

Supporting information

First Total Synthesis of Nhatrangin A

Ahmed Kamal and Saidi Reddy Vangala*

CSIR-Indian Institute of Chemical Technology, Hyderabad, India-500 007.

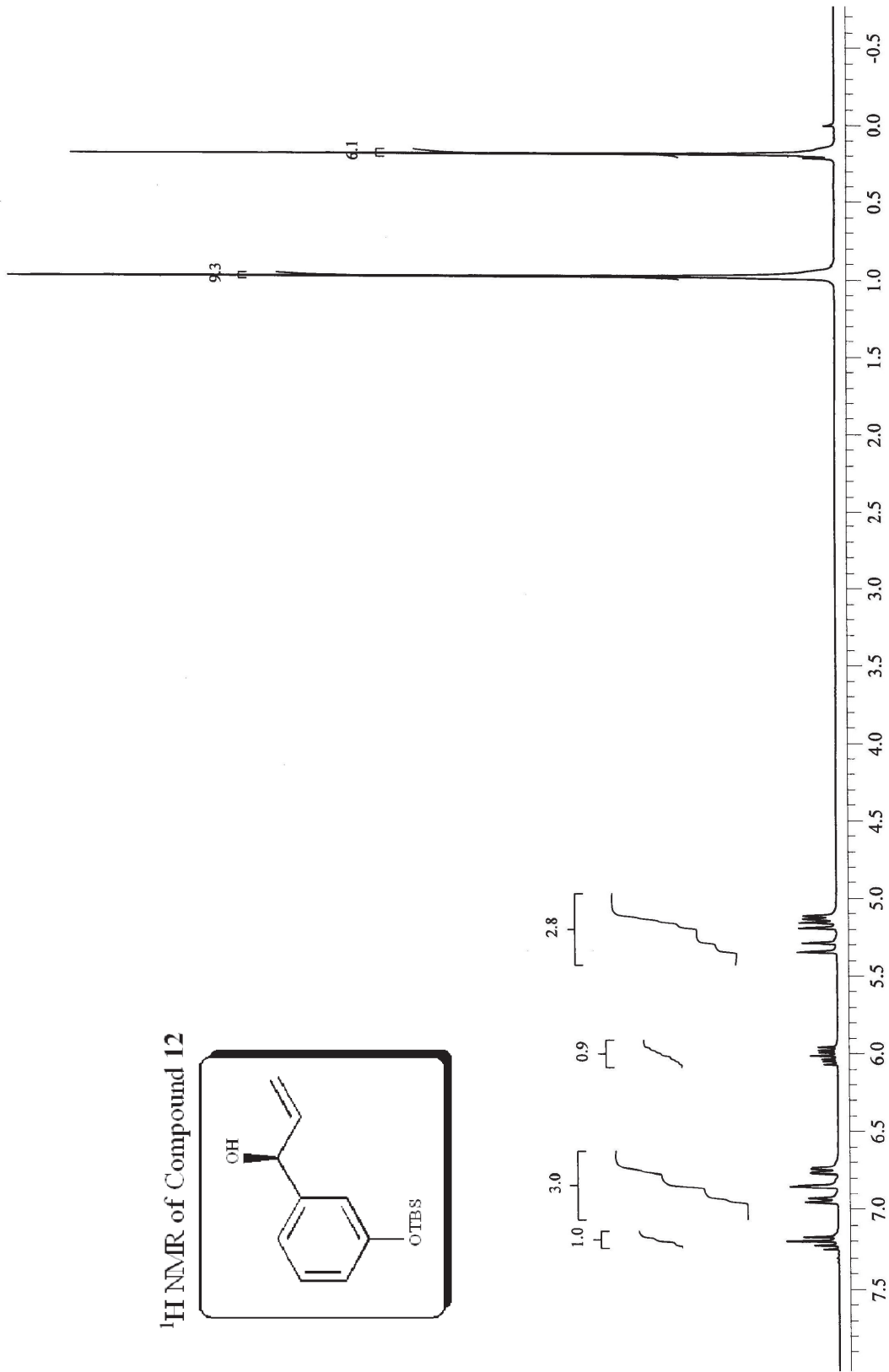
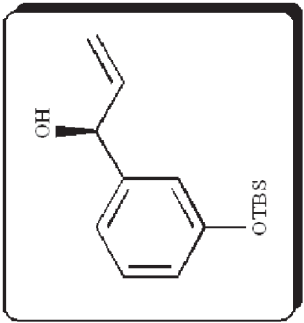
Corresponding author. Tel.: +91-40-27193157; fax: +91-40-27193189

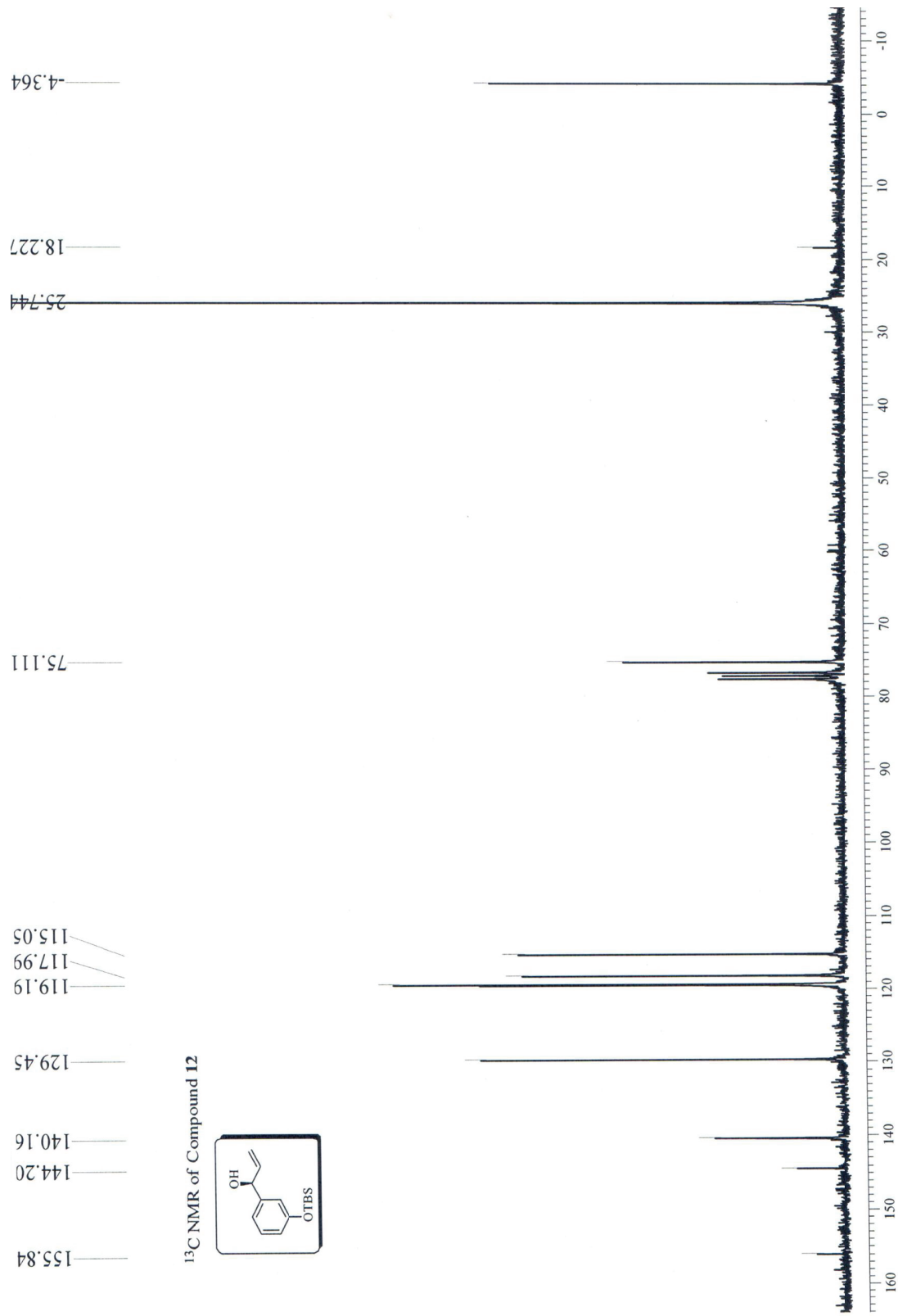
ahmedkamal@iict.res.in

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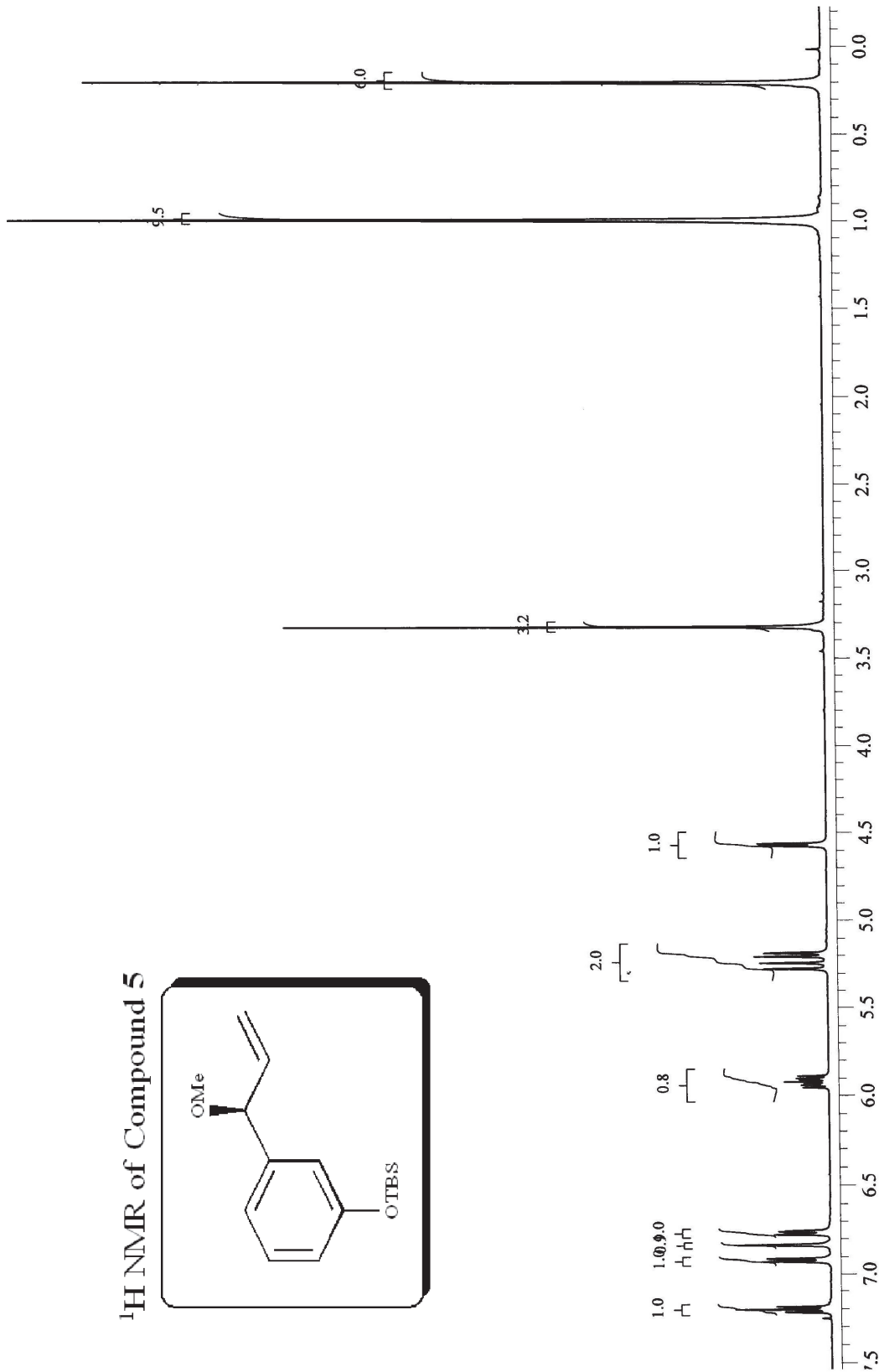
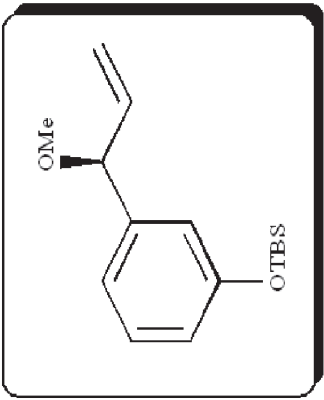
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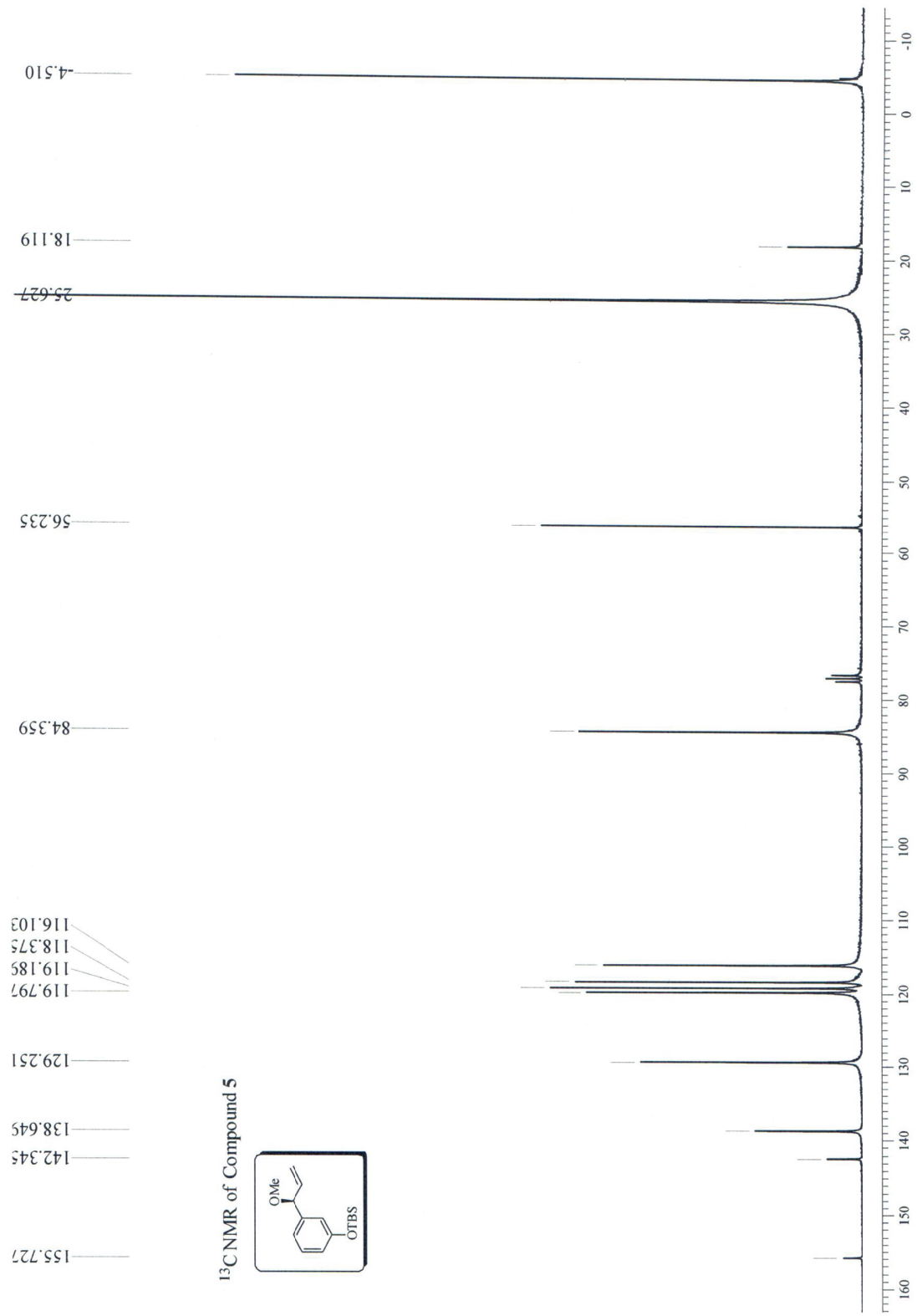
¹H NMR of Compound 12

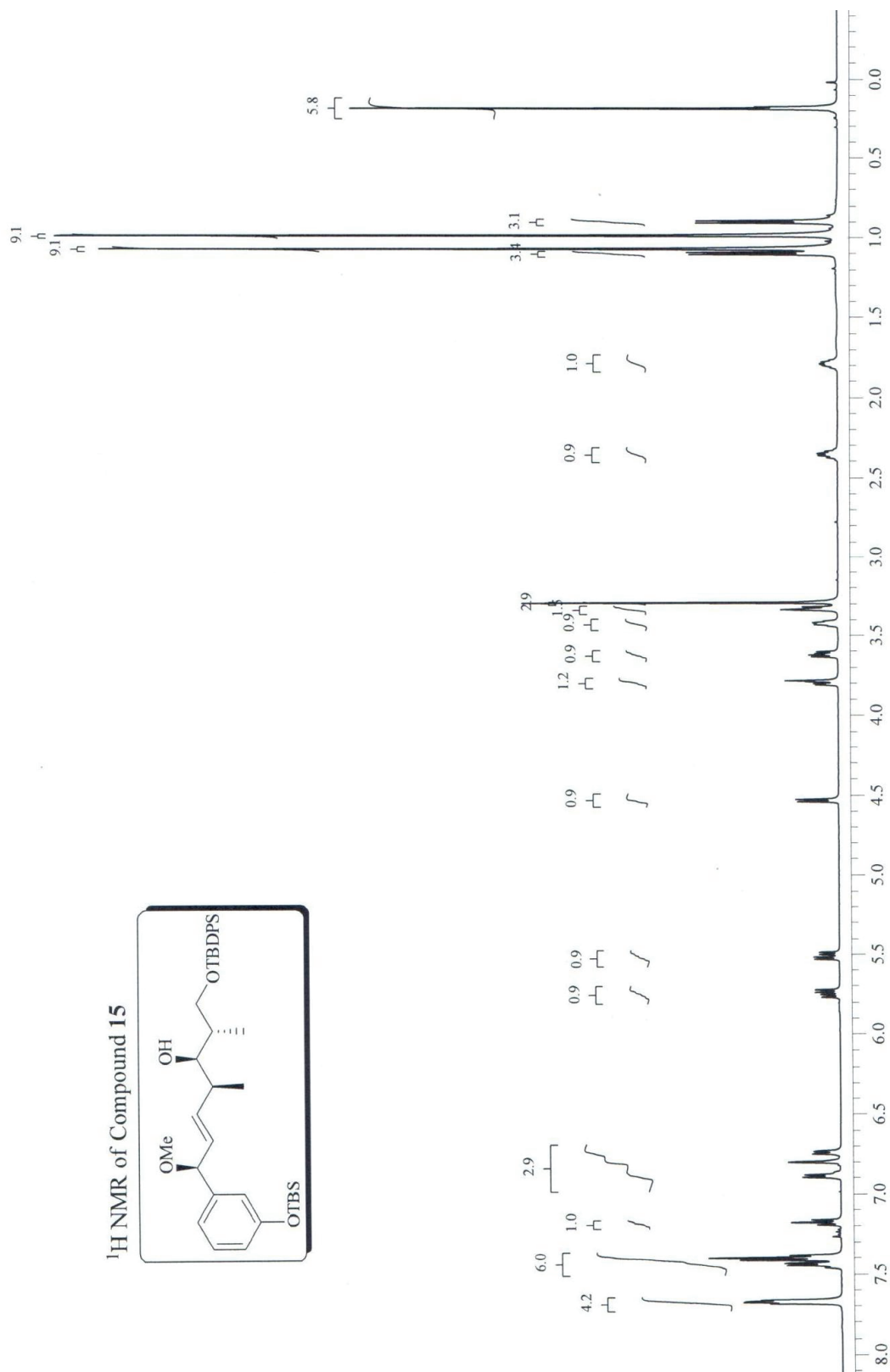


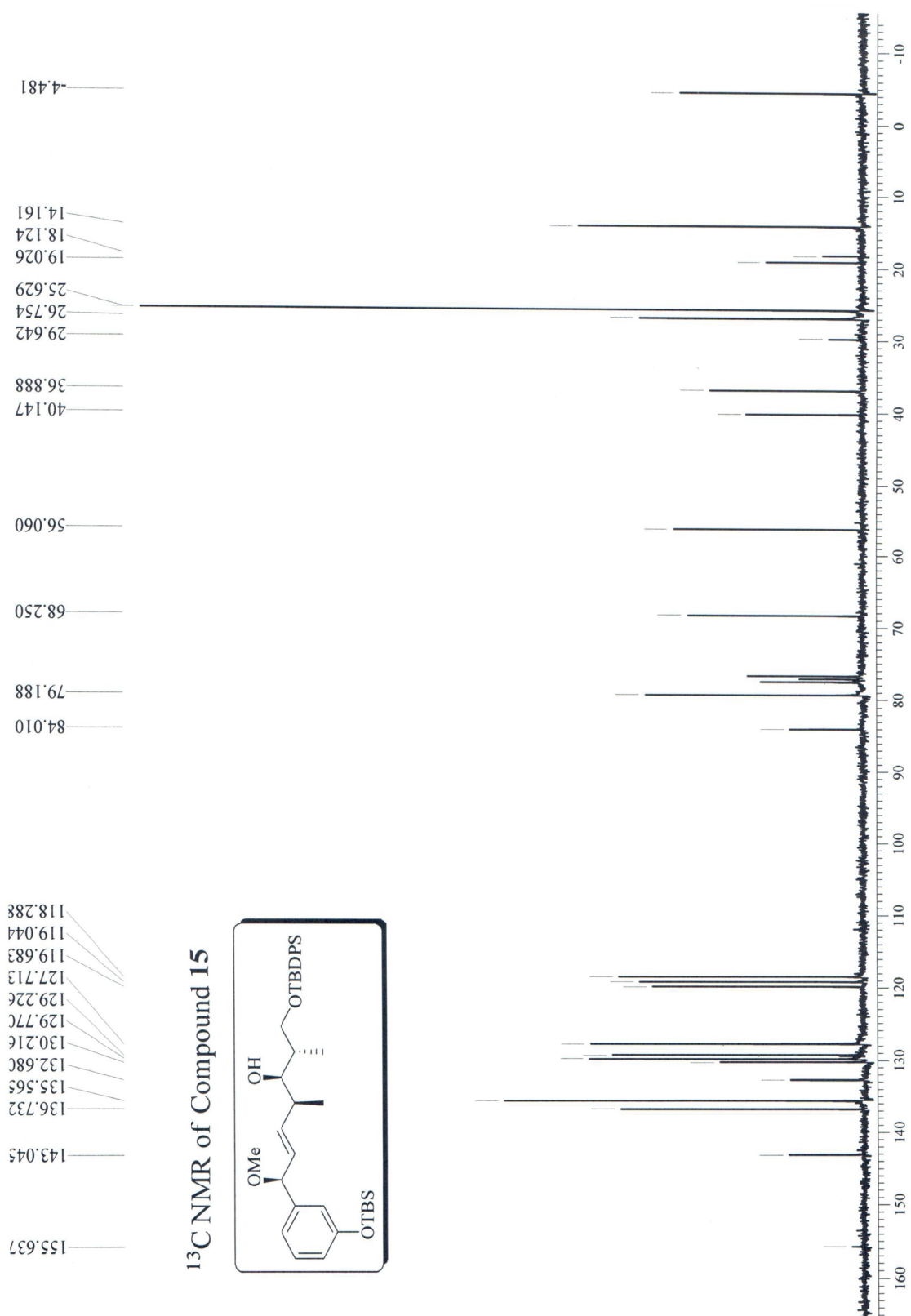


¹H NMR of Compound 5



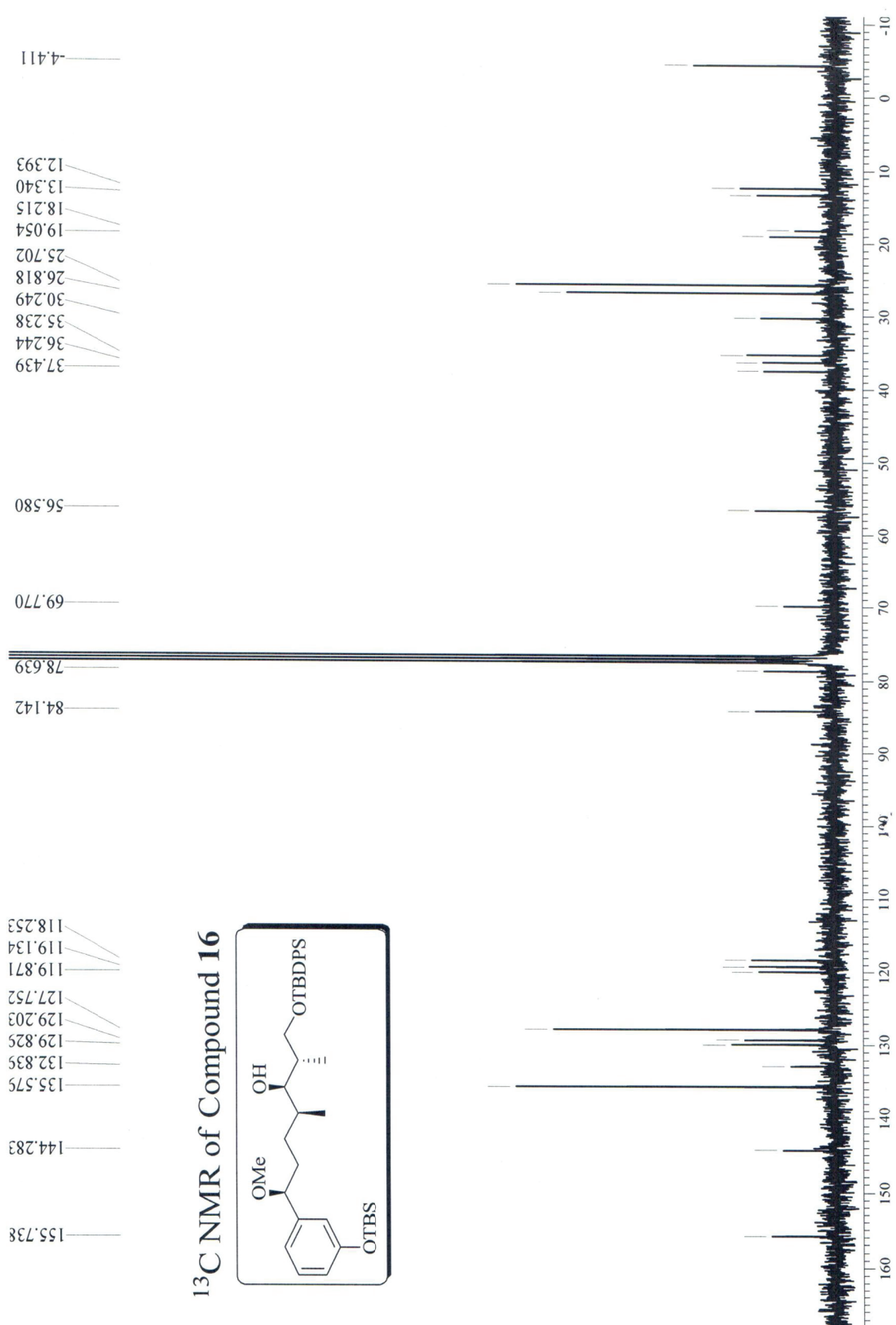




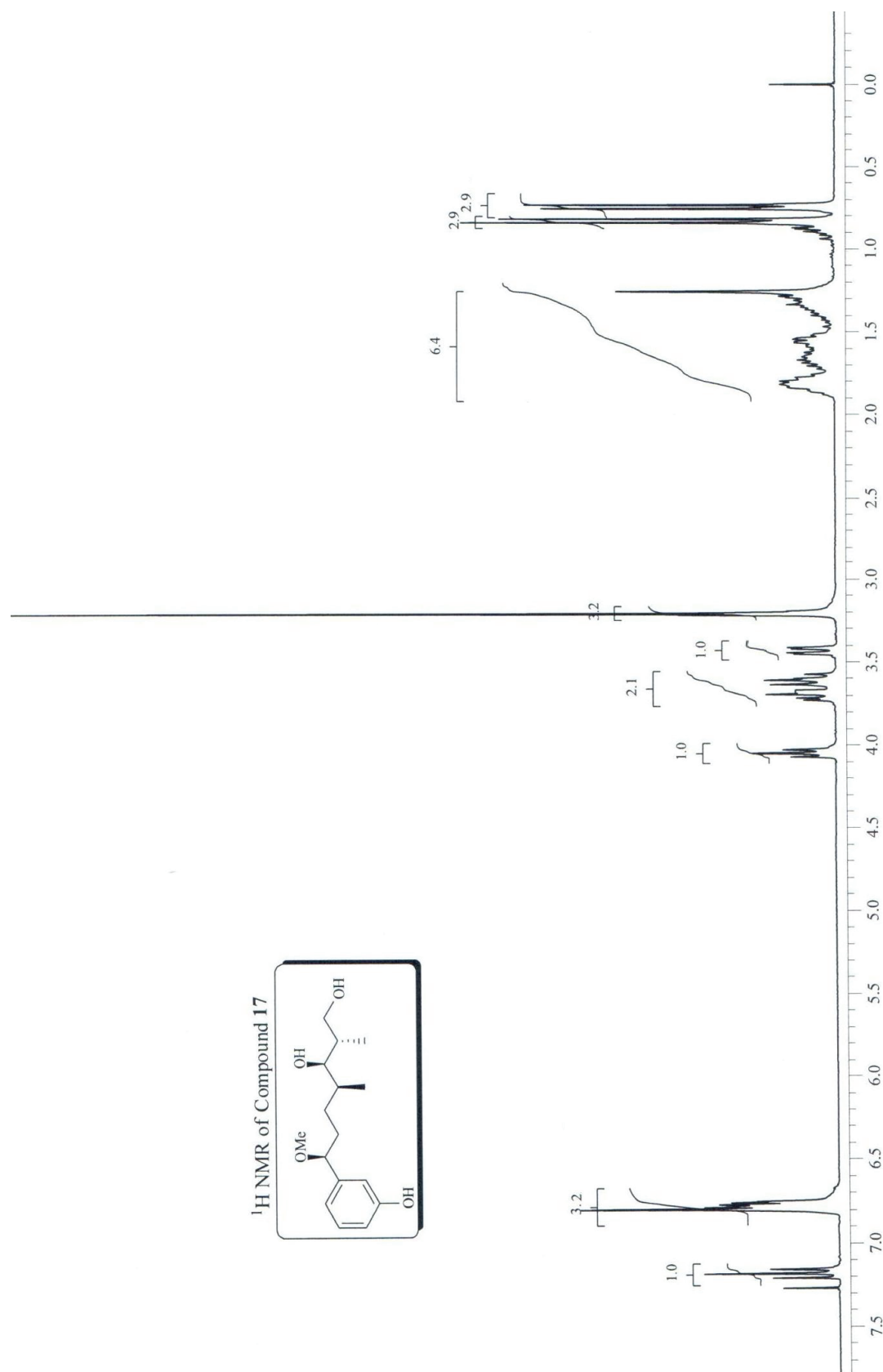


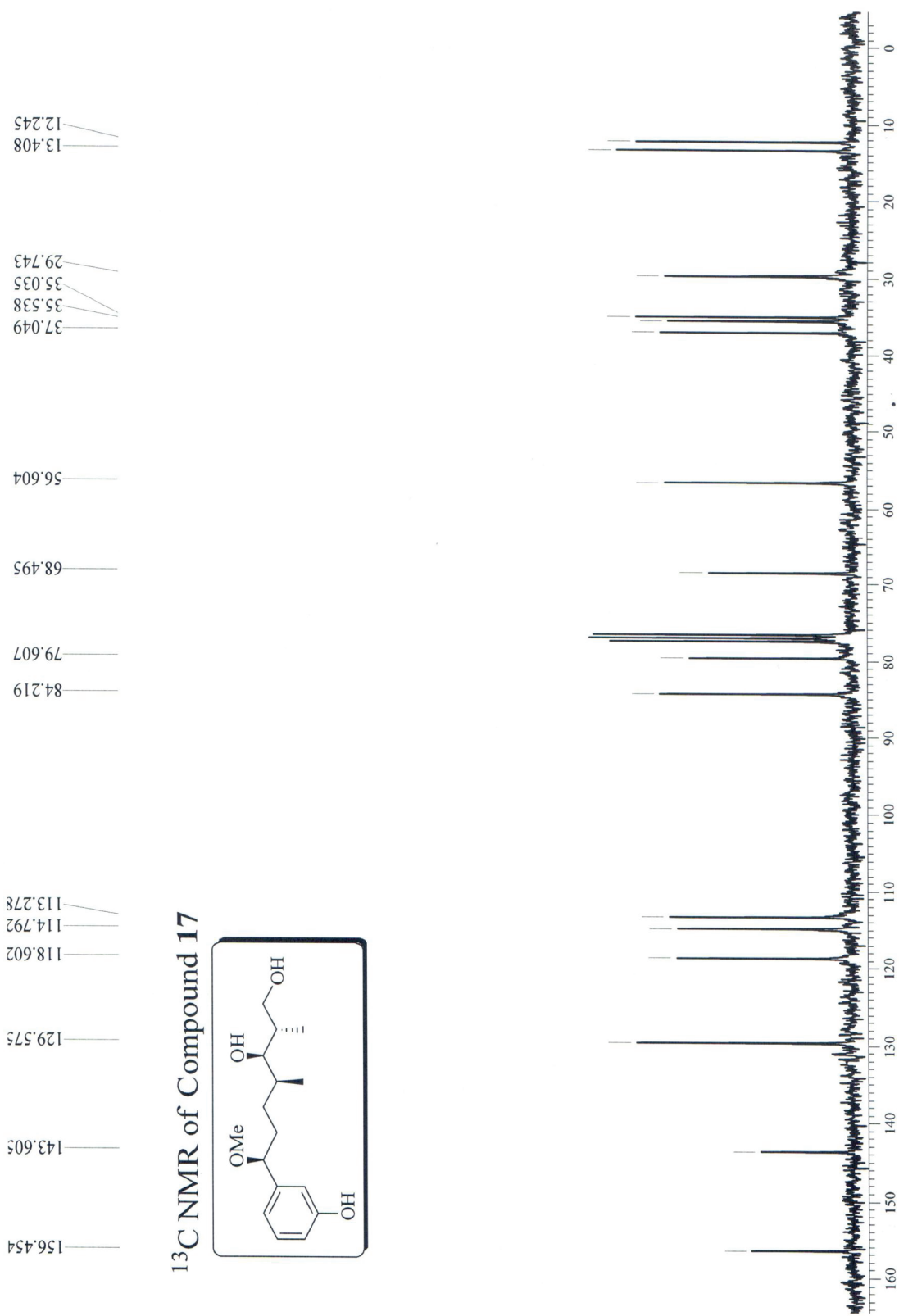
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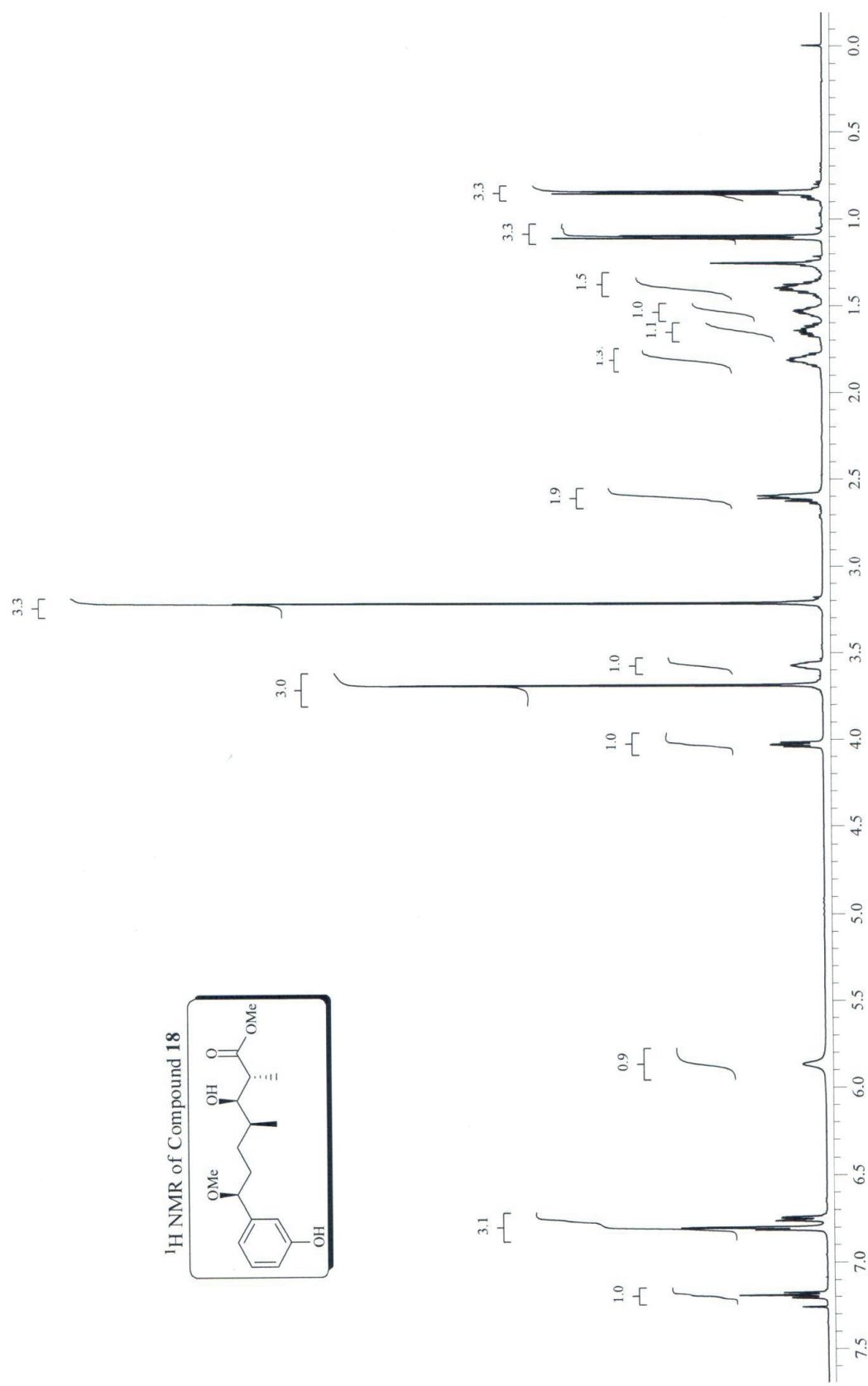


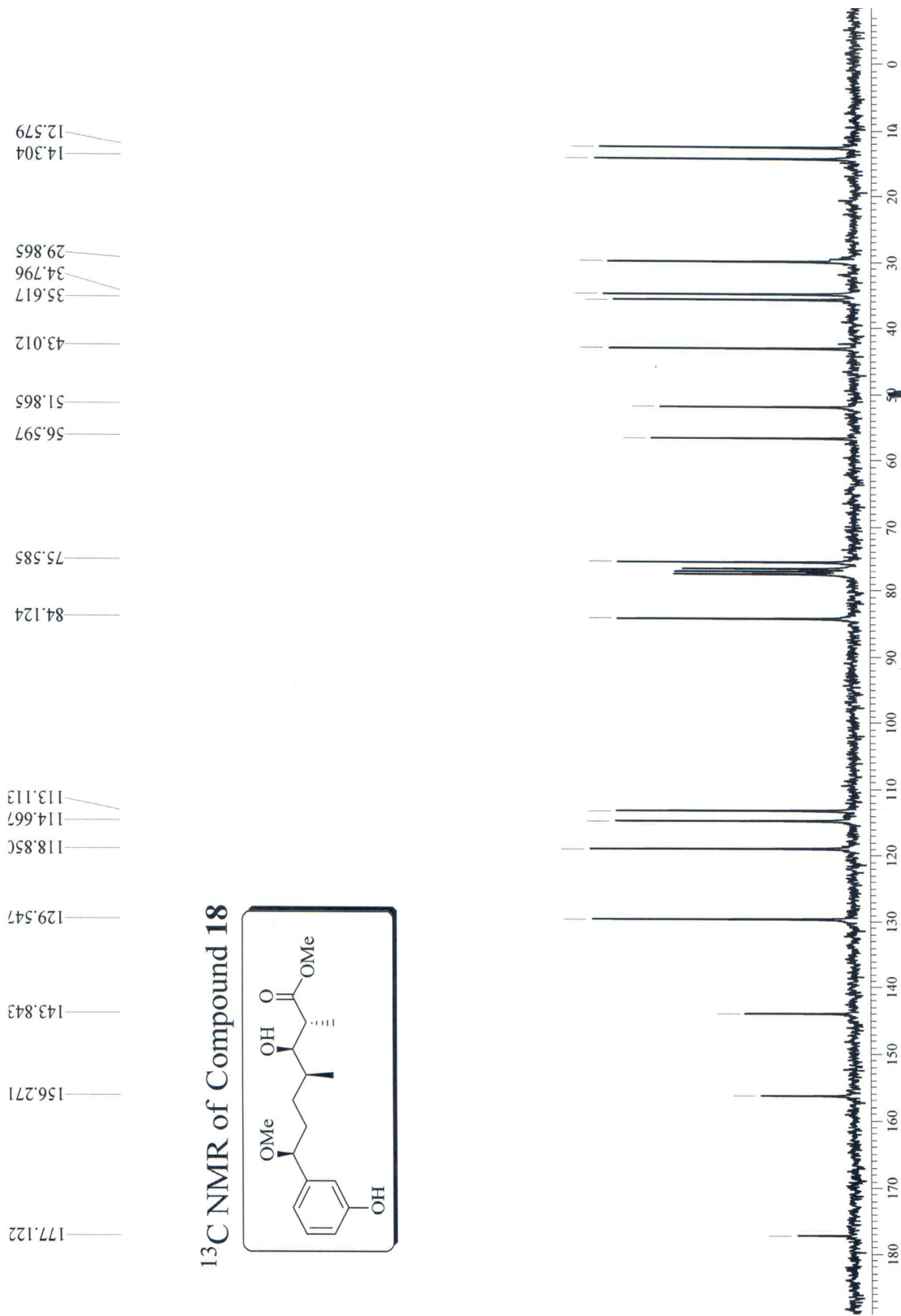


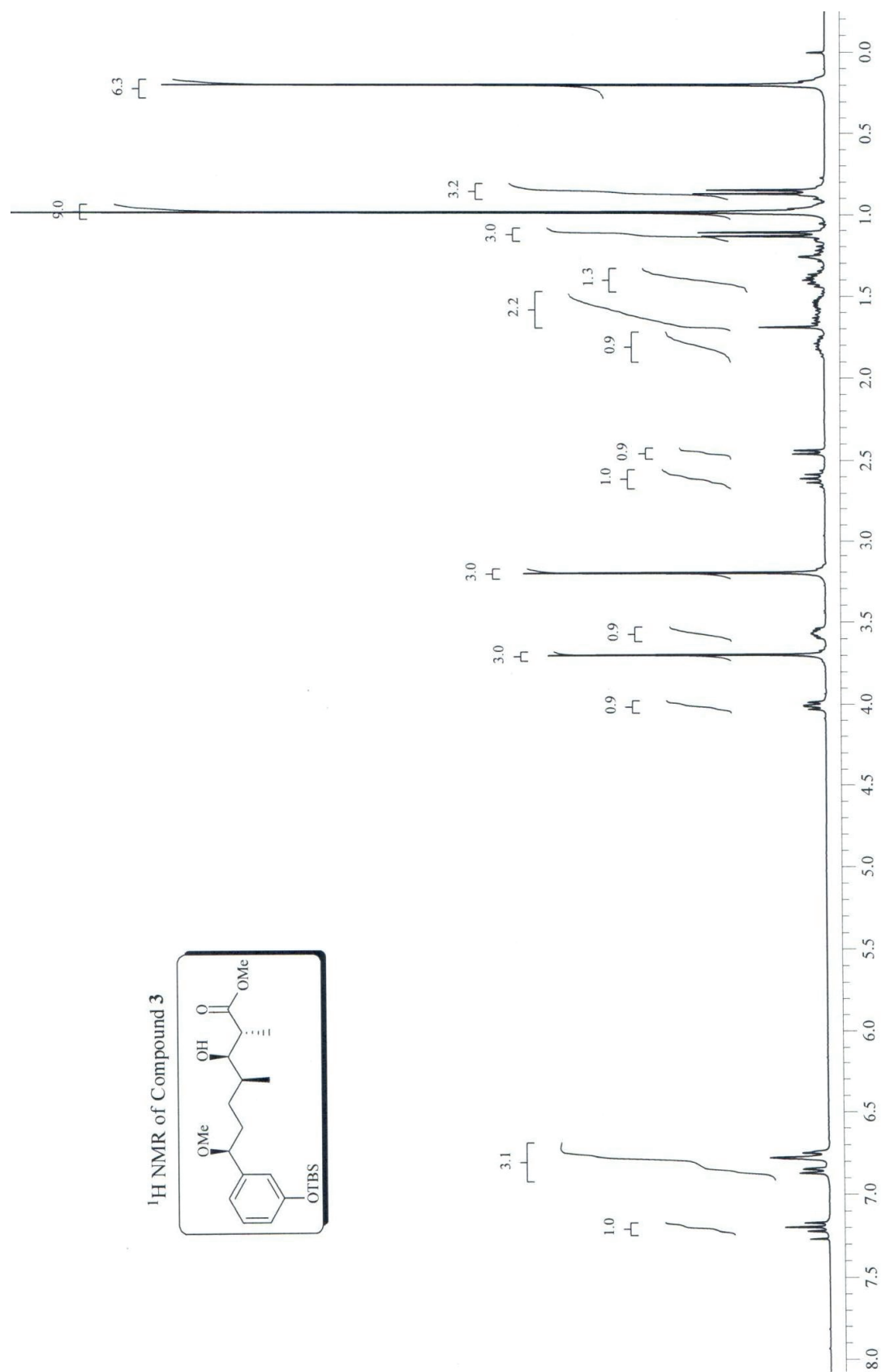
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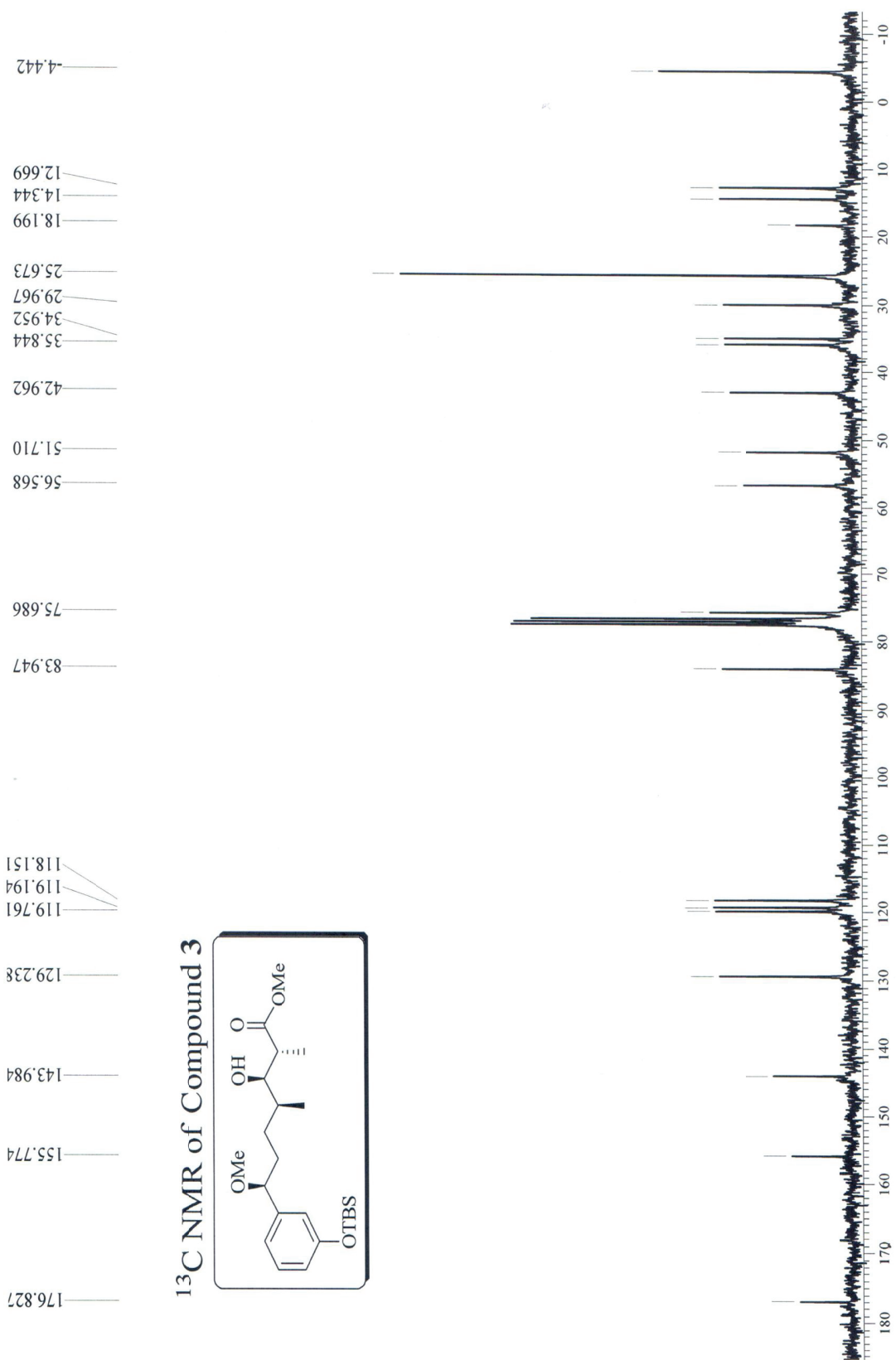


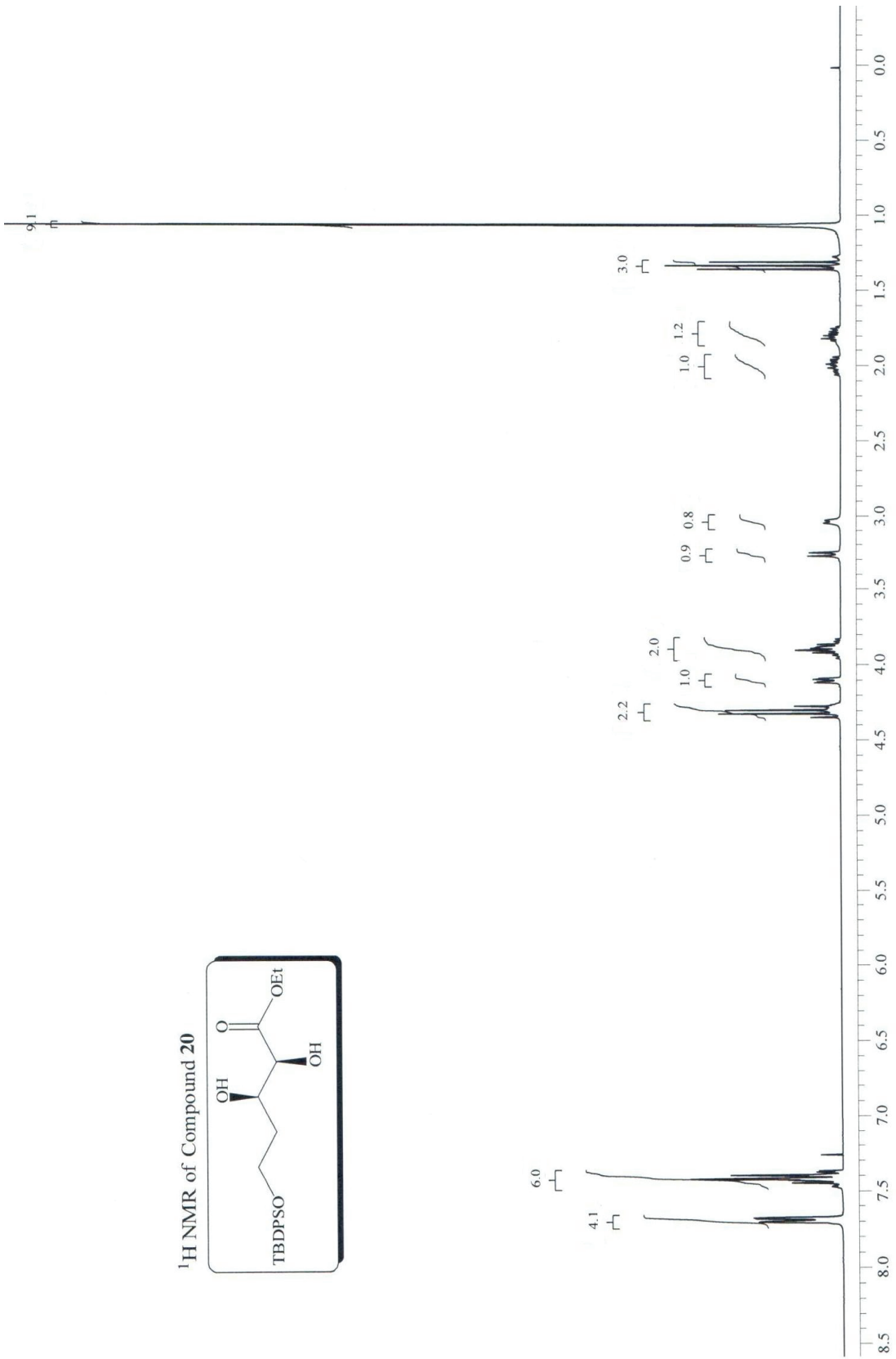
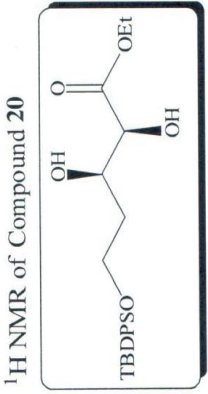


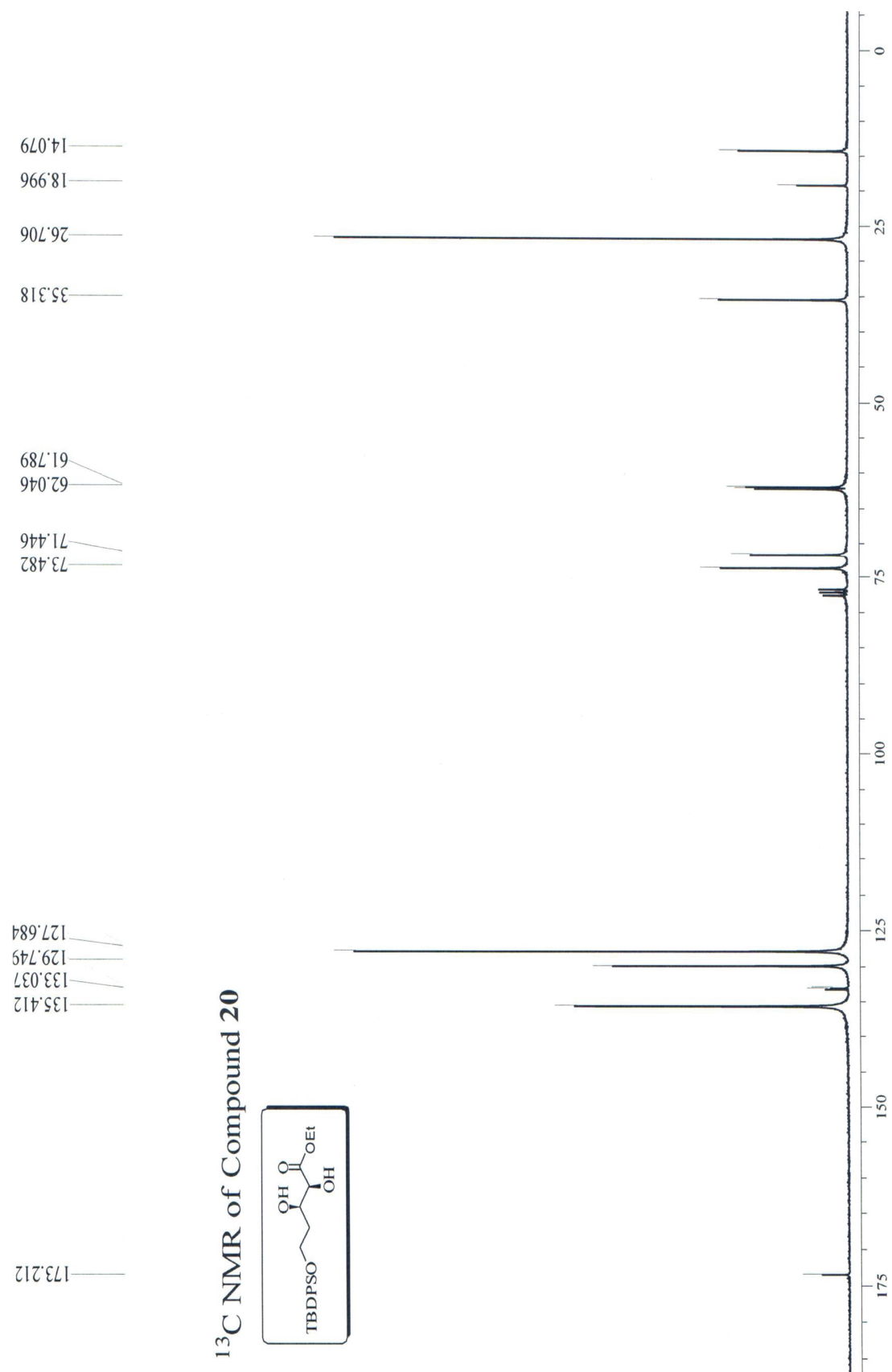




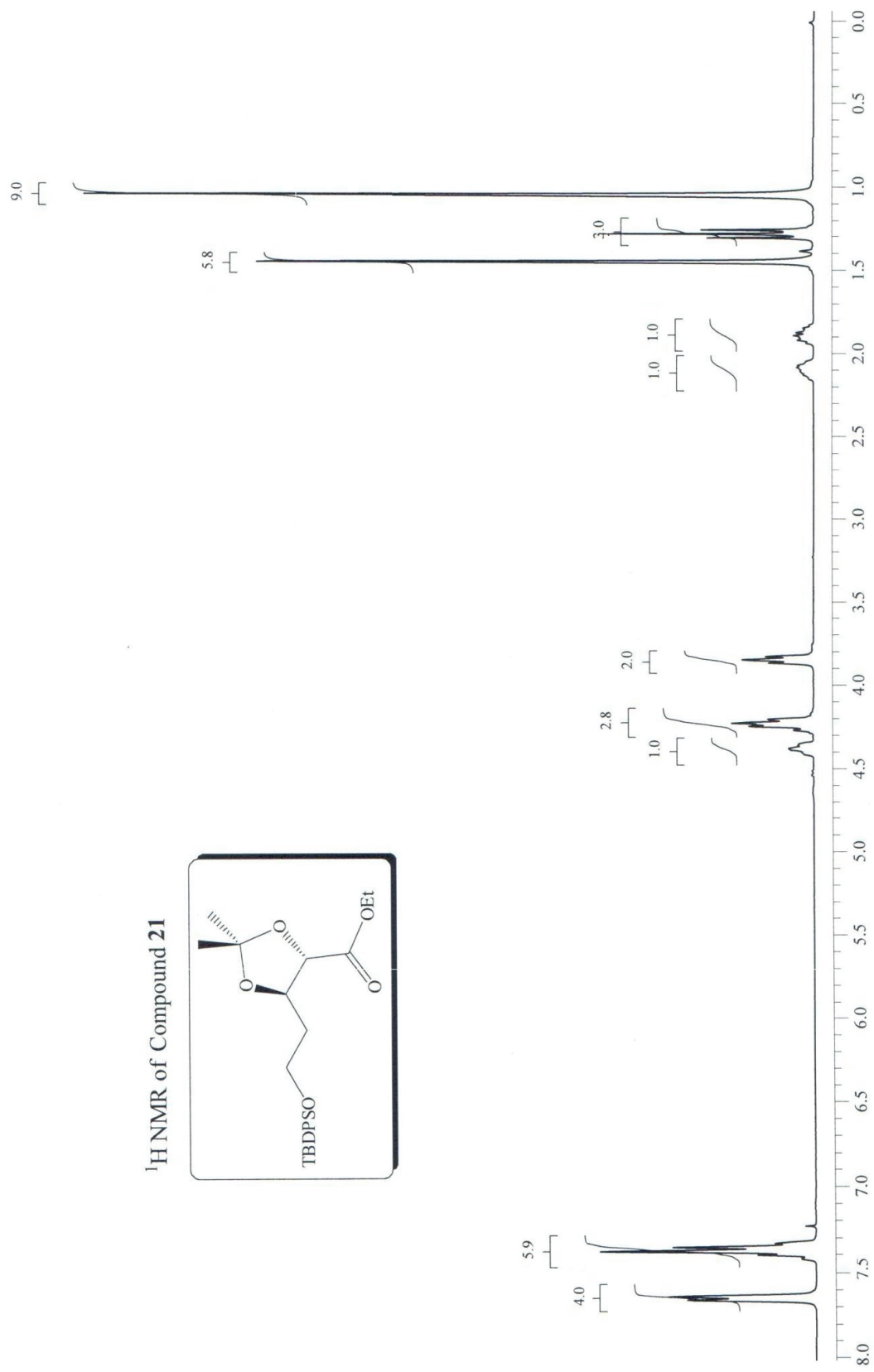


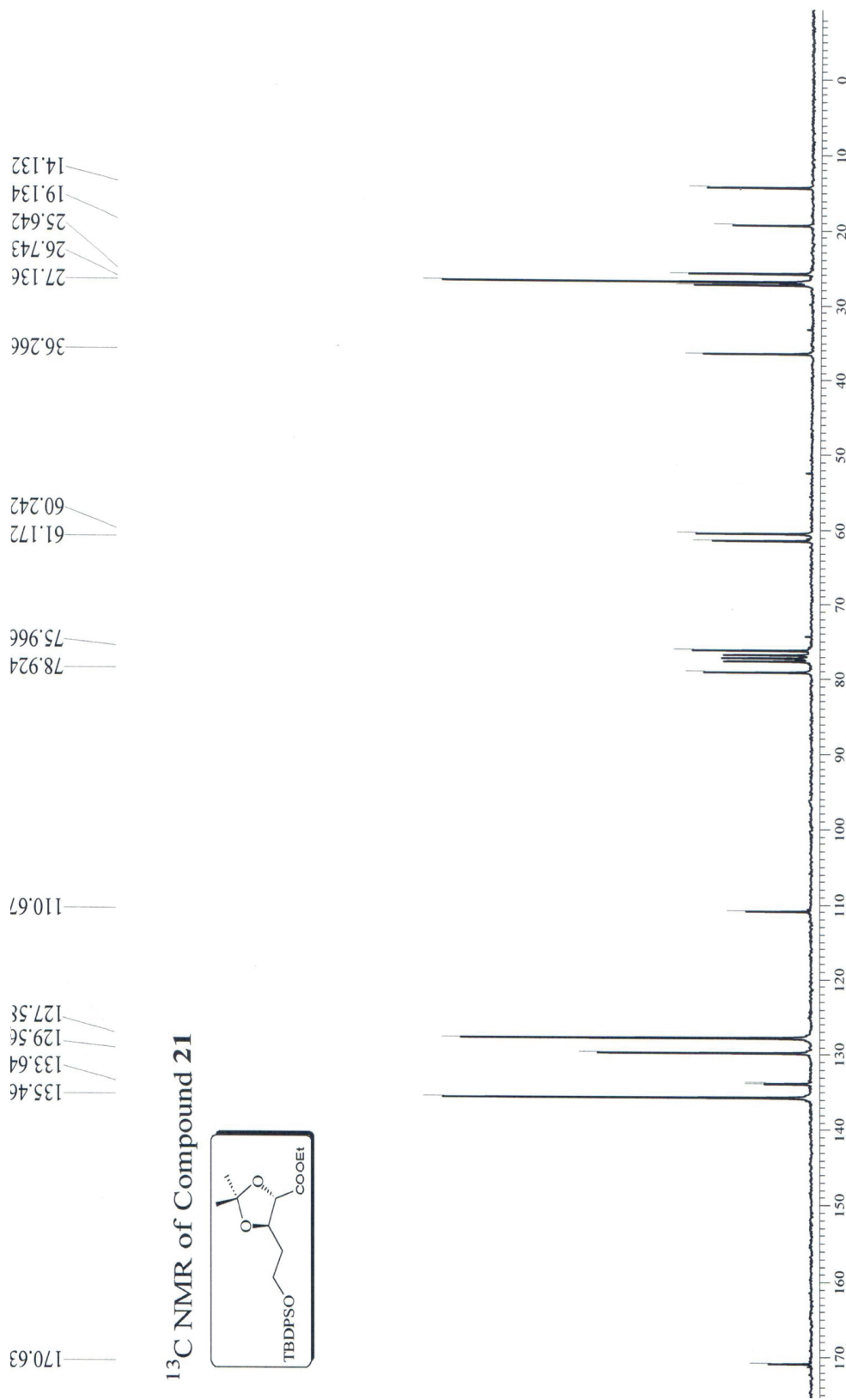




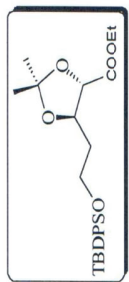


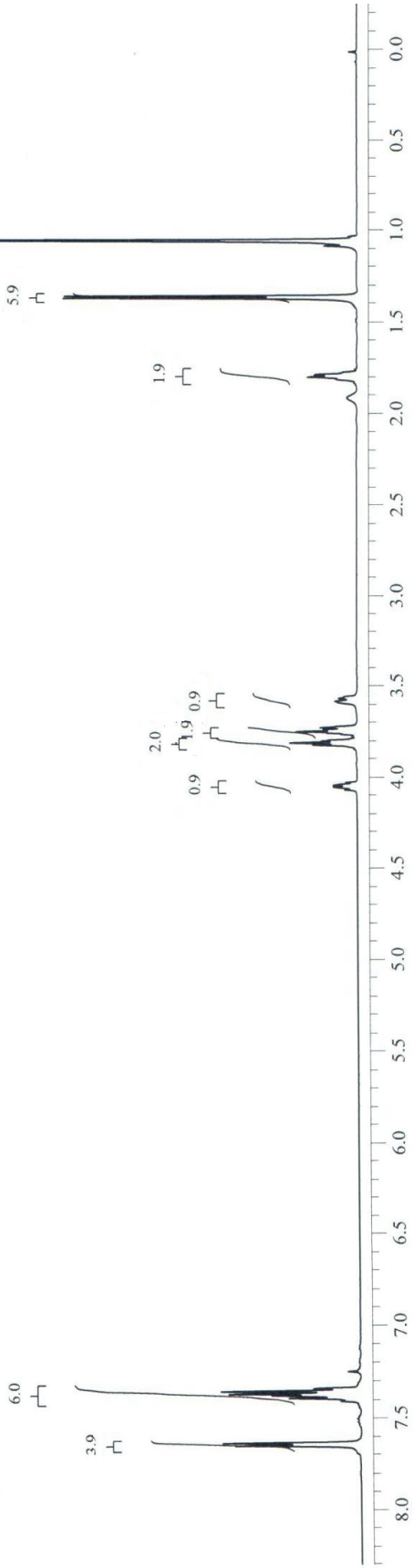
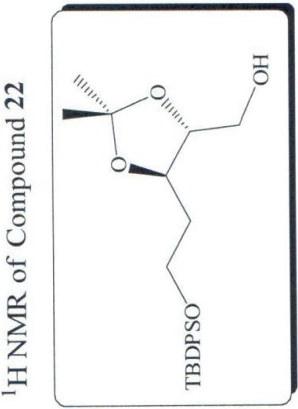
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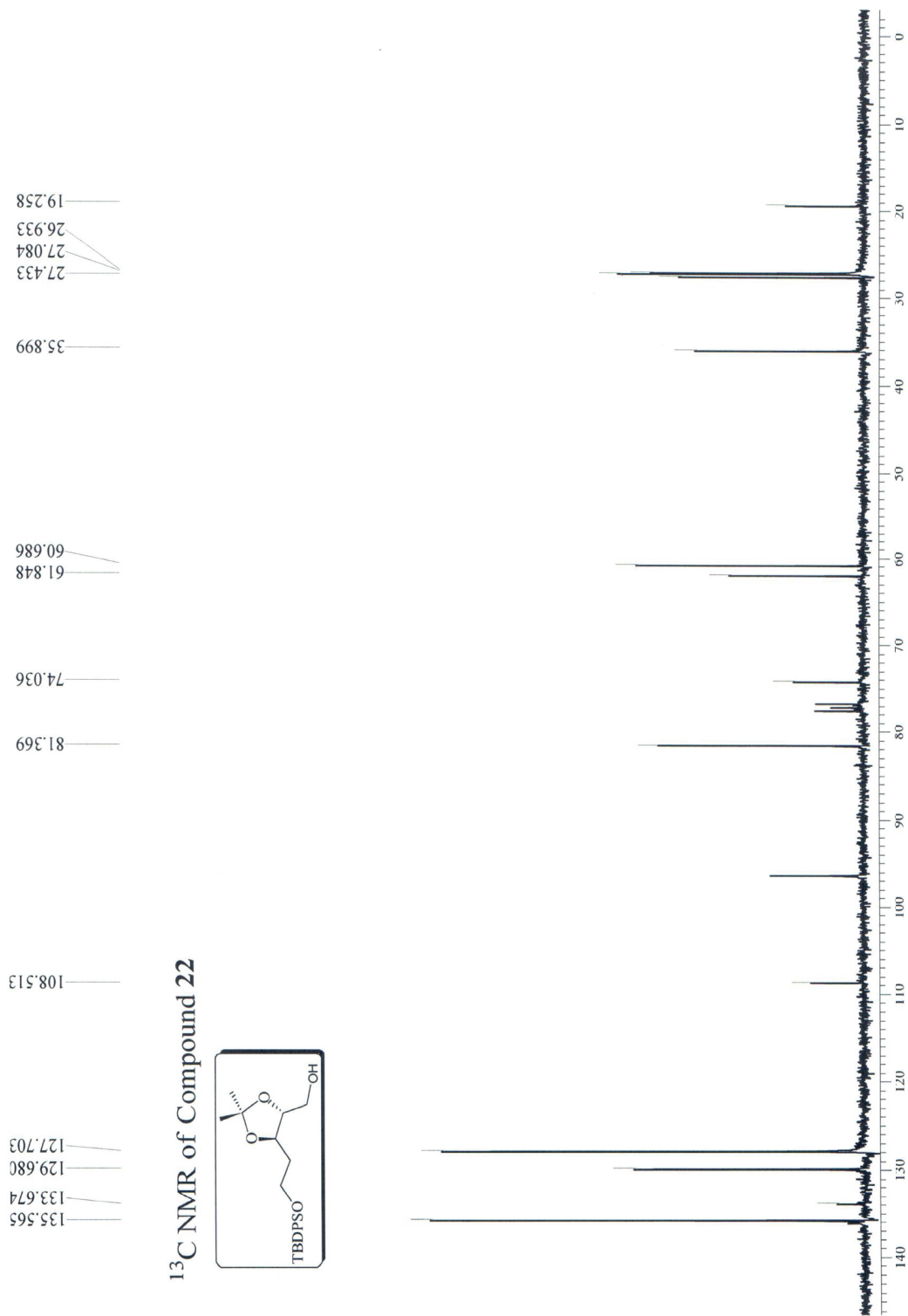




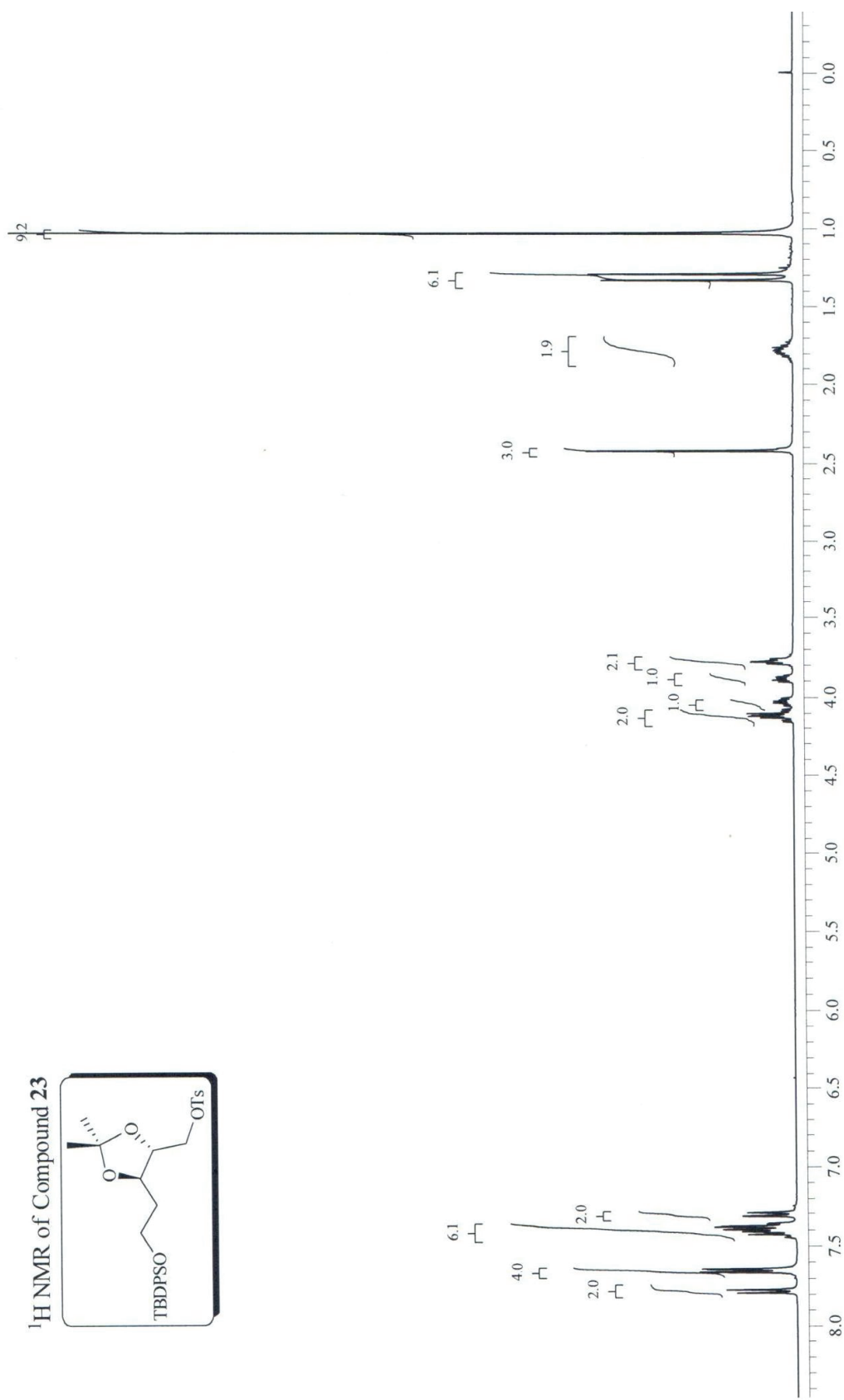
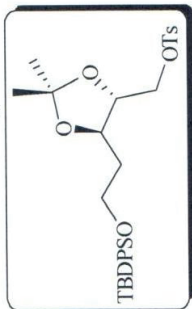
¹³C NMR of Compound 21

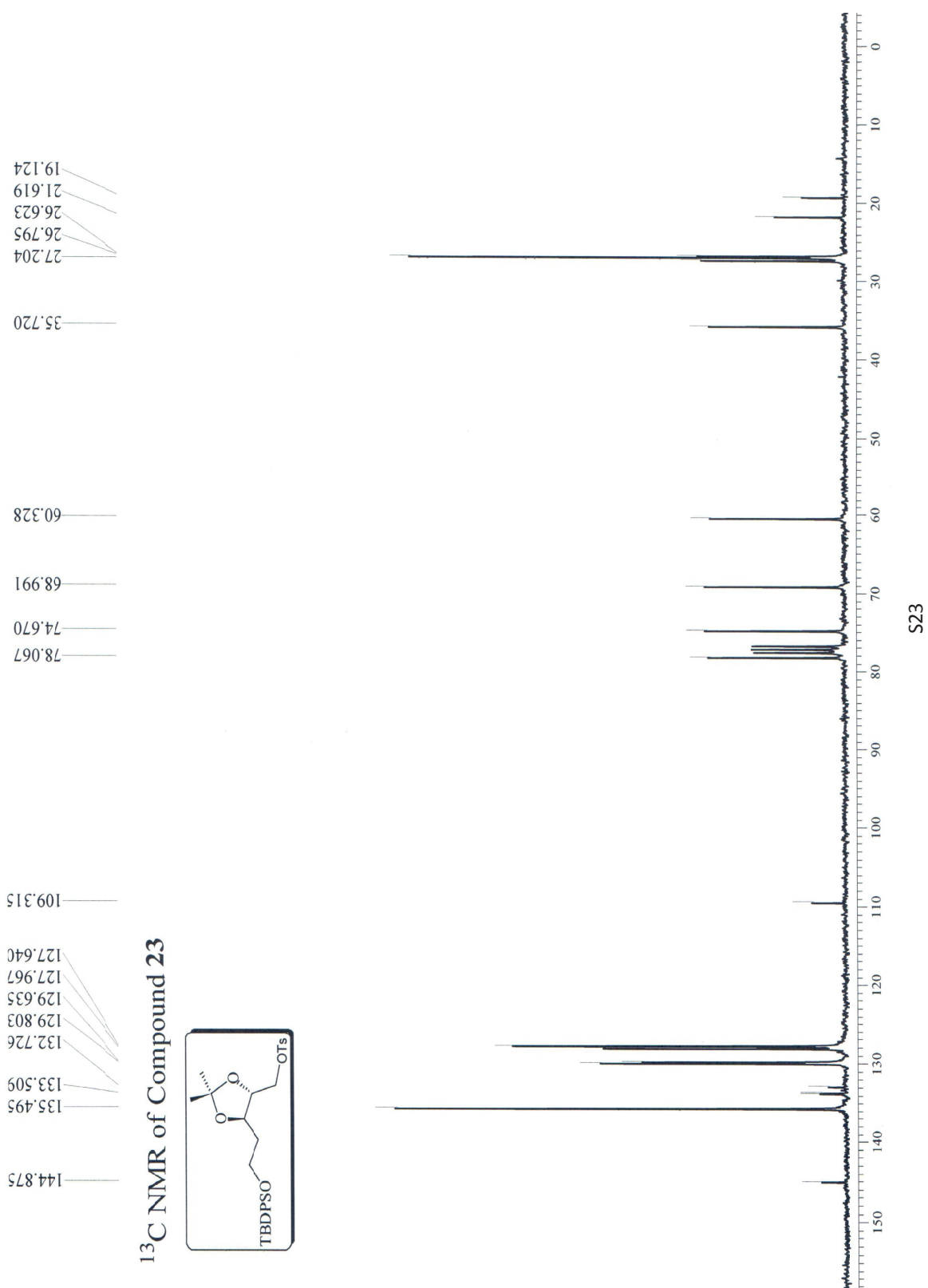


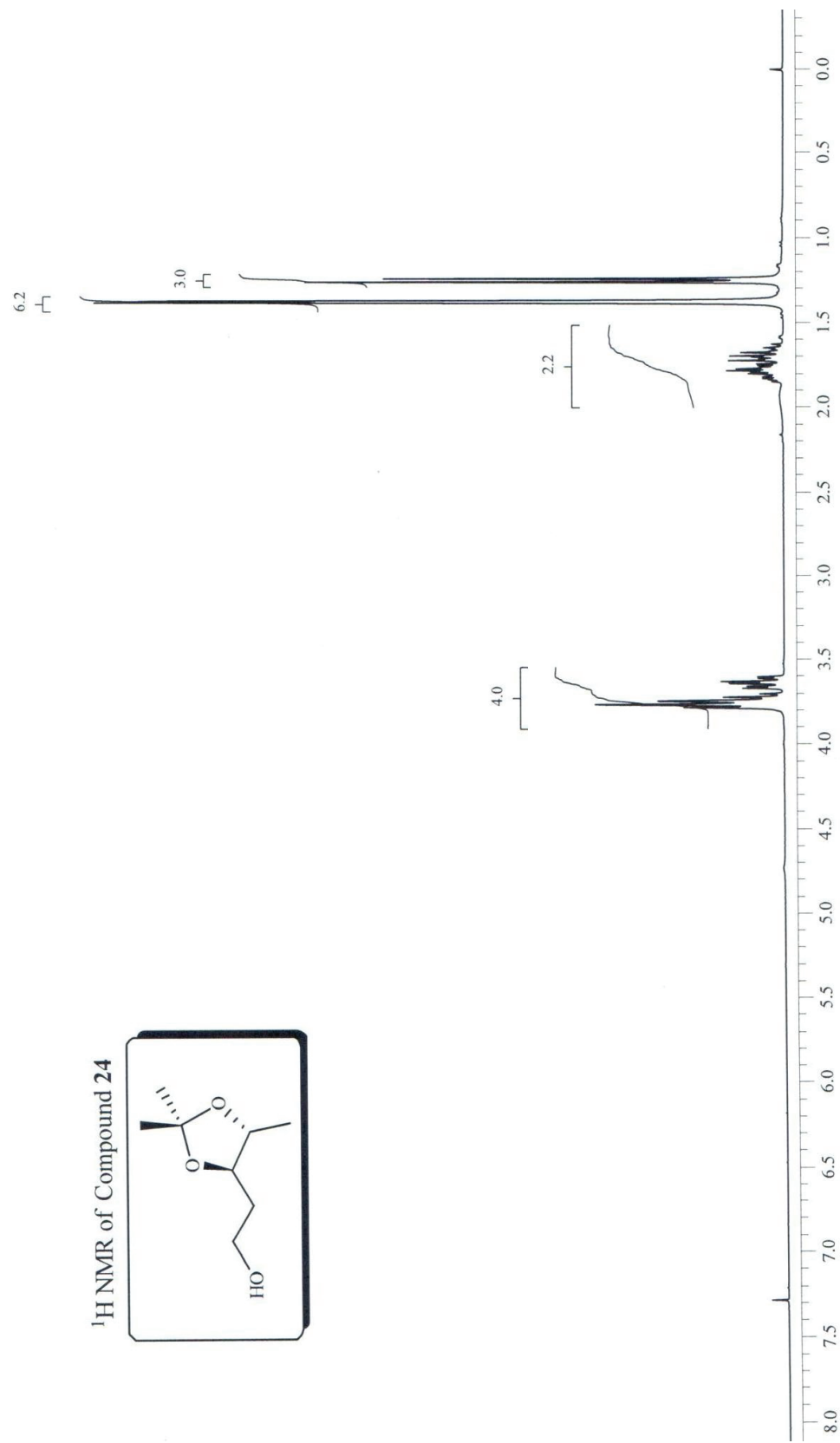


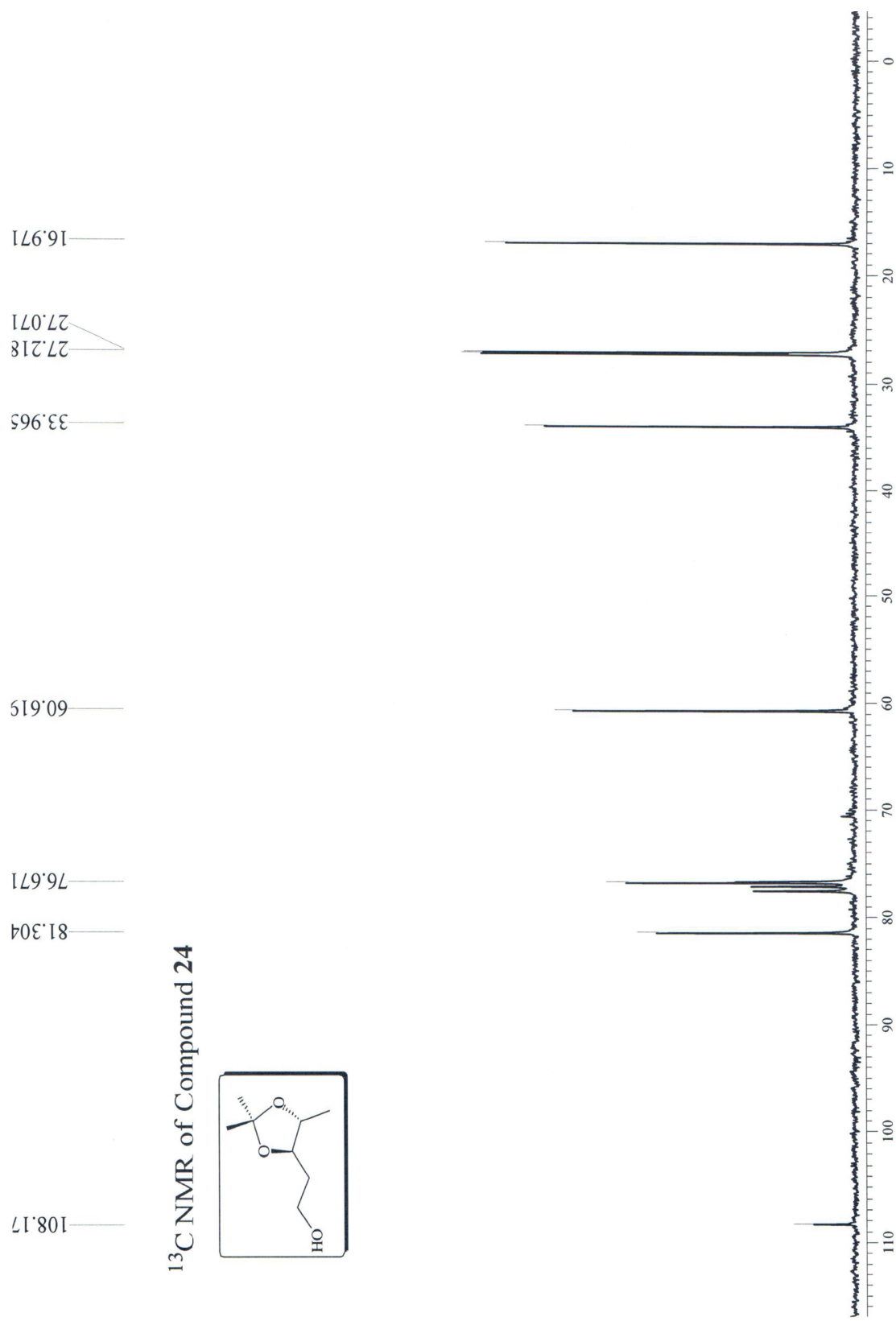


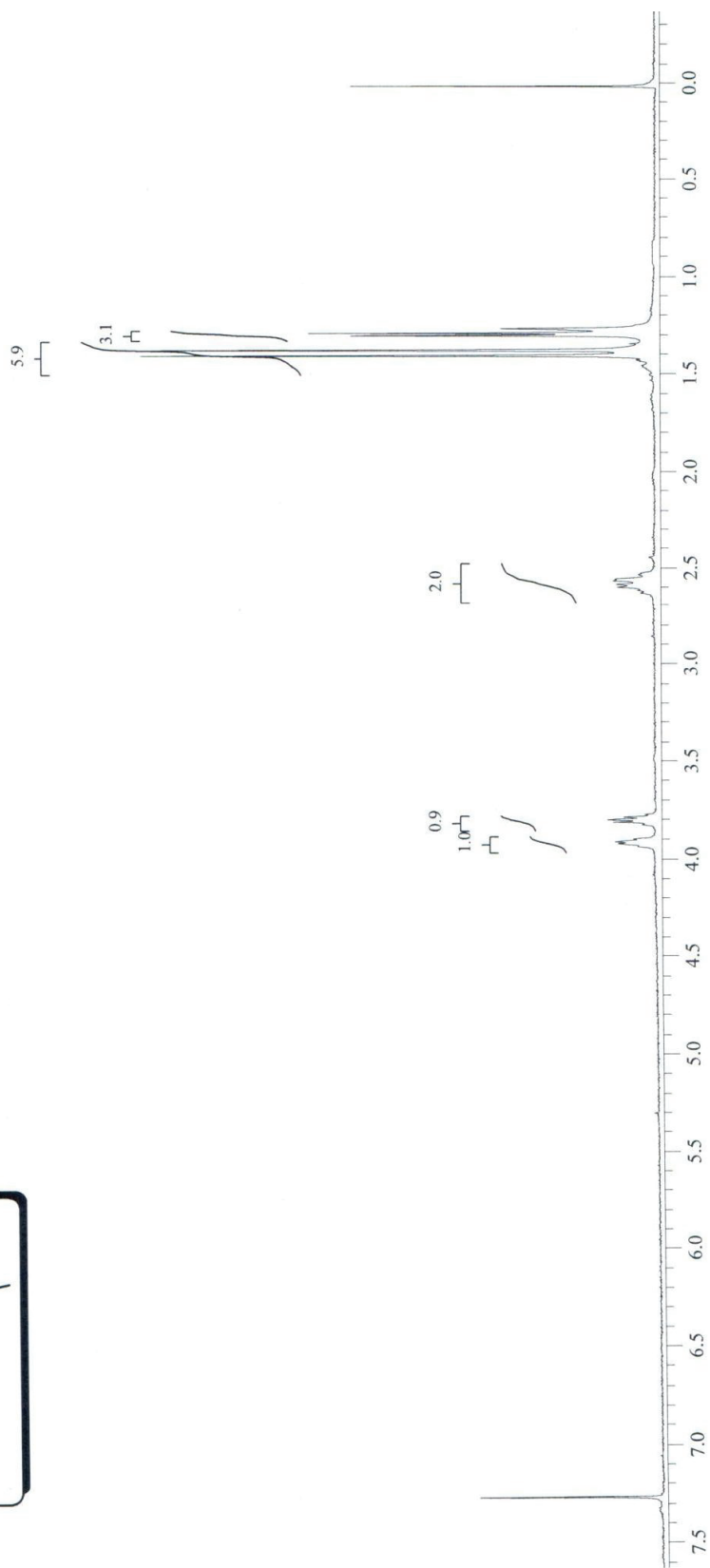
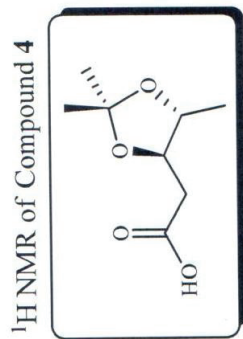
¹H NMR of Compound **23**

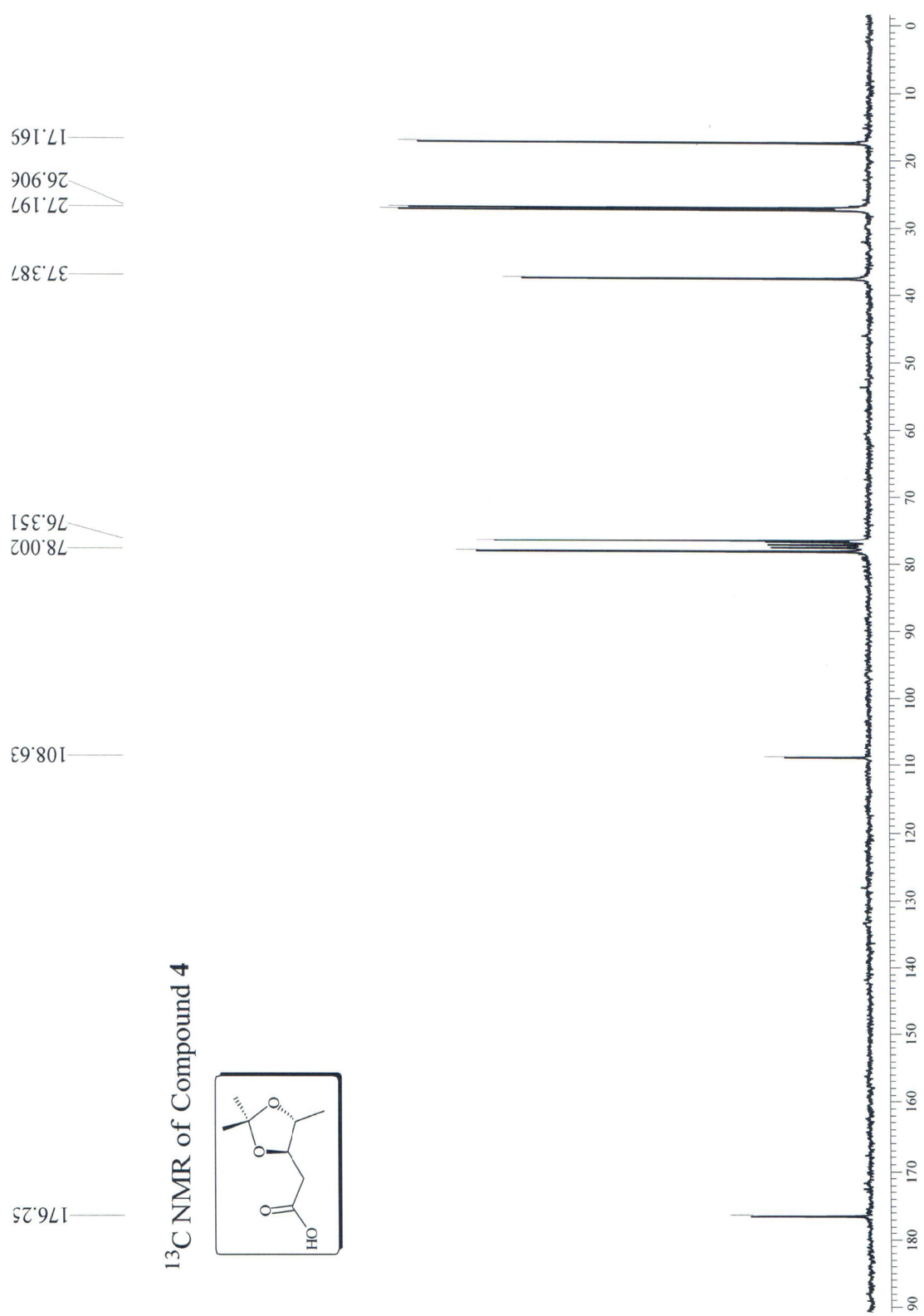


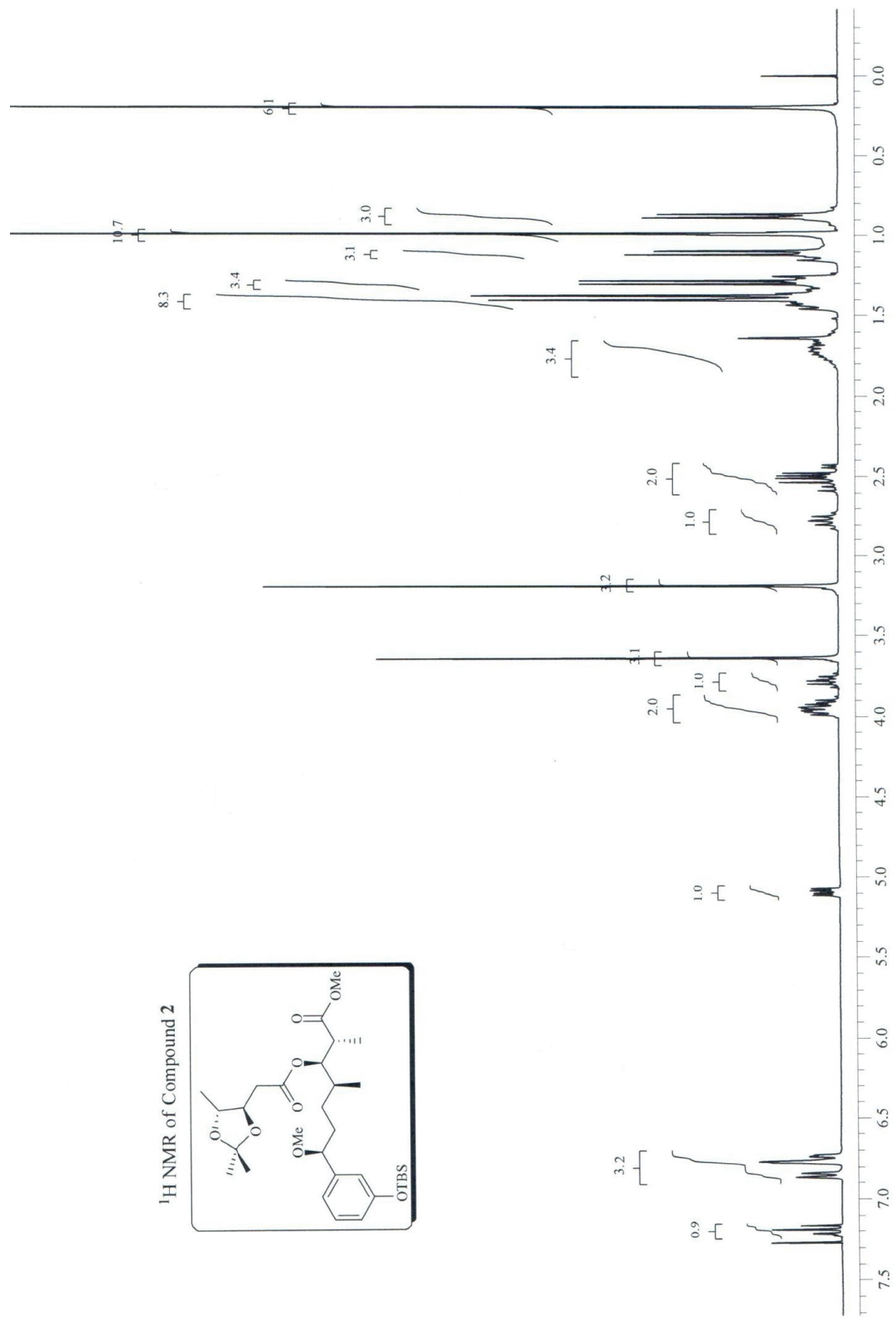


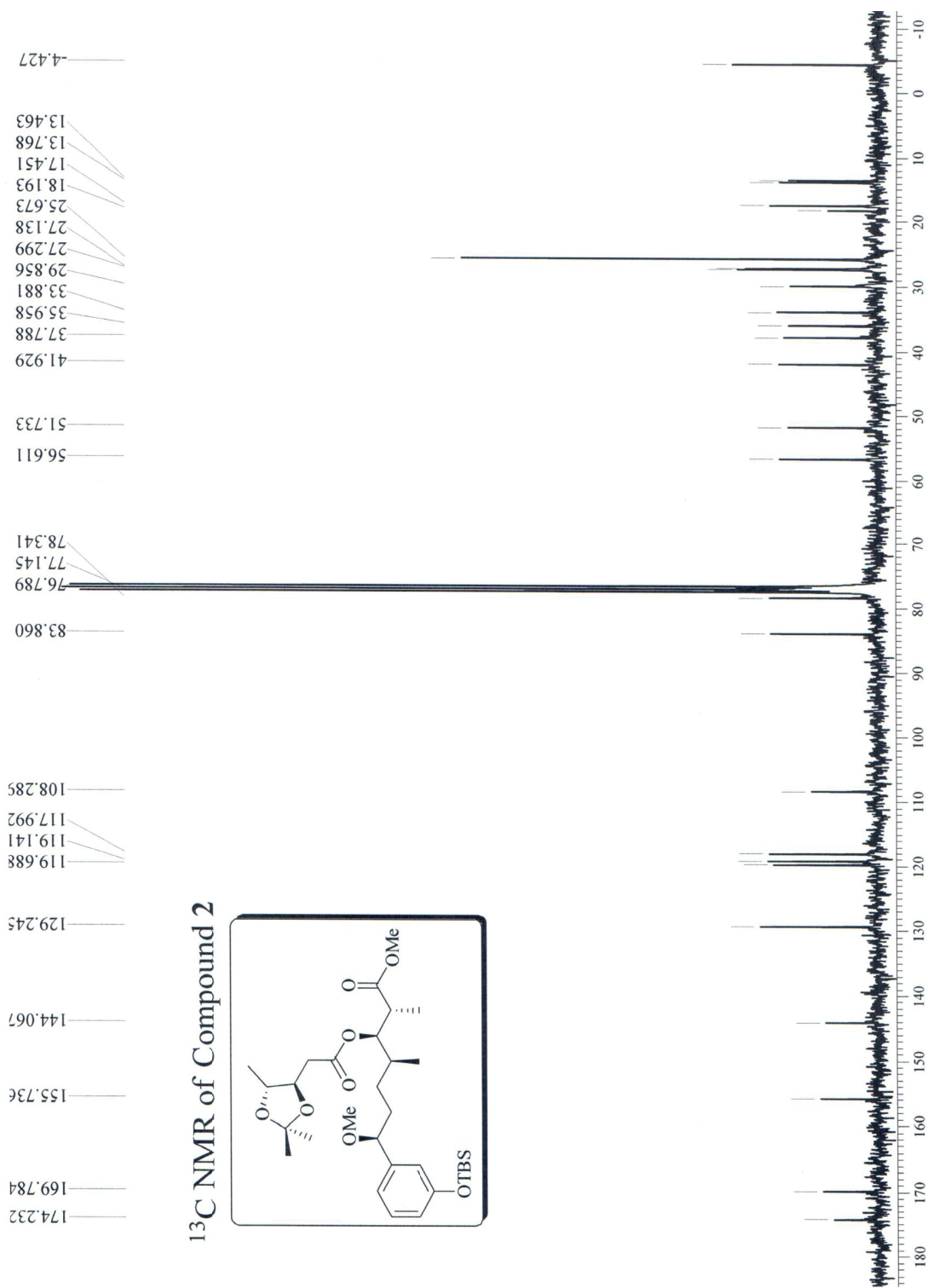


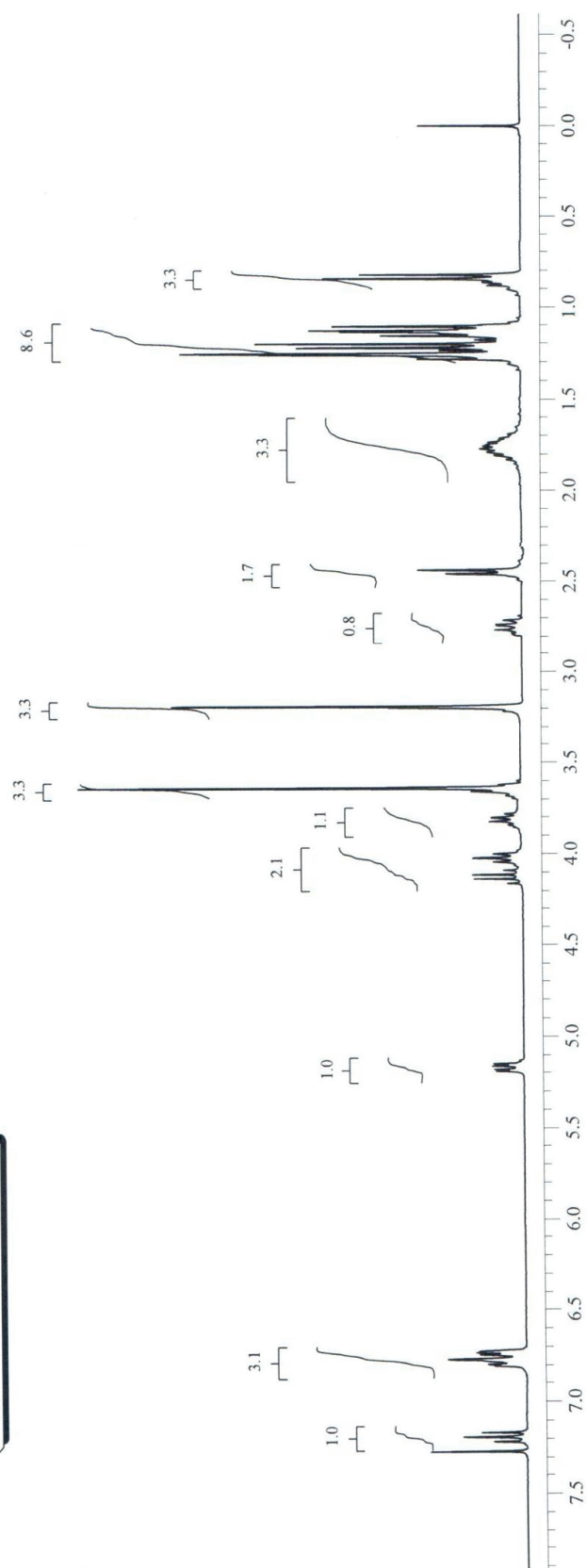
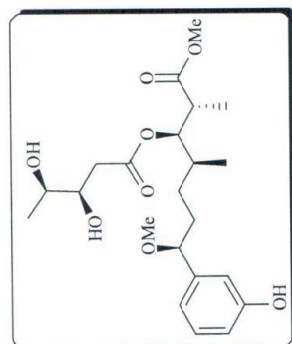


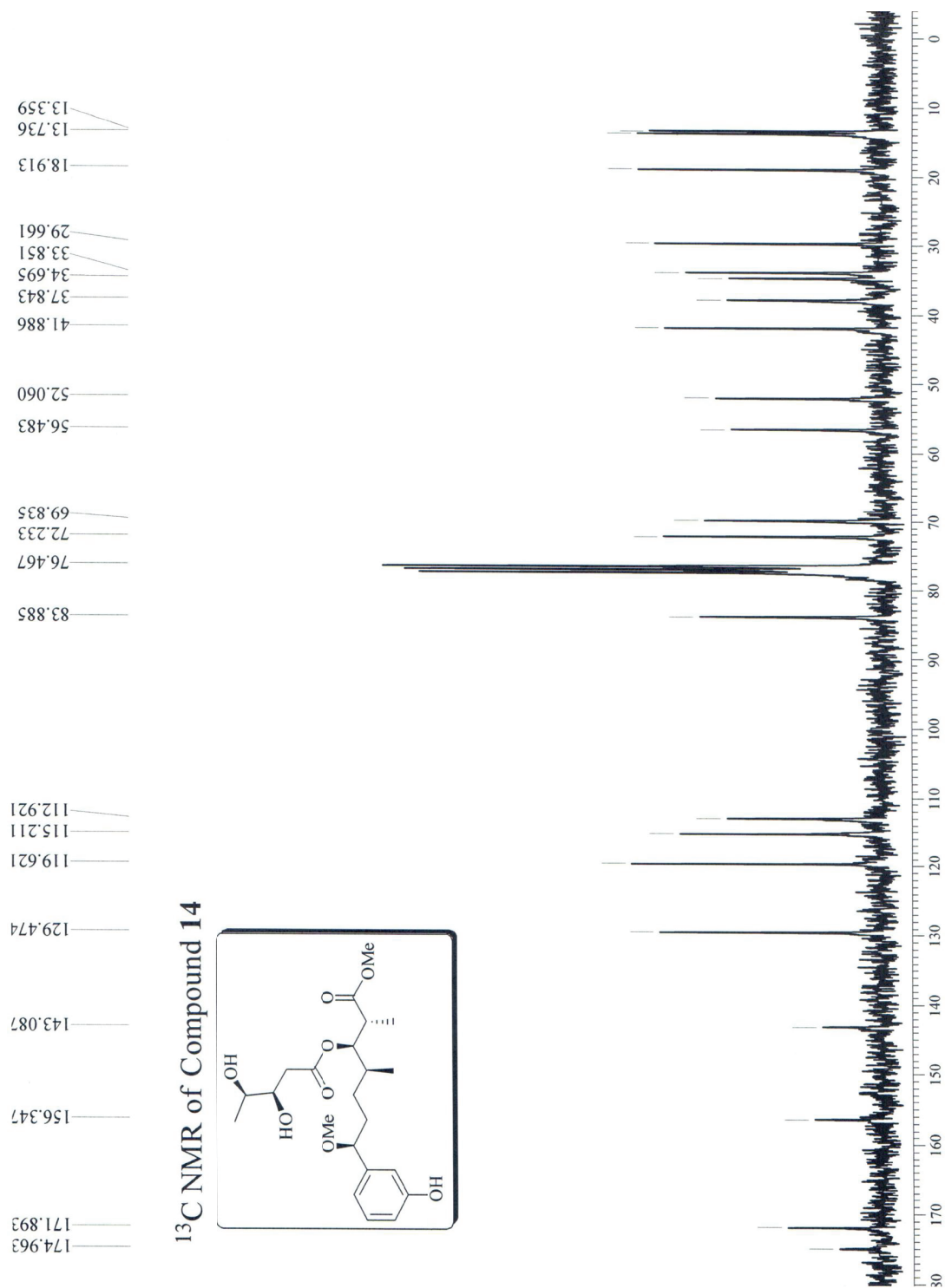


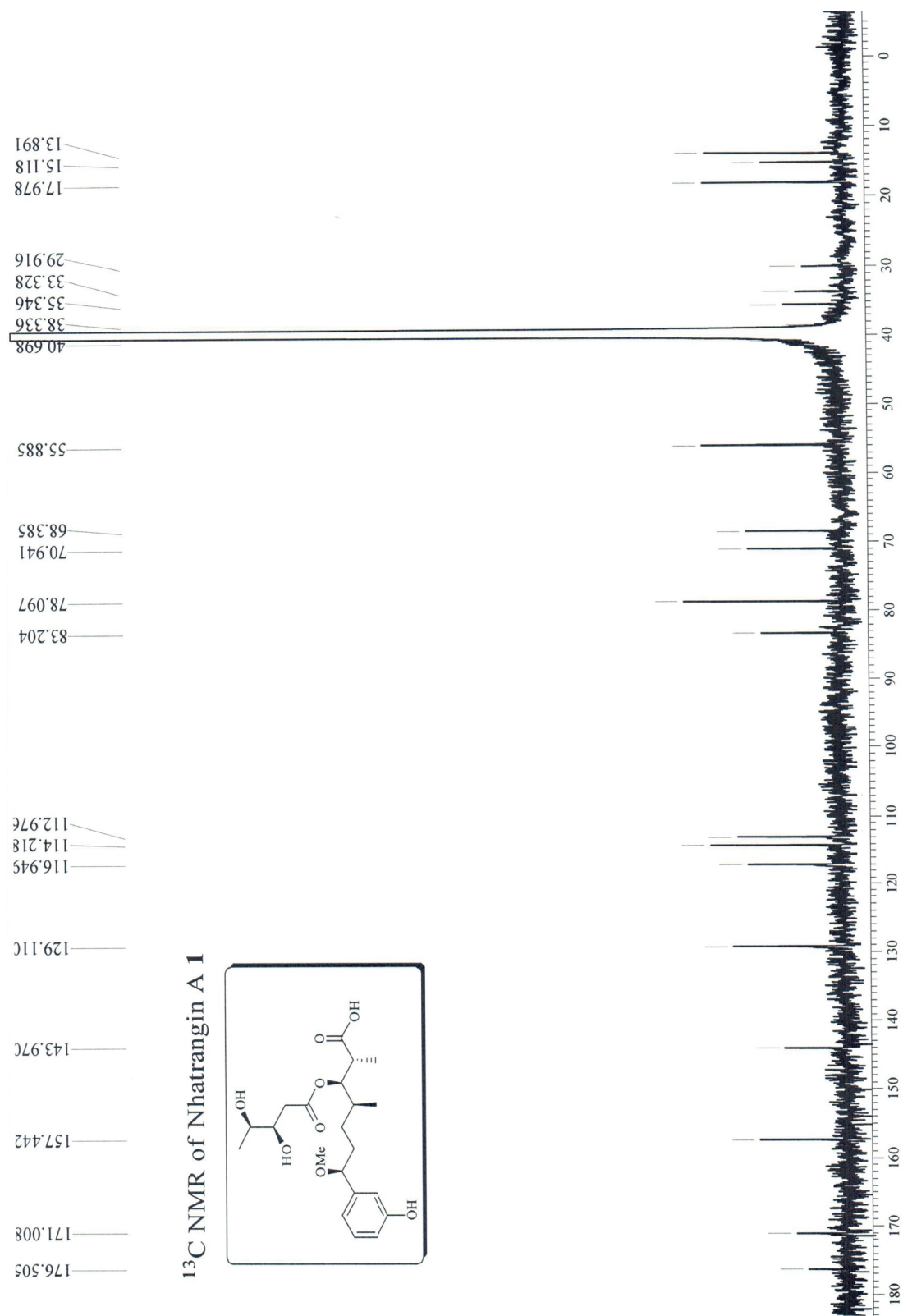


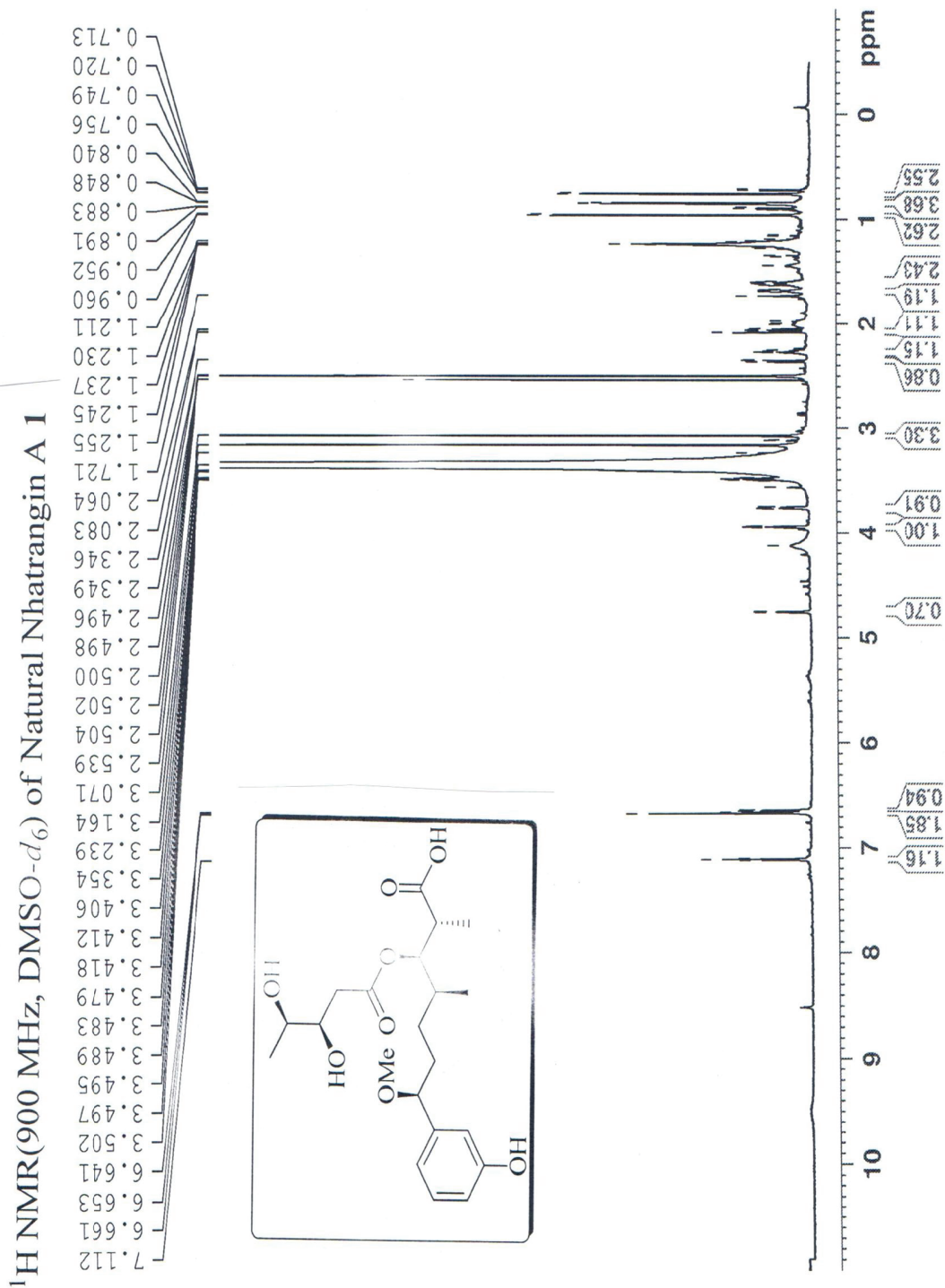




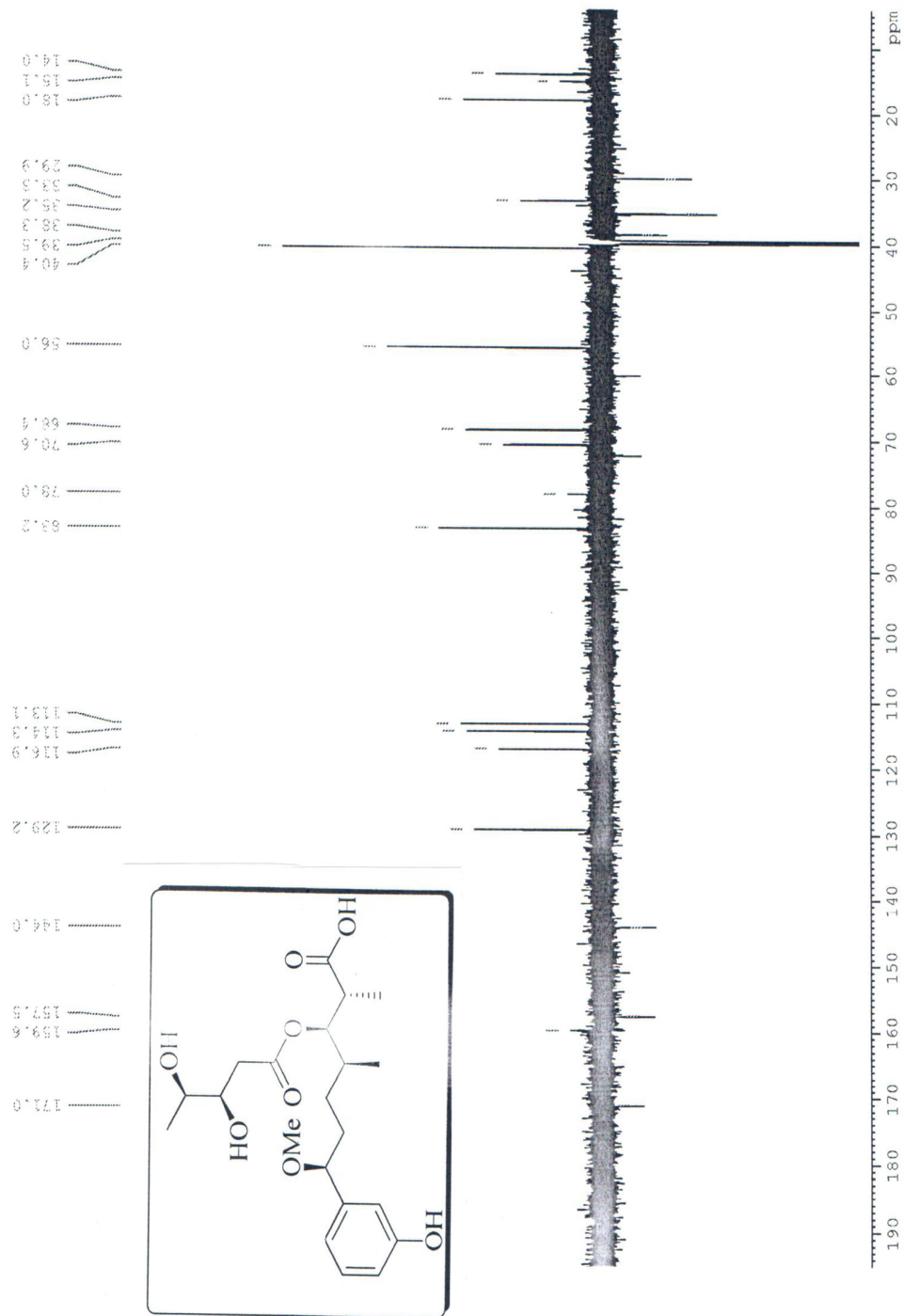




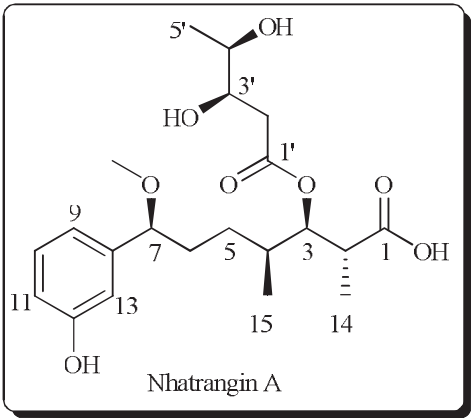




DEPTQ Spectrum (226 MHz, DMSO-*d*₆) of Natural Nhatrangin A 1



Comparison Table:



Comparison of NMR Data of Natural and Synthetic Nhatrangins A (1).

position	δ_C , natural	δ_C , synthetic	δ_H , m(in Hz) natural	δ_H , m(in Hz) , synthetic
1	176.5	176.5		9.31, s
2	40.4	40.6	2.26, dd(8.3, 3.6)	2.25, d (7.8)
3	78.0	78.0	4.74, dd (8.3, 3.6)	4.79, dd (7.8, 4.4)
4	33.3	33.3	1.67, qd (6.7, 3.6)	1.67, m
5	30.0	29.9	1.23, m	1.23, m
6	35.2	35.3	1.60, m	1.62, m
7	83.3	83.2	3.93, dd (7.4, 5.4)	3.94, dd (7.6, 4.4)
7-OMe	56.0	55.9	3.07, s	3.08, s
8	144.0	144.0		
9	113.1	113.0	6.65, m	6.65, m
10	129.2	129.1	7.10, t (7.8)	7.11, t (7.8)
11	116.9	116.9	6.63, m	6.63, m
12	157.5	157.4		
13	114.3	114.2	6.67, m	6.66, m
14	15.1	15.2	0.83, d (7.0)	0.82, d (7.8)
15	14.0	13.9	0.74, d (6.7)	0.72, d (6.6)
1'	171.1	171.0		
2'a	38.3	38.3	2.35, dd (14.3, 3.2)	2.36, dd (15.4, 4.4)
2'b			2.05, dd (14.3, 10.5)	2.17, dd (15.4, 5.5)
3'	70.6	70.9	3.75, ddd (10.5, 4.2, 3.2)	3.74, m
4'	68.4	68.4	3.48, qd (6.4, 4.2)	3.50, qd (6.5, 4.2)
5'	18.0	18.0	0.95, d (6.4)	0.93, d (6.6)

Determination of the enantiomeric excess of (S)-12 and (R)-12a: The ee was determined by chiral HPLC analysis using a Chiralcel OD-H column. The 3% iso propanol in hexane was used as mobile phase with, 0.7 mL/min flow rate. It has been established that the (S) enantiomer elutes first at 5.92 min and (R) enantiomer elutes at 6.39 min. The Acetate of (S) enantiomer elutes first at 3.10 min and acetate of (R) enantiomer elutes at 3.53 min compound.

