

## Supporting Information

### Induction of diverse secondary metabolites in *Aspergillus fumigatus* by microbial co-culture

Mostafa E. Rateb<sup>1,2</sup>, Irene Hallyburton<sup>3</sup>, Wael E. Houssen<sup>1,4</sup>, Alan T. Bull<sup>5</sup>, Michael Goodfellow<sup>6</sup>,  
Rakesh Santhanam<sup>6</sup>, Marcel Jaspars<sup>1</sup>, and Rainer Ebel<sup>1\*</sup>

<sup>1</sup>*Marine Biodiscovery Centre, Department of Chemistry, University of Aberdeen, Meston Walk, AB24 3UE, Scotland, U.K.*

<sup>2</sup>*Pharmacognosy Department, Faculty of Pharmacy, Beni-Suef University, Salah Salem St., 62111, Beni-Suef, Egypt.*

<sup>3</sup>*Drug Discovery Unit, Division of Biological Chemistry and Drug Discovery, College of Life Sciences, University of Dundee, Sir James Black Centre, Dundee, DD1 5EH, U.K.*

<sup>4</sup>*Institute of Medical Sciences, University of Aberdeen, Ashgrove Road West, Aberdeen AB25 2ZD, Scotland, UK*

<sup>5</sup>*School of Biosciences, University of Kent, Canterbury, Kent CT2 7NJ, UK*

<sup>6</sup>*School of Biology, University of Newcastle, Newcastle upon Tyne NE1 7RU, UK*

---

\* To whom correspondence should be addressed. Tel.: +44 (0)1224 272930. Fax: +44 (0)1224 272921. Email: r.ebel@abdn.ac.uk

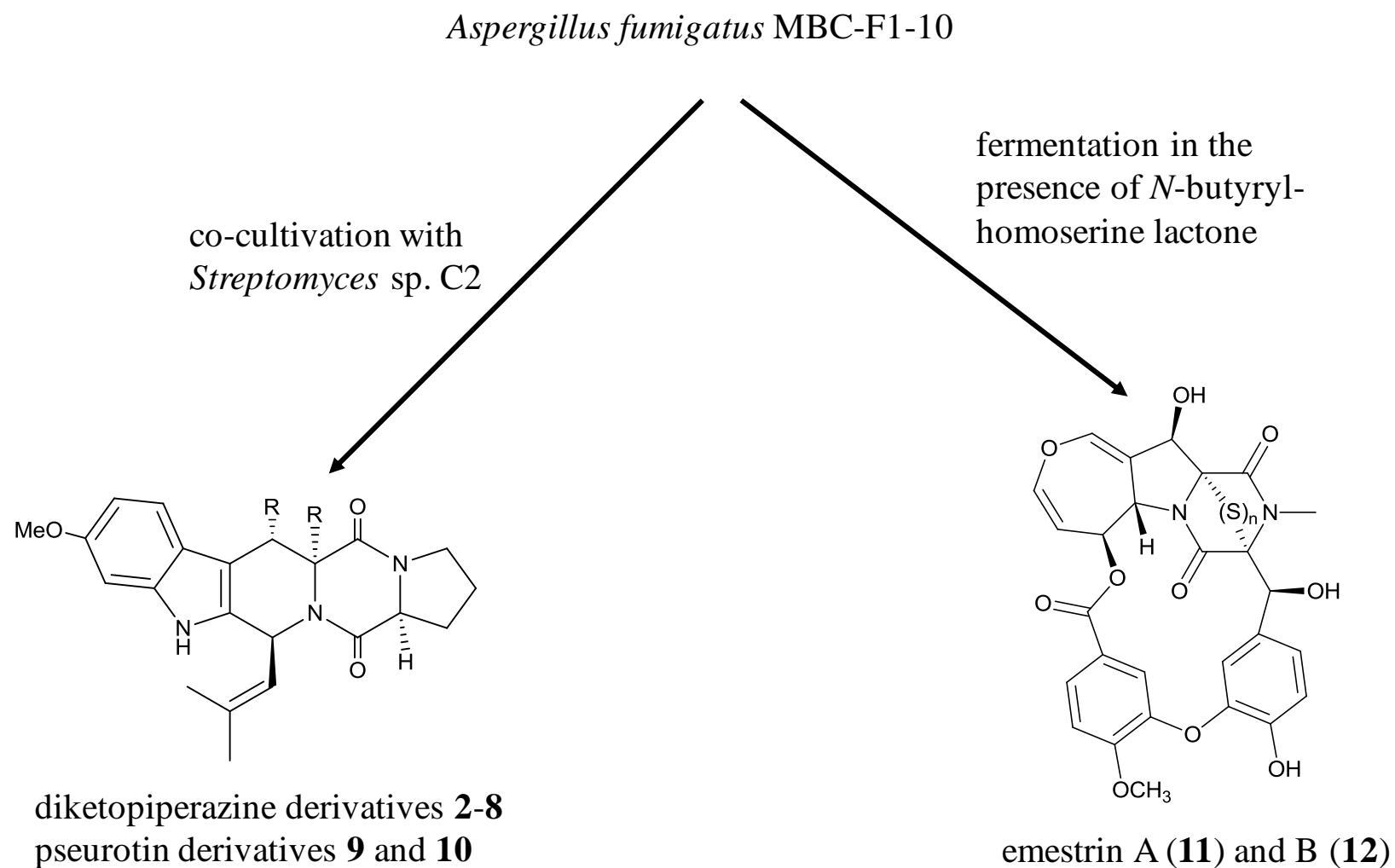
## Table of content

Content	Page
<b>Table S1.</b> NMR spectroscopic data for <b>9</b> and <b>10</b> (CDCl <sub>3</sub> , 400 MHz at 298 °K)	S3
<b>Fig. S1.</b> Induction of cryptic biogenetic pathways in <i>Aspergillus fumigatus</i> MBC-F1-10 by different strategies	S4
<b>Fig. S2.</b> HRESIMS spectrum of <b>9</b>	S5
<b>Fig. S3.</b> <sup>1</sup> H NMR spectrum of <b>9</b> in CDCl <sub>3</sub>	S6
<b>Fig. S4.</b> <sup>13</sup> C NMR spectrum of <b>9</b> in CDCl <sub>3</sub>	S7
<b>Fig. S5.</b> HSQC spectrum of <b>9</b>	S8
<b>Fig. S6.</b> COSY spectrum of <b>9</b>	S9
<b>Fig. S7.</b> HMBC spectrum of <b>9</b>	S10
<b>Fig. S8.</b> NOESY spectrum of <b>9</b>	S11
<b>Fig. S9.</b> HRESIMS spectrum of <b>10</b>	S12
<b>Fig. S10.</b> <sup>1</sup> H NMR spectrum of <b>10</b> in CDCl <sub>3</sub>	S13
<b>Fig. S11.</b> <sup>13</sup> C NMR spectrum of <b>10</b> in CDCl <sub>3</sub>	S14
<b>Fig. S12.</b> HSQC spectrum of <b>10</b>	S15
<b>Fig. S13.</b> COSY spectrum of <b>10</b>	S16
<b>Fig. S14.</b> HMBC spectrum of <b>10</b>	S17
<b>Fig. S15.</b> NOESY spectrum of <b>10</b>	S18
<b>Fig. S16.</b> <sup>1</sup> H NMR spectrum of <b>10</b> in DMSO- <i>d</i> <sub>6</sub>	S19
<b>Fig. S17.</b> <sup>13</sup> C NMR spectrum of <b>10</b> in DMSO- <i>d</i> <sub>6</sub>	S20

**Table S1.** NMR spectroscopic data for **9** and **10** (CDCl<sub>3</sub>, 400 MHz at 298 K):

Atom	<b>9</b>			<b>10</b>			<sup>13</sup> C NMR of related compounds		
	δ <sub>H</sub> , mult. ( <i>J</i> in Hz)	δ <sub>C</sub> , mult	δ <sub>C</sub> , mult <sup>a</sup>	δ <sub>H</sub> , mult. ( <i>J</i> in Hz)	δ <sub>C</sub> , mult	δ <sub>H</sub> , mult <sup>b</sup> ( <i>J</i> in Hz)	δ <sub>C</sub> , mult <sup>b</sup>	δ <sub>C</sub> , mult <sup>c</sup>	δ <sub>C</sub> , mult <sup>d</sup>
2		186.6, C	187.3, C*		184.4, C		186.8, C	186.8, C	187.6, C
3		113.4, C	113.6, C		113.3, C		111.4, C	111.6, C	111.3, C
4		197.7, C	198.0, C		198.1, C		199.8, C	196.7, C	200.0, C
5		91.8, C	92.3, C		88.5, C		88.2, C	92.4, C	88.2, C
6		166.1, C	167.2, C*		167.9, C		167.5, C	166.6, C	167.7, C
8		90.0, C	92.0, C		95.4, C		97.0, C	91.1, C	97.1, C
9	4.63, s	74.1, CH	75.0, CH	4.78, s	76.5, CH	4.62 (d, 6.2)	75.6, CH	75.0, CH	75.7, CH
10	4.69 (d, 5.7)	70.5, CH	69.7, CH	4.56 (d, 6.4)	70.3, CH	4.48 (t, 5.4)	70.4, CH	72.0, CH	72.8, CH
11	4.32 (dd, 5.2, 9.2)	77.6, CH	77.3, CH	4.28 (dd, 6.5, 9.1)	77.6, CH	4.17 (dd, 5.5, 9.3)	77.1, CH	68.3, CH	68.3, CH
12	5.33 (ddt, 10.9, 9.5, 1.3)	124.1, CH	125.1, CH	5.27 (t, 10.7)	124.7, CH	5.31 (t, 10.9)	125.6, CH	128.4, CH	129.0, CH
13	5.83, m	140.1, CH	138.4, CH	5.82, m	140.3, CH	5.62, m	136.9, CH	134.0, CH	133.8, CH
14	2.11, m	21.4, CH <sub>2</sub>	20.8, CH <sub>2</sub>	2.10, m	21.4, CH <sub>2</sub>	20.4, m	20.7, CH <sub>2</sub>	20.6, CH <sub>2</sub>	20.7, CH <sub>2</sub>
						1.97, m			
15	0.96 (t, 7.5)	14.3, CH <sub>3</sub>	13.1, CH <sub>3</sub>	0.98 (t, 7.5)	14.3, CH <sub>3</sub>	0.87 (t, 7.6)	14.1, CH <sub>3</sub>	14.1, CH <sub>3</sub>	14.2, CH <sub>3</sub>
16	1.75, s	5.8, CH <sub>3</sub>	4.3, CH <sub>3</sub>	1.77, s	5.8, CH <sub>3</sub>	1.64, s	5.6, CH <sub>3</sub>	5.6, CH <sub>3</sub>	5.7, CH <sub>3</sub>
17		194.6, C	195.8, C		193.3, C		194.7, C	196.4, C	194.8, C
18		132.5, C	133.5, C		134.0, C		134.8, C	133.6, C	134.7, C
19/23	8.29(dd, 1.2, 8.5)	130.7, CH	130.2, CH	8.21 (d, 7.9)	129.9, CH	8.11 (d, 7.7)	129.6, CH	130.2, CH	129.7, CH
20/22	7.49 (t, 8.0)	128.9, CH	128.1, CH	7.47 (t, 7.8)	128.7, CH	7.52 (t, 7.8)	128.3, CH	128.4, CH	128.4, CH
21	7.46 (t, 7.6)	134.8, CH	133.7, CH	7.60 (t, 7.2)	134.0, CH	7.63 (t, 7.6)	133.1, CH	133.6, CH	133.2, CH
8-OMe	3.38, s	51.9, CH <sub>3</sub>	51.0, CH <sub>3</sub>	3.29, s	51.6, CH <sub>3</sub>	3.12, s	51.4, CH <sub>3</sub>	51.7, CH <sub>3</sub>	51.5, CH <sub>3</sub>
11-OMe	3.31, s	56.8, CH <sub>3</sub>	55.4, CH <sub>3</sub>	3.25, s	56.7, CH <sub>3</sub>	3.15, s	55.7, CH <sub>3</sub>	---	---
9-OH						6.09 (d, 6.2)			
10-OH						5.75 (d, 5.8)			
NH-7	7.67, br s			7.40, br s		9.89, s			

<sup>a</sup> Reported <sup>13</sup>C NMR data of 11-*O*-methylpseurotin A (**9**) in CD<sub>3</sub>OD.<sup>44</sup> <sup>b</sup> NMR data of **7.10** in DMSO-*d*<sub>6</sub>. <sup>c</sup> Reported <sup>13</sup>C NMR data of pseurotin A in acetone-*d*<sub>6</sub>.<sup>45</sup> <sup>d</sup> Reported <sup>13</sup>C NMR data of pseurotin A<sub>2</sub> in DMSO-*d*<sub>6</sub>.<sup>46</sup> \*The <sup>13</sup>C shifts were interchanged as they were wrongly reported.



**Fig. S1.** Induction of cryptic biogenetic pathways in *Aspergillus fumigatus* MBC-F1-10 by different strategies

atd51 #36 RT: 0.41 AV: 1 NL: 2.12E7  
F: FTMS + p ESI Full ms [100.00-2000.00]

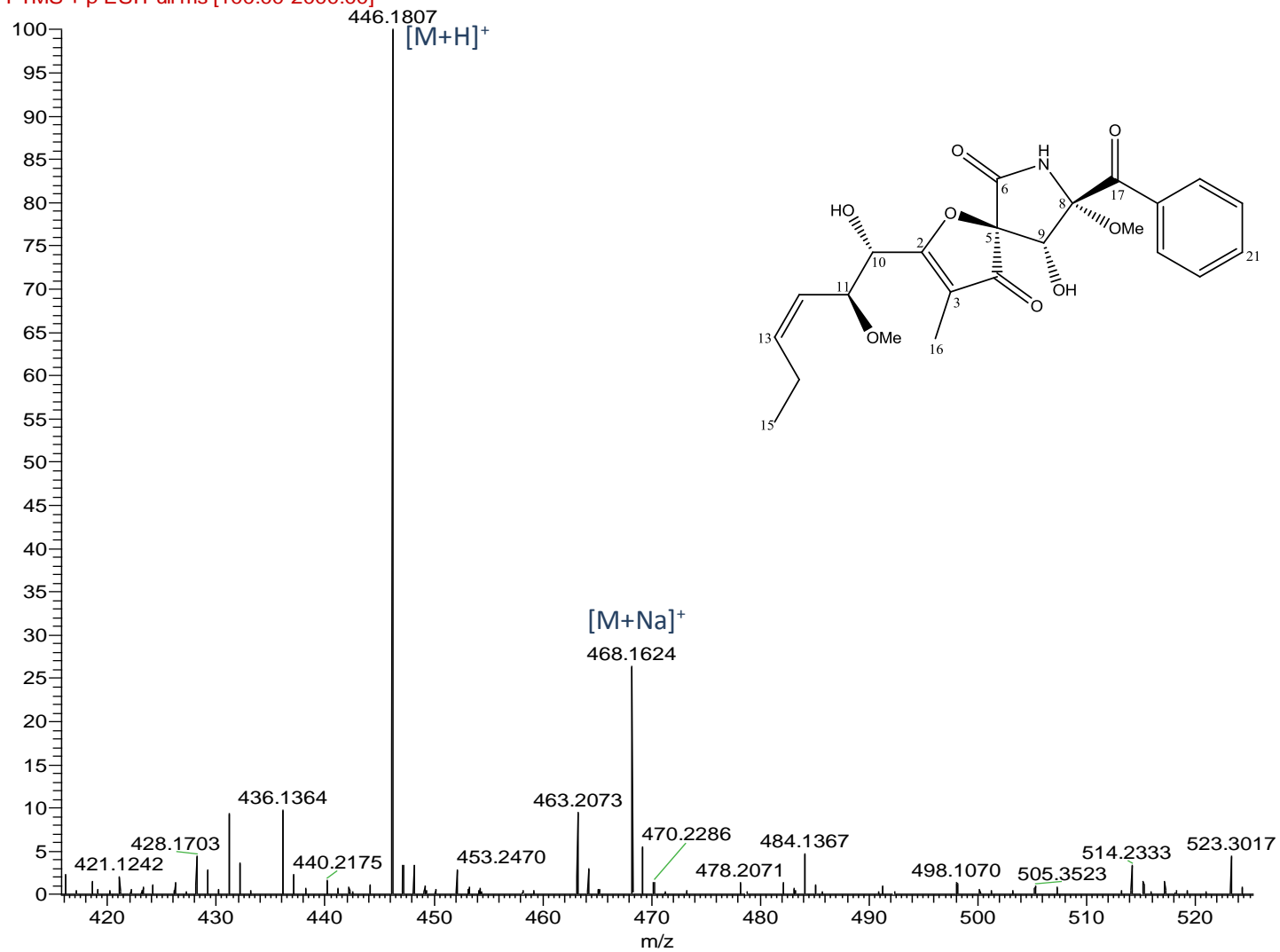


Fig. S2. HRESIMS spectrum of **9**

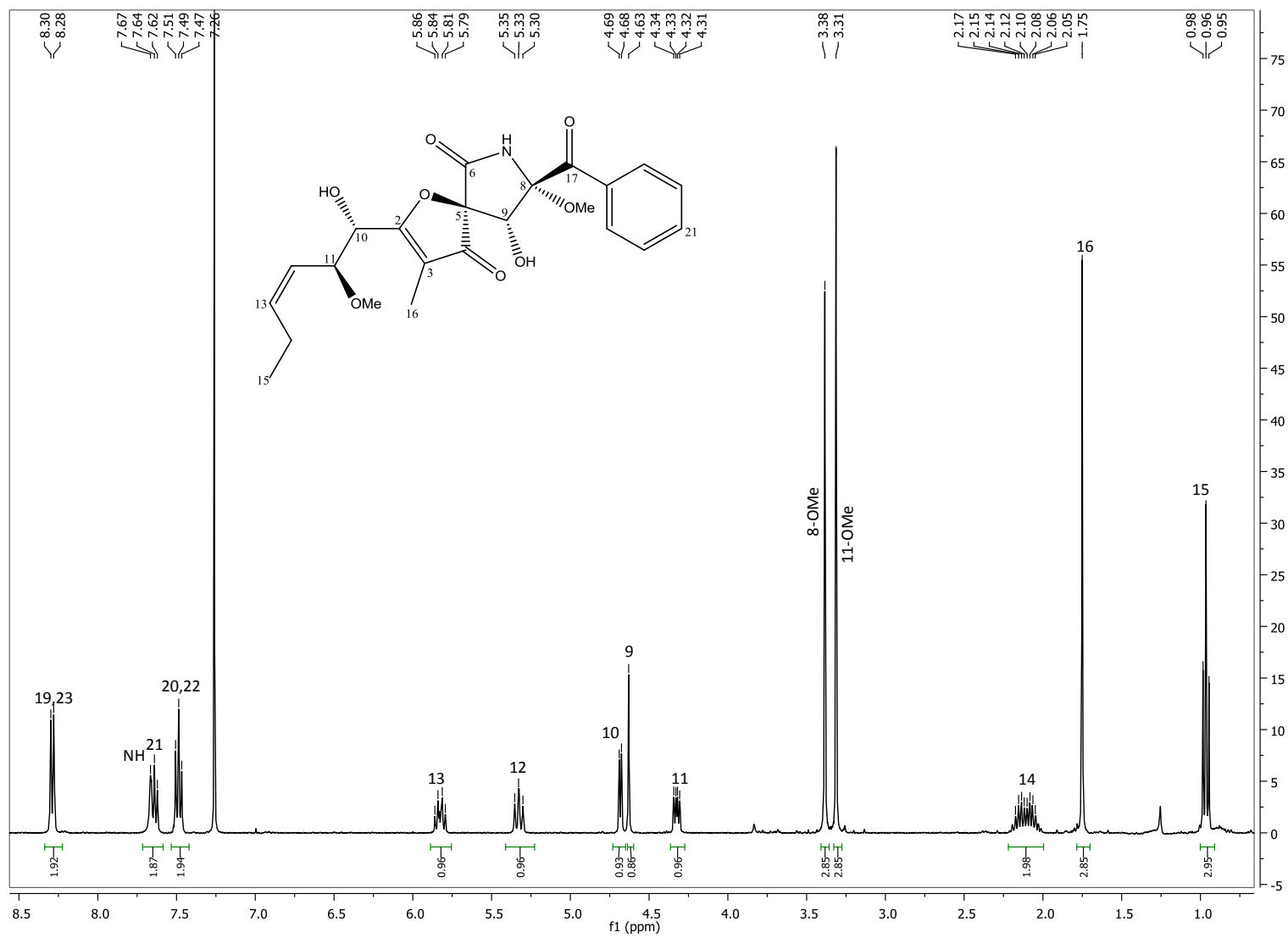


Fig. S3. <sup>1</sup>H NMR spectrum of 9

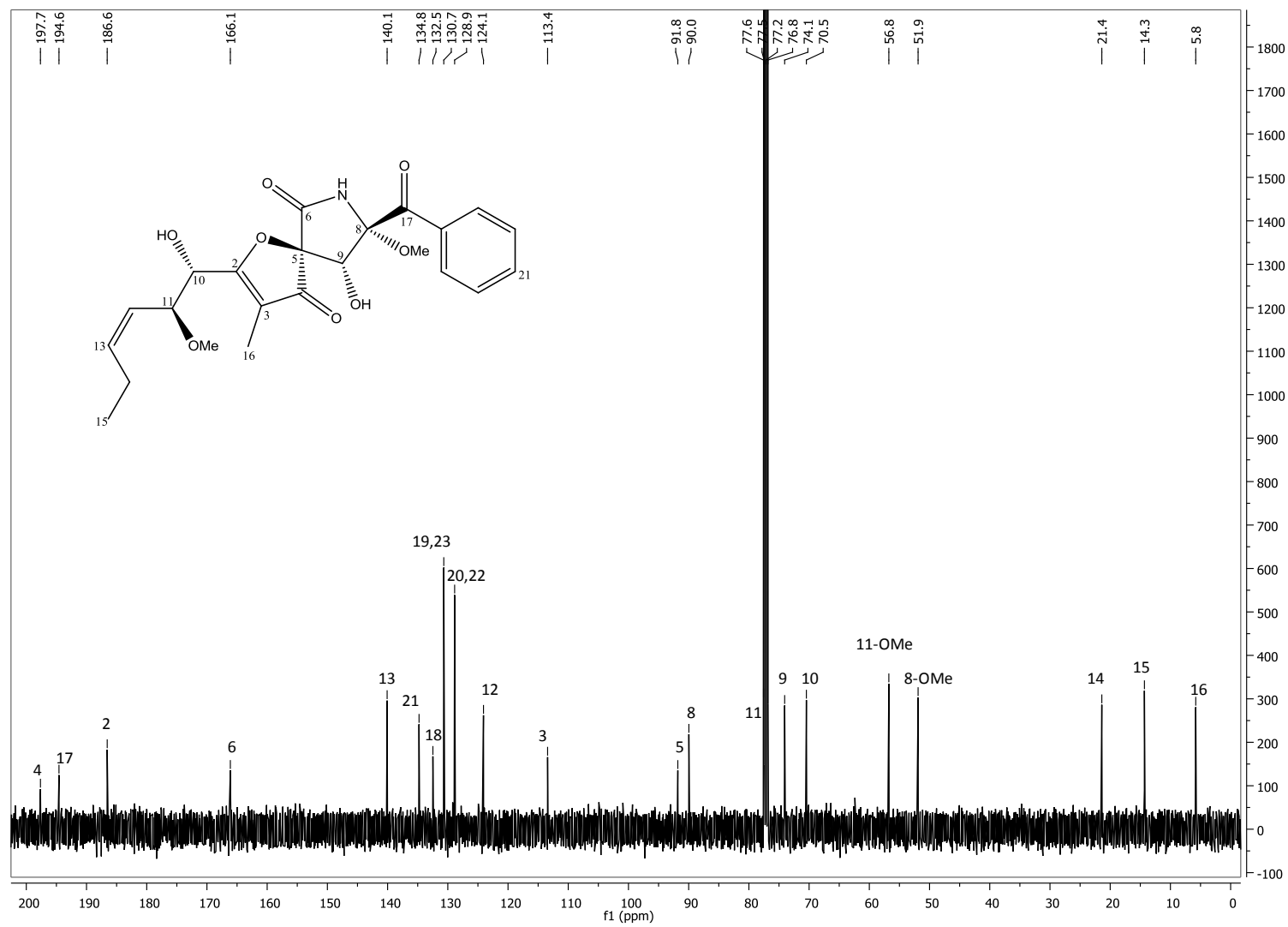


Fig. S4.  $^{13}\text{C}$  NMR spectrum of **9**

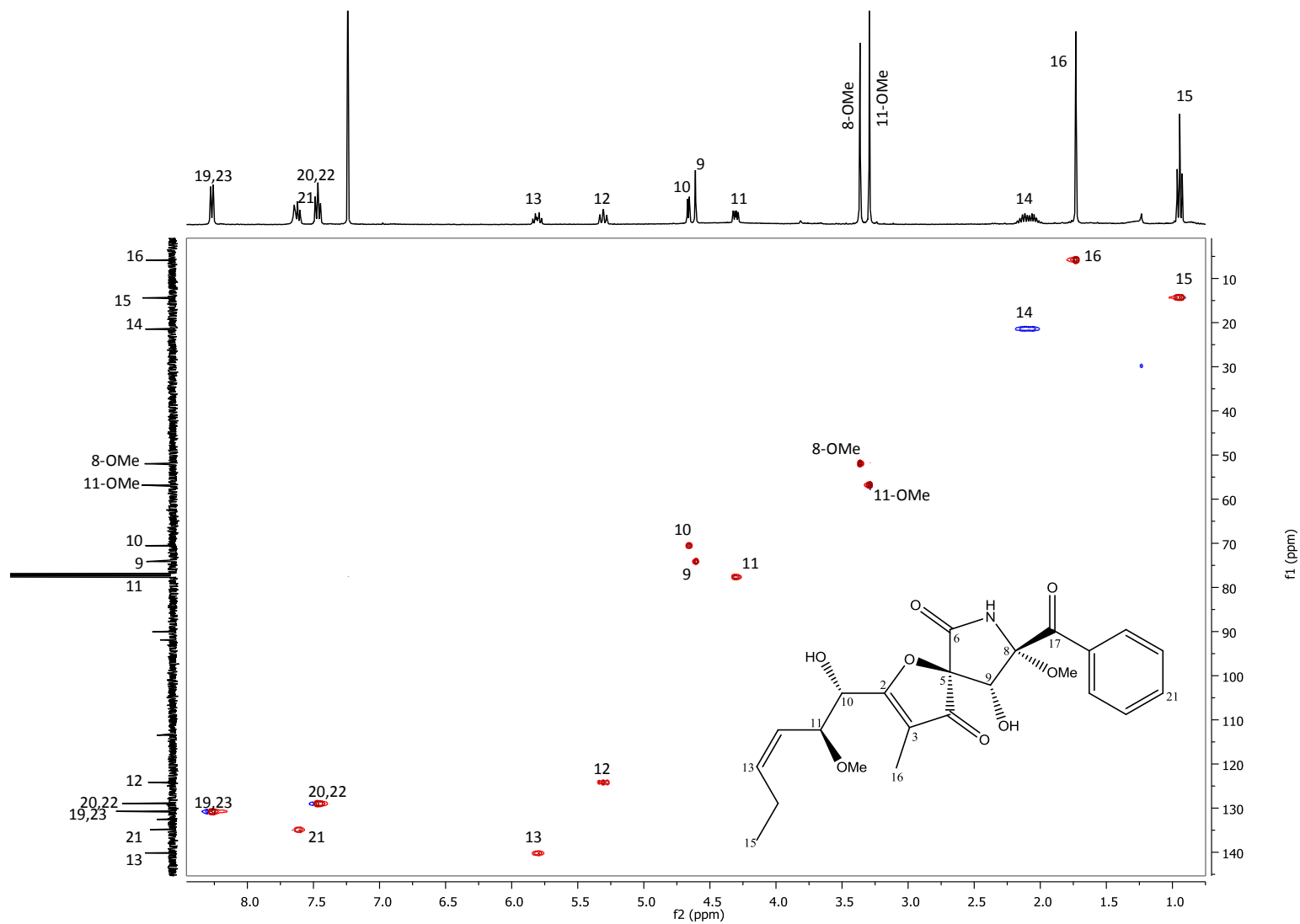




Fig. S5. HSQC spectrum of **9**

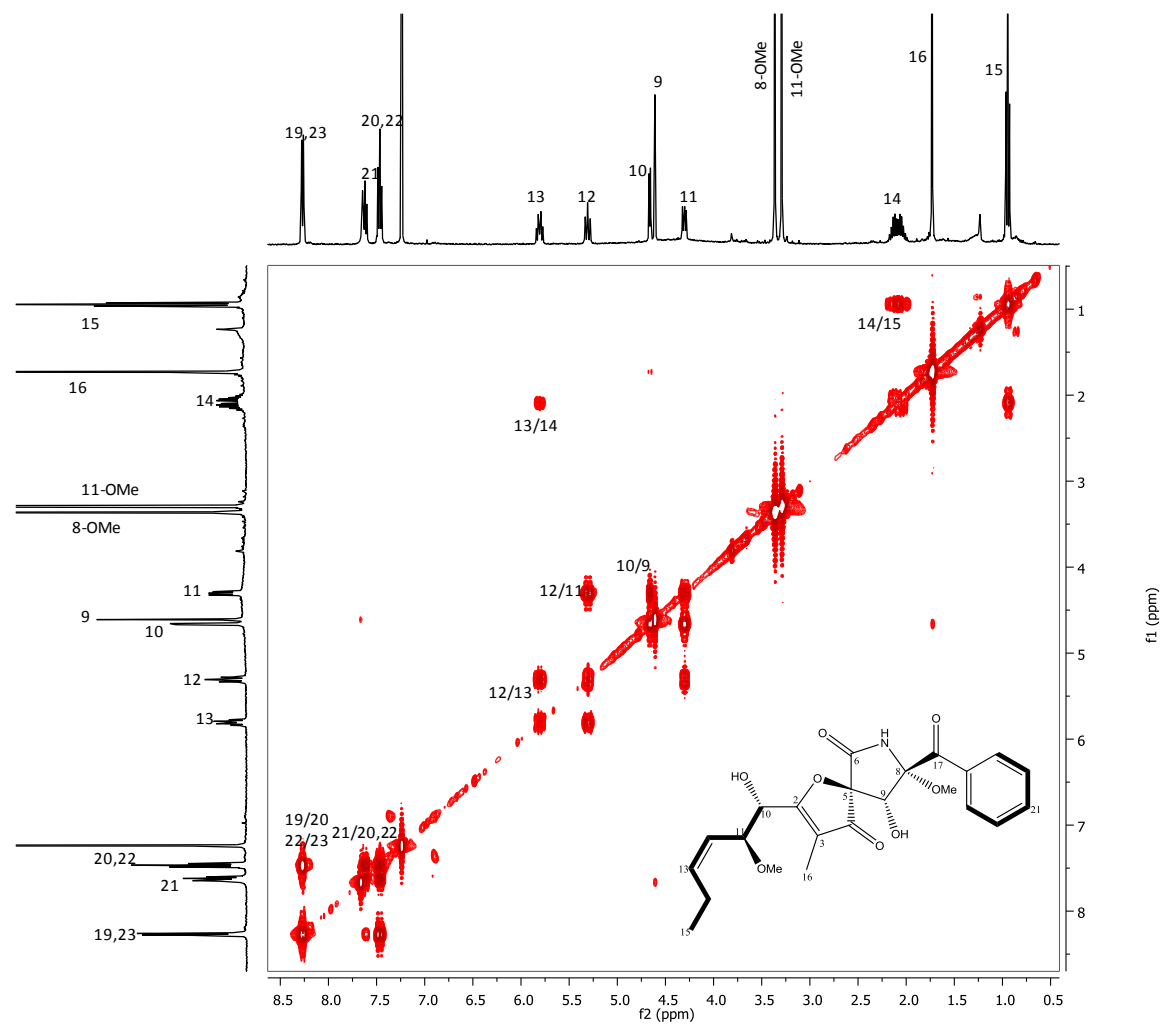


Fig. S6. COSY spectrum of **9**

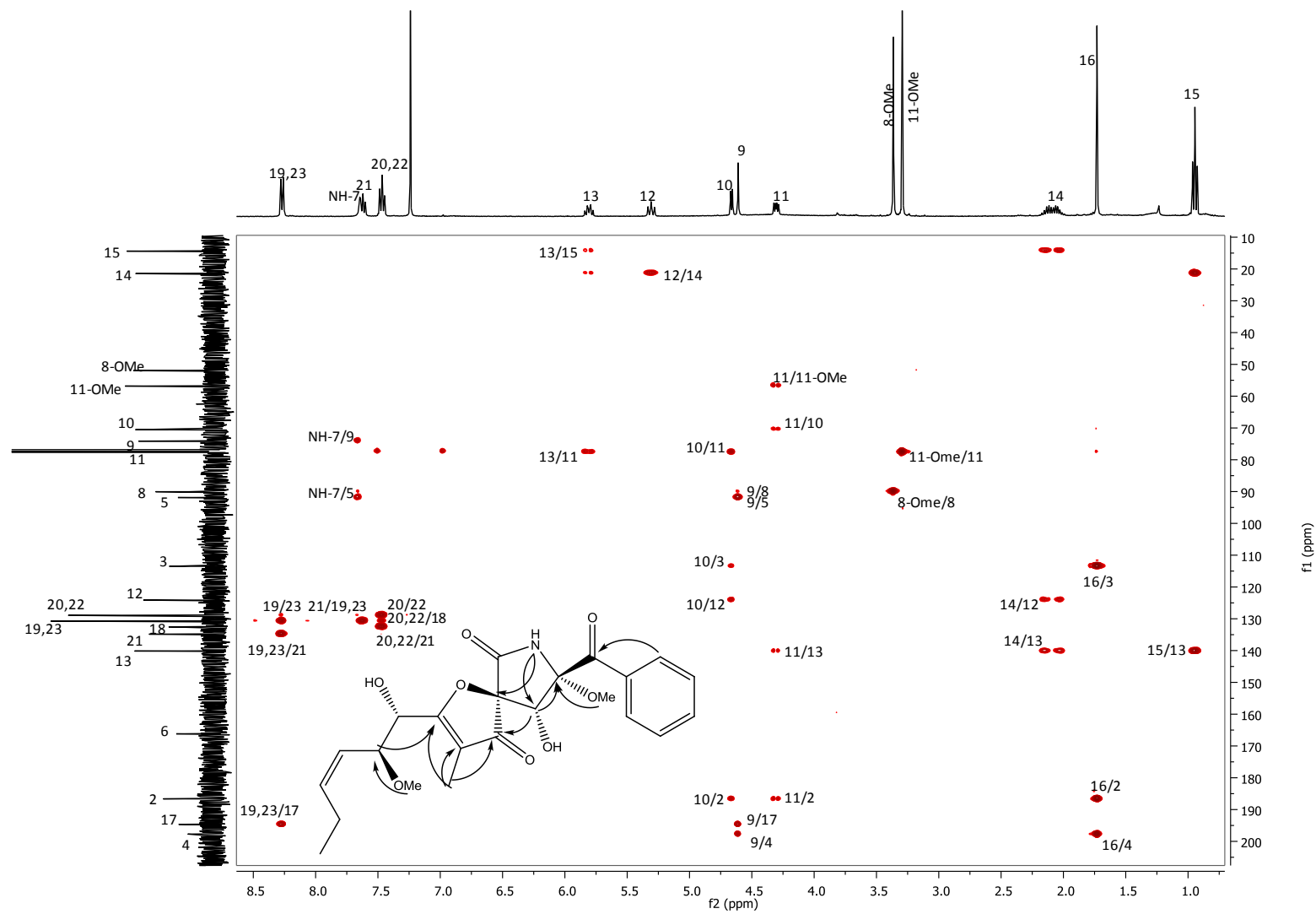


Fig. S7. HMBC spectrum of **9**

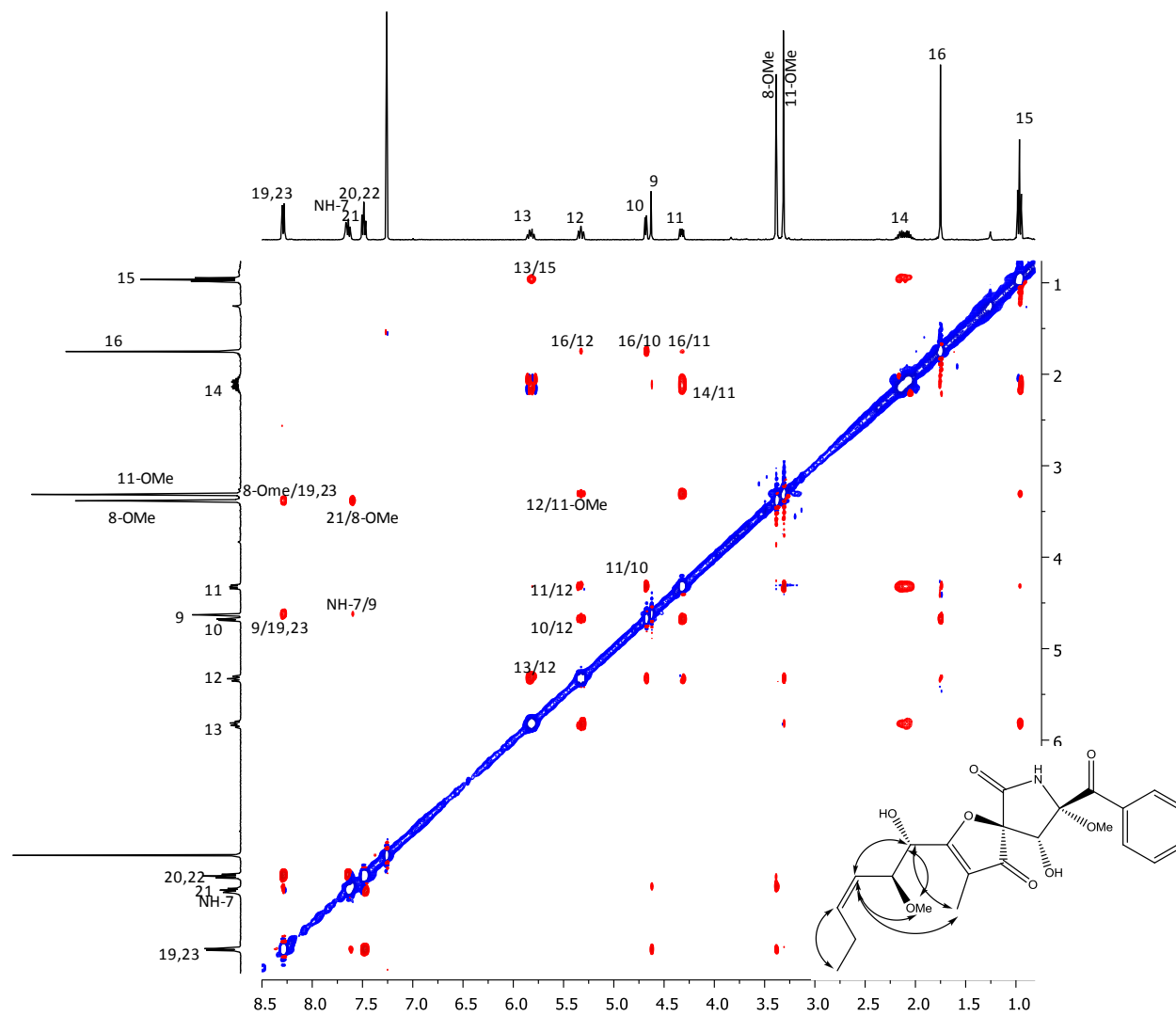


Fig. S8. NOESY spectrum of **9**

atd48 #41 RT: 0.47 AV: 1 NL: 3.55E7  
F: FTMS + p ESI Full ms [100.00-2000.00]

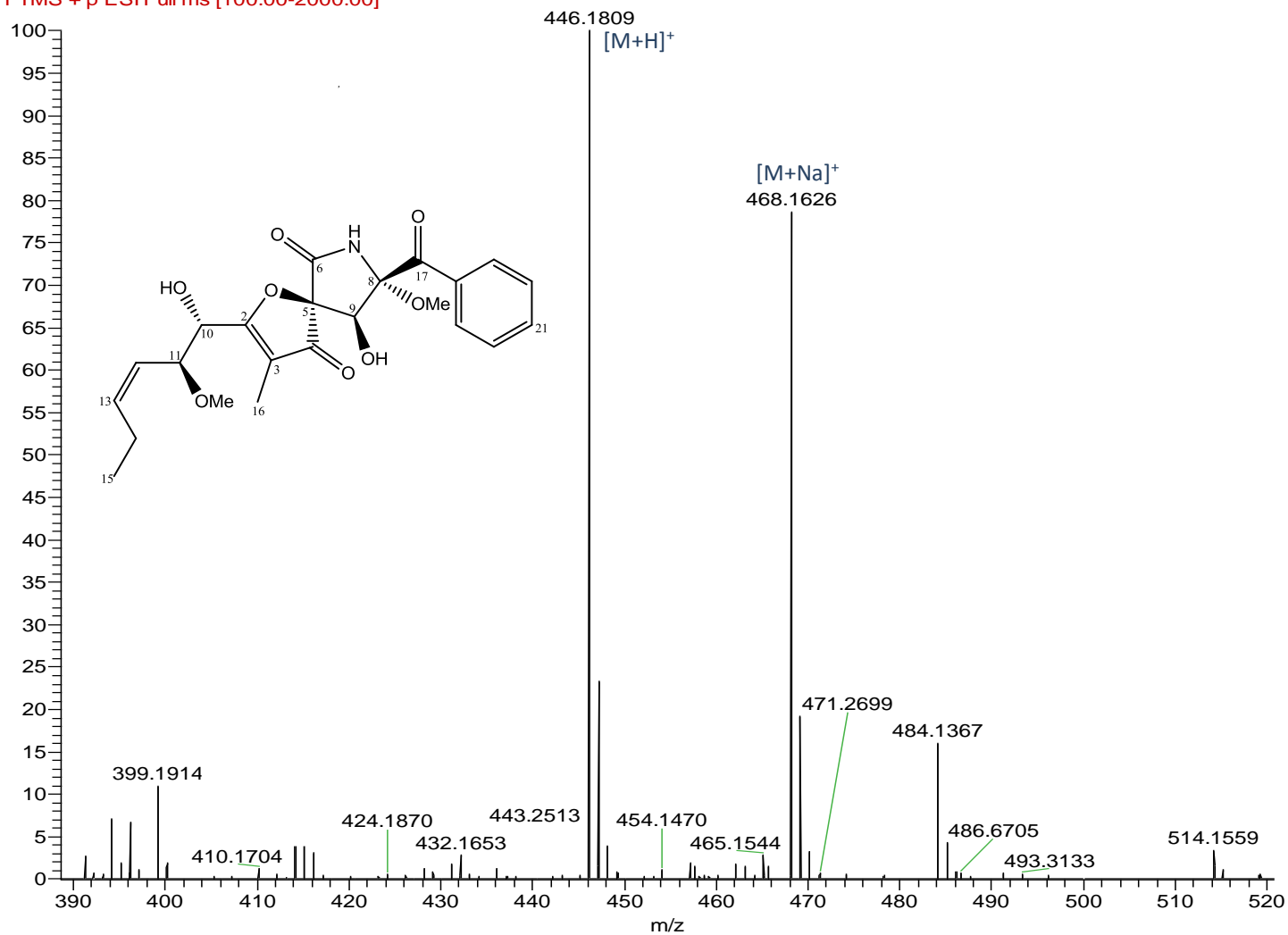


Fig. S9. HRESIMS spectrum of **10**

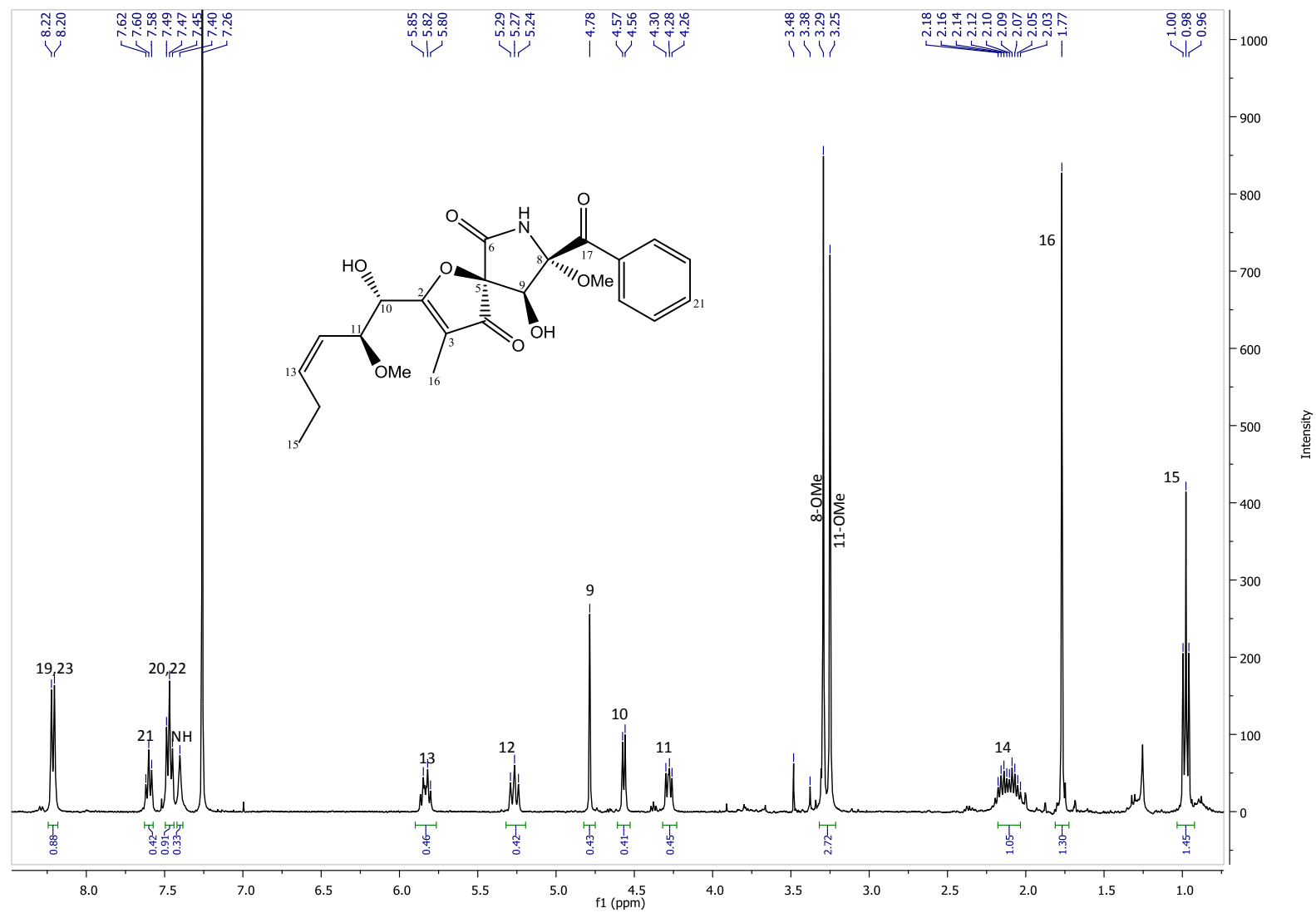


Fig. S10.  $^1\text{H}$  NMR spectrum of **10**

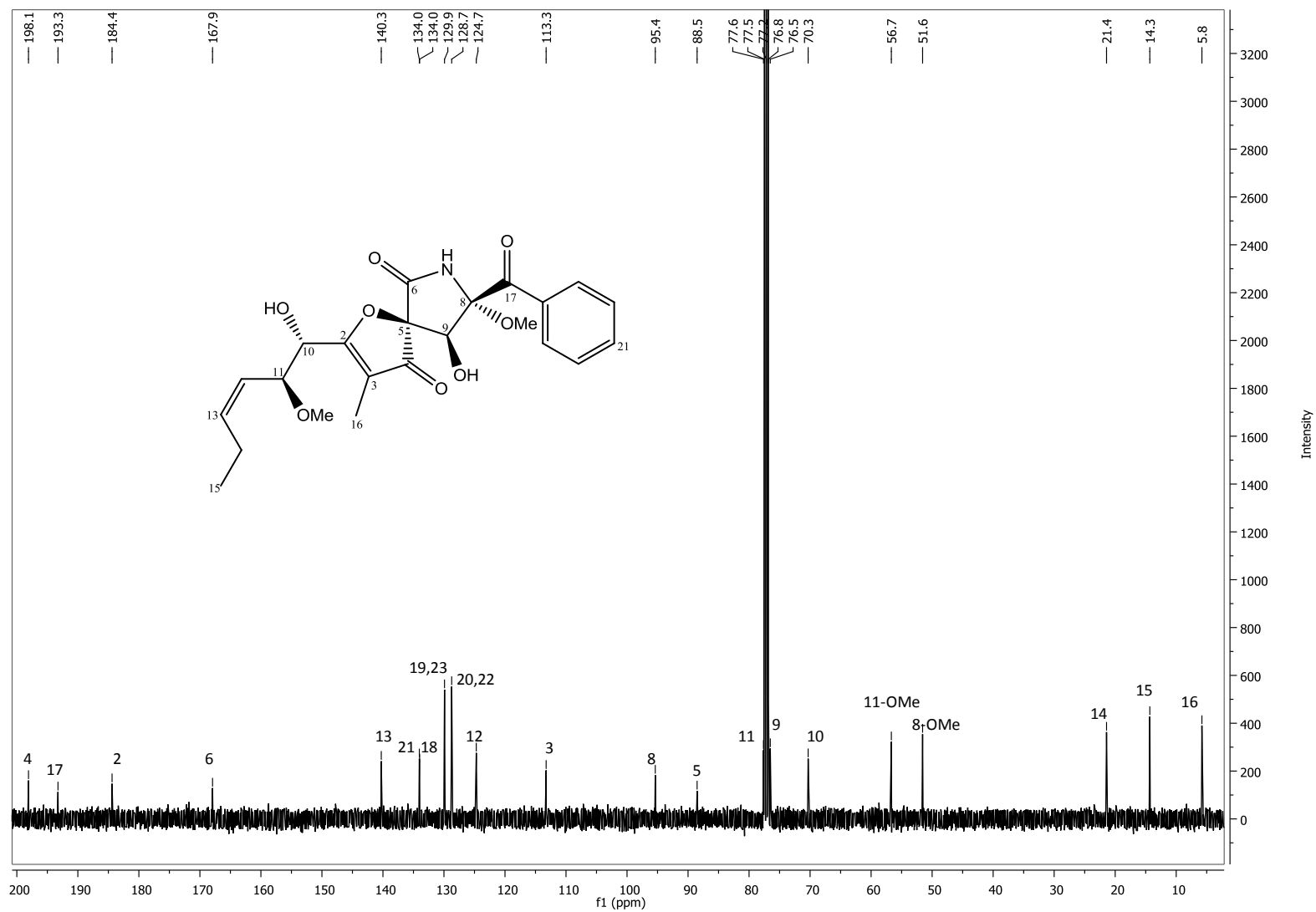


Fig. S11.  $^{13}\text{C}$  NMR spectrum of **10**

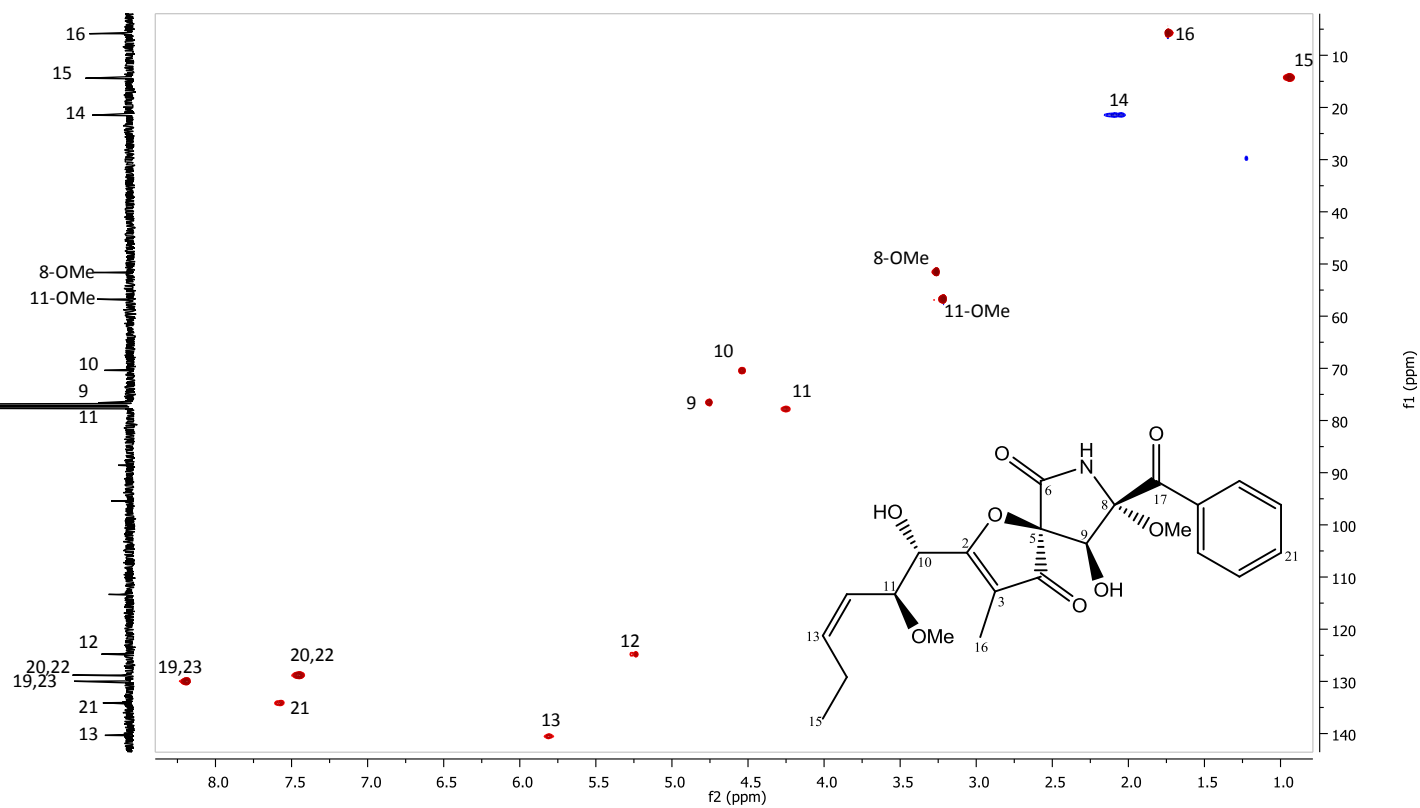
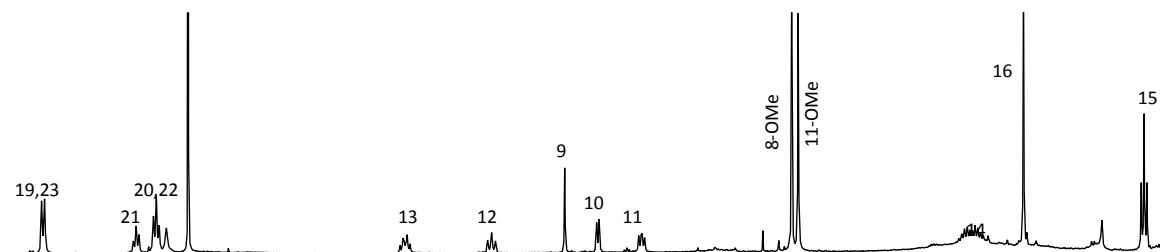
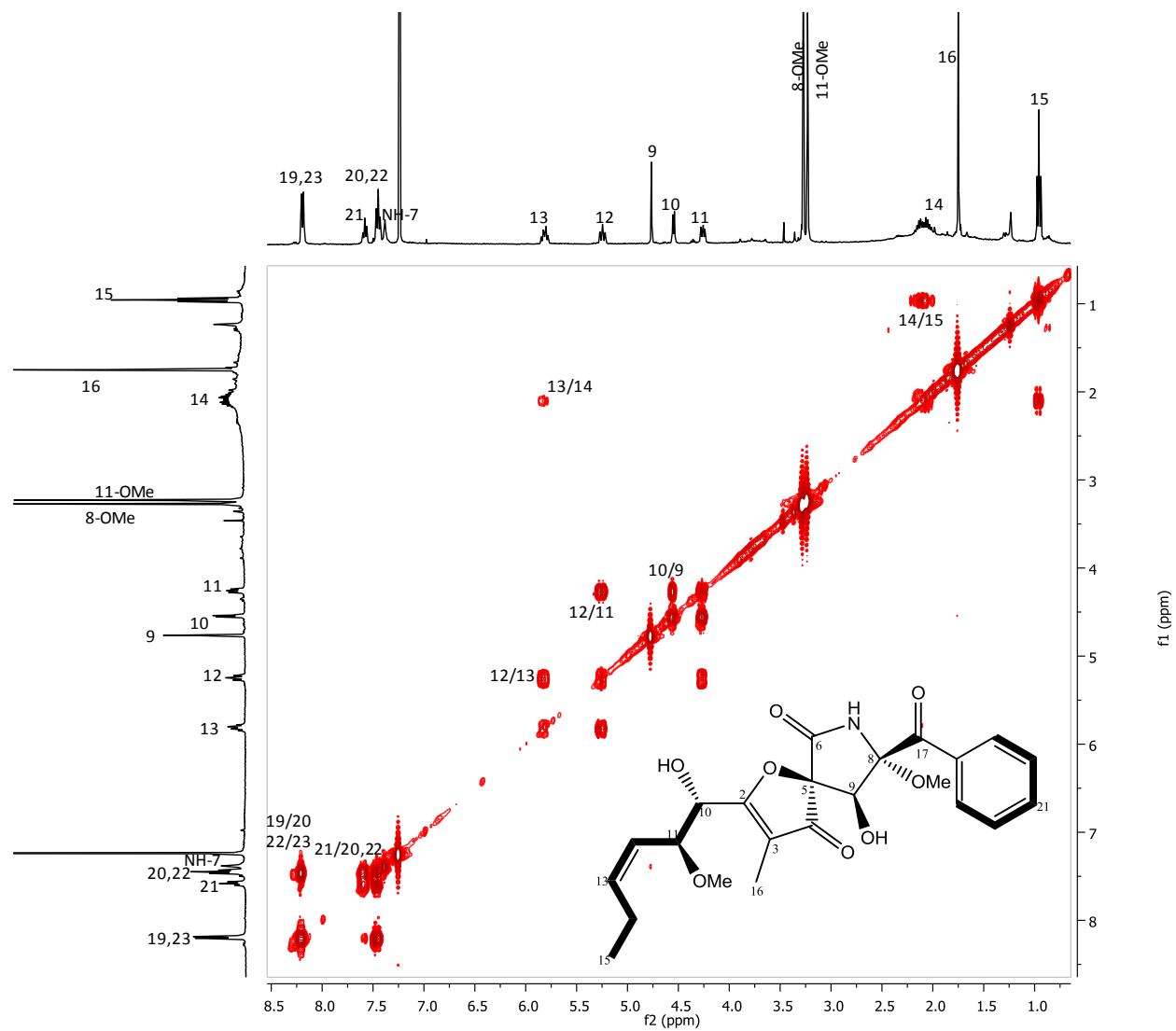
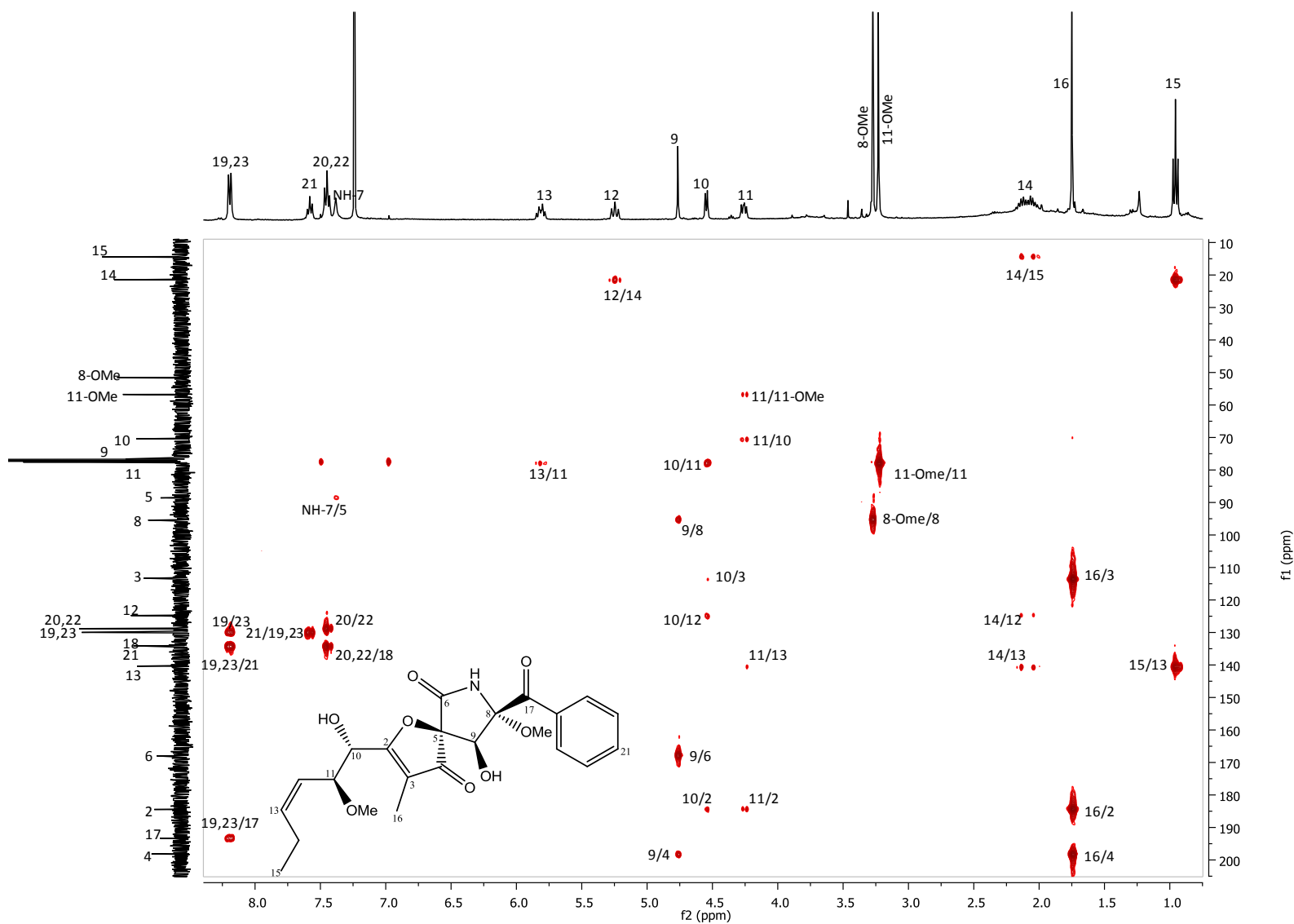


Fig. S12. HSQC spectrum of **10**





**Fig. S13.** COSY spectrum of **10**



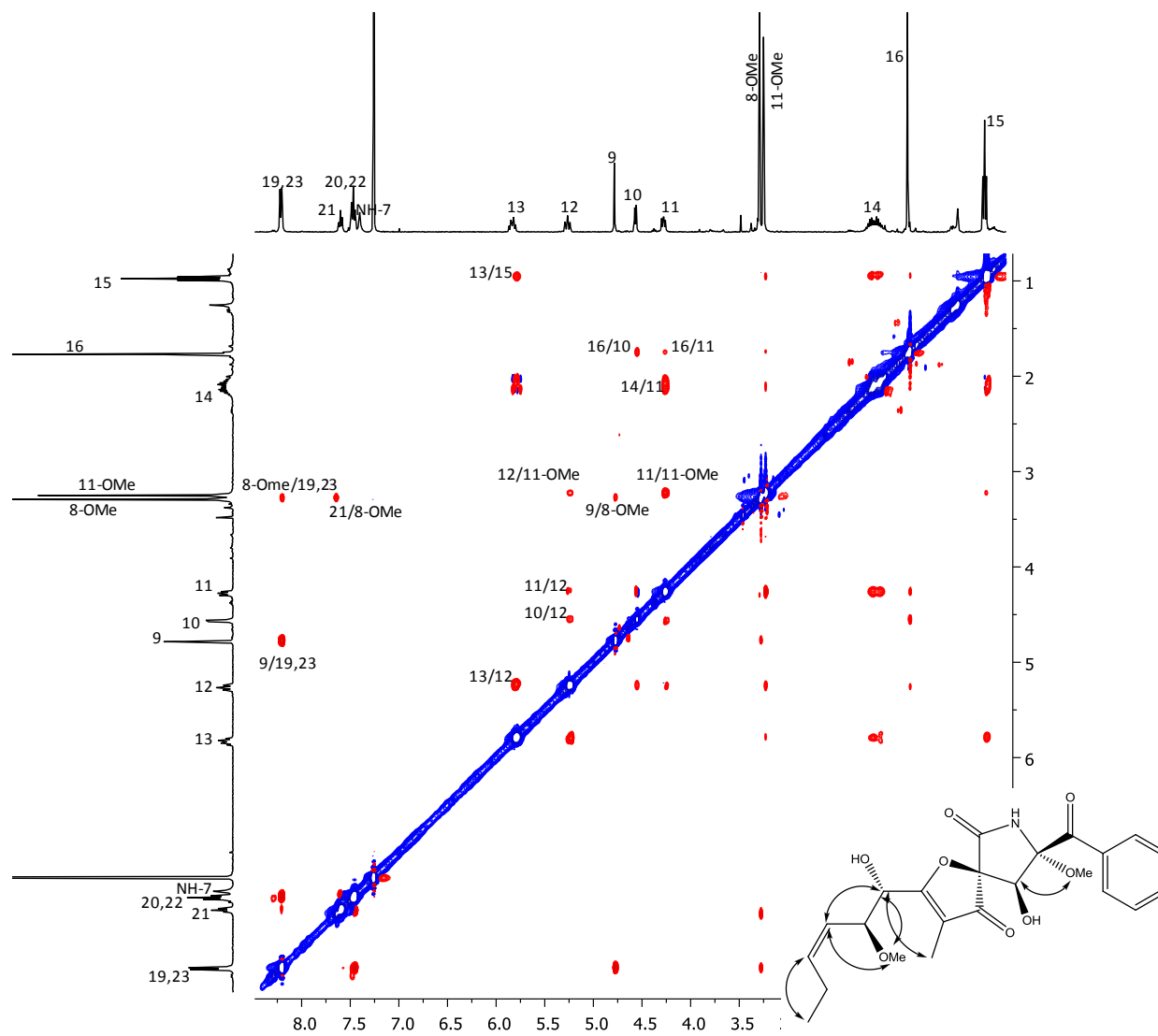


Fig. S15. NOESY spectrum of 10

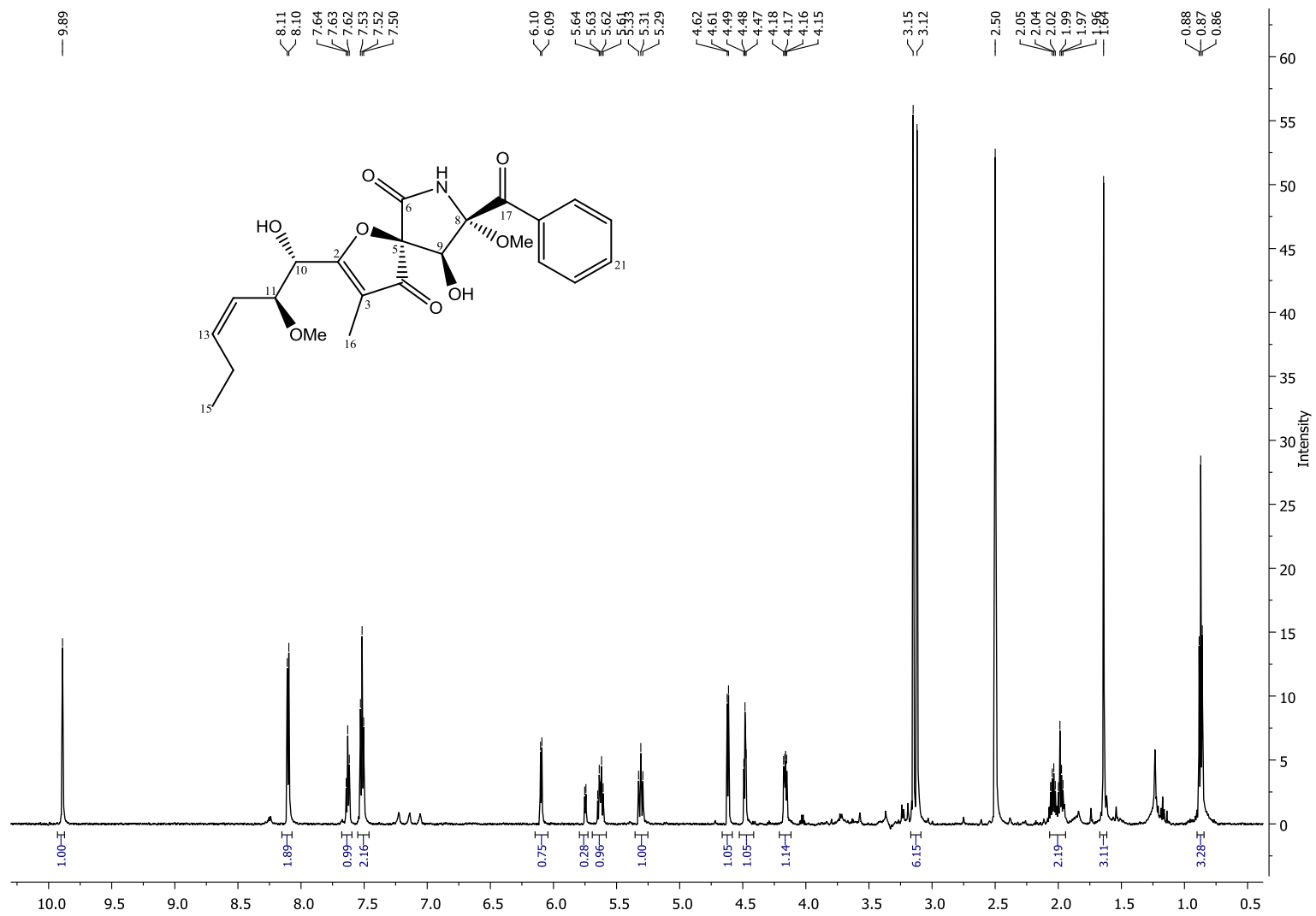


Fig. S16. <sup>1</sup>H NMR spectrum of **10** in DMSO-*d*<sub>6</sub>

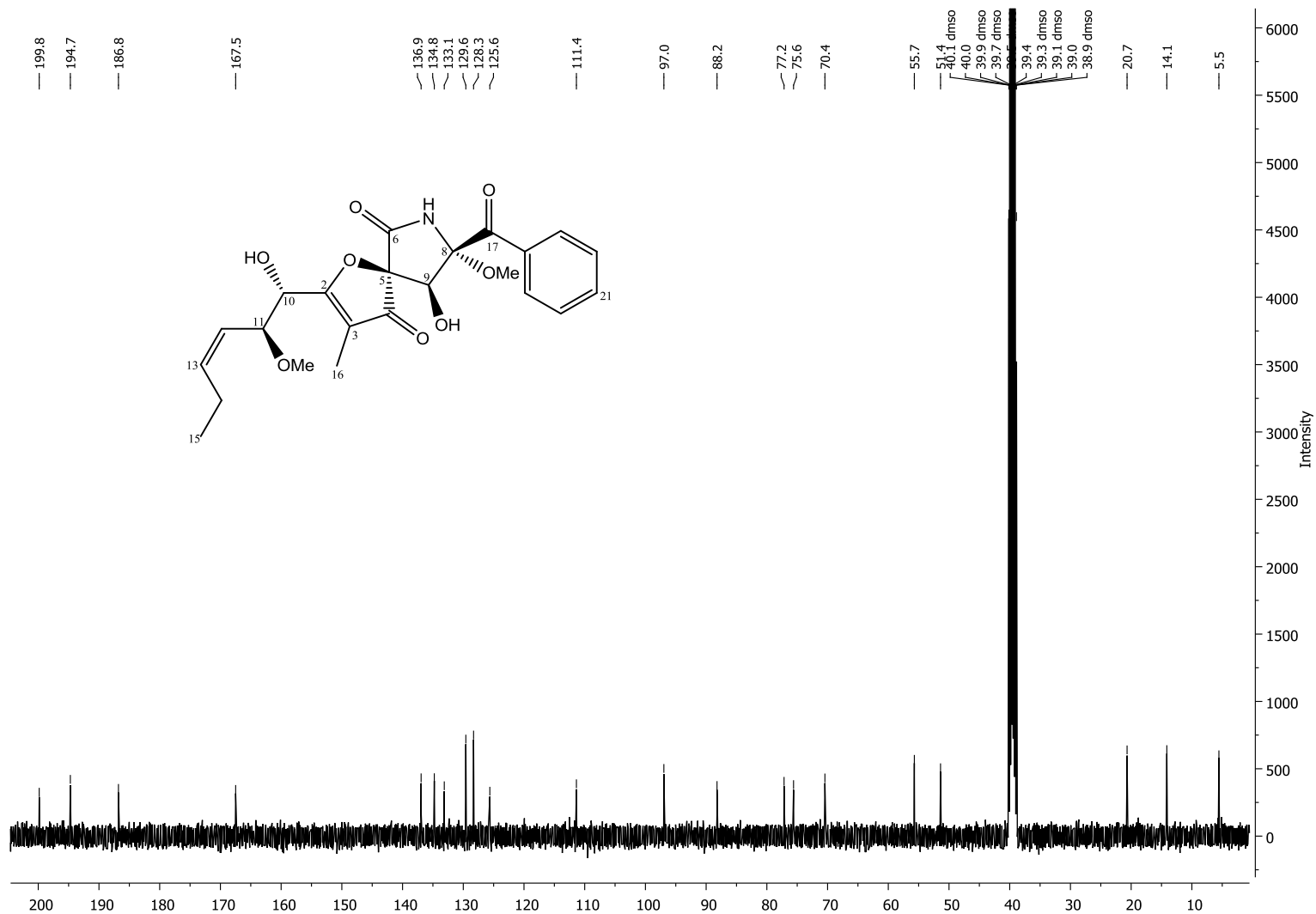


Fig. S17. <sup>13</sup>C NMR spectrum of **10** in DMSO-*d*<sub>6</sub>