

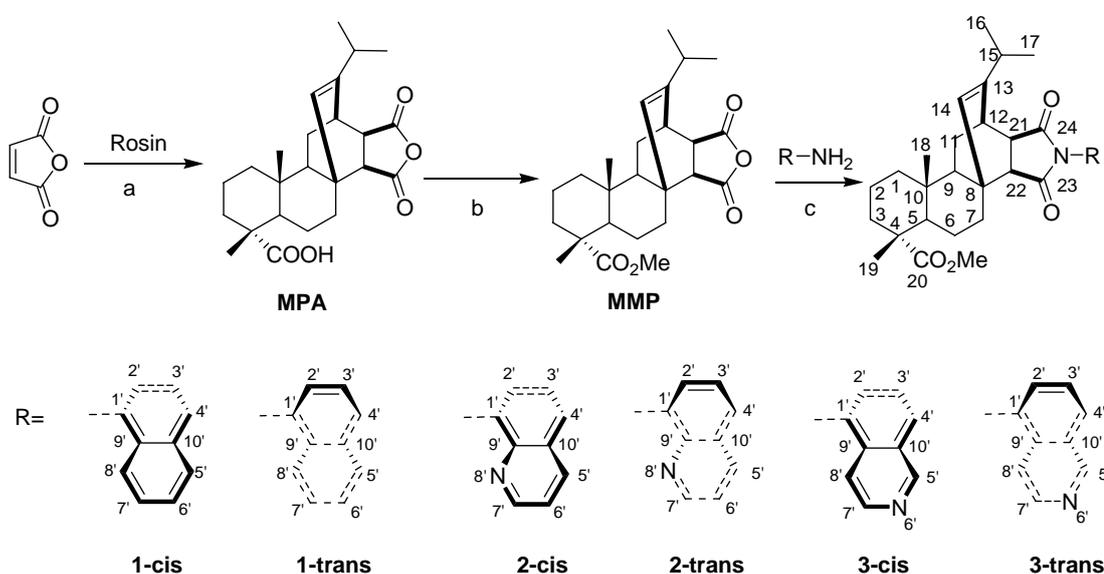
Protonation-controlled axial chirality in maleopimaric imides

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Synthesis



Scheme 1

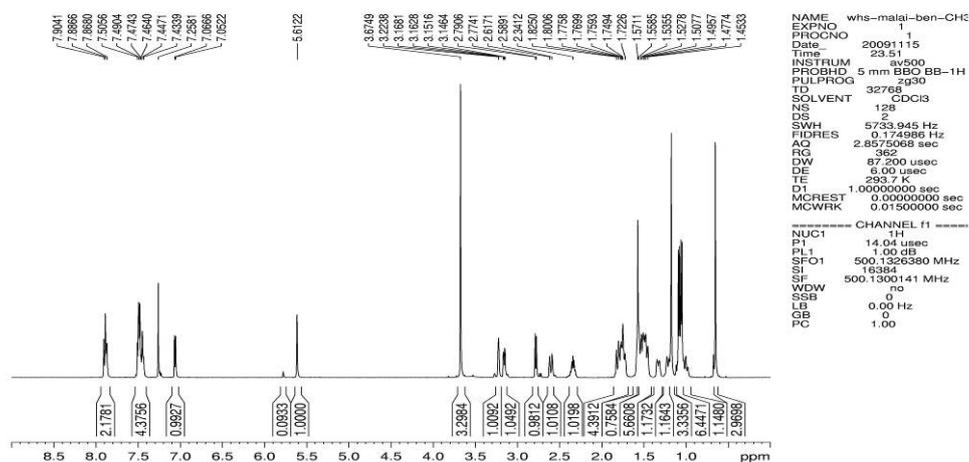


Figure S1. ¹H NMR spectrum of 1 (initial state) (CDCl₃, 500 MHz).

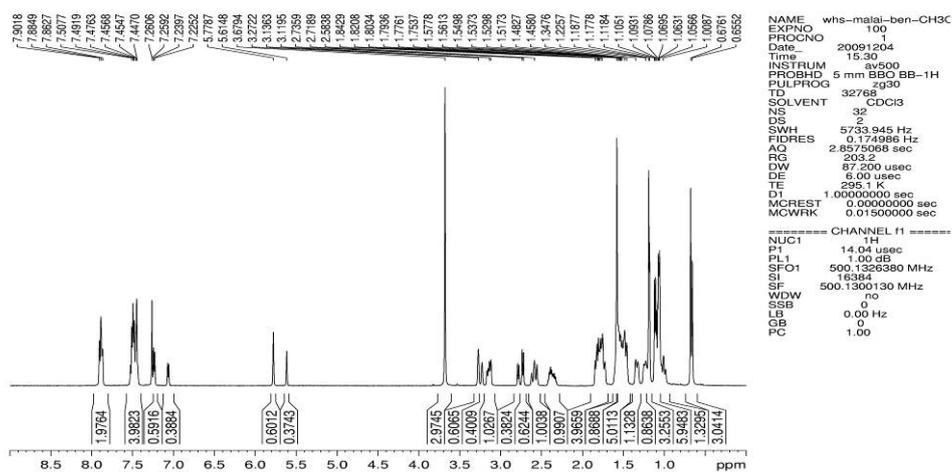


Figure S2. ¹H NMR spectrum of **1** (equilibrium state) (CDCl₃, 500 MHz).

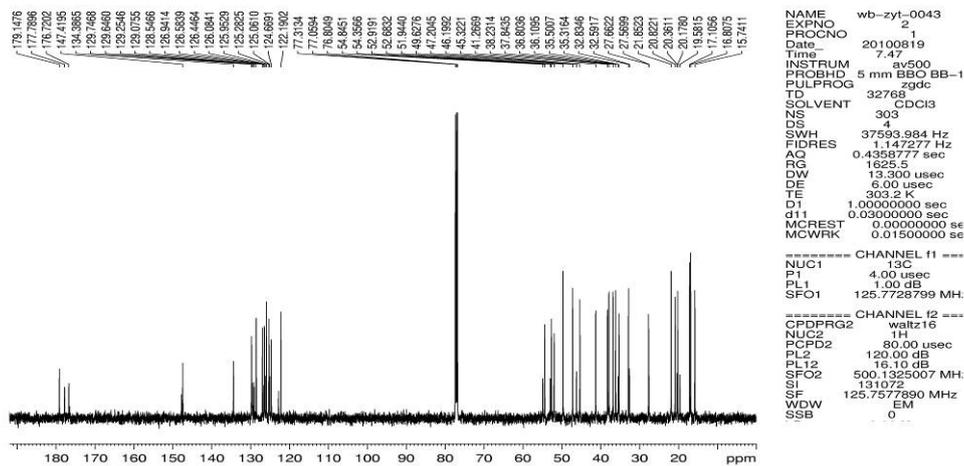


Figure S3. ¹³C NMR spectrum of **1** (initial state) (CDCl₃, 125 MHz).

Mass Spectrum List Report

Analysis Info		Acquisition Date 10/25/2007 5:06:54 PM	
Analysis Name	D:\Data\wanghengshan\zyt\APCI-whs-zyt-0009-01.d	Operator	hct
Method	APCI_POS_LOW.m	Instrument	HCT
Sample Name	090723		
Comment			
Acquisition Parameter			
Ion Source Type	APCI	Ion Polarity	Positive
Mass Range Mode	Std/Enhanced	Scan Begin	50 m/z
Capillary Exit	166.0 Volt	Skimmer	40.0 Volt
Accumulation Time	10 µs	Averages	10 Spectra
		Alternating Ion Polarity	off
		Scan End	1000 m/z
		Trap Drive	85.5
		Auto MS/MS	off

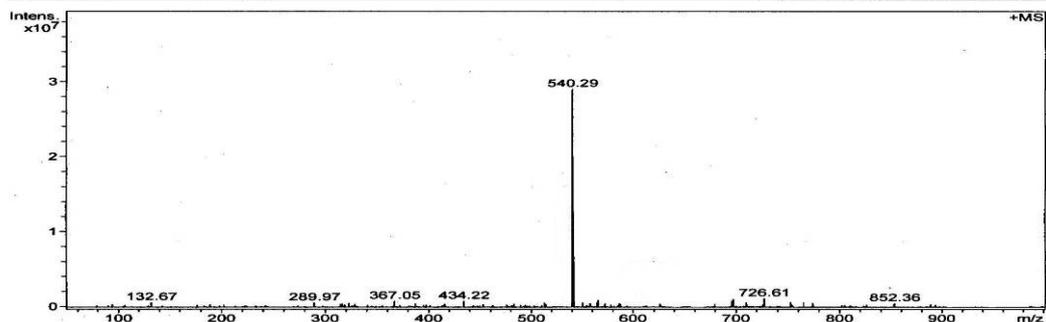
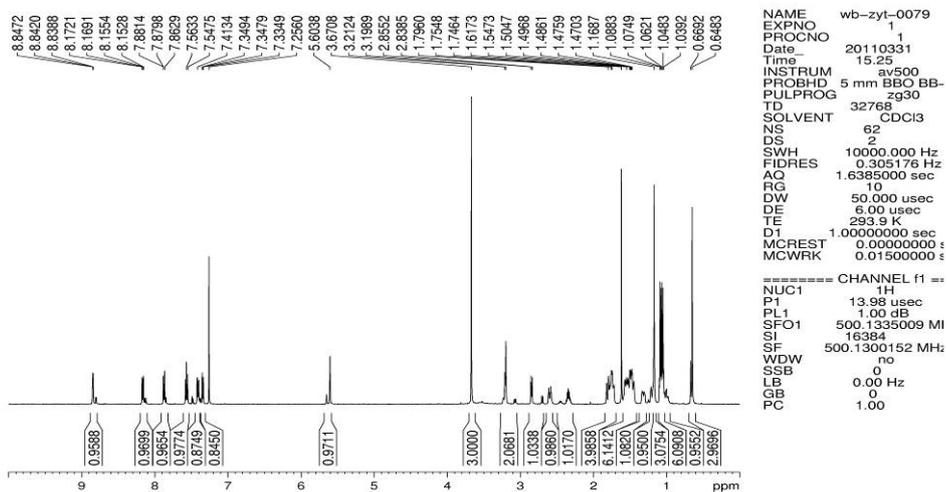


Figure S4. MS spectrum of 1.



Mass Spectrum List Report

Analysis Info		Acquisition Date		4/1/2011 3:21:17 PM	
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Method	APCI_POS_LOW.m	Instrument	HCT		
Sample Name	Dummy				
Comment					
Acquisition Parameter					
Ion Source Type	APCI	Ion Polarity	Positive	Alternating Ion Polarity	off
Mass Range Mode	Std/Enhanced	Scan Begin	200 m/z	Scan End	800 m/z
Capillary Exit	165.0 Volt	Skimmer	40.0 Volt	Trap Drive	91.1
Accumulation Time	27 µs	Averages	10 Spectra	Auto MS/MS	off

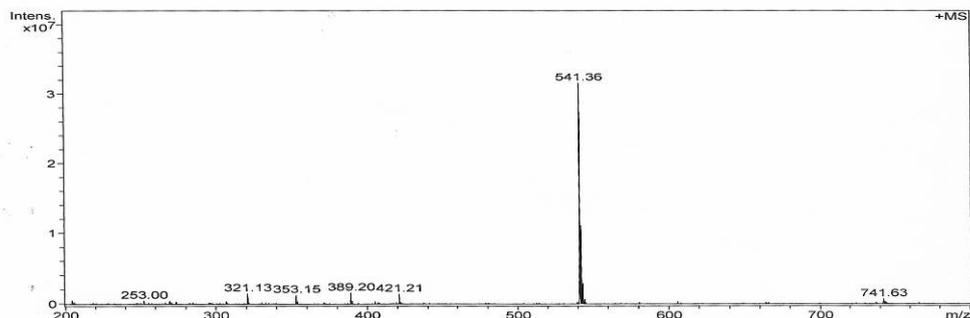


Figure S7. MS spectrum of 2.

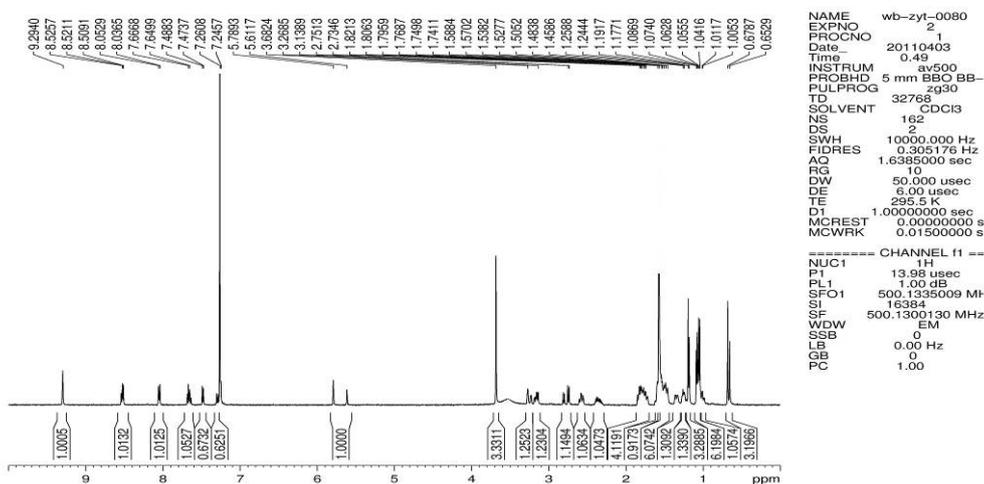


Figure S8. ¹H NMR spectrum of 3 (initial state) (CDCl₃, 500 MHz).

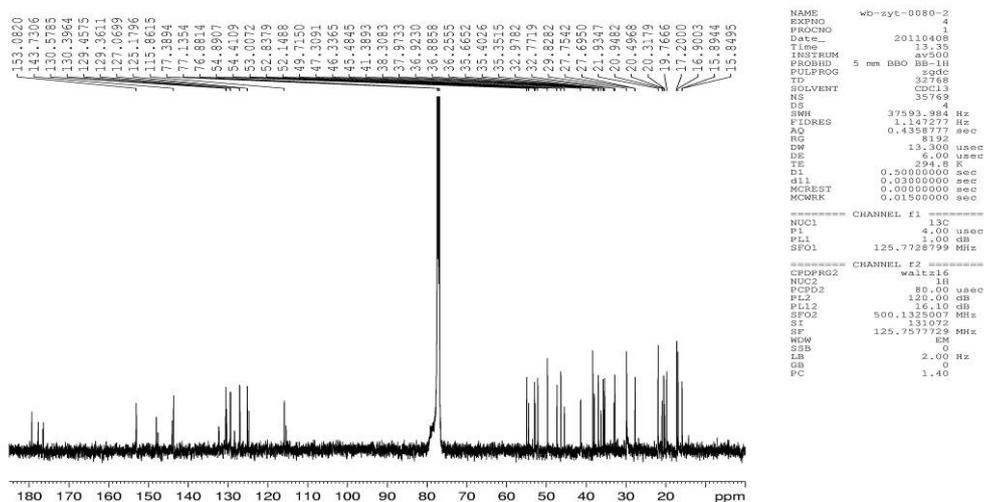


Figure S9. ¹³C NMR spectrum of 3 (initial state) (CDCl₃, 125 MHz).

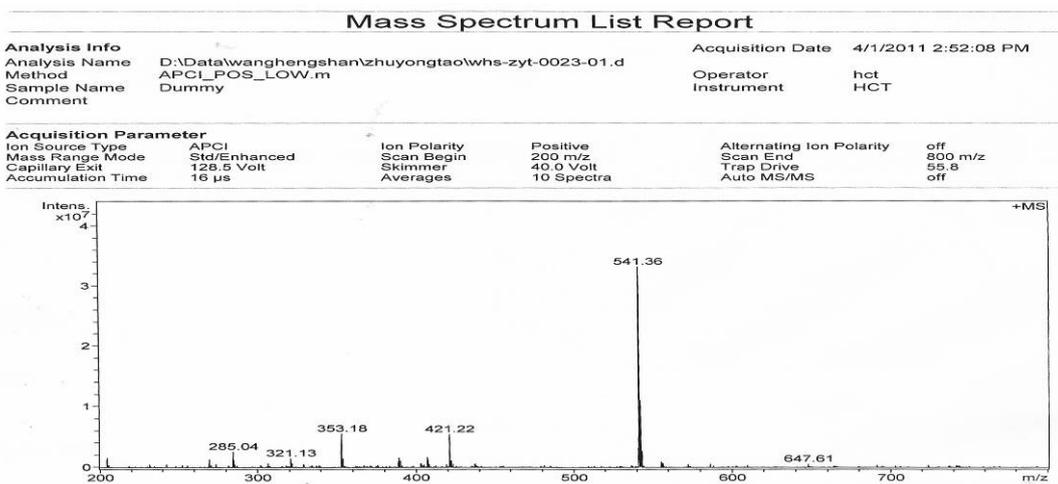


Figure S10. MS spectrum of **3**.

2D NMR

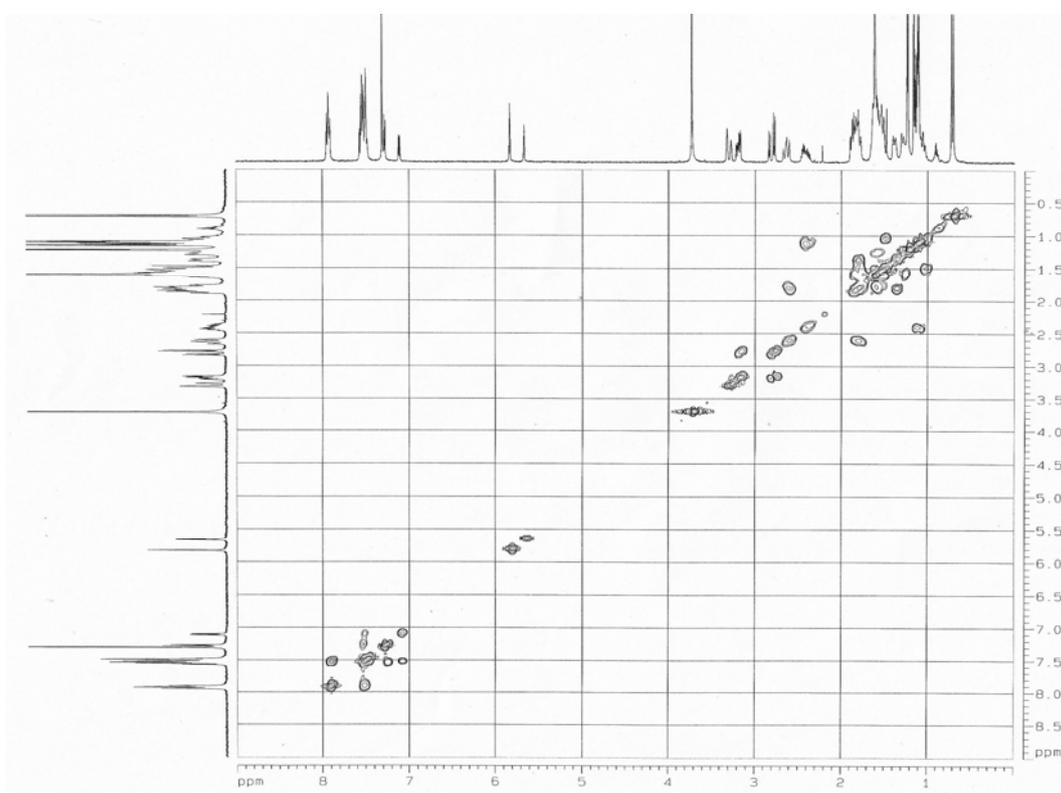


Figure S11 ^1H - ^1H COSY spectrum of **1**

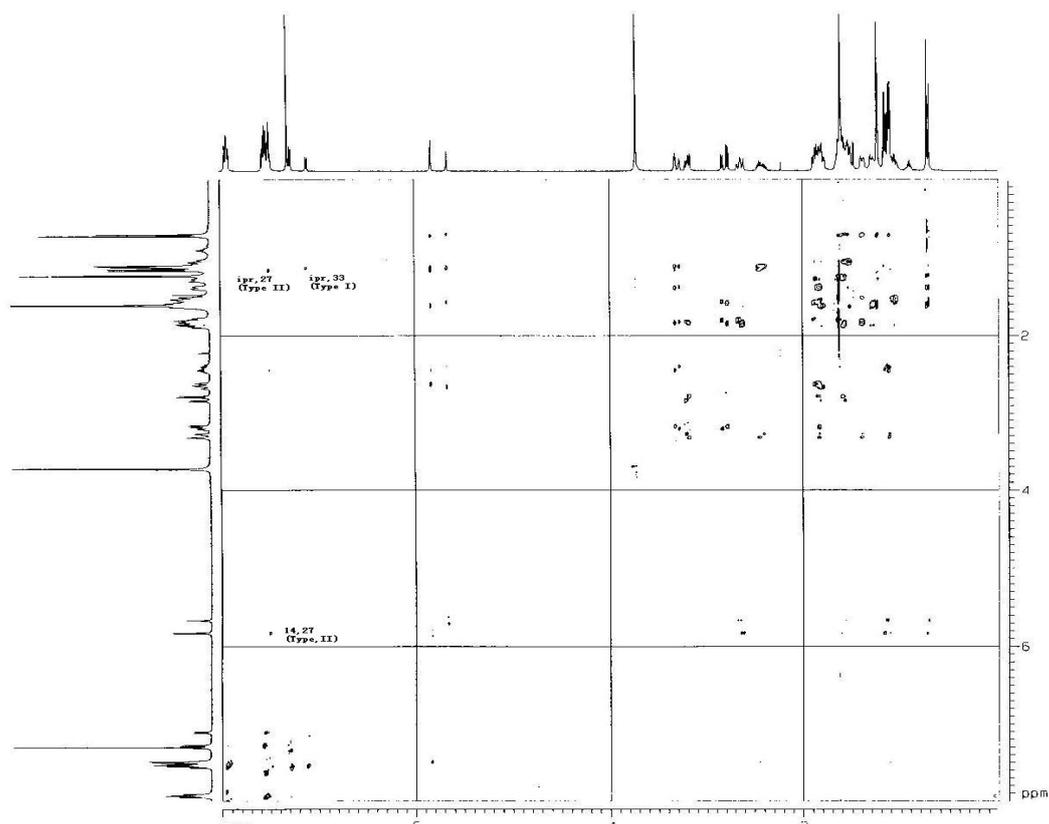


Figure S12 ^1H - ^1H NOESY spectrum of **1**

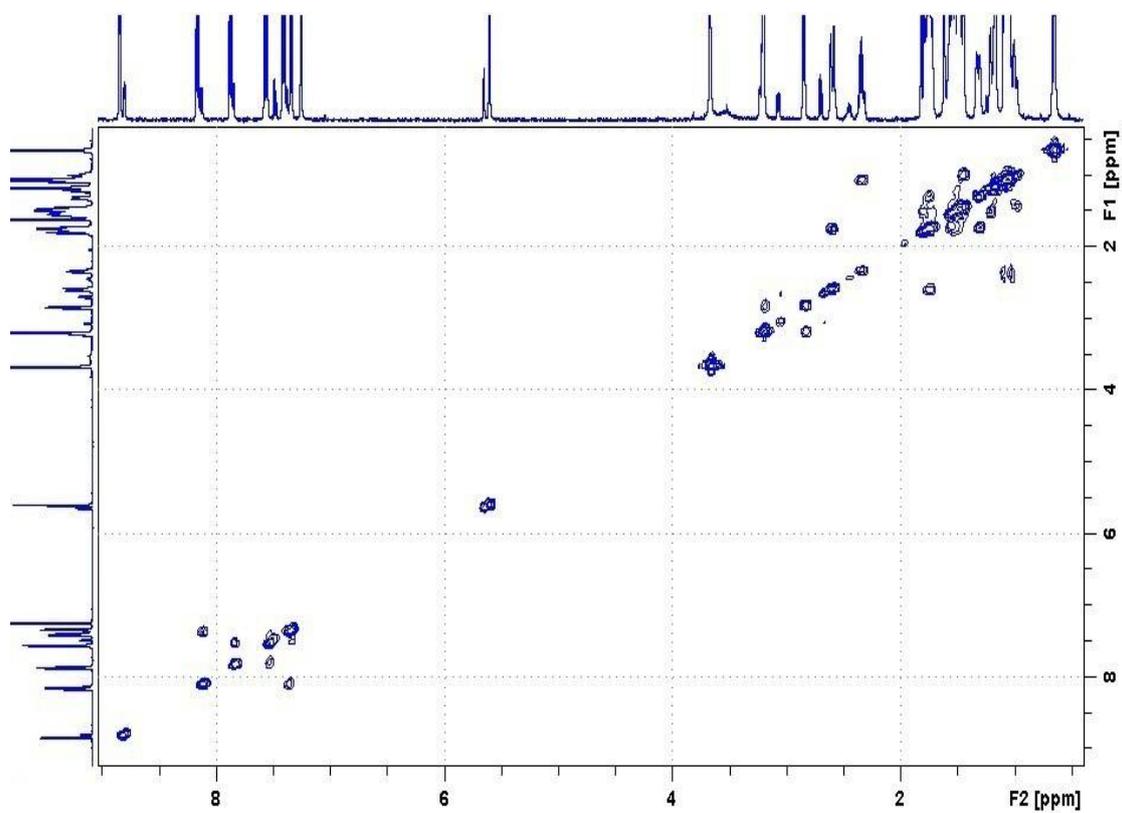


Figure S13 ^1H - ^1H COSY spectrum of **2**

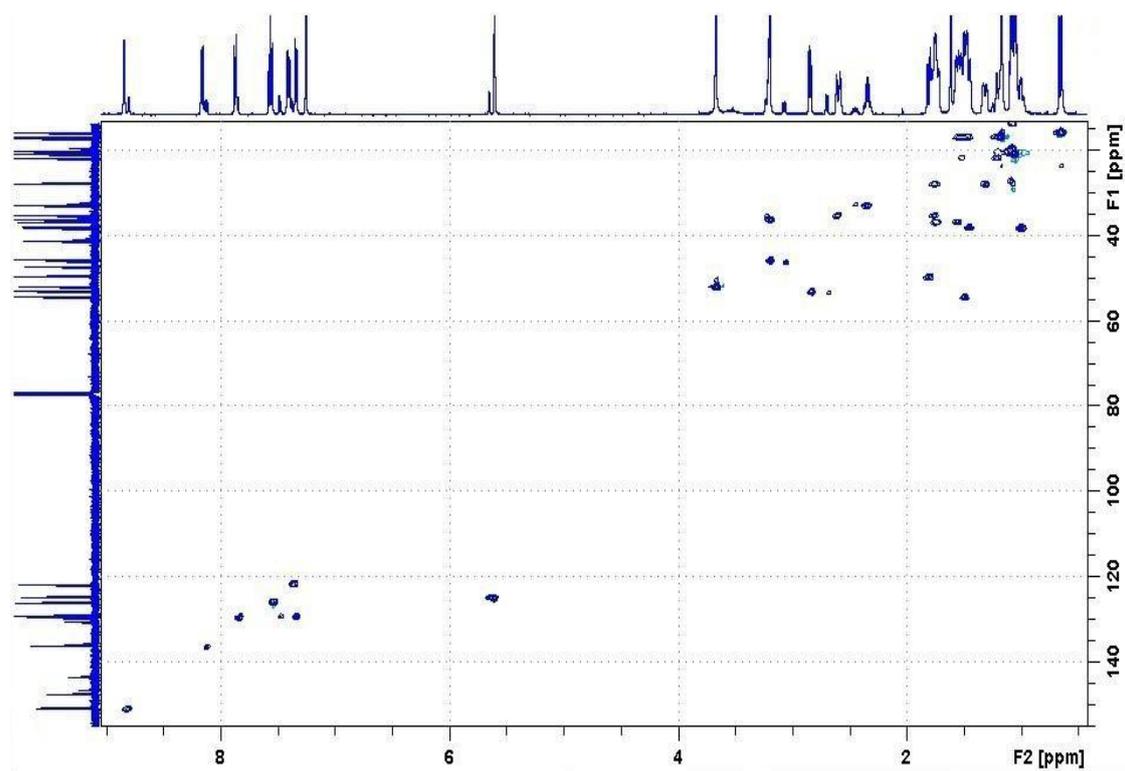


Figure S14 ^1H - ^1H HSQC spectrum of **2**.

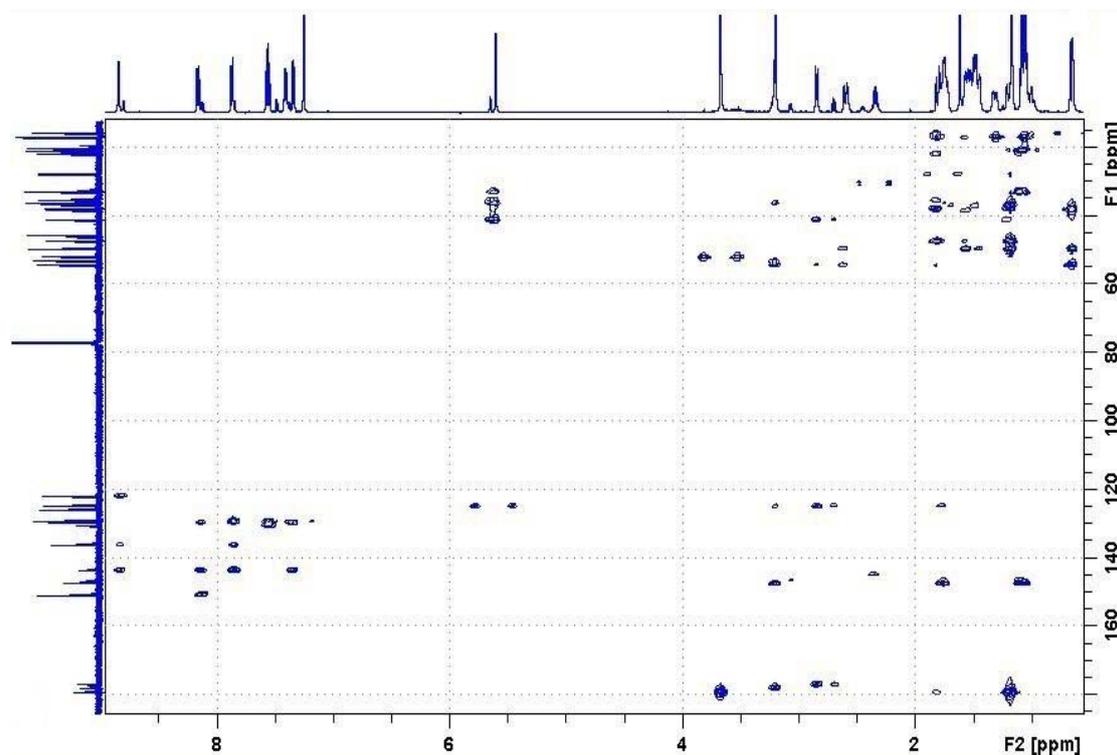


Figure S15 ^1H - ^1H HMBC spectrum of **2**.

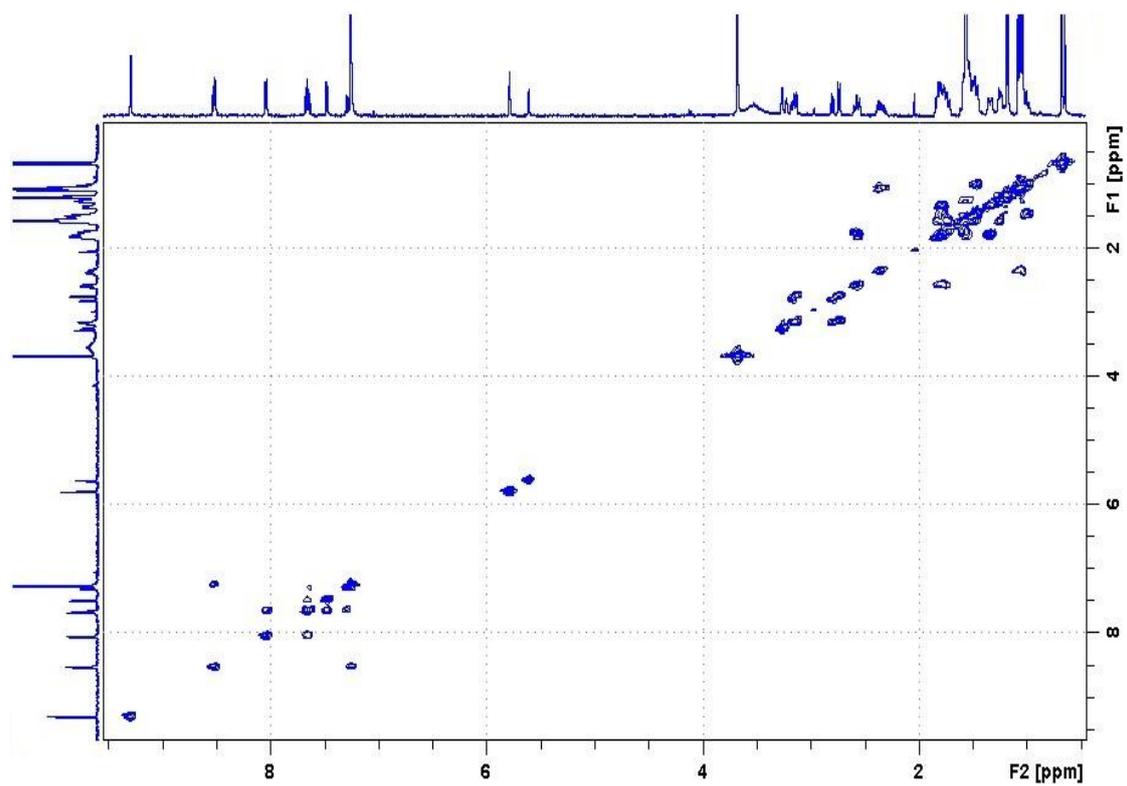


Figure S16 ^1H - ^1H COSY spectrum of **3**.

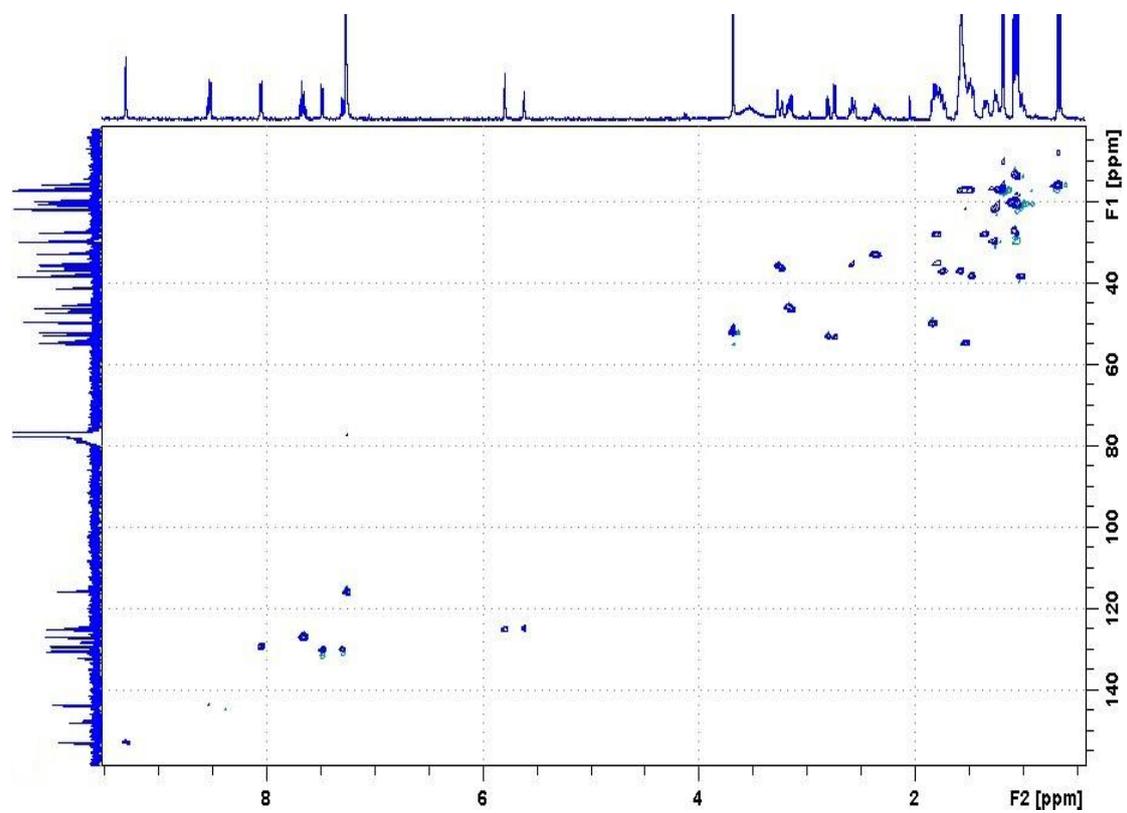


Figure S17 ^1H - ^{13}C HSQC spectrum of **3**.

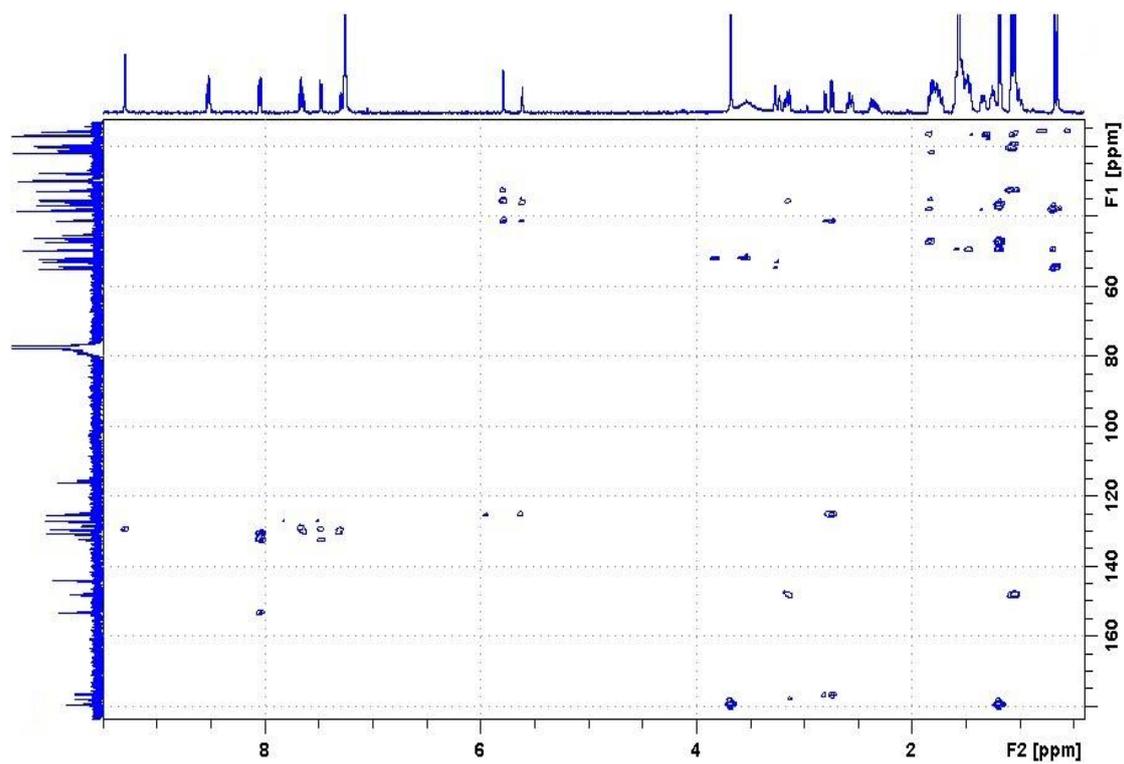


Figure S18 ^1H - ^1H HMBC spectrum of **3**.

Kinetic study

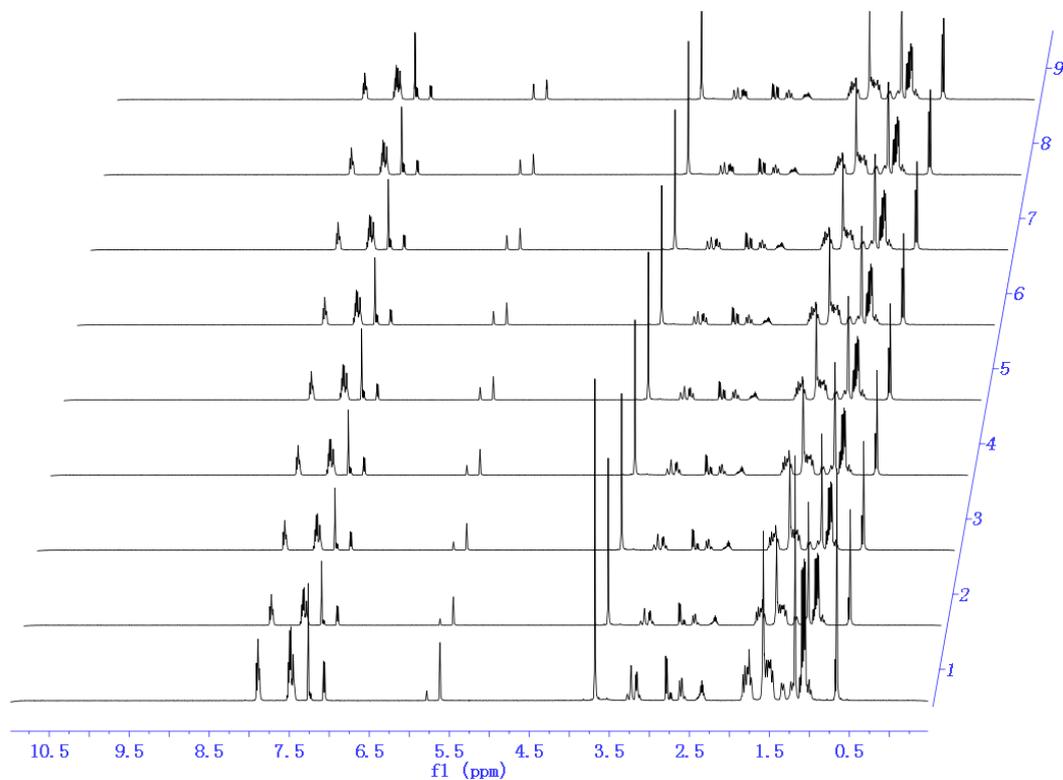


Figure S19. Rational barrier study overlay of **1** in CDCl_3 via NMR (293K)

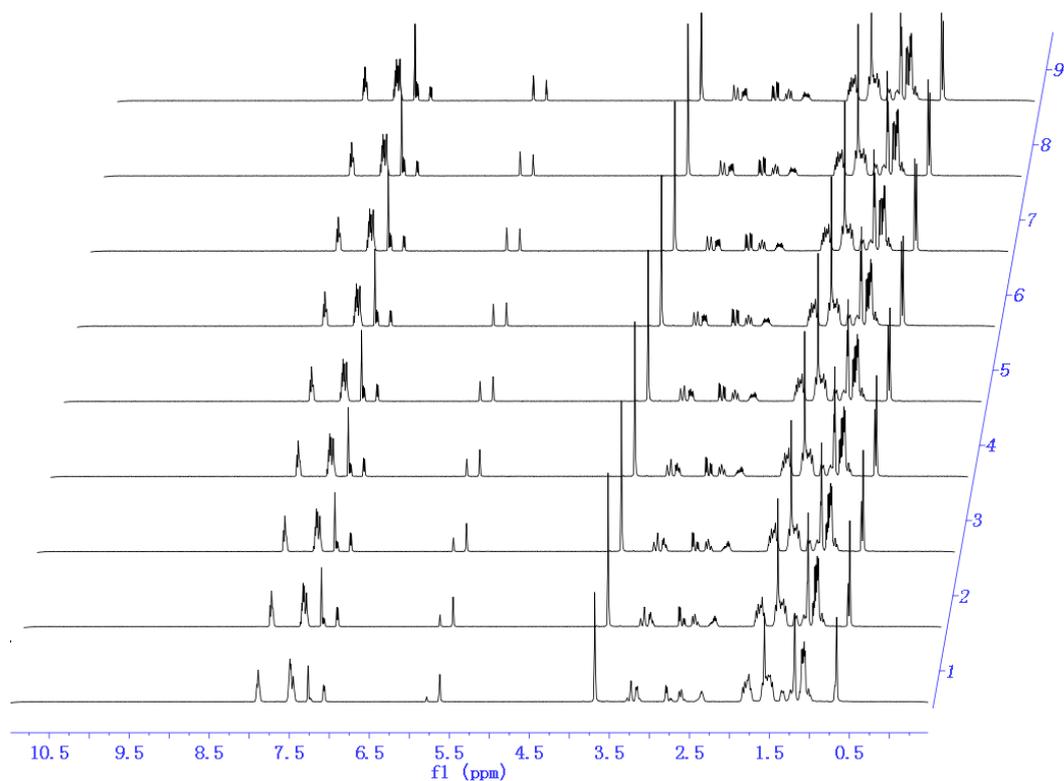


Figure S20. Rational barrier study overlay of 1 in CDCl₃ via NMR (303K)

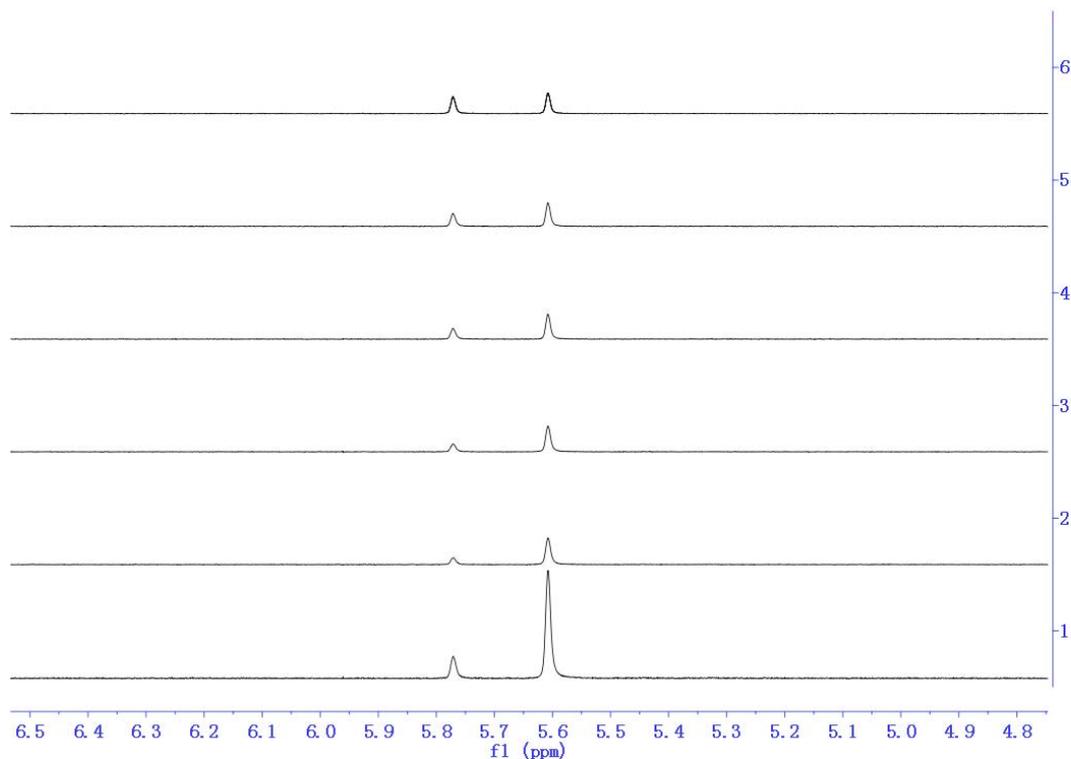


Figure S21. Rational barrier study overlay of 2 in CDCl₃ via NMR (293K)

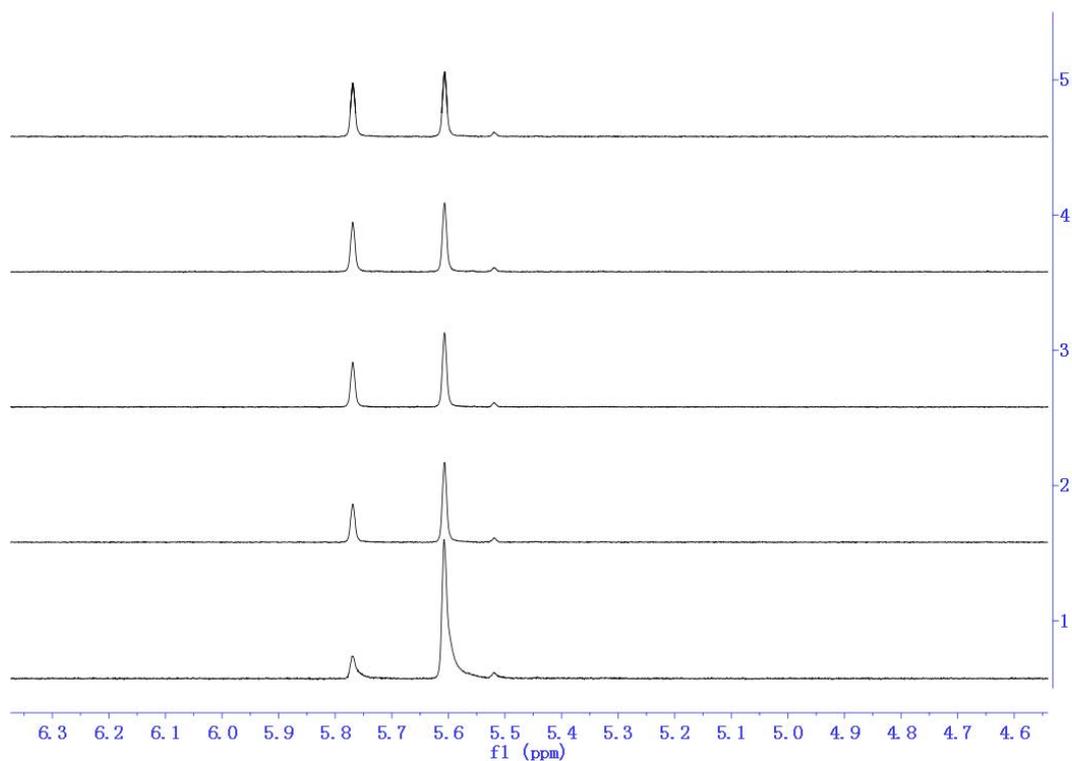


Figure S22. Rational barrier study overlay of 2 in CDCl₃ via NMR (303K)

Protonation-controlled study

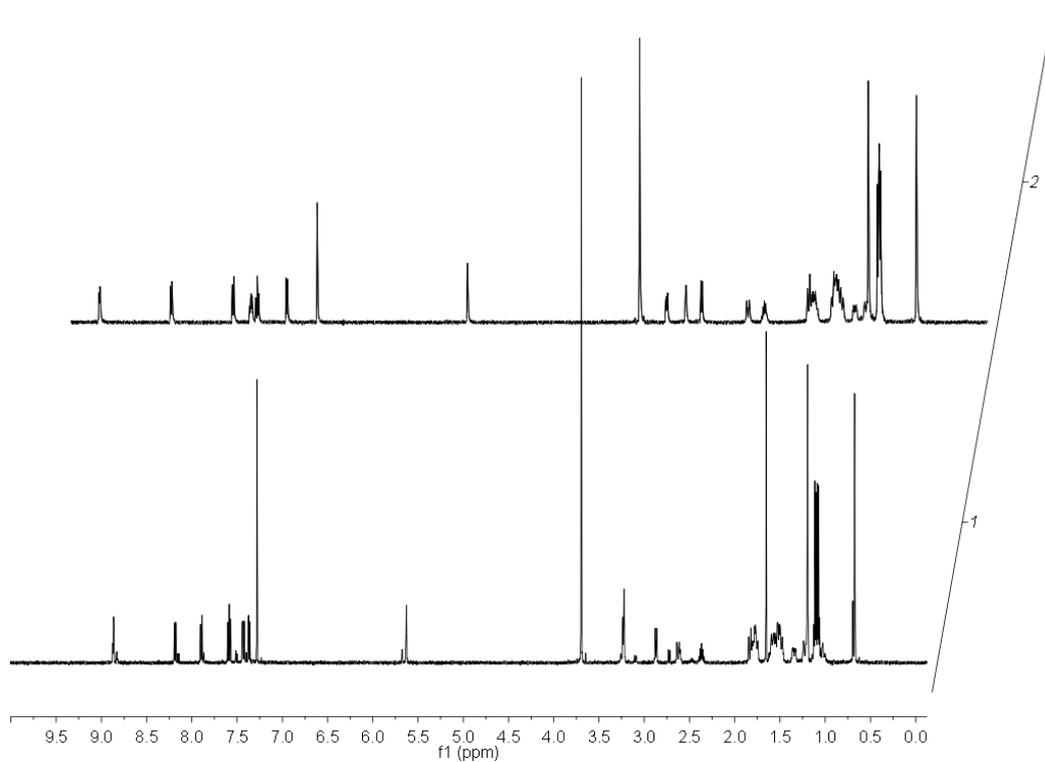


Figure S23. Full ¹H NMR (500 MHz) spectra of 2 when titrated with various equivalence of TFA in CDCl₃ at rt.

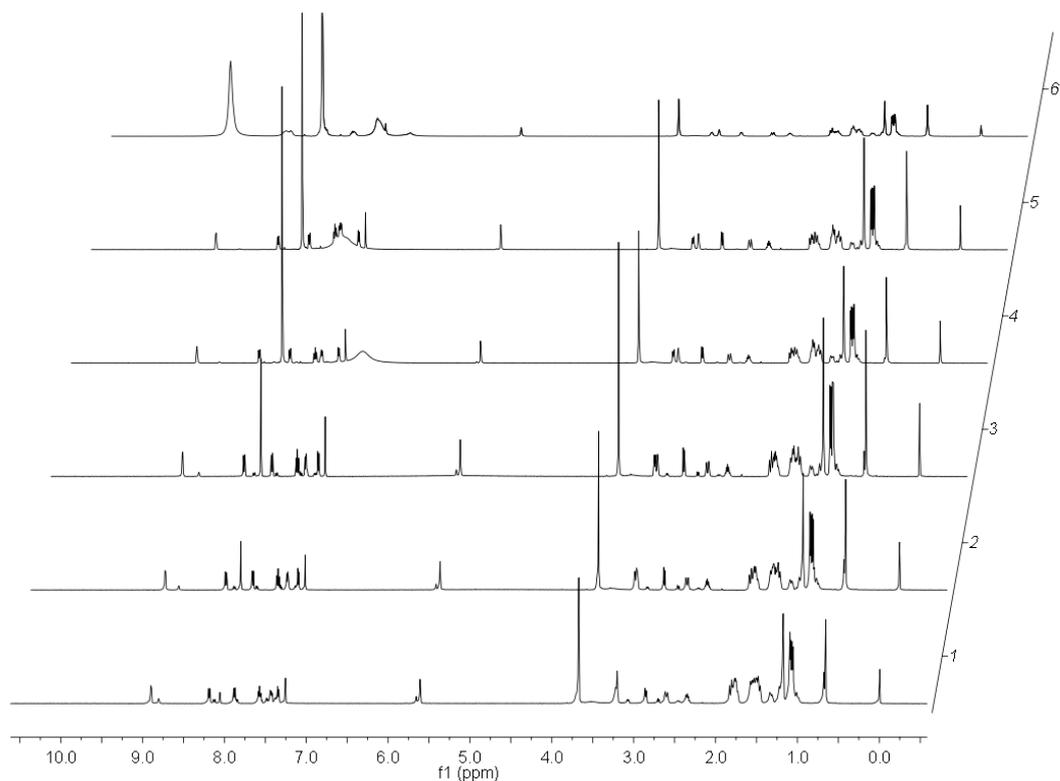


Figure S24. Full ^1H NMR (500 MHz) spectra of 2 when titrated with various equivalence of CH_3COOH in CDCl_3 at rt.

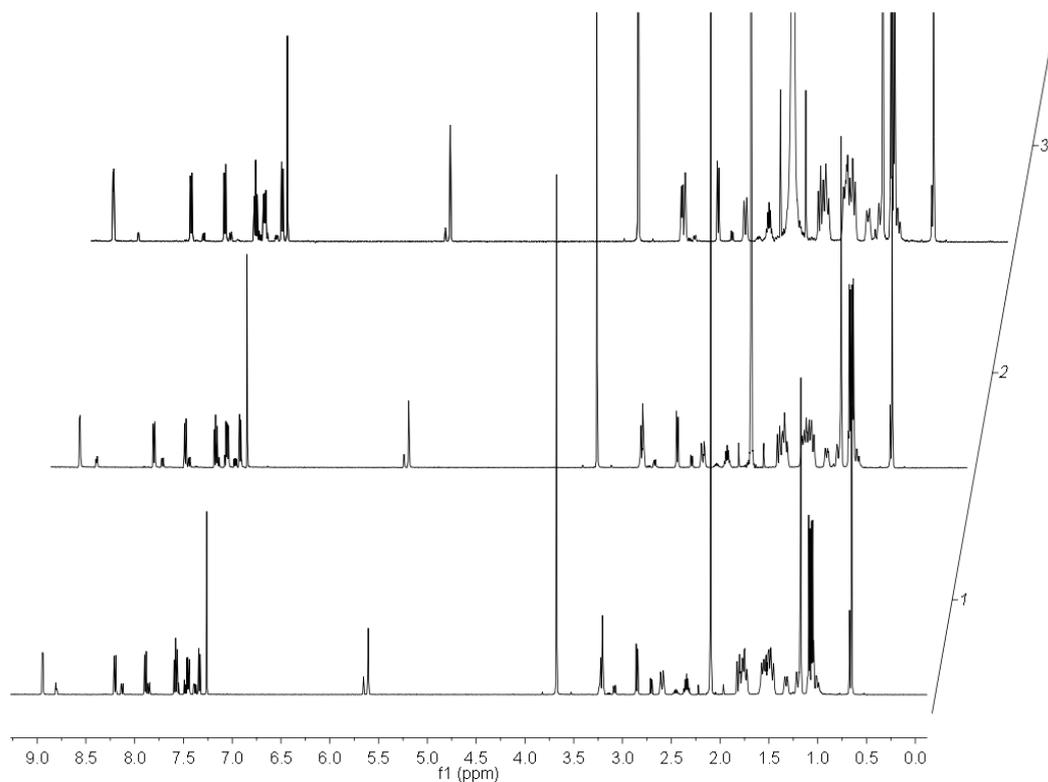


Figure S25. Full ^1H NMR (500 MHz) spectra of 2 when titrated with various equivalence of HCOOH in CDCl_3 at rt.

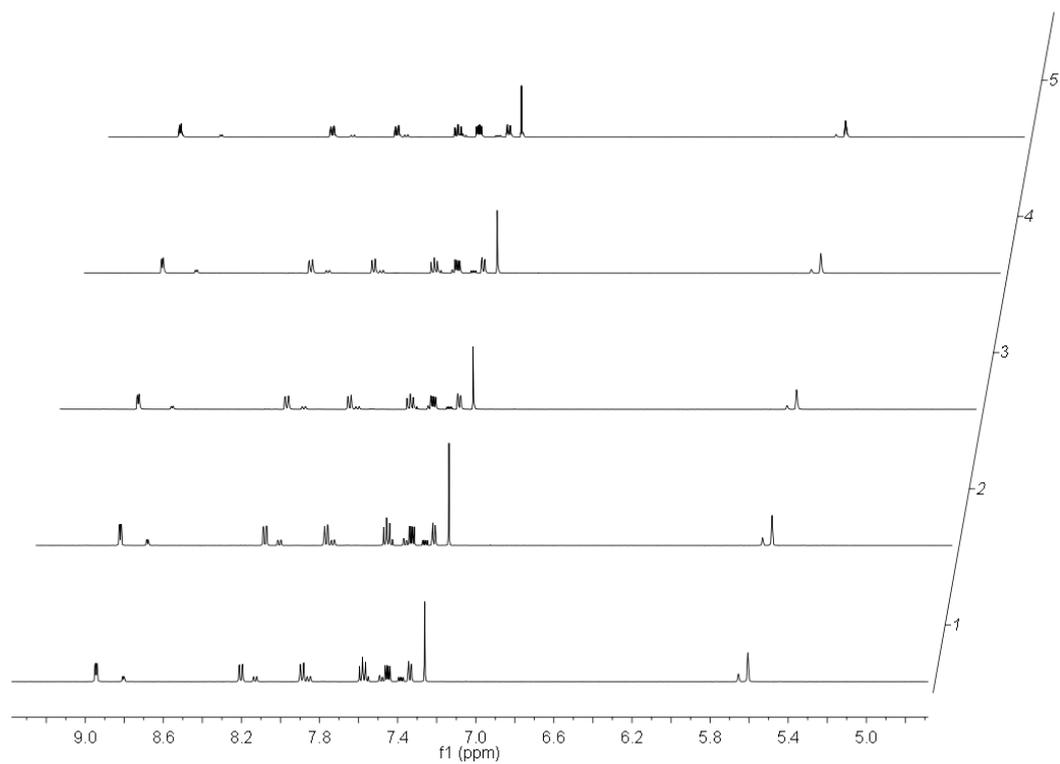


Figure S26. Full ¹H NMR (500 MHz) spectra of **2** when titrated with various equivalence of HCOOH in CDCl₃ at rt.