

Supporting Information

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Polyketides and Alkaloids from the Fungus *Penicillium* sp.

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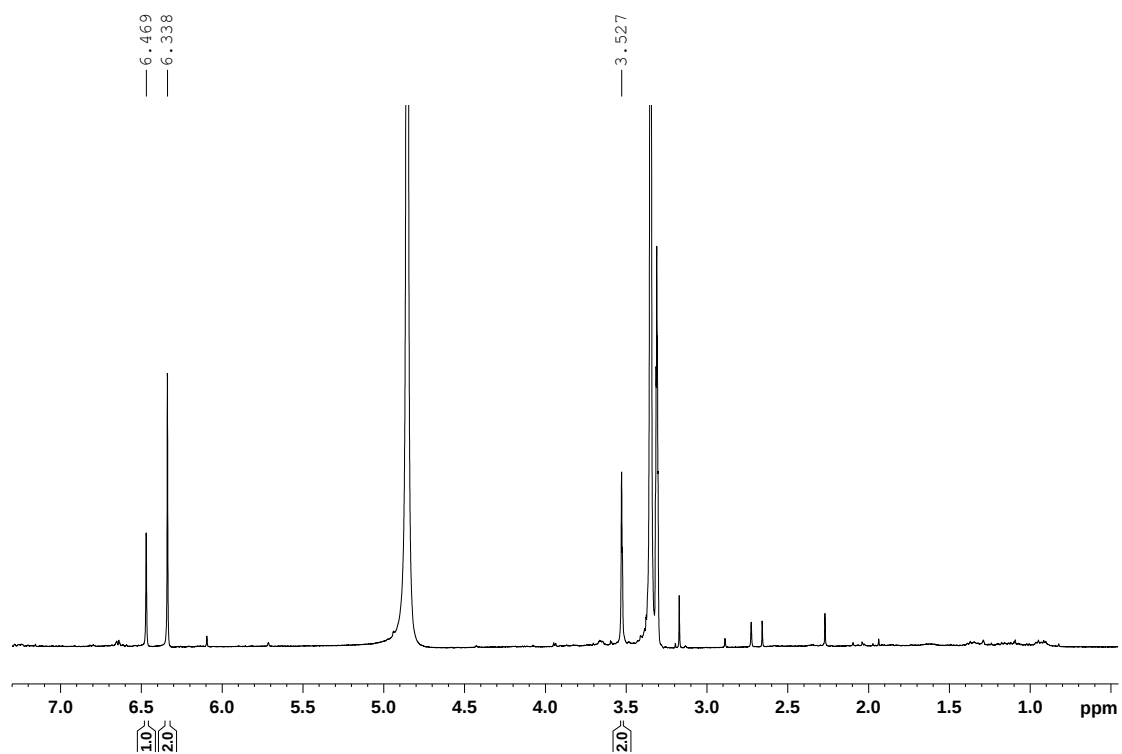


Figure S1: ^1H NMR spectrum of **1** in methanol- d_4 (400 MHz)

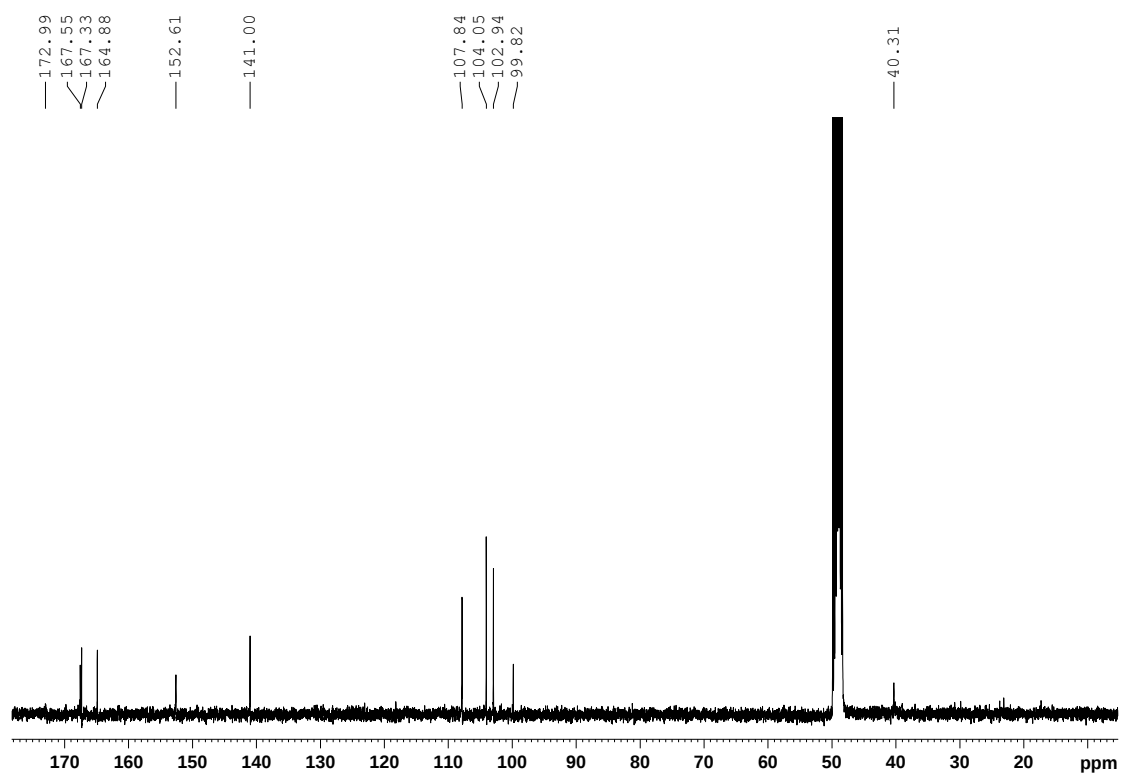


Figure S2: ^{13}C NMR spectrum of **1** in methanol- d_4 (100 MHz)

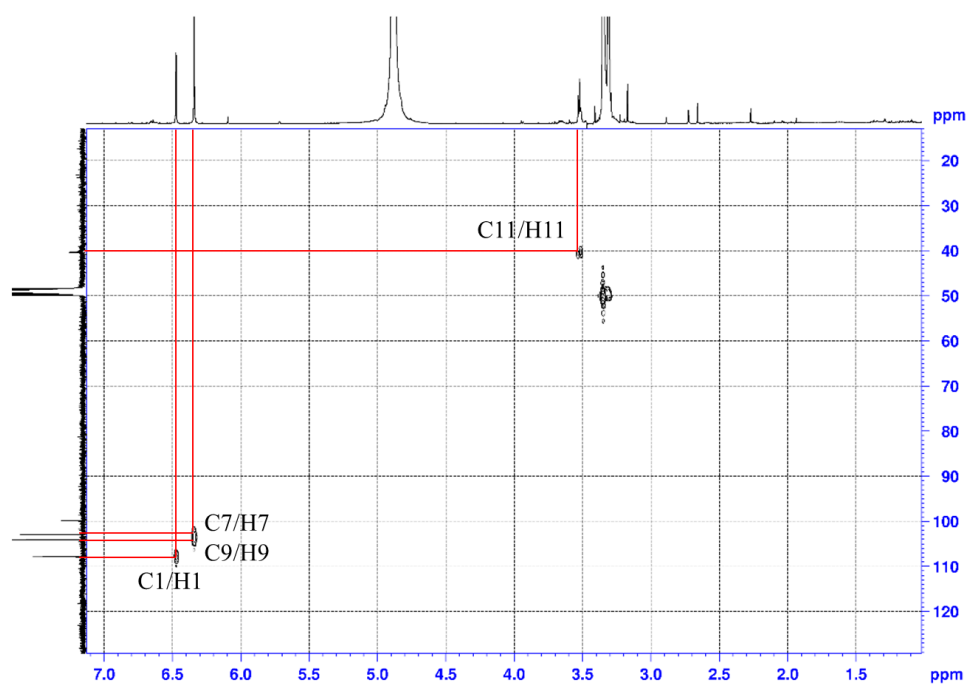


Figure S3: HSQC spectrum of **1** in methanol- d_4 .

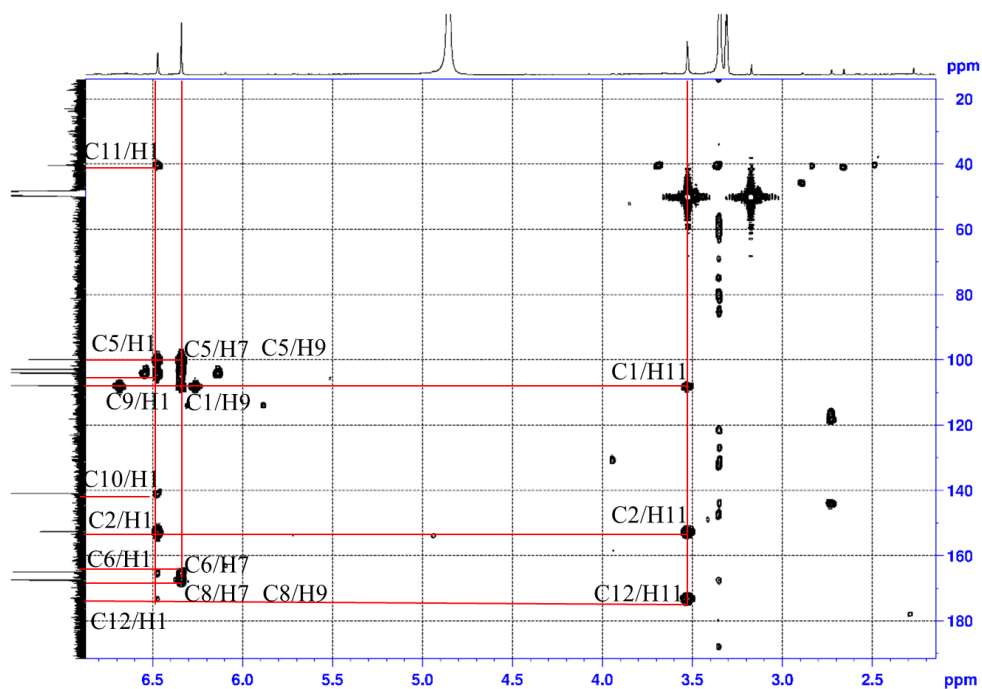


Figure S4: HMBC spectrum of **1** in methanol- d_4 .

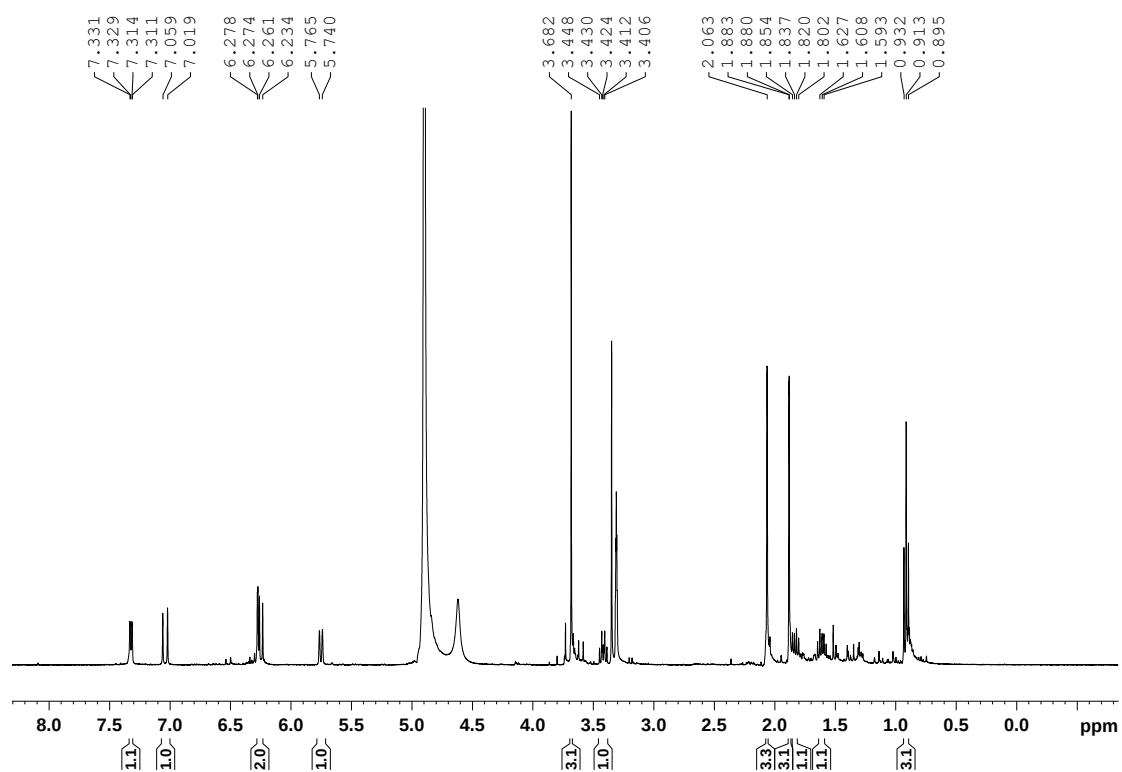


Figure S5: ¹H NMR spectrum of **2** in methanol-*d*₄ (400 MHz)

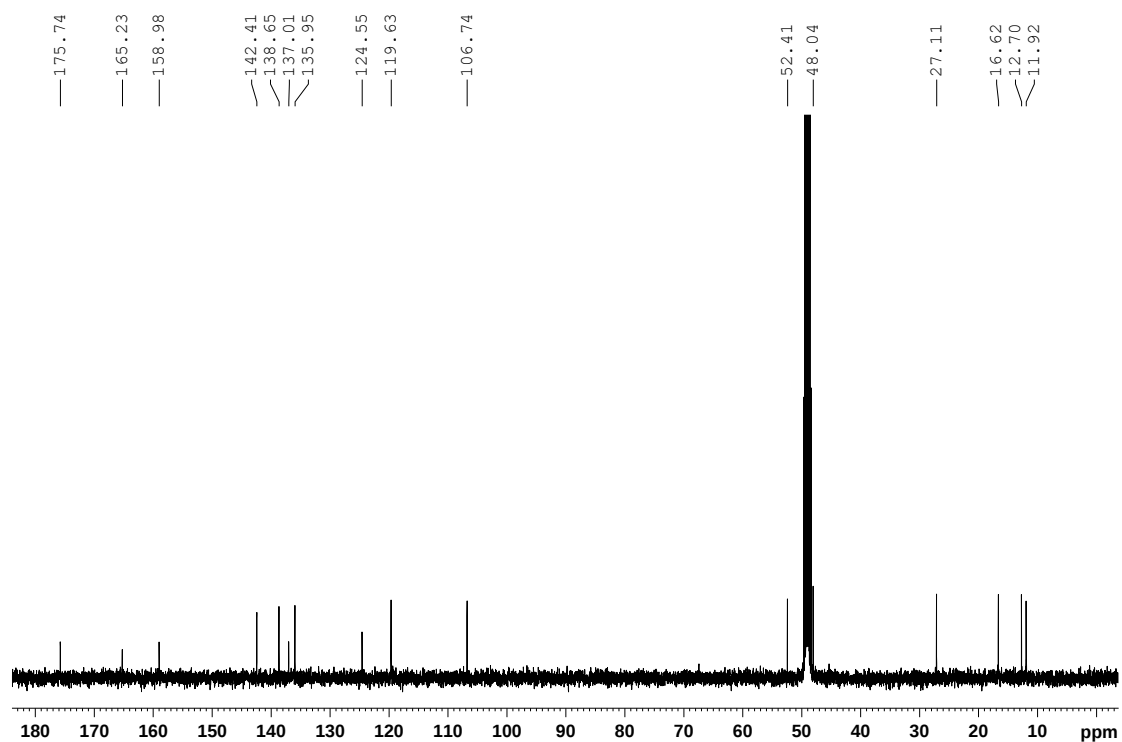


Figure S6: ¹³C NMR spectrum of **2** in methanol-*d*₄ (100 MHz)

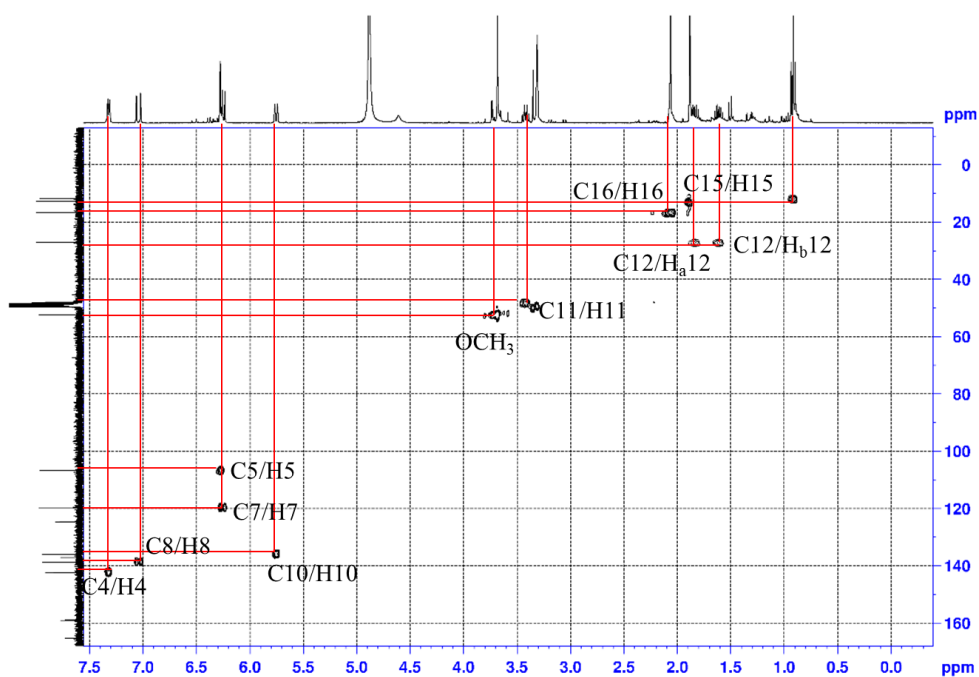


Figure S7: HSQC spectrum of **2** in methanol- d_4

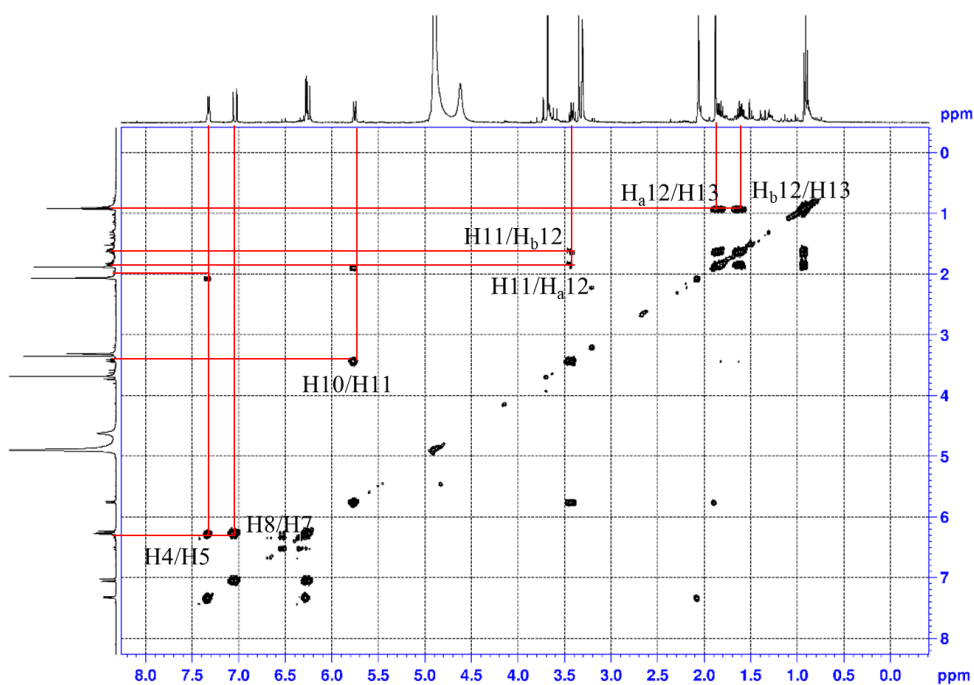


Figure S8: ^1H - ^1H COSY spectrum of **2** in methanol- d_4

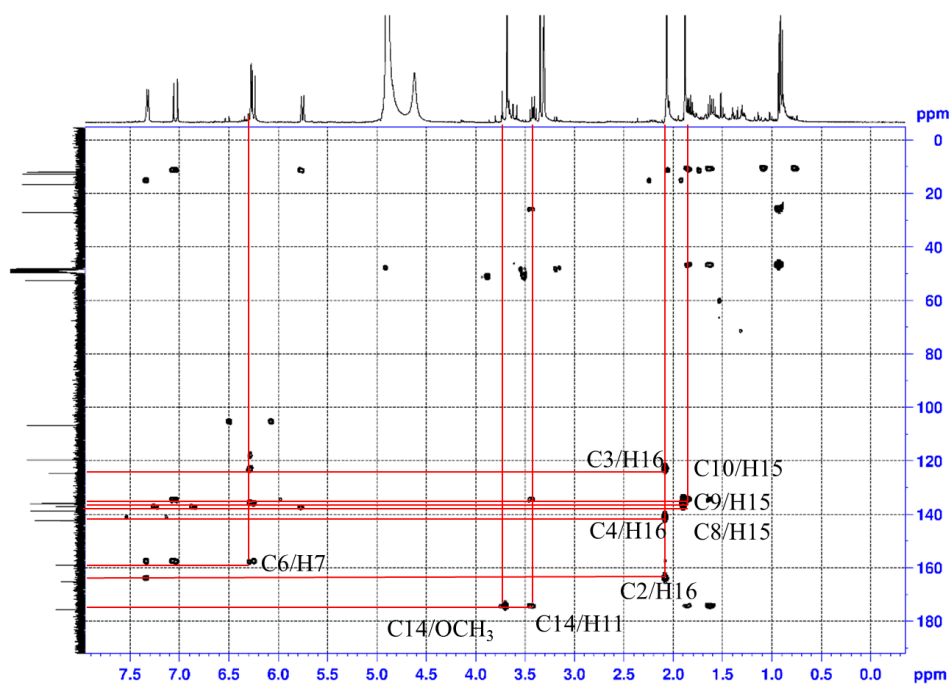


Figure S9: HMBC spectrum of **2** in methanol- d_4

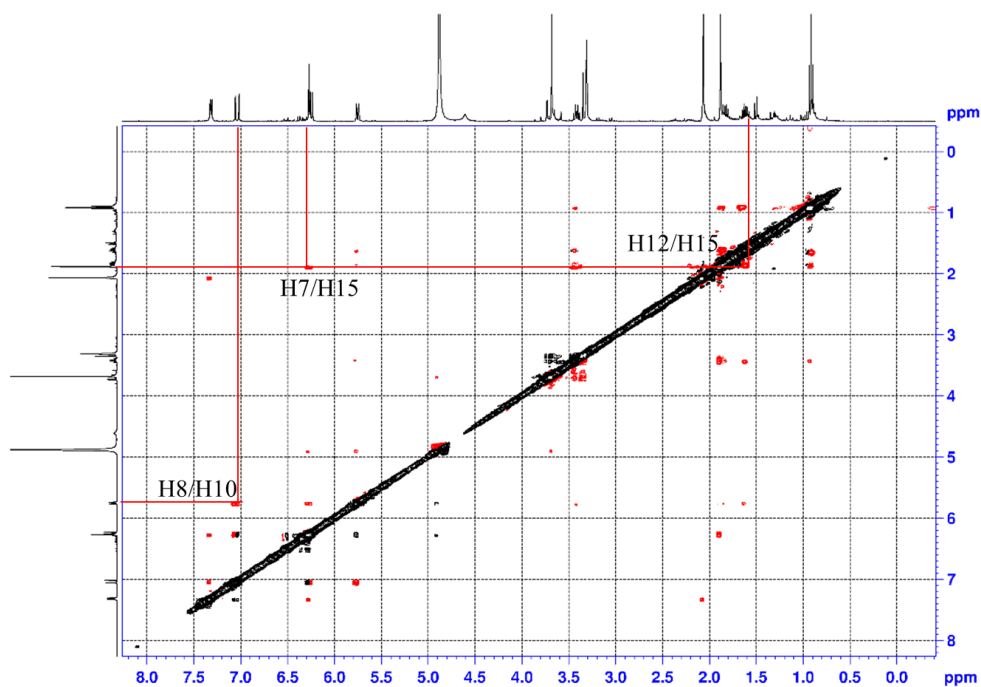


Figure S10: NOESY spectrum of **2** in methanol- d_4

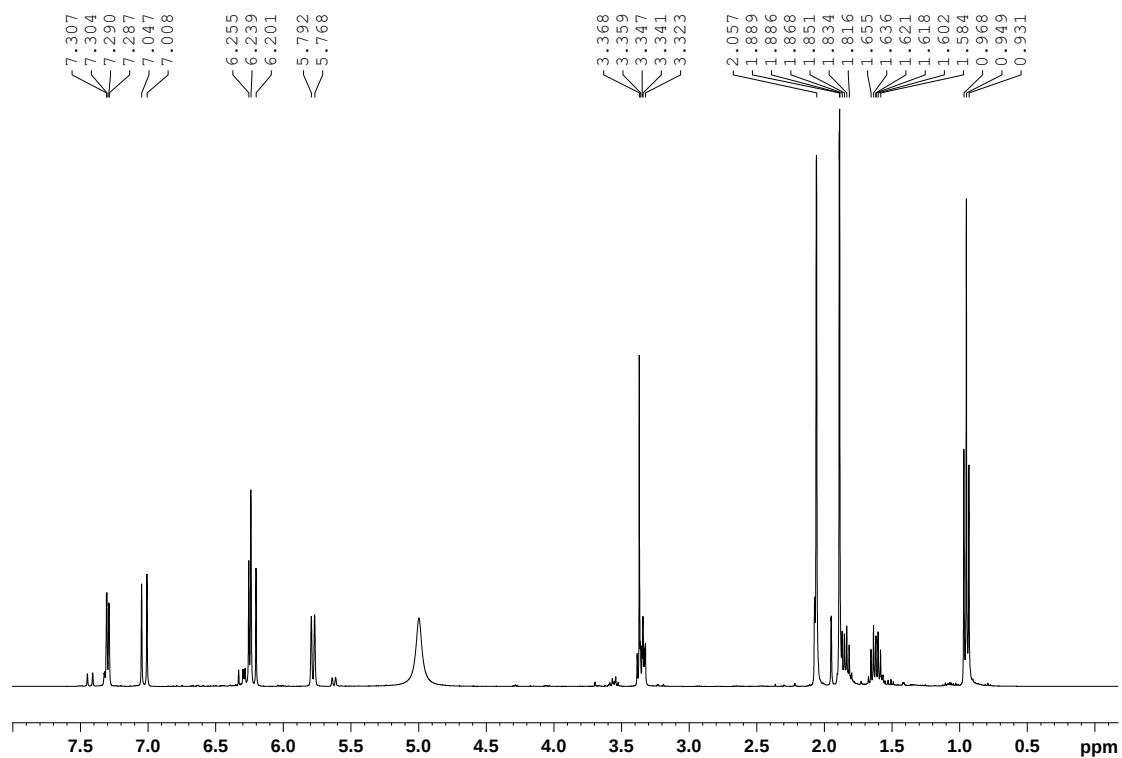


Figure S11: ^1H NMR spectrum of **3** in methanol- d_4 (400 MHz)

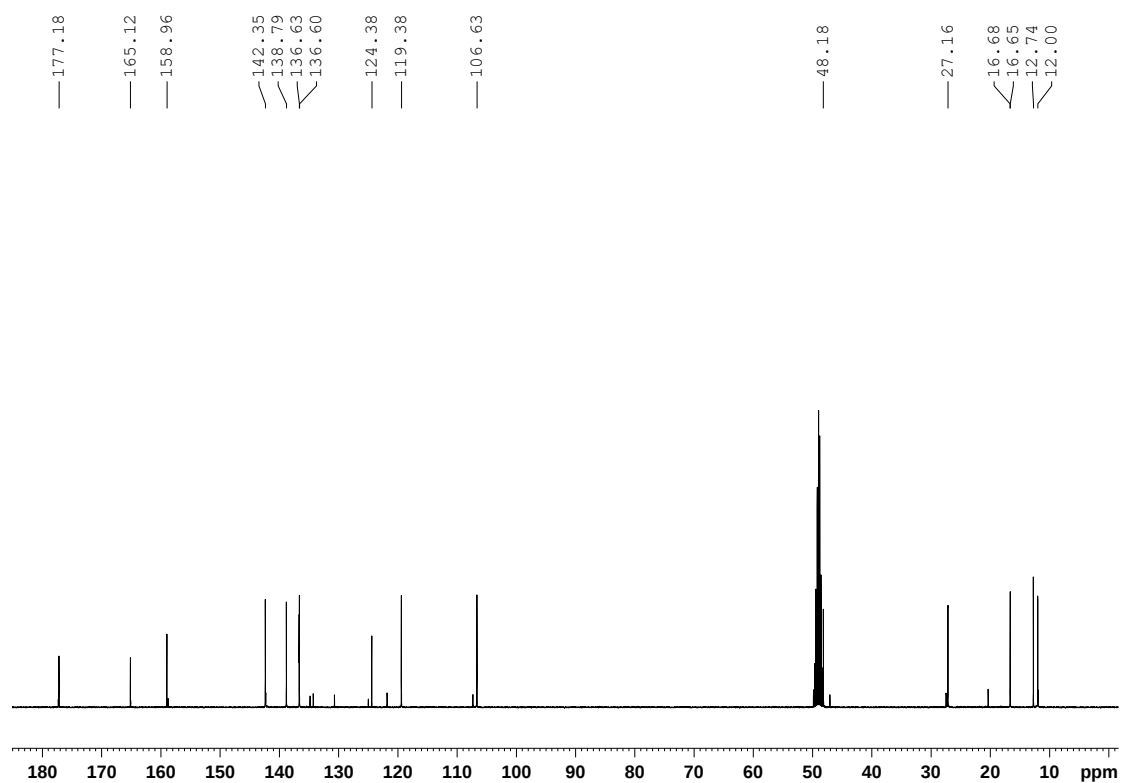
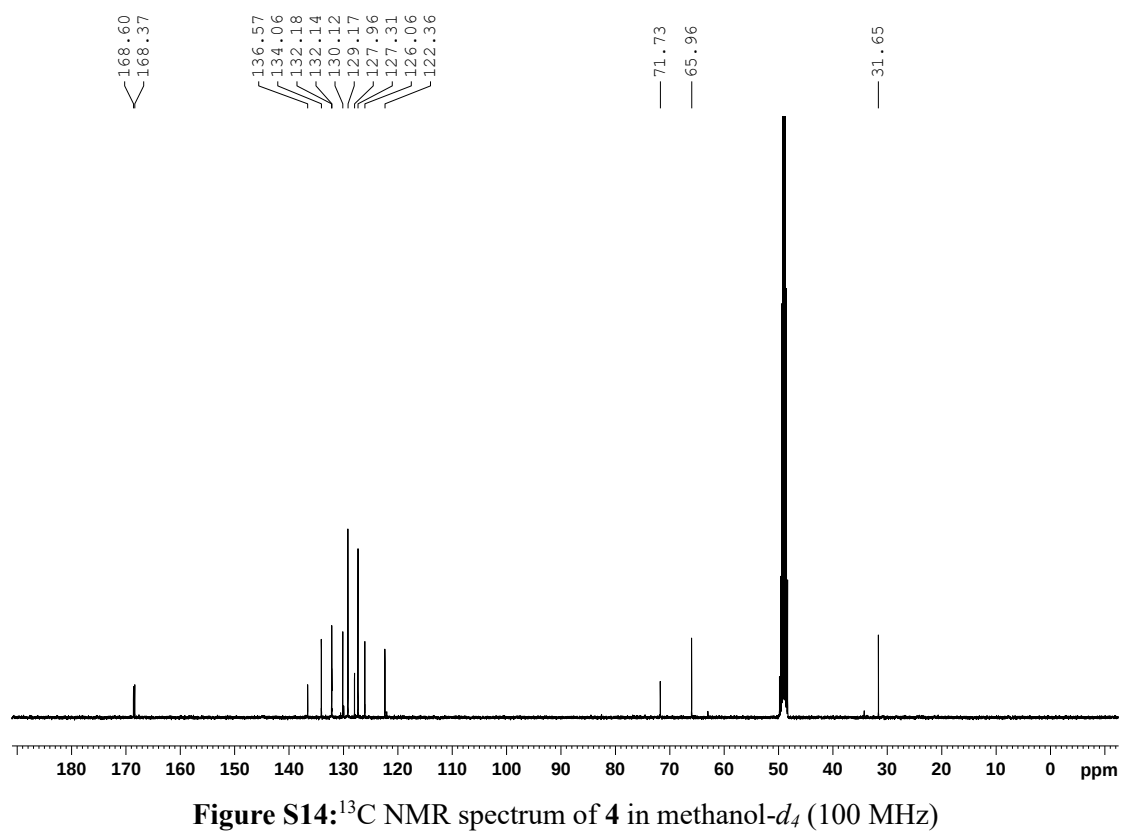
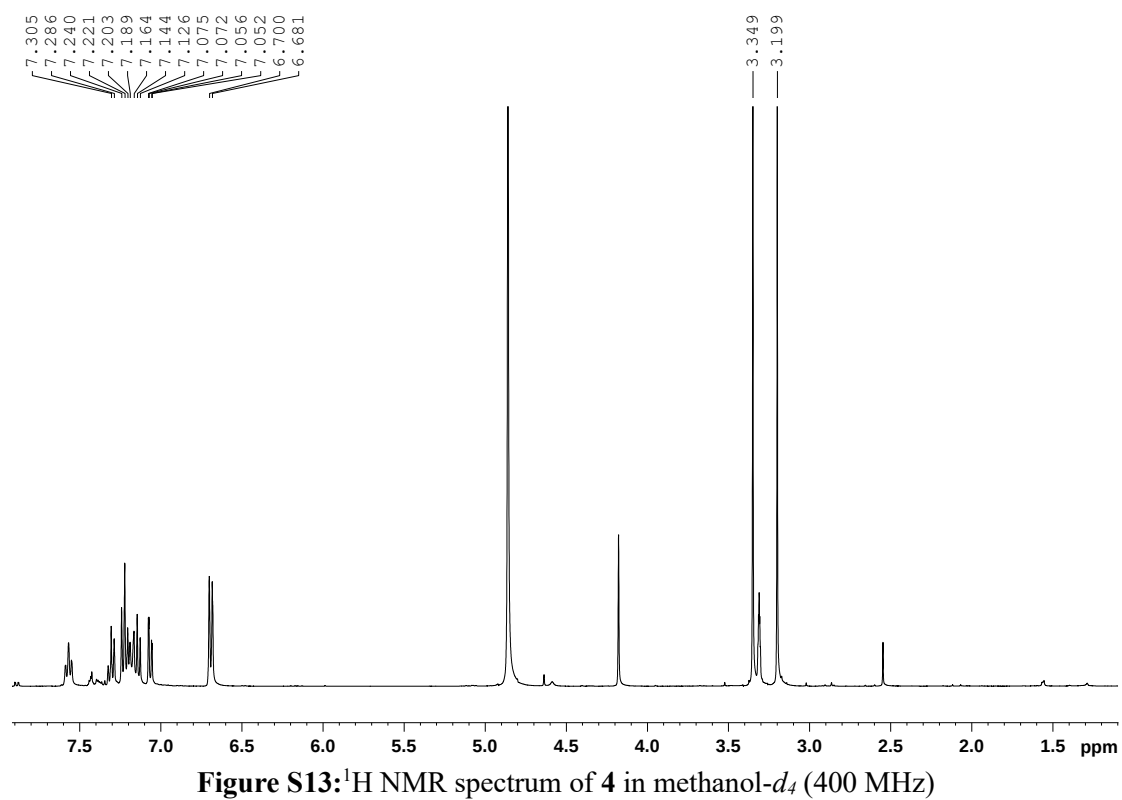


Figure S12: ^{13}C NMR spectrum of **3** in methanol- d_4 (100 MHz)



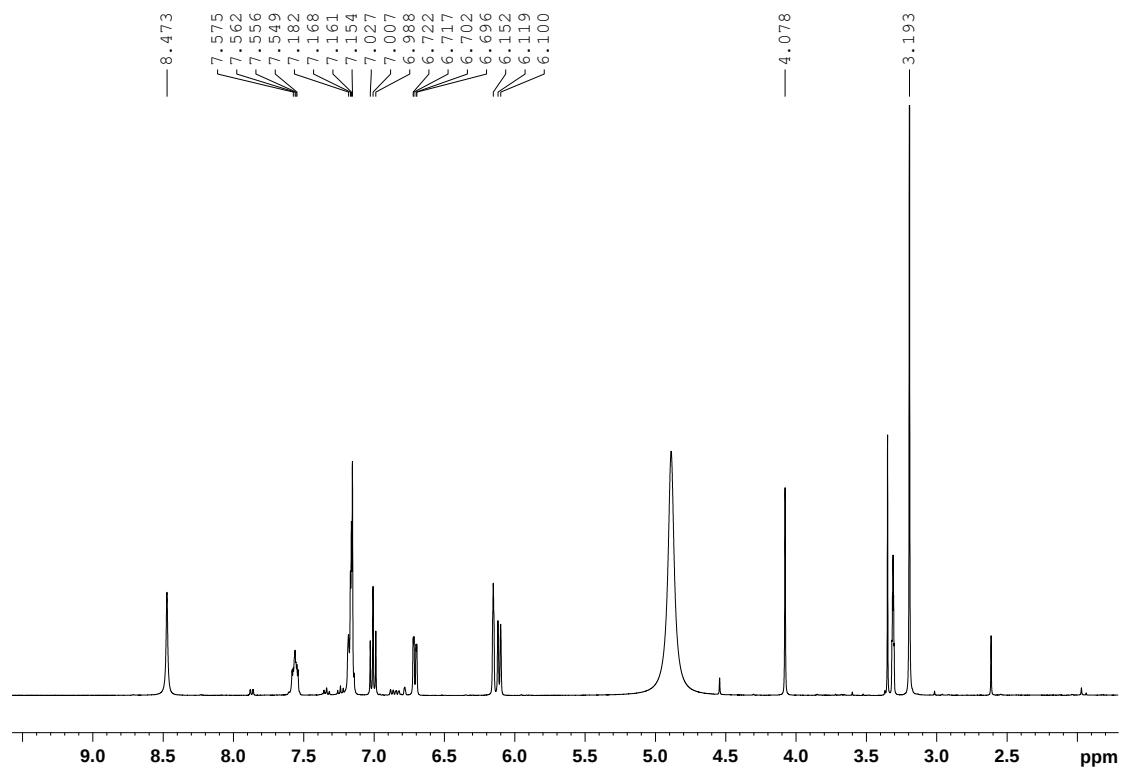


Figure S15: ^1H NMR spectrum of **5** in methanol- d_4 (400 MHz)

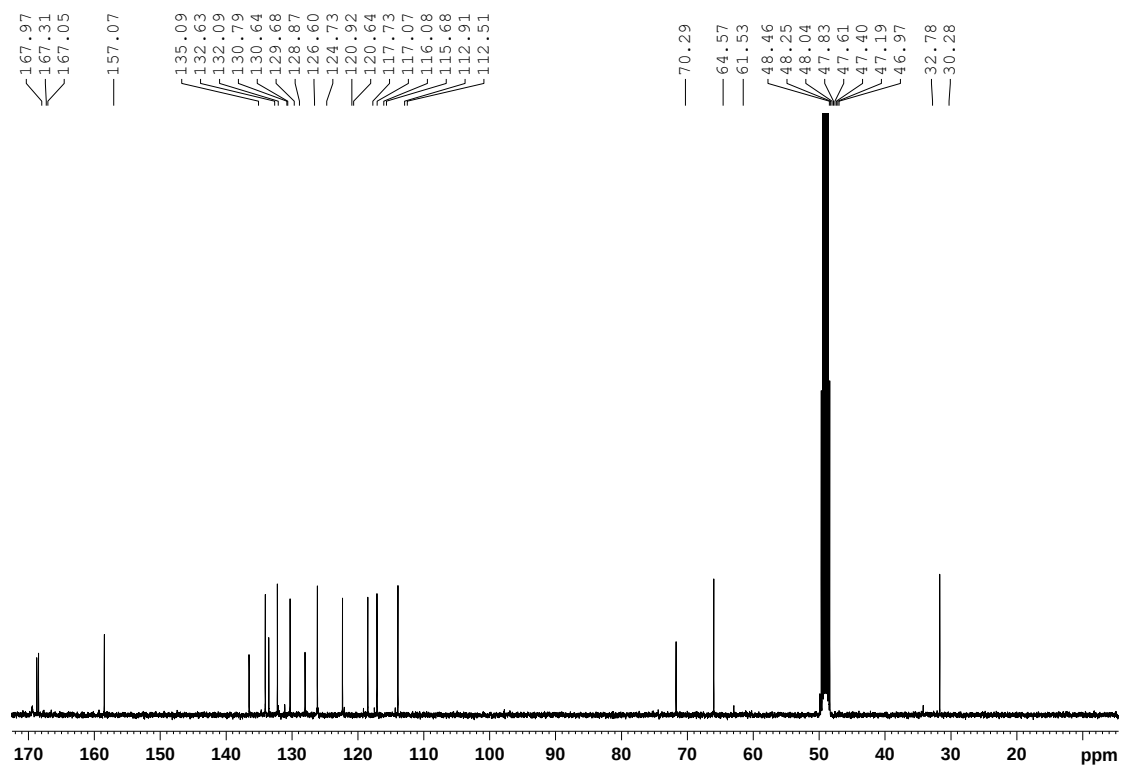


Figure S16: ^{13}C NMR spectrum of **5** in methanol- d_4 (100 MHz)

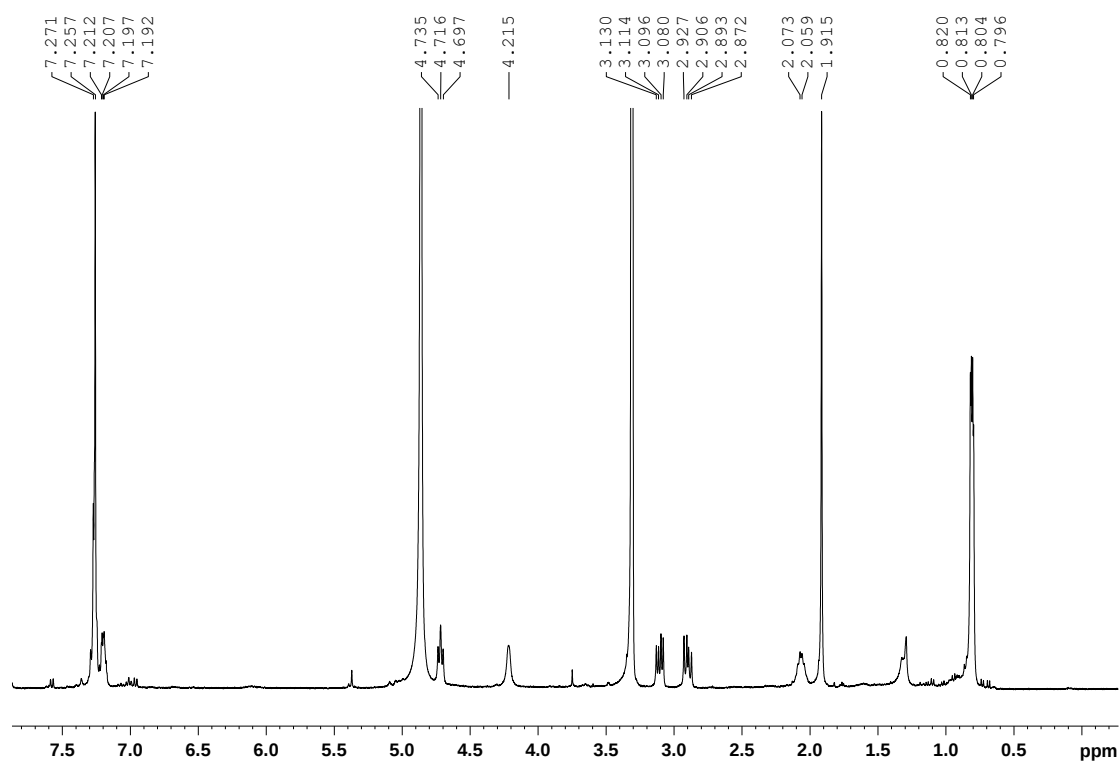


Figure S17: ¹H NMR spectrum of **6** in methanol-*d*₄ (400 MHz)

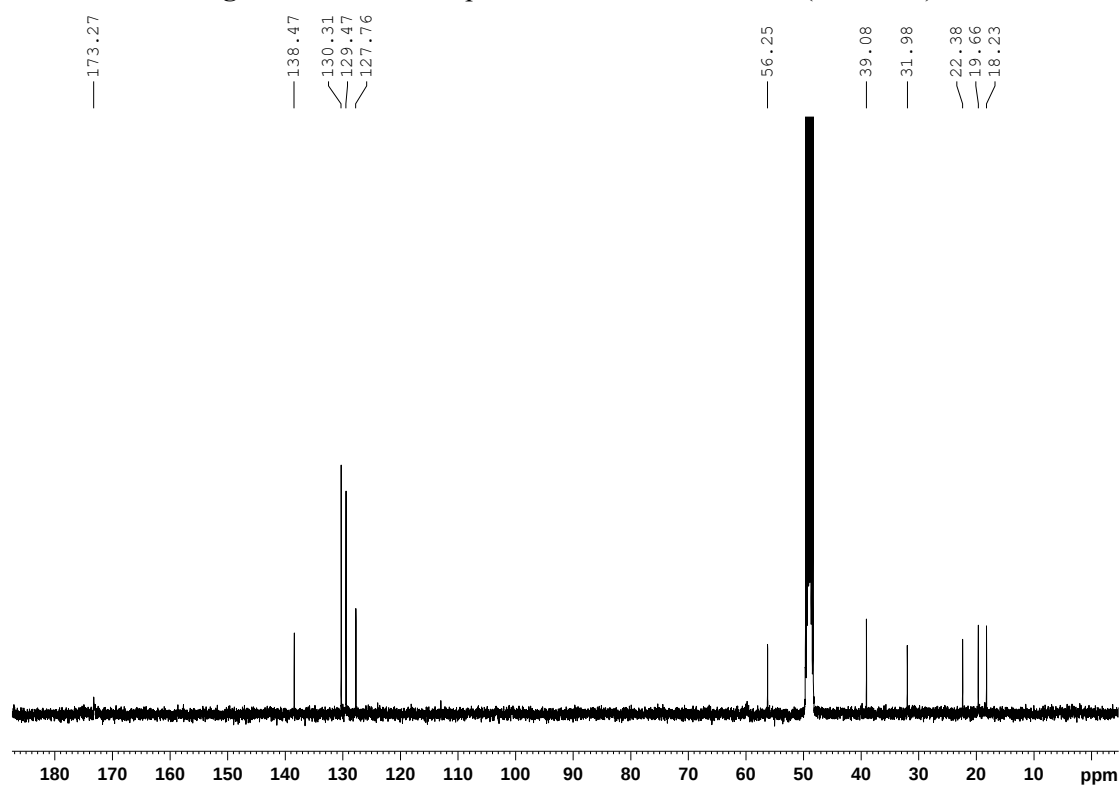


Figure S18: ¹³C NMR spectrum of **6** in methanol-*d*₄ (100 MHz)

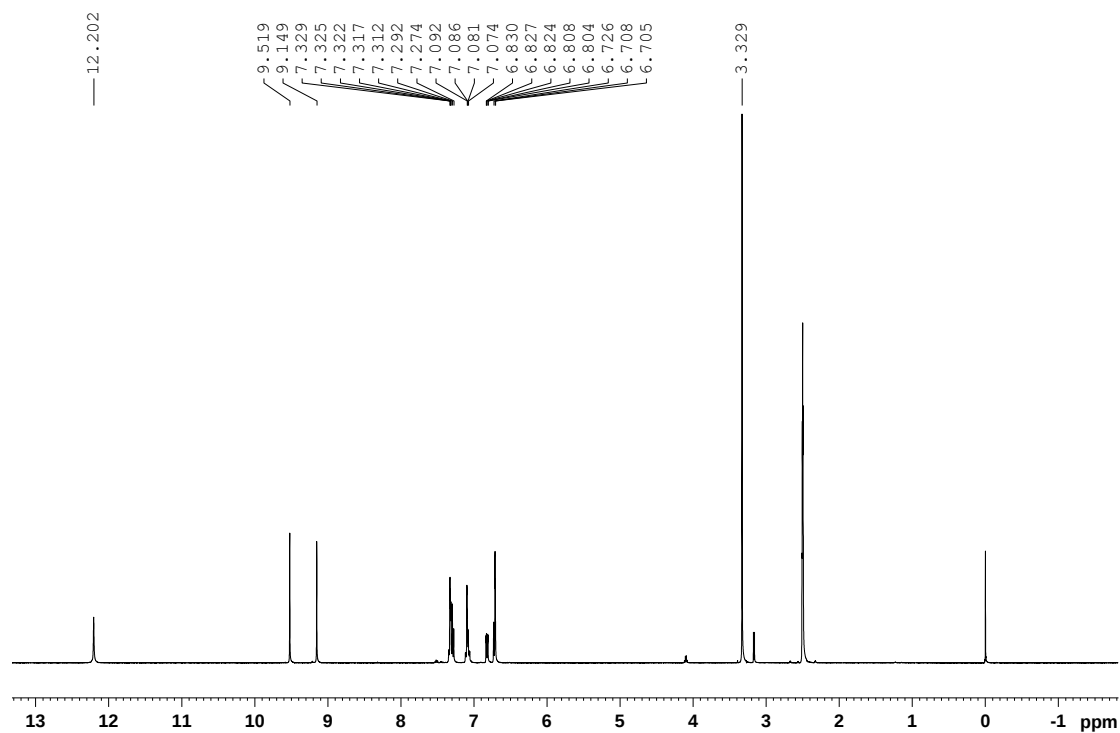


Figure S19: ^1H NMR spectrum of **7** in $\text{DMSO-}d_6$ (400 MHz)

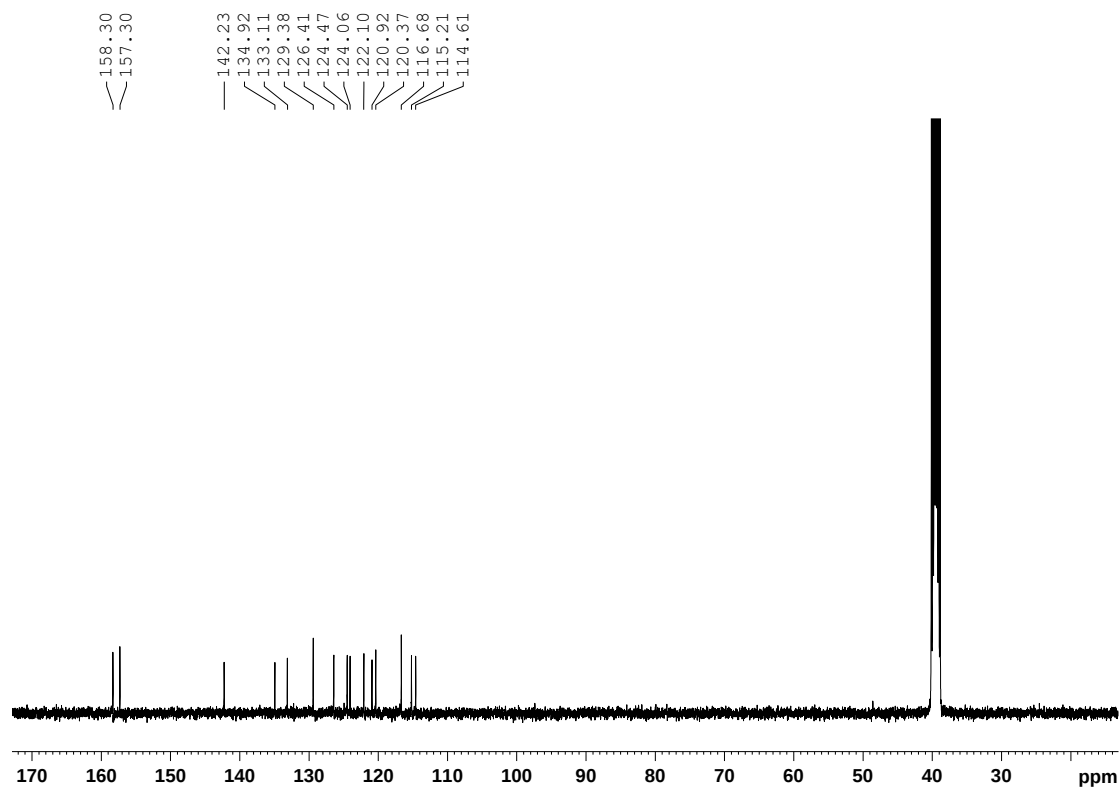


Figure S20: ^{13}C NMR spectrum of **7** in $\text{DMSO-}d_6$ (100 MHz)

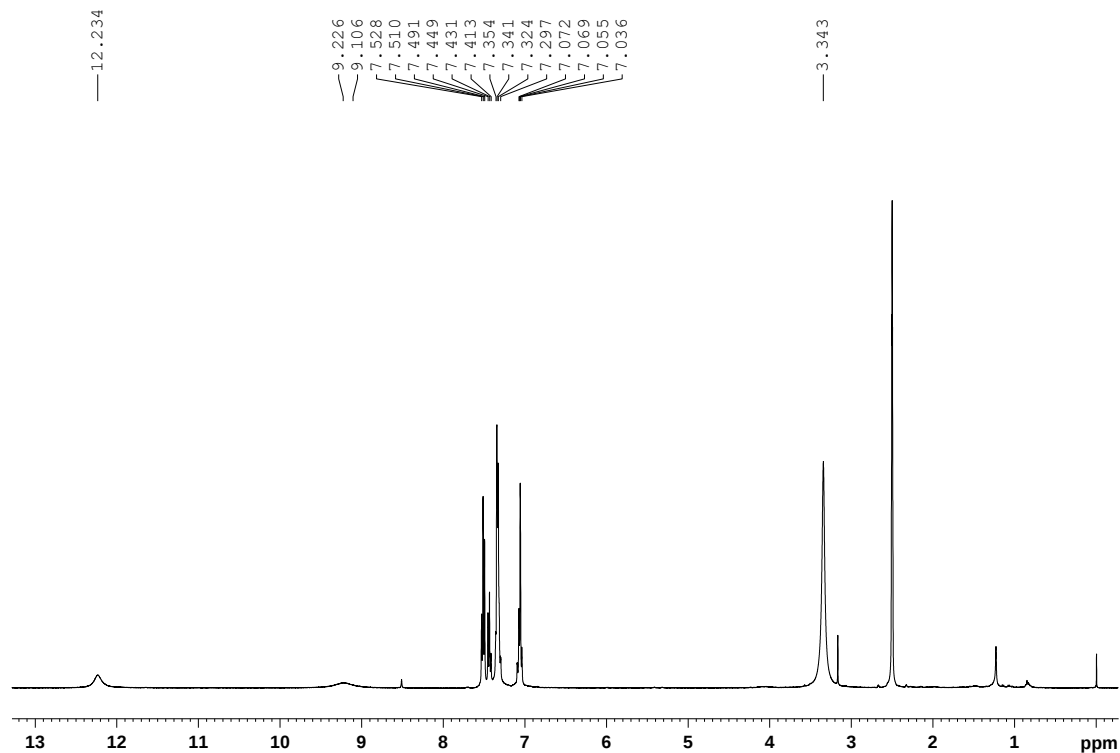


Figure S21: ^1H NMR spectrum of **8** in $\text{DMSO-}d_6$ (400 MHz)

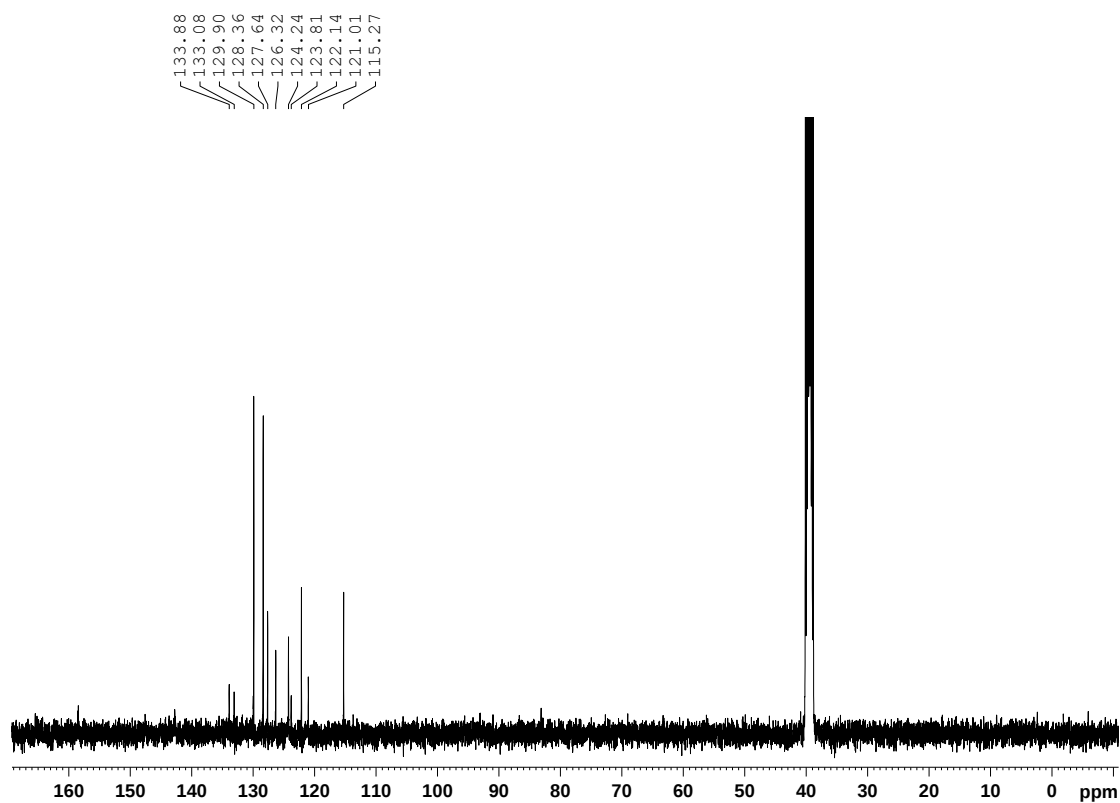


Figure S22: ^{13}C NMR spectrum of **8** in $\text{DMSO-}d_6$ (100 MHz)

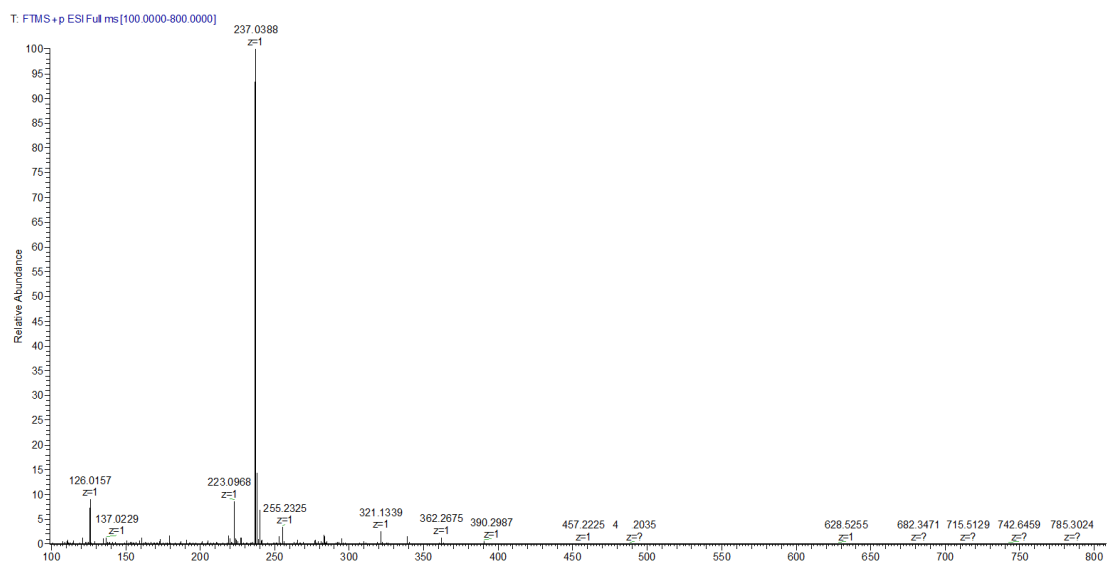


Figure S23: HRESIMS spectrum of 1

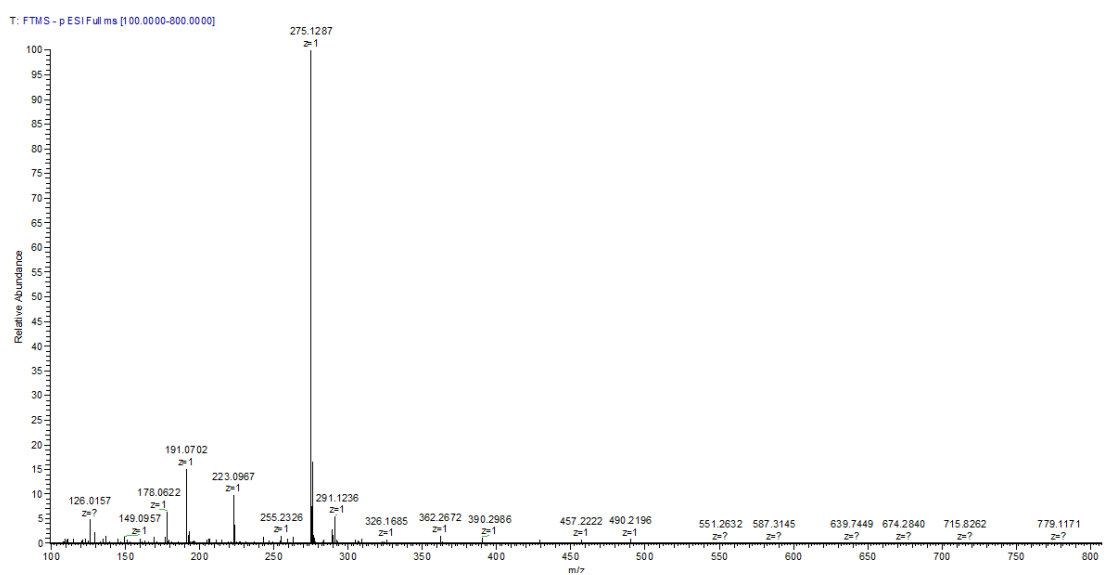


Figure S24: HRESIMS spectrum of 1

Chemical Structure similarity

REFERENCES

Research Topic
Author Name
Company Name
Document Identifier
Journal
Patent
Tags

SUBSTANCES

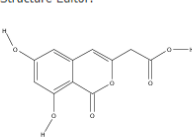
Chemical Structure
Markush
Molecular Formula
Property
Substance Identifier

REACTIONS

Reaction Structure

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Chemical Structure similarity

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☐ 95-98	1
☐ 90-94	8
☐ 85-89	9
☐ 80-84	36
☐ 75-79	120
☐ 70-74	334
☐ 65-69	734
☐ 0-64 (least similar)	3414

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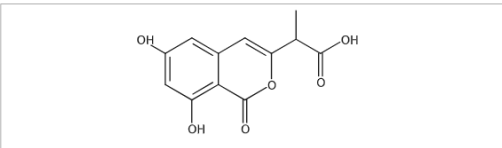
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Sort by: Similarity Score

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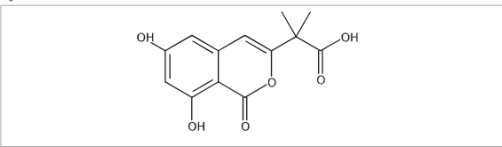
1. **215534-92-2**



C₁₂H₁₀O₆
1,7,2-Benzopyran-3-acetic acid, 6,8-dihydroxy-6-methoxy-1-oxo-
[Key Physical Properties](#)

Score: 93

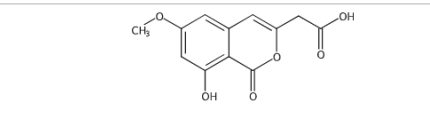
3. **215534-93-3**



C₁₃H₁₂O₆
1,7,2-Benzopyran-3-acetic acid, 6,8-dihydroxy-6-methoxy-1-oxo-
[Key Physical Properties](#)

Score: 93

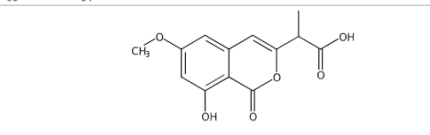
2. **181428-16-0**



C₁₂H₁₀O₆
1,7,2-Benzopyran-3-acetic acid, 8-hydroxy-6-methoxy-1-oxo-
[Key Physical Properties](#)

Score: 92

4. **181427-78-1**



C₁₃H₁₂O₆
1,7,2-Benzopyran-3-acetic acid, 8-hydroxy-6-methoxy-1-oxo-
[Key Physical Properties](#)

Figure S25: Scifinder similarity report of compound 1

REFERENCES

- Research Topic
- Author Name
- Company Name
- Document Identifier
- Journal
- Patent
- Tags

SUBSTANCES

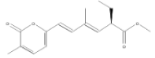
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- Substance Identifier

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☐ 95-98	0
☐ 90-94	0
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☐ 80-84	3
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Properties: 3

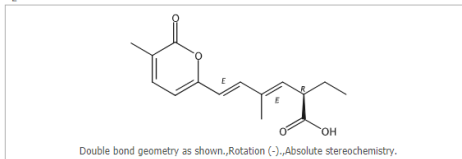
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Preparation: 2

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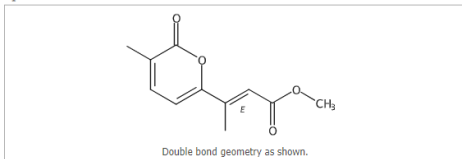
Score: 88
1. **1638619-04-1**



Double bond geometry as shown, Rotation (-), Absolute stereochemistry.

C₁₅H₁₈O₄
3,5-Hexadienoic acid, 2-ethyl-4-methyl-6-(3-methyl-2-oxo-2H-pyran-6-yl)-, (2*R*,3*E*,5*E*)-
[Key Physical Properties](#)

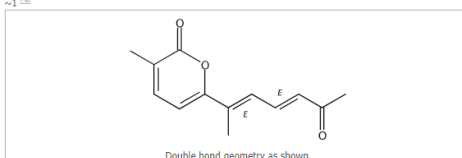
Score: 83
2. **146446-09-5**



Double bond geometry as shown.

C₁₁H₁₂O₄
2-Butenoic acid, 3-(3-methyl-2-oxo-2H-pyran-6-yl)-, methyl ester, (*E*)- (9CI)
[Key Physical Properties](#)
[Spectra](#)

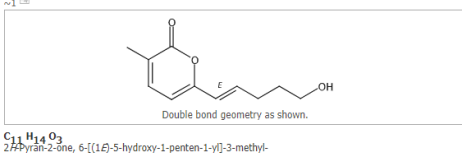
Score: 80
3. **1426258-86-7**



Double bond geometry as shown.

C₁₃H₁₄O₃

Score: 80
4. **2143532-33-4**



Double bond geometry as shown.

C₁₃H₁₄O₃
2-Pyran-2-one, 6-[(1*E*)-5-hydroxy-1-penten-1-yl]-3-methyl-
[Key Physical Properties](#)

Figure S26: Scifinder similarity report of compound 2

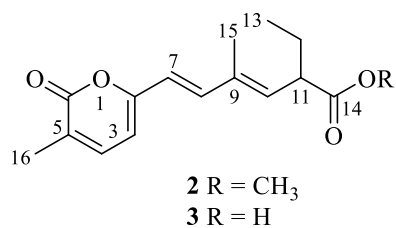
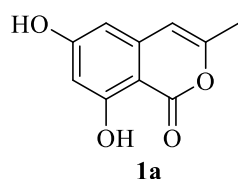
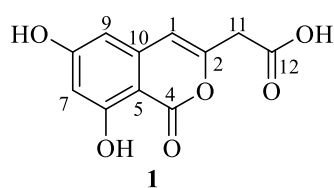


Table S1: NMR data of new compounds **1** and **2** and the similar compounds **1a** and **3**

No.	1		1a		2		3	
	δ_H	δ_C	δ_H	δ_C	δ_H	δ_C	δ_H	δ_C
1	6.47, br s	107.8	6.47	102.1				
2		152.6		155.7		165.2		165.1
3						124.6		124.4
4		167.3		166.9	7.32, d (6.9)	142.4	7.30, d (6.9)	142.3
5		99.8		99.8	6.26, d (6.9)	106.7	6.25, d (6.9)	106.6
6		164.6		165.0		159.0		159.0
7	6.34, br s	102.9	6.30	103.8	6.25, d (15.8)	119.6	6.23, d (15.8)	119.4
8		167.5		167.0	7.04, d (15.8)	138.7	7.04, d (15.8)	138.8
9	6.34, br s	104.0	6.33	105.9		137.0		136.6
10		141.0		141.8	5.75, d (9.9)	136.0	5.78, d (9.8)	136.6
11	3.52, br s	40.3	2.22	19.0	3.42, ddd (9.9, 7.2, 7.2)	48.0	3.34, ddd (9.8, 7.2, 7.2)	47.1
12		173.0			1.83, m 1.61, m	27.1	1.83, m 1.61, m	27.2
13					0.93, t (7.4)	11.9	0.94, t (7.4)	12.0
14						175.7		177.2
15					1.88, s	12.7	1.89, s	12.7
16					2.06, s	16.6	2.06, s	16.7
OCH ₃					3.70, s	52.4		