

Supporting Information

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Polyketides and Alkaloids from the Fungus *Penicillium* sp.

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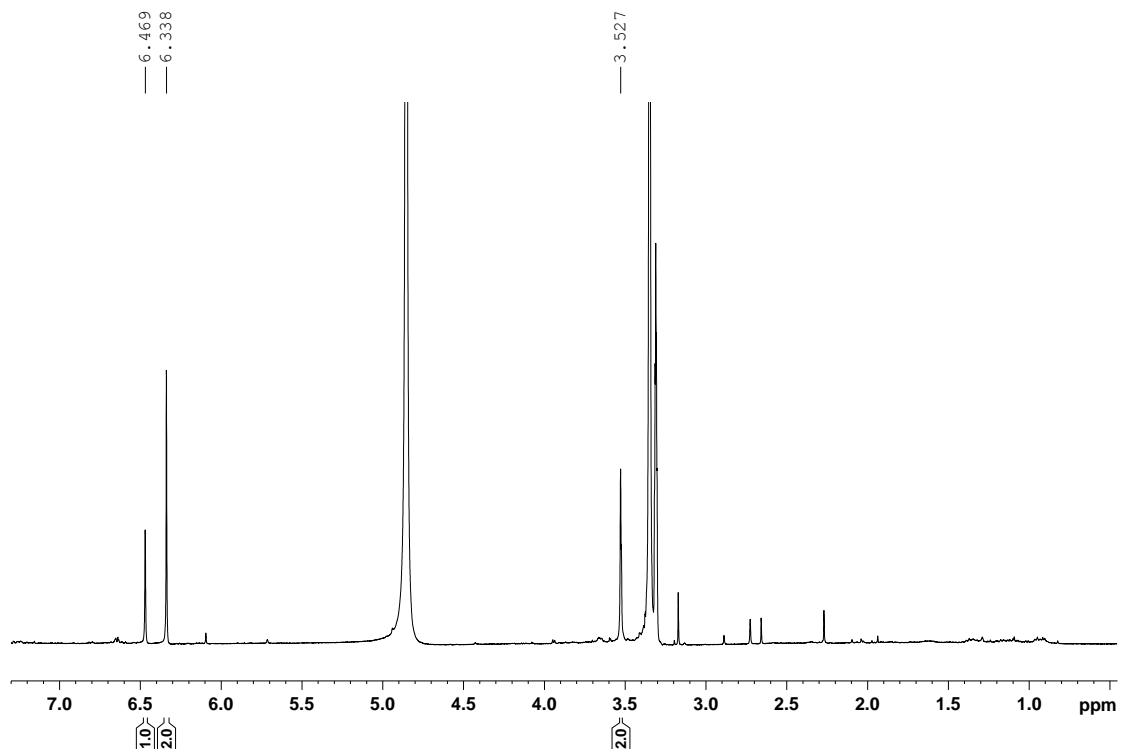


Figure S1: ^1H NMR spectrum of **1** in methanol- d_4 (400 MHz)

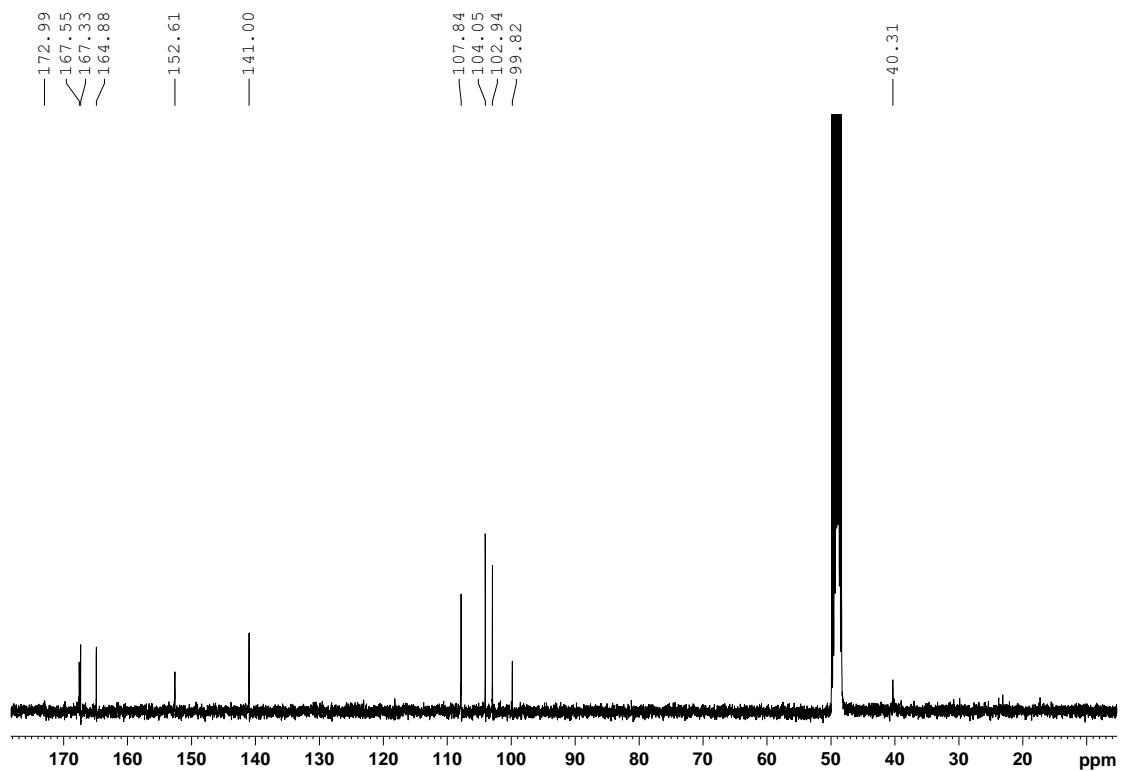


Figure S2: ^{13}C NMR spectrum of **1** in methanol- d_4 (100 MHz)

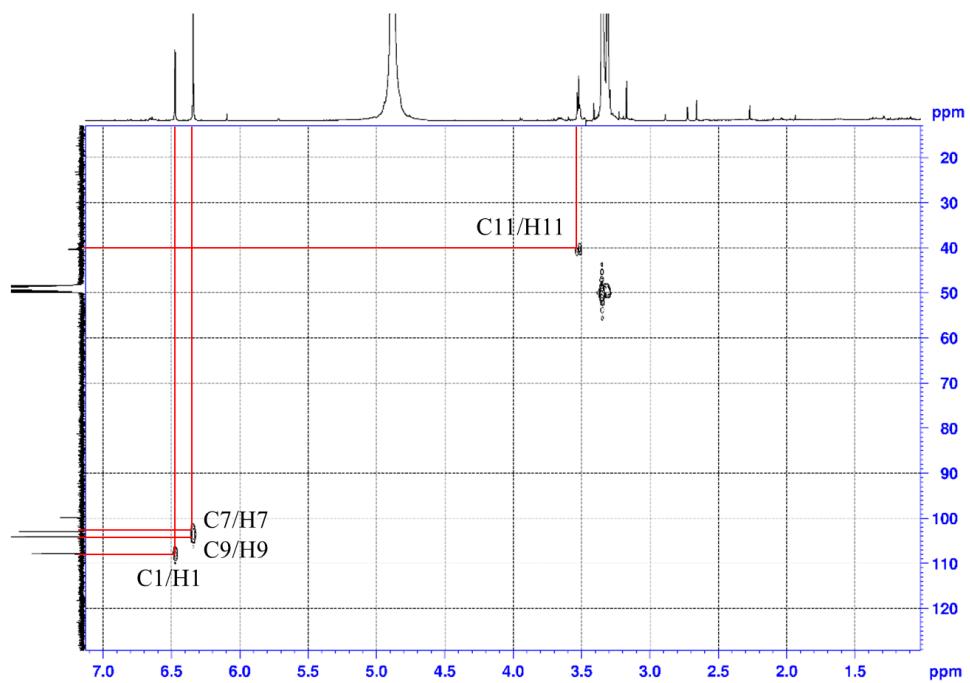


Figure S3: HSQC spectrum of **1** in methanol-*d*₄.

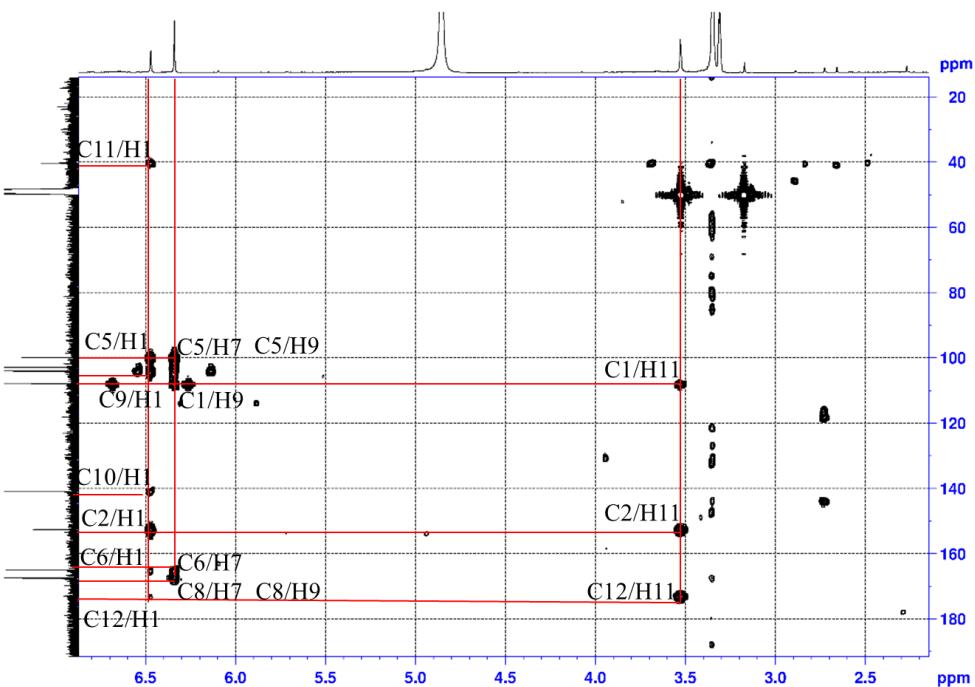


Figure S4: HMBC spectrum of **1** in methanol-*d*₄.

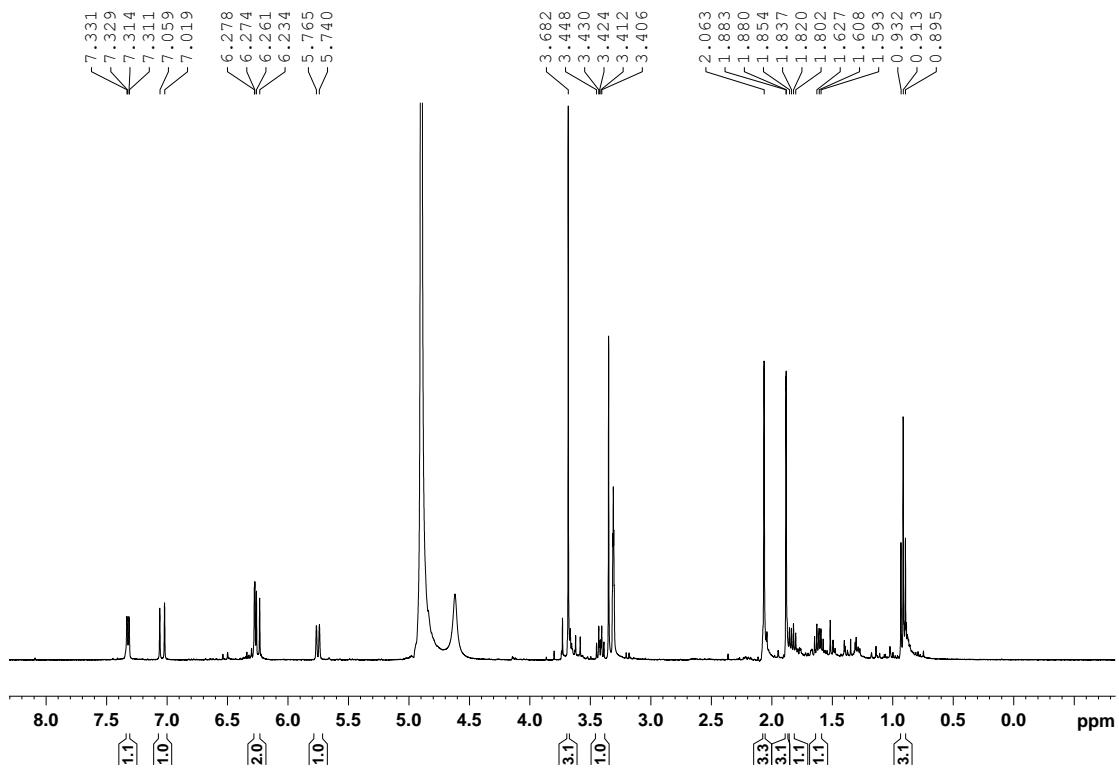


Figure S5: ^1H NMR spectrum of **2** in methanol- d_4 (400 MHz)

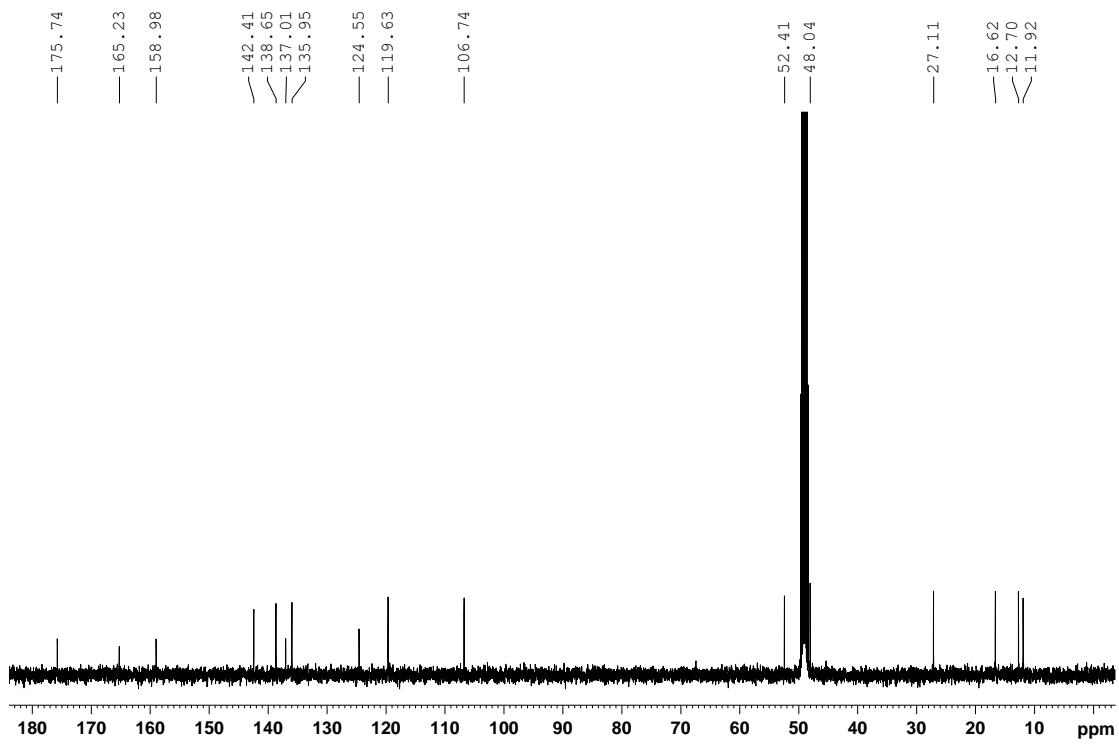


Figure S6: ^{13}C NMR spectrum of **2** in methanol- d_4 (100 MHz)

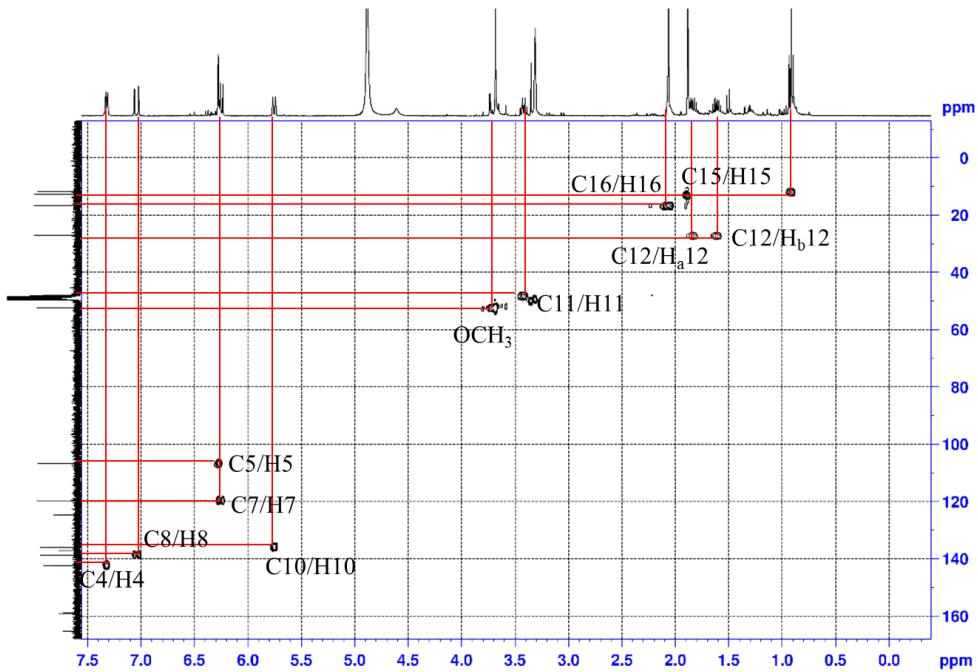


Figure S7: HSQC spectrum of **2** in methanol-*d*₄

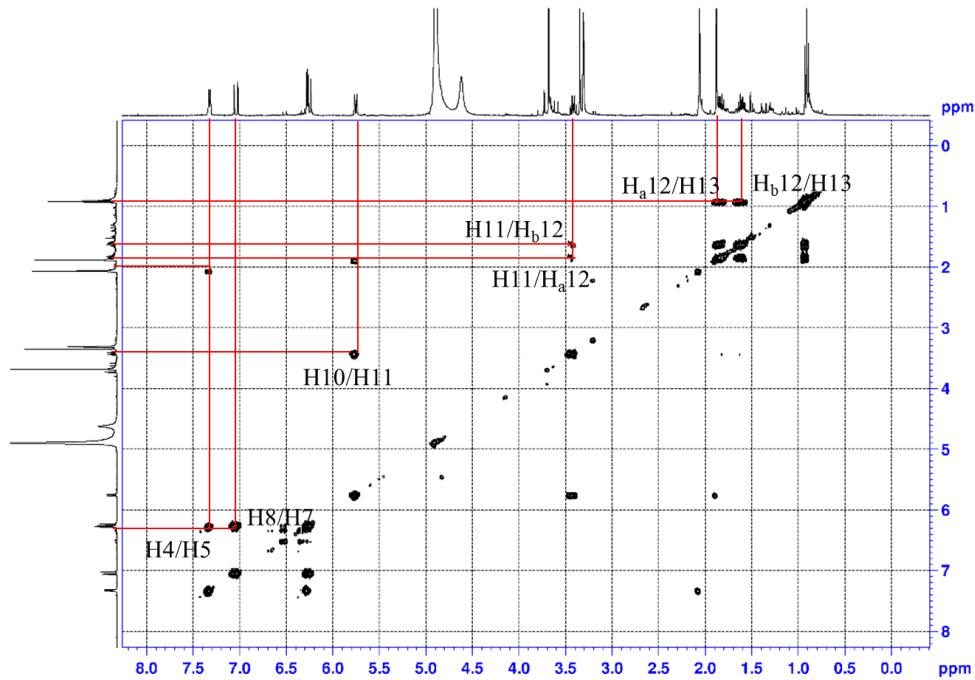


Figure S8: ¹H-¹H COSY spectrum of **2** in methanol-*d*₄

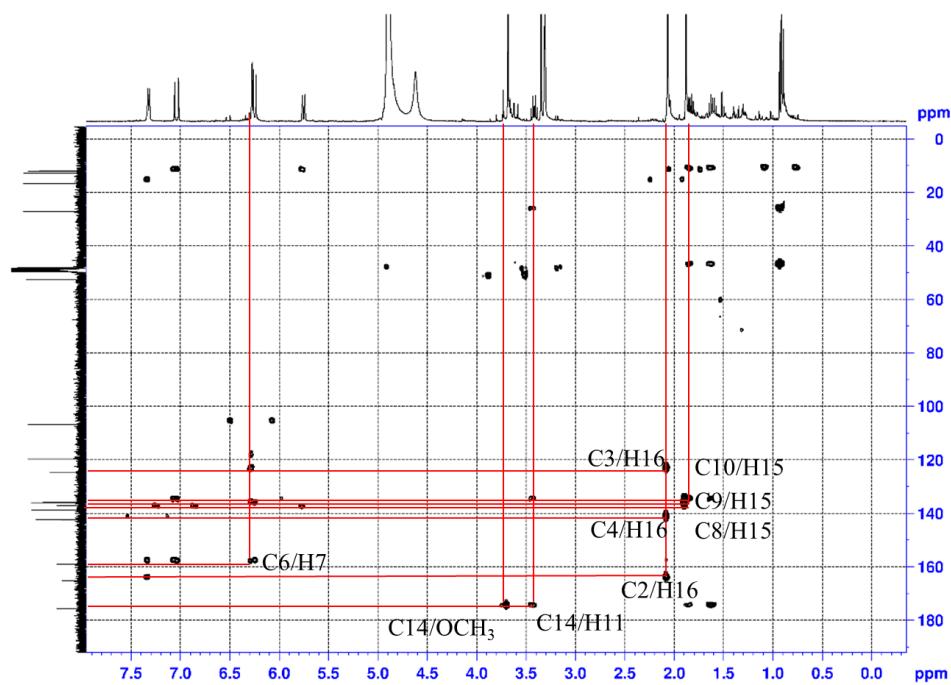


Figure S9: HMBC spectrum of **2** in methanol-*d*₄

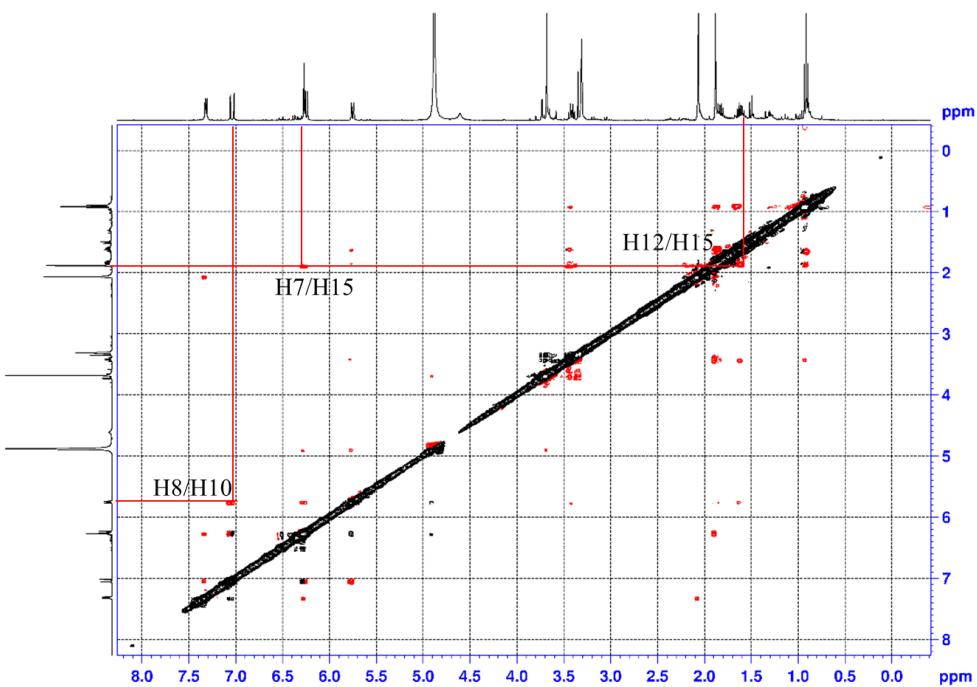


Figure S10: NOESY spectrum of **2** in methanol-*d*₄

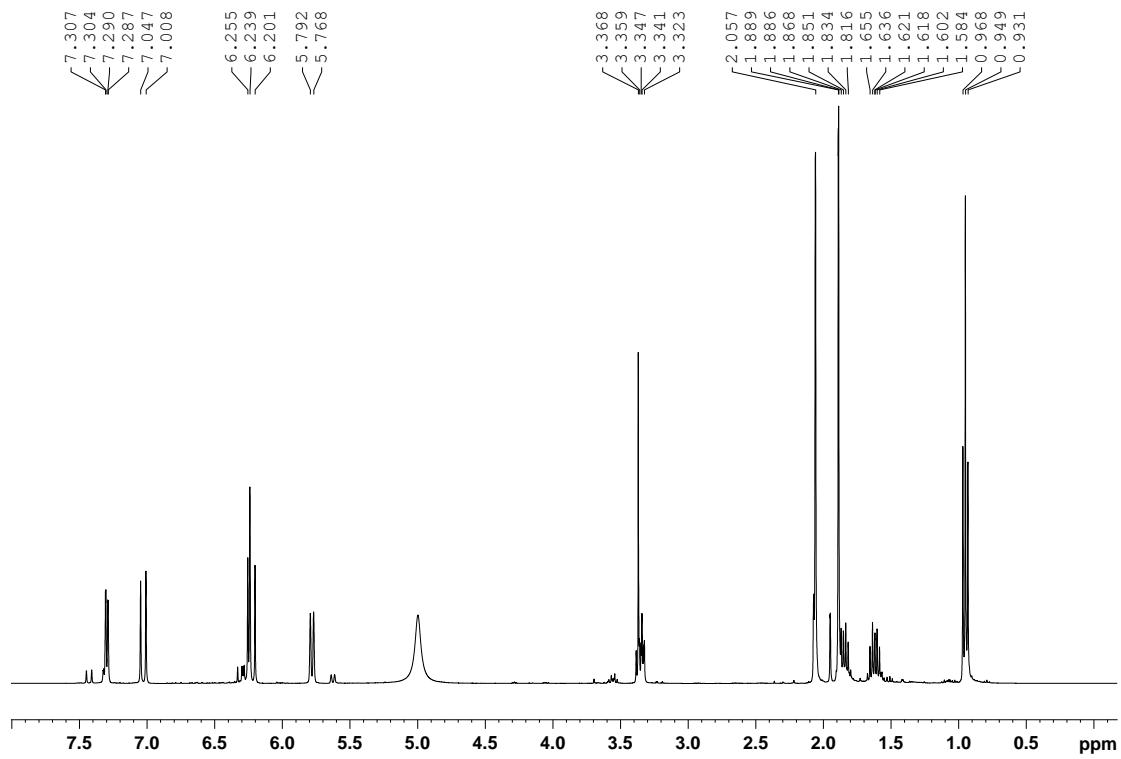


Figure S11: ^1H NMR spectrum of **3** in methanol- d_4 (400 MHz)

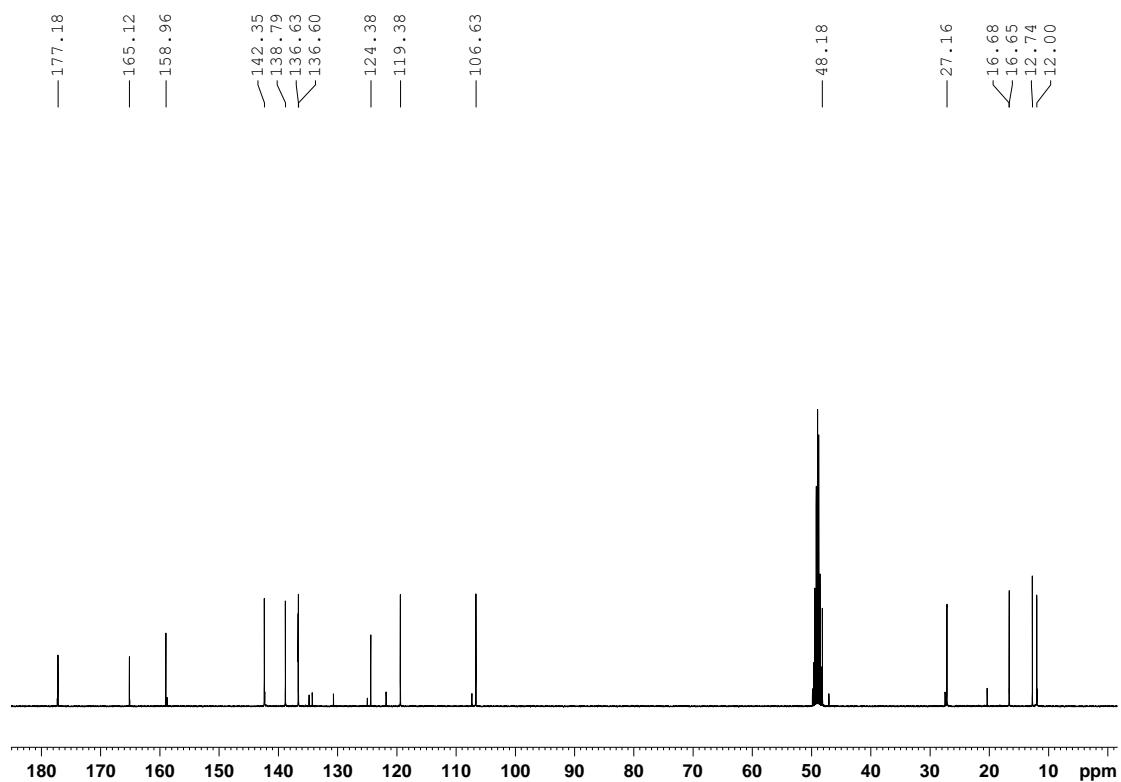


Figure S12: ^{13}C NMR spectrum of **3** in methanol- d_4 (100 MHz)

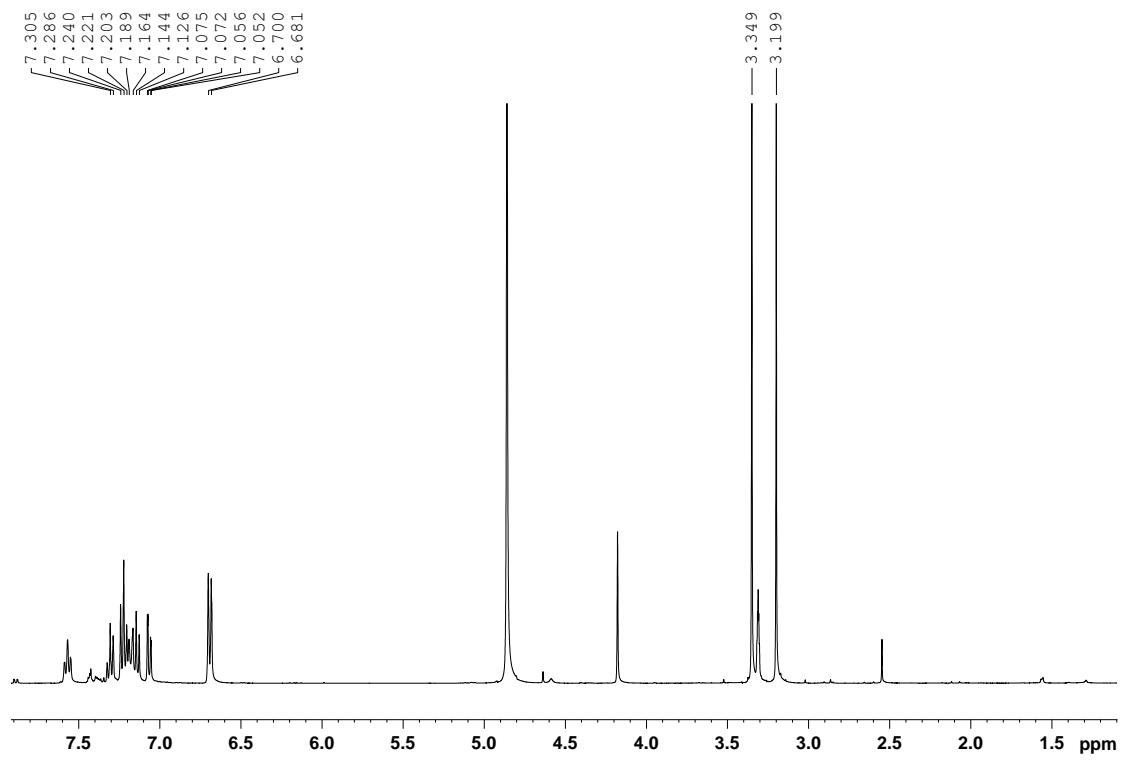


Figure S13: ^1H NMR spectrum of **4** in methanol- d_4 (400 MHz)

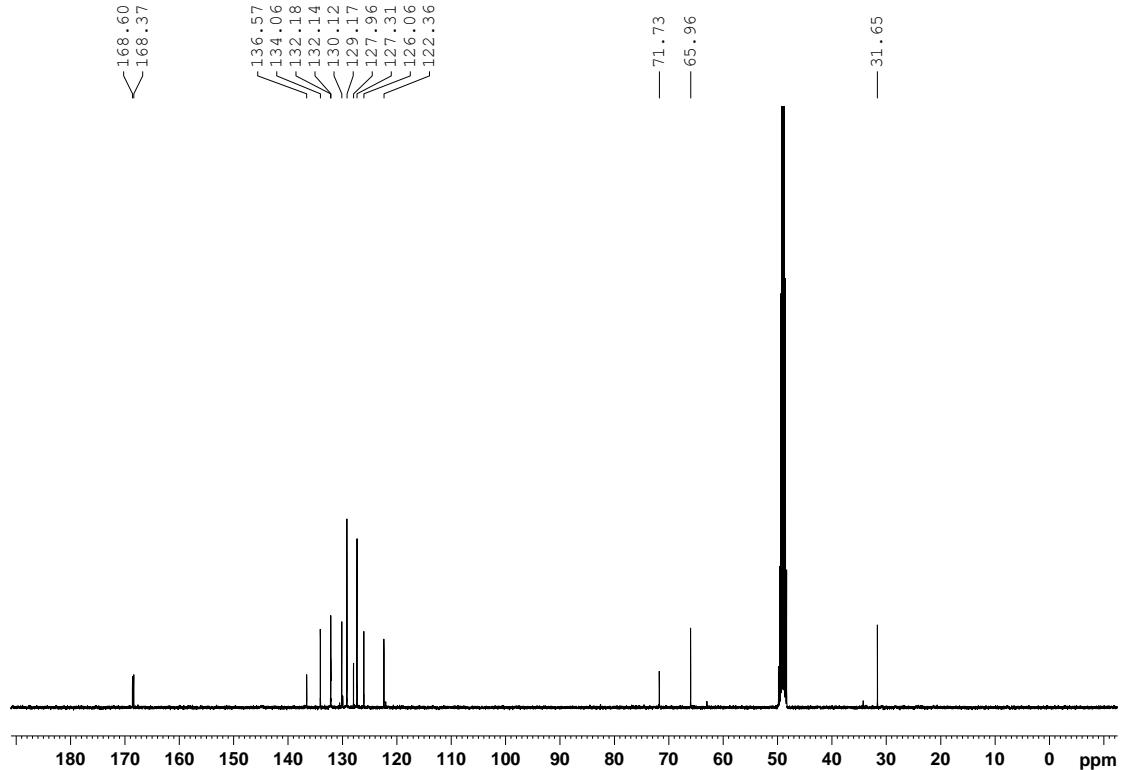


Figure S14: ^{13}C NMR spectrum of **4** in methanol- d_4 (100 MHz)

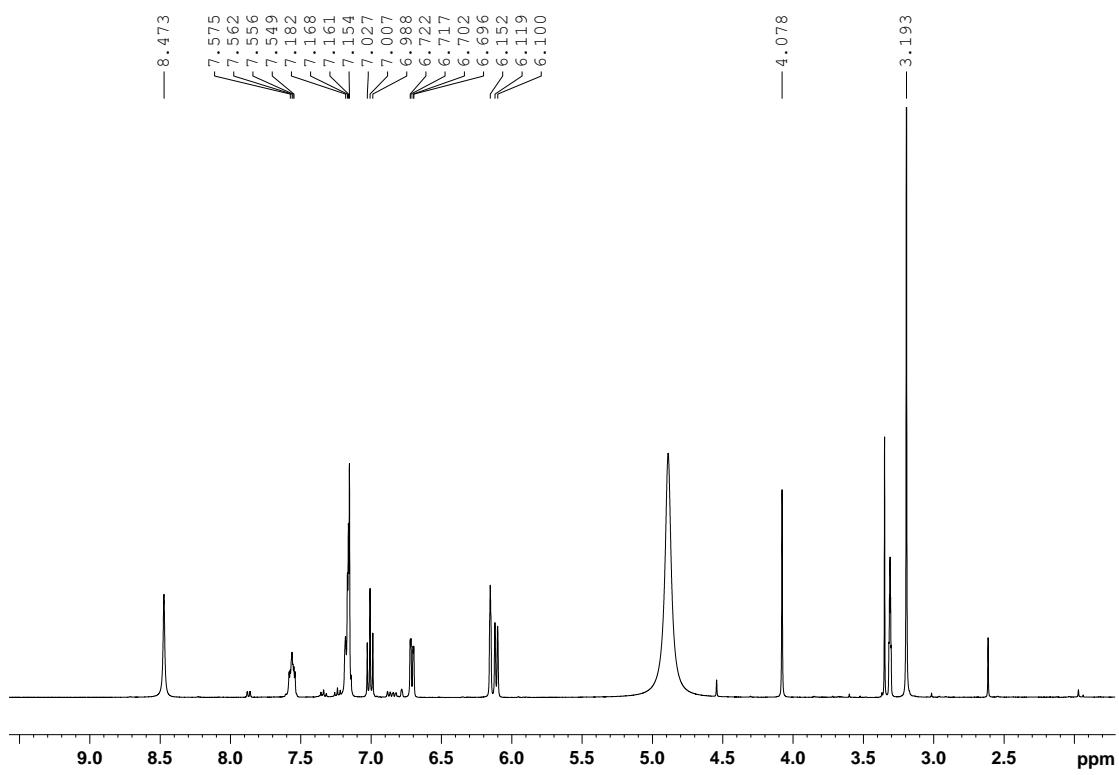


Figure S15: ^1H NMR spectrum of **5** in methanol- d_4 (400 MHz)

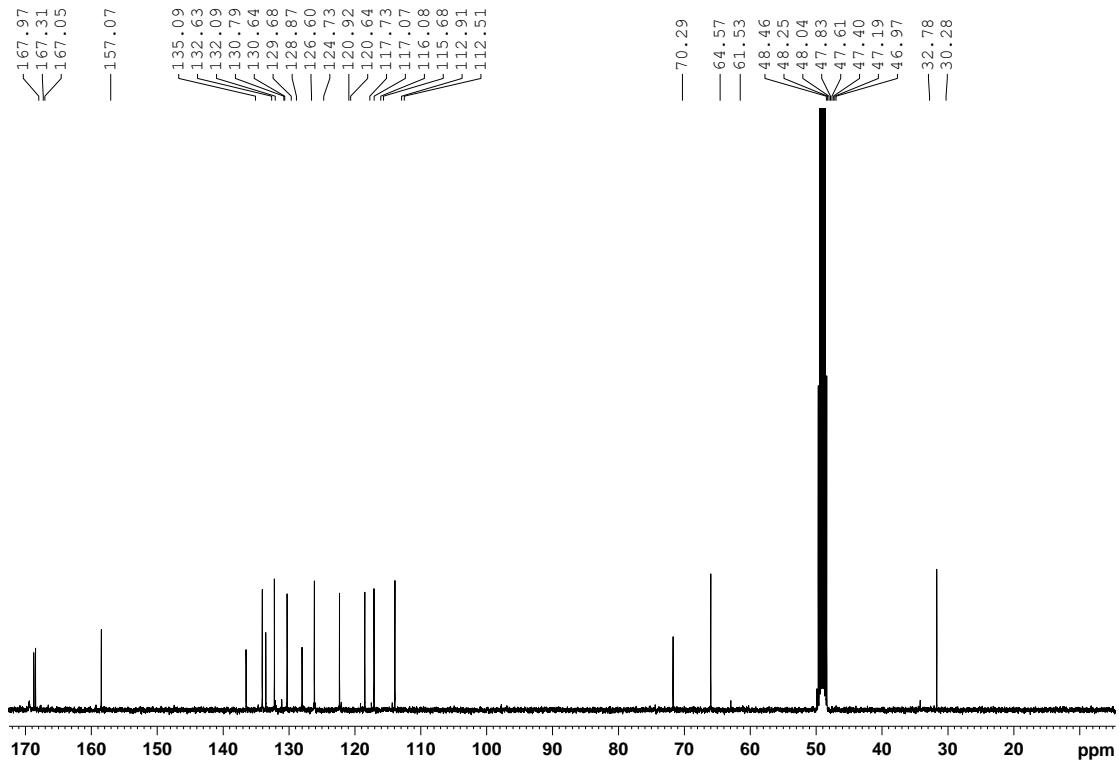


Figure S16: ^{13}C NMR spectrum of **5** in methanol- d_4 (100 MHz)

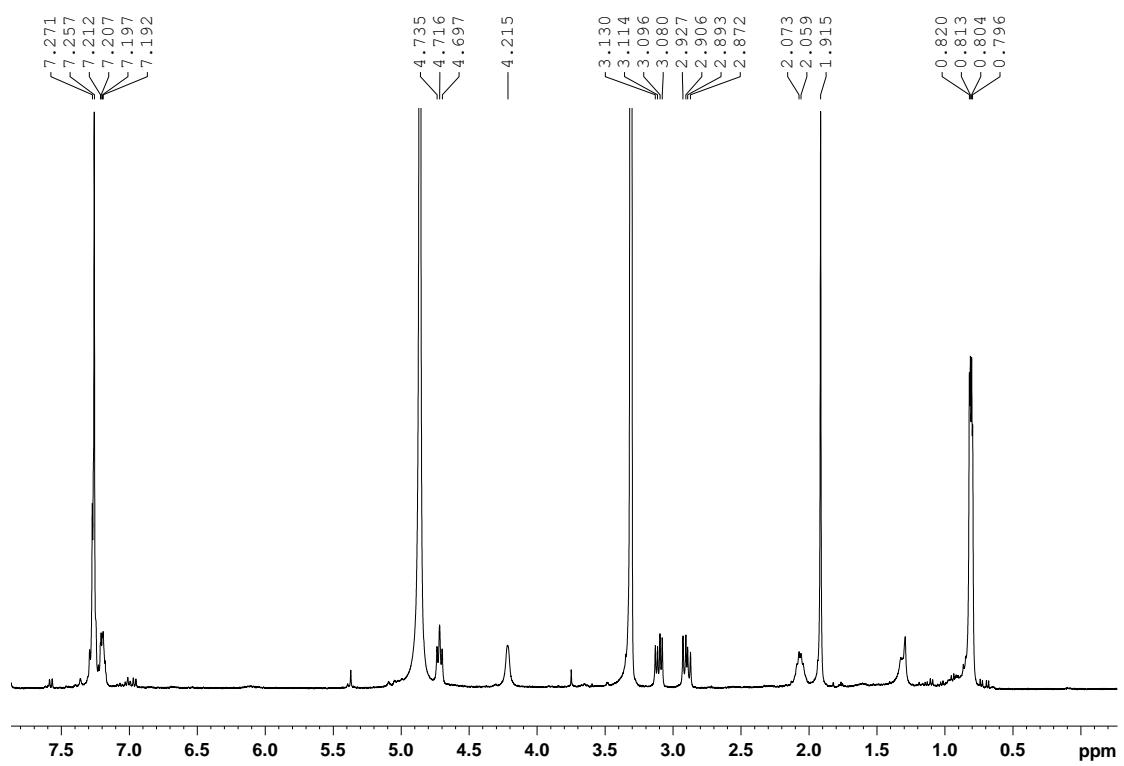


Figure S17: ^1H NMR spectrum of **6** in methanol- d_4 (400 MHz)

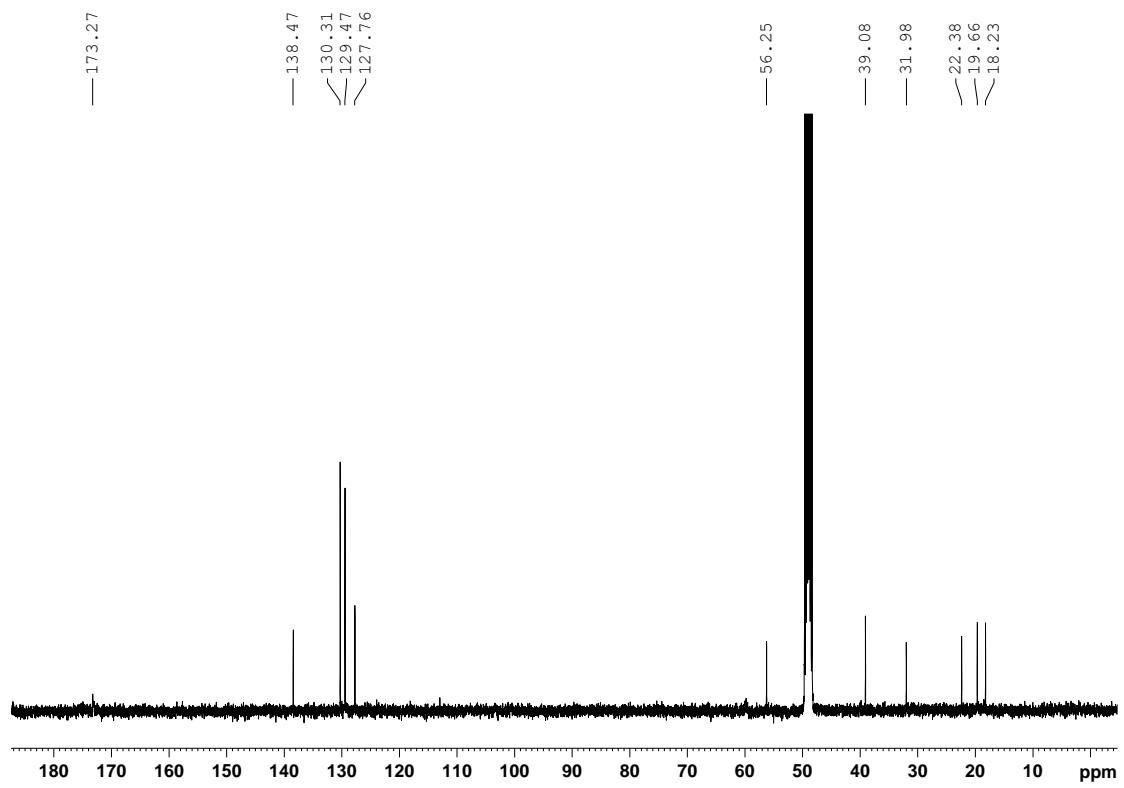


Figure S18: ^{13}C NMR spectrum of **6** in methanol- d_4 (100 MHz)

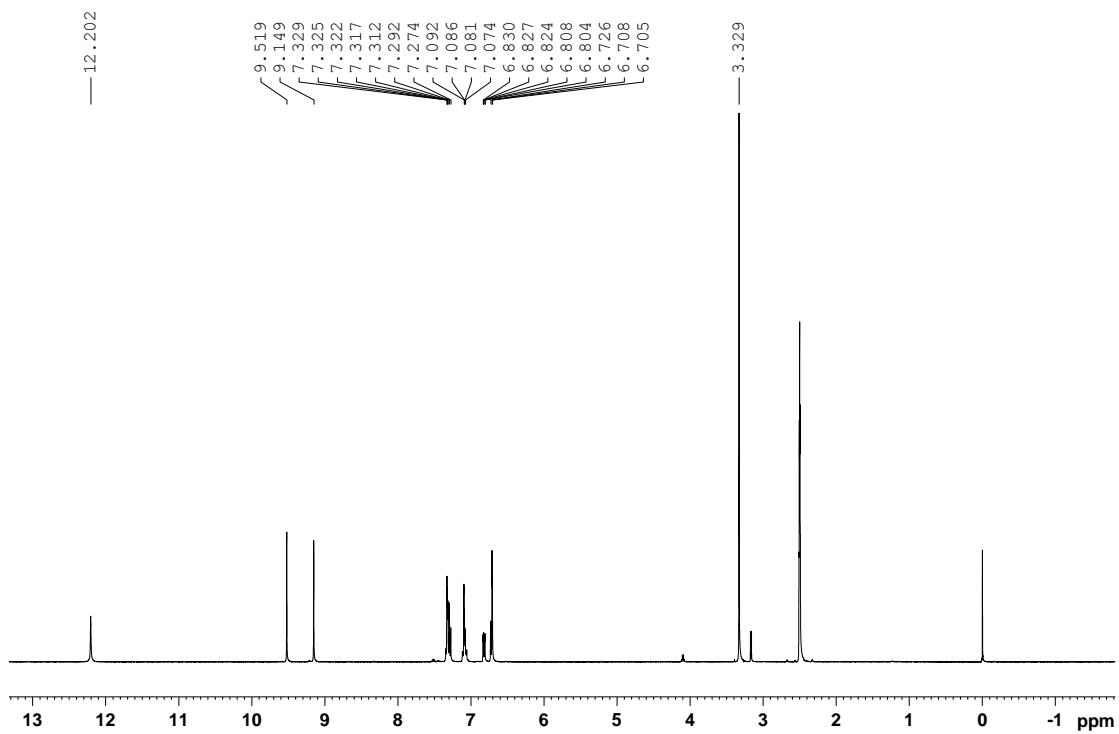


Figure S19: ^1H NMR spectrum of **7** in $\text{DMSO}-d_6$ (400 MHz)

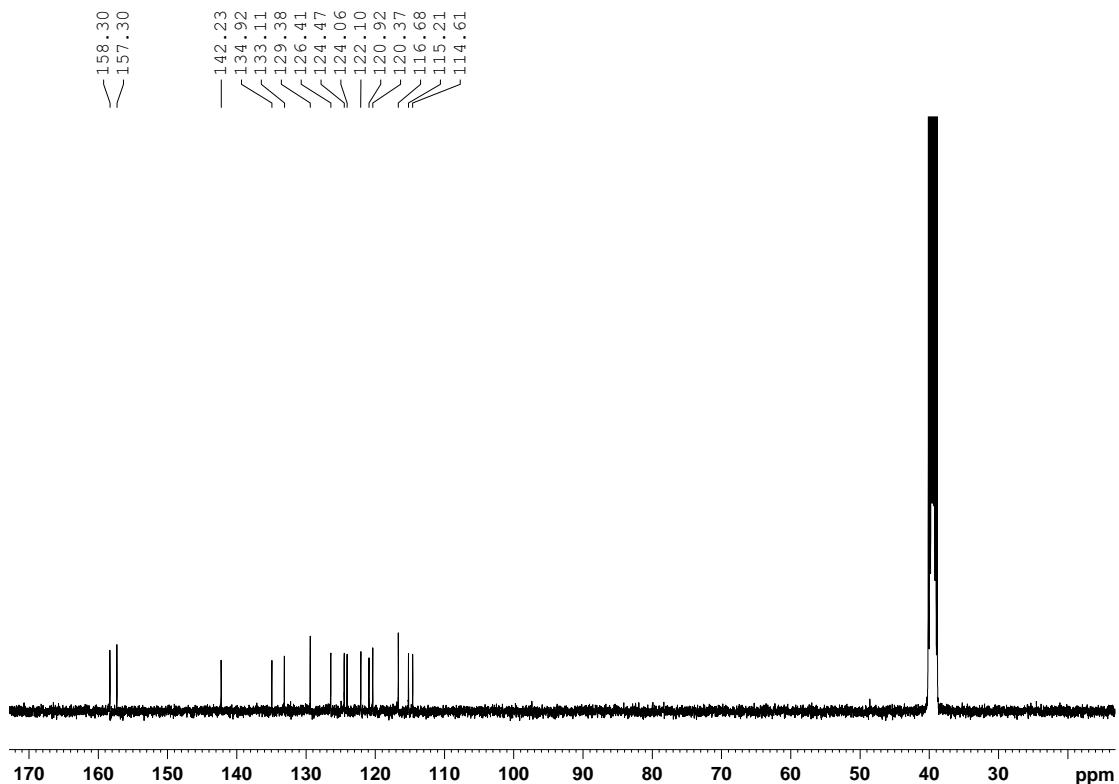


Figure S20: ^{13}C NMR spectrum of **7** in $\text{DMSO}-d_6$ (100 MHz)

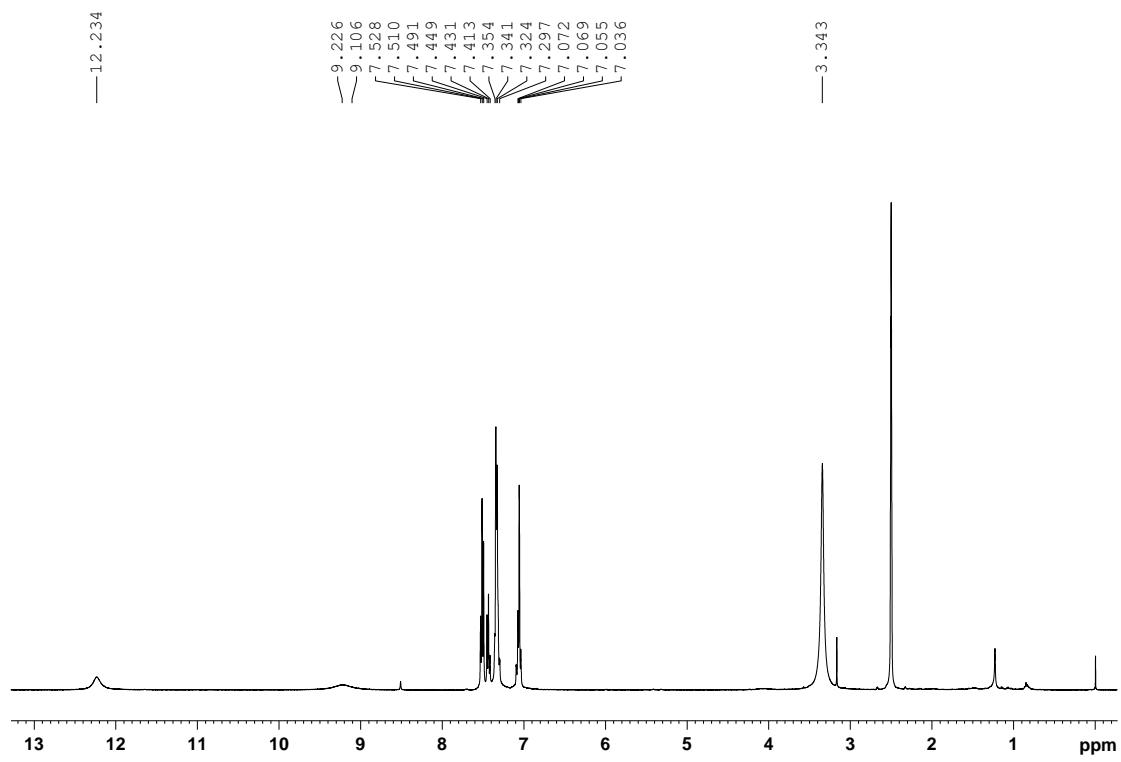


Figure S21:¹H NMR spectrum of **8** in DMSO-*d*₆ (400 MHz)

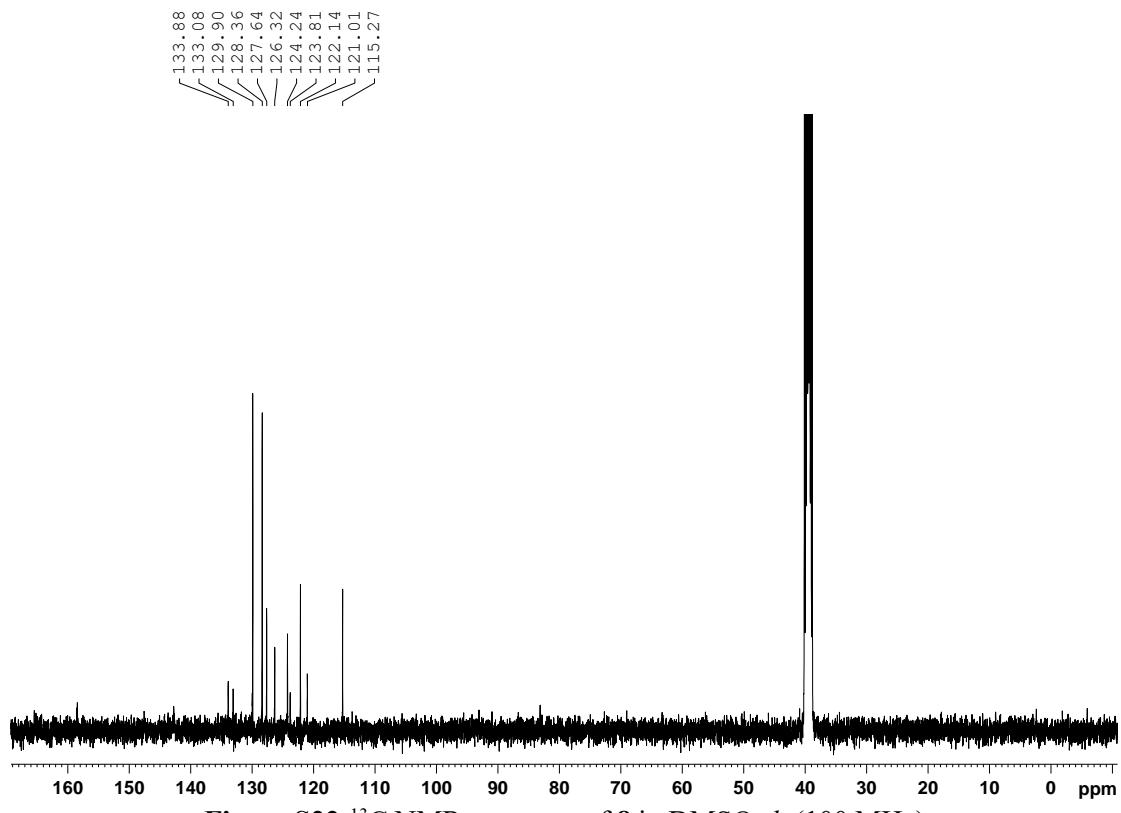


Figure S22:¹³C NMR spectrum of **8** in DMSO-*d*₆ (100 MHz)

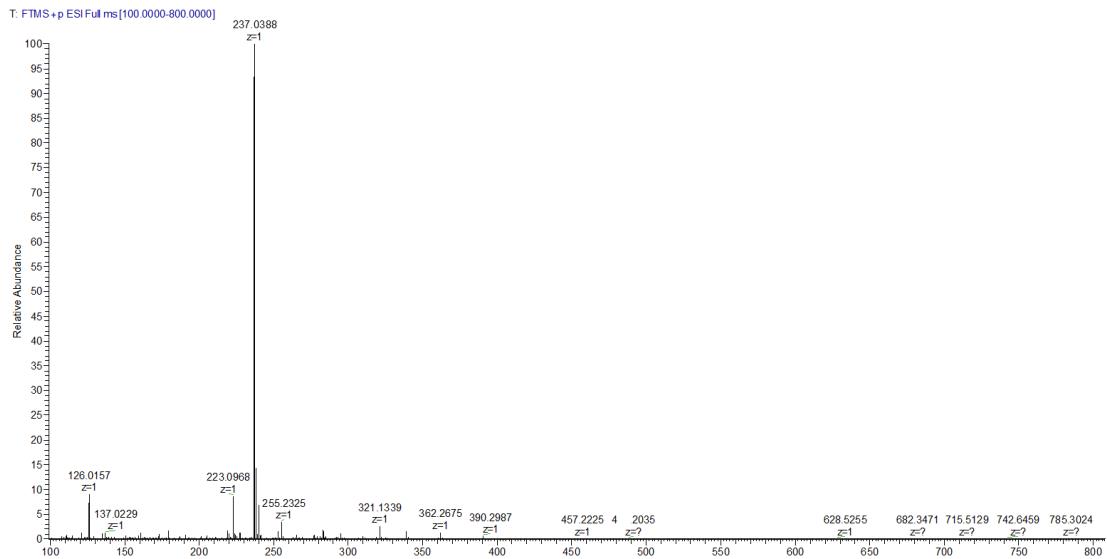


Figure S23: HRESIMS spectrum of **1**

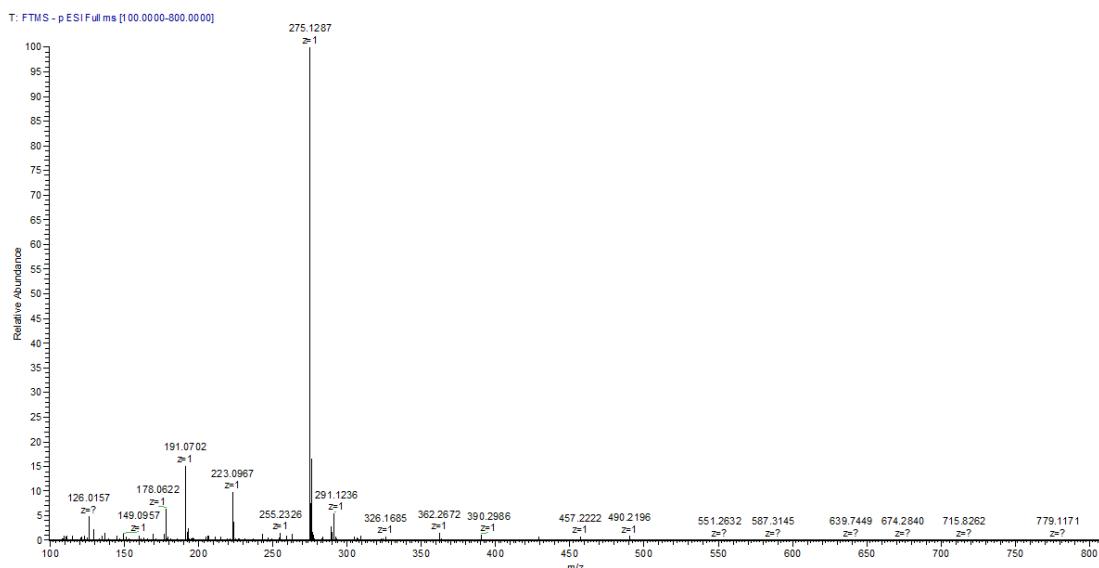


Figure S24: HRESIMS spectrum of **1**

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

SUBSTANCES: CHEMICAL STRUCTURE ?

Structure Editor:

Search Type:

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- Substructure
- Similarity

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- 90-94
- 85-89
- 80-84
- 75-79
- 70-74
- 65-69
- 0-64 (least similar)

Analyze Refine

Analyze by:

Substance Role	▼
Preparation	8
Biological Study	6
Uses	6
Reactant or Reagent	4
Process	1

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0 of 9 Substances Selected

Score: 96

1. [215534-92-2](#) ~1

C₁₂H₁₀O₆
1H2-Benzopyran-3-acetic acid, 6,8-dihydroxy-α-methyl-1-oxo-
[Key Physical Properties](#)

Score: 93

2. [181428-16-0](#) ~4

C₁₂H₁₀O₆
1H2-Benzopyran-3-acetic acid, 8-hydroxy-6-methoxy-1-oxo-
[Key Physical Properties](#)

Score: 93

3. [215534-93-3](#) ~1

C₁₃H₁₂O₆
1H2-Benzopyran-3-acetic acid, 6,8-dihydroxy-α,α-dimethyl-1-oxo-
[Key Physical Properties](#)

Score: 92

4. [181427-78-1](#) ~66

C₁₃H₁₂O₆
1H2-Benzopyran-3-acetic acid, 8-hydroxy-6-methoxy-α-methyl-1-oxo-
[Key Physical Properties](#)

Figure S25: Scifinder similarity report of compound 1

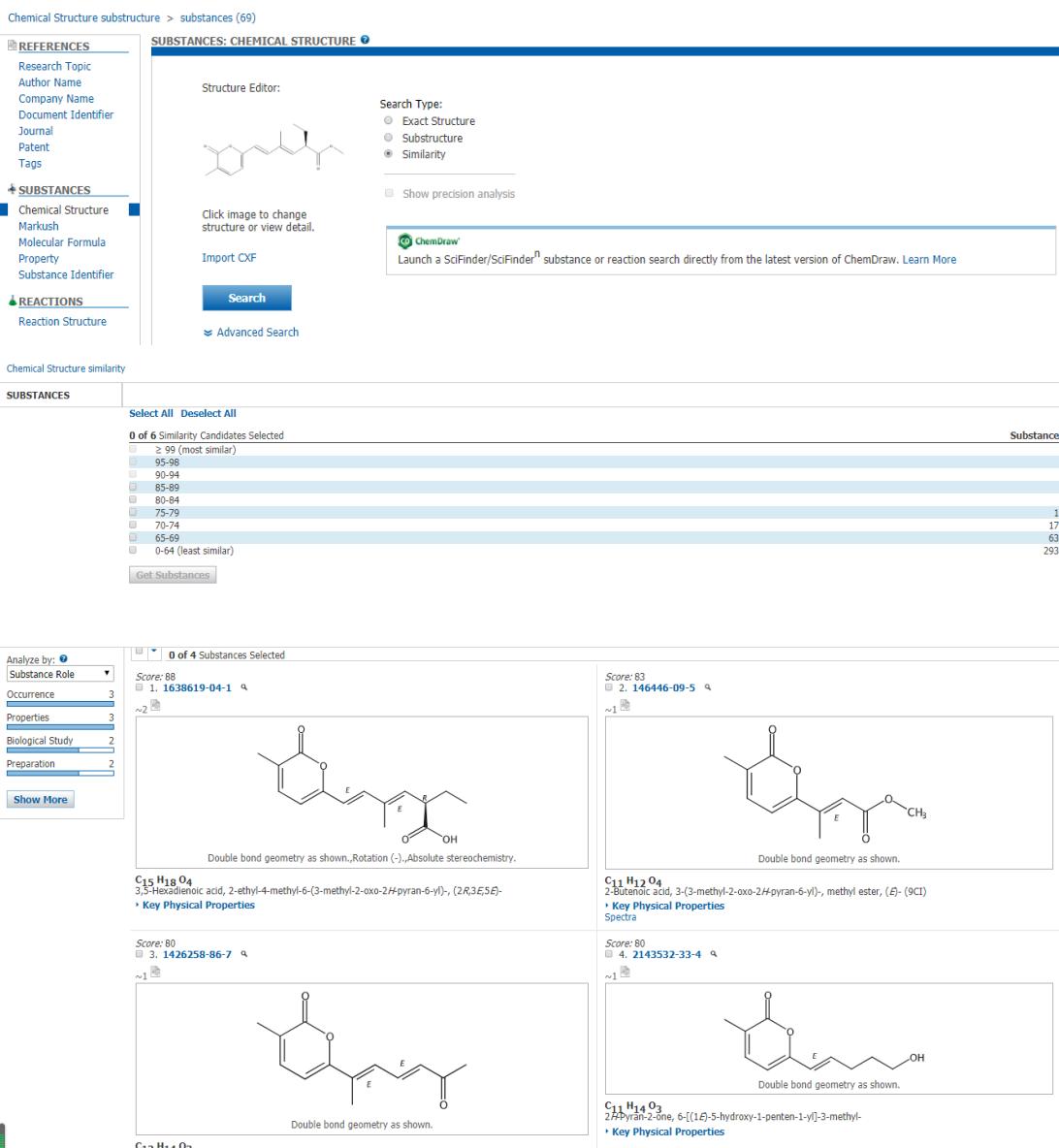


Figure S26: Scifinder similarity report of compound 2

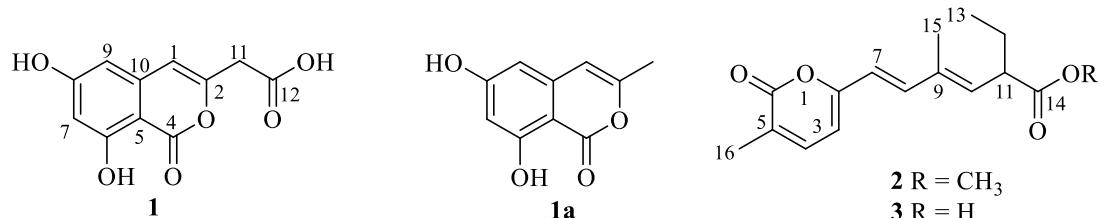


Table S1: NMR data of new compounds **1** and **2** and the similar compounds **1a** and **3**

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		