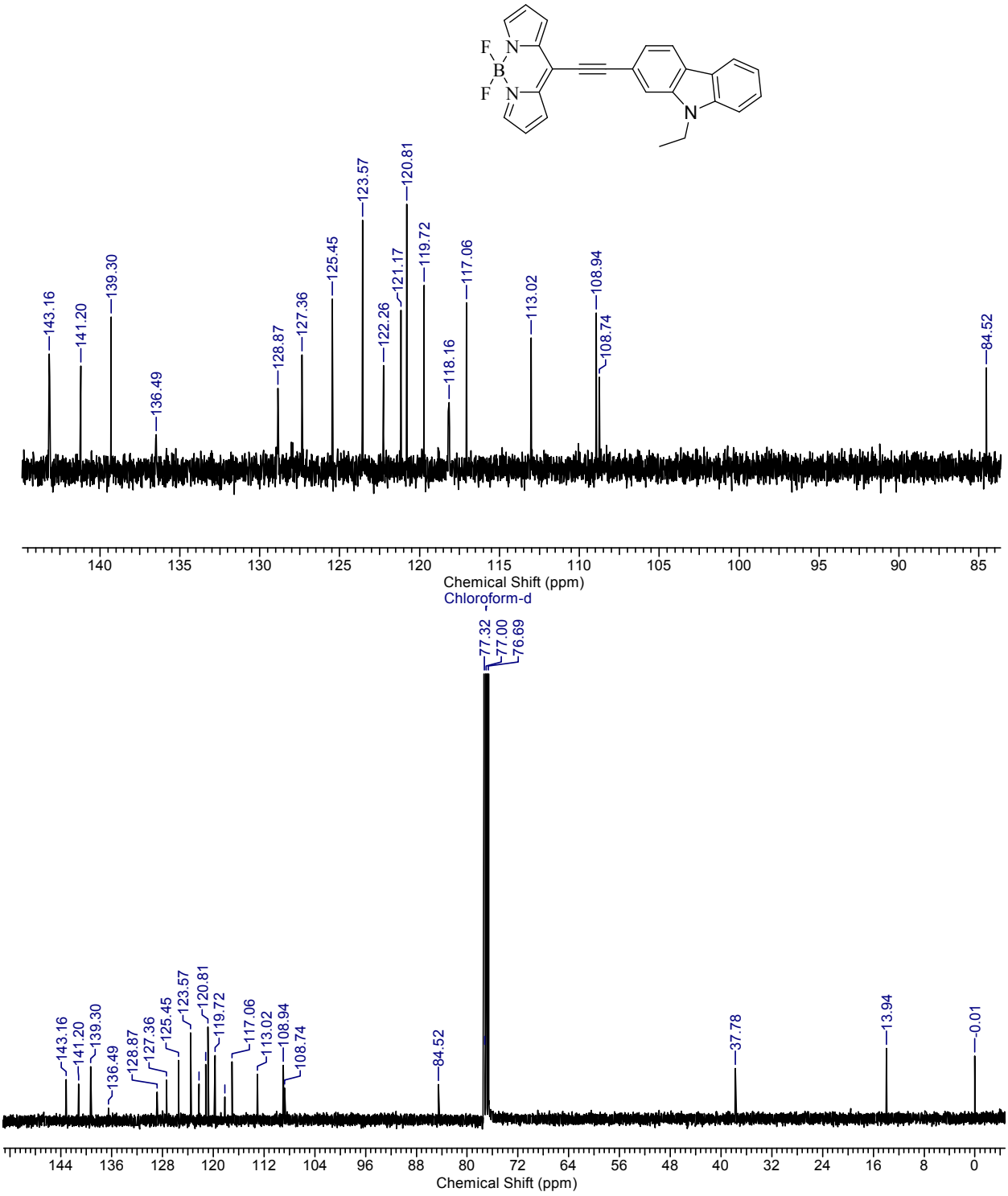
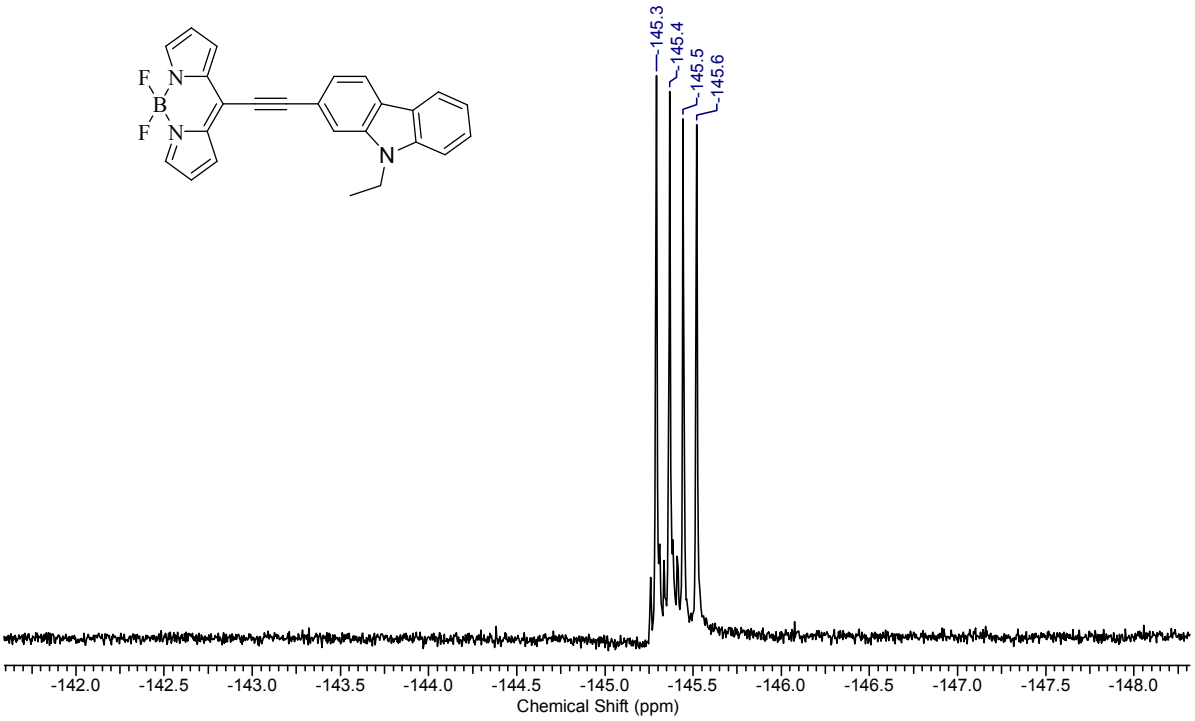
Chemical Shift (ppm)

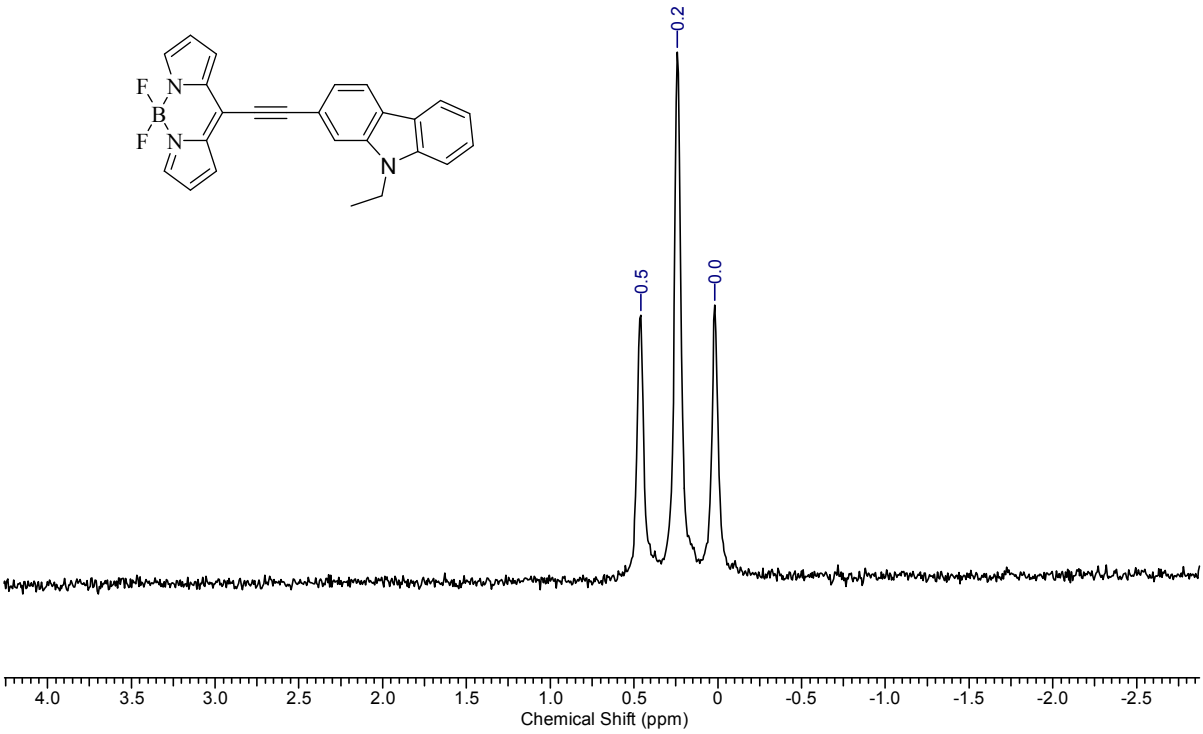
^{13}C NMR of **2b**


F
N
B
F
N
N
143.16
141.20
139.30
136.49
128.87
127.36
125.45
123.57
122.26
121.17
120.81
119.72
118.16
117.06
113.02
108.94
108.74
84.52
140
135
130
125
120
115
110
105
100
95
90
85
Chemical Shift (ppm)
Chloroform-d
77.32
77.00
76.69
143.16
141.20
139.30
136.49
128.87
127.36
125.45
123.57
120.81
119.72
117.06
113.02
108.94
108.74
84.52
37.78
13.94
-0.01
144
136
128
120
112
104
96
88
80
72
64
56
48
40
32
24
16
8
0
Chemical Shift (ppm)

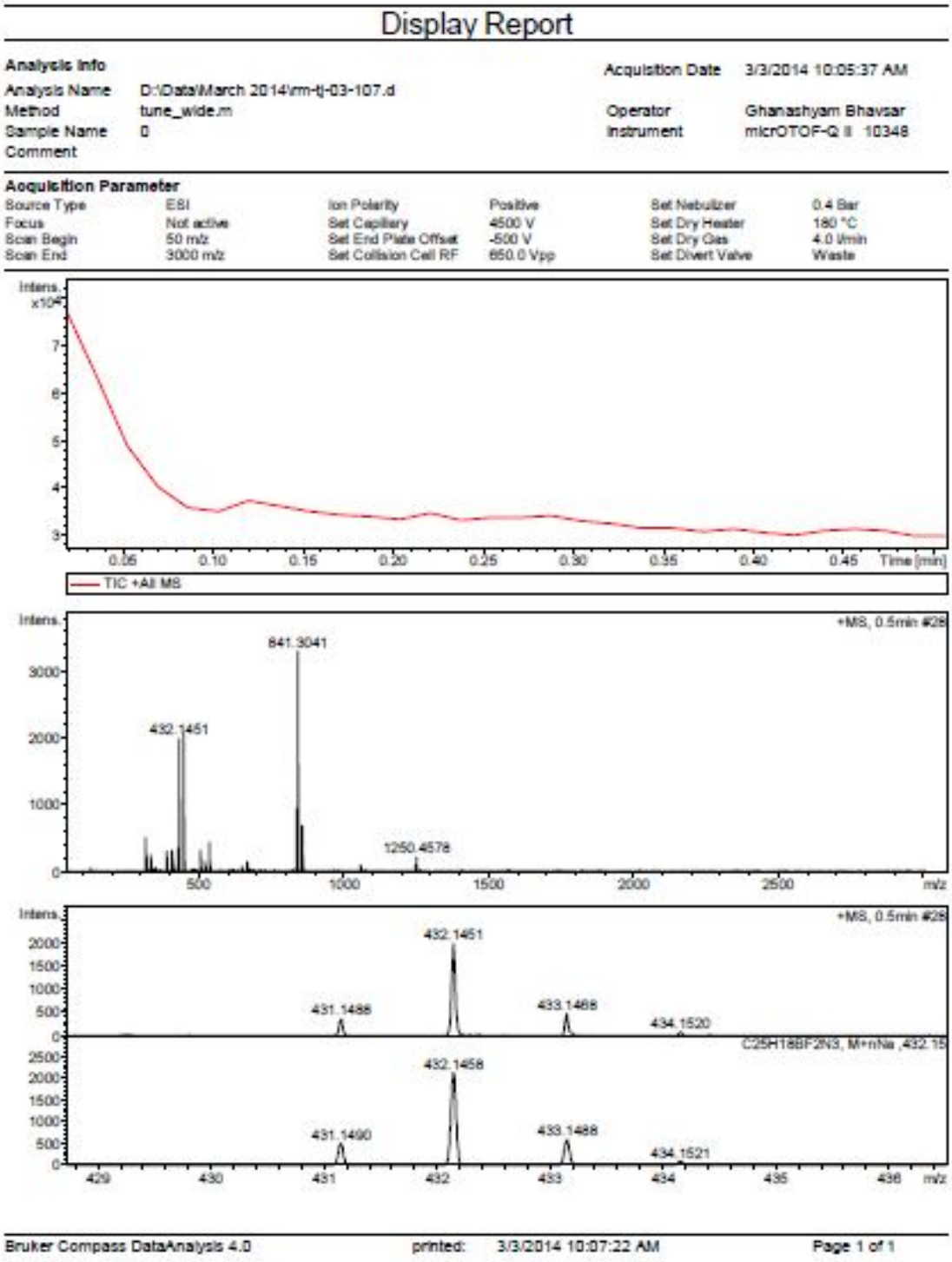
^{19}F NMR of **2b**



^{11}B NMR of **2b**



HRMS of **2b**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1250.4578
m/z
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431.1488
433.1488
434.1520
C25H18BF2N3, M+nNa ,432.15
432.1458
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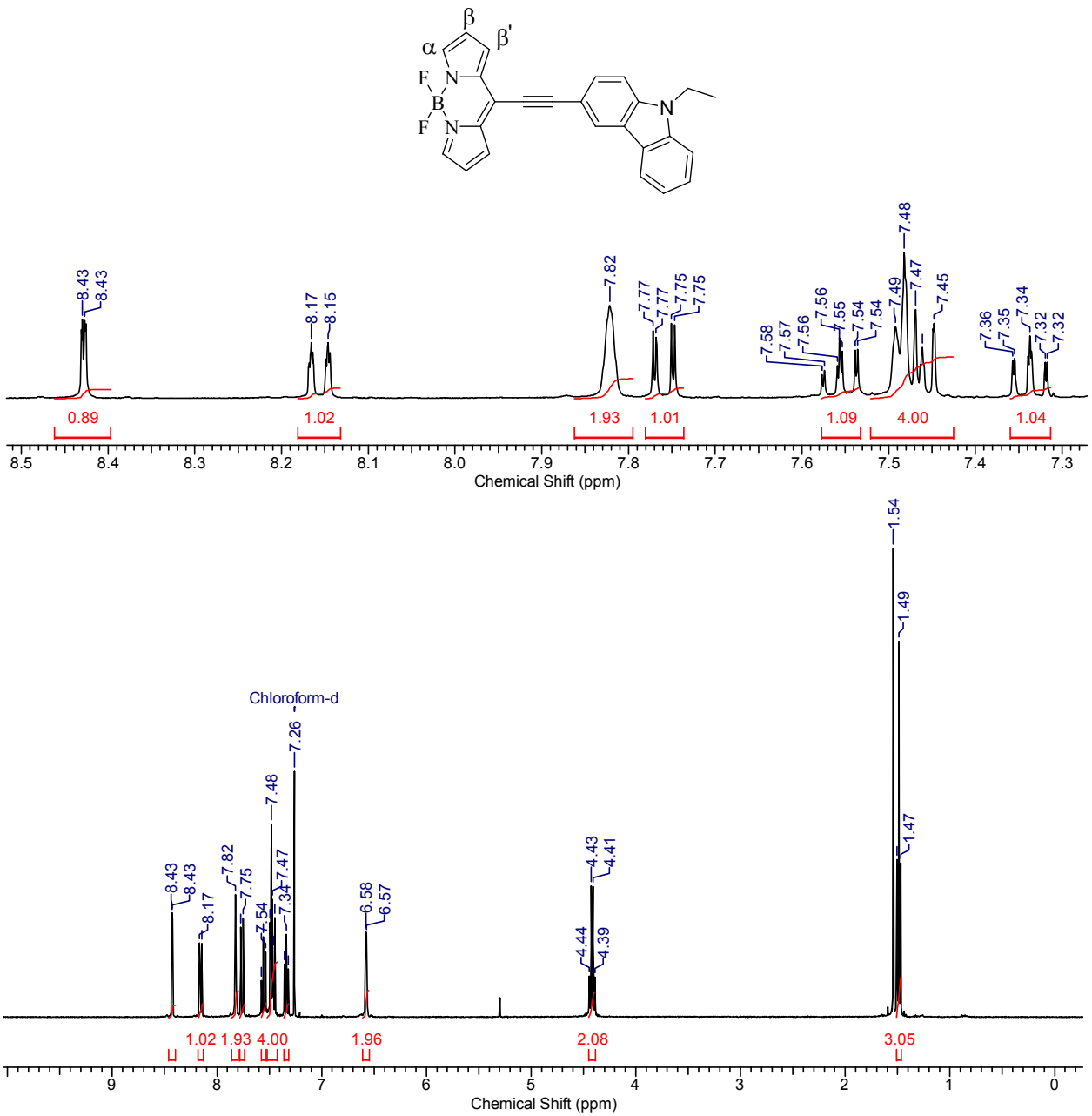
^{1}H NMR of **2c**


β
β'
α
F
N
B
F
N
N
8.43
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8.17
8.15
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7.77
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7.75
7.75
7.58
7.57
7.56
7.56
7.55
7.54
7.54
7.49
7.48
7.47
7.45
7.36
7.35
7.34
7.32
7.32
0.89
1.02
1.93
1.01
1.09
4.00
1.04
Chemical Shift (ppm)
Chloroform-d
7.26
1.54
1.49
1.47
4.43
4.41
4.44
4.39
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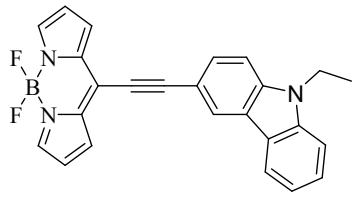
4.00
1.96
2.08
3.05
Chemical Shift (ppm)

^{13}C NMR of **2c**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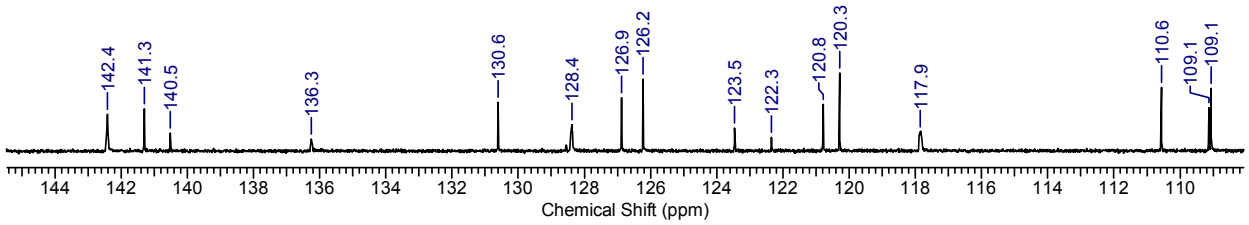
N
B
F
N
N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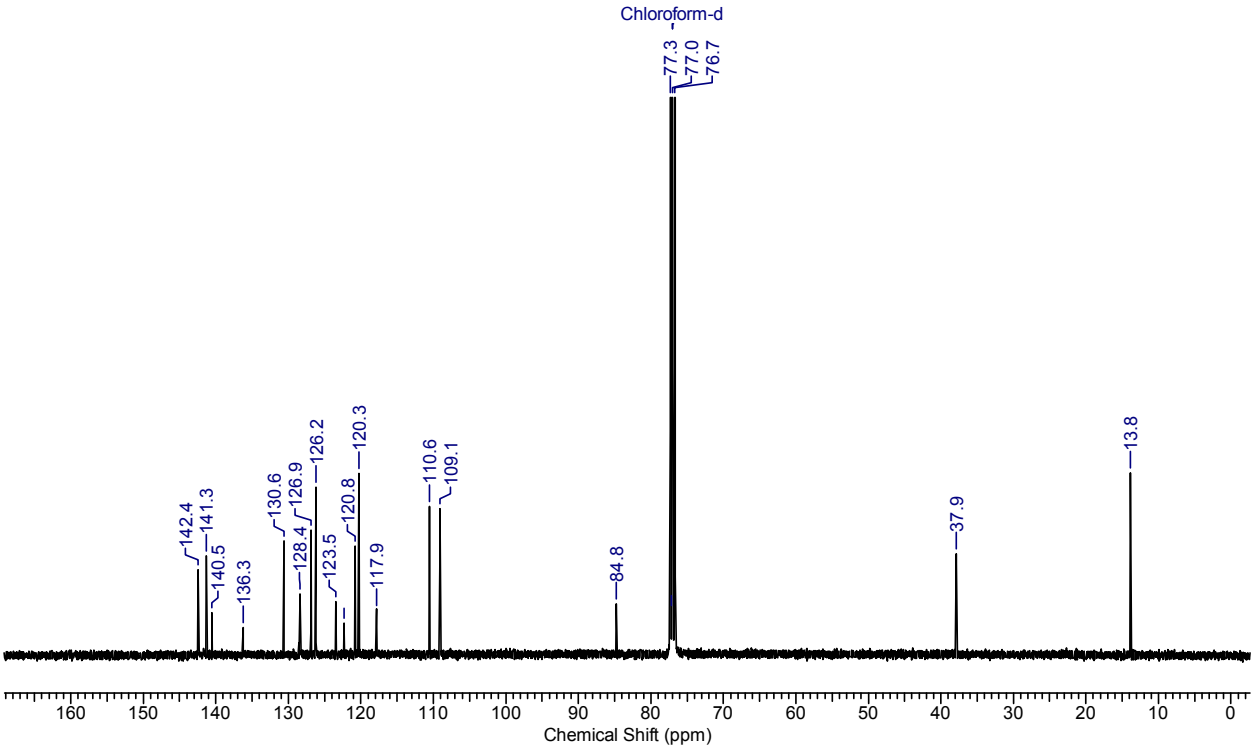
Chemical Shift (ppm)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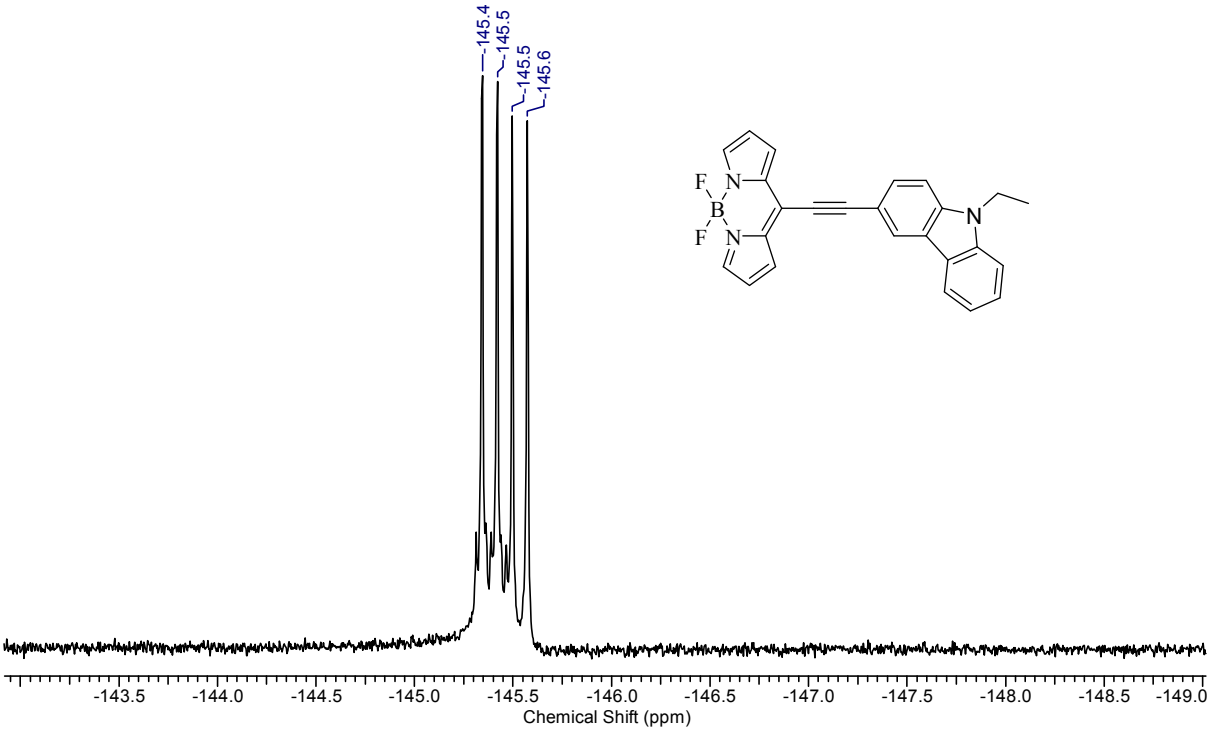
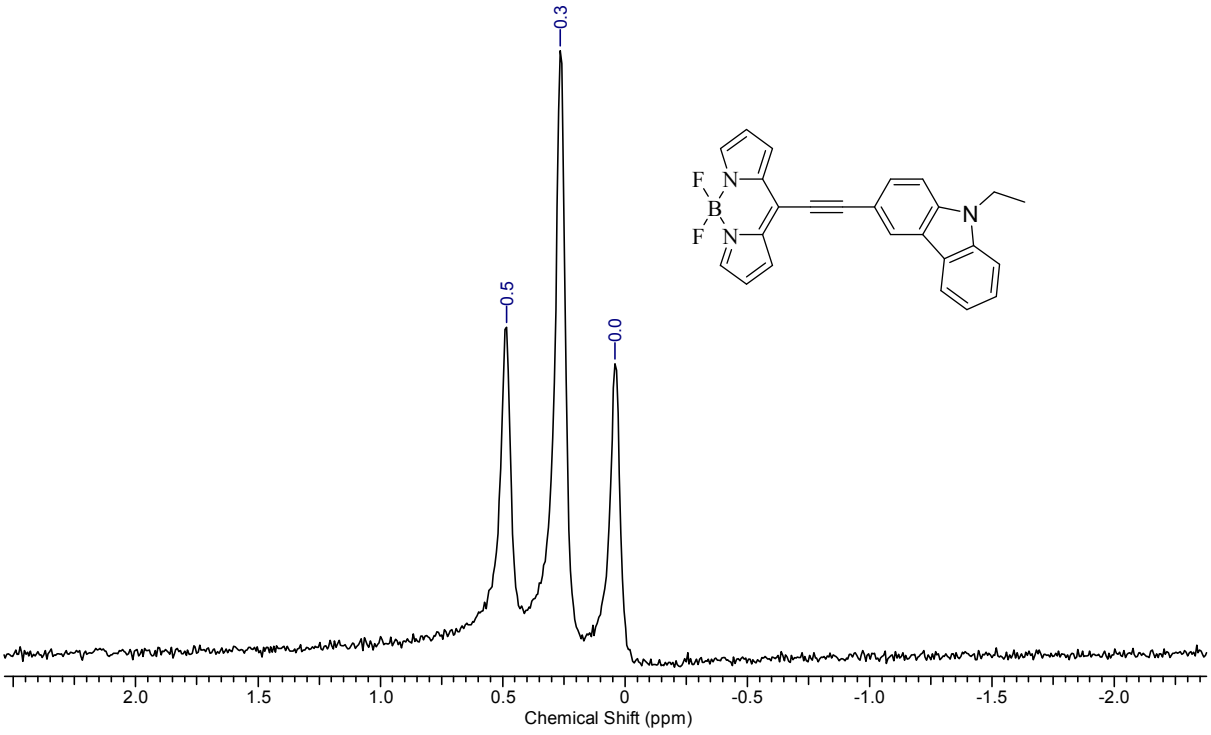
120.8
120.3
117.9
110.6
109.1
84.8
37.9
13.8
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
Chemical Shift (ppm)

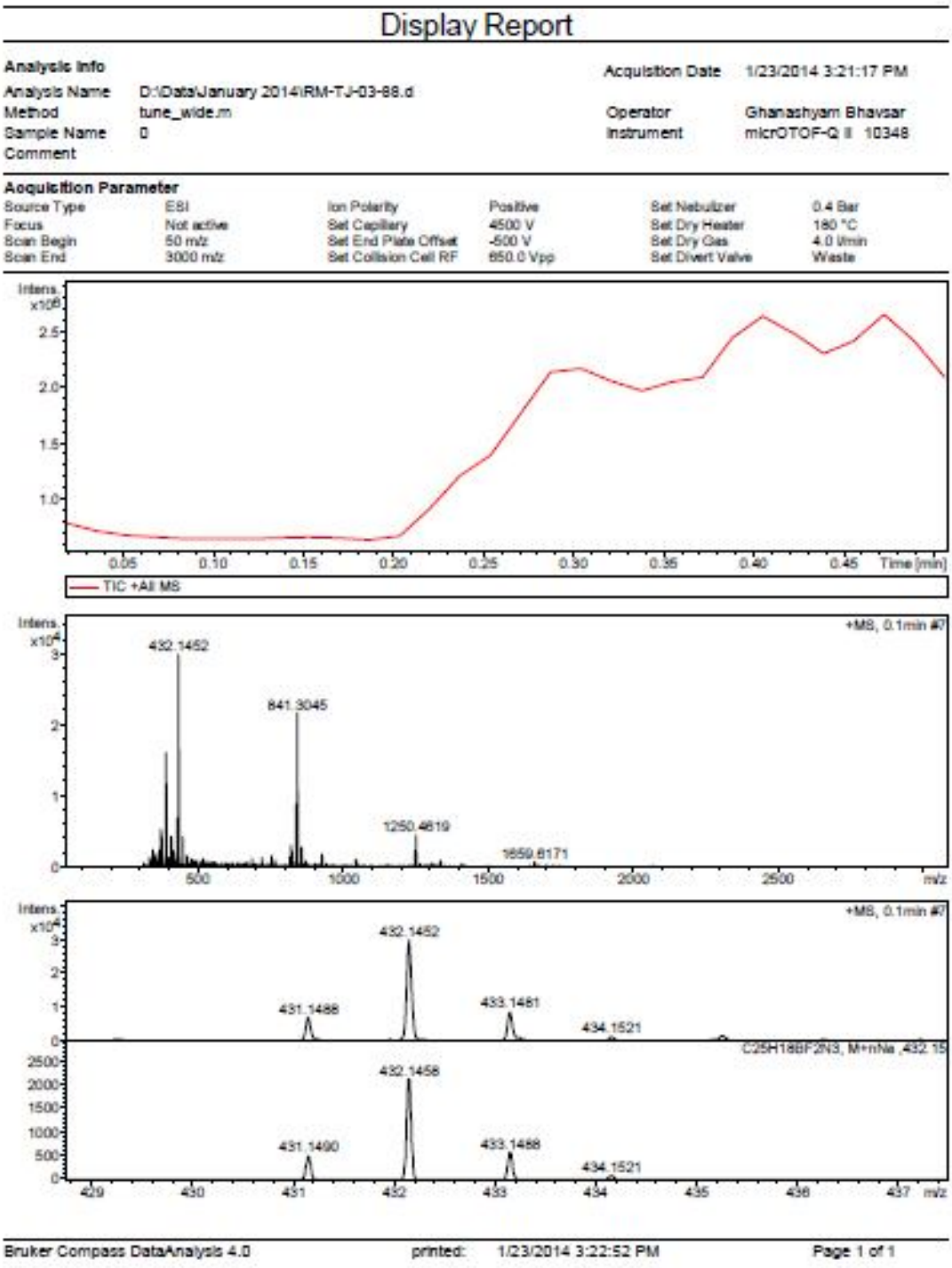
^{19}F NMR of **2c**



^{11}B NMR of **2c**



HRMS of **2c**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Set Capillary 4500 V
Set End Plate Offset -500 V
Set Collision Cell RF 650.0 Vpp
Set Nebulizer 0.4 Bar
Set Dry Heater 180 °C
Set Dry Gas 4.0 l/min
Set Divert Valve Waste
Intens.
x10^6
Time [min]
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+MS, 0.1min #7
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841.3045
1250.4619
1659.6171
m/z
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434.1521
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Page 1 of 1

Theoretical study:

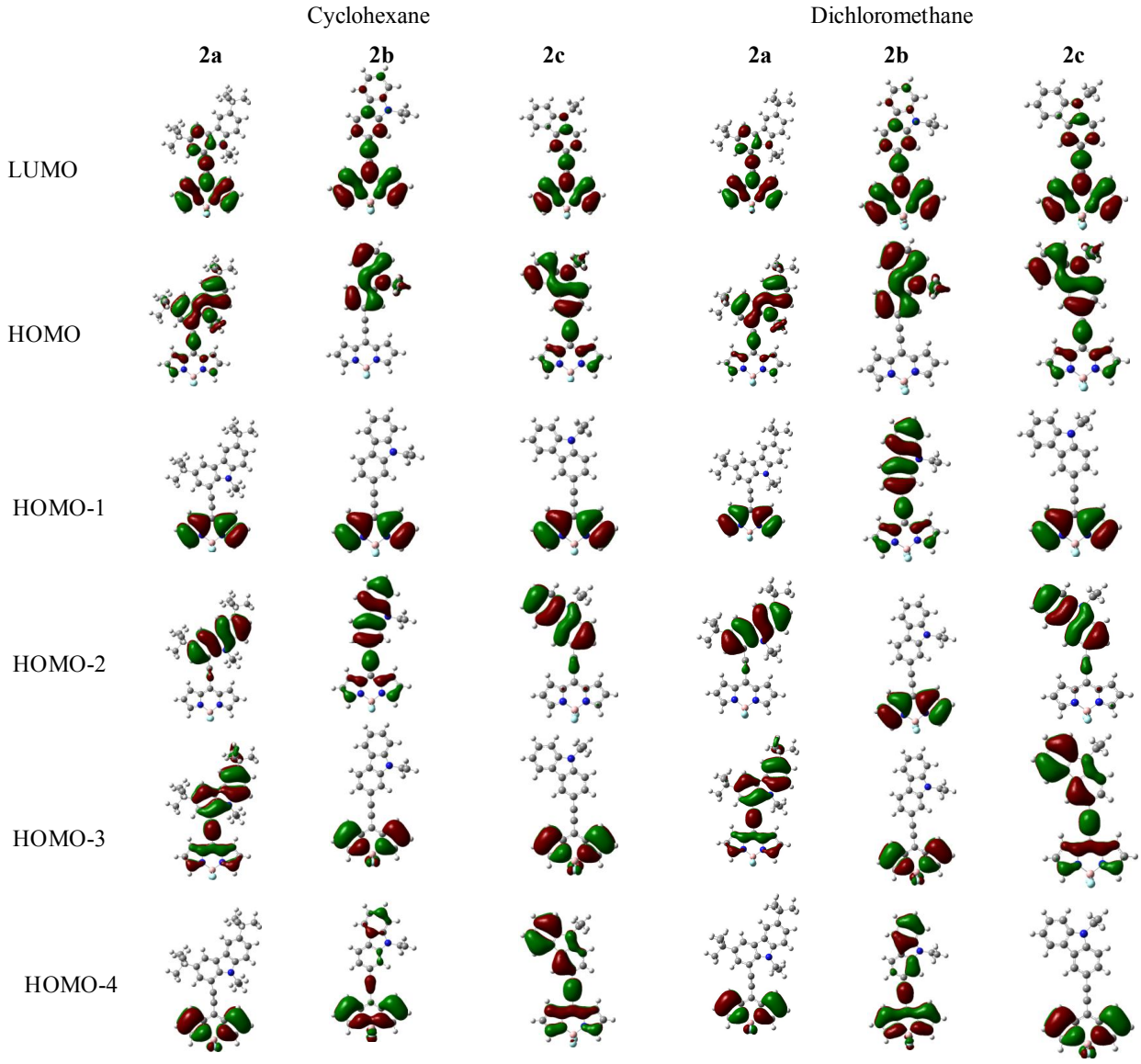

Fig. S6 Frontier molecular orbitals of BODIPYs **2a- 2c** at the B3LYP/6-31 G(d) level in dichloromethane and cyclohexane solvents using IEFPCM model.

Excitation energies and oscillator strengths:

Calculation method: B3LYP/6-31G(d) level in dichloromethane using IEFPCM model.

BODIPY **2a**- in DCM

Excited State 1: Singlet-A 1.4739 eV 841.18 nm f=0.0007 <S**2>=0.000
138 ->139 -0.70001
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1666.89641591
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.2892 eV 541.61 nm f=0.0003 <S**2>=0.000
137 ->139 -0.70311

Excited State 3: Singlet-A 2.6238 eV 472.54 nm f=0.5174 <S**2>=0.000
134 ->139 0.19082
136 ->139 0.68435

Excited State 4: Singlet-A 2.7242 eV 455.13 nm f=0.0046 <S**2>=0.000
131 ->139 -0.12460
135 ->139 -0.68335

Excited State 5: Singlet-A 2.9988 eV 413.45 nm f=0.1205 <S**2>=0.000
134 ->139 0.67993
136 ->139 -0.19424

Excited State 6: Singlet-A 3.1969 eV 387.83 nm f=0.0132 <S**2>=0.000
132 ->139 -0.28417
133 ->139 0.64170

BODIPY **2b**- DCM

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 1.9539 eV 634.54 nm f=0.0455 <S**2>=0.000

106 ->107 0.70588

This state for optimization and/or second-order correction.

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.3971 eV 517.22 nm f=1.1228 <S**2>=0.000

105 ->107 0.70434

Excited State 3: Singlet-A 2.5805 eV 480.46 nm f=0.4795 <S**2>=0.000

103 ->107 -0.15527

104 ->107 0.69229

Excited State 4: Singlet-A 3.0015 eV 413.07 nm f=0.0870 <S**2>=0.000

103 ->107 0.68861

104 ->107 0.15815

Excited State 5: Singlet-A 3.2261 eV 384.32 nm f=0.0298 <S**2>=0.000

100 ->107 -0.22487

101 ->107 0.10547

102 ->107 0.66008

Excited State 6: Singlet-A 3.4718 eV 357.12 nm f=0.0059 <S**2>=0.000

101 ->107 0.68915

102 ->107 -0.11899

Excited State 7: Singlet-A 3.6030 eV 344.12 nm f=0.1984 <S**2>=0.000

100 ->107 0.65373

102 ->107 0.20864

105 ->108 0.10162

Excited State 8: Singlet-A 3.6766 eV 337.22 nm f=0.0000 <S**2>=0.000

99 ->107 0.70435

Excited State 9: Singlet-A 3.7502 eV 330.61 nm f=0.0645 <S**2>=0.000
105 ->109 0.11293
106 ->108 0.68581

Excited State 10: Singlet-A 4.3014 eV 288.24 nm f=0.1629 <S**2>=0.000
98 ->107 -0.16211
105 ->108 0.62484
106 ->109 -0.25925

BODIPY **2c** - DCM

Excited State 1: Singlet-A 1.6874 eV 734.77 nm f=0.0000 <S**2>=0.000
106 ->107 -0.69543
This state for optimization and/or second-order correction.
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.5136 eV 493.25 nm f=0.0000 <S**2>=0.000
104 ->107 0.70242

Excited State 3: Singlet-A 2.6477 eV 468.27 nm f=0.5376 <S**2>=0.000
102 ->107 -0.17930
105 ->107 -0.68721

Excited State 4: Singlet-A 3.0352 eV 408.49 nm f=0.1144 <S**2>=0.000
102 ->107 -0.68302
105 ->107 0.18244

Excited State 5: Singlet-A 3.1215 eV 397.19 nm f=0.0000 <S**2>=0.000
98 ->107 -0.11093

103 ->107 -0.68641

106 ->107 -0.10437

Excited State 6: Singlet-A 3.2319 eV 383.63 nm f=0.0140 <S**2>=0.000

100 ->107 0.34507

101 ->107 -0.61506

Calculation method: B3LYP/6-31G(d) level in cyclohexane using IEFPCM model.

BODIPY **2a** - in cyclohexane

Excited State 1: Singlet-A 1.5444 eV 802.79 nm f=0.0003 <S**2>=0.000

138 ->139 -0.70024

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -1666.88790575

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.3437 eV 529.01 nm f=0.0002 <S**2>=0.000

137 ->139 0.70317

Excited State 3: Singlet-A 2.7512 eV 450.65 nm f=0.2777 <S**2>=0.000

134 ->139 -0.30622

135 ->139 0.24261

136 ->139 0.58965

Excited State 4: Singlet-A 2.7833 eV 445.46 nm f=0.0442 <S**2>=0.000

131 ->139 0.11398

134 ->139 0.15224

135 ->139 0.63859

136 ->139 -0.20419

Excited State 5: Singlet-A 3.0433 eV 407.40 nm f=0.2000 <S**2>=0.000

134 ->139 0.61773

136 ->139 0.34555

Excited State 6: Singlet-A 3.2023 eV 387.17 nm f=0.0036 <S**2>=0.000

132 ->139 -0.23454

133 ->139 0.66423

BODIPY **2b** - in cyclohexane

Excited State 1: Singlet-A 2.1049 eV 589.02 nm f=0.0300 <S**2>=0.000

106 ->107 0.70555

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -1352.36557282

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.5838 eV 479.85 nm f=0.9528 <S**2>=0.000

104 ->107 0.70526

Excited State 3: Singlet-A 2.7088 eV 457.72 nm f=0.3378 <S**2>=0.000

103 ->107 0.25489

105 ->107 0.66410

Excited State 4: Singlet-A 3.0285 eV 409.39 nm f=0.1138 <S**2>=0.000

103 ->107 0.65791

105 ->107 -0.25915

Excited State 5: Singlet-A 3.2196 eV 385.09 nm f=0.0335 <S**2>=0.000
105 ->107 -0.10538
102 ->107 0.69592

Excited State 6: Singlet-A 3.6035 eV 344.06 nm f=0.0059 <S**2>=0.000
101 ->107 -0.69013
106 ->108 0.11027

BODIPY **2c** - in cyclohexane

Excited State 1: Singlet-A 1.8454 eV 671.87 nm f=0.0001 <S**2>=0.000
102 ->107 -0.10077
106 ->107 0.69473
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1352.37214855
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.6653 eV 465.19 nm f=0.0001 <S**2>=0.000
104 ->107 -0.70229

Excited State 3: Singlet-A 2.7838 eV 445.38 nm f=0.3512 <S**2>=0.000
103 ->107 -0.32036
105 ->107 -0.63474
105 <-107 0.10009

Excited State 4: Singlet-A 3.0751 eV 403.19 nm f=0.1916 <S**2>=0.000
103 ->107 -0.62915
105 ->107 0.32614

Excited State 5: Singlet-A 3.2373 eV 382.98 nm f=0.0038 <S**2>=0.000

100 ->107 0.29773

101 ->107 -0.63952

Excited State 6: Singlet-A 3.2587 eV 380.47 nm f=0.0002 <S**2>=0.000

98 ->107 0.11046

102 ->107 0.68571

106 ->107 0.10824

Calculation method: B3LYP/6-31G(d) level

Data for BODIPY **2a**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.458350	-2.849062	-0.140716
2	1	0	2.382911	-2.950034	-0.130927
3	6	0	4.405450	-3.866777	-0.181133
4	1	0	4.226359	-4.932699	-0.212799
5	6	0	5.667463	-3.242599	-0.166213
6	1	0	6.653223	-3.687217	-0.189447
7	7	0	5.525773	-1.907344	-0.118216
8	5	0	6.694954	-0.862563	-0.169153
9	6	0	5.696222	2.754369	0.272720
10	6	0	4.437430	2.168574	0.203461
11	1	0	3.474922	2.657758	0.257954
12	6	0	4.636632	0.773992	0.060381
13	6	0	3.706748	-0.288396	-0.022429
14	6	0	4.165359	-1.624013	-0.100045
15	7	0	6.004208	0.528533	0.042633
16	9	0	7.595784	-1.107010	0.849560
17	6	0	6.634238	1.708394	0.169212

18	1	0	7.714991	1.752579	0.179155
19	9	0	7.306879	-0.902083	-1.408937
20	1	0	5.928734	3.803965	0.388870
21	6	0	2.327547	0.008175	-0.014153
22	6	0	1.145765	0.318981	-0.018232
23	6	0	-0.173274	0.837936	-0.023861
24	6	0	-1.362286	0.070259	-0.043046
25	6	0	-0.311739	2.249664	-0.011797
26	6	0	-2.624916	0.731180	-0.046182
27	7	0	-1.572319	-1.298184	-0.064625
28	6	0	-1.541786	2.911025	-0.018750
29	1	0	0.608913	2.819495	0.001395
30	6	0	-3.639280	-0.303194	-0.057838
31	6	0	-2.703533	2.119229	-0.036818
32	6	0	-2.949037	-1.536685	-0.059275
33	6	0	-0.570490	-2.355567	0.005230
34	6	0	-1.660050	4.447079	-0.008297
35	6	0	-5.034936	-0.284564	-0.067944
36	1	0	-3.683032	2.589409	-0.041409
37	6	0	-3.647422	-2.743166	-0.061990
38	1	0	-0.957760	-3.206820	-0.564147
39	1	0	0.322040	-2.005294	-0.515961
40	6	0	-0.234995	-2.773197	1.440603
41	6	0	-2.452308	4.894079	1.243238
42	6	0	-2.405833	4.913375	-1.281124
43	6	0	-0.285360	5.141595	0.022354
44	6	0	-5.764193	-1.481068	-0.075684
45	1	0	-5.552770	0.670826	-0.068751
46	6	0	-5.041725	-2.692716	-0.071735
47	1	0	-3.138059	-3.701877	-0.053406
48	1	0	-1.132913	-3.107880	1.970070
49	1	0	0.487739	-3.596786	1.437862
50	1	0	0.202781	-1.938564	1.996785
51	1	0	-2.553769	5.985934	1.260602
52	1	0	-3.460887	4.467410	1.263033
53	1	0	-1.941101	4.585446	2.162169

54	1	0	-2.509299	6.005229	-1.284789
55	1	0	-1.859569	4.620568	-2.184897
56	1	0	-3.411679	4.484712	-1.345511
57	1	0	0.287125	4.876213	0.918660
58	1	0	0.318305	4.893332	-0.858151
59	1	0	-0.422745	6.228552	0.030163
60	6	0	-7.305384	-1.436566	-0.085841
61	1	0	-5.577433	-3.634895	-0.074117
62	6	0	-7.809824	-0.695515	1.175229
63	6	0	-7.935426	-2.842688	-0.094971
64	6	0	-7.792447	-0.687043	-1.348763
65	1	0	-7.433098	0.331674	1.222845
66	1	0	-8.905775	-0.648331	1.179421
67	1	0	-7.488326	-1.211045	2.087375
68	1	0	-9.027648	-2.755385	-0.103048
69	1	0	-7.644321	-3.415925	-0.982643
70	1	0	-7.658181	-3.421560	0.793503
71	1	0	-7.457920	-1.196106	-2.259829
72	1	0	-8.888241	-0.640235	-1.367900
73	1	0	-7.415629	0.340622	-1.384068

Total Energy (HF) = -1666.9466894 Hartree

Data for BODIPY **2b**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.469168	-2.663789	0.204349
2	1	0	2.477525	-3.093218	0.238472
3	6	0	4.690065	-3.324025	0.278433
4	1	0	4.858964	-4.387087	0.381304
5	6	0	5.690234	-2.334148	0.199333
6	1	0	6.766222	-2.443813	0.219382
7	7	0	5.133713	-1.117086	0.083229

8	5	0	5.908183	0.235438	-0.101327
9	6	0	3.787560	3.365722	-0.110672
10	6	0	2.785890	2.401632	-0.090961
11	1	0	1.715548	2.554299	-0.090300
12	6	0	3.427260	1.140161	-0.058611
13	6	0	2.892753	-0.165951	0.003067
14	6	0	3.753752	-1.281922	0.083667
15	7	0	4.801134	1.347227	-0.061337
16	9	0	6.801725	0.417125	0.936583
17	6	0	5.014623	2.673359	-0.092062
18	1	0	6.022992	3.064769	-0.100649
19	9	0	6.544867	0.249357	-1.328922
20	1	0	3.667823	4.440195	-0.131671
21	6	0	1.494152	-0.354861	-0.000346
22	6	0	0.286045	-0.519942	-0.009457
23	6	0	-1.119167	-0.714694	-0.021738
24	6	0	-1.650676	-2.029477	0.055965
25	6	0	-1.978220	0.398337	-0.108949
26	6	0	-3.020240	-2.243409	0.048542
27	1	0	-0.964242	-2.866780	0.122905
28	6	0	-3.350858	0.168851	-0.120934
29	1	0	-1.559712	1.397545	-0.161406
30	6	0	-3.888937	-1.147529	-0.037593
31	1	0	-3.414069	-3.254059	0.110514
32	7	0	-4.393875	1.081553	-0.213083
33	6	0	-5.324944	-1.008546	-0.066860
34	6	0	-5.595810	0.383421	-0.166529
35	6	0	-4.252358	2.530036	-0.253532
36	6	0	-6.387846	-1.920228	-0.020075
37	6	0	-6.906907	0.869170	-0.211099
38	1	0	-3.340908	2.761020	-0.815080
39	1	0	-5.085441	2.929632	-0.840972
40	6	0	-4.210443	3.178258	1.134259
41	6	0	-7.691904	-1.440431	-0.068352
42	1	0	-6.194640	-2.987112	0.054167
43	6	0	-7.943664	-0.059295	-0.162572

44	1	0	-7.119023	1.931788	-0.278133
45	1	0	-3.367332	2.796601	1.719185
46	1	0	-4.101150	4.264614	1.041830
47	1	0	-5.130451	2.971311	1.690412
48	1	0	-8.525698	-2.135247	-0.031754
49	1	0	-8.970656	0.293931	-0.195834

Total Energy (HF) = -1352.4417111 Hartree

Data for BODIPY **2c**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.827008	2.470083	0.151835
2	1	0	-1.757112	2.625984	0.151209
3	6	0	-3.830974	3.428280	0.239612
4	1	0	-3.713350	4.500169	0.320328
5	6	0	-5.056011	2.733344	0.209359
6	1	0	-6.065275	3.120049	0.253186
7	7	0	-4.839424	1.410971	0.109003
8	5	0	-5.944780	0.305347	-0.022280
9	6	0	-4.717193	-3.269983	-0.017138
10	6	0	-3.497948	-2.601632	-0.043414
11	1	0	-2.505210	-3.029329	-0.065934
12	6	0	-3.786009	-1.216210	-0.023156
13	6	0	-2.926687	-0.094694	-0.004124
14	6	0	-3.465157	1.209398	0.071536
15	7	0	-5.165728	-1.056116	0.012922
16	9	0	-6.820862	0.379582	1.043993
17	6	0	-5.719357	-2.280539	0.016805
18	1	0	-6.794784	-2.394169	0.042086
19	9	0	-6.604164	0.439726	-1.230964
20	1	0	-4.882806	-4.338574	-0.017397
21	6	0	-1.529281	-0.277900	-0.042984

22	6	0	-0.320220	-0.436446	-0.078707
23	6	0	1.084298	-0.620120	-0.119108
24	6	0	1.627118	-1.930858	-0.199914
25	6	0	1.949443	0.490900	-0.076338
26	6	0	2.994989	-2.149899	-0.238610
27	1	0	0.945498	-2.774771	-0.228947
28	6	0	3.324903	0.289530	-0.113618
29	1	0	1.532498	1.491255	-0.012734
30	6	0	3.843901	-1.034929	-0.199158
31	1	0	3.385646	-3.161068	-0.293465
32	6	0	4.467946	1.179441	-0.083773
33	7	0	5.224090	-0.980077	-0.235687
34	6	0	5.620928	0.355889	-0.152200
35	6	0	4.613659	2.568539	-0.007178
36	6	0	6.121167	-2.127555	-0.263411
37	6	0	6.909018	0.897673	-0.137466
38	6	0	5.894536	3.113885	0.004103
39	1	0	3.739867	3.212680	0.044190
40	1	0	5.633098	-2.919283	-0.840979
41	1	0	7.013500	-1.838112	-0.827906
42	6	0	6.504421	-2.633608	1.131183
43	6	0	7.026919	2.284184	-0.060187
44	1	0	7.793261	0.269143	-0.180514
45	1	0	6.022146	4.190654	0.064502
46	1	0	5.617409	-2.948120	1.690494
47	1	0	7.181731	-3.490949	1.049292
48	1	0	7.008653	-1.850627	1.706499
49	1	0	8.017390	2.730486	-0.047138

Total Energy (HF) = -1352.4428201 Hartree