

Supporting information

Development and Applications of a Near-infrared Dye-Benzylguanine Conjugate to Specifically Label SNAP Tagged Proteins

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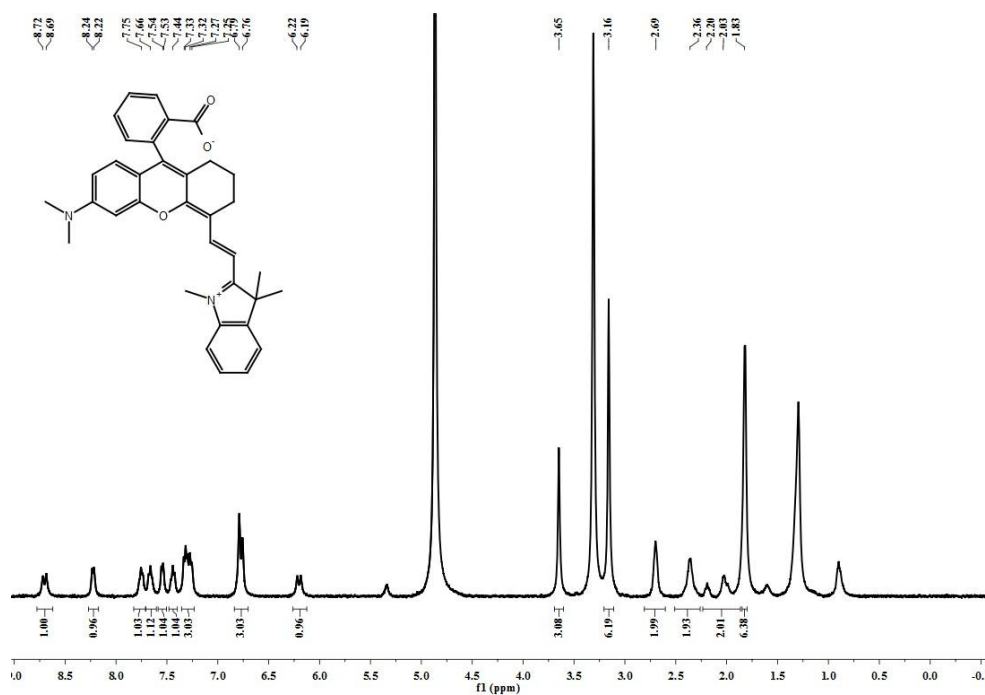


Figure S1. N-NIR ¹H NMR

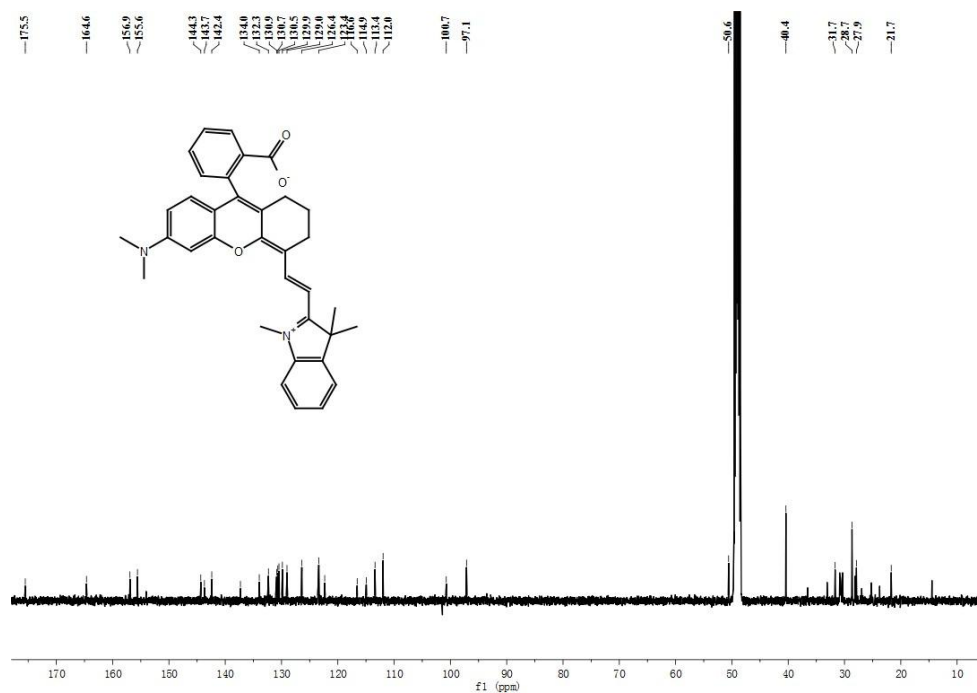


Figure S2. N-NIR $^{13}\text{C-NMR}$

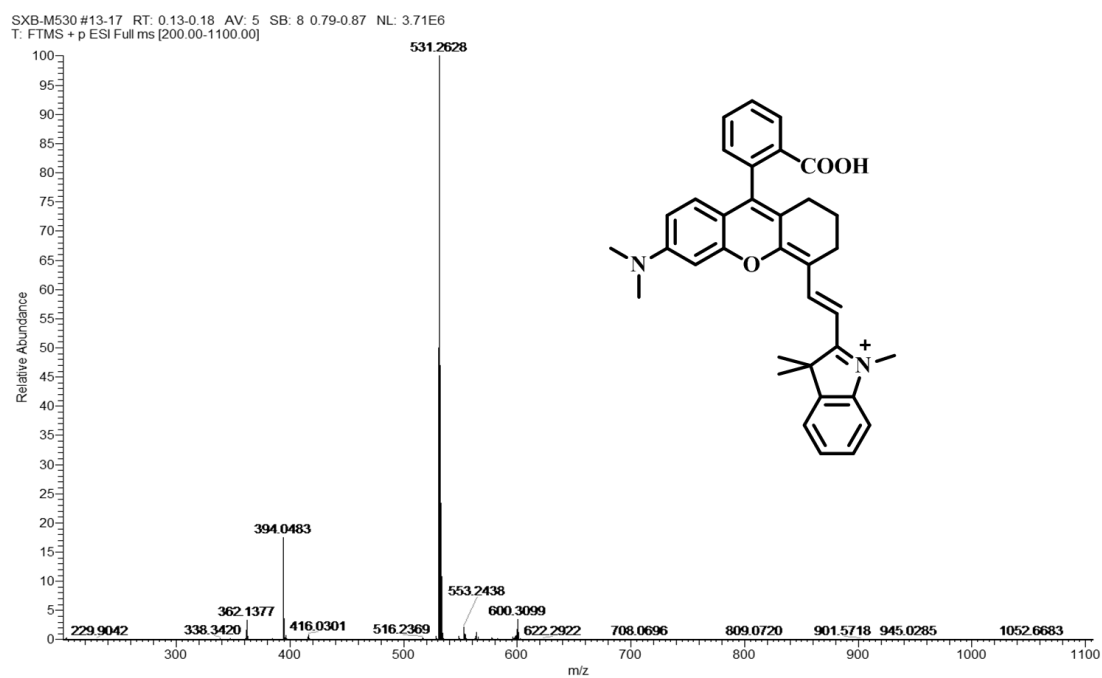


Figure S3. MS Spectrum N-NIR

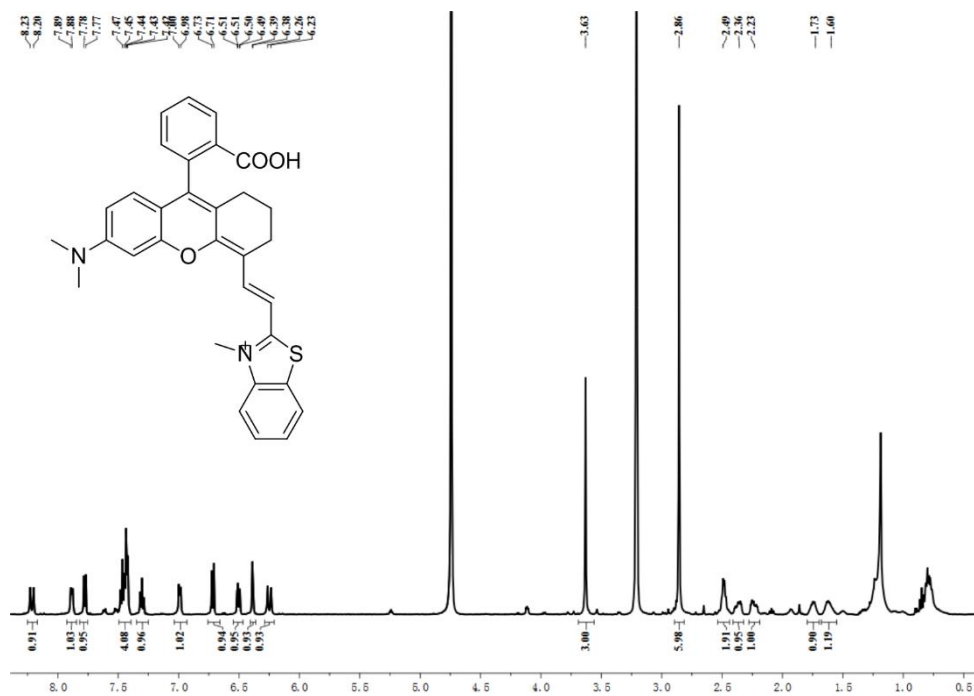


Figure S4. S-NIR $^1\text{H NMR}$



Figure S5. S-NIR $^{13}\text{C NMR}$

SXB-2

16051314 3 (0.098)

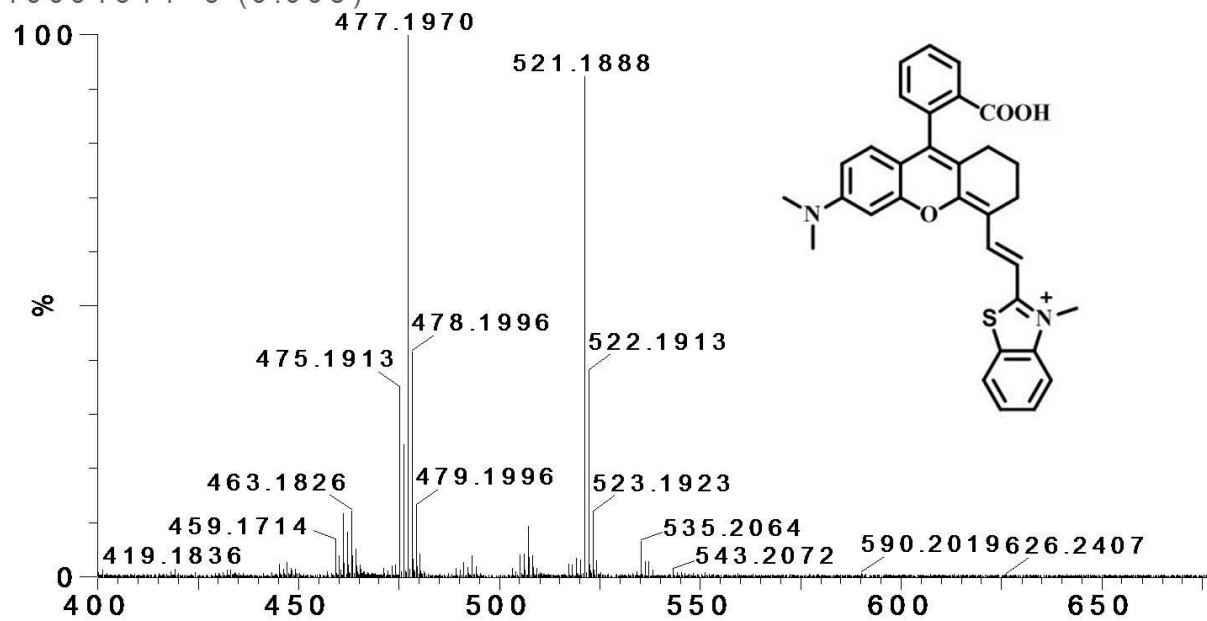


Figure S6. MS Spectrum S-NIR

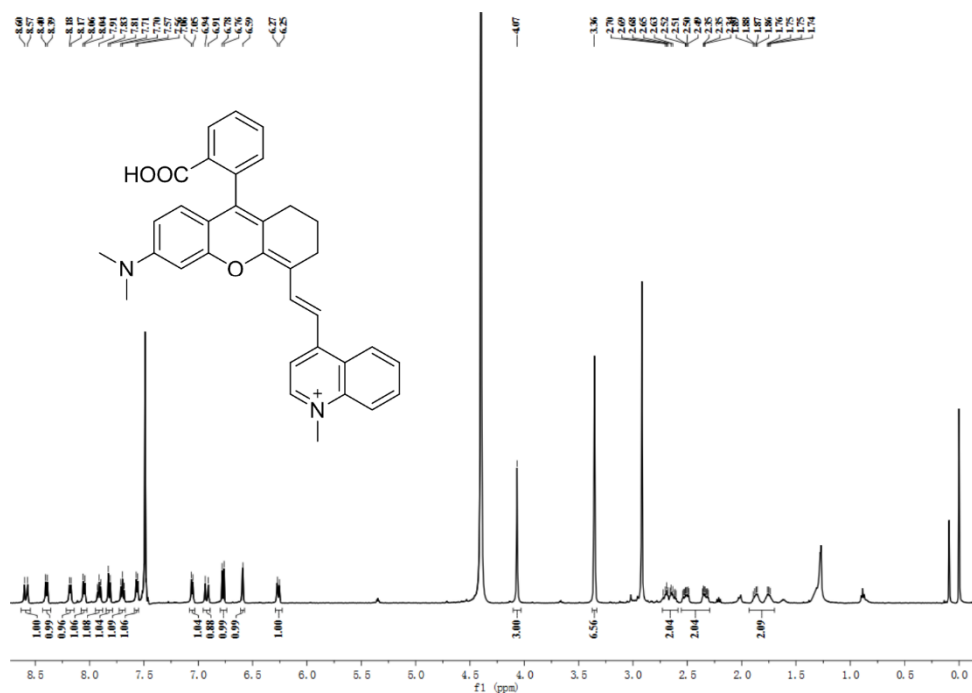


Figure S7. K-NIR ^1H NMR

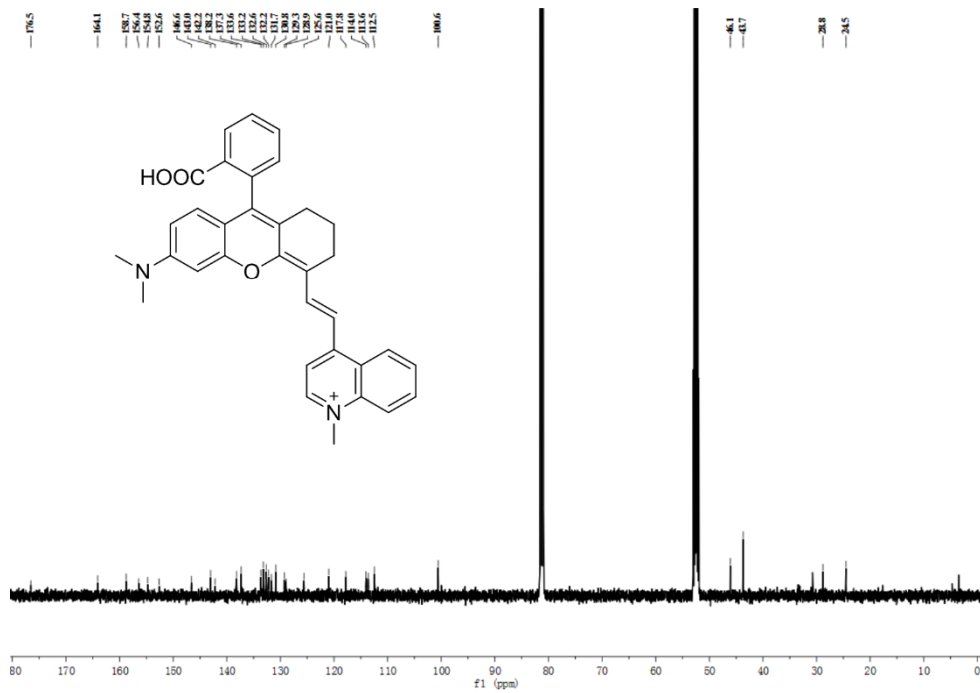


Figure S8. K-NIR ^{13}C NMR

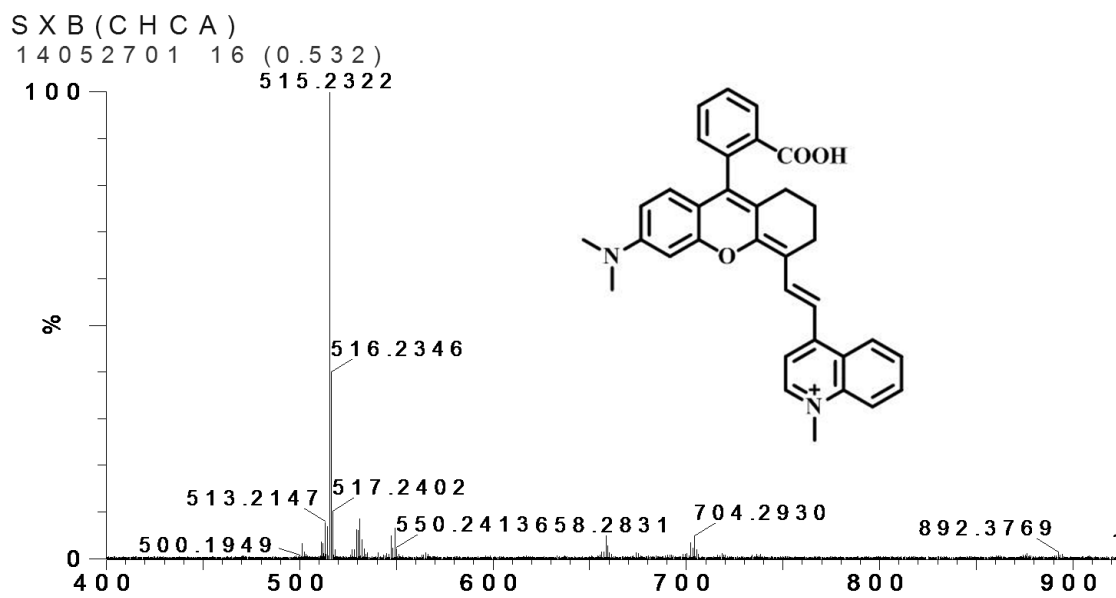


Figure S9. MS Spectrum K-NIR

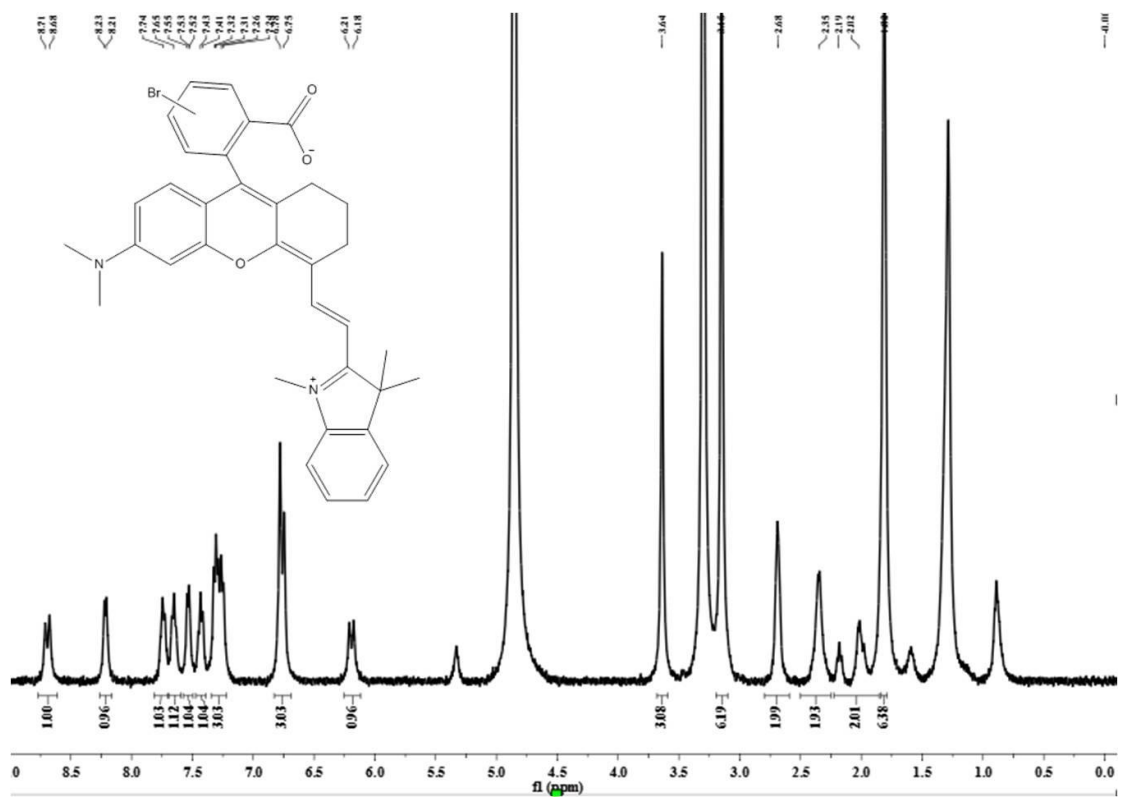


Figure S10. Br-N-NIR ^1H NMR
 SXB-2(CHCA)
 14052308 44 (1.465)

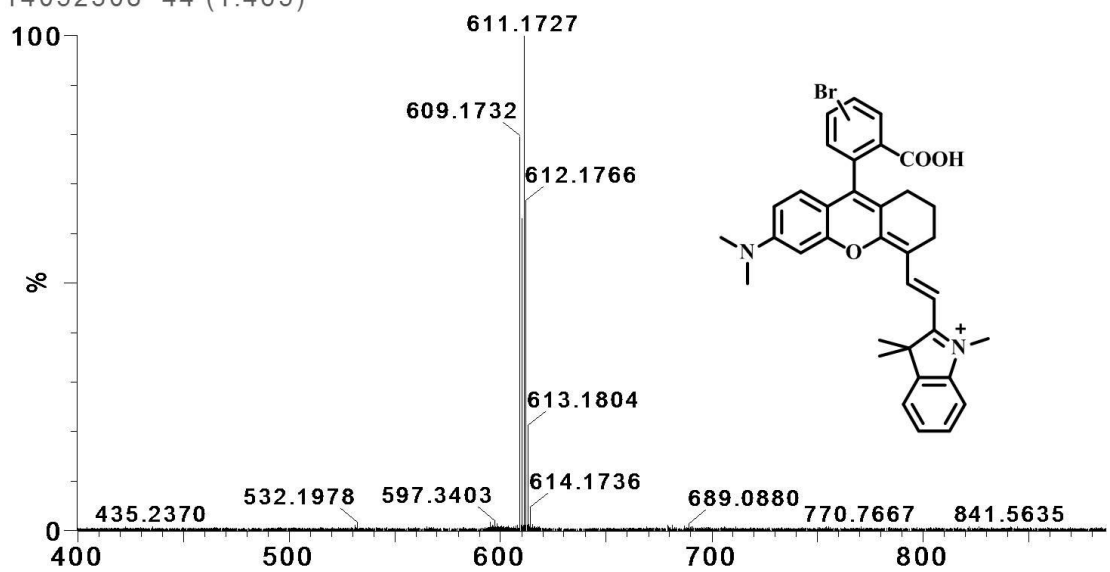


Figure S11. MS Spectrum Br-N-NIR

SXB-1

16051313 43 (1.432)

TOF LD+
394

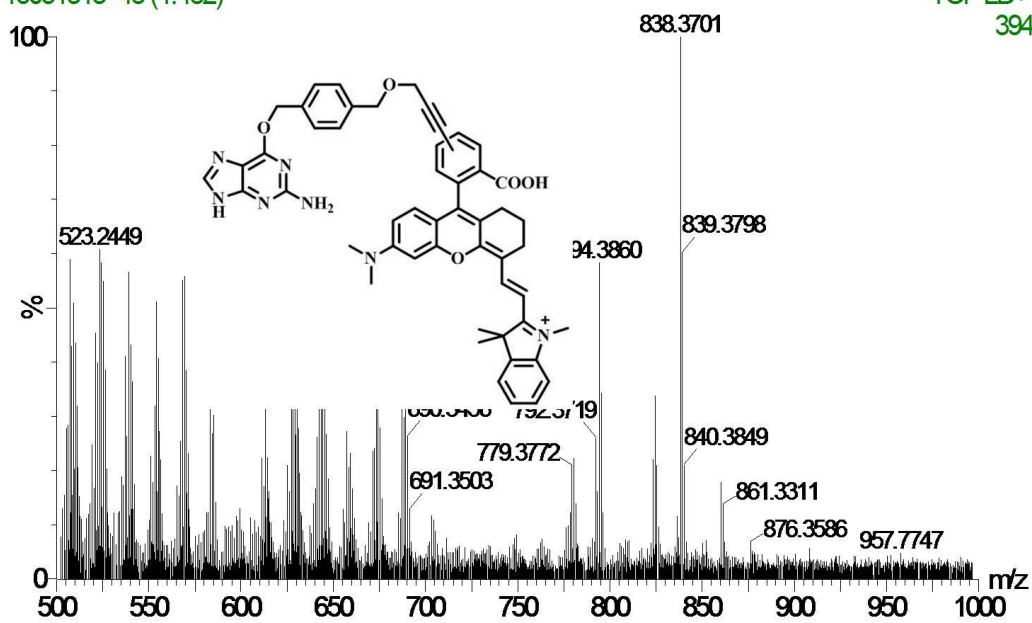
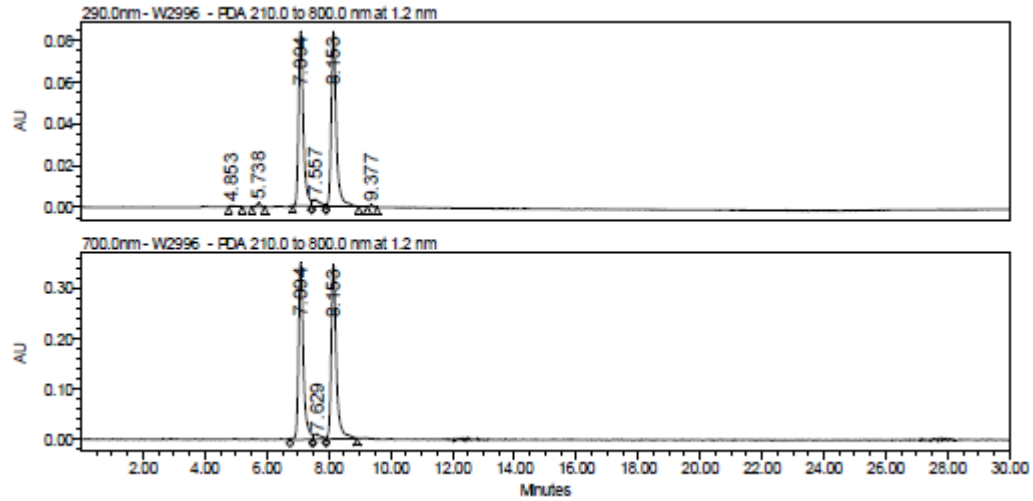


Figure S12. MS Spectrum PYBG-D



Processed Channel Descr.: PDA 290.0 nm

	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 290.0 nm	4.853	6748	0.35	539
2	PDA 290.0 nm	5.738	15701	0.82	1774
3	PDA 290.0 nm	7.094	885205	46.14	84229
4	PDA 290.0 nm	7.557	53677	2.80	3255
5	PDA 290.0 nm	8.153	950224	49.53	83903
6	PDA 290.0 nm	9.377	6887	0.36	697

Processed Channel Descr.: PDA 700.0 nm

	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 700.0 nm	7.094	3791392	47.75	352380
2	PDA 700.0 nm	7.629	177288	2.23	10181
3	PDA 700.0 nm	8.153	3971125	50.02	347144

Figure 13. HPLC spectrum **PYBG-D**

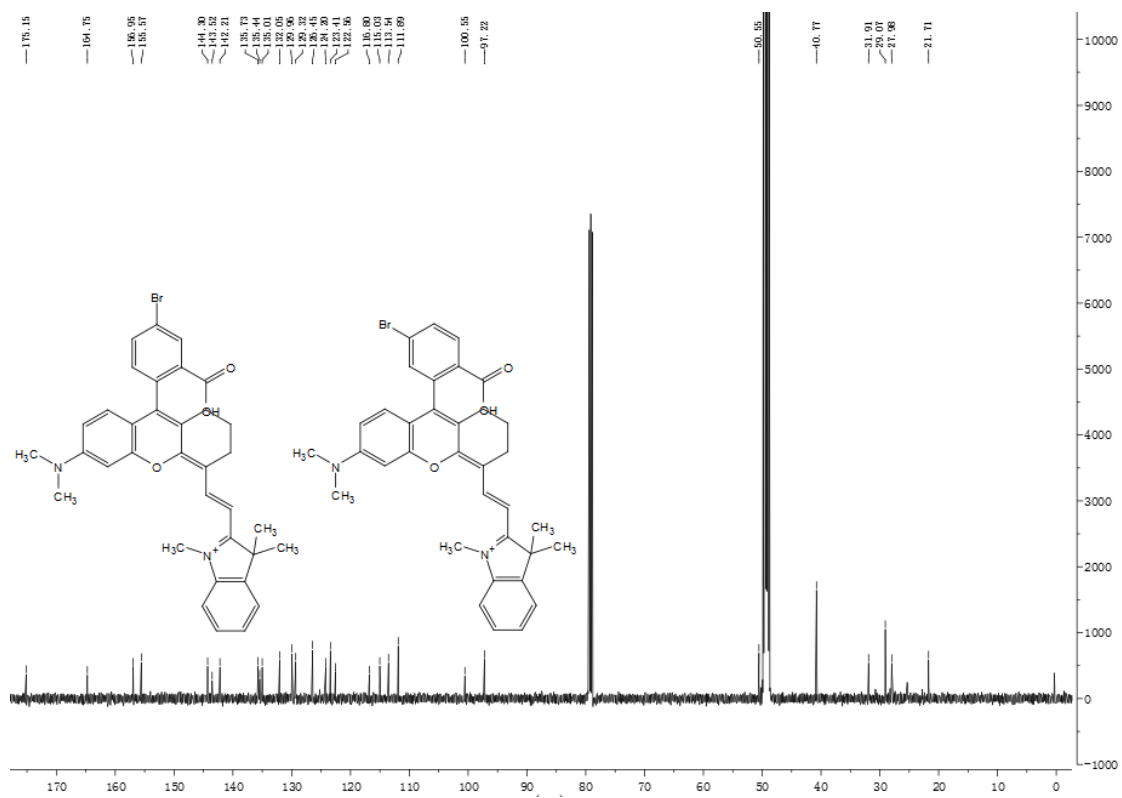


Figure 14. Br-N-NIR ^{13}C NMR

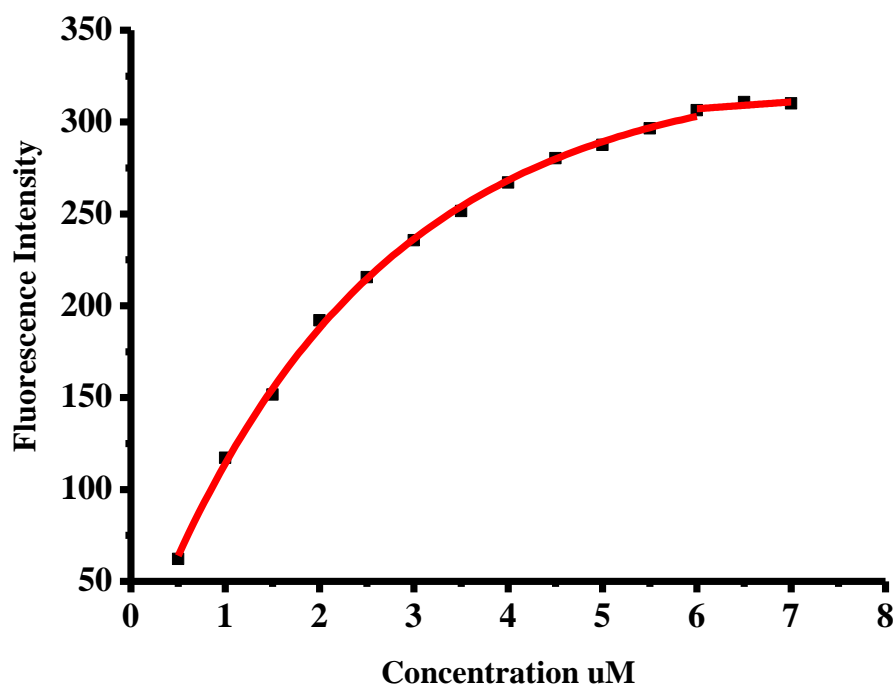


Figure 15. The water solubility of N-NIR

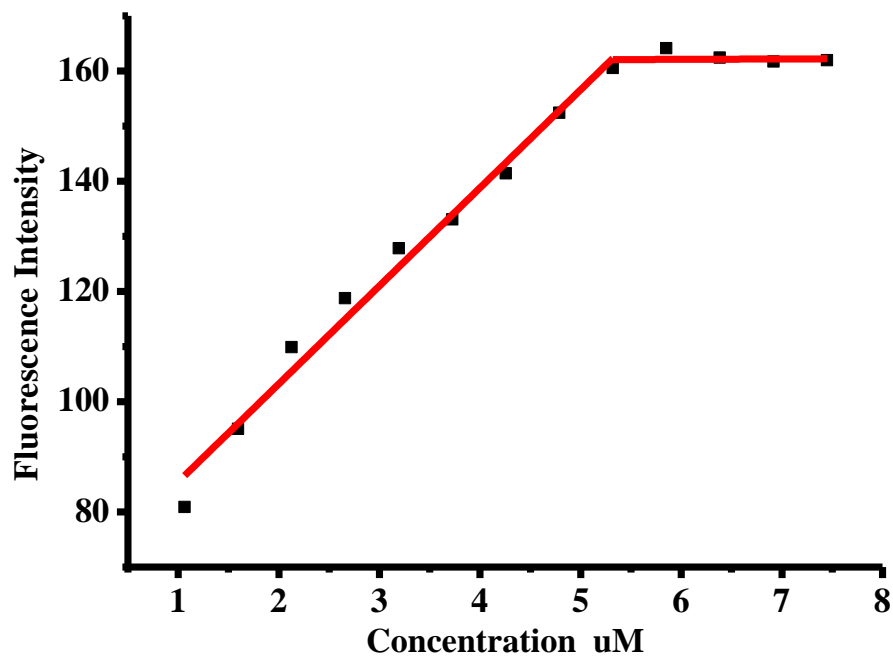


Figure 16. The water solubility of S-NIR

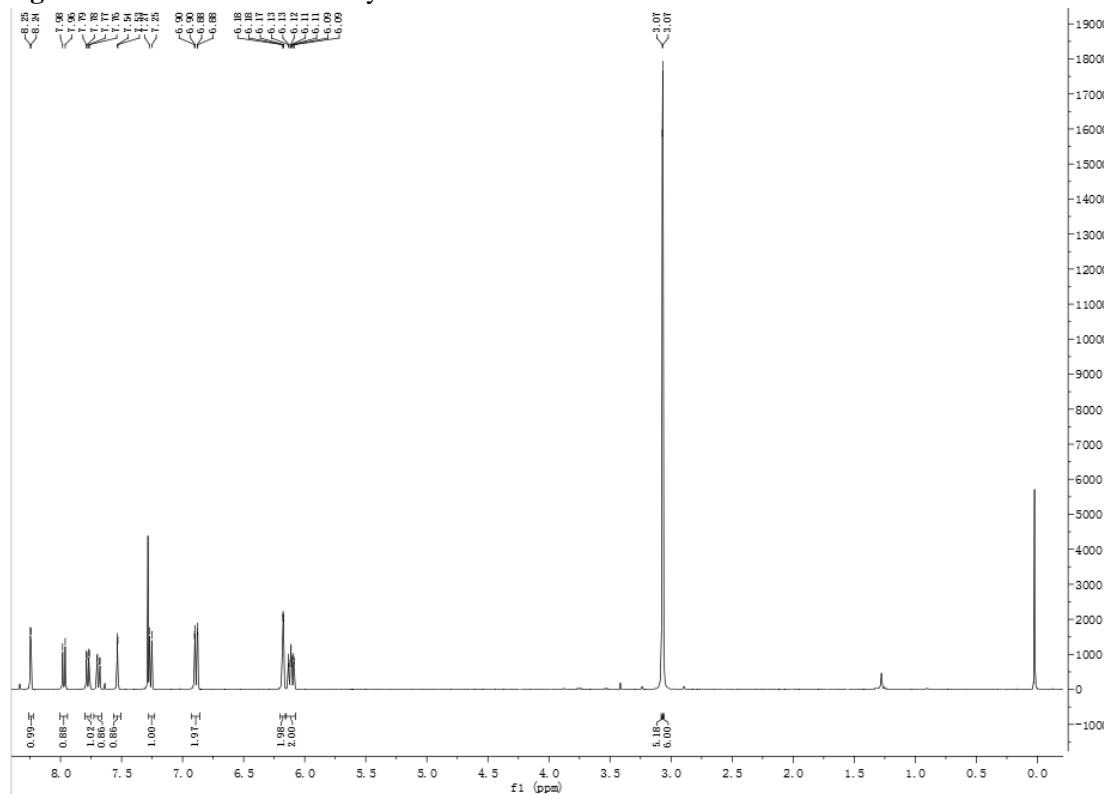


Figure 17. ^1H NMR

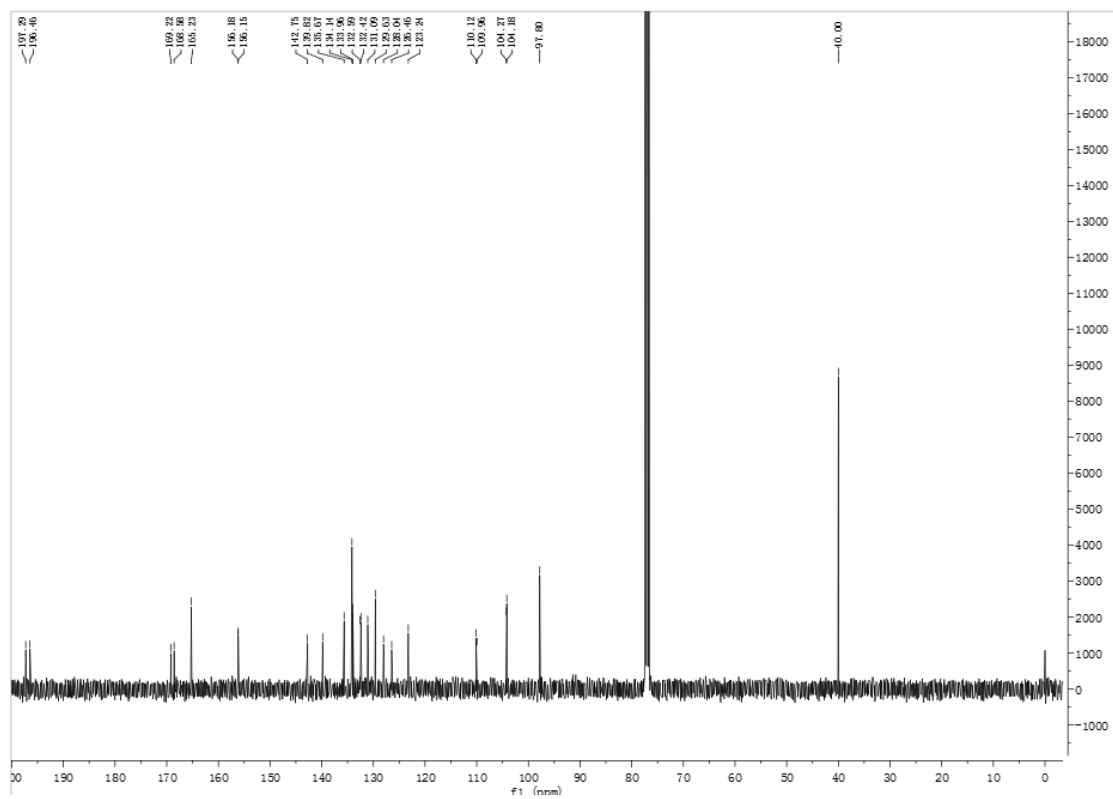


Figure 18. r ^{13}C NMR



Figure 19. the compounds before r ^1H NMR

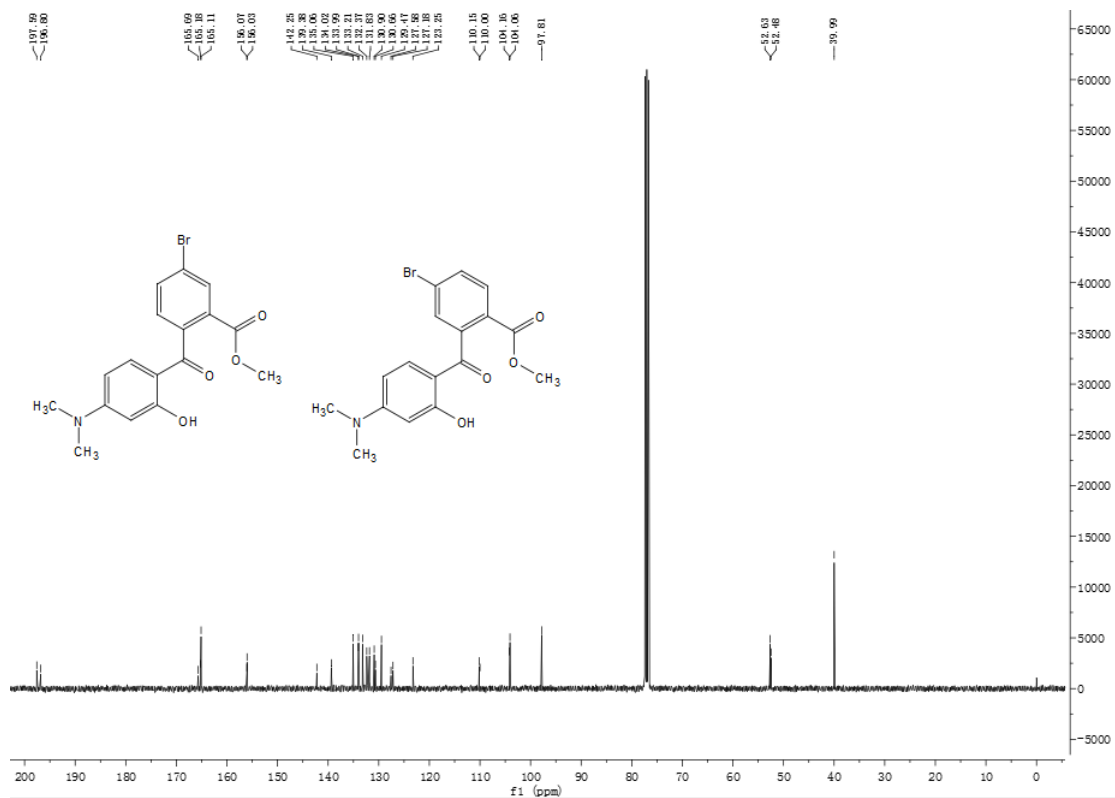


Figure 20. the compounds before r ^{13}C NMR



Figure 21. h ^1H NMR in DMSO

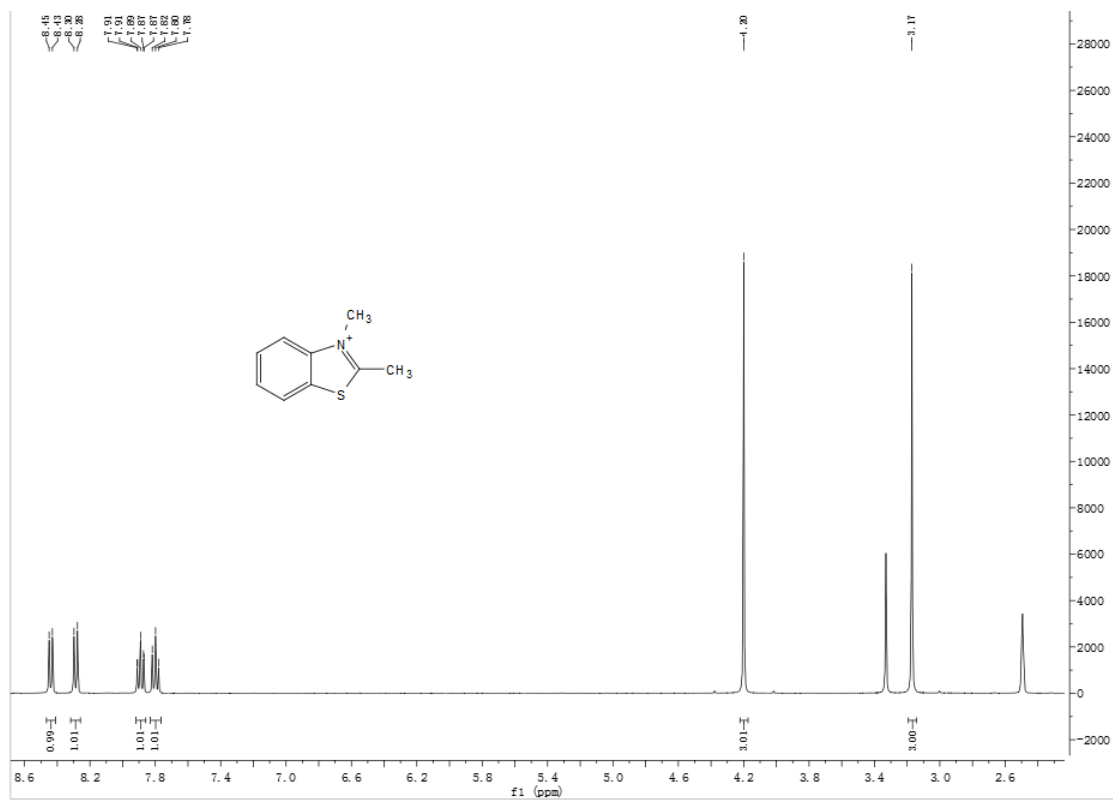


Figure 22. f ^1H NMR in DMSO

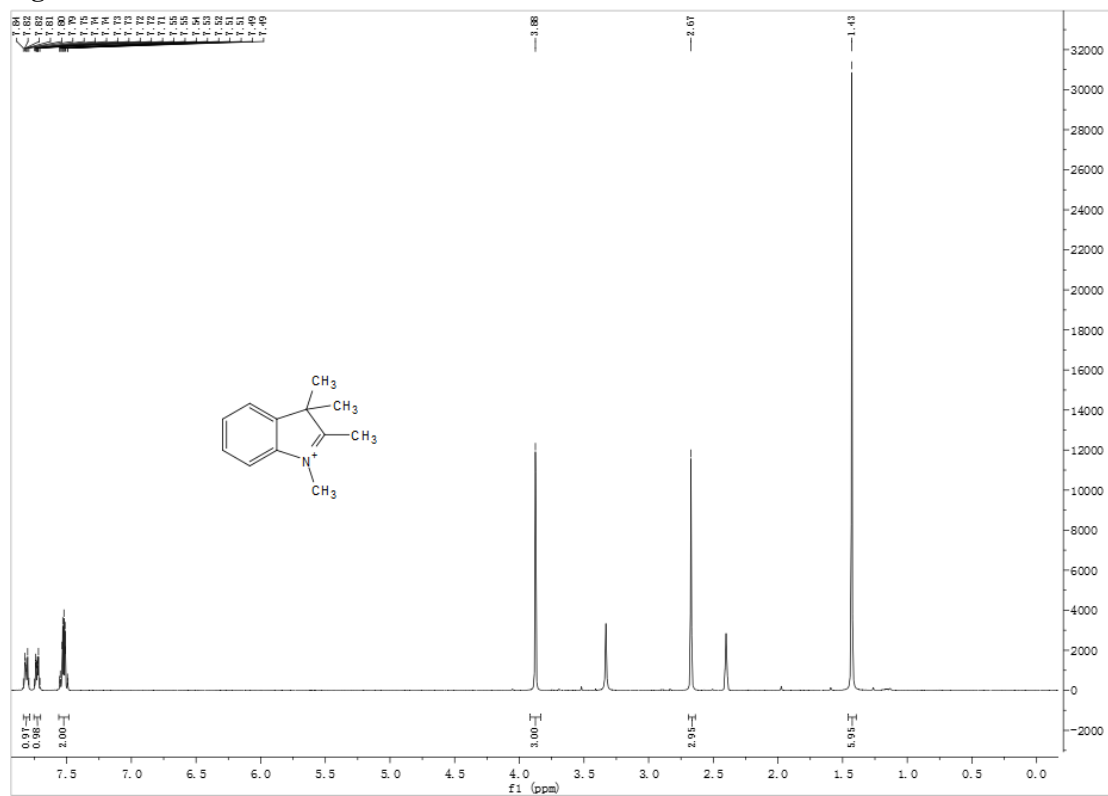


Figure 23. b ^1H NMR in DMSO

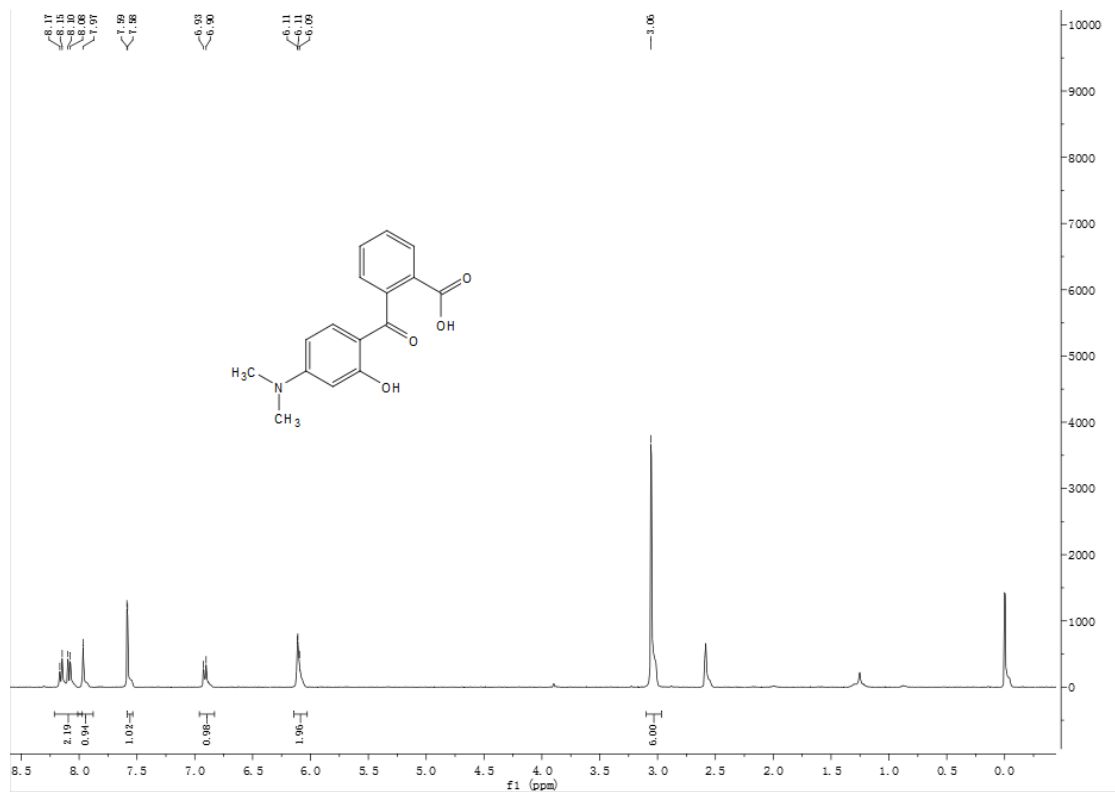


Figure 24. j ^1H NMR in DMSO

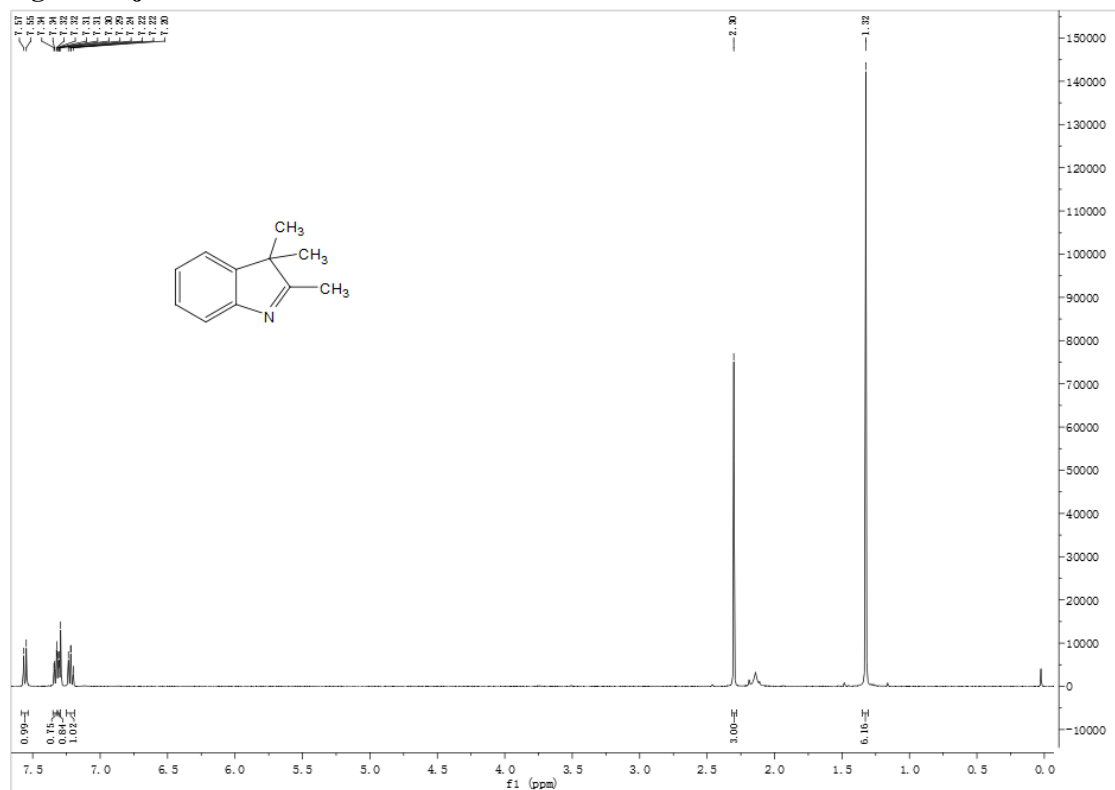


Figure 25.a ^1H NMR in CDCl_3

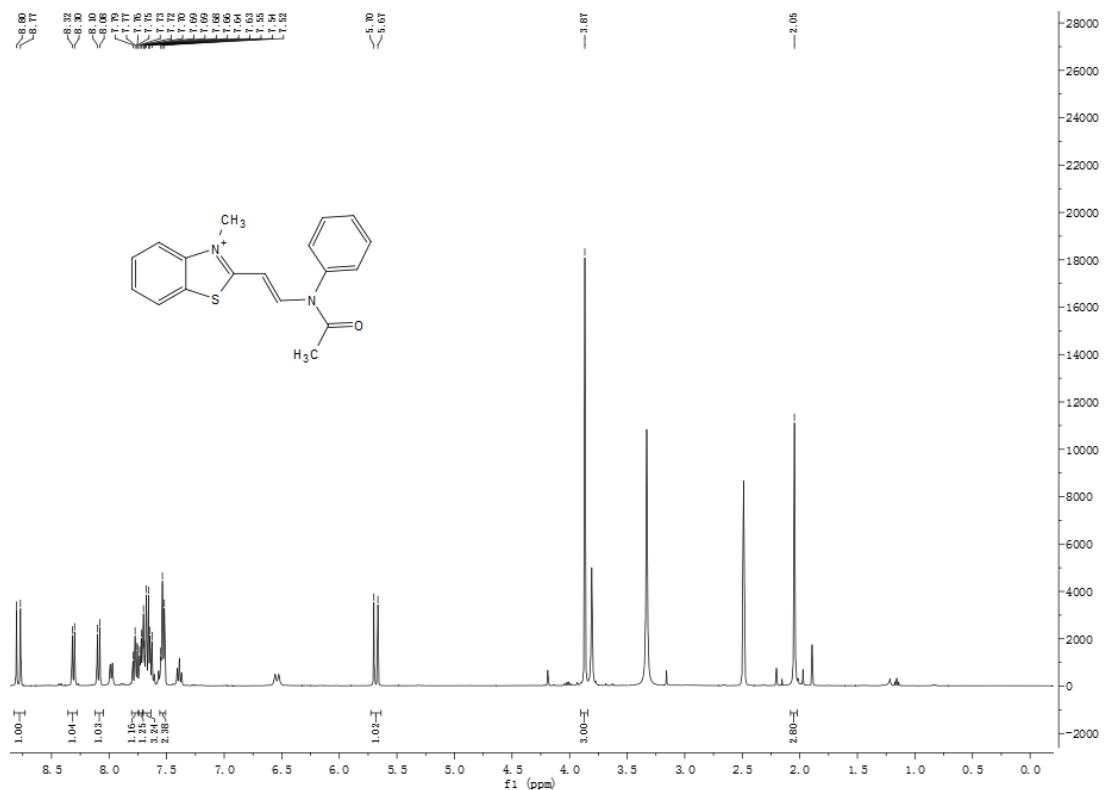


Figure 26.g ¹HNMR in DMSO

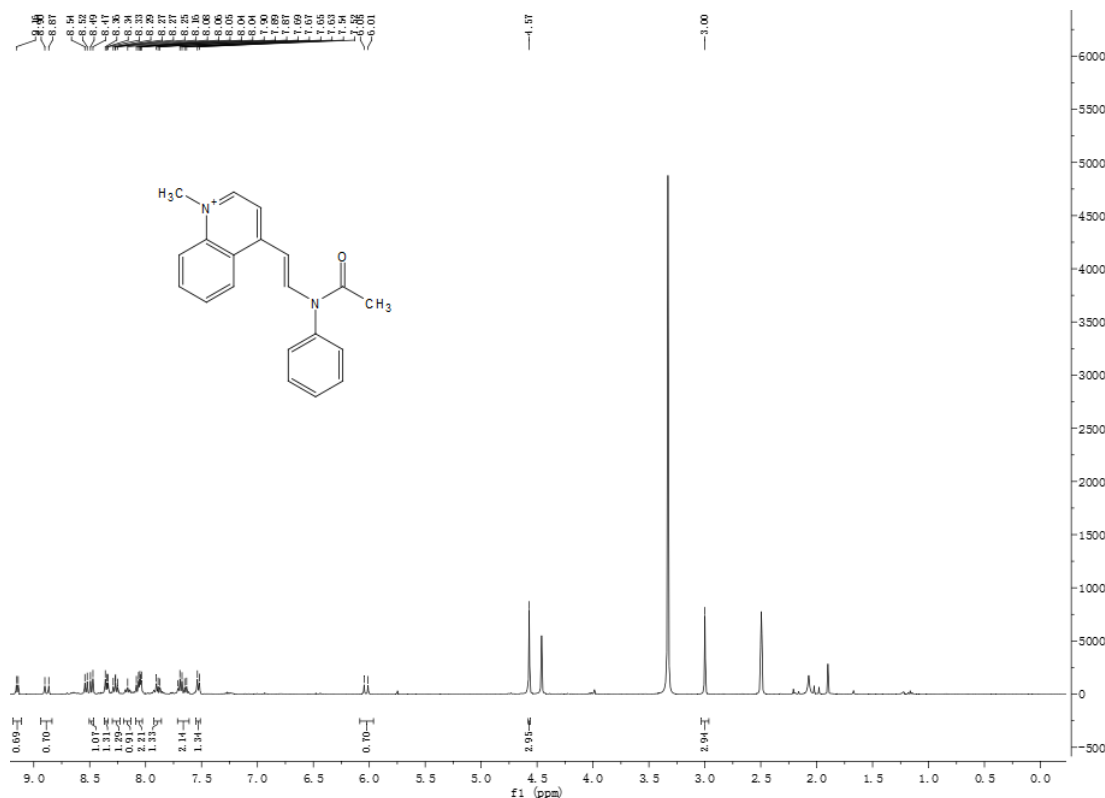


Figure 27.i ¹HNMR in DMSO

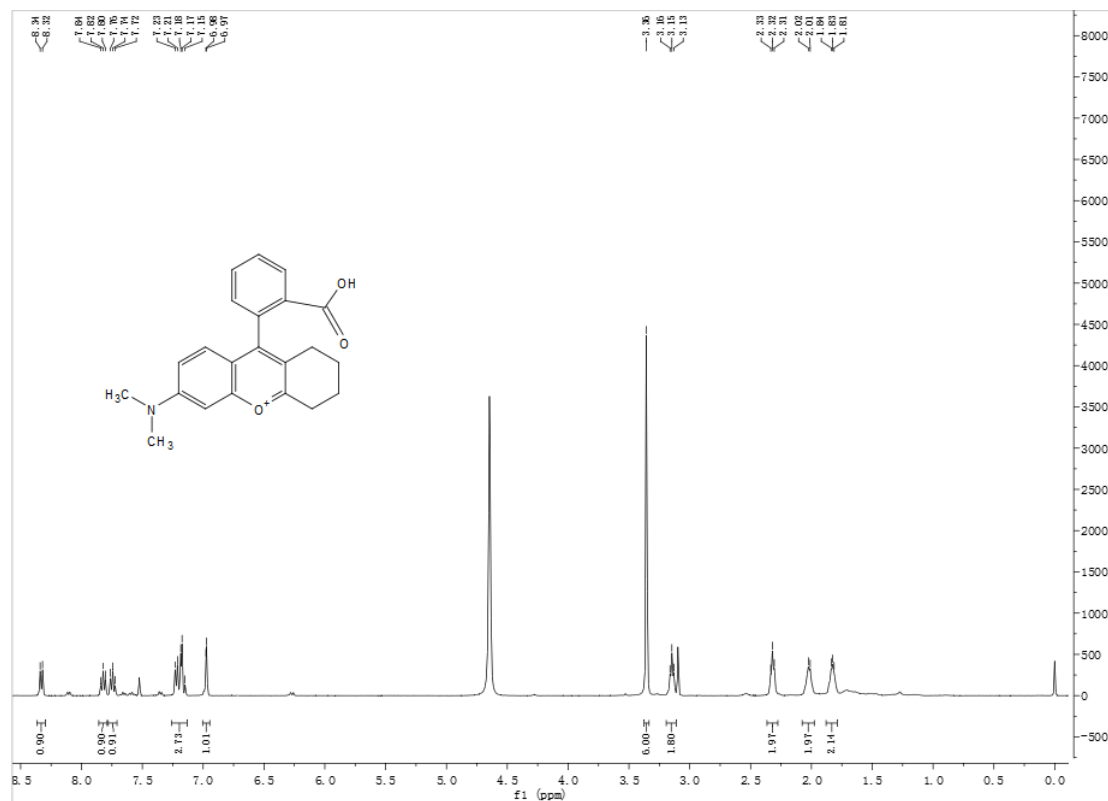


Figure 28.k ¹H NMR

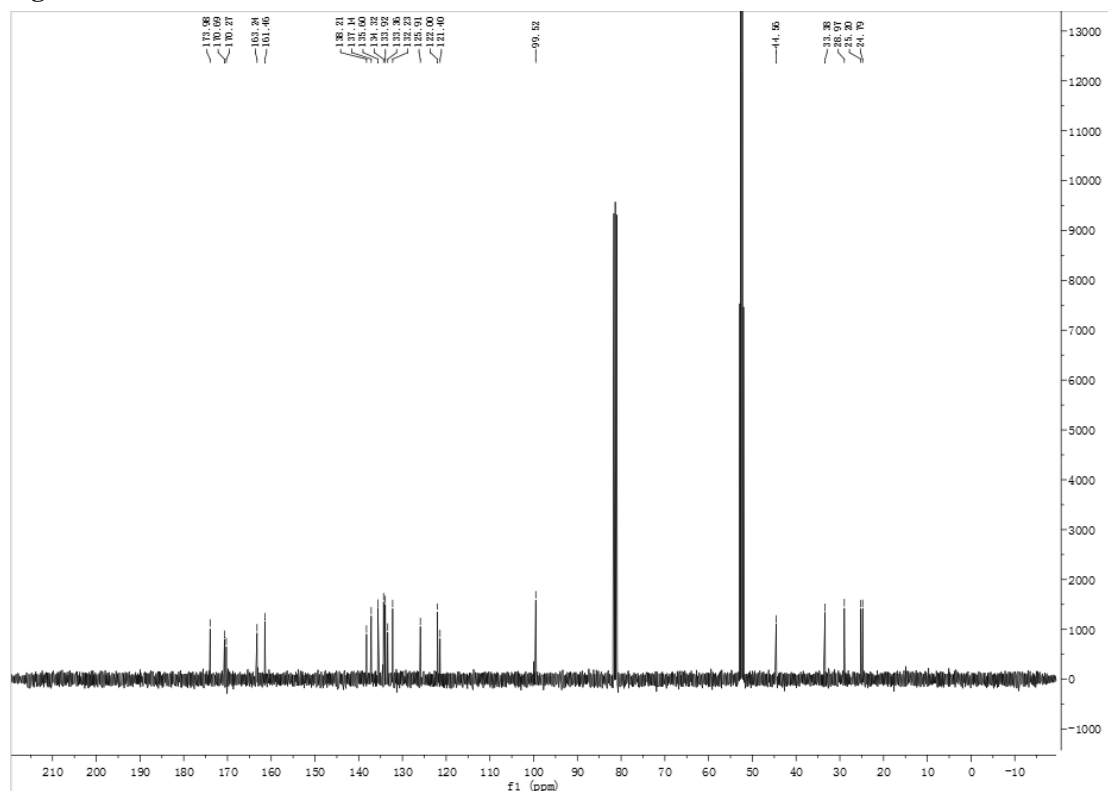


Figure 29.k ¹³C NMR

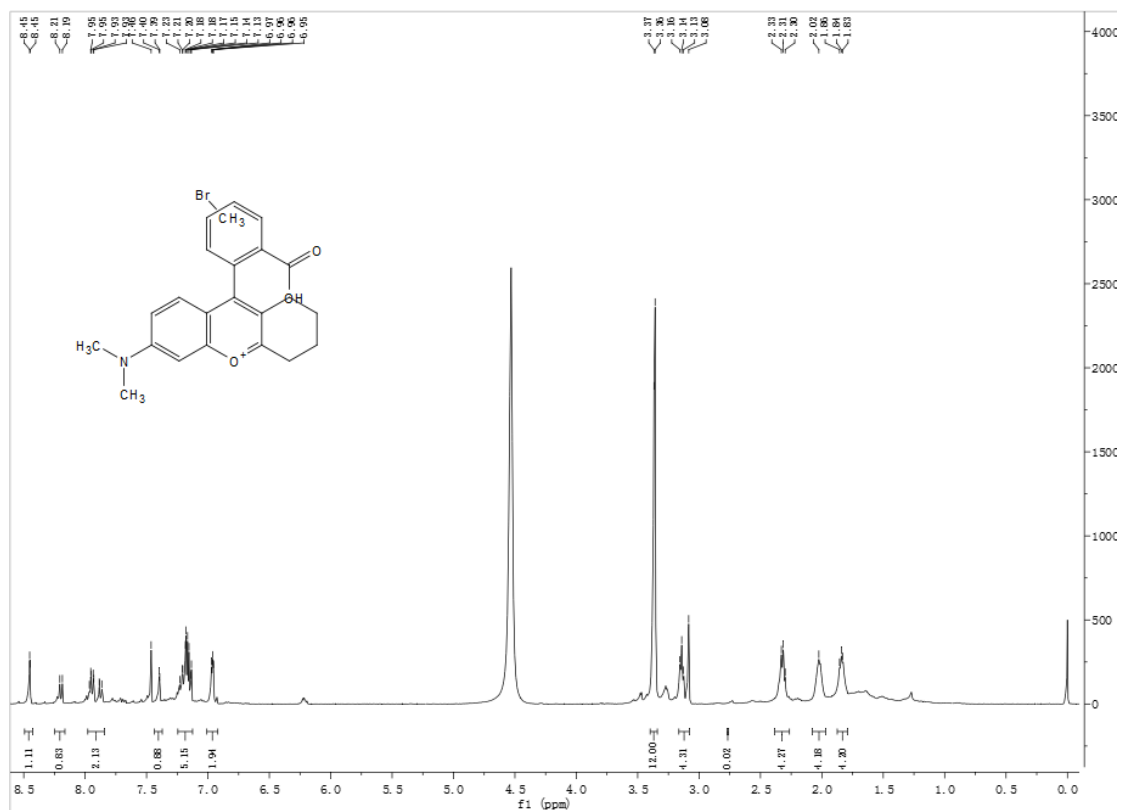
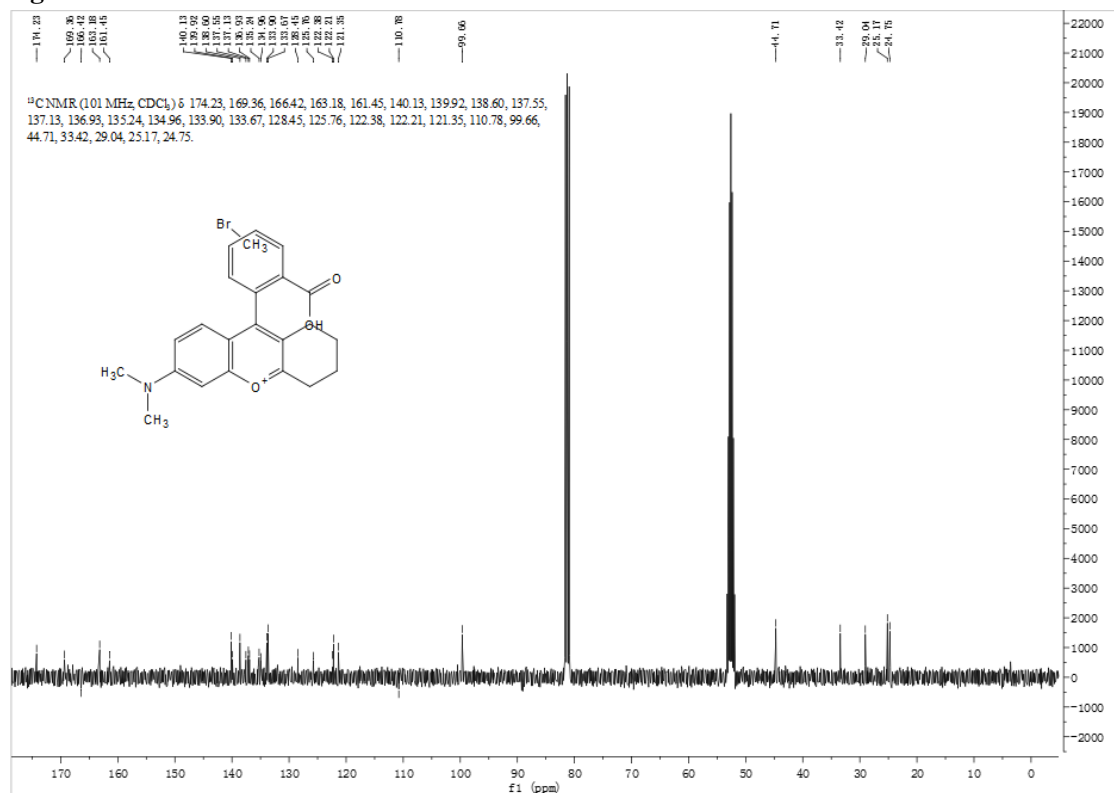


Figure 30.s ^1H NMR



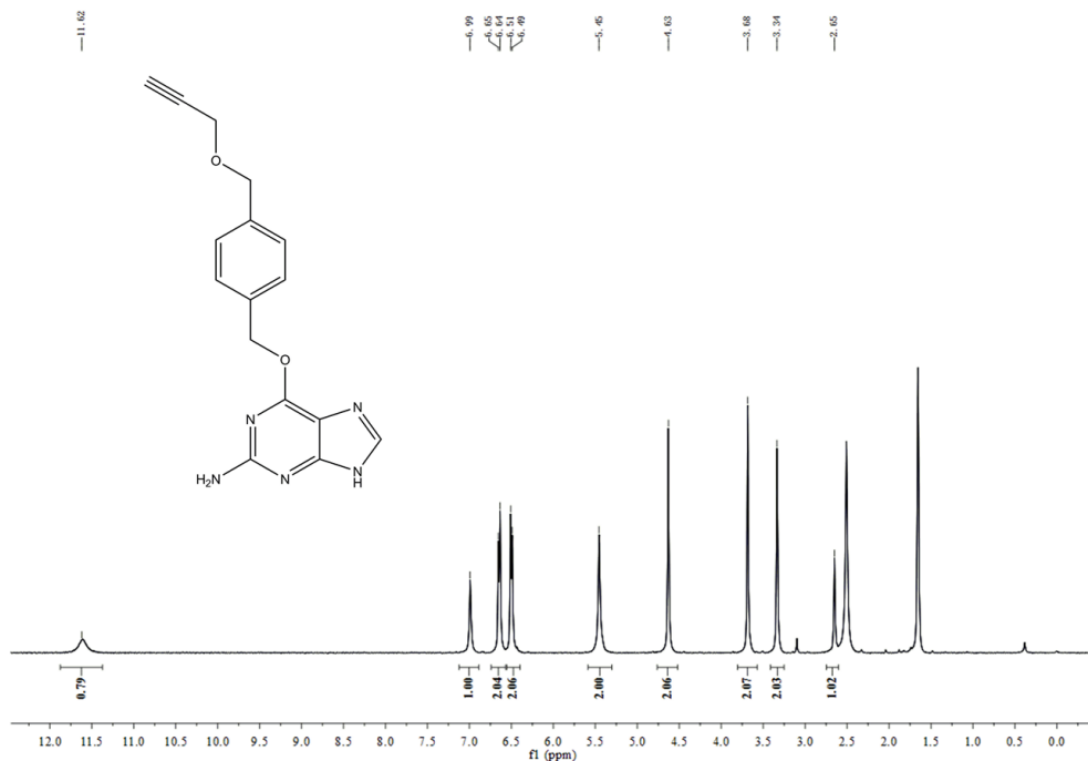


Figure 32. PYBG ¹H NMR

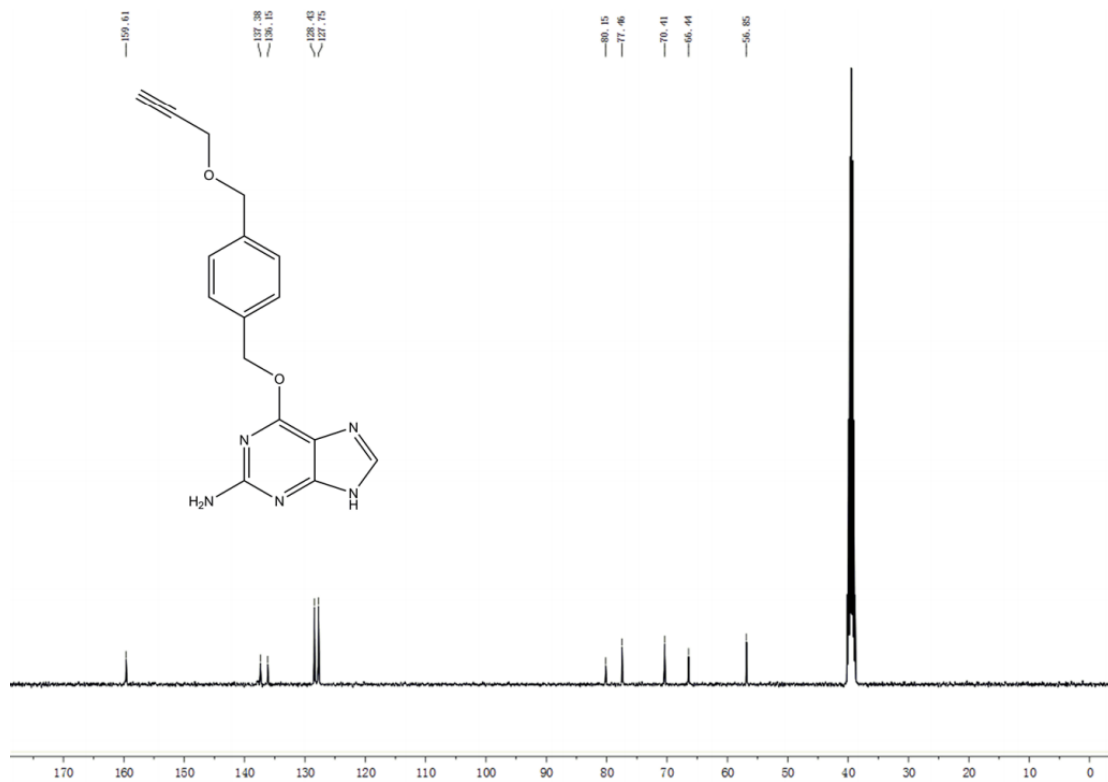


Figure 33. PYBG ¹³C NMR

SXB-M732 #14-16 RT: 0.10-0.12 AV: 3 SB: 7 0.82-0.87 NL: 3.06E6
T: FTMS + p ESI Full ms [200.00-1000.00]

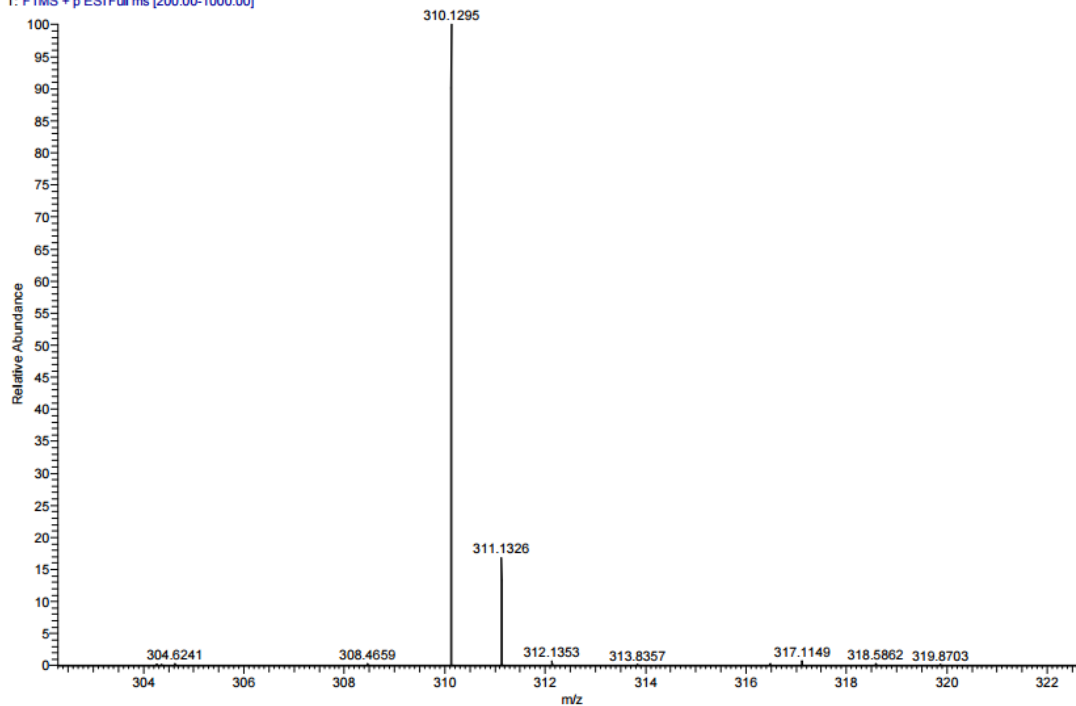


Figure 34.PYBG ESI MS spectrum