Electronic Supporting Information

Rational Design and Synthesis of Large Stokes Shift 2,6-Sulphur-Disubstituted BODIPYs for Cell Imaging

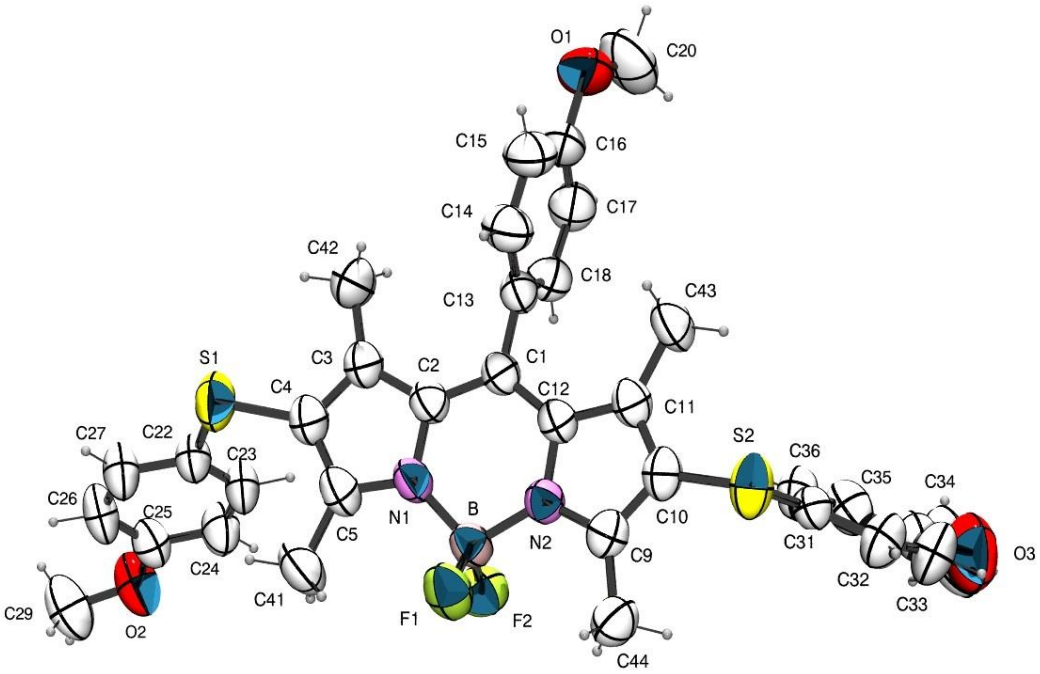


Figure S1. ORTEP-3 projection of **2d**, showing the atom numbering and displacement ellipsoids at the 50% probability level.

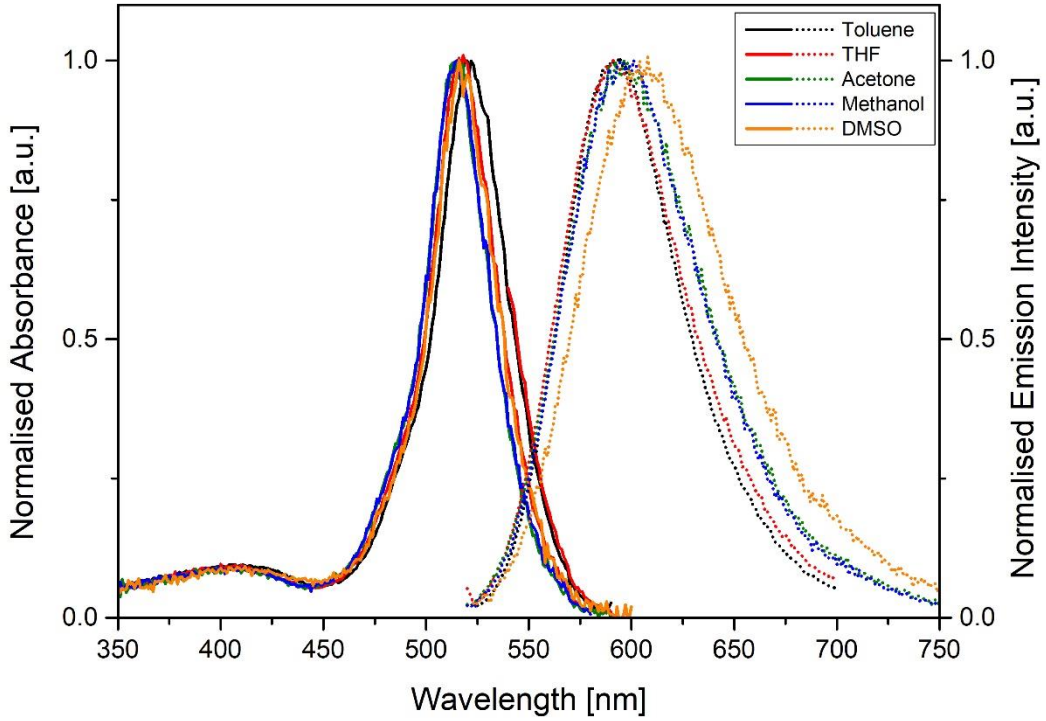


Figure S2. Normalized absorption and emission spectra of BODIPY **2a** in different organic solvents.

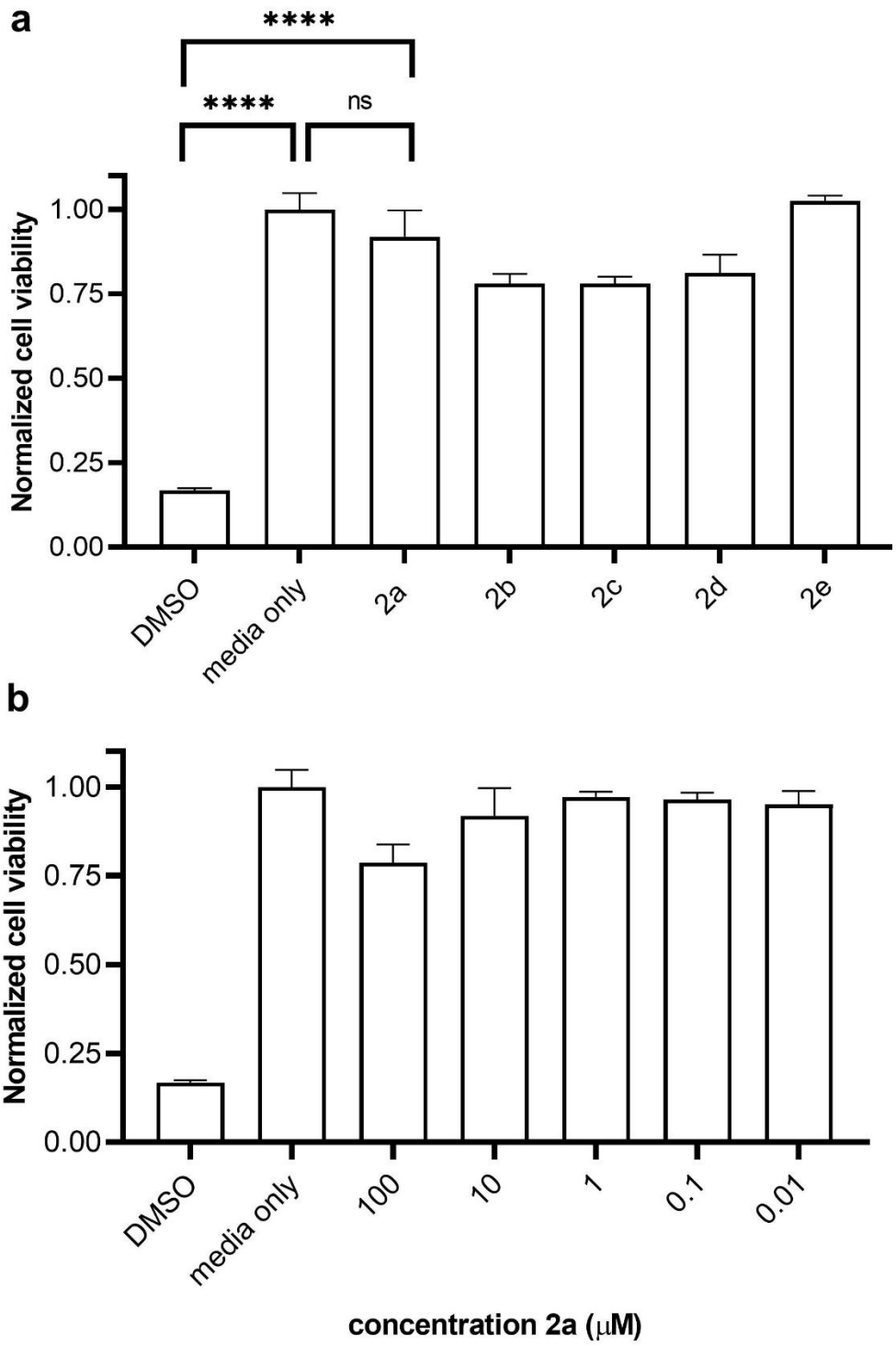


Figure S3. Viability assays in MDA-MB-231 cells. a) Cell viability after incubation with compounds **2a**-**2e** (all at 10 μM). Values were normalized against cells incubated in media only. b) Cell viability after incubation with compound **2a** at different concentrations. Values were normalized against cells incubated in media only. All values are represented as means±SD (n=3). P values were determined by one-way ANOVA using multiple comparisons (**** for $p<0.0001$, ns for $p>0.05$).

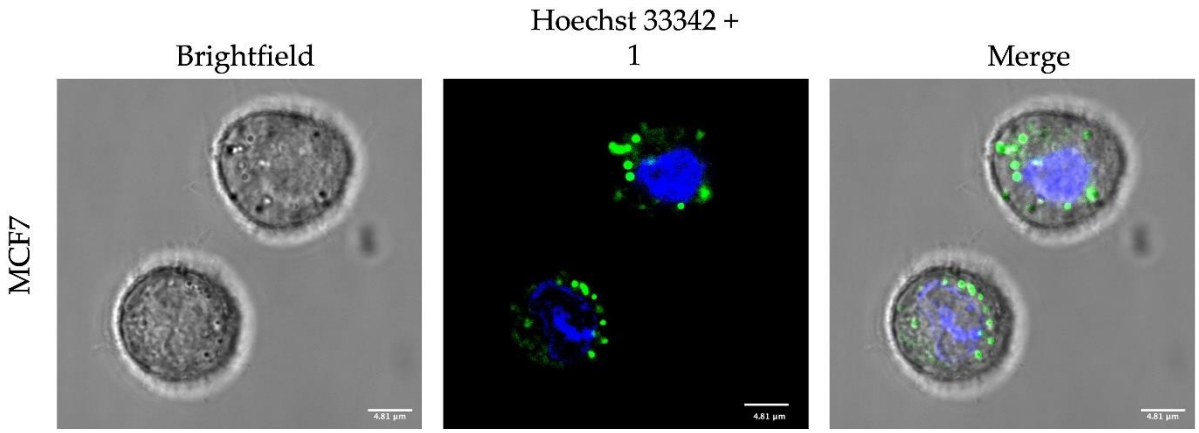
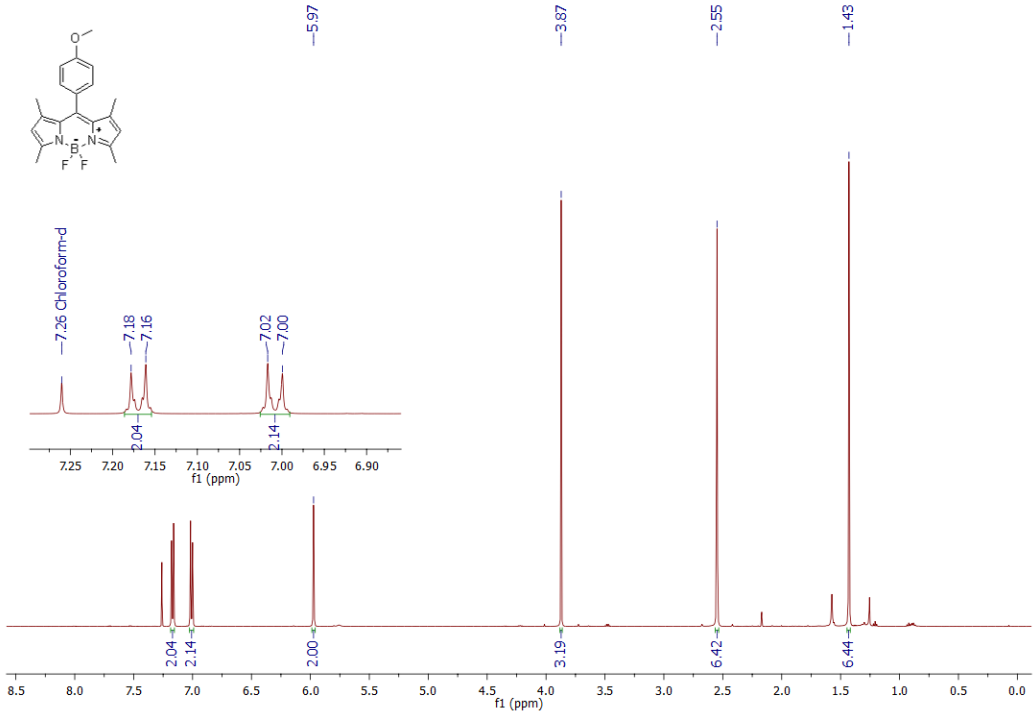


Figure S4. Confocal fluorescence microscopy images of compound **1** (10 μM, λ_{exc} = 488 nm, λ_{em} = 500-550 nm) in MCF7 (breast cancer cells). Cells were counterstained with Hoechst 33342 for nuclear labelling. Scale bar: 5 μm.

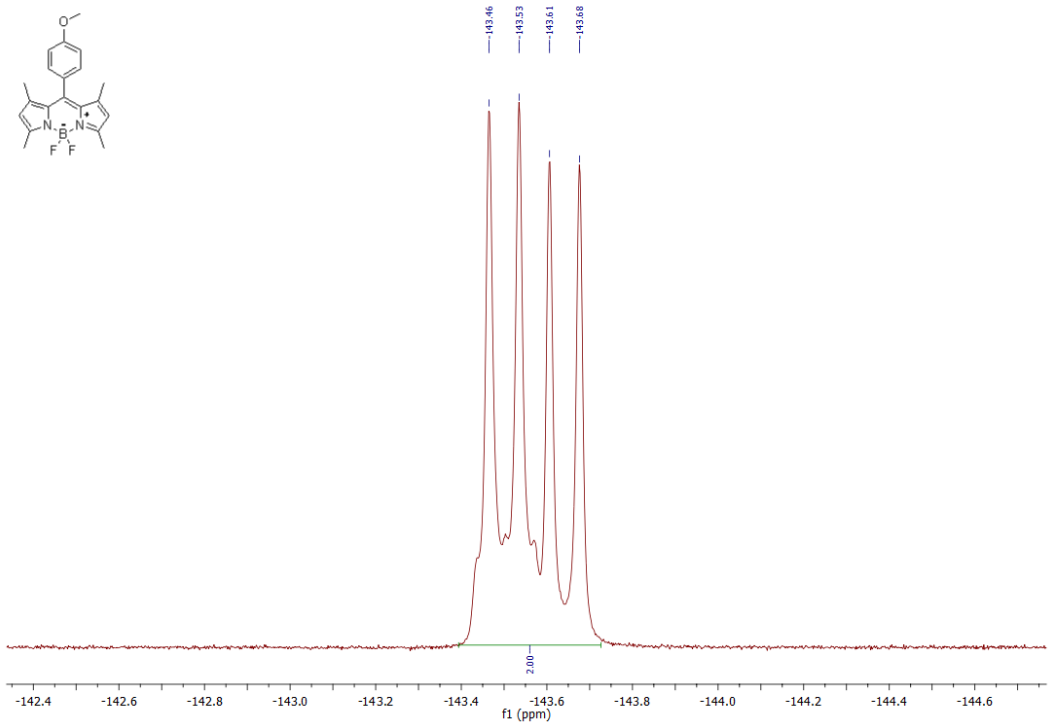
Table S1. ORTEP-3 projection of compound **2d**, showing the atom numbering and displacement ellipsoids at the 50% probability level.

Compound	**2d**
CCDC#	2122460
Formula	$C_{34}H_{33}BF_2N_2O_3S_2$
$D_{calc.}$/ g cm^{-3}	1.334
μ/mm^{-1}	0.219
Formula Weight	630.55
Colour	clear light colourless
Shape	block
Size/mm^3	0.22×0.20×0.15
T/K	293(2)
Crystal System	monoclinic
Space Group	$P2_1/c$
a/Å	15.3643(9)
b/Å	10.9746(7)
c/Å	18.6763(10)
α/°	90
β/°	94.625(5)
γ/°	90
V/Å^3	3138.9(3)
Z	4
Z'	1
Wavelength/Å	0.71073
Radiation type	Mo K
Θ_{min}/°	2.578
Θ_{max}/°	26.499
Measured Refl.	15703
Independent Refl.	6510
Reflections with I > 2(I)	4195
R_{int}	0.0308
Parameters	404
Restraints	0
Largest Peak	0.429
Deepest Hole	-0.243
GooF	1.014
wR_2 (all data)	0.1477
wR_2	0.1223
R_1 (all data)	0.0844
R_1	0.0489

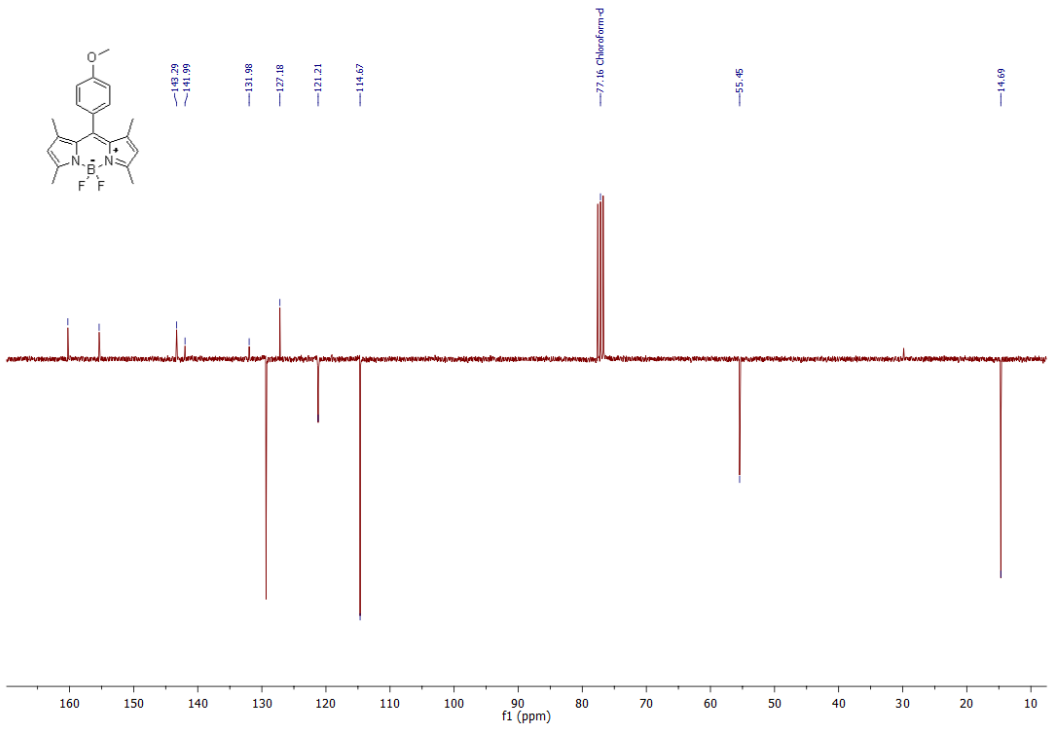
NMR spectra



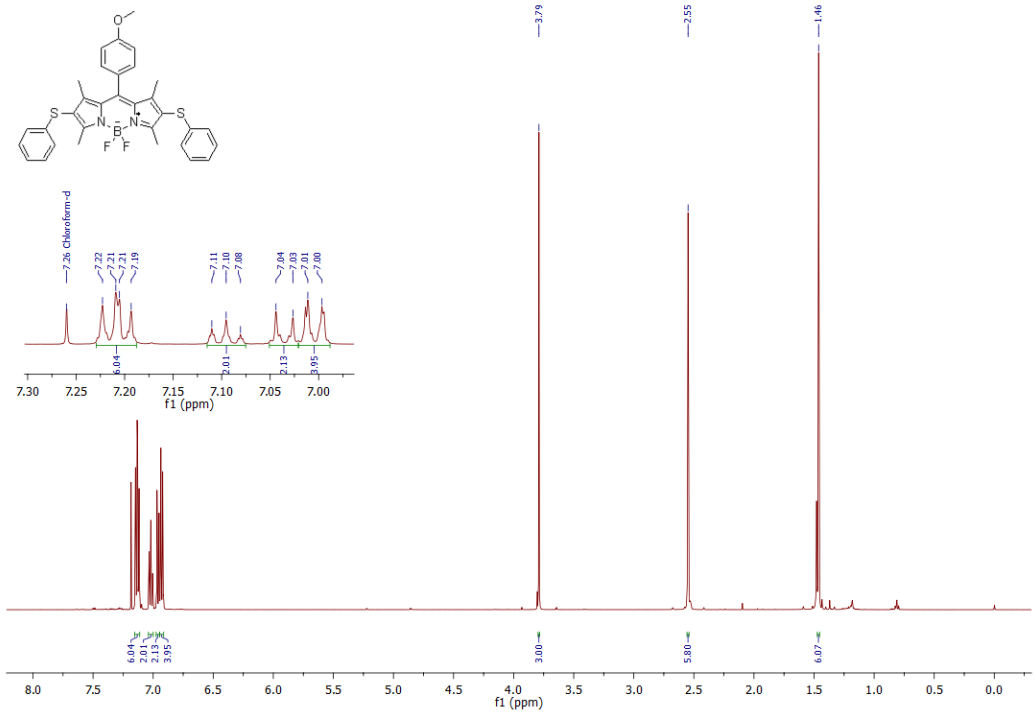
^{1}H NMR Spectrum (500 MHz, $CDCl_3$) of compound **1**



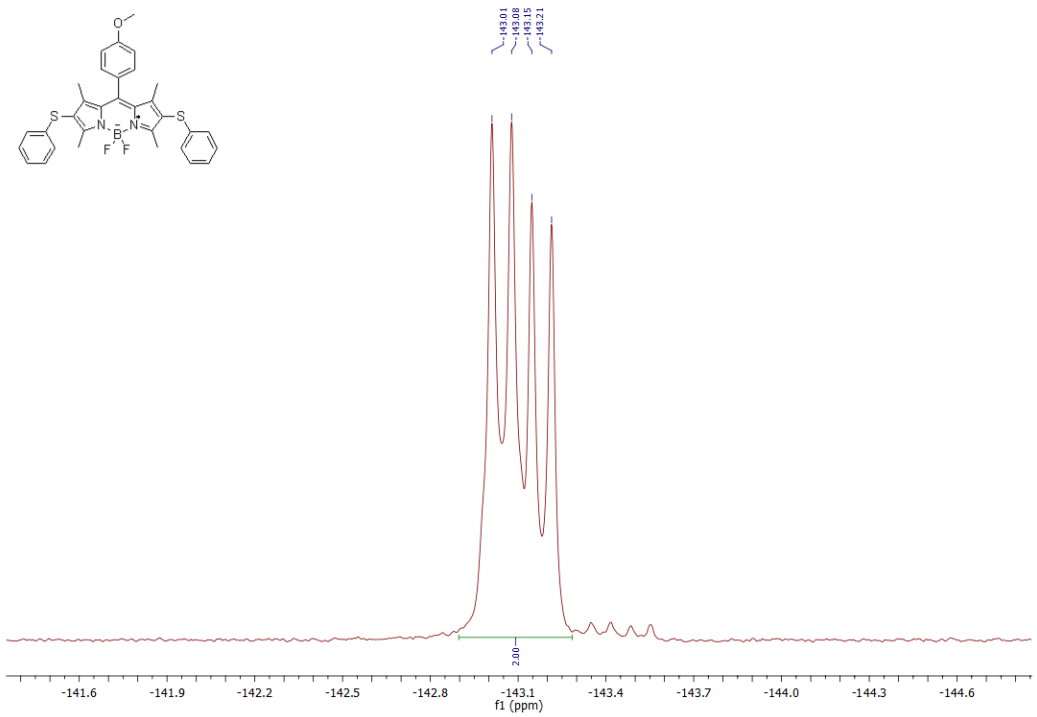
^{19}F NMR Spectrum (470 MHz, $CDCl_3$) of compound **1**



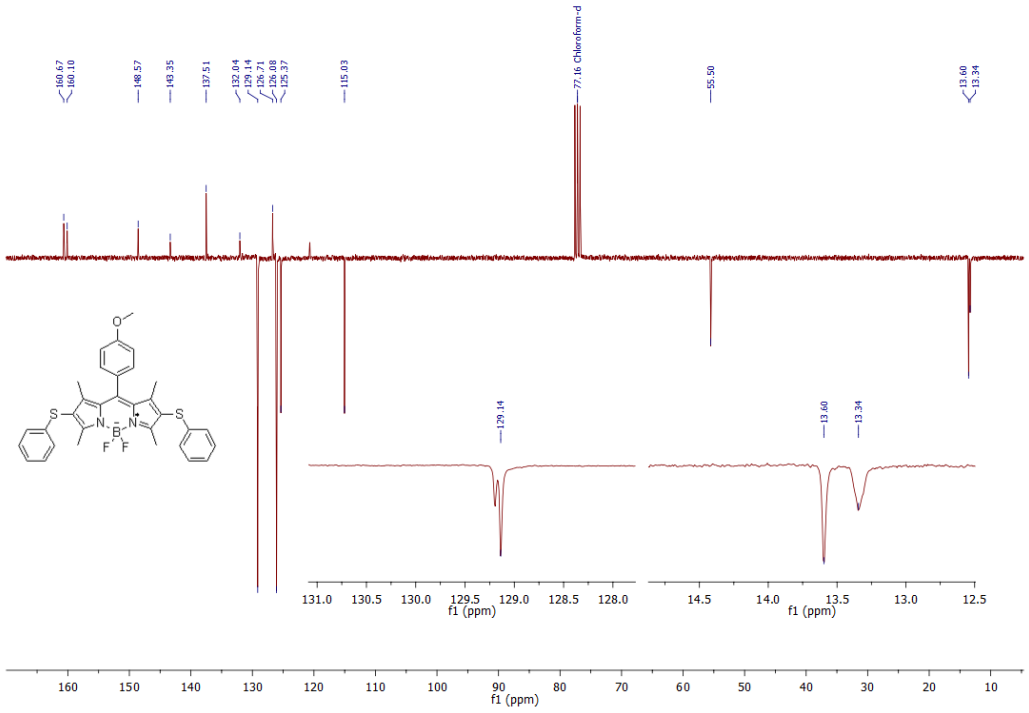
^{13}C-APT NMR Spectrum (75,0 MHz, $CDCl_3$) of compound **1**



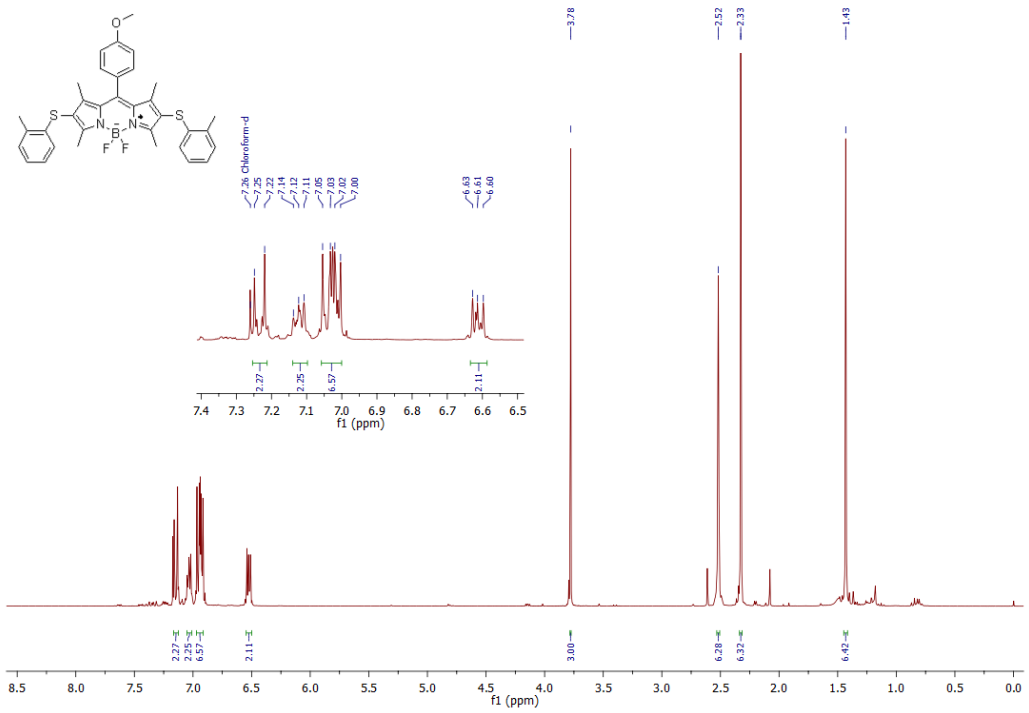
^{1}H NMR Spectrum (500 MHz, $CDCl_3$) of compound **2a**



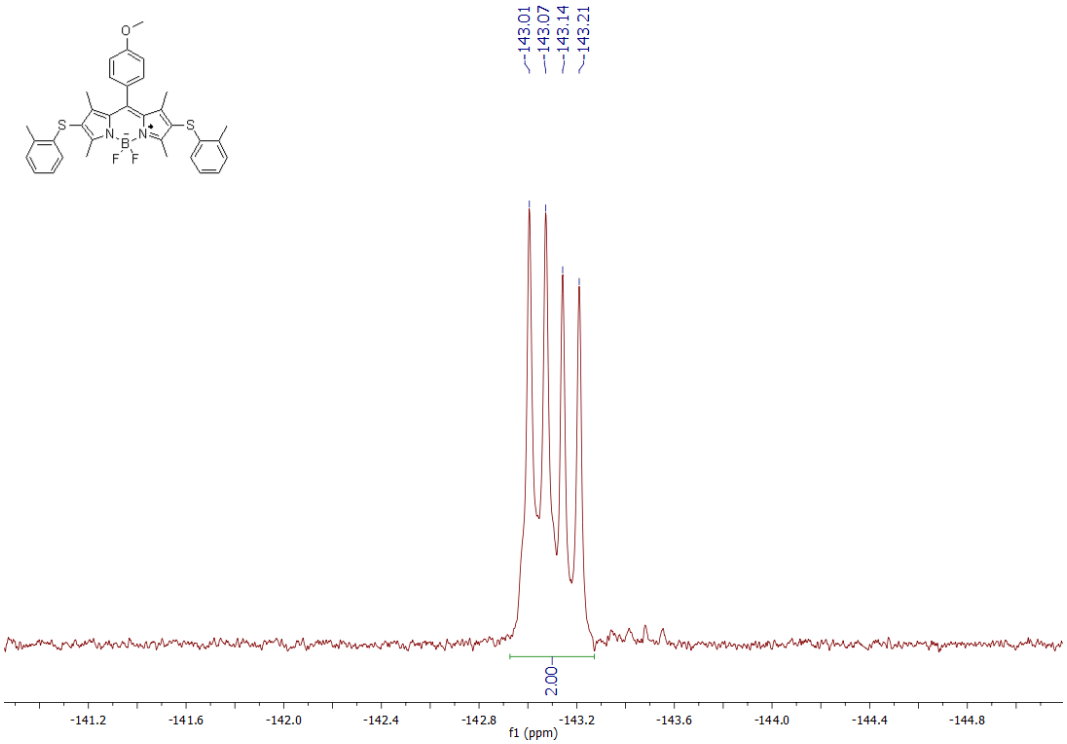
^{19}F NMR Spectrum (470 MHz, $CDCl_3$) of compound **2a**



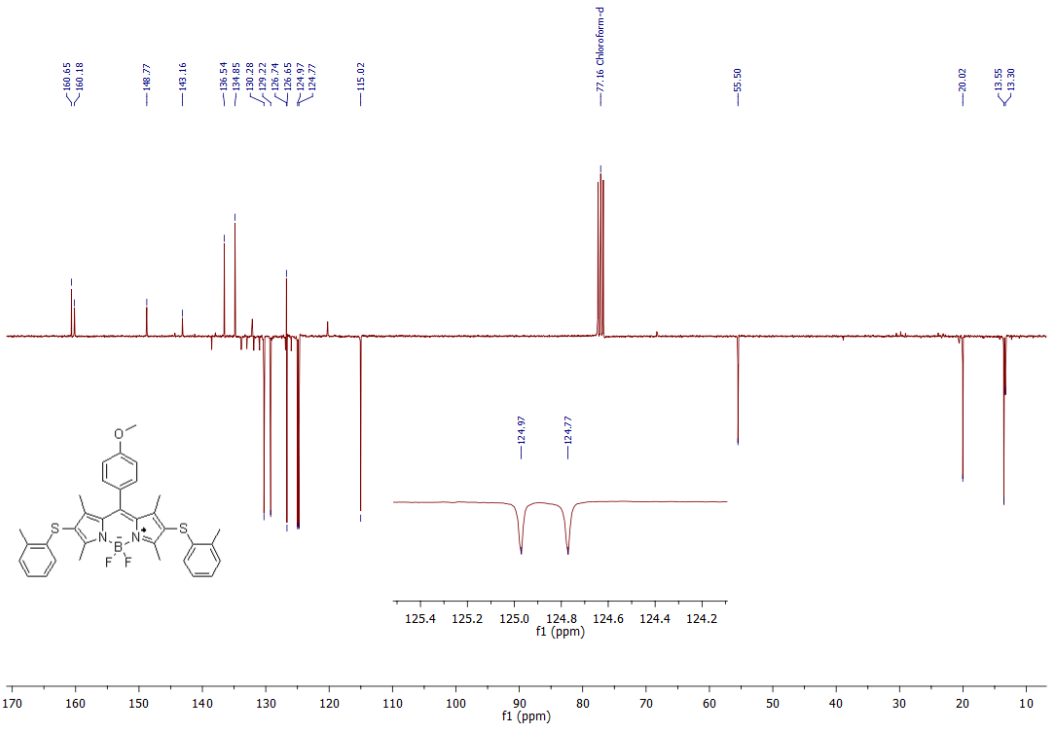
^{13}C-APT NMR Spectrum (75,0 MHz, $CDCl_3$) of compound **2a**



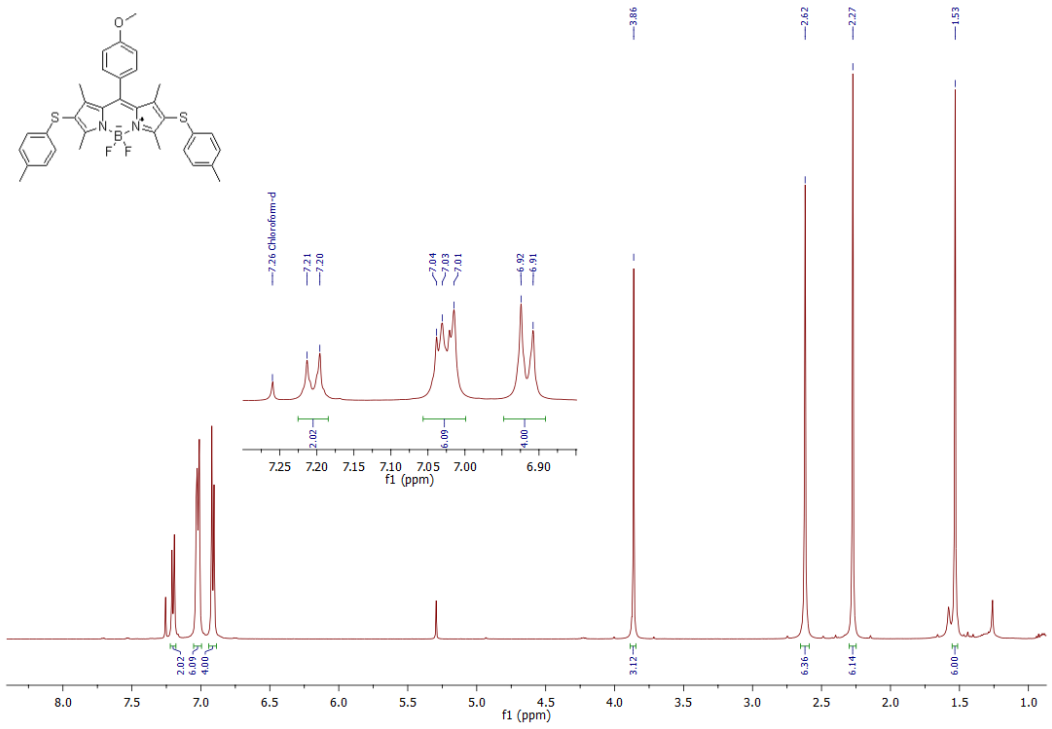
^{1}H NMR Spectrum (300 MHz, $CDCl_3$) of compound **2b**



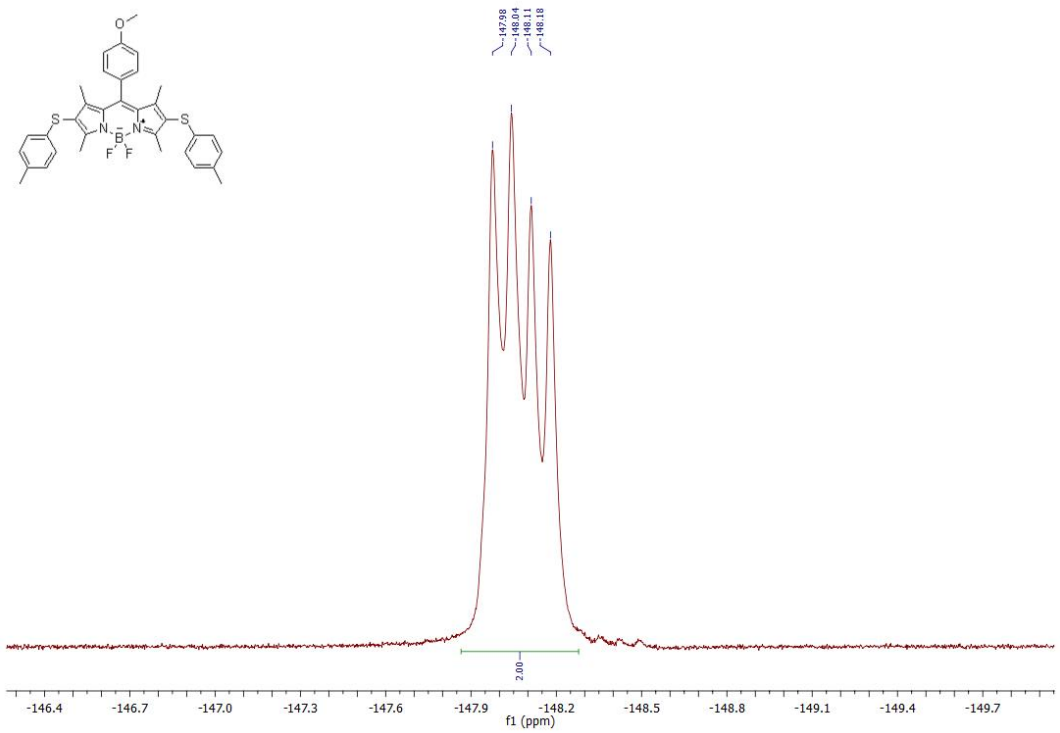
^{19}F NMR Spectrum (470 MHz, $CDCl_3$) of compound **2b**



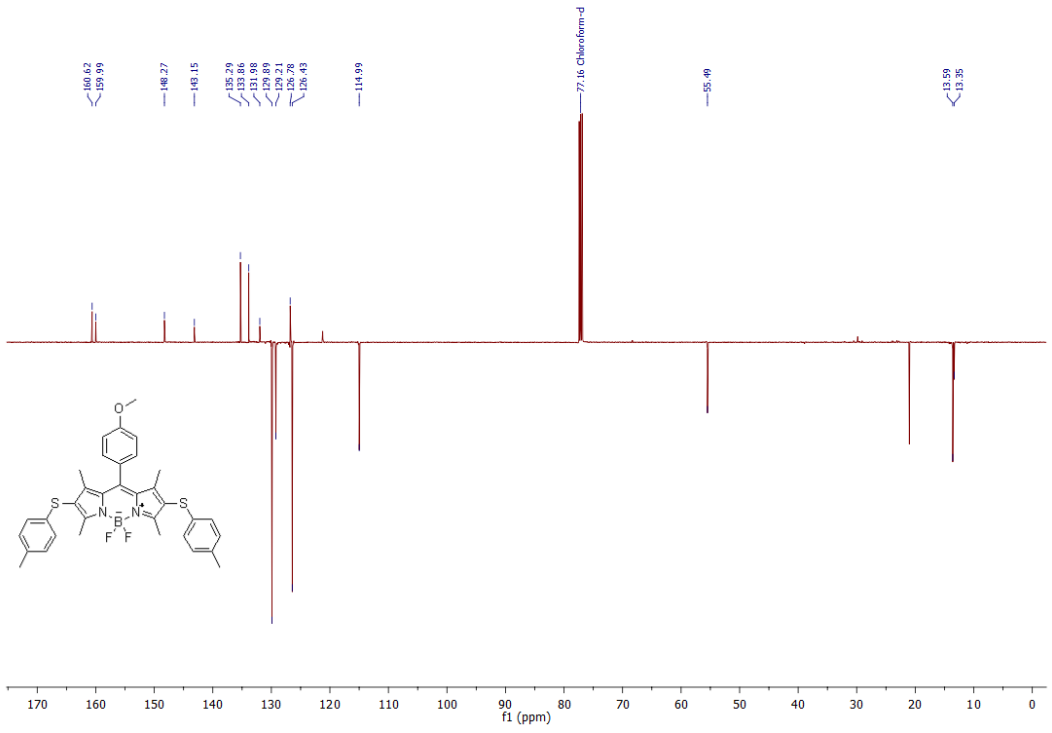
^{13}C-APT NMR Spectrum (75,0 MHz, $CDCl_3$) of compound **2b**



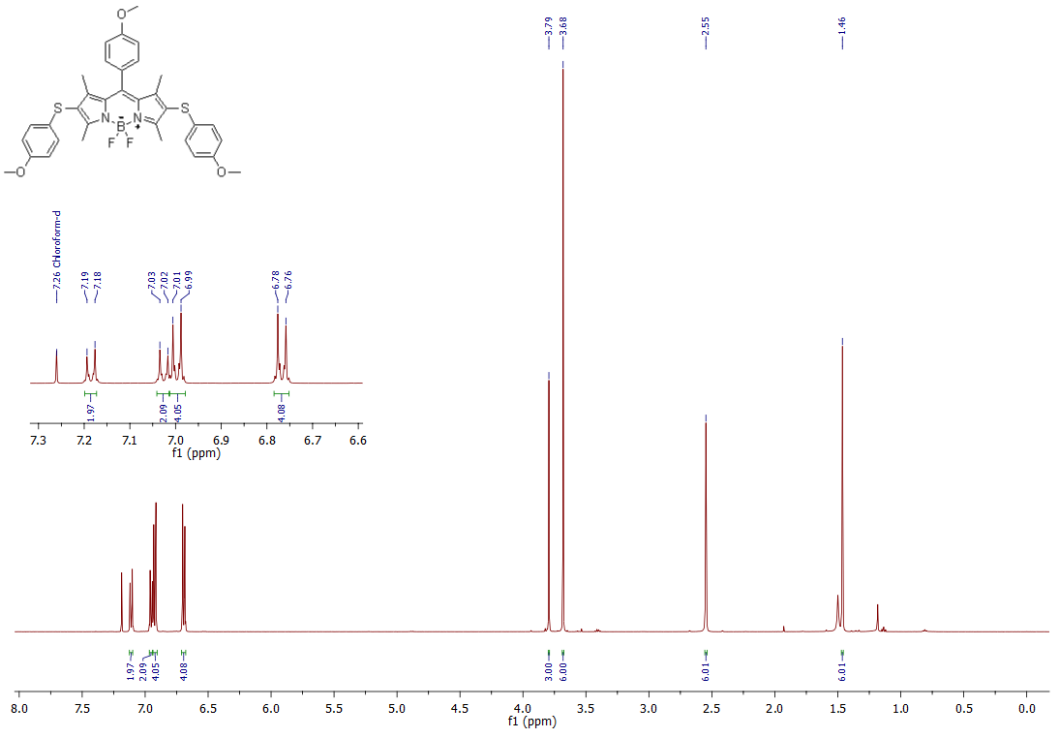
^{1}H NMR Spectrum (500 MHz, $CDCl_3$) of compound **2c**



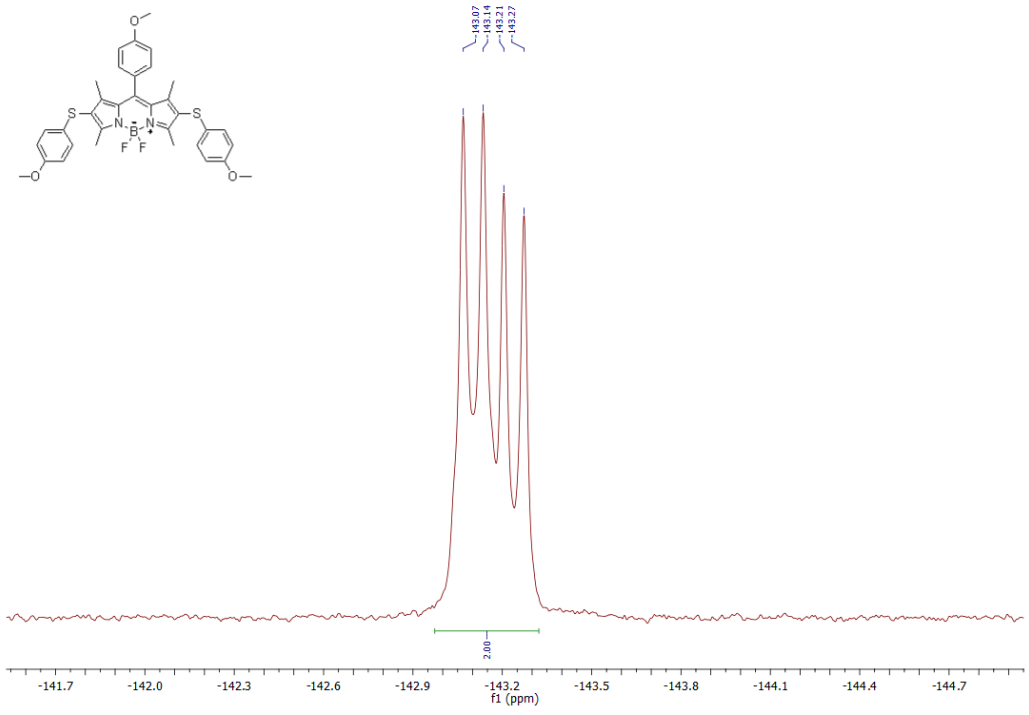
^{19}F NMR Spectrum (470 MHz, $CDCl_3$) of compound **2c**



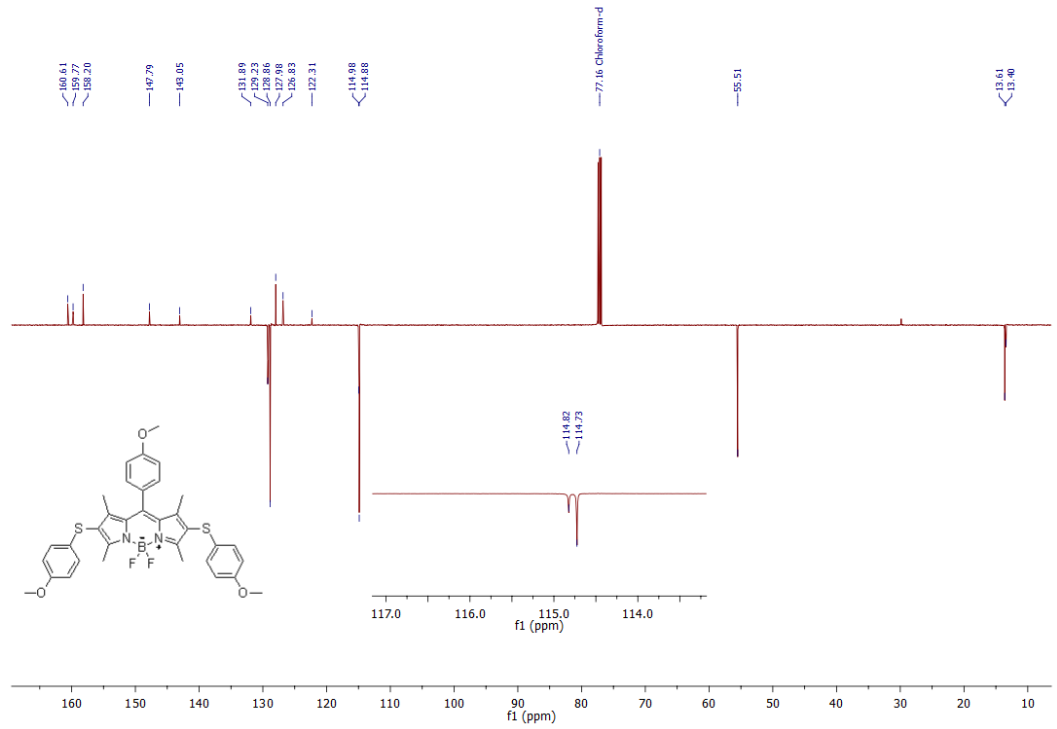
^{13}C-APT NMR Spectrum (125,0 MHz, $CDCl_3$) of compound **2c**



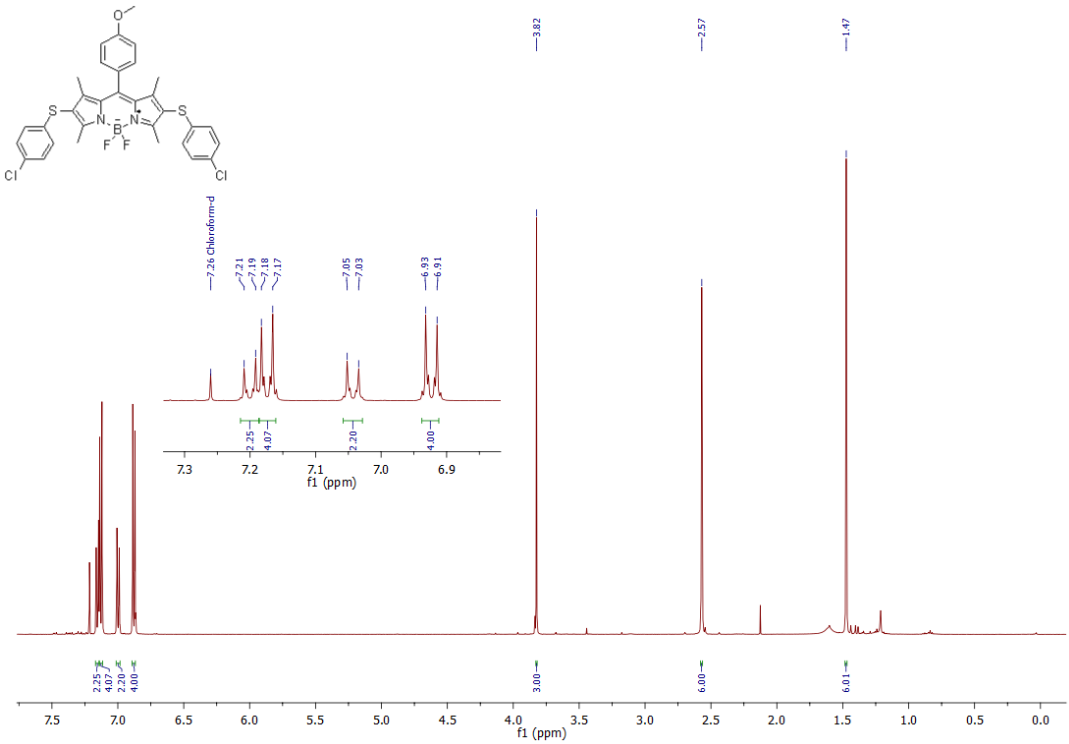
^{1}H NMR Spectrum (500 MHz, $CDCl_3$) of compound **2d**



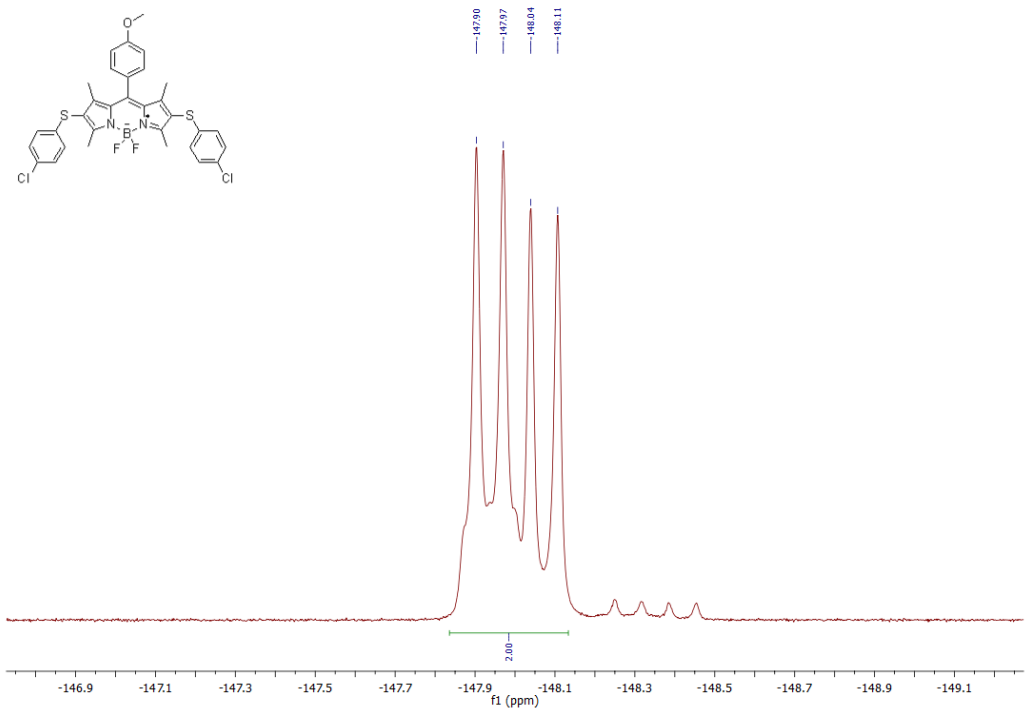
^{19}F NMR Spectrum (470 MHz, $CDCl_3$) of compound **2d**



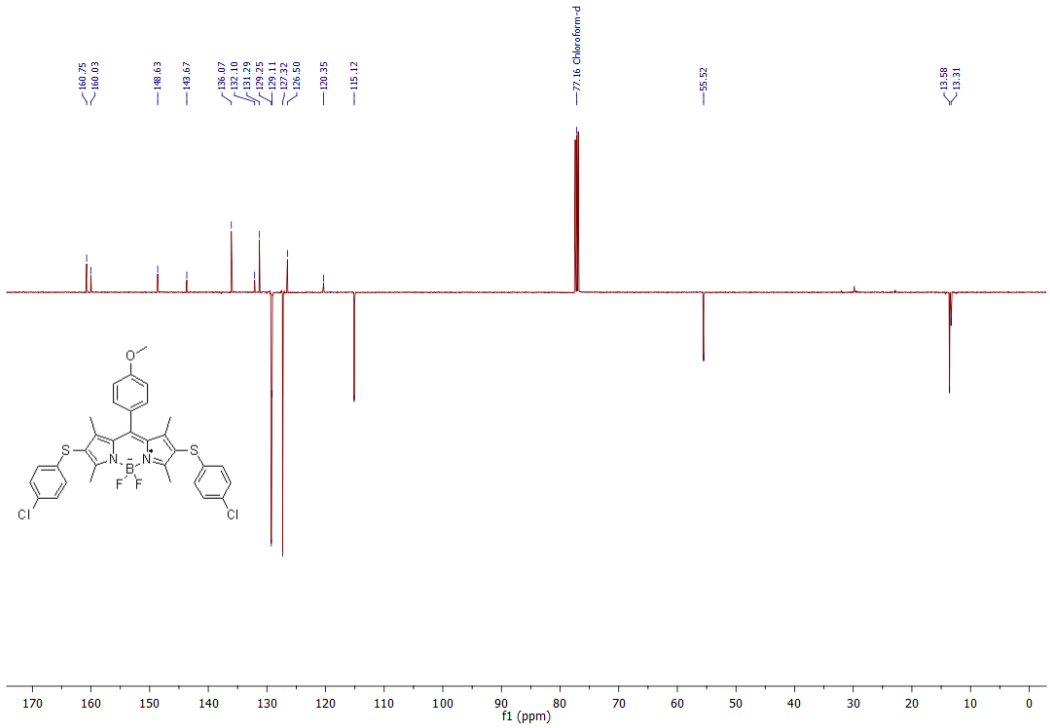
^{13}C-APT NMR Spectrum (125,0 MHz, $CDCl_3$) of compound **2d**



^{1}H NMR Spectrum (500 MHz, $CDCl_3$) of compound **2e**

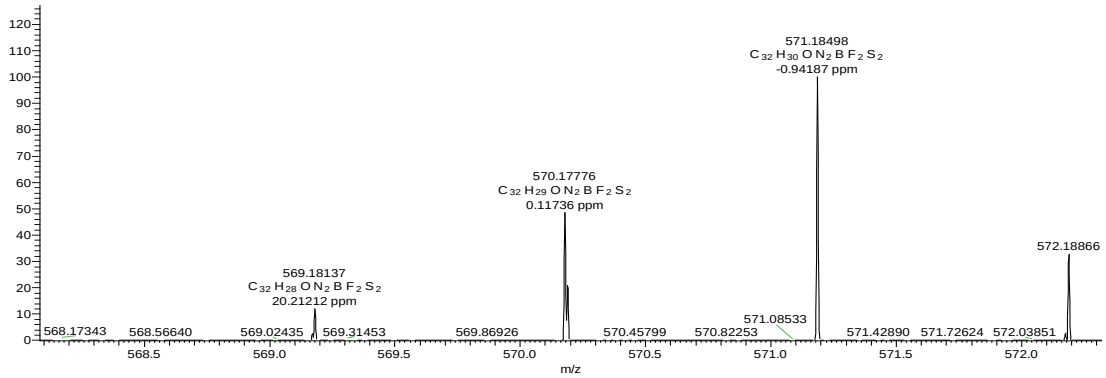


^{19}F NMR Spectrum (470 MHz, $CDCl_3$) of compound **2e**

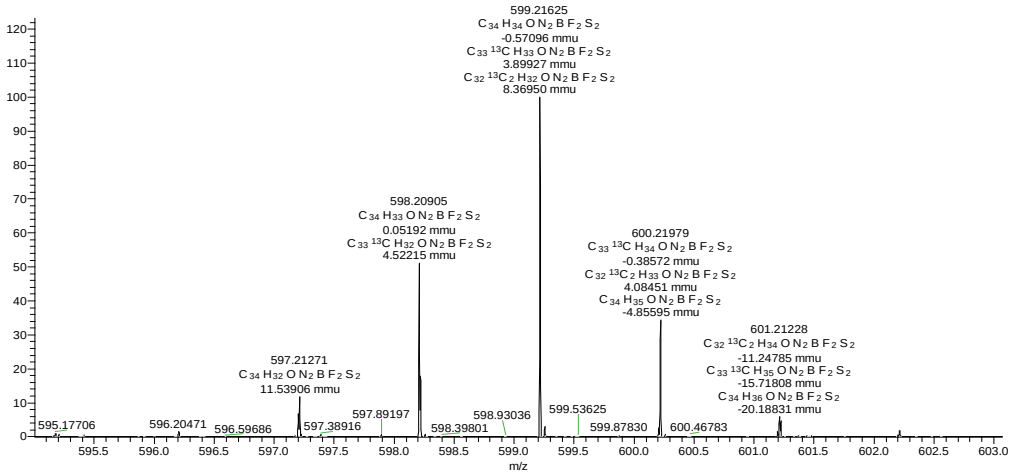


^{13}C-APT NMR Spectrum (125,0 MHz, $CDCl_3$) of compound **2e**

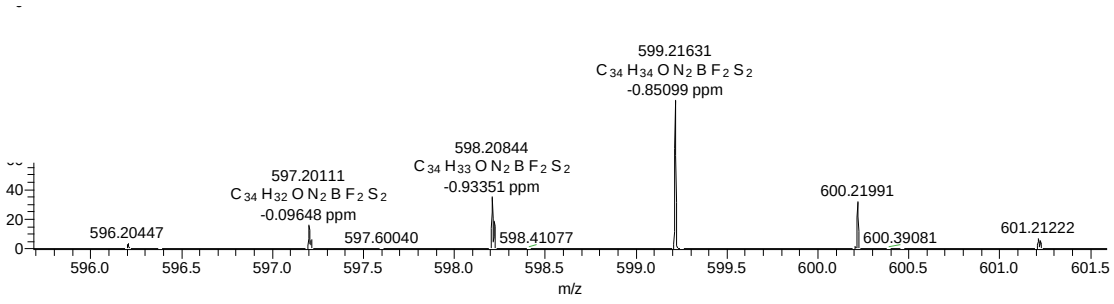
HRMS Data



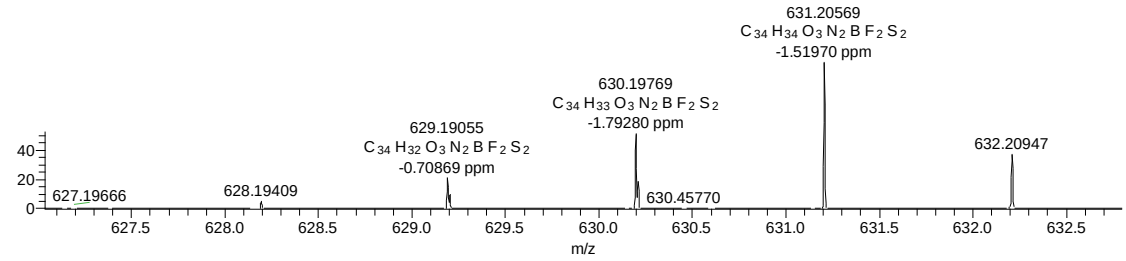
HRMS (ESI$^+$) of compound **2a**



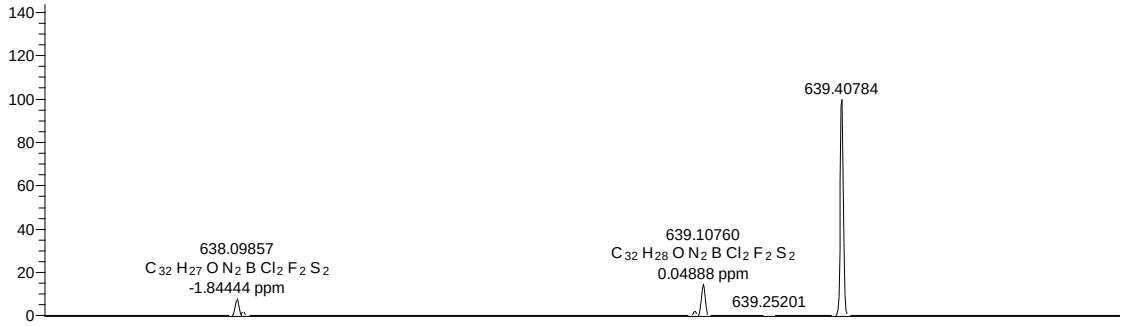
HRMS (ESI$^+$) of compound **2b**



HRMS (ESI$^+$) of compound **2c**



HRMS (ESI$^+$) of compound **2d**



HRMS (ESI$^+$) of compound **2e**