

Synthesis, Fluorine-18 Radiolabeling, and In Vivo PET Imaging of a Hydrophilic Fluorosulfotetrazine

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¹H NMR (16 scans, 500.13 MHz, 294.6 K, CDCl₃)

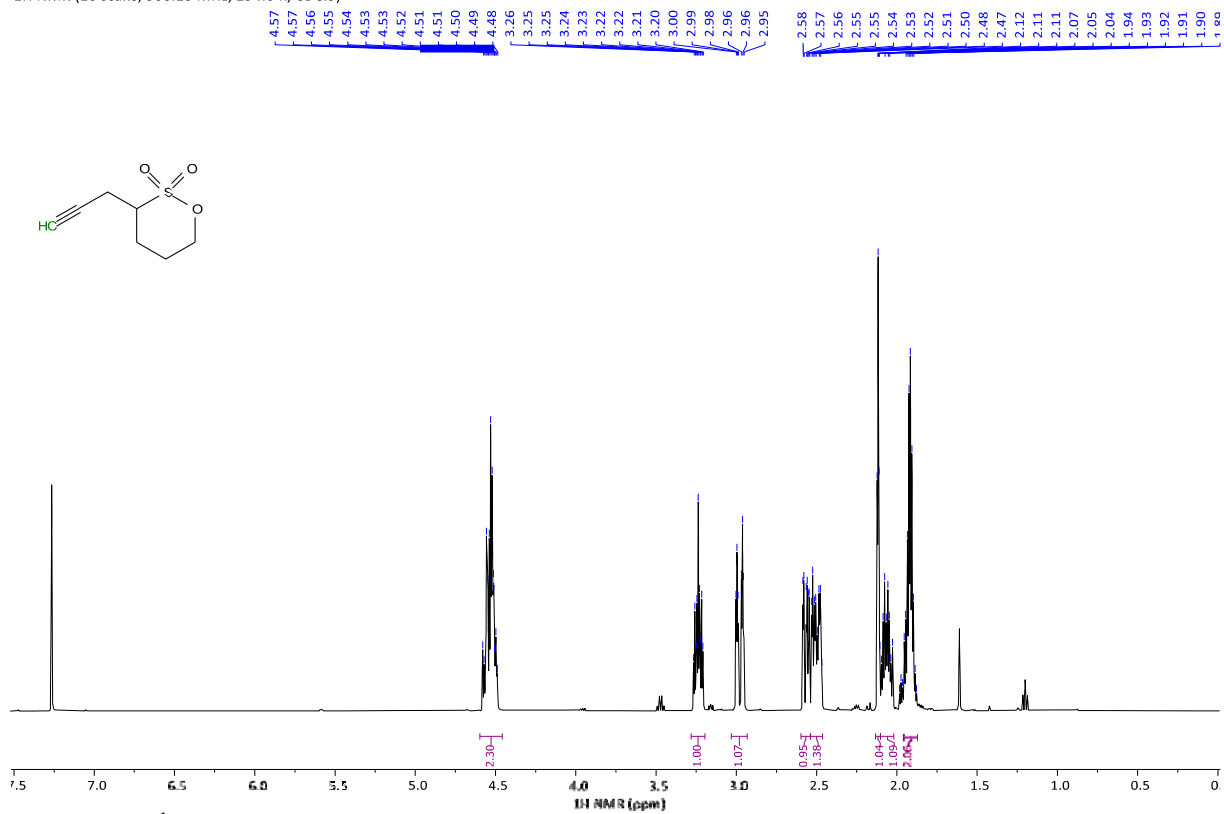


Figure S1. ¹H NMR spectrum of compound 3.

¹³C NMR (128 scans, 125.76 MHz, 295.8 K, CDCl₃)

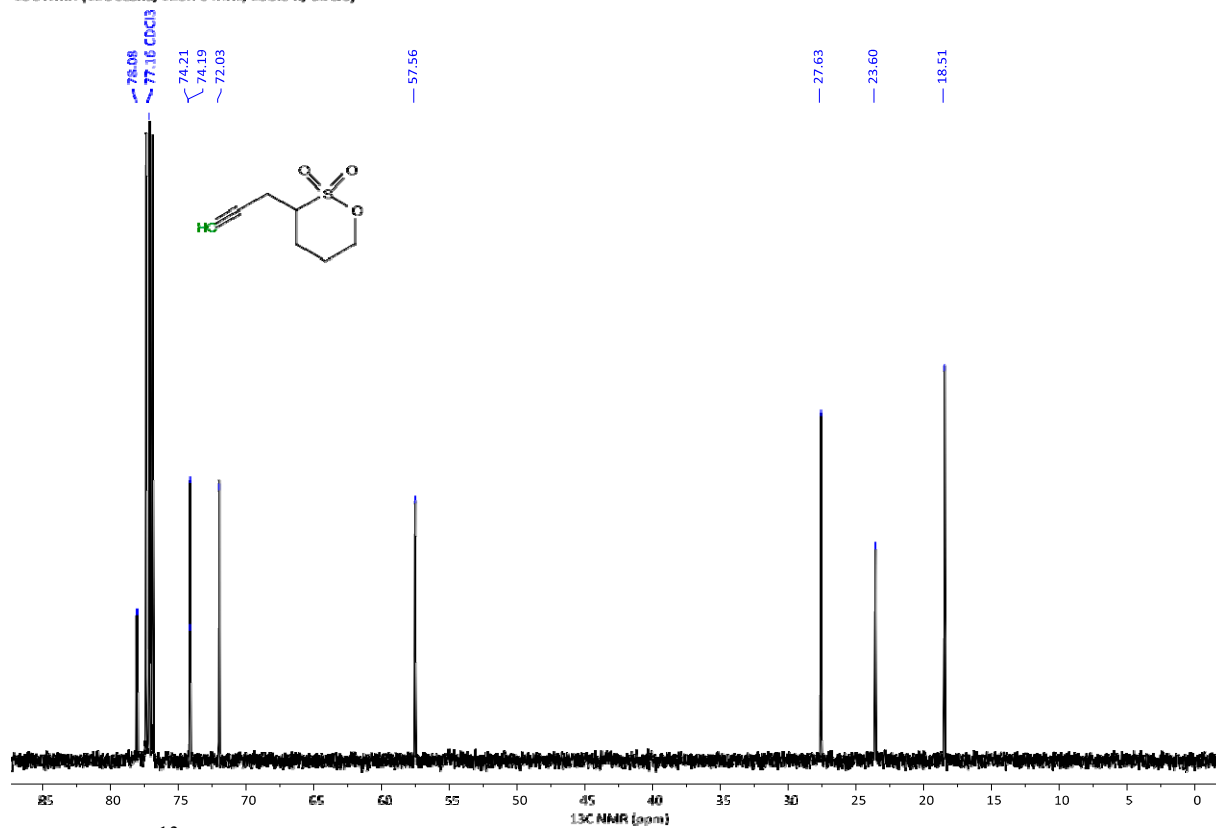


Figure S2. ¹³C NMR spectrum of compound 3.

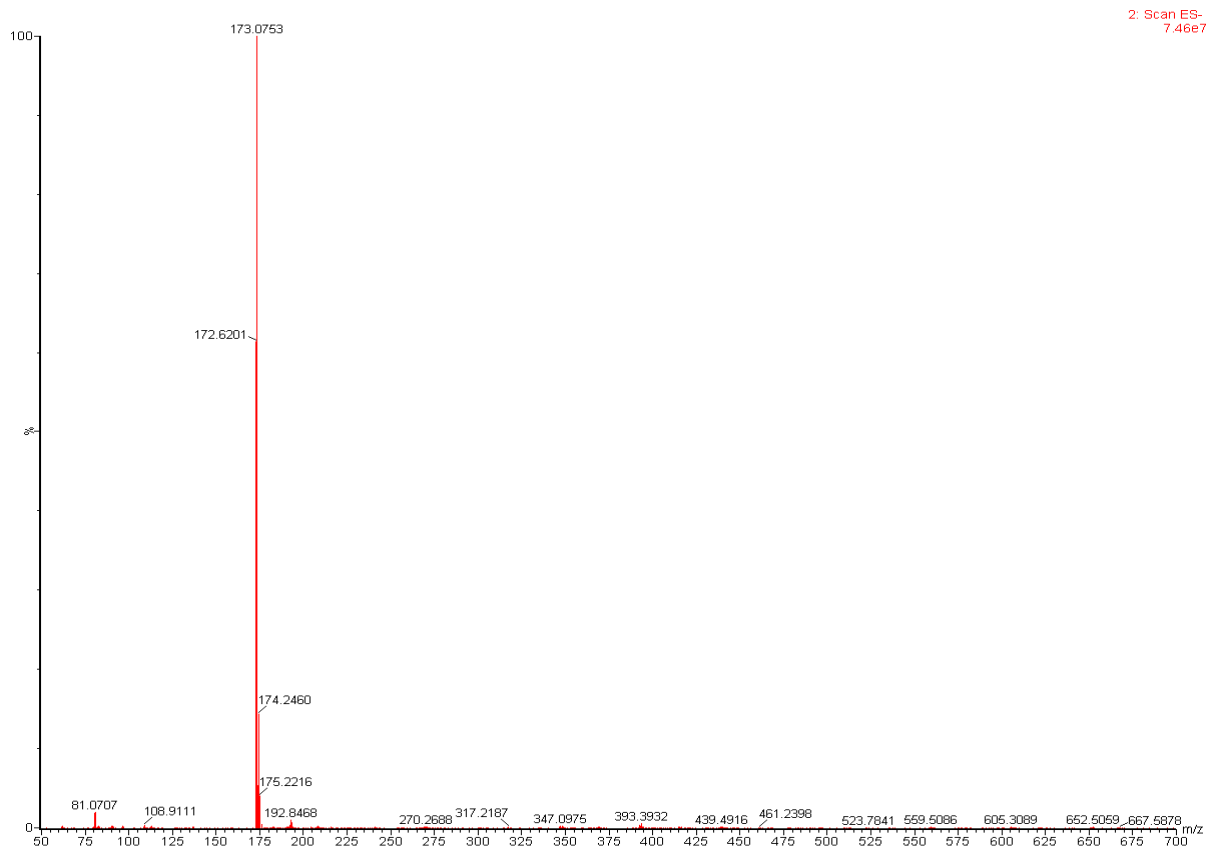


Figure S3. MS and HRMS analysis of compound **3**.

¹H NMR (16 scans, 500.13 MHz, 294.8 K, CDCl₃)

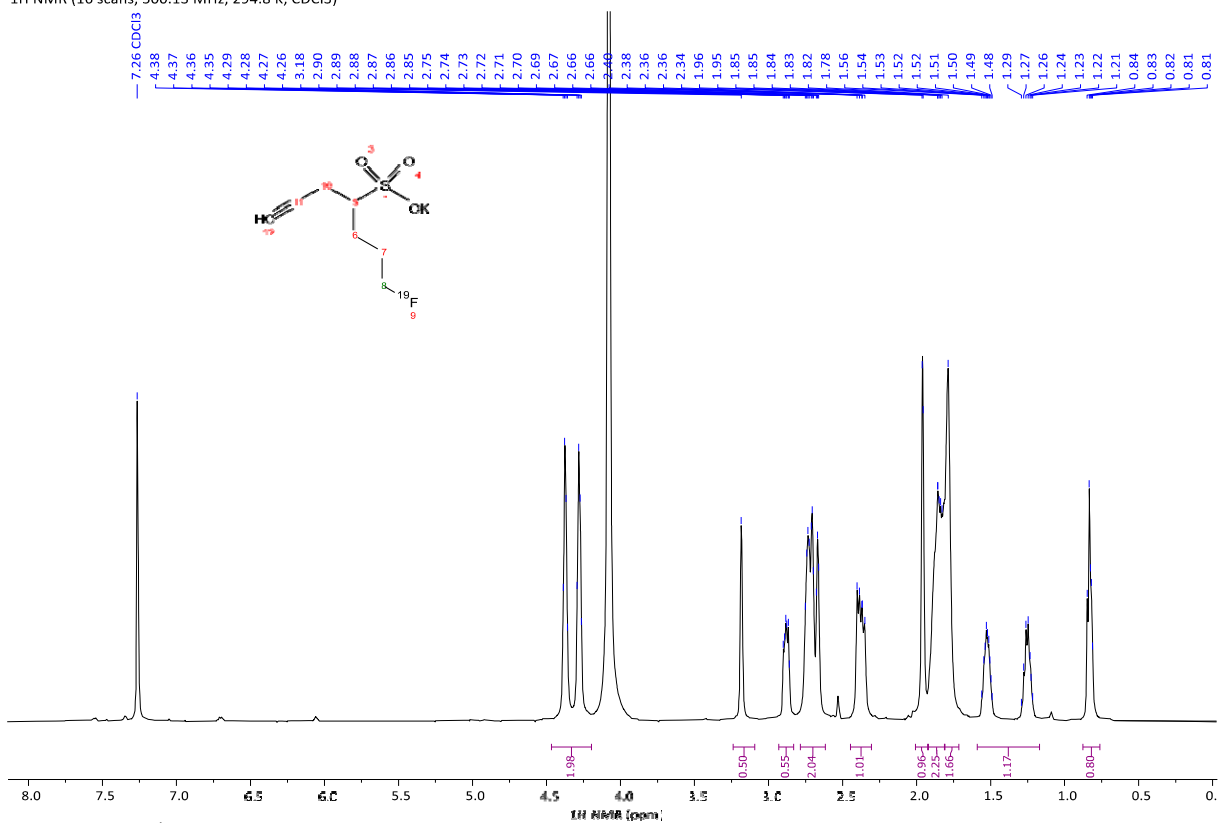


Figure S4. ¹H NMR spectrum of compound **4**.

¹³C NMR (176 scans, 124 °F, 400 MHz, 295.3 K, CDCl₃)

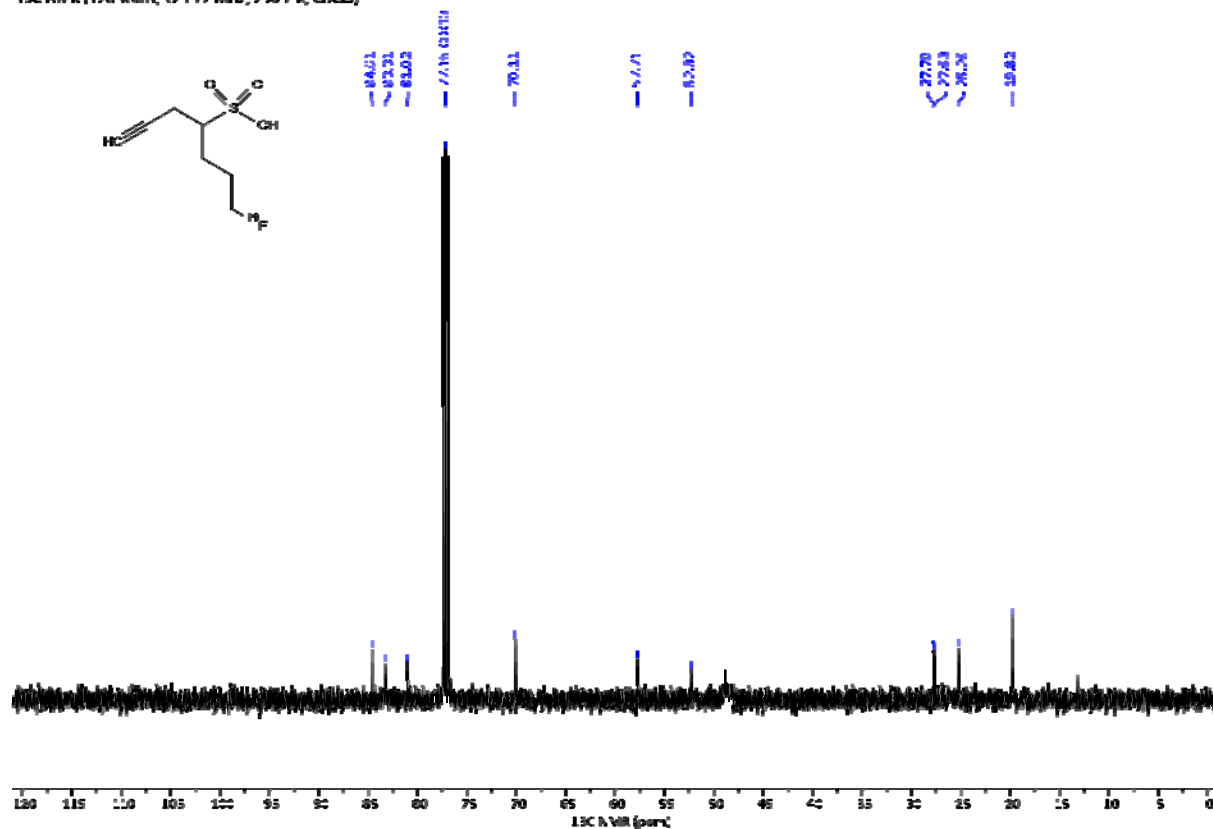


Figure S5. ¹³C NMR spectrum of compound 4.

¹⁹F NMR (64 scans, 470.54 MHz, 295.3 K, CDCl₃)

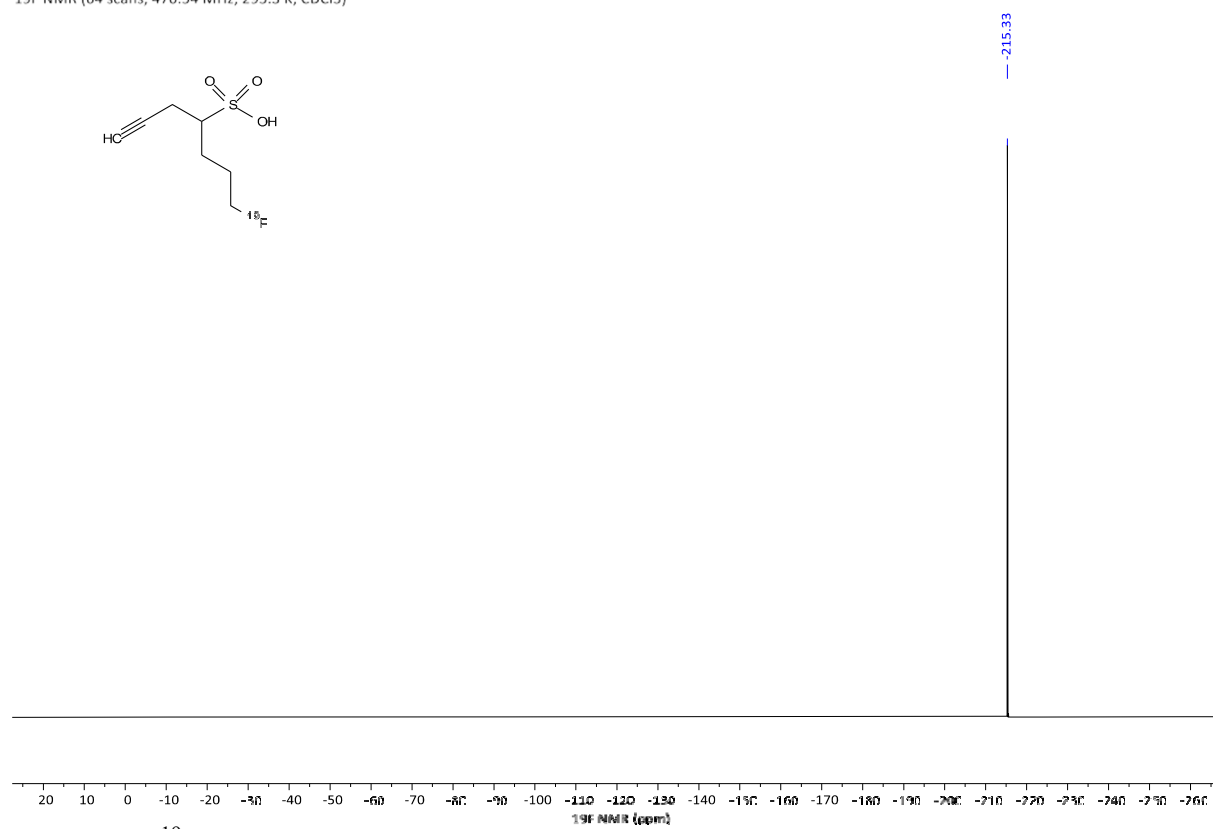


Figure S6. ¹⁹F NMR spectrum of compound 4.

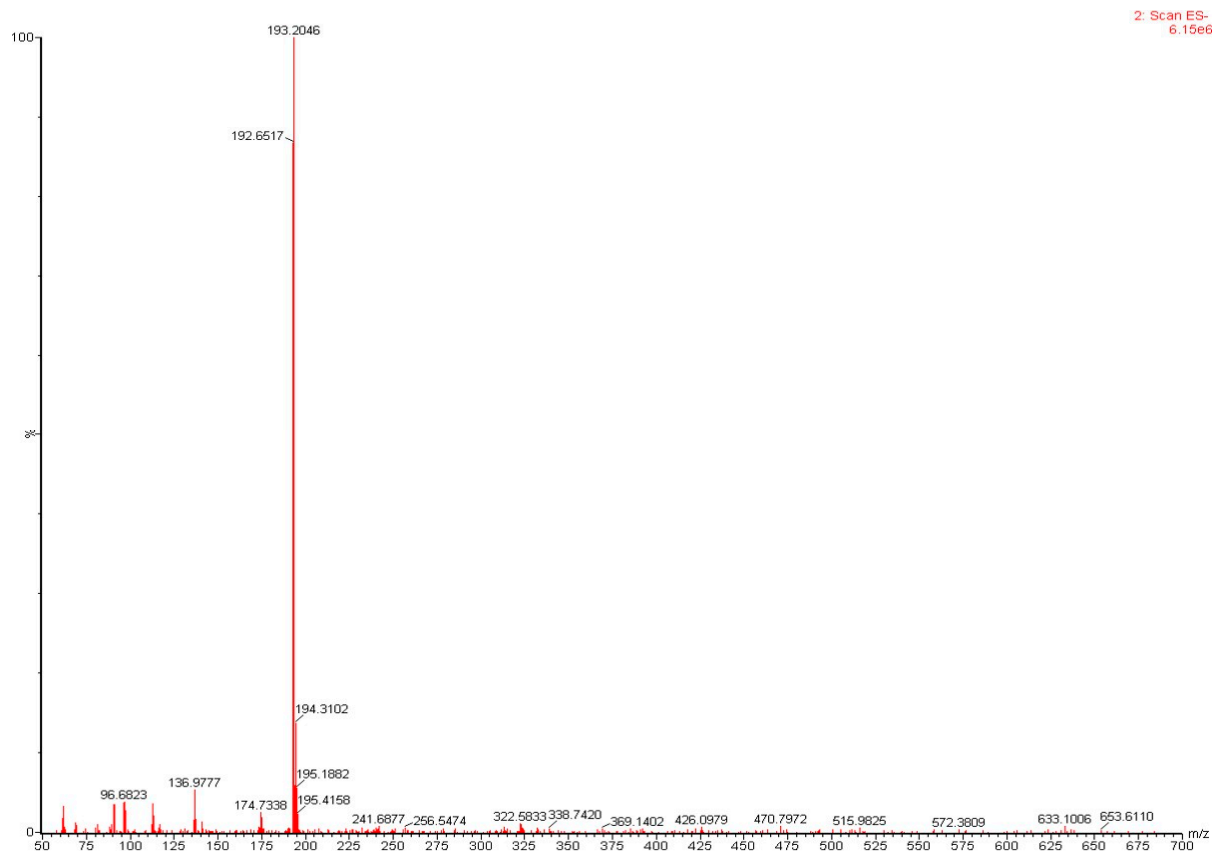


Figure S7. MS and HRMS analysis of compound **4**.

¹H NMR (16 scans, 500.13 MHz, 294.2 K, CDCl₃)

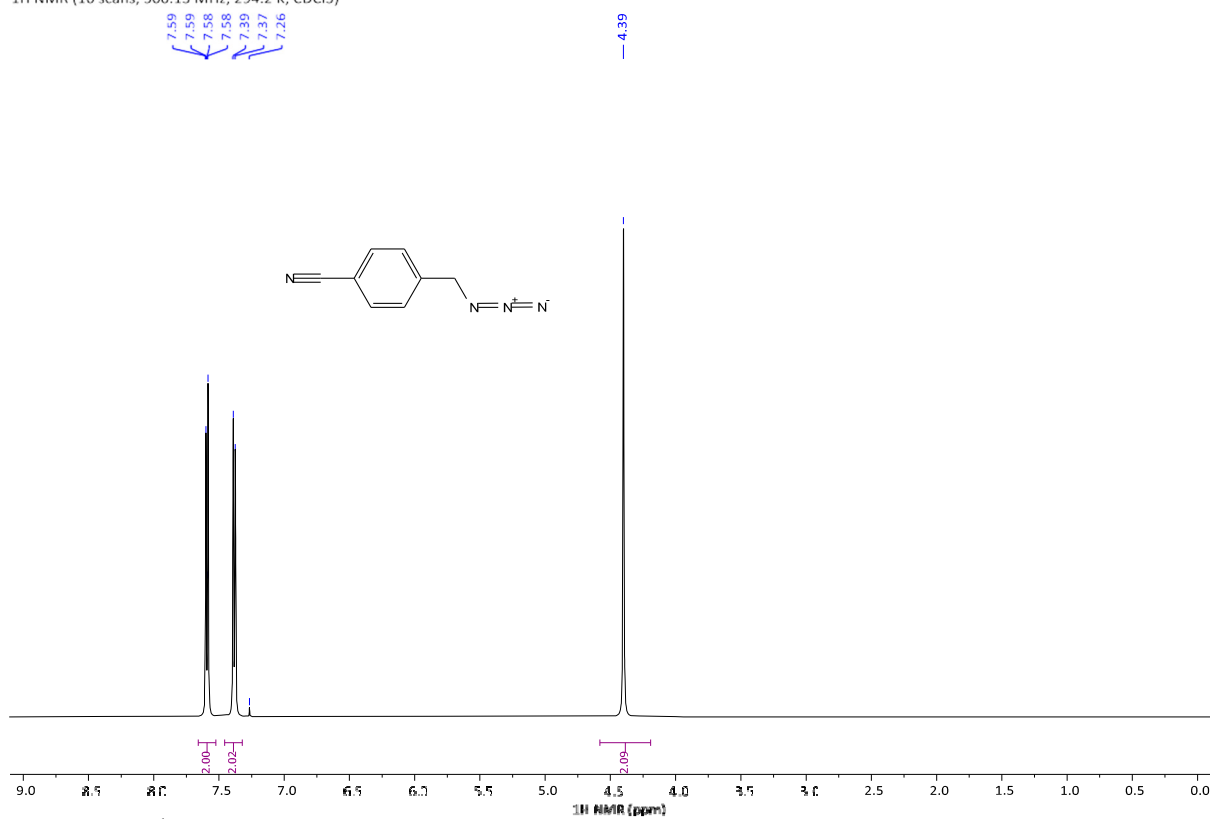


Figure S8. ¹H NMR spectrum of compound **6**.

¹³C NMR (128 scans, 125.76 MHz, 295.7 K, CDCl₃)

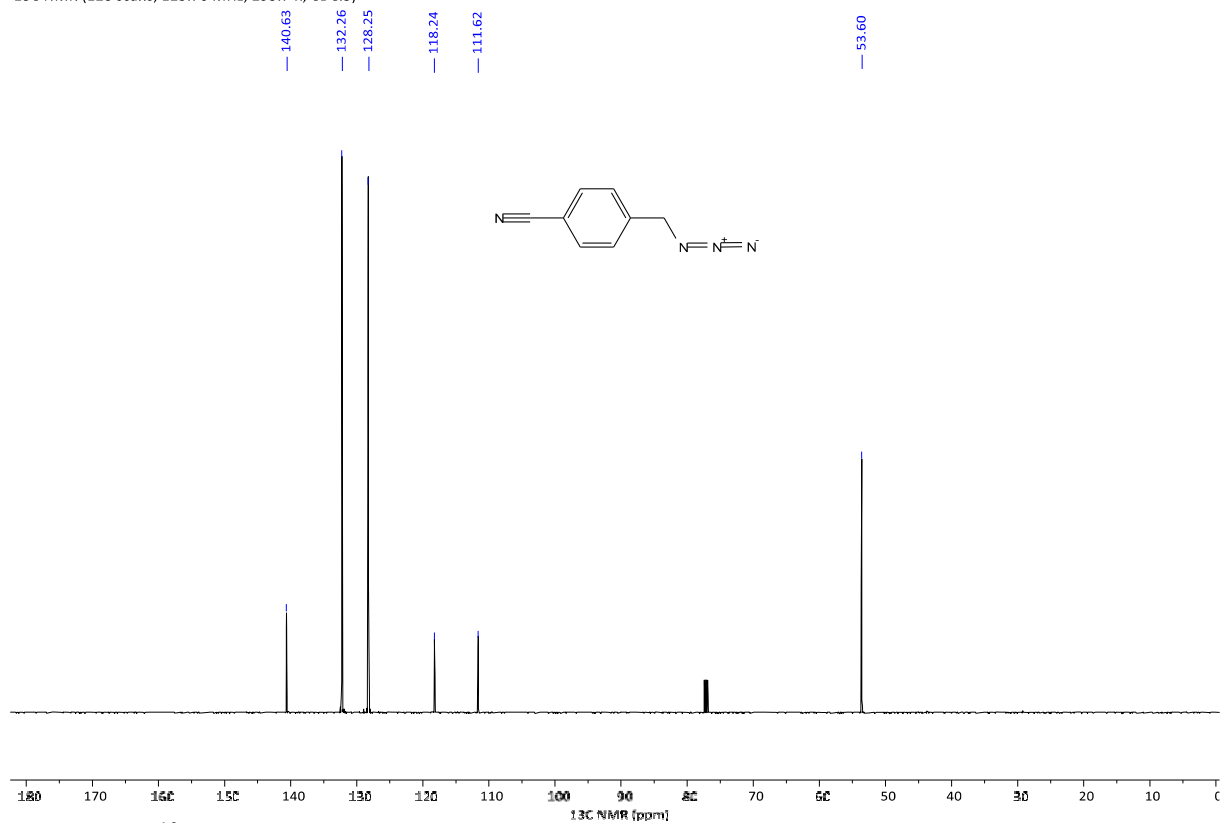
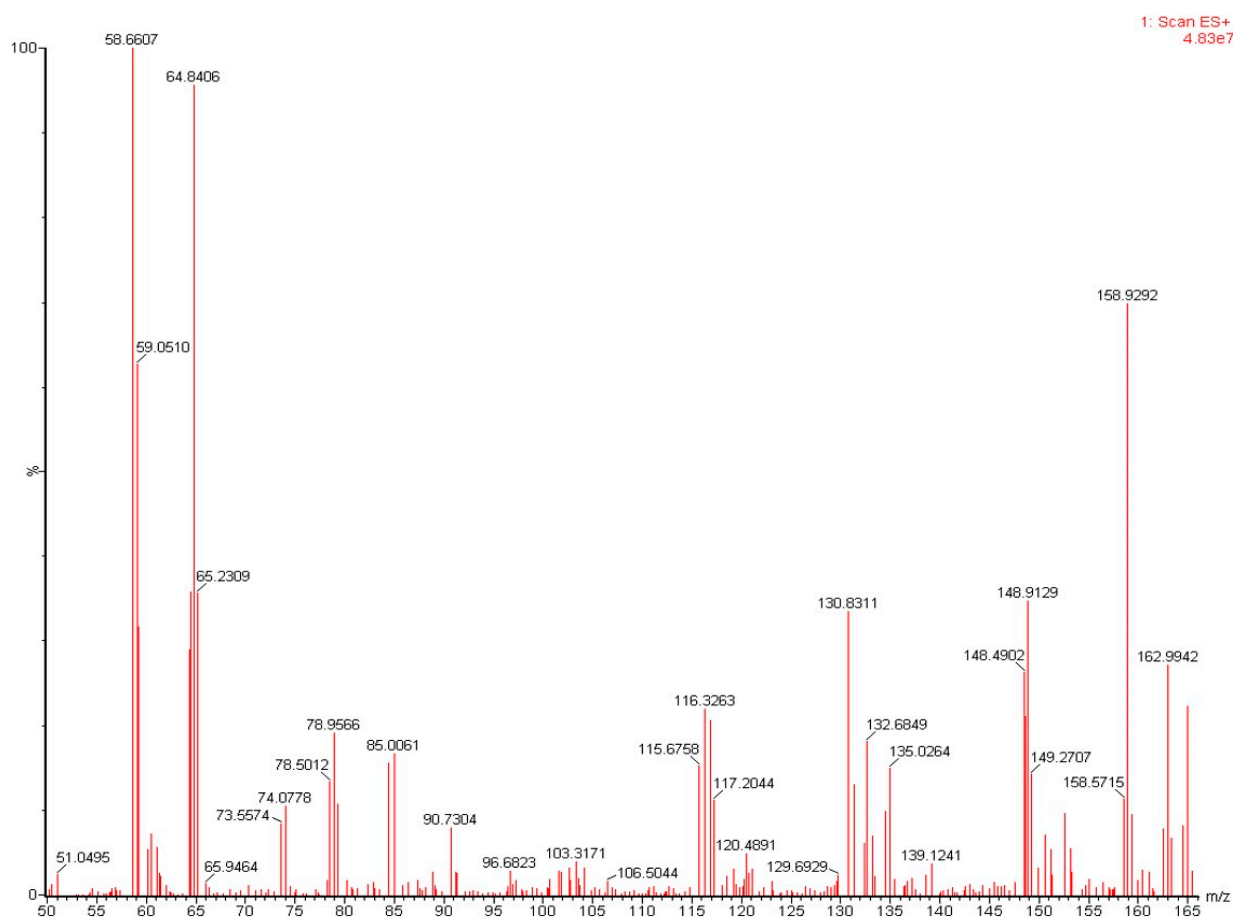


Figure S9. ¹³C NMR spectrum of compound 6.



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
158.9929	159.0671	-74.2	-466.7	7.5	100.0	13.900	0.00	C ₈ H ₇ N ₄

Figure S10. MS and HRMS analysis of compound 6.

¹H NMR (16 scans, 500.13 MHz, 293.8 K, CDCl₃)

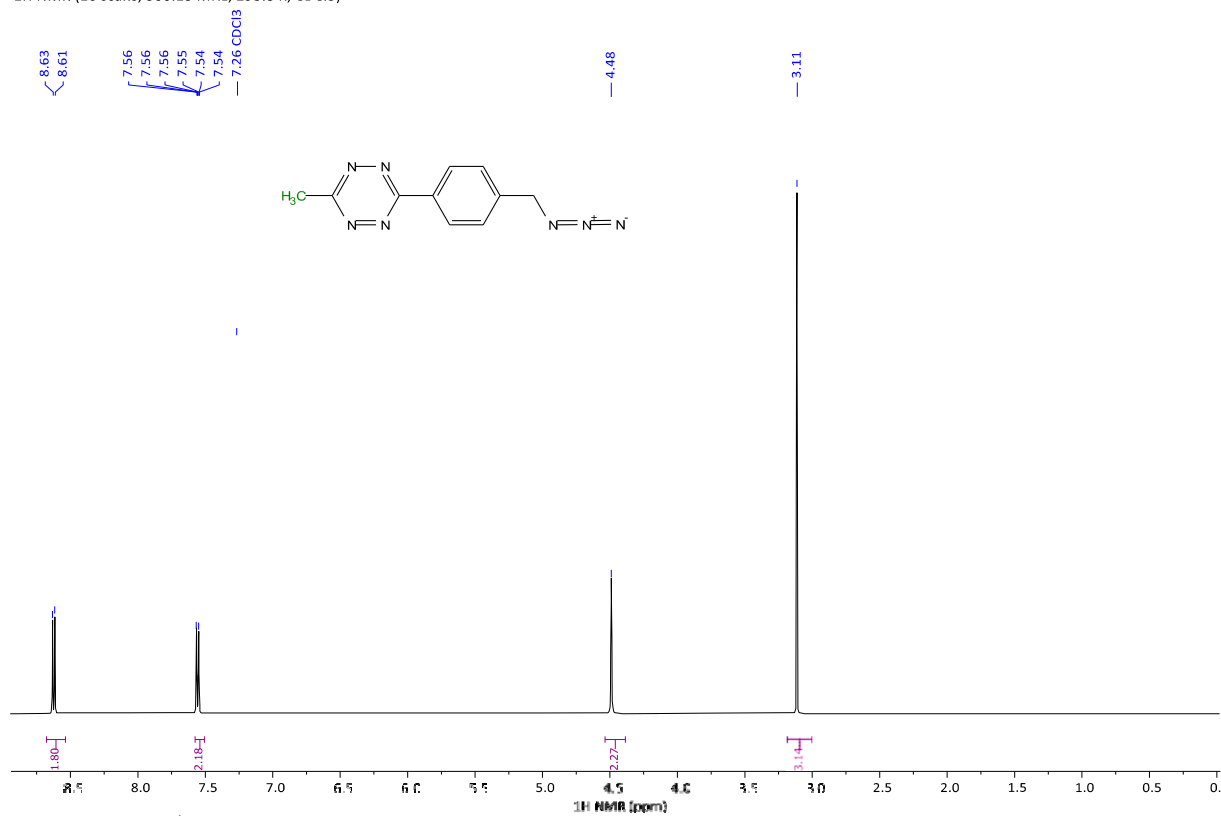


Figure S11. ¹H NMR spectrum of compound 7.

¹³C NMR (1024 scans, 125.77 MHz, 295.8 K, CDCl₃)

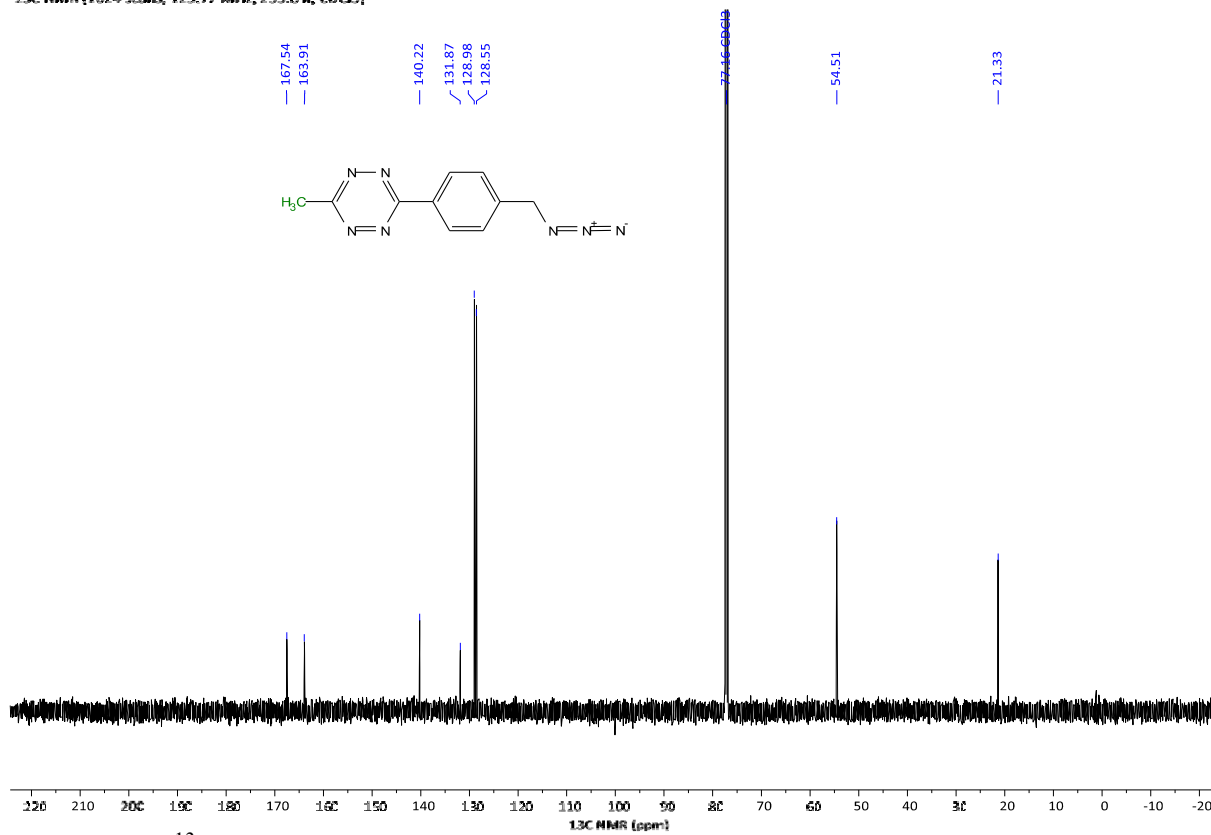


Figure S12. ¹³C NMR spectrum of compound 7.

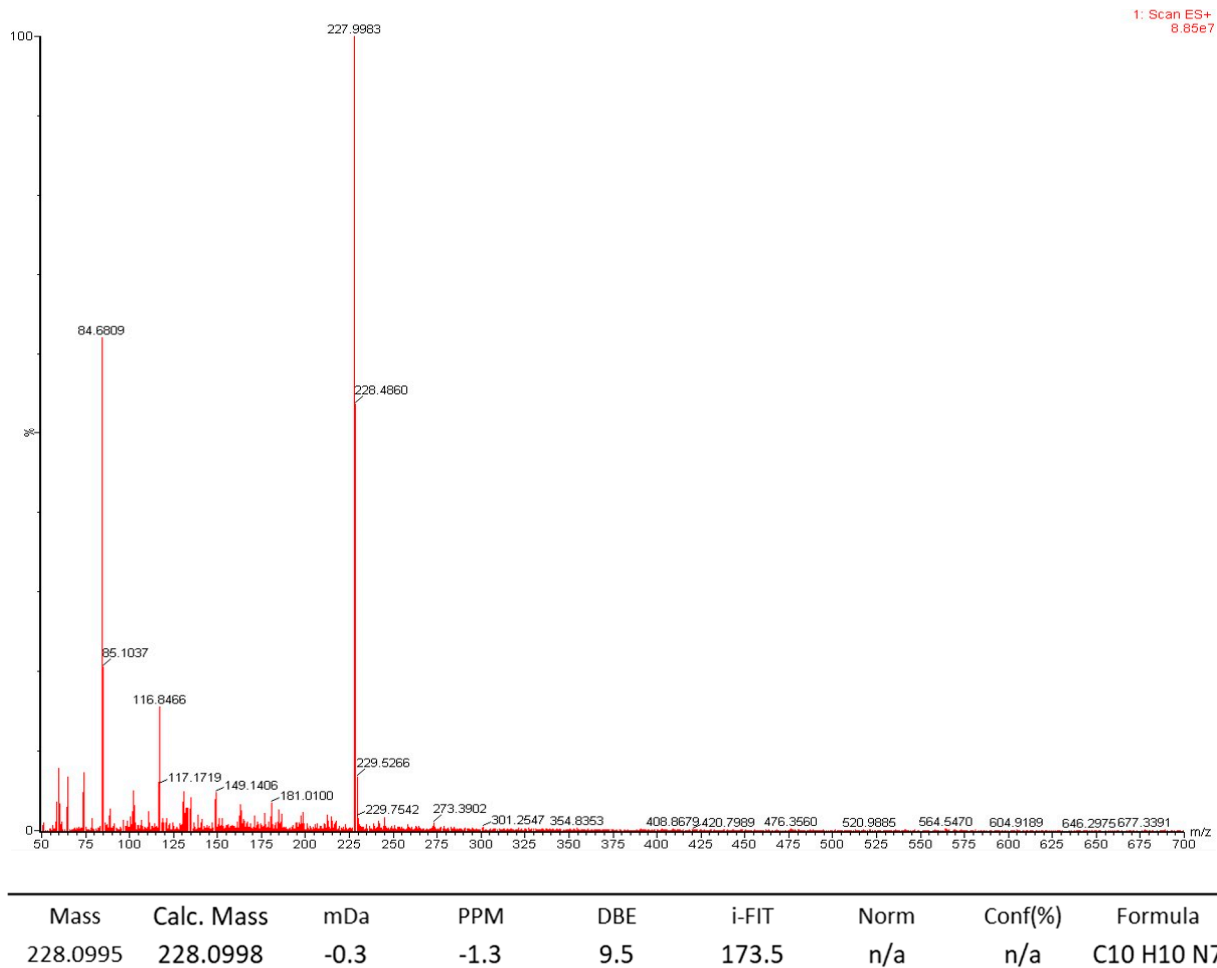


Figure S13. MS and HRMS analysis of compound 7.

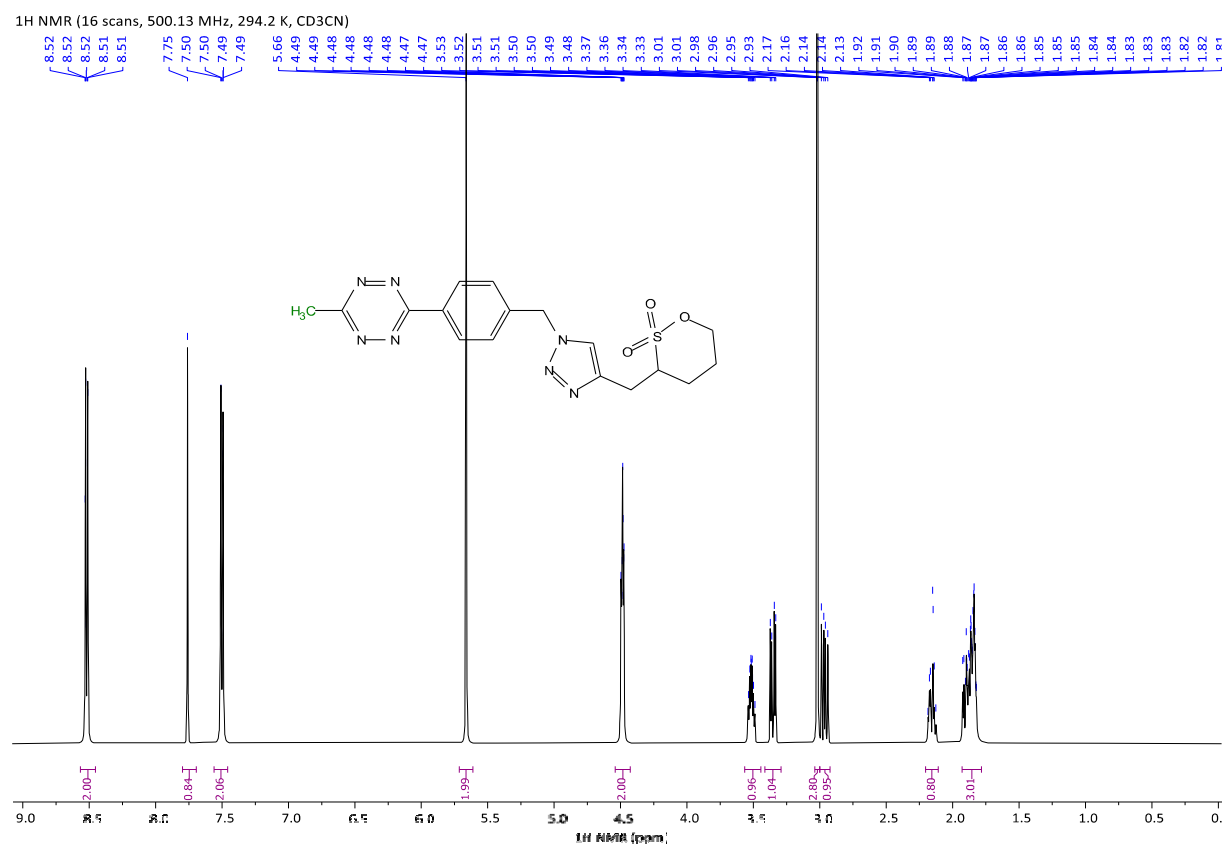


Figure S14. ¹H NMR spectrum of compound 8.

¹³C NMR (1024 scans, 125.76 MHz, 295.2 K, CDCl₃)

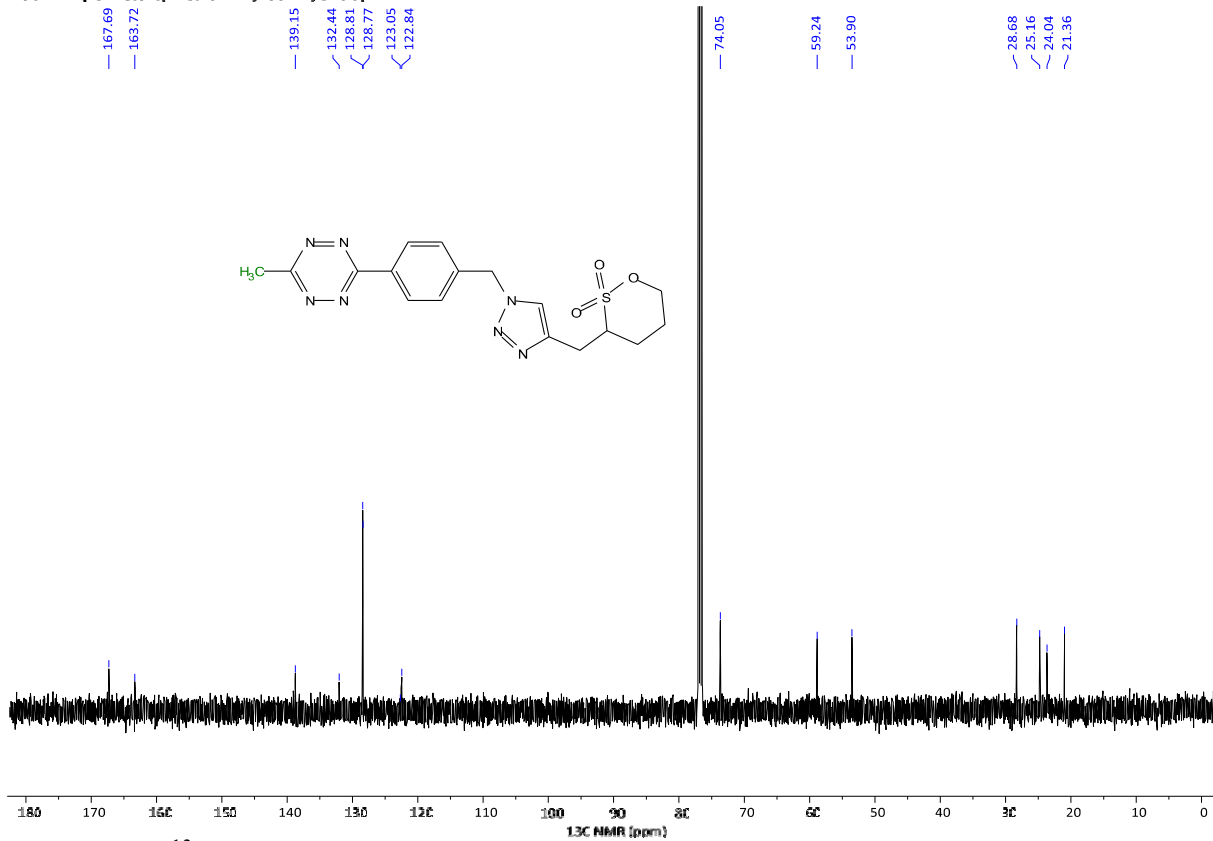
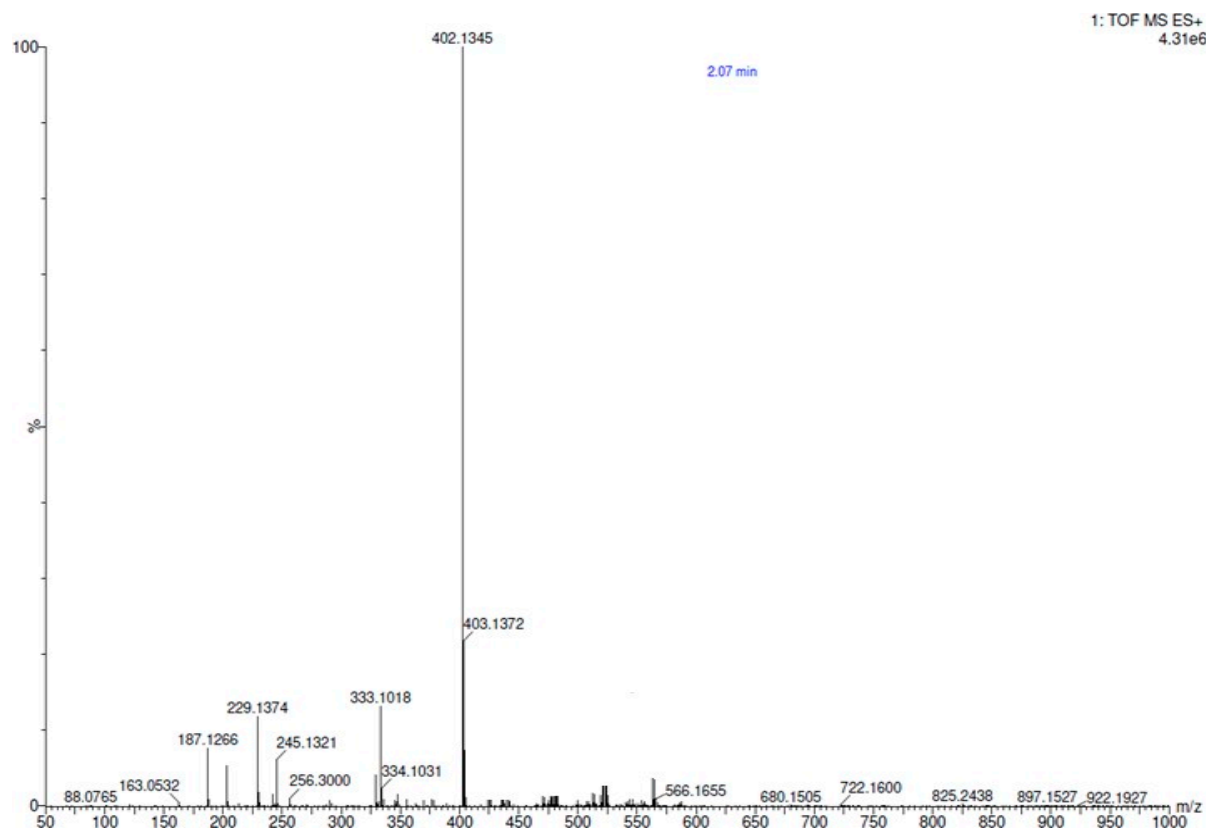
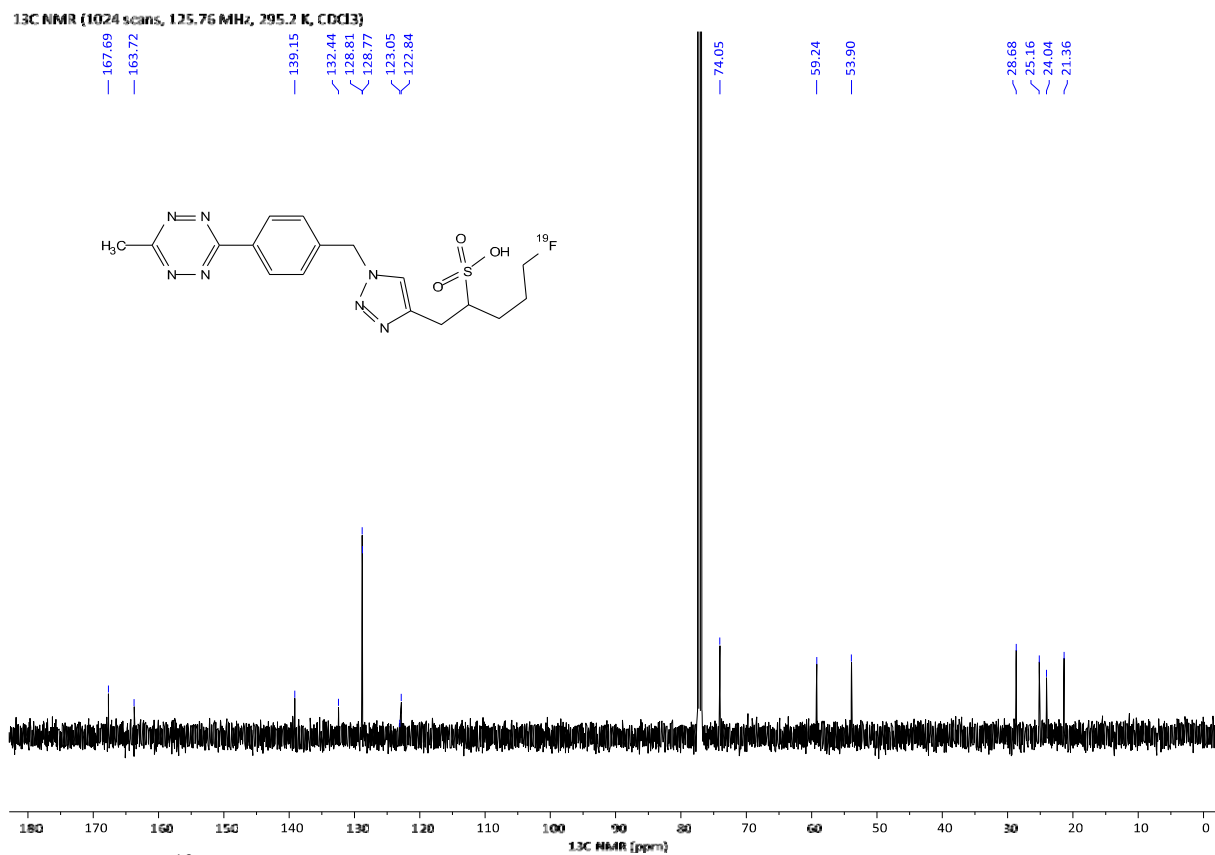
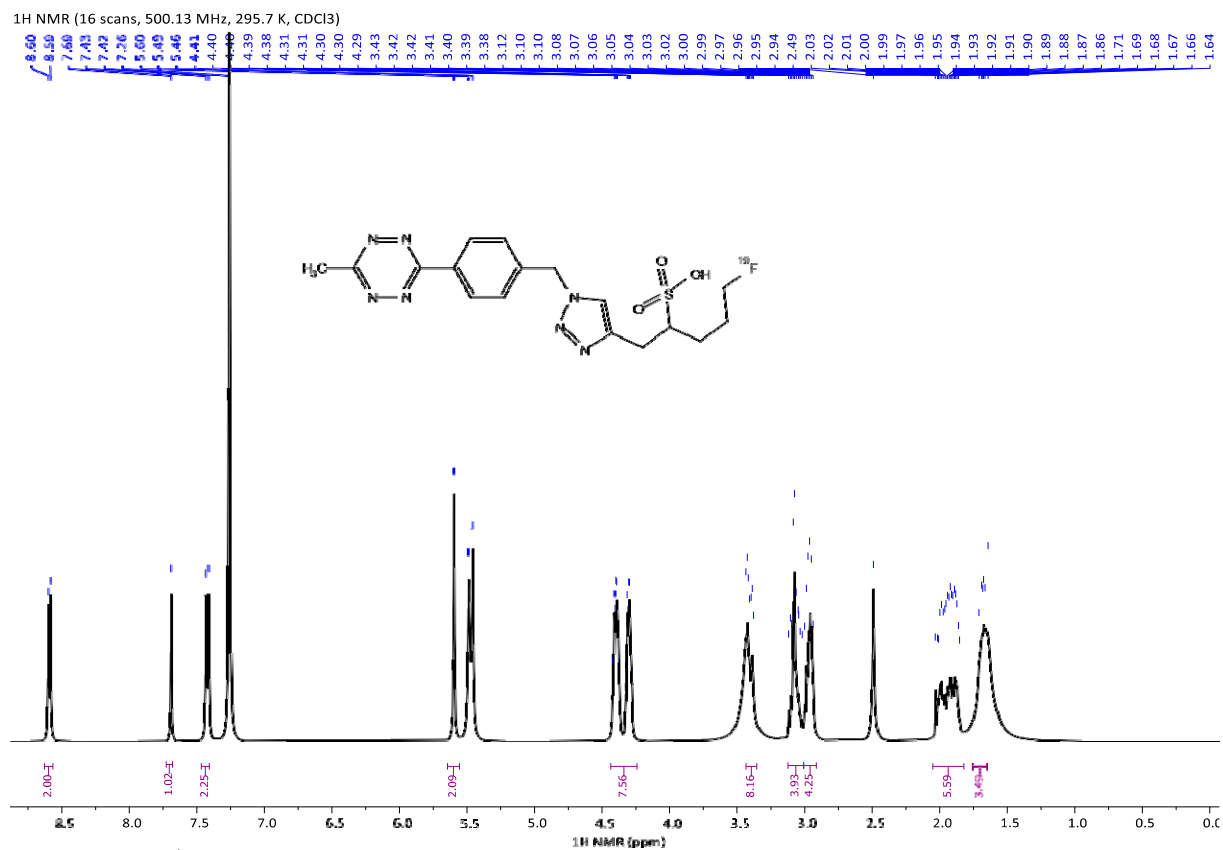


Figure S15. ¹³C NMR spectrum of compound 8.



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
402.1345	402.1348	-0.3	-0.7	11.5	220.8	n/a	n/a	C17 H20 N7 O3 S

Figure S16. MS and HRMS analysis of compound 8.



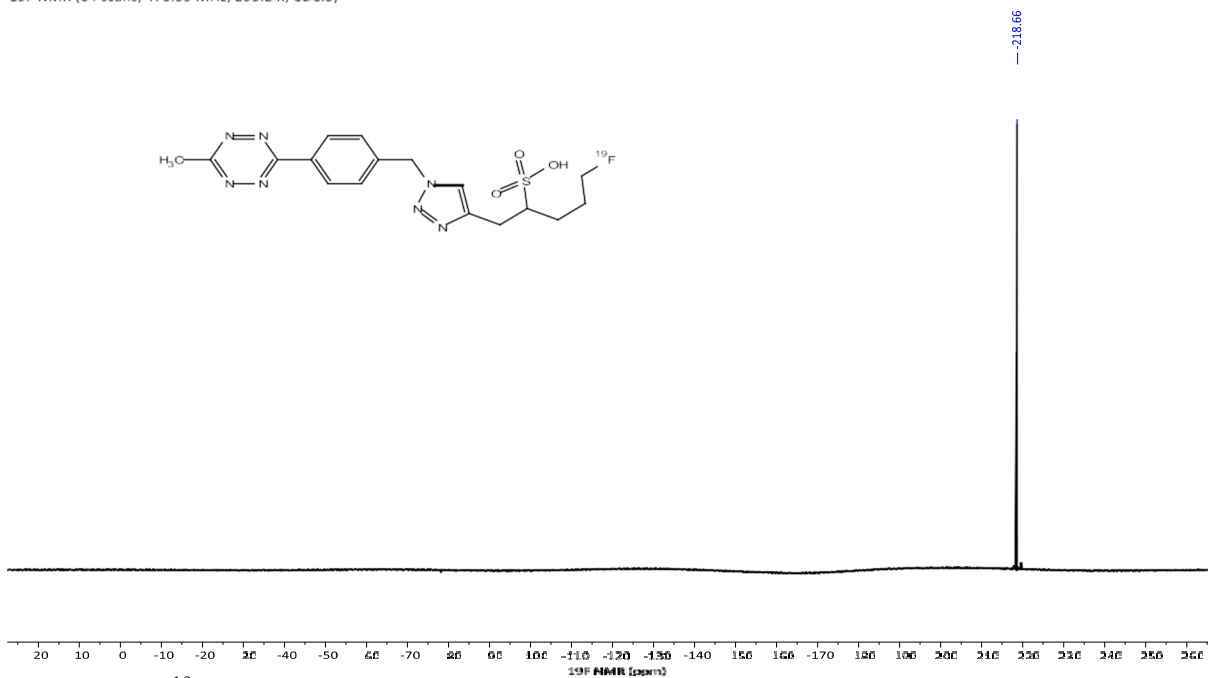


Figure S19. ¹⁹F NMR spectrum of compound 1.

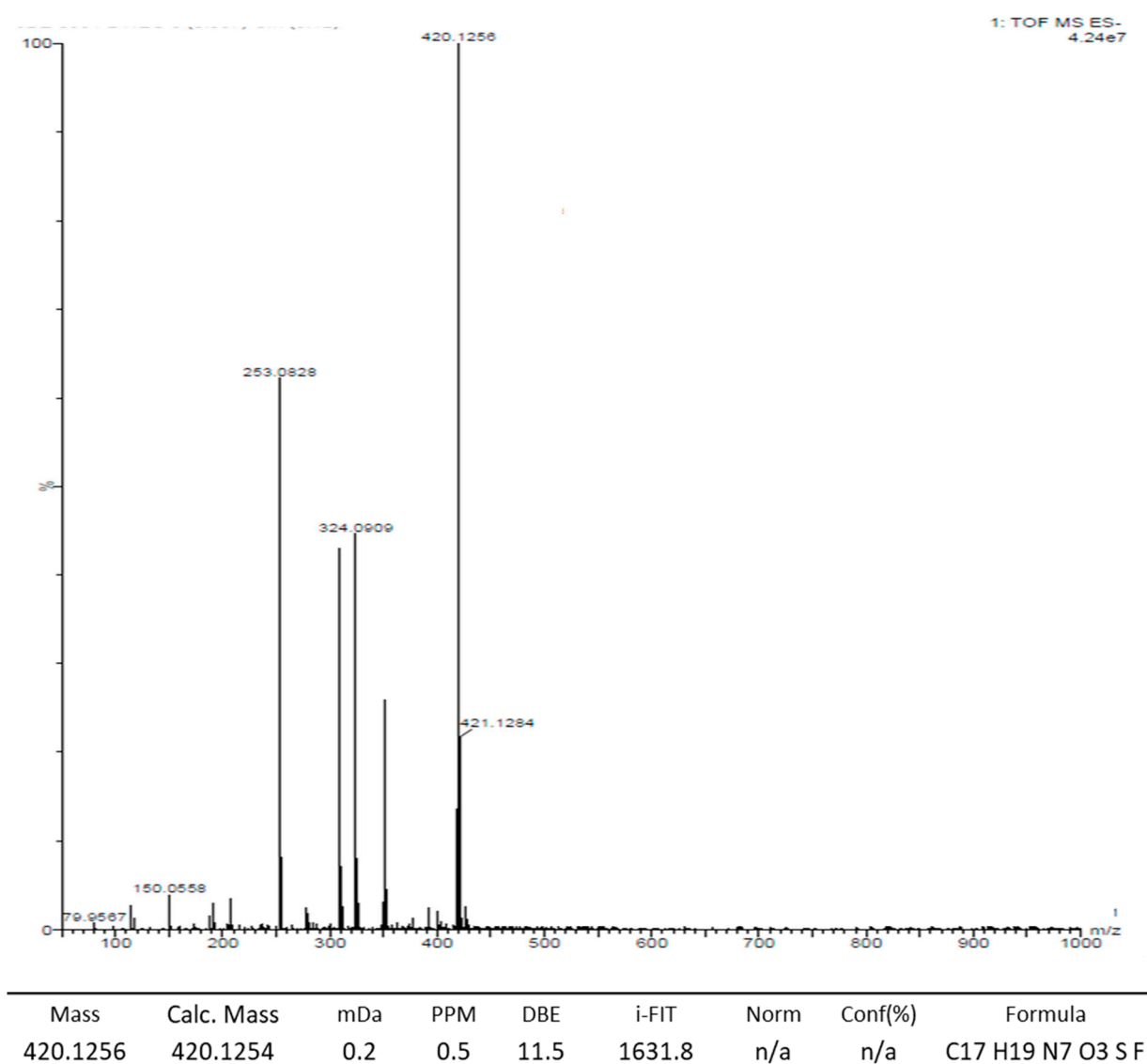


Figure S20. MS and HRMS analysis of compound 1.

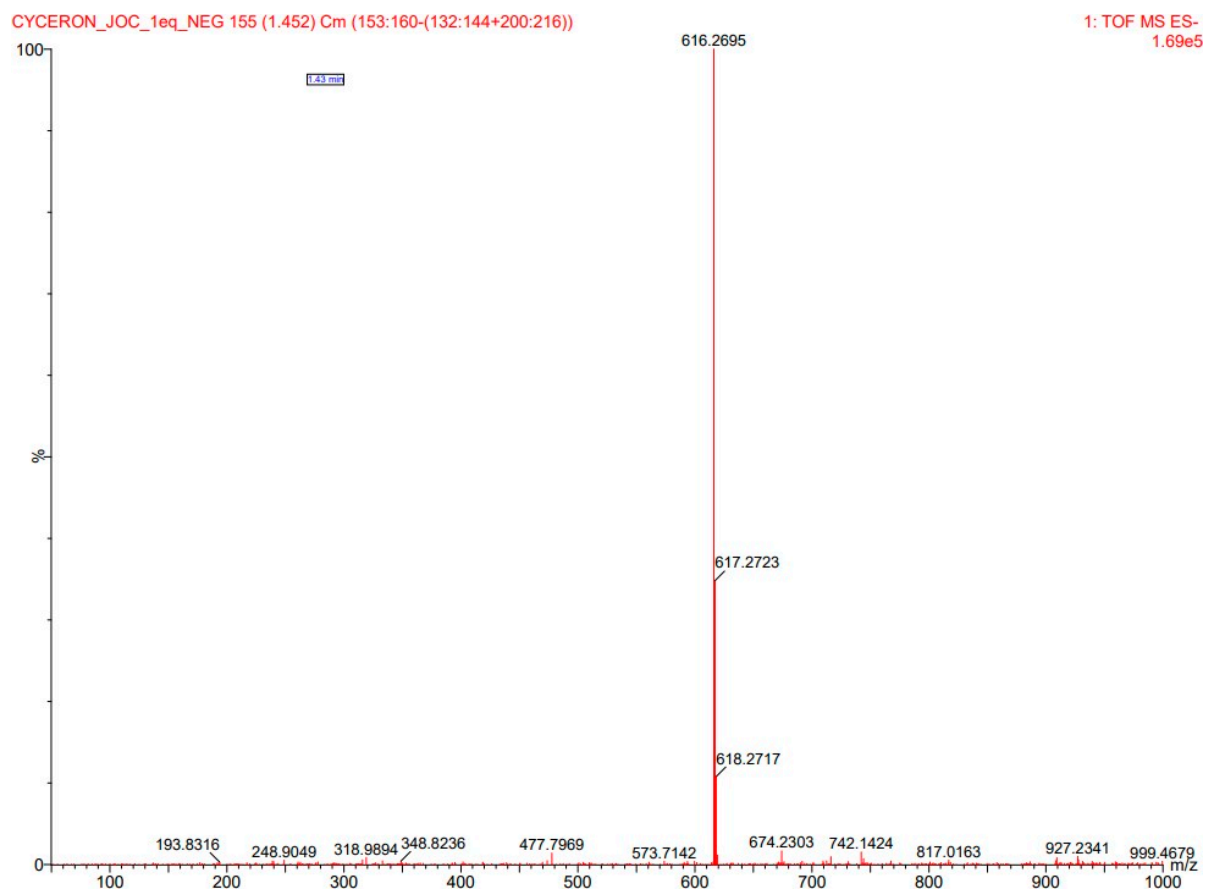


Figure S21. MS analysis of compound **10**.

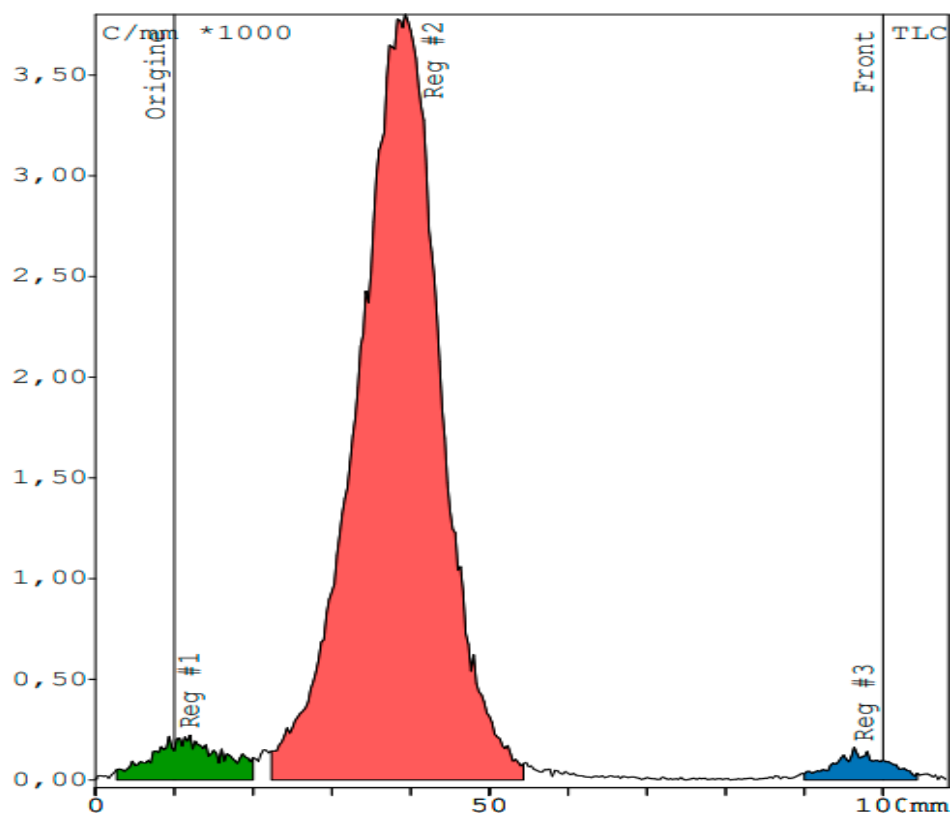


Figure S22. RadioTLC analysis of crude compound $[^{18}\text{F}]\mathbf{4}$ obtained by radiofluorination of **3**.

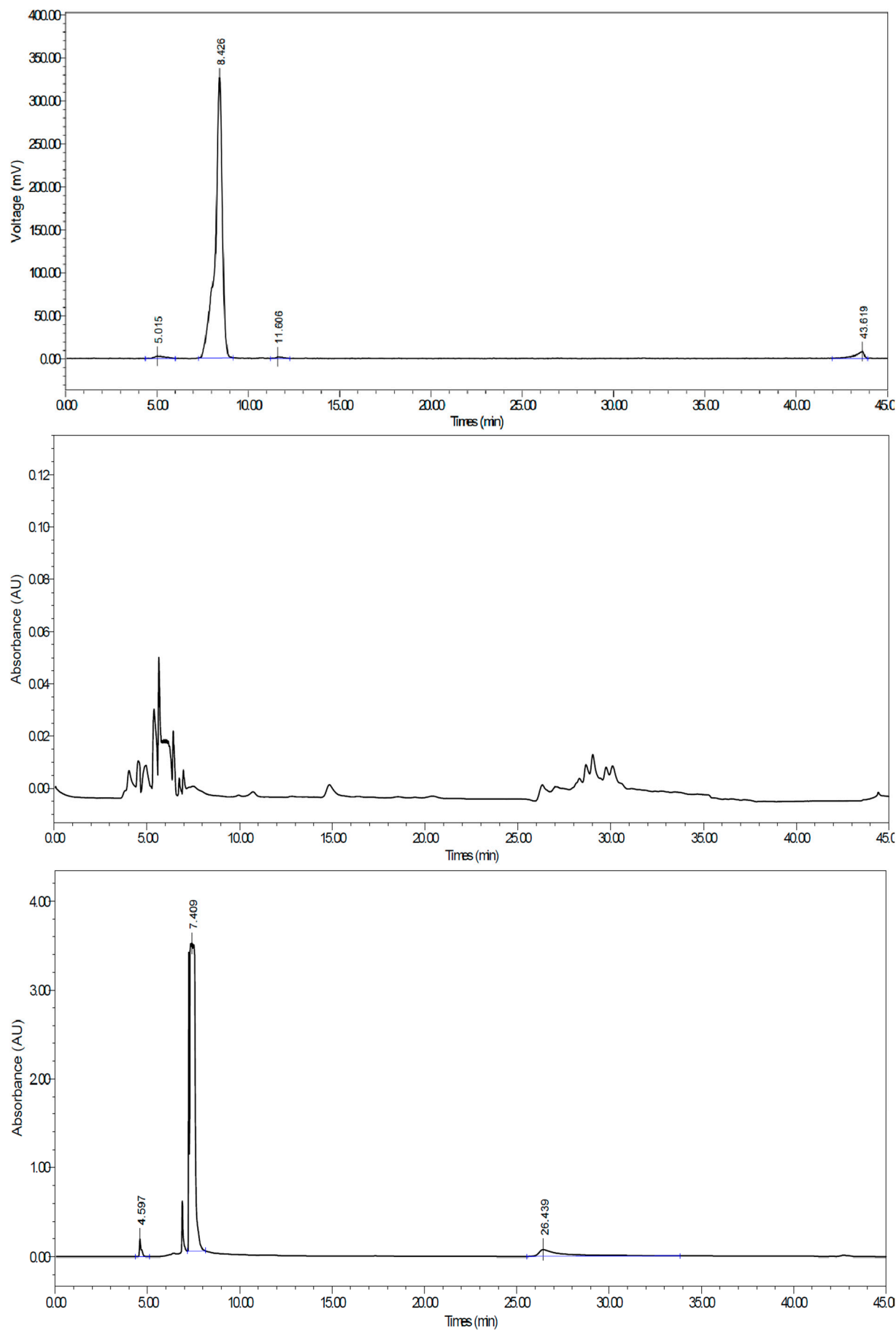


Figure S23. HPLC analysis of crude compound $[^{18}\text{F}]\mathbf{4}$ obtained by radiofluorination of **3**. Top) Gamma detection, Middle) UV detection at 254 nm ; Down) UV Chromatogram of the non radioactive reference compound **4**.