

Bioactive Steroids with Methyl Ester Group in the Side Chain from a Reef Soft Coral *Sinularia brassica* Cultured in a Tank

**Chiung-Yao Huang ¹, Jui-Hsin Su ^{2,3}, Chih-Chuang Liaw ¹, Ping-Jyun Sung ^{1,2}, Pei-Lun Chiang ⁴, Tsong-Long Hwang ^{5,6,7},
Chang-Feng Dai ⁸ and Jyh-Horng Sheu ^{1,9,10,11,*}**

¹Department of Marine Biotechnology and Resources, National Sun Yat-sen University, Kaohsiung 804, Taiwan

²National Museum of Marine Biology & Aquarium, Pingtung 944, Taiwan

³Institute of Marine Biotechnology, National Dong Hwa University, Pingtung 944, Taiwan

⁴Department of Biochemistry, University of Toronto, Toronto M5G2R3, Canada

⁵Graduate Institute of Natural Products, College of Medicine, Chang Gung University, Taoyuan 333, Taiwan

⁶Research Center for Chinese Herbal Medicine, Research Center for Food and Cosmetic Safety, and Graduate Institute of Health Industry Technology, College of Human Ecology, Chang Gung University of Science and Technology, Taoyuan 333, Taiwan

⁷Department of Anesthesiology, Chang Gung Memorial Hospital, Taoyuan 333, Taiwan

⁸ Institute of Oceanography, National Taiwan University, Taipei 112, Taiwan

⁹Department of Medical Research, China Medical University Hospital, China Medical University, Taichung 404, Taiwan

¹⁰Graduate Institute of Natural Products, Kaohsiung Medical University, Kaohsiung 807, Taiwan

¹¹Frontier Center for Ocean Science and Technology, 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.

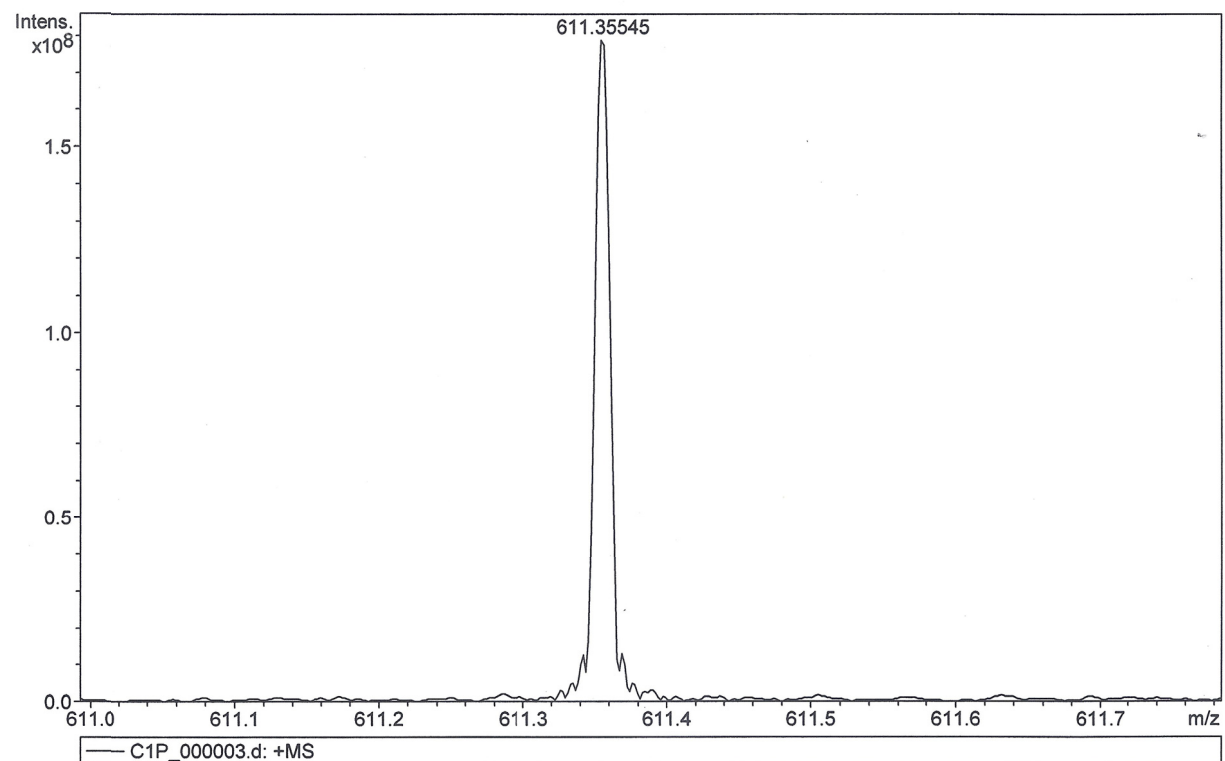
No	Content	page
Figure S1	HRESIMS spectrum of 1 .	3
Figure S2	¹ H NMR spectrum (500 MHz) of compound 1 in CDCl ₃ .	4
Figure S3	¹³ C NMR spectrum (100 MHz) of compound 1 in CDCl ₃ .	5
Figure S4	HRESIMS spectrum of 2 .	6
Figure S5	¹ H NMR spectrum (500 MHz) of compound 2 in CDCl ₃ .	7
Figure S6	¹³ C NMR spectrum (125 MHz) of compound 2 in CDCl ₃ .	8
Figure S7	HRESIMS spectrum of 3 .	9
Figure S8	¹ H NMR spectrum (400 MHz) of compound 3 in CDCl ₃ .	10
Figure S9	¹³ C NMR spectrum (100 MHz) of compound 3 in CDCl ₃ .	11
Figure S10	HRESIMS spectrum of 4 .	12
Figure S11	¹ H NMR spectrum (500 MHz) of compound 4 in CDCl ₃ .	13
Figure S12	¹³ C NMR spectrum (125 MHz) of compound 4 in CDCl ₃ .	14

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name D:\Data\1\C1P_000003.d
Method broadband first signal
Sample Name C1-P
Comment ESI Positive

4/25/2017 3:05:58 PM
Operator: YU HSIAO-CHING
Instrument: BRUKER FT-MS solariX



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
611.35545	1	C ₃₄ H ₅₂ NaO ₈	100.00	611.35544	-0.02	-0.02	15.5	8.5	even	ok

Figure S1. HRESIMS spectrum of **1**.

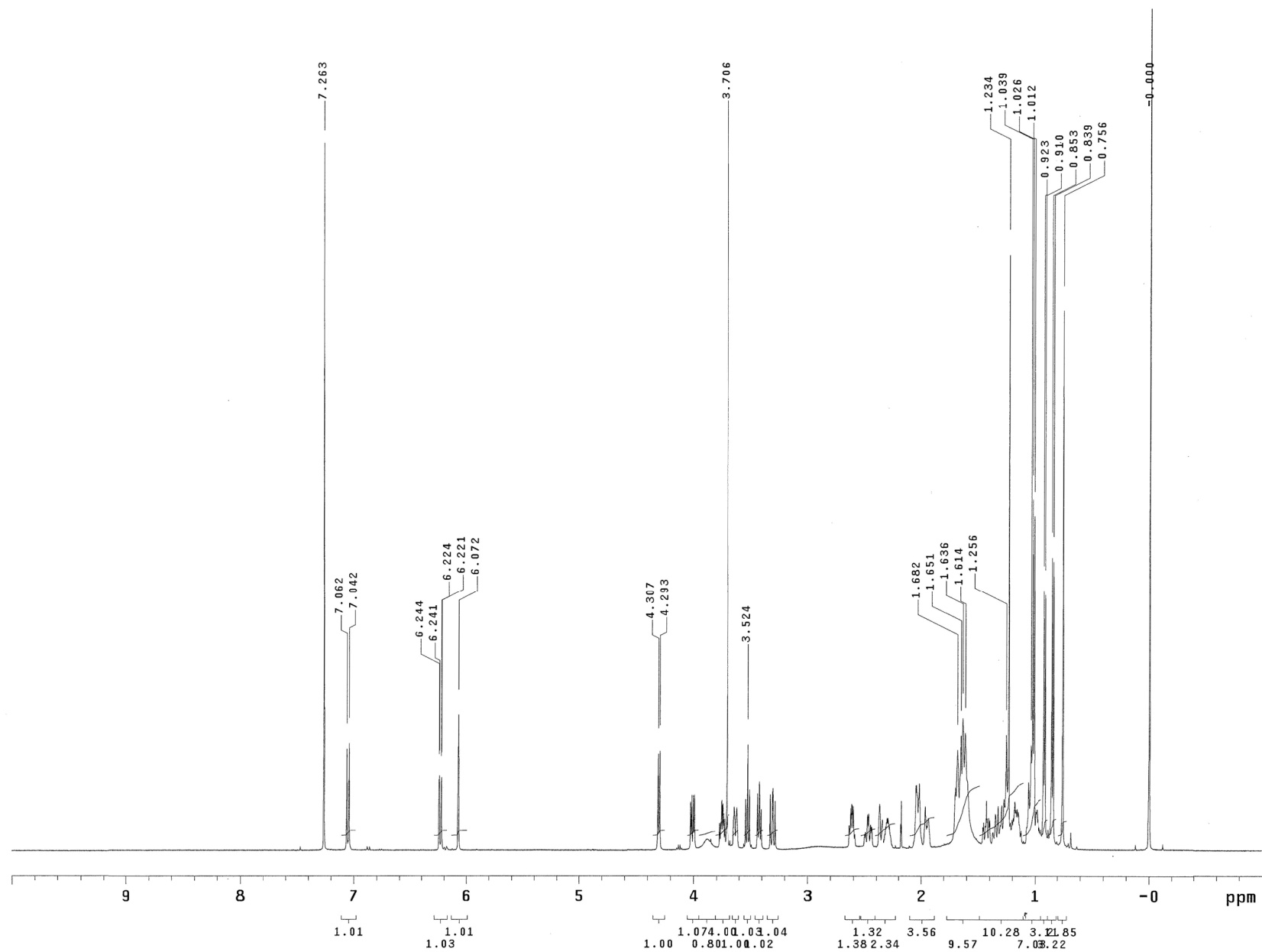


Figure S2. ^1H NMR spectrum (500 MHz) of compound **1** in CDCl_3 .

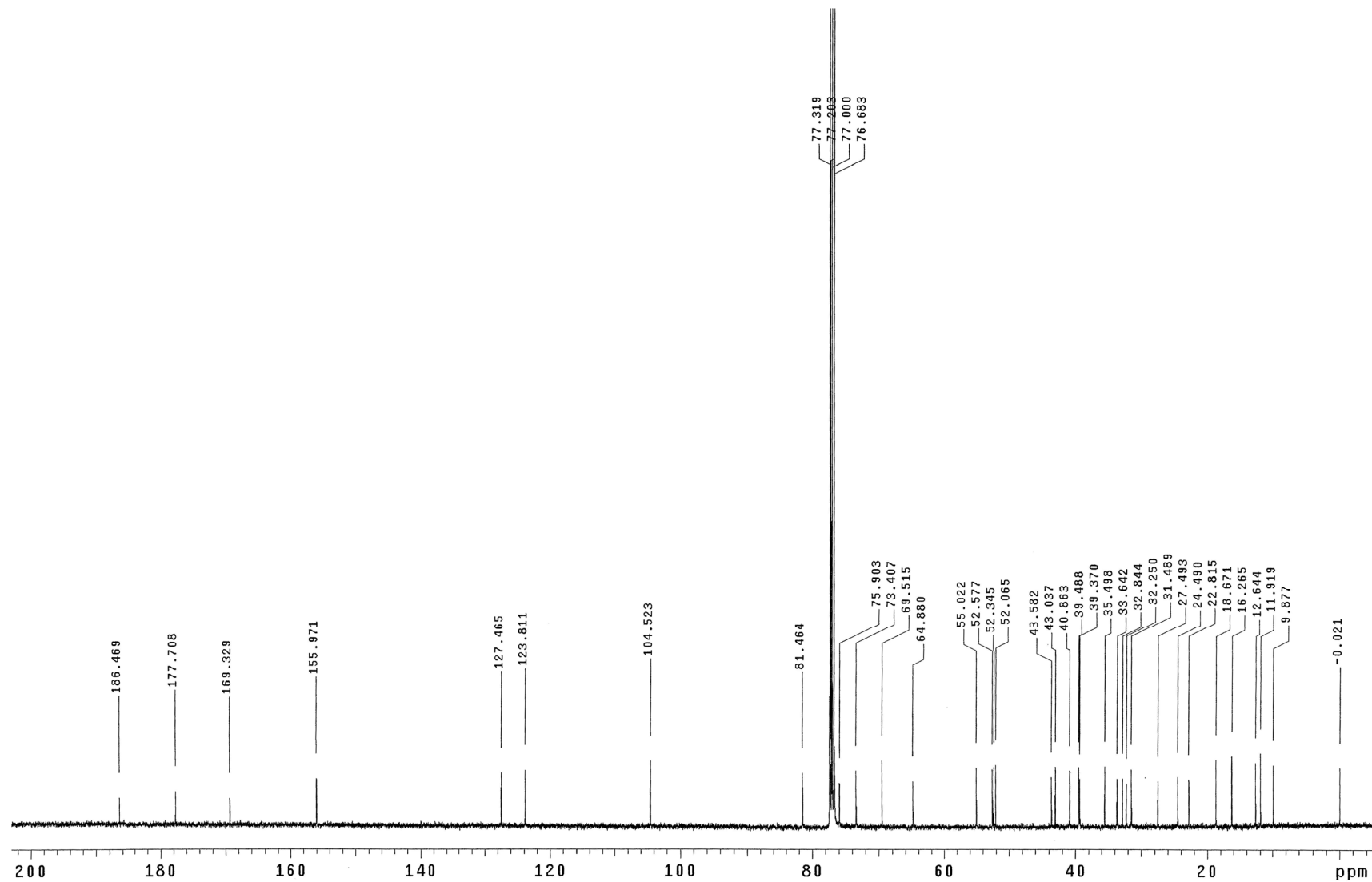


Figure S3. ¹³C NMR spectrum (100 MHz) of compound **1** in CDCl₃.

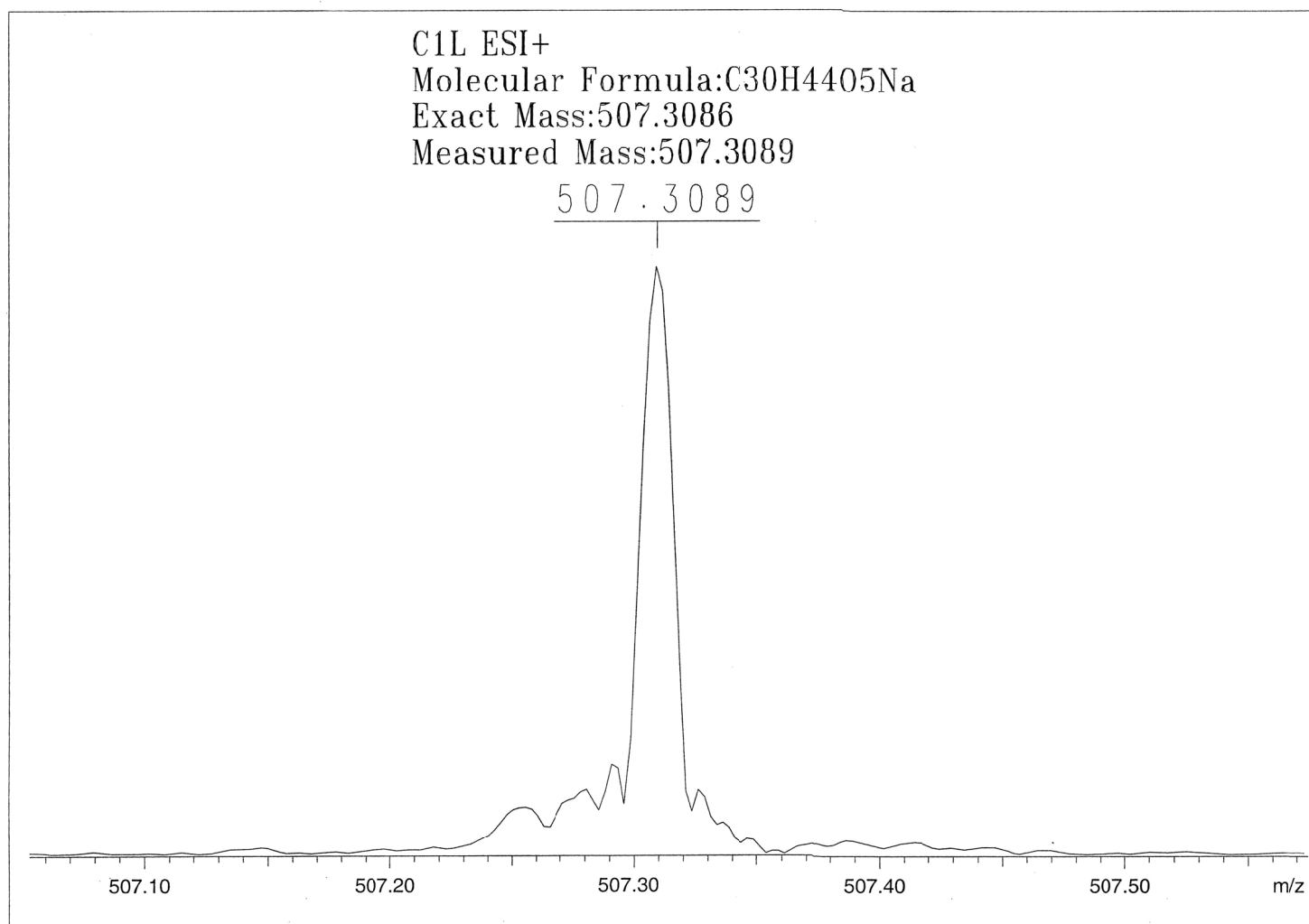


Figure S4. HRESIMS spectrum of **2**.

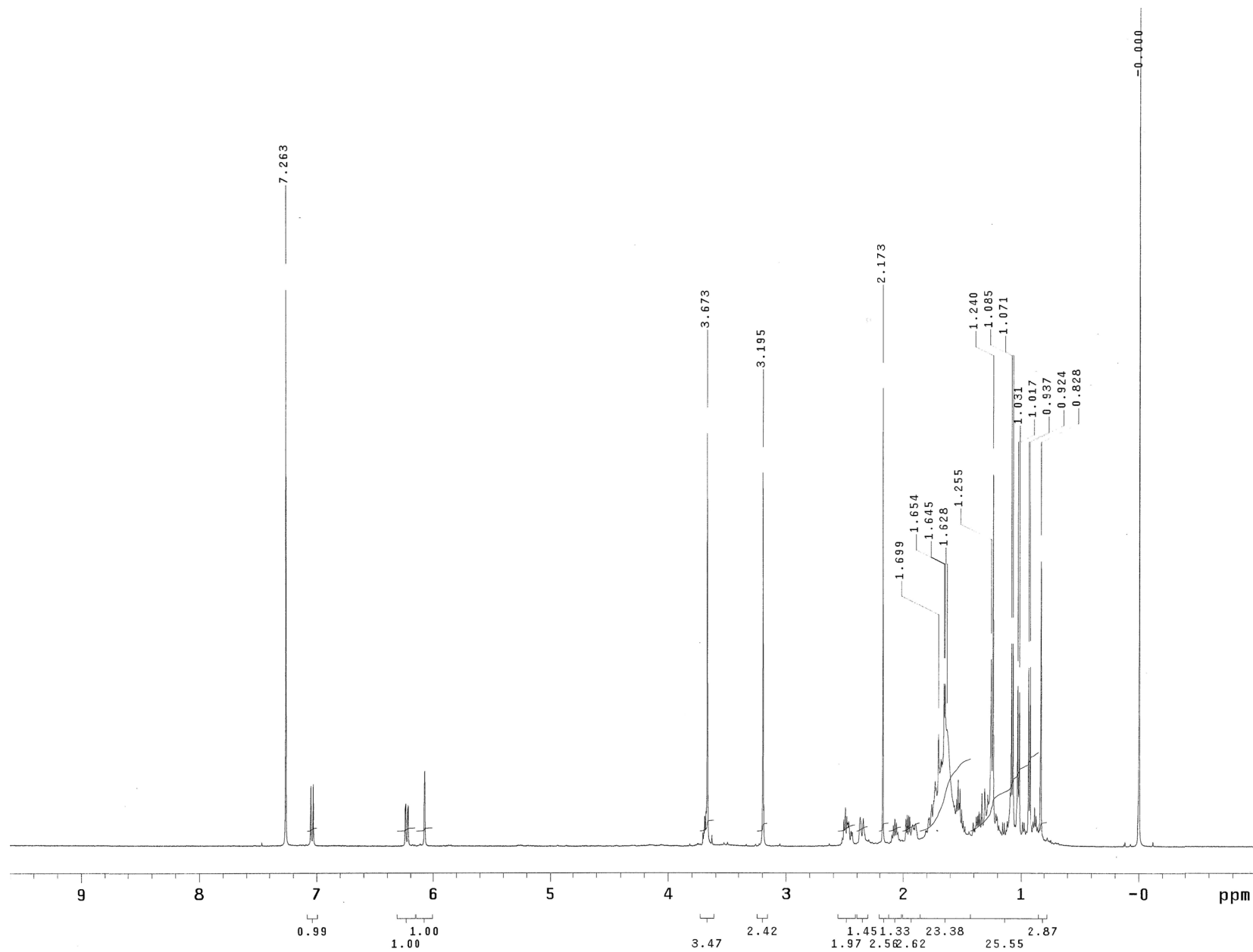


Figure S5. ¹H NMR spectrum (500 MHz) of compound **2** in CDCl₃.

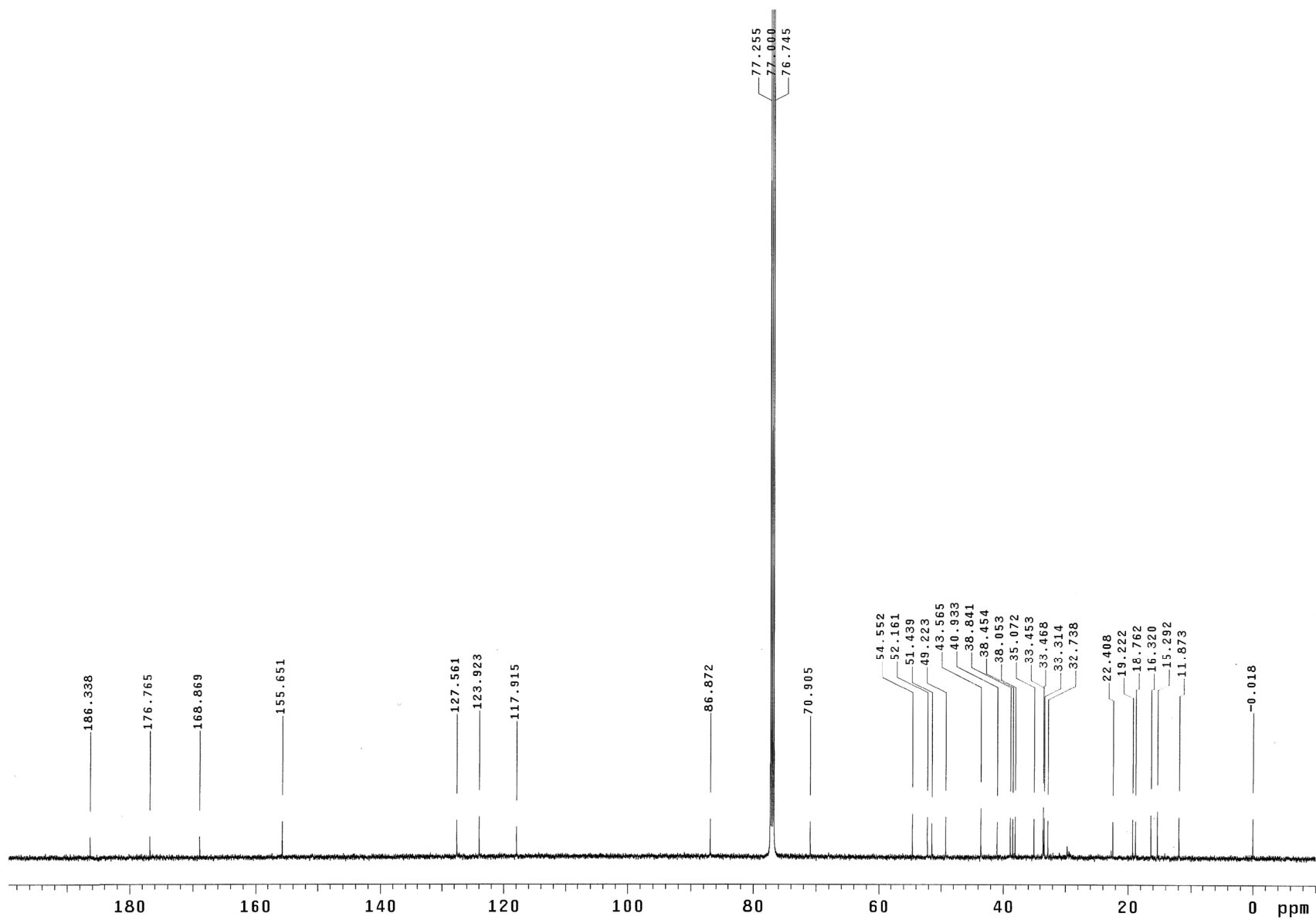


Figure S6. ¹³C NMR spectrum (125 MHz) of compound **2** in CDCl₃.

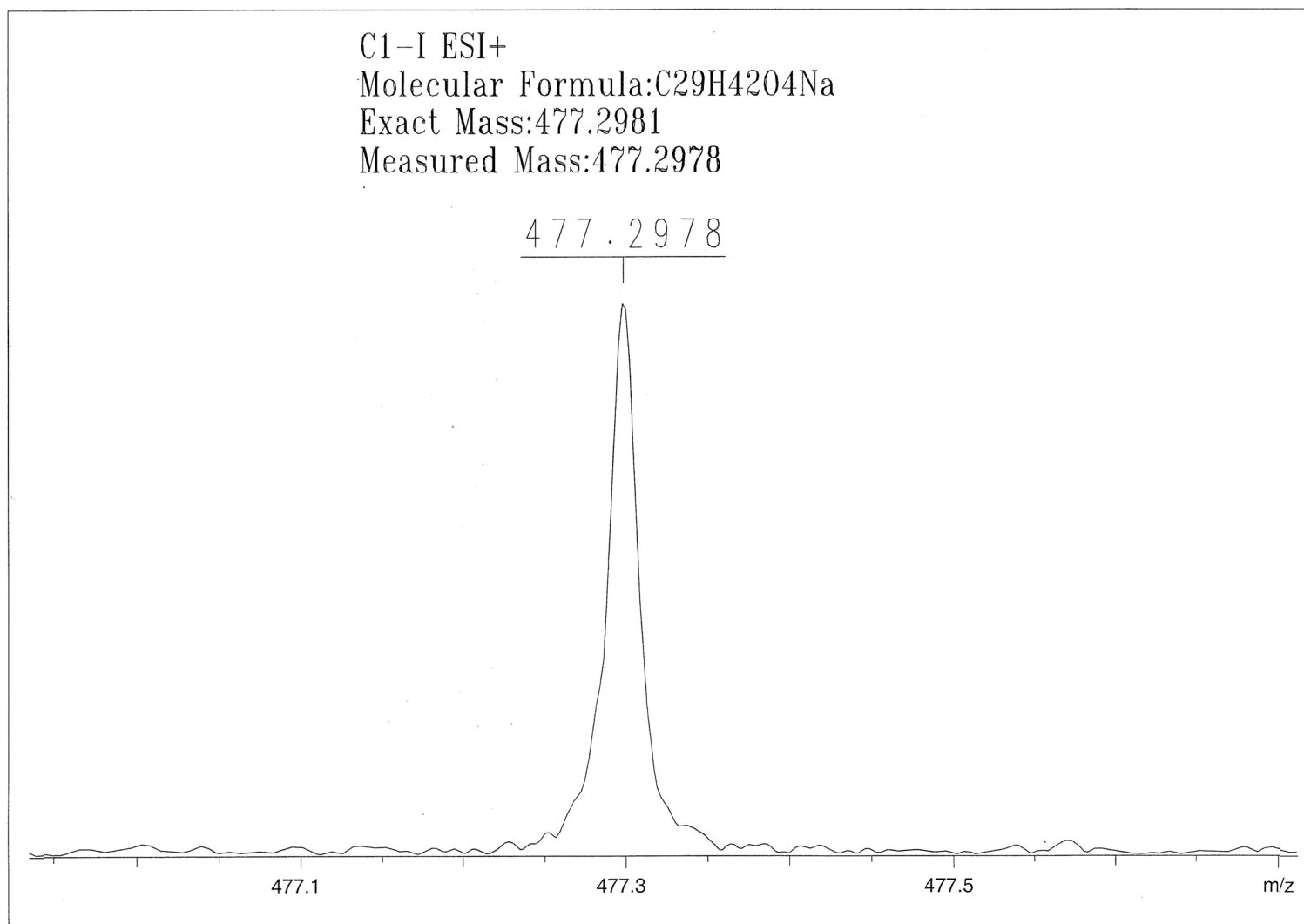


Figure S7. HRESIMS spectrum of **3**.

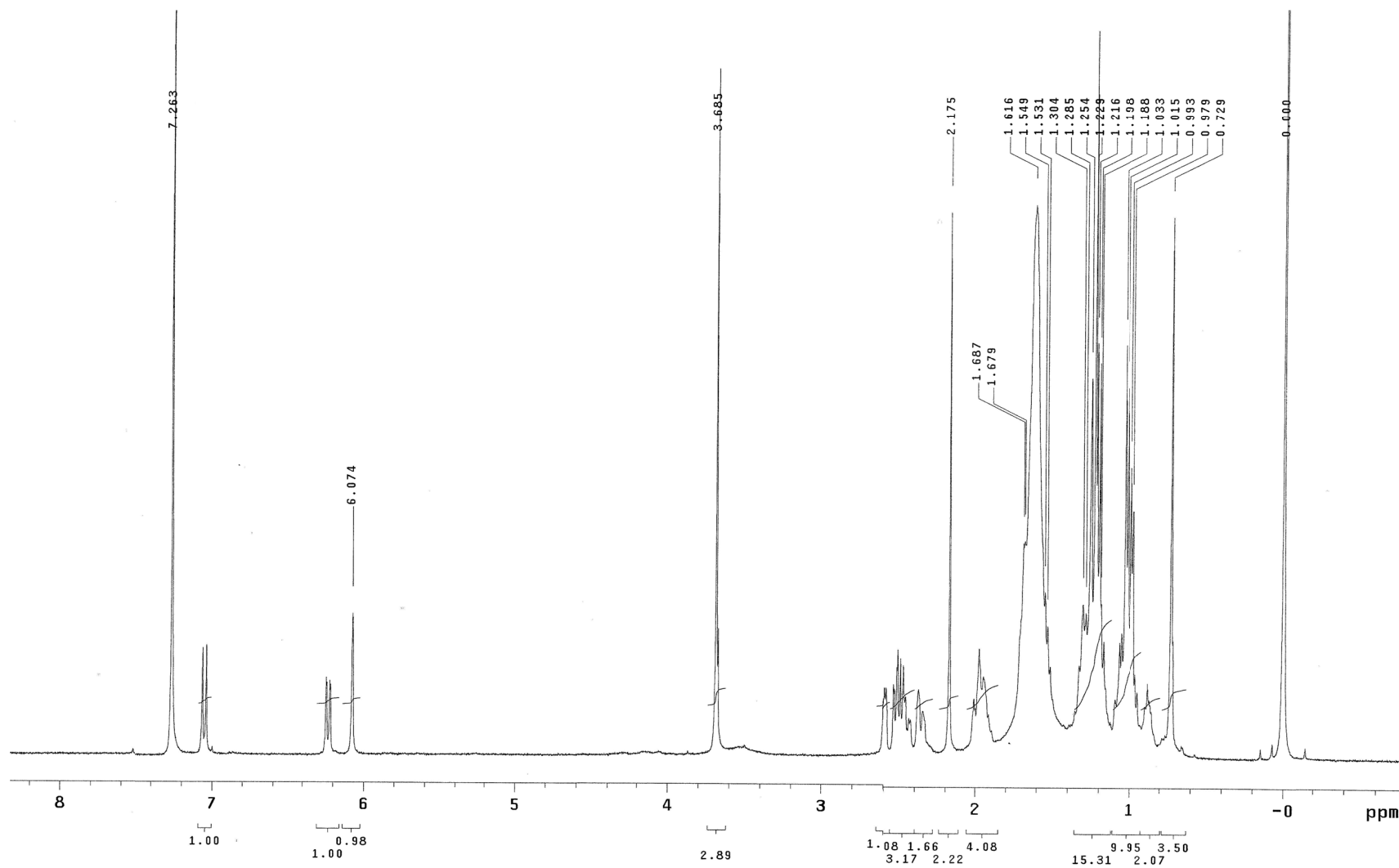


Figure S8. ¹H NMR spectrum (400 MHz) of compound **3** in CDCl₃.

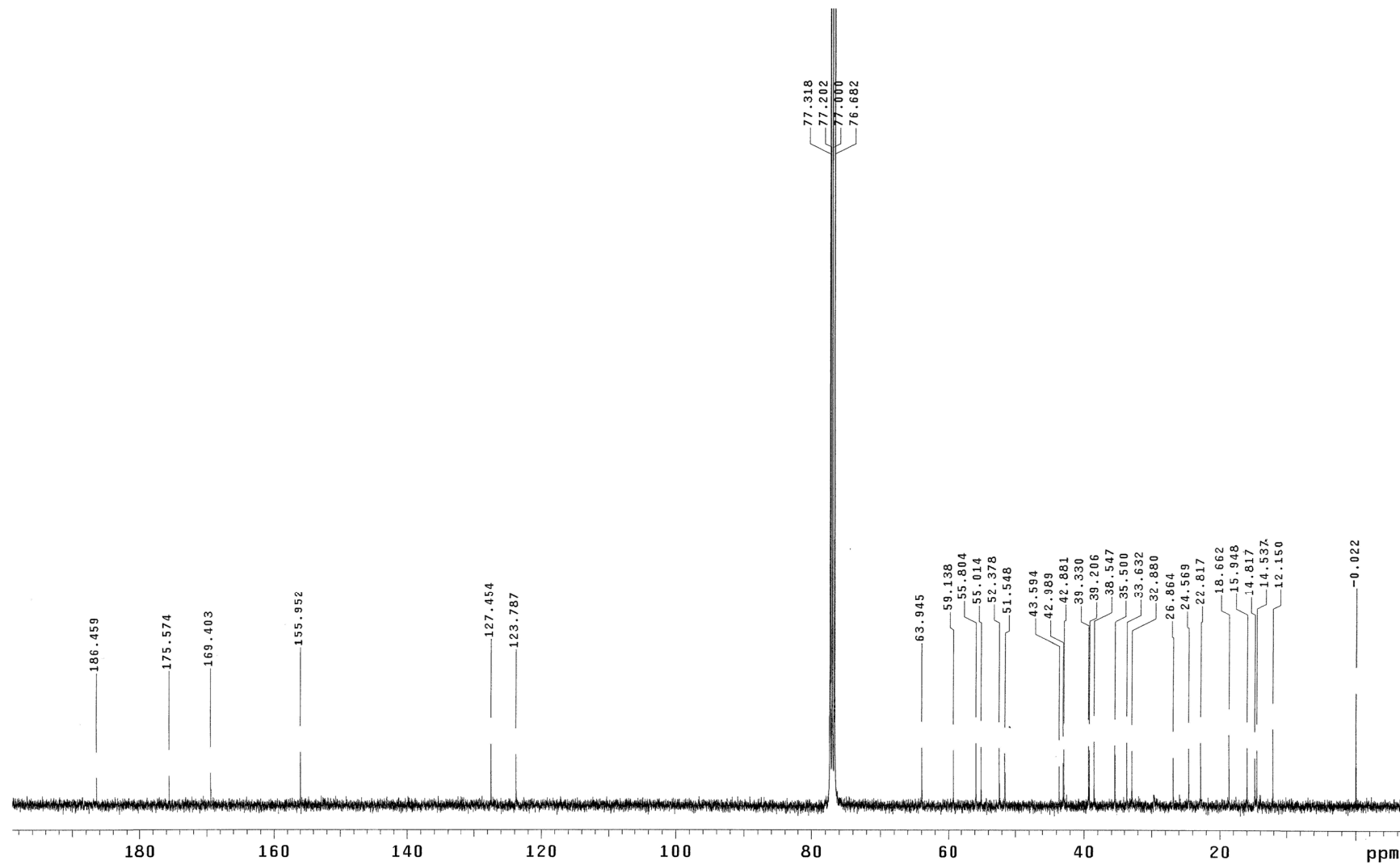


Figure S9 ¹³C NMR spectrum (100 MHz) of compound **3** in CDCl₃.

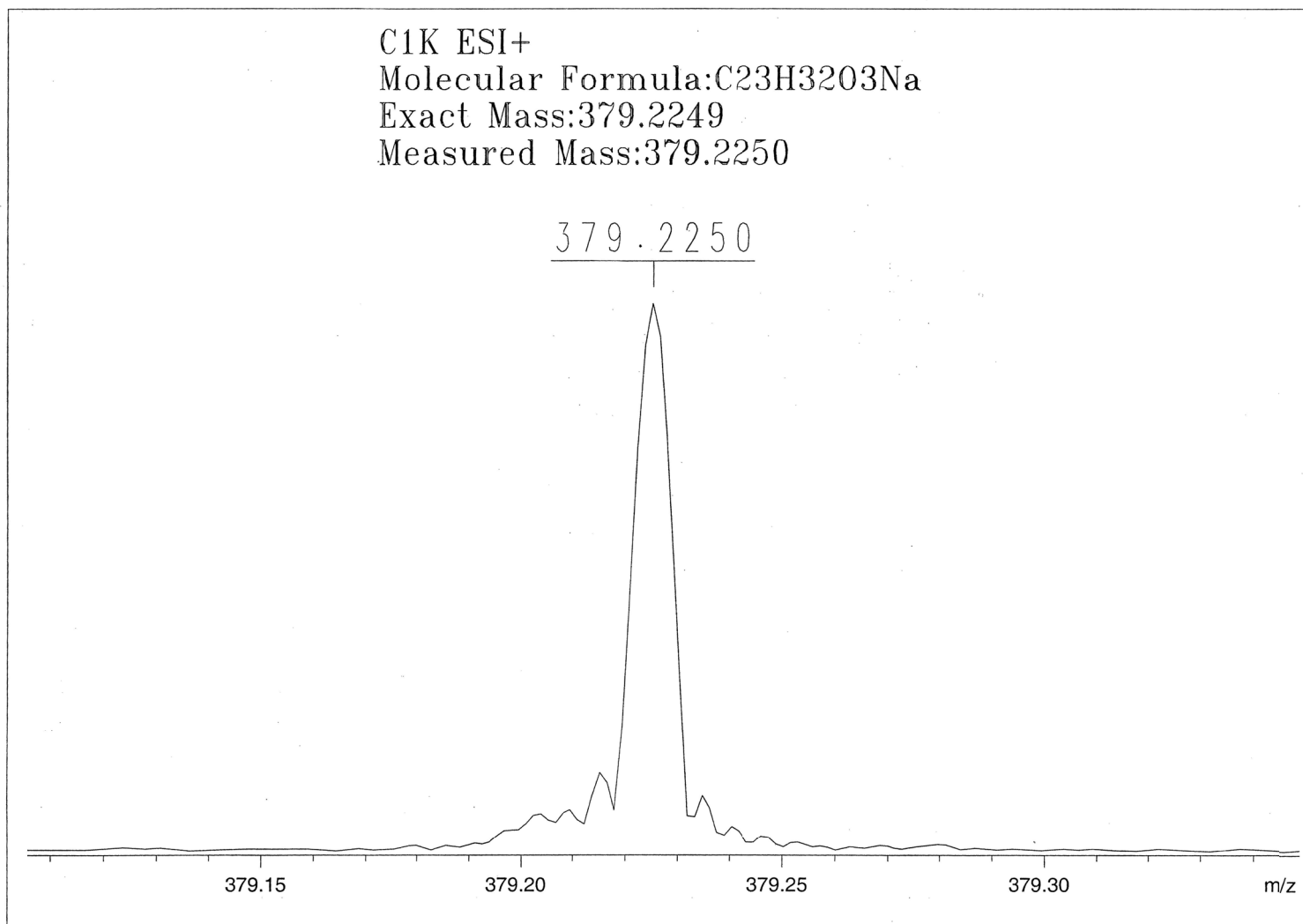


Figure S10. HRESIMS spectrum of **4**.

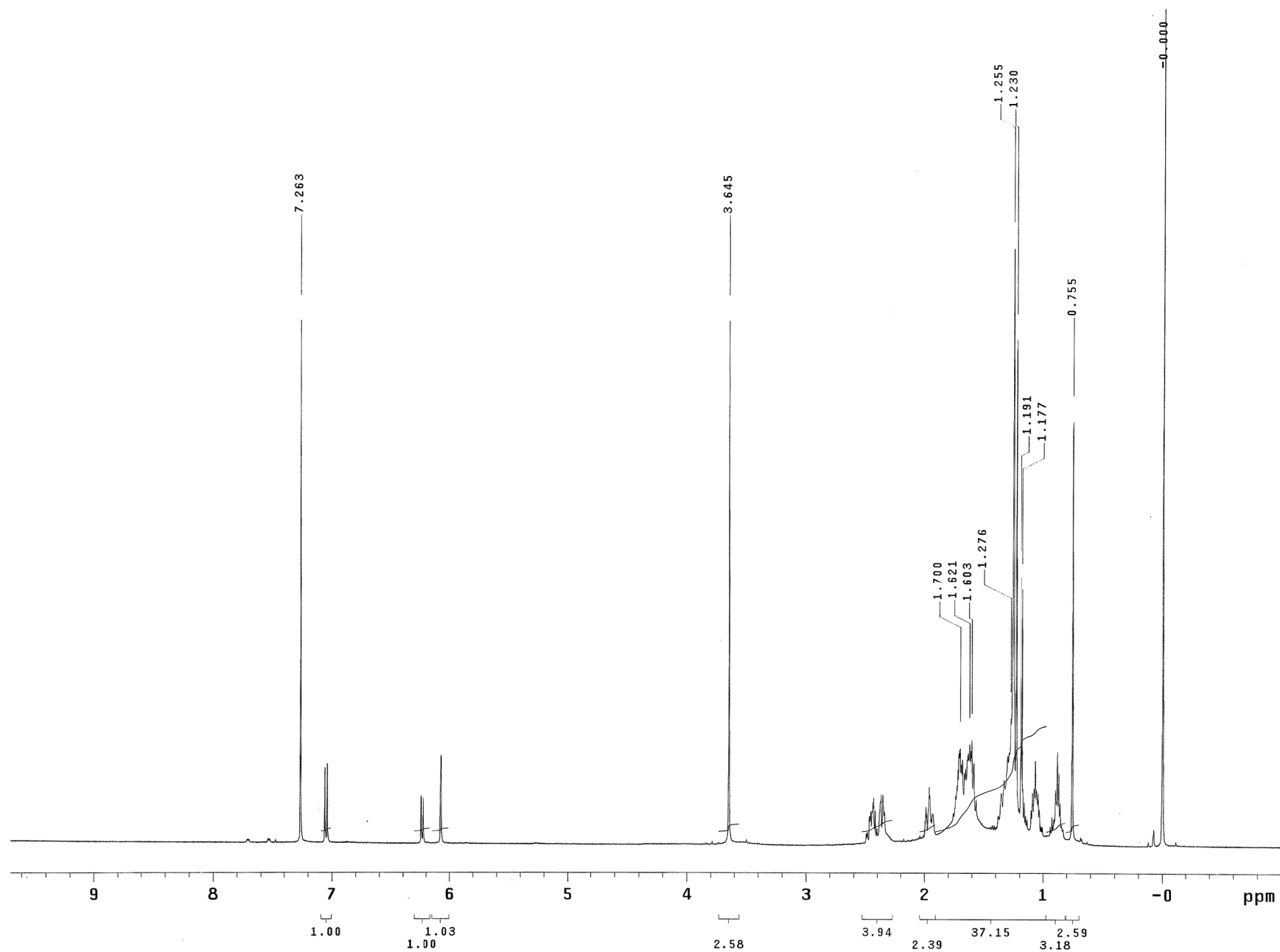


Figure S11. ¹H NMR spectrum (500 MHz) of compound **4** in CDCl₃.

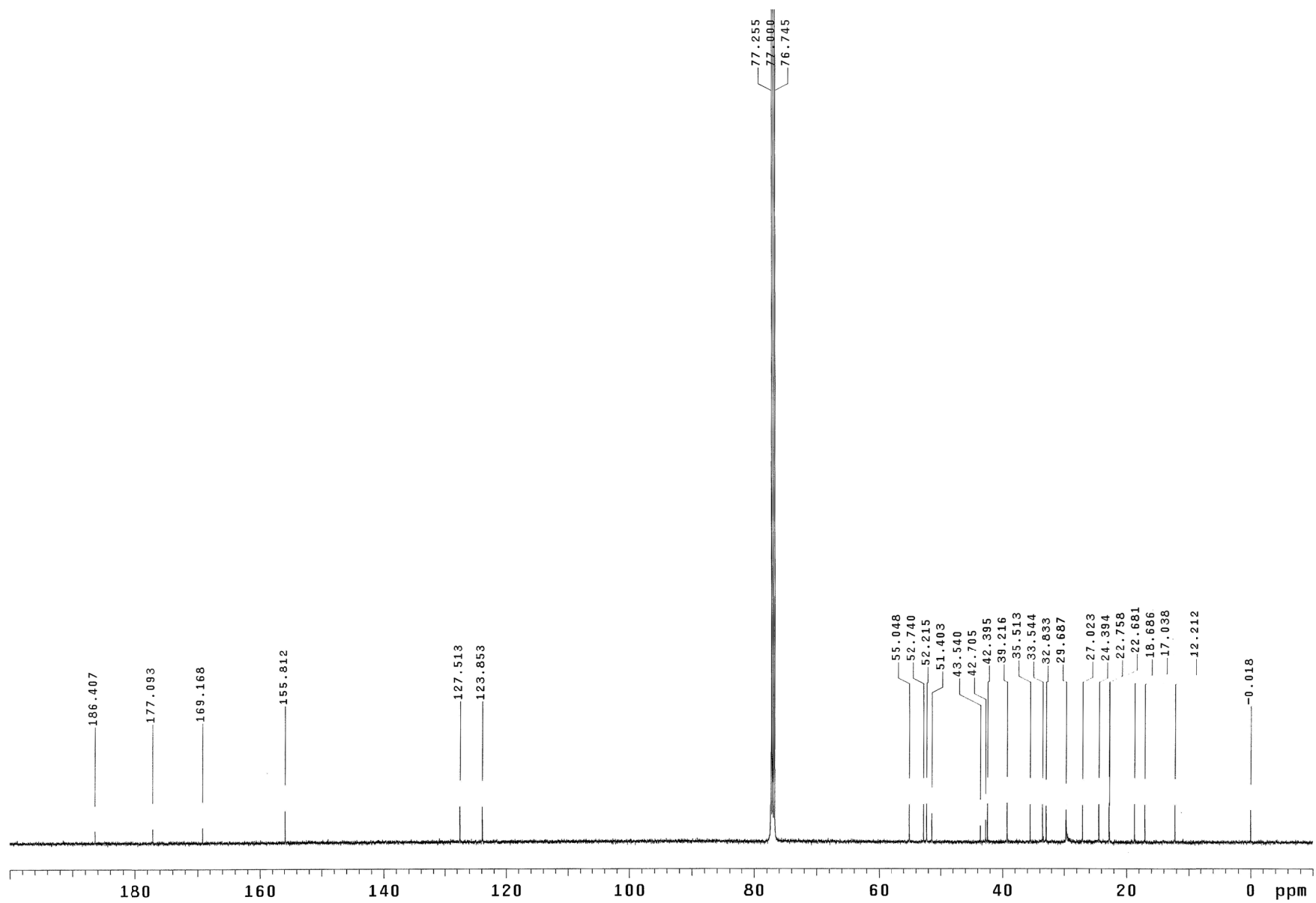


Figure S12. ¹³C NMR spectrum (125 MHz) of compound 4 in CDCl₃.