

## Supporting Information

# Cyclohumulanolide Sesquiterpenes from the Culture Broth of the Basidiomycetous Fungus *Daedaleopsis tricolor*

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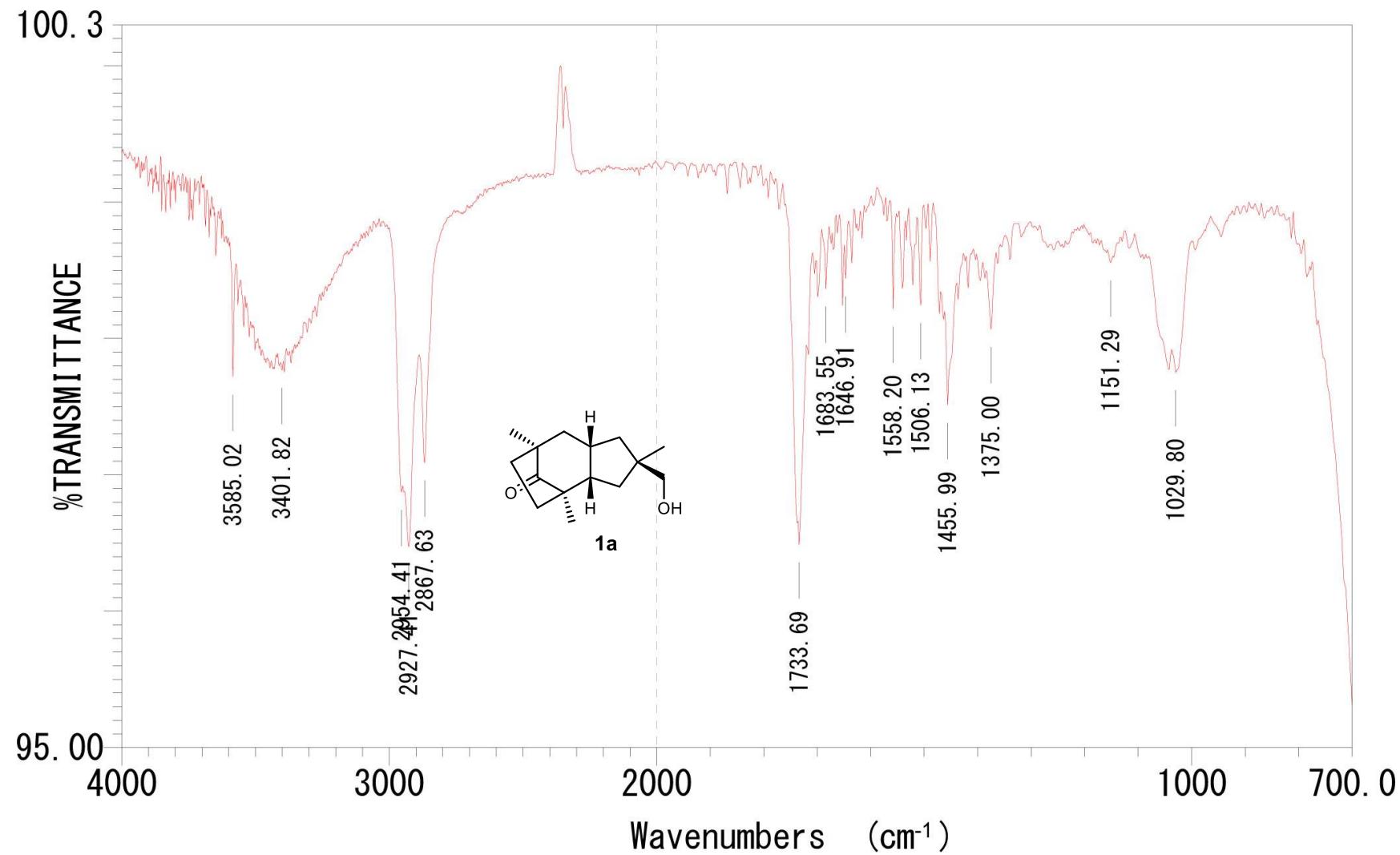
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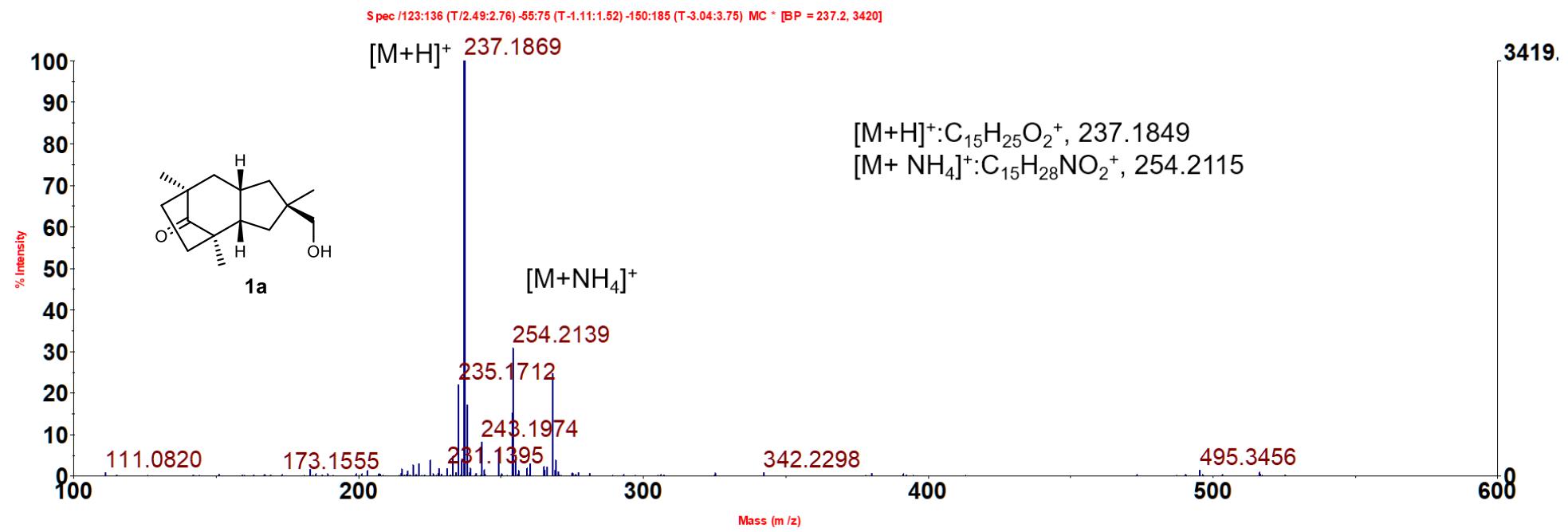
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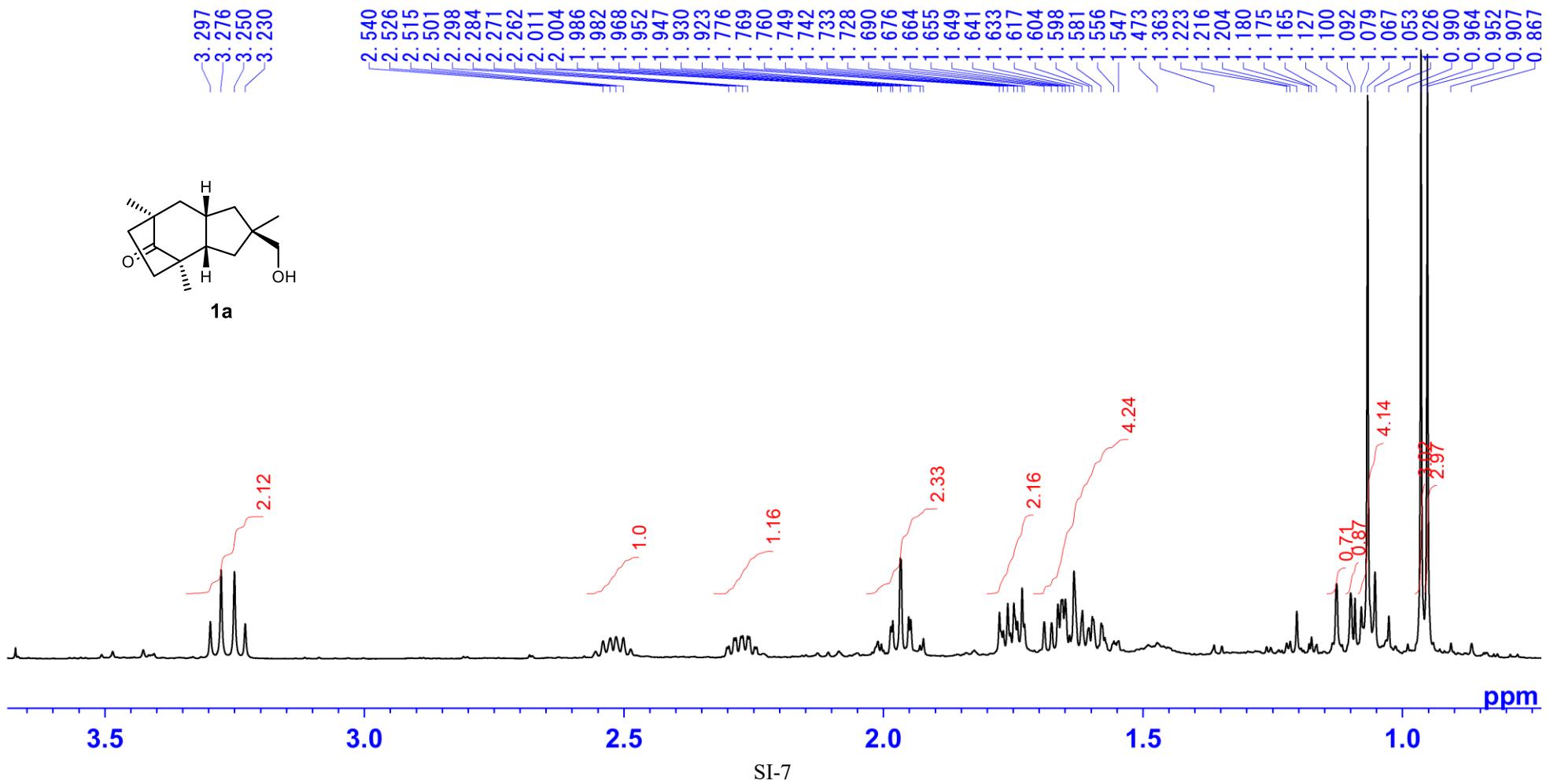
IR spectrum of **1a** (film)



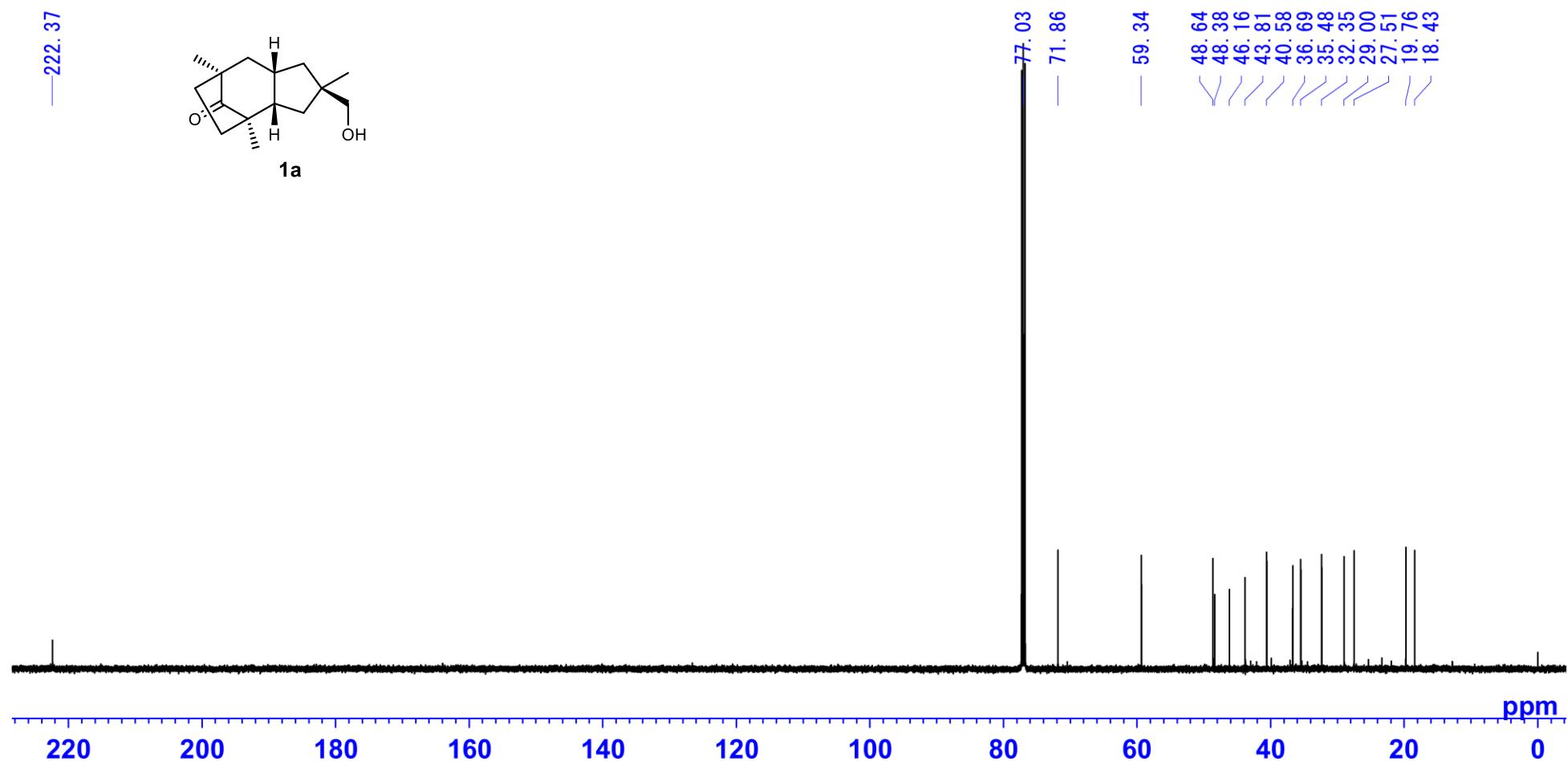
ESI-TOFMS spectrum of **1a**



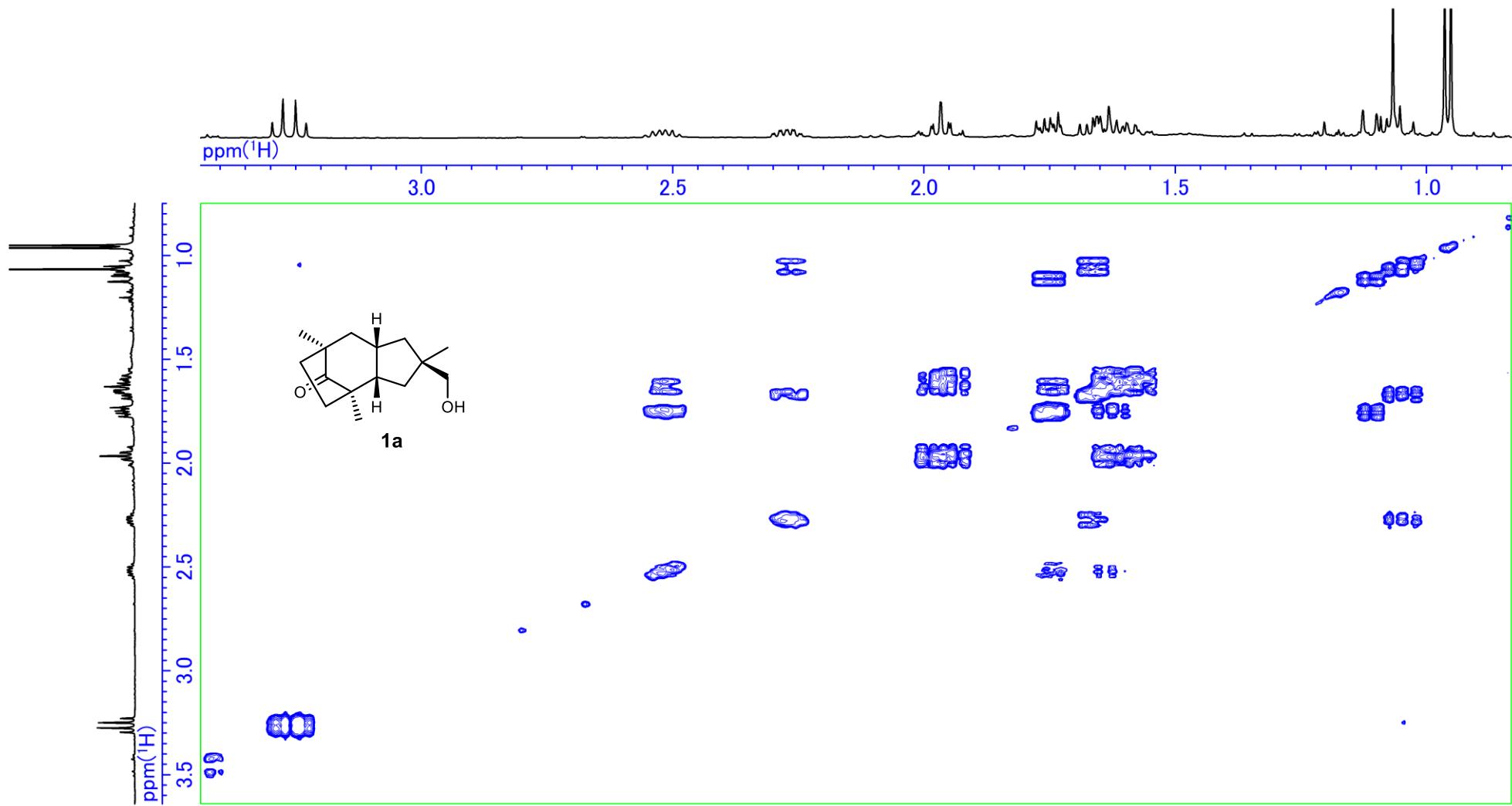
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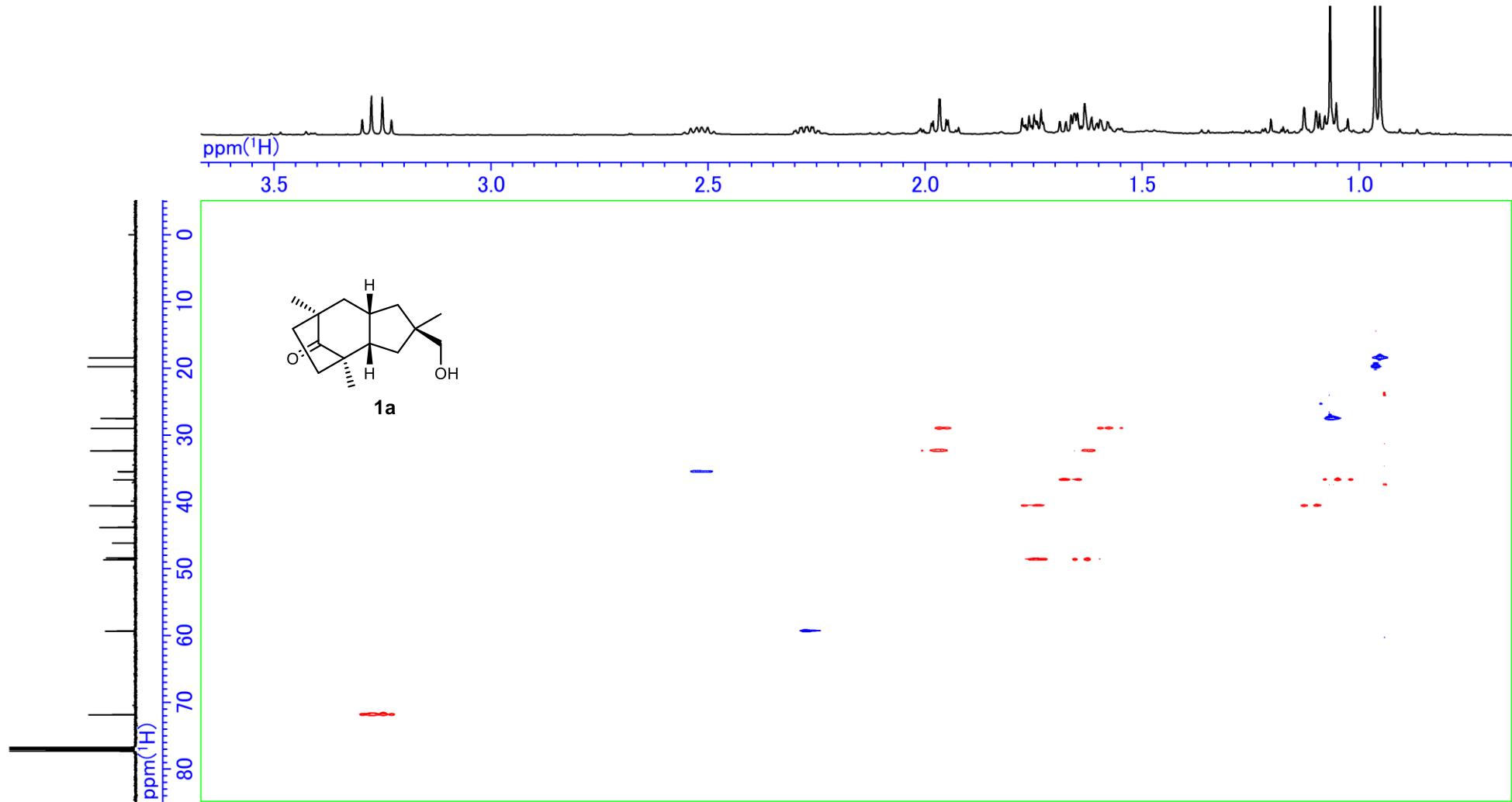
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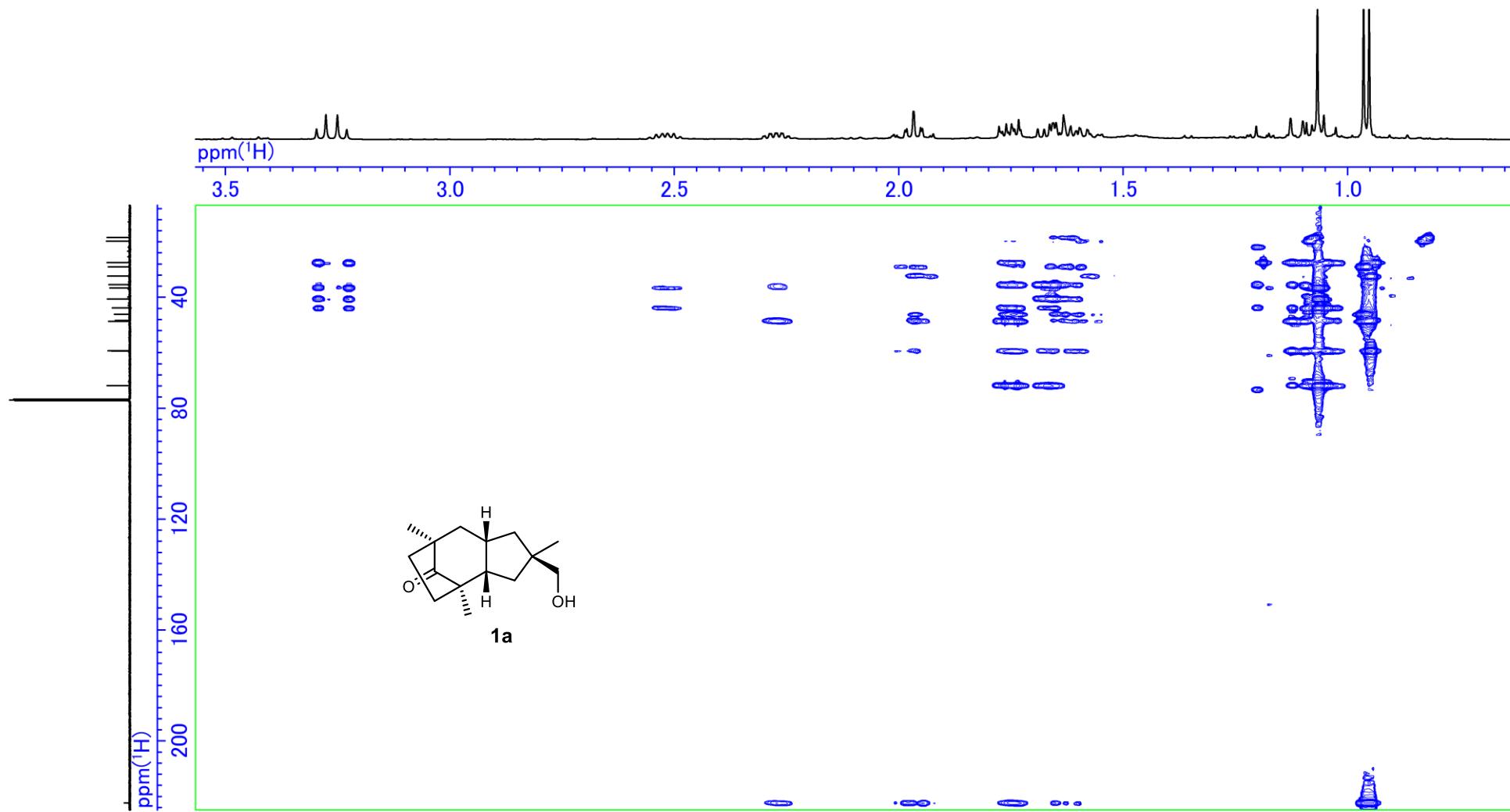
DQF COSY spectrum of **1a** (500 MHz, CDCl<sub>3</sub>)



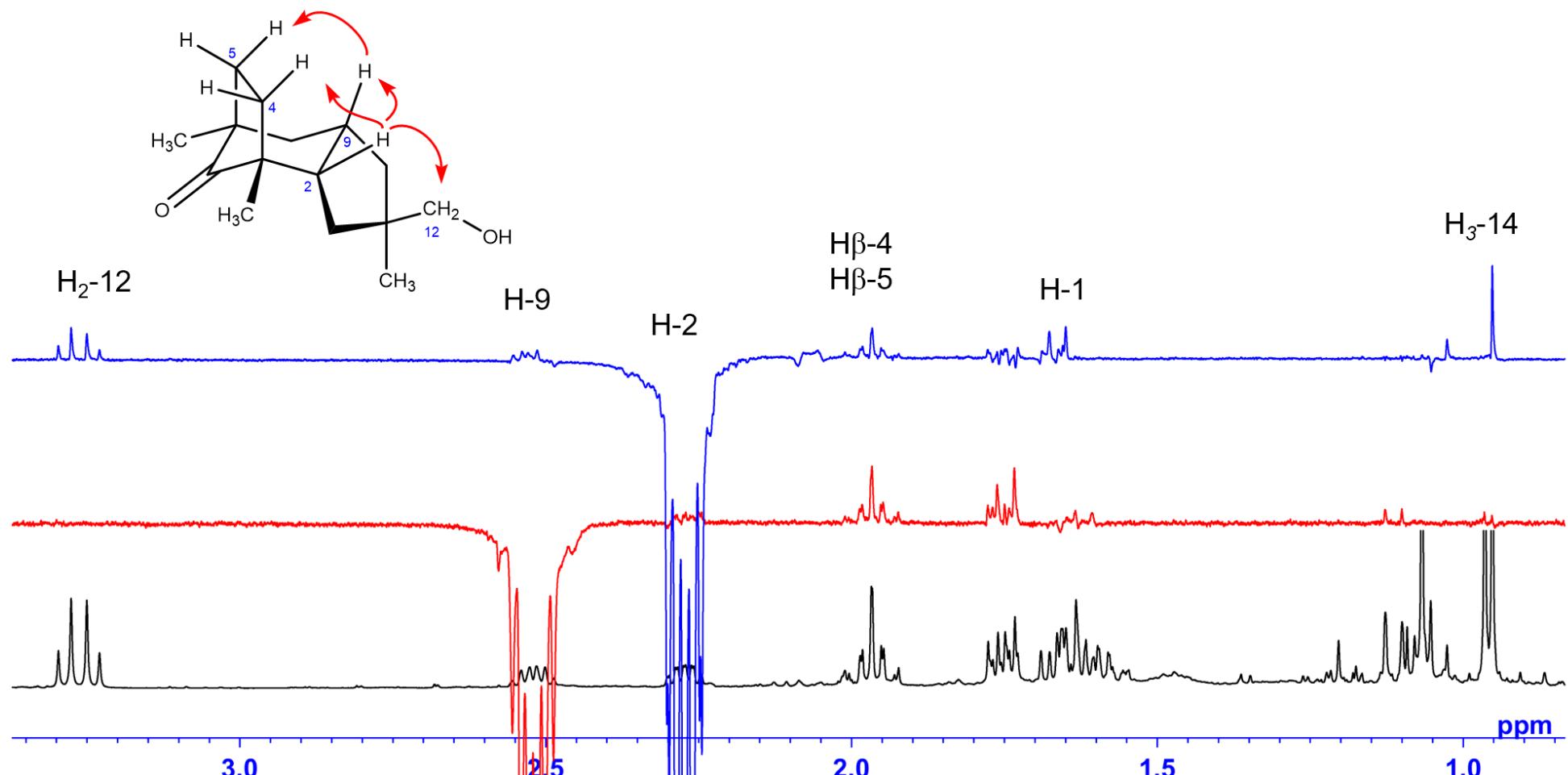
HSQC spectrum of **1a** (500 MHz, CDCl<sub>3</sub>)



HMBC spectrum of **1a** (500 MHz, CDCl<sub>3</sub>)

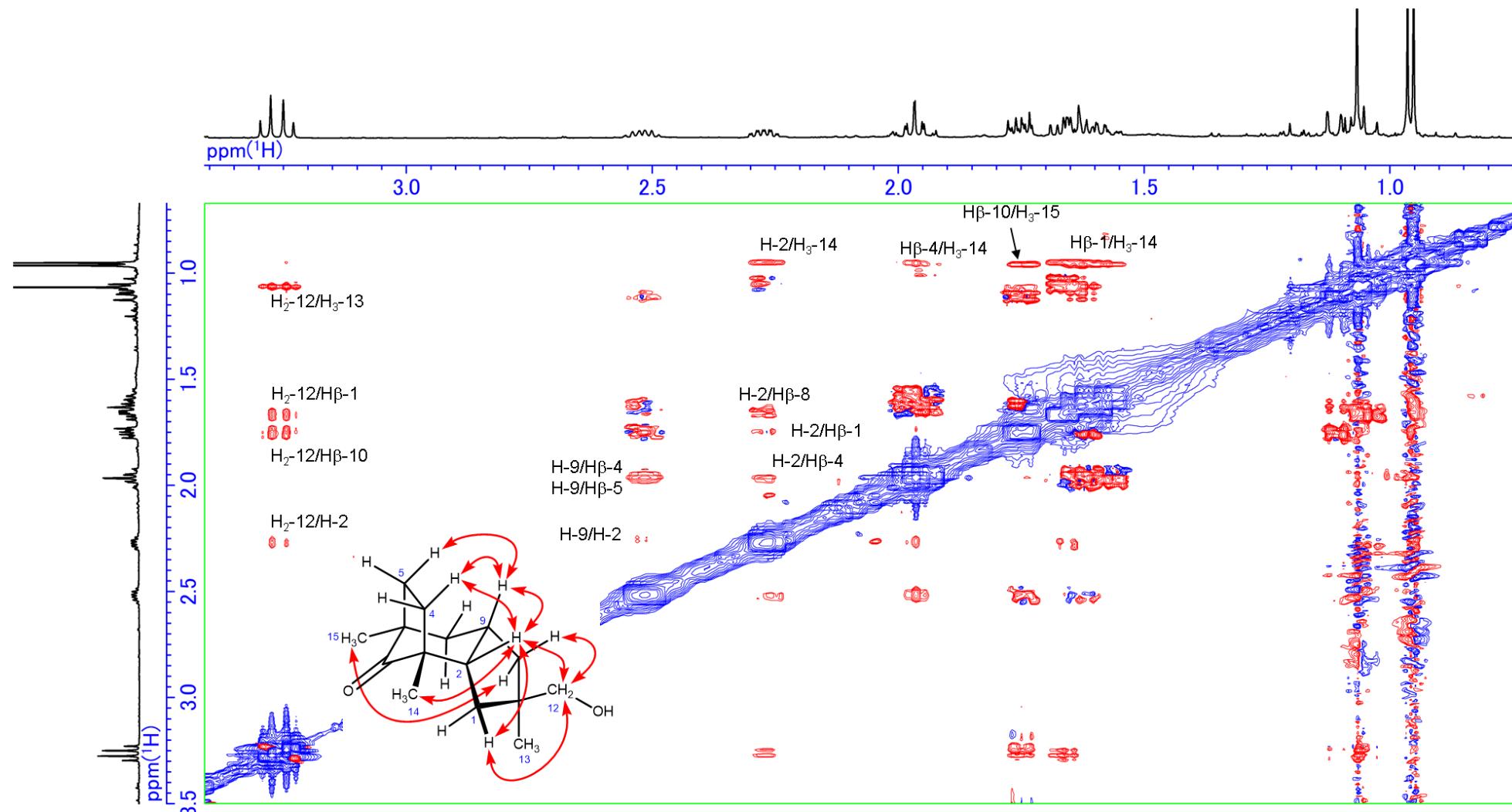


NOE 1D spectra of **1a** (500 MHz, CDCl<sub>3</sub>)

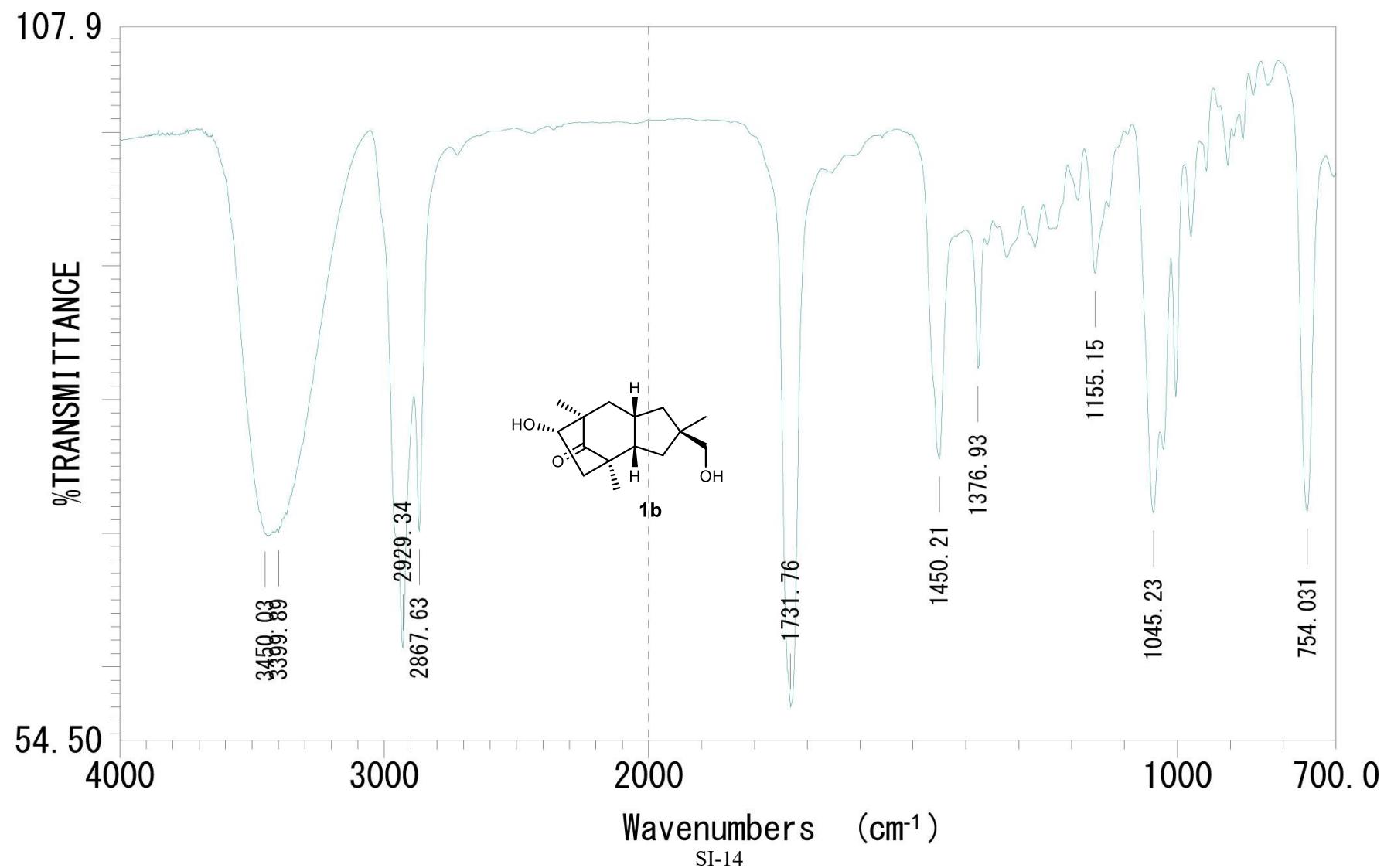


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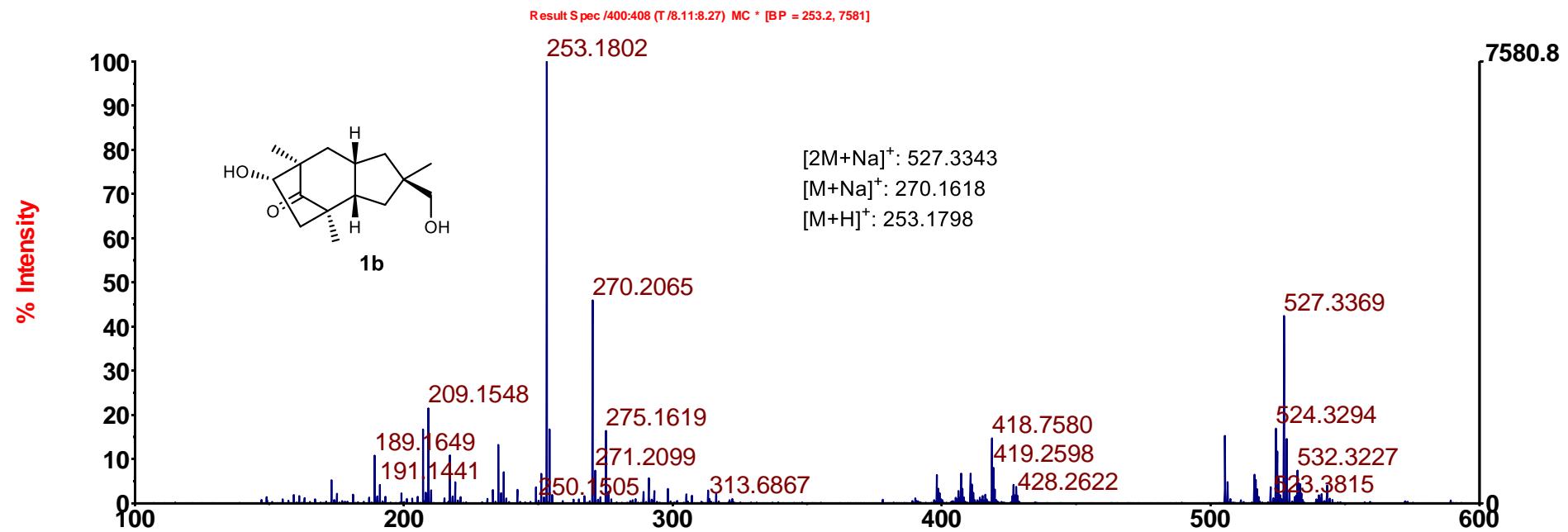
NOESY spectrum of **1a** (500 MHz, CDCl<sub>3</sub>)



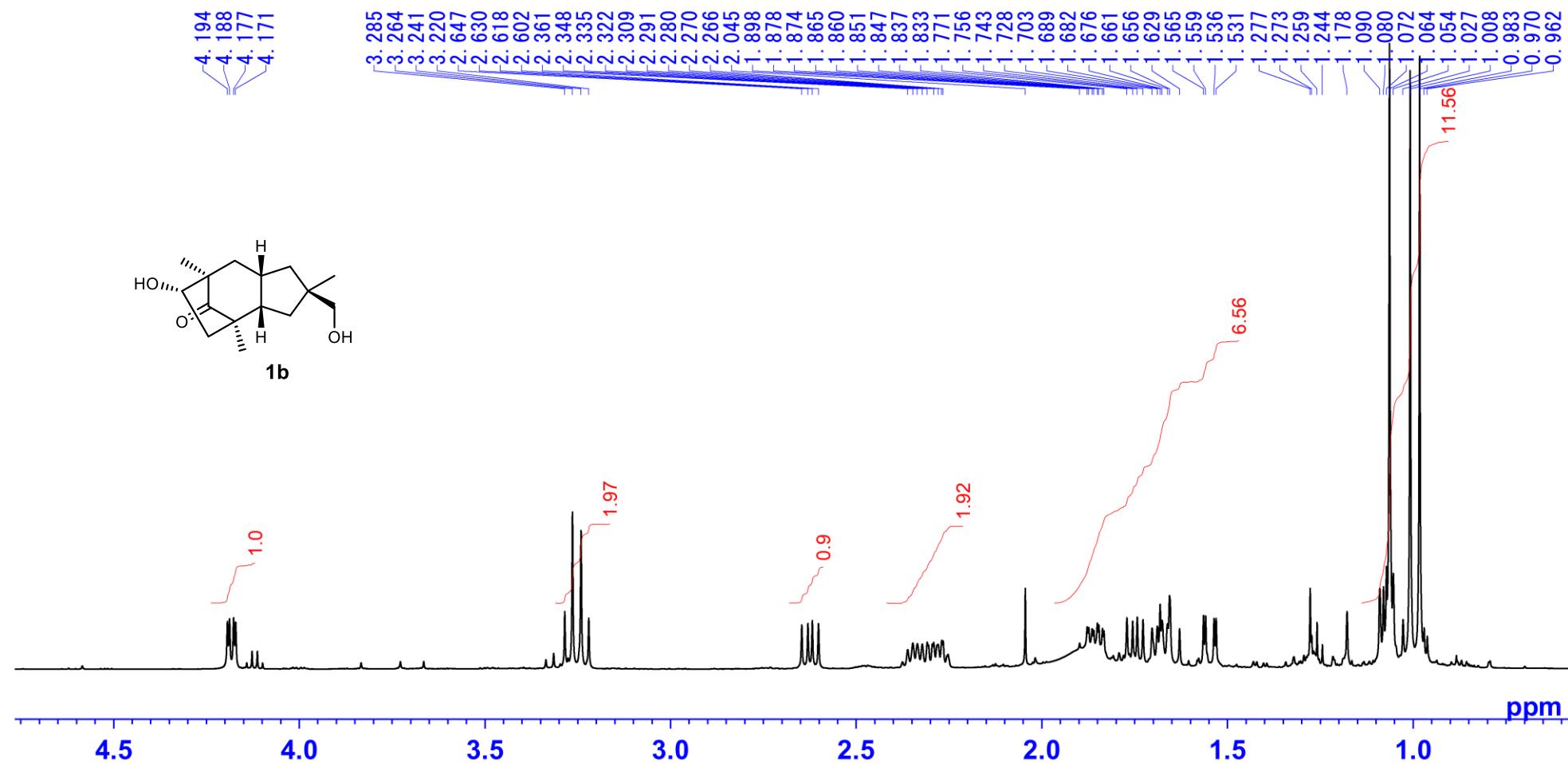
IR spectrum of **1b** (film)



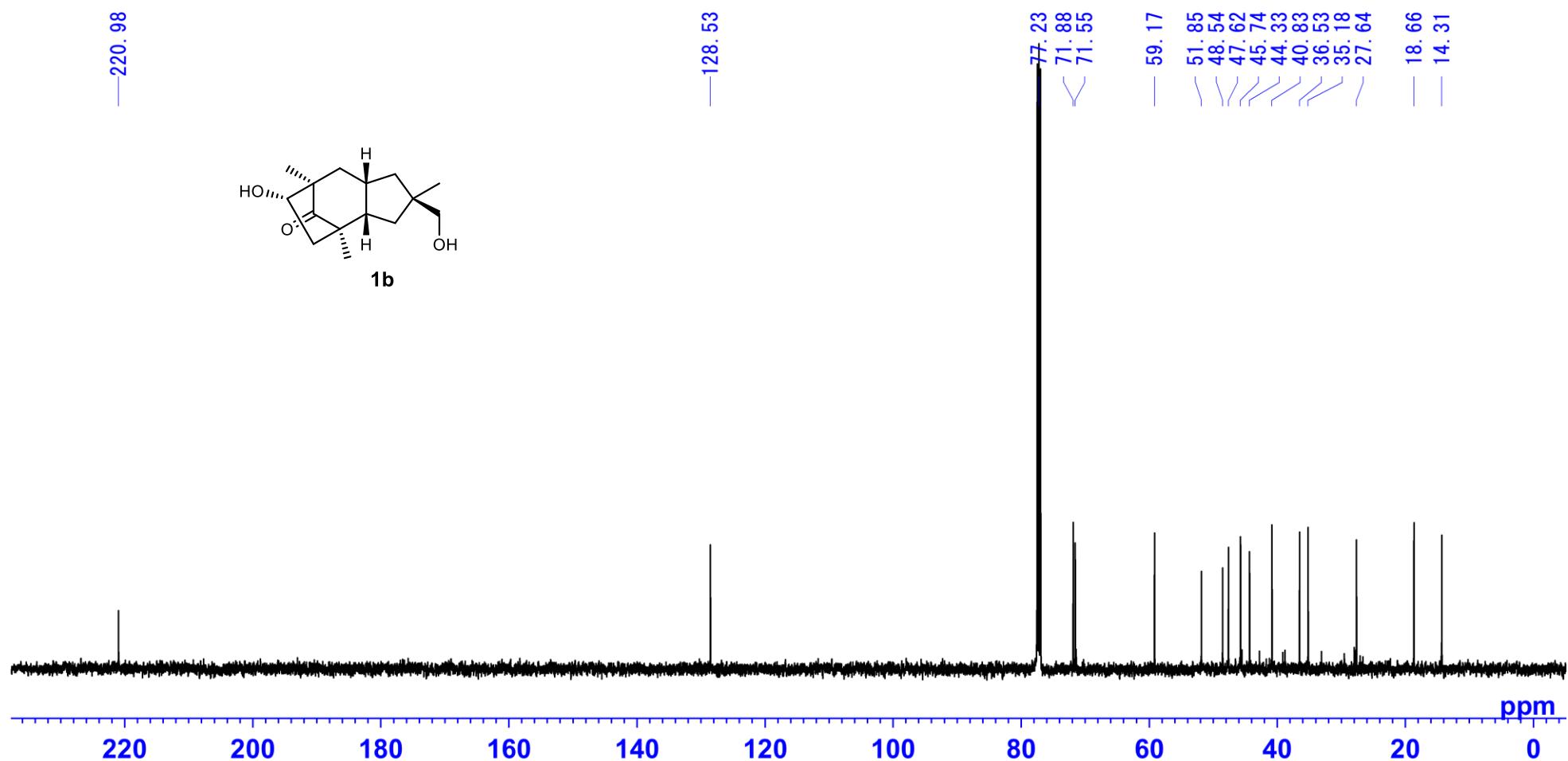
ESI-TOFMS spectrum of **1b**



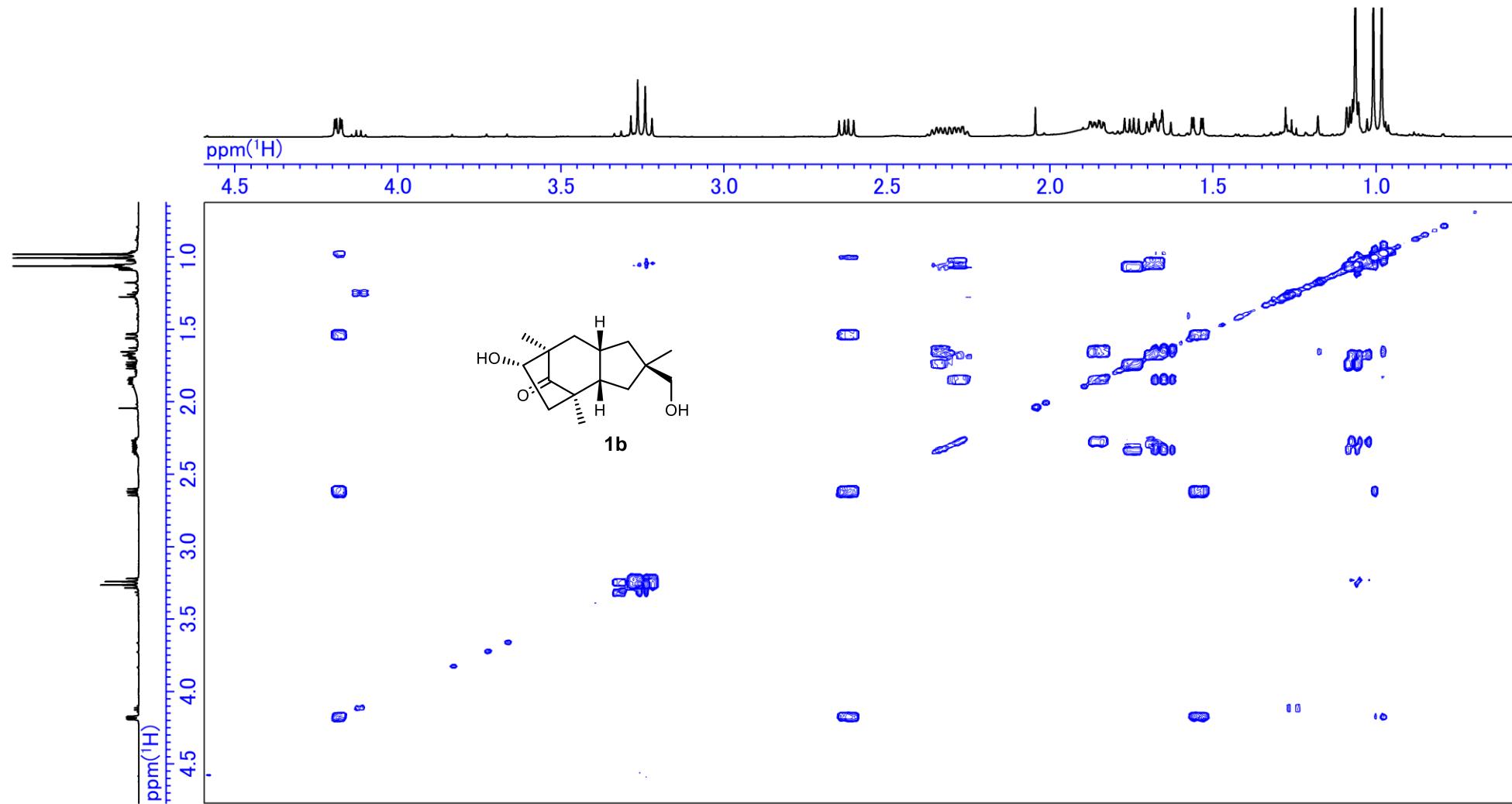
<sup>1</sup>H NMR spectrum of **1b** (500 MHz, CDCl<sub>3</sub>)



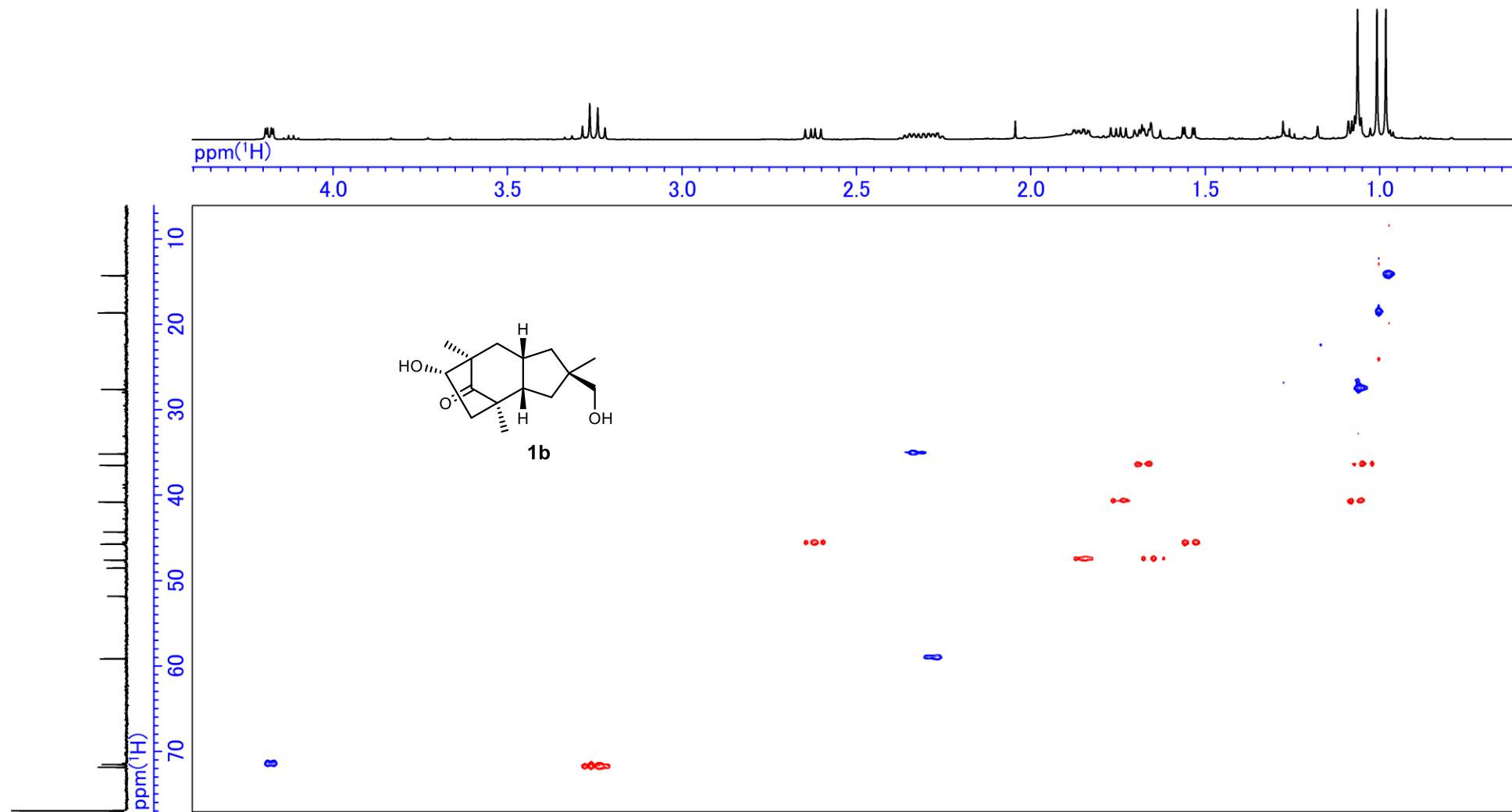
$^{13}\text{C}$  NMR spectrum of **1b** (125 MHz,  $\text{CDCl}_3$ )



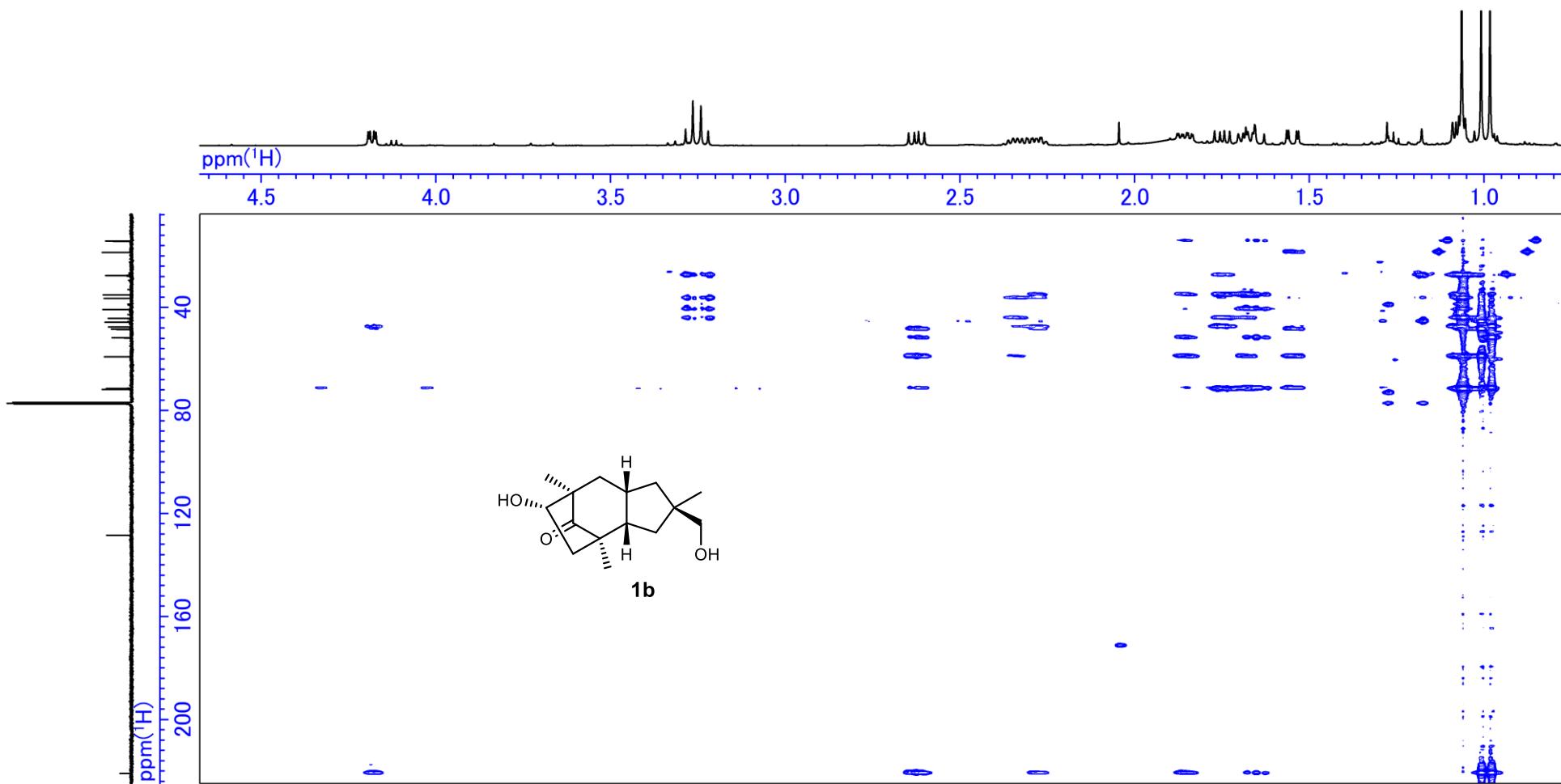
DQF COSY spectrum of **1b** (500 MHz, CDCl<sub>3</sub>)



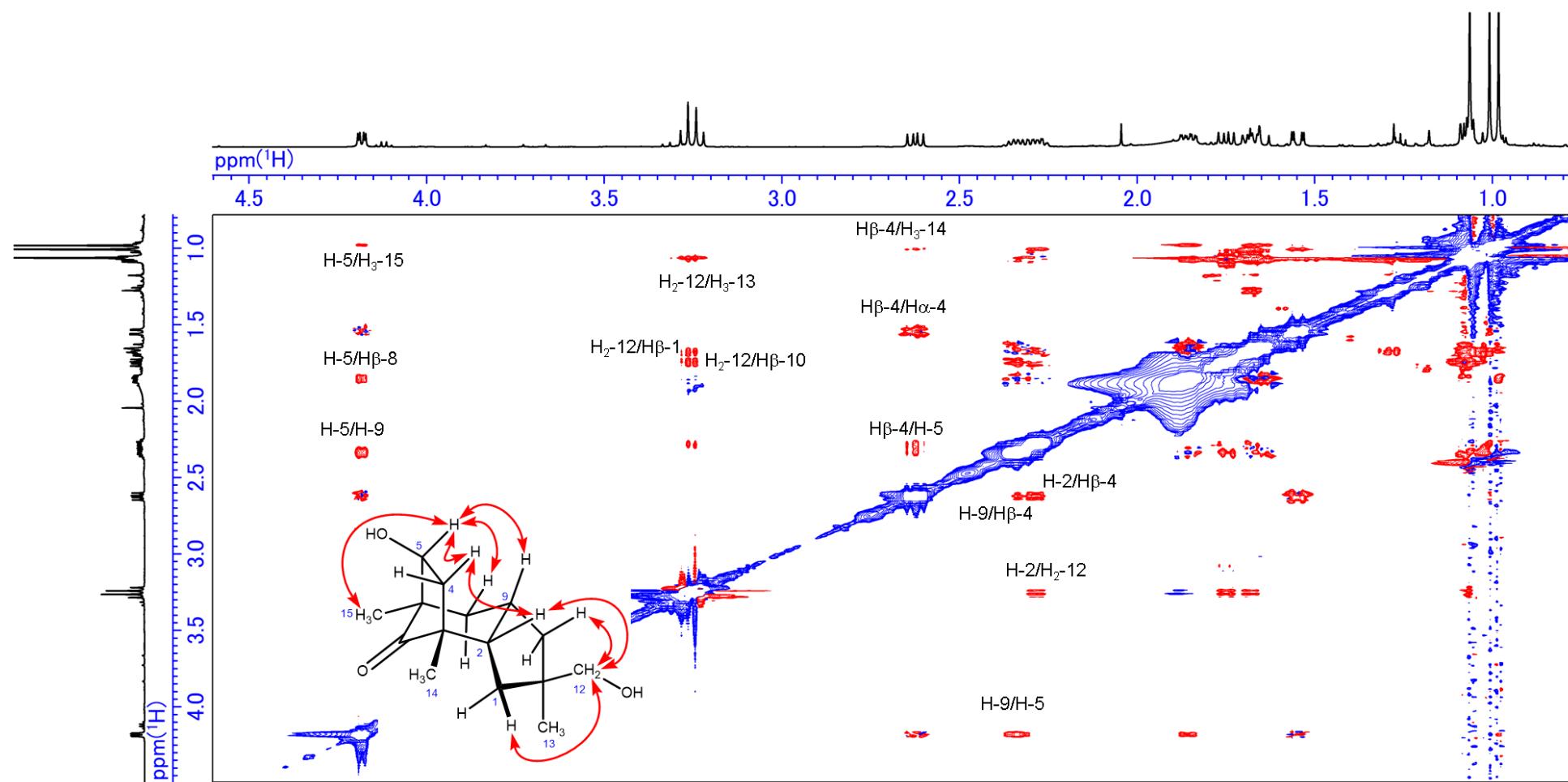
HSQC spectrum of **1b** (500 MHz, CDCl<sub>3</sub>)



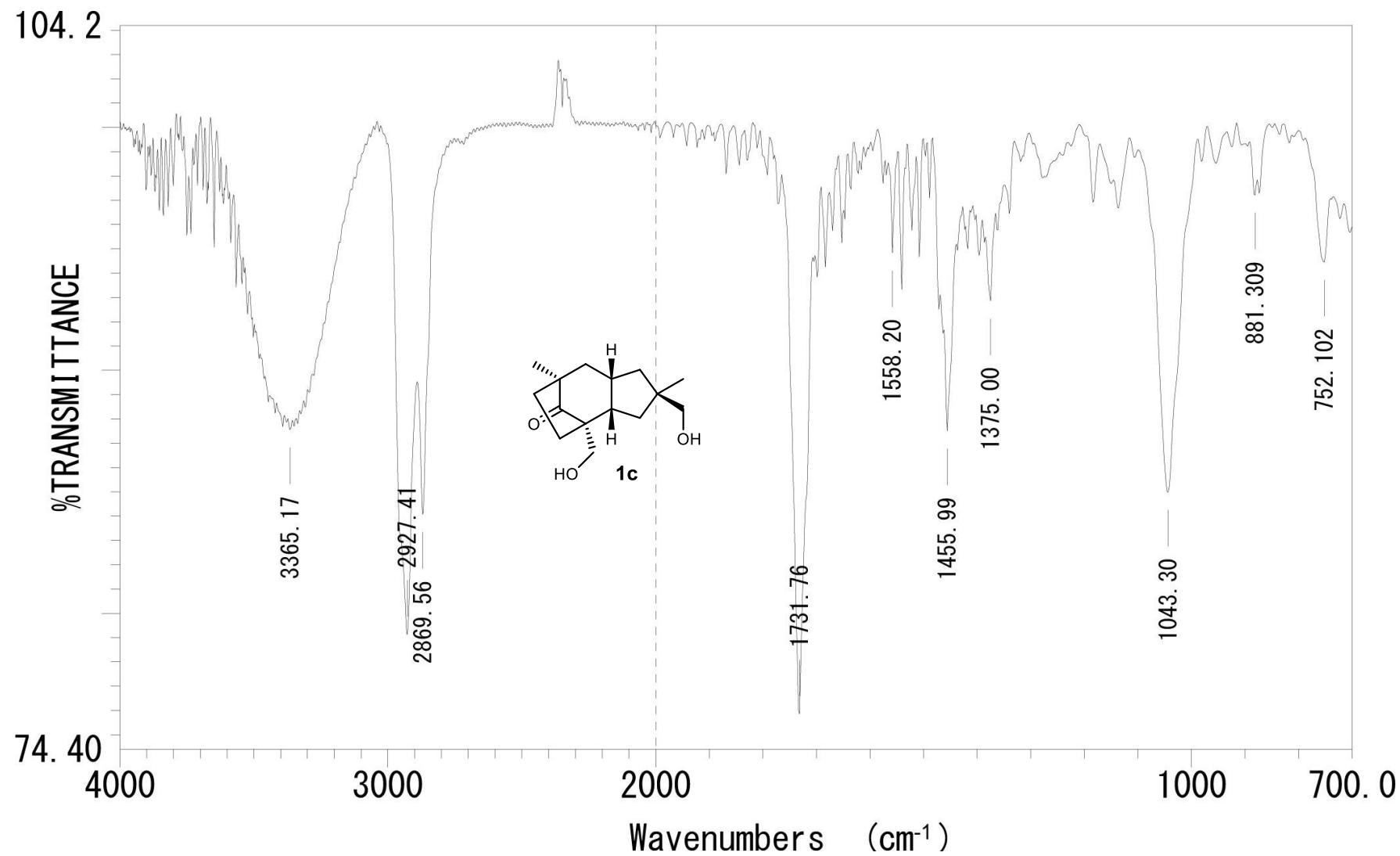
HMBC spectrum of **1b** (500 MHz, CDCl<sub>3</sub>)



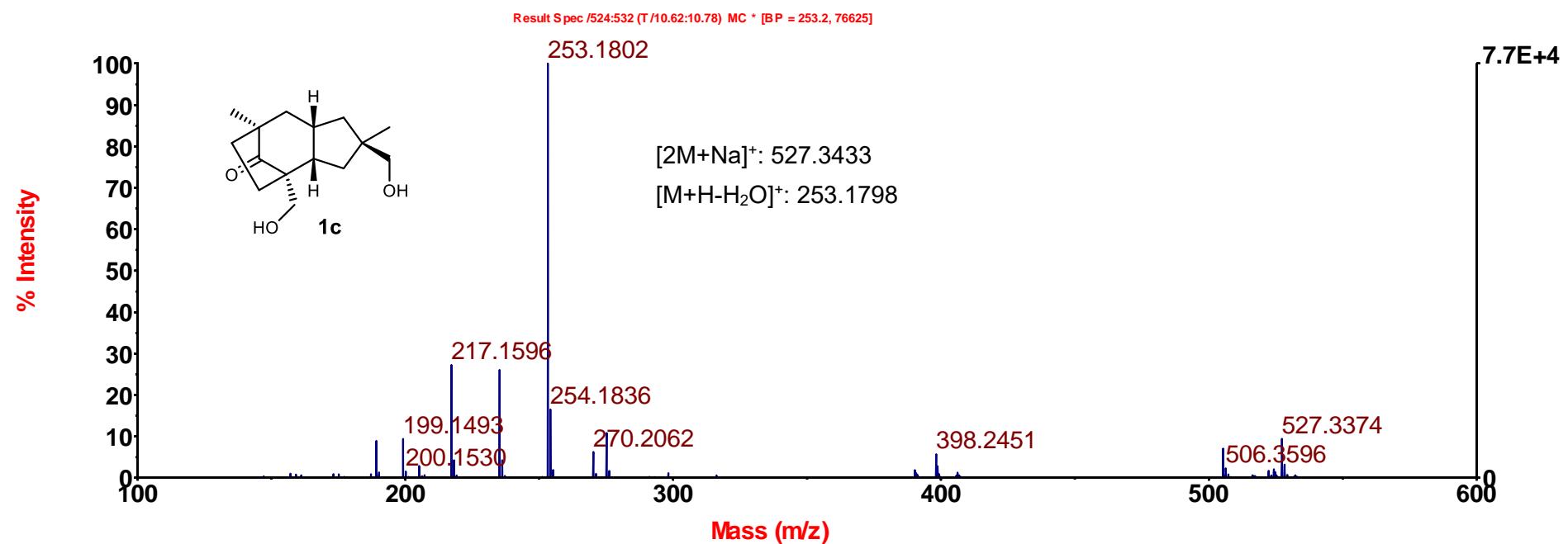
NOESY spectrum of **1b** (500 MHz,  $\text{CDCl}_3$ )



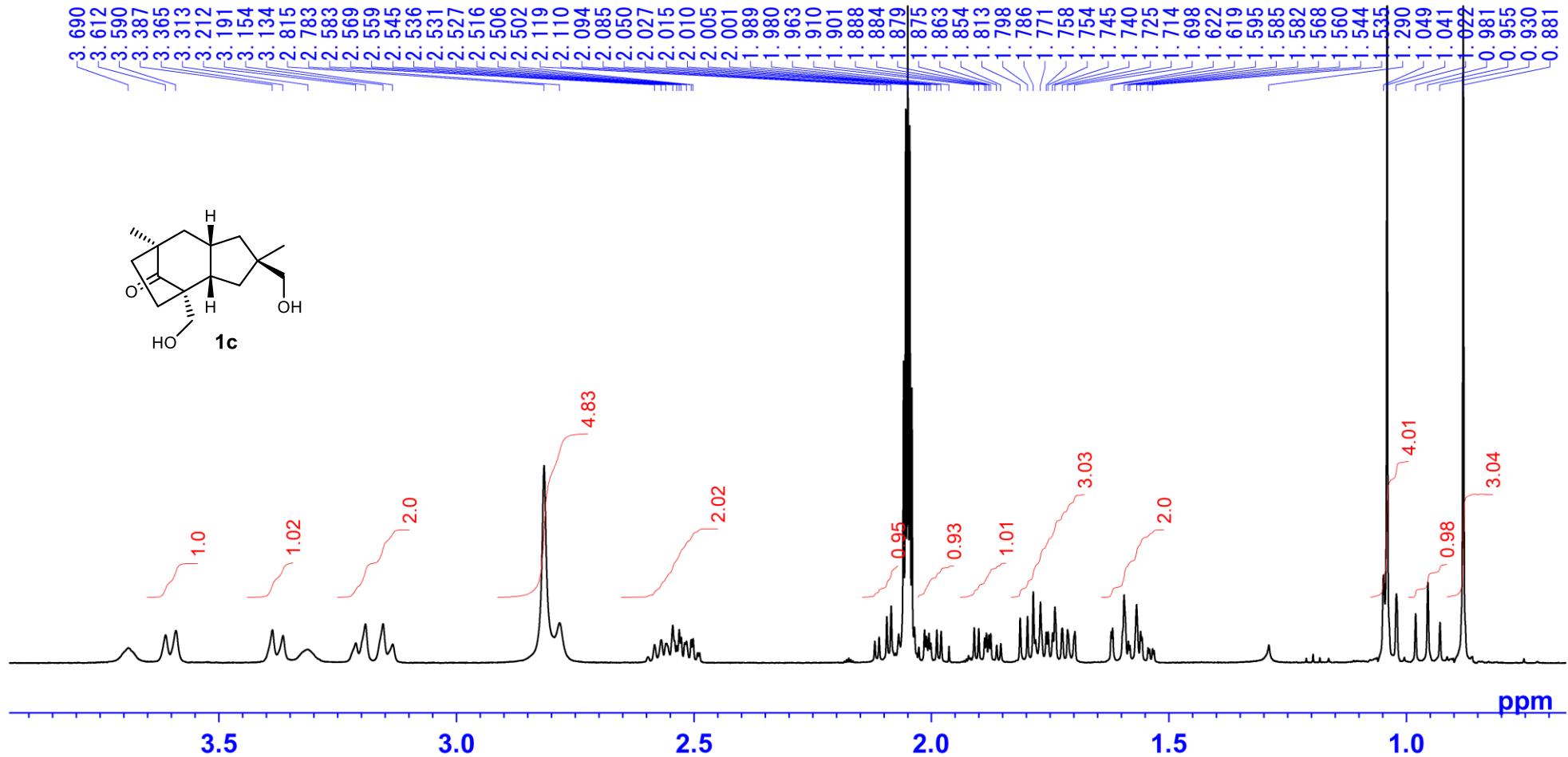
IR spectrum of **1c** (film).



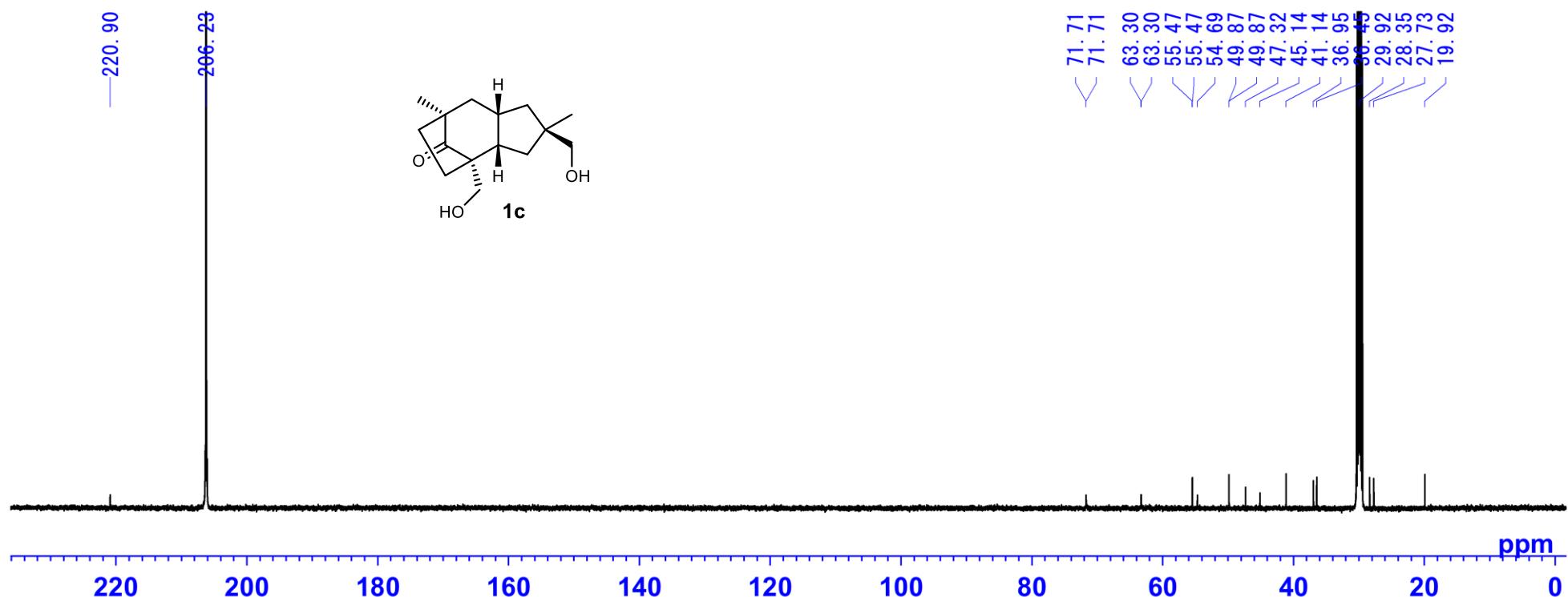
### ESI-TOFMS spectrum of **1c**



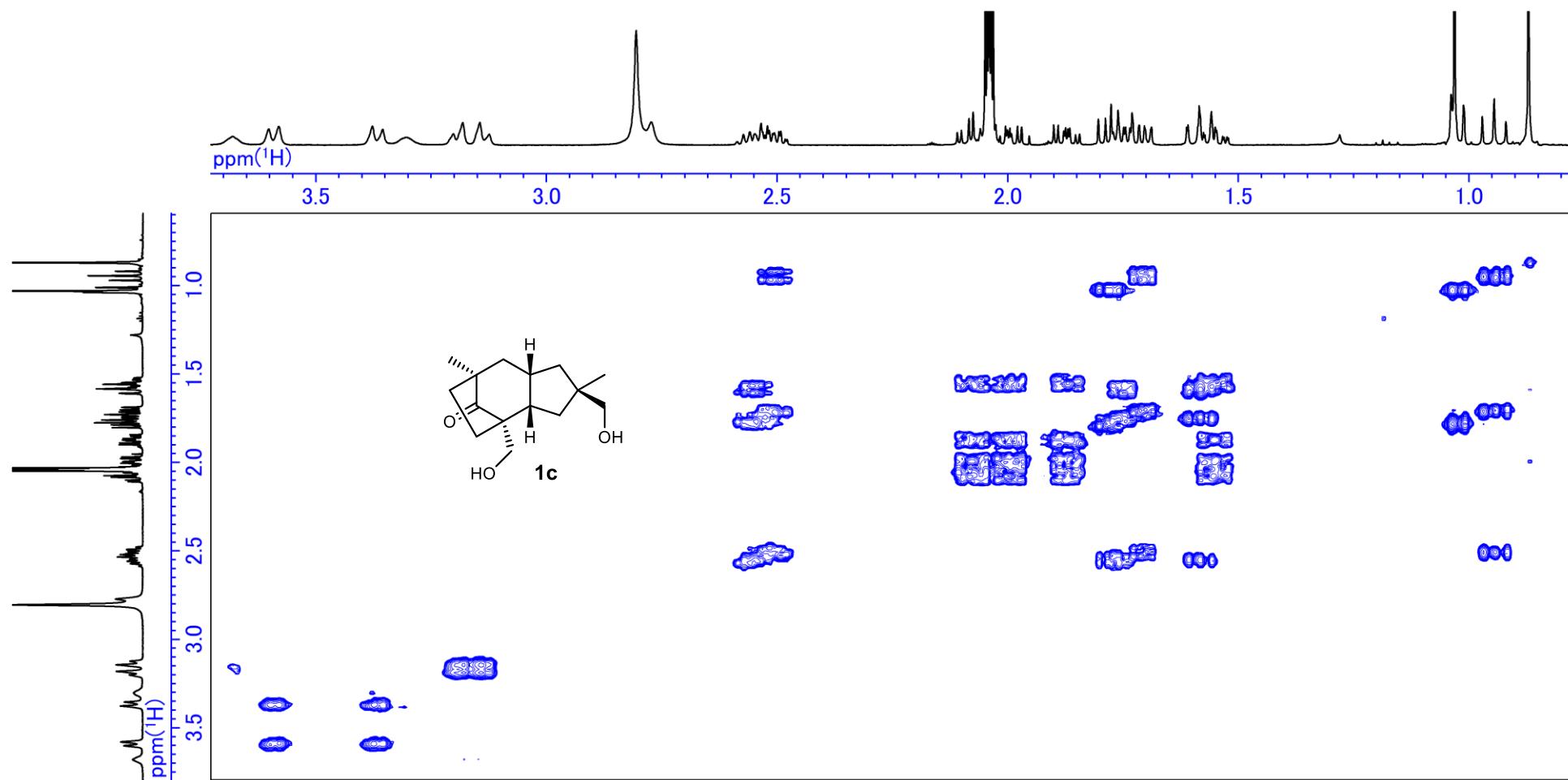
<sup>1</sup>H NMR spectrum of **1c** (500 MHz, acetone-*d*<sub>6</sub>)



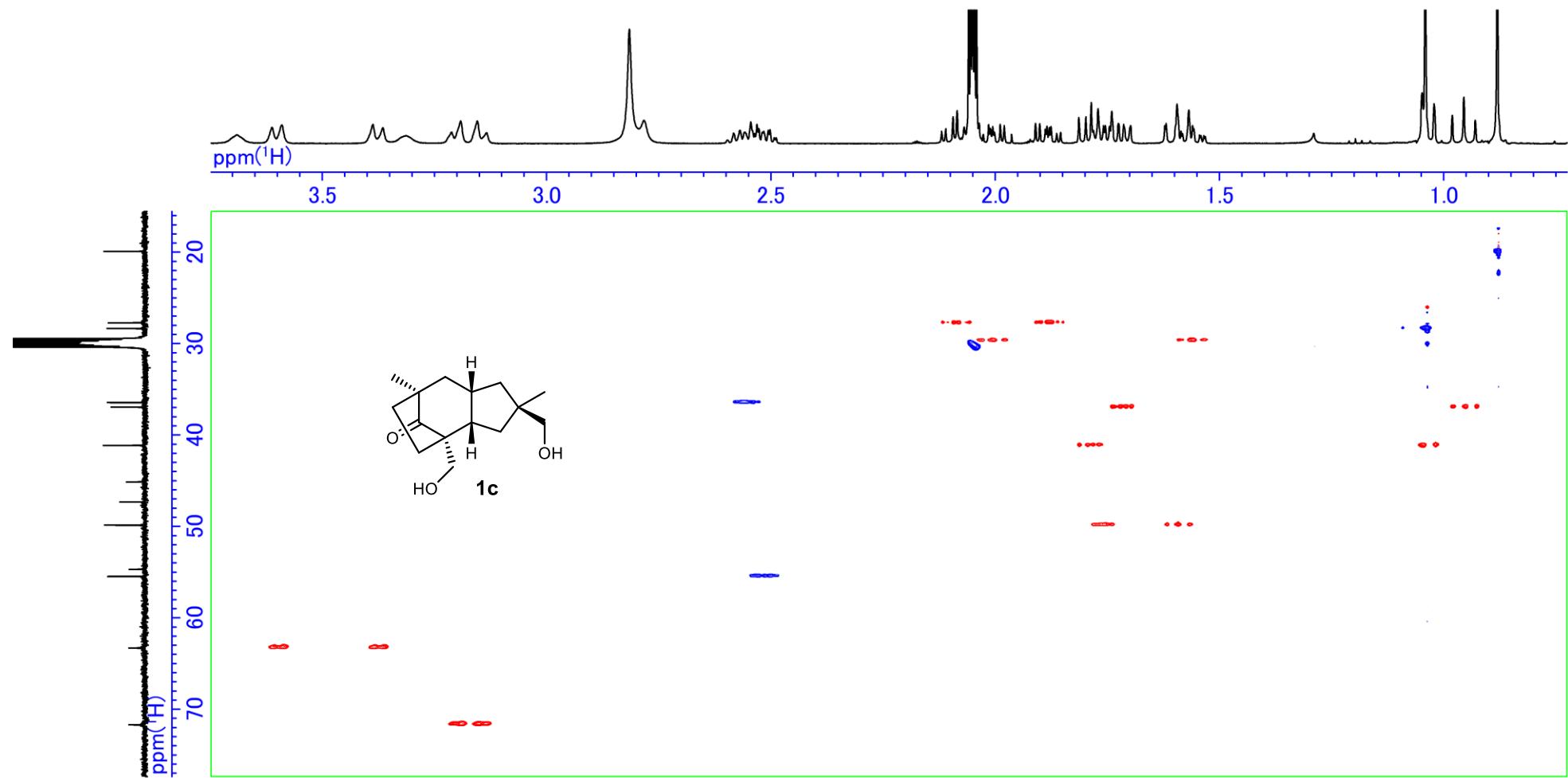
<sup>13</sup>C NMR spectrum of **1c** (125 MHz, acetone-*d*<sub>6</sub>)



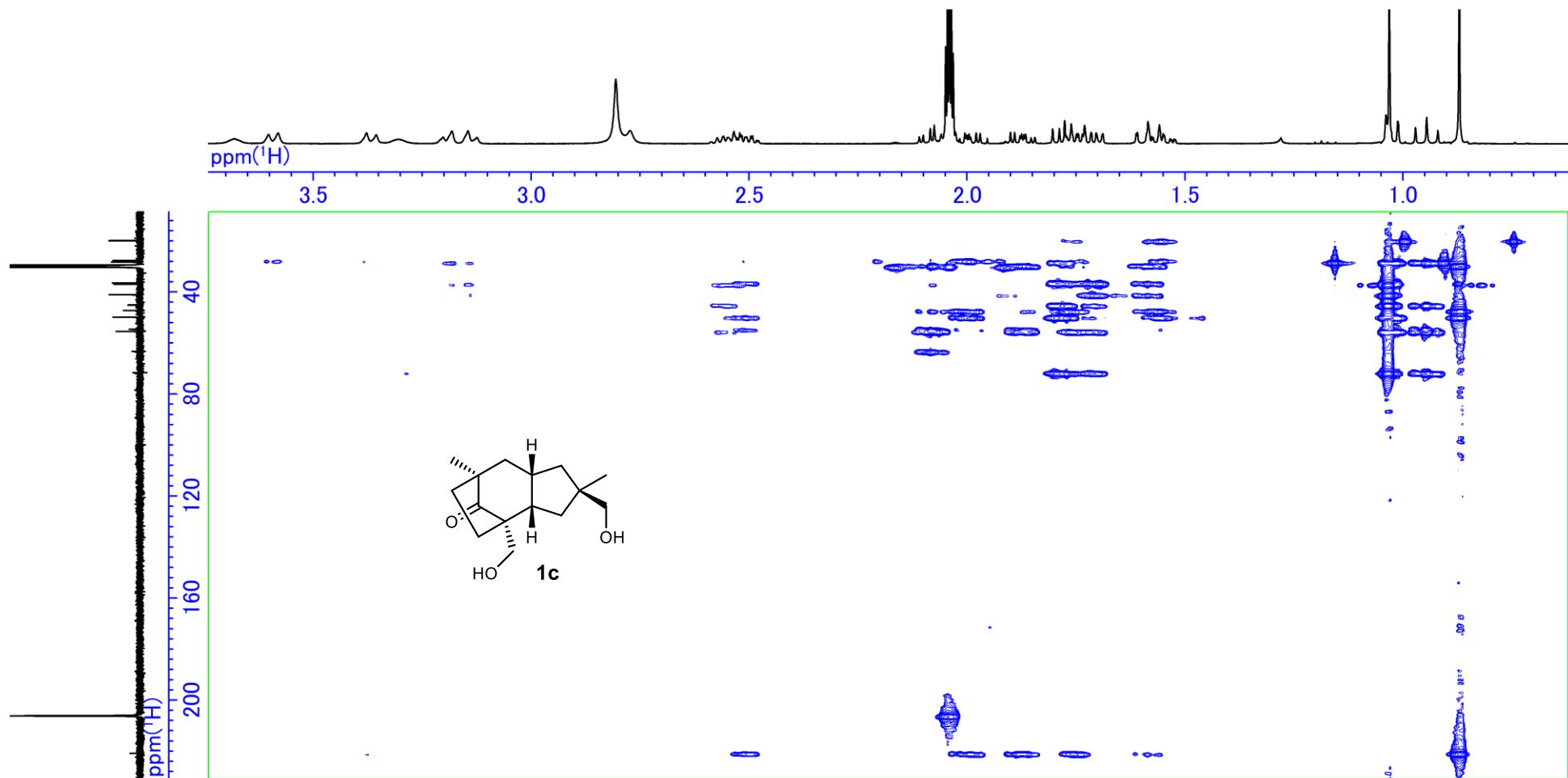
DQF COSY spectrum of **1c** (500 MHz, acetone-*d*<sub>6</sub>)



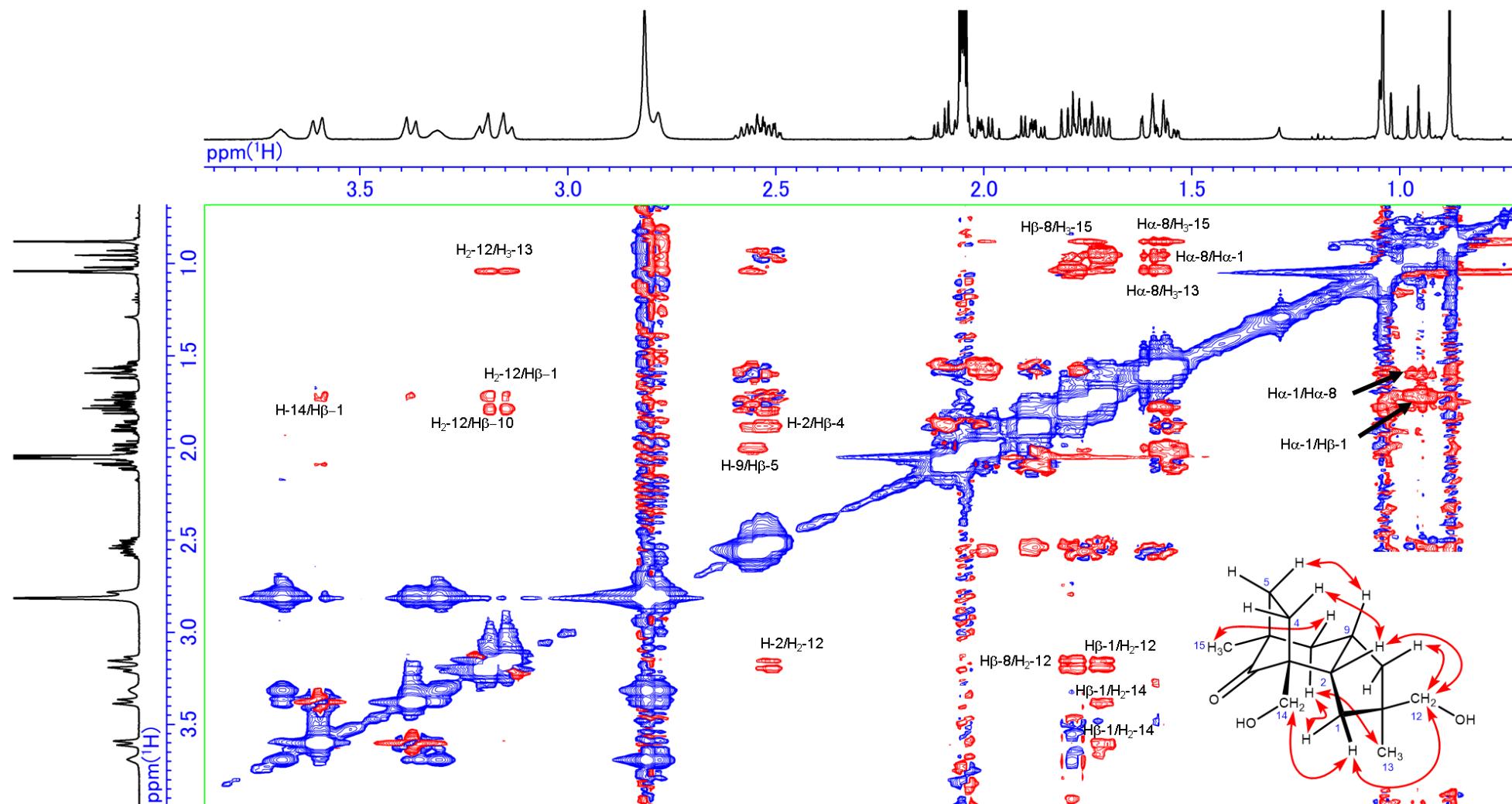
HSQC spectrum of **1c** (500 MHz, acetone-*d*<sub>6</sub>)



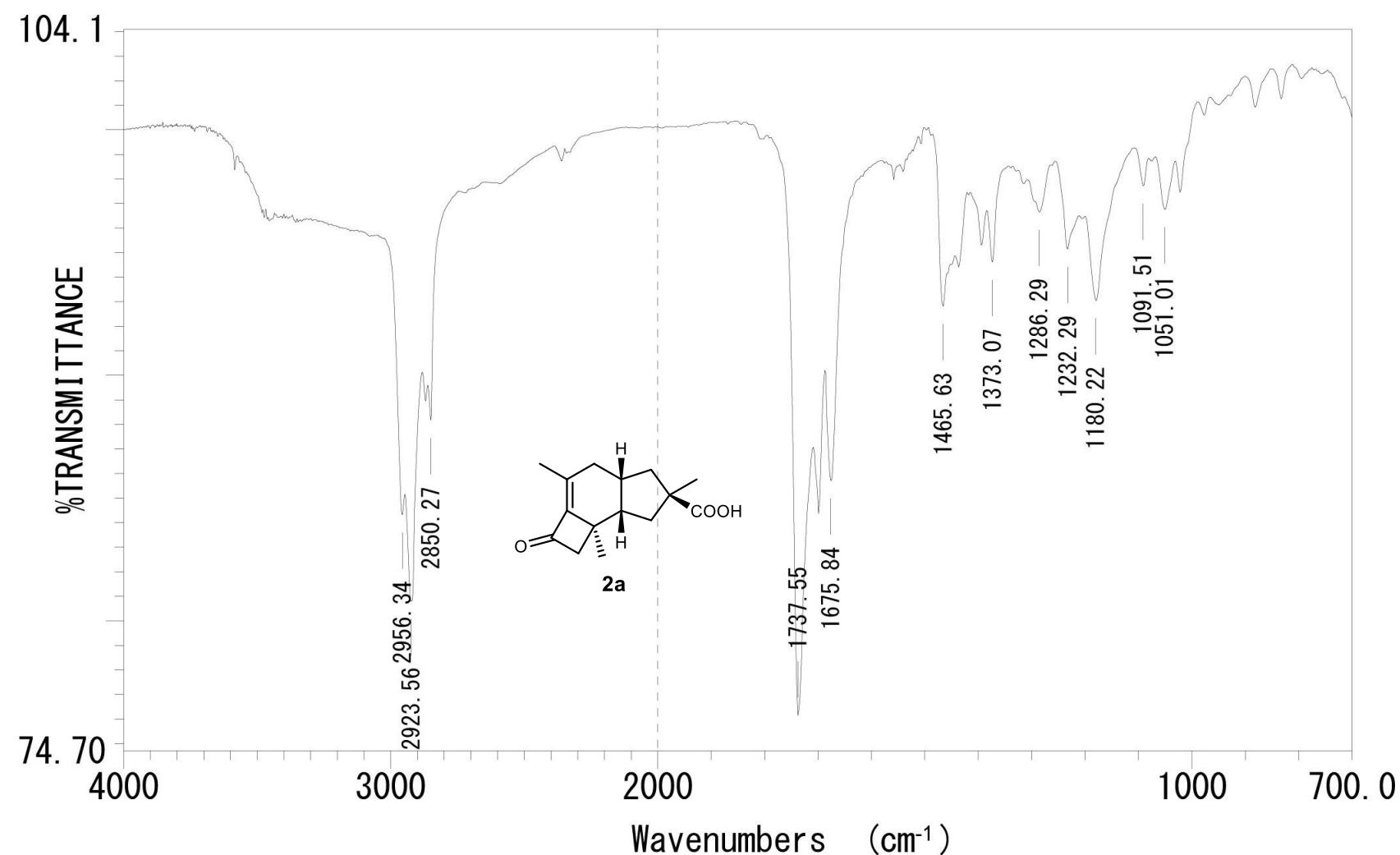
HMBC spectrum of **1c** (500 MHz, acetone-*d*<sub>6</sub>)



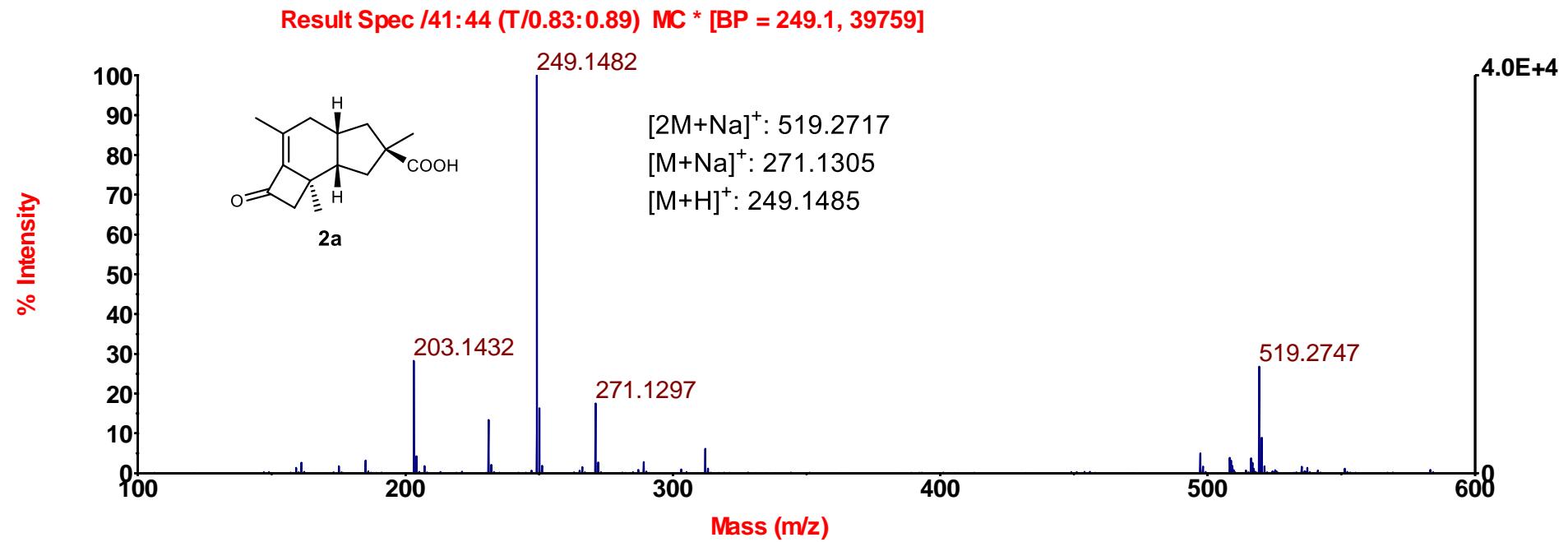
NOESY spectrum of **1c** (500 MHz, acetone-*d*<sub>6</sub>)



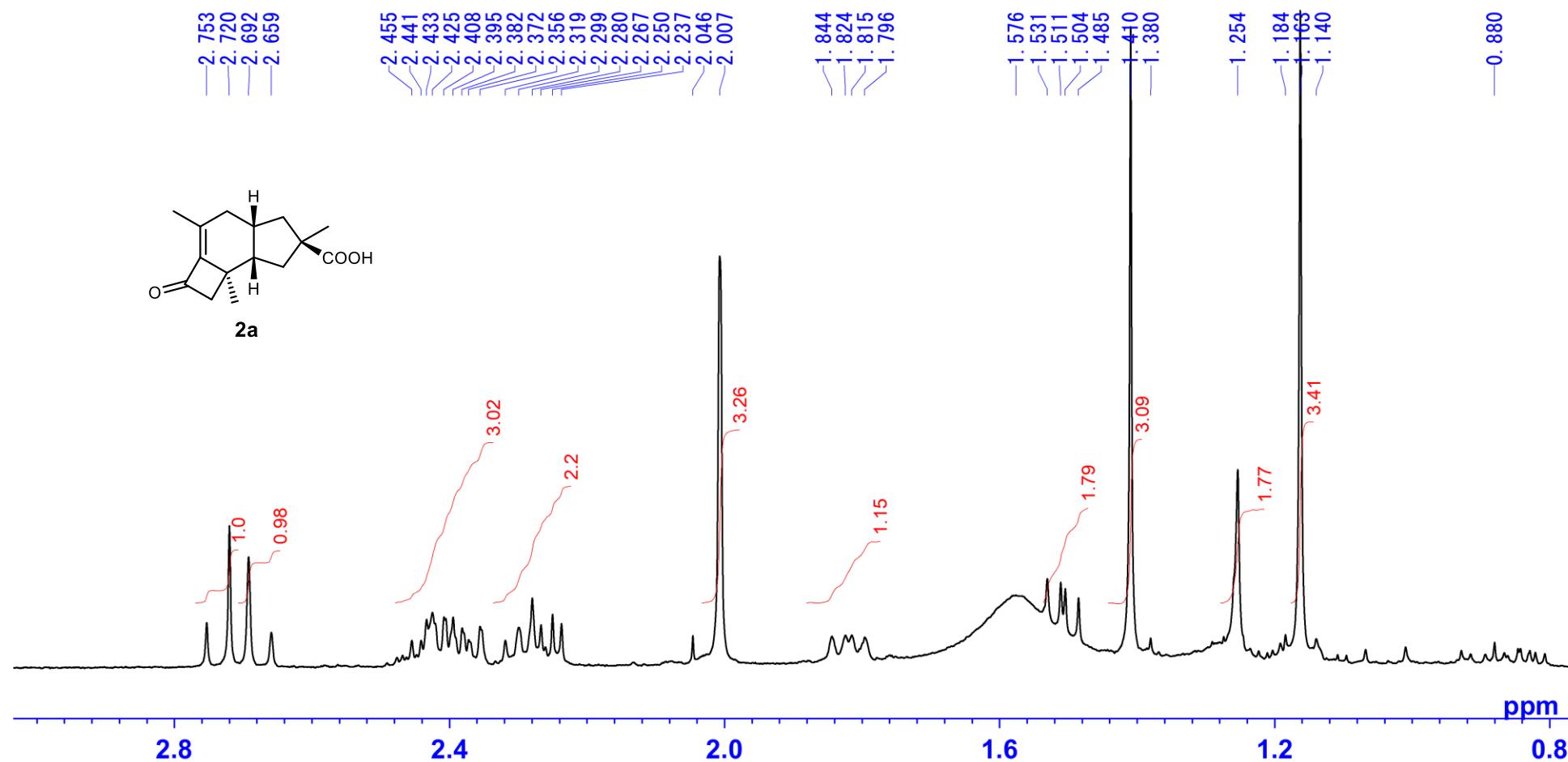
IR spectrum (film) of **2a**



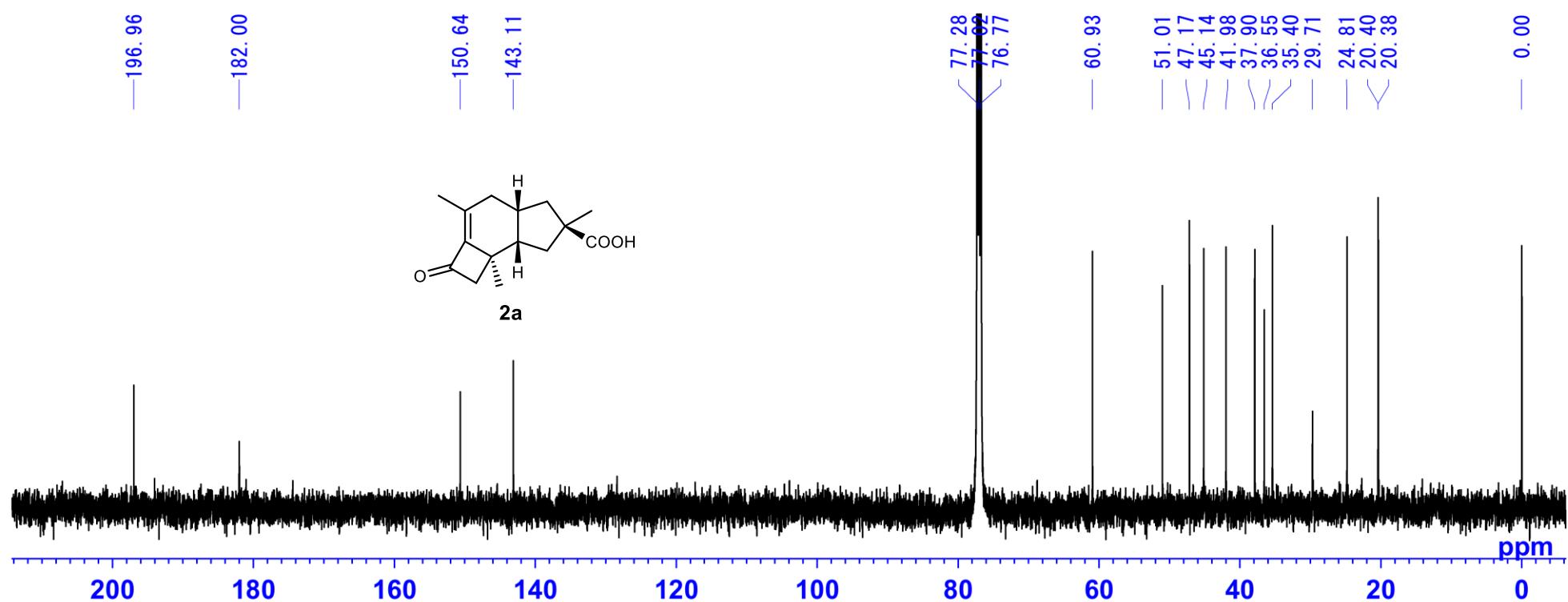
ESI-TOFMS spectrum of **2a**,



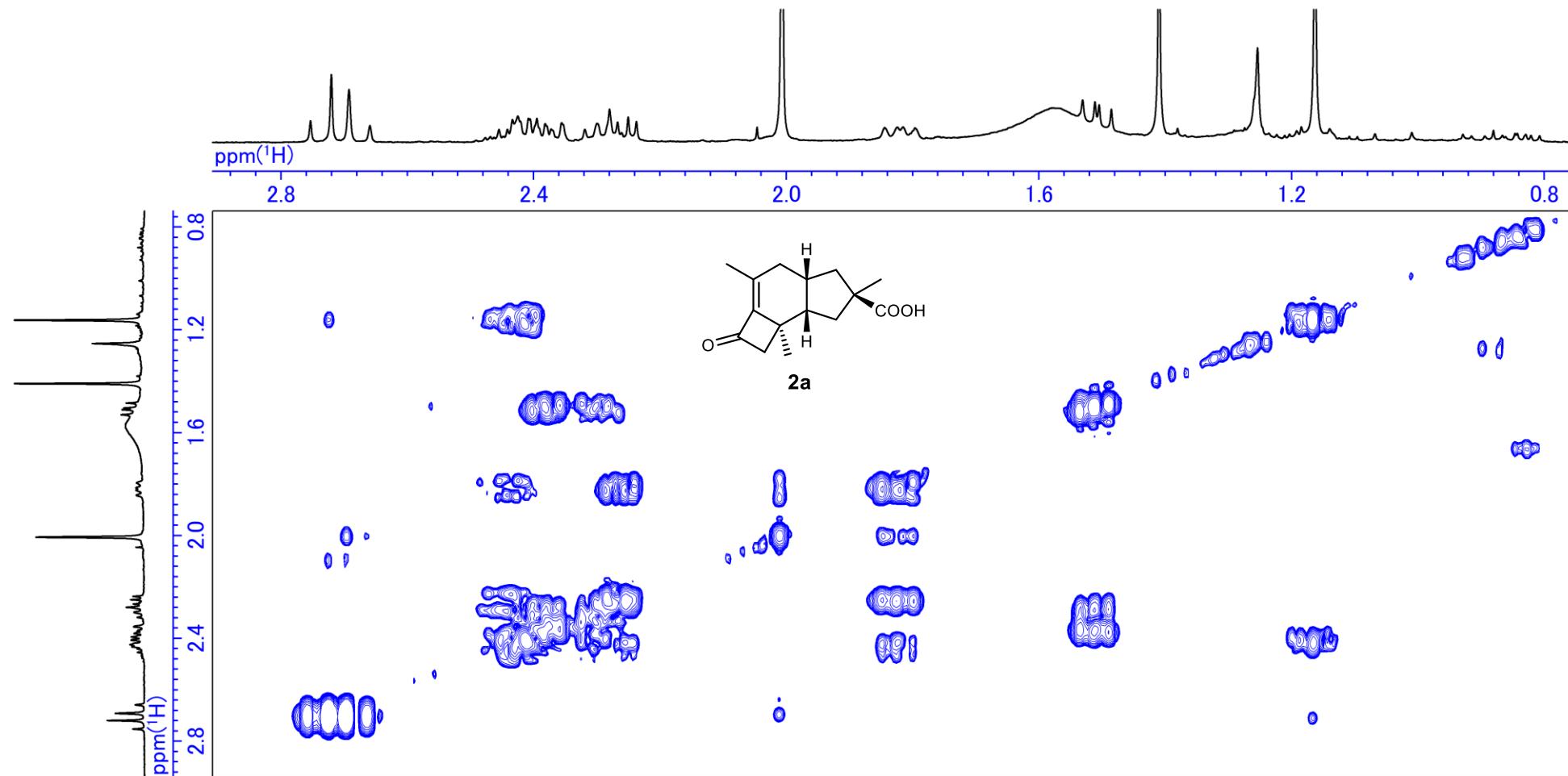
<sup>1</sup>H NMR spectrum of **2a** (500 MHz, CDCl<sub>3</sub>)



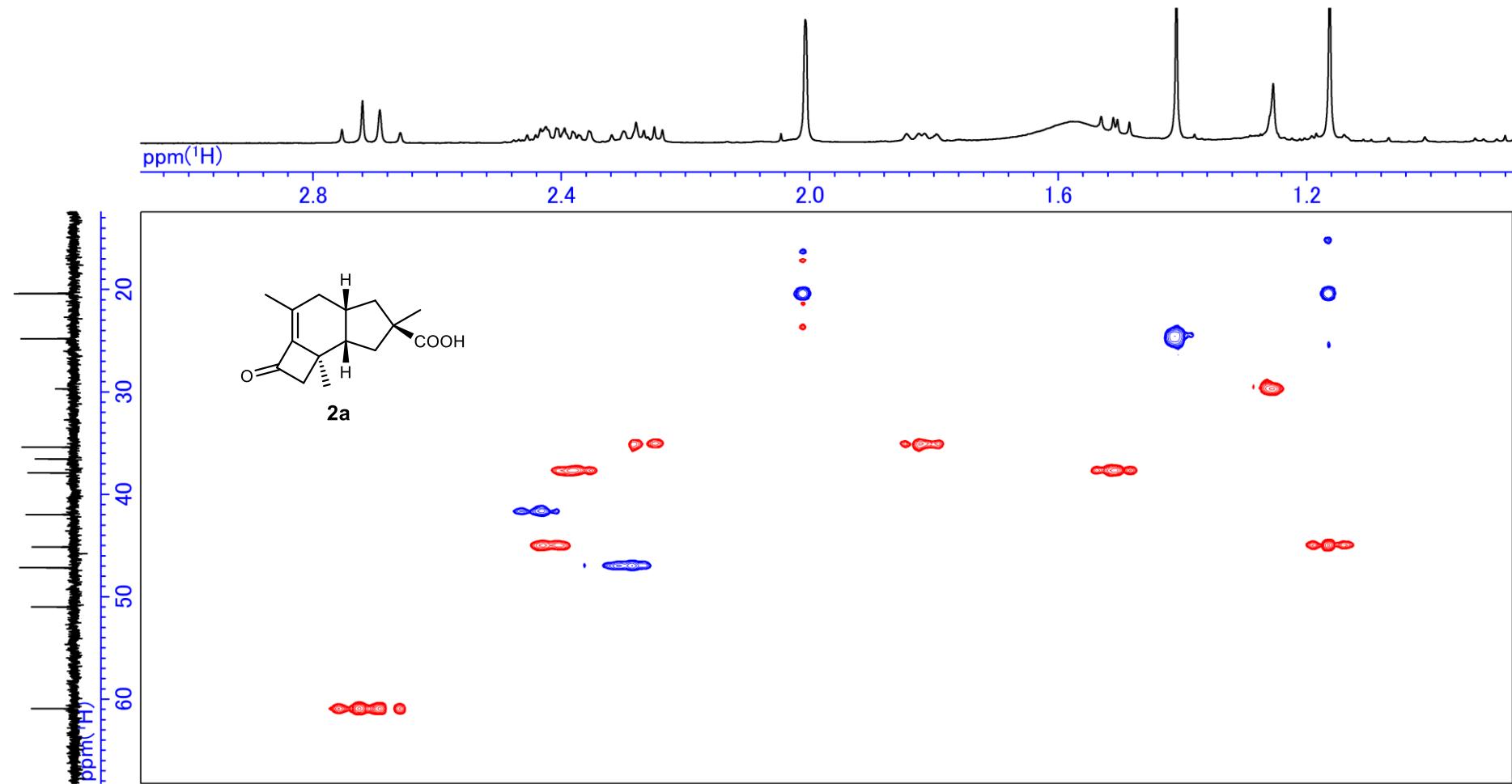
<sup>13</sup>C NMR spectrum of **2a** (125 MHz, CDCl<sub>3</sub>)



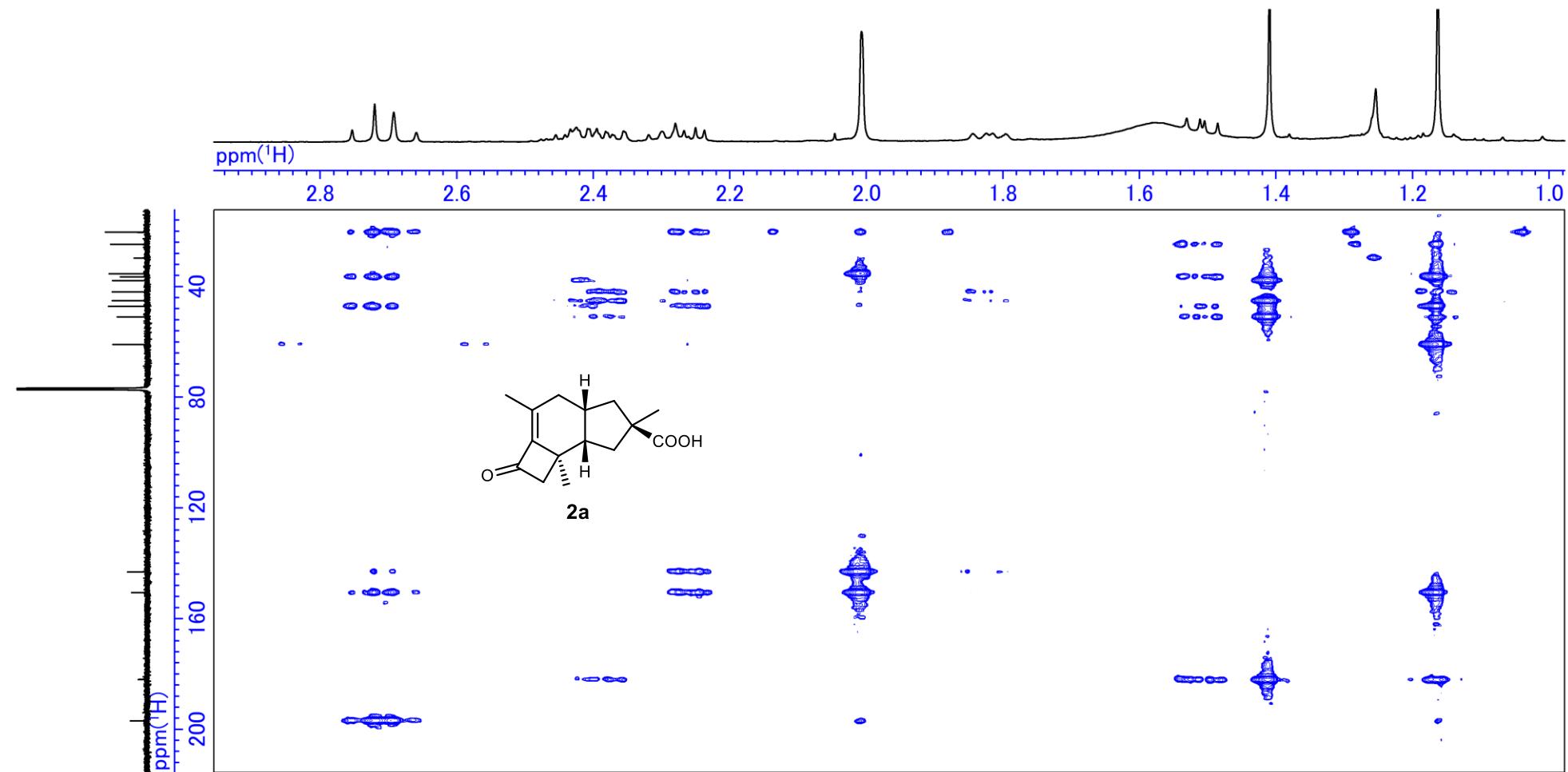
DQF COSY spectrum of **2a** (500 MHz, CDCl<sub>3</sub>)



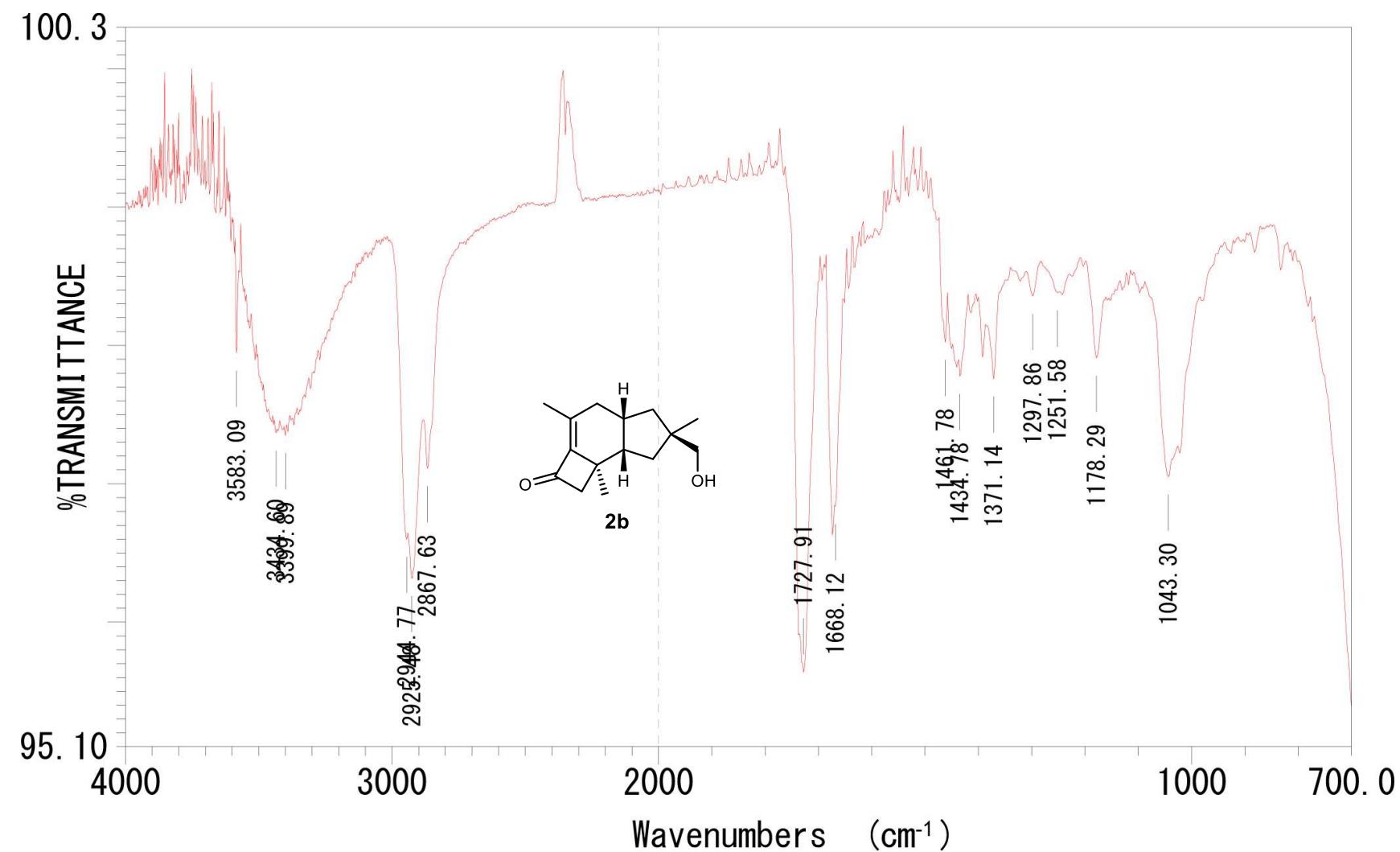
HSQC spectrum of **2a** (500 MHz, CDCl<sub>3</sub>)



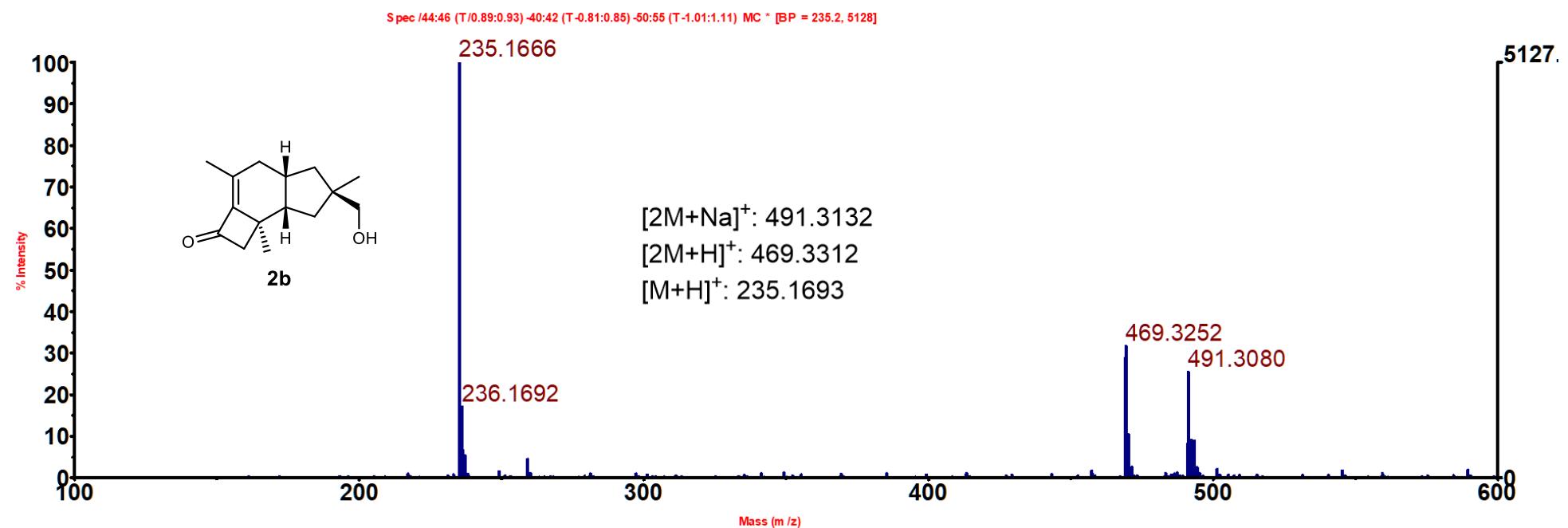
HMBC spectrum of **2a** (500 MHz, CDCl<sub>3</sub>)



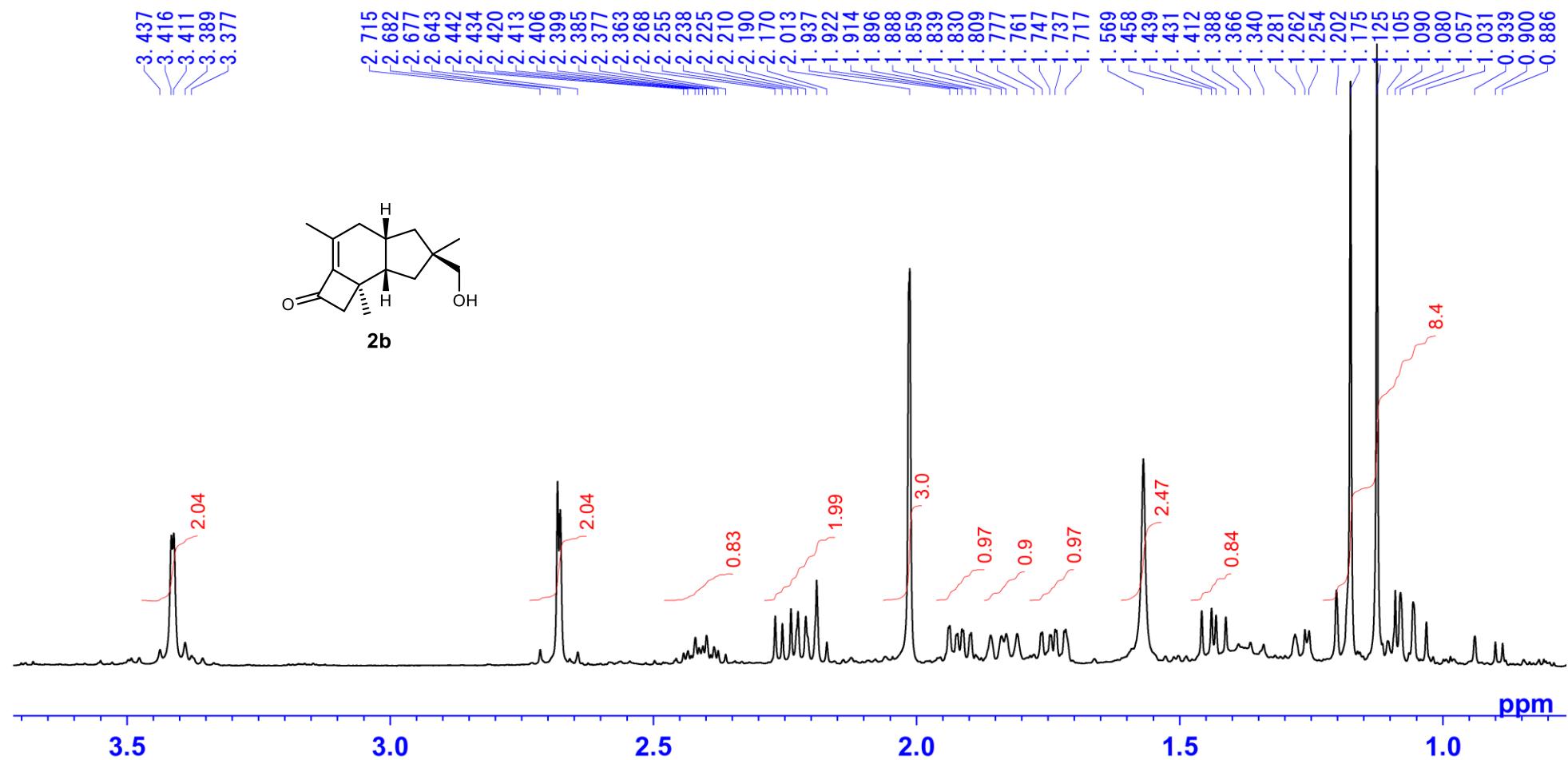
IR spectrum of **2b** (film)



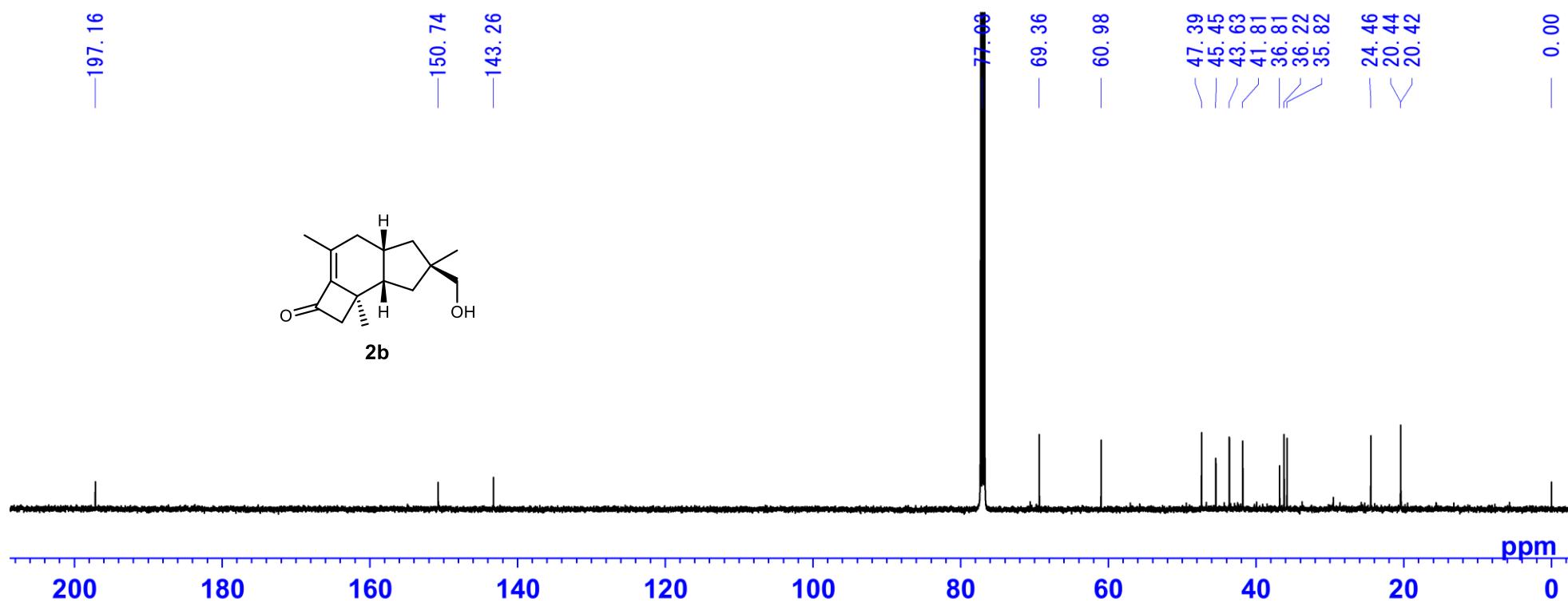
ESI-TOFMS spectrum of **2b**



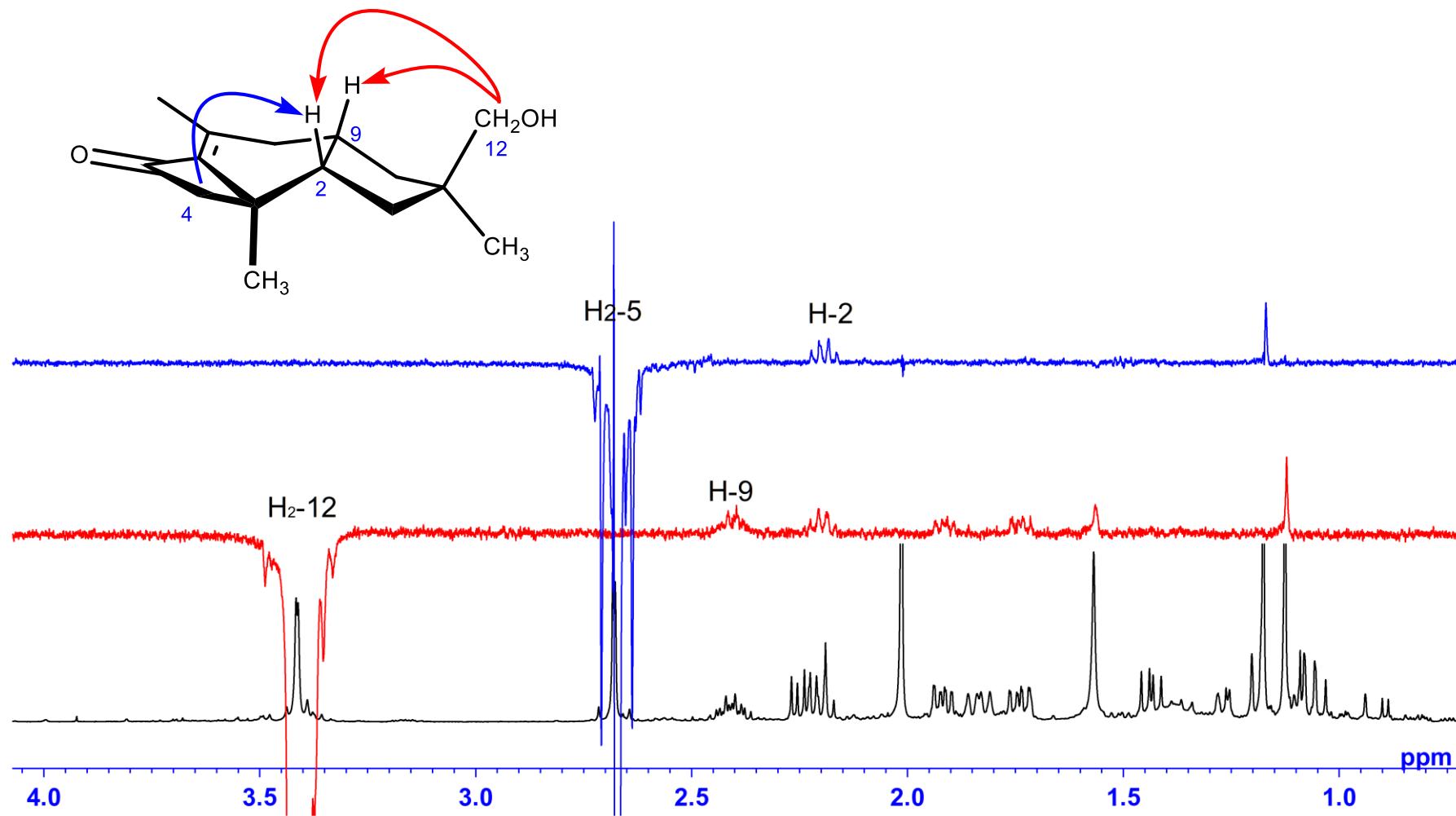
<sup>1</sup>H NMR spectrum of **2b** (500 MHz, CDCl<sub>3</sub>)



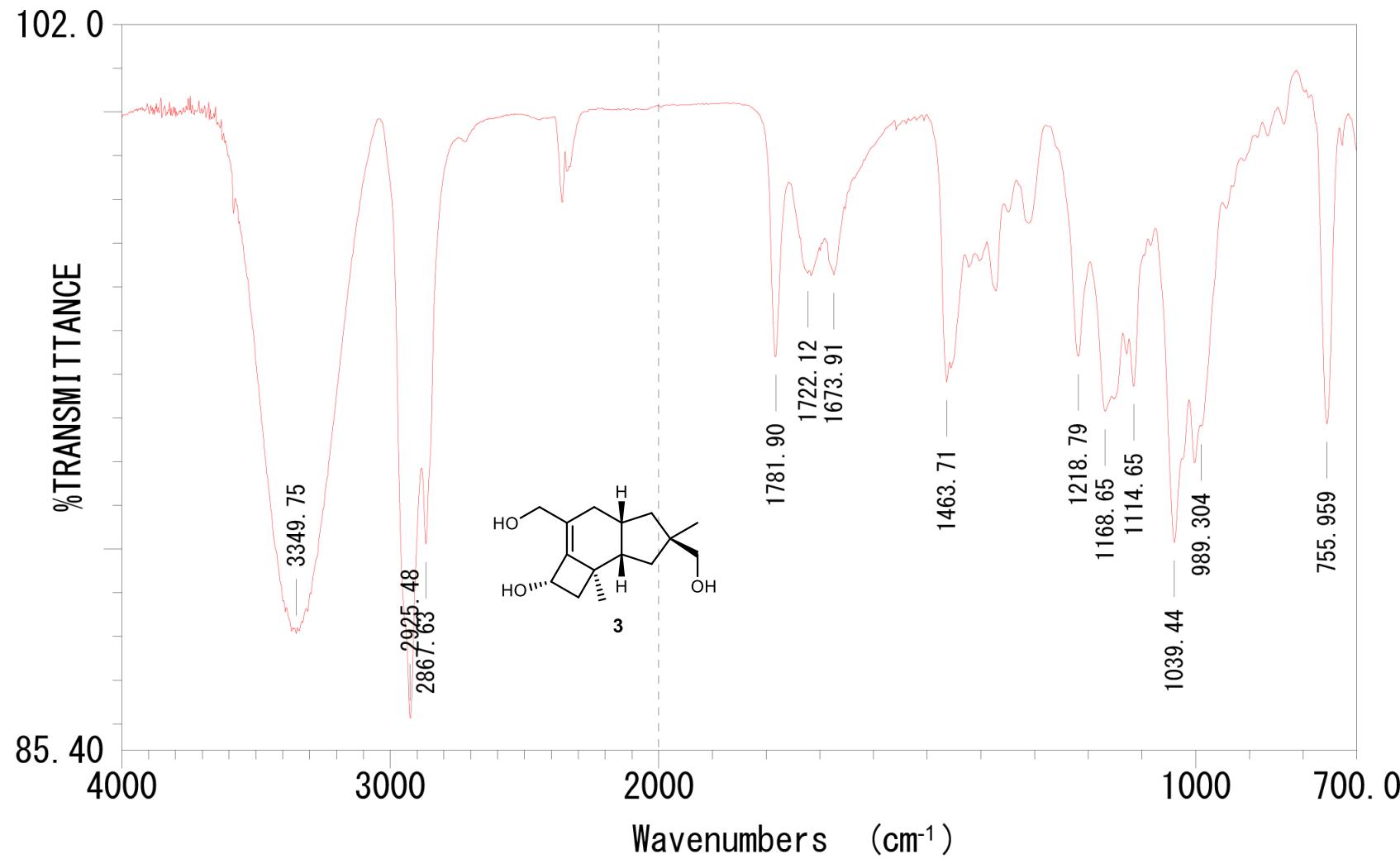
<sup>13</sup>C NMR spectrum of **2b** (125 MHz, CDCl<sub>3</sub>)



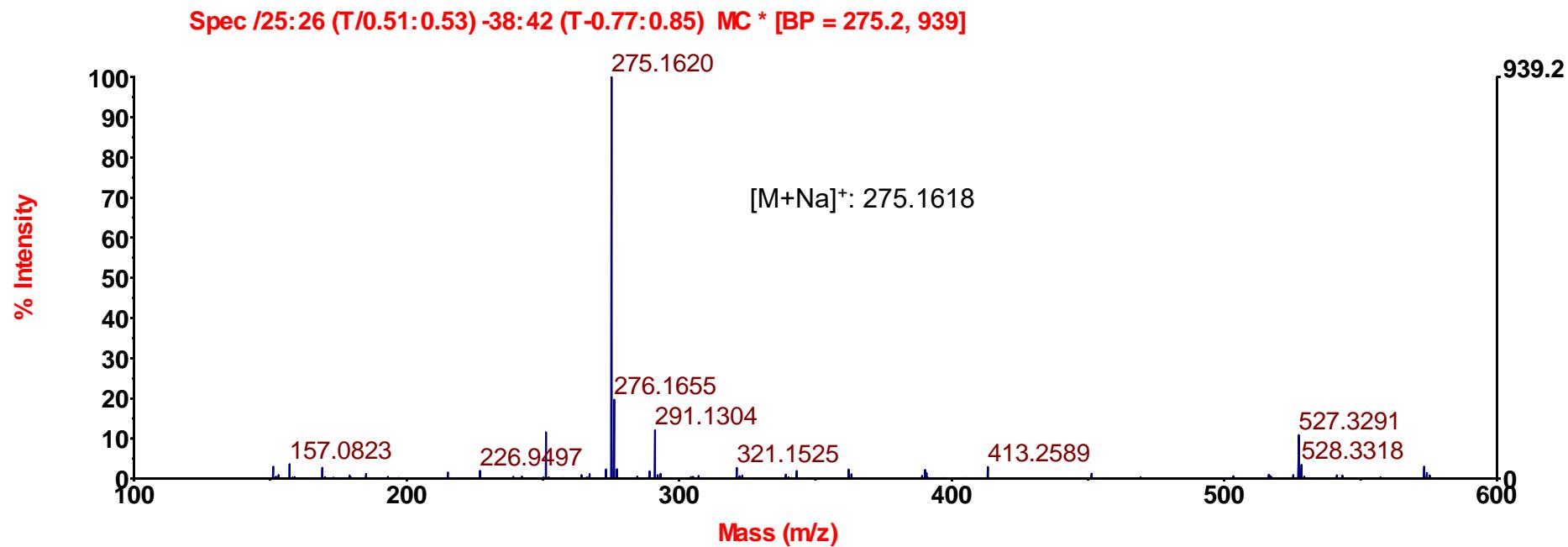
NOE 1D spectra of **2b** (500 MHz, CDCl<sub>3</sub>)



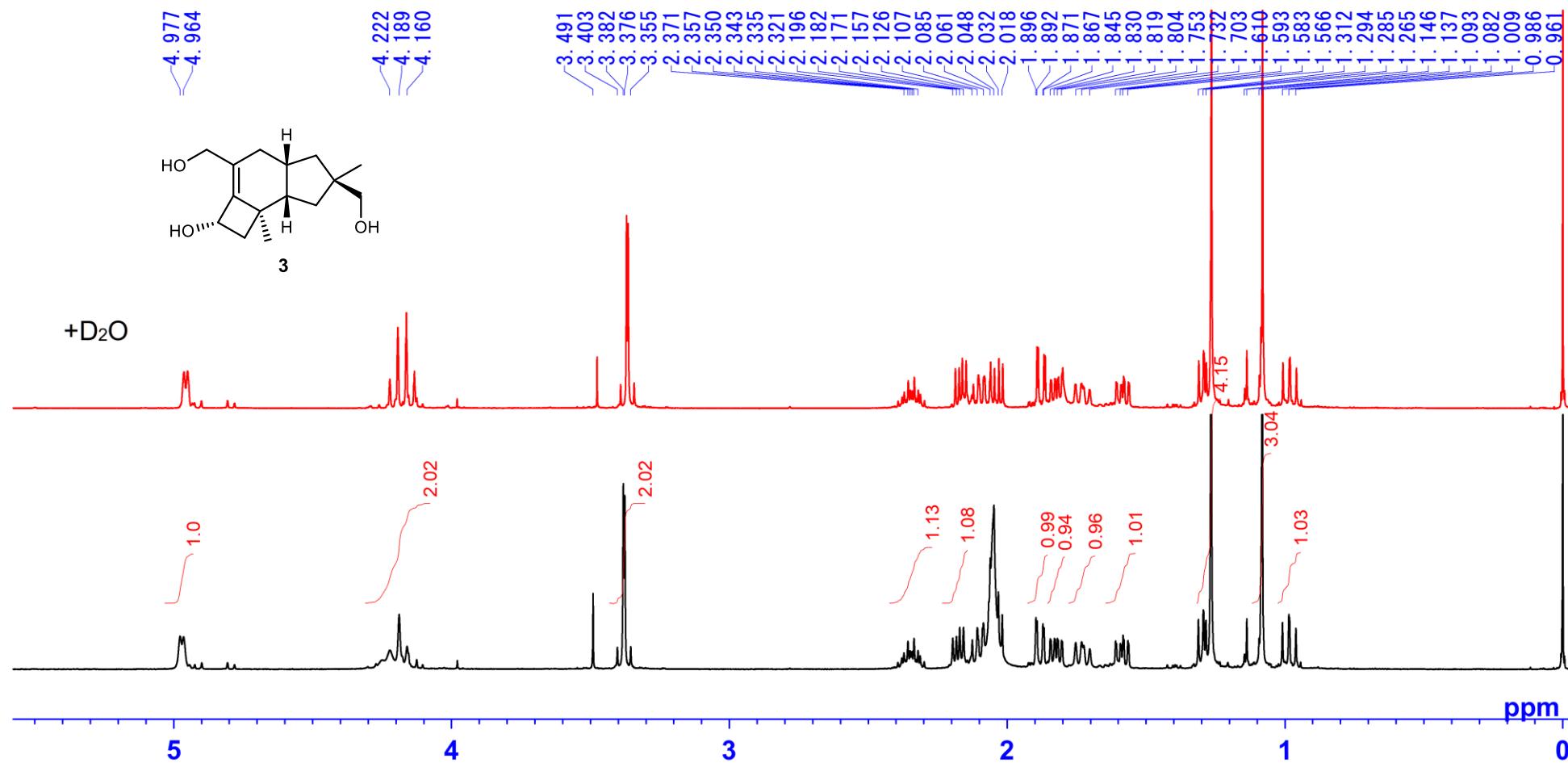
IR spectrum of **3** (film)



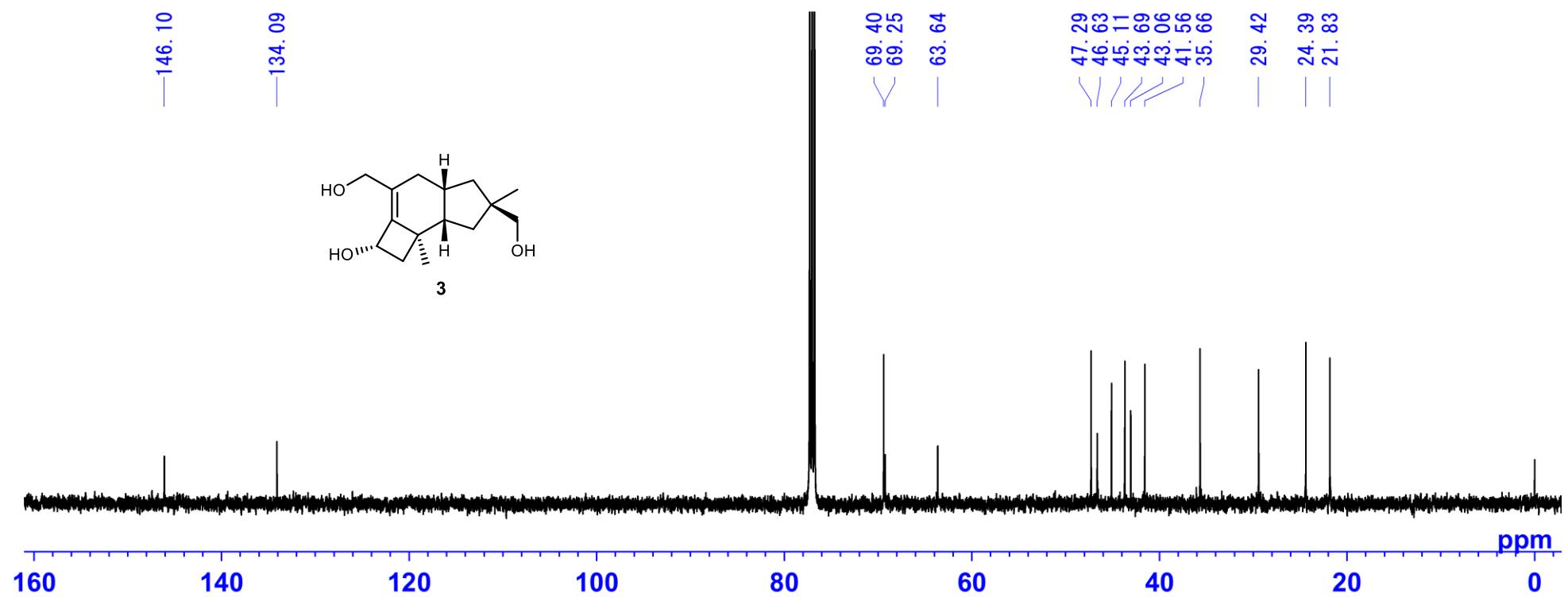
ESI-TOFMS spectrum of **3**.



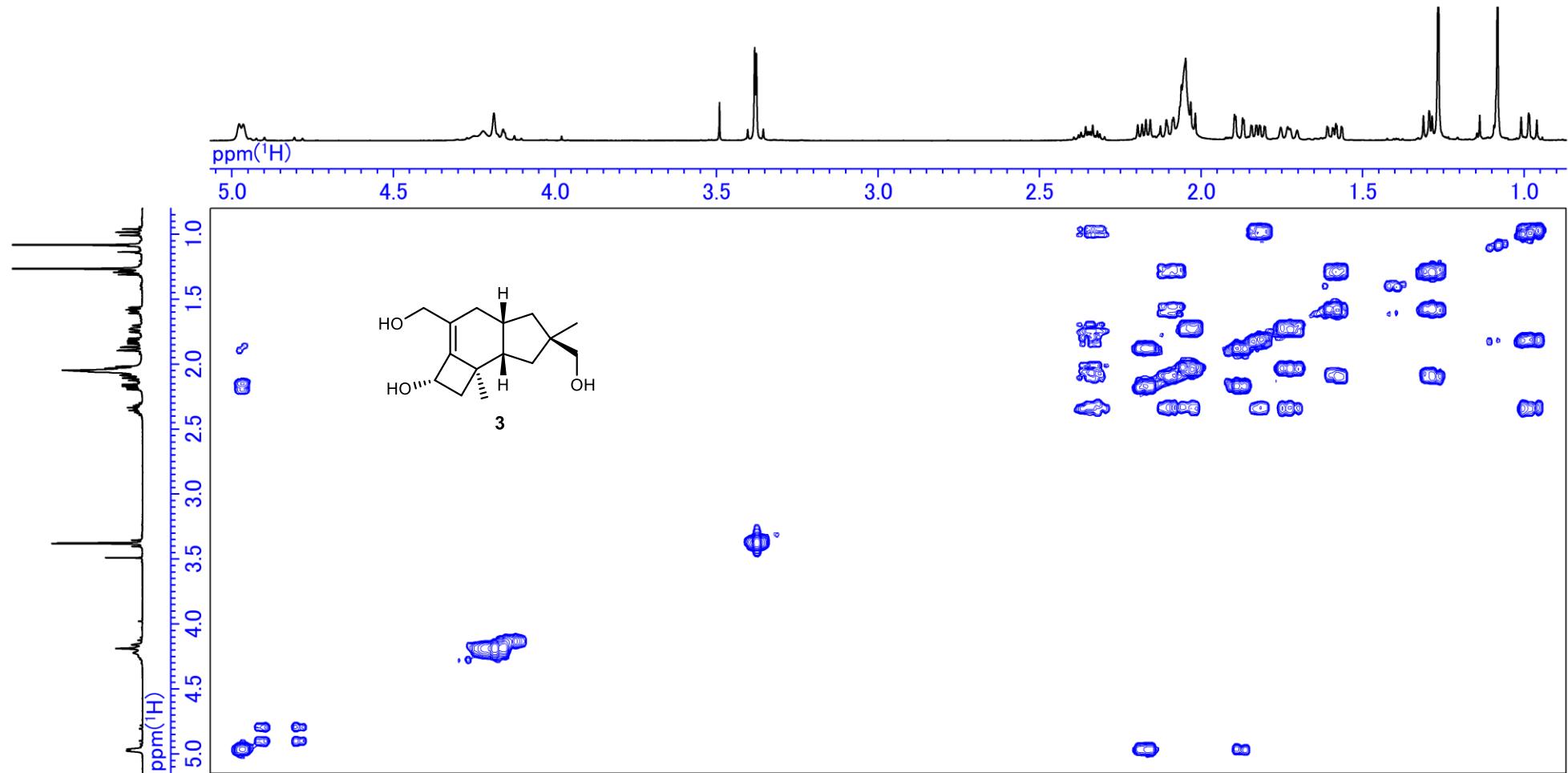
<sup>1</sup>H NMR spectrum of **3** (500 MHz, CDCl<sub>3</sub>)



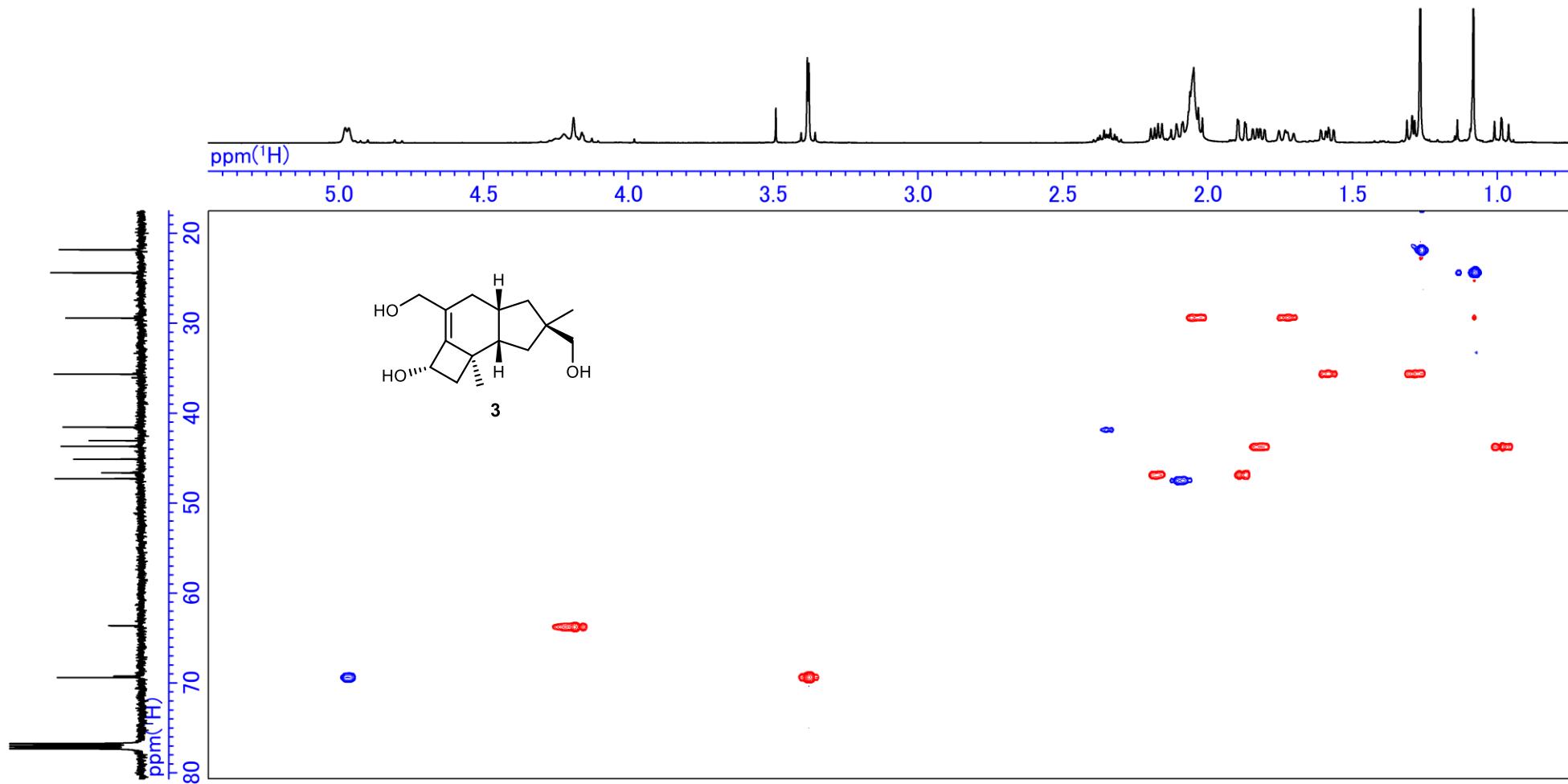
$^{13}\text{C}$  NMR spectrum of **3** (125 MHz,  $\text{CDCl}_3$ )



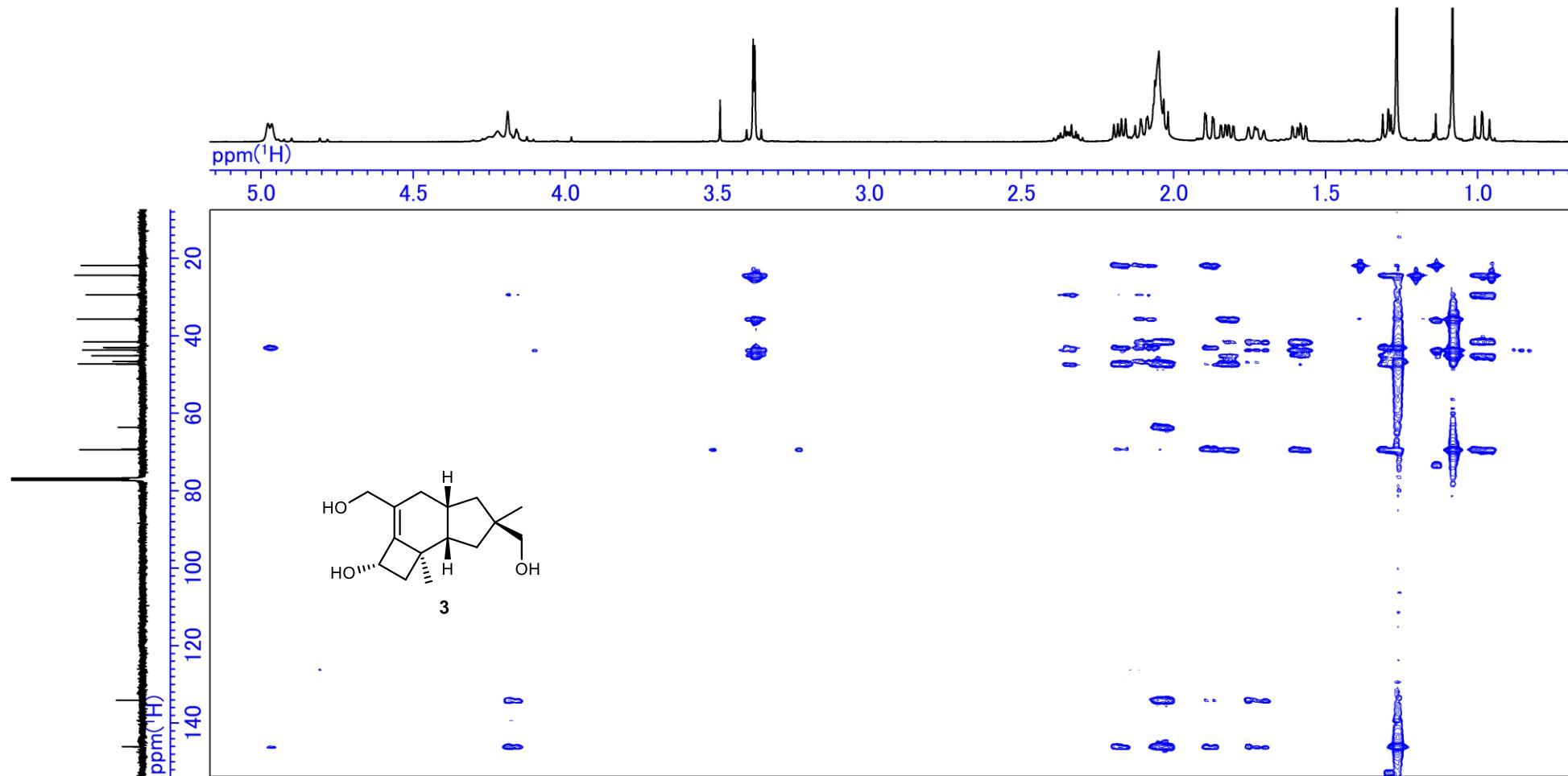
DQF COSY spectrum of **3** (500 MHz, CDCl<sub>3</sub>)



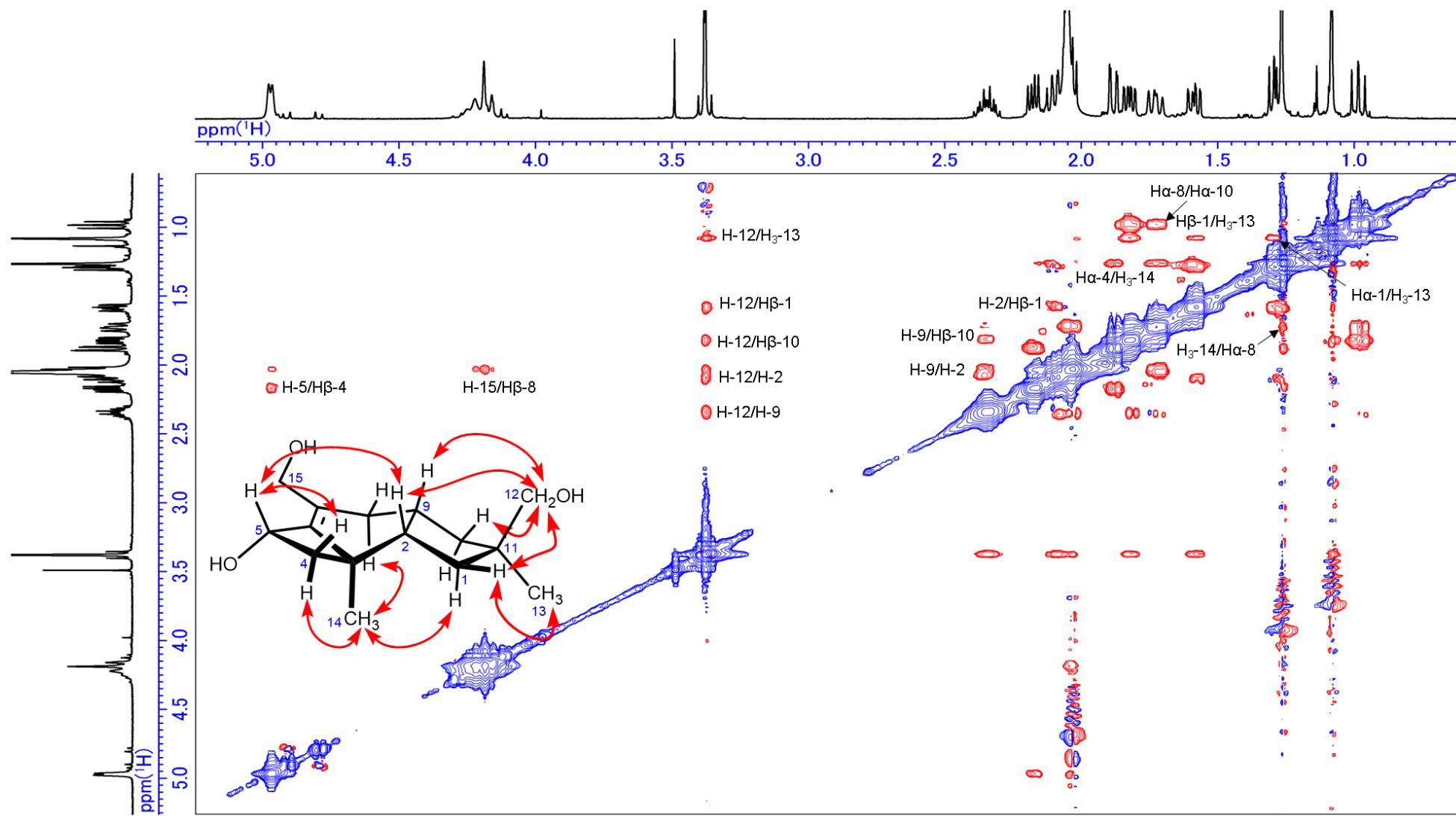
HSQC spectrum of **3** (500 MHz, CDCl<sub>3</sub>)



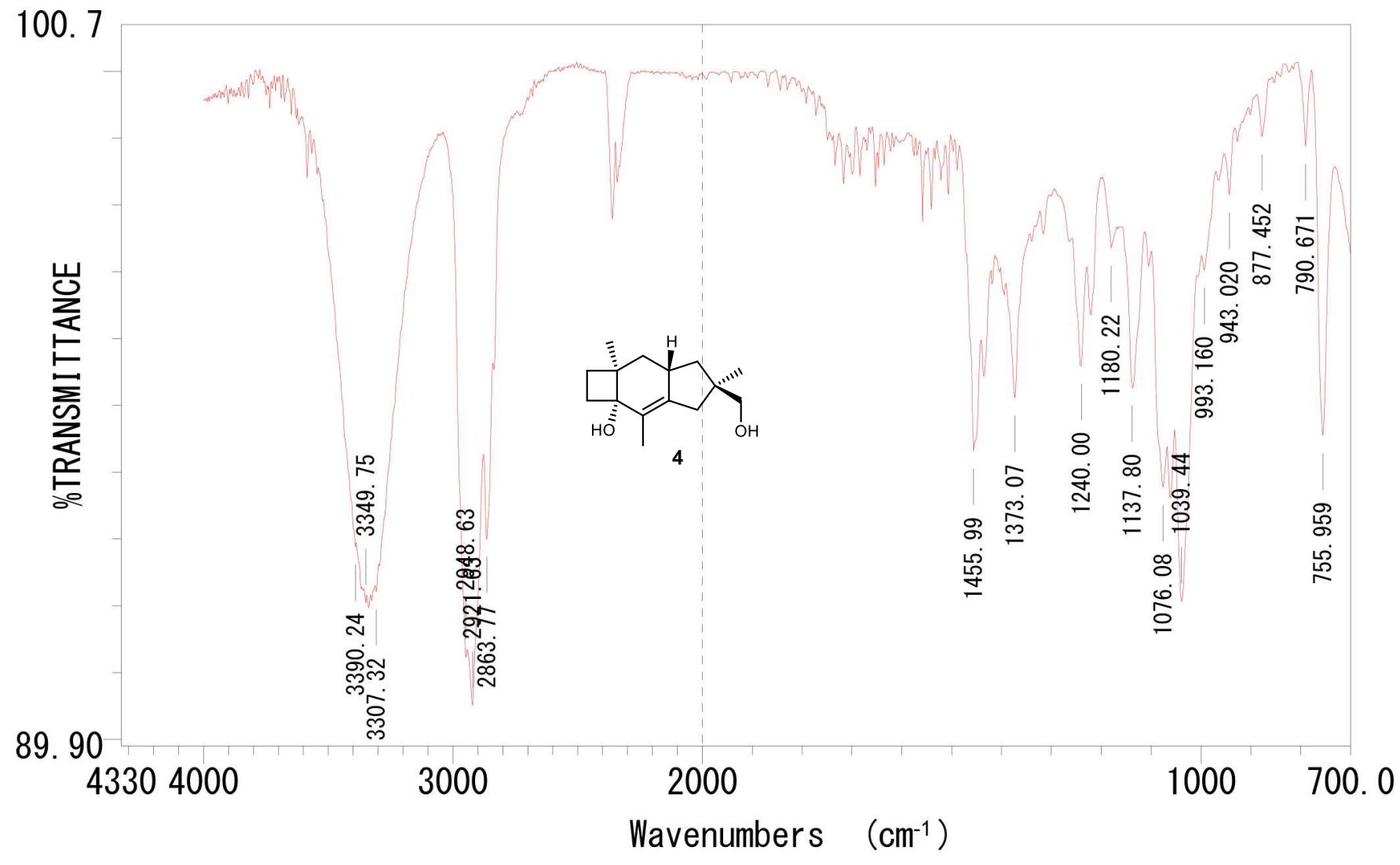
HMBC spectrum of **3** (500 MHz, CDCl<sub>3</sub>)



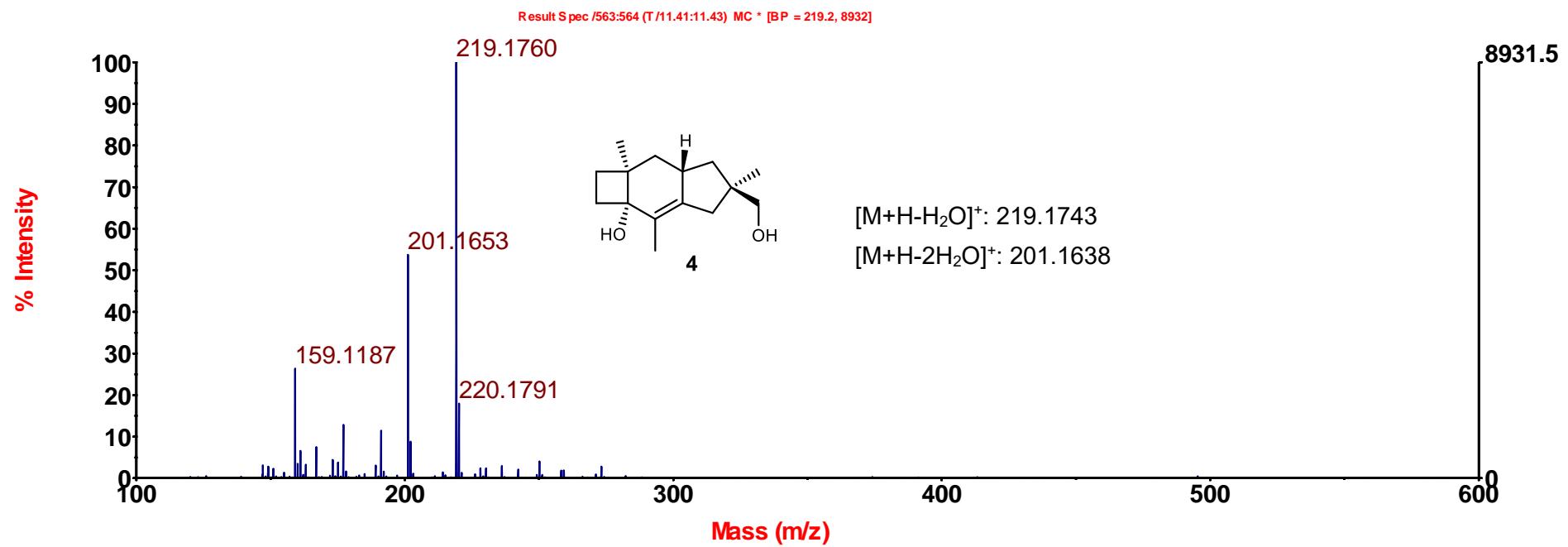
NOESY spectrum of **3** (500 MHz,  $\text{CDCl}_3$ )



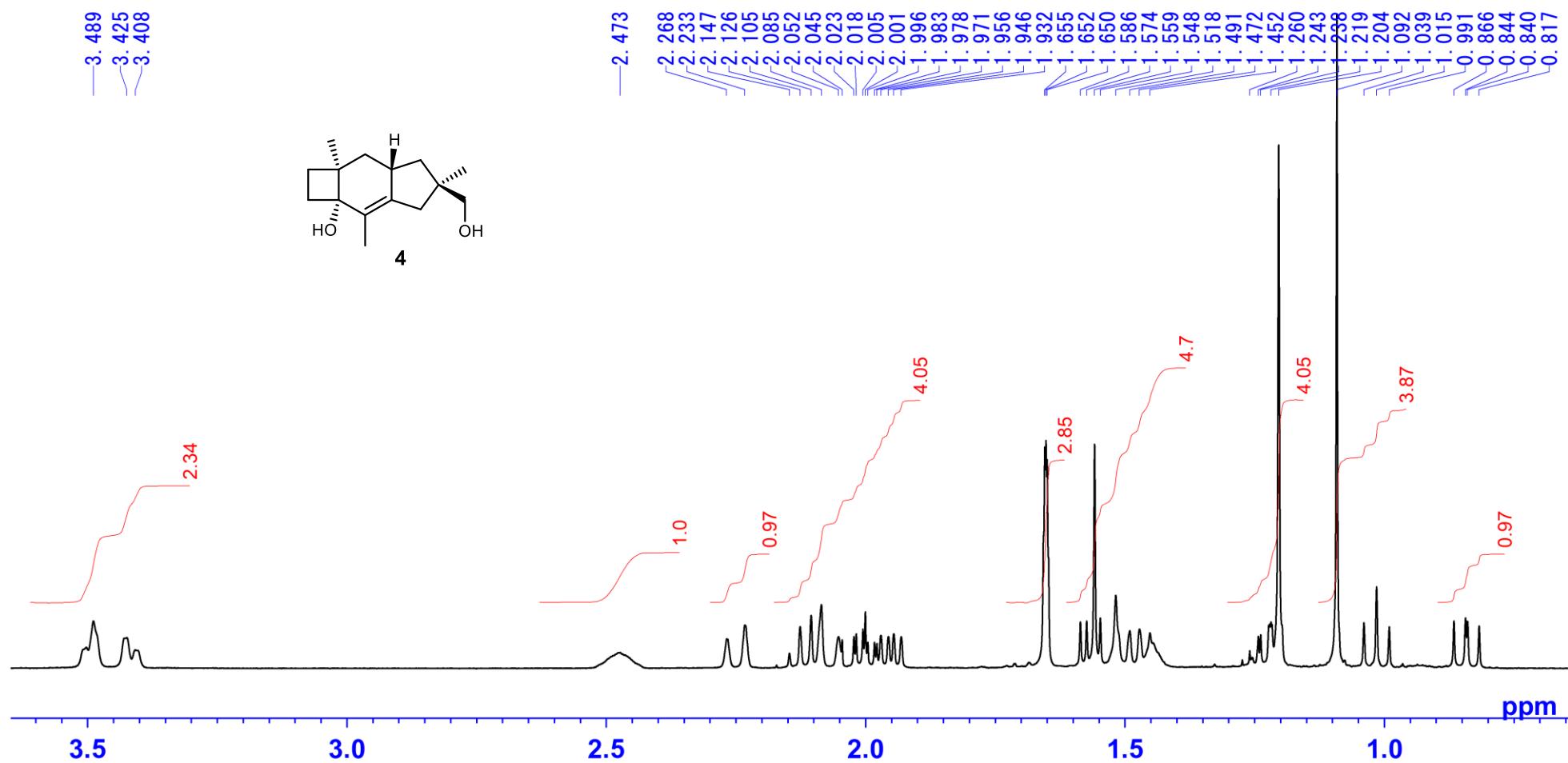
IR spectrum of **4** (film)



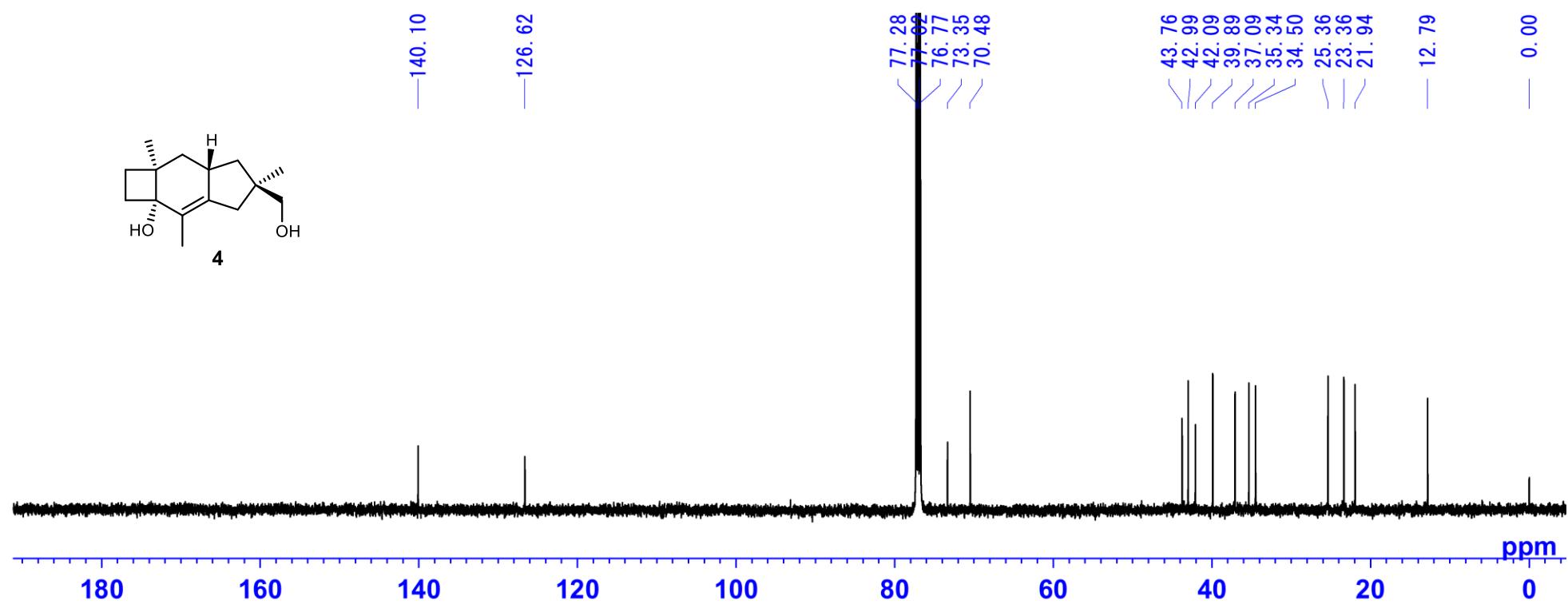
ESI-TOFMS spectrum of **4**.



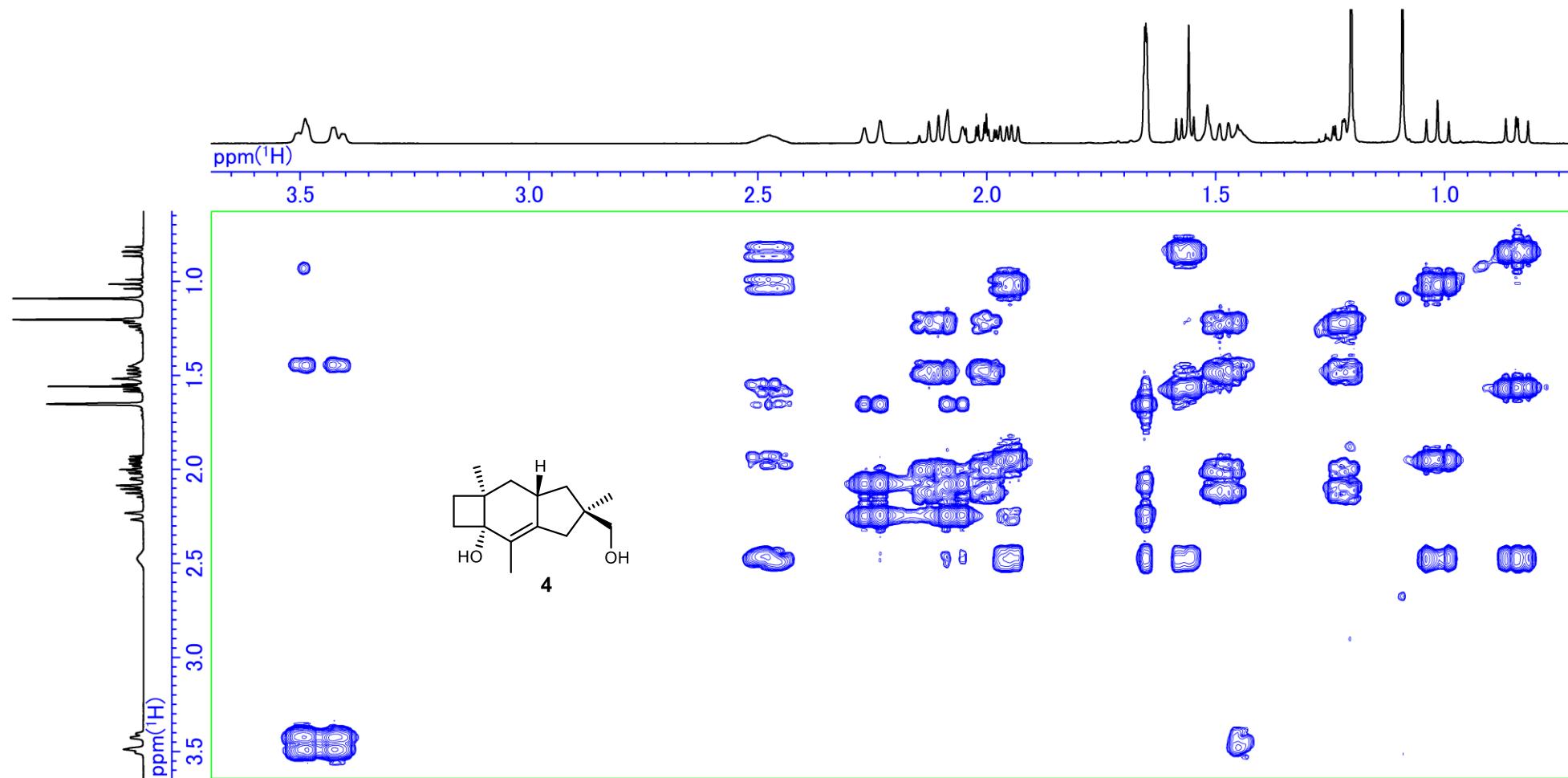
<sup>1</sup>H NMR spectrum of **4** (500 MHz, CDCl<sub>3</sub>)



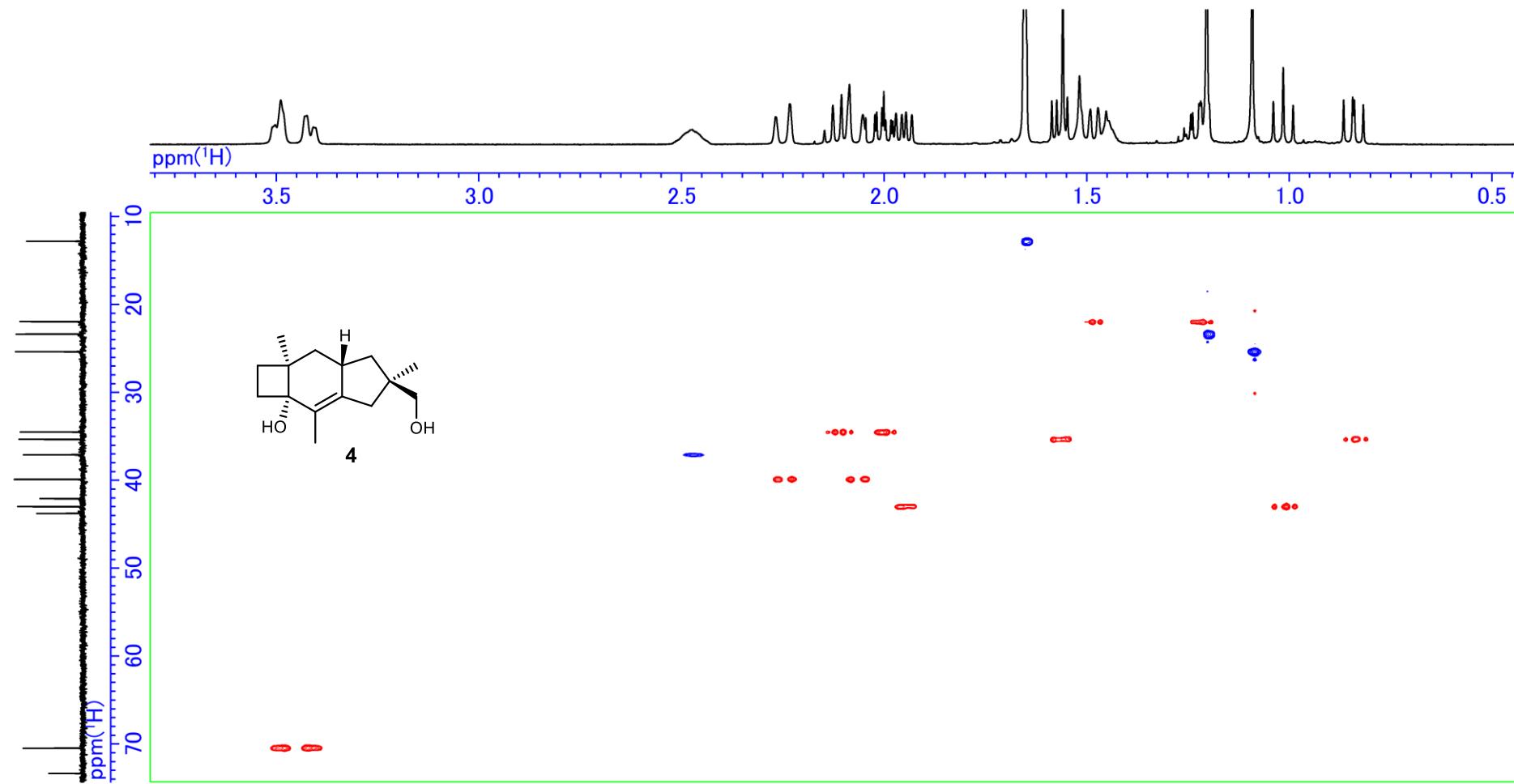
$^{13}\text{C}$  NMR spectrum of **4** (125 MHz,  $\text{CDCl}_3$ )



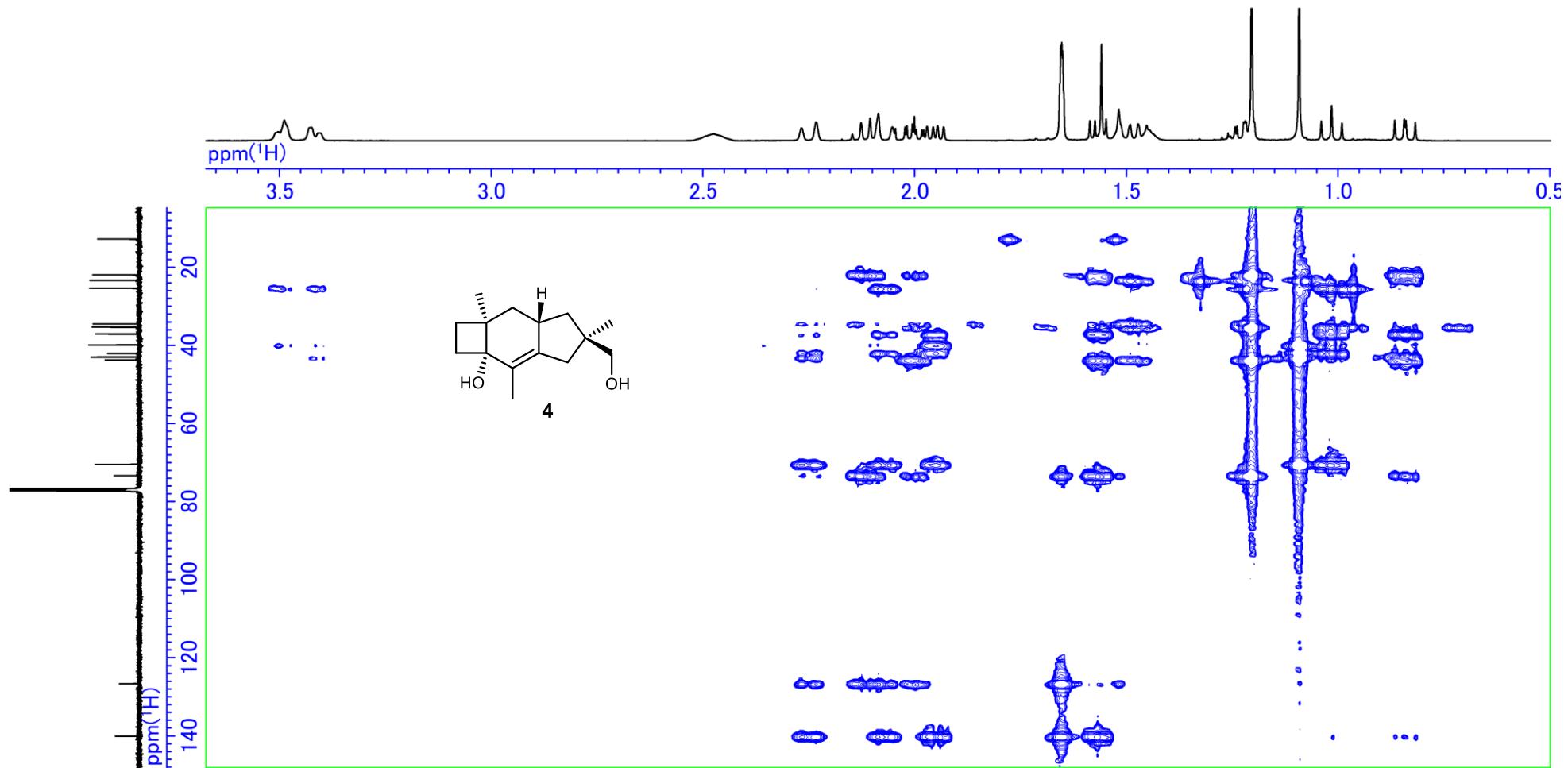
DQF COSY spectrum of **4** (500 MHz, CDCl<sub>3</sub>)



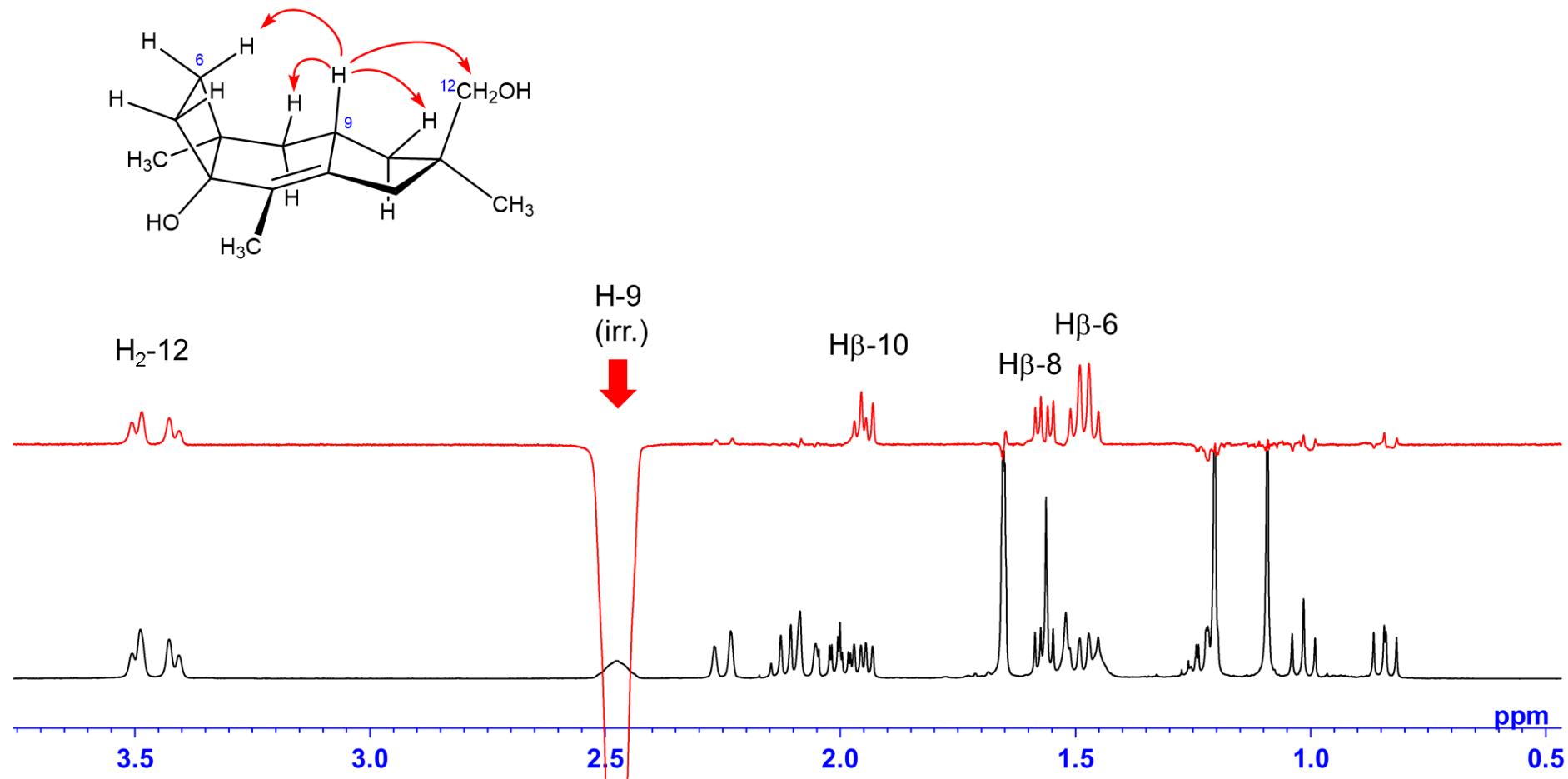
HSQC spectrum of **4** (500 MHz,  $\text{CDCl}_3$ )



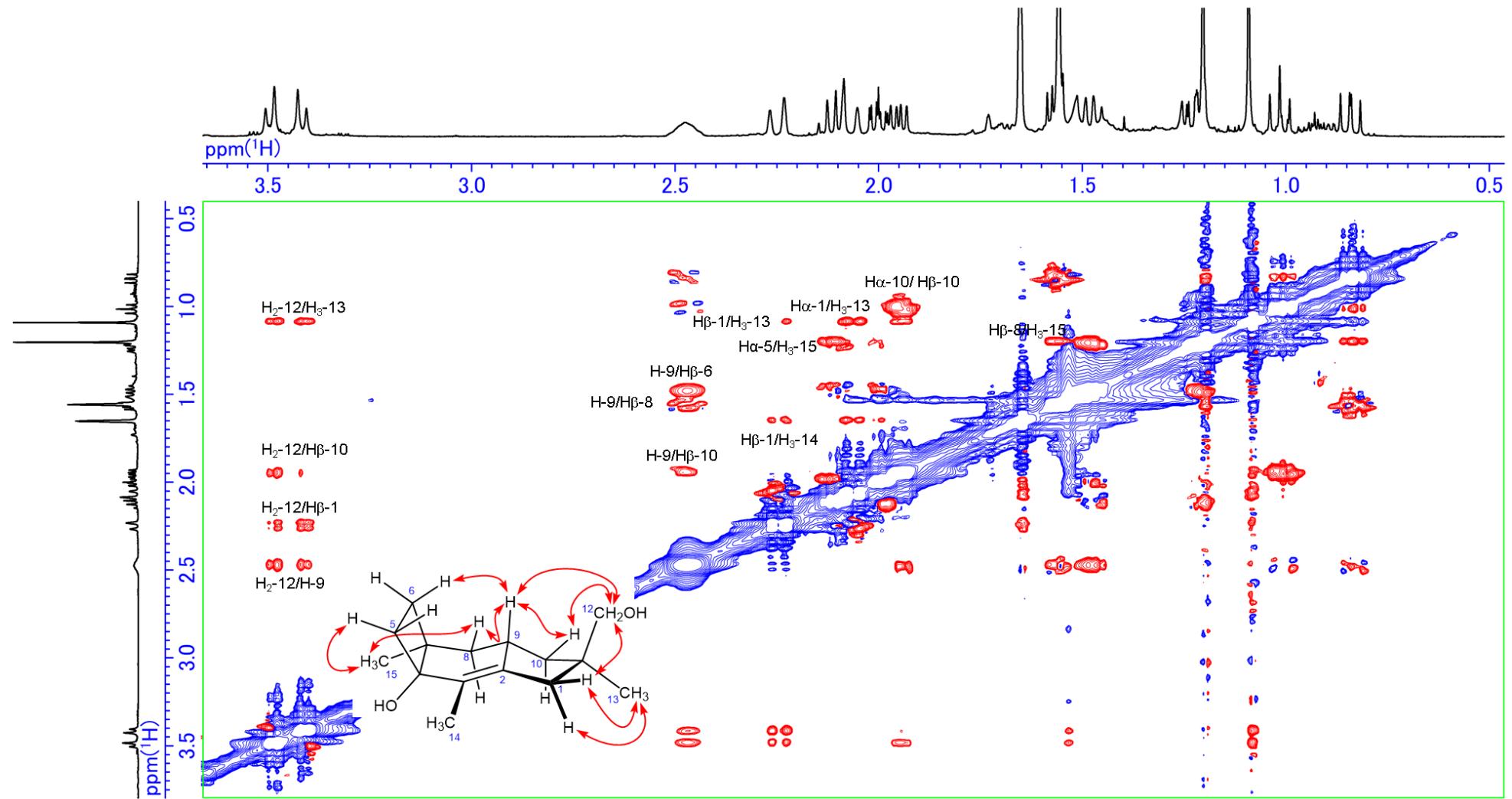
HMBC spectrum of **4** (500 MHz, CDCl<sub>3</sub>)



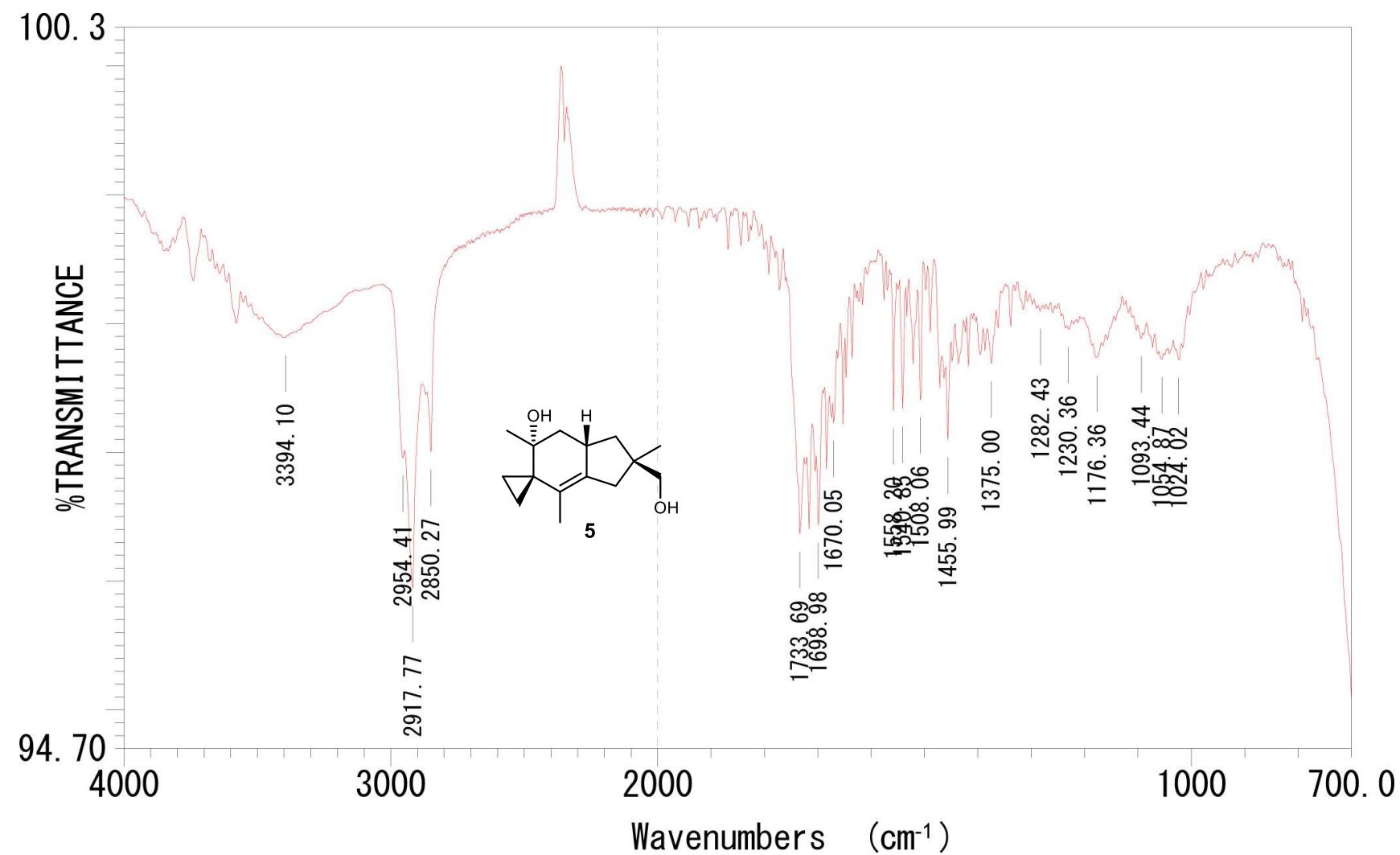
NOE 1D spectra of **4** (500 MHz,  $\text{CDCl}_3$ )



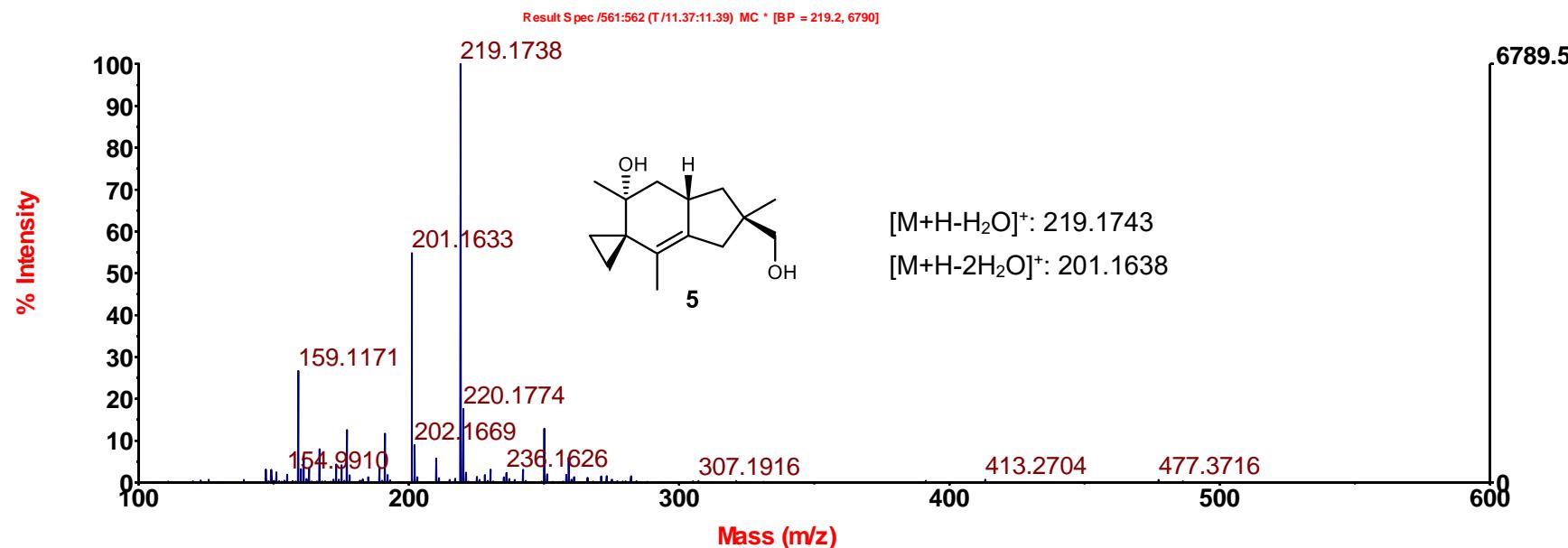
NOESY spectrum of **4** (500 MHz,  $\text{CDCl}_3$ )



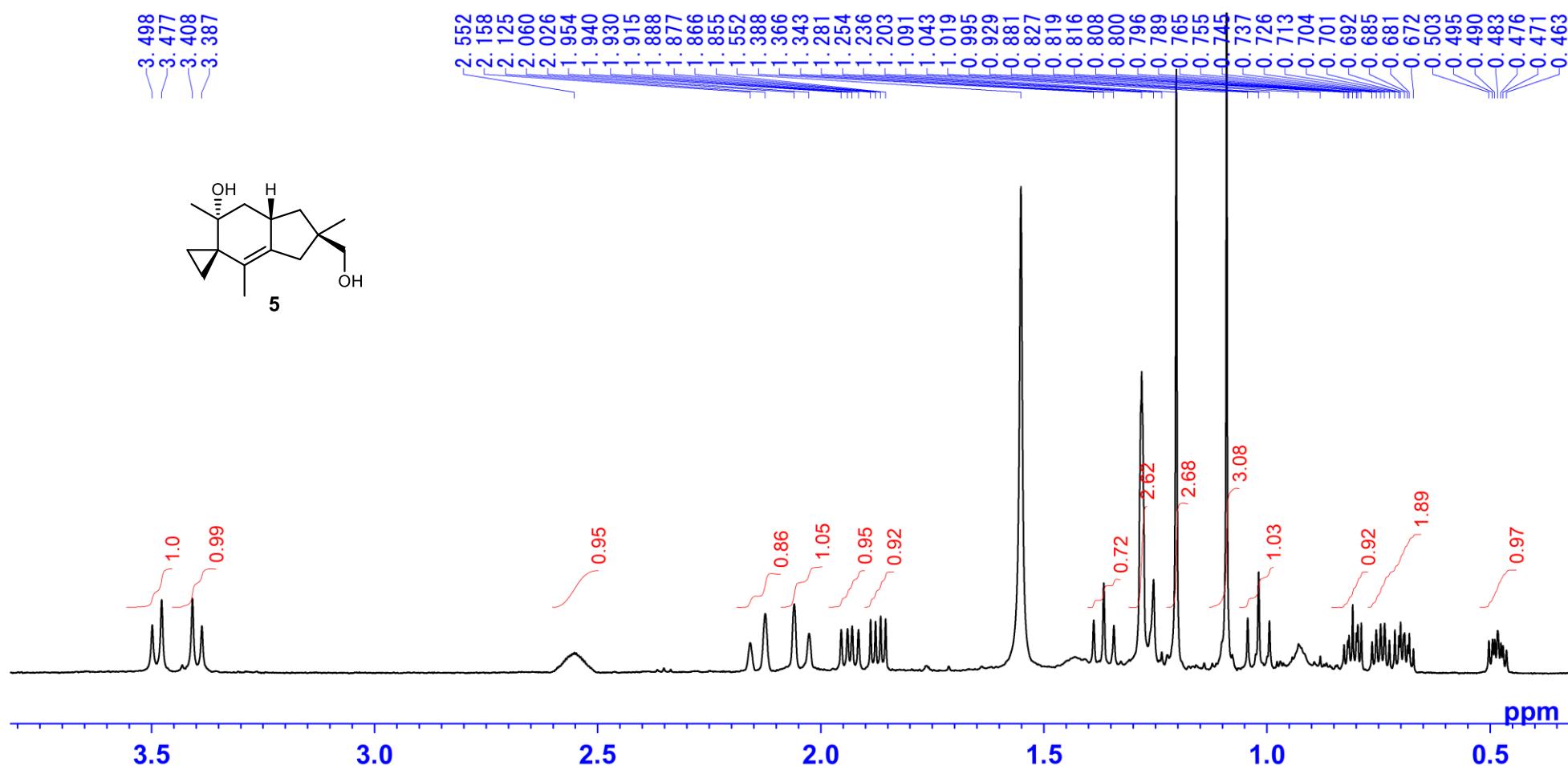
IR spectrum of **5** (film)



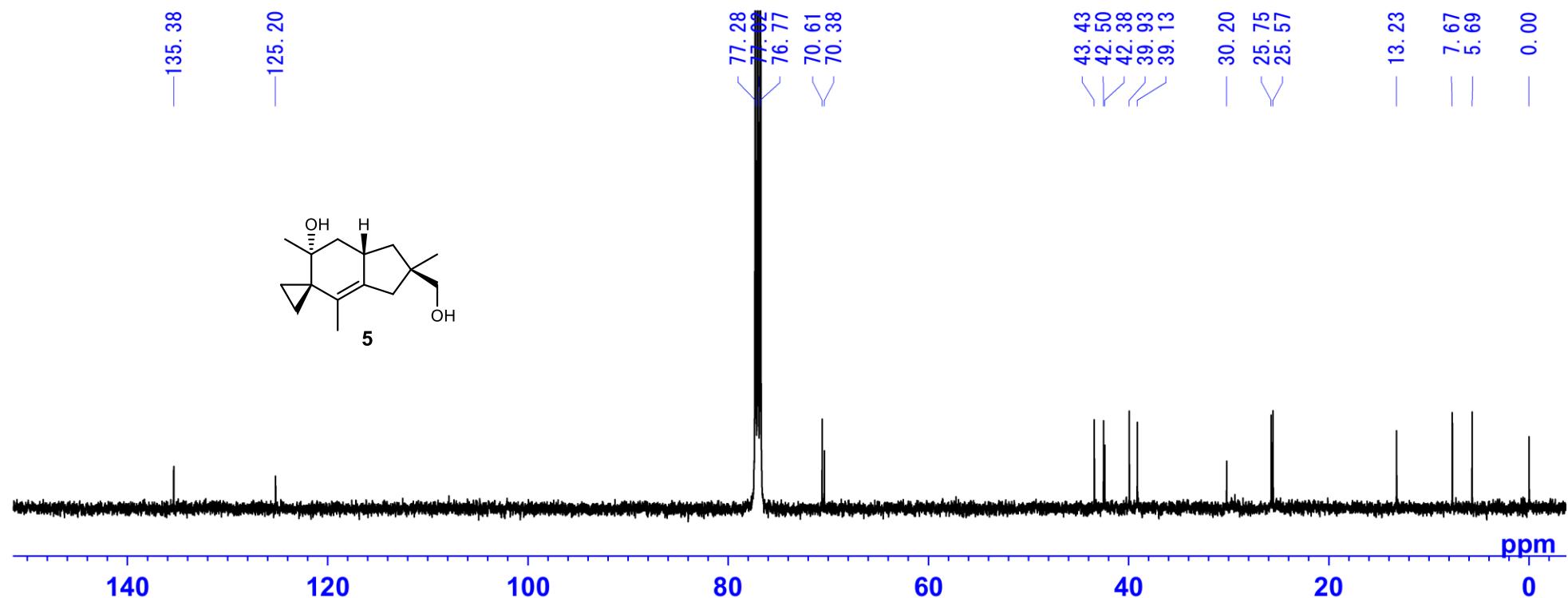
ESI-TOFMS spectrum of **5**.



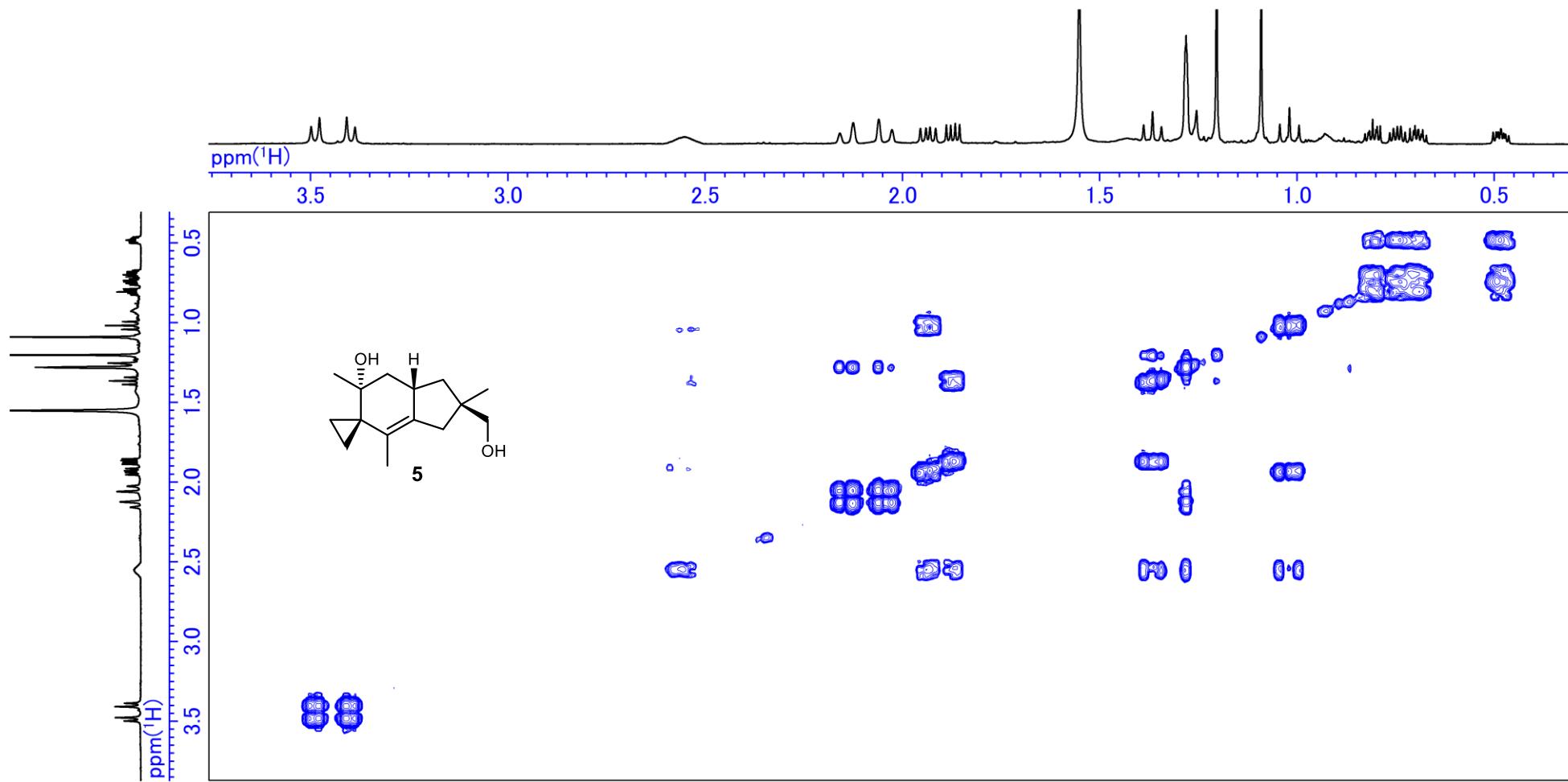
<sup>1</sup>H NMR spectrum of **5** (500 MHz, CDCl<sub>3</sub>)



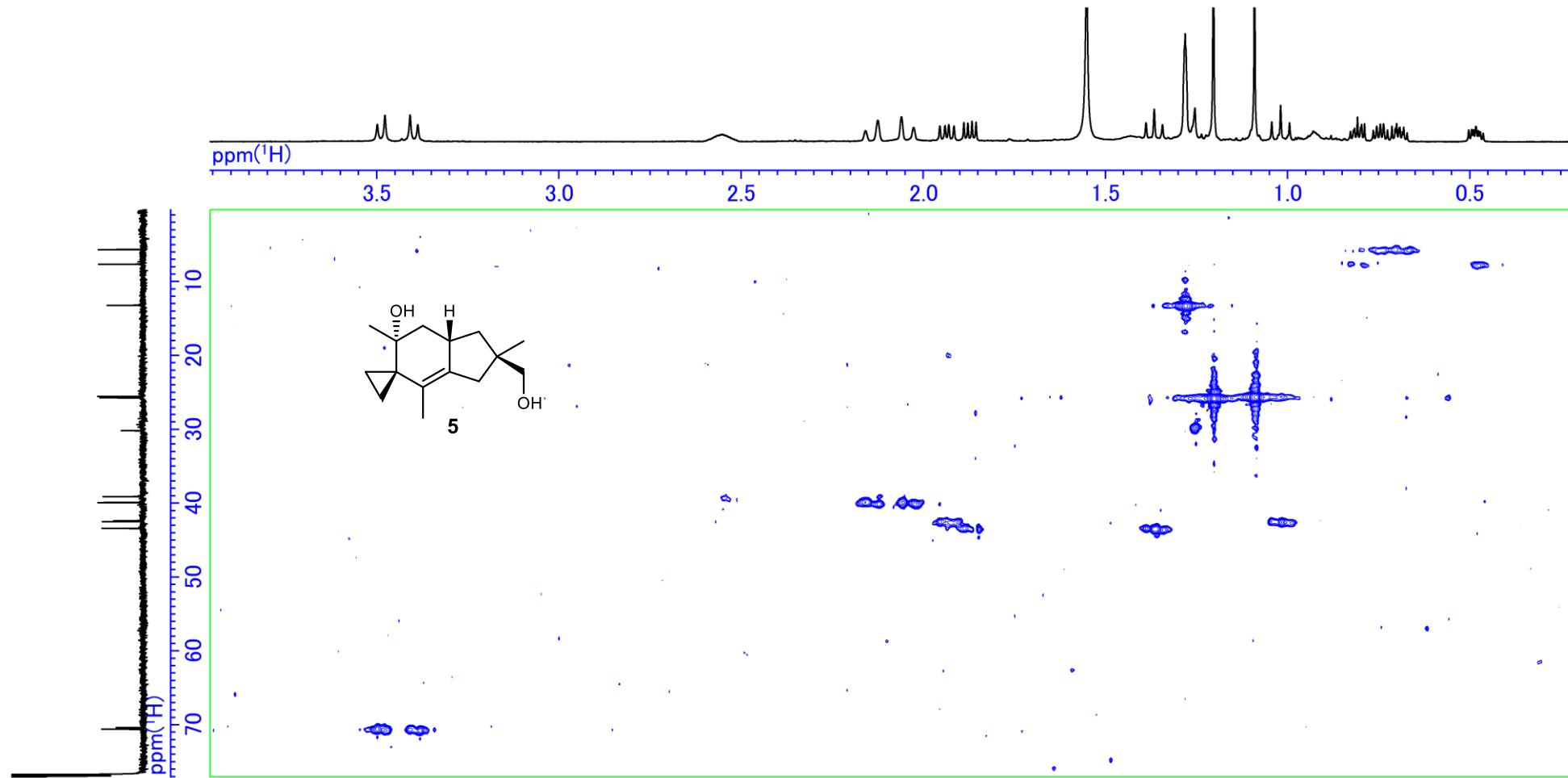
$^{13}\text{C}$  NMR spectrum of **5** (125 MHz,  $\text{CDCl}_3$ )



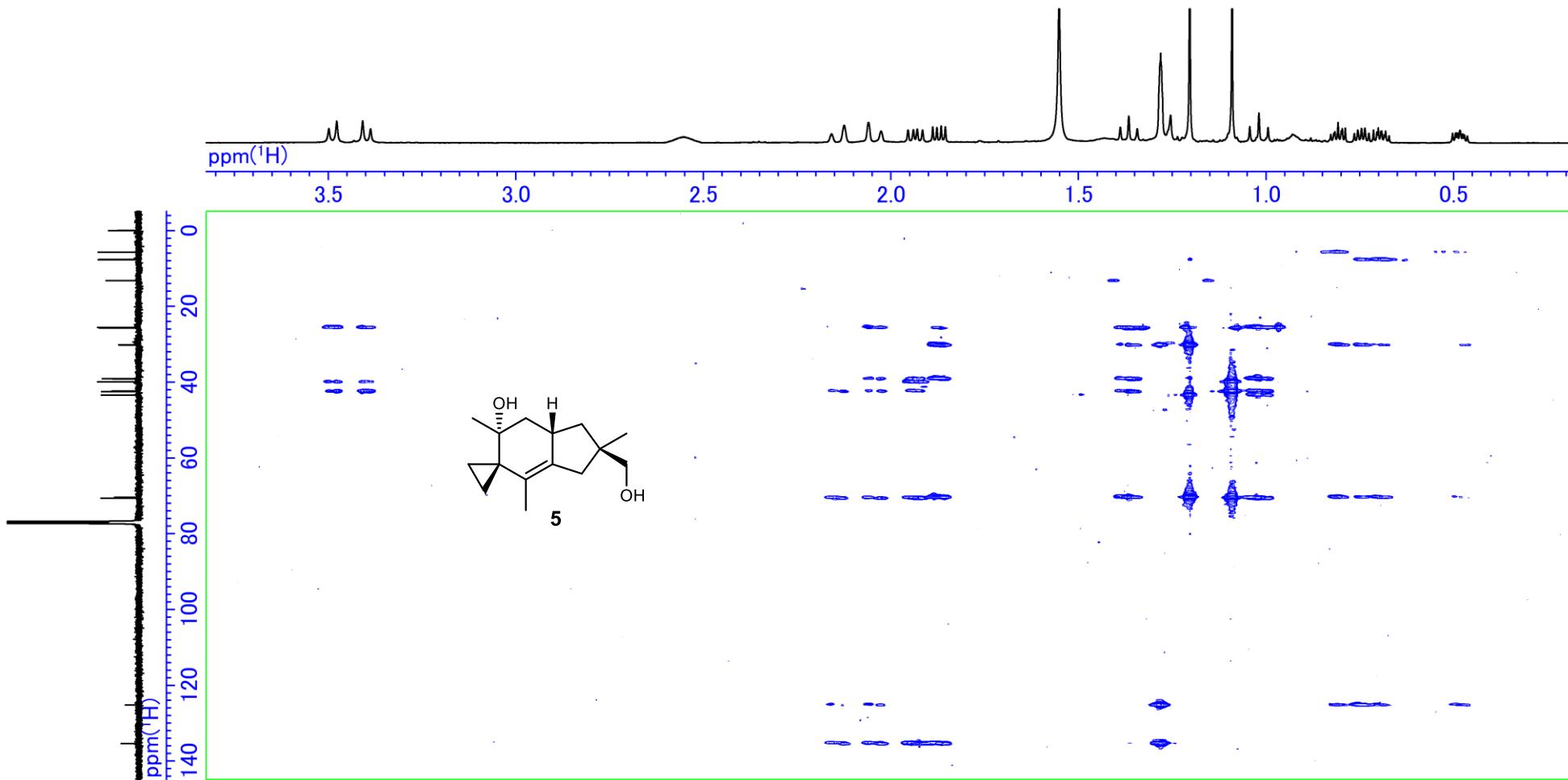
DQF COSY spectrum of **5** (500 MHz, CDCl<sub>3</sub>)



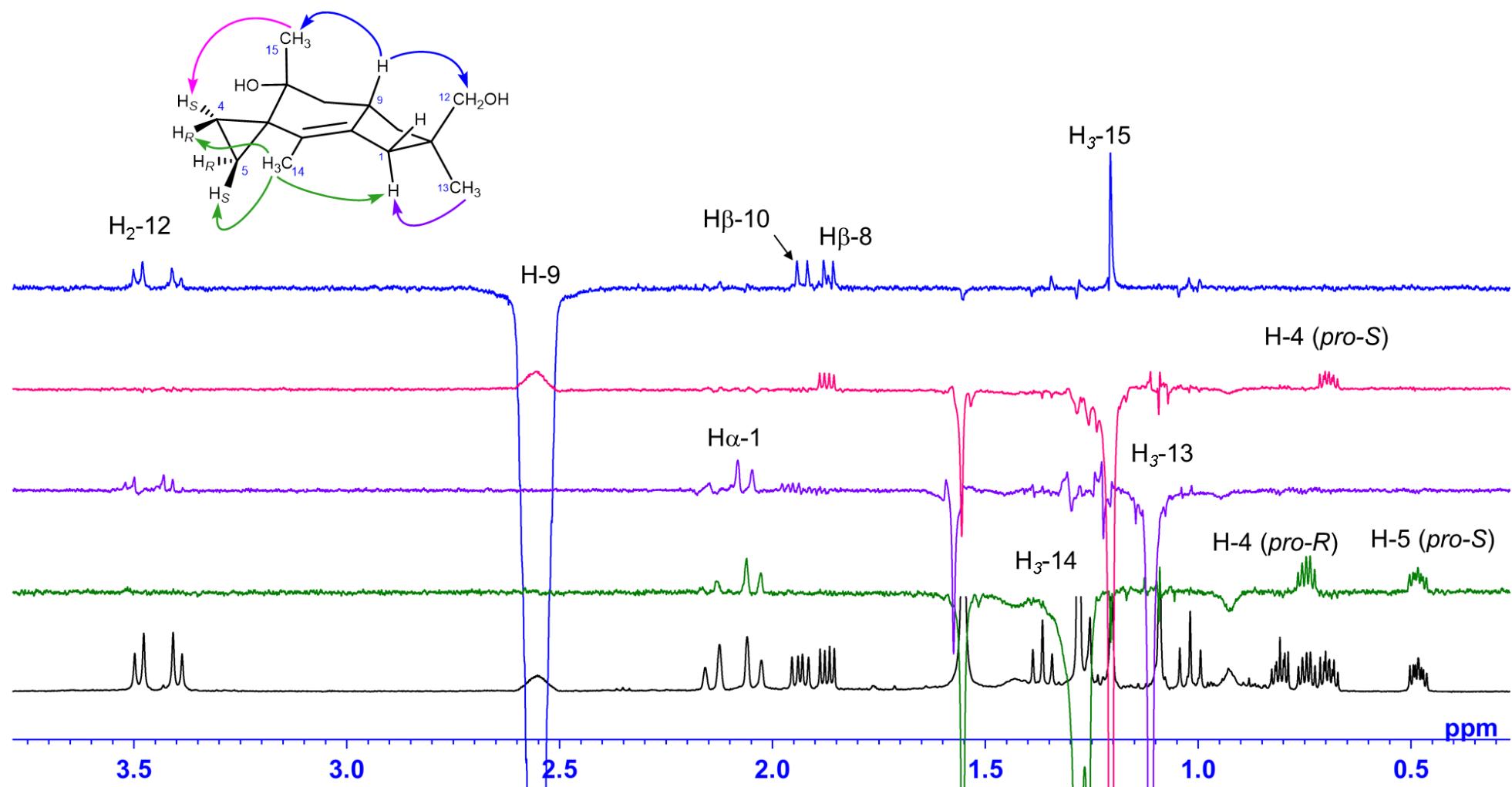
HMQC spectrum of **5** (500 MHz, CDCl<sub>3</sub>)



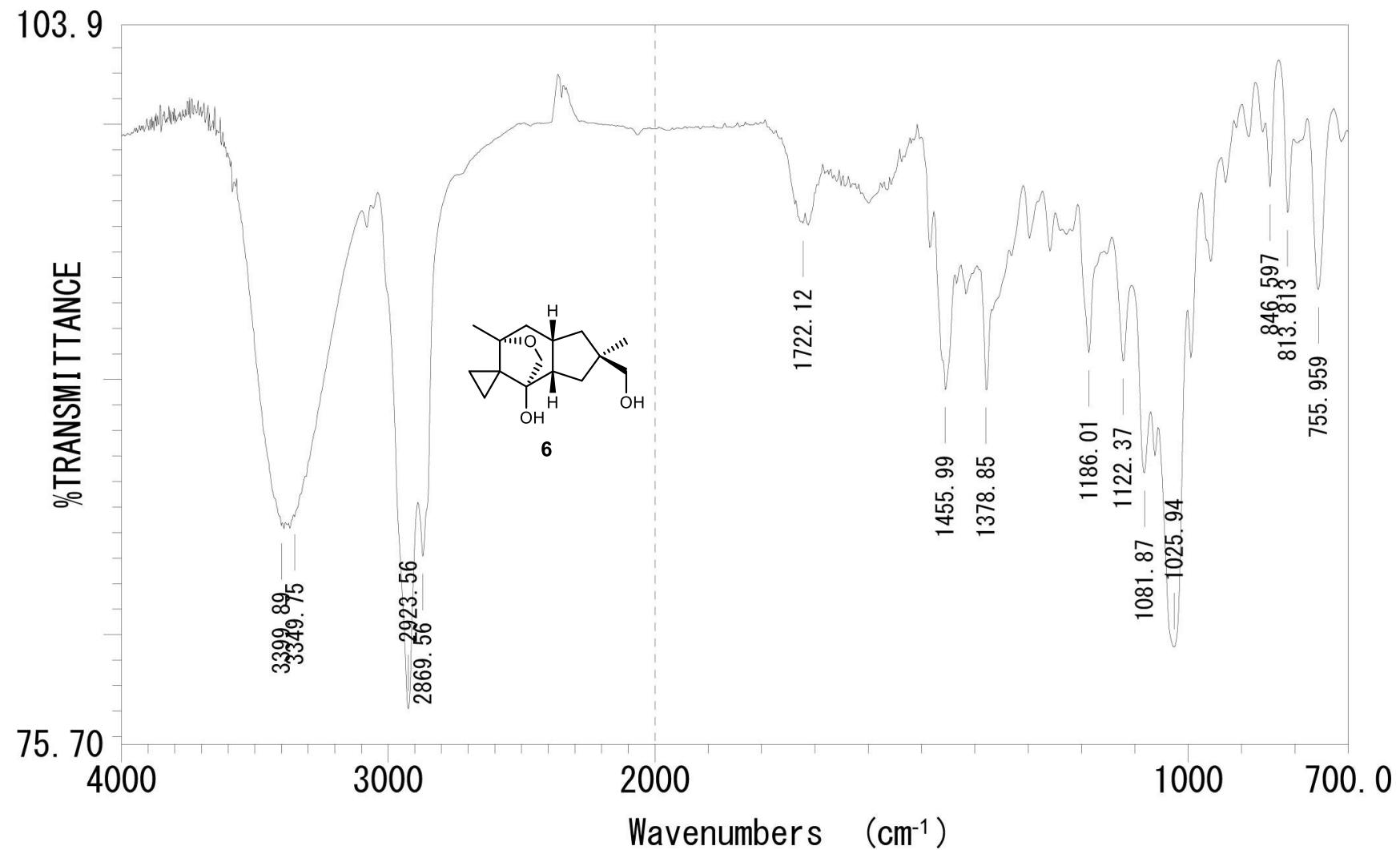
HMBC spectrum of **5** (500 MHz, CDCl<sub>3</sub>)



NOE 1D spectra of **5** (500 MHz,  $\text{CDCl}_3$ )

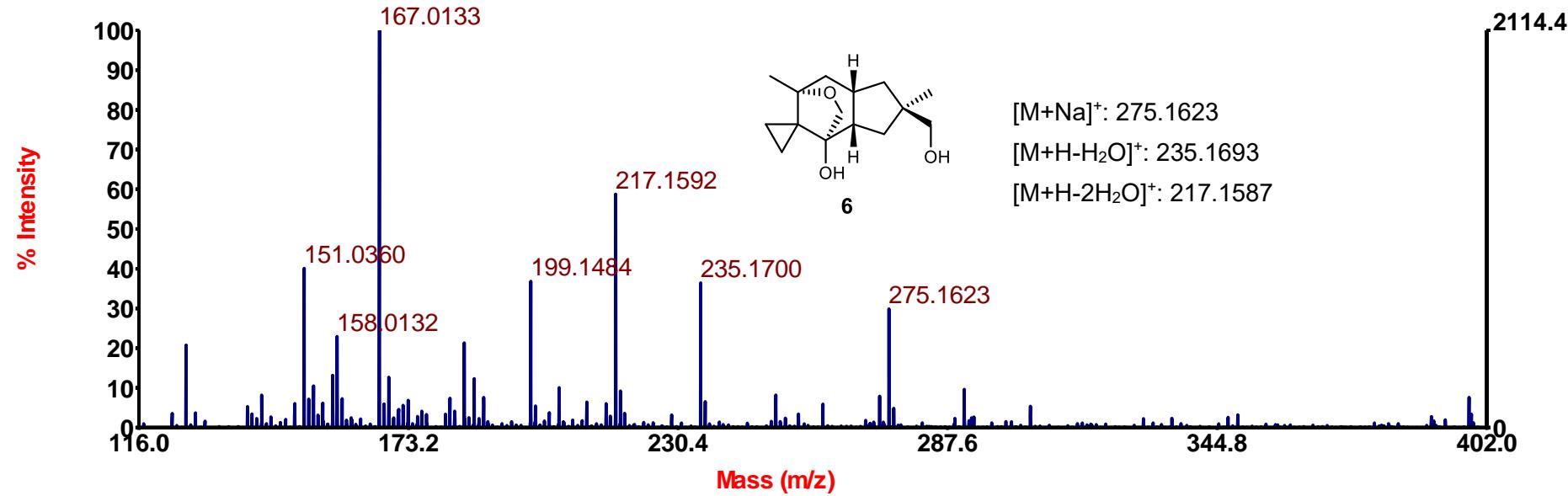


IR spectrum of **6** (film)

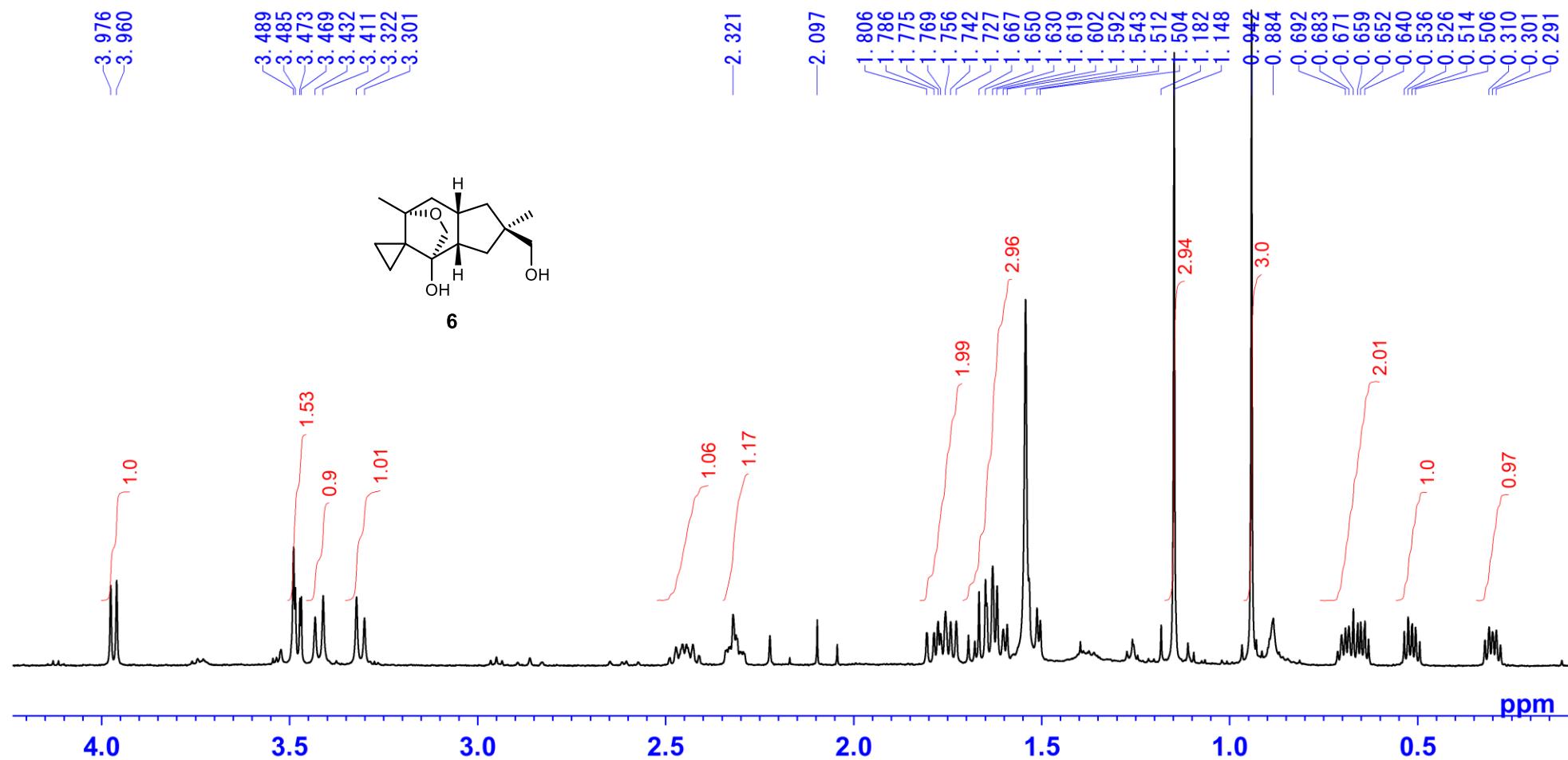


ESI-TOFMS spectrum of 6

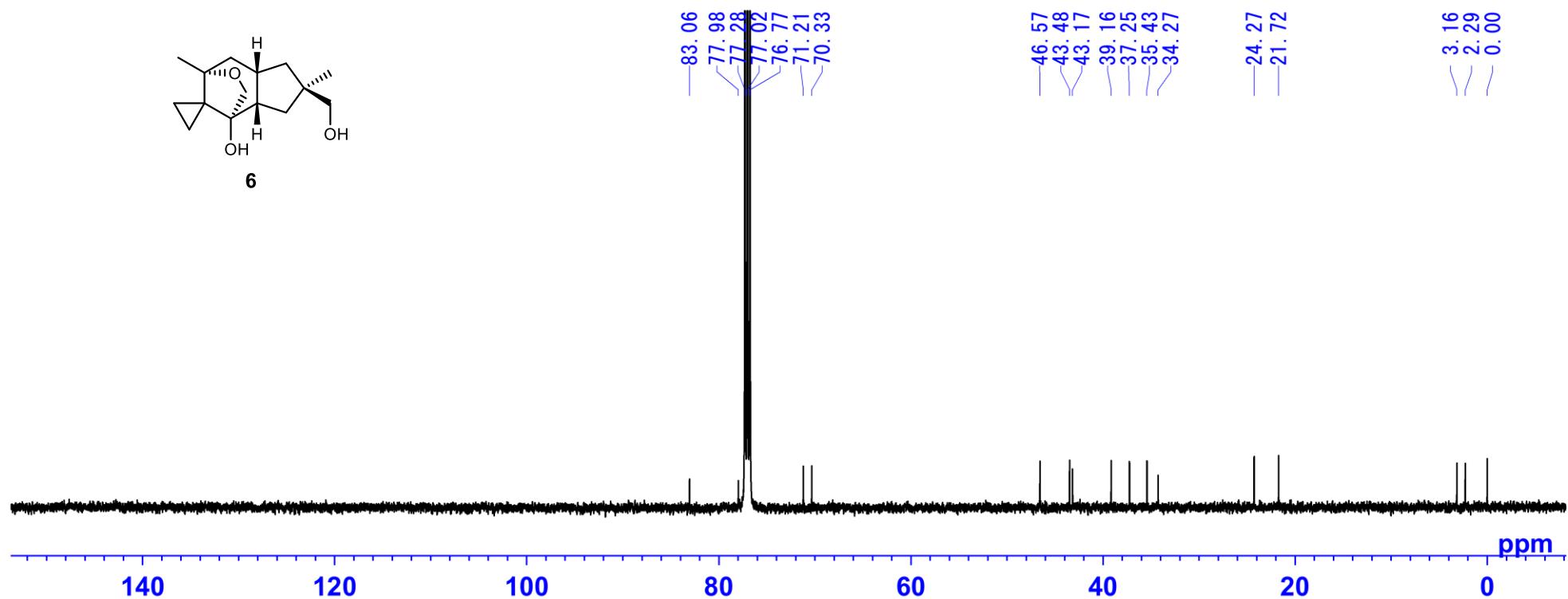
Result Spec /34:36 (T/0.69:0.73) -42:49 (T-0.85:0.99) MC \* [BP = 167.0, 2114]



<sup>1</sup>H NMR spectrum of **6** (500 MHz, CDCl<sub>3</sub>)

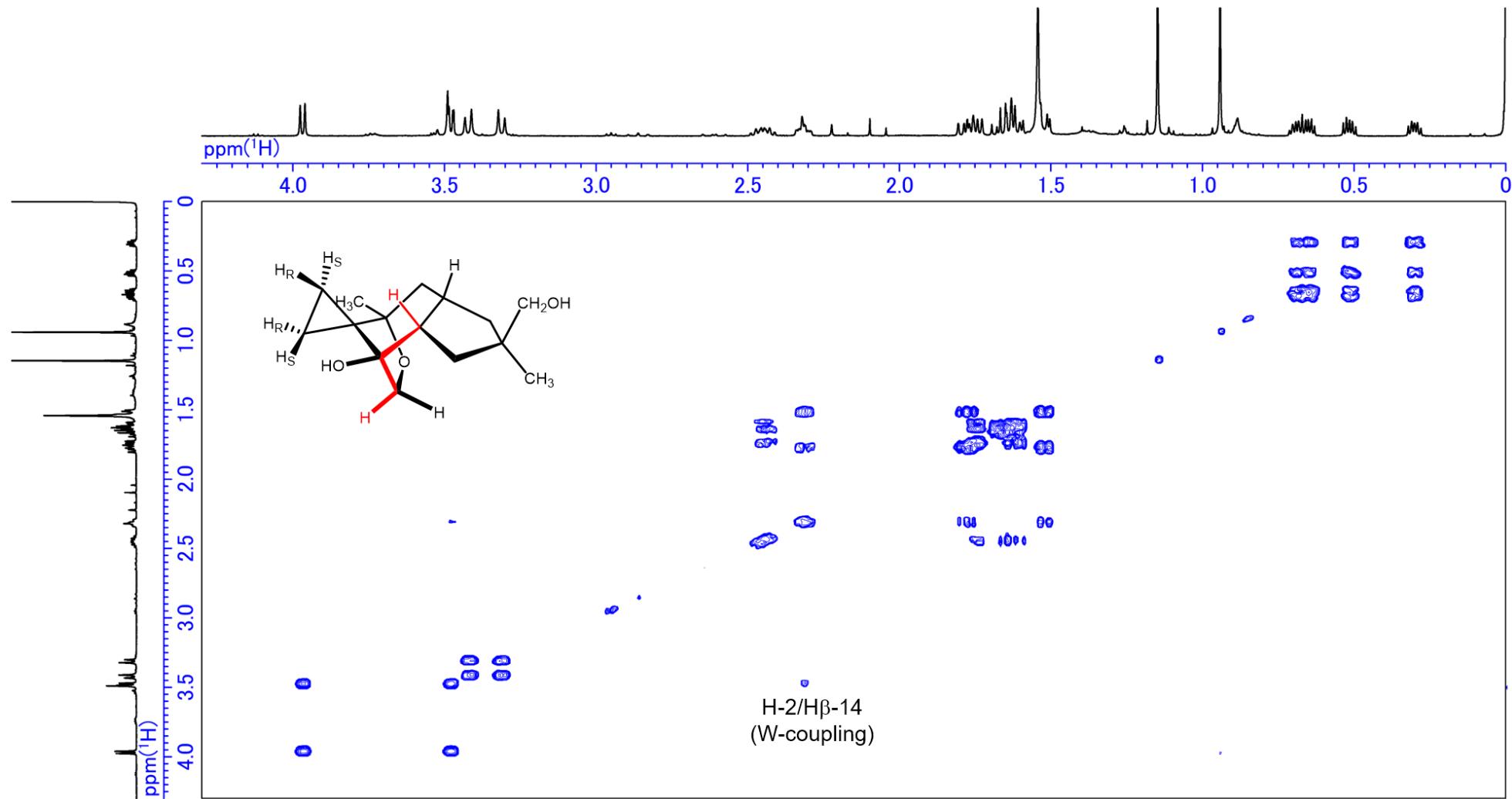


$^{13}\text{C}$  NMR spectrum of **6** (125 MHz,  $\text{CDCl}_3$ )

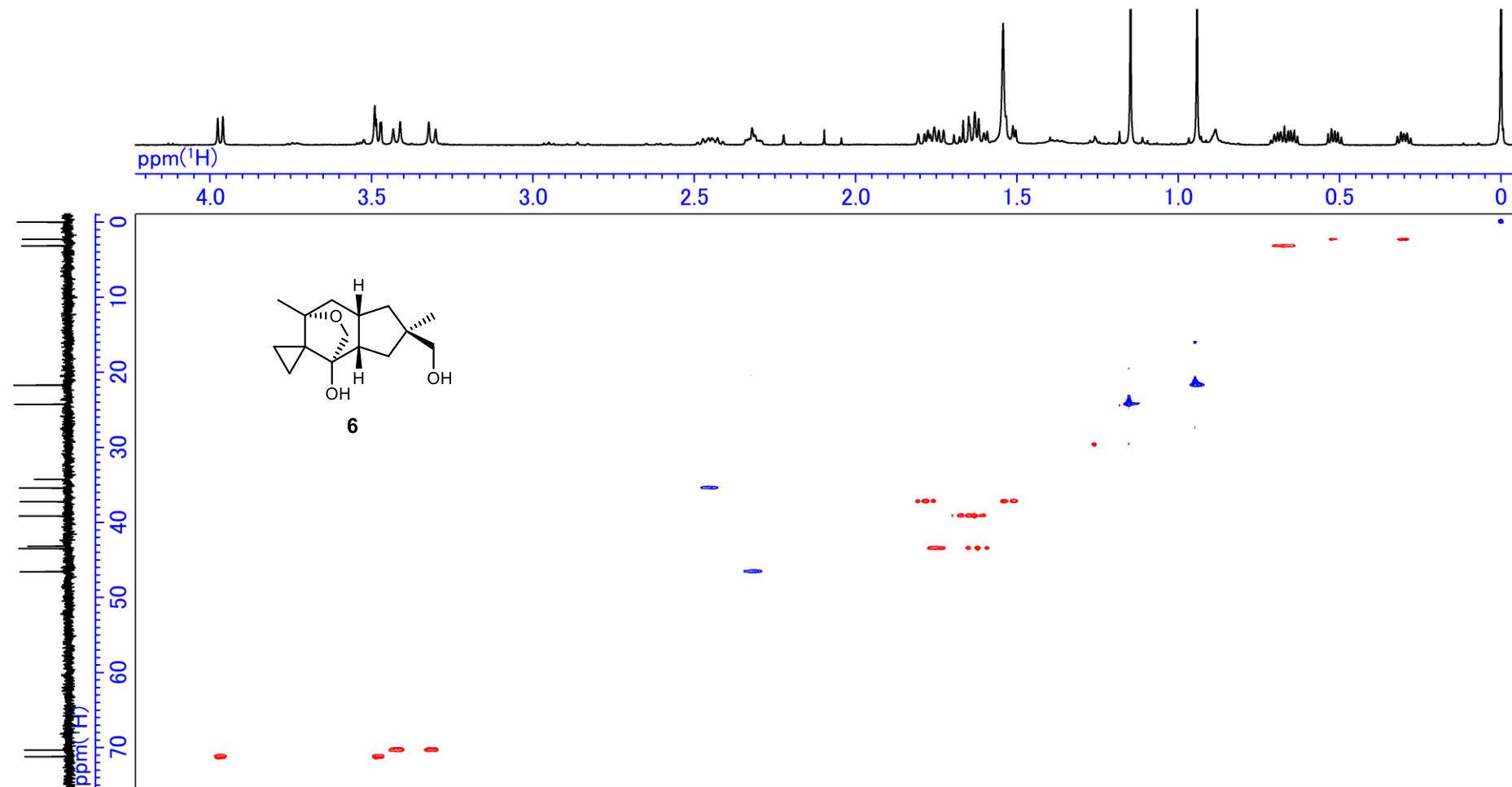


SI-70

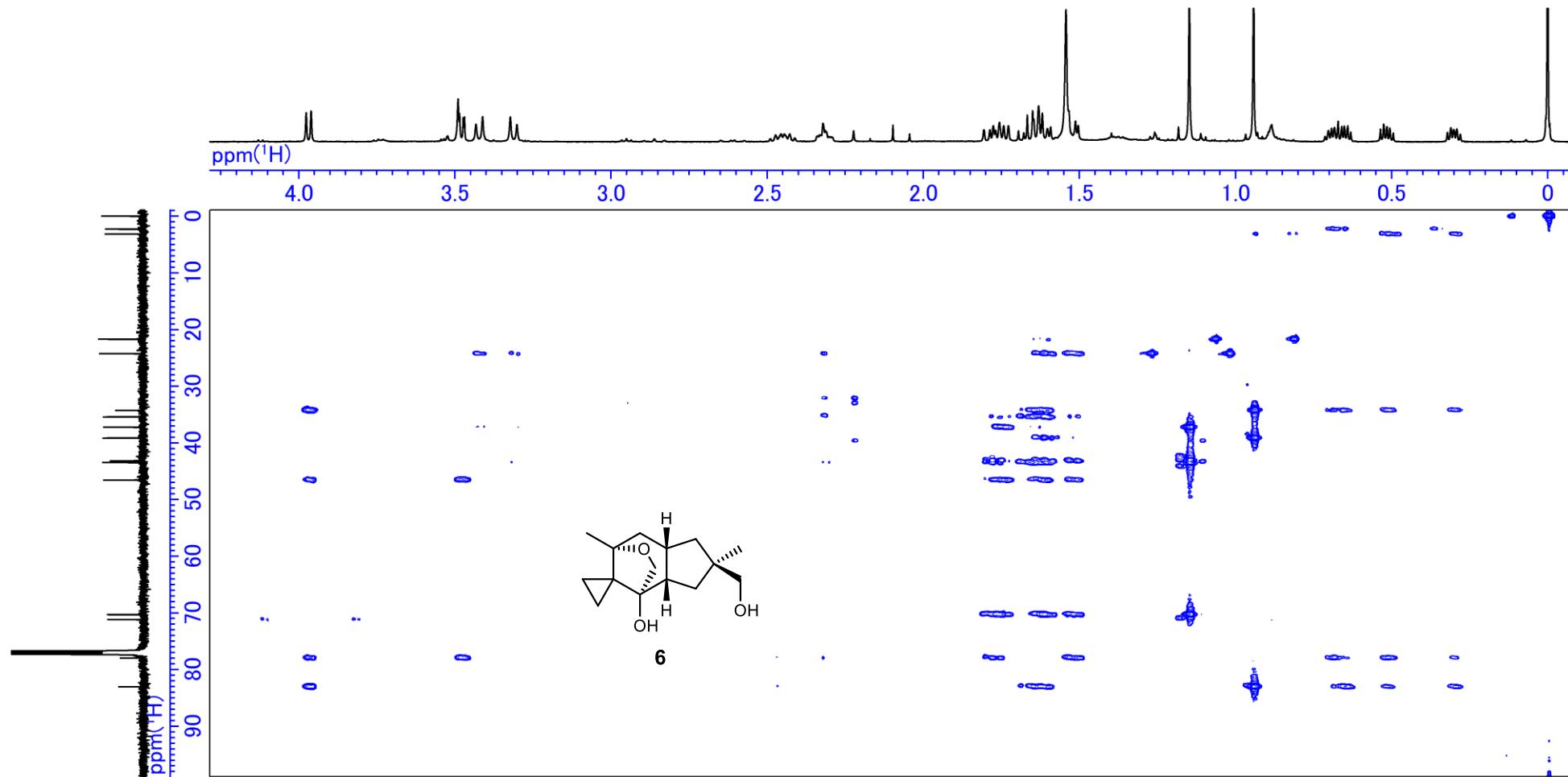
DQF COSY spectrum of **6** (500 MHz, CDCl<sub>3</sub>)



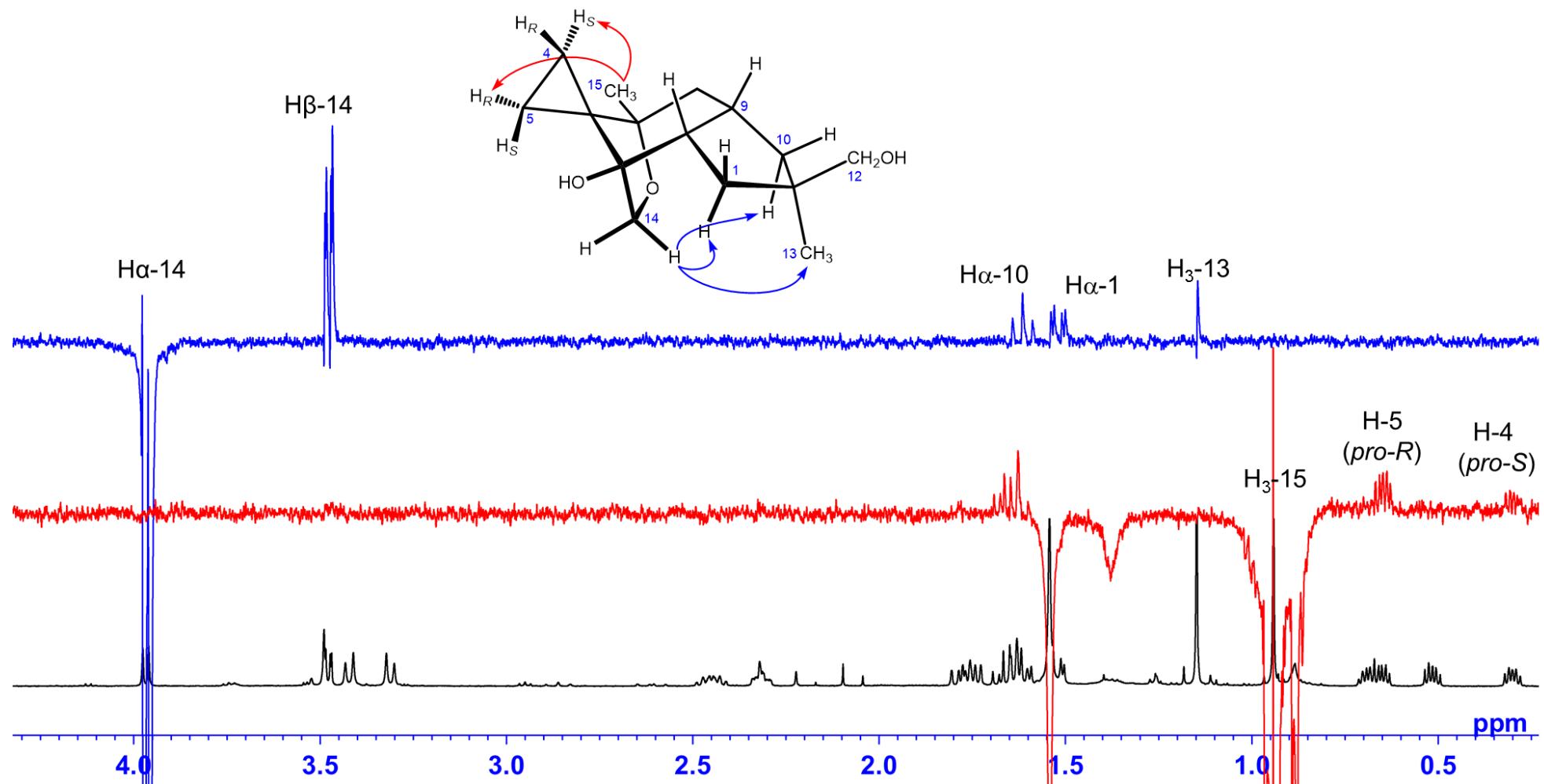
HSQC spectrum of **6** (500 MHz,  $\text{CDCl}_3$ )



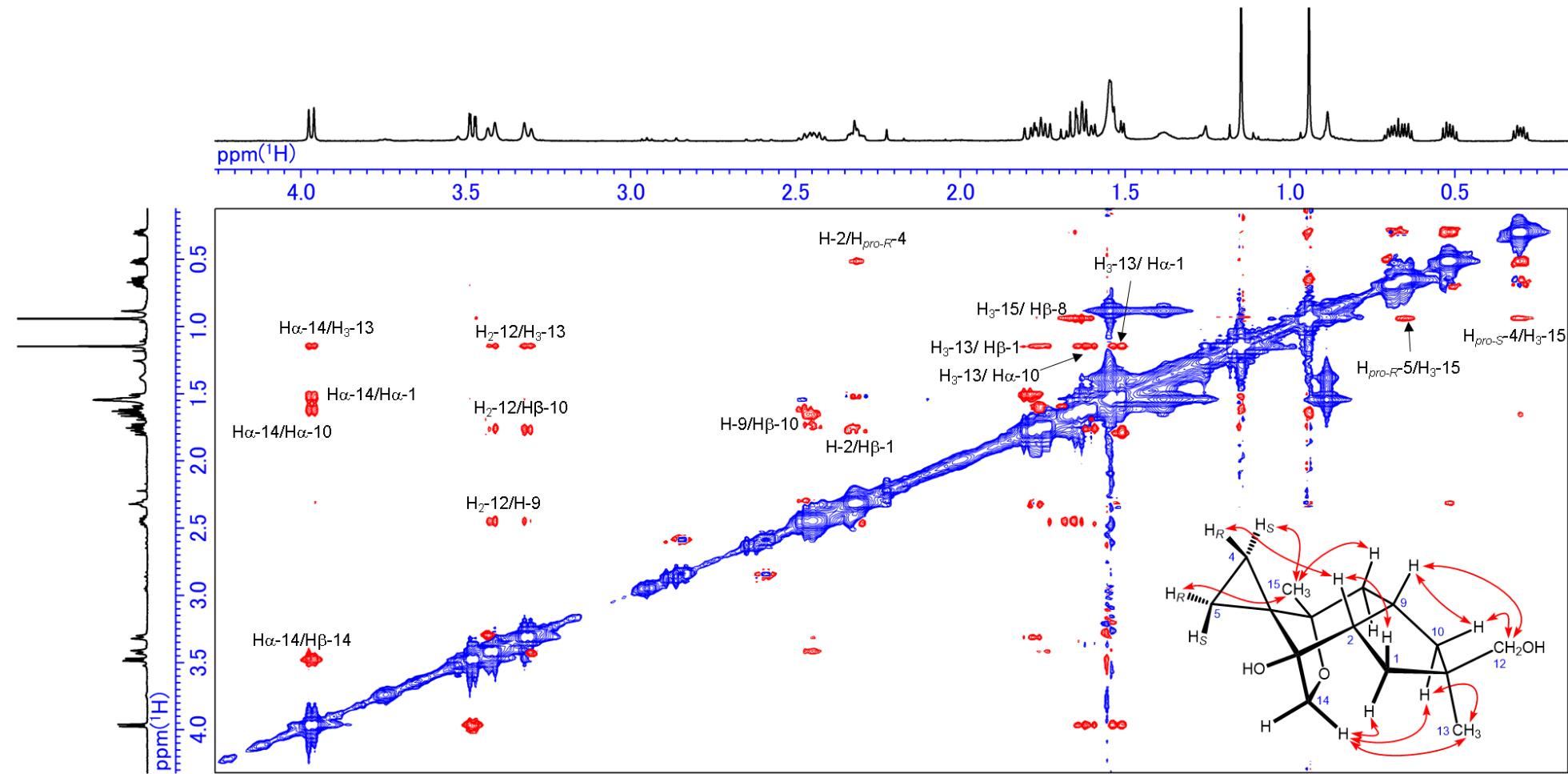
HMBC spectrum of **6** (500 MHz,  $\text{CDCl}_3$ )



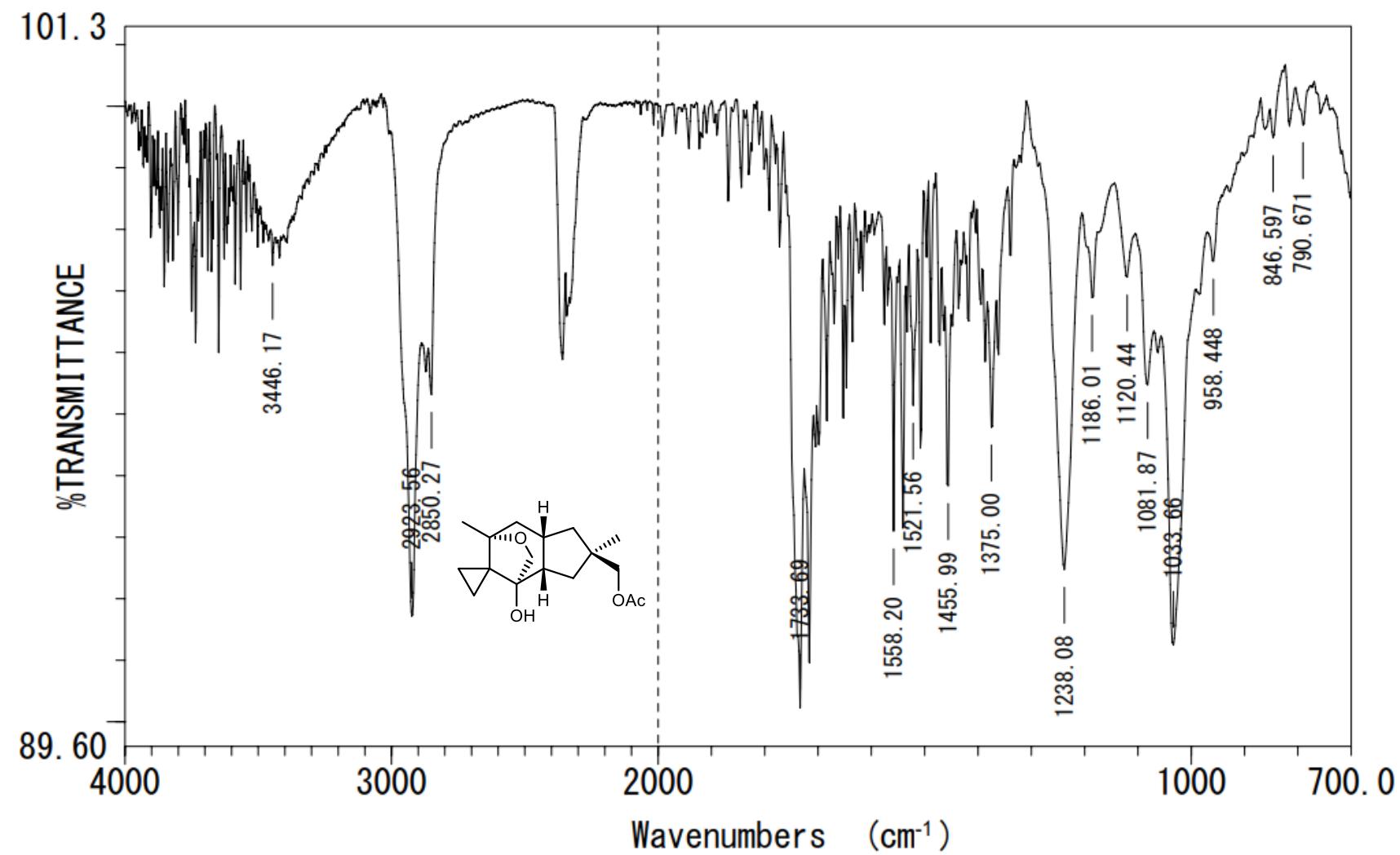
NOE 1D spectra of **6** (500 MHz,  $\text{CDCl}_3$ )



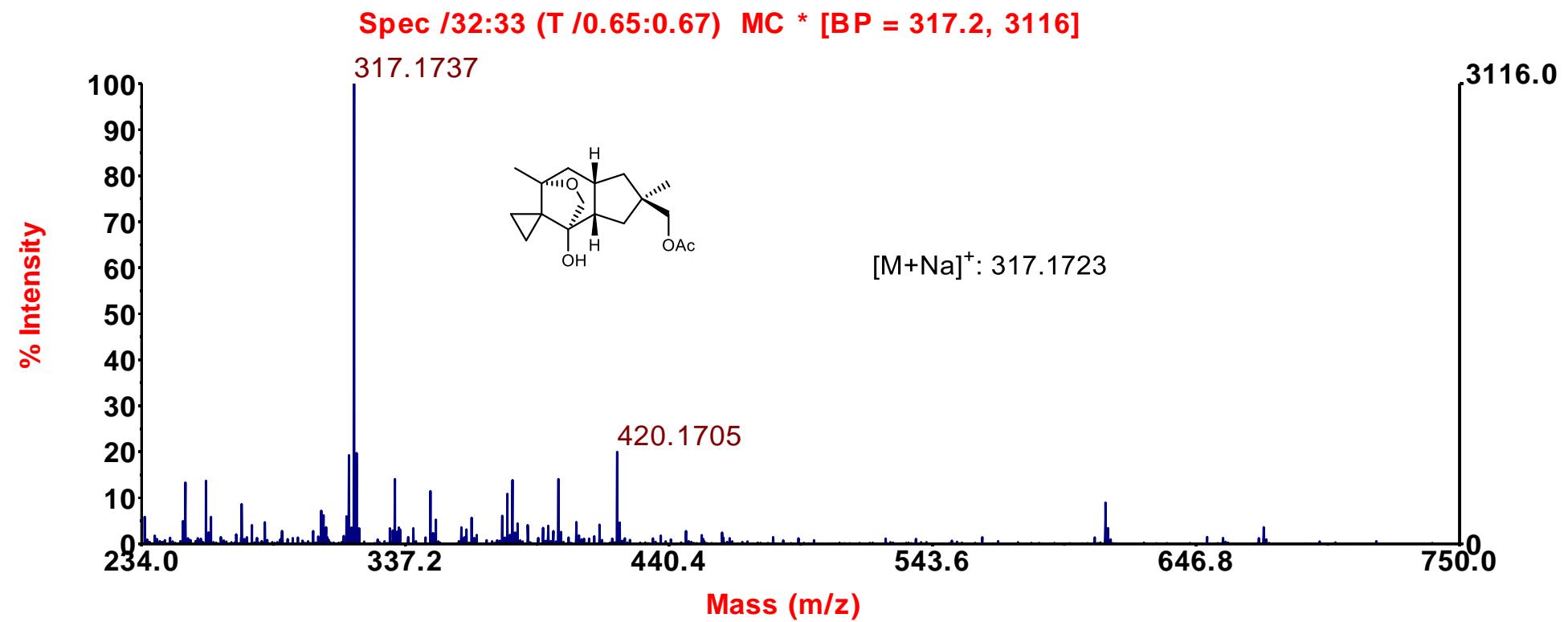
NOESY spectrum of **6** (500 MHz, CDCl<sub>3</sub>)



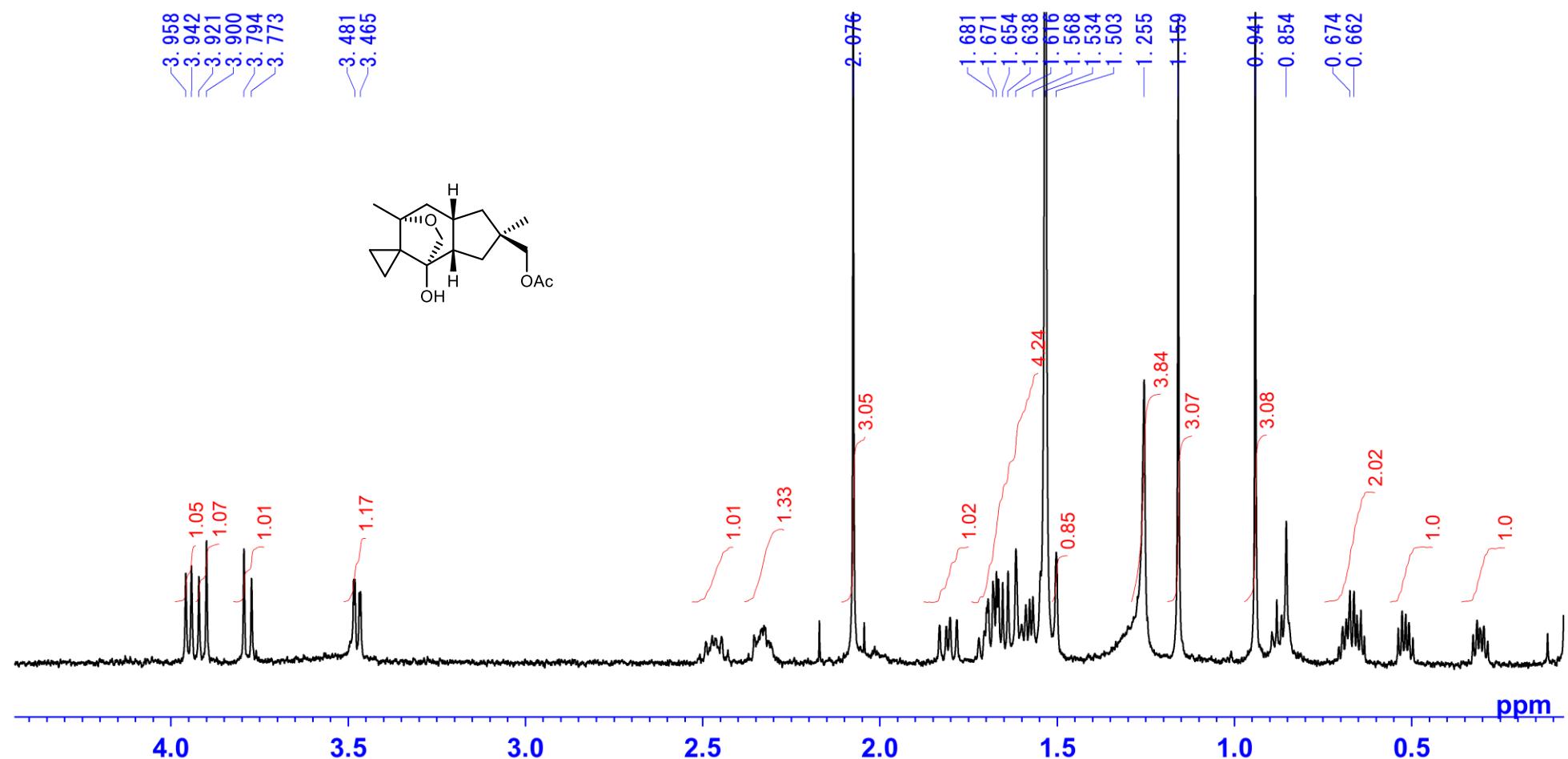
IR spectrum of 12-*O*-acetate of **6** (film)



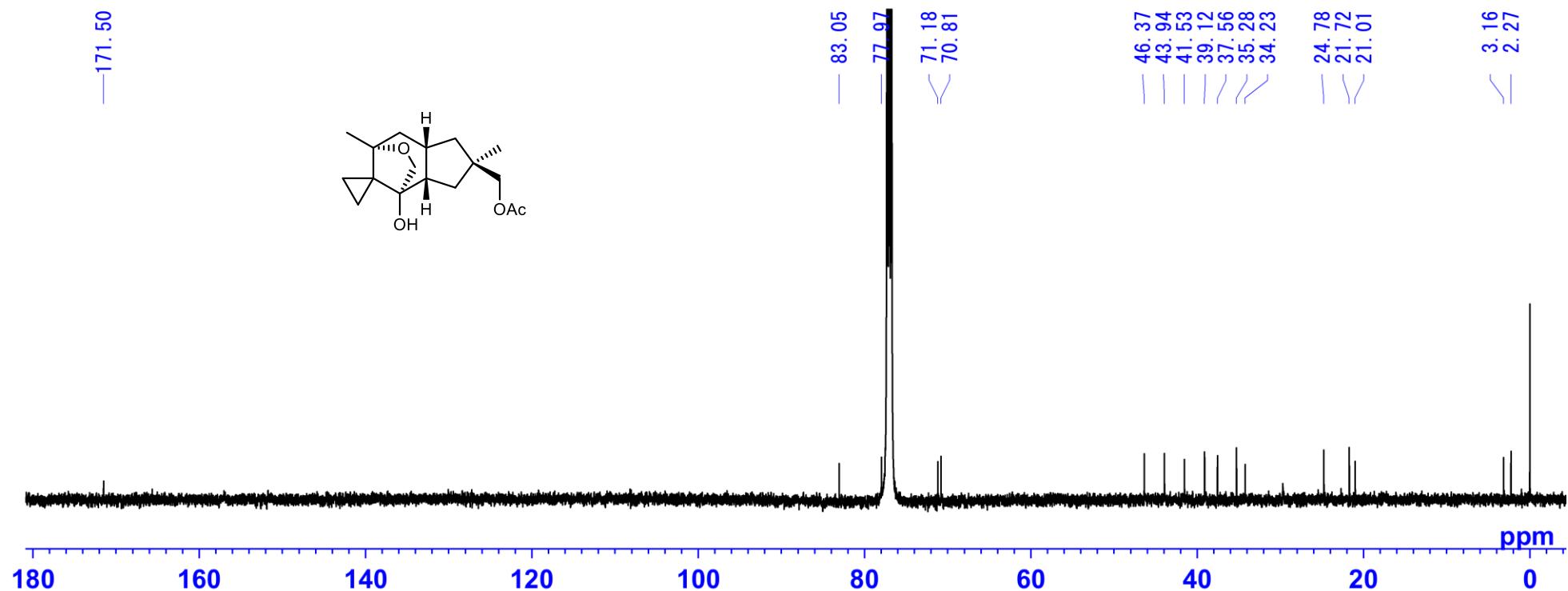
ESI-TOFMS spectrum of 12-*O*-acetate of **6**.



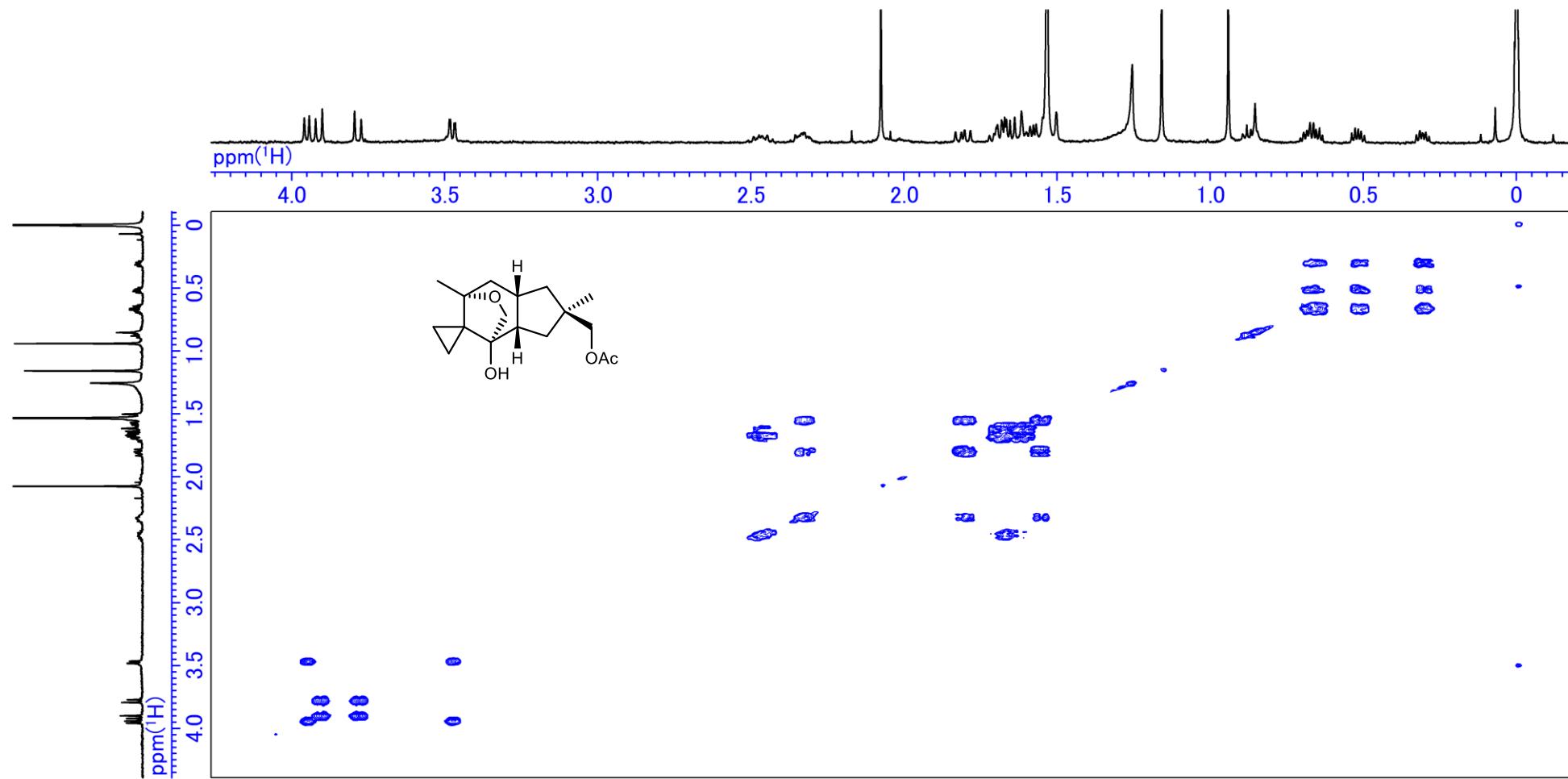
<sup>1</sup>H NMR spectrum of 12-*O*-acetate of **6** (500 MHz, CDCl<sub>3</sub>)



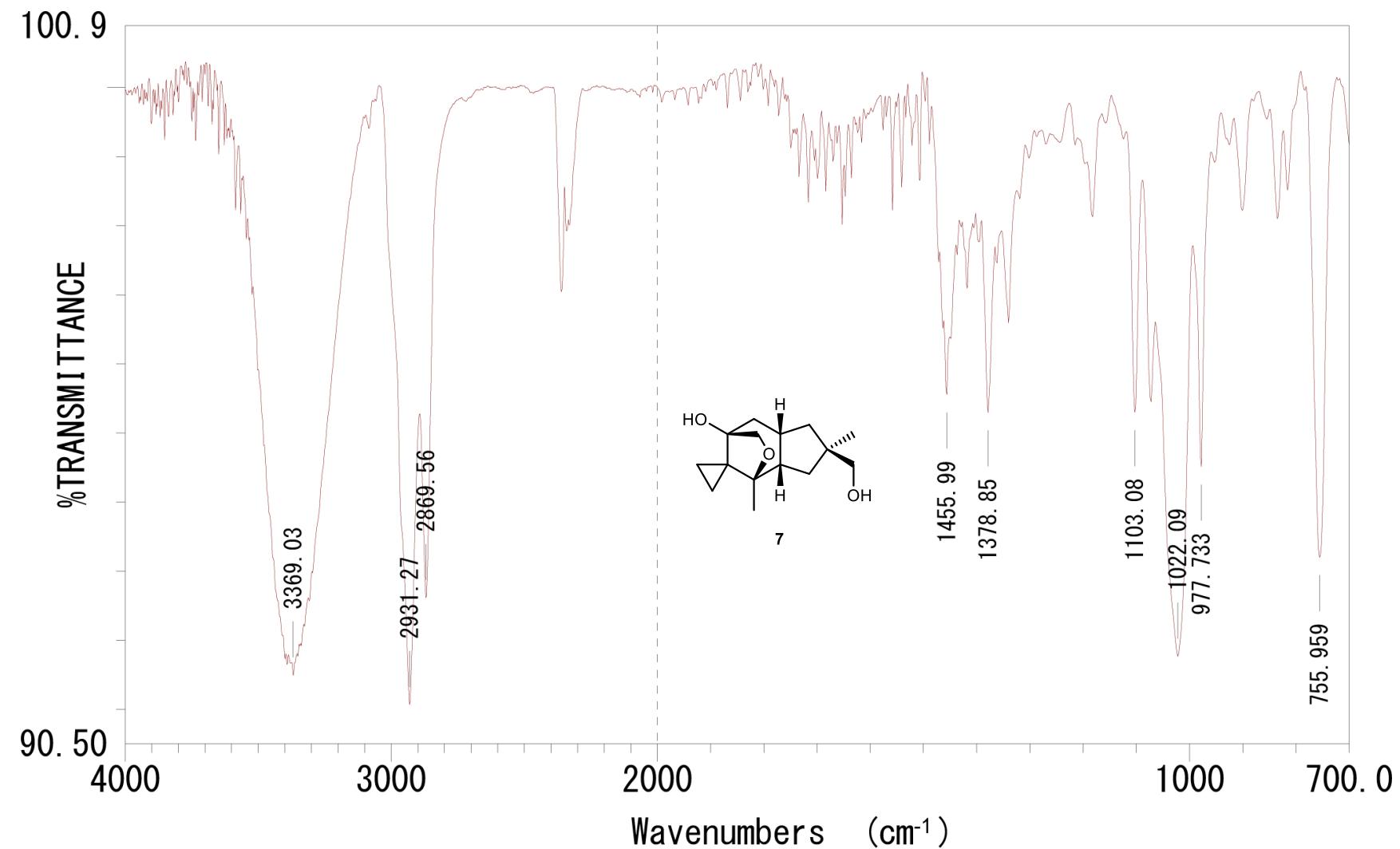
$^{13}\text{C}$  NMR spectrum of 12-*O*-acetate of **6** (125 MHz,  $\text{CDCl}_3$ )



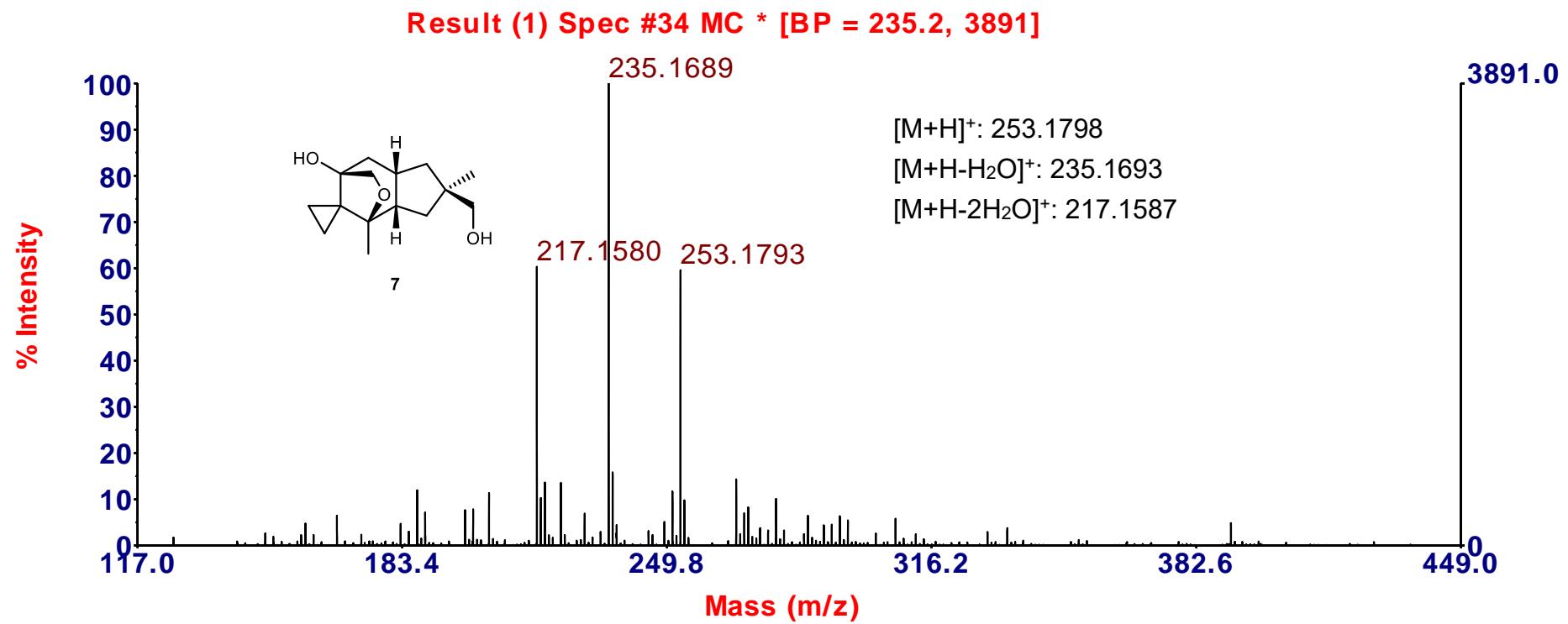
DQF COSY spectrum of 12-*O*-acetate of **6** (500 MHz, CDCl<sub>3</sub>)



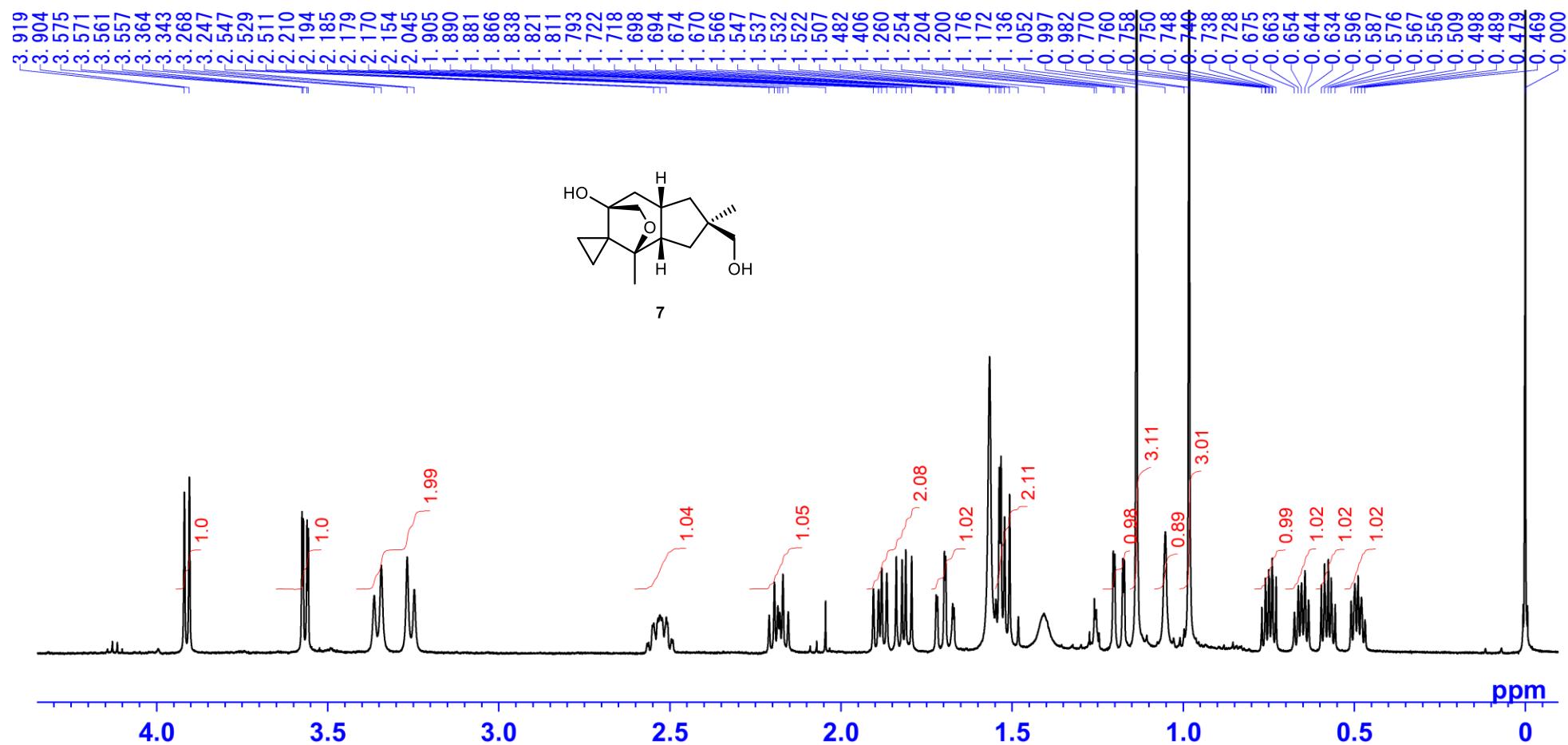
IR spectrum of 7 (film)



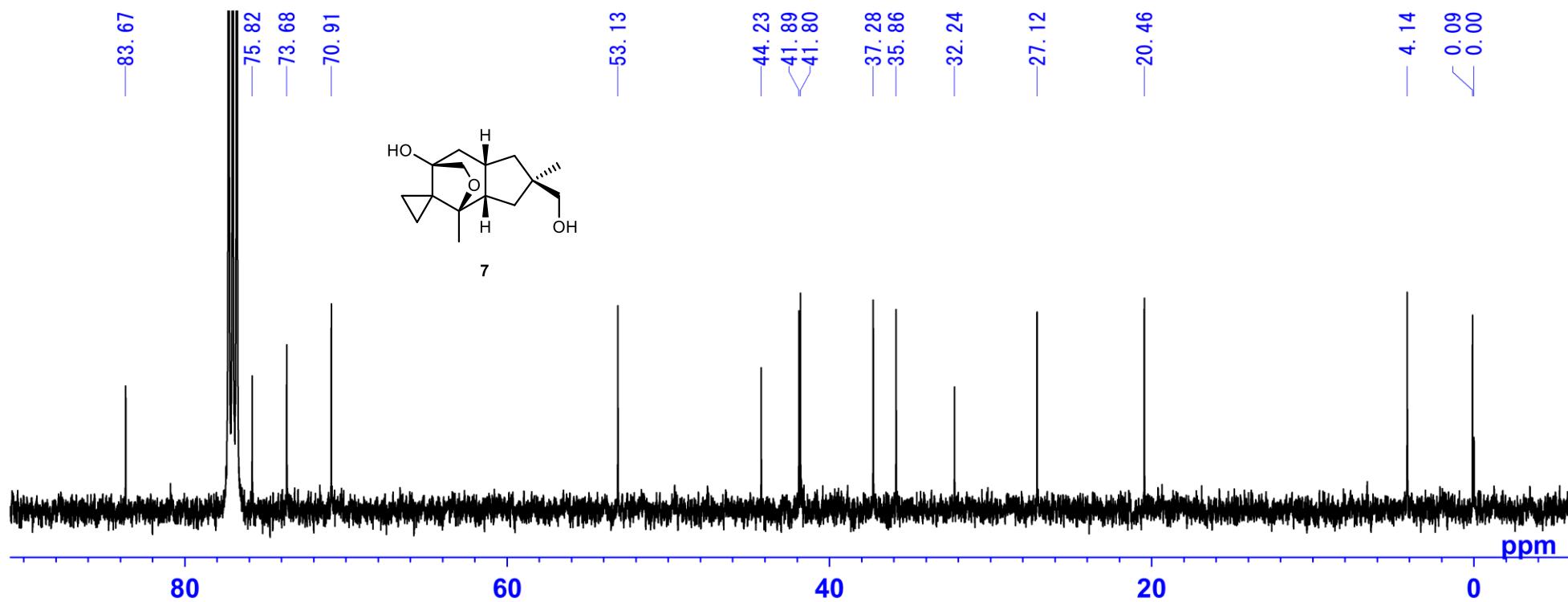
ESI-TOFMS spectrum of 7



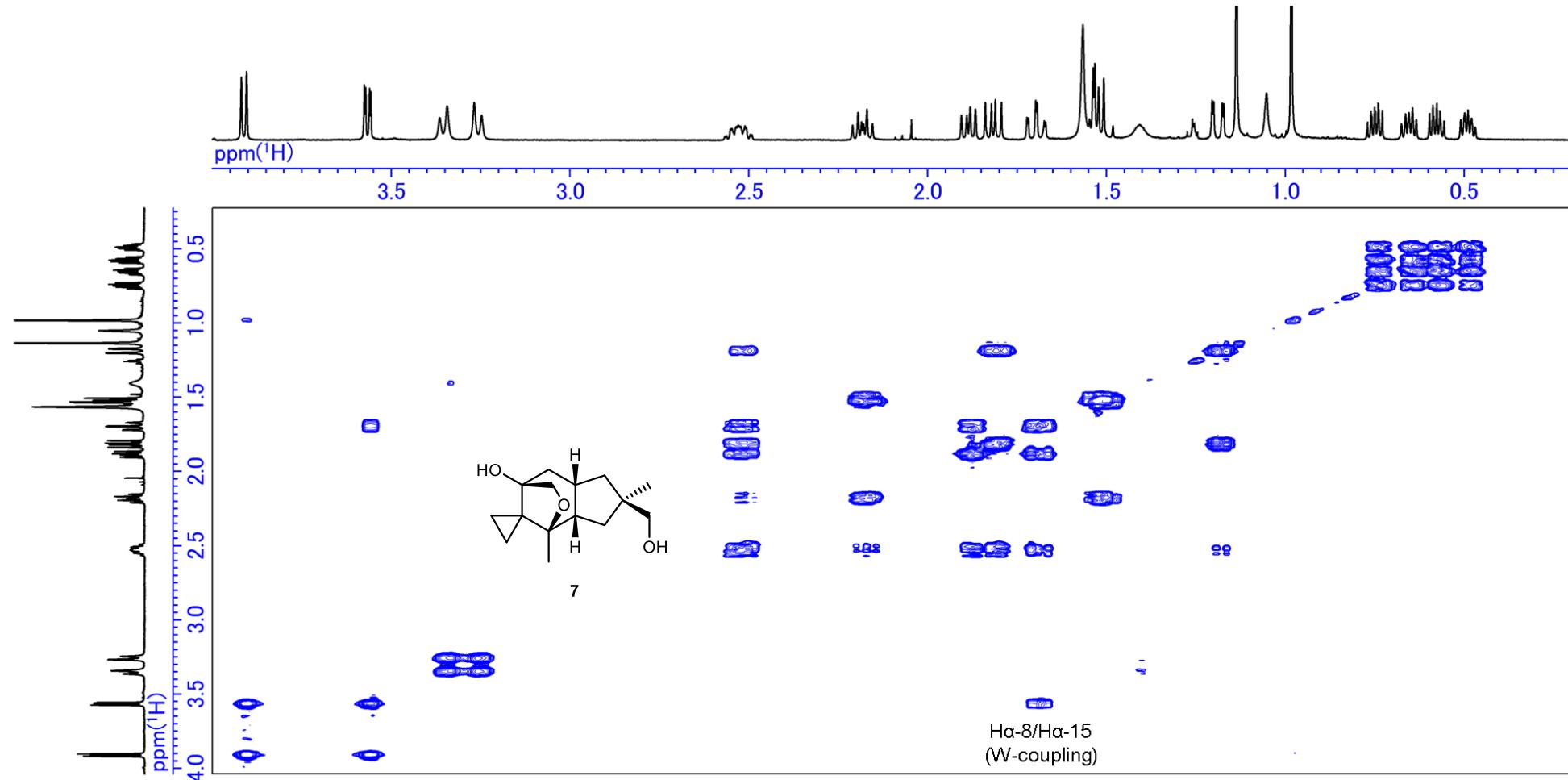
<sup>1</sup>H NMR spectrum of 7 (500 MHz, CDCl<sub>3</sub>)



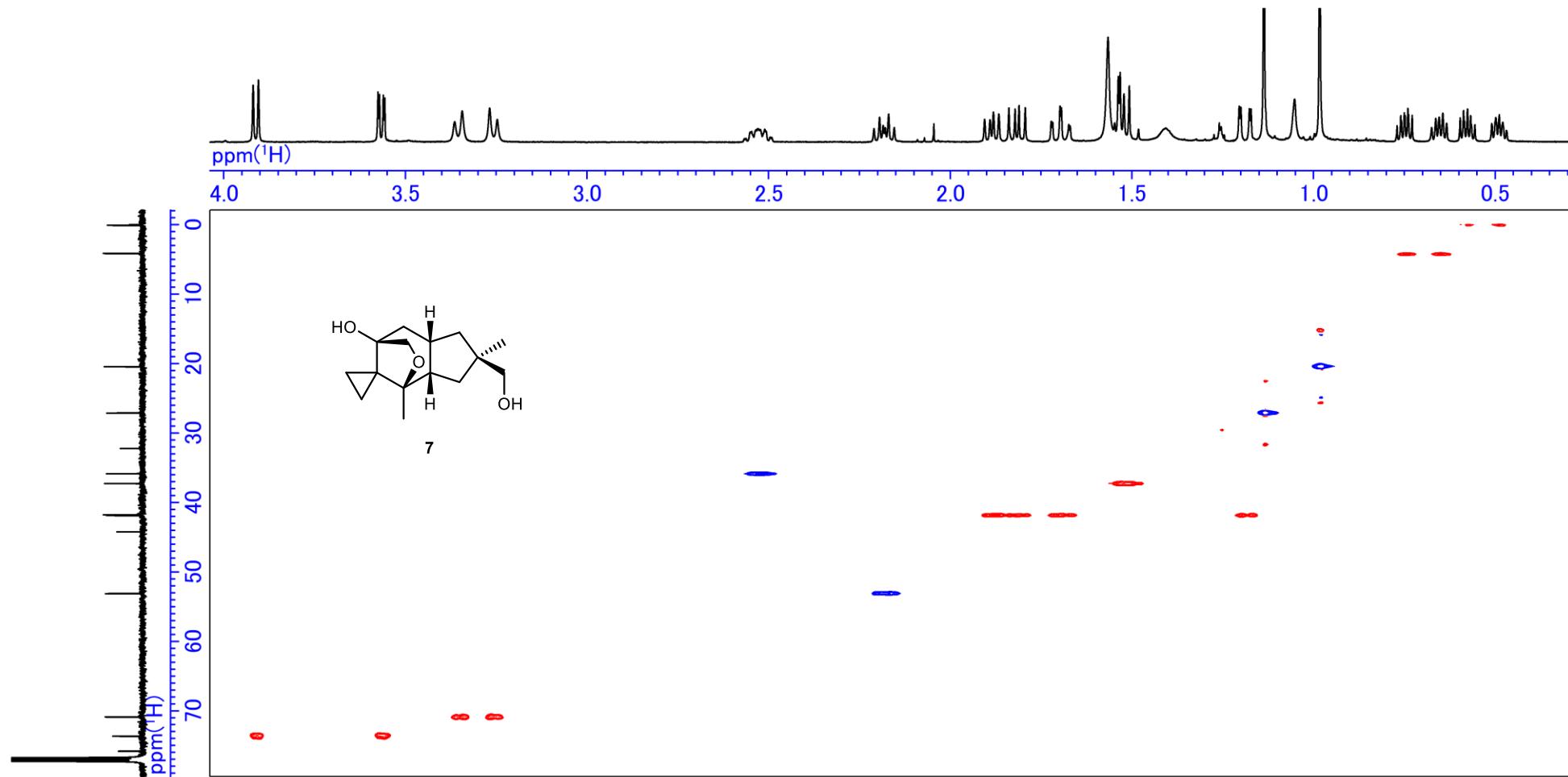
<sup>13</sup>C NMR spectrum of **7** (125 MHz, CDCl<sub>3</sub>)



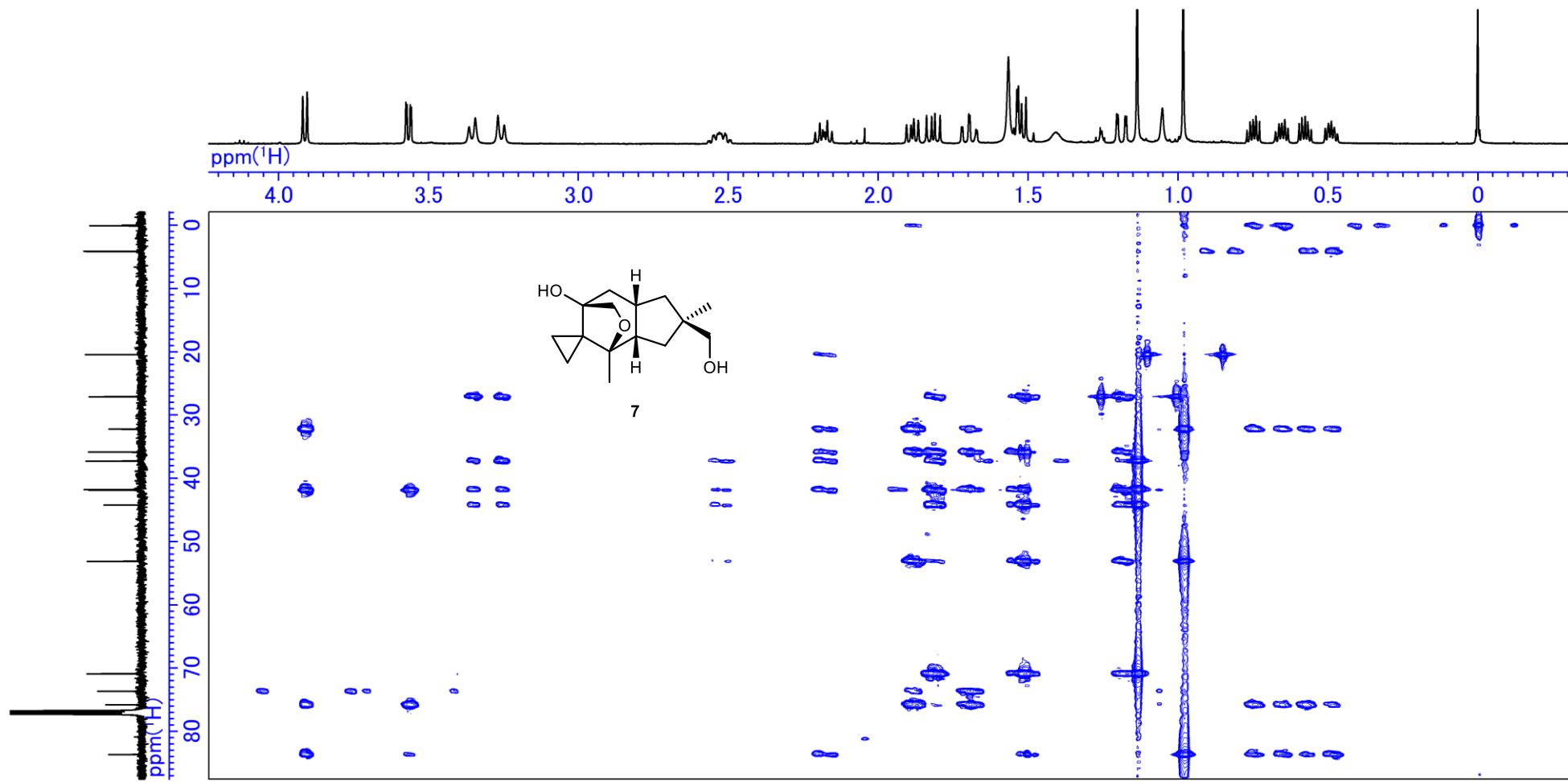
DQF COSY spectrum of **7** (500 MHz, CDCl<sub>3</sub>)



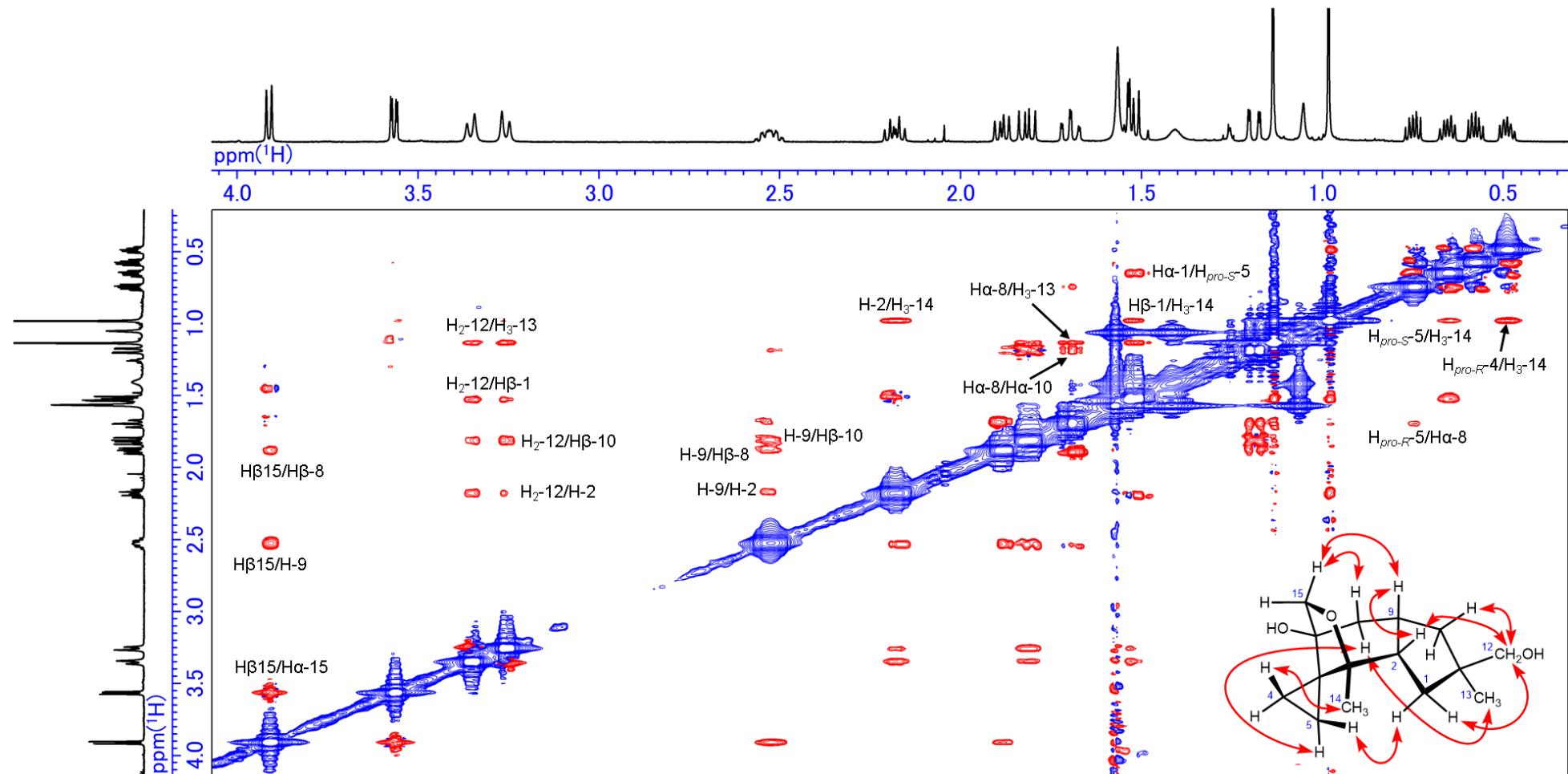
HSQC spectrum of **7** (500 MHz, CDCl<sub>3</sub>)



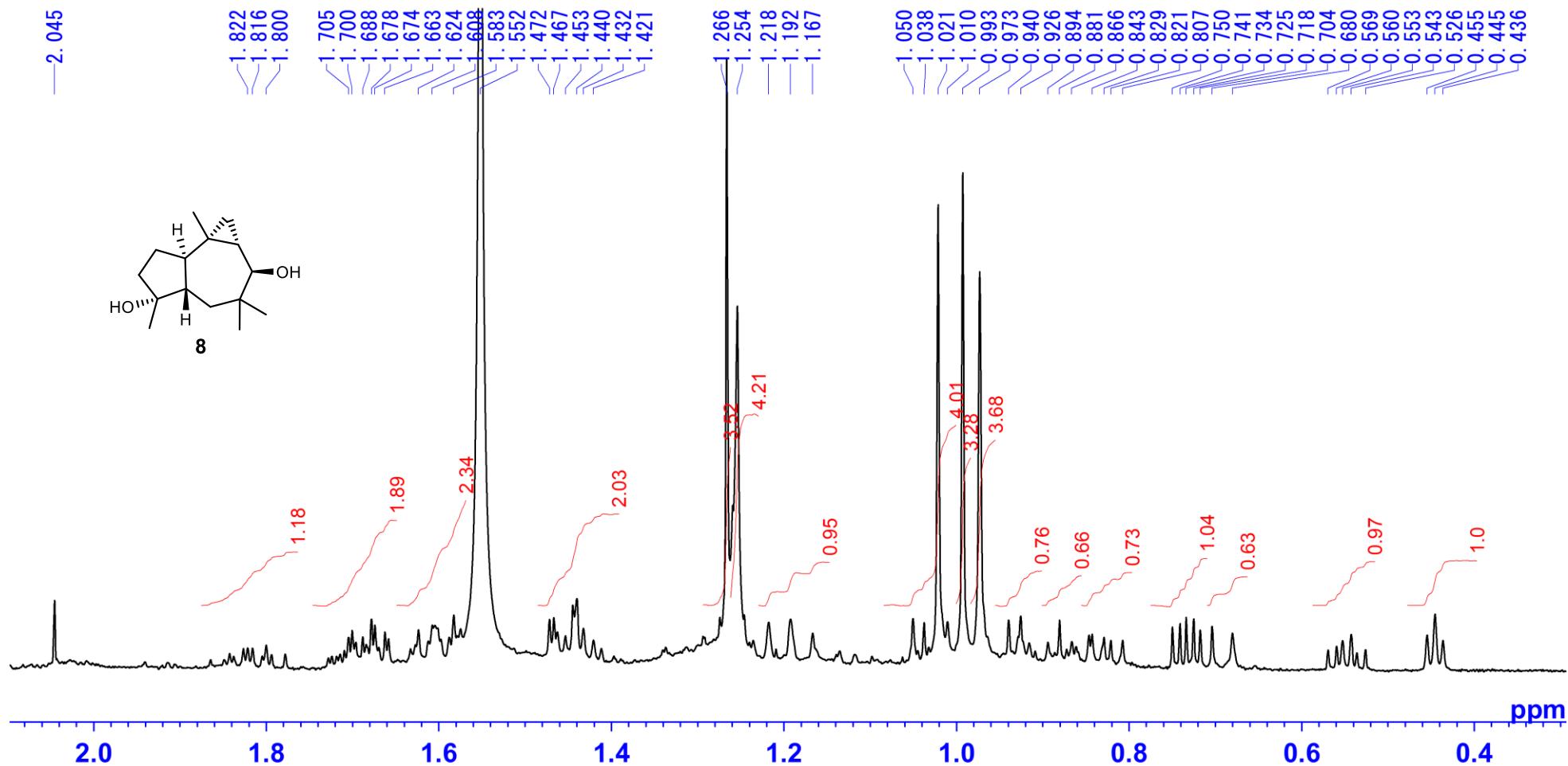
HMBC spectrum of 7 (500 MHz, CDCl<sub>3</sub>)



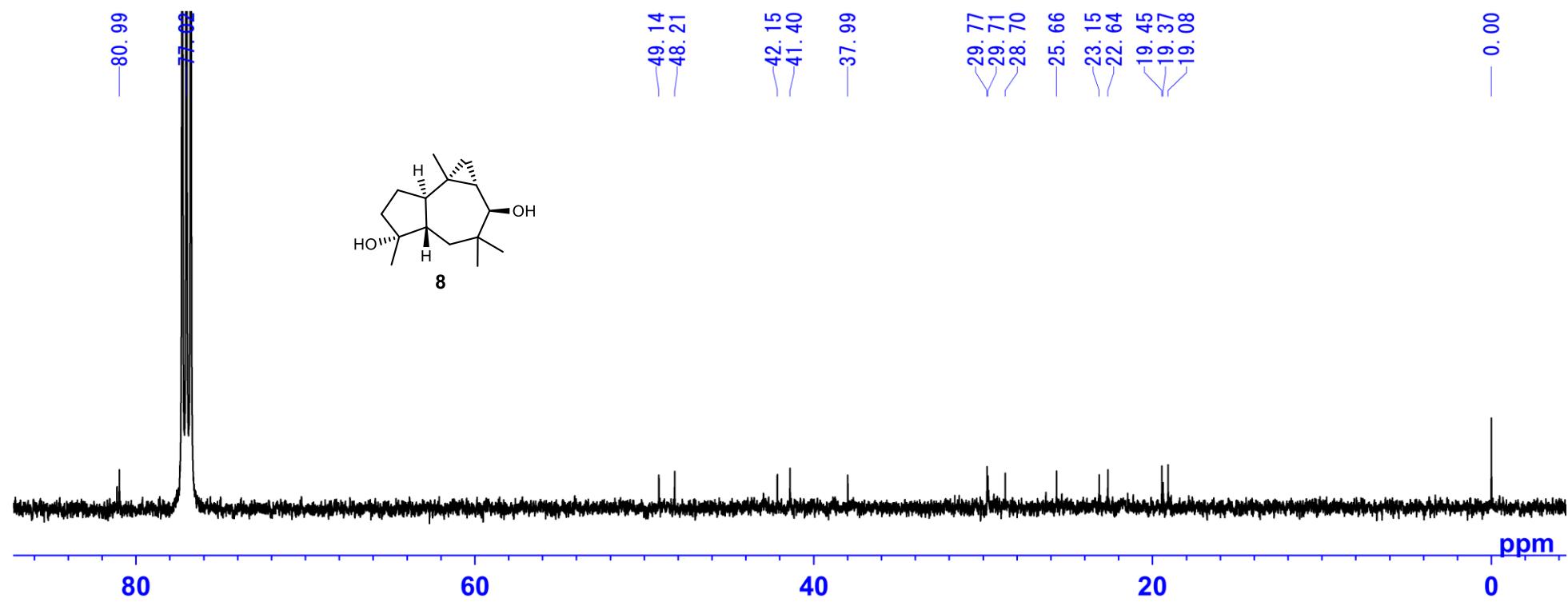
NOESY spectrum of **7** (500 MHz,  $\text{CDCl}_3$ )



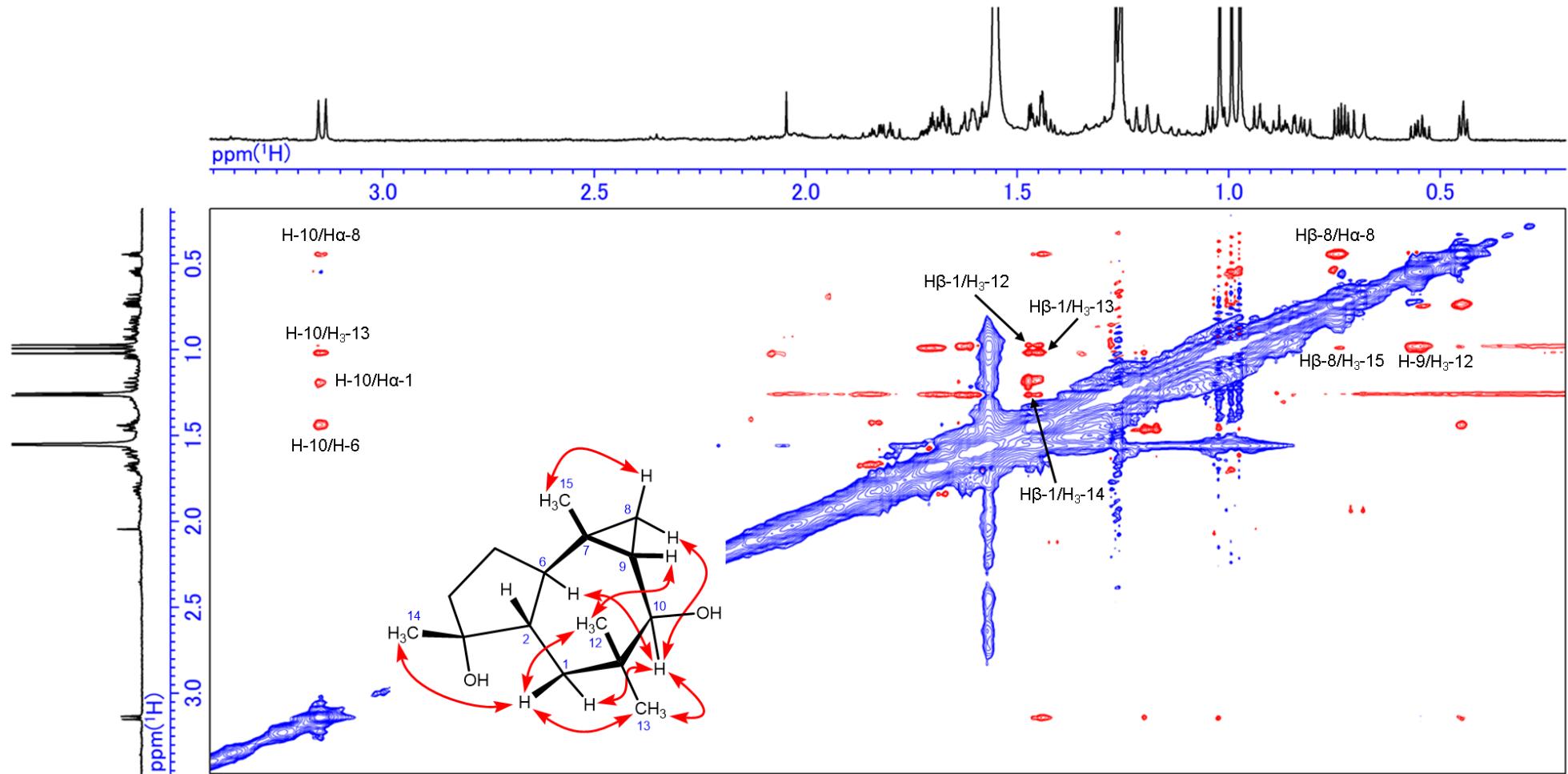
$^1\text{H}$  NMR spectrum of **8** (500 MHz,  $\text{CDCl}_3$ )



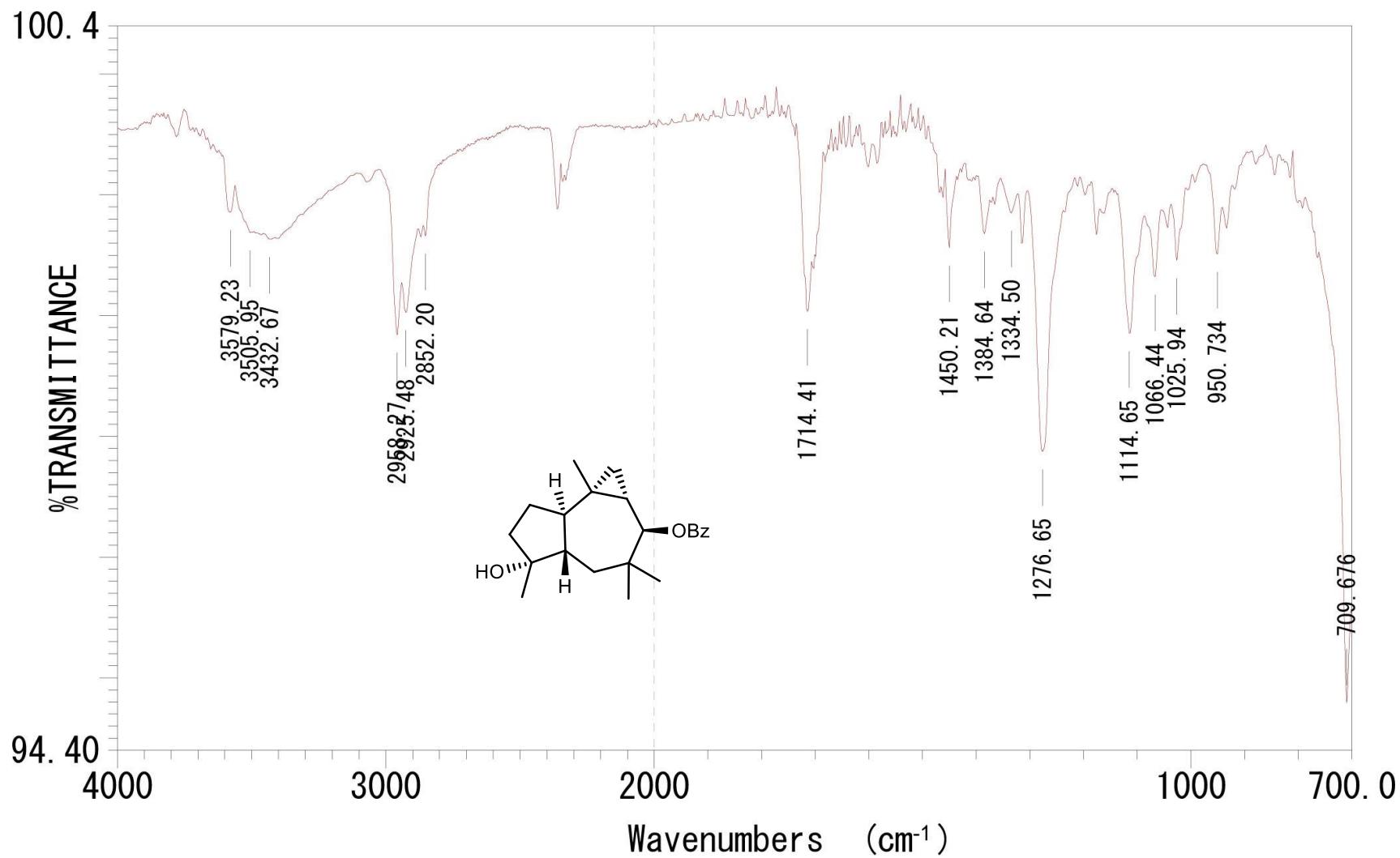
$^{13}\text{C}$  NMR spectrum of **8** (125 MHz,  $\text{CDCl}_3$ )



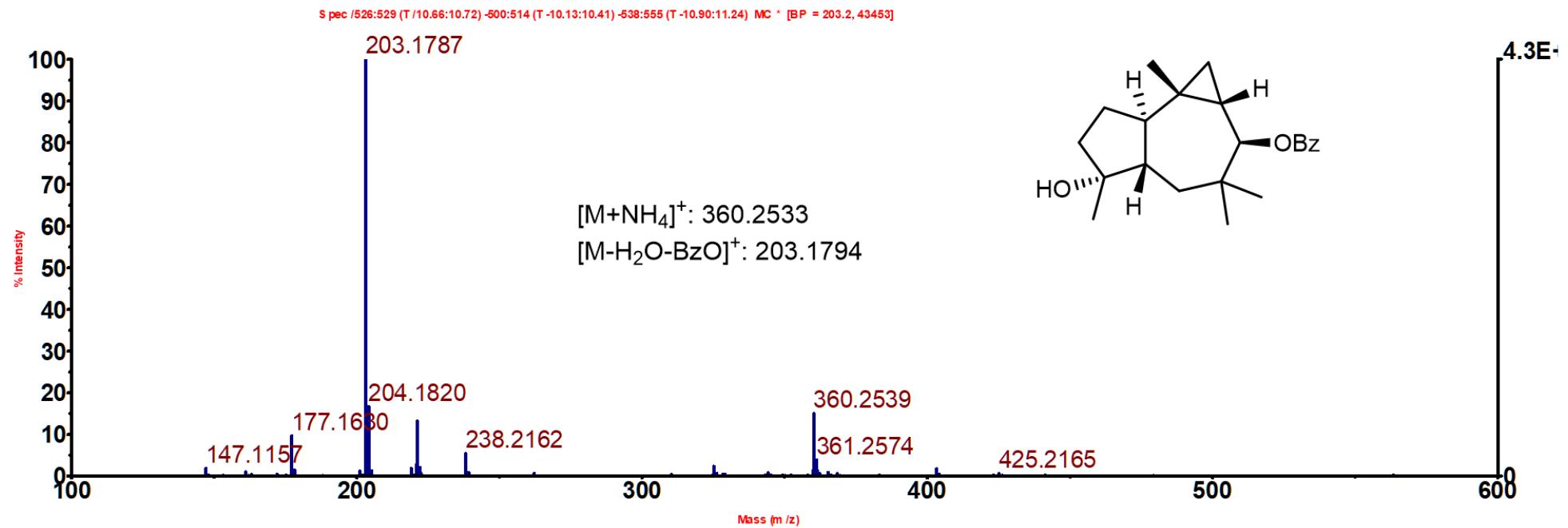
NOESY spectrum of **8** (500 MHz,  $\text{CDCl}_3$ ).



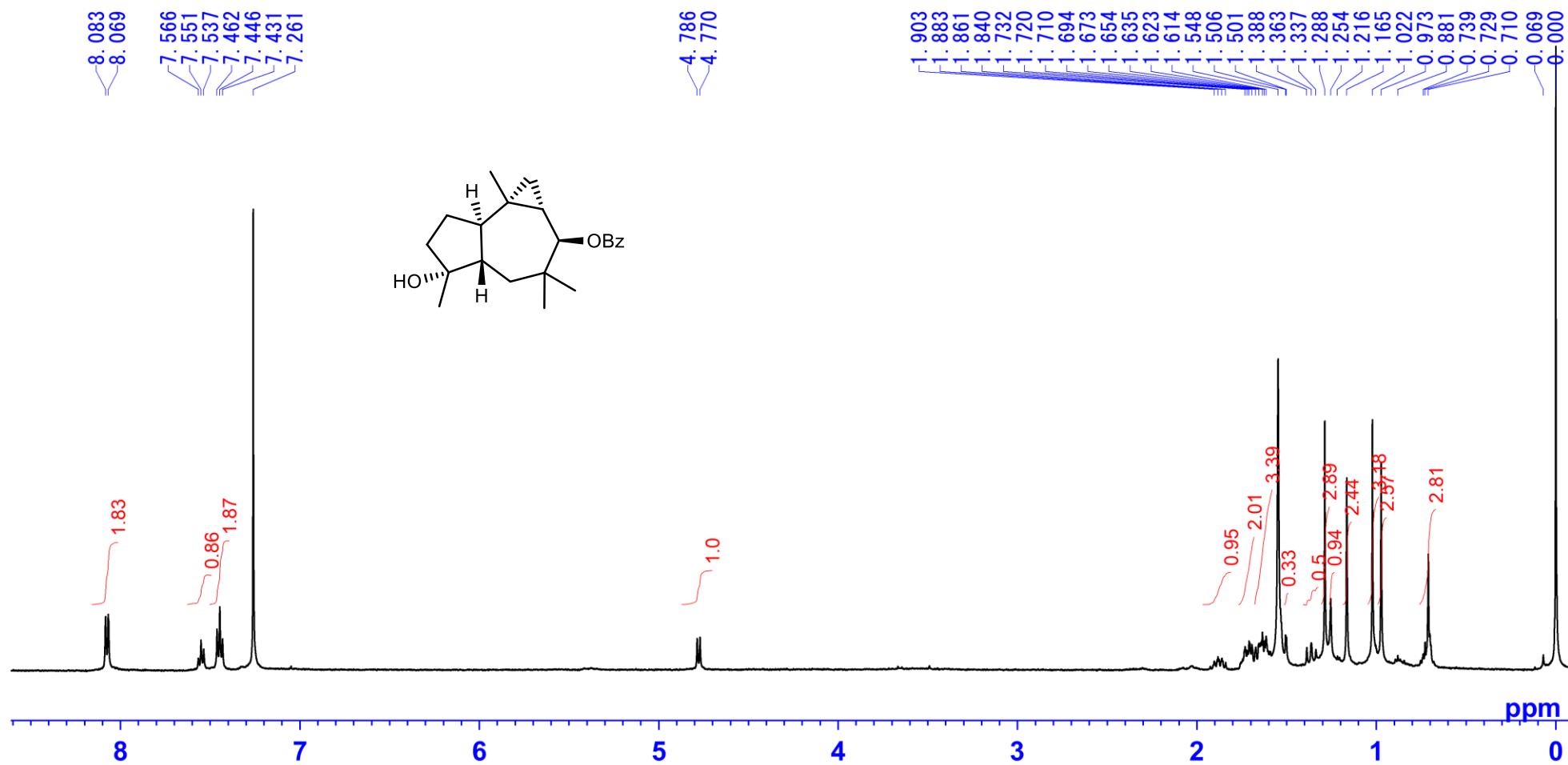
IR spectrum of **8-OBz** (film)



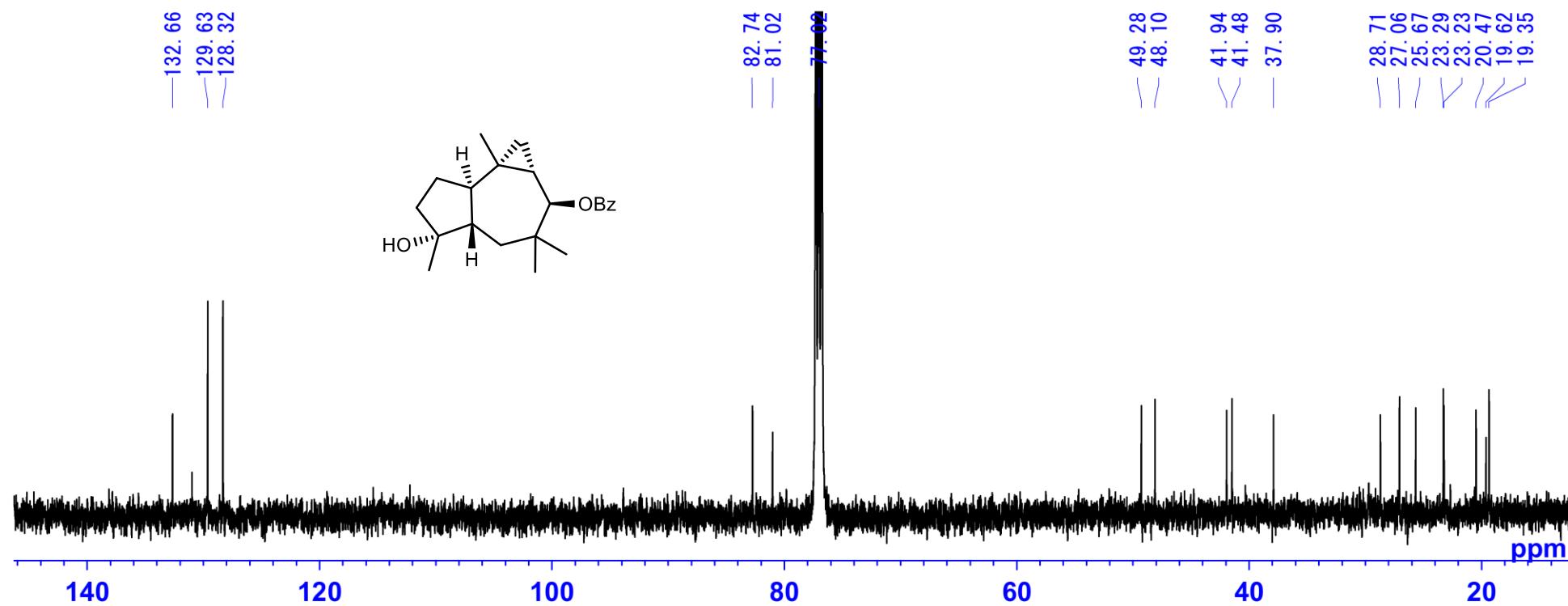
ESI-TOFMS spectrum of **8-OBz**



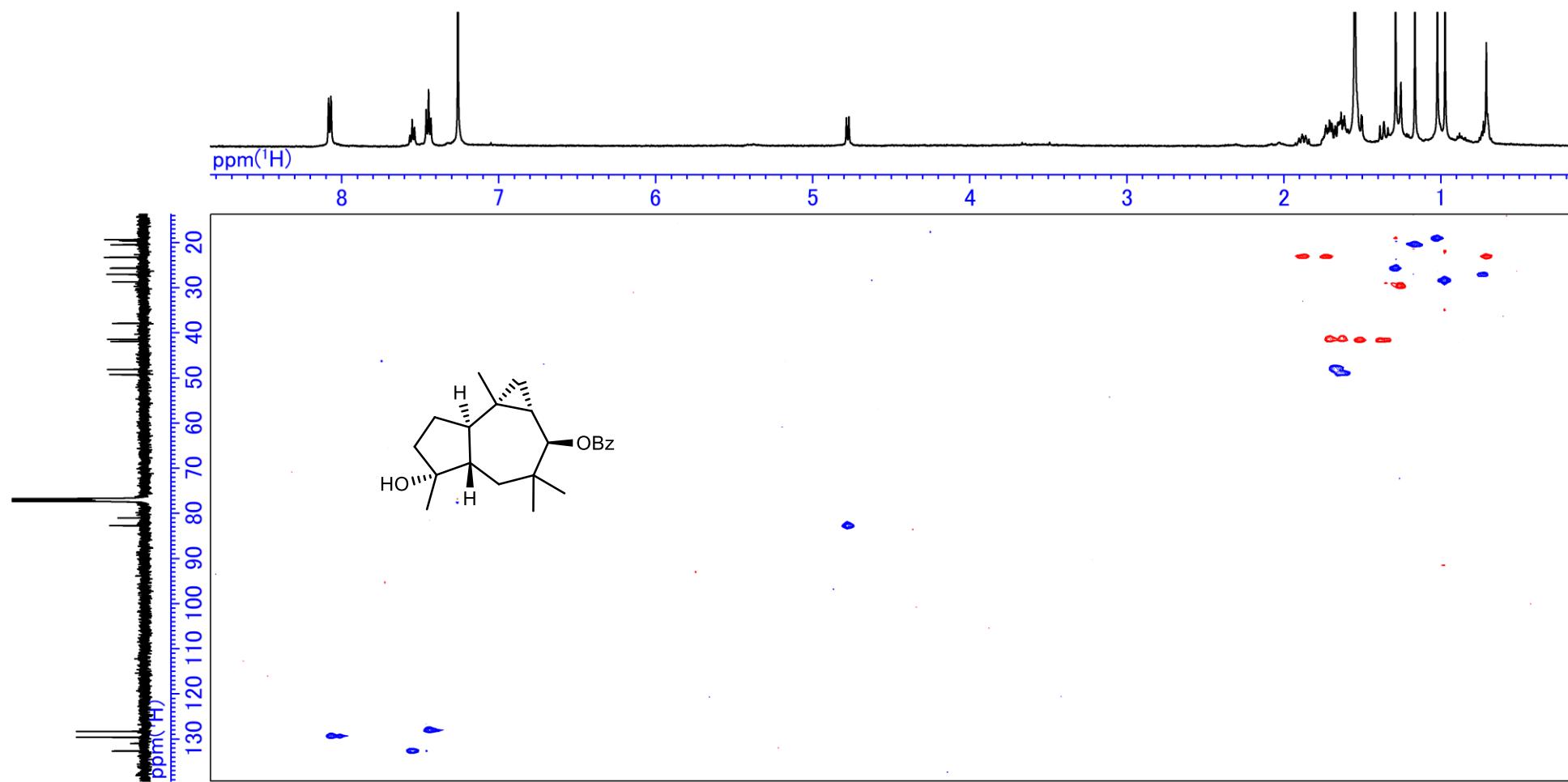
<sup>1</sup>H NMR spectrum of **8-OBz** (500 MHz, CDCl<sub>3</sub>)



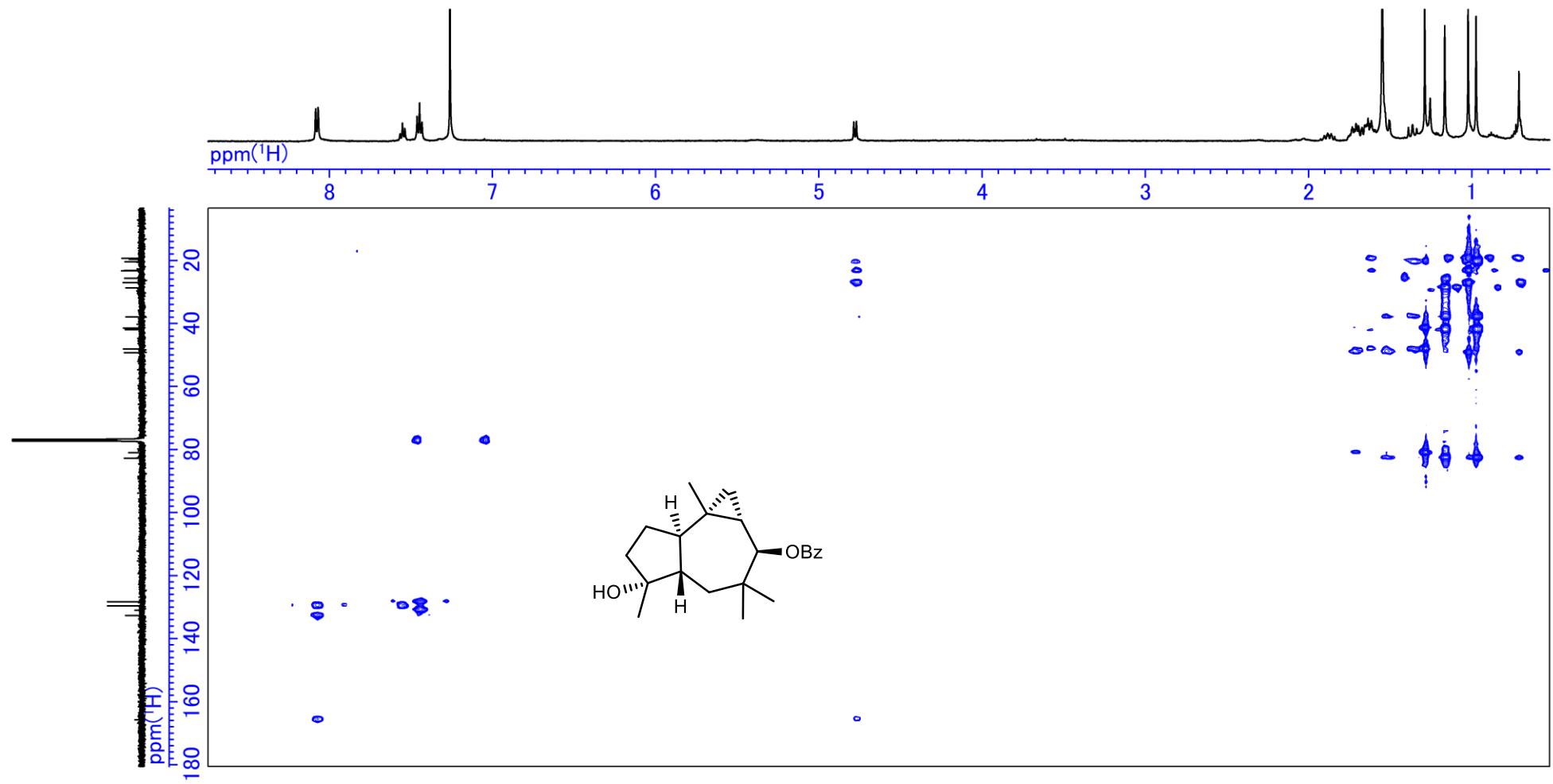
$^{13}\text{C}$  NMR spectrum of **8-OBz** (125 MHz,  $\text{CDCl}_3$ )



HSQC spectrum of **8-OBz** (500 MHz,  $\text{CDCl}_3$ )



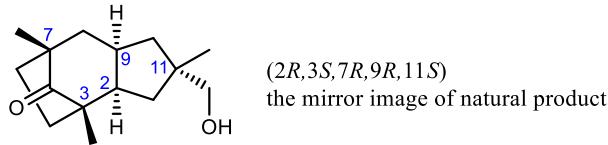
HMBC spectrum of **8-OBz** (500 MHz, CDCl<sub>3</sub>)



Chemical shift calculations.

- Calculations were performed with Spartan'18 Parallel Suite for Windows (Wavefunction Inc.) was used with default setting.
- All calculation results were checked manually. If abnormal conformers were found, these were recalculated after updating the initial conformation.
- Boltzmann distributions were obtained based on the SCF energy using  $\omega$ B97X-V/6-311+G(2df,2p)[6-311G\*]// $\omega$ B97X-D/6-31G\*
- Solvent effect was not considered in all calculations.
- The original parameters by Goodman ( $^{13}\text{C}$ :  $\sigma = 2.306$  ppm,  $\nu = 11.38$ ,  $^1\text{H}$ :  $\sigma = 0.185$  ppm,  $\nu = 14.18$ ) by Goodman (*J. Am. Chem. Soc.* 2010, 132, 12946) was used for DP4 analysis, although the present protocol was proved to give much accurate  $^{13}\text{C}$  chemical shifts.
- Although DP4 analysis requires empirical correction for both  $\delta^{13}\text{C}$  and  $\delta^1\text{H}$ , it was skipped because the protocol involves similar correction.
- For proposed diastereomers, prochiral methylene  $^1\text{H}$  signals were strictly arranged based on NOEs except for H<sub>2</sub>-5 and H<sub>2</sub>-6 of **8**. Their orientation could not be elucidated by NOE experiments. Thus, these were arranged to become the chemical shift differences from the calculated values smaller).
- Prochiral methylene protons in other diastereomers were arranged to become the chemical shift differences from the calculated values smaller.
- Details such as conformation search, chemical shift of individual conformers, conformational distributions, obtained geometries (SDF format) are seen in the associated Excel files

Calculated  $^{13}\text{C}$  NMR chemical shift of **1a** and its isomers.



	C-1	C-2	C-3	C-4	C-5	C-6	C-7	C-8	C-9	C-10	C-11	C-12	C-13	C-14	C-15
experimental	36.7	59.3	48.4	32.3	29.0	222.4	46.2	48.6	35.5	40.6	43.8	71.9	27.5	18.4	19.8
repreasentin B <sup>a</sup>	36.8	58.6	48.5	32.5	29.0	222.3	46.2	48.2	35.2	40.6	44.4	72.7	26.7	18.5	19.7
<b>(2R,3S,7R,9R,11S)</b>	37.2	58.5	48.5	32.5	29.2	221.4	46.0	47.3	36.3	39.9	43.5	73.2	27.5	19.8	20.7
(2R,3S,7R,9R,11R)	35.9	57.5	48.2	32.4	29.2	221.5	46.0	46.0	35.9	40.2	44.2	72.1	27.1	19.8	20.6
(2R,3S,7R,9S,11R)	38.5	54.2	47.1	34.6	35.3	220.9	41.6	47.2	38.7	41.6	42.9	72.4	26.5	16.5	22.2
(2R,3S,7R,9S,11S)	39.4	55.0	47.2	34.5	35.3	221.2	41.7	47.2	37.8	40.6	42.8	72.6	26.4	16.5	22.2
(2S,3S,7R,9R,11R)	36.2	55.7	48.7	25.9	31.0	221.4	45.4	43.0	37.4	39.6	43.2	72.4	26.5	18.4	20.9
(2S,3S,7R,9R,11S)	35.0	55.1	48.8	26.0	31.0	221.7	45.5	43.1	38.5	40.8	43.0	72.8	26.4	18.5	21.0
(2S,3S,7R,9S,11S)	38.0	53.0	50.6	25.0	30.4	223.2	45.5	43.6	34.7	41.6	43.4	70.9	25.2	20.4	21.8
(2S,3S,7R,9S,11R)	39.3	54.1	50.2	26.5	30.3	223.0	45.4	43.5	34.7	42.9	43.4	71.1	24.6	20.2	21.6

Calculated  $^1\text{H}$  NMR chemical shift of **1a** and its isomers.

	H $\beta$ -1	H $\alpha$ -1	H-2	H $\beta$ -4	H $\alpha$ -4	H $\beta$ -5	H $\alpha$ -5	H $\alpha$ -8	H $\beta$ -8	H-9	H $\beta$ -10	H $\alpha$ -10	H-12	H-12	H-13	H-14	H-15
experimental	1.67	1.05	2.27	1.98	1.63	1.95	1.58	1.64	1.74	2.52	1.75	1.11	3.24	3.29	1.06	0.95	0.96
repreasentin B <sup>a</sup>	1.32	1.19	2.37	2.01	1.64	1.95	1.59	1.58	1.7	2.55	1.54	1.33	3.34	3.34	0.99	0.97	0.94
<b>(2R,3S,7R,9R,11S)</b>	1.68	1.37	2.33	1.93	1.61	1.90	1.58	1.64	1.74	2.40	1.97	1.18	3.30	3.30	1.00	0.96	0.95
(2R,3S,7R,9R,11R)	1.50	1.30	2.33	1.94	1.63	1.89	1.58	1.50	1.91	2.40	1.52	1.51	3.33	3.35	0.97	0.96	0.93
(2R,3S,7R,9S,11R)	1.59	1.42	2.23	1.78	1.31	1.95	1.84	1.48	1.83	1.60	1.79	0.90	3.34	3.36	1.01	0.99	1.03
(2R,3S,7R,9S,11S)	1.80	1.29	2.30	1.77	1.29	1.97	1.83	1.52	1.84	1.63	1.40	1.32	3.39	3.36	0.97	0.98	1.03
(2S,3S,7R,9R,11R)	1.59	1.14	1.69	1.92	1.39	1.79	1.58	1.61	1.35	2.04	1.39	1.31	3.39	3.37	1.07	0.95	0.97
(2S,3S,7R,9R,11S)	1.69	1.45	2.30	2.06	1.45	1.97	1.68	1.79	1.88	2.24	1.86	1.81	3.44	3.28	1.11	0.89	0.96
(2S,3S,7R,9S,11S)	2.02	1.50	2.35	2.57	1.31	1.95	1.64	1.81	1.91	2.28	2.40	1.20	3.53	3.53	0.93	0.90	0.96
(2S,3S,7R,9S,11R)	1.77	1.45	2.30	2.07	1.46	1.97	1.68	1.79	1.88	2.25	1.83	1.80	3.44	3.31	1.13	0.89	0.96

a: Hirota, M.; Shimizu, Y.; Kamo, T.; Makabe, H.; Shibata, H. *Bioscience, Biotechnology, and Biochemistry* **2003**, 67, 1597-1600.

Statistical analysis of  $\delta^{13}\text{C}$  for **1a** and its isomers.

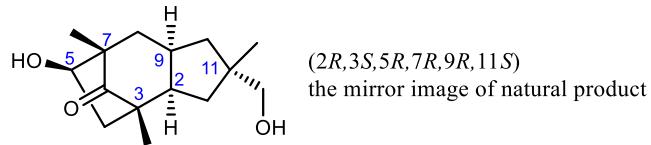
vs experimental			repaesentin B <sup>b</sup>				
RMSD	max deviation	DP4	RMSD	max deviation	DP4		
<b>(2R,3S,7R,9R,11S)</b>	<b>0.8</b>	<b>1.4</b>	<b>66.7%</b>	<b>0.7</b>	<b>1.3</b>	<b>64.3%</b>	proposed diastereomer
(2R,3S,7R,9R,11R)	1.0	2.6	33.3%	0.9	2.2	35.7%	the 11-epimer
(2R,3S,7R,9S,11R)	2.9	6.3	0.0%	2.9	6.3	0.0%	
(2R,3S,7R,9S,11S)	2.8	6.3	0.0%	2.8	6.3	0.0%	
(2S,3S,7R,9R,11R)	2.6	6.4	0.0%	2.6	6.6	0.0%	
(2S,3S,7R,9R,11S)	2.7	6.3	0.0%	2.7	6.5	0.0%	
(2S,3S,7R,9S,11S)	3.1	7.4	0.0%	3.1	7.5	0.0%	
(2S,3S,7R,9S,11R)	2.9	5.9	0.0%	2.8	6.0	0.0%	

Statistical analysis of  $\delta^1\text{H}$  for **1a** and its isomers.

vs experimental			vs. repaesentin B				
RMSD	max deviation	DP4	RMSD	max deviation	DP4		
<b>(2R,3S,7R,9R,11S)</b>	<b>0.10</b>	<b>0.32</b>	<b>99.5%</b>	<b>0.16</b>	<b>0.70</b>	<b>1.5%</b>	proposed diastereomer
(2R,3S,7R,9R,11R)	0.15	0.40	0.5%	0.10	0.70	98.5%	the 11-epimer
(2R,3S,7R,9S,11R)	0.28	0.91	0.0%	0.30	0.71	0.0%	
(2R,3S,7R,9S,11S)	0.28	0.88	0.0%	0.29	0.70	0.0%	
(2S,3S,7R,9R,11R)	0.24	0.58	0.0%	0.25	0.69	0.0%	
(2S,3S,7R,9R,11S)	0.23	0.70	0.0%	0.22	0.68	0.0%	
(2S,3S,7R,9S,11S)	0.30	0.65	0.0%	0.34	0.71	0.0%	
(2S,3S,7R,9S,11R)	0.23	0.69	0.0%	0.22	0.68	0.0%	

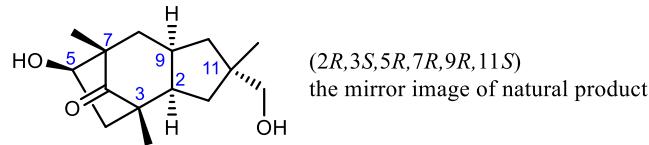
b: Hirota, M.; Shimizu, Y.; Kamo, T.; Makabe, H.; Shibata, H. *Bioscience, Biotechnology, and Biochemistry* **2003**, 67, 1597-1600.

Calculated  $^{13}\text{C}$  NMR chemical shift of **1b** and its isomers.



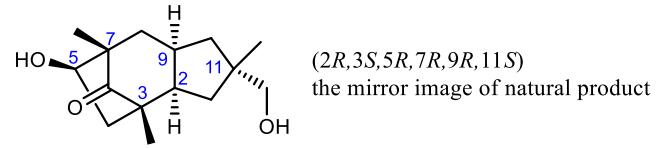
	C-1	C-2	C-3	C-4	C-5	C-6	C-7	C-8	C-9	C-10	C-11	C-12	C-13	C-14	C-15
	36.5	59.2	48.5	45.7	71.6	221.0	51.8	47.6	35.2	40.8	44.3	71.9	27.6	18.7	14.3
(2 <i>R</i> ,3 <i>S</i> ,5 <i>R</i> ,7 <i>S</i> ,9 <i>R</i> ,11 <i>S</i> )	37.0	58.3	48.6	44.5	72.9	220.6	51.8	45.9	35.8	39.9	43.7	73.1	27.5	19.7	15.2
(2 <i>R</i> ,3 <i>S</i> ,5 <i>R</i> ,7 <i>S</i> ,9 <i>R</i> ,11 <i>R</i> )	35.4	57.5	48.3	44.2	73.0	221.0	51.9	44.0	35.5	40.3	44.5	71.2	27.3	19.8	15.0
(2 <i>R</i> ,3 <i>S</i> ,5 <i>R</i> ,7 <i>S</i> ,9 <i>S</i> ,11 <i>R</i> )	38.5	55.0	47.7	46.9	78.9	220.4	47.6	46.3	39.1	41.6	43.0	72.6	26.5	16.6	15.6
(2 <i>R</i> ,3 <i>S</i> ,5 <i>R</i> ,7 <i>S</i> ,9 <i>S</i> ,11 <i>S</i> )	39.4	55.5	47.5	46.7	78.4	219.6	47.4	46.0	38.0	40.2	42.7	72.5	26.3	16.5	15.6
(2 <i>R</i> ,3 <i>S</i> ,5 <i>S</i> ,7 <i>S</i> ,9 <i>R</i> ,11 <i>S</i> )	37.7	59.7	50.4	44.1	73.5	222.5	52.1	43.6	35.9	40.5	44.0	73.7	27.9	19.8	19.5
(2 <i>S</i> ,3 <i>S</i> ,5 <i>R</i> ,7 <i>S</i> ,9 <i>R</i> ,11 <i>S</i> )	35.1	54.6	49.1	38.1	74.1	221.0	51.1	41.7	38.0	40.9	43.1	72.7	26.3	18.3	15.5
(2 <i>S</i> ,3 <i>S</i> ,5 <i>R</i> ,7 <i>S</i> ,9 <i>S</i> ,11 <i>S</i> )	38.0	52.5	50.7	37.1	73.9	222.6	51.8	42.1	34.2	41.6	43.6	70.4	25.4	20.3	15.8
(2 <i>S</i> ,3 <i>S</i> ,5 <i>R</i> ,7 <i>S</i> ,9 <i>R</i> ,11 <i>R</i> )	36.6	55.4	49.3	38.2	74.6	221.9	51.3	41.7	37.2	39.8	43.6	72.7	26.6	18.4	15.6
(2 <i>S</i> ,3 <i>S</i> ,5 <i>R</i> ,7 <i>S</i> ,9 <i>S</i> ,11 <i>R</i> )	39.6	53.7	50.4	38.8	74.1	223.1	51.9	42.0	34.2	43.3	43.6	71.4	24.6	20.2	15.7
(2 <i>R</i> ,3 <i>S</i> ,5 <i>S</i> ,7 <i>S</i> ,9 <i>R</i> ,11 <i>R</i> )	36.1	58.6	49.6	43.6	72.9	221.1	51.8	41.4	35.2	40.4	44.3	71.3	27.2	19.8	19.2
(2 <i>R</i> ,3 <i>S</i> ,5 <i>S</i> ,7 <i>S</i> ,9 <i>S</i> ,11 <i>S</i> )	39.2	55.2	47.4	46.0	74.1	220.6	48.1	35.5	37.4	40.3	42.9	72.6	26.3	16.5	21.3
(2 <i>R</i> ,3 <i>S</i> ,5 <i>S</i> ,7 <i>S</i> ,9 <i>S</i> ,11 <i>R</i> )	38.4	54.0	47.3	45.6	74.2	220.5	48.0	35.7	38.5	41.0	43.0	72.5	26.4	16.5	21.3
(2 <i>S</i> ,3 <i>S</i> ,5 <i>S</i> ,7 <i>S</i> ,9 <i>R</i> ,11 <i>S</i> )	35.2	55.7	50.2	37.5	73.8	221.2	50.9	38.5	37.4	40.6	43.0	72.8	26.3	18.3	19.5
(2 <i>S</i> ,3 <i>S</i> ,5 <i>S</i> ,7 <i>S</i> ,9 <i>S</i> ,11 <i>S</i> )	38.4	54.3	51.8	35.8	73.4	222.8	51.1	38.6	34.0	40.2	43.7	70.4	25.9	20.4	20.3
(2 <i>S</i> ,3 <i>S</i> ,5 <i>S</i> ,7 <i>S</i> ,9 <i>S</i> ,11 <i>R</i> )	38.4	54.3	51.8	35.8	73.4	222.8	51.1	38.6	34.0	40.1	43.7	70.4	25.8	20.4	20.3
(2 <i>S</i> ,3 <i>S</i> ,5 <i>S</i> ,7 <i>S</i> ,9 <i>R</i> ,11 <i>R</i> )	35.2	55.7	50.2	37.5	73.8	221.2	50.9	38.5	37.4	40.6	43.0	72.8	26.3	18.3	19.5

Calculated  $^1\text{H}$  NMR chemical shift of **1b** and its isomers.



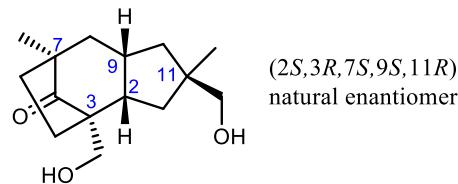
	H $\alpha$ -1	H $\beta$ -1	H-2	H $\alpha$ -4	H $\beta$ -4	H-5	H $\alpha$ -8	H $\beta$ -8	H-9	H $\alpha$ -10	H $\beta$ -10	H-12	H-12	H-13	H-14	H-15
	1.07	1.67	2.28	1.55	2.62	4.18	1.66	1.85	2.35	1.05	1.75	3.23	3.28	1.06	1.01	0.98
(2R,3S,5R,7S,9R,11S)	1.36	1.68	2.32	1.68	2.45	4.08	1.63	1.70	2.21	1.12	1.96	3.28	3.30	0.98	1.02	0.90
(2R,3S,5R,7S,9R,11R)	1.25	1.55	2.32	1.72	2.45	4.07	1.45	2.03	2.21	1.48	1.61	3.30	3.32	0.92	1.02	0.86
(2R,3S,5R,7S,9S,11R)	1.39	1.57	2.08	1.24	2.47	4.18	1.43	1.85	1.58	0.86	1.77	3.34	3.36	0.99	1.02	0.94
(2R,3S,5R,7S,9S,11S)	1.25	1.78	2.15	1.20	2.45	4.16	1.47	1.84	1.59	1.32	1.34	3.34	3.37	0.95	1.01	0.94
(2R,3S,5S,7S,9R,11S)	1.37	1.75	2.48	2.00	2.03	3.95	1.63	2.07	2.88	1.21	1.92	3.33	3.33	1.03	0.96	0.93
(2S,3S,5R,7S,9R,11S)	1.20	1.66	1.64	1.50	2.52	3.94	1.24	1.59	1.94	0.94	1.76	3.42	3.45	0.96	1.02	0.91
(2S,3S,5R,7S,9S,11S)	1.49	2.04	2.33	1.37	3.23	4.15	1.77	1.89	2.24	1.14	2.32	3.52	3.53	0.90	0.96	0.92
(2S,3S,5R,7S,9R,11R)	1.10	1.59	1.66	1.52	2.44	3.98	1.31	1.60	1.80	1.29	1.35	3.38	3.41	1.05	1.02	0.92
(2S,3S,5R,7S,9S,11R)	1.44	1.77	2.29	1.54	2.66	4.17	1.74	1.86	2.24	1.66	1.78	3.31	3.42	1.12	0.96	0.92
(2R,3S,5S,7S,9R,11R)	1.27	1.57	2.49	2.00	2.04	3.91	1.85	1.92	2.85	1.51	1.61	3.32	3.34	0.94	0.95	0.87
(2R,3S,5S,7S,9S,11S)	1.22	1.79	2.49	1.59	1.77	3.90	1.35	2.30	1.60	1.30	1.39	3.37	3.38	0.97	0.95	1.01
(2R,3S,5S,7S,9S,11R)	1.51	1.38	2.51	1.60	1.83	3.90	1.33	2.25	1.54	1.00	1.73	3.33	3.35	1.02	0.96	0.99
(2S,3S,5S,7S,9R,11S)	1.22	1.70	1.74	1.77	2.05	3.90	1.18	1.99	2.55	0.96	1.73	3.43	3.46	0.99	0.96	0.93
(2S,3S,5S,7S,9S,11S)	1.51	2.26	2.46	1.67	2.80	3.96	1.74	2.26	2.32	1.03	3.01	3.49	3.49	0.89	0.90	0.91
(2S,3S,5S,7S,9S,11R)	1.51	2.26	2.46	1.67	2.79	3.96	1.74	2.26	2.32	1.02	3.00	3.49	3.49	0.89	0.90	0.91
(2S,3S,5S,7S,9R,11R)	1.22	1.70	1.74	1.77	2.05	3.90	1.18	1.99	2.55	0.96	1.73	3.43	3.46	0.99	0.96	0.93

Statistical analysis of  $\delta^{13}\text{C}$  and  $^1\text{H}$  for **1b** and its isomers.



	$^{13}\text{C}$			$^1\text{H}$			$^1\text{H} + ^{13}\text{C}$	
	RMSD (ppm)	max dev (ppm)	DP4	RMSD (ppm)	max dev (ppm)	DP4	DP4	
(2R,3S,5R,7S,9R,11S)	0.9	1.7	77.3%	0.12	0.29	94.9%	99.7%	proposed diasteromer
(2R,3S,5R,7S,9R,11 <u>R</u> )	1.3	3.6	22.2%	0.17	0.43	0.9%	0.3%	11-epimer
(2R,3S,5R,7S,9S,11R)	2.9	7.3	0.0%	0.25	0.77	0.0%	0.0%	
(2R,3S,5R,7S,9S,11S)	2.7	6.8	0.0%	0.26	0.76	0.0%	0.0%	
(2R,3S,5S,7S,9R,11S)	2.0	5.2	0.1%	0.27	0.59	0.0%	0.0%	
(2S,3S,5R,7S,9R,11S)	3.0	7.6	0.0%	0.25	0.64	0.0%	0.0%	
(2S,3S,5R,7S,9S,11S)	3.4	8.6	0.0%	0.28	0.61	0.0%	0.0%	
(2S,3S,5R,7S,9R,11R)	2.9	7.5	0.0%	0.27	0.62	0.0%	0.0%	
(2S,3S,5R,7S,9S,11R)	3.2	6.9	0.0%	0.19	0.61	4.3%	0.0%	
(2R,3S,5S,7S,9R,11R)	2.2	6.2	0.3%	0.28	0.58	0.0%	0.0%	
(2R,3S,5S,7S,9S,11S)	4.1	12.1	0.0%	0.35	0.85	0.0%	0.0%	
(2R,3S,5S,7S,9S,11R)	4.2	11.9	0.0%	0.35	0.81	0.0%	0.0%	
(2S,3S,5S,7S,9R,11S)	3.7	9.1	0.0%	0.27	0.57	0.0%	0.0%	
(2S,3S,5S,7S,9S,11S)	4.3	9.9	0.0%	0.40	1.26	0.0%	0.0%	
(2S,3S,5S,7S,9S,11R)	4.3	9.9	0.0%	0.40	1.25	0.0%	0.0%	
(2S,3S,5S,7S,9R,11R)	3.7	9.1	0.0%	0.27	0.57	0.0%	0.0%	

Calculated  $^{13}\text{C}$  NMR chemical shift of **1c** and its isomers.

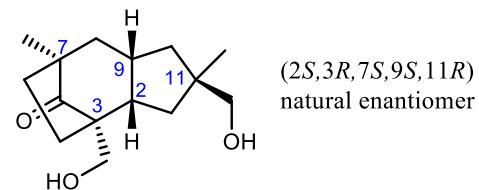


	C-1	C-2	C-3	C-4	C-5	C-6	C-7	C-8	C-9	C-10	C-11	C-12	C-13	C-14	C-15
	36.5	55.5	54.6	27.7	29.7	220.9	47.3	49.9	36.5	41.1	45.1	71.7	28.4	63.3	19.9
(2 <i>R</i> ,3 <i>R</i> ,7 <i>S</i> ,9 <i>R</i> ,11 <i>R</i> )	37.0	48.2	55.5	20.1	30.3	229.8	46.3	43.9	34.2	41.5	43.5	70.3	25.2	65.3	21.1
(2 <i>R</i> ,3 <i>R</i> ,7 <i>S</i> ,9 <i>R</i> ,11 <i>S</i> )	38.6	49.4	55.2	21.9	30.3	229.5	46.2	43.7	34.2	43.3	43.5	71.1	24.5	65.1	21.0
(2 <i>R</i> ,3 <i>R</i> ,7 <i>S</i> ,9 <i>S</i> ,11 <i>R</i> )	34.1	51.5	54.2	21.4	30.9	227.6	46.4	43.3	37.9	40.5	43.4	72.8	26.2	64.7	20.2
(2 <i>R</i> ,3 <i>R</i> ,7 <i>S</i> ,9 <i>S</i> ,11 <i>S</i> )	35.9	52.2	53.8	21.4	31.0	227.6	46.5	43.5	37.0	38.7	43.4	72.6	26.3	64.6	20.2
(2 <i>S</i> ,3 <i>R</i> ,7 <i>S</i> ,9 <i>R</i> ,11 <i>R</i> )	36.7	55.4	52.1	29.4	35.1	228.4	42.8	47.5	38.8	40.3	43.3	72.6	26.4	65.4	21.5
(2 <i>S</i> ,3 <i>R</i> ,7 <i>S</i> ,9 <i>R</i> ,11 <i>S</i> )	35.5	53.9	53.6	28.7	35.3	228.0	42.8	47.1	40.2	43.9	45.0	75.6	26.1	66.6	21.5
(2 <i>S</i> ,3 <i>R</i> ,7 <i>S</i> ,9 <i>S</i> ,11 <i>R</i> )	37.8	55.6	54.2	26.7	29.0	226.8	46.7	46.8	36.7	39.0	43.6	73.1	27.7	65.3	20.2
(2 <i>S</i> ,3 <i>R</i> ,7 <i>S</i> ,9 <i>S</i> ,11 <i>S</i> )	36.0	55.0	53.6	26.8	29.2	227.0	46.7	45.2	36.3	39.2	44.4	71.1	27.1	65.6	20.0

Calculated  $^1\text{H}$  NMR chemical shift of **1c** and its isomers.

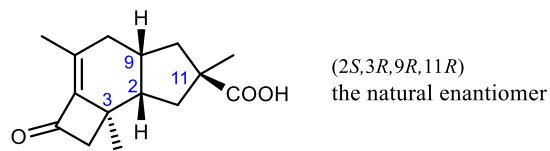
	H $\alpha$ -1	H $\beta$ -1	H-2	H $\alpha$ -4	H $\beta$ -H	H $\alpha$ -5	H $\beta$ -5	H-8	H-8	H-9	H $\alpha$ -10	H $\beta$ -10	H-12	H-12	H-13	H-14	H-14	H-15
	0.96	1.71	2.52	2.06	1.88	1.56	2.01	1.58	1.75	2.56	1.03	1.78	3.13	3.19	1.03	3.37	3.59	0.87
(2 <i>R</i> ,3 <i>R</i> ,7 <i>S</i> ,9 <i>R</i> ,11 <i>R</i> )	1.52	2.02	2.98	2.48	1.41	1.63	1.99	1.91	1.85	2.34	1.20	2.54	3.53	3.53	0.92	3.39	3.46	0.94
(2 <i>R</i> ,3 <i>R</i> ,7 <i>S</i> ,9 <i>R</i> ,11 <i>S</i> )	1.36	1.78	2.93	1.84	1.58	1.67	1.99	1.88	1.82	2.33	1.82	1.87	3.33	3.46	1.11	3.38	3.44	0.94
(2 <i>R</i> ,3 <i>R</i> ,7 <i>S</i> ,9 <i>S</i> ,11 <i>R</i> )	1.36	1.62	2.14	1.75	1.49	1.55	1.81	1.32	1.62	2.21	1.00	1.80	3.44	3.46	1.00	3.51	3.55	0.94
(2 <i>R</i> ,3 <i>R</i> ,7 <i>S</i> ,9 <i>S</i> ,11 <i>S</i> )	1.12	1.64	2.26	1.65	1.38	1.57	1.82	1.43	1.65	2.05	1.39	1.56	3.36	3.43	1.02	3.41	3.60	0.95
(2 <i>S</i> ,3 <i>R</i> ,7 <i>S</i> ,9 <i>R</i> ,11 <i>R</i> )	1.77	2.30	2.36	1.49	1.41	1.81	1.97	1.88	1.58	1.75	1.39	1.40	3.36	3.41	0.98	3.66	3.75	1.02
(2 <i>S</i> ,3 <i>R</i> ,7 <i>S</i> ,9 <i>R</i> ,11 <i>S</i> )	1.59	2.11	2.33	1.47	1.13	1.80	1.98	1.87	1.40	2.73	1.16	1.85	3.37	3.45	0.88	3.66	3.82	1.03
(2 <i>S</i> ,3 <i>R</i> ,7 <i>S</i> ,9 <i>S</i> ,11 <i>R</i> )	1.34	1.90	2.30	2.07	1.64	1.56	1.90	1.78	1.66	2.47	1.15	1.97	3.29	3.31	1.00	3.32	3.73	0.94
(2 <i>S</i> ,3 <i>R</i> ,7 <i>S</i> ,9 <i>S</i> ,11 <i>S</i> )	1.57	2.31	2.31	2.03	1.65	1.56	1.89	2.12	1.50	2.46	1.63	1.47	3.32	3.35	0.92	3.36	3.71	0.92

Statistical analysis of  $\delta^{13}\text{C}$  and  ${}^1\text{H}$  for **1c** and its isomers.



	${}^{13}\text{C}$			${}^1\text{H}$			${}^1\text{H}+{}^{13}\text{C}$	
	RMSD	max dev	DP4	RMSD	max dev	DP4	DP4	
(2R,3R,7S,9R,11R)	4.1	8.9	0.0%	0.34	0.76	0.0%	0.0%	
(2R,3R,7S,9R,11S)	3.8	8.6	0.0%	0.28	0.79	0.0%	0.0%	
(2R,3R,7S,9S,11R)	3.3	6.7	0.0%	0.24	0.40	0.0%	0.0%	
(2R,3R,7S,9S,11S)	3.2	6.7	0.0%	0.25	0.51	0.0%	0.0%	
(2S,3R,7S,9R,11R)	3.1	7.5	0.0%	0.40	0.81	0.0%	0.0%	
(2S,3R,7S,9R,11S)	3.3	7.1	0.0%	0.34	0.75	0.0%	0.0%	
(2S,3R,7S,9S,11R)	2.0	5.9	69.5%	0.16	0.38	100.0%	100.0%	proposed diastereomer
(2S,3R,7S,9S,11S)	2.2	6.1	30.5%	0.31	0.61	0.0%	0.0%	11-epimer

Calculated  $^{13}\text{C}$  NMR chemical shift of **2a** and its isomers.

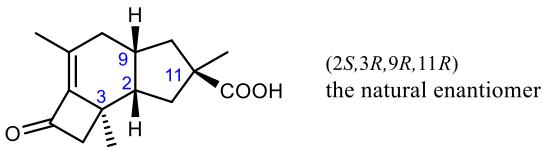


	C-1	C-2	C-3	C-4	C-5	C-6	C-7	C-8	C-9	C-10	C-11	C-12	C-13	C-14	C-15
experimental	37.8	47.2	36.5	60.9	197.0	150.6	143.1	35.4	42.0	45.1	51.0	182.0	24.8	20.4	20.4
(2R,3R,9R11R)	38.1	49.9	39.3	47.9	195.0	147.3	138.8	35.5	44.6	41.5	47.5	178.4	26.6	28.6	19.9
(2R,3R,9S,11R)	40.1	45.2	35.9	53.1	195.0	143.8	139.0	32.5	37.4	43.2	47.5	178.7	25.3	26.4	19.4
(2R,3R,9R,11S)	39.2	50.2	39.0	47.9	195.2	147.5	138.7	35.5	44.1	40.1	47.5	178.4	26.4	28.6	19.9
(2R,3R,9S,11S)	42.0	45.1	36.2	54.3	195.2	146.7	139.9	33.3	38.4	45.4	48.7	178.1	24.0	24.2	20.6
(2S,3R,9R,11R)	37.7	47.8	36.7	58.6	194.3	150.3	142.0	34.7	41.9	45.9	50.6	178.2	24.2	20.8	19.3
(2S,3R,9S,11R)	40.0	49.8	36.4	54.3	195.4	146.8	137.7	37.4	37.3	42.2	47.3	178.9	26.3	21.2	18.5
(2S,3R,9R,11S)	38.0	49.0	37.1	58.7	194.3	150.3	141.5	34.7	42.1	45.5	49.2	177.7	23.6	20.7	19.3
(2S,3R,9S,11S)	37.0	50.4	36.9	54.4	195.4	147.3	137.5	36.8	37.6	44.7	47.3	179.1	26.1	21.4	18.5

Calculated  $^1\text{H}$  NMR chemical shift of **2a** and its isomers.

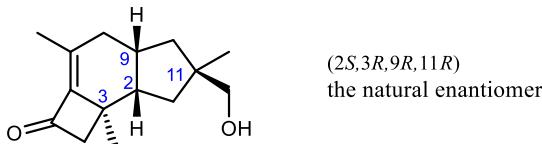
	H $\beta$ -1	H $\alpha$ -1	H-2	H $\beta$ -4	H $\alpha$ -4	H $\beta$ -8	H $\alpha$ -8	H-9	H $\alpha$ -10	H $\beta$ -10	H-13	H-14	H-15
experimental	1.51	2.37	2.29	2.74	2.68	2.25	1.82	2.45	1.17	2.41	1.40	1.16	2.01
(2R,3R,9R11R)	1.8	2.0	1.80	2.66	1.97	1.85	1.77	1.86	1.13	2.26	1.35	1.32	1.86
(2R,3R,9S,11R)	1.7	1.8	2.36	2.74	2.31	2.13	2.14	2.41	1.64	2.28	1.33	1.28	1.87
(2R,3R,9R,11S)	1.2	2.5	2.02	2.54	1.96	1.86	1.86	1.62	1.58	2.01	1.31	1.32	1.86
(2R,3R,9S,11S)	1.2	2.3	2.51	2.85	2.40	2.13	1.80	2.72	1.03	2.51	1.27	1.22	1.94
(2S,3R,9R,11R)	1.5	2.4	2.40	2.66	2.47	2.11	1.81	2.49	1.19	2.38	1.37	1.16	1.92
(2S,3R,9S,11R)	1.4	2.3	1.85	2.59	2.30	2.29	1.73	1.98	1.76	2.12	1.35	1.16	1.82
(2S,3R,9R,11S)	1.7	2.5	2.17	2.59	2.50	2.16	1.93	2.51	1.83	2.07	1.28	1.23	1.93
(2S,3R,9S,11S)	1.6	2.3	1.66	2.55	2.32	2.27	1.60	2.24	1.09	2.42	1.34	1.24	1.82

Statistical analysis of  $\delta^{13}\text{C}$  and  ${}^1\text{H}$  for **2a** and its isomers.



	${}^{13}\text{C}$			${}^1\text{H}$			${}^1\text{H}+{}^{13}\text{C}$	
	RMSD (ppm)	max dev (ppm)	DP4	RMSD (ppm)	max dev (ppm)	DP4	DP4	
( <i>2R,3R,9R,11R</i> )	4.7	13.0	0.0%	0.34	0.71	0.0%	0.0%	
( <i>2R,3R,9S,11R</i> )	3.9	7.8	0.0%	0.27	0.62	0.0%	0.0%	
( <i>2R,3R,9R,11S</i> )	4.8	13.0	0.0%	0.39	0.83	0.0%	0.0%	
( <i>2R,3R,9S,11S</i> )	3.1	6.6	0.0%	0.18	0.34	0.1%	0.0%	
( <i>2S,3R,9R,11R</i> )	1.5	3.8	87.3%	0.09	0.21	99.9%	100.0%	proposed diastereomer
( <i>2S,3R,9S,11R</i> )	3.3	6.6	0.0%	0.29	0.59	0.0%	0.0%	
( <i>2S,3R,9R,11S</i> )	1.7	4.3	12.7%	0.24	0.66	0.0%	0.0%	11-epimer
( <i>2S,3R,9S,11S</i> )	3.2	6.5	0.0%	0.24	0.63	0.0%	0.0%	

Calculated  $^{13}\text{C}$  NMR chemical shift of **2b** and its isomers.

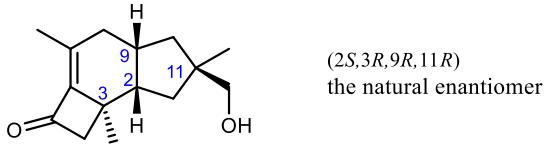


	C-1	C-2	C-3	C-4	C-5	C-6	C-7	C-8	C-9	C-10	C-11	C-12	C-13	C-14	C-15
experiential	36.2	47.4	36.8	60.9	197.2	150.7	143.3	35.8	41.8	43.6	45.5	69.4	24.5	20.4	20.4
(2R,3R,9R,11R)	36.3	49.8	39.4	47.8	195.4	147.2	139.1	35.9	44.9	39.9	43.3	72.5	26.5	28.7	19.9
(2R,3R,9S,11R)	37.6	45.2	36.0	53.4	195.3	144.8	139.2	33.4	37.5	43.1	43.3	71.4	24.5	26.0	19.8
(2R,3S,9R,11R)	35.7	50.1	36.8	54.5	195.7	147.2	137.6	37.5	38.0	43.4	42.7	72.9	26.7	21.5	18.5
(2R,3S,9S,11R)	35.2	47.9	36.9	58.8	194.5	150.4	142.2	35.3	42.4	42.6	45.6	71.5	22.4	20.9	19.2
(2S,3R,9R,11R)	35.9	48.8	36.9	58.7	194.5	150.3	142.4	35.3	42.5	43.8	45.5	69.9	24.3	20.7	19.3
(2S,3R,9S,11R)	37.1	50.6	36.5	54.5	195.7	147.1	137.5	37.4	37.0	42.2	42.6	72.8	26.6	21.5	18.5
(2S,3S,9R,11R)	39.0	45.7	36.2	53.6	195.4	145.6	138.6	34.3	38.0	43.6	43.2	71.0	25.6	25.6	20.0
(2S,3S,9S,11R)	37.4	50.2	39.3	47.8	195.3	147.3	139.1	35.8	44.0	38.7	43.2	72.6	26.3	28.7	20.0

Calculated  $^1\text{H}$  NMR chemical shift of **2b** and its isomers.

	H $\alpha$ -1	H $\beta$ -1	H-2	H-4	H-4	H-8	H-8	H-9	H $\alpha$ -10	H $\beta$ -10	H-12	H-12	H-13	H-14	H-15
experiential	1.43	1.73	2.18	2.66	2.69	1.43	2.25	2.41	1.06	1.92	3.4	3.43	1.13	1.18	2.01
(2R,3R,9R,11R)	1.43	1.73	2.18	2.66	2.69	1.43	2.25	2.41	1.06	1.92	3.4	3.43	1.13	1.18	2.01
(2R,3R,9S,11R)	1.54	1.54	1.82	2.62	1.95	1.76	1.83	1.71	1.07	1.79	3.40	3.42	1.05	1.31	1.85
(2R,3S,9R,11R)	1.33	1.46	2.45	2.32	2.78	2.07	2.10	2.48	1.53	1.59	3.40	3.41	1.02	1.27	1.89
(2R,3S,9S,11R)	1.46	1.79	1.70	2.31	2.56	1.60	2.27	2.07	1.02	2.04	1.04	3.42	3.45	1.20	1.81
(2S,3R,9R,11R)	1.44	1.83	2.30	2.48	2.60	1.86	2.12	2.55	1.43	1.53	3.49	3.50	1.05	1.18	1.93
(2S,3R,9S,11R)	1.52	1.74	2.18	2.48	2.59	1.83	2.12	2.51	1.13	1.99	3.49	3.52	1.08	1.18	1.92
(2S,3S,9R,11R)	1.32	1.81	1.73	2.30	2.56	1.65	2.28	2.02	1.43	1.65	3.44	3.43	1.06	1.19	1.81
(2S,3S,9S,11R)	1.17	1.77	2.43	2.34	2.83	1.80	2.17	2.48	1.16	1.93	3.44	3.45	1.01	1.25	1.91
(2R,3R,9R,11R)	1.09	1.90	1.86	1.94	2.56	1.84	1.83	1.64	1.37	1.54	3.43	3.45	1.04	1.30	1.86

Statistical analysis of  $\delta^{13}\text{C}$  and  ${}^1\text{H}$  for **2b** and its isomers.

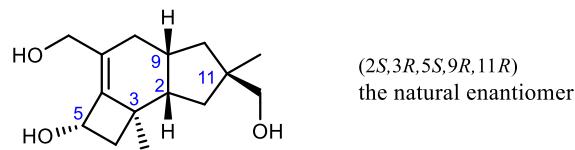


	${}^{13}\text{C}$			${}^1\text{H}$			${}^1\text{H}+{}^{13}\text{C}$	
	RMSD (ppm)	max dev (ppm)	DP4	RMSD (ppm)	max dev (ppm)	DP4	${}^1\text{H}$	DP4
2R3R9R11R	4.7	13.1	0.0%	0.32	0.74	0.0%	0.0%	
(2R3R9S11R)	3.5	7.5	0.0%	0.27	0.64	0.0%	0.0%	
(2R3S9R11R)	3.1	6.4	0.0%	0.88	2.36	0.0%	0.0%	
(2R3S9S11R)	1.3	2.7	12.3%	0.20	0.43	0.2%	0.0%	11-epimer
(2S3R9R11R)	1.1	2.7	87.7%	0.14	0.40	97.2%	100.0%	proposed diastereomer
(2S3R9S11R)	3.2	6.4	0.0%	0.24	0.45	0.0%	0.0%	
(2S3S9R11R)	3.4	7.3	0.0%	0.17	0.37	2.6%	0.0%	
(2S3S9S11R)	4.7	13.1	0.0%	0.37	0.77	0.0%	0.0%	

Calculated  $^{13}\text{C}$  NMR chemical shift of **3** and its isomers.

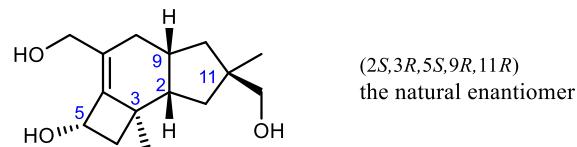
	C-1	C-2	C-3	C-4	C-5	C-6	C-7	C-8	C-9	C-10	C-11	C-12	C-13	C-14	C-15
experiential	35.7	47.3	43.1	46.6	69.3	146.1	134.1	29.4	41.6	43.7	45.1	69.4	24.4	21.8	63.7
2S3R5R9S11R	36.1	50.3	37.0	48.0	68.8	143.6	135.6	30.2	40.5	43.1	45.2	69.5	24.4	21.6	64.5
2S3R5S9S11R	35.8	48.0	40.8	44.8	69.3	144.2	137.4	30.1	41.8	43.6	45.1	69.8	24.4	22.1	65.6
2S3S5R9S11R	41.2	45.1	40.9	39.9	69.4	141.6	136.8	27.9	39.0	44.1	43.5	69.6	24.2	25.3	66.7
2R3R5R9R11R	39.6	47.4	39.7	41.5	70.4	146.8	134.2	33.1	37.8	45.3	43.3	71.8	27.7	24.6	64.2
2R3R5R9S11R	35.2	51.1	40.6	38.0	72.9	147.3	131.9	31.8	44.8	39.8	43.2	72.6	26.4	27.0	64.6
2R3R5S9R11R	39.4	45.7	42.9	40.0	69.5	143.7	135.7	28.7	38.7	43.3	43.2	70.9	24.2	24.7	64.4
2R3S5R9R11R	35.2	47.3	40.8	44.8	69.3	144.2	137.5	30.0	41.6	43.1	45.1	72.5	22.2	22.1	65.6
2R3S5R9S11R	35.3	50.1	43.8	42.2	73.2	141.7	134.0	32.2	37.4	43.2	42.5	72.8	26.6	21.9	65.7
2R3S5S9R11R	35.1	49.6	36.8	48.4	69.0	143.2	136.1	30.2	40.4	42.2	45.2	71.6	22.2	21.8	64.4
2S3R5R9R11R	36.3	52.0	37.4	43.9	72.2	143.9	130.2	33.3	37.0	41.9	42.5	72.8	26.5	21.2	64.5
2S3R5S9R11R	36.4	51.1	43.6	42.2	73.2	141.5	134.4	32.0	36.8	42.0	42.4	72.6	26.7	21.7	65.7
2S3S5R9R11R	36.2	52.2	47.3	36.5	74.9	141.8	137.5	30.5	44.7	38.4	43.3	72.6	26.3	28.8	65.4
2S3S5S9R11R	36.2	52.0	40.8	37.8	72.8	148.2	130.9	31.8	43.8	38.5	43.2	72.6	26.3	26.9	64.7
2R3R5S9S11R	34.9	51.5	47.6	36.1	75.2	143.1	137.3	30.8	45.7	40.0	43.2	72.7	26.4	28.6	65.2
2R3S5S9S11R	34.9	51.3	37.8	43.8	72.1	145.0	129.2	33.4	37.8	43.4	42.5	73.0	26.6	21.3	64.5
2S3S5S9S11R	38.0	46.3	37.0	40.4	71.3	140.2	129.0	31.2	35.6	42.1	42.3	73.4	27.8	27.3	64.1

Calculated  $^1\text{H}$  NMR chemical shift of **3** and its isomers.



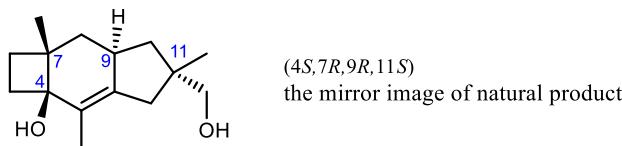
	H $\alpha$ -1	H $\beta$ -1	H-2	H $\alpha$ -4	H $\beta$ -4	H-5	H $\alpha$ -8	H $\beta$ -8	H-9	H $\alpha$ -10	H $\beta$ -10	H-12A	H-12B	H-13	H-14	H-15A	H-15B
experimental	1.29	1.59	2.09	1.88	2.18	4.97	1.72	2.04	2.35	0.98	1.82	3.37	3.38	1.05	1.25	4.15	4.21
2S3R5R9S11R	1.39	1.58	2.14	1.74	2.38	4.90	1.64	1.72	2.34	0.98	1.96	3.53	3.44	1.06	1.06	4.02	4.17
2S3R5S9S11R	1.38	1.62	2.17	1.86	2.07	4.95	1.74	1.72	2.43	1.04	1.90	3.49	3.45	1.03	1.29	4.14	4.15
2S3S5R9S11R	1.11	1.82	2.22	1.73	2.35	4.89	1.38	2.03	2.46	1.02	1.82	3.45	3.45	1.01	1.31	4.08	4.20
2R3R5R9R11R	1.31	1.82	2.14	1.94	2.07	4.91	2.12	2.35	2.33	1.73	1.90	3.31	3.42	0.91	1.12	3.59	4.43
2R3R5R9S11R	1.36	1.43	1.53	1.59	1.95	4.97	1.57	1.65	1.65	1.01	1.70	3.37	3.39	1.01	1.18	4.05	4.07
2R3R5S9R11R	1.23	1.54	2.26	1.74	2.29	4.87	1.81	2.02	2.51	1.57	1.66	3.40	3.36	0.94	1.35	3.91	4.25
2R3S5R9R11R	1.34	1.53	2.25	1.85	2.08	4.96	1.72	1.76	2.47	1.30	1.52	3.45	3.46	1.04	1.26	4.14	4.16
2R3S5R9S11R	1.31	1.54	1.65	1.83	1.90	5.07	1.41	1.96	1.98	0.92	1.97	3.38	3.39	1.01	1.40	4.00	4.14
2R3S5S9R11R	1.34	1.68	2.27	1.74	2.41	4.91	1.66	1.71	2.37	1.25	1.44	3.45	3.45	1.03	1.05	4.01	4.16
2S3R5R9R11R	1.19	1.65	1.65	1.58	2.25	5.01	1.56	1.94	1.92	1.43	1.54	3.38	3.35	0.99	1.07	3.97	4.07
2S3R5S9R11R	1.23	1.68	1.67	1.82	1.90	5.07	1.47	1.96	1.96	1.42	1.54	3.34	3.38	1.39	4.00	4.15	
2S3S5R9R11R	0.99	1.75	1.56	1.50	1.89	5.12	1.56	1.66	1.54	1.26	1.35	3.34	3.38	0.96	1.61	4.11	4.10
2S3S5S9R11R	1.06	1.79	1.56	1.55	1.95	4.97	1.58	1.69	1.65	1.31	1.34	3.36	3.39	0.99	1.17	4.08	4.08
2R3R5S9S11R	1.35	1.56	1.57	1.56	1.99	5.07	1.58	1.61	1.58	1.02	1.65	3.35	3.39	0.96	1.62	4.10	4.05
2R3S5S9S11R	1.34	1.71	1.65	1.61	2.26	5.01	1.50	1.93	1.97	0.98	1.91	3.40	3.38	1.00	1.10	3.98	4.08
2S3S5S9S11R	1.41	1.61	1.91	1.73	2.11	5.00	1.65	1.95	2.16	1.33	1.86	3.36	3.34	1.07	1.73	4.02	3.99

Statistical analysis of  $\delta^{13}\text{C}$  and  ${}^1\text{H}$  for **3** and its isomers



	${}^{13}\text{C}$			${}^1\text{H}$			${}^1\text{H}+{}^{13}\text{C}$	
	RMSD (ppm)	max dev (ppm)	DP4	RMSD (ppm)	max dev (ppm)	DP4	DP4	
2S3R5R9S11R	2.0	6.1	3.6%	0.13	0.32	4.1%	0.2%	
2S3R5S9S11R	1.4	3.3	88.5%	0.10	0.32	90.4%	99.5%	proposed diastereomer
2S3S5R9S11R	3.1	6.7	0.0%	0.14	0.34	2.4%	0.0%	
2R3R5R9R11R	2.7	5.1	0.0%	0.28	0.75	0.0%	0.0%	
2R3R5R9S11R	3.6	8.6	0.0%	0.27	0.70	0.0%	0.0%	
2R3R5S9R11R	2.5	6.6	0.0%	0.18	0.59	0.1%	0.0%	
2R3S5R9R11R	1.7	3.4	7.6%	0.14	0.32	2.9%	0.3%	enantiomer of the 11-epimer
2R3S5R9S11R	2.8	4.4	0.0%	0.19	0.44	0.0%	0.0%	
2R3S5S9R11R	2.3	6.3	0.2%	0.17	0.38	0.0%	0.0%	
2S3R5R9R11R	3.2	5.7	0.0%	0.23	0.45	0.0%	0.0%	
2S3R5S9R11R	3.0	4.8	0.0%	0.61	2.33	0.0%	0.0%	
2S3S5R9R11R	4.6	10.1	0.0%	0.34	0.81	0.0%	0.0%	
2S3S5S9R11R	3.8	8.8	0.0%	0.30	0.70	0.0%	0.0%	
2R3R5S9S11R	4.5	10.5	0.0%	0.29	0.77	0.0%	0.0%	
2R3S5S9S11R	3.1	5.3	0.0%	0.18	0.44	0.0%	0.0%	
2S3S5S9S11R	4.1	6.2	3.6%	0.18	0.48	4.1%	0.2%	

Calculated  $^{13}\text{C}$  NMR chemical shift of **4** and its isomers.

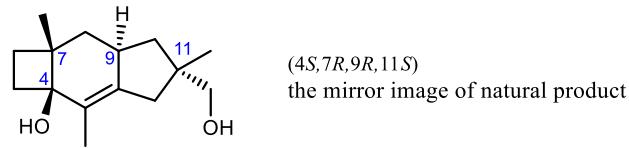


	C-1	C-2	C-3	C-4	C-5	C-6	C-7	C-8	C-9	C-10	C-11	C-12	C-13	C-14	C-15
experimental	39.9	140.1	126.6	73.4	34.5	22.0	43.8	35.4	37.1	43.0	42.1	70.5	25.4	12.8	23.4
(4 <i>S</i> ,7 <i>R</i> ,9 <i>R</i> ,11 <i>S</i> )	39.4	140.2	131.1	73.1	34.2	21.6	42.6	35.1	37.5	42.6	42.1	71.3	24.9	14.8	24.0
(4 <i>S</i> ,7 <i>R</i> ,9 <i>S</i> ,11 <i>S</i> )	39.5	141.8	132.2	78.5	29.6	28.6	40.7	43.7	35.8	41.6	42.5	72.4	24.0	13.2	19.9
(4 <i>S</i> ,7 <i>R</i> ,9 <i>R</i> ,11 <i>R</i> )	40.1	140.8	130.9	73.0	34.2	21.6	42.5	34.7	37.1	41.6	42.5	72.8	24.5	14.8	23.9
(4 <i>S</i> ,7 <i>R</i> ,9 <i>S</i> ,11 <i>R</i> )	39.0	141.5	132.4	78.6	29.7	28.6	40.8	44.4	36.0	42.1	42.4	71.0	24.5	13.3	19.9
(4 <i>R</i> ,7 <i>R</i> ,9 <i>R</i> ,11 <i>S</i> )	37.2	140.0	134.4	79.5	30.0	31.4	43.1	31.6	38.5	44.7	41.4	71.0	25.2	15.0	26.3
(4 <i>R</i> ,7 <i>R</i> ,9 <i>S</i> ,11 <i>S</i> )	40.4	140.4	132.0	79.1	31.1	32.3	42.4	35.5	39.2	40.6	41.7	76.6	25.4	14.0	24.3
(4 <i>R</i> ,7 <i>R</i> ,9 <i>R</i> ,11 <i>R</i> )	36.8	139.7	134.7	79.6	30.1	31.4	43.2	31.7	38.4	43.7	41.8	71.8	24.2	15.1	26.2
(4 <i>R</i> ,7 <i>R</i> ,9 <i>S</i> ,11 <i>R</i> )	36.3	139.4	135.9	80.1	31.0	32.3	42.6	33.7	40.0	43.2	41.7	72.3	26.3	14.1	24.3

Calculated  $^1\text{H}$  NMR chemical shift of **4** and its isomers.

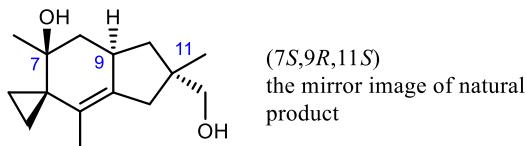
	H $\beta$ -1	H $\alpha$ -1	H $\beta$ -5	H $\alpha$ -5	H $\beta$ -6	H $\alpha$ -6	H $\beta$ -8	H $\alpha$ -8	H-9	H $\beta$ -10	H $\alpha$ -10	H-12	H-12	H-13	H-14	H-15
experimental	2.25	2.07	2.00	2.12	1.48	1.21	1.57	0.84	2.47	1.95	1.05	3.41	3.49	1.09	1.65	1.20
(4 <i>S</i> ,7 <i>R</i> ,9 <i>R</i> ,11 <i>S</i> )	2.30	2.05	2.01	2.10	1.58	1.28	1.47	0.86	2.68	1.93	1.13	3.43	3.53	1.04	1.64	1.17
(4 <i>S</i> ,7 <i>R</i> ,9 <i>S</i> ,11 <i>S</i> )	2.33	1.98	1.91	1.99	1.49	1.99	1.80	1.69	2.56	1.51	1.35	3.43	3.44	1.01	1.59	1.07
(4 <i>S</i> ,7 <i>R</i> ,9 <i>R</i> ,11 <i>R</i> )	2.29	2.10	2.02	2.09	1.60	1.29	1.46	0.99	2.68	1.58	1.40	3.42	3.45	1.07	1.67	1.17
(4 <i>S</i> ,7 <i>R</i> ,9 <i>S</i> ,11 <i>R</i> )	2.20	2.05	1.92	1.98	1.99	1.48	1.83	1.57	2.55	1.86	1.09	3.38	3.46	1.02	1.58	1.07
(4 <i>R</i> ,7 <i>R</i> ,9 <i>R</i> ,11 <i>S</i> )	2.27	2.11	2.25	1.83	2.47	1.58	2.29	1.10	2.74	1.88	1.25	3.38	3.47	1.02	1.66	0.89
(4 <i>R</i> ,7 <i>R</i> ,9 <i>S</i> ,11 <i>S</i> )	2.13	2.01	2.24	1.84	1.48	2.51	2.13	1.55	2.64	1.79	1.71	3.53	3.37	0.91	1.68	1.17
(4 <i>R</i> ,7 <i>R</i> ,9 <i>R</i> ,11 <i>R</i> )	2.43	1.96	2.27	1.84	1.58	2.47	2.32	1.12	2.77	1.45	1.44	3.40	3.41	1.04	1.65	0.87
(4 <i>R</i> ,7 <i>R</i> ,9 <i>S</i> ,11 <i>R</i> )	2.20	1.87	2.29	1.89	1.51	2.52	1.97	1.48	2.66	1.89	0.89	3.42	3.41	0.96	1.68	1.18

Statistical analysis of  $\delta^{13}\text{C}$  and  $^1\text{H}$  for **4** and its isomers.



	$^{13}\text{C}$			$^1\text{H}$			$^1\text{H}+^{13}\text{C}$	
	RMSD (ppm)	max dev (ppm)	DP4	RMSD (ppm)	max dev (ppm)	DP4	DP4	DP4
(4 <i>S</i> ,7 <i>R</i> ,9 <i>R</i> ,11 <i>S</i> )	1.4	4.5	83.5%	0.07	0.21	99.7%	99.9%	proposed diastereomer
(4 <i>S</i> ,7 <i>R</i> ,9 <i>S</i> ,11 <i>S</i> )	3.9	8.3	0.0%	0.33	0.85	0.0%	0.0%	11-epimer
(4 <i>S</i> ,7 <i>R</i> ,9 <i>R</i> ,11 <i>R</i> )	1.5	4.3	16.5%	0.15	0.37	0.3%	0.1%	
(4 <i>S</i> ,7 <i>R</i> ,9 <i>S</i> ,11 <i>R</i> )	4.0	9.0	0.0%	0.25	0.73	0.0%	0.0%	
(4 <i>R</i> ,7 <i>R</i> ,9 <i>R</i> ,11 <i>S</i> )	4.1	9.4	0.0%	0.36	0.99	0.0%	0.0%	
(4 <i>R</i> ,7 <i>R</i> ,9 <i>S</i> ,11 <i>S</i> )	3.9	10.3	0.0%	0.45	1.30	0.0%	0.0%	
(4 <i>R</i> ,7 <i>R</i> ,9 <i>R</i> ,11 <i>R</i> )	4.1	9.4	0.0%	0.44	1.26	0.0%	0.0%	
(4 <i>R</i> ,7 <i>R</i> ,9 <i>S</i> ,11 <i>R</i> )	4.3	10.3	0.0%	0.40	1.31	0.0%	0.0%	

Calculated  $^{13}\text{C}$  NMR chemical shift of **5** and its isomers.



	C-1	C-2	C-3	C-4	C-5	C-6	C-7	C-8	C-9	C-10	C-11	C-12	C-13	C-14	C-15
experimental	39.9	135.4	125.2	5.7	7.7	30.2	70.4	43.4	39.1	42.5	42.4	70.6	25.6	13.2	25.8
(7S,9S,11S)	40.7	141.2	125.1	6.7	11.4	31.0	72.0	41.9	36.0	40.8	42.7	72.6	24.4	14.1	26.3
(7S,9S,11R)	40.2	140.5	125.4	7.0	11.0	30.7	71.8	42.1	36.7	42.1	42.1	71.4	25.3	14.4	26.0
(7S,9R,11R)	39.0	136.7	128.5	7.5	8.9	30.6	70.0	42.7	39.3	42.0	42.5	72.5	25.2	15.2	25.8
(7S,9R,11S)	39.1	136.8	128.5	7.3	9.0	30.6	69.8	43.3	39.8	42.3	42.3	71.7	25.6	15.1	25.8

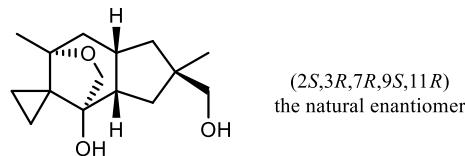
Calculated  $^{13}\text{C}$  NMR chemical shift of **5** and its isomers.

	H $\alpha$ -1	H $\beta$ -1	H <sub>S</sub> -4	H <sub>R</sub> -4	H <sub>S</sub> -5	H <sub>R</sub> -5	H $\beta$ -8	H $\alpha$ -8	H-9	Ha-10	Hb10	H-12a	H-12b	H-13	H-14	H-15
experimental	2.05	2.14	0.75	0.69	0.81	0.48	1.37	1.87	2.55	1.02	1.94	3.49	3.40	1.09	1.28	1.20
(7S,9S,11S)	2.07	2.36	0.73	0.68	0.79	0.65	1.33	1.89	3.15	1.44	1.55	3.46	3.43	1.07	1.21	0.80
(7S,9S,11R)	2.04	2.29	0.64	0.84	0.71	0.66	1.26	1.87	3.05	1.19	1.98	3.57	3.41	1.05	1.20	0.83
(7S,9R,11R)	1.96	2.34	0.85	0.72	0.45	0.82	1.44	1.68	2.76	1.34	1.48	3.44	3.43	1.09	1.24	1.22
(7S,9R,11S)	2.02	2.20	0.84	0.43	0.89	0.73	1.40	1.65	2.73	1.13	1.90	3.51	3.41	1.05	1.24	1.22

Statistical analysis of  $\delta^{13}\text{C}$  and  $^1\text{H}$  for **5** and its isomers.

	$\delta^{13}\text{C}$			$\delta^1\text{H}$			$^1\text{H} + ^{13}\text{C}$		
	RMSD	max dev	DP4	RMSD	max dev	DP4	DP4		
(7S,9S,11S)	2.2	5.8	0.1%	0.24	0.60	0.0%	0.0		
(7S,9S,11R)	1.8	5.1	2.5%	0.18	0.50	0.6%	0.0		
(7S,9R,11R)	1.3	3.3	30.3%	0.21	0.46	0.0%	0.0	11-epimer	
(7S,9R,11S)	1.2	3.3	67.0%	0.12	0.26	99.3%	100.0	proposed diastereomer	

Calculated  $^{13}\text{C}$  NMR chemical shift of **6** and its isomers.

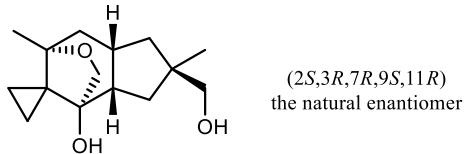


	C-1	C-2	C-3	C-4	C-5	C-6	C-7	C-8	C-9	C-10	C-11	C-12	C-13	C-14	C-15
experimental	37.2	46.6	78.0	2.3	3.2	34.3	83.1	39.2	35.4	43.5	43.2	70.3	24.3	71.2	21.7
(2S,3R,7R,9S,11R)	37.3	47.7	78.2	4.1	4.8	35.3	83.7	39.0	36.7	43.4	42.9	72.2	24.5	73.1	22.7
(2S,3R,7R,9S,11S)	36.6	46.7	78.4	4.1	4.9	35.4	83.6	39.1	36.5	42.2	43.1	71.0	26.0	72.4	22.8
(2S,3R,7R,9R,11R)	36.0	51.5	76.8	4.8	4.6	38.1	83.6	41.7	38.6	39.9	42.2	72.5	26.4	72.9	22.2
(2S,3R,7R,9R,11S)	34.9	50.5	76.7	4.6	4.9	38.0	83.5	41.8	39.6	41.0	42.2	72.6	26.4	73.1	22.1
(2R,3R,7R,9S,11R)	36.1	51.5	74.5	2.2	4.9	32.5	83.1	41.6	39.1	40.9	42.5	72.6	26.3	78.4	23.3
(2R,3R,7R,9R,11S)	35.5	51.0	76.3	2.1	6.6	33.1	82.8	43.4	36.6	39.9	43.7	72.2	27.2	78.5	21.9
(2R,3R,7R,9R,11R)	34.4	50.6	76.4	2.1	6.7	33.1	83.1	41.7	36.8	40.0	44.2	71.6	26.7	78.4	21.9
(2R,3R,7R,9S,11S)	37.2	52.4	74.4	2.1	4.9	32.4	83.1	41.6	38.0	39.9	42.5	72.5	26.5	78.5	23.4
7,12,14-triol (2S,3R,7R,9S,11R)	34.7	46.2	73.4	6.4	6.0	29.5	74.7	46.4	33.6	41.8	44.2	69.5	24.5	71.3	27.8

Calculated  $^1\text{H}$  NMR chemical shift of **6** and its isomers.

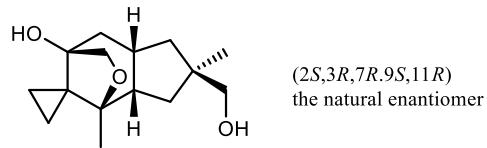
	H $\alpha$ -1	H $\beta$ -1	H-2	H <sub>R</sub> -4	H <sub>S</sub> -4	H <sub>R</sub> -5	H <sub>S</sub> -5	H $\alpha$ -8	H $\beta$ -8	H-9	H $\alpha$ -10	H $\beta$ -10	H-12	H-12	H-13	H $\beta$ -14	H $\alpha$ -14	H-15
experimental	1.53	1.78	2.32	0.52	0.30	0.65	0.68	1.63	1.67	2.45	1.62	1.75	3.31	3.42	1.15	3.48	3.97	1.2
(2S,3R,7R,9S,11R)	1.80	1.60	2.19	0.33	0.55	0.65	0.74	1.48	1.59	2.45	1.70	2.08	3.35	3.44	1.08	3.53	3.95	0.88
(2S,3R,7R,9S,11S)	1.50	2.15	2.29	0.59	0.32	0.64	0.73	1.53	1.60	2.50	1.20	2.34	3.50	3.50	0.97	3.39	4.34	0.87
(2S,3R,7R,9R,11R)	1.18	1.70	1.95	0.75	0.64	0.36	0.54	1.21	1.60	2.24	1.48	1.41	3.42	3.39	1.05	3.48	3.89	0.87
(2S,3R,7R,9R,11S)	1.31	1.55	1.95	0.59	0.35	0.65	0.79	1.17	1.58	2.21	1.08	1.76	3.43	3.46	1.02	3.48	3.91	0.86
(2R,3R,7R,9S,11R)	1.41	1.63	2.11	0.58	0.43	0.77	0.51	1.38	1.56	2.37	1.02	1.76	3.38	3.42	1.01	3.39	3.51	0.89
(2R,3R,7R,9R,11S)	1.95	1.72	2.32	0.61	0.51	0.61	0.86	1.50	1.56	2.56	1.21	1.84	3.28	3.38	1.07	3.65	3.70	0.83
(2R,3R,7R,9R,11R)	1.22	2.45	2.38	0.54	0.49	0.64	0.85	1.42	1.67	2.58	1.49	1.57	3.39	3.39	0.96	3.63	3.73	0.81
(2R,3R,7R,9S,11S)	1.24	1.80	2.09	0.58	0.43	0.53	0.79	1.42	1.59	2.38	1.29	1.41	3.39	3.41	1.03	3.48	3.36	0.90
7,12,14-triol (2S,3R,7R,9S,11R)	1.79	1.28	2.40	0.91	0.18	0.66	0.73	1.65	1.70	2.23	0.86	1.92	3.42	3.48	1.03	3.50	4.10	0.82

Statistical analysis of  $\delta^{13}\text{C}$  and  $^1\text{H}$  for **6** and its isomers.



	$^{13}\text{C}$			$^1\text{H}$			$^1\text{H}+^{13}\text{C}$	
	RMSD (ppm)	max dev (ppm)	DP4	RMSD (ppm)	max dev (ppm)	DP4	DP4	DP4
(2 <i>S</i> ,3 <i>R</i> ,7 <i>R</i> ,9 <i>S</i> ,11 <i>R</i> )	1.07	1.9	47.9%	0.16	0.33	98.5%	99.9%	proposed diastereomer
(2 <i>S</i> ,3 <i>R</i> ,7 <i>R</i> ,9 <i>S</i> ,11 <i>S</i> )	1.01	1.7	52.1%	0.24	0.59	0.1%	0.1%	11-epimer
(2 <i>S</i> ,3 <i>R</i> ,7 <i>R</i> ,9 <i>R</i> ,11 <i>R</i> )	2.44	4.9	0.0%	0.24	0.42	0.0%	0.0%	
(2 <i>S</i> ,3 <i>R</i> ,7 <i>R</i> ,9 <i>R</i> ,11 <i>S</i> )	2.41	4.2	0.0%	0.23	0.54	0.1%	0.0%	
(2 <i>R</i> ,3 <i>R</i> ,7 <i>R</i> ,9 <i>S</i> ,11 <i>R</i> )	3.01	7.2	0.0%	0.23	0.60	0.1%	0.0%	
(2 <i>R</i> ,3 <i>R</i> ,7 <i>R</i> ,9 <i>R</i> ,11 <i>S</i> )	3.01	7.3	0.0%	0.20	0.42	1.1%	0.0%	
(2 <i>R</i> ,3 <i>R</i> ,7 <i>R</i> ,9 <i>R</i> ,11 <i>R</i> )	2.84	7.2	0.0%	0.24	0.67	0.1%	0.0%	
(2 <i>R</i> ,3 <i>R</i> ,7 <i>R</i> ,9 <i>S</i> ,11 <i>S</i> )	3.11	7.3	0.0%	0.23	0.61	0.1%	0.0%	
7,12,14-triol (2 <i>S</i> ,3 <i>R</i> ,7 <i>R</i> ,9 <i>S</i> ,11 <i>R</i> )	3.99	8.4	0.0%	0.27	0.76	0.0%	0.0%	

Calculated  $^{13}\text{C}$  NMR chemical shift of **7** and its isomers.

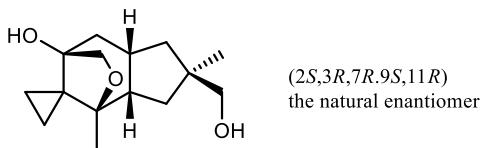


	C-1	C-2	C-3	C-4	C-5	C-6	C-7	C-8	C-9	C-10	C-11	C-12	C-13	C-14	C-15
experimental	37.3	53.1	83.7	0.1	4.1	32.2	75.8	41.9	35.9	41.8	44.2	70.9	27.1	20.5	73.7
( <i>2R,3S,7S,9R,11R</i> )	36.3	53.2	83.7	2.0	6.2	33.3	75.6	40.3	36.7	40.2	44.6	71.3	26.7	21.8	74.9
( <i>2R,3S,7S,9S,11R</i> )	37.8	55.0	83.3	4.6	1.2	33.0	76.9	41.7	38.0	40.3	42.7	72.6	26.2	19.0	79.7
( <i>2R,3S,7S,9S,11S</i> )	38.9	55.8	83.1	4.5	1.1	33.0	76.9	41.6	36.8	39.5	42.7	72.4	26.5	18.9	79.7
( <i>2S,3R,7R,9S,11R</i> )	37.4	53.6	83.8	1.9	6.1	33.5	75.7	41.8	36.7	40.4	44.2	72.2	27.3	21.8	74.9
( <i>2S,3S,7S,9R,11R</i> )	35.9	53.8	83.2	4.6	4.9	38.0	76.6	39.6	37.8	40.1	42.3	72.7	26.2	19.1	77.1
( <i>2S,3S,7S,9S,11R</i> )	37.3	46.7	85.5	3.7	4.8	35.0	74.7	38.5	34.5	43.1	43.0	70.0	24.3	20.6	76.1
( <i>2S,3S,7S,9S,11S</i> )	37.7	49.5	87.9	4.6	5.2	36.2	74.8	37.8	37.2	43.1	43.0	71.4	28.3	19.9	75.7
( <i>2S,3S,7S,9R,11S</i> )	35.4	52.6	83.2	4.6	4.8	37.9	76.3	39.9	38.8	40.6	42.3	72.6	26.4	19.1	77.3

Calculated  $^1\text{H}$  NMR chemical shift of **7** and its isomers.

	H $\alpha$ -1	H $\beta$ -1	H-2	H $R$ -4	H $S$ -4	H $R$ -5	H $S$ -5	H $\alpha$ -8	H $\beta$ -8	H-9	H $\alpha$ -10	H $\beta$ -10	H-12	H-12	H-13	H-14	H $\alpha$ -15	H $\beta$ -15
experimental	1.54	1.51	2.18	0.49	0.58	0.75	0.65	1.7	1.89	2.53	1.19	1.82	3.25	3.35	1.17	0.98	3.57	3.91
( <i>2R,3S,7S,9R,11R</i> )	1.02	2.19	2.29	0.49	0.66	0.78	0.62	1.91	1.45	2.53	1.52	1.58	3.35	3.37	0.95	0.93	3.57	3.79
( <i>2R,3S,7S,9S,11R</i> )	1.41	1.35	2.01	0.59	0.75	0.44	0.33	1.68	1.92	2.31	0.98	1.69	3.34	3.39	0.98	0.90	3.67	3.47
( <i>2R,3S,7S,9S,11S</i> )	1.79	0.90	1.98	0.56	0.77	0.44	0.34	1.72	1.94	2.29	1.26	1.36	3.38	3.37	0.99	0.88	3.47	3.67
( <i>2S,3R,7R,9S,11R</i> )	1.70	1.56	2.23	0.51	0.58	0.80	0.68	1.74	1.64	2.48	1.19	1.82	3.27	3.37	1.08	0.92	3.51	3.80
( <i>2S,3S,7S,9R,11R</i> )	1.50	1.31	1.65	0.35	0.56	0.68	0.67	1.45	1.75	2.21	1.34	1.43	3.34	3.37	1.05	0.83	3.59	3.83
( <i>2S,3S,7S,9S,11R</i> )	1.84	1.47	1.90	0.35	0.57	0.63	0.74	1.69	1.81	2.47	1.65	1.80	3.30	3.47	1.06	0.77	3.63	3.85
( <i>2S,3S,7S,9S,11S</i> )	2.26	1.41	1.88	0.34	0.66	0.70	0.79	1.72	1.85	2.50	1.39	2.30	3.36	3.41	0.90	0.95	3.62	3.94
( <i>2S,3S,7S,9R,11S</i> )	1.48	1.15	1.66	0.36	0.63	0.68	0.72	1.48	1.67	2.15	1.03	1.83	3.42	3.42	0.99	0.83	3.60	3.79

Statistical analysis of  $\delta^{13}\text{C}$  and  $^1\text{H}$  for **7** and its isomers.



	$^{13}\text{C}$			$^1\text{H}$			$^1\text{H}+^{13}\text{C}$	
	RMSD (ppm)	max dev (ppm)	DP4	RMSD (ppm)	max dev (ppm)	DP4		
(2 <i>R</i> ,3 <i>S</i> ,7 <i>S</i> ,9 <i>R</i> ,11 <i>R</i> )	1.1	2.1	30.4%	0.25	0.65	0.0%	11-epimer	
(2 <i>R</i> ,3 <i>S</i> ,7 <i>S</i> ,9 <i>S</i> ,11 <i>R</i> )	2.4	6.0	0.0%	0.19	0.44	0.0%		
(2 <i>R</i> ,3 <i>S</i> ,7 <i>S</i> ,9 <i>S</i> ,11 <i>S</i> )	2.5	6.0	0.0%	0.25	0.64	0.0%		
(2 <i>S</i> ,3 <i>R</i> ,7 <i>R</i> ,9 <i>S</i> ,11 <i>R</i> )	1.1	2.0	69.6%	0.09	0.25	100.0%		proposed diastereomer
(2 <i>S</i> ,3 <i>S</i> ,7 <i>S</i> ,9 <i>R</i> ,11 <i>R</i> )	2.5	5.8	0.0%	0.21	0.53	0.0%		
(2 <i>S</i> ,3 <i>S</i> ,7 <i>S</i> ,9 <i>S</i> ,11 <i>R</i> )	2.6	6.4	0.0%	0.17	0.46	0.0%		
(2 <i>S</i> ,3 <i>S</i> ,7 <i>S</i> ,9 <i>S</i> ,11 <i>S</i> )	2.6	4.5	0.0%	0.24	0.72	0.0%		
(2 <i>S</i> ,3 <i>S</i> ,7 <i>S</i> ,9 <i>R</i> ,11 <i>S</i> )	2.5	5.7	0.0%	0.21	0.52	0.0%		

Calculated  $^{13}\text{C}$  NMR chemical shift of **8** and its isomers.

	C-1	C-2	C-3	C-4	C-5	C-6	C-7	C-8	C-9	C-10	C-11	C-12	C-13	C-14	C-15
	42.1	48.2	81.1	41.4	23.2	49.0	19.5	22.6	29.7	81	38	19.1	28.7	25.7	19.4
(2 <i>R</i> ,3 <i>R</i> ,6 <i>R</i> ,7 <i>R</i> ,9 <i>R</i> ,10 <i>R</i> )	35.2	48.8	82.3	36.5	25.3	44.7	18.6	14.7	28.2	75.9	38.0	24.0	32.1	26.2	30.2
(2 <i>R</i> ,3 <i>R</i> ,6 <i>R</i> ,7 <i>R</i> ,9 <i>S</i> ,10 <i>R</i> )	41.2	55.4	82.4	38.5	22.4	45.5	17.3	18.9	24.6	76.0	42.2	28.9	28.7	25.8	25.2
(2 <i>R</i> ,3 <i>R</i> ,6 <i>R</i> ,7 <i>S</i> ,9 <i>R</i> ,10 <i>R</i> )	37.3	52.6	79.3	42.8	25.7	52.2	17.7	21.6	29.2	78.0	41.8	26.0	28.3	25.3	21.0
(2 <i>R</i> ,3 <i>R</i> ,6 <i>R</i> ,7 <i>S</i> ,9 <i>S</i> ,10 <i>R</i> )	37.4	47.8	79.2	41.4	26.3	45.1	17.4	21.5	27.3	79.1	37.5	23.4	25.1	23.3	24.0
(2 <i>R</i> ,3 <i>R</i> ,6 <i>S</i> ,7 <i>R</i> ,9 <i>R</i> ,10 <i>R</i> )	36.8	48.2	78.9	42.2	23.8	45.1	21.6	17.0	27.3	76.8	37.7	23.9	31.3	23.3	20.1
(2 <i>R</i> ,3 <i>R</i> ,6 <i>S</i> ,7 <i>R</i> ,9 <i>S</i> ,10 <i>R</i> )	40.2	52.8	77.0	40.1	21.9	52.8	16.5	20.7	31.7	76.3	41.5	28.5	28.7	25.1	18.7
(2 <i>R</i> ,3 <i>R</i> ,6 <i>S</i> ,7 <i>S</i> ,9 <i>R</i> ,10 <i>R</i> )	36.0	57.6	75.1	40.1	23.4	48.7	16.8	22.7	24.0	78.5	41.9	27.7	27.4	25.5	30.2
(2 <i>R</i> ,3 <i>R</i> ,6 <i>S</i> ,7 <i>S</i> ,9 <i>S</i> ,10 <i>R</i> )	37.4	46.9	79.0	40.3	27.1	44.1	23.7	14.5	32.4	78.1	36.3	26.8	27.7	22.4	27.1
(2 <i>R</i> ,3 <i>S</i> ,6 <i>R</i> ,7 <i>R</i> ,9 <i>R</i> ,10 <i>R</i> )	31.9	46.4	80.1	37.9	25.7	45.7	20.1	13.9	28.7	75.8	37.5	24.0	31.8	29.9	30.3
(2 <i>R</i> ,3 <i>S</i> ,6 <i>R</i> ,7 <i>R</i> ,9 <i>S</i> ,10 <i>R</i> )	38.8	55.7	79.1	41.3	25.5	45.5	19.3	20.1	23.3	77.6	42.5	25.0	32.7	27.5	25.8
(2 <i>R</i> ,3 <i>S</i> ,6 <i>R</i> ,7 <i>S</i> ,9 <i>R</i> ,10 <i>R</i> )	35.1	52.1	78.9	42.3	25.8	54.6	17.7	20.7	29.6	78.1	41.2	28.5	26.2	26.9	19.7
(2 <i>R</i> ,3 <i>S</i> ,6 <i>R</i> ,7 <i>S</i> ,9 <i>S</i> ,10 <i>R</i> )	36.2	47.2	79.8	40.7	26.3	47.4	17.9	20.1	28.3	79.1	37.3	23.5	25.5	26.1	23.2
(2 <i>S</i> ,3 <i>R</i> ,6 <i>R</i> ,7 <i>R</i> ,9 <i>R</i> ,10 <i>R</i> )	35.5	44.4	80.7	39.3	29.2	45.0	26.0	9.9	30.5	76.9	36.1	28.0	31.4	25.6	27.5
(2 <i>S</i> ,3 <i>R</i> ,6 <i>R</i> ,7 <i>R</i> ,9 <i>S</i> ,10 <i>R</i> )	37.4	56.4	76.1	40.4	23.6	46.6	17.3	24.1	23.6	77.4	41.1	20.5	29.9	27.2	29.5
(2 <i>S</i> ,3 <i>R</i> ,6 <i>R</i> ,7 <i>S</i> ,9 <i>R</i> ,10 <i>R</i> )	40.9	53.0	78.1	40.4	23.0	53.8	16.2	19.2	30.8	77.4	41.0	22.9	34.5	27.1	17.9
(2 <i>S</i> ,3 <i>R</i> ,6 <i>R</i> ,7 <i>S</i> ,9 <i>S</i> ,10 <i>R</i> )*	41.5	47.9	80.1	41.2	24.3	49.3	19.9	21.6	29.8	80.8	37.4	19.9	28.8	25.6	19.8
(2 <i>S</i> ,3 <i>R</i> ,6 <i>S</i> ,7 <i>R</i> ,9 <i>R</i> ,10 <i>R</i> )	35.5	46.9	79.8	41.1	26.4	44.2	17.7	16.2	27.0	74.4	37.3	24.3	30.5	26.2	24.1
(2 <i>S</i> ,3 <i>R</i> ,6 <i>S</i> ,7 <i>R</i> ,9 <i>S</i> ,10 <i>R</i> )	37.9	51.4	79.1	42.0	26.2	53.0	18.1	21.3	30.5	76.5	40.8	19.1	30.4	26.9	20.4
(2 <i>S</i> ,3 <i>R</i> ,6 <i>S</i> ,7 <i>S</i> ,9 <i>R</i> ,10 <i>R</i> )	39.9	53.7	79.2	39.8	22.1	47.0	18.2	17.8	23.5	77.3	41.9	25.1	33.7	29.3	25.4
(2 <i>S</i> ,3 <i>R</i> ,6 <i>S</i> ,7 <i>S</i> ,9 <i>S</i> ,10 <i>R</i> )	38.8	46.2	80.0	37.3	26.8	45.6	17.0	18.2	30.5	80.2	38.1	19.4	29.2	30.5	29.5
(2 <i>S</i> ,3 <i>S</i> ,6 <i>R</i> ,7 <i>R</i> ,9 <i>R</i> ,10 <i>R</i> )	37.2	45.3	79.3	40.4	27.7	44.5	25.7	10.2	30.5	76.9	36.4	28.8	30.1	22.2	27.1
(2 <i>S</i> ,3 <i>S</i> ,6 <i>R</i> ,7 <i>R</i> ,9 <i>S</i> ,10 <i>R</i> )	37.9	57.1	75.2	39.7	23.5	46.7	17.3	23.8	23.5	77.2	41.3	20.5	30.0	25.3	23.5
(2 <i>S</i> ,3 <i>S</i> ,6 <i>R</i> ,7 <i>S</i> ,9 <i>R</i> ,10 <i>R</i> )	41.6	53.7	76.9	40.6	22.9	53.5	16.4	19.2	30.6	77.3	40.8	22.5	34.2	25.7	17.8
(2 <i>S</i> ,3 <i>S</i> ,6 <i>R</i> ,7 <i>S</i> ,9 <i>S</i> ,10 <i>R</i> )	46.2	48.7	80.2	42.8	26.2	54.6	18.6	21.3	29.9	81.1	38.0	19.5	28.9	25.9	20.7
(2 <i>S</i> ,3 <i>S</i> ,6 <i>S</i> ,7 <i>R</i> ,9 <i>R</i> ,10 <i>R</i> )	36.6	47.7	79.3	41.8	26.4	41.7	17.1	17.4	25.8	74.5	37.6	24.1	30.2	22.9	17.4
(2 <i>S</i> ,3 <i>S</i> ,6 <i>S</i> ,7 <i>R</i> ,9 <i>S</i> ,10 <i>R</i> )	40.0	53.1	79.7	42.4	25.7	50.2	18.1	22.4	29.8	76.4	41.4	18.9	30.4	24.9	21.6
(2 <i>S</i> ,3 <i>S</i> ,6 <i>S</i> ,7 <i>S</i> ,9 <i>R</i> ,10 <i>R</i> )	43.5	55.3	82.6	38.6	22.3	46.8	16.8	17.5	23.3	76.9	41.6	22.2	34.8	25.5	24.6
(2 <i>S</i> ,3 <i>S</i> ,6 <i>S</i> ,7 <i>S</i> ,9 <i>S</i> ,10 <i>R</i> )	41.6	48.6	82.0	36.2	27.2	44.2	16.2	18.7	30.4	79.8	38.3	19.6	29.2	25.9	29.3
(2 <i>R</i> ,3 <i>S</i> ,6 <i>S</i> ,7 <i>R</i> ,9 <i>R</i> ,10 <i>R</i> )	35.5	47.6	80.0	41.5	24.3	45.7	21.6	17.3	27.2	76.8	37.5	24.3	31.3	25.9	19.9
(2 <i>R</i> ,3 <i>S</i> ,6 <i>S</i> ,7 <i>R</i> ,9 <i>S</i> ,10 <i>R</i> )	39.7	52.9	78.0	40.1	23.5	52.8	16.2	20.7	31.7	76.2	41.6	28.7	28.9	27.4	18.8
(2 <i>R</i> ,3 <i>S</i> ,6 <i>S</i> ,7 <i>S</i> ,9 <i>S</i> ,10 <i>R</i> )	36.8	46.4	80.8	39.0	28.7	45.1	23.5	14.5	32.7	78.2	36.1	26.0	28.4	25.7	14.5
(2 <i>R</i> ,3 <i>S</i> ,6 <i>S</i> ,7 <i>S</i> ,9 <i>R</i> ,10 <i>R</i> )	35.8	57.2	75.8	40.2	23.4	48.5	16.6	22.9	24.5	78.5	41.8	27.5	27.8	27.3	30.3

Calculated  $^1\text{H}$  NMR chemical shift of **8** and its isomers.

	H-1 1.45	H-1 1.19	H-2 2.61	H-4 1.60	H-4 1.70	H-5 1.80	H-5 1.70	H-6 1.42	H-8 0.45	H-8 0.74	H-9 0.55	H-10 3.14	H-12 0.97	H-13 1.02	H-13 1.27	H-15 0.99
(2 <i>R</i> ,3 <i>R</i> ,6 <i>R</i> ,7 <i>R</i> ,9 <i>R</i> ,10 <i>R</i> )	1.88	1.07	2.02	1.53	1.67	2.17	1.43	3.12	0.36	0.57	0.72	3.91	1.25	1.09	1.13	1.19
(2 <i>R</i> ,3 <i>R</i> ,6 <i>R</i> ,7 <i>R</i> ,9 <i>S</i> ,10 <i>R</i> )	1.69	1.15	2.19	1.64	1.75	1.61	0.97	3.12	0.58	0.76	0.86	3.48	1.10	1.15	1.13	1.12
(2 <i>R</i> ,3 <i>R</i> ,6 <i>R</i> ,7 <i>S</i> ,9 <i>R</i> ,10 <i>R</i> )	2.19	1.19	2.37	1.60	1.79	1.72	1.64	1.96	0.84	0.91	0.42	4.06	1.01	1.03	1.16	1.37
(2 <i>R</i> ,3 <i>R</i> ,6 <i>R</i> ,7 <i>S</i> ,9 <i>S</i> ,10 <i>R</i> )	1.64	1.45	1.87	1.60	1.63	1.72	1.71	1.74	0.23	0.56	0.77	3.00	1.11	1.08	1.12	0.98
(2 <i>R</i> ,3 <i>R</i> ,6 <i>S</i> ,7 <i>R</i> ,9 <i>R</i> ,10 <i>R</i> )	1.80	1.36	2.09	1.66	1.52	1.75	1.52	2.05	0.53	0.47	0.62	3.87	1.14	1.12	1.08	1.11
(2 <i>R</i> ,3 <i>R</i> ,6 <i>S</i> ,7 <i>R</i> ,9 <i>S</i> ,10 <i>R</i> )	1.73	1.35	2.17	1.83	1.75	1.63	1.44	1.30	0.87	0.66	0.60	3.42	1.13	1.11	1.03	1.01
(2 <i>R</i> ,3 <i>R</i> ,6 <i>S</i> ,7 <i>S</i> ,9 <i>R</i> ,10 <i>R</i> )	2.02	1.32	1.58	1.74	1.73	1.37	1.03	1.90	1.00	1.10	0.53	4.09	1.08	1.02	1.07	1.41
(2 <i>R</i> ,3 <i>R</i> ,6 <i>S</i> ,7 <i>S</i> ,9 <i>S</i> ,10 <i>R</i> )	1.52	1.33	1.14	1.57	1.54	1.78	1.60	2.04	0.54	0.71	0.89	3.68	1.15	0.96	1.03	1.05
(2 <i>R</i> ,3 <i>S</i> ,6 <i>R</i> ,7 <i>R</i> ,9 <i>R</i> ,10 <i>R</i> )	1.92	1.37	2.09	1.66	1.55	2.23	1.31	2.26	0.31	0.63	0.78	3.89	1.10	1.23	1.23	1.14
(2 <i>R</i> ,3 <i>S</i> ,6 <i>R</i> ,7 <i>R</i> ,9 <i>S</i> ,10 <i>R</i> )	1.88	1.60	2.13	1.46	1.42	1.38	1.30	2.31	0.76	0.95	1.21	3.34	1.19	1.15	1.16	1.09
(2 <i>R</i> ,3 <i>S</i> ,6 <i>R</i> ,7 <i>S</i> ,9 <i>R</i> ,10 <i>R</i> )	2.43	0.89	2.11	1.74	1.57	2.20	1.48	1.78	0.89	0.94	0.38	4.08	1.04	0.99	1.11	1.49
(2 <i>R</i> ,3 <i>S</i> ,6 <i>R</i> ,7 <i>S</i> ,9 <i>S</i> ,10 <i>R</i> )	1.85	1.16	1.70	1.67	1.48	2.25	1.65	1.67	0.25	0.59	0.77	3.01	1.12	1.06	1.12	1.15
(2 <i>S</i> ,3 <i>R</i> ,6 <i>R</i> ,7 <i>R</i> ,9 <i>R</i> ,10 <i>R</i> )	1.60	1.39	1.86	1.57	1.52	2.17	1.59	2.72	0.26	0.80	0.93	4.00	1.16	1.12	1.07	0.26
(2 <i>S</i> ,3 <i>R</i> ,6 <i>R</i> ,7 <i>R</i> ,9 <i>S</i> ,10 <i>R</i> )	1.58	1.52	1.12	1.72	1.71	1.53	0.80	2.42	1.01	1.10	0.40	3.52	1.00	1.18	1.06	1.14
(2 <i>S</i> ,3 <i>R</i> ,6 <i>R</i> ,7 <i>S</i> ,9 <i>R</i> ,10 <i>R</i> )	1.74	1.20	2.00	1.83	1.82	1.60	1.44	1.86	0.70	0.99	0.56	4.30	1.16	1.16	1.11	1.27
(2 <i>S</i> ,3 <i>R</i> ,6 <i>R</i> ,7 <i>S</i> ,9 <i>S</i> ,10 <i>R</i> ) <sup>*</sup>	1.33	1.43	1.83	1.56	1.60	1.66	2.01	1.57	0.42	0.69	0.64	3.20	1.14	1.08	1.12	0.97
(2 <i>S</i> ,3 <i>R</i> ,6 <i>S</i> ,7 <i>R</i> ,9 <i>R</i> ,10 <i>R</i> )	1.97	1.13	1.97	1.63	1.53	2.22	1.63	2.48	0.47	0.50	0.89	3.78	1.04	1.03	1.13	1.22
(2 <i>S</i> ,3 <i>R</i> ,6 <i>S</i> ,7 <i>R</i> ,9 <i>S</i> ,10 <i>R</i> )	1.83	1.03	2.13	1.71	1.54	2.12	1.52	1.72	0.73	0.94	0.94	3.34	1.02	1.15	1.11	1.13
(2 <i>S</i> ,3 <i>R</i> ,6 <i>S</i> ,7 <i>S</i> ,9 <i>R</i> ,10 <i>R</i> )	1.90	1.54	2.32	1.60	1.59	1.37	1.07	2.50	0.66	0.84	0.97	4.21	1.16	1.20	1.25	1.43
(2 <i>S</i> ,3 <i>R</i> ,6 <i>S</i> ,7 <i>S</i> ,9 <i>S</i> ,10 <i>R</i> )	1.55	1.29	2.03	1.67	1.60	1.34	1.40	2.21	0.40	0.57	0.79	3.19	1.22	1.05	1.22	1.11
(2 <i>S</i> ,3 <i>S</i> ,6 <i>R</i> ,7 <i>R</i> ,9 <i>R</i> ,10 <i>R</i> )	1.75	1.19	1.96	1.59	1.55	1.81	1.63	2.14	0.29	0.92	0.93	3.97	1.11	1.11	1.03	1.06
(2 <i>S</i> ,3 <i>S</i> ,6 <i>R</i> ,7 <i>R</i> ,9 <i>S</i> ,10 <i>R</i> )	1.61	1.41	1.60	1.73	1.72	1.37	1.02	1.75	0.96	1.11	0.56	3.53	1.07	1.19	1.03	1.73
(2 <i>S</i> ,3 <i>S</i> ,6 <i>R</i> ,7 <i>S</i> ,9 <i>R</i> ,10 <i>R</i> )	1.59	1.42	2.34	1.76	1.84	1.67	1.43	1.25	0.70	0.91	0.42	4.27	1.17	1.15	1.00	1.32
(2 <i>S</i> ,3 <i>S</i> ,6 <i>R</i> ,7 <i>S</i> ,9 <i>S</i> ,10 <i>R</i> )	1.67	0.98	2.10	1.51	1.40	2.03	1.43	1.02	0.37	0.70	0.67	3.16	1.18	1.05	1.07	1.07
(2 <i>S</i> ,3 <i>S</i> ,6 <i>S</i> ,7 <i>R</i> ,9 <i>R</i> ,10 <i>R</i> )	1.73	1.46	2.06	1.62	1.60	1.70	1.68	2.53	0.46	0.57	0.90	3.77	1.04	1.02	1.13	1.04
(2 <i>S</i> ,3 <i>S</i> ,6 <i>S</i> ,7 <i>R</i> ,9 <i>S</i> ,10 <i>R</i> )	1.59	1.32	2.23	1.65	1.61	1.72	1.61	1.93	0.72	0.89	0.44	3.32	1.03	1.14	1.12	1.00
(2 <i>S</i> ,3 <i>S</i> ,6 <i>S</i> ,7 <i>S</i> ,9 <i>R</i> ,10 <i>R</i> )	1.50	1.21	2.37	1.68	1.62	1.60	0.89	3.19	0.59	0.78	0.71	4.26	1.23	1.13	1.10	1.46
(2 <i>S</i> ,3 <i>S</i> ,6 <i>S</i> ,7 <i>S</i> ,9 <i>S</i> ,10 <i>R</i> )	1.36	1.03	1.94	1.61	1.60	1.59	1.59	3.14	0.42	0.60	0.76	3.19	1.24	1.03	1.12	1.15
(2 <i>R</i> ,3 <i>S</i> ,6 <i>S</i> ,7 <i>R</i> ,9 <i>R</i> ,10 <i>R</i> )	1.96	1.15	1.89	1.64	1.59	1.97	1.61	2.36	0.49	0.59	0.61	3.88	1.11	1.14	1.13	1.03
(2 <i>R</i> ,3 <i>S</i> ,6 <i>S</i> ,7 <i>R</i> ,9 <i>S</i> ,10 <i>R</i> )	1.66	1.33	1.77	1.86	1.79	1.62	1.36	1.85	0.67	0.94	0.72	3.42	1.14	1.09	1.11	0.94
(2 <i>R</i> ,3 <i>S</i> ,6 <i>S</i> ,7 <i>S</i> ,9 <i>S</i> ,10 <i>R</i> )	1.44	1.32	0.97	1.61	1.51	2.13	1.55	2.57	0.53	0.53	0.88	3.60	1.19	0.98	1.05	1.09
(2 <i>R</i> ,3 <i>S</i> ,6 <i>S</i> ,7 <i>S</i> ,9 <i>R</i> ,10 <i>R</i> )	1.73	1.54	1.09	1.73	1.82	1.53	0.81	2.54	1.01	1.10	0.43	4.08	0.98	1.09	1.07	1.44

Statistical analysis of  $\delta^{13}\text{C}$  and  ${}^1\text{H}$  for **8** and its isomers.

	${}^{13}\text{C}$			${}^1\text{H}$			${}^1\text{H}+{}^{13}\text{C}$	
	RMSD (ppm)	max dev (ppm)	DP4	RMSD (ppm)	max dev (ppm)	DP4	DP4	
(2R,3R,6R,7R,9R,10R)	4.8	10.8	0.0%	0.54	1.98	0.0%	0.0%	
(2R,3R,6R,7R,9S,10R)	4.4	9.8	0.0%	0.52	1.87	0.0%	0.0%	
(2R,3R,6R,7S,9R,10R)	3.1	6.9	0.0%	0.36	2.01	0.0%	0.0%	
(2R,3R,6R,7S,9S,10R)	2.9	4.7	0.0%	0.25	1.73	3.4%	0.0%	
(2R,3R,6S,7R,9R,10R)	3.1	5.6	0.0%	0.32	1.97	0.0%	0.0%	
(2R,3R,6S,7R,9S,10R)	3.6	9.4	0.0%	0.23	1.85	1.5%	0.0%	
(2R,3R,6S,7S,9R,10R)	5.3	10.8	0.0%	0.49	2.02	0.0%	0.0%	
(2R,3R,6S,7S,9S,10R)	4.5	8.1	0.0%	0.46	1.92	0.0%	0.0%	
(2R,3S,6R,7R,9R,10R)	5.2	10.9	0.0%	0.39	1.97	0.0%	0.0%	
(2R,3S,6R,7R,9S,10R)	4.2	7.5	0.0%	0.41	1.83	0.0%	0.0%	
(2R,3S,6R,7S,9R,10R)	3.9	9.4	0.0%	0.44	2.02	0.0%	0.0%	
(2R,3S,6R,7S,9S,10R)	2.7	5.9	0.0%	0.31	1.73	0.0%	0.0%	
(2S,3R,6R,7R,9R,10R)	5.7	12.7	0.0%	0.48	2.00	0.0%	0.0%	
(2S,3R,6R,7R,9S,10R)	4.4	10.1	0.0%	0.57	1.88	0.0%	0.0%	
(2S,3R,6R,7S,9R,10R)	3.2	5.8	0.0%	0.40	2.07	0.0%	0.0%	
(2S,3R,6R,7S,9S,10R)*	0.6	1.1	99.9%	0.24	1.79	30.7%	100.0%	proposed diastereomer
(2S,3R,6S,7R,9R,10R)	3.9	6.6	0.0%	0.42	1.95	0.0%	0.0%	
(2S,3R,6S,7R,9S,10R)	2.5	4.5	0.0%	0.26	1.83	0.0%	0.0%	
(2S,3R,6S,7S,9R,10R)	4.1	6.2	0.0%	0.49	2.05	0.0%	0.0%	
(2S,3R,6S,7S,9S,10R)	3.7	10.1	0.0%	0.31	1.79	0.0%	0.0%	
(2S,3S,6R,7R,9R,10R)	5.5	12.4	0.0%	0.37	1.99	0.0%	0.0%	
(2S,3S,6R,7R,9S,10R)	3.9	8.9	0.0%	0.41	1.88	0.0%	0.0%	
(2S,3S,6R,7S,9R,10R)	3.2	5.5	0.0%	0.35	2.07	0.0%	0.0%	
(2S,3S,6R,7S,9S,10R)	2.1	5.6	0.1%	0.24	1.78	1.4%	0.0%	
(2S,3S,6S,7R,9R,10R)	3.9	7.3	0.0%	0.39	1.94	0.0%	0.0%	
(2S,3S,6S,7R,9S,10R)	2.3	4.9	0.0%	0.21	1.82	63.0%	0.0%	
(2S,3S,6S,7S,9R,10R)	4.0	7.1	0.0%	0.59	2.06	0.0%	0.0%	
(2S,3S,6S,7S,9S,10R)	3.6	9.9	0.0%	0.49	1.79	0.0%	0.0%	
(2R,3S,6S,7R,9R,10R)	3.2	6.6	0.0%	0.40	1.97	0.0%	0.0%	
(2R,3S,6S,7R,9S,10R)	3.7	9.6	0.0%	0.31	1.85	0.0%	0.0%	
(2R,3S,6S,7S,9S,10R)	4.1	8.1	0.0%	0.56	1.90	0.0%	0.0%	
(2R,3S,6S,7S,9R,10R)	5.2	10.9	0.0%	0.64	2.02	0.0%	0.0%	

## ECD calculations

- Sets of stable conformers obtained in the chemical shift calculations were used as the initial geometries.
- Geometries were further optimized with B3LYP/def2-TZVP and the ECD calculations were performed with the same level.
- Relative Gibbs free energy was calculated by summing the SCF energy and the chemical potential obtained by the vibrational analysis.
- The UV ECD spectra were build based on the oscillator strength (UV) and rotatory strength (ECD) using the normal distribution function in Microsoft Excel (NORM.DIST) for Office365.
- The widths were set to appropriately reproduce the spectra.
- The UV/ECD spectra of individual conformers were composed by Boltzmann averaging based on the free energy.
- The wavelengths UV spectra were corrected based on the experimental spectra, and those of ECD spectra were also corrected using identical parameters.
- The ECD spectra of **1a**, **1b**, **2**, and **4** were reversed by using negative magnitude for the intensities.

SCF energy (au), chemical potential (kJ/mol), relative free energy, and Boltzmann distribution of *ent*-**1a** based on B3LYP/def2-TZVP.

	M0001	M0002	M0003	M0004	M0005	M0006	M0007	M0008	M0009
SCF (au)	-736.2984287	-736.2980099	-736.298485	-736.2975939	-736.2980739	-736.2979987	-736.2978283	-736.297762	-736.2976151
CP (kJ/mol)	850.59	850.56	848.17	850.79	846.85	846.36	847.6	847.6	850.4
rel G (kJ/mol)	3.1	4.17	0.53	5.49	0.29	0	1.69	1.86	5.05
Boltzmann dist.	6.5%	4.2%	18.4%	2.5%	20.3%	22.8%	11.5%	10.8%	3.0%

Wavelength (nm) oscillator strength (UV), and rotatory strength (CD) of *ent*-**1a** based on B3LYP/def2-TZVP.

M0001			M0002			M0003			M0004			M0005		
$\lambda$	UV	CD	$\lambda$	UV	CD	$\lambda$	UV	CD	$\lambda$	UV	CD	$\lambda$	UV	CD
158.1	5.8.E-03	-20.1	159.2	2.1.E-03	-0.4	158.0	2.7.E-03	1.1	159.3	2.E-03	0.3	158.5	3.E-03	-0.2
158.9	1.4.E-02	19.3	159.9	5.0.E-03	-7.9	159.4	1.8.E-03	-2.7	159.5	2.E-02	-3.0	159.5	6.E-04	2.0
158.9	8.5.E-04	-3.1	160.5	1.2.E-03	-0.4	159.7	7.1.E-03	4.6	160.2	1.E-03	3.7	159.7	7.E-04	0.9
159.8	4.5.E-04	-0.1	160.6	1.6.E-03	0.8	161.9	2.7.E-03	-4.4	161.5	1.E-03	1.2	160.4	1.E-02	-7.8
161.6	1.2.E-03	1.5	161.1	4.4.E-03	-3.2	162.4	5.4.E-03	12.9	161.7	8.E-03	3.7	160.7	1.E-03	-2.2
163.0	3.6.E-03	2.8	162.1	3.0.E-02	15.2	164.7	3.2.E-03	-2.9	162.6	2.E-02	15.0	165.5	5.E-03	2.0
164.0	4.7.E-03	-4.7	165.9	1.0.E-03	5.0	167.1	7.2.E-03	1.4	165.8	5.E-03	-0.6	168.0	5.E-03	0.1
169.2	2.5.E-03	0.3	169.4	1.4.E-03	3.2	168.8	3.2.E-03	-2.4	168.7	3.E-03	-3.8	168.5	6.E-03	6.9
172.9	8.1.E-03	4.3	170.5	7.9.E-03	-5.3	168.9	2.5.E-03	-1.0	171.5	1.E-02	-6.4	171.7	1.E-02	-1.6
175.2	8.1.E-03	2.7	172.0	1.5.E-02	-0.8	170.8	7.0.E-03	-3.2	172.3	8.E-03	5.4	172.4	3.E-03	-2.0
177.1	6.0.E-03	-6.8	176.5	6.3.E-03	-6.3	175.4	8.1.E-03	0.4	176.2	5.E-03	-4.6	175.4	7.E-03	2.2
177.7	2.4.E-03	-2.9	176.8	5.5.E-03	0.8	176.5	1.0.E-02	-5.1	176.4	1.E-02	-3.0	176.7	1.E-02	-8.1
178.8	2.8.E-03	-15.6	180.4	1.5.E-02	5.1	179.3	1.5.E-02	5.9	179.0	2.E-02	9.7	179.9	5.E-03	8.5
181.0	1.8.E-02	2.4	182.7	3.5.E-03	-6.3	179.7	1.3.E-03	-6.6	182.2	4.E-03	-8.6	180.1	7.E-03	1.4
183.5	1.1.E-03	-2.4	183.8	4.6.E-03	1.6	183.1	1.2.E-02	4.7	183.9	5.E-03	3.3	182.9	1.E-02	3.3
185.9	1.1.E-02	-2.1	184.5	2.7.E-03	-14.5	184.4	2.4.E-03	-6.0	185.1	2.E-03	-1.4	184.2	3.E-03	-6.4
187.2	1.5.E-03	7.1	187.5	9.6.E-03	-3.7	189.4	6.2.E-03	-3.0	189.8	6.E-03	2.1	189.3	4.E-03	-1.2
189.9	3.5.E-03	-0.6	195.9	2.3.E-03	-0.8	194.1	2.5.E-04	0.0	195.3	4.E-03	7.1	194.4	1.E-04	-0.8
198.3	4.4.E-03	2.9	204.0	8.7.E-03	2.0	199.2	5.0.E-03	2.6	204.0	6.E-03	6.9	197.9	6.E-03	2.1
294.0	3.5.E-05	2.2	294.2	4.3.E-05	1.7	294.1	4.1.E-05	1.9	294.3	4.E-05	1.6	294.1	5.E-05	1.7

M0006			M0007			M0008			M0009		
$\lambda$	UV	CD									
158.3	2.6.E-03	2.0	158.3	2.6.E-03	2.0	158.5	1.6.E-04	-2.0	158.5	2.5.E-03	5.7
158.8	1.5.E-03	1.8	158.8	1.5.E-03	1.8	159.4	9.7.E-04	1.2	158.9	3.0.E-03	-0.3
160.3	1.0.E-02	-4.6	160.3	1.0.E-02	-4.6	160.4	5.0.E-03	-7.5	159.3	1.0.E-03	1.2
160.6	7.2.E-04	-3.2	160.6	7.2.E-04	-3.2	161.4	9.2.E-03	-5.0	160.4	1.2.E-02	-3.4
164.8	2.9.E-03	-7.7	164.8	2.9.E-03	-7.7	162.6	9.6.E-04	3.0	161.2	6.7.E-04	0.5
165.3	3.9.E-03	0.4	165.3	3.9.E-03	0.4	165.1	1.3.E-02	4.3	165.7	7.3.E-03	6.9
166.0	3.2.E-03	3.5	166.0	3.2.E-03	3.5	165.4	5.3.E-03	5.9	165.7	2.3.E-03	1.3
167.0	5.6.E-03	-1.7	167.0	5.6.E-03	-1.7	165.9	2.4.E-03	4.8	167.9	8.2.E-03	-8.4
173.5	1.7.E-02	6.7	173.5	1.7.E-02	6.7	169.7	4.7.E-03	-3.4	171.6	1.8.E-02	0.9
174.0	3.4.E-03	0.5	174.0	3.4.E-03	0.5	171.4	1.5.E-02	0.9	173.1	3.7.E-03	-0.5
177.2	9.6.E-03	-8.7	177.2	9.6.E-03	-8.7	176.3	5.9.E-03	-2.9	177.1	9.7.E-03	-7.0
177.8	2.1.E-03	-0.2	177.8	2.1.E-03	-0.2	177.5	2.1.E-03	-2.2	177.7	1.3.E-03	-3.4
179.9	1.8.E-03	2.1	179.9	1.8.E-03	2.1	179.6	1.5.E-02	1.2	179.2	1.5.E-02	2.1
180.5	1.2.E-02	-1.4	180.5	1.2.E-02	-1.4	183.8	8.6.E-03	11.4	182.3	4.2.E-03	-4.7
183.8	1.6.E-02	-3.0	183.8	1.6.E-02	-3.0	183.9	9.7.E-03	-6.6	183.1	1.1.E-02	-9.2
185.4	2.5.E-03	-2.6	185.4	2.5.E-03	-2.6	184.5	2.1.E-03	-0.3	183.6	3.0.E-03	-7.8
187.0	8.4.E-04	0.8	187.0	8.4.E-04	0.8	185.4	5.3.E-03	-0.2	186.3	2.2.E-03	1.9
188.8	8.7.E-04	3.0	188.8	8.7.E-04	3.0	196.8	3.3.E-04	2.5	196.8	5.7.E-04	1.2
198.8	7.3.E-03	2.1	198.8	7.3.E-03	2.1	202.7	6.1.E-03	4.1	200.5	6.8.E-03	2.7
294.0	4.6.E-05	1.5	294.0	4.6.E-05	1.5	294.1	4.2.E-05	1.7	294.3	3.7.E-05	1.4

Parameters used for ECD reproduction of *ent-1a*.

wavelength 3 nm  
 UV width 15 nm  
 UV intensity 40000  
 CD width 12 nm  
 CD intensity -100 (because the enantiomer was applied for the calculations)

SCF energy (au), chemical potential (kJ/mol), relative free energy, and Boltzmann distribution of *ent*-**1b** based on B3LYP/def2-TZVP.

	M0001	M0002	M0003	M0004	M0005	M0006	M0007	M0008	M0009	M0010	M0014
SCF (au)	-811.516922	-811.516468	-811.516919	-811.516603	-811.515945	-811.516378	-811.5165	-811.516228	-811.515979	-811.515459	-811.515448
CP (kJ/mol)	856.71	857.12	856.45	856.59	856.49	855.38	855.66	855.6	856.5	855.84	855.52
rel. G (kJ/mol)	0	1.6	-0.25	0.72	2.35	0.1	0.06	0.71	2.27	2.97	2.68
Boltz. dist.	13.35%	6.98%	14.78%	9.98%	5.17%	12.82%	13.03%	10.01%	5.34%	4.01%	4.52%

Wavelength (nm) oscillator strength (UV), and rotatory strength (CD) of *ent*-**1b** based on B3LYP/def2-TZVP.

M0001			M0002			M0003			M0004			M0005		
$\lambda$	UV	CD	$\lambda$	UV	CD	$\lambda$	UV	CD	$\lambda$	UV	CD	$\lambda$	UV	CD
169.0	2.6.E-03	-1.8	169.3	5.1.E-03	3.0	168.0	4.5.E-03	-0.8	168.5	3.2.E-03	-3.8	167.9	3.E-03	-4.6
172.8	4.2.E-04	-4.0	171.5	7.9.E-04	-1.1	171.3	3.7.E-03	-6.2	171.5	3.5.E-03	-3.6	170.6	2.E-03	-3.9
174.6	5.5.E-03	6.7	172.4	2.7.E-03	4.1	171.8	2.6.E-03	-7.2	173.2	2.6.E-03	-8.0	172.8	5.E-03	-2.6
175.3	9.1.E-03	-8.8	173.8	2.3.E-03	-2.2	174.2	3.6.E-03	1.8	173.4	4.3.E-03	-1.6	174.6	9.E-03	-3.9
175.7	8.2.E-03	-4.2	175.3	3.3.E-03	-3.8	174.9	5.3.E-03	-5.4	175.0	6.9.E-03	3.9	175.6	4.E-03	-2.3
177.1	9.4.E-03	-1.4	177.2	2.8.E-02	-0.2	176.0	5.5.E-03	-2.9	176.1	3.0.E-02	-0.3	176.7	3.E-02	1.2
178.7	8.3.E-03	-25.4	178.2	2.7.E-03	-7.5	176.6	3.1.E-02	4.0	178.6	2.9.E-03	-9.8	178.4	1.E-03	-1.8
180.3	1.1.E-02	1.4	180.1	7.3.E-03	-9.8	179.8	1.7.E-03	-2.8	179.8	1.2.E-03	7.5	180.0	5.E-03	-8.2
181.8	2.4.E-04	-2.2	184.0	4.1.E-03	-10.4	180.0	3.8.E-03	-12.6	180.2	5.4.E-03	-7.9	185.1	4.E-03	15.4
185.5	1.9.E-03	5.4	184.9	8.2.E-03	-5.9	189.1	9.9.E-03	-4.5	188.5	1.1.E-02	-2.7	185.8	5.E-03	-9.9
186.6	9.2.E-03	-6.4	193.8	6.9.E-04	-2.6	191.7	1.6.E-03	2.2	190.7	8.6.E-04	1.7	193.1	3.E-03	-2.7
193.6	2.8.E-03	2.0	195.7	7.4.E-03	-6.2	193.4	4.8.E-05	-0.5	193.5	4.4.E-04	-1.4	196.9	5.E-03	2.1
201.6	1.1.E-03	-0.2	203.8	1.6.E-03	9.0	201.9	1.0.E-03	2.0	201.6	4.7.E-03	-2.5	202.9	2.E-03	16.3
203.2	8.7.E-03	23.6	205.1	1.1.E-02	17.2	203.6	9.1.E-03	20.6	203.4	5.5.E-03	25.1	206.1	9.E-03	13.2
293.8	1.6.E-05	0.4	294.2	2.2.E-05	-0.2	293.9	2.1.E-05	0.0	293.9	2.4.E-05	-0.3	294.3	2.E-05	-0.2

M0006			M0007			M0008			M0009			M0010		
$\lambda$	UV	CD												
167.8	4.1.E-03	1.6	166.8	9.7.E-03	-9.8	166.7	2.3.E-03	-12.1	168.5	4.6.E-03	-12.7	170.7	4.7.E-03	1.3
172.0	1.2.E-03	-6.5	171.2	4.3.E-04	-4.6	170.7	2.6.E-03	0.9	171.2	7.0.E-04	-5.1	171.5	6.6.E-03	-0.3
174.5	2.8.E-03	-4.1	174.3	4.9.E-03	11.1	171.5	6.3.E-04	-2.2	173.5	9.1.E-03	-11.3	175.9	5.7.E-03	-16.7
175.2	7.8.E-03	-0.8	175.1	2.1.E-02	-6.6	174.4	1.6.E-02	-3.3	174.5	2.1.E-02	2.0	176.3	3.6.E-03	-7.5
176.1	3.3.E-02	-0.5	175.3	1.0.E-03	-2.7	175.0	2.0.E-03	-4.0	175.2	8.8.E-03	-4.6	176.8	6.9.E-03	-8.7
177.1	5.1.E-03	-1.4	176.6	2.1.E-02	-5.3	177.3	5.9.E-03	5.4	177.3	1.1.E-02	1.8	178.5	9.6.E-03	-24.7
179.5	3.6.E-04	5.3	178.4	3.9.E-03	-5.2	177.6	1.8.E-02	-10.6	179.5	5.5.E-03	-11.5	179.3	1.2.E-02	4.3
180.0	6.8.E-03	-19.0	180.2	2.7.E-03	-10.3	179.6	4.3.E-03	-10.7	180.4	1.5.E-03	-5.1	181.9	4.3.E-03	12.3
180.7	1.9.E-03	-5.3	180.6	8.5.E-04	4.3	184.2	5.1.E-03	17.2	182.7	3.4.E-03	-7.5	183.1	3.0.E-03	-6.8
185.5	5.4.E-03	-0.4	186.1	7.1.E-03	-9.3	185.2	8.3.E-03	-11.3	183.6	7.9.E-03	-7.3	184.7	1.6.E-03	7.5
188.8	7.8.E-04	1.7	188.4	4.5.E-04	-0.6	193.6	4.7.E-03	3.7	192.6	3.4.E-03	3.1	185.9	8.2.E-03	-2.9
191.4	5.4.E-03	1.2	193.0	4.4.E-03	4.4	196.1	1.8.E-04	-0.4	195.7	1.1.E-03	-3.0	193.0	1.3.E-03	-1.5
201.8	3.5.E-03	-3.8	201.7	1.5.E-03	7.8	203.0	1.8.E-03	9.4	202.7	2.4.E-03	-1.6	199.7	6.4.E-03	5.7
203.2	7.7.E-03	27.3	204.1	9.6.E-03	16.4	204.8	8.8.E-03	15.9	203.9	8.5.E-03	25.0	200.7	1.0.E-03	-0.6
293.9	2.5.E-05	-0.5	293.8	2.3.E-05	-0.1	293.9	2.2.E-05	-0.2	294.2	2.0.E-05	-0.5	293.7	4.9.E-05	3.1

M0014		
$\lambda$	UV	CD
168.4	2.5.E-03	-2.9
168.9	6.9.E-03	-0.7
173.4	7.1.E-03	2.6
175.7	5.5.E-03	-6.4
176.0	5.7.E-03	-23.6
177.7	7.7.E-03	-15.1
178.5	1.8.E-02	-0.9
179.6	1.7.E-03	-3.4
180.2	4.4.E-03	10.2
186.3	7.9.E-03	-1.4
192.2	1.7.E-03	-3.5
193.2	2.1.E-04	0.8
200.6	7.4.E-03	4.2
201.0	9.6.E-04	1.0
293.7	5.6.E-05	2.6

Parameters used for ECD reproduction of *ent*-**1b**.

wavelength	-7 nm
UV width	15 nm
UV intensity	40000
CD width	12 nm
CD intensity	-50 (because the enantiomer was applied for the calculations)

SCF energy (au), chemical potential (kJ/mol), relative free energy, and Boltzmann distribution of **1c** based on B3LYP/def2-TZVP.

	M0001	M0002	M0003	M0004	M0005	M0006	M0007	M0008	M0009	M0010
SCF (au)	-736.26236	-736.26196	-736.26213	-736.26209	-736.2616	-736.26158	-736.26177	-736.26186	-736.26132	-736.26122
CP (kJ/mol)	840.16	841.15	839.38	840.48	840.29	841.16	839.64	840.49	840.46	840.37
Boltz. Dist.	12.6%	5.6%	13.6%	8.3%	5.4%	3.7%	8.4%	6.6%	3.7%	3.5%
	M0011	M0012	M0013	M0014	M0015	M0016	M0017	M0018	M0019	
SCF (au)	-736.26089	-736.26113	-736.26051	-736.26133	-736.26057	-736.26091	-736.26059	-736.26011	-736.26039	
CP (kJ/mol)	839.63	838.83	840.43	839.1	839.67	840.08	838.9	839.76	839.98	
Boltz. Dist.	3.3%	5.9%	1.6%	6.5%	2.3%	2.8%	3.2%	1.4%	1.7%	

Wavelength (nm) oscillator strength (UV), and rotatory strength (CD) of **1c** based on B3LYP/def2-TZVP.

M0001			M0002			M0003			M0004			M0005		
$\lambda$	UV	CD												
165.3	1.4.E-02	-37.4	165.7	4.3.E-03	-6.0	165.6	1.2.E-02	-6.9	165.1	2.3.E-04	-2.3	165.8	4.6.E-03	1.1
166.3	3.6.E-03	4.2	168.3	7.2.E-03	-4.9	165.8	8.6.E-03	-22.7	166.1	1.3.E-03	-6.9	168.7	7.7.E-03	-1.5
169.9	1.5.E-02	5.2	170.0	1.2.E-02	-4.8	170.2	1.6.E-02	8.8	170.0	1.2.E-02	1.4	169.9	5.8.E-03	-2.1
173.3	4.5.E-03	2.2	172.8	4.6.E-04	1.3	172.0	5.1.E-03	0.9	174.4	6.8.E-02	28.4	170.7	1.1.E-02	-4.5
174.2	1.1.E-03	-4.1	173.9	1.4.E-02	0.8	173.9	1.9.E-02	33.1	174.8	4.2.E-03	0.5	172.9	3.6.E-03	8.0
175.3	4.3.E-02	15.8	175.8	3.8.E-02	-16.5	174.4	3.8.E-02	7.7	175.8	3.2.E-03	7.4	176.1	3.6.E-02	-19.8
176.1	4.2.E-02	33.0	177.3	8.1.E-03	0.2	176.1	1.5.E-02	-5.0	176.6	4.2.E-03	5.5	178.2	5.1.E-02	36.1
178.0	4.9.E-02	51.7	179.1	8.6.E-02	108.3	180.2	4.0.E-02	49.1	178.9	5.2.E-02	31.4	181.6	3.3.E-02	47.2
181.0	5.6.E-03	7.5	180.8	4.8.E-03	5.4	182.0	5.9.E-04	5.6	180.0	4.5.E-03	0.4	182.2	3.3.E-03	6.6
183.9	1.4.E-02	3.1	184.2	1.5.E-03	-10.4	183.9	1.0.E-02	-0.4	183.3	3.5.E-02	30.9	184.6	3.8.E-03	-7.8
188.0	2.9.E-03	-8.2	188.7	1.7.E-02	-9.7	188.0	6.1.E-03	1.0	187.8	2.9.E-03	-9.6	188.3	1.6.E-02	17.3
193.4	5.1.E-02	1.9	192.6	7.9.E-02	35.5	190.8	1.1.E-01	22.0	196.7	1.6.E-02	-4.9	191.8	1.1.E-01	17.0
199.5	9.4.E-02	36.4	197.1	2.7.E-02	-13.5	200.3	4.9.E-02	27.1	199.1	9.6.E-02	44.3	195.9	3.4.E-02	-5.5
206.5	1.3.E-01	-81.6	202.7	6.1.E-02	-41.3	206.8	8.6.E-02	-72.5	206.6	1.5.E-01	-76.1	203.3	4.6.E-02	-32.7
207.3	9.6.E-03	10.4	206.8	9.7.E-02	-3.8	208.6	5.7.E-02	-2.7	208.4	4.4.E-03	1.4	209.2	8.7.E-02	-14.5

M0006			M0007			M0008			M0009			M0010		
$\lambda$	UV	CD												
166.0	4.0.E-03	6.5	165.7	1.2.E-02	4.4	164.8	9.7.E-03	-11.6	165.8	9.7.E-03	4.1	165.6	5.5.E-03	2.0
170.0	2.2.E-02	-2.0	166.5	1.3.E-02	-24.4	165.4	9.0.E-03	-41.8	168.2	9.0.E-03	-1.3	170.5	2.6.E-02	1.3
171.0	4.7.E-03	-7.4	168.7	1.2.E-02	7.1	171.4	1.6.E-02	0.7	171.4	1.6.E-02	-3.8	171.5	2.7.E-03	0.2
173.0	3.4.E-04	0.2	173.2	3.1.E-02	33.7	173.5	2.5.E-03	-0.4	171.8	2.5.E-03	-1.3	172.1	2.2.E-03	-6.6
174.2	1.4.E-02	-5.2	173.9	1.3.E-03	-4.5	174.5	8.2.E-04	2.2	173.2	8.2.E-04	15.6	173.1	2.7.E-03	5.1
175.4	2.7.E-02	-2.8	174.0	6.2.E-04	-5.6	174.9	5.1.E-02	14.7	176.1	5.1.E-02	7.5	175.5	2.4.E-02	-21.1
177.7	4.6.E-02	69.5	176.9	4.0.E-02	7.5	178.3	7.2.E-02	73.9	177.6	7.2.E-02	-10.4	179.3	9.6.E-02	94.0
179.8	1.2.E-03	-9.5	180.3	3.6.E-02	43.5	180.6	1.4.E-02	6.3	181.8	1.4.E-02	62.5	181.3	2.2.E-04	-2.7
181.5	2.4.E-02	-1.7	183.9	1.1.E-02	0.8	181.1	1.8.E-03	-0.4	184.1	1.8.E-03	-5.5	182.8	1.0.E-02	16.0
184.5	3.2.E-03	-6.7	187.2	1.1.E-01	48.0	181.6	2.7.E-02	23.0	186.4	2.7.E-02	29.4	184.8	3.4.E-03	-8.1
187.6	8.3.E-02	22.3	188.5	1.2.E-02	-10.2	187.7	2.0.E-03	-6.9	188.3	2.0.E-03	-12.7	187.2	4.7.E-02	-6.7
192.9	3.5.E-02	32.6	188.7	1.4.E-02	-17.4	194.5	5.3.E-02	-4.3	190.8	5.3.E-02	-18.7	192.6	4.6.E-02	29.0
199.8	8.1.E-03	-7.6	201.8	4.6.E-02	20.9	200.0	4.8.E-02	33.9	196.1	4.8.E-02	17.0	198.0	3.7.E-02	-18.1
203.7	9.2.E-02	-56.9	206.2	4.1.E-02	-43.8	207.0	1.2.E-01	-85.4	202.4	1.2.E-01	-23.6	204.1	6.6.E-02	-37.5
207.2	9.1.E-02	6.2	212.1	9.7.E-02	-27.5	209.3	4.7.E-02	10.2	213.1	4.7.E-02	-24.5	210.0	9.0.E-02	-5.0

M0011			M0012			M0013			M0014			M0015		
$\lambda$	UV	CD												
166.8	0.0	2.8	166.5	0.0	12.7	167.2	0.0	-7.0	165.3	0.0	-2.2	166.2	0.0	-2.2
167.2	0.0	0.6	167.5	0.0	-0.4	167.5	0.0	10.4	166.2	0.0	-36.4	168.5	0.0	20.4
167.4	0.0	5.7	169.7	0.0	-4.6	169.8	0.0	-2.6	169.4	0.0	4.8	168.8	0.0	2.4
170.4	0.0	4.2	170.1	0.0	18.1	175.5	0.0	1.1	173.5	0.1	33.9	170.7	0.0	1.8
176.4	0.1	45.2	172.1	0.0	7.1	175.8	0.0	-0.8	174.7	0.0	10.8	175.3	0.0	-5.8
177.0	0.0	3.3	175.7	0.0	-4.7	177.2	0.0	-3.5	176.6	0.0	-4.4	176.0	0.0	-12.6
177.6	0.0	-0.3	177.4	0.0	-4.5	177.8	0.0	4.2	177.3	0.0	0.4	179.3	0.1	32.0
179.1	0.0	3.7	180.6	0.0	12.1	178.6	0.0	33.7	178.8	0.0	-0.7	180.7	0.0	5.3
187.0	0.0	14.3	181.4	0.0	17.6	185.6	0.0	-8.4	180.4	0.1	57.8	183.1	0.0	3.6
187.8	0.0	-8.3	187.7	0.0	-6.9	187.1	0.0	-7.2	187.4	0.0	10.6	185.6	0.0	-13.8
189.7	0.0	10.9	188.9	0.0	20.0	188.5	0.0	29.0	188.2	0.0	-3.1	190.8	0.0	59.2
192.3	0.1	-3.0	194.6	0.1	24.3	192.9	0.1	21.6	192.5	0.1	-18.4	191.8	0.0	3.0
200.9	0.1	30.1	200.2	0.0	24.7	197.0	0.0	-3.5	200.6	0.1	36.6	198.9	0.1	-26.8
207.1	0.1	-78.7	206.6	0.1	-83.3	203.2	0.1	-57.9	206.5	0.1	-72.1	204.1	0.1	-34.0
215.3	0.0	20.7	209.2	0.0	14.9	215.7	0.0	18.3	211.6	0.1	18.0	210.1	0.1	8.4

M0016			M0017			M0018			M019		
$\lambda$	UV	CD	$\lambda$	UV	CD	$\lambda$	UV	CD	$\lambda$	UV	CD
165.5	0.0	-5.1	166.9	0.0	-0.8	166.0	0.0	10.6	165.5	0.0	0.0
168.5	0.0	0.8	167.6	0.0	-1.1	167.2	0.0	8.9	166.4	0.0	0.0
171.4	0.0	-9.2	167.9	0.0	1.3	168.6	0.0	12.2	170.3	0.0	0.0
173.6	0.0	11.2	171.2	0.0	13.7	169.2	0.0	3.8	172.0	0.0	0.0
174.8	0.1	30.6	171.3	0.0	6.0	173.0	0.0	6.0	174.7	0.0	0.0
175.3	0.0	-9.9	174.1	0.0	0.1	177.3	0.0	-2.2	175.0	0.0	0.0
177.3	0.0	-6.2	177.8	0.0	5.4	178.2	0.0	-0.7	176.1	0.1	0.1
180.4	0.0	14.0	180.1	0.0	20.0	180.8	0.0	21.4	180.3	0.0	0.0
183.9	0.0	29.7	186.0	0.1	52.1	185.0	0.0	-8.1	181.3	0.1	0.1
184.8	0.0	0.5	187.4	0.0	-1.7	186.6	0.1	63.6	182.6	0.0	0.0
186.7	0.0	13.7	188.6	0.0	-9.5	189.1	0.0	12.3	183.4	0.0	0.0
193.2	0.1	12.6	189.6	0.0	8.2	191.1	0.1	-38.8	192.9	0.1	0.1
196.6	0.0	-0.1	202.2	0.1	20.0	196.7	0.0	21.9	195.8	0.0	0.0
202.4	0.1	-54.0	205.7	0.0	-30.7	202.4	0.0	-20.6	202.8	0.1	0.1
211.7	0.1	15.8	215.1	0.1	-33.5	215.9	0.1	-26.0	205.3	0.1	0.1

Parameters used for ECD reproduction of **1c**.

wavelength	-0 nm
UV width	8 nm
UV intensity	40000
CD width	6 nm
CD intensity	+10

SCF energy (au), chemical potential (kJ/mol), relative free energy, and Boltzmann distribution of **2a** based on B3LYP/def2-TZVP

	M0001	M0002	M0003
SCF (au)	-809.1107141	-809.1107323	-809.1107375
CP (kJ/mol)	728.38	728.04	728.47
rel G (kJ/mol)	0.00	-0.39	0.03
Boltzmann dist.	31.7%	37.0%	31.3%

Wavelength (nm) oscillator strength (UV), and rotatory strength (CD) of **2a** based on B3LYP/def2-TZVP.

M0001				M0002				M0003			
$\lambda$	UV	CD	$\lambda$	UV	CD	$\lambda$	UV	CD	UV	CD	UV
173.6	1.3.E-02	173.6	-17.1	172.8	6.3.E-03	172.8	-12.0	172.8	6.4.E-03	172.8	
173.9	6.6.E-03	173.9	2.9	174.1	3.5.E-03	174.1	1.7	174.1	3.3.E-03	174.1	
174.1	1.5.E-03	174.1	-2.3	174.9	5.2.E-03	174.9	-9.1	174.9	5.5.E-03	174.9	
175.3	3.6.E-03	175.3	-5.8	175.2	4.2.E-03	175.2	4.5	175.1	4.1.E-03	175.1	
177.2	3.6.E-03	177.2	7.2	177.2	6.5.E-03	177.2	8.5	177.2	6.5.E-03	177.2	
178.0	3.3.E-03	178.0	-6.1	177.9	1.8.E-03	177.9	-6.5	177.9	1.7.E-03	177.9	
179.2	7.0.E-03	179.2	-4.0	178.7	7.7.E-03	178.7	-4.8	178.7	7.6.E-03	178.7	
183.6	5.9.E-03	183.6	4.3	184.1	6.7.E-03	184.1	-2.8	184.1	6.6.E-03	184.1	
186.7	2.9.E-03	186.7	15.4	187.5	3.0.E-03	187.5	6.7	187.5	3.0.E-03	187.5	
188.4	2.5.E-03	188.4	1.1	187.8	3.6.E-03	187.8	10.9	187.8	3.6.E-03	187.8	
193.5	3.9.E-03	193.5	3.2	193.0	5.1.E-03	193.0	6.1	192.9	5.1.E-03	192.9	
200.9	1.0.E-03	200.9	1.1	200.9	2.4.E-04	200.9	-0.1	200.9	2.3.E-04	200.9	
201.1	1.6.E-02	201.1	-2.0	201.2	1.5.E-02	201.2	-1.8	201.2	1.5.E-02	201.2	
207.2	7.1.E-04	207.2	-1.2	206.7	1.2.E-05	206.7	0.0	206.7	1.4.E-05	206.7	
211.9	7.8.E-03	211.9	-1.5	210.5	5.3.E-03	210.5	2.0	210.4	5.0.E-03	210.4	
215.3	3.2.E-03	215.3	4.4	215.6	1.7.E-03	215.6	6.4	215.6	1.7.E-03	215.6	
217.0	5.3.E-03	217.0	-18.8	218.0	1.1.E-02	218.0	-15.9	218.1	1.2.E-02	218.1	
221.6	4.1.E-02	221.6	-34.6	221.2	3.8.E-02	221.2	-34.7	221.2	3.8.E-02	221.2	
245.4	2.0.E-01	245.4	32.0	245.7	2.1.E-01	245.7	40.4	245.7	2.1.E-01	245.7	
346.8	6.3.E-04	346.8	-13.7	346.0	6.1.E-04	346.0	-13.5	345.9	6.1.E-04	345.9	

Parameters used for ECD reproduction of **2a**.

wavelength	7 nm
UV width	12 nm
UV intensity	6000
CD width	10 nm
CD intensity	+0.63

SCF energy (au), chemical potential (kJ/mol), relative free energy, and Boltzmann distribution of **2b** based on B3LYP/def2-TZVP

	M0001	M0002	M0003	M0004	M0005	M0006	M0007	M0008	M0009
SCF (au)	-735.0551692	-735.0549887	-735.0548794	-735.0546431	-735.0543656	-735.0542393	-735.0532329	-735.0537391	-735.0527031
CP (kJ/mol)	780.16	779.47	780.71	779.5	779.72	780.07	780.61	779.62	778.11
rel G (kJ/mol)	0.00	-0.22	1.31	0.72	1.67	2.35	5.53	3.21	4.42
Boltzmann dist.	20.54%	22.42%	12.09%	15.34%	10.45%	7.93%	2.19%	5.60%	3.43%

Wavelength (nm) oscillator strength (UV), and rotatory strength (CD) of **2b** based on B3LYP/def2-TZVP.

M0001			M0002			M0003			M0004			M0005		
$\lambda$	UV	CD												
168.9	9.3.E-03	-12.5	168.6	1.7.E-02	-6.2	168.6	1.2.E-02	-4.8	169.6	1.3.E-02	-1.1	169.0	4.3.E-03	-4.8
170.3	4.2.E-03	-1.9	170.9	4.7.E-03	-5.9	170.1	6.4.E-03	-4.9	170.0	4.5.E-03	1.4	170.8	4.0.E-03	0.6
174.2	1.9.E-03	-3.1	174.9	4.4.E-03	3.0	171.7	3.4.E-03	-8.2	172.9	5.3.E-03	-11.0	174.1	3.5.E-03	0.5
175.1	7.9.E-03	15.2	175.4	2.8.E-03	-5.4	175.1	7.8.E-03	6.4	175.3	5.8.E-03	-0.8	174.4	6.2.E-03	0.6
176.2	4.3.E-03	-6.8	177.5	9.6.E-03	7.9	175.7	1.3.E-03	5.9	178.4	7.3.E-03	11.0	175.9	4.5.E-04	-2.8
178.3	2.4.E-03	-4.5	178.2	1.6.E-03	-7.8	178.1	1.1.E-02	-4.8	179.0	4.2.E-03	-11.1	177.4	6.6.E-03	6.0
179.1	3.3.E-03	3.3	179.9	7.6.E-03	-9.4	179.5	4.5.E-03	-4.1	179.9	1.0.E-02	-2.9	178.2	1.3.E-03	-8.3
180.7	1.4.E-03	-8.0	181.5	1.2.E-03	5.6	180.4	9.2.E-04	4.8	181.5	1.6.E-04	0.1	179.4	9.5.E-03	-9.9
182.1	5.6.E-03	10.0	183.3	7.7.E-03	5.2	182.8	8.8.E-03	1.0	182.2	1.4.E-03	-1.3	182.5	5.2.E-03	0.6
183.5	3.4.E-03	3.4	184.1	2.8.E-03	4.8	184.2	3.1.E-03	-3.1	184.8	3.1.E-03	0.2	184.3	5.1.E-03	11.2
184.2	5.3.E-03	-8.3	188.1	2.1.E-03	1.7	186.2	3.0.E-04	-1.3	190.1	3.1.E-03	-2.3	187.3	3.0.E-03	13.0
189.5	3.7.E-03	0.1	190.5	4.1.E-03	1.8	189.7	4.9.E-03	7.5	191.1	6.3.E-03	-1.5	194.5	6.3.E-03	1.6
193.5	2.4.E-03	4.6	194.5	2.4.E-03	7.9	190.1	3.4.E-03	9.2	192.1	4.1.E-03	17.5	195.5	3.9.E-03	13.3
194.6	6.5.E-03	11.0	195.3	7.2.E-03	1.7	194.9	4.4.E-03	3.6	195.9	4.8.E-03	1.7	199.2	4.0.E-03	-2.4
202.3	1.5.E-02	-2.1	203.1	1.5.E-02	-4.6	202.3	1.7.E-02	-3.1	203.1	1.8.E-02	-3.2	201.2	1.5.E-02	-1.3
212.2	4.7.E-03	3.2	213.9	8.0.E-03	3.8	213.6	5.4.E-03	3.5	212.1	4.0.E-03	1.3	213.4	5.3.E-03	2.6
220.5	4.6.E-02	-49.0	218.5	8.0.E-03	-9.2	219.7	4.0.E-02	-41.8	220.5	2.0.E-02	-17.0	221.7	5.0.E-02	-50.4
226.2	5.2.E-03	-0.6	224.0	4.0.E-02	-35.2	226.5	1.2.E-02	-6.6	224.0	3.3.E-02	-26.9	228.4	2.4.E-03	-0.6
246.2	2.0.E-01	36.8	246.7	2.0.E-01	35.7	246.2	2.0.E-01	38.5	246.8	2.0.E-01	38.8	246.1	2.0.E-01	38.5
346.4	6.0.E-04	-13.4	346.3	6.0.E-04	-13.5	346.9	6.0.E-04	-13.5	346.8	5.9.E-04	-13.5	347.0	6.1.E-04	-13.6

M0006			M0007			M0008			M0009		
$\lambda$	UV	CD									
167.7	1.3.E-02	9.1	167.7	1.1.E-02	2.2	168.6	4.5.E-03	-0.2	168.3	9.5.E-03	2.0
169.7	2.1.E-03	8.8	169.8	1.4.E-03	4.3	170.6	1.4.E-03	4.3	169.7	2.6.E-03	7.5
170.8	9.9.E-03	-17.7	170.4	1.3.E-03	-4.9	175.7	7.2.E-03	-10.6	170.7	1.9.E-03	-3.0
174.2	4.5.E-03	2.3	171.8	1.3.E-02	-11.4	177.6	7.7.E-03	-5.2	175.0	1.5.E-02	-19.5
175.1	5.7.E-03	-1.5	176.7	5.6.E-03	-7.0	178.6	7.6.E-03	-2.7	177.0	3.0.E-03	-8.9
177.8	5.9.E-03	2.4	177.3	1.1.E-02	-8.2	179.8	2.6.E-03	-2.4	178.5	1.1.E-02	-4.7
179.0	7.3.E-03	-7.4	179.3	5.3.E-03	-2.1	181.0	3.6.E-04	-1.2	180.1	4.6.E-03	-1.5
179.7	5.9.E-04	-1.2	180.9	9.9.E-04	8.1	181.1	9.4.E-03	-5.0	180.8	9.0.E-04	5.0
183.0	4.4.E-03	1.3	182.4	1.7.E-03	1.8	181.5	2.1.E-03	-1.5	183.1	1.6.E-03	1.6
186.0	3.2.E-03	4.2	186.6	2.8.E-03	6.0	185.7	9.4.E-04	-7.3	186.3	3.6.E-03	4.5
186.7	2.7.E-03	-15.0	187.5	4.2.E-03	15.8	186.5	7.5.E-03	15.5	187.9	3.1.E-03	-6.7
193.7	6.9.E-03	-0.4	192.7	6.0.E-03	19.0	191.3	4.2.E-03	-3.9	190.1	5.4.E-03	21.2
194.7	5.1.E-03	18.5	196.7	3.8.E-03	-1.5	192.7	5.3.E-03	10.9	197.6	5.8.E-03	-7.2
199.5	4.8.E-03	-0.9	201.7	3.2.E-03	-2.1	196.0	3.3.E-03	2.1	201.6	2.6.E-03	-3.1
201.4	1.7.E-02	-5.4	204.3	1.3.E-02	-5.7	202.1	9.9.E-03	-4.1	204.5	1.5.E-02	0.7
213.7	8.6.E-03	1.9	215.3	1.3.E-02	0.8	211.7	1.3.E-03	-2.7	214.4	7.1.E-03	3.1
221.0	4.3.E-02	-44.3	222.2	4.6.E-02	-45.0	220.9	8.8.E-03	8.8	222.5	5.7.E-02	-50.7
229.3	1.4.E-03	-0.9	226.7	6.9.E-03	-1.0	223.9	5.1.E-02	-46.7	225.9	1.0.E-02	-3.3
246.2	2.0.E-01	38.5	247.6	1.9.E-01	39.5	247.3	2.0.E-01	38.9	247.5	1.8.E-01	45.0
346.6	5.9.E-04	-13.5	346.0	6.1.E-04	-13.5	346.0	6.2.E-04	-13.7	347.1	6.1.E-04	-13.8

Parameters used for ECD reproduction of **2b**.

wavelength	8 nm
UV width	12 nm
UV intensity	6000
CD width	15 nm
CD intensity	+1.1

SCF energy (au), chemical potential (kJ/mol), relative free energy, and Boltzmann distribution of **3** based on BHLYP/def2-TZVP.

	M0001	M0002	M0003	M0004	M0005	M0006	M0007	M0008	M0009	M0010
SCF (au)	-811.47736	-811.47722	-811.47736	-811.47676	-811.47714	-811.4766	-811.47678	-811.47627	-811.47601	-811.47613
CP (kJ/mol)	891.24	890.98	890.73	890.84	890.47	890.68	889.67	890.35	891.25	890.76
rel G (kJ/mol)	0.0	0.4	0.0	1.6	0.6	2.0	1.5	2.8	3.5	3.2
Boltzmann dist	16.6%	14.4%	16.7%	8.8%	13.3%	7.5%	9.0%	5.2%	4.0%	4.5%

Wavelength (nm) oscillator strength (UV), and rotatory strength (CD) of **3** based on BHLYP/def2-TZVP.

M0001			M0002			M0003			M0004			M0005		
$\lambda$	UV	CD												
144.5	7.4.E-03	5.8	144.7	9.4.E-03	-3.6	144.8	1.3.E-03	-2.5	145.9	1.5.E-03	-1.2	145.1	3.3.E-04	-0.5
146.9	8.1.E-03	6.0	147.1	1.3.E-02	-16.5	147.2	1.3.E-02	5.4	147.1	8.4.E-03	11.2	147.4	1.5.E-02	-16.9
147.6	1.5.E-02	0.8	147.5	1.6.E-02	5.5	148.3	8.8.E-03	-3.2	149.0	2.3.E-02	9.0	148.4	2.2.E-02	5.5
149.3	1.1.E-02	14.2	148.5	1.8.E-02	16.3	149.4	1.0.E-02	8.2	149.4	7.8.E-04	-3.3	148.5	7.3.E-03	6.1
150.6	4.9.E-03	-6.0	150.4	1.6.E-03	4.2	150.7	1.2.E-02	-14.6	151.2	2.0.E-02	-15.7	150.3	2.4.E-03	5.0
151.6	1.2.E-02	-12.0	151.5	1.6.E-02	-11.7	151.7	7.5.E-03	-5.2	152.5	3.1.E-03	-3.2	151.5	1.4.E-02	-8.3
156.5	1.9.E-02	-21.5	156.6	1.8.E-02	-16.2	155.4	1.5.E-02	-23.3	155.2	1.7.E-02	-22.4	155.4	1.8.E-02	-23.6
158.9	8.4.E-03	2.4	158.6	9.3.E-03	-5.0	159.8	8.2.E-03	7.2	159.7	7.0.E-03	12.2	159.9	8.4.E-03	4.0
160.4	3.0.E-03	3.7	160.2	2.3.E-03	9.8	160.7	8.8.E-03	17.8	160.6	9.1.E-03	19.9	160.7	8.6.E-03	19.2
160.6	6.2.E-03	5.7	160.6	7.1.E-03	16.0	162.9	1.3.E-03	7.3	164.1	2.7.E-02	35.5	163.1	6.3.E-04	-1.6
163.9	3.2.E-02	7.4	164.0	3.0.E-02	6.0	163.9	3.5.E-02	-1.3	164.4	1.1.E-02	-29.3	164.1	3.2.E-02	-1.9
166.1	1.3.E-02	-33.3	166.1	1.4.E-02	-34.4	166.1	1.4.E-02	-35.4	166.0	1.4.E-02	-36.8	166.2	1.5.E-02	-36.2
171.5	2.9.E-02	-6.4	172.1	2.8.E-02	-5.2	172.5	2.7.E-02	-2.9	174.4	2.5.E-02	3.0	173.0	2.8.E-02	-2.4
177.4	3.5.E-03	-0.8	177.8	3.1.E-03	-1.8	177.6	3.5.E-03	-0.8	177.6	2.7.E-03	-1.8	177.9	3.1.E-03	-2.1
192.7	2.4.E-01	20.3	192.7	2.4.E-01	23.7	192.8	2.4.E-01	19.1	192.6	2.4.E-01	19.5	192.8	2.4.E-01	23.0

M0006			M0007			M0008			M0009			M0010		
$\lambda$	UV	CD	$\lambda$	UV	CD	$\lambda$	UV	CD	$\lambda$	UV	CD	$\lambda$	UV	CD
145.7	1.6.E-03	-4.6	144.3	3.E-03	7.9	144.5	2.E-02	-13.6	144.3	4.E-03	14.6	144.6	8.E-03	13.2
146.9	6.2.E-03	-7.2	146.0	4.E-03	0.8	146.0	2.E-02	19.3	147.3	1.E-02	29.7	147.7	2.E-02	22.2
148.1	3.8.E-02	17.3	148.5	1.E-02	-21.8	149.0	1.E-02	-6.5	147.7	1.E-02	14.0	148.2	1.E-02	8.5
150.5	2.6.E-03	-1.8	151.5	5.E-04	3.2	150.0	1.E-03	-6.9	151.0	3.E-03	-1.9	150.2	4.E-03	-8.2
150.6	1.2.E-03	5.3	152.4	1.E-02	-8.4	150.7	9.E-03	-4.1	151.7	2.E-02	-37.1	151.7	2.E-02	-38.3
151.5	1.4.E-02	-10.1	155.7	8.E-03	14.8	154.4	2.E-02	-4.7	152.9	1.E-02	-19.3	152.7	9.E-03	-17.6
156.0	1.4.E-02	-23.2	158.0	1.E-02	-9.6	155.1	4.E-03	12.0	157.7	1.E-02	25.9	158.2	1.E-02	33.7
160.2	7.4.E-03	13.5	158.6	9.E-04	-6.8	158.9	1.E-02	-8.0	159.5	1.E-03	-3.8	159.3	2.E-03	9.4
161.1	7.5.E-03	16.8	159.7	1.E-02	15.0	160.4	1.E-03	-7.9	160.3	3.E-03	-7.3	160.1	5.E-03	-32.9
163.9	1.7.E-02	-17.1	160.6	1.E-03	-6.7	161.9	1.E-02	-12.8	160.5	4.E-03	-15.5	162.6	3.E-04	5.9
164.2	2.2.E-02	-7.8	162.8	7.E-03	-14.6	164.4	8.E-03	-19.9	165.1	2.E-02	4.5	165.6	3.E-02	-4.5
166.1	1.3.E-02	-33.9	171.9	9.E-03	11.1	168.5	1.E-03	1.4	171.2	3.E-02	-6.2	171.5	3.E-03	0.4
173.8	2.7.E-02	1.6	181.4	7.E-02	-45.9	177.8	1.E-01	19.1	171.8	4.E-02	-13.9	172.2	5.E-02	-15.0
177.5	3.0.E-03	-2.1	183.0	9.E-03	-13.2	183.8	6.E-03	-4.8	178.6	8.E-03	-25.4	178.7	8.E-03	-25.7
192.6	2.4.E-01	21.9	189.1	2.E-01	45.6	193.1	2.E-01	12.0	195.3	2.E-01	34.4	195.3	2.E-01	33.5

Parameters used for ECD reproduction of 3.

wavelength	20 nm
UV width	12 nm
UV intensity	800000
CD width	10 nm
CD intensity	1.7

SCF energy (au), chemical potential (kJ/mol), relative free energy, and Boltzmann distribution of *ent*-4 based on B3LYP/def2-TZVP.

	M0001	M0002	M0003	M0004	M0005	M0006	M0007	M0008	M0009	M0010
SCF (AU)	-736.262356	-736.261964	-736.262126	-736.262087	-736.261596	-736.261584	-736.261771	-736.261863	-736.26132	-736.261217
CP (kJ/mol)	840.16	841.15	839.38	840.48	840.29	841.16	839.64	840.49	840.46	840.37
rel. ΔG (kJ/mol)	0.00	2.02	-0.18	1.03	2.12	3.02	1.01	1.62	3.02	3.20
Boltz. Dist.	12.6%	5.6%	13.6%	8.3%	5.4%	3.7%	8.4%	6.6%	3.7%	3.5%

	M0011	M0012	M0013	M0014	M0015	M0016	M0017	M0018	M0019
SCF (AU)	-736.260887	-736.261129	-736.260512	-736.261326	-736.260573	-736.260905	-736.260587	-736.26011	-736.260385
CP (kJ/mol)	839.63	838.83	840.43	839.1	839.67	840.08	838.9	839.76	839.98
rel. ΔG (kJ/mol)	3.32	1.89	5.11	1.64	4.19	3.73	3.38	5.49	4.99
Boltz. Dist.	3.3%	5.9%	1.6%	6.5%	2.3%	2.8%	3.2%	1.4%	1.7%

Wavelength (nm) oscillator strength (UV), and rotatory strength (CD) of *ent*-4 based on B3LYP/def2-TZVP.

M0001			M0002			M0003			M0004			M0005		
λ	UV	CD												
165.3	1.4.E-02	-37.4	165.7	4.3.E-03	-6.0	165.6	1.2.E-02	-6.9	165.1	2.3.E-04	-2.3	165.8	4.6.E-03	1.1
166.3	3.6.E-03	4.2	168.3	7.2.E-03	-4.9	165.8	8.6.E-03	-22.7	166.1	1.3.E-03	-6.9	168.7	7.7.E-03	-1.5
169.9	1.5.E-02	5.2	170.0	1.2.E-02	-4.8	170.2	1.6.E-02	8.8	170.0	1.2.E-02	1.4	169.9	5.8.E-03	-2.1
173.3	4.5.E-03	2.2	172.8	4.6.E-04	1.3	172.0	5.1.E-03	0.9	174.4	6.8.E-02	28.4	170.7	1.1.E-02	-4.5
174.2	1.1.E-03	-4.1	173.9	1.4.E-02	0.8	173.9	1.9.E-02	33.1	174.8	4.2.E-03	0.5	172.9	3.6.E-03	8.0
175.3	4.3.E-02	15.8	175.8	3.8.E-02	-16.5	174.4	3.8.E-02	7.7	175.8	3.2.E-03	7.4	176.1	3.6.E-02	-19.8
176.1	4.2.E-02	33.0	177.3	8.1.E-03	0.2	176.1	1.5.E-02	-5.0	176.6	4.2.E-03	5.5	178.2	5.1.E-02	36.1
178.0	4.9.E-02	51.7	179.1	8.6.E-02	108.3	180.2	4.0.E-02	49.1	178.9	5.2.E-02	31.4	181.6	3.3.E-02	47.2
181.0	5.6.E-03	7.5	180.8	4.8.E-03	5.4	182.0	5.9.E-04	5.6	180.0	4.5.E-03	0.4	182.2	3.3.E-03	6.6
183.9	1.4.E-02	3.1	184.2	1.5.E-03	-10.4	183.9	1.0.E-02	-0.4	183.3	3.5.E-02	30.9	184.6	3.8.E-03	-7.8
188.0	2.9.E-03	-8.2	188.7	1.7.E-02	-9.7	188.0	6.1.E-03	1.0	187.8	2.9.E-03	-9.6	188.3	1.6.E-02	17.3
193.4	5.1.E-02	1.9	192.6	7.9.E-02	35.5	190.8	1.1.E-01	22.0	196.7	1.6.E-02	-4.9	191.8	1.1.E-01	17.0
199.5	9.4.E-02	36.4	197.1	2.7.E-02	-13.5	200.3	4.9.E-02	27.1	199.1	9.6.E-02	44.3	195.9	3.4.E-02	-5.5
206.5	1.3.E-01	-81.6	202.7	6.1.E-02	-41.3	206.8	8.6.E-02	-72.5	206.6	1.5.E-01	-76.1	203.3	4.6.E-02	-32.7
207.3	9.6.E-03	10.4	206.8	9.7.E-02	-3.8	208.6	5.7.E-02	-2.7	208.4	4.4.E-03	1.4	209.2	8.7.E-02	-14.5

M0006			M0007			M0008			M0009			M0010		
$\lambda$	UV	CD												
166.0	4.0.E-03	6.5	165.7	1.2.E-02	4.4	164.8	9.7.E-03	-11.6	165.8	2.8.E-03	4.1	165.6	5.5.E-03	2.0
170.0	2.2.E-02	-2.0	166.5	1.3.E-02	-24.4	165.4	9.0.E-03	-41.8	168.2	1.2.E-02	-1.3	170.5	2.6.E-02	1.3
171.0	4.7.E-03	-7.4	168.7	1.2.E-02	7.1	171.4	1.6.E-02	0.7	171.4	8.5.E-03	-3.8	171.5	2.7.E-03	0.2
173.0	3.4.E-04	0.2	173.2	3.1.E-02	33.7	173.5	2.5.E-03	-0.4	171.8	7.6.E-04	-1.3	172.1	2.2.E-03	-6.6
174.2	1.4.E-02	-5.2	173.9	1.3.E-03	-4.5	174.5	8.2.E-04	2.2	173.2	6.3.E-03	15.6	173.1	2.7.E-03	5.1
175.4	2.7.E-02	-2.8	174.0	6.2.E-04	-5.6	174.9	5.1.E-02	14.7	176.1	5.1.E-02	7.5	175.5	2.4.E-02	-21.1
177.7	4.6.E-02	69.5	176.9	4.0.E-02	7.5	178.3	7.2.E-02	73.9	177.6	6.0.E-03	-10.4	179.3	9.6.E-02	94.0
179.8	1.2.E-03	-9.5	180.3	3.6.E-02	43.5	180.6	1.4.E-02	6.3	181.8	4.7.E-02	62.5	181.3	2.2.E-04	-2.7
181.5	2.4.E-02	-1.7	183.9	1.1.E-02	0.8	181.1	1.8.E-03	-0.4	184.1	8.0.E-03	-5.5	182.8	1.0.E-02	16.0
184.5	3.2.E-03	-6.7	187.2	1.1.E-01	48.0	181.6	2.7.E-02	23.0	186.4	4.8.E-02	29.4	184.8	3.4.E-03	-8.1
187.6	8.3.E-02	22.3	188.5	1.2.E-02	-10.2	187.7	2.0.E-03	-6.9	188.3	6.0.E-03	-12.7	187.2	4.7.E-02	-6.7
192.9	3.5.E-02	32.6	188.7	1.4.E-02	-17.4	194.5	5.3.E-02	-4.3	190.8	1.1.E-01	-18.7	192.6	4.6.E-02	29.0
199.8	8.1.E-03	-7.6	201.8	4.6.E-02	20.9	200.0	4.8.E-02	33.9	196.1	1.3.E-02	17.0	198.0	3.7.E-02	-18.1
203.7	9.2.E-02	-56.9	206.2	4.1.E-02	-43.8	207.0	1.2.E-01	-85.4	202.4	2.8.E-02	-23.6	204.1	6.6.E-02	-37.5
207.2	9.1.E-02	6.2	212.1	9.7.E-02	-27.5	209.3	4.7.E-02	10.2	213.1	9.9.E-02	-24.5	210.0	9.0.E-02	-5.0
M0011			M0012			M0013			M0014			M0015		
$\lambda$	UV	CD												
166.8	4.3.E-03	2.8	166.5	2.7.E-02	12.7	167.2	5.8.E-03	-7.0	165.3	5.1.E-03	-2.2	166.2	3.8.E-03	-2.2
167.2	2.5.E-03	0.6	167.5	3.0.E-03	-0.4	167.5	8.4.E-03	10.4	166.2	1.4.E-02	-36.4	168.5	3.0.E-02	20.4
167.4	1.1.E-02	5.7	169.7	3.4.E-03	-4.6	169.8	1.2.E-02	-2.6	169.4	1.1.E-02	4.8	168.8	7.1.E-03	2.4
170.4	1.0.E-02	4.2	170.1	3.2.E-02	18.1	175.5	9.9.E-03	1.1	173.5	5.0.E-02	33.9	170.7	1.9.E-02	1.8
176.4	7.2.E-02	45.2	172.1	4.5.E-02	7.1	175.8	2.4.E-02	-0.8	174.7	7.0.E-03	10.8	175.3	4.8.E-03	-5.8
177.0	3.5.E-03	3.3	175.7	8.7.E-03	-4.7	177.2	6.7.E-03	-3.5	176.6	2.3.E-02	-4.4	176.0	4.1.E-03	-12.6
177.6	4.8.E-03	-0.3	177.4	2.7.E-03	-4.5	177.8	2.2.E-02	4.2	177.3	2.9.E-04	0.4	179.3	6.5.E-02	32.0
179.1	4.9.E-04	3.7	180.6	8.8.E-04	12.1	178.6	2.7.E-02	33.7	178.8	1.3.E-03	-0.7	180.7	4.2.E-04	5.3
187.0	5.2.E-03	14.3	181.4	1.8.E-02	17.6	185.6	2.7.E-03	-8.4	180.4	5.8.E-02	57.8	183.1	2.3.E-03	3.6
187.8	3.0.E-03	-8.3	187.7	1.4.E-03	-6.9	187.1	2.2.E-03	-7.2	187.4	2.8.E-03	10.6	185.6	4.3.E-03	-13.8
189.7	1.3.E-02	10.9	188.9	6.9.E-03	20.0	188.5	1.9.E-02	29.0	188.2	1.5.E-03	-3.1	190.8	4.3.E-02	59.2
192.3	9.9.E-02	-3.0	194.6	1.4.E-01	24.3	192.9	1.1.E-01	21.6	192.5	5.8.E-02	-18.4	191.8	4.8.E-02	3.0
200.9	7.3.E-02	30.1	200.2	2.2.E-02	24.7	197.0	2.0.E-02	-3.5	200.6	9.4.E-02	36.6	198.9	8.9.E-02	-26.8
207.1	1.1.E-01	-78.7	206.6	1.3.E-01	-83.3	203.2	1.2.E-01	-57.9	206.5	7.7.E-02	-72.1	204.1	6.4.E-02	-34.0
215.3	2.8.E-02	20.7	209.2	3.1.E-02	14.9	215.7	4.0.E-02	18.3	211.6	6.6.E-02	18.0	210.1	6.7.E-02	8.4

M0016			M0017			M0018			M0019		
$\lambda$	UV	CD	$\lambda$	UV	CD	$\lambda$	UV	CD	$\lambda$	UV	CD
165.5	4.1.E-03	-5.1	166.9	1.1.E-02	-0.8	166.0	2.5.E-03	10.6	165.5	1.1.E-02	0.0
168.5	2.0.E-02	0.8	167.6	5.7.E-03	-1.1	167.2	9.0.E-03	8.9	166.4	3.4.E-04	0.0
171.4	9.8.E-03	-9.2	167.9	1.5.E-03	1.3	168.6	3.1.E-02	12.2	170.3	2.3.E-02	0.0
173.6	8.1.E-03	11.2	171.2	3.2.E-02	13.7	169.2	4.3.E-03	3.8	172.0	2.5.E-03	0.0
174.8	5.2.E-02	30.6	171.3	9.6.E-03	6.0	173.0	1.7.E-03	6.0	174.7	5.9.E-03	0.0
175.3	5.2.E-03	-9.9	174.1	5.4.E-05	0.1	177.3	2.7.E-02	-2.2	175.0	7.6.E-03	0.0
177.3	1.2.E-03	-6.2	177.8	3.0.E-02	5.4	178.2	2.0.E-03	-0.7	176.1	7.5.E-02	0.1
180.4	7.1.E-03	14.0	180.1	3.5.E-02	20.0	180.8	4.4.E-02	21.4	180.3	1.8.E-02	0.0
183.9	4.0.E-02	29.7	186.0	1.1.E-01	52.1	185.0	2.4.E-03	-8.1	181.3	5.3.E-02	0.1
184.8	3.6.E-02	0.5	187.4	2.6.E-02	-1.7	186.6	1.3.E-01	63.6	182.6	1.6.E-02	0.0
186.7	4.4.E-03	13.7	188.6	1.1.E-02	-9.5	189.1	2.6.E-03	12.3	183.4	1.4.E-02	0.0
193.2	9.0.E-02	12.6	189.6	2.1.E-03	8.2	191.1	5.0.E-02	-38.8	192.9	6.3.E-02	0.1
196.6	1.1.E-02	-0.1	202.2	5.2.E-02	20.0	196.7	1.3.E-02	21.9	195.8	5.1.E-03	0.0
202.4	7.6.E-02	-54.0	205.7	2.4.E-02	-30.7	202.4	2.1.E-02	-20.6	202.8	1.2.E-01	0.1
211.7	9.3.E-02	15.8	215.1	1.3.E-01	-33.5	215.9	1.3.E-01	-26.0	205.3	5.0.E-02	0.1

Parameters used for ECD reproduction of *ent-4*.

wavelength	0 nm
UV width	8 nm
UV intensity	4000
CD width	6 nm
CD intensity	-0.2 (because the enantiomer was applied for the calculations)

SCF energy (au), chemical potential (kJ/mol), relative free energy, and Boltzmann distribution of *ent*-5 based on B3LYP/def2-TZVP.

	M0001	M0002	M0003	M0004	M0005	M0006	M0007	M0008	M0009	M0010
SCF (au)	-736.2551045	-736.254876	-736.2548473	-736.2546731	-736.2545079	-736.2545639	-736.2544778	-736.2542072	-736.2543734	-736.254286
CP (kJ/mol)	840.06	839.74	838.66	840.08	839.61	838.9	838.33	838.06	838.93	838.52
rel G (kJ/mol)	0.72	1.00	0.00	1.88	1.84	0.98	0.64	1.08	1.51	1.33
Boltz. Dist.	12.4%	8.3%	35.0%	2.4%	2.5%	8.6%	14.0%	7.5%	4.0%	5.2%

Wavelength (nm) oscillator strength (UV), and rotatory strength (CD) of *ent*-5 based on B3LYP/def2-TZVP.

M0001			M0002			M0003			M0004			M0005		
$\lambda$	UV	CD												
176.1	9.0.E-03	9.0	176.0	9.1.E-03	7.4	178.1	2.2.E-03	-8.7	176.2	9.0.E-03	11.3	176.0	8.7.E-03	8.0
179.4	1.4.E-02	-1.7	180.0	1.2.E-02	-1.9	179.1	2.2.E-02	2.3	176.3	3.1.E-03	-3.1	179.3	4.8.E-03	0.6
180.4	1.4.E-03	6.9	181.6	2.6.E-04	3.1	180.4	1.9.E-03	7.2	179.9	1.1.E-03	-8.3	185.5	1.1.E-03	-2.6
184.3	2.0.E-04	1.1	185.3	6.5.E-03	13.0	184.3	4.2.E-03	0.2	184.3	6.8.E-03	11.5	186.7	4.7.E-03	12.7
185.2	7.8.E-03	14.0	187.0	1.1.E-02	13.1	185.4	2.4.E-02	37.0	188.3	2.8.E-03	-4.9	187.5	1.2.E-02	-3.3
189.4	7.7.E-02	87.6	190.1	2.9.E-02	46.5	189.8	1.7.E-02	29.6	190.5	1.1.E-01	94.5	190.2	1.6.E-02	31.3
199.4	6.6.E-02	4.4	197.4	1.6.E-01	35.3	197.5	1.3.E-01	58.7	199.5	9.0.E-03	0.0	194.7	2.2.E-01	52.8
203.4	6.5.E-02	-32.2	204.3	3.3.E-02	-4.2	204.8	1.6.E-01	-65.3	203.2	1.4.E-01	-36.1	202.9	3.1.E-02	-12.2
205.3	1.3.E-01	-57.2	204.9	9.8.E-02	-68.8	208.1	1.7.E-02	-21.6	208.9	8.9.E-02	-56.7	204.7	5.0.E-02	-43.2
216.0	9.8.E-02	20.0	217.7	1.1.E-01	3.4	219.6	8.9.E-02	0.8	216.5	9.2.E-02	26.2	221.6	1.3.E-01	-11.7

M0006			M0007			M0008			M0009			M0010		
$\lambda$	UV	CD												
176.5	9.7.E-03	7.0	178.2	2.6.E-03	-11.5	176.9	8.9.E-03	8.7	176.3	6.5.E-03	-3.8	176.9	1.1.E-02	-16.5
177.0	2.3.E-03	3.5	179.9	1.9.E-02	2.2	180.1	9.1.E-04	-2.9	177.8	1.9.E-03	-10.3	180.1	2.2.E-02	-0.7
180.8	4.3.E-04	0.4	181.9	3.8.E-04	3.0	181.4	1.5.E-03	0.6	179.9	1.0.E-03	-7.7	180.5	9.1.E-03	9.7
184.4	6.9.E-03	9.5	185.9	2.2.E-02	34.8	184.2	1.1.E-02	25.3	185.1	2.5.E-02	37.8	181.7	3.3.E-03	3.2
190.3	1.5.E-02	-5.7	187.5	6.1.E-03	3.4	185.4	4.2.E-02	33.9	188.5	1.5.E-02	-8.2	183.0	6.2.E-03	11.0
190.7	1.1.E-01	103.8	188.8	2.7.E-03	3.9	195.5	2.2.E-02	-4.1	191.3	6.6.E-02	56.7	190.3	6.0.E-02	70.0
198.4	1.6.E-03	4.0	198.1	2.0.E-01	87.1	199.5	1.3.E-01	49.2	196.9	2.0.E-02	21.7	198.9	5.1.E-02	19.5
203.7	1.8.E-01	-75.6	205.3	1.1.E-01	-76.3	203.6	1.6.E-01	-97.5	203.8	2.3.E-01	-37.9	204.5	2.2.E-01	-89.6
207.2	2.6.E-02	-13.7	206.8	1.9.E-02	-3.1	207.3	1.7.E-02	2.5	211.9	1.6.E-02	-28.7	208.1	1.8.E-03	6.1
218.0	1.1.E-01	9.7	222.0	8.7.E-02	-10.8	218.8	8.4.E-02	24.4	220.6	8.9.E-02	-0.9	217.6	8.8.E-02	10.3

Parameters used for ECD reproduction of *ent*-**5**.

wavelength	0 nm
UV width	12 nm
UV intensity	10000
CD width	10 nm
CD intensity	-3.2 (because the enantiomer was applied for the calculations)

SCF energy (au), chemical potential (kJ/mol), relative free energy, and Boltzmann distribution of **8-OBz** based on B3LYP/def2-TZVP.

	M0001	M0002	M0003	M0004	M0005	M0006
SCF (au)	-1081.801	-1081.801	-1081.799	-1081.799	-1081.798	-1081.798
CP (kJ/mol)	1113.44	1114.89	1113.65	1112.42	1112.2	1112.94
rel G (kJ/mol)	0	1.71	3.90	3.82	4.77	6.30
Boltzmann dist	46.7%	23.3%	9.6%	9.9%	6.8%	3.7%

Wavelength (nm) oscillator strength (UV), and rotatory strength (CD) of **8-OBz** based on B3LYP/def2-TZVP.

M0001			M0002			M0003			M0004			M0005		
$\lambda$	UV	CD												
176.1	3.1.E-03	4.3	177.5	1.3.E-03	-0.8	176.0	5.6.E-04	-0.1	175.7	3.3.E-04	1.0	175.8	2.4.E-03	1.2
176.3	6.6.E-03	-15.6	180.0	4.8.E-04	-0.2	178.0	2.2.E-03	-8.9	175.8	5.5.E-03	-9.3	177.2	8.2.E-04	-0.6
179.7	7.8.E-04	-1.0	181.2	8.7.E-03	1.6	179.5	4.1.E-04	-0.7	179.3	1.3.E-03	-1.2	179.5	3.0.E-03	0.9
183.9	5.8.E-03	16.8	182.5	3.9.E-03	-1.6	184.2	3.3.E-03	-1.5	184.2	1.9.E-02	-8.5	180.4	9.6.E-04	-0.4
183.9	5.3.E-03	-7.5	184.5	2.2.E-02	0.6	185.3	5.4.E-02	-7.2	184.6	1.9.E-01	0.9	185.5	1.4.E-01	36.0
185.1	3.4.E-01	11.4	185.5	7.7.E-02	-15.6	185.6	5.5.E-01	3.2	186.3	4.5.E-02	32.0	185.7	4.3.E-01	-43.0
186.9	3.9.E-01	-10.3	185.9	6.3.E-01	5.3	187.6	1.5.E-02	10.2	186.7	4.9.E-01	-20.2	187.7	1.7.E-01	-6.4
188.9	3.2.E-02	-12.5	190.0	1.7.E-01	-26.2	188.2	1.2.E-01	-7.4	187.4	1.4.E-03	-1.1	188.5	3.8.E-03	5.9
190.4	9.1.E-02	-19.7	190.6	1.1.E-02	15.0	189.6	6.6.E-02	-4.2	190.3	1.8.E-01	-14.1	190.2	1.4.E-01	-27.1
190.5	7.2.E-02	21.5	191.4	5.3.E-02	-10.6	189.9	9.8.E-04	4.8	191.0	5.8.E-03	6.7	190.9	3.0.E-02	13.0
192.0	3.2.E-02	-7.8	192.9	1.6.E-03	0.2	191.1	1.6.E-01	-19.1	192.0	4.2.E-02	-7.8	191.7	5.5.E-02	-5.4
197.7	1.3.E-02	2.6	197.9	2.2.E-02	1.7	197.4	1.3.E-02	2.3	198.0	9.9.E-03	2.7	197.2	1.0.E-02	2.1
201.1	1.1.E-02	5.6	201.9	2.1.E-03	-1.4	201.5	3.1.E-03	-1.2	201.2	1.1.E-02	5.8	201.8	4.2.E-03	-1.7
202.7	3.6.E-03	-1.5	202.8	1.3.E-02	5.8	201.6	1.1.E-02	5.5	202.6	3.5.E-03	-1.5	203.1	1.3.E-02	4.8
216.2	2.3.E-03	-1.0	214.1	2.7.E-04	-0.2	219.5	2.4.E-03	-0.5	215.0	3.2.E-03	-0.5	218.8	1.9.E-03	0.8
226.3	1.6.E-01	-7.0	225.7	2.9.E-02	-3.7	224.1	2.2.E-02	-5.9	226.0	1.3.E-01	-8.6	226.2	8.5.E-02	-11.5
227.6	1.1.E-01	16.6	226.2	2.2.E-01	8.5	227.3	2.5.E-01	15.7	227.8	1.4.E-01	19.0	227.6	1.8.E-01	21.8
238.2	4.9.E-02	3.0	236.0	7.1.E-02	7.0	236.4	4.9.E-02	3.3	238.0	4.6.E-02	1.6	236.7	5.4.E-02	1.0
248.9	1.2.E-02	-0.6	248.6	1.2.E-02	0.4	249.0	1.2.E-02	-0.1	248.9	1.2.E-02	-0.6	249.1	1.2.E-02	-1.3
255.4	3.4.E-05	-0.5	256.0	1.1.E-04	-1.2	255.1	1.6.E-04	-1.5	255.3	1.6.E-05	-0.3	254.8	1.2.E-05	0.1

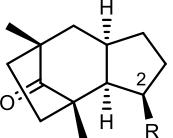
## M0006

$\lambda$	UV	CD
176.6	8.4.E-03	3.1
177.7	1.2.E-03	-0.8
179.9	1.5.E-04	-0.5
182.0	7.4.E-03	1.8
183.0	5.1.E-03	3.6
185.8	6.6.E-01	-2.8
187.8	6.2.E-02	-3.4
189.5	2.4.E-02	-12.1
190.3	1.5.E-01	2.8
191.3	5.4.E-02	-12.5
193.4	1.7.E-03	1.2
196.8	2.7.E-02	1.5
201.4	1.1.E-03	-1.3
203.3	1.3.E-02	5.8
218.3	7.1.E-04	-0.1
225.5	1.0.E-03	0.1
226.1	2.3.E-01	4.7
234.3	9.0.E-02	8.1
248.7	1.2.E-02	-0.2
255.5	2.1.E-04	-1.7

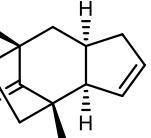
Parameters used for ECD reproduction of **8-OBz**.

wavelength	4 nm
UV width	10 nm
UV intensity	35000
CD width	6 nm
CD intensity	+3.0

Wavelength (nm) and rotatory strength (CD) of *ent*-model **I**, *ent*-model **II**, and *ent*-model **III** based on B3LYP/def2-TZVP, and their calculated ECD spectra



*ent*-model **I** (R = H)

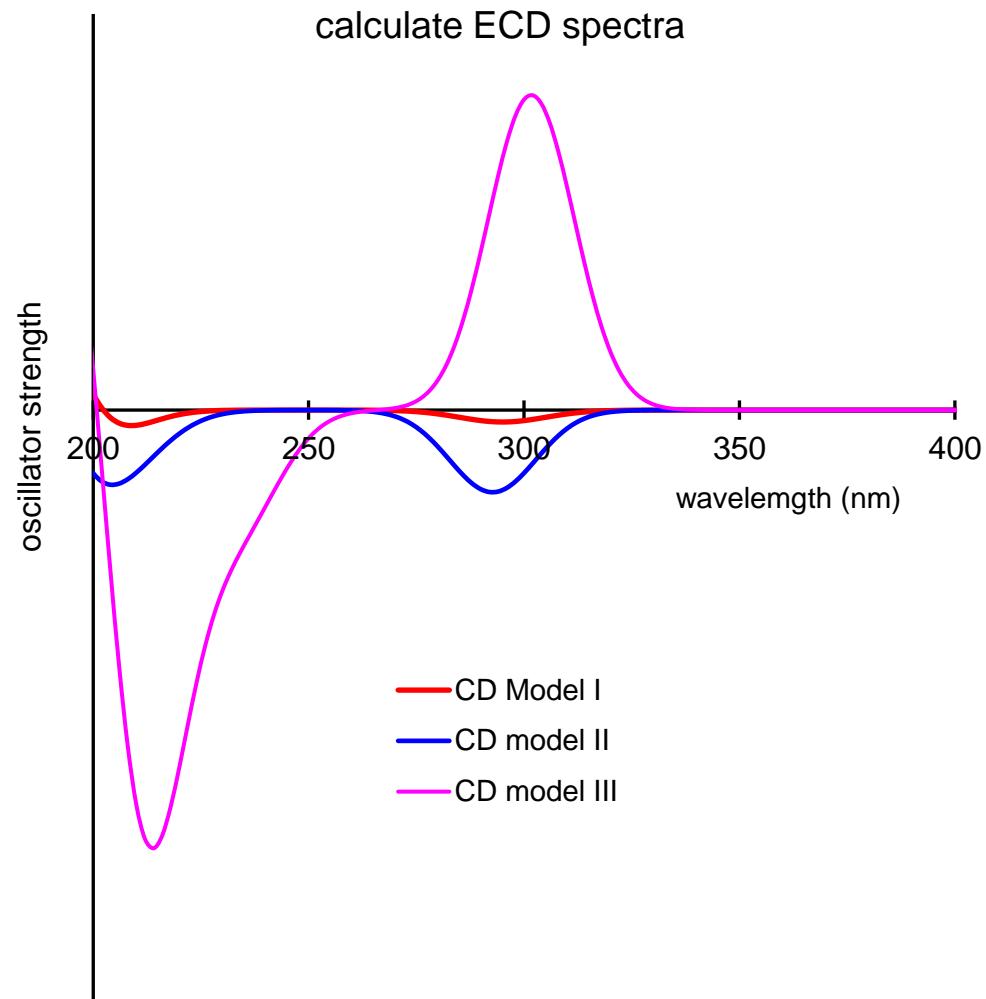


*ent*-model **II** (R = Cl)



*ent*-model **III**

<i>ent</i> -model <b>I</b>		<i>ent</i> -model <b>II</b>		<i>ent</i> -model <b>III</b>	
$\lambda$	CD	$\lambda$	CD	$\lambda$	CD
157.5	1.6	166.6	-0.1	170.4	-5.0
159.1	2.1	168.0	11.2	171.0	0.0
159.6	-1.4	170.0	9.3	171.1	0.6
161.8	-3.0	173.2	-18.4	172.1	-3.2
166.5	7.2	174.4	-10.4	175.5	-0.6
170.0	-1.0	179.1	33.1	176.4	18.9
171.6	1.0	180.2	-45.6	177.2	-7.8
175.6	-3.0	181.8	-11.7	177.8	-7.1
176.9	-4.7	182.6	-3.0	179.4	-4.0
177.1	2.4	184.9	-1.0	185.7	-5.4
180.3	3.2	187.9	13.7	189.1	-1.0
185.1	-14.6	198.7	-26.4	194.1	3.6
185.5	3.5	209.7	37.8	197.6	2.8
199.7	2.4	233.3	7.2	209.1	2.1
295.0	0.8	301.7	-19.9	292.7	5.2



Parameters used for ECD reproduction of *ent*-model **I**, *ent*-model **II**, and *ent*-model **III**.

wavelength	4 nm
CD width	6 nm
intensity	-1

XYZ data of *ent*-model **I** used for reproduction of the ECD spectrum.

34			C	0.967608	-1.261576	0.525516	H	1.593892	-1.161433	2.600991	
C	1.811005	-2.492120	0.227582	C	-0.202946	0.711515	-0.314404	H	-0.934439	0.940415	-2.340564
C	-0.613461	1.566304	-1.505766	O	1.726224	-0.179703	-1.537504	H	0.214851	2.180694	-1.858900
C	-0.544431	-1.543690	0.695973	H	2.093523	1.288110	3.727435	H	-1.442415	2.226770	-1.238342
C	-1.292361	-0.290834	0.144592	H	-0.207308	0.394307	2.670993	H	2.069153	2.176466	-0.173116
C	1.451351	1.762160	2.981635	H	-0.620637	2.178086	1.188481	H	2.851789	-2.217703	0.047944
C	1.525762	-0.479737	1.746819	H	1.079985	3.525397	0.331678	H	1.449819	-3.009790	-0.663042
C	1.438668	2.542456	0.638777	H	-0.817559	-2.430025	0.120525	H	1.780402	-3.193177	1.065365
C	0.675792	0.744418	2.131633	H	-0.797740	-1.752967	1.736760	H	0.741981	2.392676	3.524964
C	0.250372	1.579028	0.898430	H	-1.955525	0.156780	0.887031	H	3.243992	2.202783	1.821147
C	0.959715	-0.235404	-0.607775	H	-1.914312	-0.568669	-0.708488	H	2.374519	3.635983	2.314616
C	2.242089	2.611414	1.964662	H	2.550747	-0.173282	1.514135				

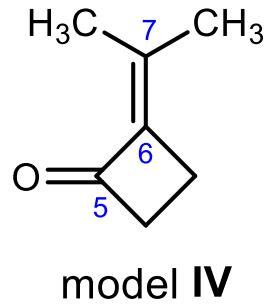
XYZ data of *ent*-model **II** used for reproduction of the ECD spectrum.

40			C	-1.096761	-1.596017	-1.213736	H	1.714946	3.548067	0.003464	
H	1.755916	0.706760	2.357815	C	-1.171015	-2.195595	0.192569	C	-1.651524	0.618922	-2.364348
C	1.645872	0.314147	1.345015	C	-2.611396	-0.191515	-0.118273	H	-2.491699	0.150809	-2.878938
C	0.199722	-0.171098	1.054026	H	-3.509148	-0.262266	-0.735015	H	-0.793732	0.570458	-3.034960
C	-0.229464	0.586378	-0.237766	H	-2.719262	0.701892	0.499487	H	-1.902310	1.669268	-2.191959
C	1.085888	1.008769	-0.906863	C	-2.441755	-1.489173	0.730545	C	-1.251111	-3.714729	0.195002
C	1.997182	1.395879	0.289534	H	-3.307216	-2.140636	0.601942	H	-0.350886	-4.154390	-0.237669
H	2.341201	-0.522555	1.253828	H	-2.360290	-1.278119	1.798194	H	-2.101046	-4.063326	-0.393931
H	-0.461075	0.139781	1.865506	C	3.493618	1.437147	-0.030376	H	-1.361036	-4.092956	1.214532
H	-0.665244	1.540182	0.076747	H	4.053747	1.717654	0.865008	O	-0.994939	-2.201420	-2.248488
H	0.960068	1.825292	-1.614263	H	3.713803	2.176769	-0.804230	H	0.553417	2.845193	1.134218
C	0.099066	-1.702749	0.930283	H	3.861432	0.472180	-0.373099	H	0.971851	-2.087607	0.396360
H	0.121222	-2.149475	1.930148	C	1.586441	2.798802	0.788725	Cl	1.813376	-0.332501	-1.913615
C	-1.366893	-0.093697	-1.049668	H	2.222547	3.087839	1.627864				

XYZ data of *ent*-model **III** used for reproduction of the ECD spectrum.

32				C	1.763653	3.000278	2.059540	H	1.495427	-1.372550	2.675023
C	1.406067	-2.920837	0.421288	C	0.856834	-1.513437	0.604521	H	-0.523270	0.753790	-2.494600
C	-0.100478	1.386984	-1.713094	C	0.116486	0.586778	-0.439349	H	0.841592	1.787366	-2.088535
C	-0.680603	-1.446004	0.784993	O	1.785434	-0.827325	-1.560302	H	-0.786487	2.218227	-1.537986
C	-1.157802	-0.130221	0.096364	H	3.039179	1.312509	2.536860	H	2.479785	-2.898507	0.228477
C	2.006540	1.621528	2.718527	H	0.113555	0.571420	2.552954	H	0.930674	-3.421185	-0.424351
C	1.587453	-0.775067	1.762369	H	-1.142623	-2.310649	0.305431	H	1.230304	-3.522446	1.316432
C	1.164205	2.638862	0.722792	H	-0.959901	-1.483624	1.839203	H	1.855989	1.633557	3.798883
C	1.052943	0.648465	1.989352	H	-1.719824	0.514198	0.772843	H	2.681807	3.586372	1.968270
C	0.767359	1.367740	0.681402	H	-1.812570	-0.359951	-0.746094	H	1.065560	3.611871	2.644632
C	1.055335	-0.623226	-0.626119	H	2.653613	-0.728849	1.517760	H	1.050251	3.356940	-0.078810

Wavelength (nm) oscillator strength (UV), and rotatory strength (CD) of model **IV** based on B3LYP/def2-TZVP when dihedral angle  $\angle O/C-5/C-9/C-7$  was set to 15°.



$\lambda$	UV	CD
134.8	9.8.E-03	21.6
135.8	5.0.E-02	-15.2
136.1	1.4.E-02	-5.1
136.9	6.0.E-03	-2.0
138.5	5.5.E-03	15.4
139.9	1.5.E-01	-0.9
140.0	1.9.E-02	0.4
141.9	2.0.E-02	-1.8
145.3	2.1.E-02	-9.2
146.3	8.3.E-02	9.9
146.5	3.7.E-02	7.7
148.3	7.4.E-02	-19.4
148.7	7.4.E-03	-17.5
149.0	3.6.E-02	17.7
152.8	1.1.E-01	4.4
153.1	3.7.E-03	-3.7
154.6	8.1.E-03	0.8
158.4	1.3.E-04	1.3
164.3	7.7.E-04	-0.1
165.5	2.7.E-02	-7.8
166.0	9.4.E-03	0.3
167.4	4.3.E-04	5.4
171.3	2.0.E-03	10.3
174.1	1.5.E-03	-18.0
181.5	8.3.E-03	2.2
183.5	3.3.E-03	1.5
185.8	3.5.E-02	-1.6
194.5	1.2.E-03	-7.7
237.2	3.5.E-01	9.5
348.4	5.8.E-04	-5.3

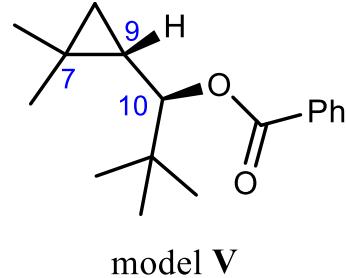
Parameters used for ECD reproduction of model V.

wavelength	20 nm
UV width	11 nm
UV intensity	30000
CD width	10 nm
CD intensity	+2.0

XYZ data of model V used for reproduction of the ECD spectrum.

C	-1.0314	1.2228	-0.8196
C	-0.356	0.096	-0.1109
C	-2.3385	0.9708	-0.0474
C	-1.6525	-0.2665	0.6126
H	-2.0871	-1.2203	0.3083
H	-1.6057	-0.2384	1.7021
O	-0.7283	1.9886	-1.6986
C	0.9194	-0.3042	-0.0283
C	2.0009	0.349	-0.8379
H	2.7889	0.7309	-0.1806
H	1.6174	1.1647	-1.4466
H	2.4763	-0.3864	-1.4957
C	1.3411	-1.4274	0.8714
H	2.0979	-1.0839	1.5842
H	1.8071	-2.2289	0.289
H	0.5062	-1.849	1.4293
H	-3.2017	0.7689	-0.6831
H	-2.5899	1.7769	0.6436

Wavelength (nm) and rotatory strength (CD) of model V based on B3LYP/def2-TZVP when dihedral angle  $\angle C-8/C-9/C-10/O$  was set to  $180^\circ$ .



model V

$\lambda$	CD
162.52	0.47
164.96	-2.58
169.72	-0.26
173.42	-0.31
178.45	-4.99
178.69	4.03
181.43	4.03
184.49	7.29
188.16	-2.09
197.38	0.84
204.85	0.10
206.42	-0.59
223.00	15.85
245.63	1.38
255.28	-1.96

Parameters used for ECD reproduction of model V.

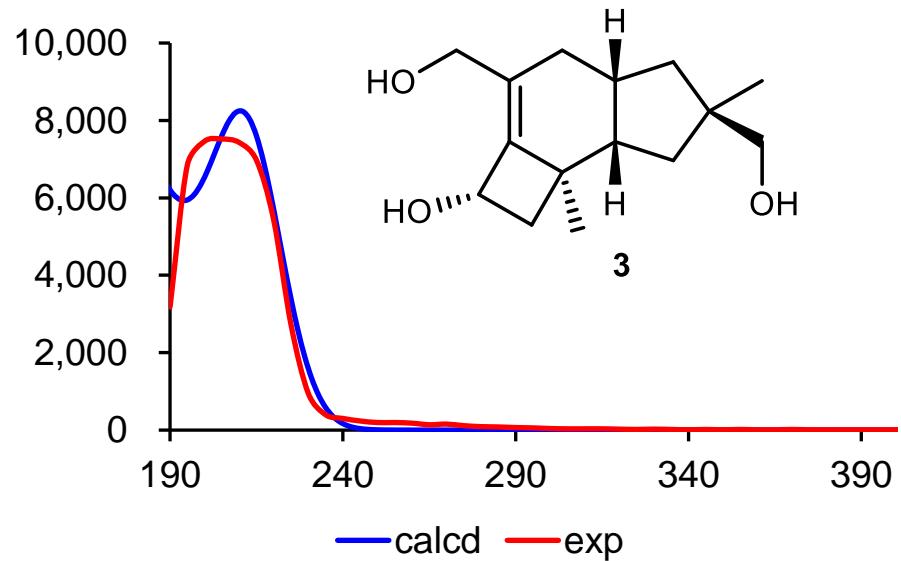
wavelength 14 nm  
CD width 8.0 nm  
CD intensity +2.8

XYZ data of model V used for reproduction of the ECD spectrum.

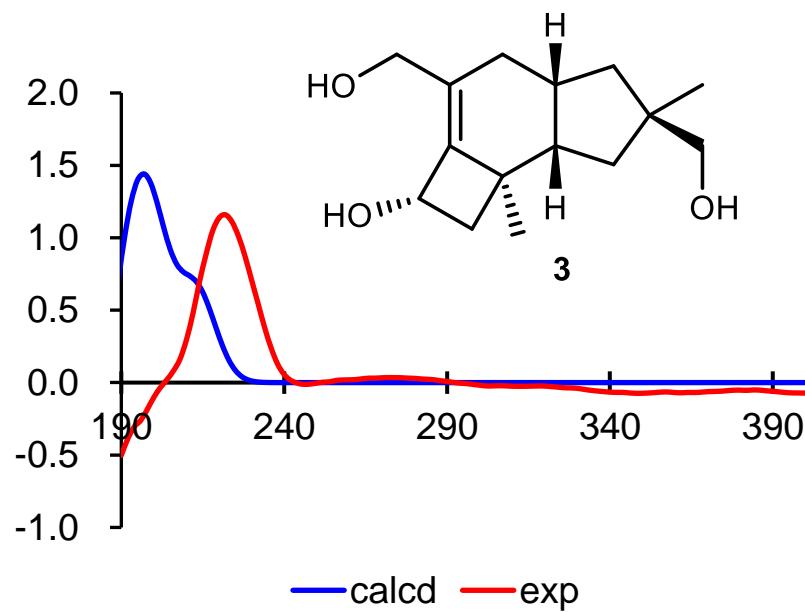
C	-2.9578	1.3481	2.639
C	-3.1552	0.9629	1.1929
H	-3.4814	-0.0481	0.9687
H	-3.5249	1.7173	0.5055
C	-1.7699	1.1253	1.7416
H	-1.2172	2.0149	1.4473
C	-0.8807	-0.0594	2.0181
H	-1.4413	-0.9981	1.9911
O	0.2131	-0.1155	1.0914
C	-0.0251	-0.7463	-0.0727
C	1.1411	-0.6781	-0.9985
C	3.2552	-0.5907	-2.806
C	1.0295	-1.3146	-2.2361
C	2.3141	0.0033	-0.6671
C	3.3685	0.0455	-1.5721
C	2.0858	-1.2715	-3.1373
H	0.1082	-1.8361	-2.4734
H	2.3944	0.4955	0.2953
H	4.28	0.5764	-1.3151
H	1.9973	-1.7672	-4.0991
H	4.0805	-0.5558	-3.5112
O	-1.0651	-1.3091	-0.3327
H	-3.1843	2.364	2.9468
H	-3.1722	0.5944	3.3929
H	-0.3924	0.0428	2.9907

Calculated and experimental UV/ECD spectra of **3** with B3LYP/def2-TZVP

UV spectra



ECD spectra



Hyphal growth inhibitions of *Cochliobolus miyabeanus* by **2a** and **5** at 5.0 µg/mL



**2a** (5.0 µg/mL)



**5** (5.0 µg/mL)