

**Racemosol Derivatives and Other Metabolites from *Bauhinia malabarica* Bark with
Antibacterial Activity**

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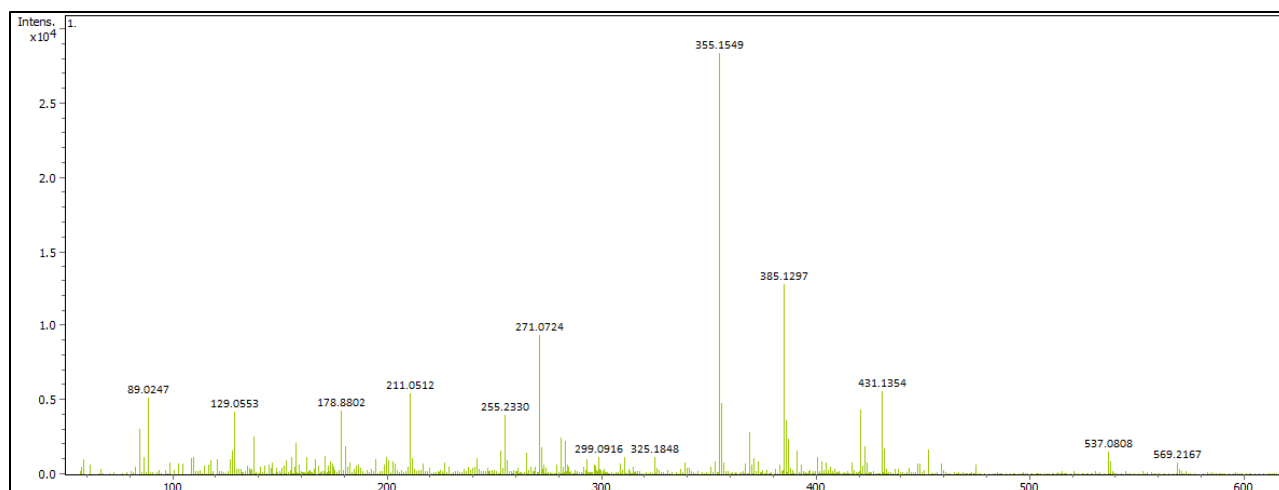


Figure S1. HR-ESIMS spectrum of 4.

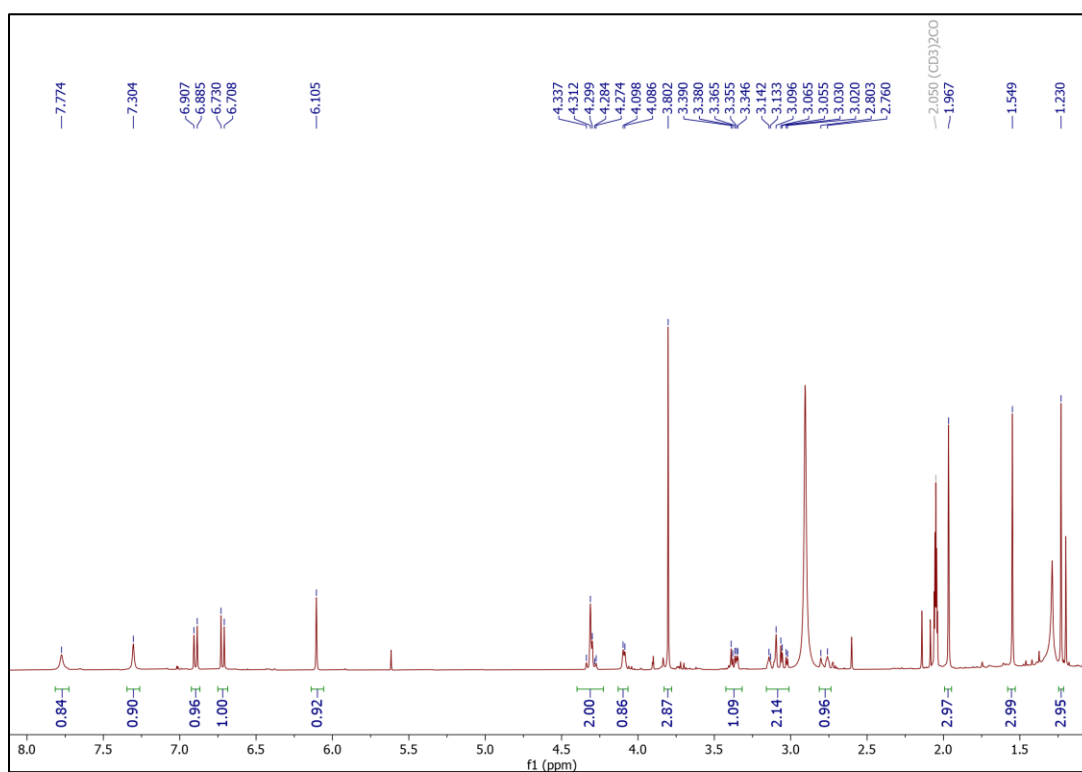


Figure S2. ¹H NMR spectrum (400 MHz, acetone-d₆) of 4.

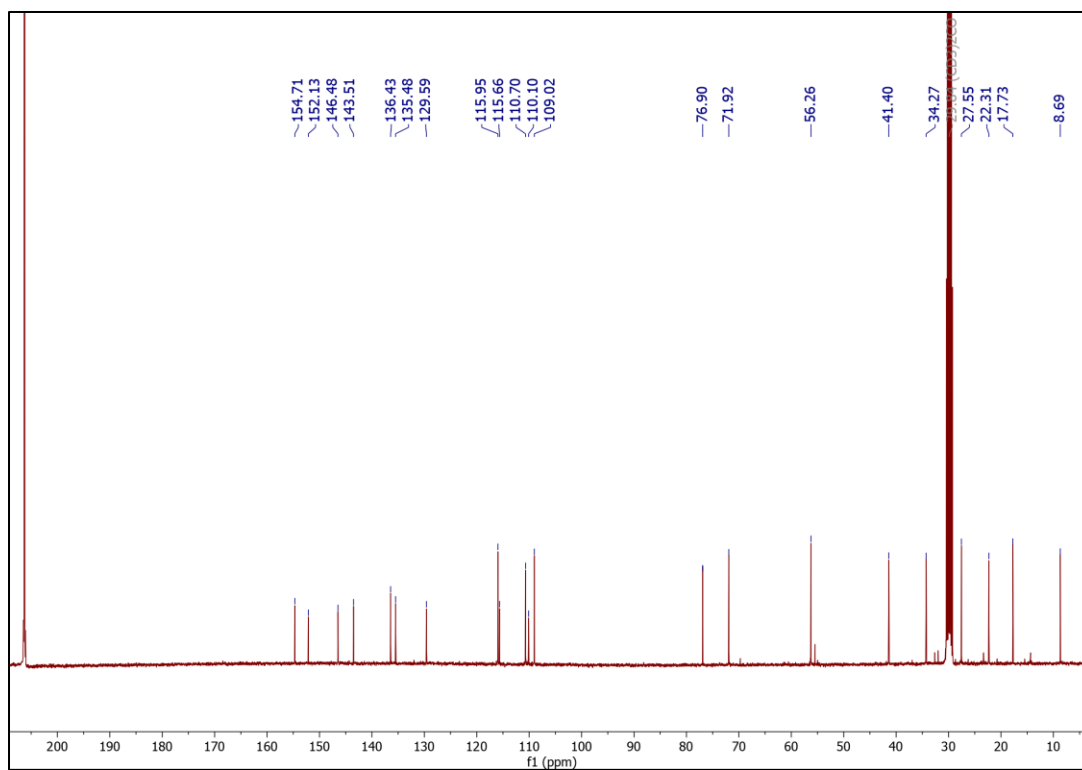


Figure S3. ^{13}C NMR spectrum (100 MHz, acetone- d_6) of 4.

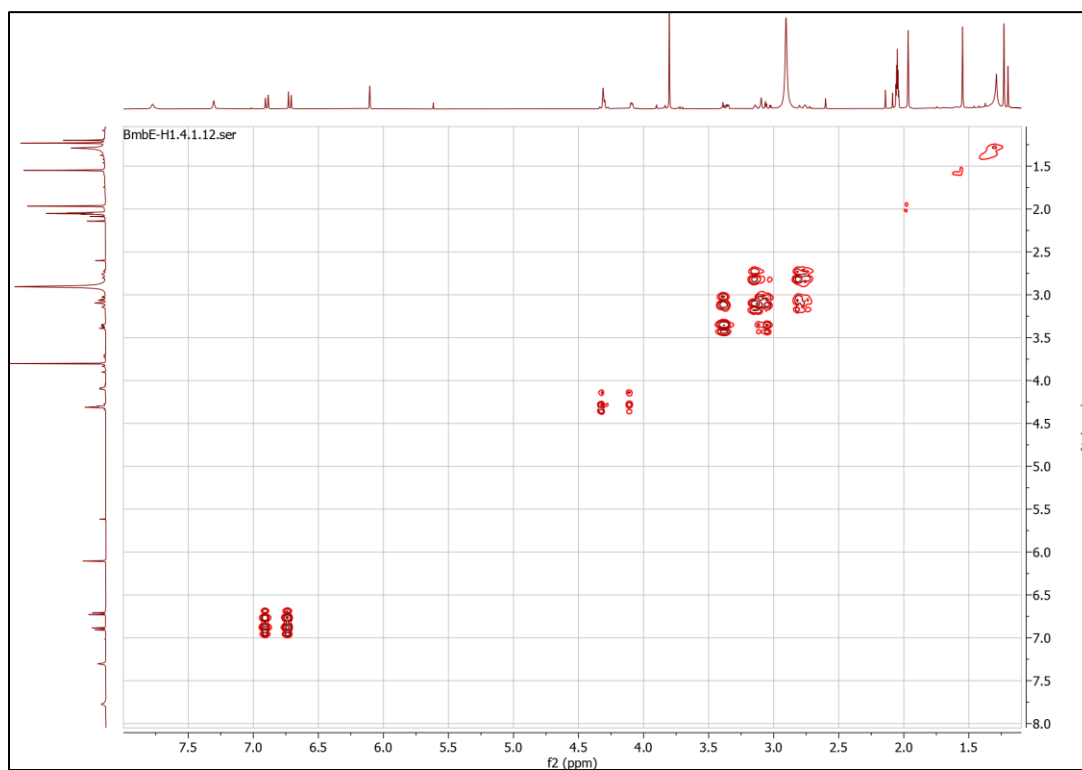


Figure S4. COSY spectrum of 4.

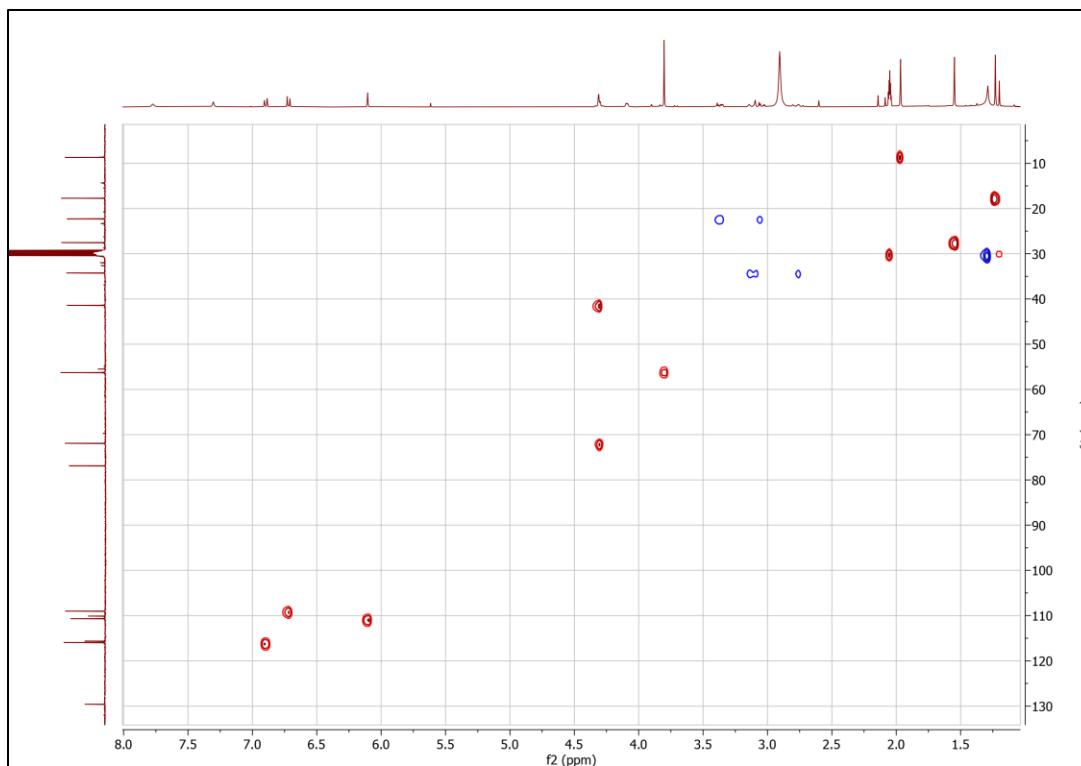


Figure S5. HSQC spectrum of **4**.

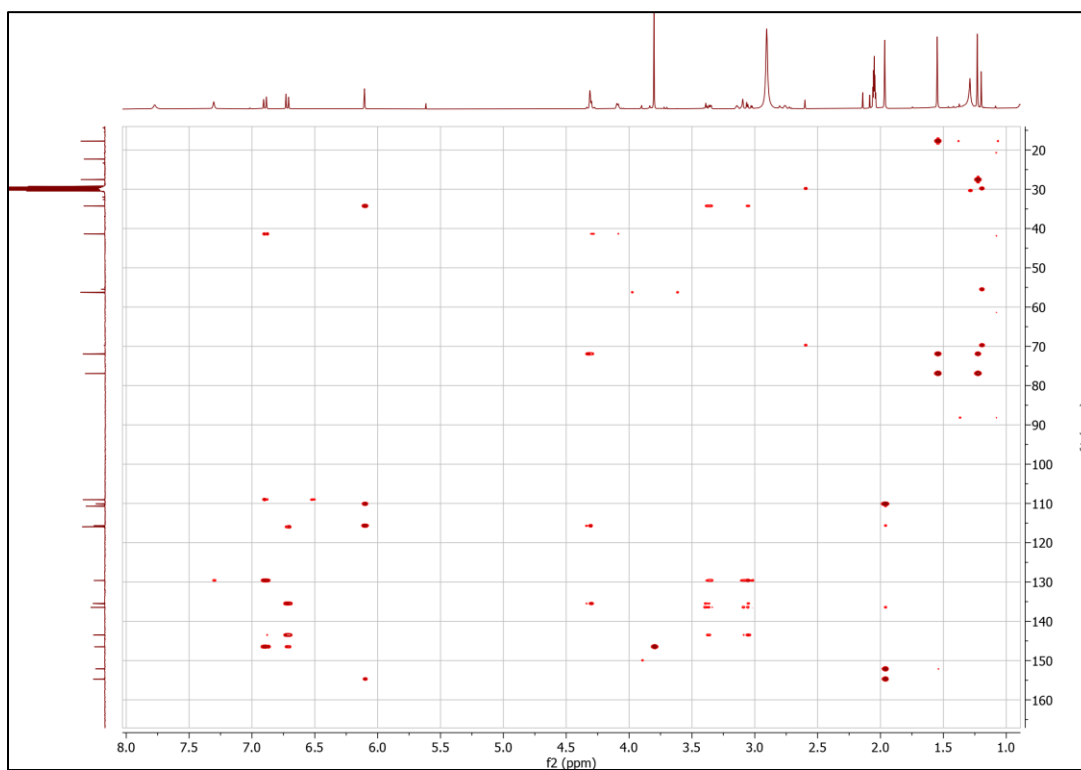


Figure S6. HMBC spectrum of **4**.

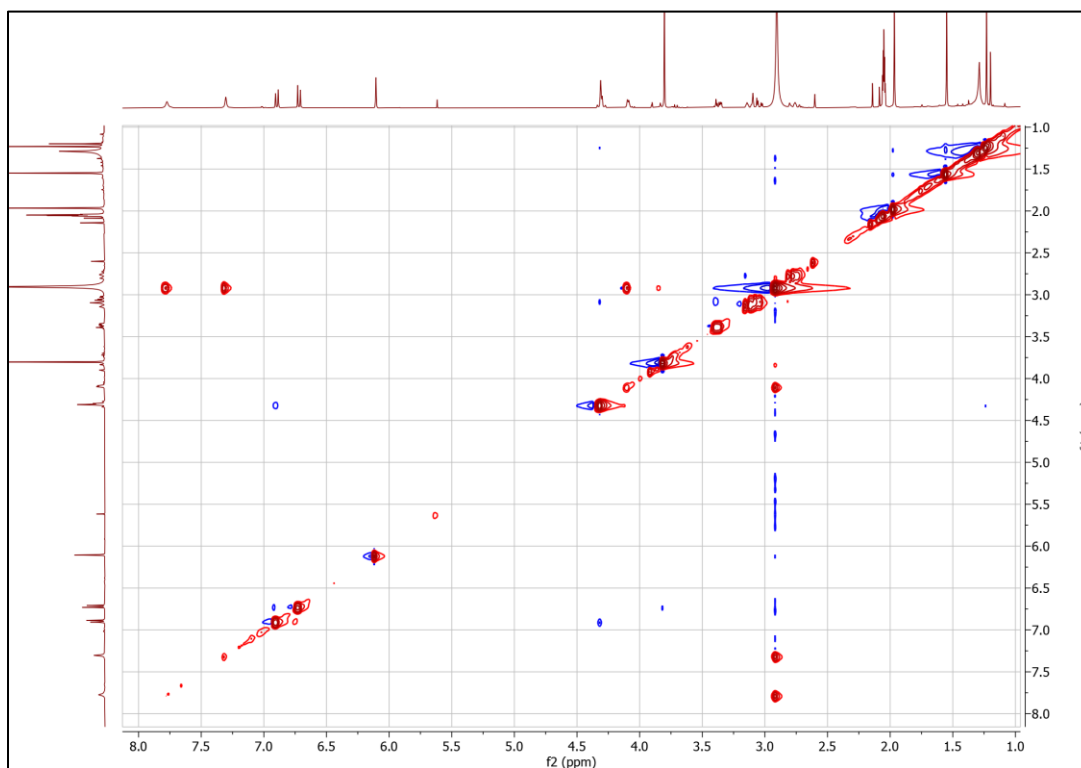


Figure S7. NOSY spectrum of **4**.

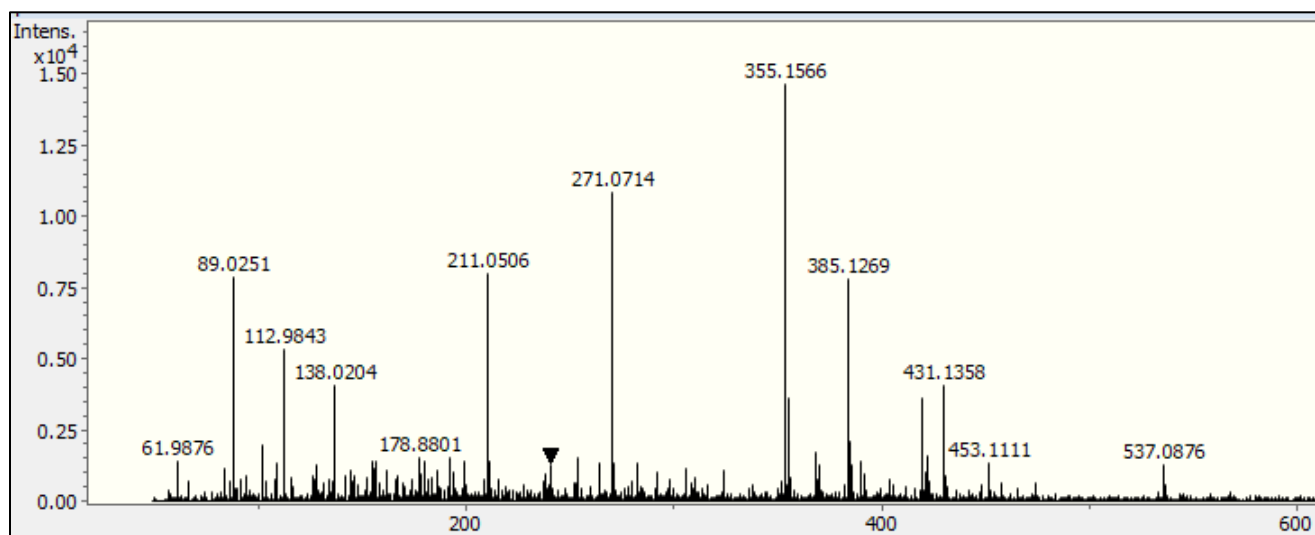


Figure S8. HR-ESIMS spectrum of **5**.

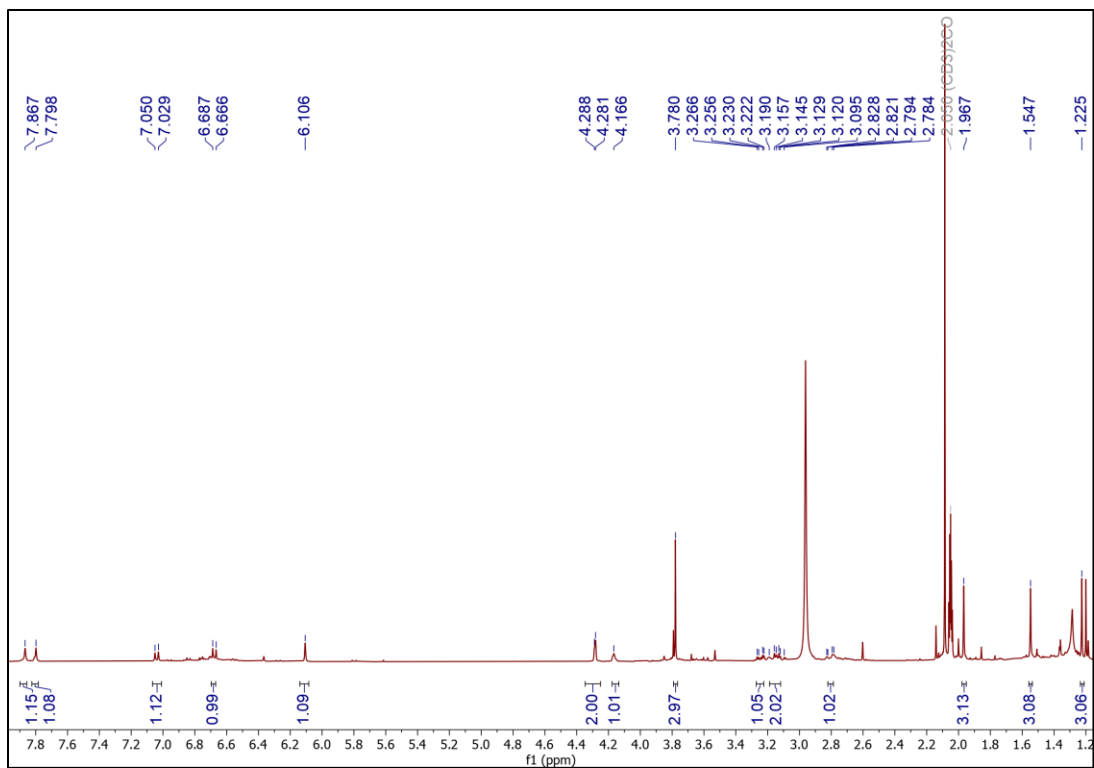


Figure S9. ¹H NMR spectrum (400 MHz, acetone-d₆) of **5**.

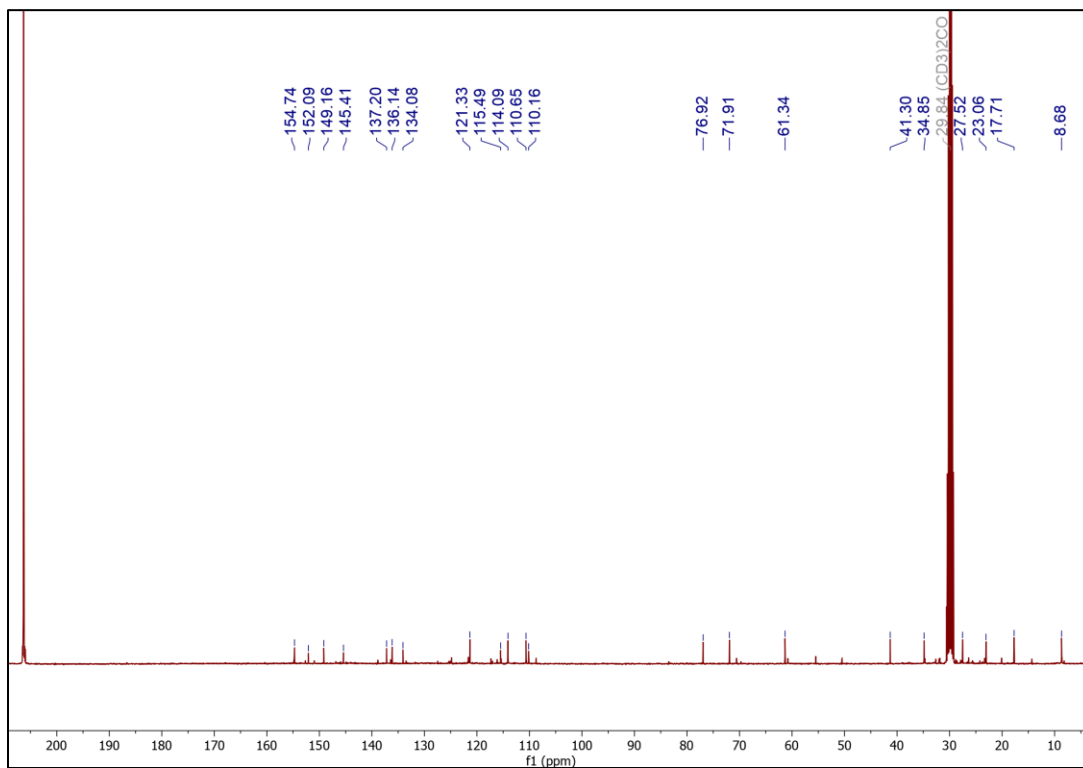


Figure S10. ¹³C NMR spectrum (100 MHz, acetone-d₆) of **5**.

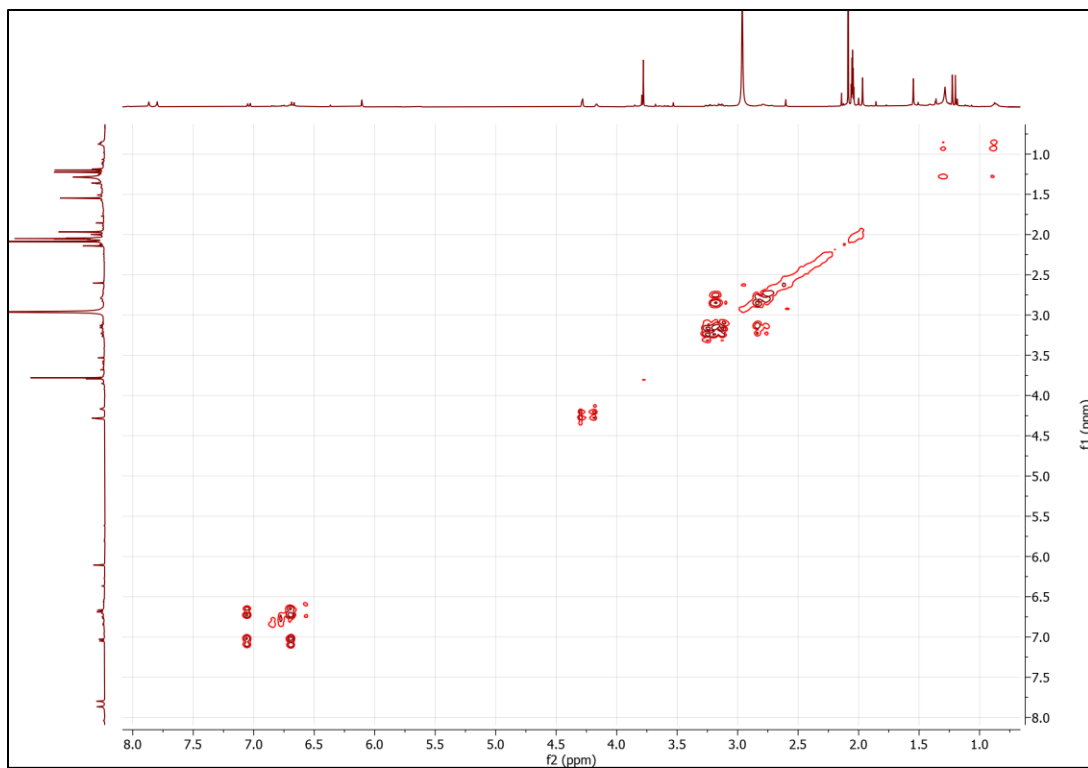


Figure S11. COSY spectrum of **5**.

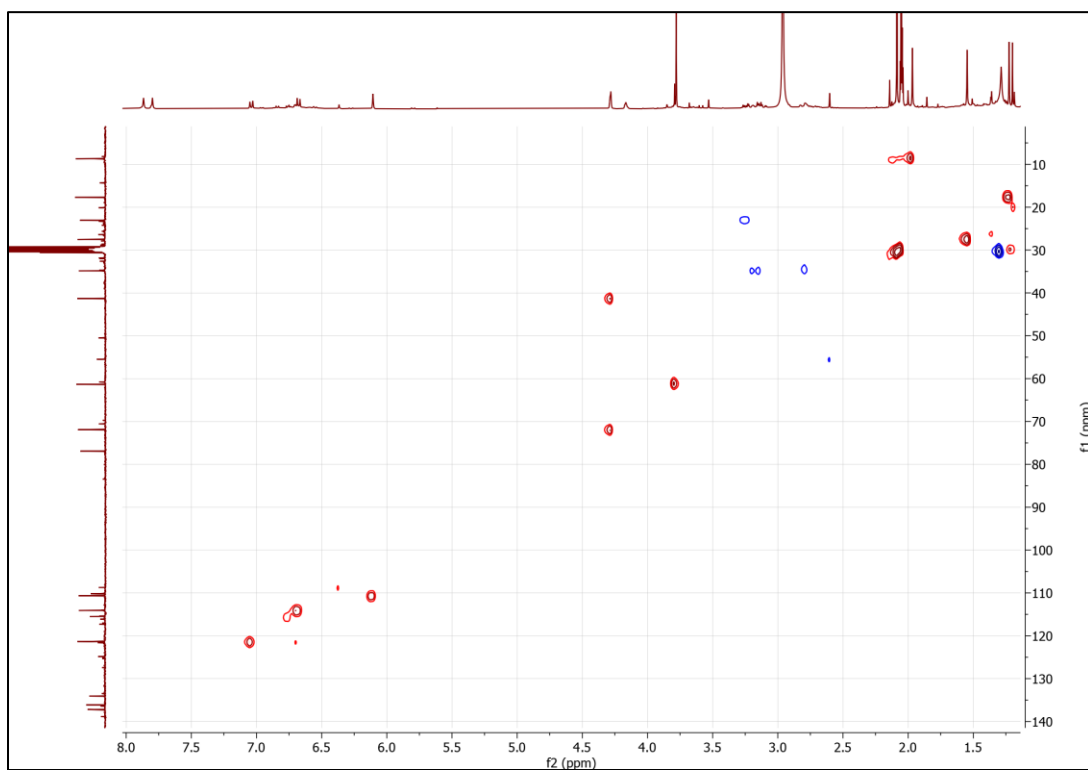


Figure S12. HSQC spectrum of **5**.

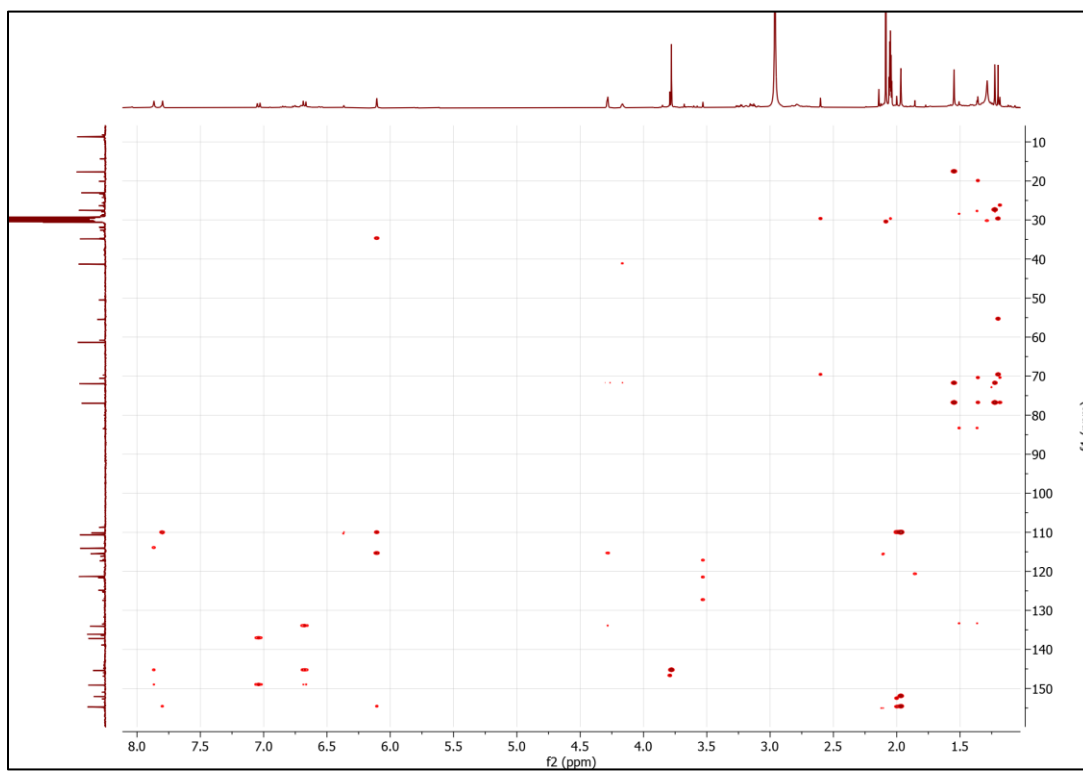


Figure S13. HMBC spectrum of **5**.

Functional		Solvent?		Basis Set		Type of Data	
mPW1PW91		PCM		6-31+G(d,p)		Shielding Tensors	
		DP4+	99.59%	0.41%	-	-	-
Nuclei	sp2?	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5
c		154.7	156.6	156.6			
c		152.1	153.5	152.1			
c		146.5	150.9	150.7			
c		143.5	147.3	147.5			
c		136.4	143.8	139.7			
c	x	135.5	134.5	134.7			
c	x	129.6	130.1	124.0			
c	x	116	122.3	122.0			
c	x	115.7	118.5	118.7			
c	x	110.7	111.2	115.8			
c	x	110.1	106.9	107.7			
c	x	109	104.55	105.78			
c		76.9	74.34	76.18			
c		71.9	68.82	72.88			
c	x	56.3	54.30	54.23			
c	x	41.4	40.01	41.58			
c	x	34.3	31.51	29.09			
c	x	27.5	25.98	24.85			
c	x	22.3	21.42	22.63			
c		17.7	17.18	12.34			
c		8.7	2.09	1.88			

Functional	Solvent?		Basis Set		Type of Data	
mPW1PW91	PCM		6-31+G(d,p)		Shielding Tensors	
	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
sDP4+ (H data)	-	-	-	-	-	-
sDP4+ (C data)	99.59%	0.41%	-	-	-	-
sDP4+ (all data)	99.59%	0.41%	-	-	-	-
uDP4+ (H data)	-	-	-	-	-	-
uDP4+ (C data)	50.07%	49.93%	-	-	-	-
uDP4+ (all data)	50.07%	49.93%	-	-	-	-
DP4+ (H data)	-	-	-	-	-	-
DP4+ (C data)	99.59%	0.41%	-	-	-	-
DP4+ (all data)	99.59%	0.41%	-	-	-	-

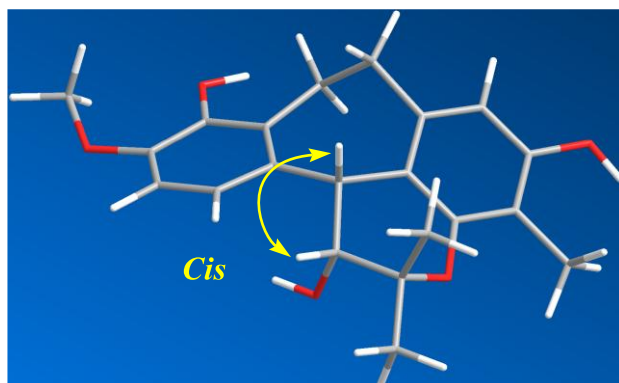
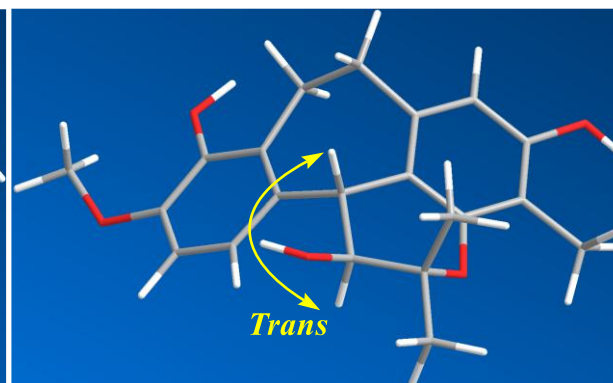
Isomer 4a (*cis*)Isomer 4b (*trans*)

Figure S14. DP4+ analysis of isomer 1 (4a) and isomer 2 (4b) of 4.