

Supplementary Information

Synthetic Analogue of the Natural Product Piperlongumine as a Potent Inhibitor of Breast Cancer Cell Line Migration

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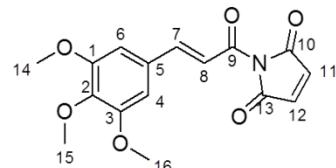
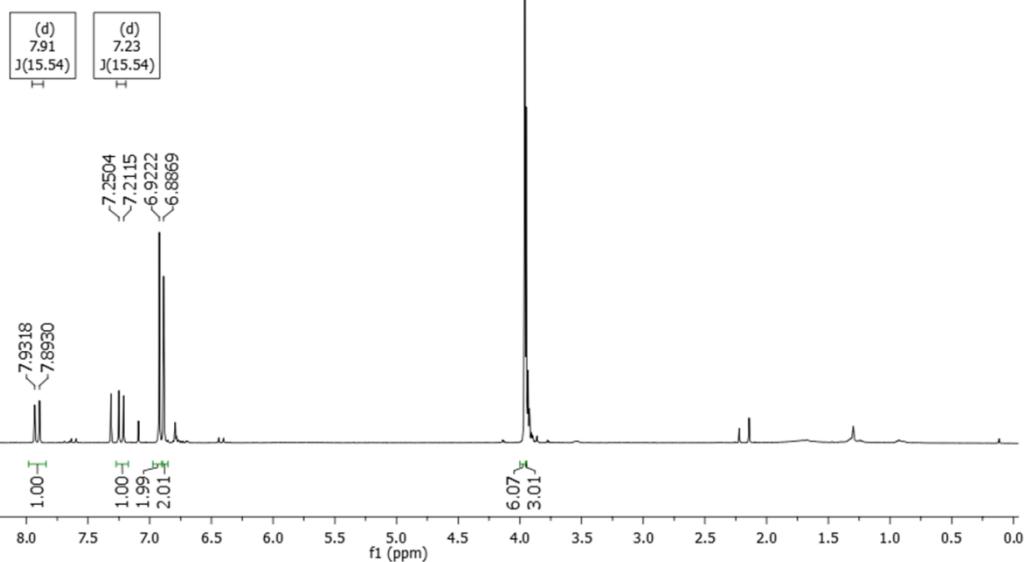
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DRMV1 - CDCl₃ - Bruker 400 MHz - 1H

Parameter	Value
Spectrometer	spect
Solvent	CDCl ₃
Temperature	294.2
Pulse Sequence	zg30
Number of Scans	8
Receiver Gain	128
Relaxation Delay	0.5000
Pulse Width	5.8000
Acquisition Time	2.7329
Acquisition Date	2013-01-10T07:40:19
Echo Delay	0.0000
Gradient Duration	0.0000
Spectrometer Frequency	400.13
Spectral Width	5995.2
Nucleus	1H



DRMV 1
C₁₆H₁₅NO₆

Figure S1. ¹H NMR (400 MHz, CDCl₃) of **2**.

DRMV1 - CDCl₃ - Bruker 300 MHz - 13C

Parameter	Value
Spectrometer	spect
Solvent	CDCl ₃
Temperature	293.6
Pulse Sequence	zgpg
Number of Scans	152
Receiver Gain	23170
Relaxation Delay	2.5000
Pulse Width	8.5000
Acquisition Time	0.7226
Acquisition Date	2012-12-20T11:51:24
Echo Delay	0.0000
Gradient Duration	0.0000
Spectrometer Frequency	75.47
Spectral Width	22675.7
Nucleus	13C

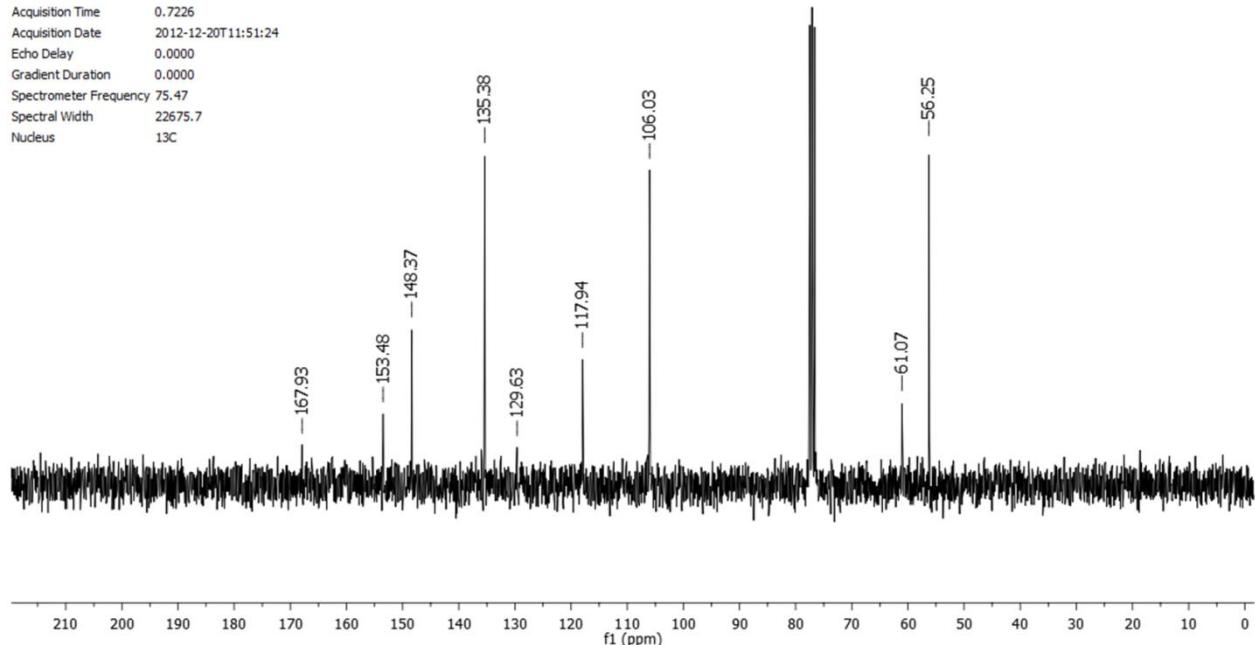


Figure S2. ¹³C NMR (75 MHz, CDCl₃) of **2**.

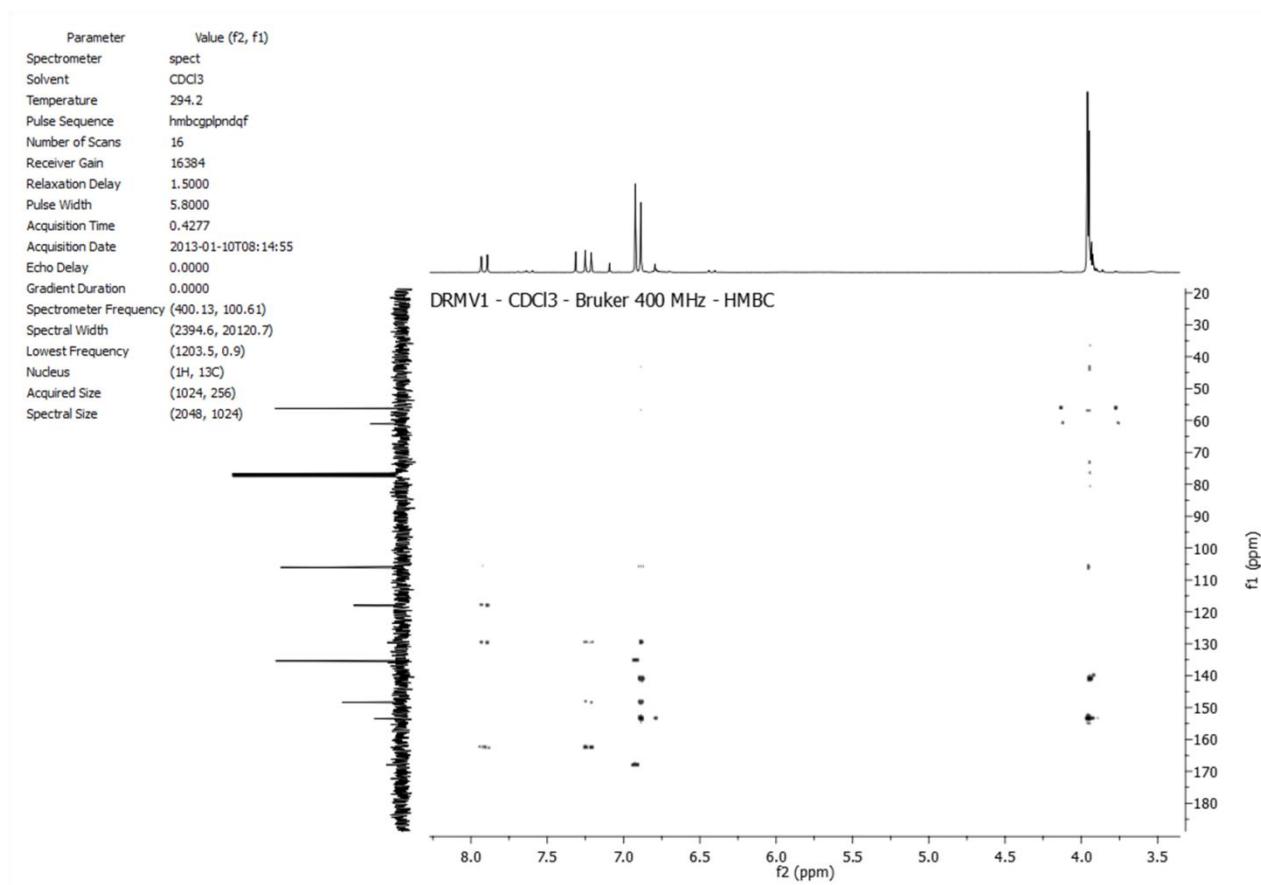


Figure S3. HMBC (400 MHz, CDCl₃) of **2**.

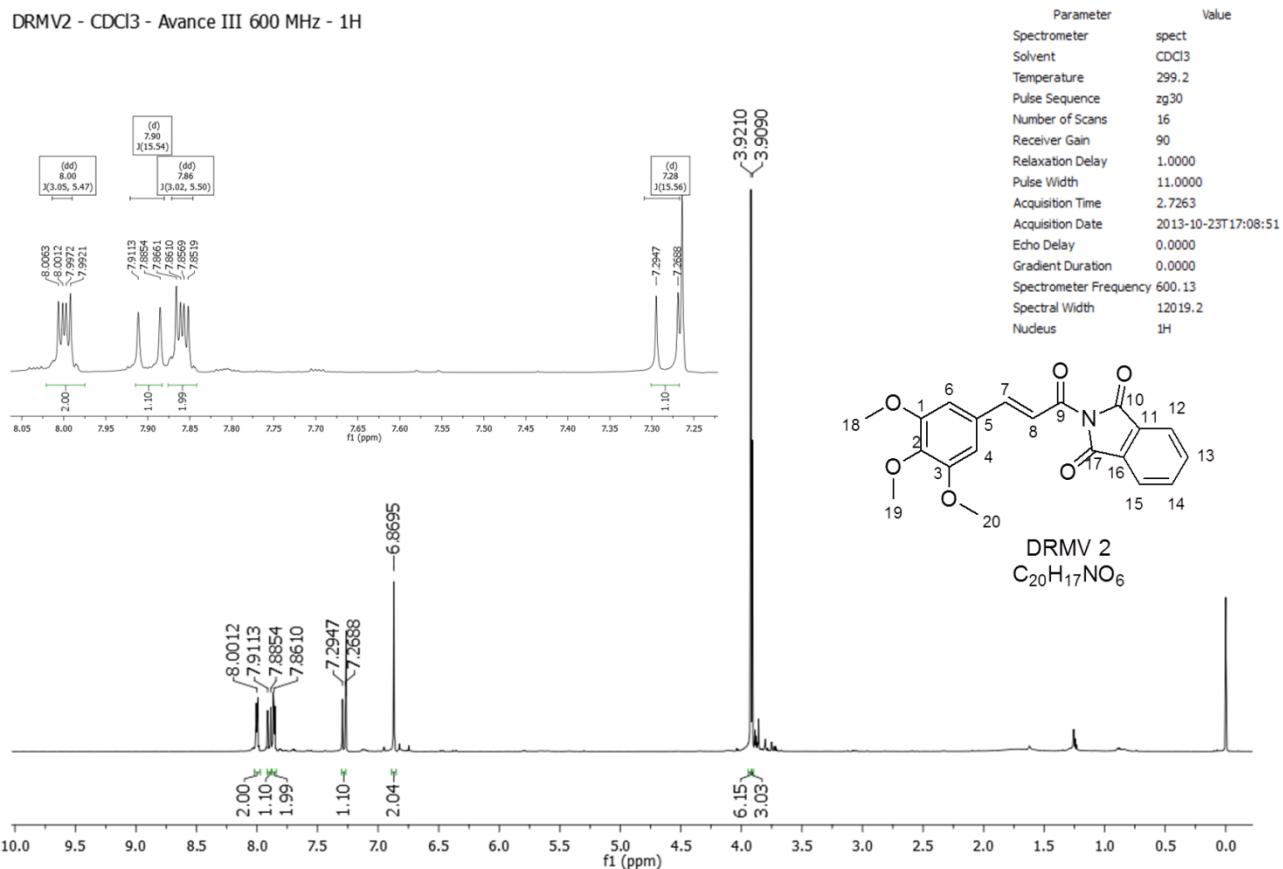


Figure S4. ¹H NMR (600 MHz, CDCl₃) of **3**.

DRMV2 - CDCl₃ - Avance III 600 MHz - 13C

Parameter	Value
Spectrometer	spect
Solvent	CDCl ₃
Temperature	299.4
Pulse Sequence	zpgg30
Number of Scans	372
Receiver Gain	81
Relaxation Delay	2.0000
Pulse Width	11.0000
Acquisition Time	0.9088
Acquisition Date	2013-10-24T13:43:35
Echo Delay	0.0000
Gradient Duration	0.0000
Spectrometer Frequency	150.90
Spectral Width	36057.7
Nucleus	13C

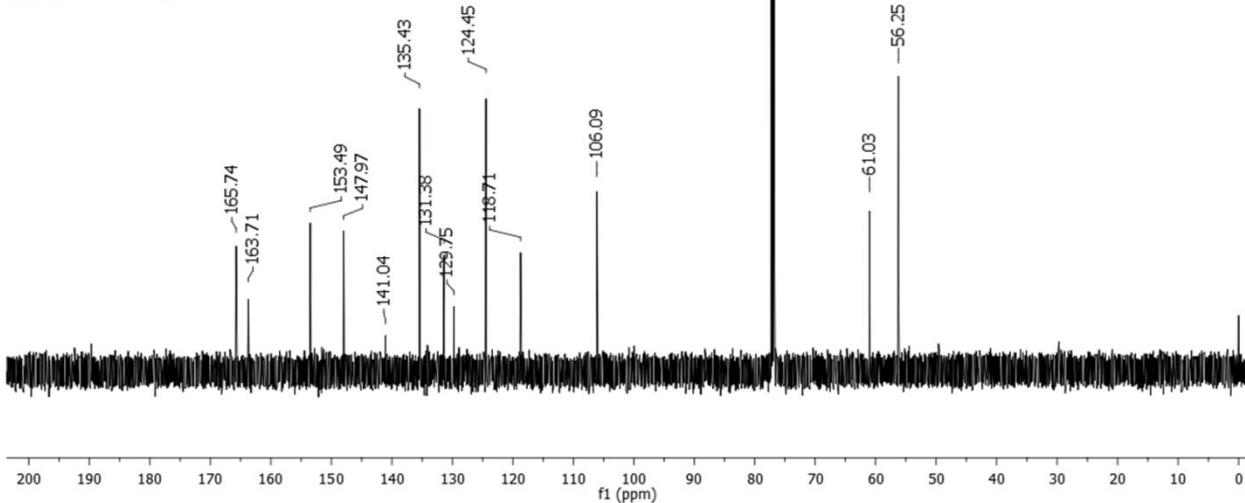


Figure S5. ¹³C NMR (150 MHz, CDCl₃) of **3**.

Parameter	Value (f ₂ , f ₁)
Spectrometer	spect
Solvent	CDCl ₃
Temperature	299.1
Pulse Sequence	hmbcgplndqf
Number of Scans	8
Receiver Gain	81
Relaxation Delay	1.5000
Pulse Width	11.0000
Acquisition Time	0.1311
Acquisition Date	2013-10-24T12:08:42
Echo Delay	0.0000
Gradient Duration	0.0000
Spectrometer Frequency (600.13, 150.90)	
Spectral Width (7812.5, 33557.0)	
Lowest Frequency (-125.4, -1713.5)	
Nucleus (¹ H, ¹³ C)	
Acquired Size (1024, 128)	
Spectral Size (2048, 1024)	

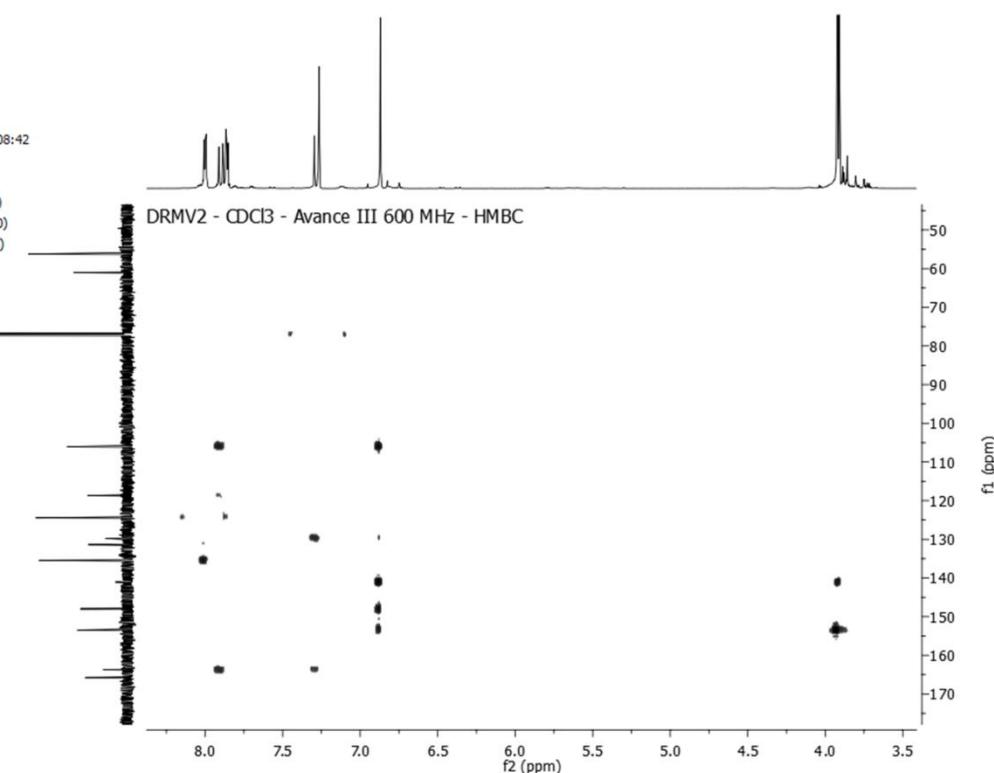


Figure S6. HMBC (600 MHz, CDCl₃) of **3**.

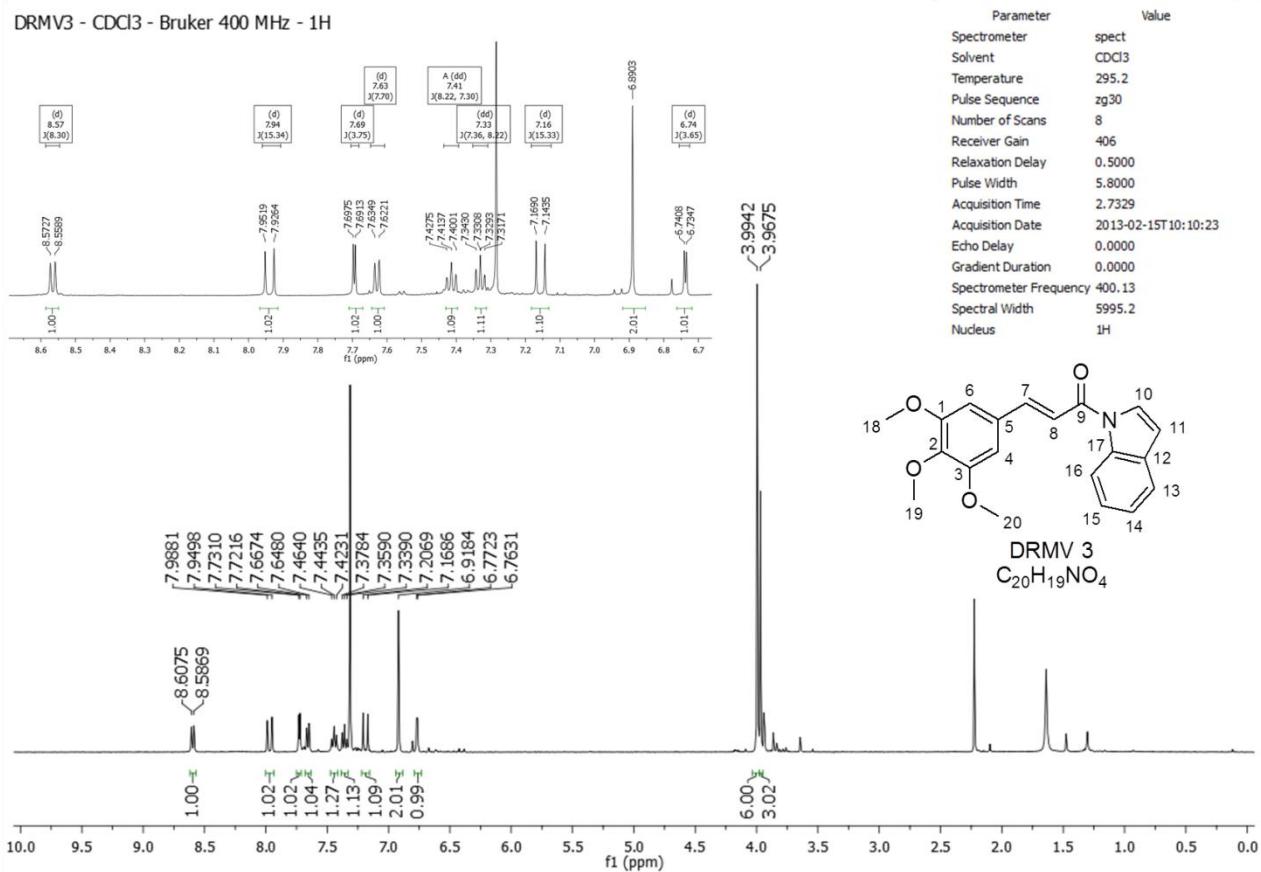


Figure S7. ¹H NMR (400 MHz, CDCl₃) of **4**.

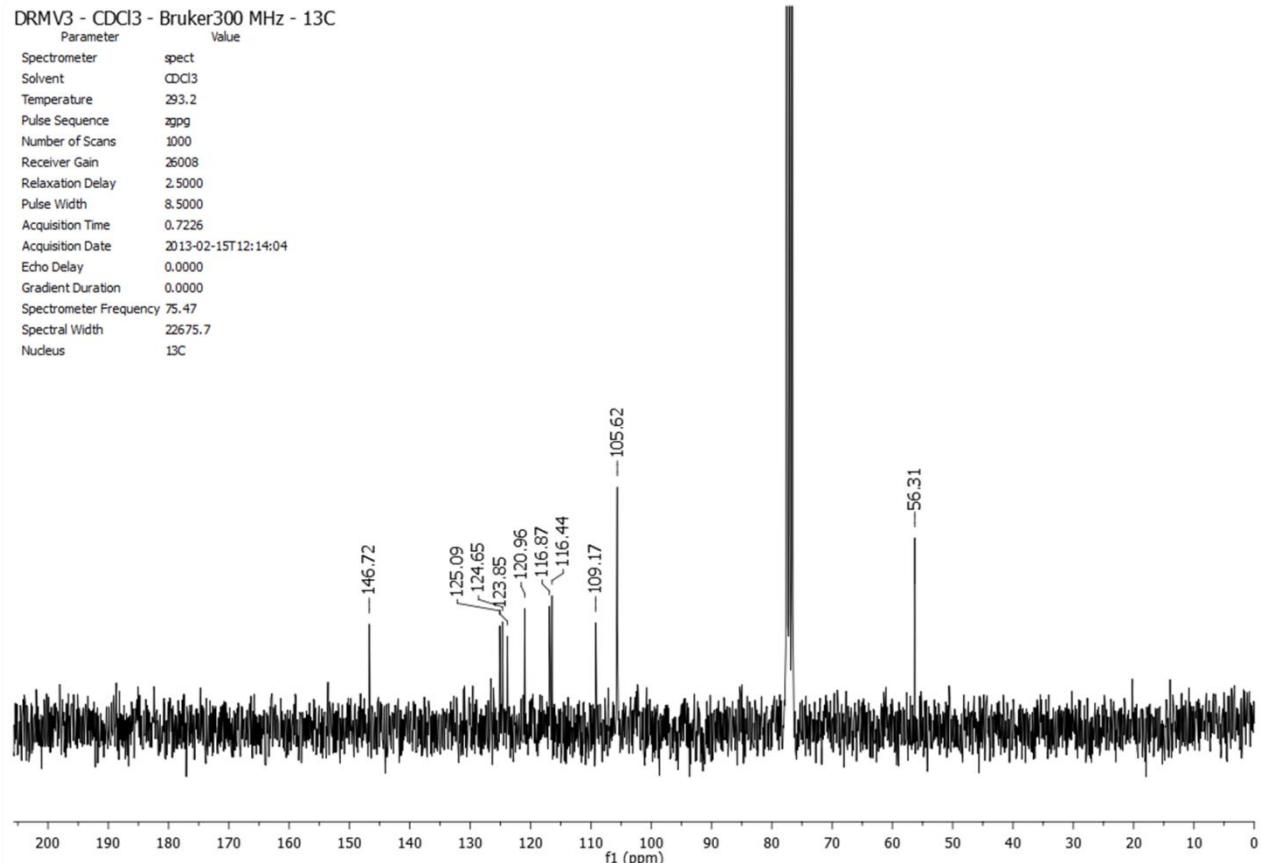


Figure S8. ¹³C NMR (75 MHz, CDCl₃) of **4**.

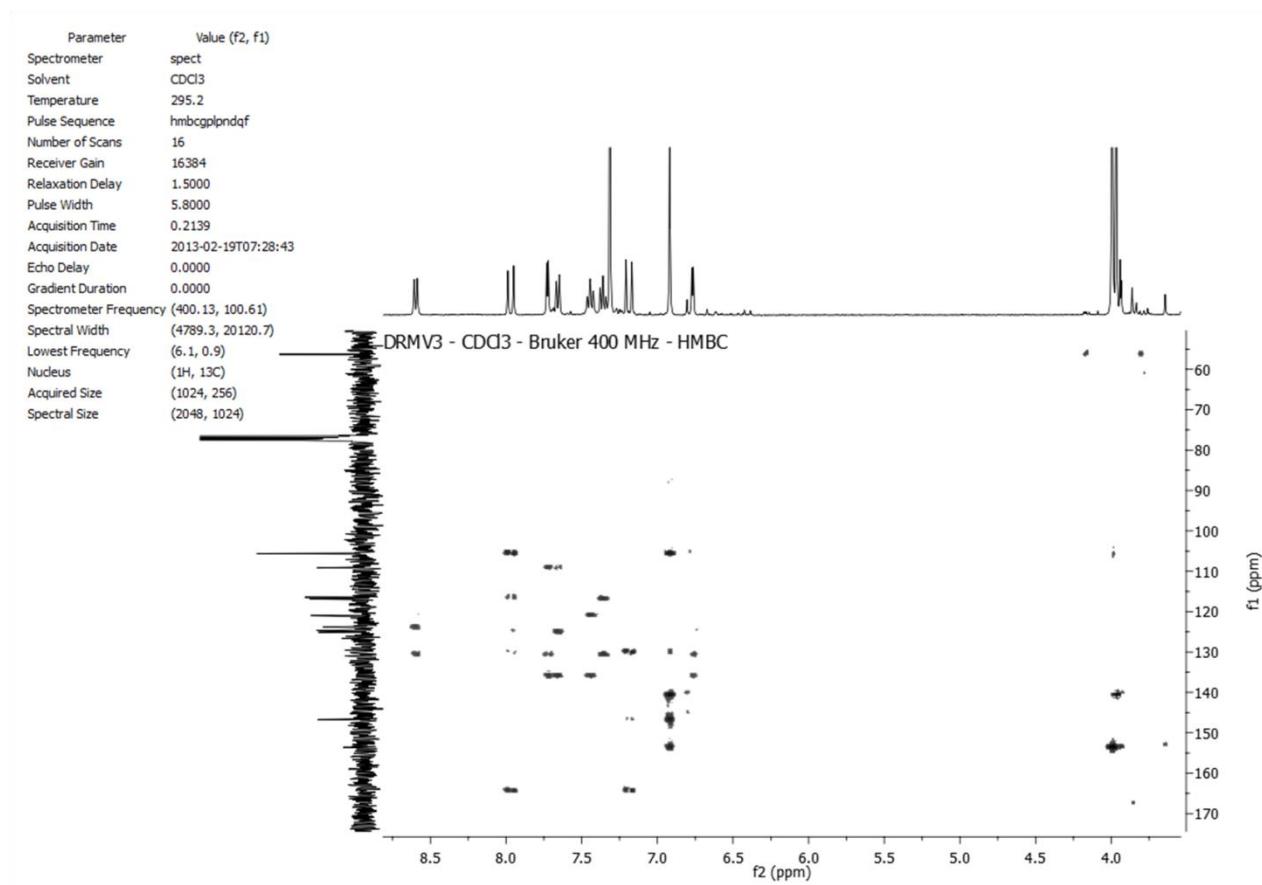


Figure S9. HMBC (400 MHz, CDCl₃) of **4**.

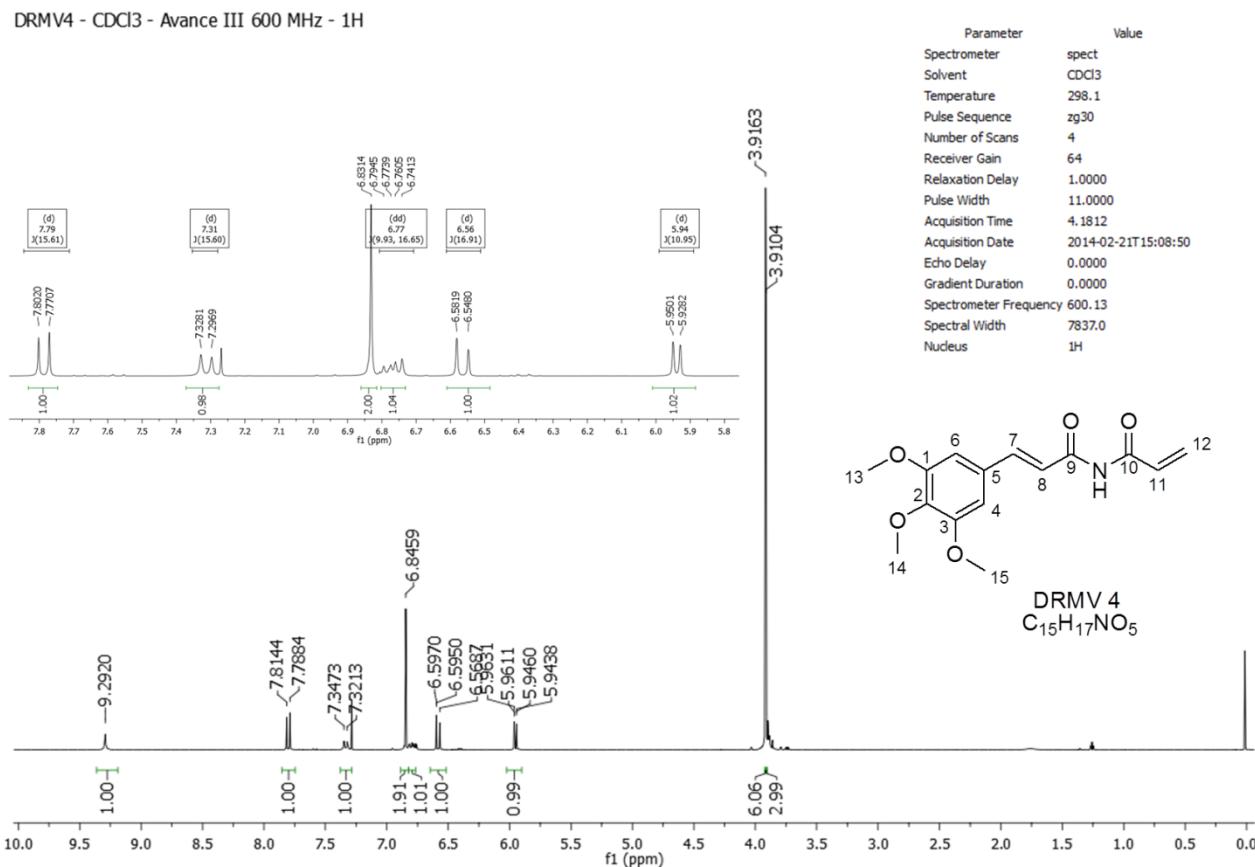


Figure S10. ¹H NMR (600 MHz, CDCl₃) of **5**.

DRMV4 - CDCl₃ - Avance 600 MHz - 13C

Parameter	Value
Spectrometer	spect
Solvent	CDCl ₃
Temperature	298.3
Pulse Sequence	zpgg30
Number of Scans	144
Receiver Gain	2050
Relaxation Delay	2.0000
Pulse Width	11.0000
Acquisition Time	0.9088
Acquisition Date	2014-02-21T15:11:28
Echo Delay	0.0000
Gradient Duration	0.0000
Spectrometer Frequency	150.90
Spectral Width	36057.7
Nucleus	13C

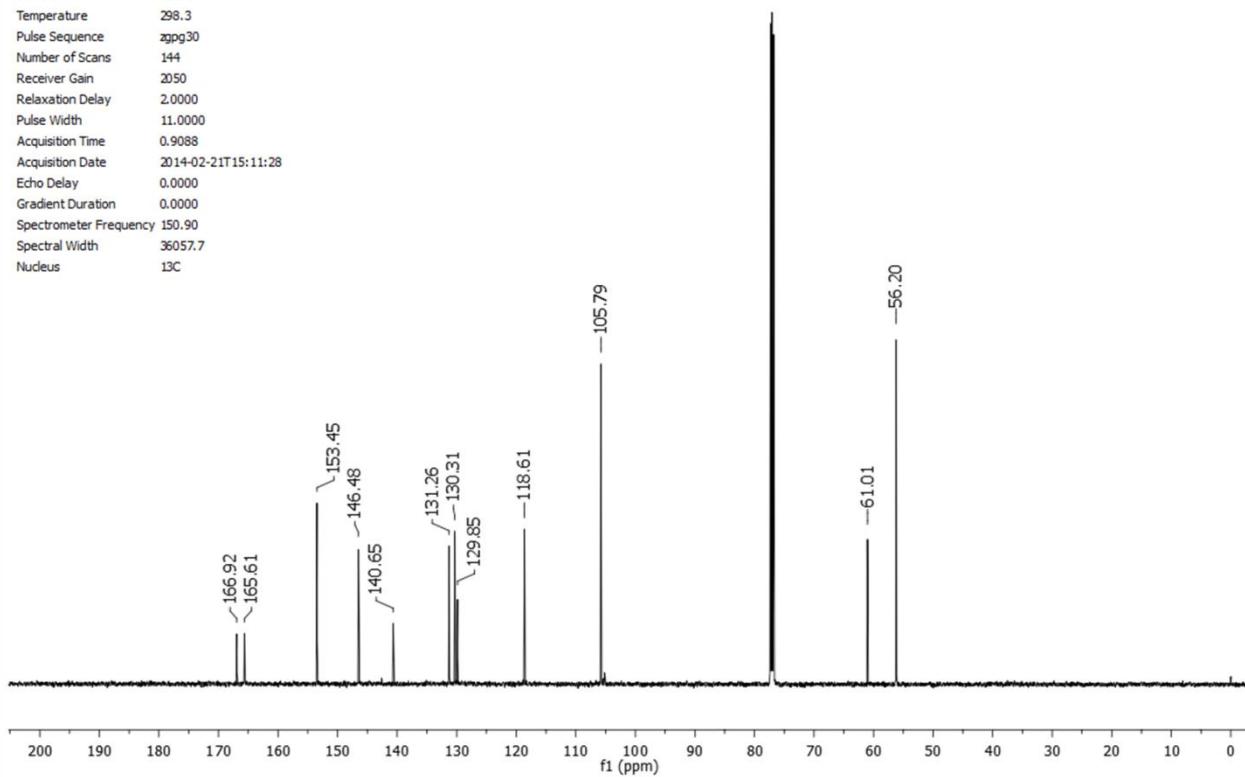


Figure S11. ¹³C NMR (150 MHz, CDCl₃) of **5**.

Parameter	Value (f2, f1)
Spectrometer	spect
Solvent	CDCl ₃
Temperature	298.1
Pulse Sequence	hmbcgplndqf
Number of Scans	8
Receiver Gain	64
Relaxation Delay	1.5000
Pulse Width	11.0000
Acquisition Time	0.1311
Acquisition Date	2014-02-21T15:35:14
Echo Delay	0.0000
Gradient Duration	0.0000
Spectrometer Frequency (600.13, 150.90)	
Spectral Width (7812.5, 33557.0)	
Lowest Frequency (-125.4, -1713.5)	
Nucleus (1H, 13C)	
Acquired Size (1024, 128)	
Spectral Size (2048, 1024)	

DRMV4 - CDCl₃ - Avance III 600 MHz - HMBC

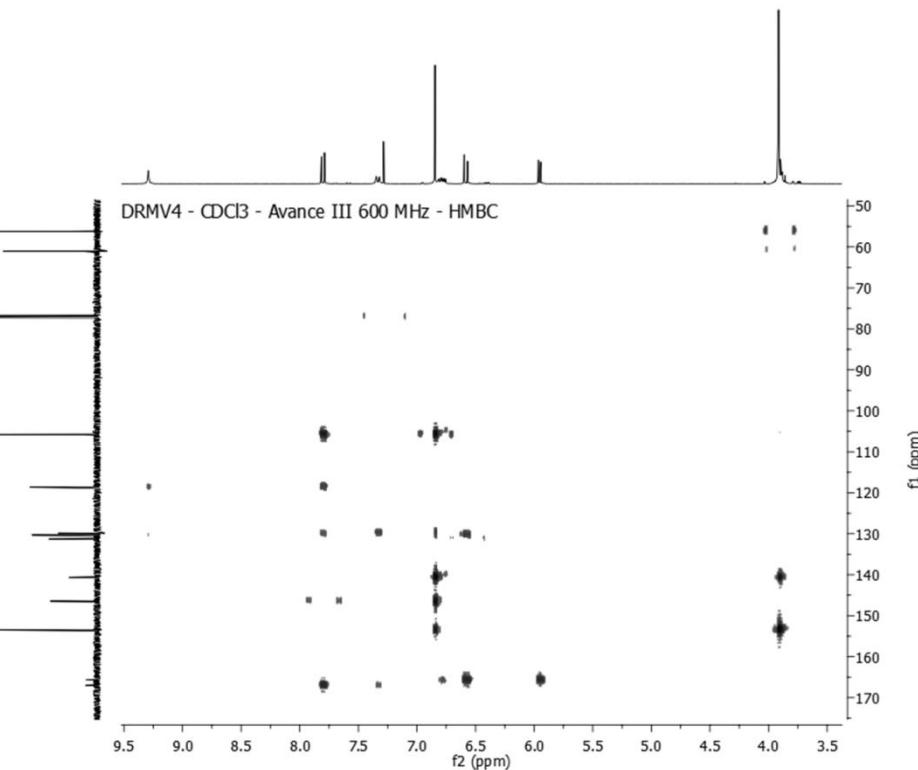


Figure S12. HMBC (600 MHz, CDCl₃) of **5**.

DRMV5 - CDCl₃ - Avance III 600 MHz - 1H

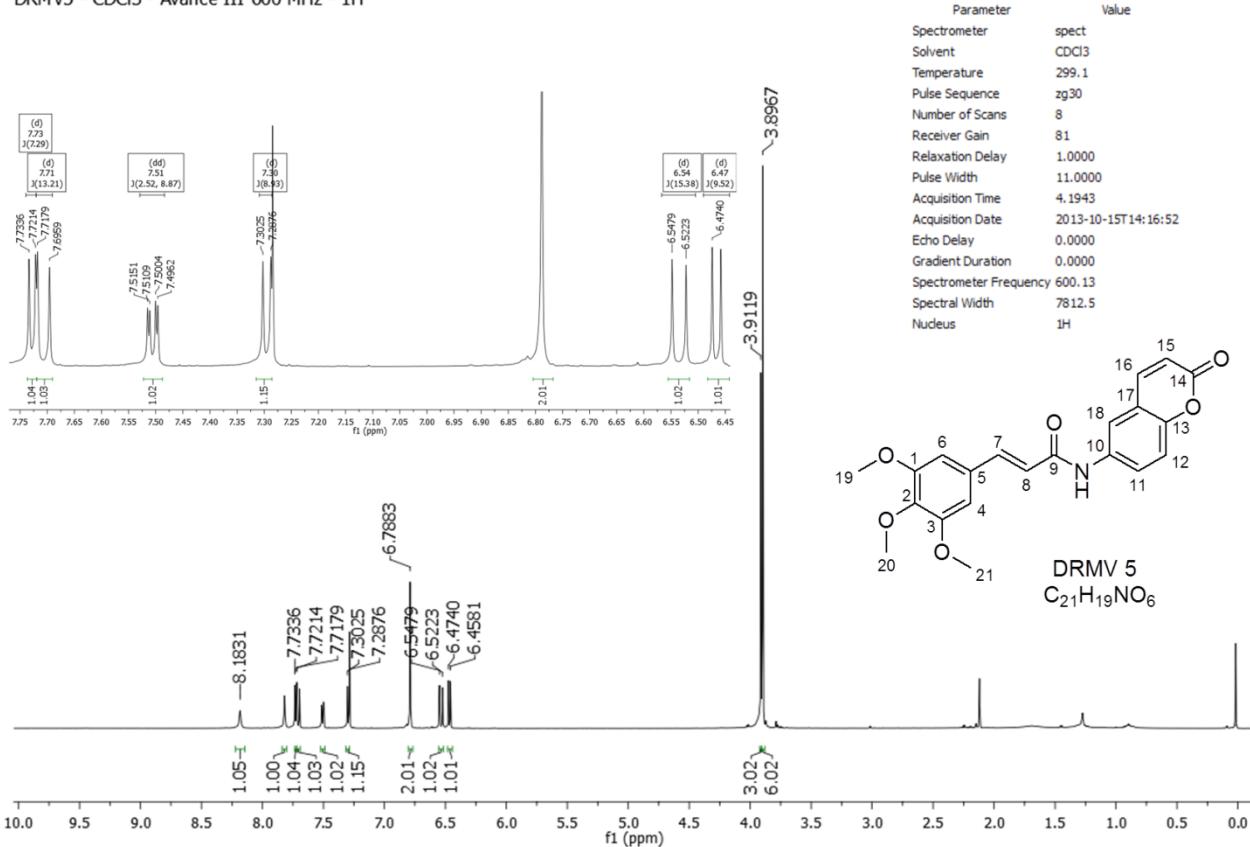


Figure S13. ¹H NMR (600 MHz, CDCl₃) of **6**.

DRMV5 - CDCl₃ - Avance III 600 MHz - 13C

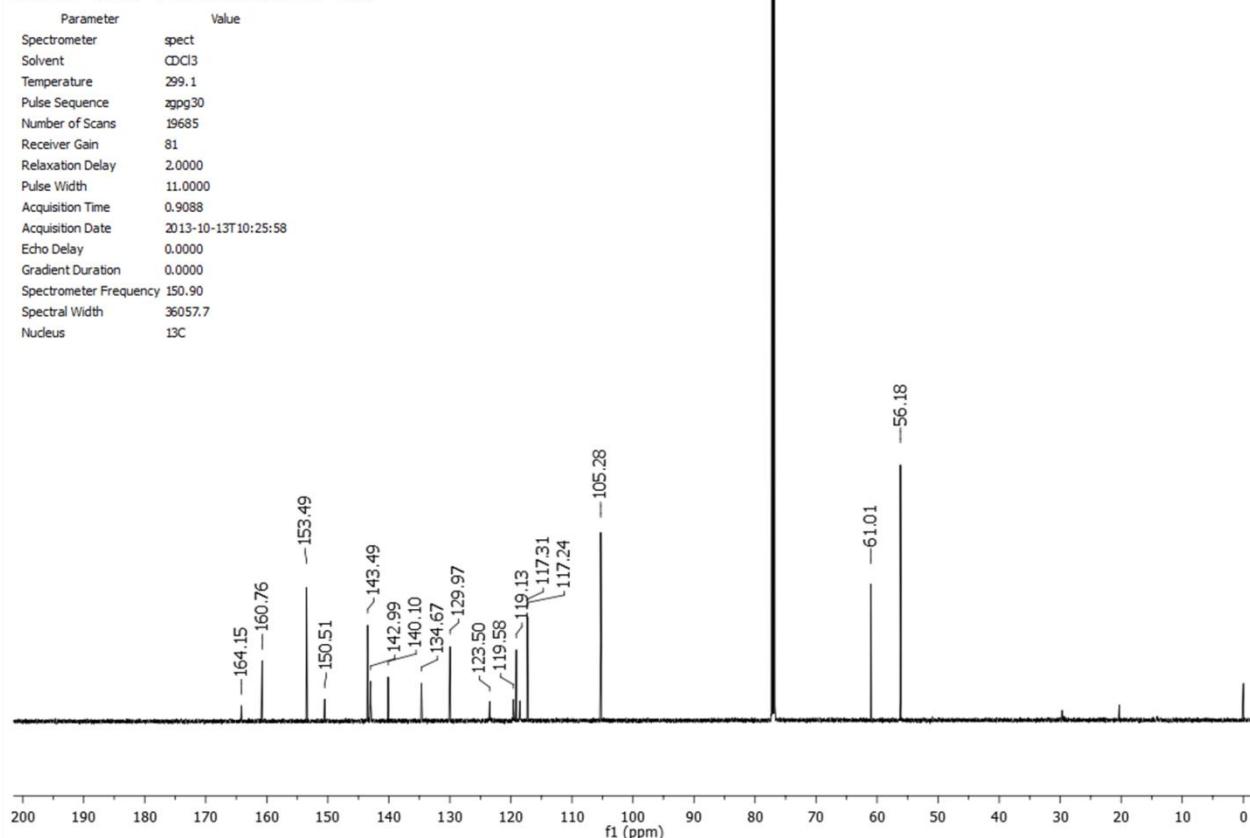


Figure S14. ¹³C NMR (150 MHz, CDCl₃) of **6**.

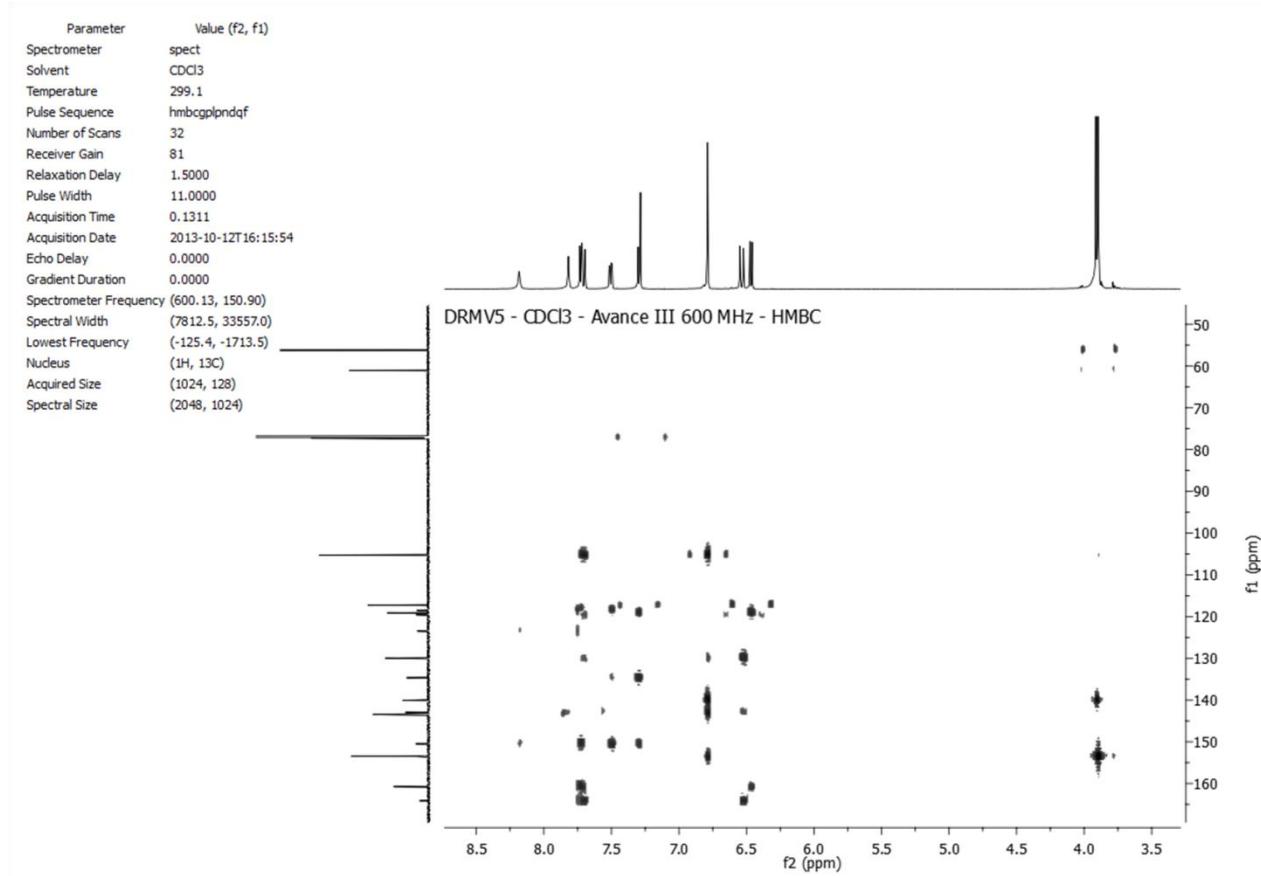


Figure S15. HMBC (600 MHz, CDCl₃) of **6**.