



Supporting Information

for

Analogs of the carotane antibiotic fulvoerruginin from submerged cultures of a Thai *Marasmius* sp.

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HRESIMS profiles and copies of NMR spectra for compounds 1–6 in CD₃OD, and for metabolite 3 also in CDCl₃; minimum inhibitory concentrations (MIC) of 1–6 for bacteria, yeasts and fungi as well as half inhibitory concentrations (IC₅₀) for different cell lines

Table S1. NMR chemical shifts (^1H 700 MHz, ^{13}C 176 MHz) of Fulvoerruginin C (3) in chloroform- d .	S4
Table S2. Minimum inhibitory concentration (MIC) for bacteria, yeasts and fungi and half-inhibitory concentration (IC_{50}) for cell lines, in $\mu\text{g/ml}$.	S5
Table S3. NMR chemical shifts (^1H 500 MHz, ^{13}C 125 MHz) of Fulvoerruginin (A) (1) in methanol- d_4 .	S6
Figure S1. ECD spectra of Fulvoerruginin (1), Fulvoerruginin C (3) and D (4) in methanol.	S7
HRESIMS of Fulvoerruginin A (1).	S8
^1H NMR spectrum (500 MHz, methanol- d_4) of Fulvoerruginin (A) (1).	S9
^{13}C NMR spectrum (125 MHz, methanol- d_4) of Fulvoerruginin A (1).	S10
HSQC-dept NMR spectrum (500 MHz, methanol- d_4) of Fulvoerruginin A (1).	S11
HMBC NMR spectrum (500 MHz, methanol- d_4) of Fulvoerruginin A (1).	S12
COSY NMR spectrum (500 MHz, methanol- d_4) of Fulvoerruginin A (1).	S13
ROESY NMR spectrum (500 MHz, methanol- d_4) of Fulvoerruginin A (1).	S14
HRESIMS of Fulvoerruginin B (2).	S15
^1H NMR spectrum (700 MHz, methanol- d_4) of Fulvoerruginin B (2).	S16
^{13}C NMR spectrum (176 MHz, methanol- d_4) of Fulvoerruginin B (2).	S17
HSQC-dept NMR spectrum (700 MHz, methanol- d_4) of Fulvoerruginin B (2).	S18
HMBC NMR spectrum (700 MHz, methanol- d_4) of Fulvoerruginin B (2).	S19
COSY NMR spectrum (700 MHz, methanol- d_4) of Fulvoerruginin B (2).	S20
ROESY NMR spectrum (700 MHz, methanol- d_4) of Fulvoerruginin B (2).	S21
HRESIMS of Fulvoerruginin C (3).	S22
^1H NMR spectrum (700 MHz, methanol- d_4) of Fulvoerruginin C (3).	S23
^{13}C NMR spectrum (176 MHz, methanol- d_4) of Fulvoerruginin C (3).	S24
HSQC-dept NMR spectrum (700 MHz, methanol- d_4) of Fulvoerruginin C (3).	S25
HMBC NMR spectrum (700 MHz, methanol- d_4) of Fulvoerruginin C (3).	S26
COSY NMR spectrum (700 MHz, methanol- d_4) of Fulvoerruginin C (3).	S27
ROESY NMR spectrum (700 MHz, methanol- d_4) of Fulvoerruginin C (3).	S28
^1H NMR spectrum (700 MHz, chloroform- d) of Fulvoerruginin C (3).	S29
^{13}C NMR spectrum (176 MHz, chloroform- d) of Fulvoerruginin C (3).	S30
HSQC-dept NMR spectrum (700 MHz, chloroform- d) of Fulvoerruginin C (3).	S31
HMBC NMR spectrum (700 MHz, chloroform- d) of Fulvoerruginin C (3).	S32
COSY NMR spectrum (700 MHz, chloroform- d) of Fulvoerruginin C (3).	S33
ROESY NMR spectrum (700 MHz, chloroform- d) of Fulvoerruginin C (3).	S34

HRESIMS of Fulvoerruginin D (4).	S35
¹ H NMR spectrum (700 MHz, methanol- <i>d</i> ₄) of Fulvoerruginin D (4).	S36
¹³ C NMR spectrum (176 MHz, methanol- <i>d</i> ₄) of Fulvoerruginin D (4).	S37
HSQC-dept NMR spectrum (700 MHz, methanol- <i>d</i> ₄) of Fulvoerruginin D (4).	S38
HMBC NMR spectrum (700 MHz, methanol- <i>d</i> ₄) of Fulvoerruginin D (4).	S39
COSY NMR spectrum (700 MHz, methanol- <i>d</i> ₄) of Fulvoerruginin D (4).	S40
ROESY NMR spectrum (700 MHz, methanol- <i>d</i> ₄) of Fulvoerruginin D (4).	S41
HRESIMS of Fulvoerruginin E (5).	S42
¹ H NMR spectrum (700 MHz, methanol- <i>d</i> ₄) of Fulvoerruginin E (5).	S43
¹³ C NMR spectrum (176 MHz, methanol- <i>d</i> ₄) of Fulvoerruginin E (5).	S44
HSQC-dept NMR spectrum (700 MHz, methanol- <i>d</i> ₄) of Fulvoerruginin E (5).	S45
HMBC NMR spectrum (700 MHz, methanol- <i>d</i> ₄) of Fulvoerruginin E (5).	S46
COSY NMR spectrum (700 MHz, methanol- <i>d</i> ₄) of Fulvoerruginin E (5).	S47
ROESY NMR spectrum (700 MHz, methanol- <i>d</i> ₄) of Fulvoerruginin E (5).	S48
HRESIMS of Fulvoerruginin F (6).	S49
¹ H NMR spectrum (700 MHz, methanol- <i>d</i> ₄) of Fulvoerruginin F (6).	S50
¹³ C NMR spectrum (176 MHz, methanol- <i>d</i> ₄) of Fulvoerruginin F (6).	S51
HSQC-dept NMR spectrum (700 MHz, methanol- <i>d</i> ₄) of Fulvoerruginin F (6).	S52
HMBC NMR spectrum (700 MHz, methanol- <i>d</i> ₄) of Fulvoerruginin F (6).	S53
COSY NMR spectrum (700 MHz, methanol- <i>d</i> ₄) of Fulvoerruginin F (6).	S54
ROESY NMR spectrum (700 MHz, methanol- <i>d</i> ₄) of Fulvoerruginin F (6).	S55

Table S1. NMR chemical shifts (^1H 700 MHz, ^{13}C 176 MHz) of Fulvoferruginin C (**3**) in chloroform-*d*.

Pos.	δ_{C}	mult	δ_{H}	mult (<i>J</i> , Hz)
1	142.2	CH	6.04	d (11.2)
2	125.9	CH	5.57	d (11.2)
3	132.8	C		
4	123.7	CH	5.72	d (0.6)
5	78.1	CH	4.89	br d (12.1)
6	45.1	CH	2.57	t (12.1)
7	43.9	C		
8	39.8	CH ₂	1.77	m
9	30.4	CH ₂	1.66	m
			2.19	m
10	37.7	CH	2.75	m
11	51.6	CH	3.38	d (13.3)
12	27.7	CH ₃	1.91	m (1.7)
13	20.9	CH ₃	1.01	s
14	172.1	C		
15	170.5	C		

Table S2. Minimum inhibitory concentration (MIC) for bacteria, yeasts and fungi and half-inhibitory concentration (IC₅₀) for cell lines, in µg/ml.

A total of 2 µL and 20 µL of a 1 mg/mL stock solution (6.7 and 67 µg/mL) of **1–6** were tested. MeOH (20 µL) served as negative control and showed no inhibitory effects. Oxytetracycline served as a reference antimicrobial for bacteria; Nystatin for yeasts and filamentous fungi; Epothilon B was used as positive control for cell lines.

MIC (µg/ml)							
Organism	1	2	3	4	5	6	Ref.
<i>Schizos. pombe</i> DSM70572	66.7	-	-	-	-	-	16.7
<i>Mucor hiemalis</i> DSM2656	16.7	-	-	-	-	-	16.7
<i>Candida albicans</i> DSM1665	8.3	-	-	-	-	-	16.7
<i>Rhodoturula glutinis</i> DSM10134	33.3	-	-	-	-	-	16.7
<i>Micrococcus luteus</i> DSM1790	-	-	-	-	-	-	0.5
<i>Staph. aureus</i> DSM346	-	-	-	-	-	-	8.3
<i>Bacillus subtilis</i> DSM10	-	-	-	-	-	-	8.3
<i>Escherichia coli</i> DSM1116	-	-	-	-	-	-	4.2
<i>Pichia anomala</i> DSM6766	33.3	-	-	-	-	-	16.7
IC ₅₀ (µg/ml)							
Cell line	1	2	3	4	5	6	Ref.
L929	0.6	*	*	9.5	*	*	0.00062
KB3.1	0.7	23	*	20	*	32	0.00003
A549	0.5	n.t.	n.t.	n.t.	n.t.	n.t.	0.000016
A431	0.06	n.t.	n.t.	n.t.	n.t.	n.t.	0.000048
SKOV-3	0.7	n.t.	n.t.	n.t.	n.t.	n.t.	0.00013
MCF-7	0.3	n.t.	n.t.	n.t.	n.t.	n.t.	0.000072
PC-3	0.1	n.t.	n.t.	n.t.	n.t.	n.t.	n.t.

* showed cytotoxic effects, but no IC₅₀ determinable in conducted assays

n.t. not tested, – no inhibitory effects observed up to 67 µg/mL.

Table S3. NMR chemical shifts (^1H 500 MHz, ^{13}C 125 MHz) of Fulvoerruginin (A) (**1**) in methanol- d_4 .

Pos.	δ_{C}	mult	δ_{H}	mult (J , Hz)
1	143.6	CH	6.11	d (11.2)
2	126.6	CH	5.61	d (11.2)
3	133.9	C		
4	125.3	CH	5.70	dd (2.2, 1.14)
5	78.6	CH	4.63	dt (12.6, 2.2)
6	57.6	CH	2.40	d (12.6)
7	45.3	C		
8	38.4	CH ₂	2.10	td (13.6, 12.0, 6.5)
8			1.74	dd (12.0, 6.5)
9	36.2	CH ₂	2.40	dt (13.6, 6.6)
9			1.95	dd (13.6, 6.6)
10	80.7	C		
11	144.9	C		
12	27.9	CH ₃	1.91	t (1.9)
13	19.8	CH ₃	0.89	s
14	121.7	CH ₂	5.96	s
14			5.73	s
15	171.8	C		

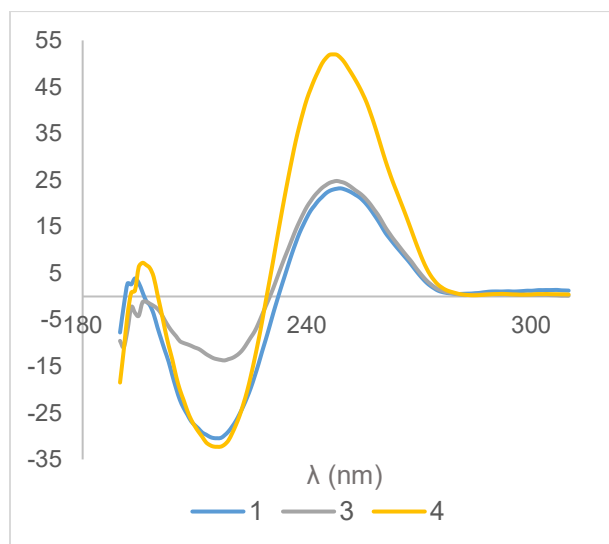
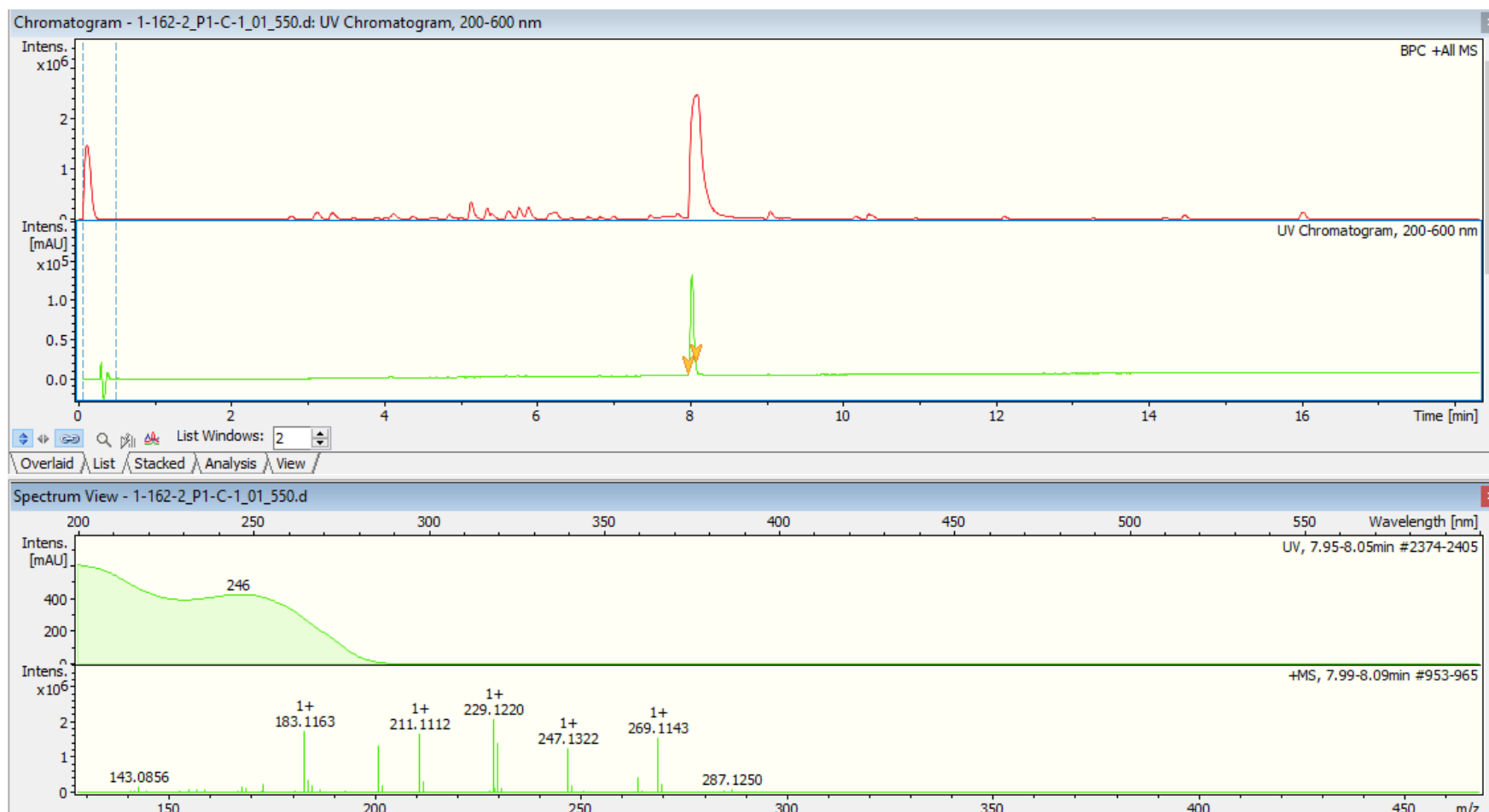
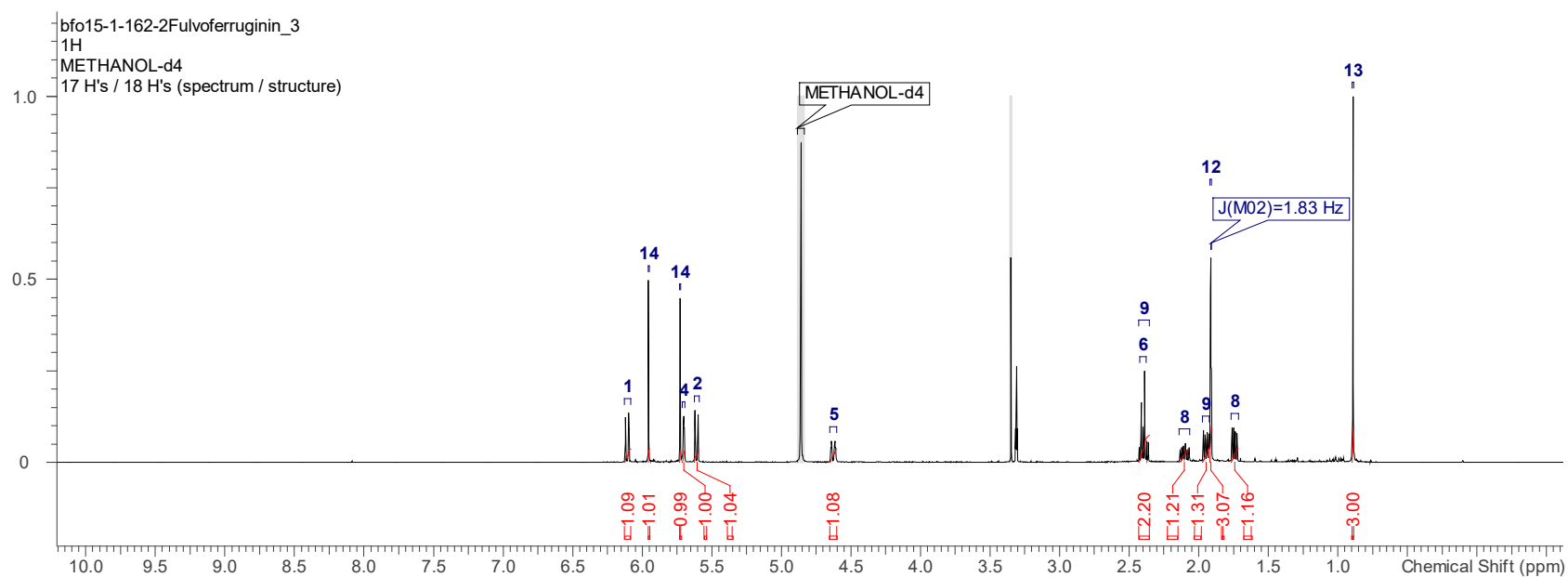
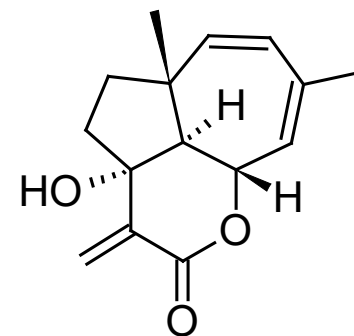


Figure S1. ECD spectra of Fulvoferruginin (**1**), Fulvoferruginin C (**3**) and D (**4**) in methanol ($\Delta\epsilon$ [cm^2/mmol], c 1.0). λ_{max} ($\Delta\epsilon$) for **1**: 216 (-30.4), 249 (23.2); for **3**: 218 (-13.7), 248 (24.8); for **4**: 216 (-32.3), 247 (52.0).

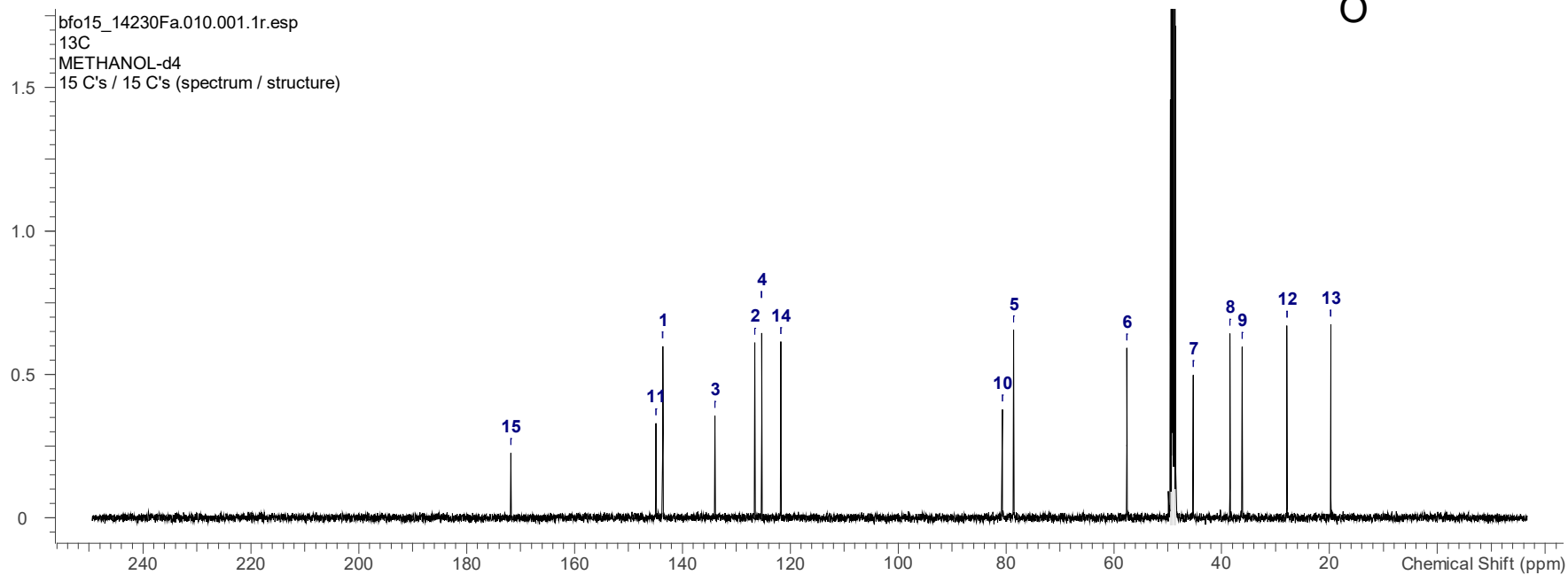
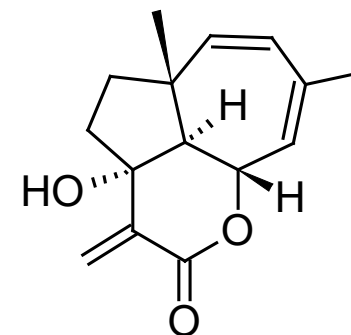


HRESIMS of Fulvoferruginin A (1).

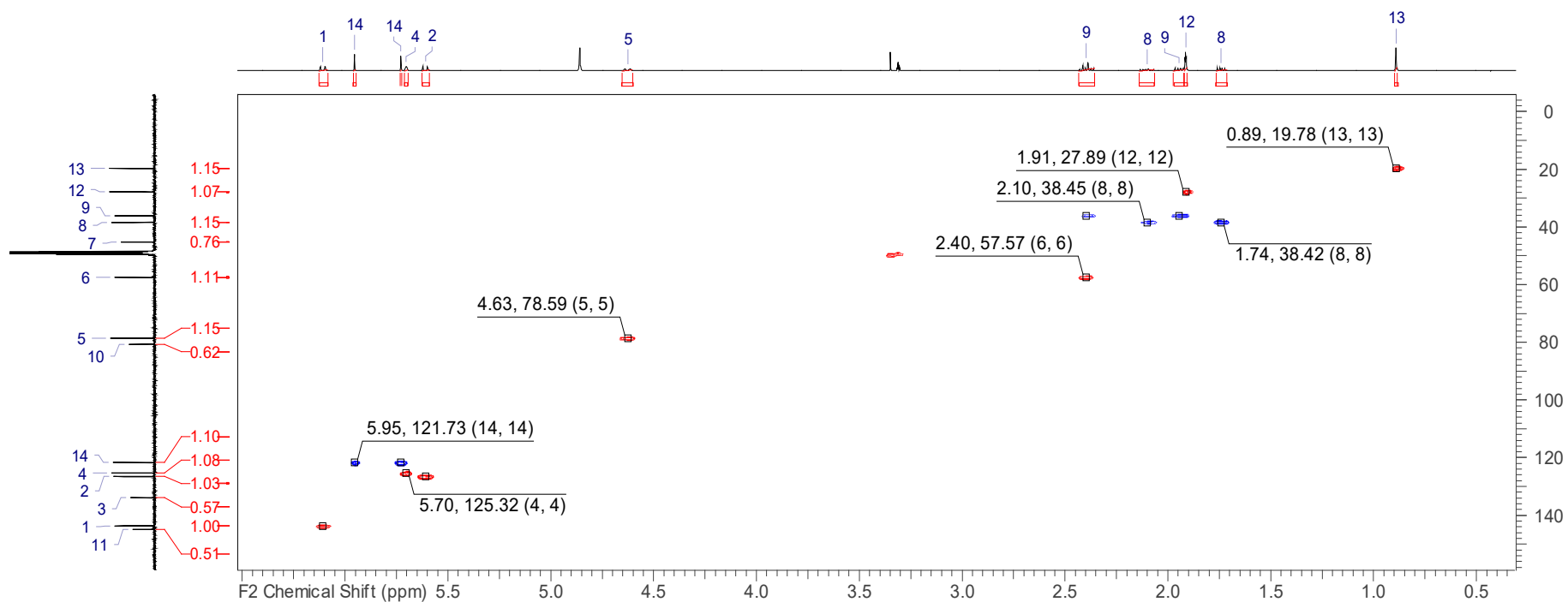
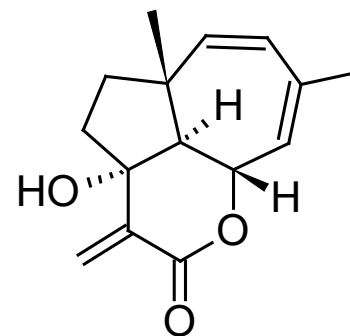
^1H NMR spectrum (500 MHz, methanol- d_4) of Fulvoferruginin (A) (**1**).



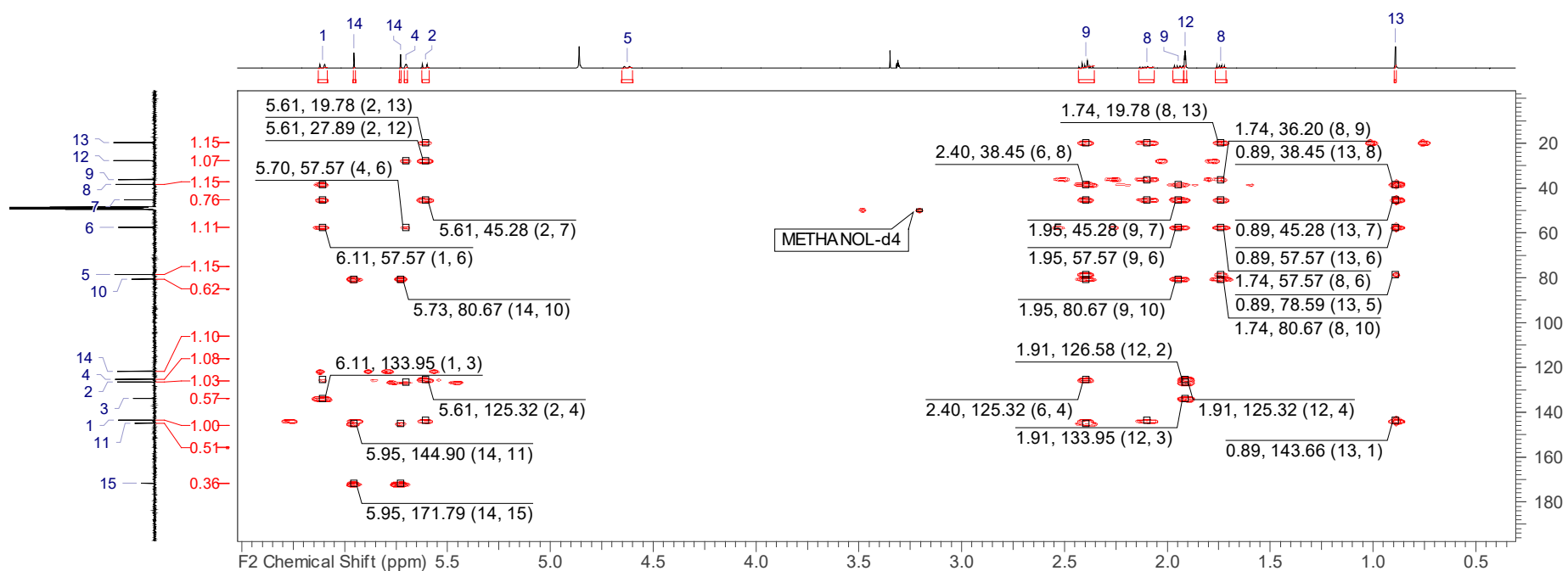
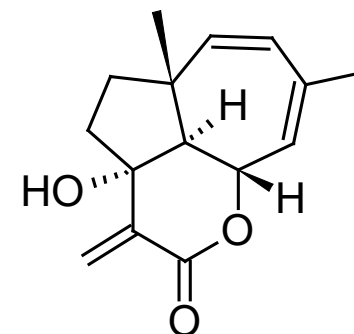
^{13}C NMR spectrum (125 MHz, methanol- d_4) of Fulvoferruginin A (**1**).



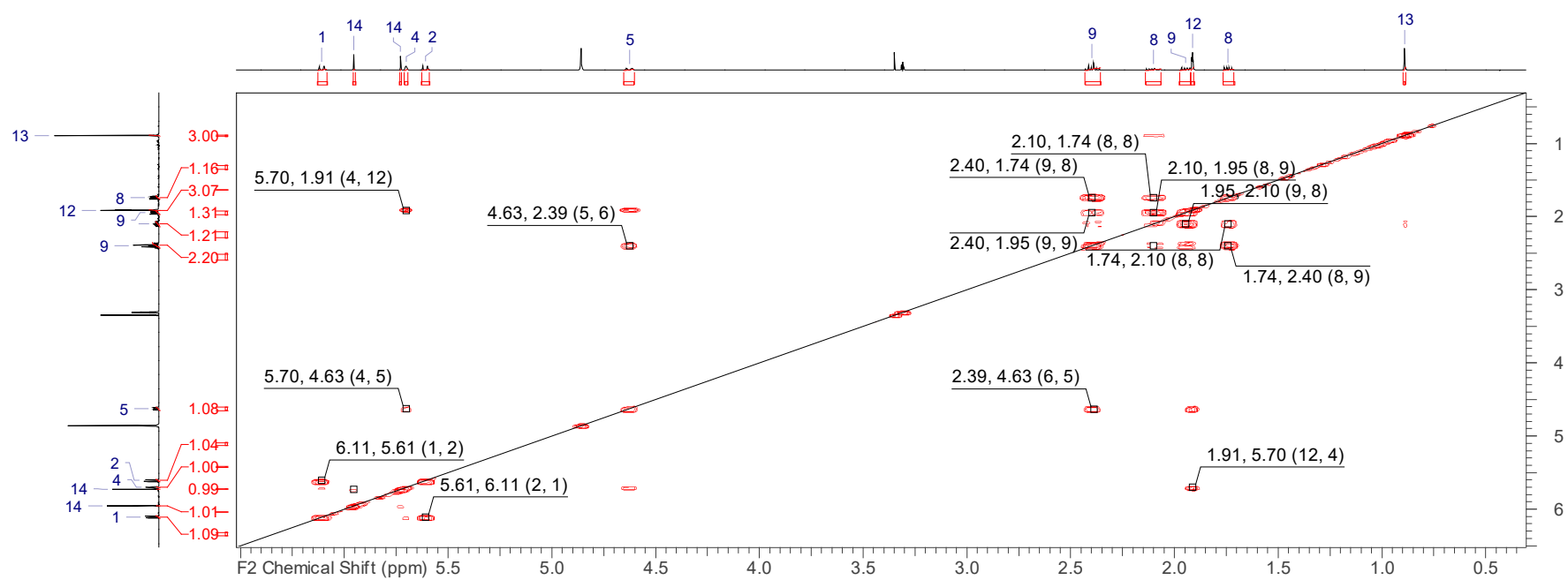
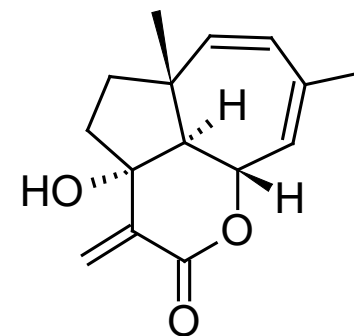
HSQC-dept NMR spectrum (500 MHz, methanol-*d*₄) of Fulvoferruginin A (**1**).



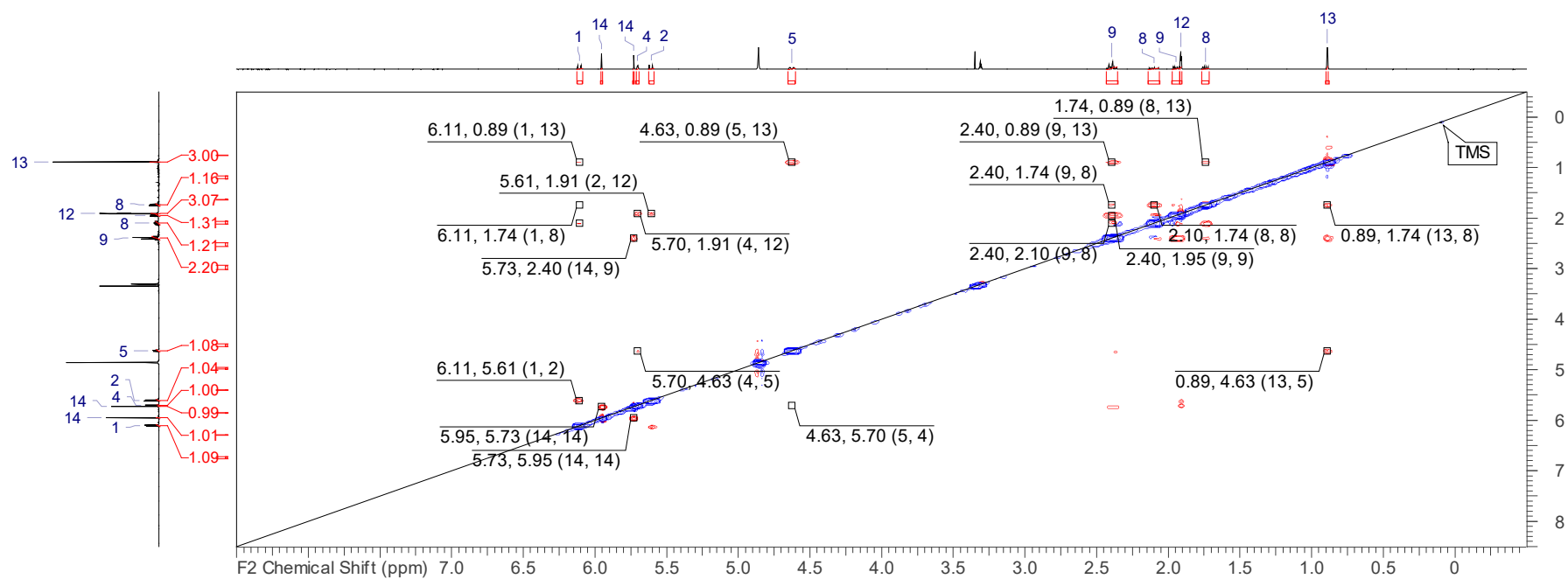
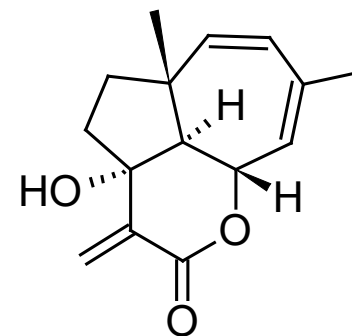
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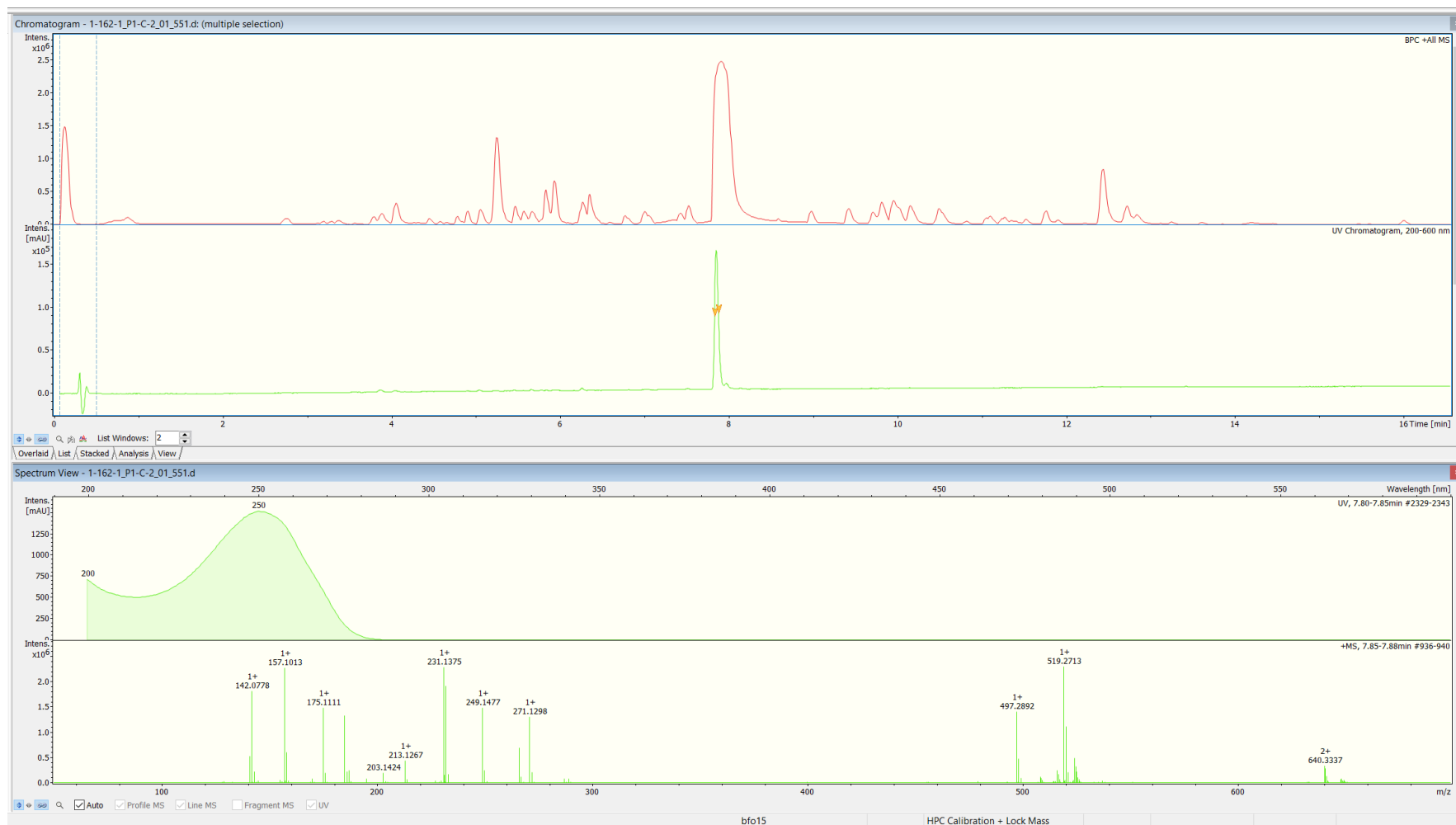


COSY NMR spectrum (500 MHz, methanol- d_4) of Fulvoferruginin A (**1**).



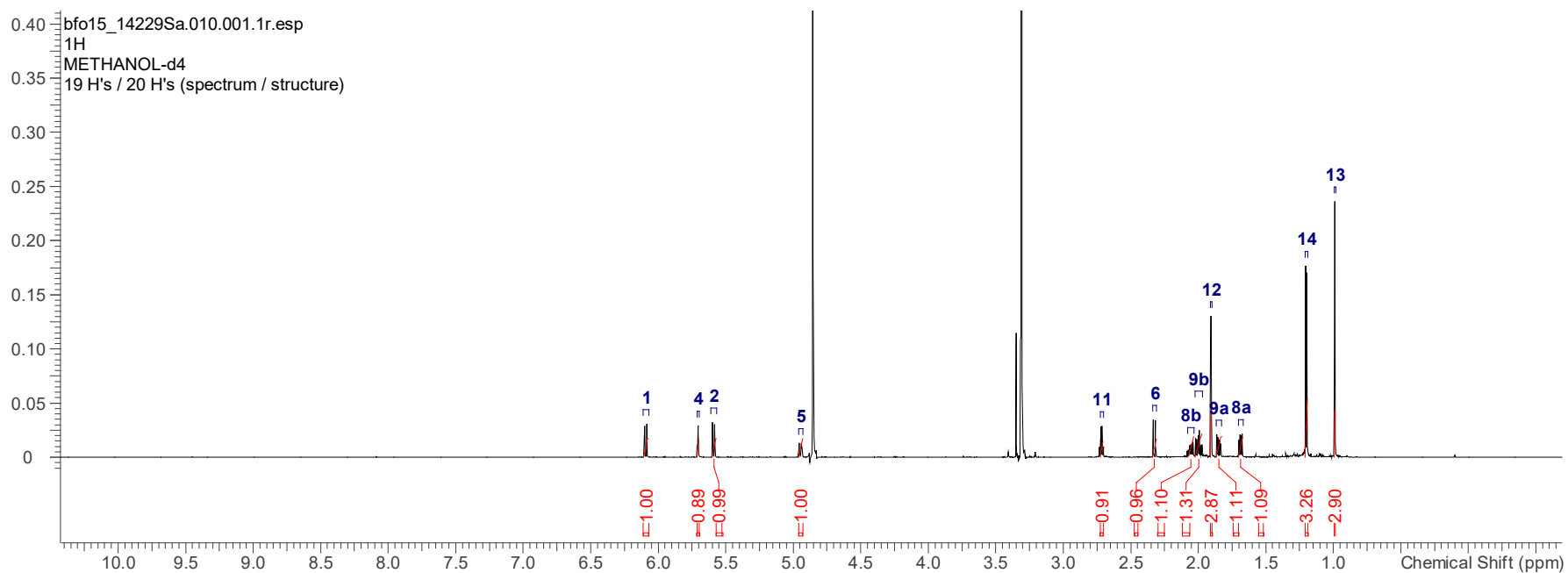
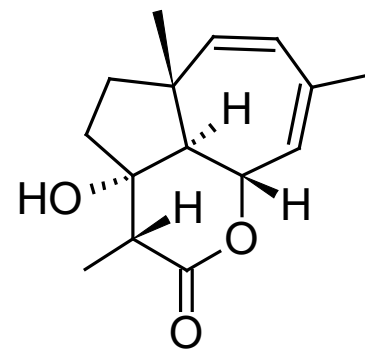
ROESY NMR spectrum (500 MHz, methanol- d_4) of Fulvoferruginin A (**1**).



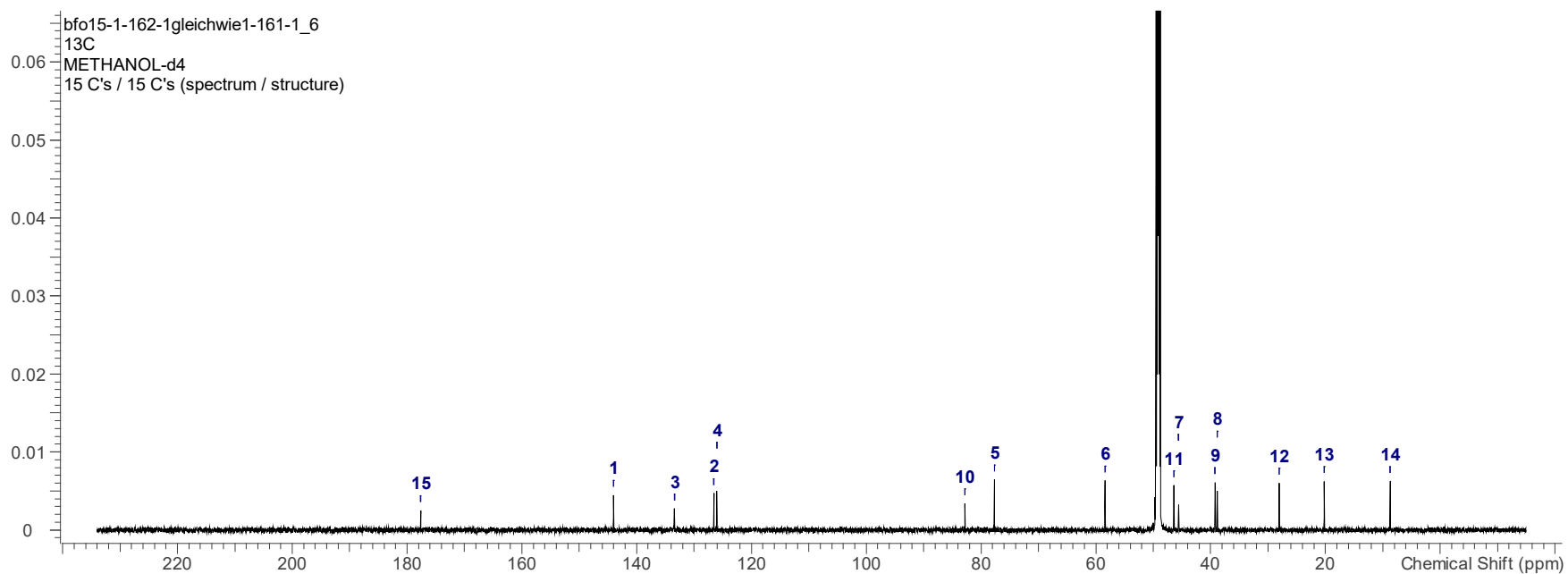
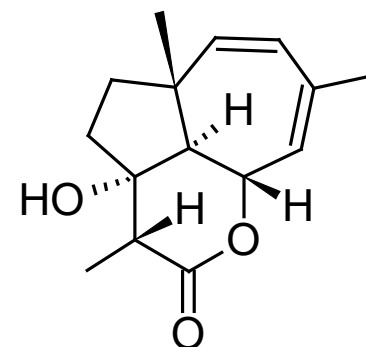


HRESIMS of Fulvoferruginin B (2).

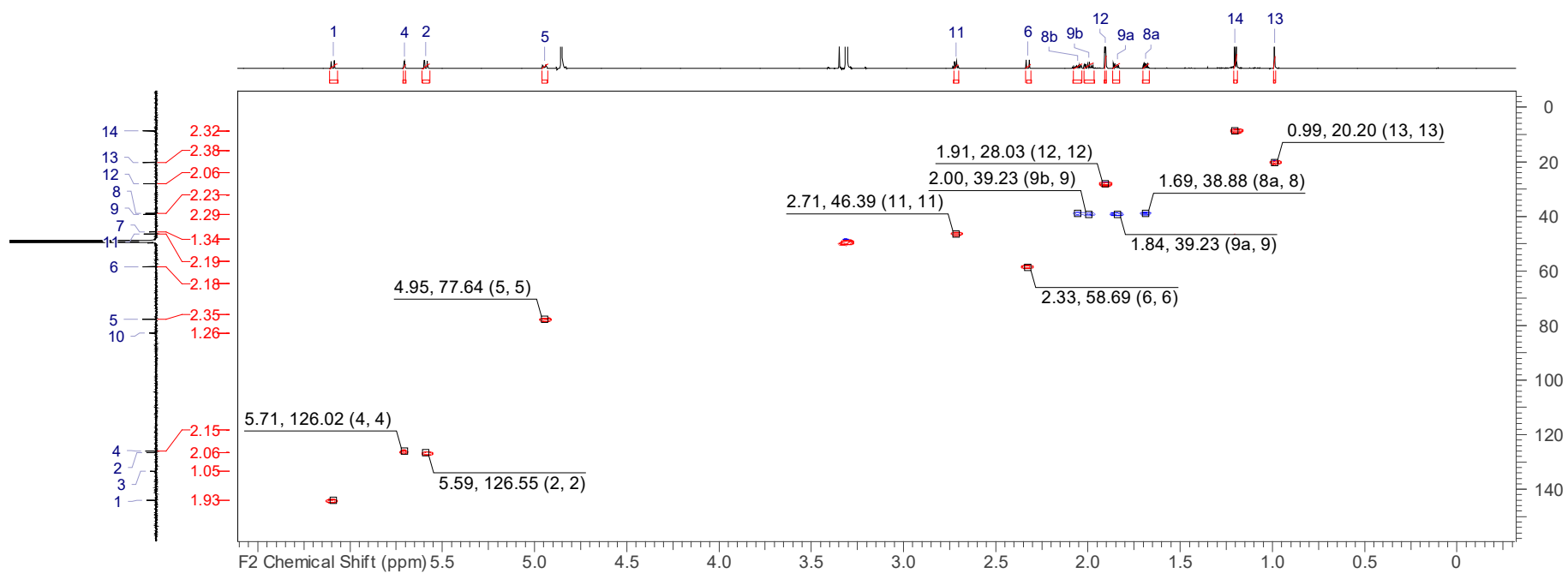
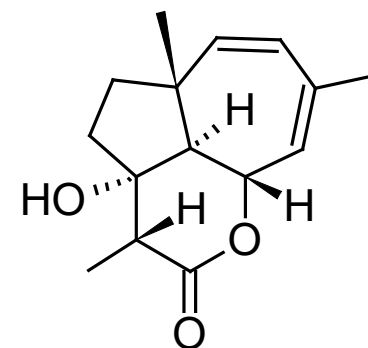
^1H NMR spectrum (700 MHz, methanol- d_4) of Fulvoferruginin B (**2**).



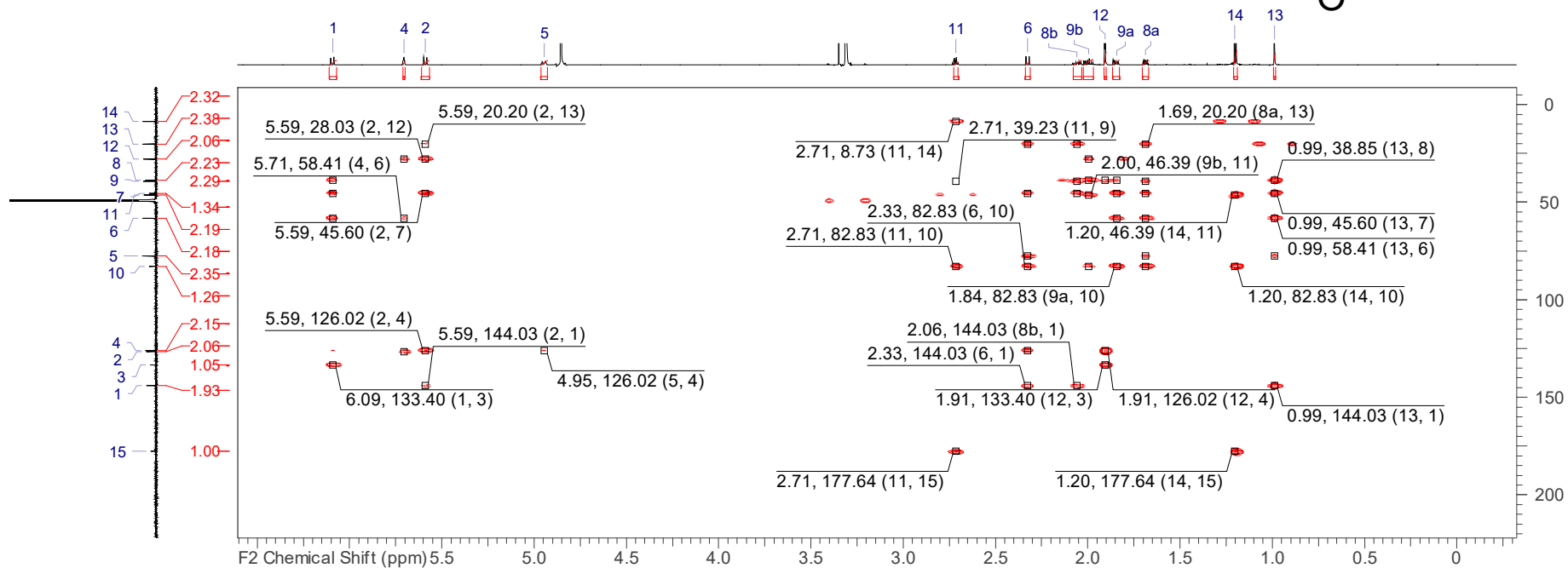
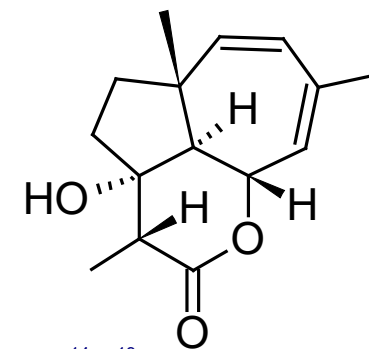
^{13}C NMR spectrum (176 MHz, methanol- d_4) of Fulvoferruginin B (**2**).



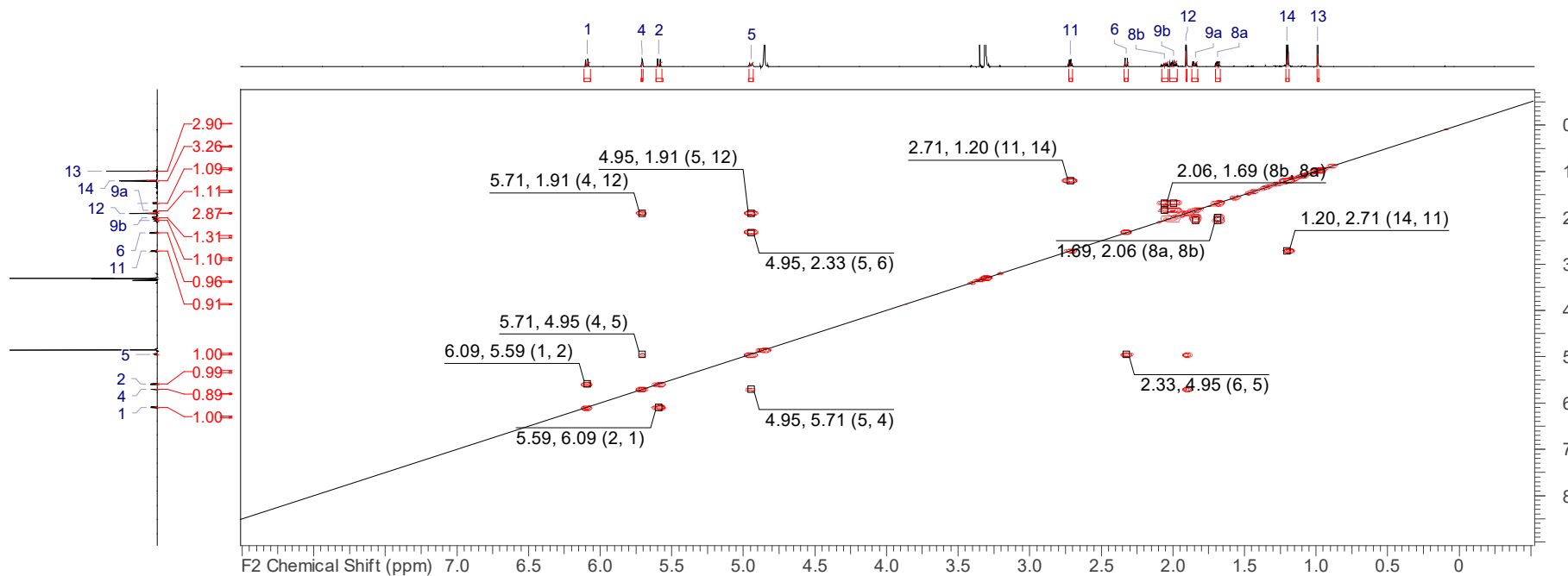
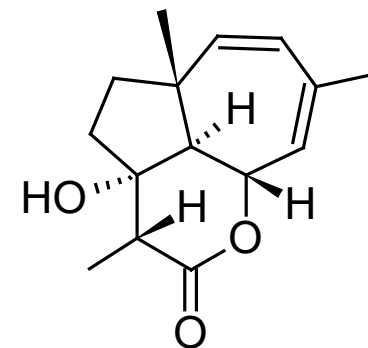
HSQC-dept NMR spectrum (700 MHz, methanol- d_4) of Fulvoferruginin B (**2**).



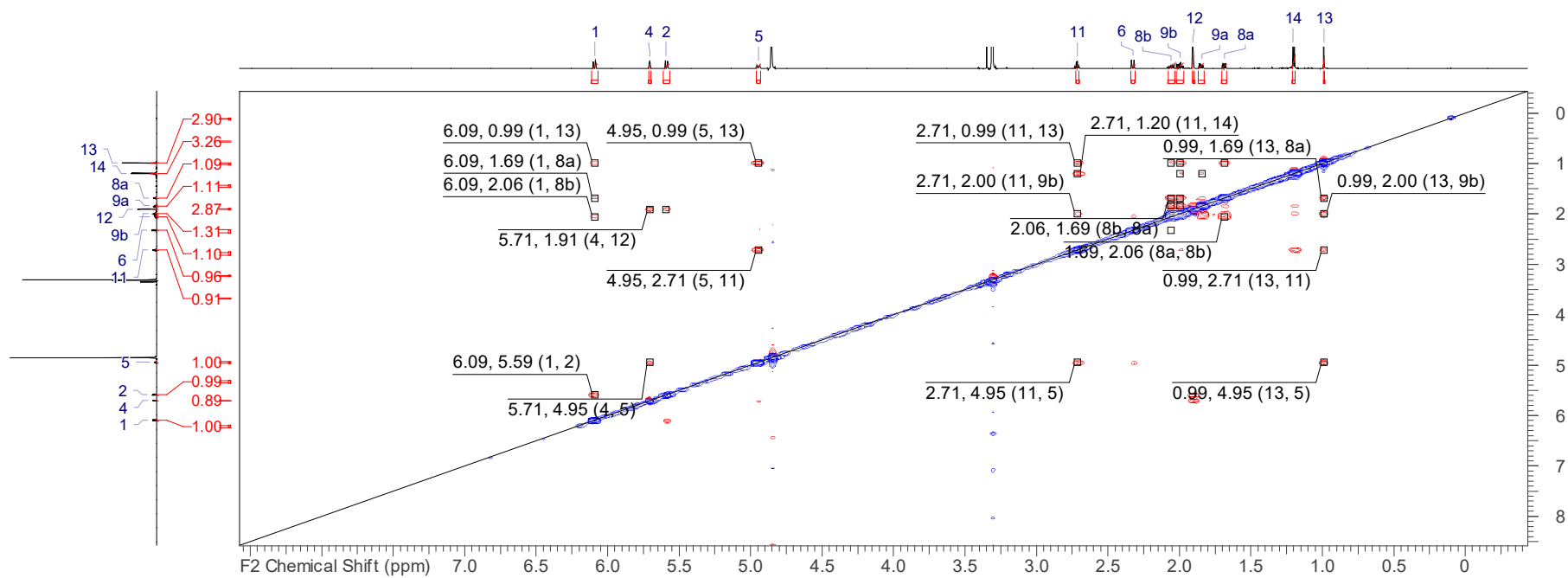
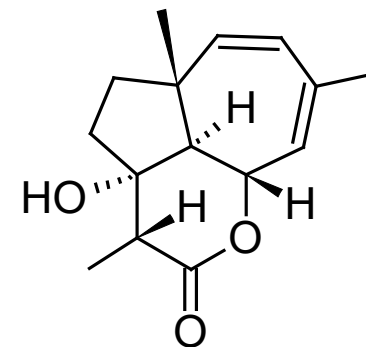
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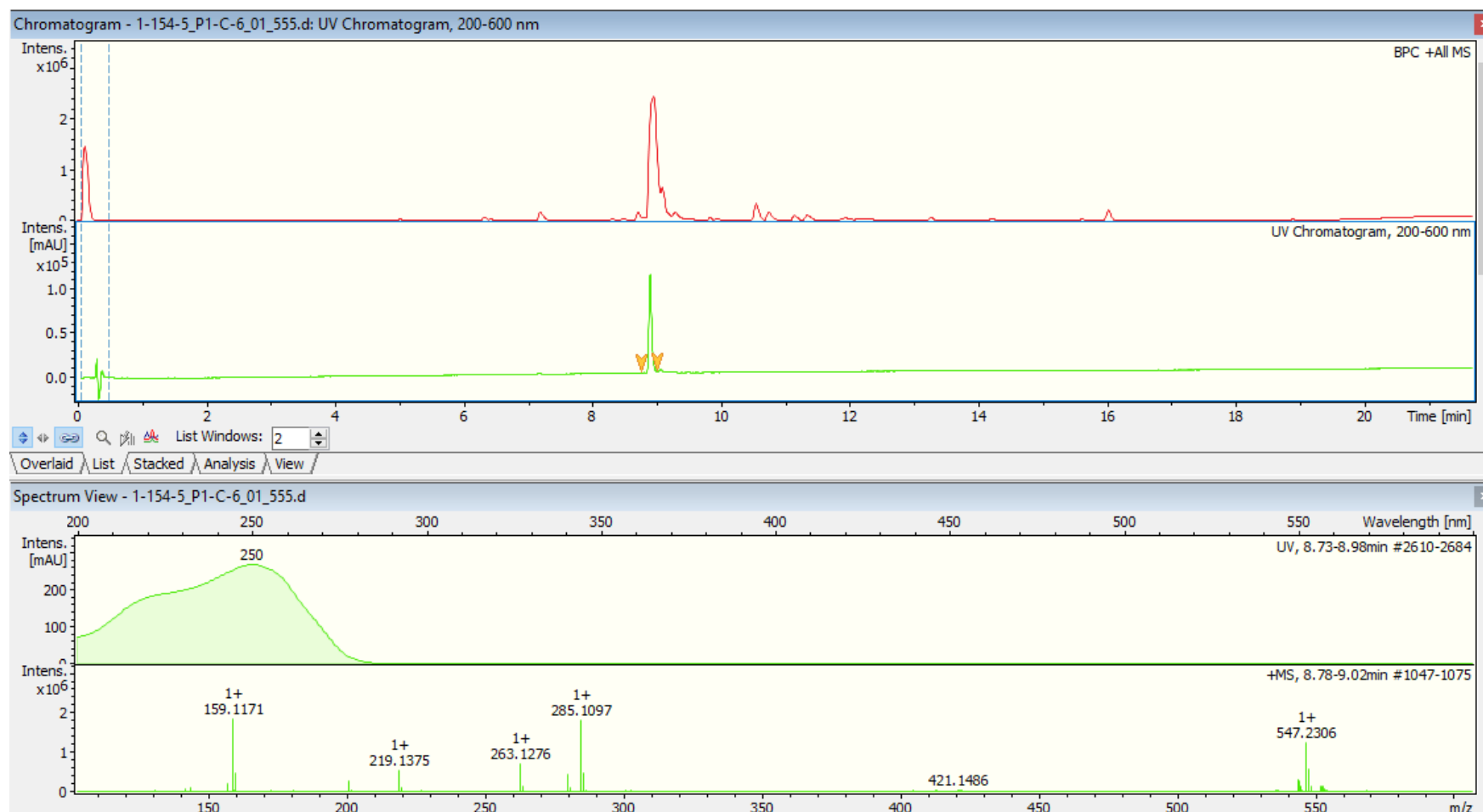


COSY NMR spectrum (700 MHz, methanol- d_4) of Fulvoferruginin B (**2**).



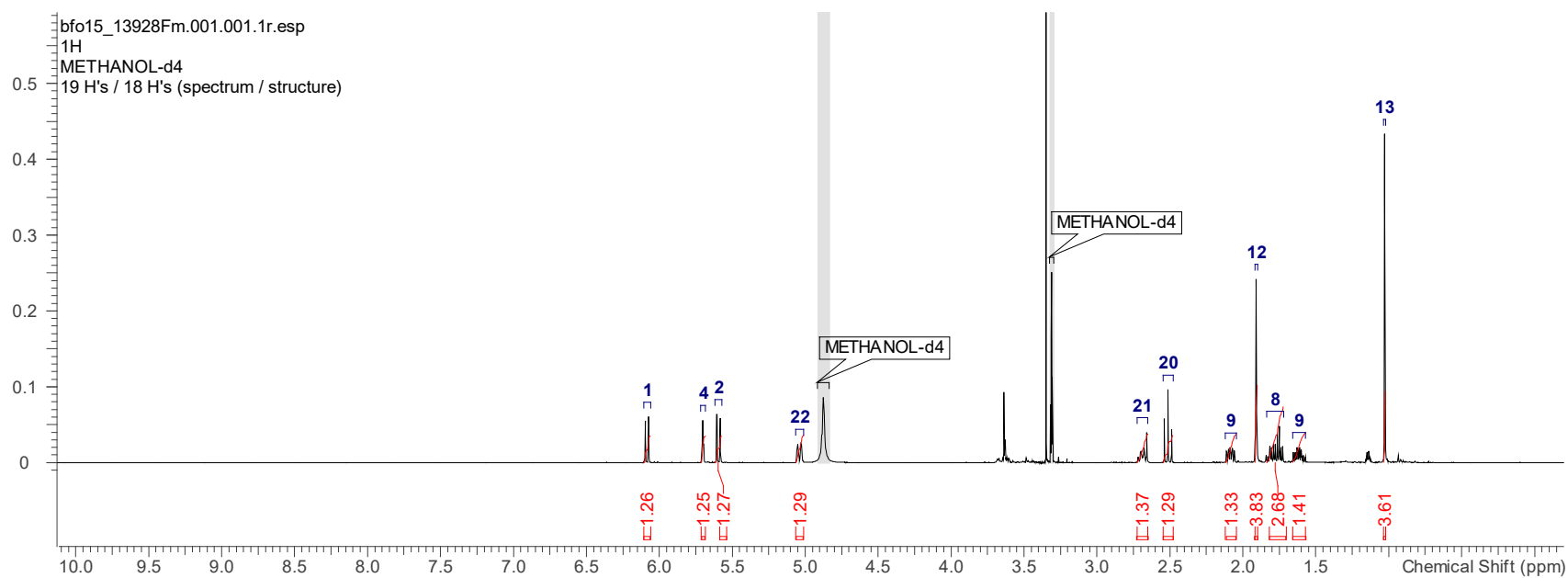
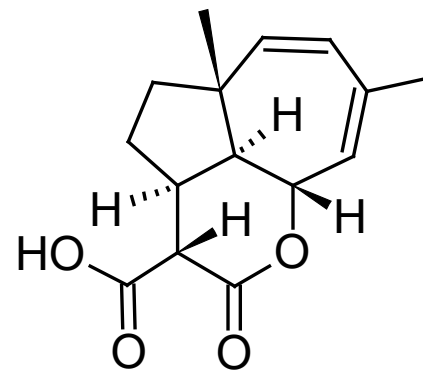
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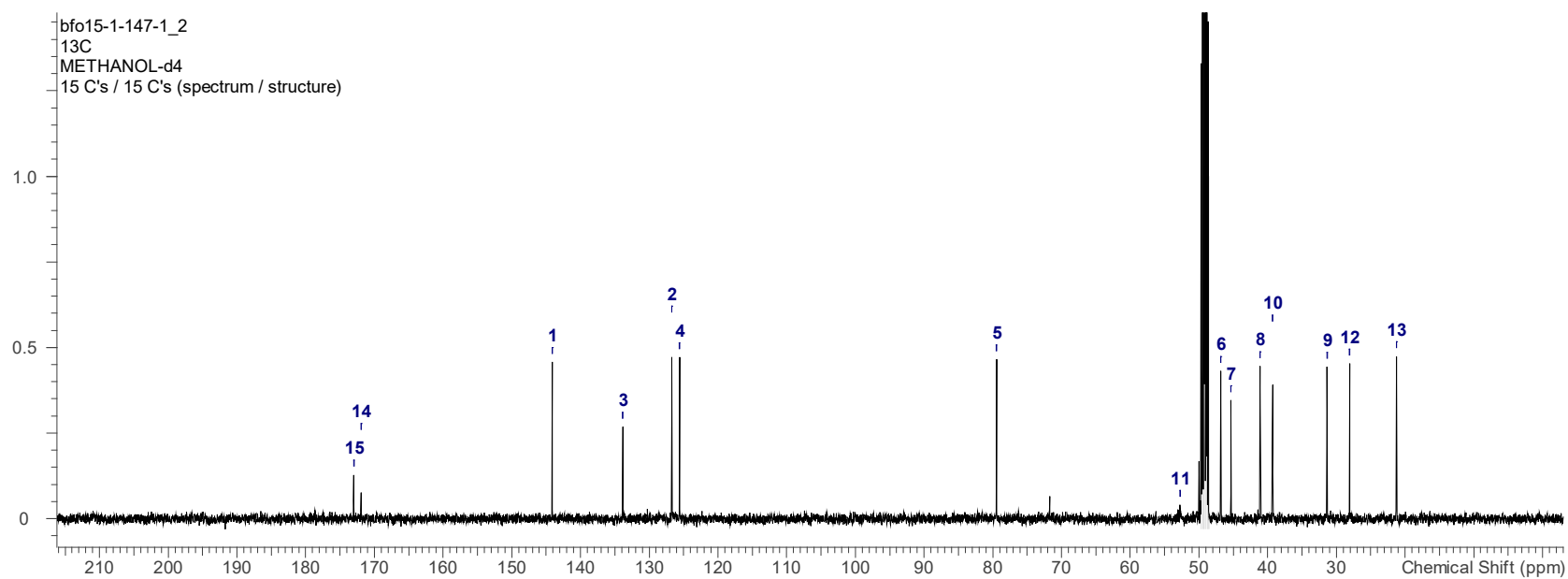
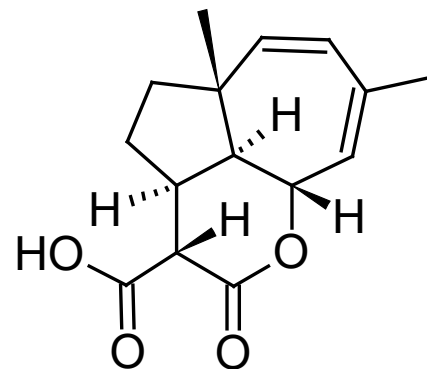


HRESIMS of Fulvoferruginin C (**3**).

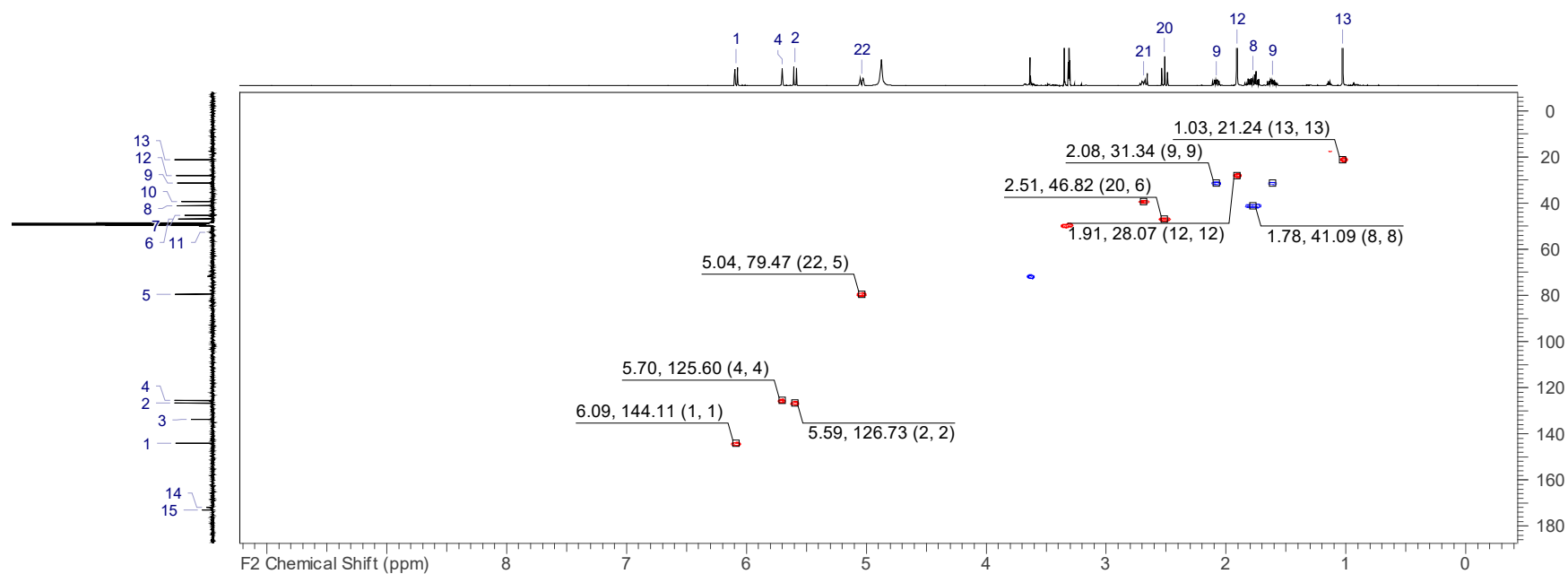
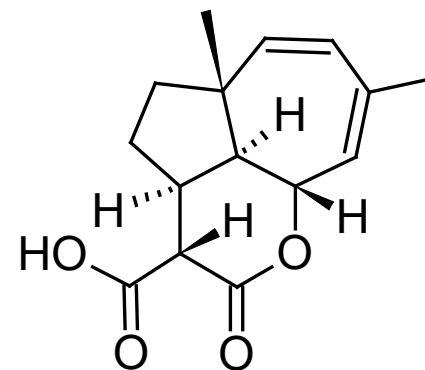
^1H NMR spectrum (700 MHz, methanol- d_4) of Fulvoferruginin C (**3**).



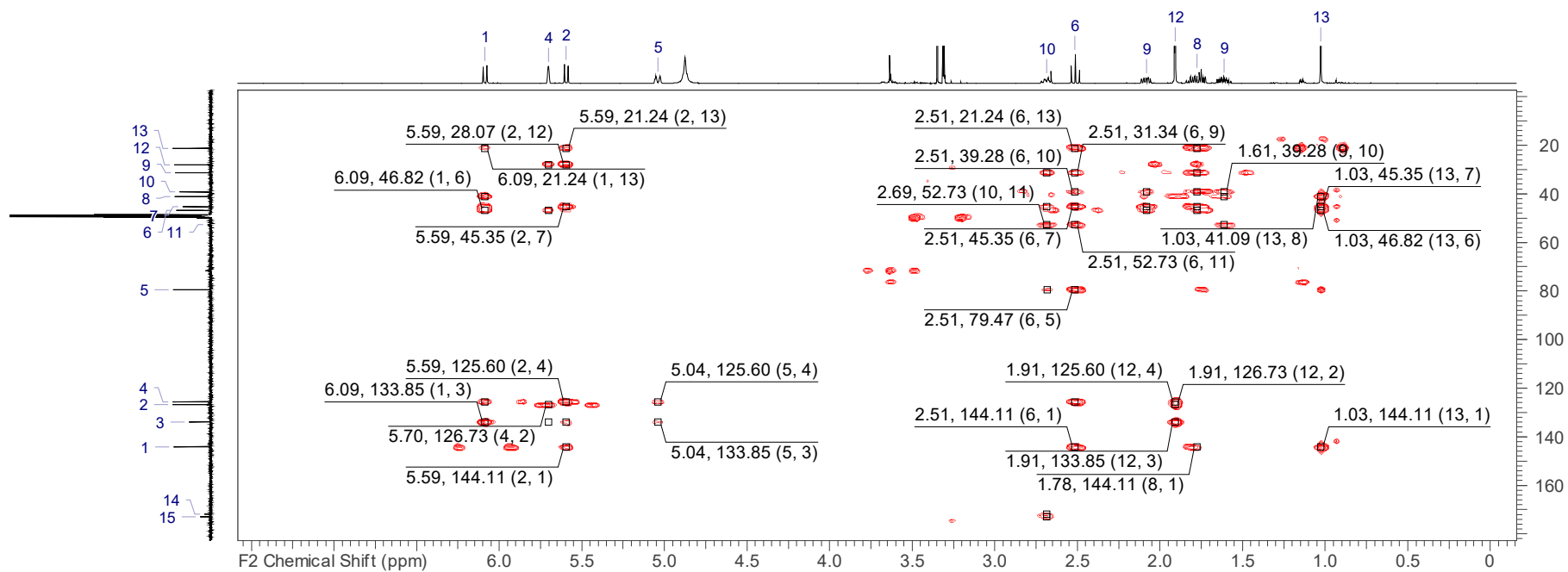
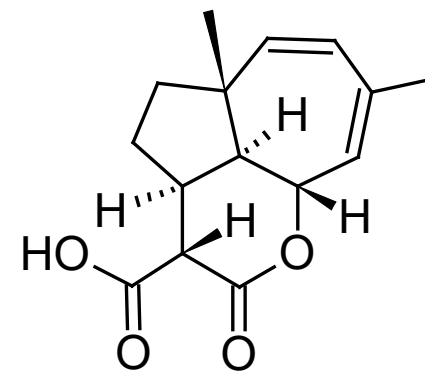
^{13}C NMR spectrum (176 MHz, methanol- d_4) of Fulvoferruginin C (**3**).



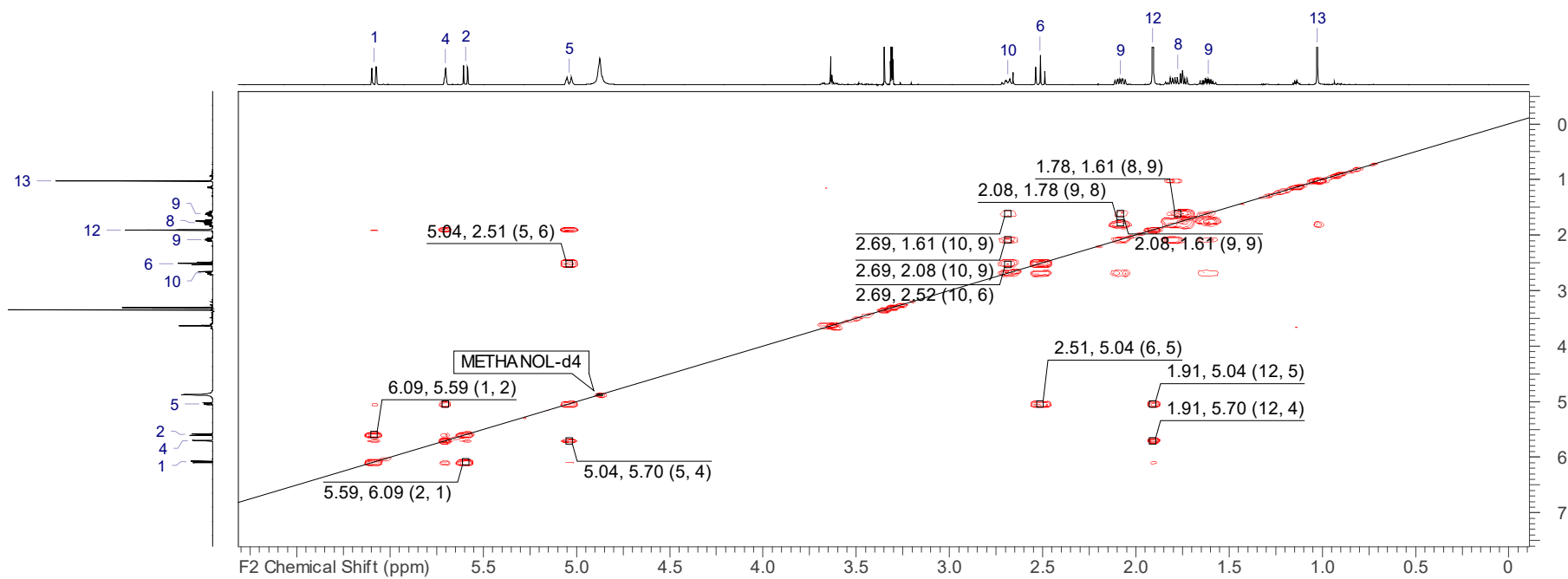
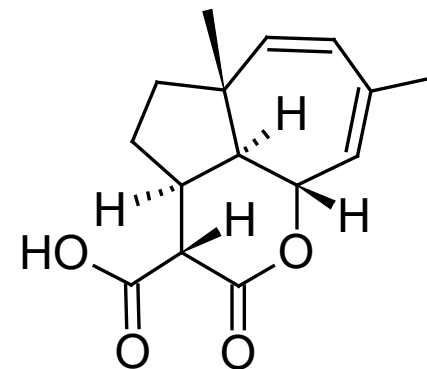
HSQC-dept NMR spectrum (700 MHz, methanol-*d*₄) of Fulvoferruginin C (**3**).



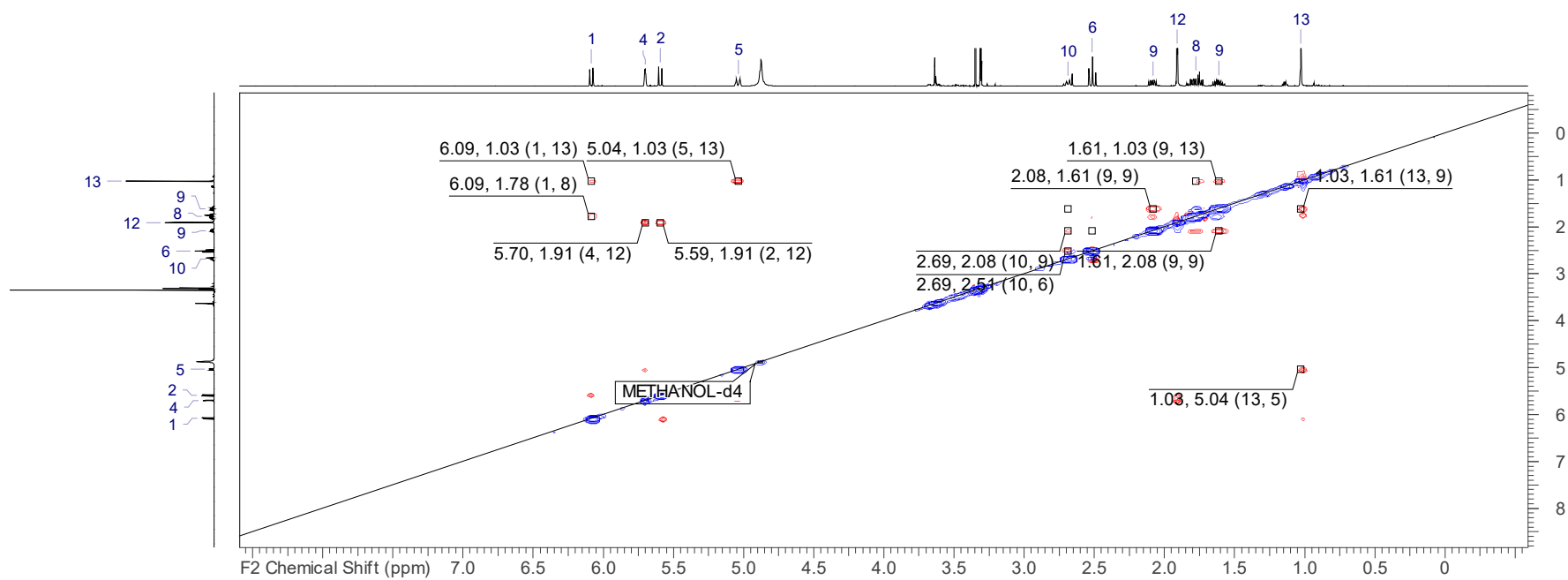
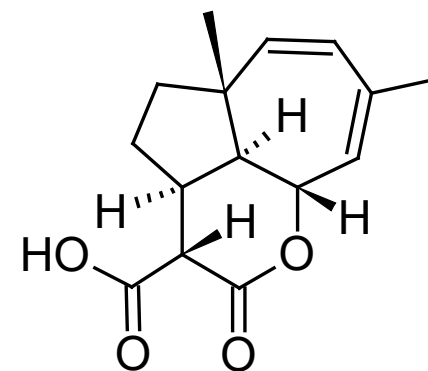
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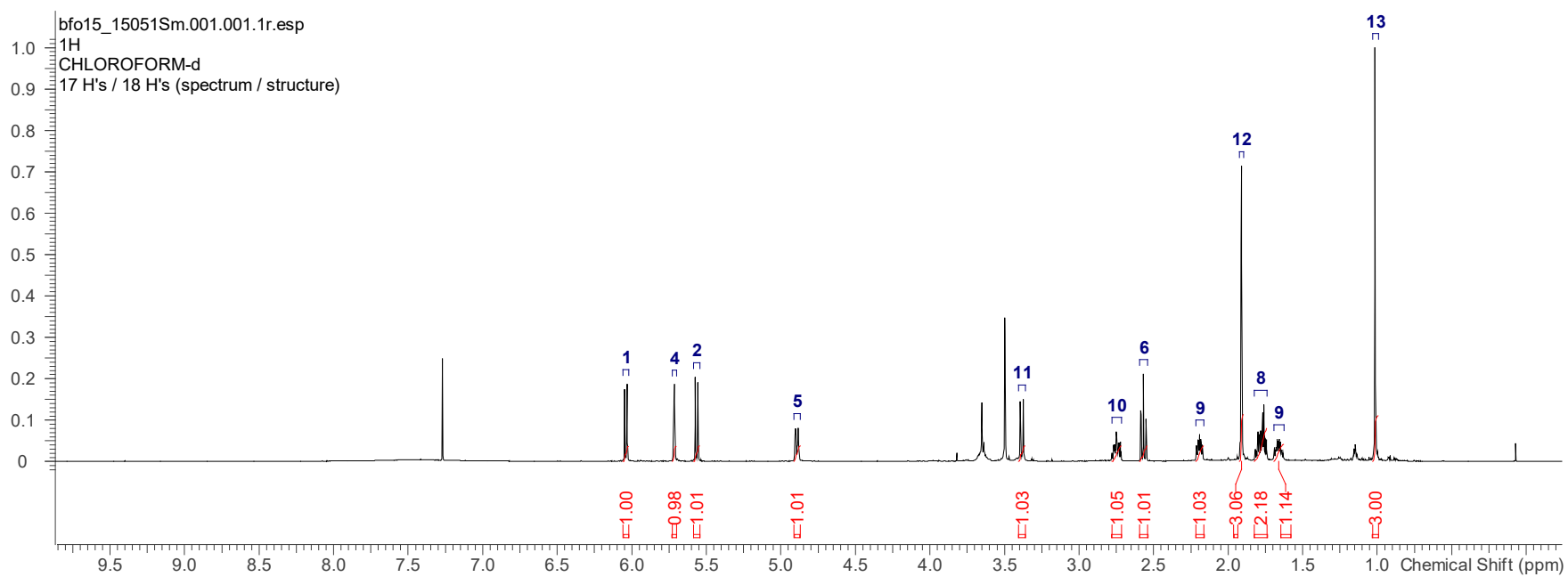
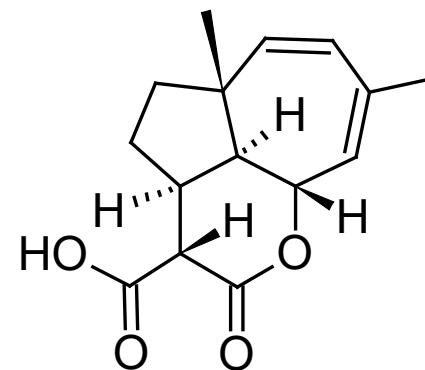
COSY NMR spectrum (700 MHz, methanol- d_4) of Fulvoferruginin C (**3**).



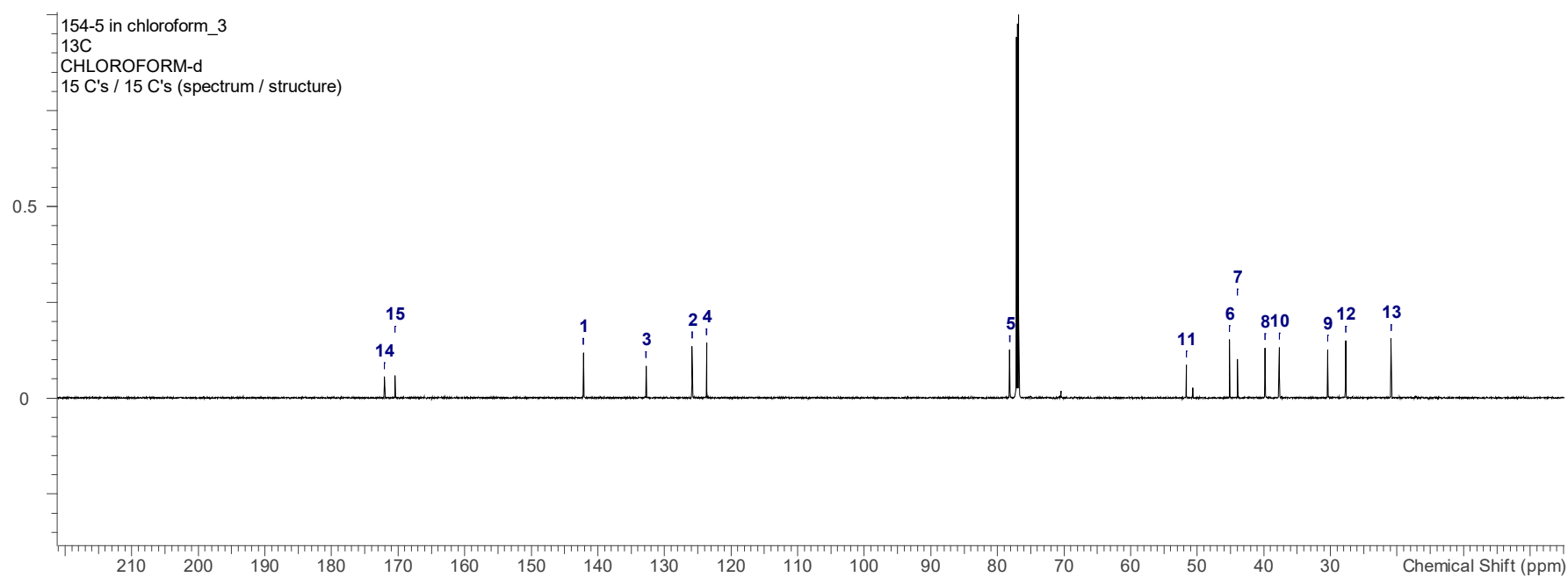
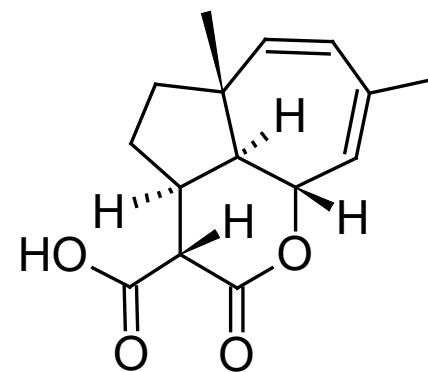
ROESY NMR spectrum (700 MHz, methanol- d_4) of Fulvoferruginin C (**3**).



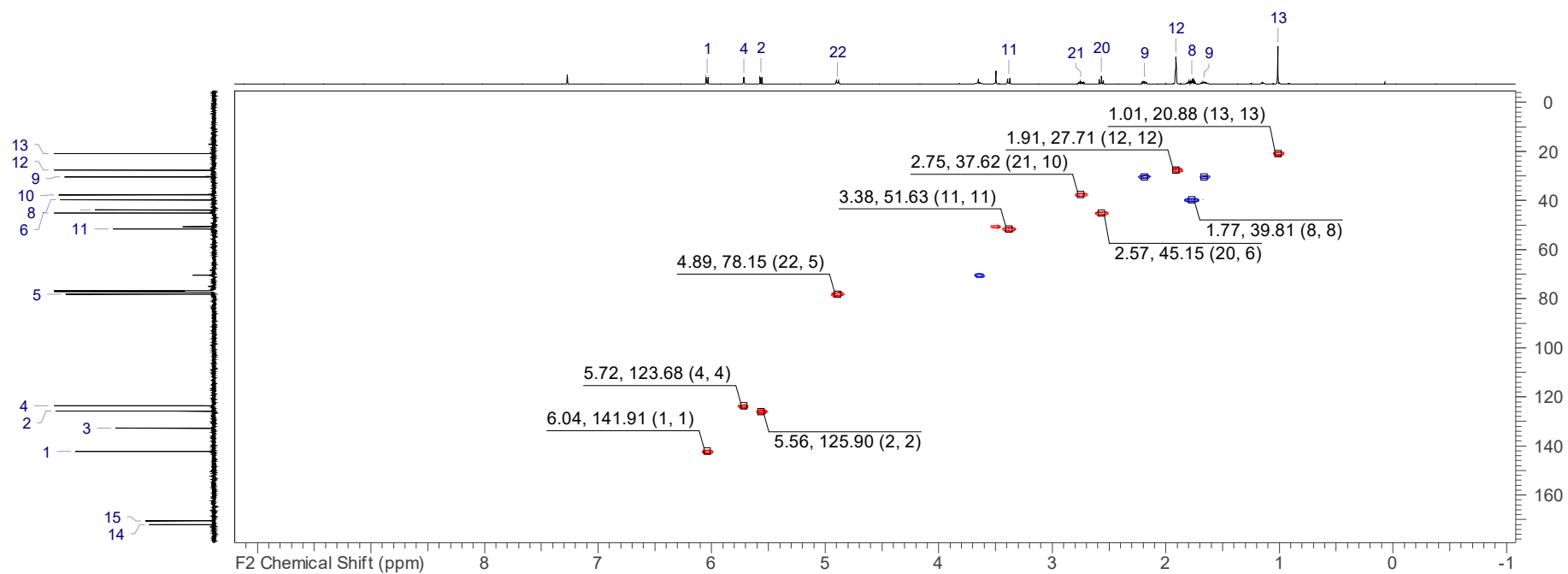
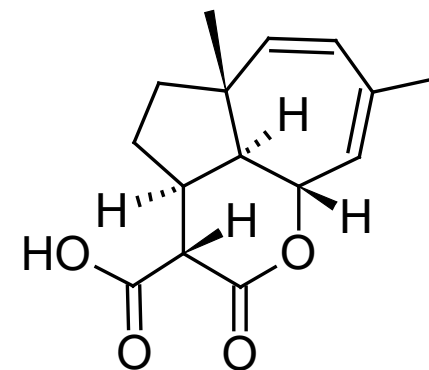
^1H NMR spectrum (700 MHz, chloroform-*d*) of Fulvoferruginin C (**3**).



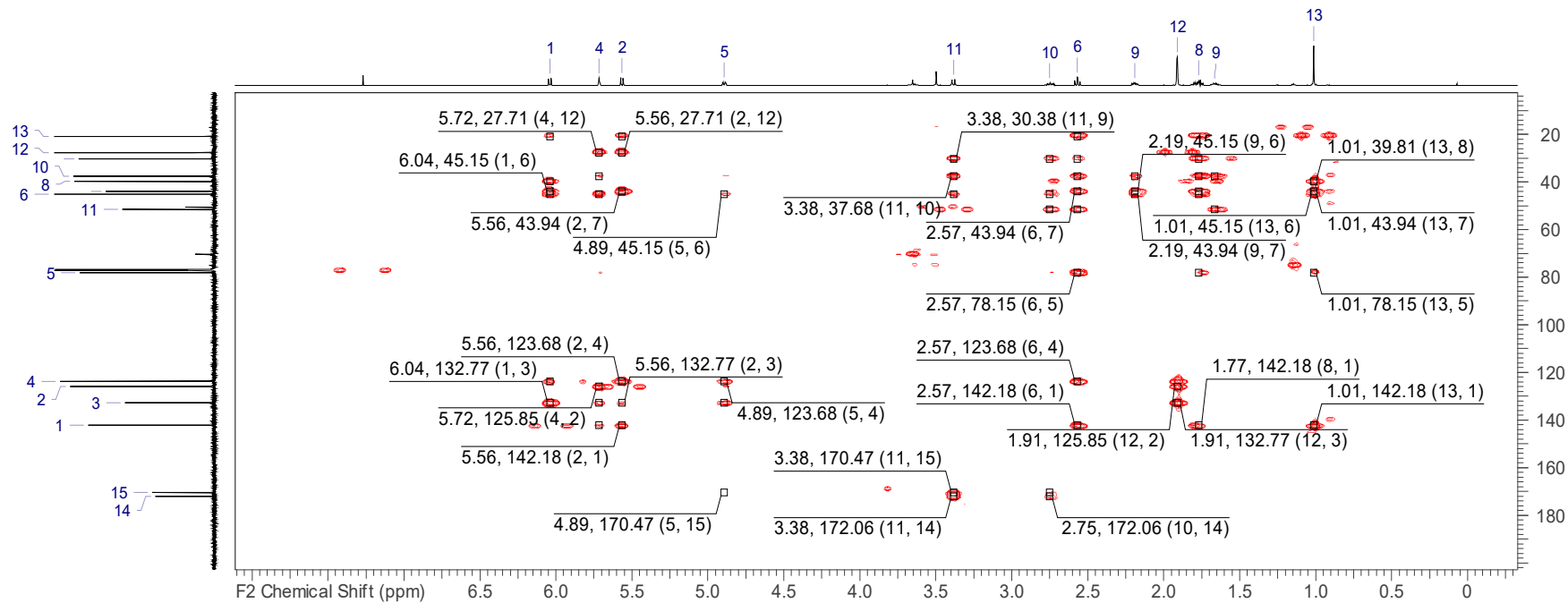
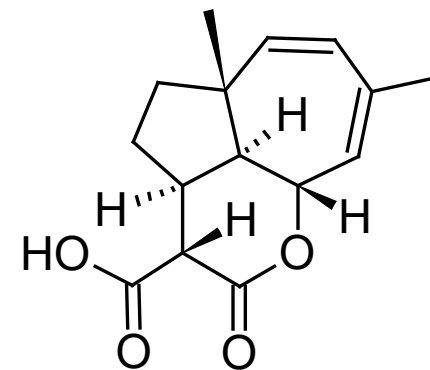
^{13}C NMR spectrum (176 MHz, chloroform-*d*) of Fulvoferruginin C (**3**).



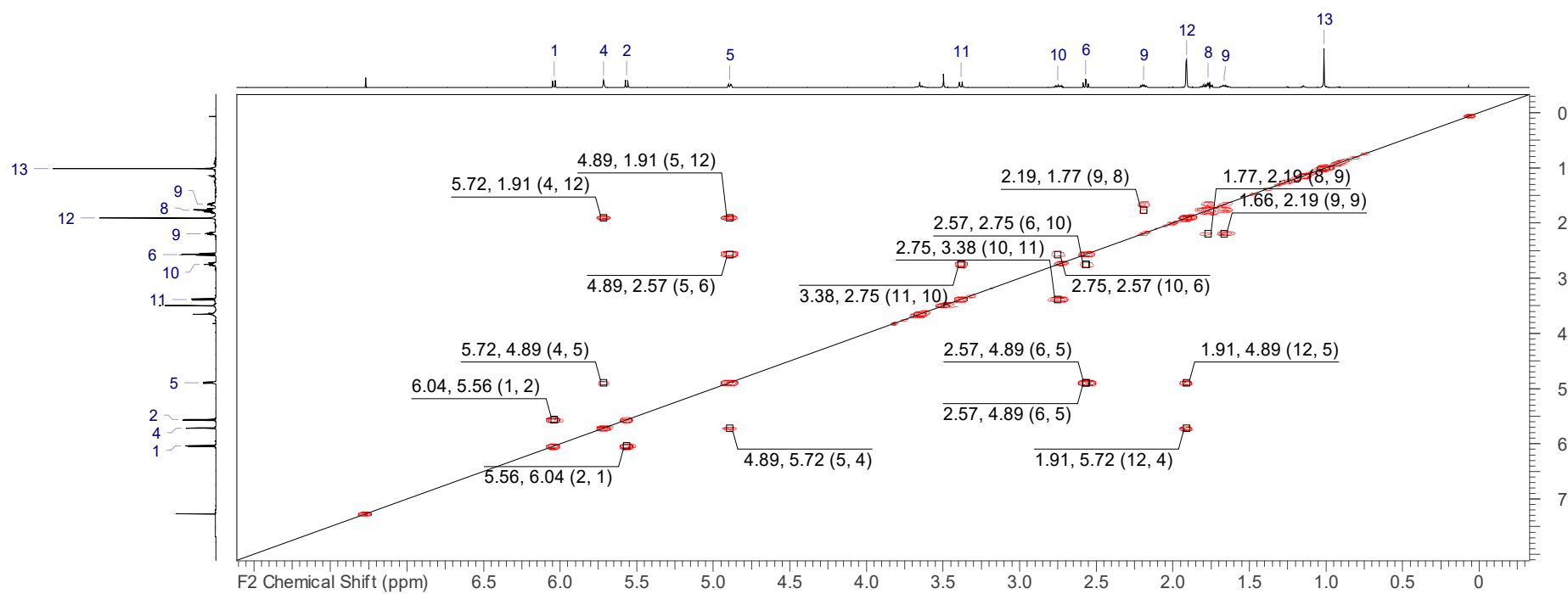
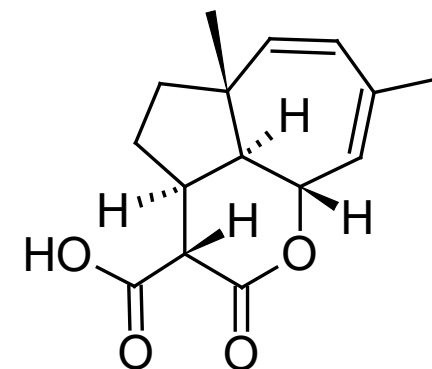
HSQC-dept NMR spectrum (700 MHz, chloroform-*d*) of Fulvoferruginin C (**3**).



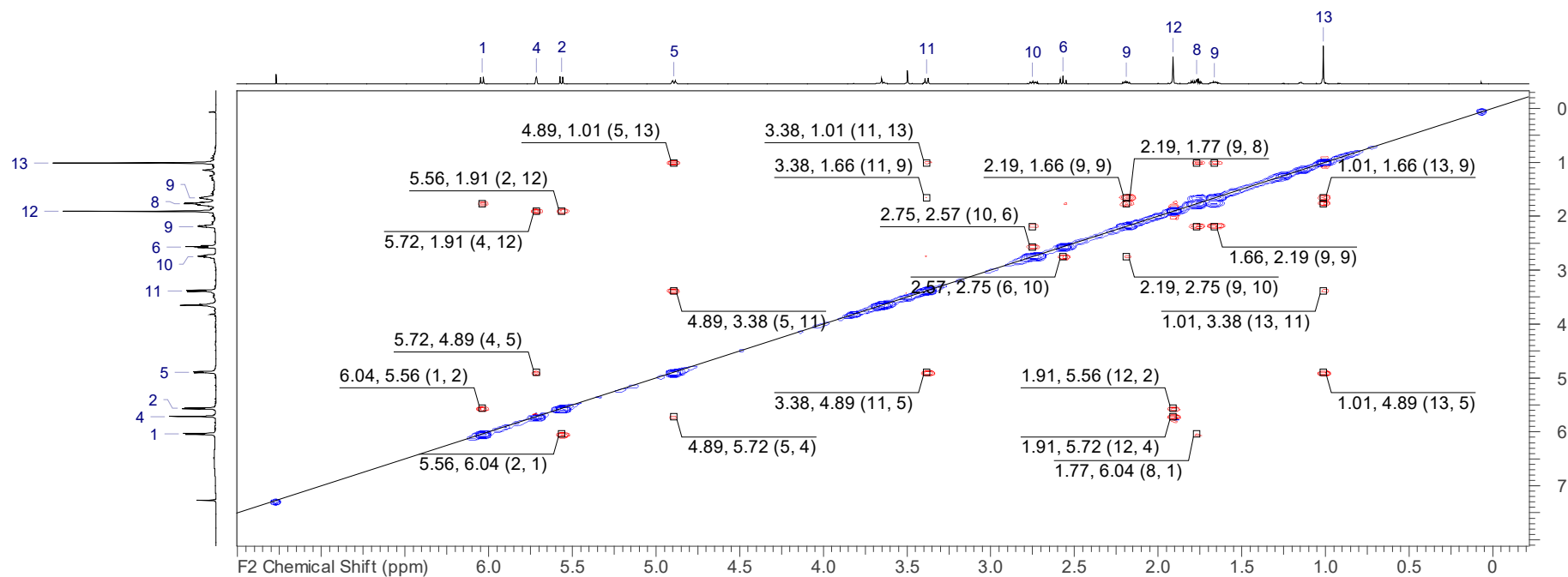
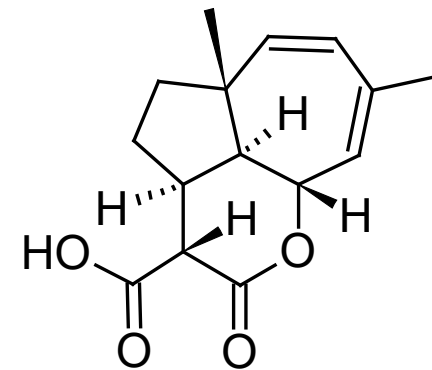
HMBC NMR spectrum (700 MHz, chloroform-*d*) of Fulvoferruginin C (**3**).

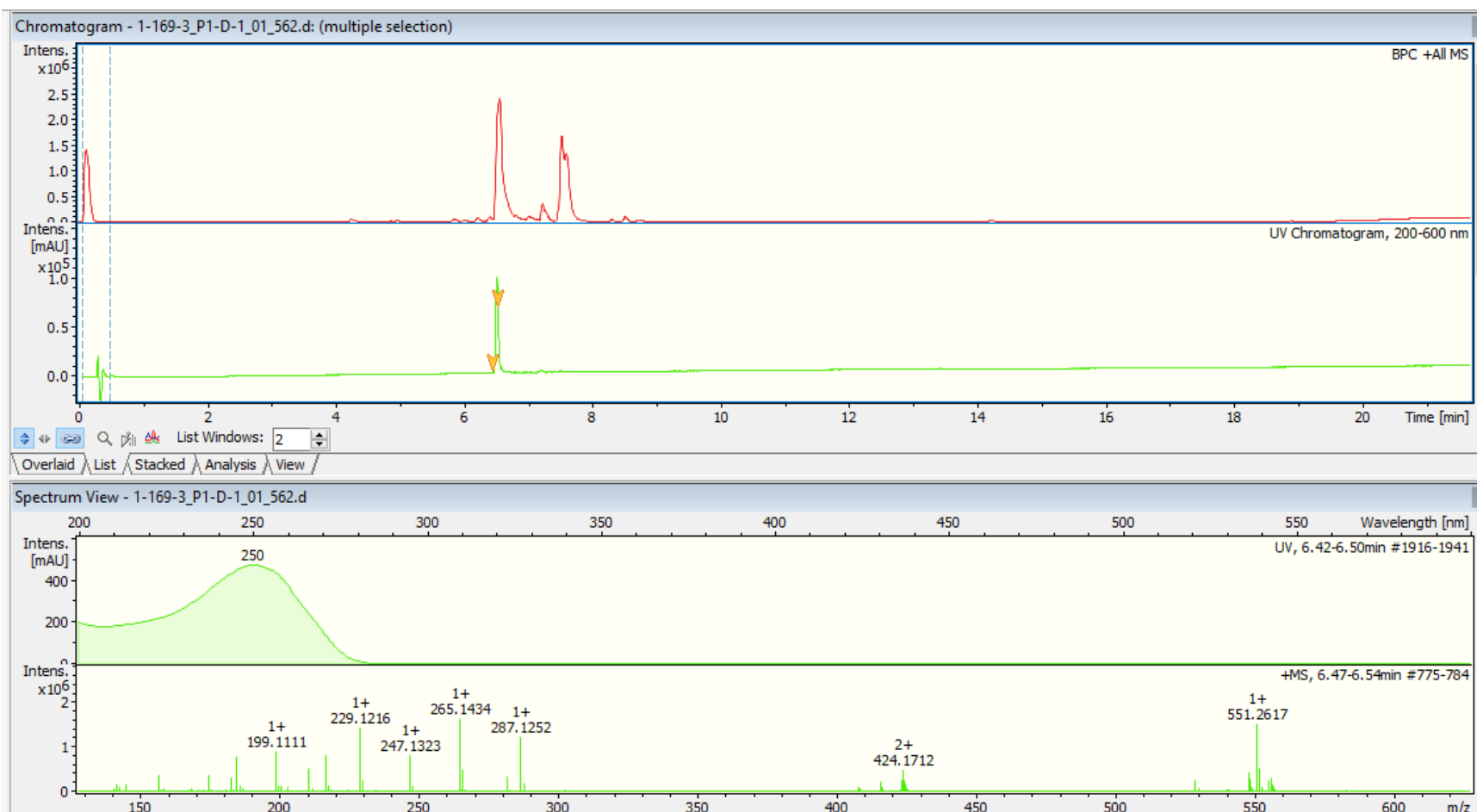


COSY NMR spectrum (700 MHz, chloroform-*d*) of Fulvoferruginin C (**3**).



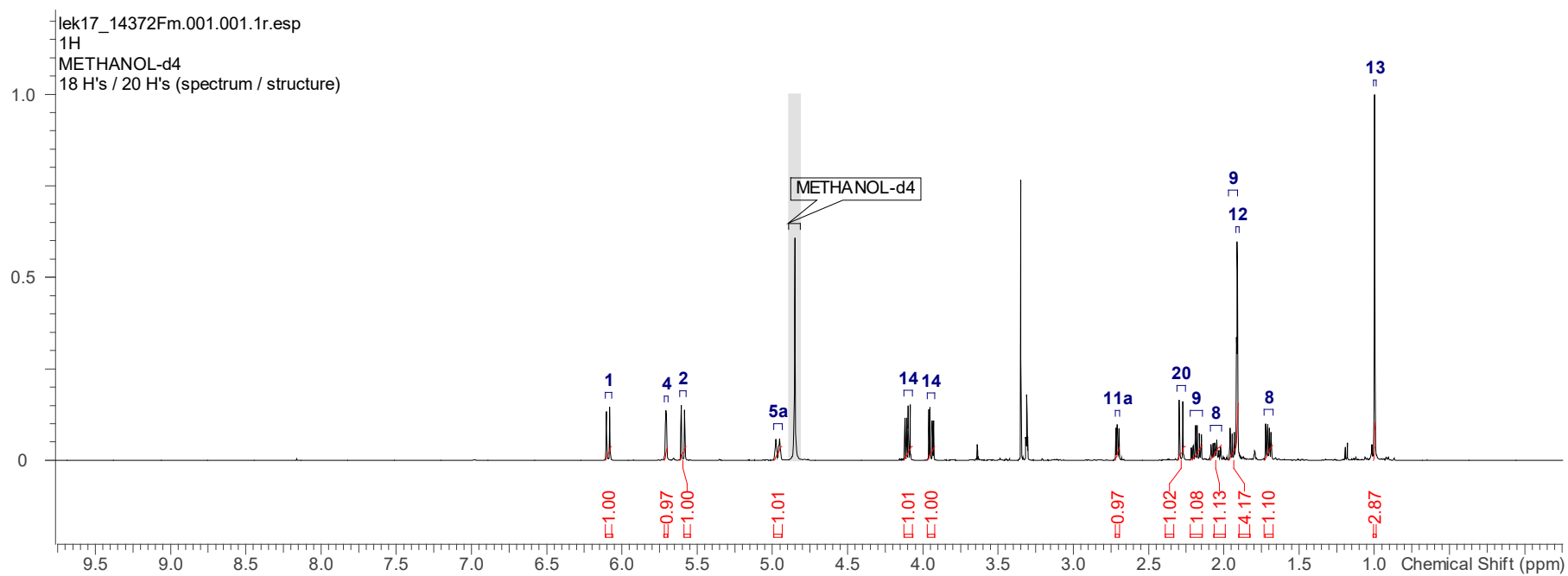
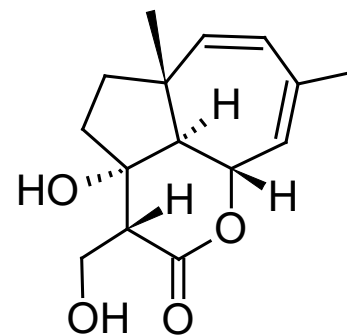
ROESY NMR spectrum (700 MHz, chloroform-*d*) of Fulvoferruginin C (**3**).



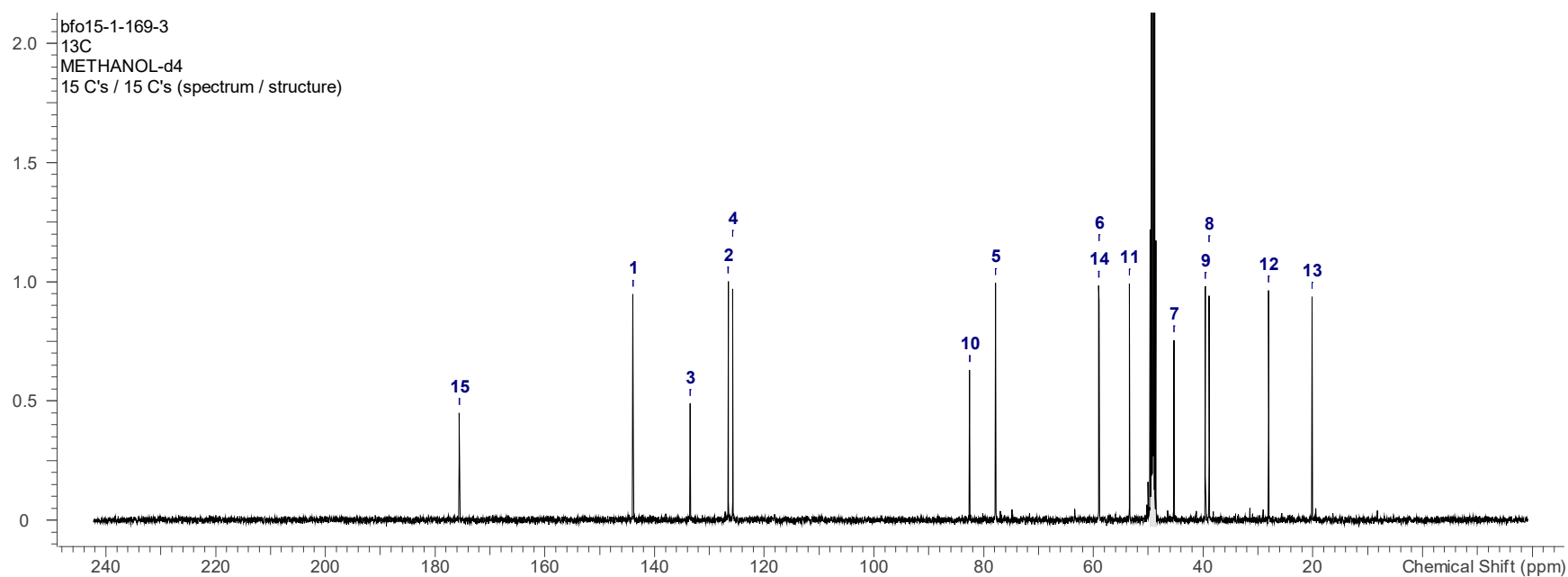
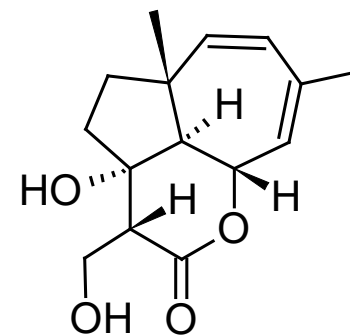


HRESIMS of Fulvoferruginin D (**4**).

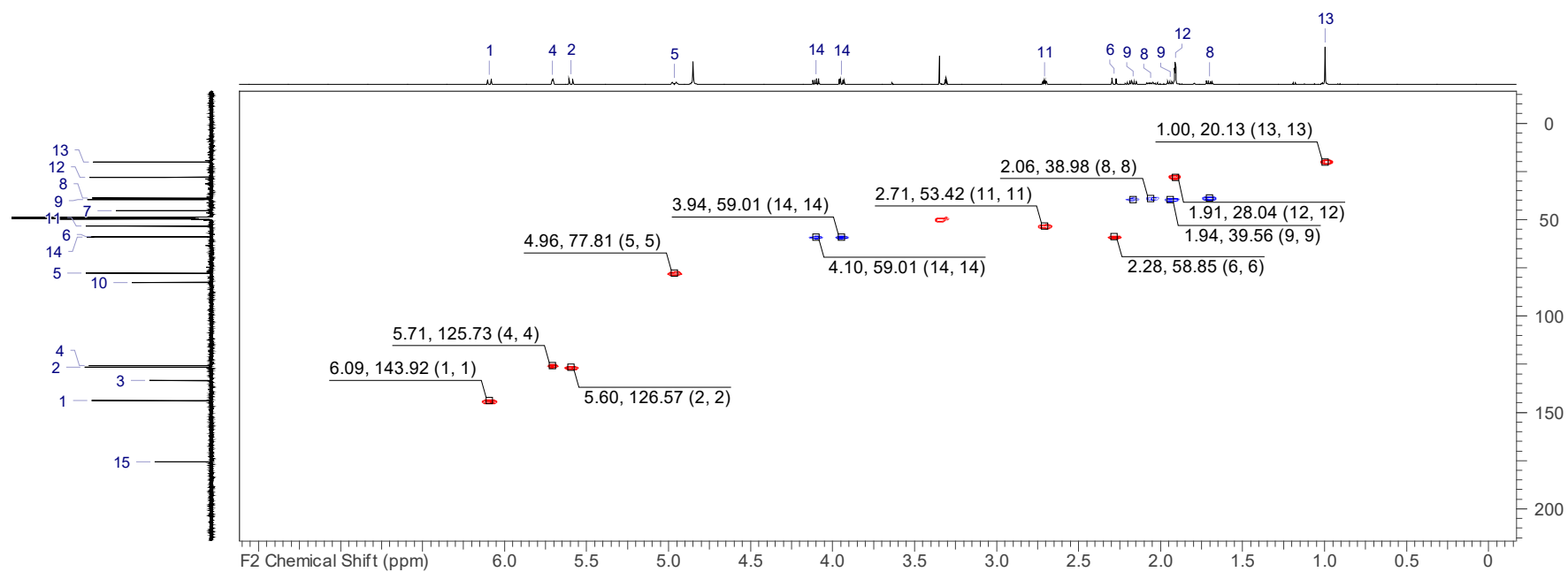
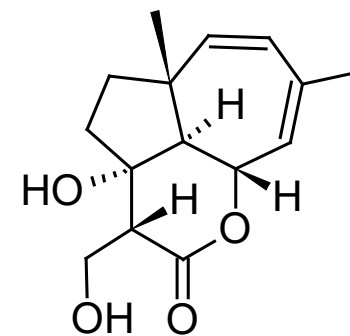
^1H NMR spectrum (700 MHz, methanol- d_4) of Fulvoferruginin D (**4**).



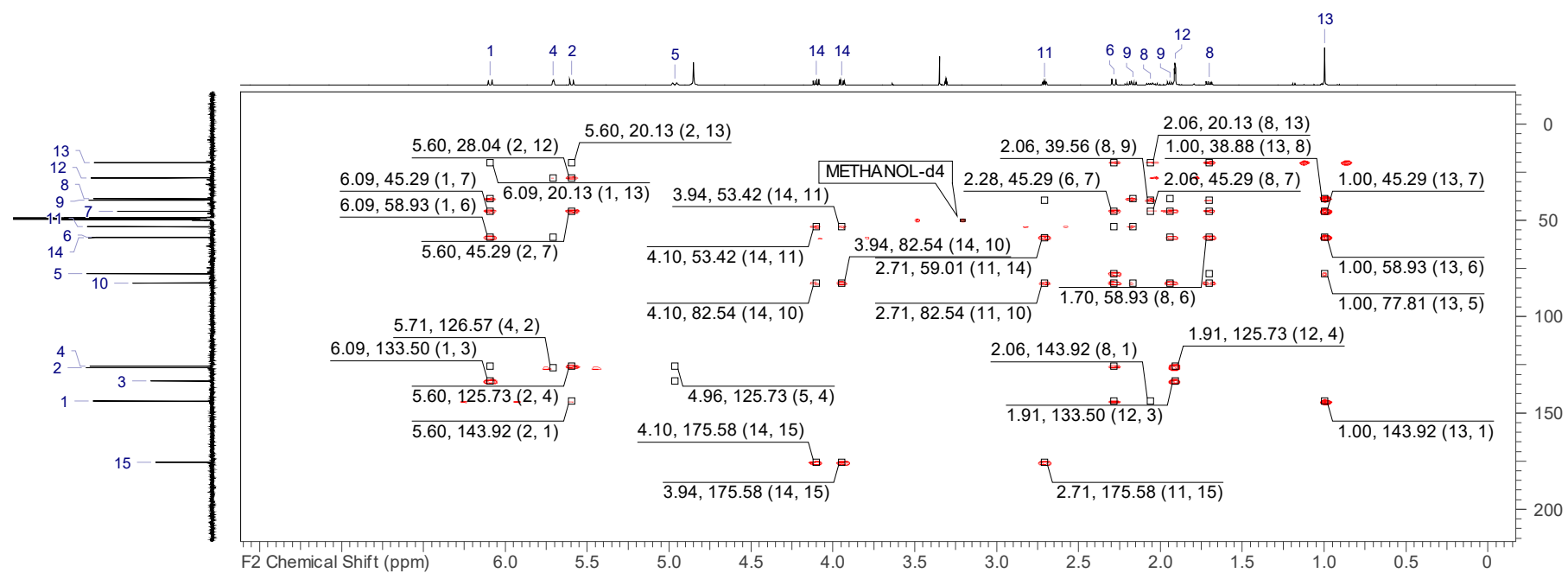
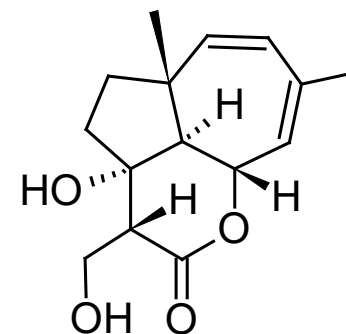
^{13}C NMR spectrum (176 MHz, methanol- d_4) of Fulvoferruginin D (**4**).



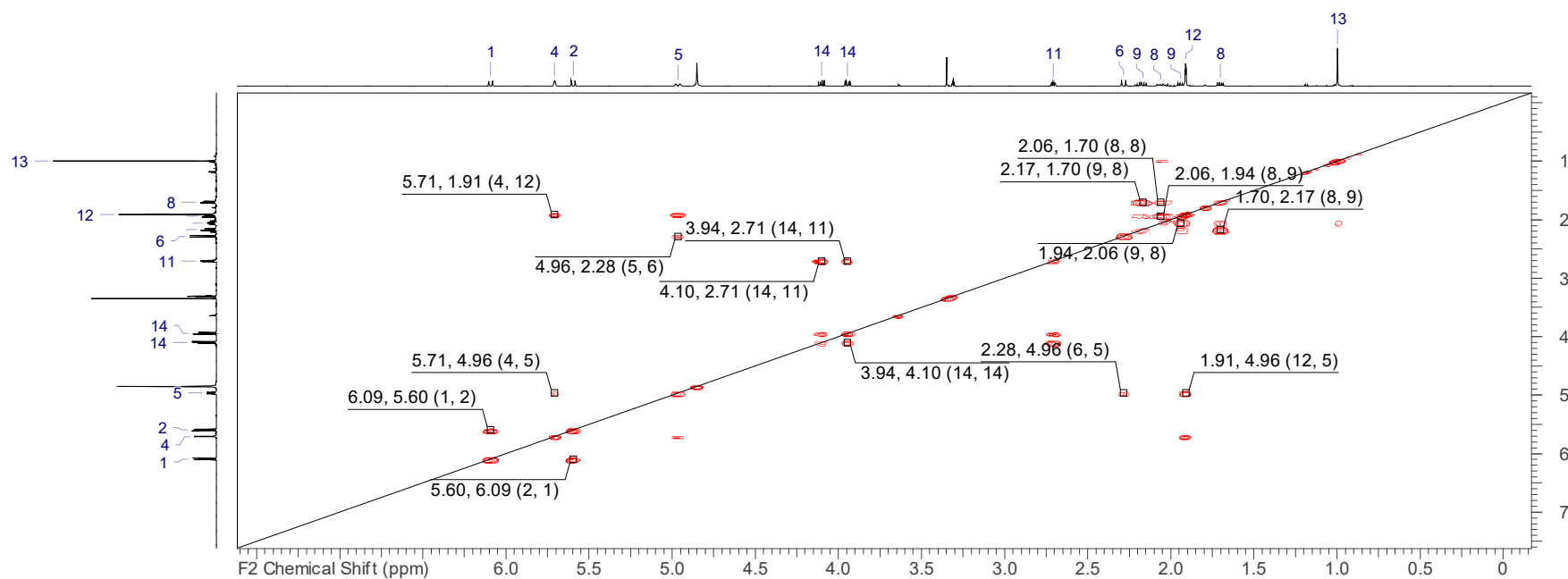
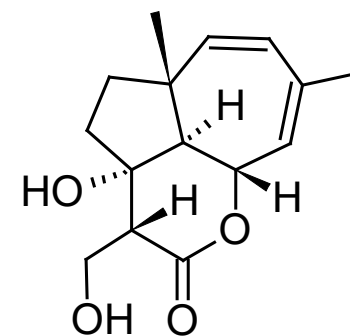
HSQC-dept NMR spectrum (700 MHz, methanol-*d*₄) of Fulvoferruginin D (**4**).



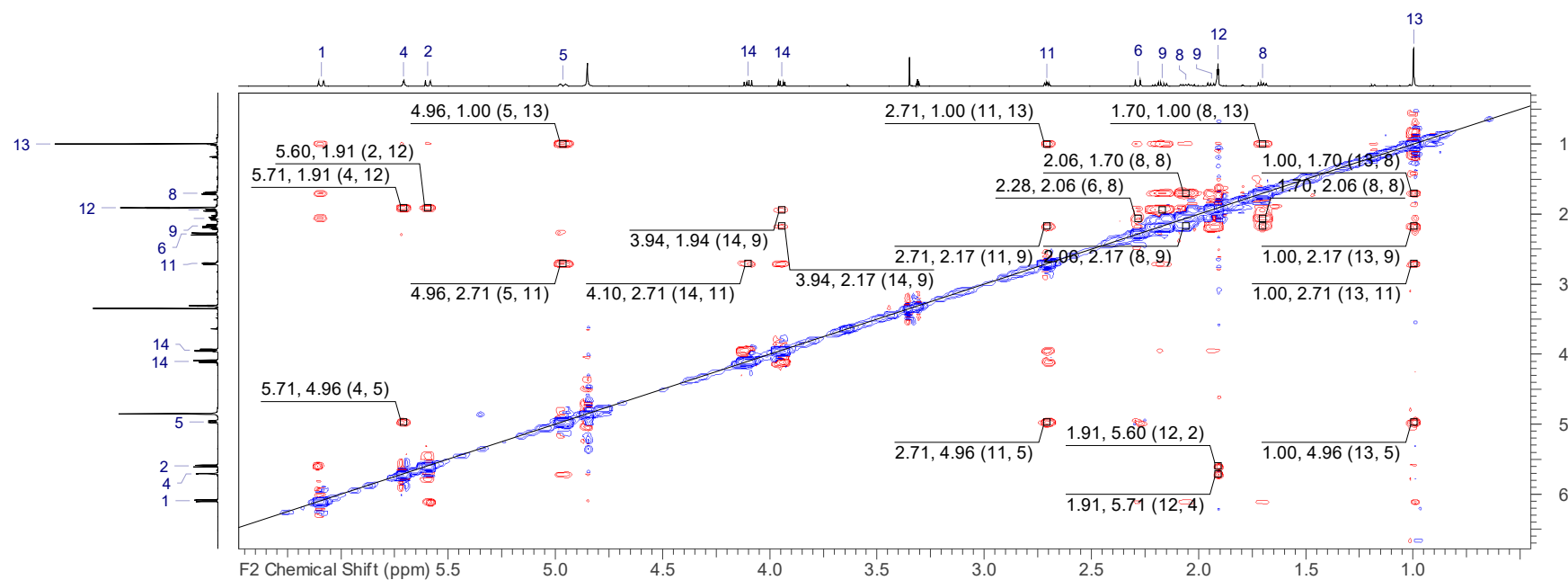
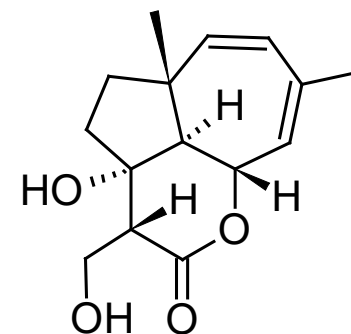
HMBC NMR spectrum (700 MHz, methanol-*d*₄) of Fulvoferruginin D (**4**).

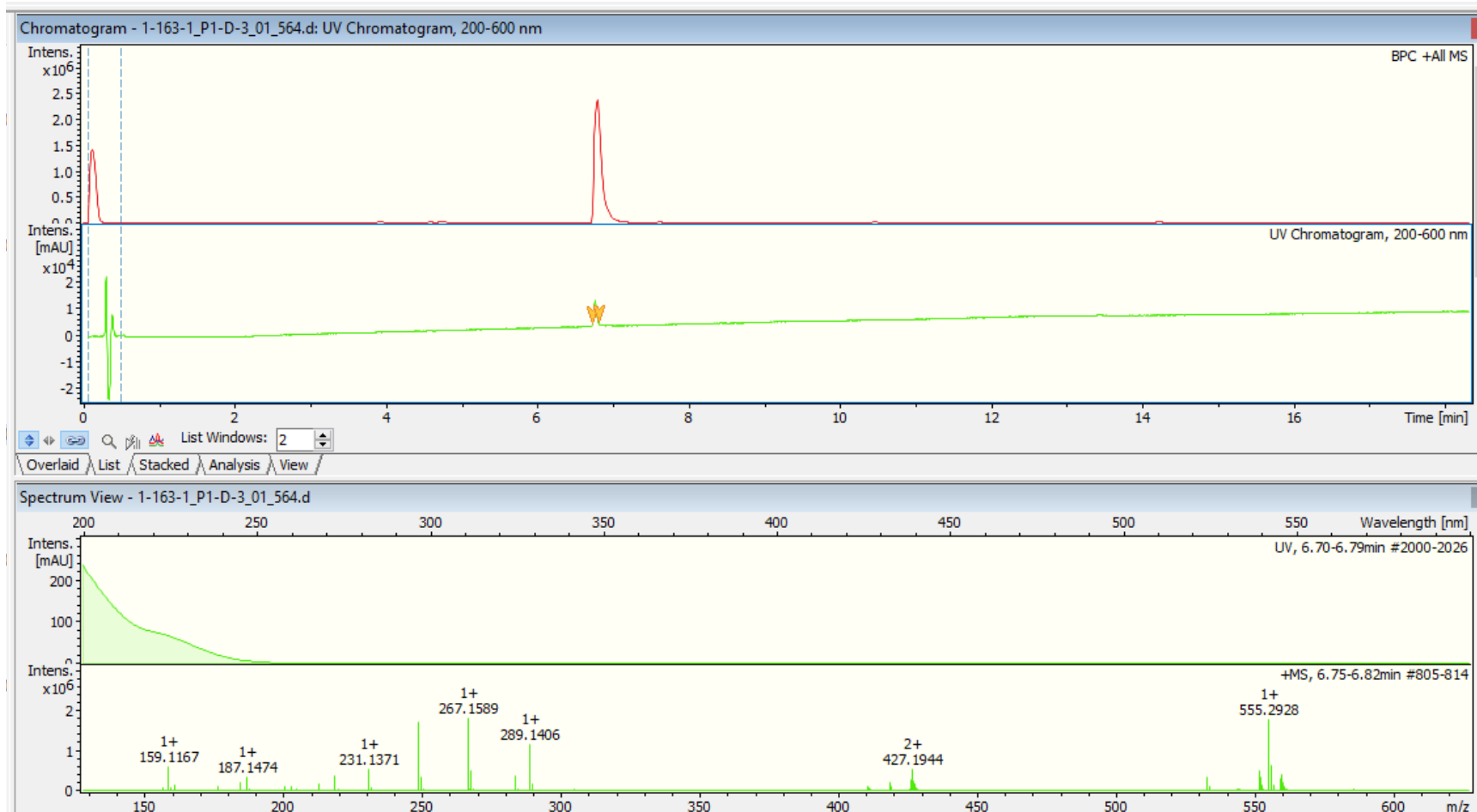


COSY NMR spectrum (700 MHz, methanol- d_4) of Fulvoferruginin D (**4**).



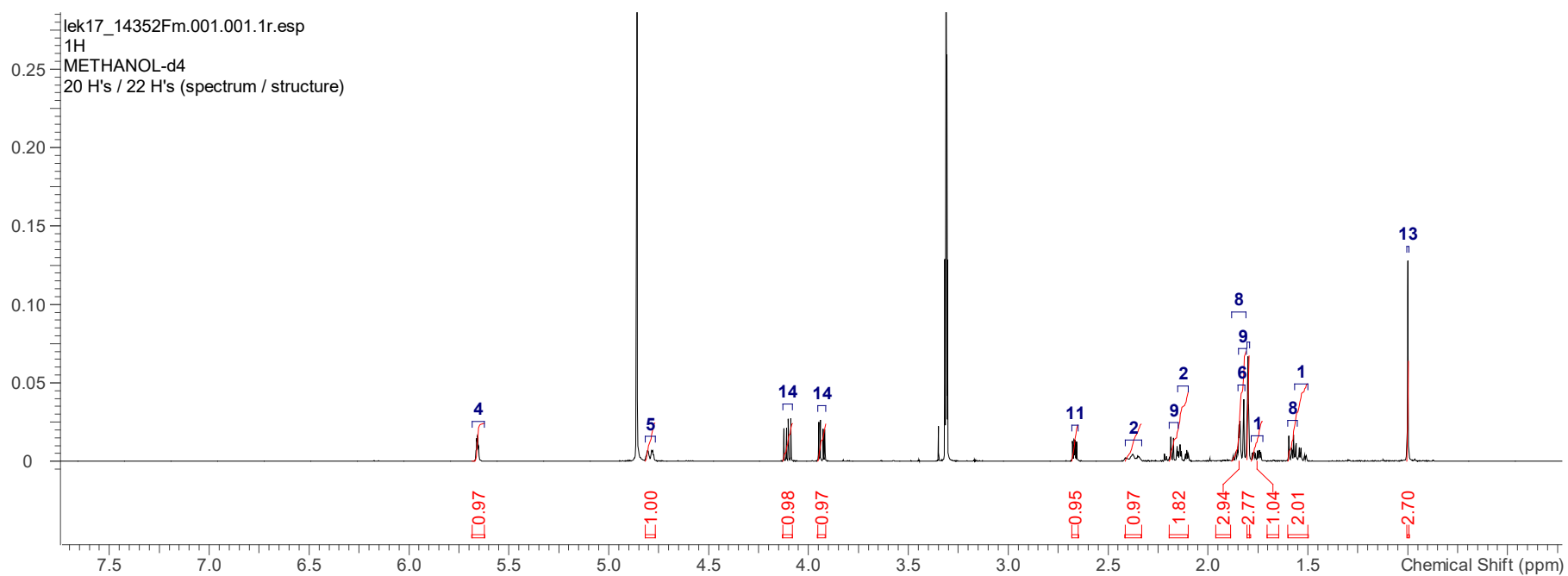
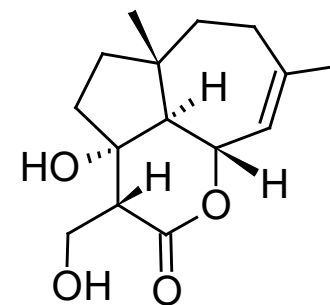
ROESY NMR spectrum (700 MHz, methanol- d_4) of Fulvoferruginin D (**4**).



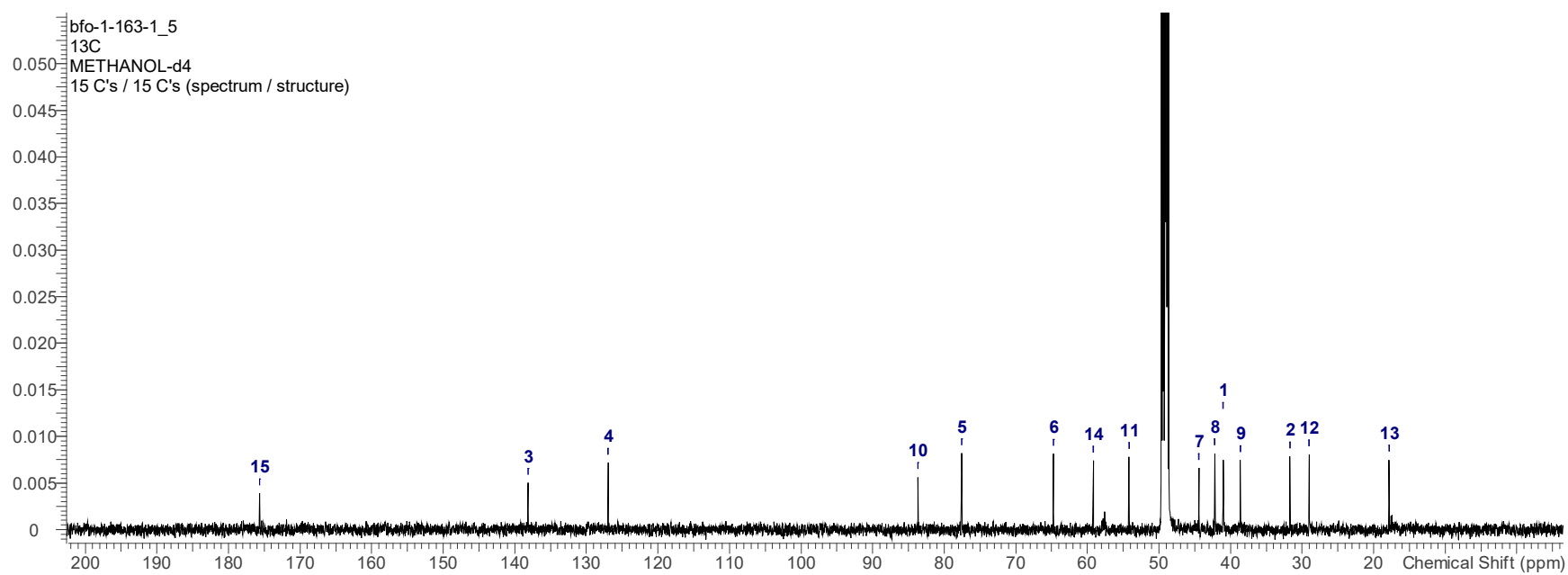
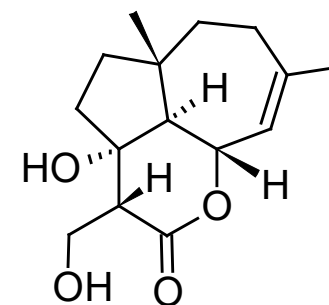


HRESIMS of Fulvoferruginin E (**5**).

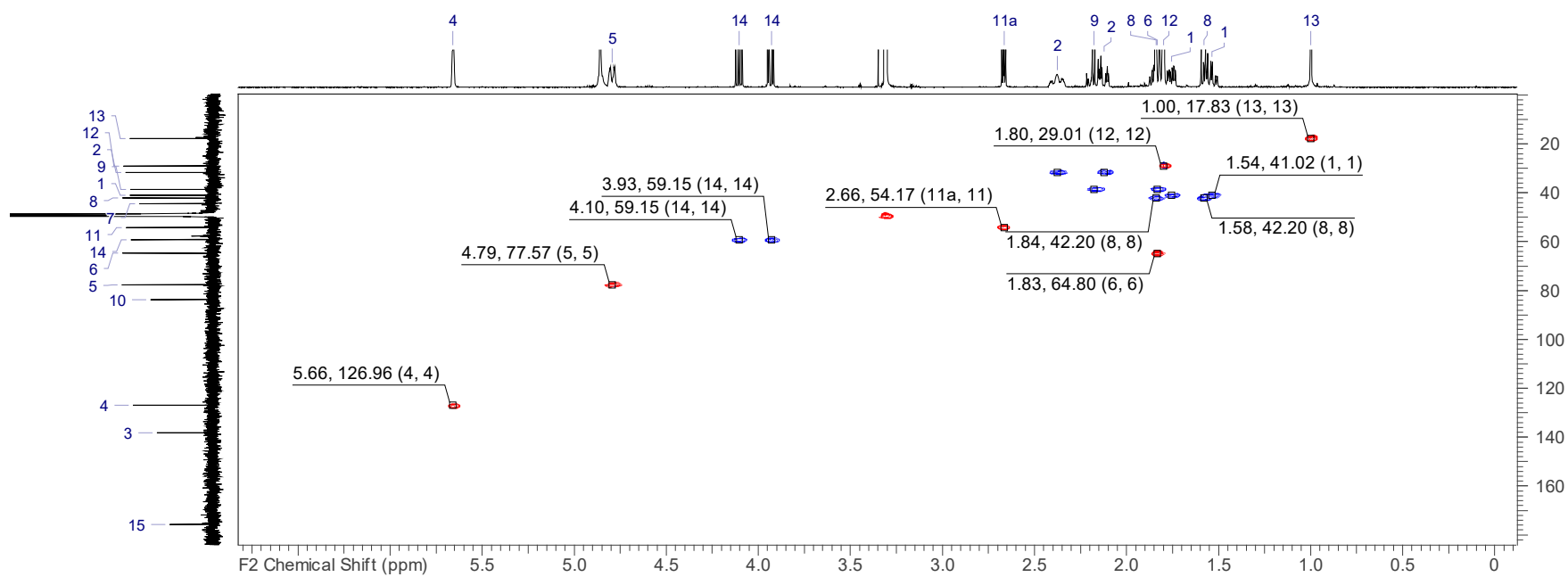
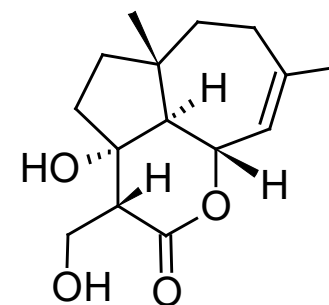
^1H NMR spectrum (700 MHz, methanol- d_4) of Fulvoferruginin E (**5**).



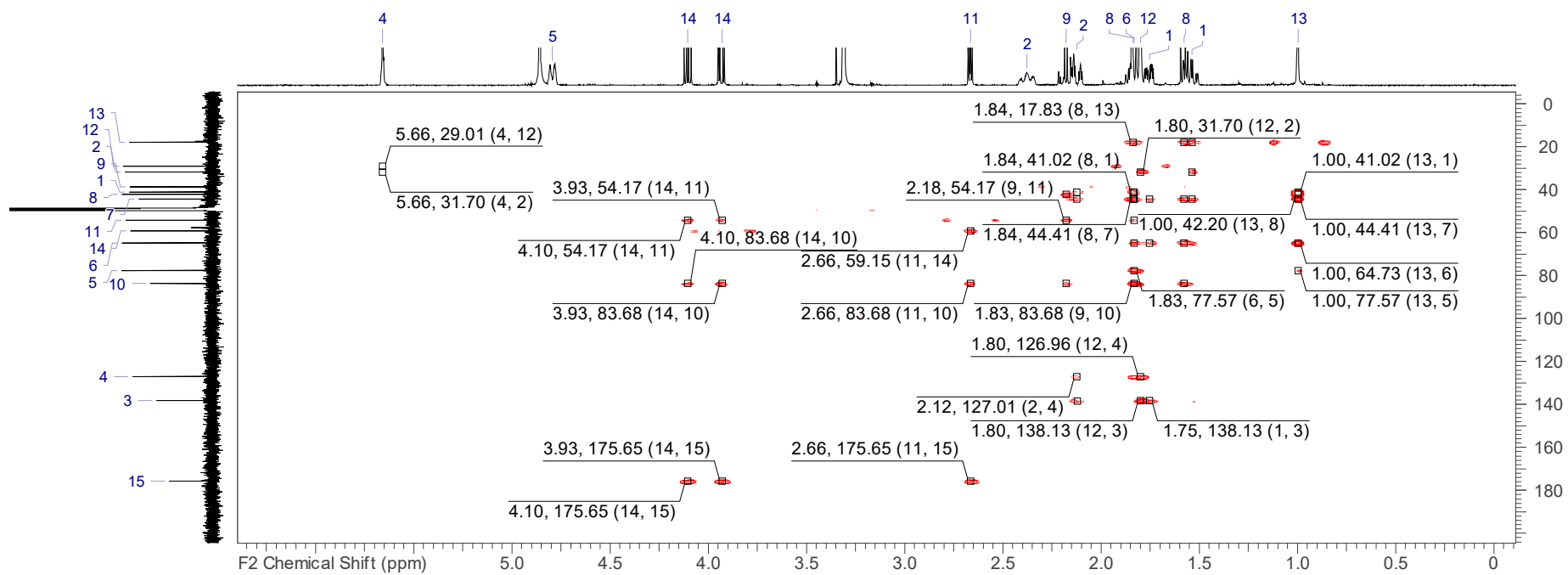
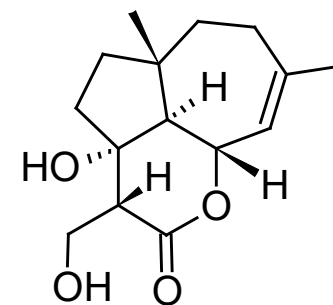
^{13}C NMR spectrum (176 MHz, methanol- d_4) of Fulvoferruginin E (**5**).



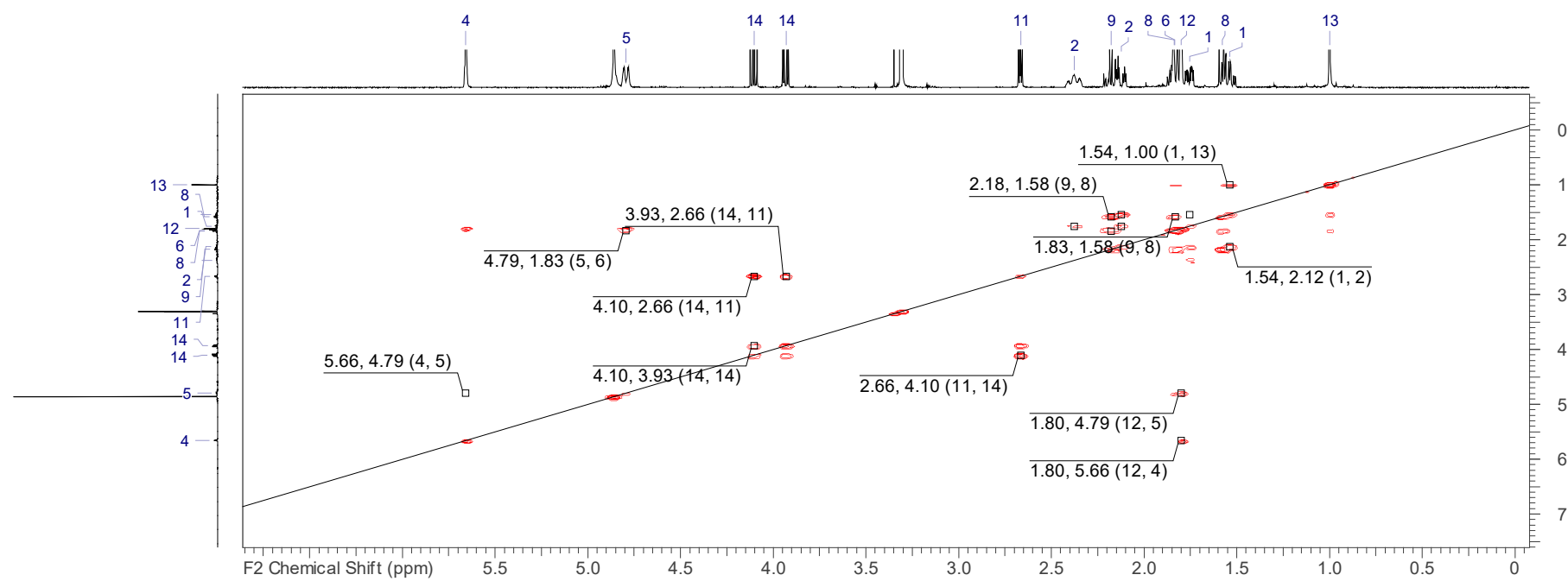
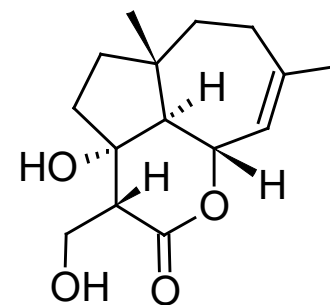
HSQC-dept NMR spectrum (700 MHz, methanol-*d*₄) of Fulvoferruginin E (**5**).



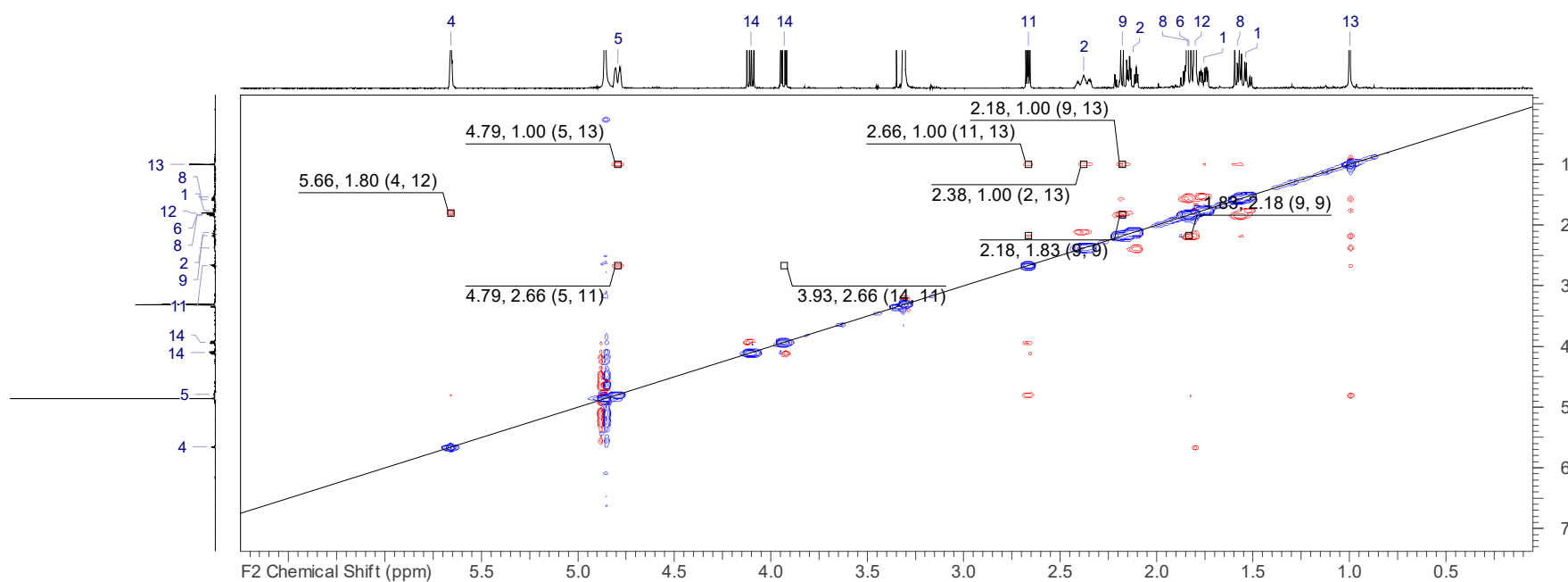
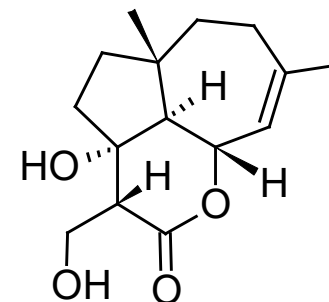
HMBC NMR spectrum (700 MHz, methanol- d_4) of Fulvoferruginin E (**5**).

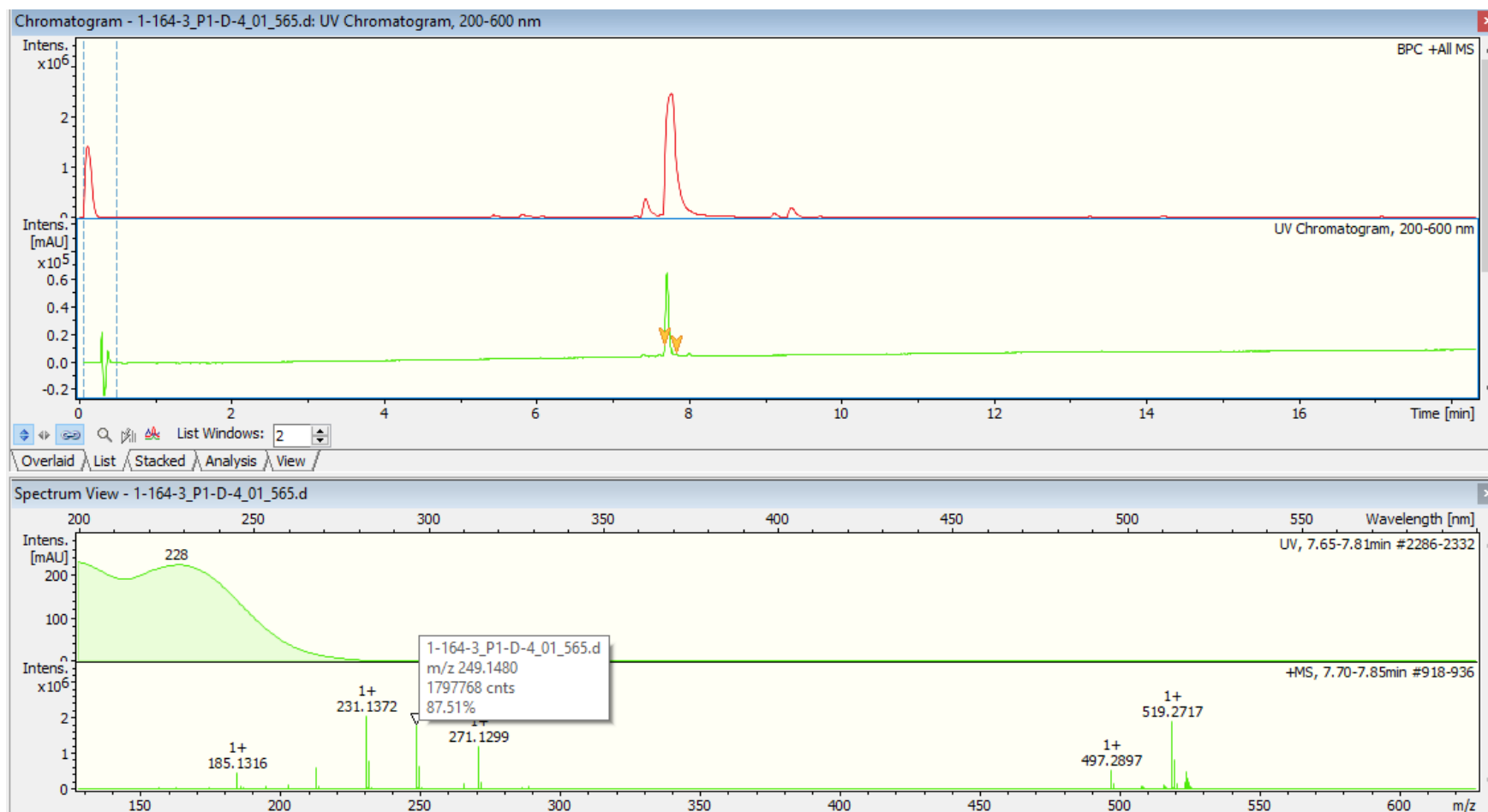


COSY NMR spectrum (700 MHz, methanol-*d*₄) of Fulvoferruginin E (**5**).



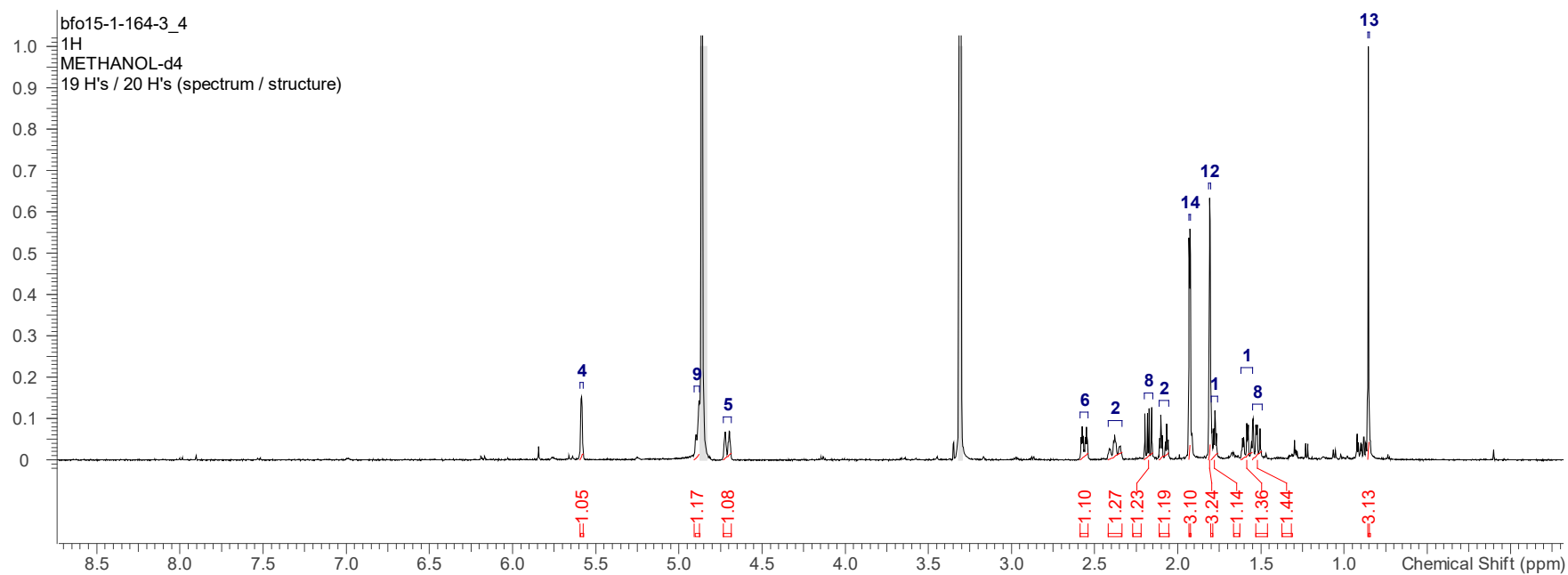
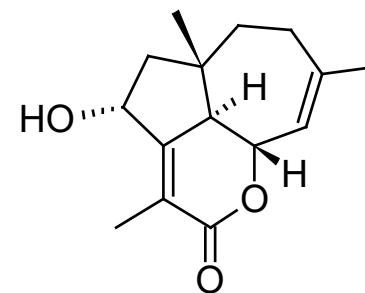
ROESY NMR spectrum (700 MHz, methanol- d_4) of Fulvoferruginin E (**5**).



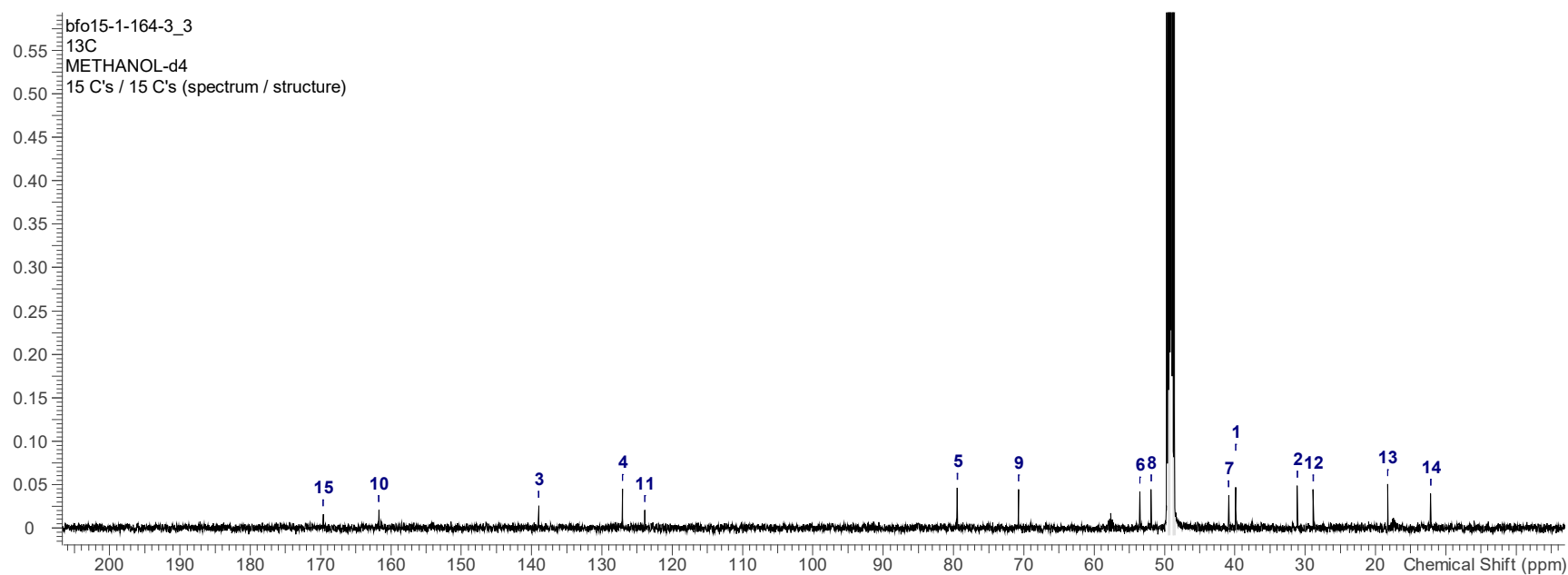
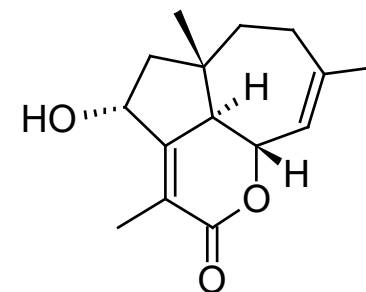


HRESIMS of Fulvoferruginin F (6).

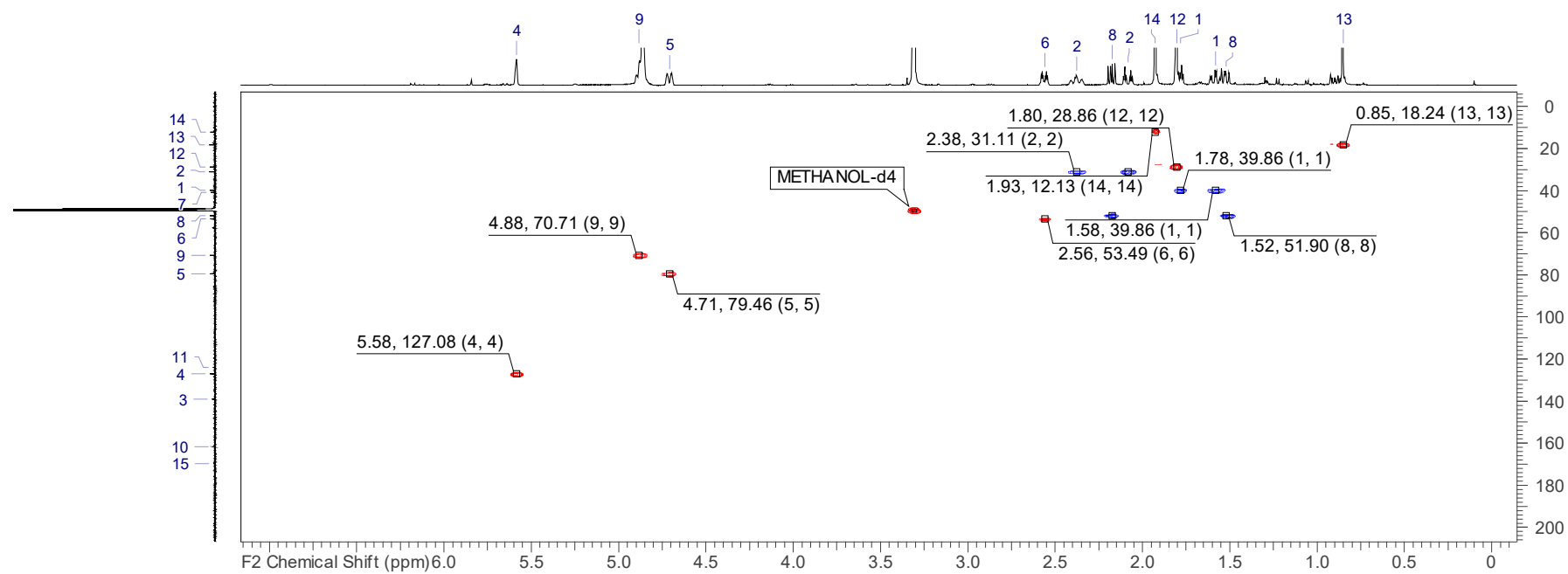
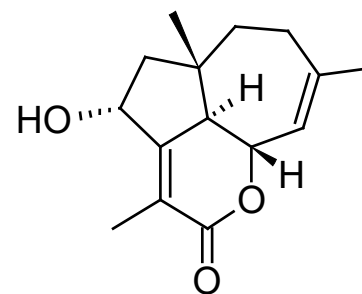
^1H NMR spectrum (700 MHz, methanol- d_4) of Fulvoferruginin F (**6**).



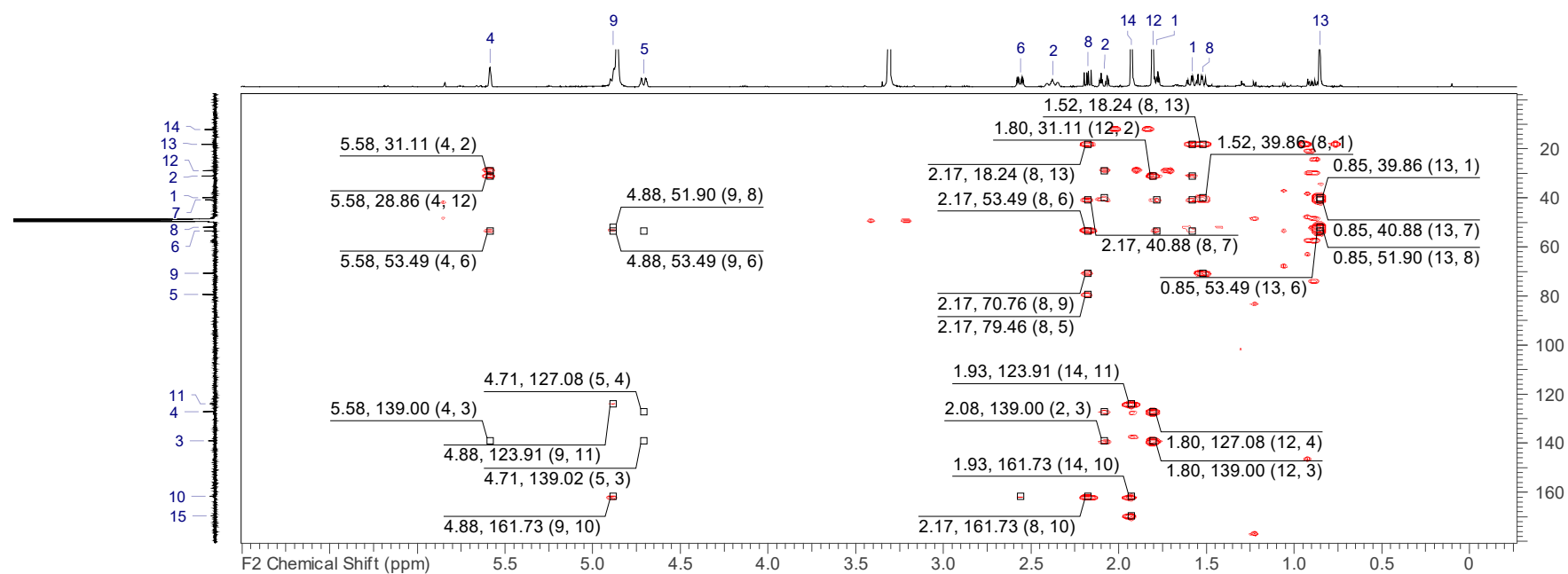
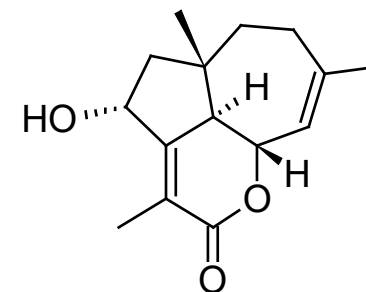
^{13}C NMR spectrum (176 MHz, methanol- d_4) of Fulvoferruginin F (**6**).



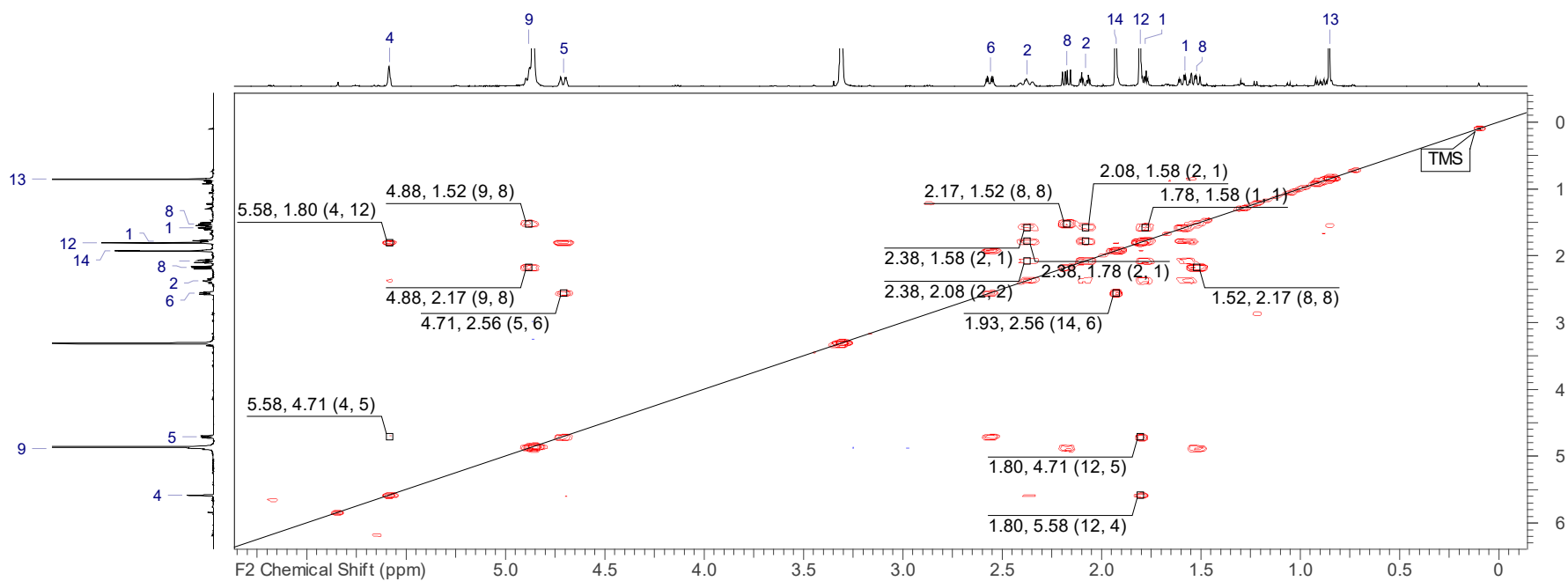
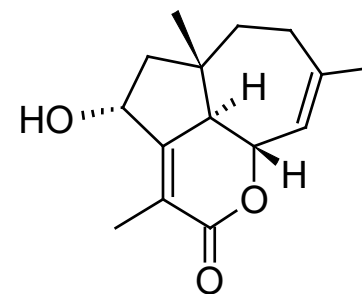
HSQC-dept NMR spectrum (700 MHz, methanol-*d*₄) of Fulvoferruginin F (**6**).



HMBC NMR spectrum (700 MHz, methanol- d_4) of Fulvoferruginin F (**6**).



COSY NMR spectrum (700 MHz, methanol- d_4) of Fulvoferruginin F (**6**).



ROESY NMR spectrum (700 MHz, methanol- d_4) of Fulvoferruginin F (**6**).

