

Supporting Information

New Monoterpenoids and Polyketides from the Deep-Sea Sediment-Derived Fungus *Aspergillus sydowii* MCCC 3A00324

Siwen Niu^{a,b,†,*}, Longhe Yang^{b,†}, Tingting Chen^b, Bihong Hong^{b,*}, Shengxiang Pei^a,
Zongze Shao^a, Gaiyun Zhang^{a,*}

^a *Key Laboratory of Marine Genetic Resources, Third Institute of Oceanography,
Ministry of Natural Resources, Xiamen 361005, People's Republic of China*

^b *Technology Innovation Center for Exploitation of Marine Biological Resources, Third
Institute of Oceanography, Ministry of Natural Resources, Xiamen 361005, People's
Republic of China*

***Corresponding authors:** Siwen Niu, Bihong Hong, and Gaiyun Zhang

E-mail addresses: niusiwen@tio.org.cn (S. Niu), bhhong@tio.org.cn (B. Hong), and
zhgyun@tio.org.cn (G. Zhang)

Author contributions

[†] S. Niu and L. Yang contributed equally to this work.

Contents	Pages
Figure S1. HPLC and TLC profiles of the extract from the deep-sea-derived <i>Aspergillus sydowii</i> MCCC 3A00324.	S3
Figure S1-1. HRESIMS spectrum of 1 .	S4
Figure S1-2. ¹ H NMR spectrum of 1 in CD ₃ OD (400 MHz).	S5
Figure S1-3. ¹³ C NMR spectrum of 1 in CD ₃ OD (100 MHz).	S6
Figure S1-4. HSQC spectrum of 1 in CD ₃ OD.	S7
Figure S1-5. COSY spectrum of 1 in CD ₃ OD.	S8
Figure S1-6. HMBC spectrum of 1 in CD ₃ OD.	S9
Figure S1-7. NOESY spectrum of 1 in CD ₃ OD.	S10
Figure S2-1. HRESIMS spectrum of 2 .	S11
Figure S2-2. ¹ H NMR spectrum of 2 in CD ₃ OD (400 MHz).	S12
Figure S2-3. ¹³ C NMR spectrum of 2 in CD ₃ OD (100 MHz).	S13
Figure S2-4. HSQC spectrum of 2 in CD ₃ OD.	S14
Figure S2-5. COSY spectrum of 2 in CD ₃ OD.	S15
Figure S2-6. HMBC spectrum of 2 in CD ₃ OD.	S16
Figure S2-7. NOESY spectrum of 2 in CD ₃ OD.	S17
Figure S3-1. HRESIMS spectrum of 3 .	S18
Figure S3-2. ¹ H NMR spectrum of 3 in CD ₃ OD (400 MHz).	S19
Figure S3-3. ¹³ C NMR spectrum of 3 in CD ₃ OD (100 MHz).	S20
Figure S3-4. HSQC spectrum of 3 in CD ₃ OD.	S21
Figure S3-5. COSY spectrum of 3 in CD ₃ OD.	S22
Figure S3-6. HMBC spectrum of 3 in CD ₃ OD.	S23
Figure S4-1. HRESIMS spectrum of 4 .	S24
Figure S4-2. ¹ H NMR spectrum of 4 in DMSO- <i>d</i> ₆ (400 MHz).	S25
Figure S4-3. ¹³ C NMR spectrum of 4 in DMSO- <i>d</i> ₆ (100 MHz).	S26
Figure S4-4. HSQC spectrum of 4 in DMSO- <i>d</i> ₆ .	S27
Figure S4-5. COSY spectrum of 4 in DMSO- <i>d</i> ₆ .	S28
Figure S4-6. HMBC spectrum of 4 in DMSO- <i>d</i> ₆ .	S29

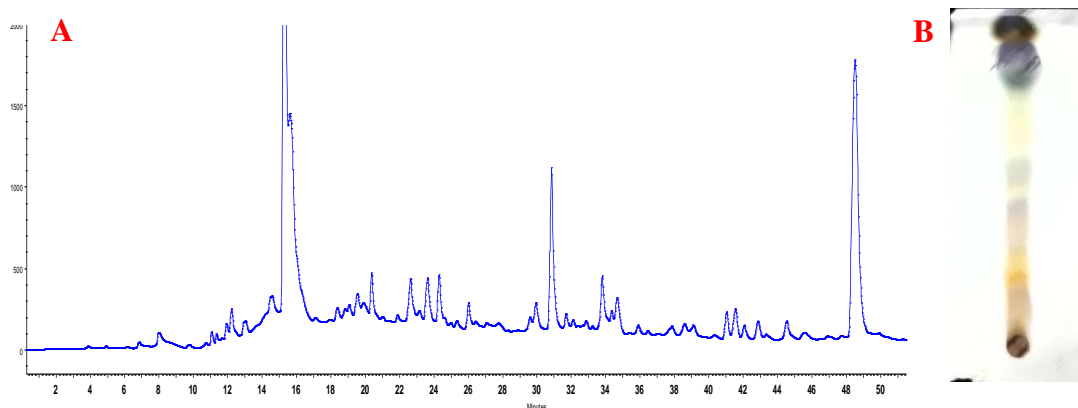


Figure S1. HPLC profile of the EtOAc extracts from the *Aspergillus sydowii* 3A00324 detected by UV absorption at 254 nm (Chromatographic conditions: MeOH/H₂O, 5%–100% 0–35 min, 100%–100% 35–45 min, 100%–5% 45–46 min, 5% 46–52 min) (A). TLC profile of the EtOAc extracts of the above fungus analyzed by vanillin sulfuric acid chromogenic reagent after heating (Mobile phase, CH₂Cl₂:MeOH = 10:1) (B).

P51-Sep-2 109 (0.429) Cm (104:115)

1: TOF MS ES+
6.17e6

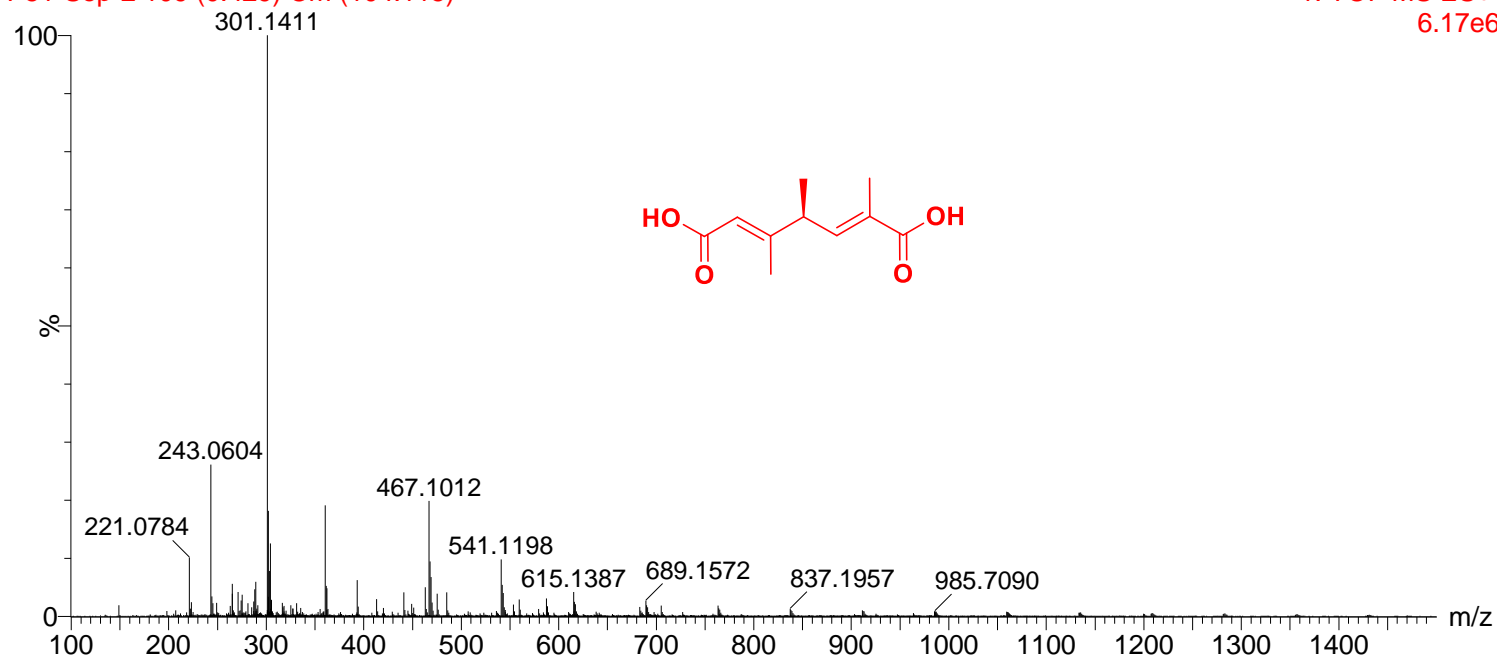


Figure S1-1. HRESIMS spectrum of 1.

^1H NMR spectrum of P51 in CD_3OD 400 MHz

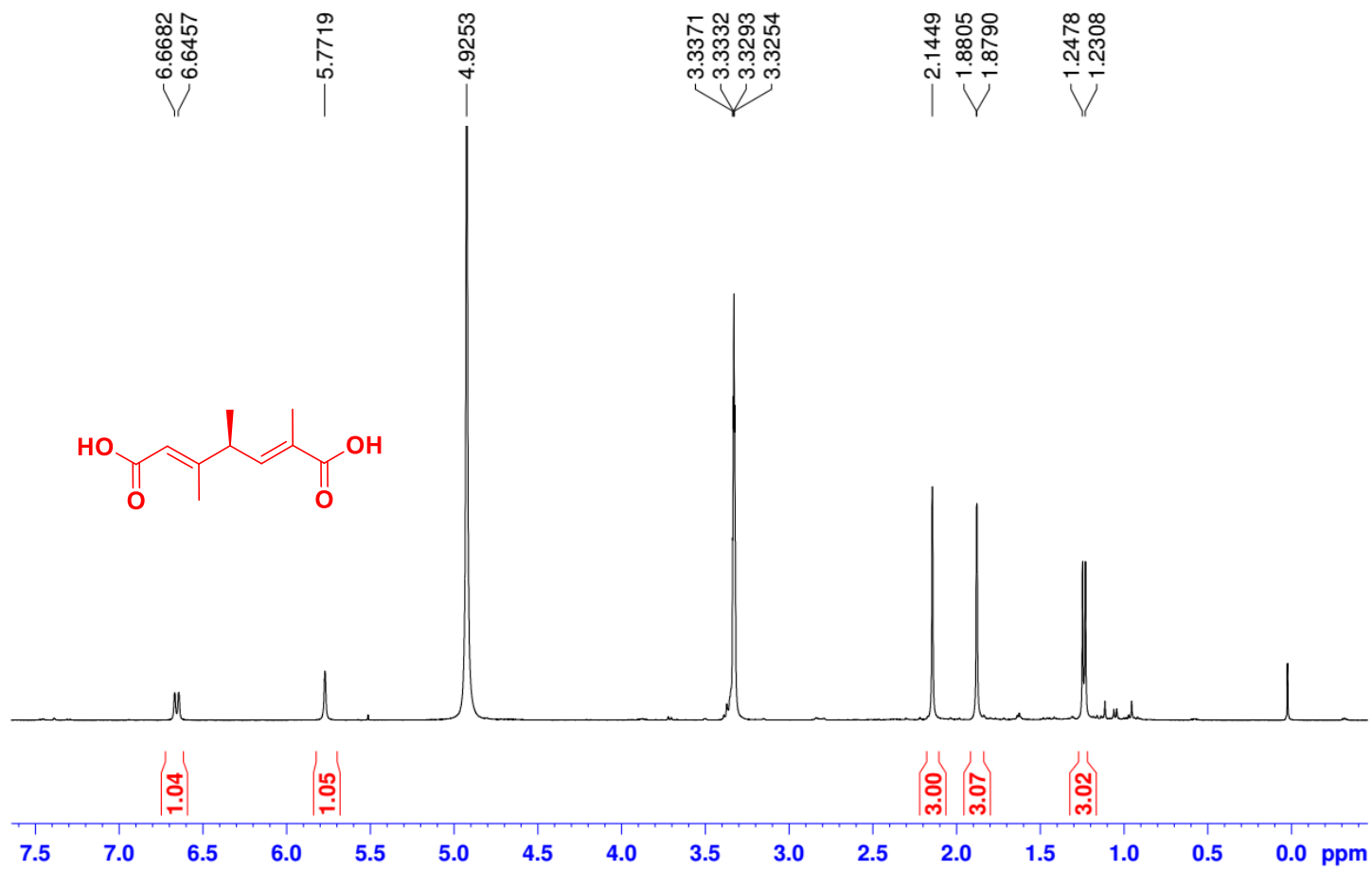


Figure S1-2. ^1H NMR spectrum of **1** in CD_3OD (400 MHz).

^{13}C NMR spectrum of P51 in CD_3OD 100 MHz

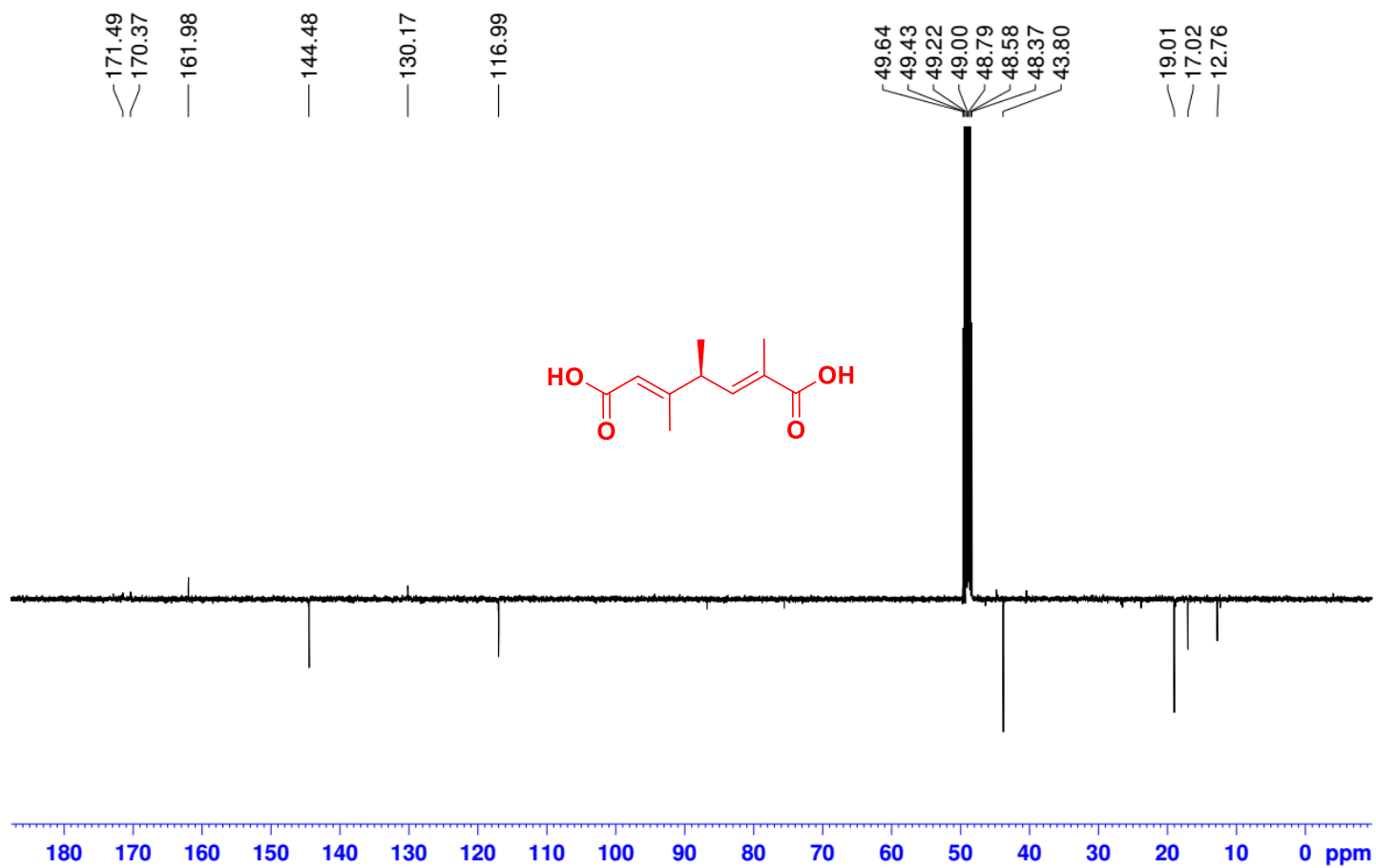


Figure S1-3. ^{13}C NMR spectrum of **1** in CD_3OD (100 MHz).

HSQC spectrum of P51 in CD3OD

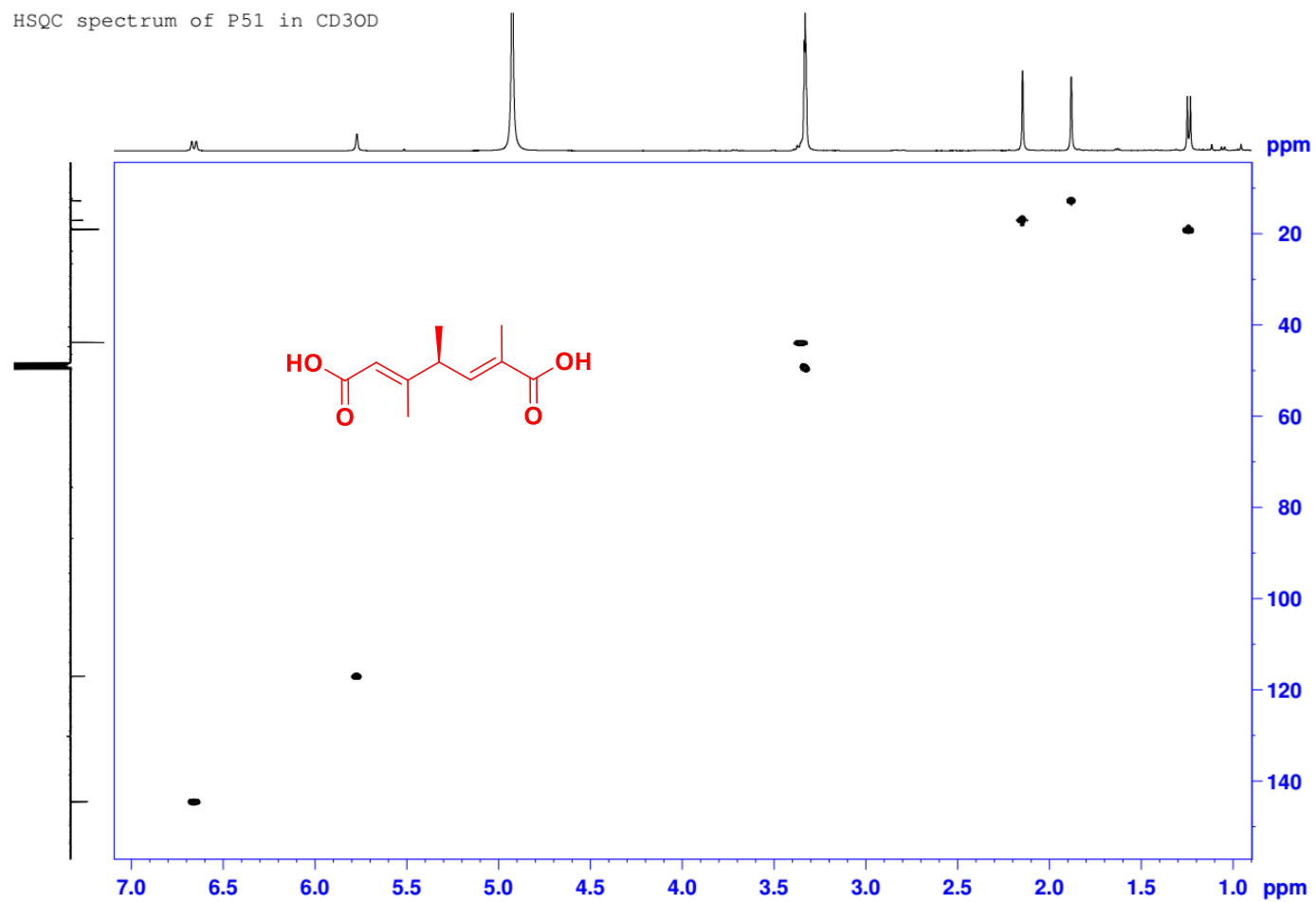


Figure S1-4. HSQC spectrum of **1** in CD₃OD.

COSY spectrum of P51 in CD3OD

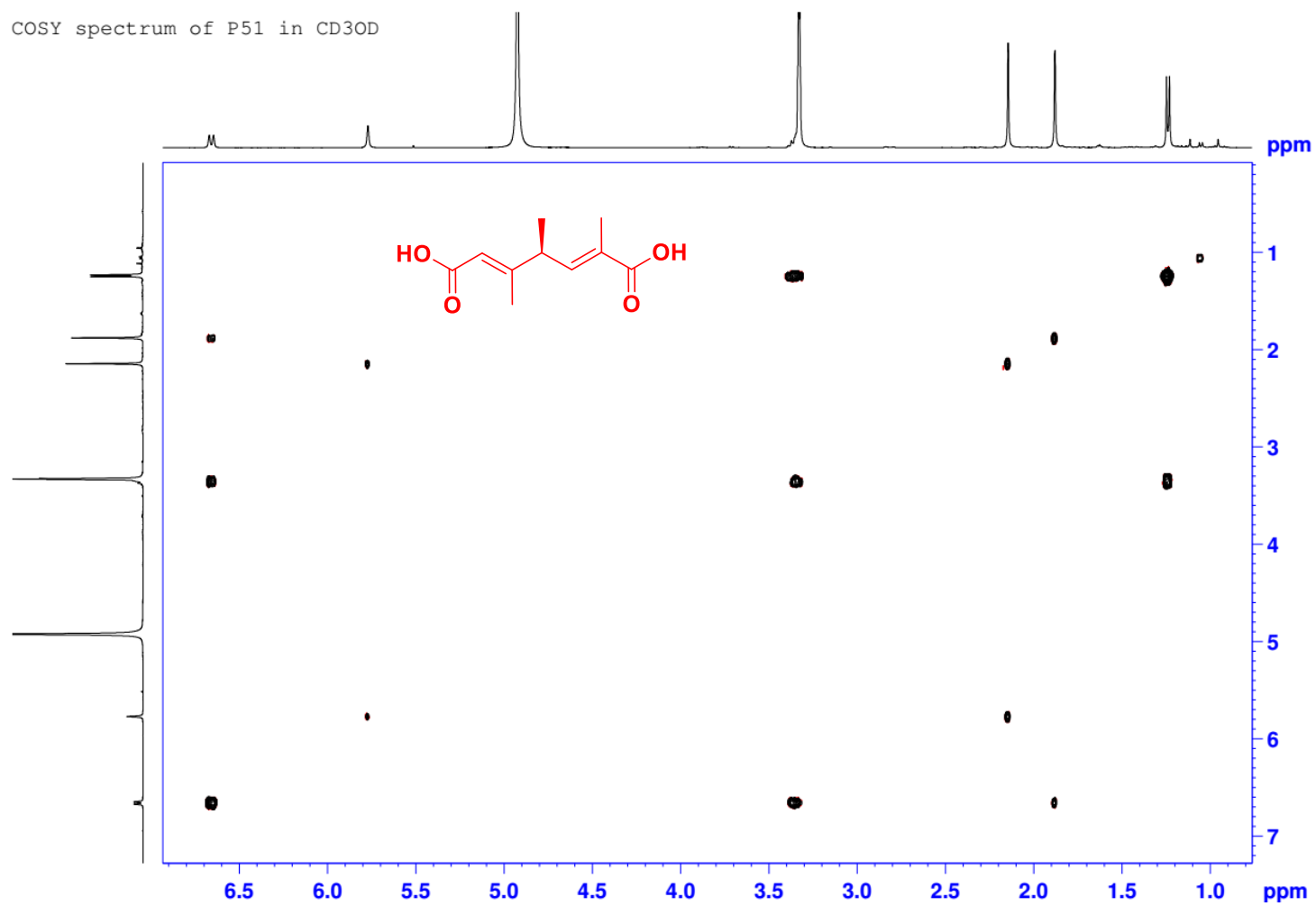


Figure S1-5. COSY spectrum of 1 in CD₃OD.

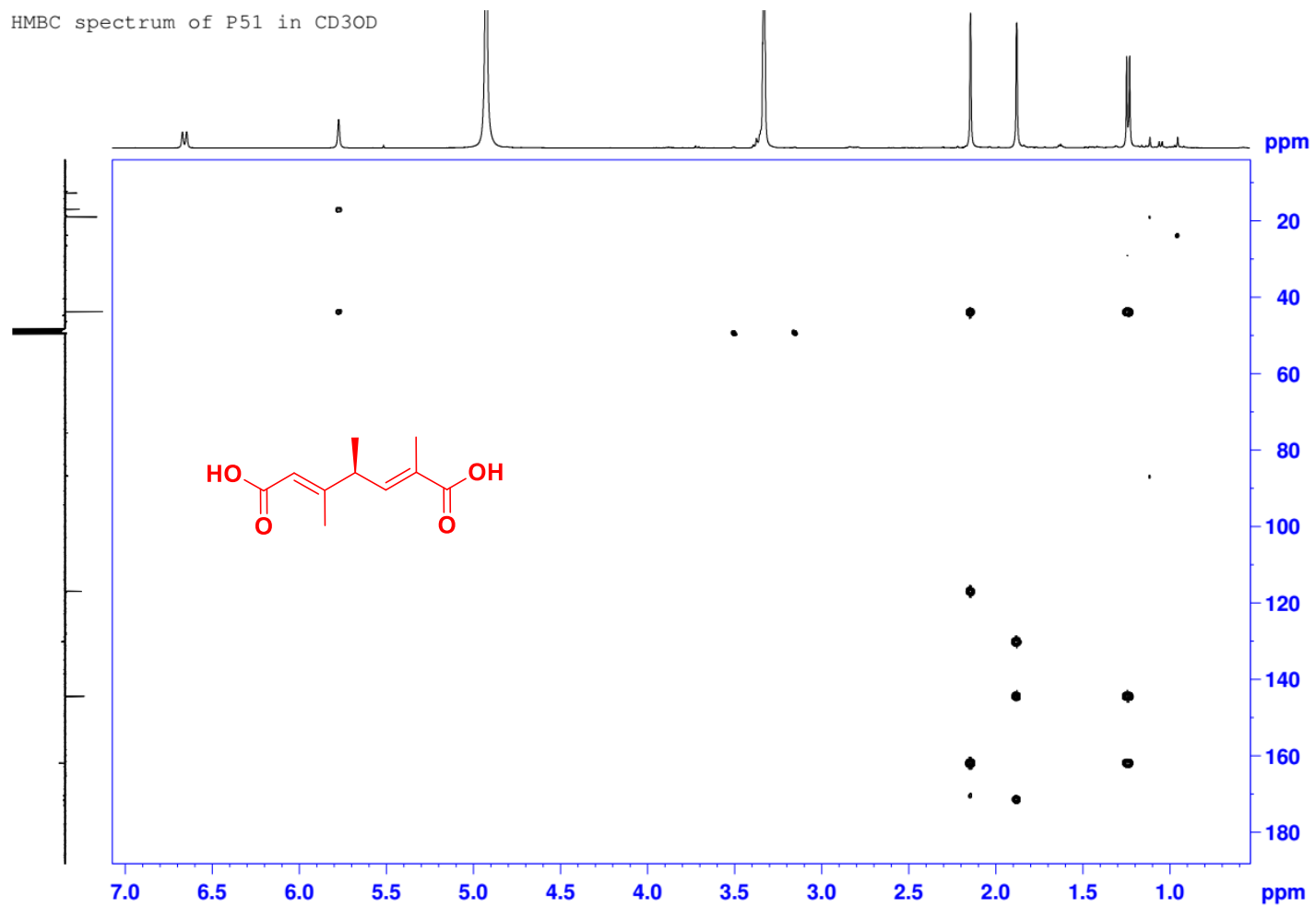


Figure S1-6. HMBC spectrum of **1** in CD₃OD.

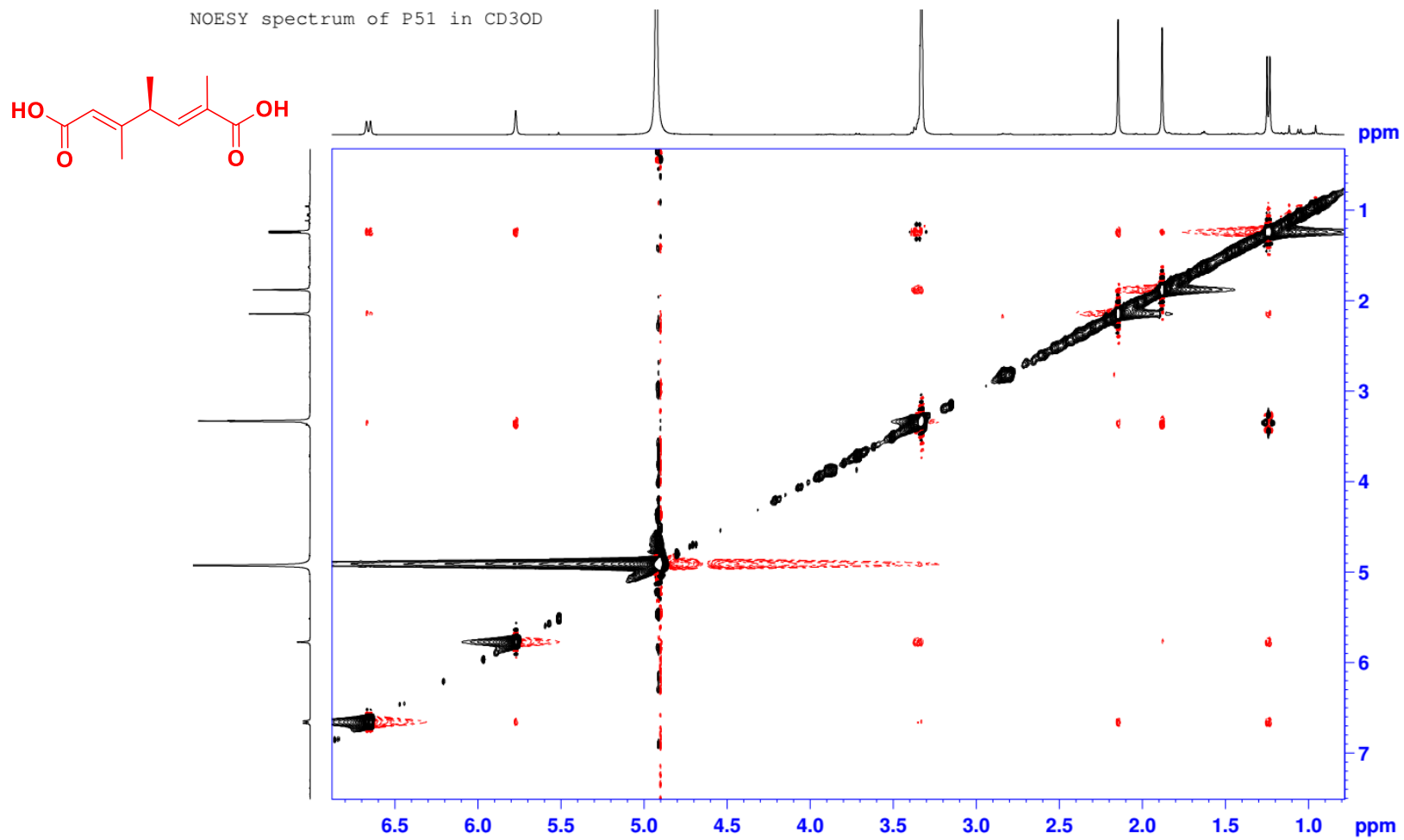


Figure S1-7. NOESY spectrum of 1 in CD₃OD.

P52-Sep-2 113 (0.443) Cm (108:118)

1: TOF MS ES+
1.79e7

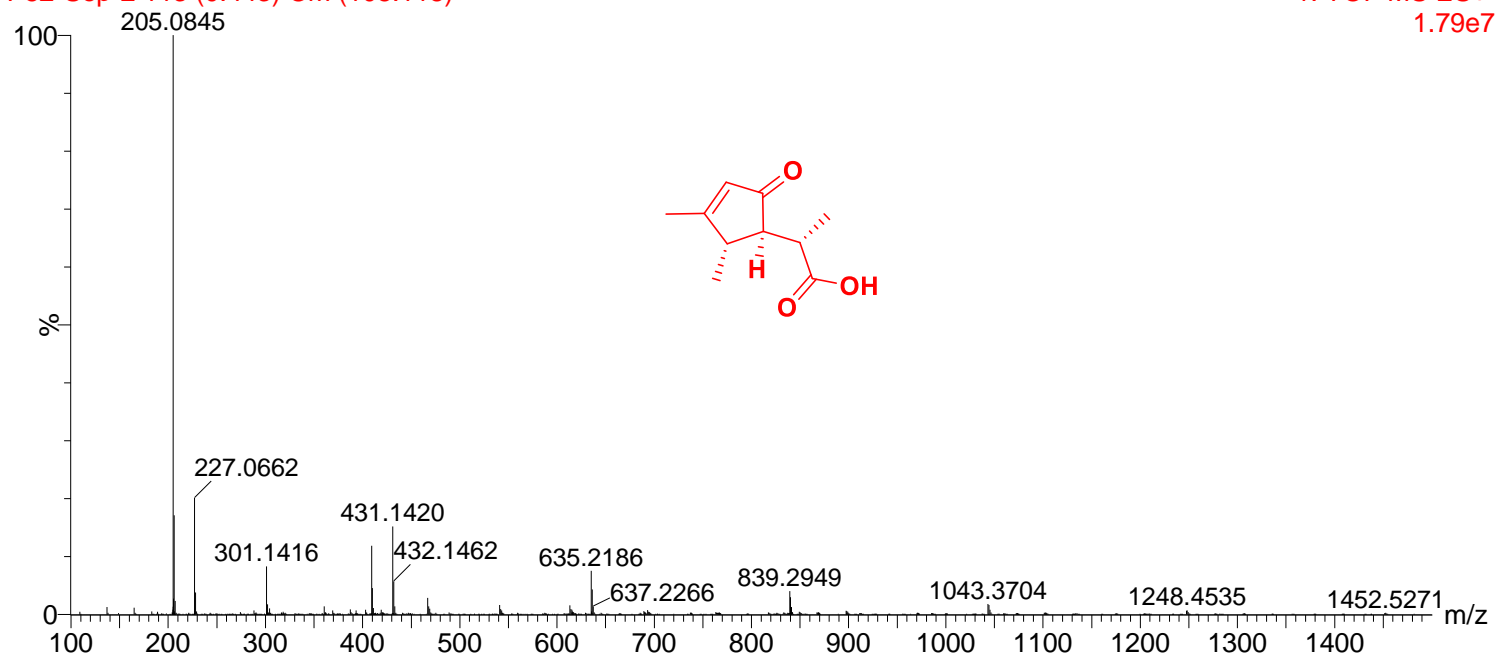


Figure S2-1. HRESIMS spectrum of 2.

¹H NMR spectrum of P52 in CD₃OD 400 MHz

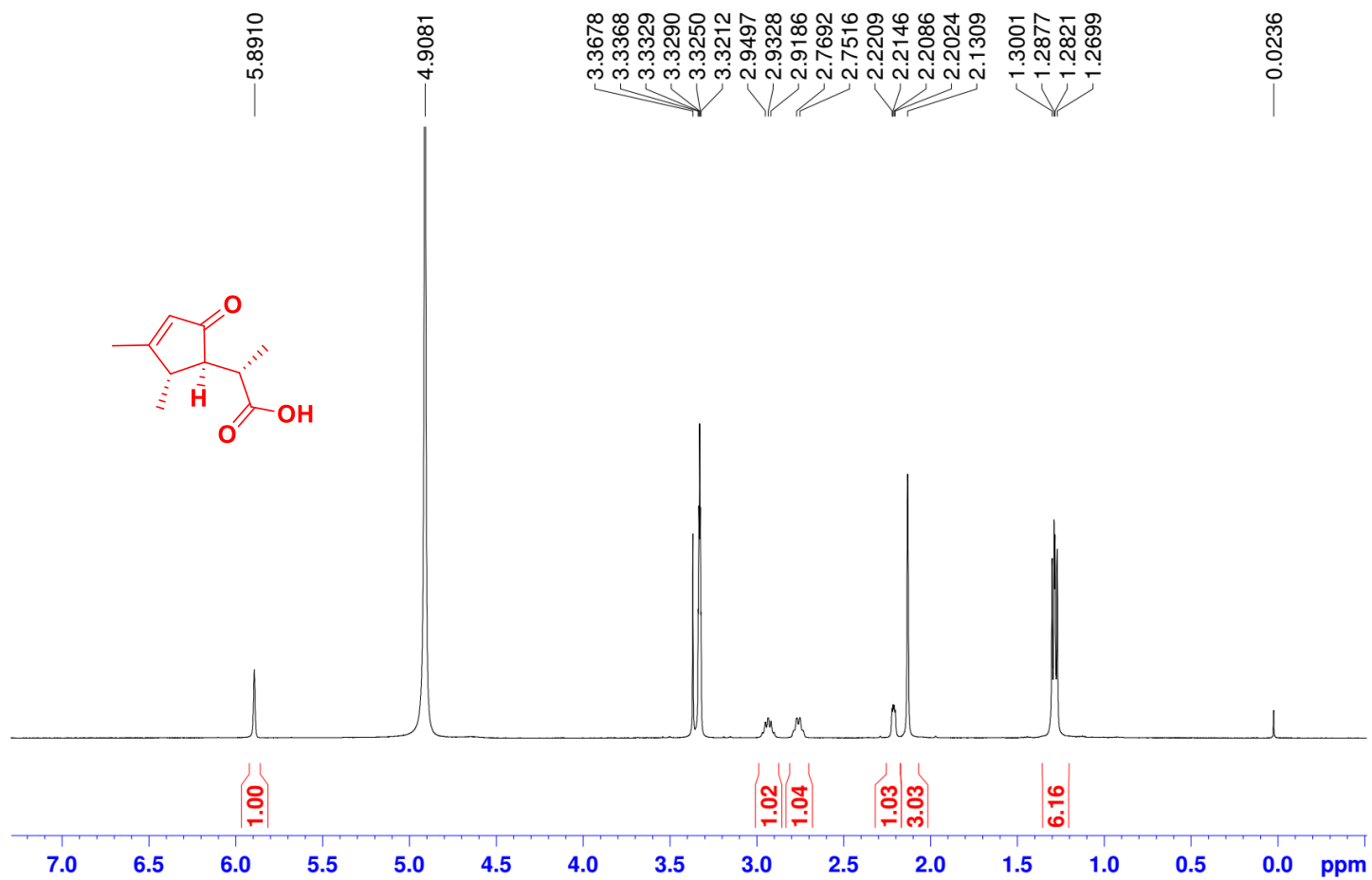


Figure S2-2. ¹H NMR spectrum of **2** in CD₃OD (400 MHz).

^{13}C NMR spectrum of P52 in CD_3OD 100 MHz

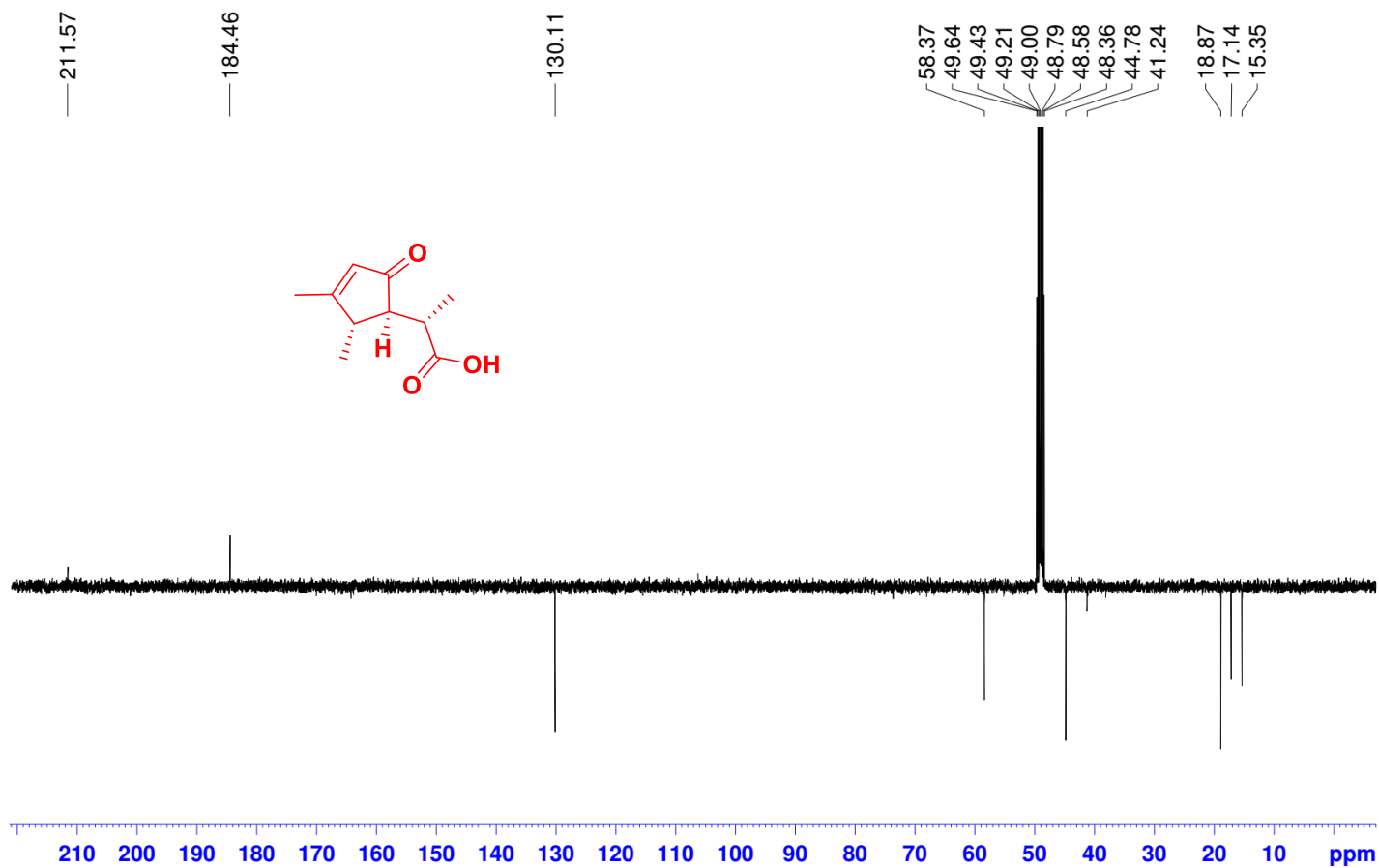


Figure S2-3. ^{13}C NMR spectrum of **2** in CD_3OD (100 MHz).

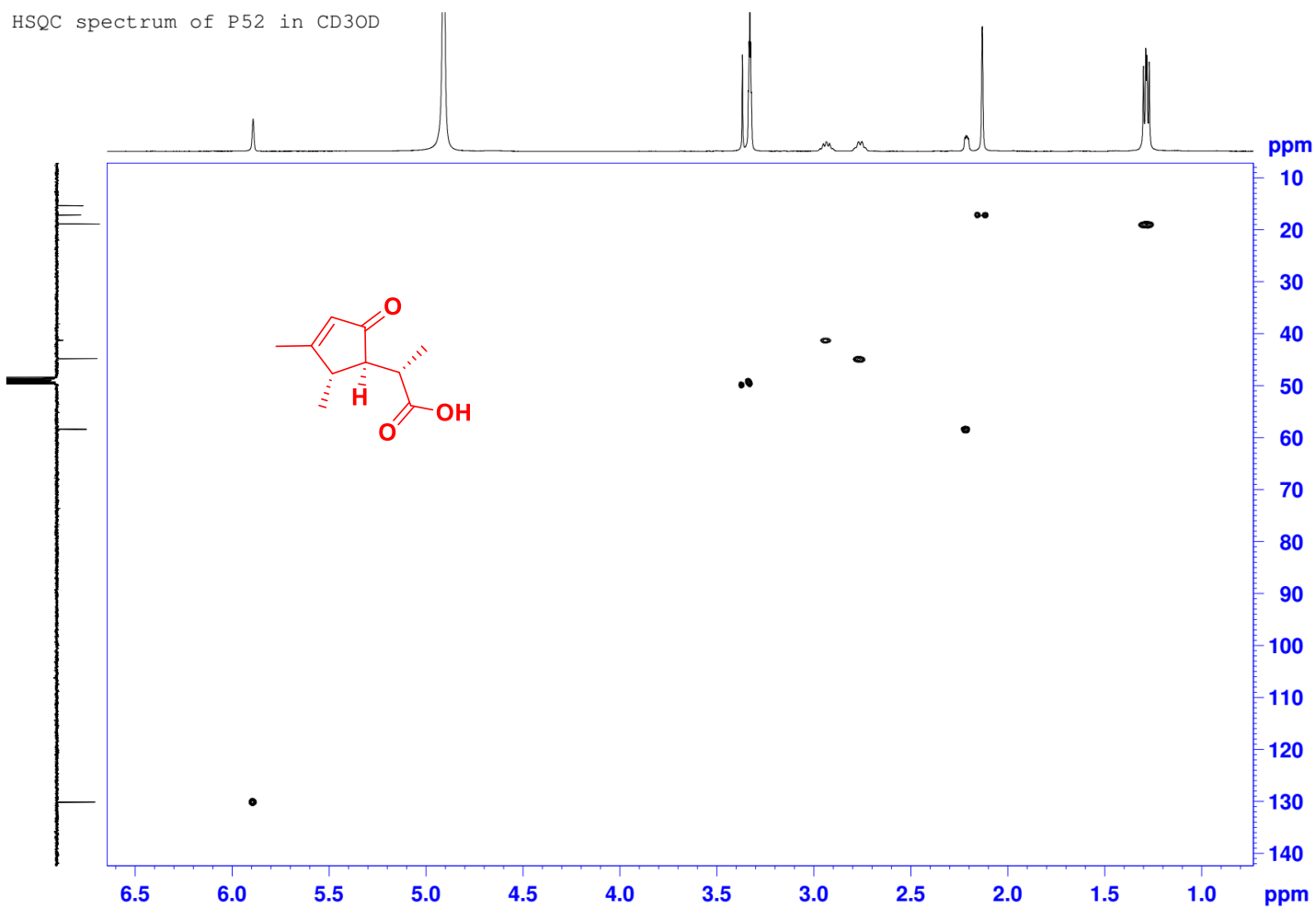


Figure S2-4. HSQC spectrum of **2** in CD₃OD.

COSY spectrum of P52 in CD3OD

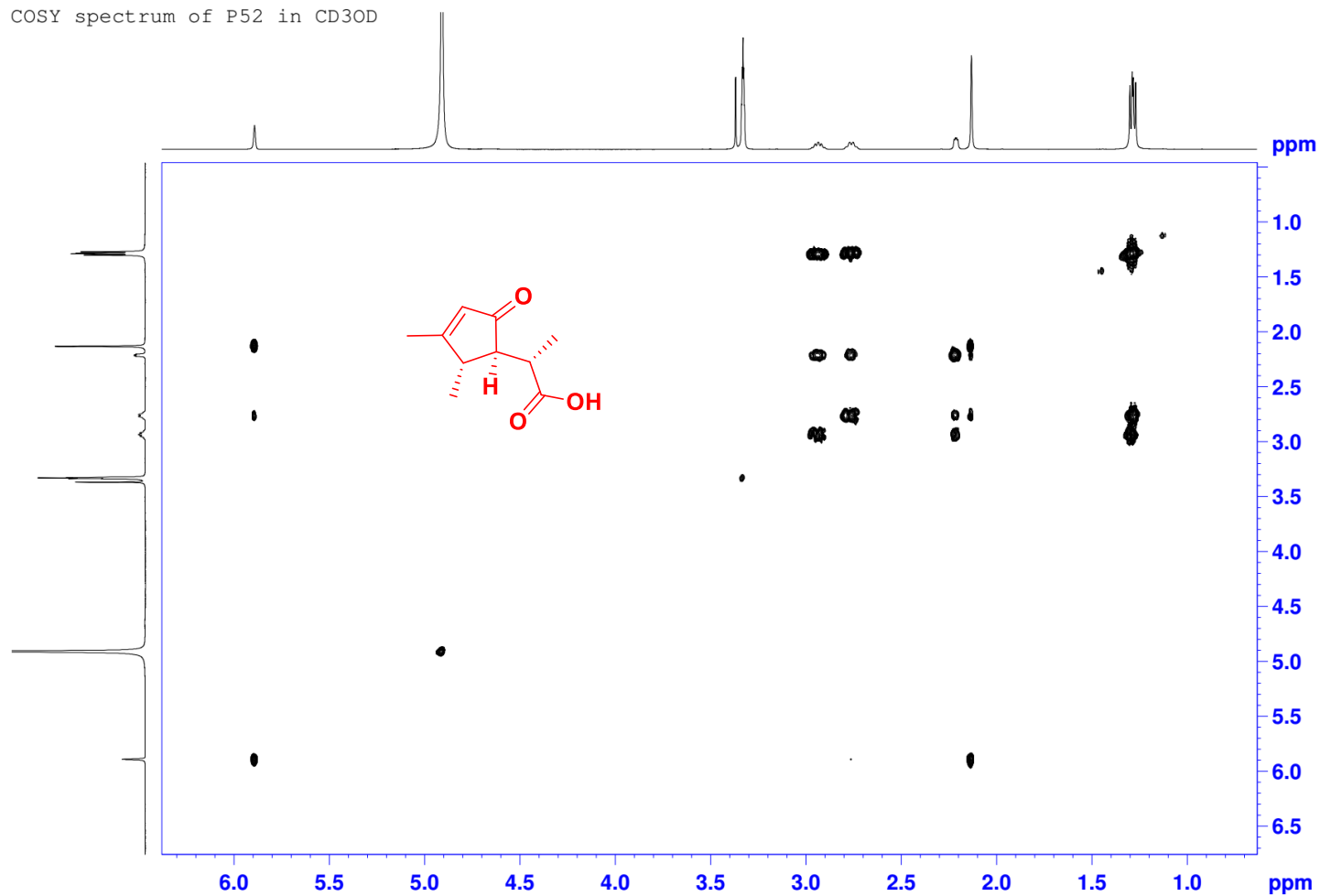


Figure S2-5. COSY spectrum of 2 in CD₃OD.

HMBC spectrum of P52 in CD3OD

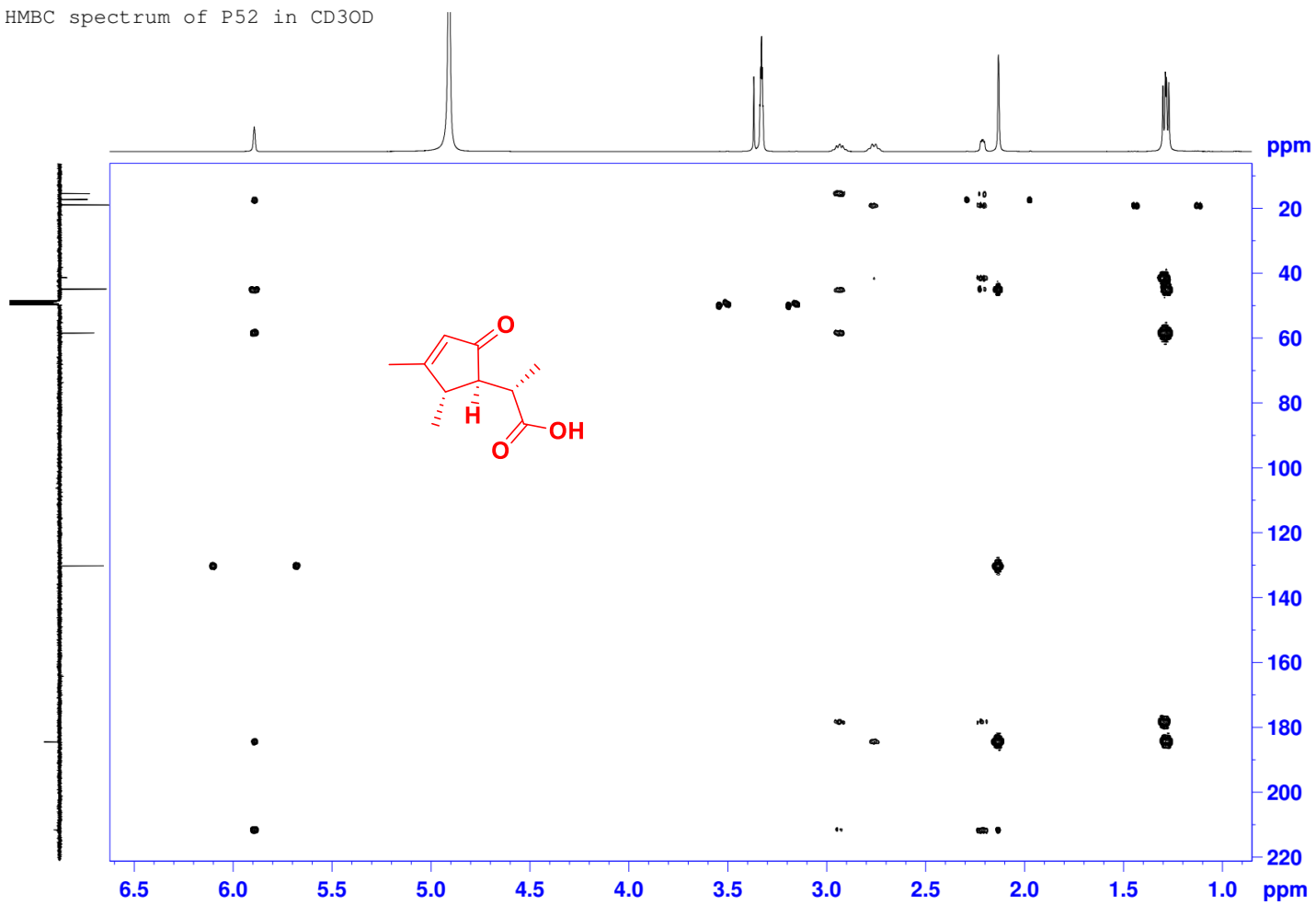


Figure S2-6. HMBC spectrum of 2 in CD₃OD.

NOESY spectrum of P52 in CD3OD

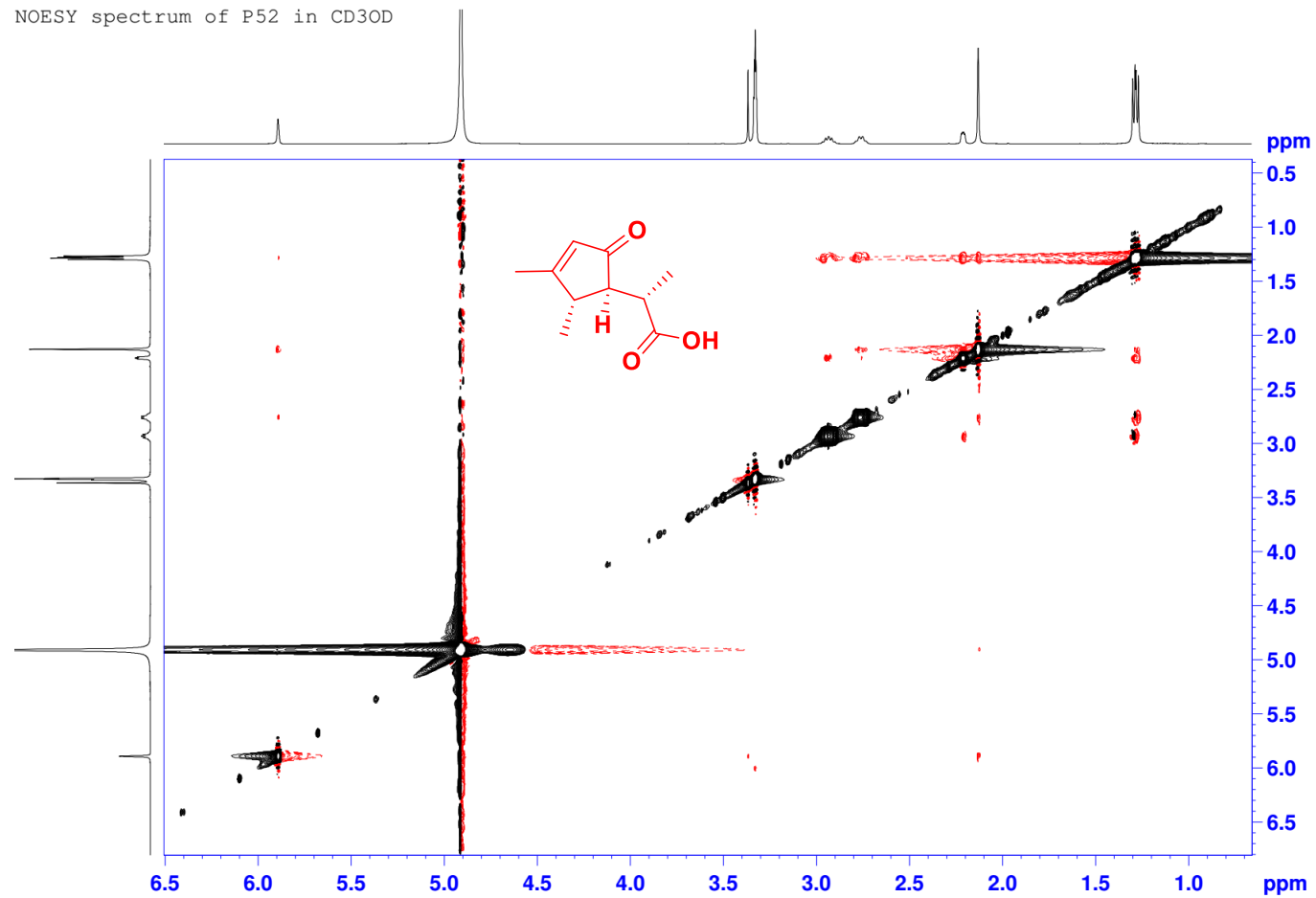


Figure S2-7. NOESY spectrum of **2** in CD₃OD.

P53-Sep-2 111 (0.436) Cm (97:113)

1: TOF MS ES+
1.12e7

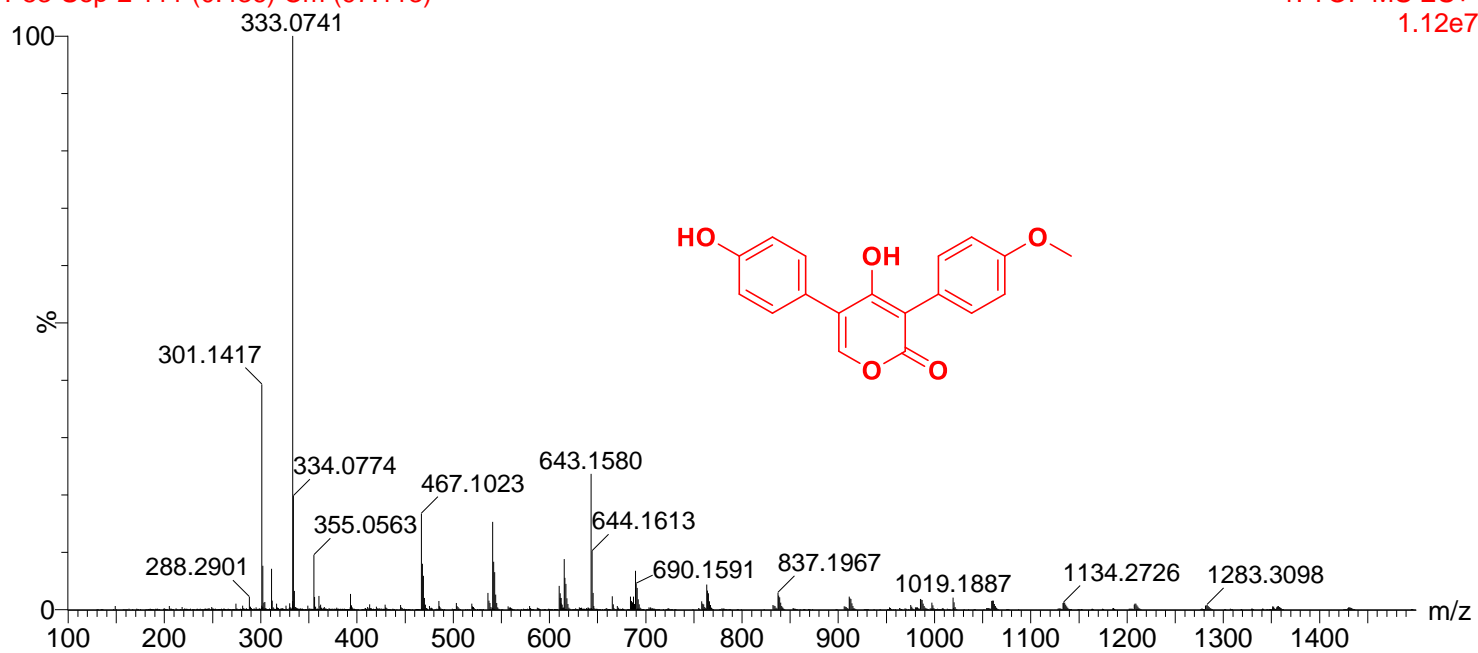


Figure S3-1. HRESIMS spectrum of **3**.

¹H NMR spectrum of P53 in CD₃OD 400 MHz

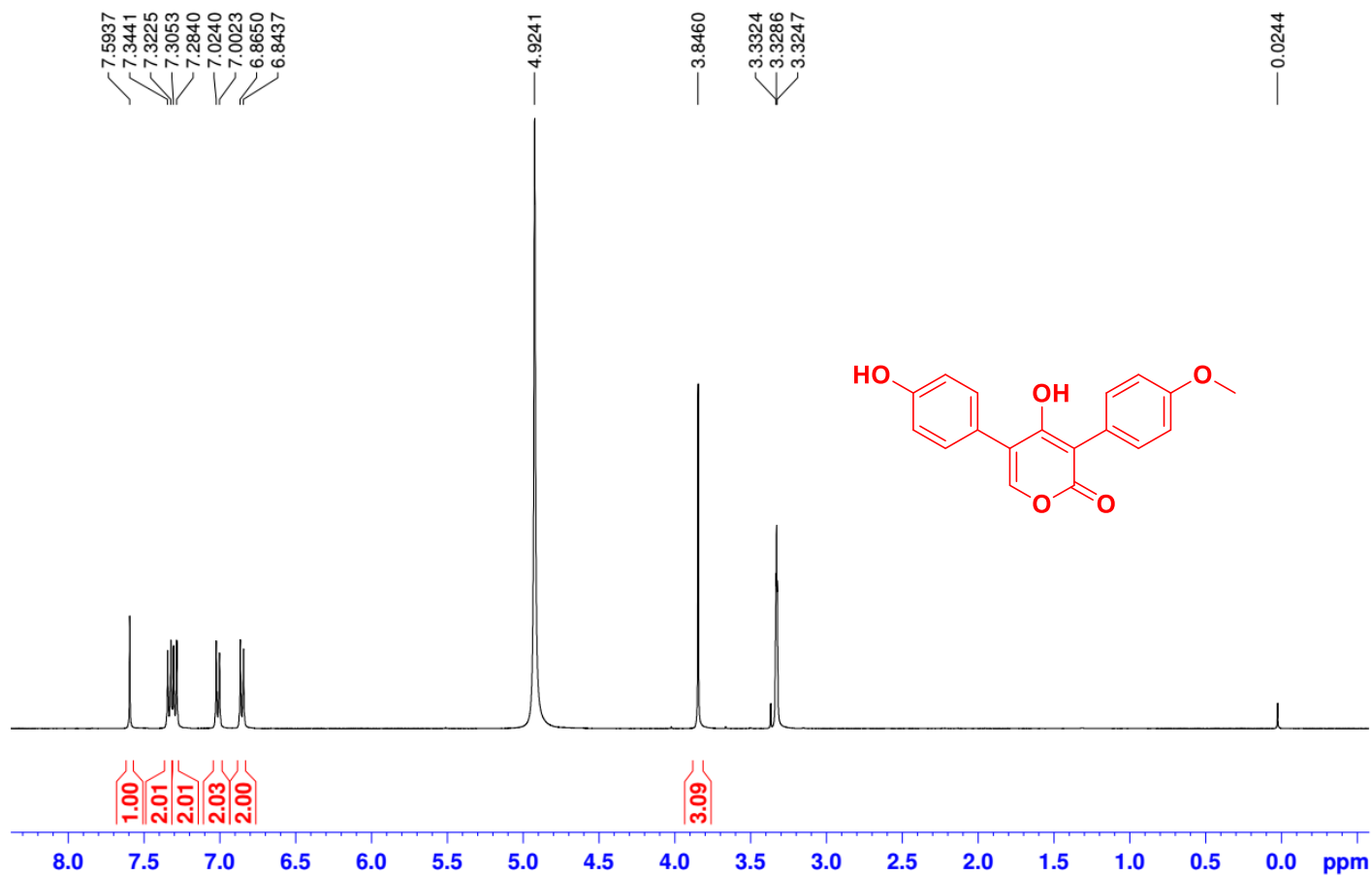


Figure S3-2. ¹H NMR spectrum of **3** in CD₃OD (400 MHz).

^{13}C NMR spectrum of P53 in CD_3OD 100 MHz

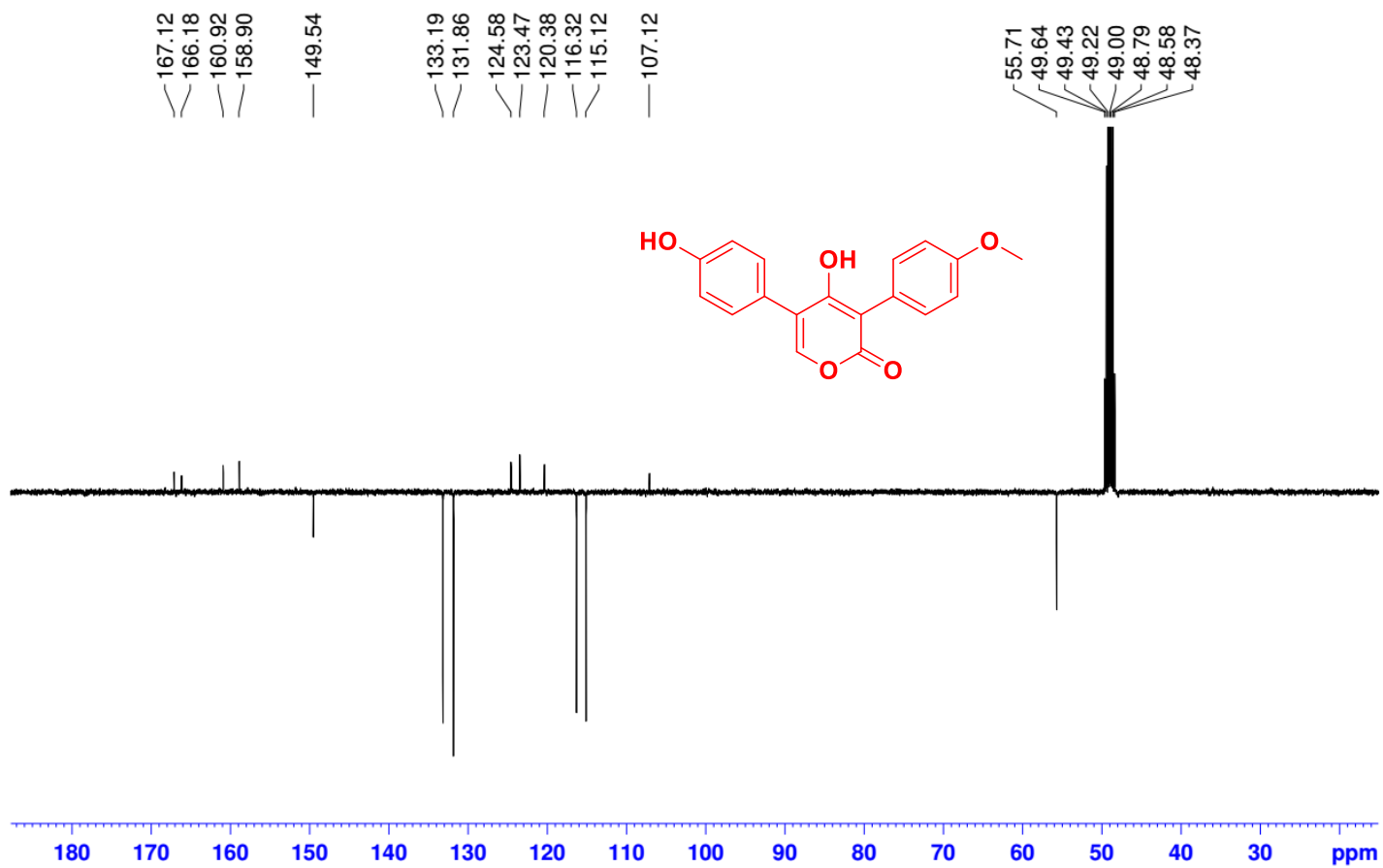


Figure S3-3. ^{13}C NMR spectrum of **3** in CD_3OD (100 MHz).

HSQC spectrum of P53 in CD3OD

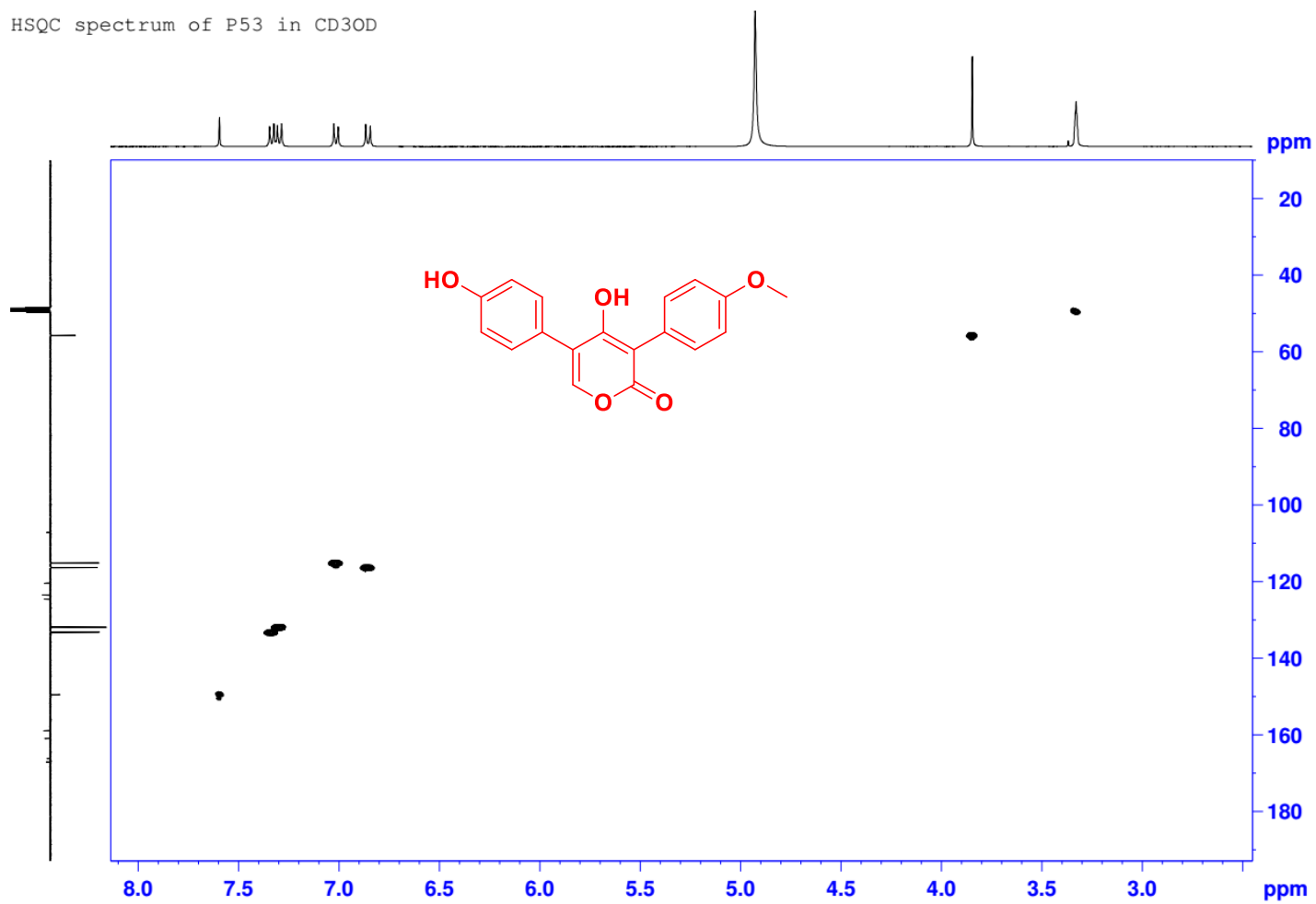


Figure S3-4. HSQC spectrum of 3 in CD₃OD.

COSY spectrum of P53 in CD3OD

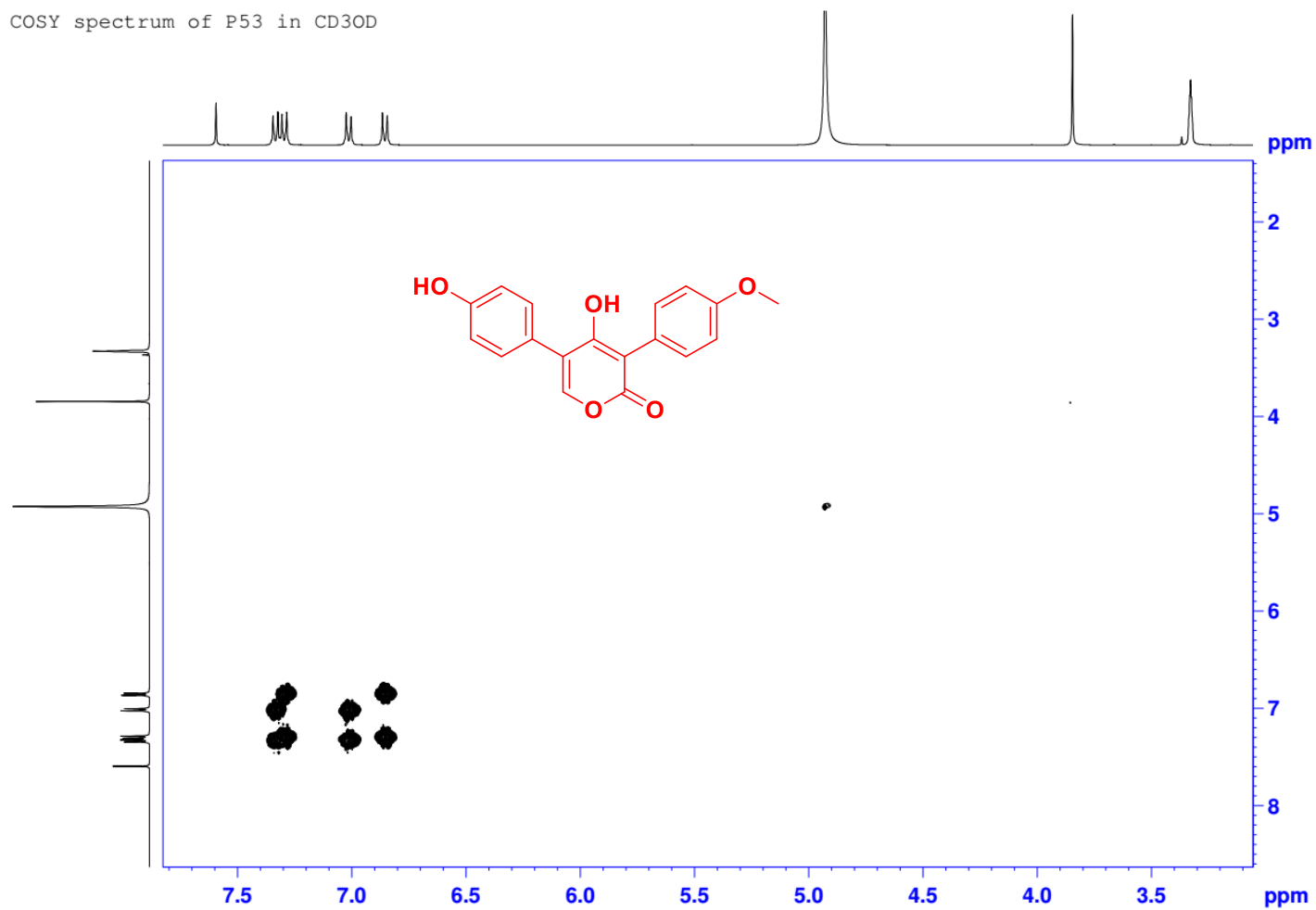


Figure S3-5. COSY spectrum of 3 in CD₃OD.

HMBC spectrum of P53 in CD3OD

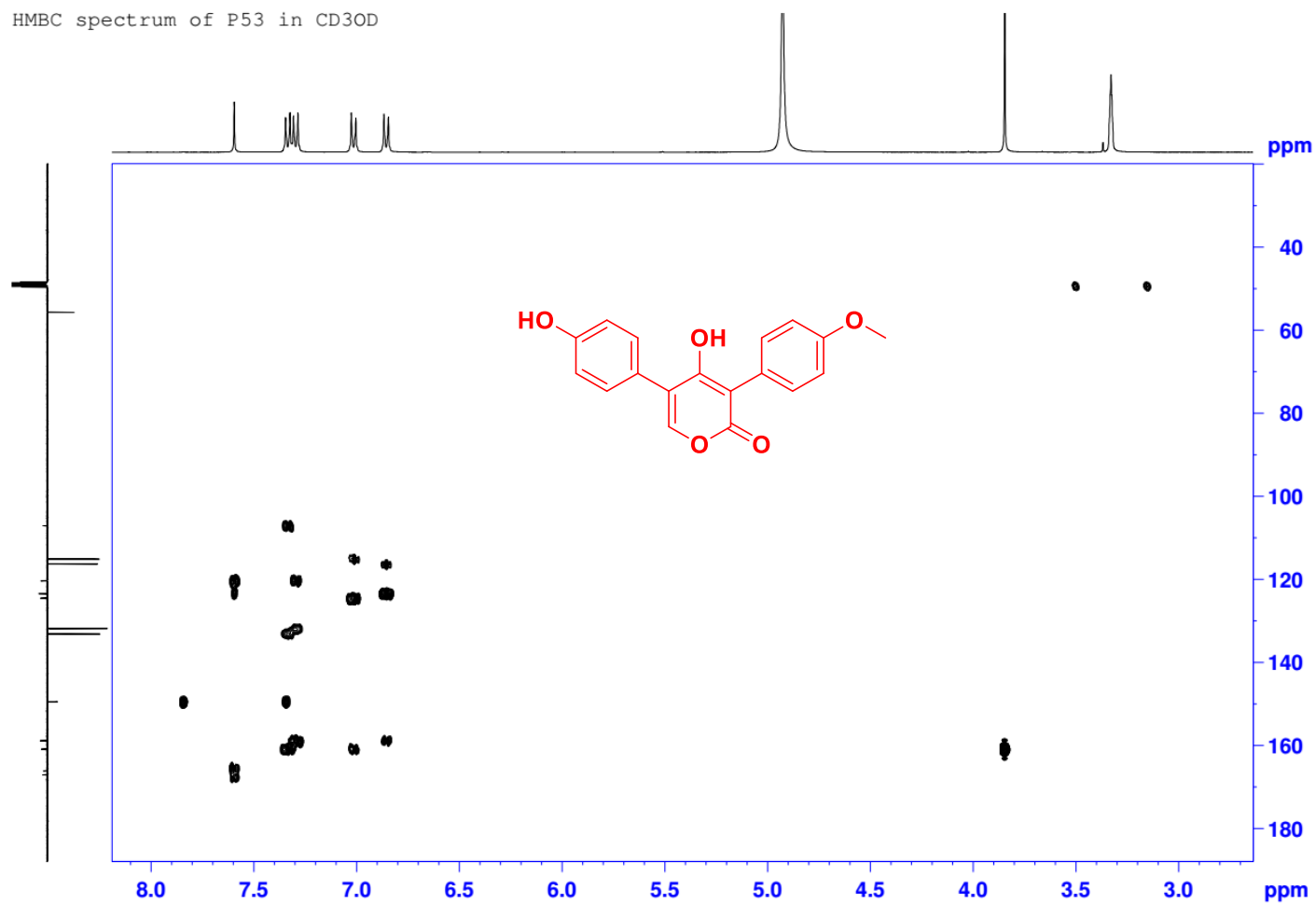


Figure S3-6. HMBC spectrum of **3** in CD₃OD.

P54-Sep-2 105 (0.415) Cm (102:121)

1: TOF MS ES+
5.56e6

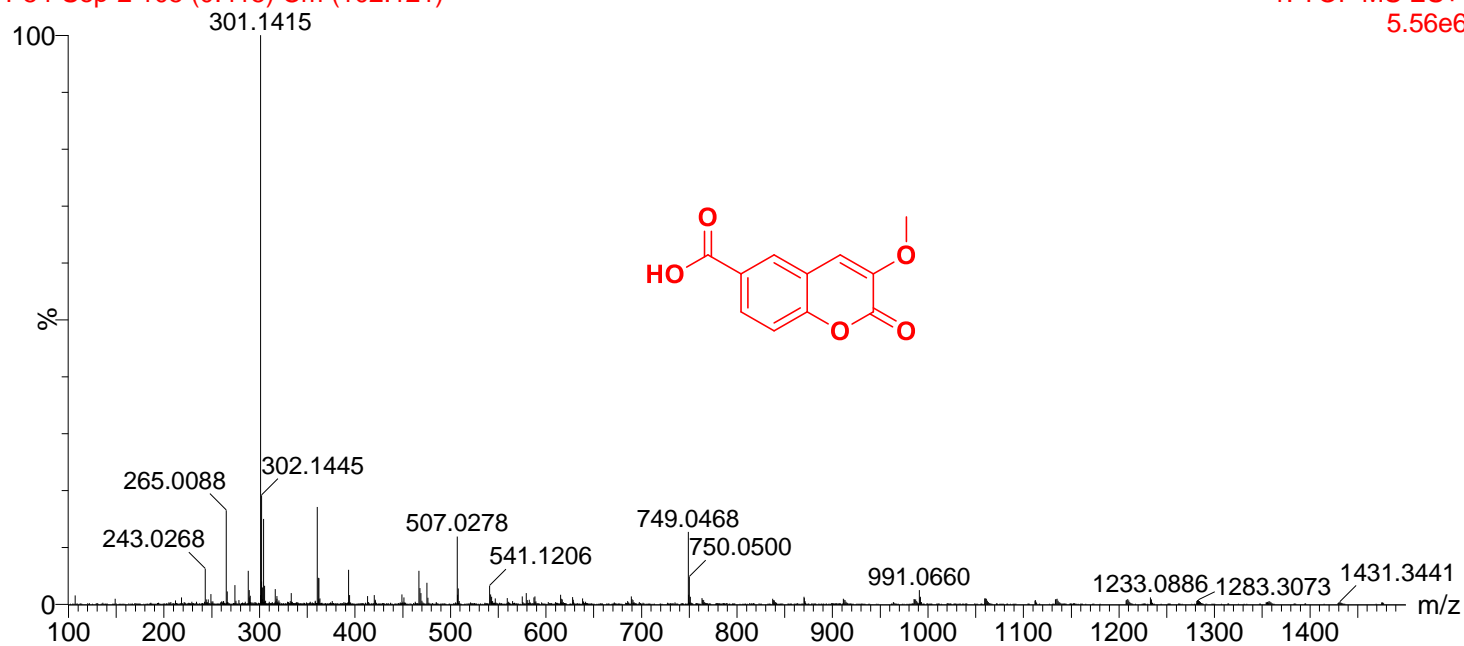


Figure S4-1. HRESIMS spectrum of **4**.

¹H NMR spectrum of P54 in DMSO-d₆ 400 MHz

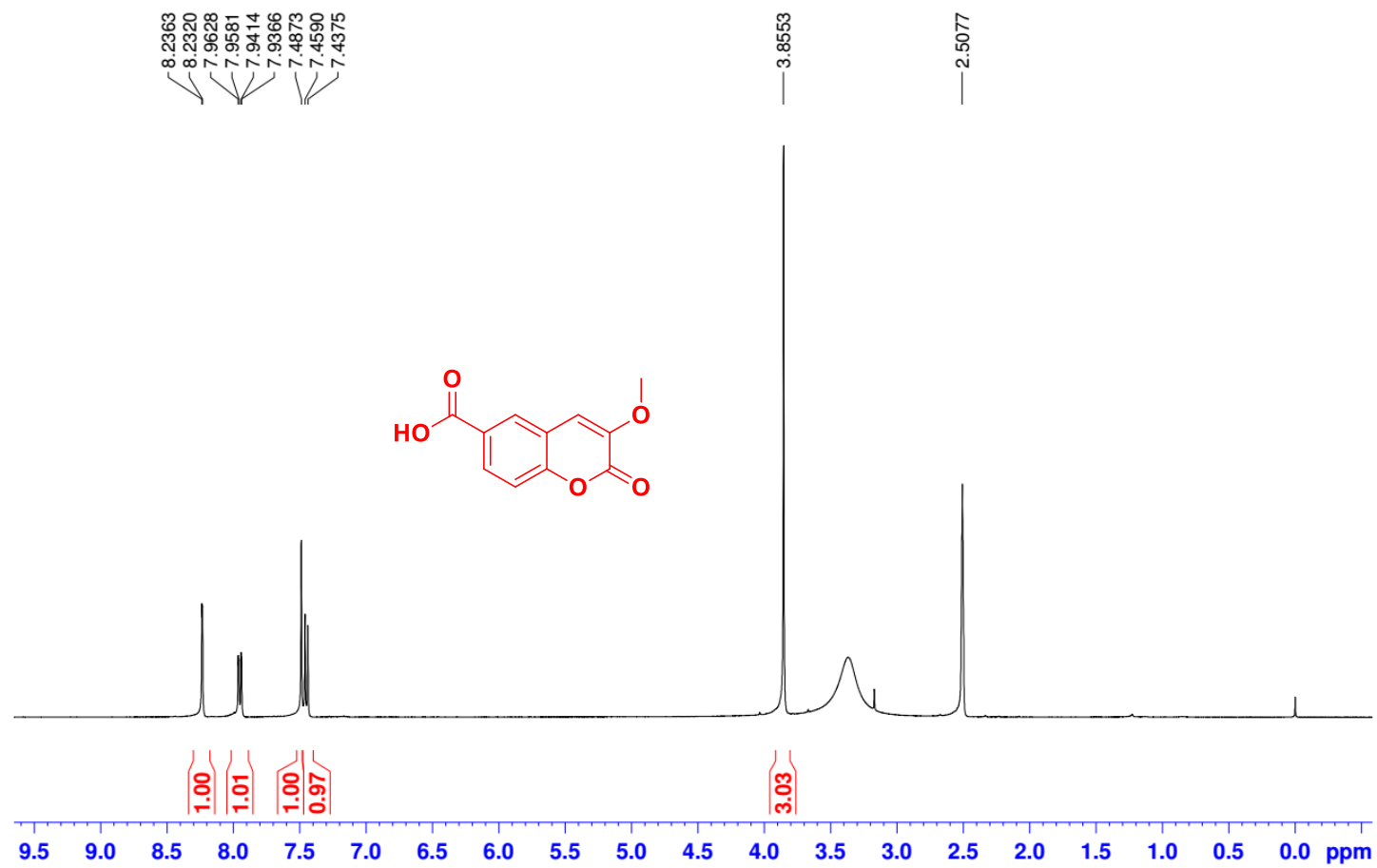


Figure S4-2. ¹H NMR spectrum of **4** in DMSO-*d*₆ (400 MHz).

^{13}C NMR spectrum of P54 in DMSO- d_6 100 MHz

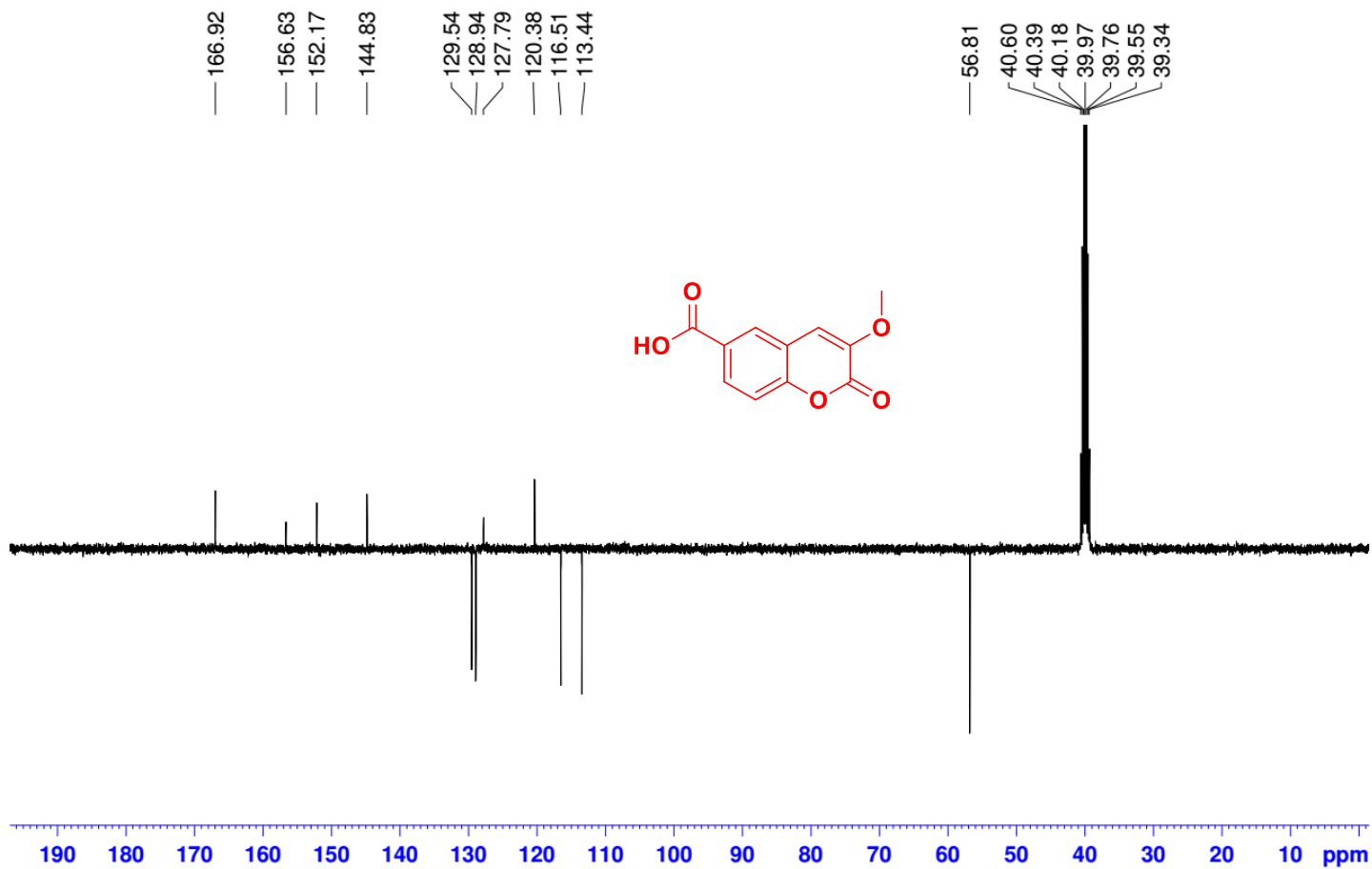


Figure S4-3. ^{13}C NMR spectrum of **4** in DMSO- d_6 (100 MHz).

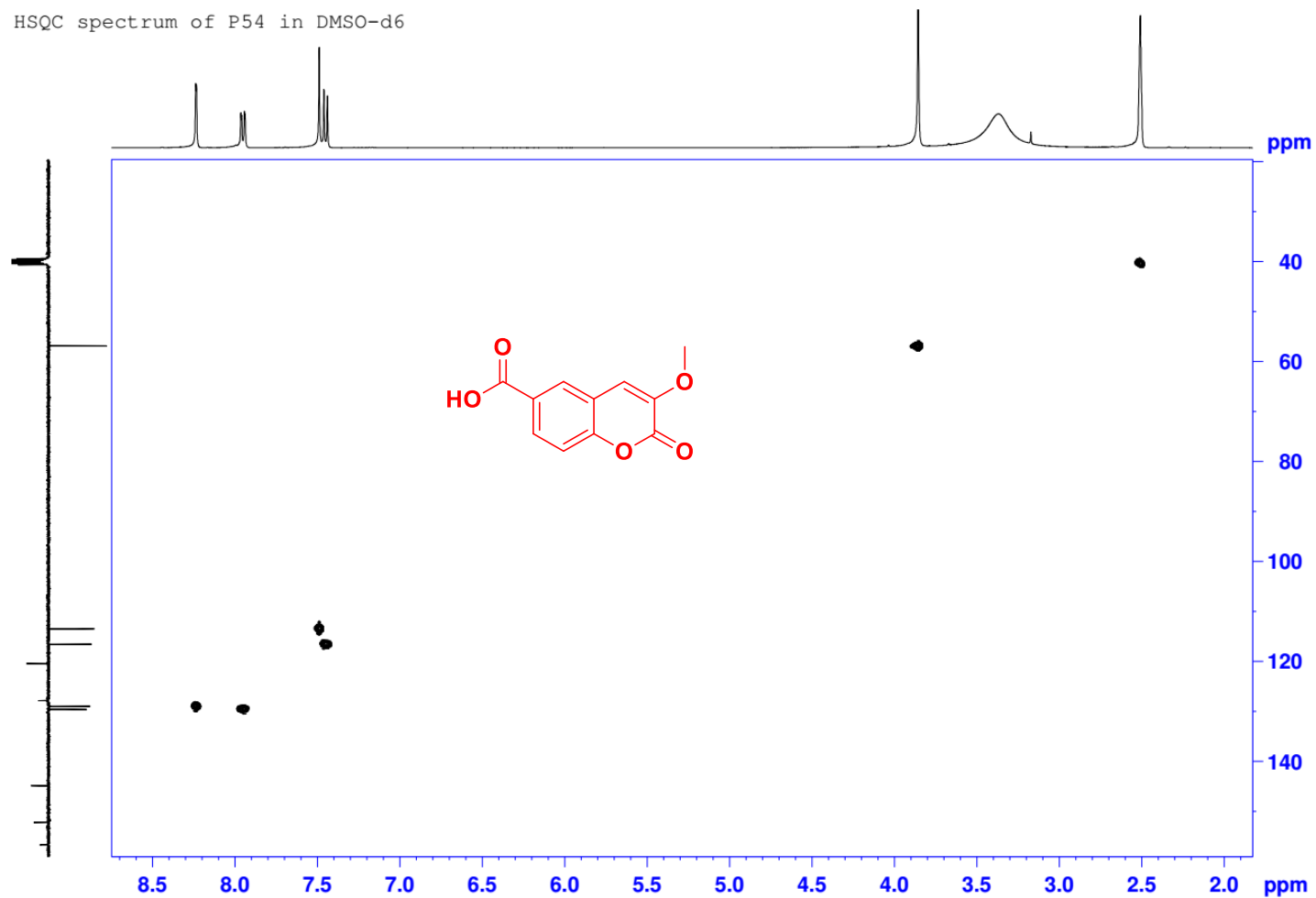


Figure S4-4. HSQC spectrum of **4** in DMSO- d_6 .

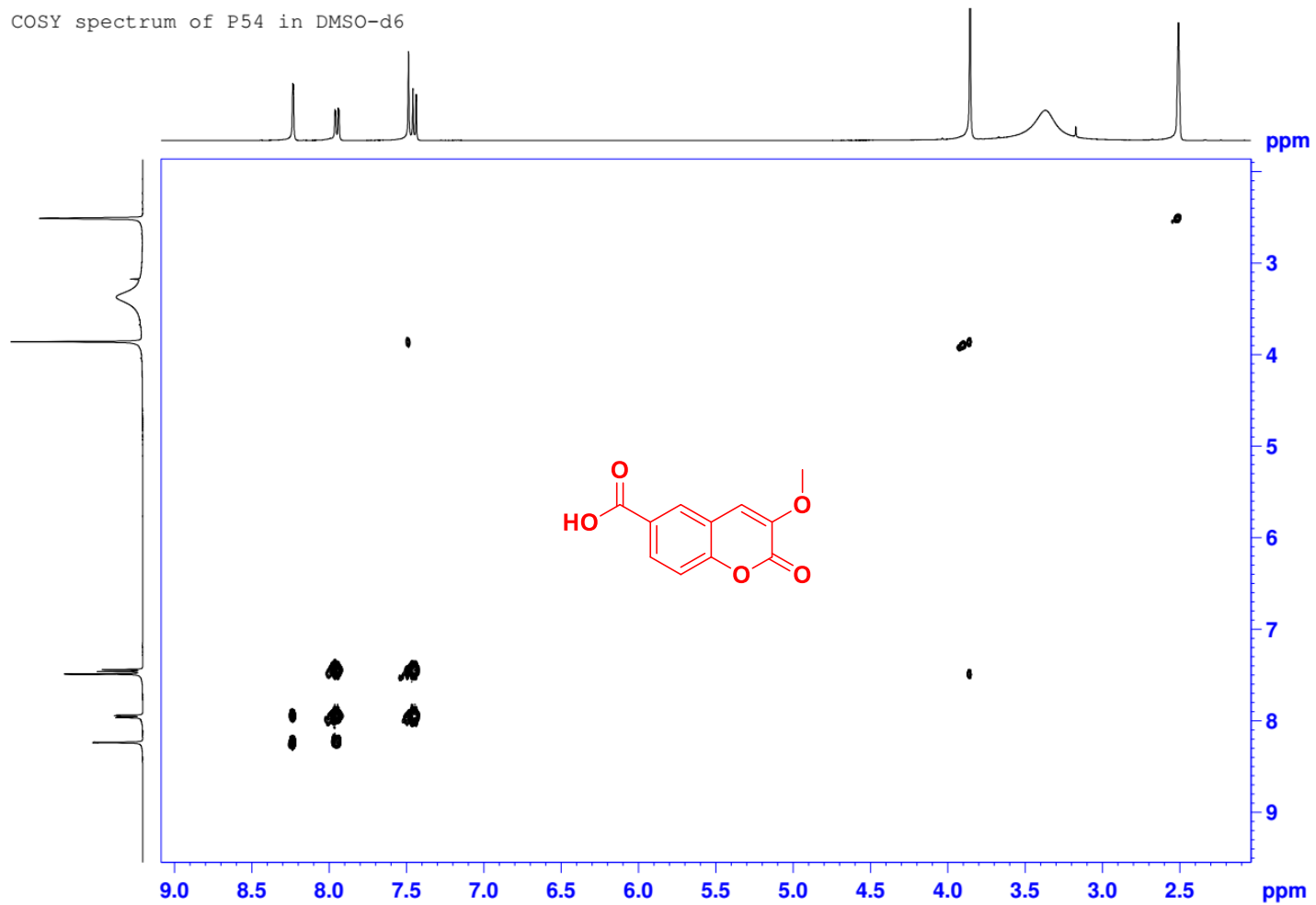


Figure S4-5. COSY spectrum of **4** in DMSO- d_6 .

HMBC spectrum of P54 in DMSO-d6

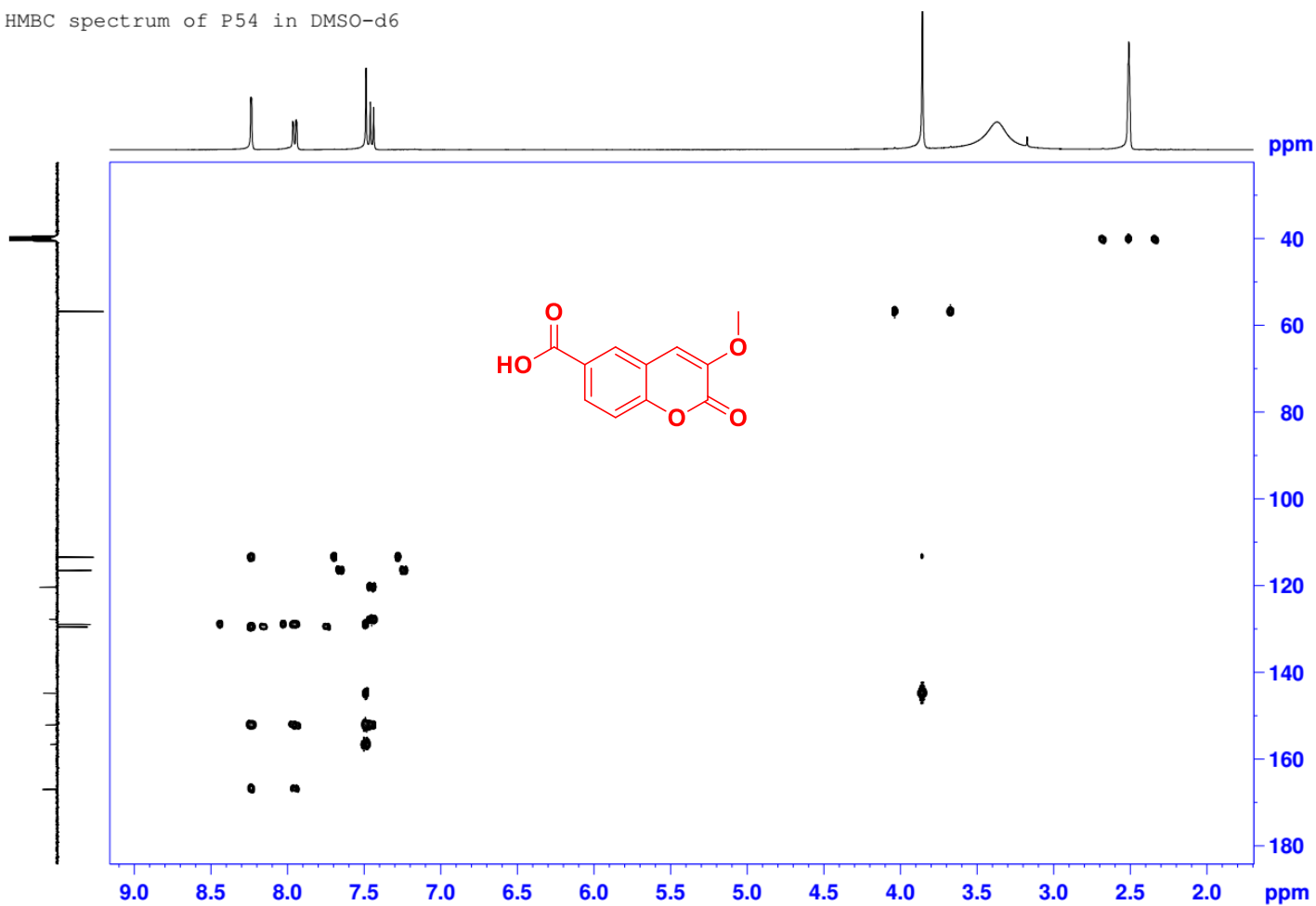


Figure S4-6. HMBC spectrum of 4 in DMSO-*d*₆.