

Supporting Information

Rec. Nat. Prod. 9:3 (2015) 336-341

Four New Cycloheximide Derivatives from *Streptomyces* sp.

h-119

Dou Yang^{1,2,3}, **Qing Yan Xu**^{1,2,3}, **Xian Ming Deng**^{1,2,3}, **Si Yang Son**^{1,2,3},
Zhi Yu Hu^{1,2,3} and **Zhong Hui Zheng**^{1,2,3*}

¹ *State Key Laboratory of Cellular Stress Biology, School of Life Sciences, Xiamen University,
Xiamen, Fujian 361102, China*

² *State-Province Joint Engineering Laboratory of Targeted Drugs from Natural Products,
Xiamen University, Xiamen, Fujian, 361102, China*

³ *School of Life Sciences, Xiamen University, Xiamen, Fujian 361102, China*

Table of Contents	Page
S1: HRESI-MS Spectrum of Compound 1	3
S2: ¹ H-NMR (600 MHz, CDCl ₃) Spectrum of Compound 1	4
S3: Expansion of the ¹ H-NMR Spectrum of Compound 1	5
S4: Expansion of the ¹ H-NMR Spectrum of Compound 1	6
S5: ¹³ C-NMR and DEPT (600 MHz, CDCl ₃) Spectrum of Compound 1	7
S6: Expansion of the ¹³ C-NMR and DEPT Spectrum of Compound 1	8
S7: HSQC Spectrum (600MHz, CDCl ₃) of Compound 1	9
S8: Expansion of the HSQC Spectrum of Compound 1	10
S9: HMBC Spectrum (600MHz, CDCl ₃) of Compound 1	11

* Corresponding author: E-Mail: zhzheng@xmu.edu.cn; Tel. /Fax: 086-592-2181722

S10: Expansion of the HMBC Spectrum of Compound 1	12
S11: ^1H - ^1H COSY Spectrum (600MHz, CDCl_3) of Compound 1	13
S12: Expansion of the ^1H - ^1H COSY Spectrum of Compound 1	14
S13: NOESY spectrum (600MHz, CDCl_3) of compound 1	15
S14: HRESI-MS Spectrum of Compound 2	16
S15: ^1H -NMR (600 MHz, CDCl_3) Spectrum of Compound 2	17
S16: Expansion of the ^1H -NMR Spectrum of Compound 2	18
S17: Expansion of the ^1H -NMR Spectrum of Compound 2	19
S18: ^{13}C -NMR and DEPT (600 MHz, CDCl_3) Spectrum of Compound 2	20
S19: Expansion of the ^{13}C -NMR and DEPT Spectrum of Compound 2	21
S20: HSQC Spectrum (600MHz, CDCl_3) of Compound 2	22
S21: Expansion of the HSQC Spectrum of Compound 2	23
S22: HMBC Spectrum (600MHz, CDCl_3) of Compound 2	24
S23: Expansion of the HMBC Spectrum of Compound 2	25
S24: Expansion of the HMBC Spectrum of Compound 2	26
S25: ^1H - ^1H COSY Spectrum (600MHz, CDCl_3) of Compound 2	27
S26: Expansion of the ^1H - ^1H COSY Spectrum of Compound 2	28
S27: NOESY spectrum (600MHz, CDCl_3) of compound 2	29
S28: HRESI-MS Spectrum of Compound 3	30
S29: ^1H -NMR (600 MHz, CDCl_3) Spectrum of Compound 3	31
S30: ^{13}C -NMR and DEPT (600 MHz, CDCl_3) Spectrum of Compound 3	32
S31: HSQC Spectrum (600MHz, CDCl_3) of Compound 3	33
S32: Expansion of the HSQC Spectrum of Compound 3	34
S33: HMBC Spectrum (600MHz, CDCl_3) of Compound 3	35
S34: Expansion of the HMBC Spectrum of Compound 3	36
S35: Expansion of the HMBC Spectrum of Compound 3	37
S36: ^1H - ^1H COSY Spectrum (600MHz, CDCl_3) of Compound 3	38

S37: NOESY spectrum (600MHz, CDCl ₃) of compound 3	39
S38: HRESI-MS Spectrum of Compound 4	40
S39: ¹ H-NMR (600 MHz, CDCl ₃) Spectrum of Compound 4	41
S40: Expansion of the ¹ H-NMR Spectrum of Compound 4	42
S41: Expansion of the ¹ H-NMR Spectrum of Compound 4	43
S42: ¹³ C-NMR and DEPT (600 MHz, CDCl ₃) Spectrum of Compound 4	44
S43: Expansion of the ¹³ C-NMR and DEPT Spectrum of Compound 4	45
S44: HSQC Spectrum (600MHz, CDCl ₃) of Compound 4	46
S45: Expansion of the HSQC Spectrum of Compound 4	47
S46: HMBC Spectrum (600MHz, CDCl ₃) of Compound 4	48
S47: Expansion of the HMBC Spectrum of Compound 4	49
S48: ¹ H- ¹ H COSY Spectrum (600MHz, CDCl ₃) of Compound 4	50
S49: Expansion of the ¹ H- ¹ H COSY Spectrum of Compound 4	52
S50: NOESY spectrum (600MHz, CDCl ₃) of compound 4	53

Shanghai Mass Spectrometry Center
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
High Resolution MS Data Report



Instrument

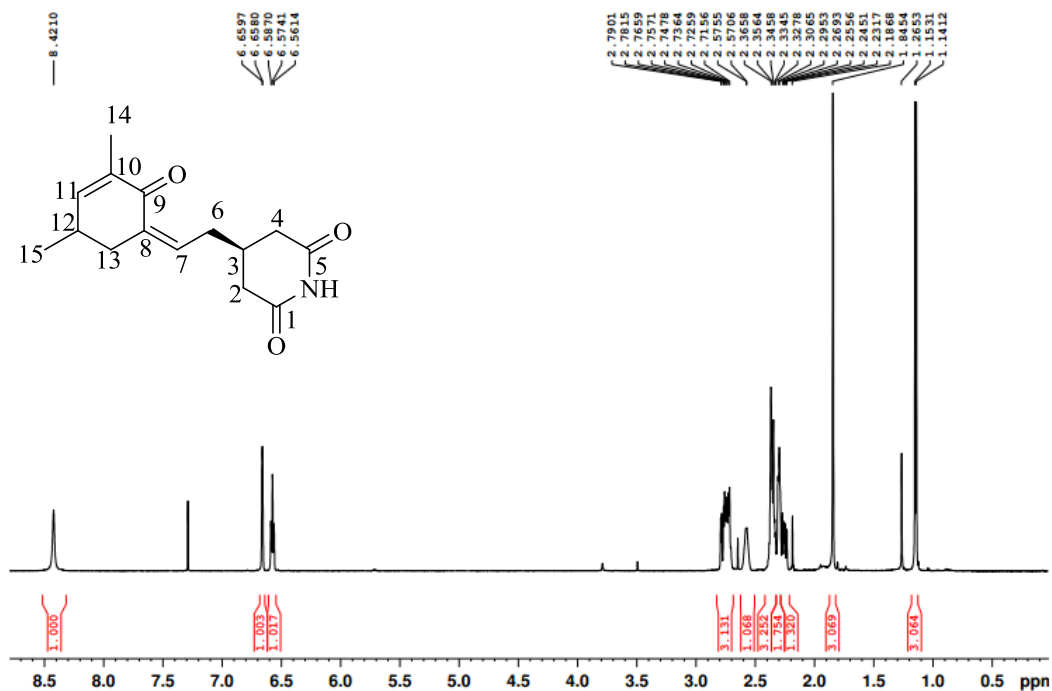


Bruker Daltonics, Inc. APEXIII 7.0 TESLA FTMS

Card Serial Number F140258
Analysis Name D:\Data\zjf\2014\20140225_000002.d
Sample Name **P-42** → **Compound 1**
Acquisition Date 2/26/2014 10:26:30 AM
Operator: zjf
Ionization Mode ESI-Positive
Ion Mass (Measured) 284.1257

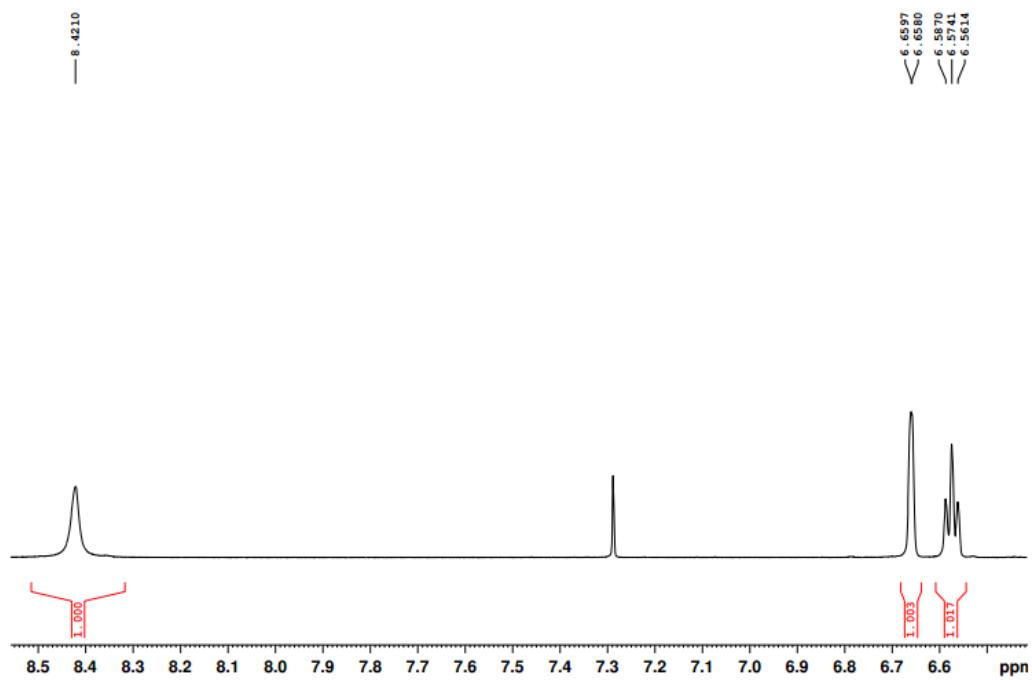
Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e ⁻
C 15 H 19 N 1 Na 1 O 3	0.039	284.1257	0.17	0.26	0.05	6.50	ok	even

S1: HRESIMS Spectrum of Compound 1

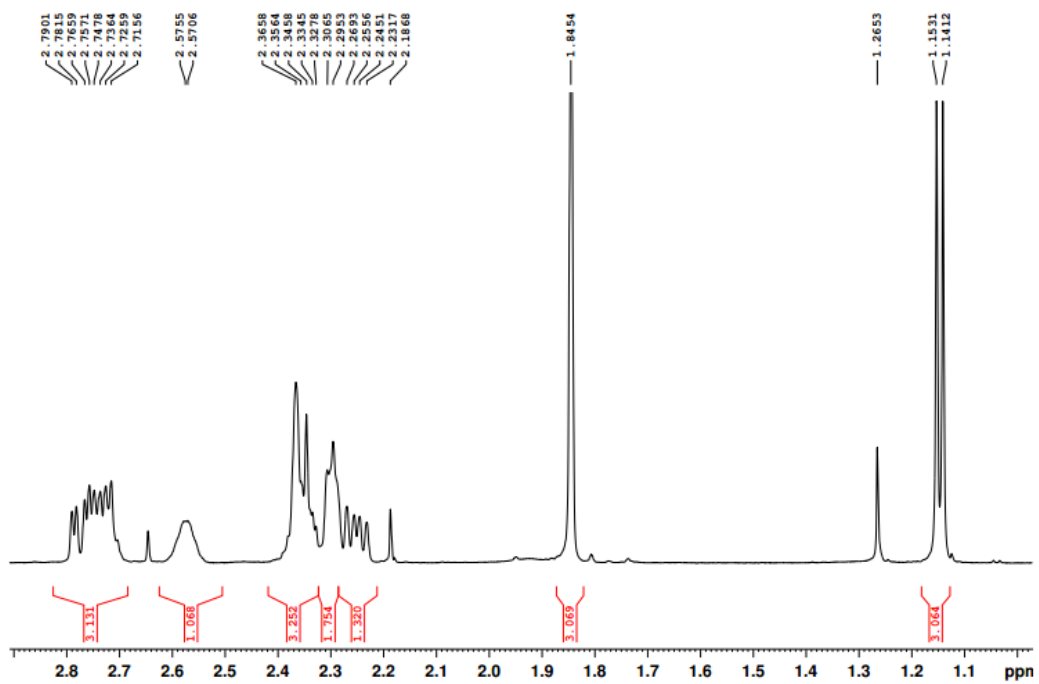


S2: $^1\text{H-NMR}$ Spectrum (600MHz, CDCl_3) of Compound **1**

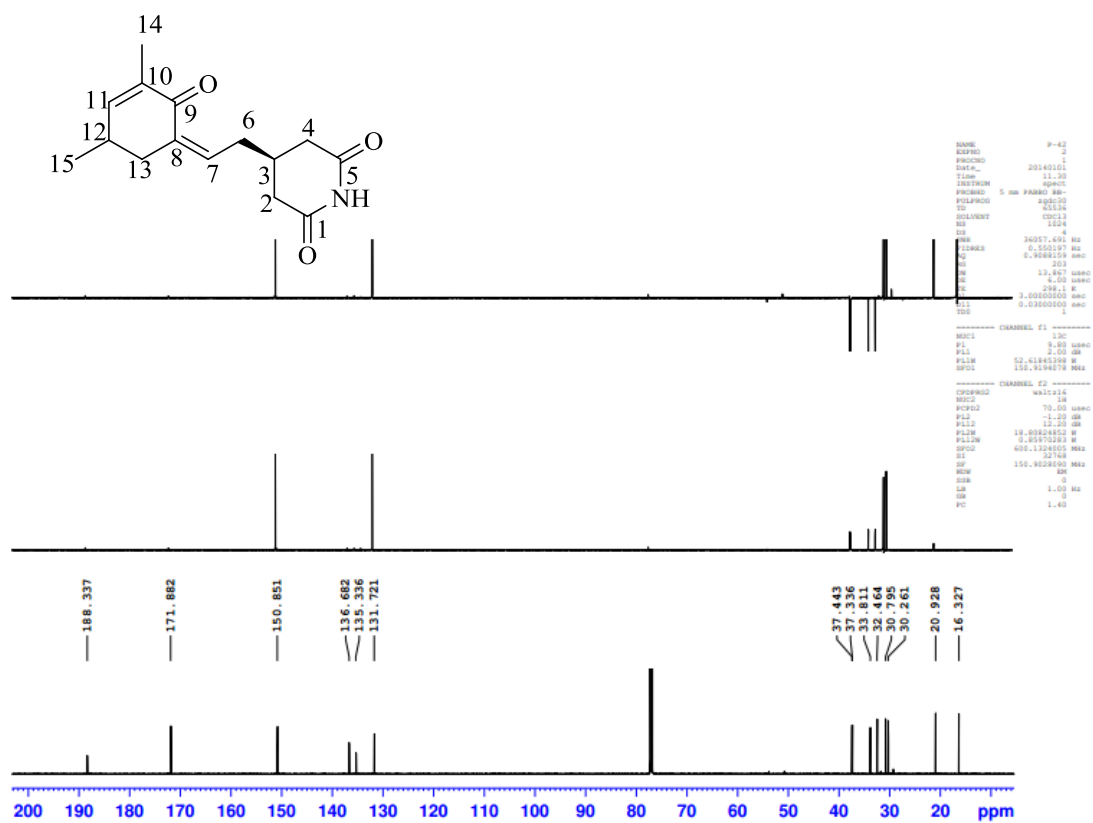
Compound **1** : $^1\text{H-NMR}$ (CDCl_3 , 600 MHz), δ : 1.20(3H, d, H-15), 1.77(3H, brs, H-14), 2.25(1H, dd, H-13 β), 2.29(2H, m, H-6), 2.35(2H, m, H-2), 2.36(1H, m, H-3), 2.57(1H, br s, H-12), 2.73(2H, m, H-4), 2.77(1H, m, H-13 α), 6.58(1H, t, H-7), 6.66(1H, br s, H-11). $^{13}\text{C-NMR}$ (CDCl_3 , 600 MHz), δ : 16.4 (C-14), 20.9 (C-15), 30.3 (C-3), 30.8 (C-12), 32.5 (C-6), 33.9 (C-13), 37.3 (C-4), 37.4 (C-2), 131.8 (C-7), 135.5 (C-10), 136.9 (C-8), 151.0 (C-11), 172.0 (C-1/5), 188.5 (C-9). EIMS: m/z = 261[M] $^+$ for formula $\text{C}_{15}\text{H}_{19}\text{NO}_3$.



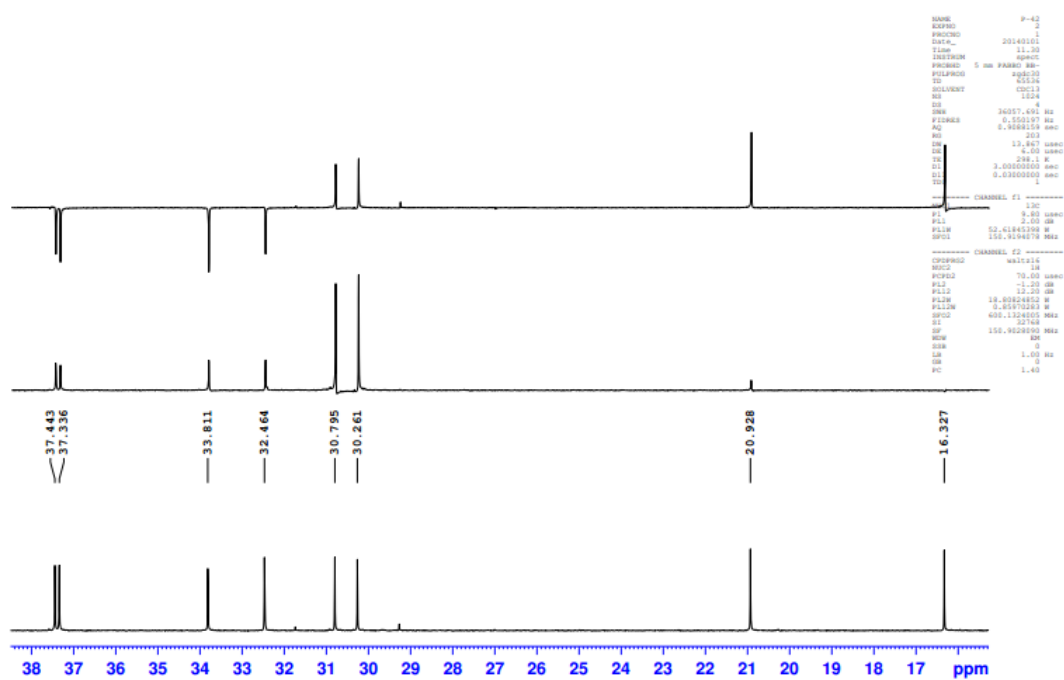
S3: Expansion of the $^1\text{H-NMR}$ Spectrum of Compound 1



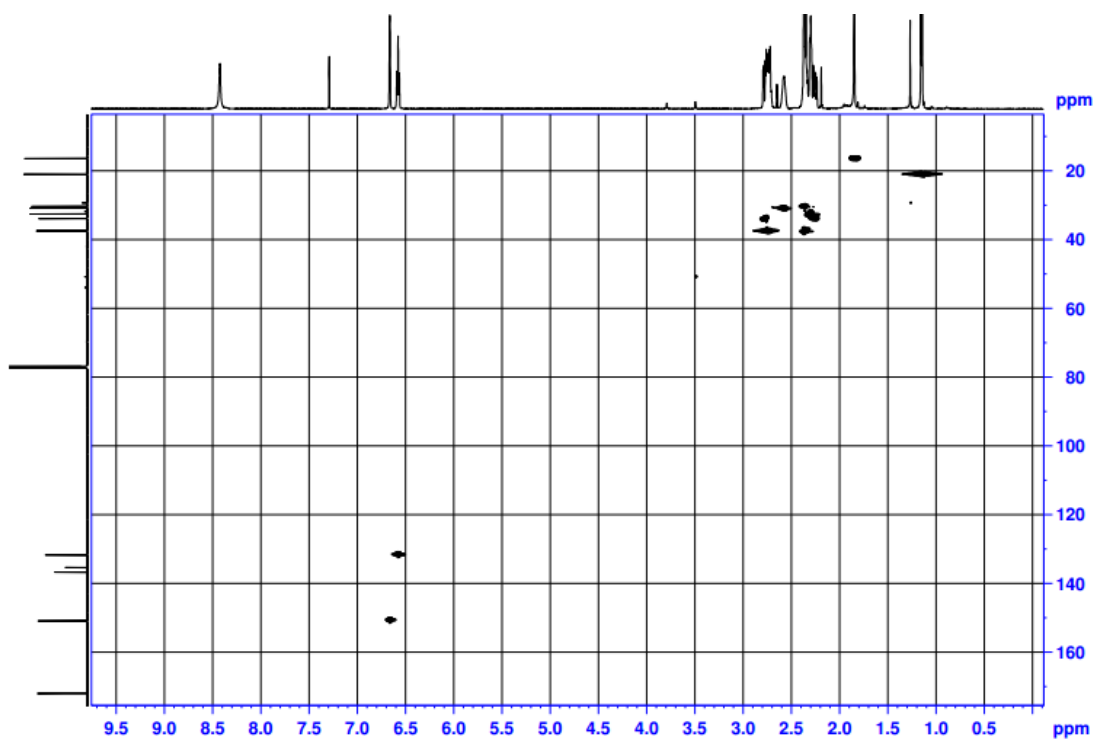
S4: Expansion of the $^1\text{H-NMR}$ Spectrum of Compound 1



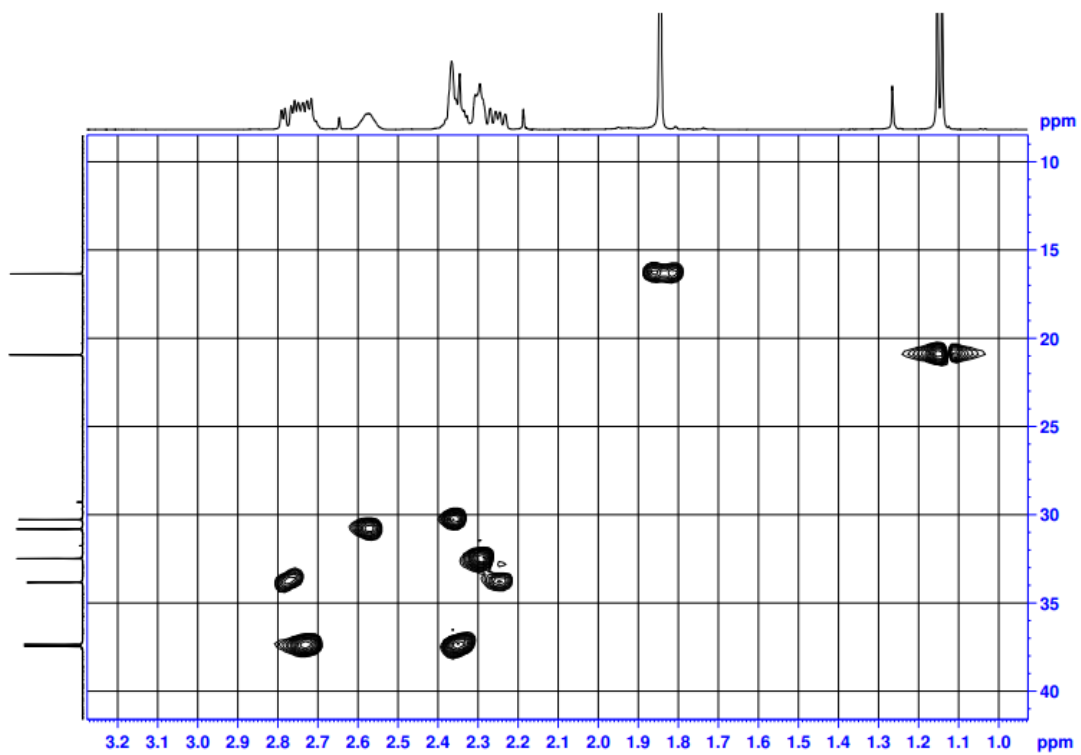
S5: ^{13}C -NMR and DEPT Spectrum (600MHz, CDCl_3) of Compound 1



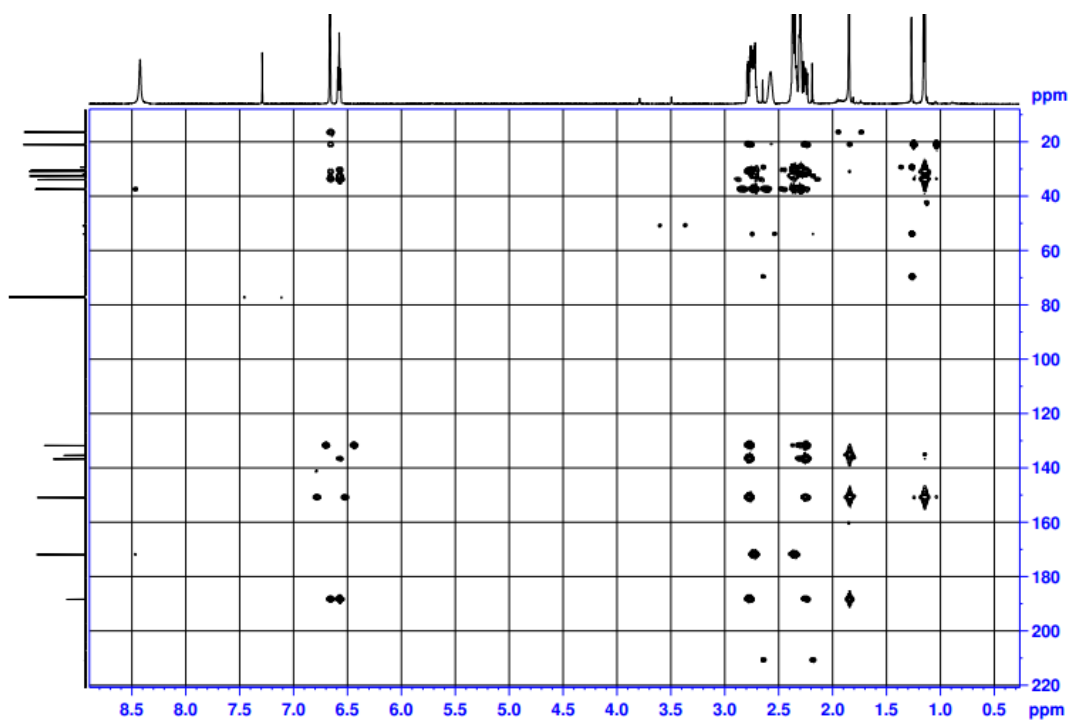
S6: Expansion of the ^{13}C -NMR and DEPT Spectrum of Compound **1**



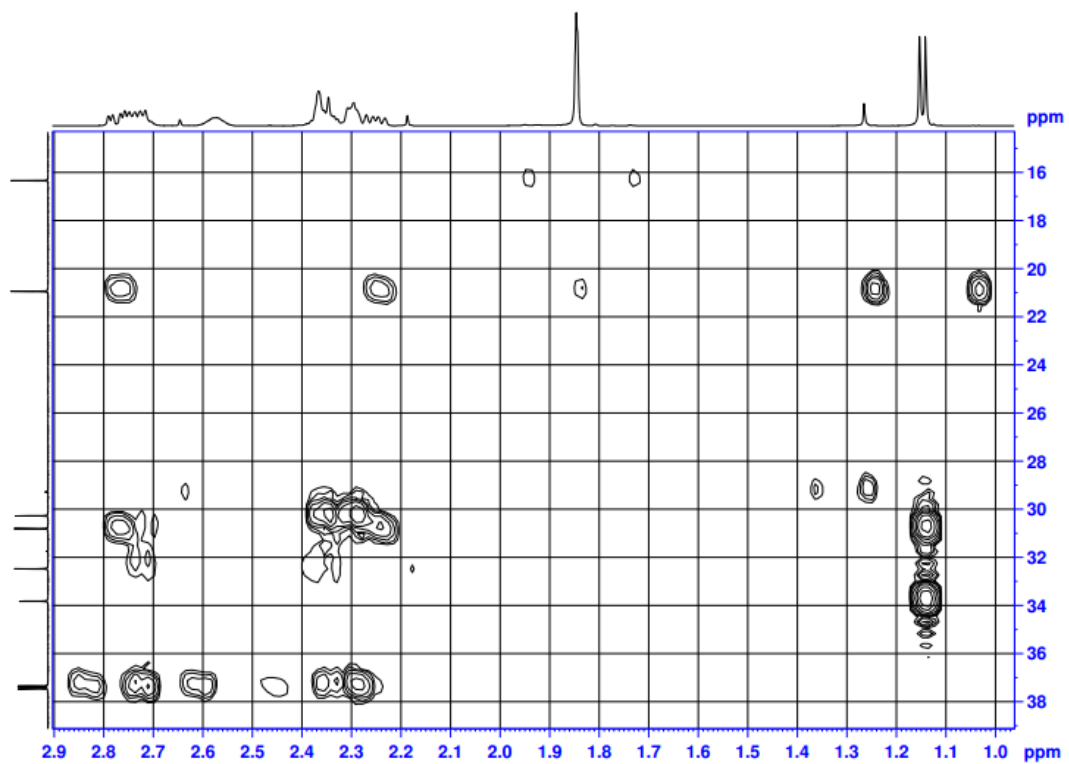
S7: HSQC Spectrum (600MHz, CDCl_3) of Compound **1**



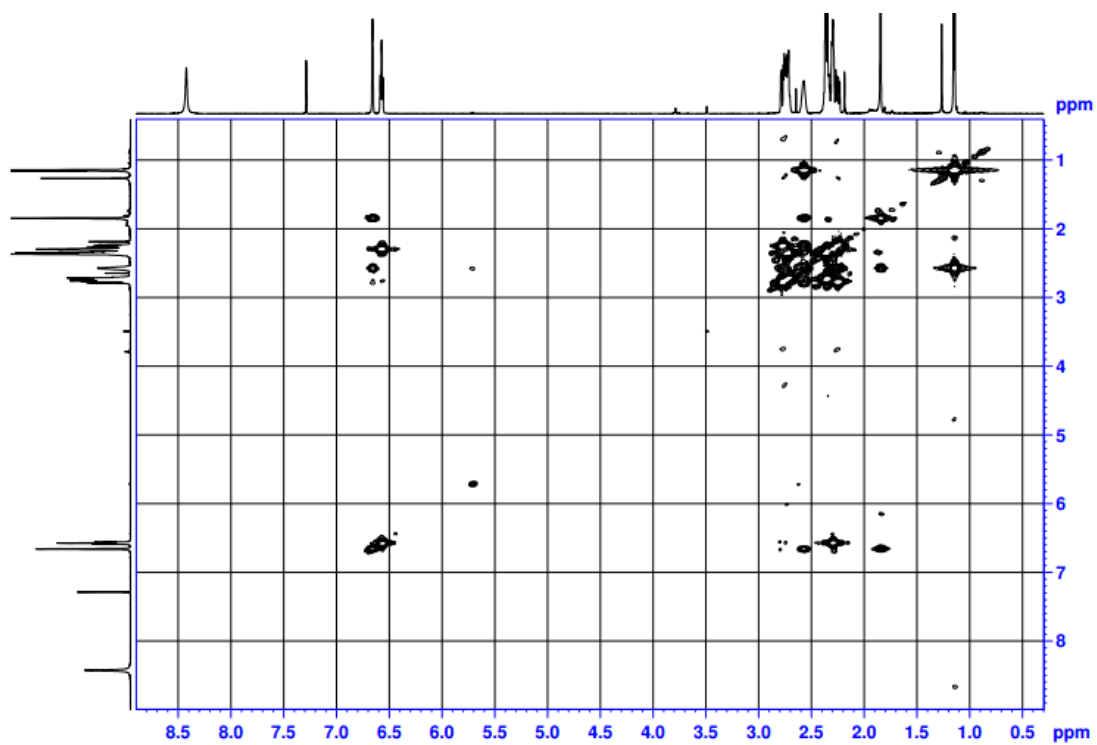
S8: Expansion of the COSY Spectrum of Compound **1**



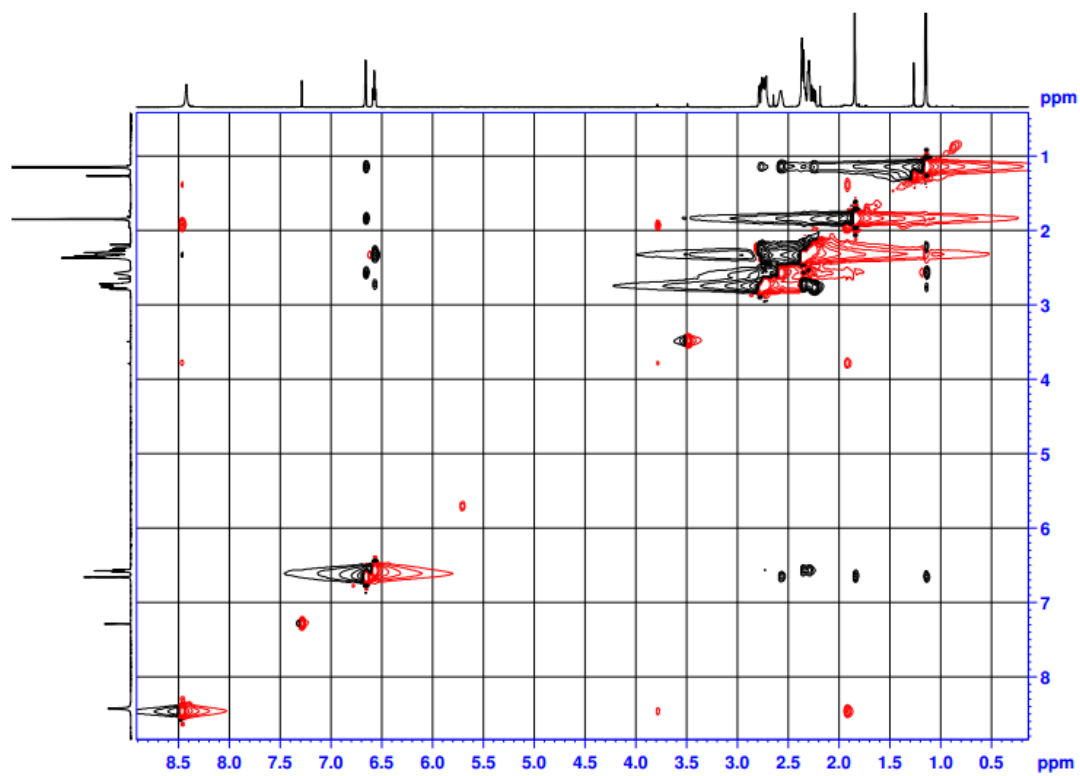
S9: HMBC Spectrum (600MHz, CDCl_3) of Compound **1**



S10: Expansion of the HMBC Spectrum of Compound **1**



S11: ^1H - ^1H COSY Spectrum (600MHz, CDCl_3) of Compound **1**



S13: NOESY spectrum (600MHz, CDCl_3) of compound **1**

Shanghai Mass Spectrometry Center
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
High Resolution MS Data Report



Instrument

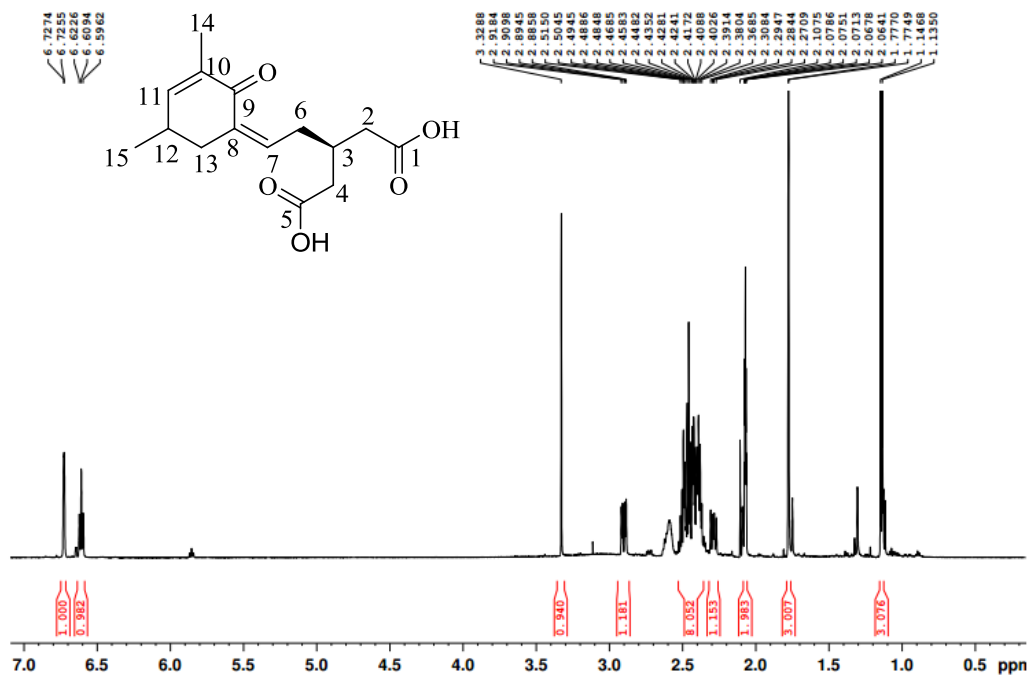


Bruker Daltonics, Inc. APEXIII 7.0 TESLA FTMS

Card Serial Number F140115
Analysis Name D:\Data\zjf2014\20140108_000002.d
Sample Name **h-119-24** → **Compound 2**
Acquisition Date 5/8/2013 4:00:34 PM
Operator: zjf
Ionization Mode ESI-Positive
Ion Mass (Measured) 303.1206

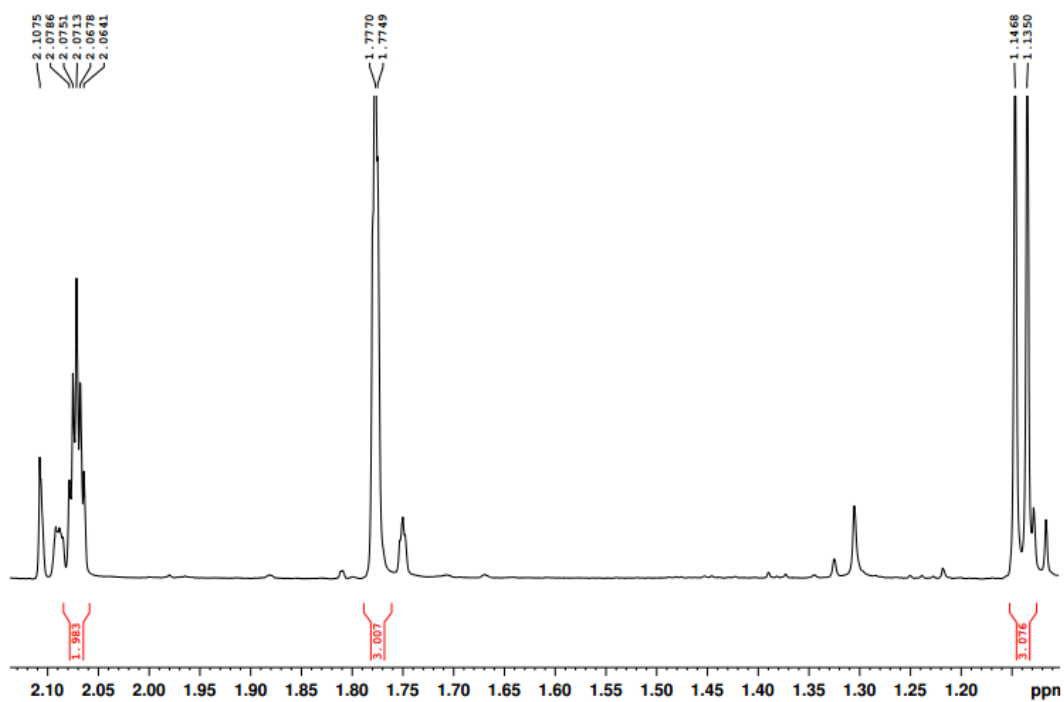
Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e ⁻
C 15 H 17 N 3 O 4	0.209	303.1214	2.62	-5.86	0.80	9.00	ok	odd
C 15 H 20 Na 1 O 5	0.208	303.1203	-0.88	-8.96	-0.27	5.50	ok	even

S14: HRESIMS Spectrum of Compound 2

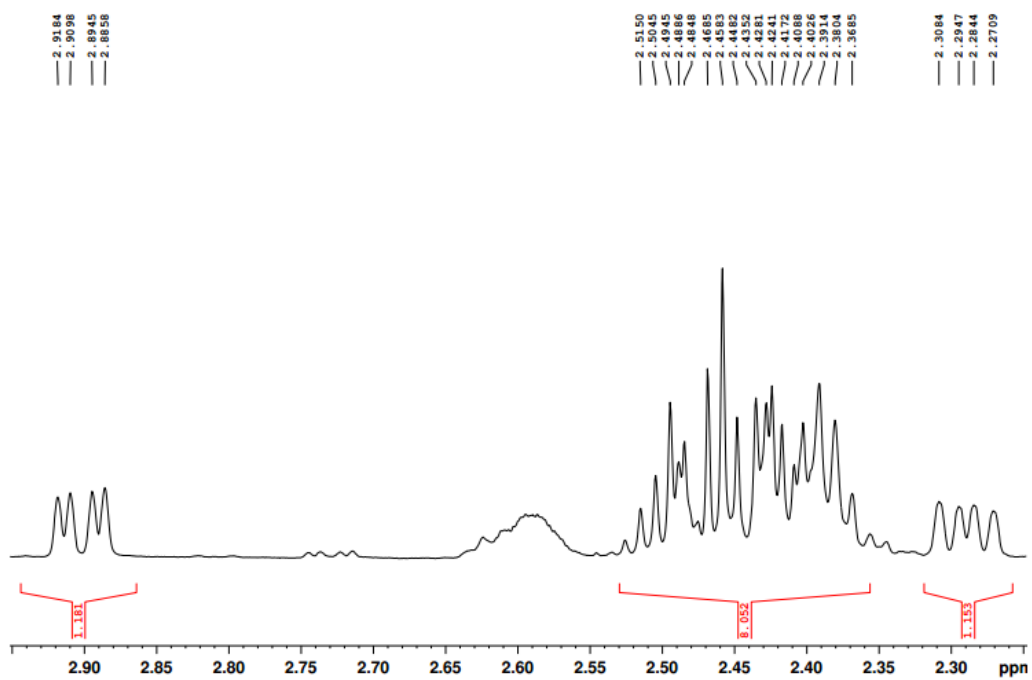


S15: $^1\text{H-NMR}$ Spectrum (600MHz, Acetone) of Compound 2

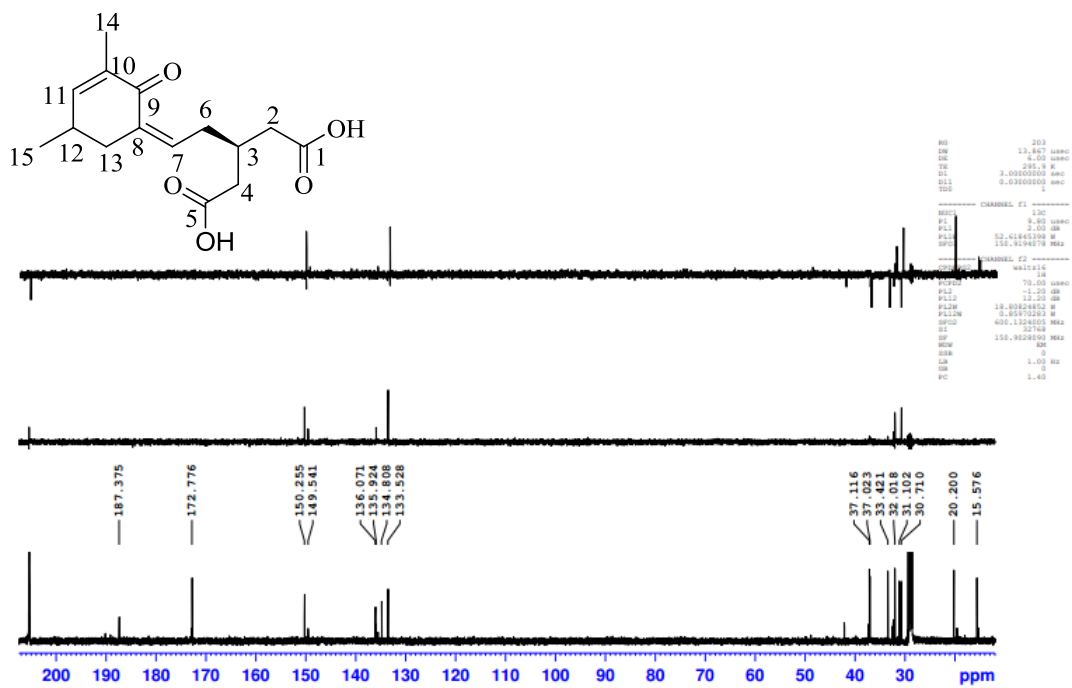
Compound 2 : $^1\text{H-NMR}$ (CDCl_3 , 600 MHz), δ : 1.14(3H, d, H-15), 1.78(3H, brs, H-14), 2.29(1H, dd, H-13 β), 2.39(2H, m, H-6), 2.43(2H, m, H-4), 2.46(2H, m, H-2), 2.50(1H, m, H-3), 2.59(1H, br s, H-12), 2.90(1H, m, H-13 α), 6.61(1H, t, H-7), 6.73(1H, br s, H-11). $^{13}\text{C-NMR}$ (CDCl_3 , 600 MHz), δ : 15.7 (C-14), 20.3 (C-15), 30.7 (C-12), 31.1 (C-6), 32.0 (C-3), 33.5 (C-13), 37.0 (C-4), 37.1 (C-2), 133.6 (C-7), 134.8 (C-10), 136.1 (C-8), 150.4 (C-11), 172.9 (C-1/5), 187.4 (C-9). EIMS: $m/z = 280[\text{M}]^+$ for formula $\text{C}_{15}\text{H}_{20}\text{O}_5$.



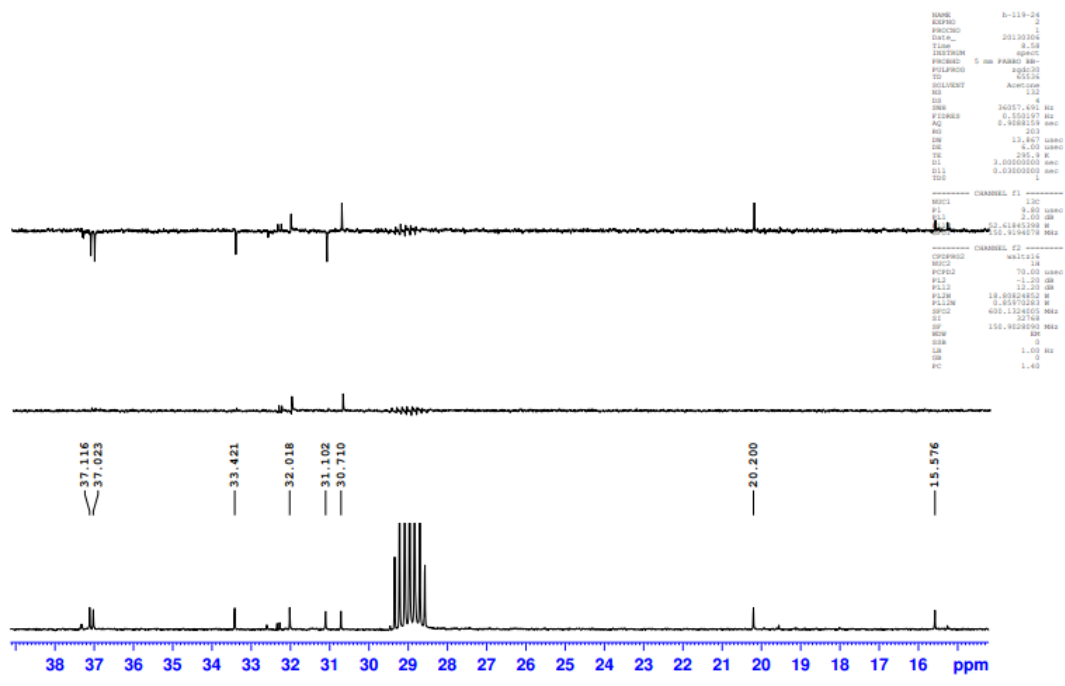
S16: Expansion of the $^1\text{H-NMR}$ Spectrum of Compound 2



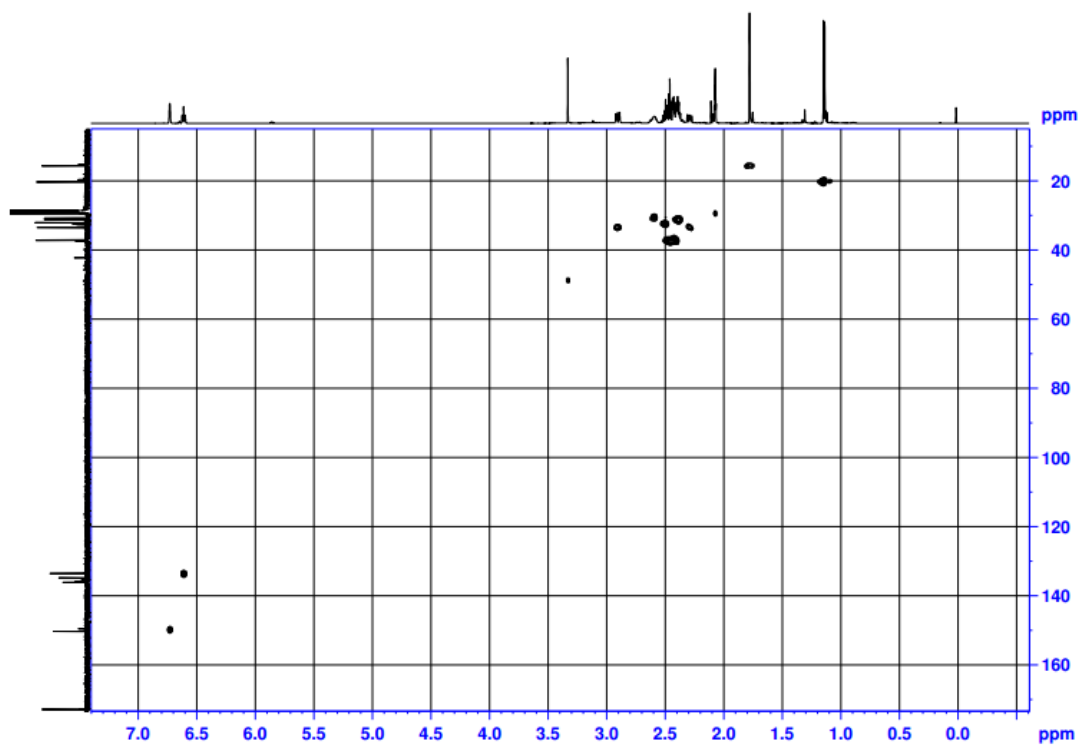
S17: Expansion of the ¹H-NMR Spectrum of Compound 2



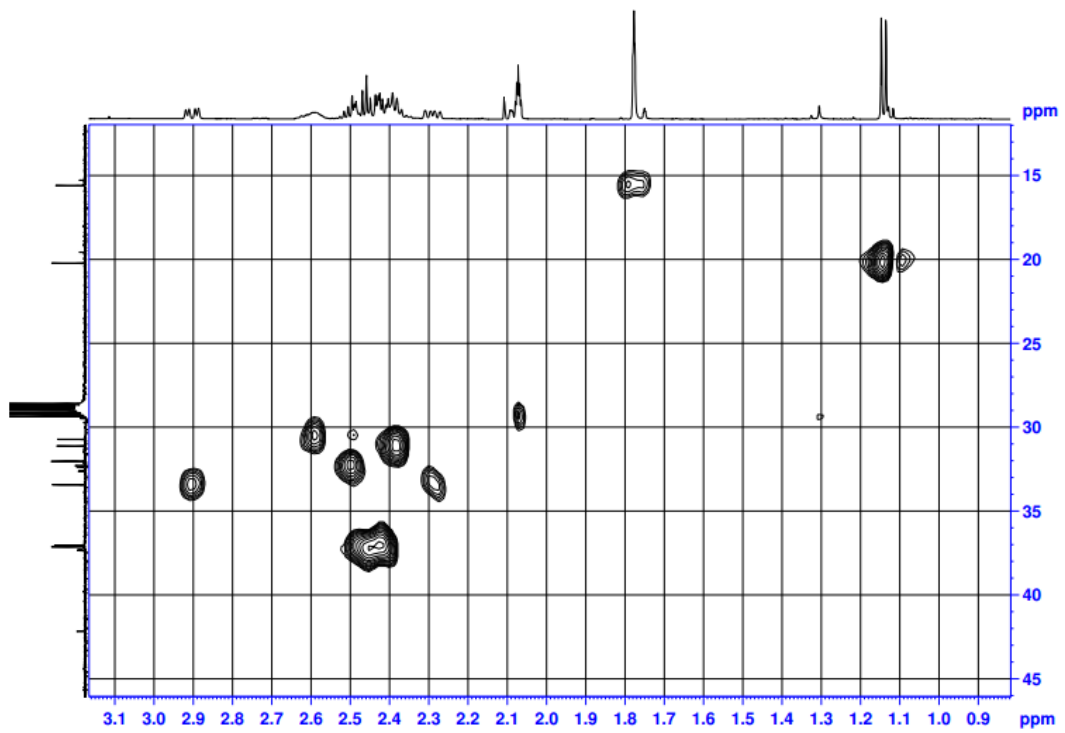
S18: ¹³C-NMR and DEPT Spectrum (600MHz, Acetone) of Compound 2



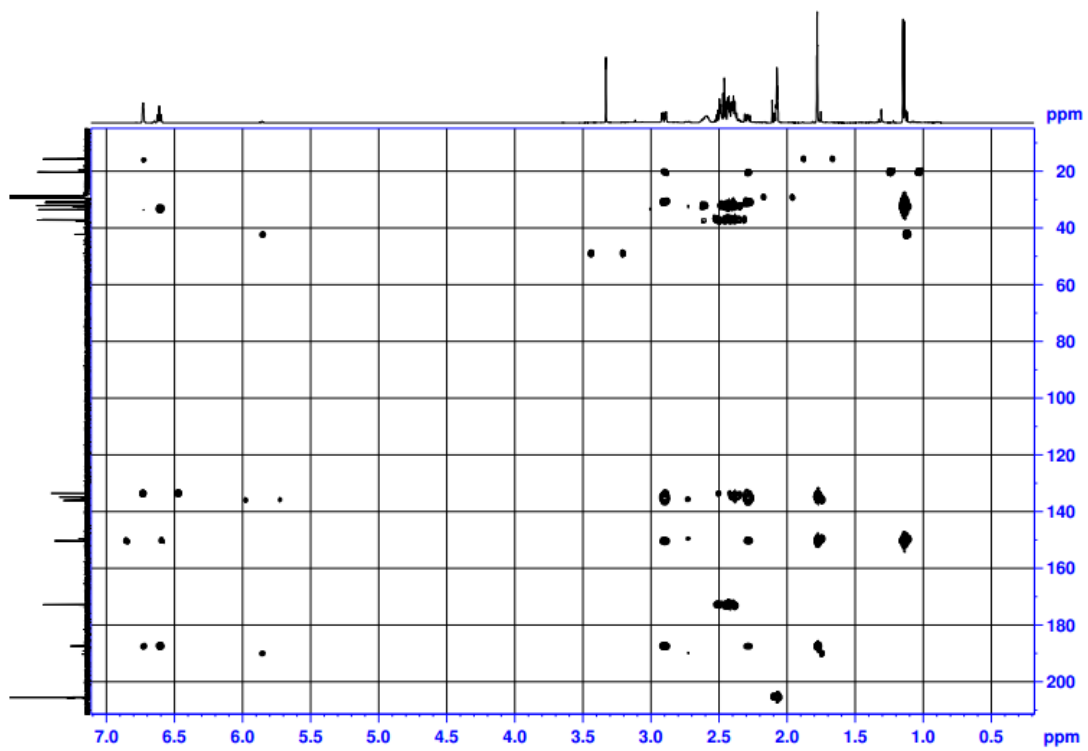
S19: Expansion of the ^{13}C -NMR and DEPT Spectrum of Compound **2**



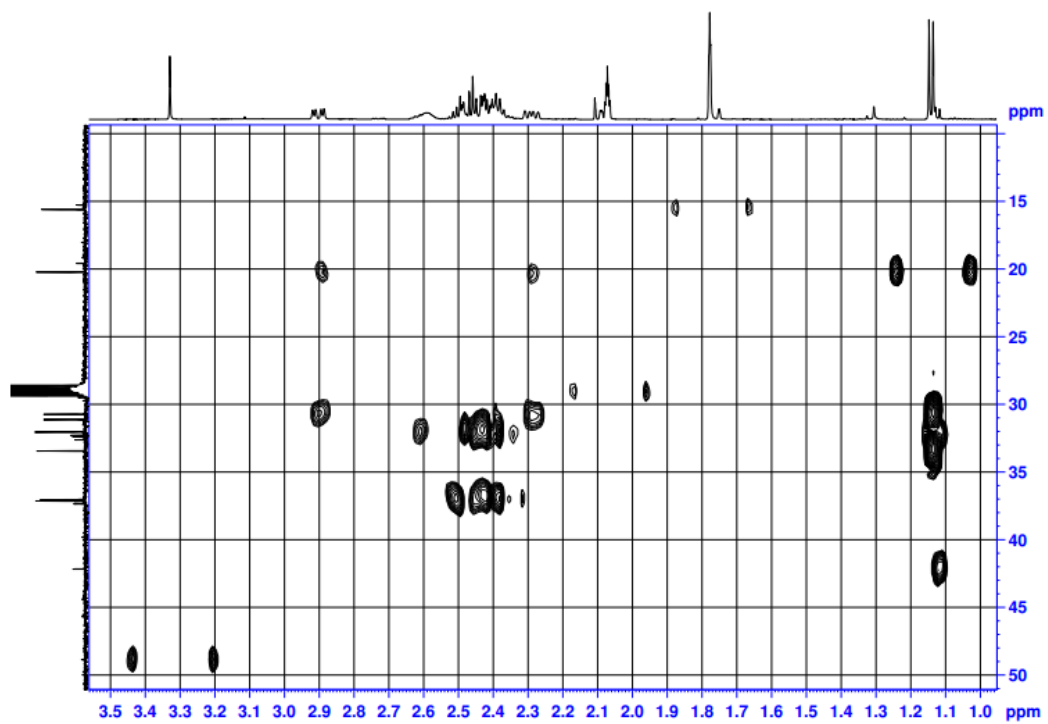
S20: HSQC Spectrum (600MHz, CDCl₃) of Compound **2**



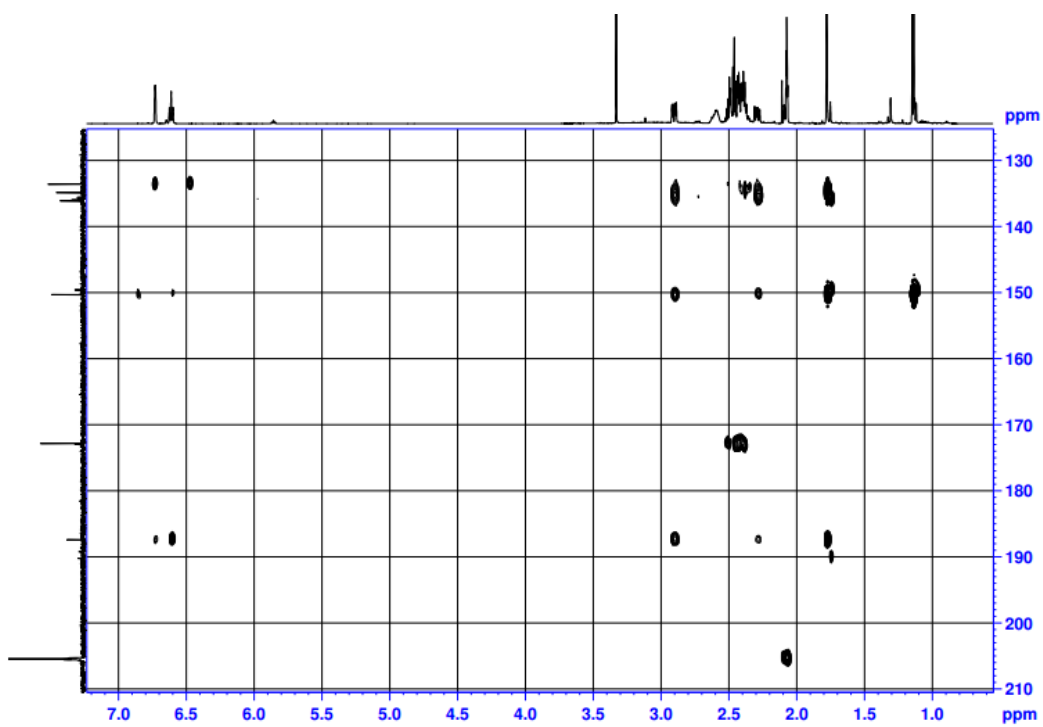
S21: Expansion of the HSQC Spectrum of Compound 2



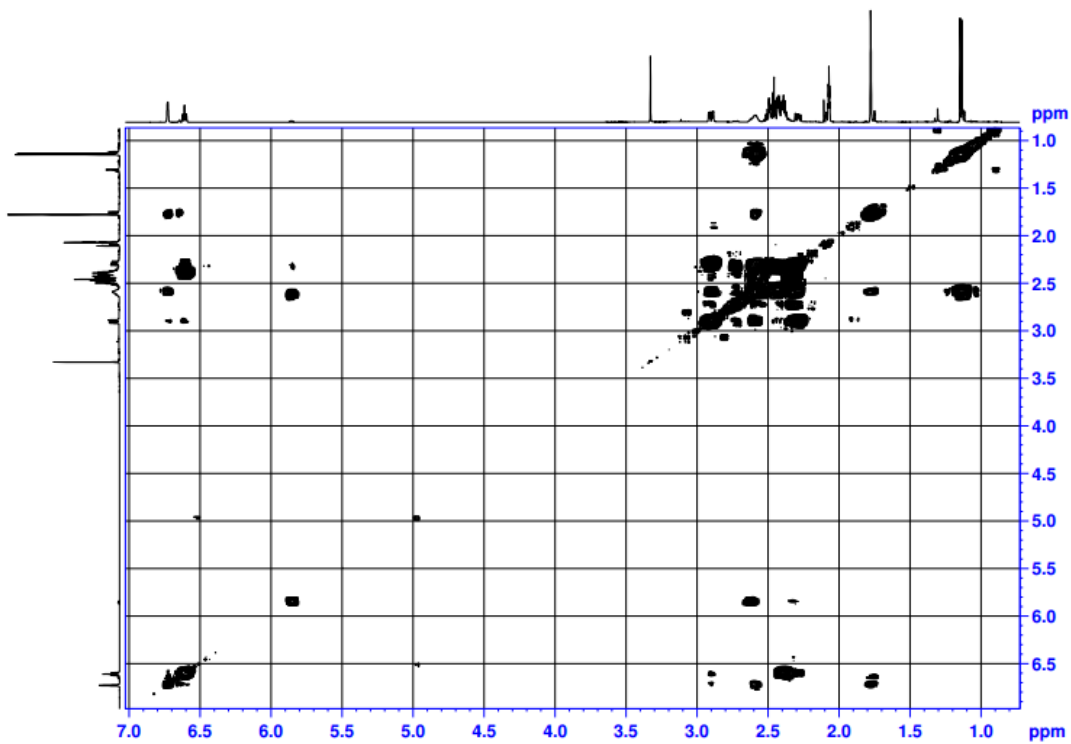
S22: HMBC Spectrum (600MHz, Acetone) of Compound **2**



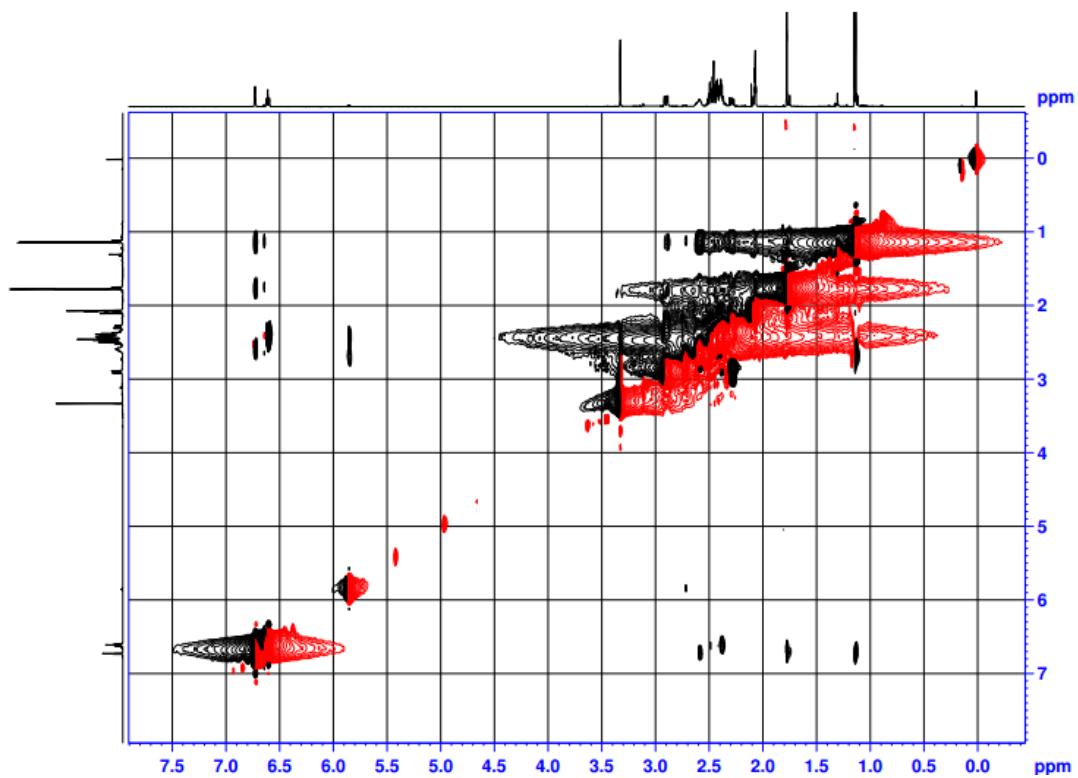
S23: Expansion of the HMBC Spectrum of Compound 2



S24: Expansion of the HMBC Spectrum of Compound 2



S25: ^1H - ^1H COSY Spectrum (600MHz, Acetone) of Compound 2



S27: NOESY Spectrum (600MHz, Acetone) of Compound 2

Shanghai Mass Spectrometry Center
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
High Resolution MS Data Report



Instrument

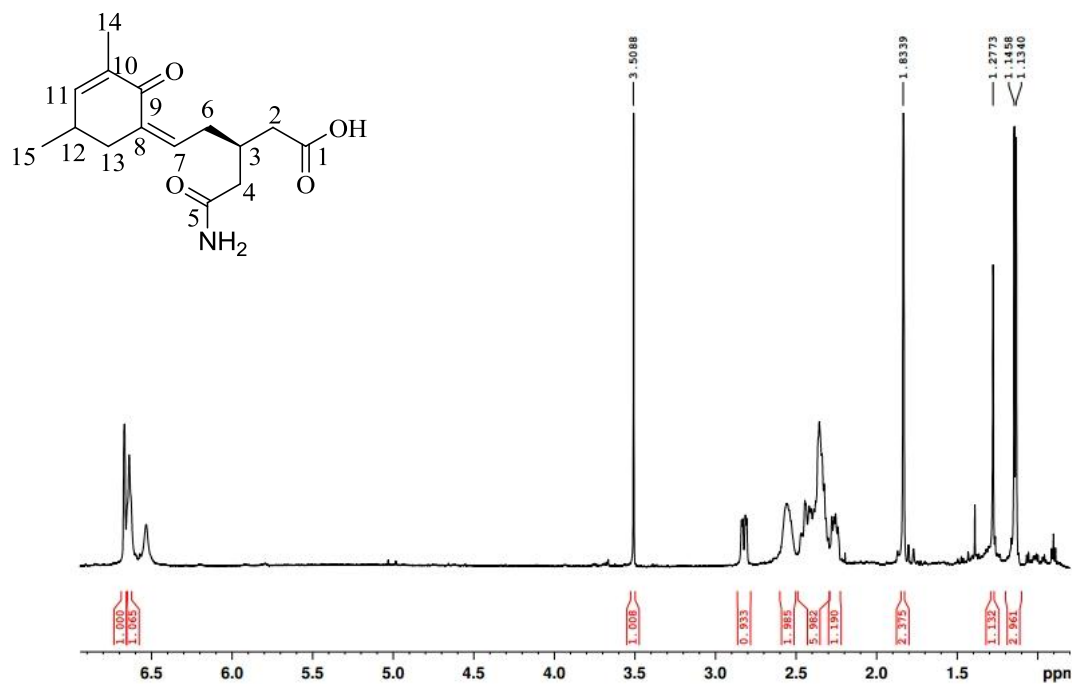


Bruker Daltonics, Inc. APEXIII 7.0 TESLA FTMS

Card Serial Number F140112
Analysis Name D:\Data\zjf\2014\20140106_000032.d
Sample Name **h-119-14** → **Compound 3**
Acquisition Date 5/8/2013 3:13:36 PM
Operator: zjf
Ionization Mode ESI-Positive
Ion Mass (Measured) 302.1354

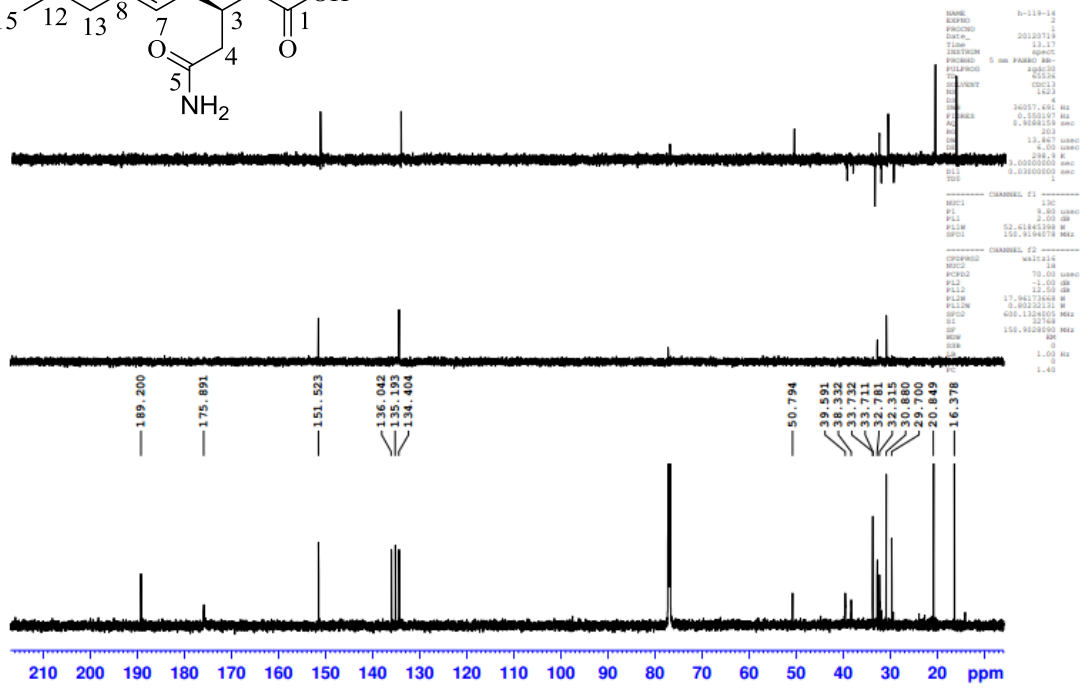
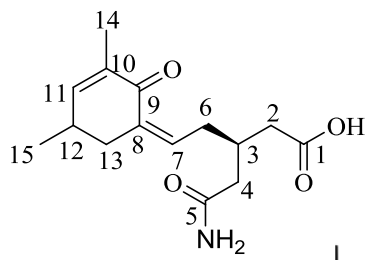
Sum	Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e ⁻
C 12 H 20 N 3 O 6		0.021	302.1347	-2.37	-3.57	-0.72	4.50	ok	even
C 14 H 22 O 7		0.016	302.1360	2.08	0.86	0.63	4.00	ok	odd
C 15 H 21 N 1 Na 1 O 4		0.019	302.1363	2.99	1.61	0.90	5.50	ok	even

S28: HRESIMS Spectrum of Compound 3

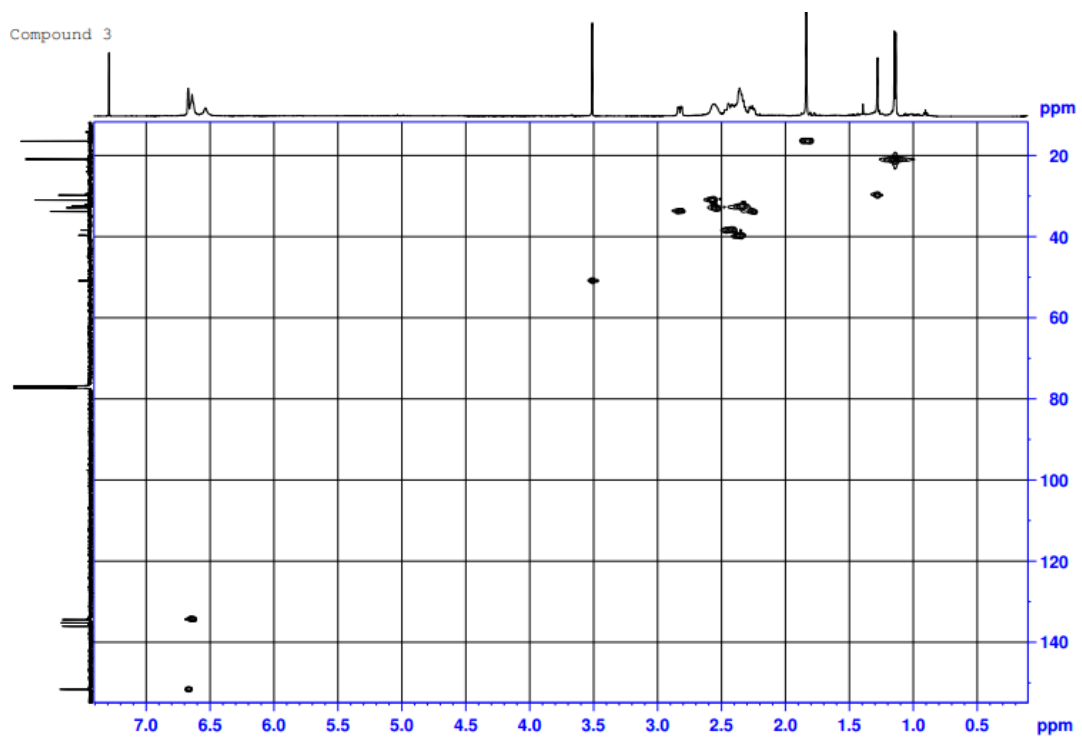


S29: $^1\text{H-NMR}$ Spectrum (600MHz, CDCl_3) of Compound **3**

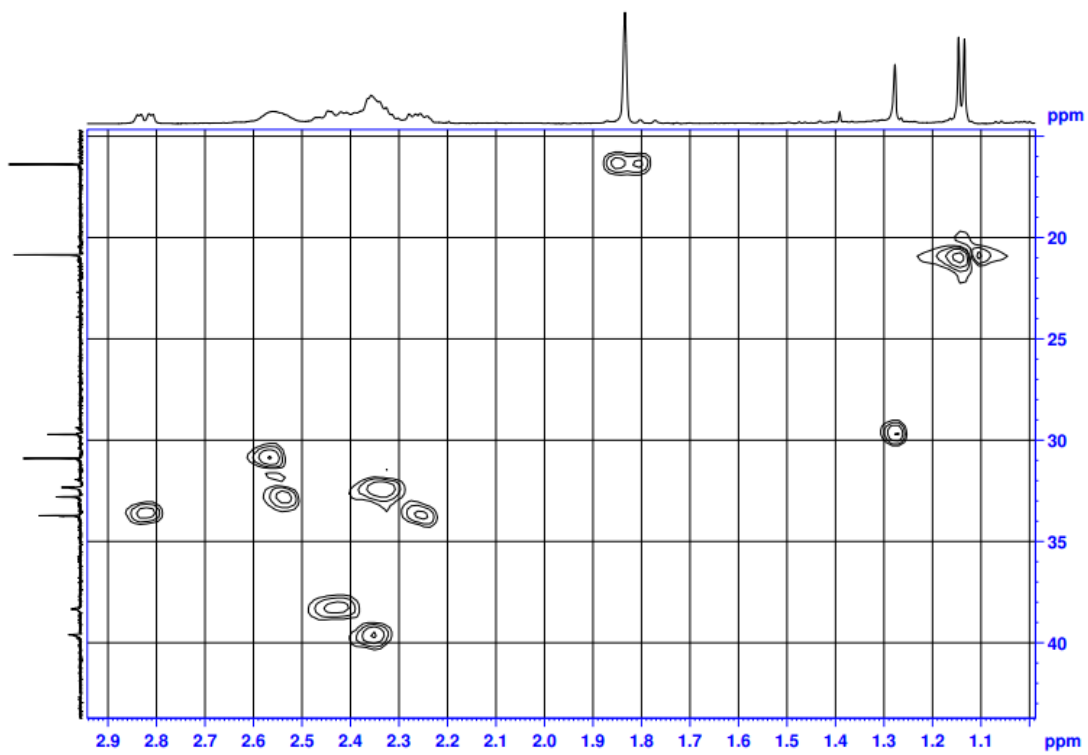
Compound **3** : $^1\text{H-NMR}$ (CDCl_3 , 600 MHz), δ : 1.15(3H, d, H-15), 1.83(3H, brs, H-14), 2.25(1H, dd, H-13 β), 2.33(2H, m, H-6), 2.35(2H, m, H-4), 2.43(2H, m, H-2), 2.54(1H, m, H-3), 2.57(1H, m, H-12), 2.83(1H, dd, H-13 α), 6.64(1H, br s, H-7), 6.67(1H, br s, H-11). $^{13}\text{C-NMR}$ (CDCl_3 , 600 MHz), δ : 16.4 (C-14), 20.9 (C-15), 30.8 (C-12), 33.3 (C-6), 32.8 (C-3), 33.8 (C-13), 38.4 (C-2), 39.7 (C-4), 134.3 (C-7), 135.2 (C-10), 136.1 (C-8), 151.6 (C-11), 176.1 (C-1/5), 189.3(C-9). EIMS: $m/z = 279[\text{M}]^+$ for formula $\text{C}_{15}\text{H}_{21}\text{NO}_4$.



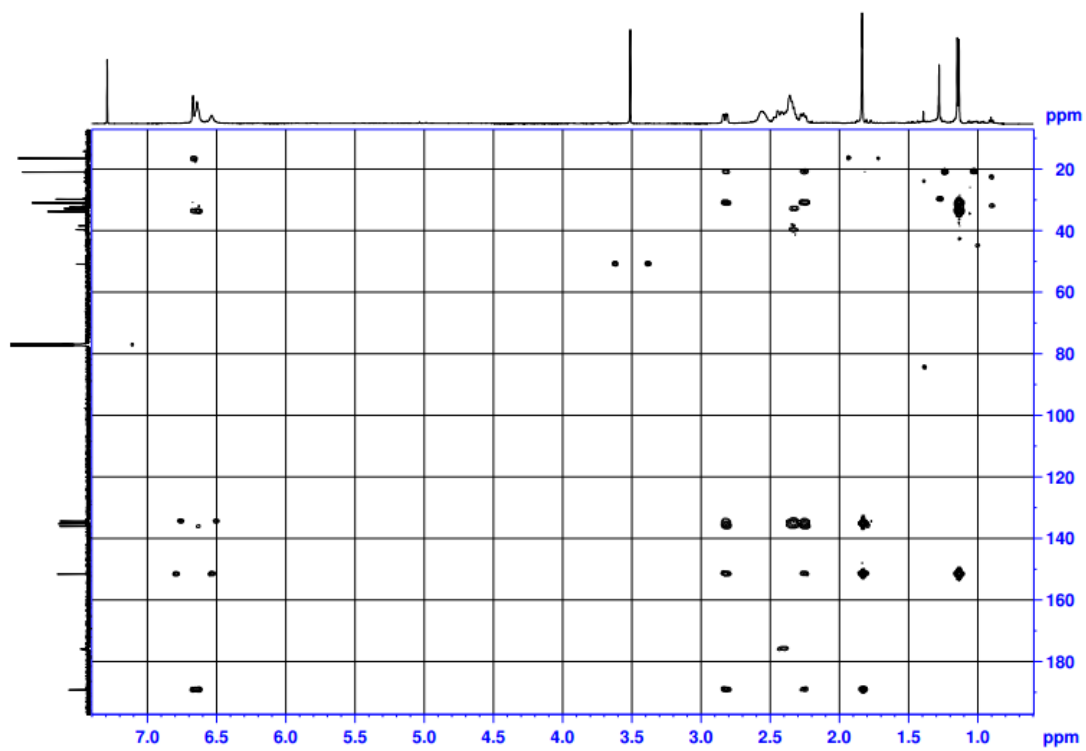
S30: ¹³C-NMR and DEPT Spectrum (600MHz, CDCl₃) of Compound 3



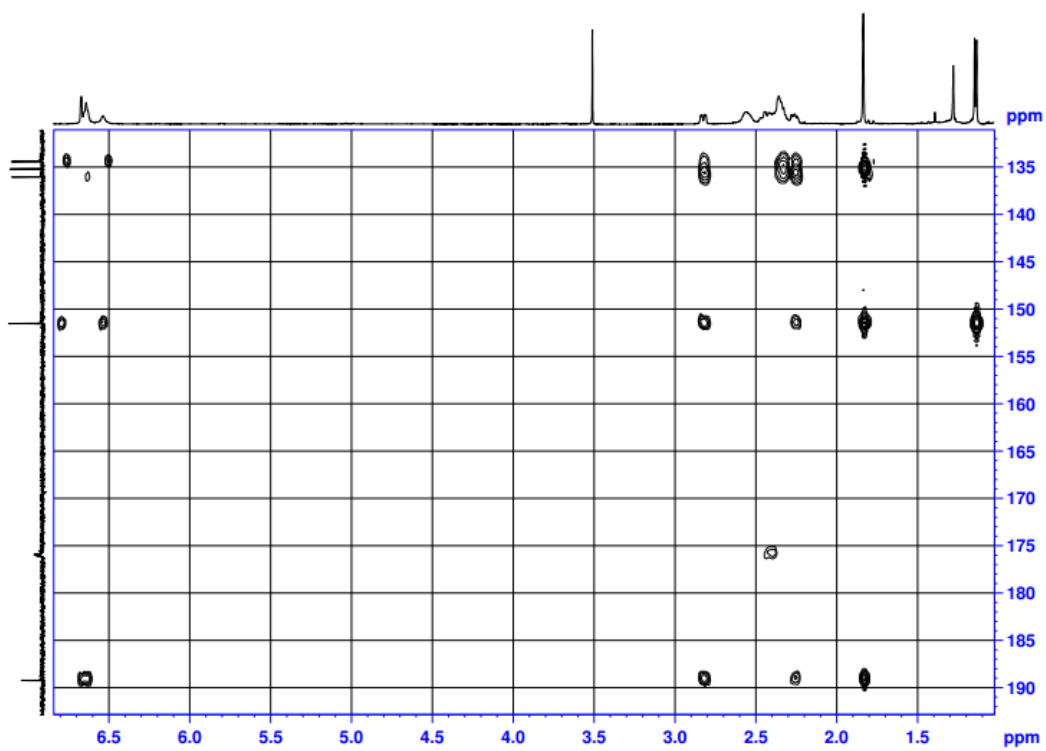
S31: HSQC Spectrum (600MHz, CDCl₃) of Compound 3



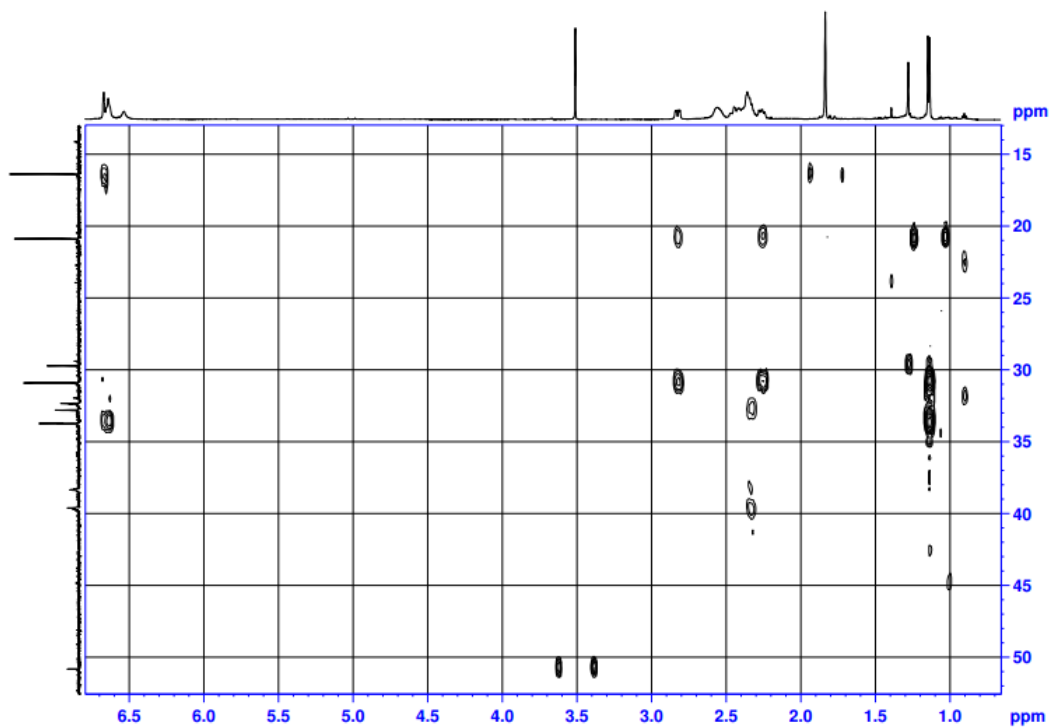
S32: Expansion of the HSQC Spectrum of Compound 3



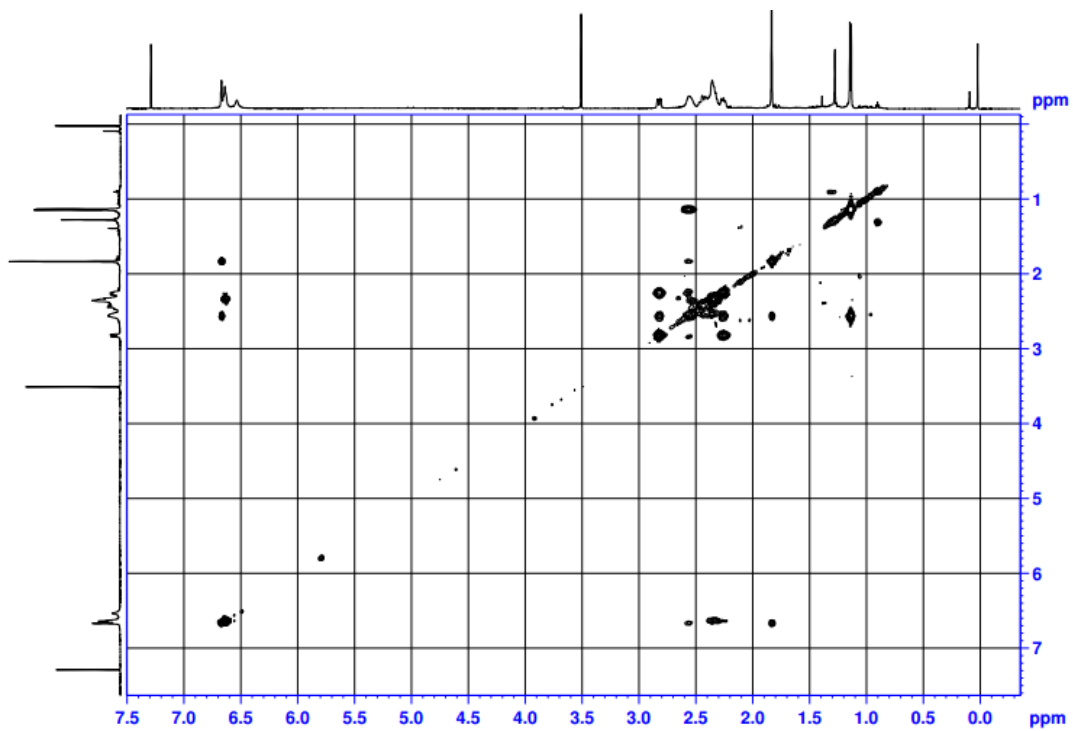
S33: HMBC Spectrum (600MHz, CDCl₃) of Compound 3



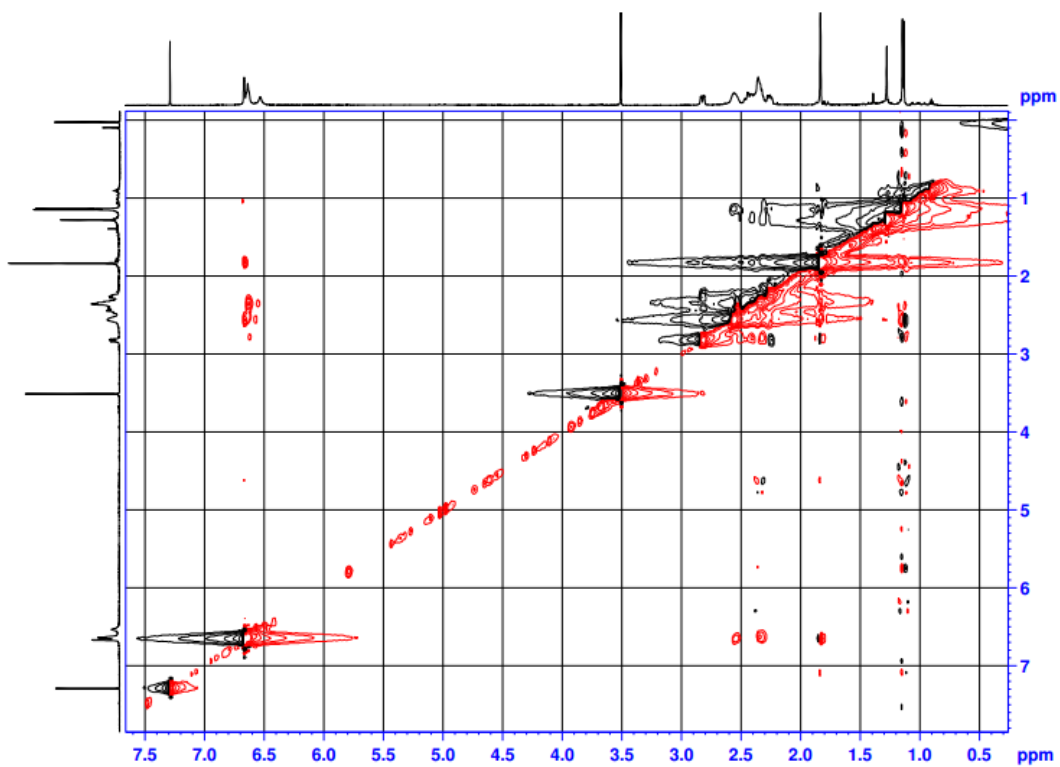
S34: Expansion of the HMBC Spectrum of Compound 3



S35: Expansion of the HMBC Spectrum of Compound **3**



S36: ^1H - ^1H COSY Spectrum (600MHz, CDCl_3) of Compound **3**



S37: NOESY Spectrum (600MHz, CDCl₃) of Compound **3**

Shanghai Mass Spectrometry Center
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
High Resolution MS Data Report



Instrument

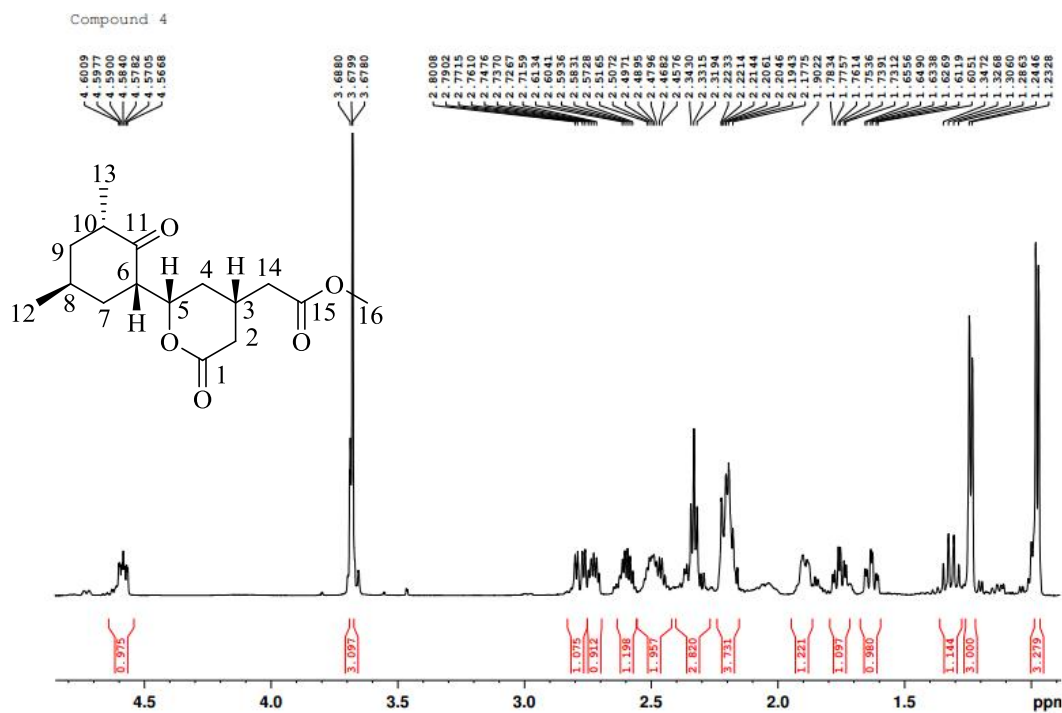


Bruker Daltonics, Inc. APEXIII 7.0 TESLA FTMS

Card Serial Number F140114
Analysis Name D:\Data\zjf\2014\20140108_000002.d
Sample Name h-119-22 → Compound 4
Acquisition Date 5/8/2013 4:00:34 PM
Operator: zjf
Ionization Mode ESI-Positive
Ion Mass (Measured) 319.1512

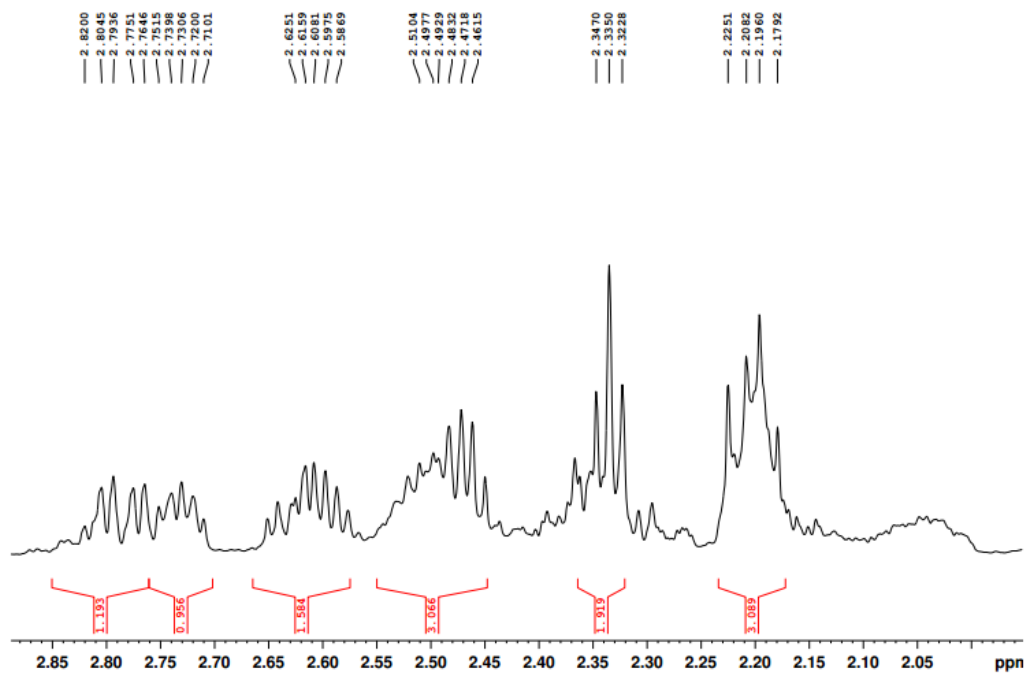
Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e ⁻
C 13 H 23 N 2 O 7	0.015	319.1500	-3.70	-3.94	-1.18	3.50	ok	even
C 14 H 22 N 3 Na 1 O 4	0.007	319.1503	-2.83	-3.14	-0.90	5.00	ok	odd
C 16 H 21 N 3 O 4	0.005	319.1527	4.70	4.40	1.50	8.00	ok	odd
C 16 H 24 Na 1 O 5	0.002	319.1516	1.37	1.28	0.44	4.50	ok	even

S38: HRESIMS Spectrum of Compound 4

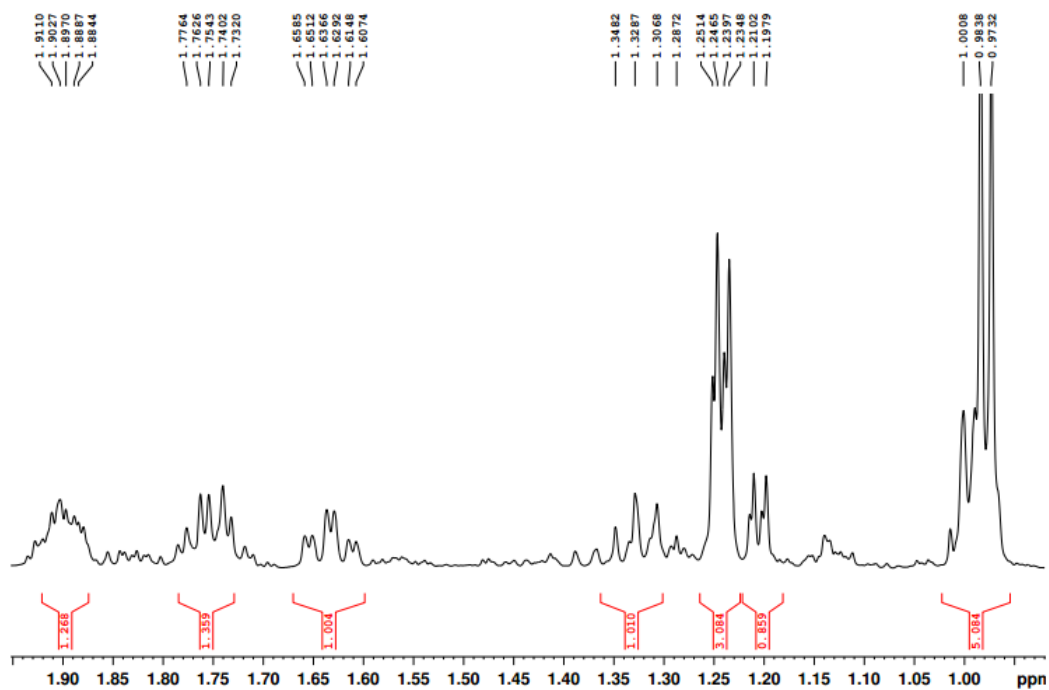


S39: $^1\text{H-NMR}$ Spectrum (600MHz, CDCl_3) of Compound 4

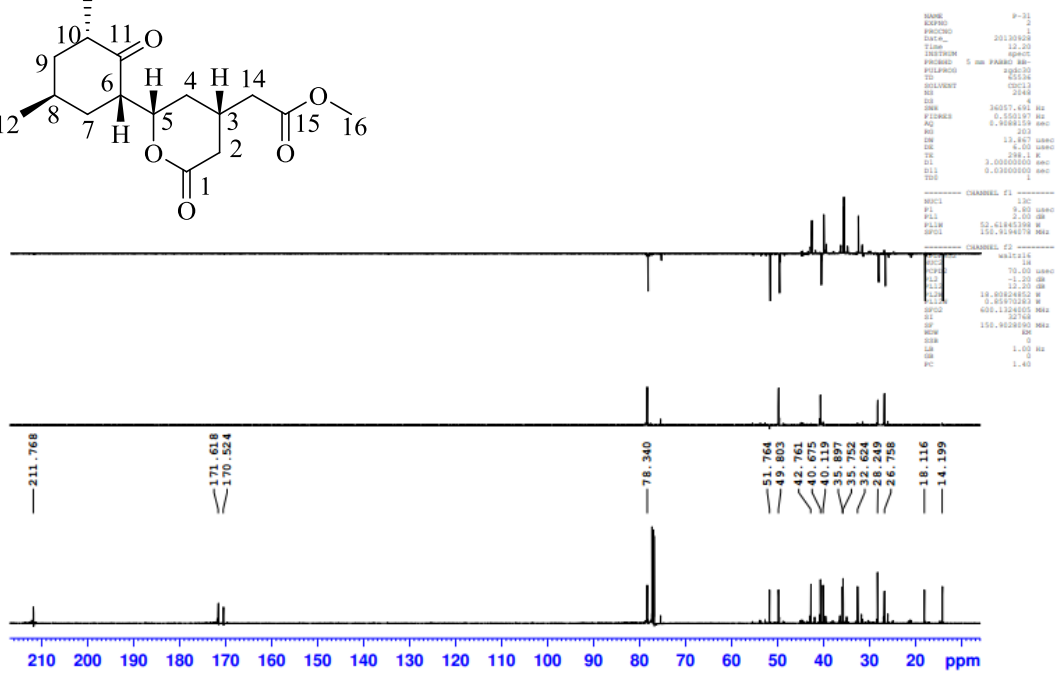
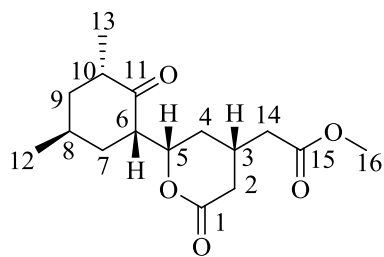
Compound 4: $^1\text{H-NMR}$ (CDCl_3 , 600 MHz), δ : 0.98(3H, d, H-13), 1.24(3H, d, H-12), 1.32(1H, dd, H-4 β), 1.63(1H, td, H-9 β), 1.78(1H, td, H-7 β), 1.89(1H, m, H-9 α), 2.19(1H, m, H-7 α), 2.19(1H, m, H-8), 2.22(1H, m, H-2 β), 2.22(1H, m, H-4 α), 2.34(2H, t, H-14), 2.49(1H, m, H-3), 2.60(1H, m, H-10), 2.73(1H, m, H-6), 2.78(1H, m, H-2 α), 3.68(3H, d, O-Me), 4.58(1H, ddd, H-5). $^{13}\text{C-NMR}$ (CDCl_3 , 600 MHz), δ : 16.4 (C-14), 20.9 (C-15), 30.8 (C-12), 33.3 (C-6), 32.8 (C-3), 33.8 (C-13), 38.4 (C-2), 39.7 (C-4), 134.3 (C-7), 135.2 (C-10), 136.1 (C-8), 151.6 (C-11), 176.1 (C-1/5), 189.3(C-9). EIMS: $m/z = 296[\text{M}]^+$ for formula $\text{C}_{16}\text{H}_{24}\text{O}_5$.



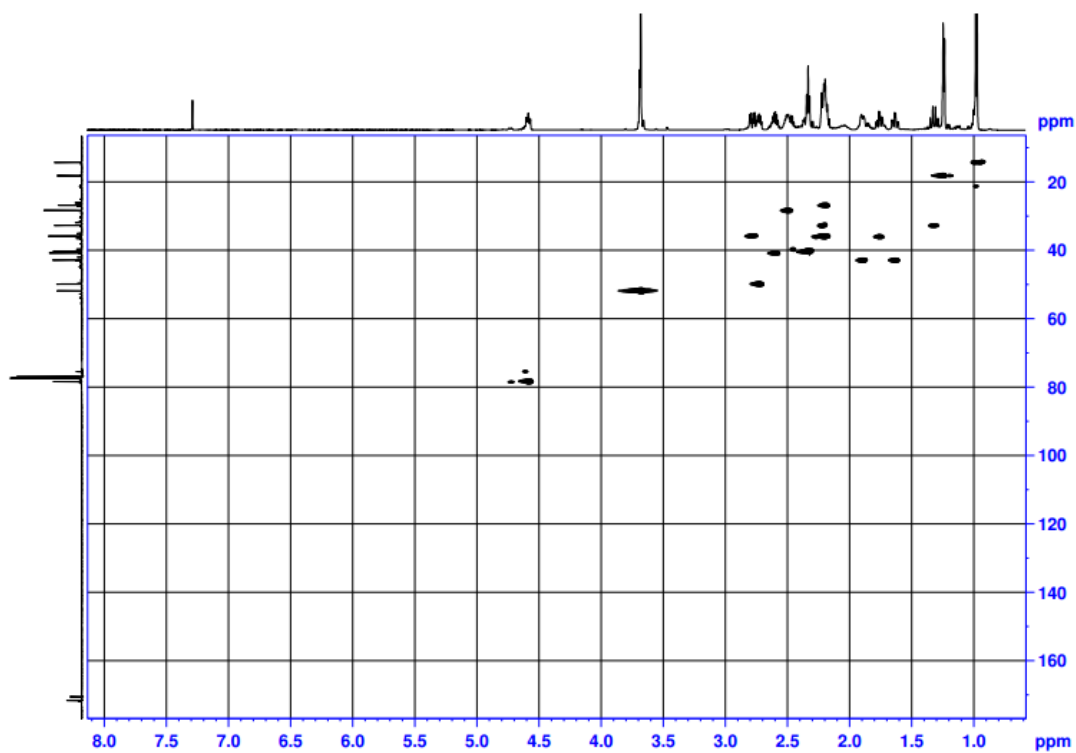
S40: Expansion of the ¹H-NMR Spectrum of Compound 4



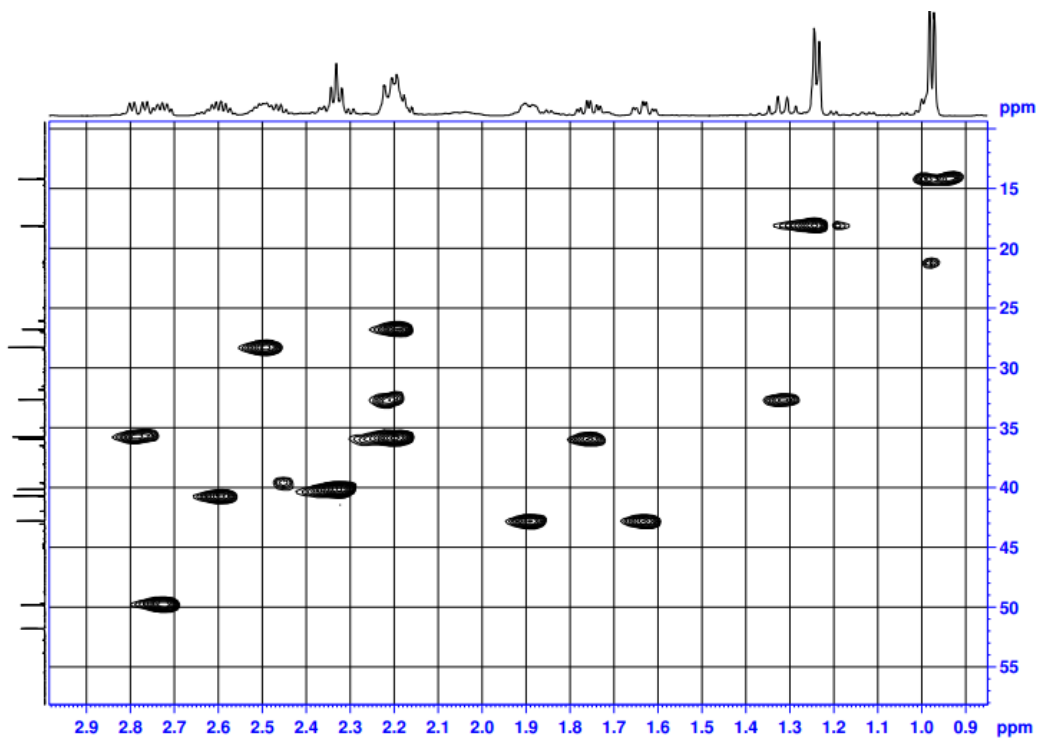
S41: Expansion of the ¹H-NMR Spectrum of Compound 4



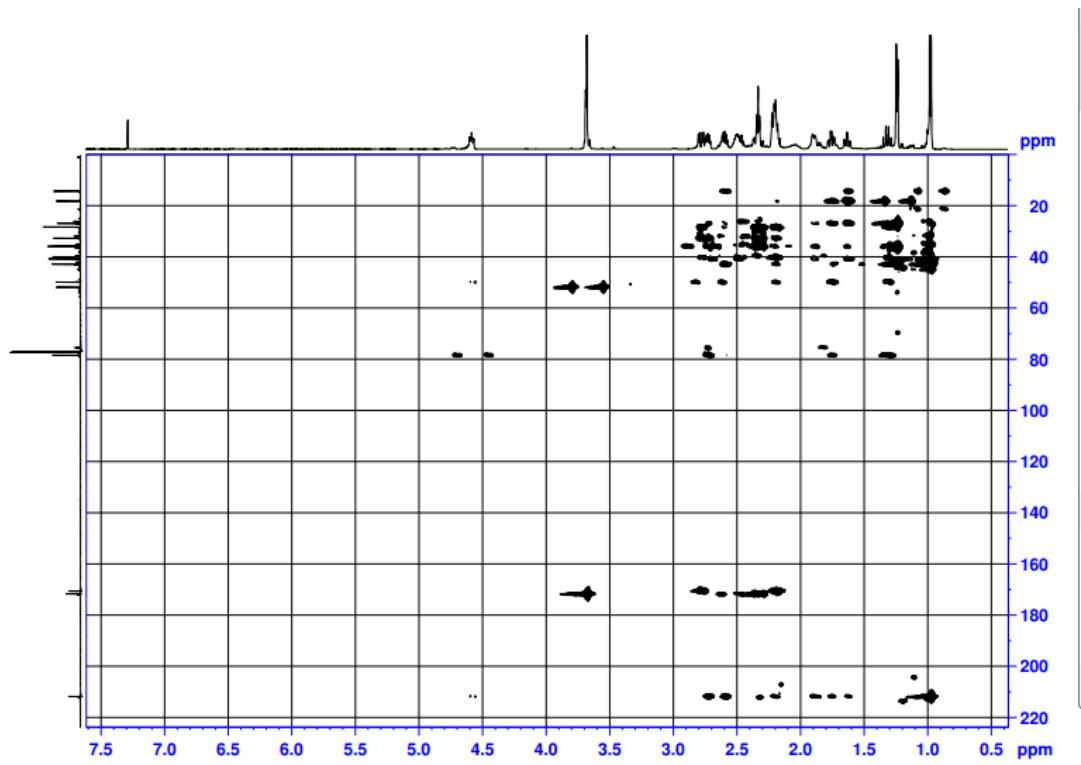
S42: ¹³C-NMR Spectrum (600MHz, CDCl₃) of Compound 4



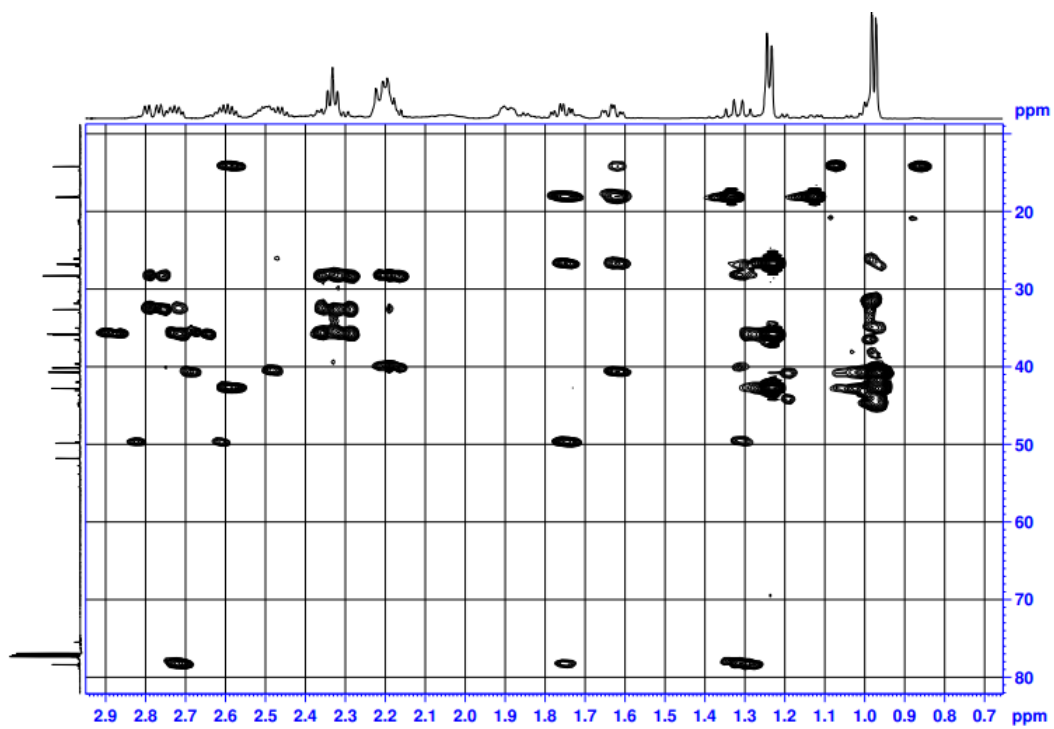
S44: HSQC Spectrum (600MHz, CDCl₃) of Compound **4**



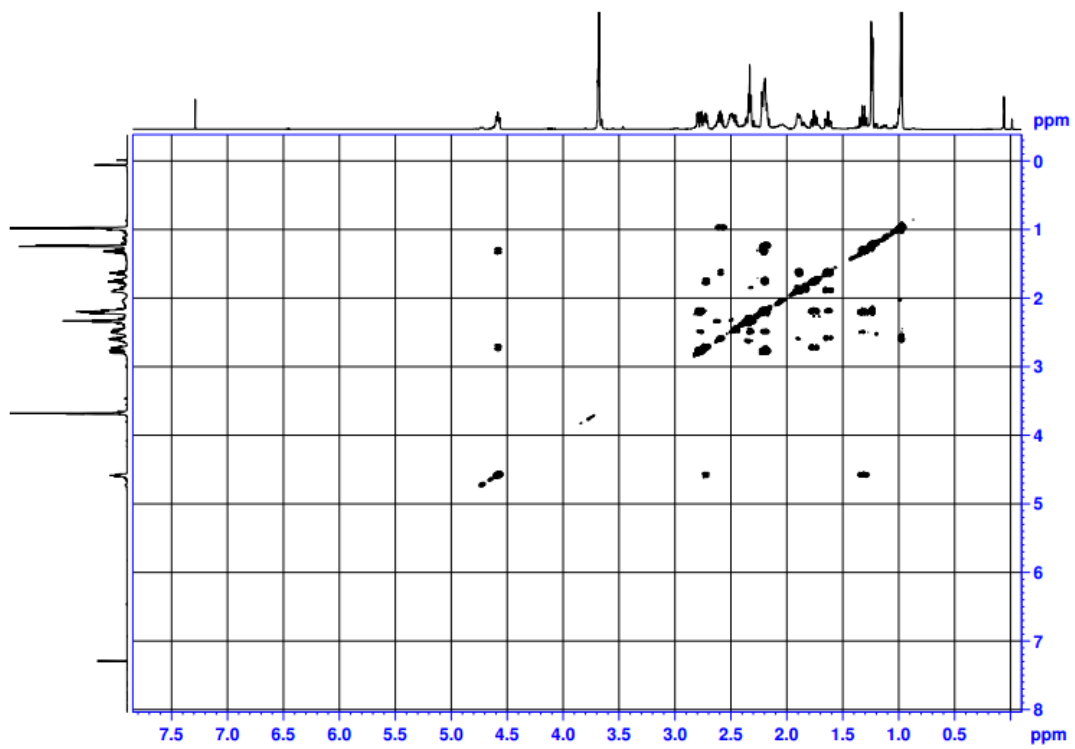
S45: Expansion of the HSQC Spectrum of Compound 4



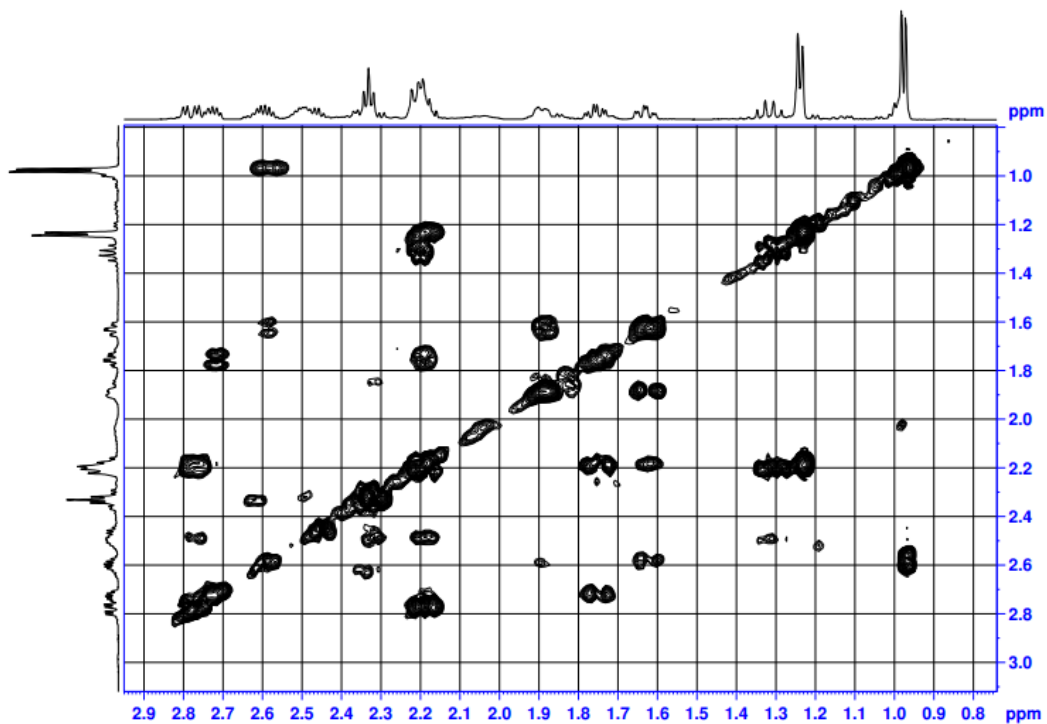
S46: HMBC Spectrum (600MHz, CDCl₃) of Compound 4



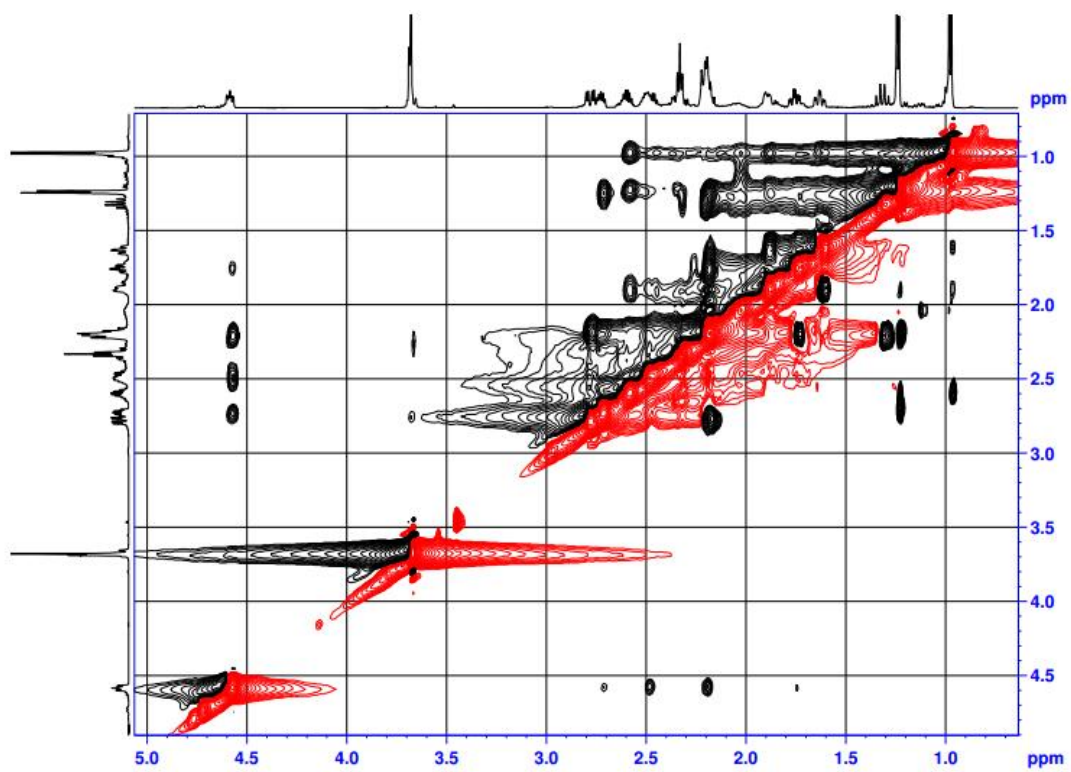
S47: Expansion of the HMBC Spectrum of Compound **4**



S48: ^1H - ^1H COSY Spectrum (600MHz, CDCl_3) of Compound **4**



S49: Expansion of the ^1H - ^1H COSY Spectrum of Compound **4**



S50: NOESY Spectrum (600MHz, CDCl₃) of Compound 4