

Supporting Information

Rec. Nat. Prod. 17:1 (2023) 174-178

Three New Chromone Derivatives from the Deep-Sea-Derived

Fungus *Penicillium thomii*

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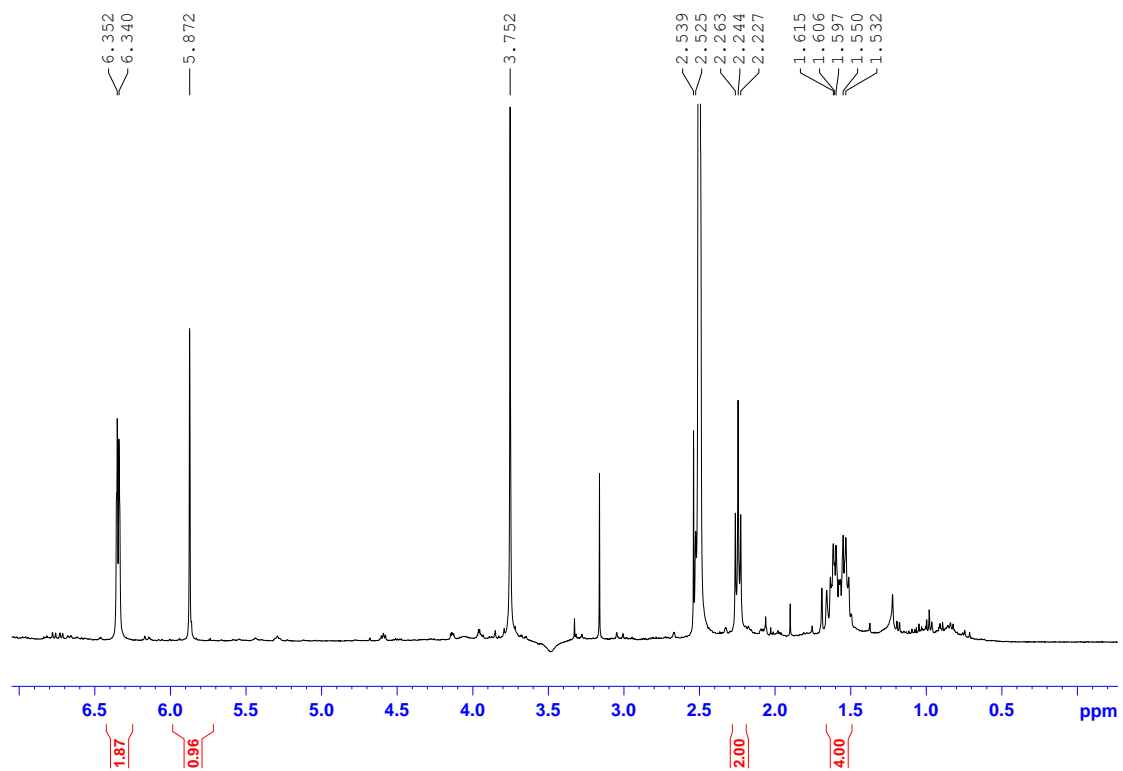


Figure S1: ^1H NMR spectrum of **1** in $\text{DMSO-}d_6$ (400 MHz)

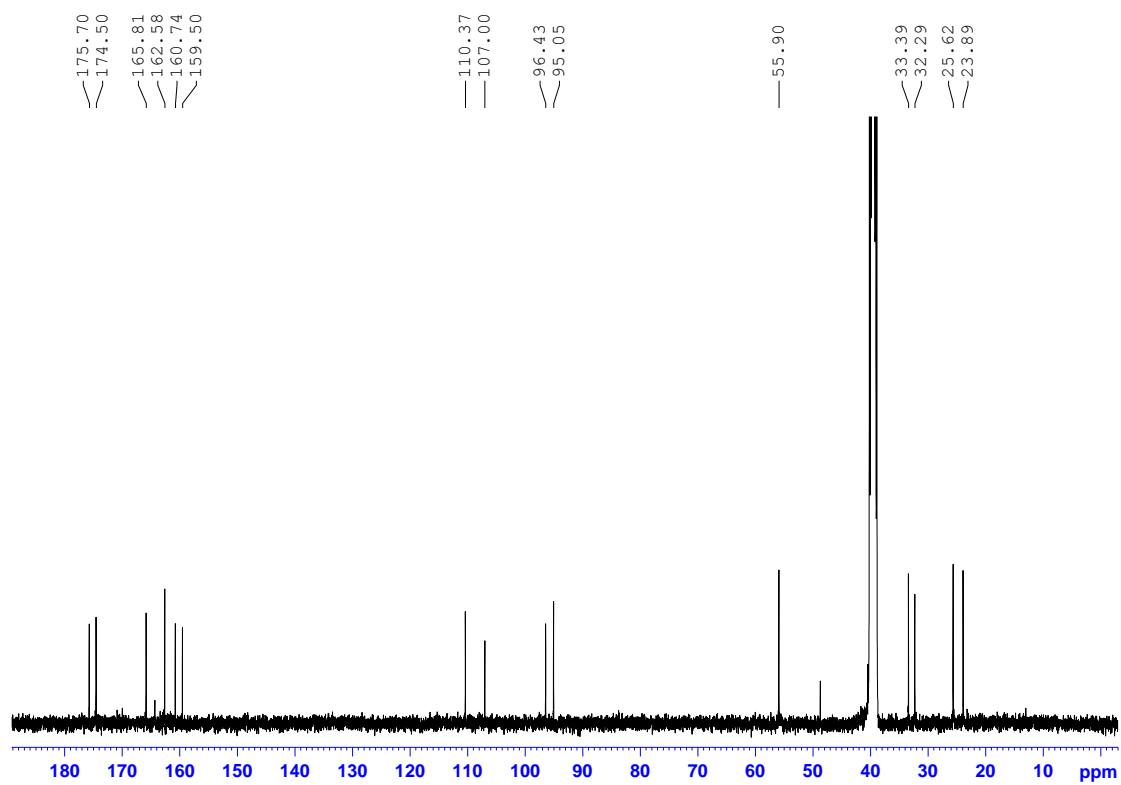


Figure S2: ^{13}C NMR spectrum of **1** in $\text{DMSO-}d_6$ (100 MHz)

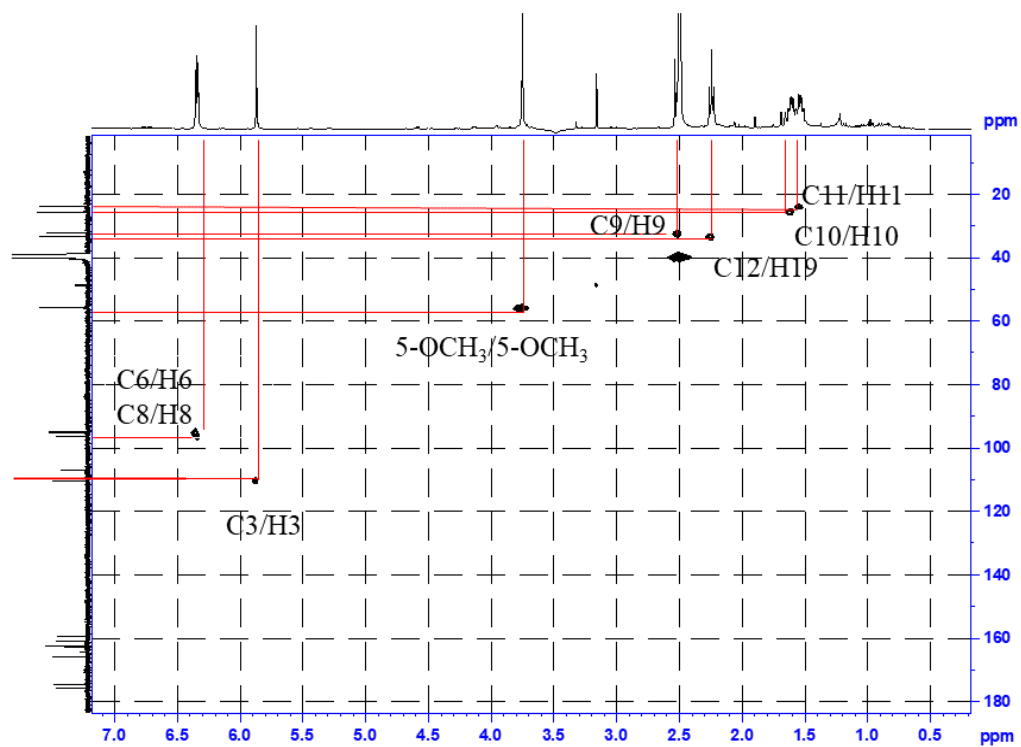


Figure S3: HSQC spectrum of **1** in $\text{DMSO-}d_6$

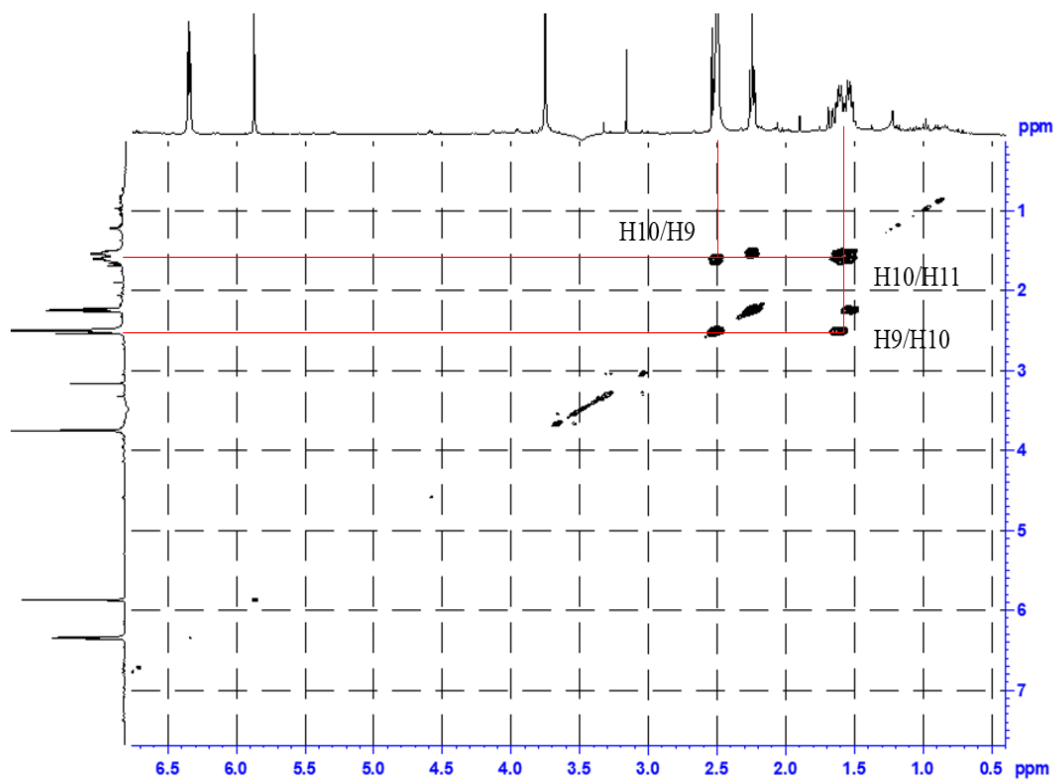


Figure S4: ^1H - ^1H COSY spectrum of **1** in CD_3OD

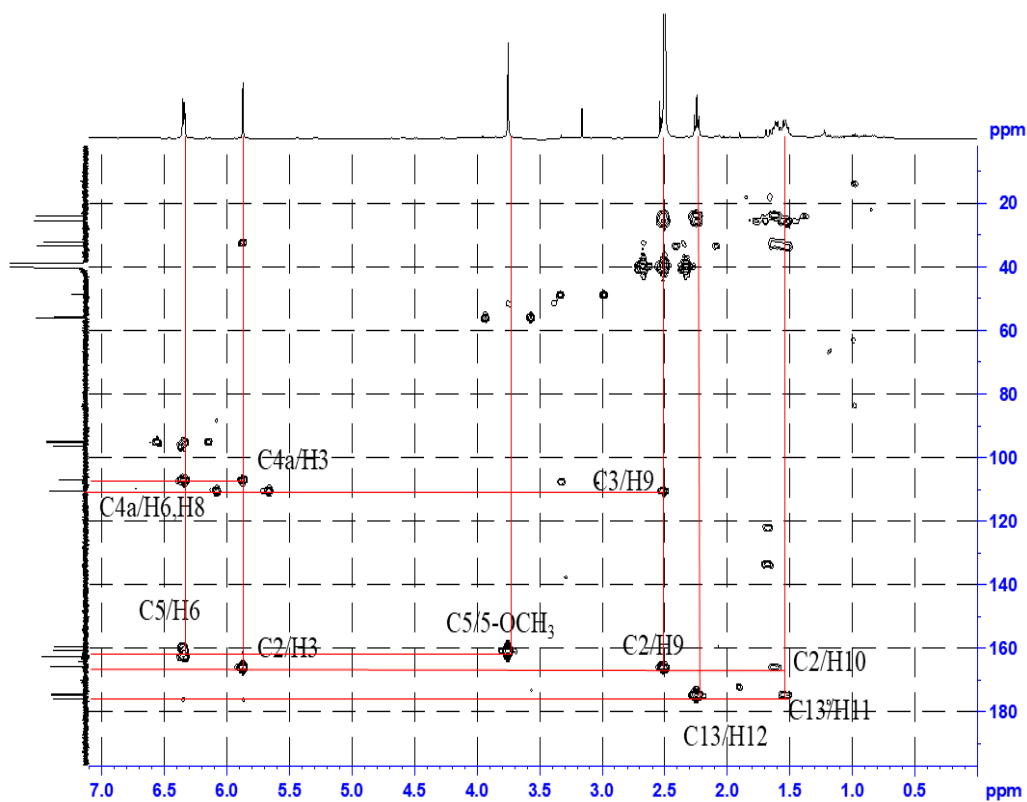


Figure S5: HMBC spectrum of **1** in CD_3OD

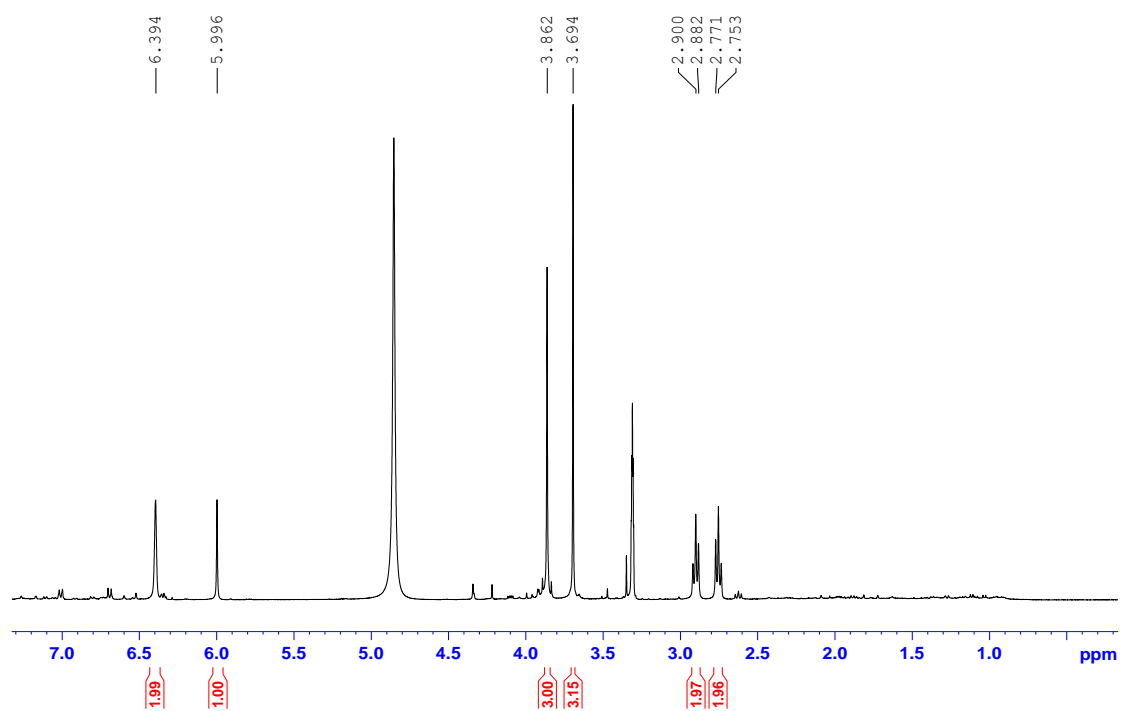


Figure S6: ^1H NMR spectrum of **2** in CD_3OD

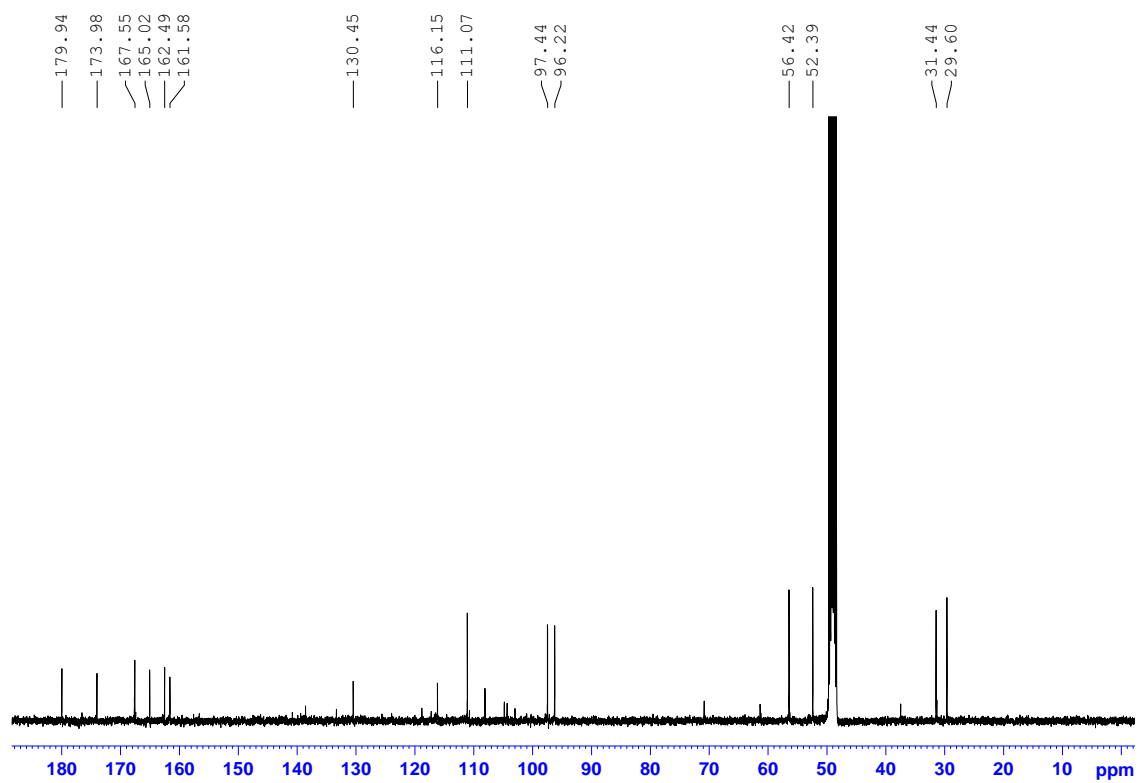


Figure S7: ^{13}C NMR spectrum of **2** in CD_3OD

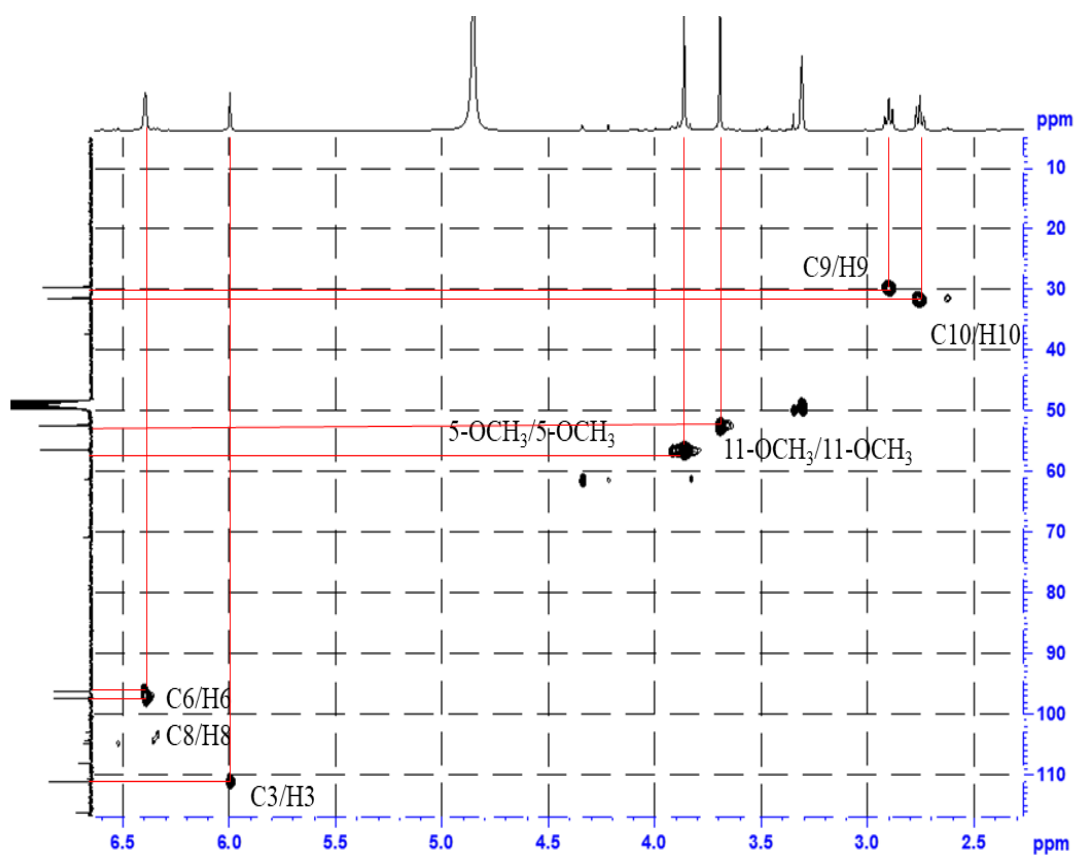


Figure S8: HSQC spectrum of **2** in CD₃OD

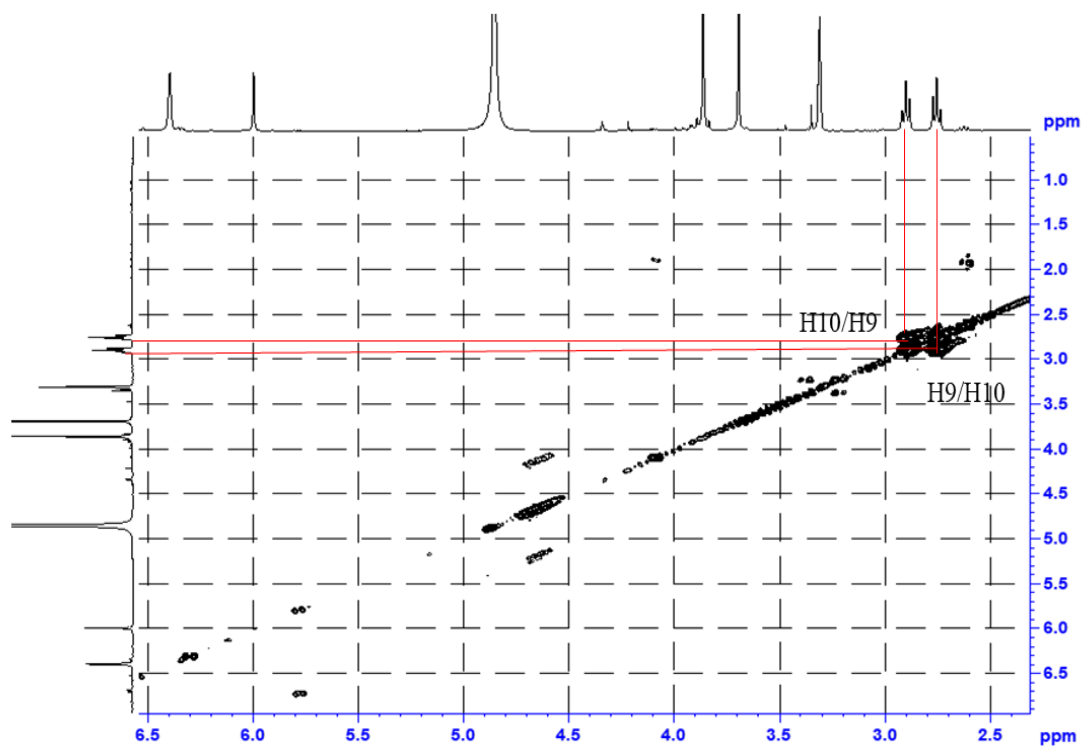


Figure S9: COSY spectrum of **2** in CD₃OD

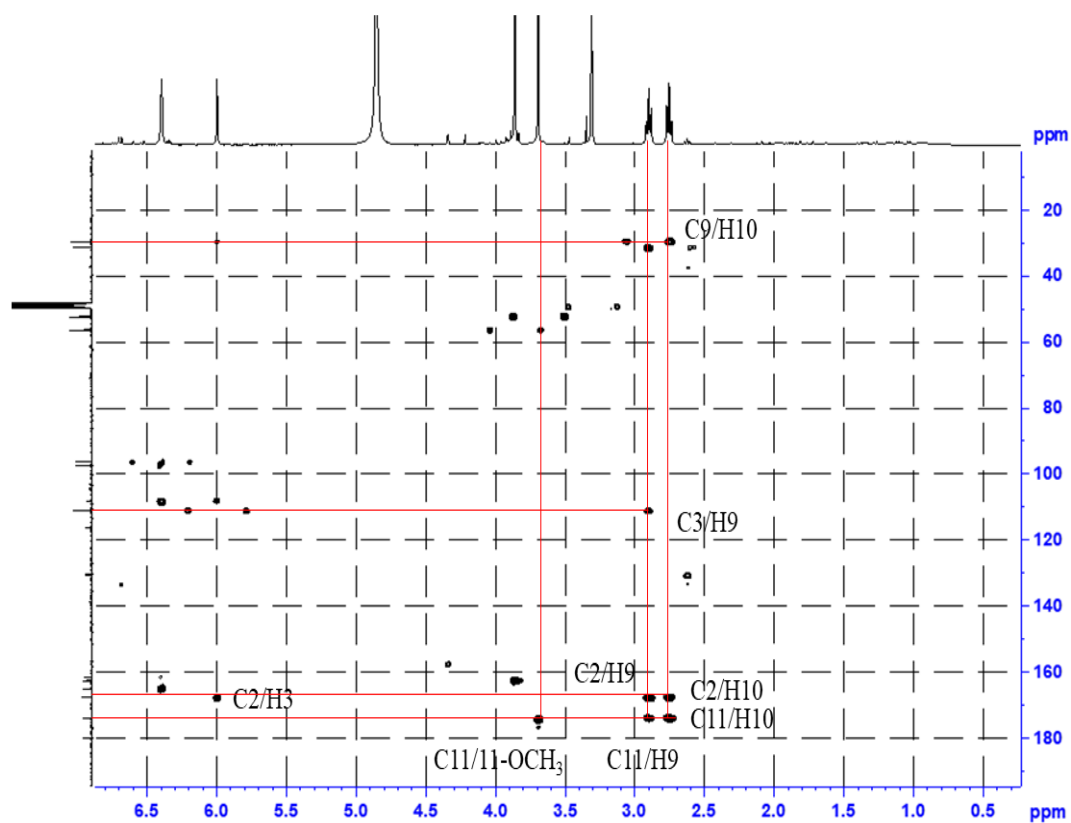


Figure S10: HMBC spectrum of **2** in CD₃OD

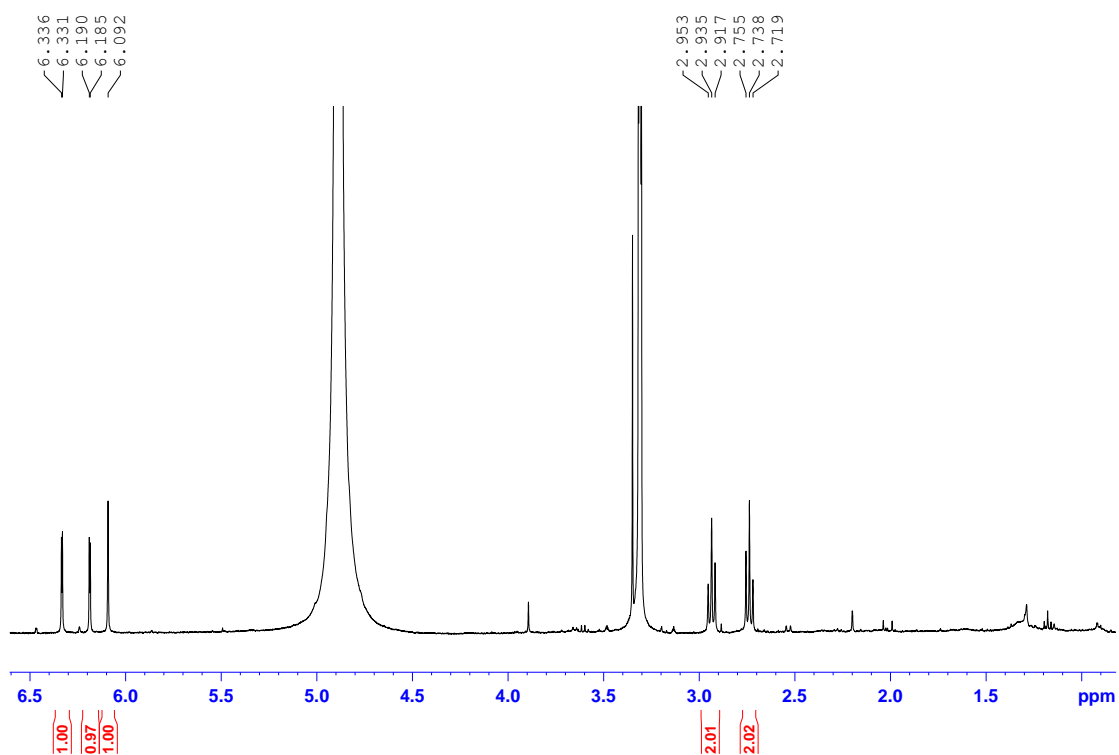


Figure S11: ¹H NMR spectrum of **3** in CD₃OD (400 MHz)

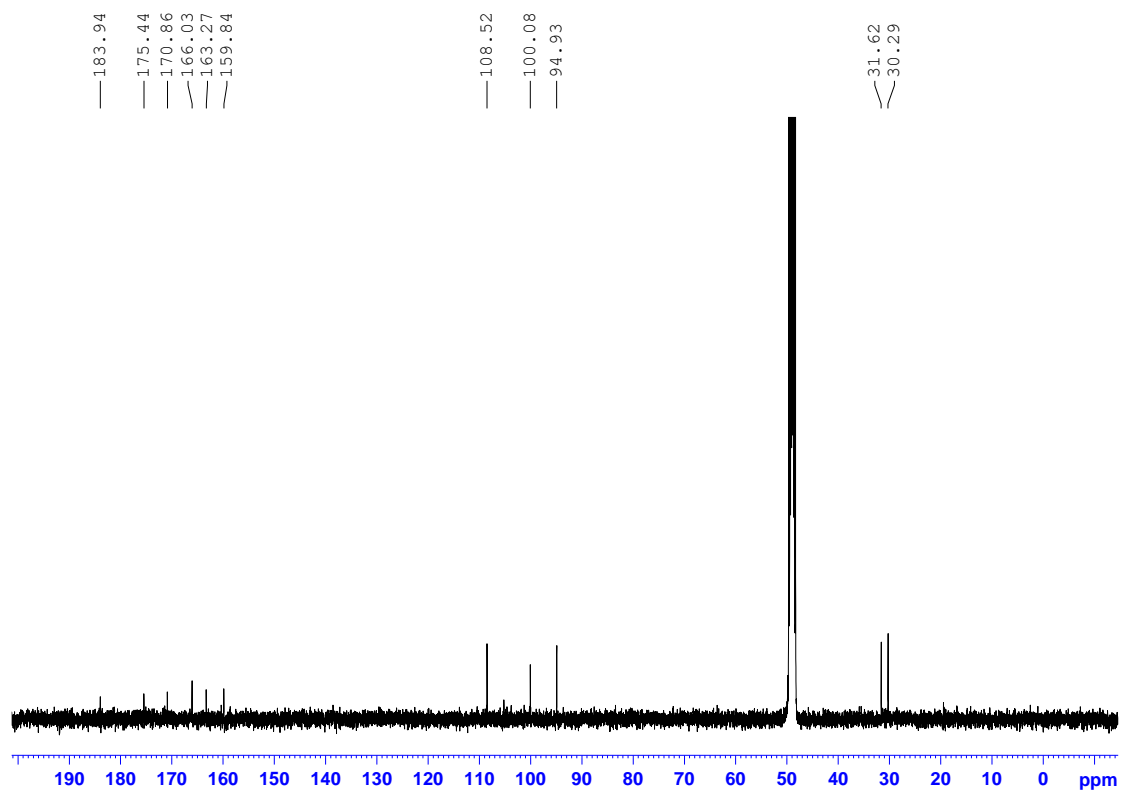


Figure S12: ^{13}C NMR spectrum of **3** in CD_3OD (100 MHz)

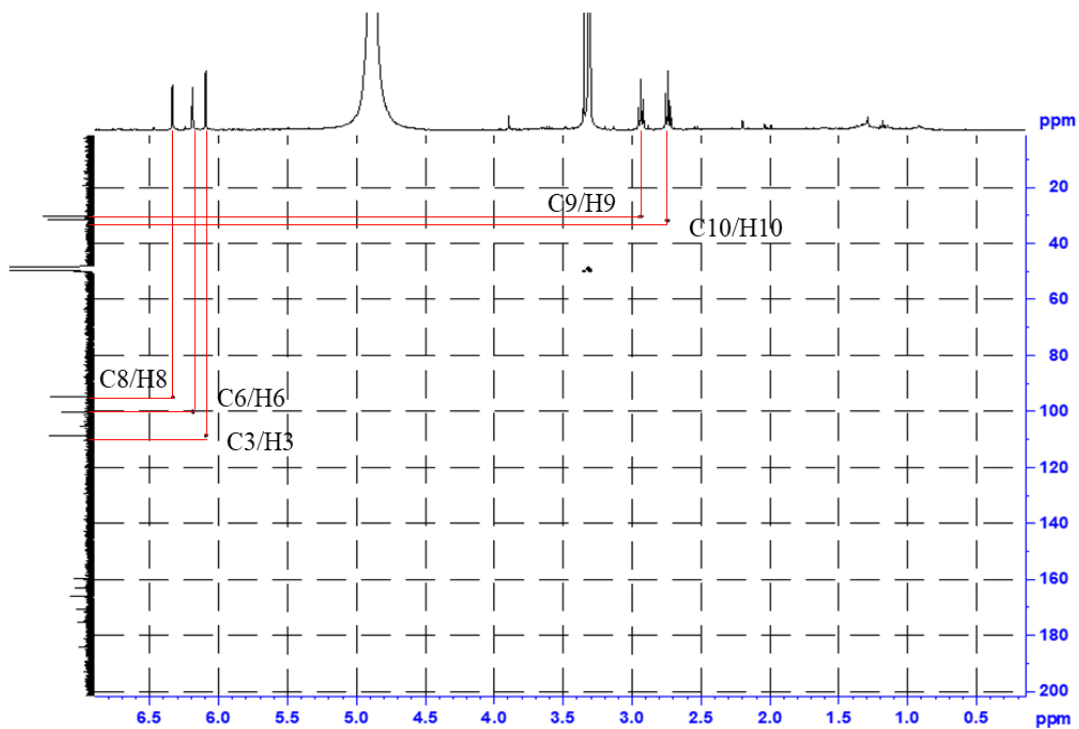


Figure S13: HSQC spectrum of **3** in CD_3OD

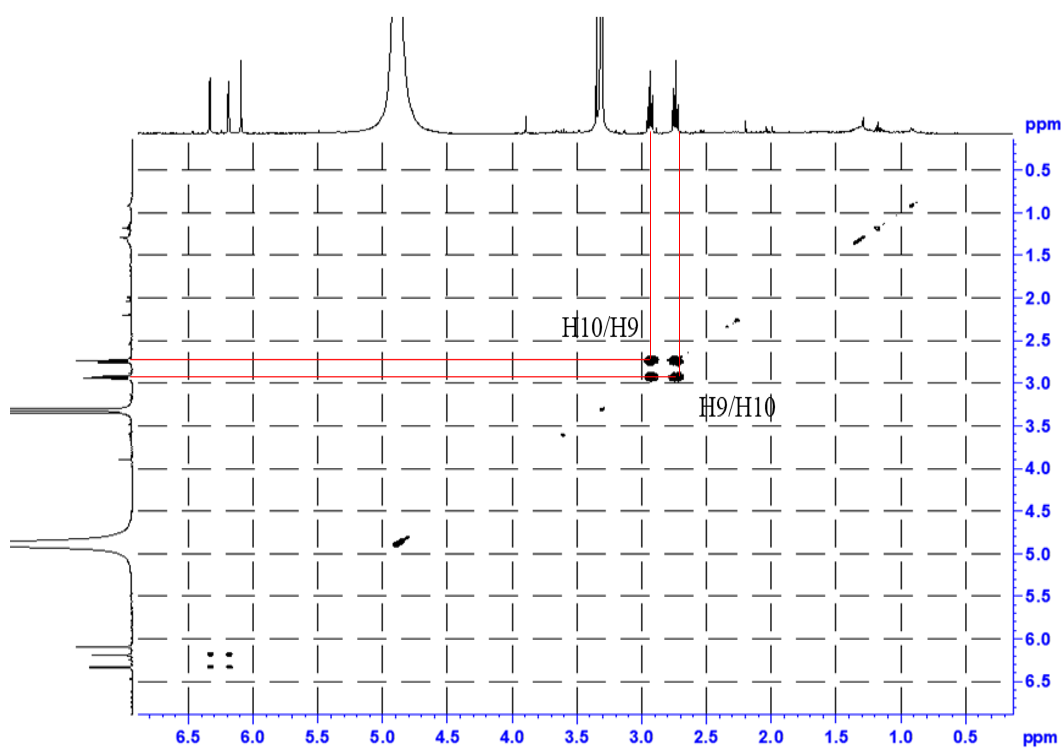


Figure S14: ^1H - ^1H COSY spectrum of **3** in CD_3OD

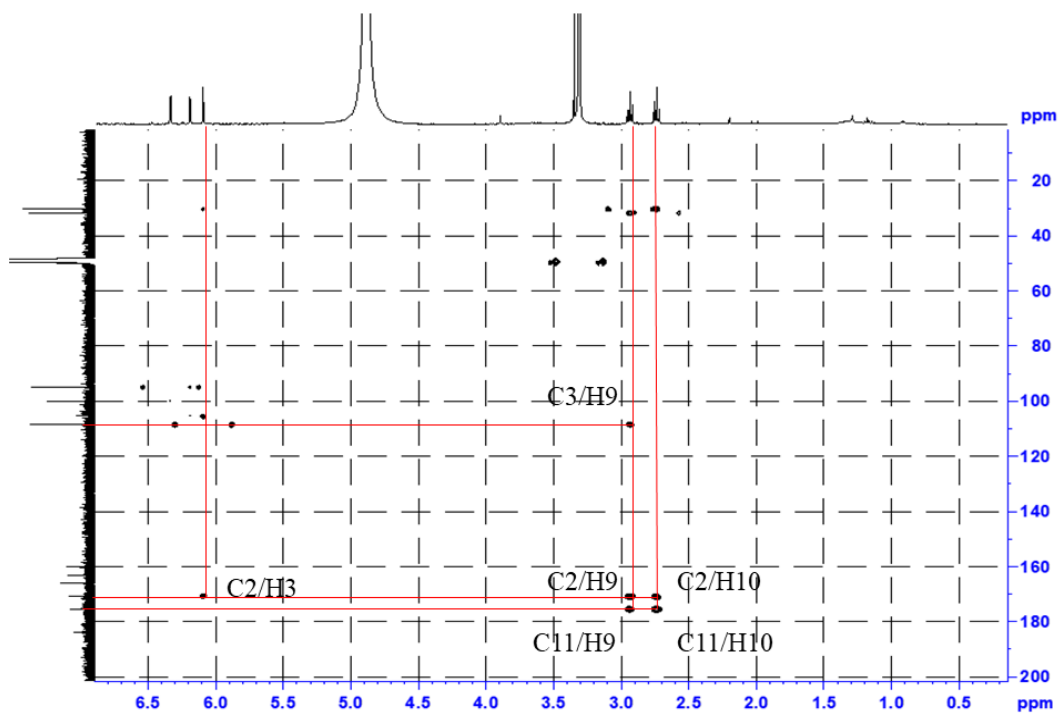


Figure S15: HMBC spectrum of **3** in CD_3OD

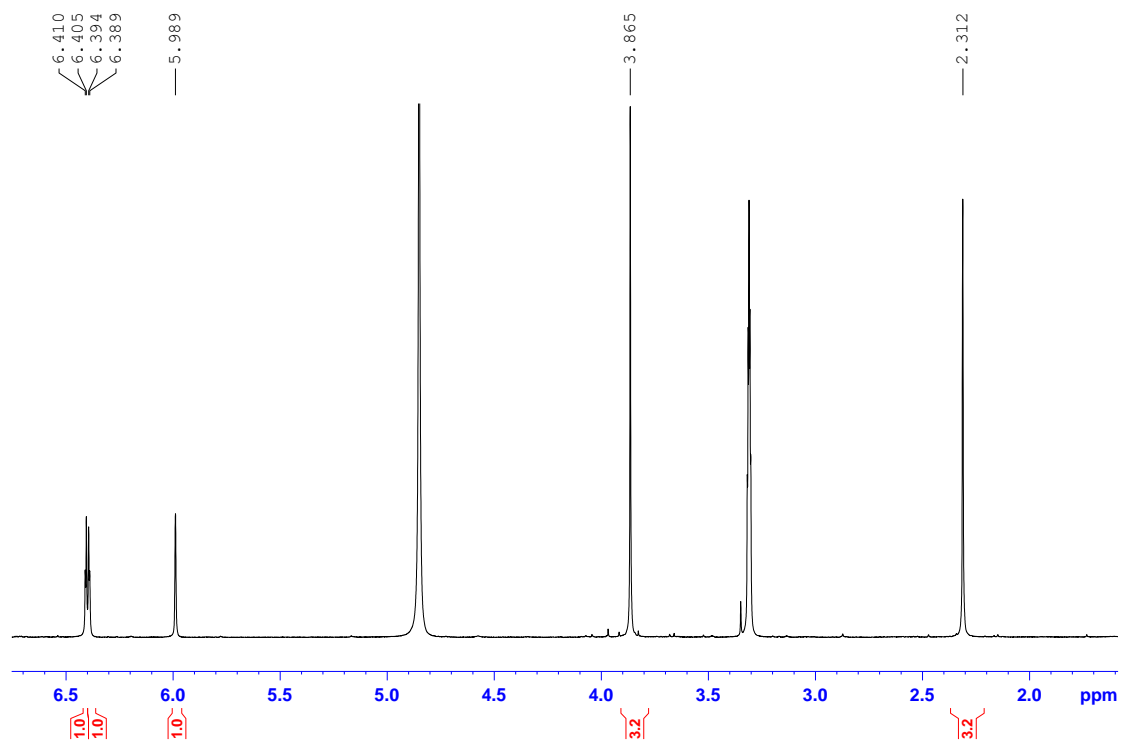


Figure S16: ^1H NMR spectrum of **4** in CD_3OD

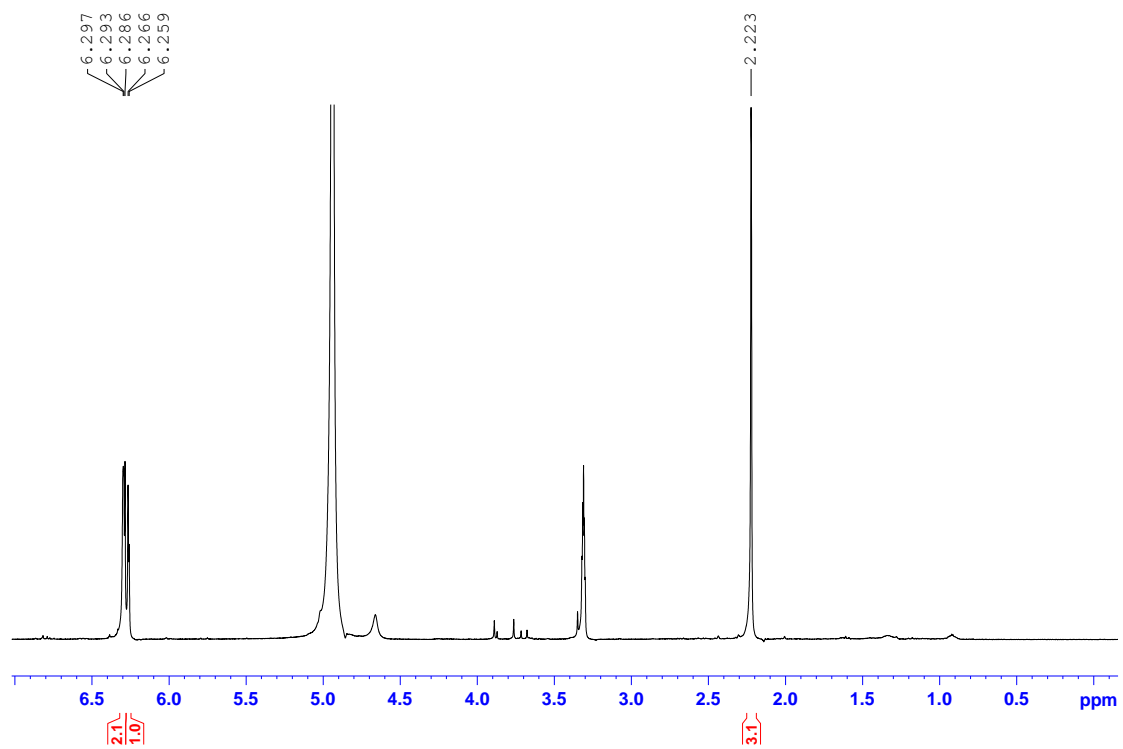


Figure S17: ^1H NMR spectrum of **5** in CD_3OD

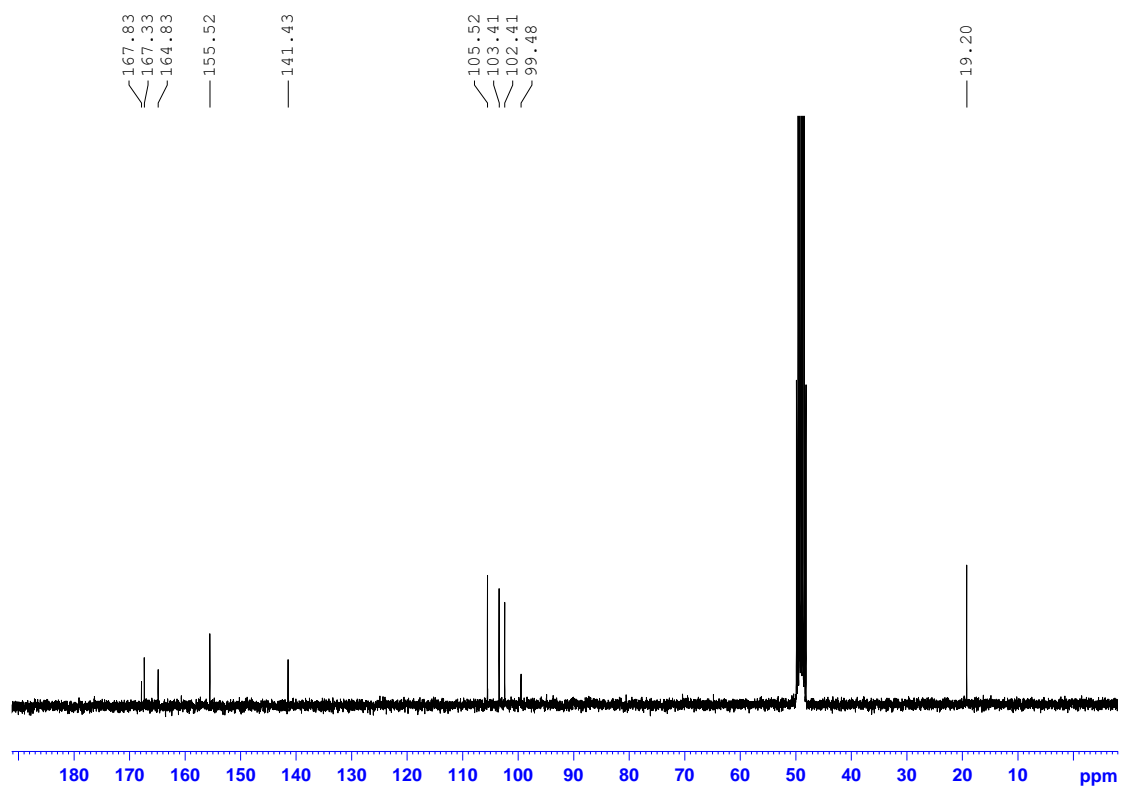


Figure S18: ^{13}C NMR spectrum of **5** in CD_3OD

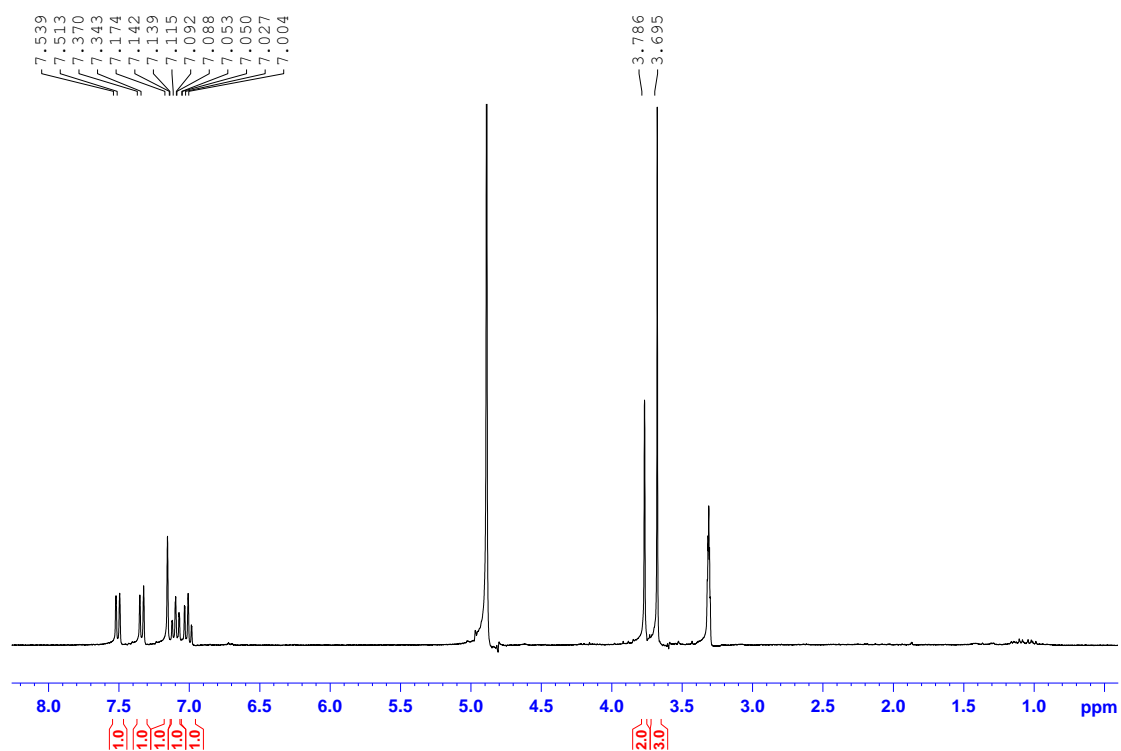


Figure S19: ^1H NMR spectrum of **6** in CD_3OD

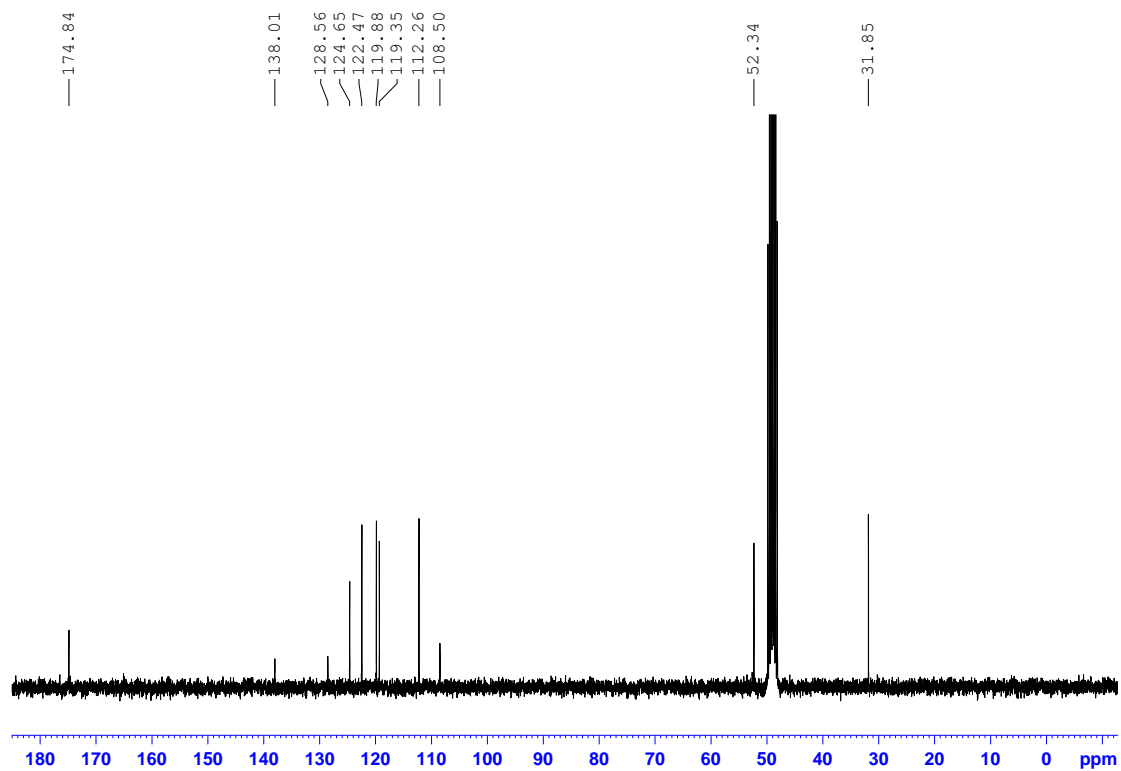


Figure S20: ^{13}C NMR spectrum of **6** in CD_3OD

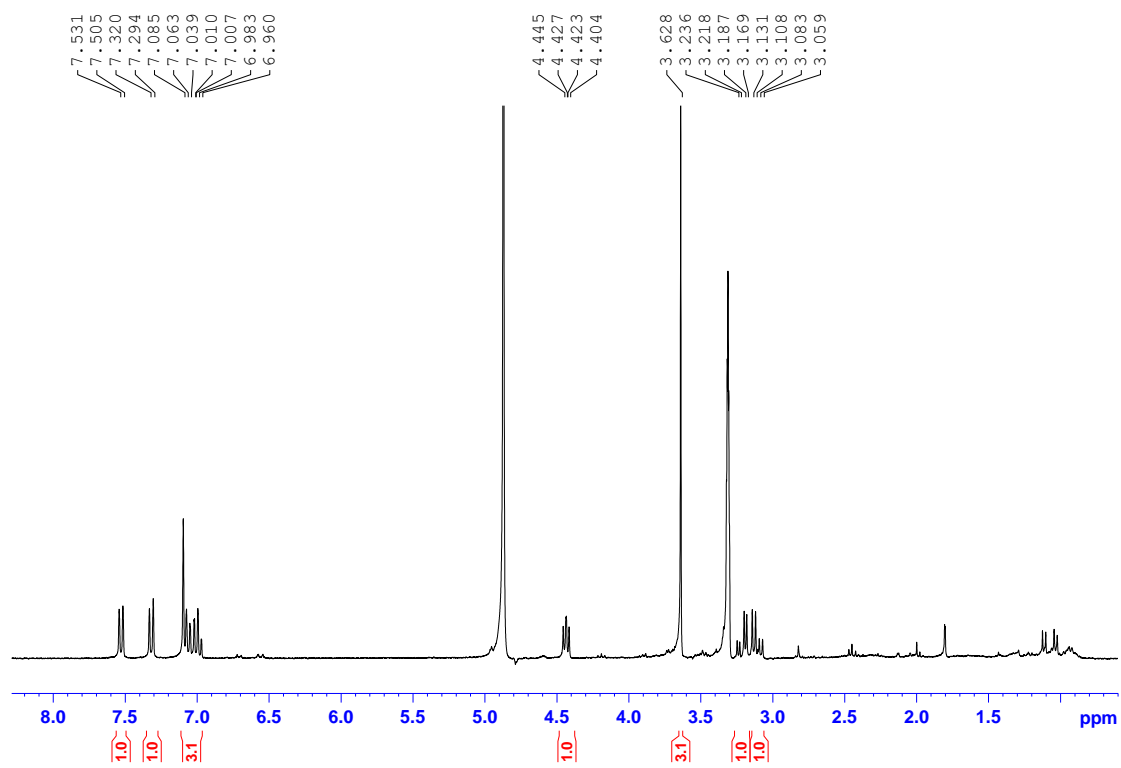
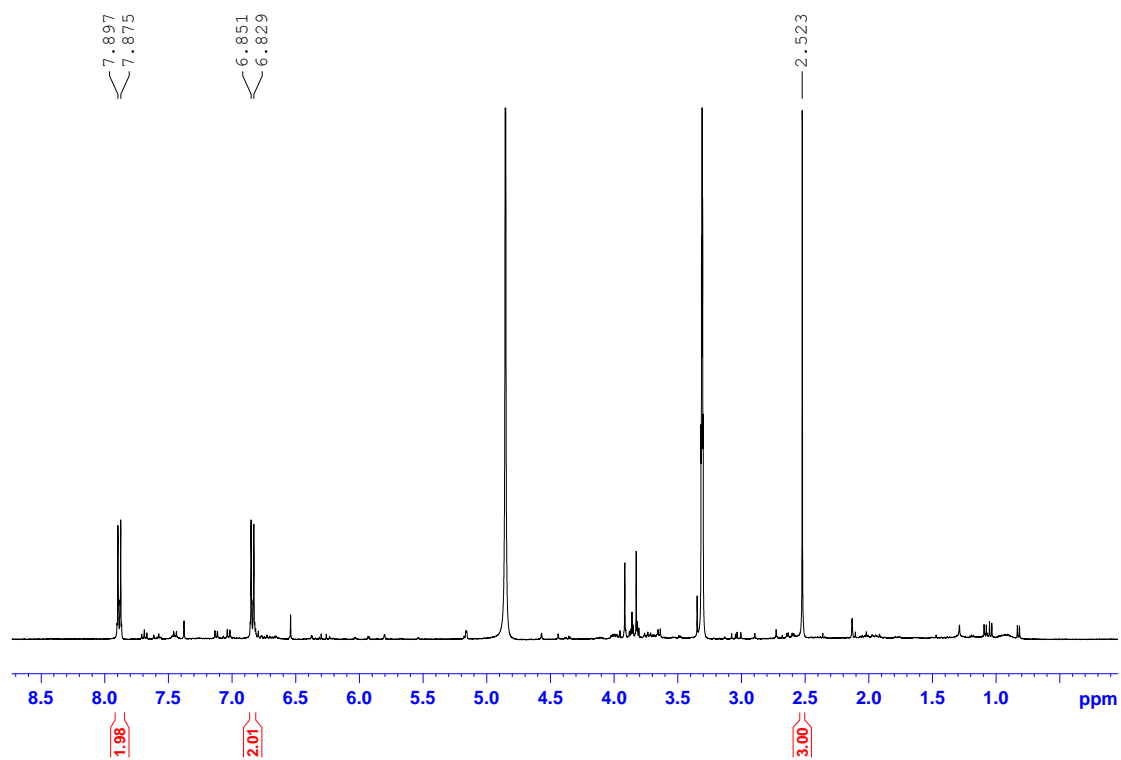
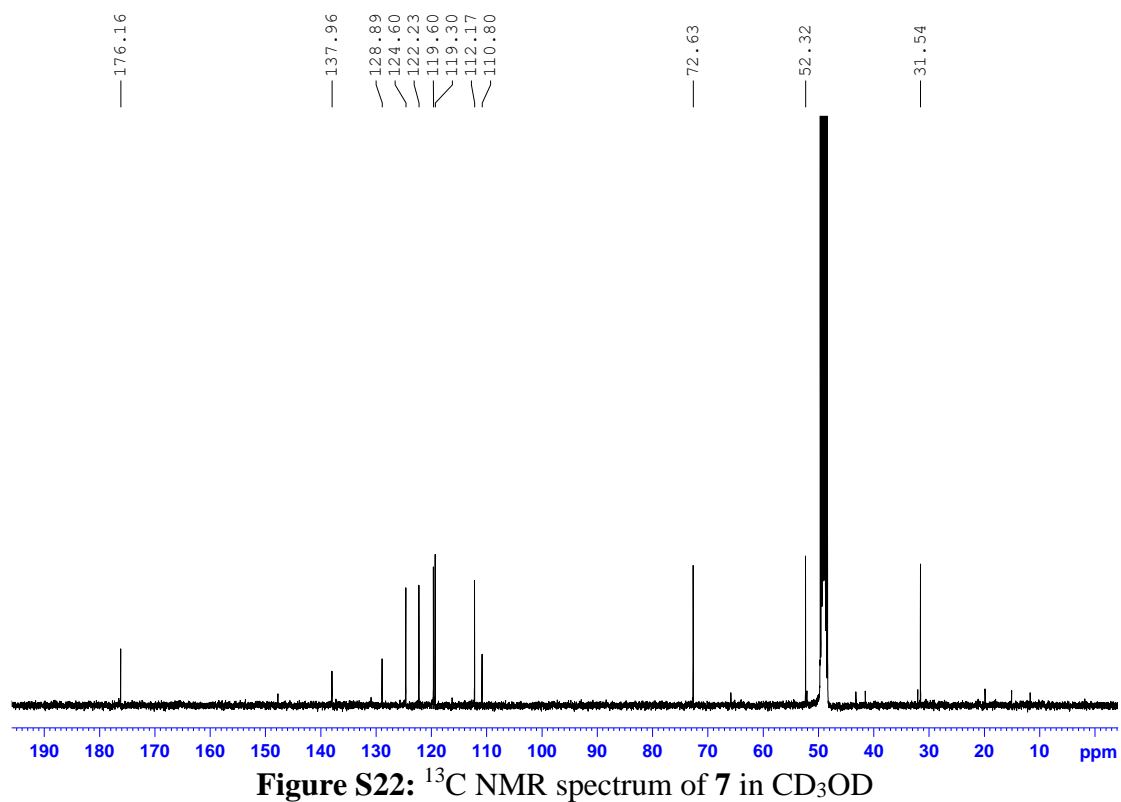


Figure S21: ^1H NMR spectrum of **7** in CD_3OD



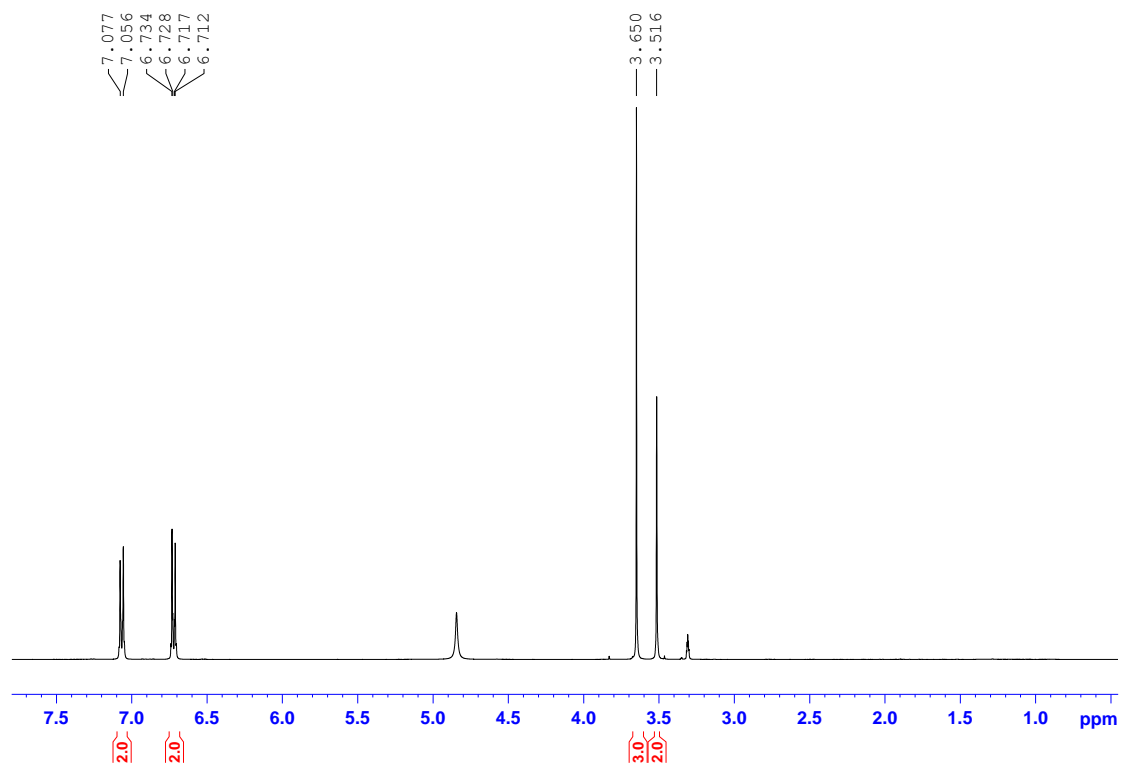


Figure S24: ^1H NMR spectrum of **9** in CD_3OD

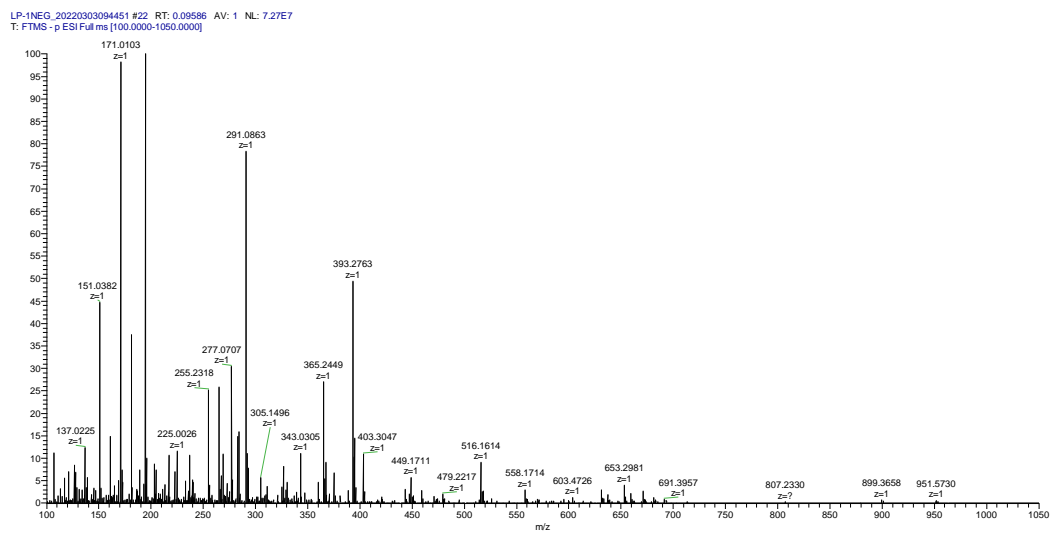


Figure S25: HRESIMS spectrum of **1**

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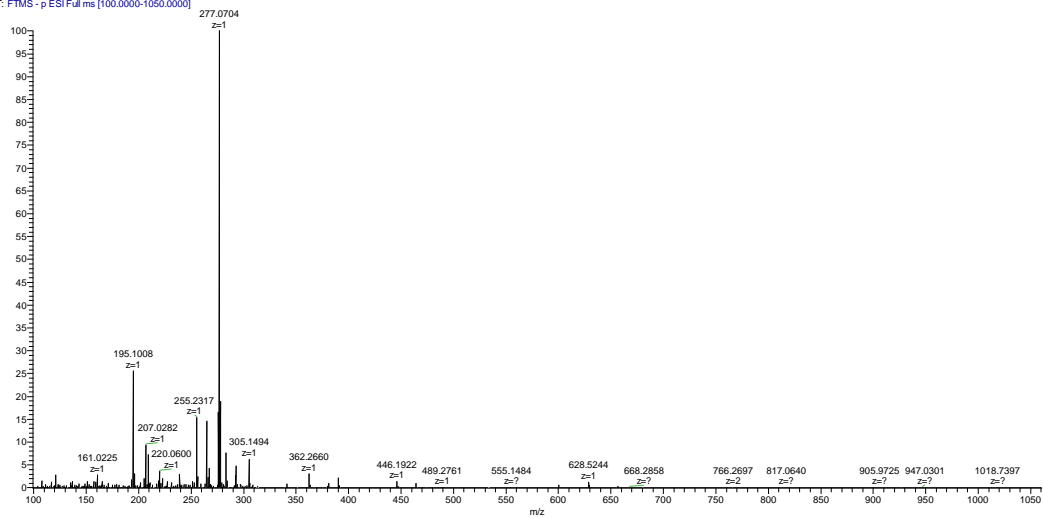


Figure S26: HRESIMS spectrum of 2

LP-4NEG_20220303094907 #33-34 RT: 0.14420-0.14858 AV: 2 NL: 4.31E8
T: FTMS - p ESI Full ms [100.0000-1050.0000]

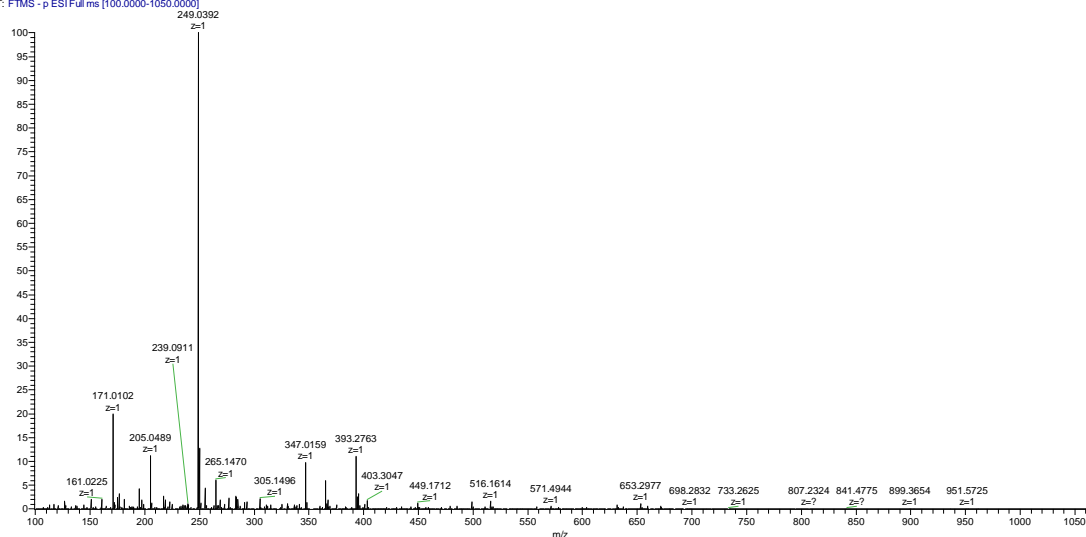


Figure S27: HRESIMS spectrum of 3

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REFERENCES

- Research Topic
- Author Name
- Company Name
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SUBSTANCES

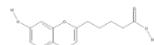
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- Markush
- Molecular Formula
- Property
- Substance Identifier

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- Reaction Structure

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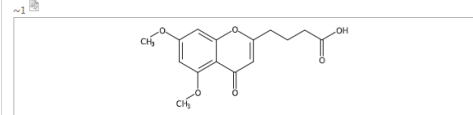
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- Occurrence
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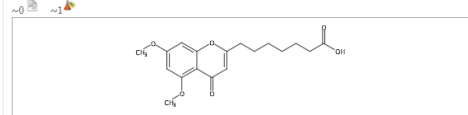
1. 1621594-60-2



C₁₅H₁₆O₆
4,7-Dimethoxy-2-butanoylbenzopyran-4-oxo-5,7-dimethoxy-4-oxo-
Key Physical Properties

Score: 96

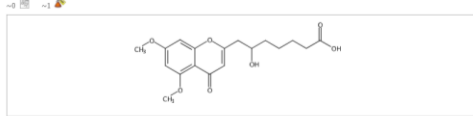
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C₁₈H₂₂O₆
4,7-Dimethoxy-2-heptanoylbenzopyran-4-oxo-5,7-dimethoxy-4-oxo-
Key Physical Properties

Score: 93

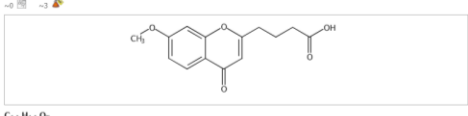
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C₁₈H₂₂O₇
4,7-Dimethoxy-2-(4-hydroxyheptanoyl)benzopyran-4-oxo-5,7-dimethoxy-4-oxo-
Key Physical Properties

Score: 91

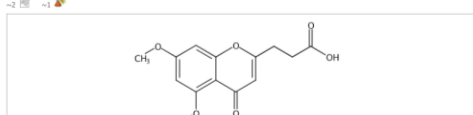
4. 927978-07-2



C₁₄H₁₄O₆
4,7-Dimethoxy-2-butanoylbenzopyran-4-oxo-7-methoxy-4-oxo-
Key Physical Properties

Score: 90

5. 1083202-36-1



C₁₄H₁₄O₆
4,7-Dimethoxy-2-propanoylbenzopyran-4-oxo-5,7-dimethoxy-4-oxo-
Key Physical Properties

Figure S28: Search report of SciFinder for compound 1
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REFERENCES

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- Company Name
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- Journal
- Patent
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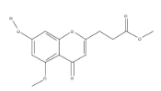
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- Molecular Formula
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- Substance Identifier

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- Reaction Structure

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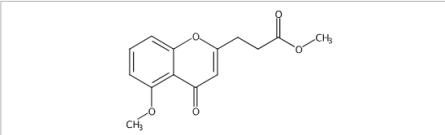
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- Preparation: 2

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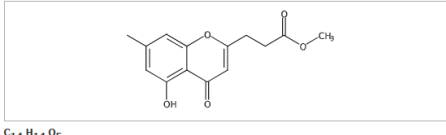
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$C_{14}H_{14}O_5$
471-Benzopyran-2-propanoic acid, 5-methoxy-4-oxo-, methyl ester
Key Physical Properties

Score: 90
2. 1660953-60-5



$C_{14}H_{14}O_5$
473-Benzopyran-2-propanoic acid, 5-hydroxy-7-methyl-4-oxo-, methyl ester
Key Physical Properties

Score: 90
3. 2376784-45-9

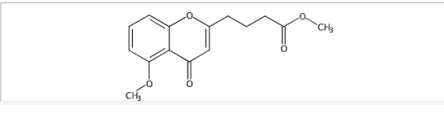


Figure S29: Search report of SciFinder for compound 2

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- Company Name
- Document Identifier
- Journal
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- Tags

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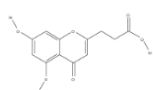
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- Molecular Formula
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- Substance Identifier

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85-89	14
80-84	39
75-79	144
70-74	493
65-69	2460
0-64 (least similar)	8767

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Substance Role

Biological Study 1

Occurrence 1

Properties 1

Reactant or Reagent 1

Uses 1

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Score: 95
1. 1660953-61-6



$C_{13}H_{12}O_5$
4H-1-Benzopyran-2-propanoic acid, 5-hydroxy-7-methyl-4-oxo-
Key Physical Properties

Score: 92
2. 927971-89-9



$C_{13}H_{12}O_5$
4H-1-Benzopyran-2-propanoic acid, 7-methoxy-4-oxo-
Key Physical Properties

Score: 92
3. 1083202-36-1



$C_{14}H_{14}O_6$
4H-1-Benzopyran-2-propanoic acid, 5,7-dimethoxy-4-oxo-
Key Physical Properties

Figure S30: Search report of SciFinder for compound 3

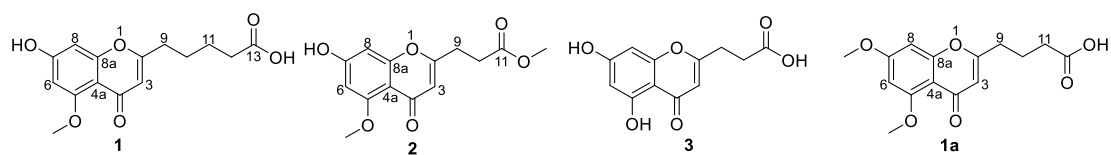


Table S1: NMR data of compounds **1–3** and the known analog **1a**

No.	1		2		3		1a ^[1]	
	δ_{H}	δ_{C}	δ_{H}	δ_{C}	δ_{H}	δ_{C}	δ_{H}	δ_{C}
2		165.8		167.6		170.9		166.2
3	5.87, s	110.4	6.00, s	111.1	6.09, s	108.5	5.95, s	110.7
4		175.7		179.9		183.9		178.3
4a		107.0		108.1		105.2		108.2
5		160.7		162.5		163.3		160.5
6	6.34, d (1.9)	95.1	6.39, d (1.9)	96.2	6.19, d (2.1)	100.1	6.25, br s	95.9
7		162.6		165.0		166.0		164.1
8	6.35, d (1.9)	96.4	6.39, d (1.9)	97.4	6.33, d (2.1)	94.9	6.36, br s	92.5
8a		159.5		161.6		159.8		160.0
9	2.53, t (7.0)	32.3	2.90, t (7.1)	29.6	2.93, t (7.2)	30.3	2.53, t (8.0)	32.5
10	1.61, m	25.6	2.75, t (7.1)	31.4	2.73, t (7.2)	31.6	1.94, qunit (8.0)	21.6
11	1.53, m	23.9		174.0		175.4	2.32, t (8.0)	32.6
12	2.24, t (7.2)	33.4						
13		174.5						
5-OCH ₃	3.75, s	55.9	3.86, s	56.4			3.80, s	55.8
11-OCH ₃			3.69, s	52.4				
7-OCH ₃							3.78, s	55.5

References

- [1] W. H. Yuan, Z. W. Wei, P. Dai, H. Wu, Y. X. Zhao, M. M. Zhang, N. Jiang and W. F. Zheng (2014). Halogenated metabolites isolated from *Penicillium citreonigrum*, *Chem. Biodivers.* **11**, 1078-1087.