Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Non-symmetric thieno[3, 2-b]thiophene-fused BODIPYs: Synthesis, Spectroscopic properties and providing a functional strategy for NIR probes

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Supporting Information

Content

Experimental Details

All reagents come from commercial suppliers and are not further purified for use unless otherwise specified. CH_2Cl_2 was distilled with calcium hydride. THF and toluene were dried and distilled with sodium metal. ^{1}H NMR, ^{13}C NMR spectra were obtained using a Bruker DRX400 spectrometer and referenced to the residual proton signals of the solvent. HR-MS were obtained by a Bruker Daltonics microTOF-Q II spectrometer. All the solvents employed for the spectroscopic measurements were of UV spectroscopic grade (Aldrich).

Spectroscopic measurements

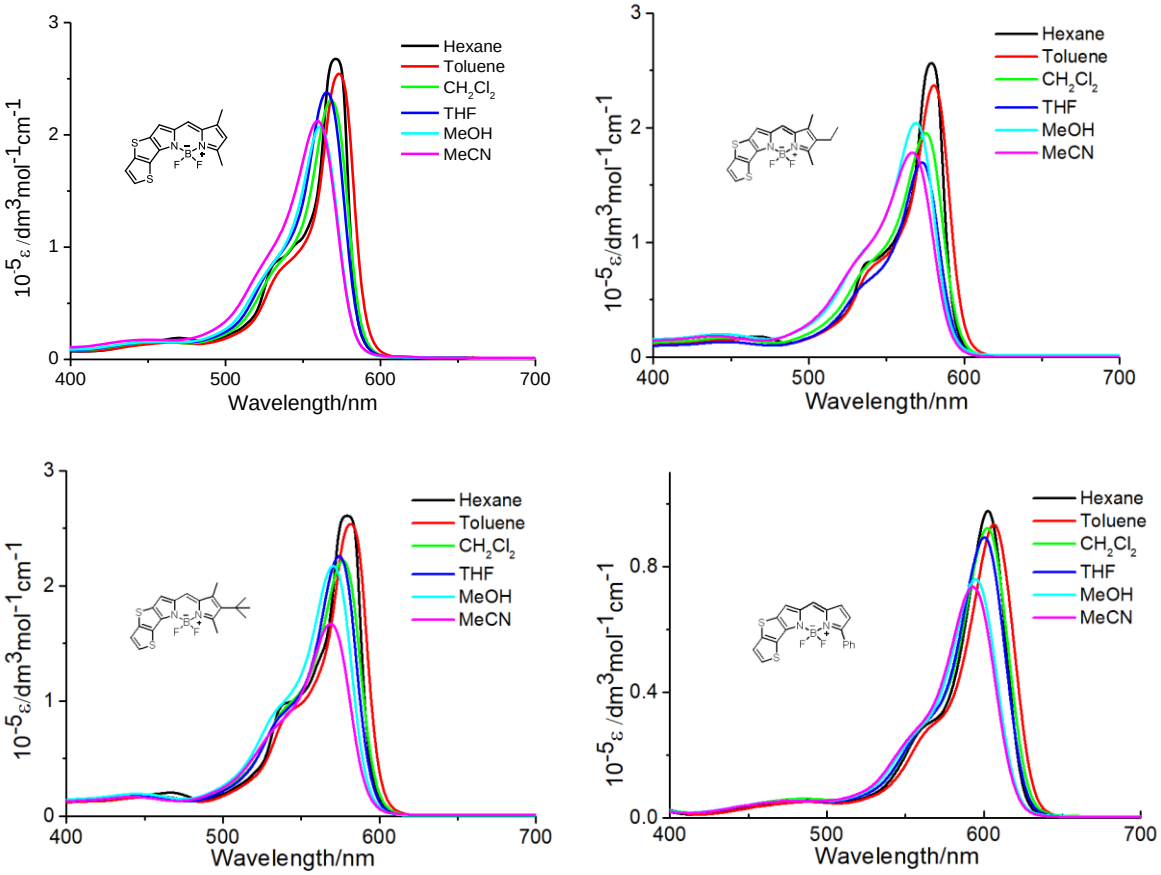


Fig S1. The absorption spectra of **4**-**7** in hexane, toluene, CH_2Cl_2, THF, MeOH, MeCN.

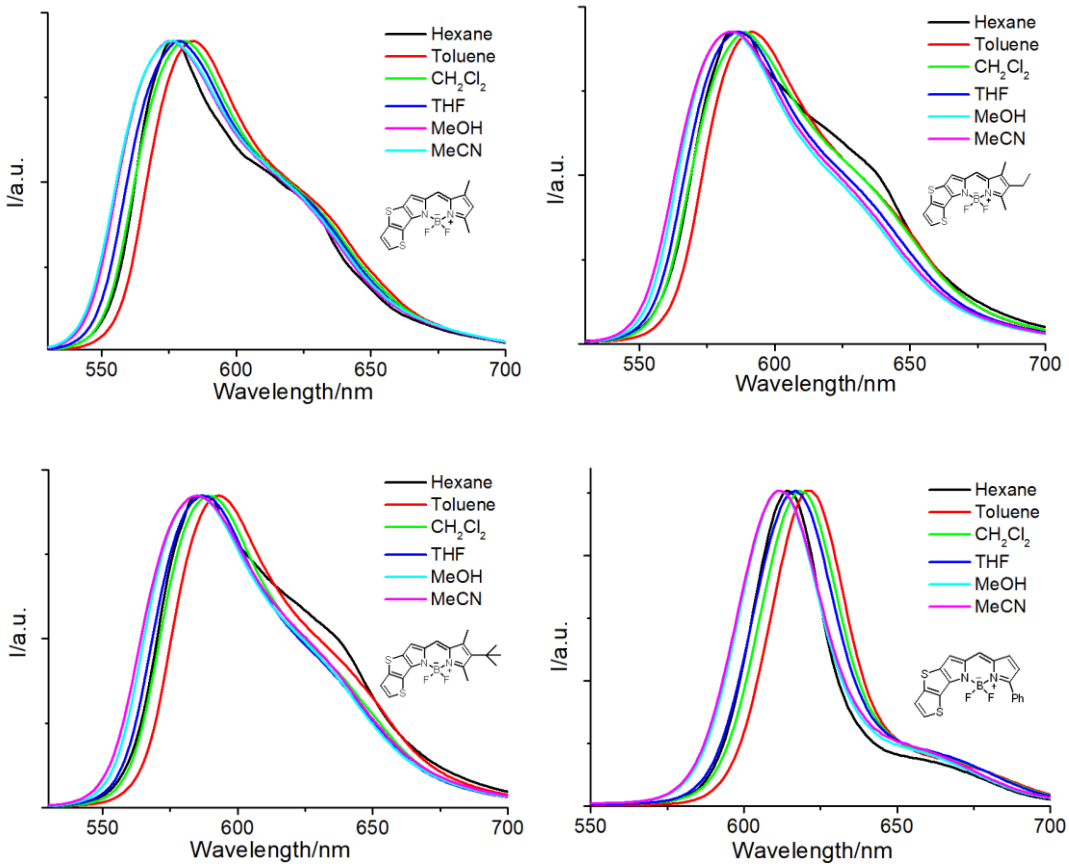


Fig S2. The emission spectra of **4-7** in hexane, toluene, CH_2Cl_2, THF, MeOH, MeCN

Photostability

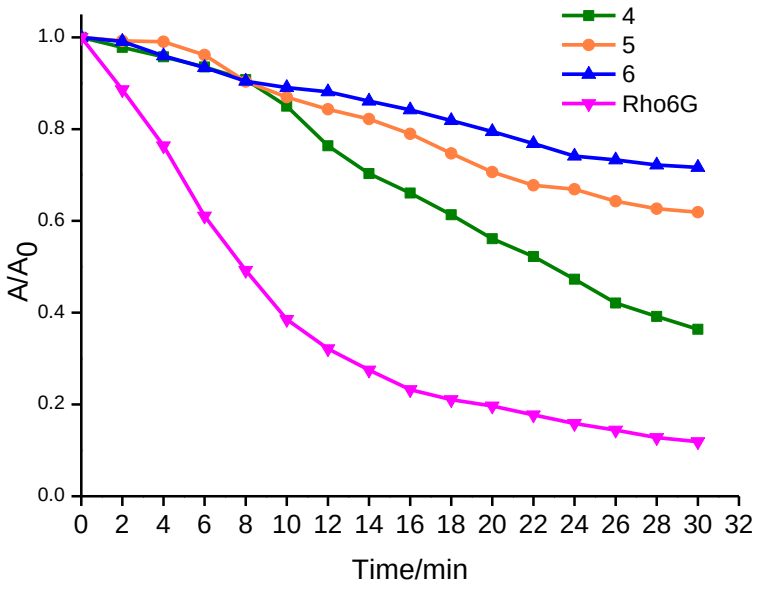


Fig. S3 Photostability of **4-6** and Methylene Blue (MB) in dichloromethane at 2 min intervals determined using a laser beam (525 nm,1.5 W cm^{-2}) over an irradiation period of 30 min (c = 10^{-5} M, 298 K).

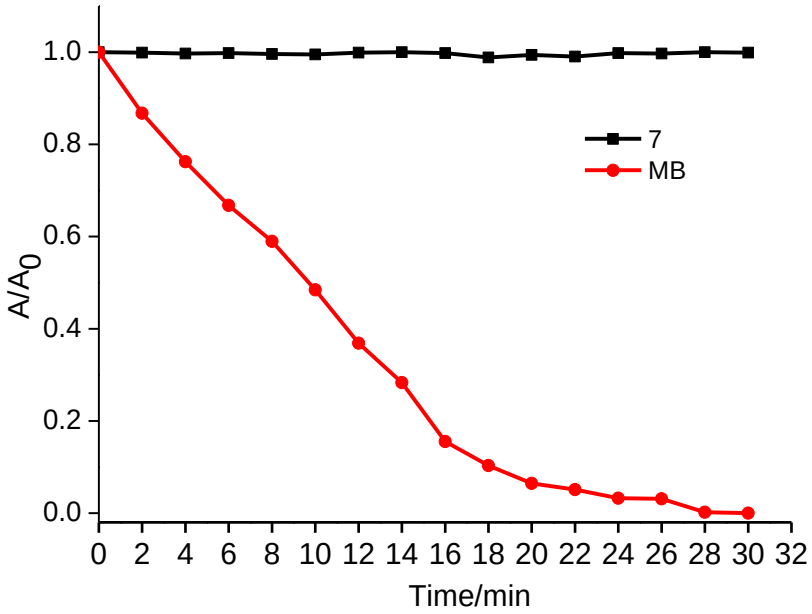


Fig. S4 Photostability of **7** and Methylene Blue (MB) in dichloromethane at 2 min intervals determined using a laser beam (635 nm, 660 mW cm^{-2}) over an irradiation period of 30 min (c = 10^{-5} M, 298 K).

The sensing properties of compounds 8

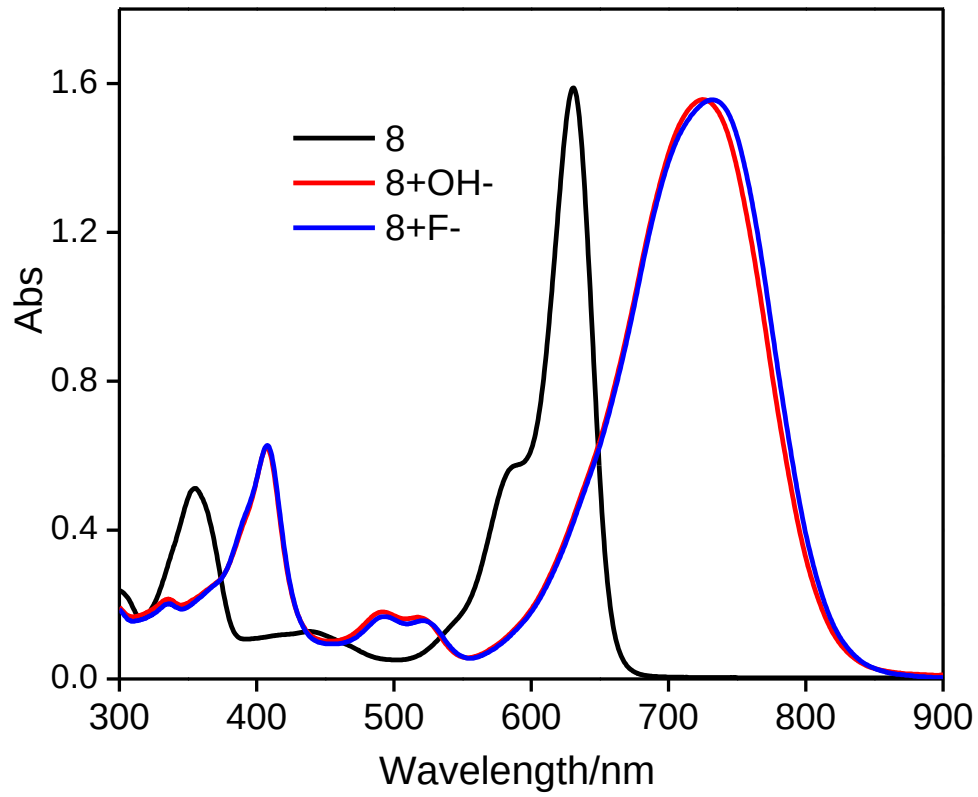


Fig S5. The absorption spectra of **8** (10 mM) in CH_3CN after the addition of 20 eq. of OH^- or F^-

^{1}H and ^{13}C NMR spectra

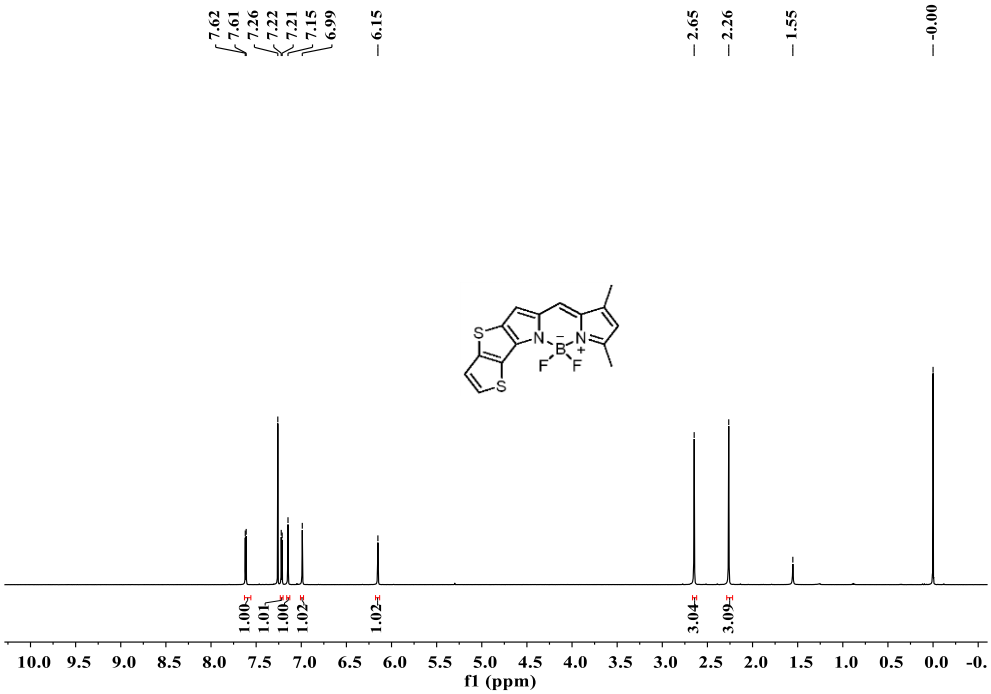


Fig. S6 ^{1}H NMR spectra of compound **4** recorded in $CDCl_3$

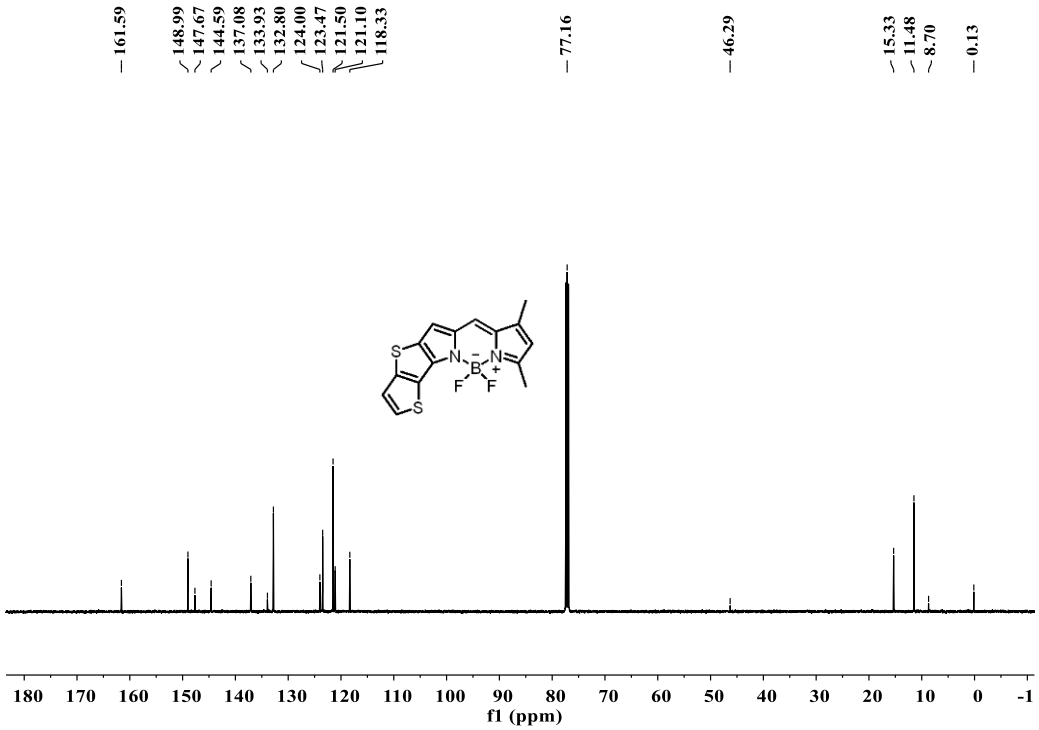


Fig. S7 ^{13}C NMR spectra of compound **4** recorded in $CDCl_3$

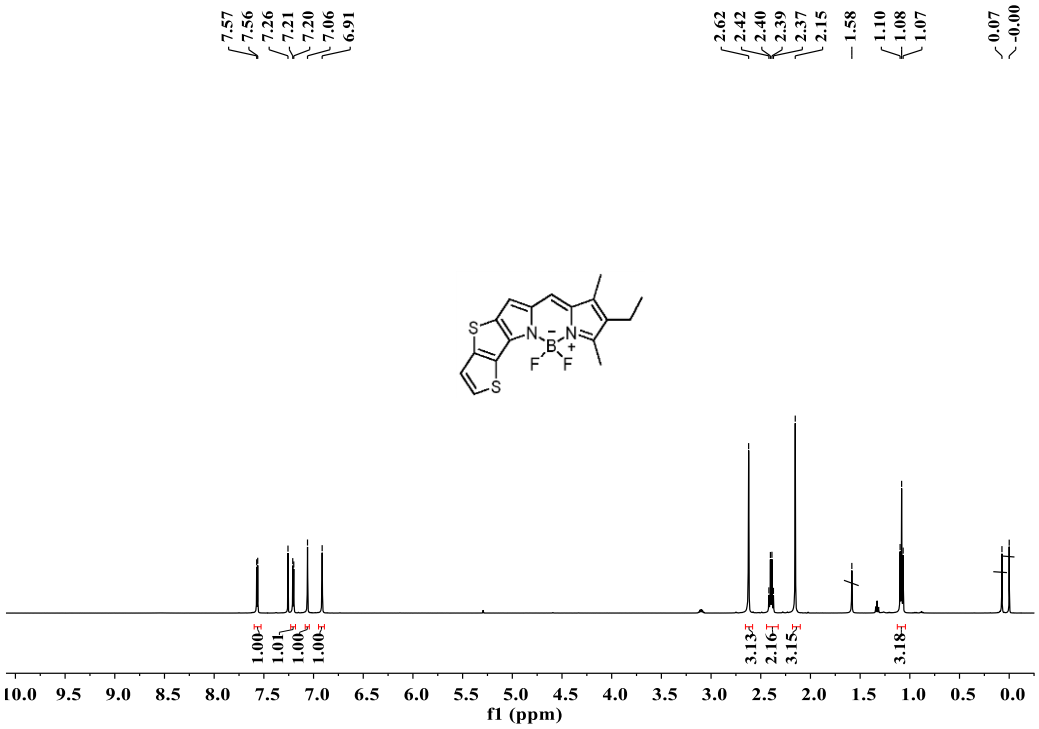


Fig. S8 ^{1}H NMR spectra of compound **5** recorded in $CDCl_3$

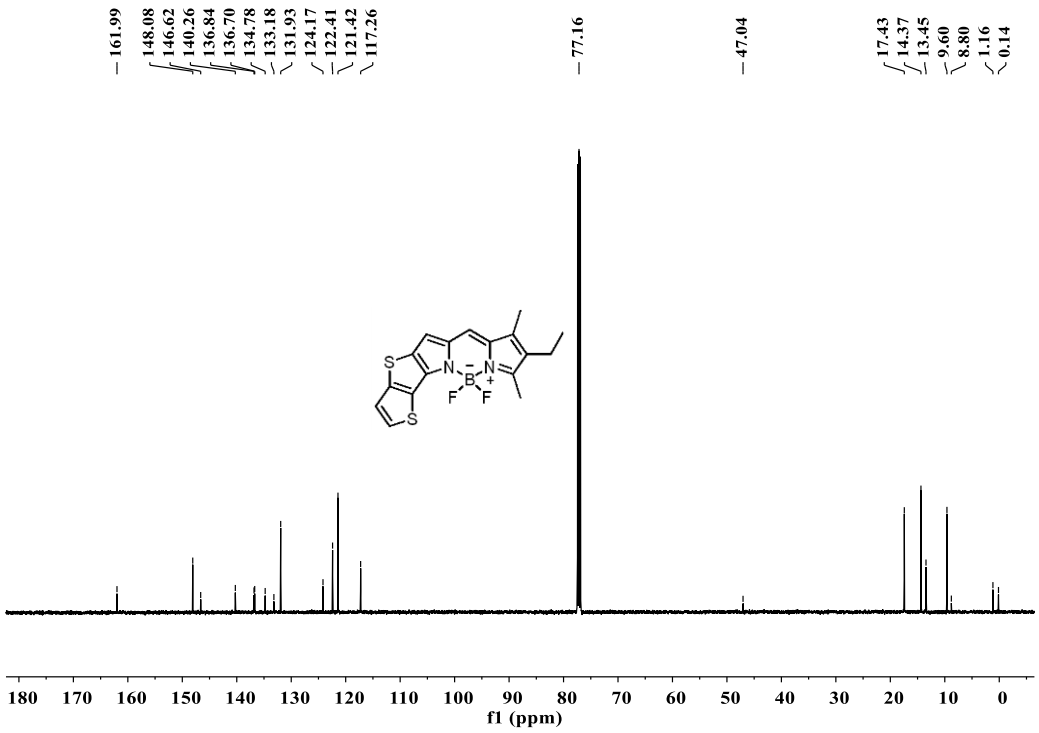


Fig. S9 ^{13}C NMR spectra of compound **5** recorded in $CDCl_3$

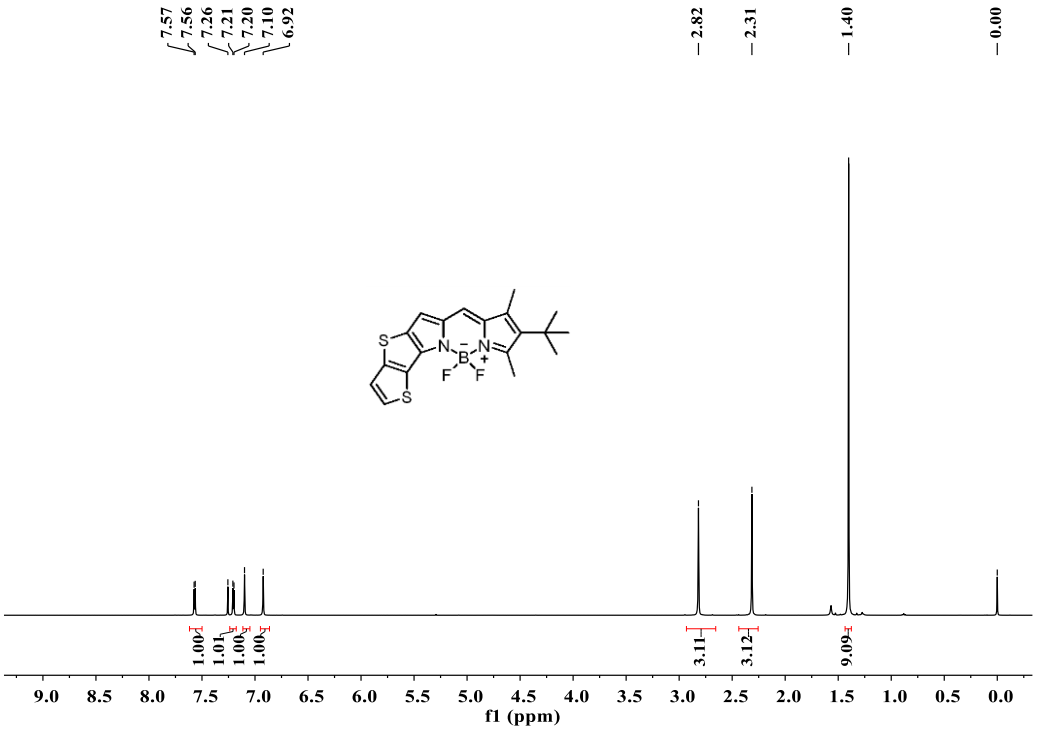


Fig. S10 ^{1}H NMR spectra of compound **6** recorded in $CDCl_3$

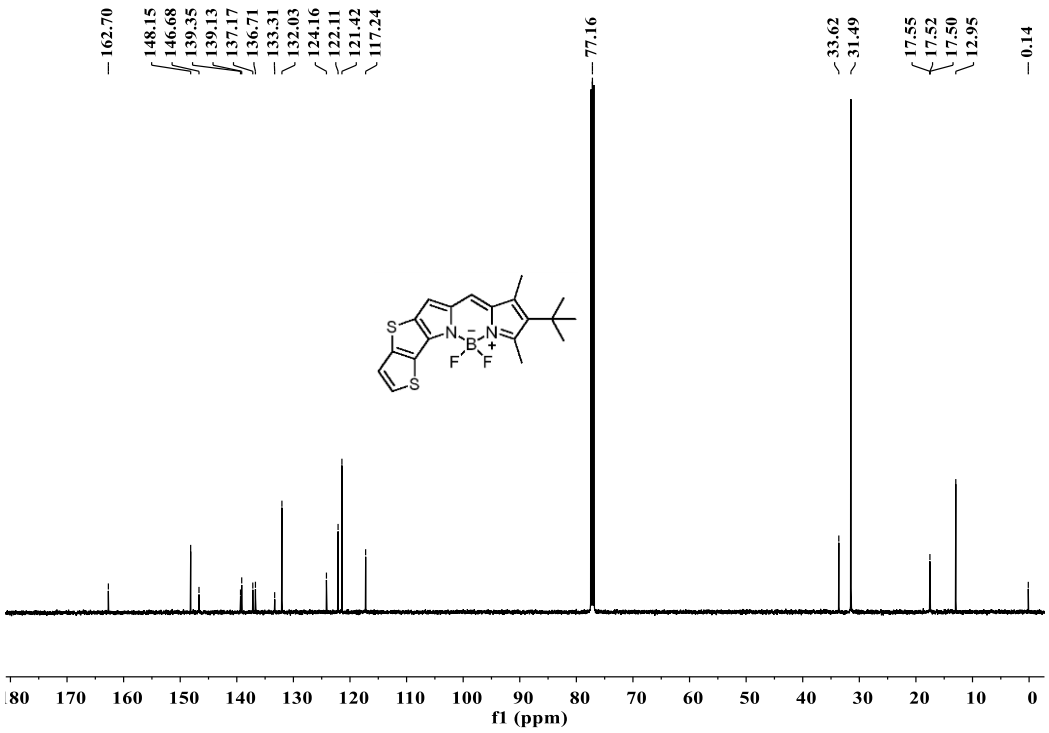


Fig. S11 ^{13}C NMR spectra of compound **6** recorded in $CDCl_3$

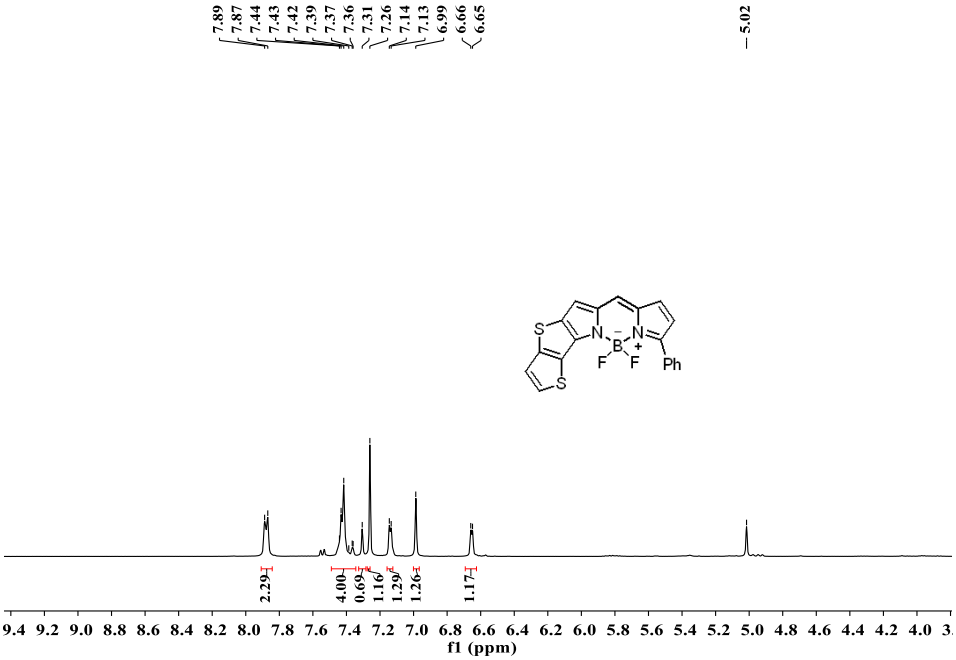


Fig. S12 ^{1}H NMR spectra of compound **7** recorded in $CDCl_3$

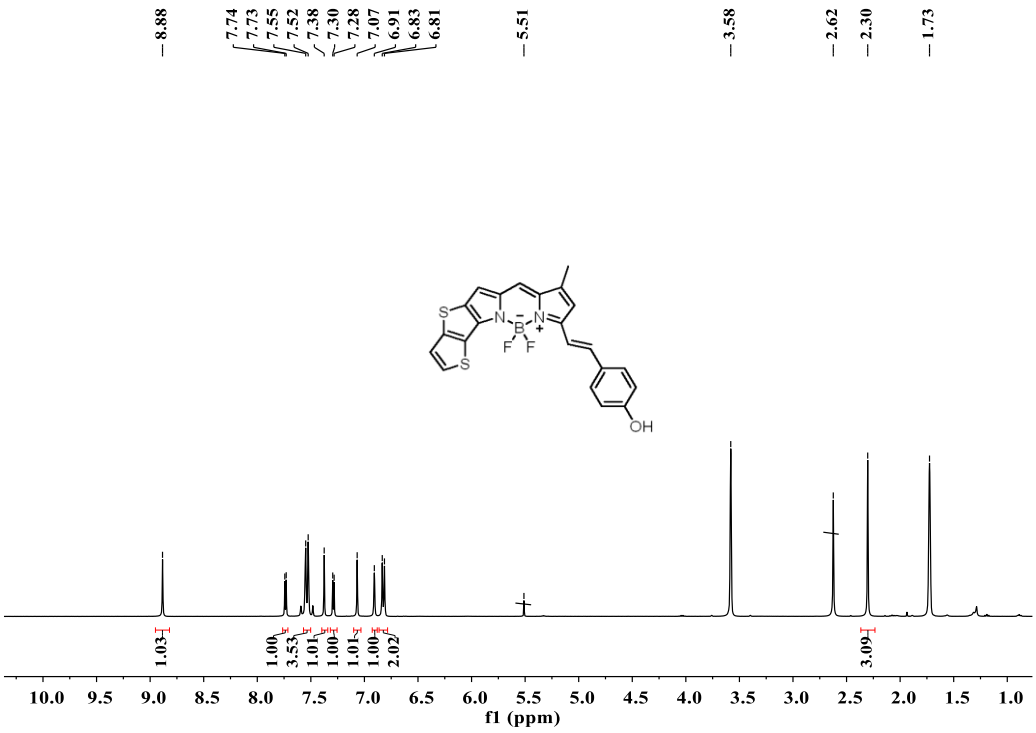


Fig. S13 ^{1}H NMR spectra of compound **8** recorded in THF-d_8

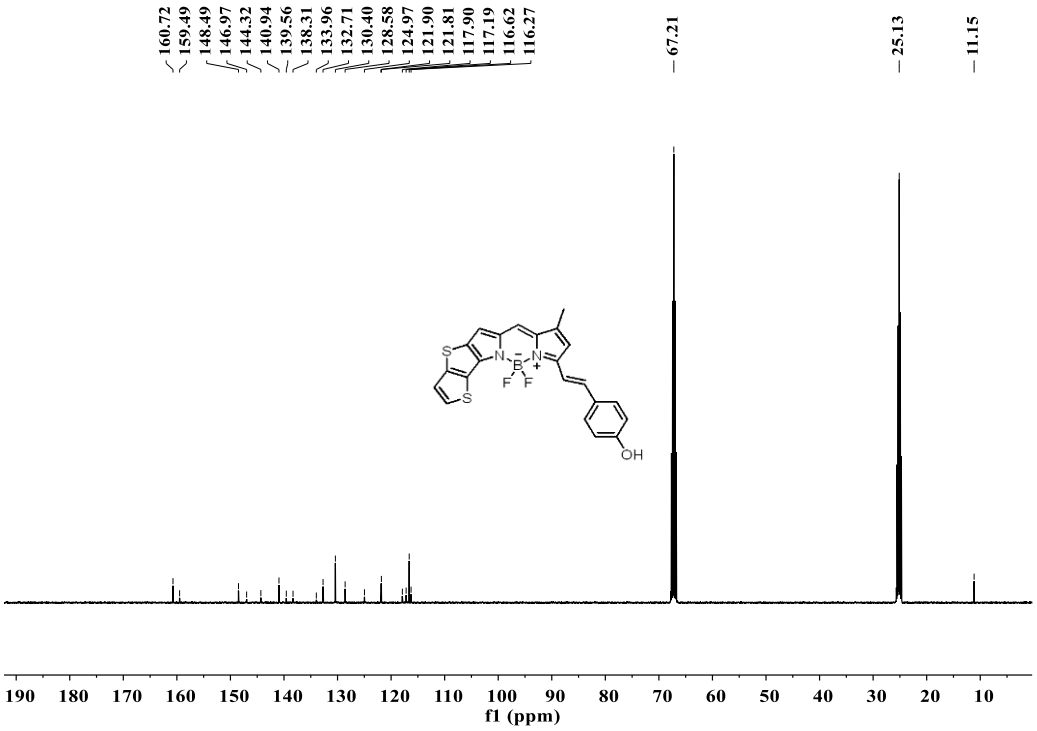


Fig. S14 ^{13}C NMR spectra of compound **8** recorded in THF-d_8

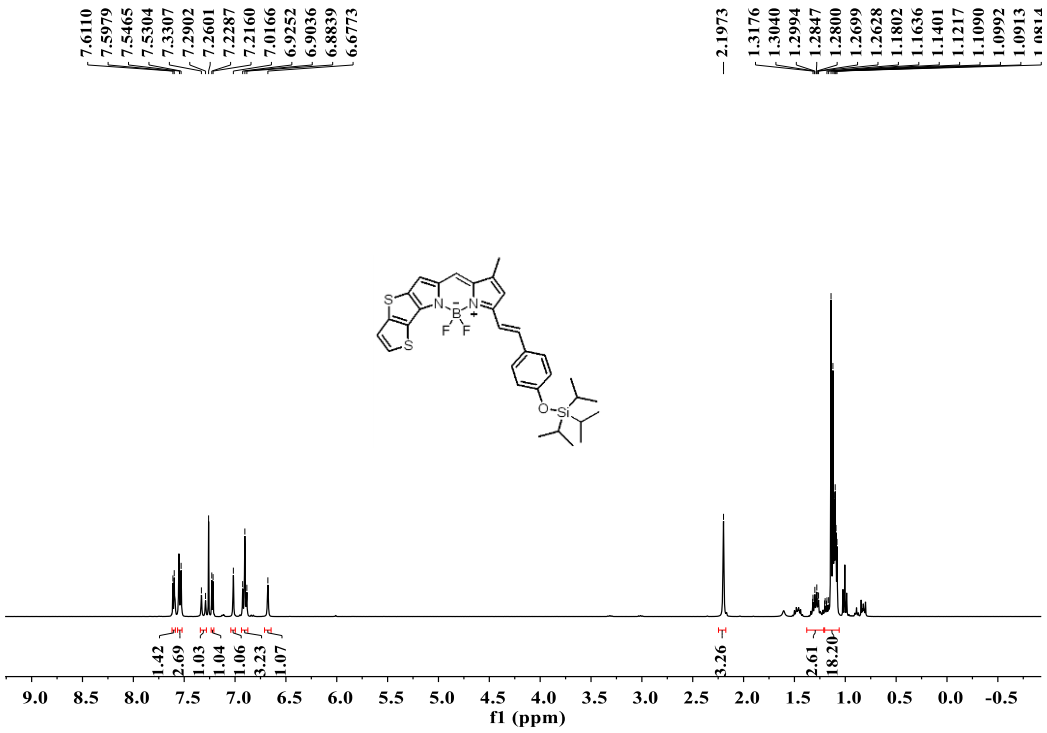


Fig. S15 ^{1}H NMR spectra of compound **9** recorded in $CDCl_3$

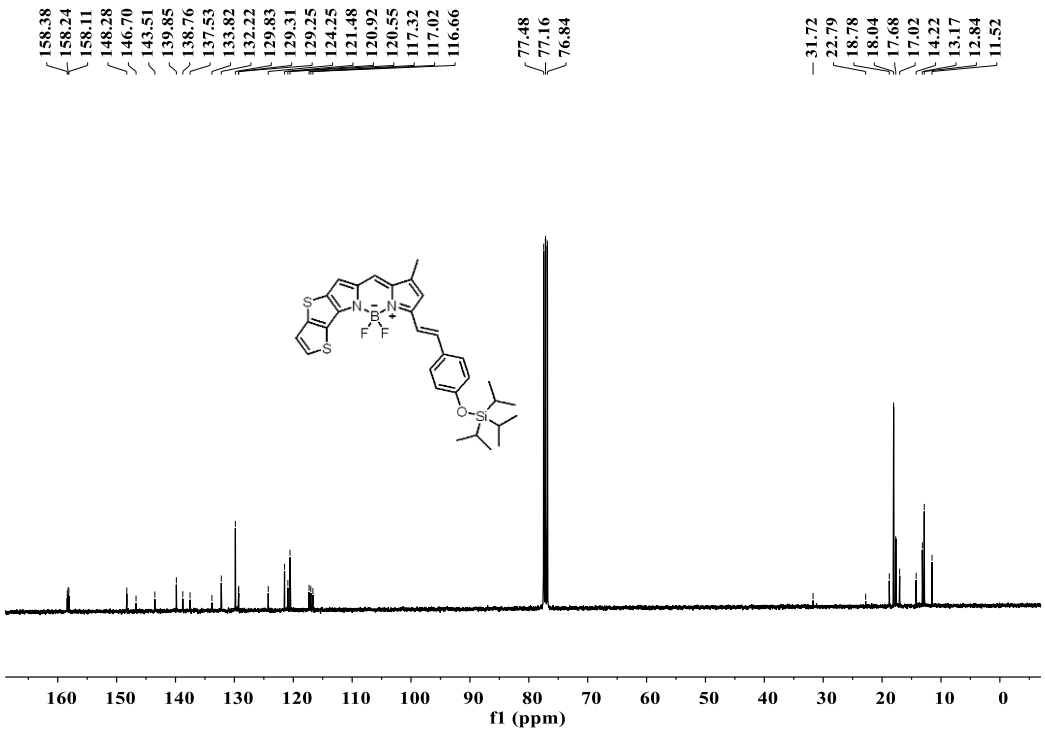
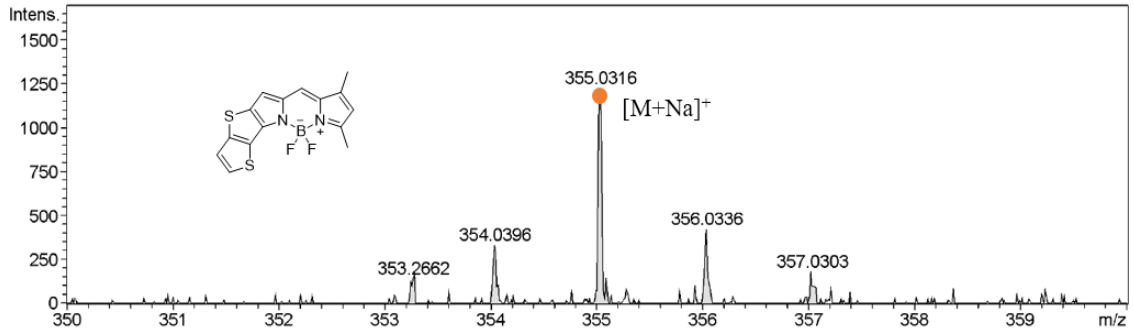
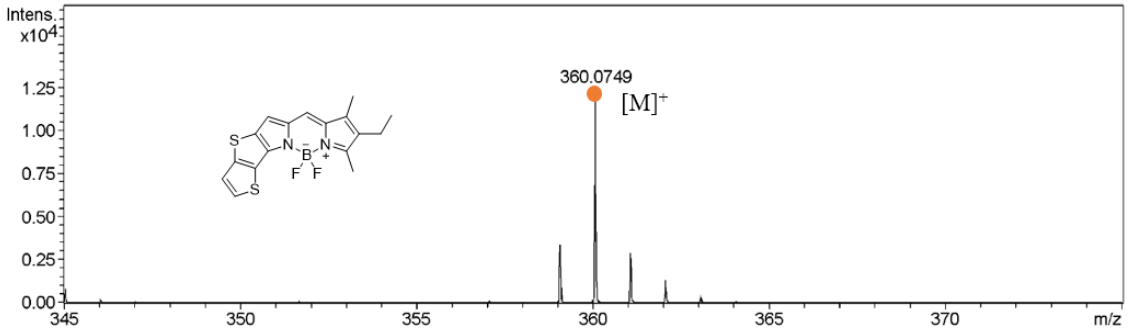


Fig. S16 ^{13}C NMR spectra of compound **9** recorded in $CDCl_3$

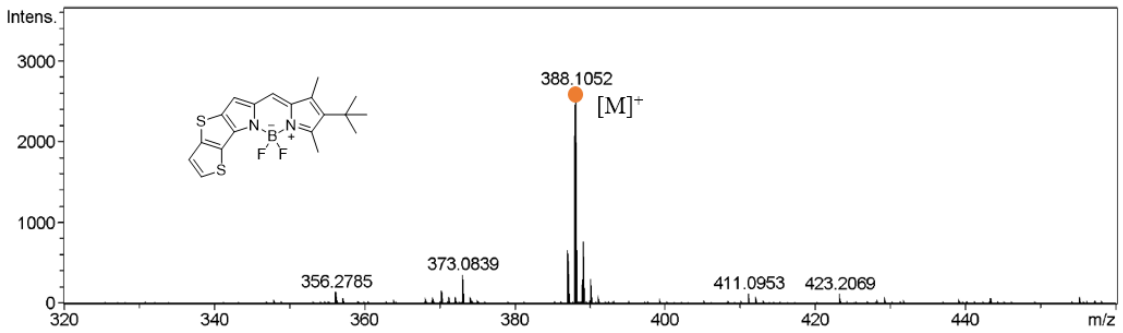
HRMS-ESI spectra



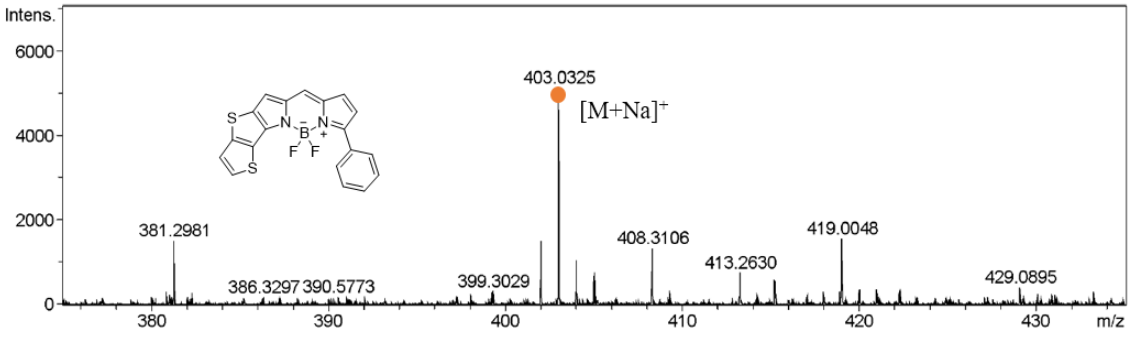
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e¯ Conf	N-Rule
355.0316	1	C15H11BF2N2NaS2	355.0320	1.1	62.7	1	100.00	10.5	even	ok



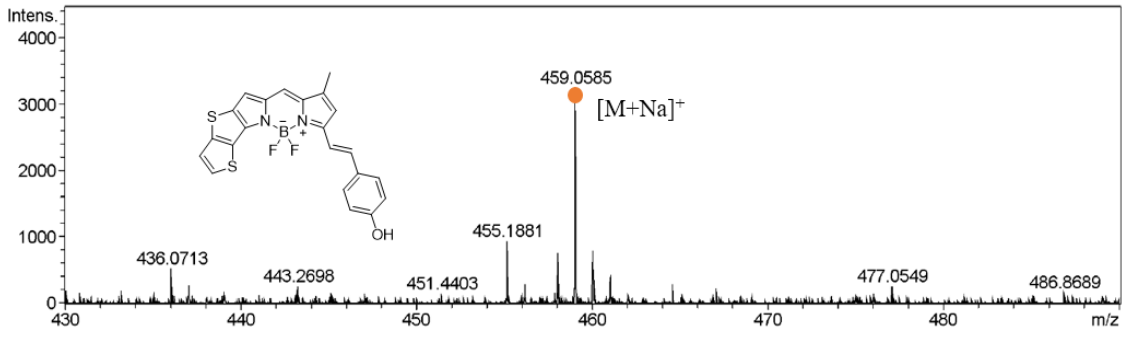
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e¯ Conf	N-Rule
360.0749	1	C17H15BF2N2S2	360.0735	-3.7	16.1	1	100.00	11.0	odd	ok



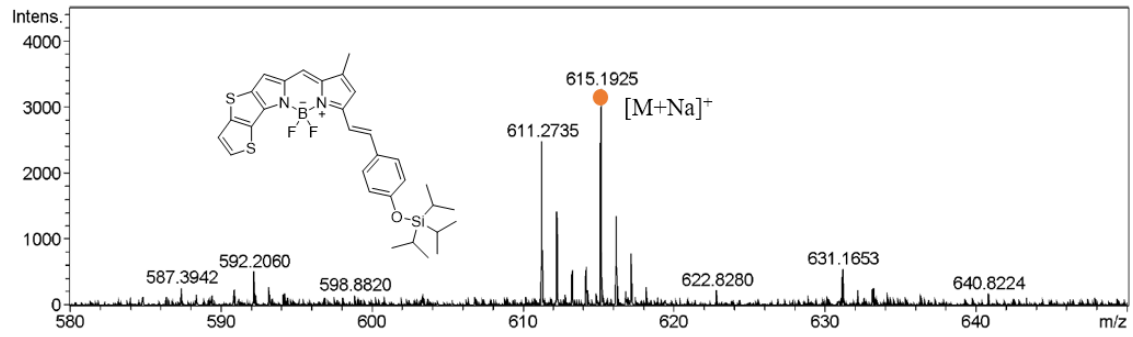
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e¯ Conf	N-Rule
388.1052	1	C19H19BF2N2S2	388.1049	-0.9	23.0	1	100.00	11.0	odd	ok



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e¯ Conf	N-Rule
403.0325	1	C19H11BF2N2NaS2	403.0321	-1.2	34.0	2	100.00	14.5	even	ok



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e¯ Conf	N-Rule
459.0585	1	C22H15BF2N2NaOS2	459.0583	-0.5	23.6	1	100.00	15.5	even	ok



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e¯ Conf	N-Rule
615.1925	1	C31H35BF2N2NaOS2Si	615.1919	-1.0	27.7	1	100.00	15.5	even	ok