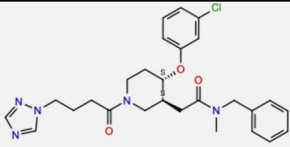
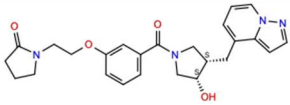
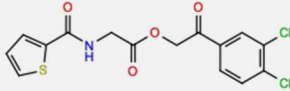
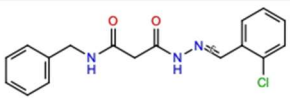
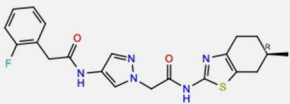
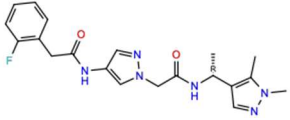
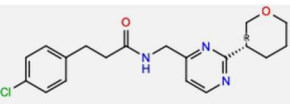


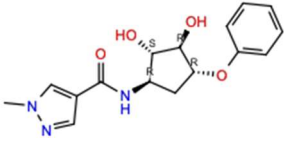
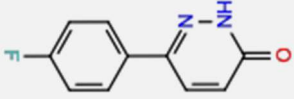
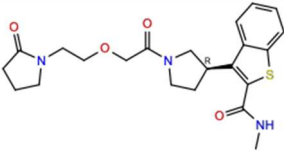
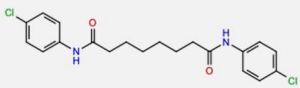
Supporting information

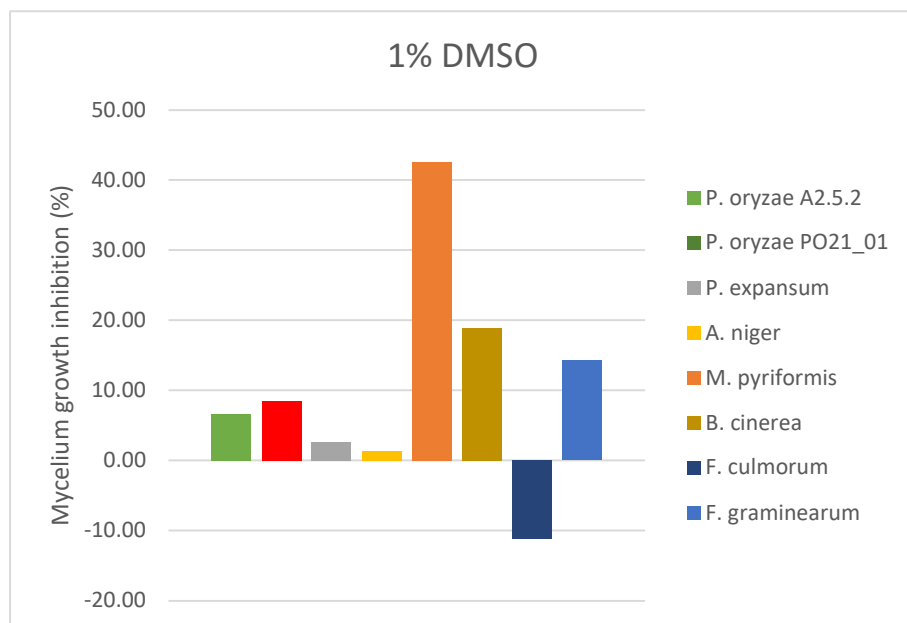
Exploration of novel scaffolds targeting cytochrome *b* of *Pyricularia oryzae*

Cecilia Pinna^{1†}, Tommaso Laurenzi^{2†}, Fabio Forlani¹, Luca Palazzolo², Claire Beatrice Nolan¹, Michael S. Christodoulou¹, Paolo Cortesi¹, Andrea Pinto¹, Ivano Eberini^{2,3*}, Andrea Kunova^{1*}, and Sabrina Dallavalle¹

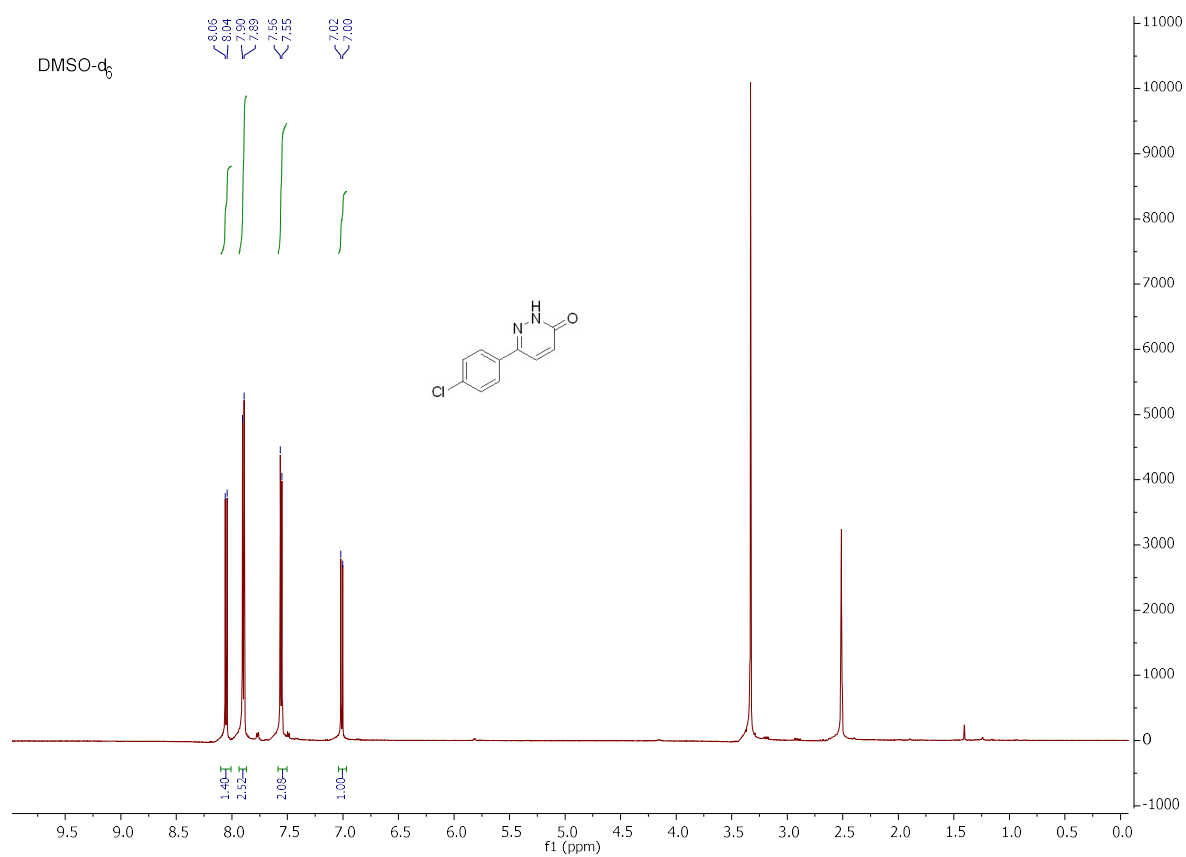
Supplementary Table S1. Compounds selected after high-throughput virtual screening (HTVS) and interaction fingerprint clustering (SIFT)

Title	XPGscore [Kcal/mol]	mw	XPGscore/m w	Interactions
 BioDesign:122364	-12.91	510.03	-0.025	-Glu273 H-bond
 BioDesign:88775	-11.73	448.52	-0.026	-Glu273 H-bond -Met296 H-bond
 Agrochem:9387	-11.10	372.22	-0.029	-Glu273 H-bond -Tyr280 $\pi-\pi$ stacking
 Agrochem:6989_mod	-10.08	329.79	-0.031	-Glu273 H-bond -Tyr280 $\pi-\pi$ stacking
 Biodesign:7778	-11.44	427.5	-0.027	-Glu273 H-bond -Tyr275 H-bond -Tyr280 $\pi-\pi$ stacking
 Biodesign:7763	-10.90	398.44	-0.027	-Glu273 H-bond -Met125 H-bond -Tyr279 $\pi-\pi$ stacking -Tyr280 $\pi-\pi$ stacking
 Biodesign:61594	-10.80	359.85	-0.030	-Tyr275 H-bond

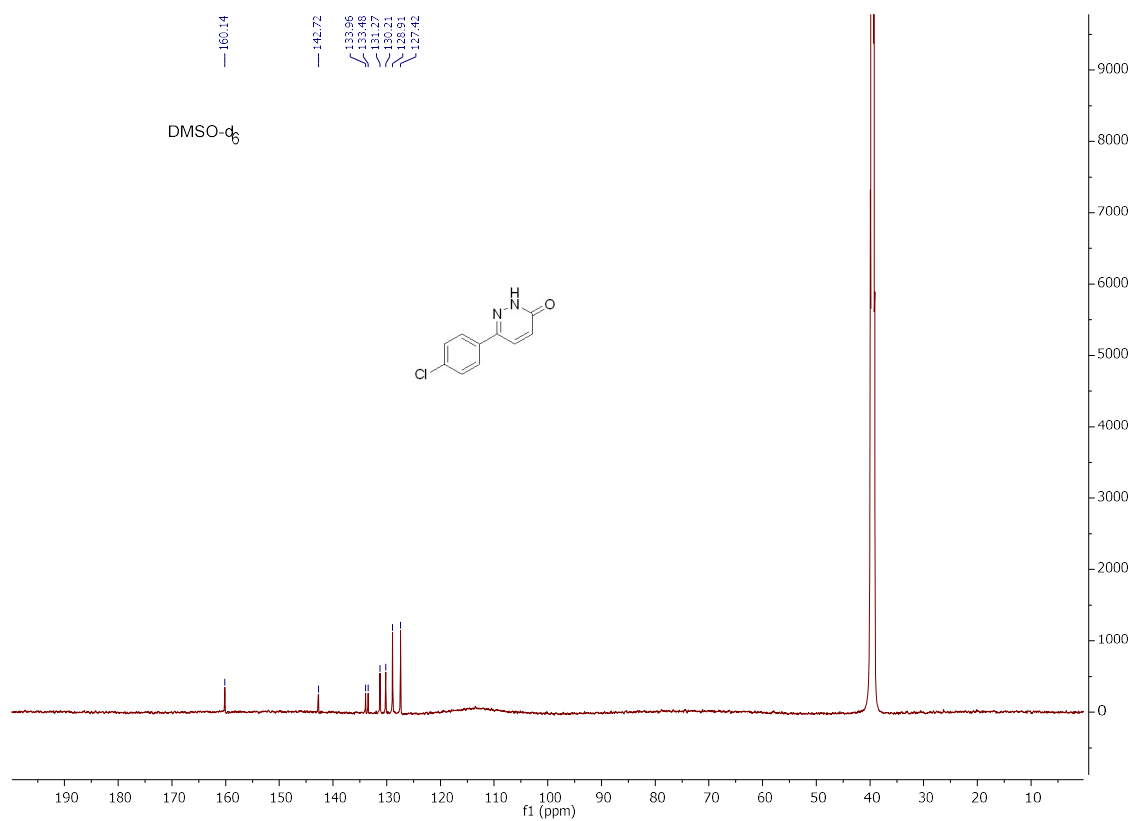
	-10.56	317.34	-0.033	-Glu273 H-bond -Tyr275 H-bond
Biodesign:101550				
	-10.22	190.18	-0.054	-Tyr132 π - π stacking -Tyr275 H-bond
Biodesign:1678				
	-11.35	429.53	-0.026	-Glu273 H-bond
Biodesign:14185				
	-10.83	393.31	-0.028	-Glu273 H-bond -Phe279 π - π stacking
Agrochem:6151				



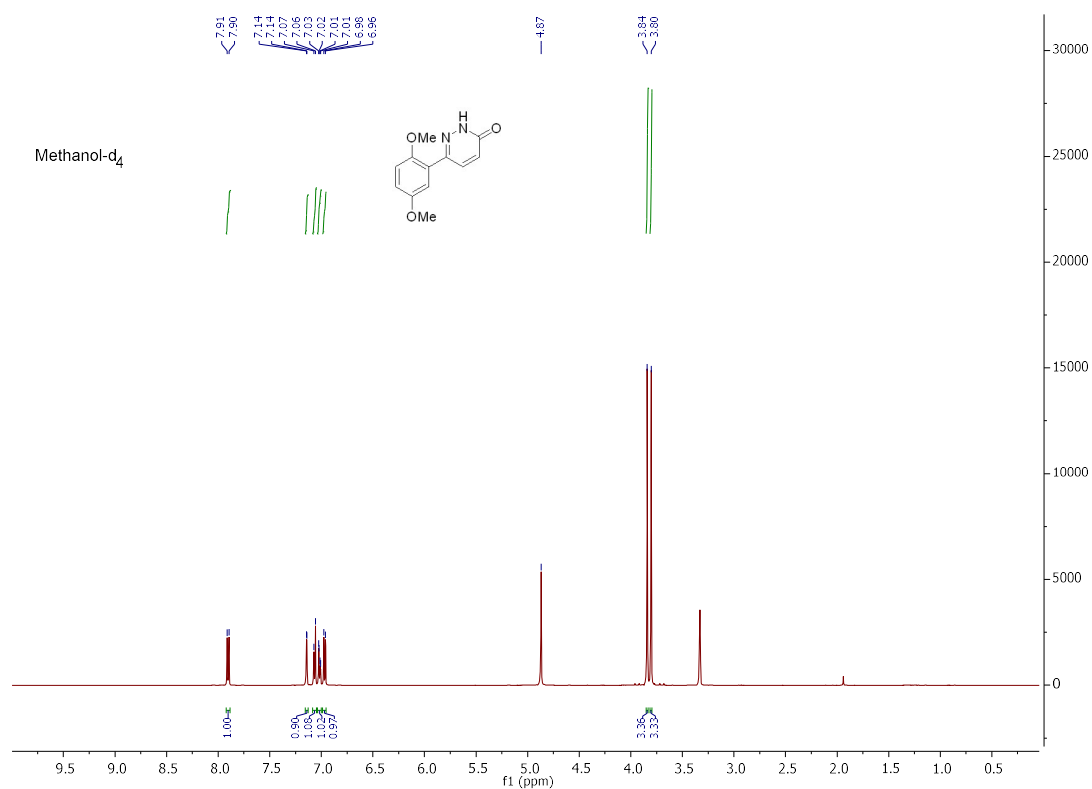
Supplementary Figure S1. Inhibition of mycelium growth of diverse fungi by 1% DMSO.



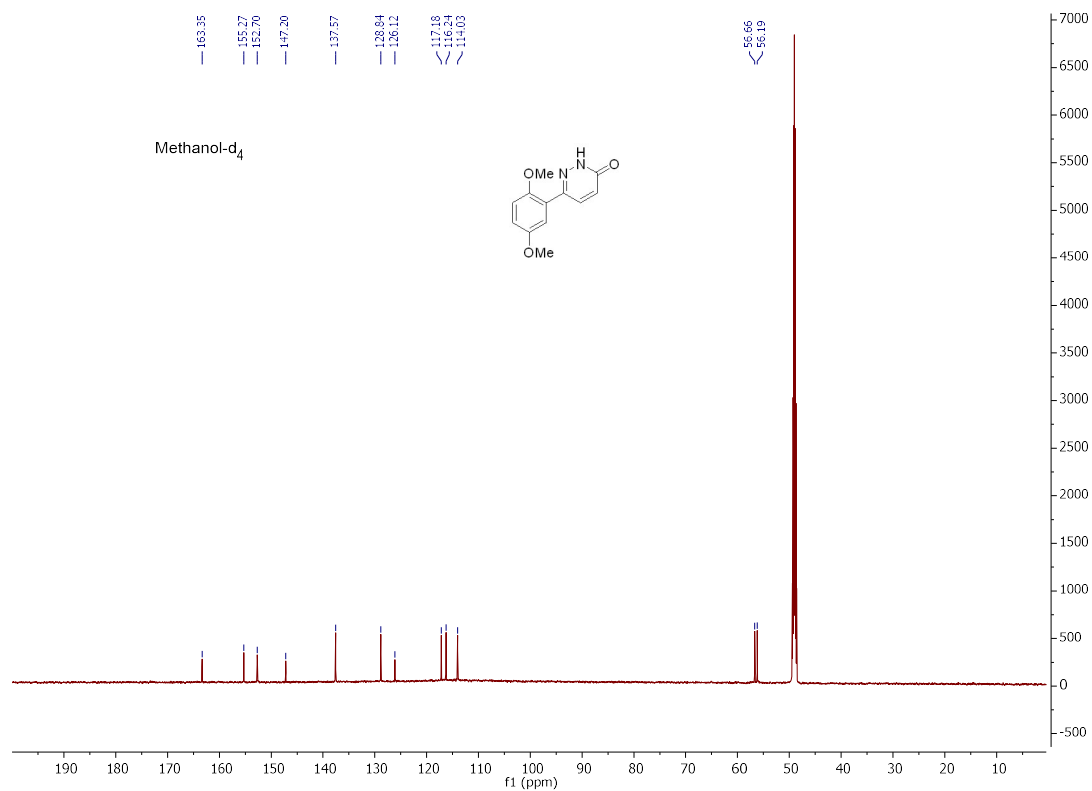
Supplementary Figure S4. ^1H -NMR 1b.



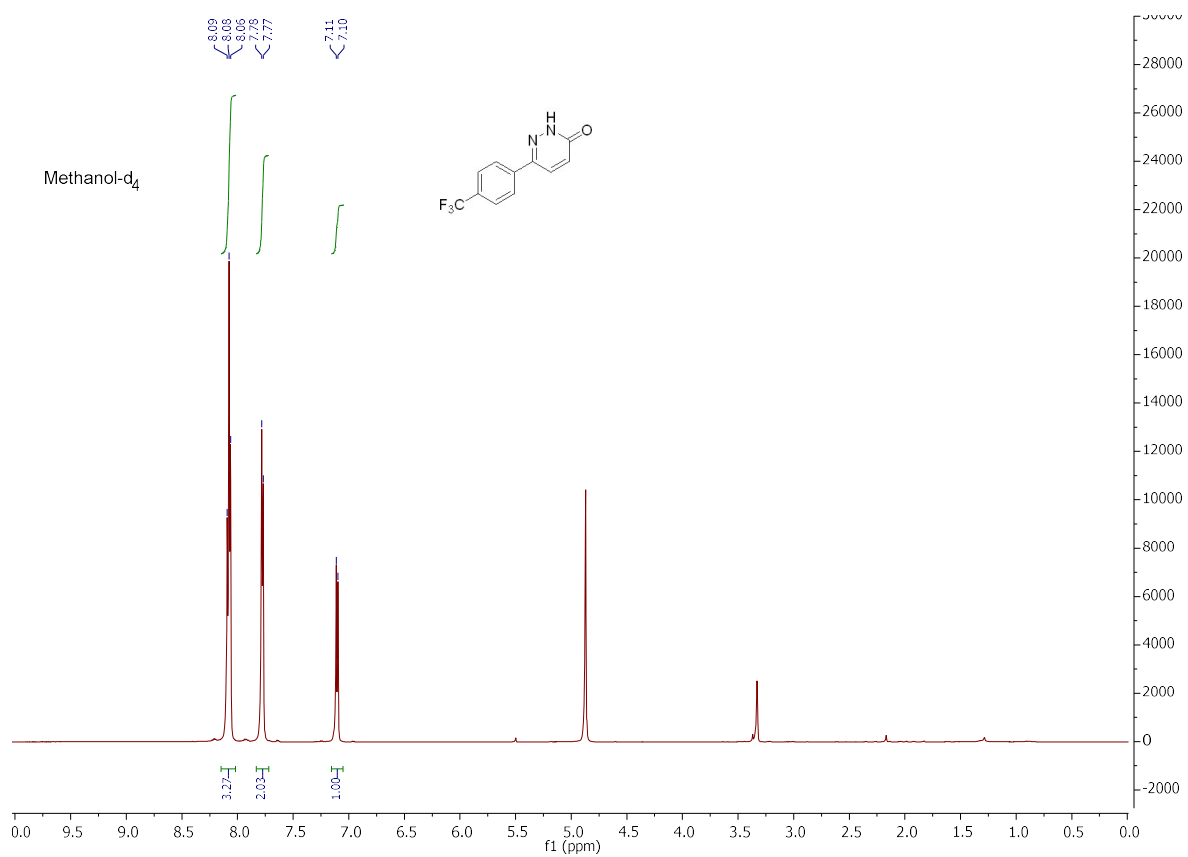
Supplementary Figure S5. ^{13}C -NMR 1b.



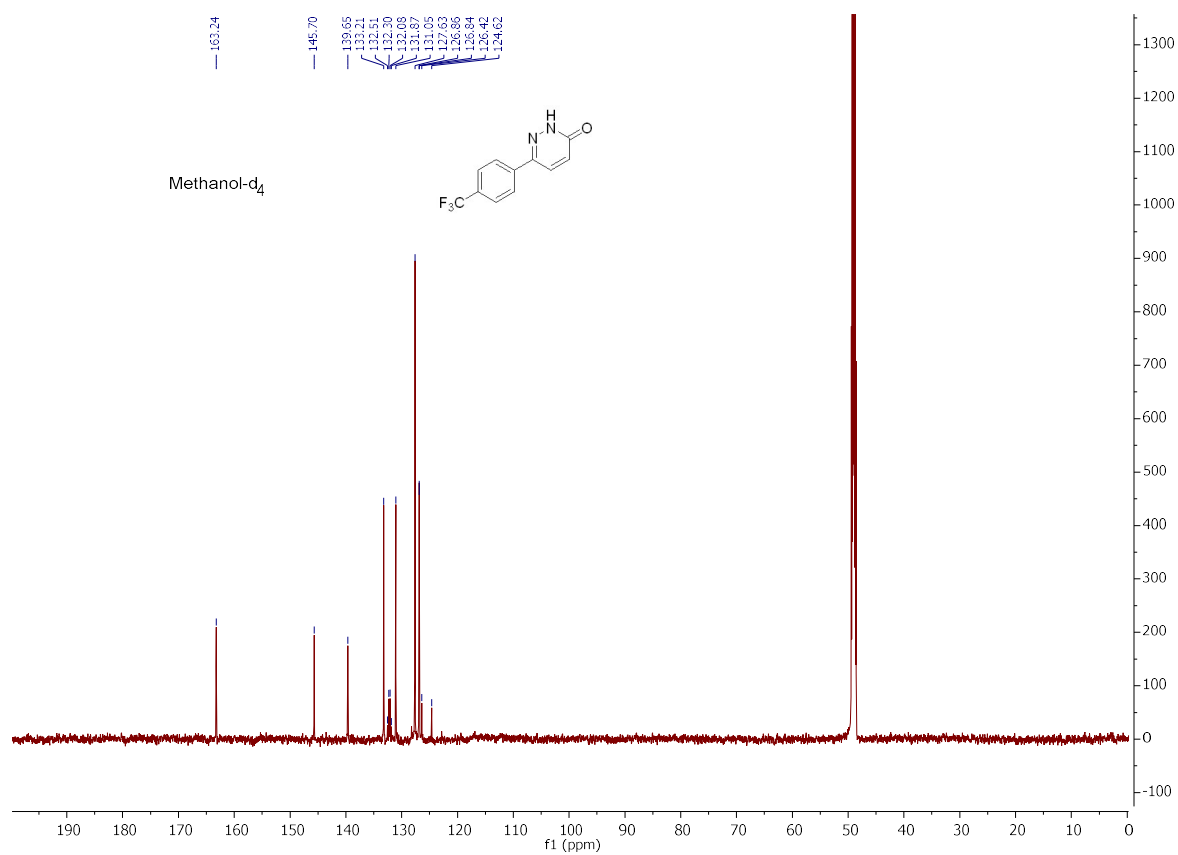
Supplementary Figure S6. ¹H-NMR 1c.



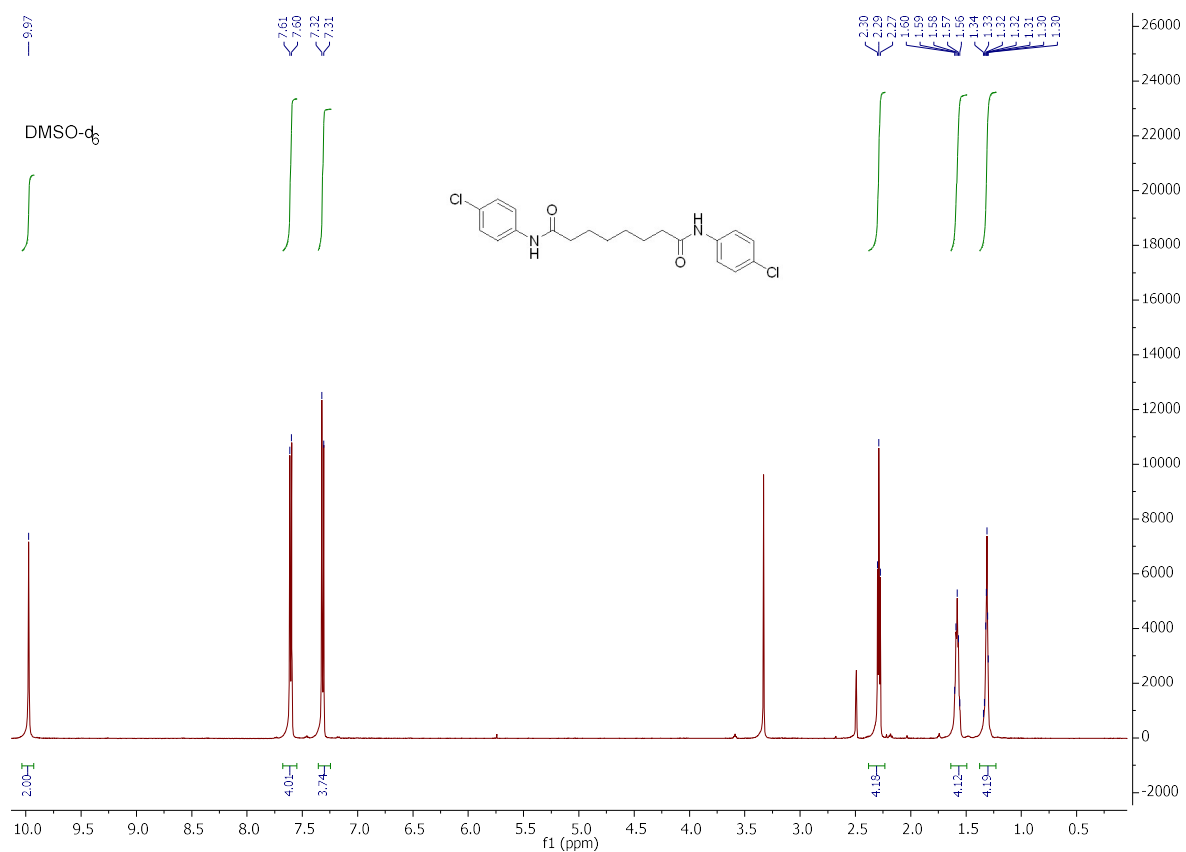
Supplementary Figure S7. ¹³C-NMR 1c.



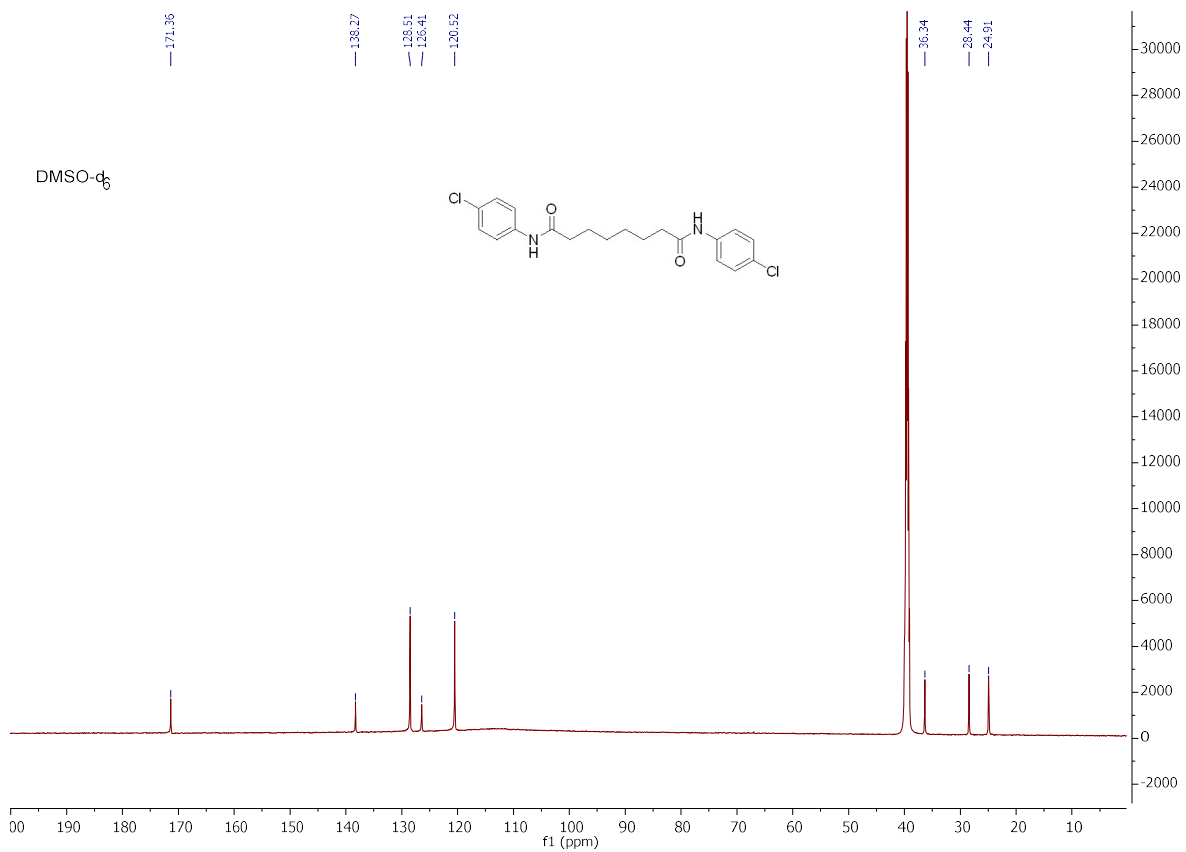
Supplementary Figure S8. ^1H -NMR 1d.



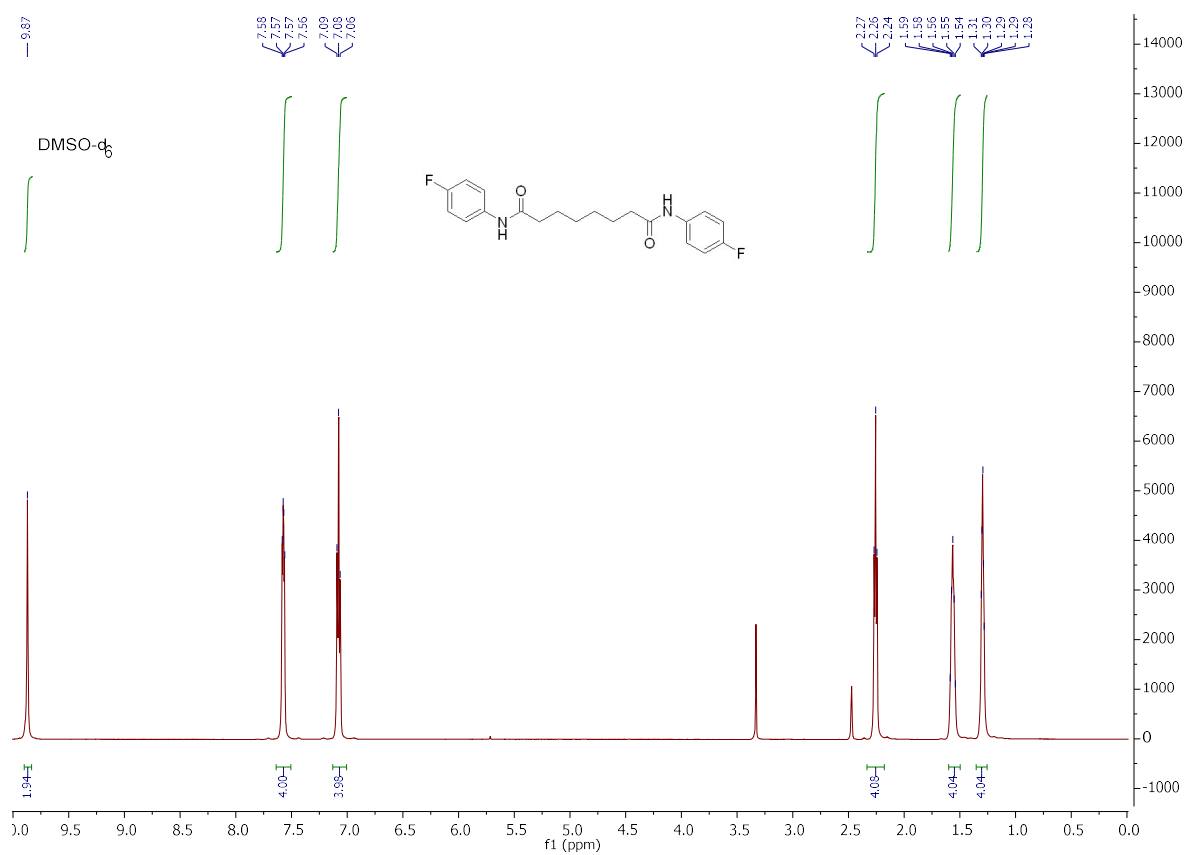
Supplementary Figure S9. ^{13}C -NMR 1d.



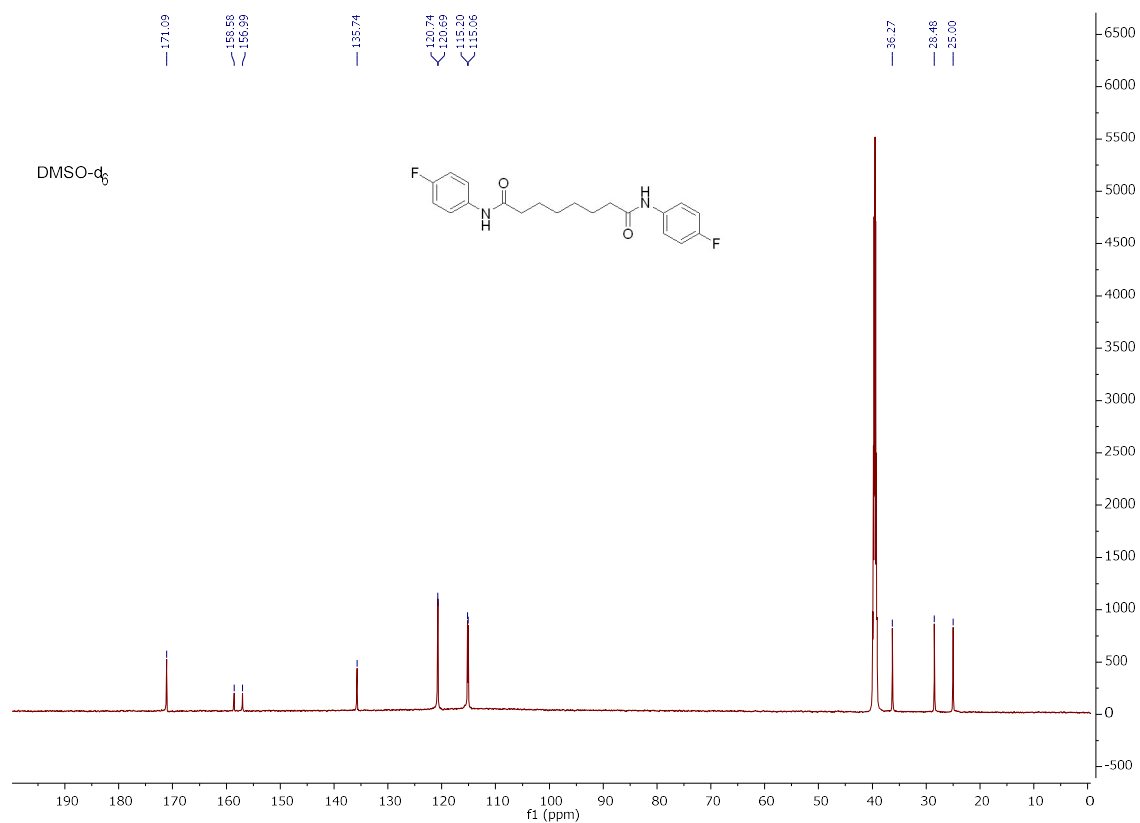
Supplementary Figure S12. ¹H-NMR 2a.



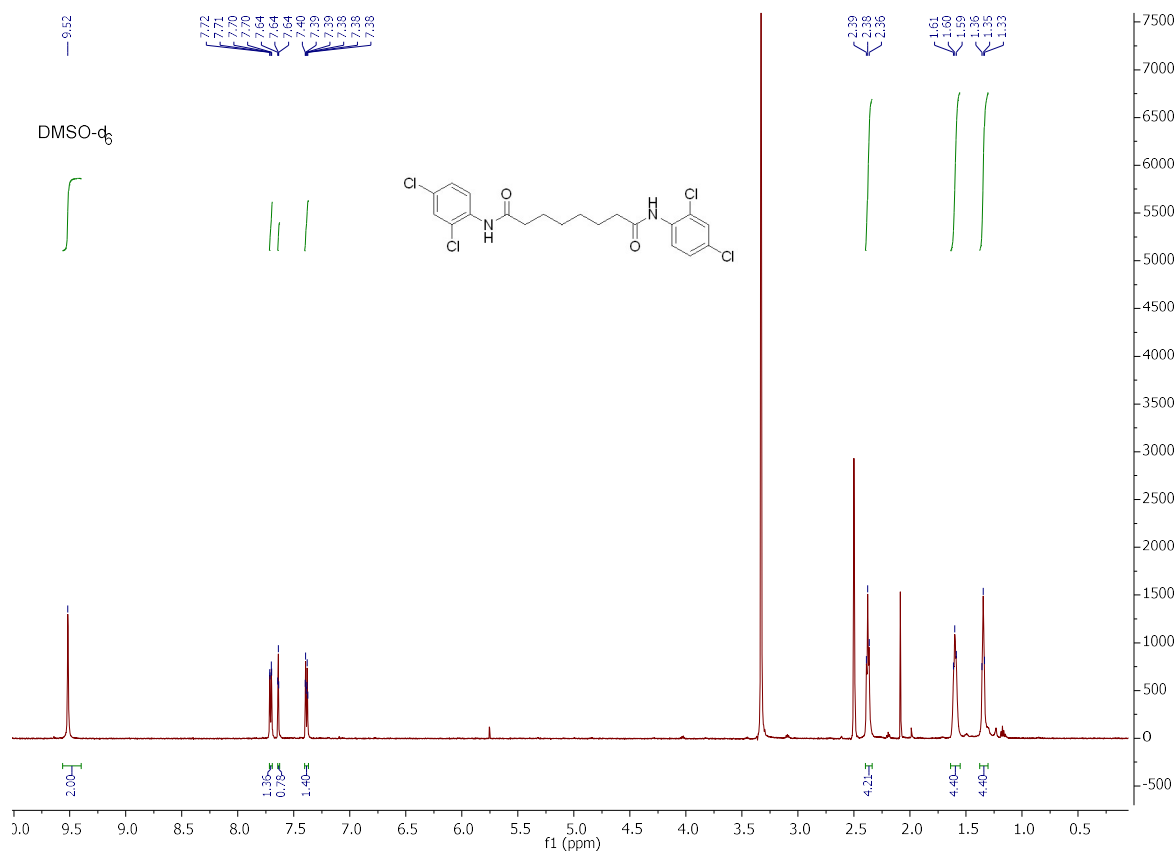
Supplementary Figure S13. ¹³C-NMR 2a.



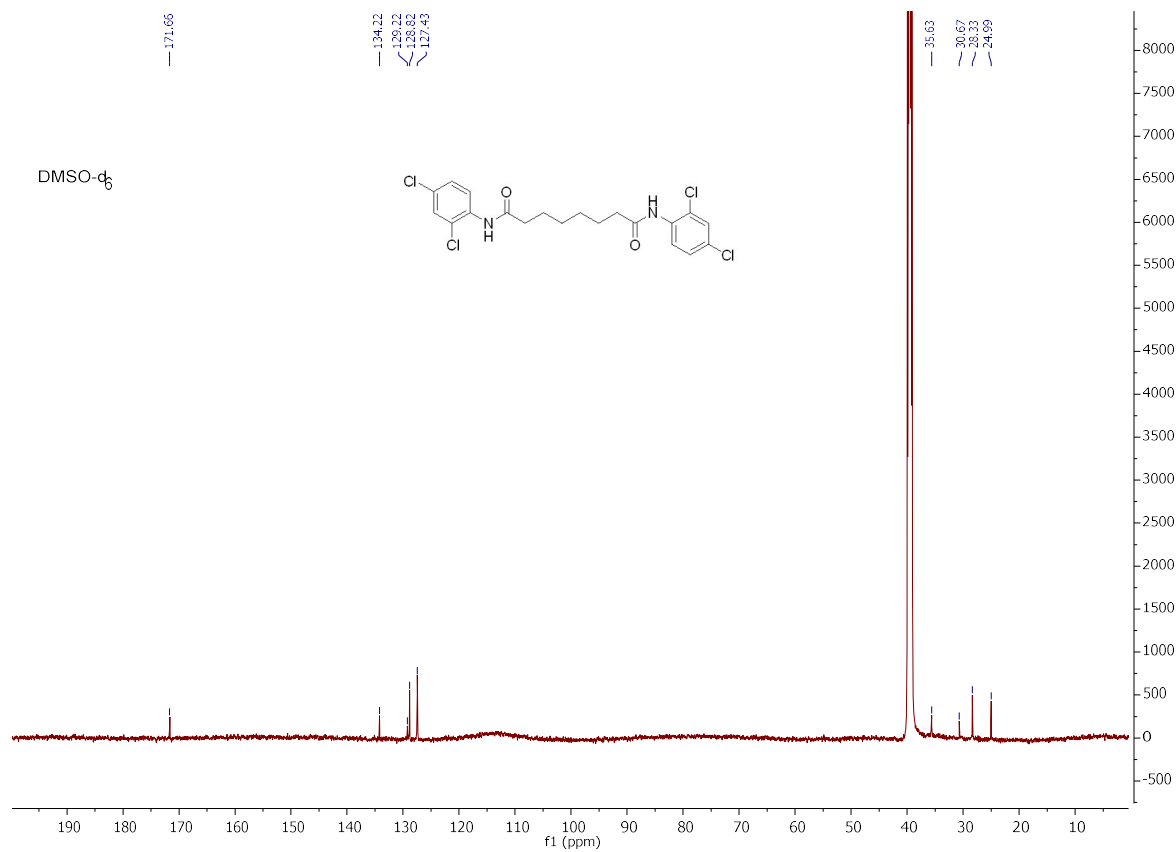
Supplementary Figure S14. ¹H-NMR 2b.



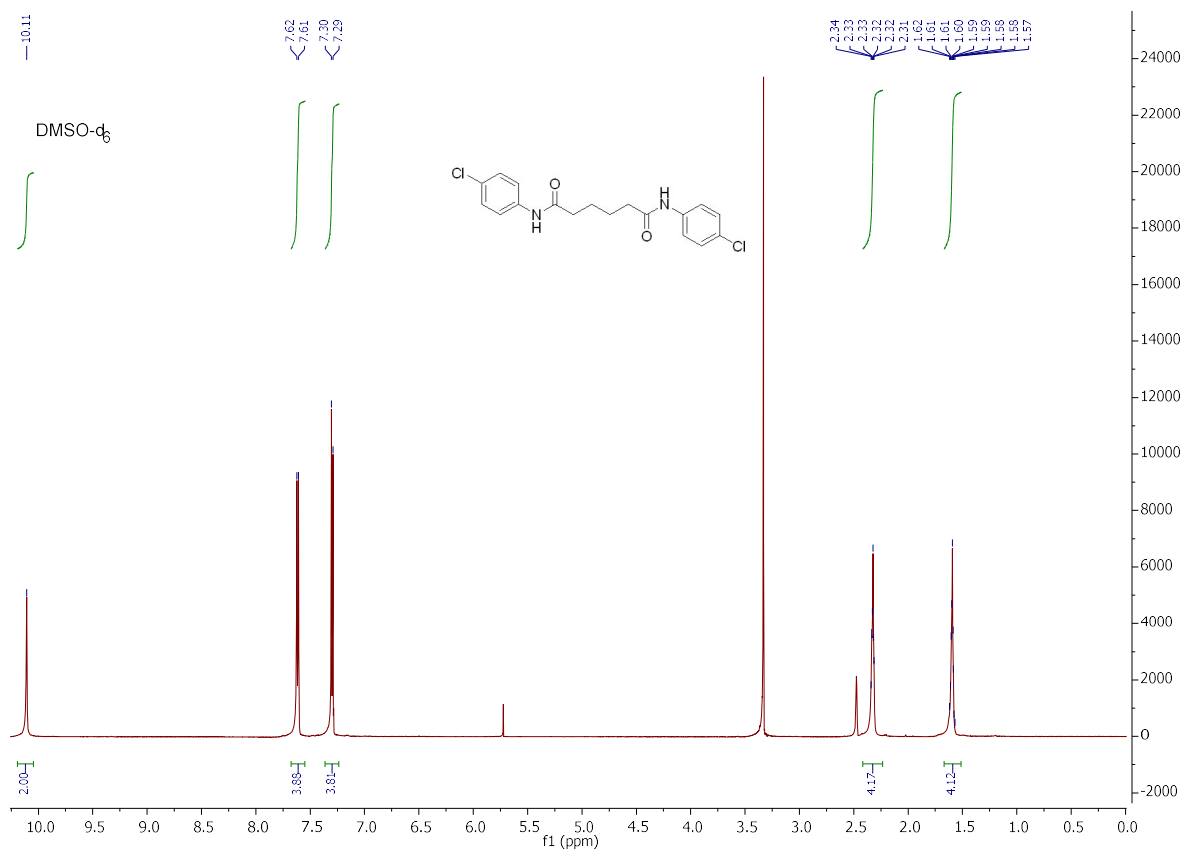
Supplementary Figure S15. ¹³C-NMR 2b.



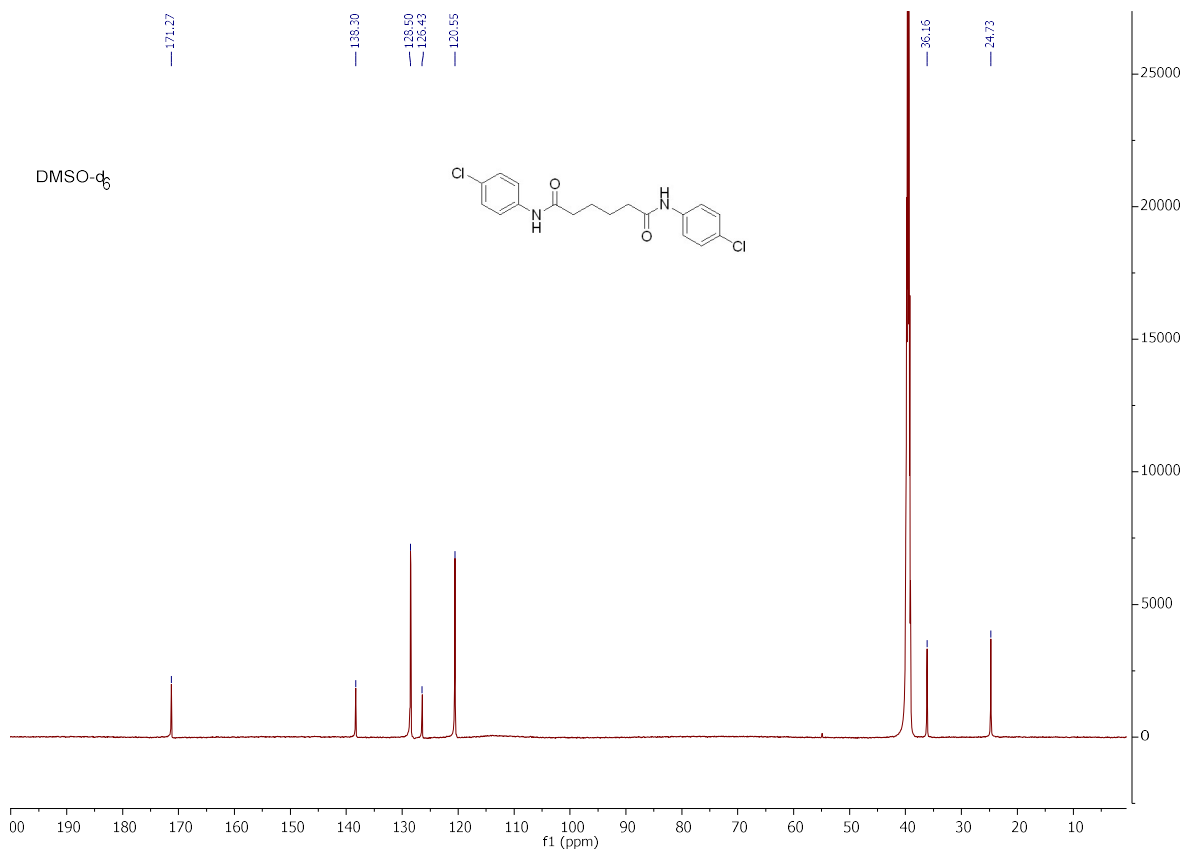
Supplementary Figure S16. ¹H-NMR 2c.



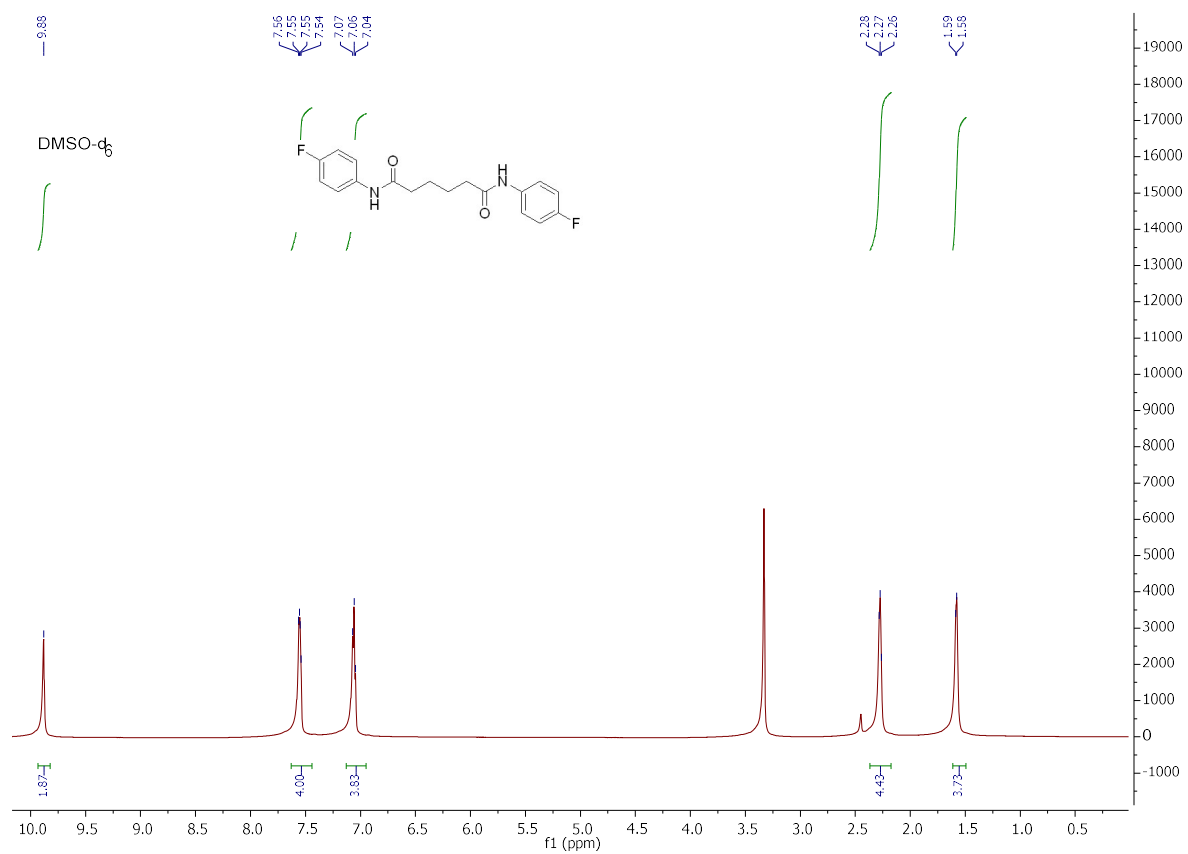
Supplementary Figure S17. ¹³C-NMR 2c.



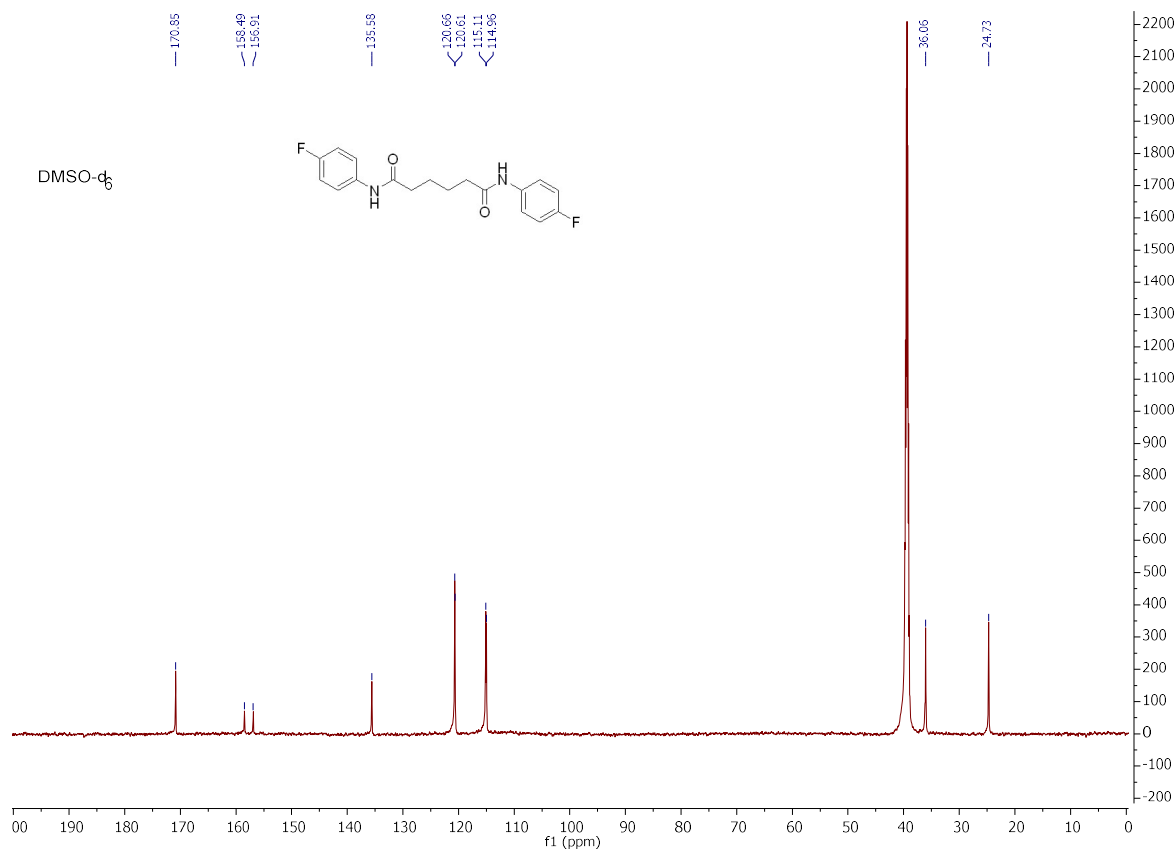
Supplementary Figure S18. ¹H-NMR 2d.



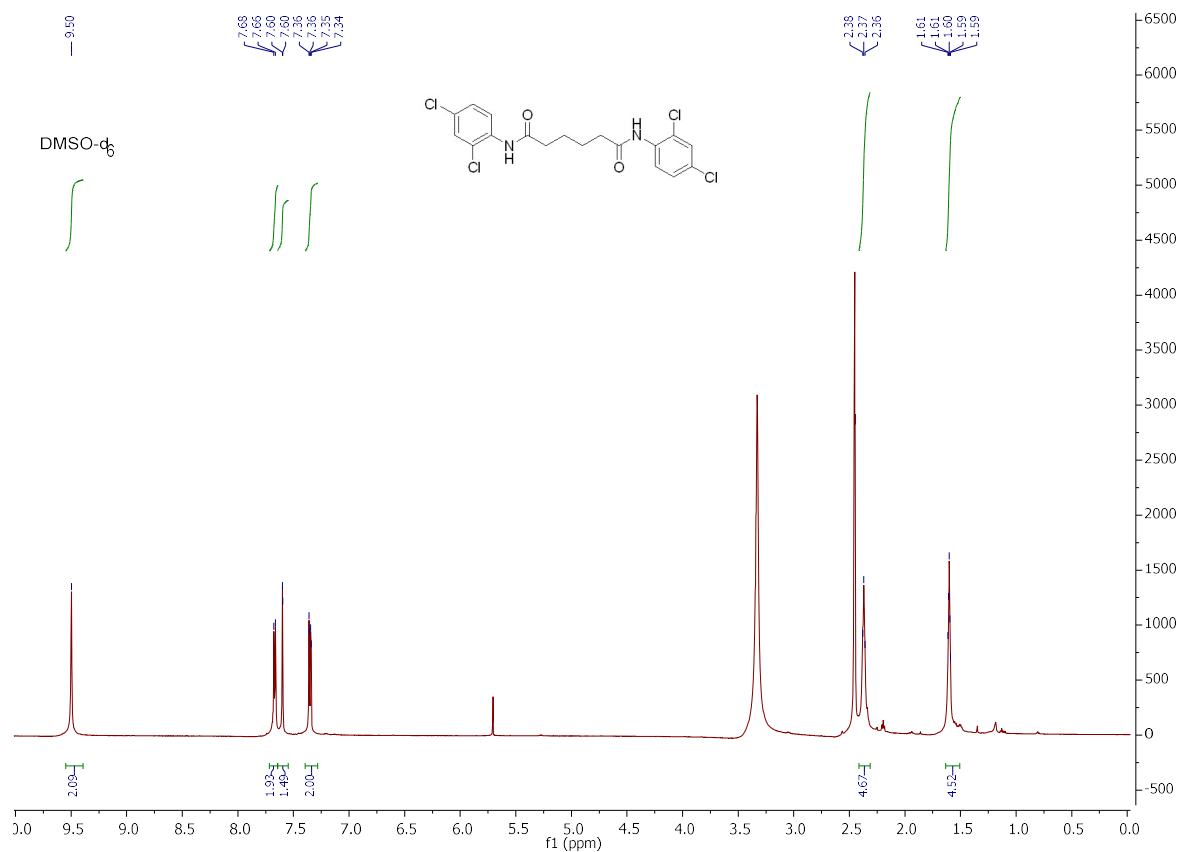
Supplementary Figure S19. ¹³C-NMR 2d.



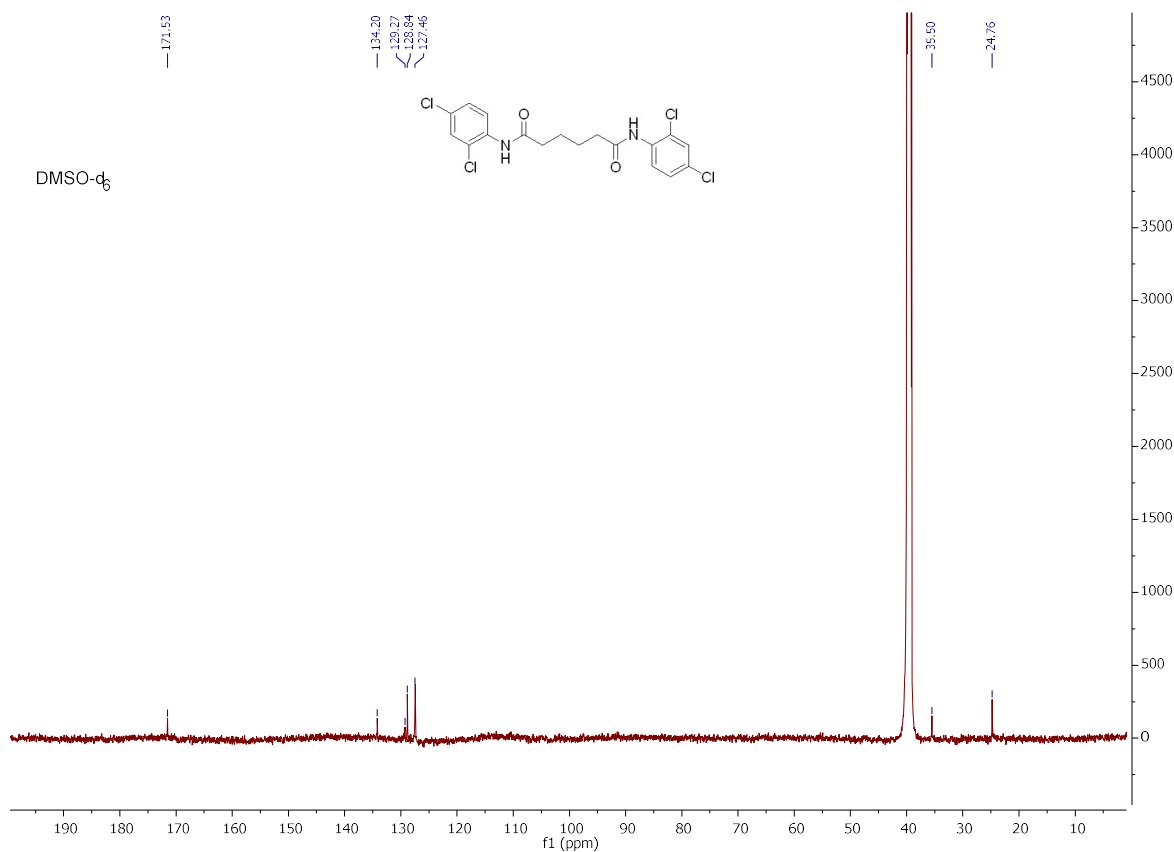
Supplementary Figure S20. ¹H-NMR 2e.



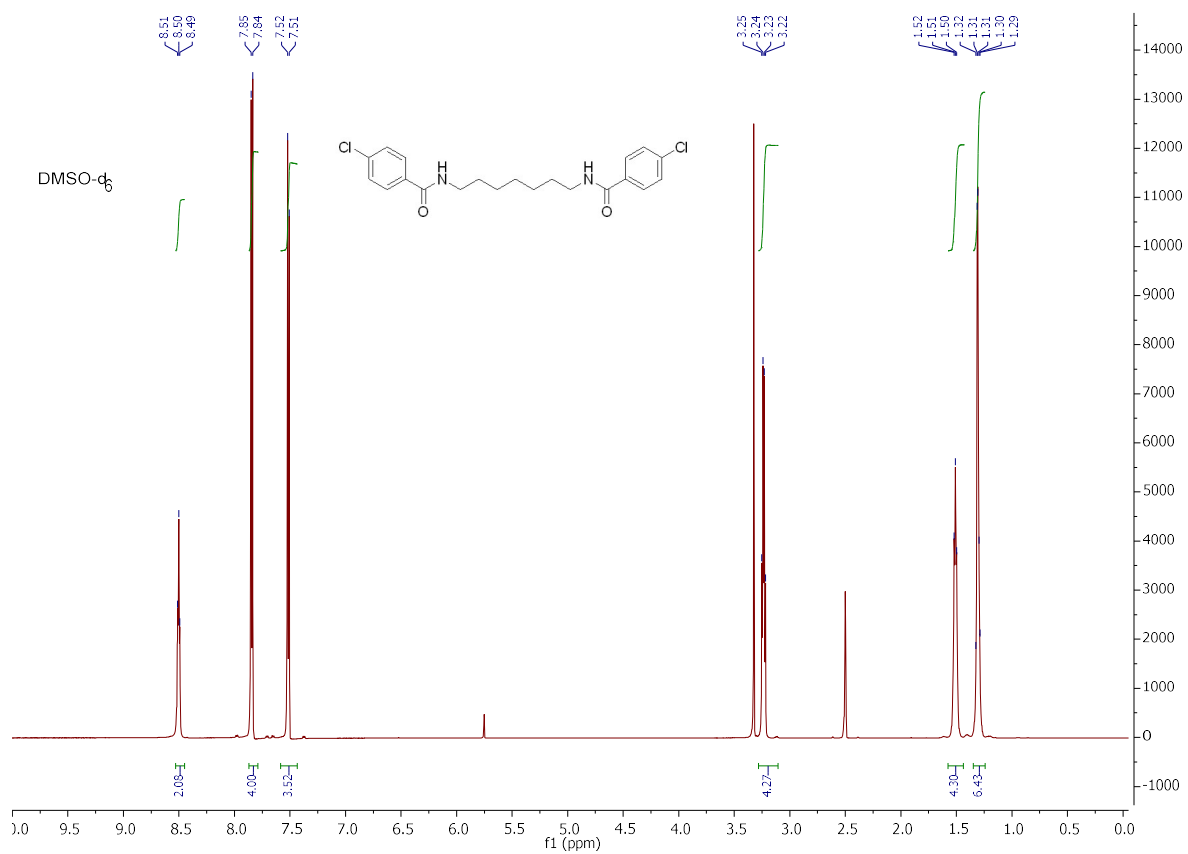
Supplementary Figure S21. ¹³C-NMR 2e.



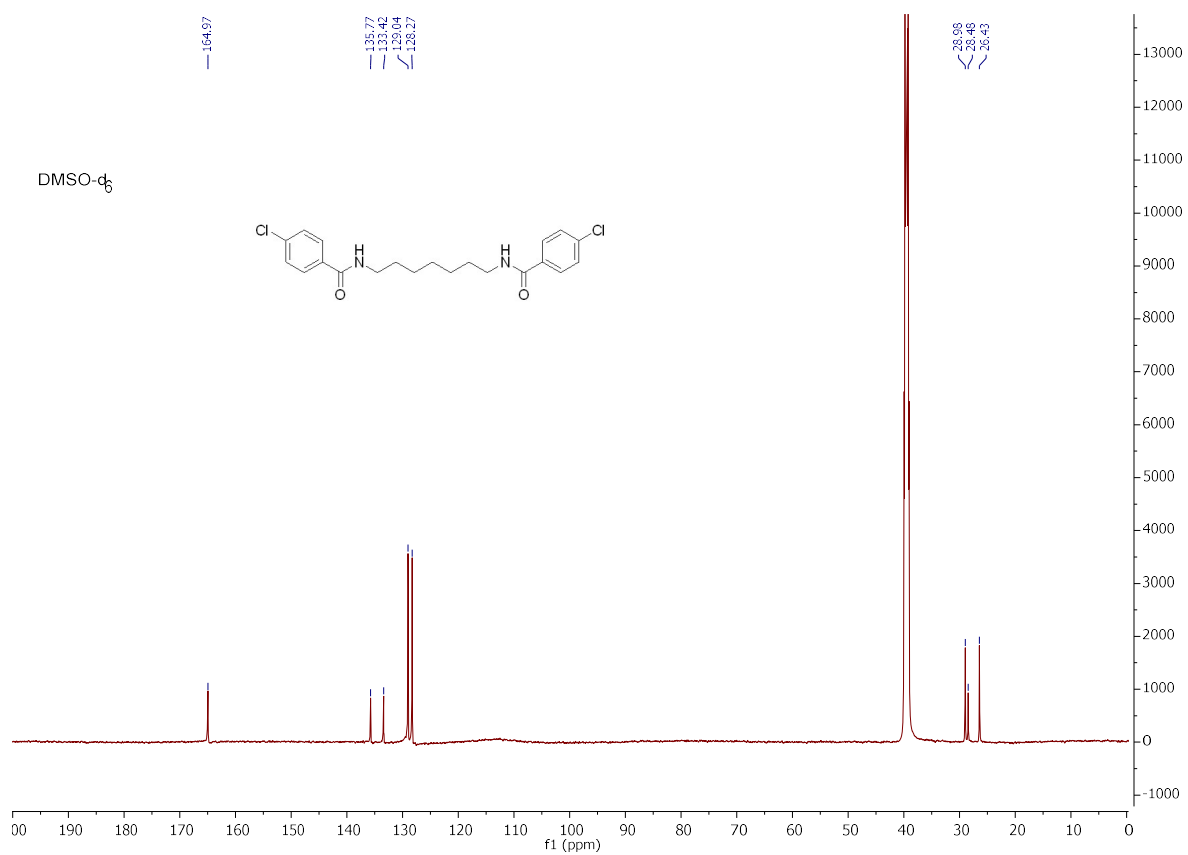
Supplementary Figure S22. ¹H-NMR 2f.



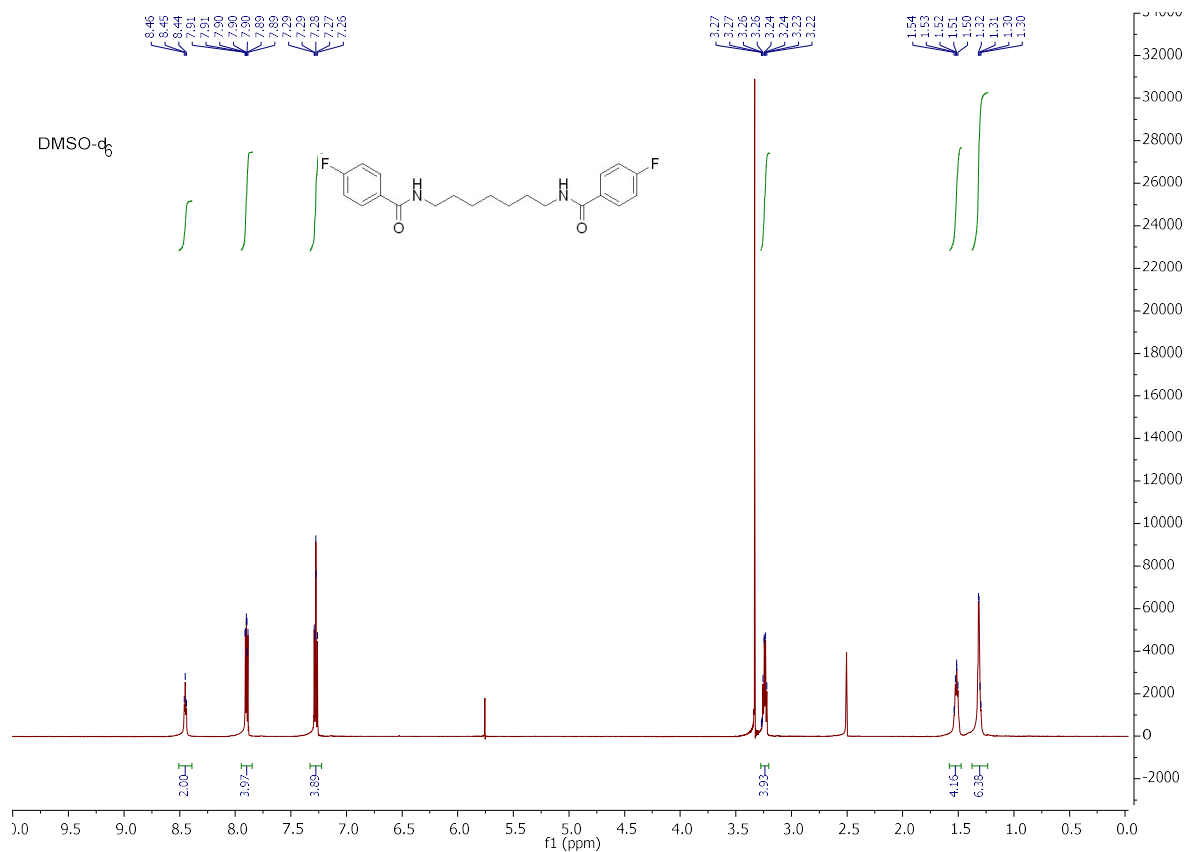
Supplementary Figure S23. ¹³C-NMR 2f.



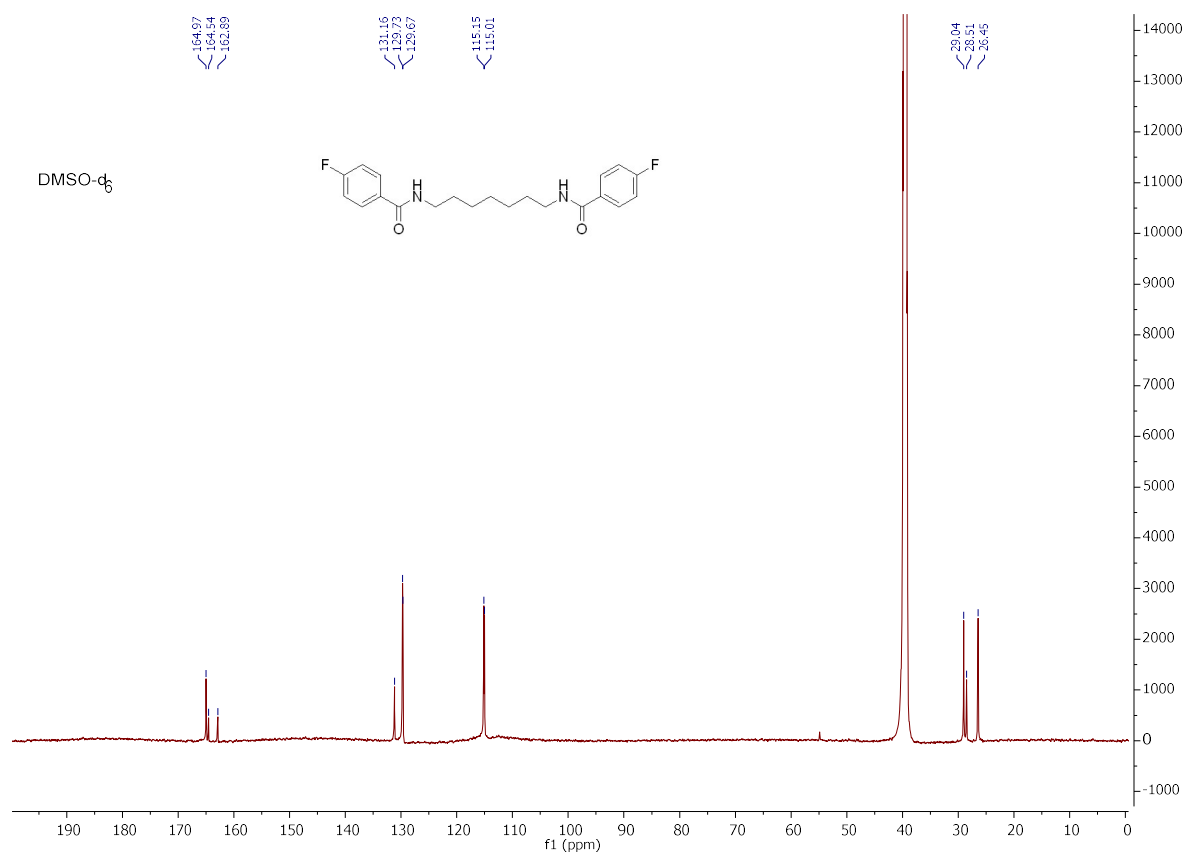
Supplementary Figure S24. ¹H-NMR 5a.



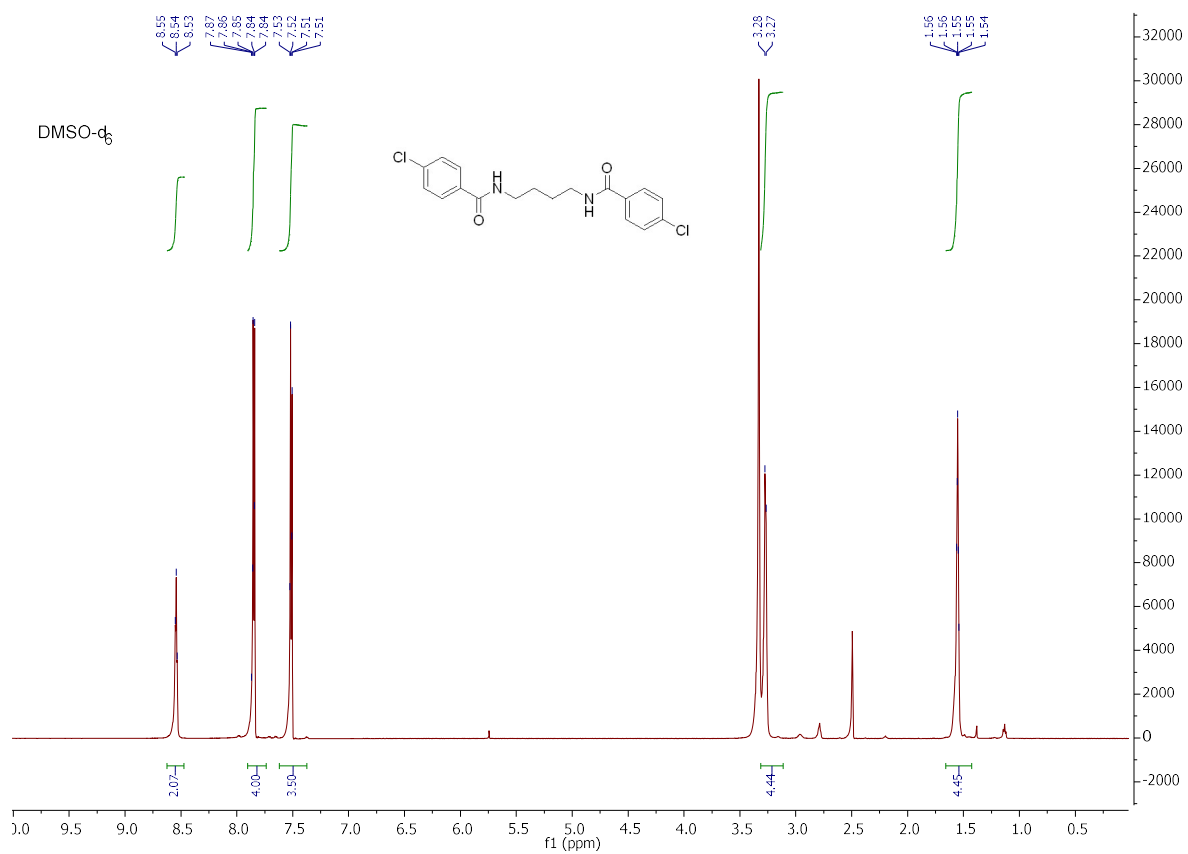
Supplementary Figure S25. ¹³C-NMR 5a.



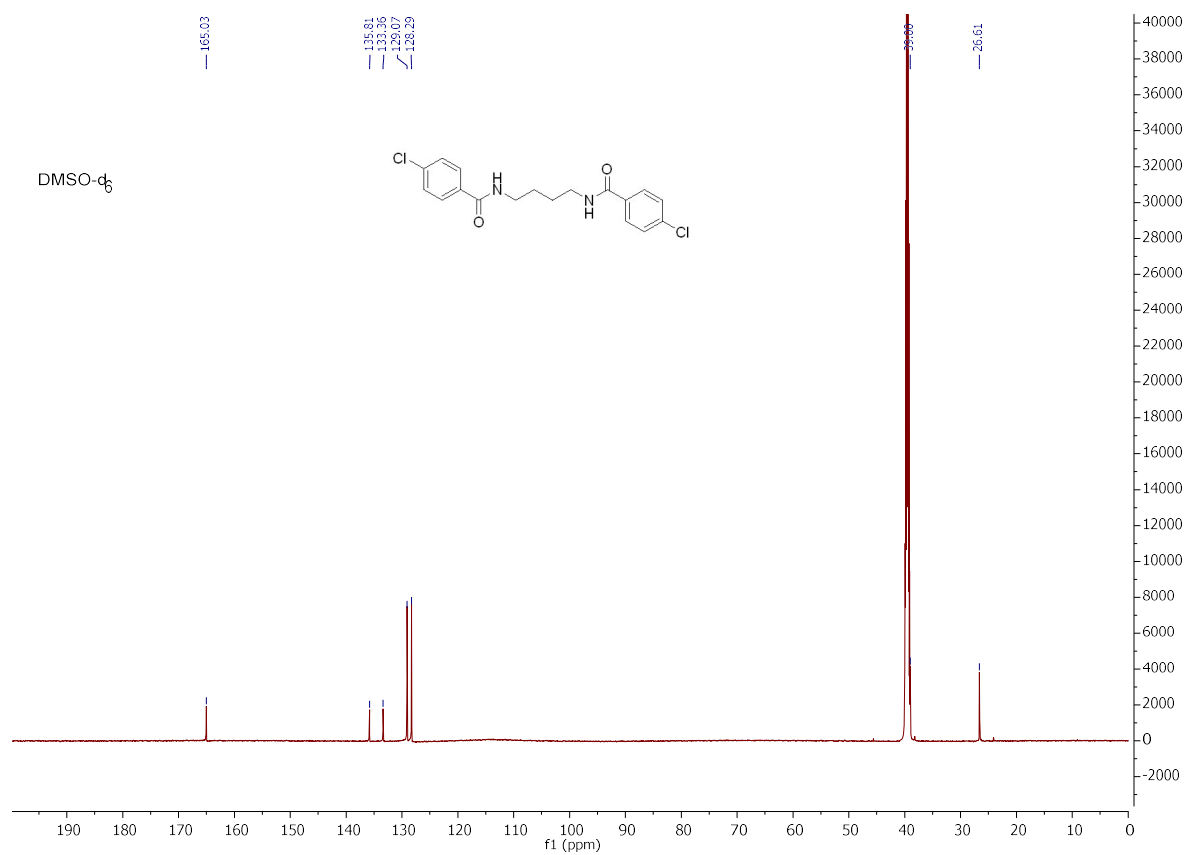
Supplementary Figure S26. ^1H -NMR 5b.



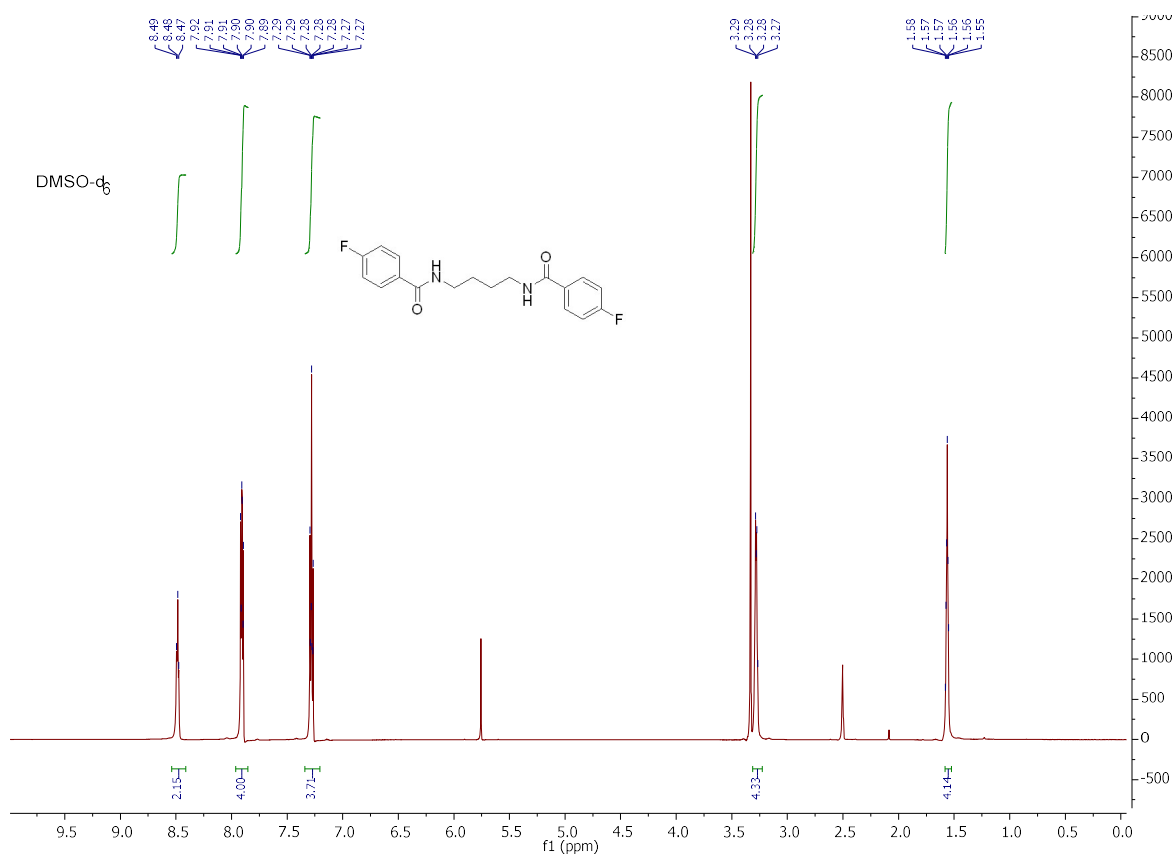
Supplementary Figure S27. ^{13}C -NMR 5b.



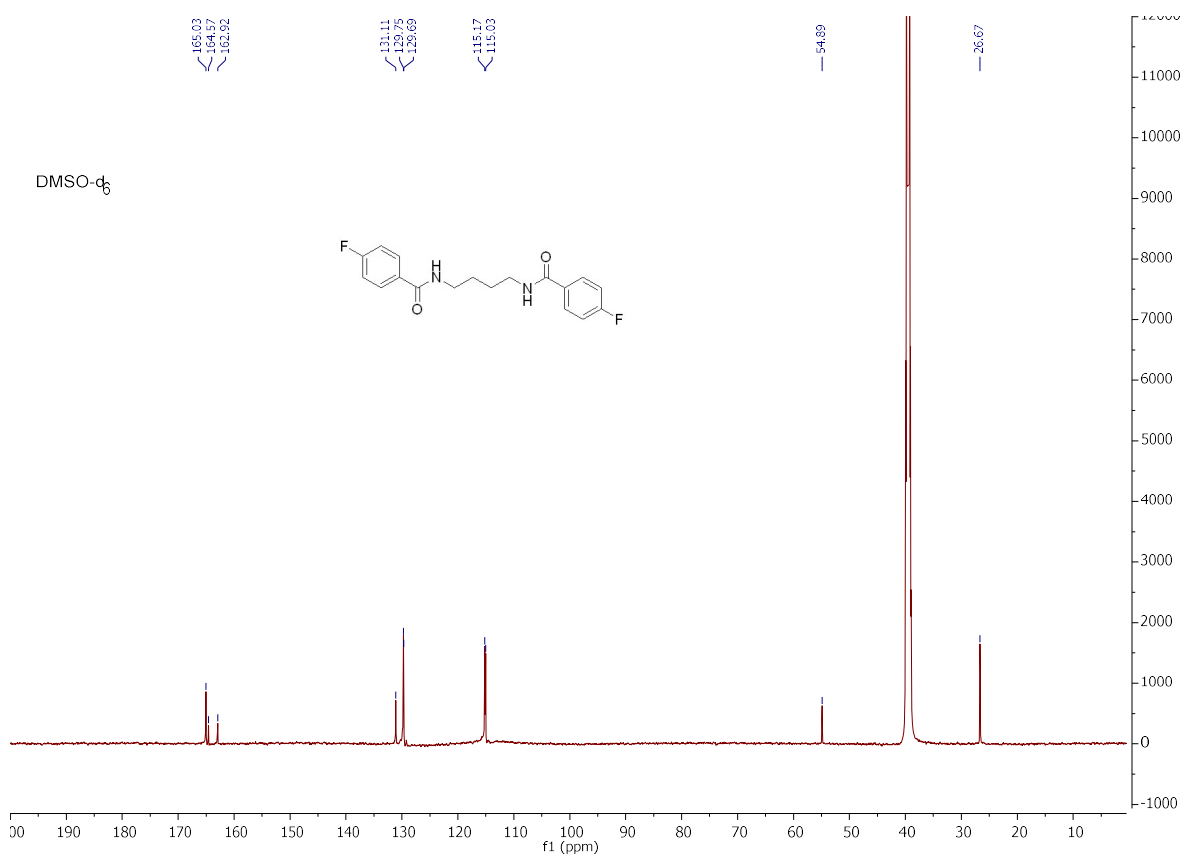
Supplementary Figure S28. ¹H-NMR 5c.



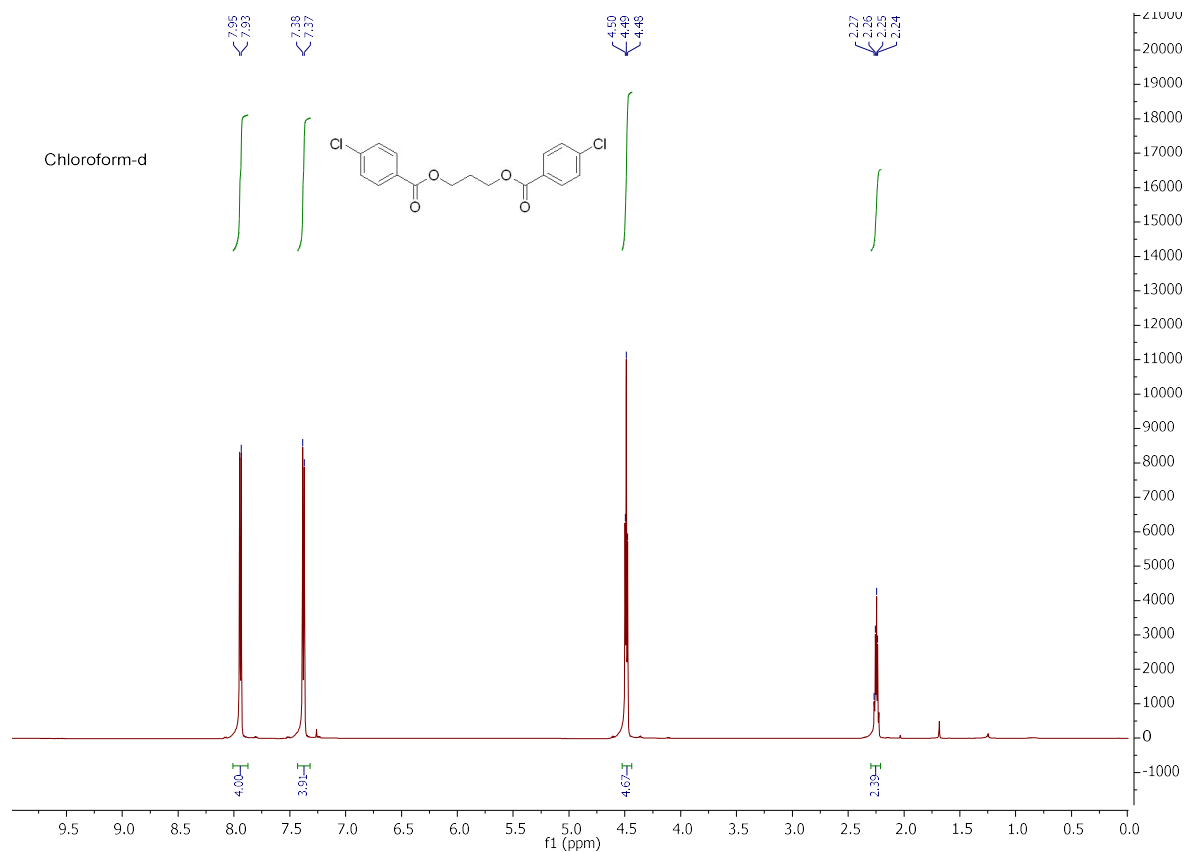
Supplementary Figure S29. ¹³C-NMR 5c.



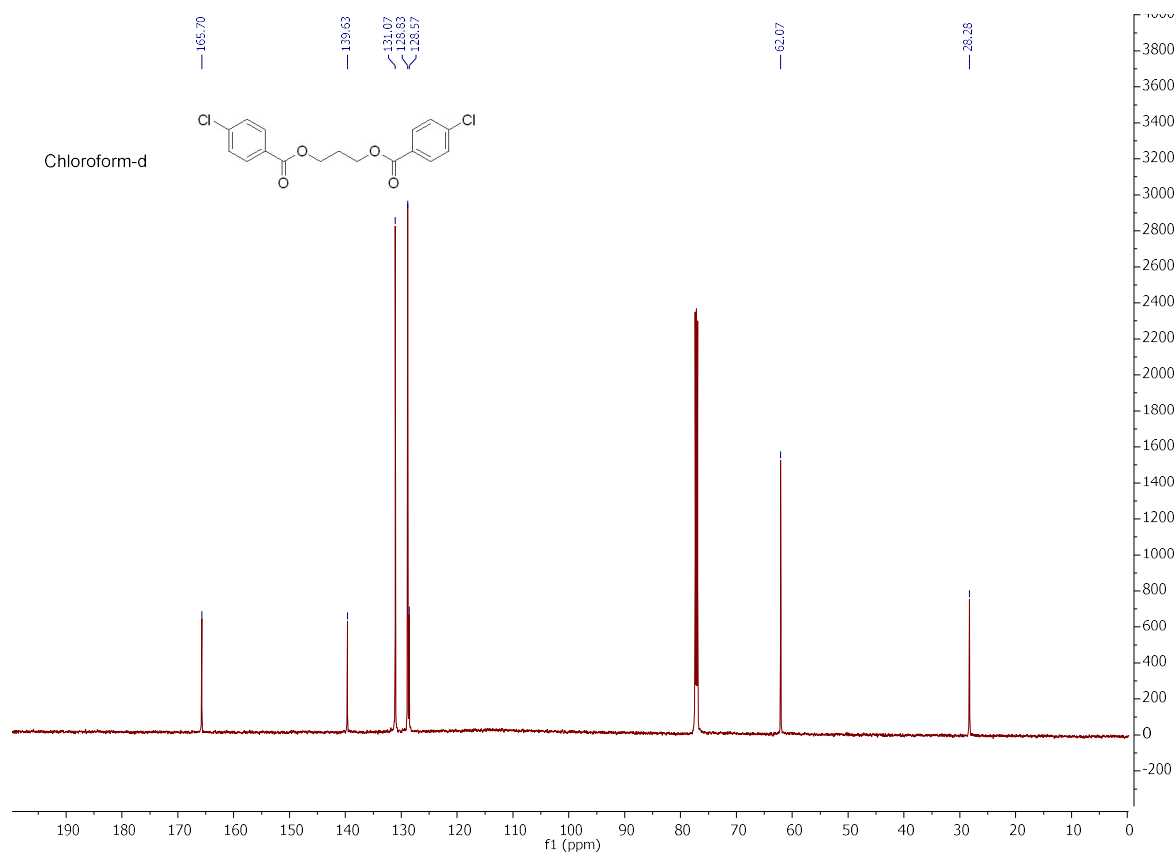
Supplementary Figure S30. ¹H-NMR 5d.



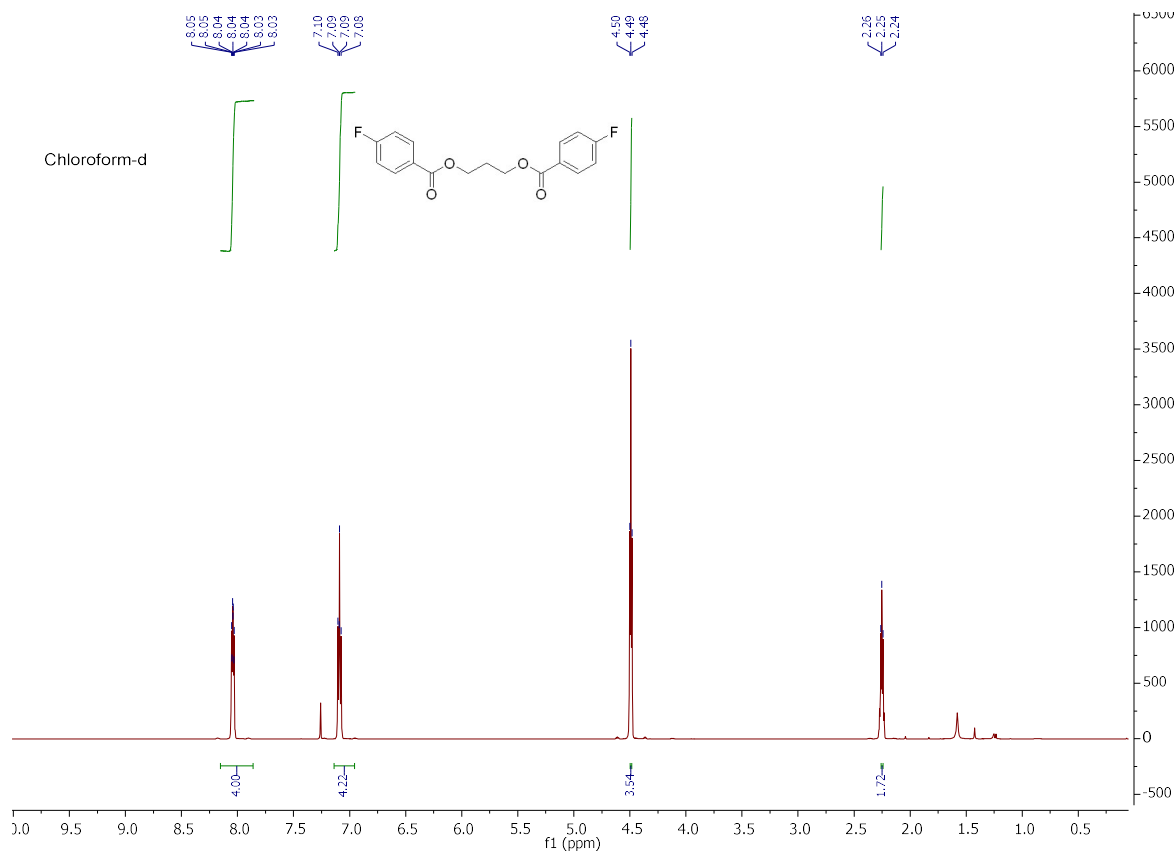
Supplementary Figure S31. ¹³C-NMR 5d.



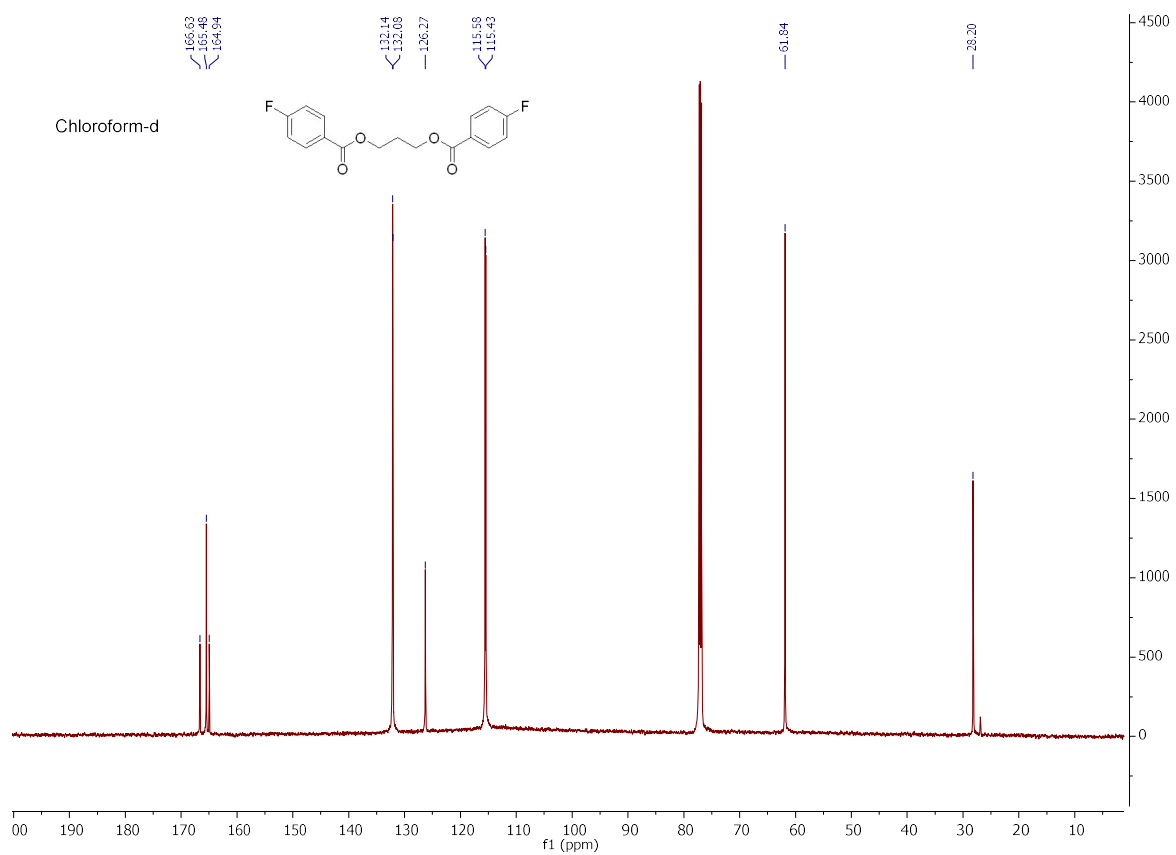
Supplementary Figure S32. ^1H -NMR 6a.



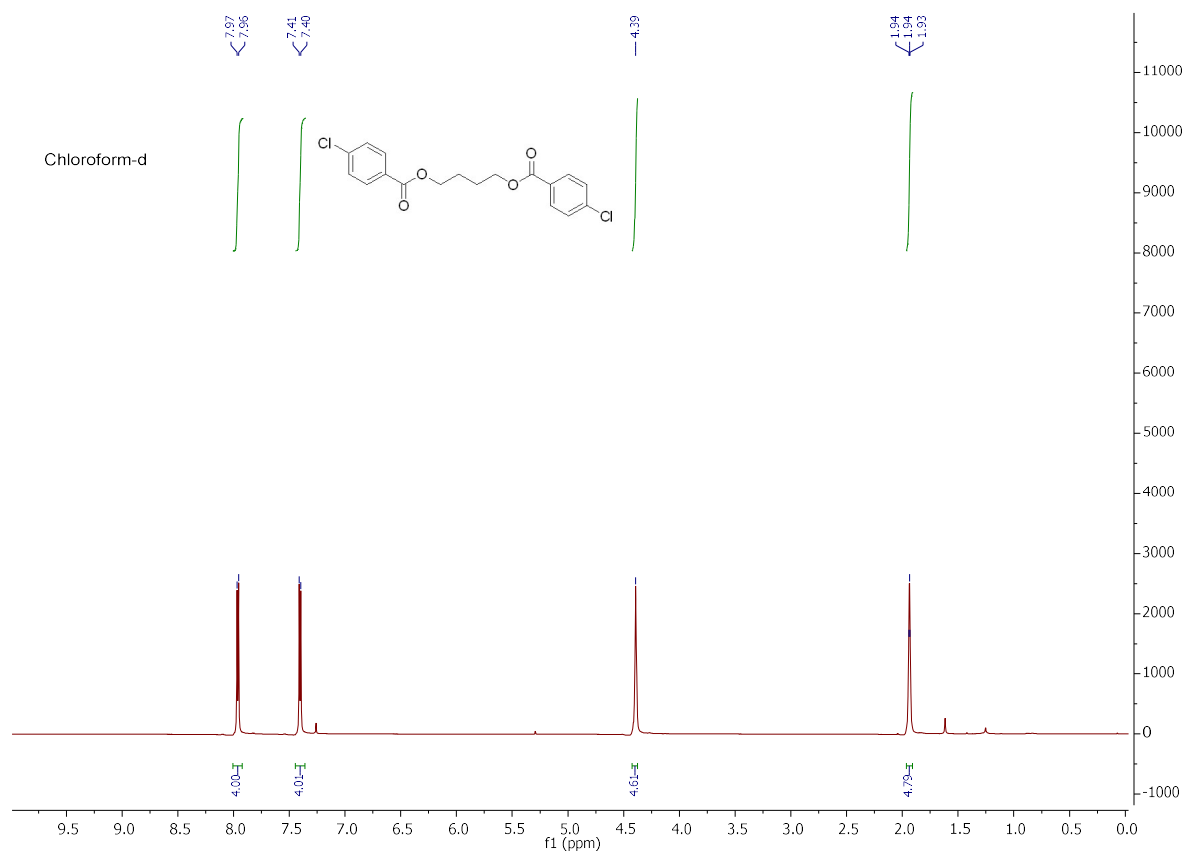
Supplementary Figure S33. ^{13}C -NMR 6a.



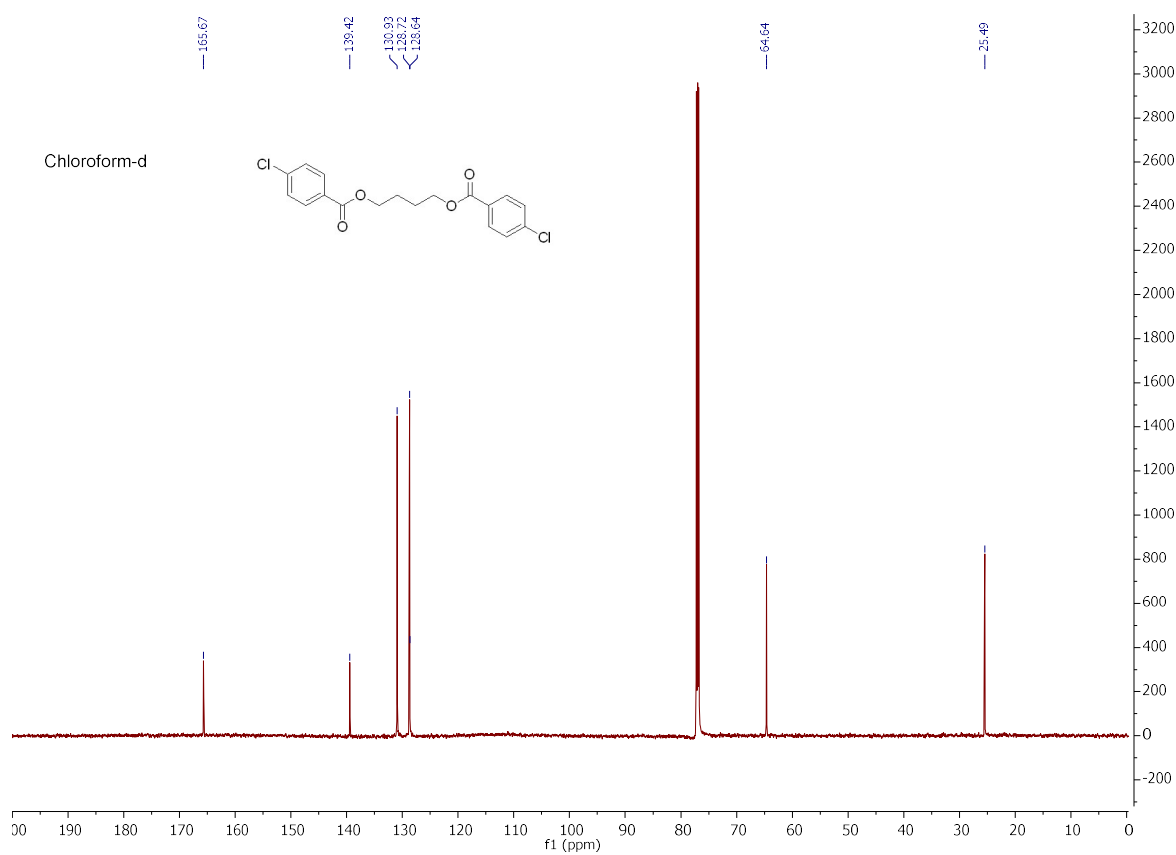
Supplementary Figure S34. ^1H -NMR 6b.



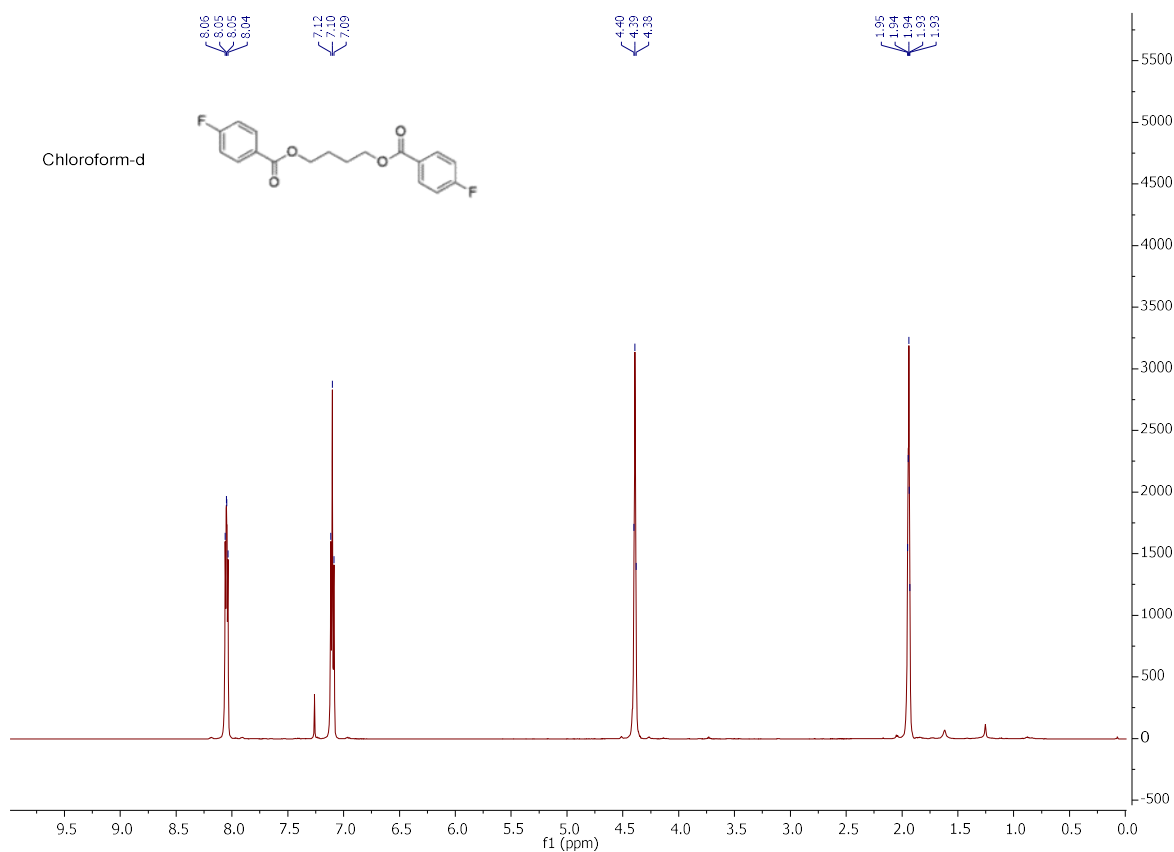
Supplementary Figure S35. ^{13}C -NMR 6b.



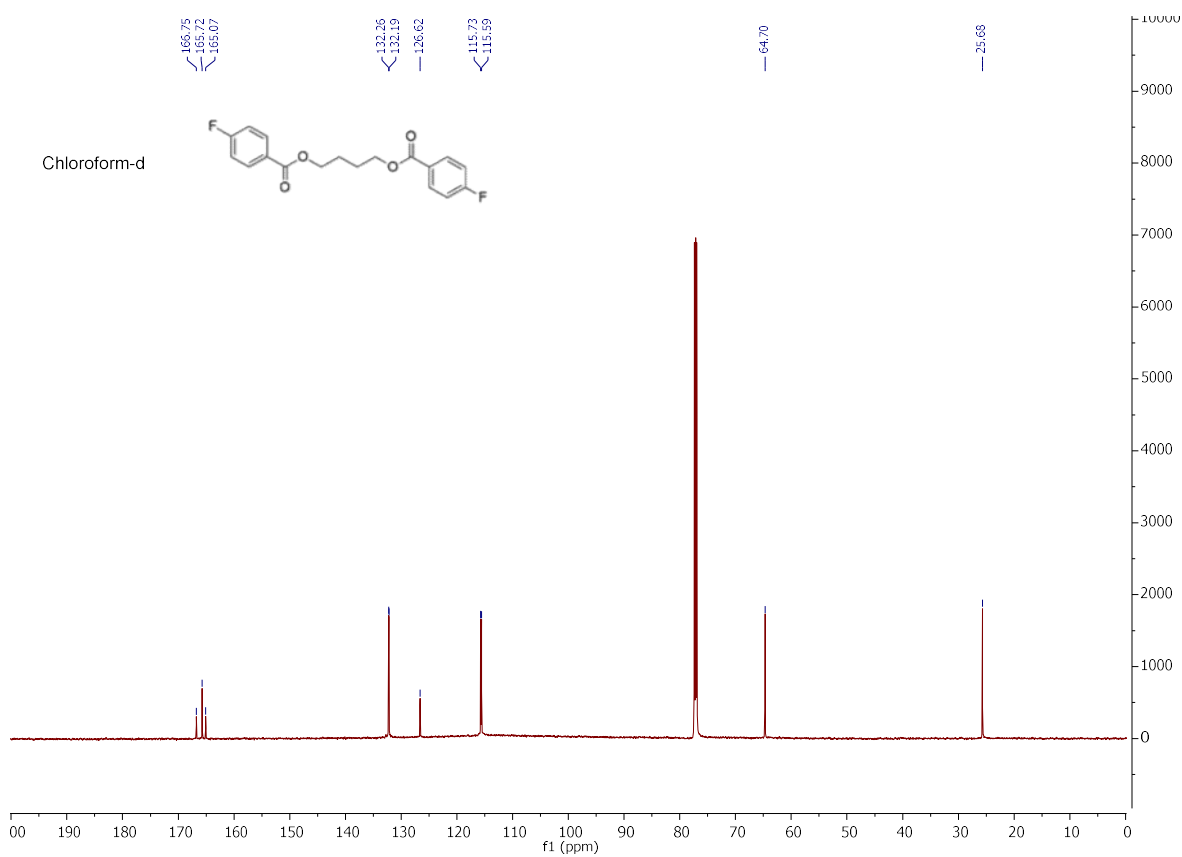
Supplementary Figure S36. ^1H -NMR 6c.



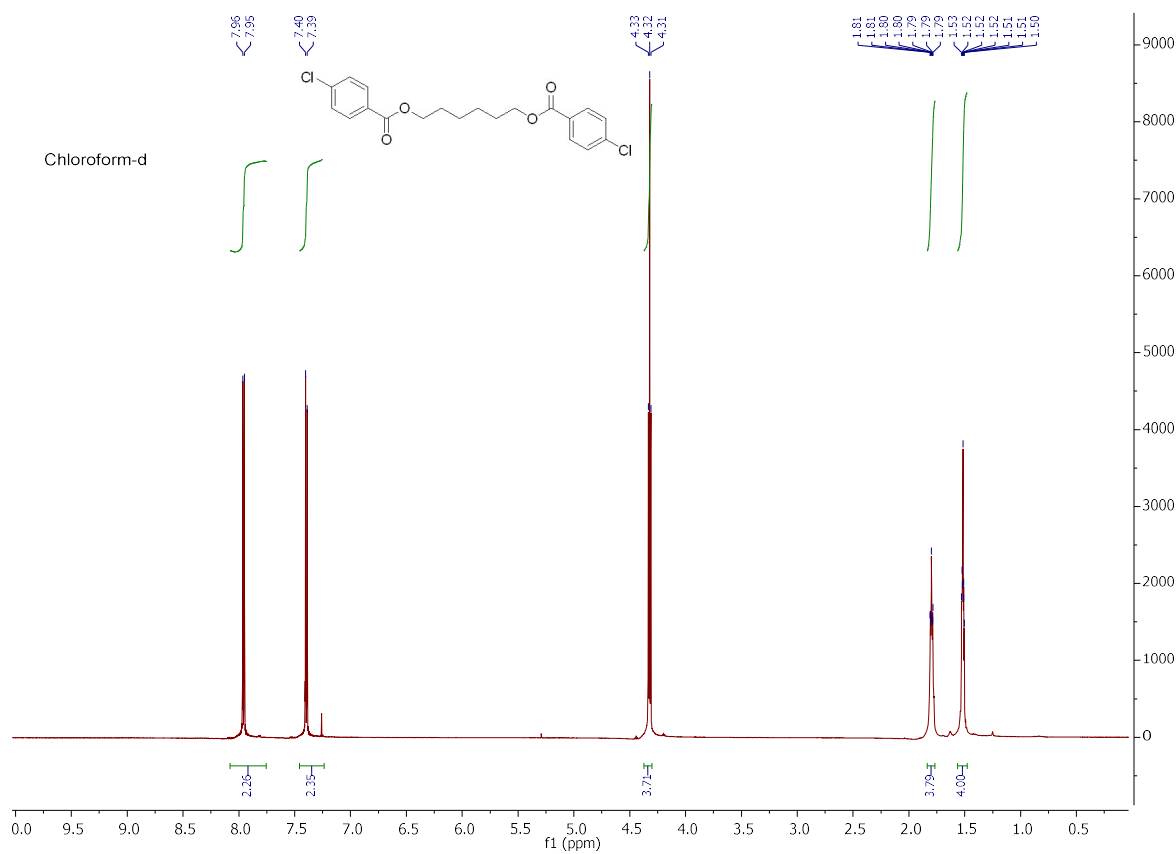
Supplementary Figure S37. ^{13}C -NMR 6c.



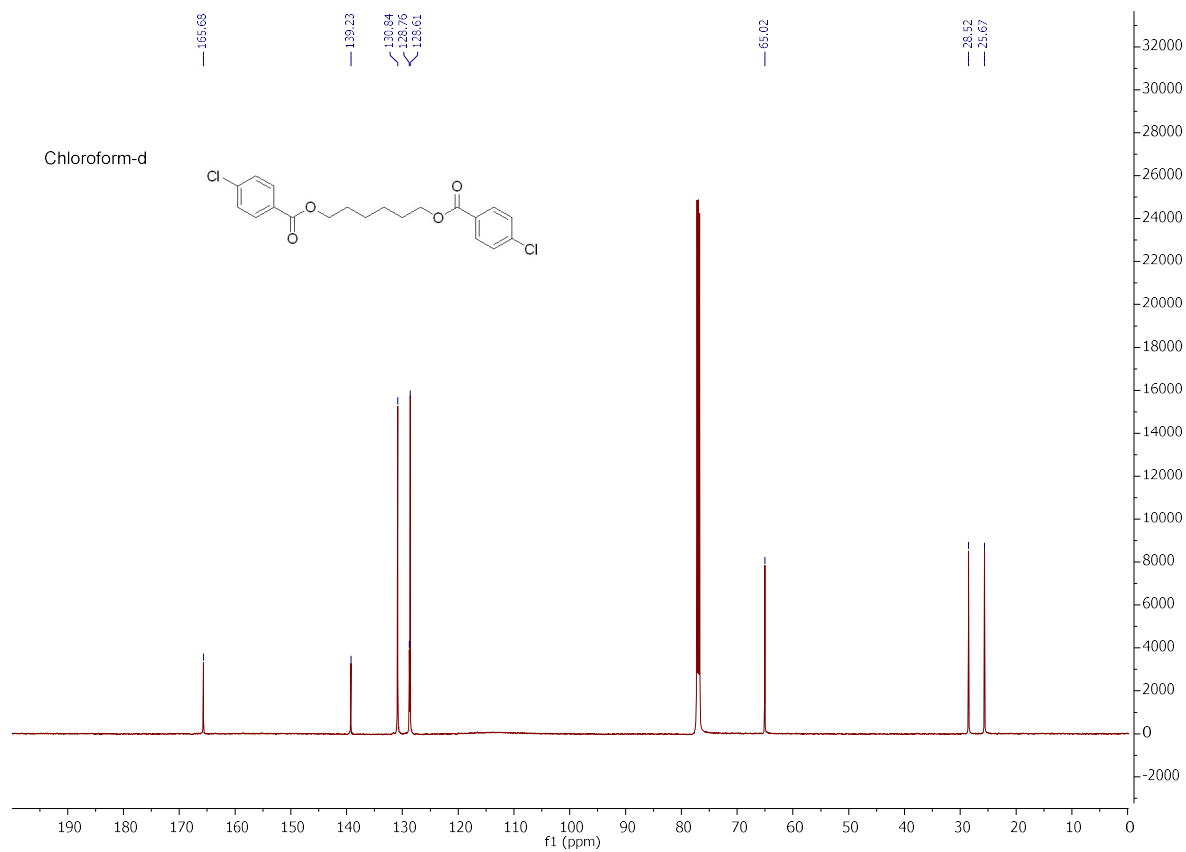
Supplementary Figure S38. ¹H-NMR 6d.



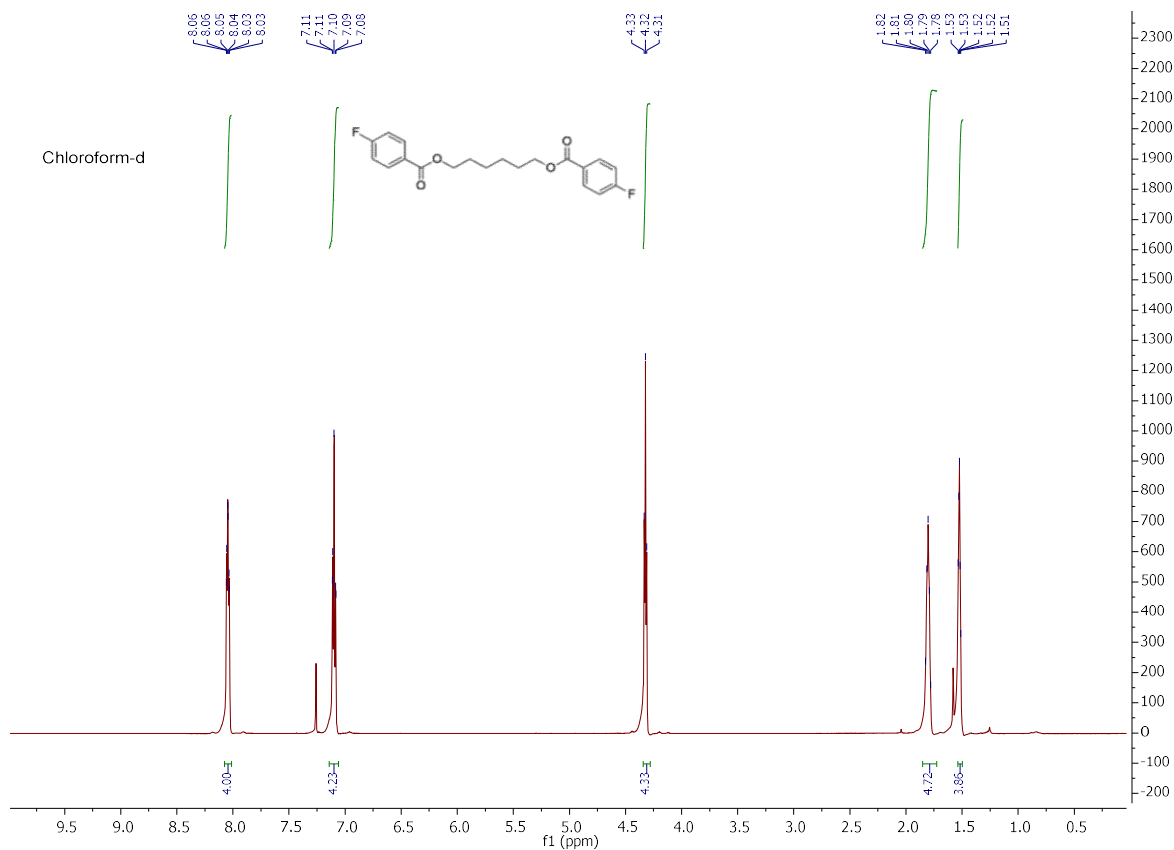
Supplementary Figure S39. ¹³C-NMR 6d.



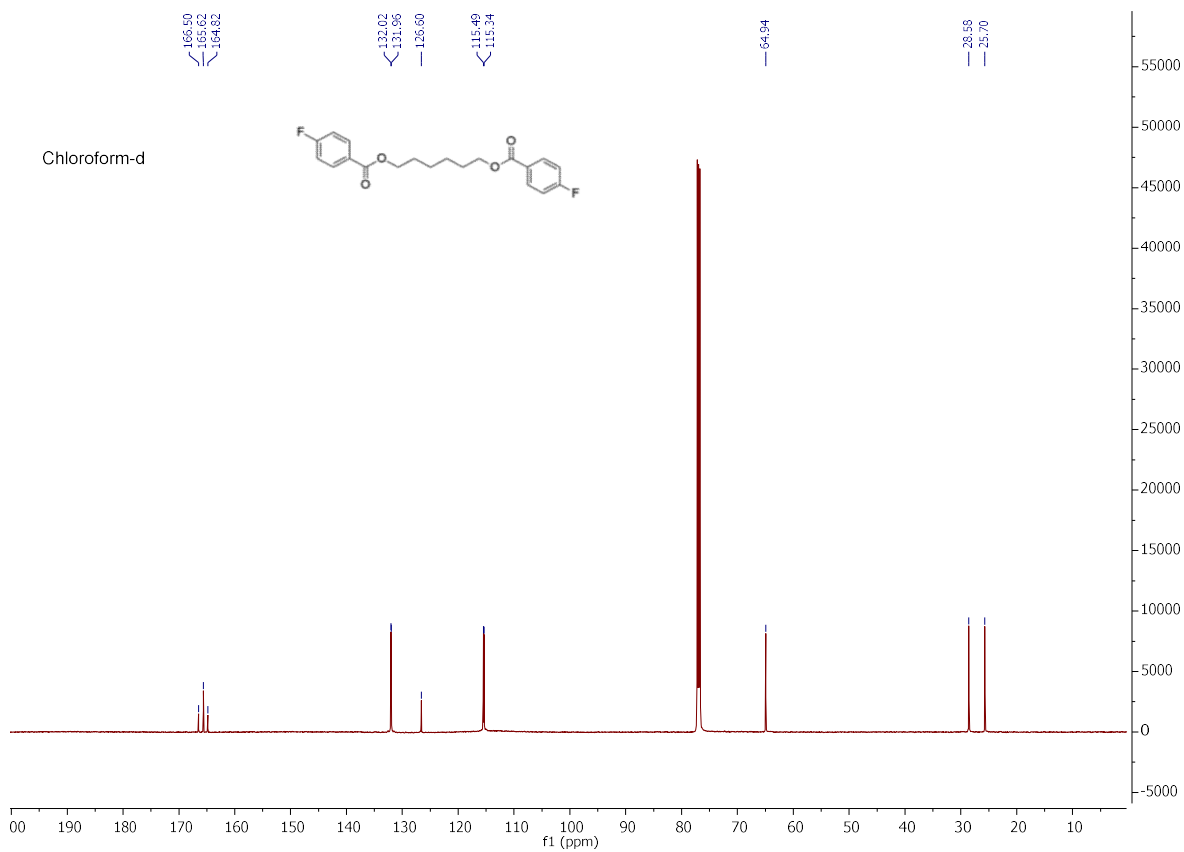
Supplementary Figure S40. ¹H-NMR 6e.



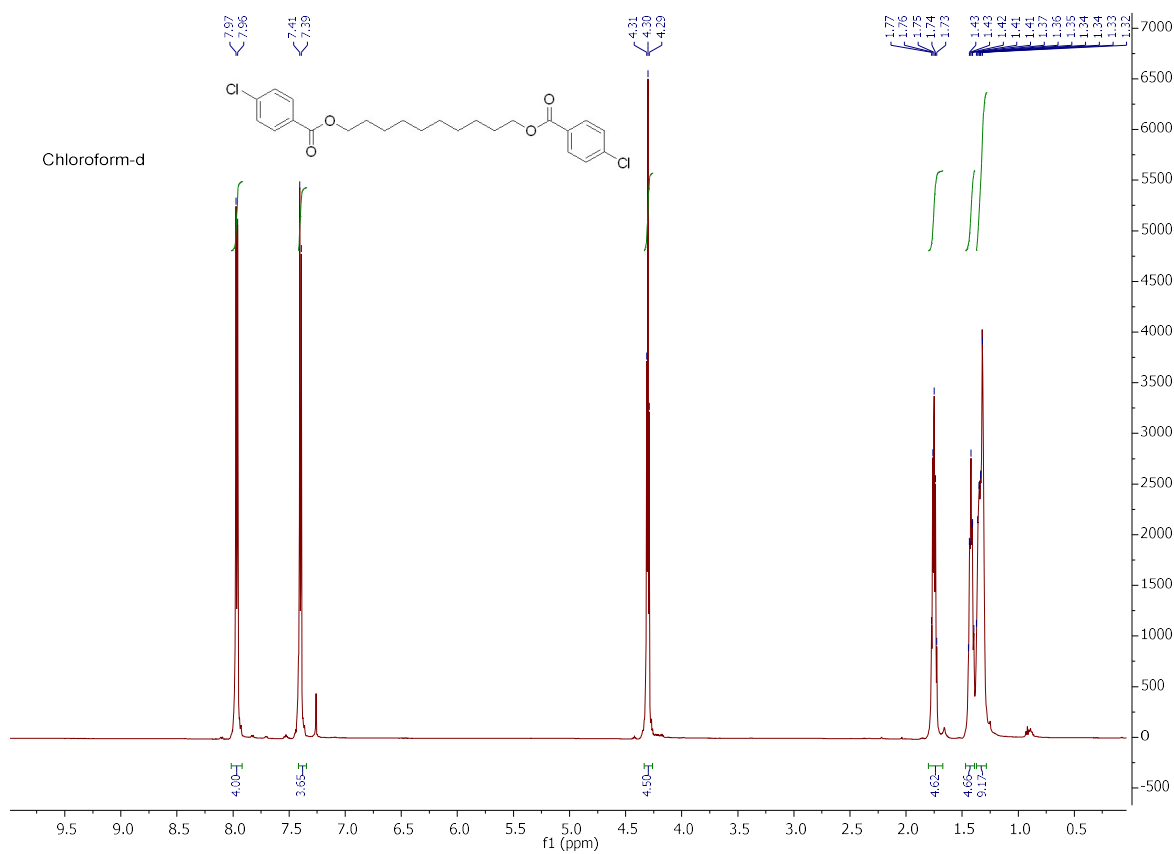
Supplementary Figure S41. ¹³C-NMR 6e.



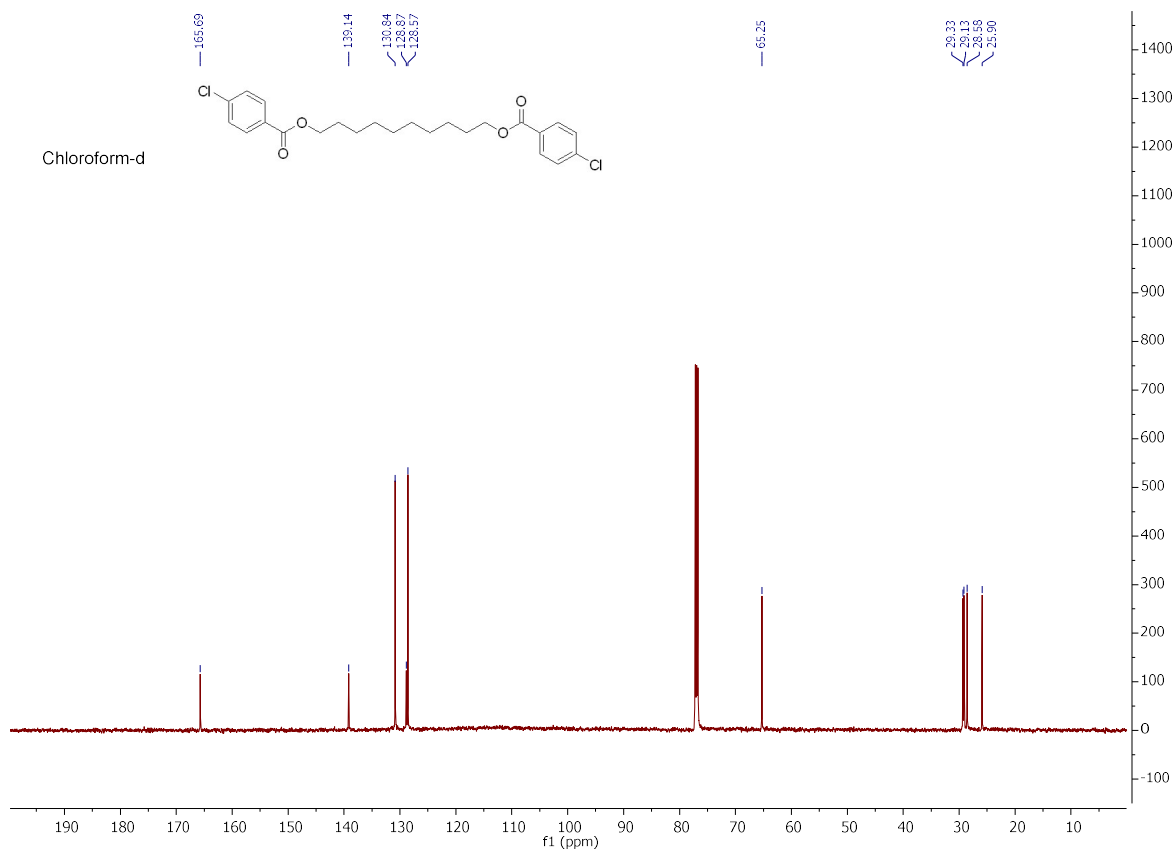
Supplementary Figure S42. ^1H -NMR 6f.



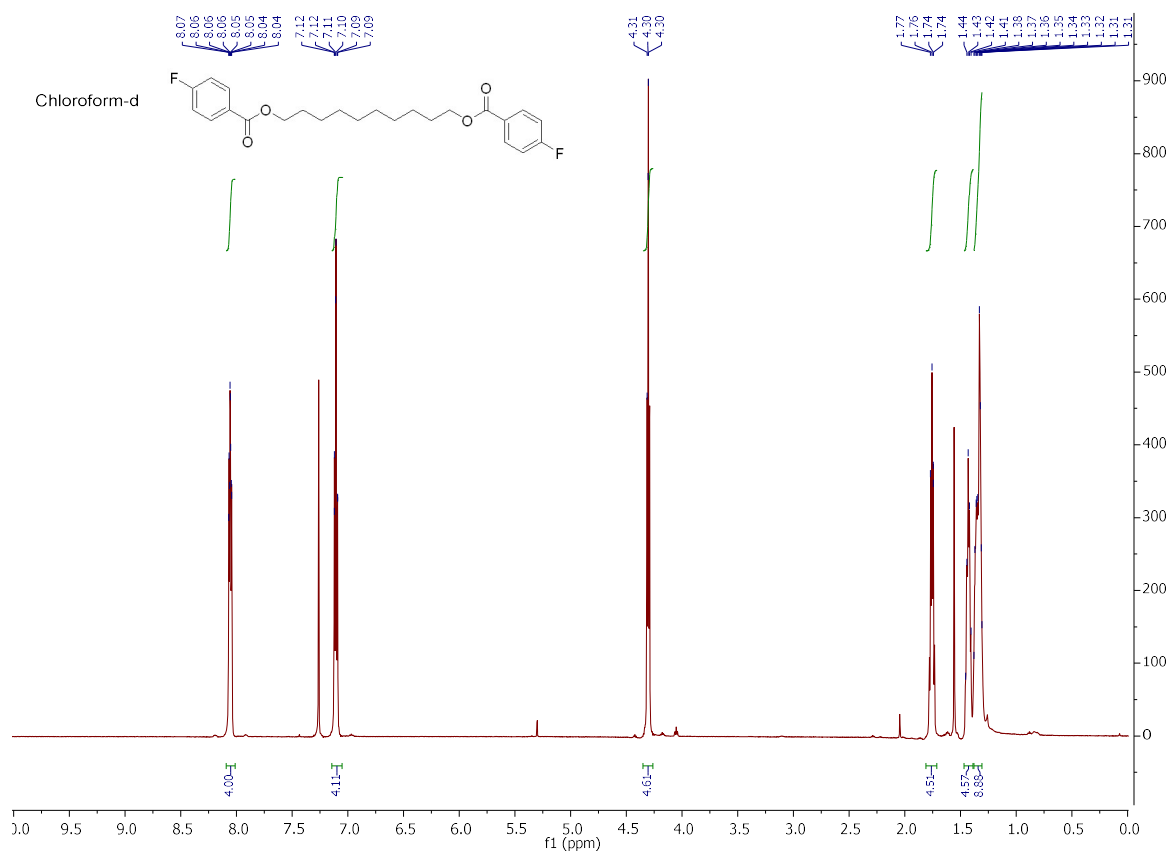
Supplementary Figure S43. ^{13}C -NMR 6f.



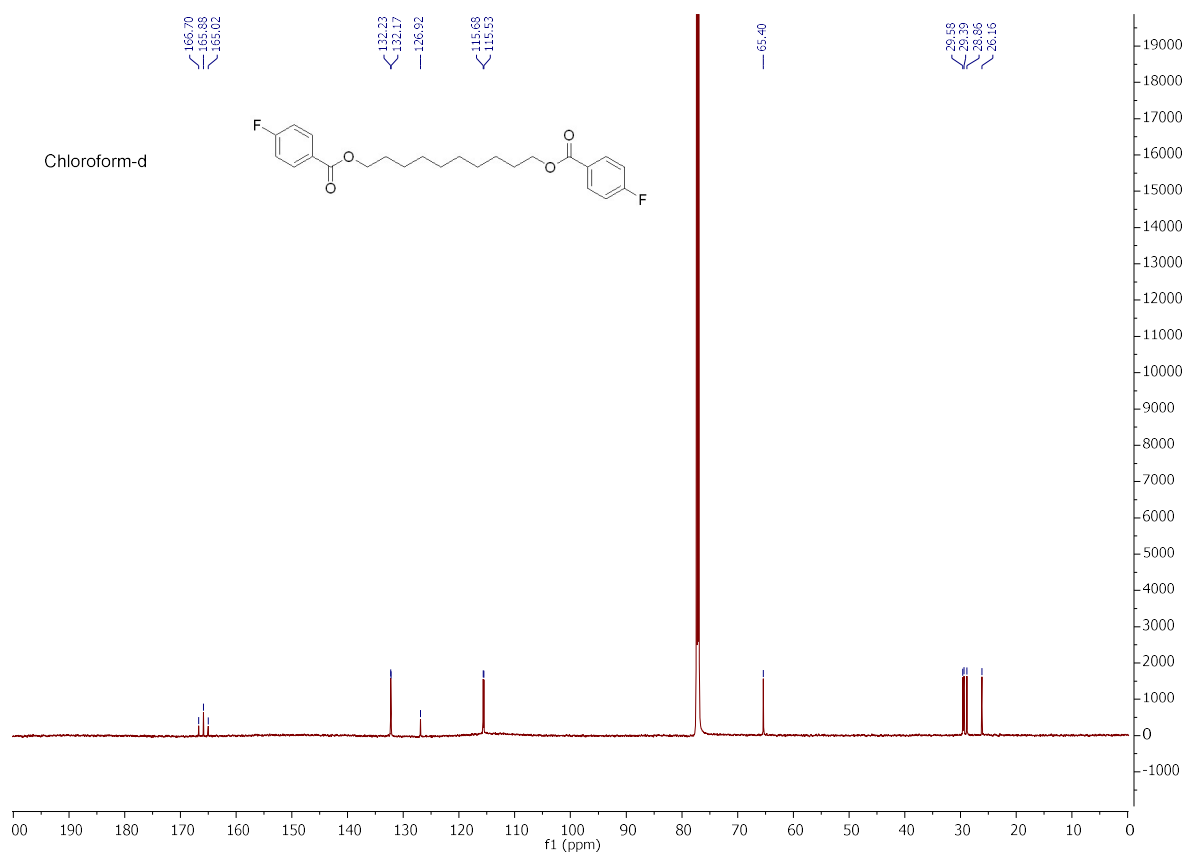
Supplementary Figure S44. ¹H-NMR 6g.



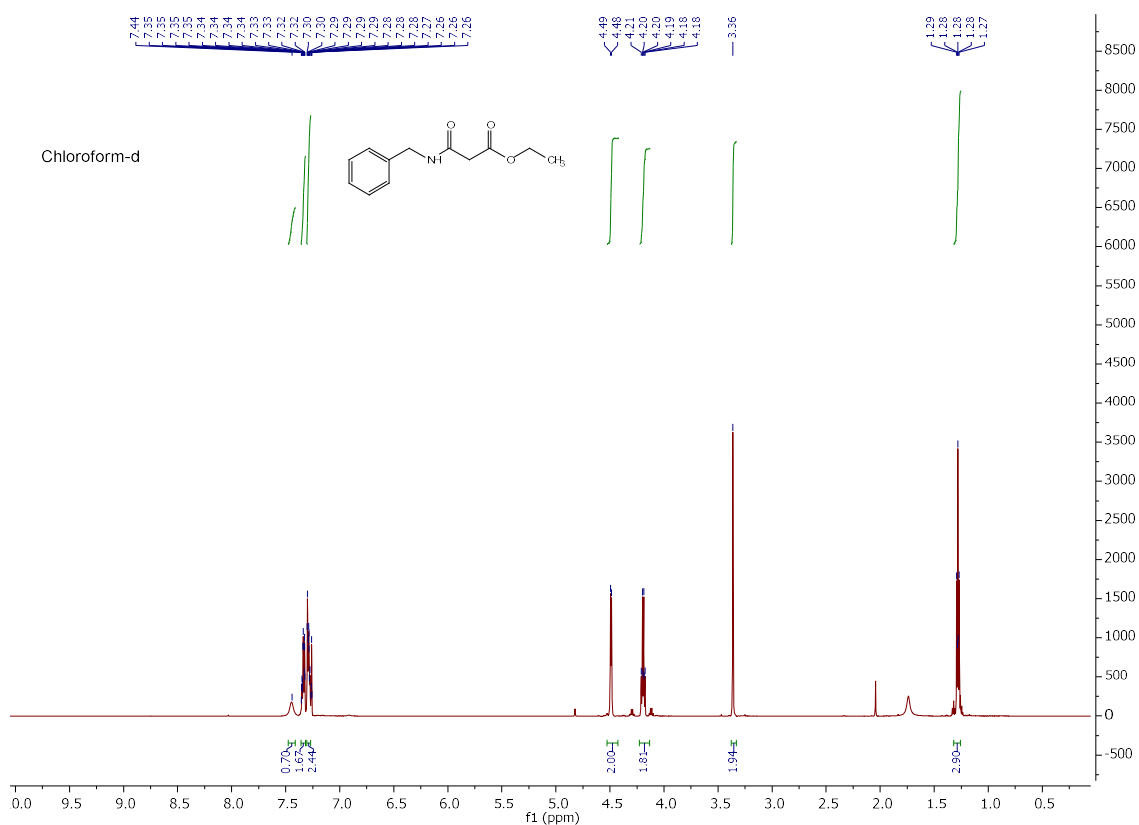
Supplementary Figure S45. ¹³C-NMR 6g.



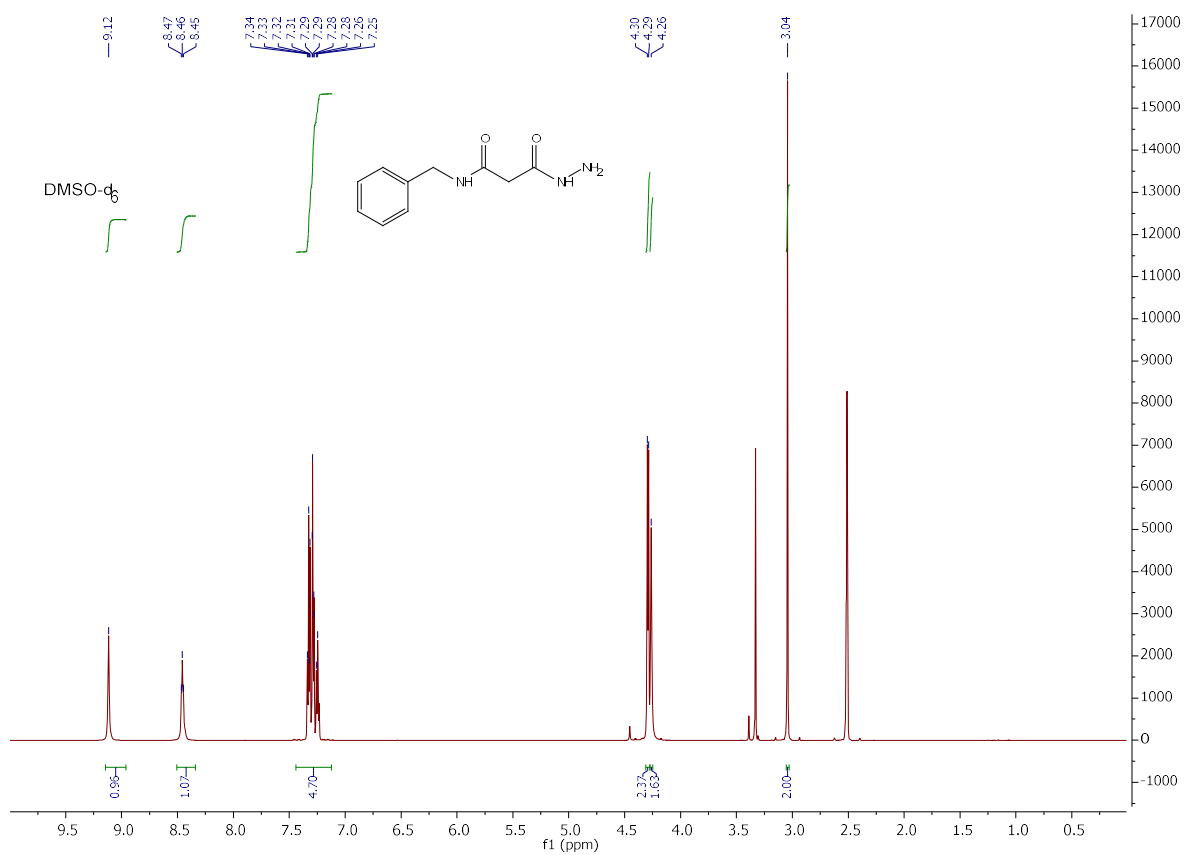
Supplementary Figure S46. ^1H -NMR 6h.



Supplementary Figure S47. ^{13}C -NMR 6h.



Supplementary Figure S48. ^1H -NMR 9.



Supplementary Figure S49. ^1H -NMR 10.

