

Supporting information
for
Synthesis of Novel Multifunctional *bora*-Ibuprofen
Derivatives

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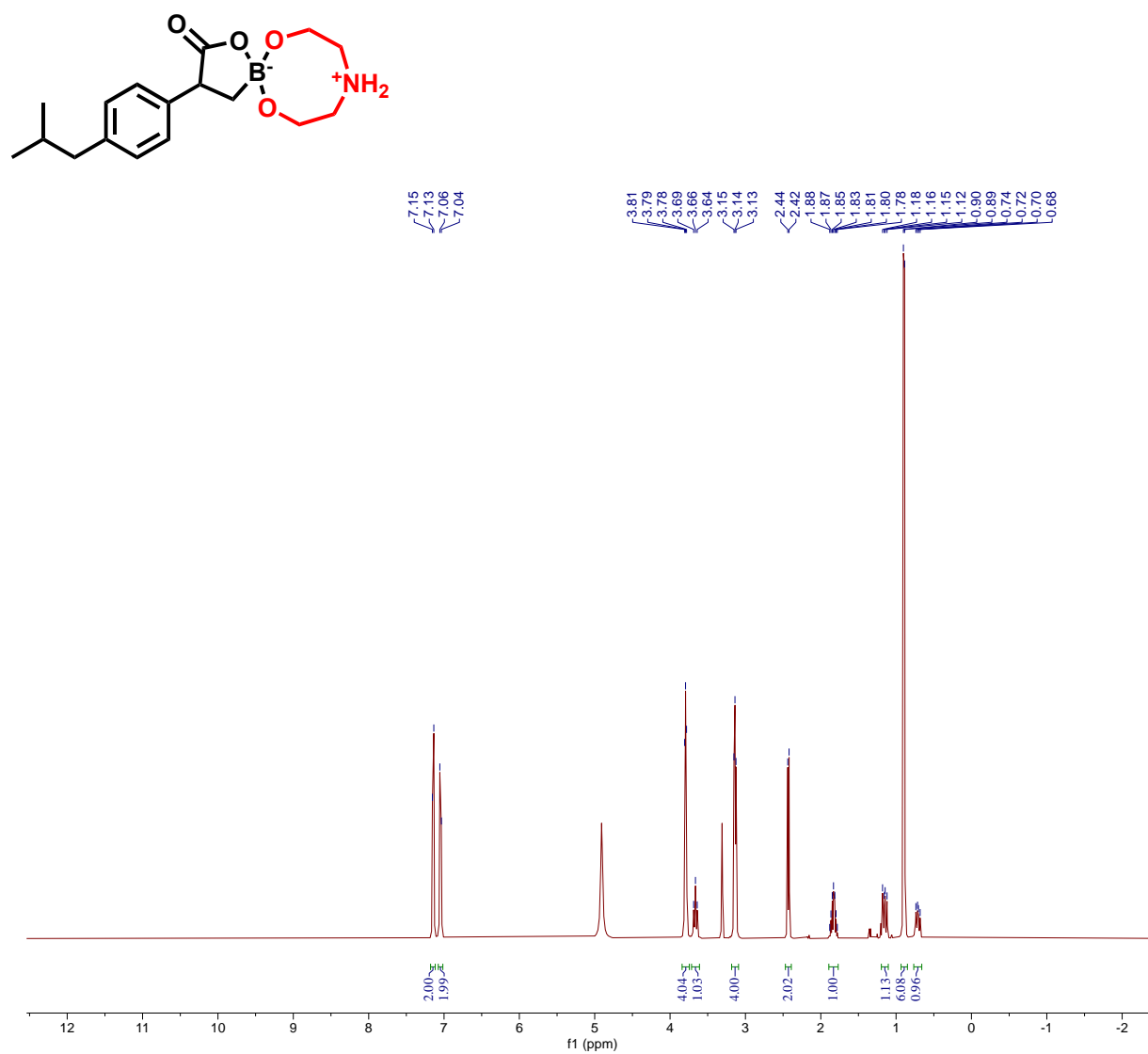


Figure S1. ^1H NMR Spectrum of **1^{DEA}** in CD $_3$ OD.

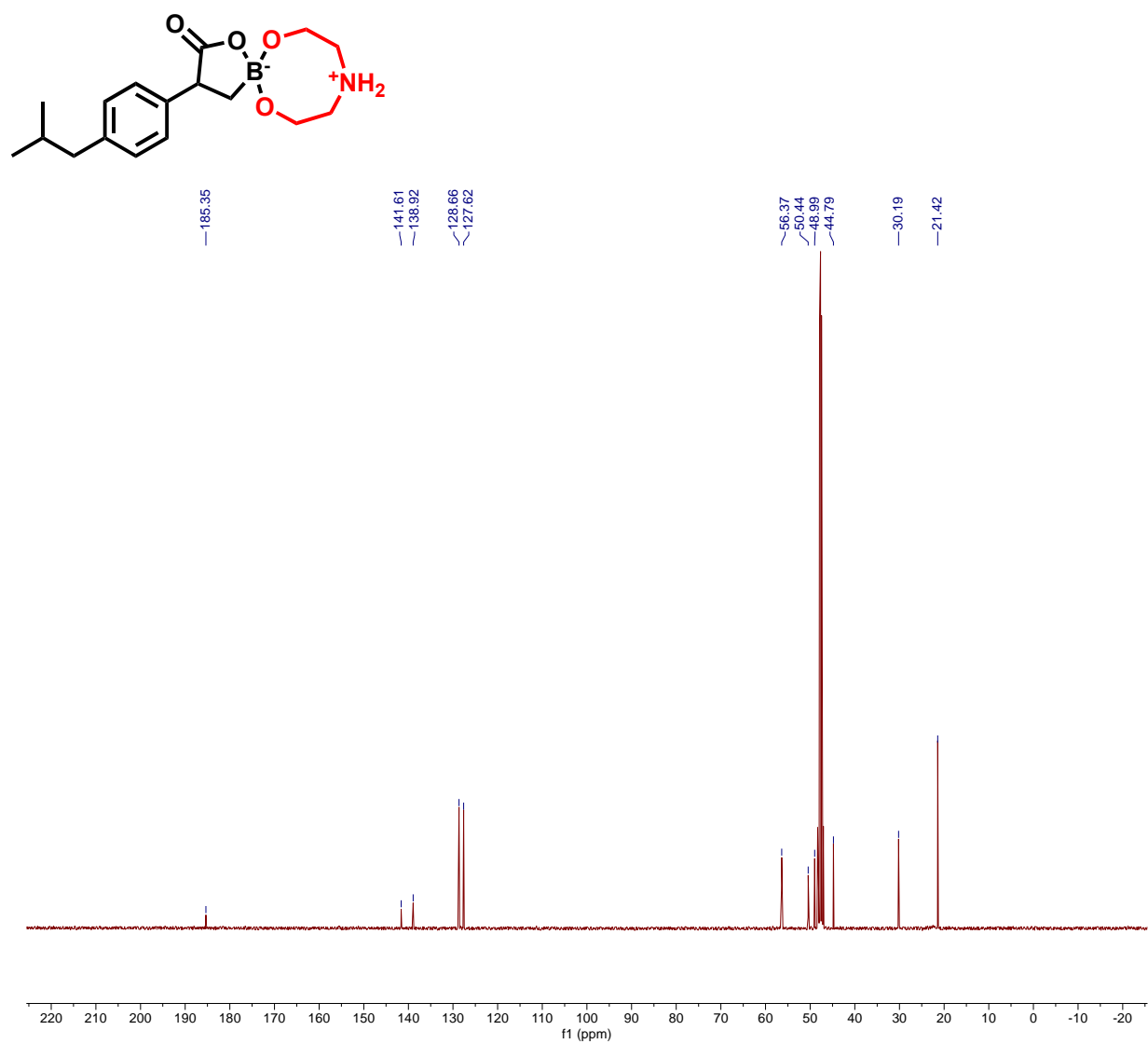


Figure S2. ¹³C NMR Spectrum of **1^{DEA}** in CD₃OD.

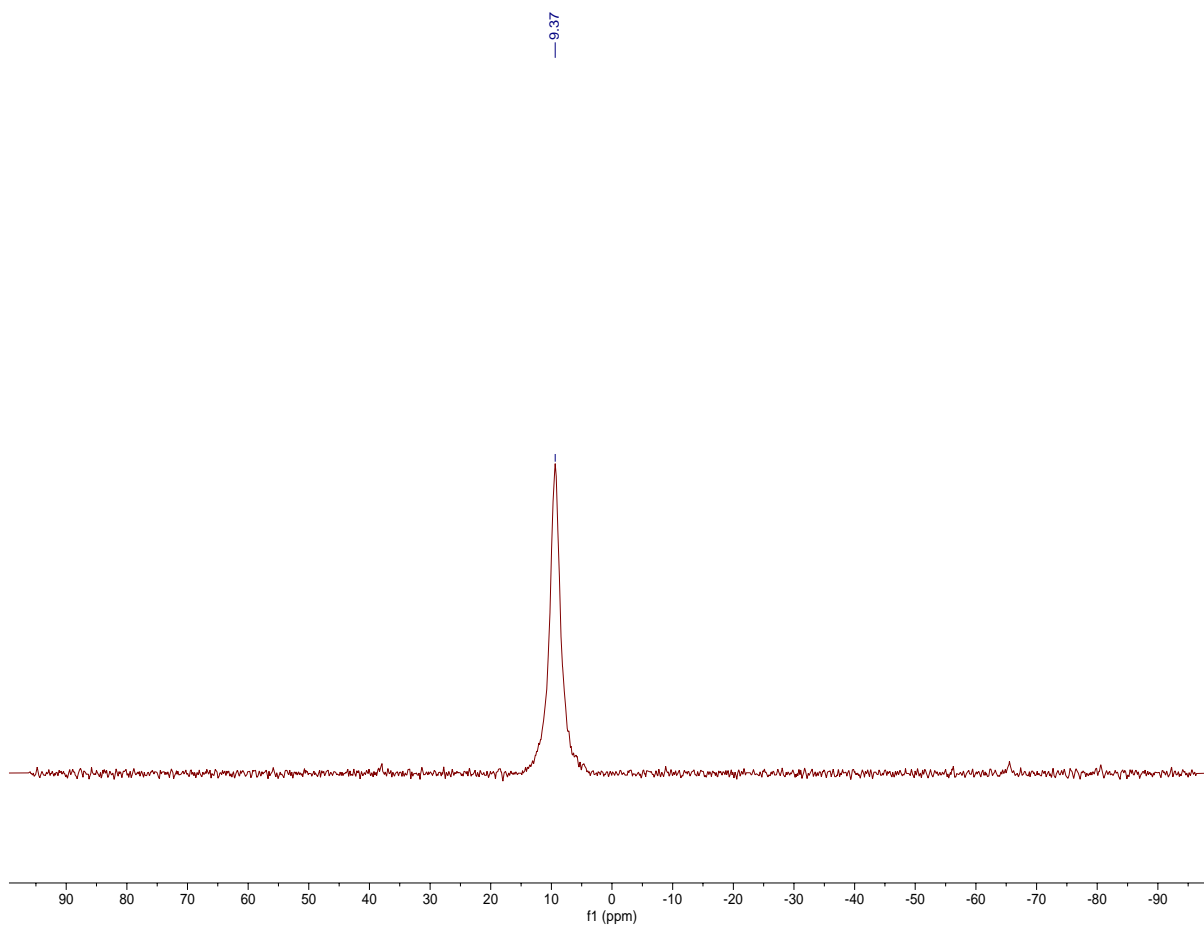
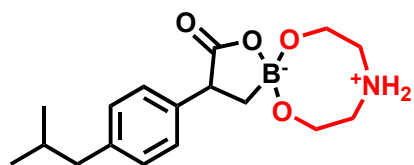
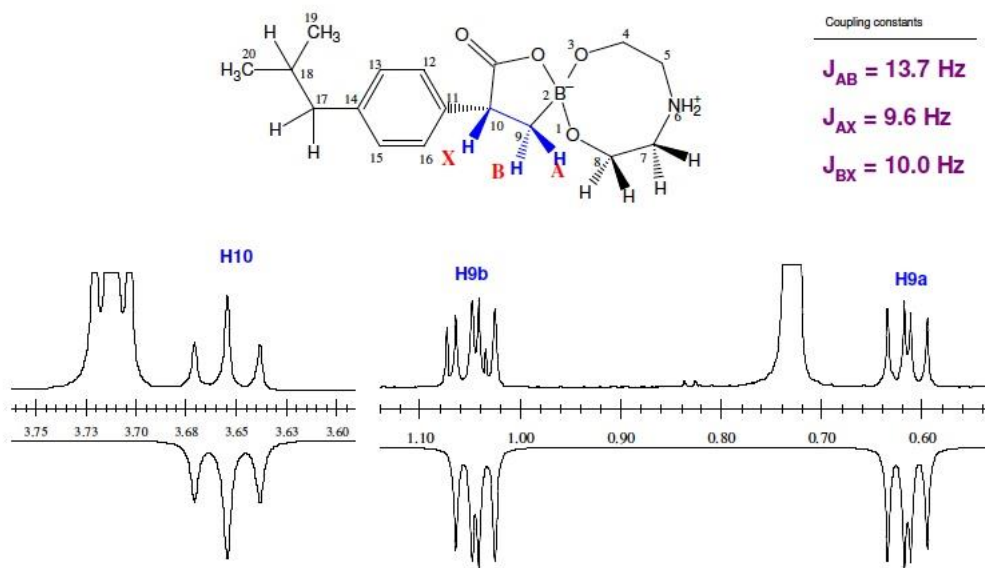
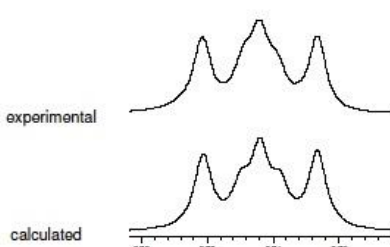


Figure S3. ^{11}B NMR Spectrum of **1**^{DEA} in CD_3OD .

ABX spin system



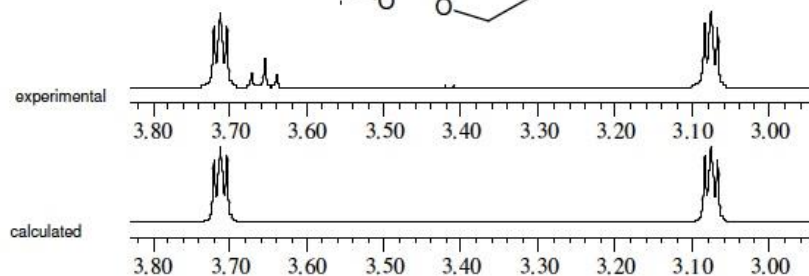
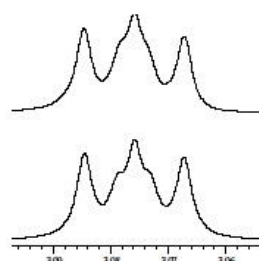
AA part of the AA'XX' spin system



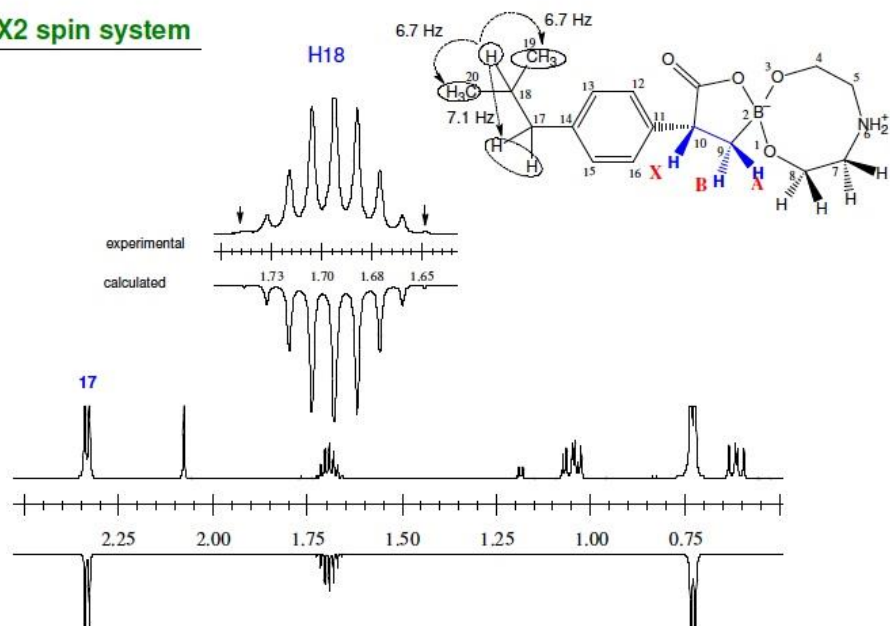
Coupling constants

- $J_{AA'} = -13.96 \text{ Hz}$
- $J_{XX'} = -13.71 \text{ Hz}$
- $J_{AX} = 3.44 \text{ Hz}$
- $J_{AX'} = 6.99 \text{ Hz}$

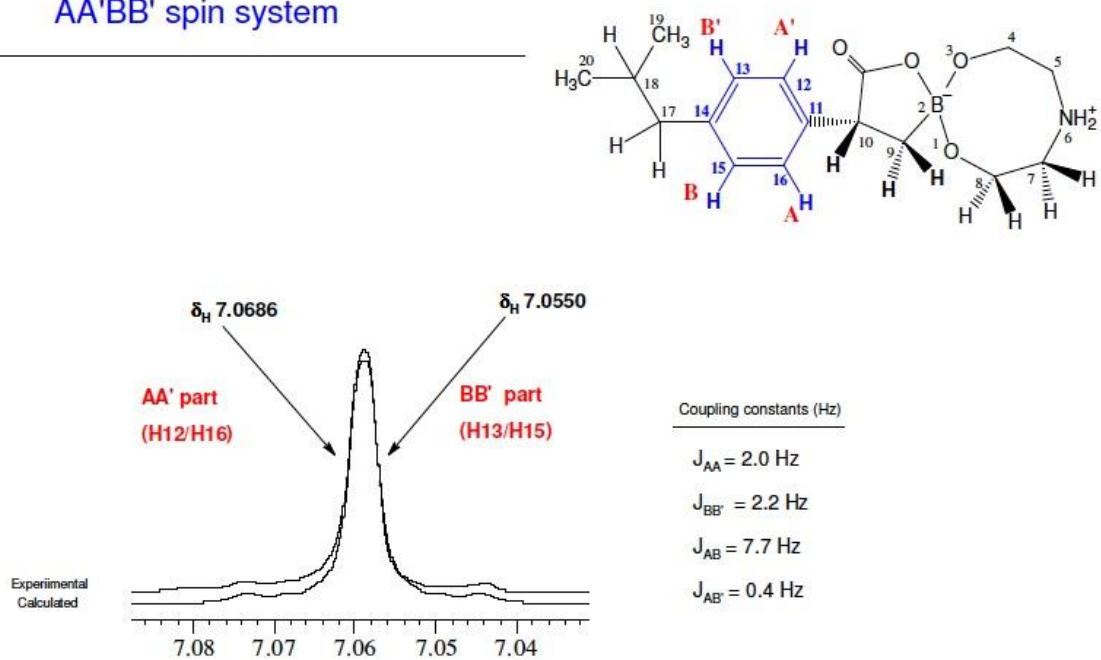
XX part of the AA'XX' spin system



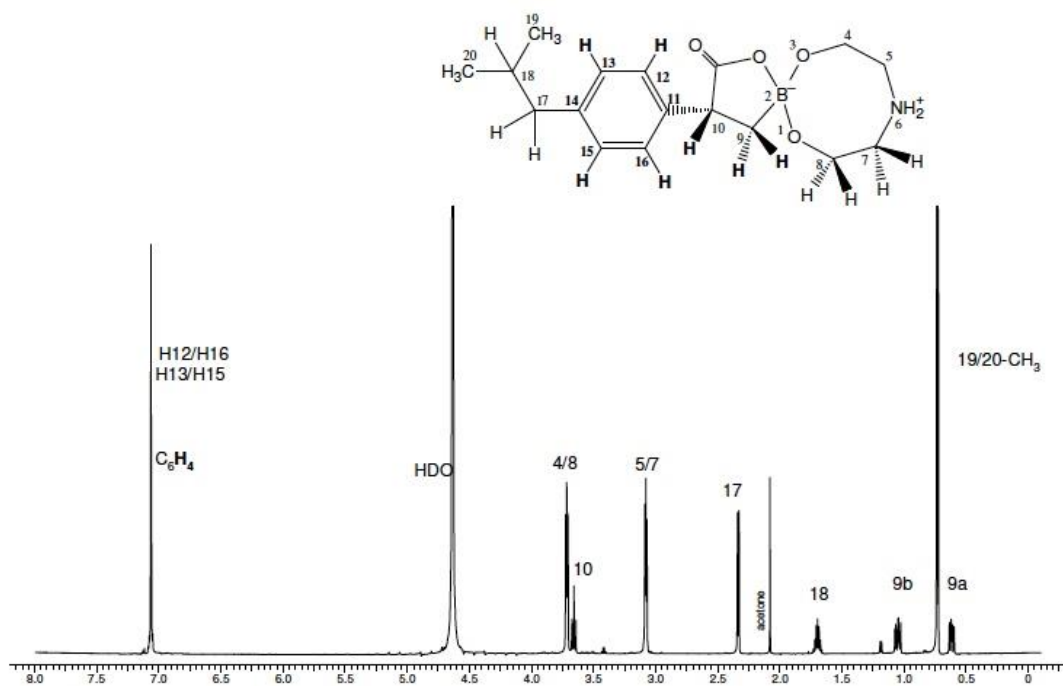
A6BX2 spin system



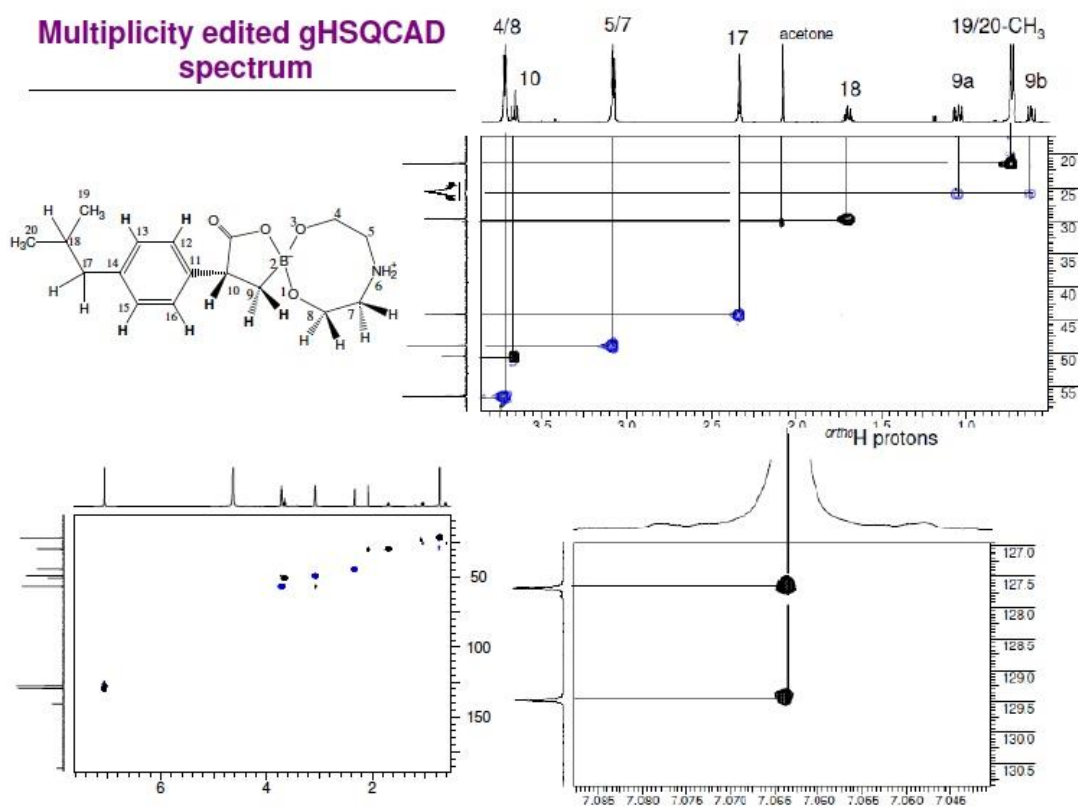
AA'BB' spin system



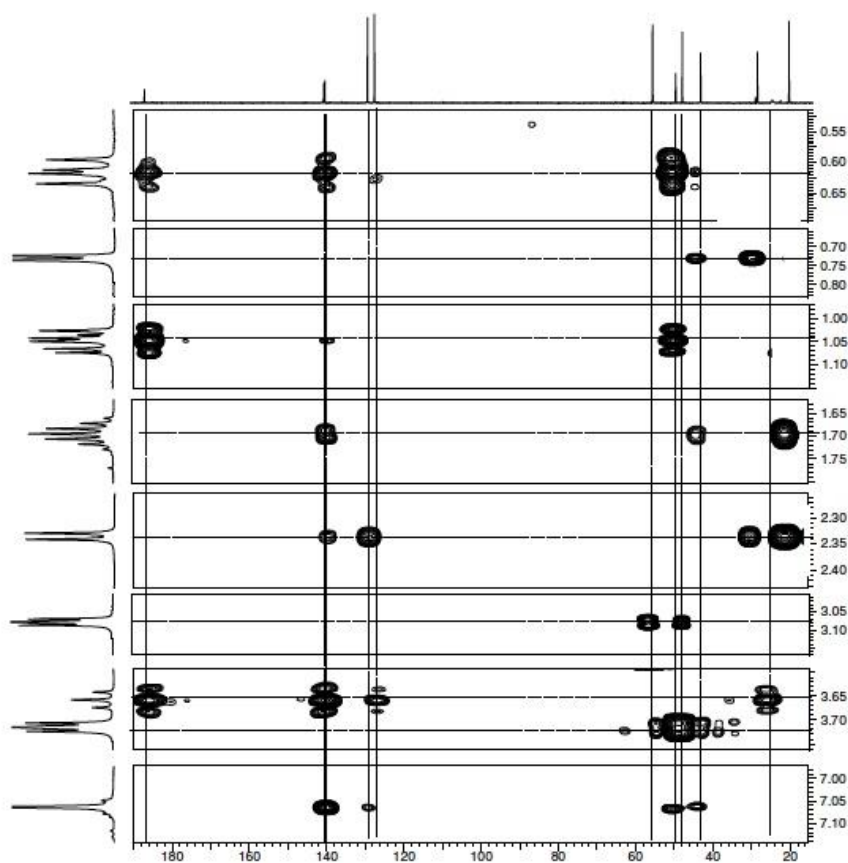
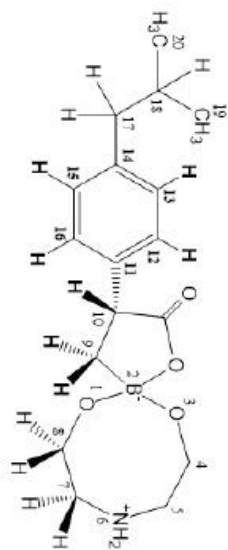
^1H NMR spectrum in D_2O



Multiplicity edited gHSQCAD spectrum

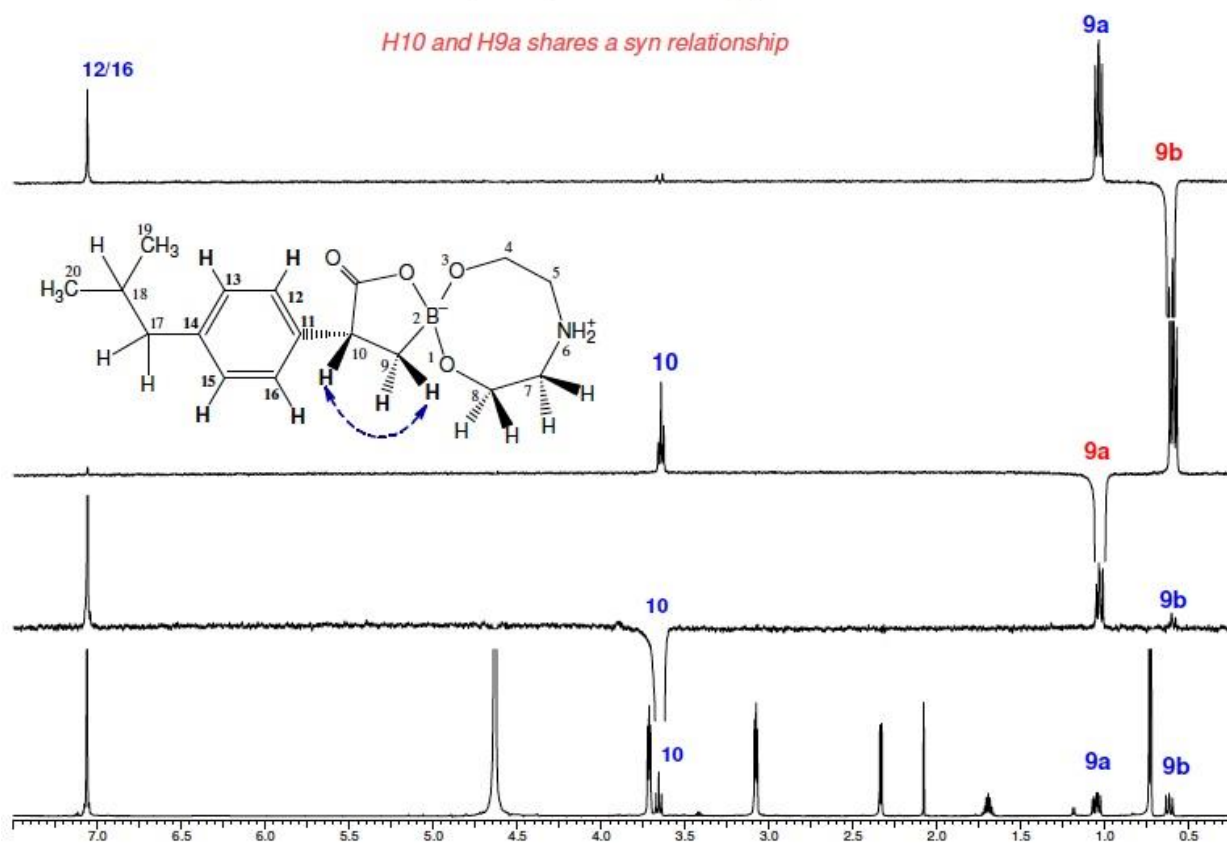


Long-range
HMBC correlations
(expanded regions)



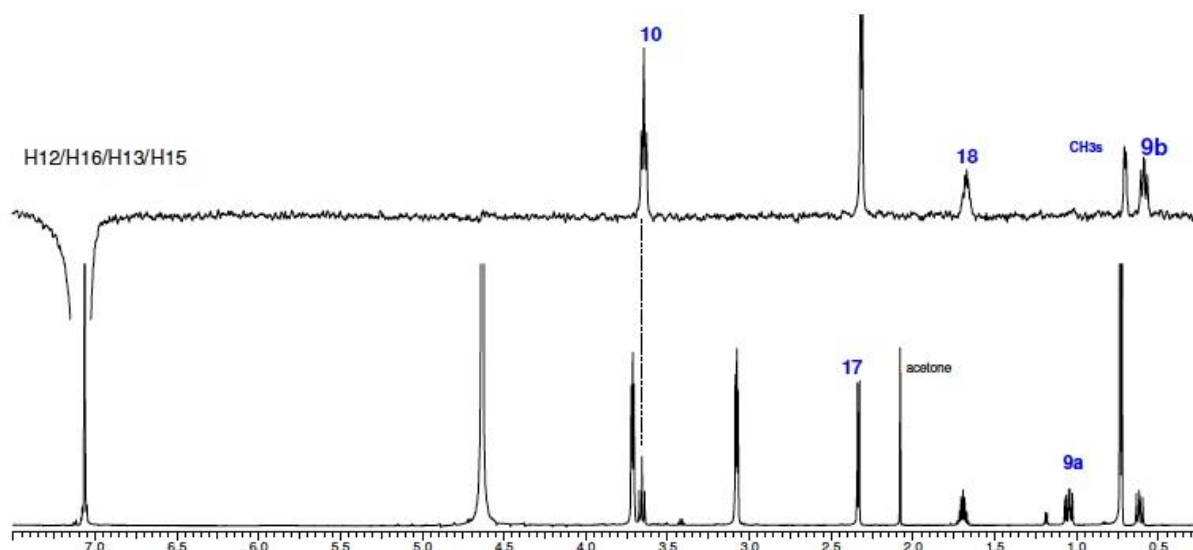
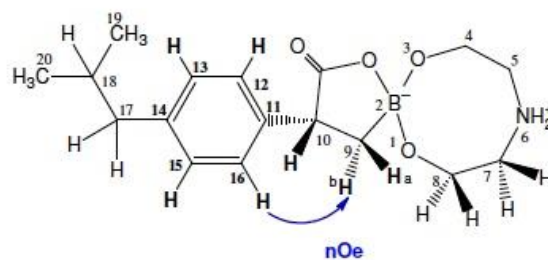
Relative stereochemistry

H10 and H9a shares a syn relationship



DPFGSENOE subspectrum

H9b in space is close to the ortho protons of the Phenyl group



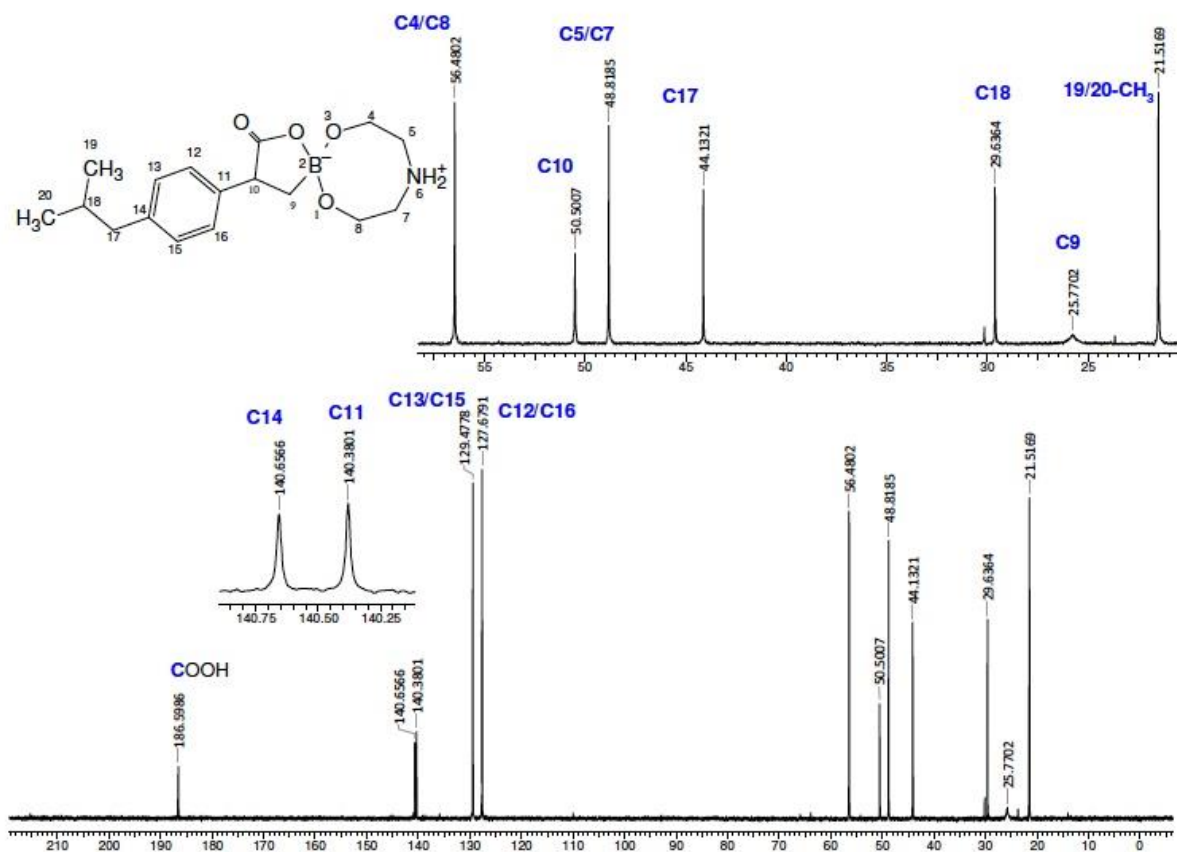


Figure S4. Full NMR characterization of **1^{DEA}** in CD₃OD.

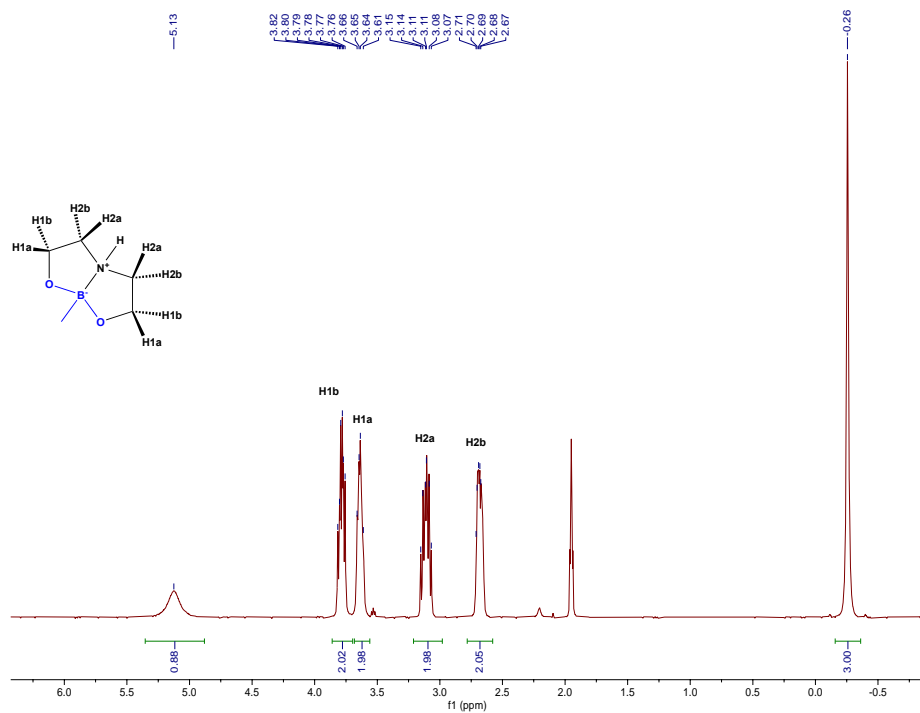


Figure S5. ¹H NMR spectrum of DABO methyl boronate in CD₃CN.

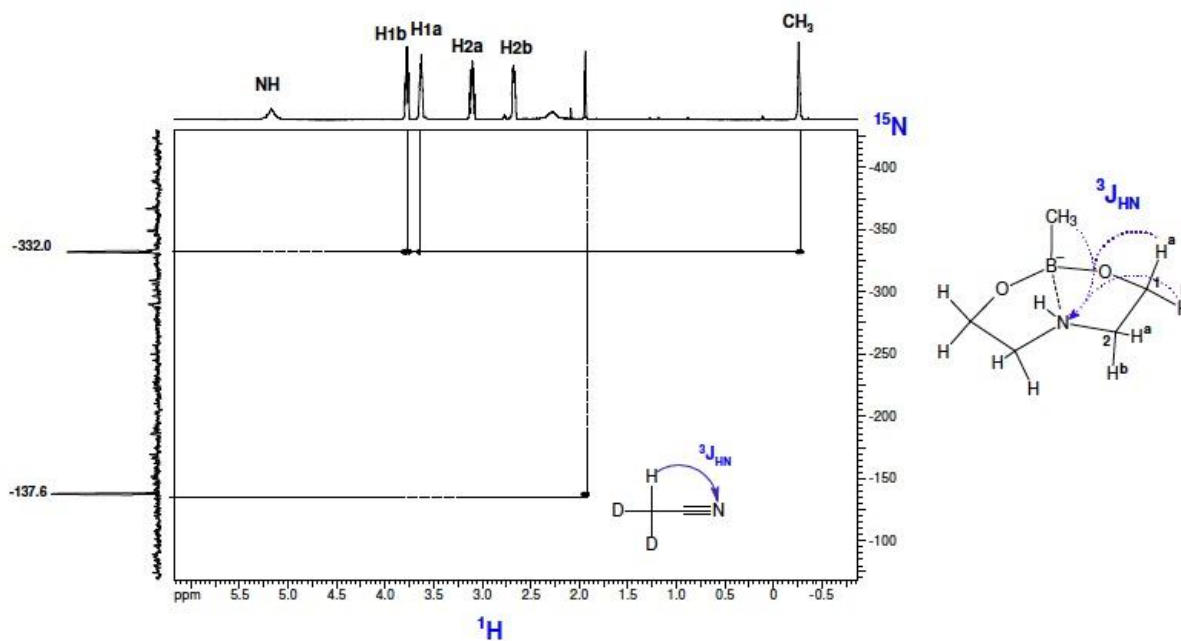


Figure S6. Two-dimensional ¹H-¹⁵N CIGAR-HMBC NMR spectrum of DABO methyl boronate in CD₃CN. The ¹¹B NMR chemical shift was observed at δ 11.2 ppm in CD₃CN.

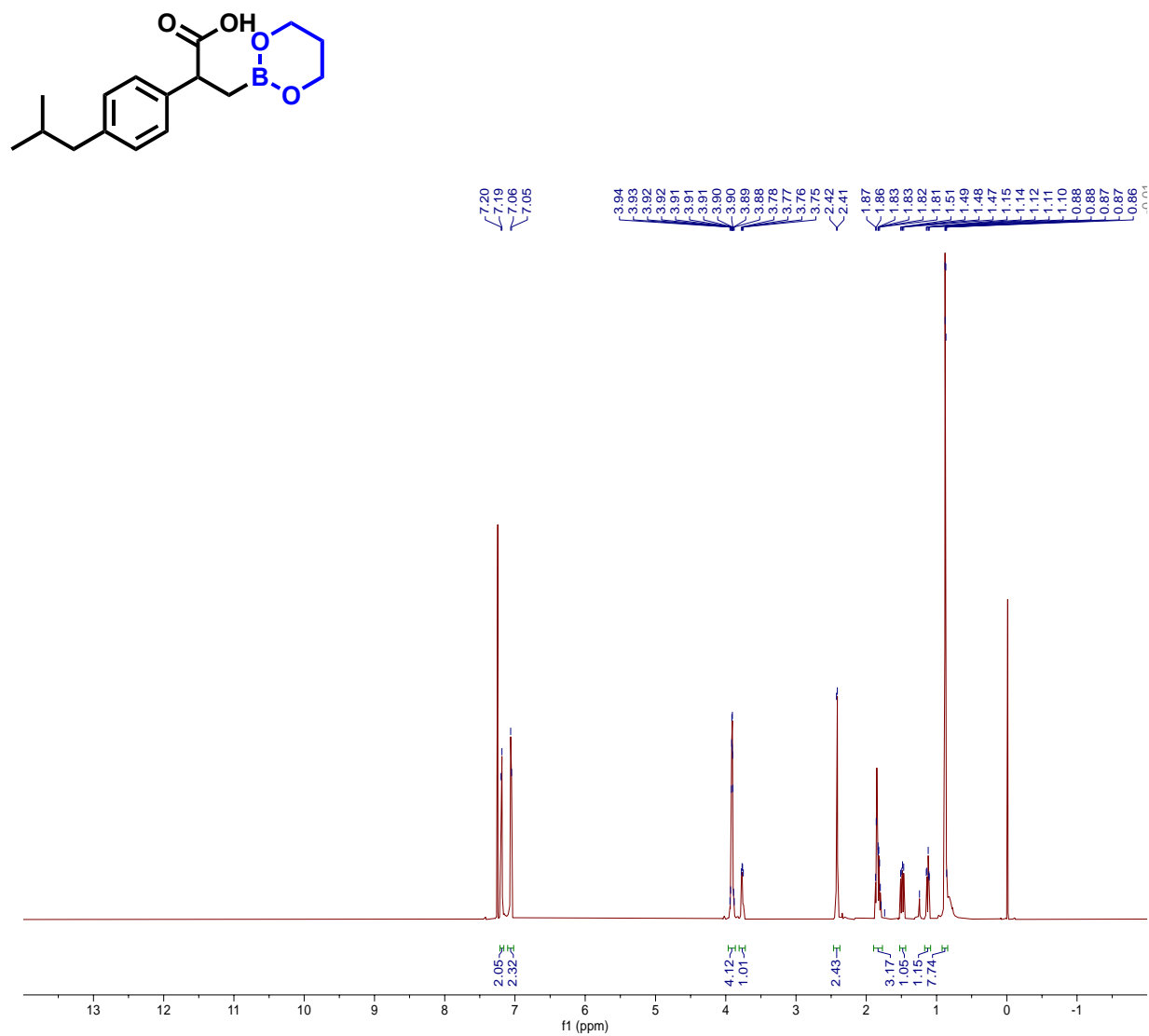


Figure S7. ¹H NMR Spectrum of **1a** in CDCl₃.

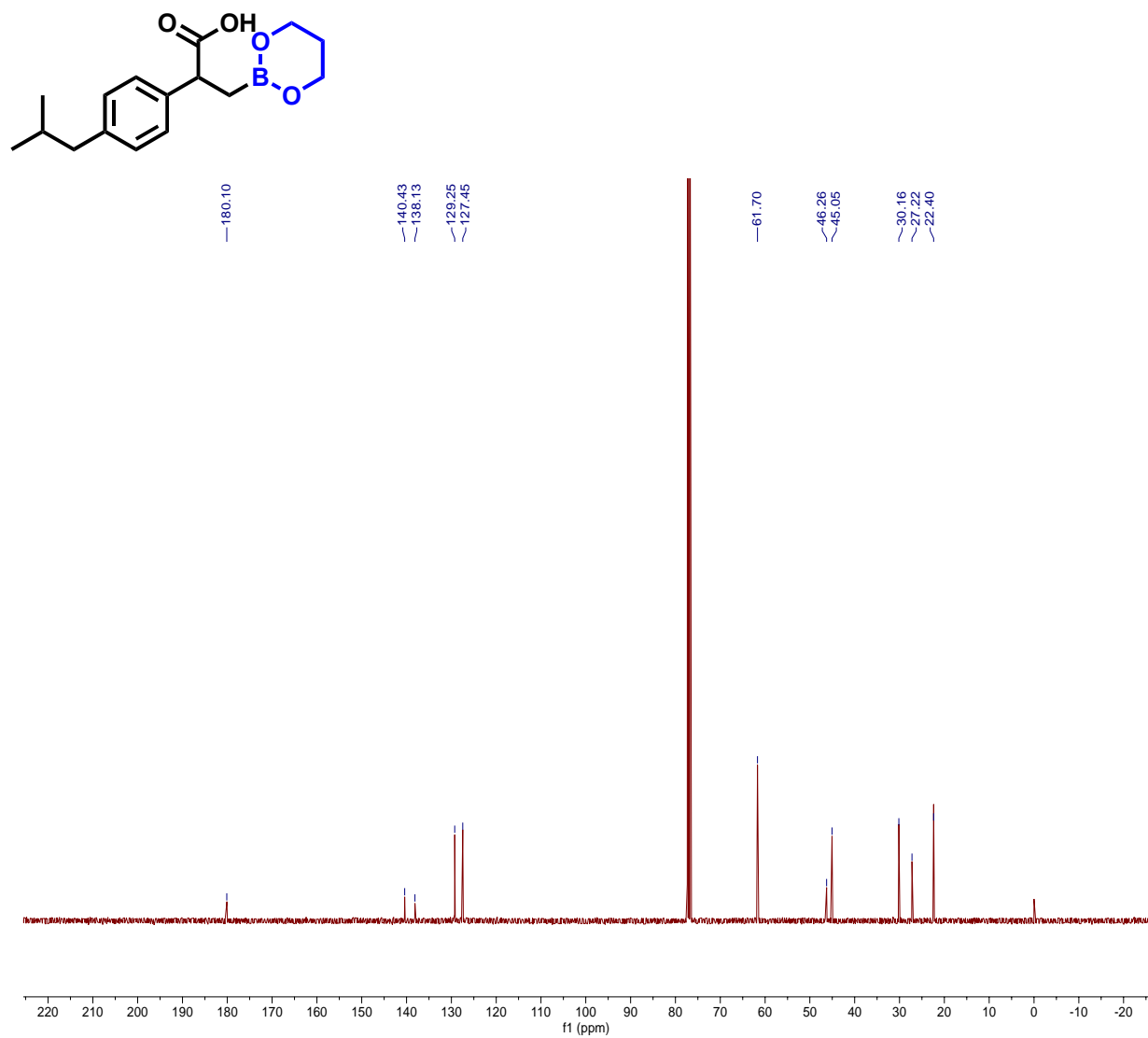


Figure S8. ¹³C NMR Spectrum of **1a** in CDCl₃.

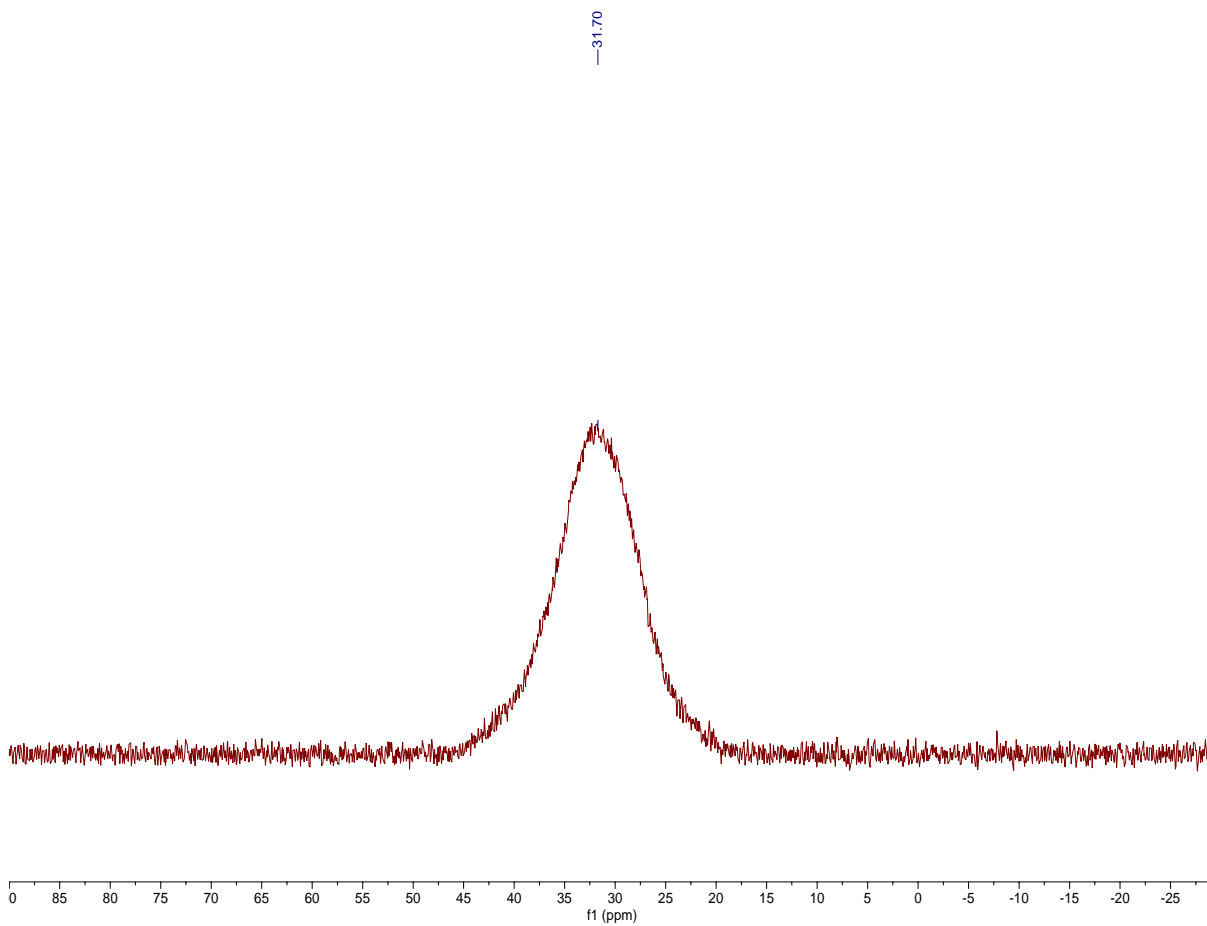
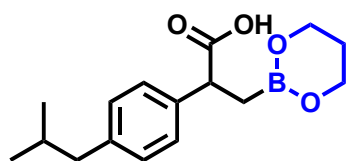


Figure S9. ^{11}B NMR Spectrum of **1a** in CDCl_3 .

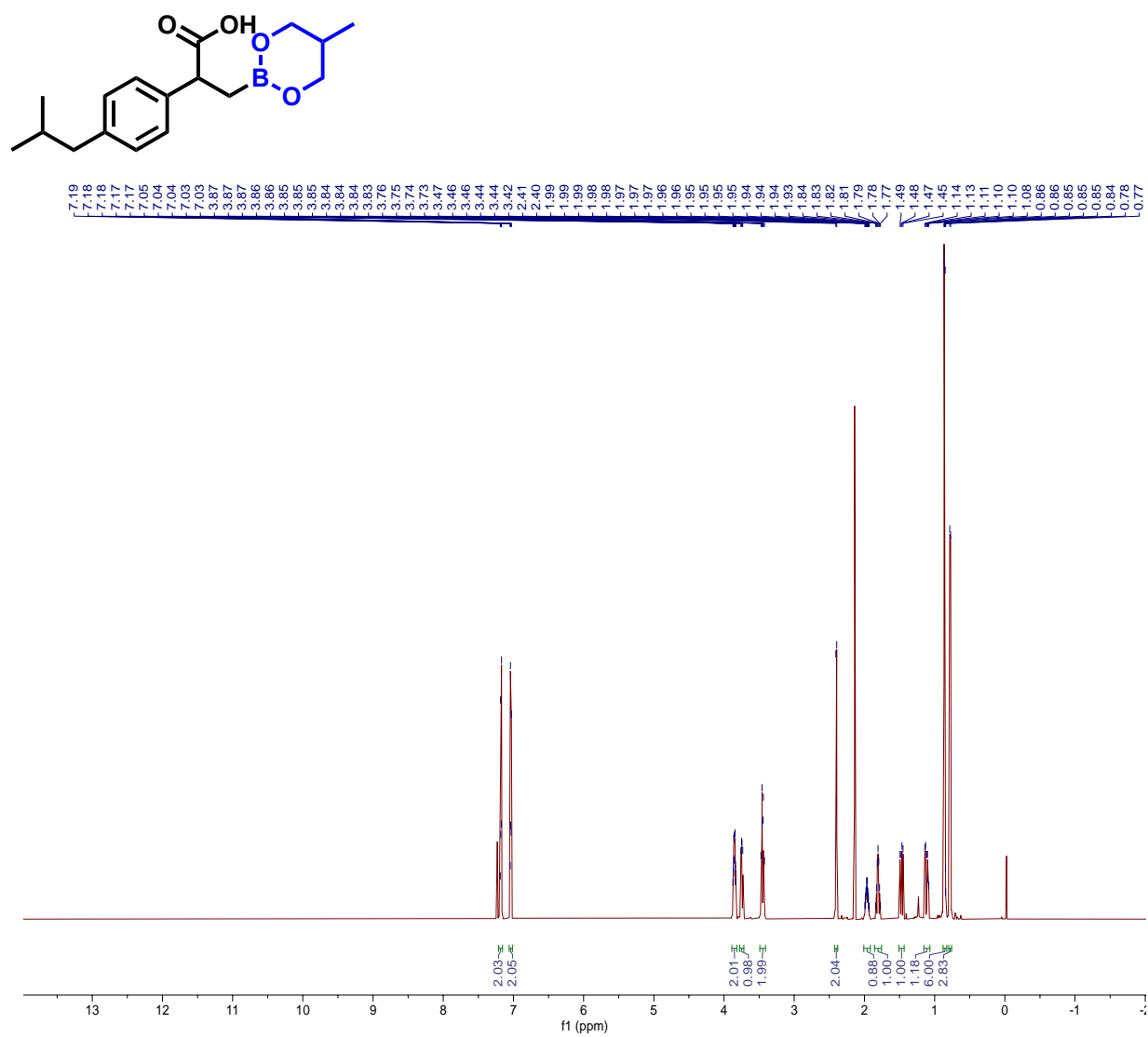


Figure S10. ¹H NMR Spectrum of **1b** in CDCl₃.

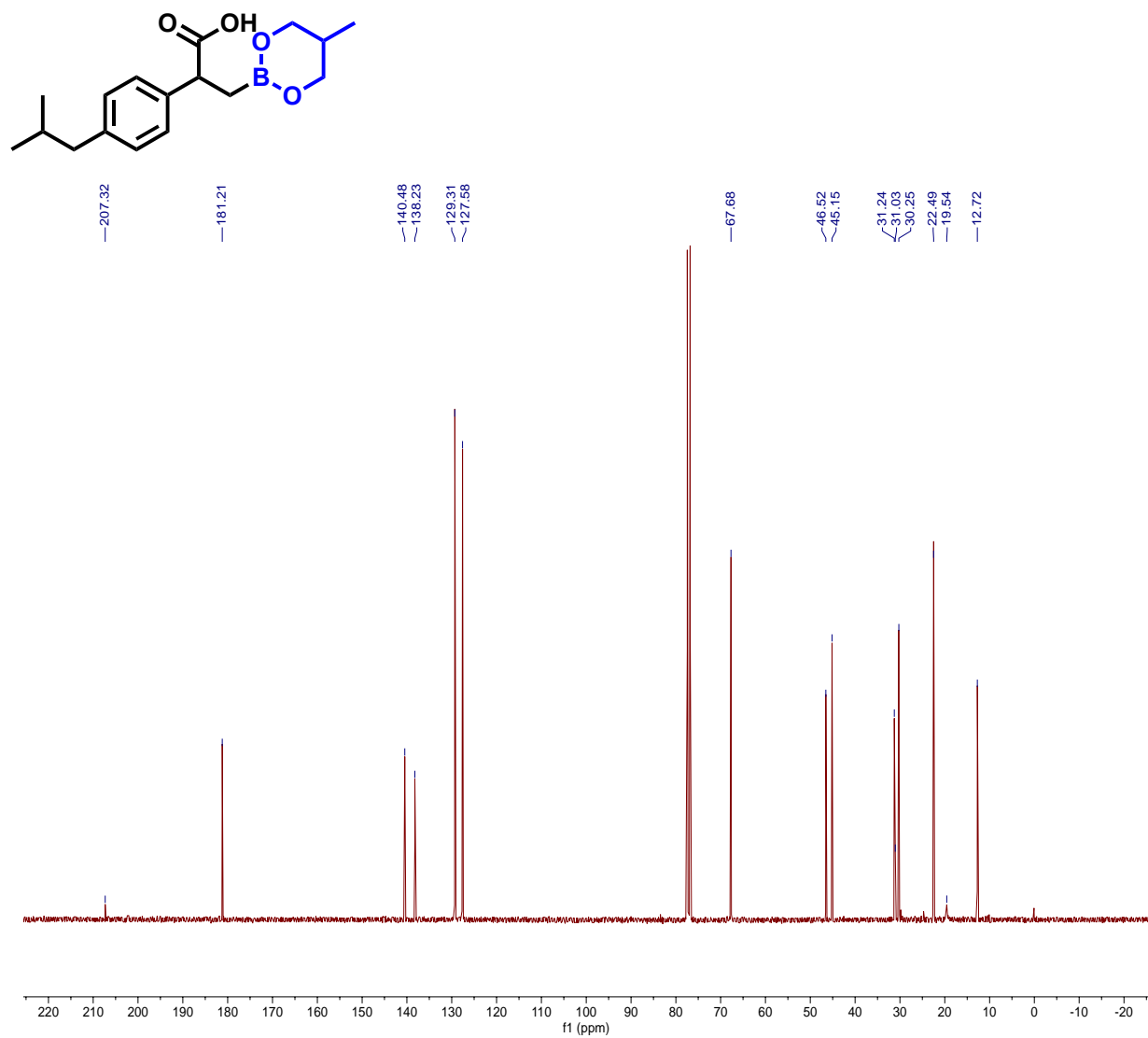


Figure S11. ^{13}C NMR Spectrum of **1b** in CDCl₃.

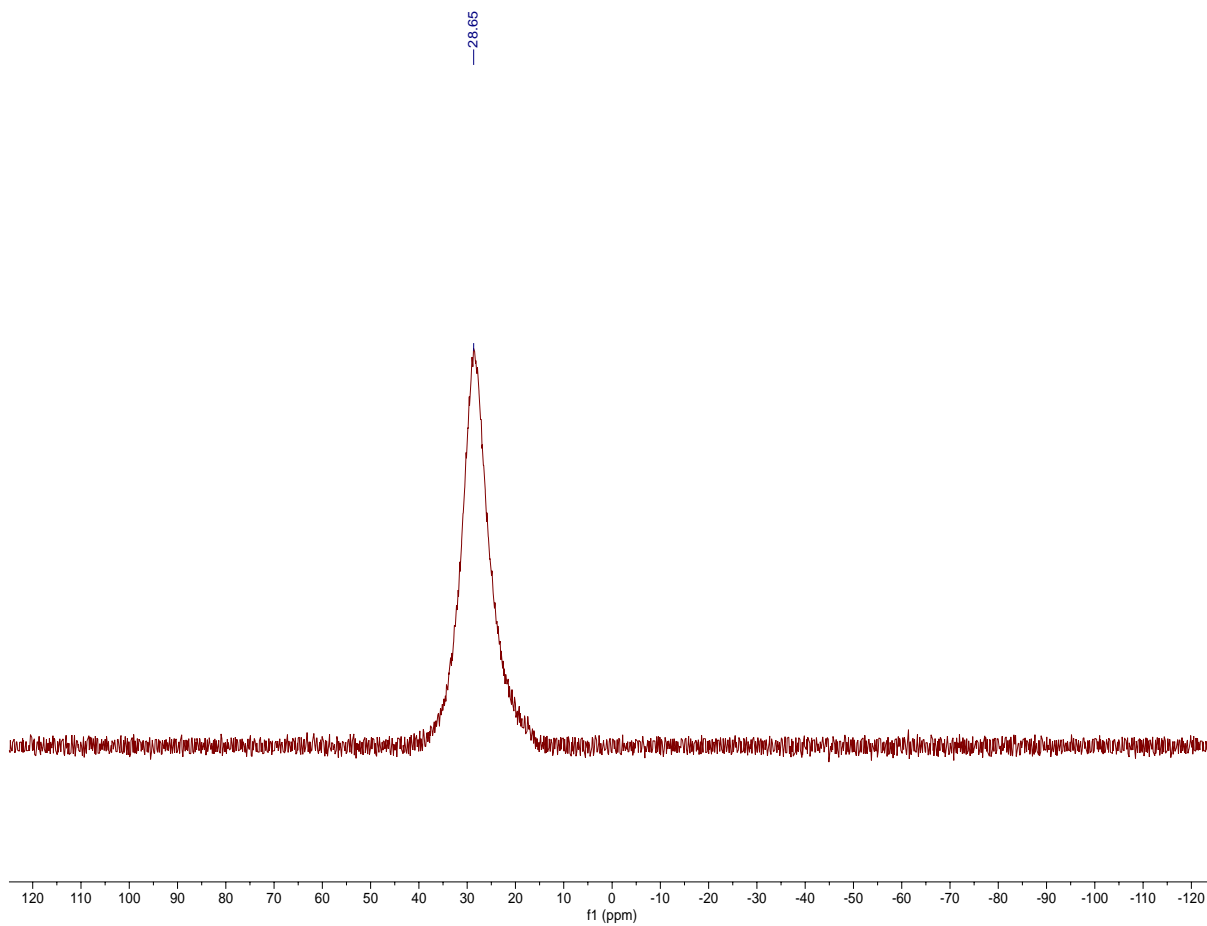
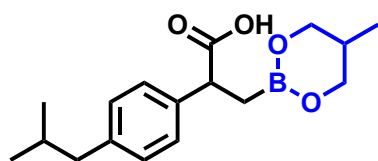


Figure S12. ^{11}B NMR Spectrum of **1b** in CDCl_3 .

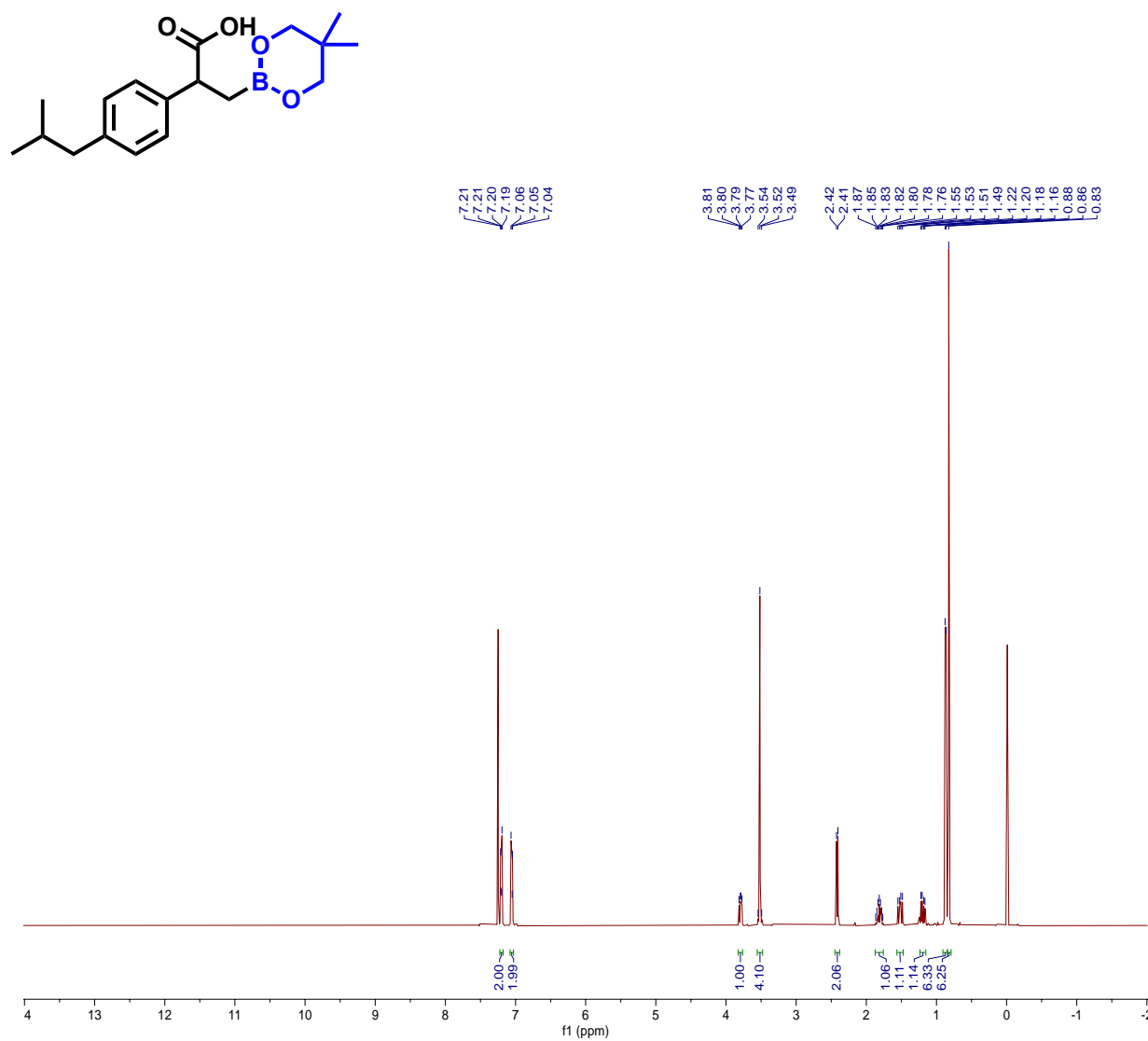


Figure S13. ¹H NMR Spectrum of **1c** in CDCl₃.

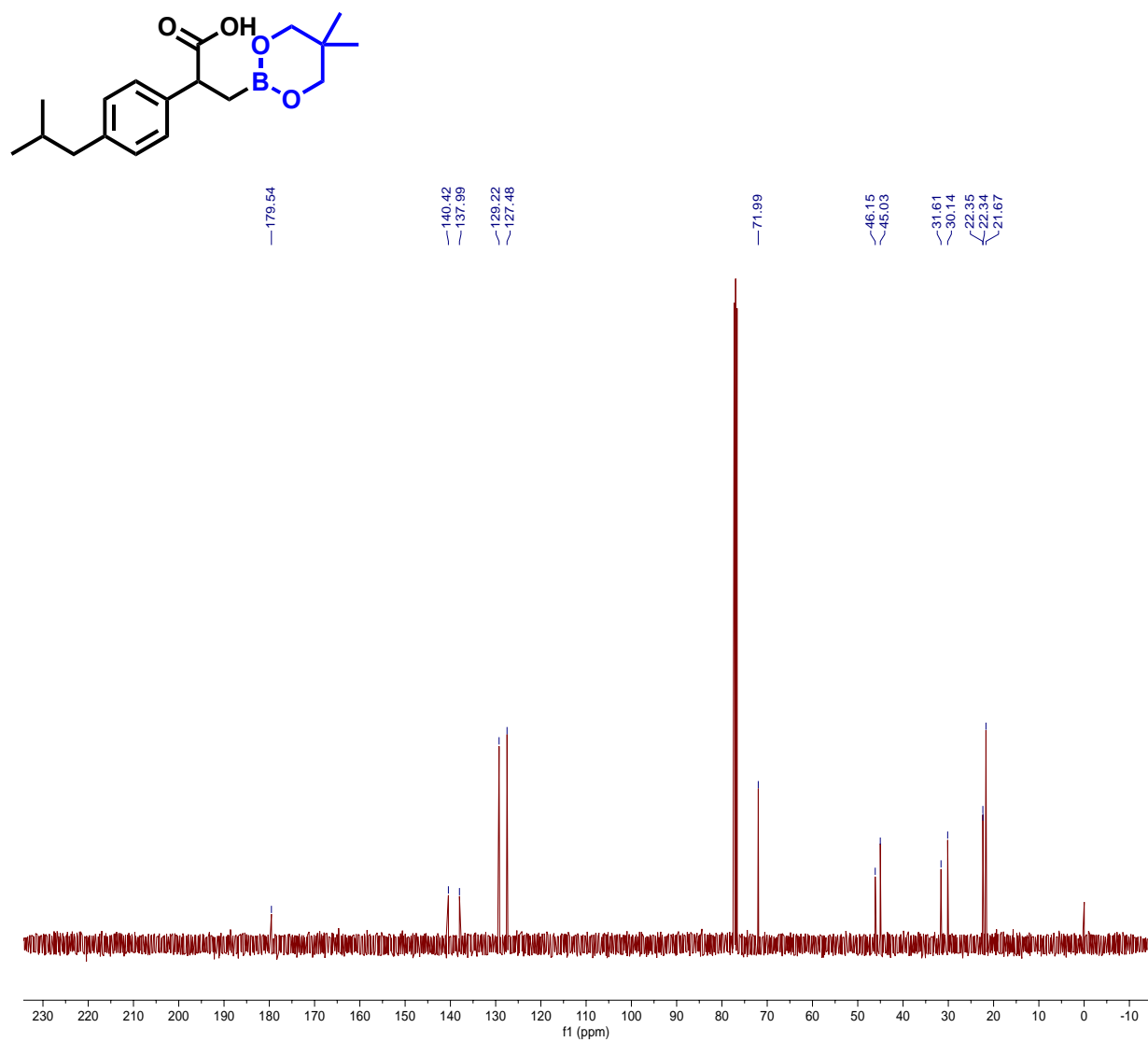


Figure S14. ^{13}C NMR Spectrum of **1c** in CDCl_3 .

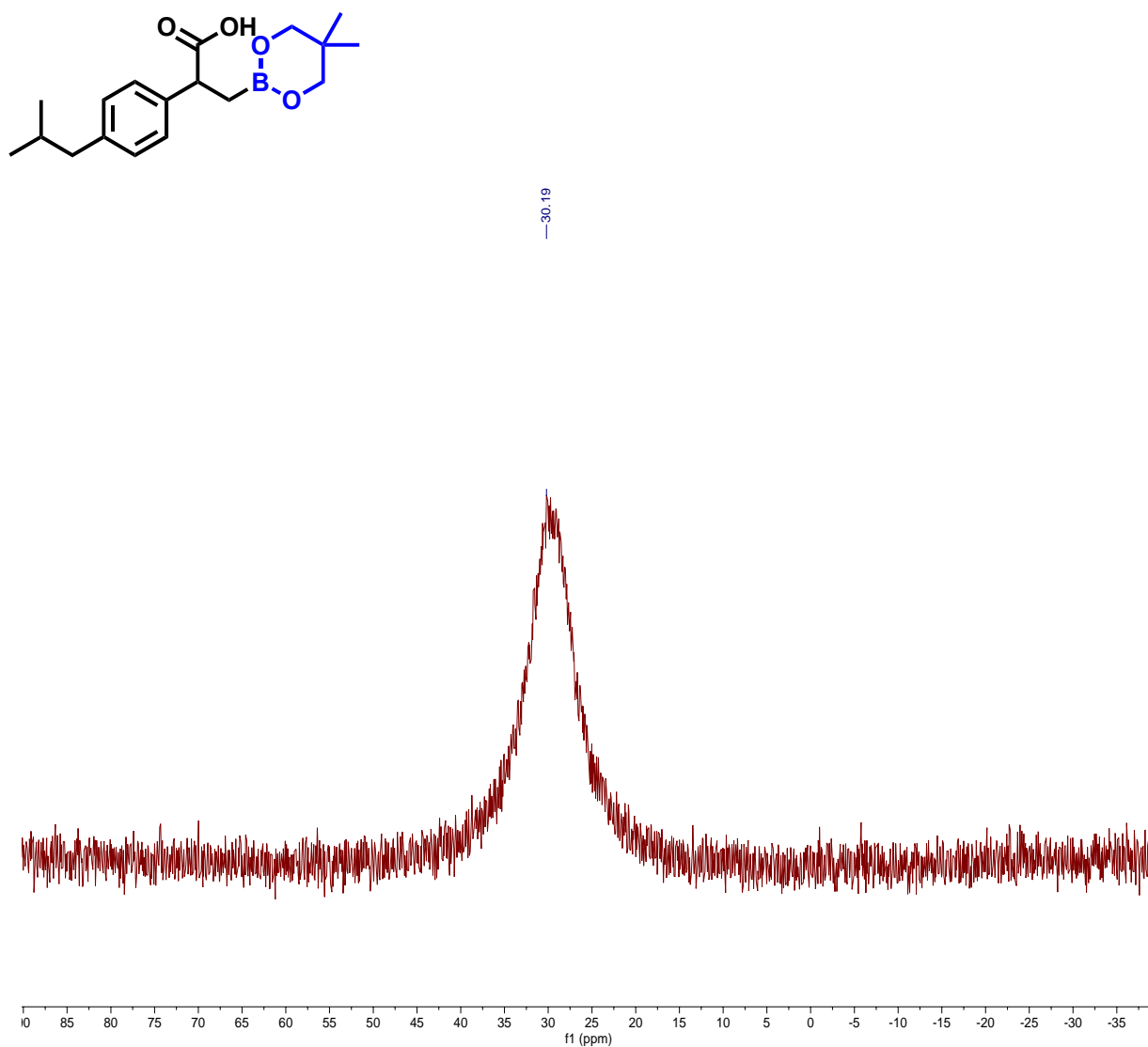


Figure S15. ^{11}B NMR Spectrum of **1c** in CDCl_3 .

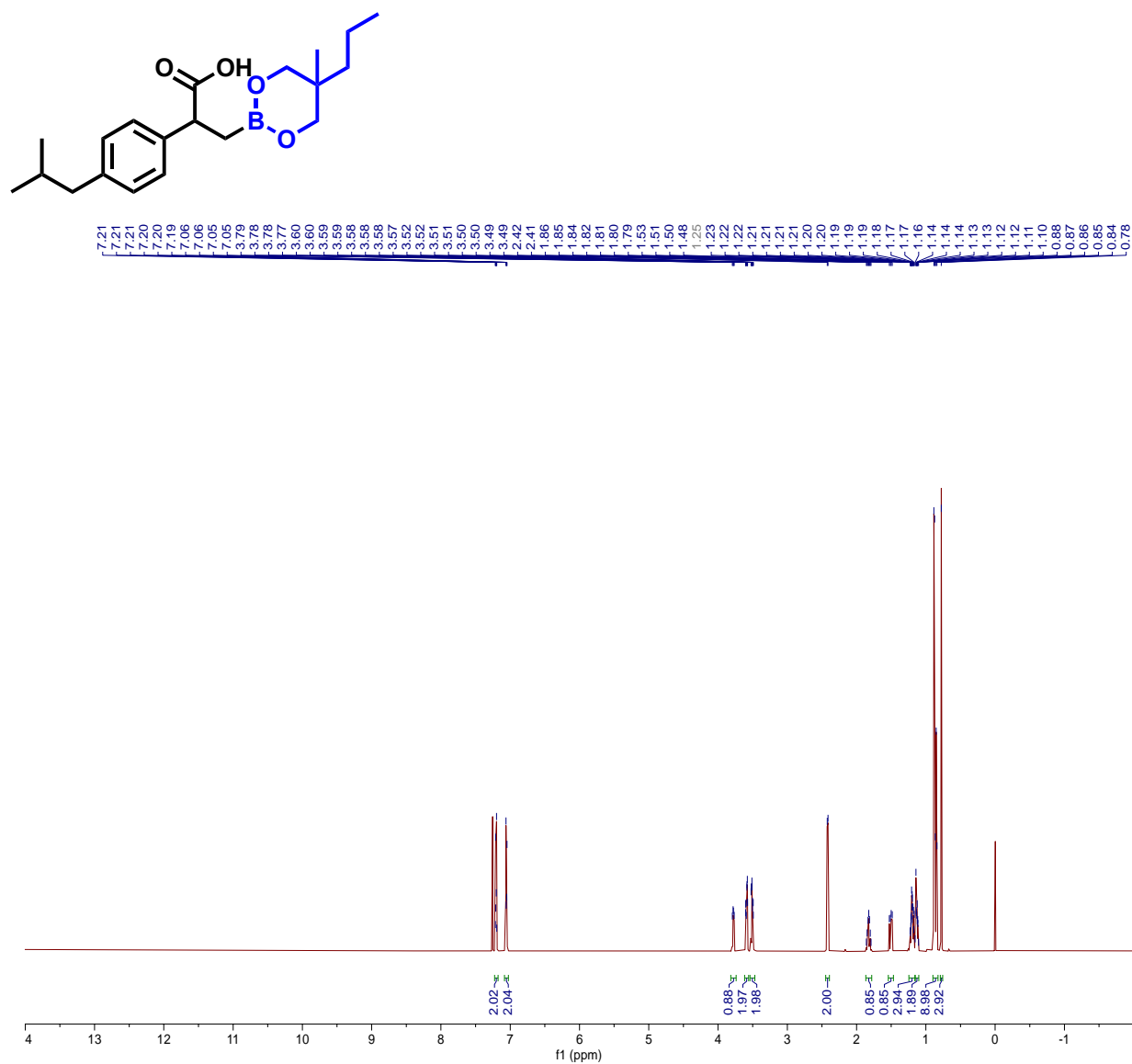


Figure S16. ¹H NMR Spectrum of **1d** in CDCl₃.

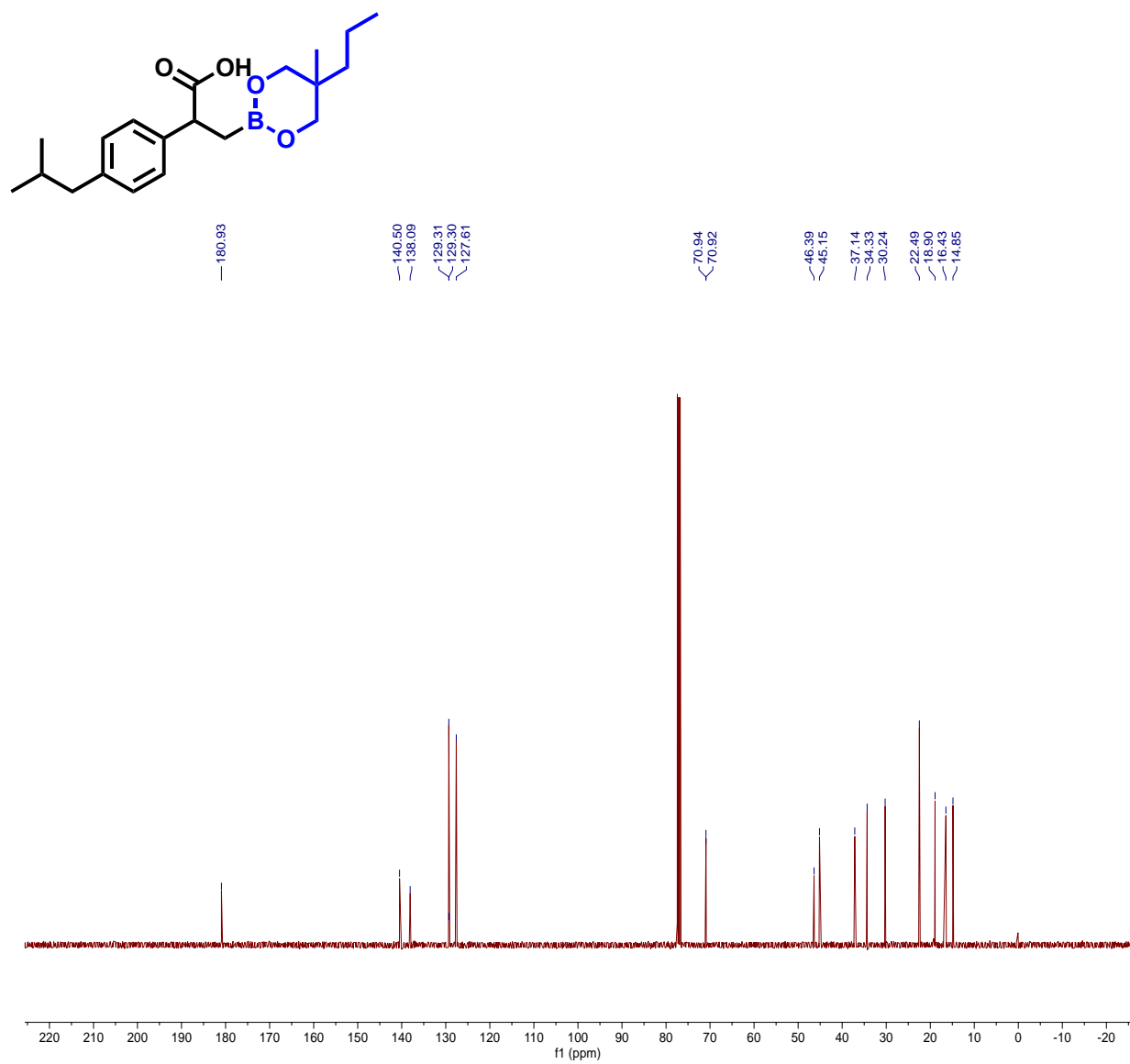


Figure S17. ¹³C NMR Spectrum of **1d** in CDCl₃.

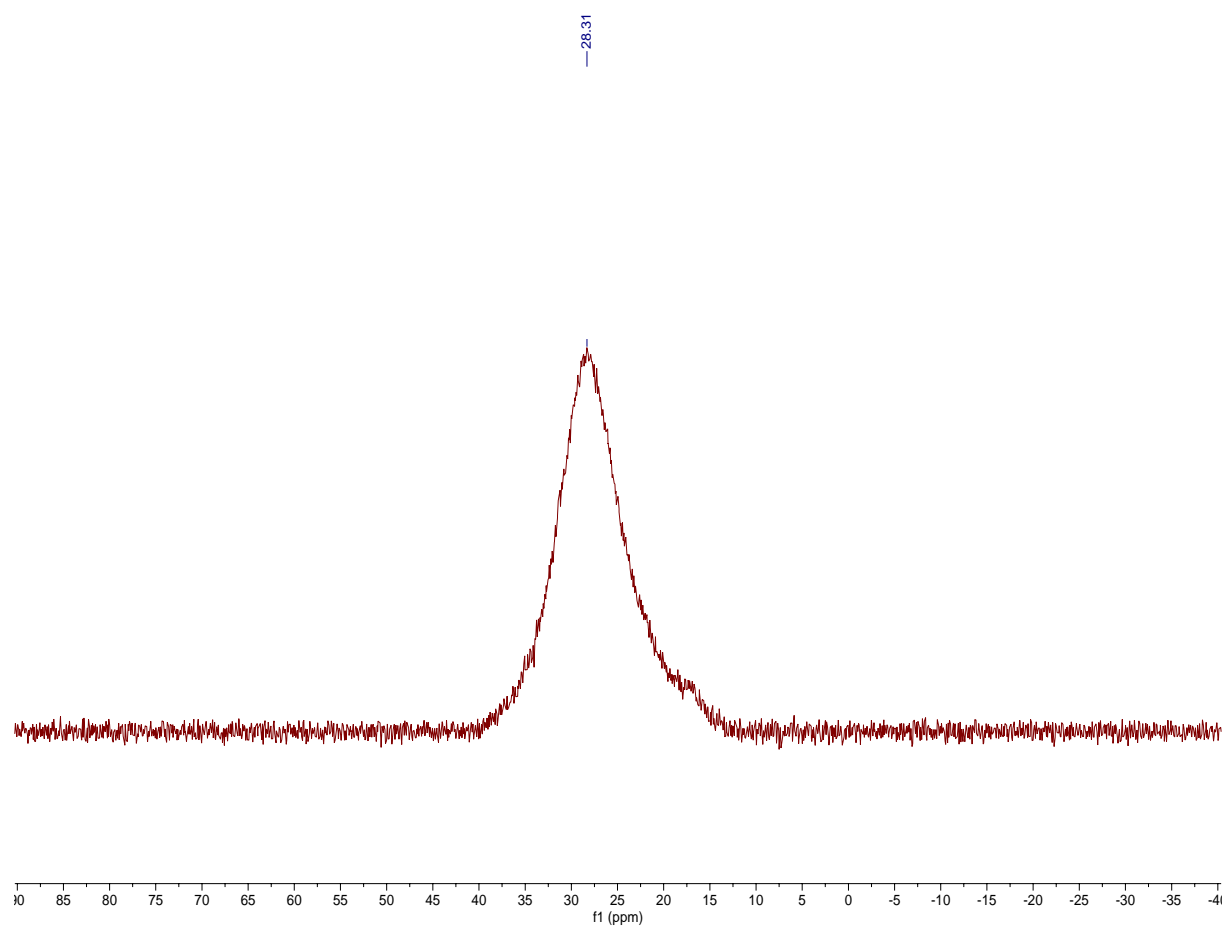
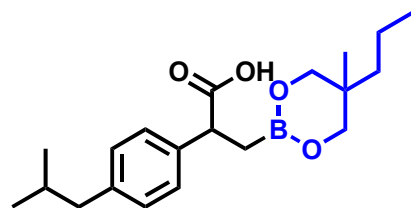


Figure S18. ^{11}B NMR Spectrum of **1d** in CDCl_3 .

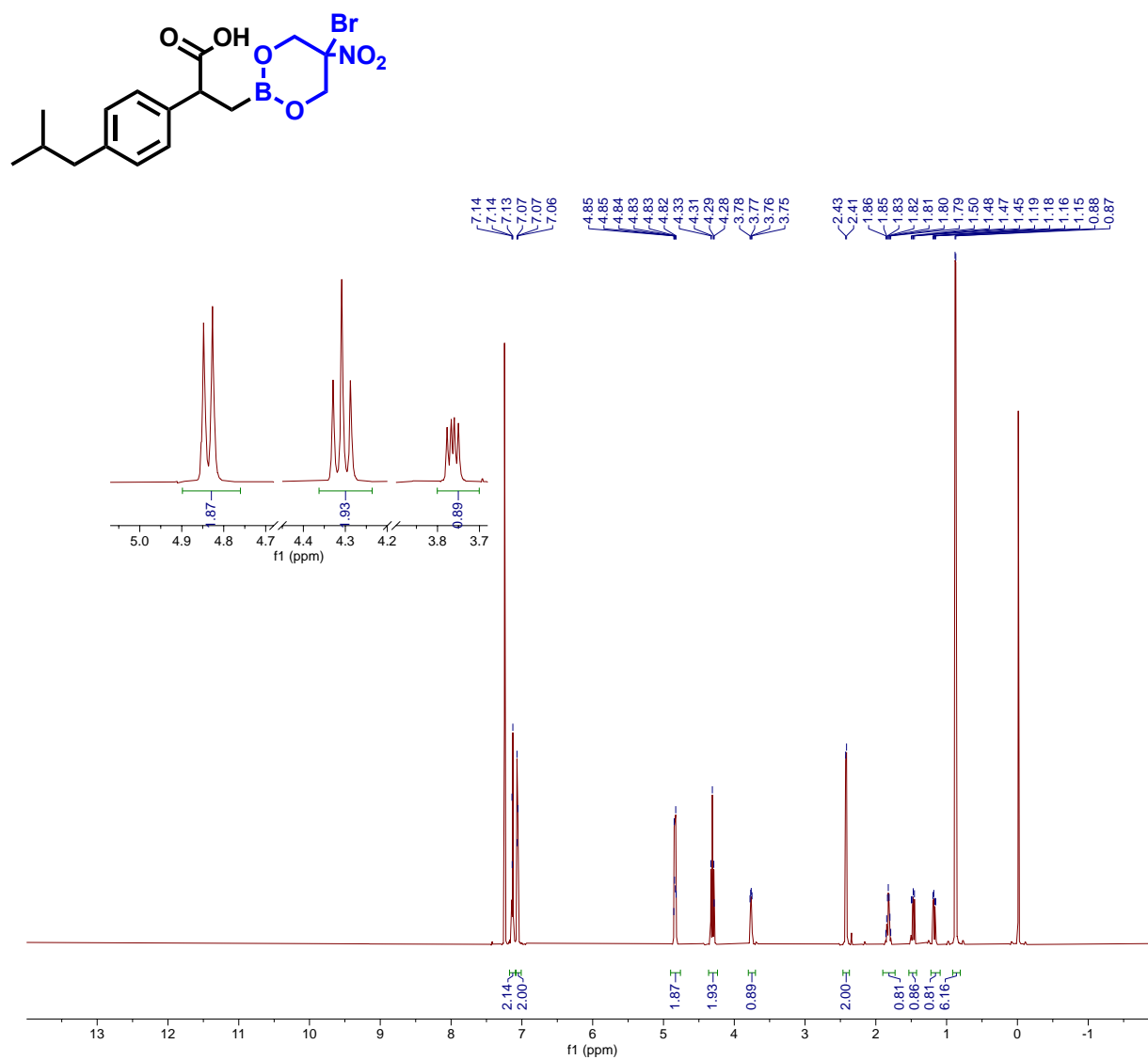


Figure S19. ¹H NMR Spectrum of **1c** in CDCl₃.

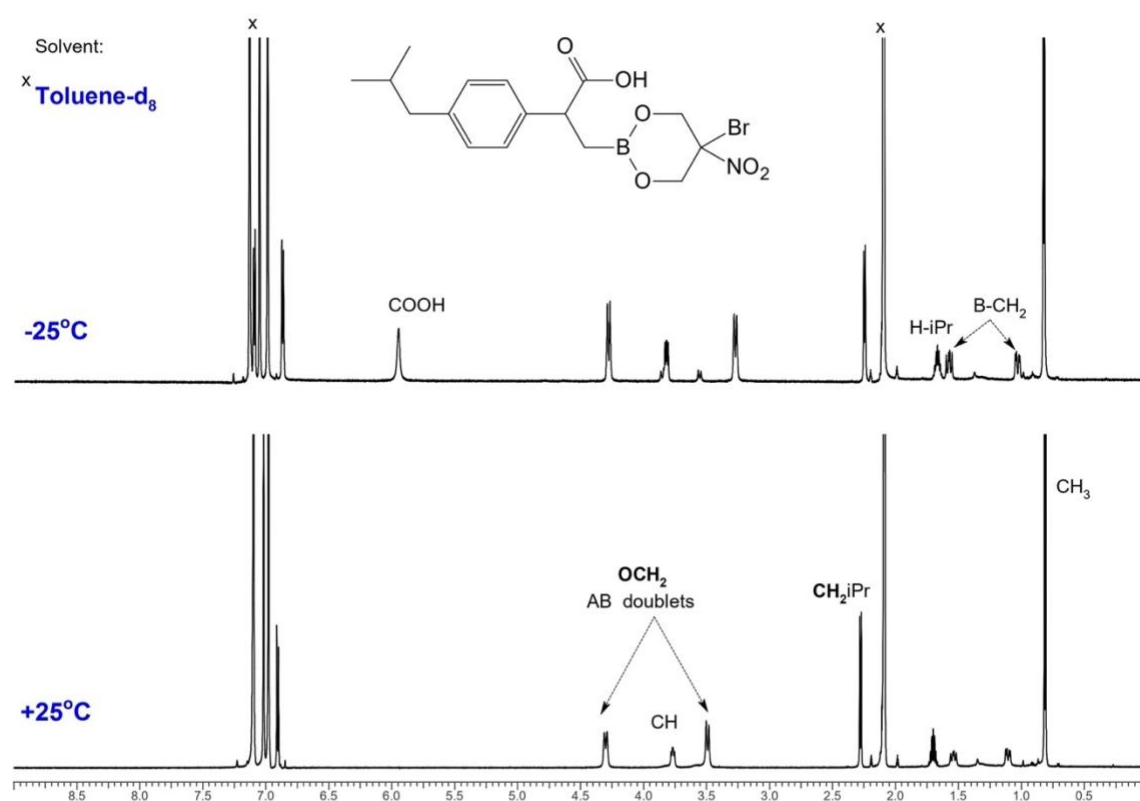


Figure S20. VT- ^1H NMR Spectrum of **1c** in Toluene- d_8 .

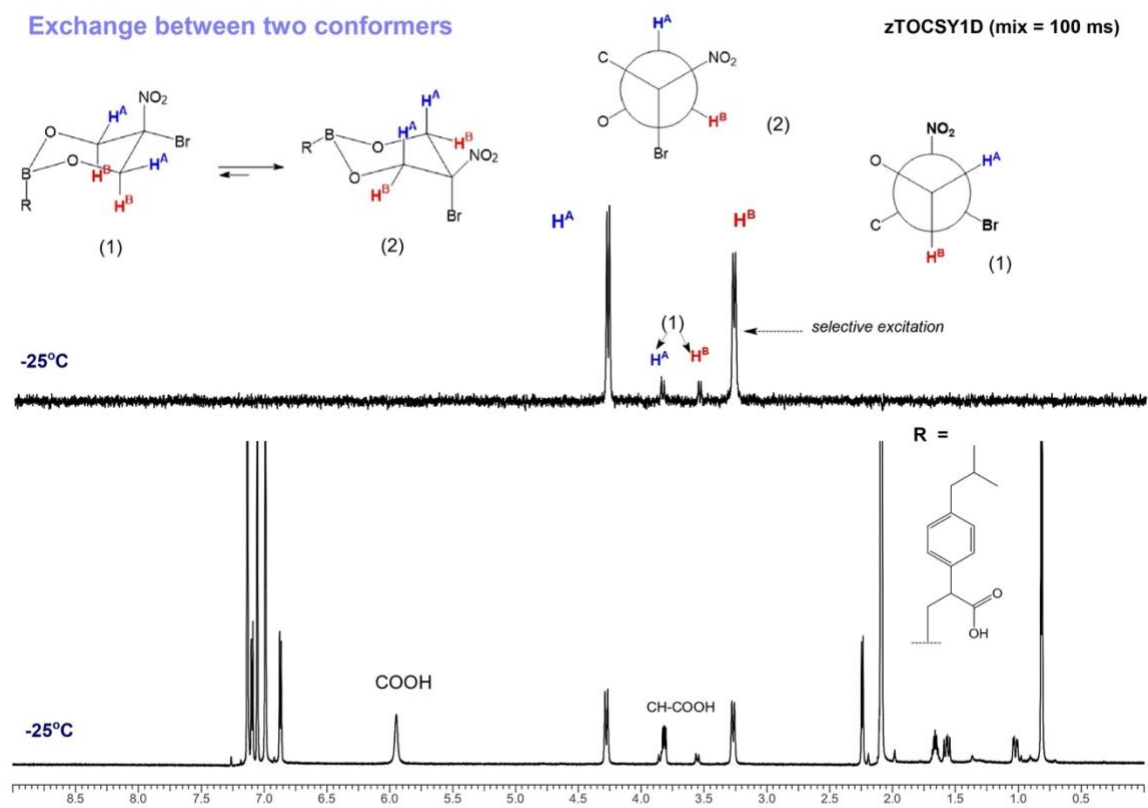


Figure S21. zTOCSY 1D ^1H NMR Spectrum of **1c** in toluene- d_8 .

Exchange between two conformers

NOESY1D (b-c)

-25°C

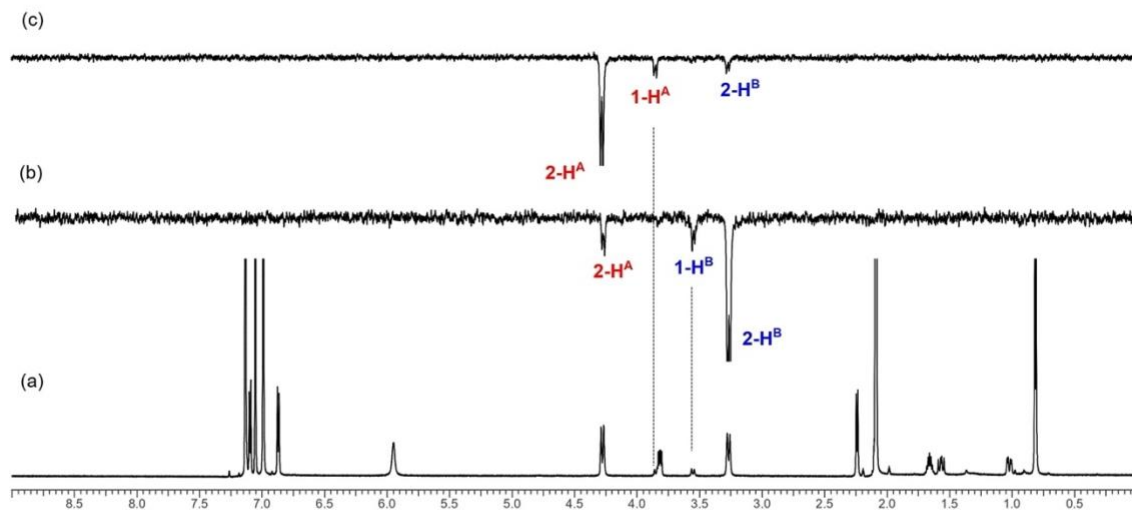
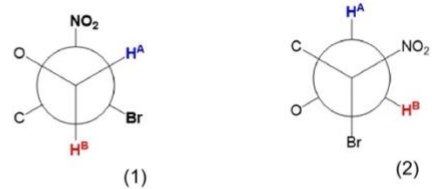


Figure S22. NOESY 1D ^1H NMR Spectrum of **1c** in toluene- d_8 .

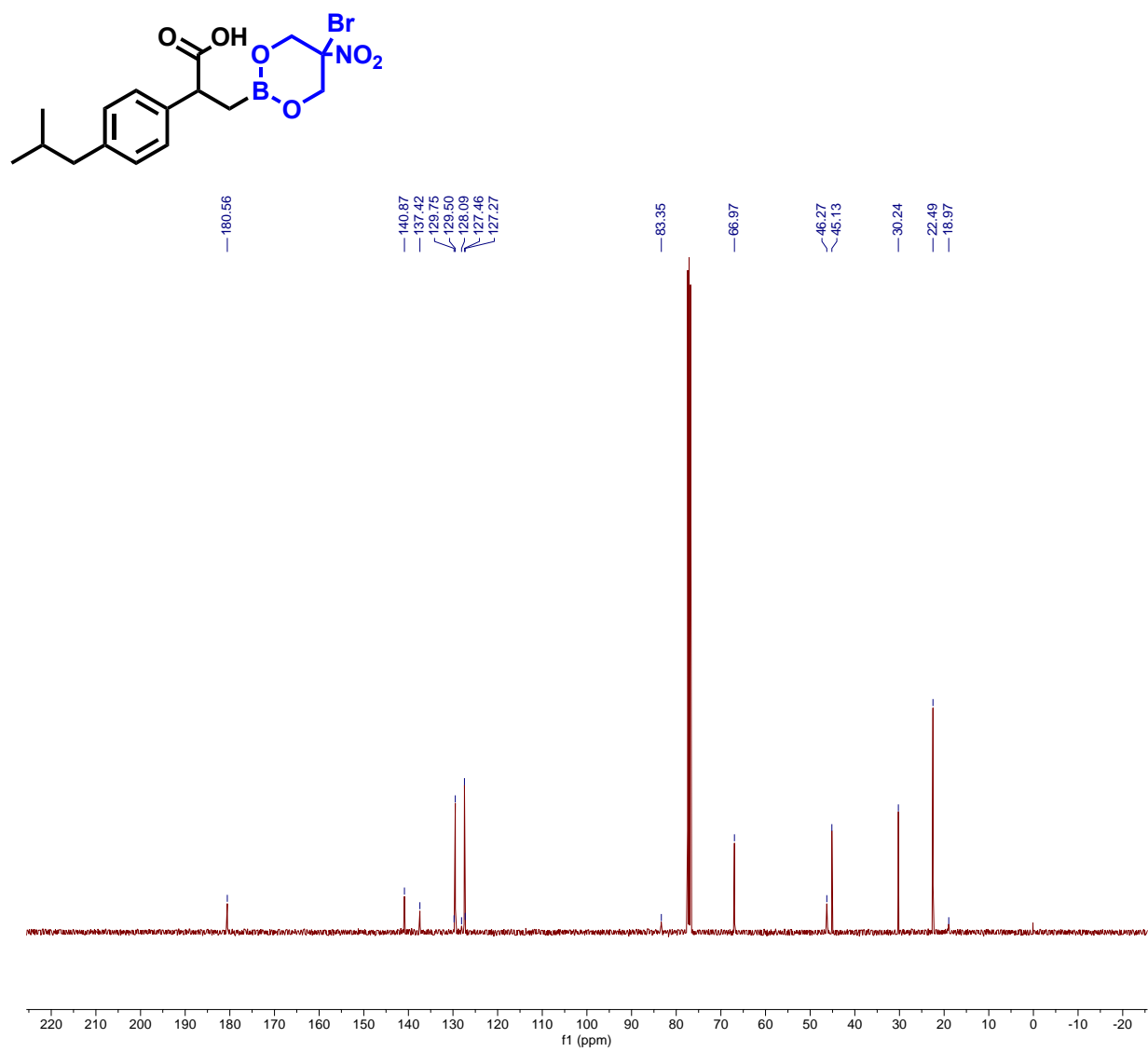


Figure S23. ^{13}C NMR Spectrum of **1c** in CDCl₃.

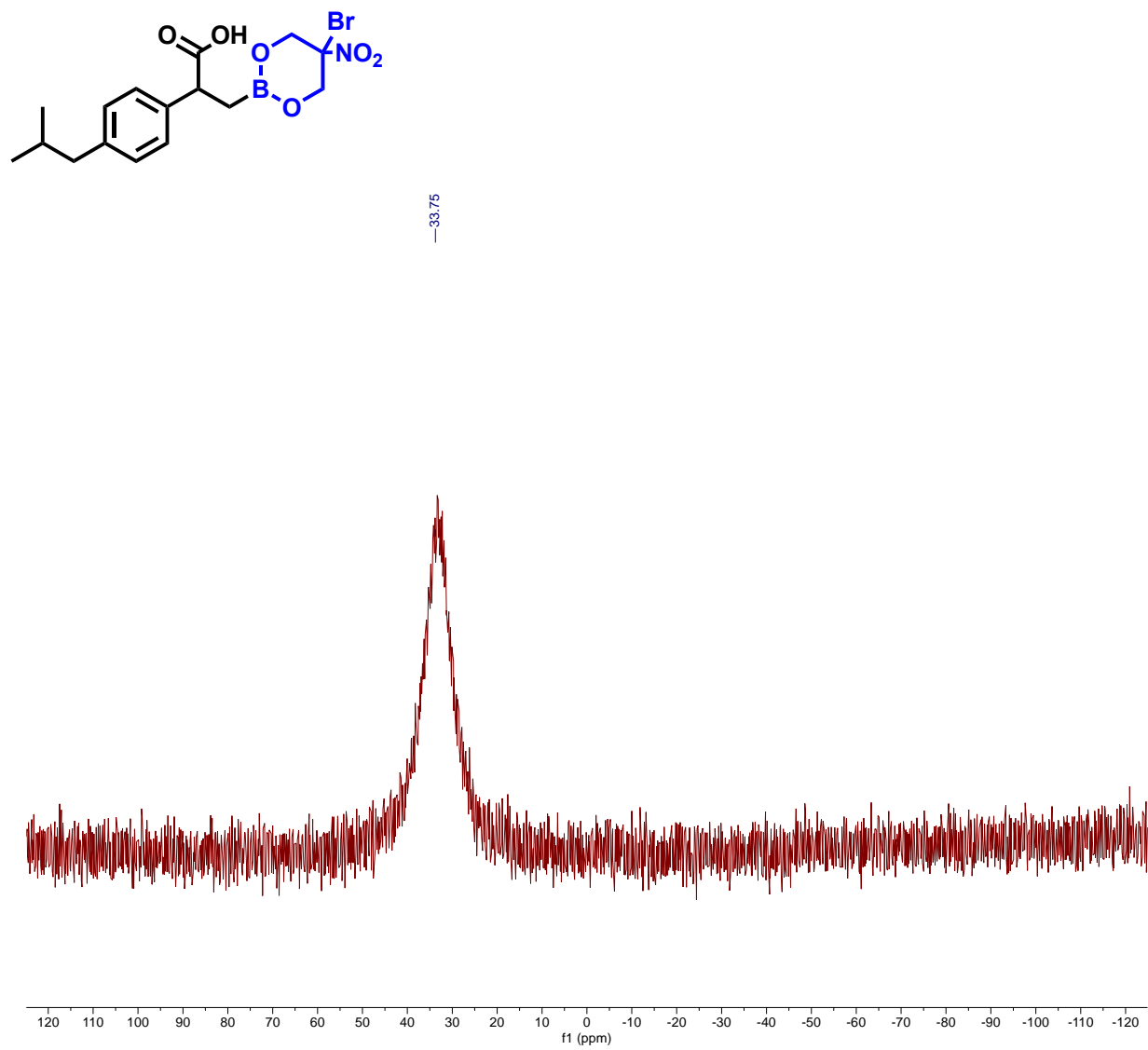


Figure S24. ^{11}B NMR Spectrum of **1c** in CDCl_3 .

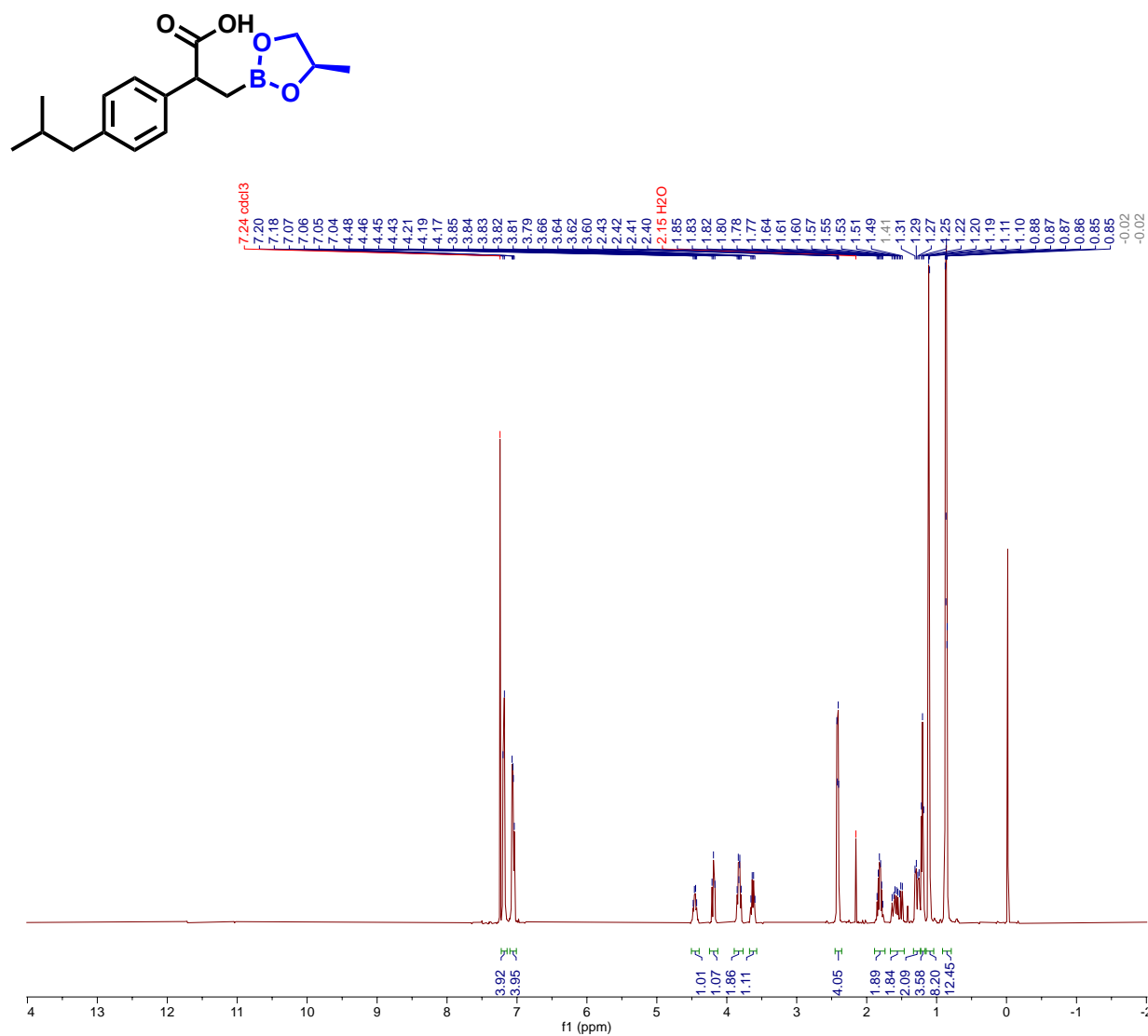


Figure S25. ¹H NMR Spectrum of **1f** in CDCl₃.

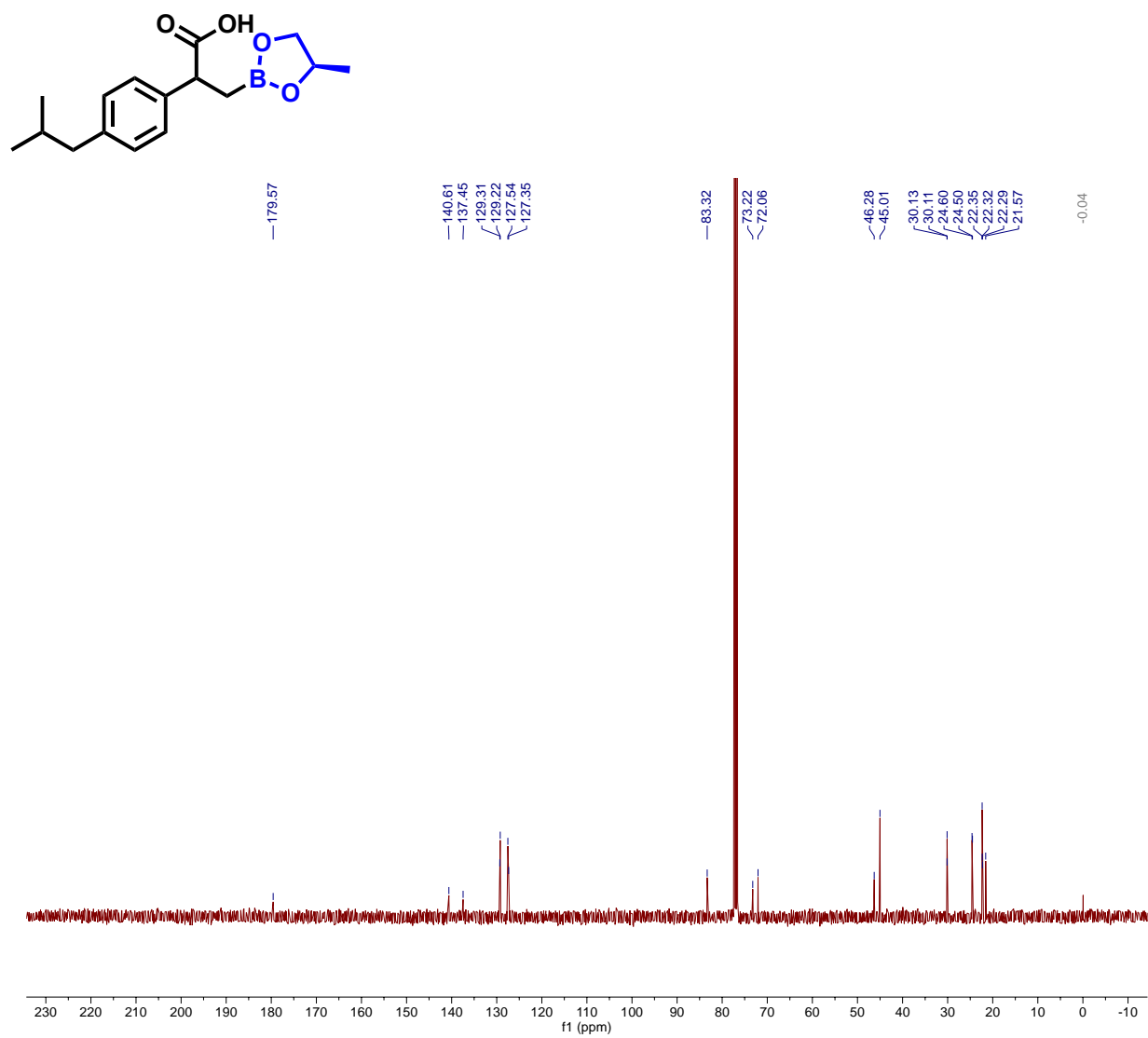
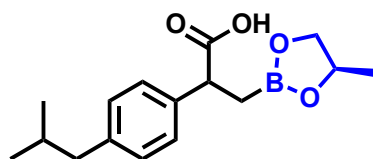


Figure S26. ^{13}C NMR Spectrum of **1f** in CDCl₃.



—34.57

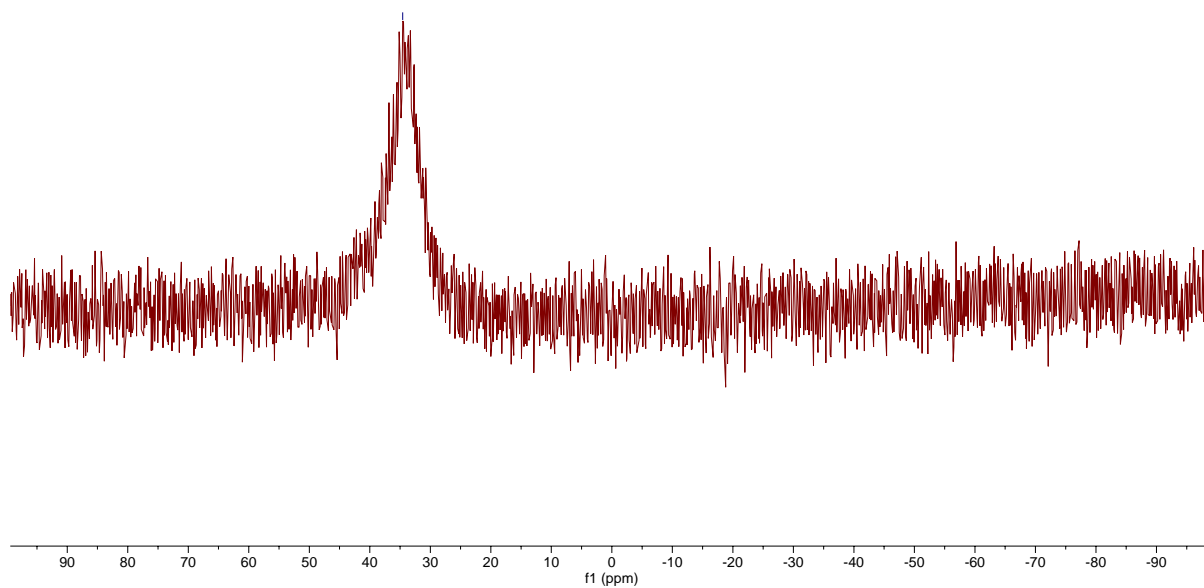


Figure S27. ^{11}B NMR Spectrum of **1f** in CDCl_3 .

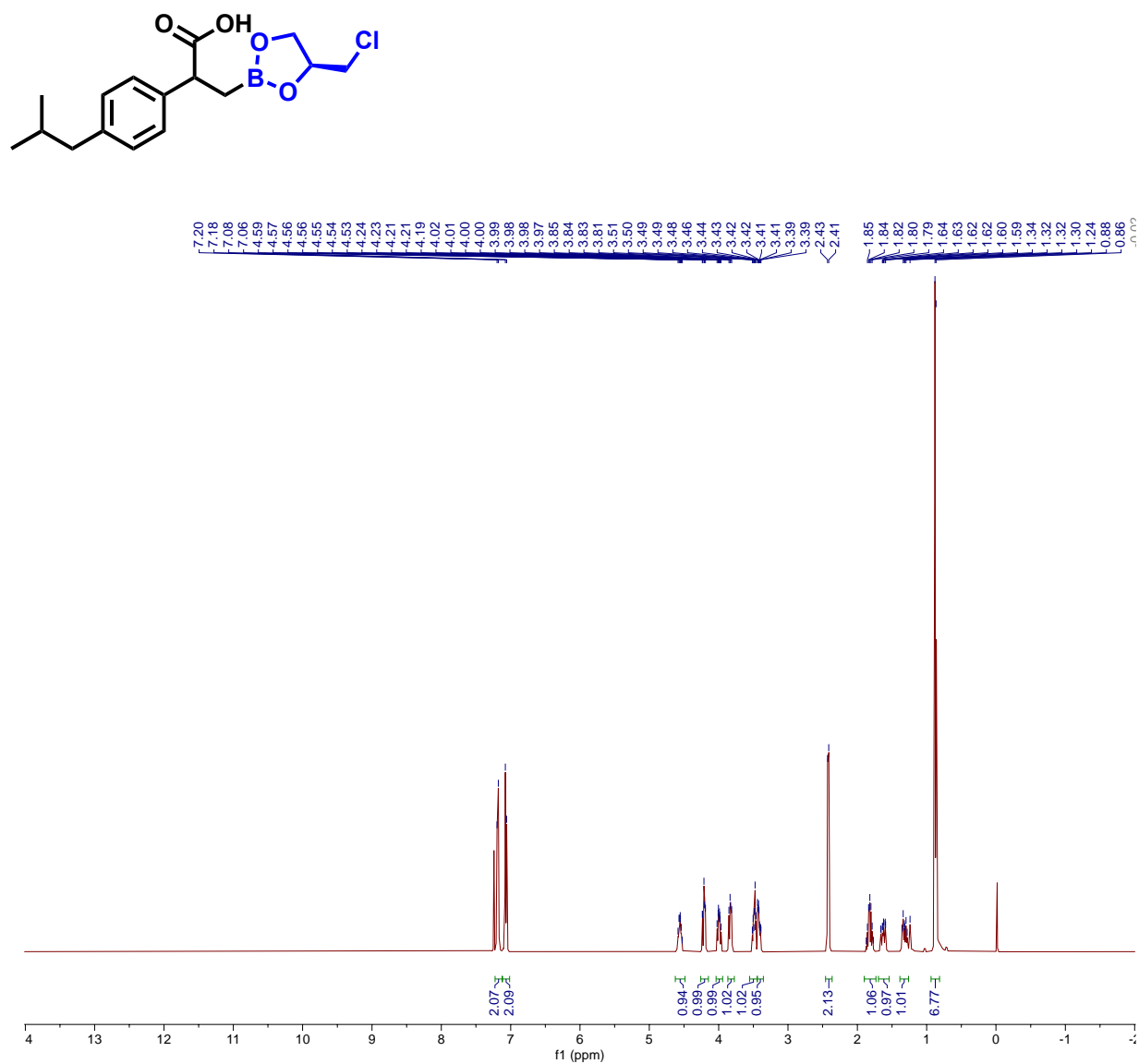


Figure S28. ¹H NMR Spectrum of **1g** in CDCl₃.

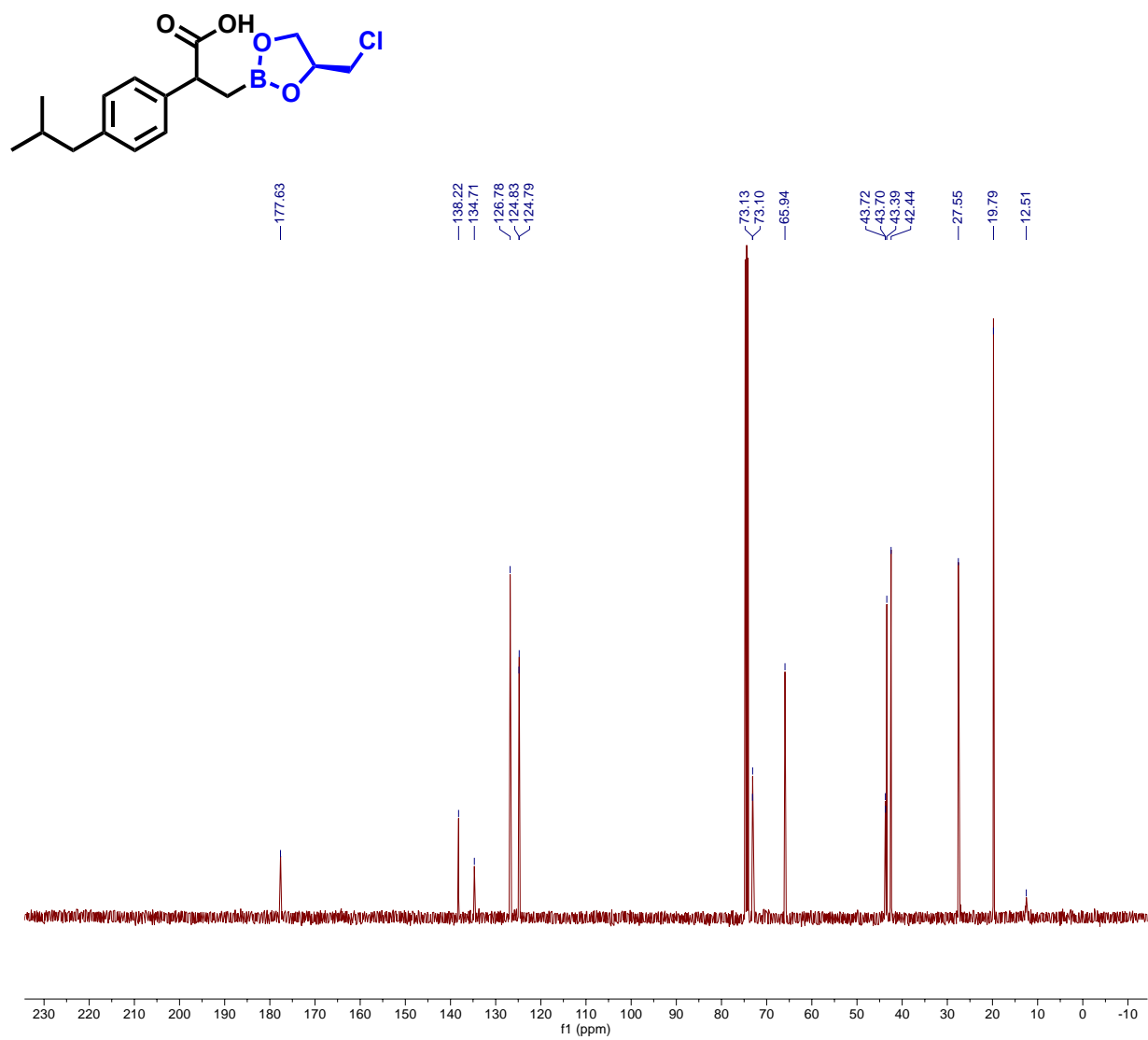
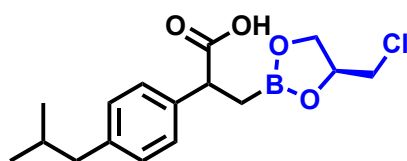


Figure S29. ^{13}C NMR Spectrum of **1g** in CDCl₃.



—32.69

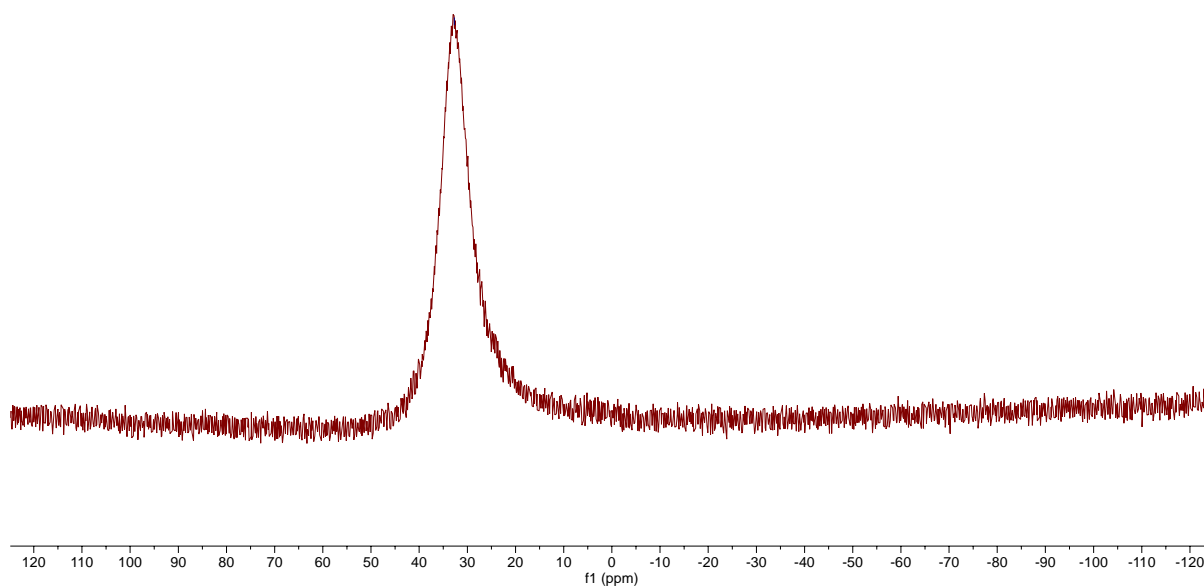


Figure S30. ^{11}B NMR Spectrum of **1g** in CDCl_3 .

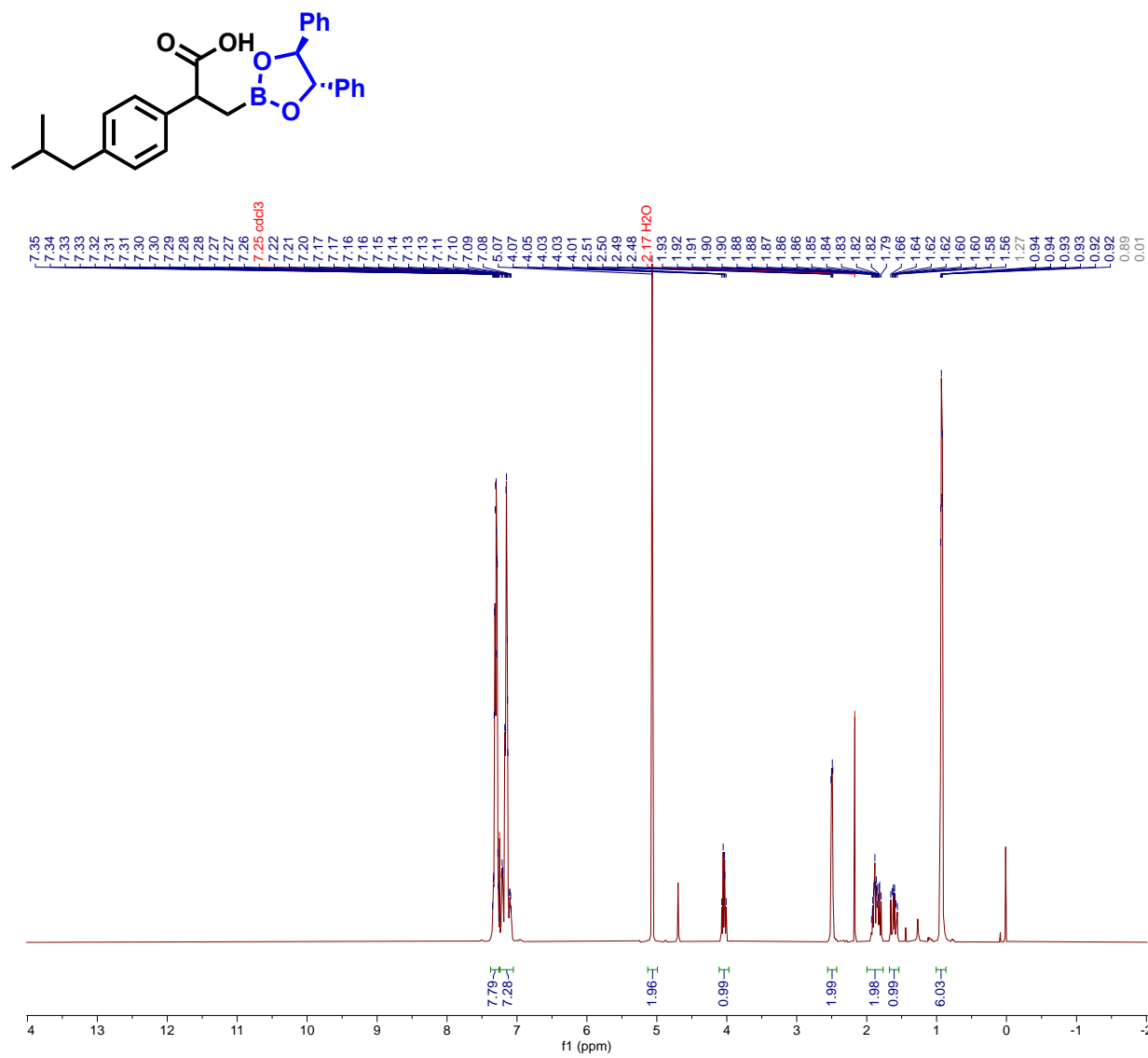


Figure S31. ¹H NMR Spectrum of **1h** in CDCl₃.

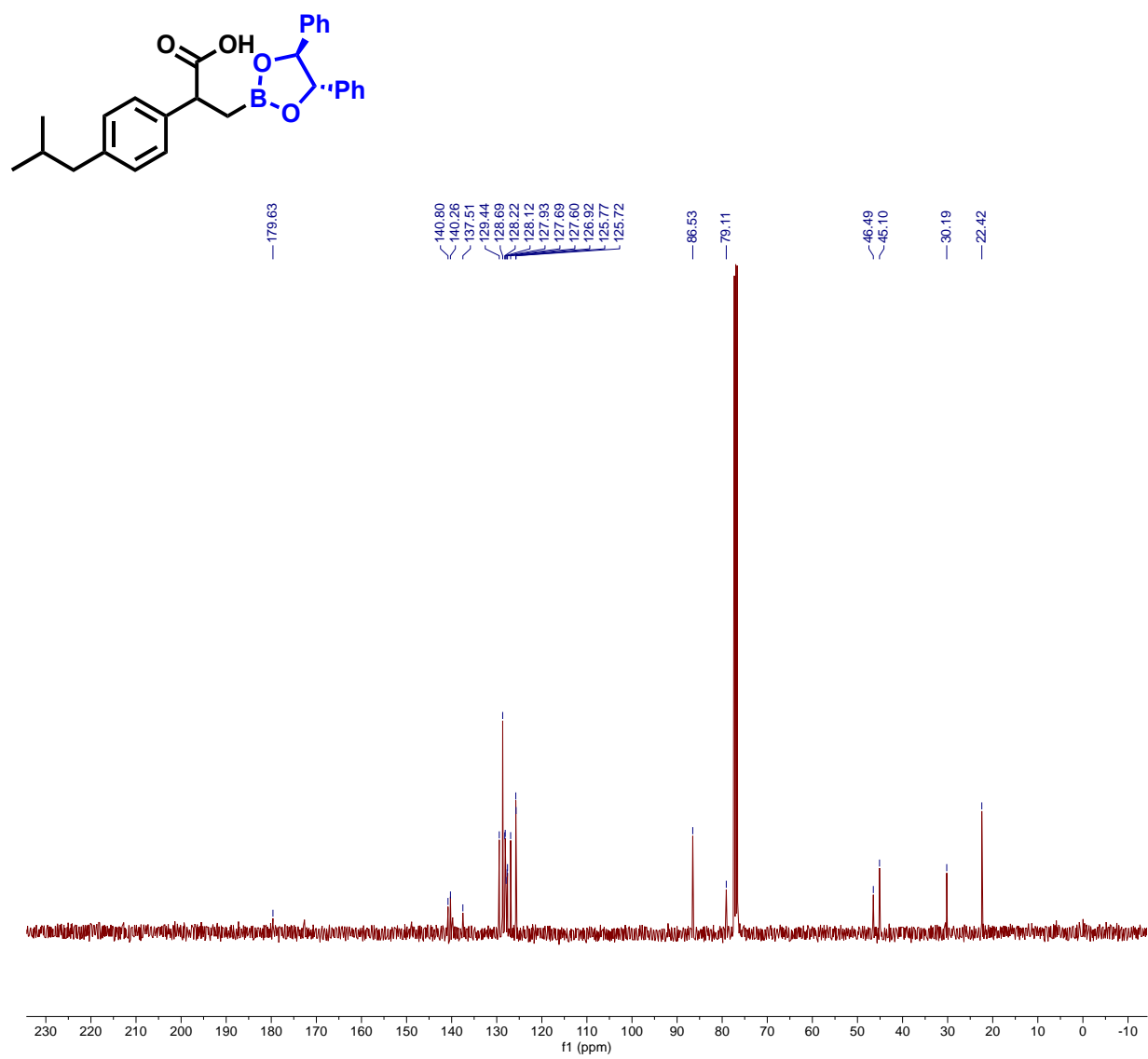
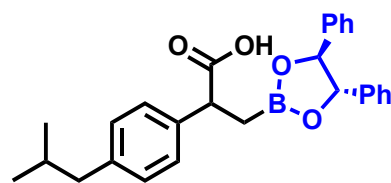


Figure S32. ¹³C NMR Spectrum of **1h** in CDCl₃.



—33.67

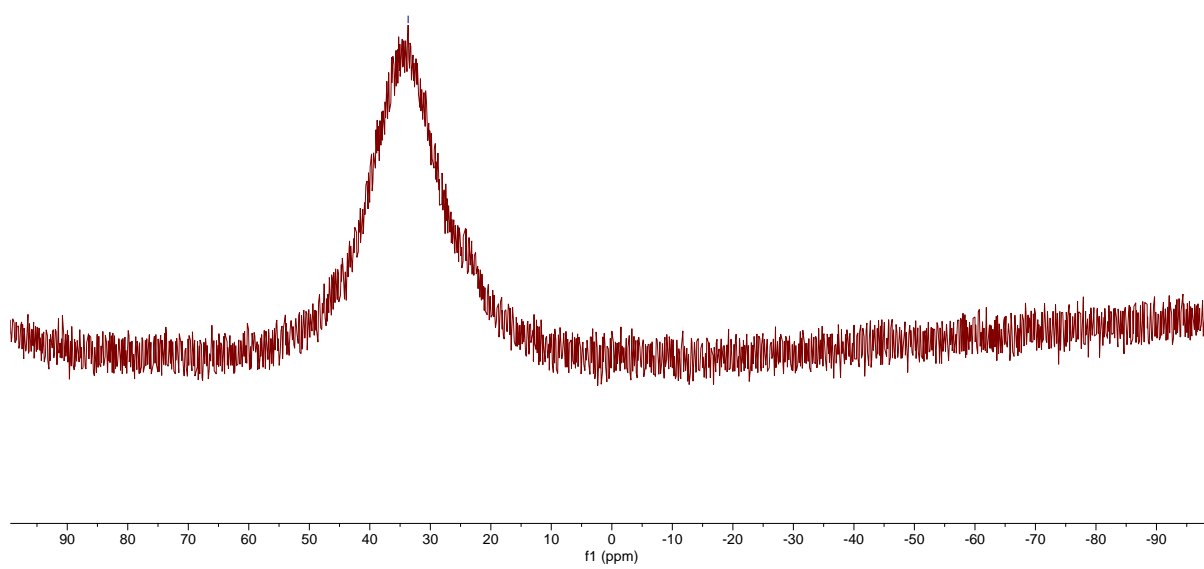


Figure S33. ^{11}B NMR Spectrum of **1h** in CDCl_3 .

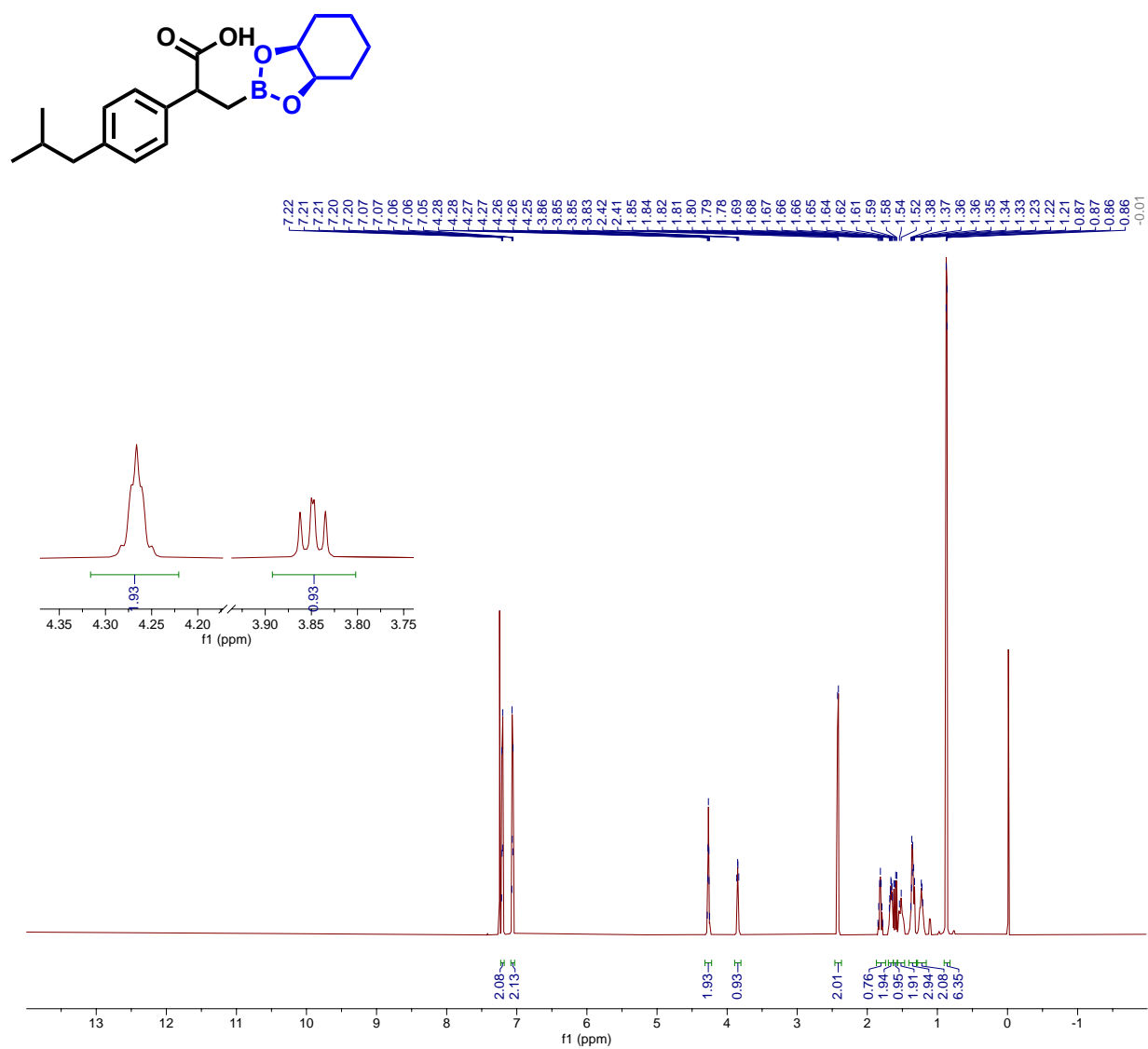
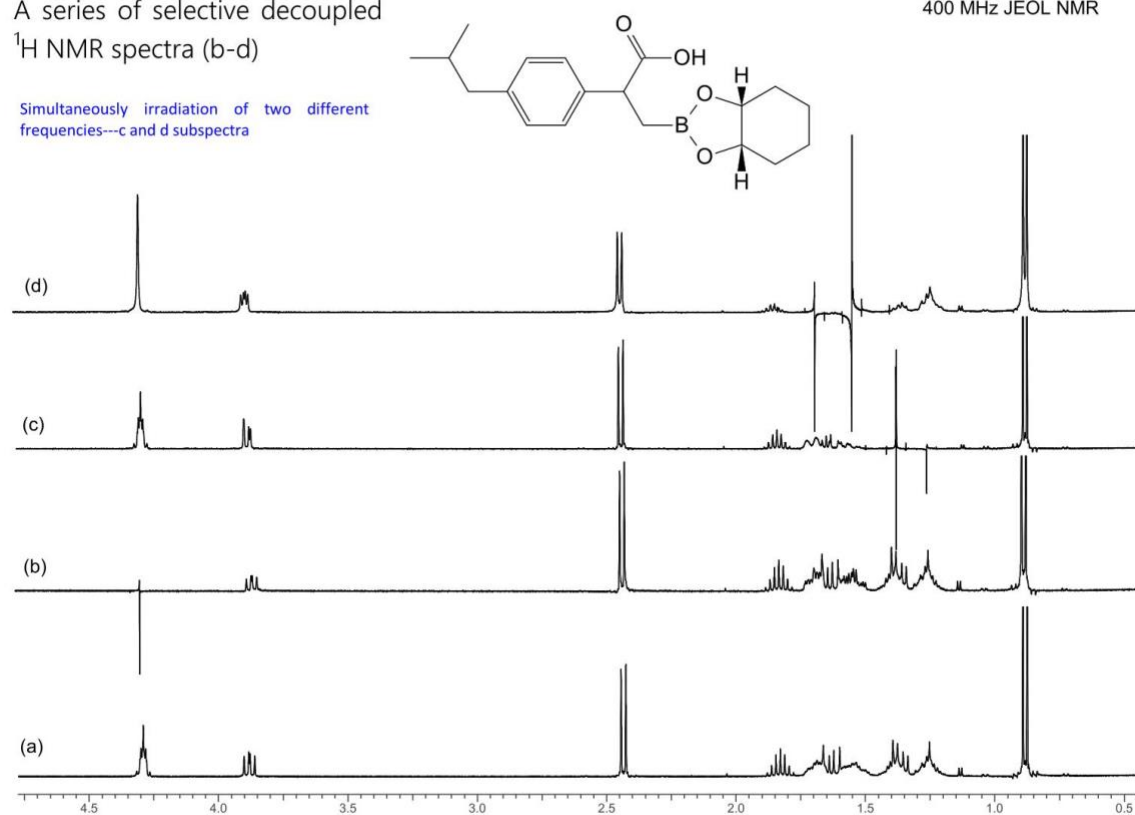


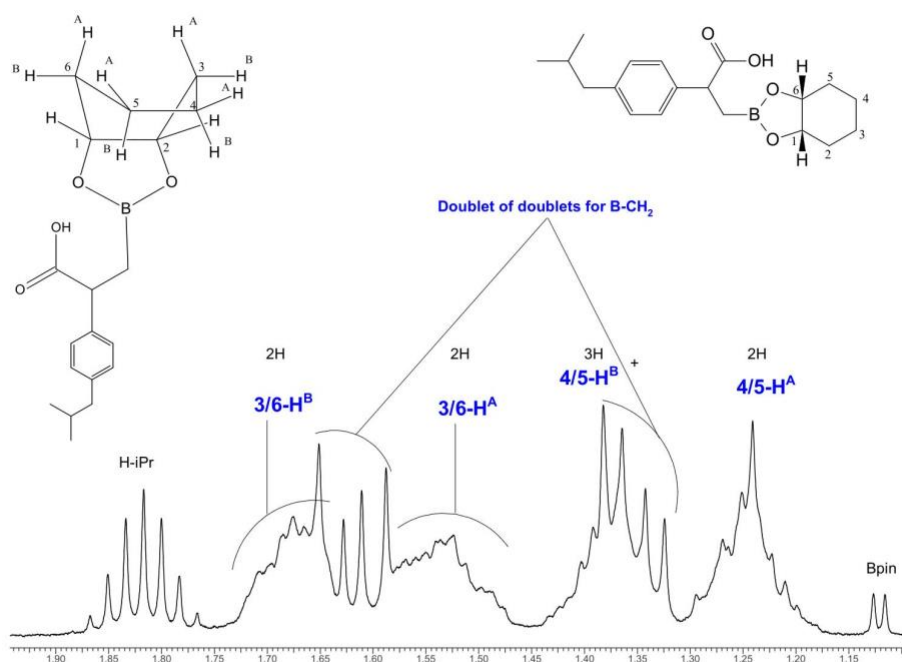
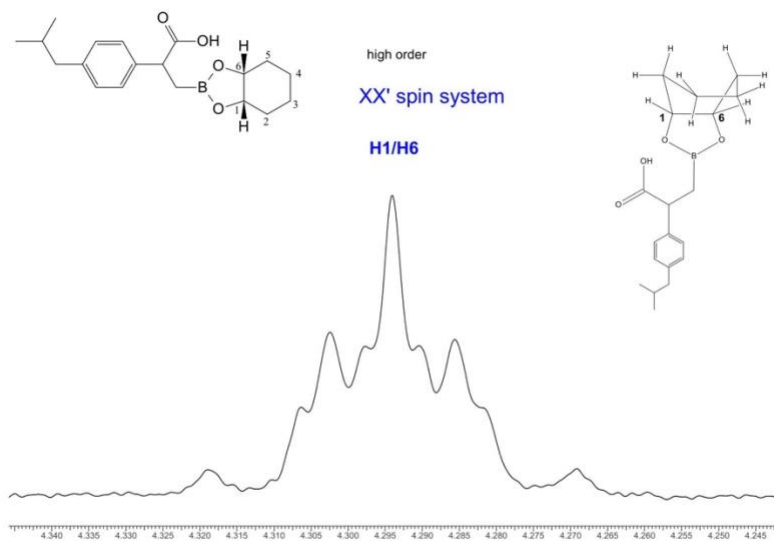
Figure S34. a) ¹H NMR Spectrum of **1i** in CDCl₃.

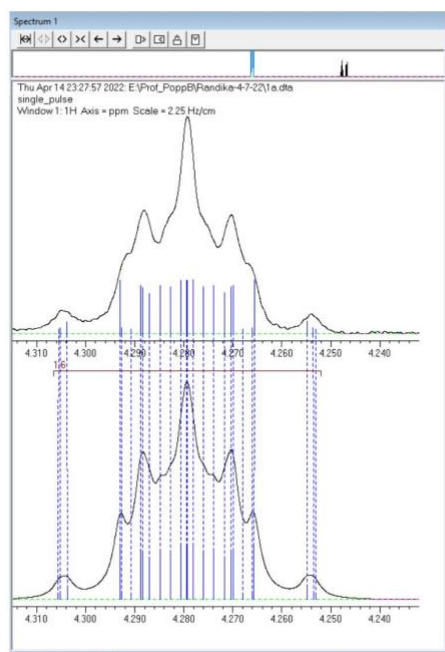
A series of selective decoupled
 ^1H NMR spectra (b-d)

Simultaneously irradiation of two different
 frequencies---c and d subspectra

400 MHz JEOL NMR

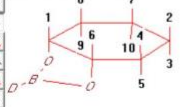






Simulation of the multiplicity patterns of OCH protons (bridge)

Coupling constants in Hz



#	n	Shift	Width	J[1]	J[2]	J[3]	J[4]	J[5]	J[6]	J[7]	J[8]	J[9]
1	1	4.279										
	x	-										
2	f	1.360		0.00								
	c	-										
3	f	1.230		0.00	-12.00							
	d	-										
4	1	1.539		0.00	7.00	7.00						
	a	-										
5	1	1.679		0.00	7.00	7.00	-13.60					
	b	-					ab					
6	1	4.279		6.70	0.00	0.00	4.97	5.98				
	x	-	xx'				ax	bx				
7	f	1.360		0.00	7.00	7.00	0.00	0.00	0.00			
	c	-										
8	1	1.539		4.97	0.00	0.00	0.00	0.00	0.00	7.00		
	a	-		ax								
9	1	1.679		5.98	0.00	0.00	0.00	0.00	0.00	7.00	-13.60	
	b	-		bx							ab	
10	f	1.230		0.00	7.00	7.00	0.00	0.00	0.00	-16.00	7.00	7.00
	d	-										

Figure S34. b) Additional ^1H NMR characterization data for **1i** in CDCl_3 .

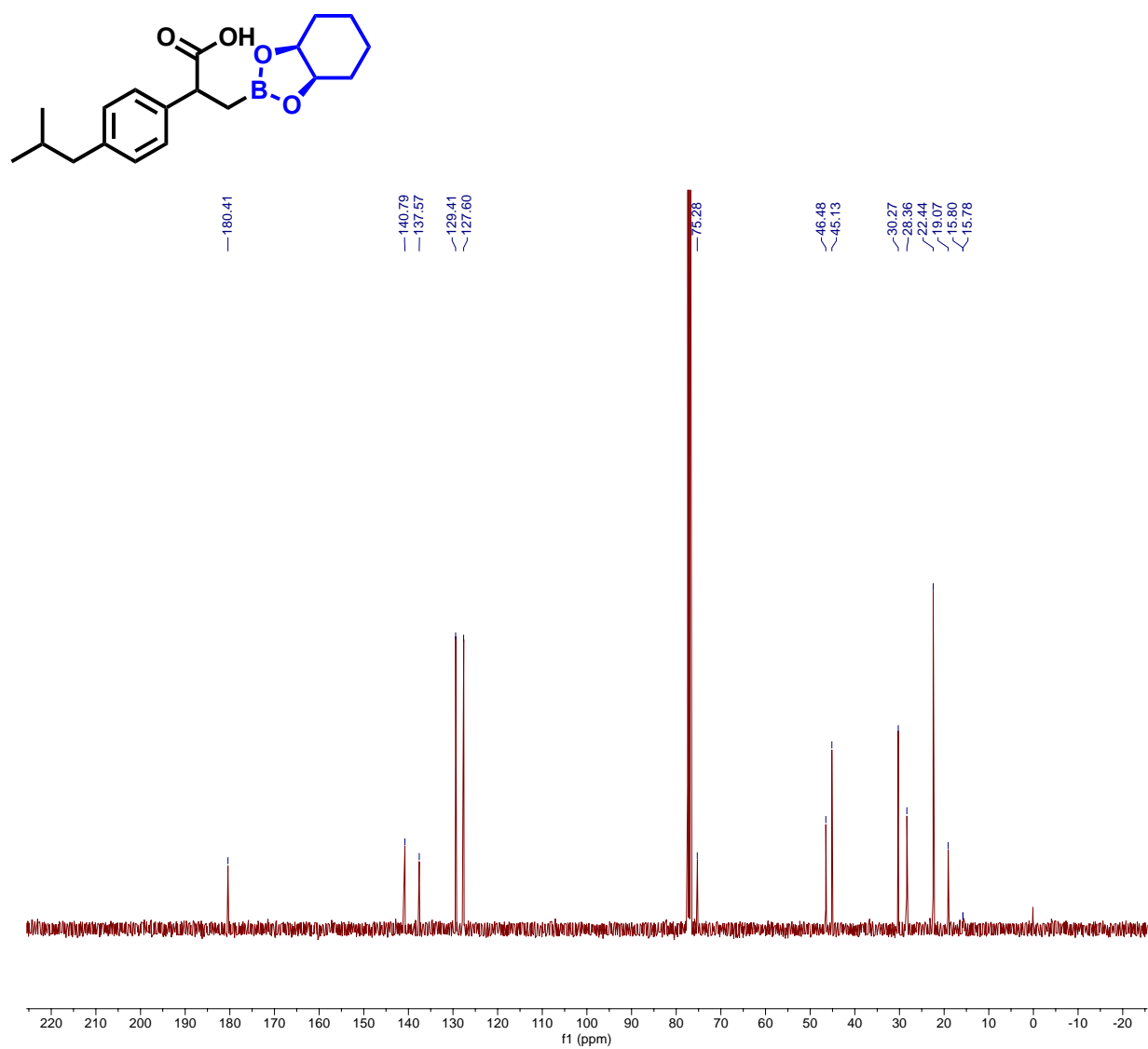


Figure S35. ^{13}C NMR Spectrum of **1i** in CDCl₃.

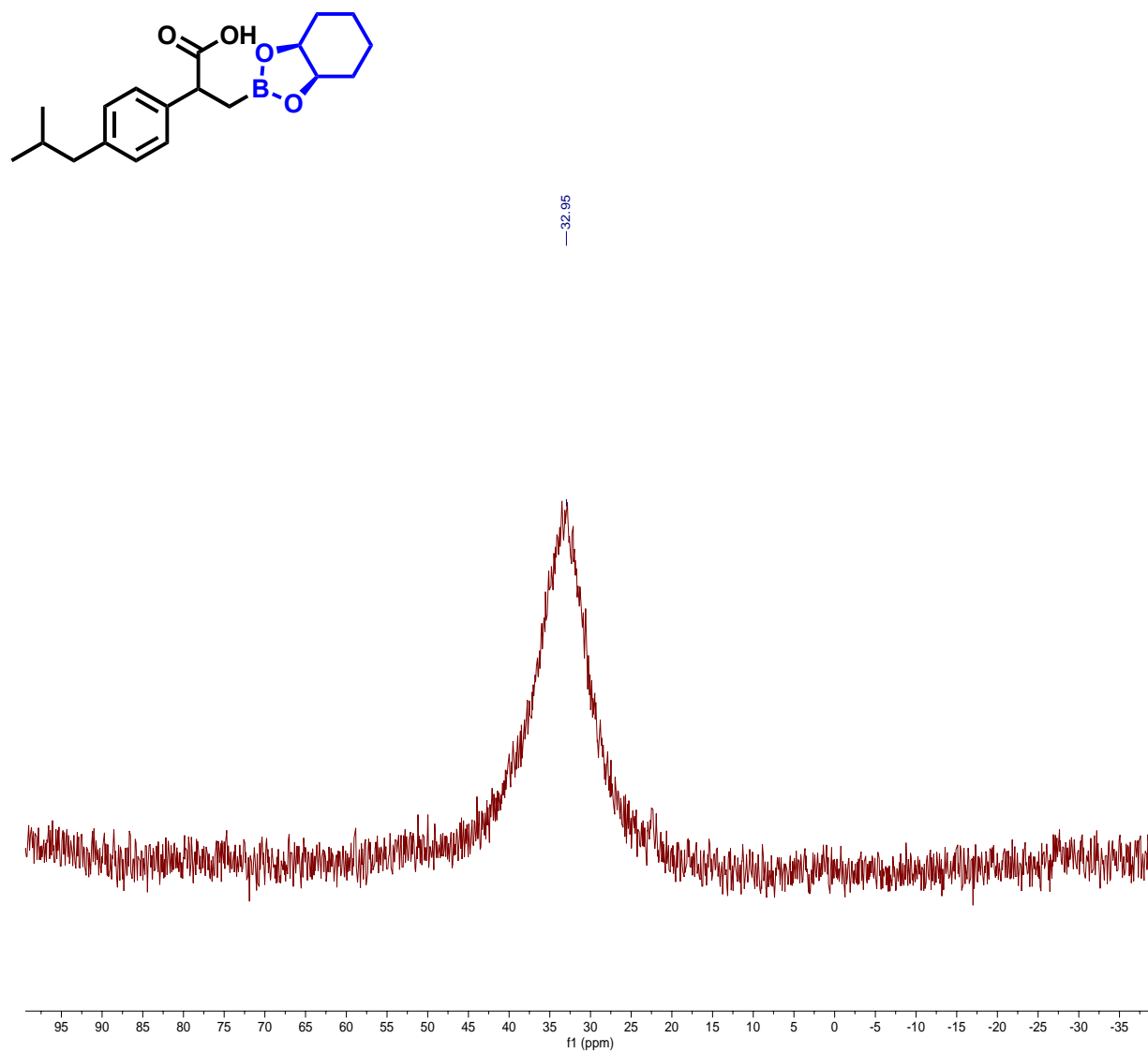


Figure S36. ^{11}B NMR Spectrum of **1i** in CDCl_3 .

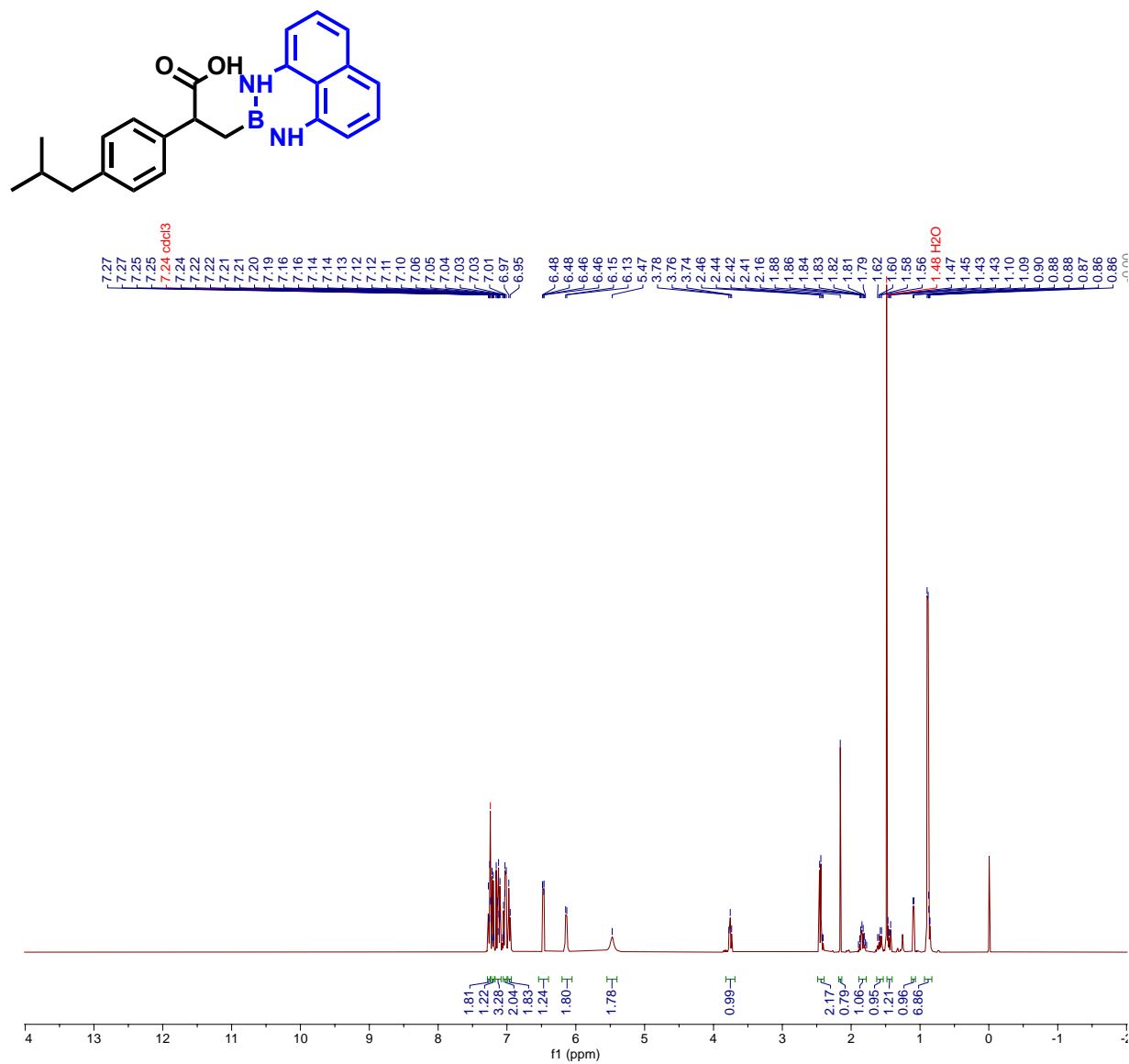


Figure S37. ¹H NMR Spectrum of **1j** in CDCl₃.

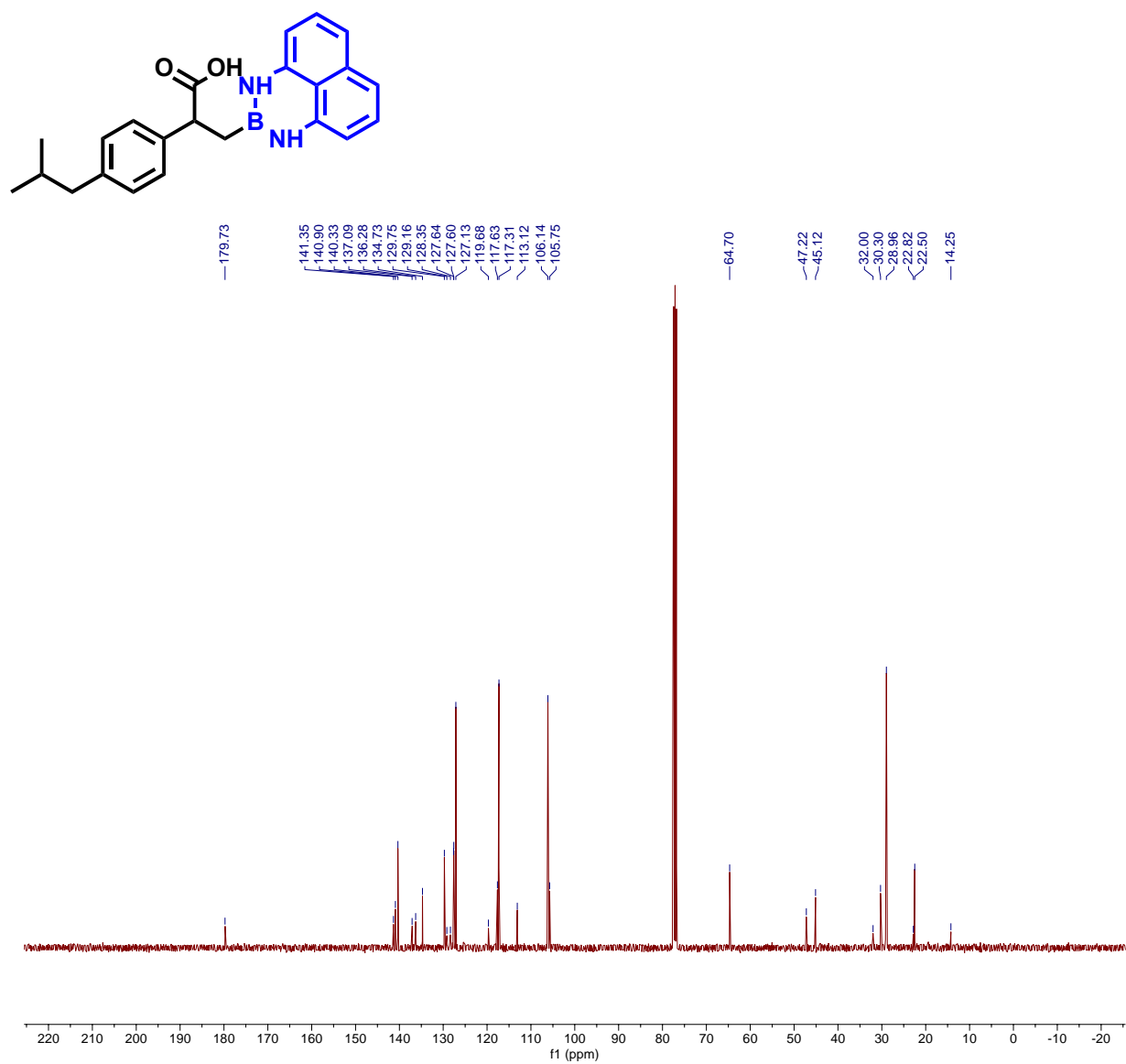
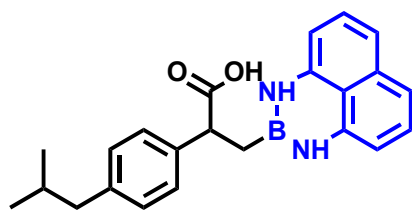


Figure S38. ^{13}C NMR Spectrum of **1j** in CDCl₃.



— 31.62

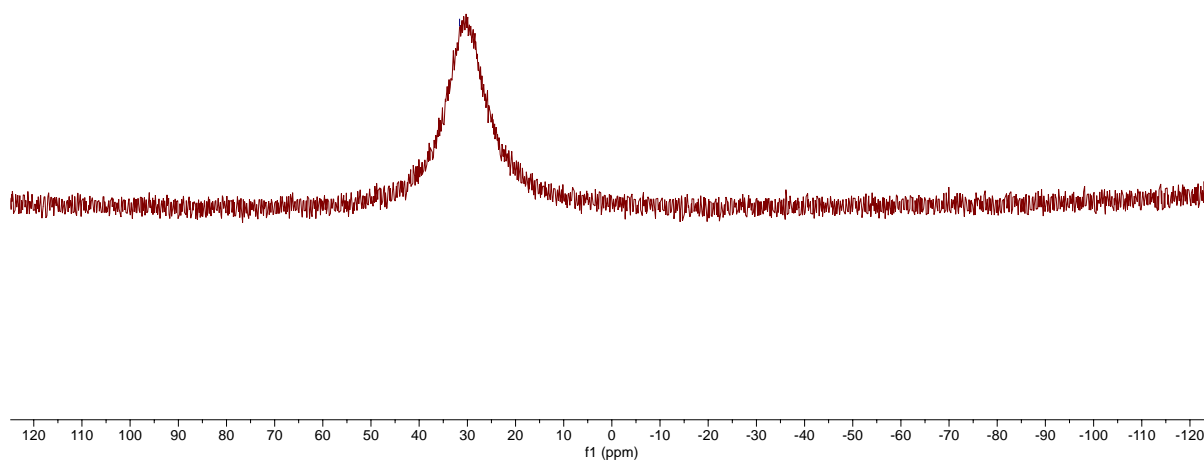


Figure S39. ^{13}C NMR Spectrum of **1j** in CDCl_3 .

Table S1. Crystal data and structure refinement for 1e (CCDC ID: 2225404).

Identification code	1e
Empirical formula	C ₁₆ H ₂₁ BBrNO ₆
Formula weight	414.06
Temperature/K	100.0
Crystal system	monoclinic
Space group	P2 ₁ /c
a/Å	15.0011(5)
b/Å	13.4984(5)
c/Å	9.1329(3)
α/°	90
β/°	102.251(2)
γ/°	90
Volume/Å ³	1807.21(11)
Z	4
ρ _{calc} /cm ³	1.522
μ/mm ⁻¹	2.306
F(000)	848.0
Crystal size/mm ³	0.3 × 0.2 × 0.1
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	5.472 to 51.462
Index ranges	-18 ≤ h ≤ 18, -16 ≤ k ≤ 16, -11 ≤ l ≤ 11
Reflections collected	55837
Independent reflections	3448 [R _{int} = 0.0922, R _{sigma} = 0.0320]
Data/restraints/parameters	3448/348/285
Goodness-of-fit on F ²	1.167
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0663, wR ₂ = 0.1408
Final R indexes [all data]	R ₁ = 0.0814, wR ₂ = 0.1472
Largest diff. peak/hole / e Å ⁻³	0.75/-0.73