

Supplementary Materials

Development of phenalenone-triazolium salts derivatives for aPDT: synthesis and antibacterial screening.

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Table S1. Molar extinction coefficient (ϵ), fluorescence quantum yield (Φ_f), and singlet oxygen quantum yield (Φ_Δ) of the tested PN in water

Compound	ϵ (L.mol ⁻¹ .cm ⁻¹)	Φ_f	Φ_Δ
PNS	9026.88	<0.01	0.97
4a	3538.81	0.02	0.80
4b	6824.01	0.01	>0.98
5a	8074.44	0.02	0.97
5b	7265.28	<0.01	0.31
6a	7818.8	<0.01	0.70
6b	4009.84	<0.01	0.59
7a	3493.81	<0.01	>0.99
7b	4421.33	<0.01	N/A – signal not good
8a	4189.9	<0.01	>0.99
8b	5932.82	<0.01	N/A – signal not good
9a	2417.86	0.02	0.93
9b	3590.89	0.01	0.23
10a	3243.01	0.02	0.87
10b	6414.40	0.02	N/A – signal not good
5	10396.61	0.02	0.87
10	2790.03	0.02	0.91
SAPyr	2834.47	0.02	0.83

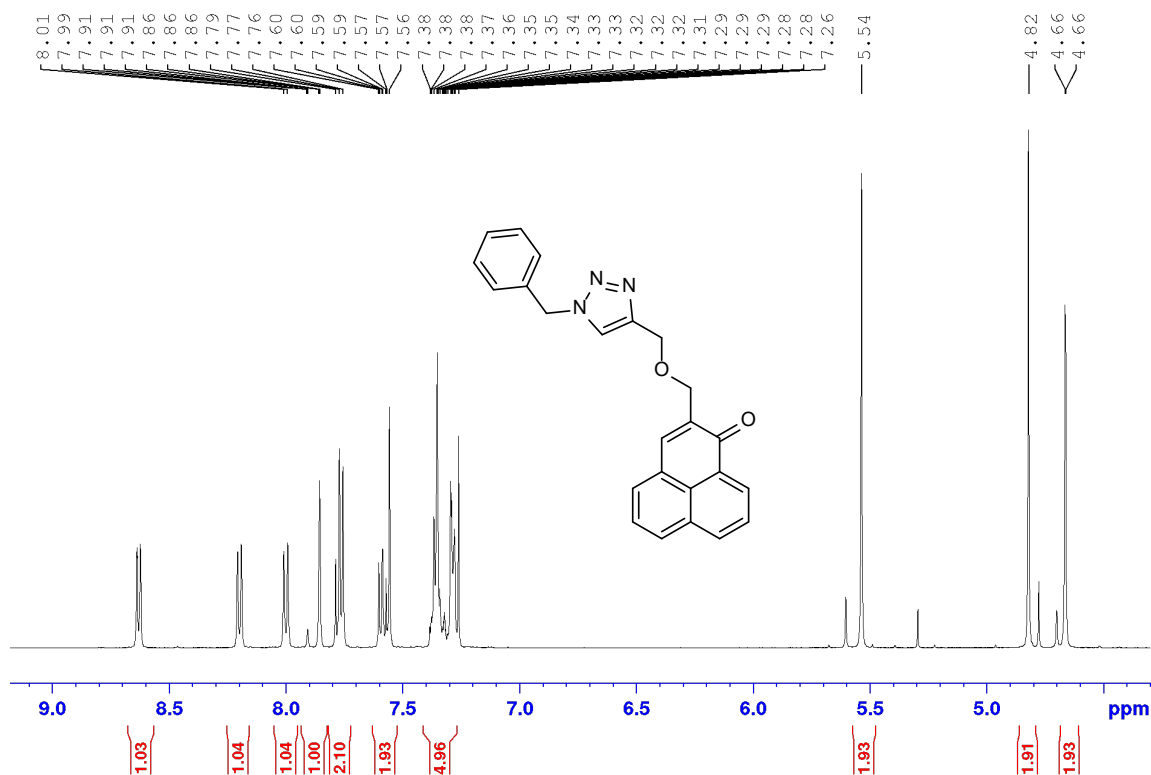


Figure S1. ¹H NMR of compound 7 in CDCl₃

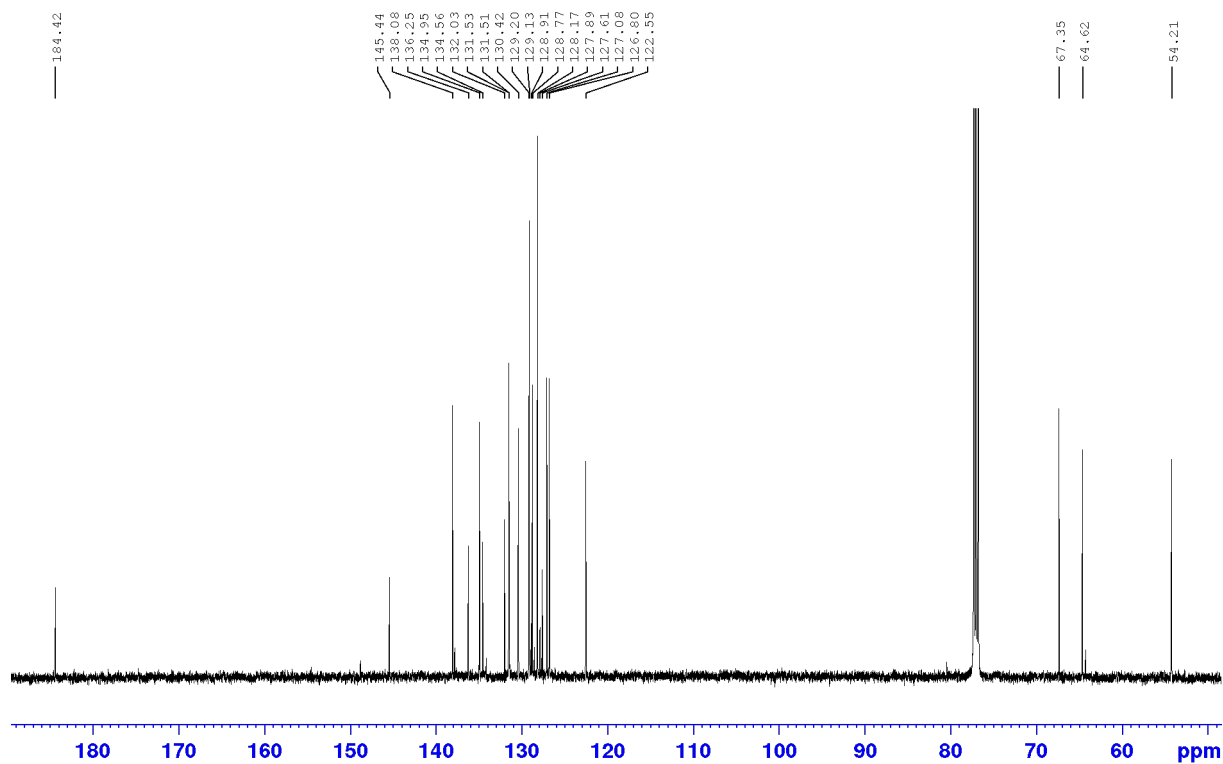


Figure S2. ¹³C NMR of compound 7 in CDCl₃

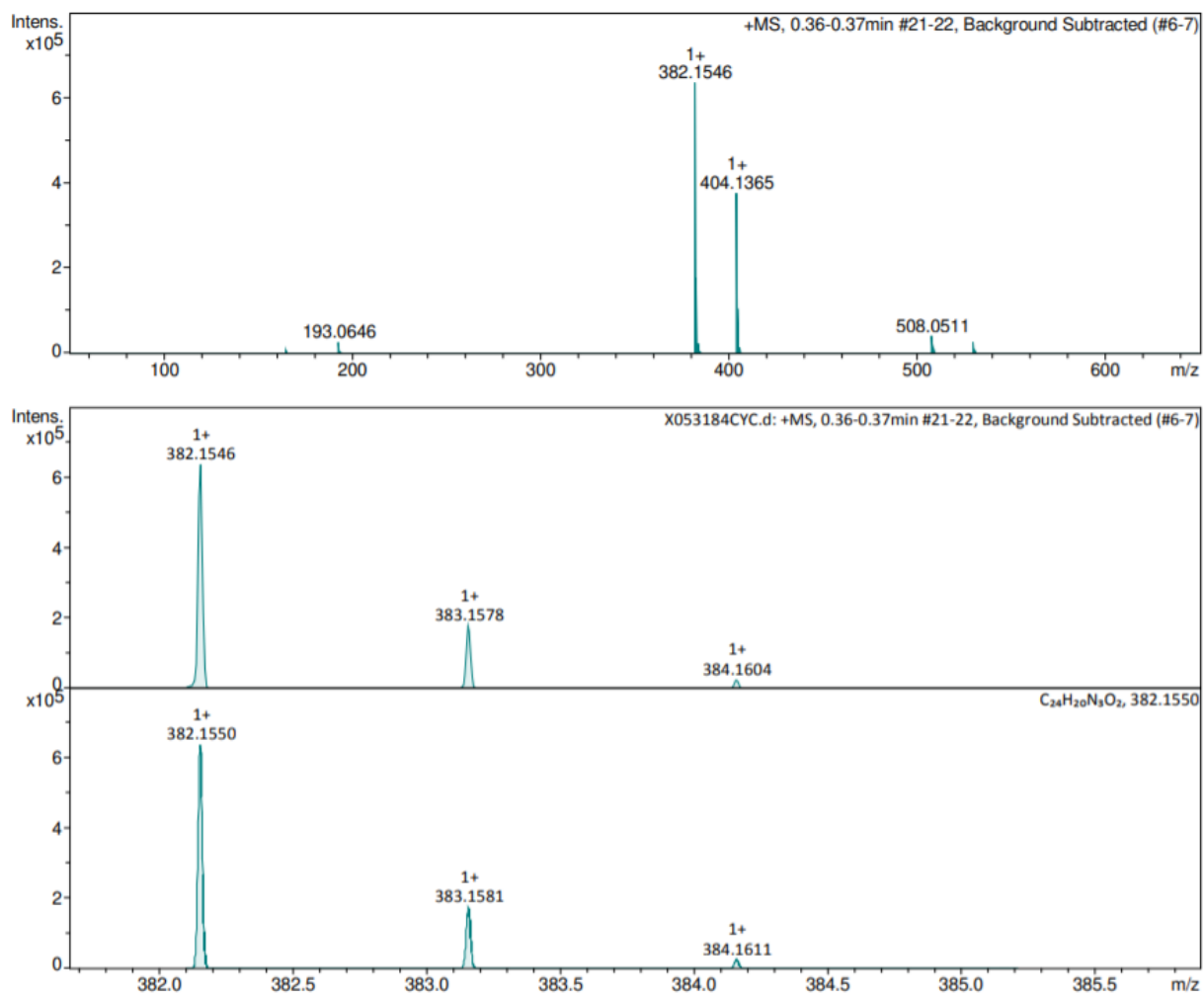


Figure S3. HRMS ESI⁺ of compound 7

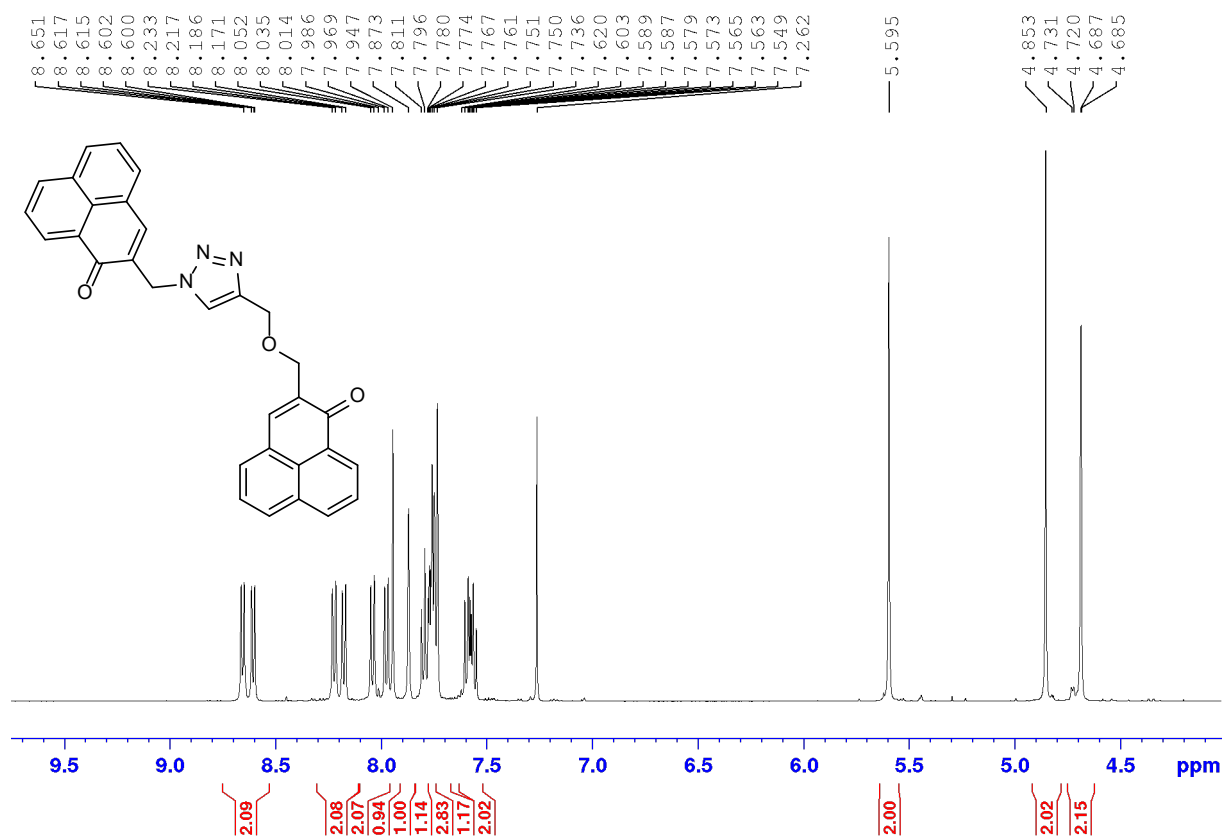


Figure S4. ¹H NMR of compound 8 in CDCl₃

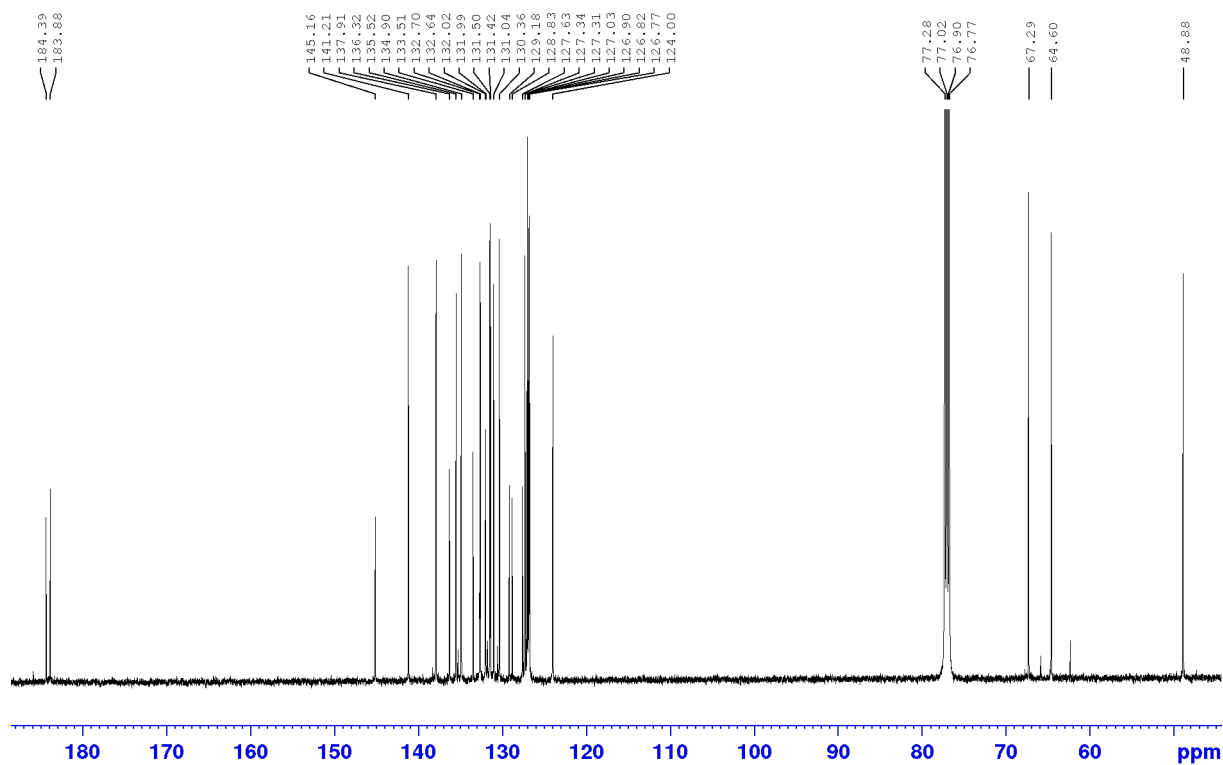


Figure S5. ¹³C NMR of compound 8 in CDCl₃

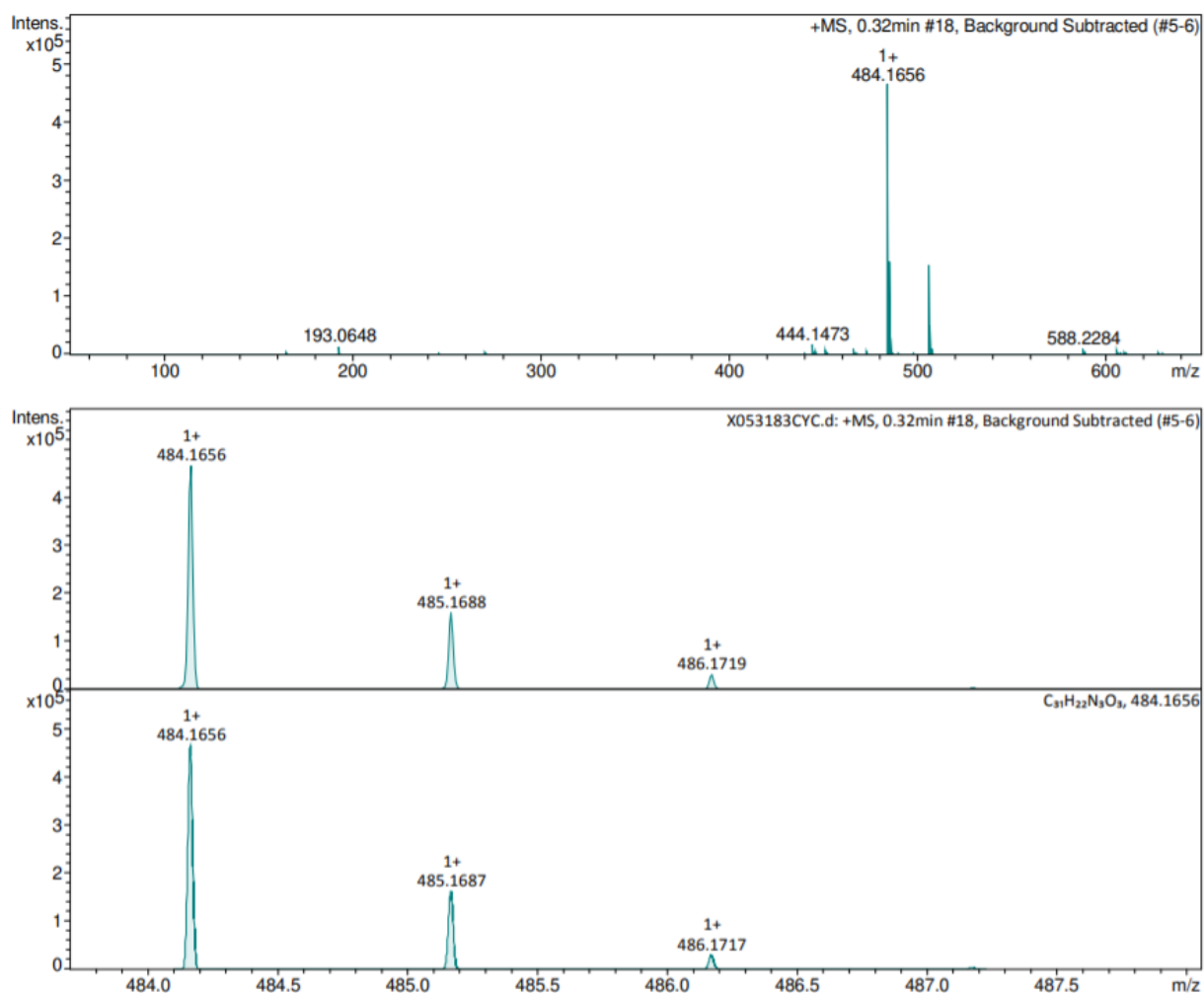


Figure S6. HRMS ESI⁺ of compound 8

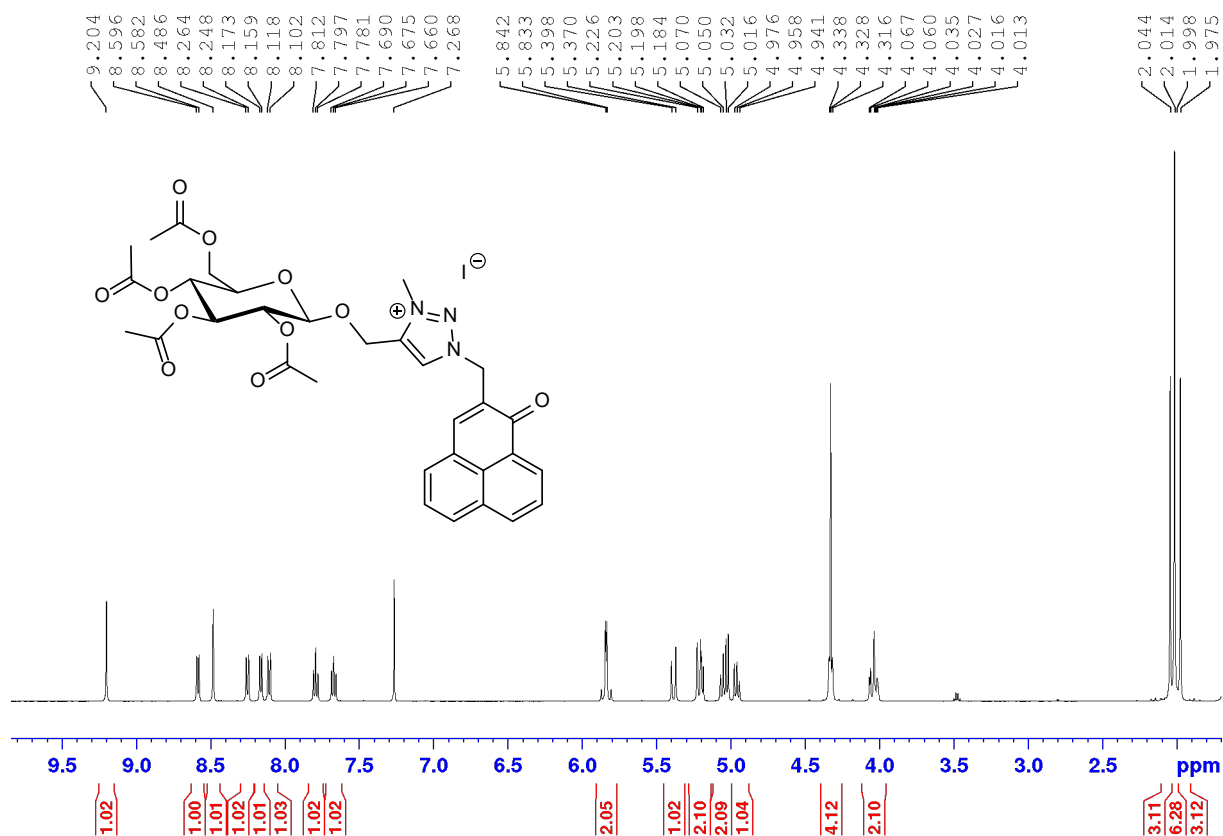


Figure S7. ¹H NMR of compound **4a** in CDCl₃

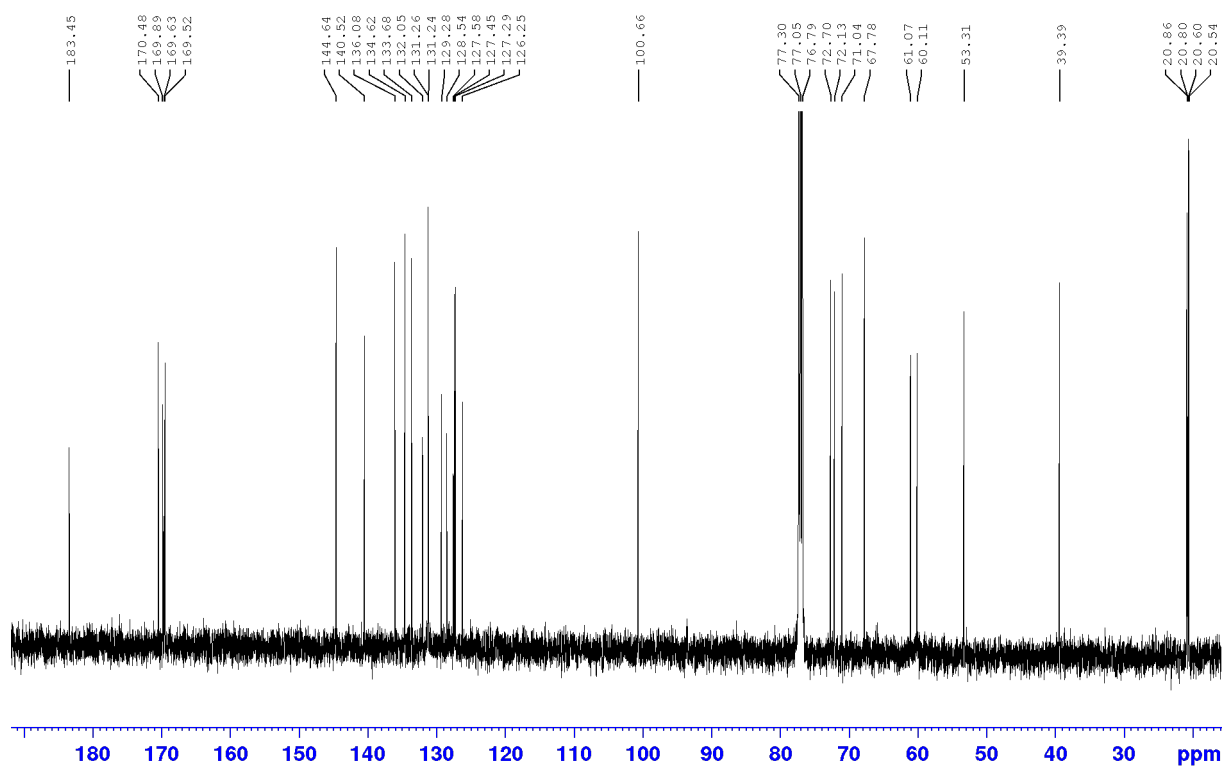


Figure S8. ¹³C NMR of compound **4a** in CDCl₃

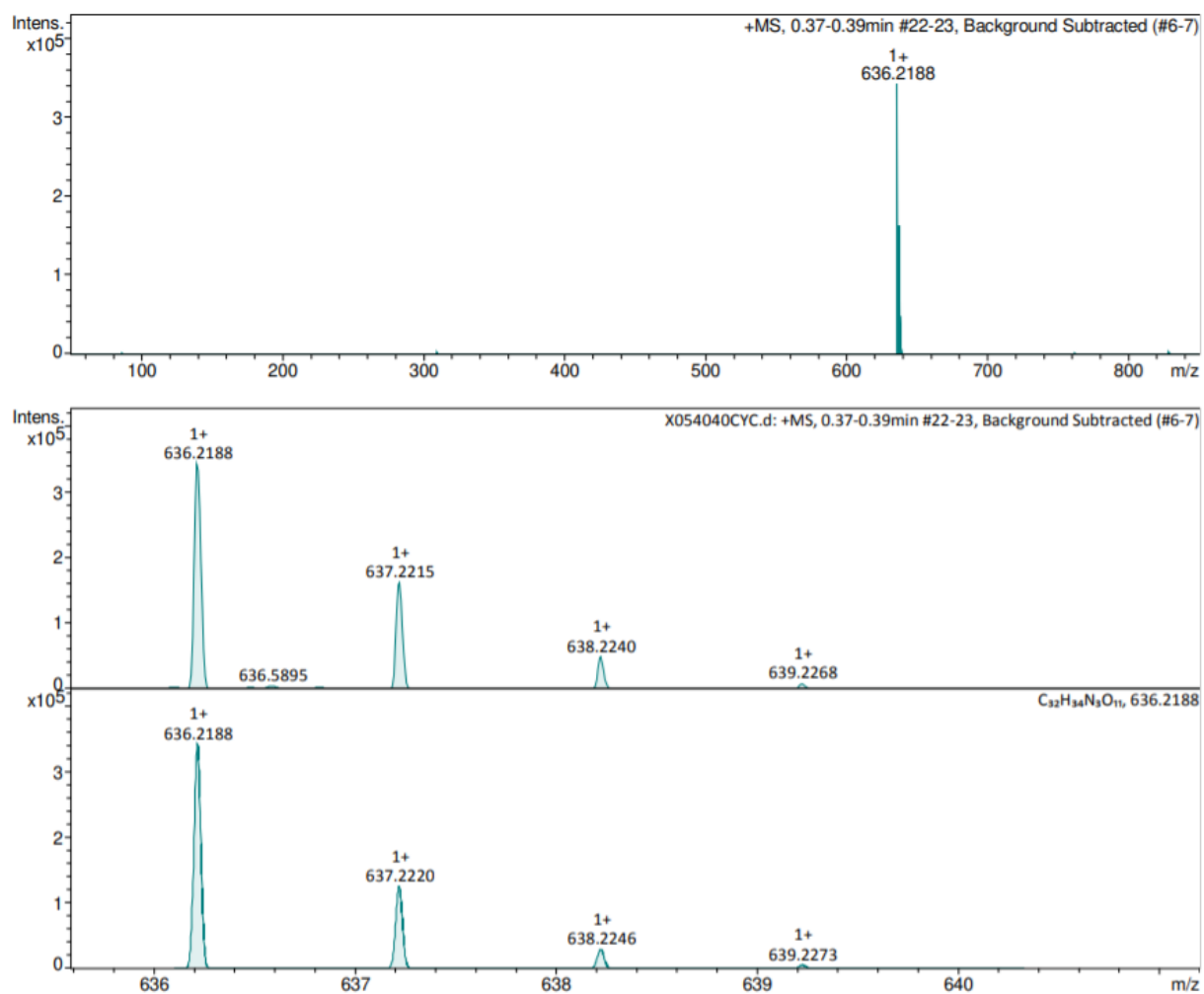


Figure S9. HRMS ESI⁺ of compound 4a

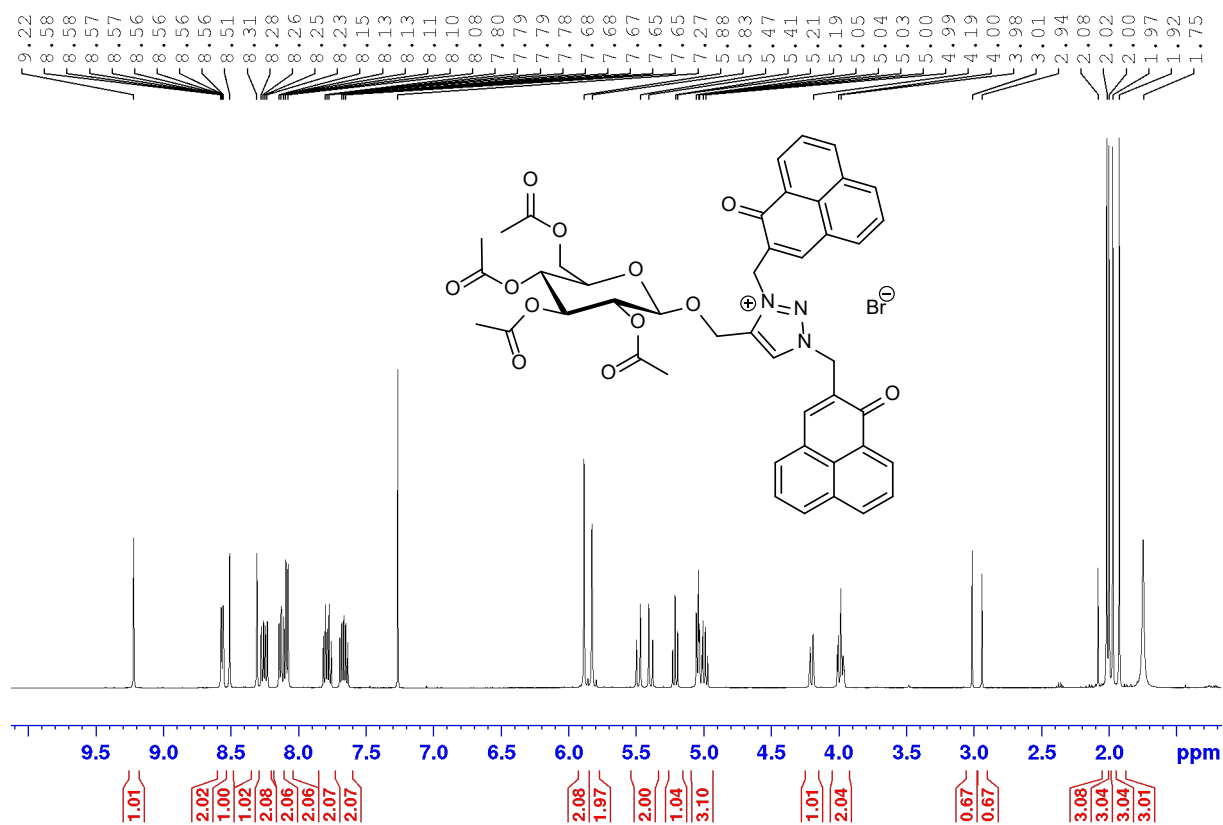


Figure S10. ¹H NMR of compound **4b** in CDCl₃

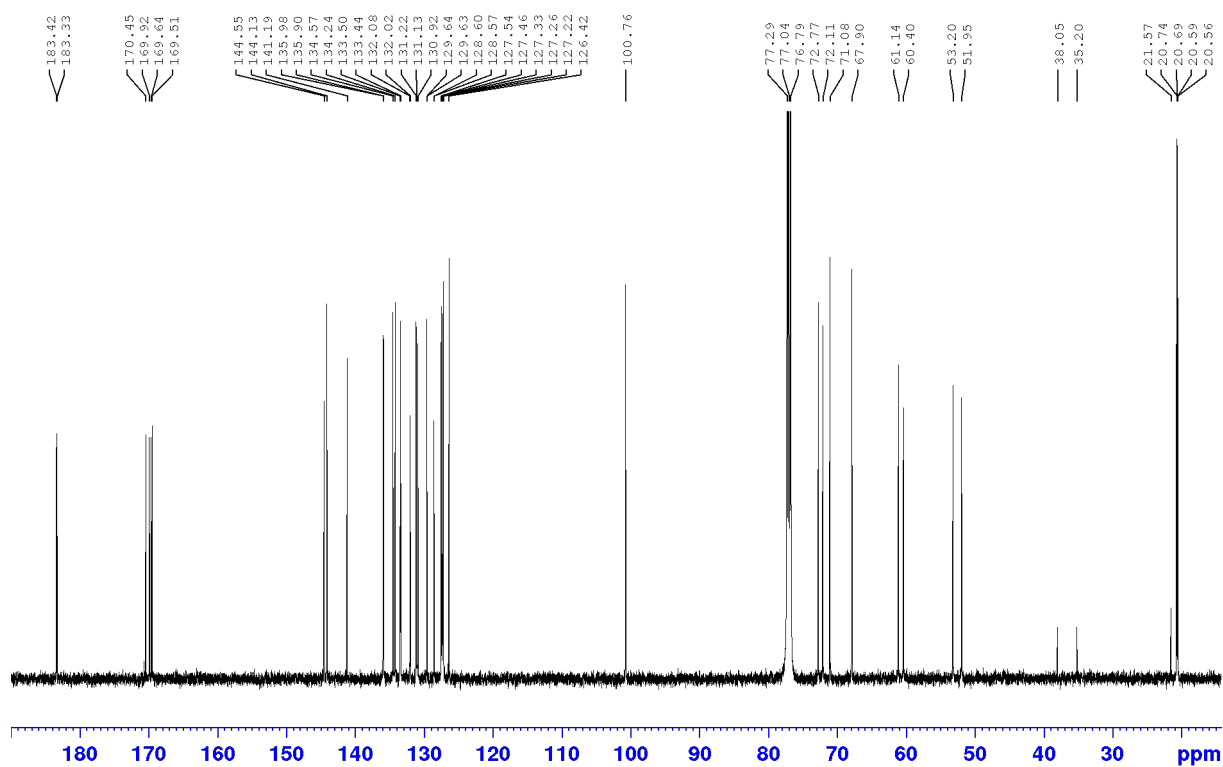


Figure S11. ¹³C NMR of compound **4b** in CDCl₃

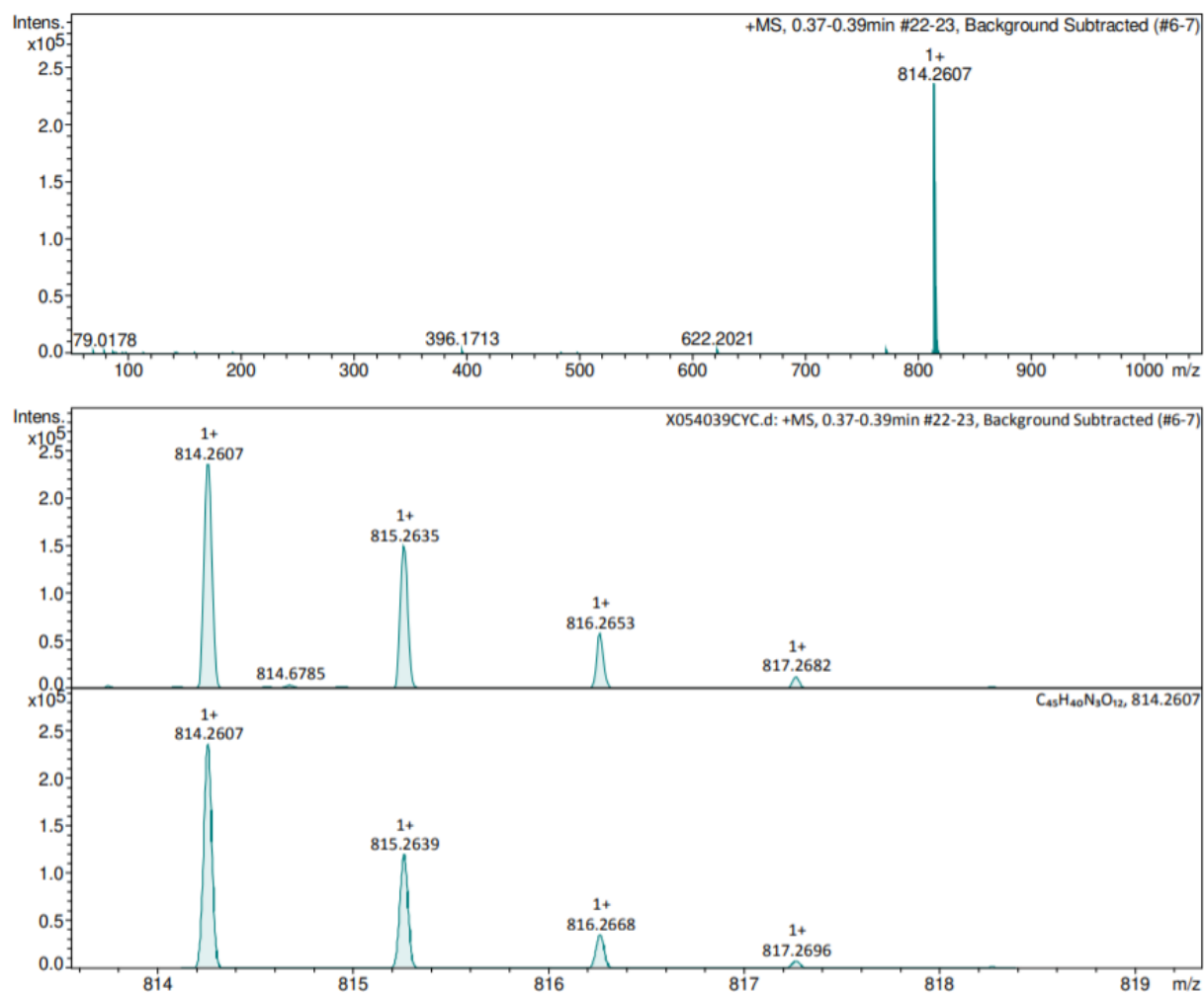


Figure S12. HRMS ESI⁺ of compound **4b**

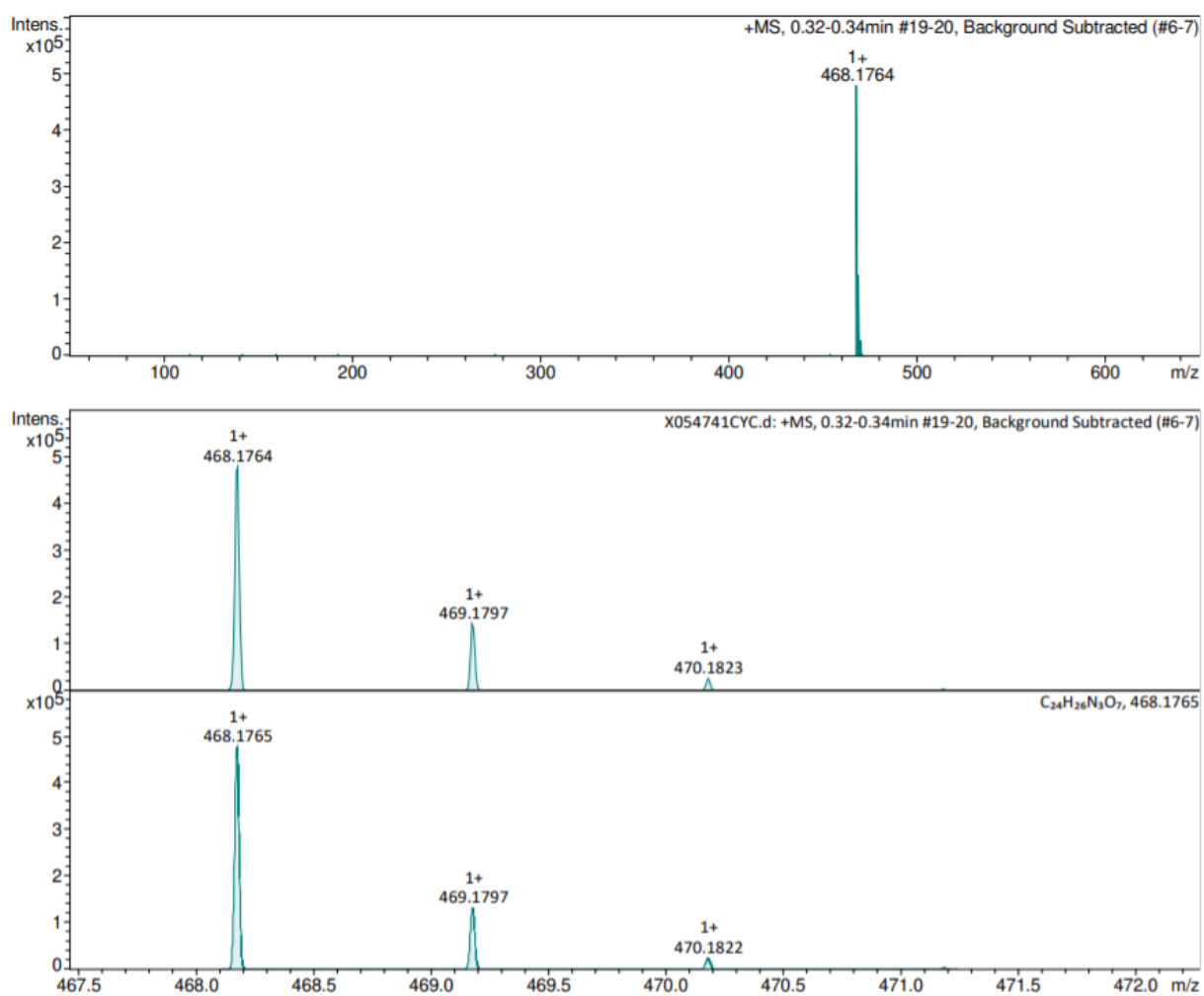


Figure S15. HRMS ESI⁺ of compound 5a

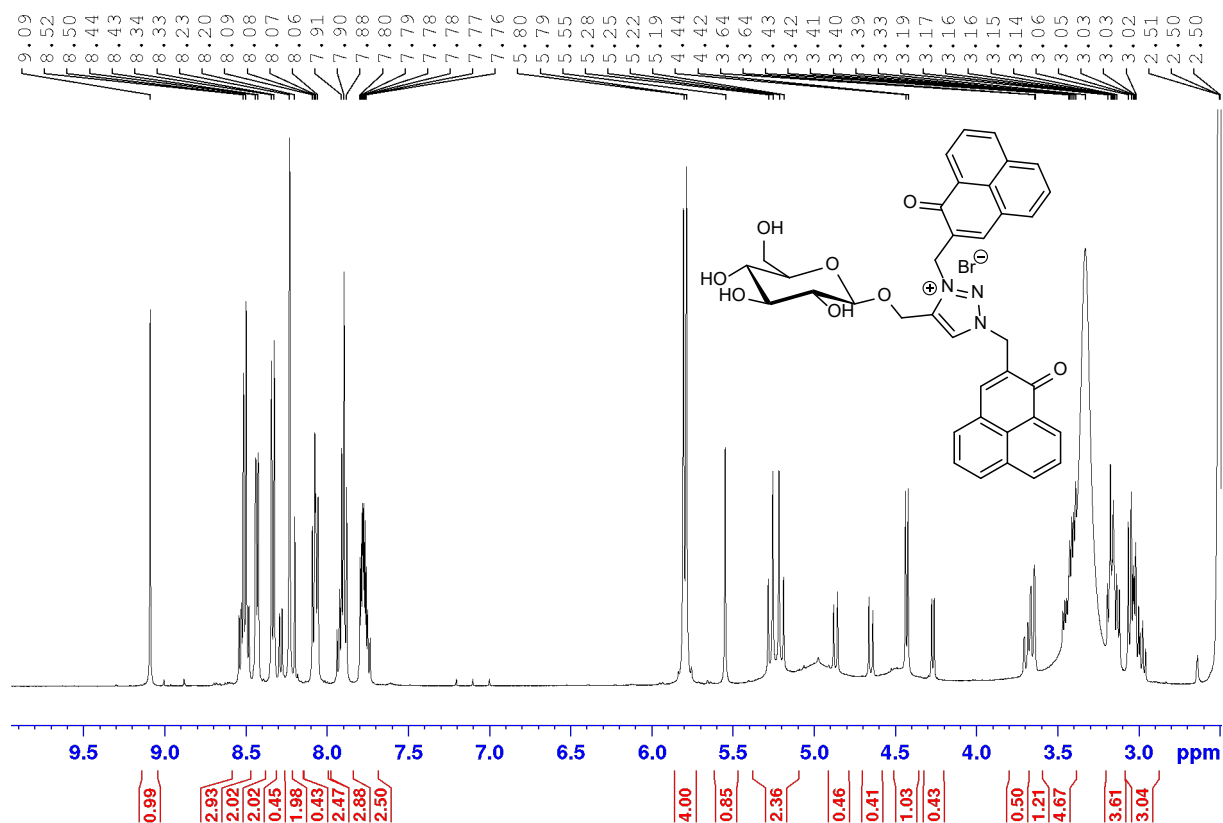


Figure S16. ¹H NMR of compound **5b** in D₂O

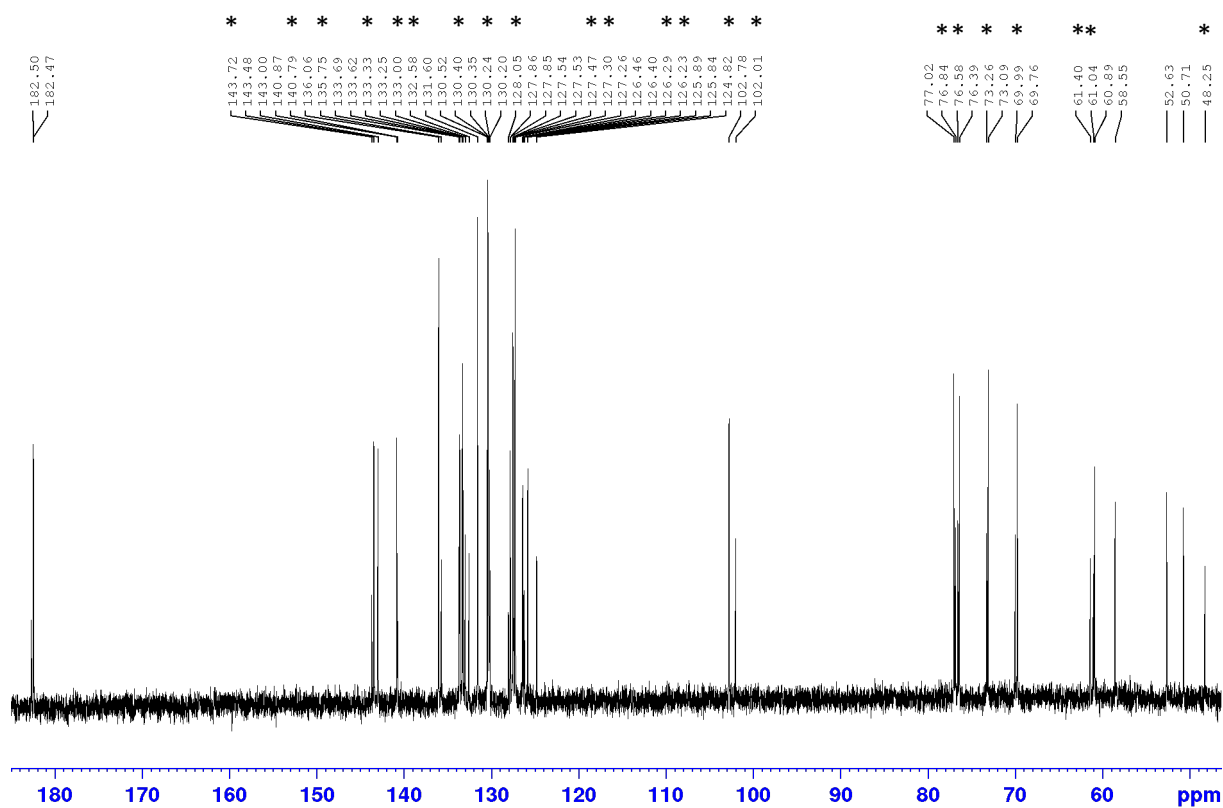


Figure S17. ¹³C NMR of compound **5b** in D₂O (*contamination by compound **5**)

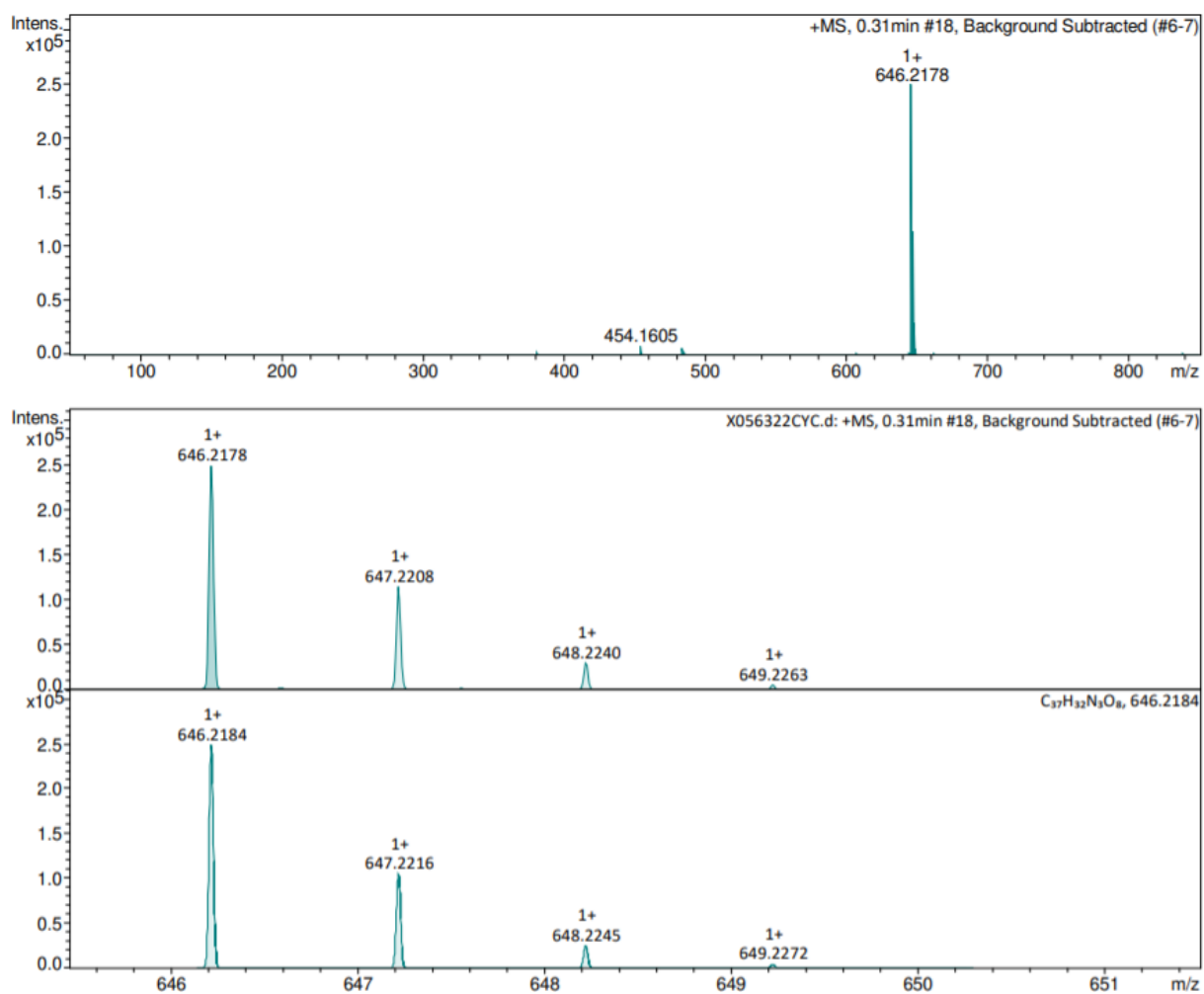


Figure S18. HRMS ESI⁺ of compound **5b**

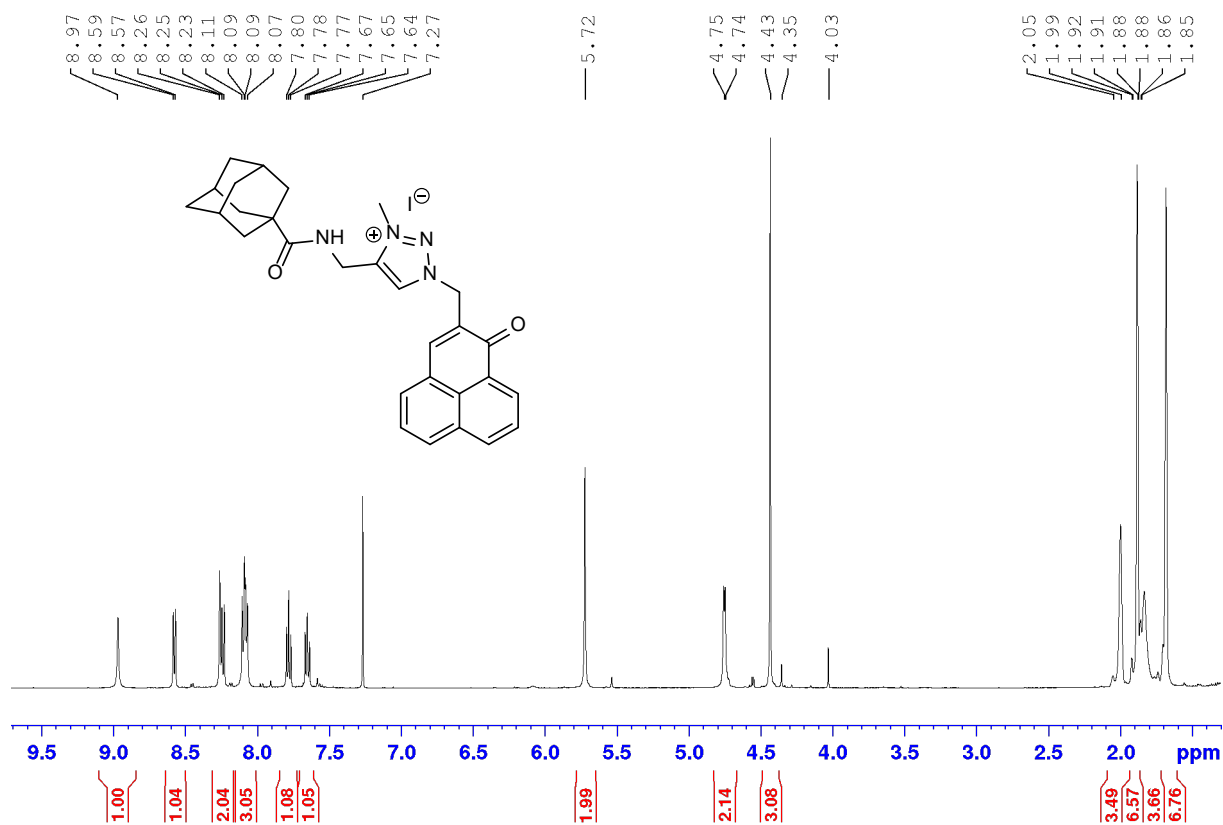


Figure S19. ¹H NMR of compound **6a** in CDCl₃

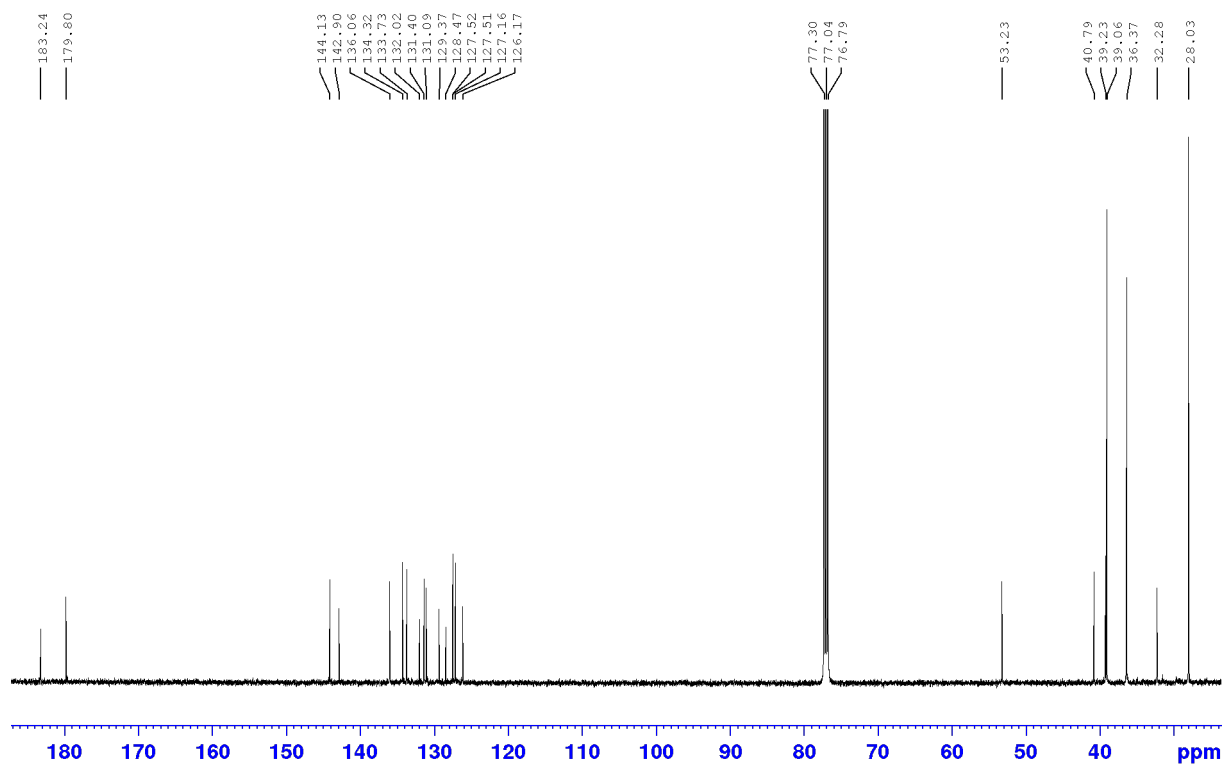


Figure S20. ¹³C NMR of compound **6a** in CDCl₃

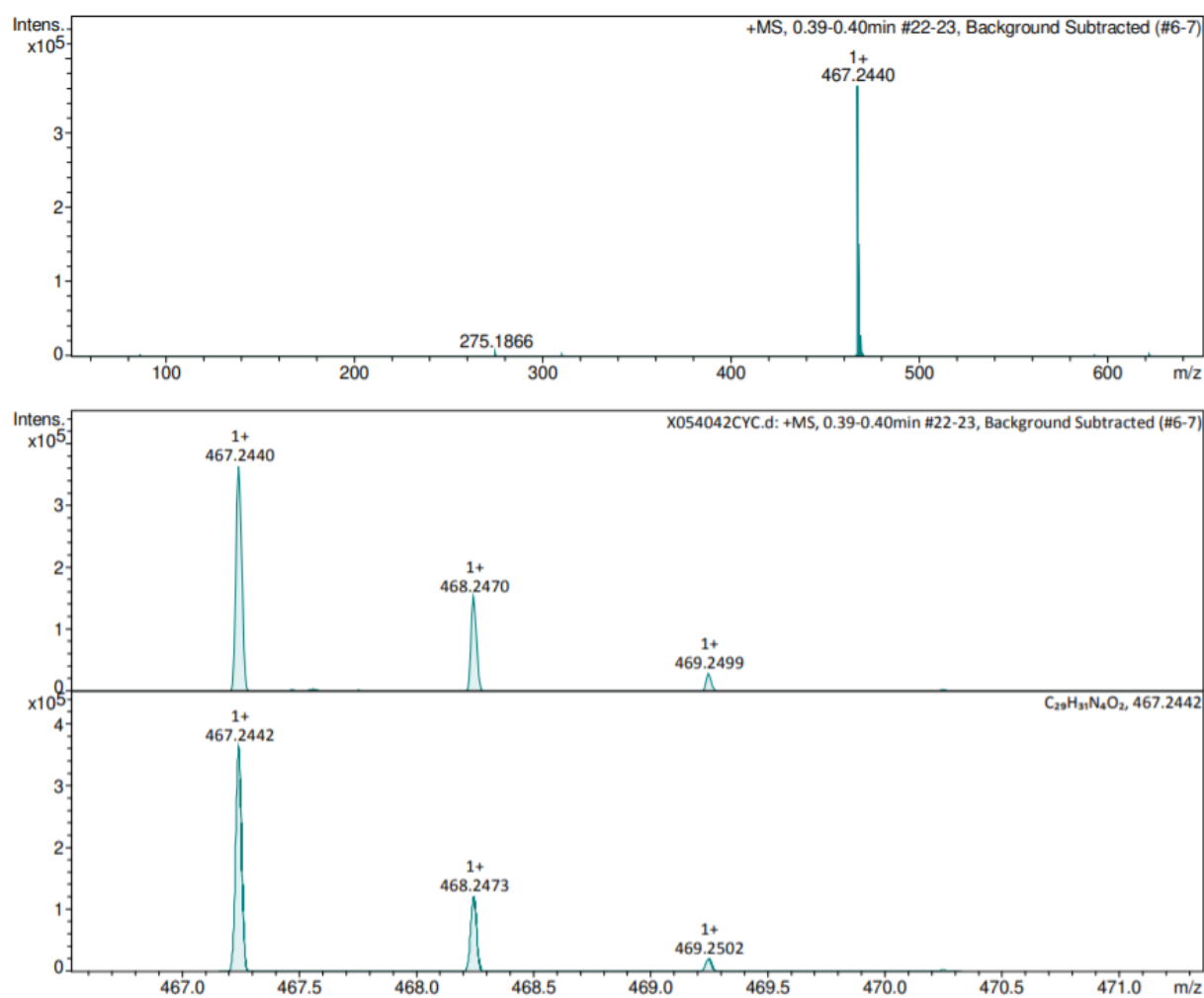


Figure S21. HRMS ESI⁺ of compound 6a

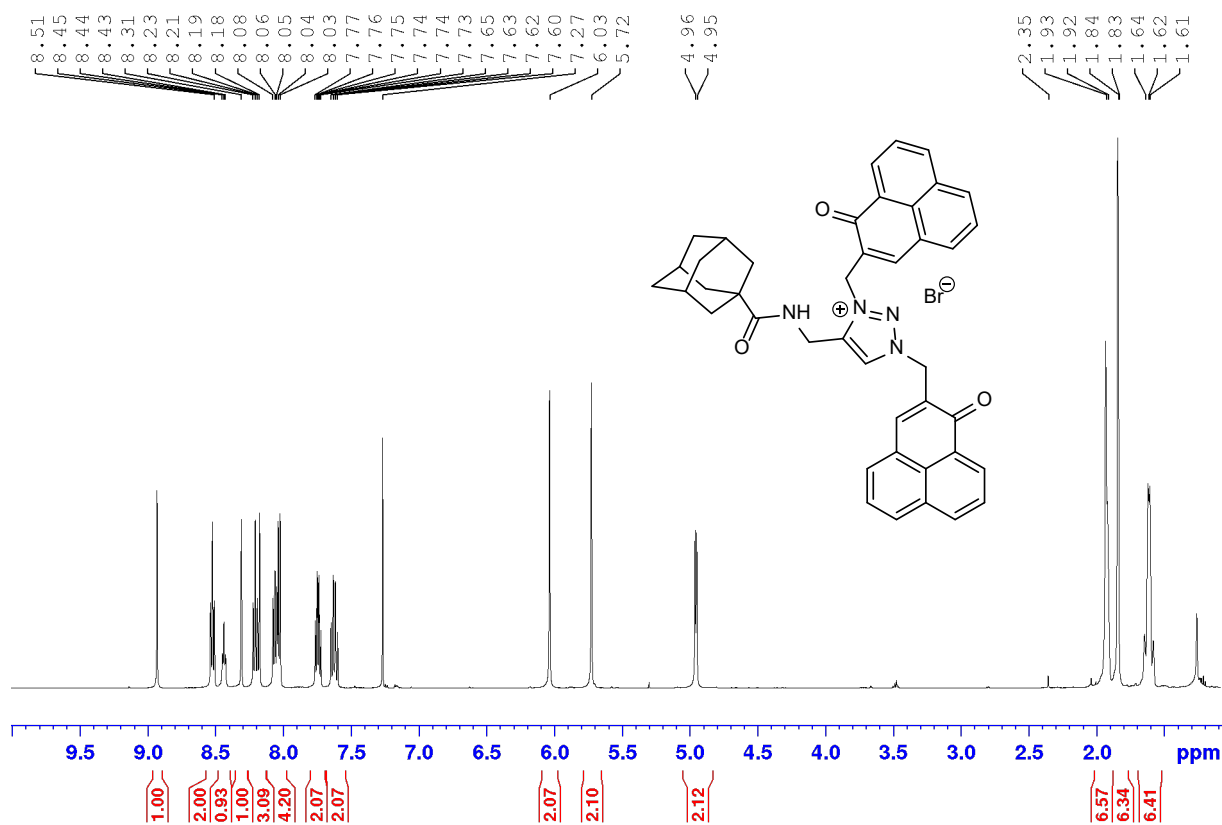


Figure S22. ¹H NMR of compound **6b** in CDCl₃

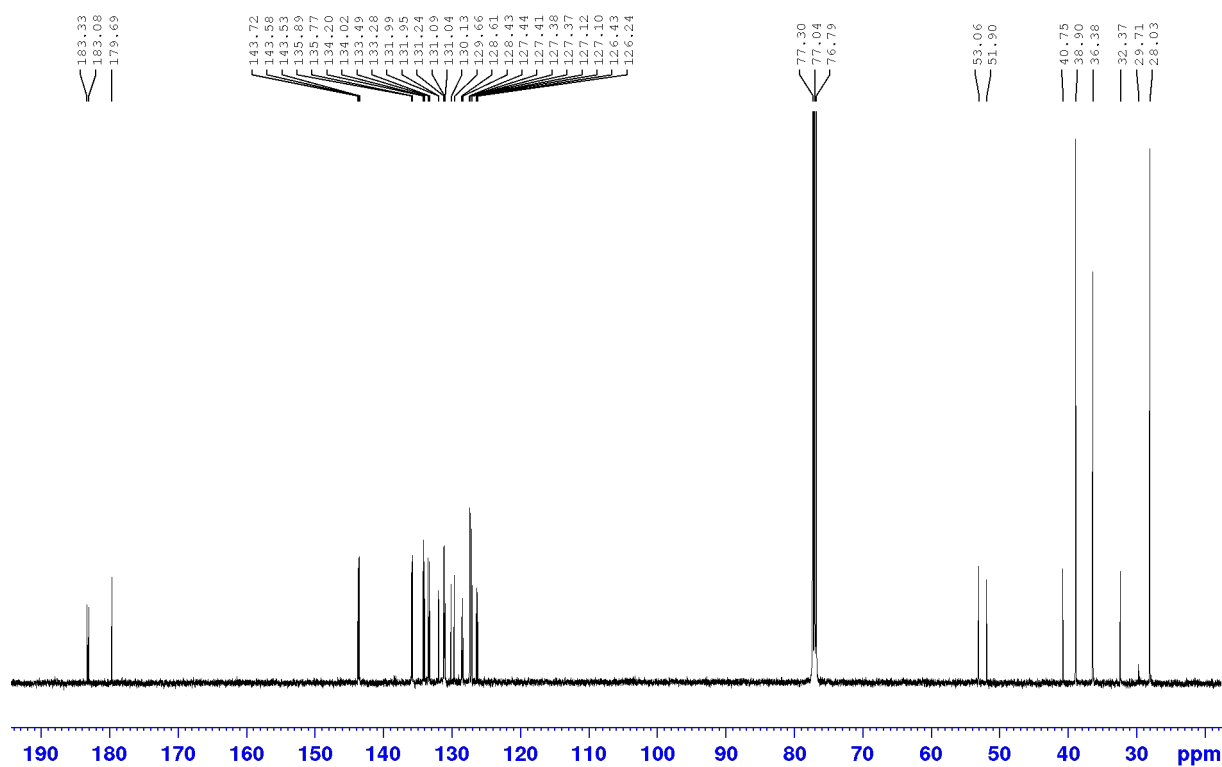


Figure S23. ¹³C NMR of compound **6b** in CDCl₃

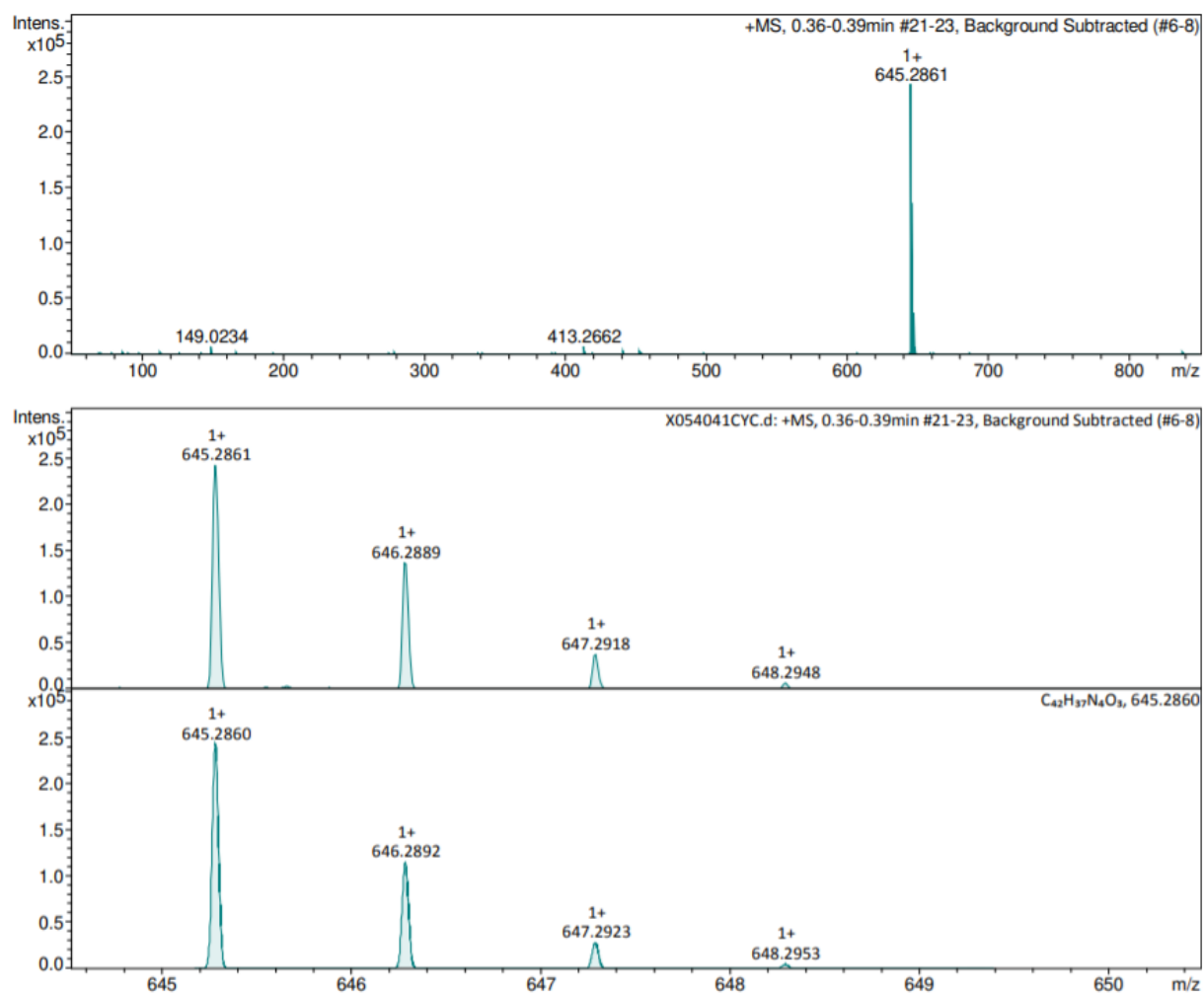


Figure S24. HRMS ESI⁺ of compound **6b**

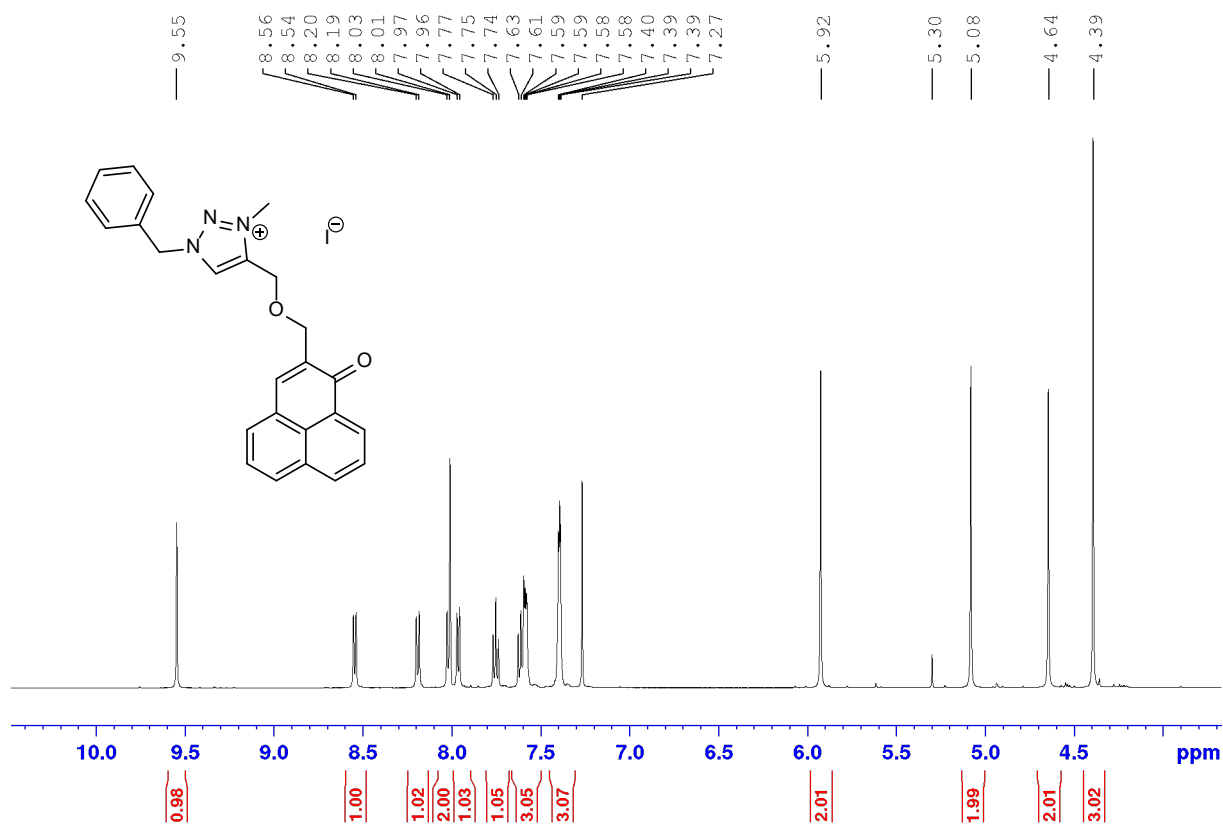


Figure S25. ¹H NMR of compound **7a** in CDCl₃

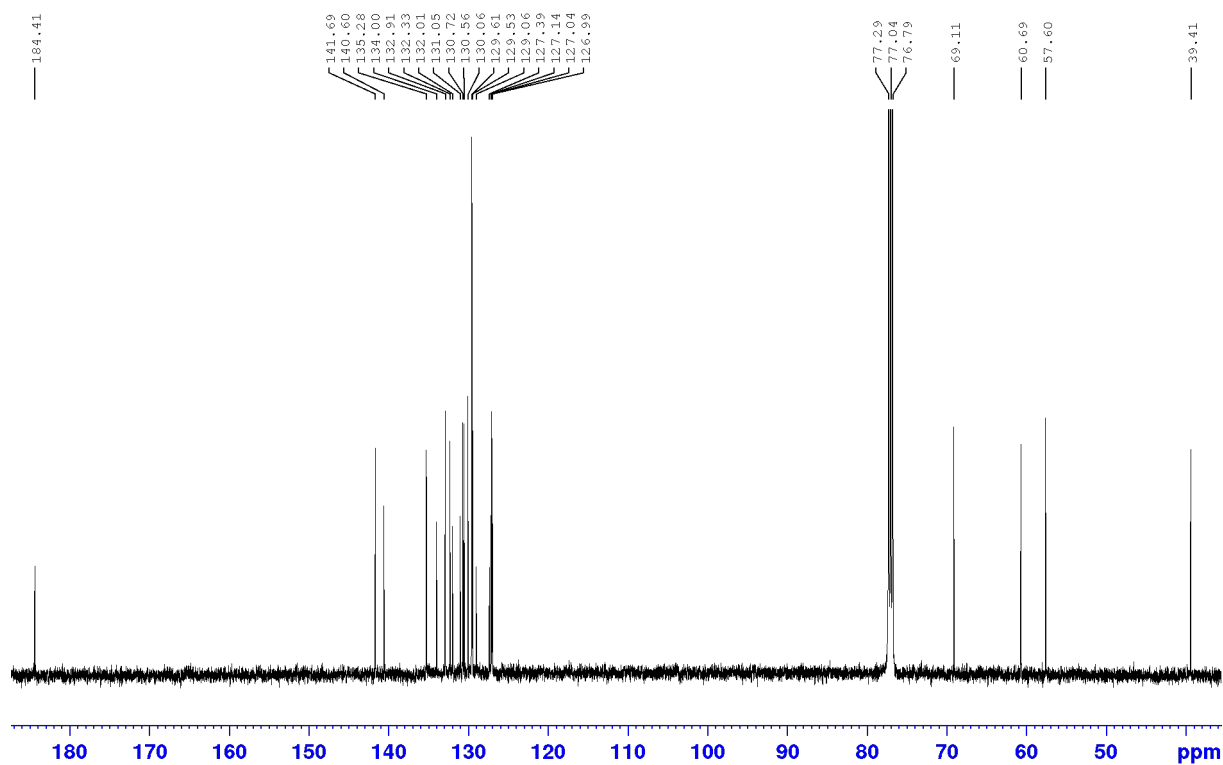


Figure S26. ¹³C NMR of compound **7a** in CDCl₃

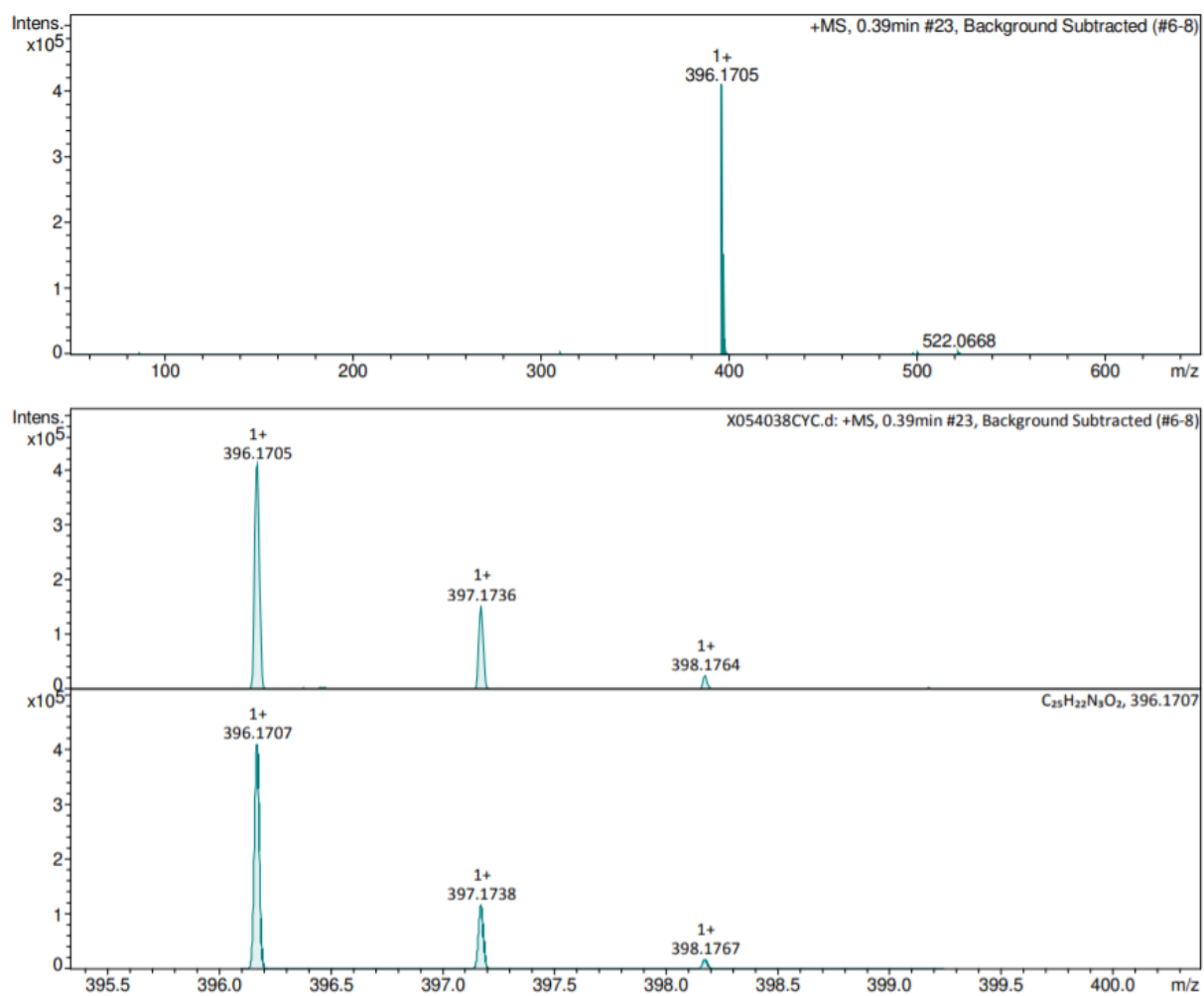


Figure S27. HRMS ESI⁺ of compound **7a**

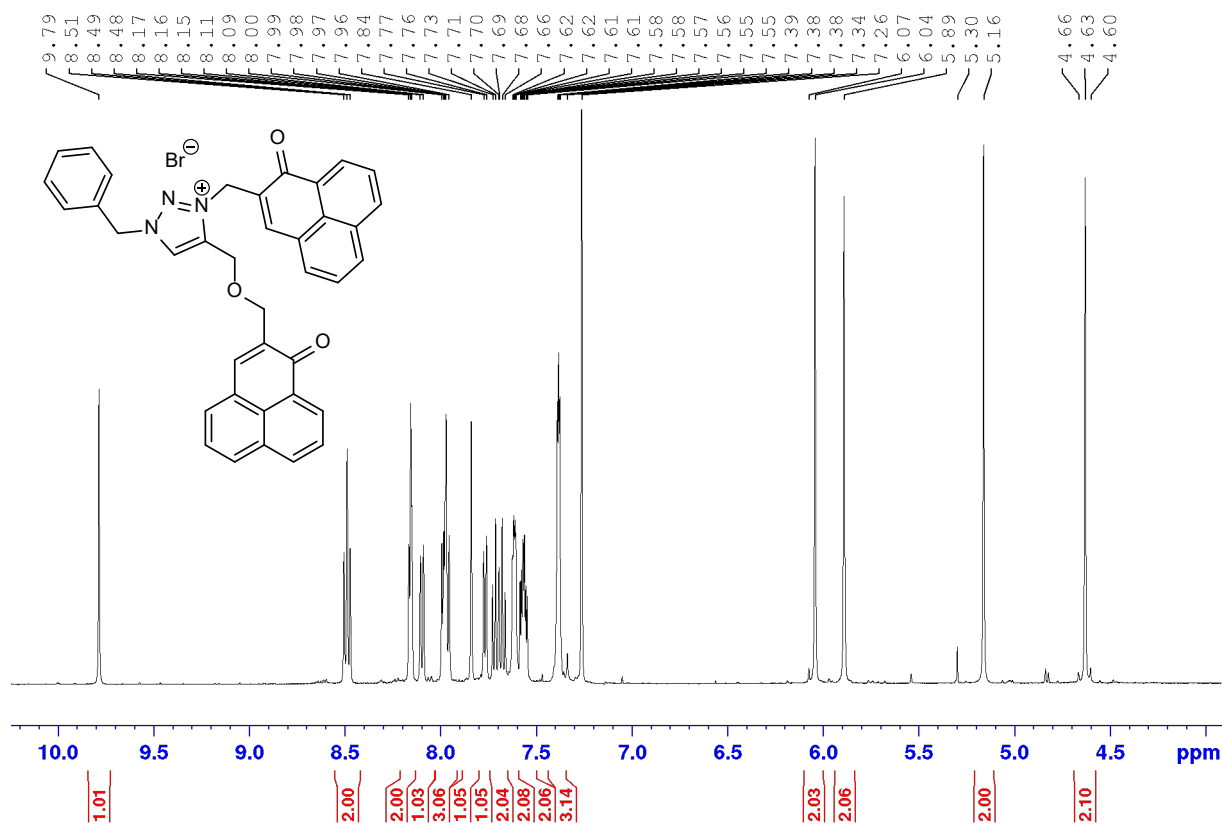


Figure S28. ¹H NMR of compound **7b** in CDCl₃

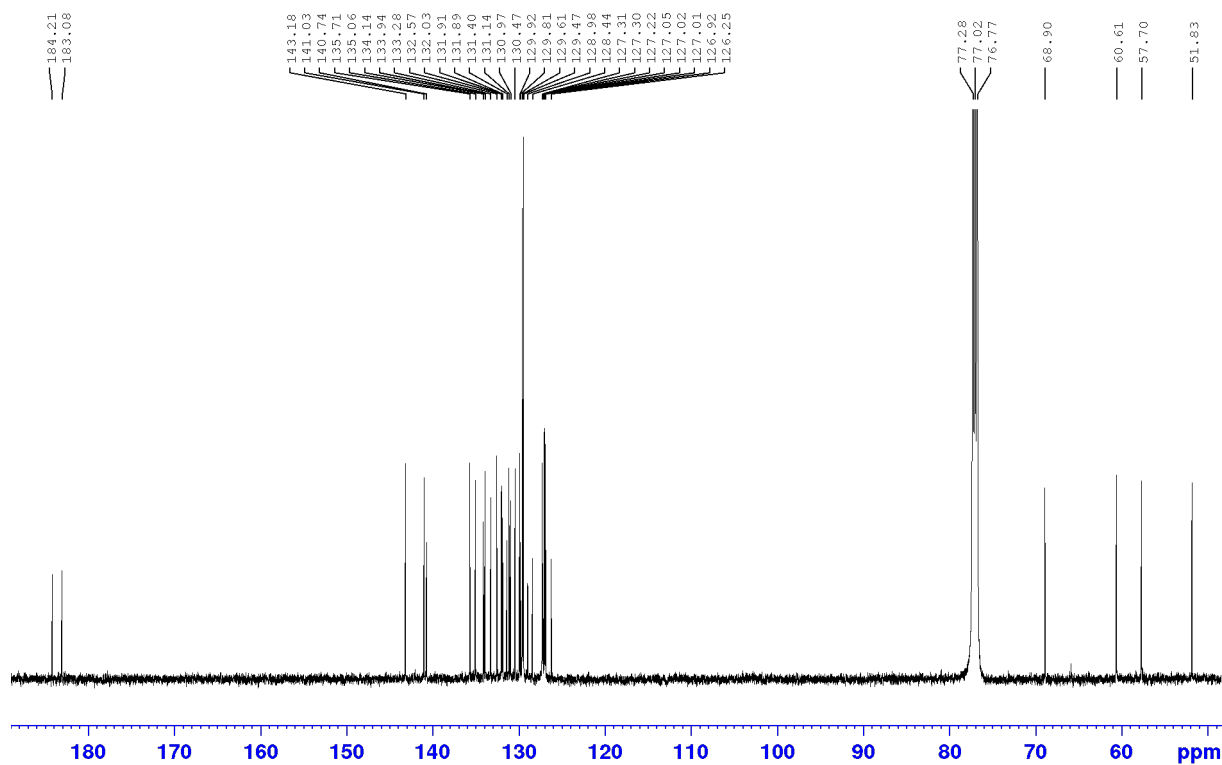


Figure S29. ¹³C NMR of compound **7b** in CDCl₃

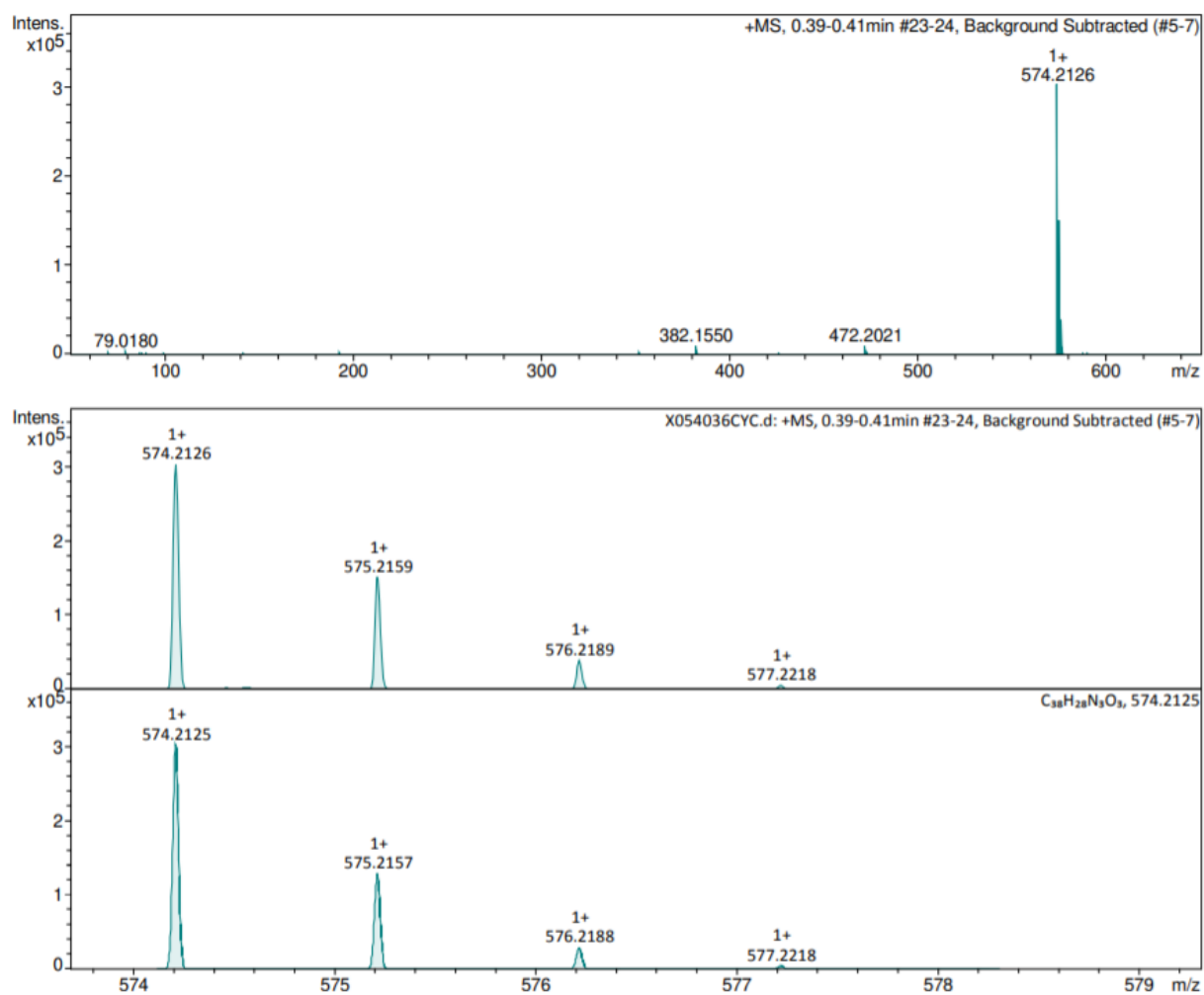


Figure S30. HRMS ESI⁺ of compound **7b**

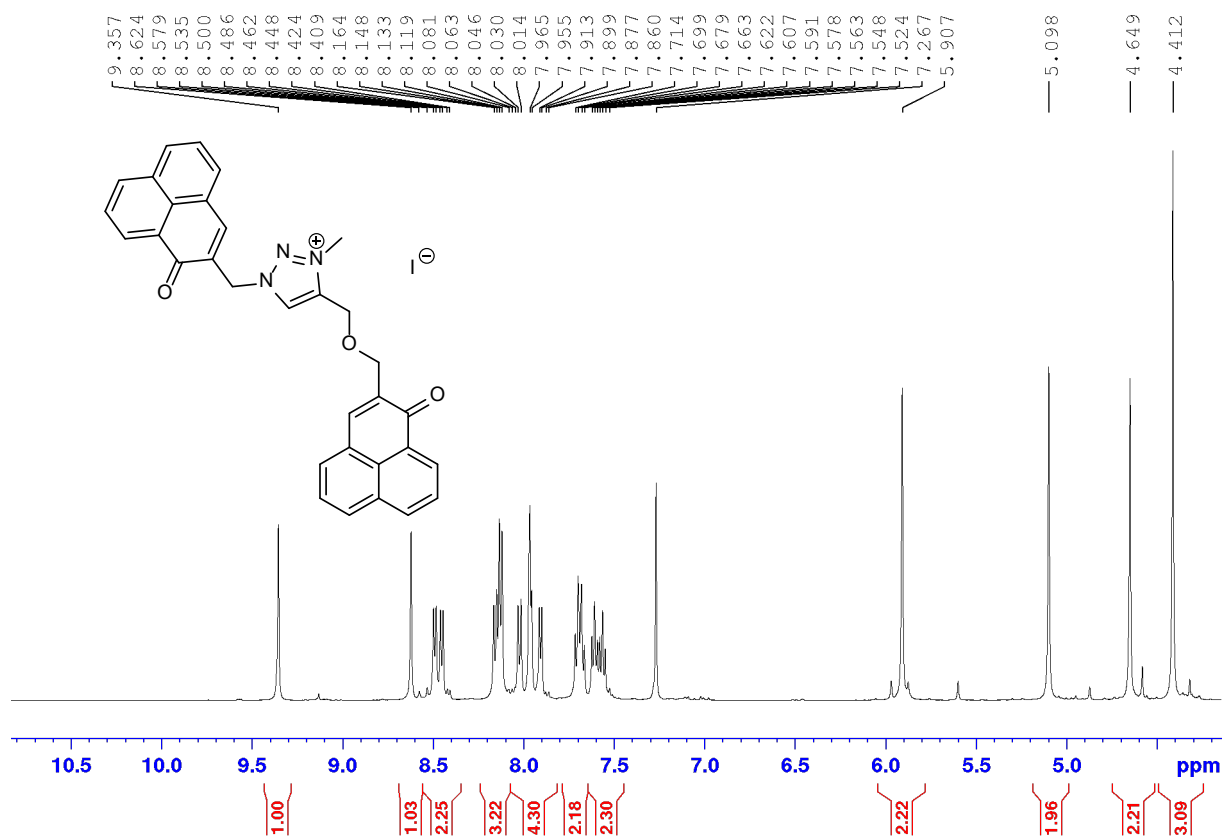


Figure S31. ¹H NMR of compound **8a** in CDCl₃

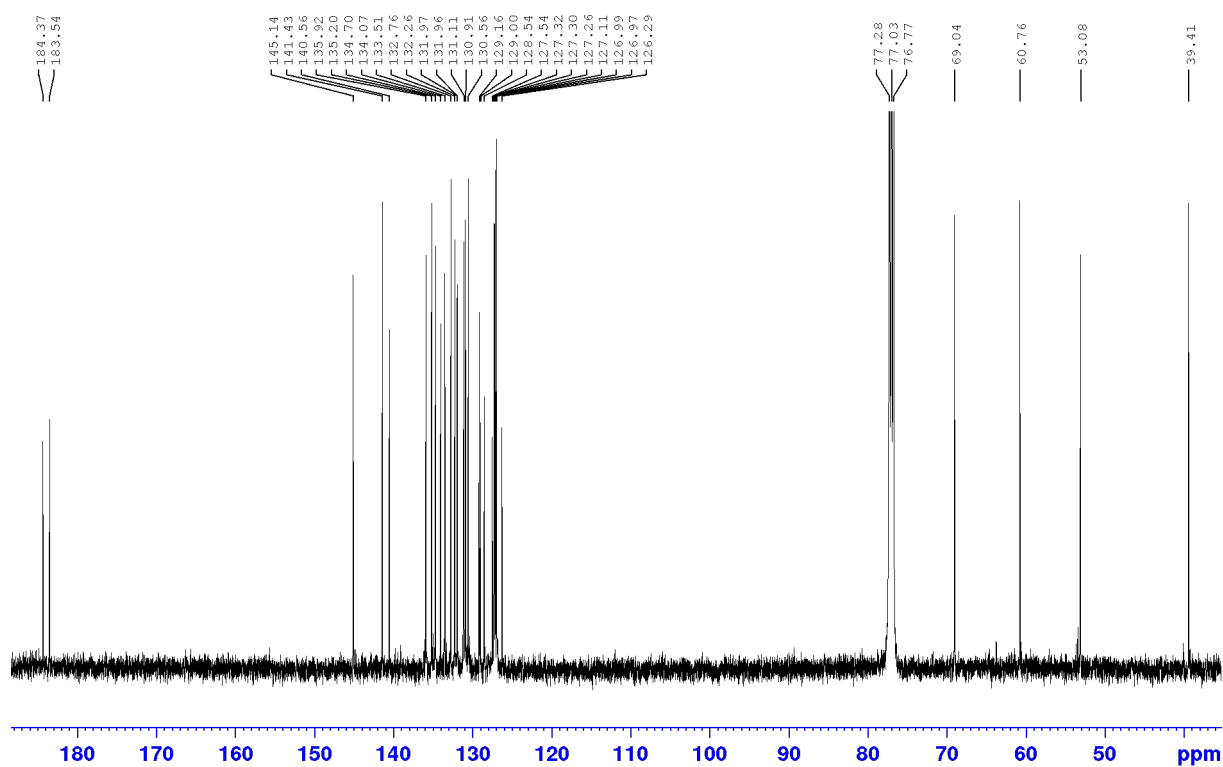


Figure S32. ¹³C NMR of compound **8a** in CDCl₃

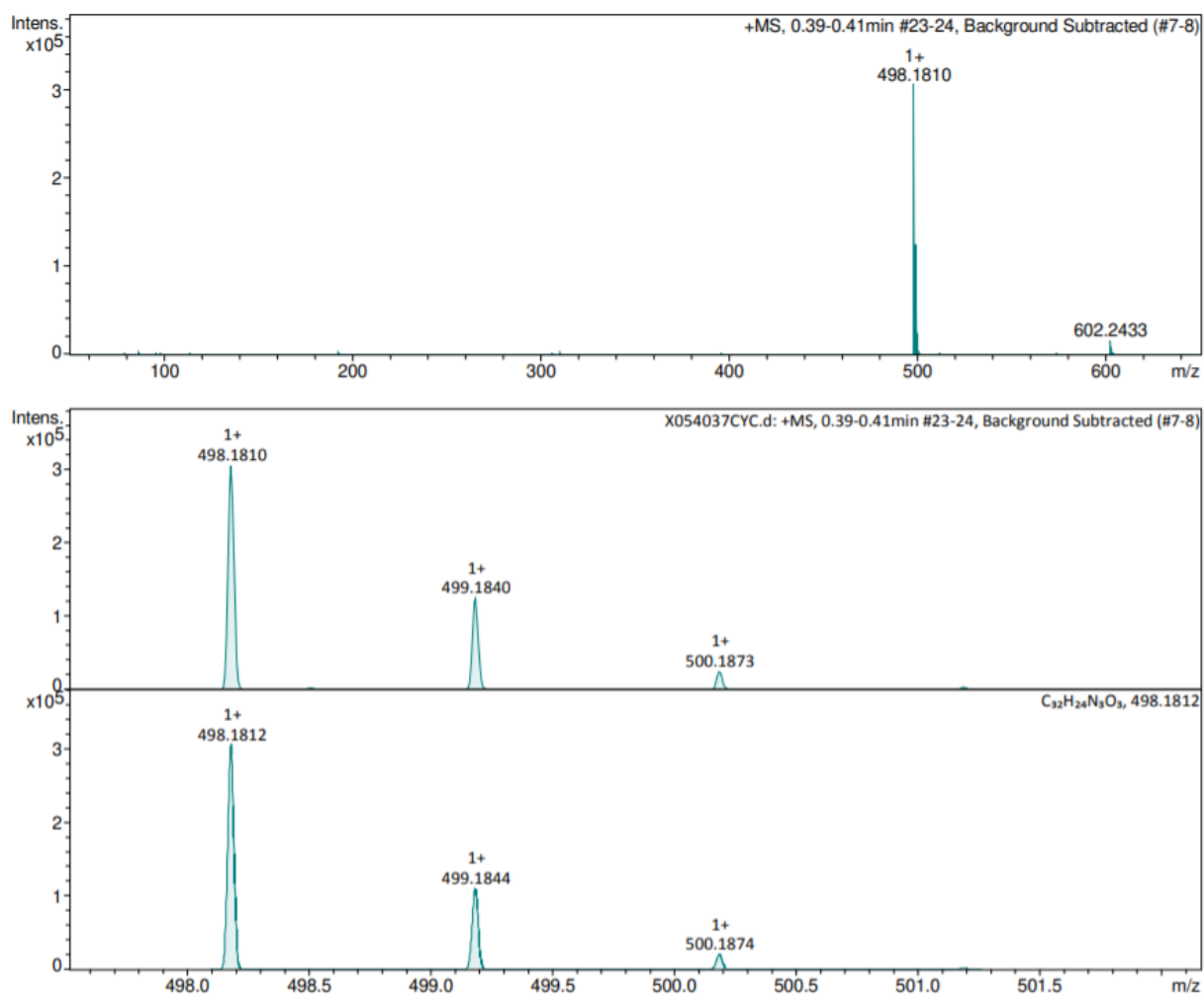
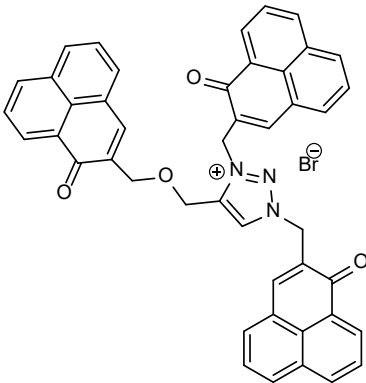


Figure S33. HRMS ESI⁺ of compound **8a**



183.94
183.65
183.05

145.53
142.86
140.77
139.89
135.77
135.48
134.88
134.64
134.33
134.10
133.33
133.11
132.23
131.97
131.78
131.74
130.99
130.97
130.93
130.34
130.06
129.50
128.79
128.65
128.34
127.55
127.26
127.16
127.03
126.98
126.97
126.91
126.78
126.48
126.33

77.28
77.03
76.78

68.64
60.84
53.33
51.44

ppm

Figure S35. ^{13}C NMR of compound **8b** in CDCl_3

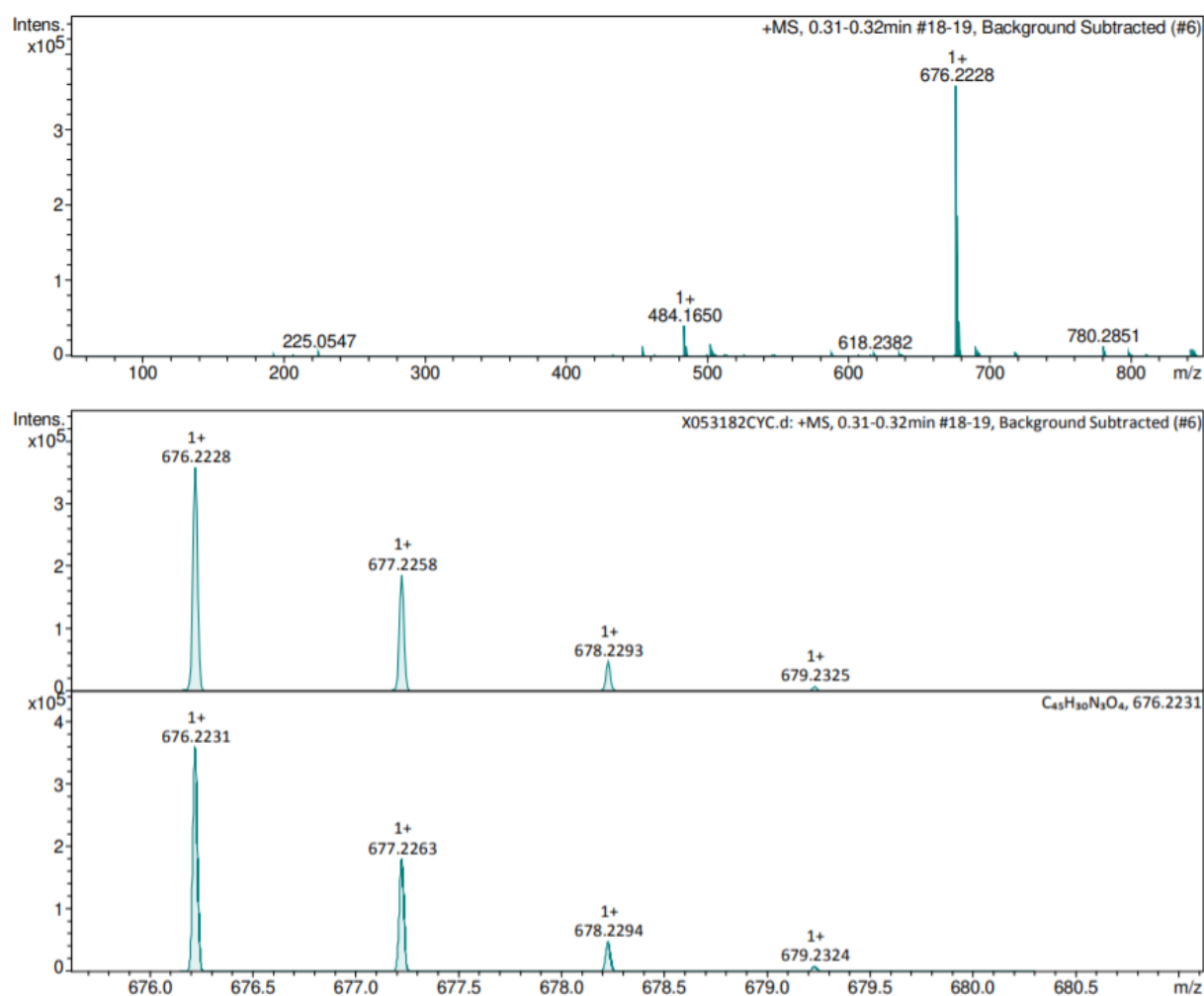


Figure S36. HRMS ESI⁺ of compound **8b**

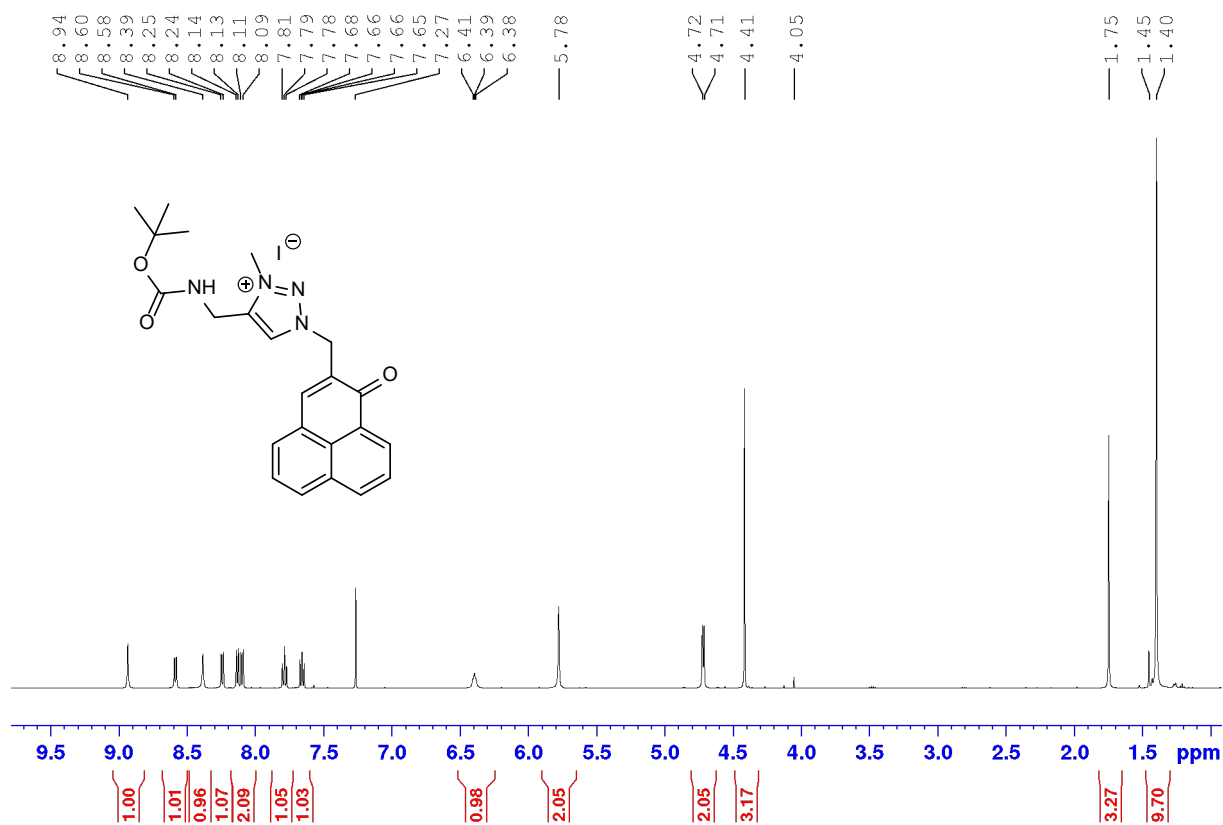


Figure S37. ¹H NMR of compound **9a** in CDCl₃

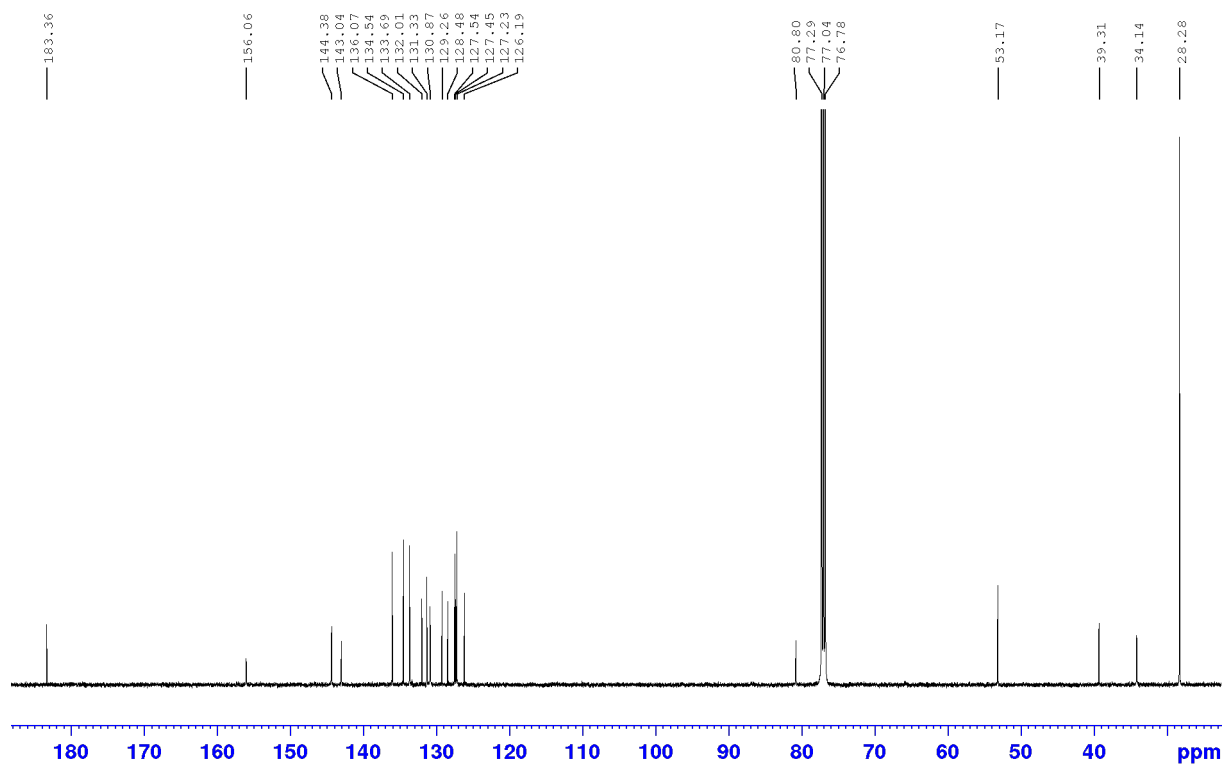


Figure S38. ¹³C NMR of compound **9a** in CDCl₃

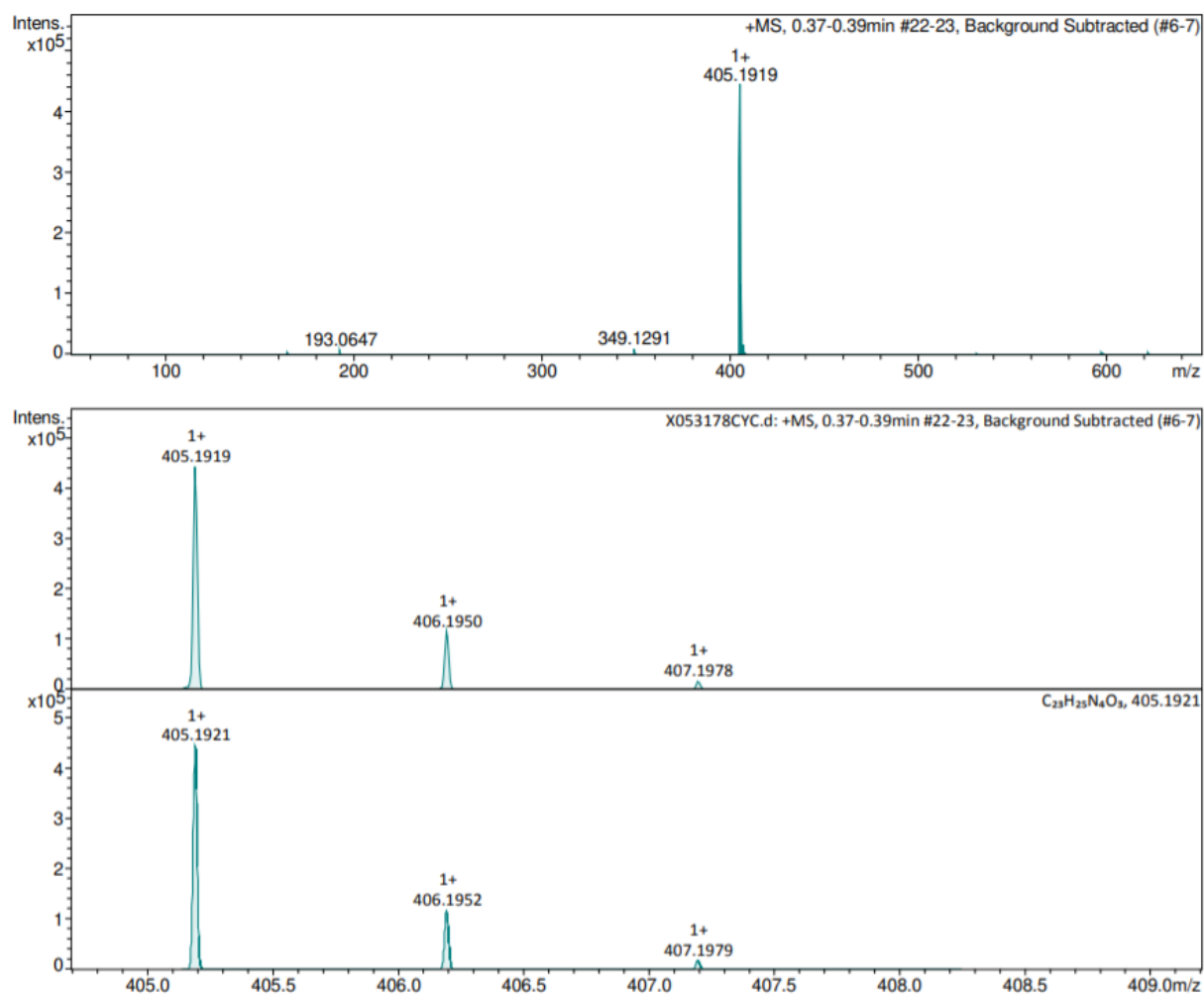


Figure S39. HRMS ESI⁺ of compound **9a**

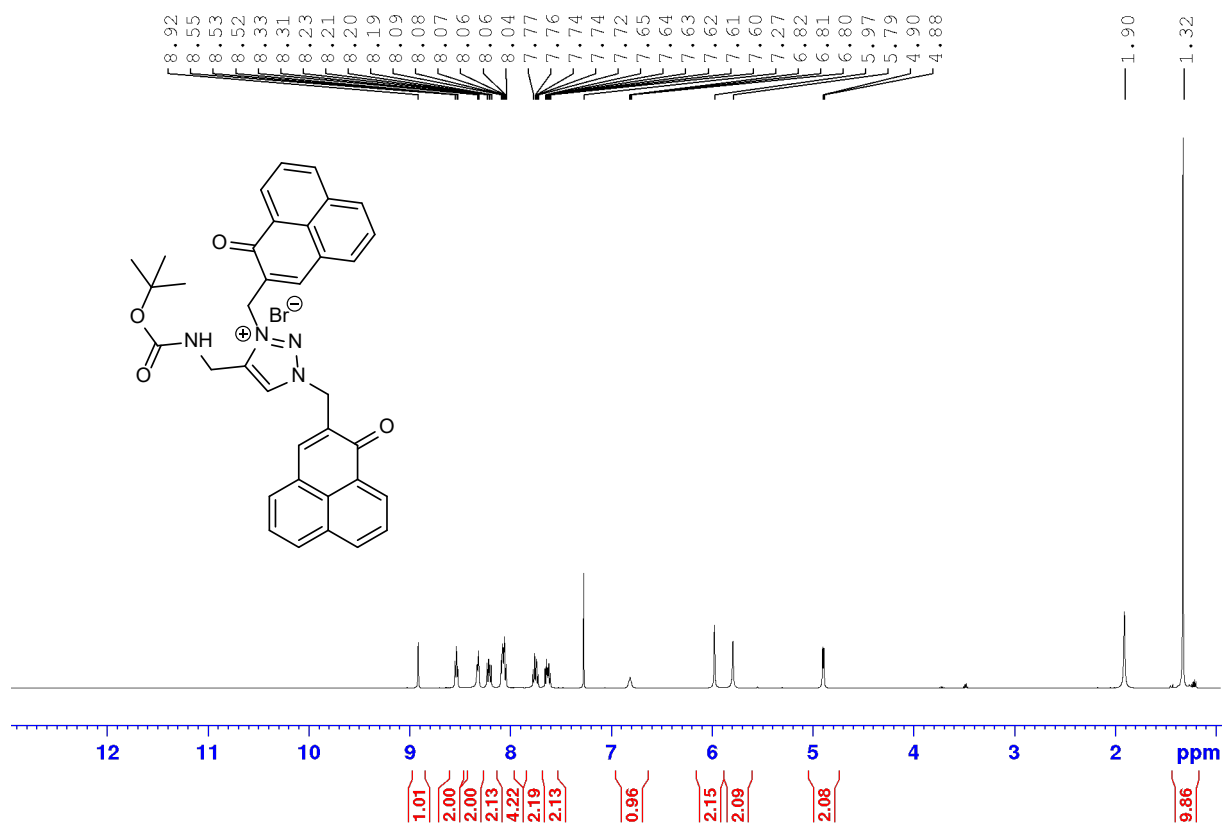


Figure S40. ¹H NMR of compound 9b in CDCl₃

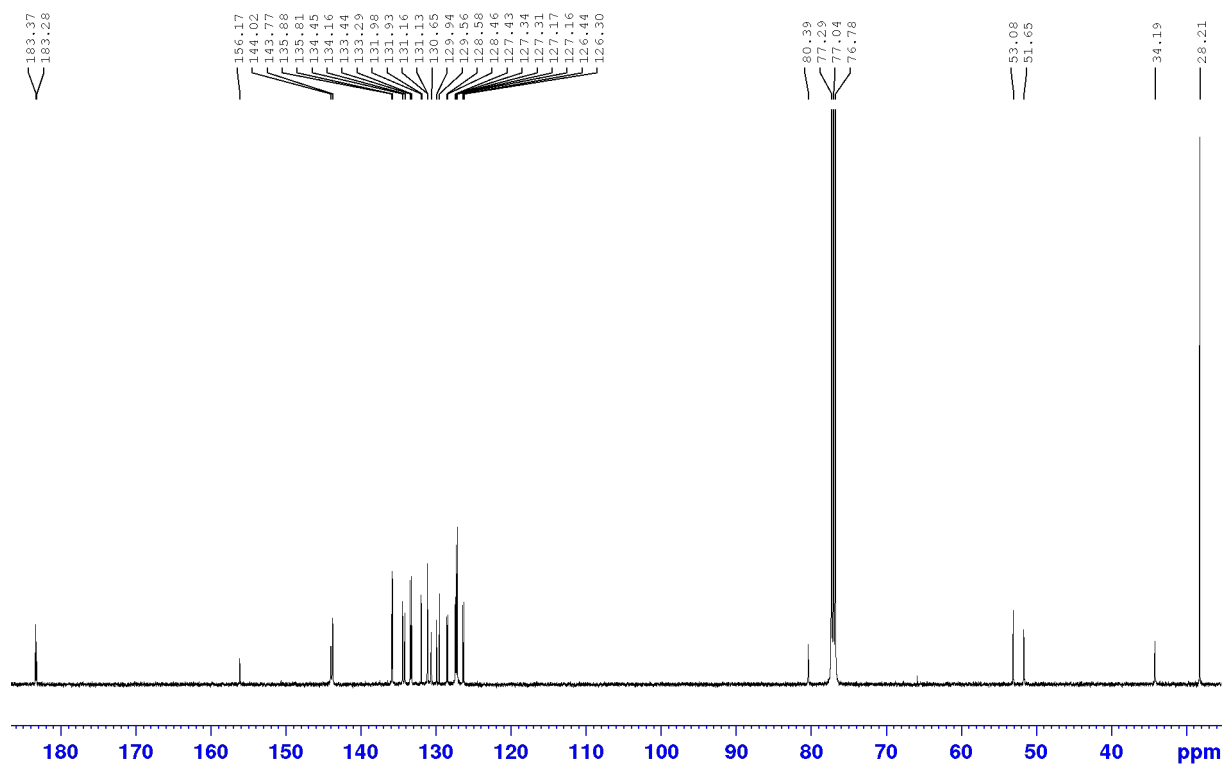


Figure S41. ¹³C NMR of compound 9b in CDCl₃

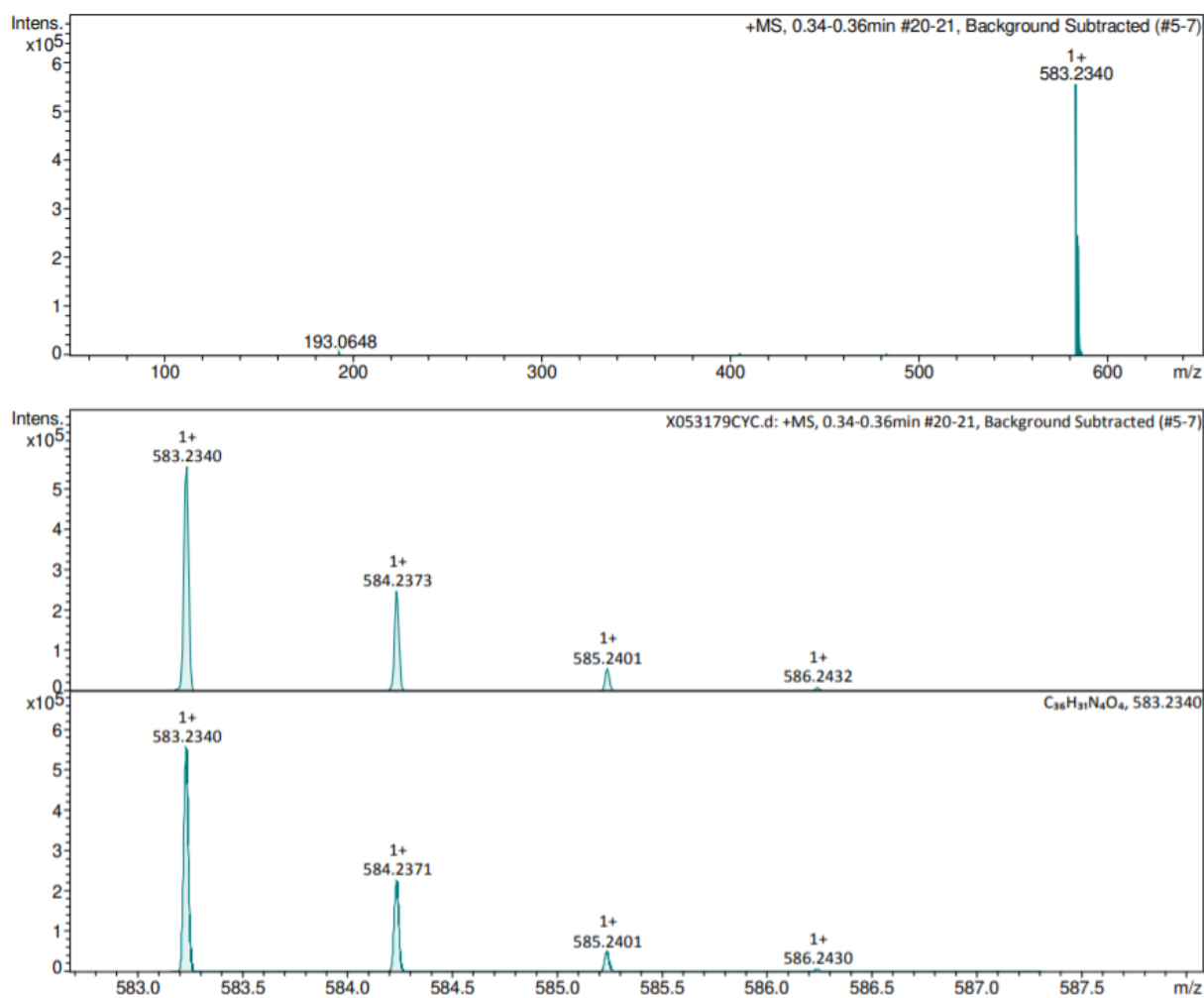


Figure S42. HRMS ESI⁺ of compound **9b**

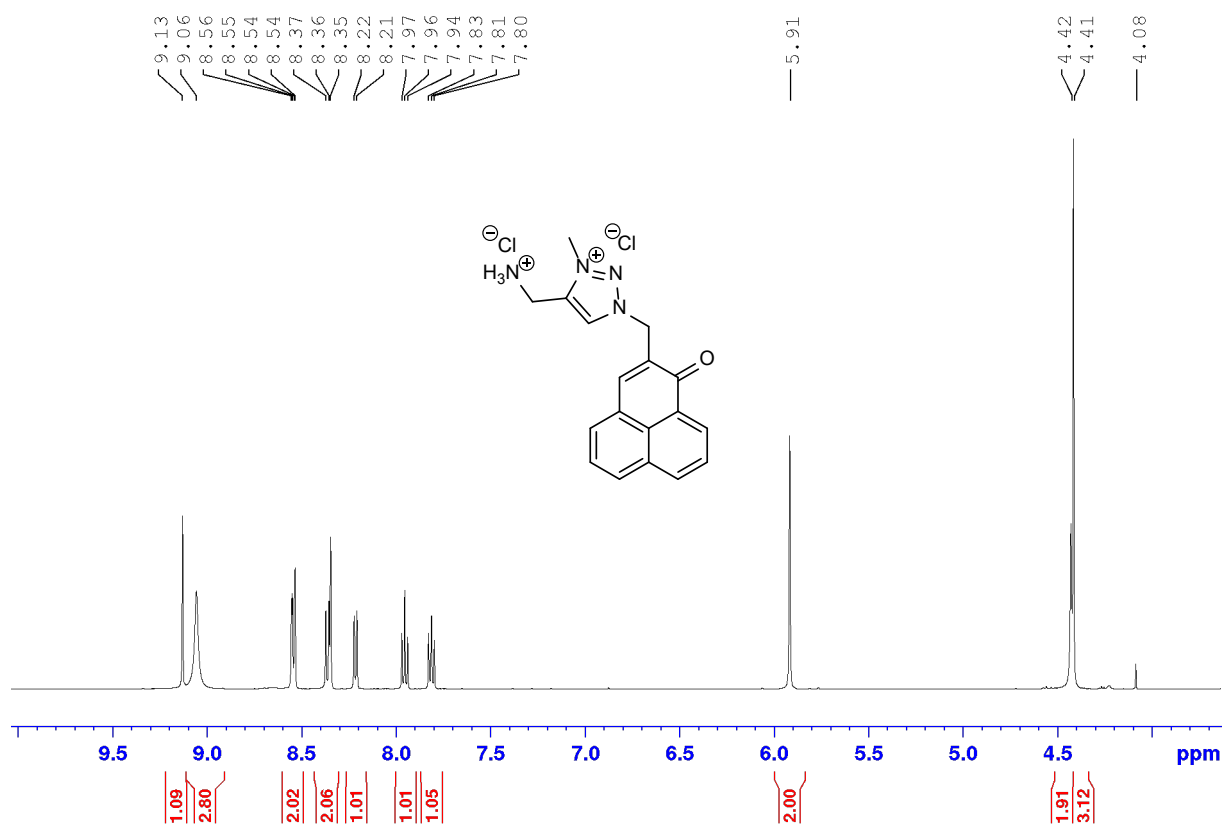


Figure S43. ¹H NMR of compound **10a** in DMSO-d₆

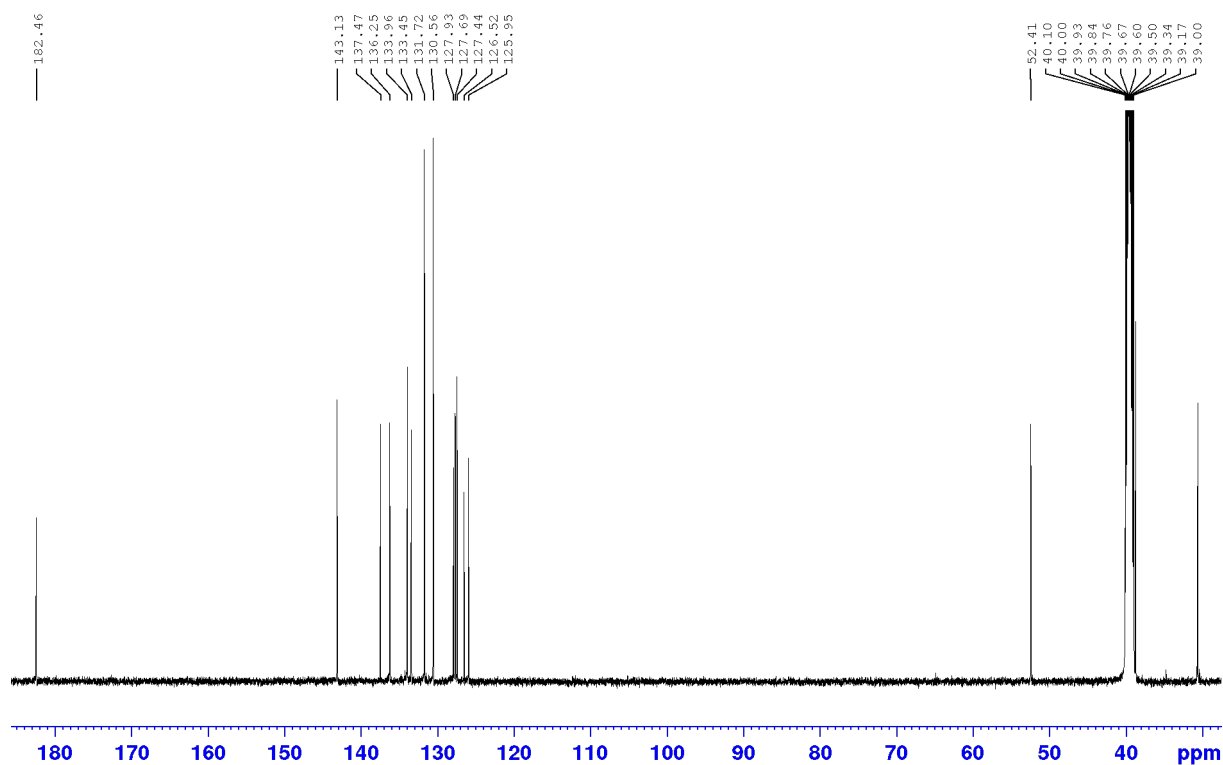


Figure S44. ¹³C NMR of compound **10a** in DMSO-d₆

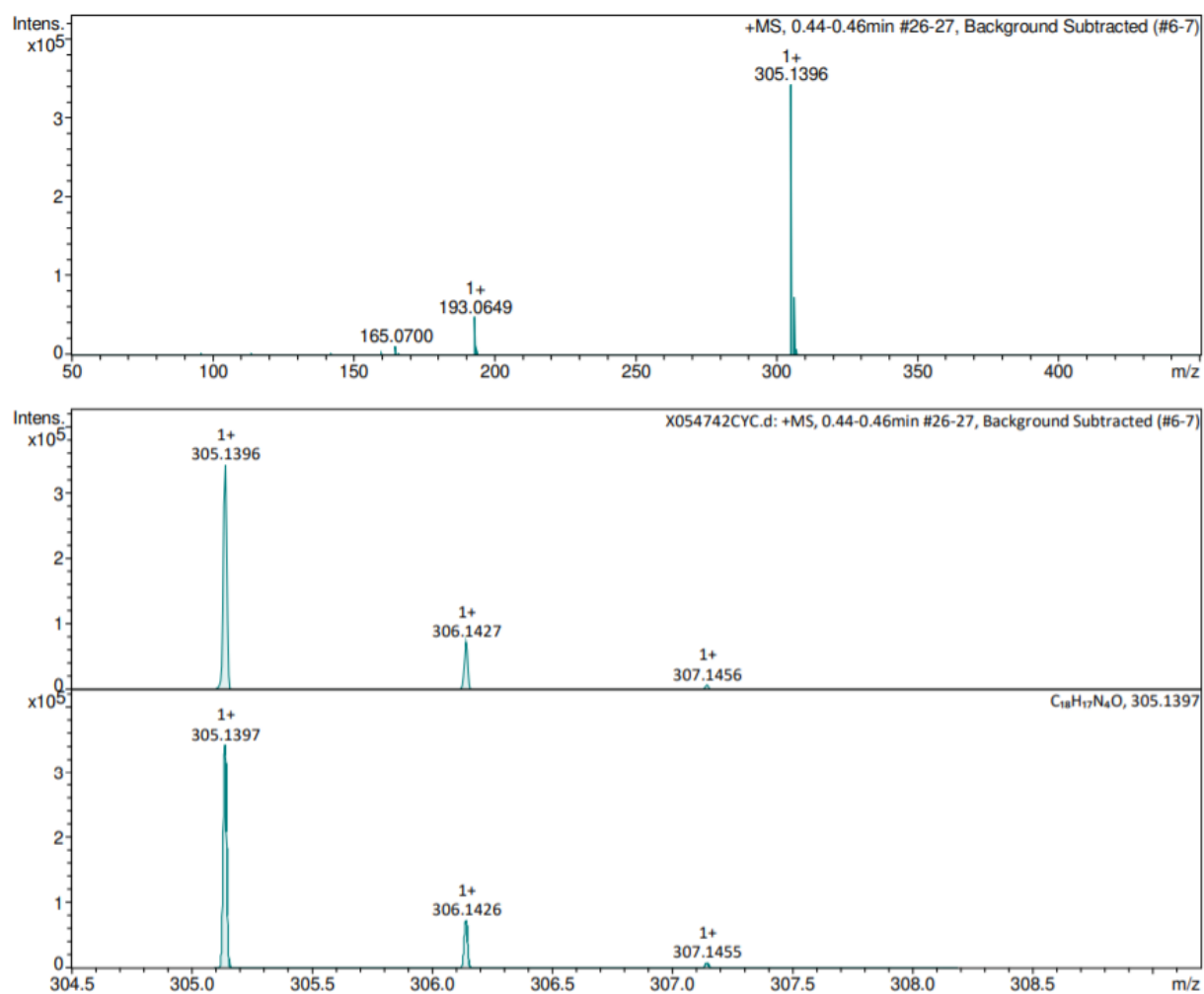


Figure S45. HRMS ESI⁺ of compound **10a**

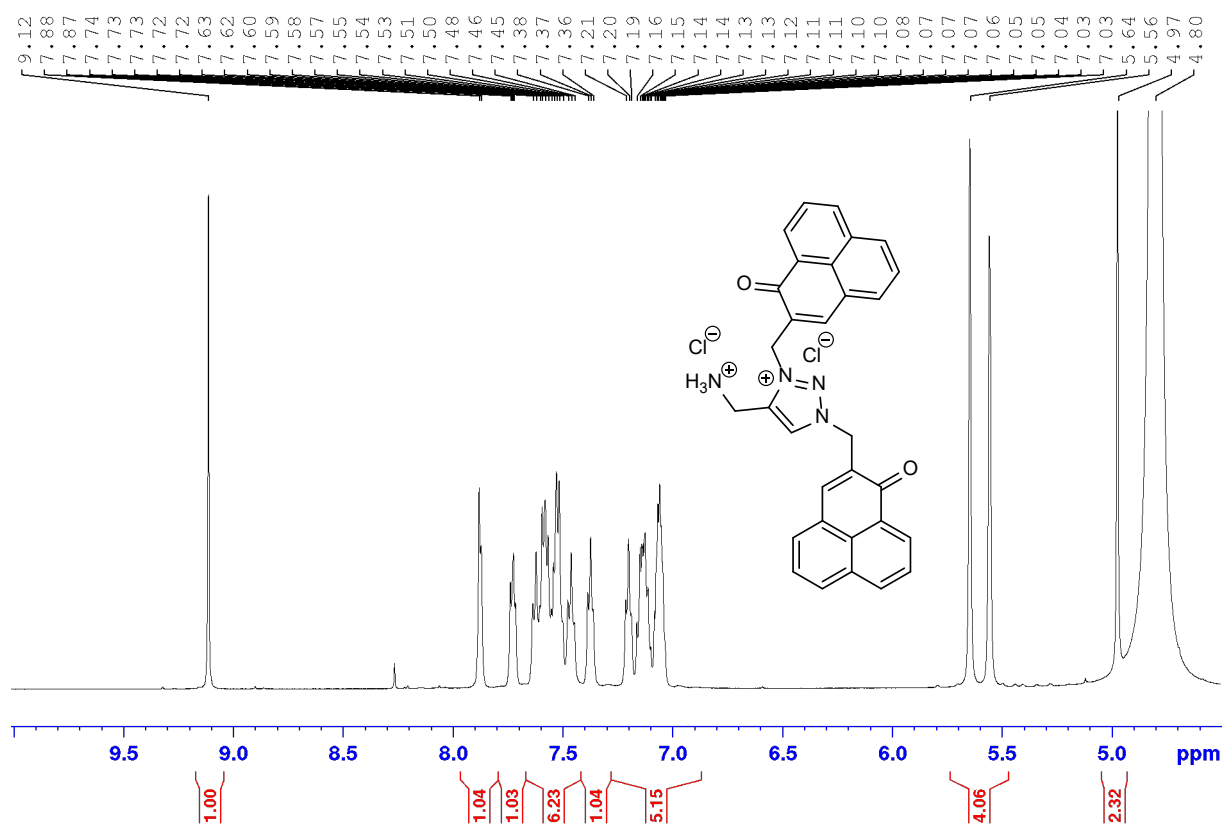


Figure S46. ^1H NMR of compound **10b** in D_2O

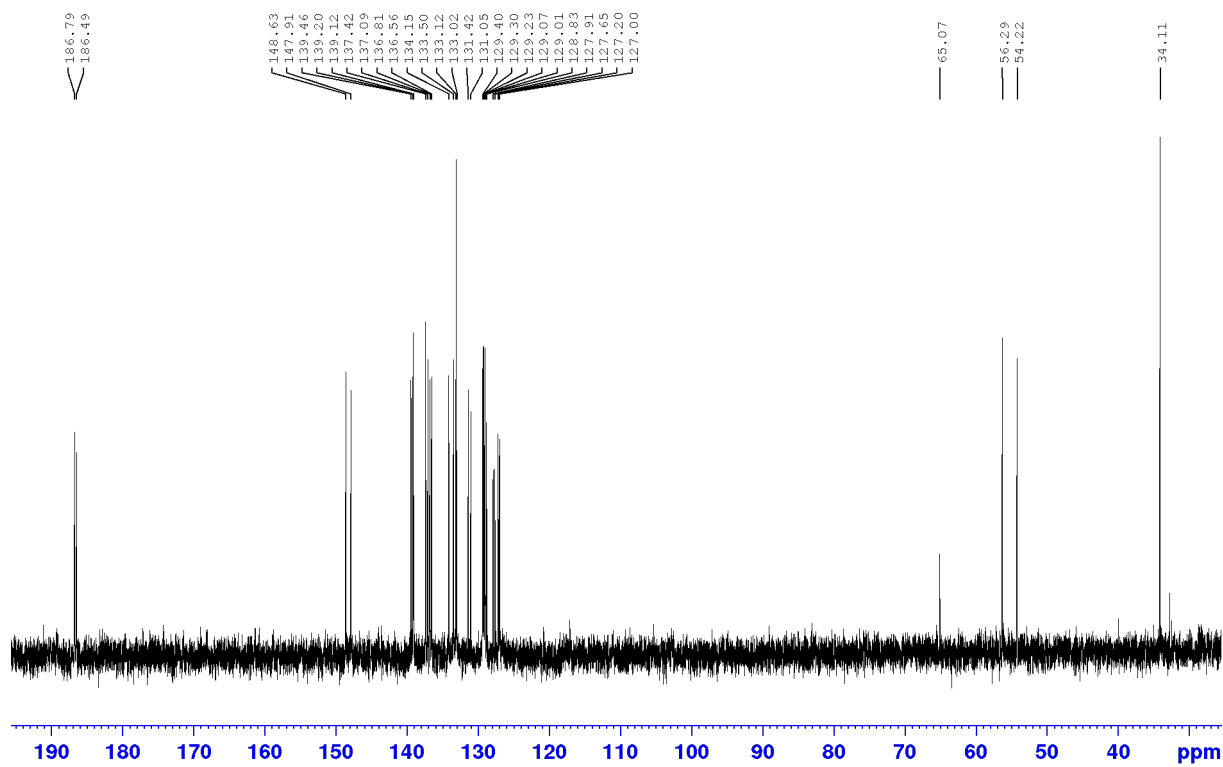


Figure S47. ^{13}C NMR of compound **10b** in D_2O

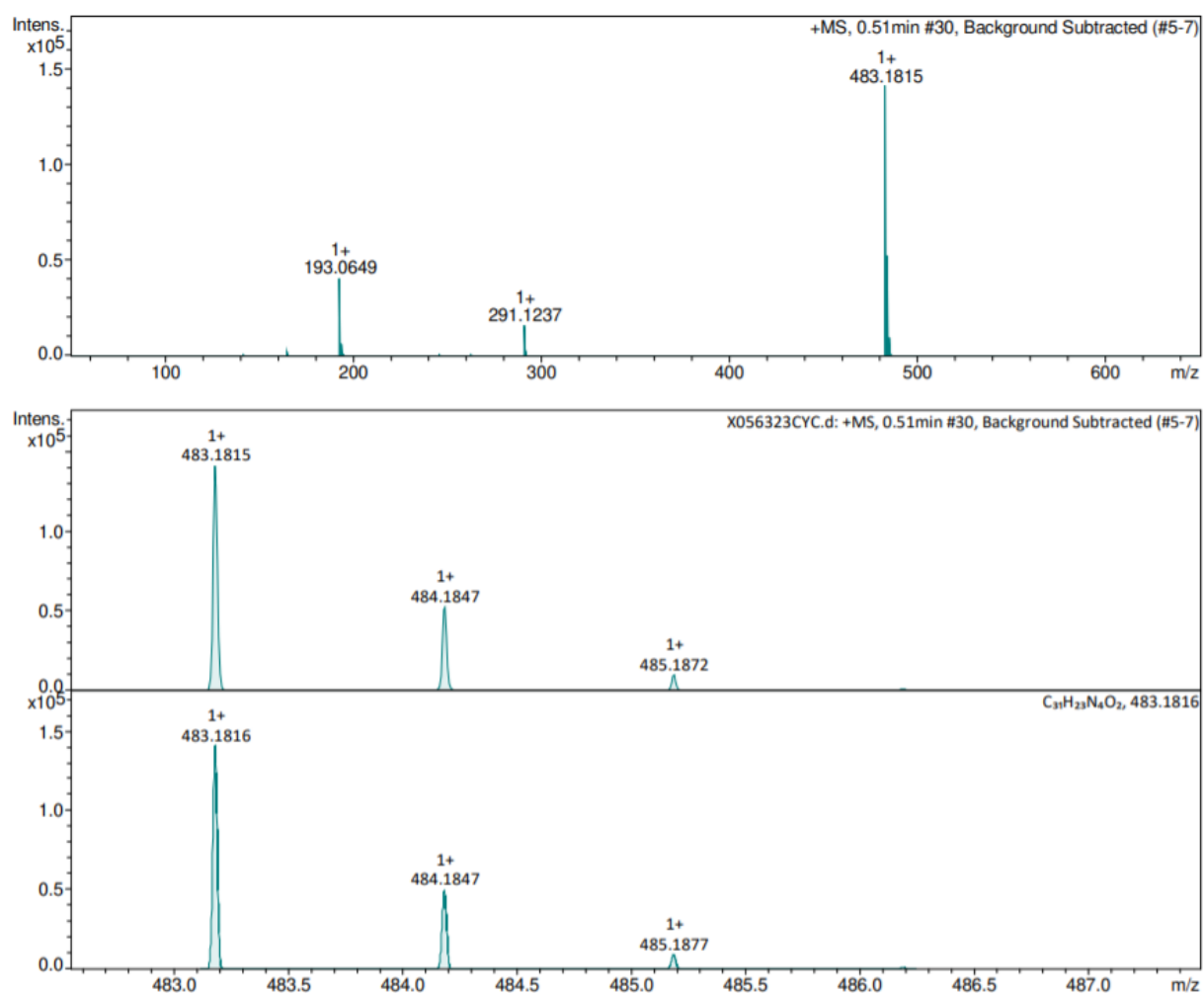


Figure S48. HRMS ESI⁺ of compound **10b**

Figure S49 : Chemical structures of all compounds

