

## Supporting Information

### **A Simple and Economic Synthesis of Propargylamines by CuI Catalyzed Three-component Coupling Reaction with Succinic Acid as Additive**

Ge-rui Ren, Jin-li Zhang, Zheng Duan, Meng-jun Cui and Yang-jie Wu\*

Department of Chemistry, Henan key Laboratory of Chemical Biology and Organic Chemistry, Key Laboratory of Applied Chemistry of Henan Universities, Zhengzhou University, Zhengzhou 450052, P. R. China

\*Corresponding authors. Email: [wyl@zsu.edu.cn](mailto:wyl@zsu.edu.cn)

### **Context**

- 1. General Methods**
- 2. General procedure for the synthesis of propargylamines**
- 3. The figures for all new compounds**

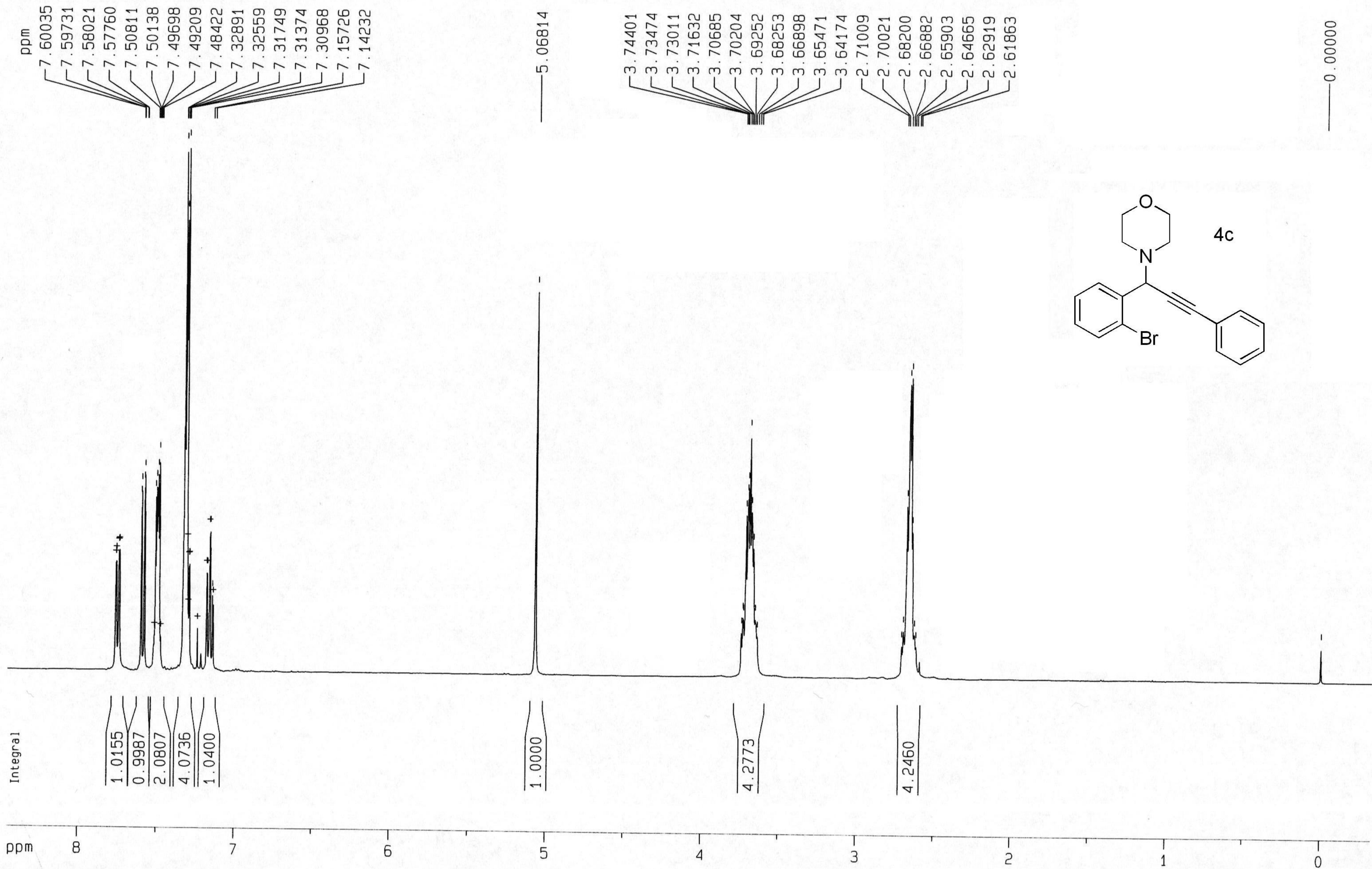
## 1. General Methods

Commercial solvents and reagents were used without further purification with the following exceptions: Toluene was freshly distilled from sodium wire, Aldehydes 1g, 1k were distilled before using. CuI was synthesized according to the literature.<sup>[10b]</sup>

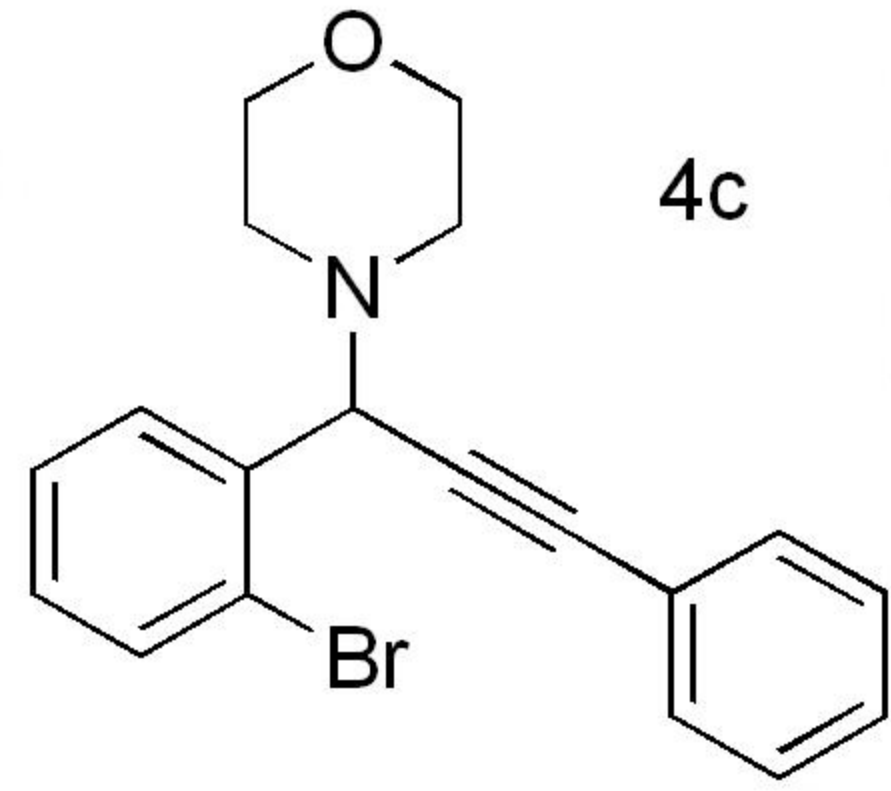
Melting points were measured on a XT-5 microscopic apparatus and uncorrected. GC analysis was performed on Agilent 4890D gas chromatograph. Proton nuclear magnetic resonance (<sup>1</sup>H NMR) and carbon nuclear magnetic resonance (<sup>13</sup>C NMR) spectroscopy were recorded on a Bruker DPX 400 instrument using CDCl<sub>3</sub> as the solvent and TMS as the internal standard. Elemental analyses was conducted with a Carlo Erba 1160 elemental analyzer. High-resolution mass spectra (HRMS) was measured on a Waters Q-T of Micro spectrometer.

**2. General procedure for the synthesis of propargylamines:** A mixture of aldehyde (1 mmol), amine (1.2 mmol), alkyne (1.5 mmol), CuI (3 mol %), succinic acid (6 mol %) and toluene (0.5 mL) was heated at 100°C under nitrogen for 6h. After completion of the reaction as monitored by GC or TLC, the reaction mixture was filtered by a pad of silica gel and washed with ethyl acetate. The combined filtrates were concentrated in vacuo. The residue was purified by chromatography on silica gel using petroleum ether / ethyl acetate as eluent. The products were characterized by <sup>1</sup>H NMR and <sup>13</sup>C NMR. New compounds were confirmed by high-resolution mass spectra or elemental analysis.

## 3. The figures for all new compounds

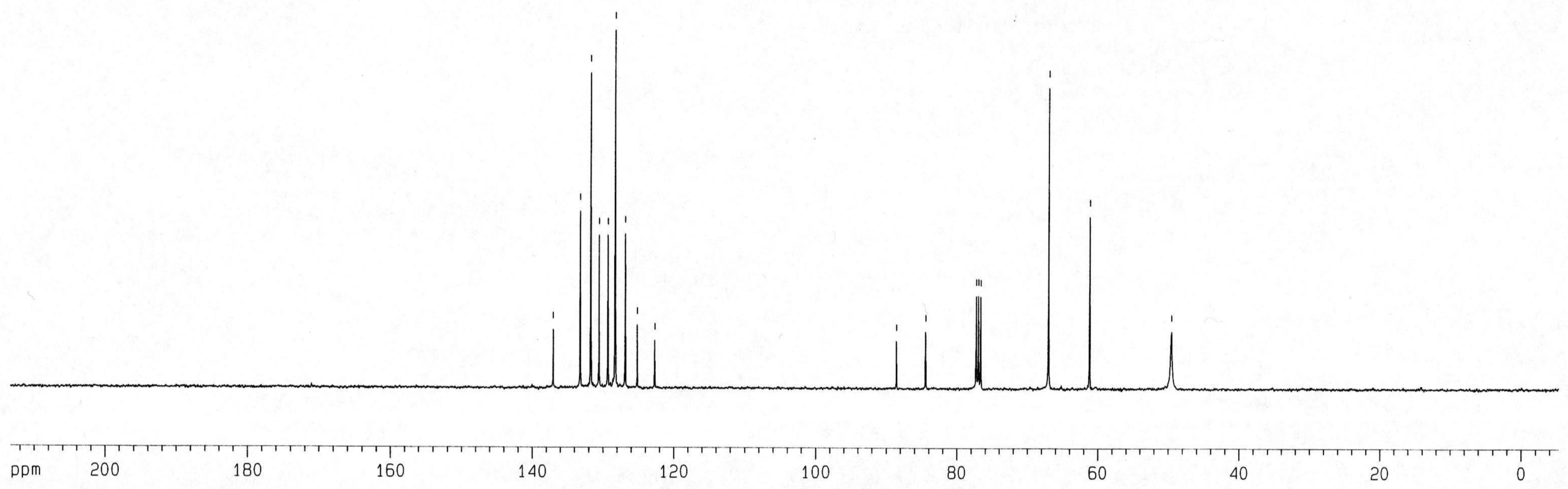


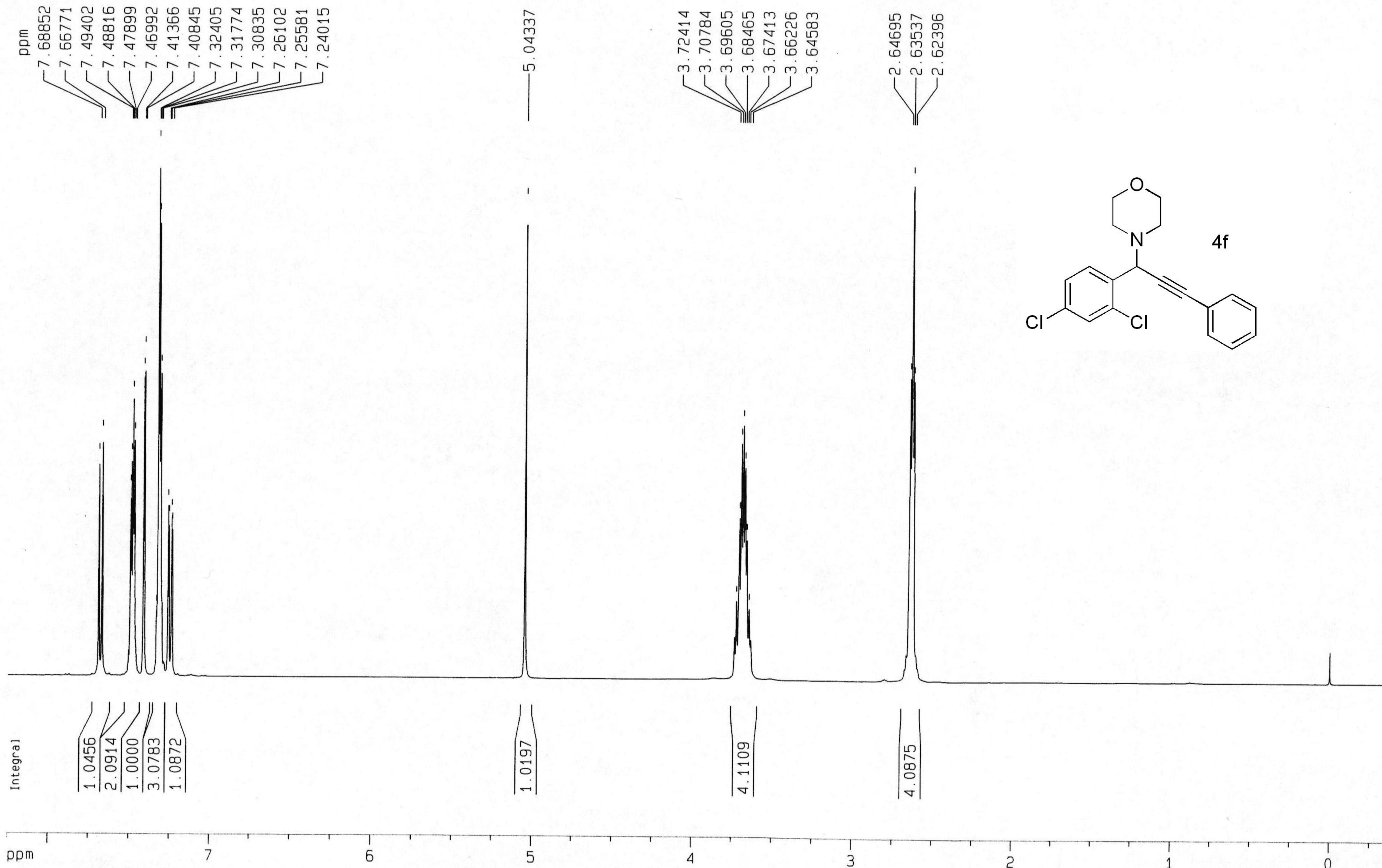
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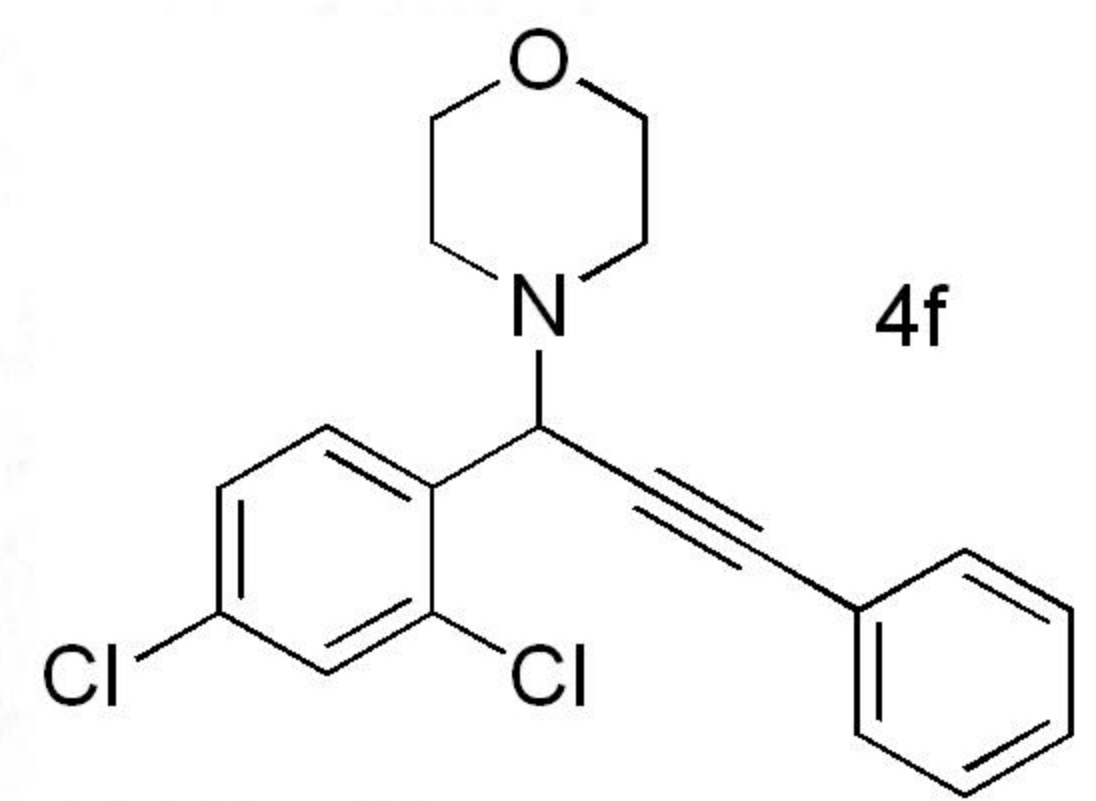
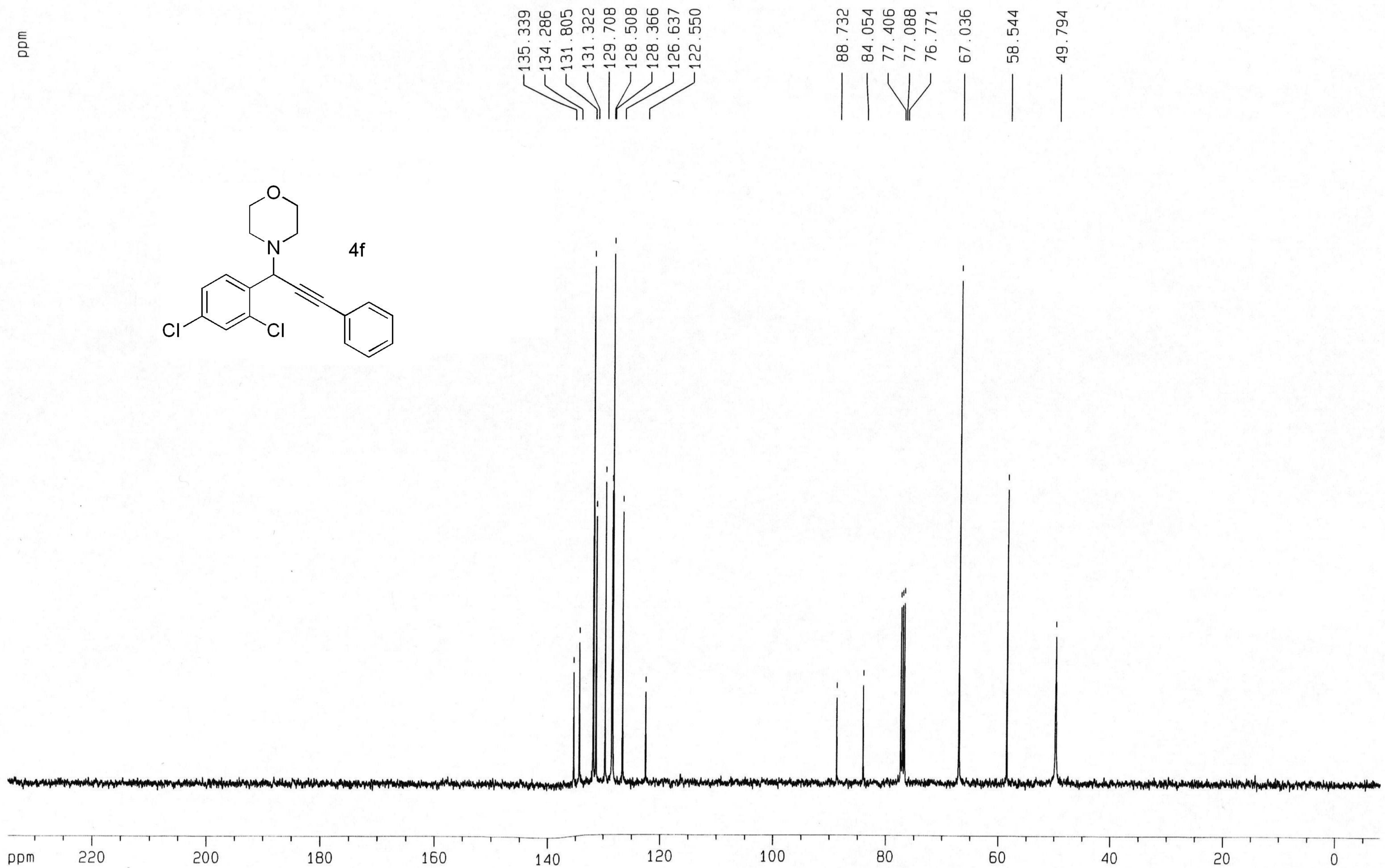


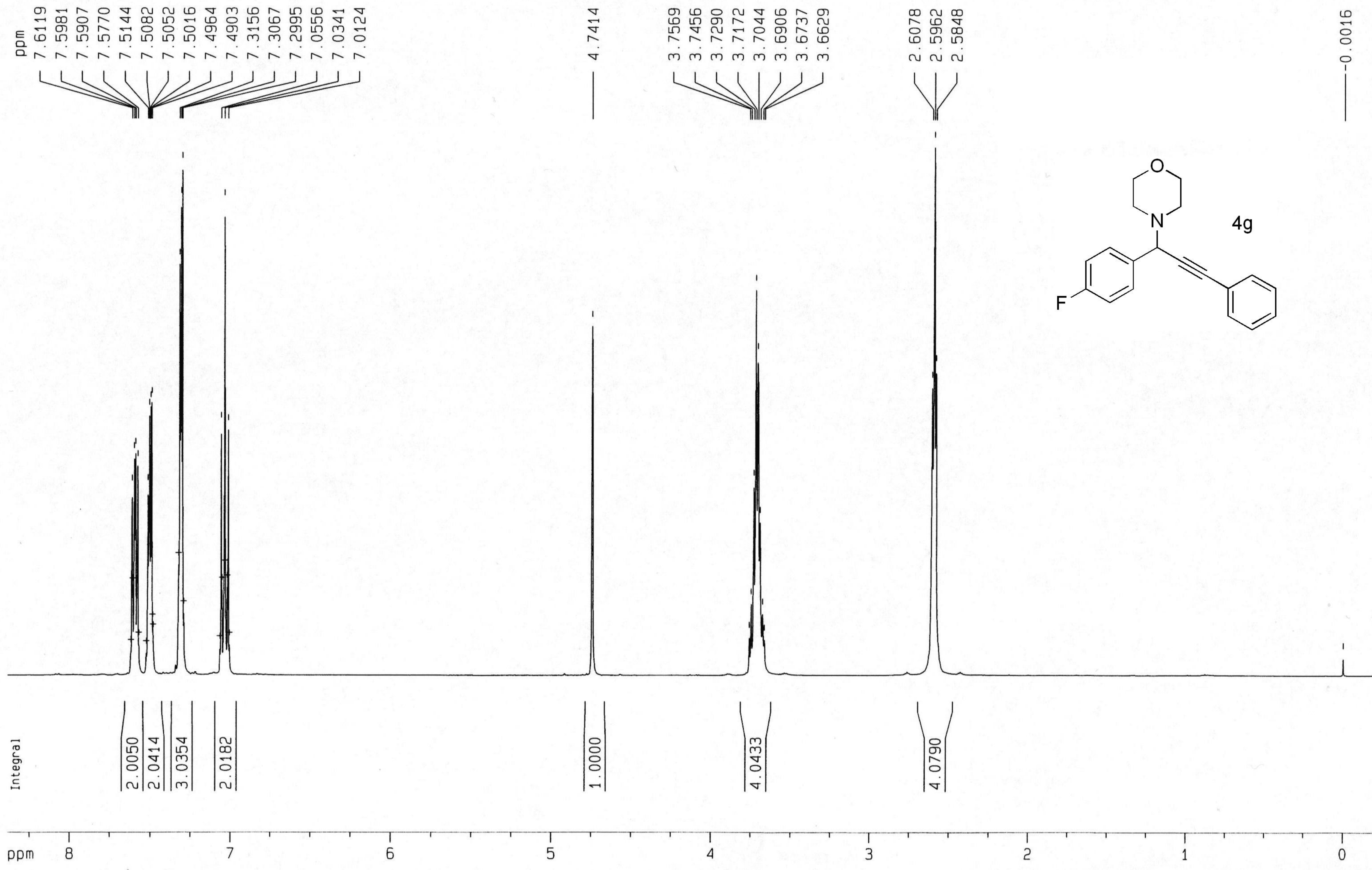
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88.541  
84.460  
77.318  
77.000  
76.682  
67.010  
61.196  
49.582



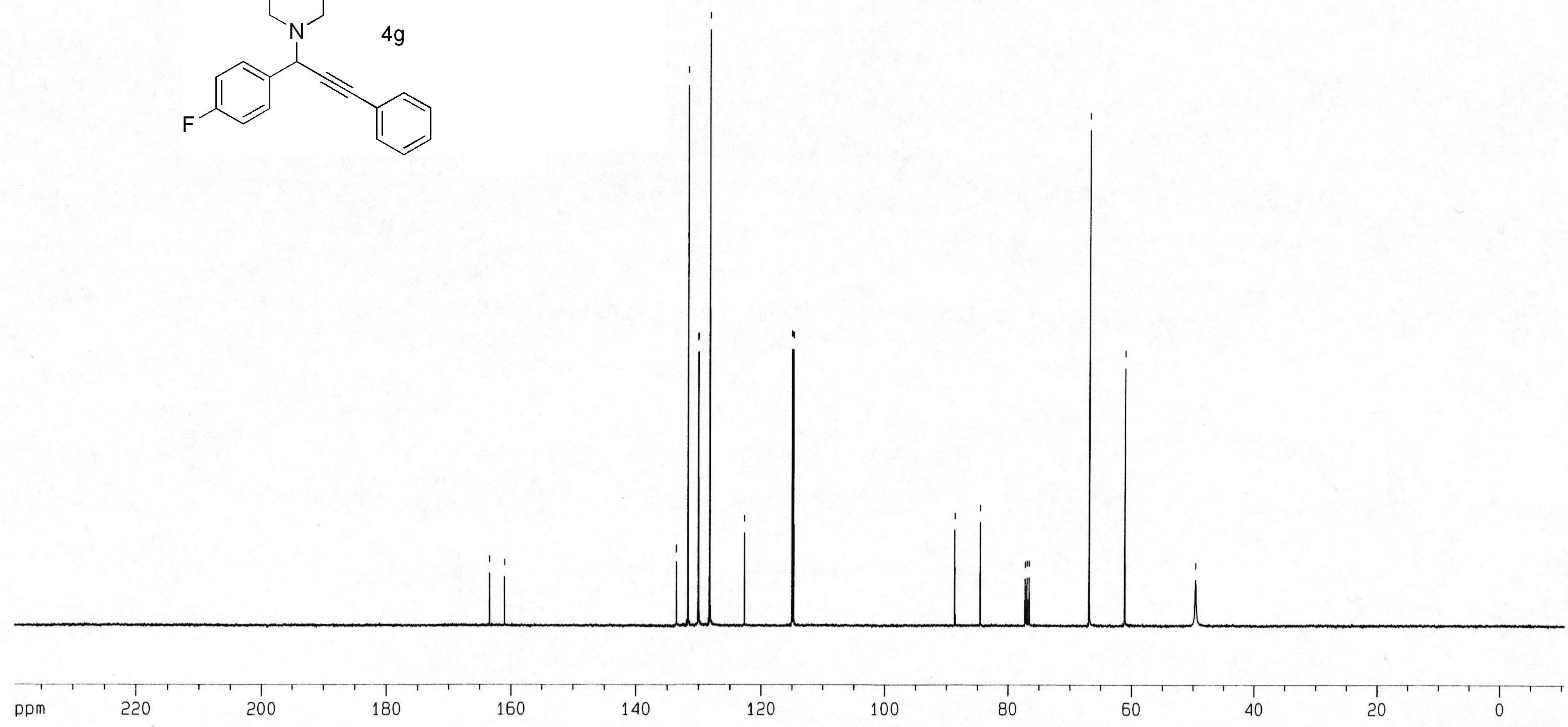
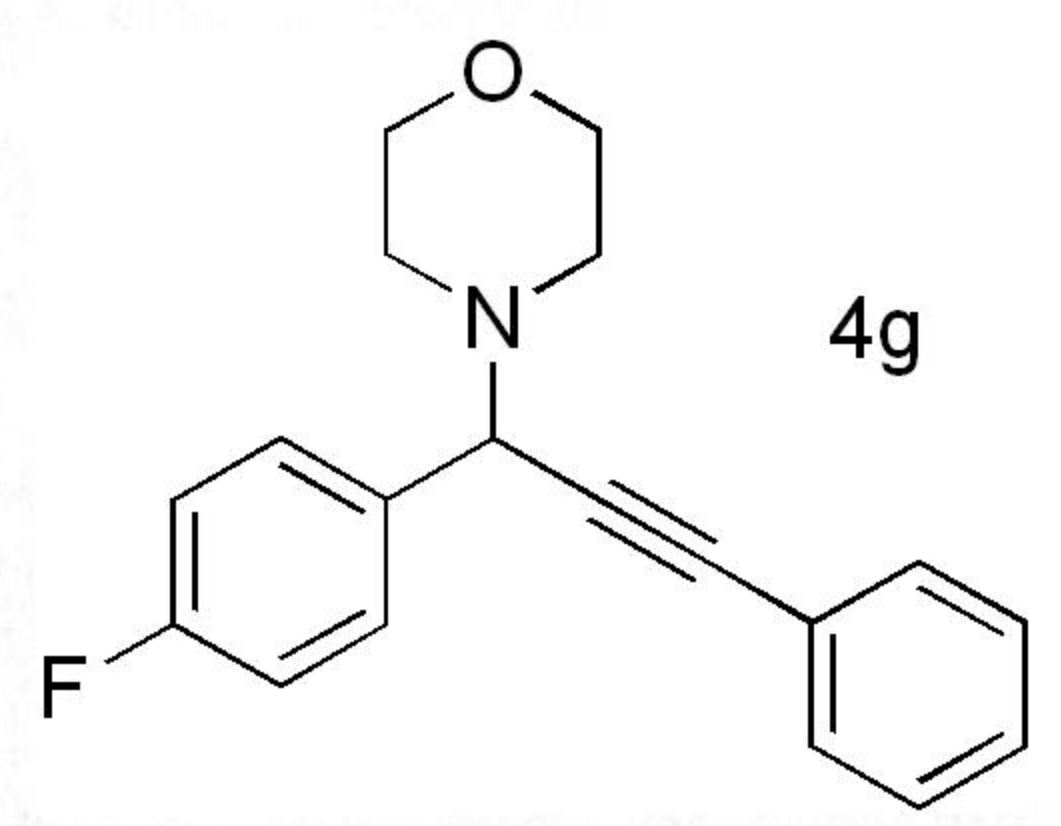




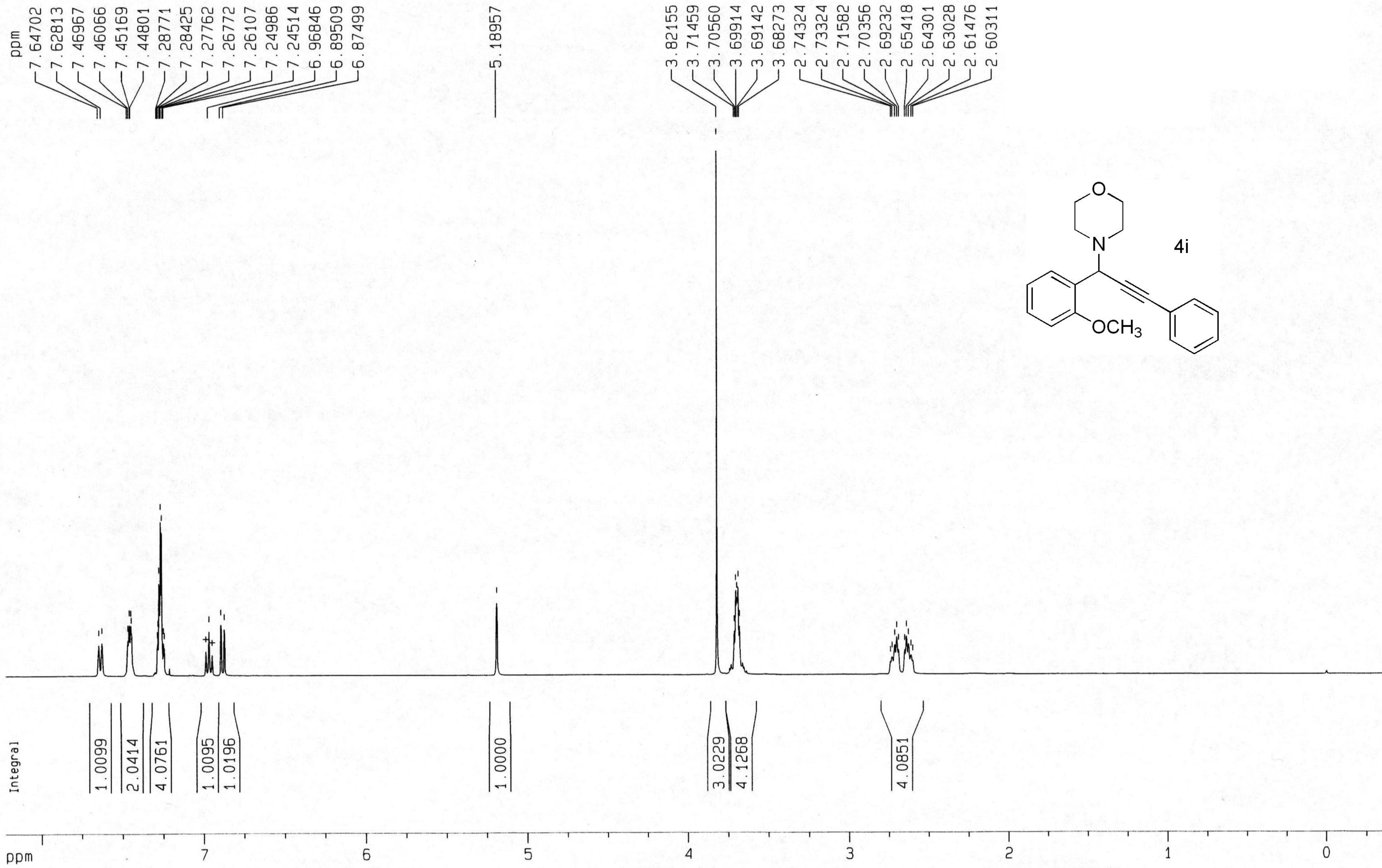


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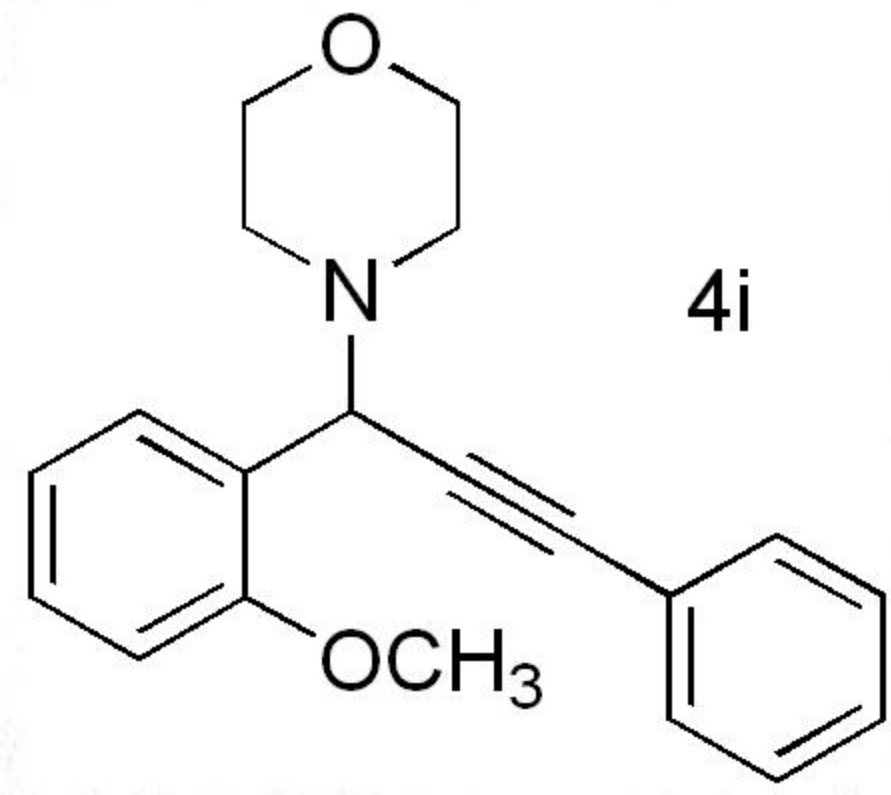
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- 128.227
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- 84.574
- 77.318
- 76.999
- 76.681
- 66.967
- 61.158
- 49.646







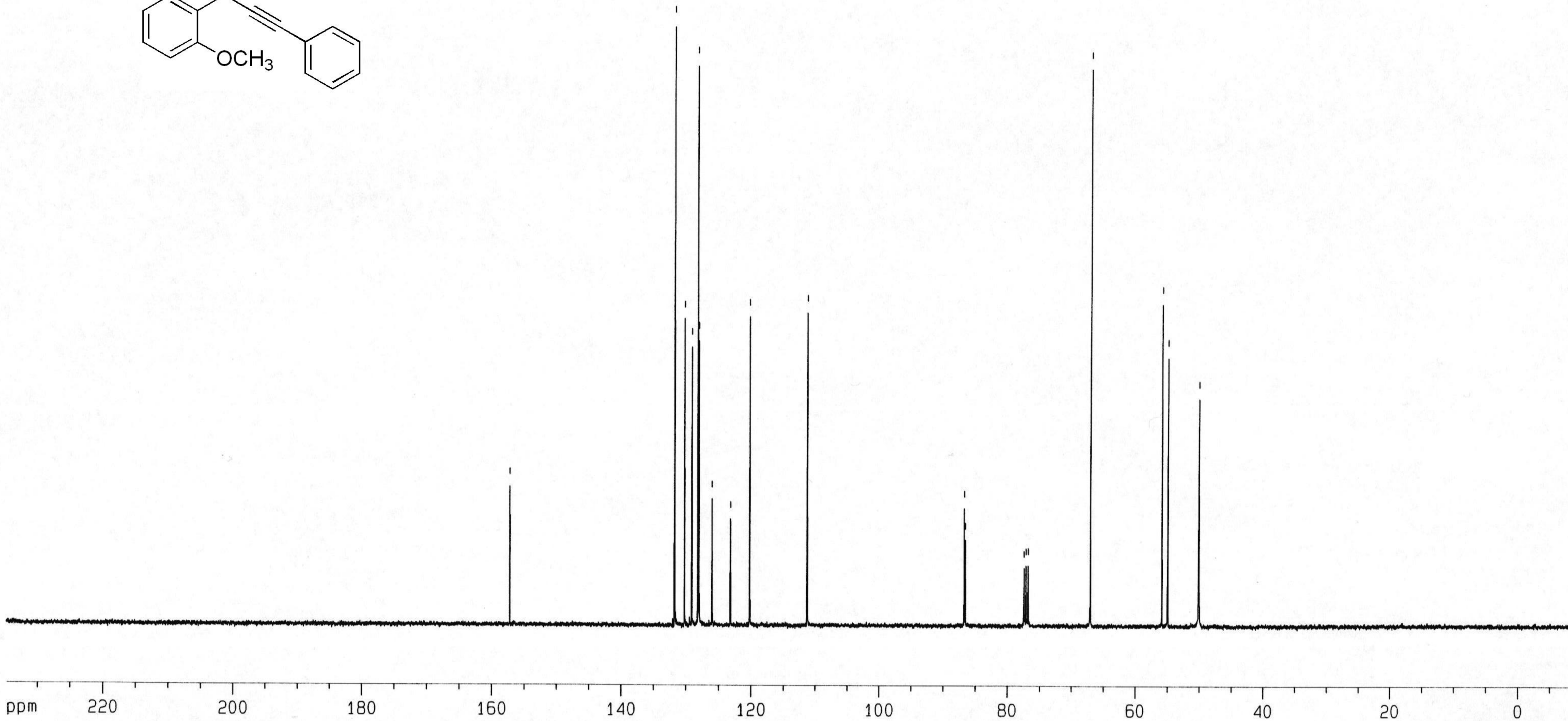
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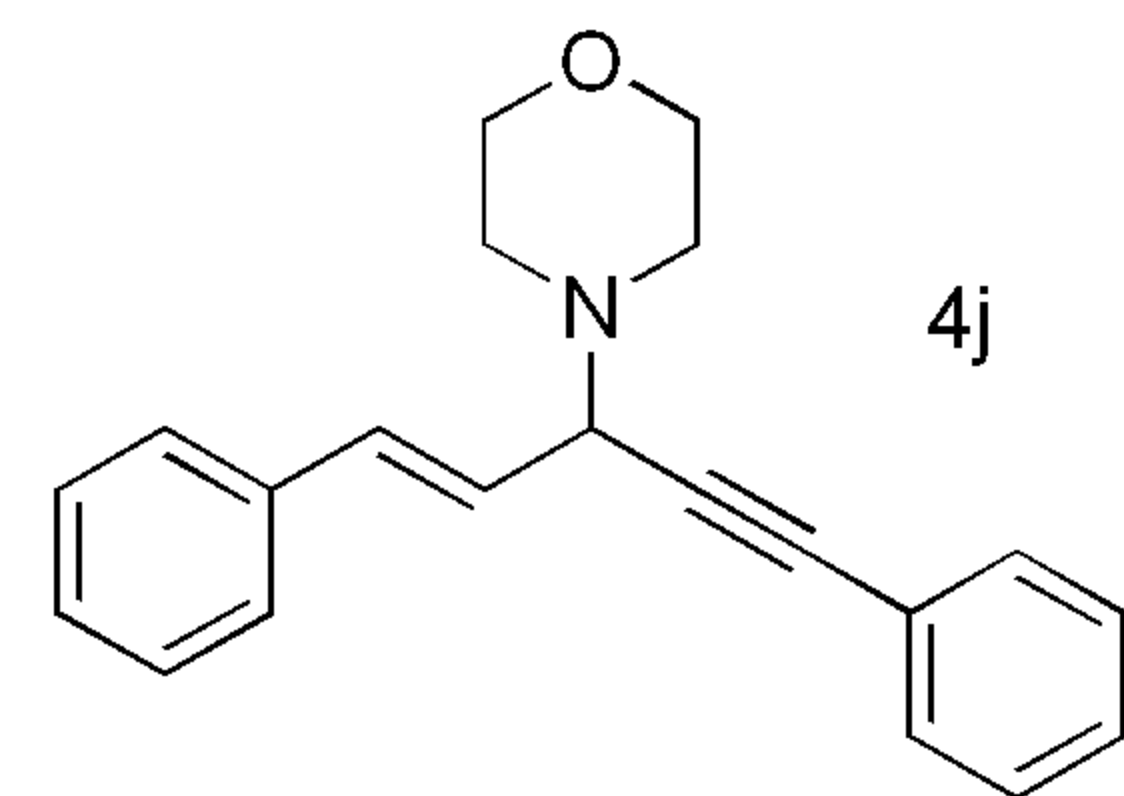
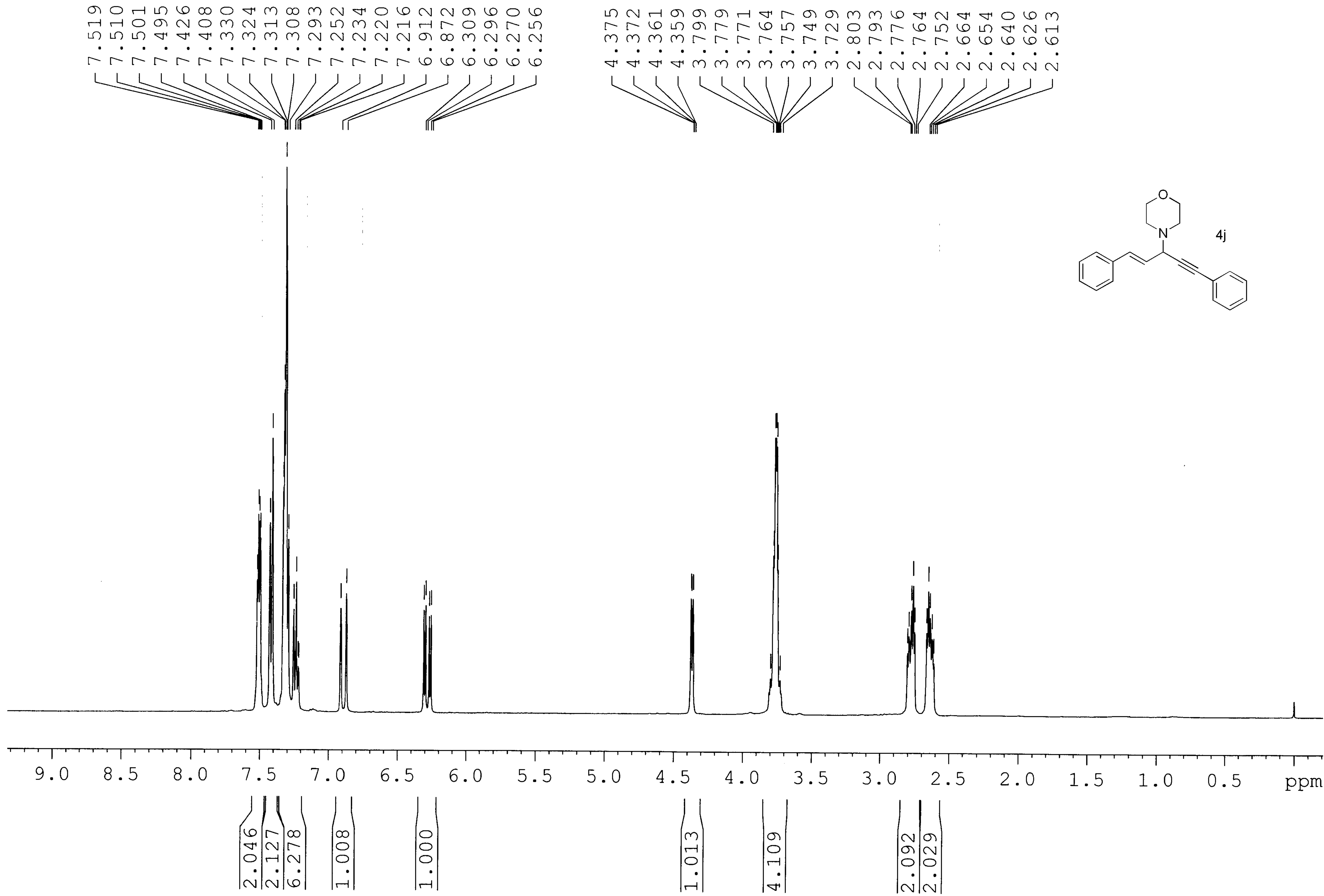


157.194

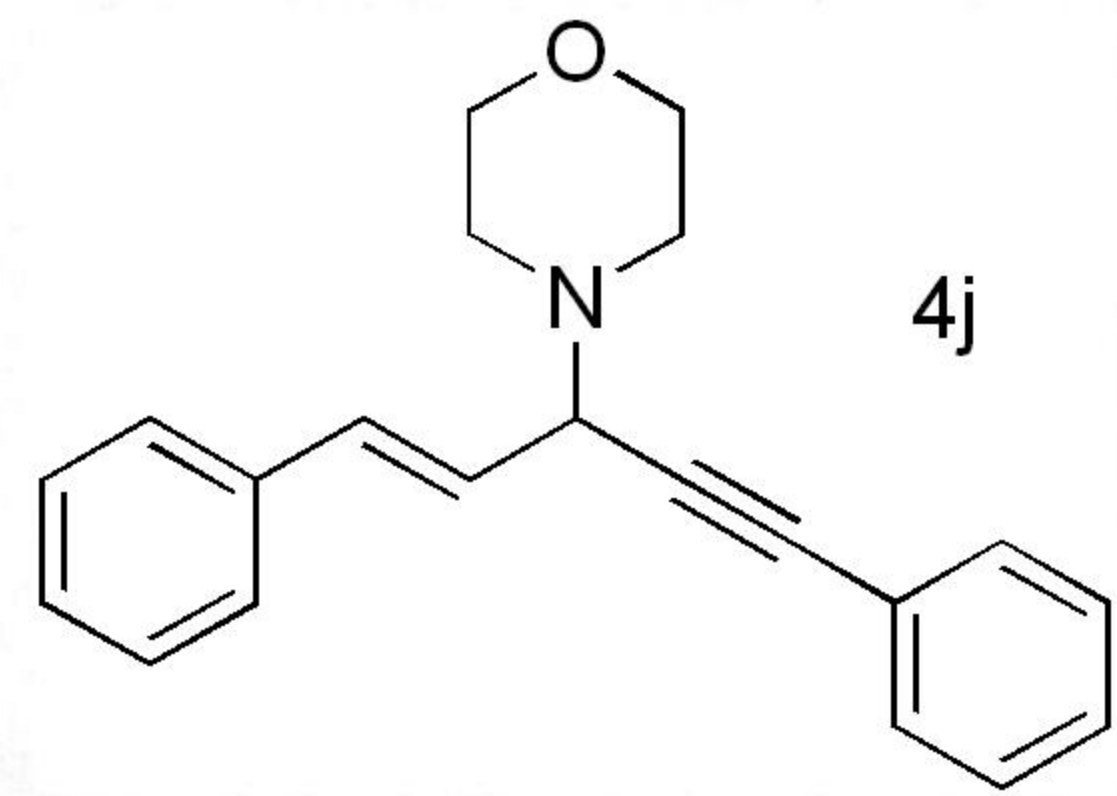
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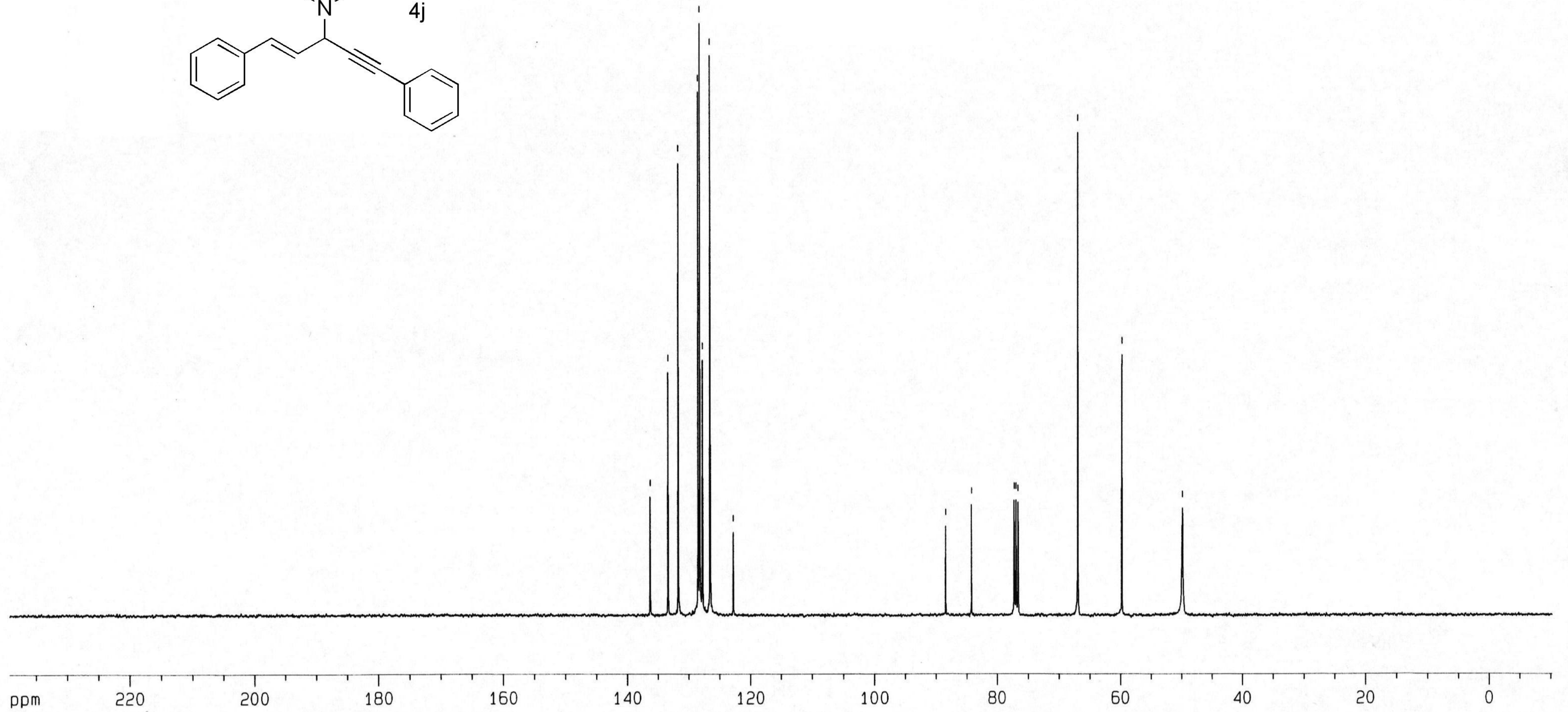


ppm



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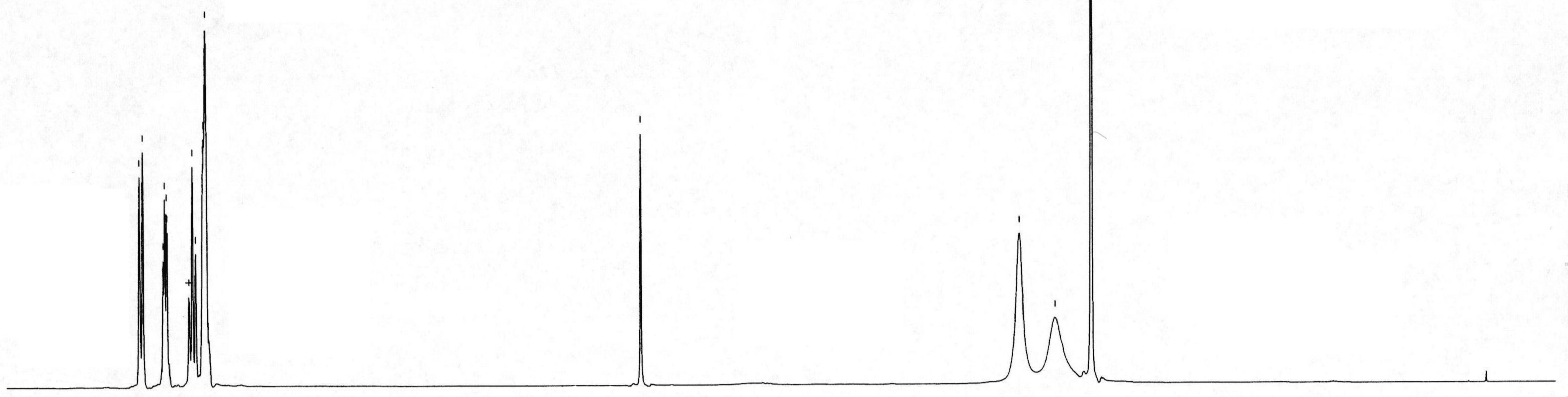
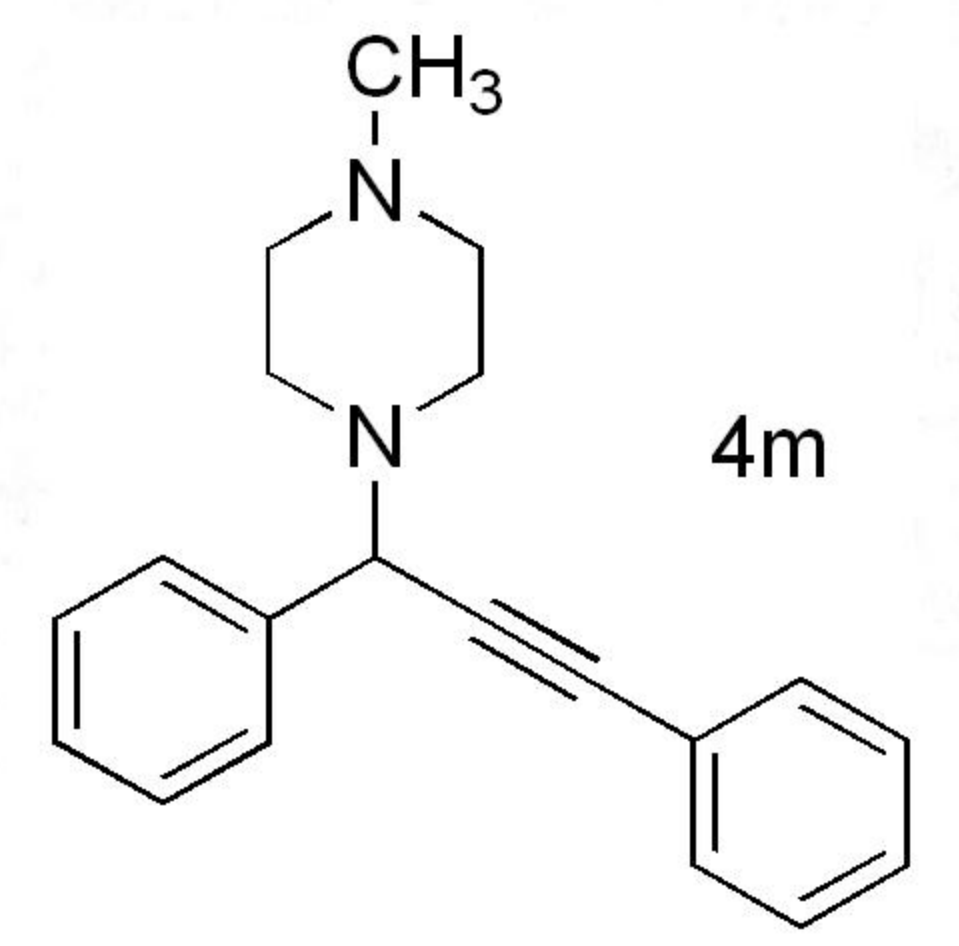
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7.27685  
7.27325  
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Integral

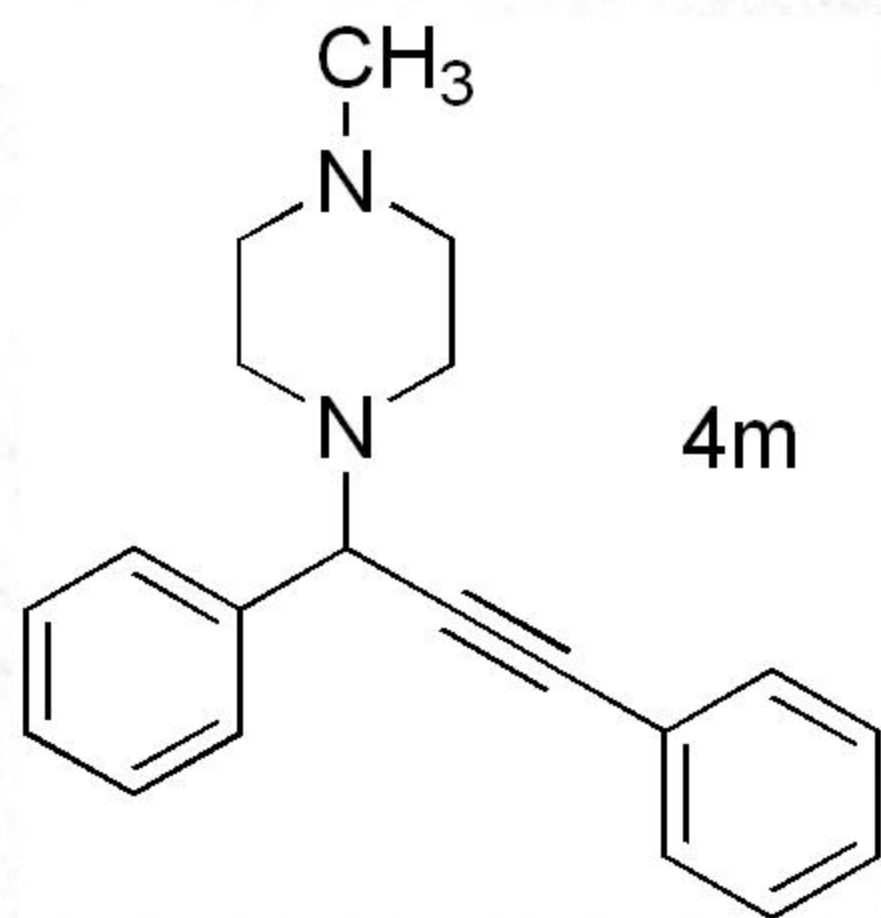
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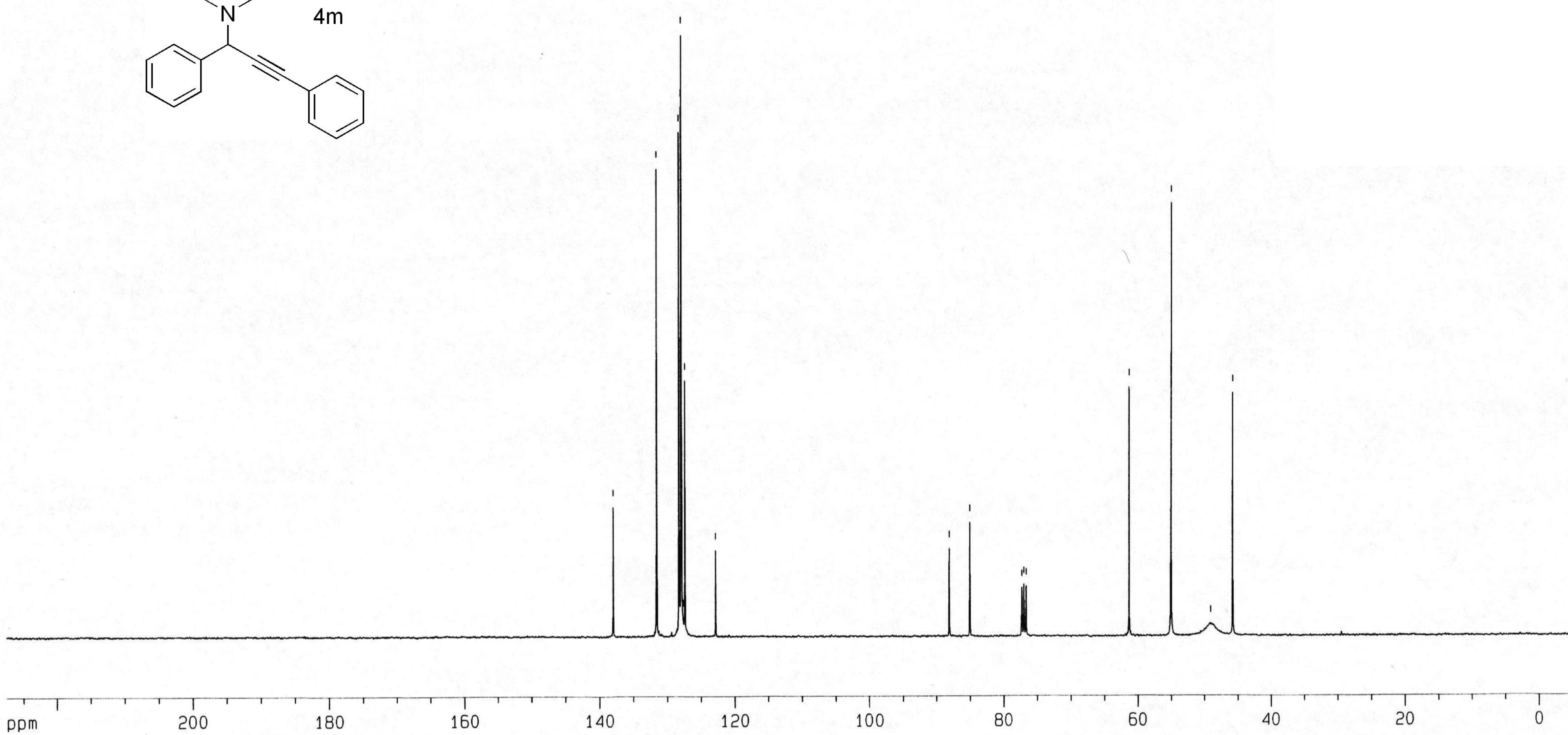
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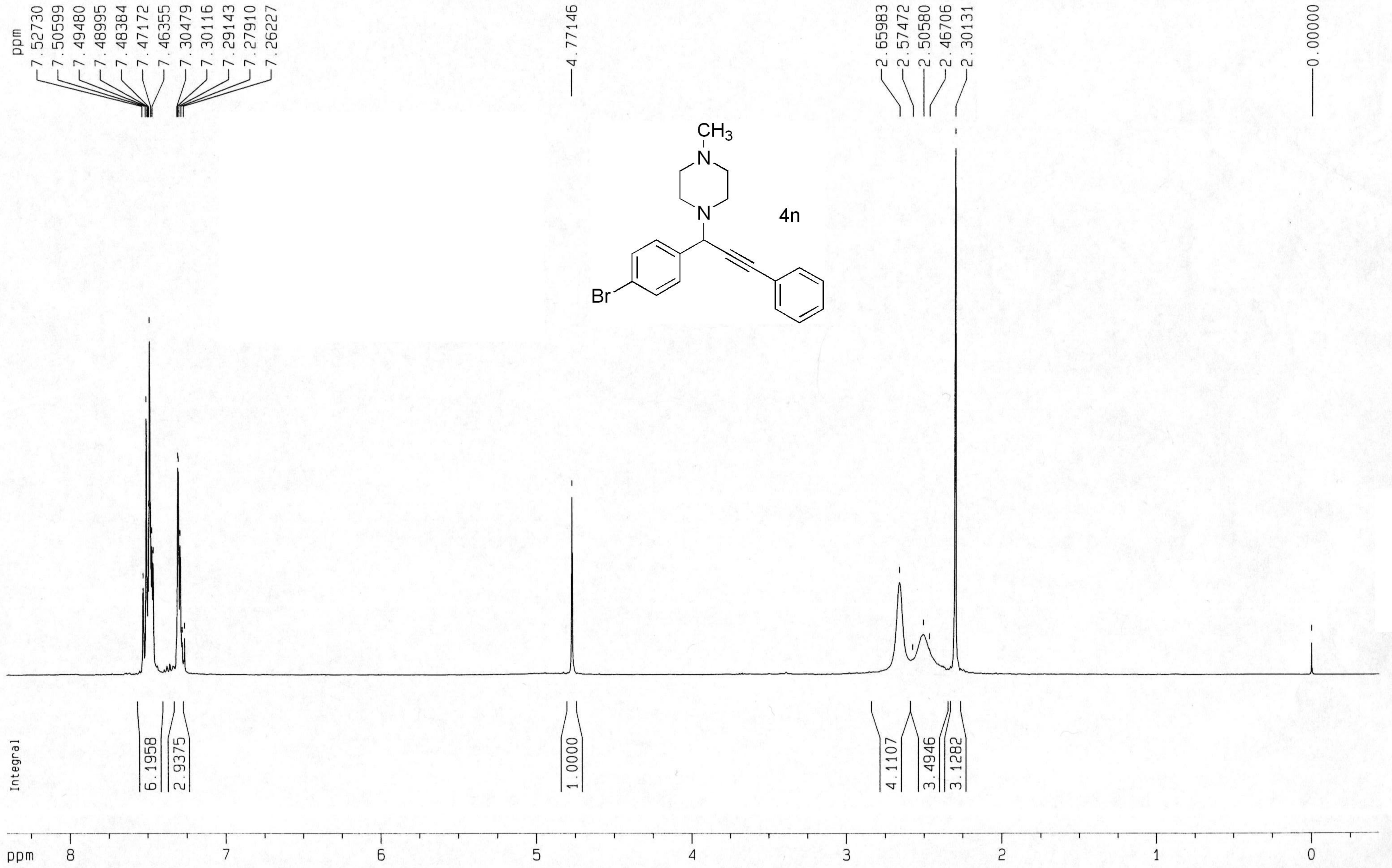
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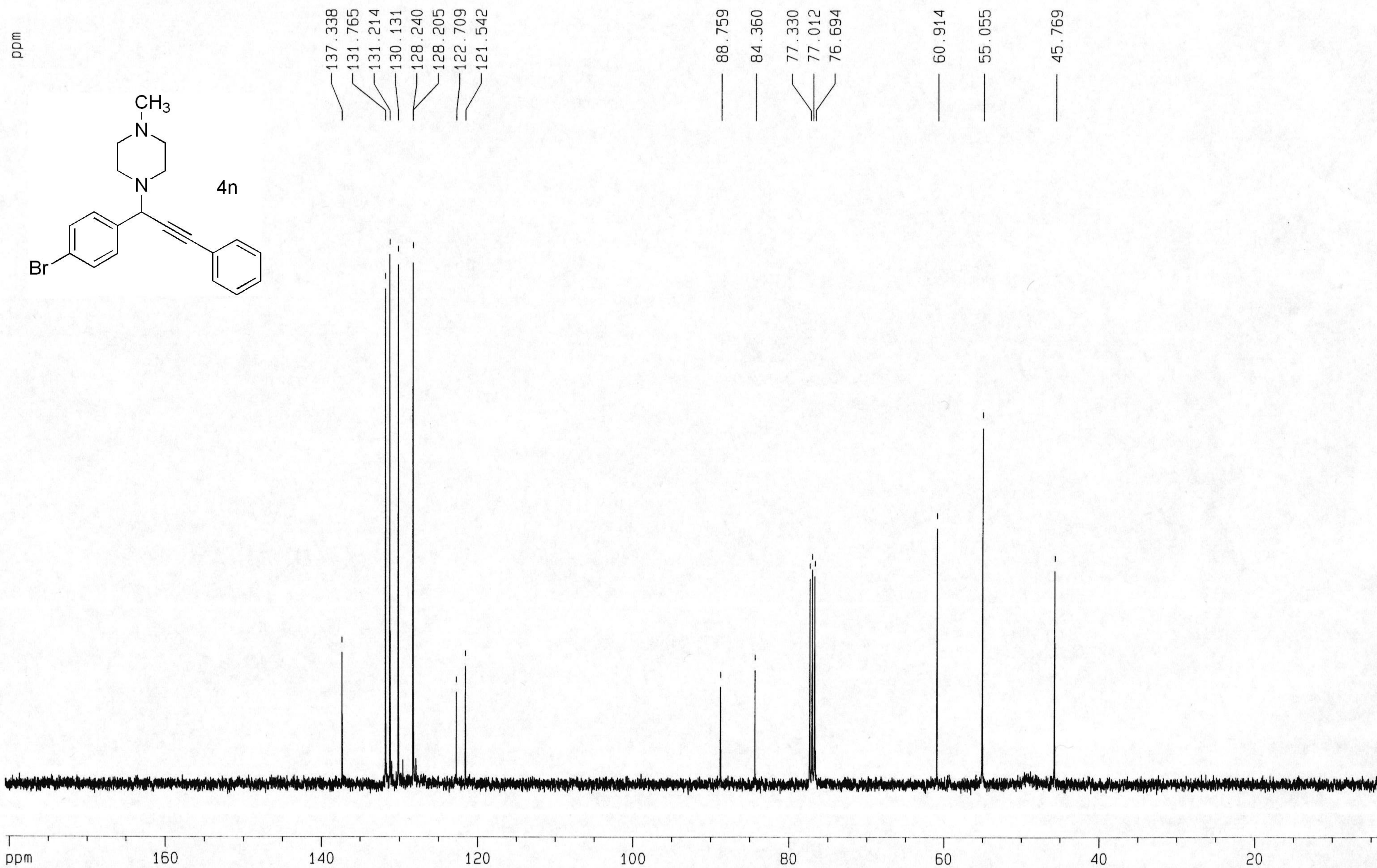
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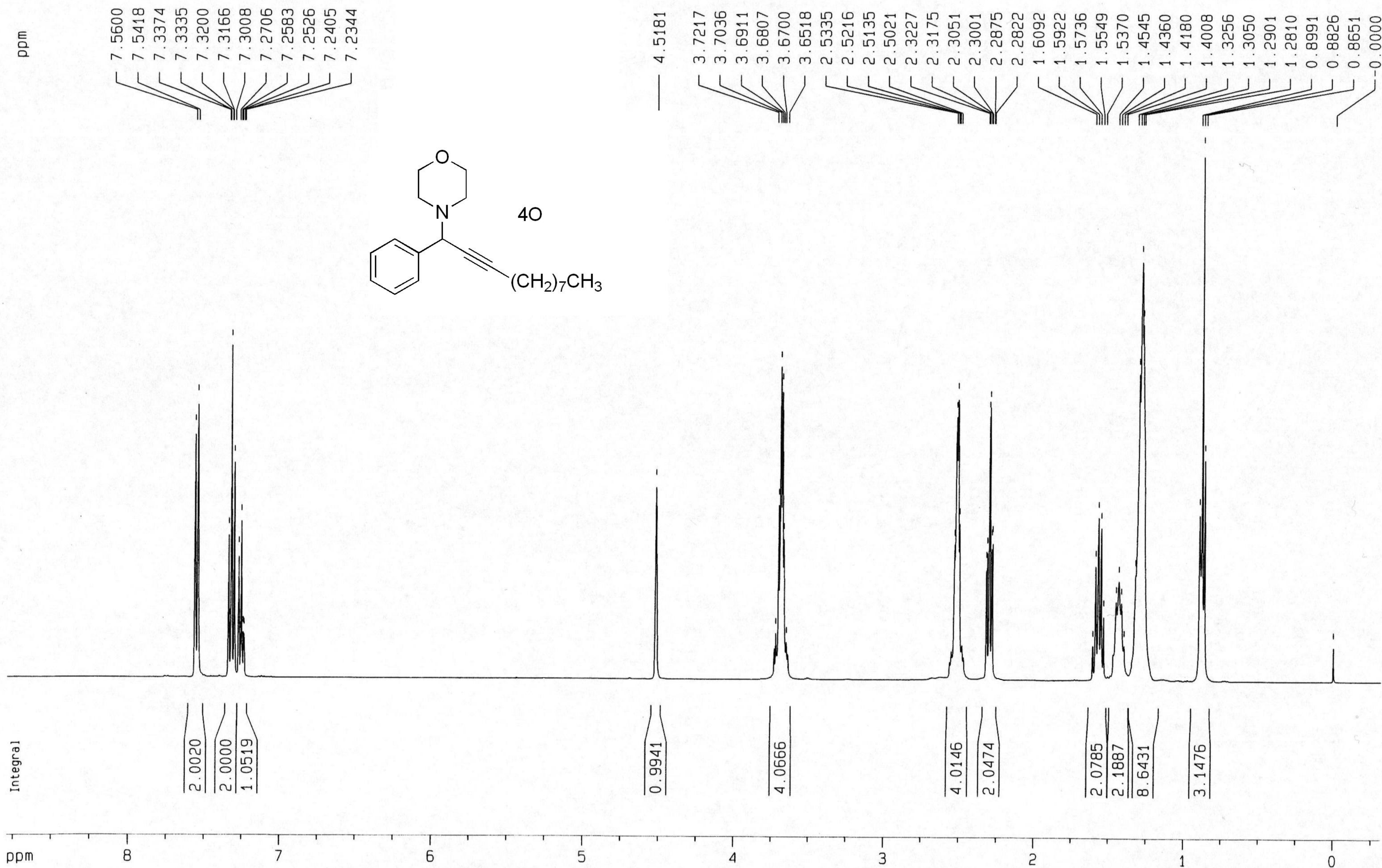


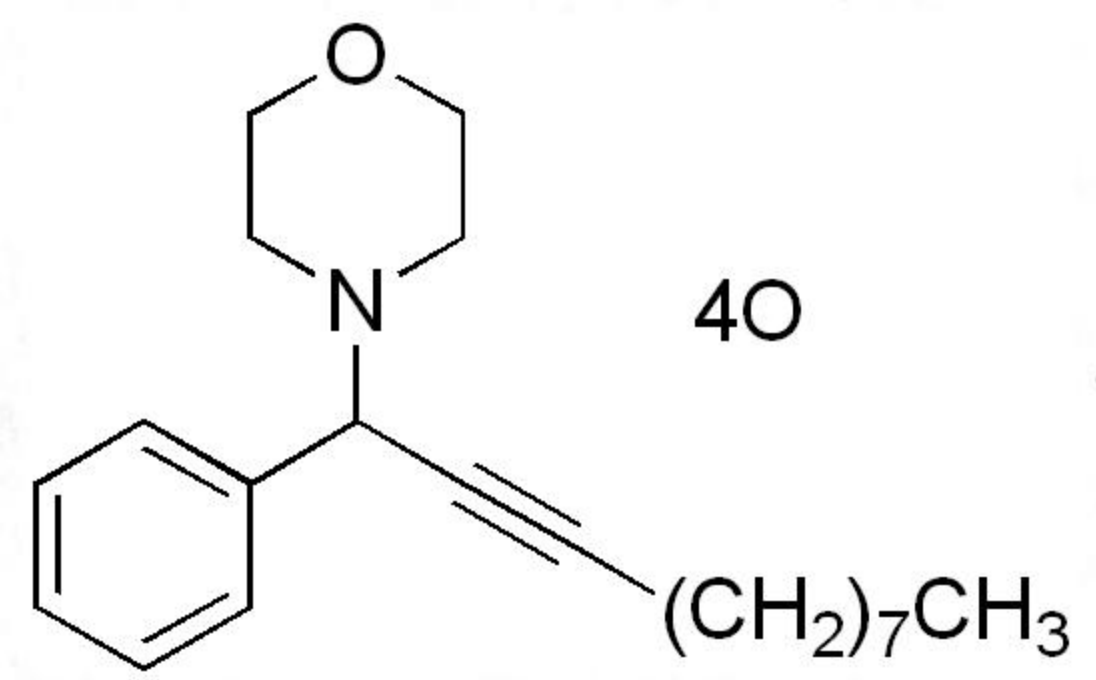
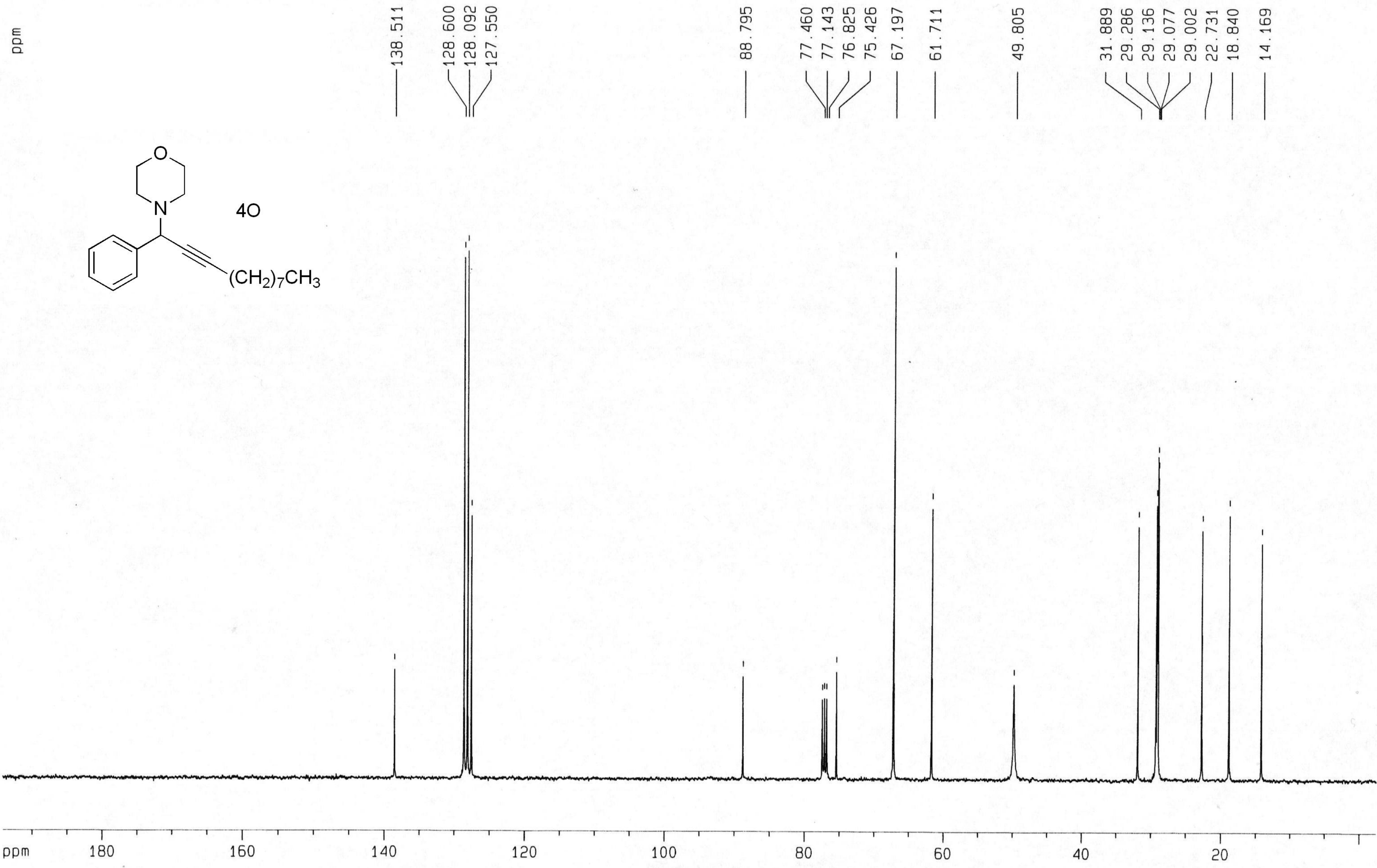
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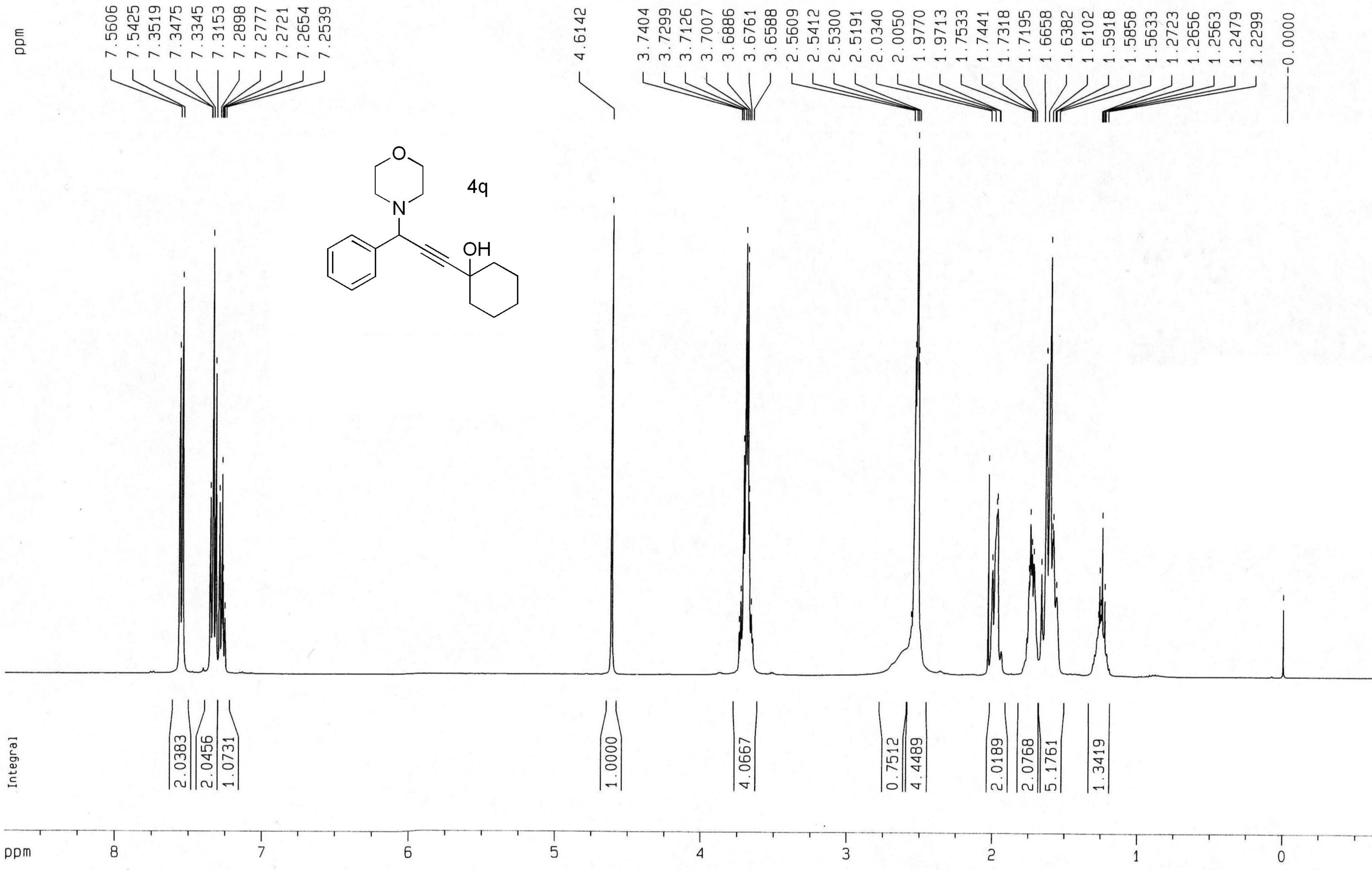


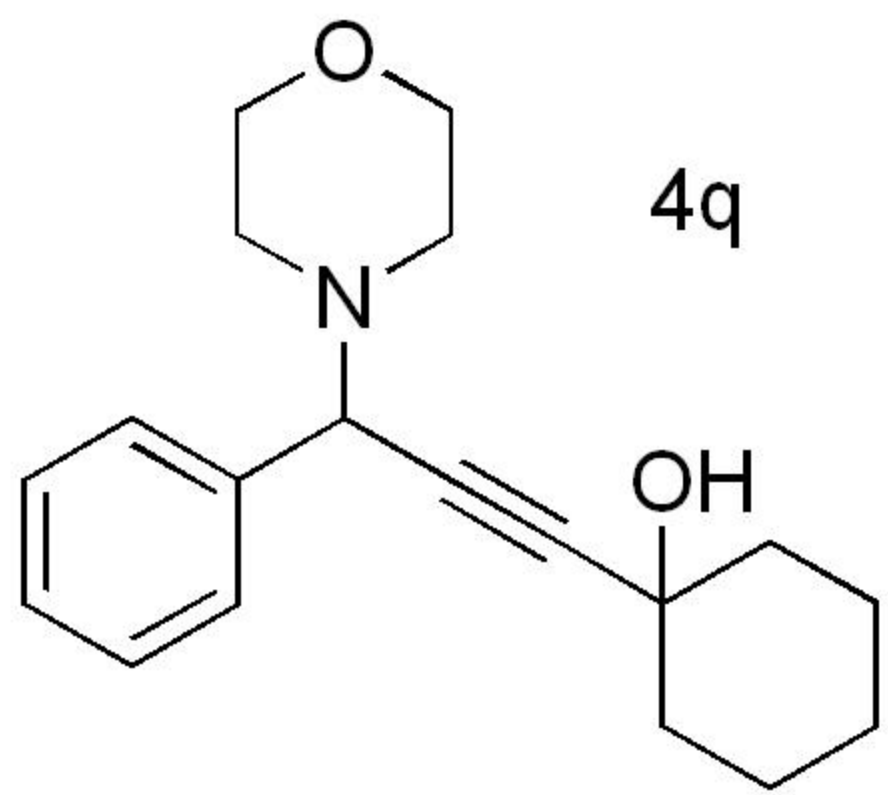
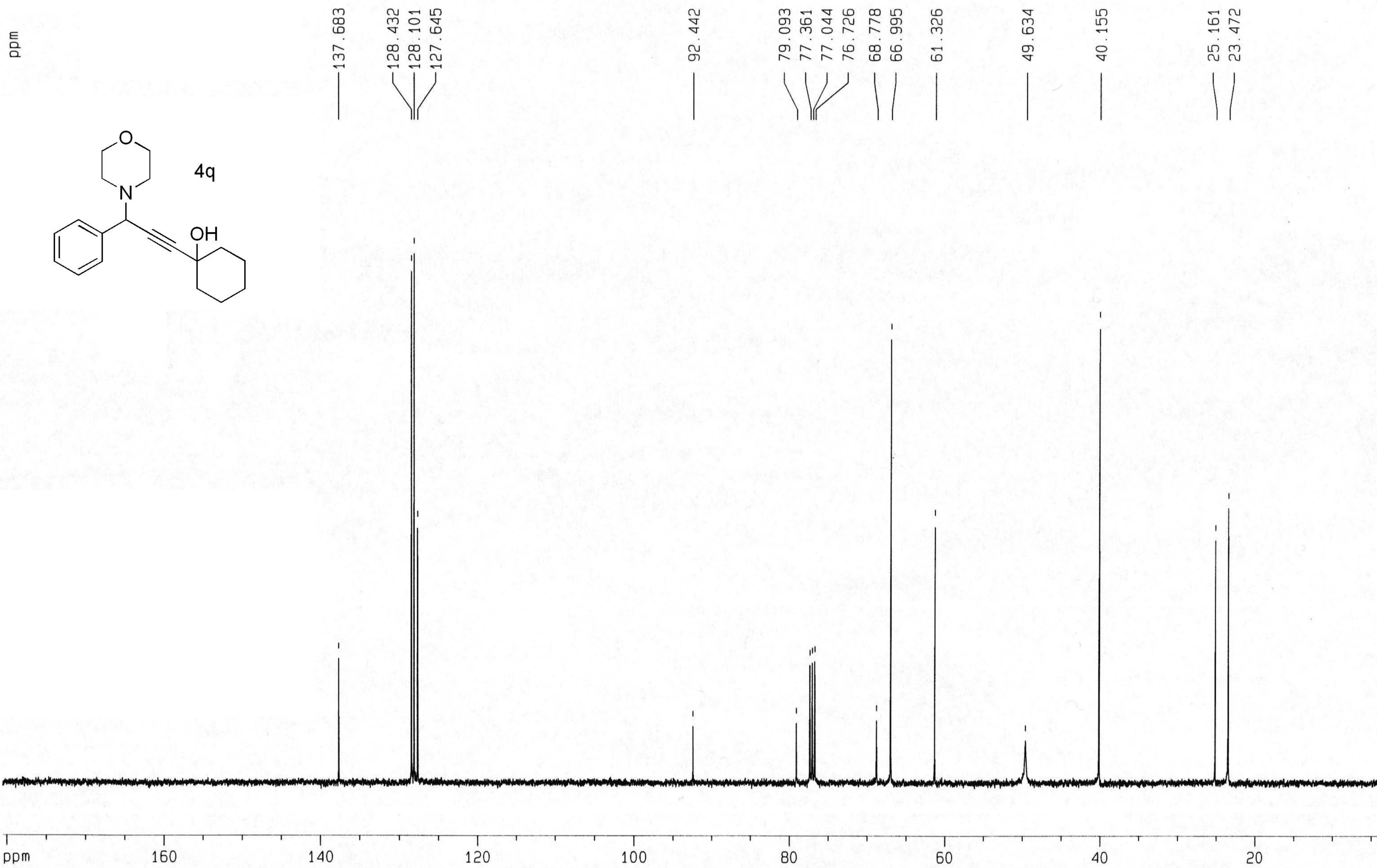






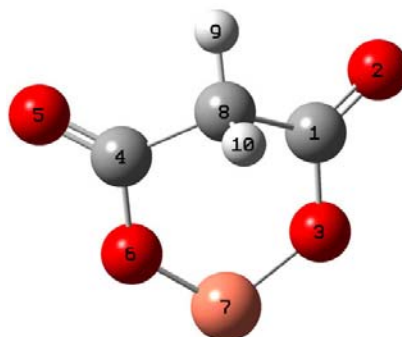






## The three Gaussian models and some data

### 1. propandioic acid



Optimized Parameters !

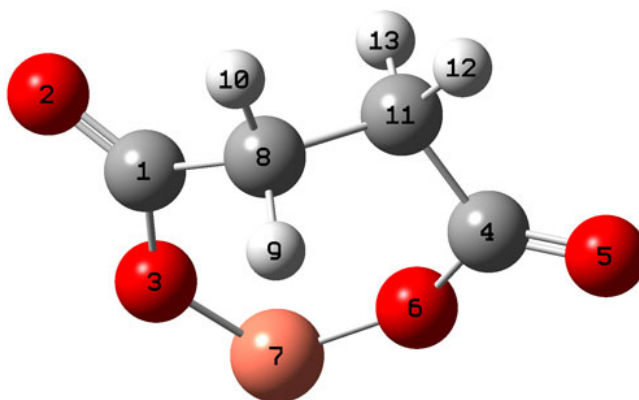
! (Angstroms and Degrees) !

! Name	Definition	Value	Derivative	Info.	!
! R1	R(1, 2)	1. 2459	-DE/DX =	-0. 0004	!
! R2	R(1, 3)	1. 4174	-DE/DX =	0. 0002	!
! R3	R(1, 8)	1. 5985	-DE/DX =	0. 0	!
! R4	R(3, 7)	1. 6288	-DE/DX =	0. 0003	!
! R5	R(4, 5)	1. 244	-DE/DX =	-0. 0001	!
! R6	R(4, 6)	1. 423	-DE/DX =	0. 0004	!
! R7	R(4, 8)	1. 5906	-DE/DX =	0. 0003	!
! R8	R(6, 7)	1. 5698	-DE/DX =	0. 0	!
! R9	R(8, 9)	1. 1034	-DE/DX =	0. 0003	!
! R10	R(8, 10)	1. 1076	-DE/DX =	0. 0001	!
! A1	A(2, 1, 3)	122. 2254	-DE/DX =	-0. 0001	!
! A2	A(2, 1, 8)	124. 5257	-DE/DX =	0. 0	!
! A3	A(3, 1, 8)	113. 2353	-DE/DX =	0. 0001	!
! A4	A(1, 3, 7)	125. 4892	-DE/DX =	-0. 0002	!
! A5	A(5, 4, 6)	122. 1261	-DE/DX =	0. 0	!
! A6	A(5, 4, 8)	126. 0669	-DE/DX =	-0. 0002	!
! A7	A(6, 4, 8)	111. 8064	-DE/DX =	0. 0002	!
! A8	A(4, 6, 7)	129. 4434	-DE/DX =	-0. 0003	!
! A9	A(3, 7, 6)	108. 7589	-DE/DX =	0. 0003	!
! A10	A(1, 8, 4)	115. 3496	-DE/DX =	0. 0	!
! A11	A(1, 8, 9)	108. 914	-DE/DX =	0. 0	!
! A12	A(1, 8, 10)	107. 6337	-DE/DX =	0. 0	!
! A13	A(4, 8, 9)	108. 7166	-DE/DX =	0. 0002	!
! A14	A(4, 8, 10)	107. 5777	-DE/DX =	-0. 0001	!
! A15	A(9, 8, 10)	108. 4569	-DE/DX =	-0. 0001	!
! D1	D(2, 1, 3, 7)	-155. 2768	-DE/DX =	0. 0001	!
! D2	D(8, 1, 3, 7)	26. 0135	-DE/DX =	0. 0001	!
! D3	D(2, 1, 8, 4)	136. 0856	-DE/DX =	0. 0001	!

! D4	D(2, 1, 8, 9)	13. 5599	-DE/DX =	-0. 0002	!
! D5	D(2, 1, 8, 10)	-103. 8322	-DE/DX =	0. 0	!
! D6	D(3, 1, 8, 4)	-45. 2393	-DE/DX =	0. 0001	!
! D7	D(3, 1, 8, 9)	-167. 765	-DE/DX =	-0. 0002	!
! D8	D(3, 1, 8, 10)	74. 843	-DE/DX =	0. 0	!
! D9	D(1, 3, 7, 6)	-4. 5375	-DE/DX =	-0. 0001	!
! D10	D(5, 4, 6, 7)	159. 1685	-DE/DX =	0. 0	!
! D11	D(8, 4, 6, 7)	-21. 0907	-DE/DX =	0. 0001	!
! D12	D(5, 4, 8, 1)	-138. 1327	-DE/DX =	0. 0	!
! D13	D(5, 4, 8, 9)	-15. 5017	-DE/DX =	0. 0001	!
! D14	D(5, 4, 8, 10)	101. 7544	-DE/DX =	0. 0	!
! D15	D(6, 4, 8, 1)	42. 1388	-DE/DX =	-0. 0001	!
! D16	D(6, 4, 8, 9)	164. 7697	-DE/DX =	0. 0	!
! D17	D(6, 4, 8, 10)	-77. 9741	-DE/DX =	-0. 0001	!
! D18	D(4, 6, 7, 3)	1. 9208	-DE/DX =	0. 0001	!

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## 2. succinic acid



! Optimized Parameters !  
! (Angstroms and Degrees) !

! Name	Definition	Value	Derivative Info.	!
! R1	R(1, 2)	1. 2472	-DE/DX = 0. 0	!
! R2	R(1, 3)	1. 4137	-DE/DX = 0. 0	!
! R3	R(1, 8)	1. 59	-DE/DX = 0. 0	!
! R4	R(3, 7)	1. 6001	-DE/DX = 0. 0	!
! R5	R(4, 5)	1. 2451	-DE/DX = 0. 0	!
! R6	R(4, 6)	1. 4121	-DE/DX = 0. 0	!
! R7	R(4, 11)	1. 5861	-DE/DX = 0. 0	!
! R8	R(6, 7)	1. 5492	-DE/DX = 0. 0	!
! R9	R(8, 9)	1. 1053	-DE/DX = 0. 0	!
! R10	R(8, 10)	1. 1041	-DE/DX = 0. 0	!

! R11	R(8, 11)	1. 578	-DE/DX =	0. 0	!
! R12	R(11, 12)	1. 1041	-DE/DX =	0. 0	!
! R13	R(11, 13)	1. 1061	-DE/DX =	0. 0	!
! A1	A(2, 1, 3)	121. 5793	-DE/DX =	0. 0	!
! A2	A(2, 1, 8)	124. 6693	-DE/DX =	0. 0	!
! A3	A(3, 1, 8)	113. 7425	-DE/DX =	0. 0	!
! A4	A(1, 3, 7)	134. 3002	-DE/DX =	0. 0	!
! A5	A(5, 4, 6)	122. 3225	-DE/DX =	0. 0	!
! A6	A(5, 4, 11)	125. 8496	-DE/DX =	0. 0	!
! A7	A(6, 4, 11)	111. 8265	-DE/DX =	0. 0	!
! A8	A(4, 6, 7)	144. 859	-DE/DX =	0. 0	!
! A9	A(3, 7, 6)	115. 375	-DE/DX =	0. 0	!
! A10	A(1, 8, 9)	109. 0014	-DE/DX =	0. 0	!
! A11	A(1, 8, 10)	106. 1676	-DE/DX =	0. 0	!
! A12	A(1, 8, 11)	115. 5285	-DE/DX =	0. 0	!
! A13	A(9, 8, 10)	107. 738	-DE/DX =	0. 0	!
! A14	A(9, 8, 11)	110. 1789	-DE/DX =	0. 0	!
! A15	A(10, 8, 11)	107. 8888	-DE/DX =	0. 0	!
! A16	A(4, 11, 8)	115. 8408	-DE/DX =	0. 0	!
! A17	A(4, 11, 12)	106. 3429	-DE/DX =	0. 0	!
! A18	A(4, 11, 13)	108. 3063	-DE/DX =	0. 0	!
! A19	A(8, 11, 12)	108. 5258	-DE/DX =	0. 0	!
! A20	A(8, 11, 13)	109. 9583	-DE/DX =	0. 0	!
! A21	A(12, 11, 13)	107. 521	-DE/DX =	0. 0	!
! D1	D(2, 1, 3, 7)	145. 7964	-DE/DX =	0. 0	!
! D2	D(8, 1, 3, 7)	-35. 2356	-DE/DX =	0. 0	!
! D3	D(2, 1, 8, 9)	124. 9823	-DE/DX =	0. 0	!
! D4	D(2, 1, 8, 10)	9. 1763	-DE/DX =	0. 0	!
! D5	D(2, 1, 8, 11)	-110. 3538	-DE/DX =	0. 0	!
! D6	D(3, 1, 8, 9)	-53. 9488	-DE/DX =	0. 0	!
! D7	D(3, 1, 8, 10)	-169. 7547	-DE/DX =	0. 0	!
! D8	D(3, 1, 8, 11)	70. 7152	-DE/DX =	0. 0	!
! D9	D(1, 3, 7, 6)	7. 17	-DE/DX =	0. 0	!
! D10	D(5, 4, 6, 7)	152. 3548	-DE/DX =	0. 0	!
! D11	D(11, 4, 6, 7)	-28. 0487	-DE/DX =	0. 0	!
! D12	D(5, 4, 11, 8)	-126. 4006	-DE/DX =	0. 0	!
! D13	D(5, 4, 11, 12)	-5. 7428	-DE/DX =	0. 0	!
! D14	D(5, 4, 11, 13)	109. 5643	-DE/DX =	0. 0	!
! D15	D(6, 4, 11, 8)	54. 0201	-DE/DX =	0. 0	!
! D16	D(6, 4, 11, 12)	174. 6779	-DE/DX =	0. 0	!
! D17	D(6, 4, 11, 13)	-70. 0151	-DE/DX =	0. 0	!
! D18	D(4, 6, 7, 3)	12. 666	-DE/DX =	0. 0	!
! D19	D(1, 8, 11, 4)	-84. 5451	-DE/DX =	0. 0	!
! D20	D(1, 8, 11, 12)	155. 9814	-DE/DX =	0. 0	!
! D21	D(1, 8, 11, 13)	38. 6276	-DE/DX =	0. 0	!
! D22	D(9, 8, 11, 4)	39. 5059	-DE/DX =	0. 0	!
! D23	D(9, 8, 11, 12)	-79. 9676	-DE/DX =	0. 0	!
! D24	D(9, 8, 11, 13)	162. 6786	-DE/DX =	0. 0	!
! D25	D(10, 8, 11, 4)	156. 8738	-DE/DX =	0. 0	!

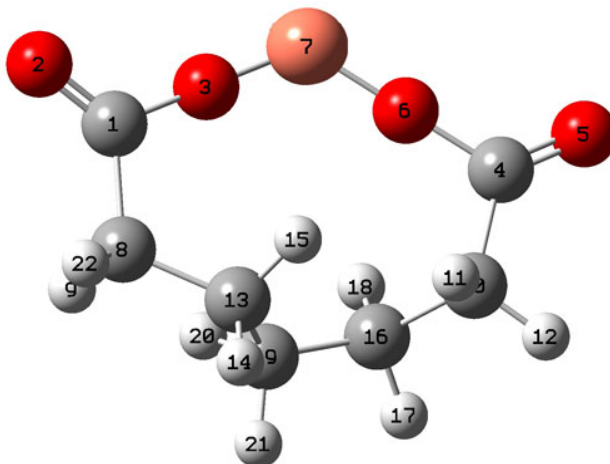
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! D26  D(10, 8, 11, 12)          37.4003      -DE/DX =   0.0      !
! D27  D(10, 8, 11, 13)        -79.9536      -DE/DX =   0.0      !

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### 3. heptandioic acid



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!  Optimized Parameters  !
!  (Angstroms and Degrees)  !

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! Name	Definition	Value	Derivative Info.	!
! R1	R(1,2)	1.2471	-DE/DX = -0.002	
! R2	R(1,3)	1.4026	-DE/DX = -0.0018	
! R3	R(1,8)	1.5879	-DE/DX = 0.0	!
! R4	R(3,7)	1.4993	-DE/DX = 0.001	!
! R5	R(4,5)	1.2462	-DE/DX = -0.0015	!
! R6	R(4,6)	1.4019	-DE/DX = -0.0002	!
! R7	R(4,10)	1.5821	-DE/DX = -0.0006	!
! R8	R(6,7)	1.5012	-DE/DX = -0.0014	!
! R9	R(8,9)	1.1059	-DE/DX = -0.0001	!
! R10	R(8,13)	1.5793	-DE/DX = 0.0006	!
! R11	R(8,22)	1.1044	-DE/DX = 0.0002	!
! R12	R(10,11)	1.1046	-DE/DX = -0.0001	!
! R13	R(10,12)	1.1031	-DE/DX = -0.0001	!
! R14	R(10,16)	1.5815	-DE/DX = -0.0003	!
! R15	R(13,14)	1.1031	-DE/DX = -0.0001	!
! R16	R(13,15)	1.0998	-DE/DX = 0.0004	!
! R17	R(13,19)	1.5797	-DE/DX = 0.0004	!
! R18	R(16,17)	1.1036	-DE/DX = -0.0003	!
! R19	R(16,18)	1.1029	-DE/DX = 0.0	!
! R20	R(16,19)	1.5888	-DE/DX = -0.0008	!
! R21	R(19,20)	1.1033	-DE/DX = -0.0001	!
! R22	R(19,21)	1.1031	-DE/DX = -0.0002	!
! A1	A(2,1,3)	123.6551	-DE/DX = 0.0004	!
! A2	A(2,1,8)	127.2688	-DE/DX = -0.0004	!



! A3	A(3,1,8)	109.0561	-DE/DX =	0.0	!
! A4	A(1,3,7)	175.5045	-DE/DX =	0.0011	!
! A5	A(5,4,6)	124.1986	-DE/DX =	0.0004	!
! A6	A(5,4,10)	128.9698	-DE/DX =	0.0003	!
! A7	A(6,4,10)	106.83	-DE/DX =	-0.0007	!
! A8	A(4,6,7)	179.9996	-DE/DX =	-0.0022	!
! A9	A(3,7,6)	122.3661	-DE/DX =	-0.0009	!
! A10	A(1,8,9)	106.8936	-DE/DX =	-0.0003	!
! A11	A(1,8,13)	115.8558	-DE/DX =	0.0007	!
! A12	A(1,8,22)	106.5391	-DE/DX =	-0.0001	!
! A13	A(9,8,13)	110.0479	-DE/DX =	-0.0003	!
! A14	A(9,8,22)	106.7567	-DE/DX =	0.0001	!
! A15	A(13,8,22)	110.2972	-DE/DX =	0.0	!
! A16	A(4,10,11)	108.3229	-DE/DX =	-0.0006	!
! A17	A(4,10,12)	107.4449	-DE/DX =	-0.0002	!
! A18	A(4,10,16)	111.7189	-DE/DX =	0.0009	!
! A19	A(11,10,12)	107.6778	-DE/DX =	0.0001	!
! A20	A(11,10,16)	111.174	-DE/DX =	-0.0001	!
! A21	A(12,10,16)	110.3371	-DE/DX =	-0.0001	!
! A22	A(8,13,14)	107.8333	-DE/DX =	0.0002	!
! A23	A(8,13,15)	109.0088	-DE/DX =	0.0003	!
! A24	A(8,13,19)	114.0839	-DE/DX =	-0.0008	!
! A25	A(14,13,15)	106.1499	-DE/DX =	-0.0001	!
! A26	A(14,13,19)	108.4655	-DE/DX =	0.0002	!
! A27	A(15,13,19)	110.9503	-DE/DX =	0.0003	!
! A28	A(10,16,17)	107.3228	-DE/DX =	0.0003	!
! A29	A(10,16,18)	108.0619	-DE/DX =	0.0004	!
! A30	A(10,16,19)	120.4067	-DE/DX =	-0.0011	!
! A31	A(17,16,18)	105.9966	-DE/DX =	-0.0002	!
! A32	A(17,16,19)	106.3127	-DE/DX =	0.0003	!
! A33	A(18,16,19)	107.8898	-DE/DX =	0.0003	!
! A34	A(13,19,16)	120.8491	-DE/DX =	-0.0006	!
! A35	A(13,19,20)	108.2943	-DE/DX =	0.0001	!
! A36	A(13,19,21)	107.4682	-DE/DX =	0.0003	!
! A37	A(16,19,20)	105.612	-DE/DX =	0.0002	!
! A38	A(16,19,21)	107.7605	-DE/DX =	0.0001	!
! A39	A(20,19,21)	105.97	-DE/DX =	-0.0001	!
! D1	D(2,1,3,7)	-32.9534	-DE/DX =	-0.0003	!
! D2	D(8,1,3,7)	145.5248	-DE/DX =	0.0014	!
! D3	D(2,1,8,9)	71.9748	-DE/DX =	0.0005	!
! D4	D(2,1,8,13)	-164.98	-DE/DX =	0.0003	!
! D5	D(2,1,8,22)	-41.8851	-DE/DX =	0.0007	!
! D6	D(3,1,8,9)	-106.4334	-DE/DX =	-0.0013	!
! D7	D(3,1,8,13)	16.6118	-DE/DX =	-0.0015	!
! D8	D(3,1,8,22)	139.7067	-DE/DX =	-0.0012	!
! D9	D(1,3,7,6)	-153.2541	-DE/DX =	0.0008	!
! D10	D(5,4,6,7)	2.0289	-DE/DX =	0.0	!
! D11	D(10,4,6,7)	-177.5487	-DE/DX =	0.0001	!
! D12	D(5,4,10,11)	113.2311	-DE/DX =	-0.0003	!
! D13	D(5,4,10,12)	-2.8325	-DE/DX =	0.0	!
! D14	D(5,4,10,16)	-123.9844	-DE/DX =	-0.0003	!
! D15	D(6,4,10,11)	-67.2183	-DE/DX =	-0.0003	!
! D16	D(6,4,10,12)	176.7181	-DE/DX =	-0.0001	!
! D17	D(6,4,10,16)	55.5662	-DE/DX =	-0.0003	!
! D18	D(4,6,7,3)	-176.973	-DE/DX =	0.0001	!
! D19	D(1,8,13,14)	136.6544	-DE/DX =	0.0005	!
! D20	D(1,8,13,15)	21.8279	-DE/DX =	0.0004	!

! D21	D(1,8,13,19)	-102.7988	-DE/DX =	0.0003	
! D22	D(9,8,13,14)	-101.9733	-DE/DX =	0.0003	!
! D23	D(9,8,13,15)	143.2002	-DE/DX =	0.0001	!
! D24	D(9,8,13,19)	18.5736	-DE/DX =	0.0001	!
! D25	D(22,8,13,14)	15.5552	-DE/DX =	0.0001	!
! D26	D(22,8,13,15)	-99.2712	-DE/DX =	0.0	!
! D27	D(22,8,13,19)	136.1021	-DE/DX =	0.0	!
! D28	D(4,10,16,17)	124.2893	-DE/DX =	0.0002	!
! D29	D(4,10,16,18)	10.3761	-DE/DX =	0.0001	!
! D30	D(4,10,16,19)	-114.0971	-DE/DX =	0.0002	!
! D31	D(11,10,16,17)	-114.5668	-DE/DX =	0.0	!
! D32	D(11,10,16,18)	131.52	-DE/DX =	-0.0002	!
! D33	D(11,10,16,19)	7.0469	-DE/DX =	-0.0001	!
! D34	D(12,10,16,17)	4.831	-DE/DX =	0.0	!
! D35	D(12,10,16,18)	-109.0822	-DE/DX =	-0.0002	!
! D36	D(12,10,16,19)	126.4446	-DE/DX =	-0.0001	!
! D37	D(8,13,19,16)	129.2439	-DE/DX =	-0.0002	!
! D38	D(8,13,19,20)	7.3989	-DE/DX =	-0.0001	!
! D39	D(8,13,19,21)	-106.6697	-DE/DX =	-0.0002	!
! D40	D(14,13,19,16)	-110.5629	-DE/DX =	-0.0004	!
! D41	D(14,13,19,20)	127.5921	-DE/DX =	-0.0003	!
! D42	D(14,13,19,21)	13.5235	-DE/DX =	-0.0004	!
! D43	D(15,13,19,16)	5.6596	-DE/DX =	-0.0003	!
! D44	D(15,13,19,20)	-116.1854	-DE/DX =	-0.0002	!
! D45	D(15,13,19,21)	129.746	-DE/DX =	-0.0003	!
! D46	D(10,16,19,13)	26.0502	-DE/DX =	0.0005	!
! D47	D(10,16,19,20)	149.1795	-DE/DX =	0.0004	!
! D48	D(10,16,19,21)	-97.8987	-DE/DX =	0.0005	!
! D49	D(17,16,19,13)	148.1552	-DE/DX =	0.0005	!
! D50	D(17,16,19,20)	-88.7155	-DE/DX =	0.0004	!
! D51	D(17,16,19,21)	24.2062	-DE/DX =	0.0004	!
! D52	D(18,16,19,13)	-98.5041	-DE/DX =	0.0006	!
! D53	D(18,16,19,20)	24.6252	-DE/DX =	0.0005	!
! D54	D(18,16,19,21)	137.5469	-DE/DX =	0.0005	!

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