

Supplementary Materials

Efficacy of Novel Quaternary Ammonium and Phosphonium Salts Differing in Cation Type and Alkyl Chain Length against Antibiotic-Resistant *Staphylococcus aureus*

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1. Experimental Section

1.1 Nuclear Magnetic Resonance Data

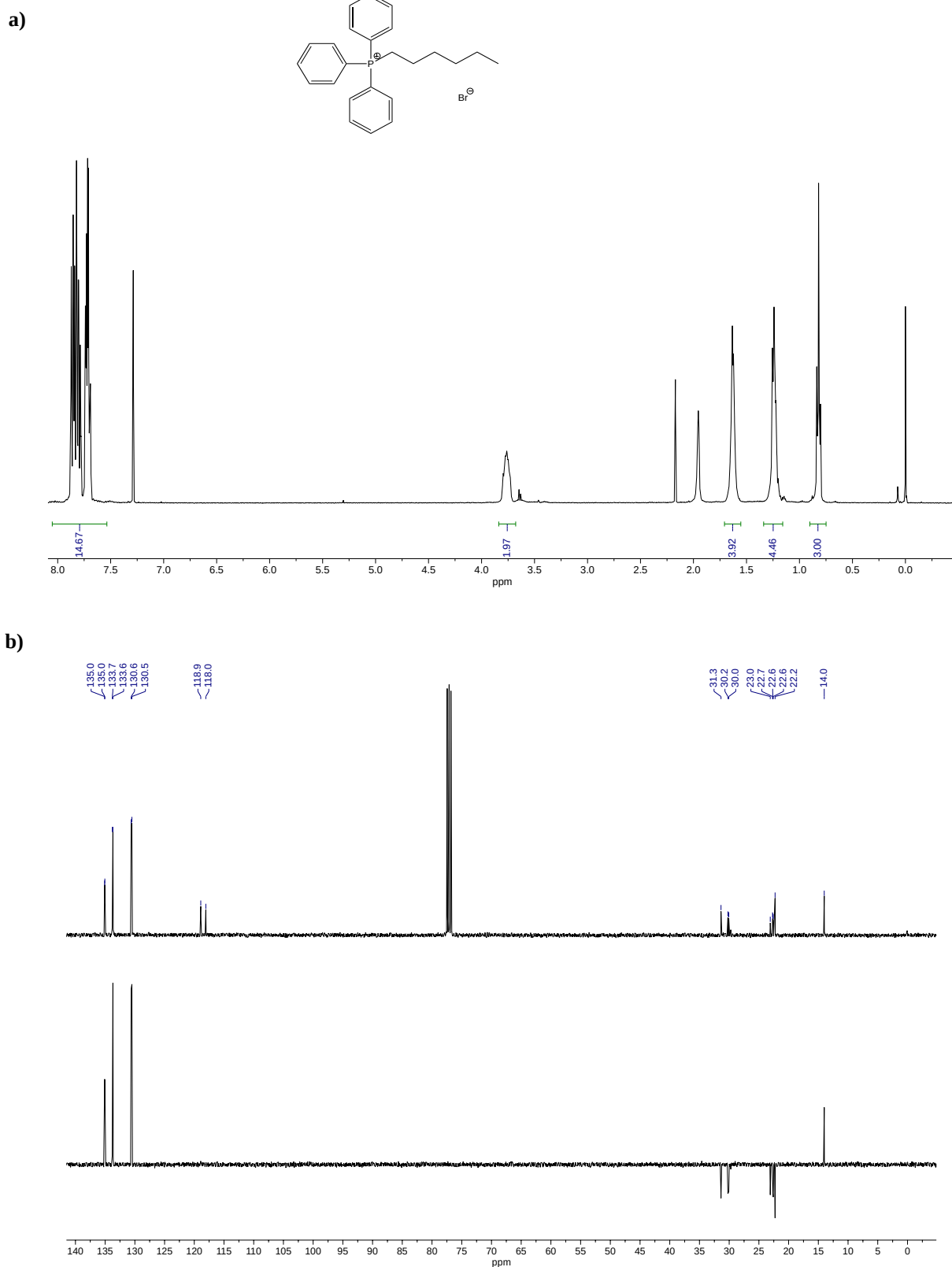
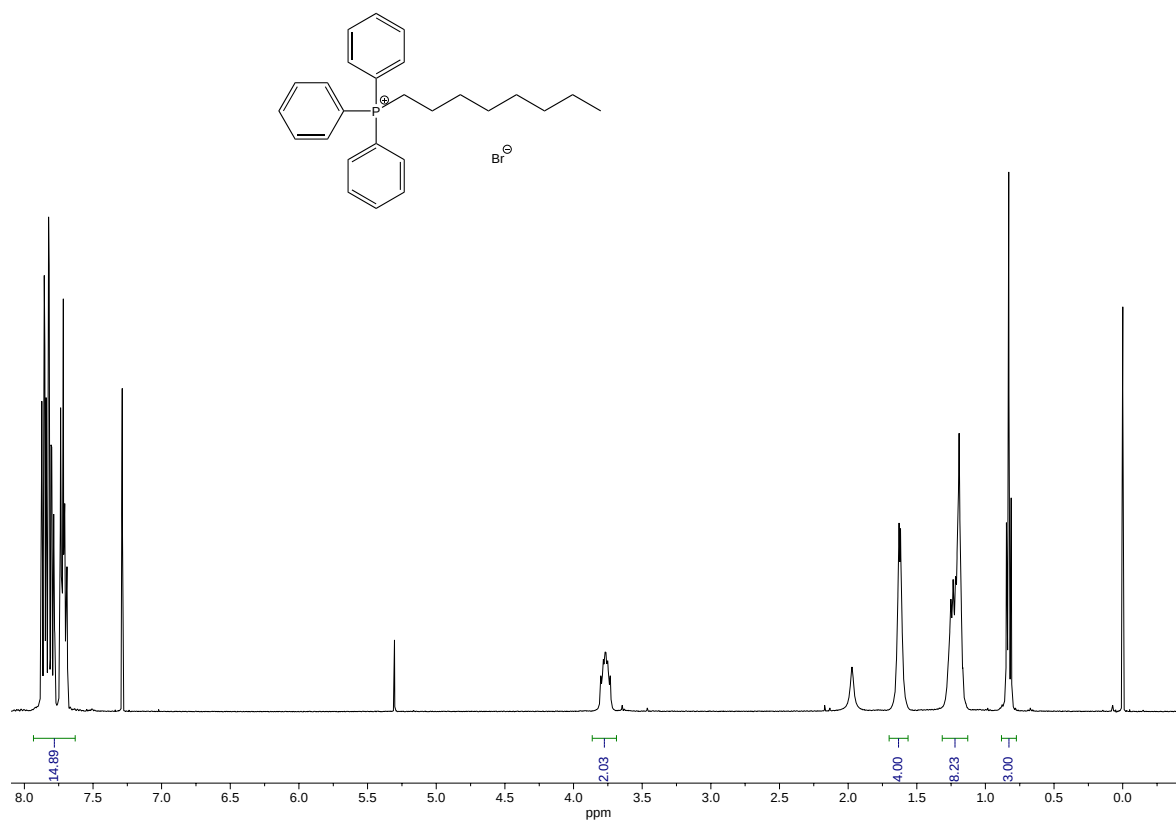


Figure S1. ¹H NMR (a), ¹³C NMR and DEPT135 (b) spectra of compound 1a.

a)



b)

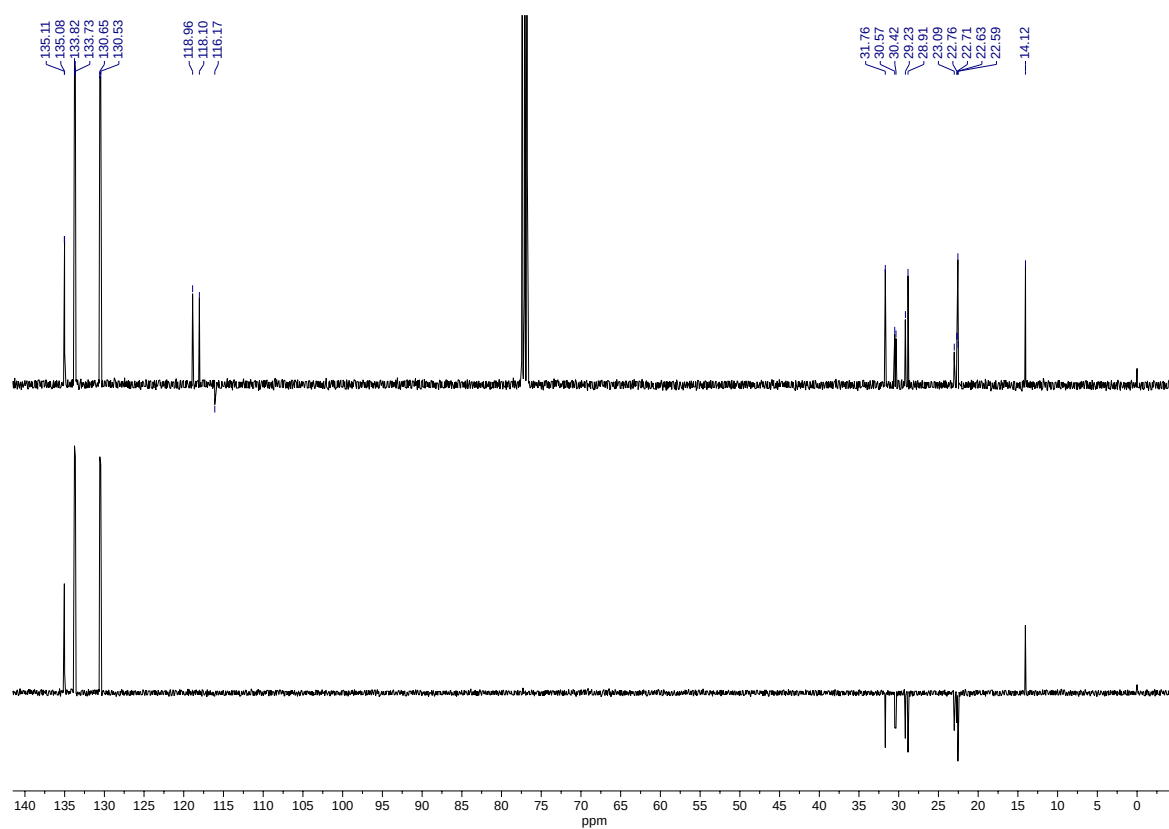
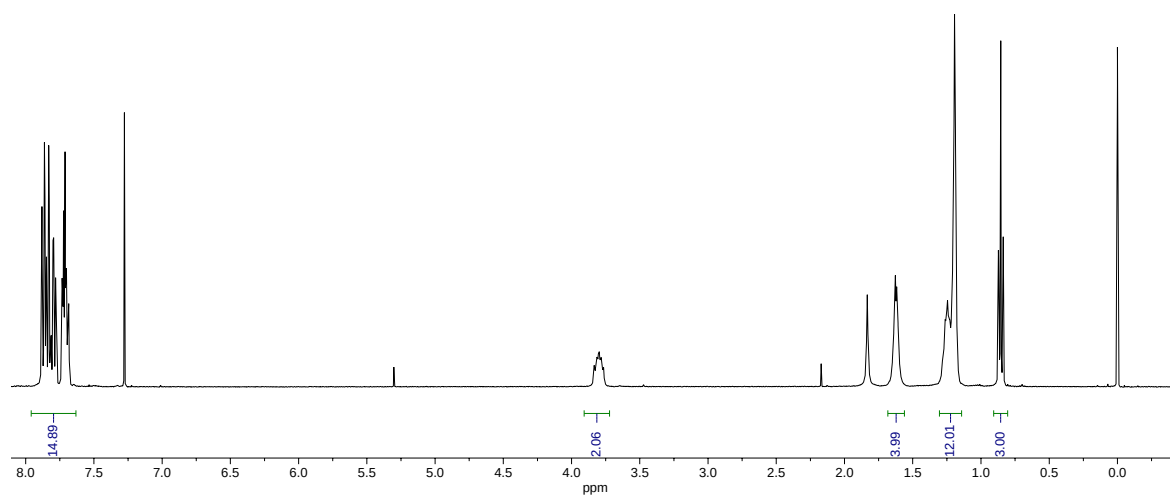
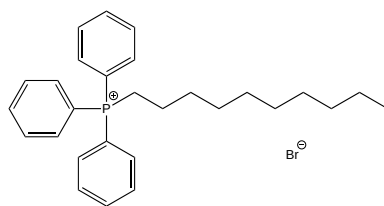


Figure S2. ¹H NMR (a), ¹³C NMR and DEPT135 (b) spectra of compound **1b**.

a)



b)

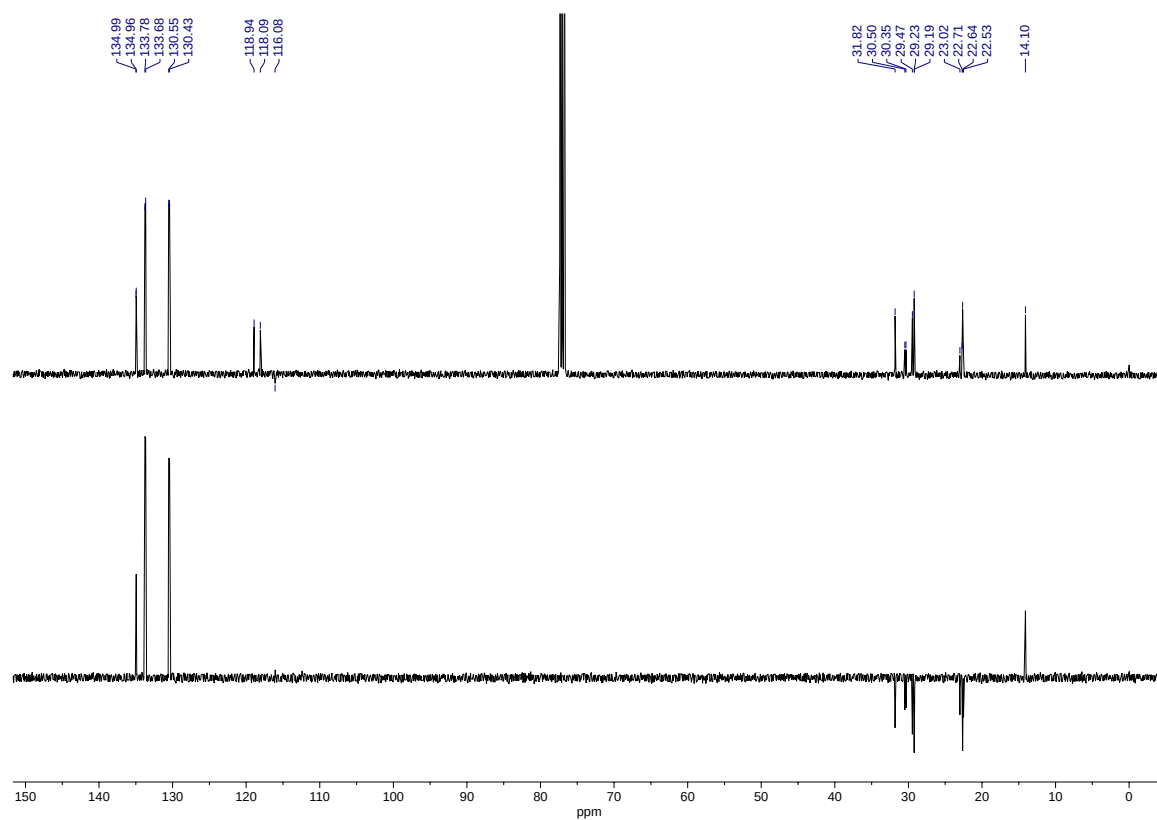
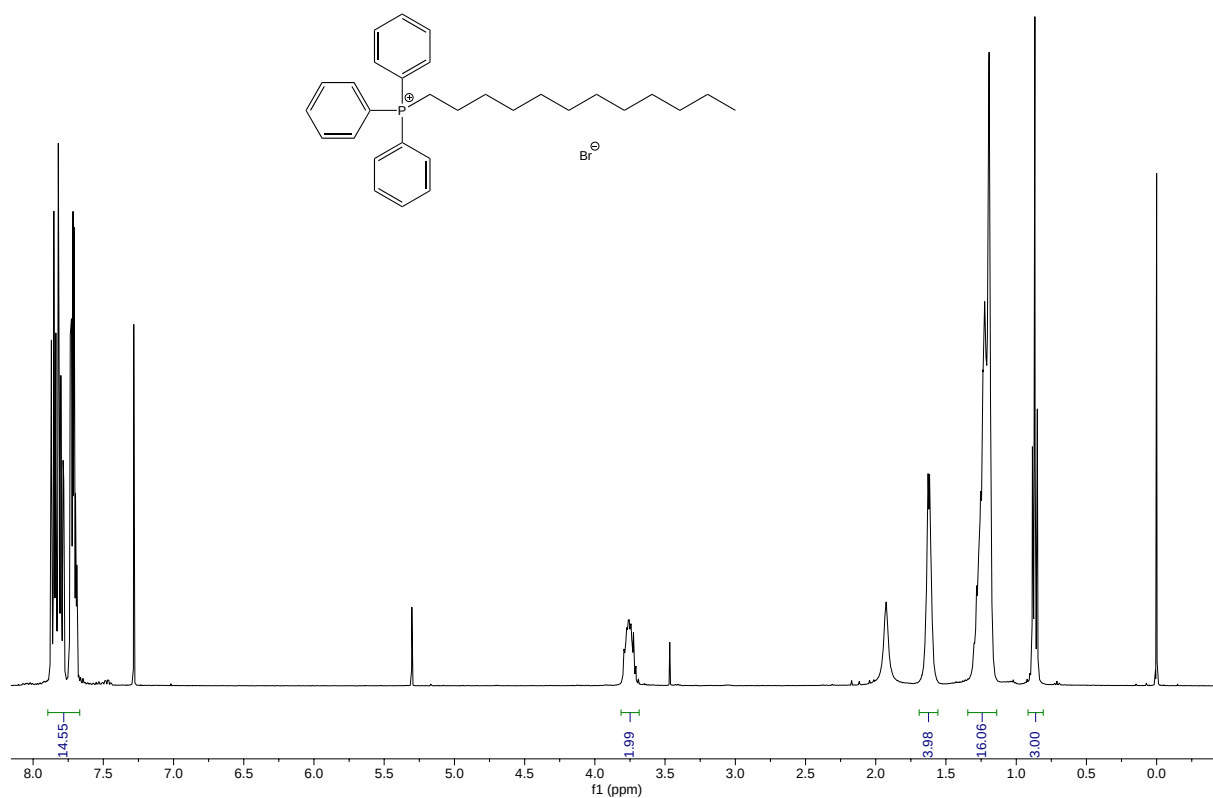


Figure S3. ¹H NMR (a), ¹³C NMR and DEPT135 (b) spectra of compound 1c.

a)



b)

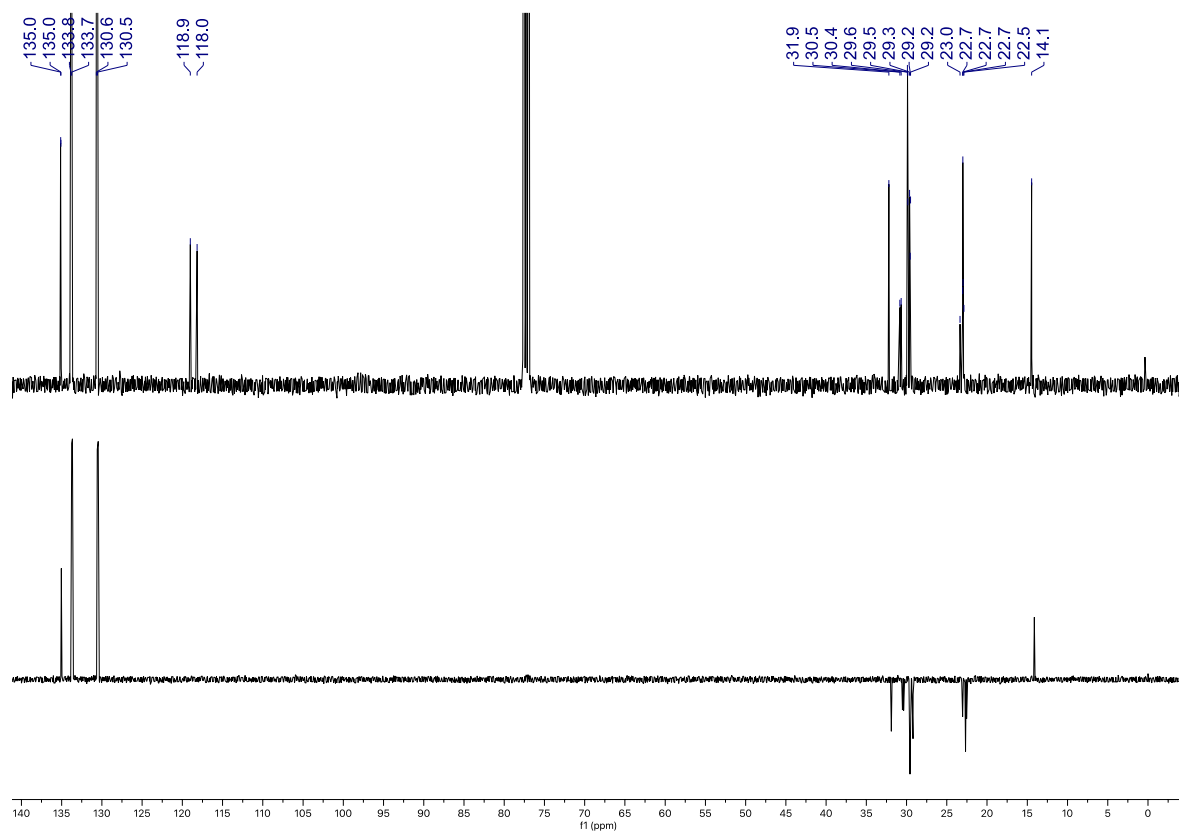
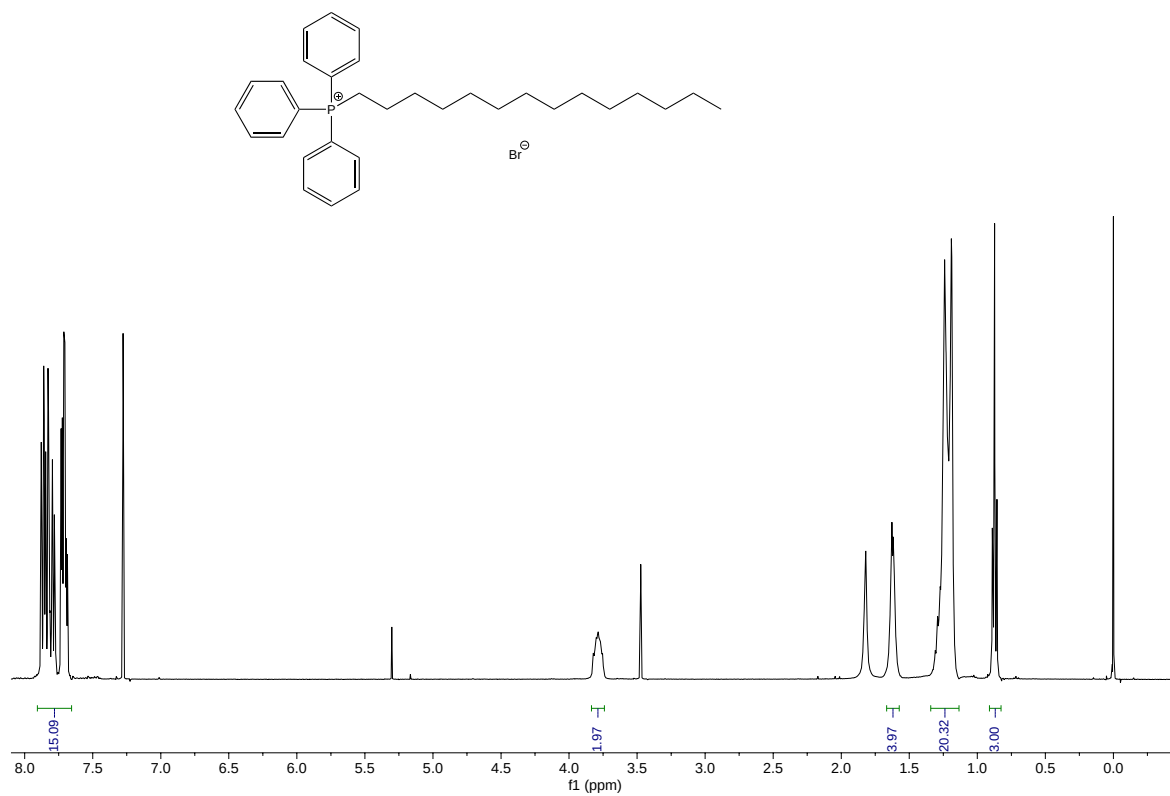


Figure S4. ¹H NMR (a), ¹³C NMR and DEPT135 (b) spectra of compound **1d**.

a)



b)

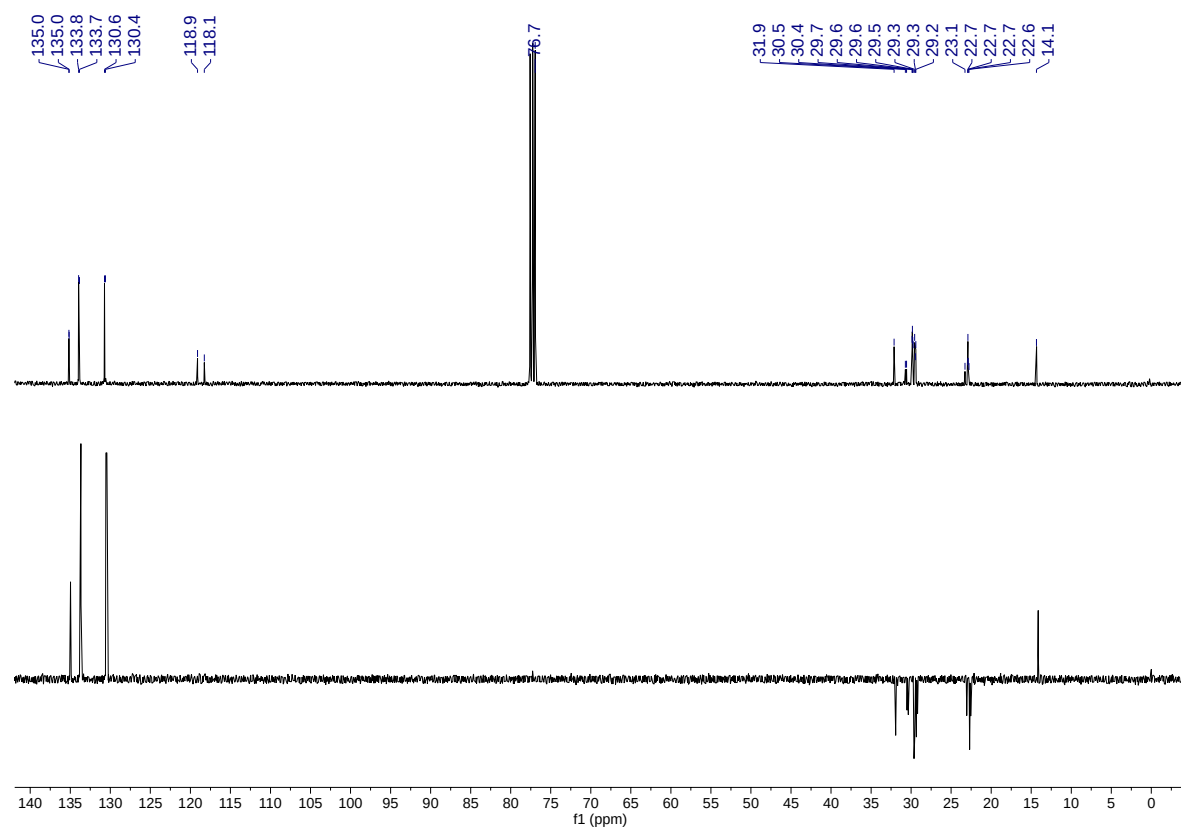
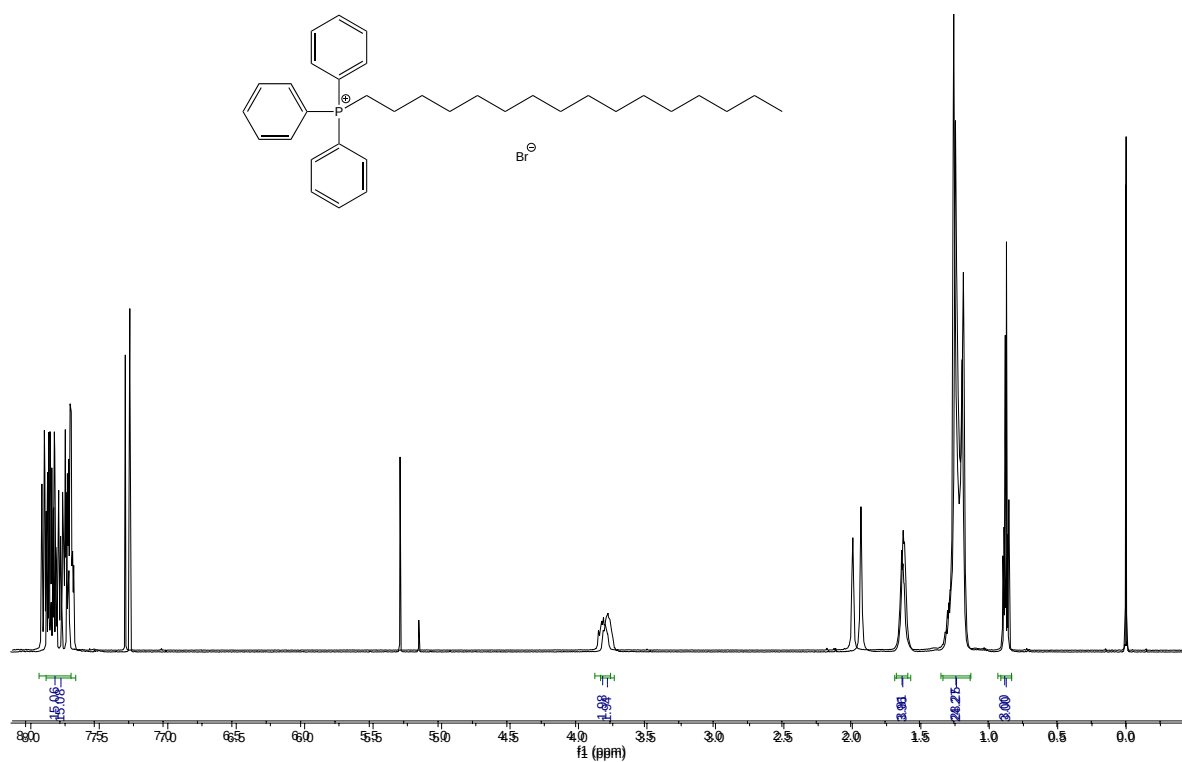


Figure S5. ¹H NMR (a), ¹³C NMR and DEPT135 (b) spectra of compound **1e**.

a)



b)

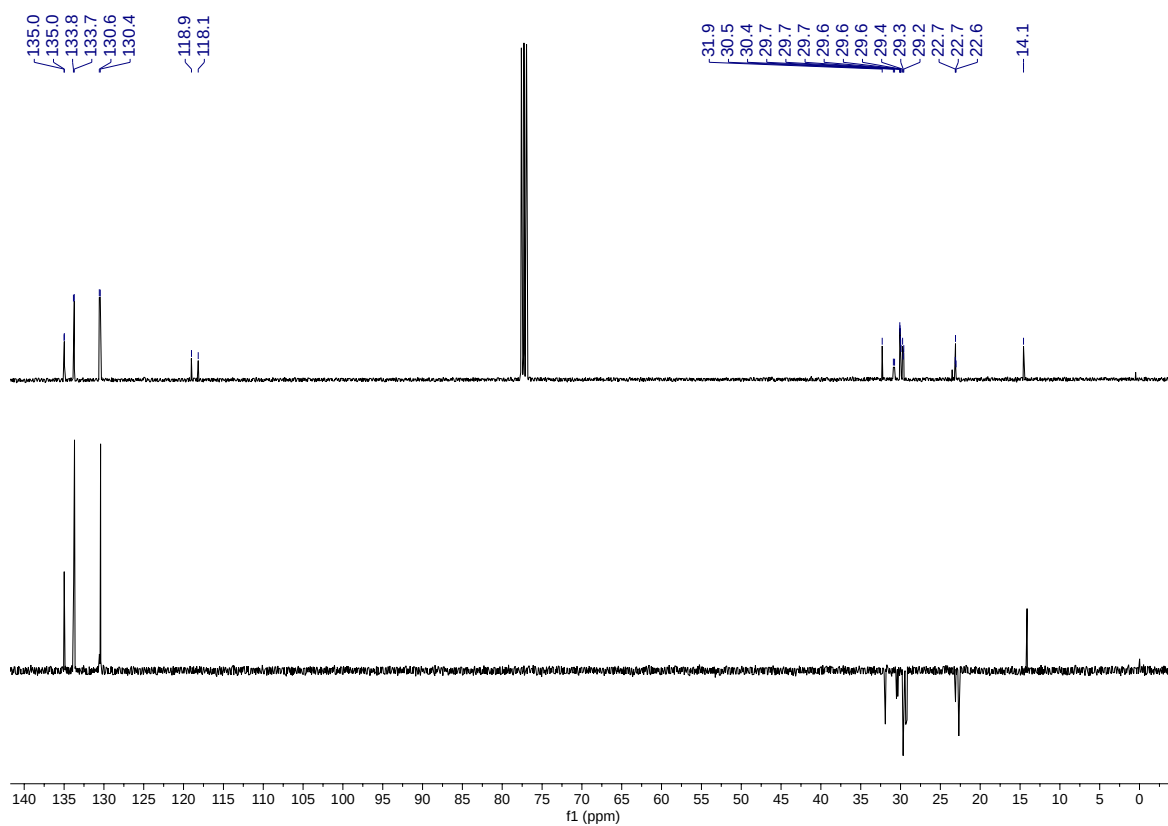
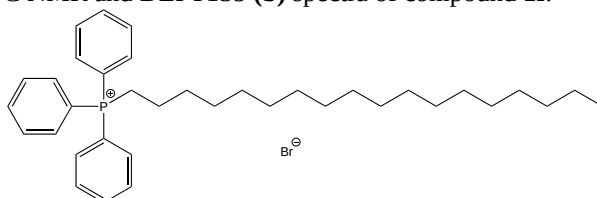


Figure S6. ^1H NMR (a), ^{13}C NMR and DEPT135 (b) spectra of compound 1f.



b)

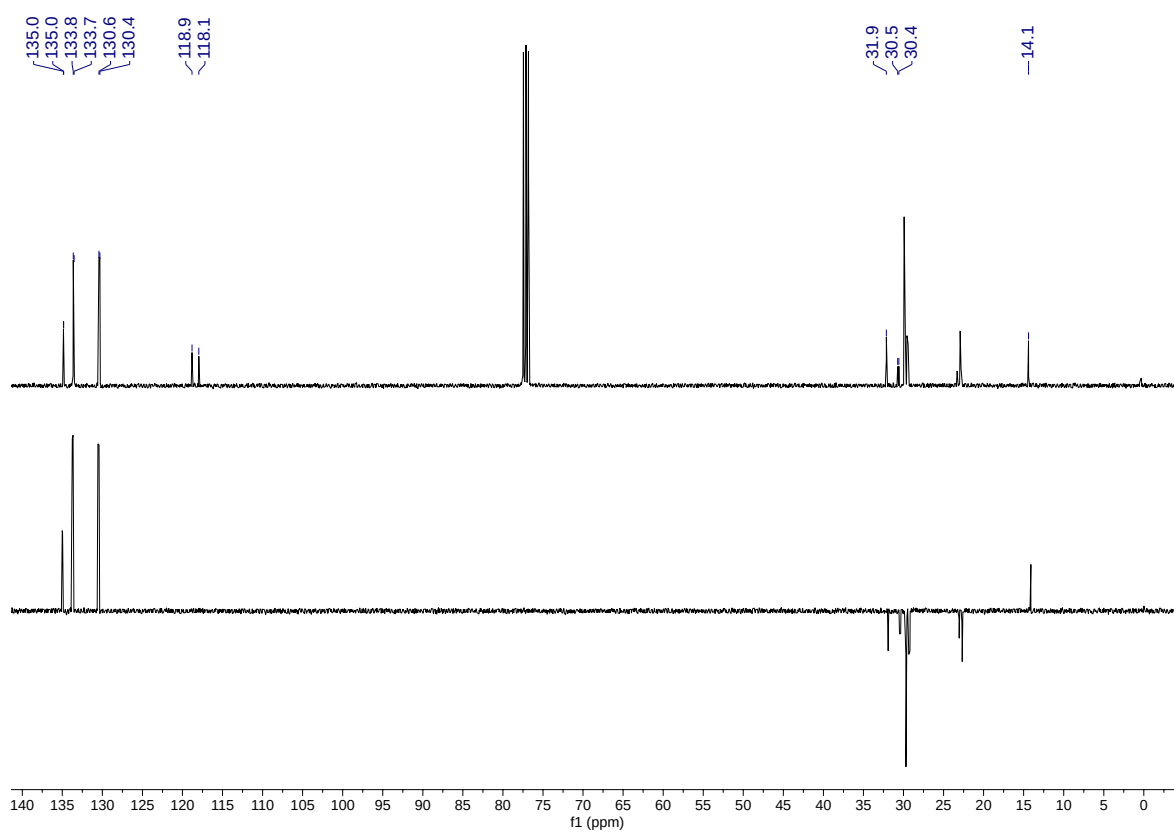
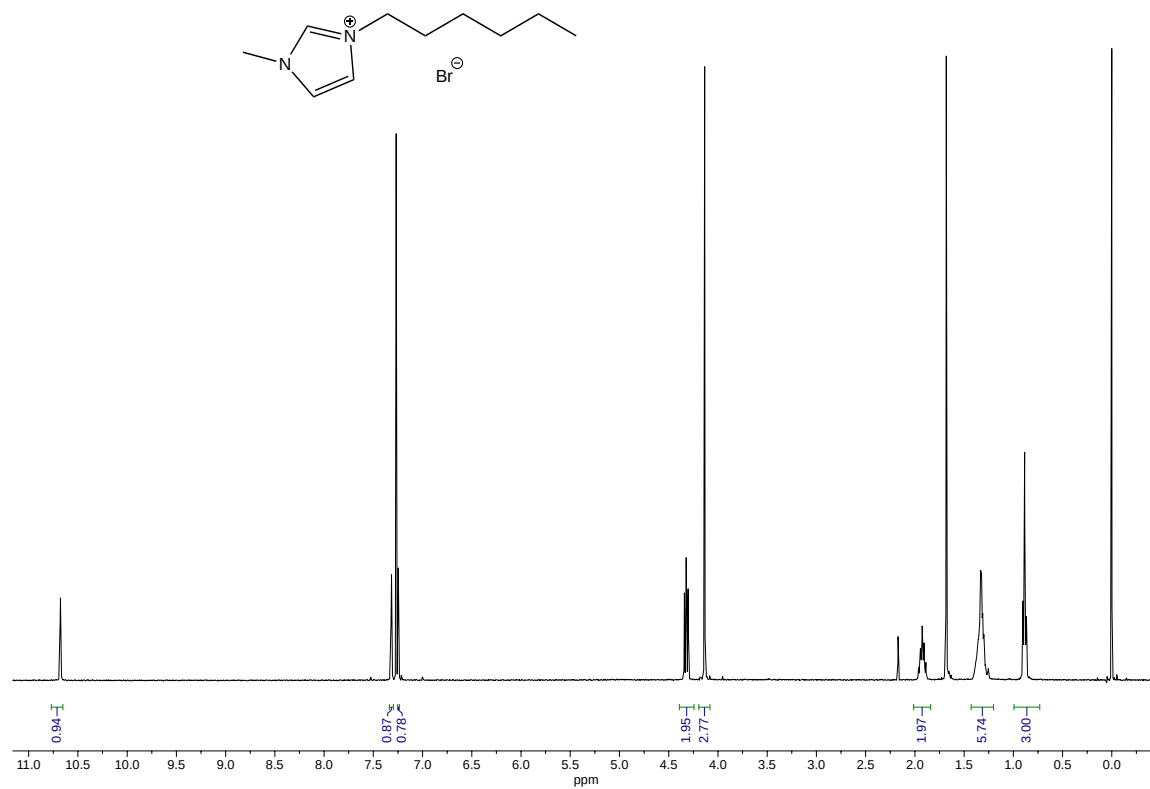


Figure S7. ^1H NMR (a), ^{13}C NMR and DEPT135 (b) spectra of compound **1g**.

a)



b)

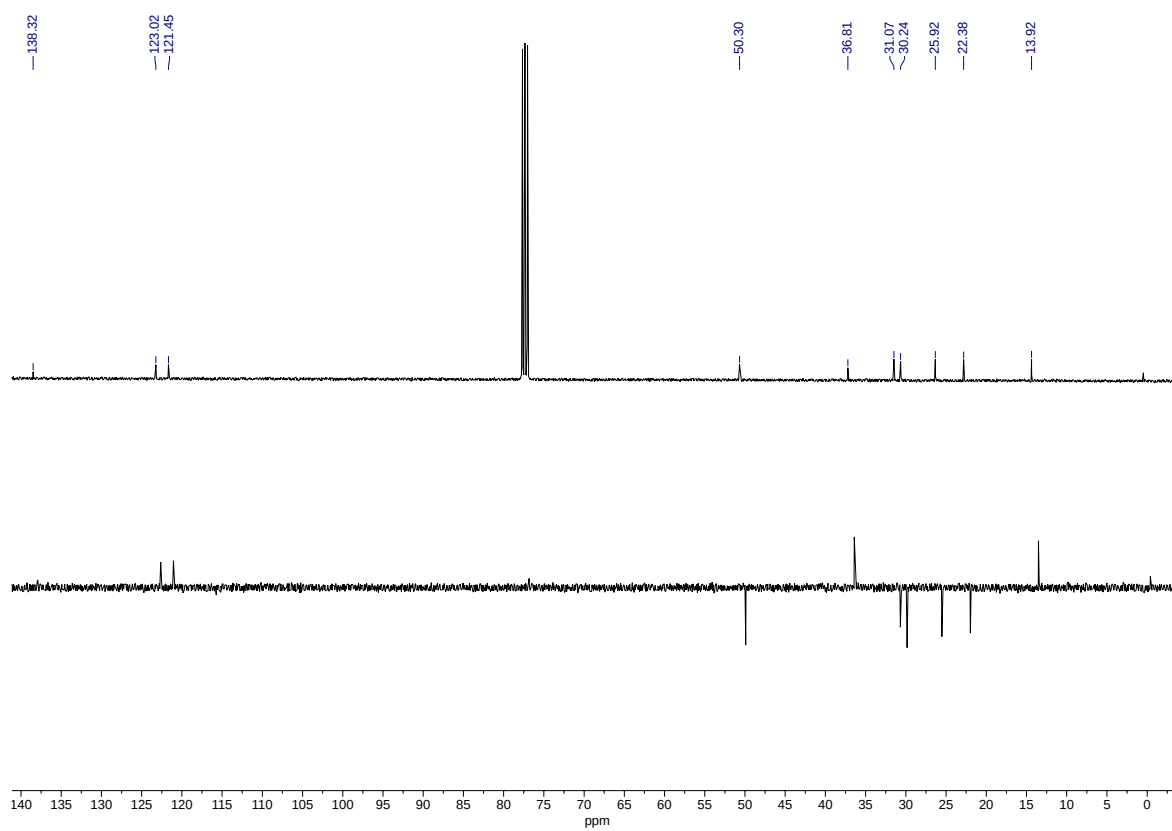
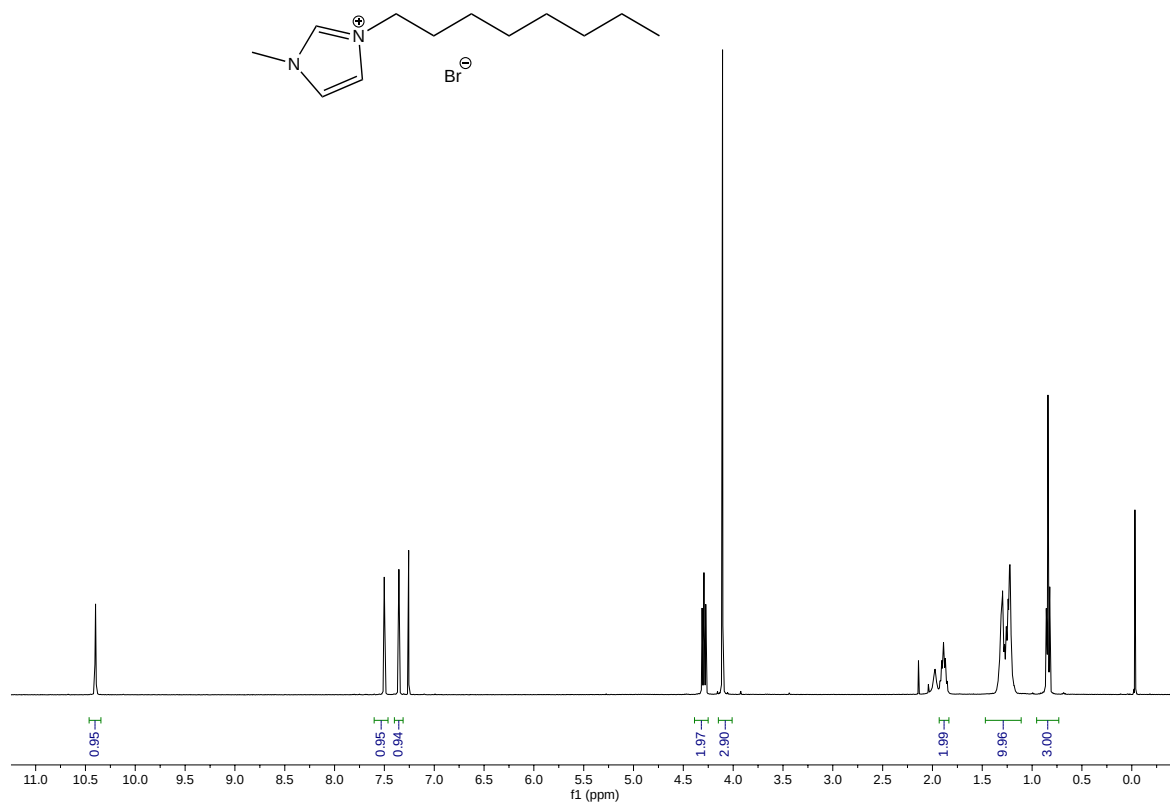


Figure S8. ¹H NMR (a), ¹³C NMR and DEPT135 (b) spectra of compound 2a.

a)



b)

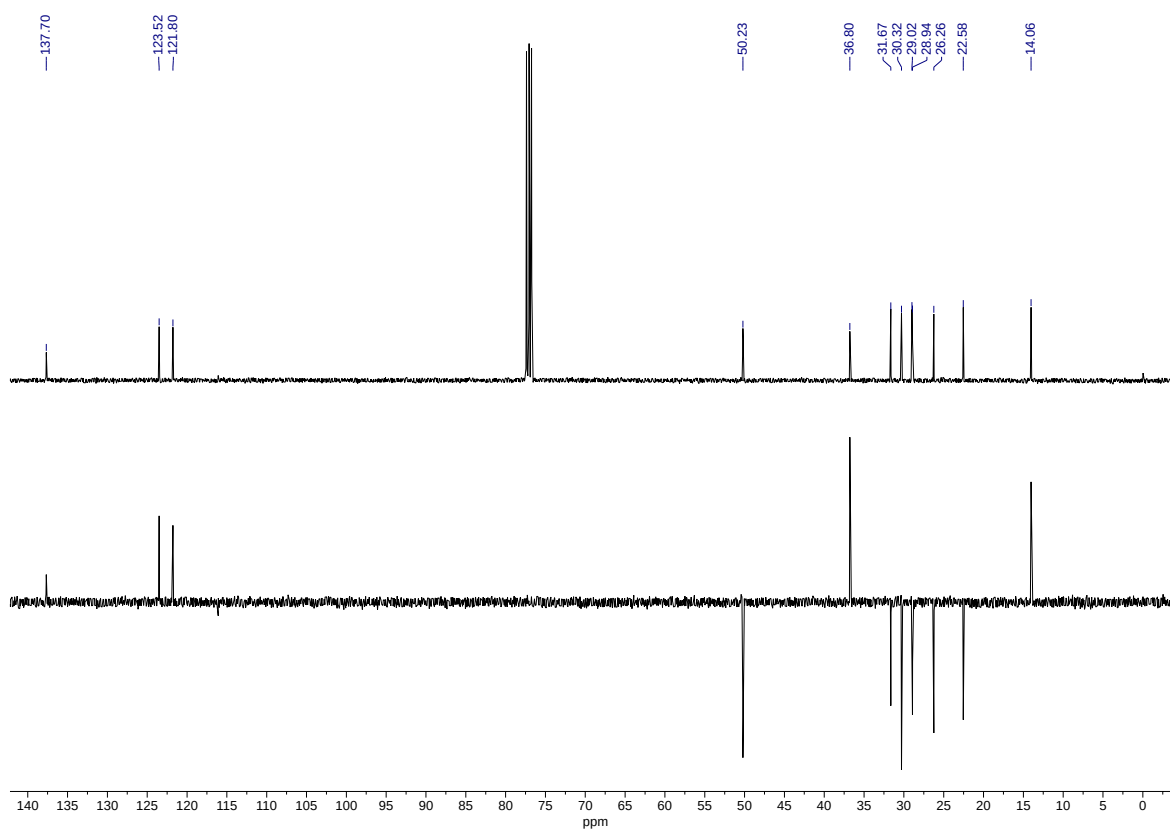


Figure S9. ¹H NMR (a), ¹³C NMR and DEPT135 (b) spectra of compound 2b.

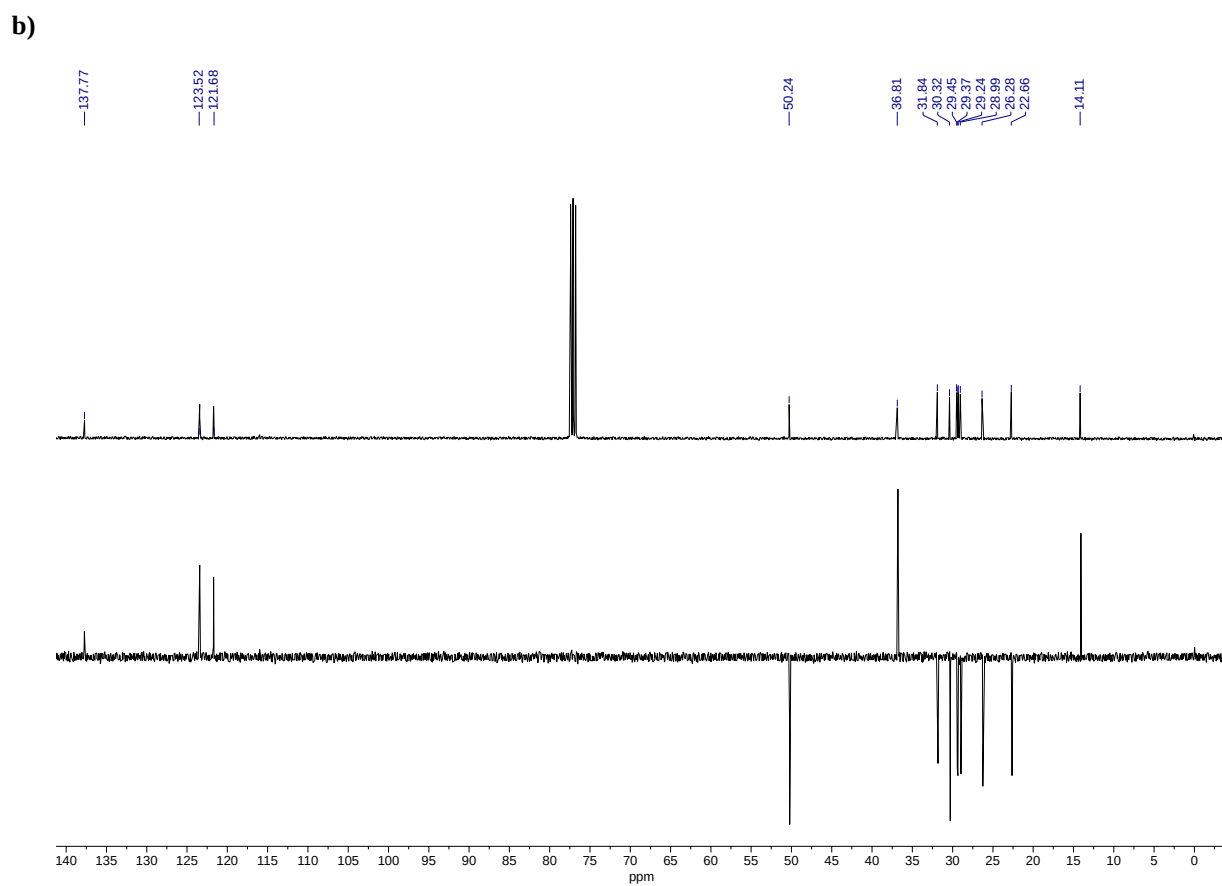
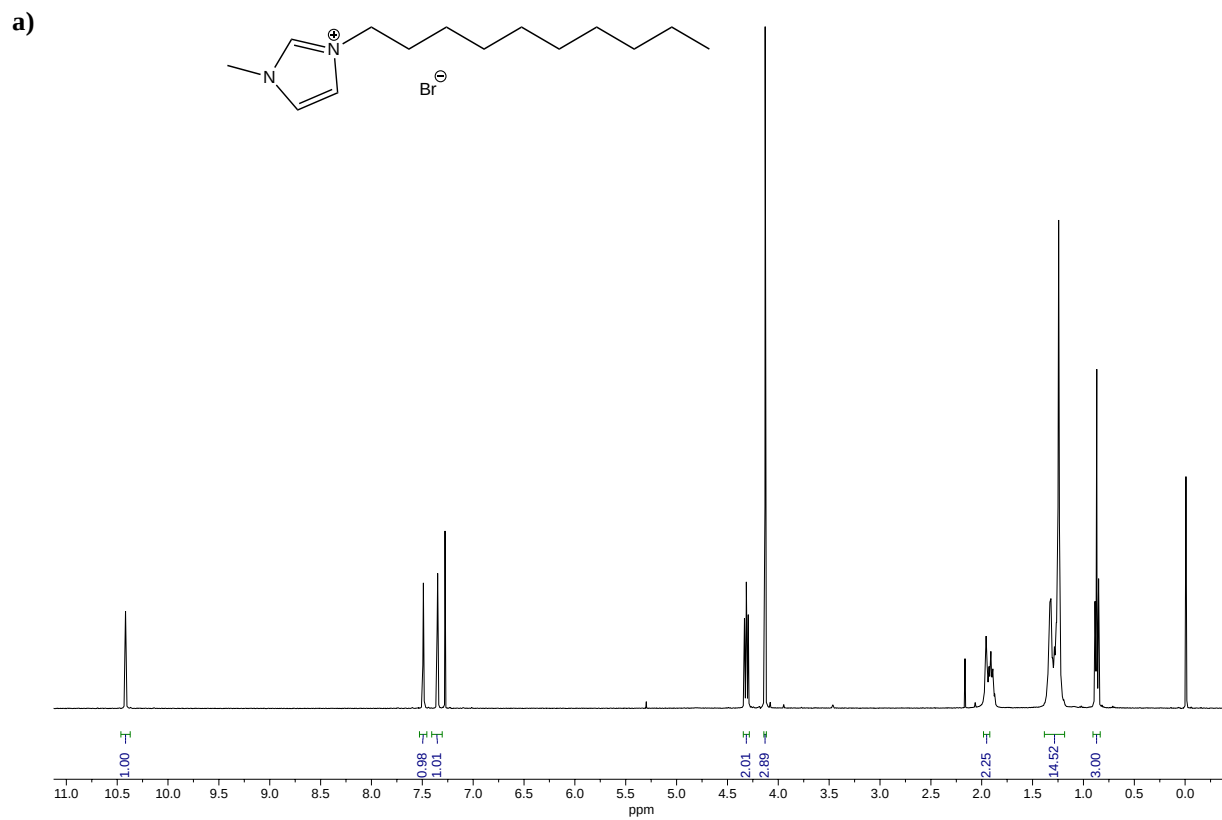
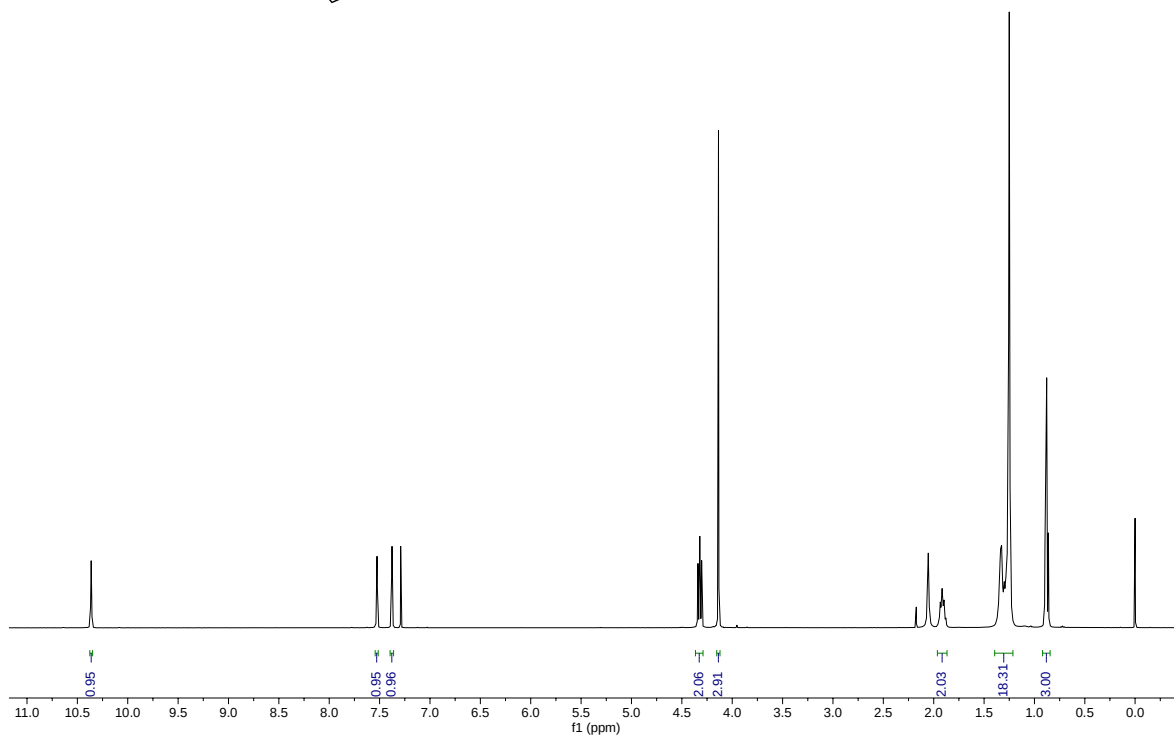
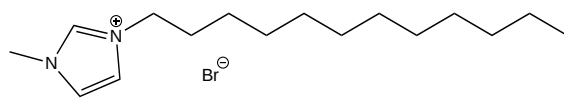


Figure S10. ¹H NMR (a), ¹³C NMR and DEPT135 (b) spectra of compound 2c.

a)



b)

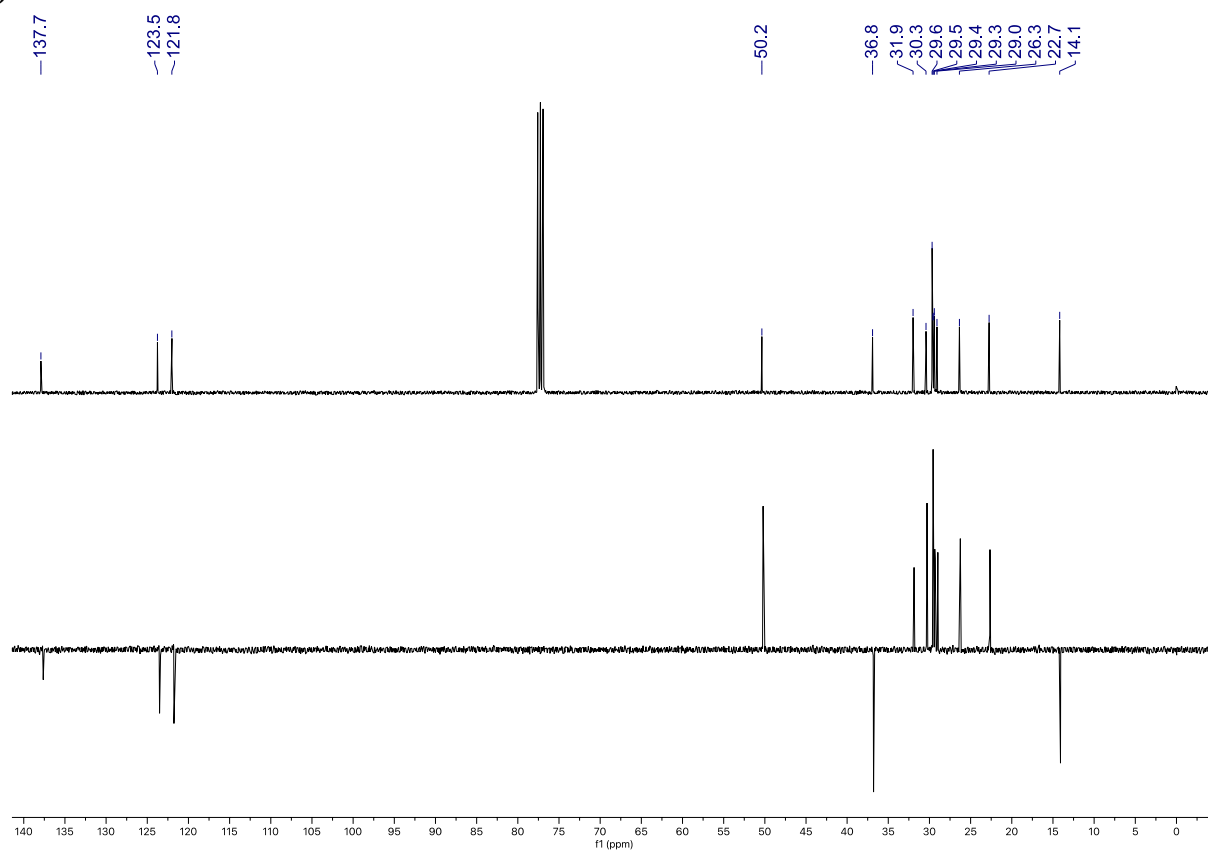


Figure S11. ¹H NMR (a), ¹³C NMR and DEPT135 (b) spectra of compound 2d.

a)



b)

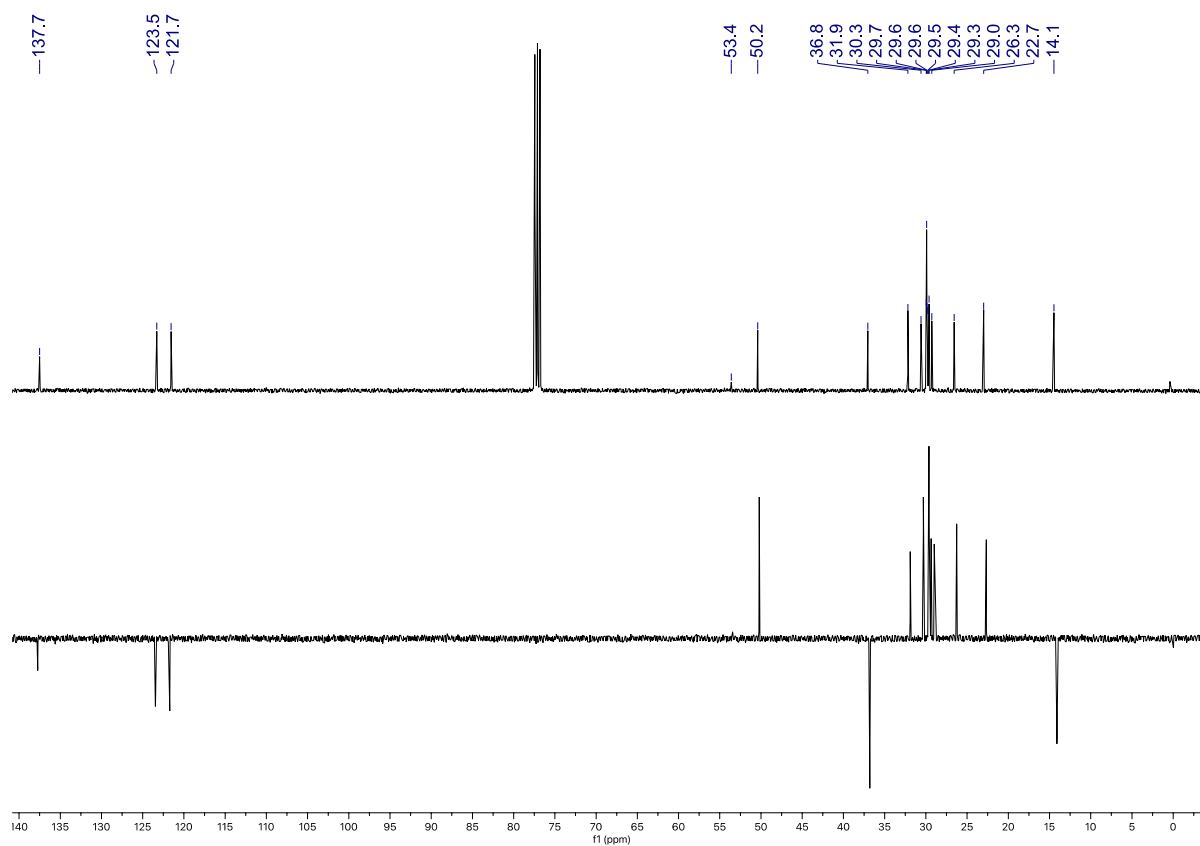
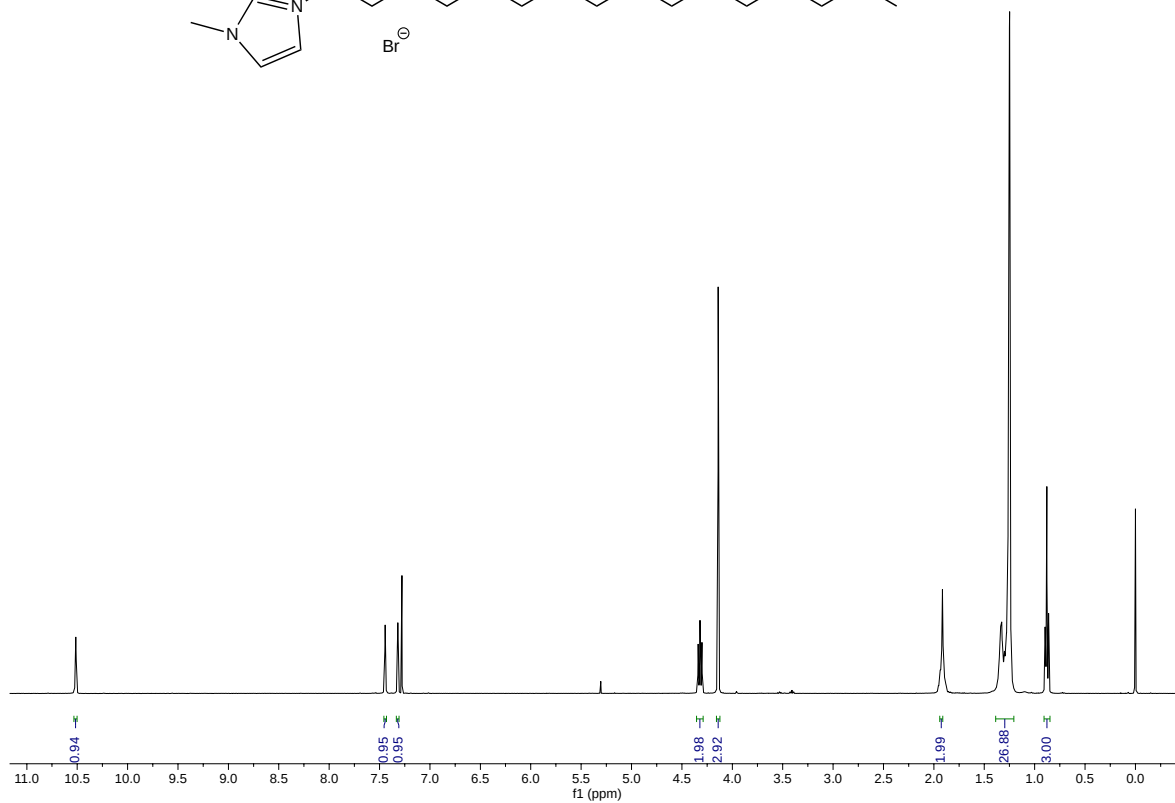
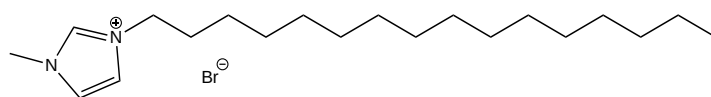


Figure S12. ^1H NMR (a), ^{13}C NMR and DEPT135 (b) spectra of compound **2e**.

a)



b)

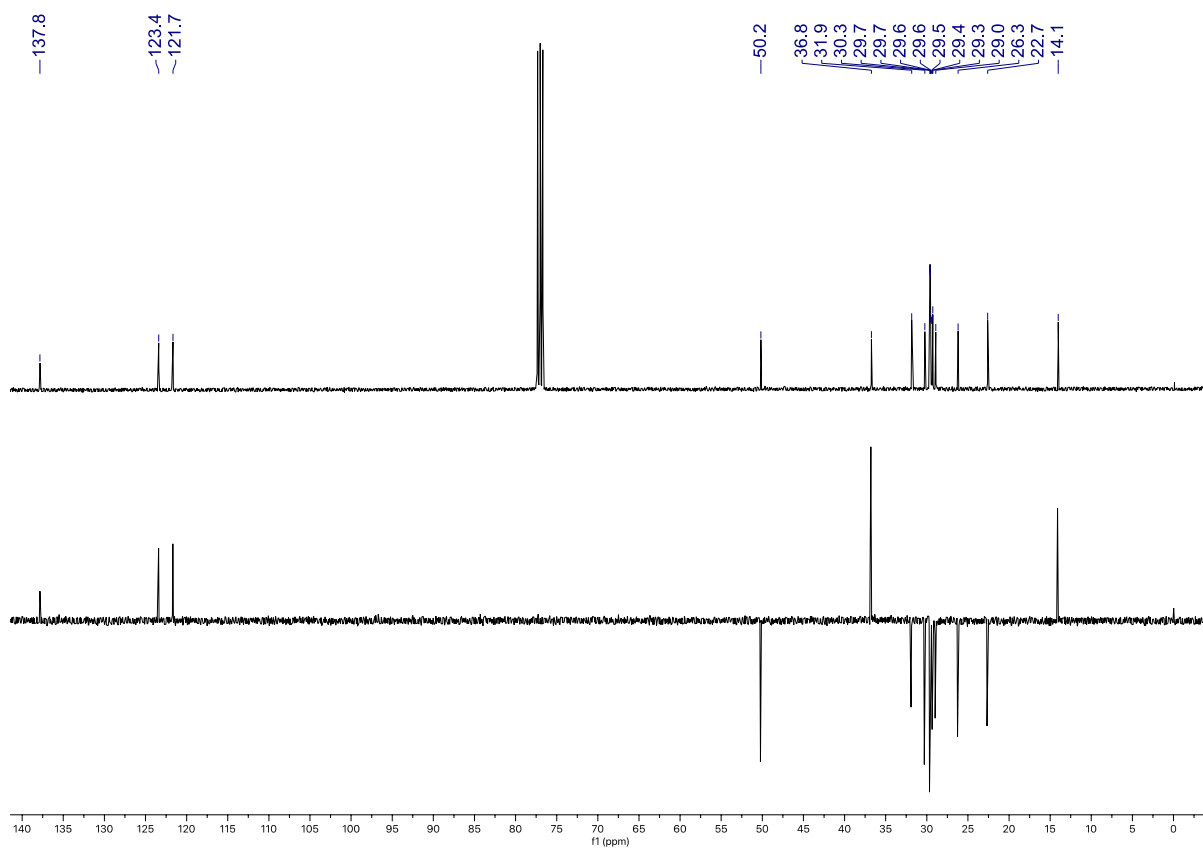
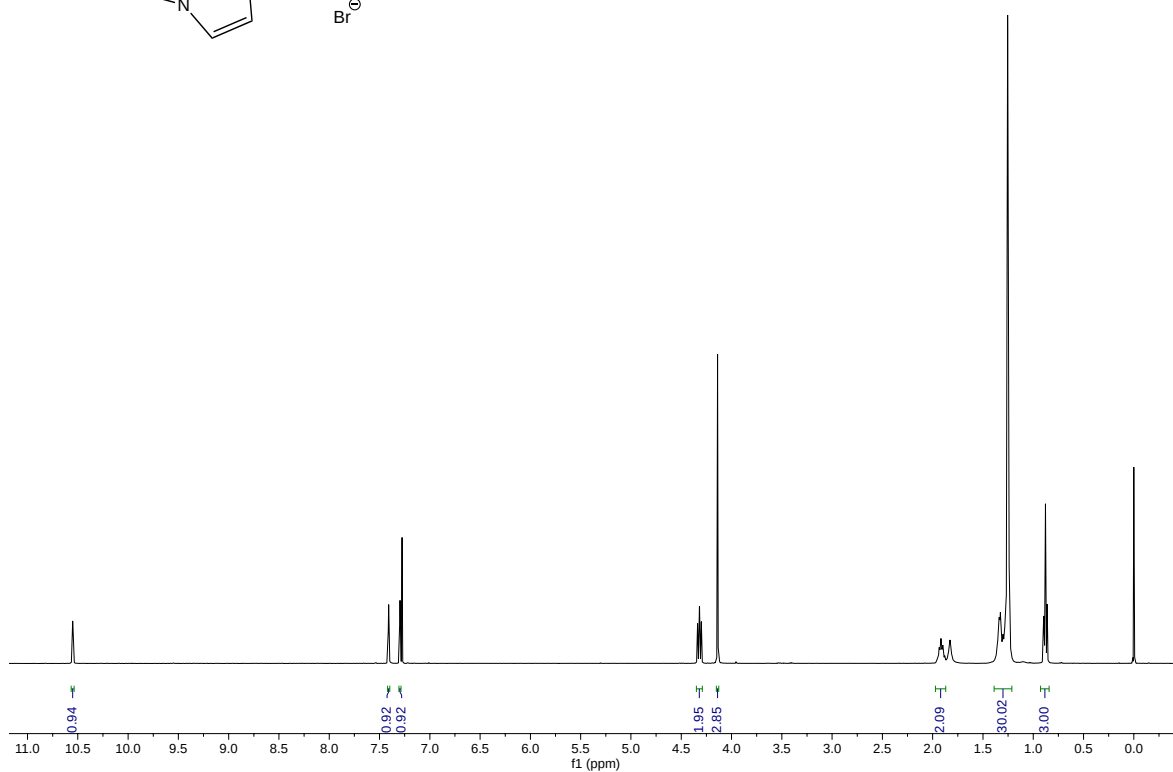
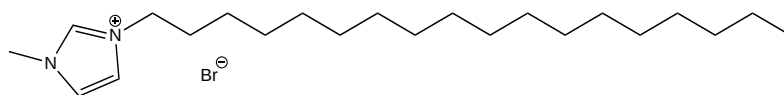


Figure S13. ^1H NMR (a), ^{13}C NMR and DEPT135 (b) spectra of compound **2f**.

a)



b)

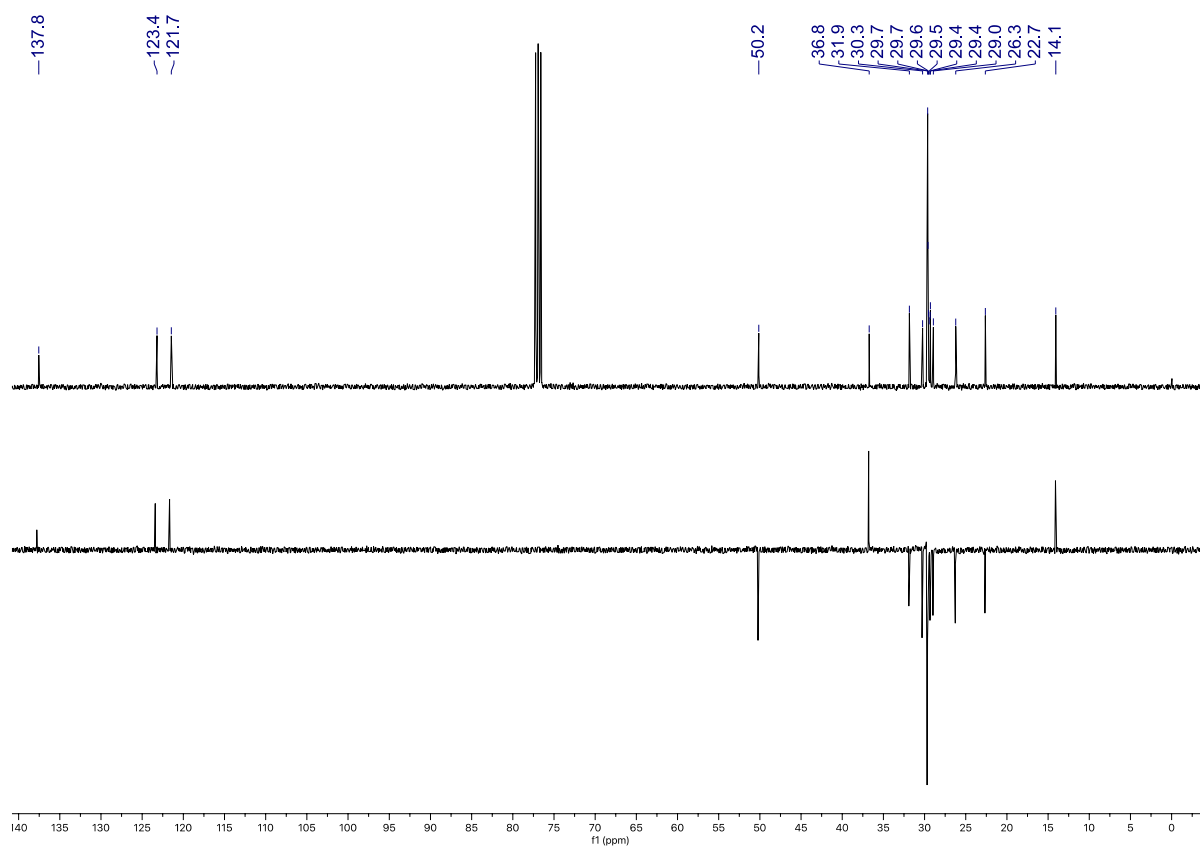
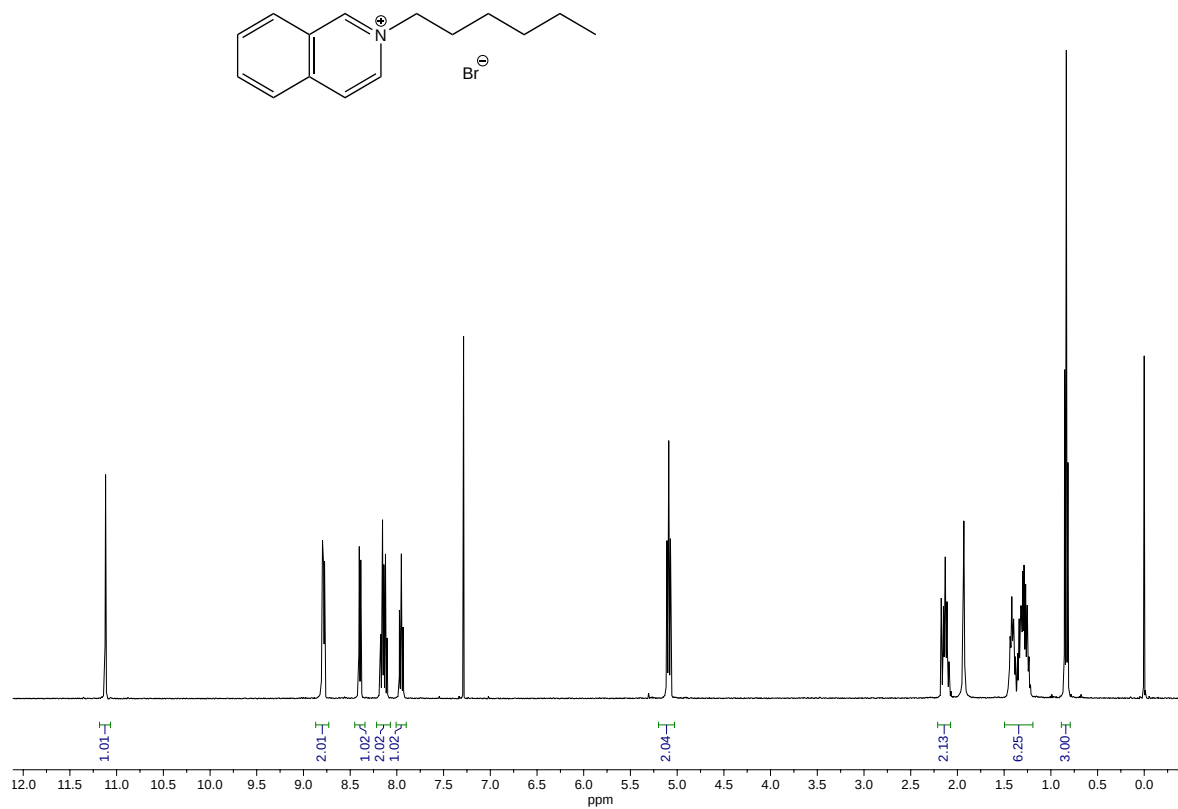


Figure S14. ¹H NMR (a), ¹³C NMR and DEPT135 (b) spectra of compound 2g.

a)



b)

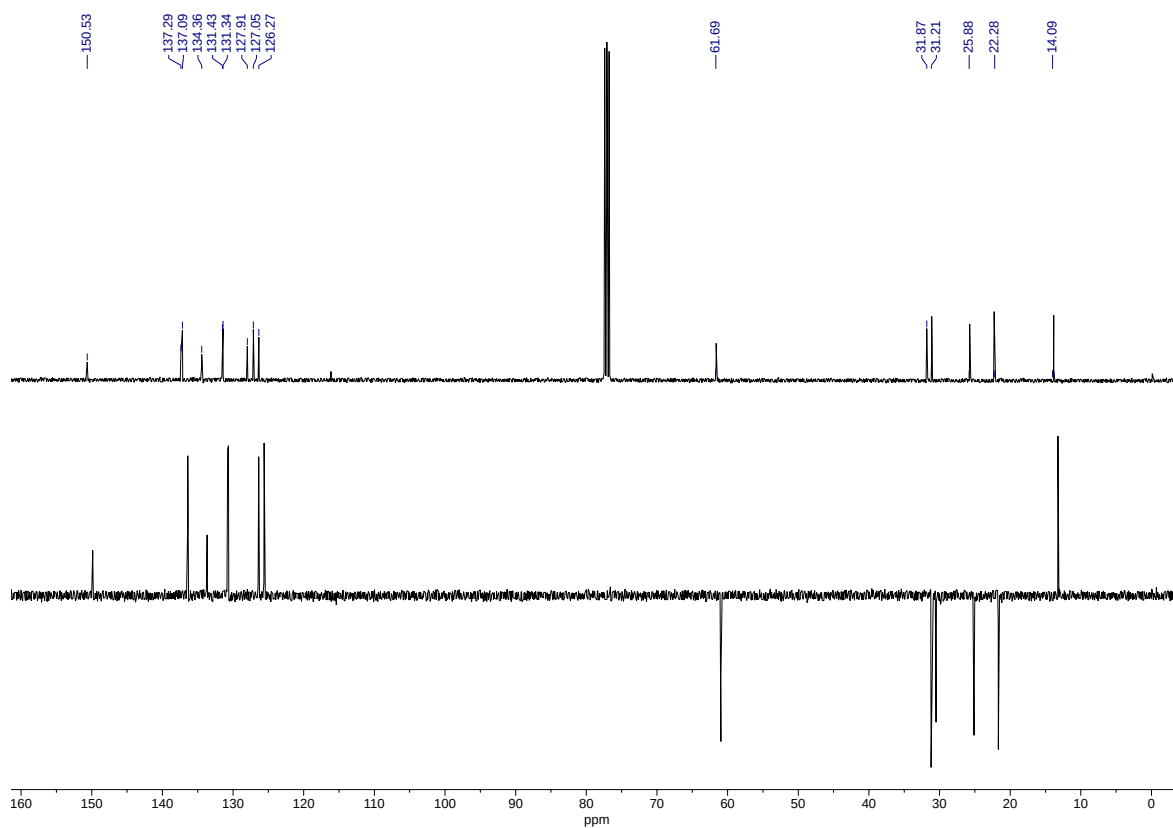
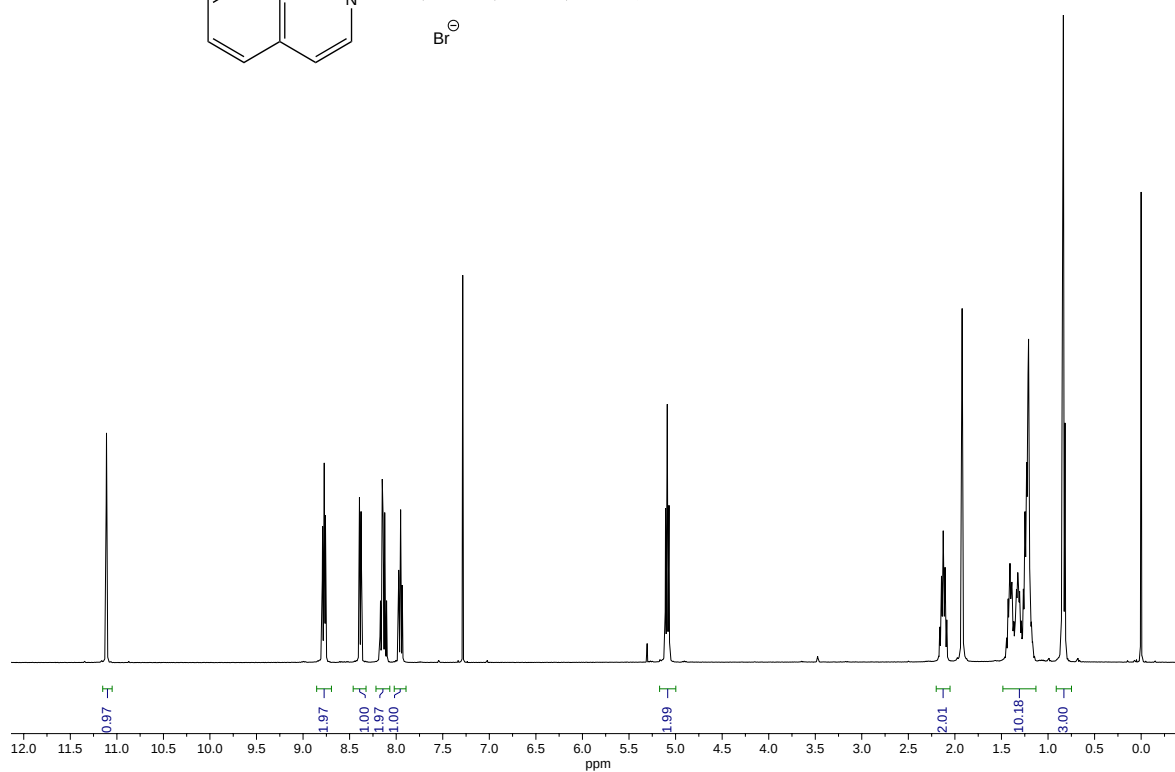
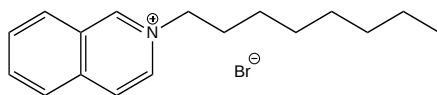


Figure S15. ¹H NMR (a), ¹³C NMR and DEPT135 (b) spectra of compound 3a.

a)



b)

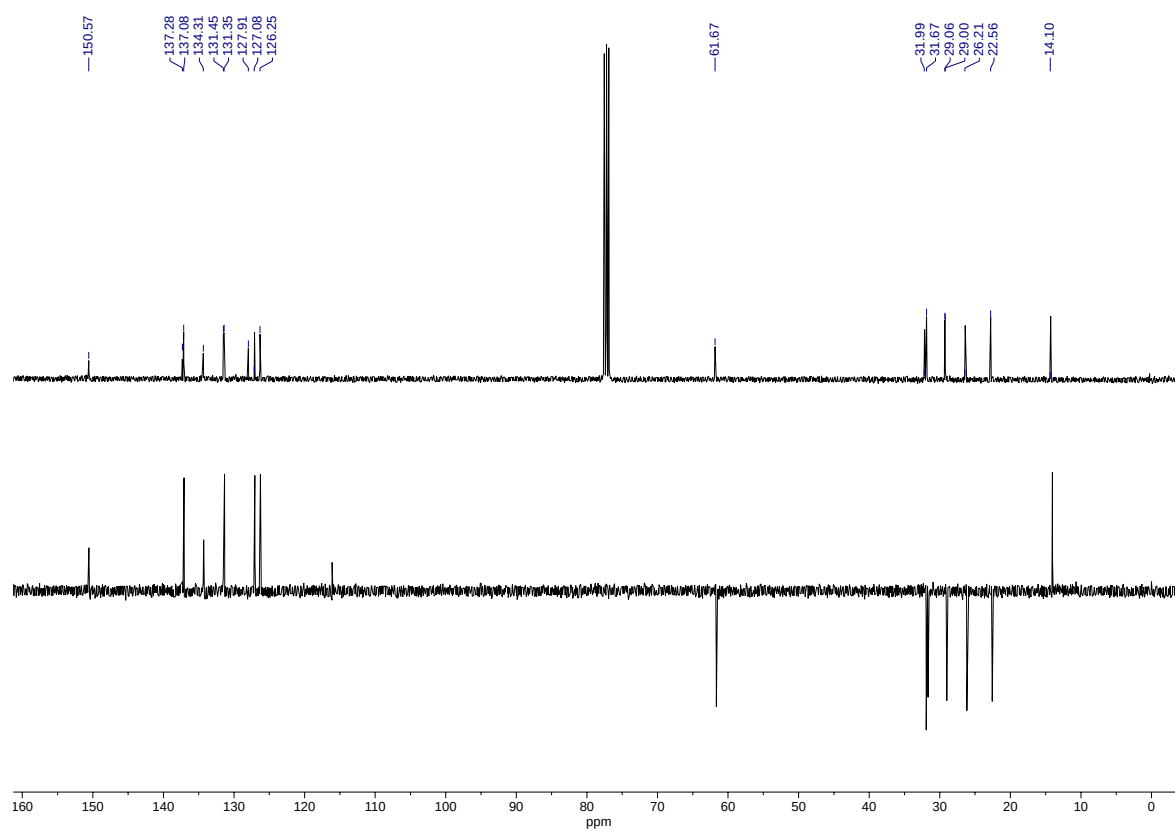
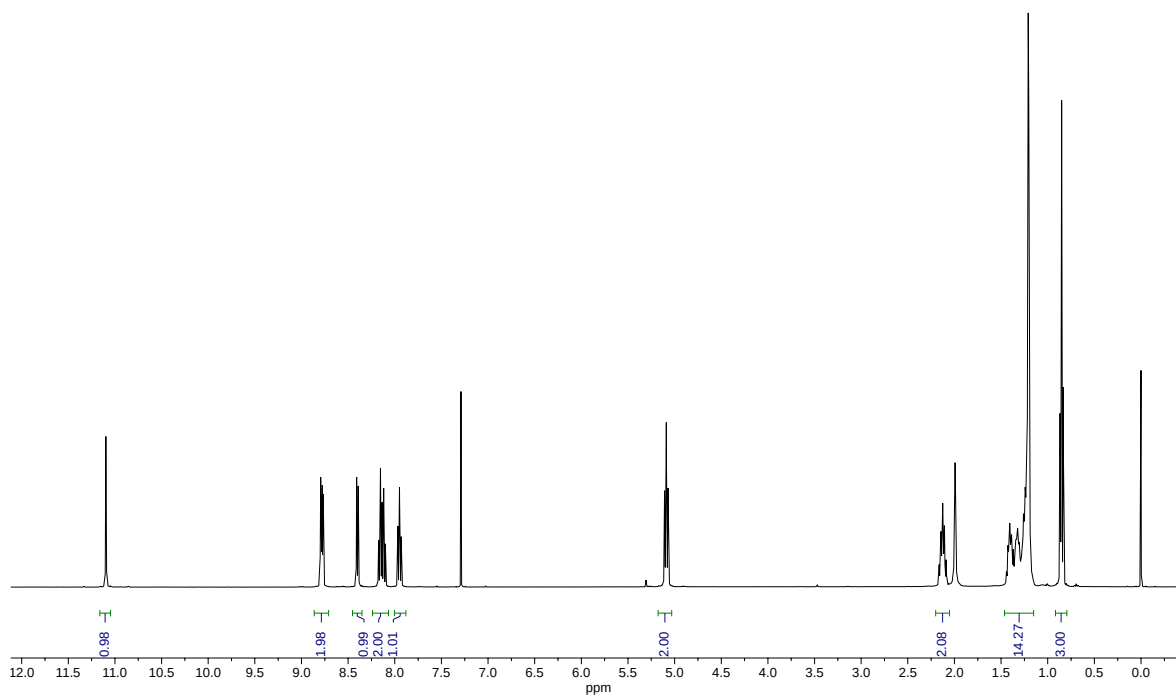
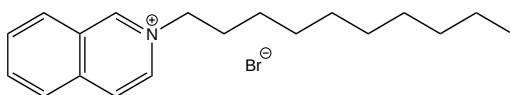


Figure S16. ^1H NMR (a), ^{13}C NMR and DEPT135 (b) spectra of compound **3b**.

a)



b)

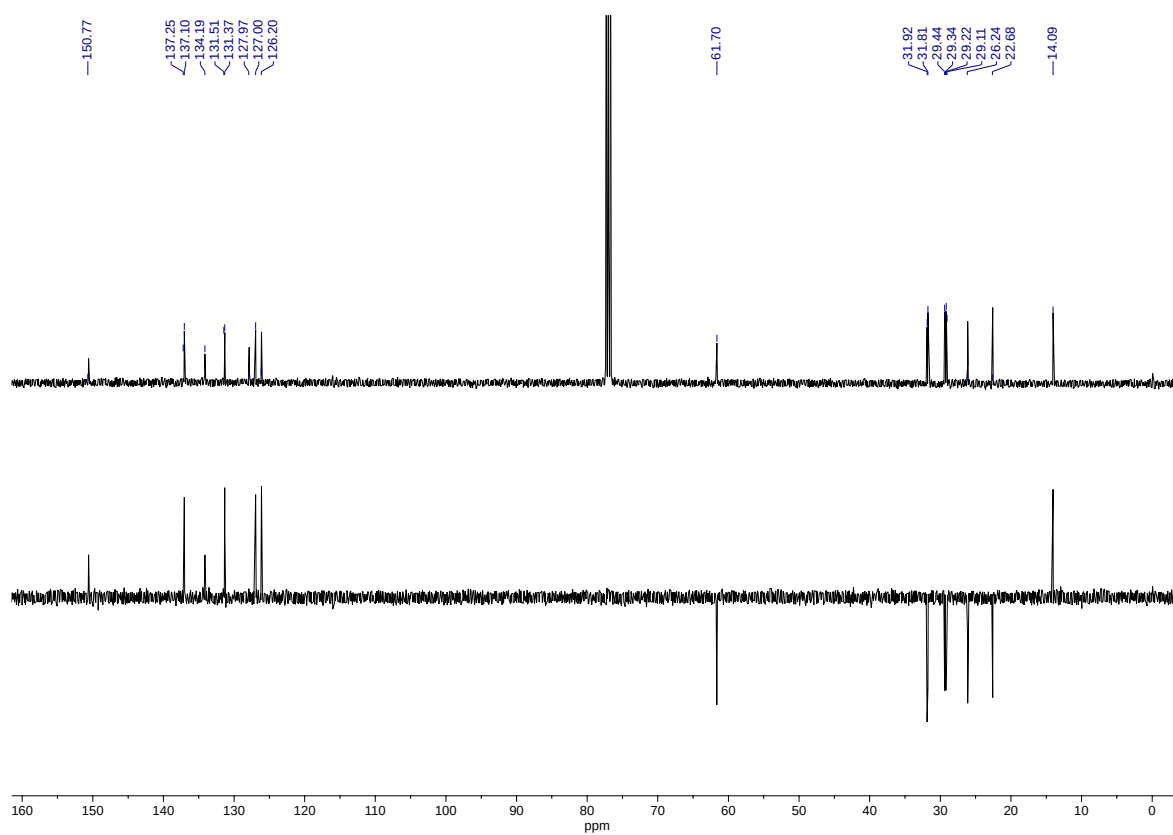
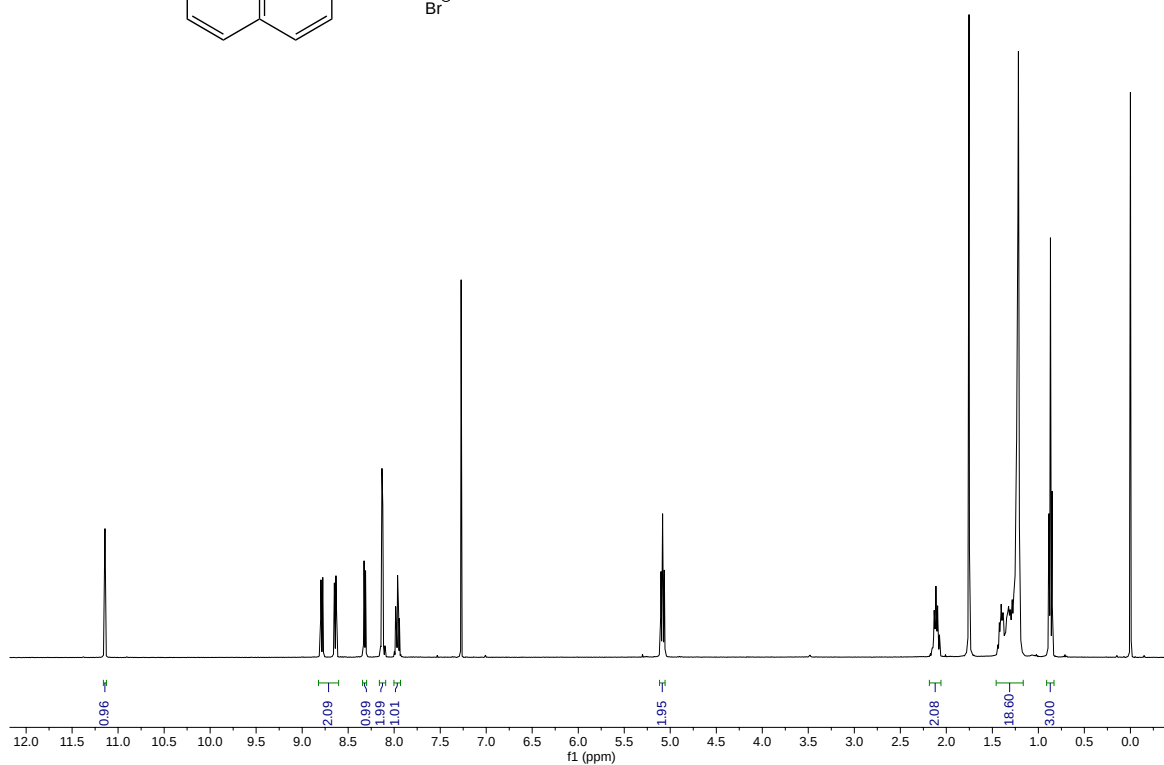
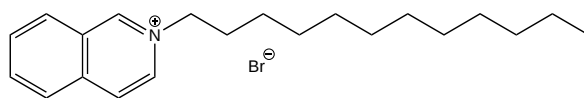


Figure S17. ¹H NMR (a), ¹³C NMR and DEPT135 (b) spectra of compound 3c.

a)



b)

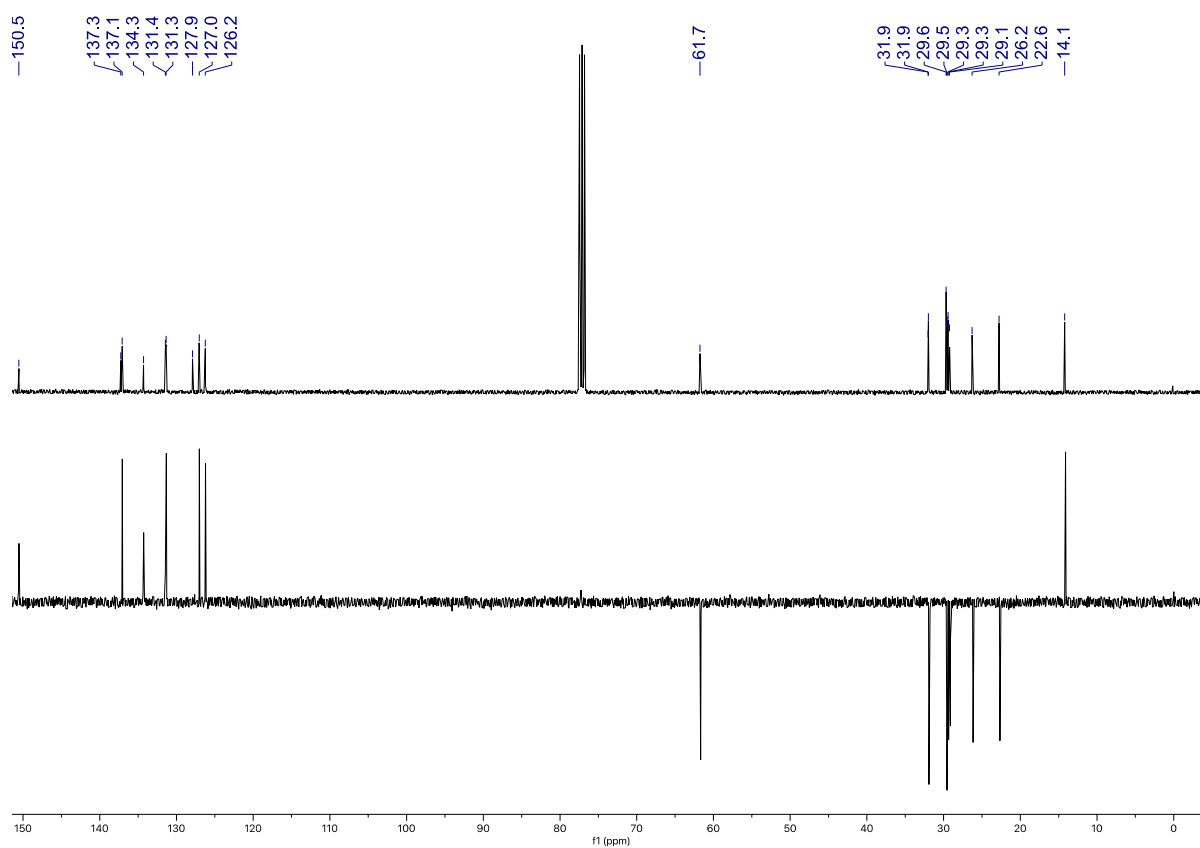
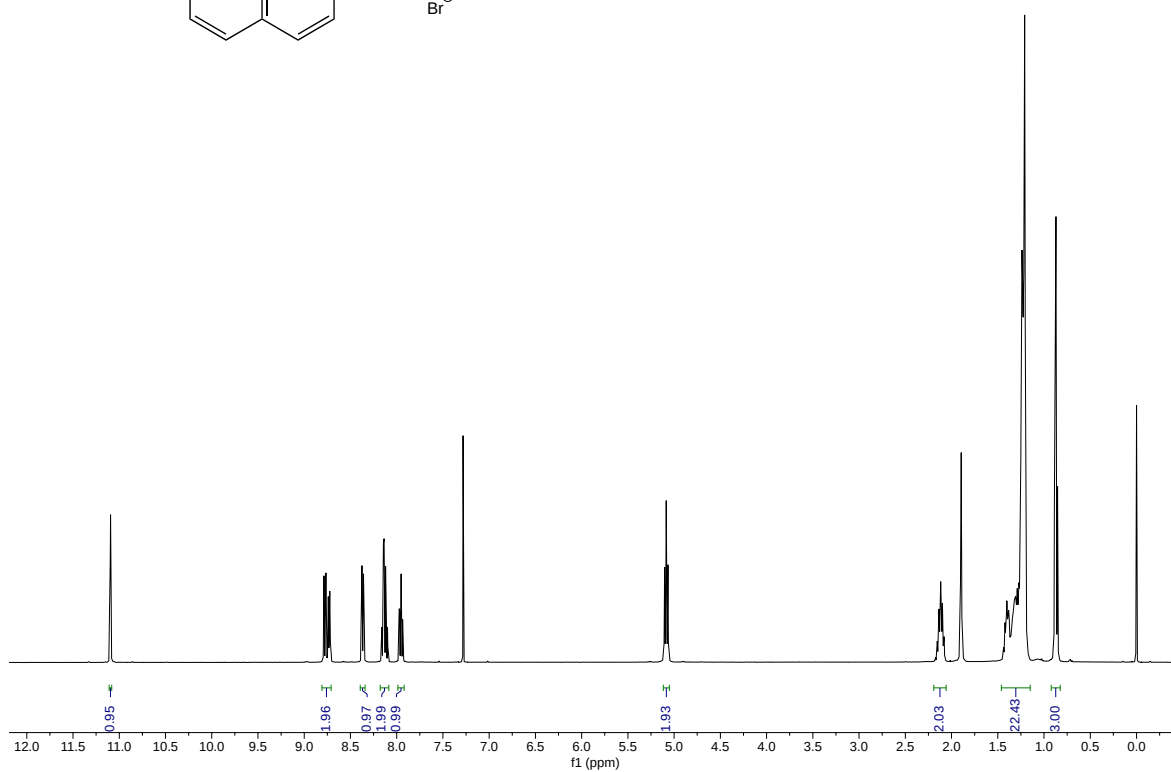
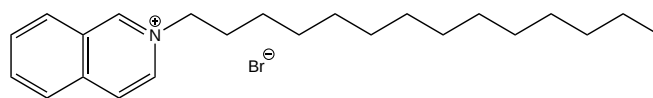


Figure S18. ^1H NMR (a), ^{13}C NMR and DEPT135 (b) spectra of compound **3d**.

a)



b)

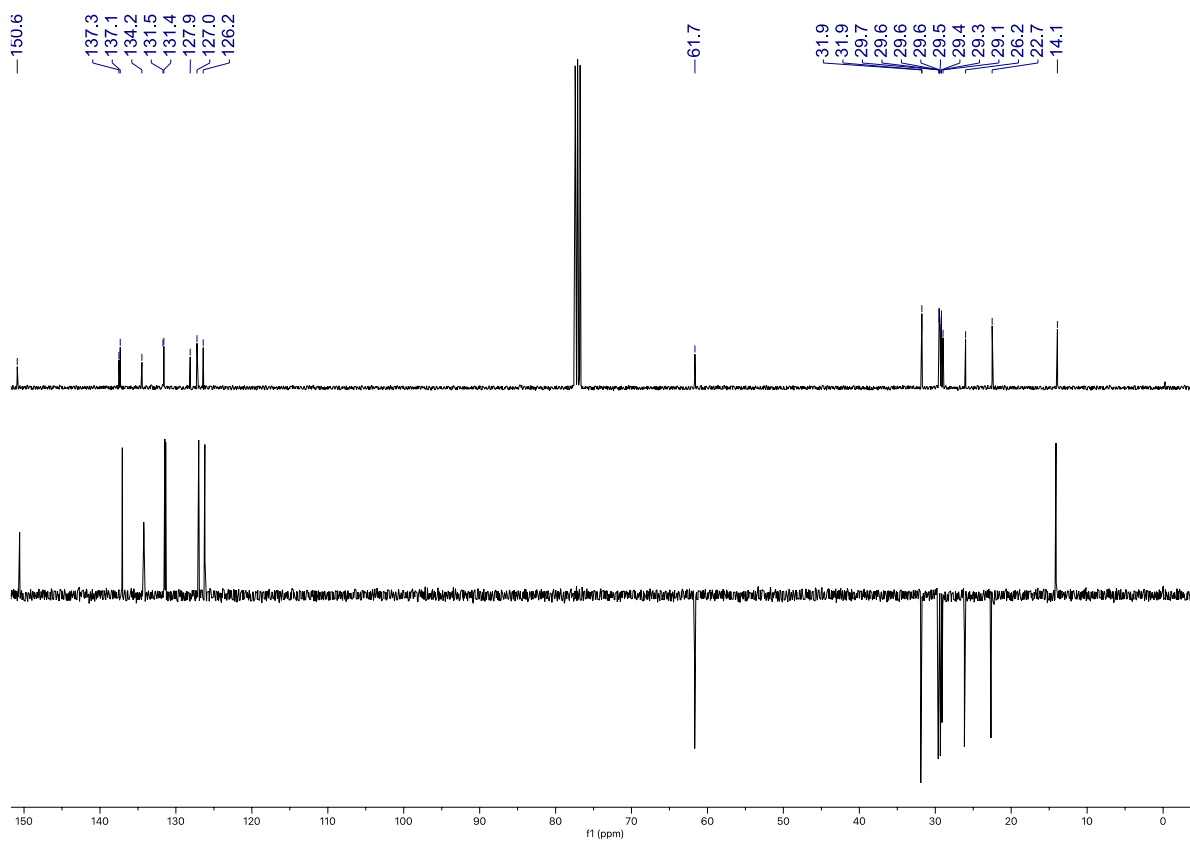
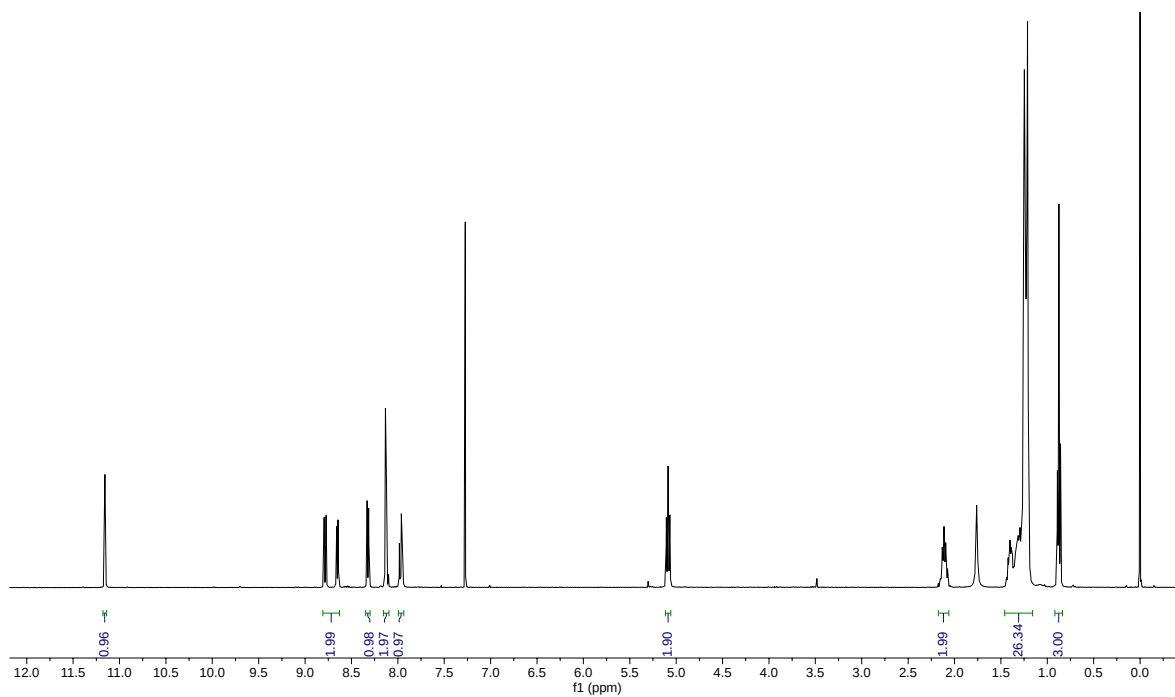
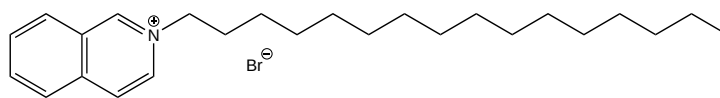


Figure S19. ^1H NMR (a), ^{13}C NMR and DEPT135 (b) spectra of compound **3e**.

a)



b)

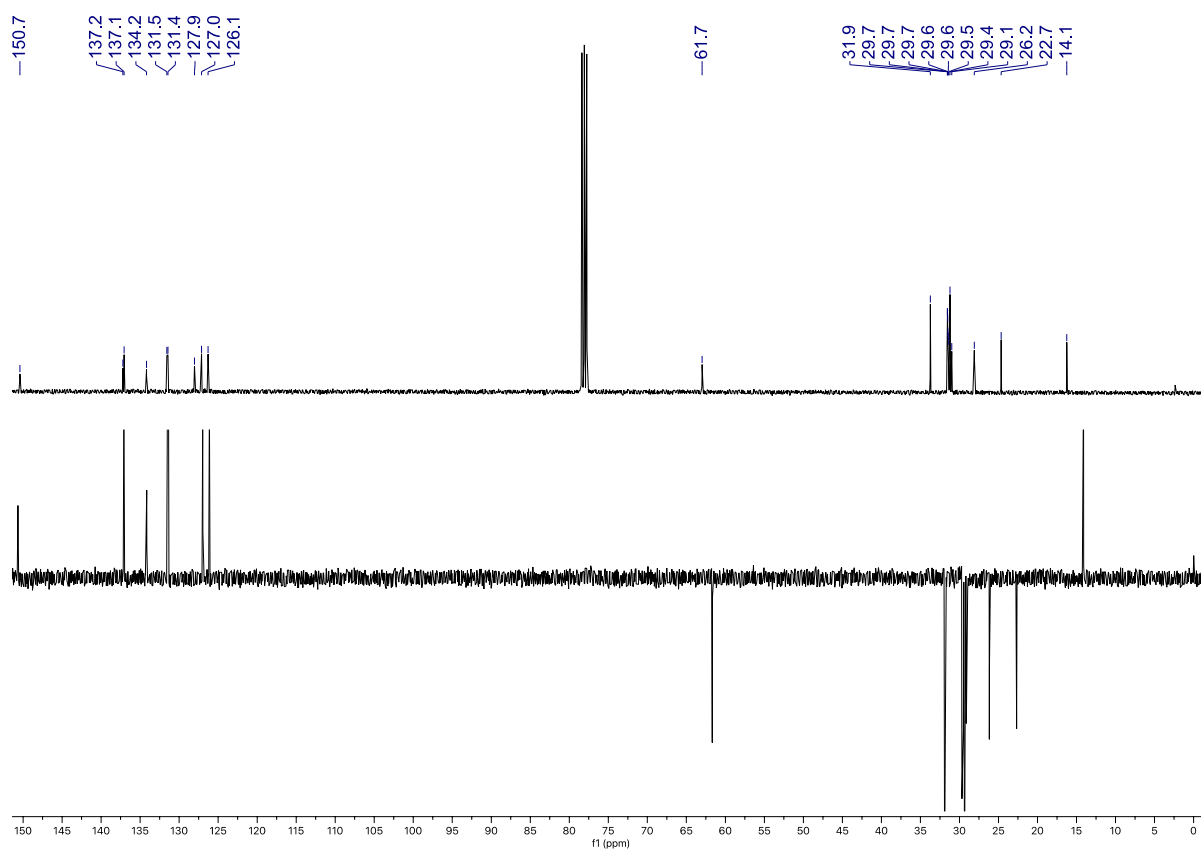
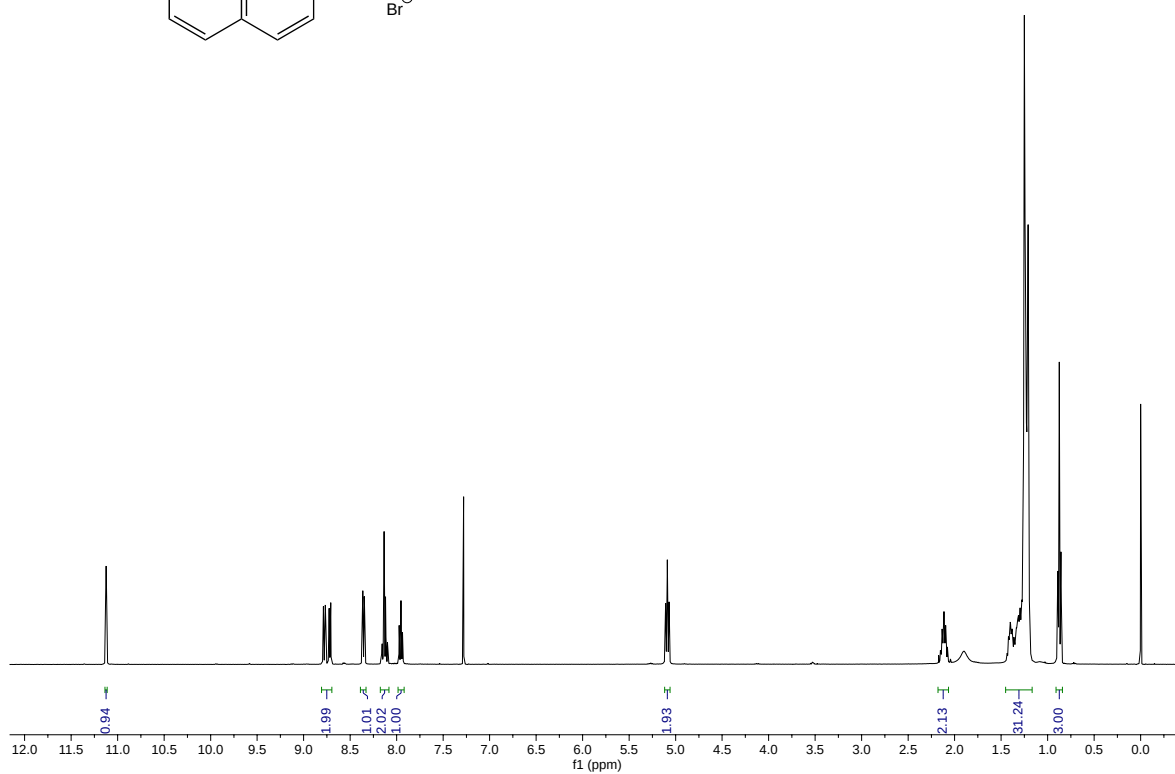
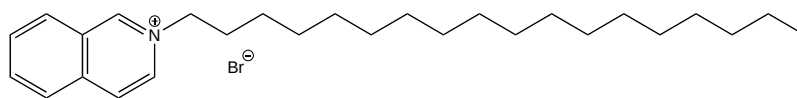


Figure S20. ¹H NMR (a), ¹³C NMR and DEPT135 (b) spectra of compound **3f**.

a)



b)

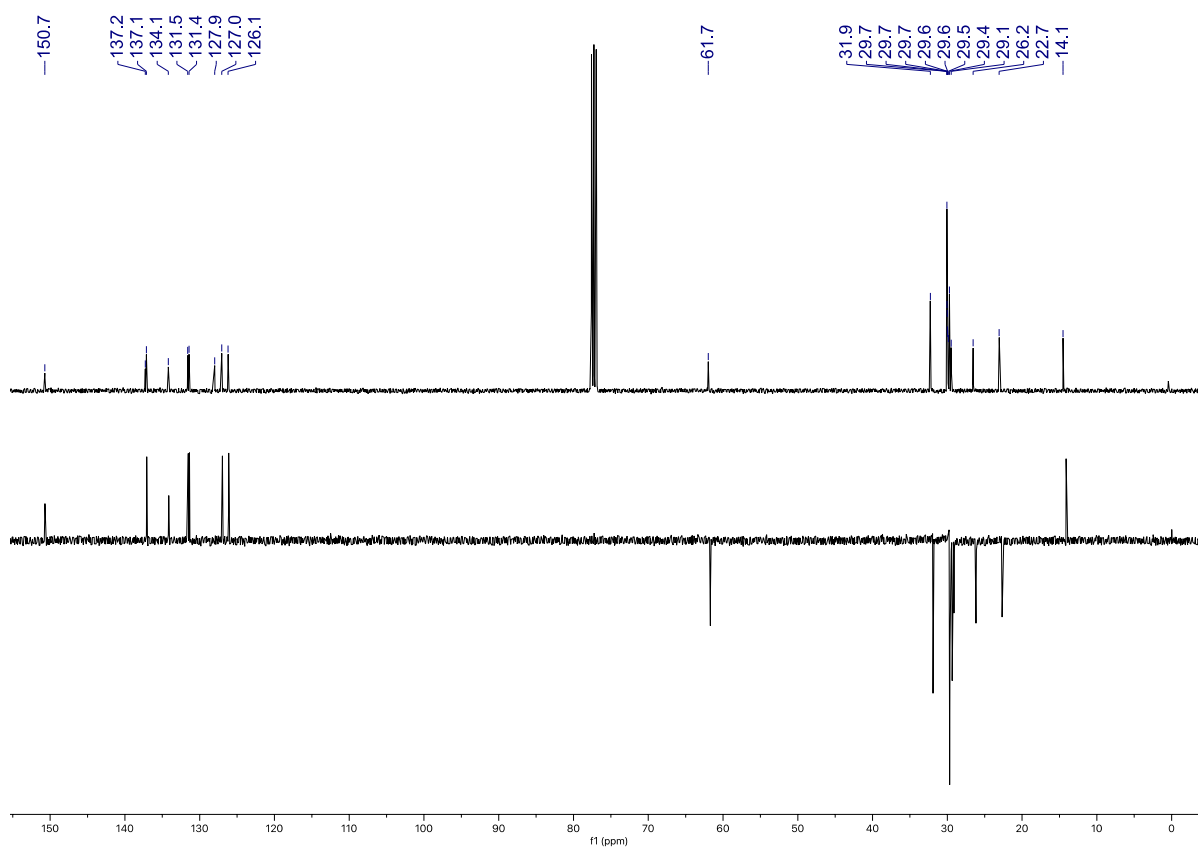
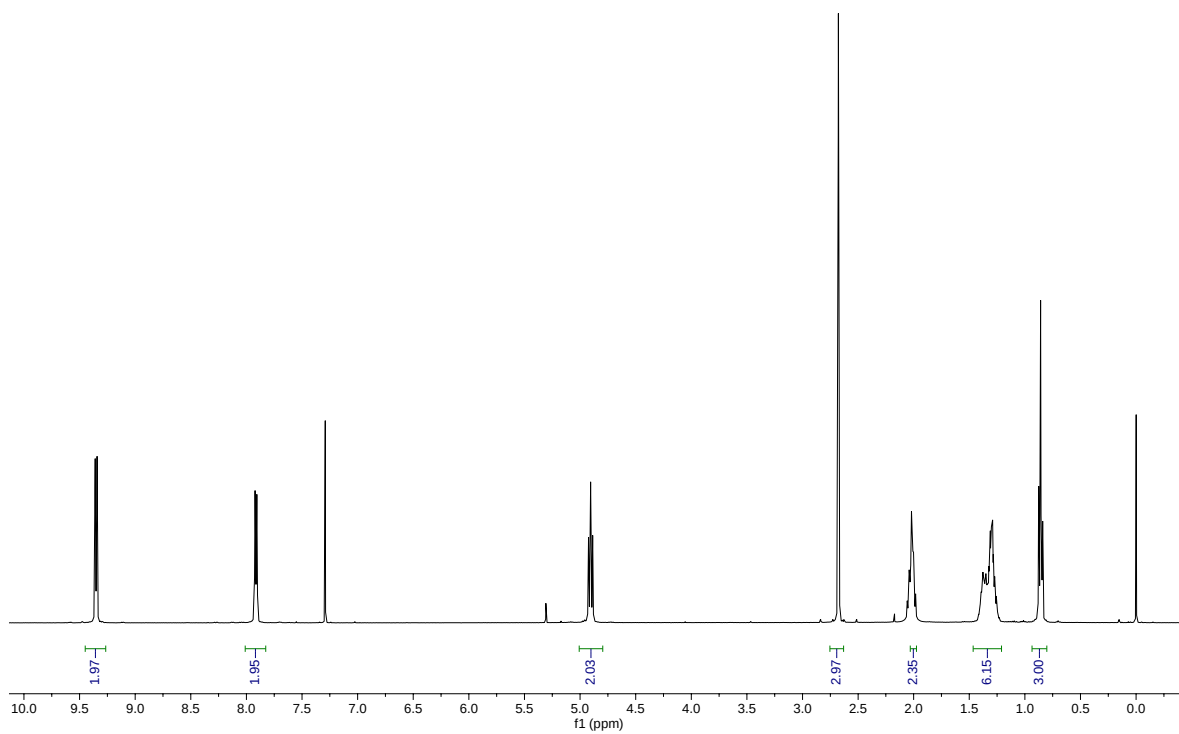
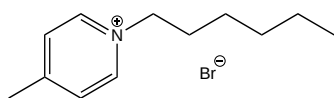


Figure S21. ^1H NMR (a), ^{13}C NMR and DEPT135 (b) spectra of compound **3g**.

a)



b)

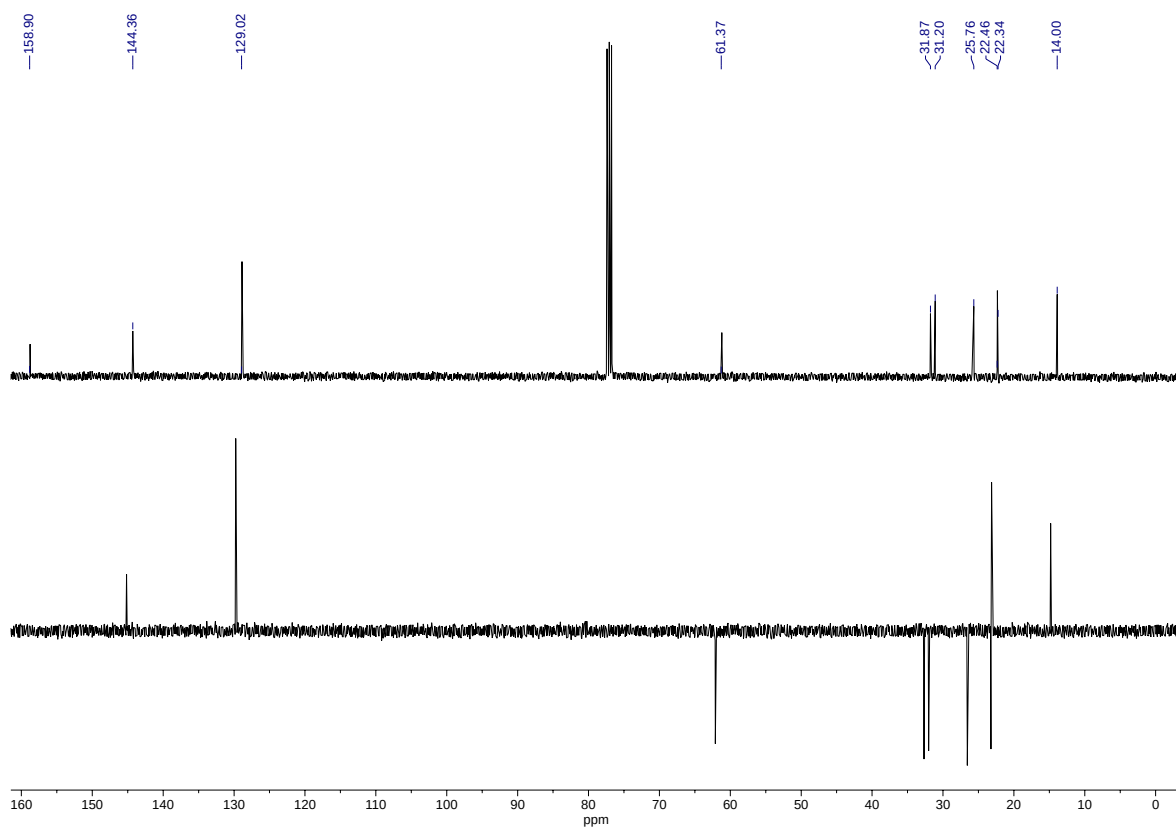
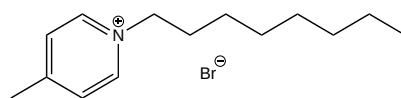


Figure S22. ¹H NMR (a), ¹³C NMR and DEPT135 (b) spectra of compound 4a.

a)



b)

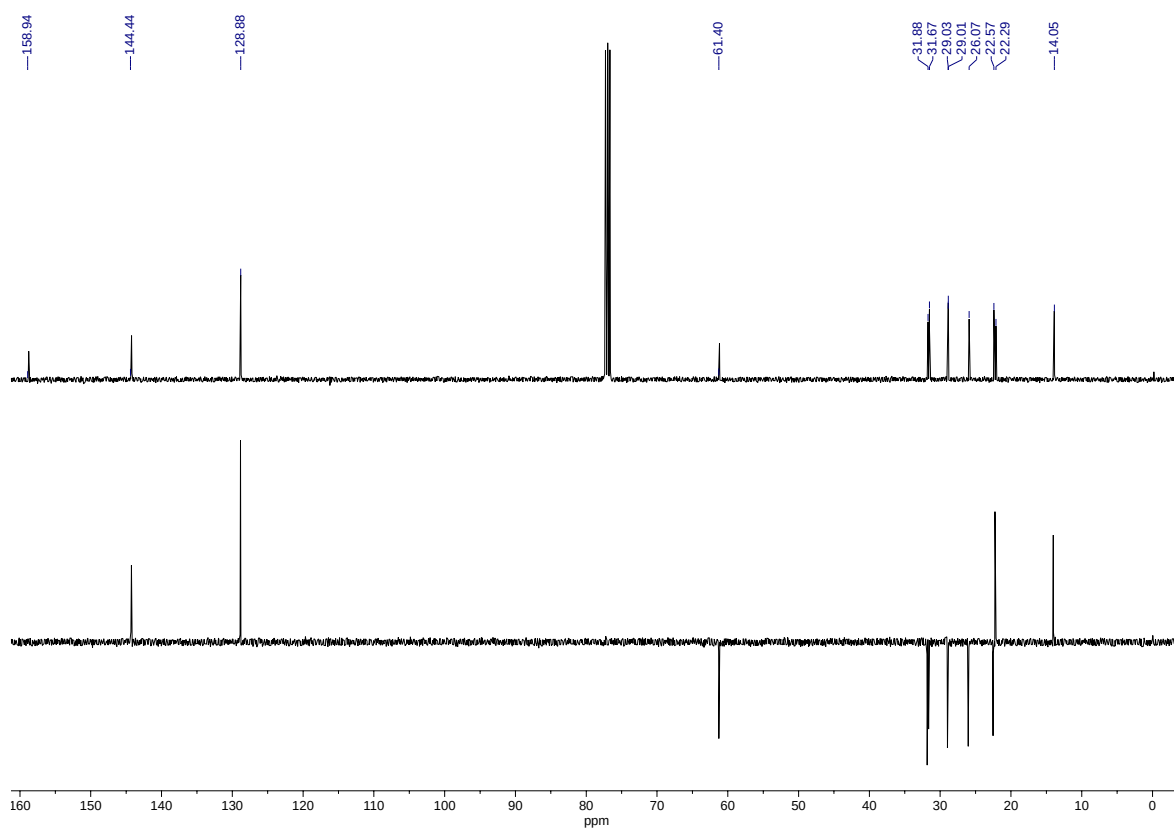
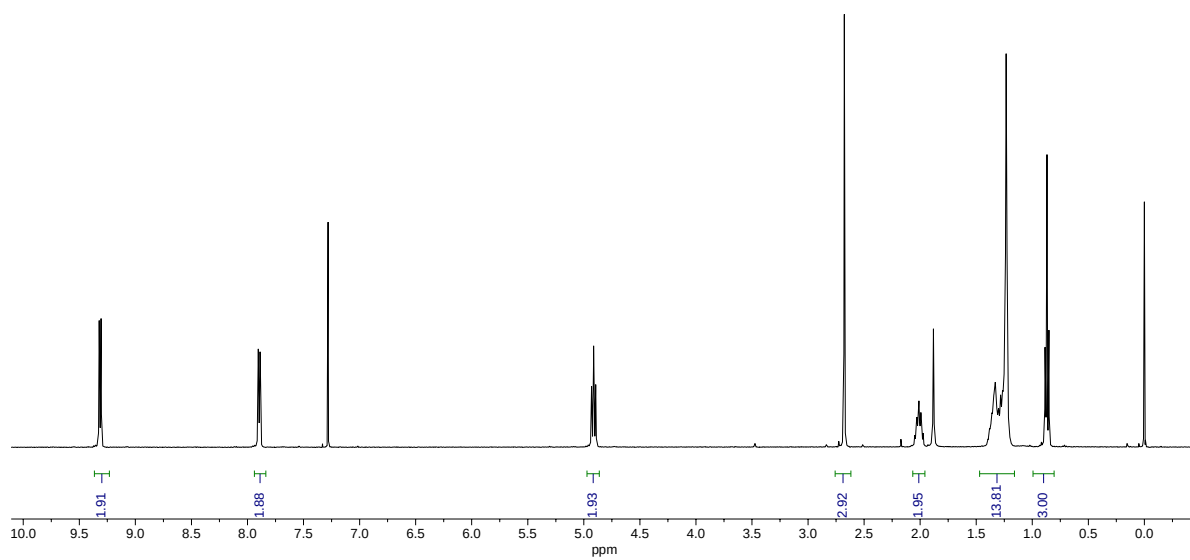
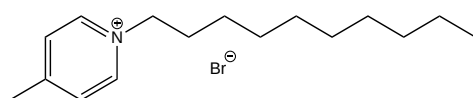


Figure S23. ¹H NMR (a), ¹³C NMR and DEPT135 (b) spectra of compound 4b.

a)



b)

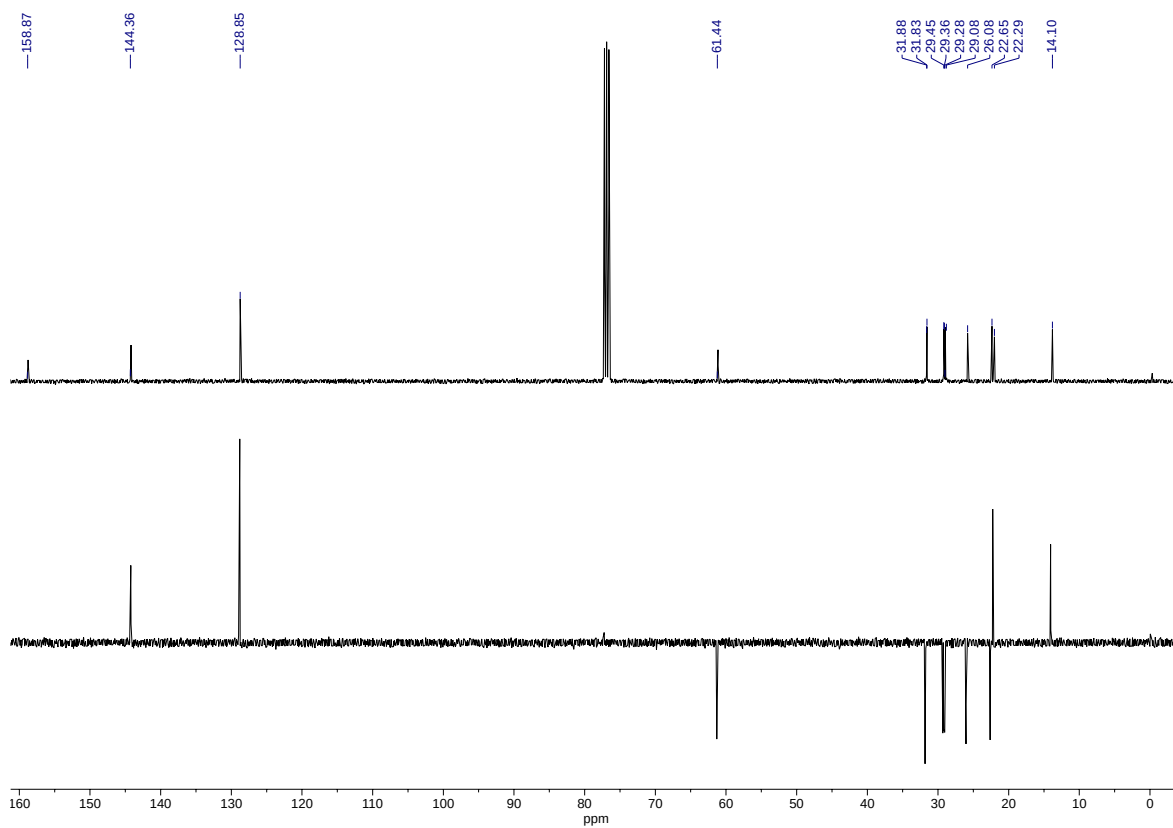
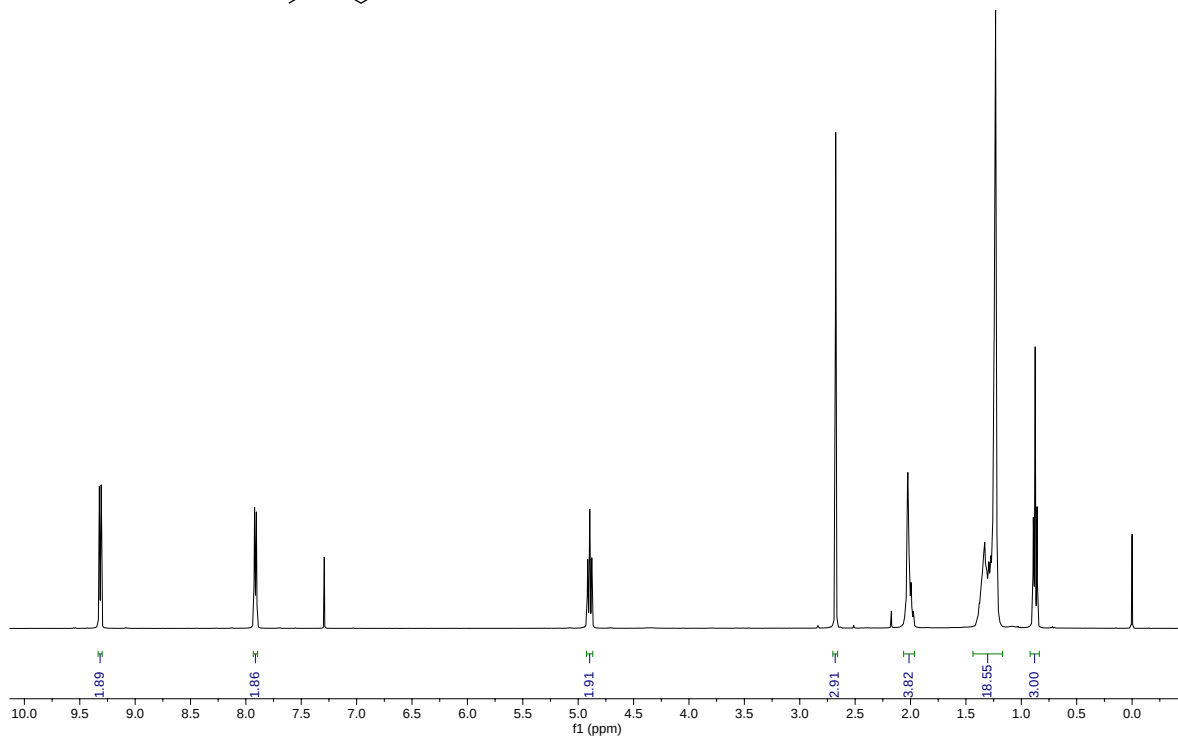
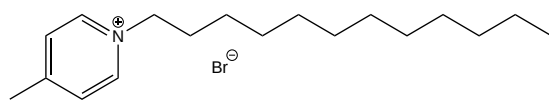


Figure S24. ¹H NMR (a), ¹³C NMR and DEPT135 (b) spectra of compound 4c.

a)



b)

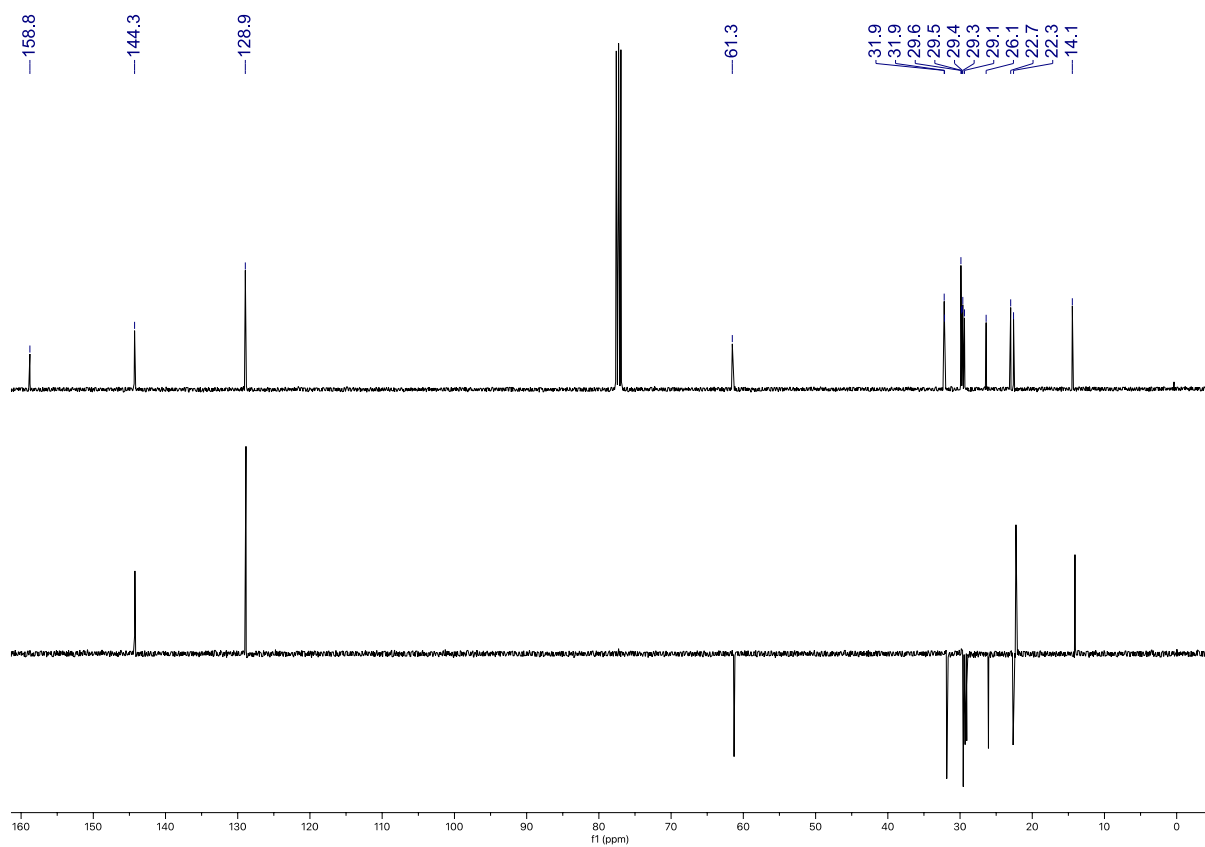
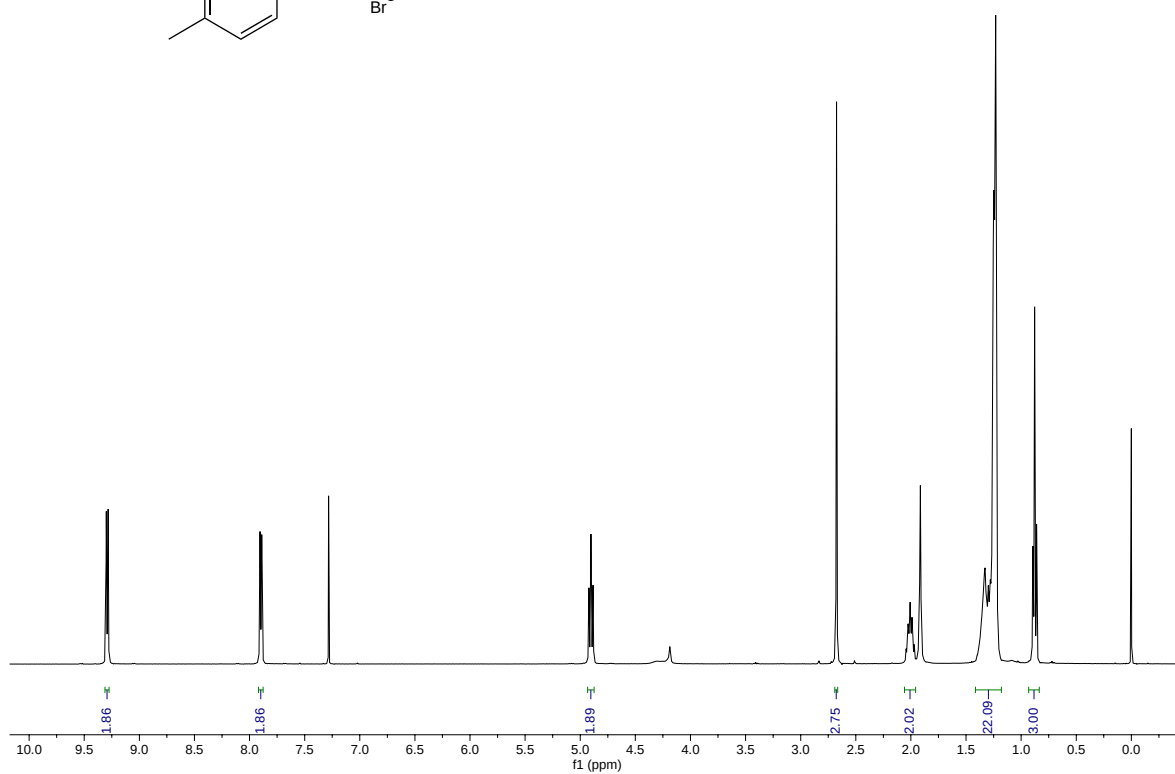
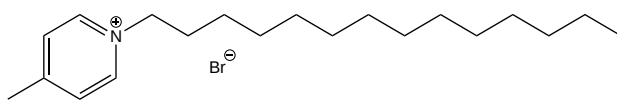


Figure S25. ¹H NMR (a), ¹³C NMR and DEPT135 (b) spectra of compound 4d.

a)



b)

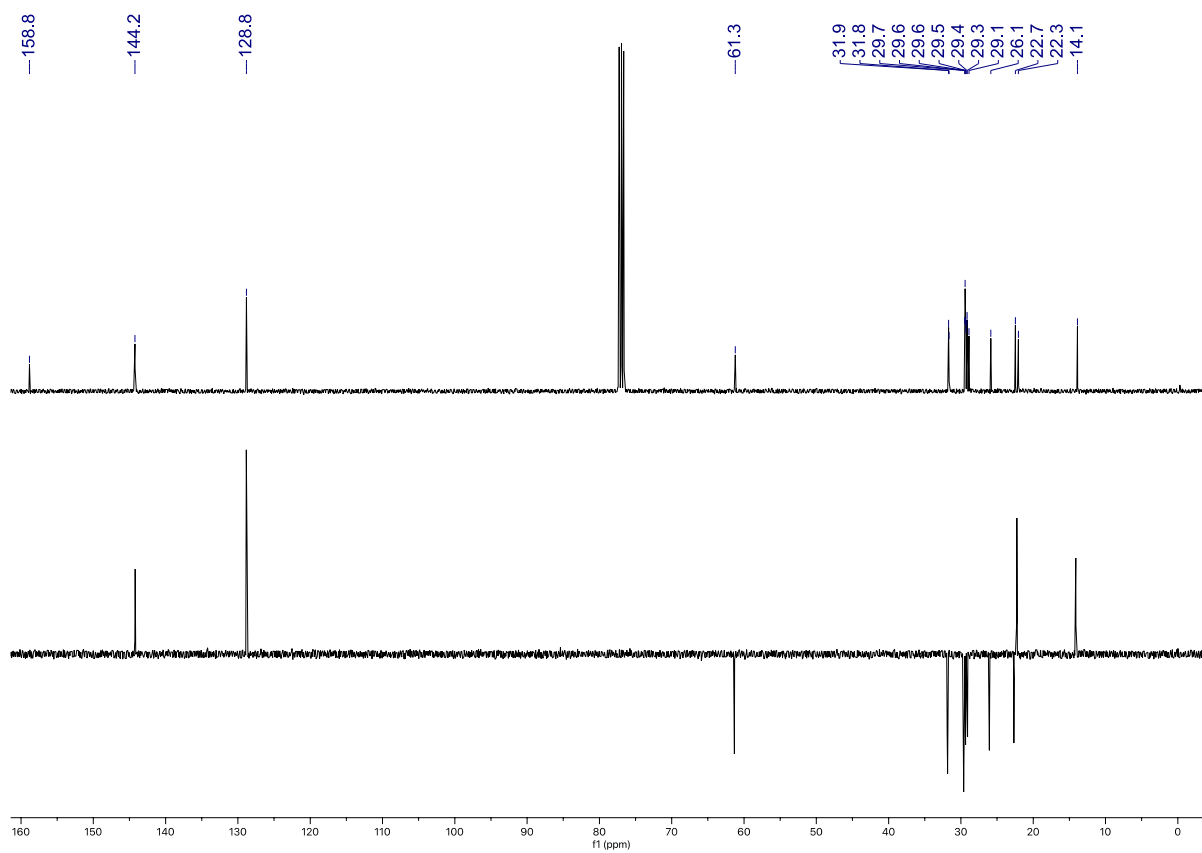
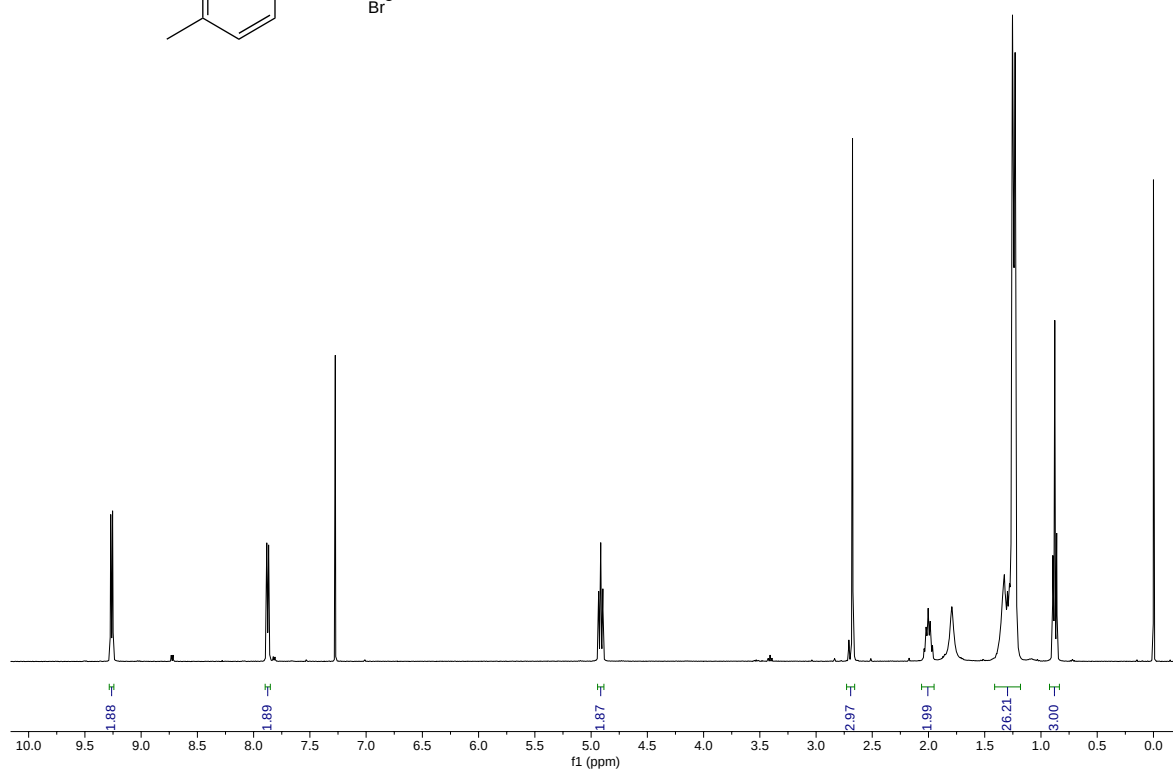
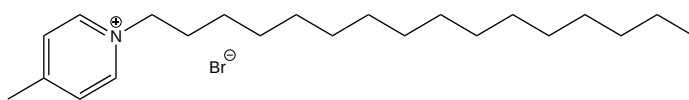


Figure S26. ¹H NMR (a), ¹³C NMR and DEPT135 (b) spectra of compound 4e.

a)



b)

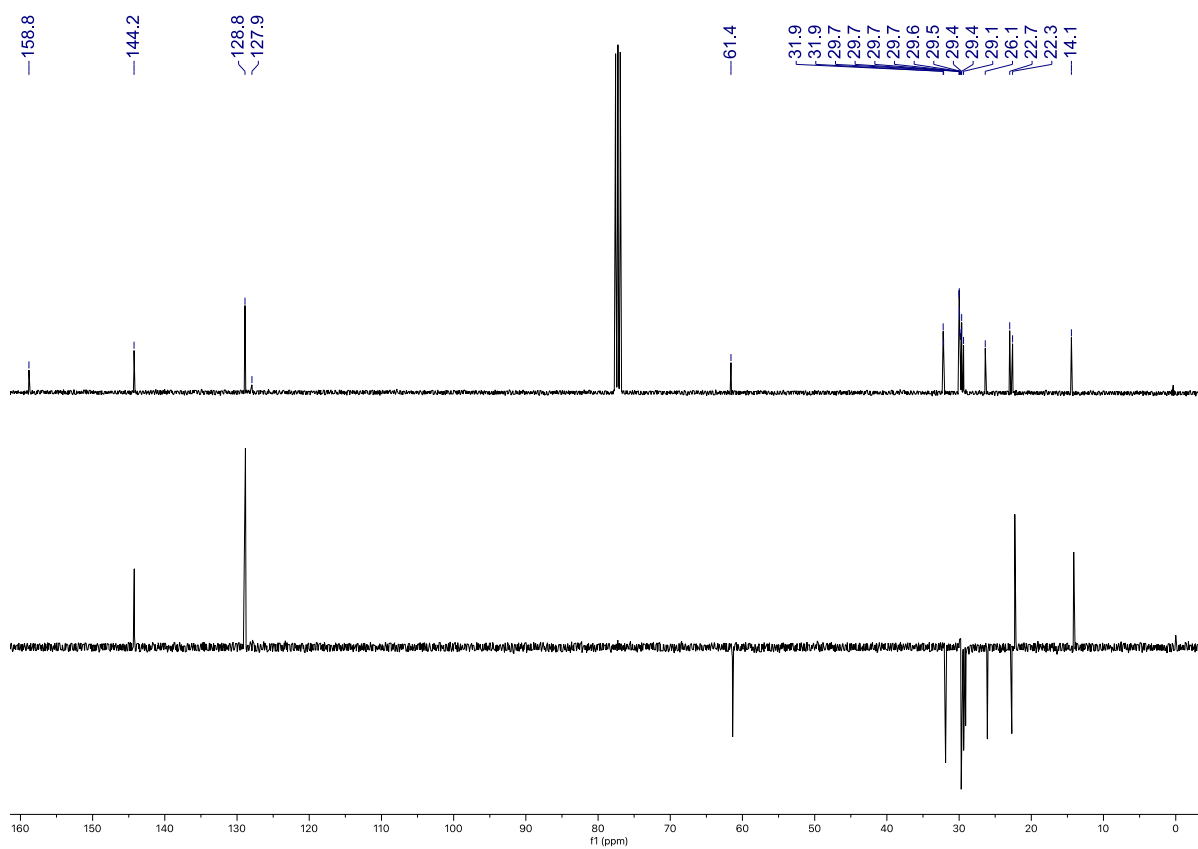
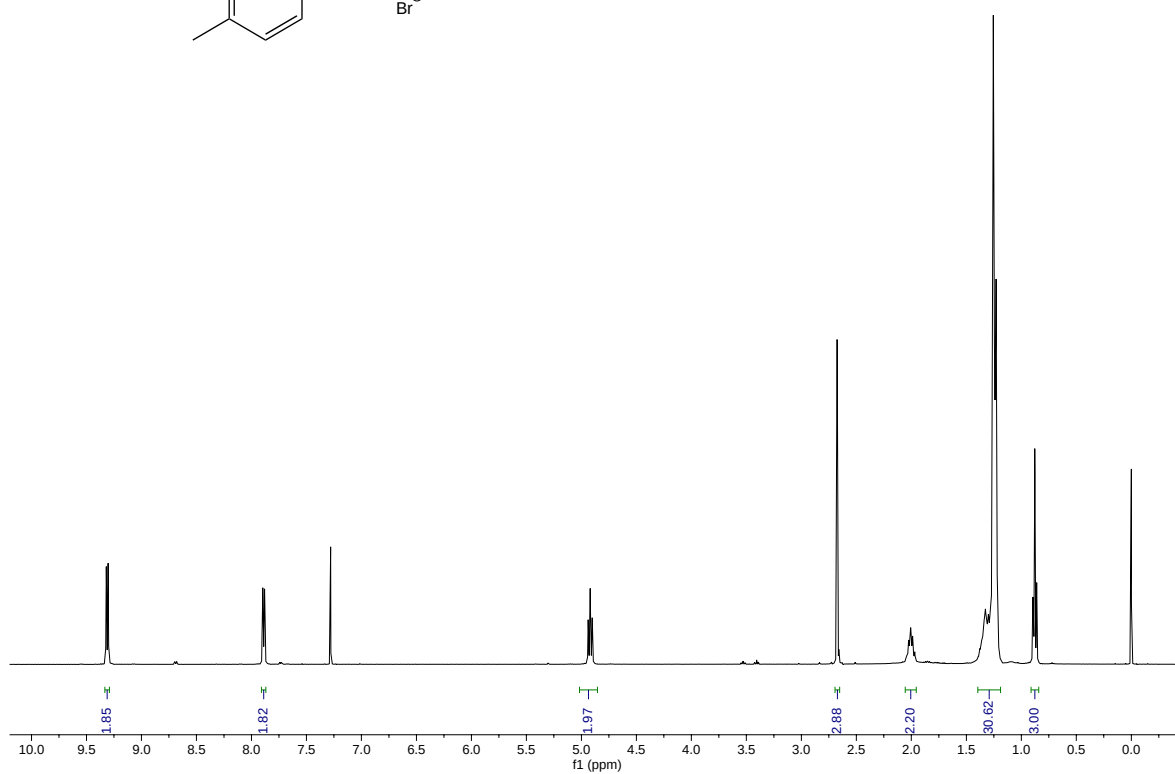
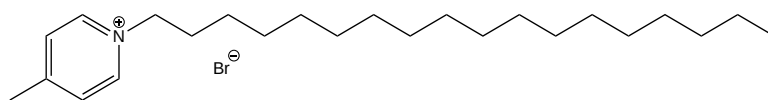


Figure S27. ^1H NMR (a), ^{13}C NMR and DEPT135 (b) spectra of compound **4f**.

a)



b)

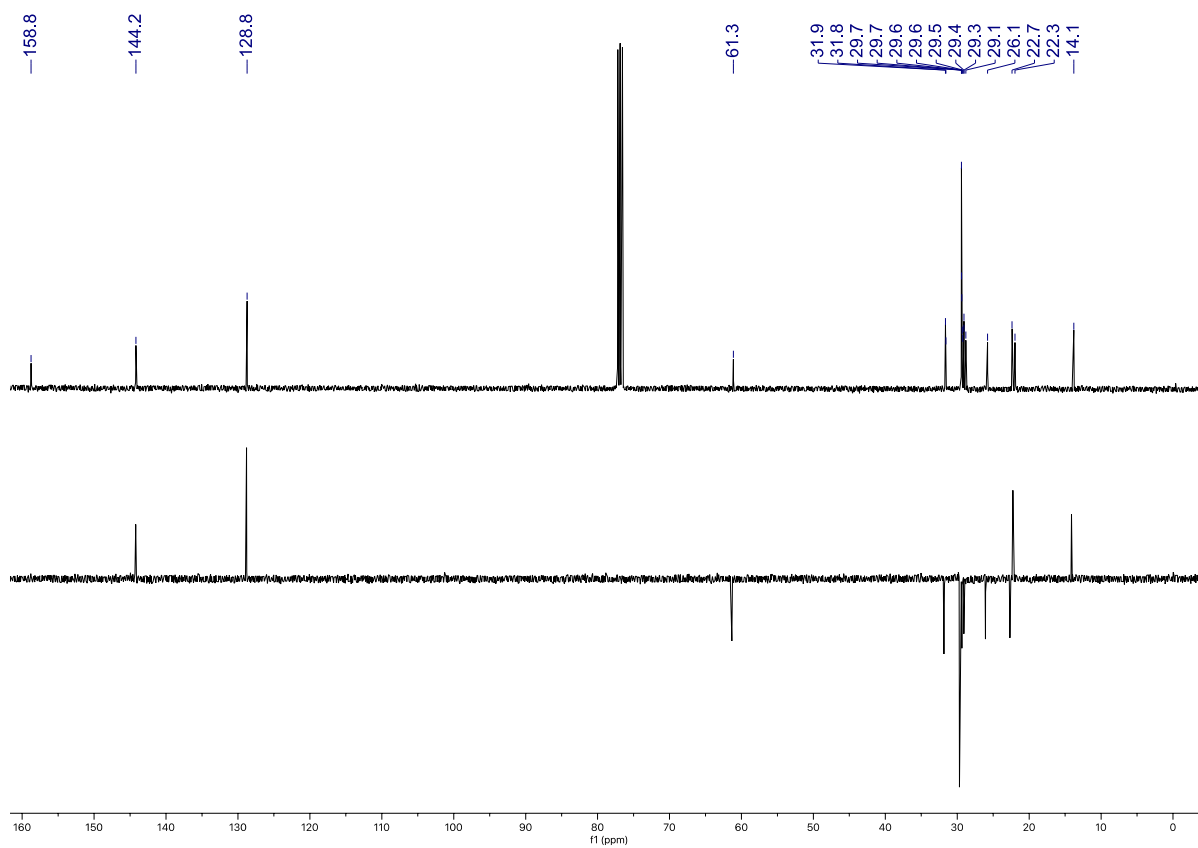
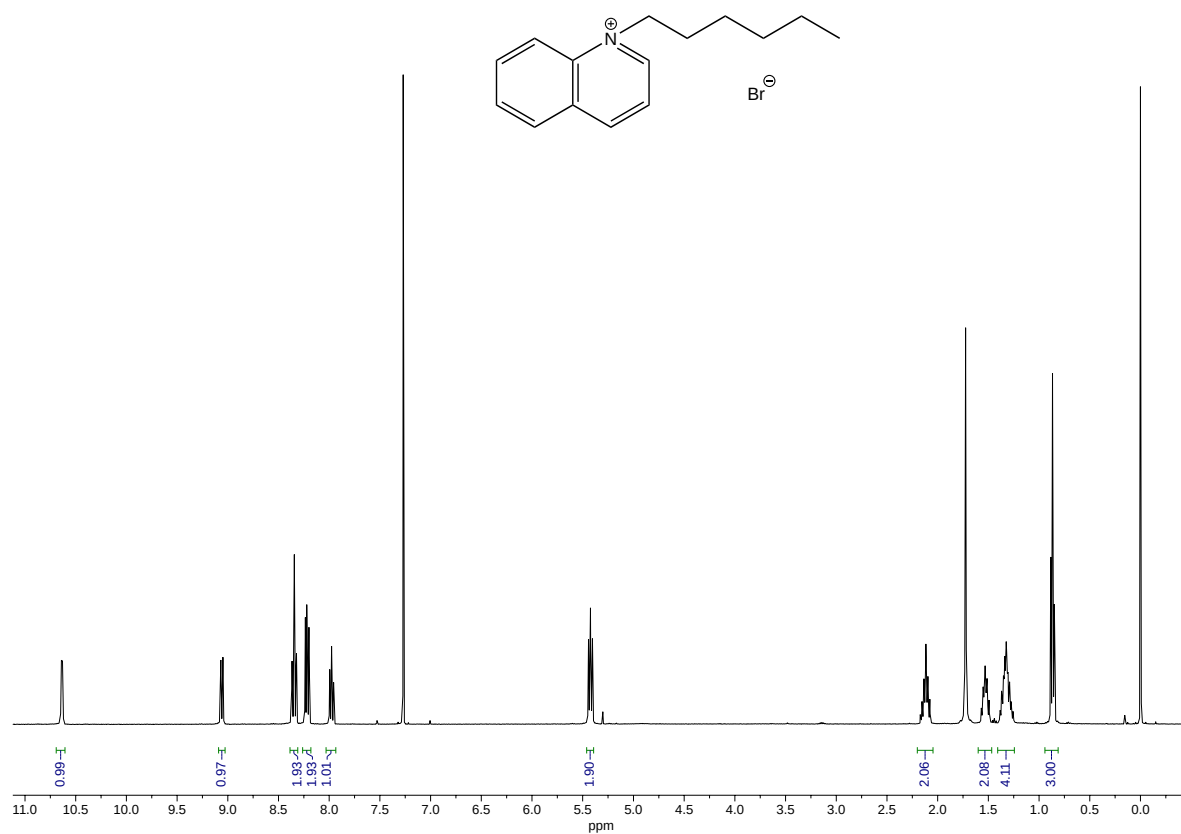


Figure S28. ¹H NMR (a), ¹³C NMR and DEPT135 (b) spectra of compound 4g.

a)



b)

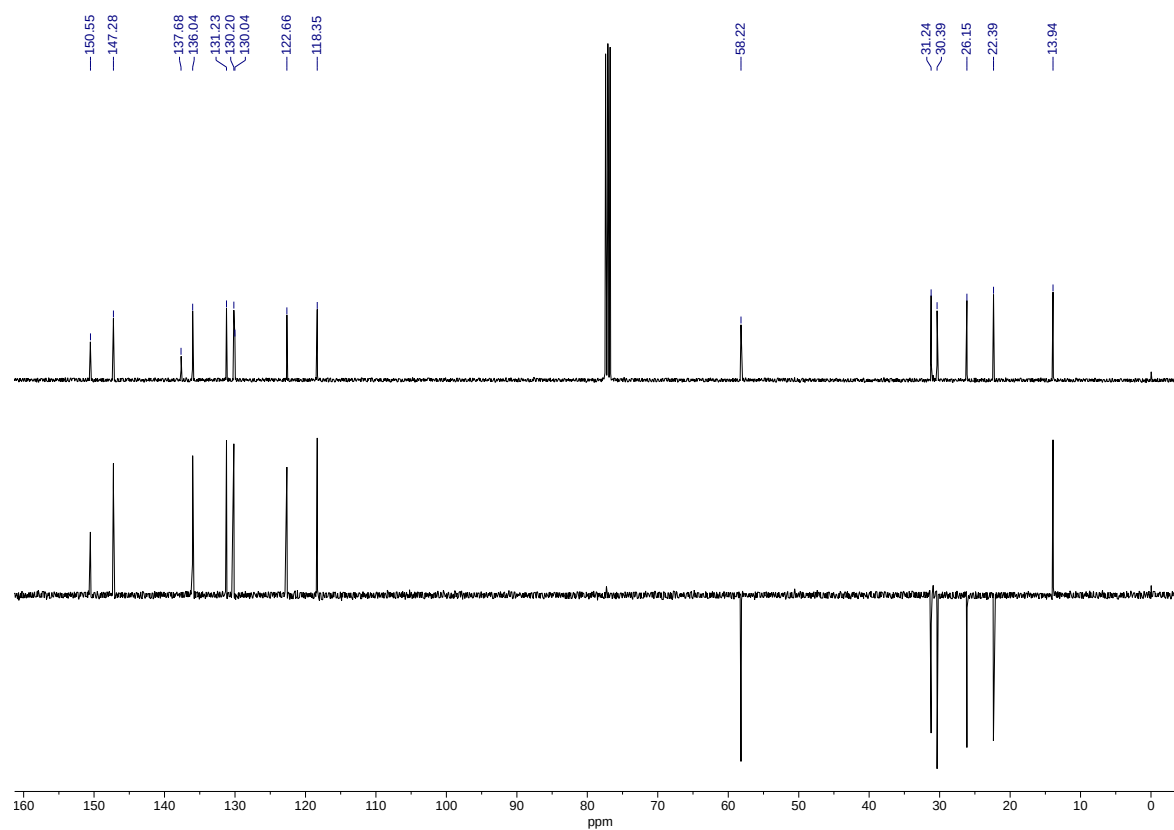
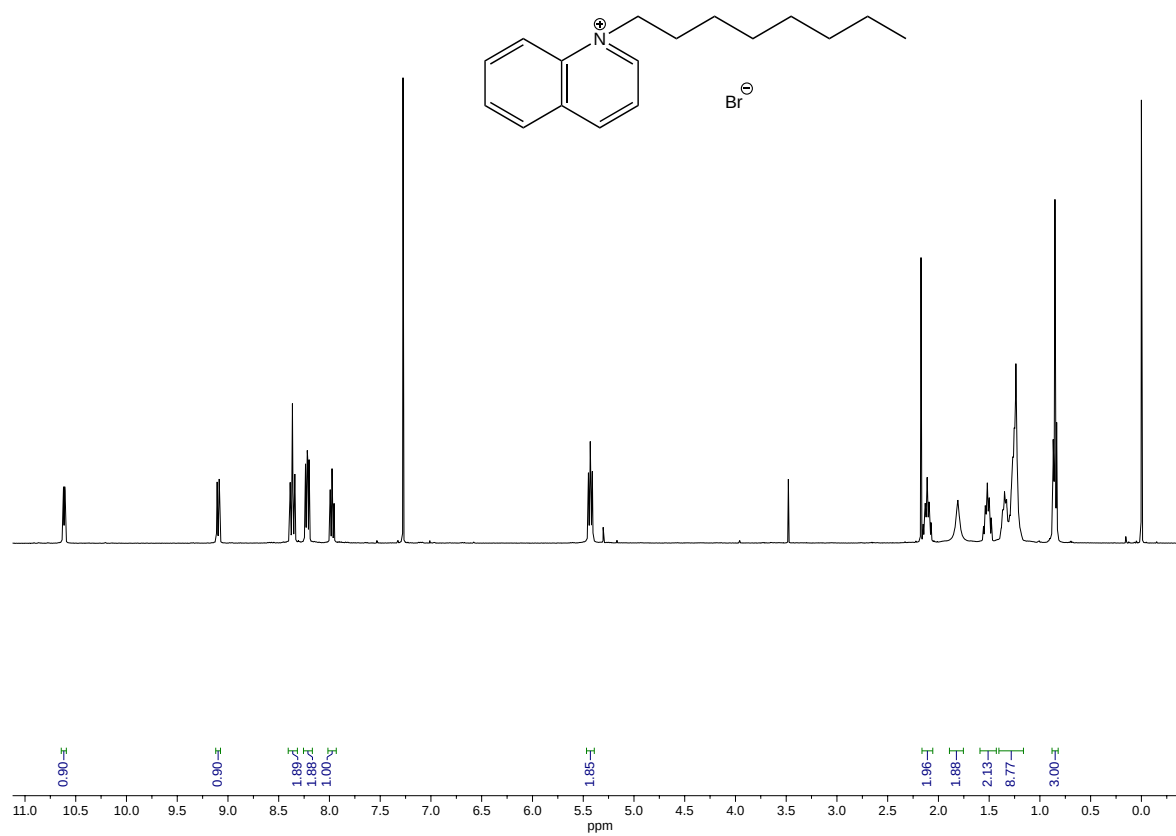


Figure S29. ¹H NMR (a), ¹³C NMR and DEPT135 (b) spectra of compound 5a.

a)



b)

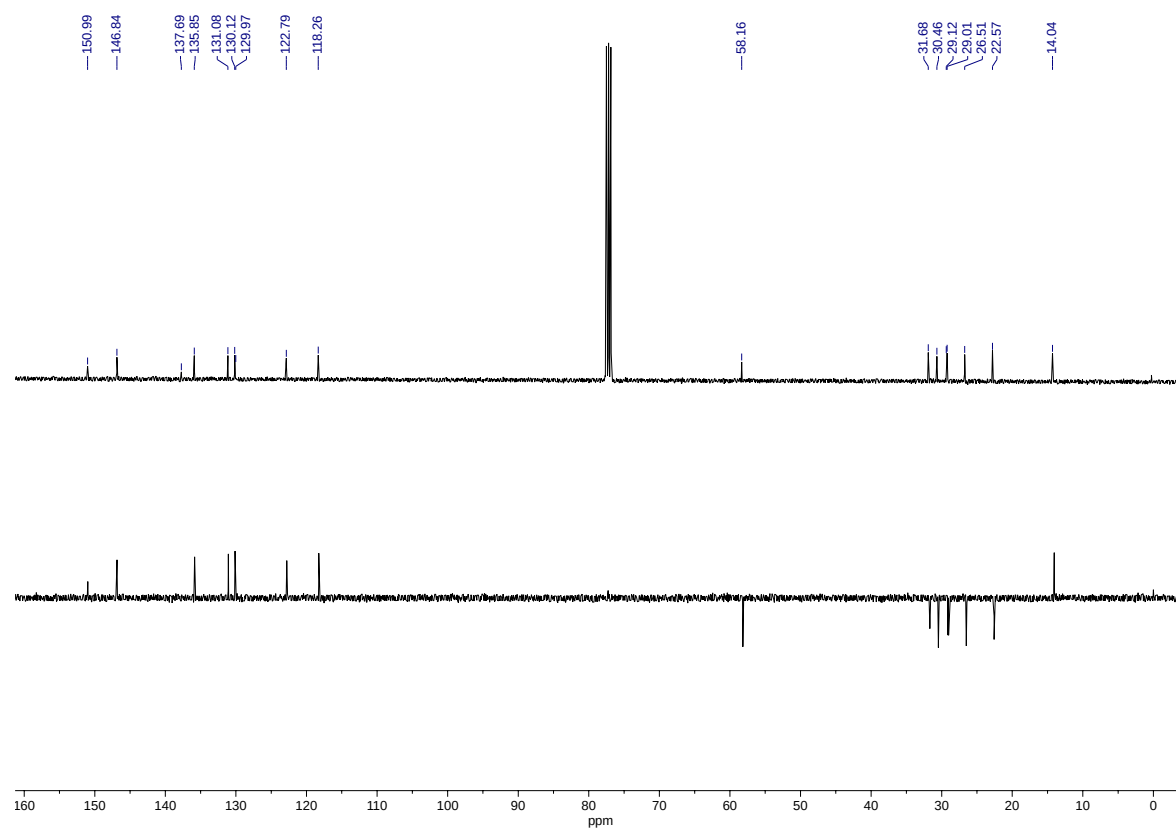
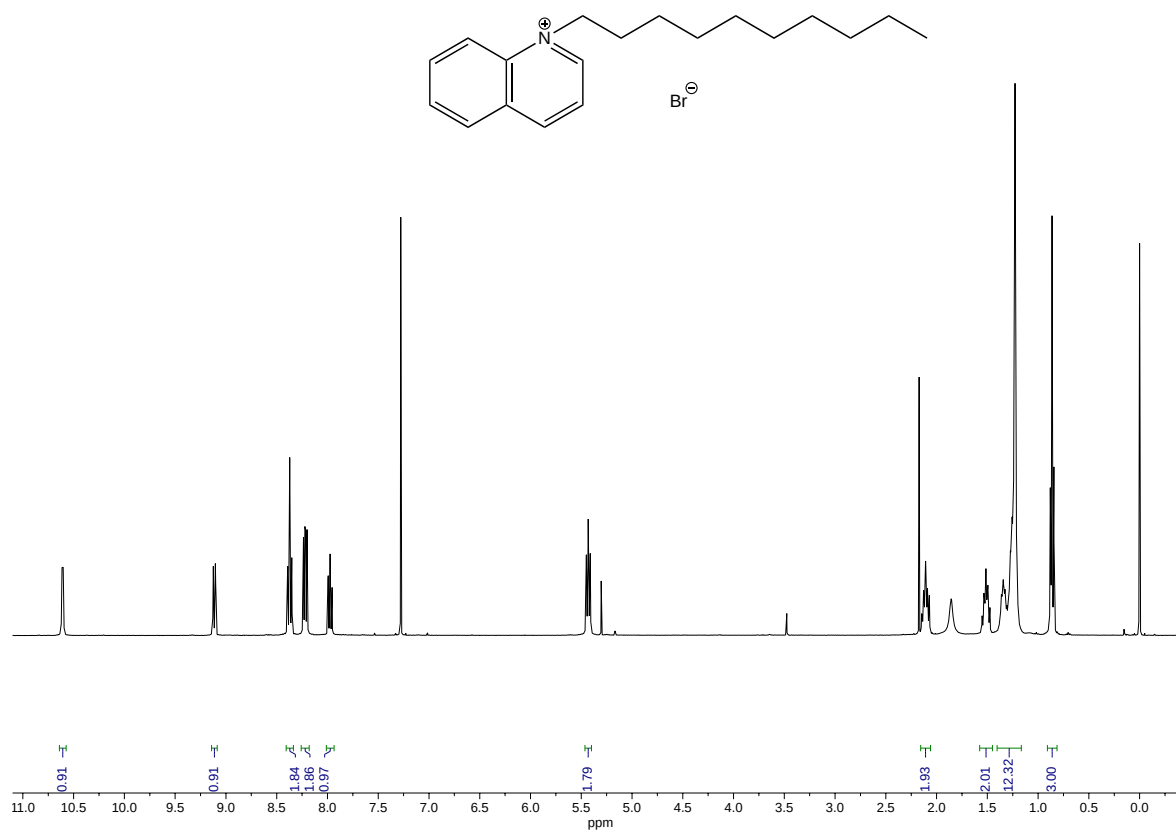


Figure S30. ¹H NMR (a), ¹³C NMR and DEPT135 (b) spectra of compound 5b.

a)



b)

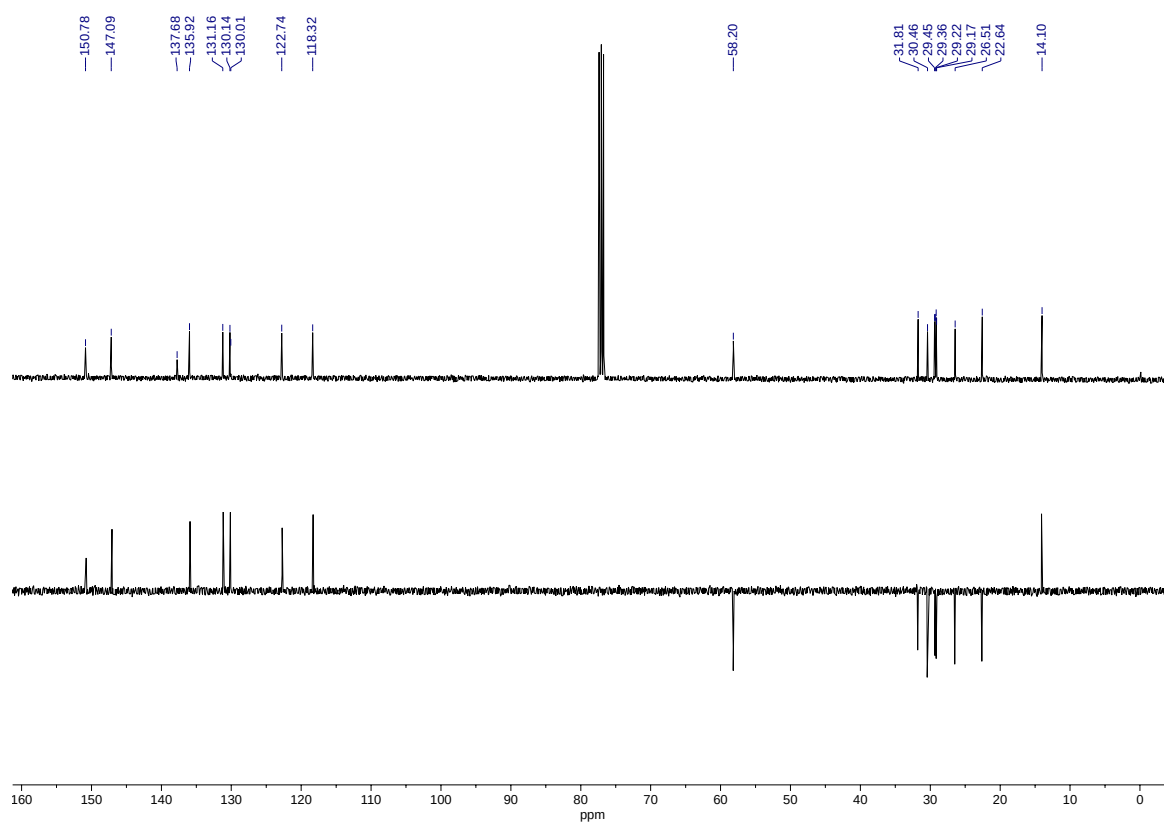
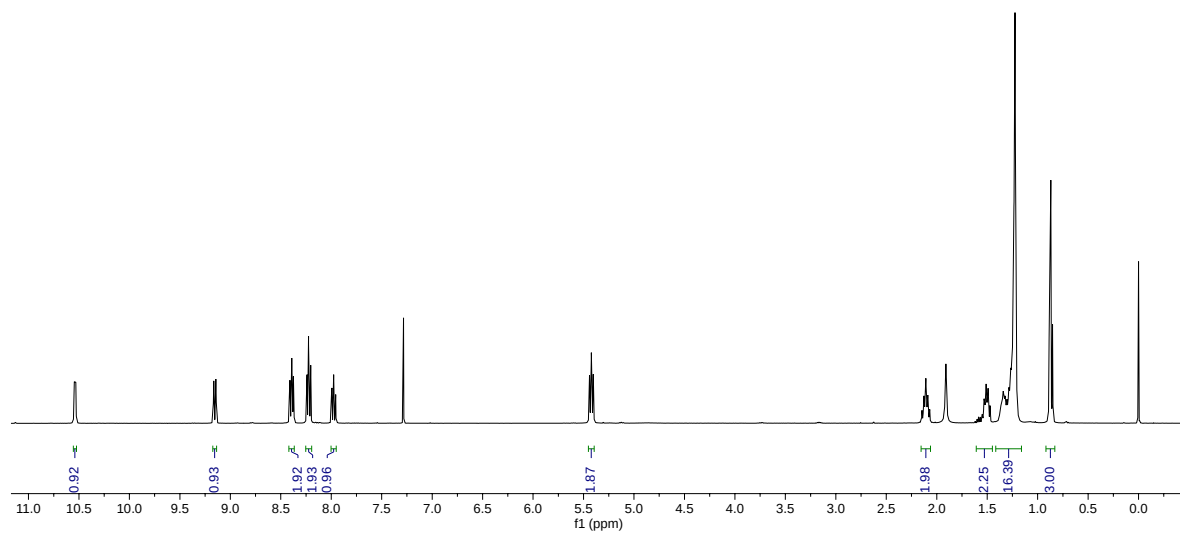
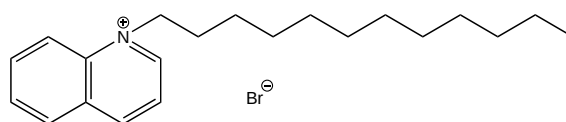


Figure S31. ^1H NMR (a), ^{13}C NMR and DEPT135 (b) spectra of compound 5c.

a)



b)

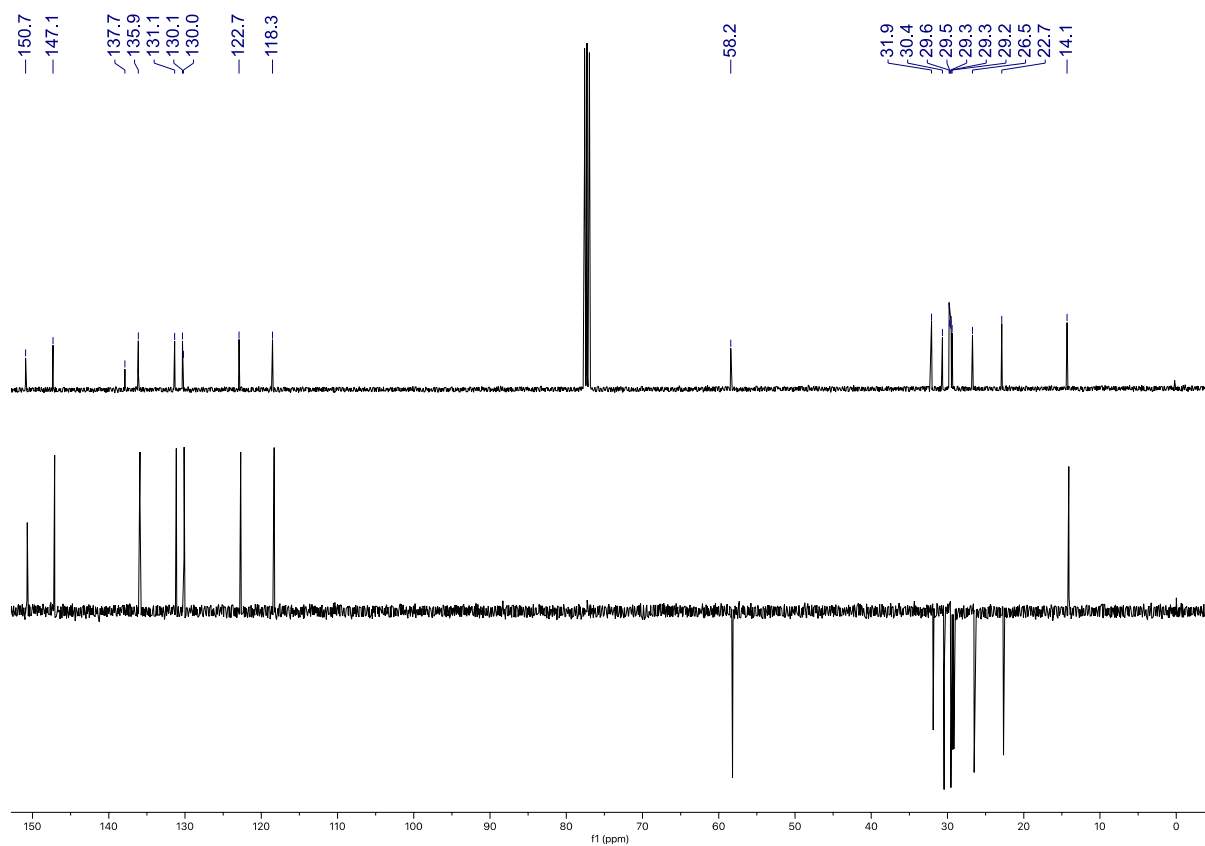
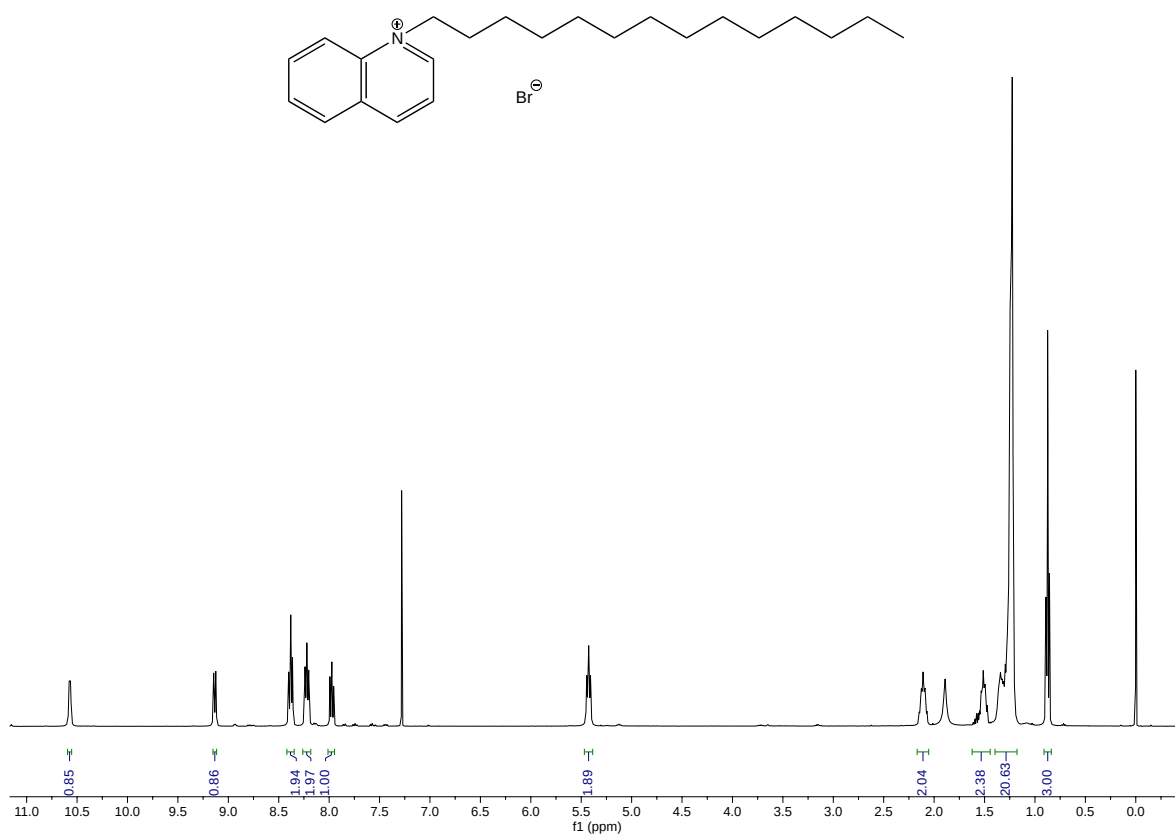


Figure S32. ^1H NMR (a), ^{13}C NMR and DEPT135 (b) spectra of compound **5d**.

a)



b)

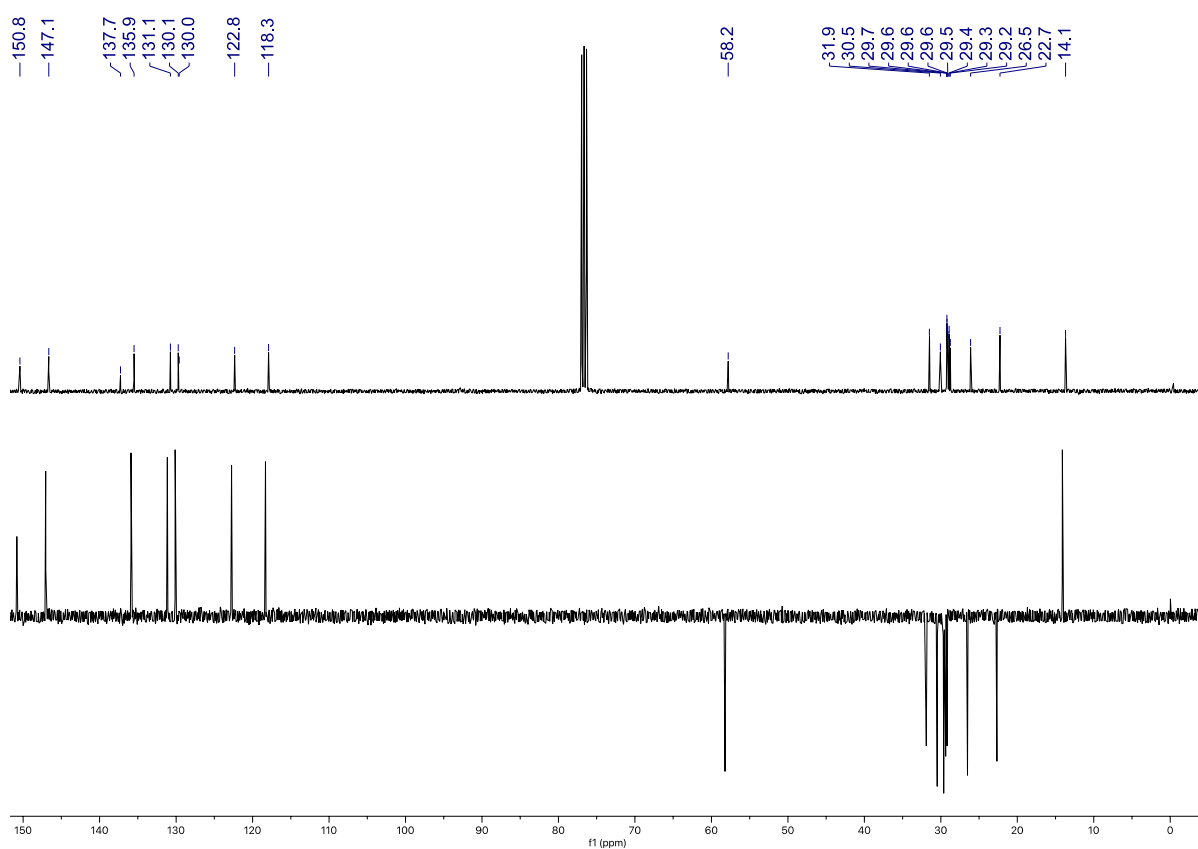
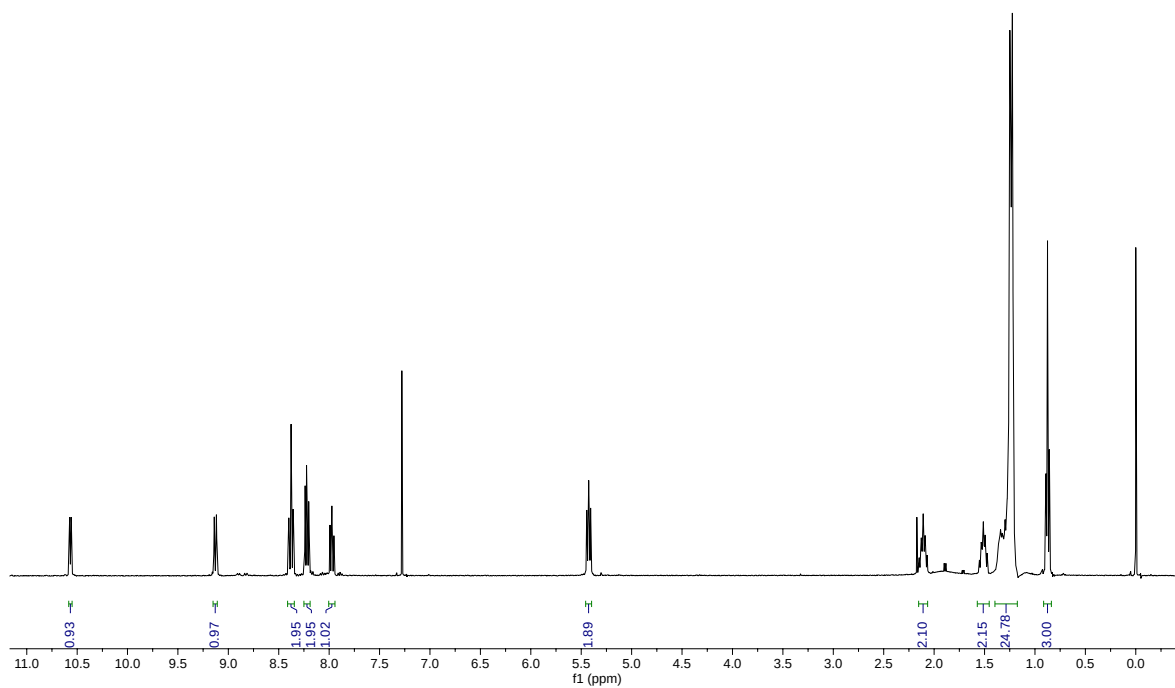
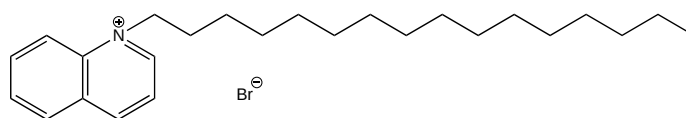


Figure S33. ¹H NMR (a), ¹³C NMR and DEPT135 (b) spectra of compound 5e.

a)



b)

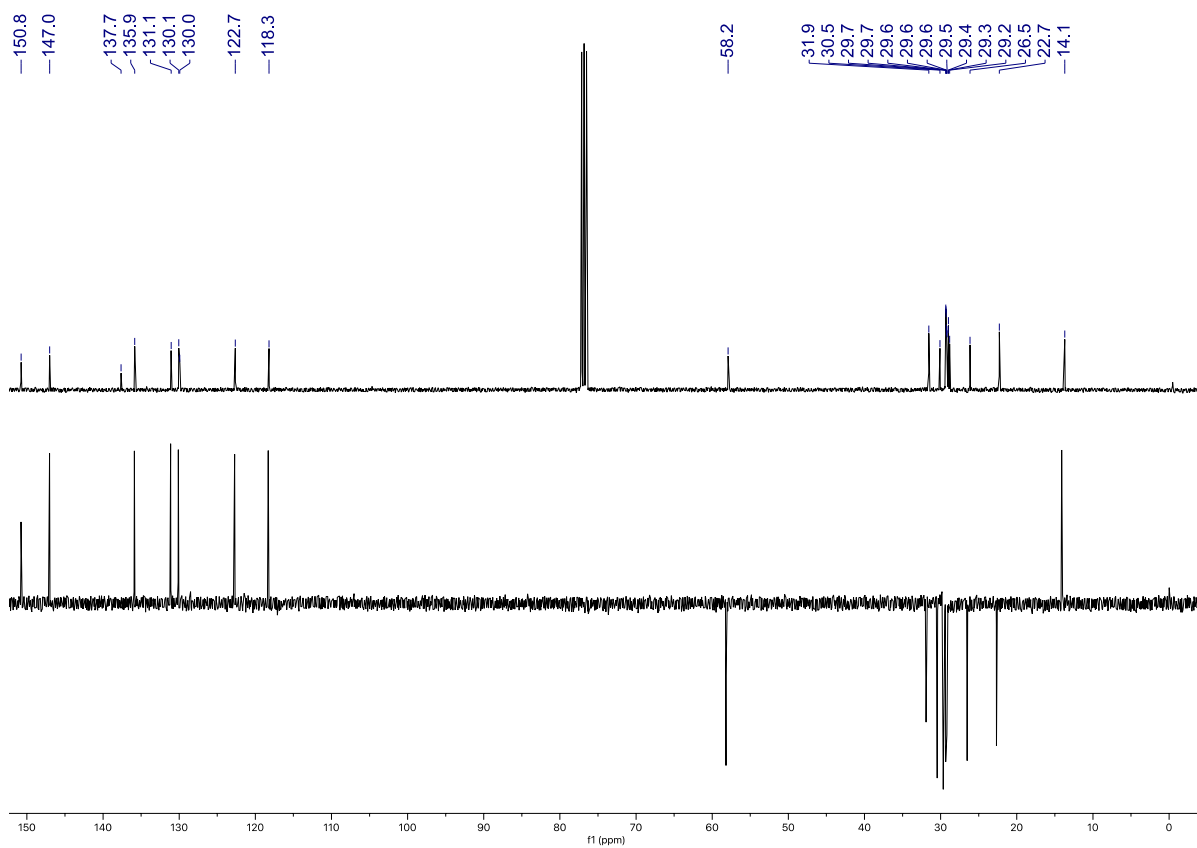
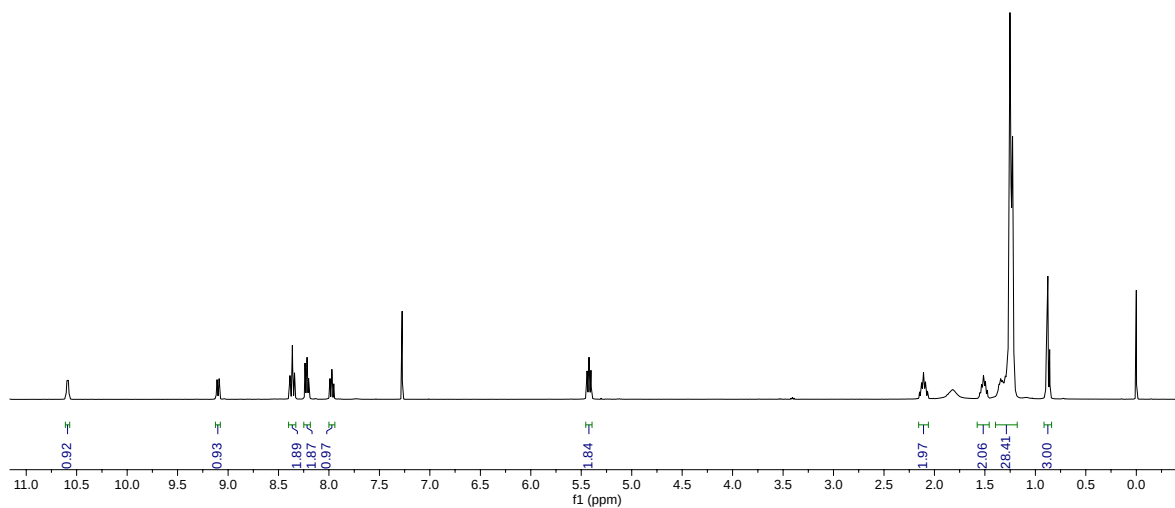
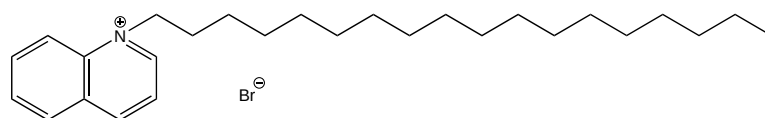


Figure S34. ^1H NMR (a), ^{13}C NMR and DEPT135 (b) spectra of compound **5f**.

a)



b)

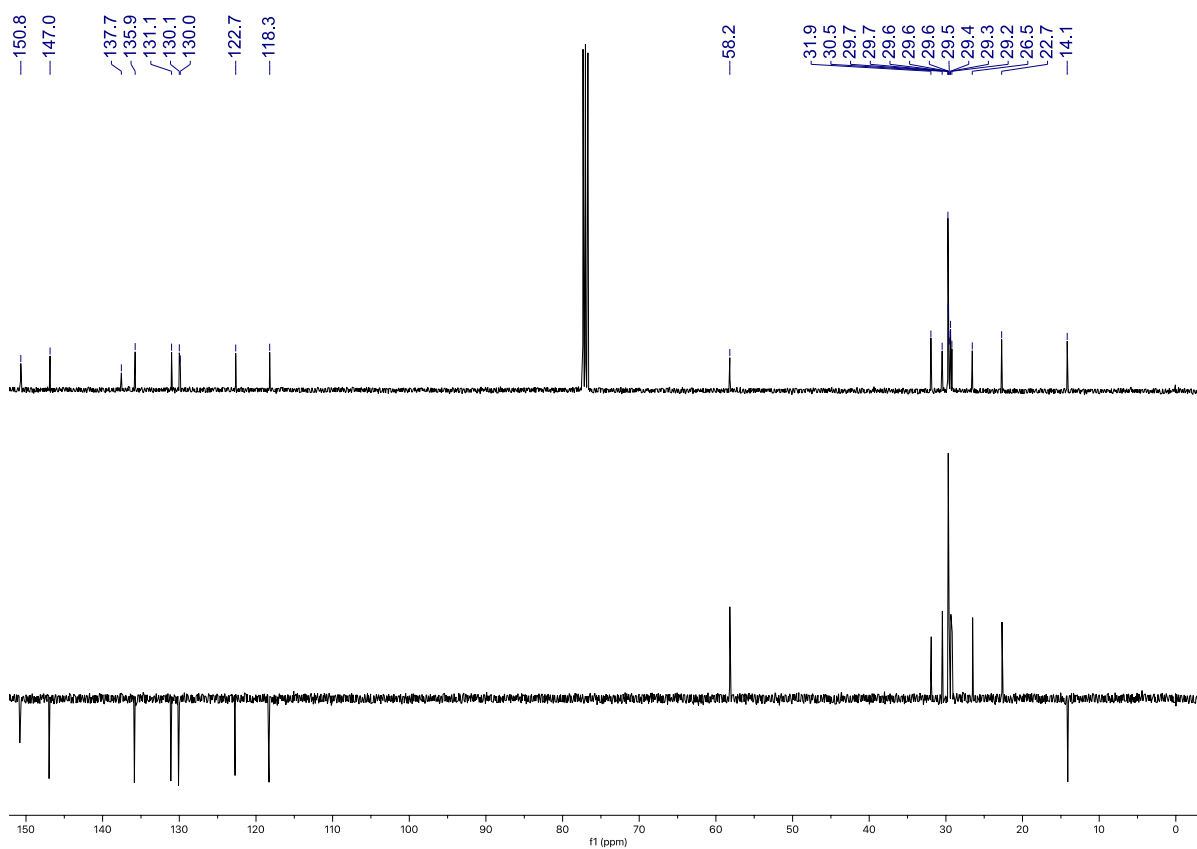
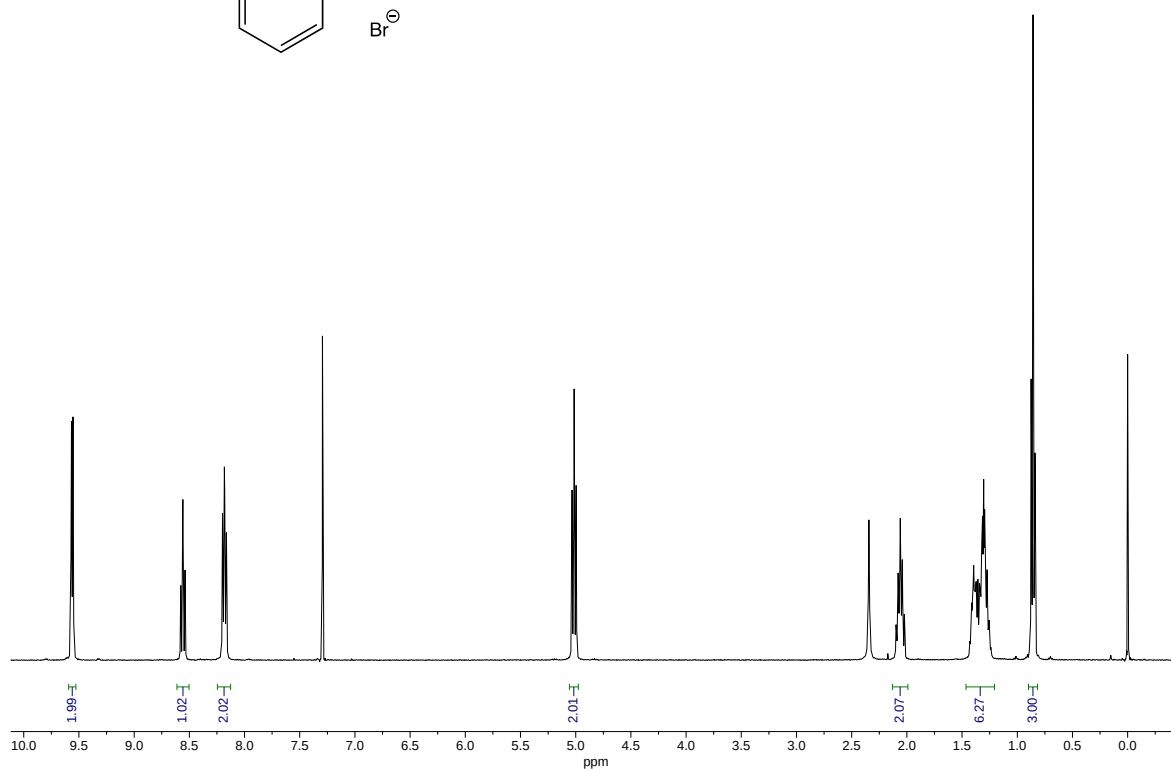
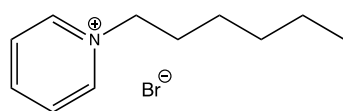


Figure S35. ¹H NMR (a), ¹³C NMR and DEPT135 (b) spectra of compound 5g.

a)



b)

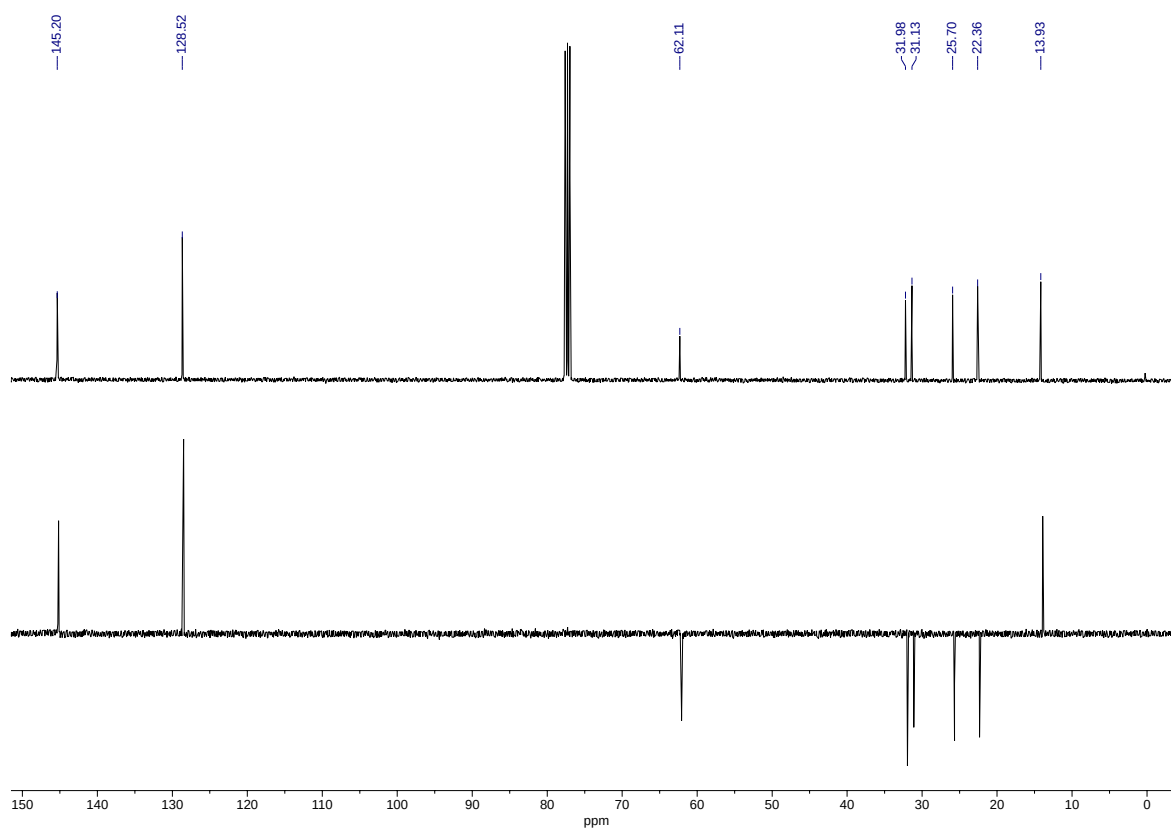
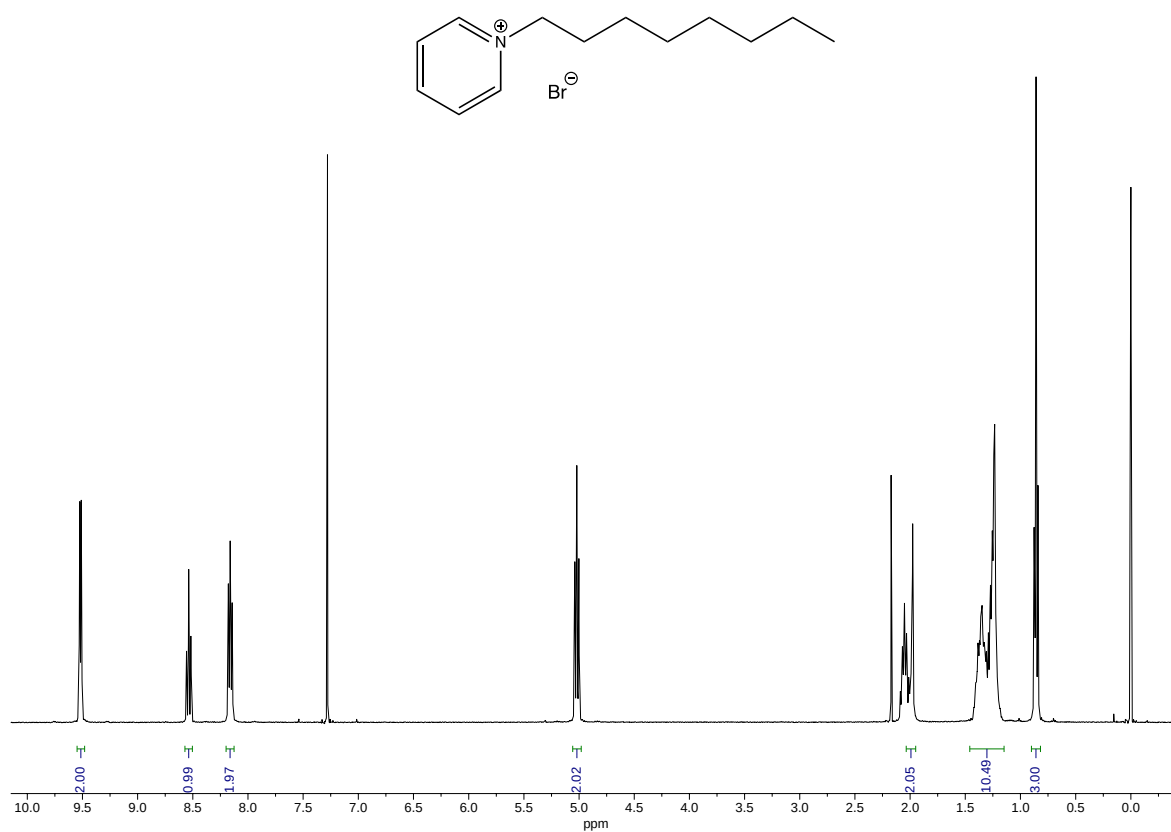


Figure S36. ¹H NMR (a), ¹³C NMR and DEPT135 (b) spectra of compound 6a.

a)



b)

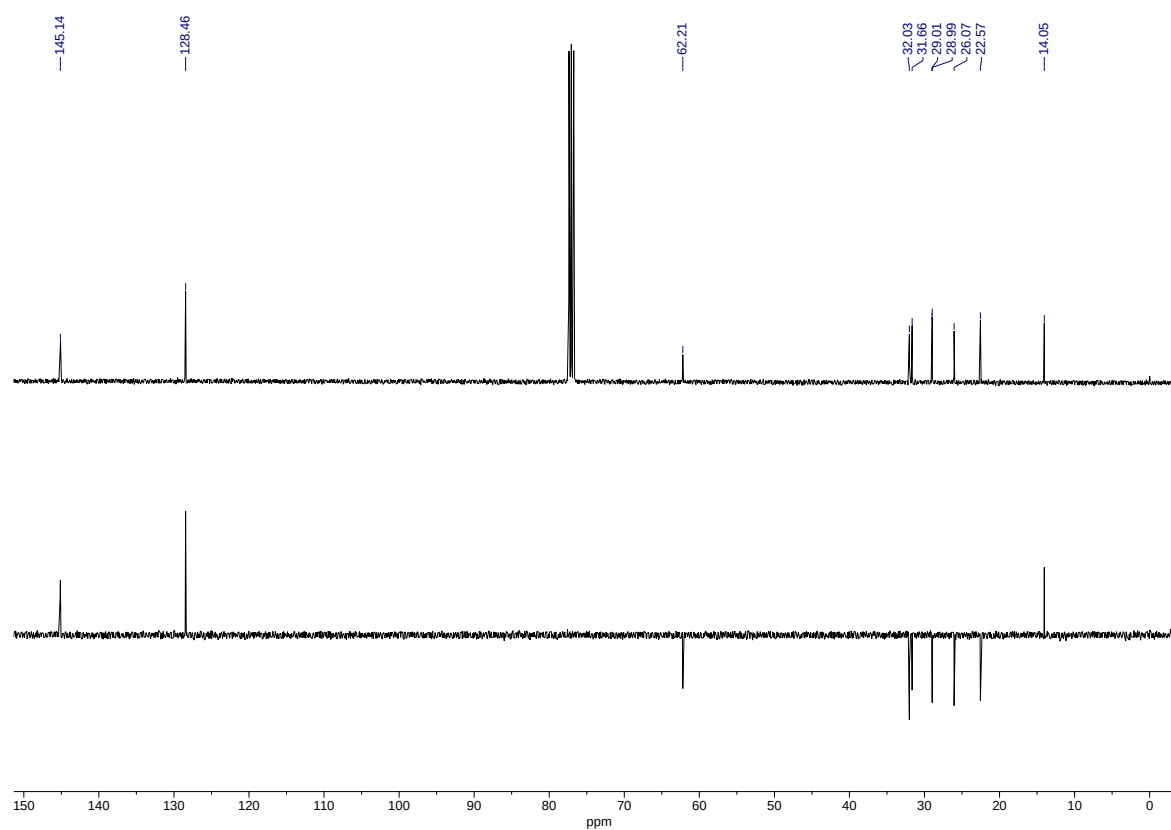
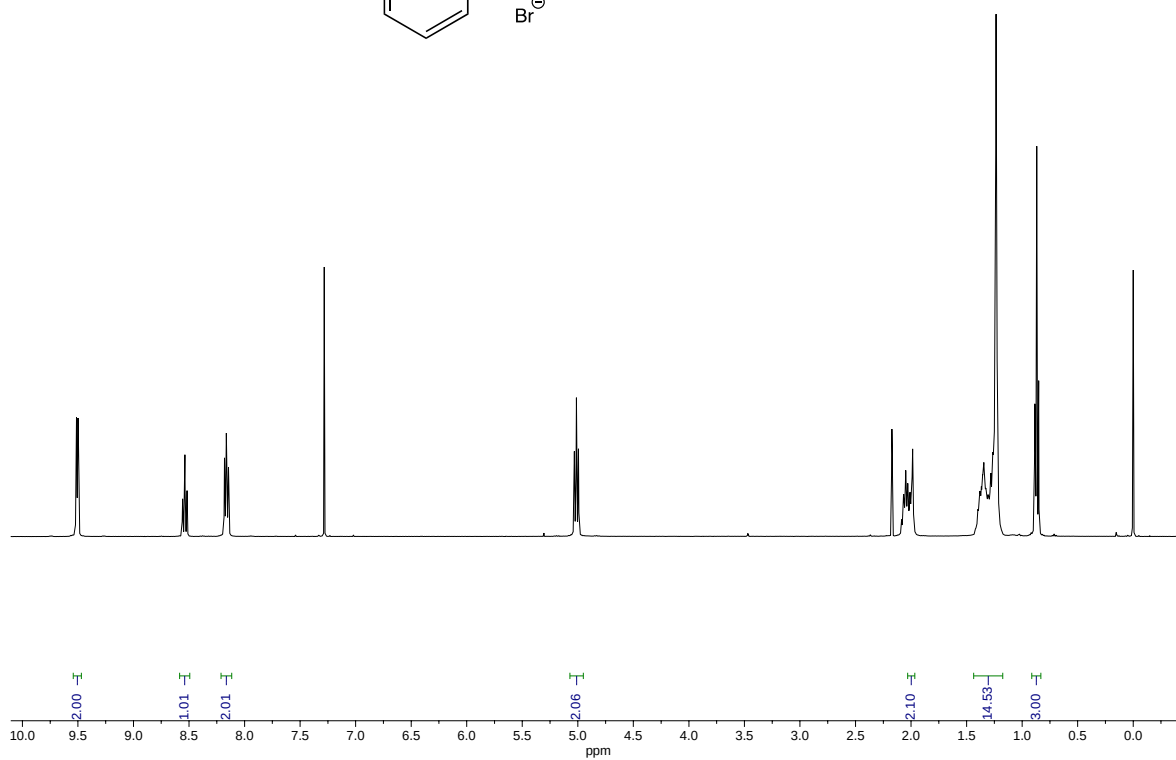
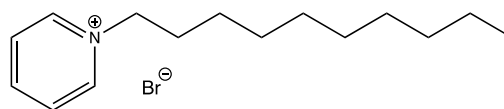


Figure S37. ¹H NMR (a), ¹³C NMR and DEPT135 (b) spectra of compound **6b**.

a)



b)

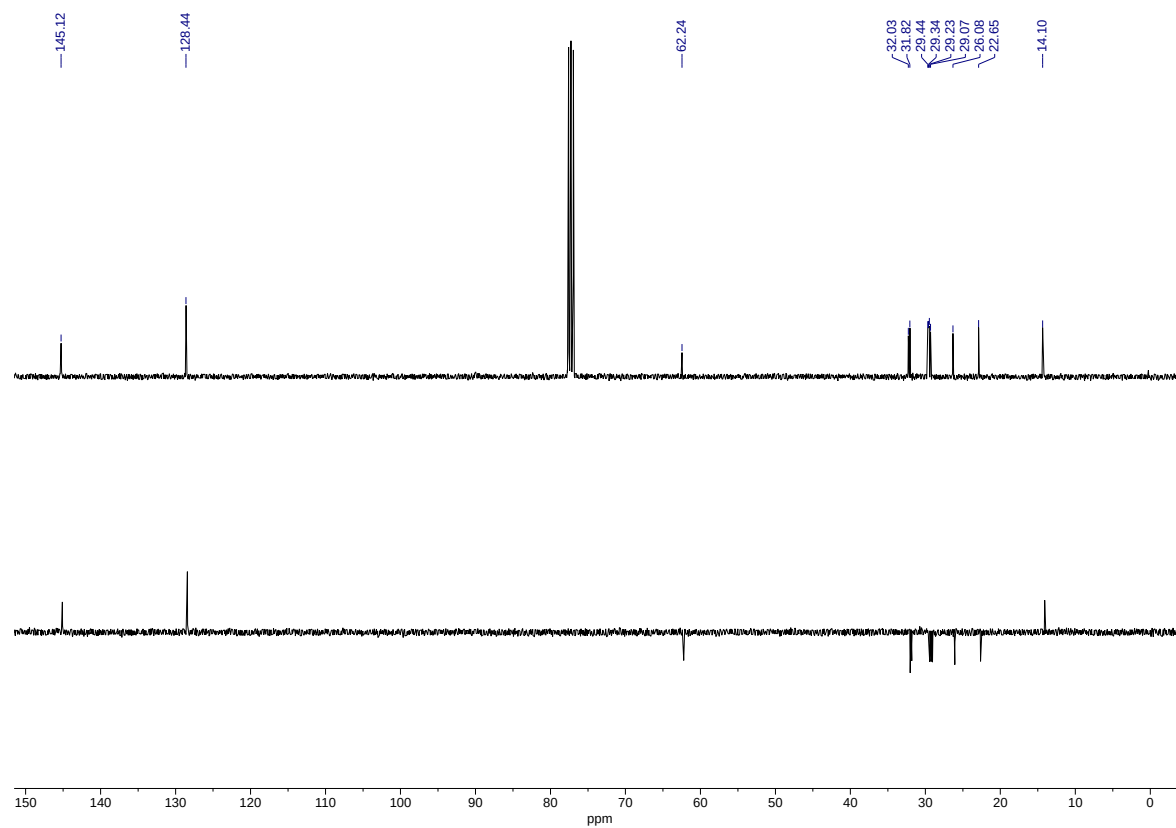
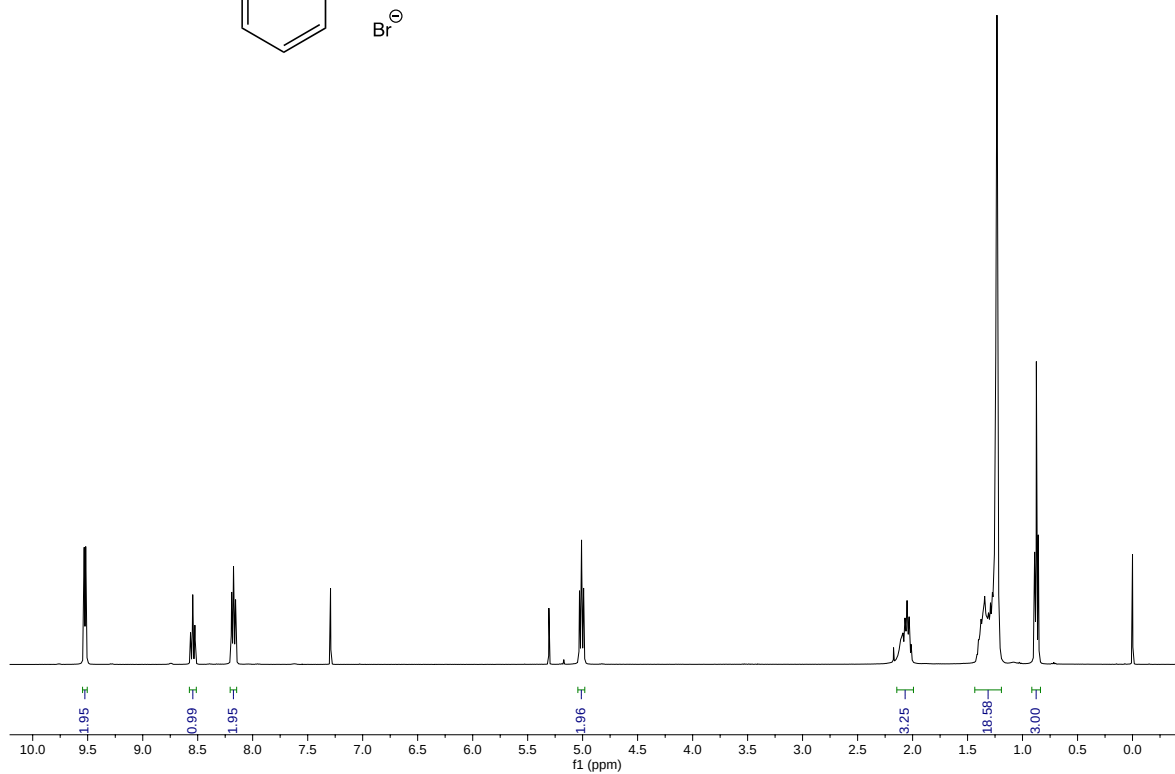
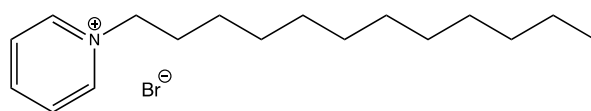


Figure S38. ^1H NMR (a), ^{13}C NMR and DEPT135 (b) spectra of compound **6c**.

a)



b)

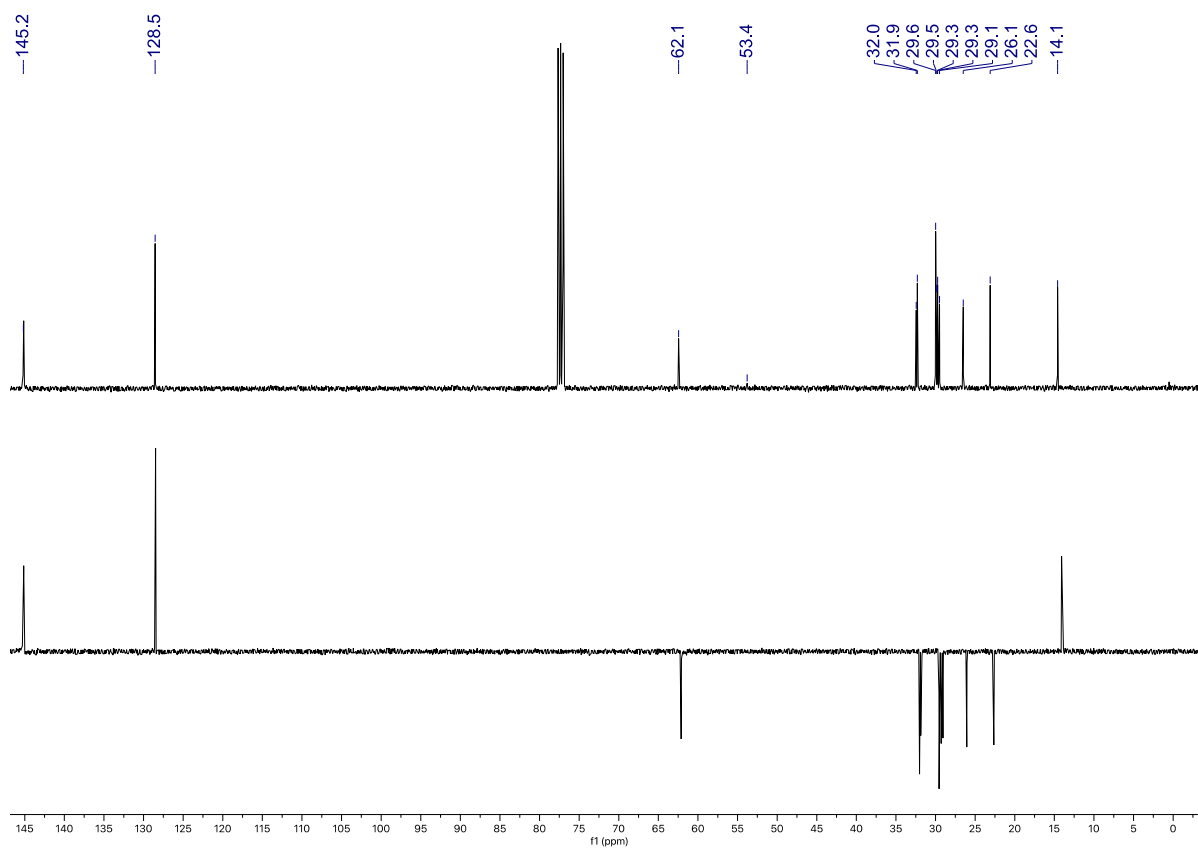
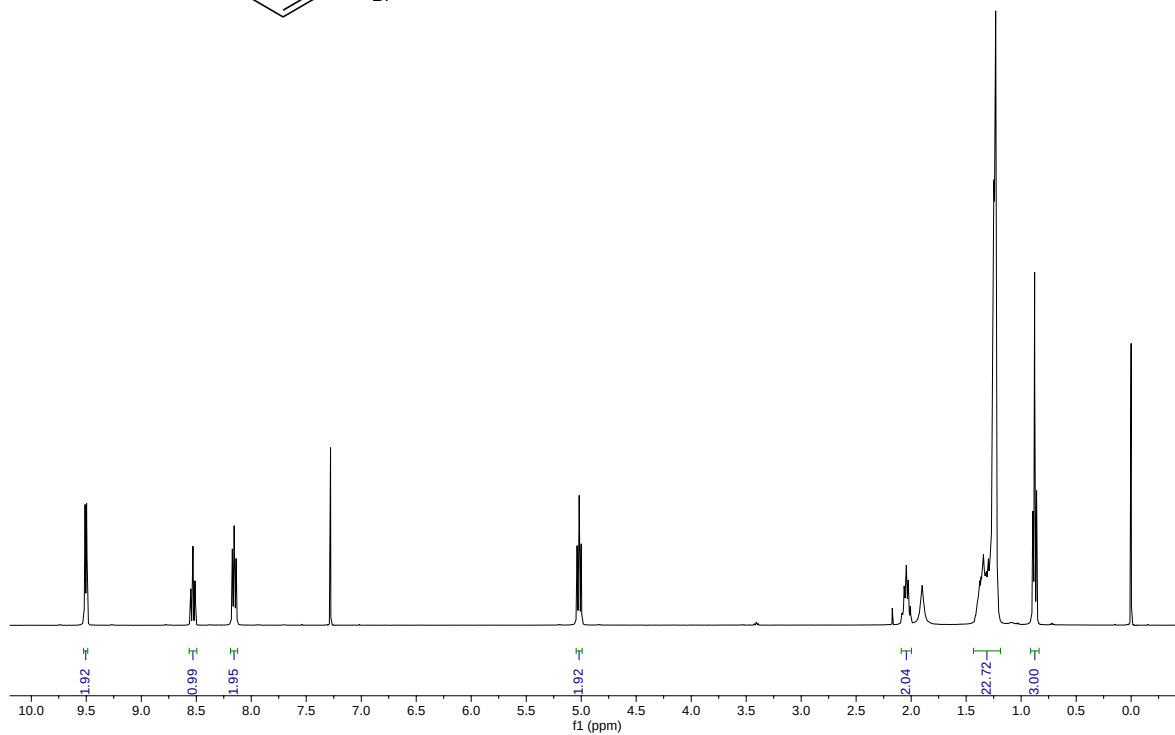
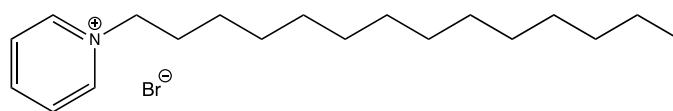


Figure S39. ^1H NMR (a), ^{13}C NMR and DEPT135 (b) spectra of compound **6d**.

a)



b)

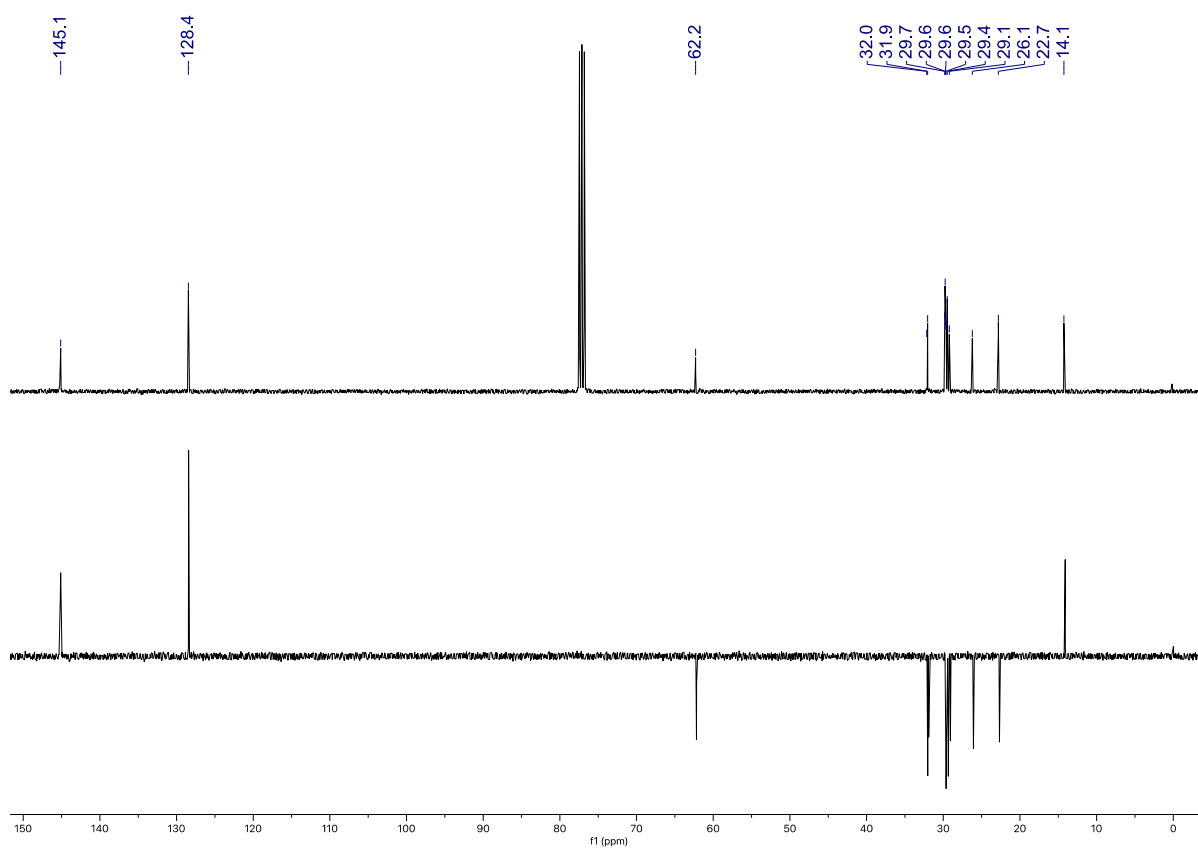


Figure S40. ^1H NMR (a), ^{13}C NMR and DEPT135 (b) spectra of compound **6e**.

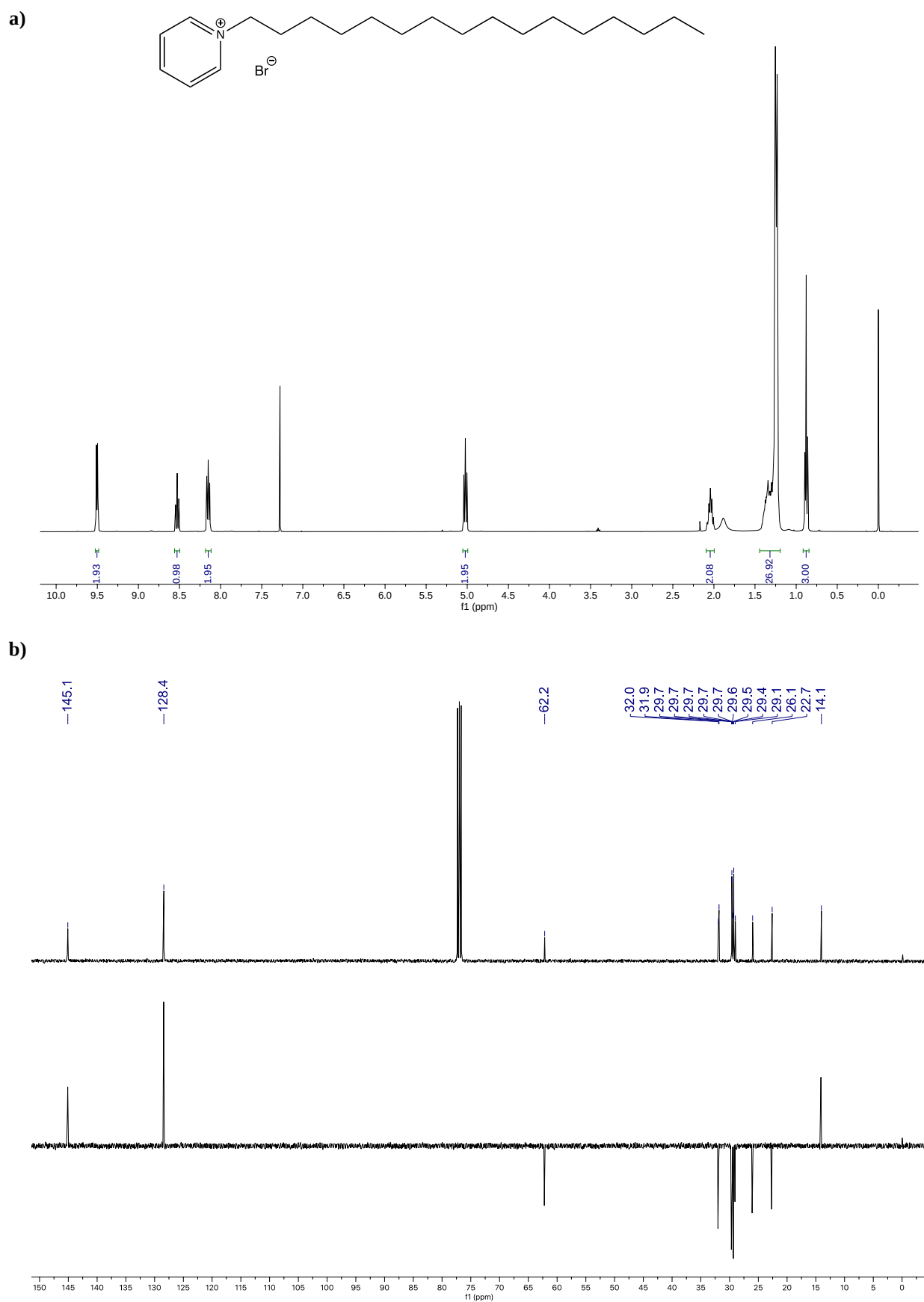
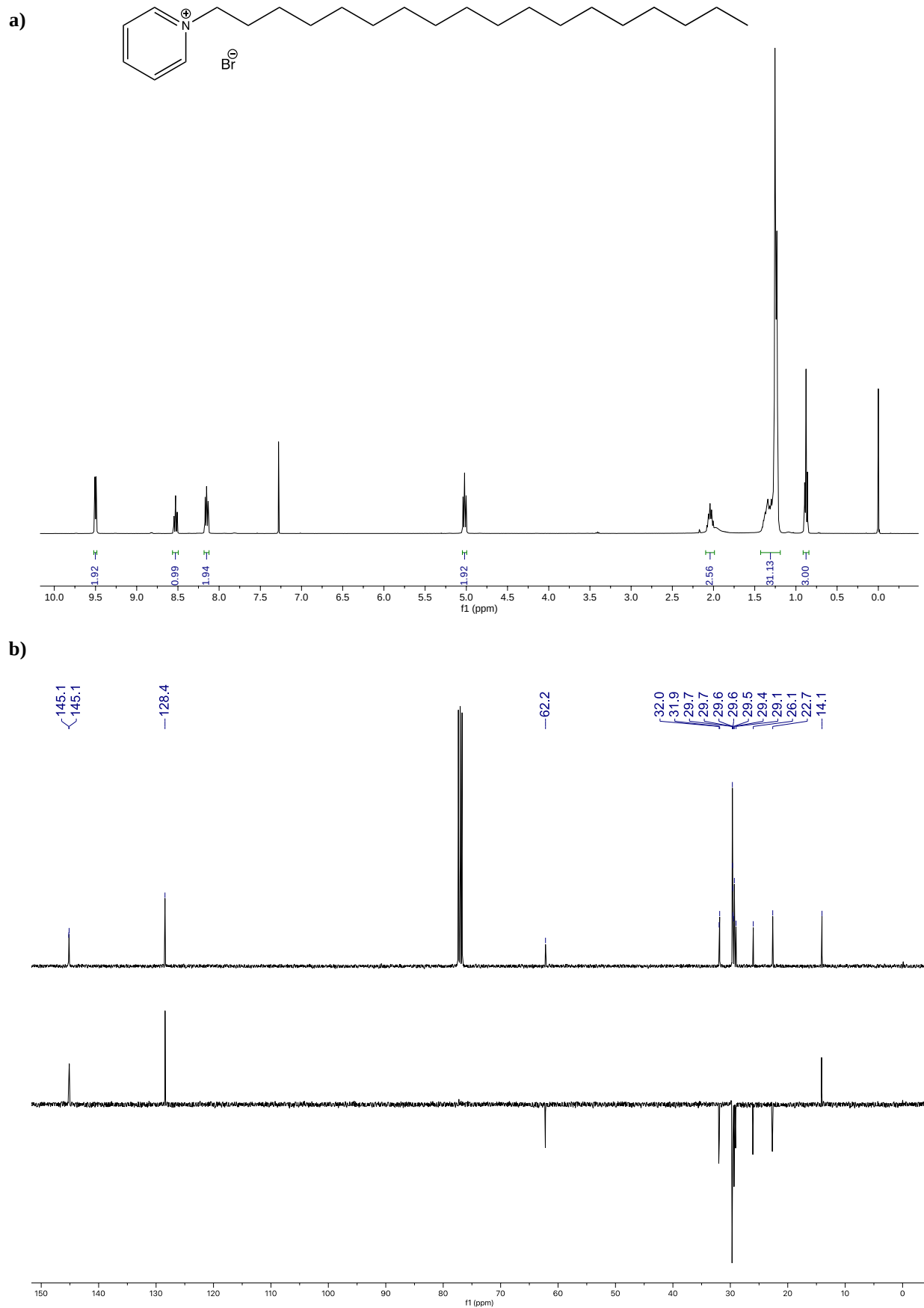
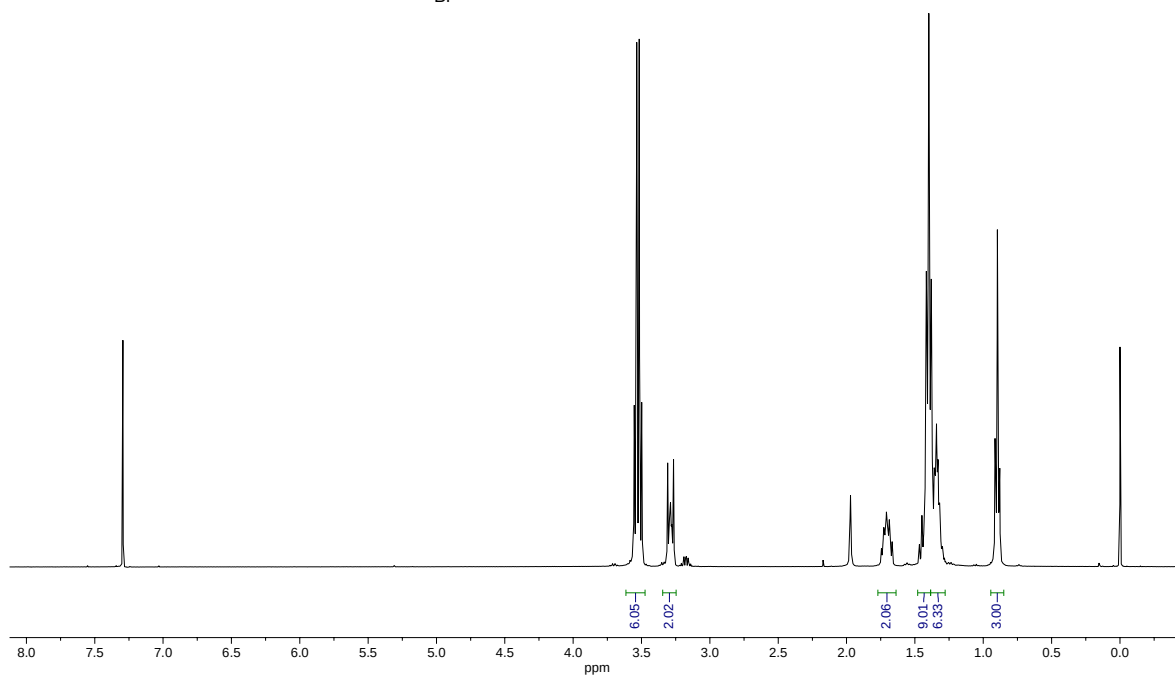
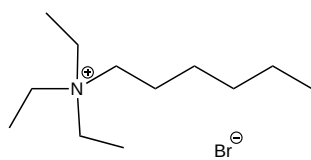


Figure S41. ¹H NMR (a), ¹³C NMR and DEPT135 (b) spectra of compound 6f.



a)



b)

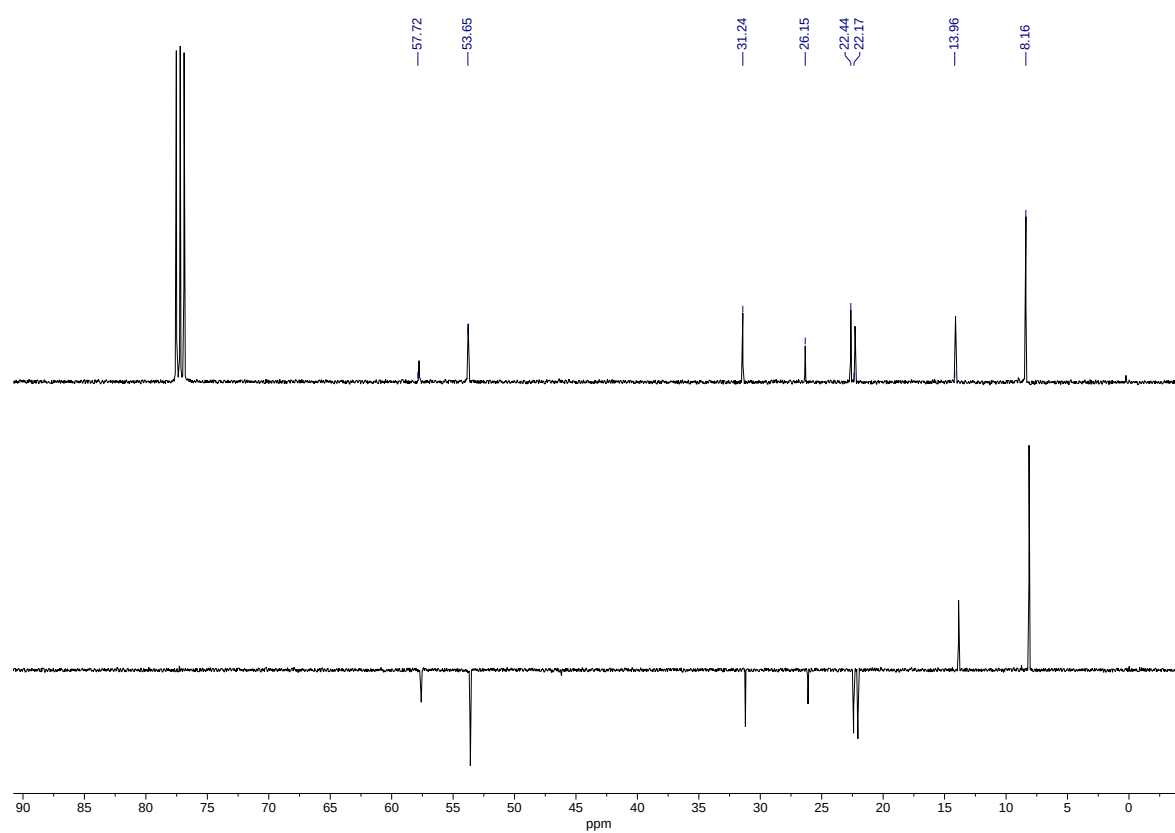
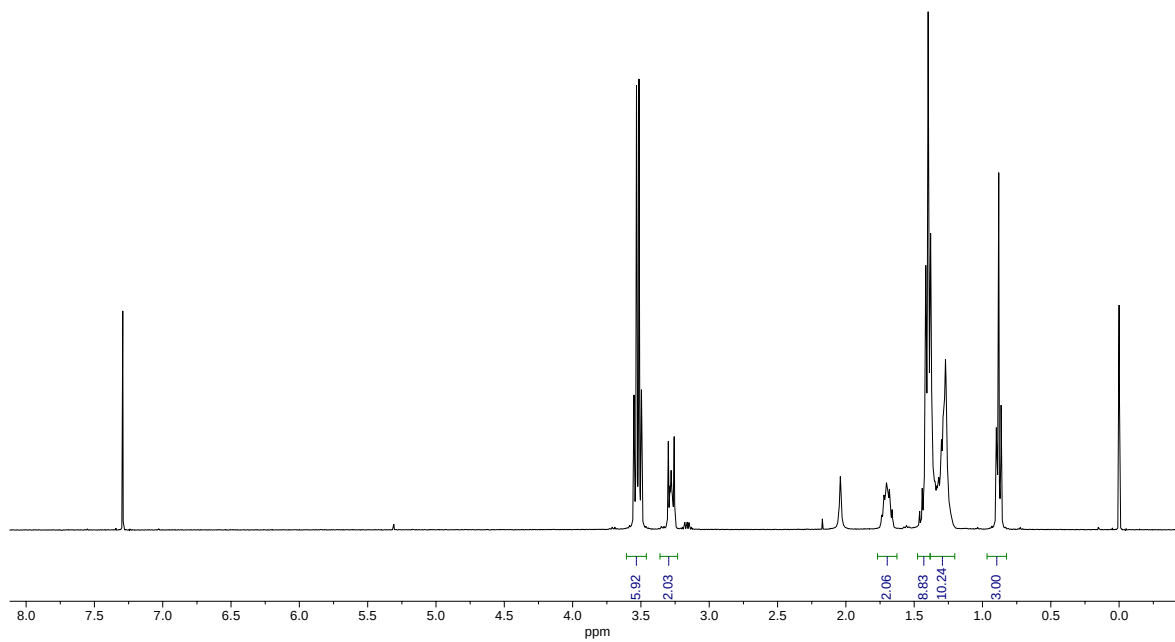
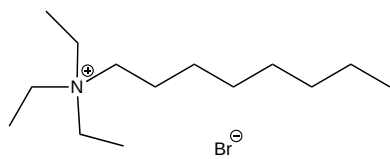


Figure S43. ^1H NMR (a), ^{13}C NMR and DEPT135 (b) spectra of compound **7a**.

a)



b)

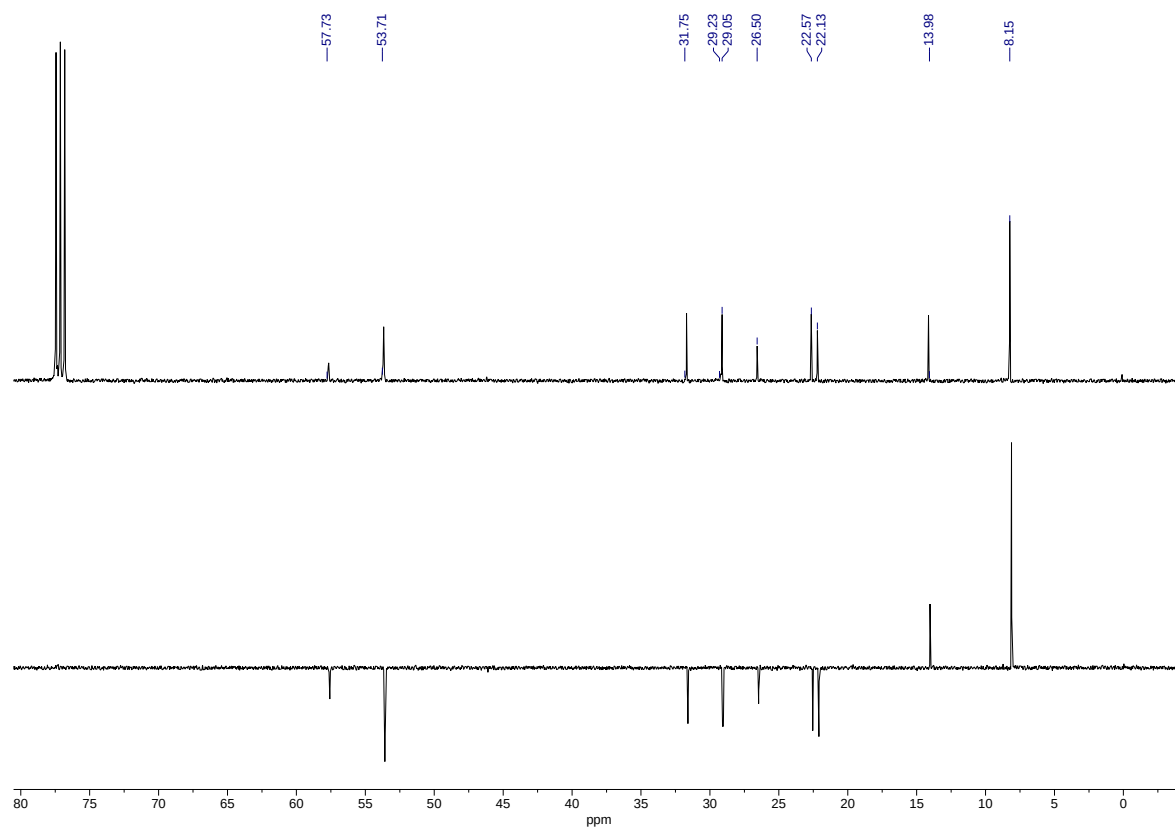


Figure S44. ¹H NMR (a), ¹³C NMR and DEPT135 (b) spectra of compound **7b**.

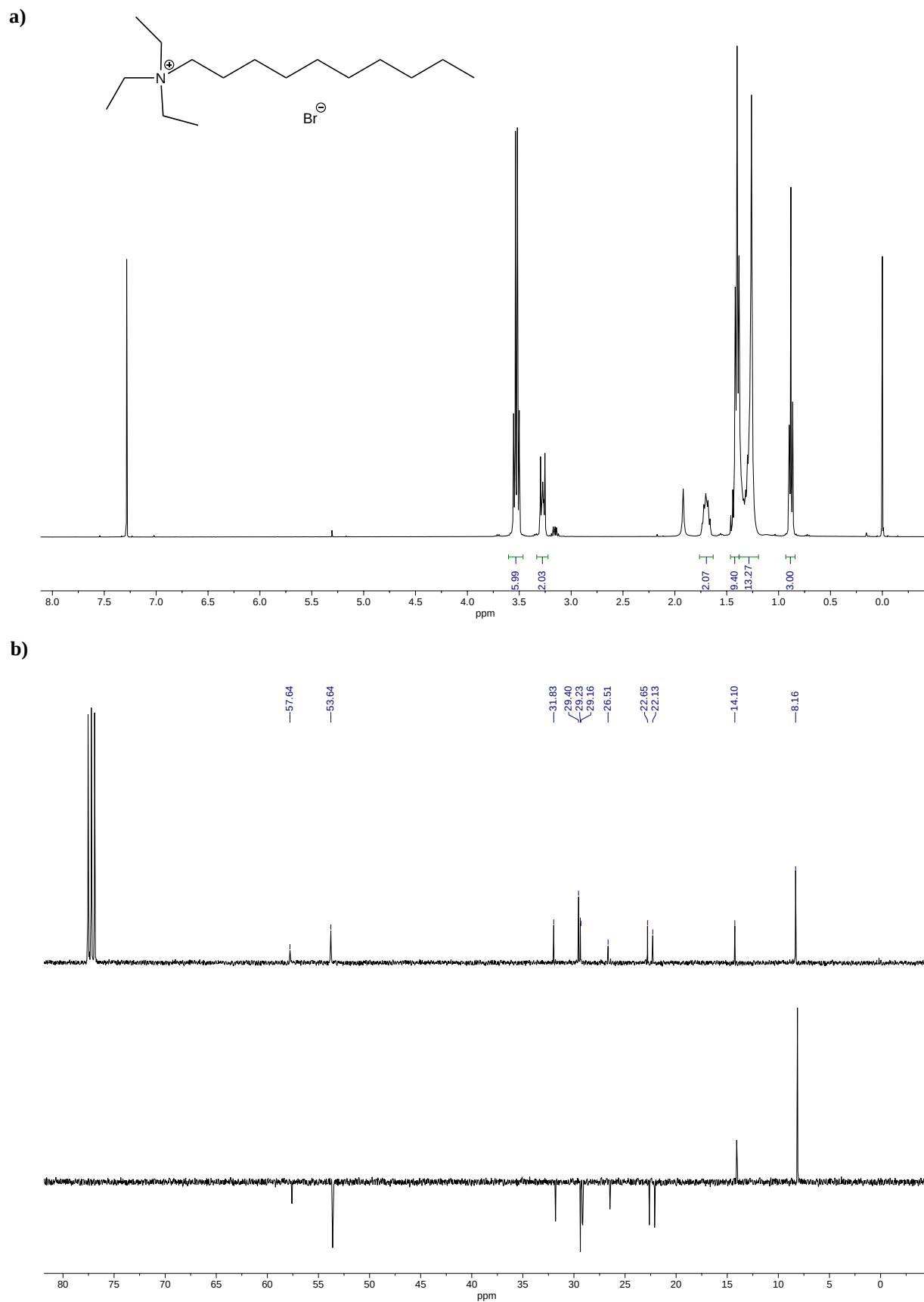
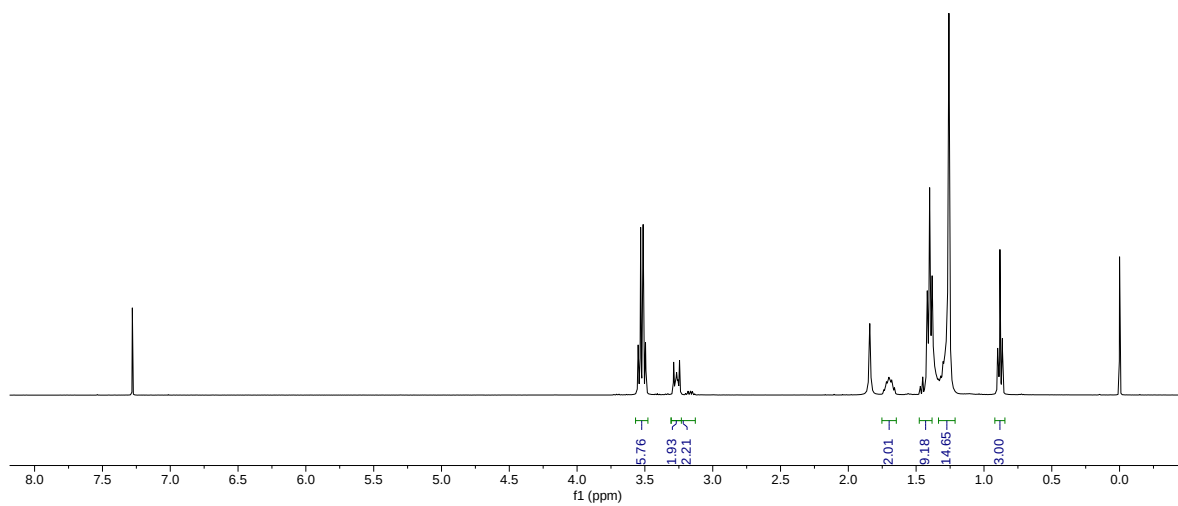
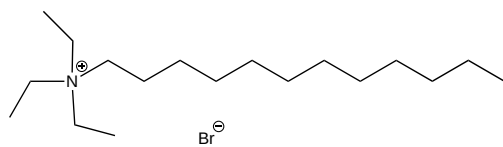


Figure S45. ^1H NMR (a), ^{13}C NMR and DEPT135 (b) spectra of compound 7c.

a)



b)

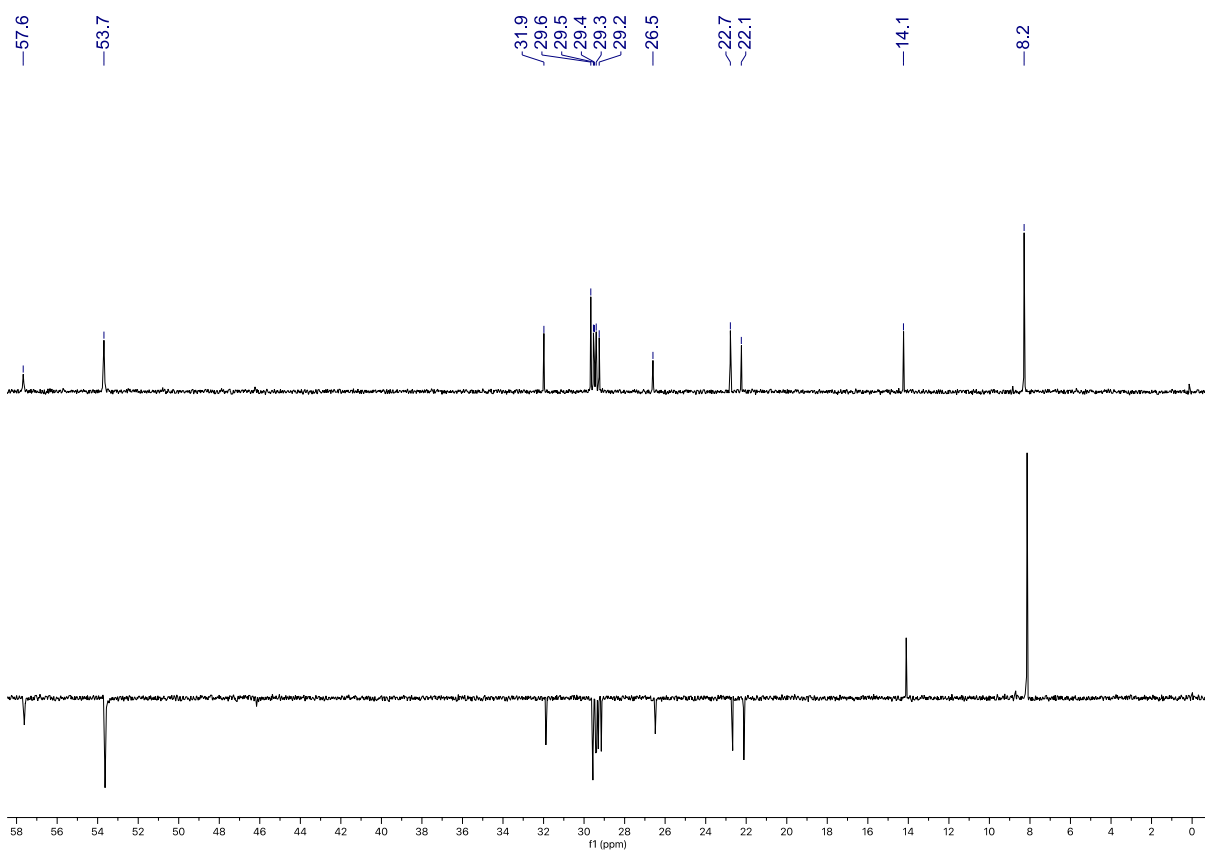
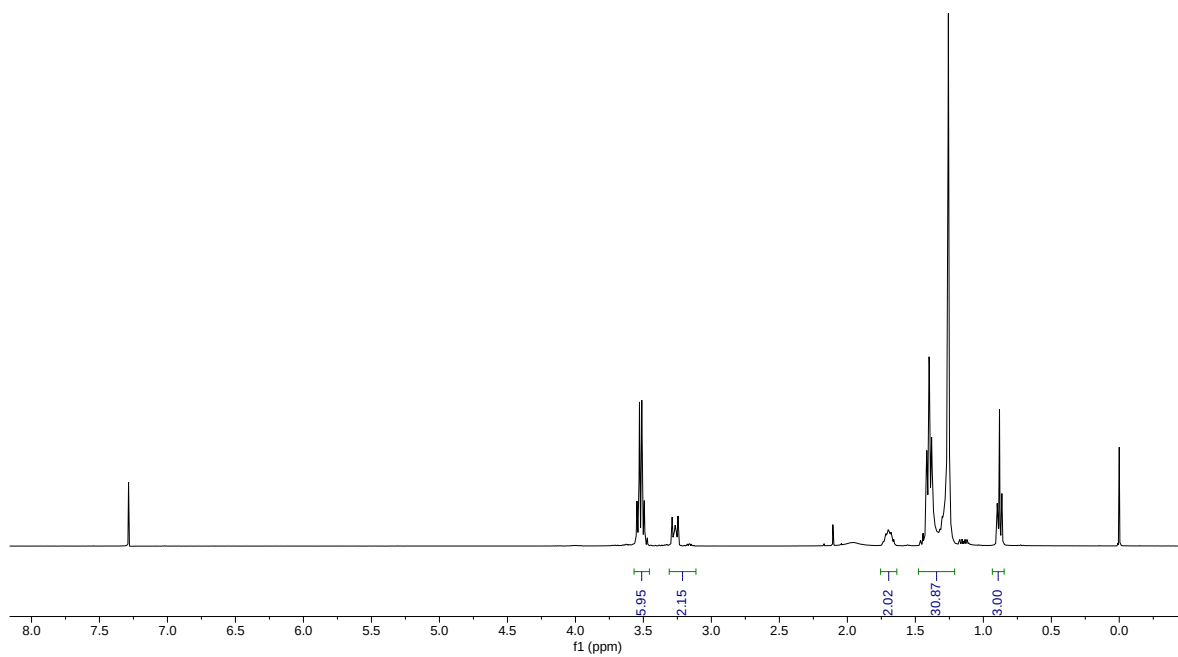
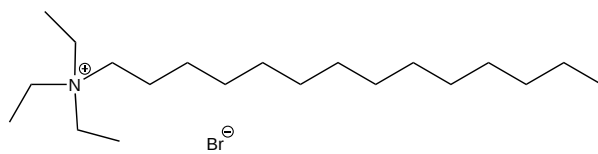


Figure S46. ^1H NMR (a), ^{13}C NMR and DEPT135 (b) spectra of compound 7d.

a)



b)

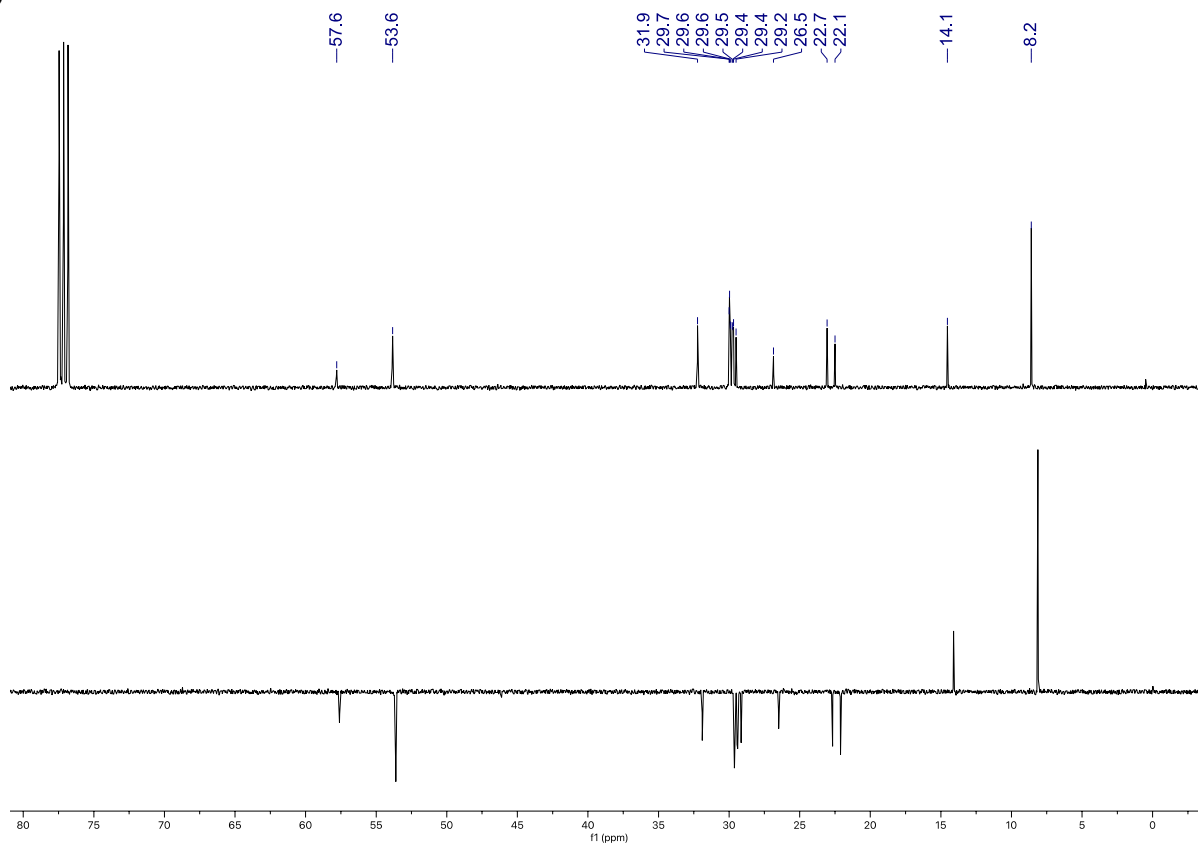


Figure S47. ^1H NMR (a), ^{13}C NMR and DEPT135 (b) spectra of compound **7e**.

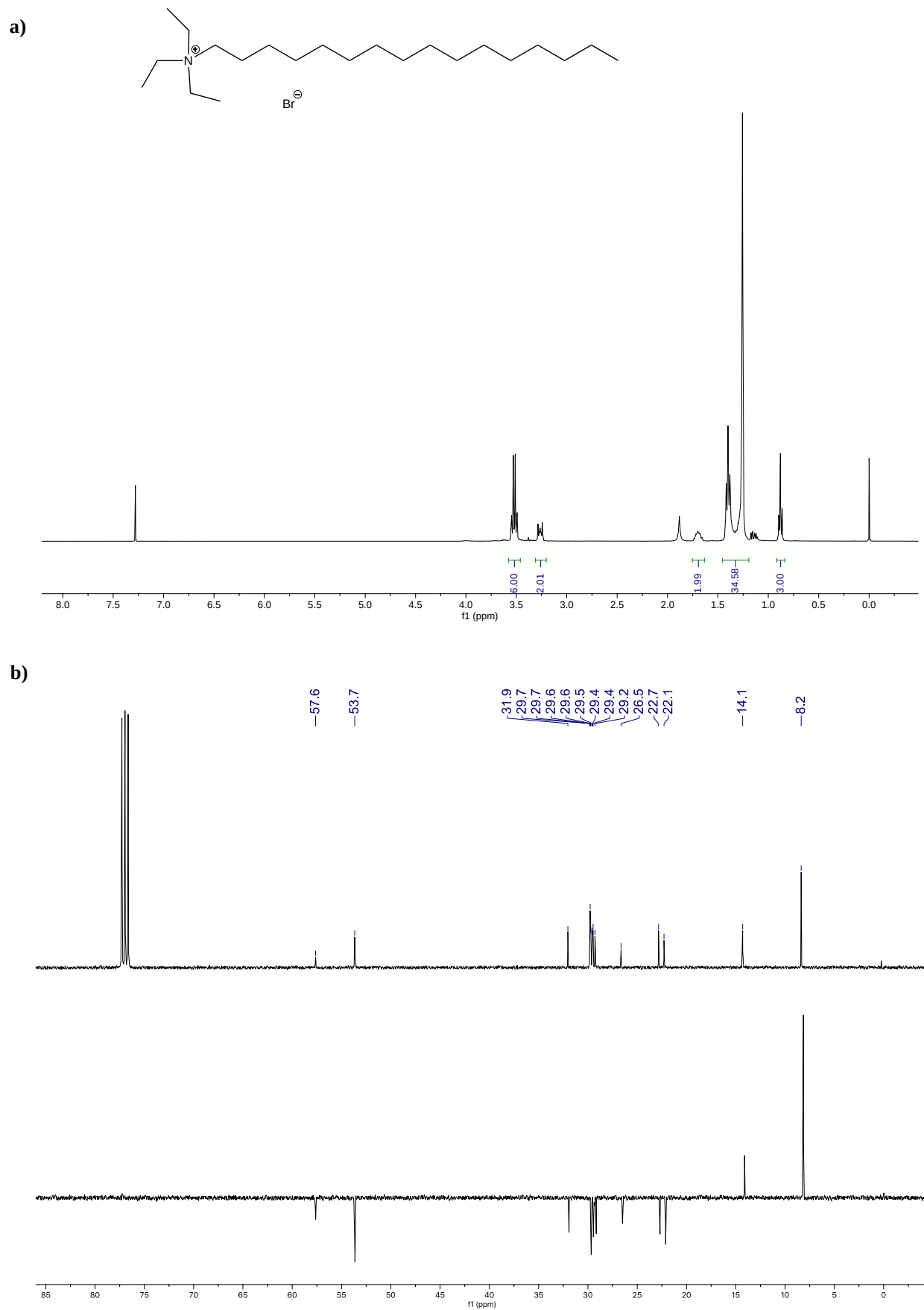
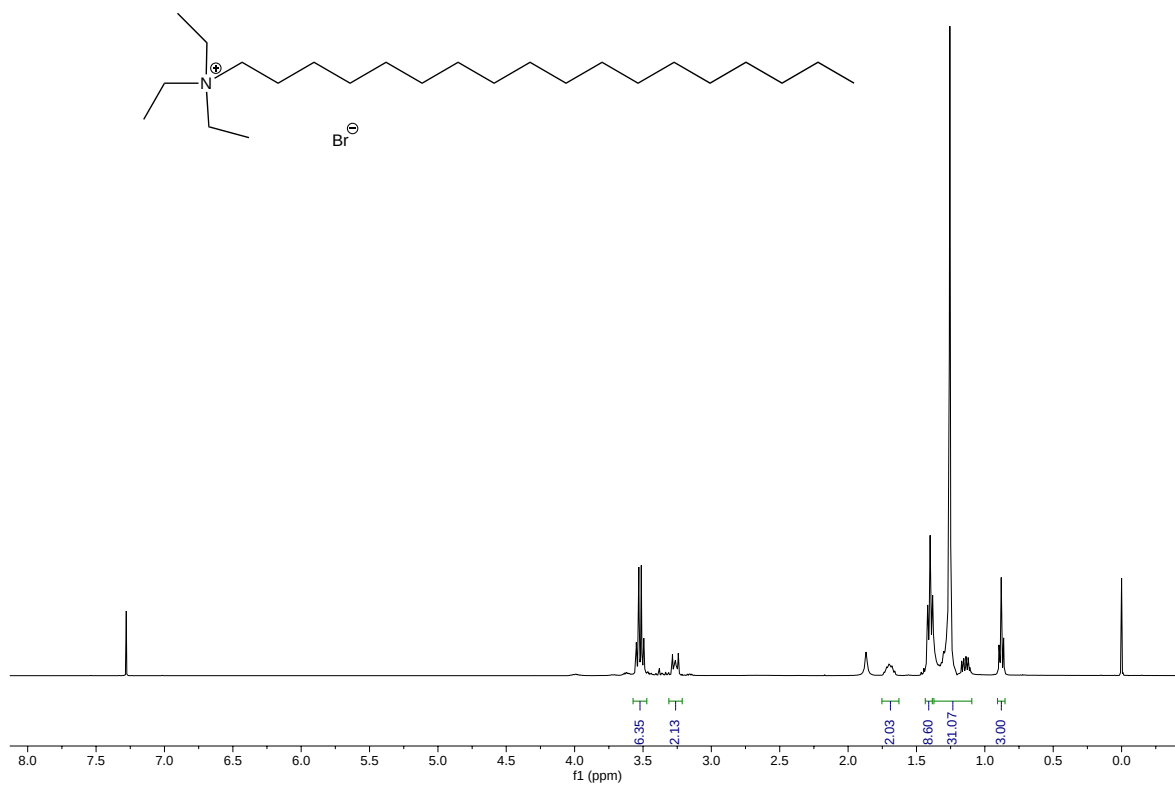


Figure S48. ¹H NMR (a), ¹³C NMR and DEPT135 (b) spectra of compound 7f.

a)



b)

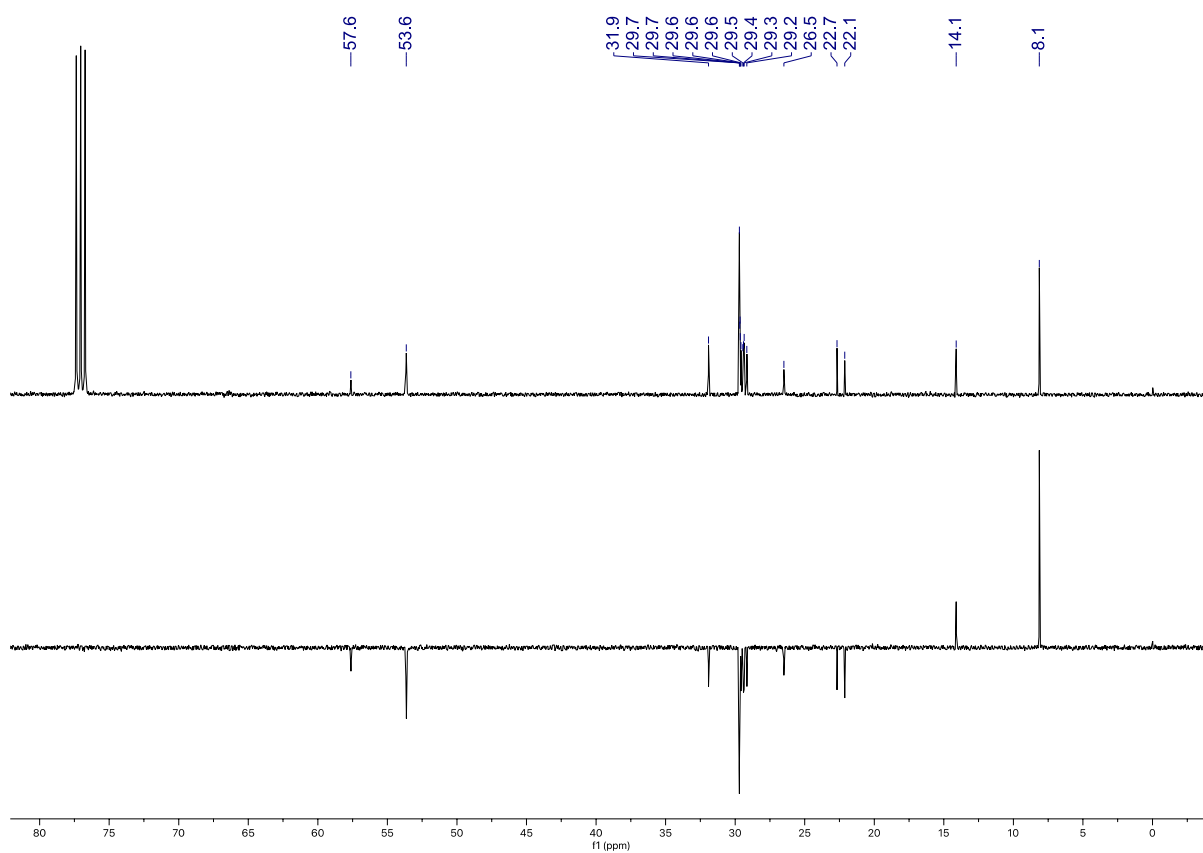


Figure S49. ¹H NMR (a), ¹³C NMR and DEPT135 (b) spectra of compound 7g.

1.2 Evaluation of the Chromatographic Hydrophobicity Index

Table S1. Retention times (t_R) of the standard mixture obtained by LC/UV at pH 2.6. CHI_0 values at pH 2.6.

Compound	t_R (min)	CHI_0 pH 2.6
Benzimidazole	4.141	6.300
Theophylline	4.532	17.90
Paracetamol	4.656	18.77
Caffeine	4.823	23.41
Colchicine	5.792	43.90
Carbamazepine	6.434	60.42
Indole	7.076	72.10
Propiophenone	7.421	77.40
Butyrophenone	7.901	87.30
Valerophenone	8.326	96.40
Heptanophenone	9.092	112.1

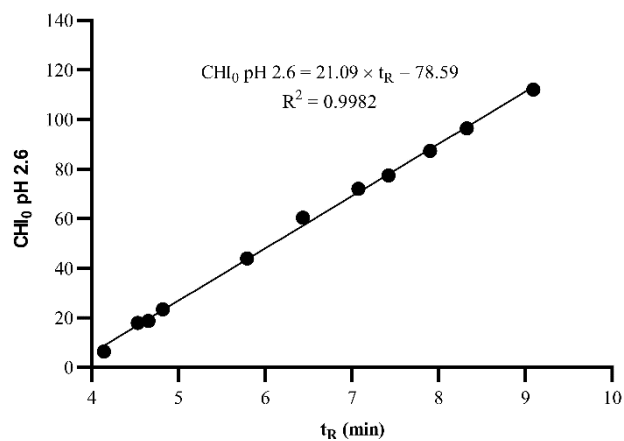


Figure S50. Linear correlation obtained by plotting the retention times (t_R) of each of the individual standard mixture compounds against the CHI values at pH 2.6 (CHI_0).