

## **Synthesis of the Antitumor Agent Mucocin: A Modular Approach Based on Olefinic Coupling Reactions**

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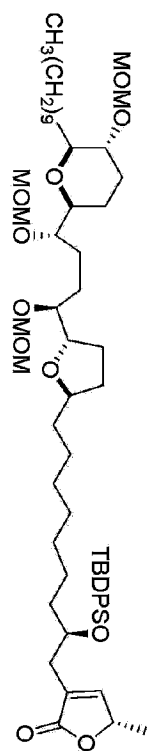
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### **Supporting Information**

<sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compounds **17**, **1** and mucocin samples

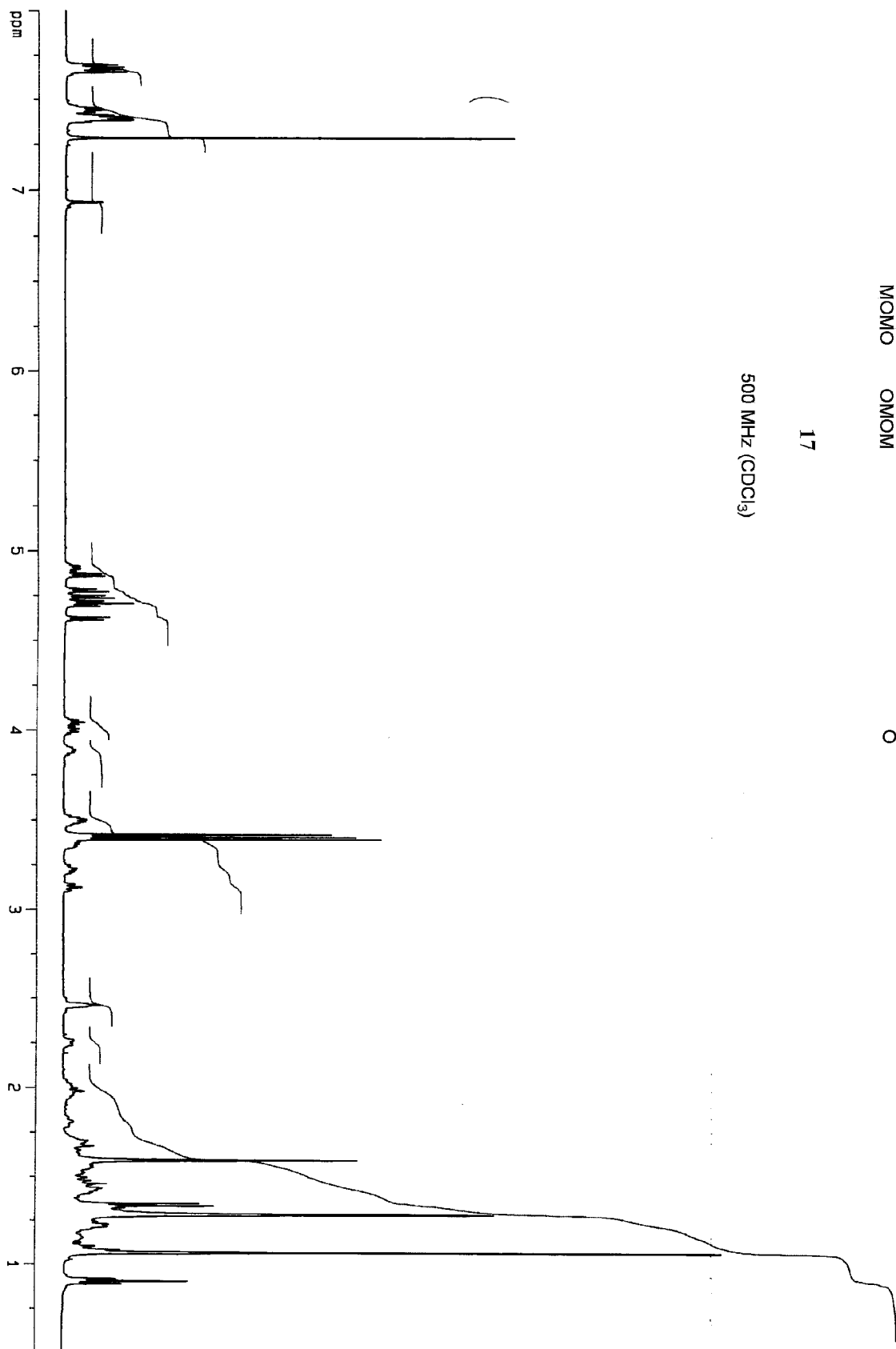
Tabulated data for natural and synthetic mucocin

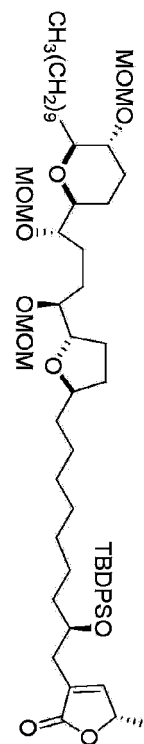
**General.** <sup>1</sup>H and <sup>13</sup>C NMR spectra were recorded at 500 and 125 MHz respectively, in CDCl<sub>3</sub> solutions, with CHCl<sub>3</sub> as internal standard.



17

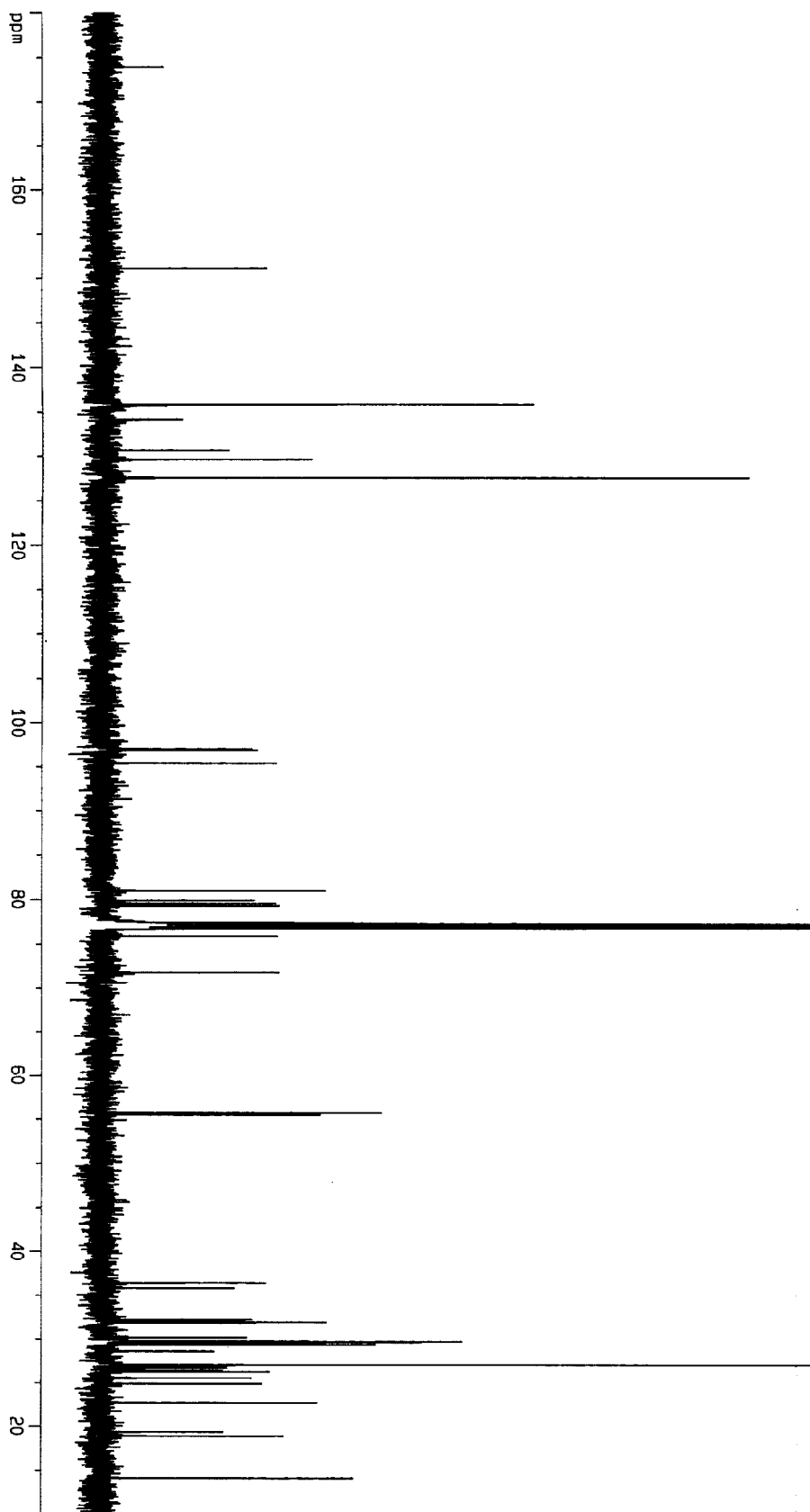
500 MHz (CDCl<sub>3</sub>)

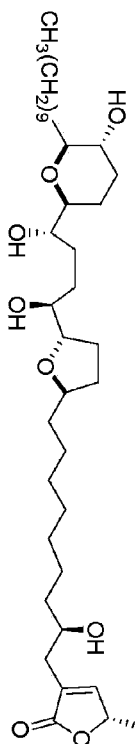




17

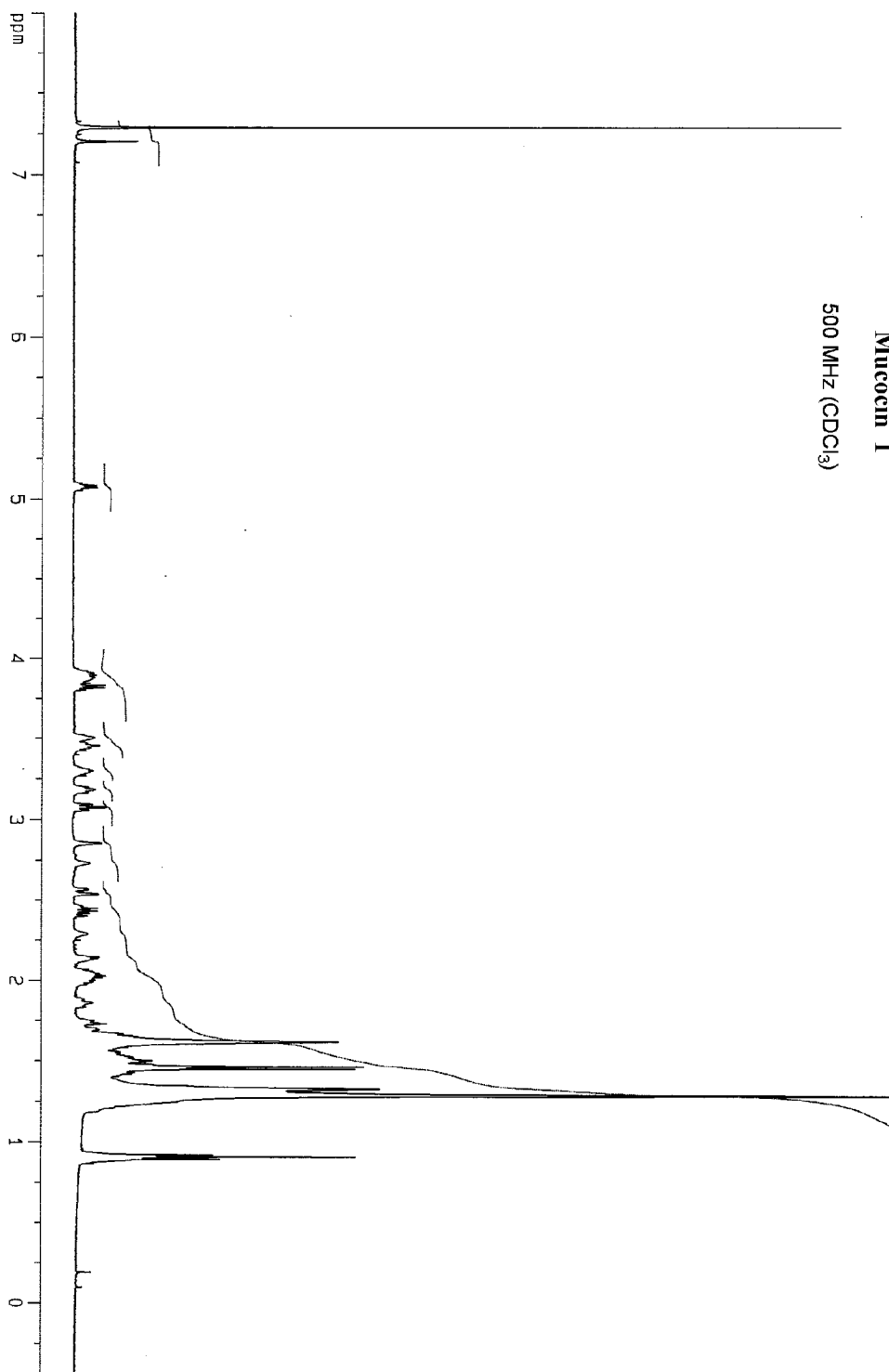
125 MHz (CDCl<sub>3</sub>)

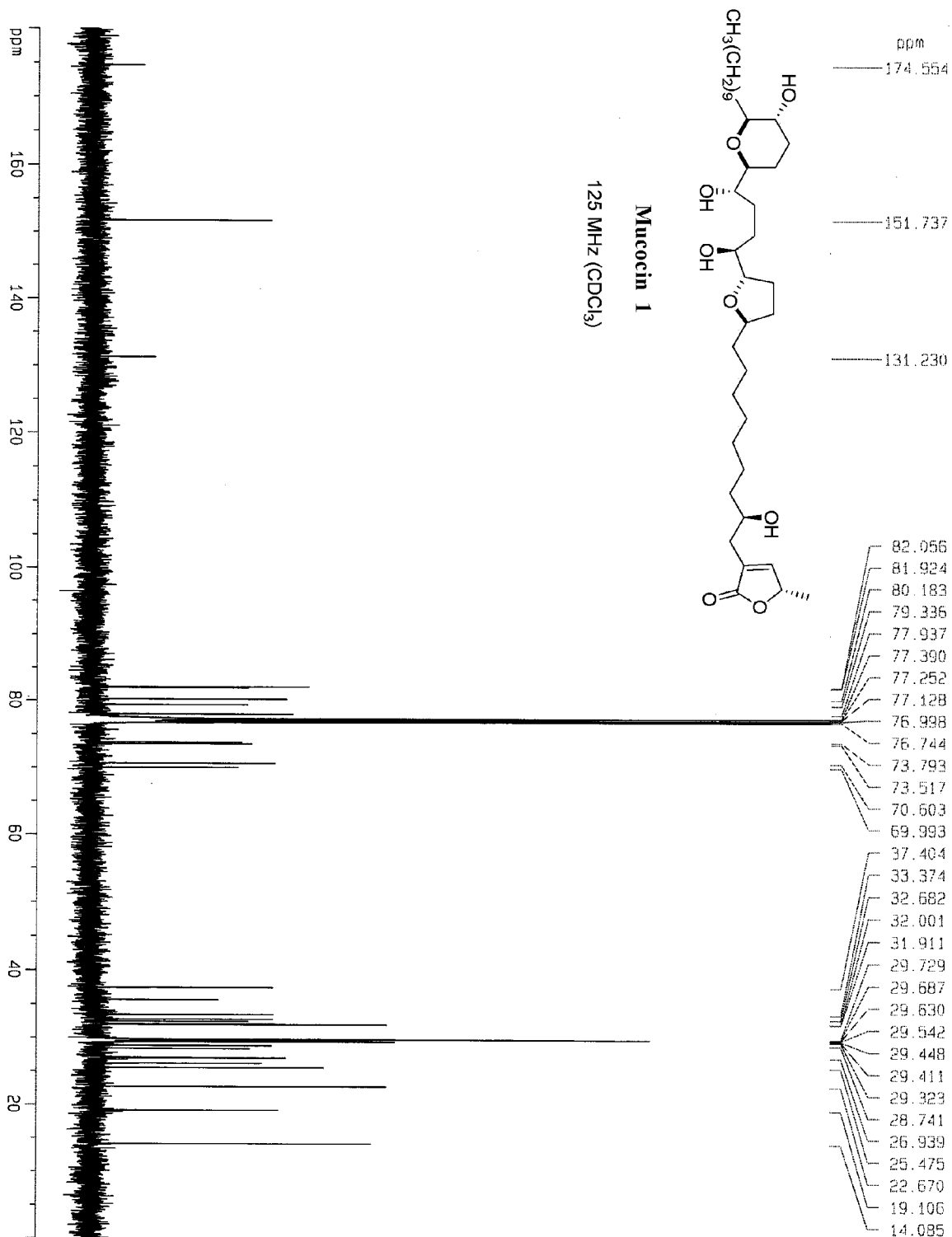


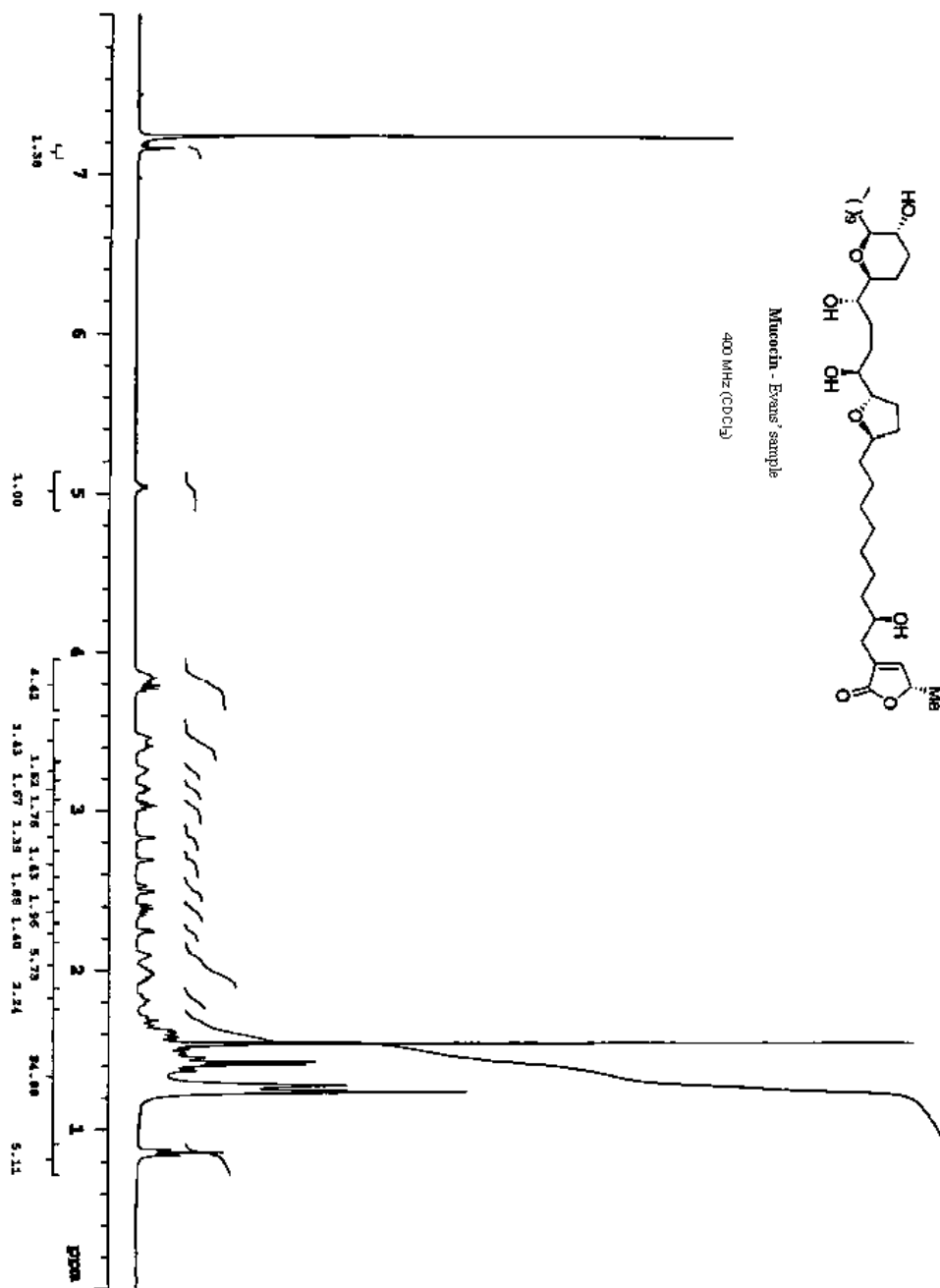


**Mucocin 1**

500 MHz (CDCl<sub>3</sub>)









### Comparison of <sup>13</sup>C NMR of Mucocin and synthetic material

<sup>13</sup>C NMR in CDCl<sub>3</sub> (Natural compound: 75 MHz; synthetic compound: 125 MHz; rel to CDCl<sub>3</sub> at 77.00 ppm, carbon assignments made by comparison to literature values)

Carbon #	Mucocin	Comp1	Comp1-Muc	Keinan	Comp1-Keinan	Evans	Comp1-Evans
1	174.61	174.55	-0.06	174.62	-0.07	174.82	-0.27
35	151.81	151.74	-0.07	151.82	-0.08	152	-0.26
2	131.15	131.23	0.08	131.16	0.07	131.3	-0.07
24	82.01	82.06	0.05	81.98	0.08	82.15	-0.09
15	81.91	81.92	0.01	81.89	0.03	82.06	-0.14
20	80.12	80.18	0.06	80.14	0.04	80.28	-0.1
12	79.31	79.34	0.03	79.3	0.04	79.47	-0.13
36	77.96	77.94	-0.02	77.98	-0.04	78.16	-0.22
16	73.77	73.79	0.02	73.76	0.03	73.93	-0.14
19	73.48	73.52	0.04	73.47	0.05	73.63	-0.11
23	70.51	70.6	0.09	70.57	0.03	70.68	-0.08
4	69.92	69.99	0.07	69.96	0.03	70.09	-0.1
5	37.33	37.4	0.07	37.37	0.03	37.52	-0.12
11	35.56	35.6	0.04	35.57	0.03	35.73	-0.13
3	33.29	33.38	0.09	33.34	0.04	33.48	-0.1
6-10, 26-33	32.6	32.68	0.08	32.61	0.07	32.75	-0.07
13	32.35	32.4	0.05	32.4	0	32.56	-0.16
6-10, 26-33	31.98	32	0.02	32	0	32.12	-0.12
22	31.87	31.91	0.04	31.96	-0.05	32.06	-0.15
6-10, 26-33				31.9			
6-10, 26-33	29.7	29.73	0.03	29.71	0.02	29.87	-0.14
6-10, 26-33		29.69		29.66	0.03	29.78	-0.09
6-10, 26-33		29.63		29.63	0	29.69	-0.06
6-10, 26-33	29.51	29.54	0.03	29.54	0	29.6	-0.06
6-10, 26-33		29.45		29.45	0	29.55	-0.1
6-10, 26-33	29.39	29.41	0.02	29.39	0.02	29.48	-0.07
6-10, 26-33	29.29	29.32	0.03	29.32	0		
18	28.77	28.84	0.07	28.75	0.09	28.9	-0.06
17	28.68	28.74	0.06	28.68	0.06	28.83	-0.09
14	28.31	28.35	0.04	28.33	0.02	28.49	-0.14
21	26.89	26.94	0.05	26.89	0.05	27.05	-0.11
6-10, 26-33	26.12	26.16	0.04	26.16	0	26.31	-0.15
6-10, 26-33		25.52		25.52	0	25.67	-0.15
25	25.48	25.48	0	25.46	0.02	25.63	-0.15
6-10, 26-33	22.63	22.67	0.04	22.67	0	22.82	-0.15
37	19.1	19.11	0.01	19.1	0.01	19.24	-0.13
34	14.1	14.09	-0.01	14.12	-0.03	14.27	-0.18