

SUPPORTING INFORMATION

Norterenoids and Related Peroxides from the Formosan Marine Sponge *Negombata corticata*

Chih-Hua Chao,[†] Kuei-Ju Chou,[†] Guey-Horng Wang,[‡] Yang-Chang Wu,[§] Li-Hsueh Wang,^{⊥, ||}
Jeng-Ping Chen,[▽] Jyh-Horng Sheu,^{*, †, °} and Ping-Jyun Sung,^{*, ⊥, ||}

Department of Marine Biotechnology and Resources, National Sun Yat-sen University, Kaohsiung 804, Taiwan, Department of Cosmetic Science, Chia-Nan University of Pharmacy and Science, Tainan 717, Taiwan, Graduate Institute of Natural Products, Kaohsiung Medical University, Kaohsiung 807, Taiwan, National Museum of Marine Biology and Aquarium, Checheng, Pingtung 944, Taiwan, Graduate Institute of Marine Biotechnology, National Dong Hwa University, Checheng, Pingtung 944, Taiwan, Taiwan Ocean Research Institute, National Applied Research Laboratories, Taipei 106, Taiwan, and Asia-Pacific Ocean Research Center, National Sun Yat-sen University, Kaohsiung 804, Taiwan

* To whom correspondence should be addressed. Tel: 886-7-5252000, ext. 5030. Fax: 886-7-5255020. E-mail: sheu@mail.nsysu.edu.tw (J.-H. S)

[†] National Sun Yat-sen University.

[‡] Chia-Nan University of Pharmacy and Science.

[§] Kaohsiung Medical University.

[⊥] National Museum of Marine Biology and Aquarium.

^{||} National Dong Hwa University.

[▽] Taiwan Ocean Research Institute, National Applied Research Laboratories.

[°] Asia-Pacific Ocean Research Center.

Table S1. Comparison of NMR data of isolates **1** and **2** with literature data.

For compound 4:

S1-1. ^1H NMR spectrum (300 MHz) of compound **4** in CDCl_3 .

S1-2. ^{13}C NMR spectrum (300 MHz) of compound **4** in CDCl_3 .

S1-3. HRESIMS spectrum of compound **4**.

For compound 5 and its methyl ester 5a:

S2-1. ^1H NMR spectrum (500 MHz) of compound **5** in CDCl_3 .

S2-2. ^{13}C NMR spectrum (500 MHz) of compound **5** in CDCl_3 .

S2-3. HRESIMS spectrum of compound **5**.

S2-4. ^1H NMR spectrum (300 MHz) of methyl ester **5a** in CDCl_3 .

S2-5. ^{13}C NMR spectrum (300 MHz) of methyl ester **5a** in CDCl_3 .

For compound 6/7 and the methyl ester 6a/7a:

S3-1. ^1H NMR spectrum (300 MHz) of compound **6/7** in CDCl_3 .

S3-2. ^{13}C NMR spectrum (300 MHz) of compound **6/7** in CDCl_3 .

S3-3. HRESIMS spectrum of compound **6/7**.

S3-4. ^1H NMR spectrum (300 MHz) of methyl ester **6a/7a** in CDCl_3 .

S3-5. ^{13}C NMR spectrum (300 MHz) of methyl ester **6a/7a** in CDCl_3 .

For compound 8 and its MTPA esters 8a and 8b:

S4-1. ^1H NMR spectrum (300 MHz) of compound **8** in CDCl_3 .

S4-2. ^{13}C NMR spectrum (300 MHz) of compound **8** in CDCl_3 .

S4-3. HRESIMS spectrum of compound **8**.

S4-4. ^1H NMR spectrum (300 MHz) of diol derived from **2** in CDCl_3 .

S4-5. ^{13}C NMR spectrum (300 MHz) of diol derived from **2** in CDCl_3 .

S4-6. ^1H NMR spectrum (300 MHz) of (*S*)-MTPA ester **8a** in CDCl_3 .

S4-7. ^1H NMR spectrum (300 MHz) of (*R*)-MTPA ester **8b** in CDCl_3 .

For compound 9:

S5-1. ^1H NMR spectrum (300 MHz) of compound **9** in CDCl_3 .

S5-2. ^{13}C NMR spectrum (300 MHz) of compound **9** in CDCl_3 .

S5-3. HRESIMS spectrum of compound **9**.

For compound 10:

S6-1. ^1H NMR spectrum (300 MHz) of compound **10** in CDCl_3 .

S6-2. ^{13}C NMR spectrum (300 MHz) of compound **10** in CDCl_3 .

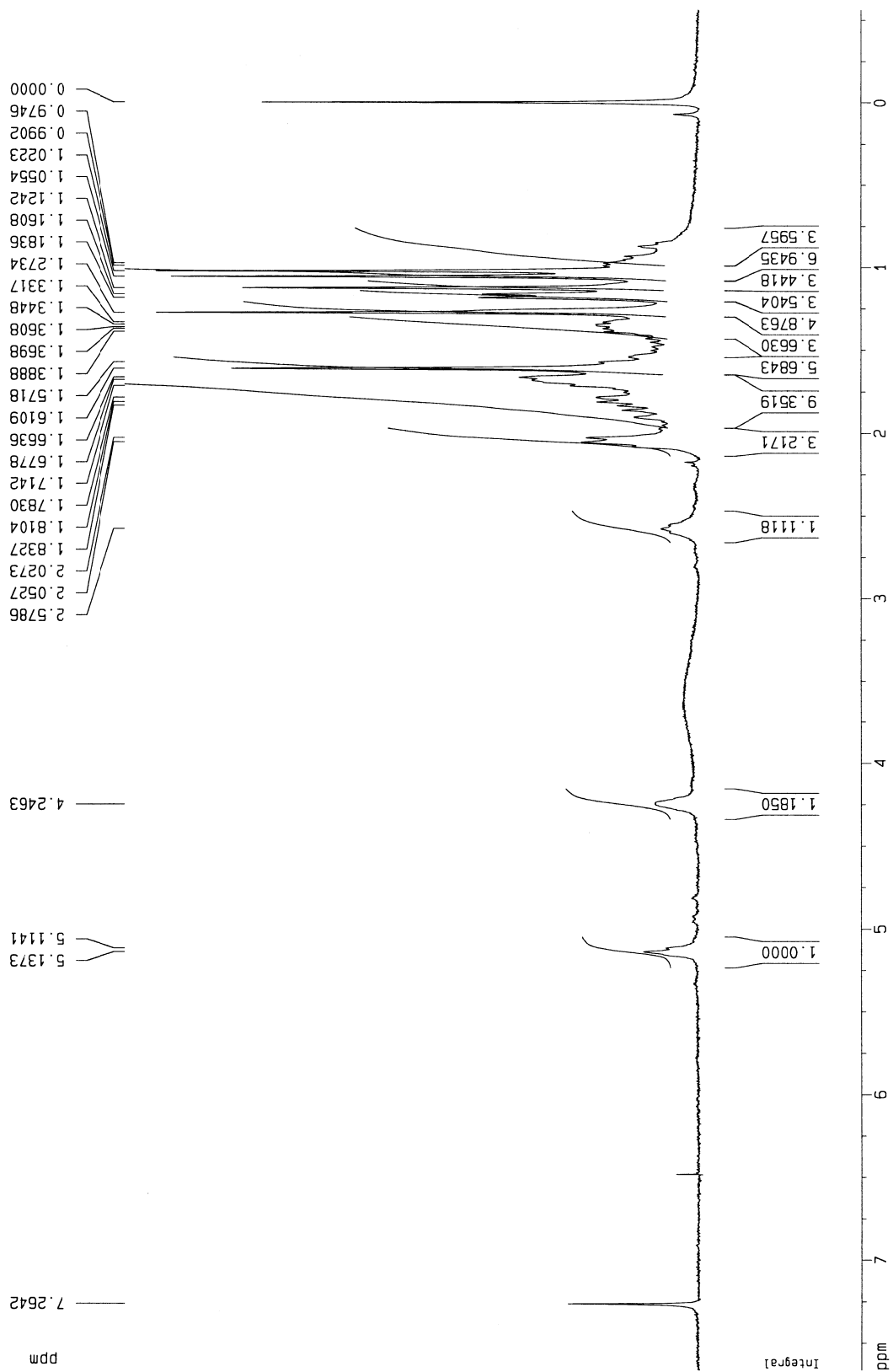
S6-3. HRESIMS spectrum of compound **10**.

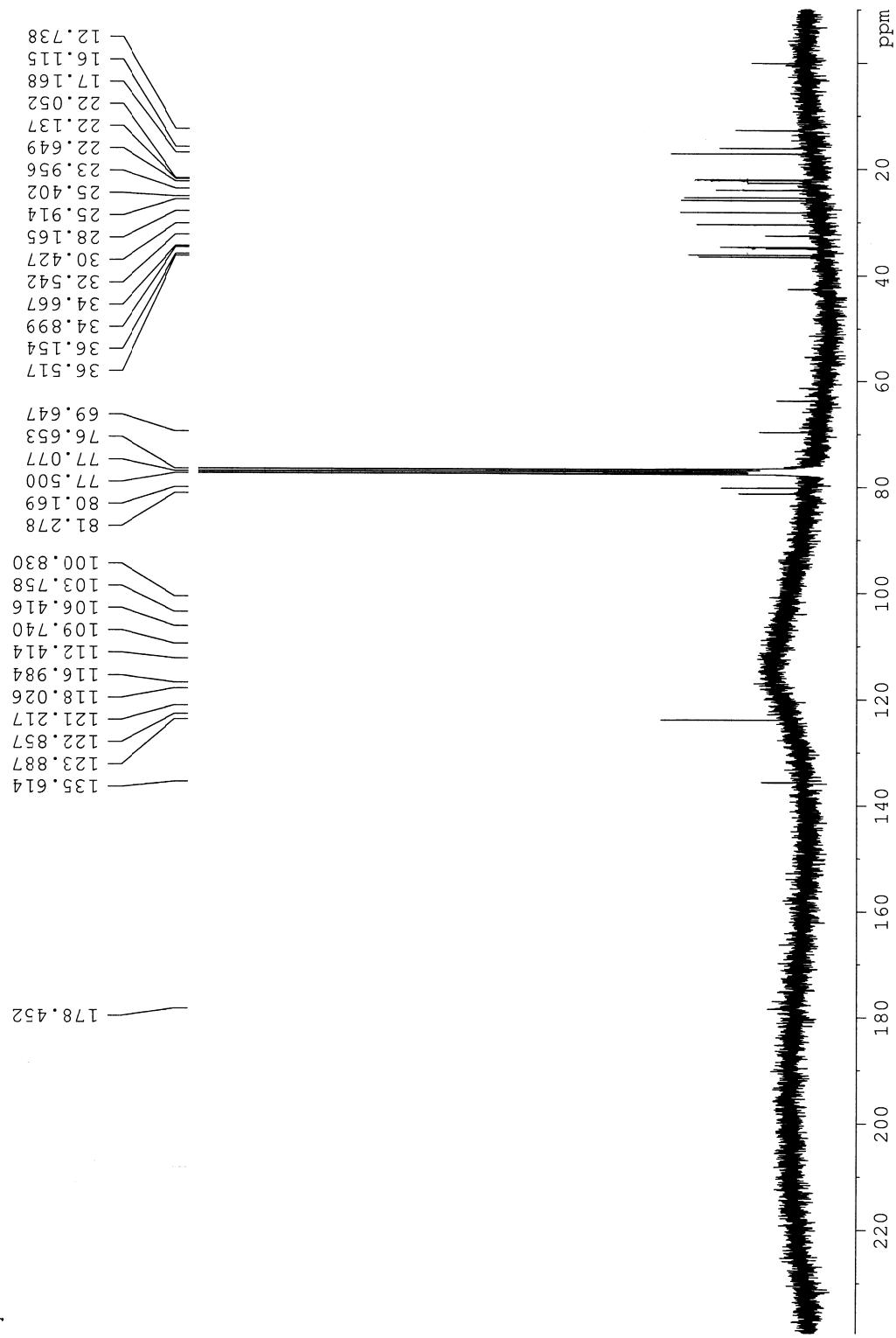
Table S1. Comparison of NMR data of isolates **1** and **2** with literature data

position	<u>2 (300 MHz, CDCl₃)</u>		<u>(+)-nuapapu B methyl ester (CDCl₃)</u>		<u>1 (300 MHz, CDCl₃)</u>		<u>1 (400MHz, CD₃OD)</u>		<u>(+)-nuapapu B (CD₃OD)</u>	
	δ_{H} (<i>J</i> in Hz)	δ_{C} , mult	δ_{H} (<i>J</i> in Hz) ^a	δ_{C} , mult ^b	δ_{H} (<i>J</i> in Hz)	δ_{C} , mult	δ_{H} (<i>J</i> in Hz)	δ_{C} , mult	δ_{H} (<i>J</i> in Hz) ^a	δ_{C} , mult ^d
1		174.2, C		174.0, C		179.9, C		177.9, C		178.0, C
2	2.58 m	42.4, CH	2.58, m	42.6, CH	2.58, m	42.6, CH	2.44, m	44.1, CH	2.39, m	44.0, CH
3	4.23 m	81.0, CH	4.22, m	81.2, CH	4.24, m	81.1, CH	4.15, m	82.9, CH	4.13, dt (8.5, 3.5)	82.8, CH
4	1.62 m	22.3, CH ₂		22.5, CH ₂	1.60, m	22.3, CH ₂	1.66, m	23.6, CH ₂		23.5, CH ₂
5	1.71 m	32.4, CH ₂		32.4, CH ₂	1.75, m	32.6, CH ₂	1.76, m	33.9, CH ₂		33.5, CH ₂
6		80.0, C		80.3, C		80.4, C		81.3, C		81.2, C
7	1.58 m	33.5, CH ₂		33.6, CH ₂	1.59, m	33.6, CH ₂	1.59, m	34.6, CH ₂		33.9, CH ₂
	1.55 m				1.55, m		1.48, m			
8	1.8 m	19.9, CH ₂		20.0, CH ₂	1.62, m	20.0, CH ₂	1.57, m	21.1, CH ₂		20.8, CH ₂
9	1.65 m	54.2, CH		54.4, CH	1.65, m	54.3, CH	1.70, m	55.8, CH		55.6, CH
10		149.3, C		149.5, C		149.5, C		150.9, C		150.7, C
11	2.01 m	32.3, CH ₂		32.4, CH ₂	2.01, m	32.4, CH ₂	2.03, m	33.3, CH ₂	2.02, m	33.2, CH ₂
12	1.53 m	23.7, CH ₂		23.9, CH ₂	1.53, m	23.9, CH ₂	1.54, m	24.8, CH ₂		24.6, CH ₂
	1.51 m				1.51, m					
13	1.51 m	36.1, CH ₂		36.2, CH ₂	1.51, m	36.2, CH ₂	1.53, m	37.2, CH ₂		37.5, CH ₂
	1.19 m				1.20, m		1.23, m			
14		34.8, C		35.0, C		35.0, C		35.8, C		35.7, C
15	1.13 d (7.2)	12.6, CH ₃	1.15, d (7.5)	12.8, CH ₃	1.17, d (7.2)	12.5, CH ₃	1.11, d	13.3, CH ₃	1.09, d	13.3, CH ₃
16	1.10 s	23.6, CH ₃	1.10, s	23.7, CH ₃	1.10, s	23.7, CH ₃	1.06, s	24.3, CH ₃	1.04, s	24.0, CH ₃
17	4.54 s	108.8, CH ₂	4.57, d (2.5)	108.9, CH ₂	4.54, s	108.9, CH ₂	4.55, d (2.5)	109.6, CH ₂	4.57, d (2.5)	109.5, CH ₂
	4.75 s		4.75, d (2.5)		4.75, s		4.76, d (2.5)		4.76, d (2.5)	
18	0.92 s	28.2, CH ₃	0.92, s	28.4, CH ₃	0.93, s	28.4, CH ₃	0.93, s	28.8, CH ₃	0.91, s	28.8, CH ₃
19	0.85 s	26.2, CH ₃	0.85, s	26.4, CH ₃	0.85, s	26.4, CH ₃	0.86, s	27.0, CH ₃	0.83, s	27.4, CH ₃
OMe	3.69 s	51.7, CH ₃	3.69, s	— ^c						

^a Only selected ¹H NMR data were provided in the literature. ^b The assignments of CH₂ carbons for C-4, C-7, and C-12 were revised according to our present work.^c The chemical shift was not found in the original literature. ^d The assignments of CH₂ carbons for C-4, C-5, C-7, C-11, and C-12 were revised according to our present work. The assignment of NMR data of isolates **1** and **2** were based on the interpretation of 2D NMR experiment.

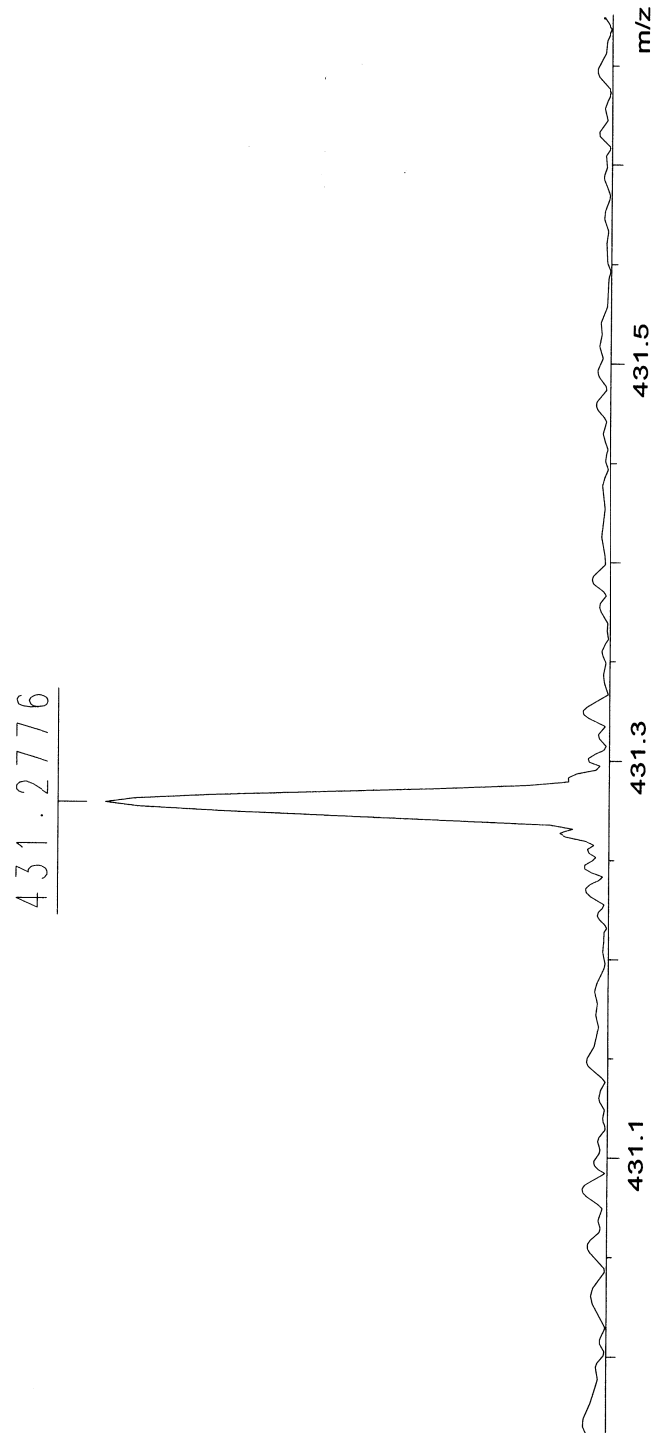
S1-1. ^1H NMR spectrum (300 MHz) of compound **4** in CDCl_3 .



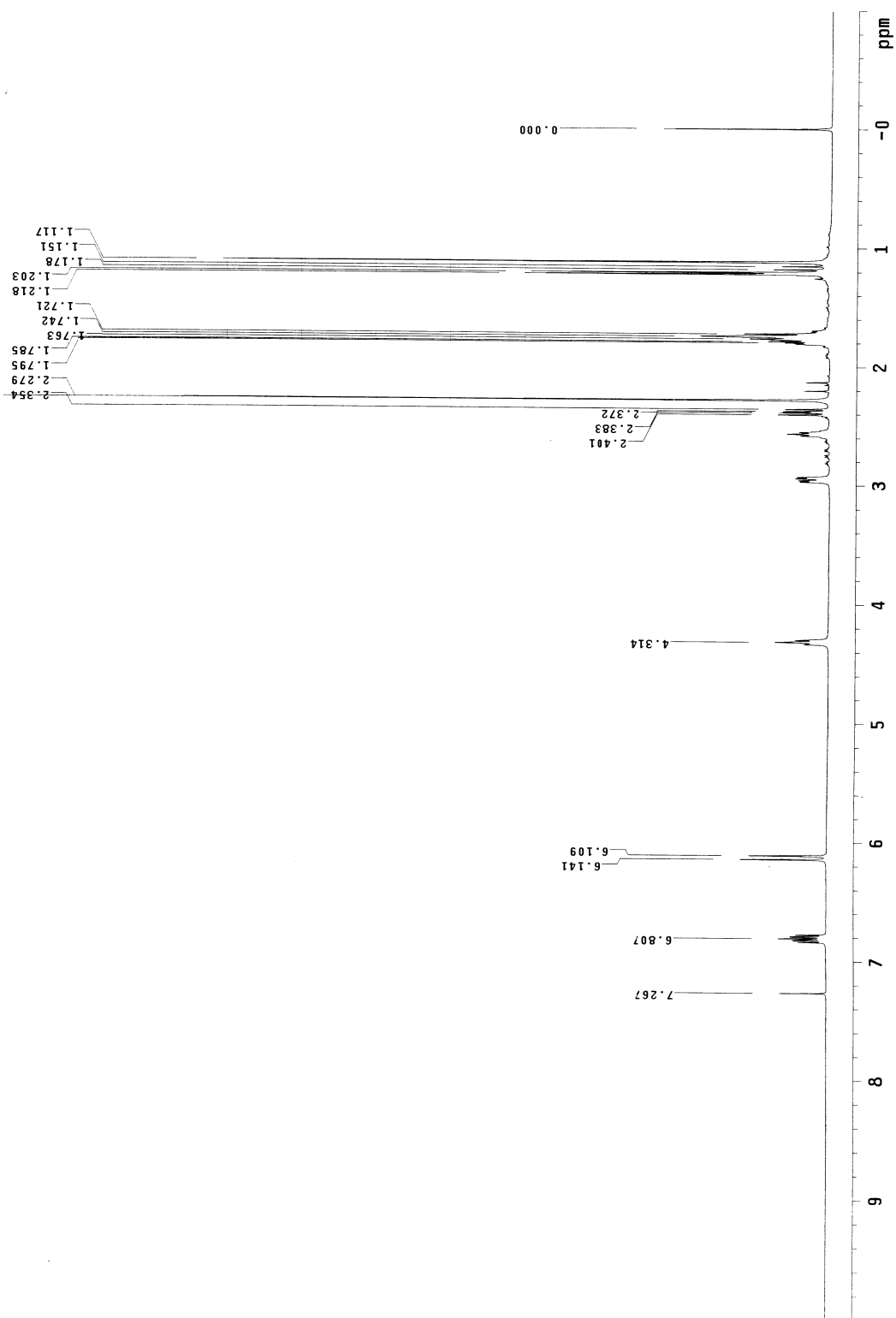


S1-2. ¹³C NMR spectrum (300 MHz) of compound **4** in CDCl₃.

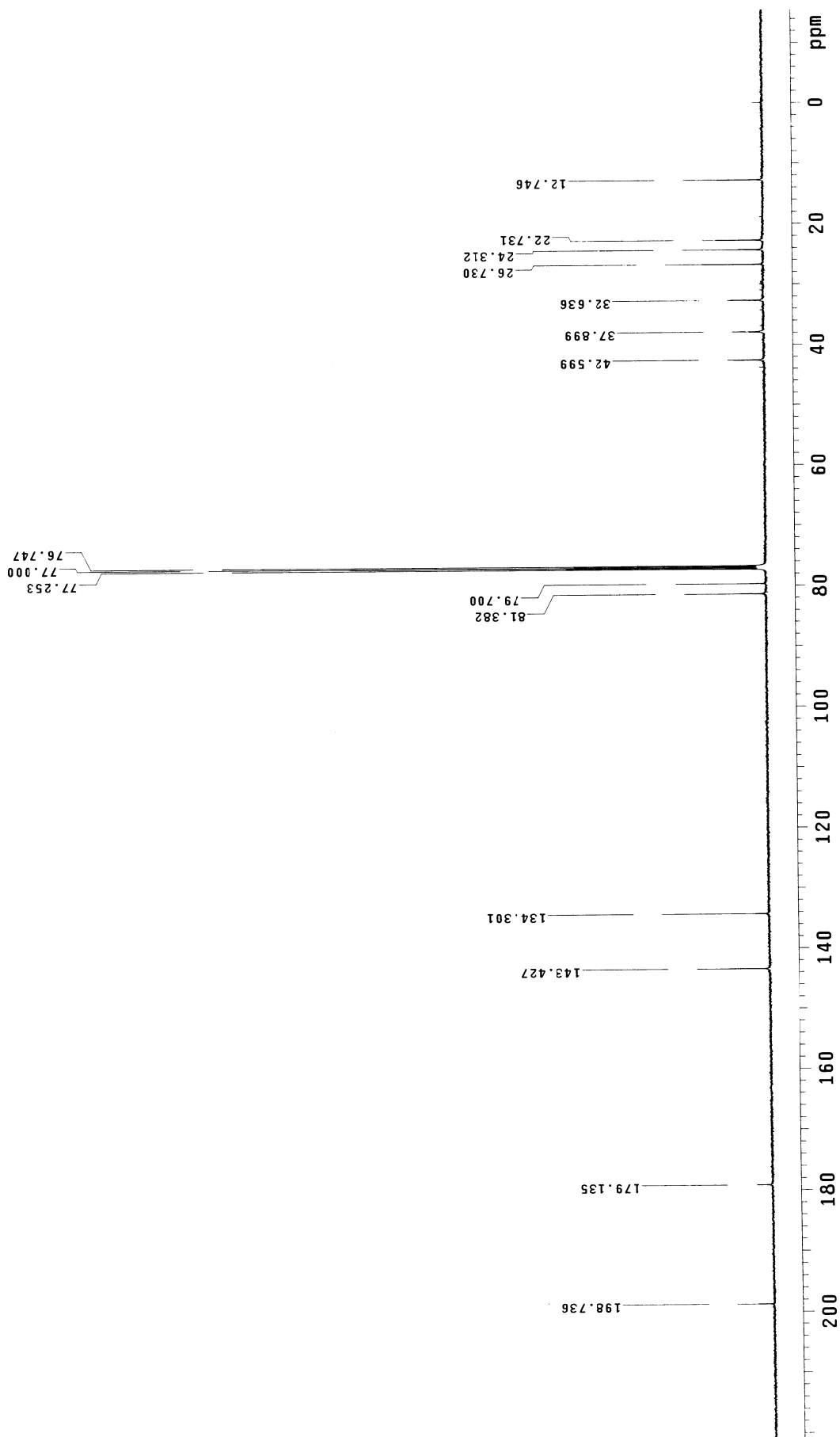
ESI+



S1-3. HRESIMS spectrum of compound **4**.

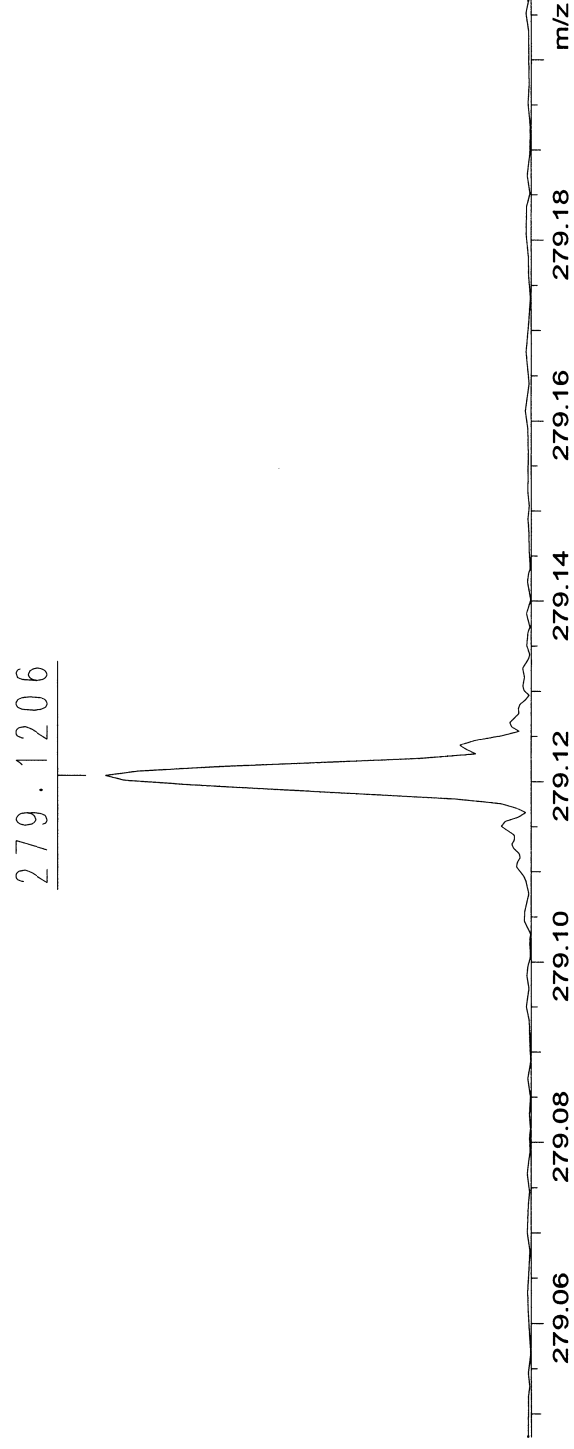


S2-1. ¹H NMR spectrum (500 MHz) of compound **5** in CDCl₃.

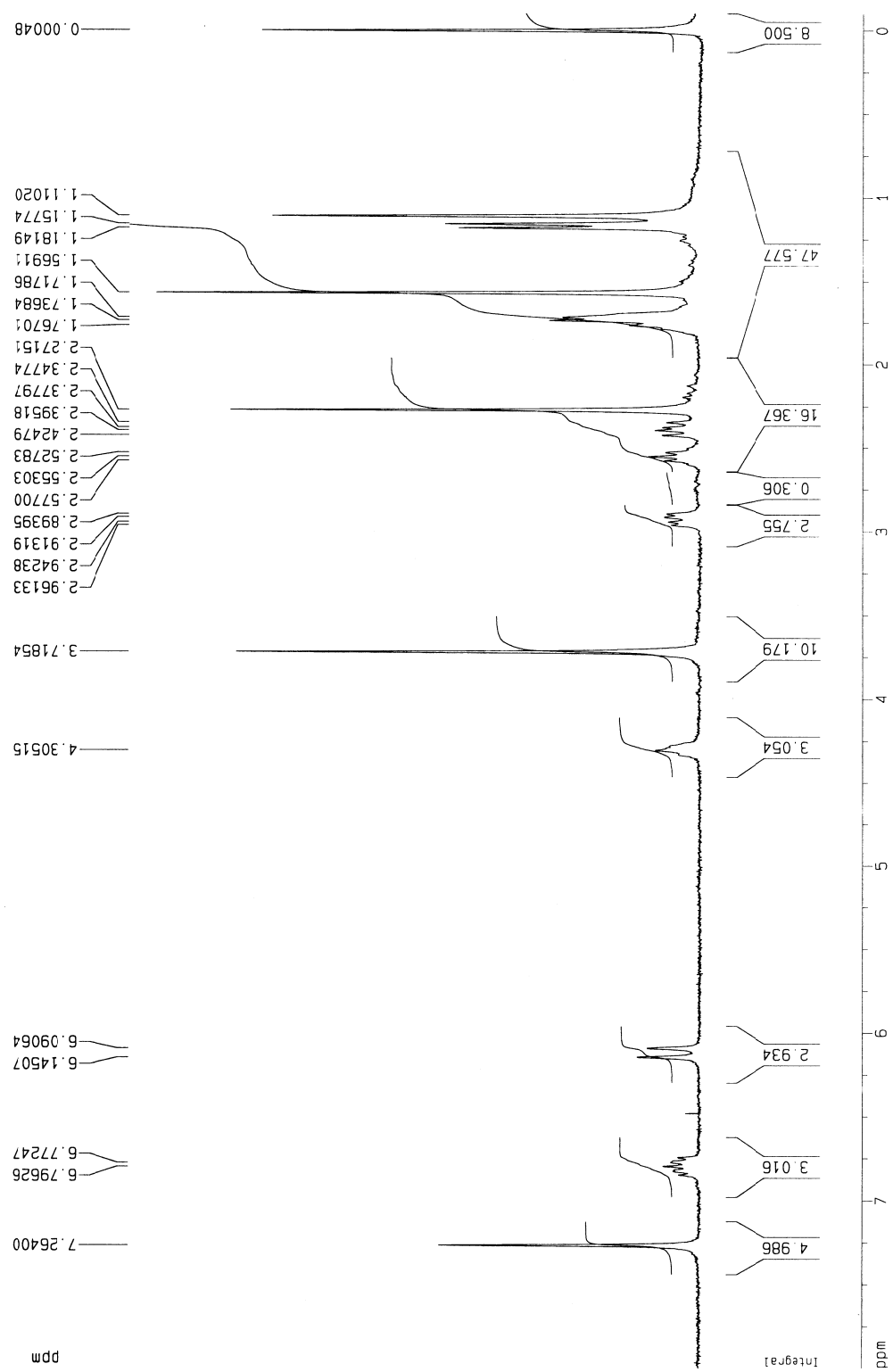


S2-2. ¹³C NMR spectrum (500 MHz) of compound **5** in CDCl₃.

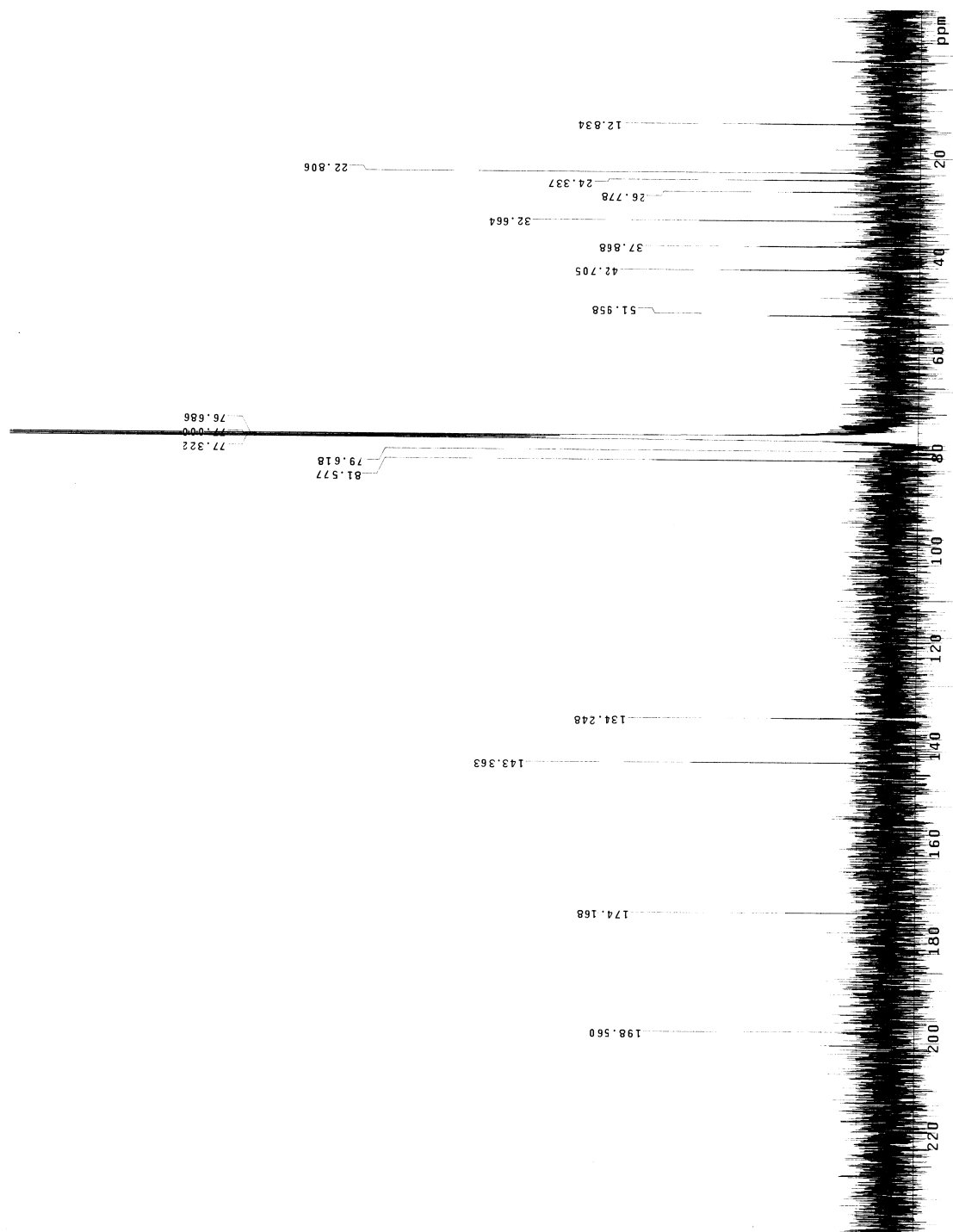
ESI+



S2-3. HRESIMS spectrum of compound 5.

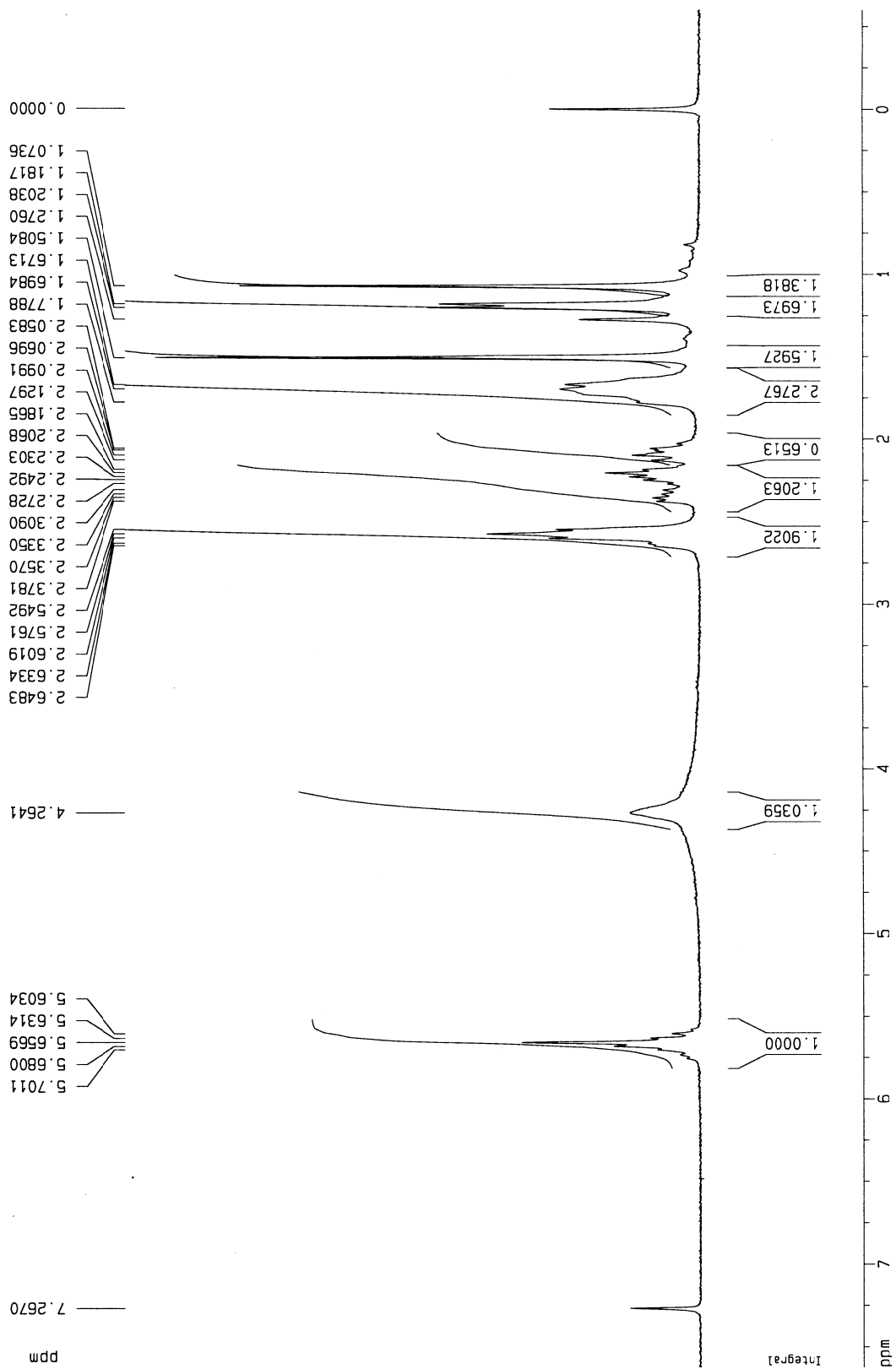


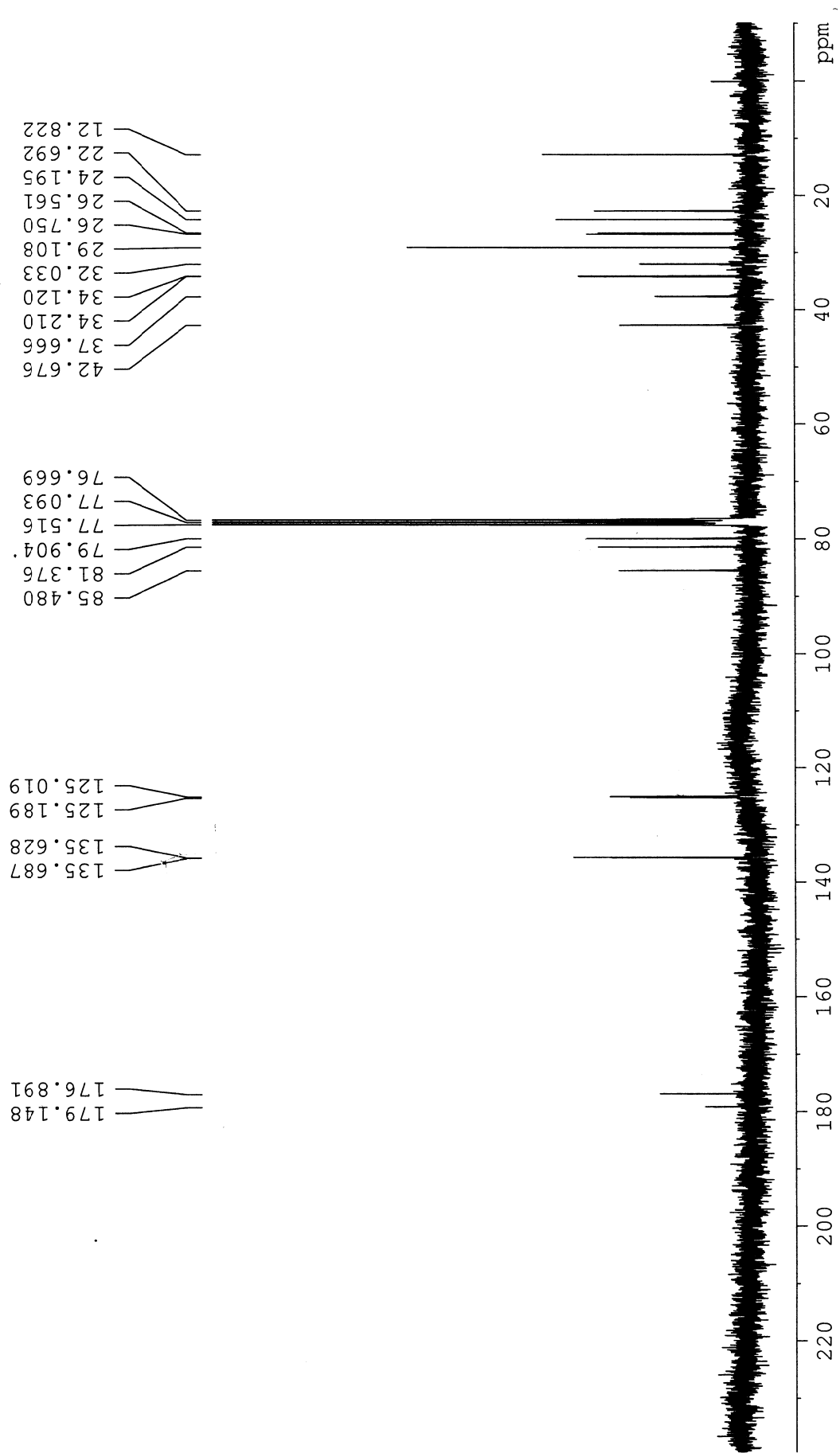
S2-4. ¹H NMR spectrum (300 MHz) of methyl ester **5a** in CDCl₃.



S2-5. ¹³C NMR spectrum (300 MHz) of methyl ester **5a** in CDCl₃.

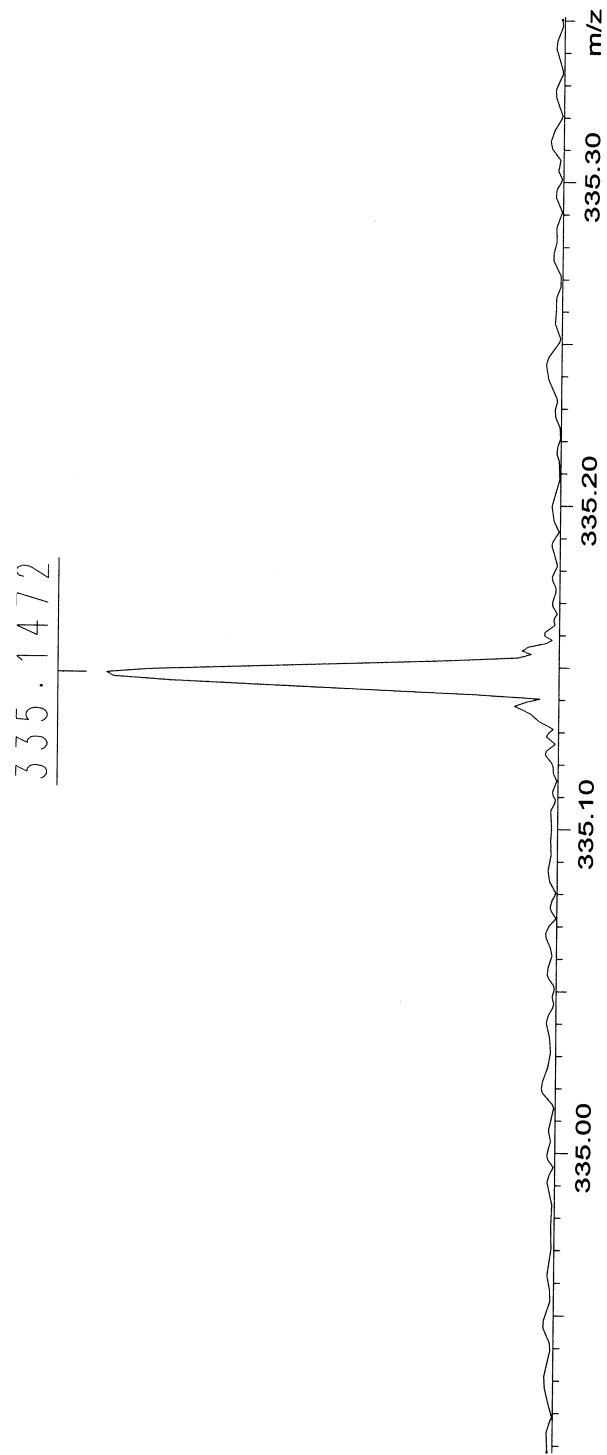
S3-1. ^1H NMR spectrum (300 MHz) of compound **6/7** in CDCl_3 .



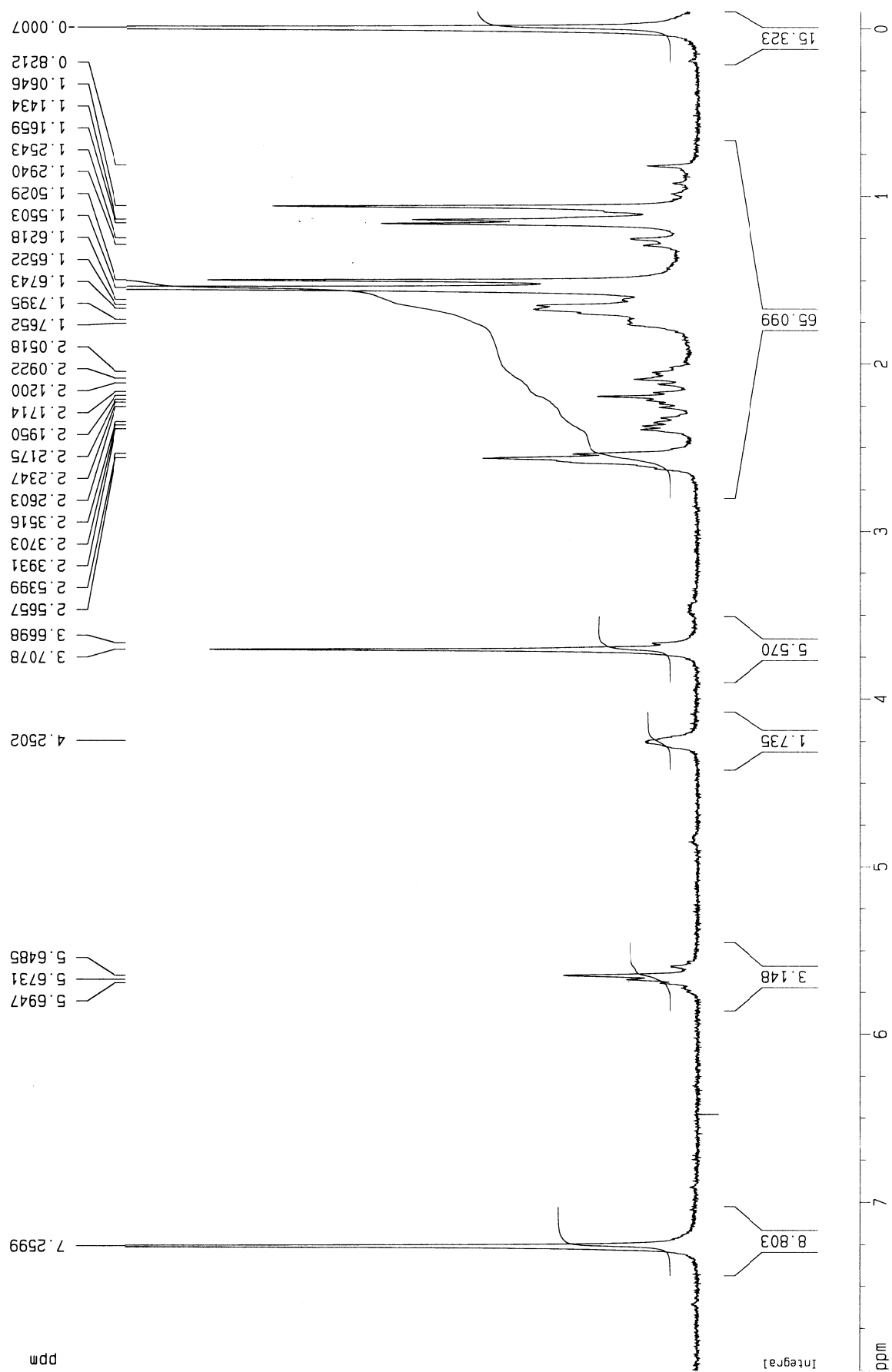


S3-2. ^{13}C NMR spectrum (300 MHz) of compound **6/7** in CDCl_3 .

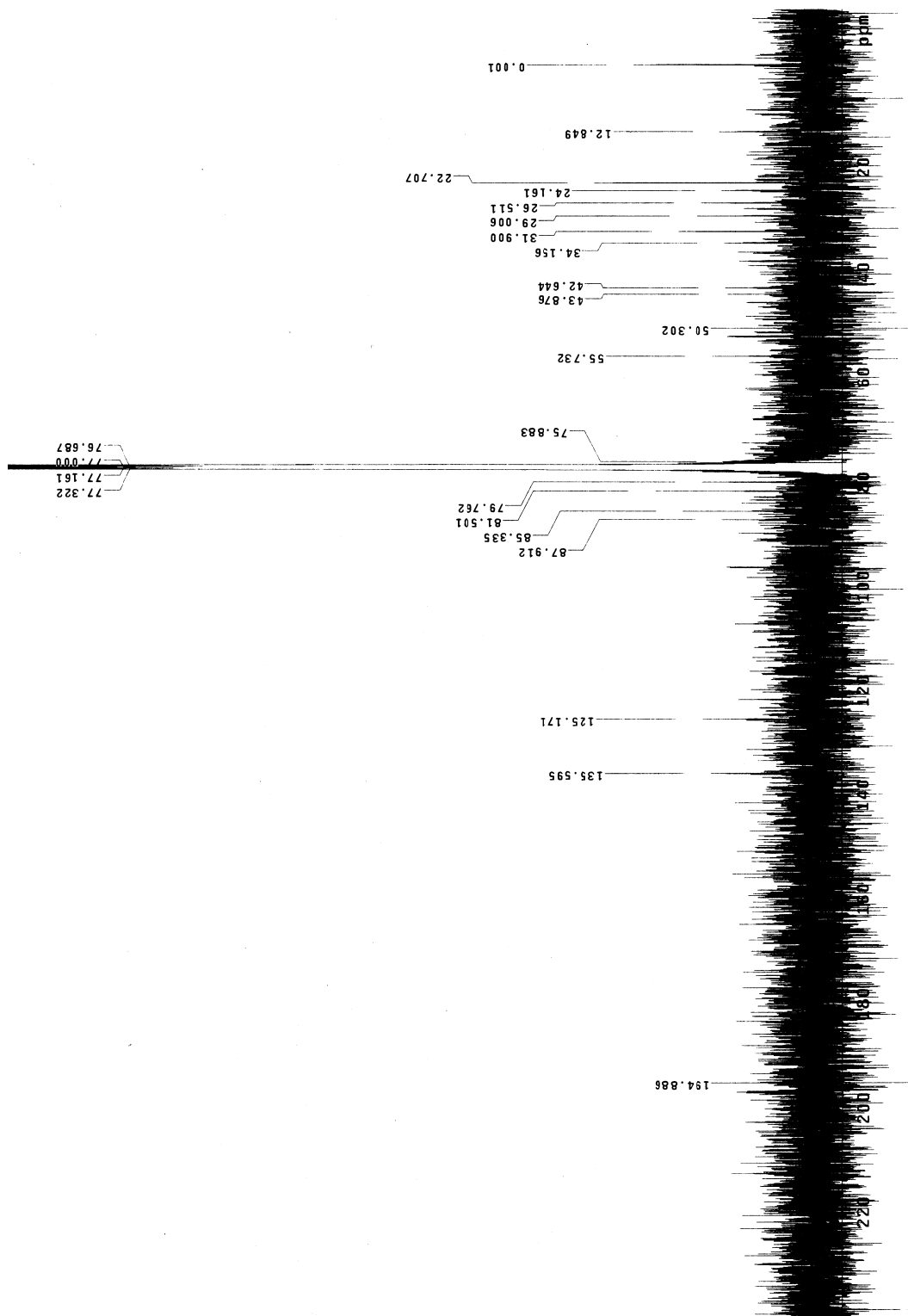
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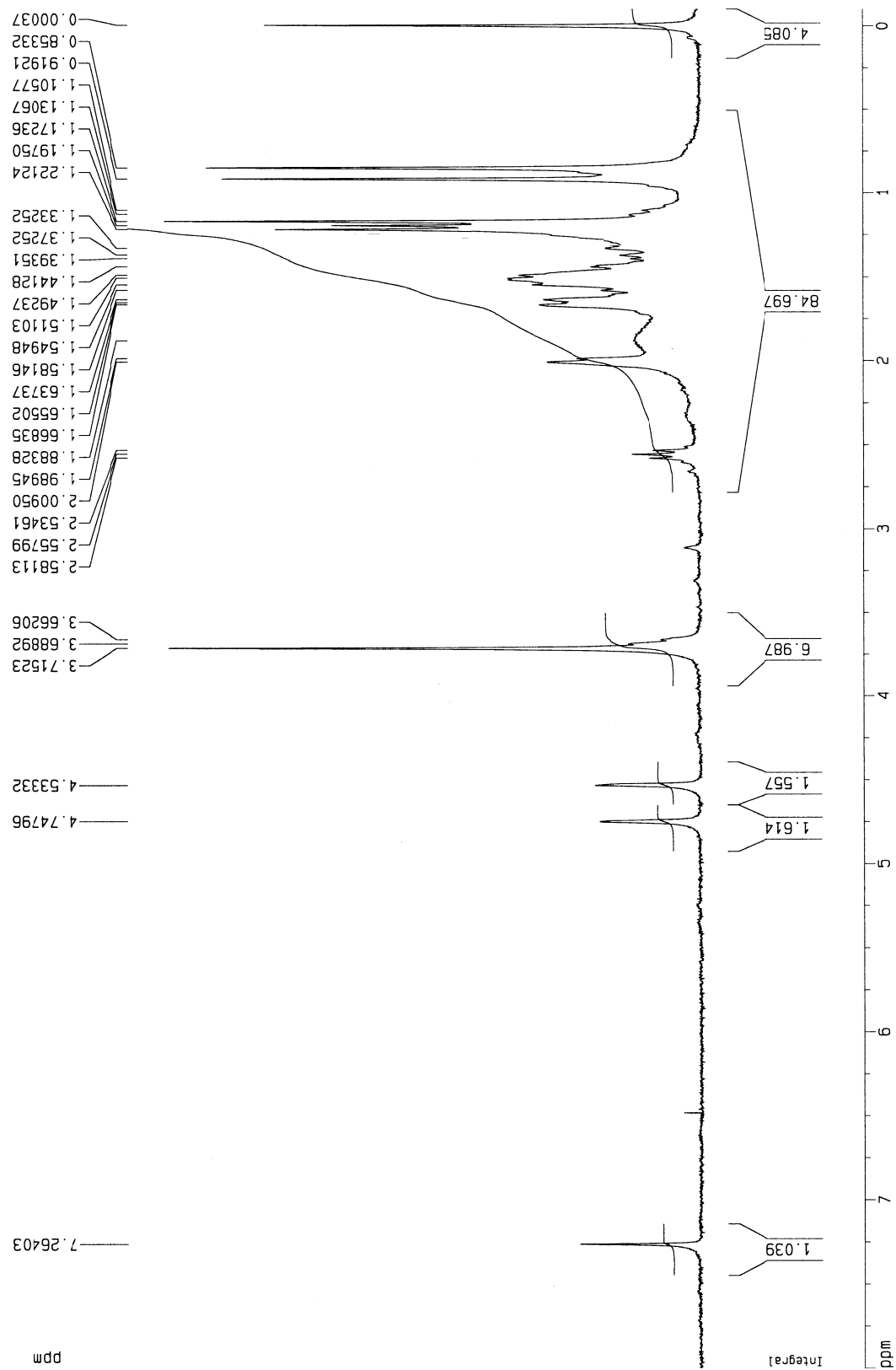
S3-3. HRESIMS spectrum of compound **6/7**.



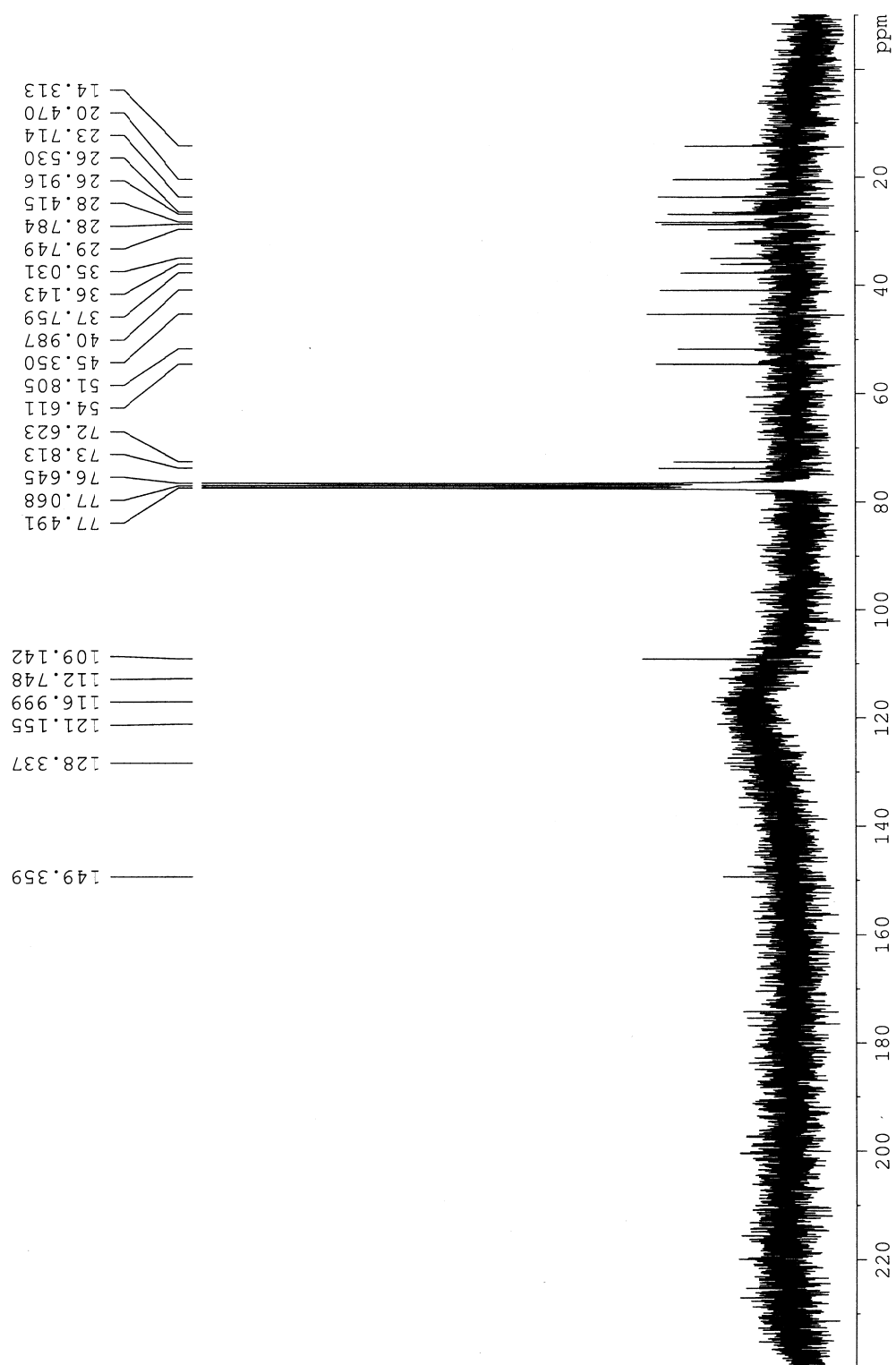
S3-4. ^1H NMR spectrum (300 MHz) of methyl ester **6a/7a** in CDCl_3 .



S3-5. ¹³C NMR spectrum (300 MHz) of methyl ester **6a/7a** in CDCl₃.

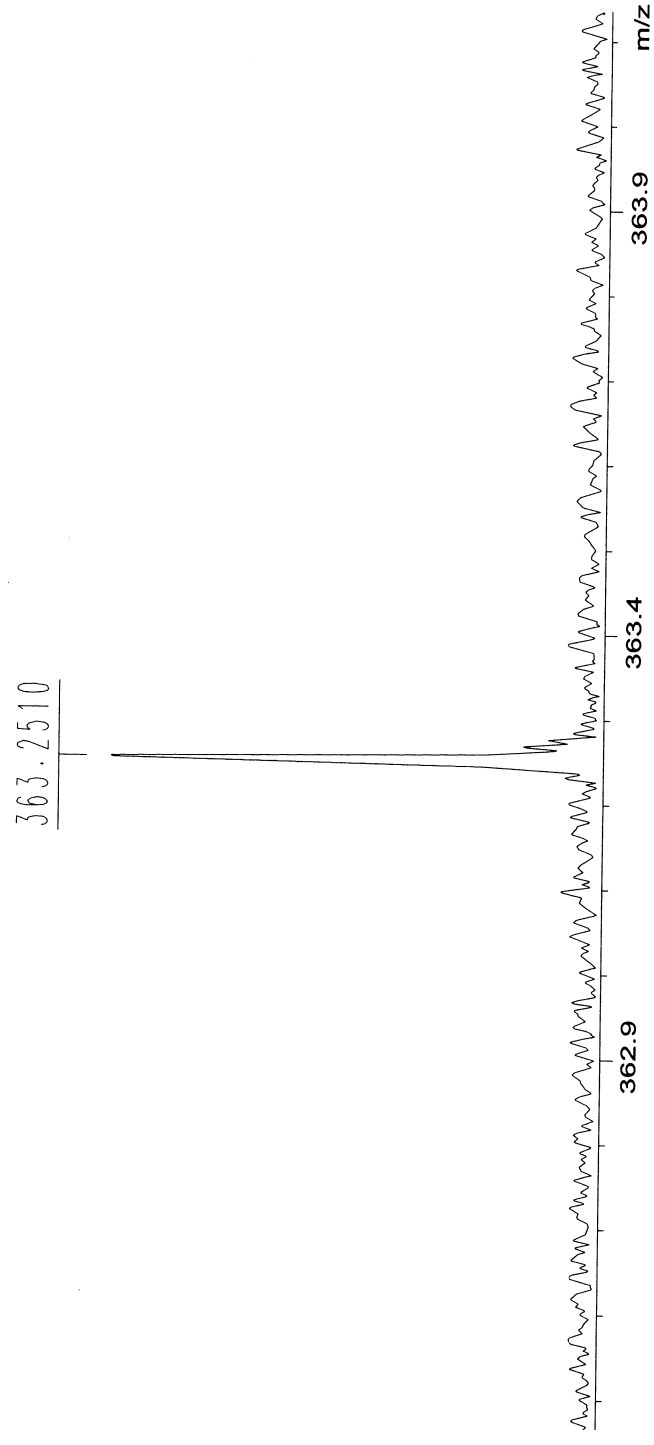


S4-1. ^1H NMR spectrum (300 MHz) of compound **8** in CDCl_3 .

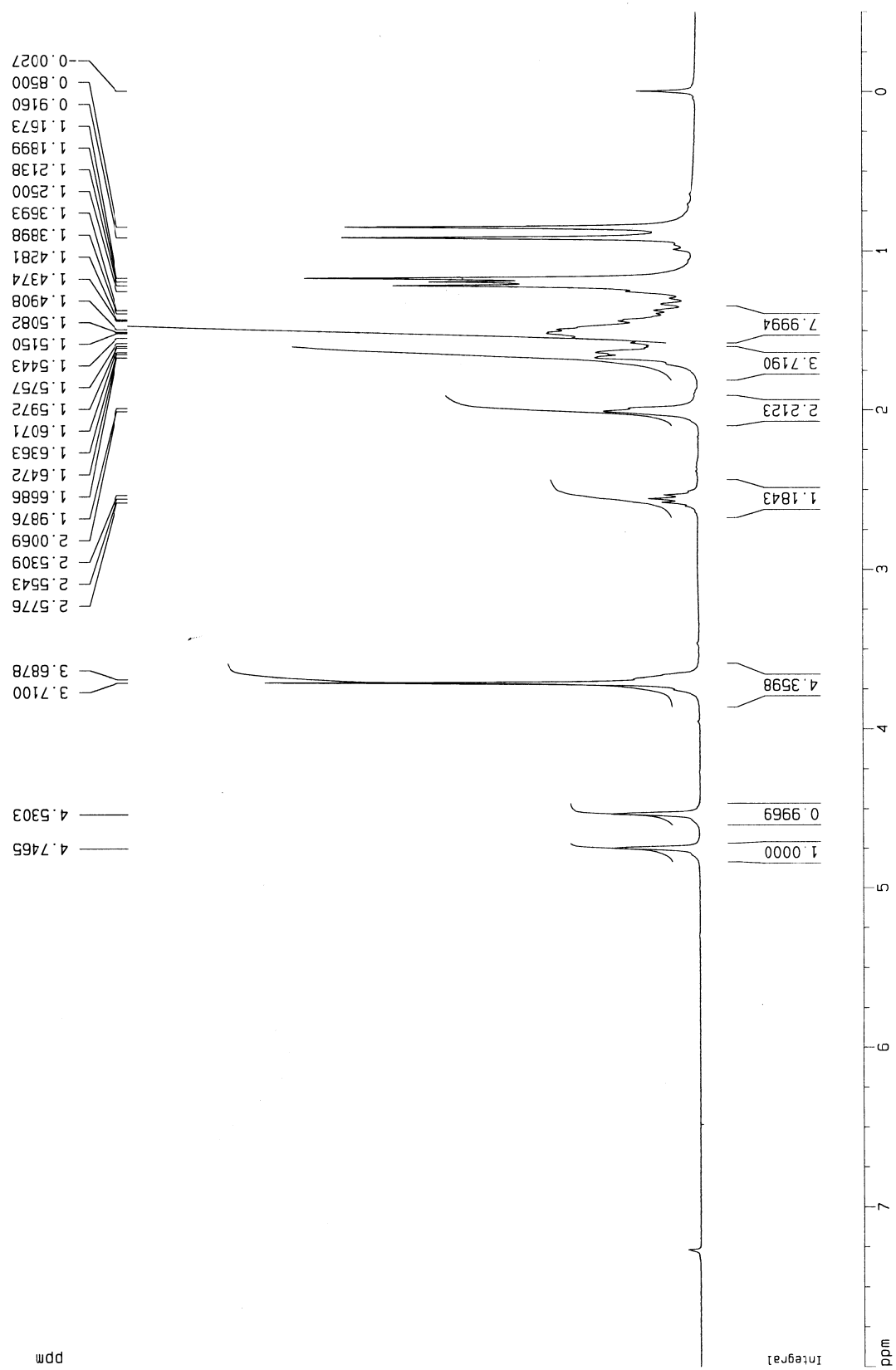


S4-2. ¹³C NMR spectrum (300 MHz) of compound **8** in CDCl₃.

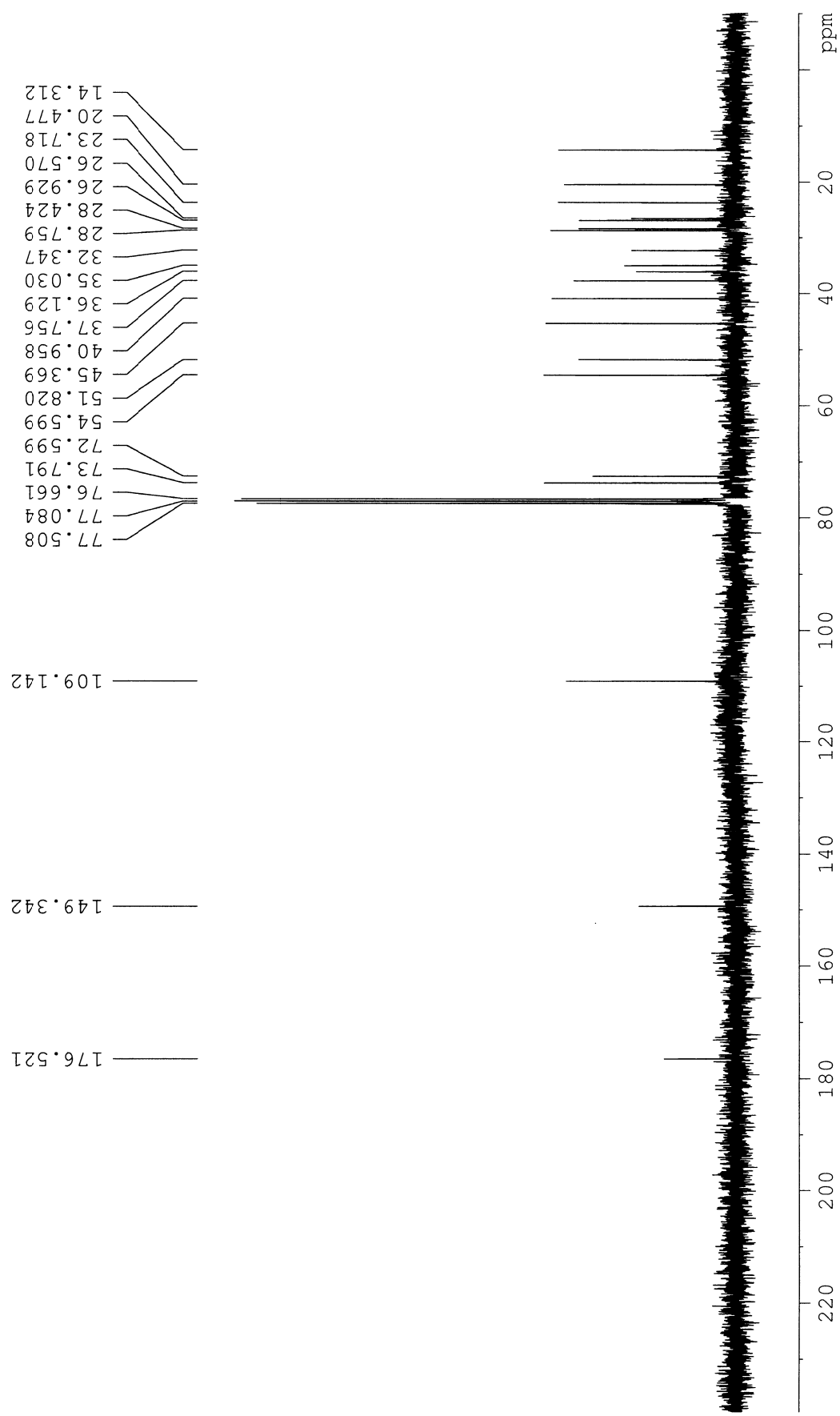
ESI+



S4-3. HRMS spectrum of compound **8**.

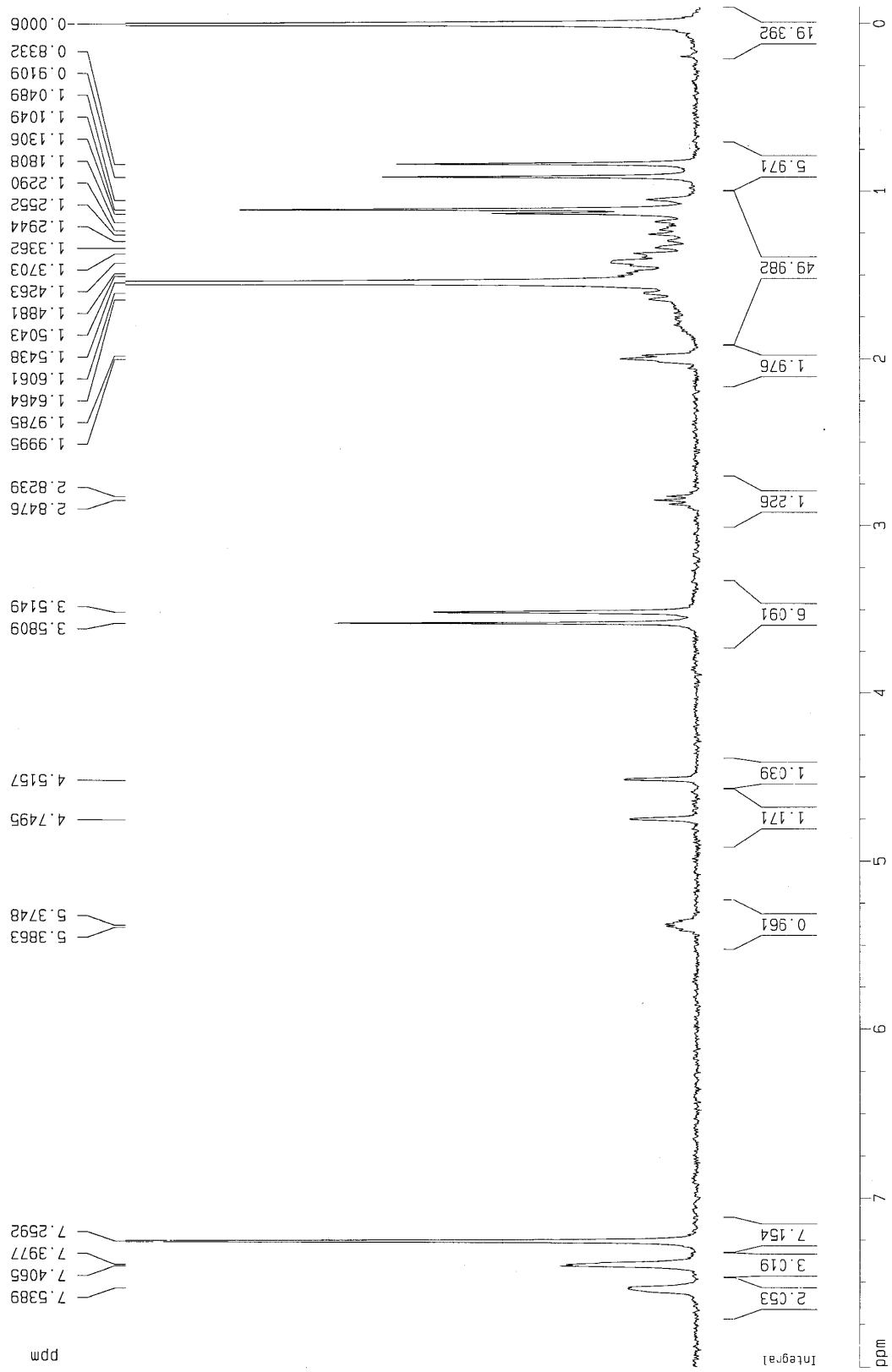


S4-4. ^1H NMR spectrum (300 MHz) of diol derived from **2** in CDCl_3 .

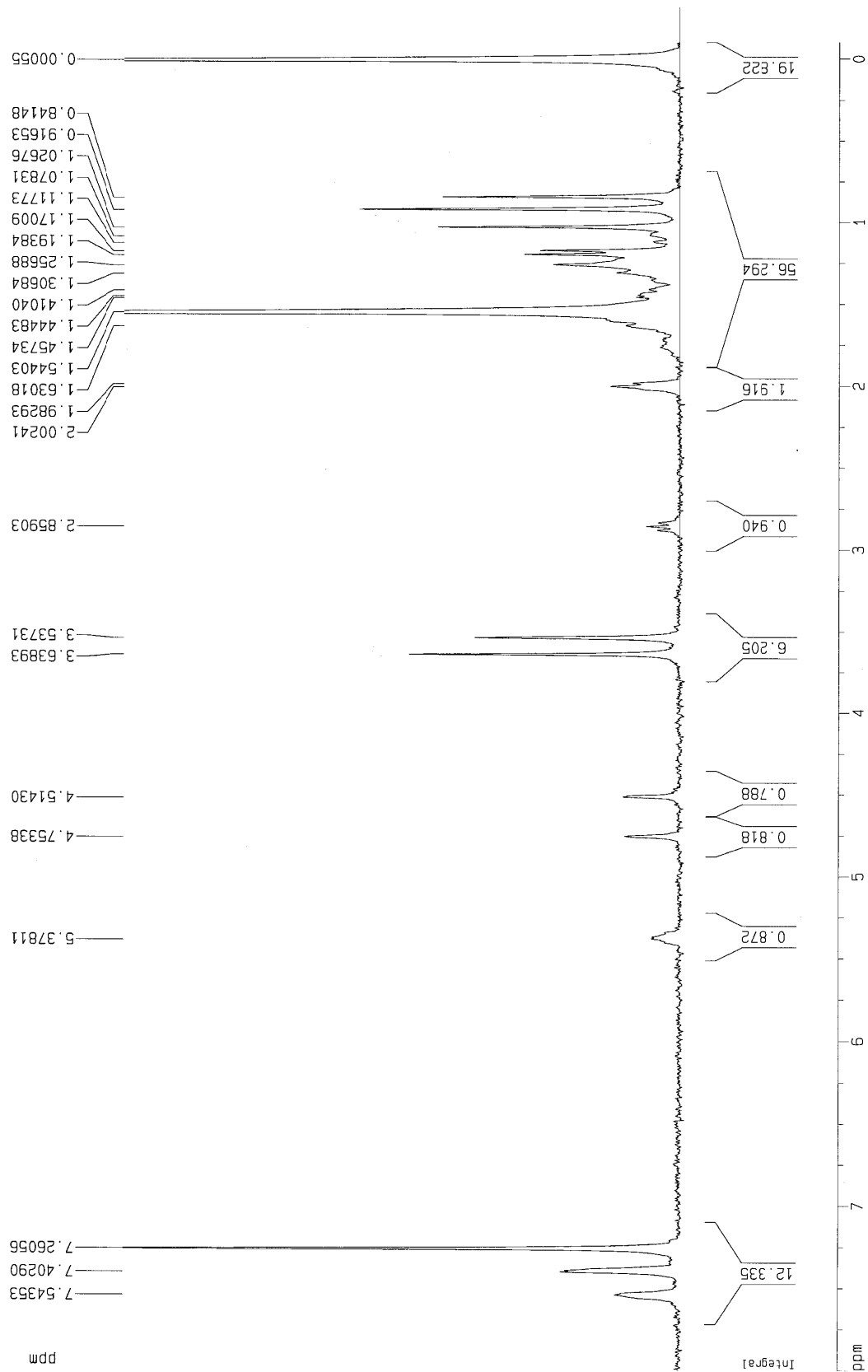


S4-5. ¹³C NMR spectrum (300 MHz) of diol derived from **2** in CDCl₃.

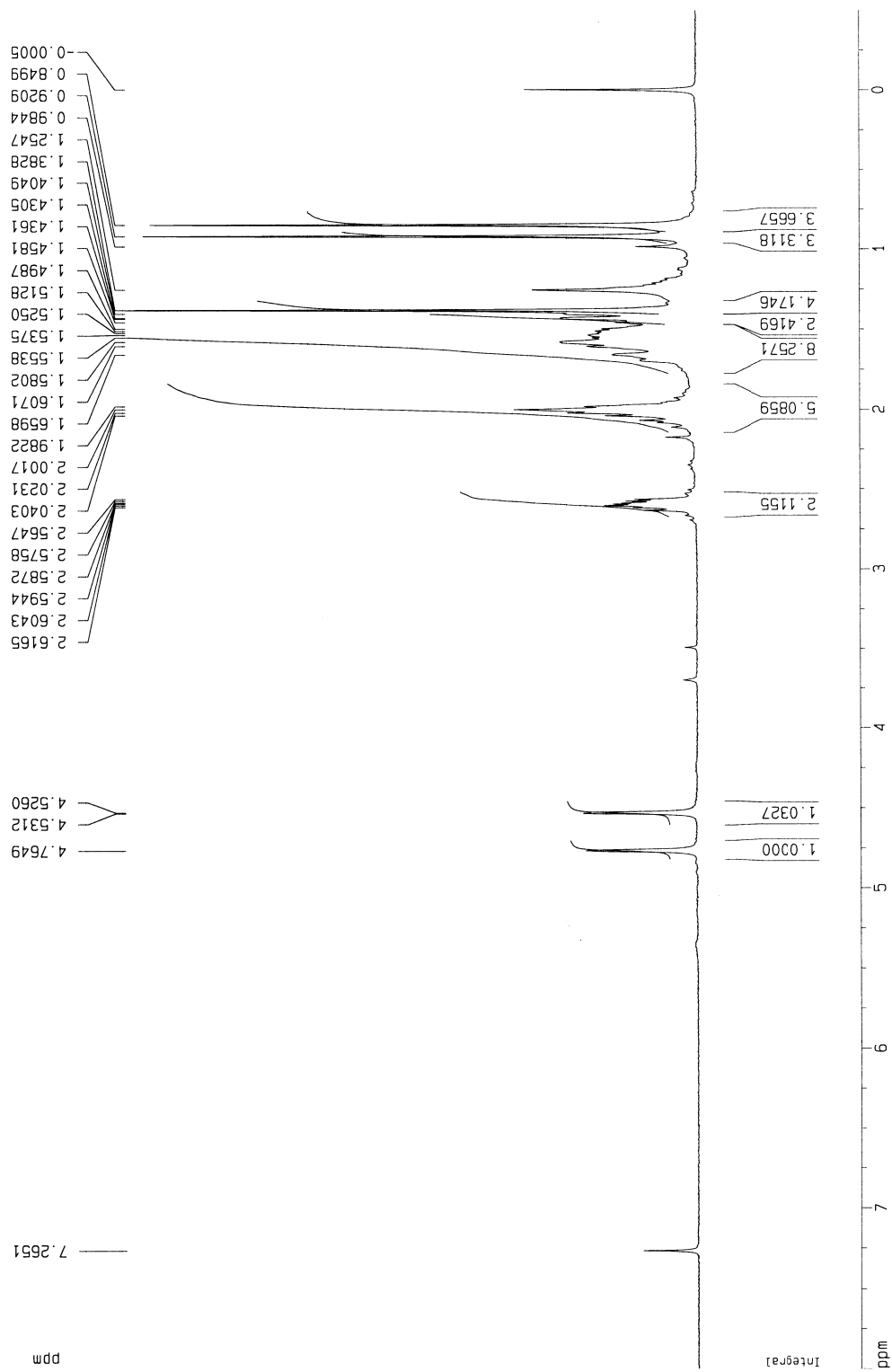
S4-6. ^1H NMR spectrum (300 MHz) of (*S*)-MTPA ester **8a** in CDCl_3 .



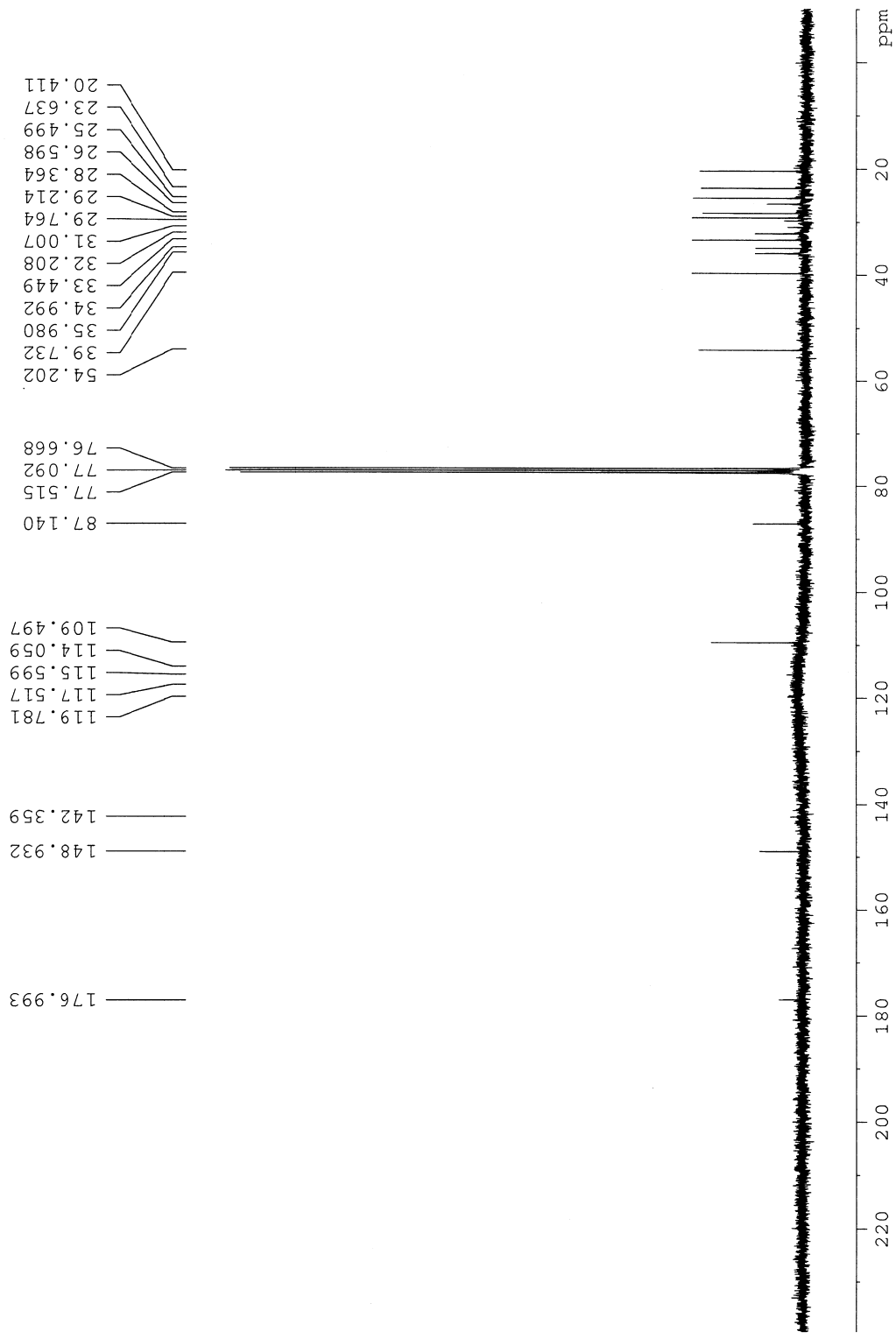
S4-7. ^1H NMR spectrum (300 MHz) of (*R*)-MTPA ester **8b** in CDCl_3 .



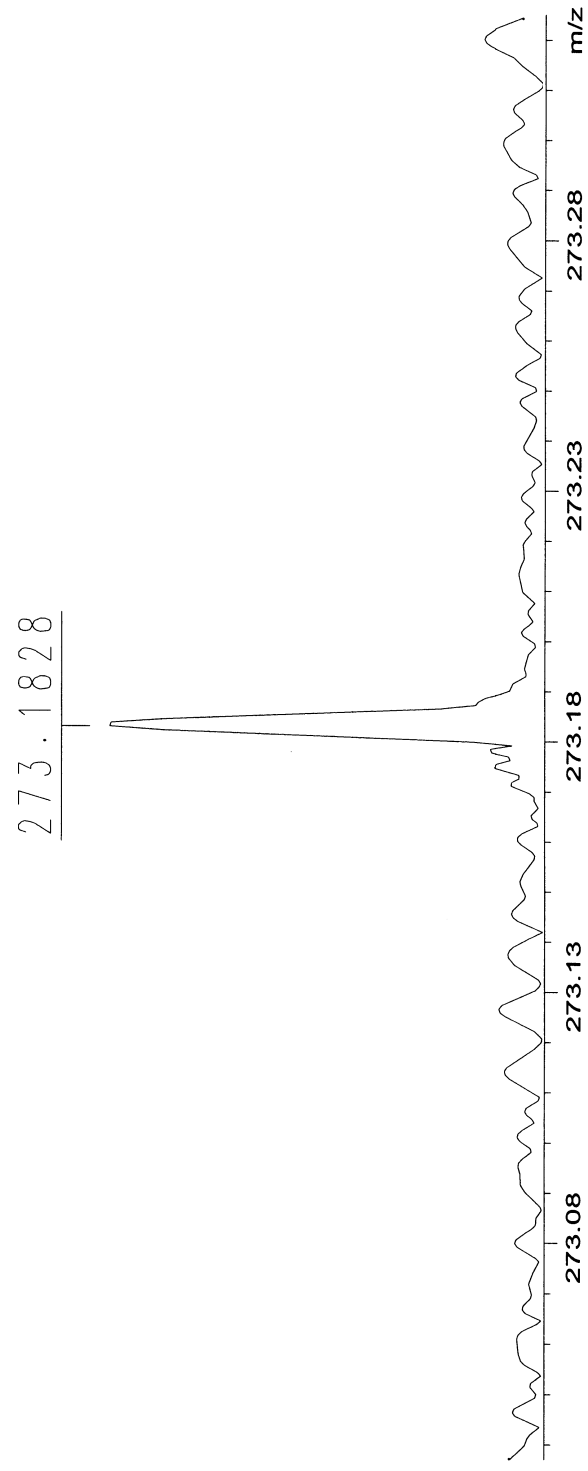
S5-1. ^1H NMR spectrum (300 MHz) of compound **9** in CDCl_3 .



S5-2. ^{13}C NMR spectrum (300 MHz) of compound **9** in CDCl_3 .

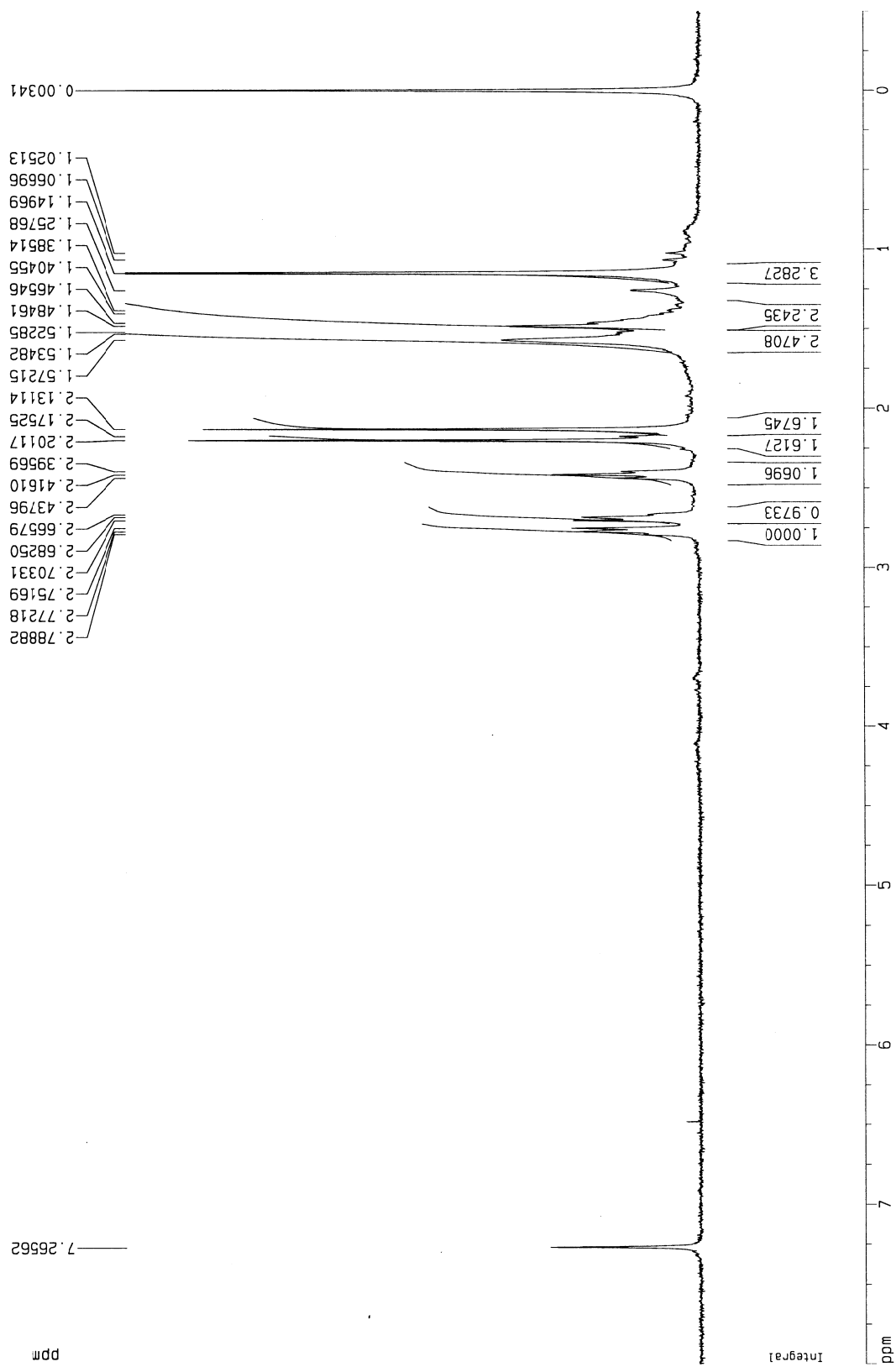


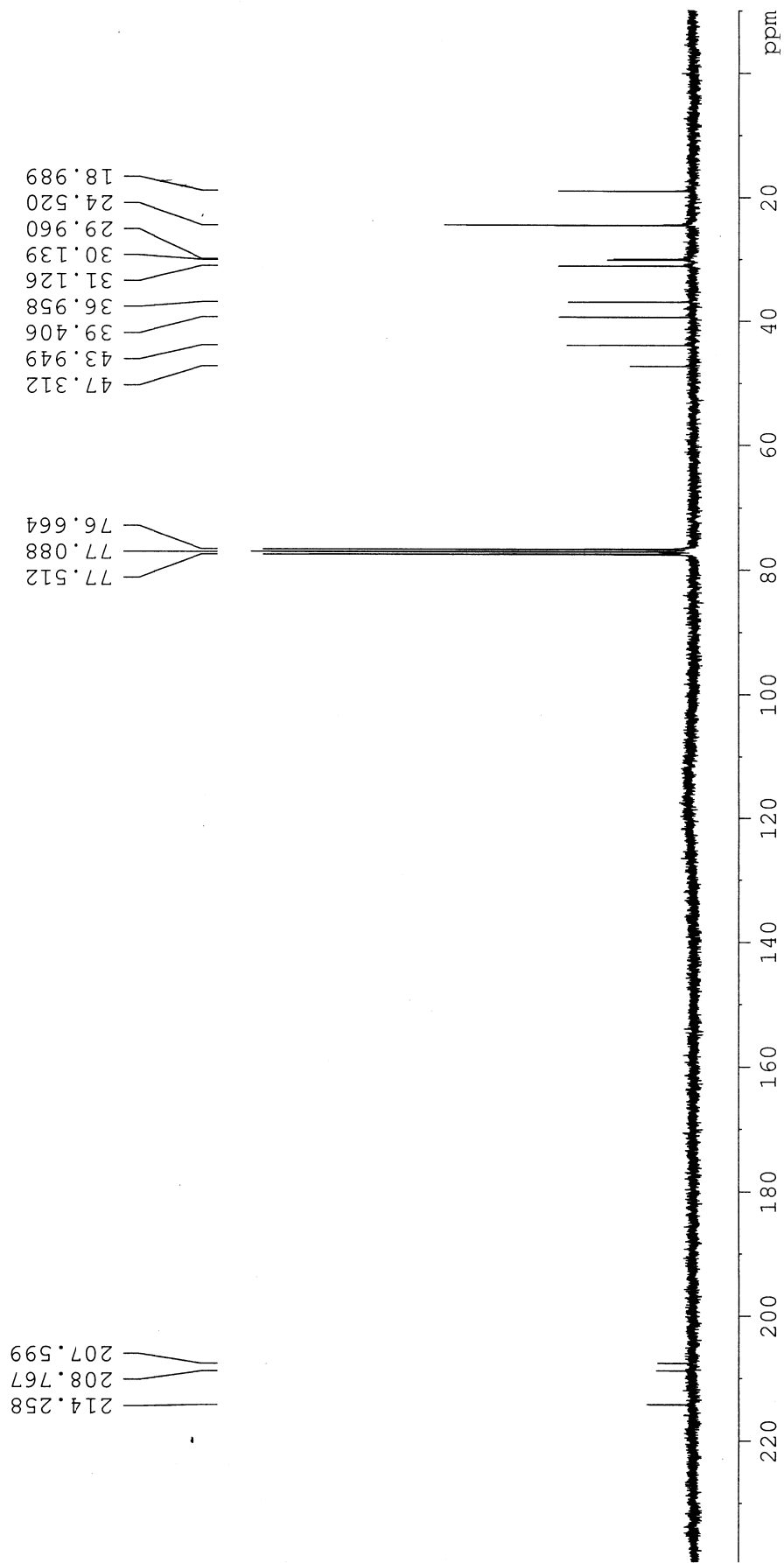
ESI+



S5-3. HRMS spectrum of compound **9**.

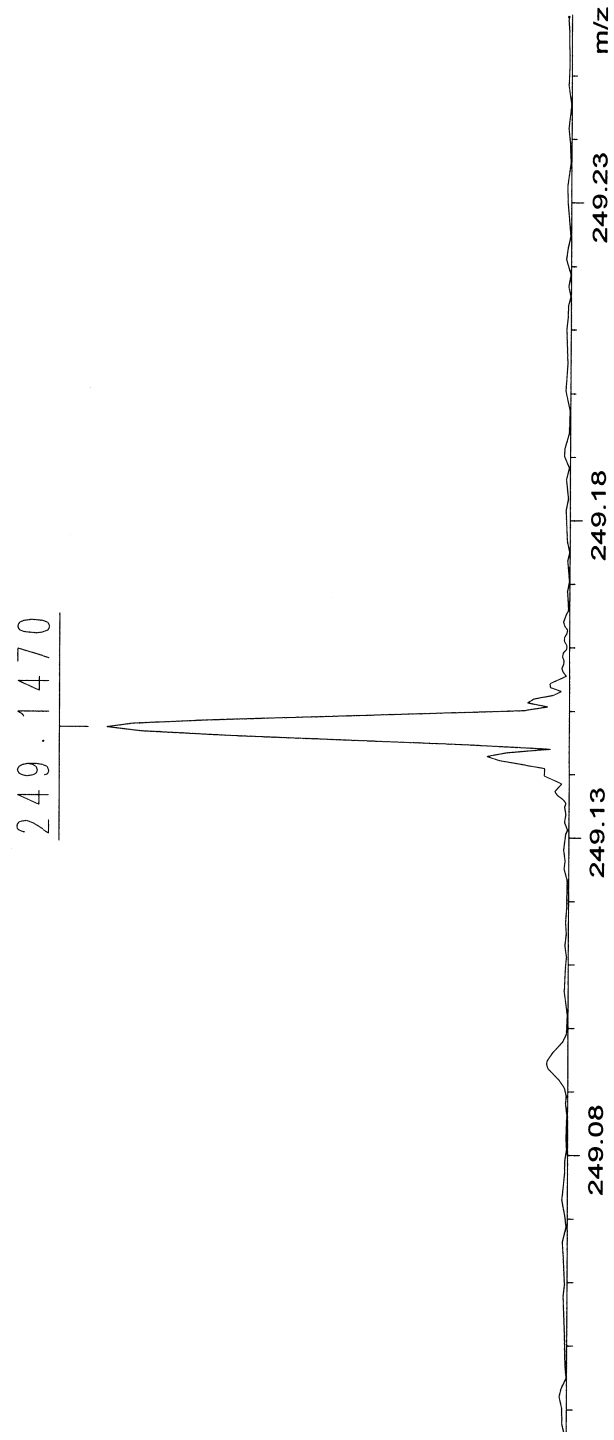
S6-1. ^1H NMR spectrum (300 MHz) of compound **10** in CDCl_3 .





S6-2. ^{13}C NMR spectrum (300 MHz) of compound **10** in CDCl_3 .

ESI+



S6-3. HRESIMS spectrum of compound **10**.