ELECTRONIC SUPPORTING INFORMATION (ESI)

Synthesis and properties of L-valine based chiral long alkyl chain appended 1,2,3-triazolium ionic liquids†

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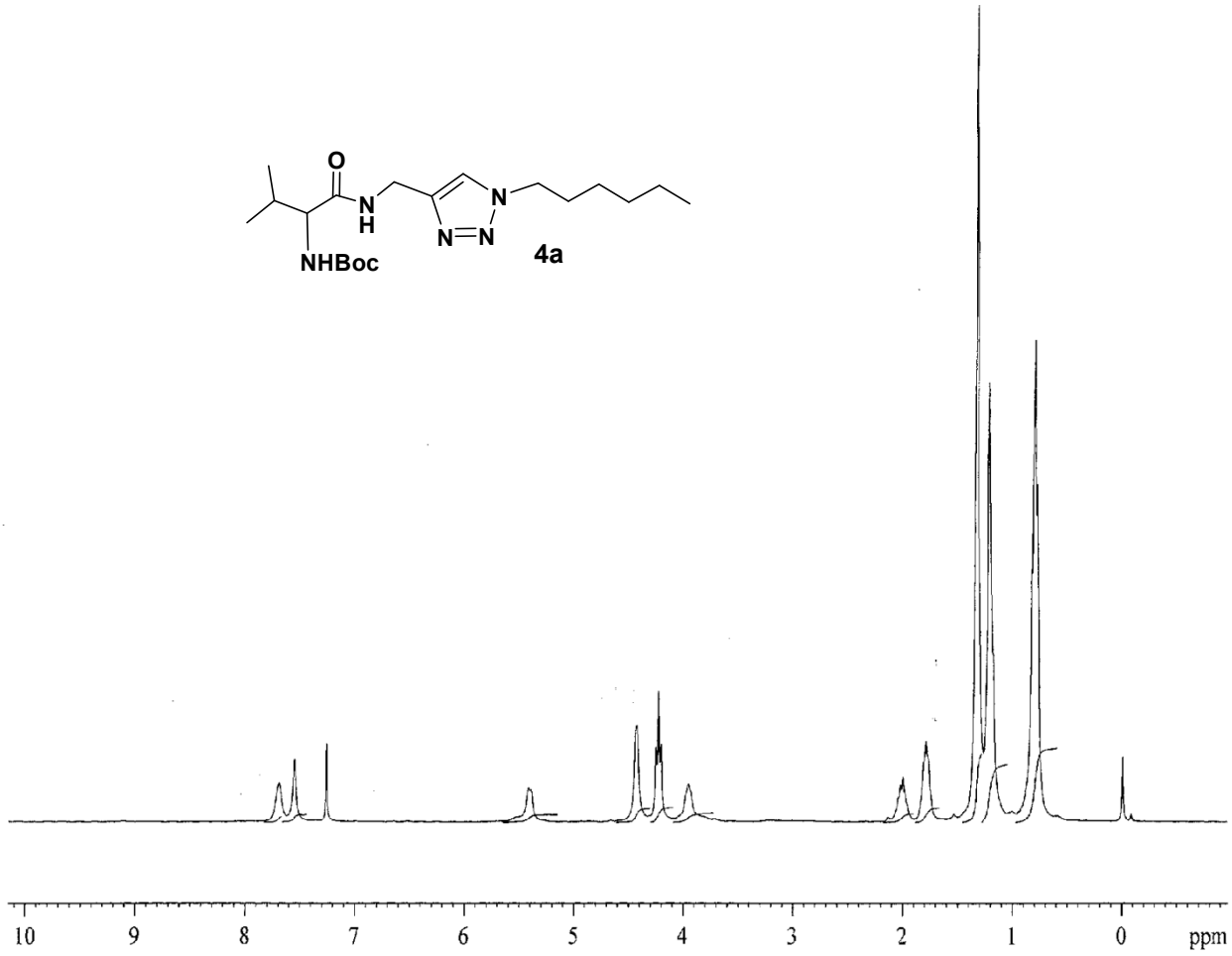


Figure S1. ^{1}H NMR Spectrum of **4a** ($CDCl_3$).

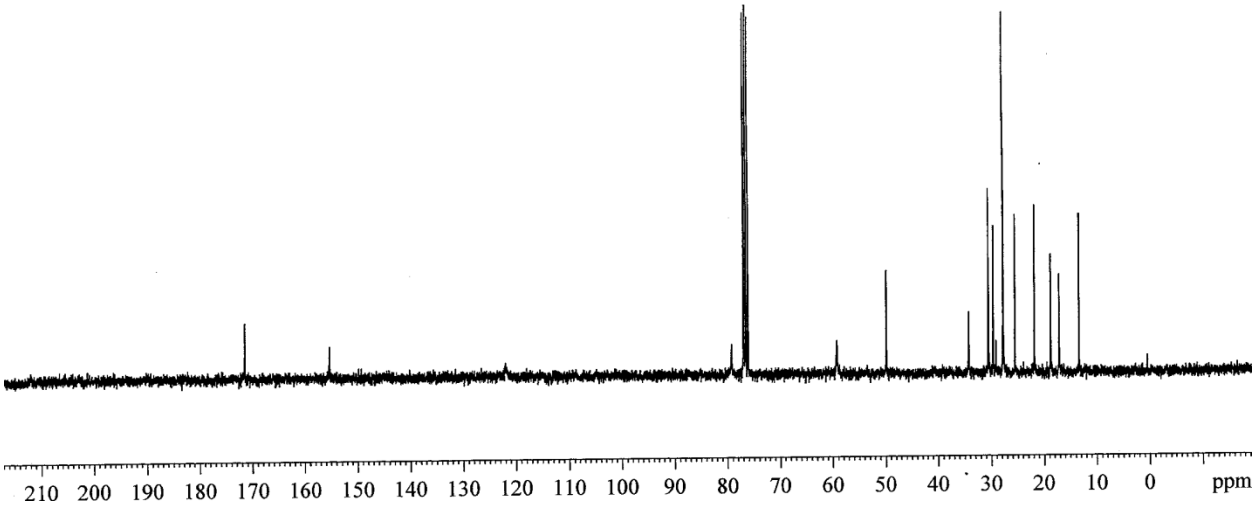
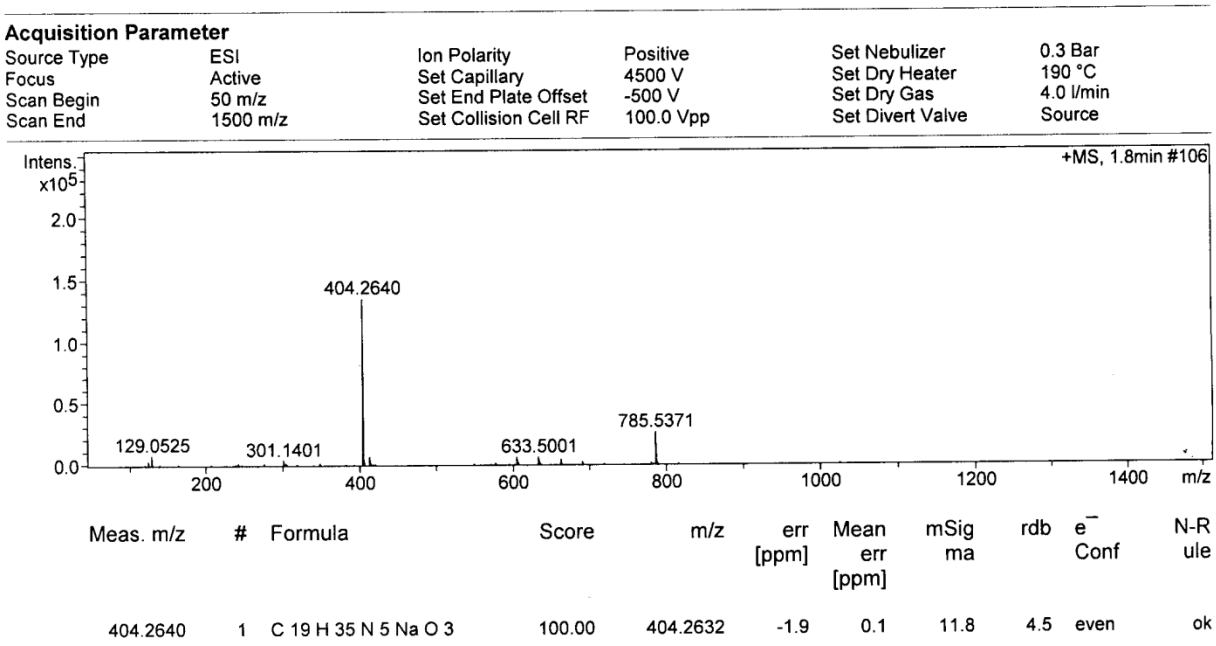


Figure S2. ^{13}C NMR Spectrum of **4a (**$CDCl_3$).



Meas. m/z	#	Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSig ma	rdb	e⁻ Conf	N-R ule
404.2640	1	C 19 H 35 N 5 Na O 3	100.00	404.2632	-1.9	0.1	11.8	4.5	even	ok

Figure S3. Mass Spectrum of **4a**.

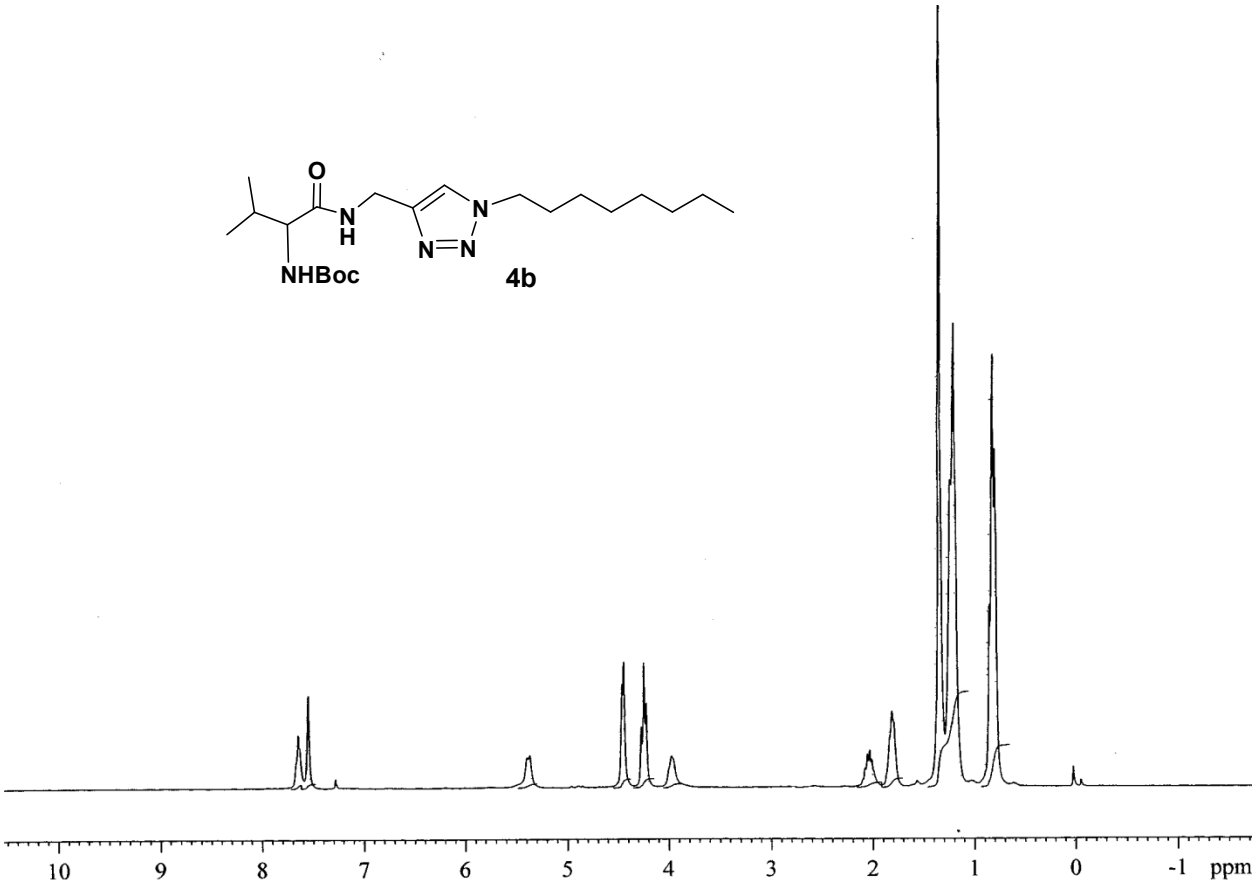


Figure S4. ^{1}H NMR Spectrum of **4b** ($CDCl_3$).

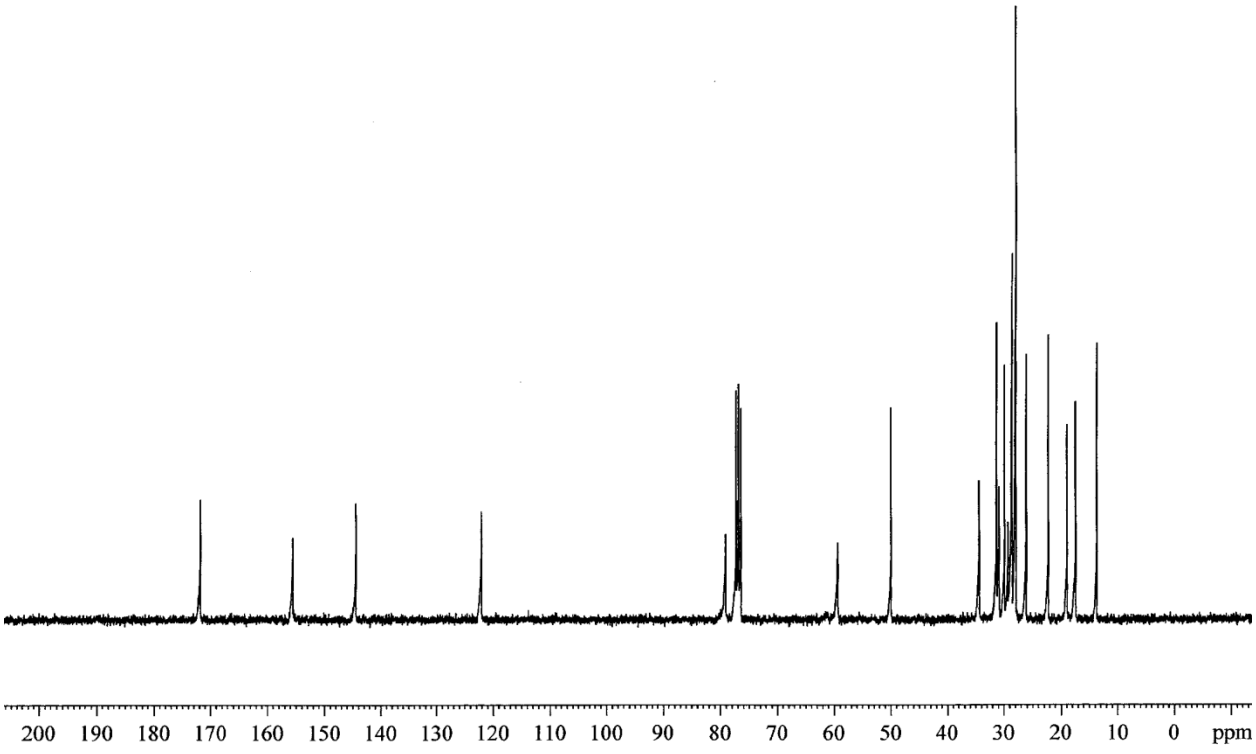
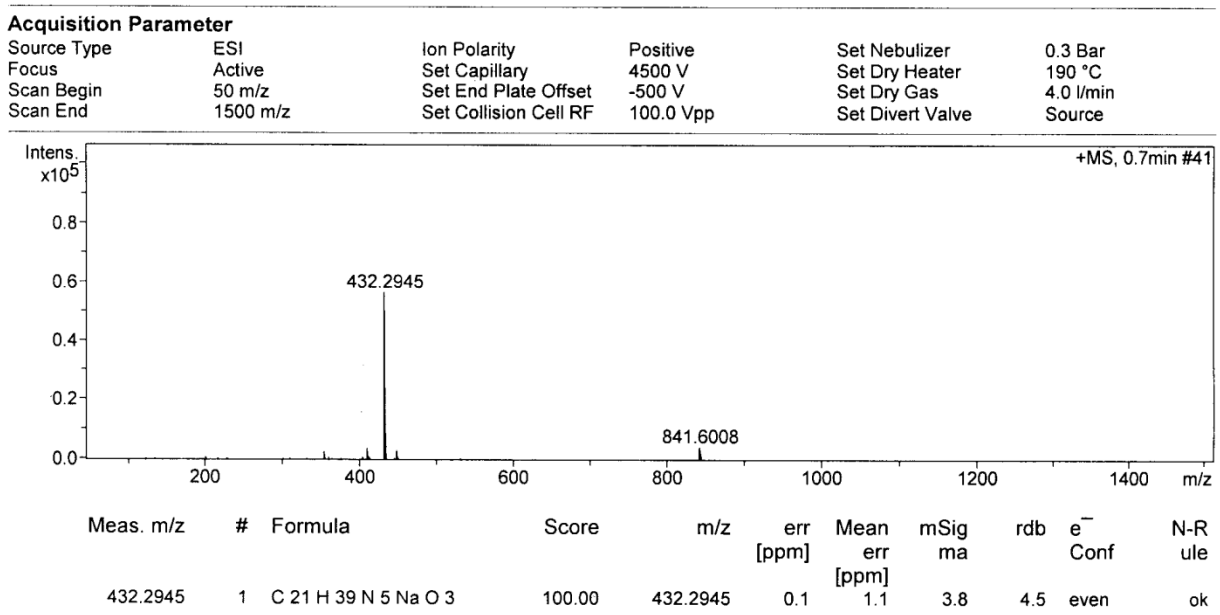


Figure S5. ^{13}C NMR Spectrum of **4b** ($CDCl_3$).



Meas. m/z	#	Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSig ma	rdb	e⁻ Conf	N-R ule
432.2945	1	C 21 H 39 N 5 Na O 3	100.00	432.2945	0.1	1.1	3.8	4.5	even	ok

Figure S6. Mass Spectrum of **4b**.

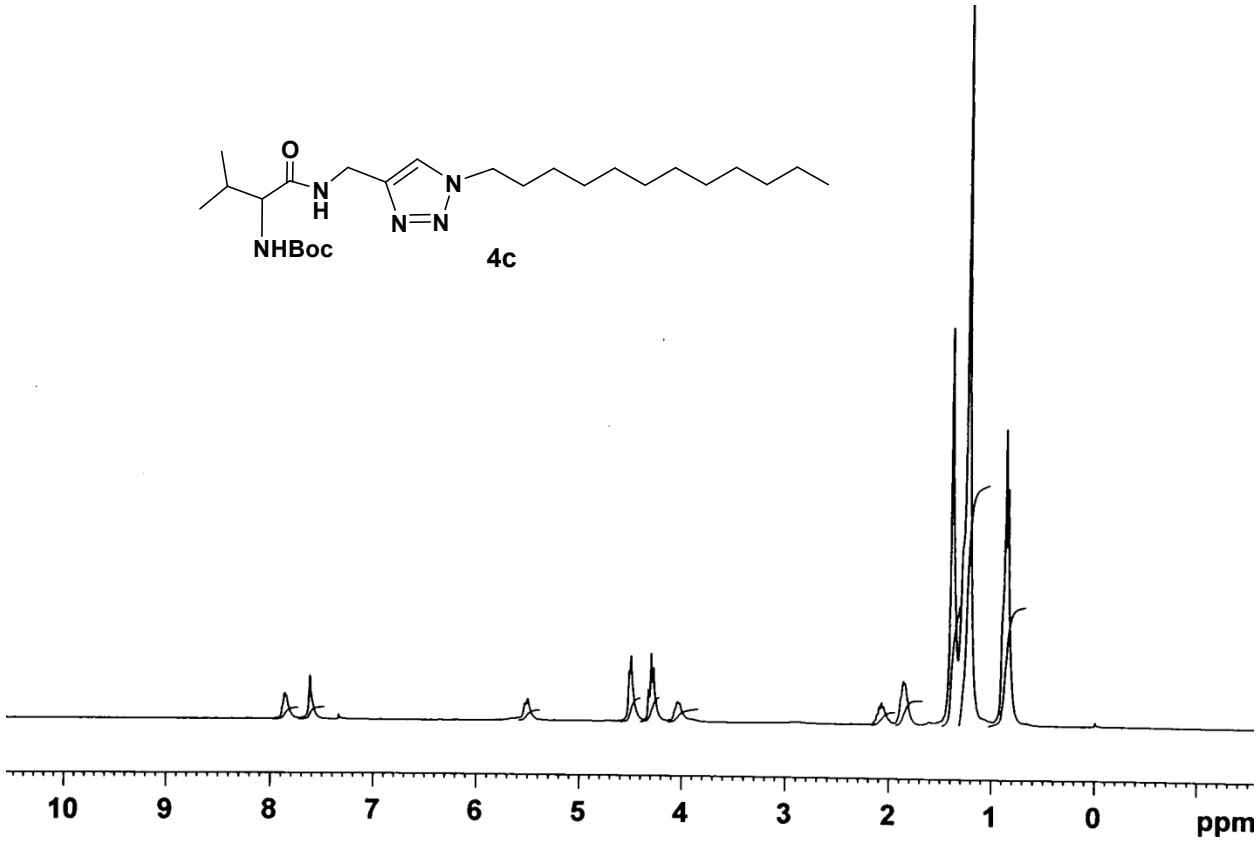


Figure S7. ^{1}H NMR Spectrum of **4c** ($CDCl_3$).

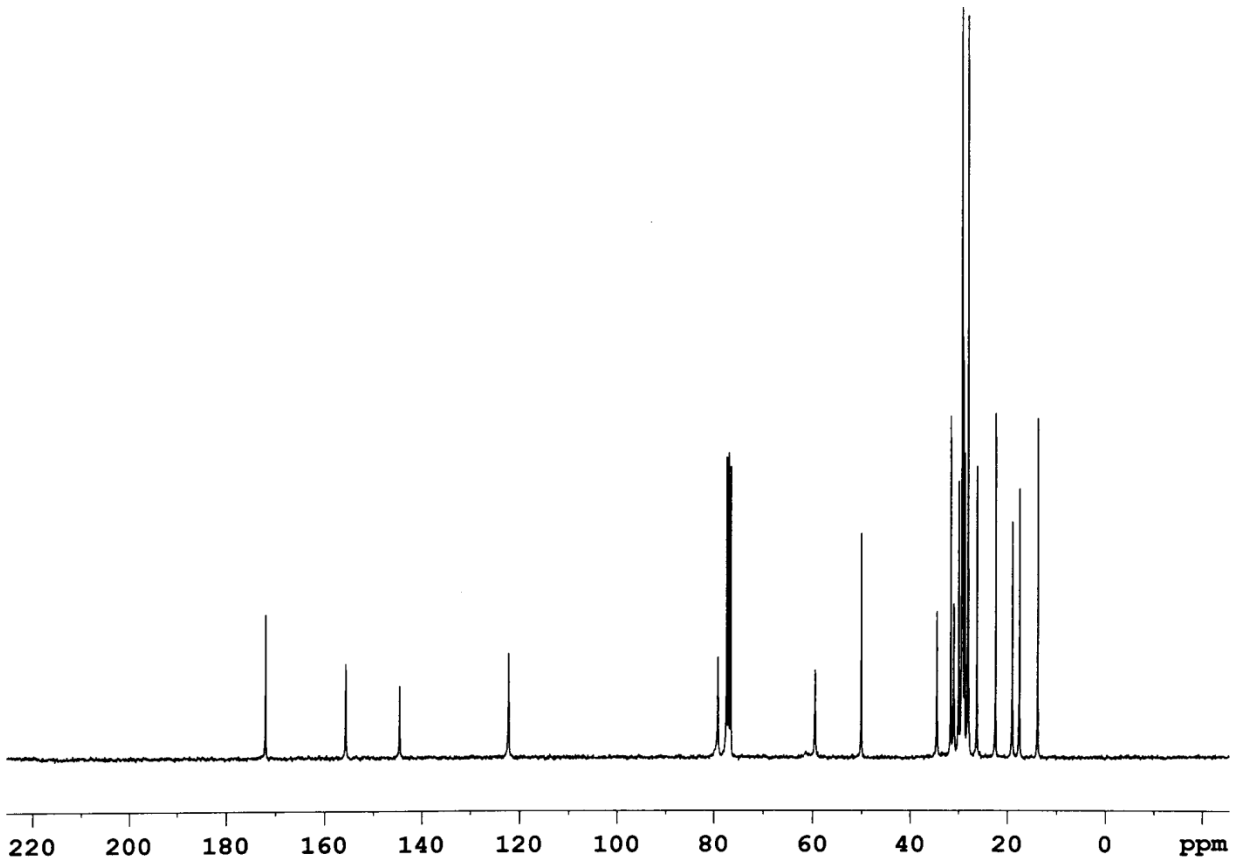
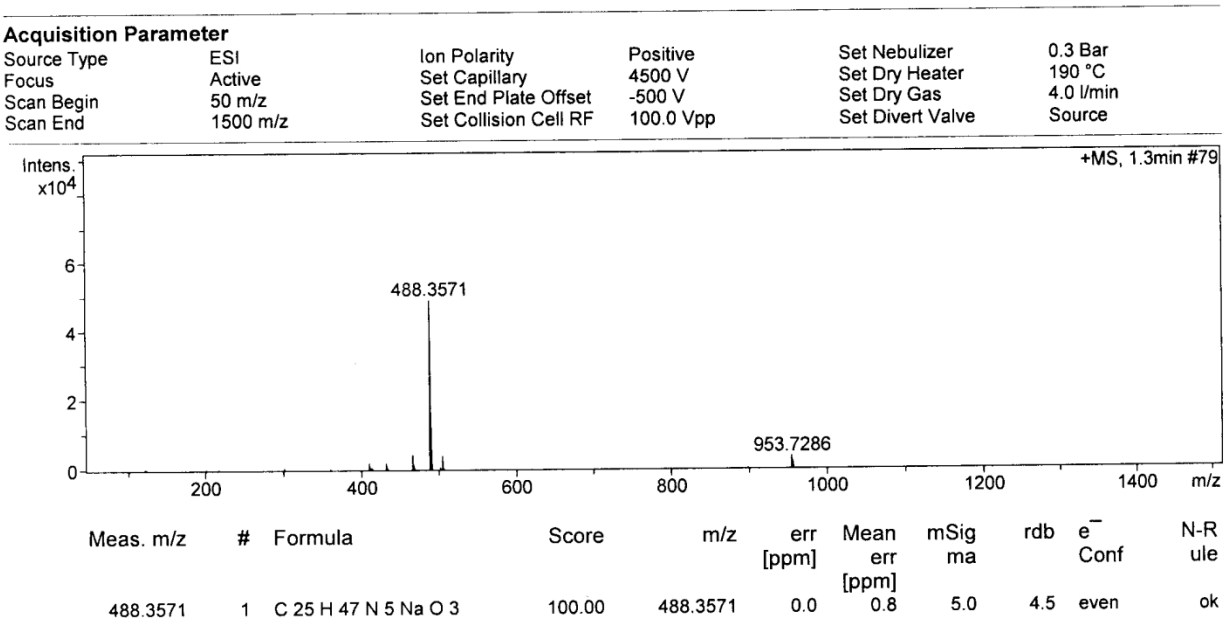


Figure S8. ^{13}CNMR Spectrum of **4c** ($CDCl_3$).



Meas. m/z	#	Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSig ma	rdb	e⁻ Conf	N-R ule
488.3571	1	C 25 H 47 N 5 Na O 3	100.00	488.3571	0.0	0.8	5.0	4.5	even	ok

Figure S9. Mass Spectrum of **4c.**

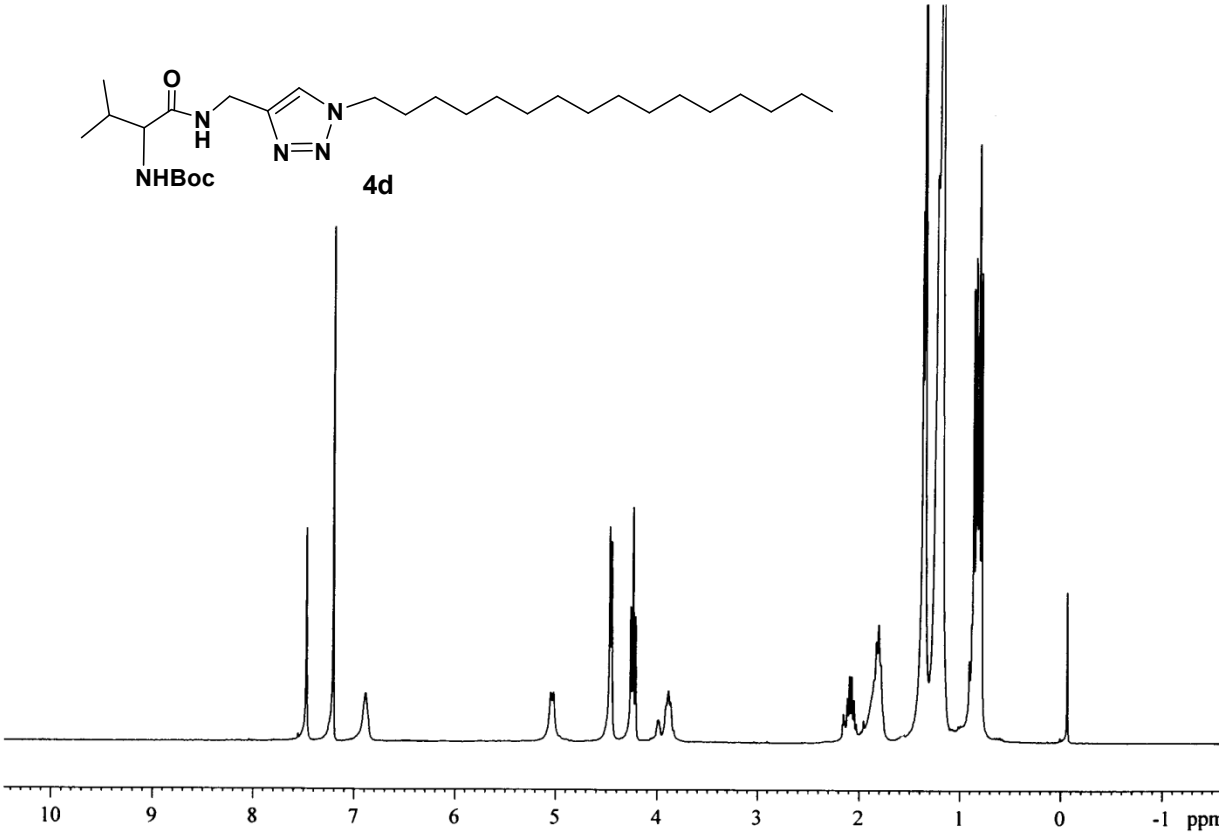


Figure S10. ^{1}H NMR Spectrum of **4d** ($CDCl_3$).

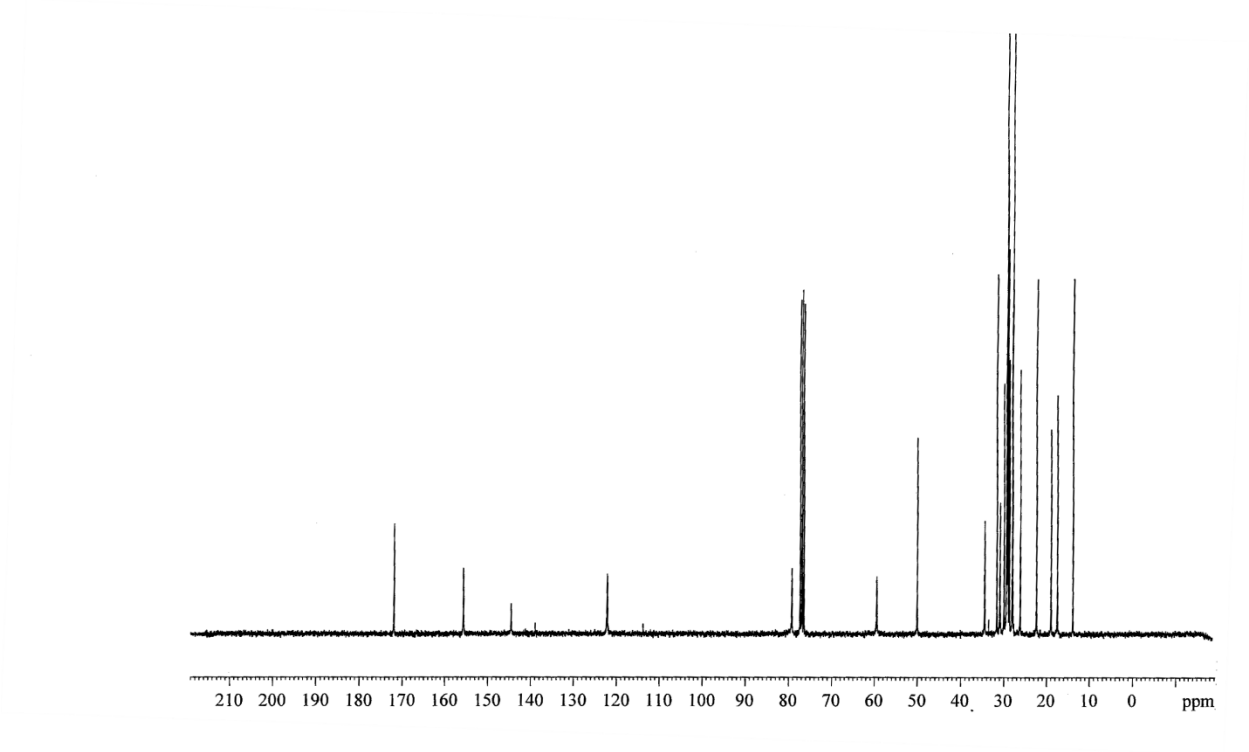
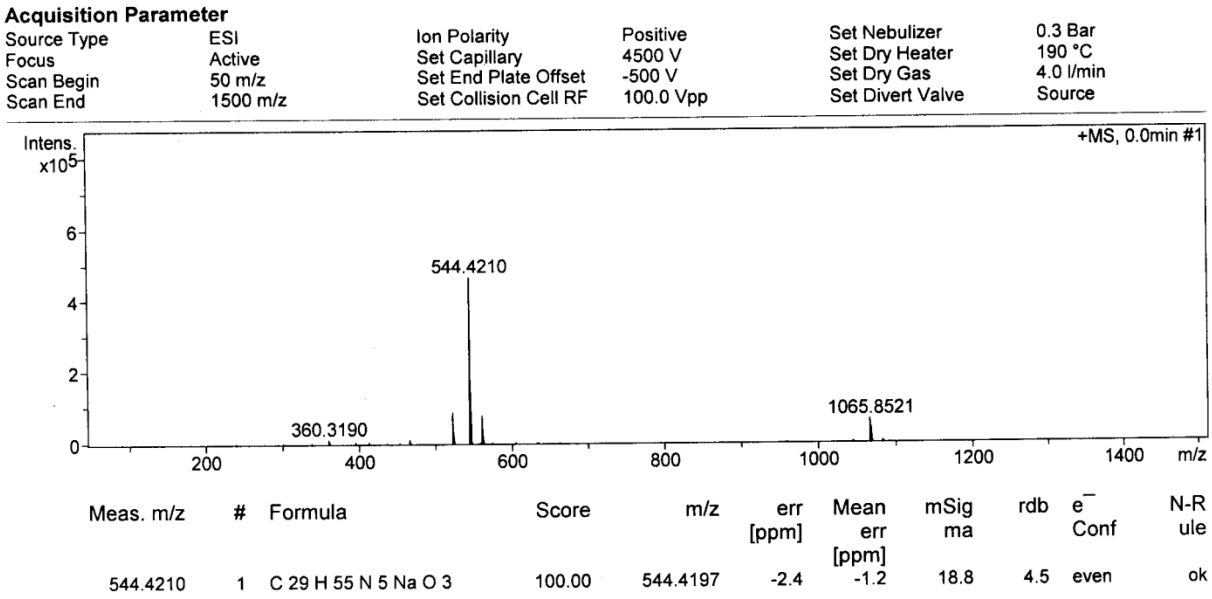


Figure S11. ^{13}C NMR Spectrum of **4d** ($CDCl_3$).



Meas. m/z	#	Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
544.4210	1	C 29 H 55 N 5 Na O 3	100.00	544.4197	-2.4	-1.2	18.8	4.5	even	ok

Figure S12. Mass Spectrum of **4d.**

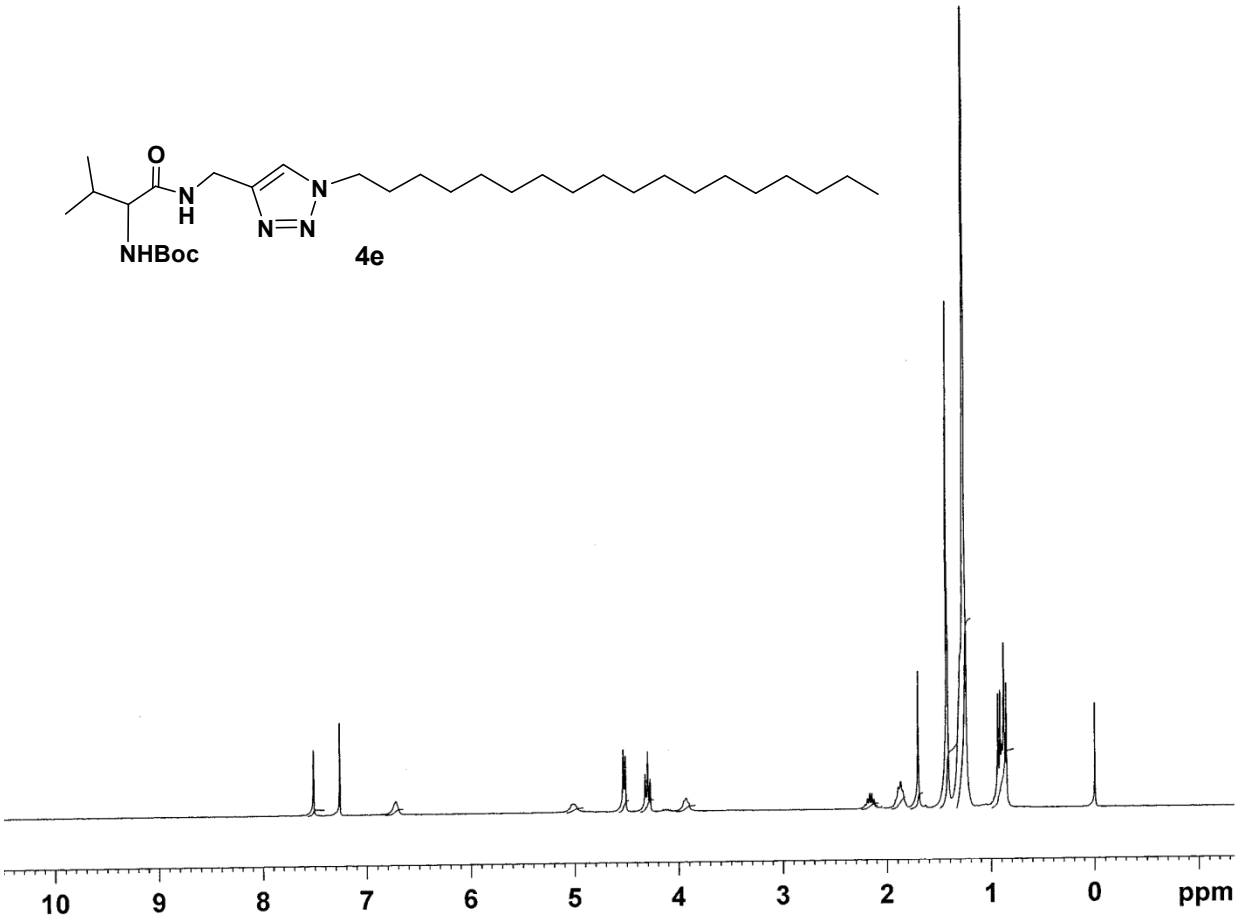


Figure S13. ^{1}H NMR Spectrum of **4e** ($CDCl_3$).

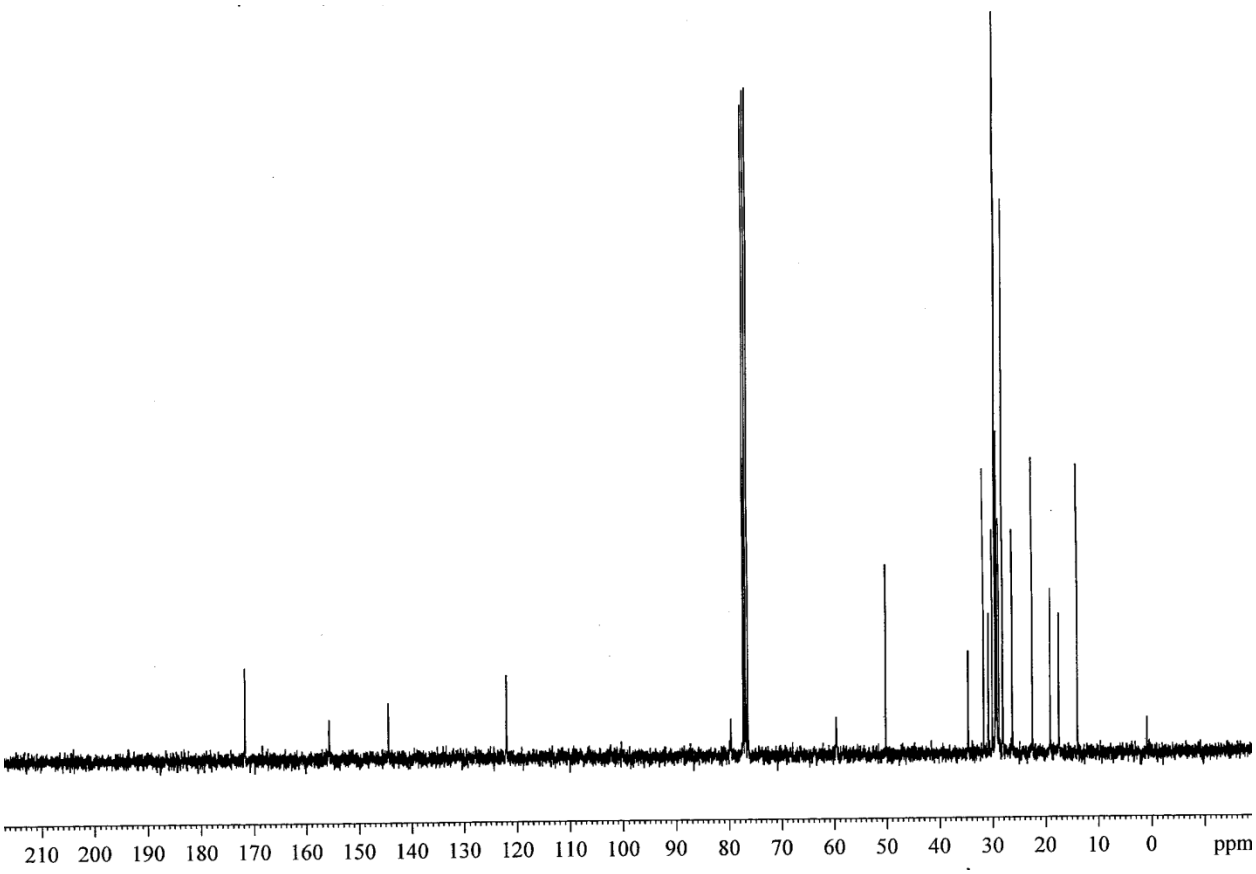


Figure S14. ^{13}C NMR Spectrum of **4e** ($CDCl_3$).

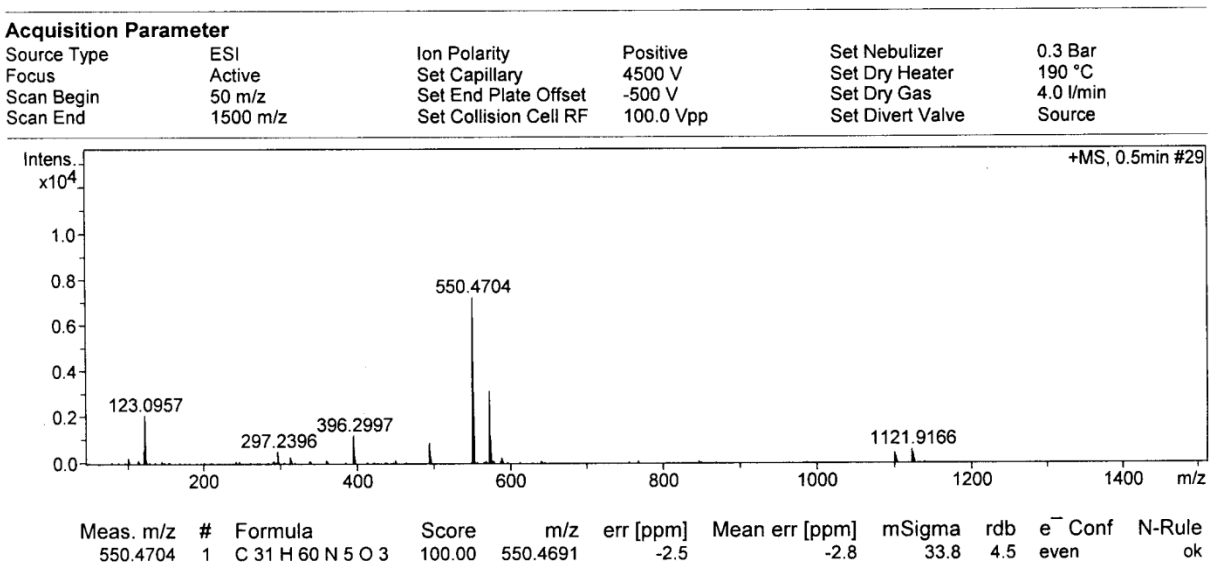


Figure S15. Mass Spectrum of **4e.**

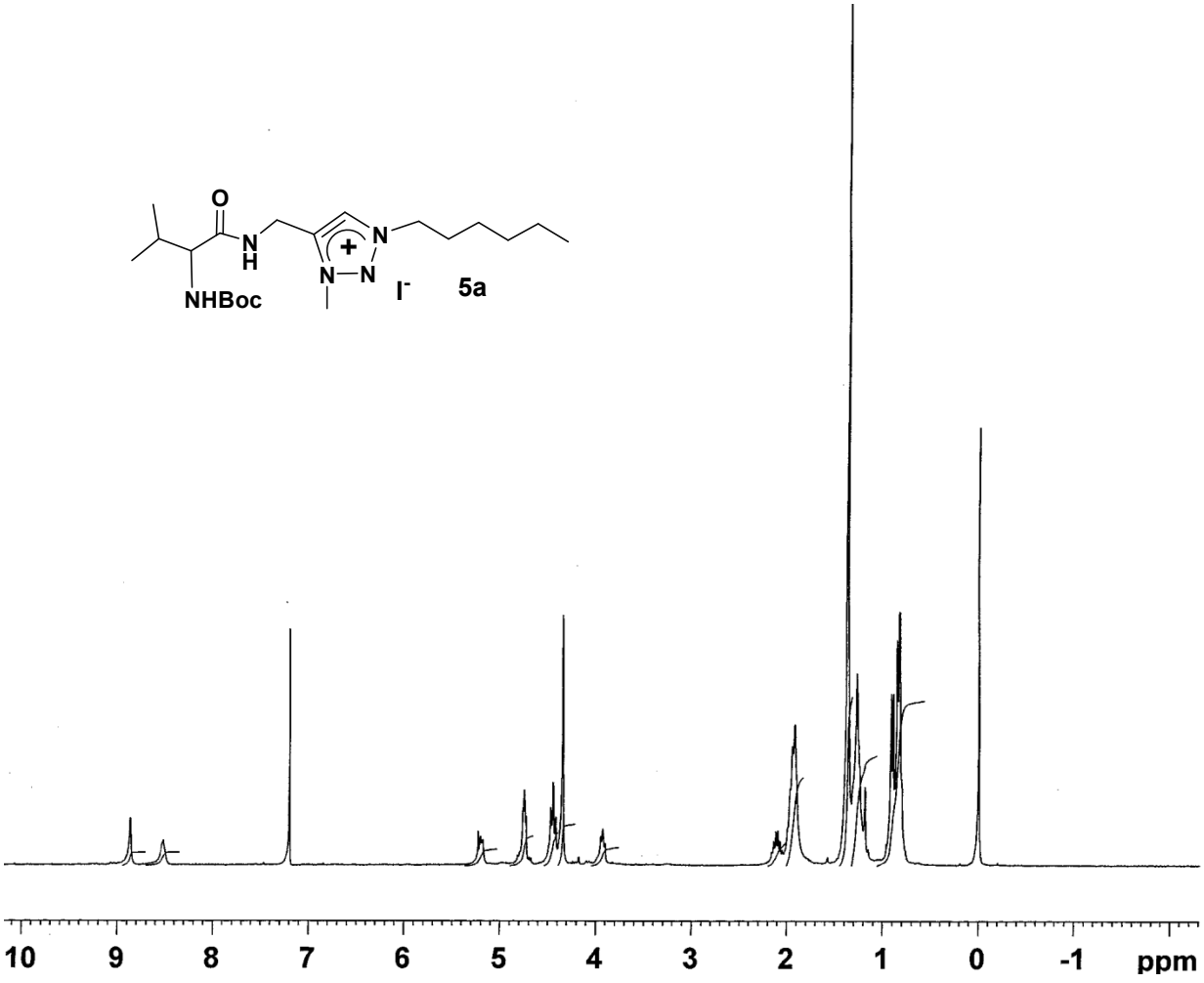


Figure S16. ^{1}H NMR Spectrum of **5a** ($CDCl_3$).

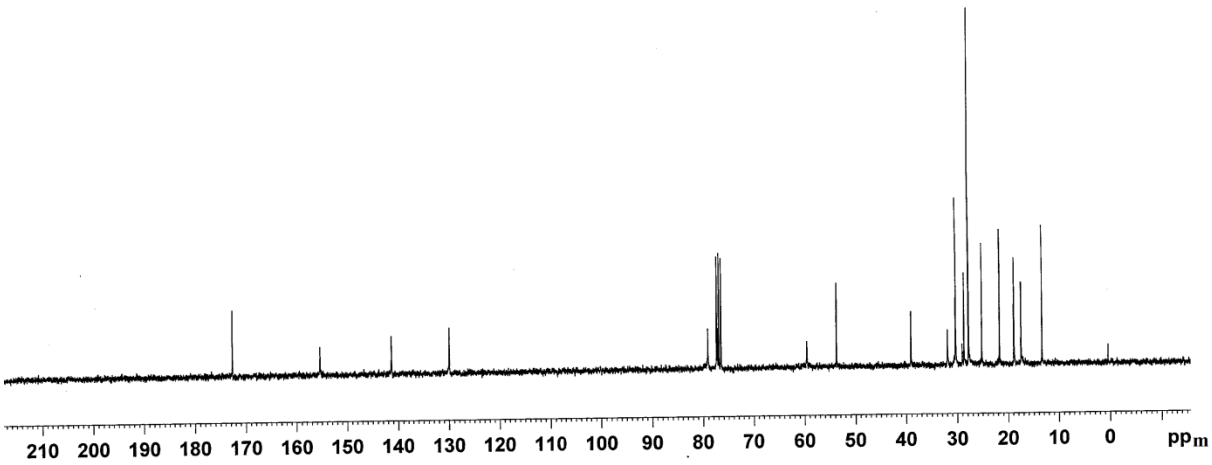


Figure S17. ^{13}C NMR Spectrum of **5a** ($CDCl_3$).

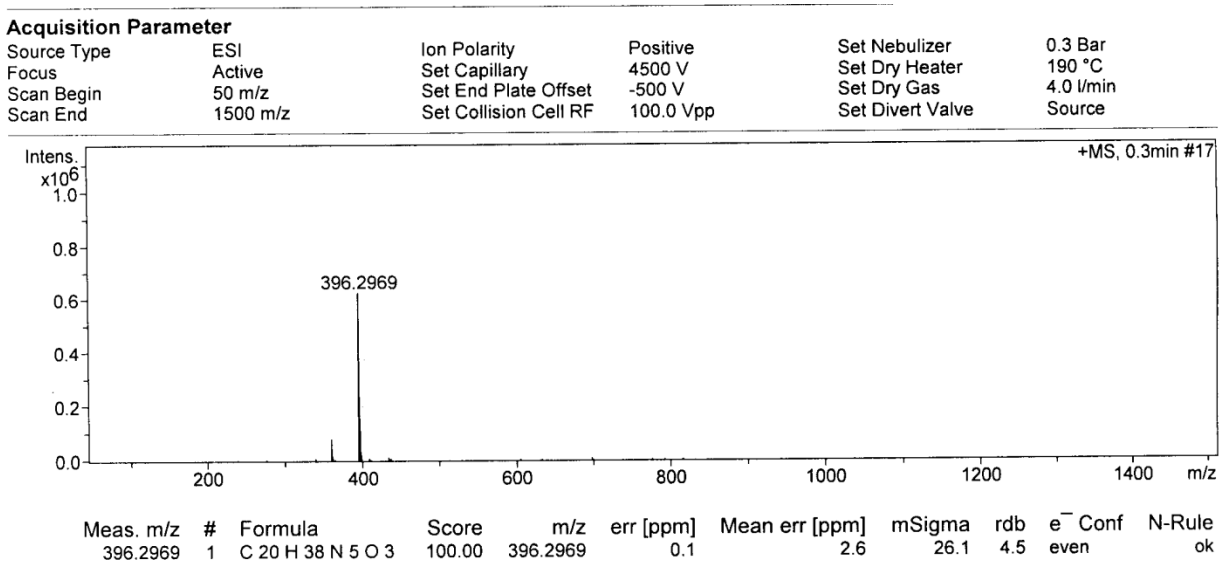


Figure S18. Mass Spectrum of **5a.**

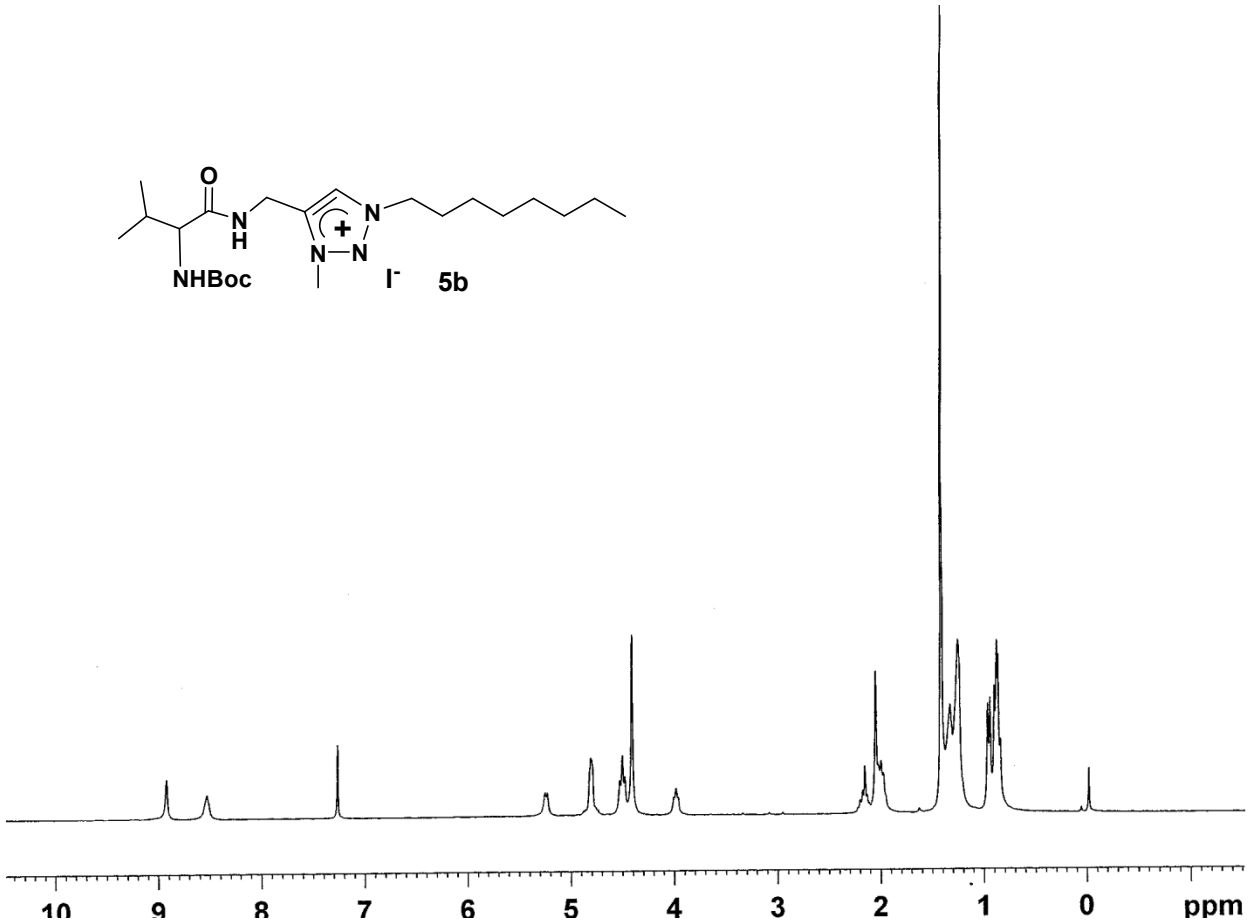


Figure S19. ^{1}H NMR Spectrum of **5b** ($CDCl_3$).

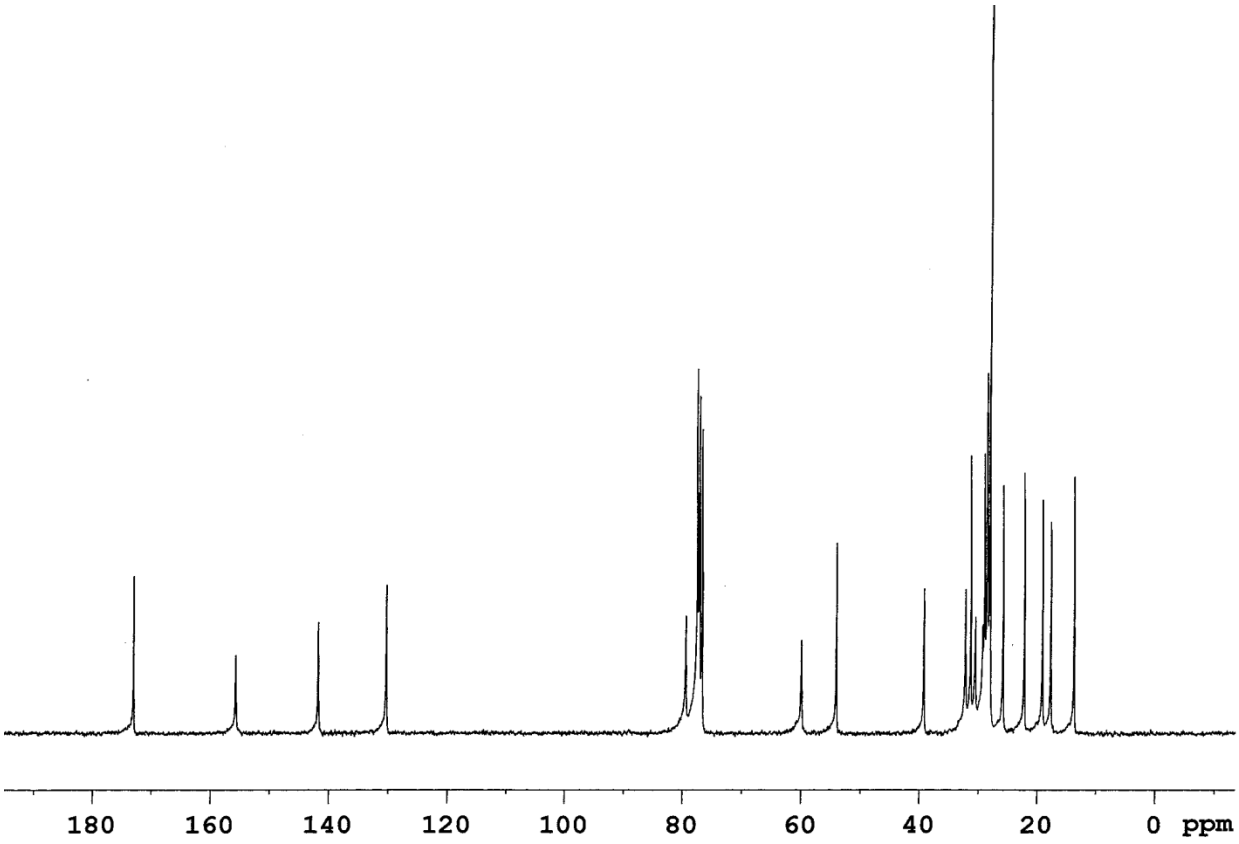


Figure S20. ^{13}C NMR Spectrum of **5b** ($CDCl_3$).

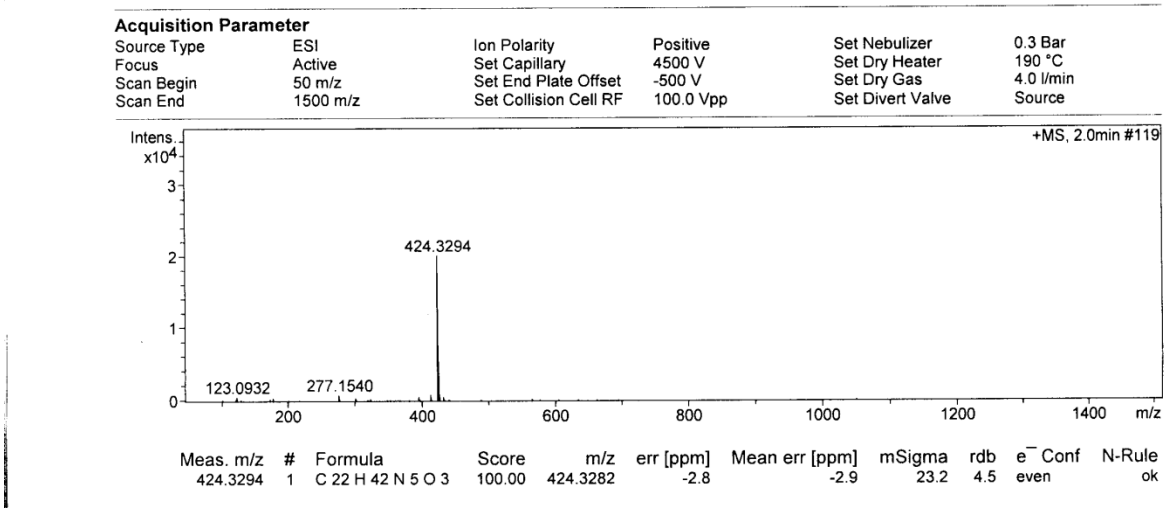


Figure S21. Mass Spectrum of **5b.**

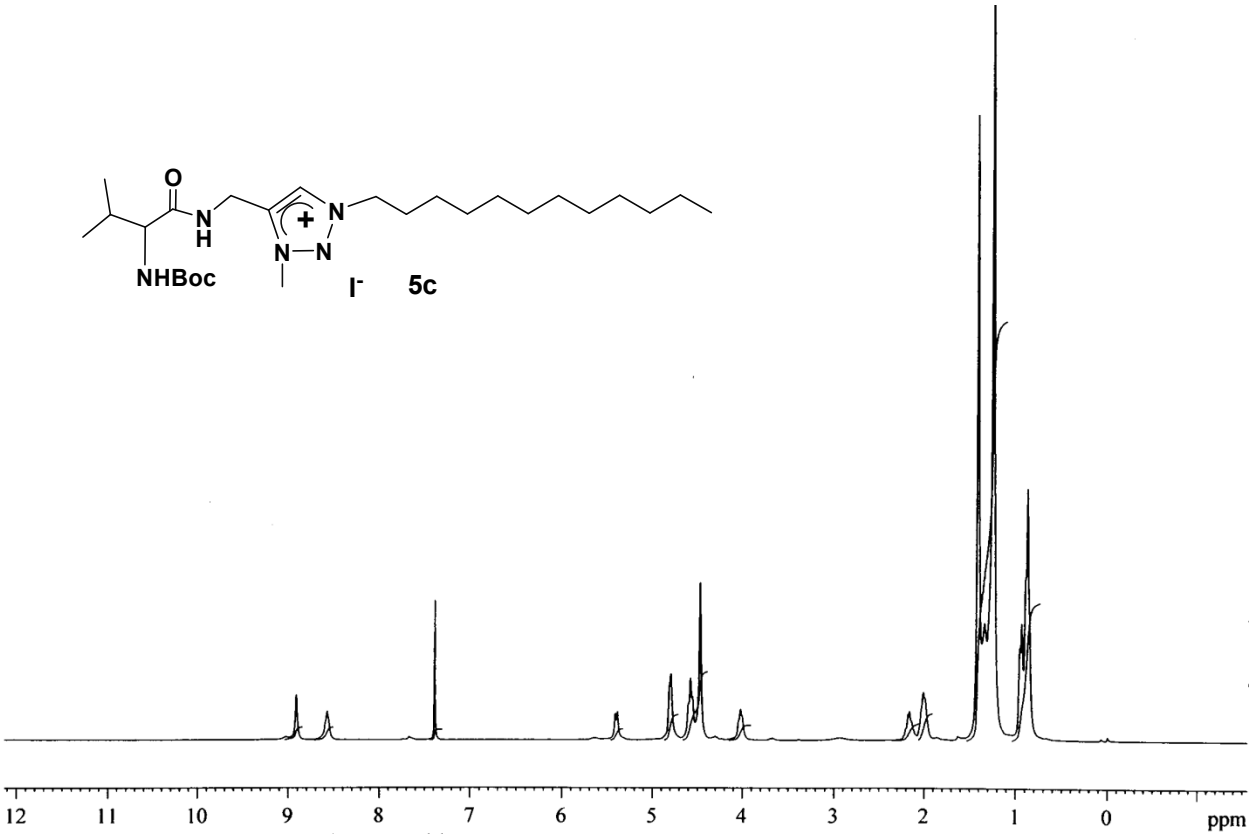


Figure S22. ^{1}H NMR Spectrum of **5c** ($CDCl_3$).

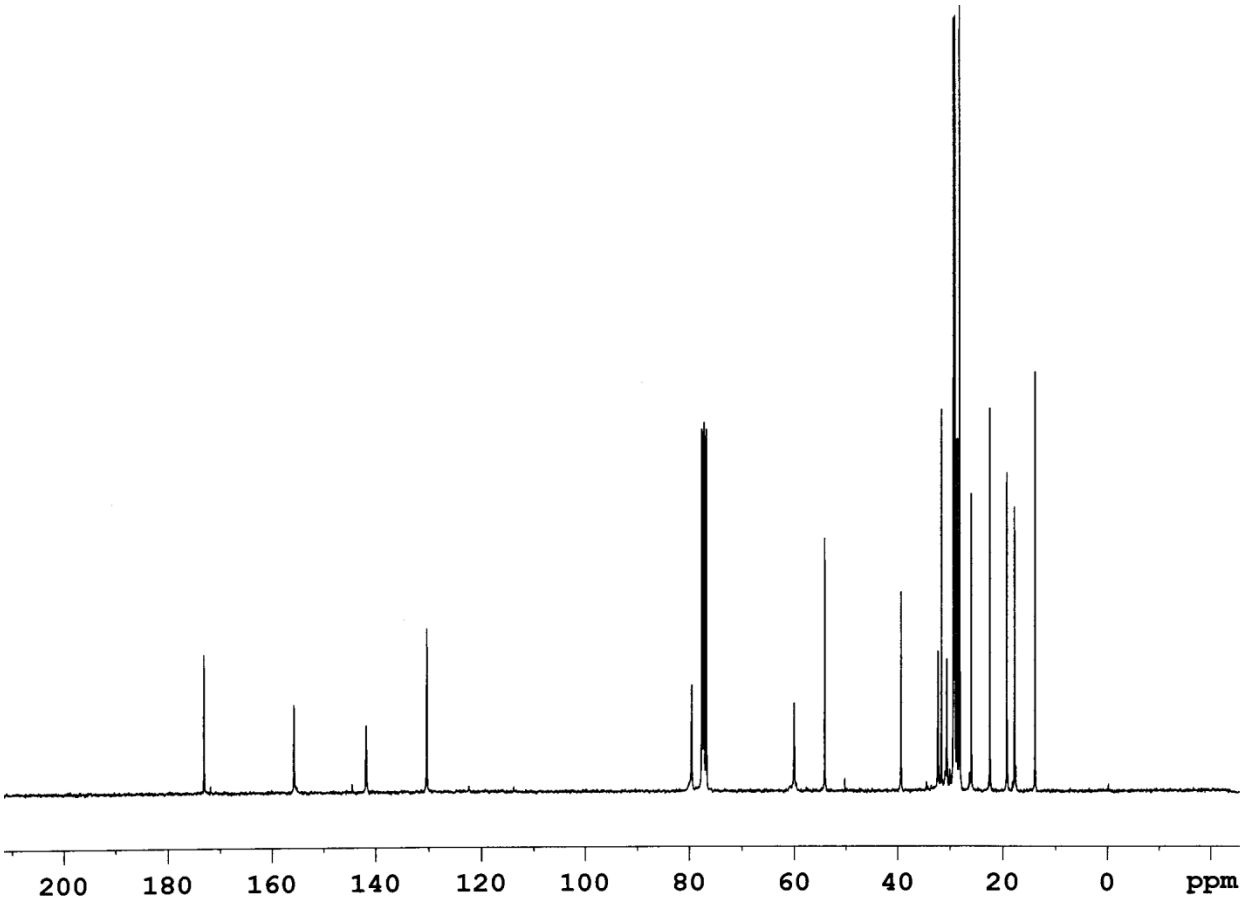


Figure S23. ^{13}C NMR Spectrum of **5c** ($CDCl_3$).

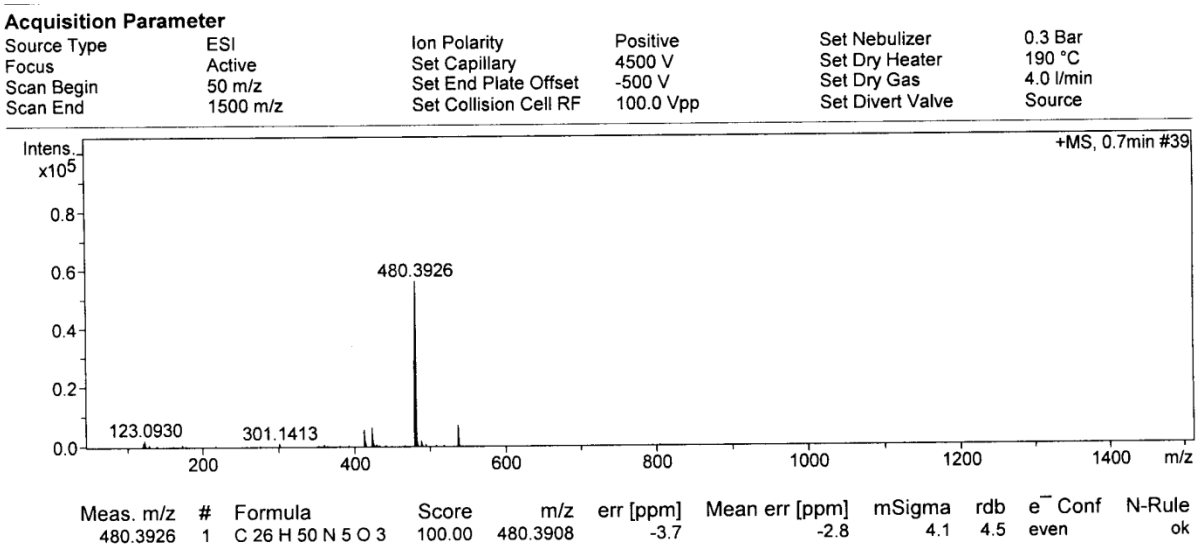


Figure S24. Mass Spectrum of **5c.**

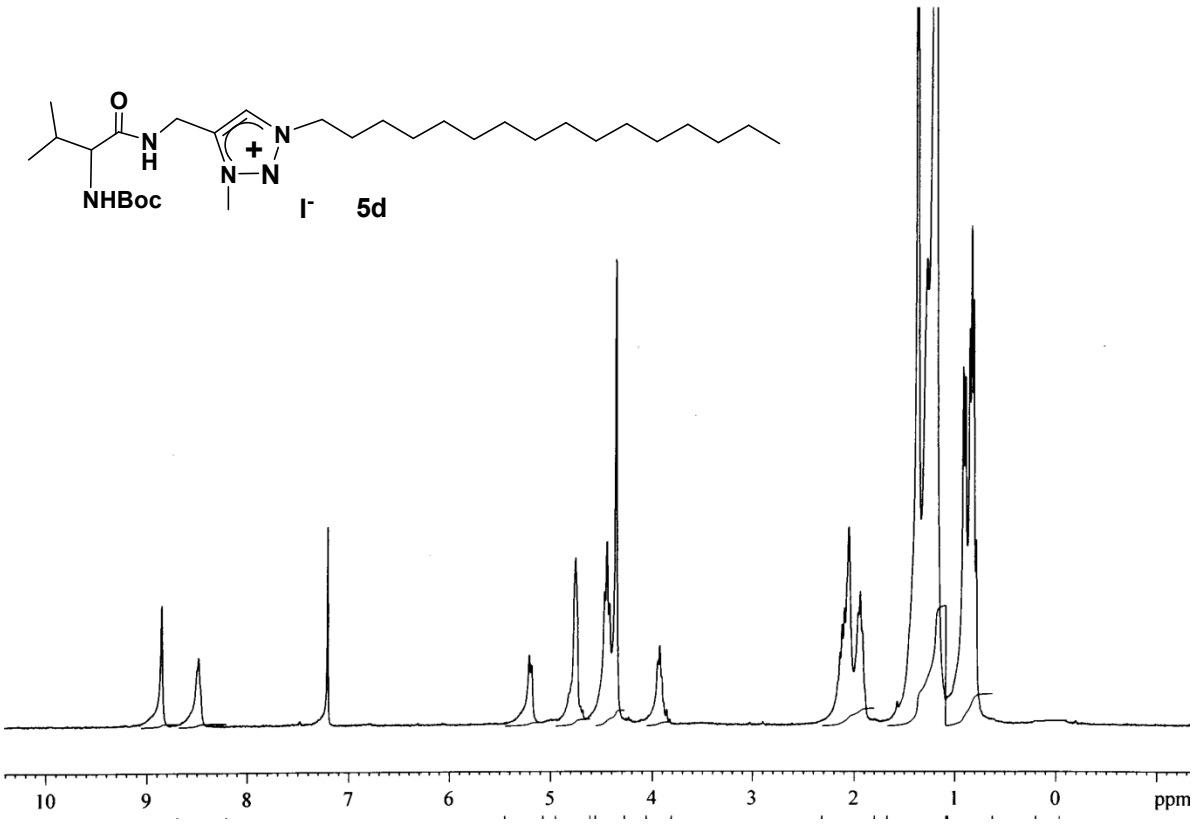


Figure S25. ^{1}HNMR Spectrum of **5d** ($CDCl_3$).

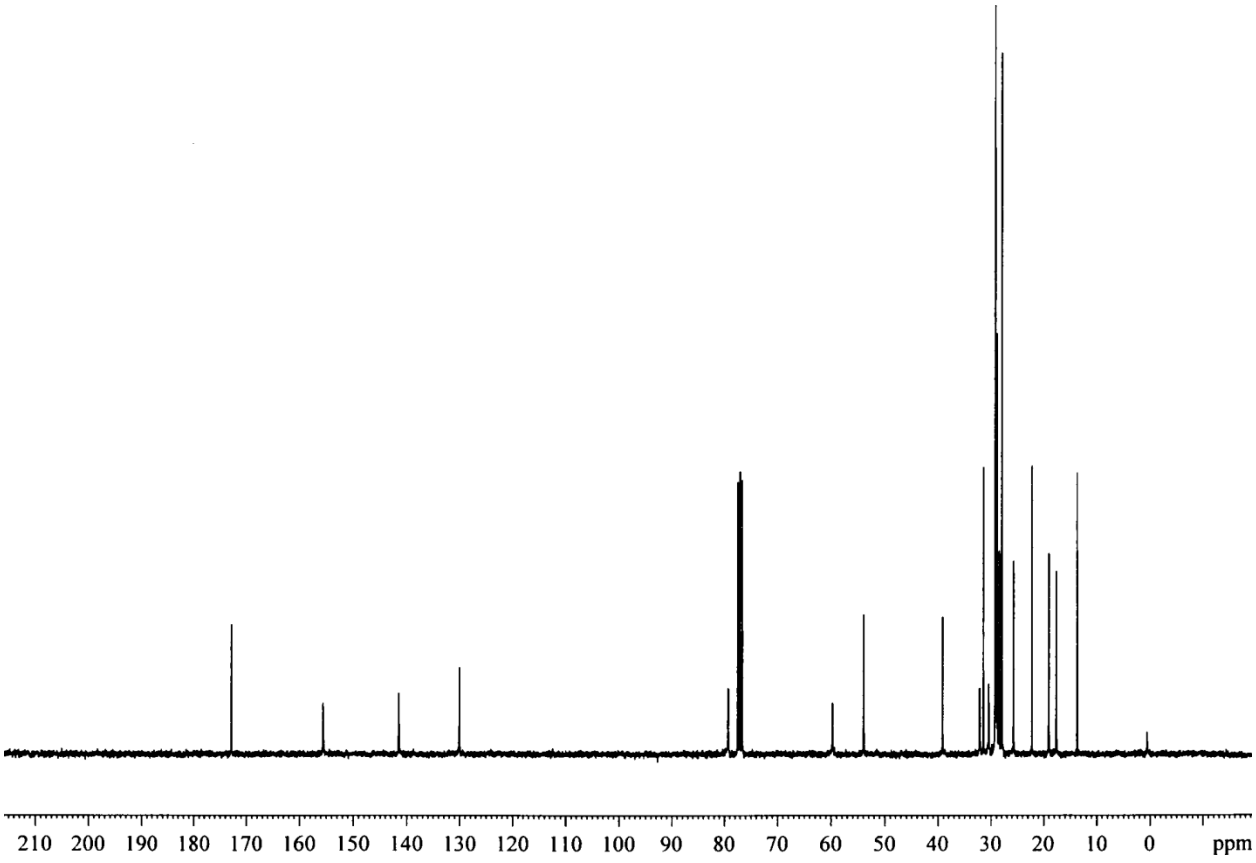


Figure S26. ^{13}C NMR Spectrum of **5d** ($CDCl_3$).

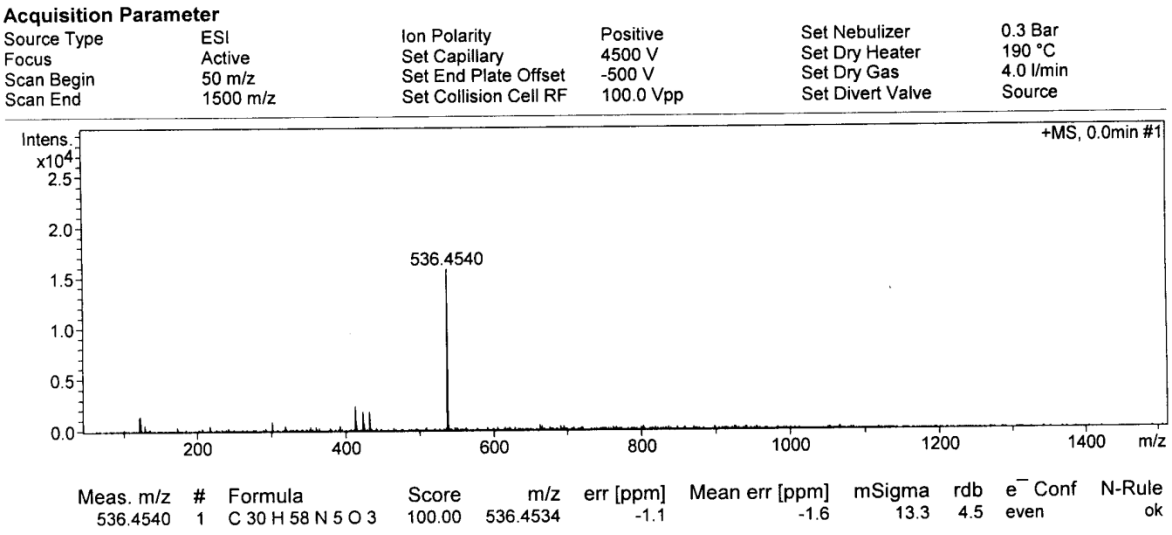


Figure S27. Mass Spectrum of **5e.**

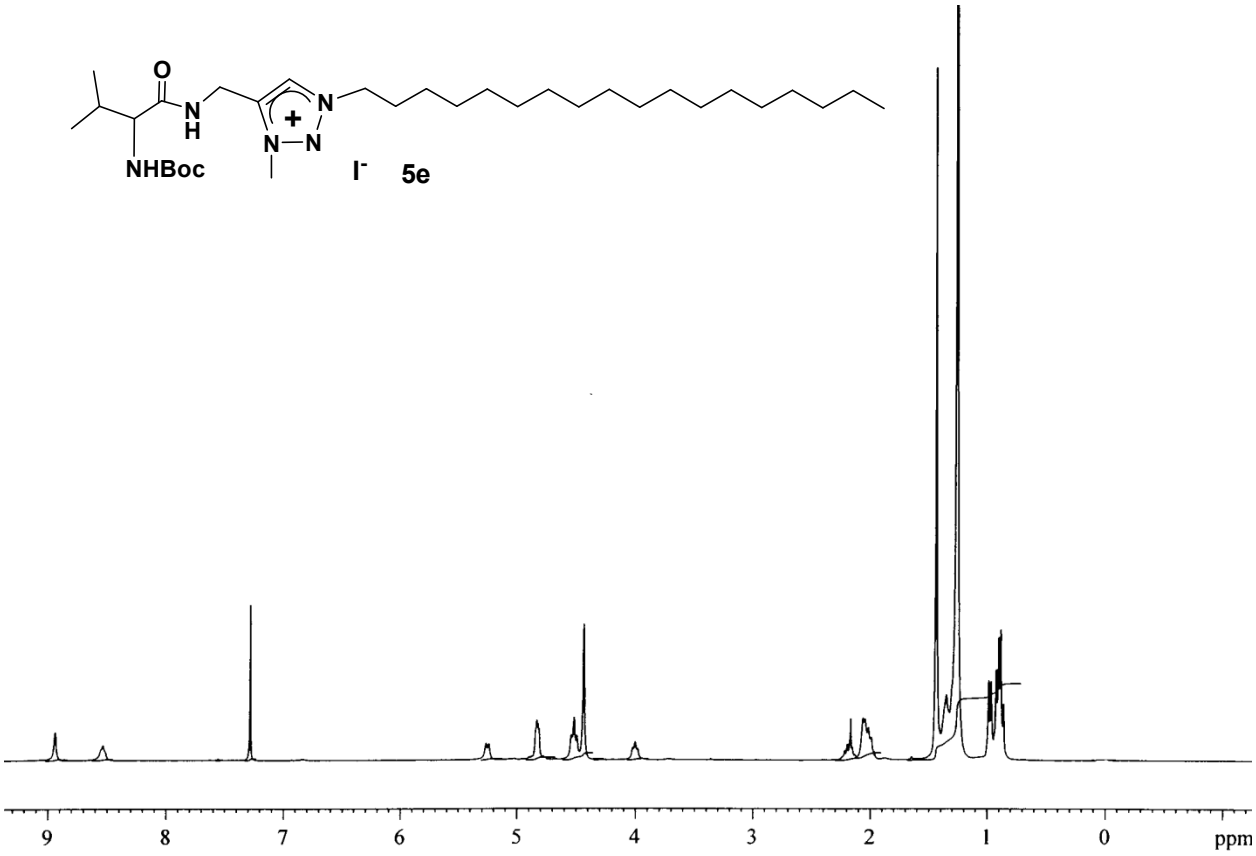


Figure S28. ^{1}H NMR Spectrum of **5e** ($CDCl_3$).

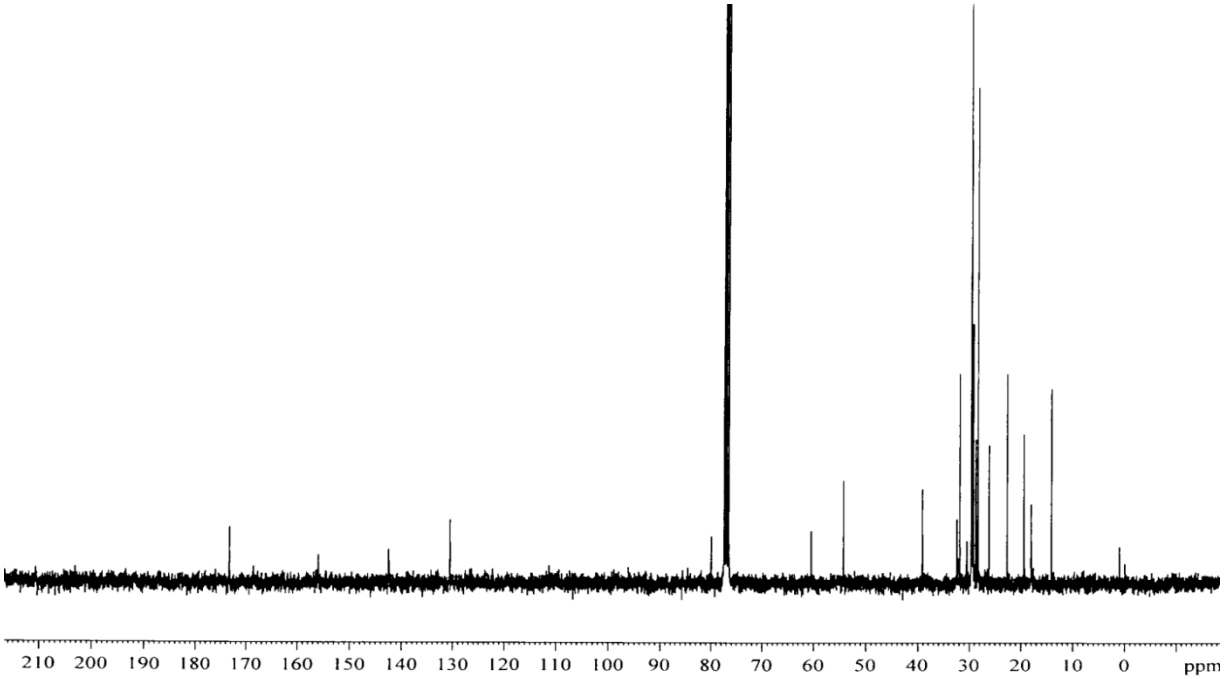
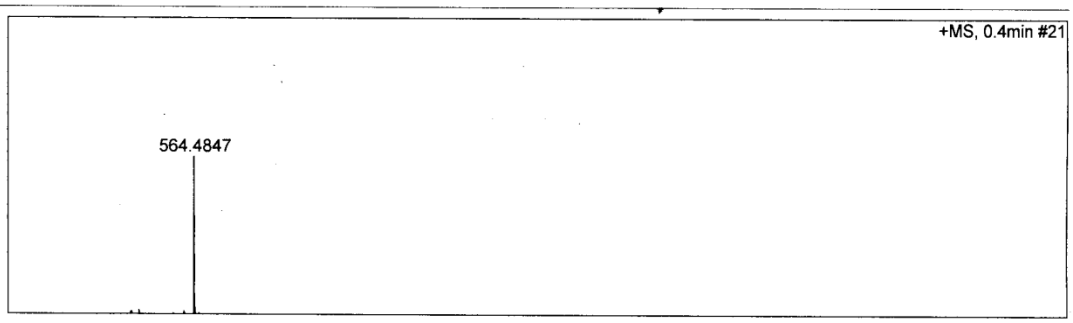


Figure S29. ^{13}C NMR Spectrum of **5e** ($CDCl_3$).

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e⁻ Conf	mSigma	Std I	Std Mean m/z	Std I Var Norm	Std m/z Diff	Std Comb Dev
564.4847	1	C 32 H 62 N 5 O 3	564.4847	-0.0	1.6	4.5	ok	even	10.3	16.1	1.7	7.0	3.5	842.7

Figure S30. Mass Spectrum of **5e.**

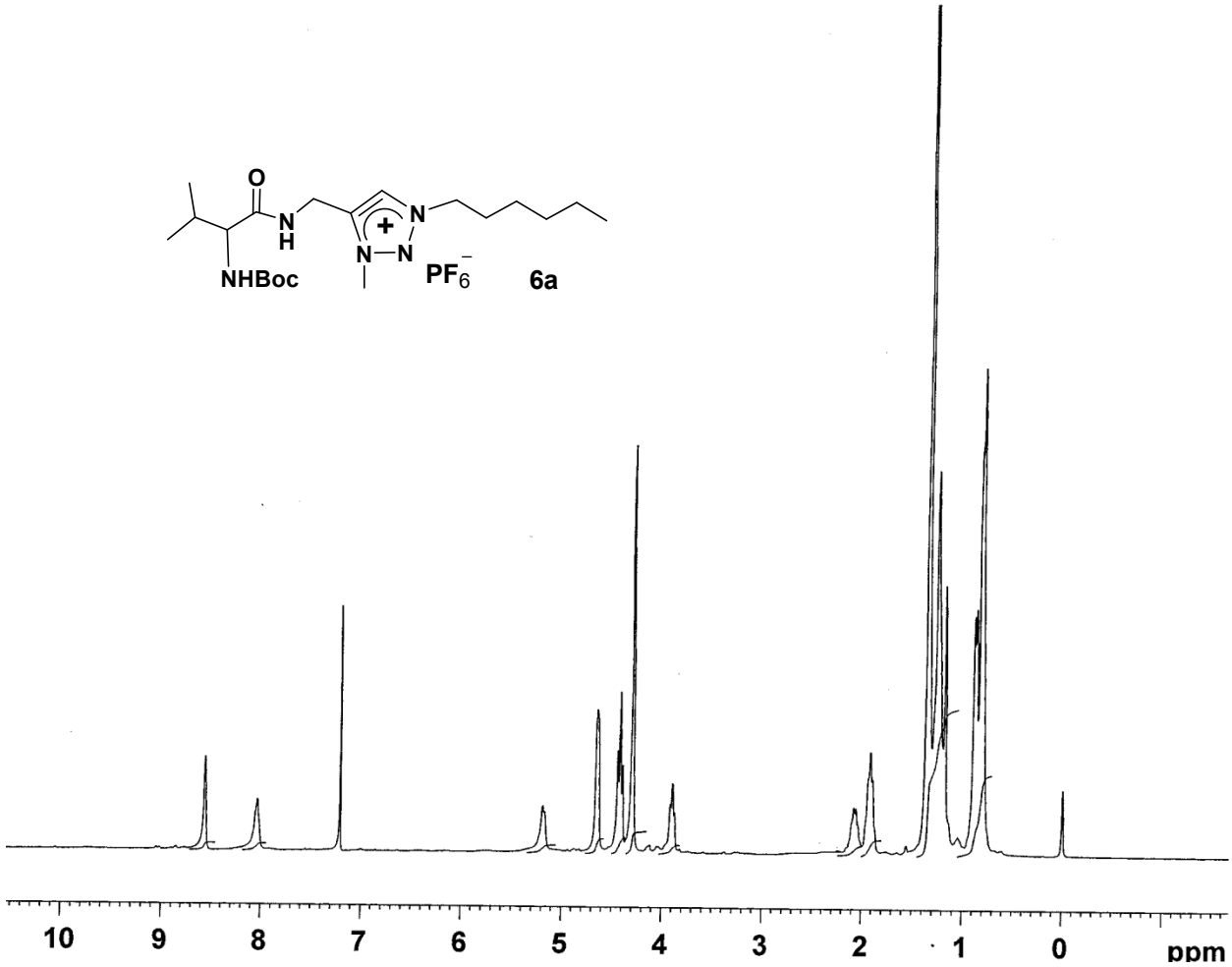


Figure S31. ^{1}H NMR Spectrum of **6a** ($CDCl_3$).

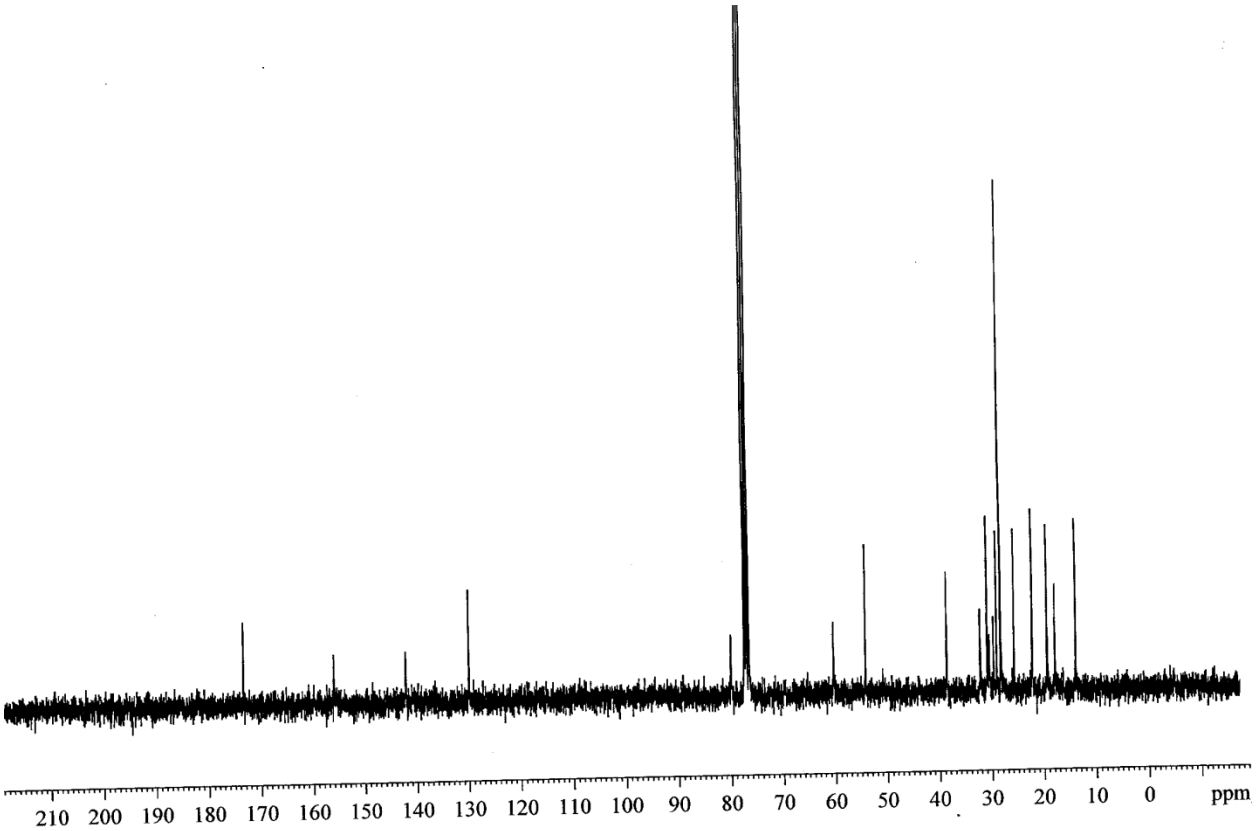


Figure S32. ^{13}C NMR Spectrum of **6a** ($CDCl_3$).

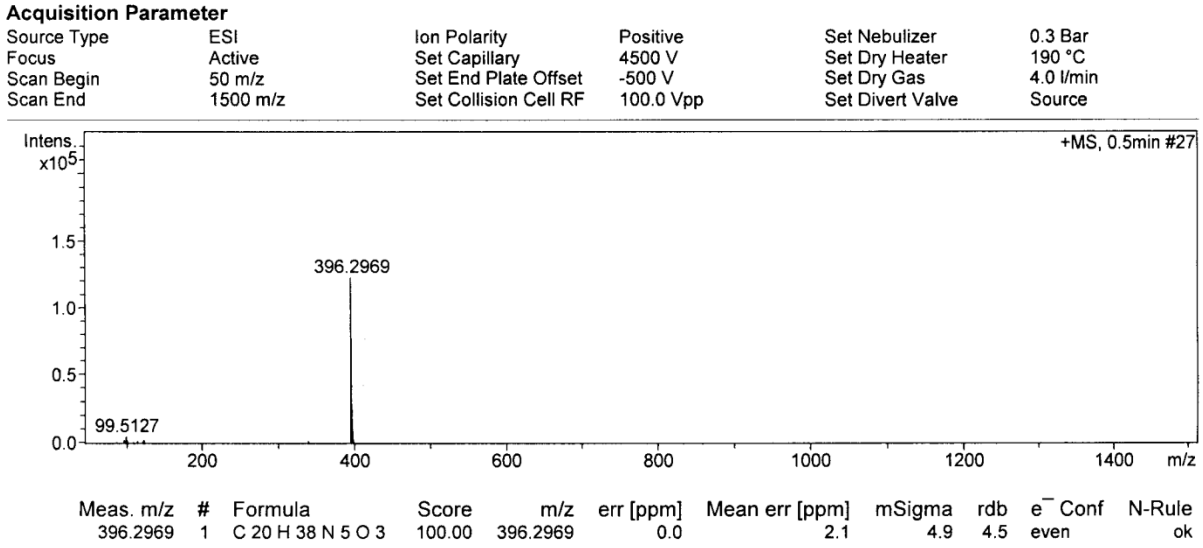


Figure S33. Mass Spectrum of **6a** ($CDCl_3$).

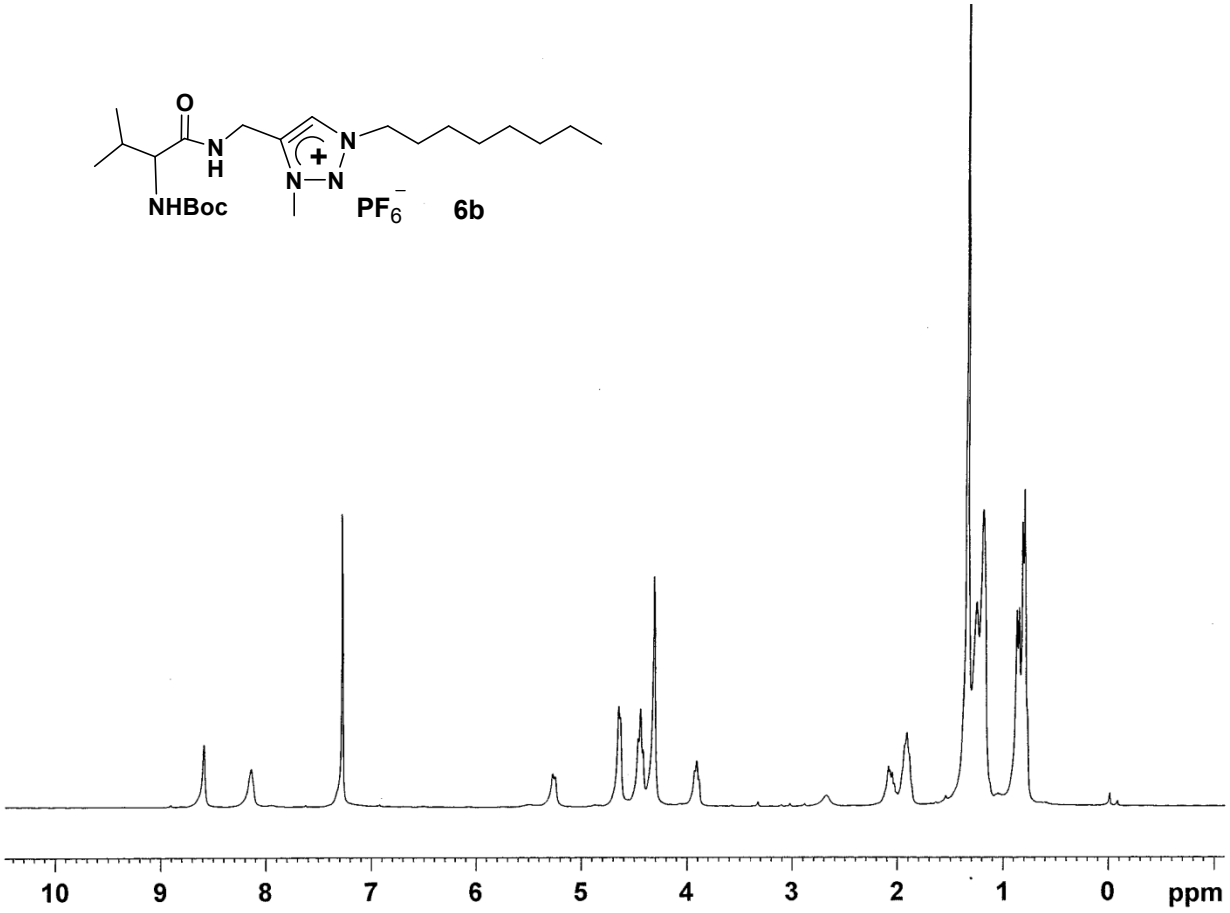


Figure S34. ^{1}H NMR Spectrum of **6b** ($CDCl_3$).

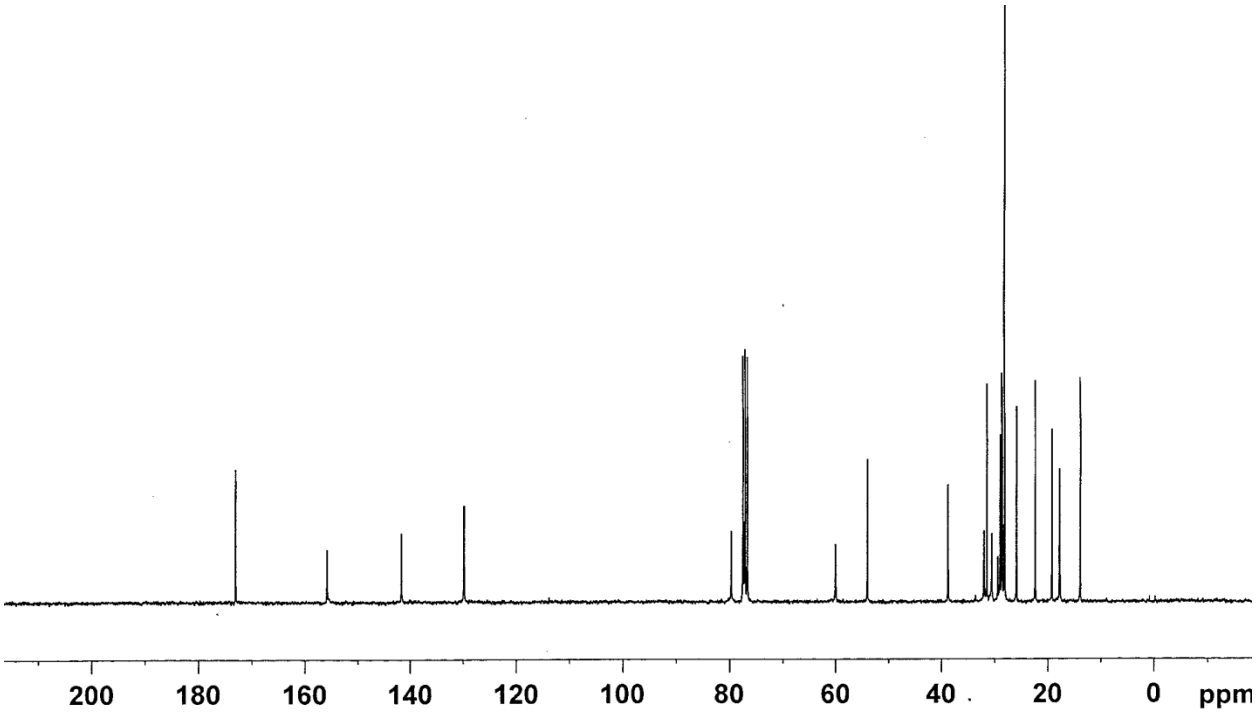


Figure S35. ^{13}C NMR Spectrum of **6b** ($CDCl_3$).

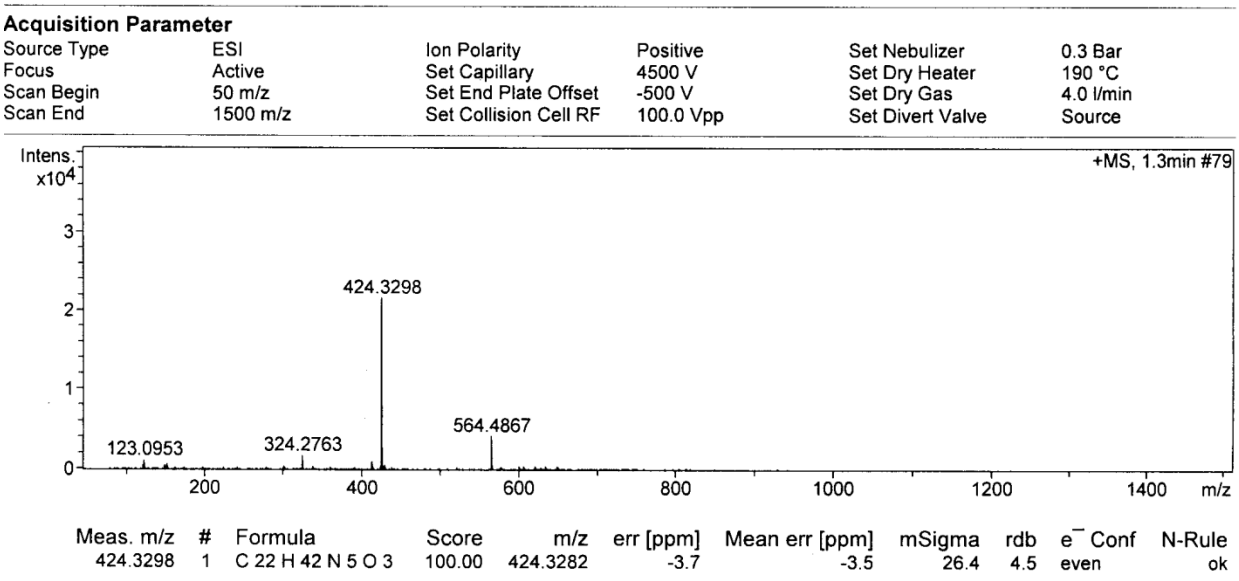


Figure S36. Mass Spectrum of **6b** ($CDCl_3$).

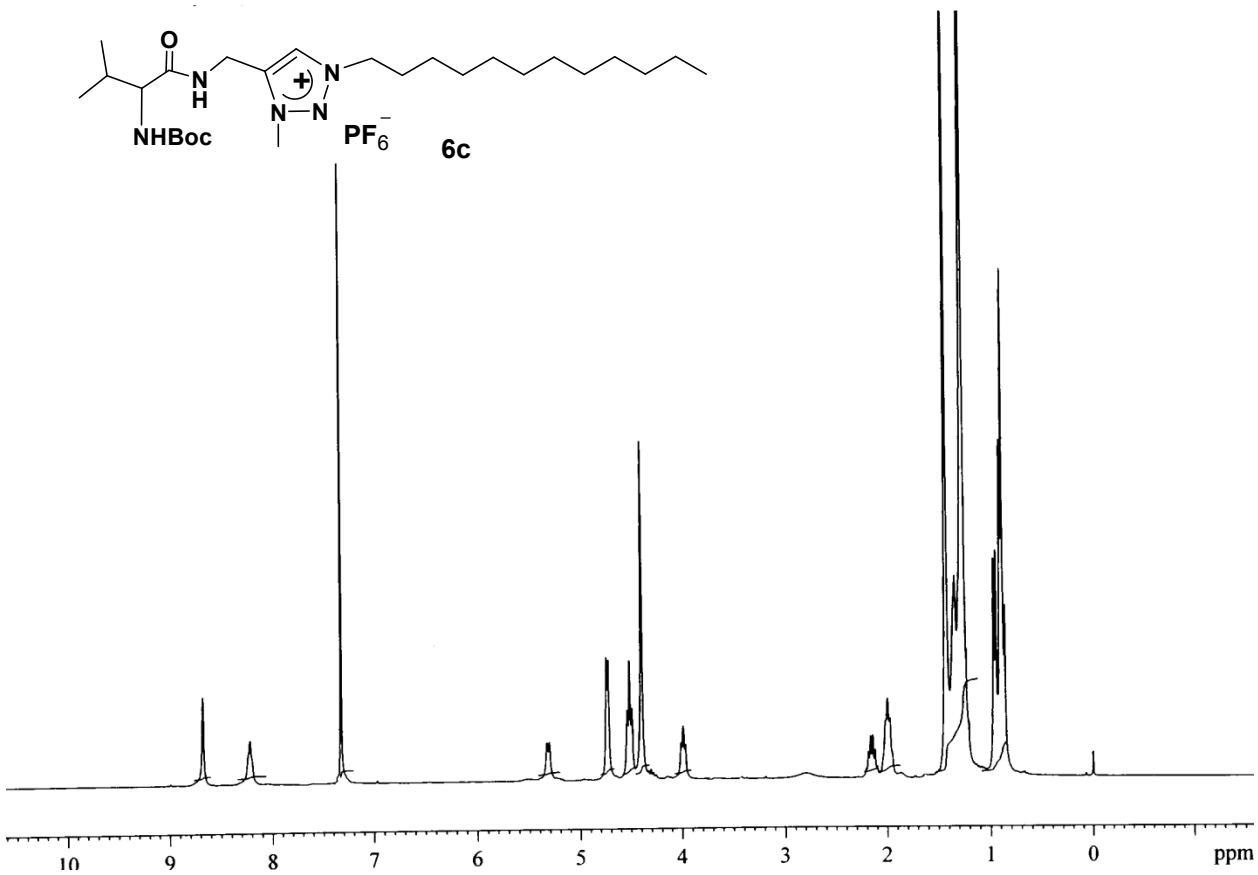


Figure S37. ^{1}H NMR Spectrum of **6c** ($CDCl_3$).

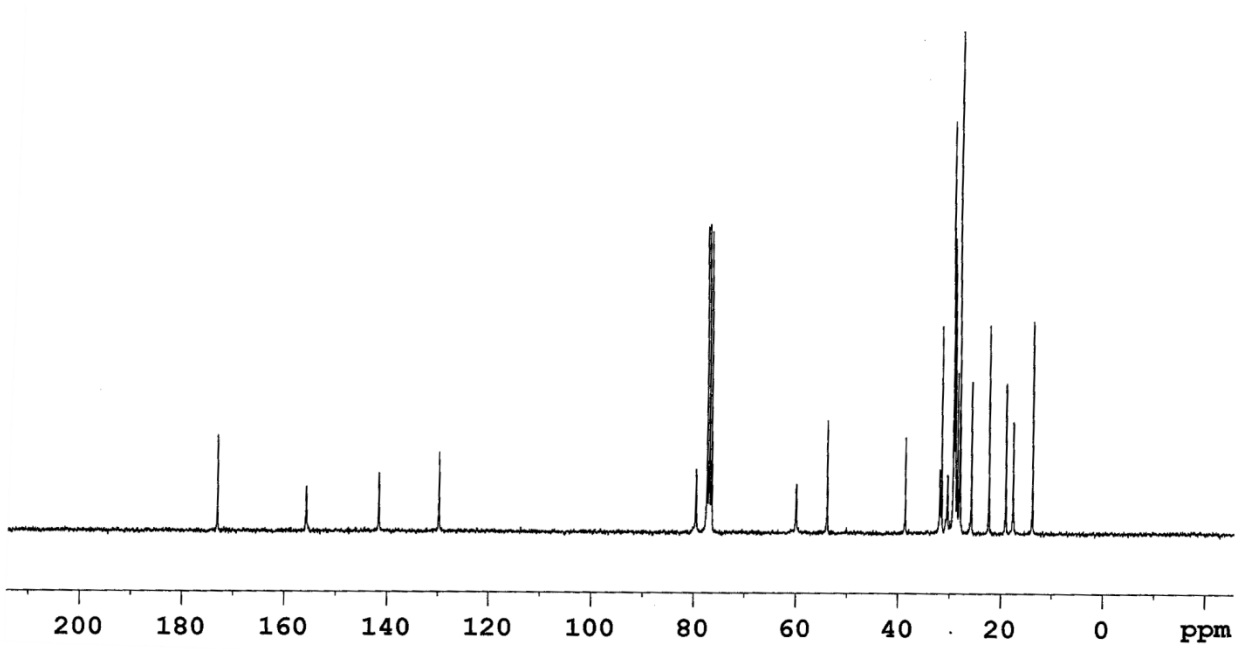


Figure S38: ^{13}C NMR Spectrum of **6c** ($CDCl_3$).

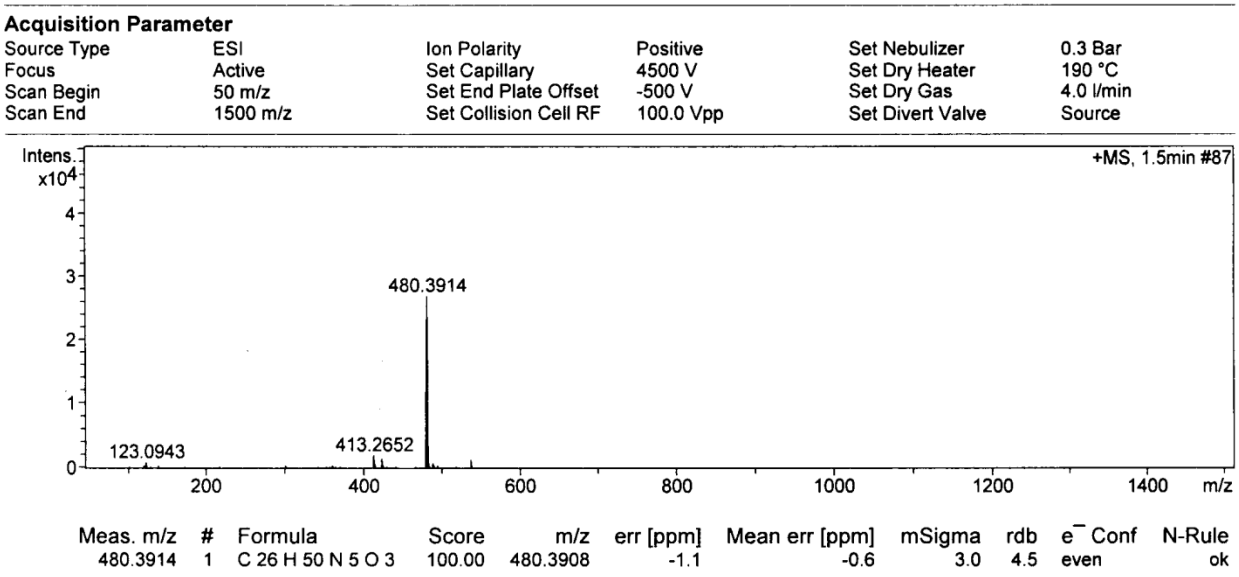


Figure S39. Mass Spectrum of **6c.**

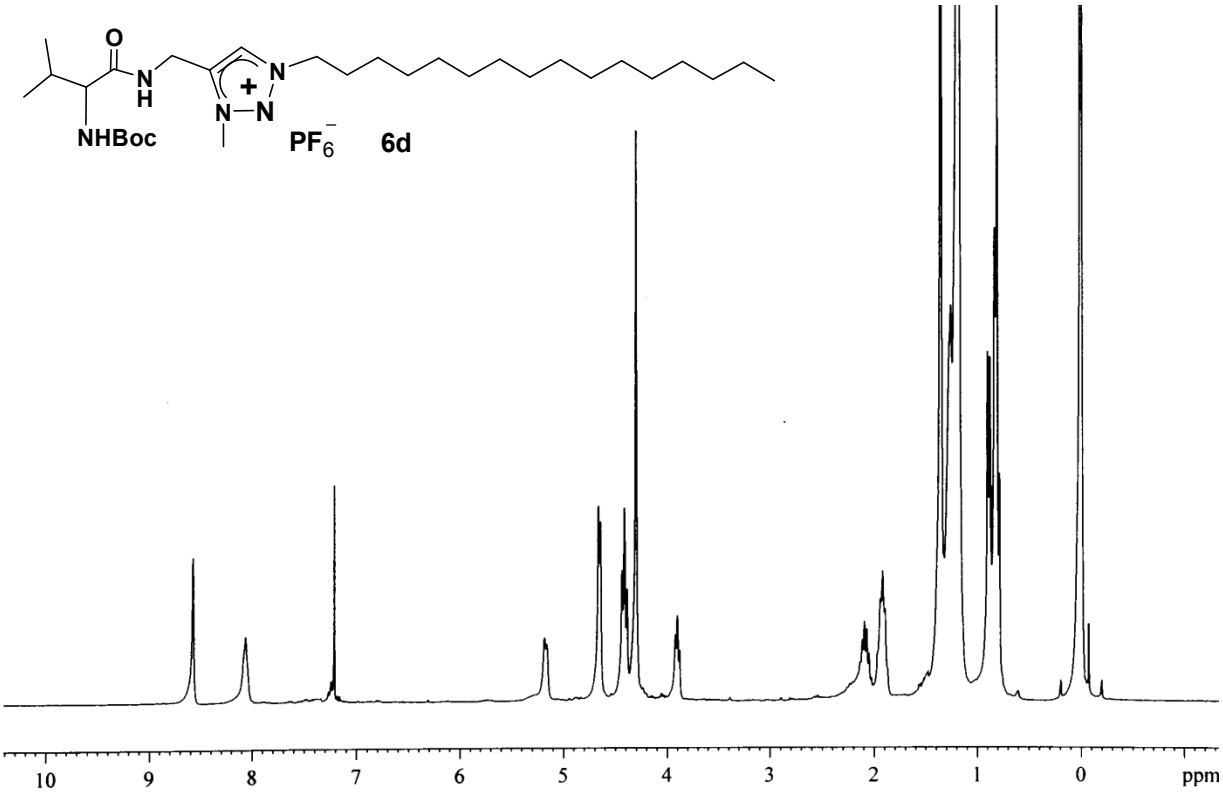


Figure S40. ^{1}H NMR Spectrum of **6d** ($CDCl_3$).

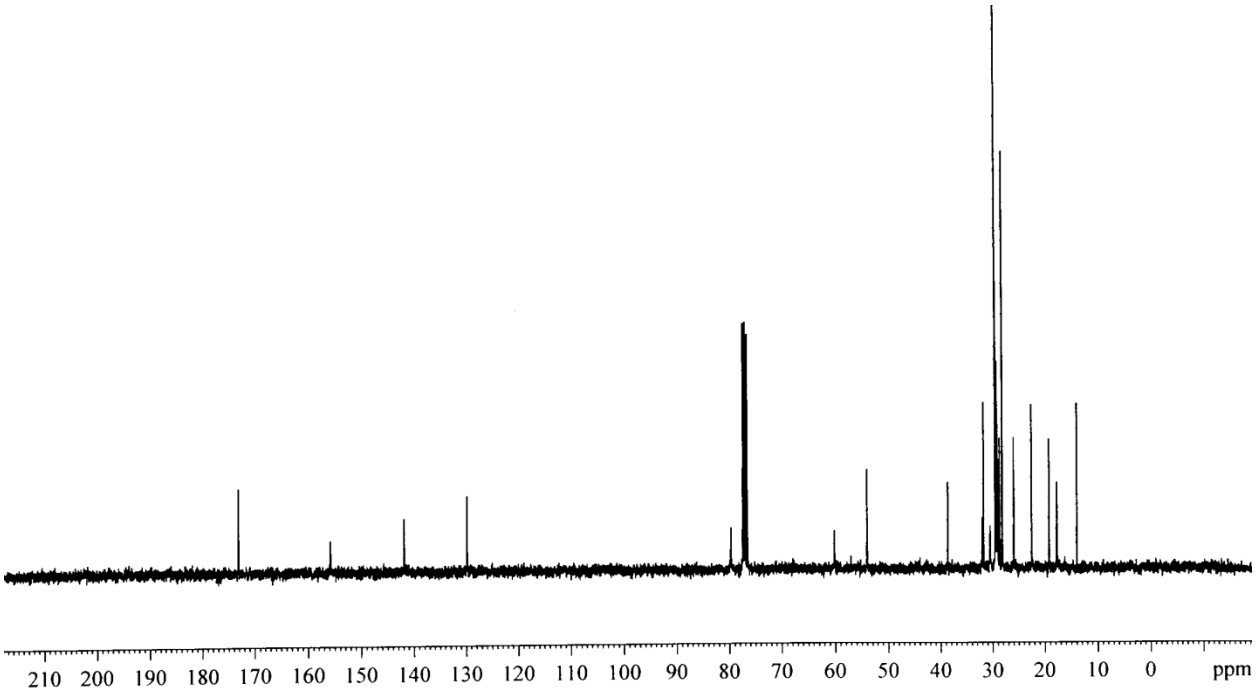


Figure S41. ^{13}C NMR Spectrum of **6d** ($CDCl_3$).

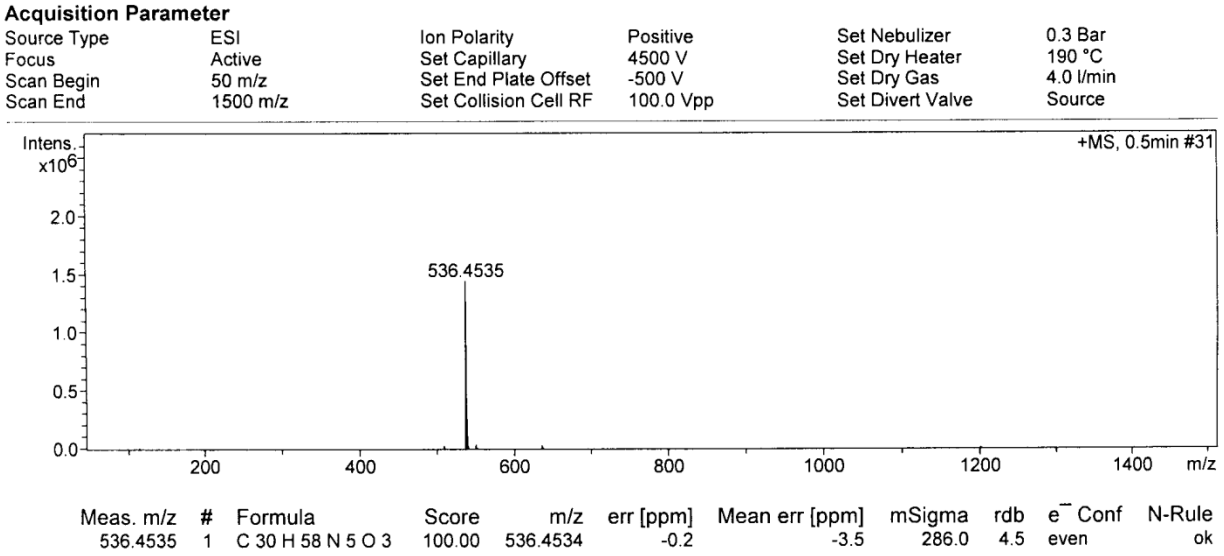


Figure S42. Mass Spectrum of **6d.**

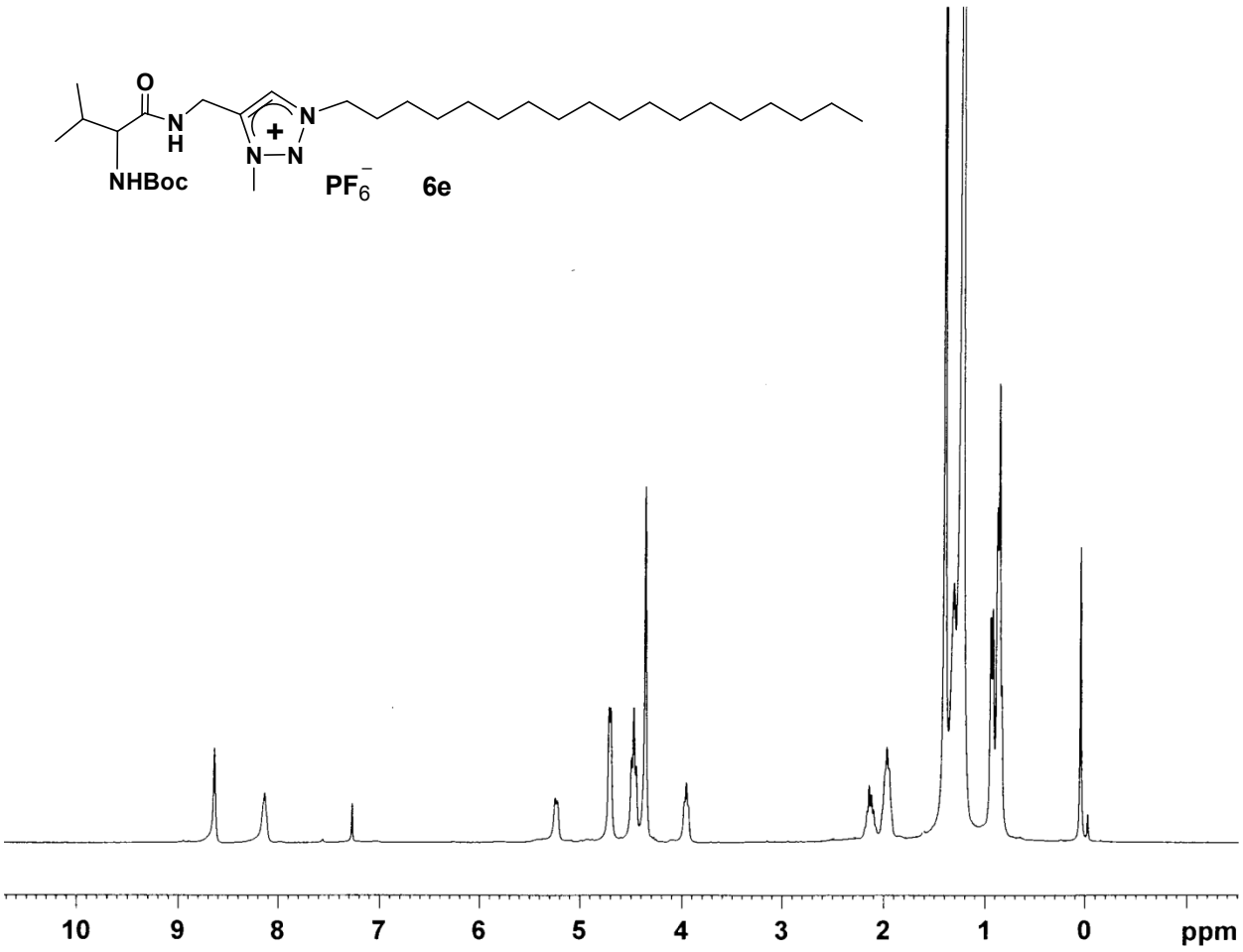


Figure S43. ^{1}H NMR Spectrum of **6e** ($CDCl_3$).

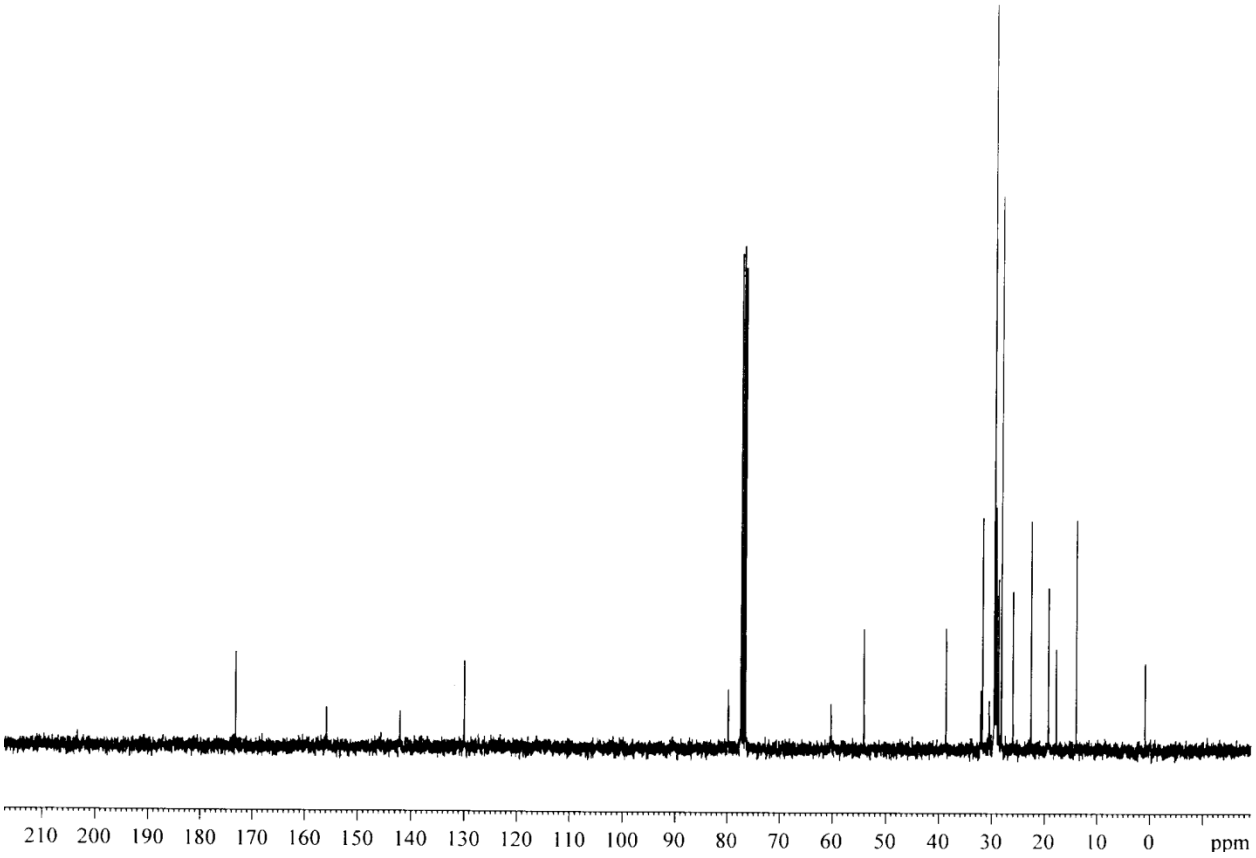


Figure S44. ^{13}C NMR Spectrum of **6e** ($CDCl_3$).

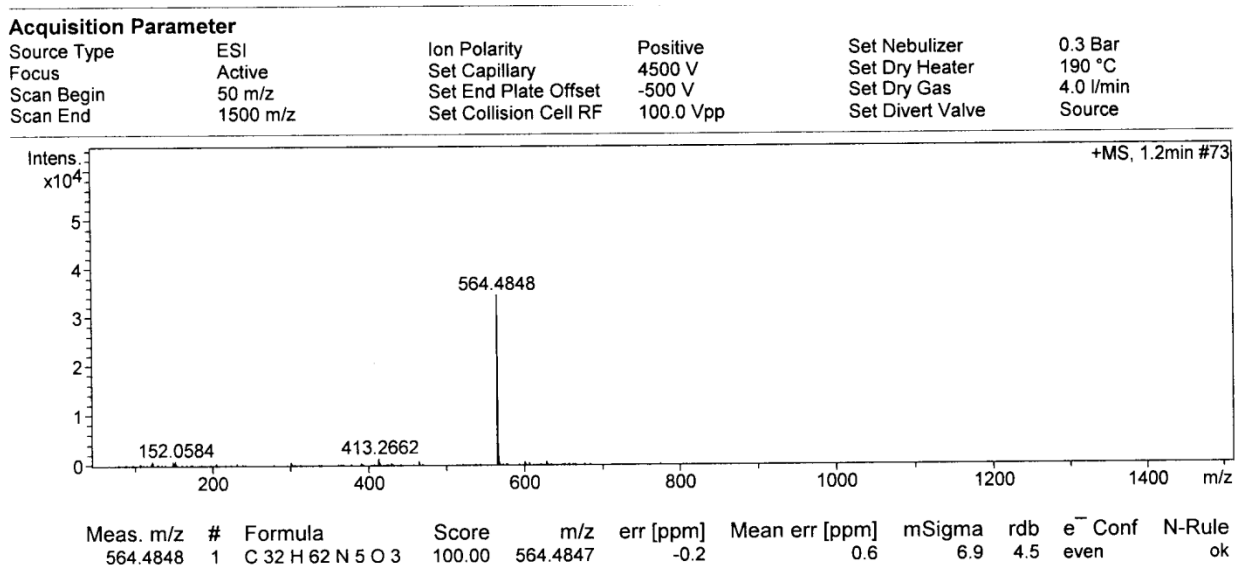


Figure S45. Mass Spectrum of **6e**.

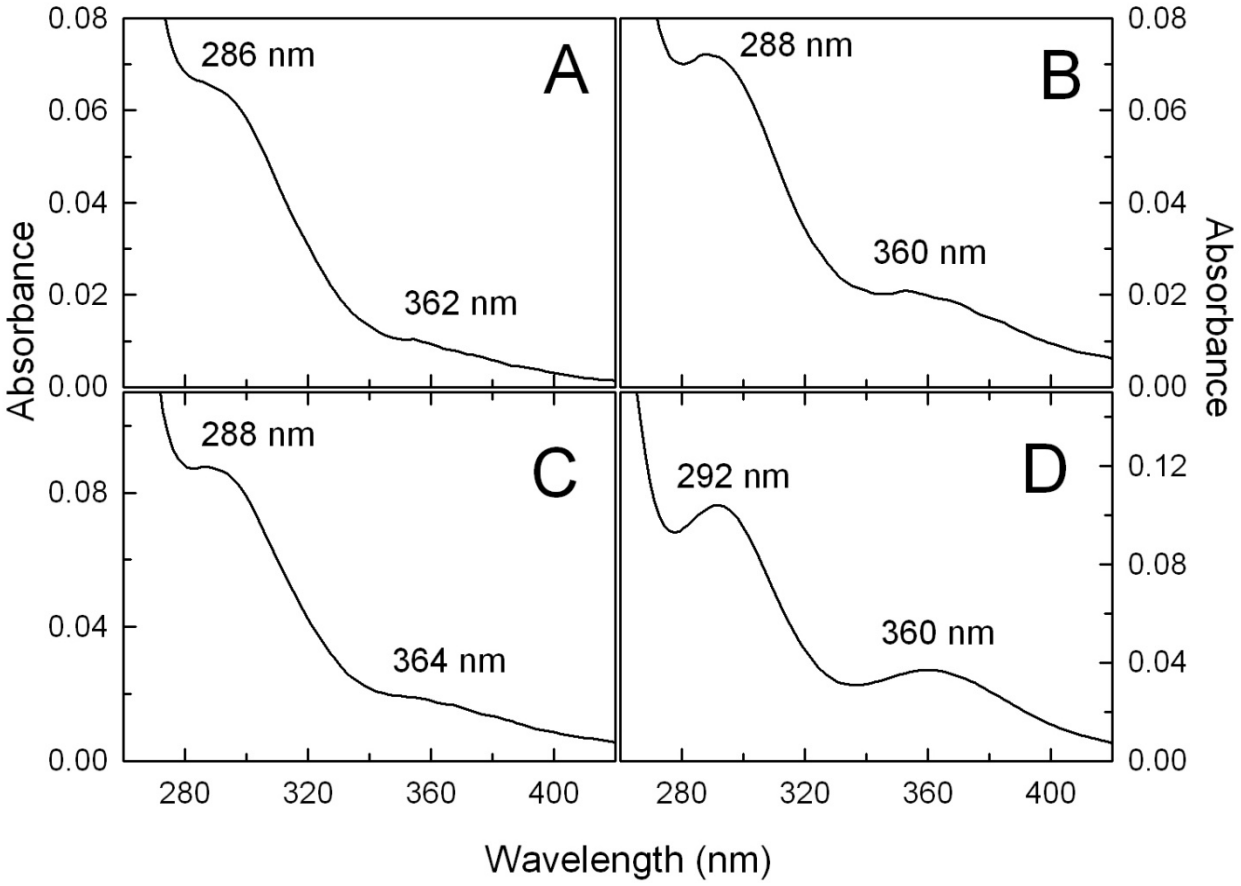


Figure S46. UV-vis absorbance spectra of 100 μM of Boc-val-[C_8-Tr][I] (panel A), Boc-val-[C_8-Tr][PF_6] (panel B), Boc-val-[C_{16}-Tr][I] (panel C), Boc-val-[C_{16}-Tr][PF_6] (panel D) dissolved in chloroform at ambient conditions.

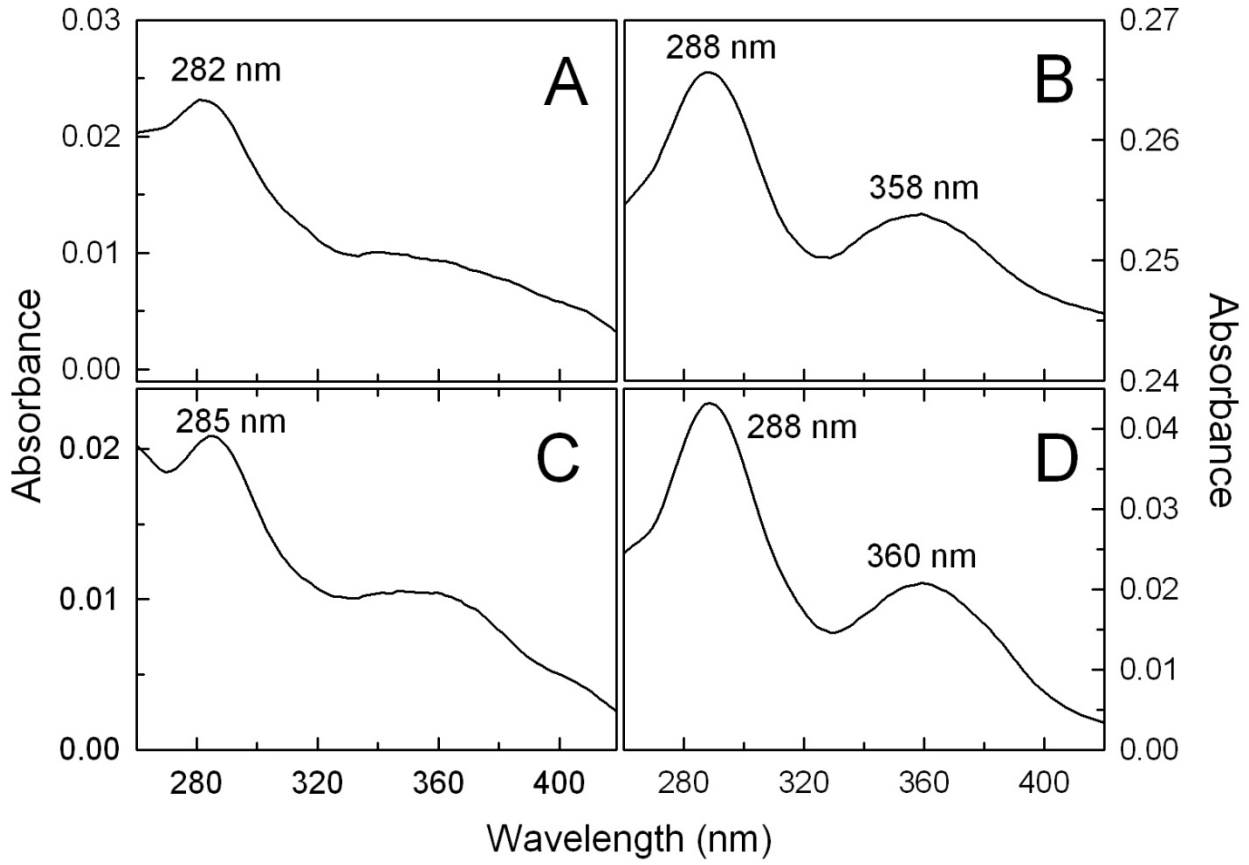


Figure S47. UV-vis absorbance spectra of 100 μM of Boc-val-[C_8-Tr][I] (panel A), Boc-val-[C_8-Tr][PF_6] (panel B), Boc-val-[C_{16}-Tr][I] (panel C), Boc-val-[C_{16}-Tr][PF_6] (panel D) dissolved in ethanol at ambient conditions.

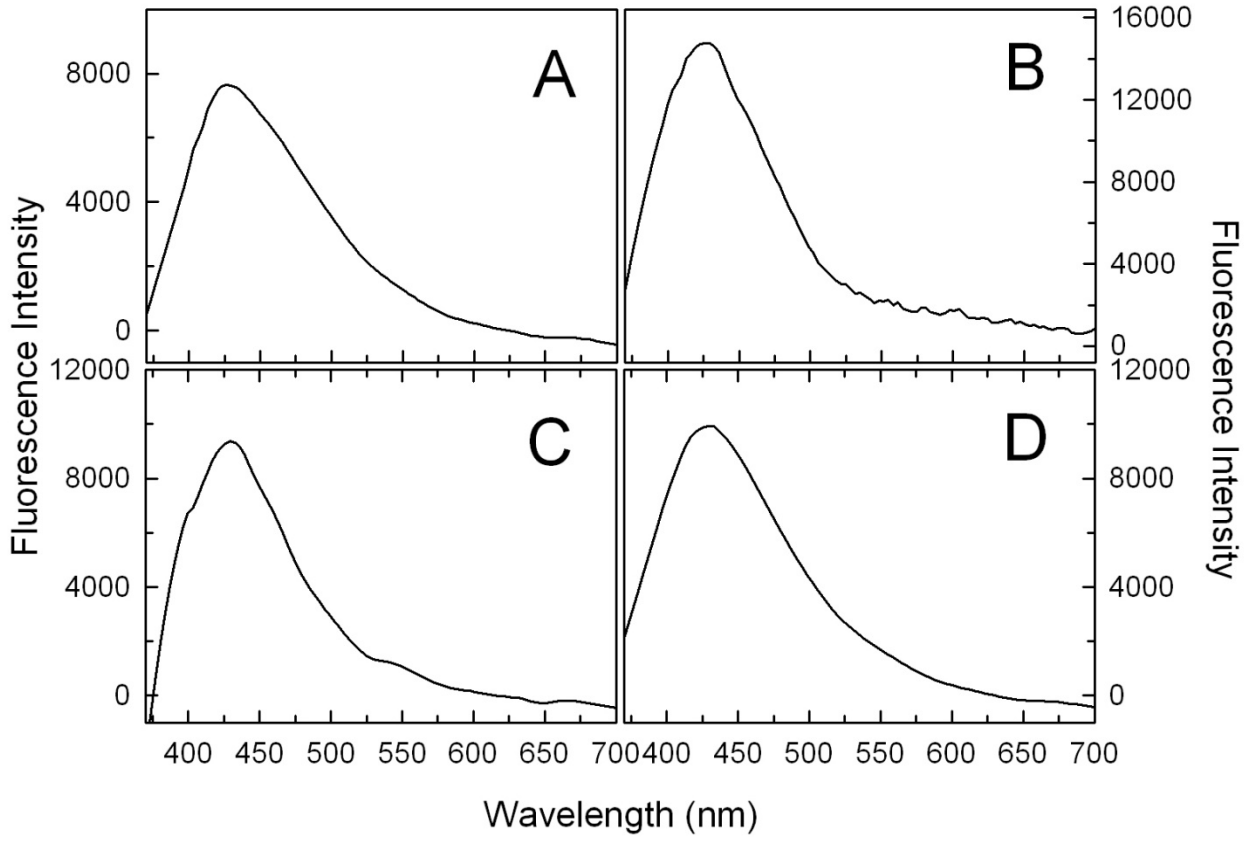


Figure S48. Emission spectra of CILs (25 μM) dissolved in ethanol: Boc-val-[C_8-Tr][I] (panel A); Boc-val-[C_8-Tr][PF_6] (panel B); Boc-val-[C_{16}-Tr][I] (panel C); Boc-val-[C_{16}-Tr][PF_6] (panel D) at ambient conditions [slits: 3/3, λ_{ex} = 360 nm].