Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Electronic Supplementary Information for

Zwitterionic indenylammonium with carbon-centred reactivity toward reversible CO_2 binding and catalytic reduction

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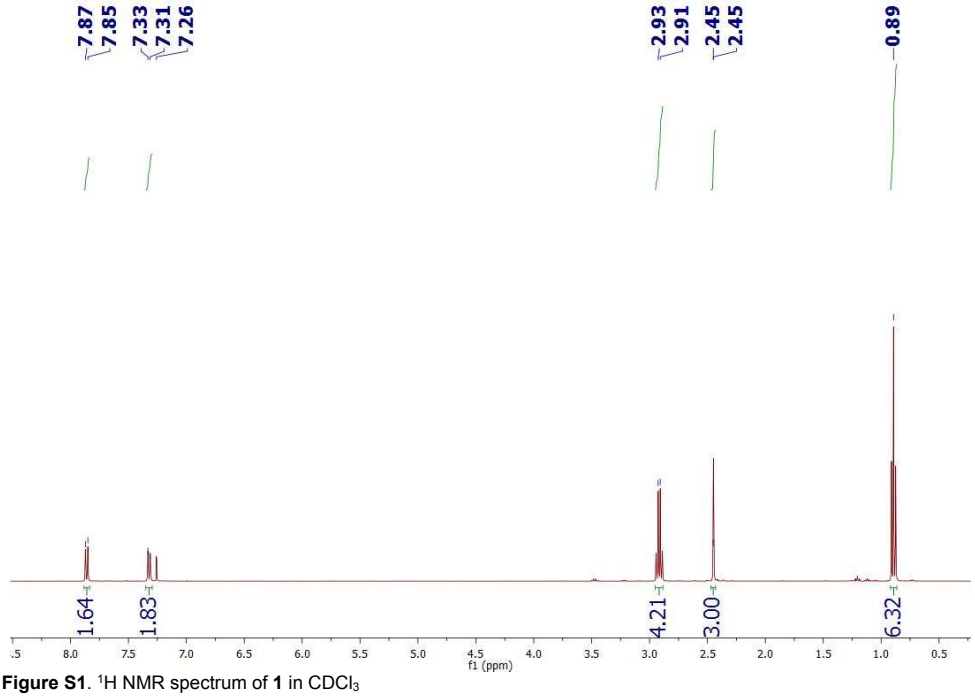
Table of Contents



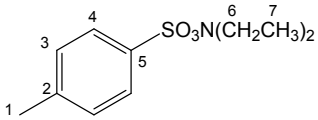


Figure S1. ^{1}H NMR spectrum of **1** in $CDCl_3$

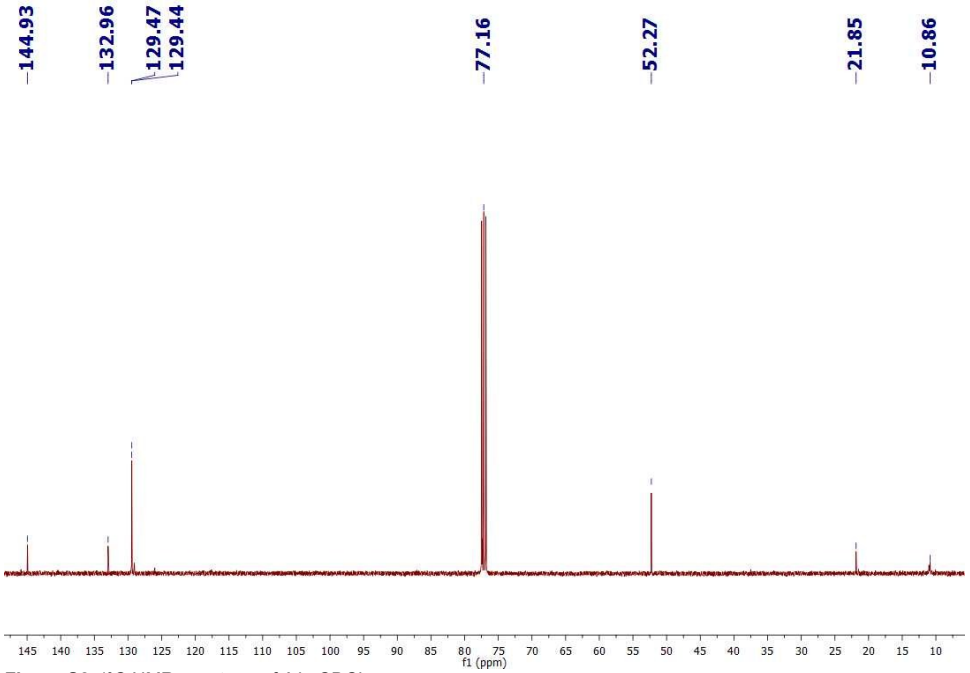
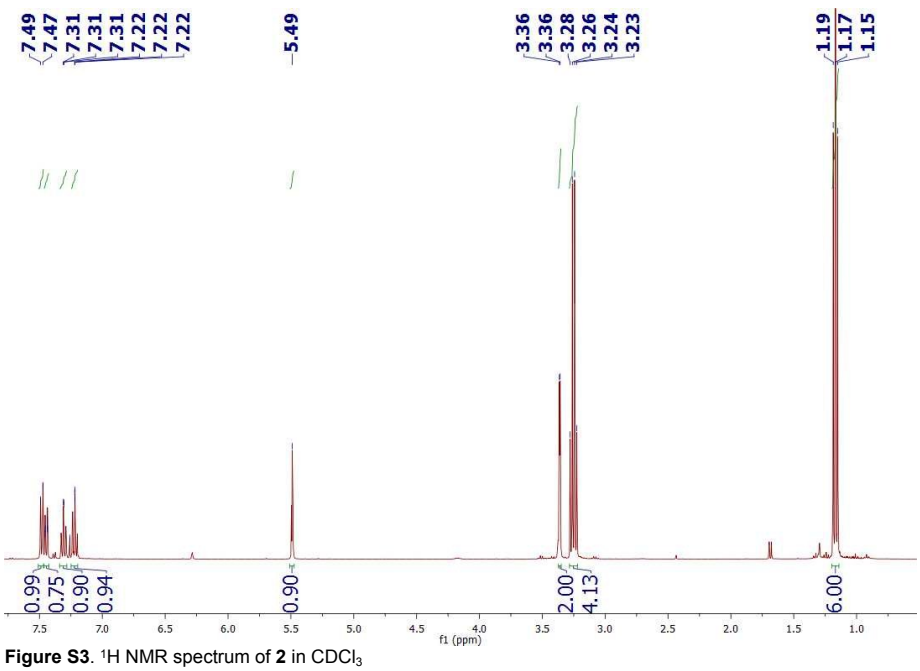


Figure S2. ^{13}C NMR spectrum of **1** in $CDCl_3$



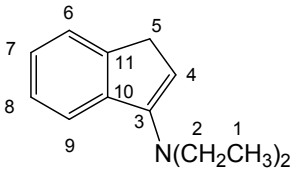


Figure S3. ^{1}H NMR spectrum of **2** in $CDCl_3$

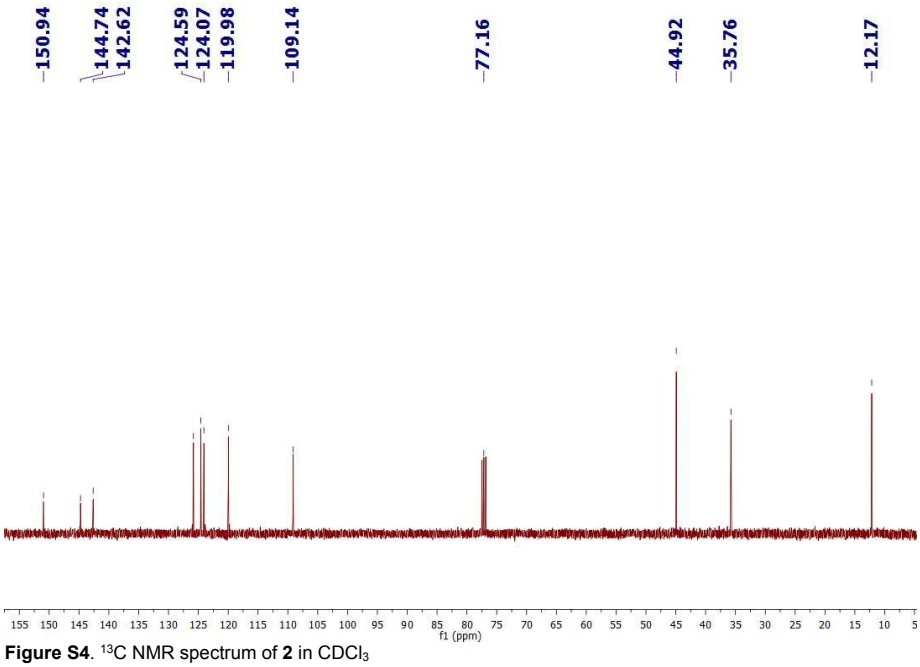
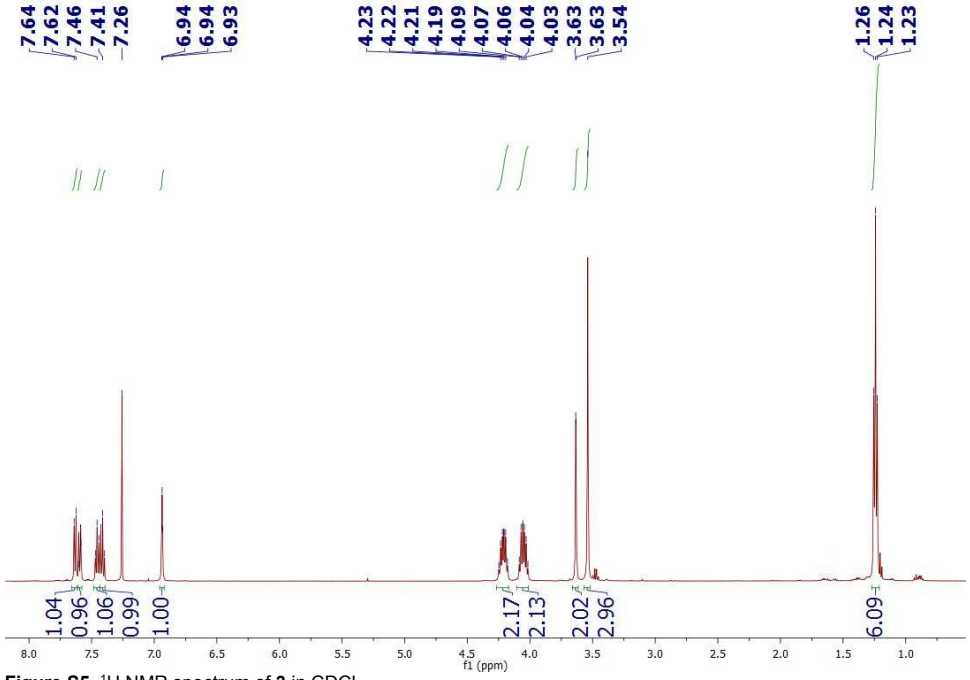


Figure S4. ^{13}C NMR spectrum of **2** in $CDCl_3$



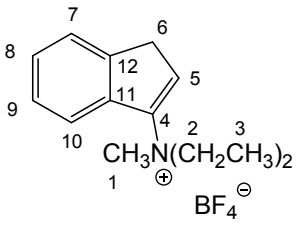


Figure S5. ^{1}H NMR spectrum of **3** in $CDCl_3$

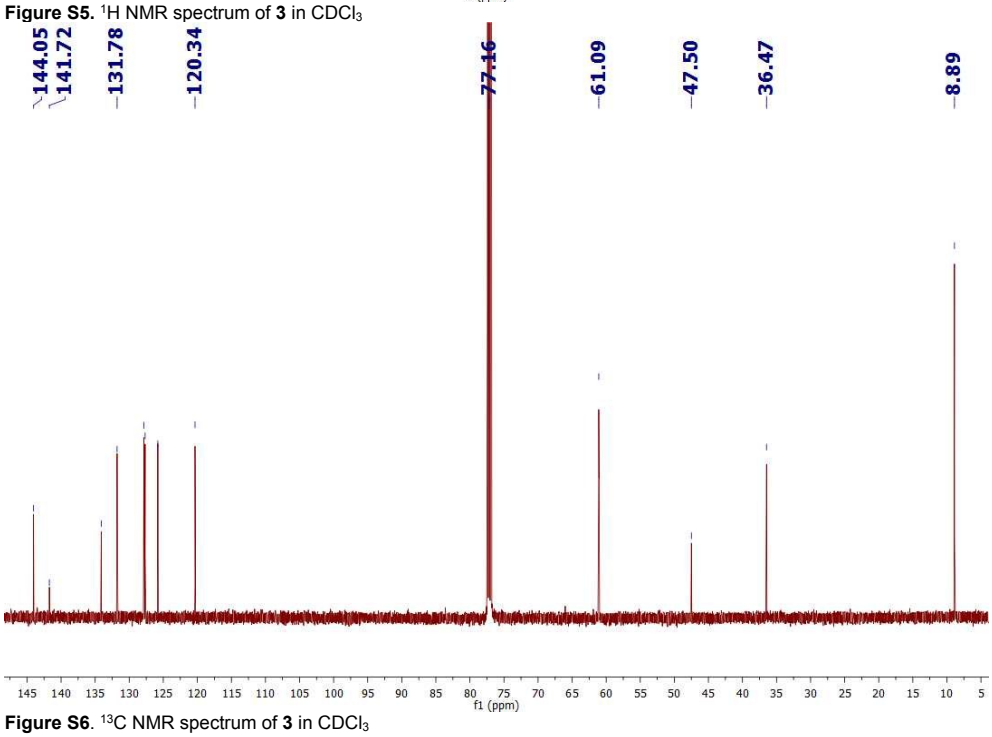
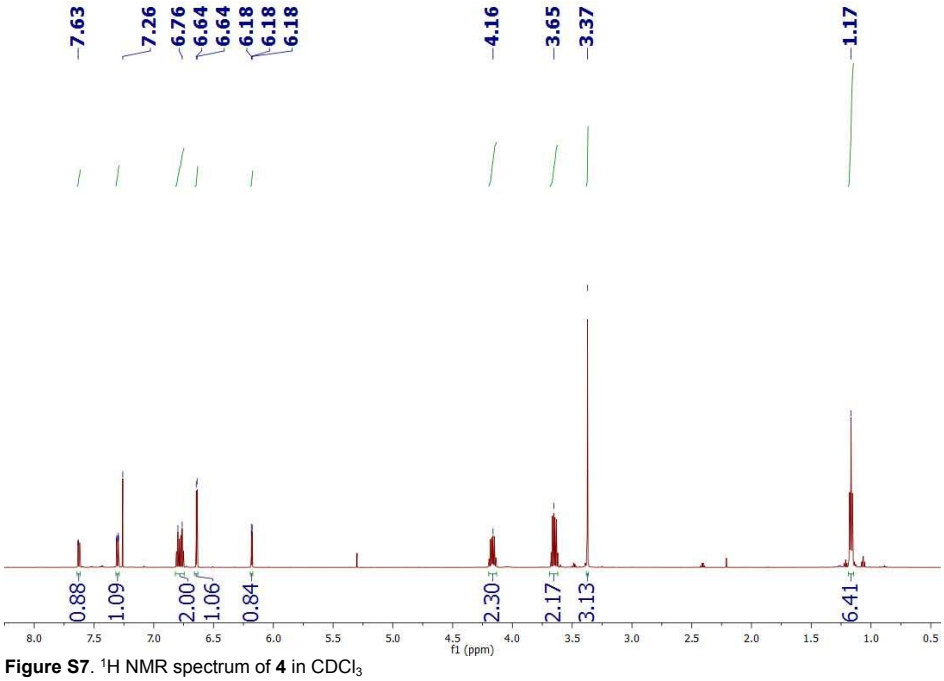


Figure S6. ^{13}C NMR spectrum of **3** in $CDCl_3$



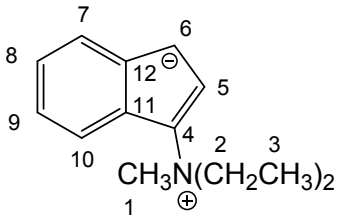


Figure S7. ^{1}H NMR spectrum of **4** in $CDCl_3$

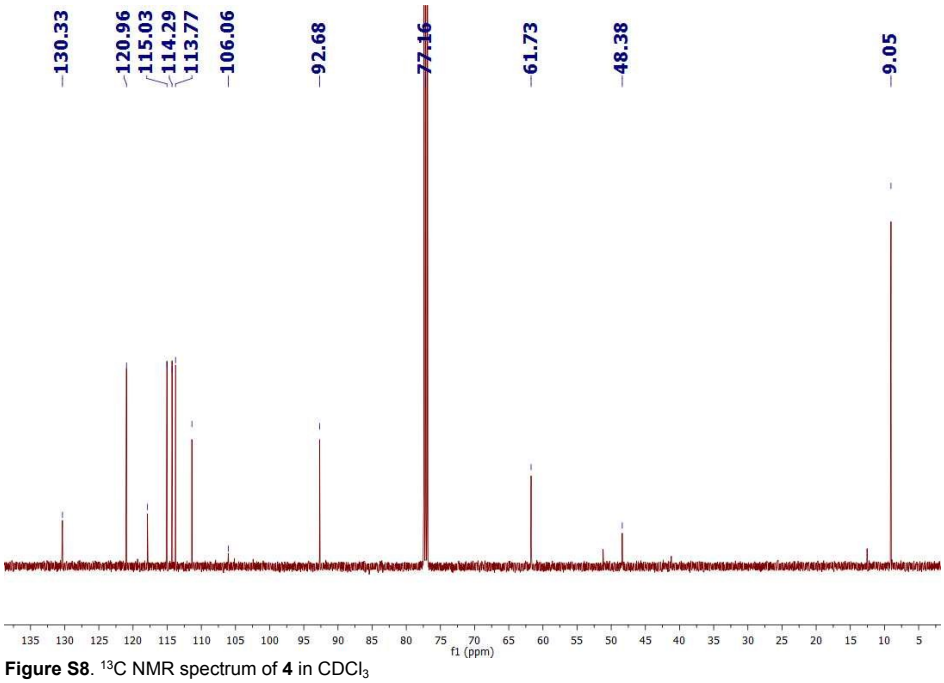


Figure S8. ^{13}C NMR spectrum of **4** in $CDCl_3$

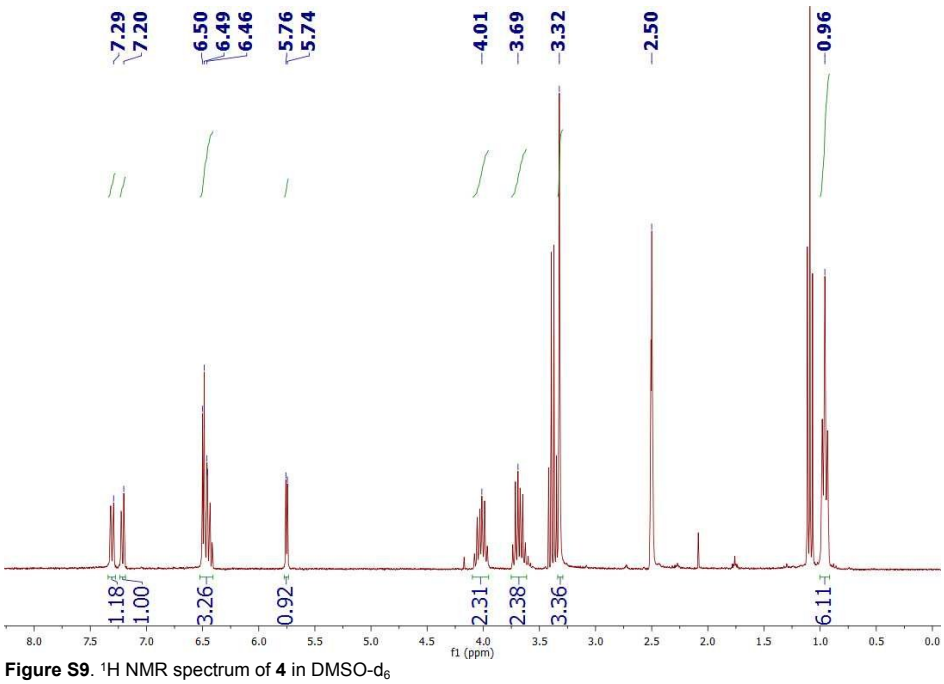
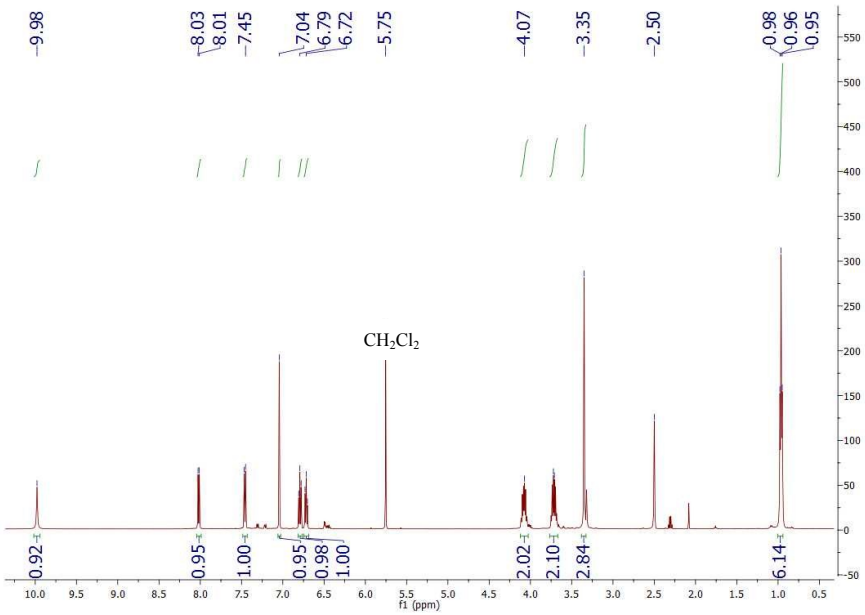


Figure S9. ^{1}H NMR spectrum of **4** in DMSO-d_6



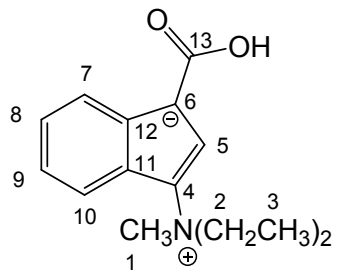


Figure S10. ^{1}H NMR spectrum of **5** in DMSO-d_6. The peak at 9.98 ppm in the ^{1}H NMR spectrum corresponds to a carboxylic acid.

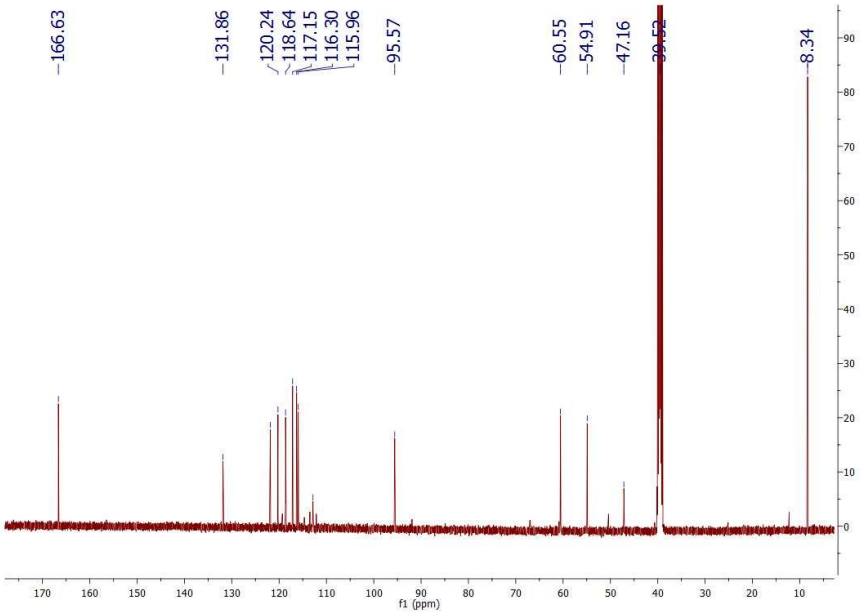


Figure S11. ^{13}C NMR spectrum of **5** in DMSO-d_6. The ^{13}C NMR spectrum confirms the formation of a carboxylic acid species with a new peak a 166.63 ppm.

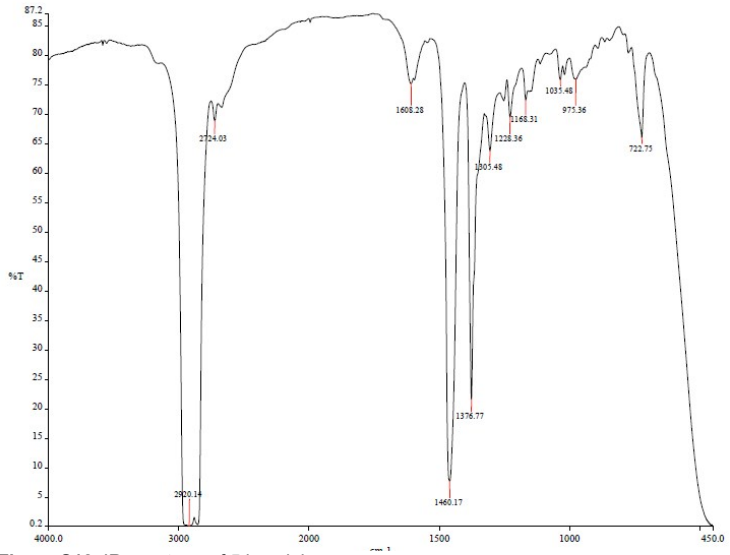


Figure S12. IR spectrum of **5** in nujol.

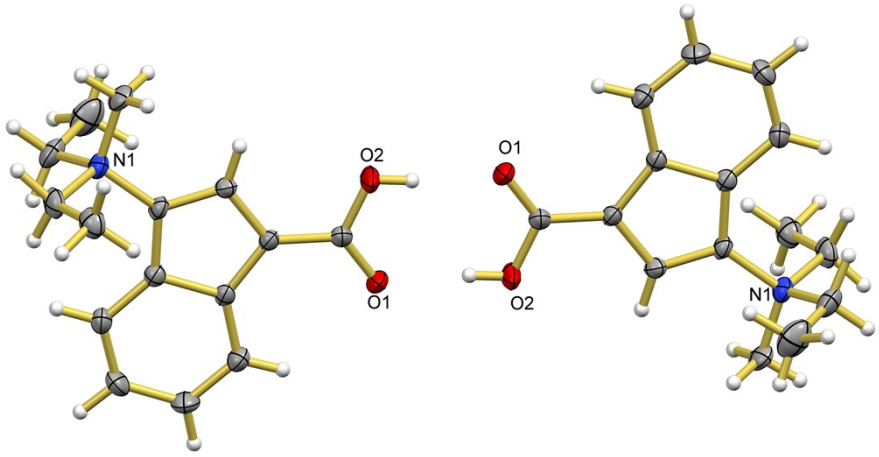
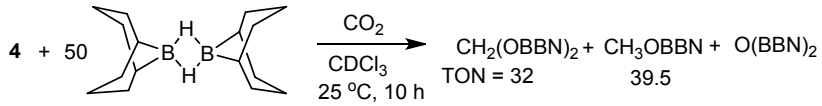


Figure S13. The hydrogen bonded pair in the crystal lattice of **5**. The intermolecular O1−O2 distance is ~2.6 Å.

Table S1. Selected crystallographic data of 5:

	5
Formula	$C_{15}H_{19}NO_2 \cdot 0.5CH_2Cl_2$
FW	287.77
T (K)	150(2)
space group	$P2_1/n$
a (Å)	7.8393(9)
b (Å)	10.837(1)
c (Å)	17.382(2)
α (deg)	90
β (deg)	94.666(5)
γ (deg)	90
V (Å^3)	1471.7(3)
Z	4
D_c (g·cm^{-3})	1.299
μ (mm^{-1})	0.259
no. of refln collected	12831
no. of indept refln	3347
GOF on F^2	1.012
R [$I > 2\sigma(I)$]	R_1 = 0.0664
	wR_2 = 0.1285
R (all data)	R_1 = 0.1588
	wR_2 = 0.1635



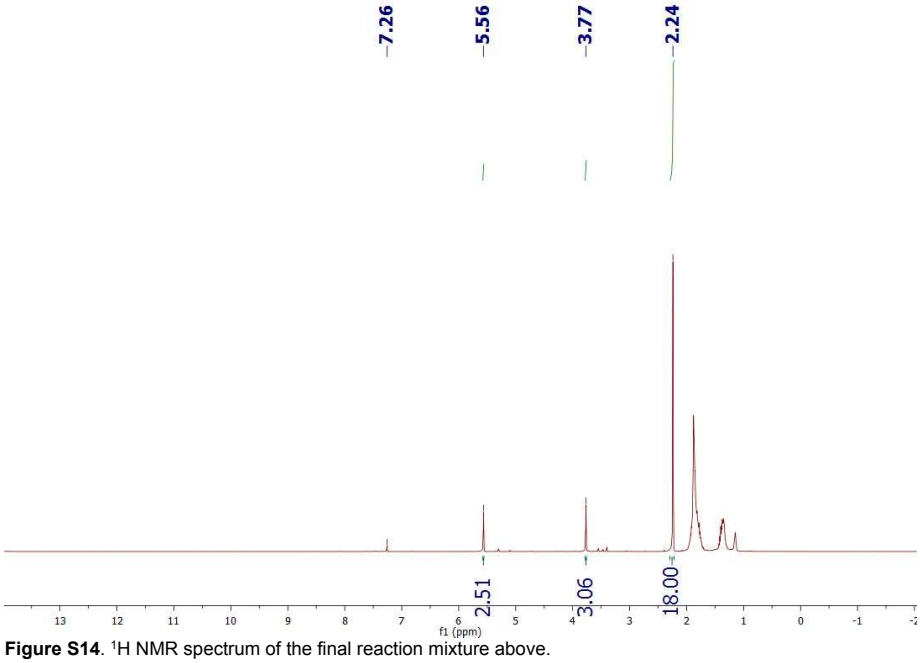


Figure S14. ^{1}H NMR spectrum of the final reaction mixture above.

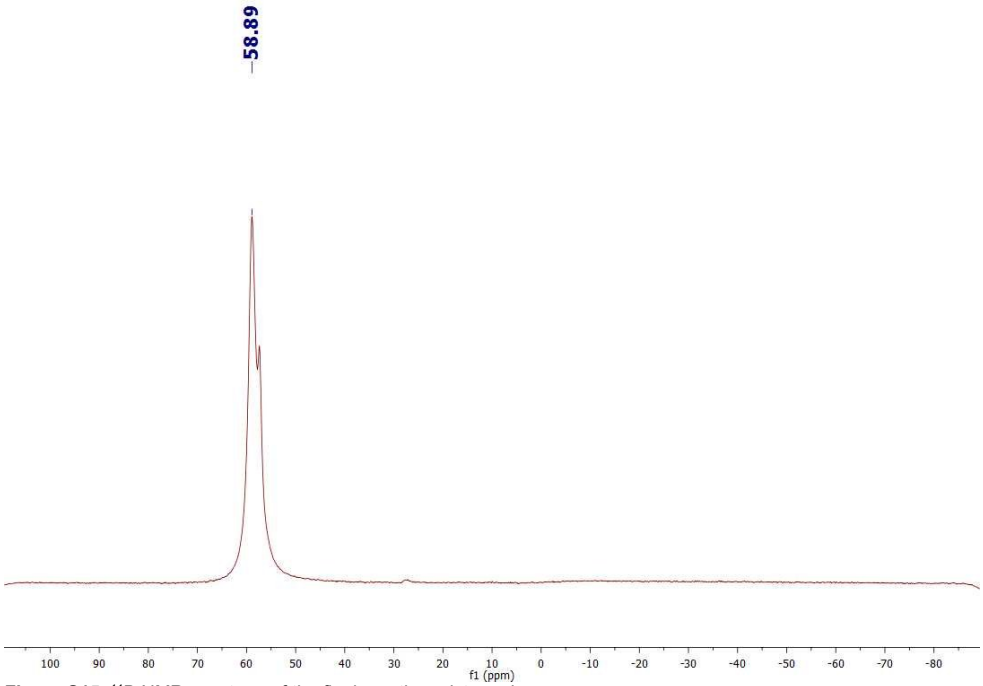
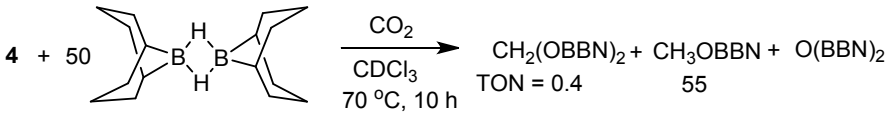


Figure S15. ^{11}B NMR spectrum of the final reaction mixture above



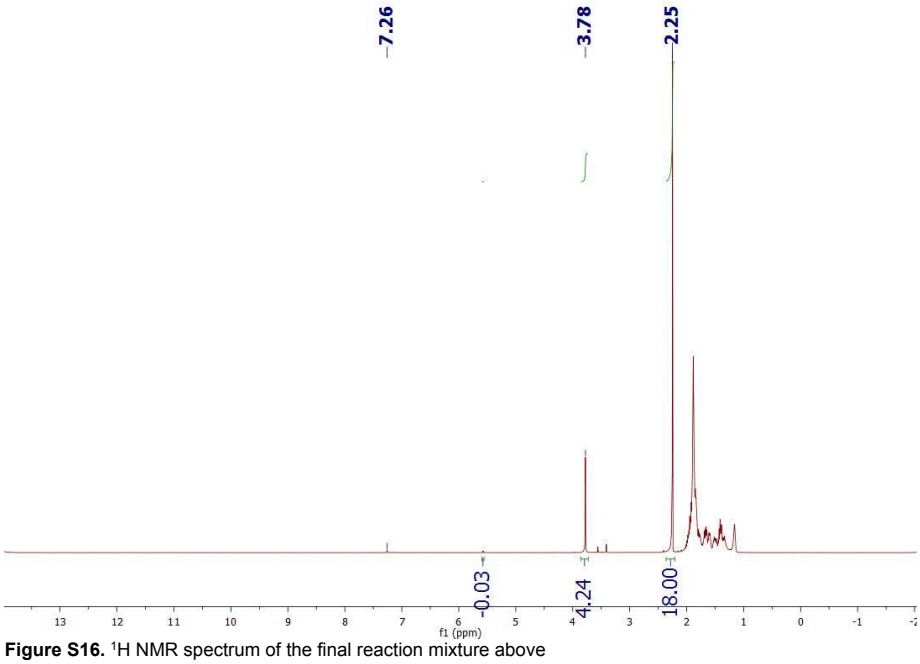


Figure S16. ^{1}H NMR spectrum of the final reaction mixture above

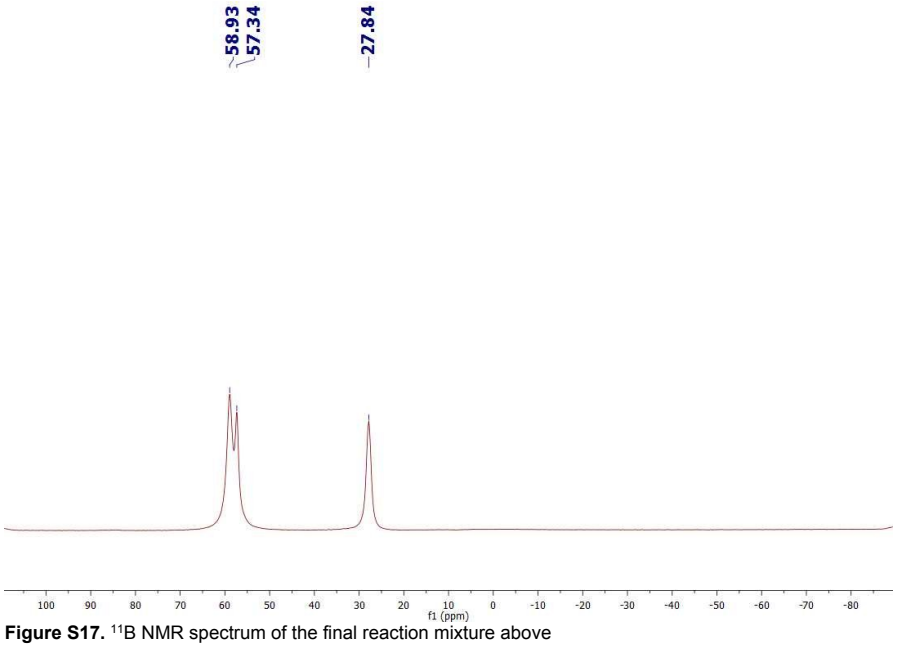
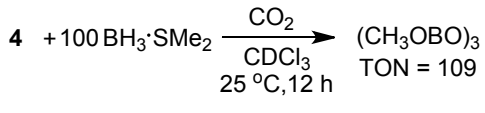


Figure S17. ^{11}B NMR spectrum of the final reaction mixture above



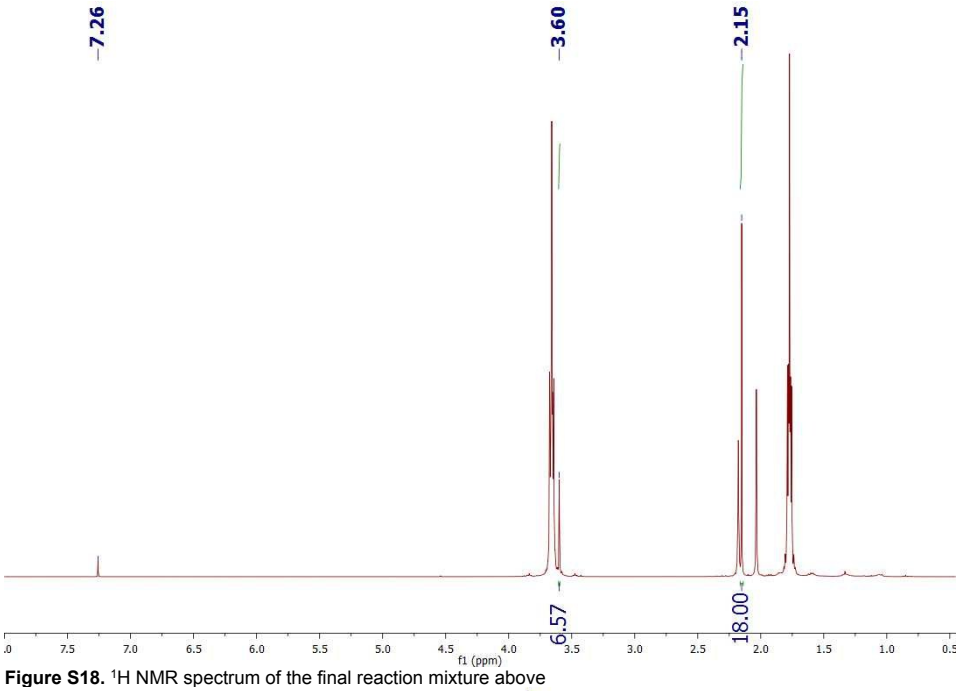


Figure S18. ^{1}H NMR spectrum of the final reaction mixture above

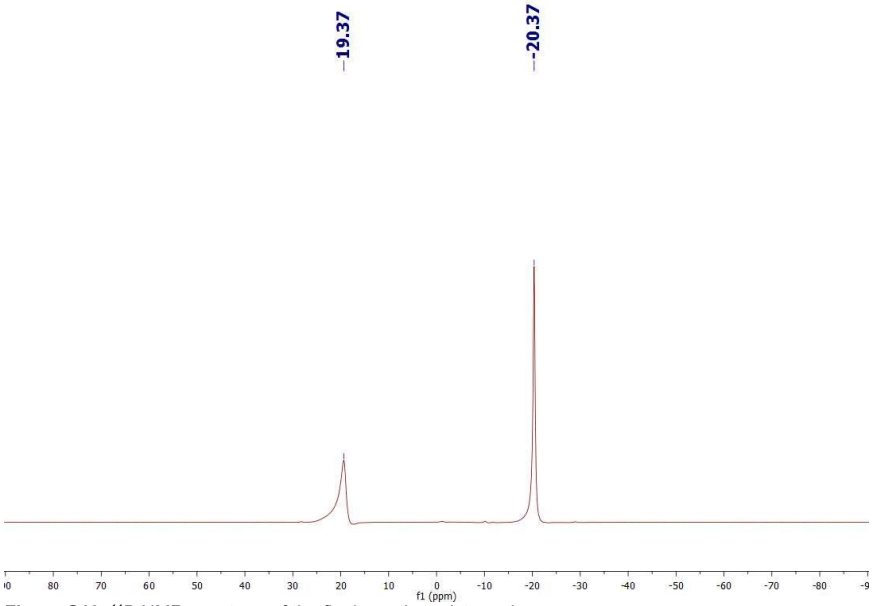
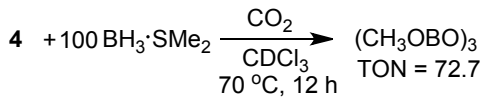


Figure S19. ^{11}B NMR spectrum of the final reaction mixture above



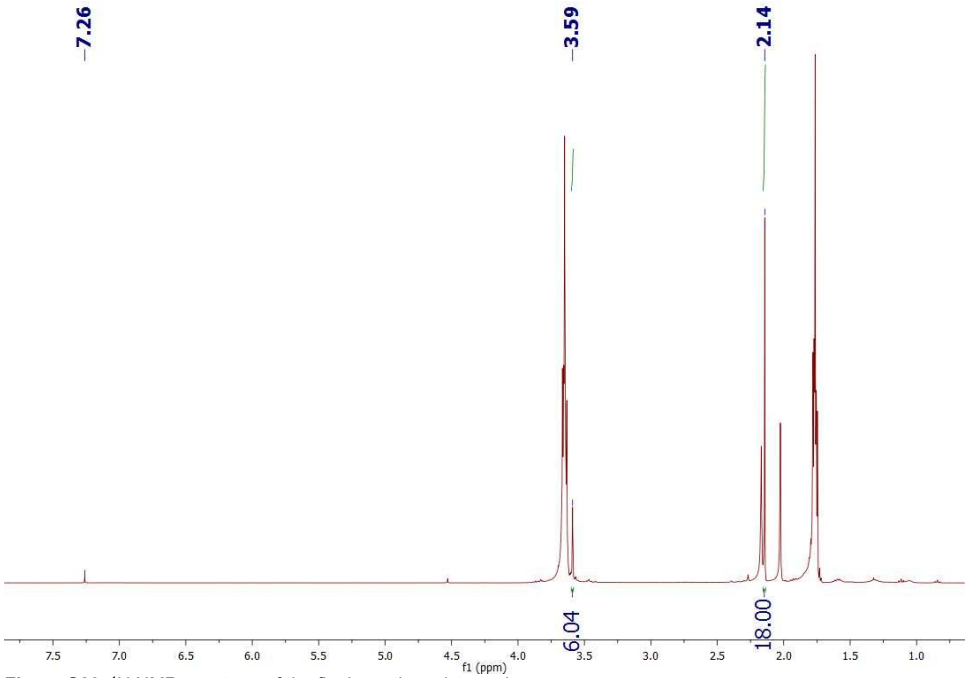


Figure S20. ^{1}H NMR spectrum of the final reaction mixture above

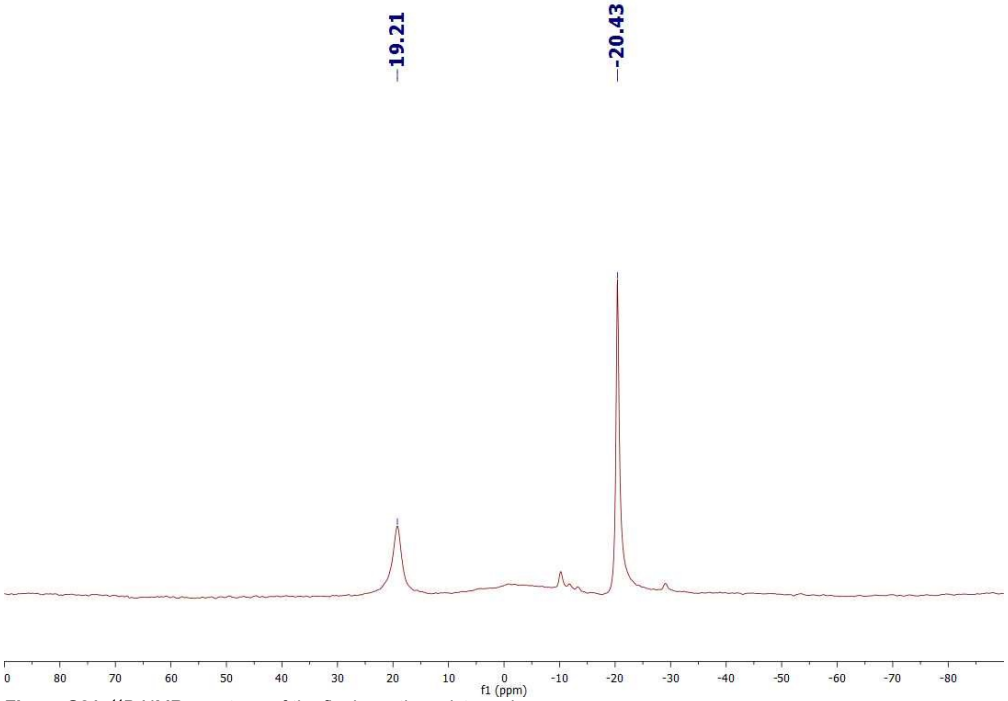
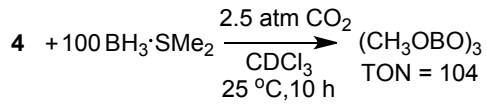


Figure S21. ^{11}B NMR spectrum of the final reaction mixture above



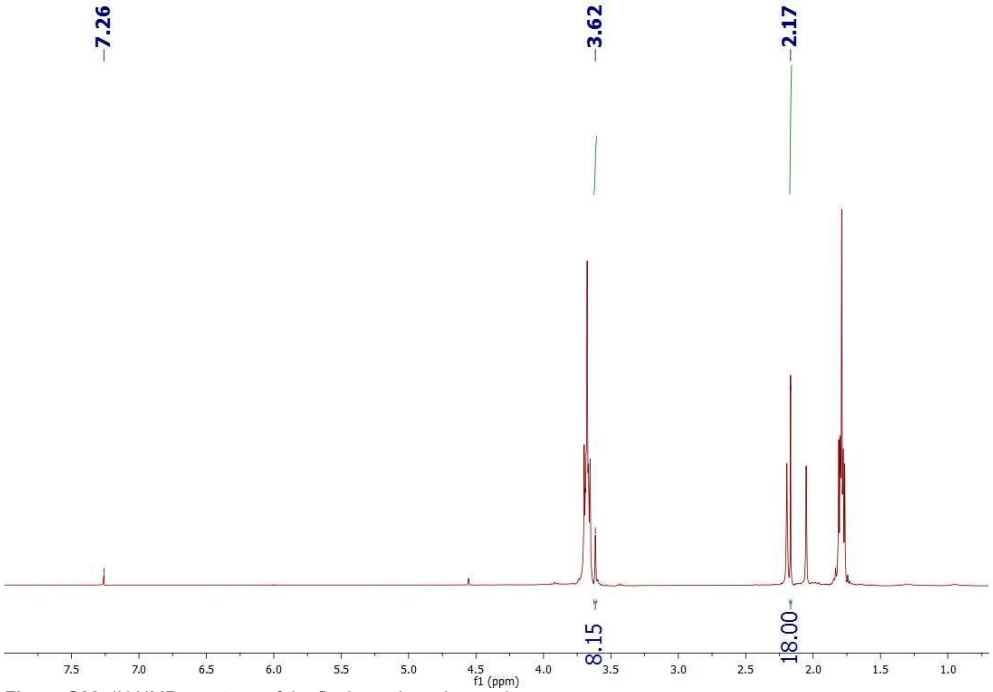


Figure S22. ^{1}H NMR spectrum of the final reaction mixture above

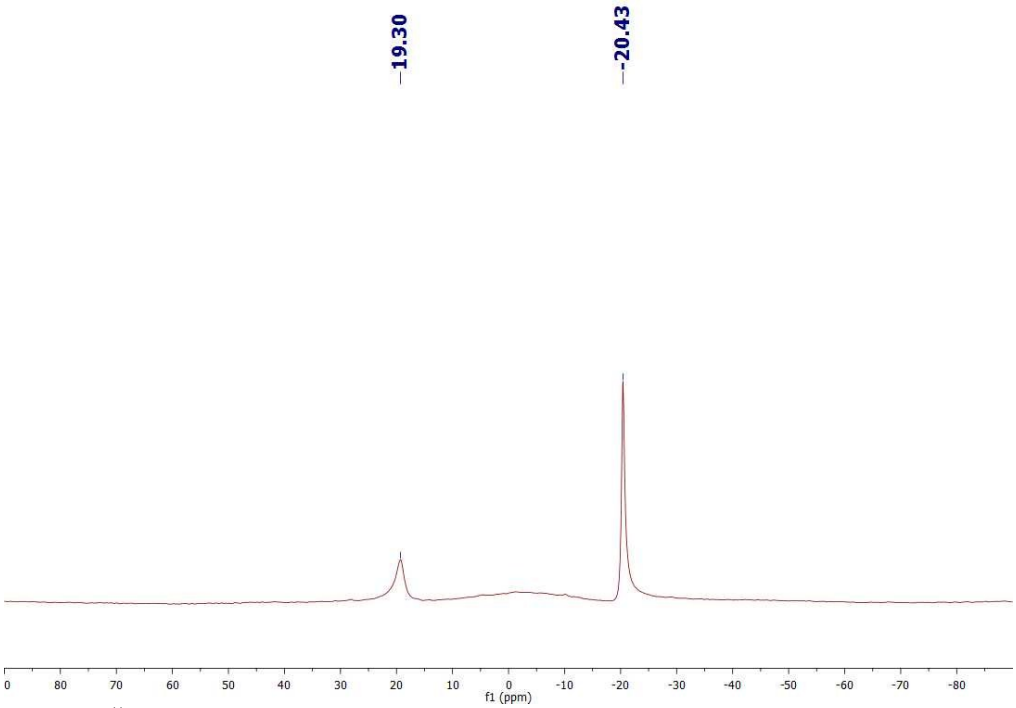
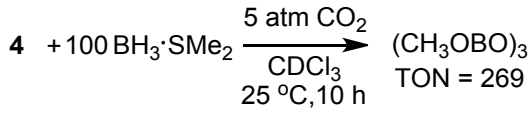


Figure S23. ^{11}B NMR spectrum of the final reaction mixture above



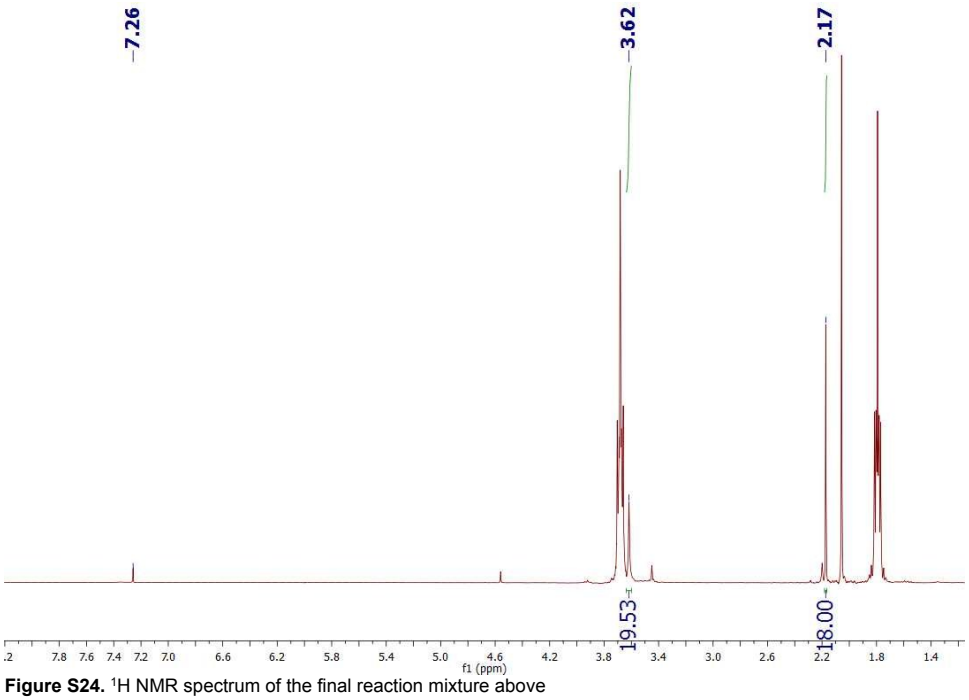


Figure S24. ^{1}H NMR spectrum of the final reaction mixture above

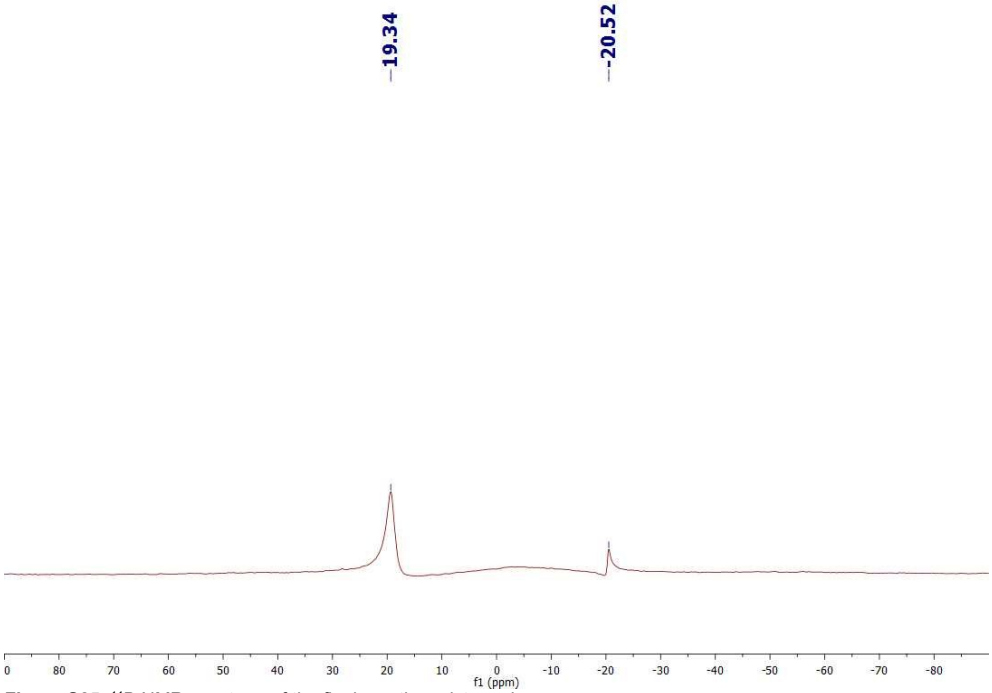
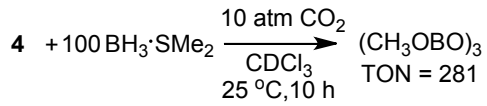


Figure S25. ^{11}B NMR spectrum of the final reaction mixture above



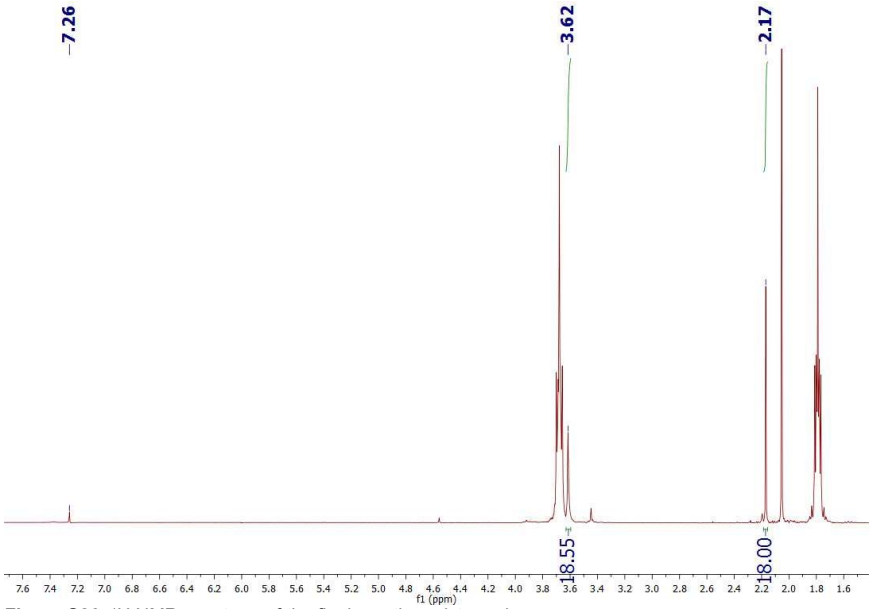


Figure S26. ^{1}H NMR spectrum of the final reaction mixture above

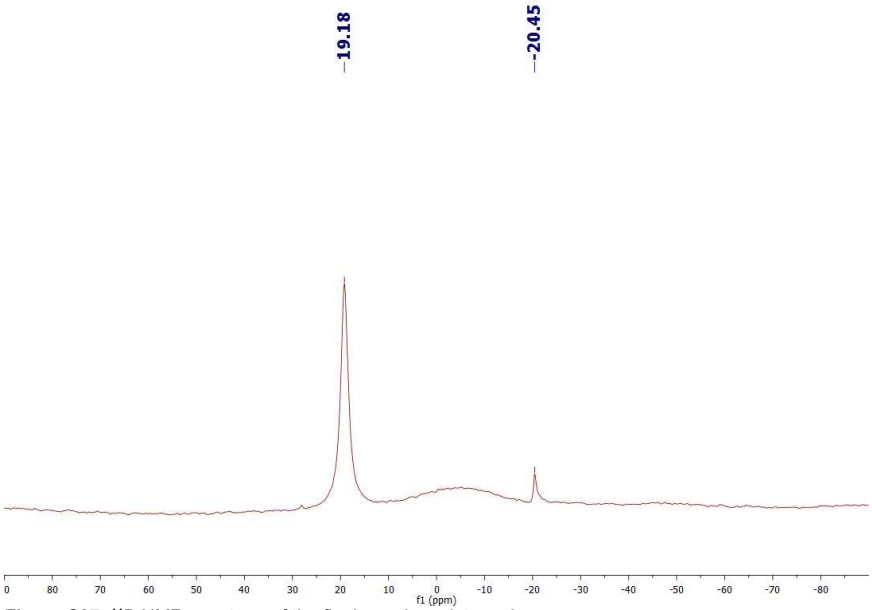


Figure S27. ^{11}B NMR spectrum of the final reaction mixture above