

Supplementary Data

A green and rapid approach for the stereoselective vinylation of phenol, thiol and amine derivatives in water

Yaghoub Sarrafi,* Marzieh sadatshahabi, Kamal Alimohammadi and Mahmood

Tajbakhsh *Department of Organic Chemistry, Faculty of Chemistry, Mazandaran University,*

Babolsar, Iran, E-mail: ysarrafi@umz.ac.ir

List of contents	Page	List of contents	Page	List of contents	Page
Title, author's name, address, general methods	S1-S2	¹³ C NMR of 1t	S24	¹³ C NMR of 2i	S46
¹ H NMR of 1g	S3	¹ H NMR of 1u	S25	¹ H NMR of 2j	S47
¹³ C NMR of 1g	S4	¹³ C NMR of 1u	S26	¹³ C NMR of 2j	S48
¹ H NMR of 1h	S5	¹ H NMR of 1x	S27	¹ H NMR of 2k	S49
¹³ C NMR of 1h	S6	¹³ C NMR of 1x	S28	¹³ C NMR of 2k	S50
¹ H NMR of 1i	S7	¹ H NMR of 2a	S29	¹ H NMR of 2l	S51
¹³ C NMR of 1i	S8	¹³ C NMR of 2a	S30	¹³ C NMR of 2l	S52
¹ H NMR of 1l	S9	¹ H NMR of 2b	S31	¹ H NMR of 2m	S53
¹³ C NMR of 1l	S10	¹³ C NMR of 2b	S32	¹³ C NMR of 2m	S54
¹ H NMR of 1m	S11	¹ H NMR of 2c	S33	¹ H NMR of 2n	S55
¹³ C NMR of 1m	S12	¹³ C NMR of 2c	S34	¹³ C NMR of 2n	S56
¹ H NMR of 1n	S13	¹ H NMR of 2d	S35	¹ H NMR of 2o	S57
¹³ C NMR of 1n	S14	¹³ C NMR of 2d	S36	¹³ C NMR of 2o	S58
¹ H NMR of 1o	S15	¹ H NMR of 2e	S37	¹ H NMR of 4a	S59
¹³ C NMR of 1o	S16	¹³ C NMR of 2e	S38	¹³ C NMR of 4a	S60
¹ H NMR of 1p	S17	¹ H NMR of 2f	S39	¹ H NMR of 4b	S61
¹³ C NMR of 1p	S18	¹³ C NMR of 2f	S40	¹³ C NMR of 4b	S62
¹ H NMR of 1q	S19	¹ H NMR of 2g	S41	¹ H NMR of 4c	S63
¹³ C NMR of 1q	S20	¹³ C NMR of 2g	S42	¹³ C NMR of 4c	S64
¹ H NMR of 1r	S21	¹ H NMR of 2h	S43	¹ H NMR of 4d	S65
¹³ C NMR of 1r	S22	¹³ C NMR of 2h	S44	¹³ C NMR of 4d	S66
¹ H NMR of 1t	S23	¹ H NMR of 2i	S45	¹ H NMR of 5a	S67

Supplementary Data

List of contents	Page	List of contents	Page	List of contents	Page
¹³ C NMR of 5a	S68	¹ H NMR of 5e	S75	¹³ C NMR of 5i	S82
¹ H NMR of 5b	S69	¹³ C NMR of 5e	S76	¹ H NMR of 5j	S83
¹³ C NMR of 5b	S70	¹ H NMR of 5f	S77	¹³ C NMR of 5j	S84
¹ H NMR of 5c	S71	¹³ C NMR of 5f	S78	¹ H NMR of 5j	S83
¹³ C NMR of 5c	S72	¹ H NMR of 5g	S79	¹³ C NMR of 5j	S84
¹ H NMR of 5d	S73	¹³ C NMR of 5g	S80	¹ H NMR of Di- <i>tert</i> -butyl 2-(phenoxy)-2-butenedioate	S85
¹³ C NMR of 5d	S74	¹ H NMR of 5i	S81	¹³ C NMR of Di- <i>tert</i> -butyl 2-(phenoxy)-2-butenedioate	S86

Experimental Section:

General Considerations

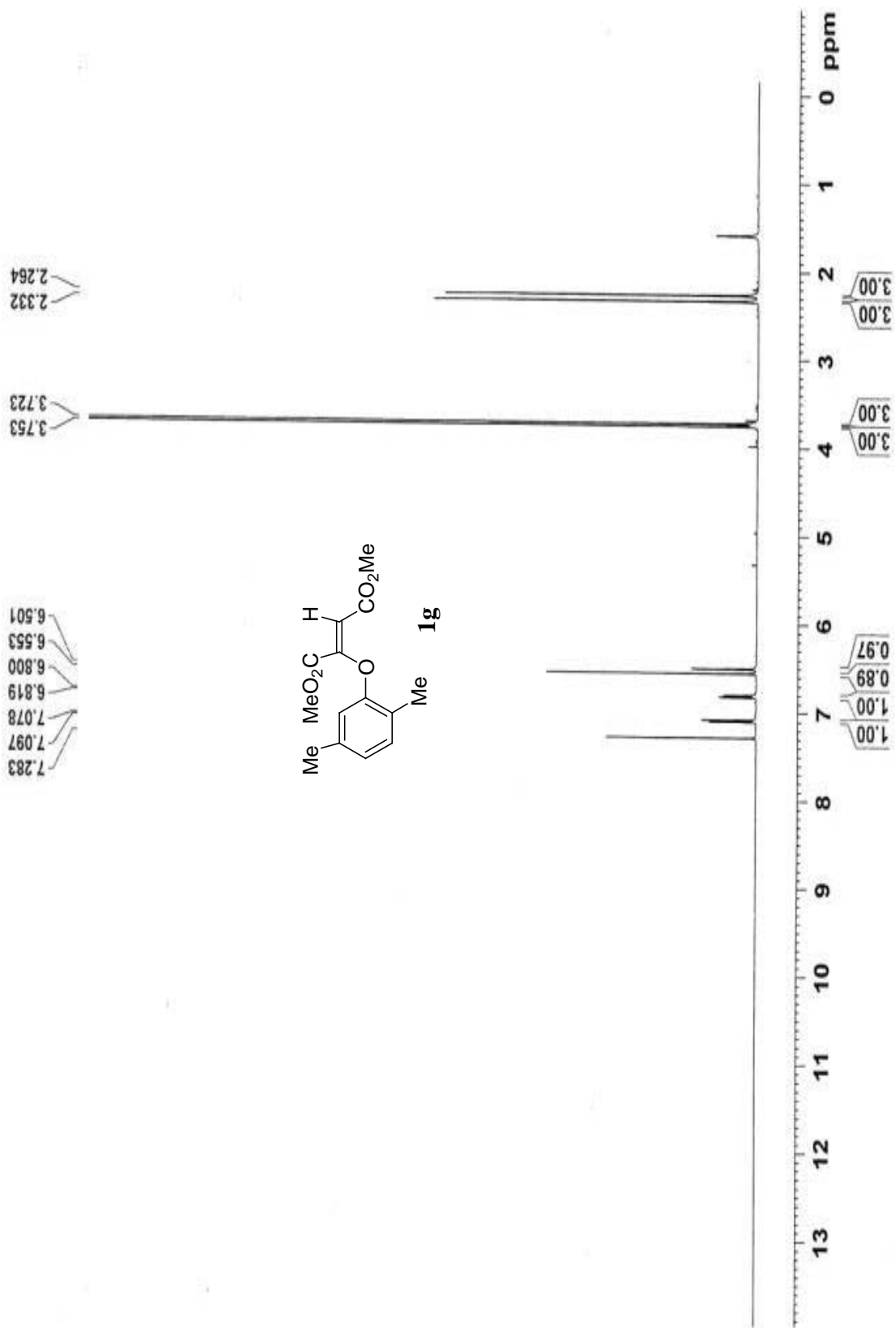
Melting points were measured on an Electrothermal 9100 apparatus. Infrared spectra were recorded on a Shimadzu IR-8300 series FT-IR spectrophotometer. ¹H NMR and ¹³C NMR spectra were recorded on a Bruker 400-MHz instrument in CDCl₃ solvent with TMS as a standard. Mass spectra were recorded by a Jeol DX303 HF mass spectrometer. Elemental analyses were carried out by Perkin-Elmer CHN 2400 instrument.

Typical procedure for synthesis of 1a

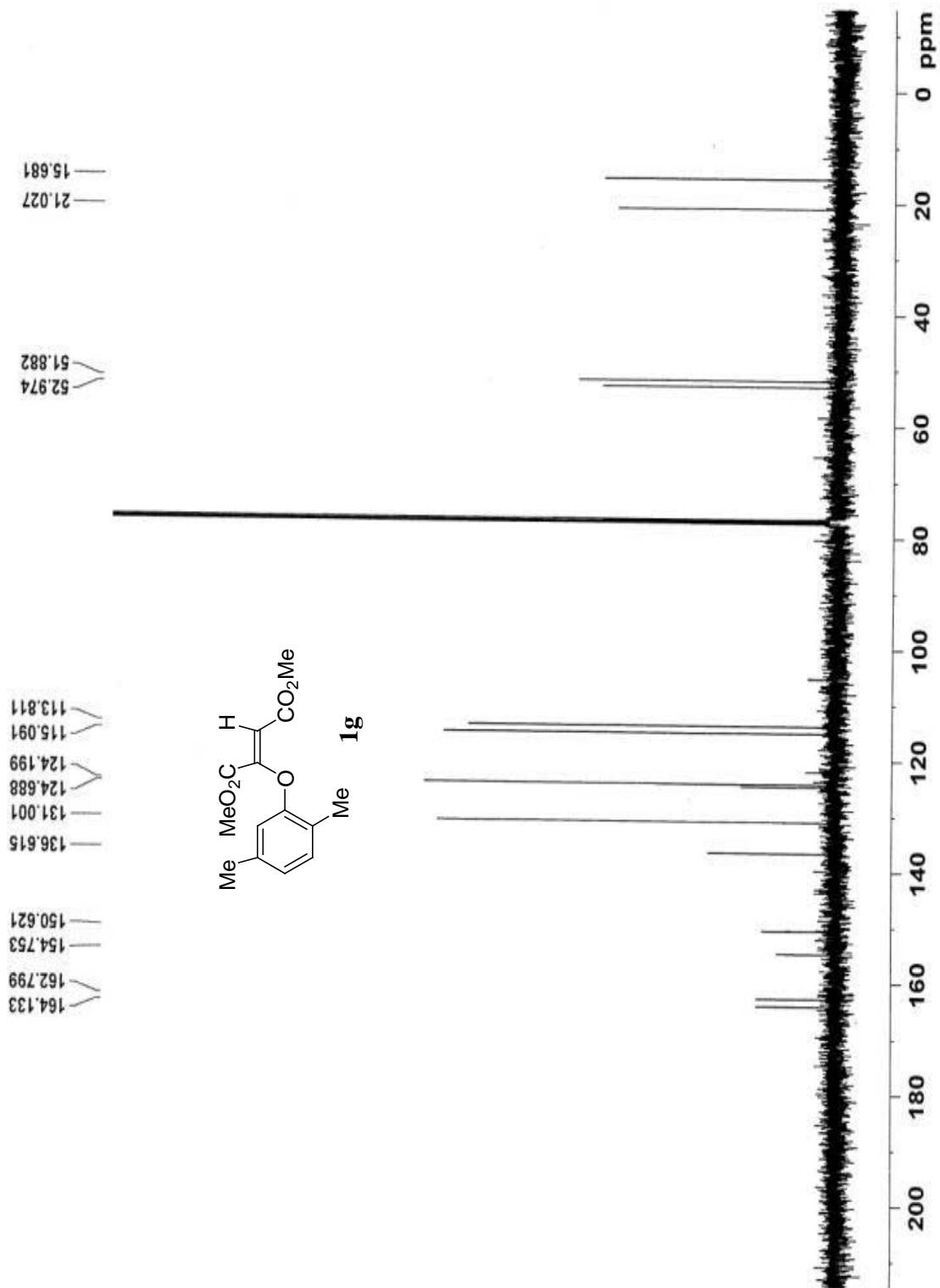
Phenol (0.188 g, 2 mmol) was dissolved in aqueous solution of K₂CO₃ (0.276 g, 2 mmol) and DMAD (0.284 g, 2 mmol) was added. The reaction mixture was stirred vigorously at room temperature. A turbid solution was formed which by consumption of phenol (monitored by TLC) in 5 min., the reaction mixture became clear and dimethyl (Z)-2-(phenoxy)-2-butenedioate **1a** existed as solid in water. The product was isolated by filtration without further purification.

Compounds **1a-f**, **j**, **k**, **s**, **v**, **w** and **5j** are known compounds and were characterized by comparison of their physical and spectroscopic data with those of reported ones.^{24n, o, 27, 30, 31, 32j, 40} Spectral data of new compounds are reported here.

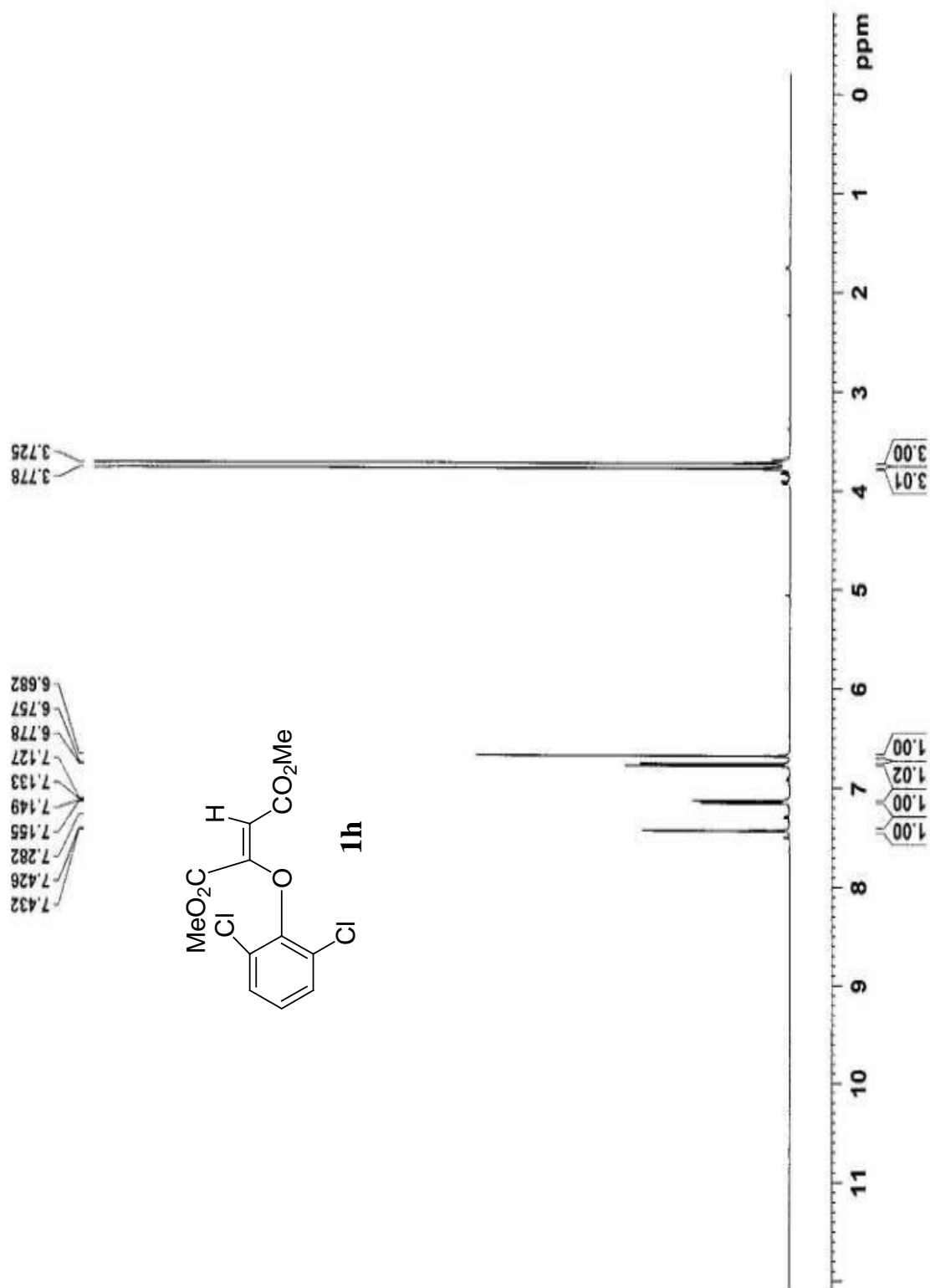
Supplementary Data



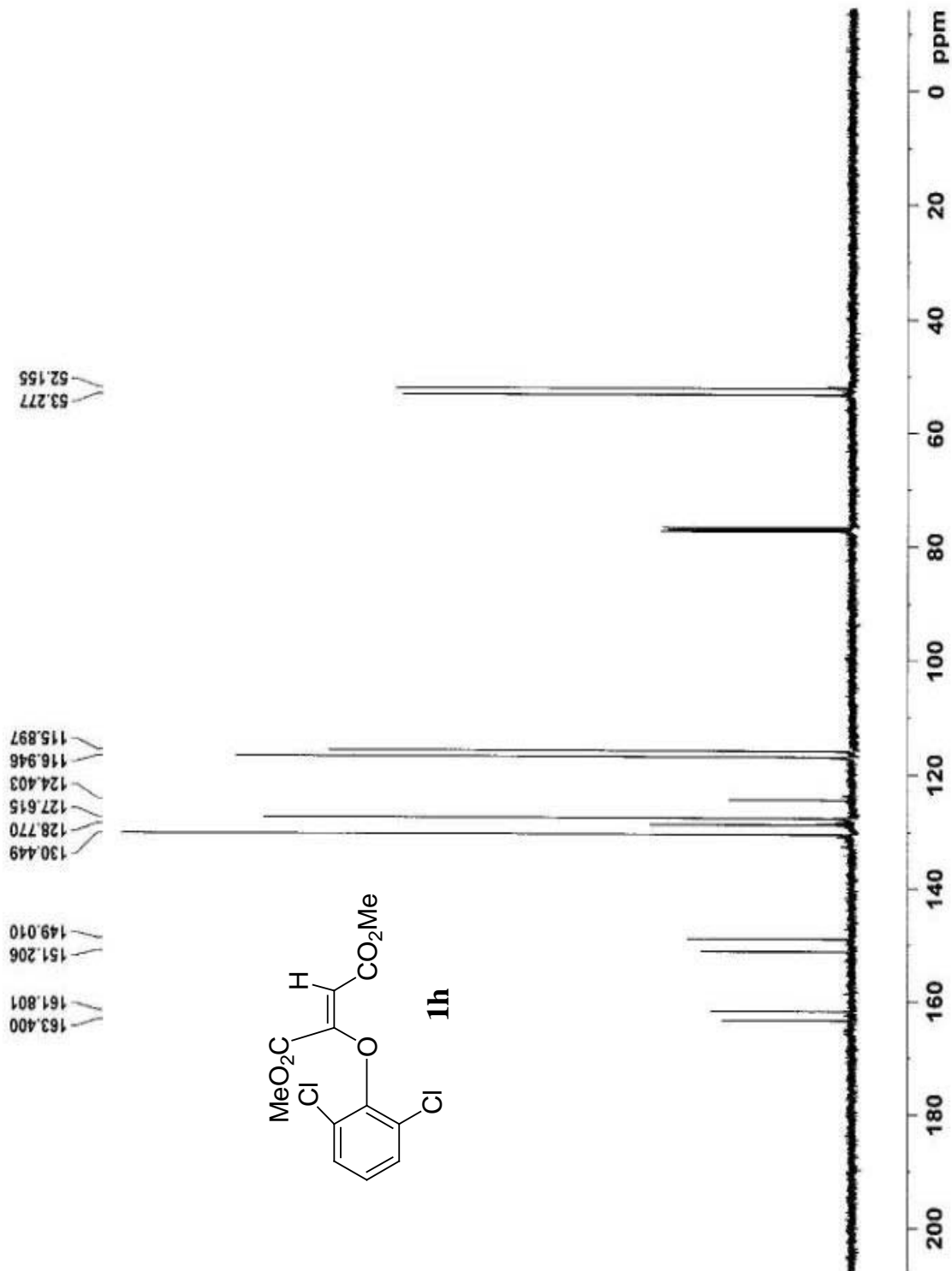
Supplementary Data



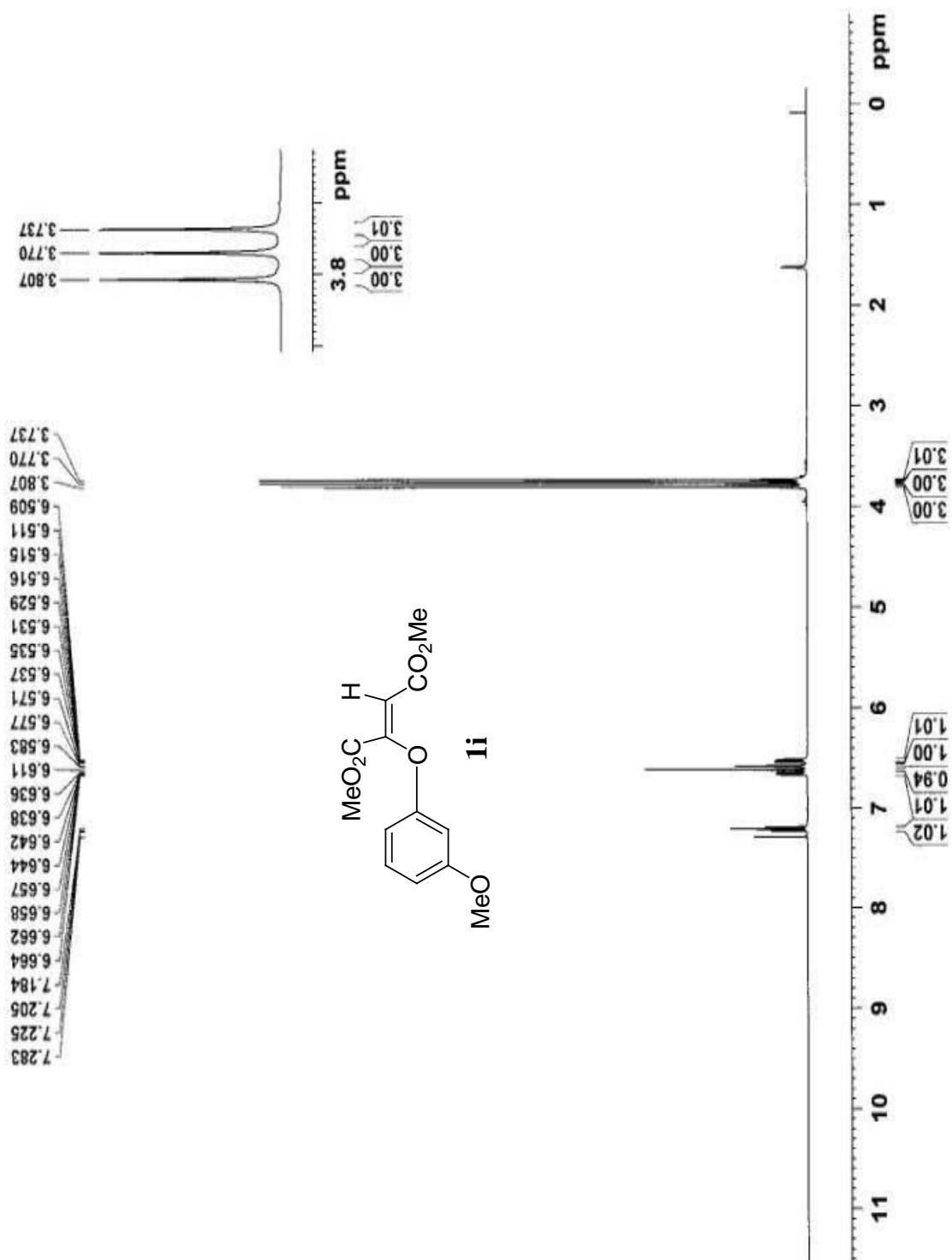
Supplementary Data



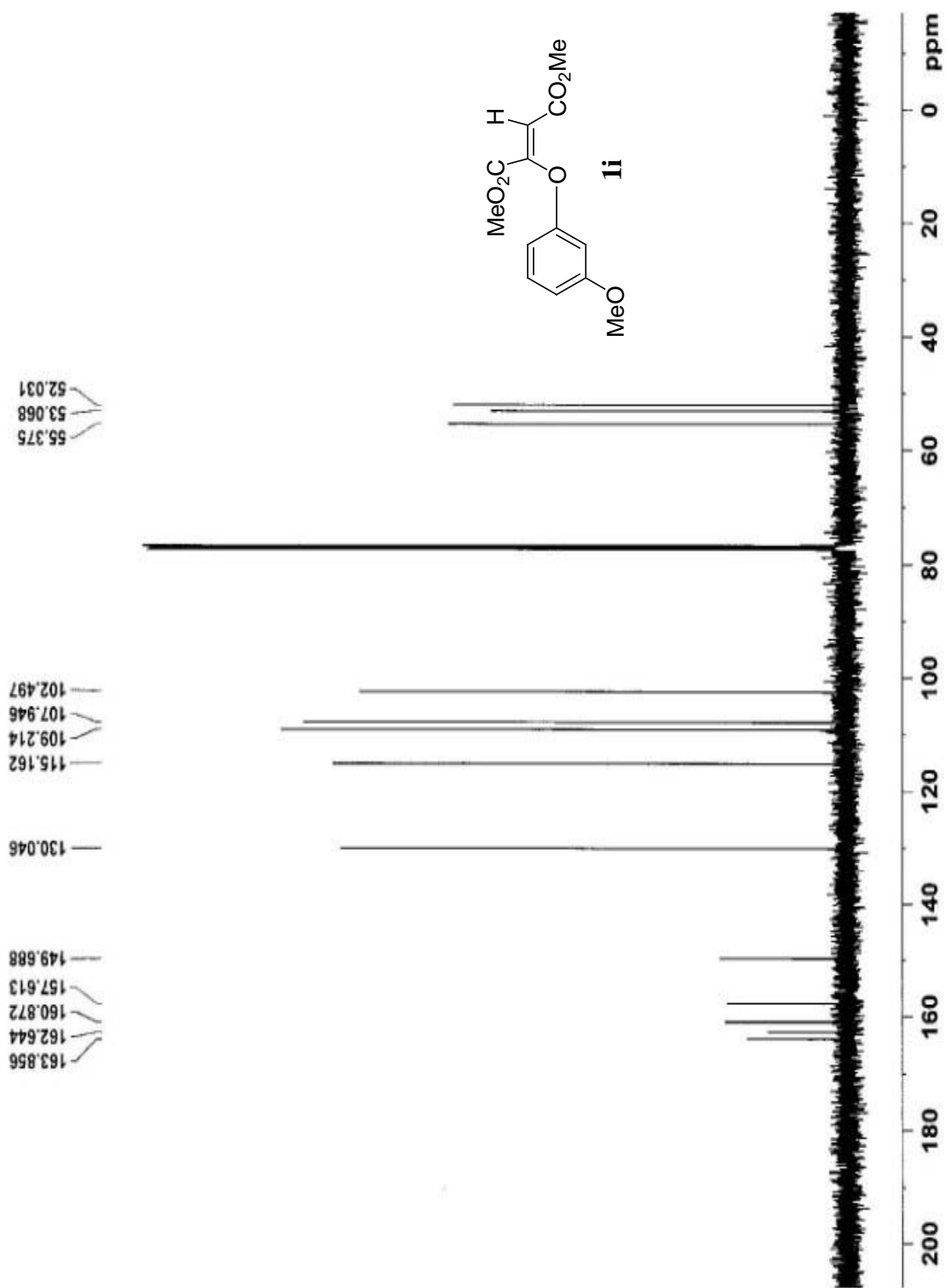
Supplementary Data



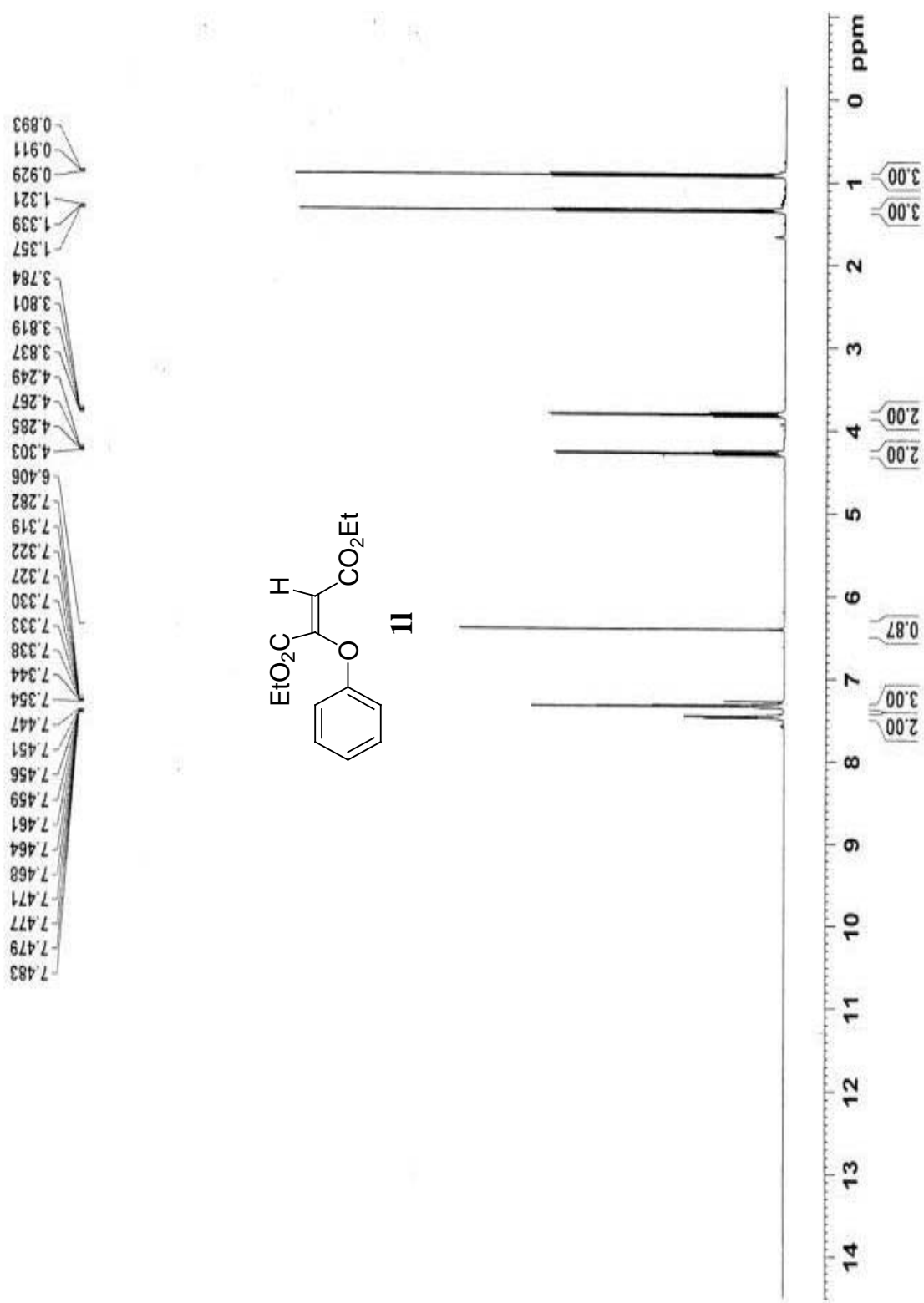
Supplementary Data



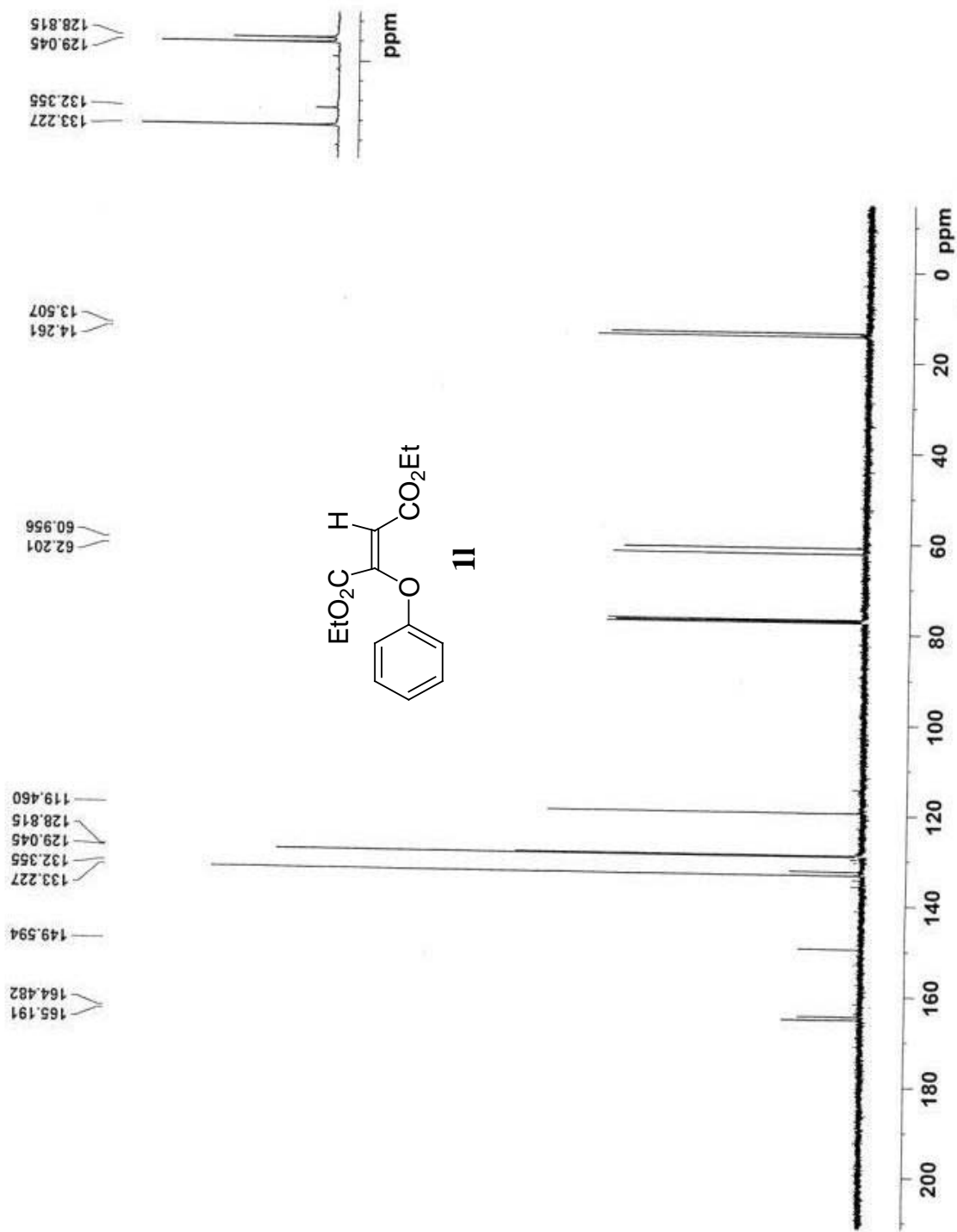
Supplementary Data



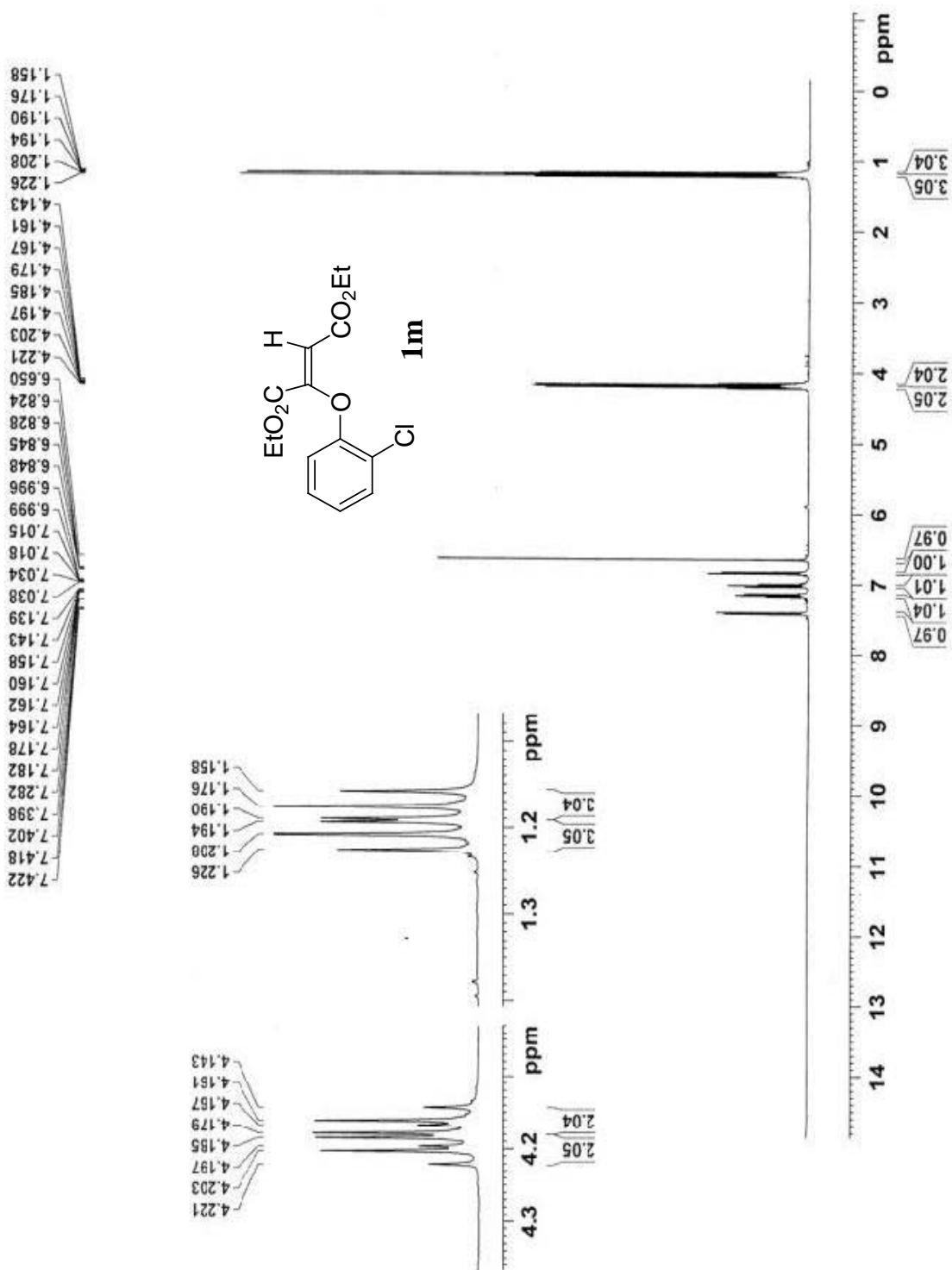
Supplementary Data



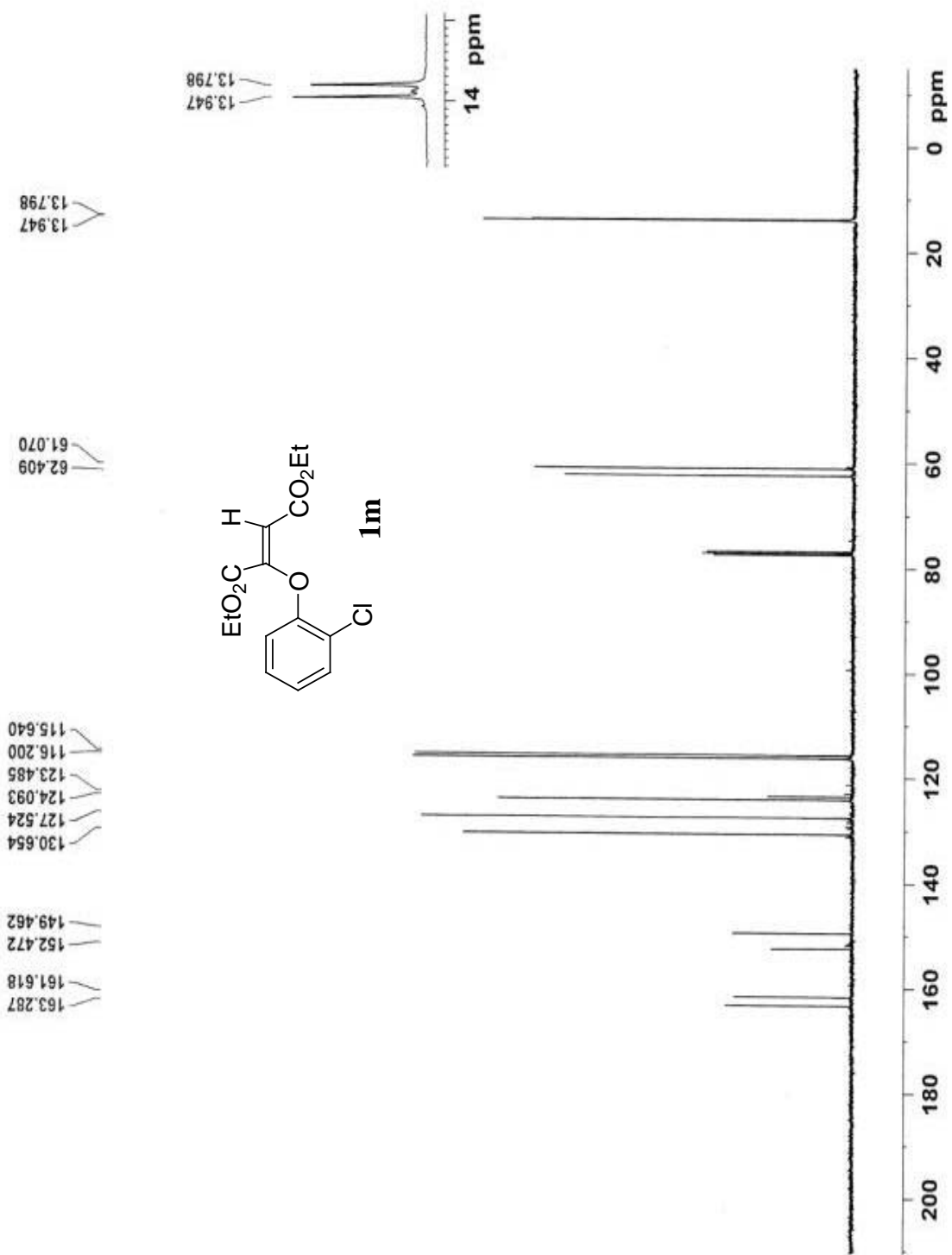
Supplementary Data



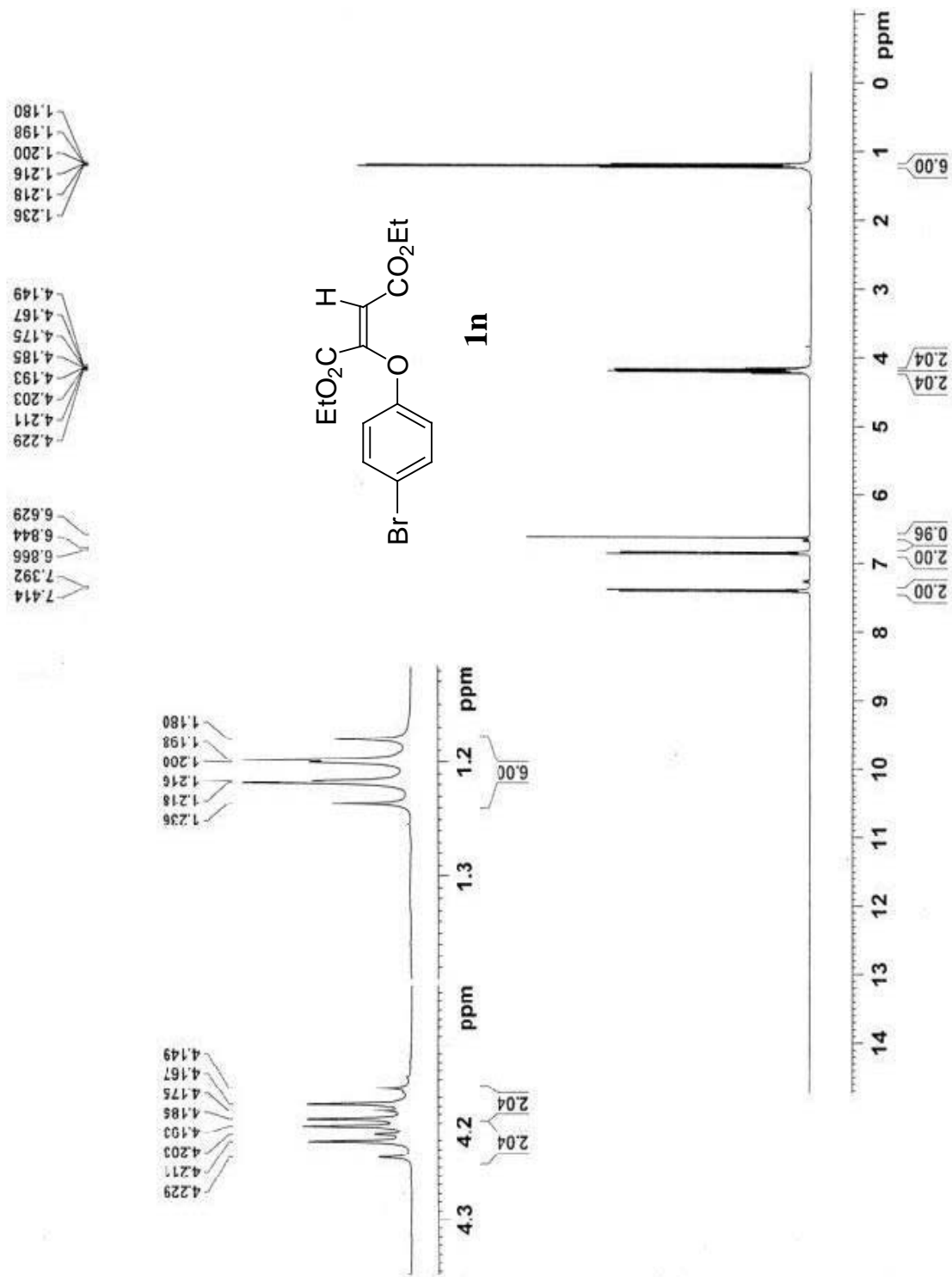
Supplementary Data



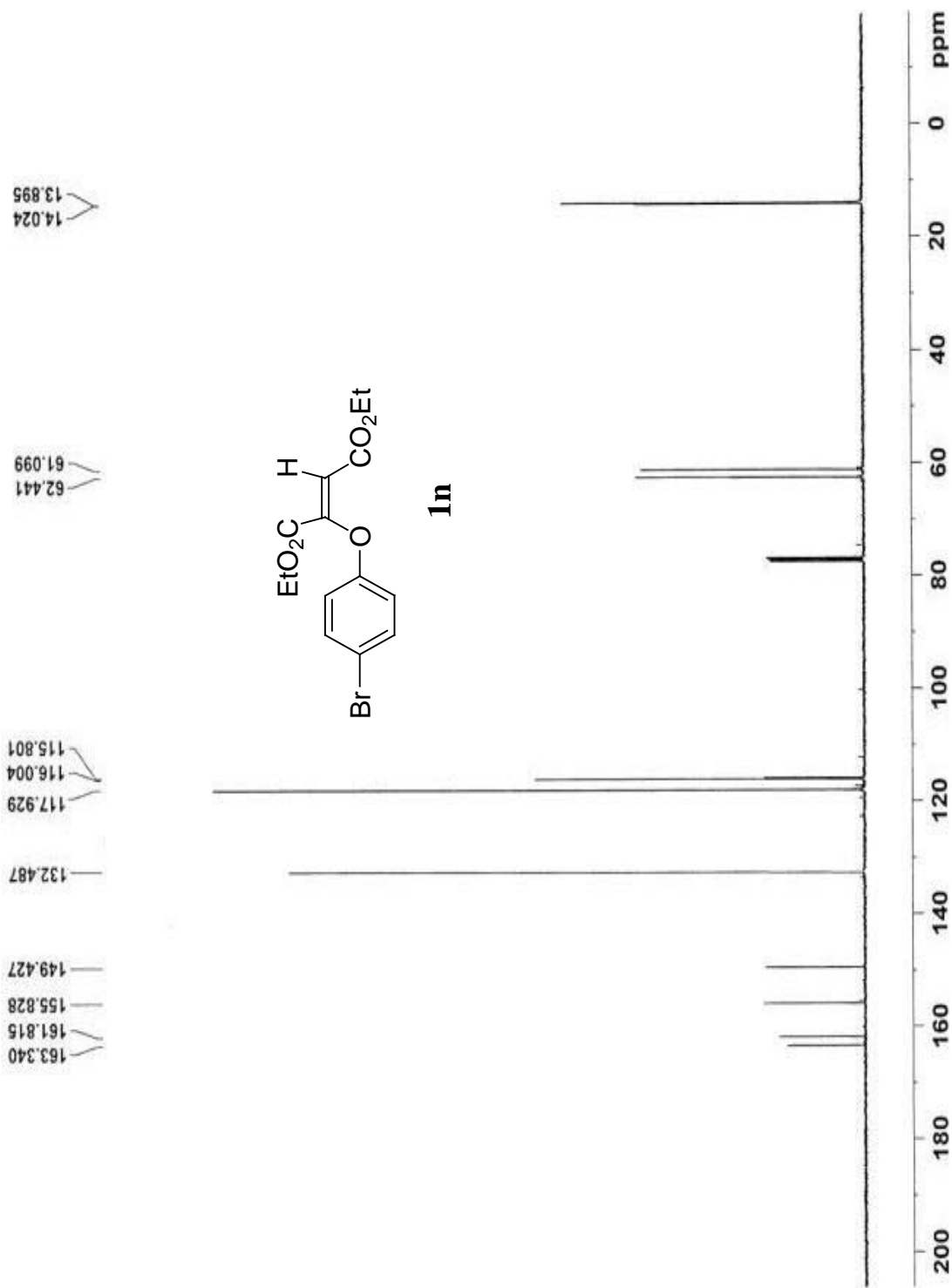
Supplementary Data



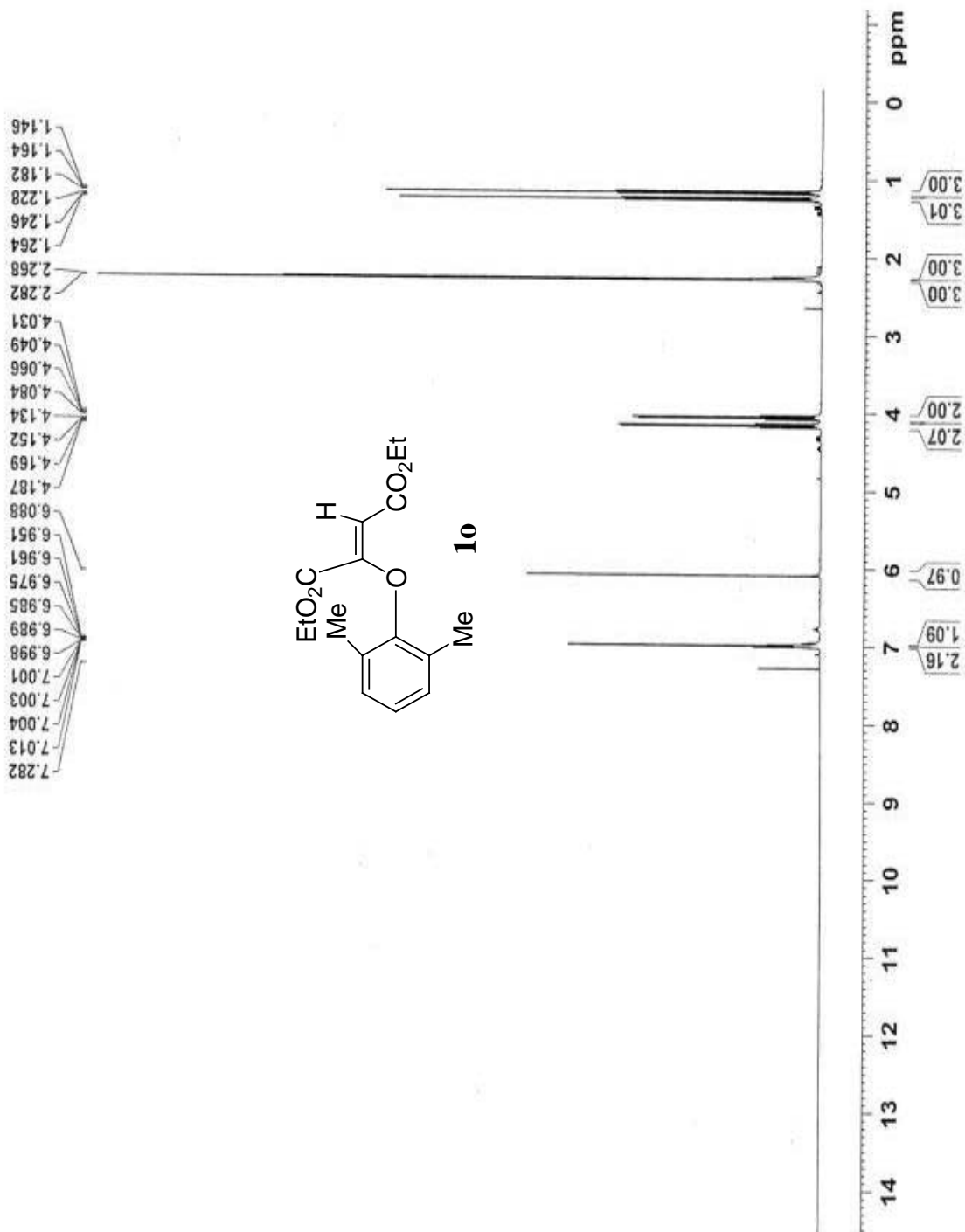
Supplementary Data



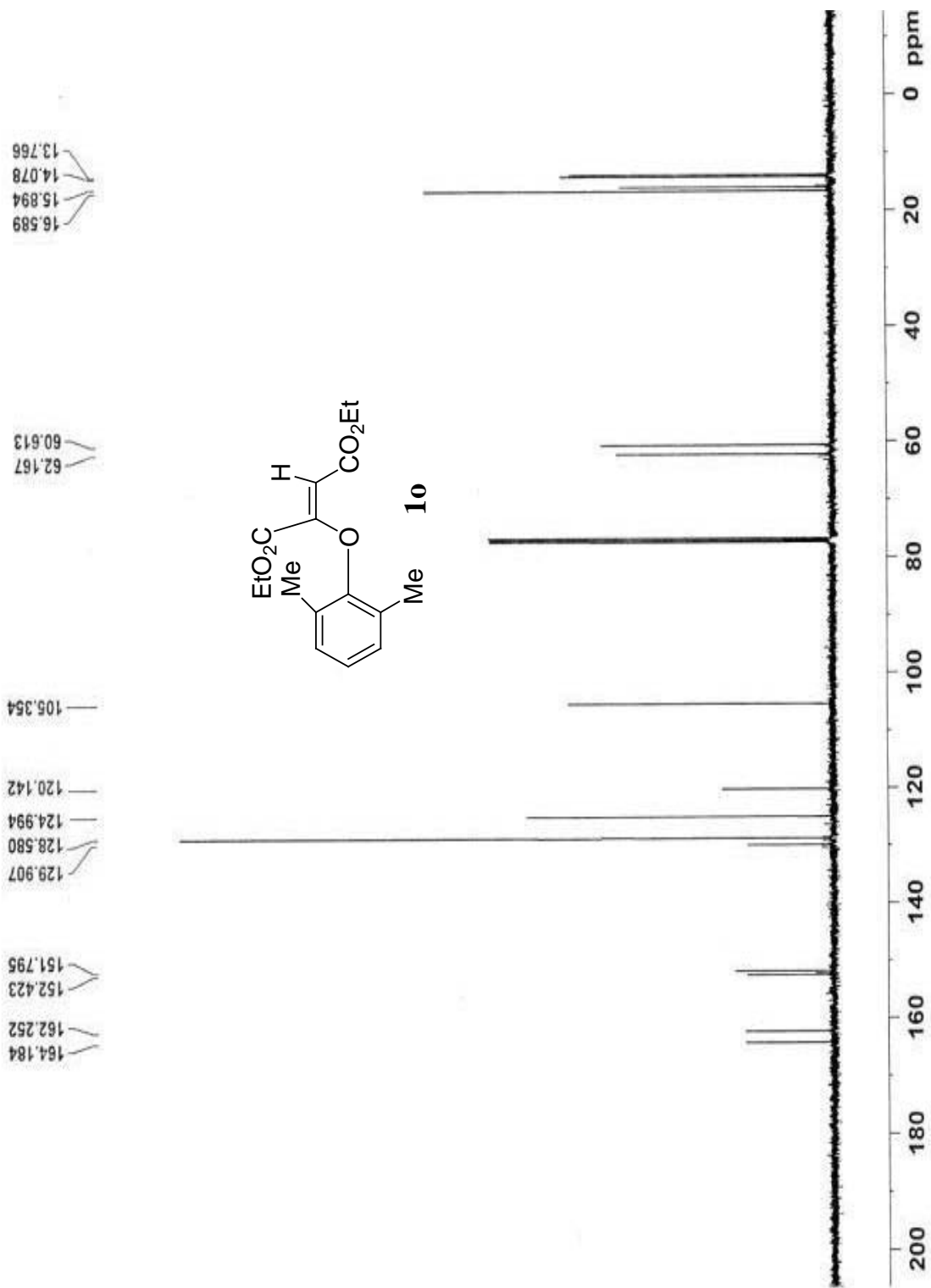
Supplementary Data



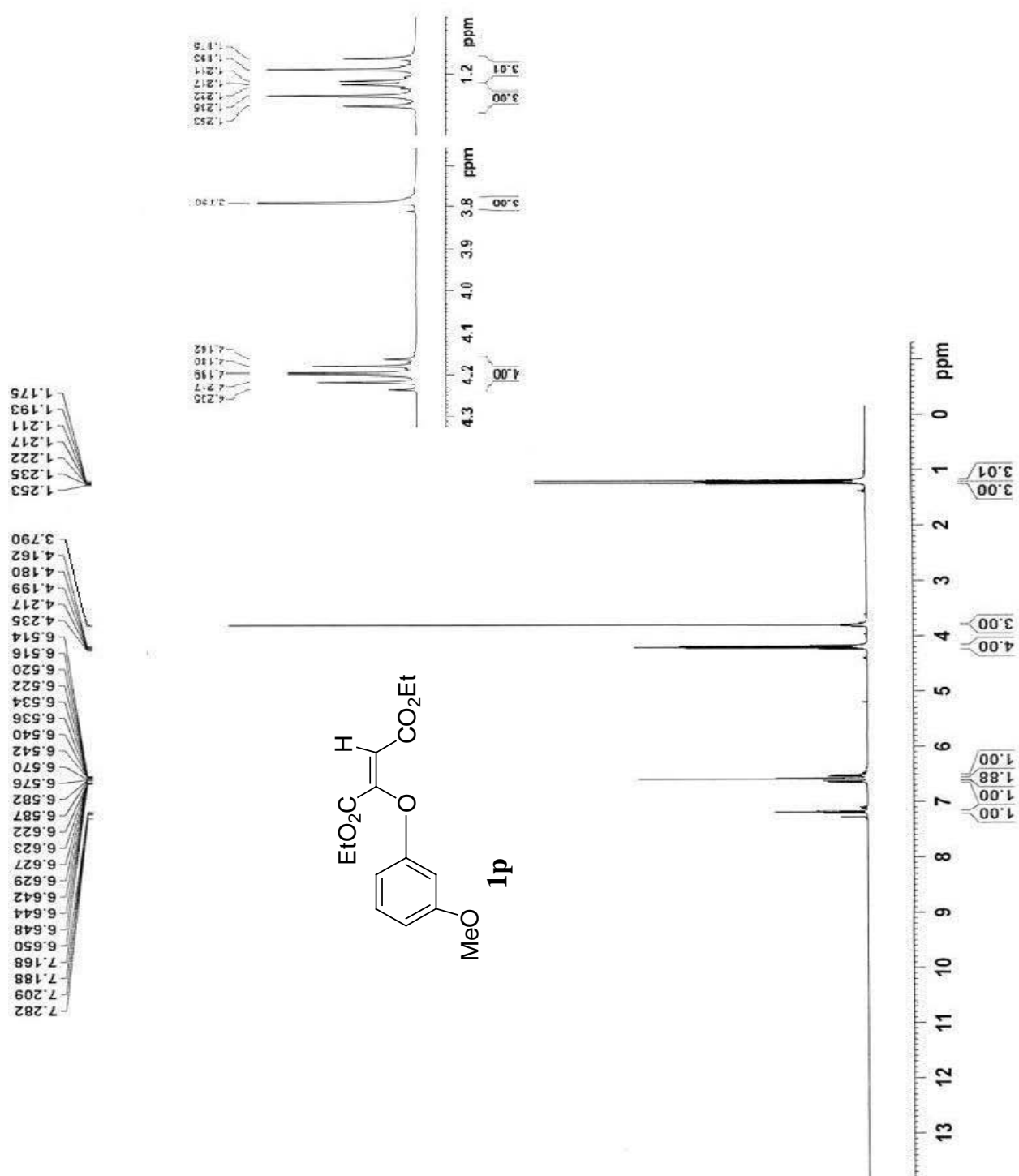
Supplementary Data



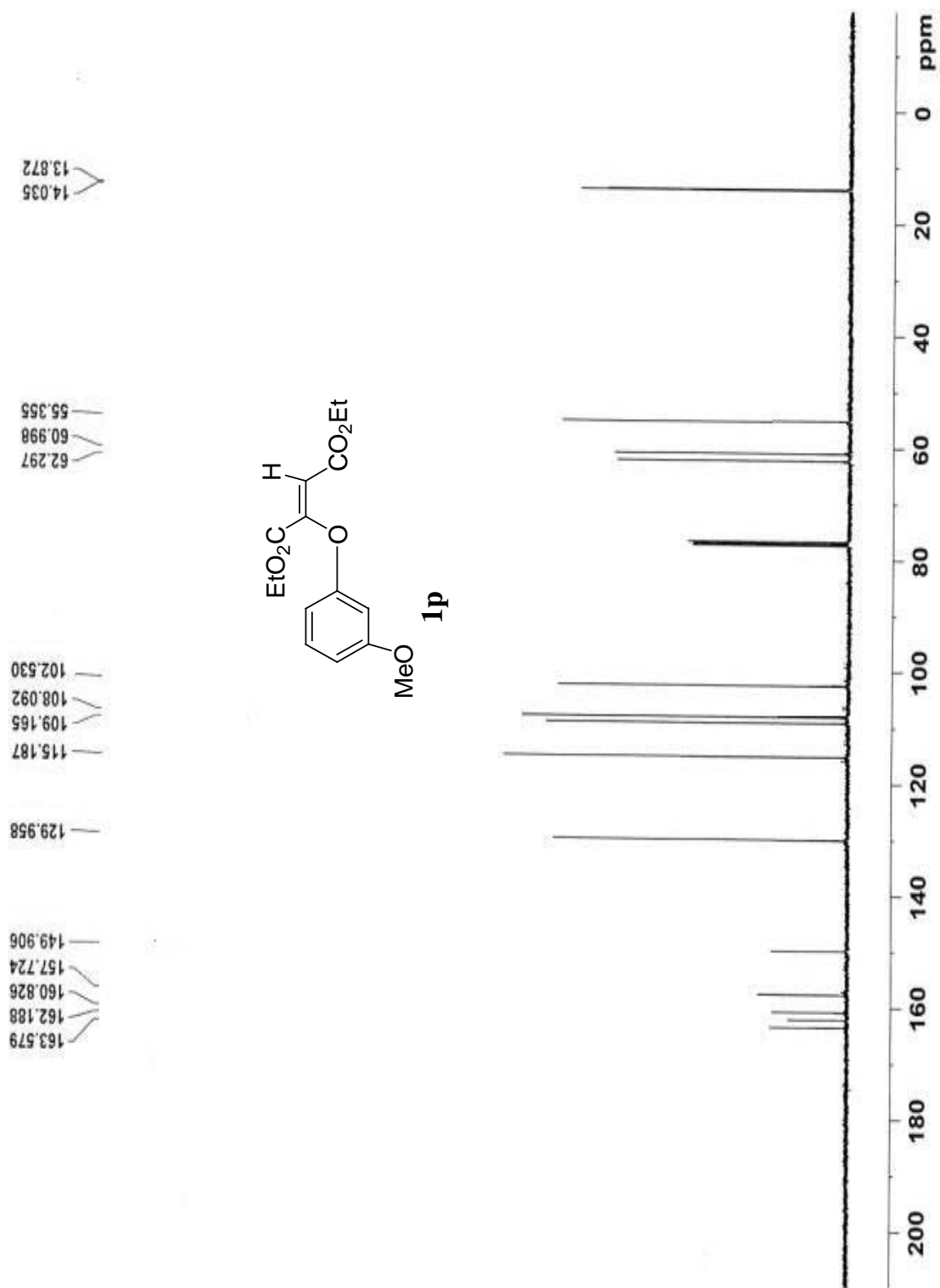
Supplementary Data



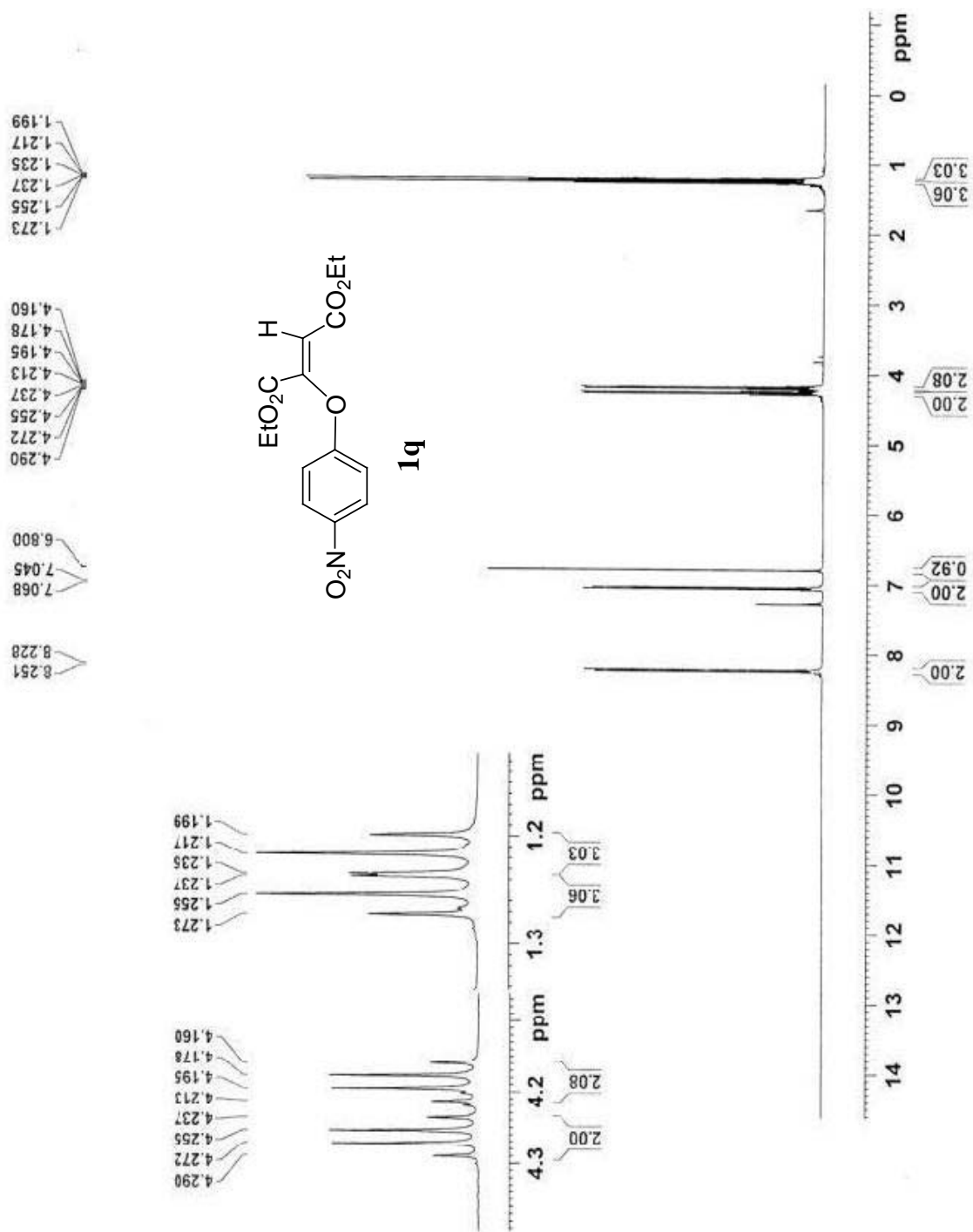
Supplementary Data



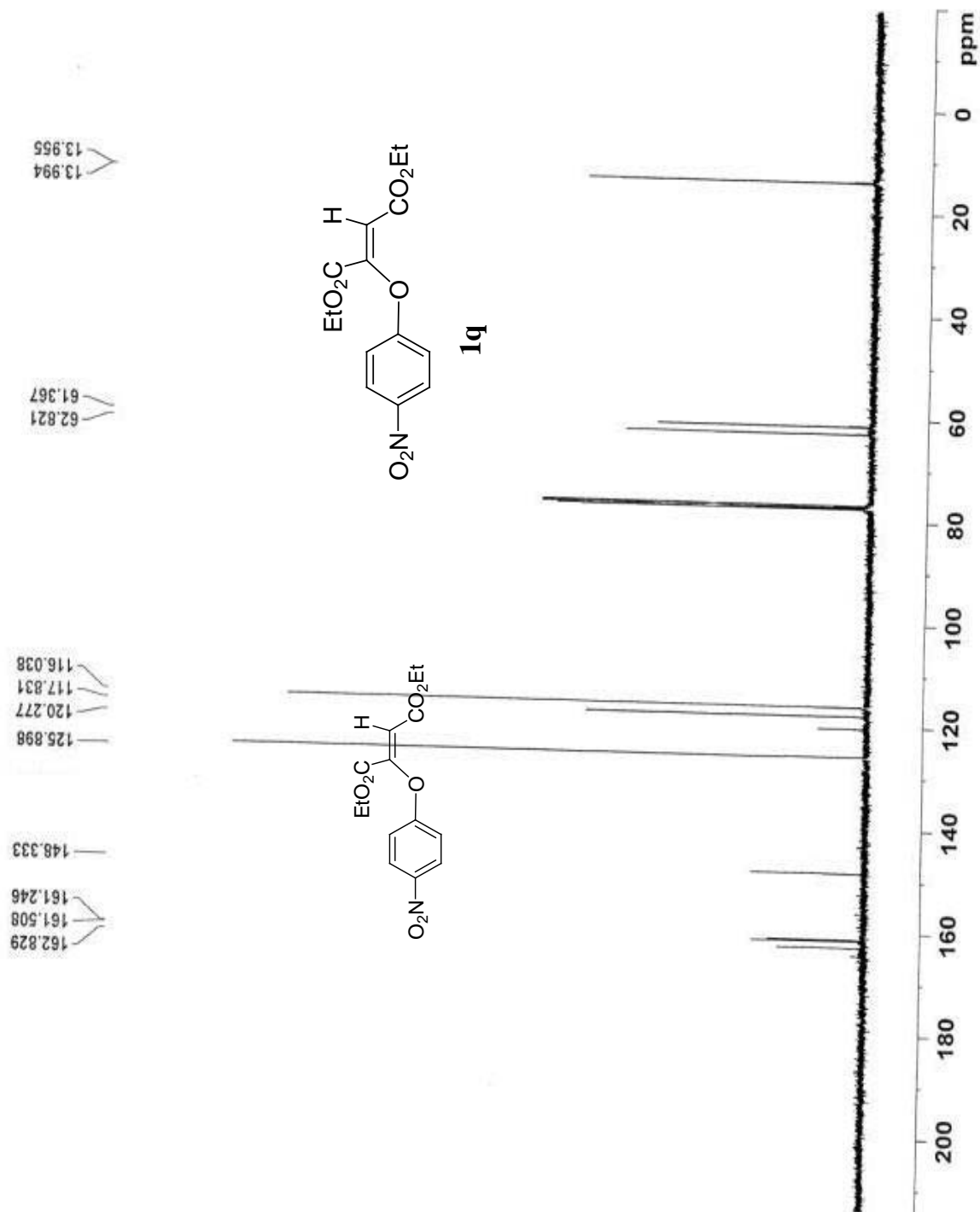
Supplementary Data



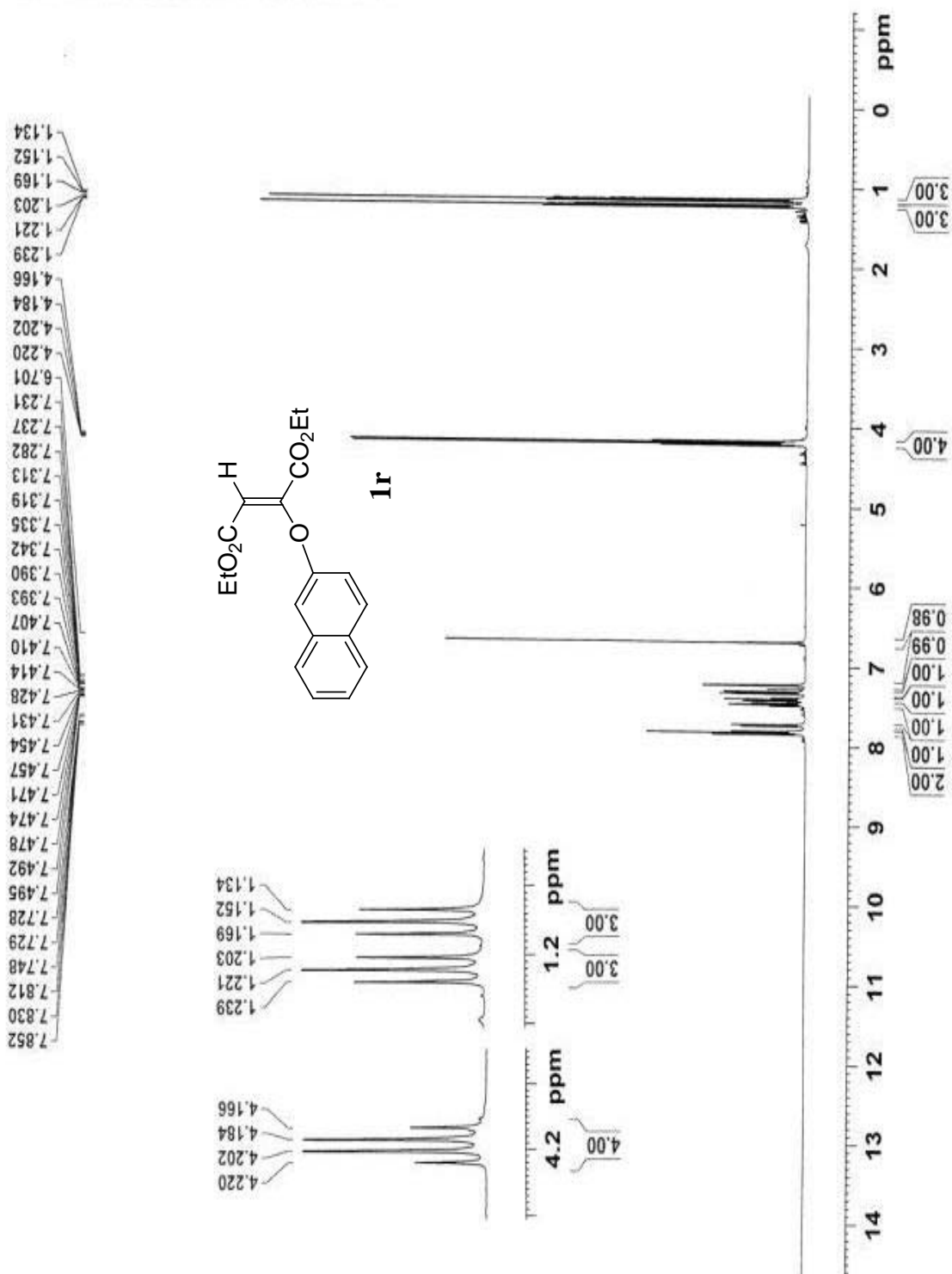
Supplementary Data



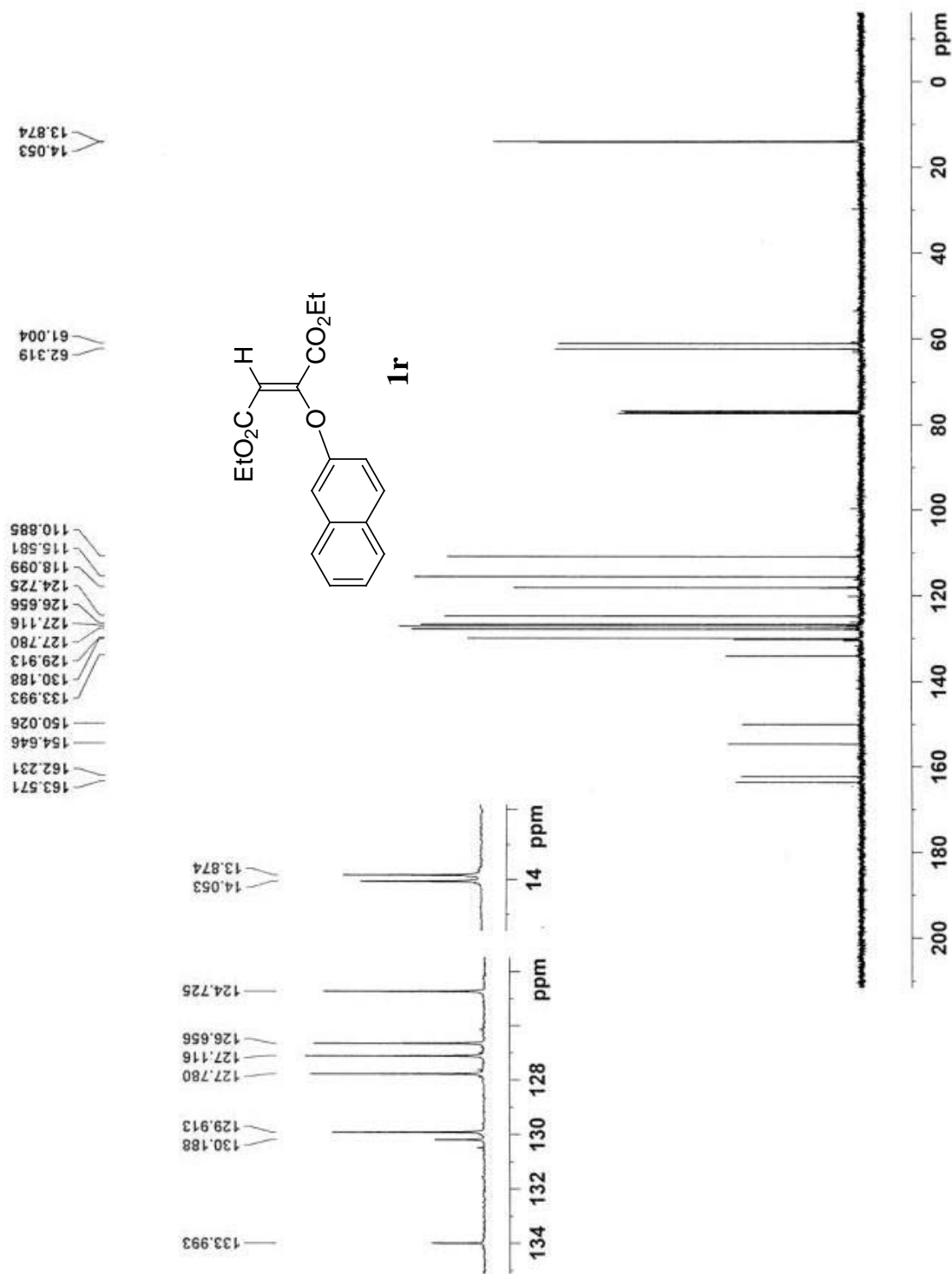
Supplementary Data



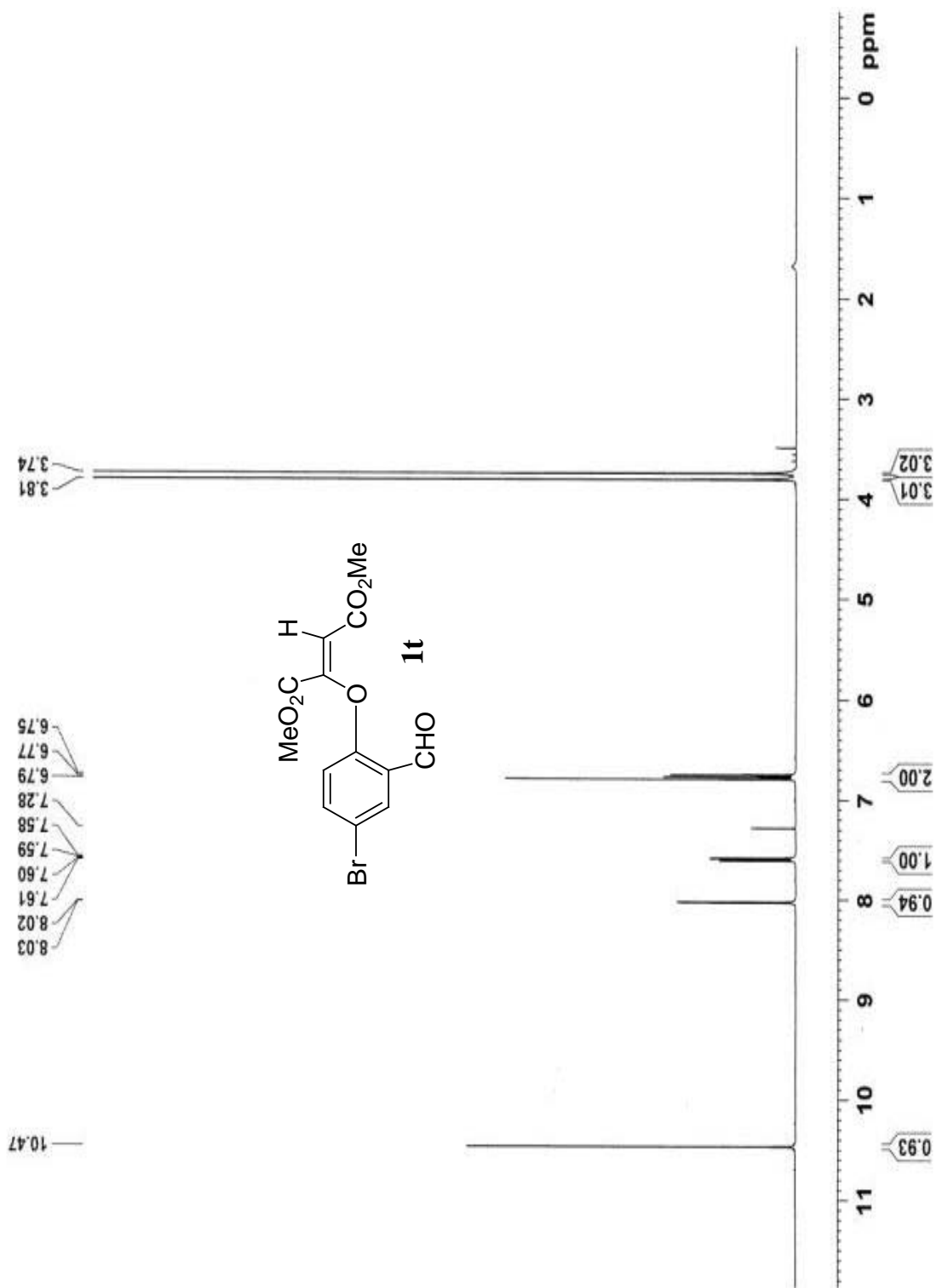
Supplementary Data



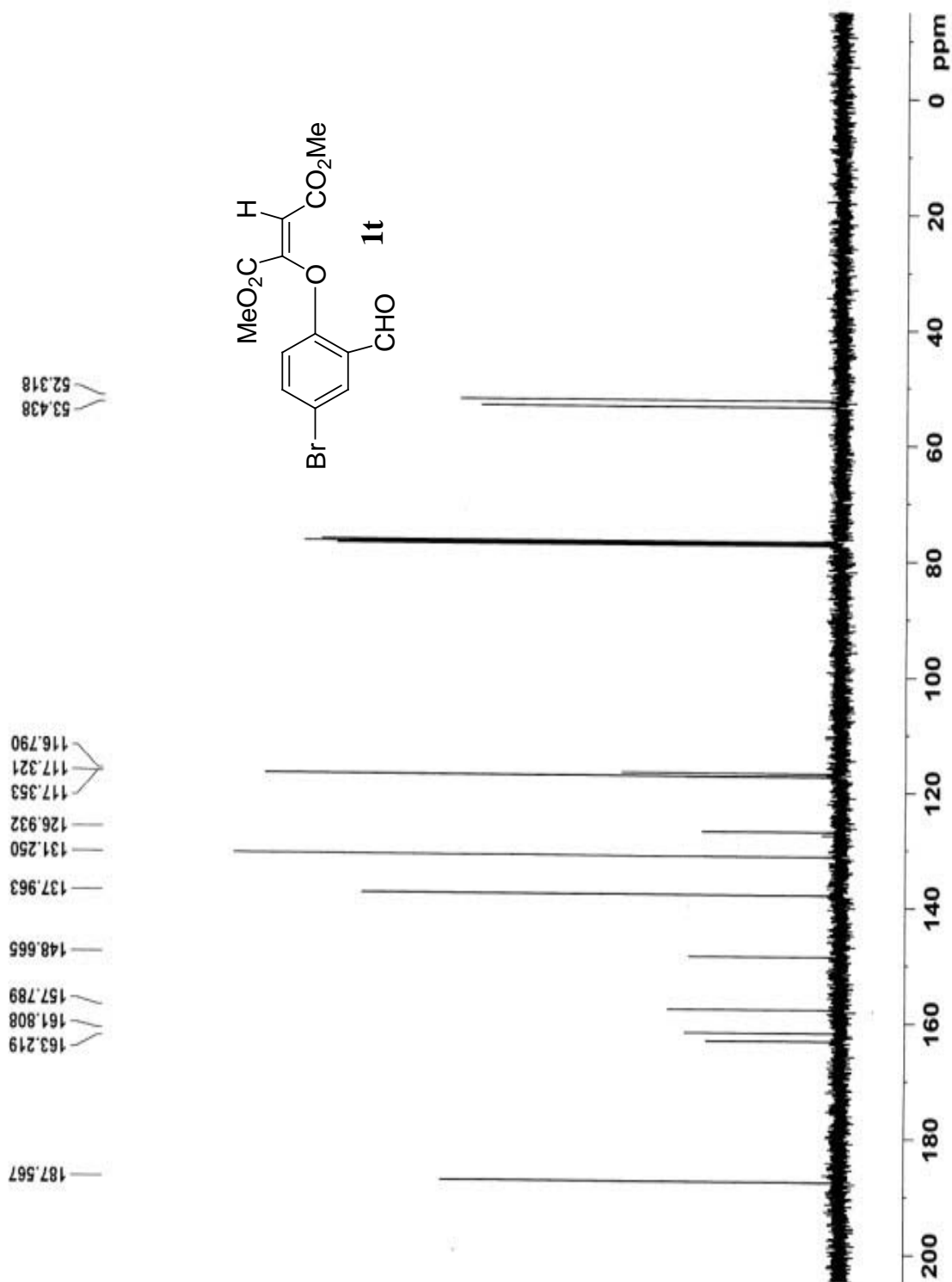
Supplementary Data



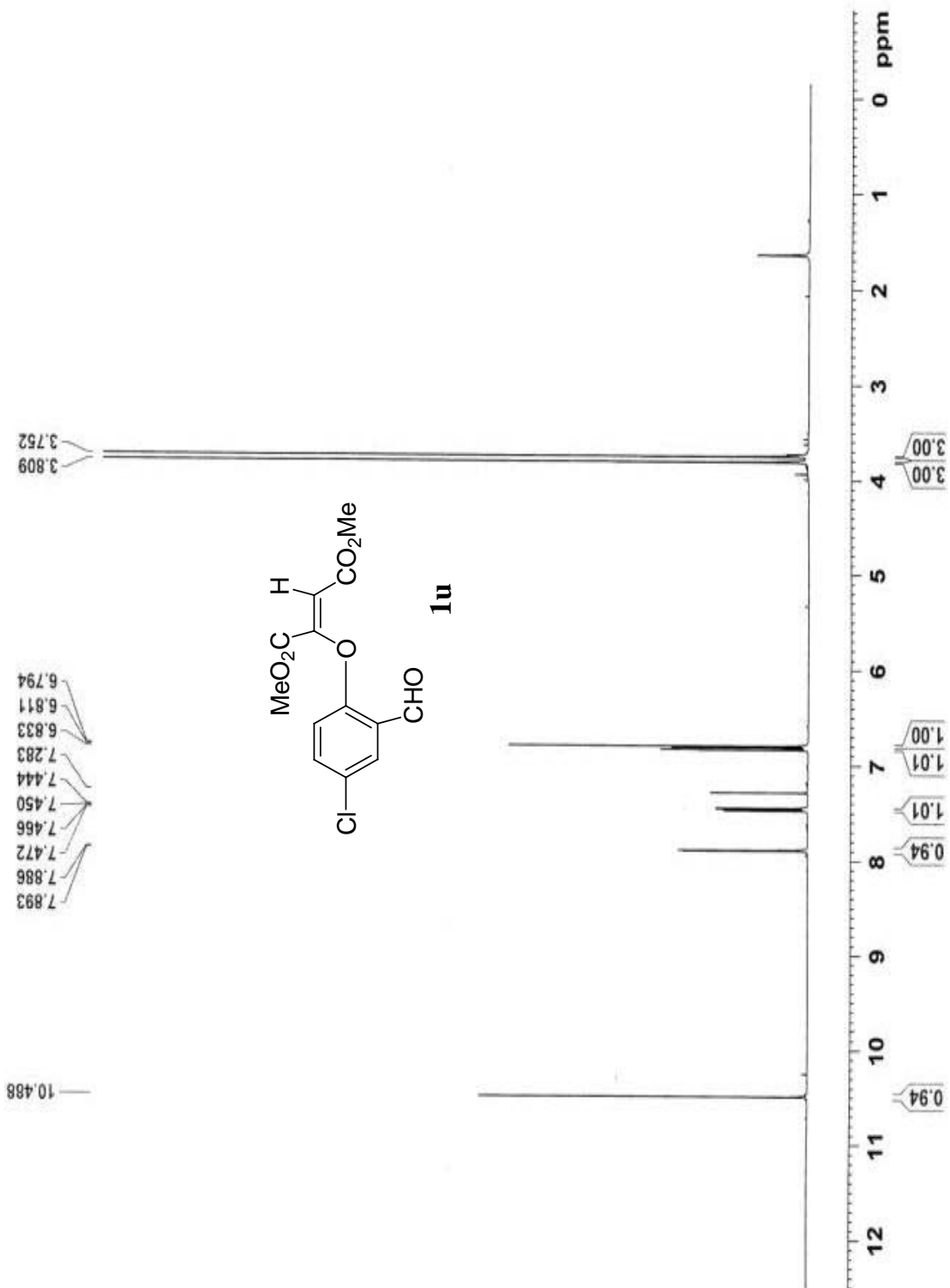
Supplementary Data



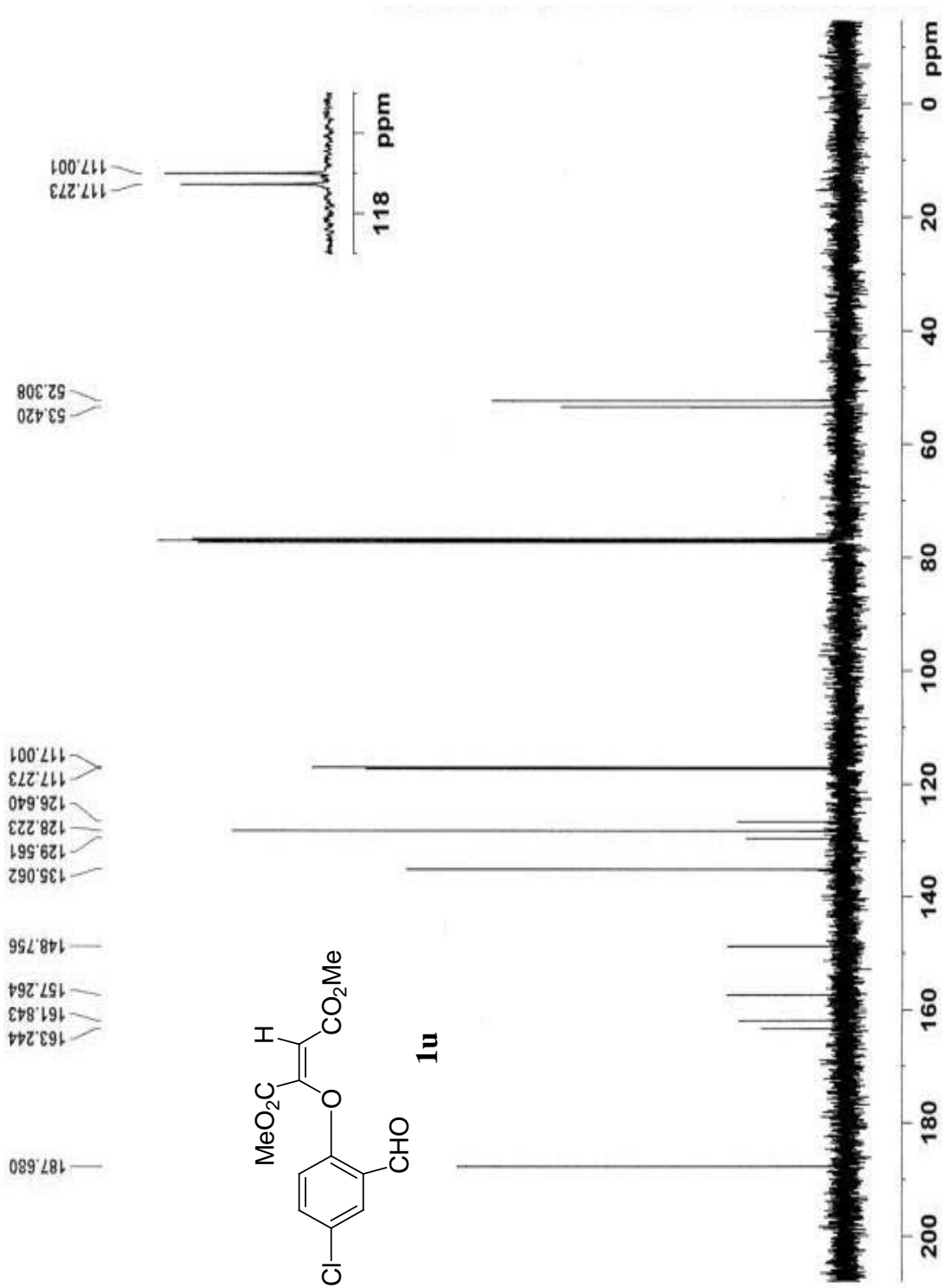
Supplementary Data



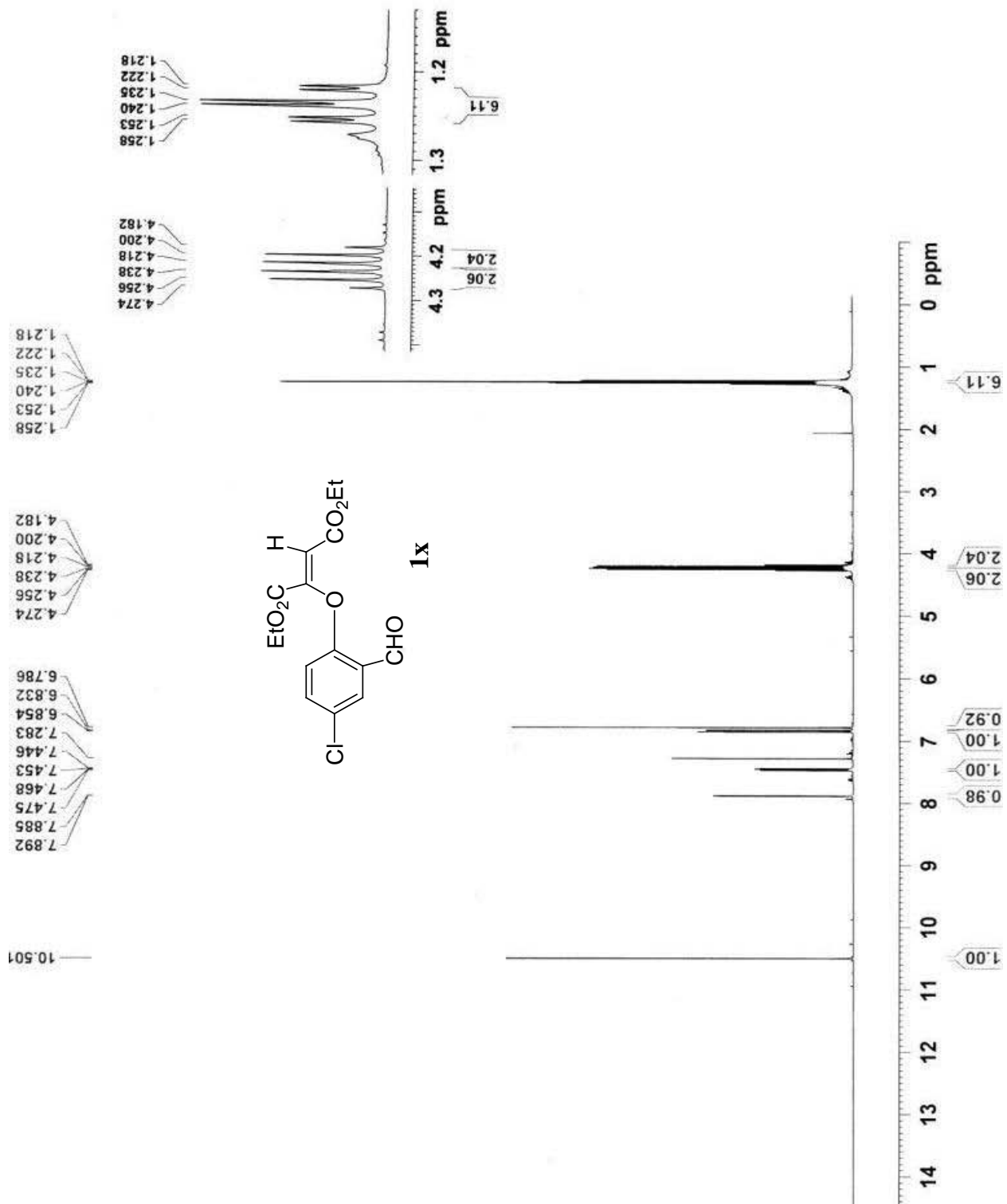
Supplementary Data



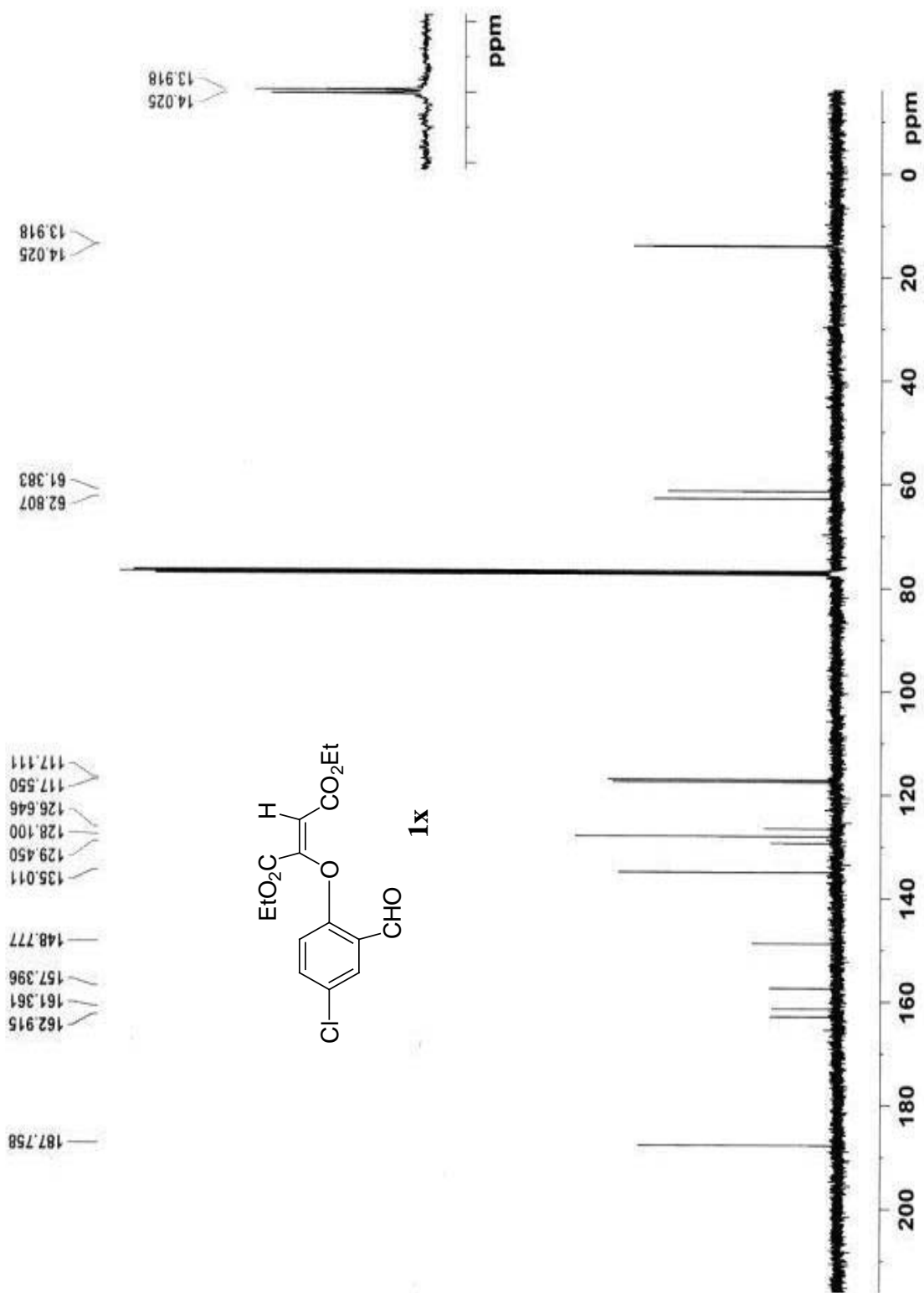
Supplementary Data



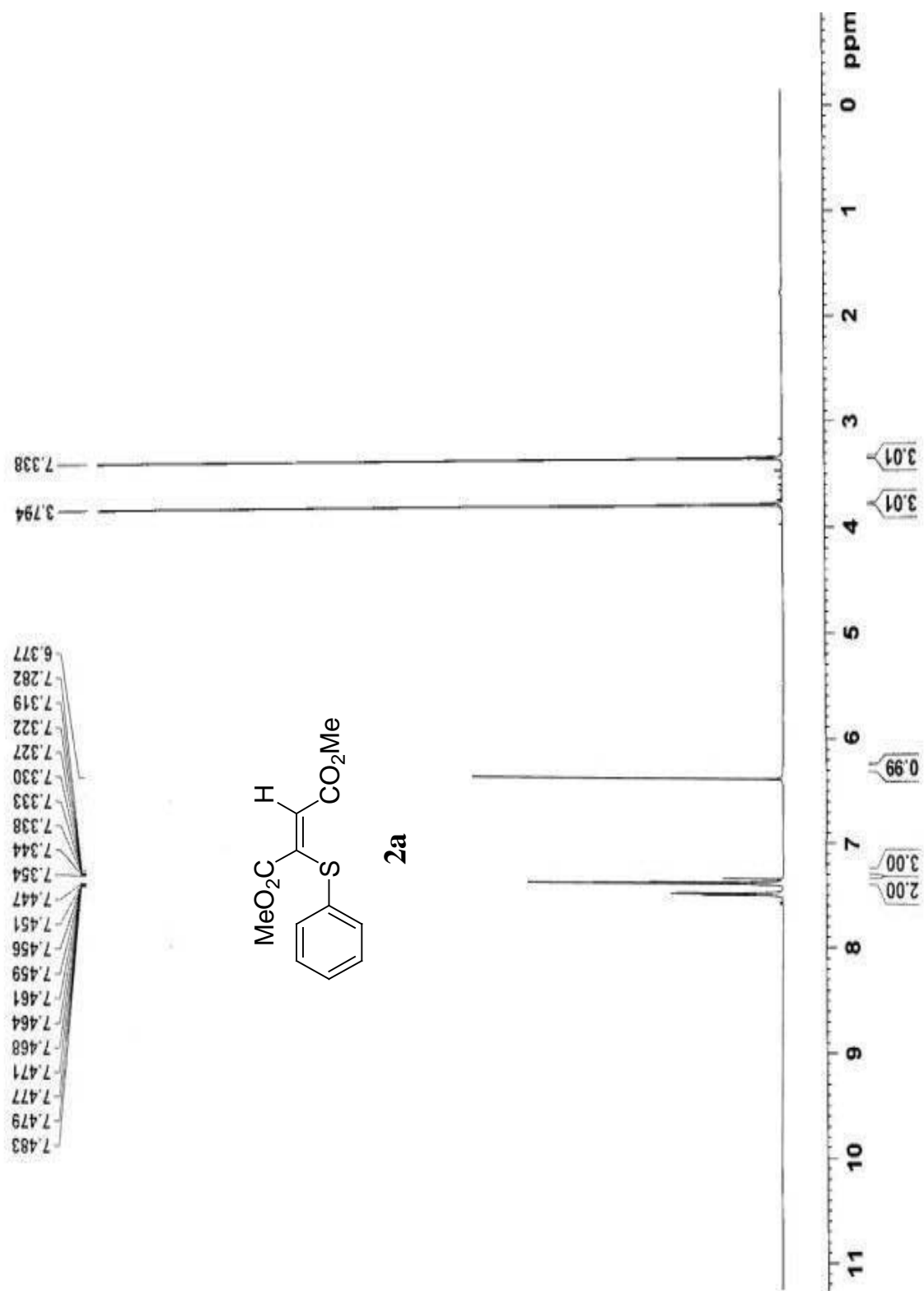
Supplementary Data



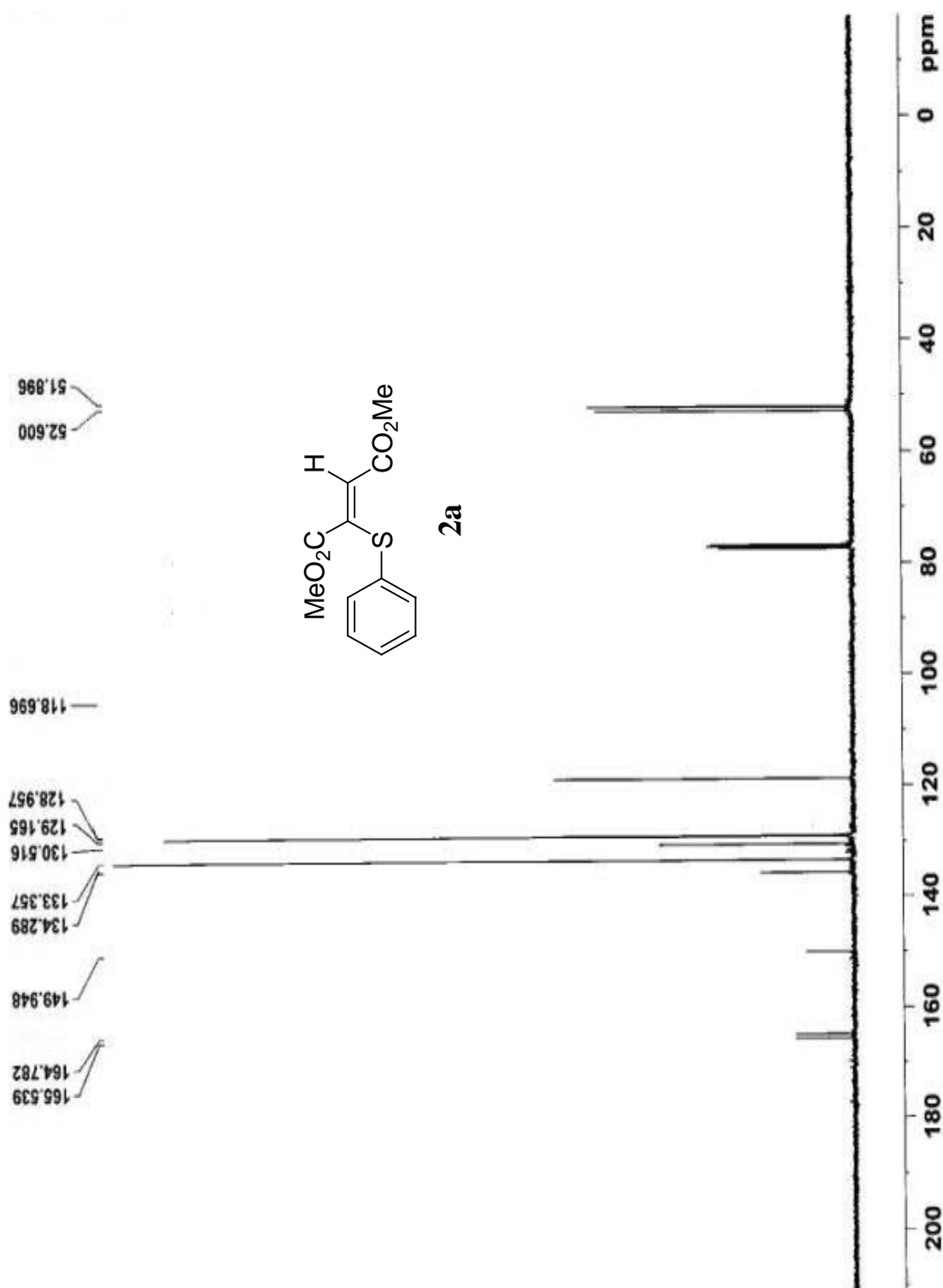
Supplementary Data



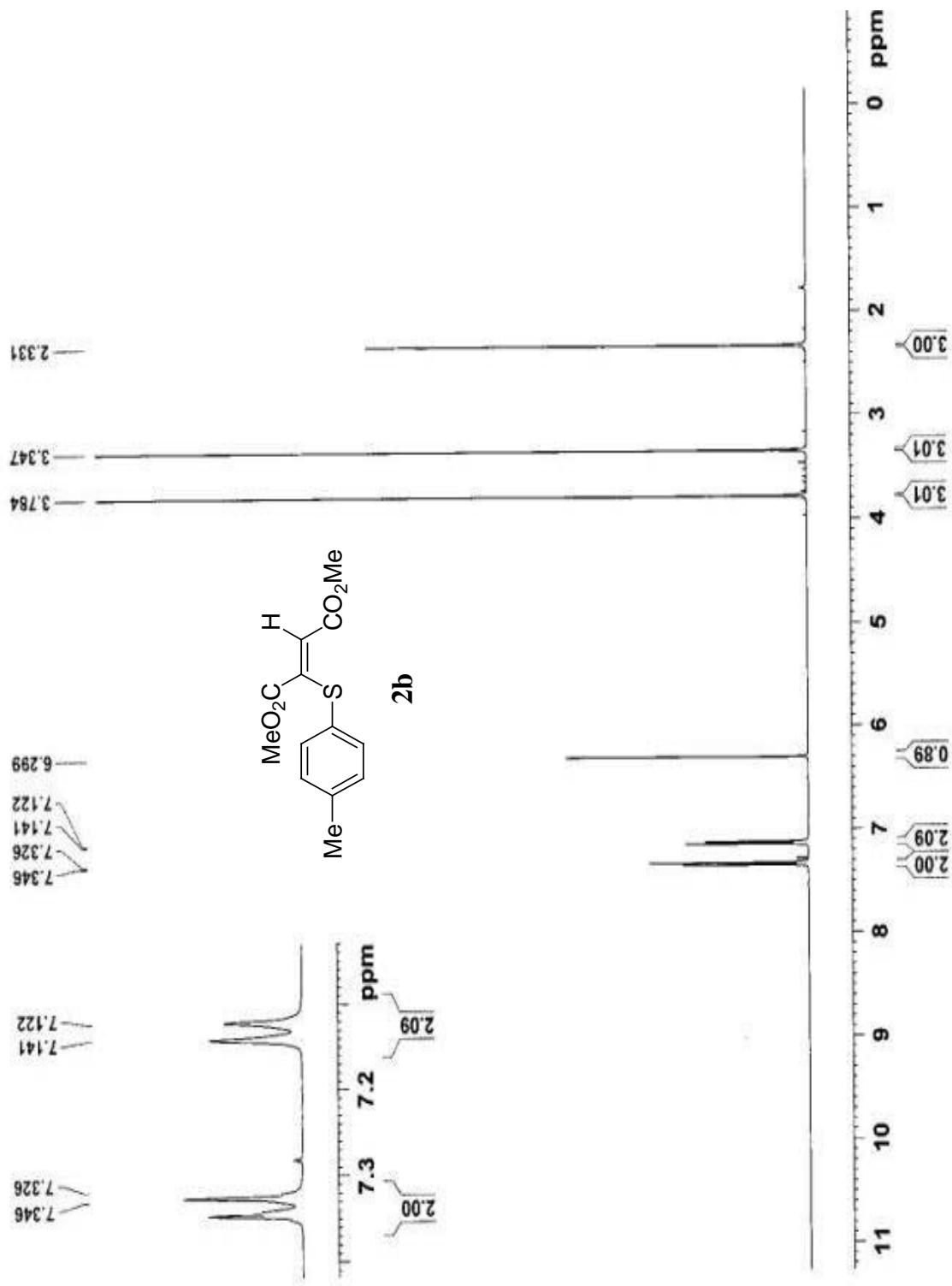
Supplementary Data



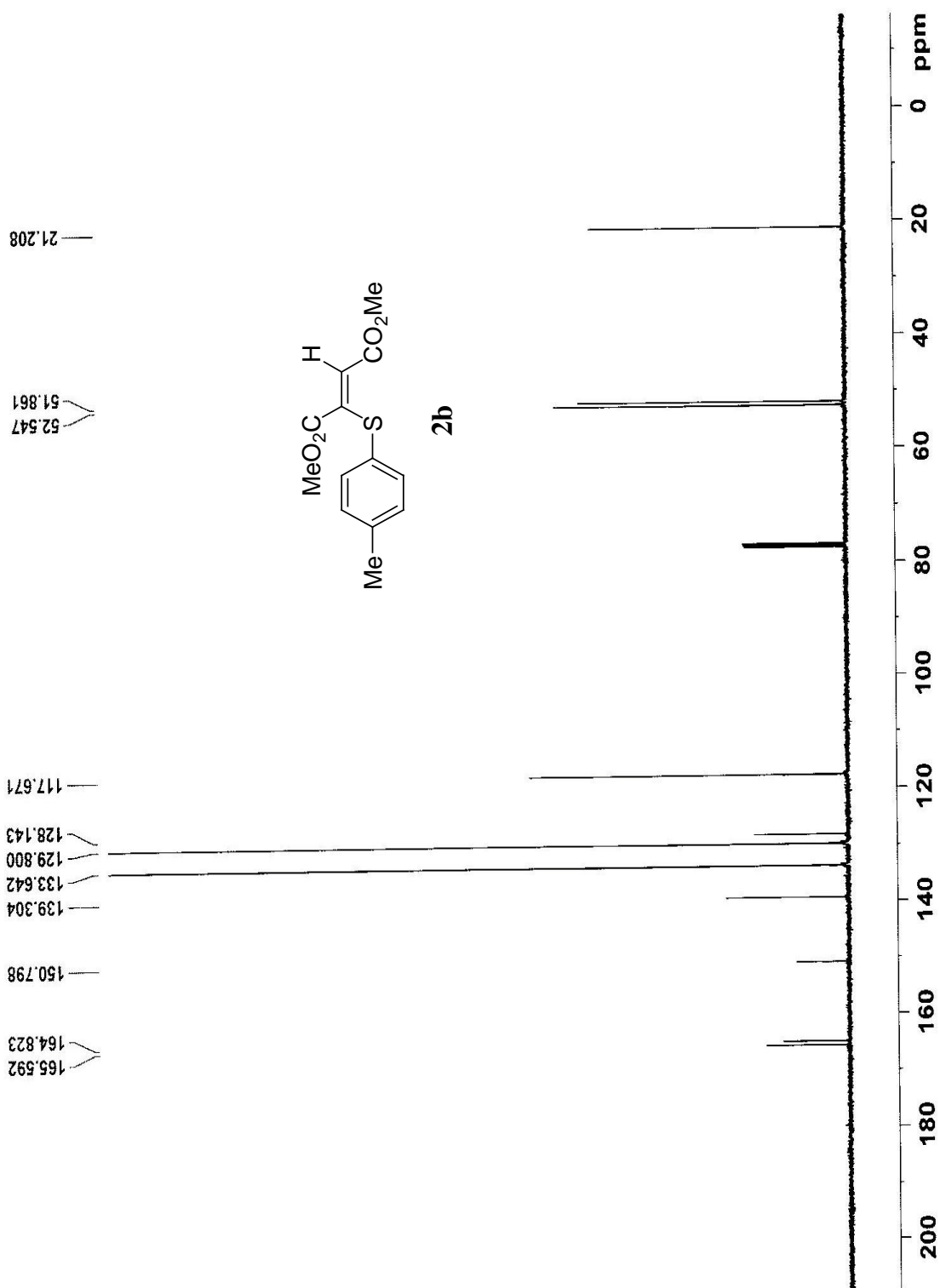
Supplementary Data



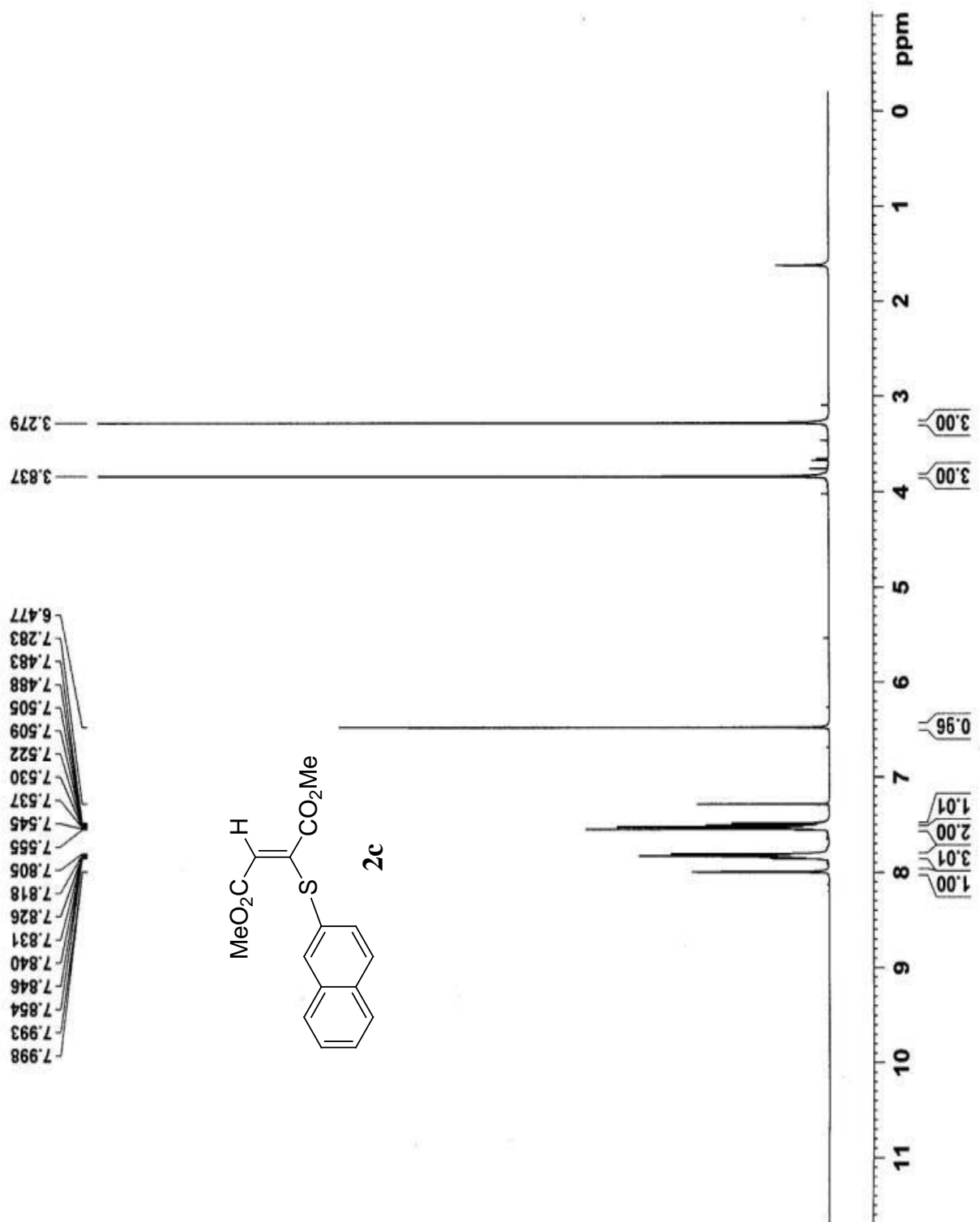
Supplementary Data



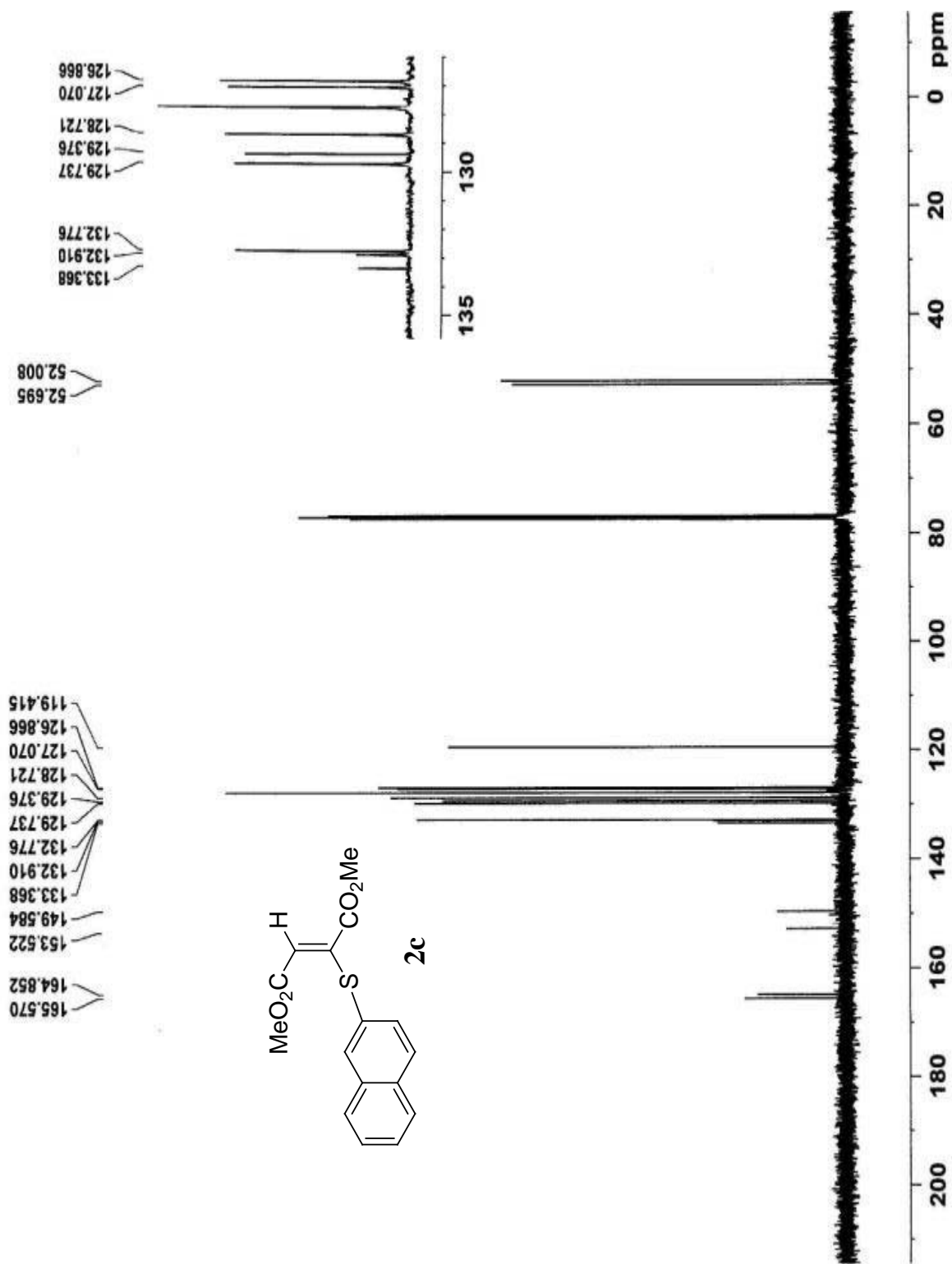
Supplementary Data



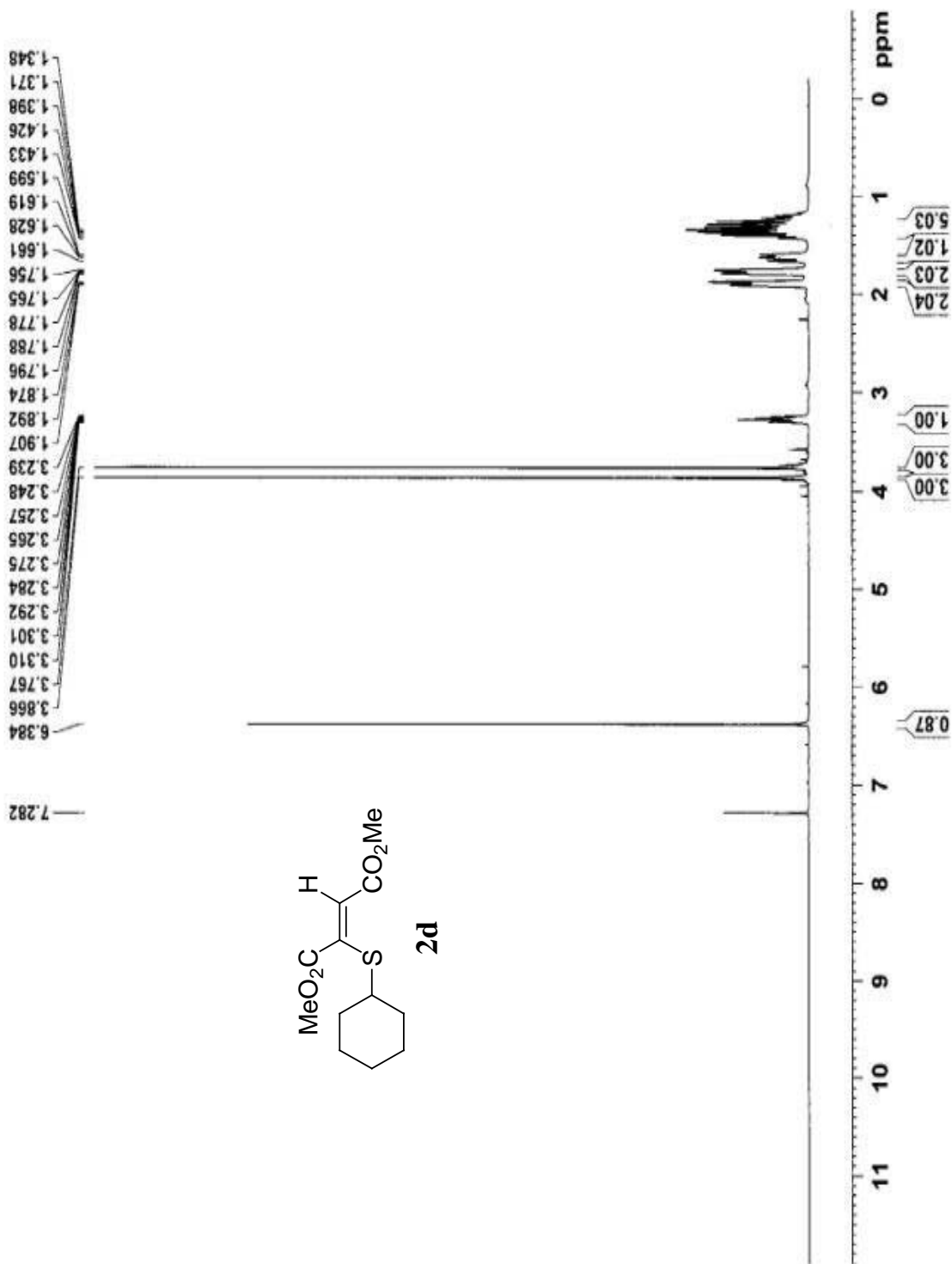
Supplementary Data



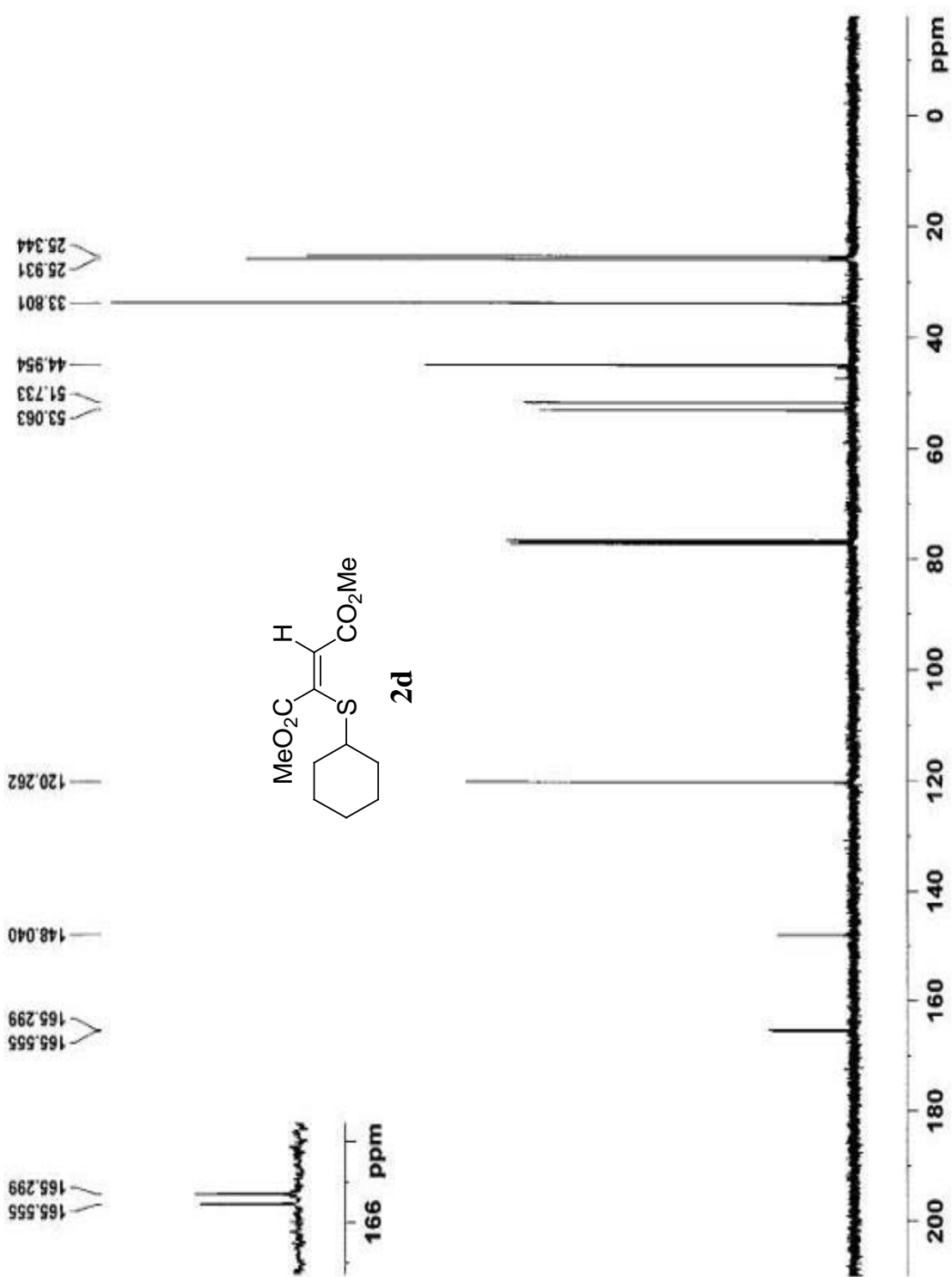
Supplementary Data



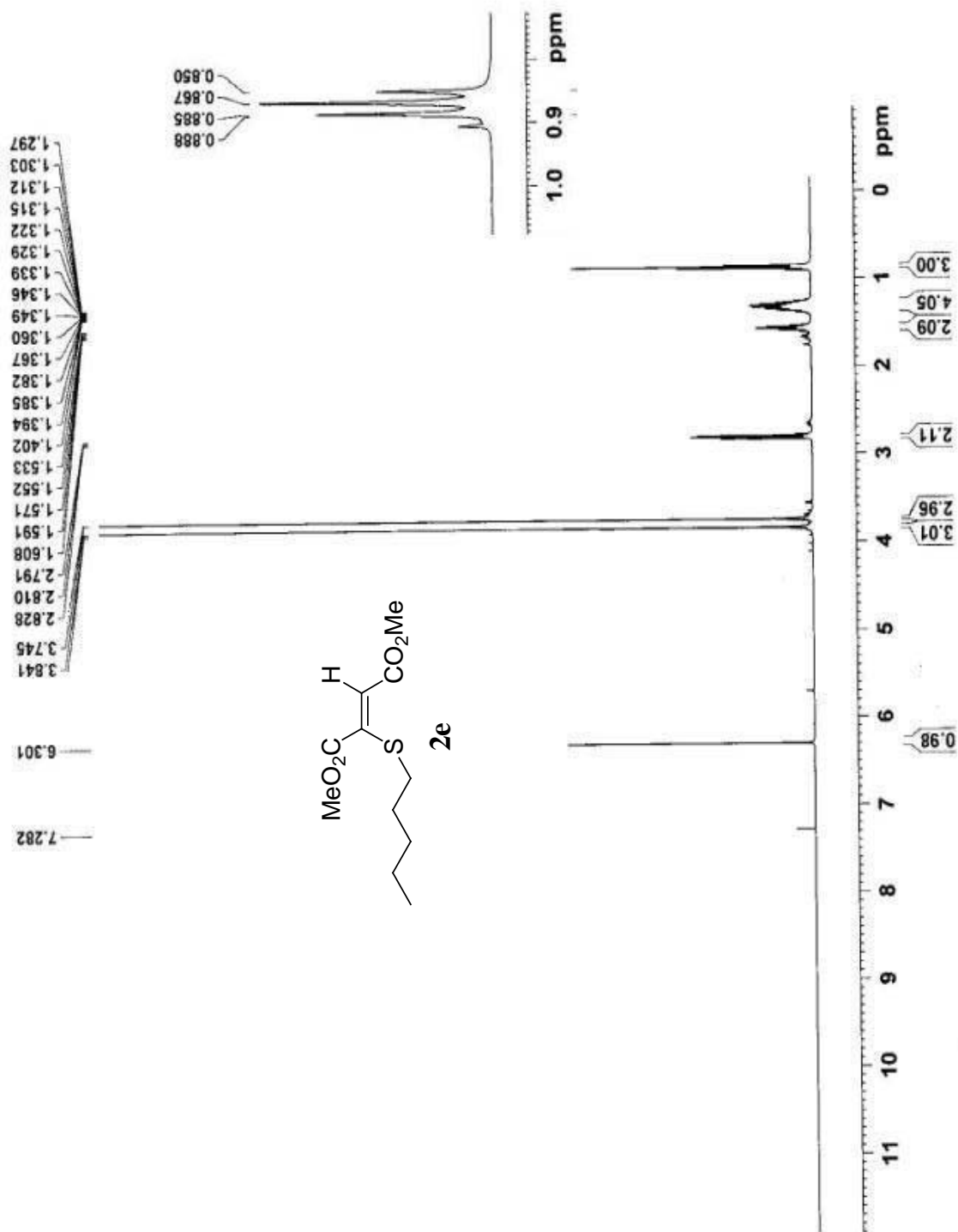
Supplementary Data



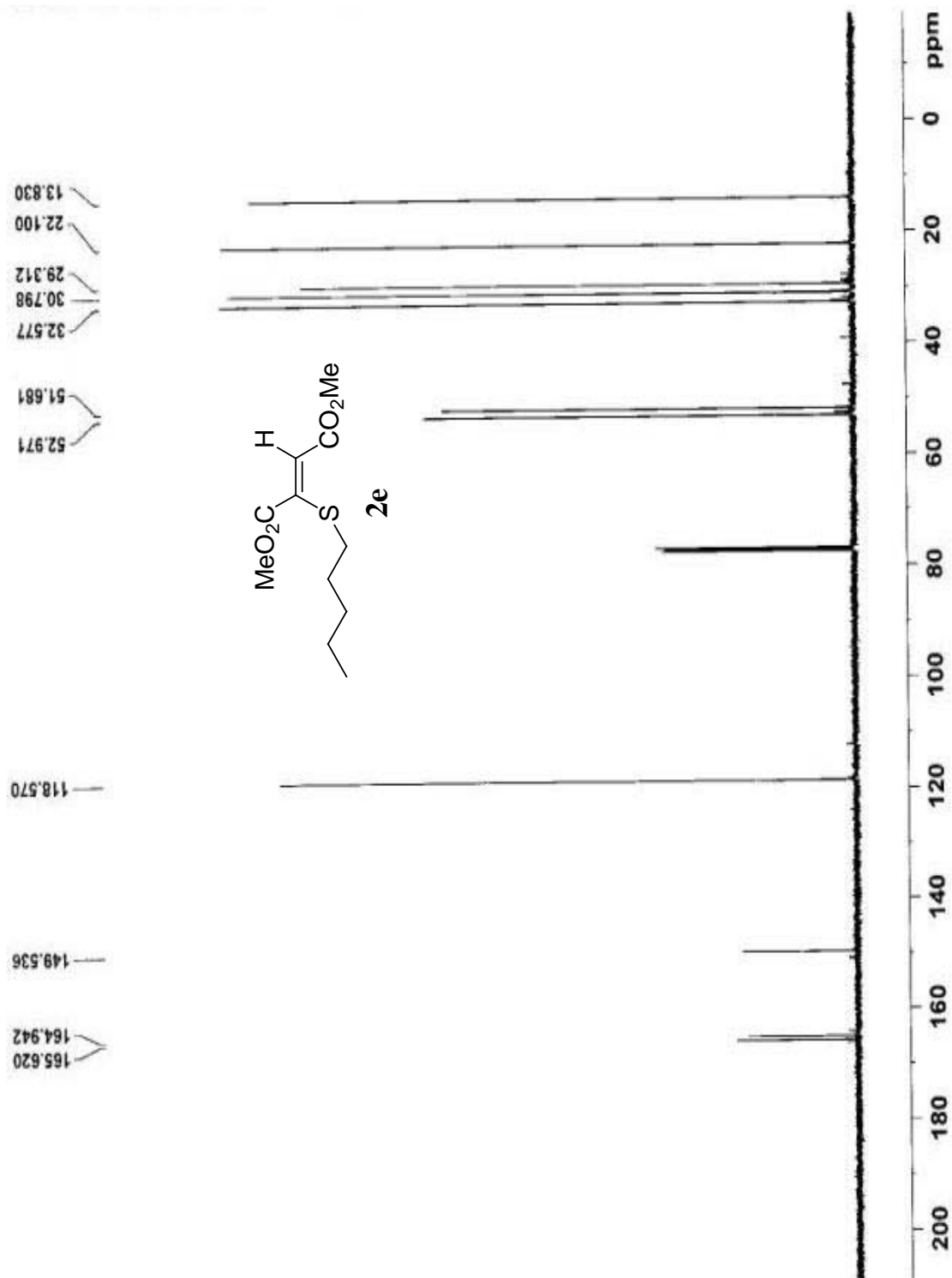
Supplementary Data



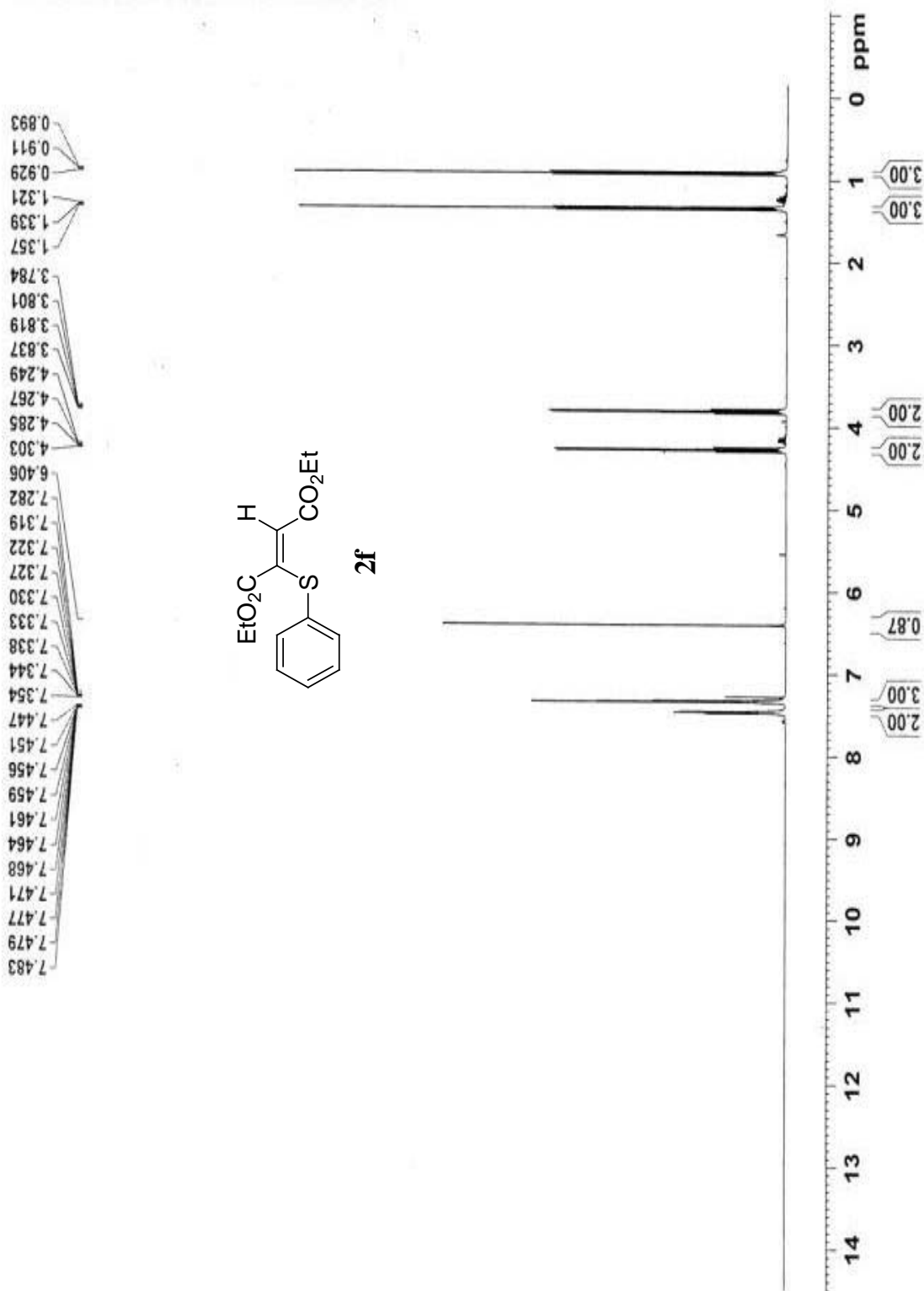
Supplementary Data



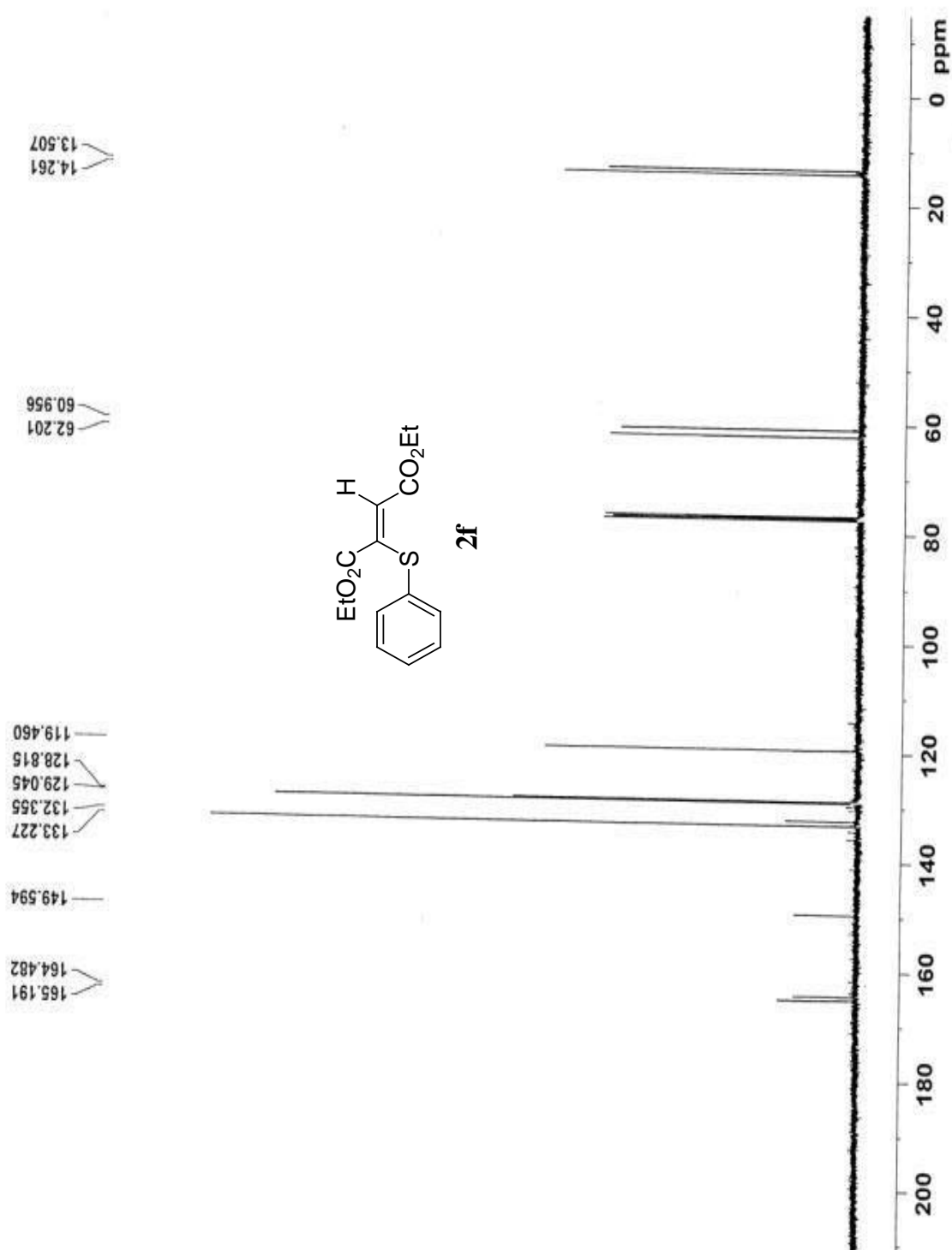
Supplementary Data



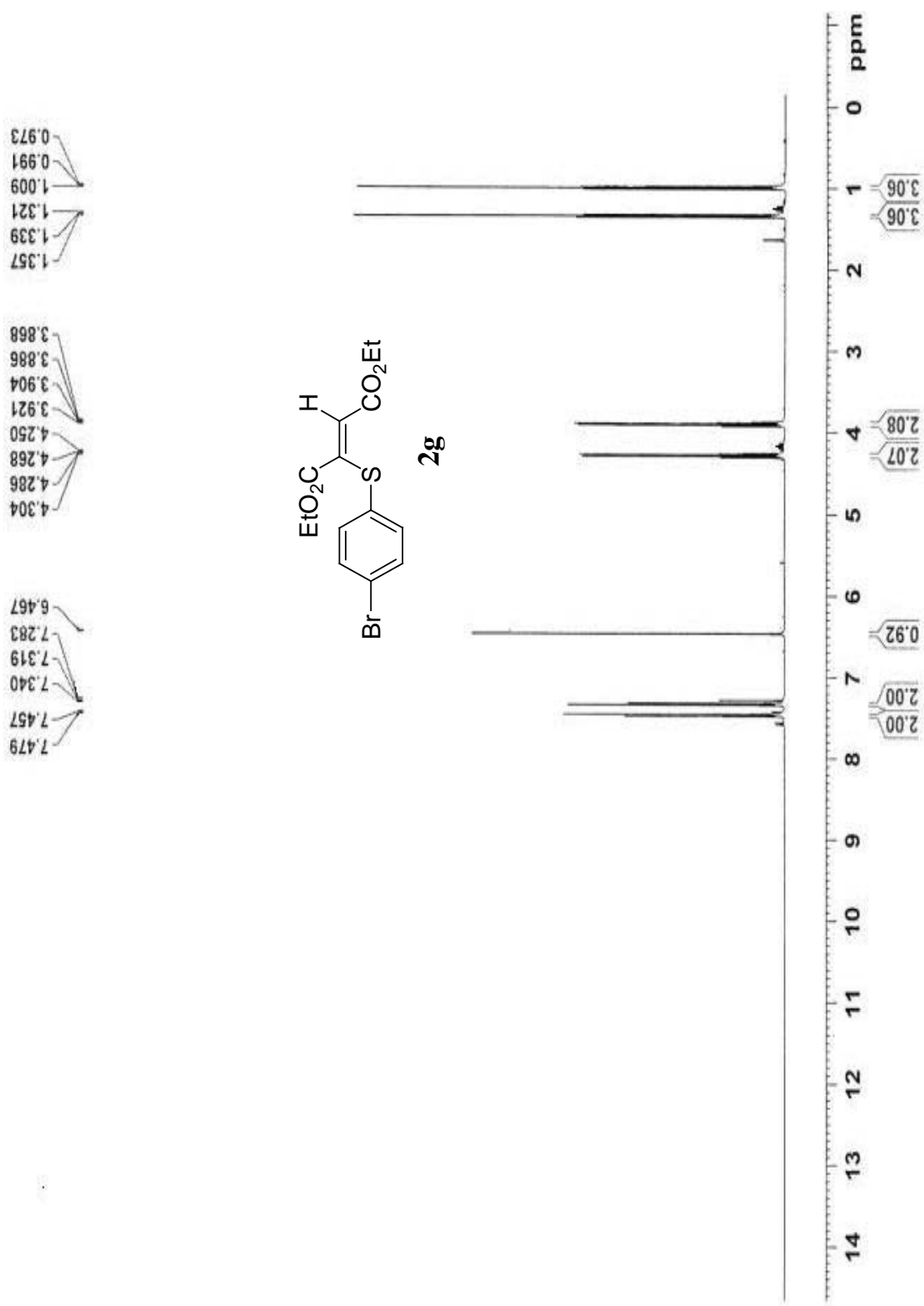
Supplementary Data



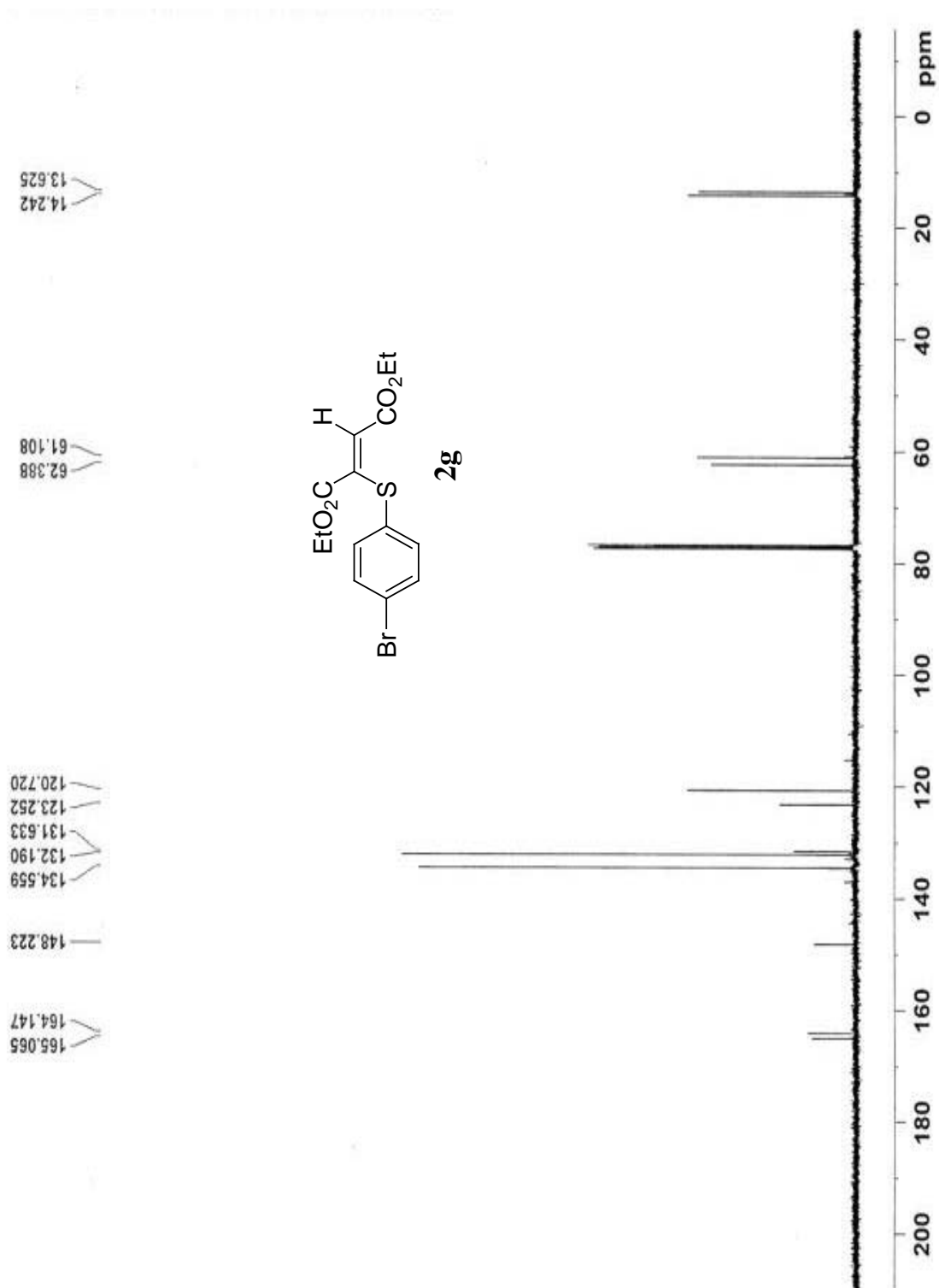
Supplementary Data



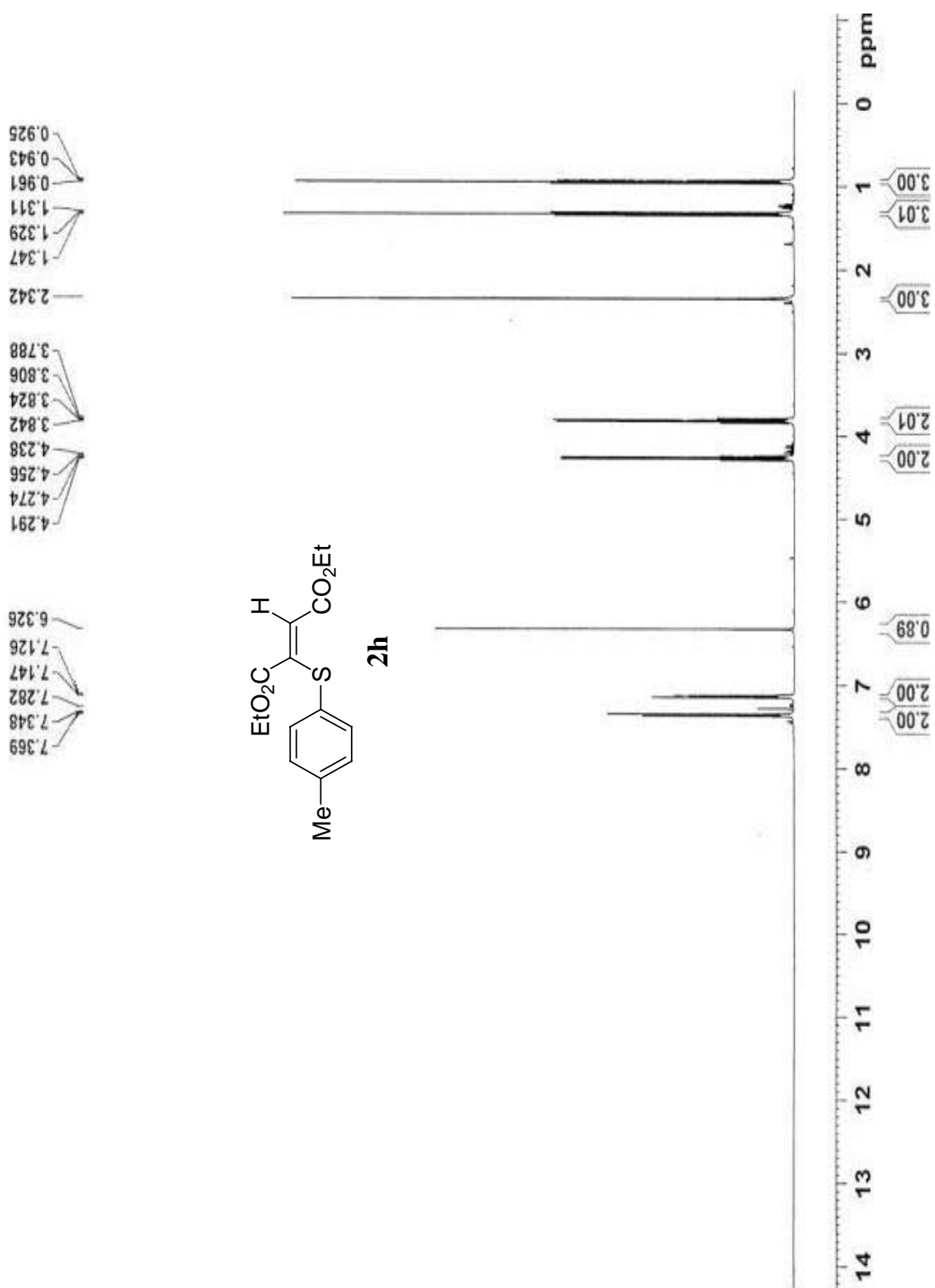
Supplementary Data



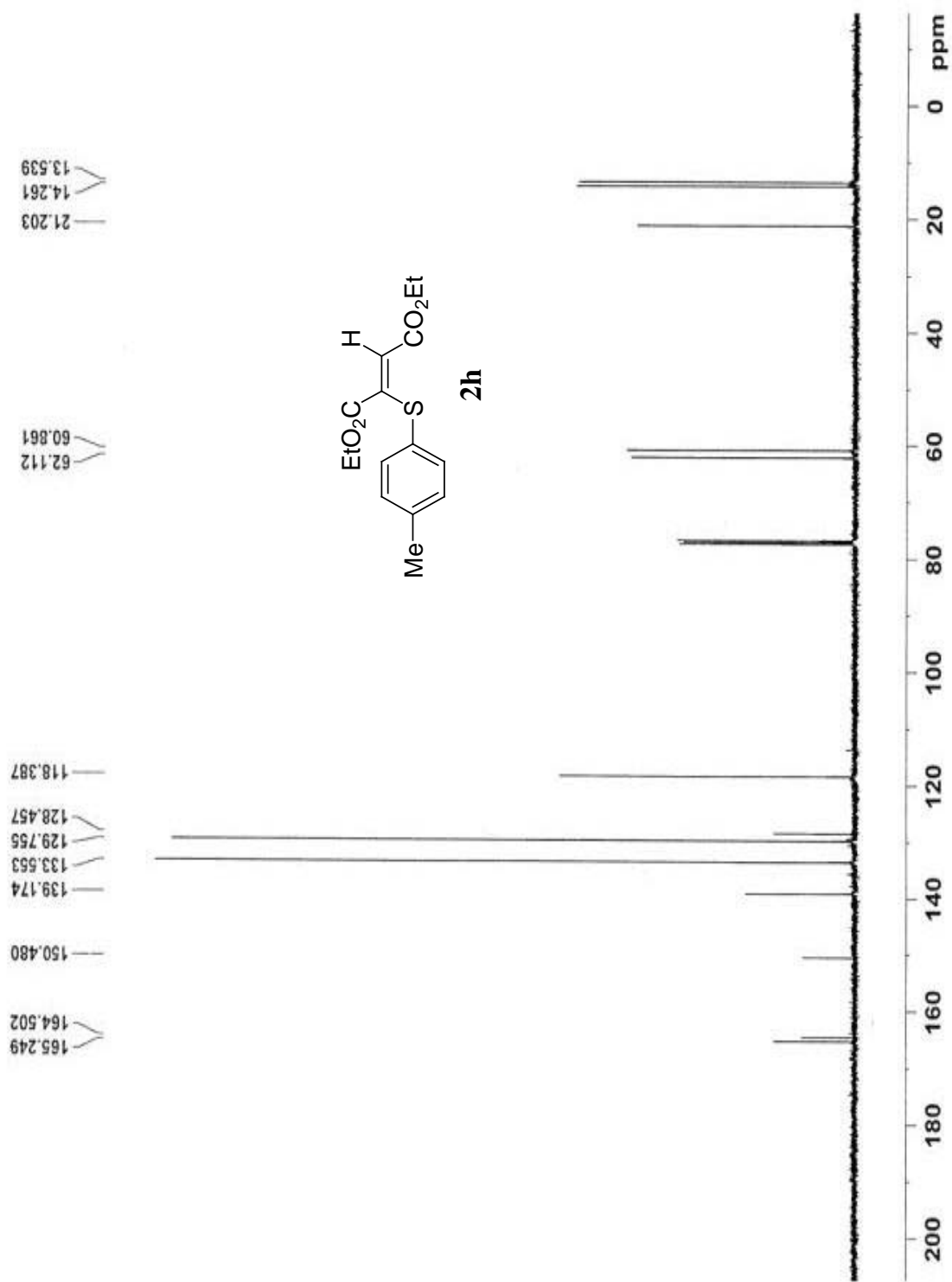
Supplementary Data



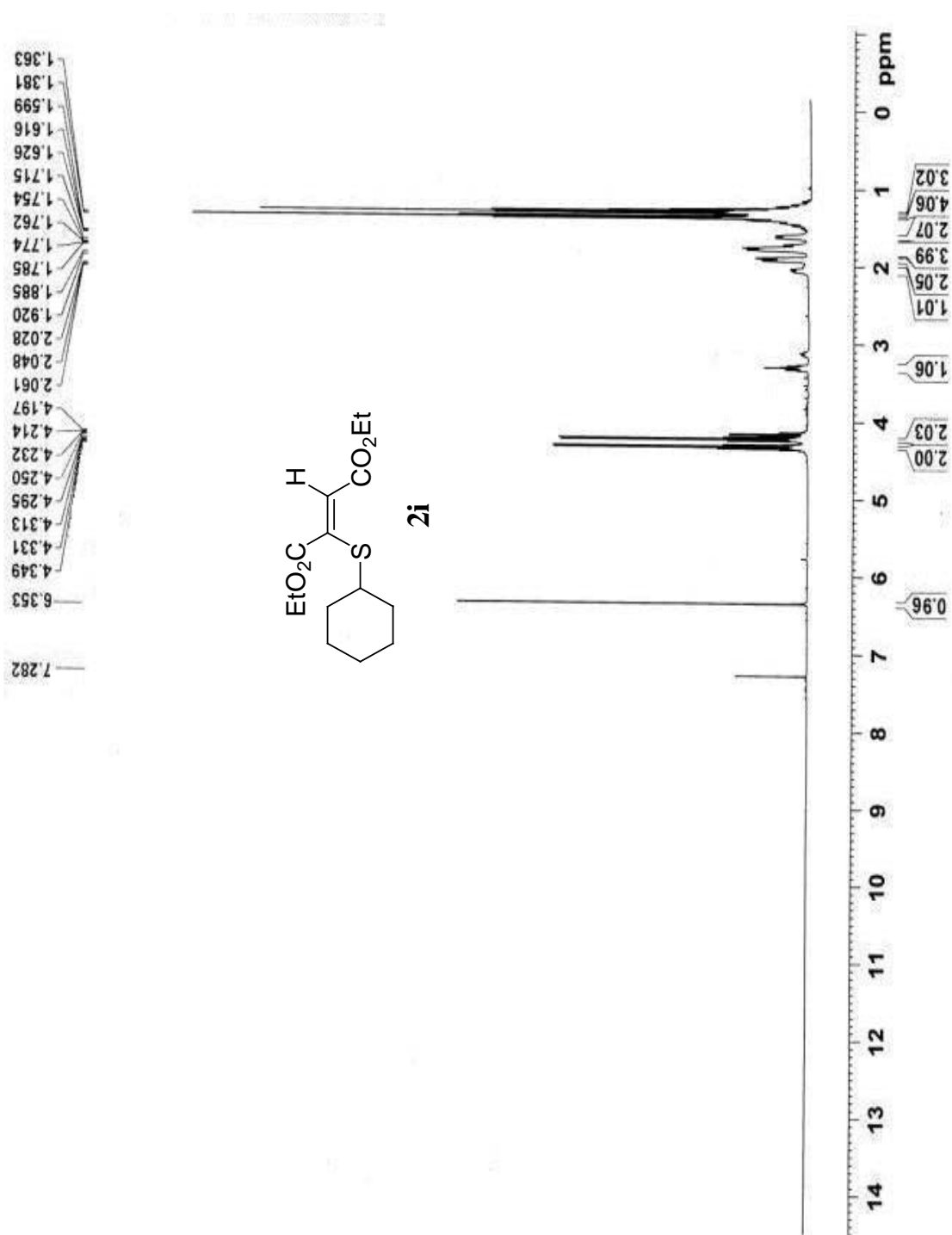
Supplementary Data



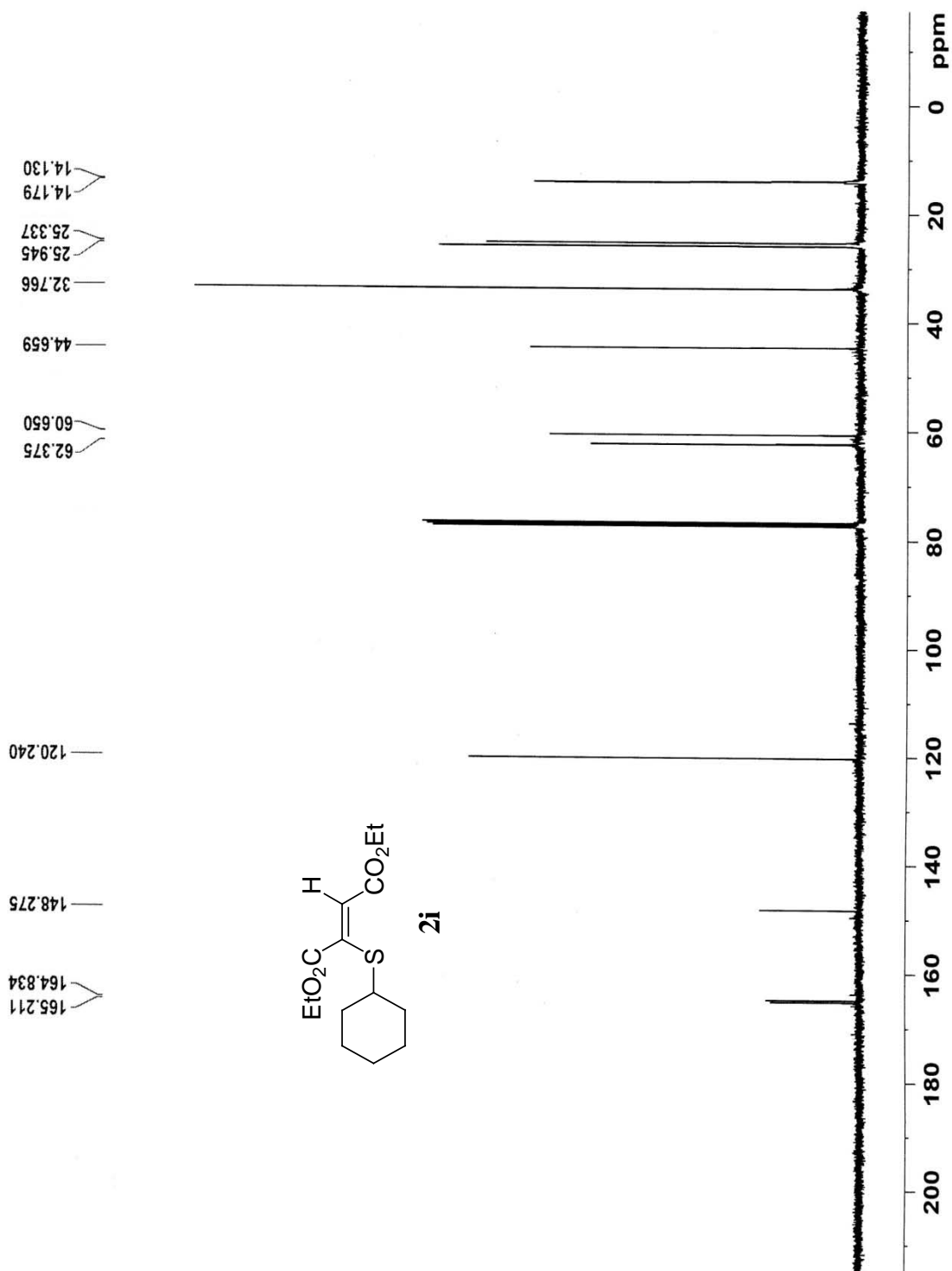
Supplementary Data



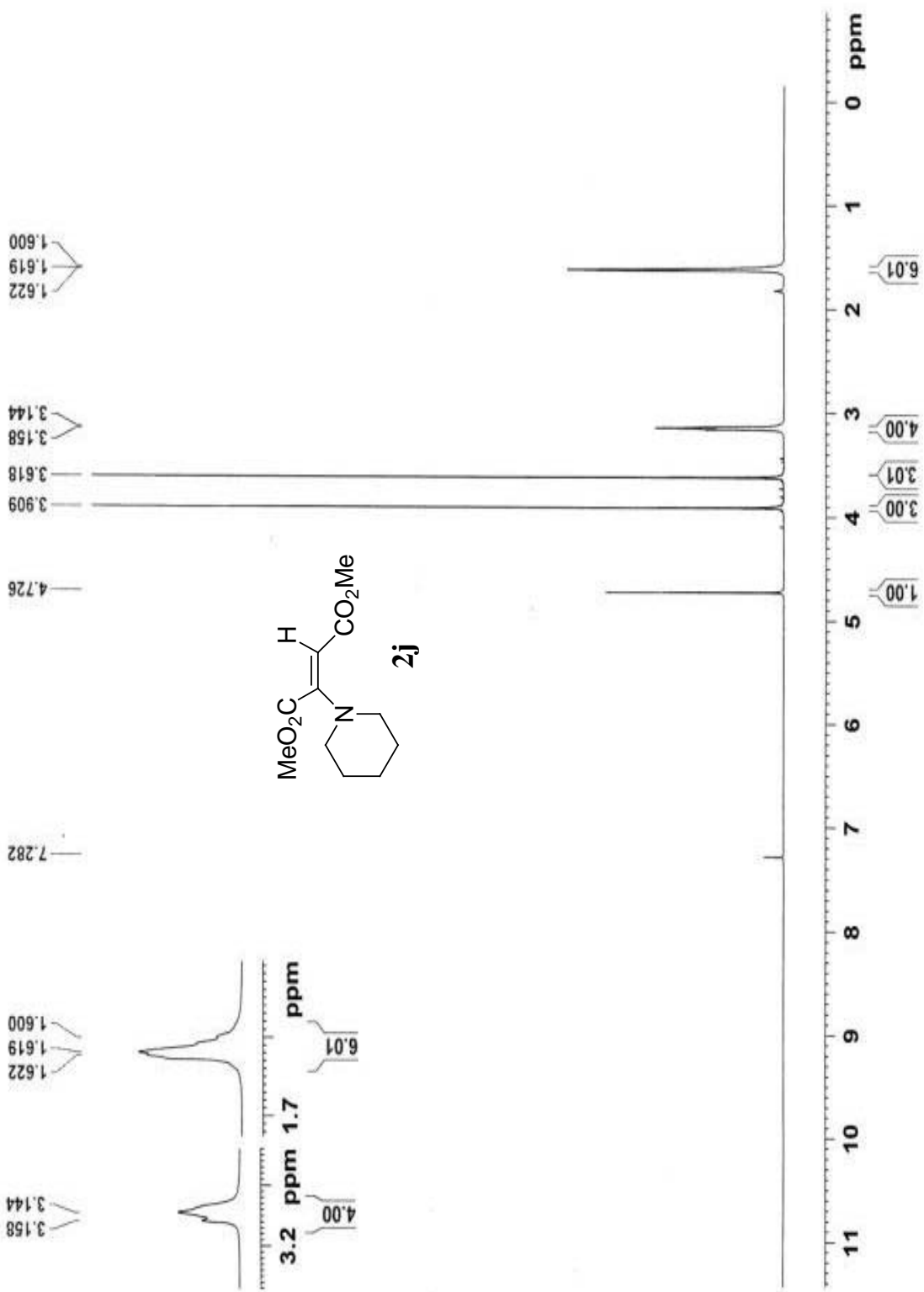
Supplementary Data



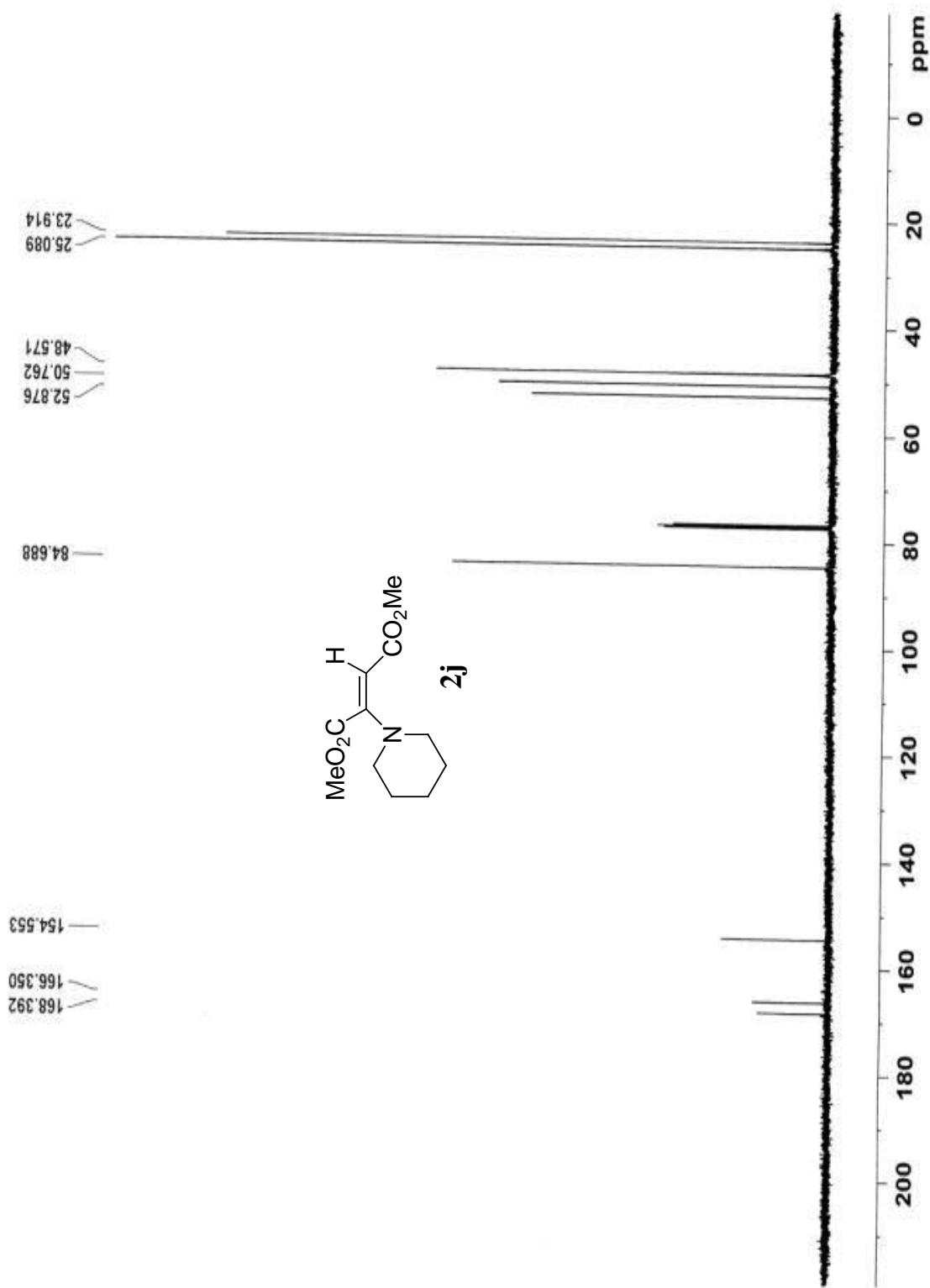
Supplementary Data



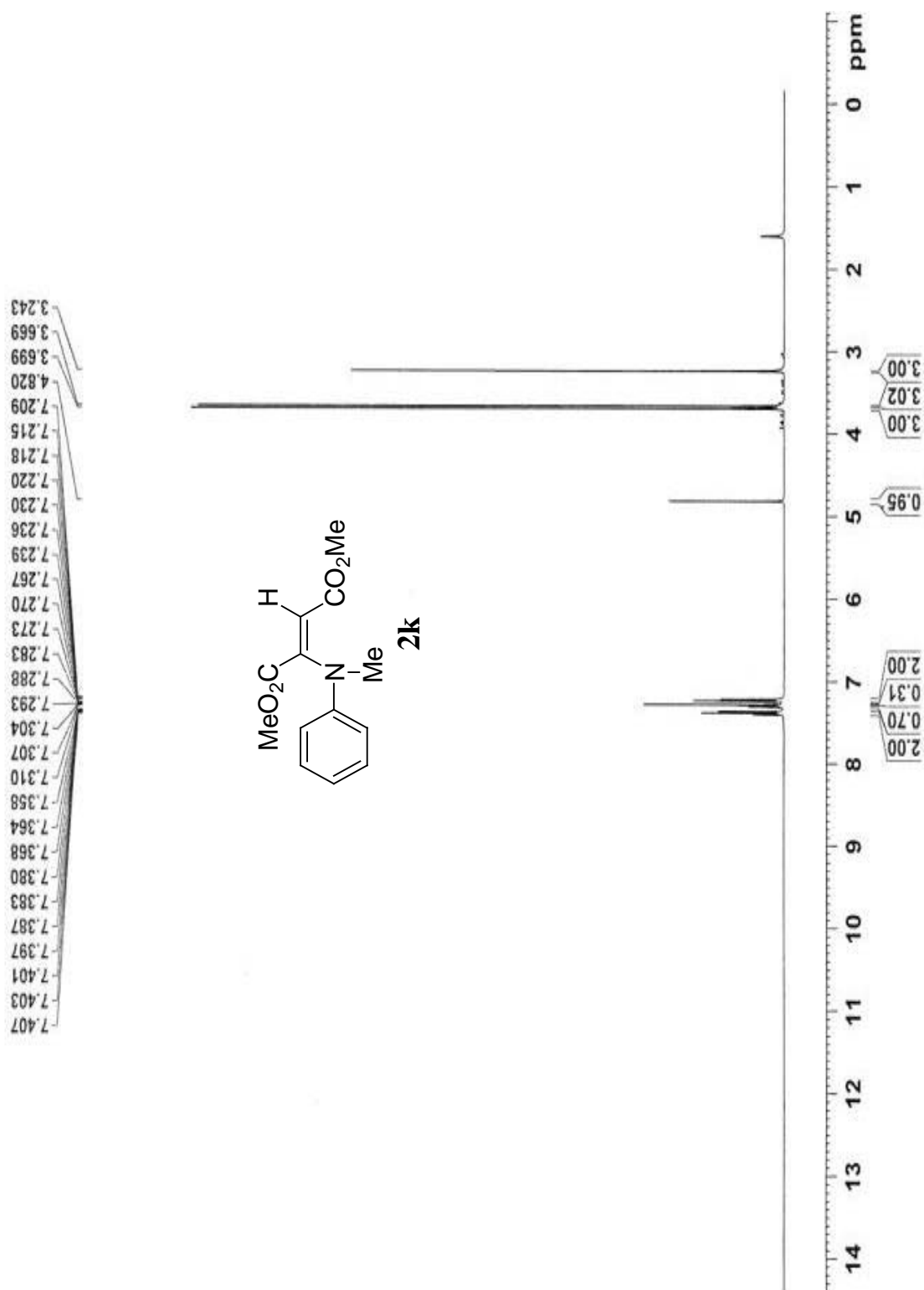
Supplementary Data



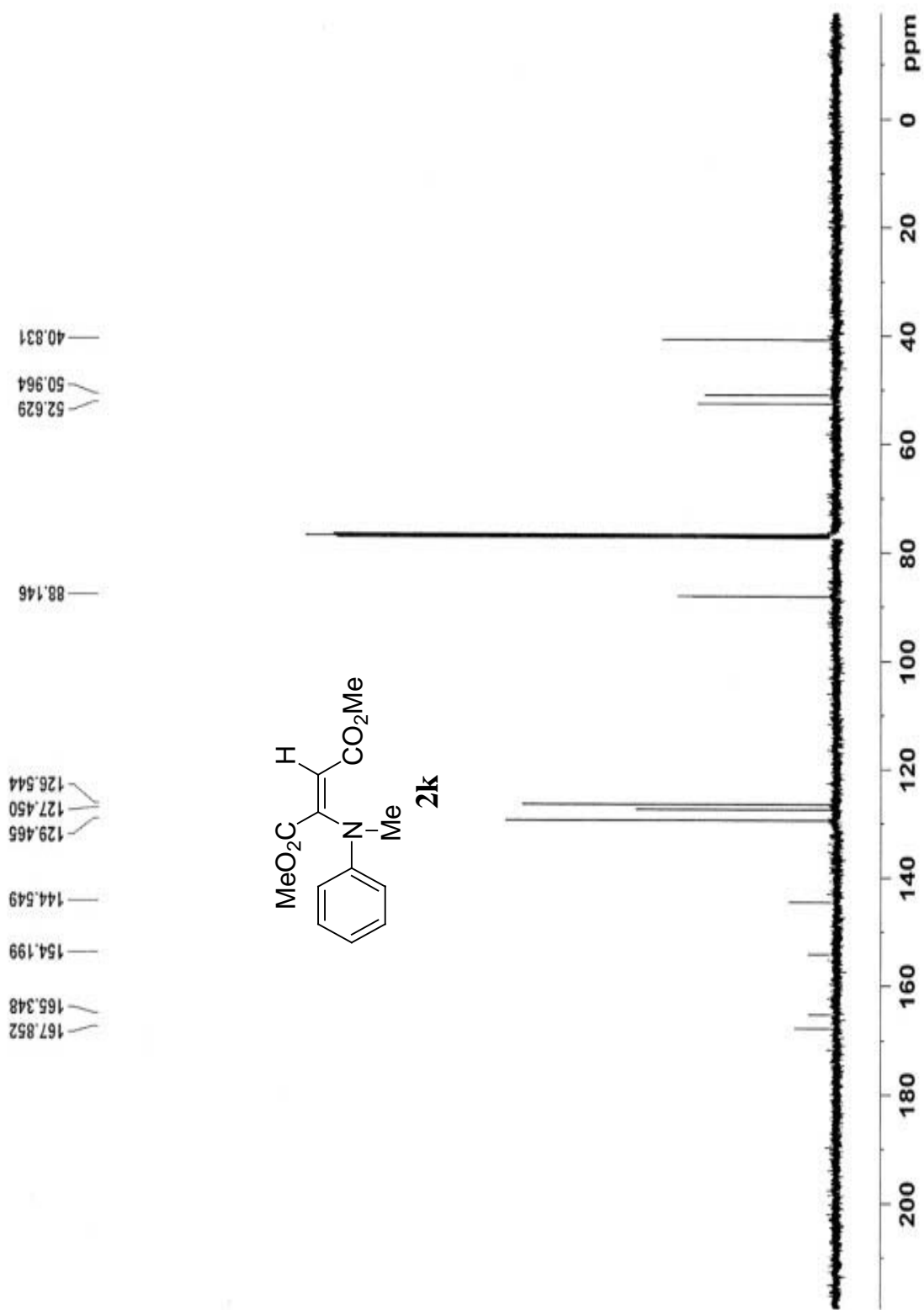
Supplementary Data



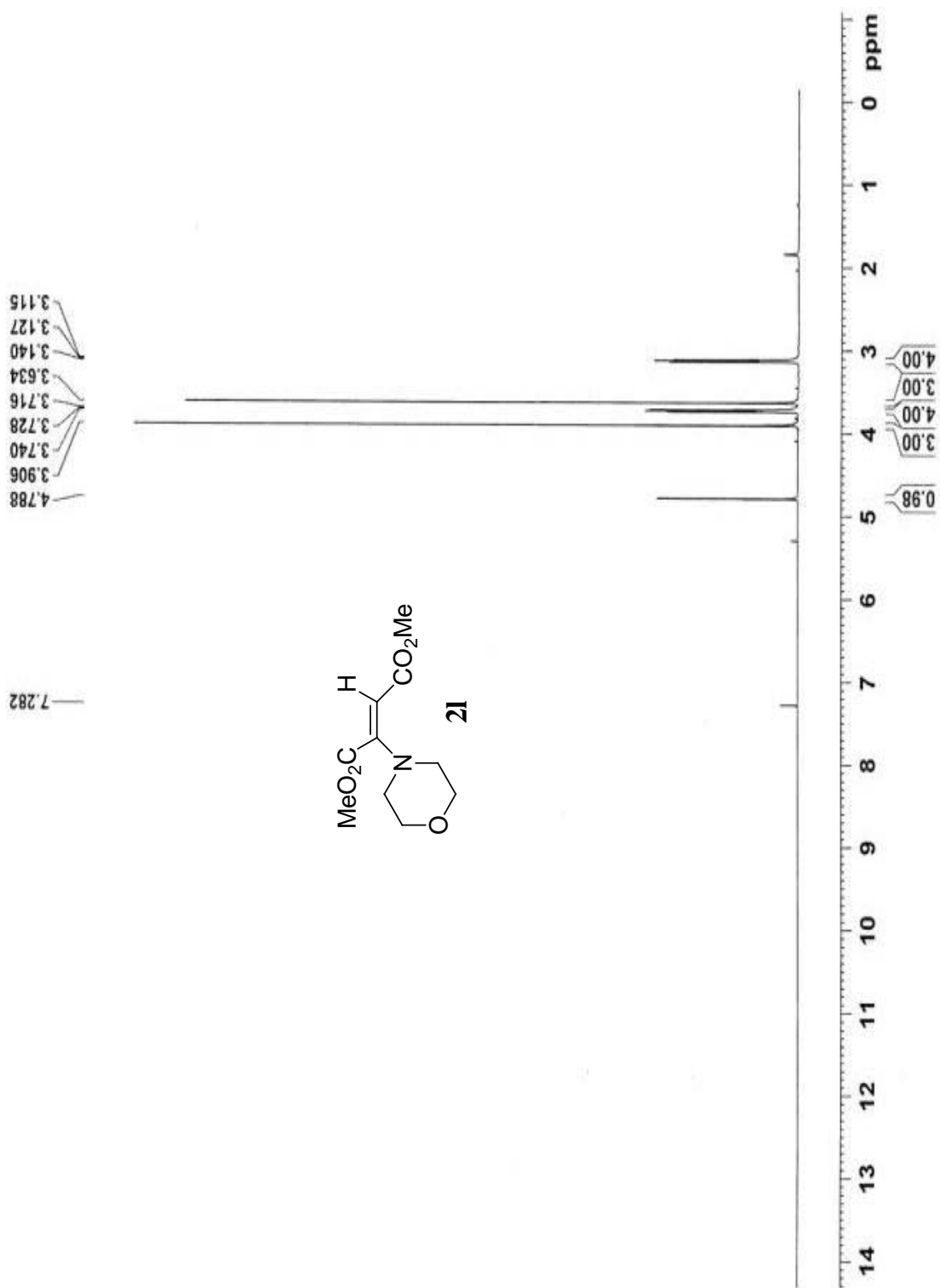
Supplementary Data



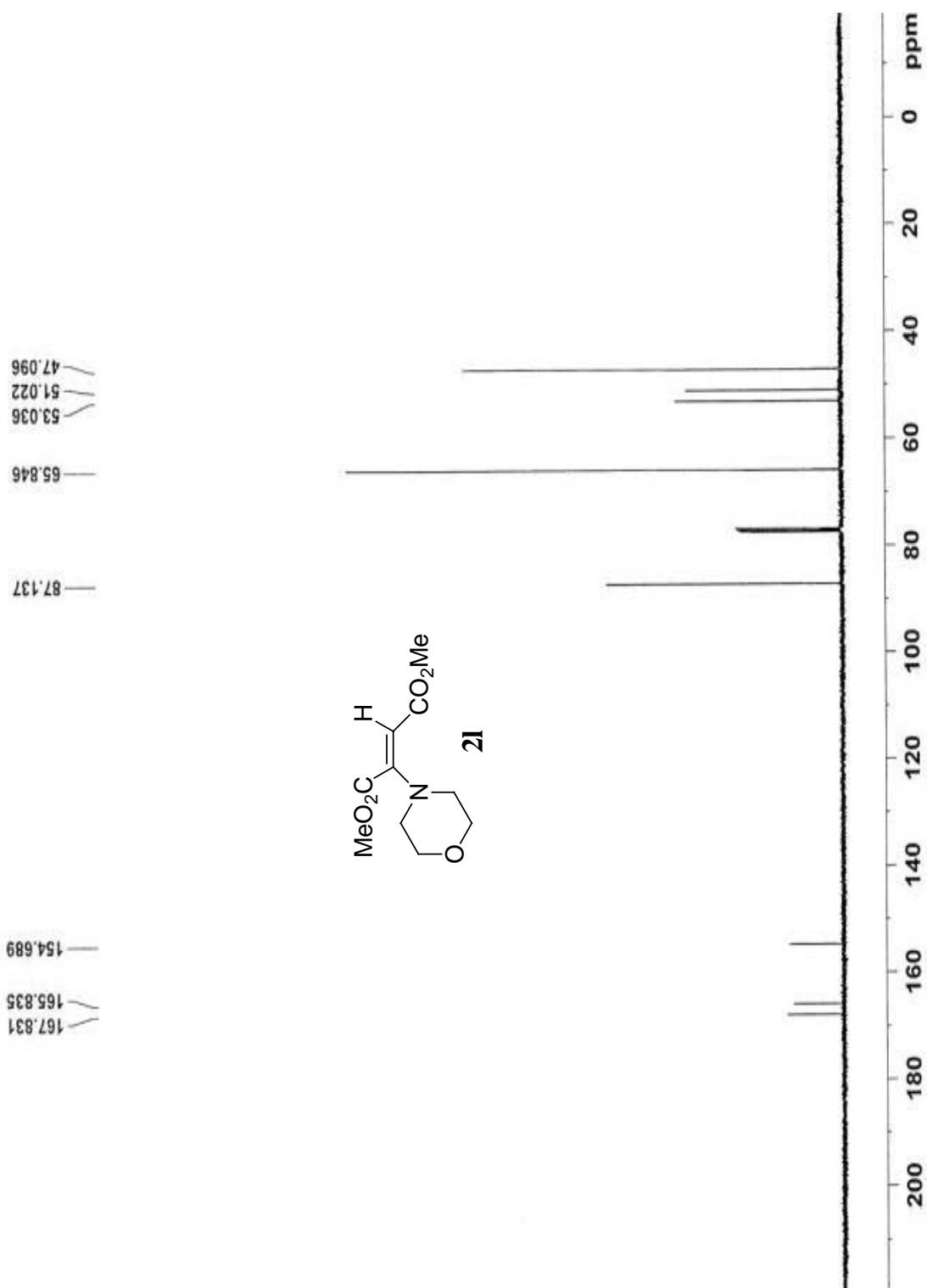
Supplementary Data



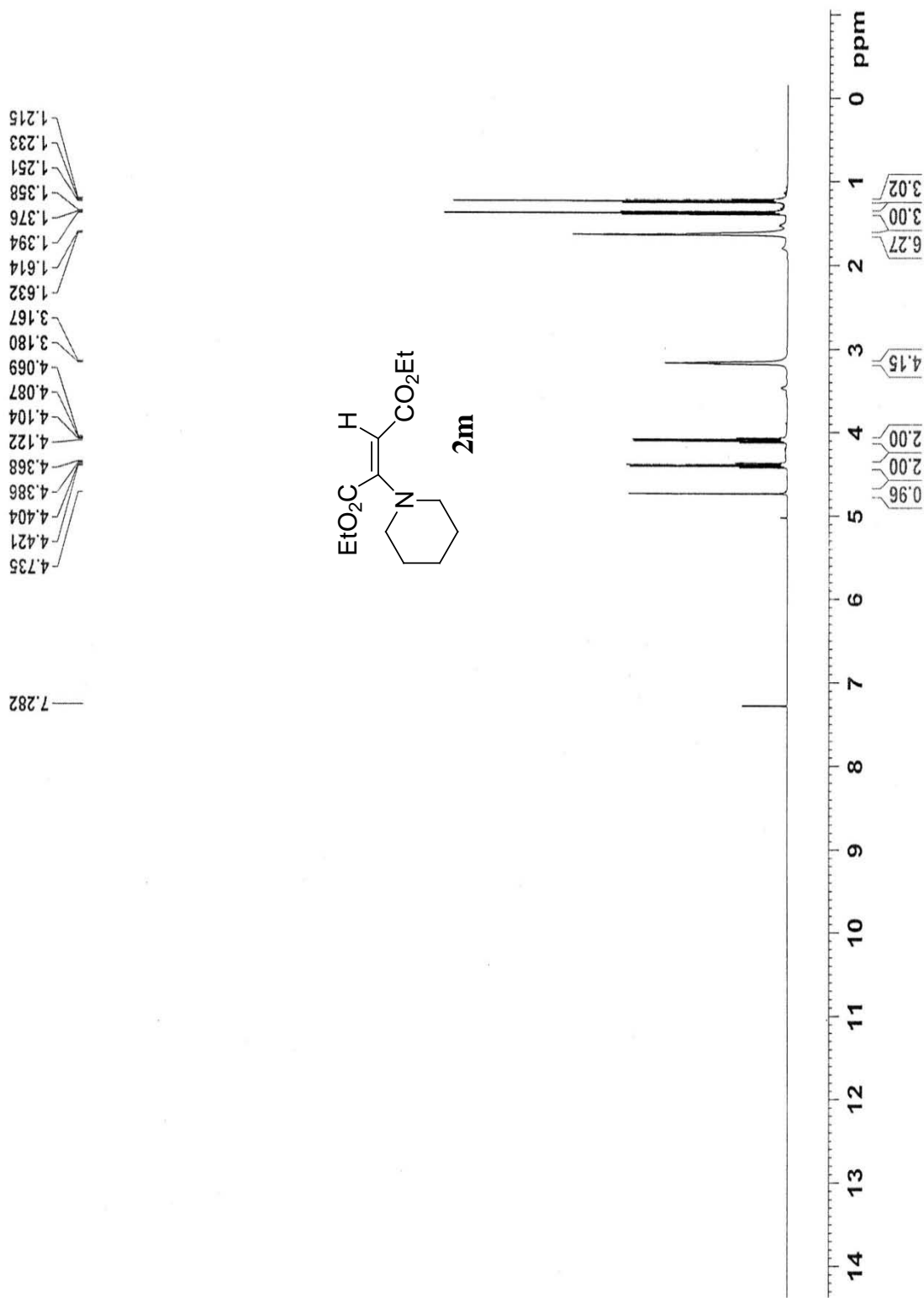
Supplementary Data



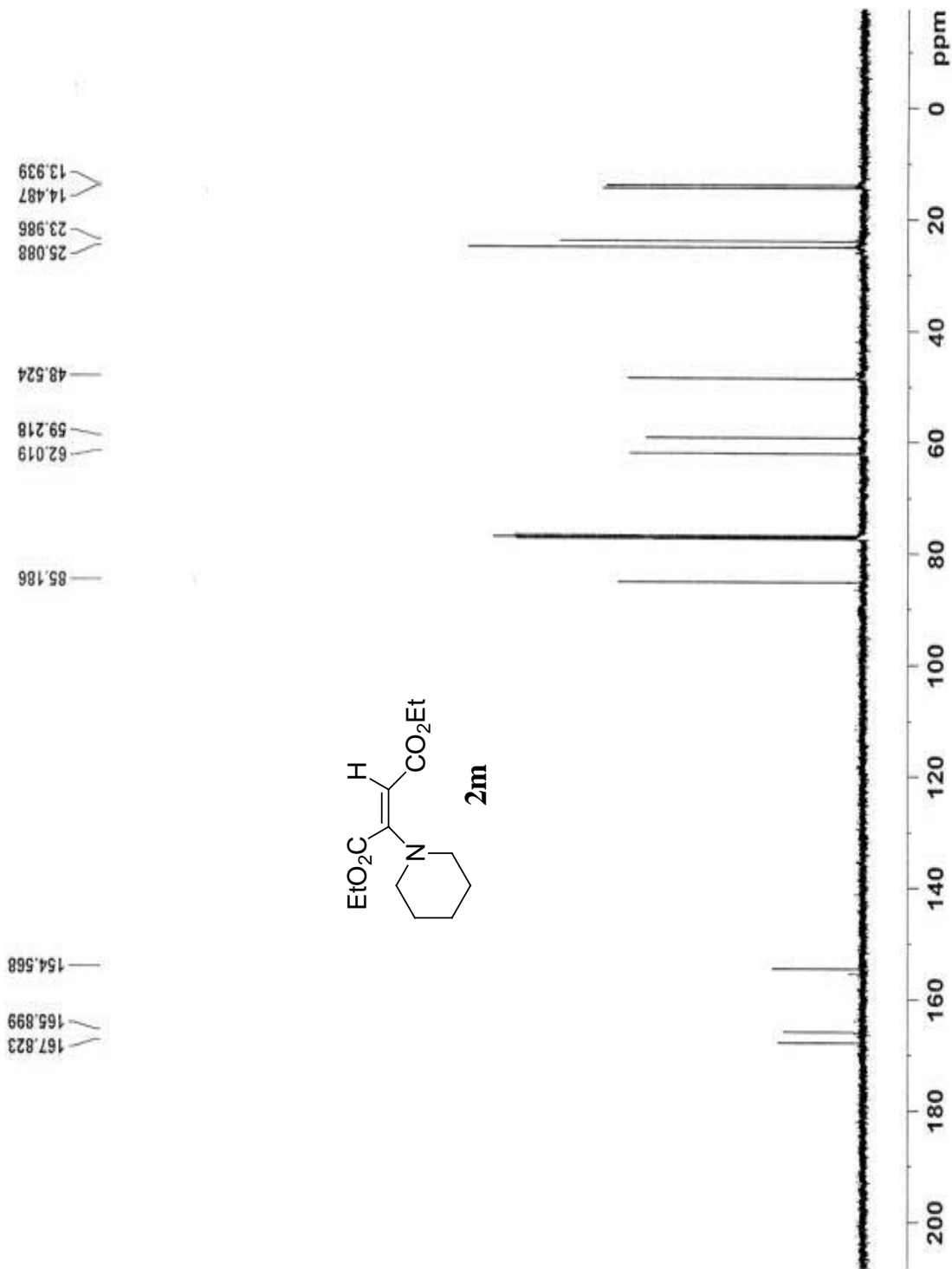
Supplementary Data



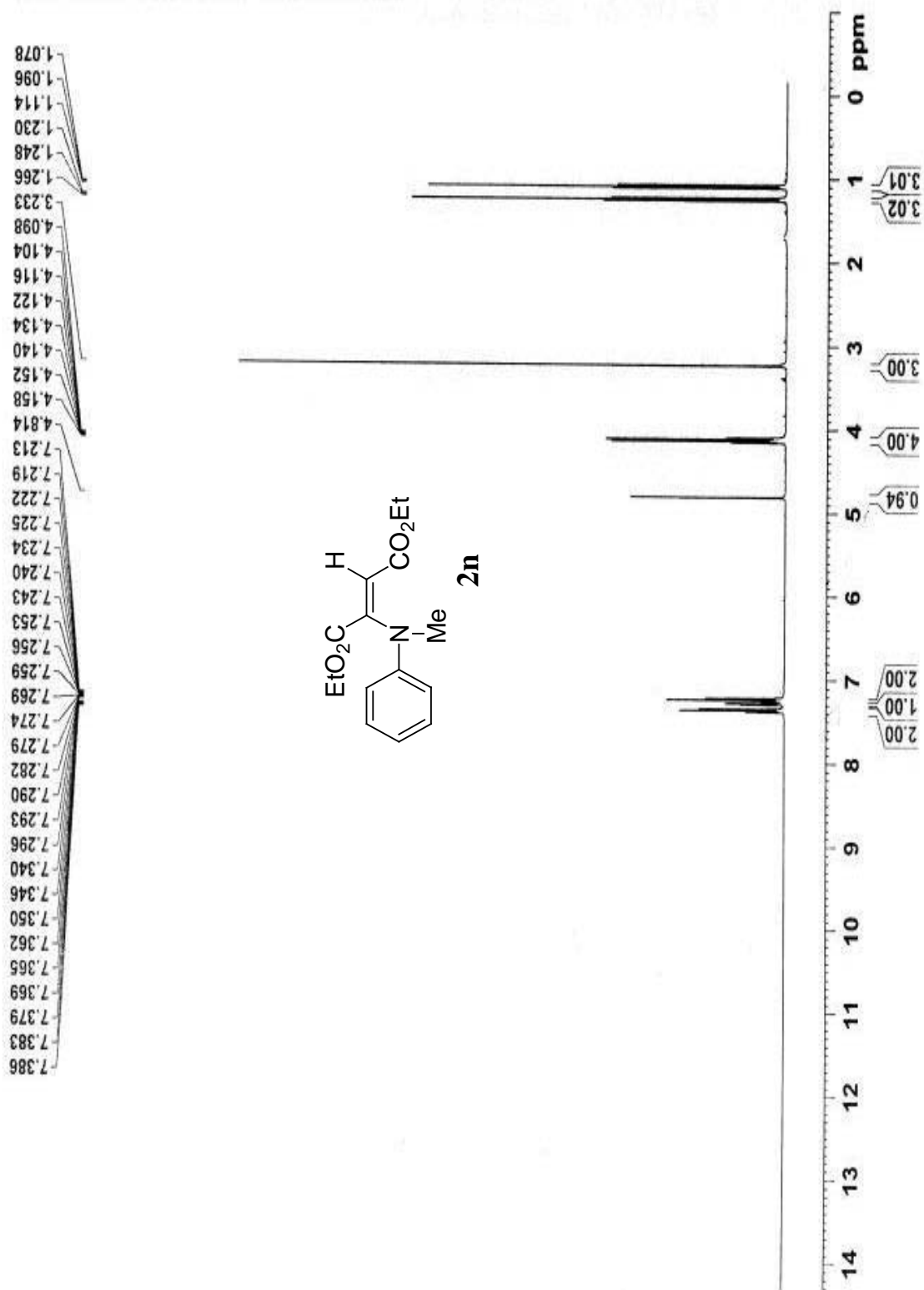
Supplementary Data



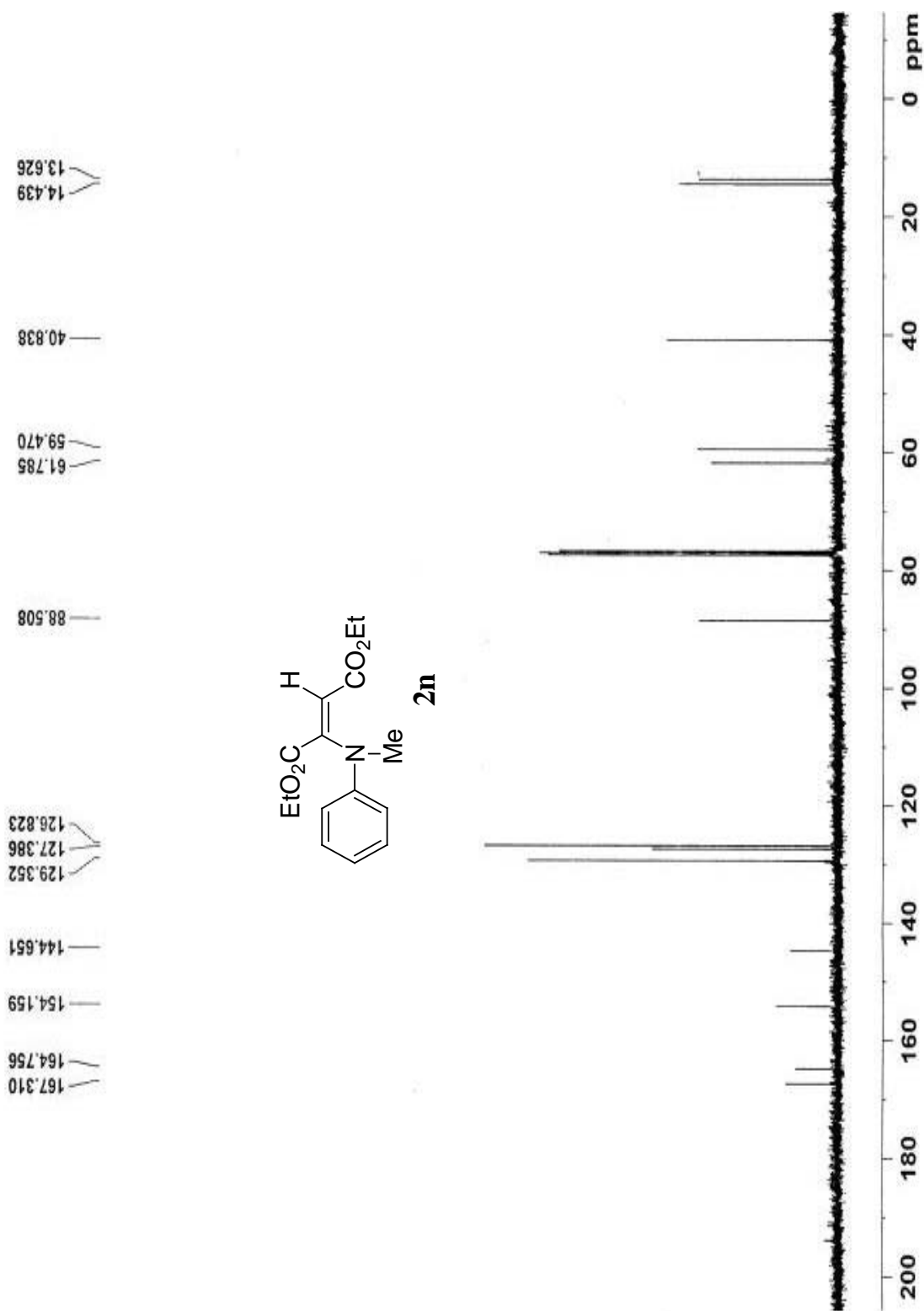
Supplementary Data



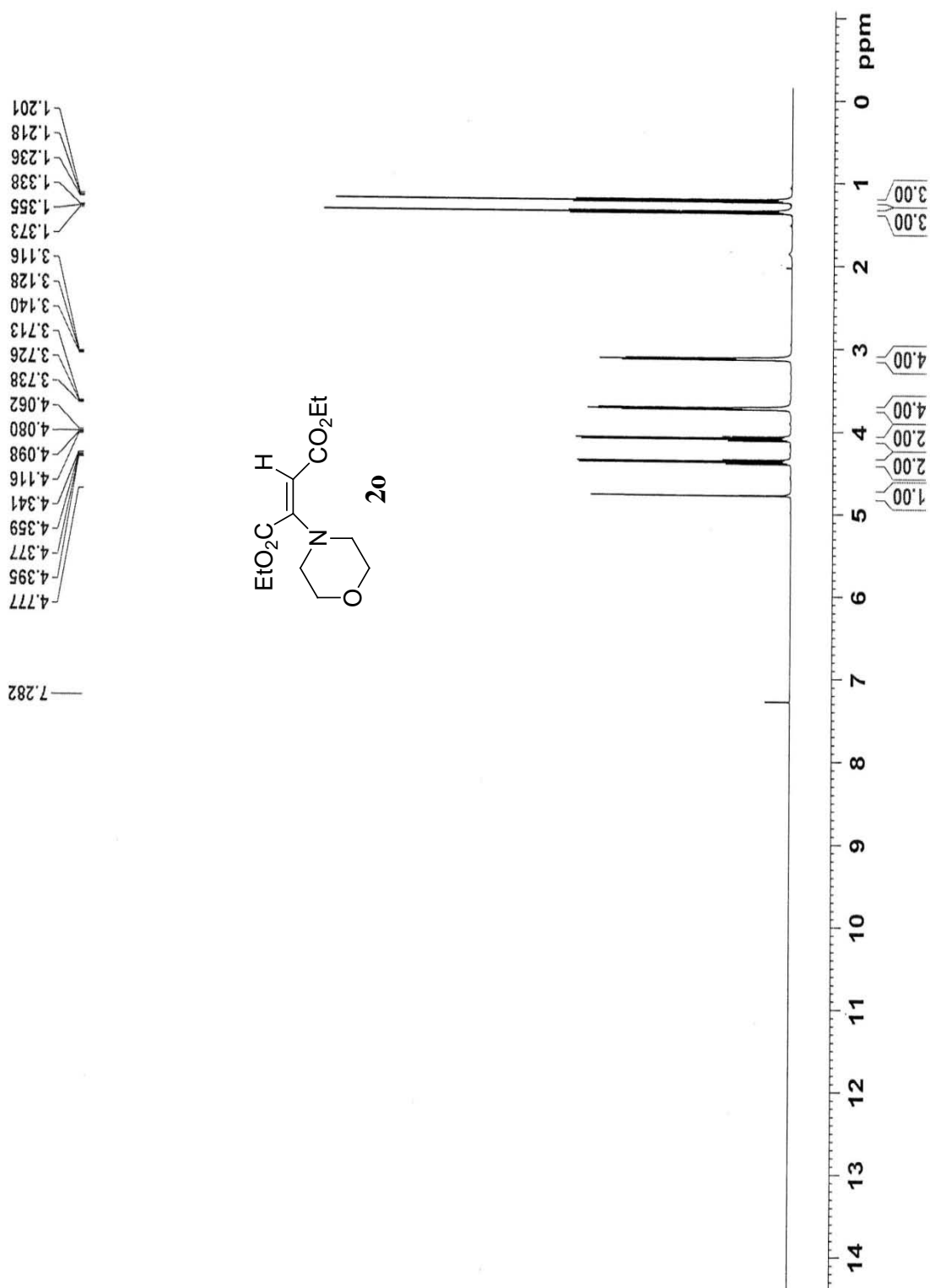
Supplementary Data



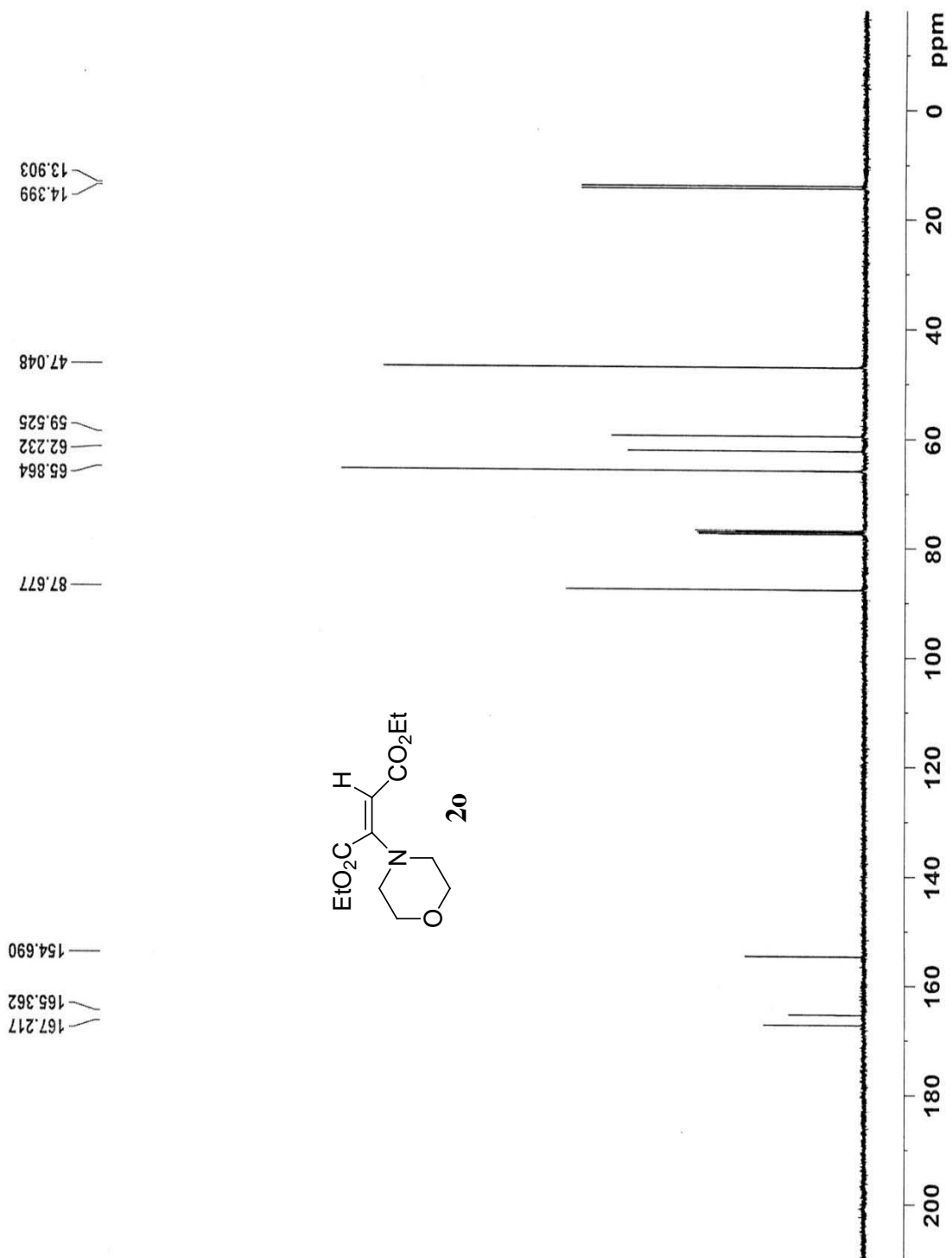
Supplementary Data



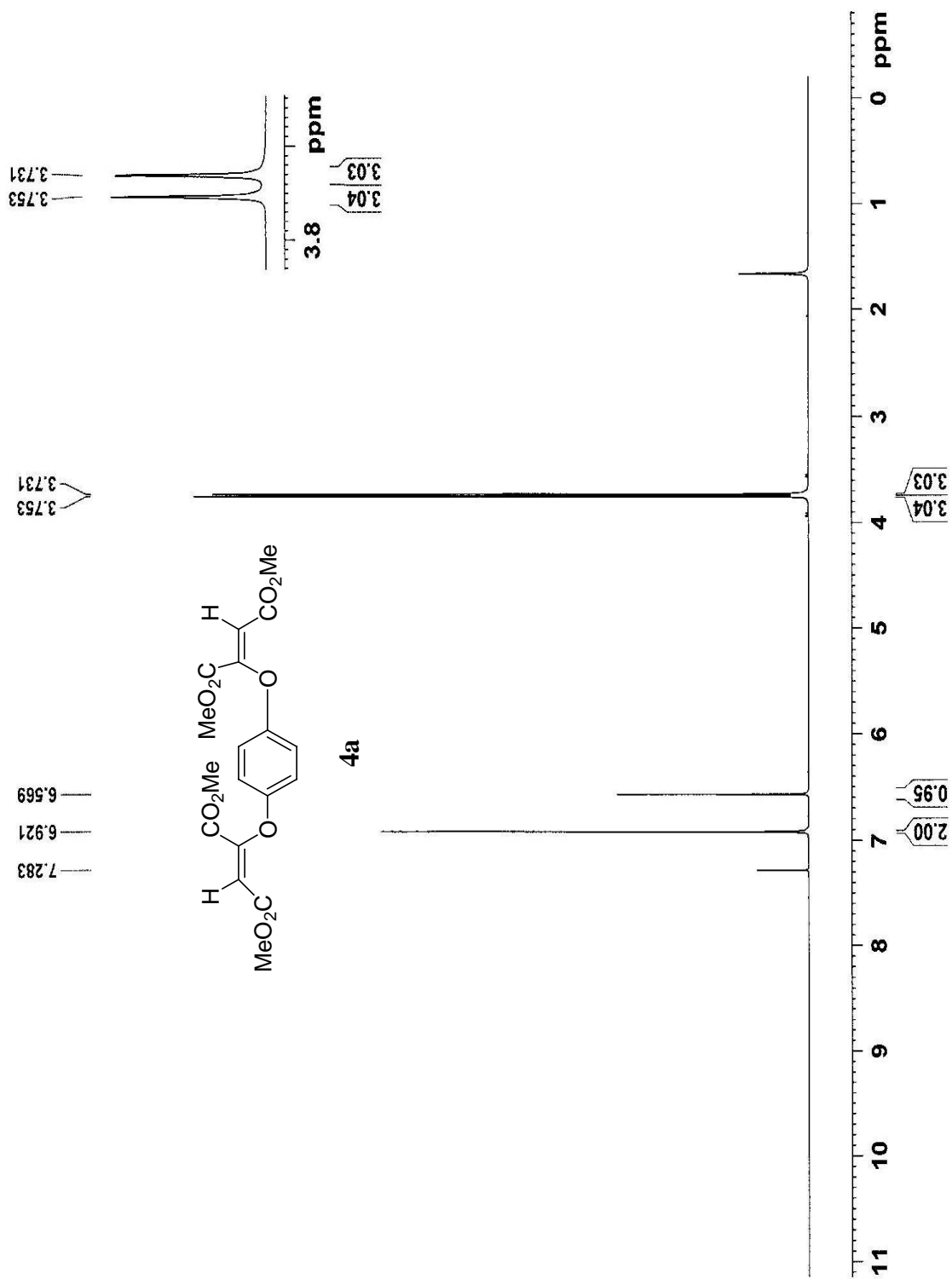
Supplementary Data



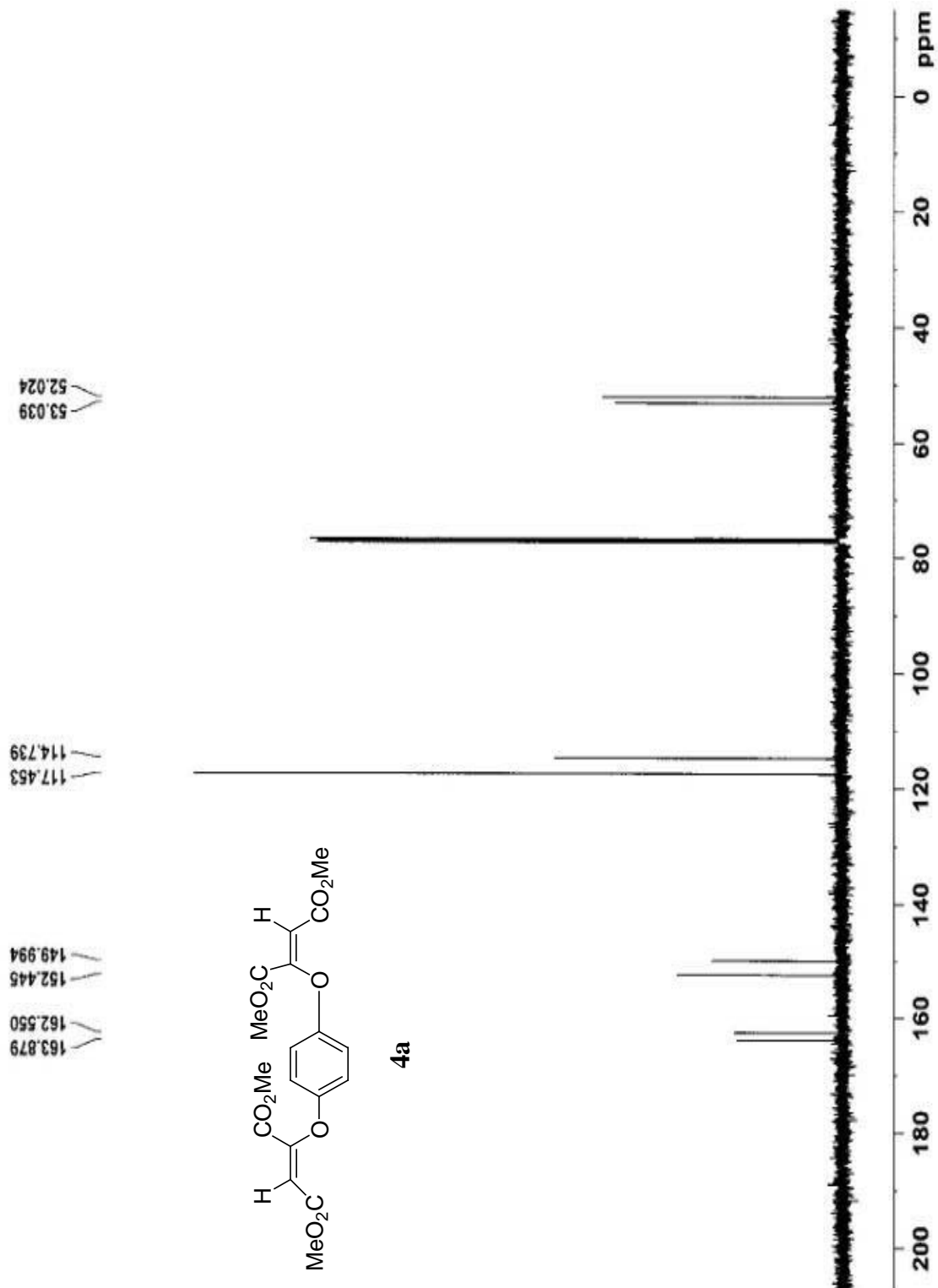
Supplementary Data



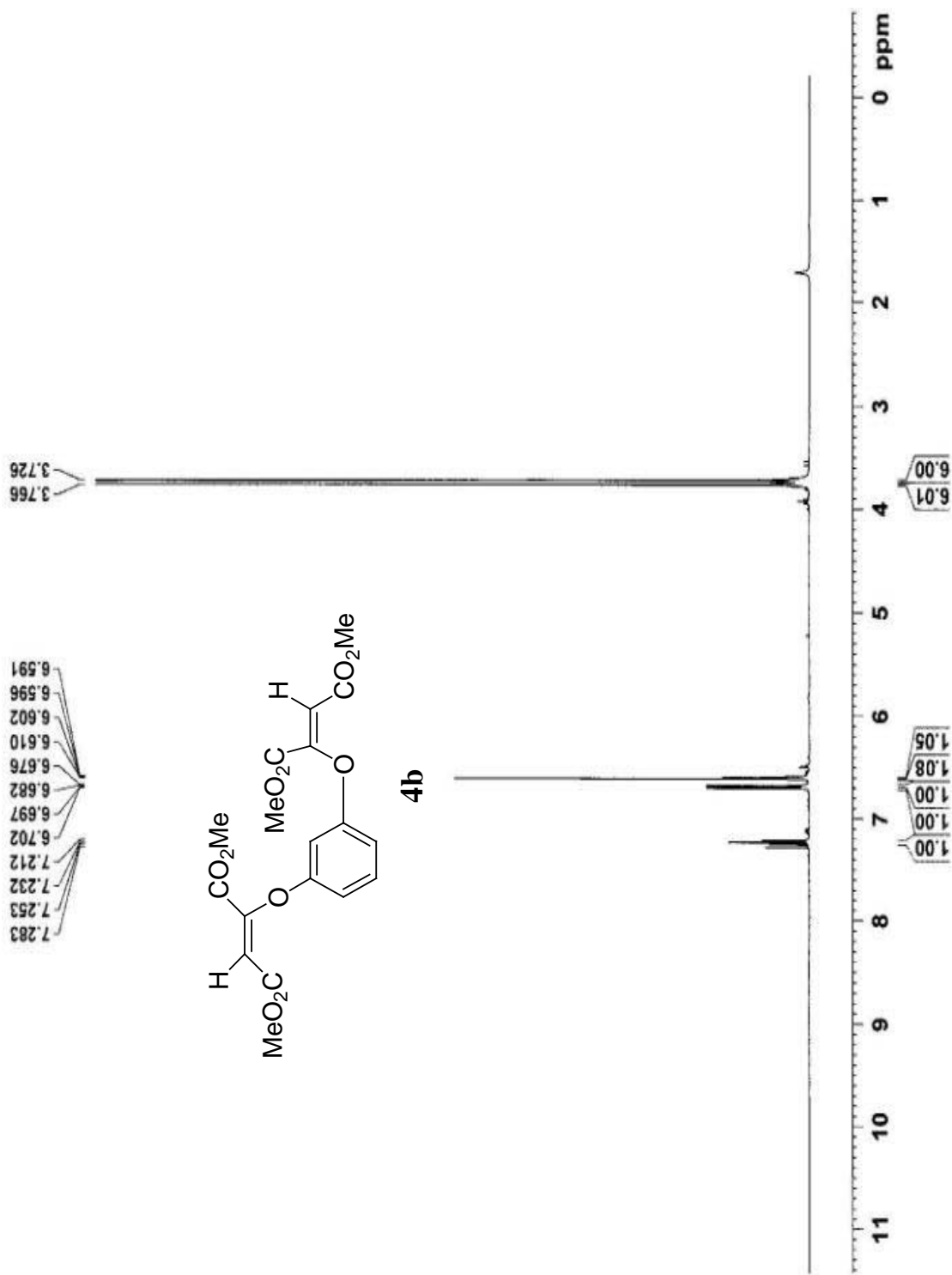
Supplementary Data



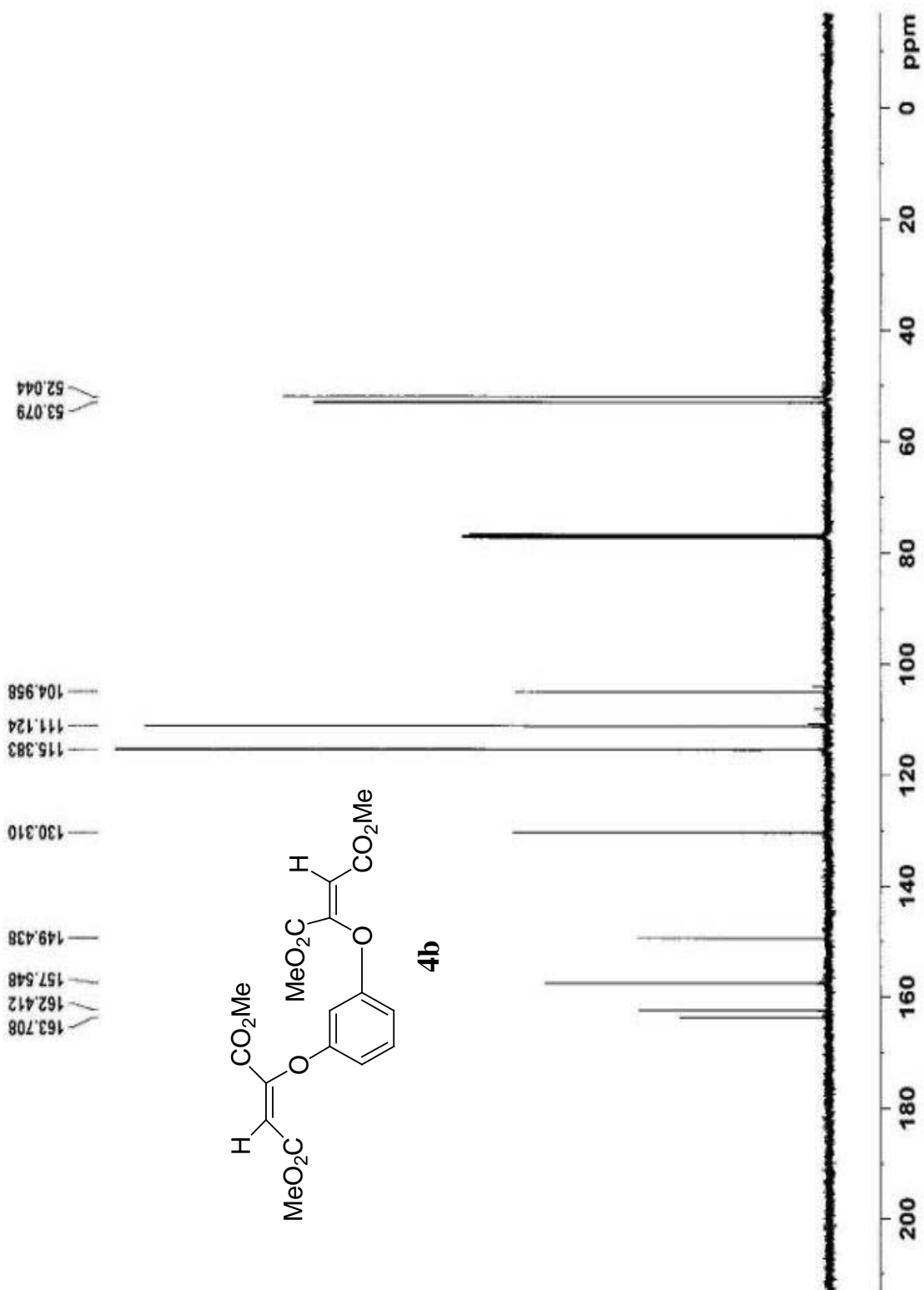
Supplementary Data



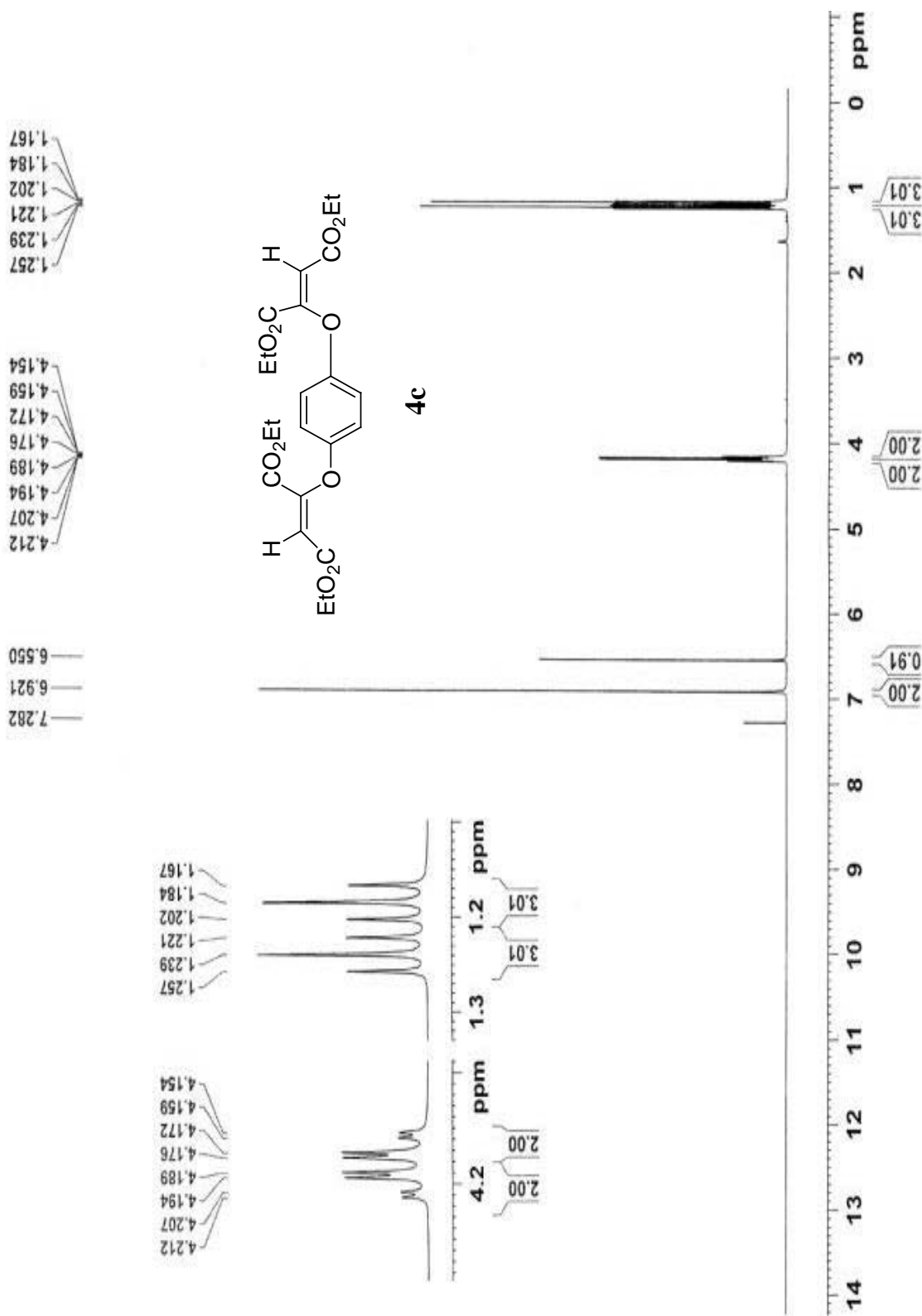
Supplementary Data



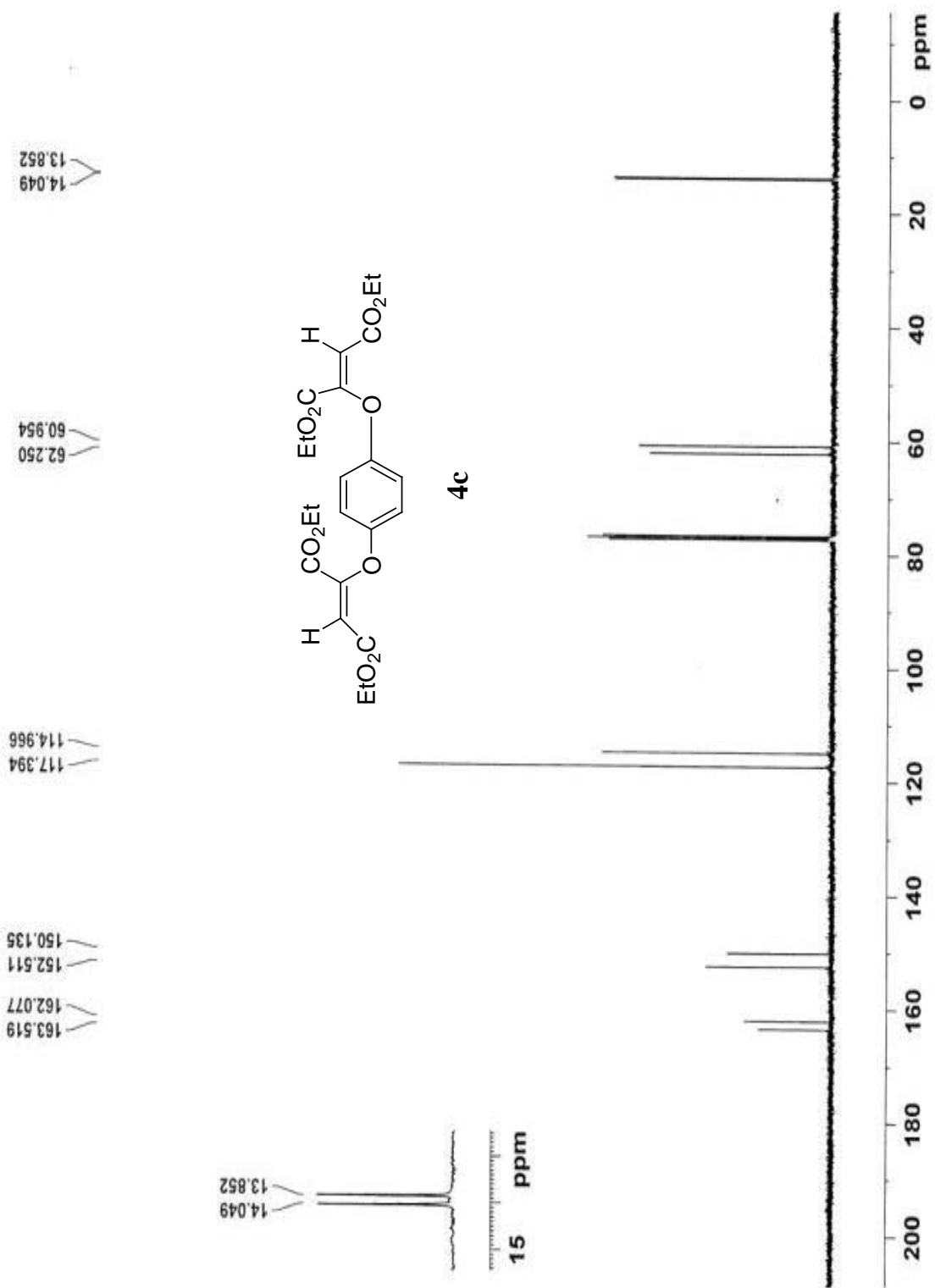
Supplementary Data



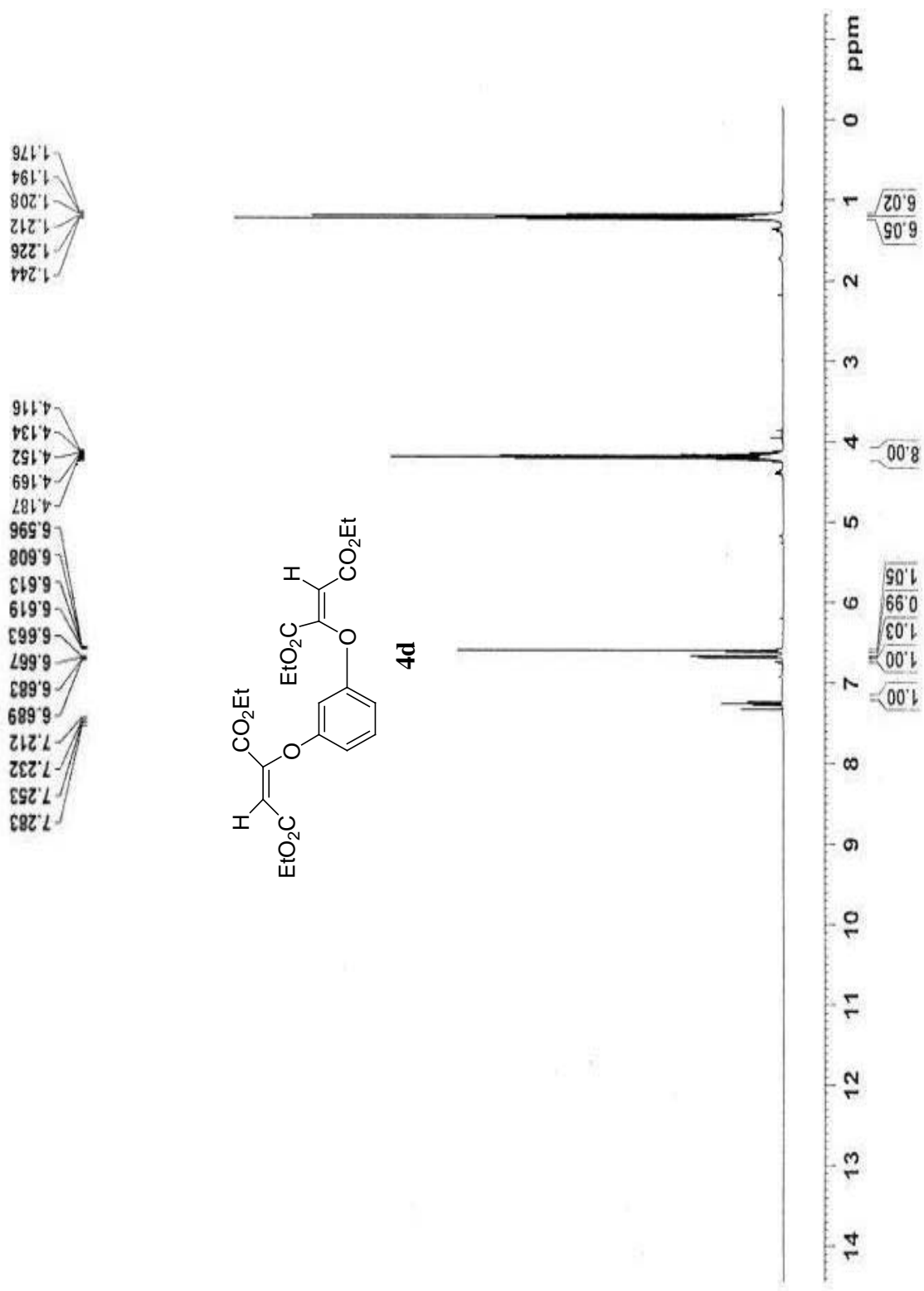
Supplementary Data



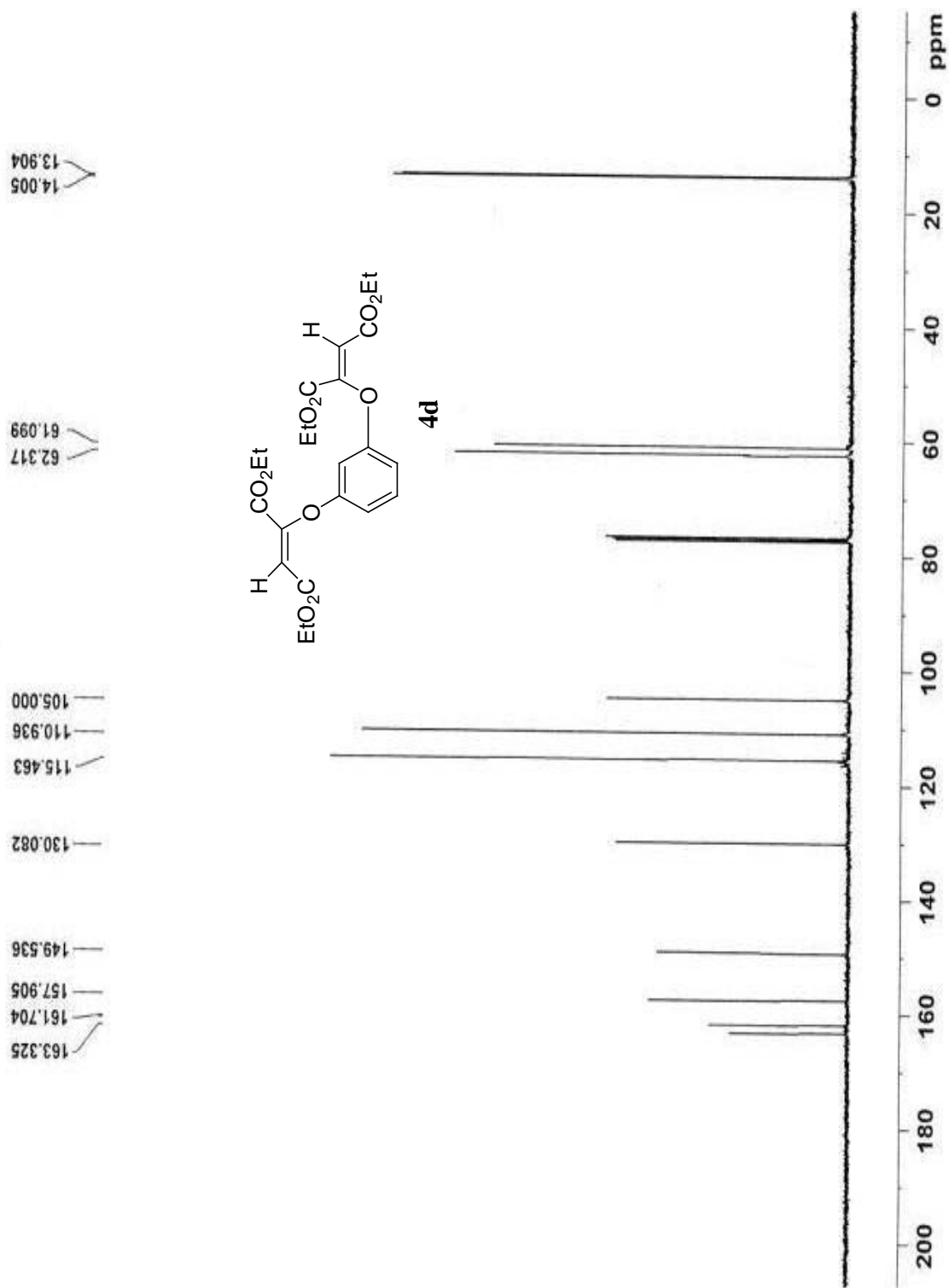
Supplementary Data



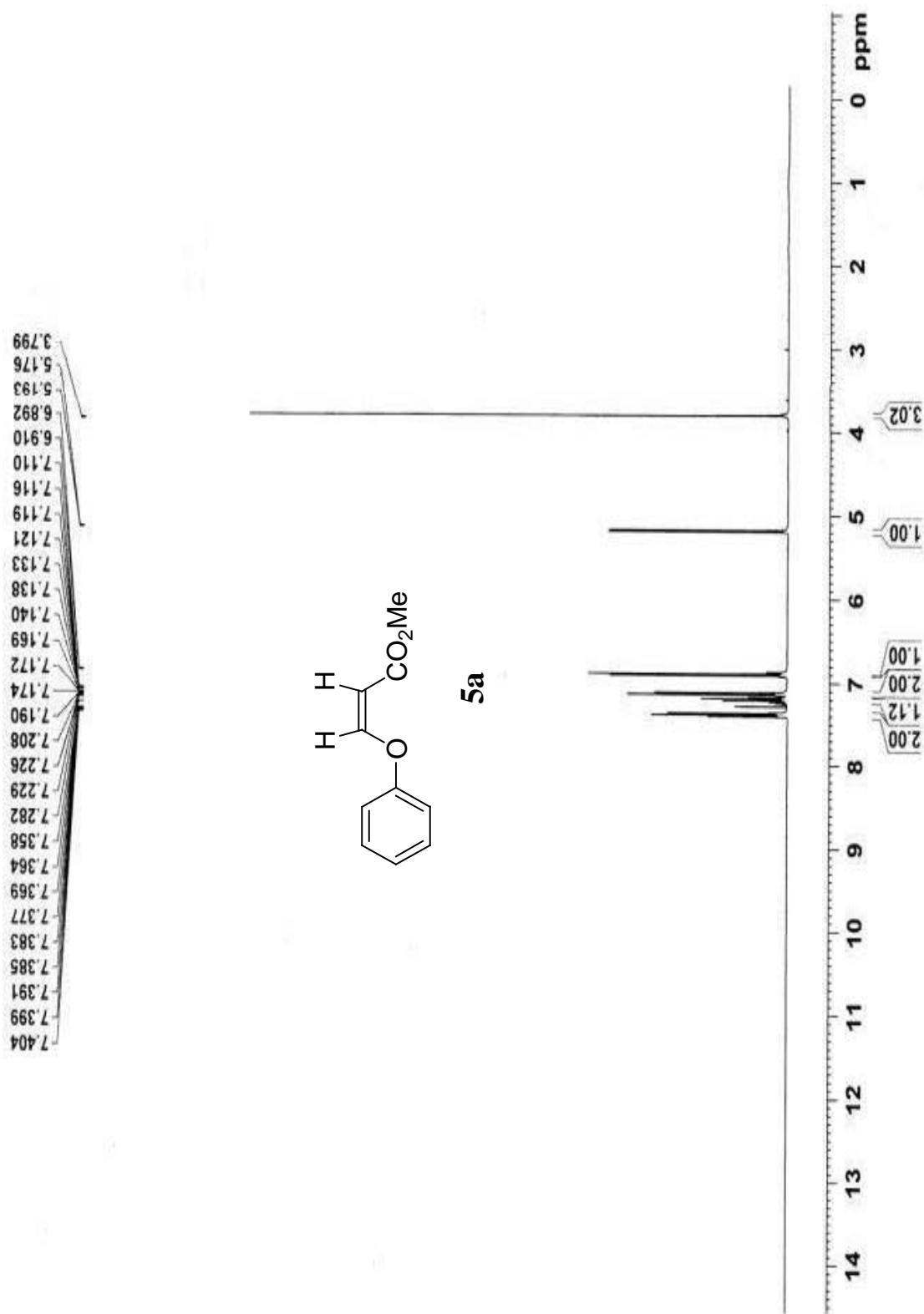
Supplementary Data



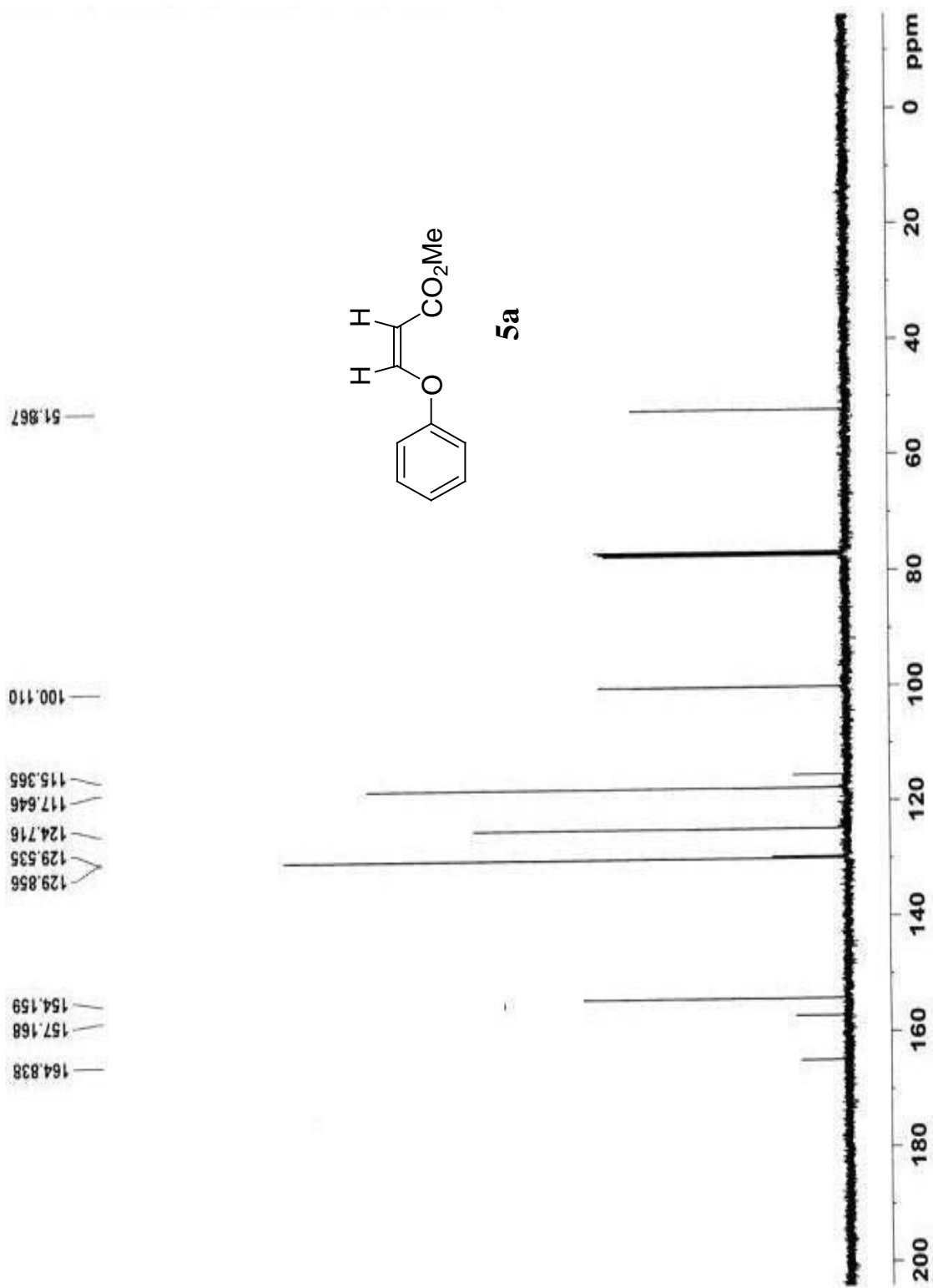
Supplementary Data



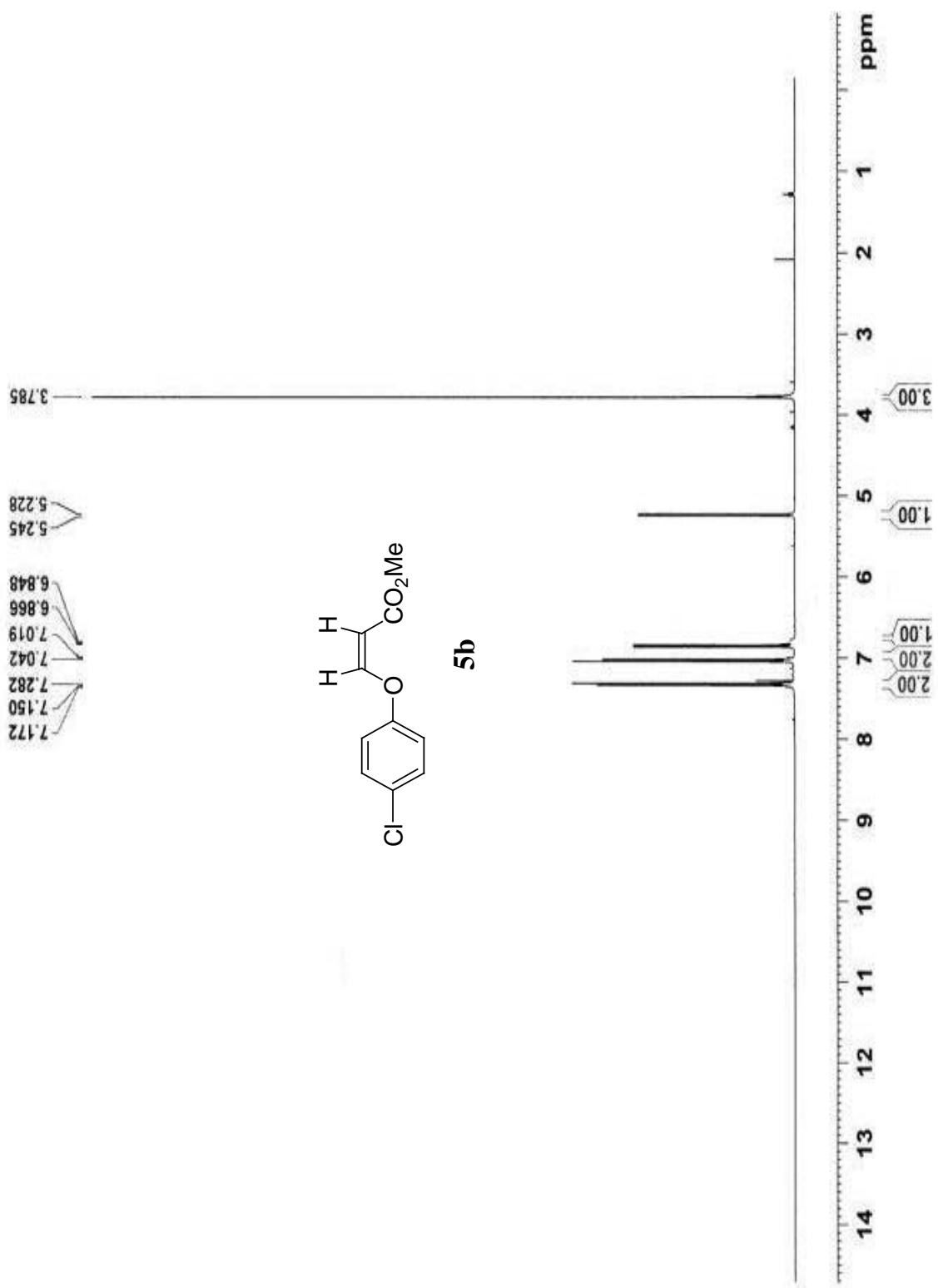
Supplementary Data



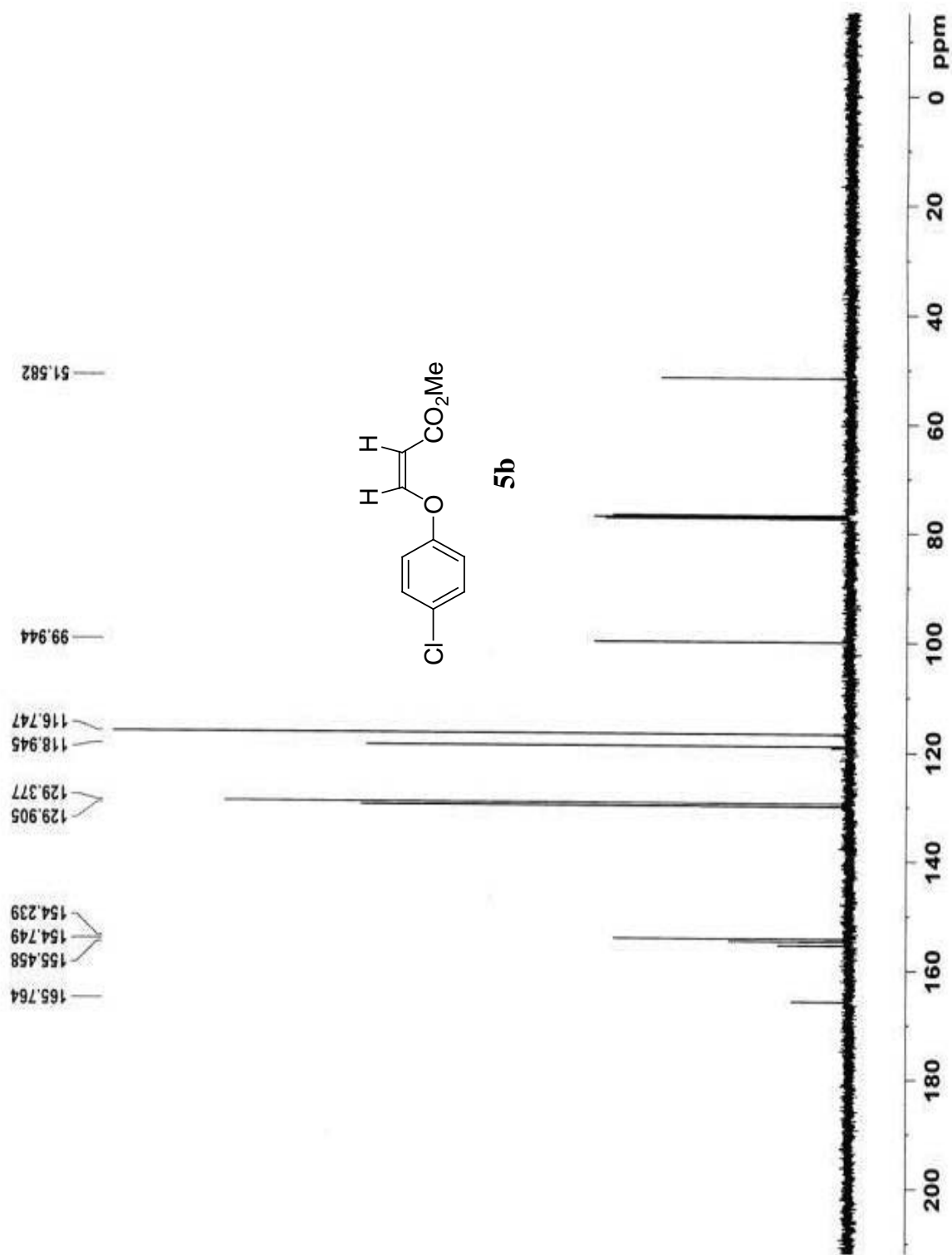
Supplementary Data



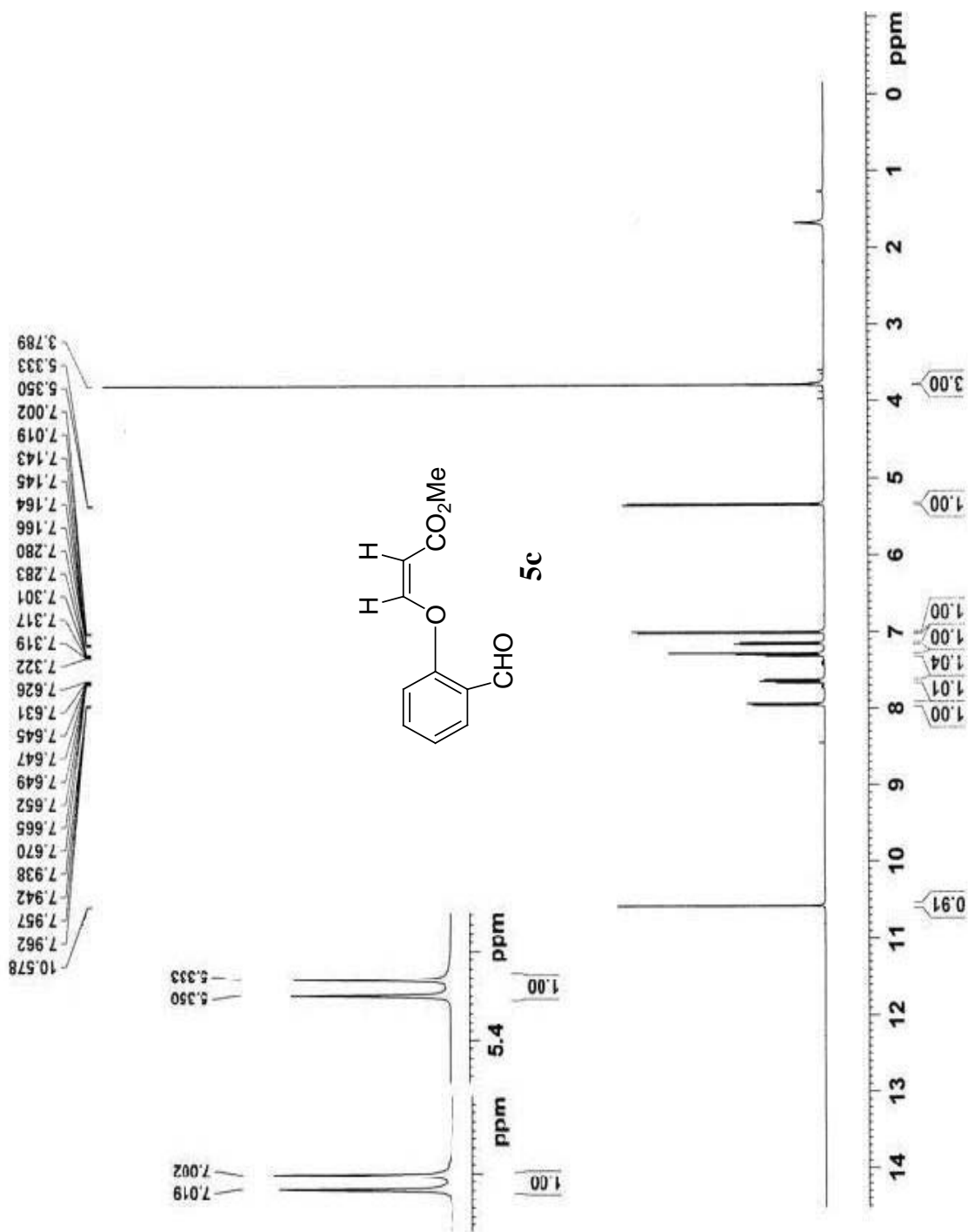
Supplementary Data



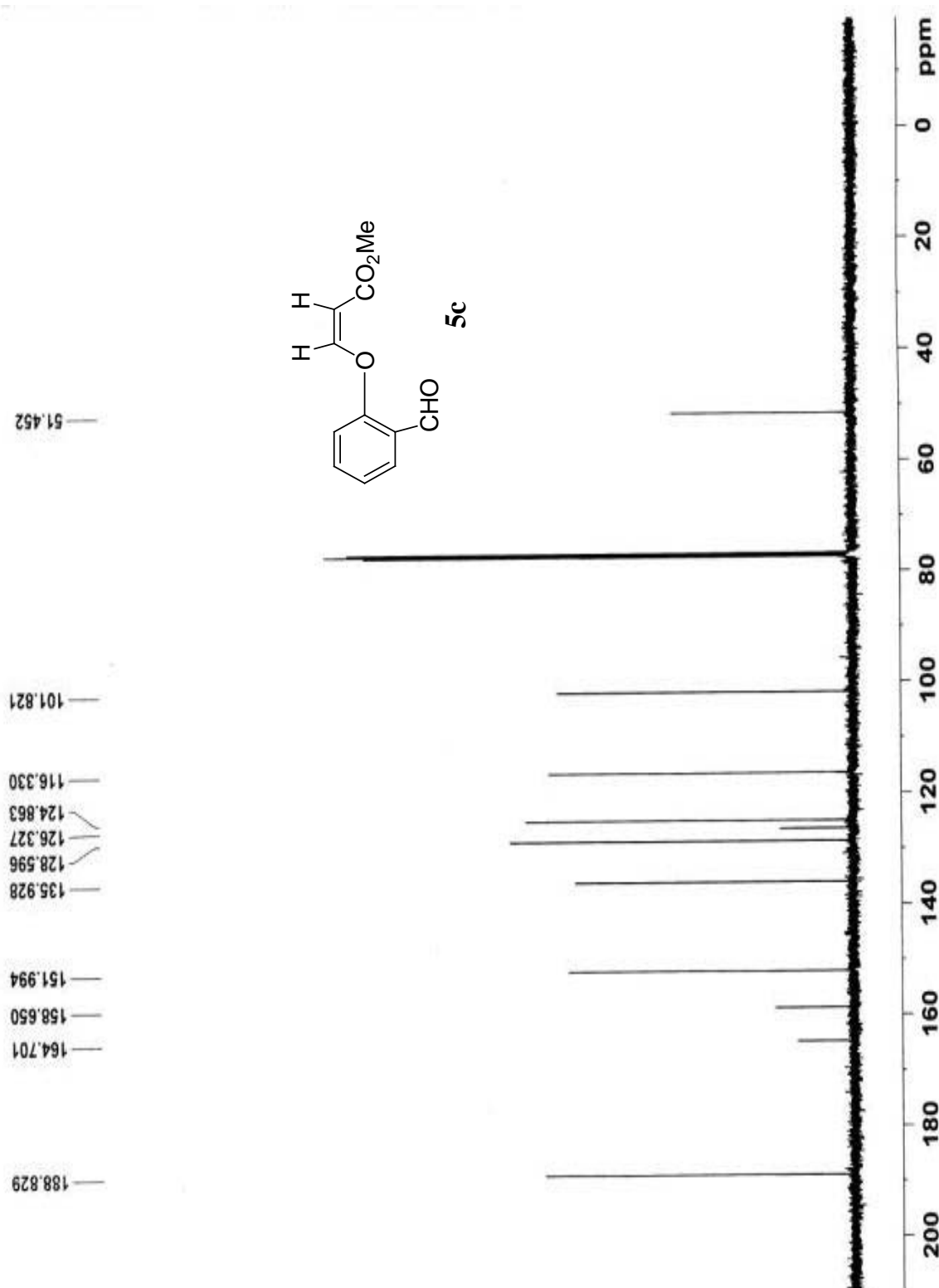
Supplementary Data



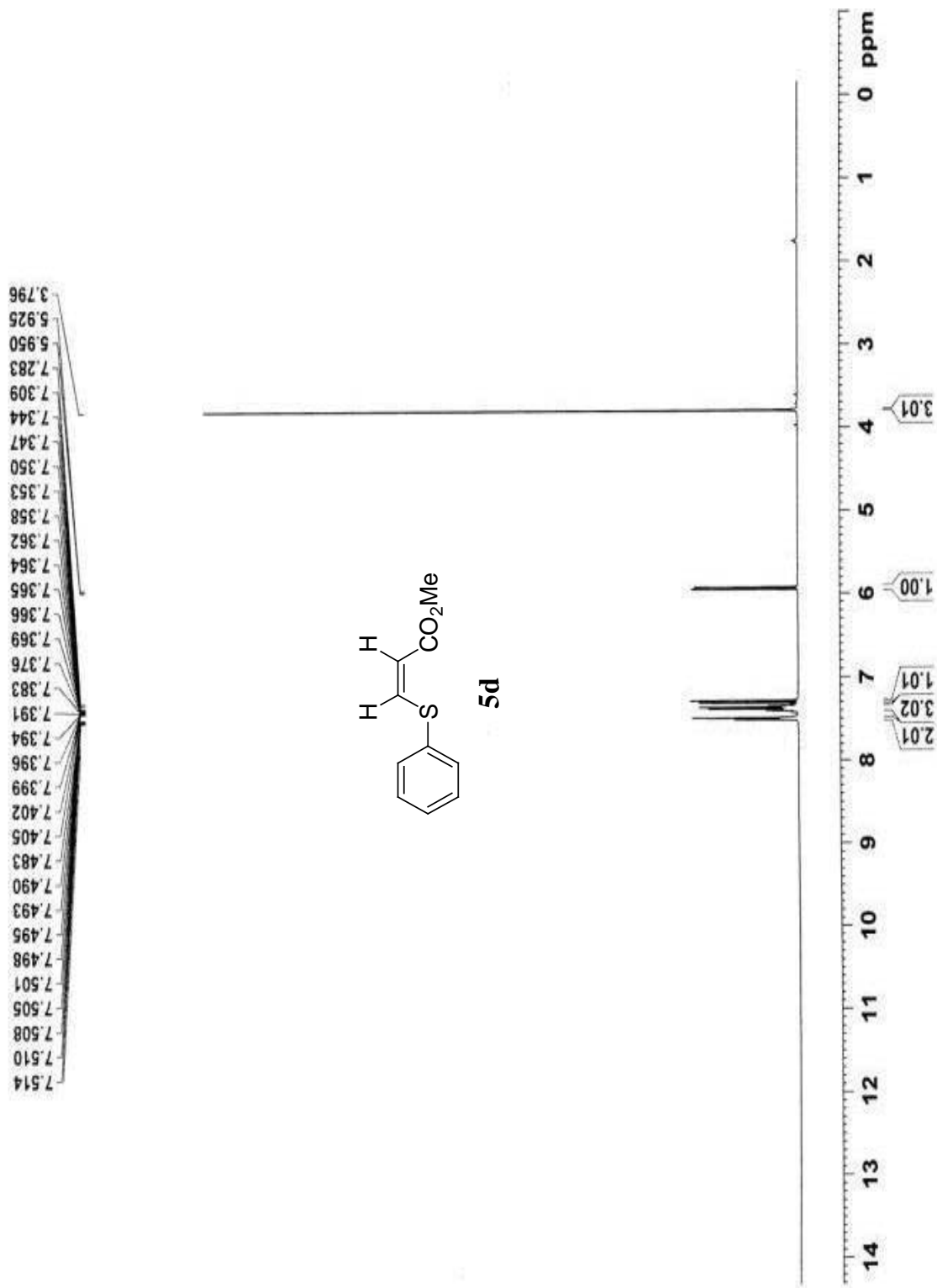
Supplementary Data



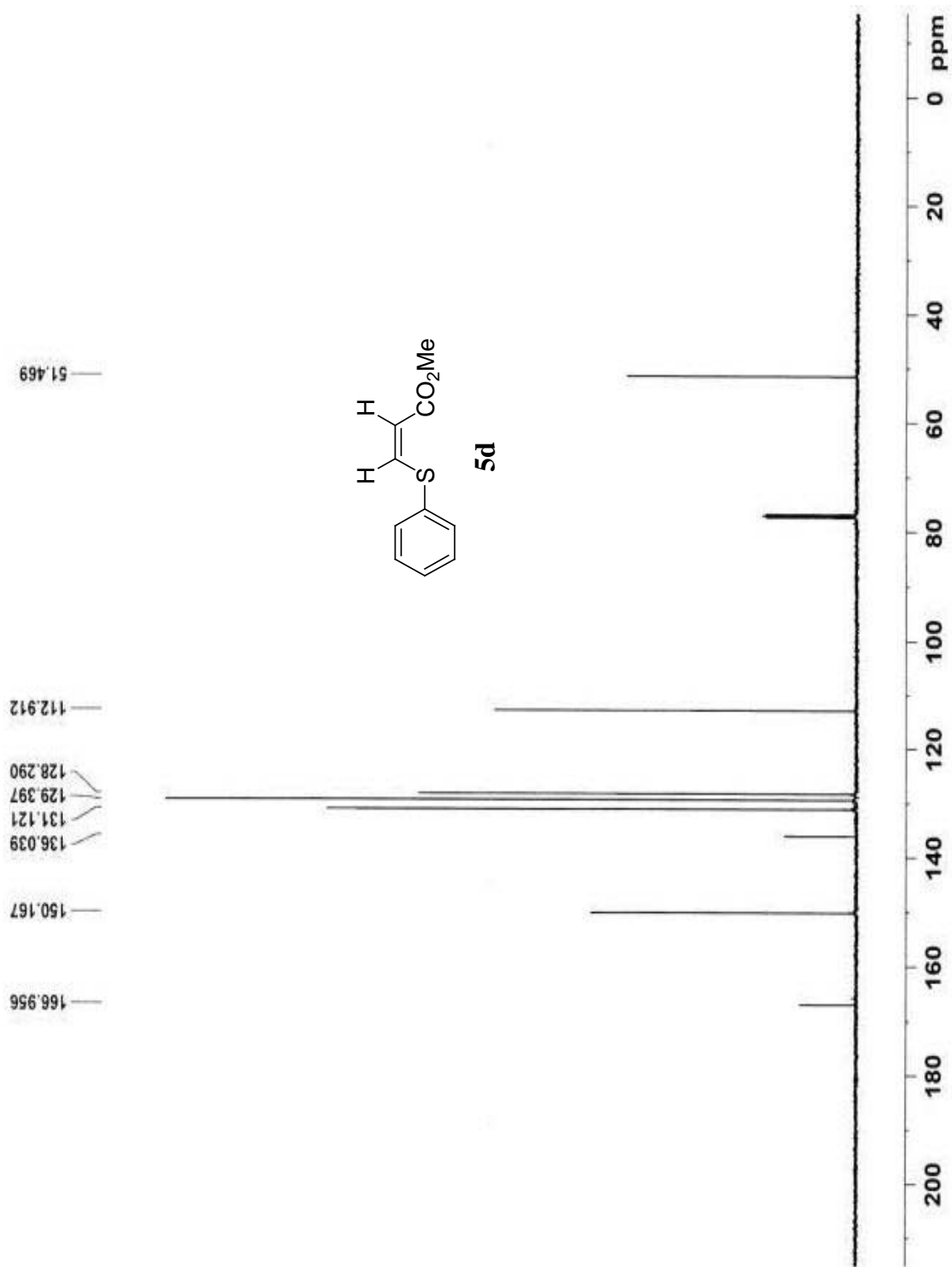
Supplementary Data



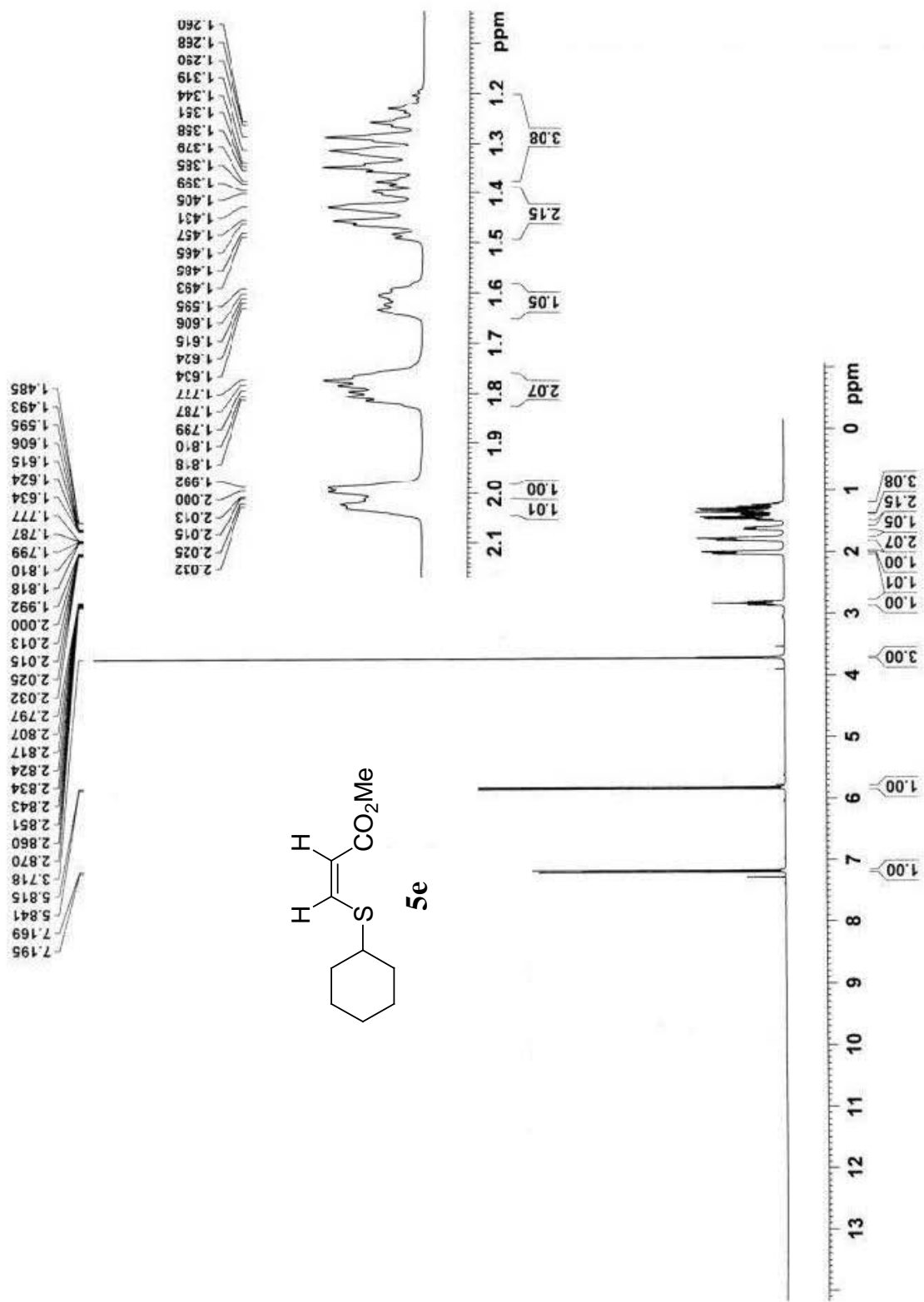
Supplementary Data



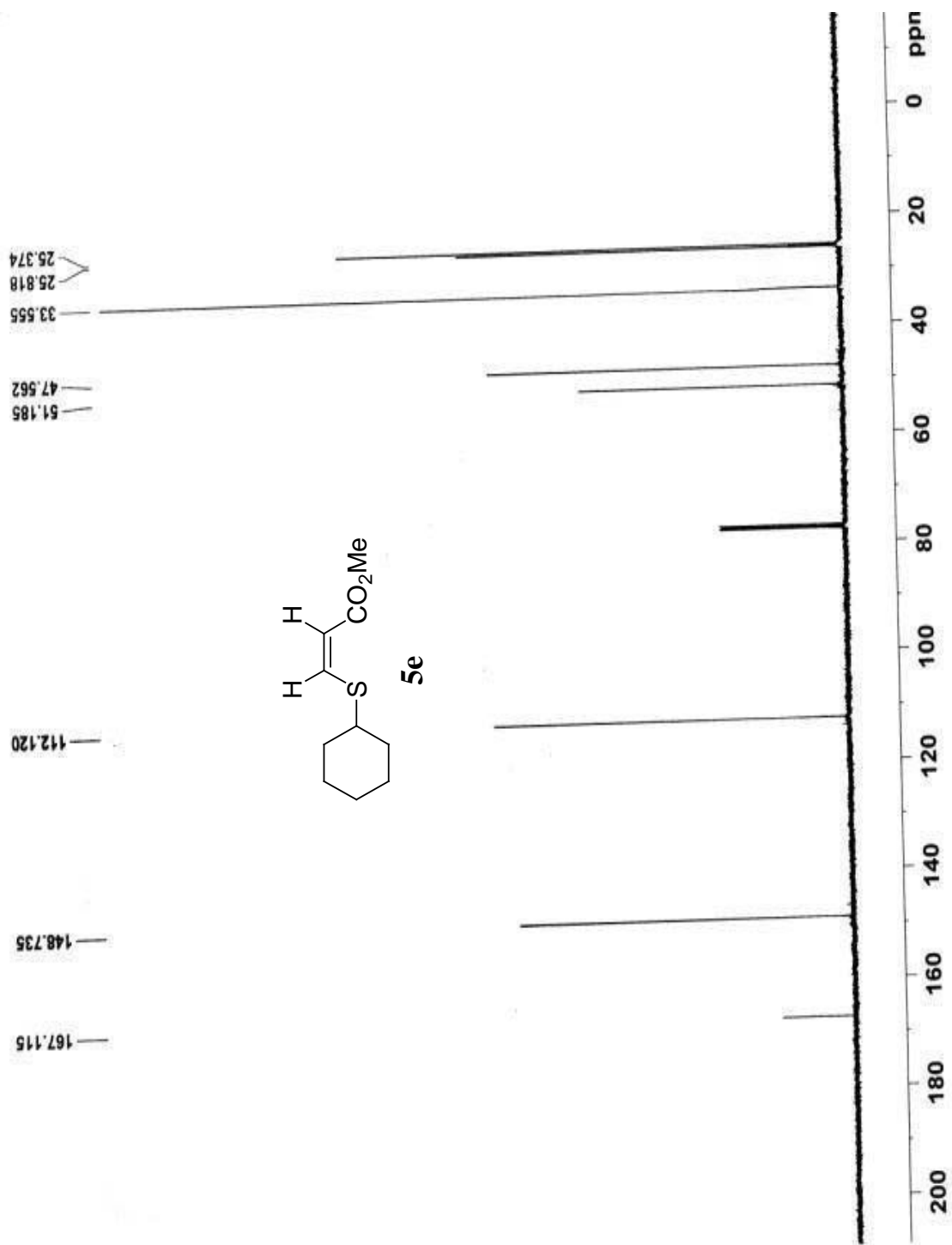
Supplementary Data



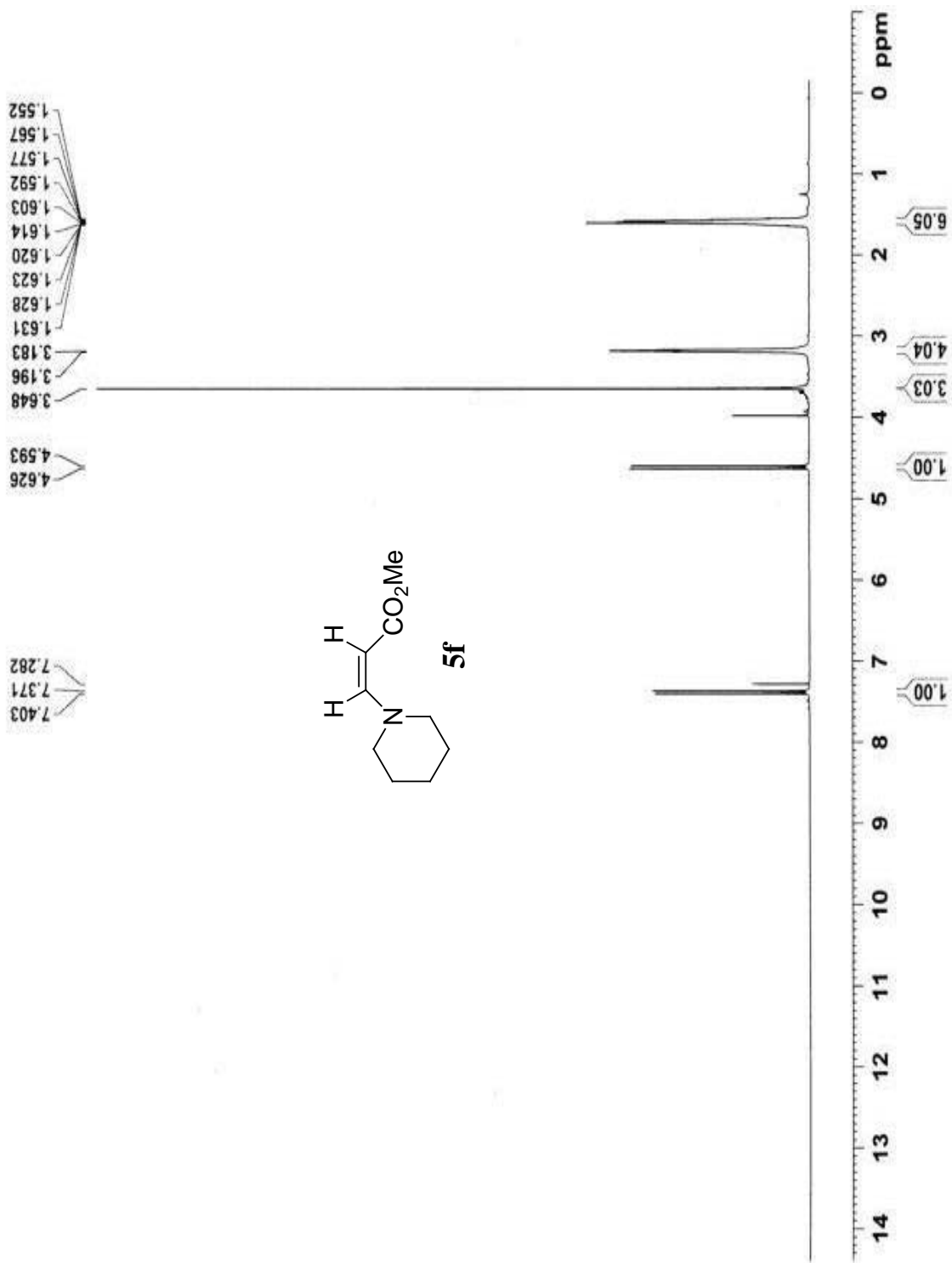
Supplementary Data



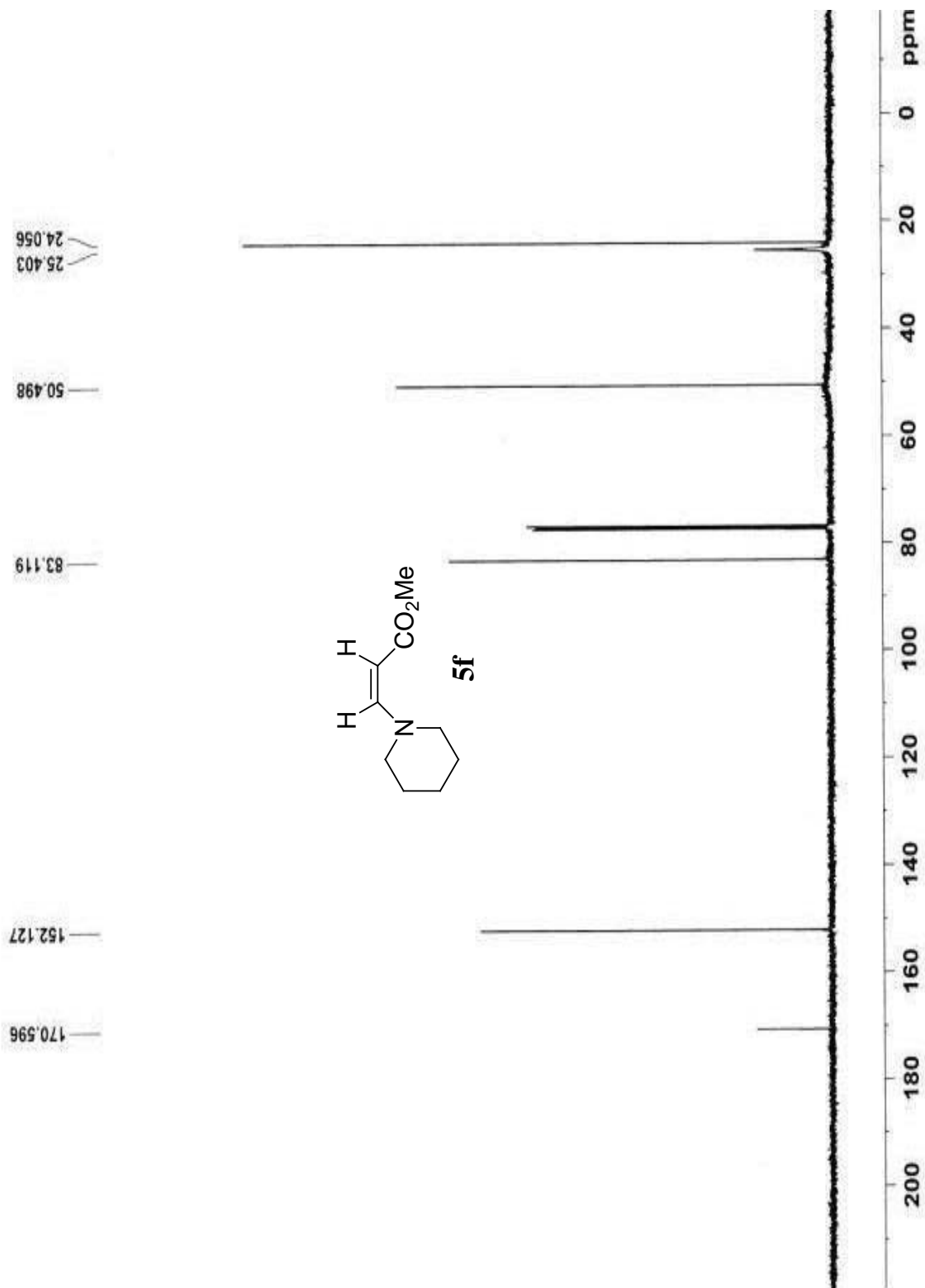
Supplementary Data



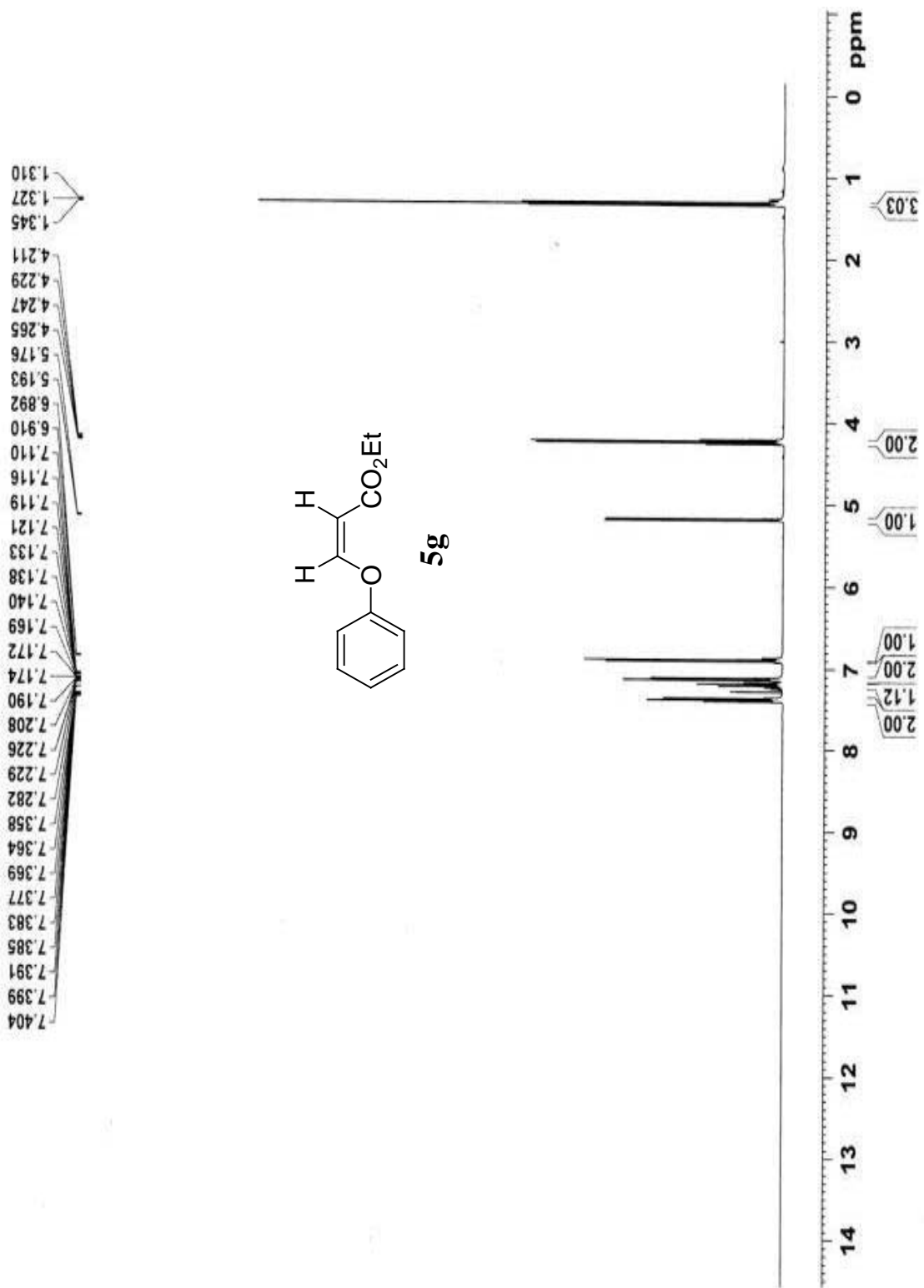
Supplementary Data



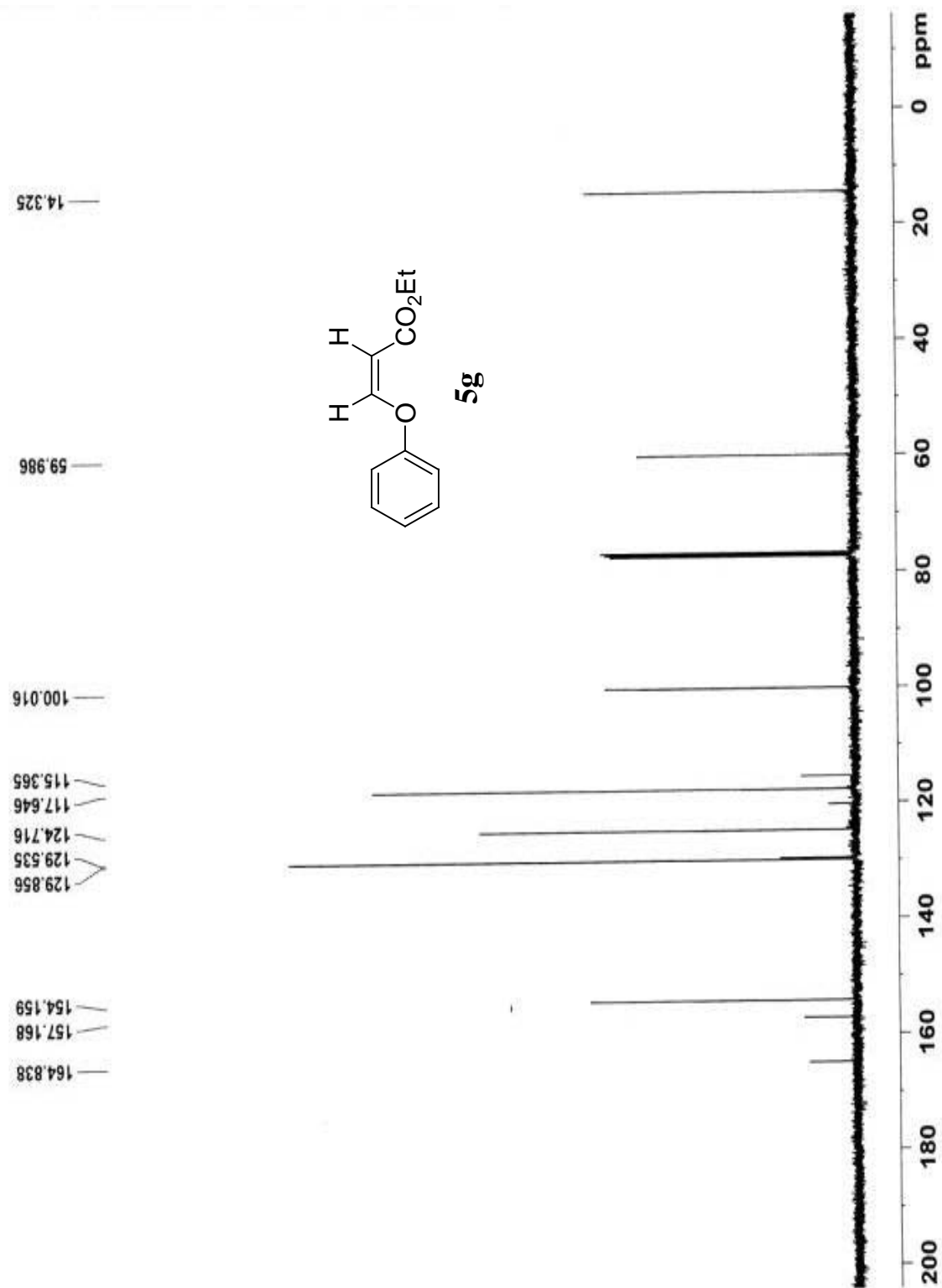
Supplementary Data



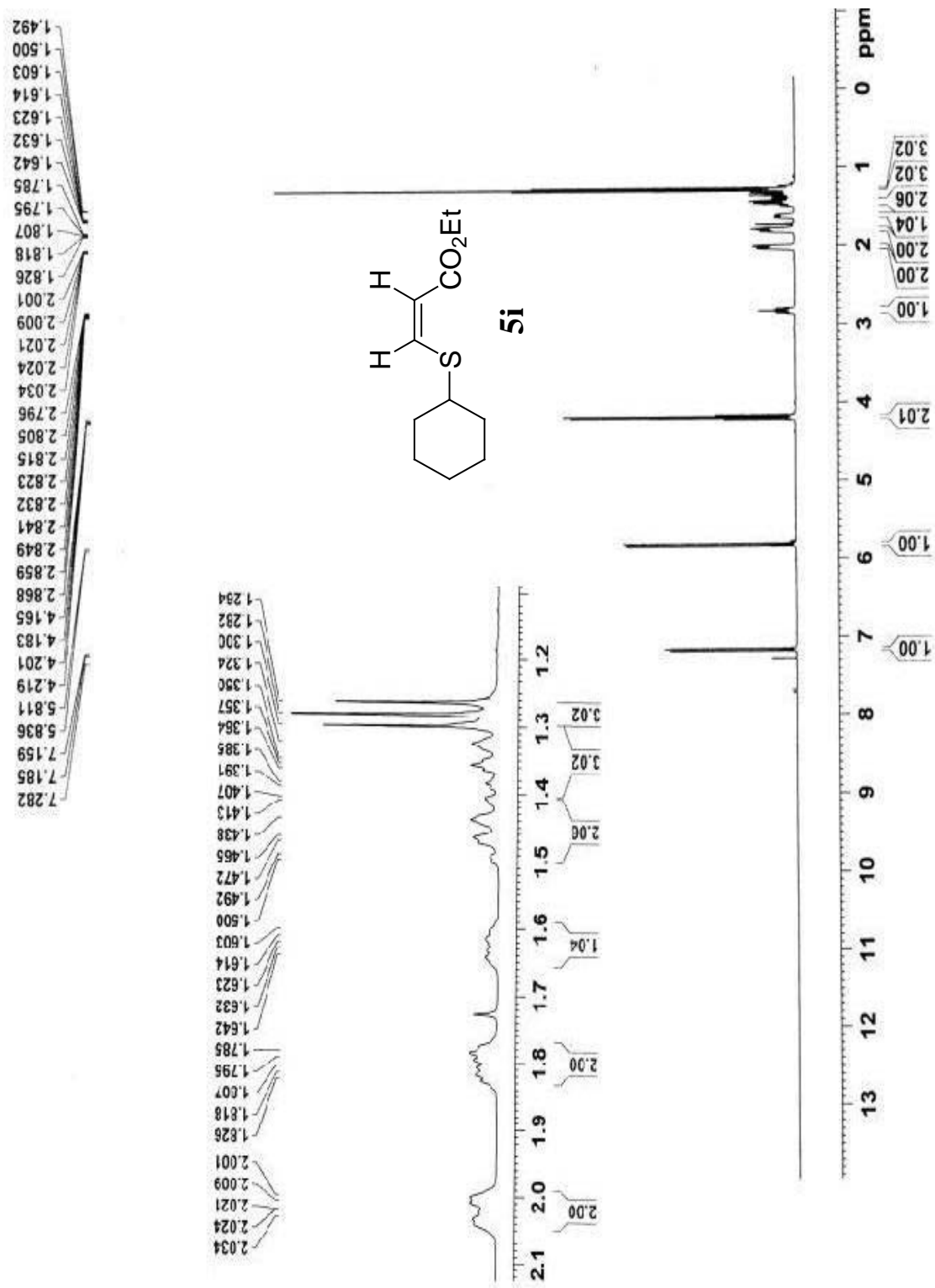
Supplementary Data



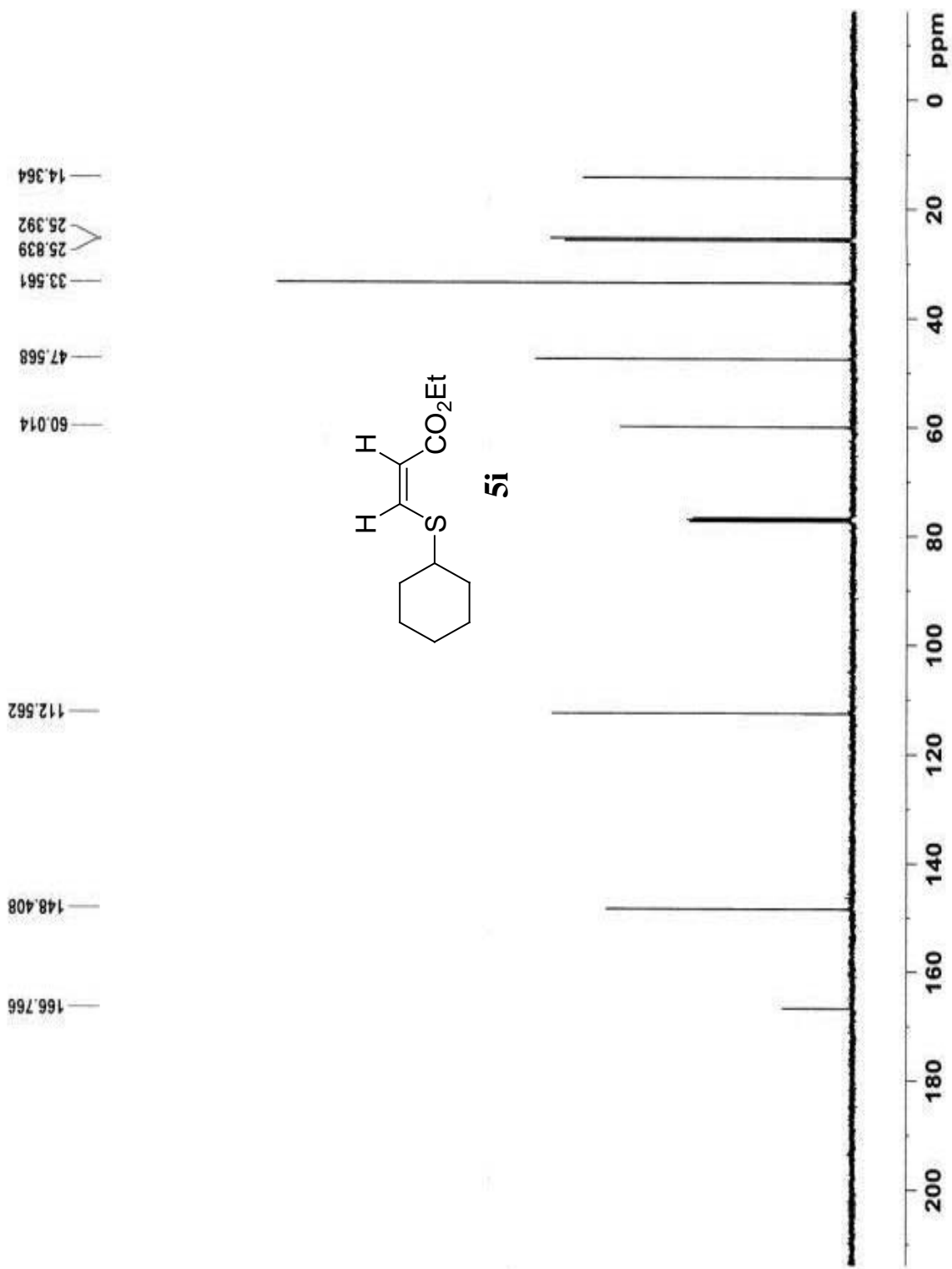
Supplementary Data



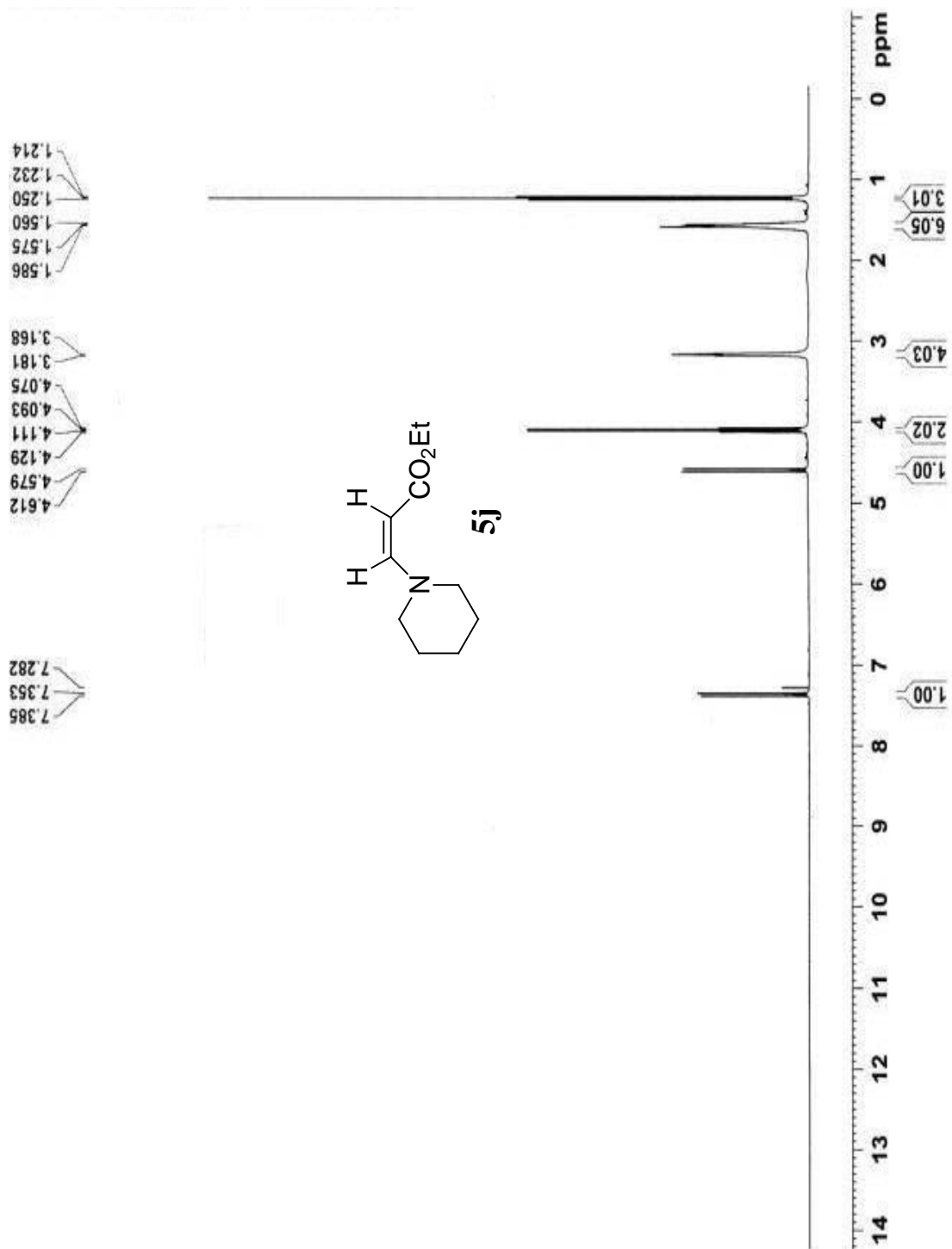
Supplementary Data



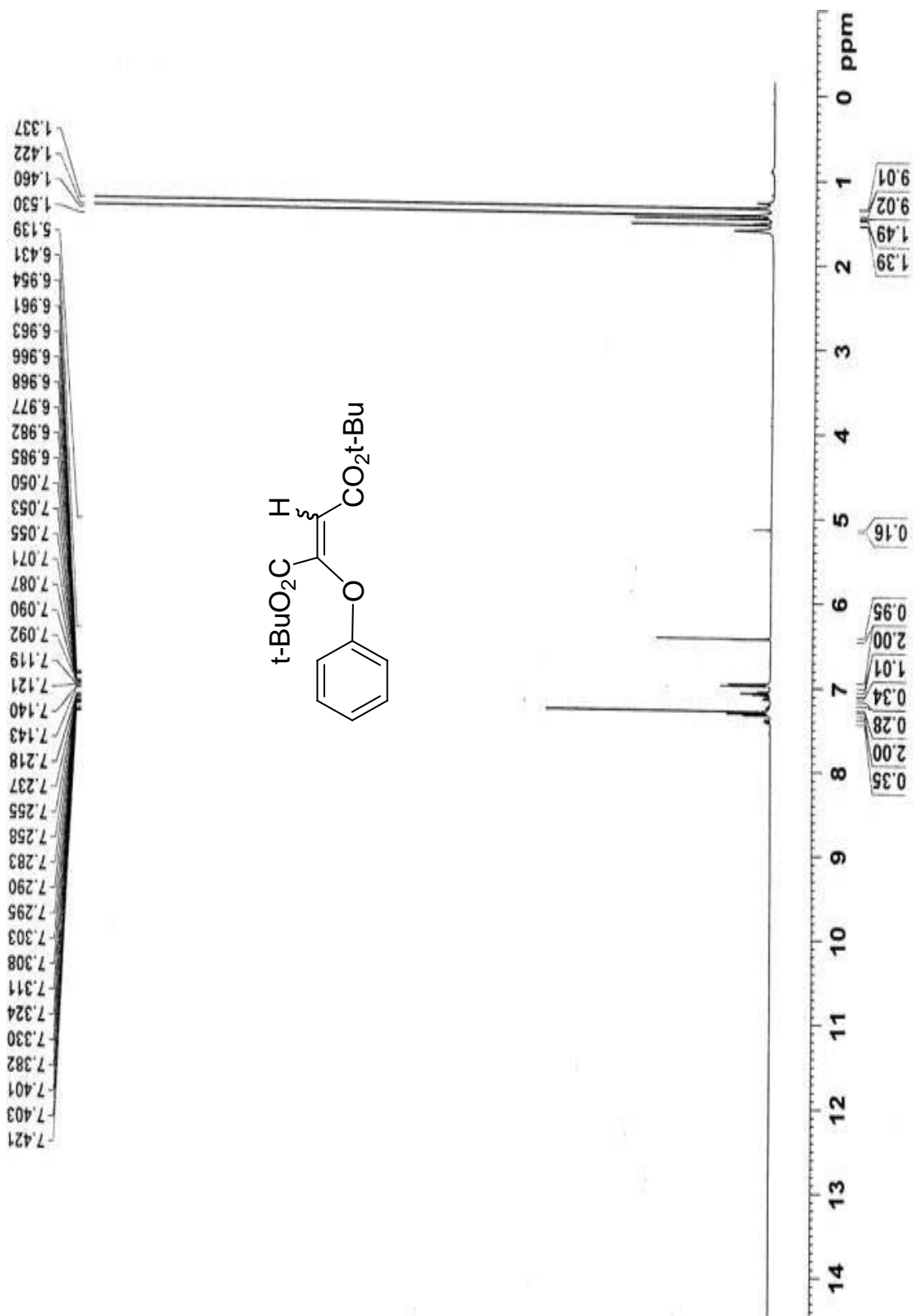
Supplementary Data



Supplementary Data



Supplementary Data



Supplementary Data

