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

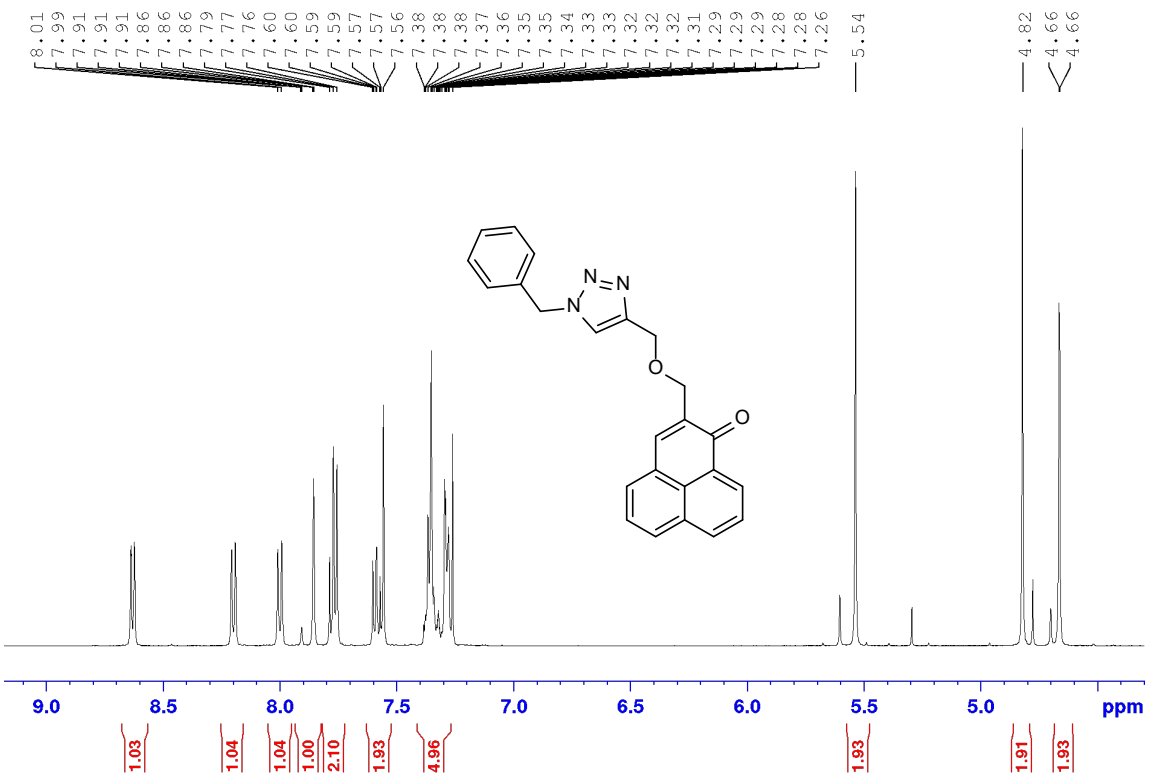

Figure S1. ^{1}H NMR of compound **7** in $CDCl_3$

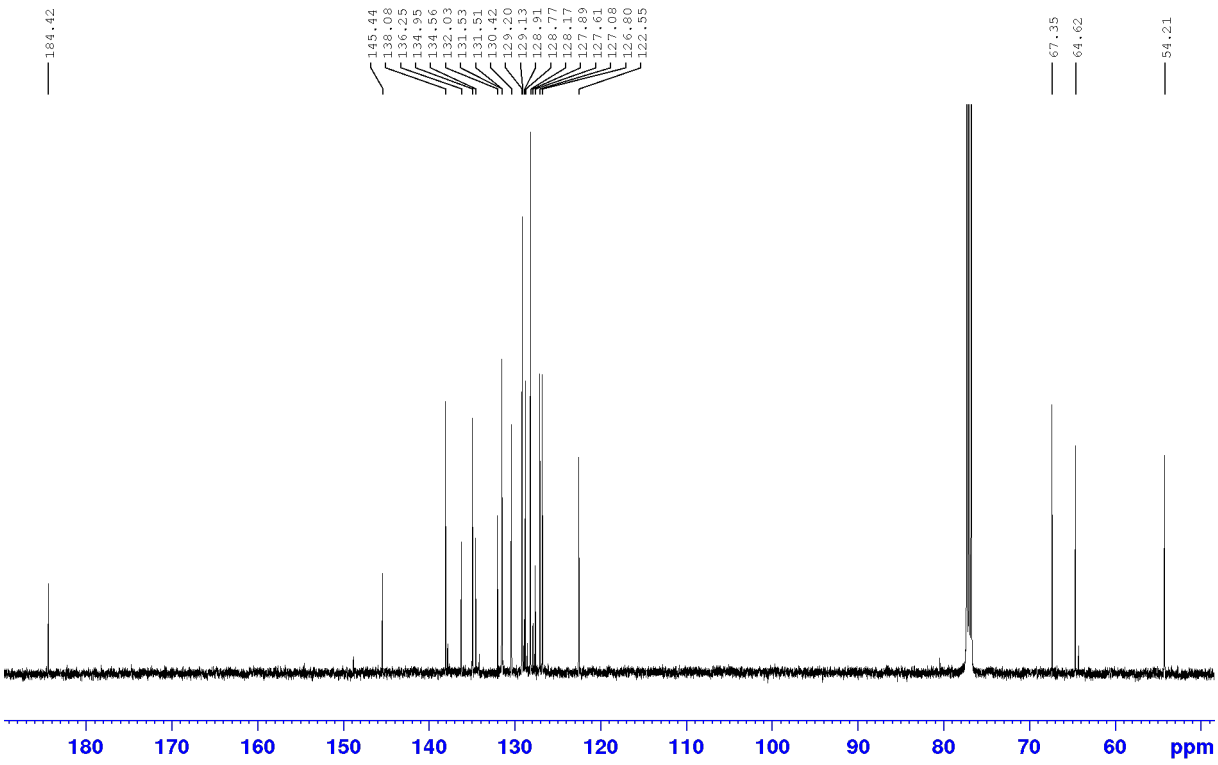

Figure S2. ^{13}C NMR of compound **7** in $CDCl_3$

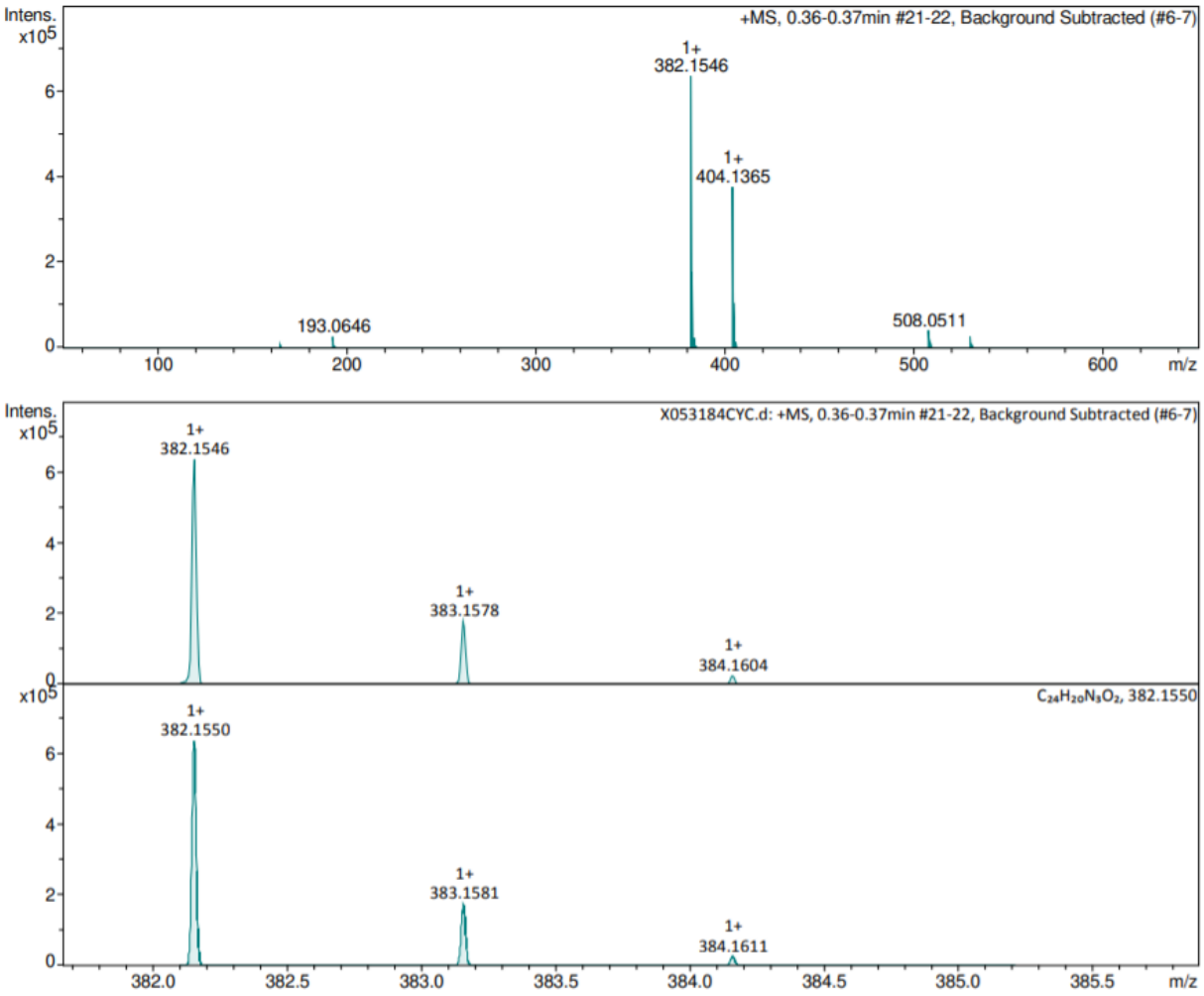

Figure S3. HRMS ESI$^+$ of compound **7**

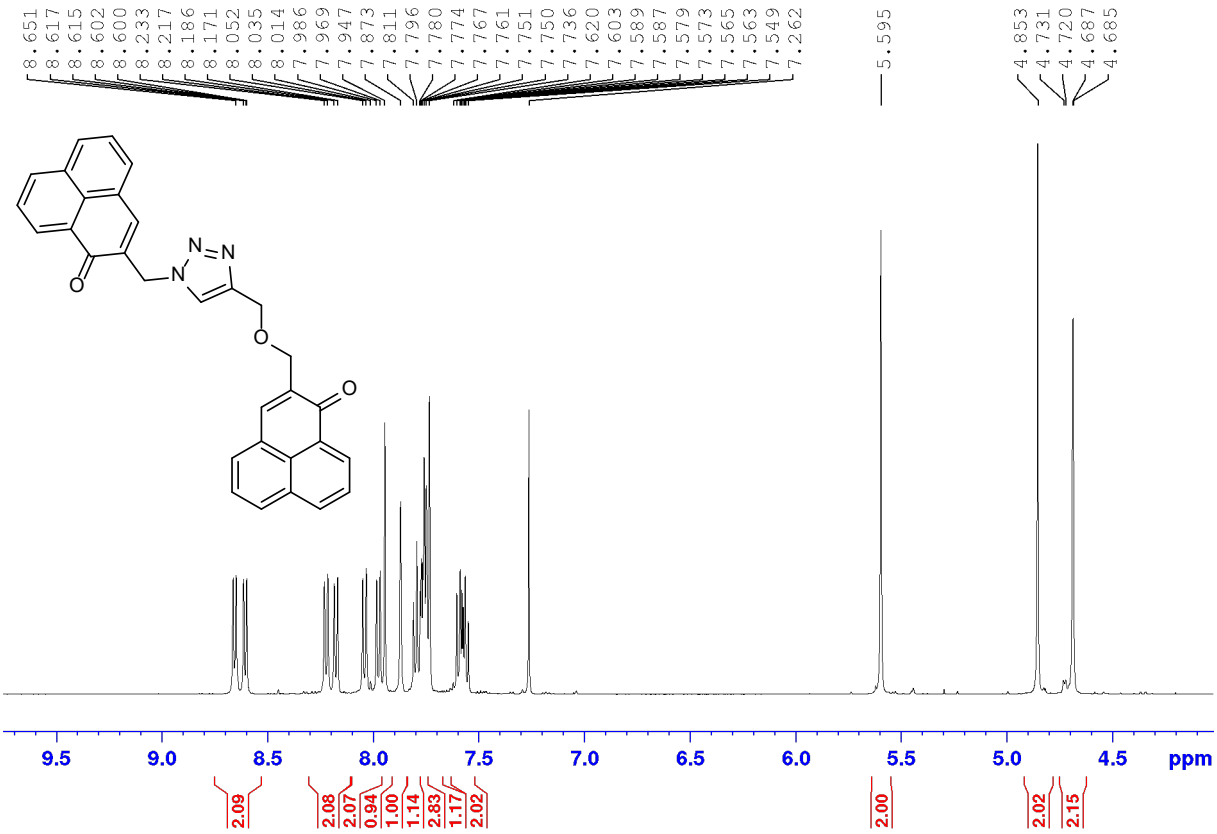

Figure S4. ^{1}H NMR of compound **8** in $CDCl_3$

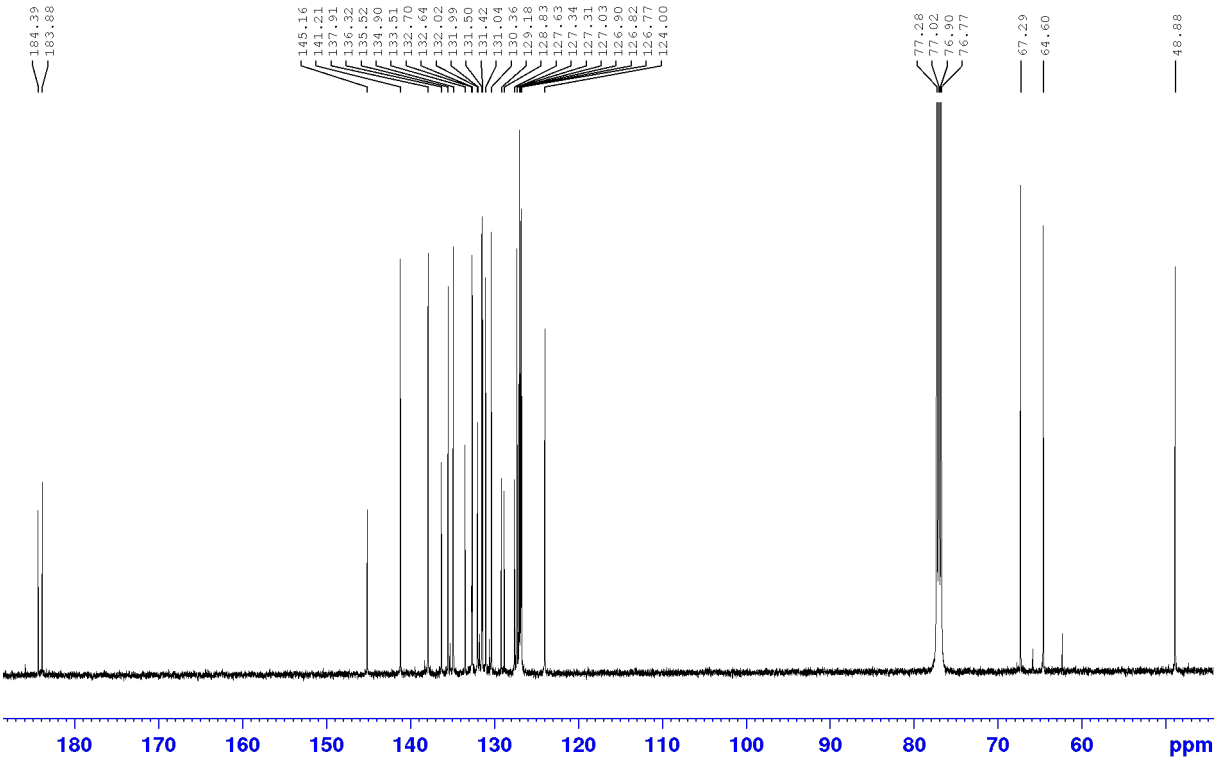

Figure S5. ^{13}C NMR of compound **8** in $CDCl_3$

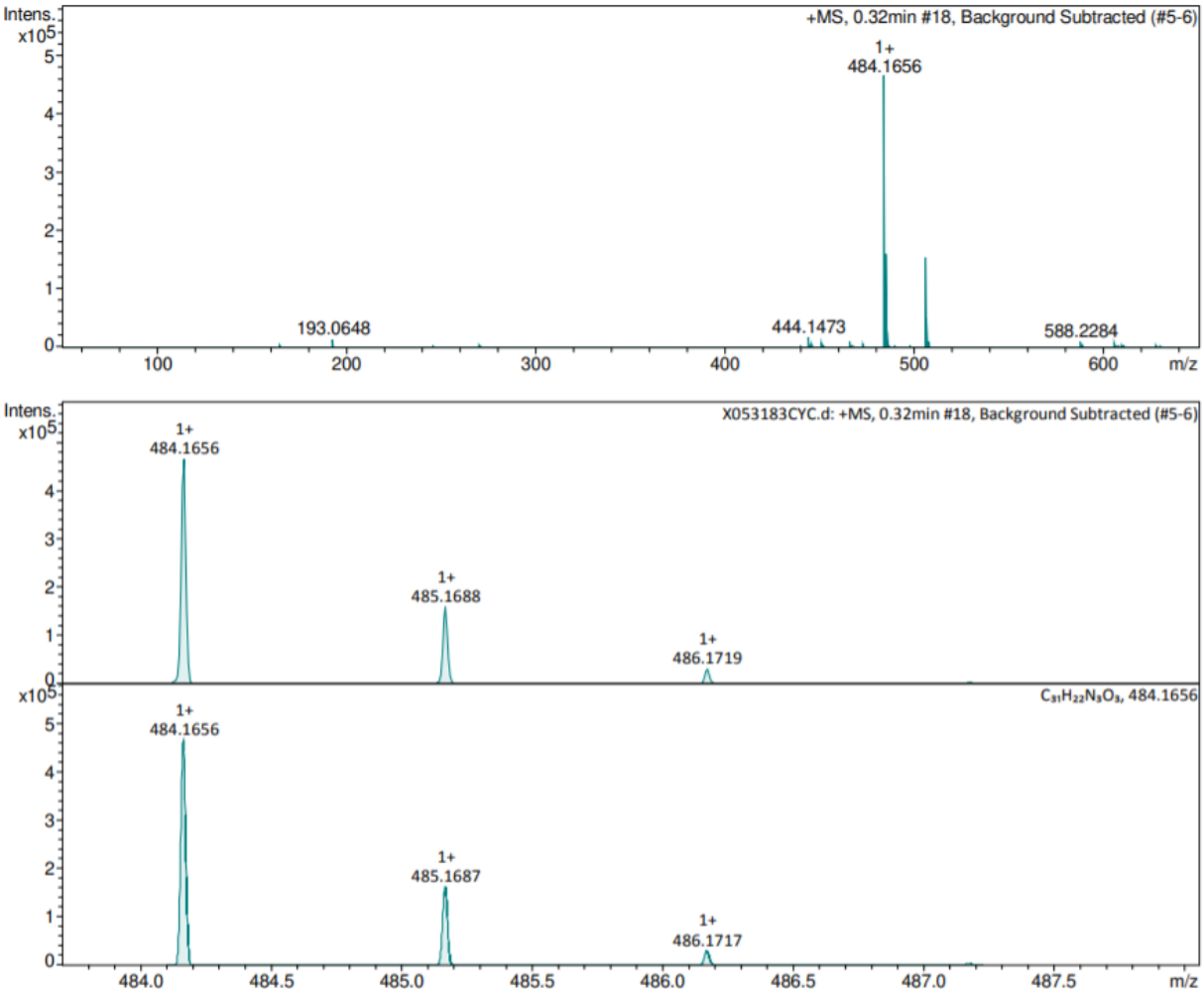

Figure S6. HRMS ESI$^+$ of compound **8**

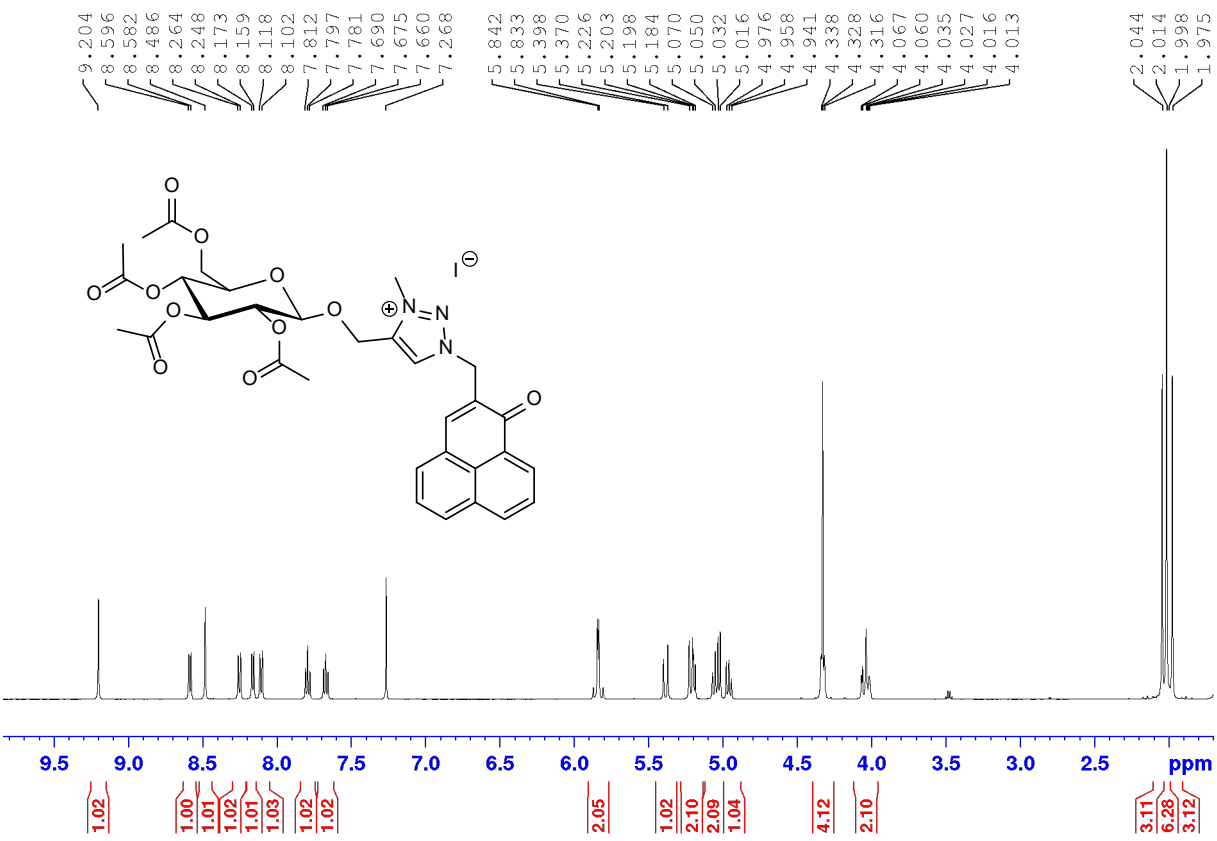

Figure S7. ^{1}H NMR of compound **4a** in $CDCl_3$

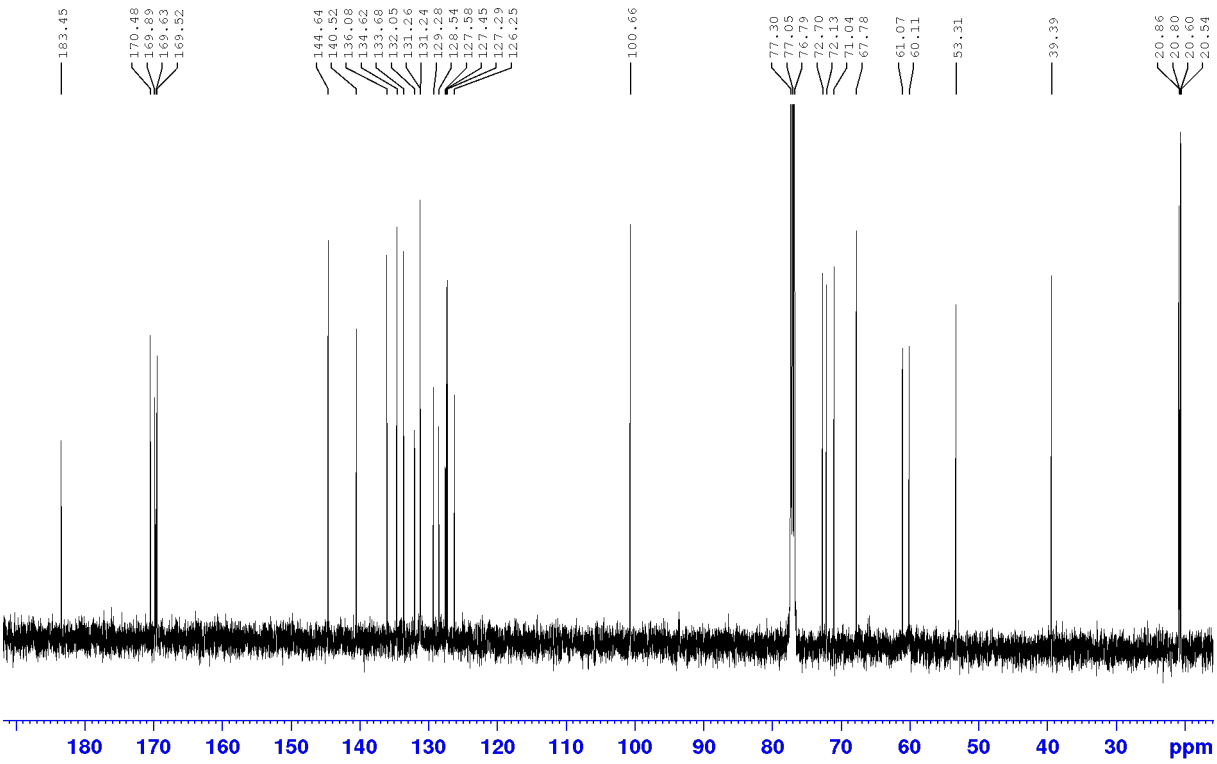

Figure S8. ^{13}C NMR of compound **4a** in $CDCl_3$

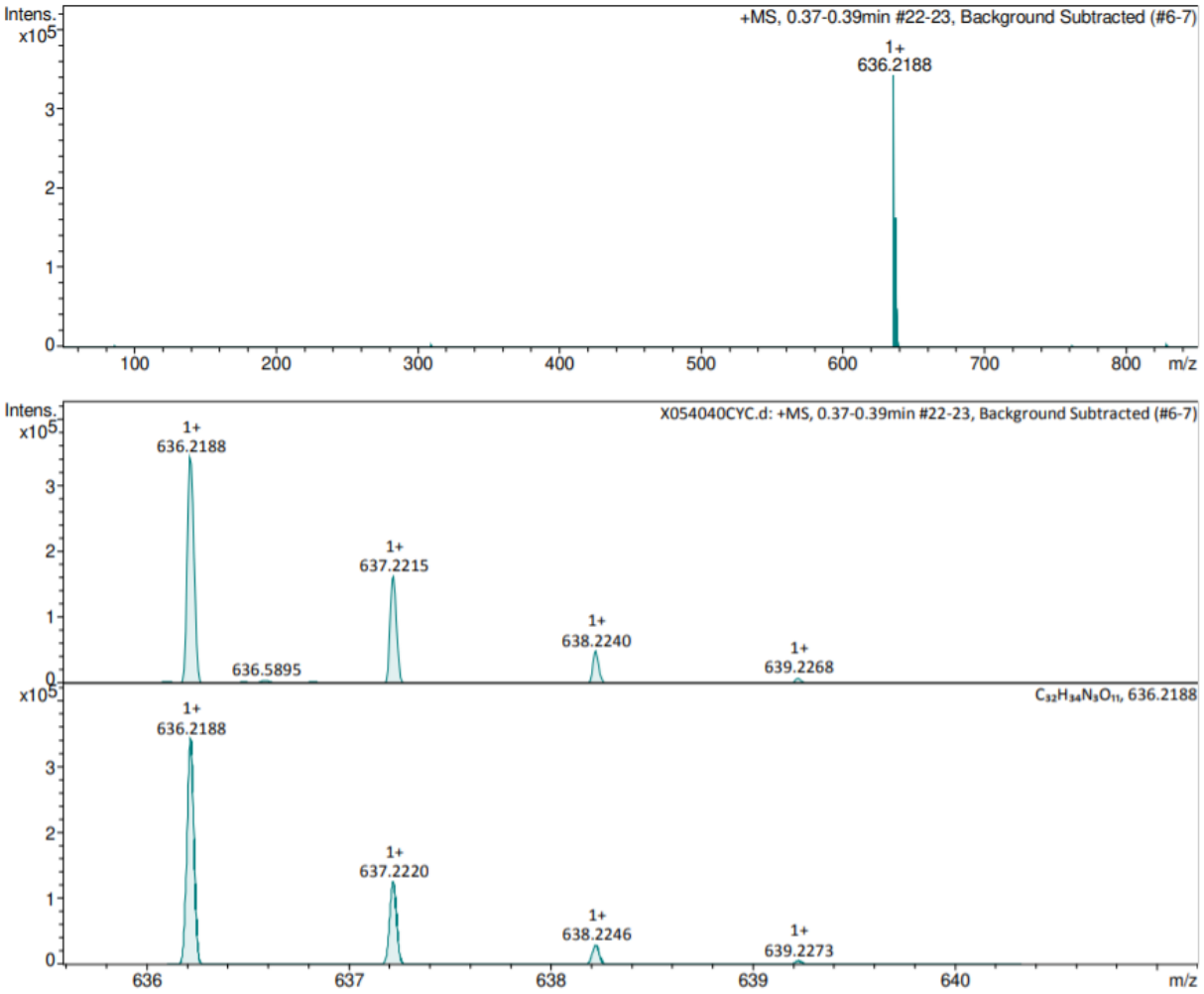

Figure S9. HRMS ESI$^+$ of compound **4a**

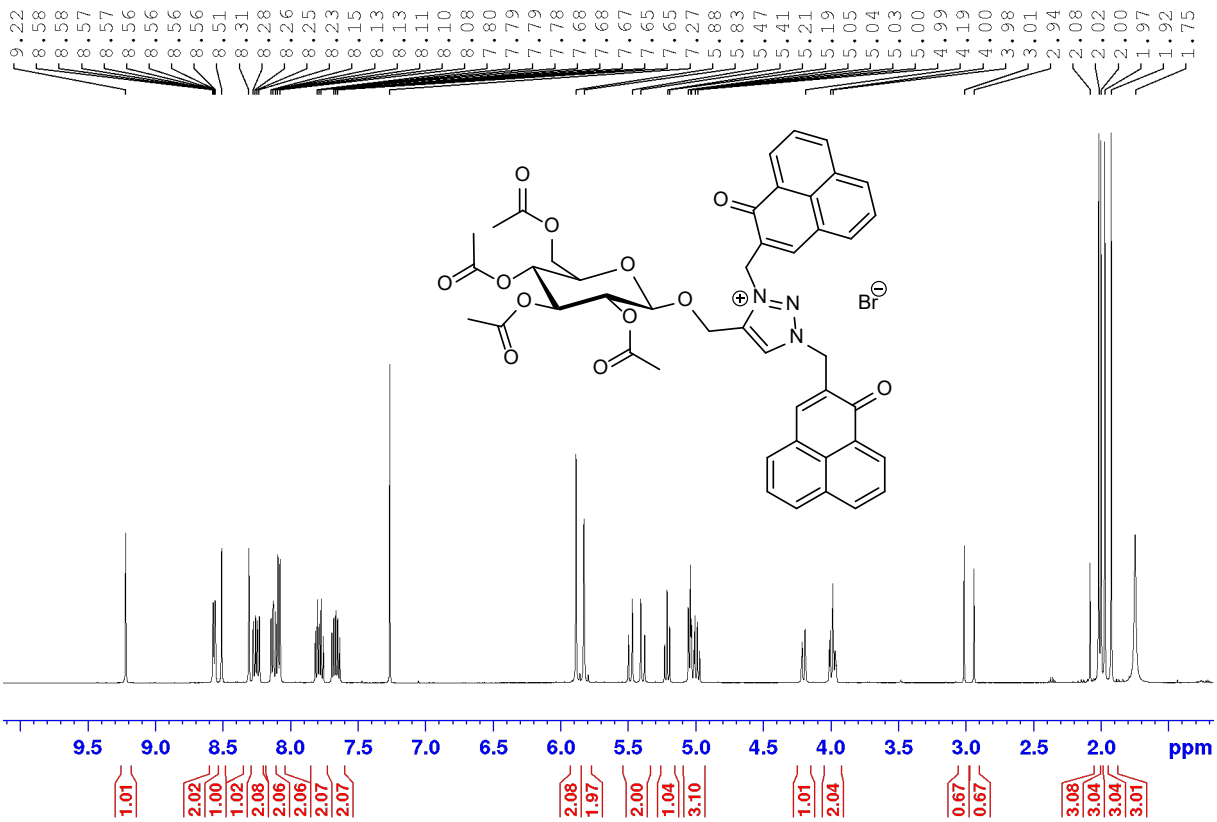

Figure S10. ^{1}H NMR of compound **4b** in $CDCl_3$

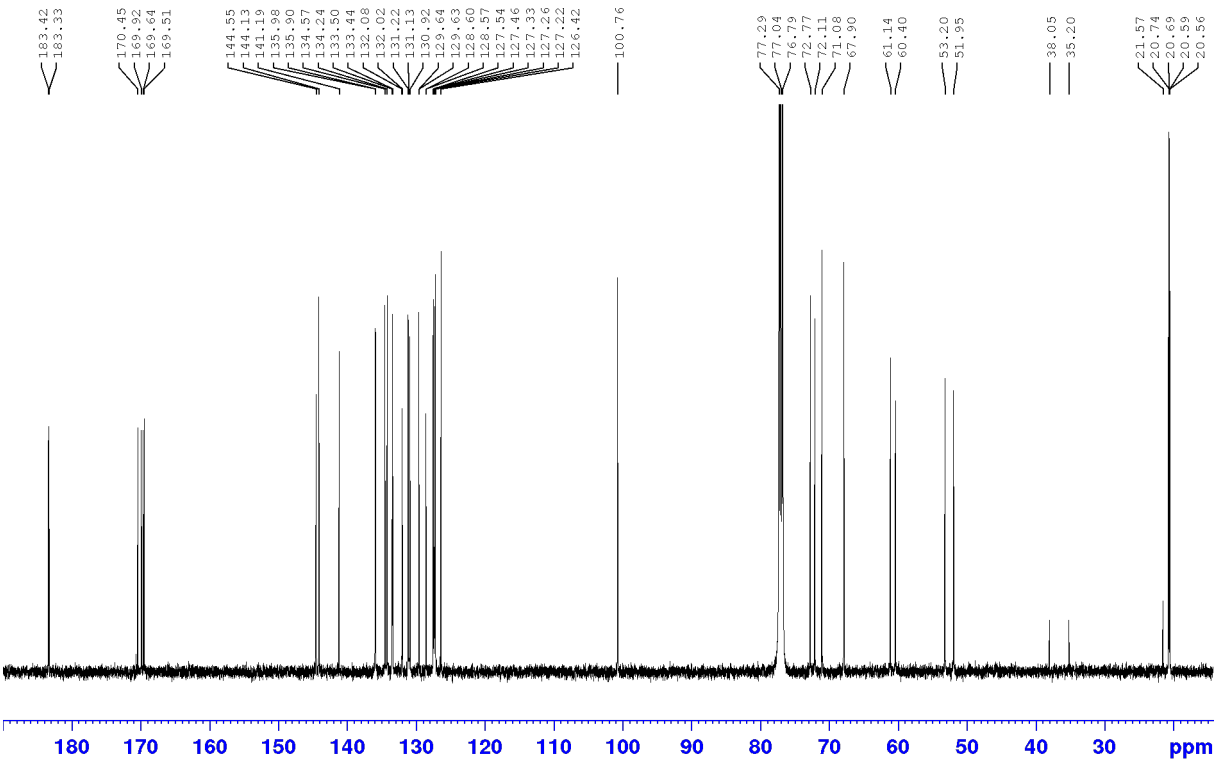

Figure S11. ^{13}C NMR of compound **4b** in $CDCl_3$

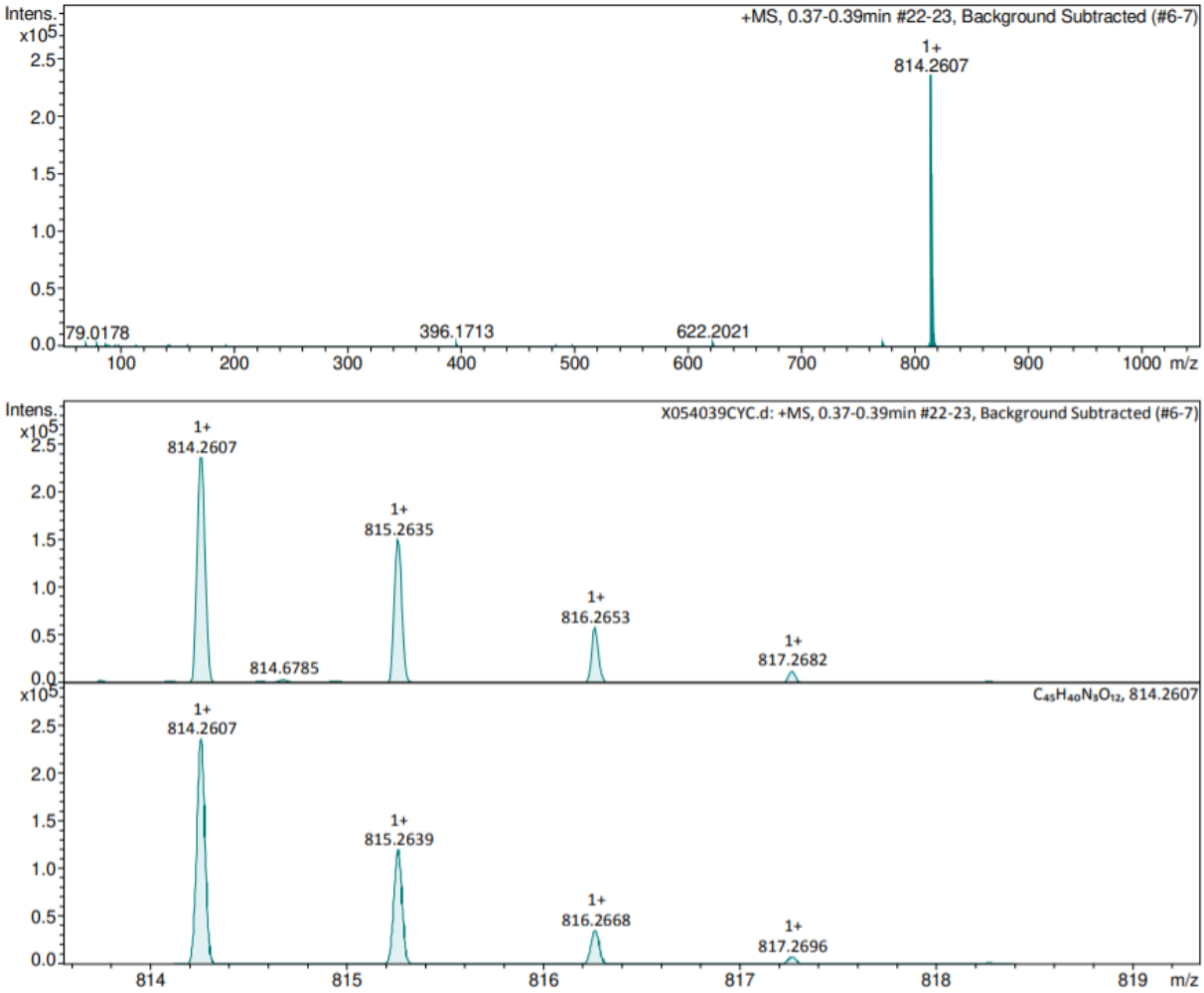

Figure S12. HRMS ESI$^+$ of compound **4b**

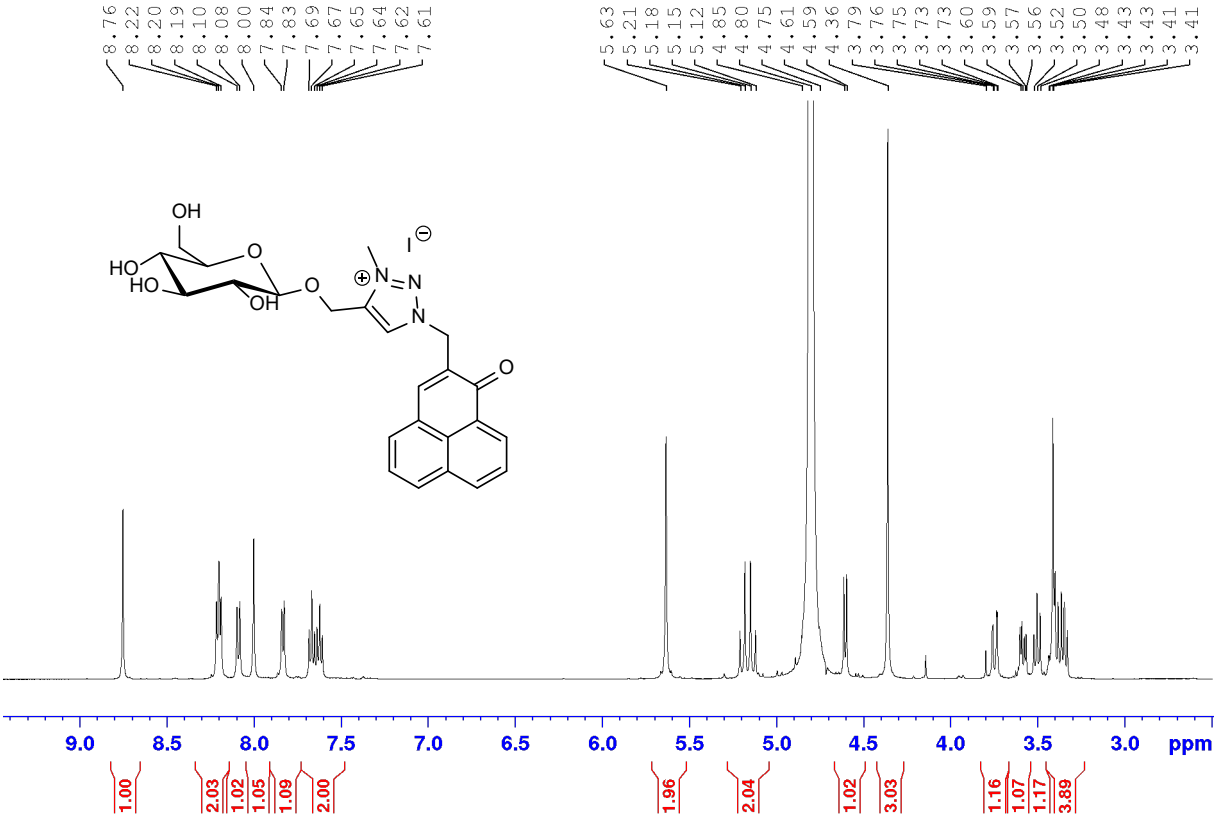

Figure S13. ^{1}H NMR of compound **5a** in D_2O

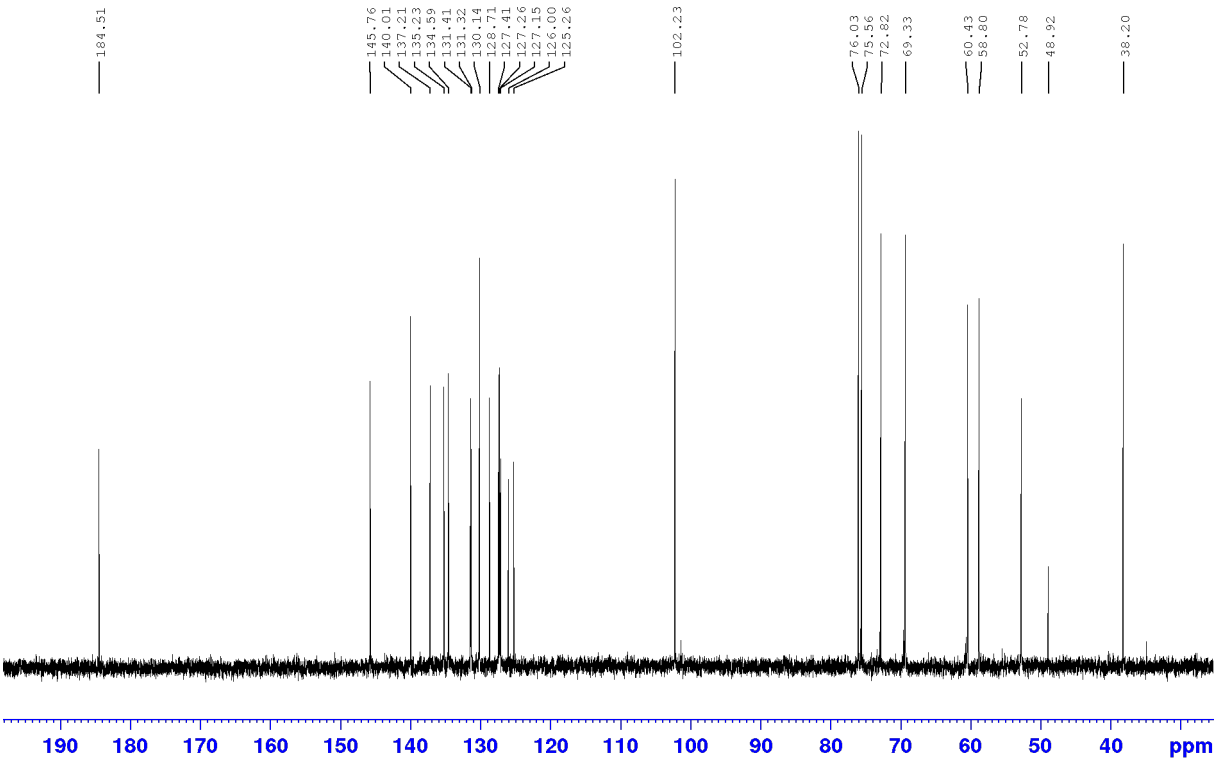

Figure S14. ^{13}C NMR of compound **5a** in D_2O

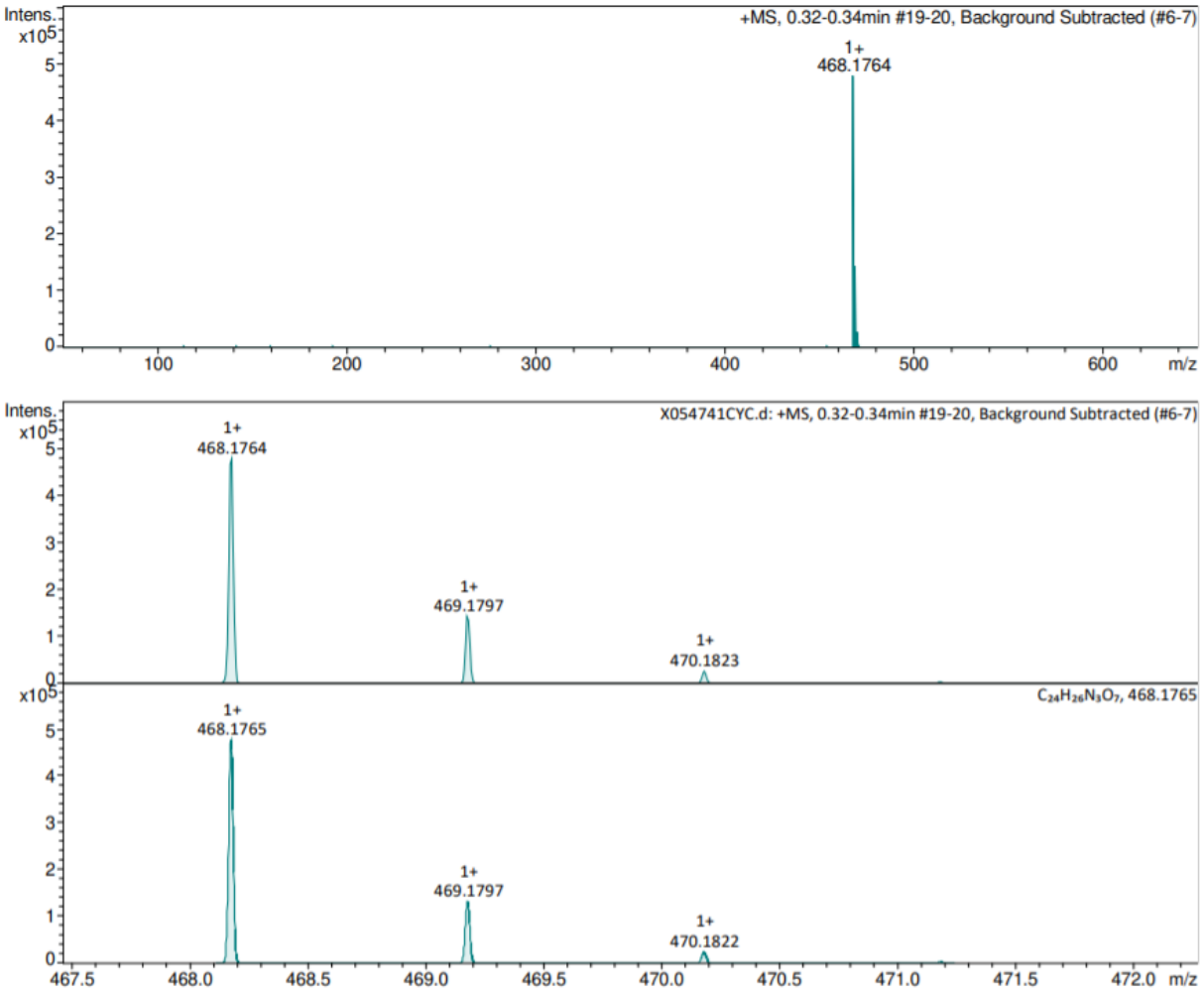

Figure S15. HRMS ESI$^+$ of compound **5a**

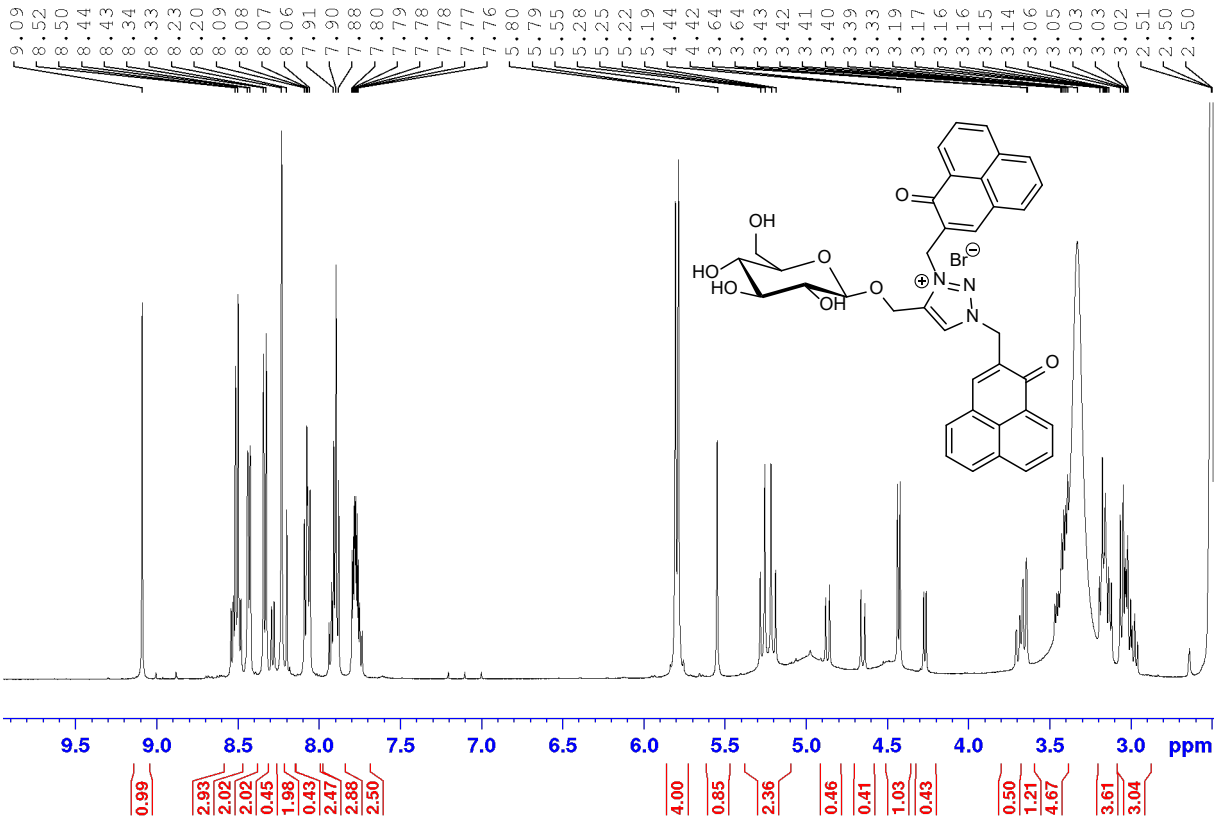

Figure S16. ^{1}H NMR of compound **5b** in D_2O

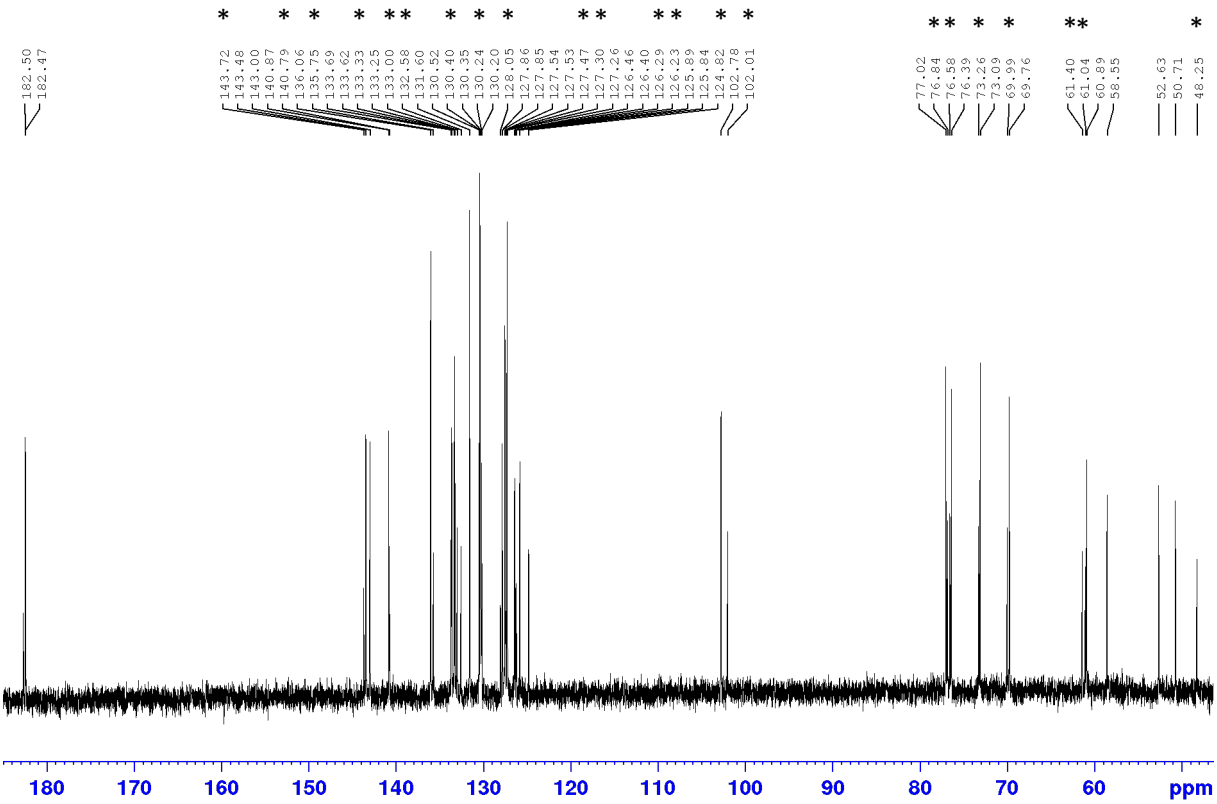

Figure S17. ^{13}C NMR of compound **5b** in D_2O (*contamination by compound **5**)

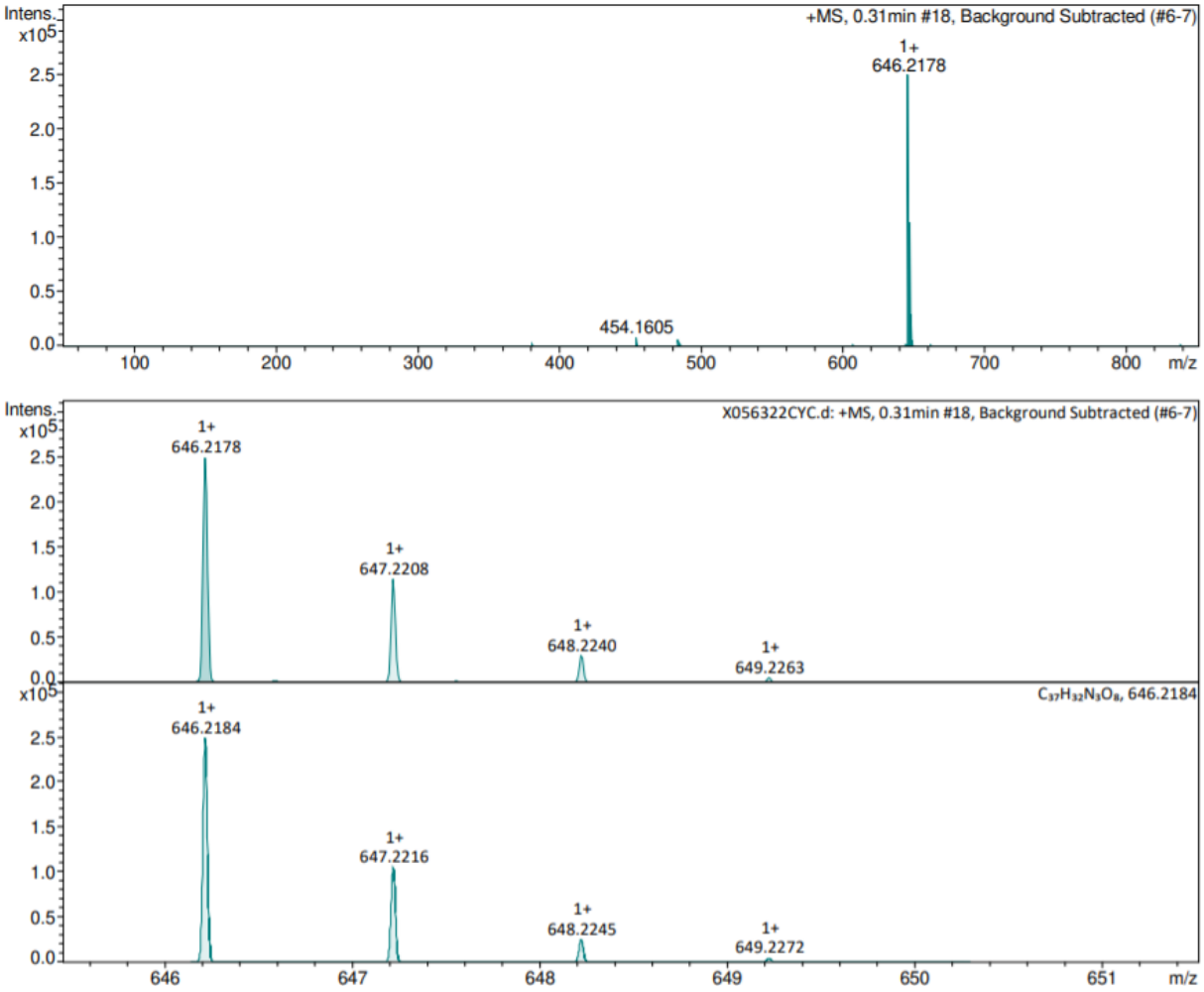

Figure S18. HRMS ESI$^+$ of compound **5b**

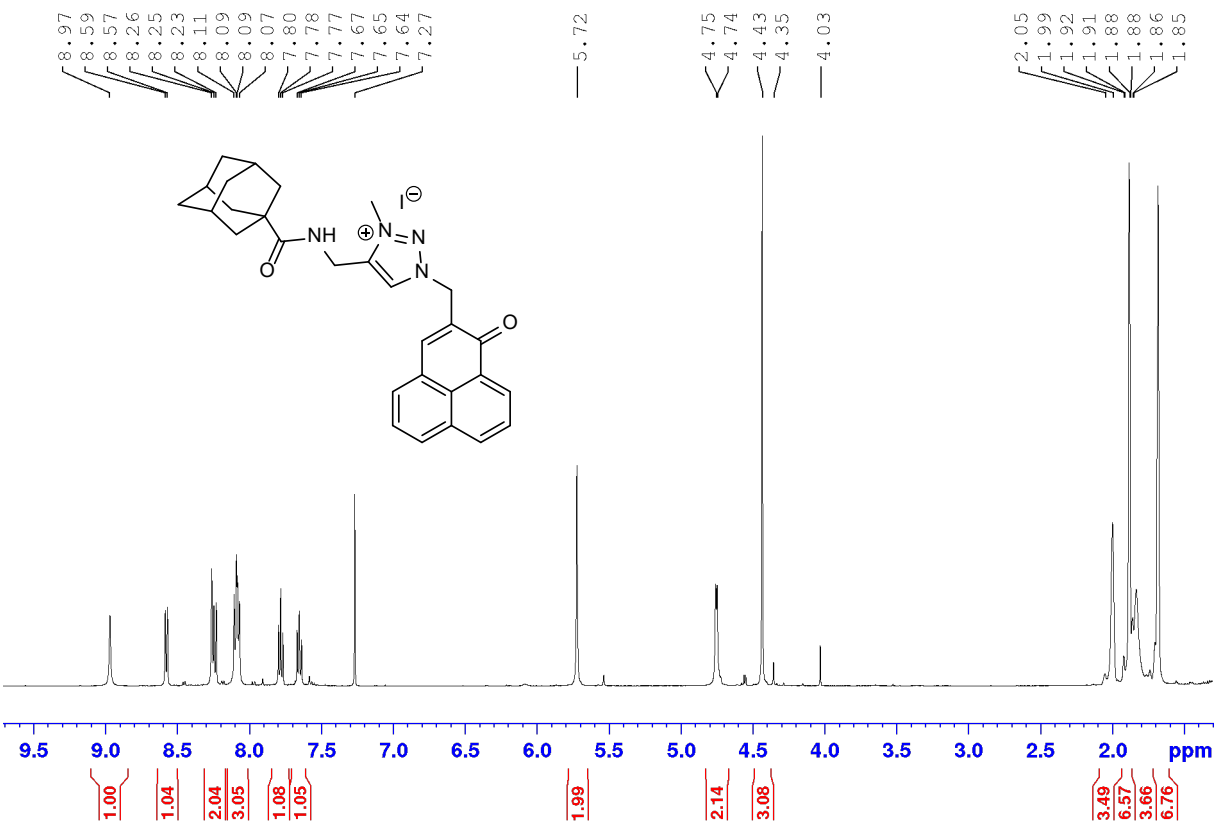

Figure S19. ^{1}H NMR of compound **6a** in $CDCl_3$

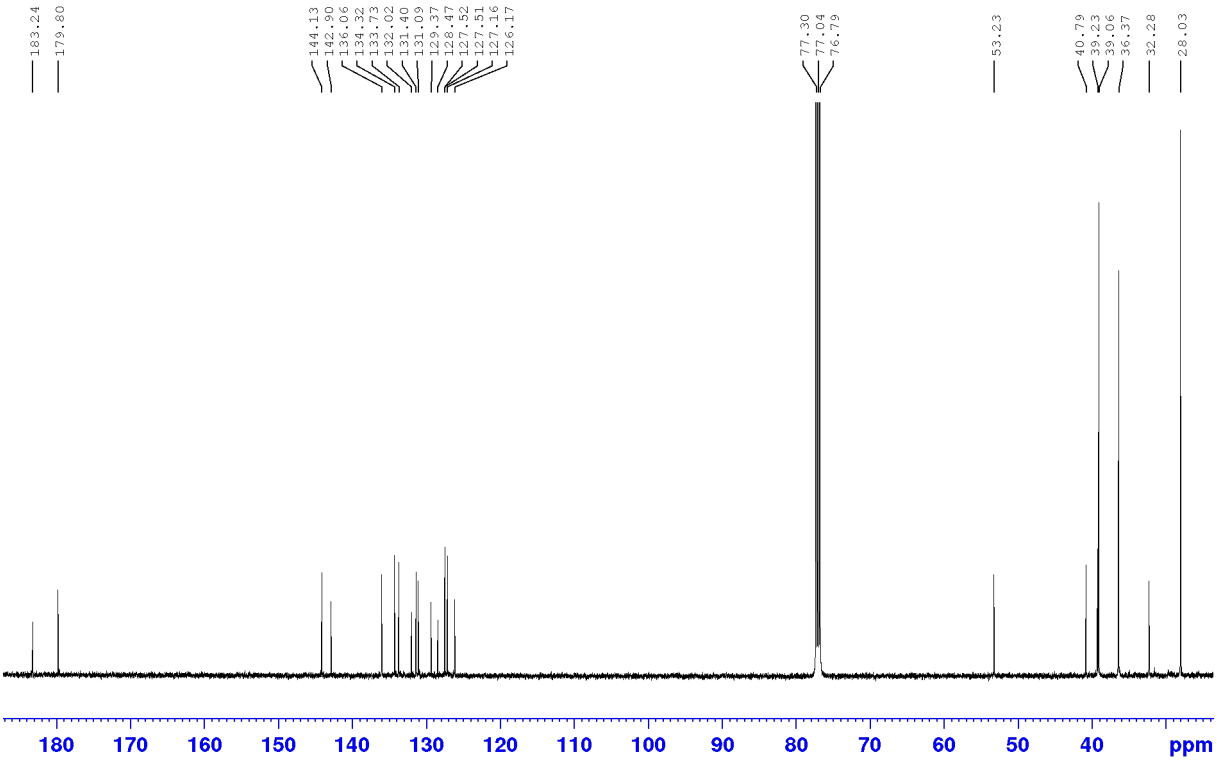

Figure S20. ^{13}C NMR of compound **6a** in $CDCl_3$

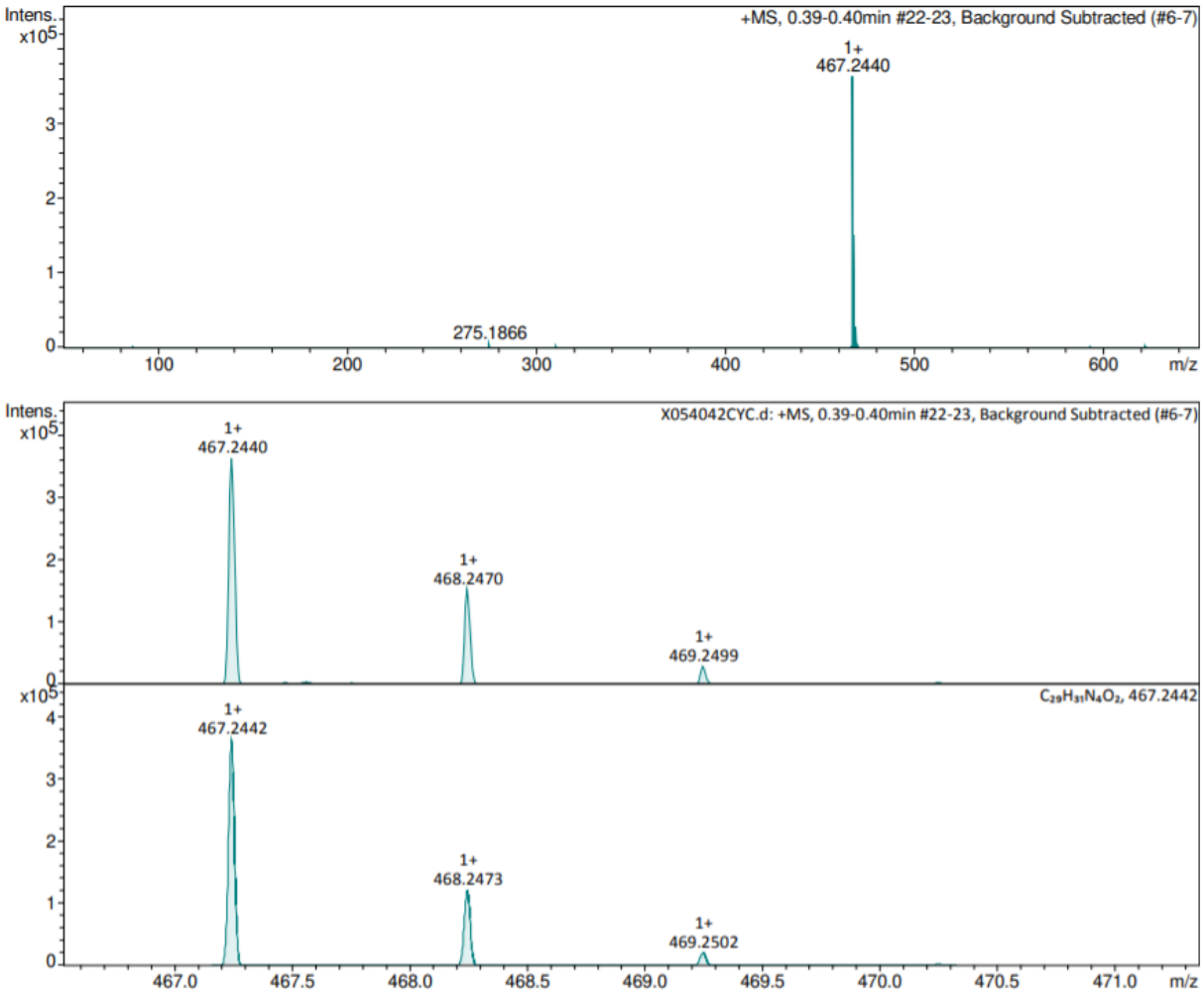

Figure S21. HRMS ESI$^+$ of compound **6a**

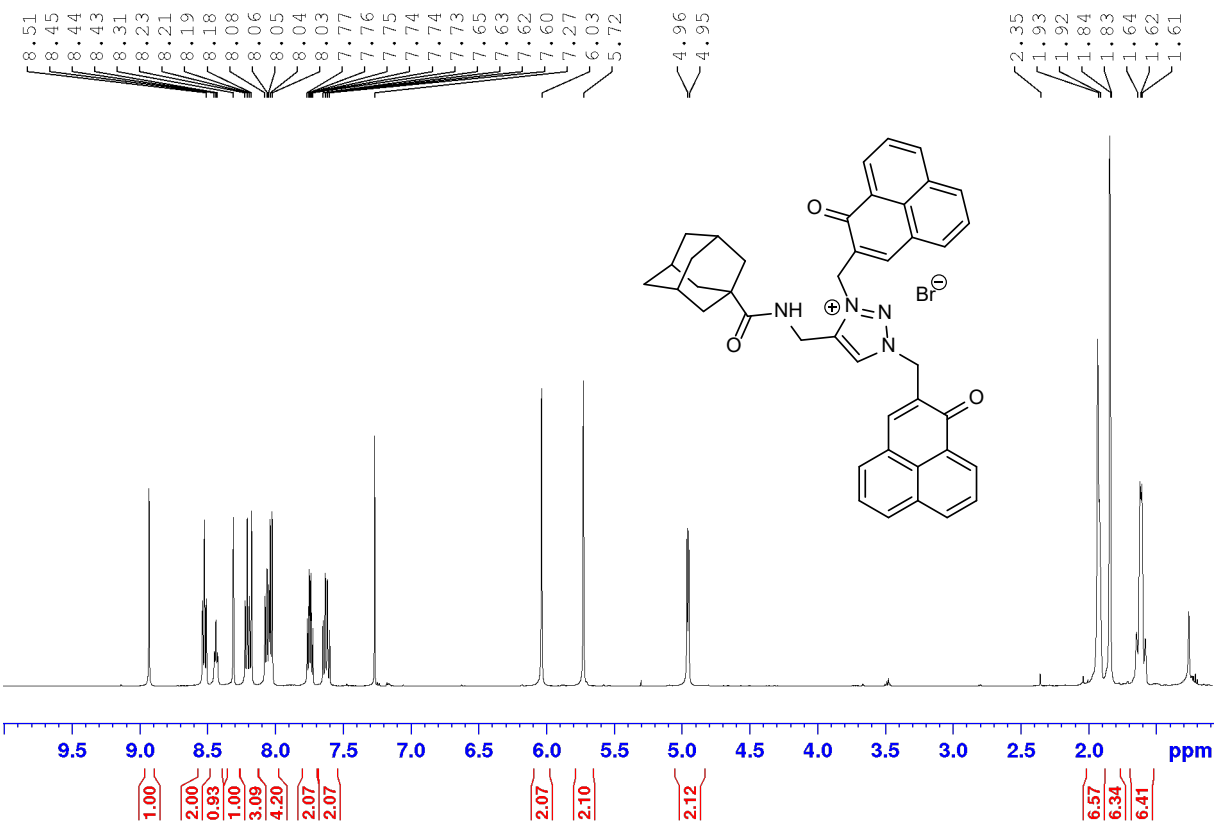

Figure S22. ^{1}H NMR of compound **6b** in $CDCl_3$

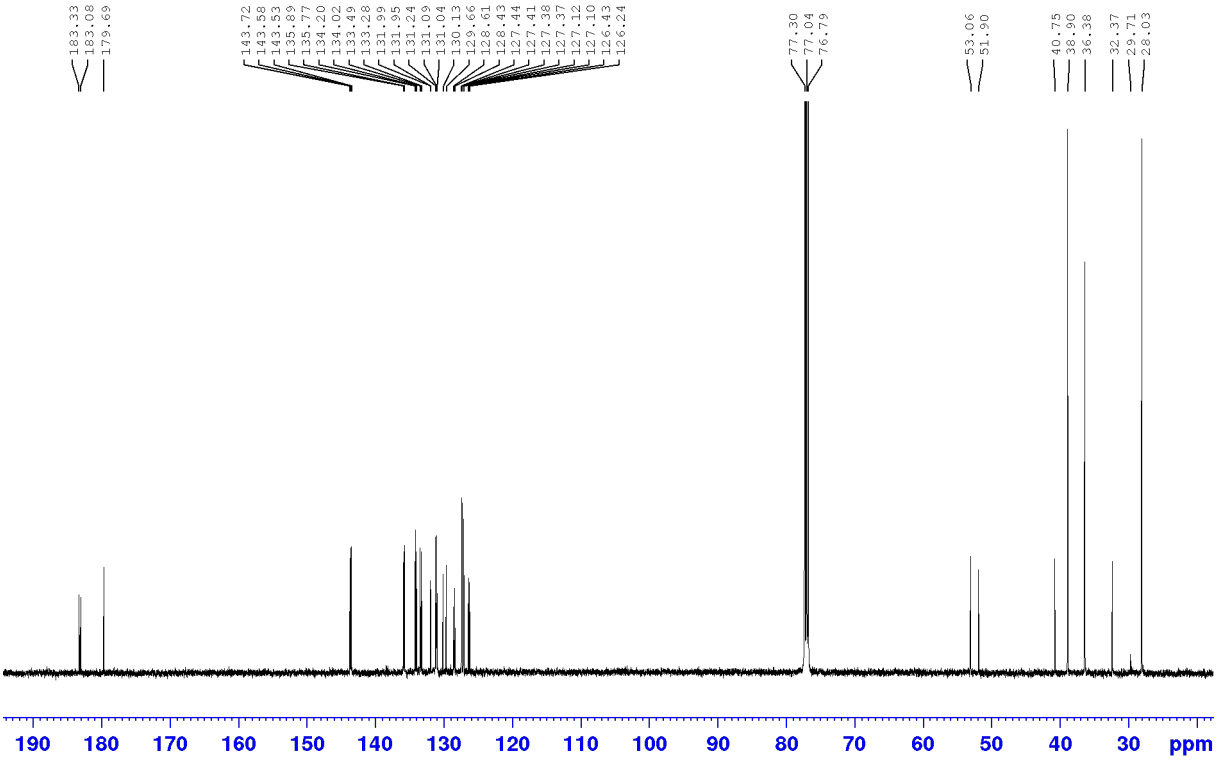

Figure S23. ^{13}C NMR of compound **6b** in $CDCl_3$

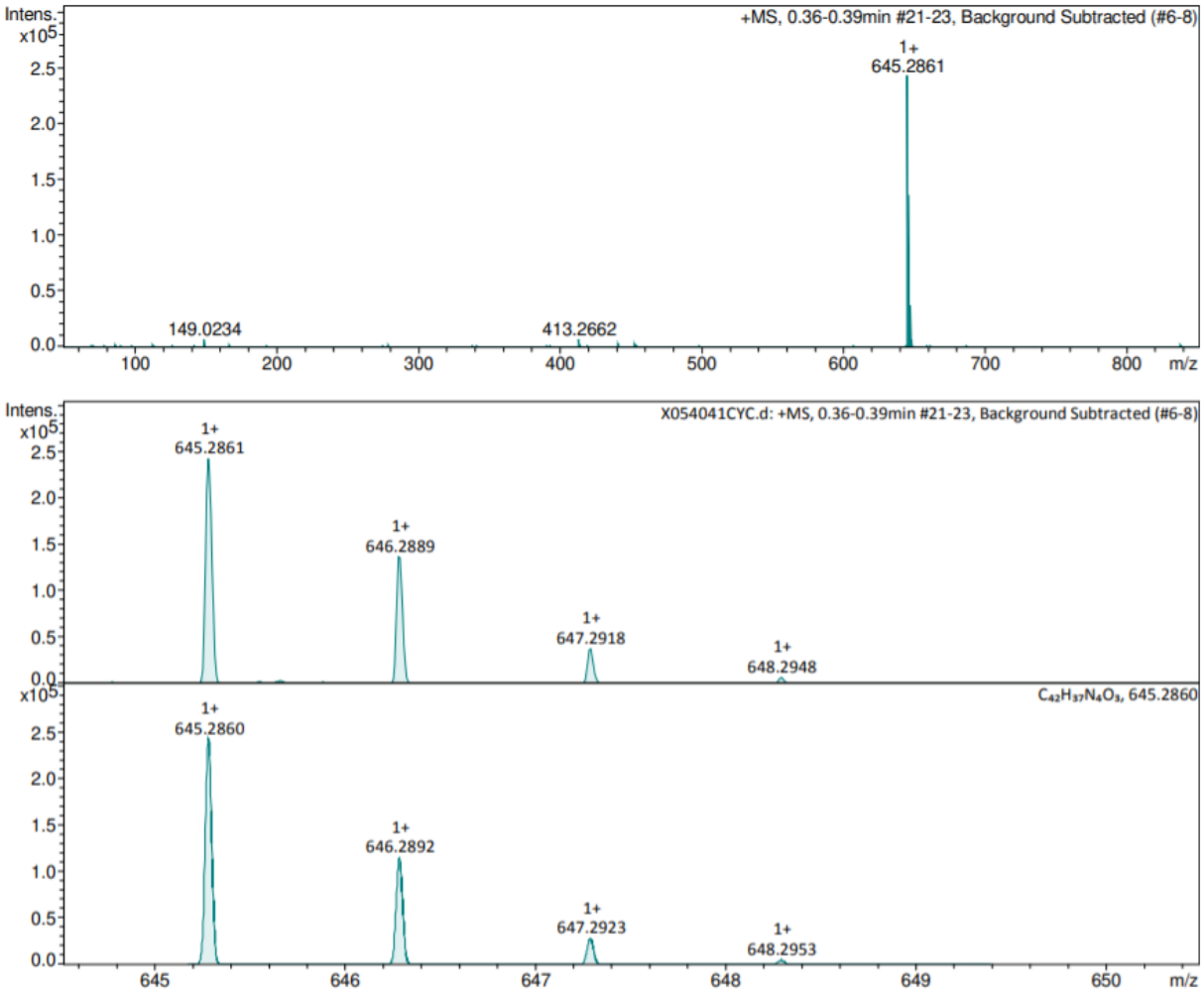

Figure S24. HRMS ESI$^+$ of compound **6b**

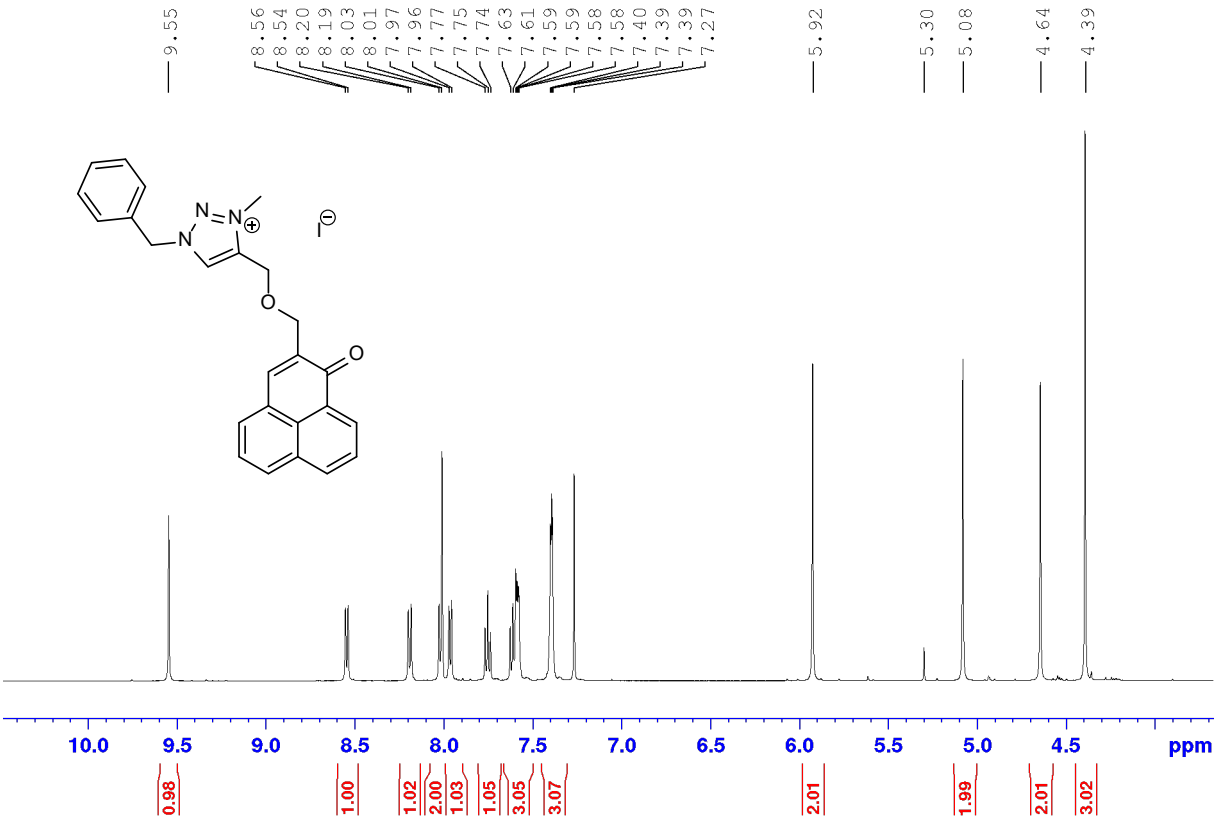

Figure S25. ^{1}H NMR of compound **7a** in $CDCl_3$

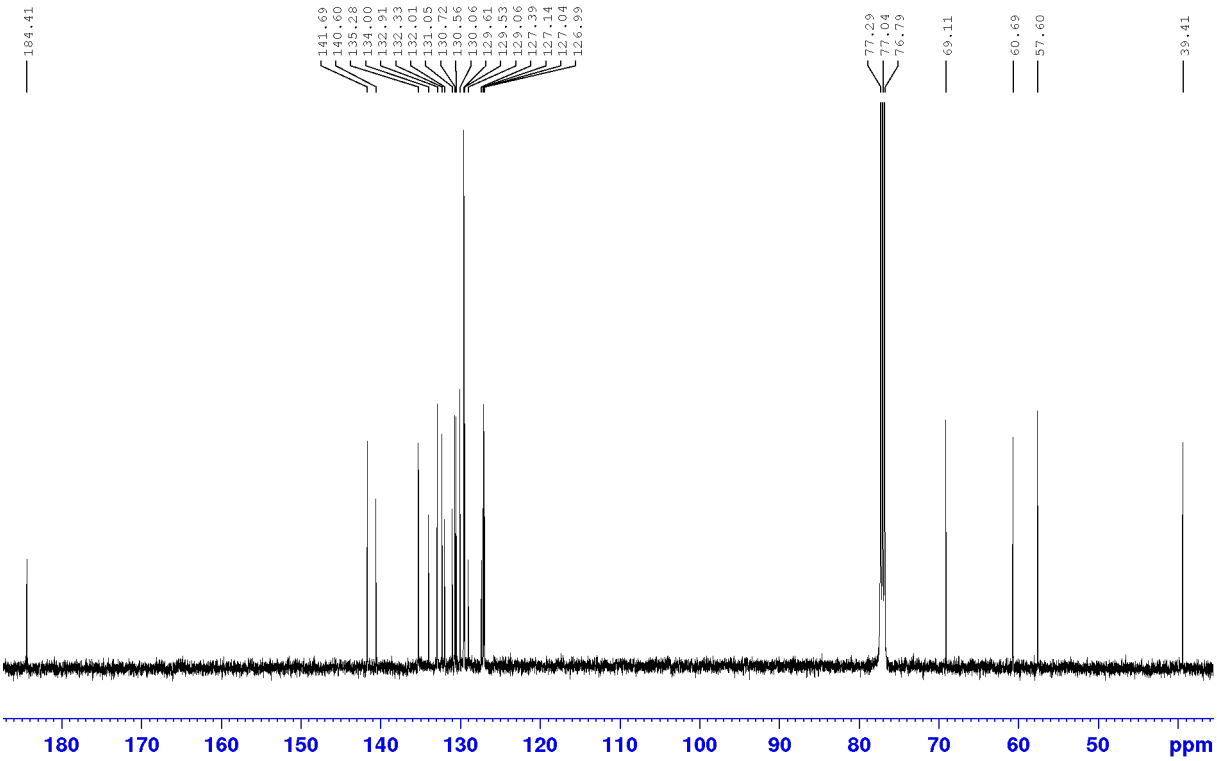

Figure S26. ^{13}C NMR of compound **7a** in $CDCl_3$

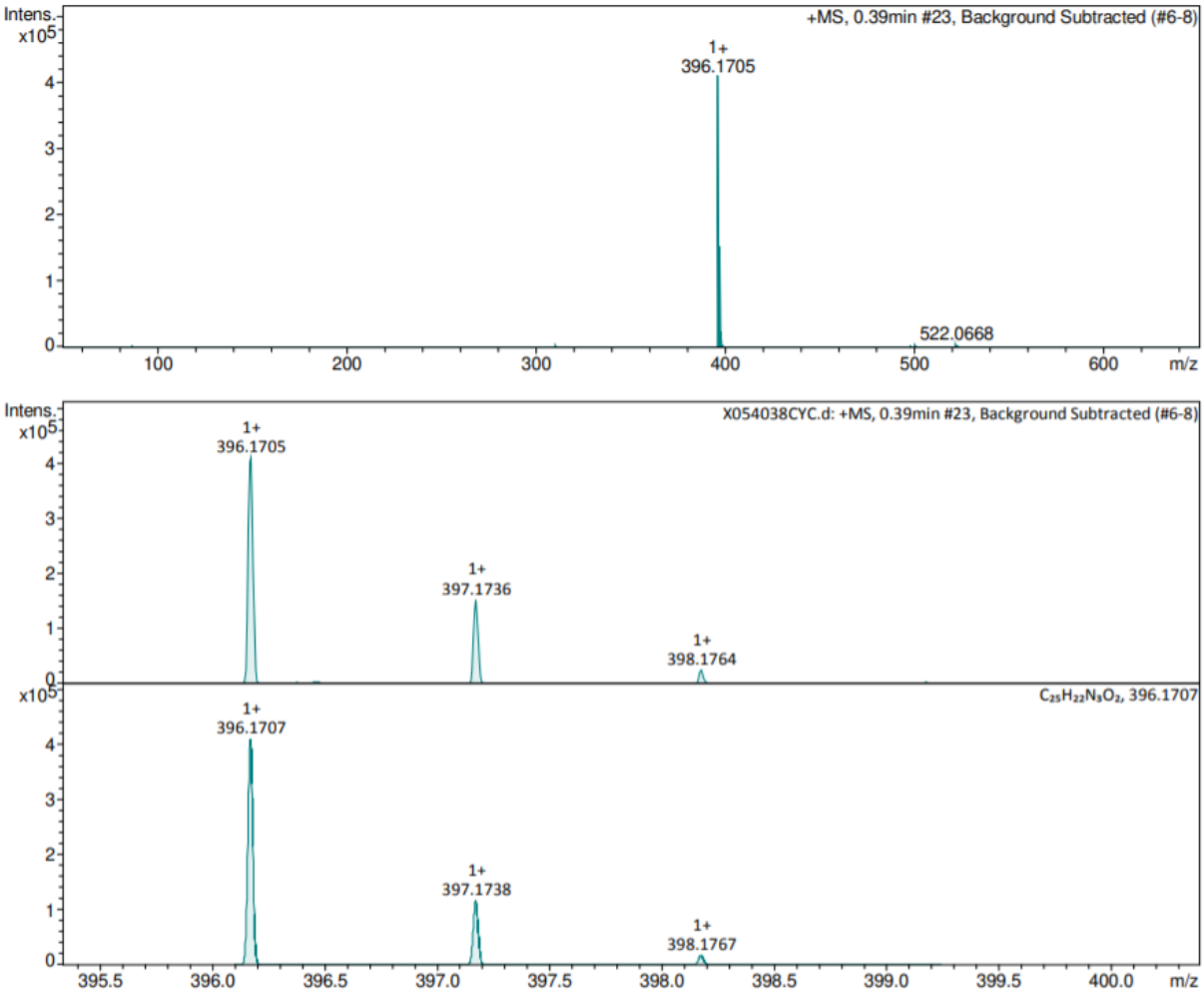

Figure S27. HRMS ESI$^+$ of compound **7a**

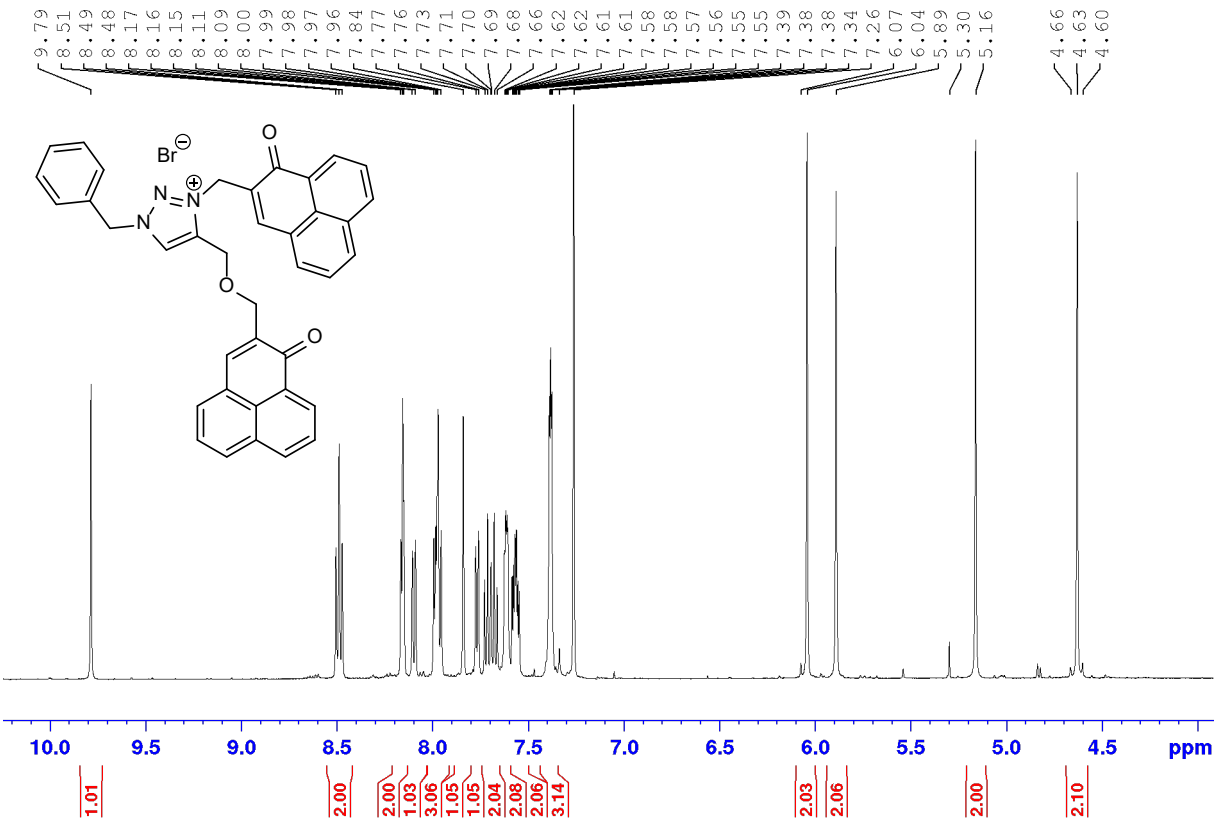

Figure S28. ^{1}H NMR of compound **7b** in $CDCl_3$

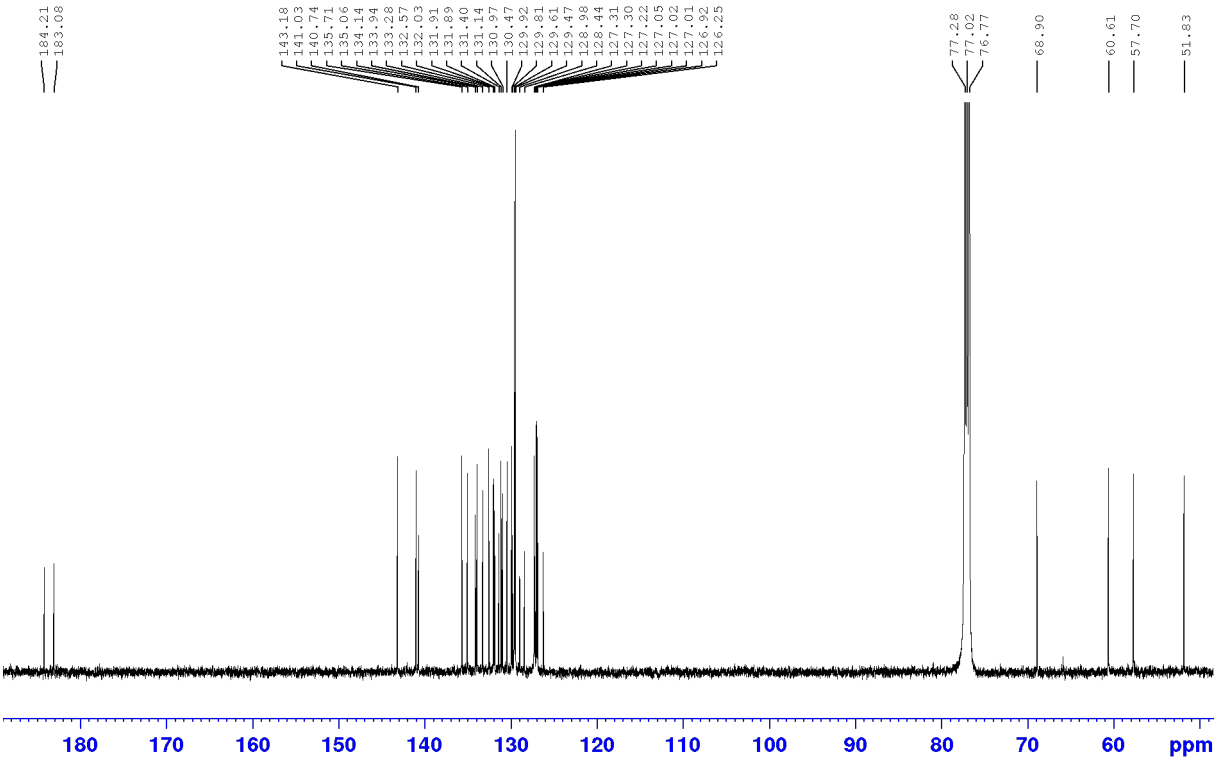

Figure S29. ^{13}C NMR of compound **7b** in $CDCl_3$

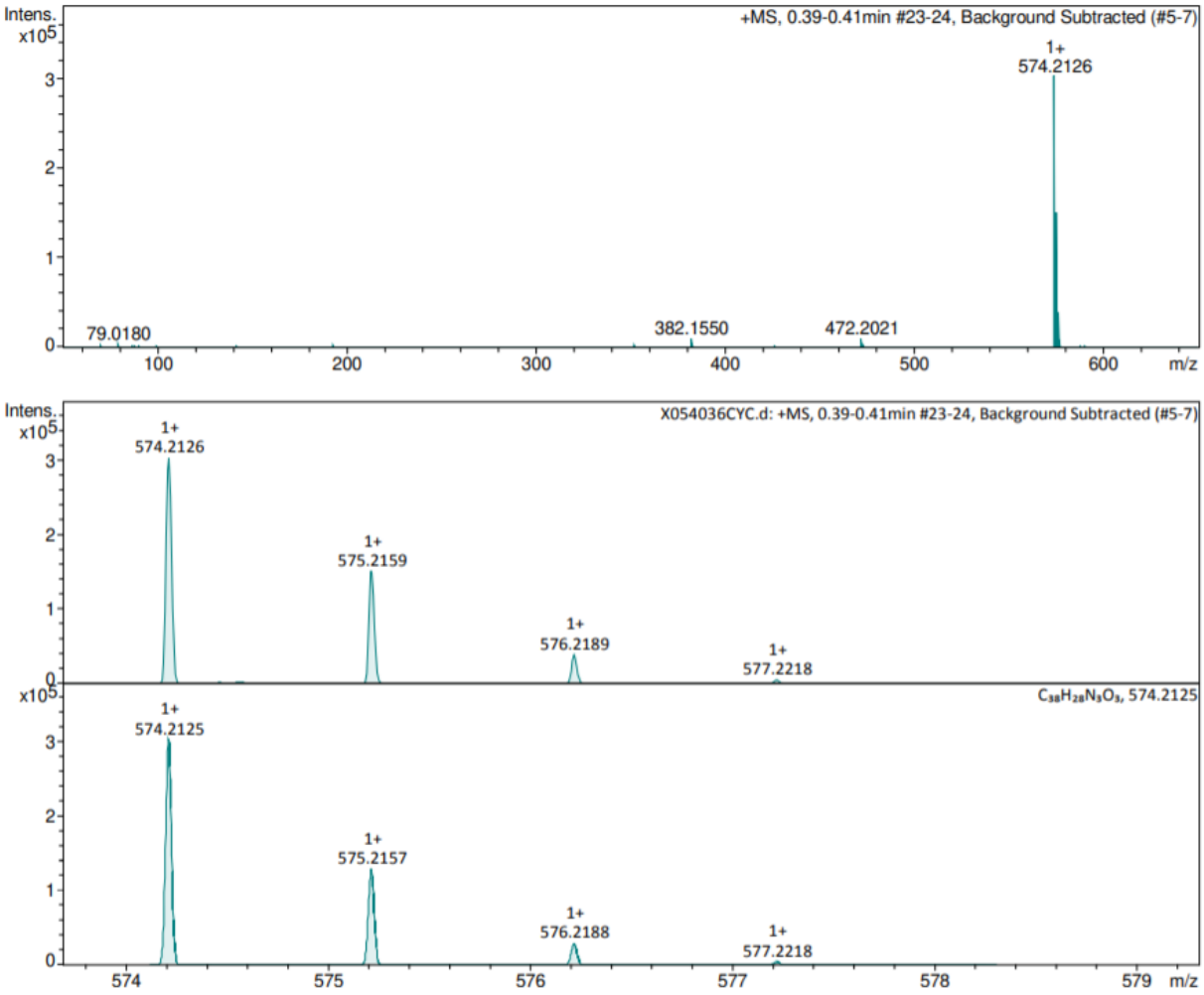

Figure S30. HRMS ESI$^+$ of compound **7b**

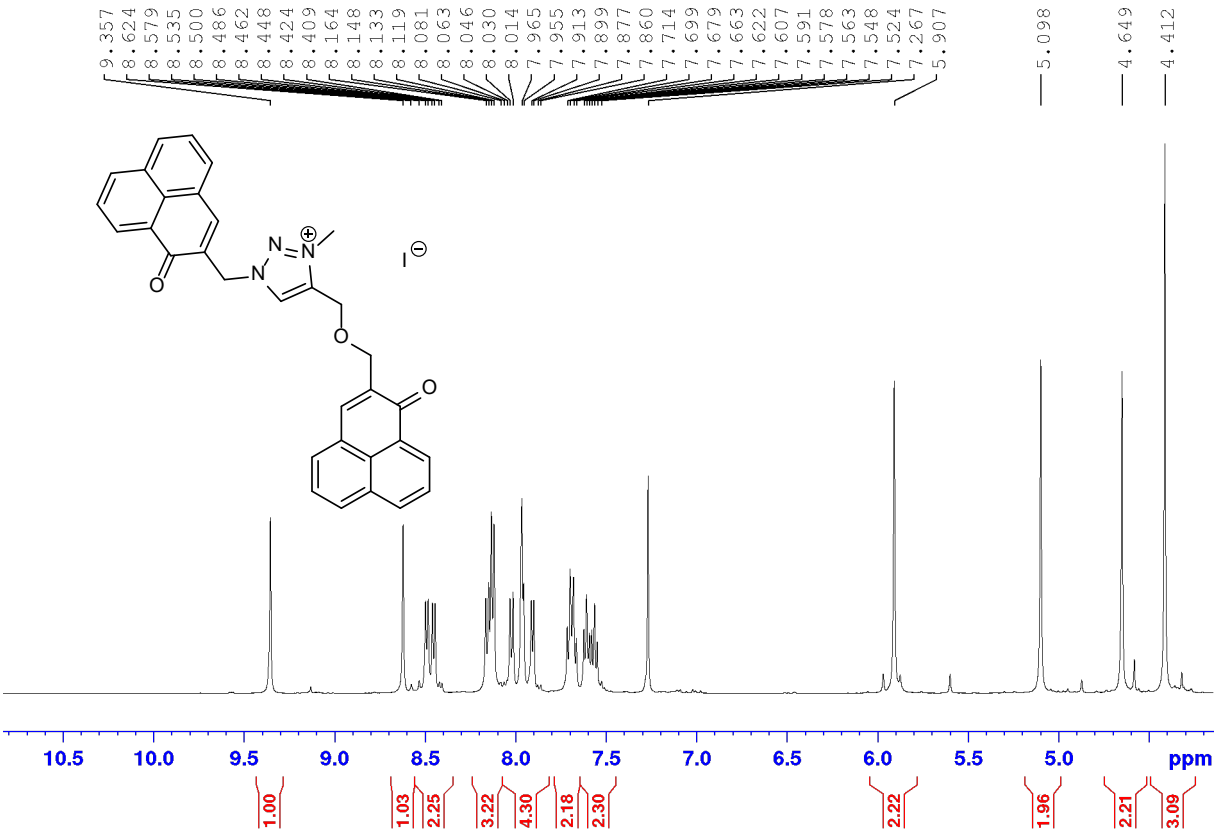

Figure S31. ^{1}H NMR of compound **8a** in $CDCl_3$

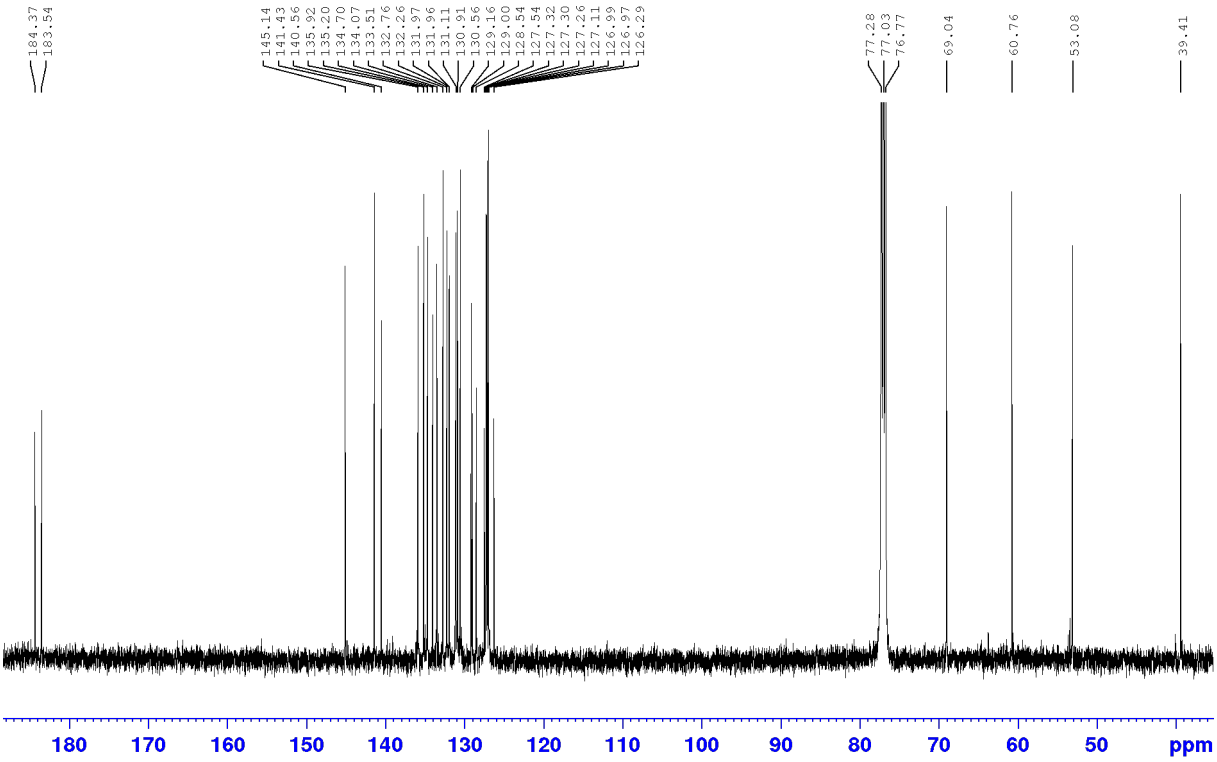

Figure S32. ^{13}C NMR of compound **8a** in $CDCl_3$

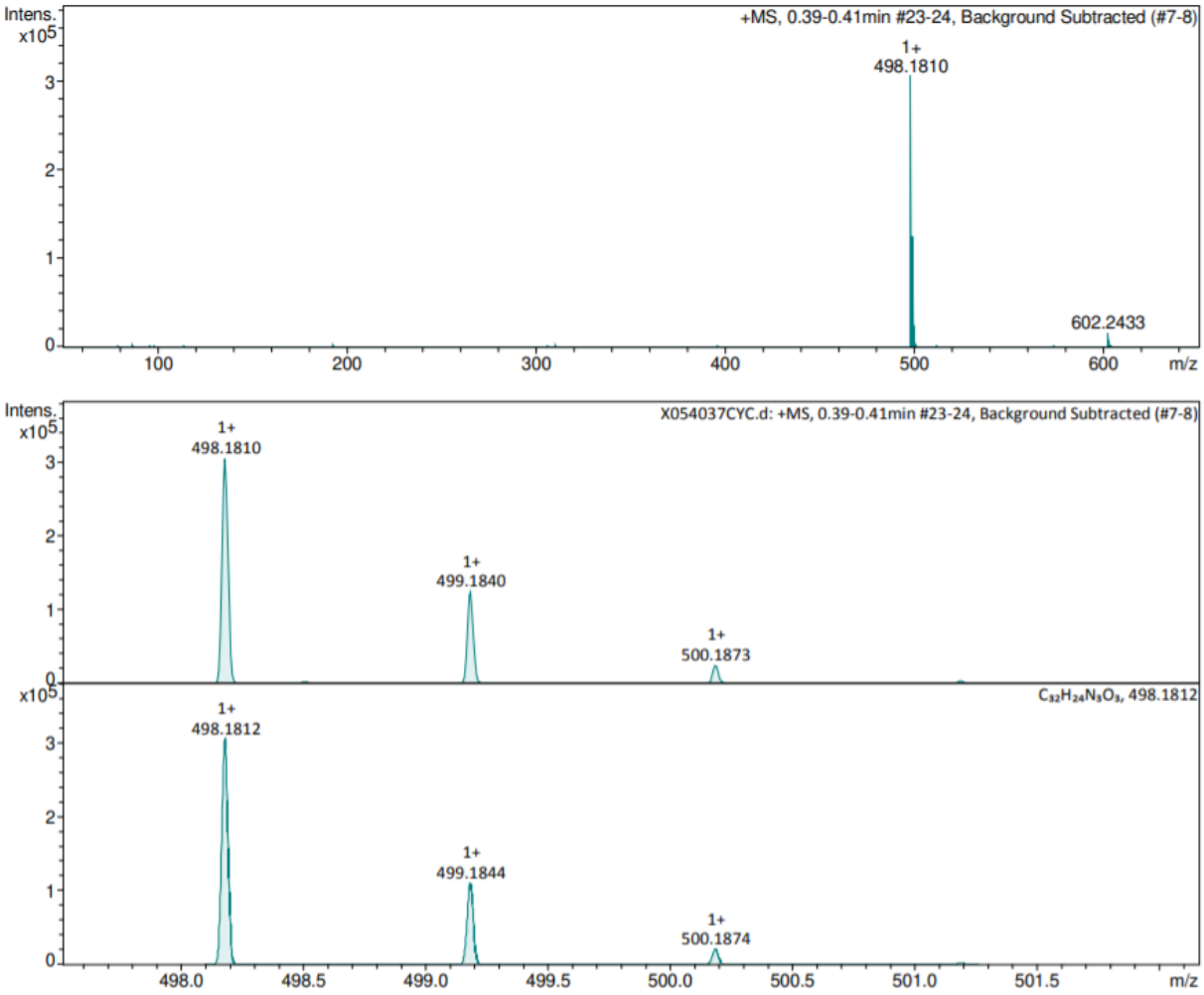

Figure S33. HRMS ESI$^+$ of compound **8a**

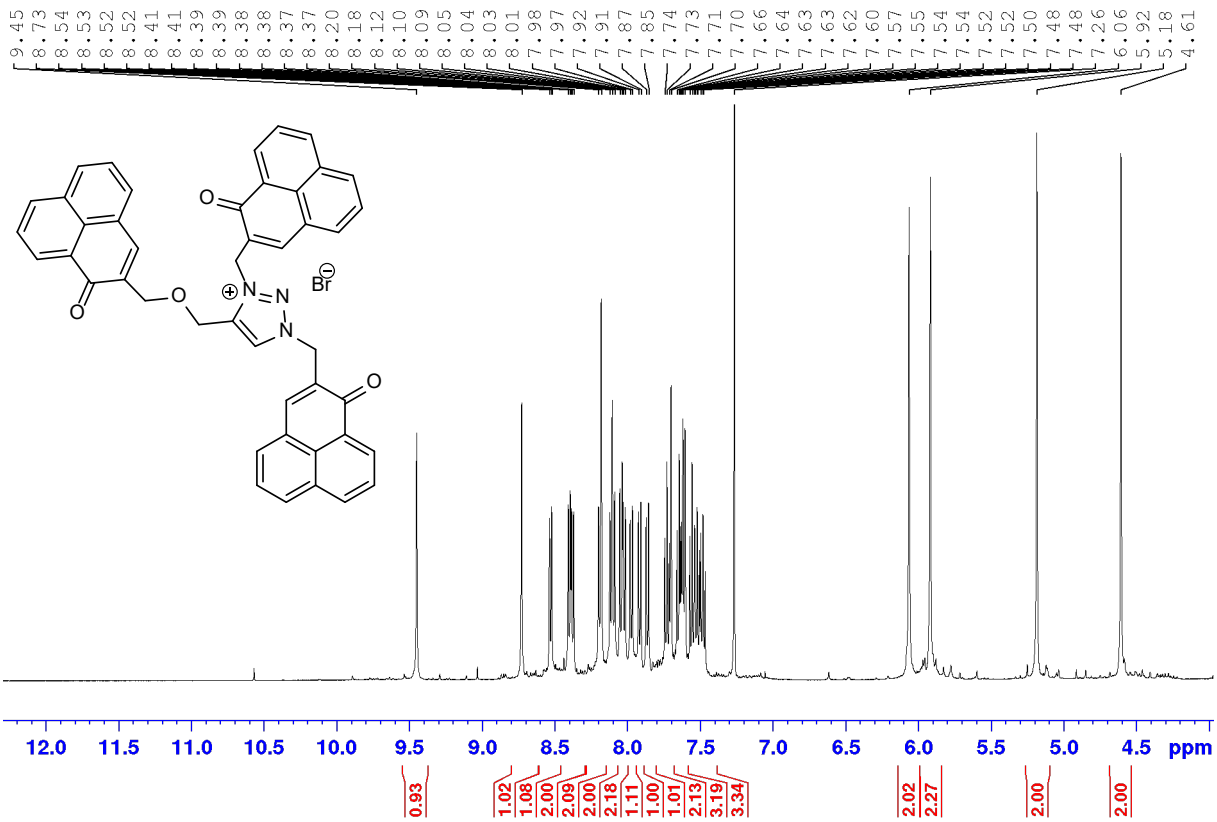

Figure S34. ^{1}H NMR of compound **8b** in $CDCl_3$

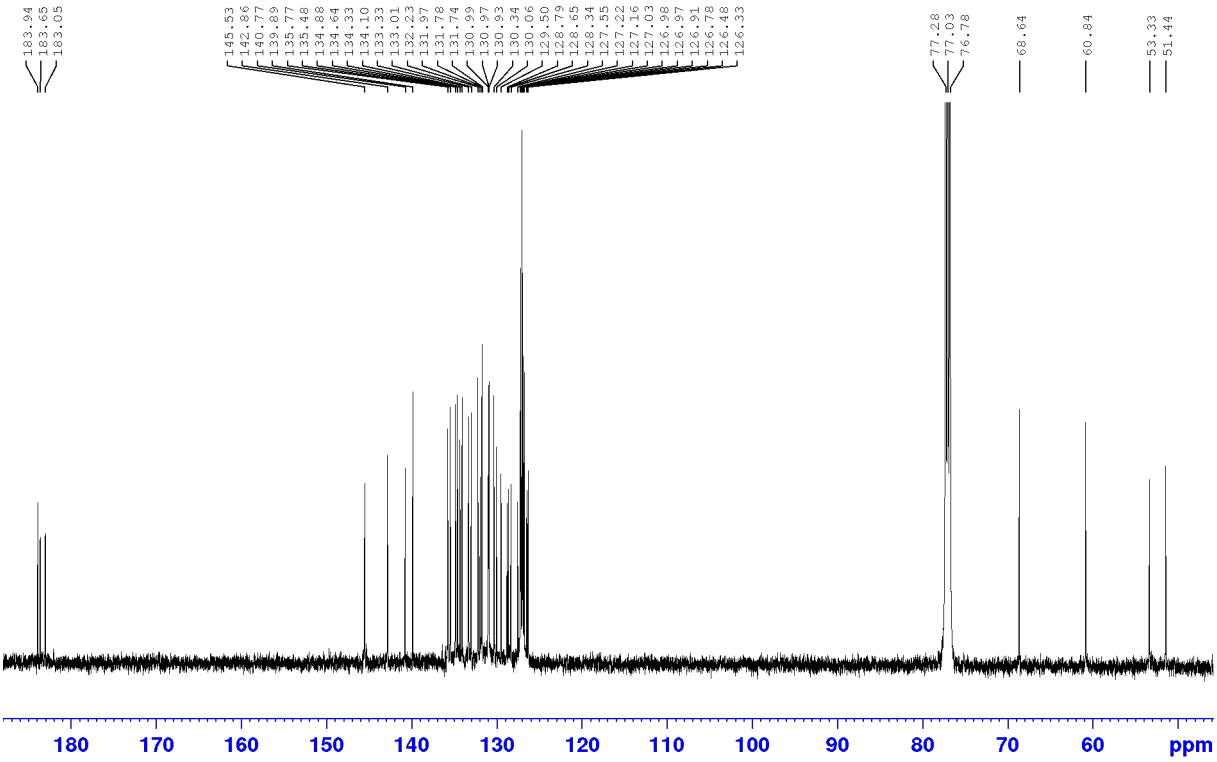

Figure S35. ^{13}C NMR of compound **8b** in $CDCl_3$

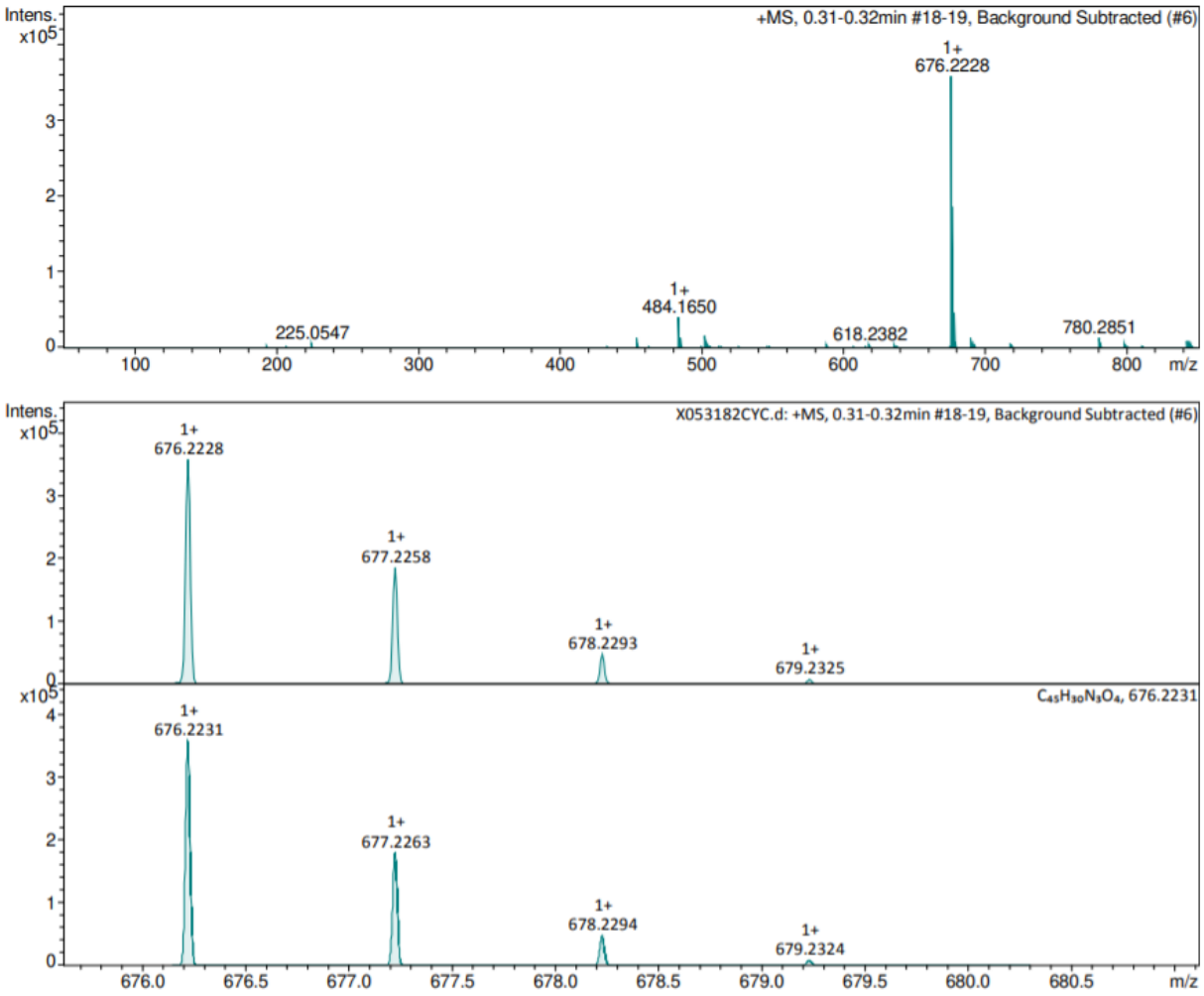

Figure S36. HRMS ESI$^+$ of compound **8b**

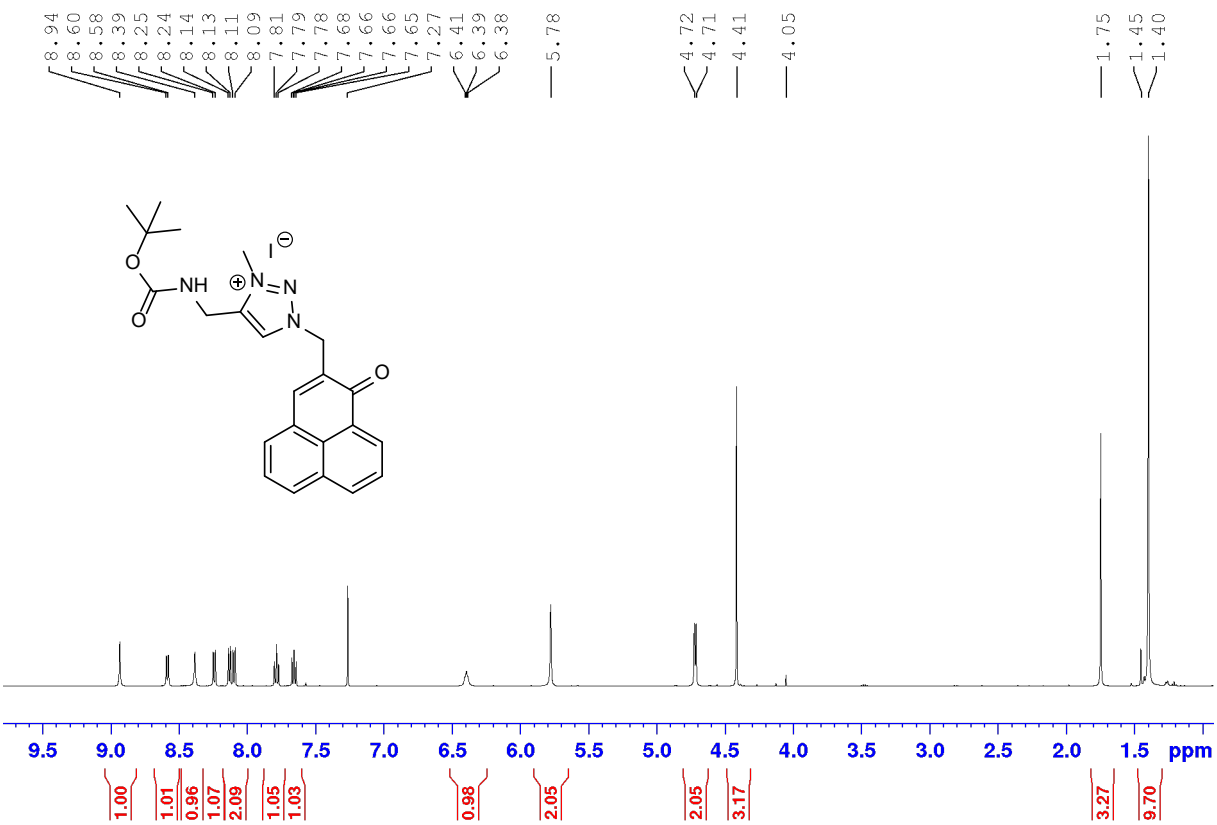

Figure S37. ^{1}H NMR of compound **9a** in $CDCl_3$

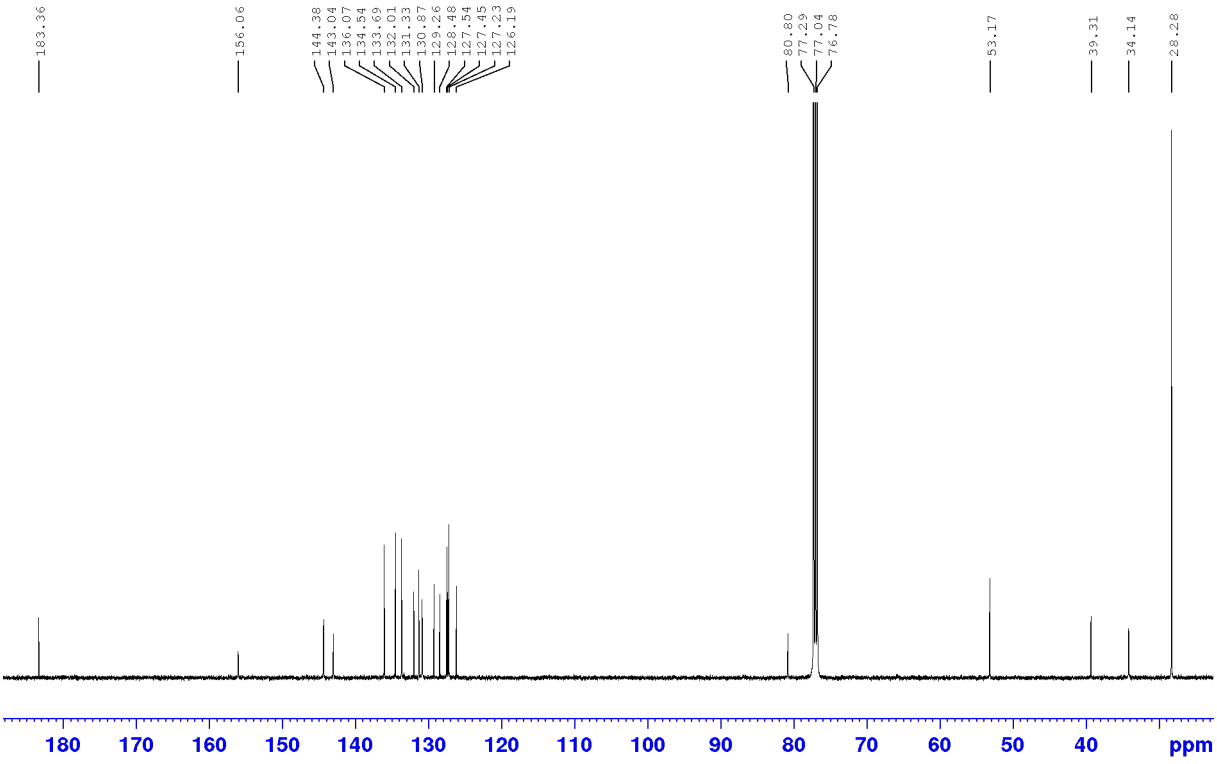

Figure S38. ^{13}C NMR of compound **9a** in $CDCl_3$

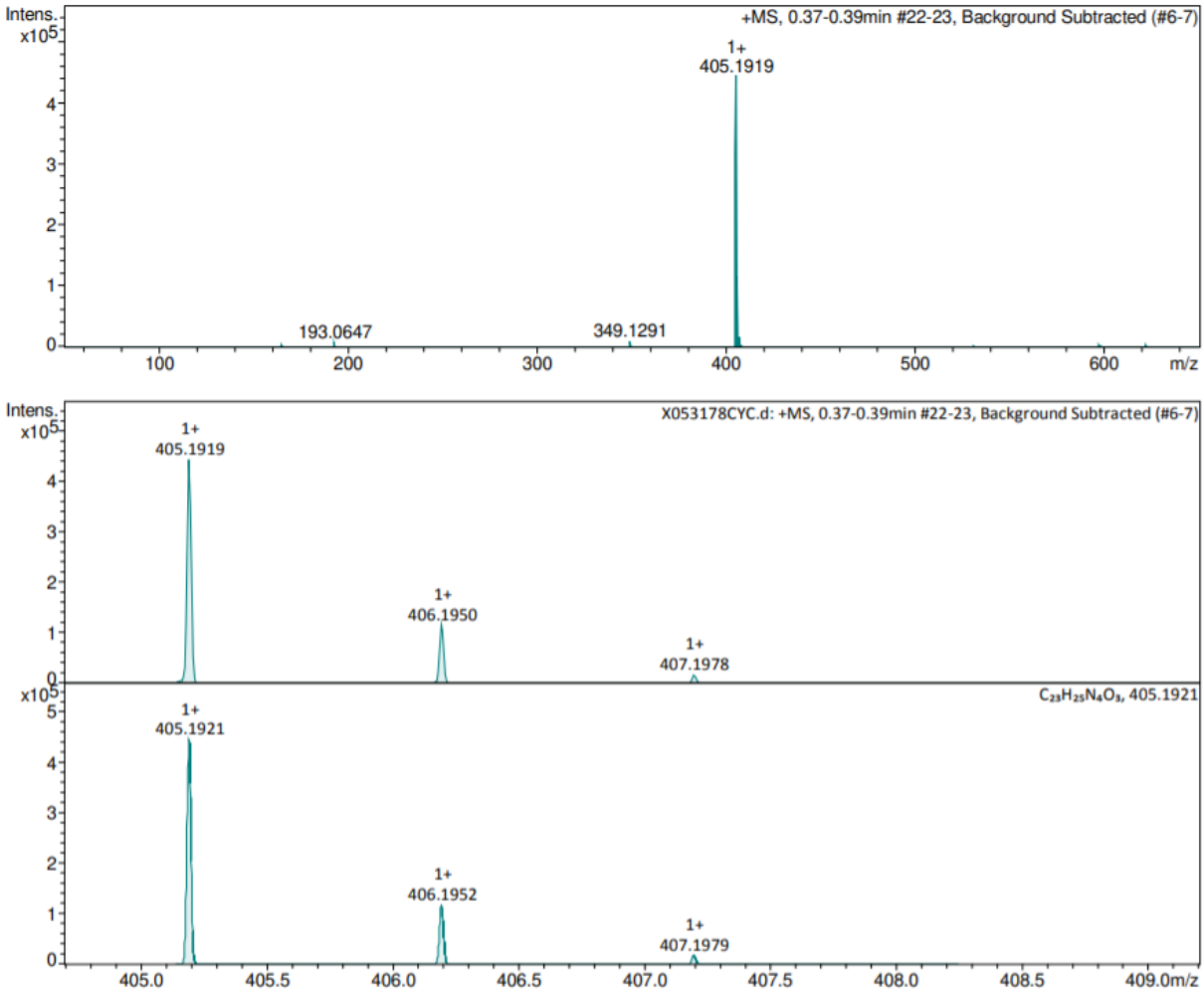

Figure S39. HRMS ESI$^+$ of compound **9a**

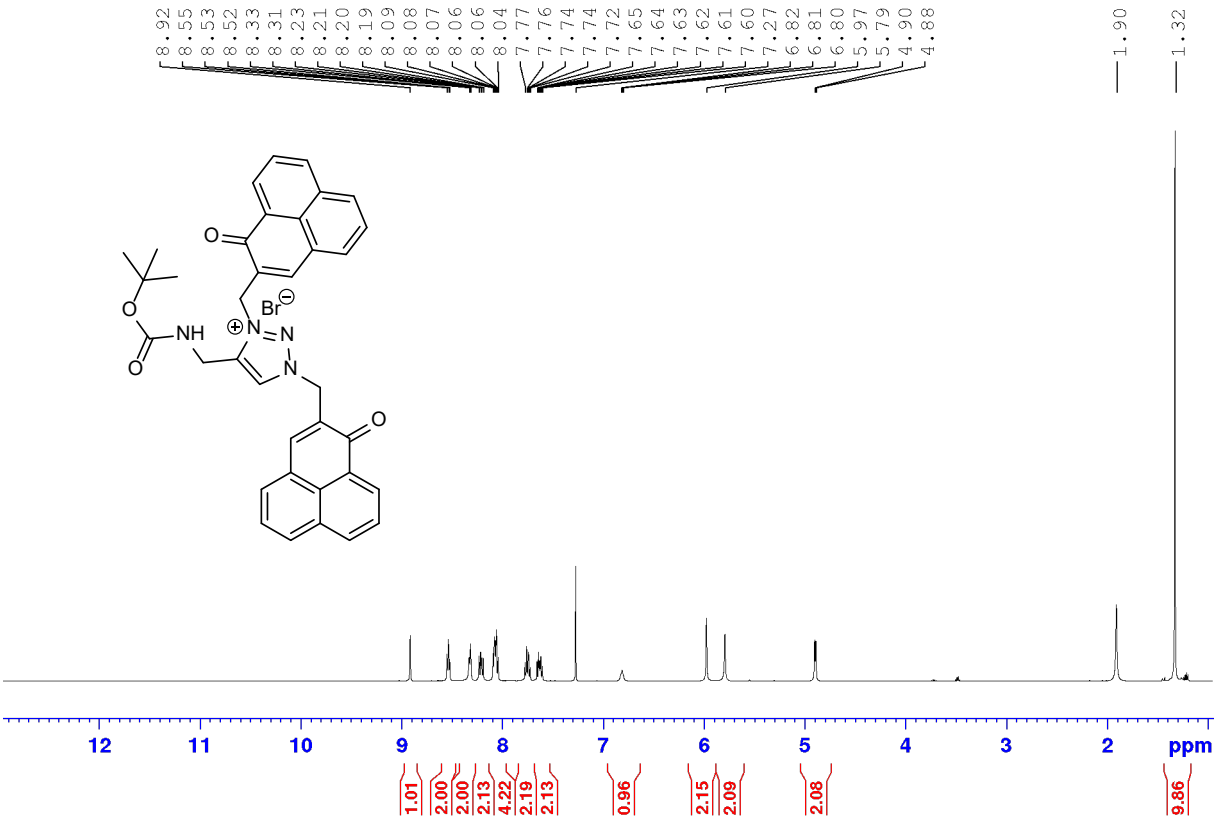

Figure S40. ^{1}H NMR of compound **9b** in $CDCl_3$

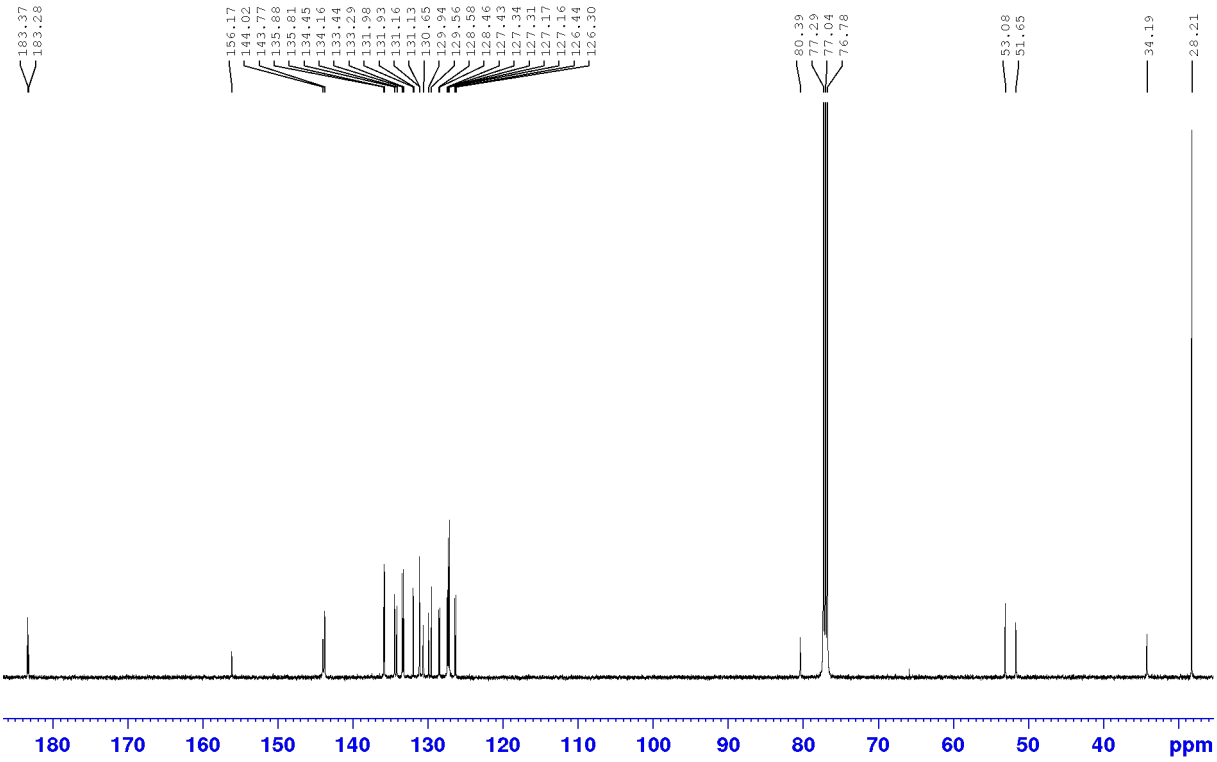

Figure S41. ^{13}C NMR of compound **9b** in $CDCl_3$

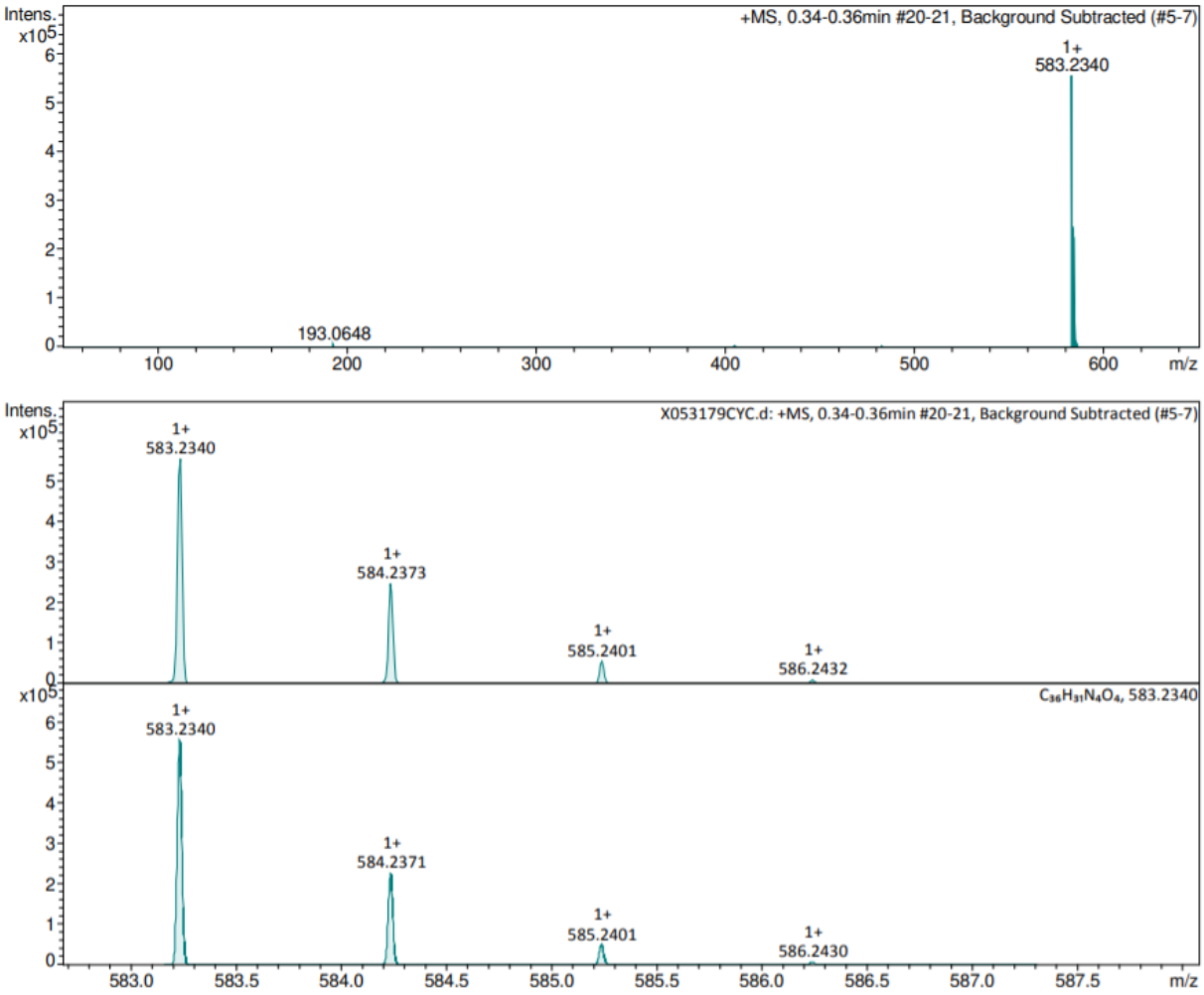

Figure S42. HRMS ESI$^+$ of compound **9b**

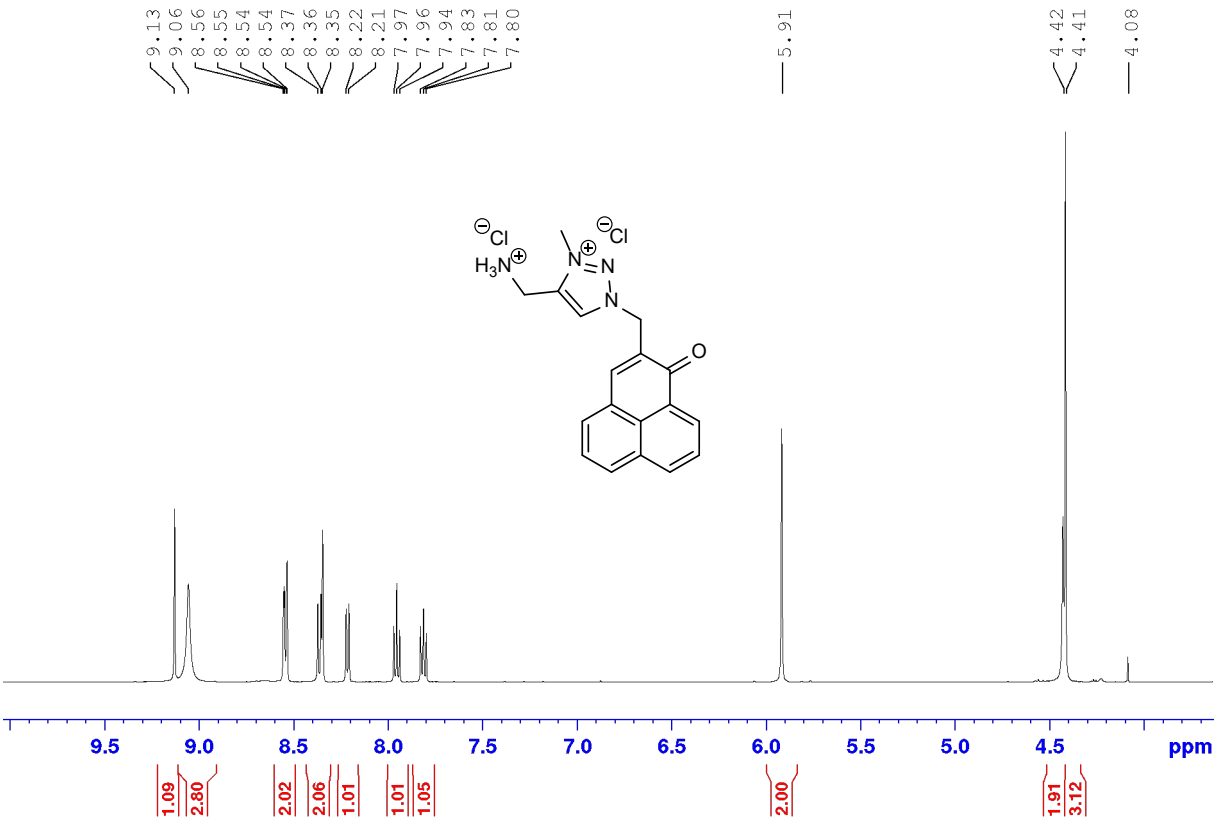

Figure S43. ^{1}H NMR of compound **10a** in DMSO-d_6

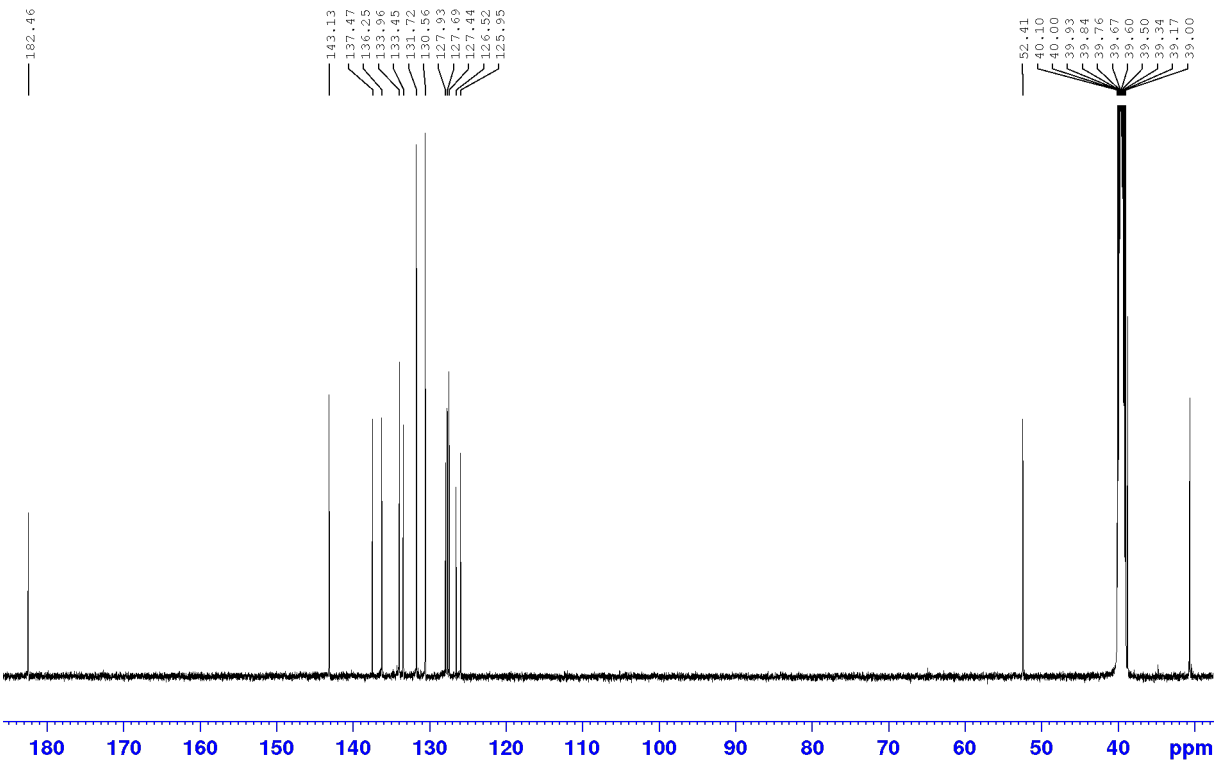

Figure S44. ^{13}C NMR of compound **10a** in DMSO-d_6

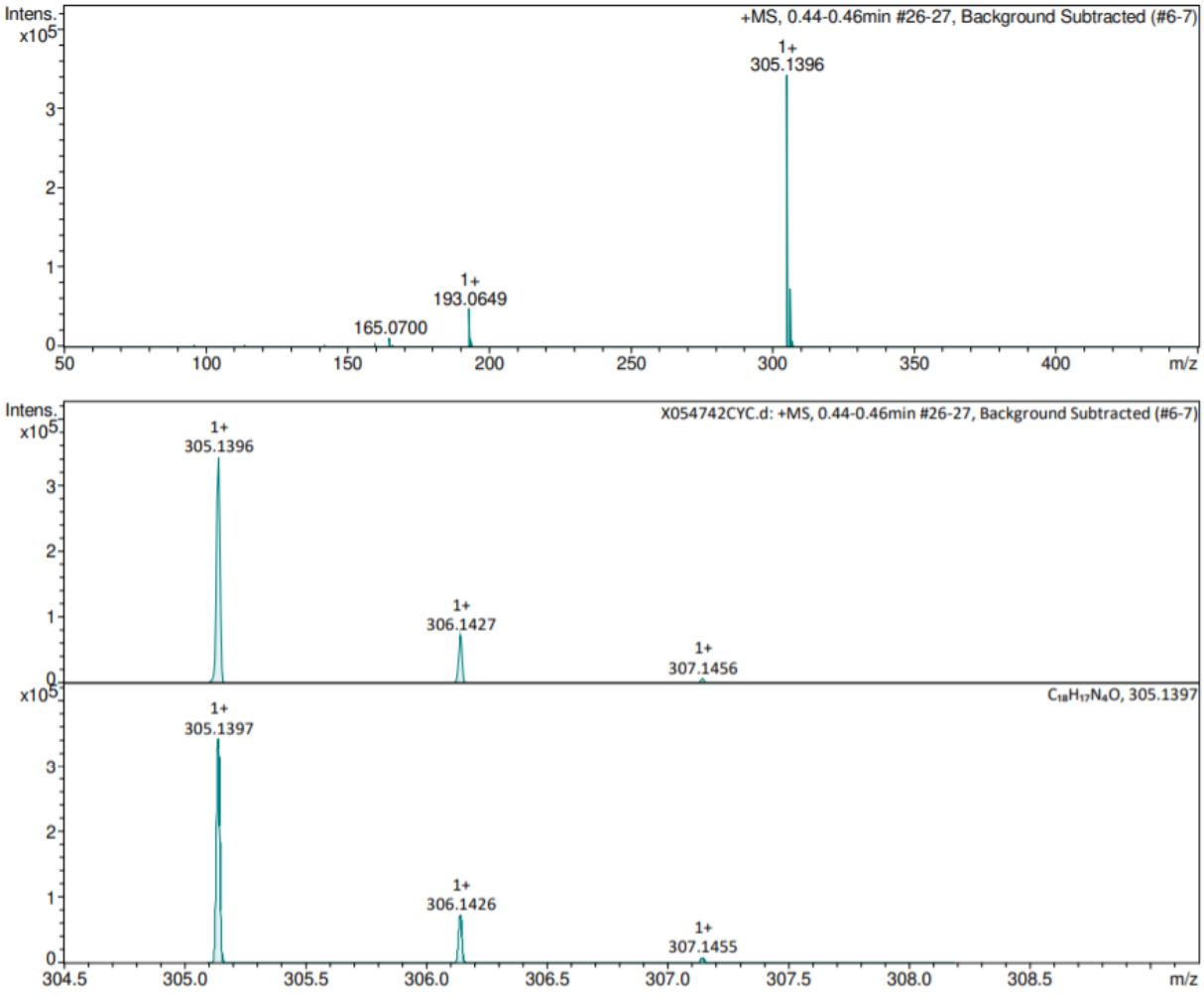

Figure S45. HRMS ESI$^+$ of compound **10a**

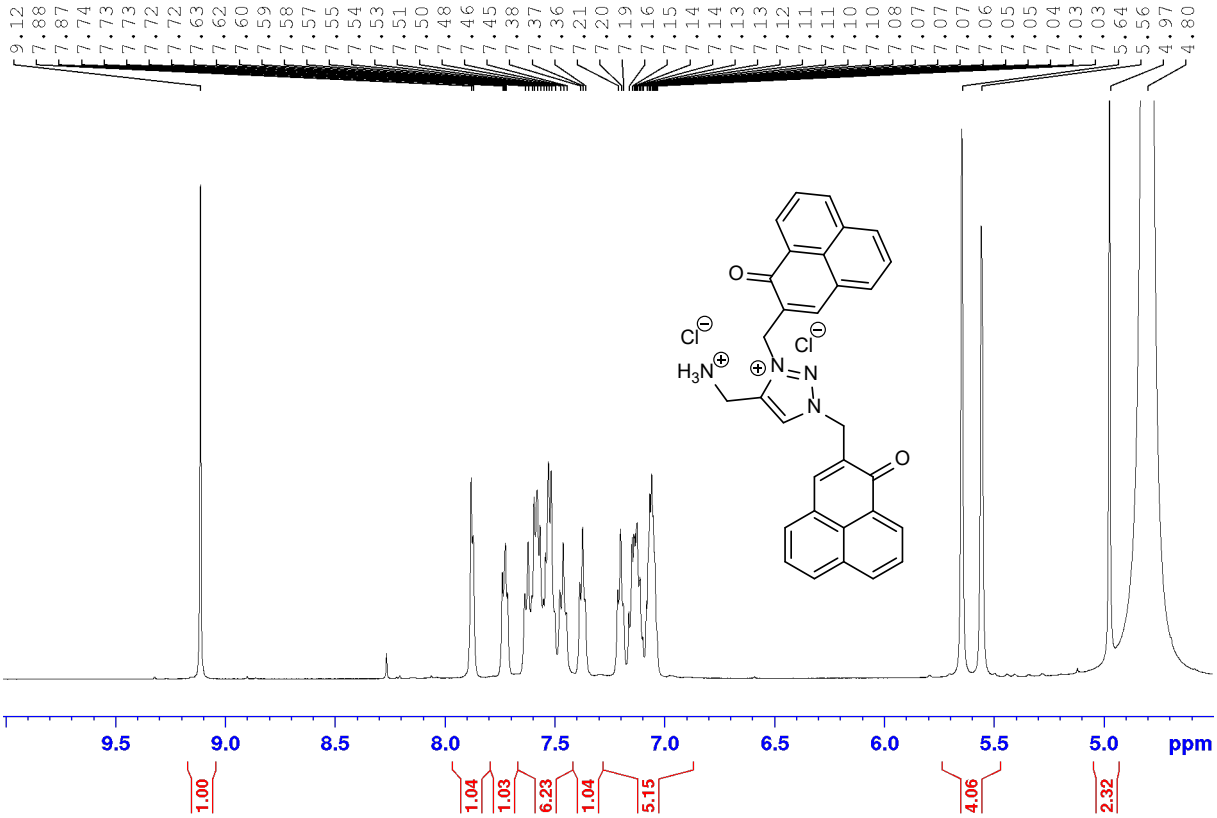

Figure S46. ^{1}H NMR of compound **10b** in D_2O

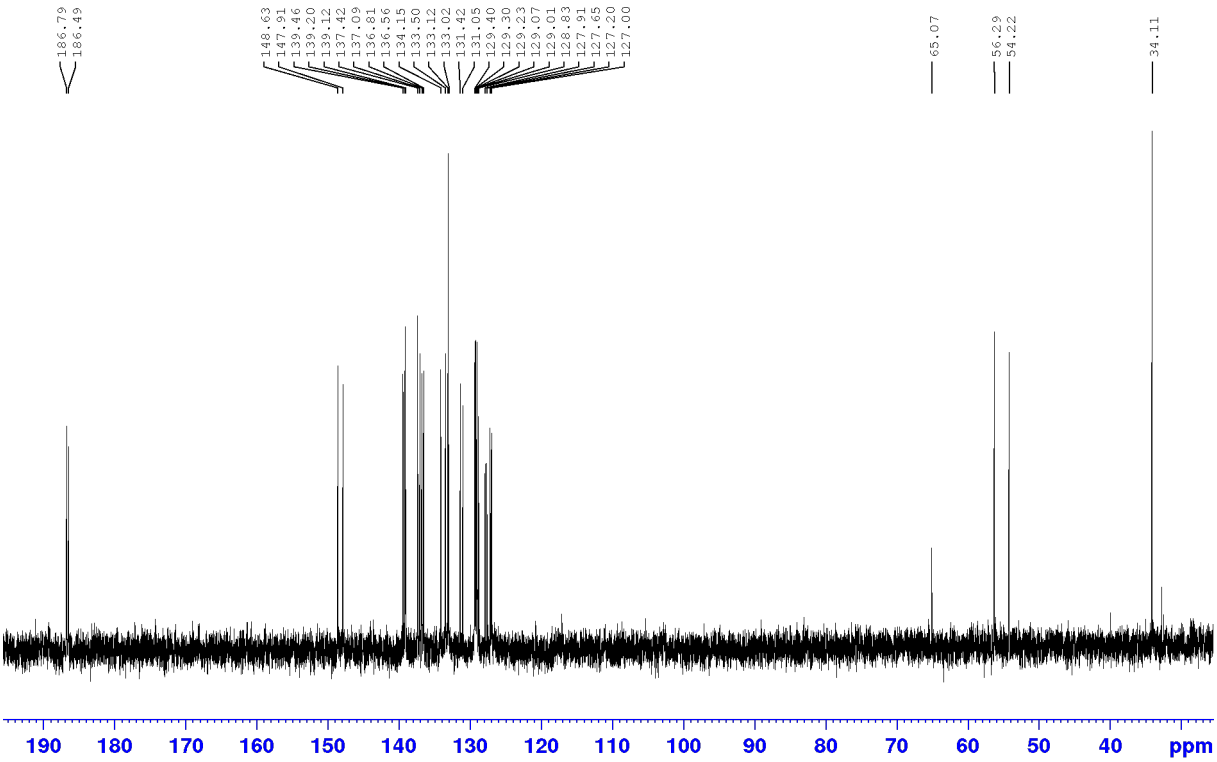

Figure S47. ^{13}C NMR of compound **10b** in D_2O

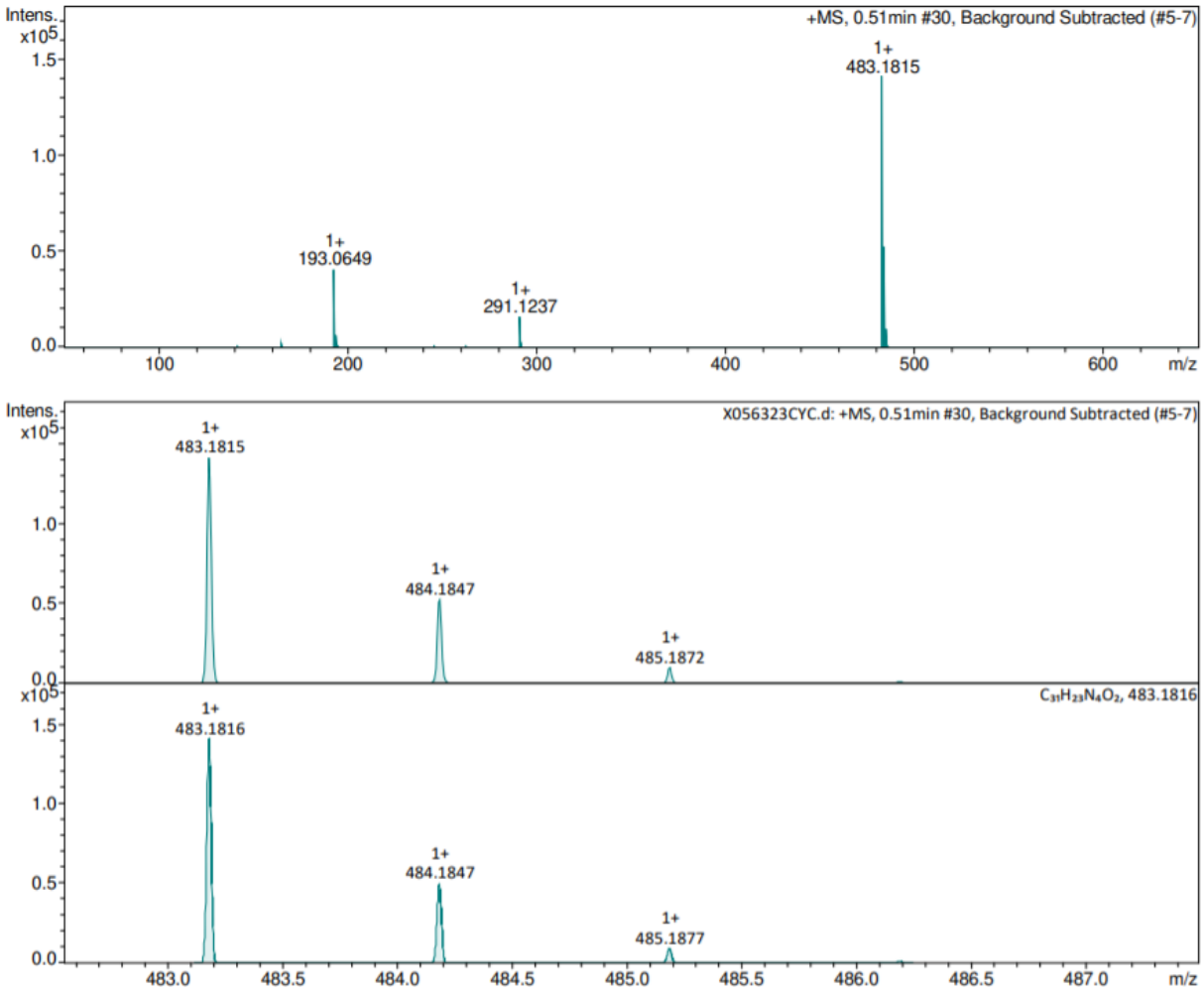

Figure S48. HRMS ESI$^+$ of compound **10b**

Figure S49 : Chemical structures of all compounds