

Synthesis of Dibenzazepinones by Palladium-Catalyzed Intramolecular Arylation of *o*-(2'-Bromophenyl)anilide Enolates

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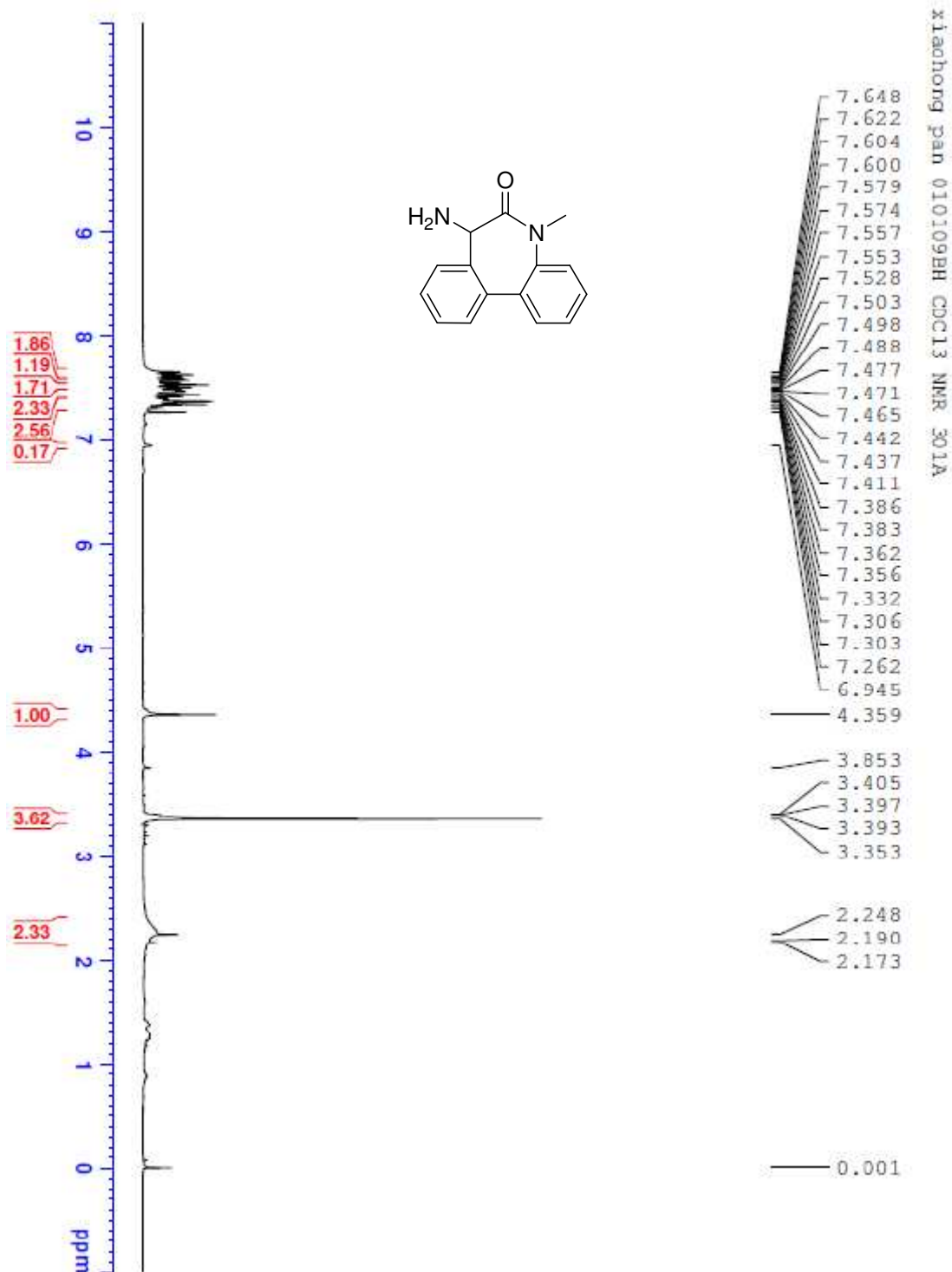
Supporting Information

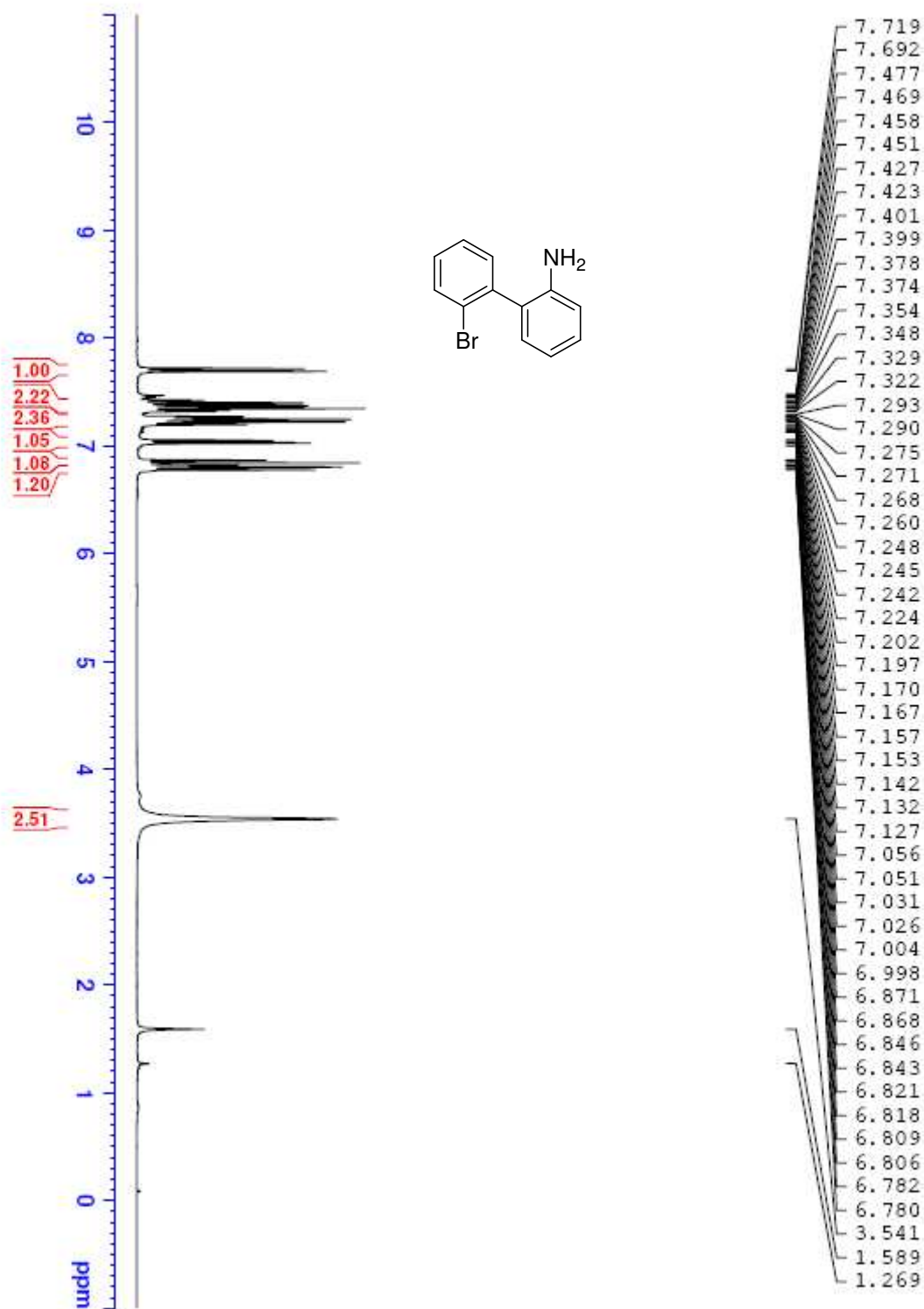
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¹ H and ¹³ C NMR spectra of compounds	S3

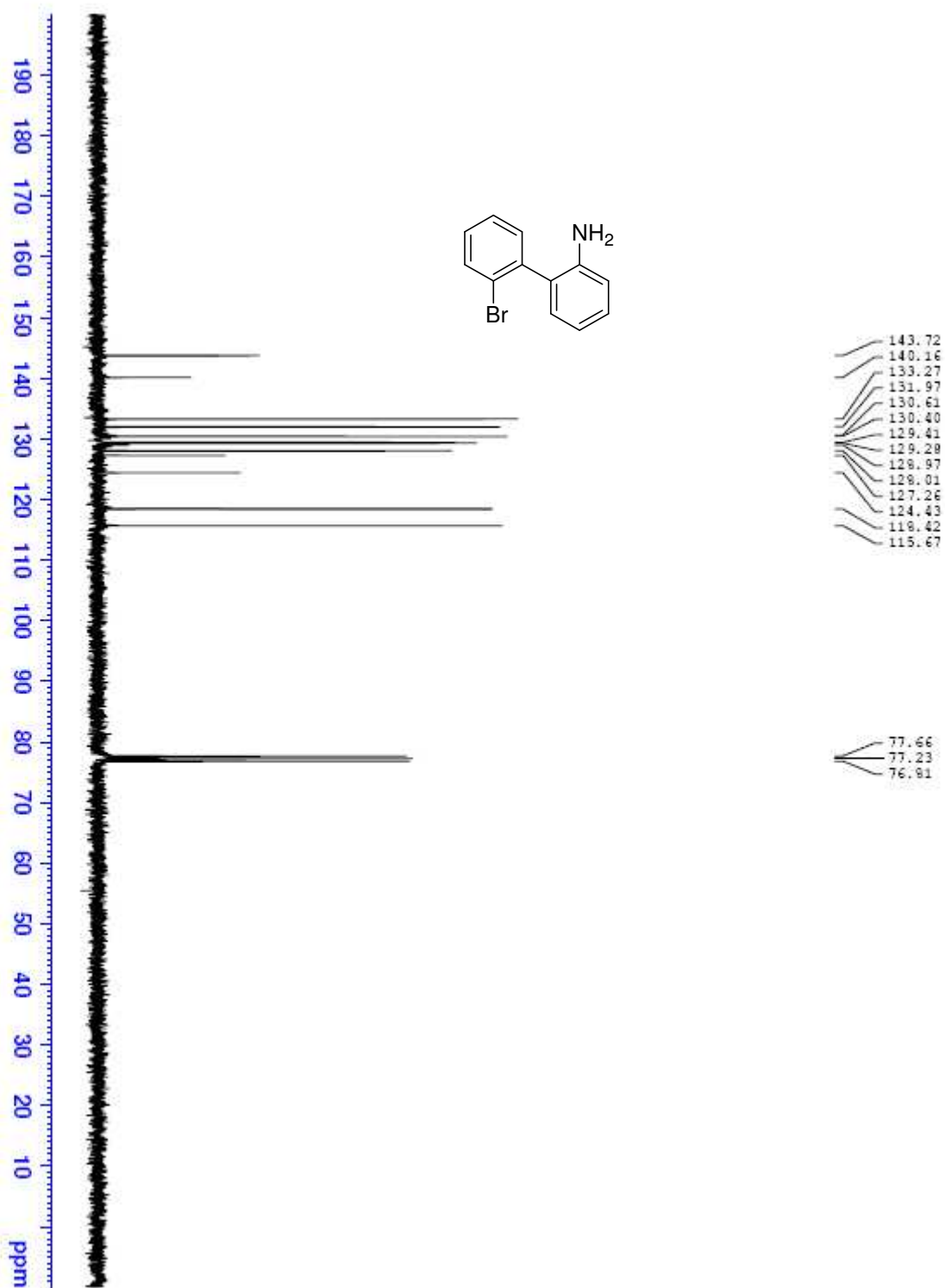
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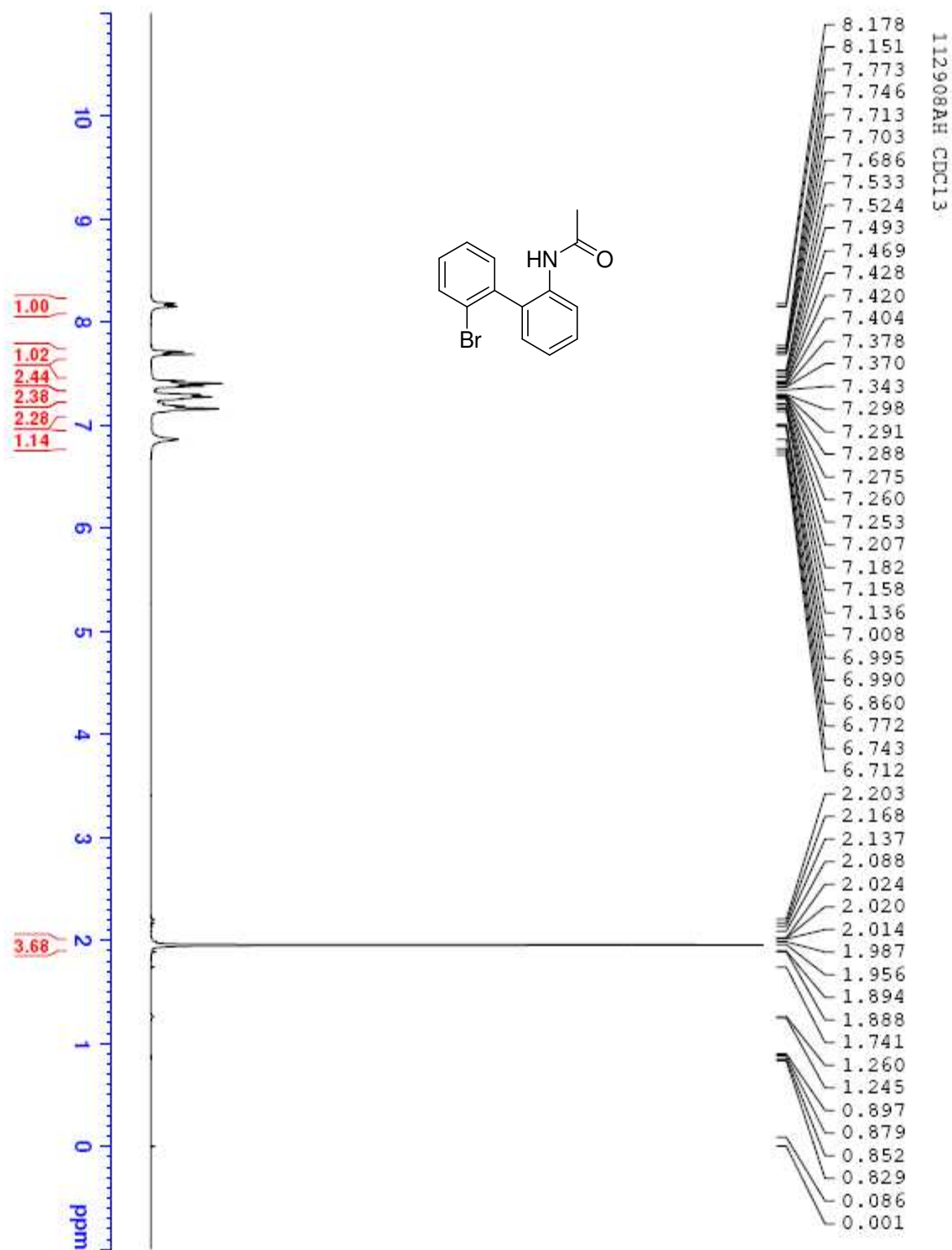
Commercially available reagents and solvents were used as received without further purification. Reactions at “room temperature” were conducted under ambient laboratory conditions T = 20-27 °C, p = 720-770 mmHg. References to “removal of volatile components” refer to rotary evaporation of the sample at 25-65 °C *in vacuo* (18-25 mmHg). Thin layer chromatography (TLC) was performed on silica gel 60 F254 glass backed plates with a layer thickness of 0.25 mm manufactured by EMD. Silica gel columns for flash chromatography, according to the method of Still, were prepared with SILICYCLE silica gel (SiliaFlash P60, 230-240 mesh). ¹H NMR spectra were recorded on a Bruker Avance 300 at 300 MHz and a Bruker DRX 500 at 500 MHz, and chemical shifts were given in parts per million (ppm) on the delta scale (δ) using TMS (Me₄Si, 0.00). ¹³C NMR spectra were recorded on a Bruker Avance 300 at 75 MHz, and chemical shifts are given in parts per million (ppm) on the delta

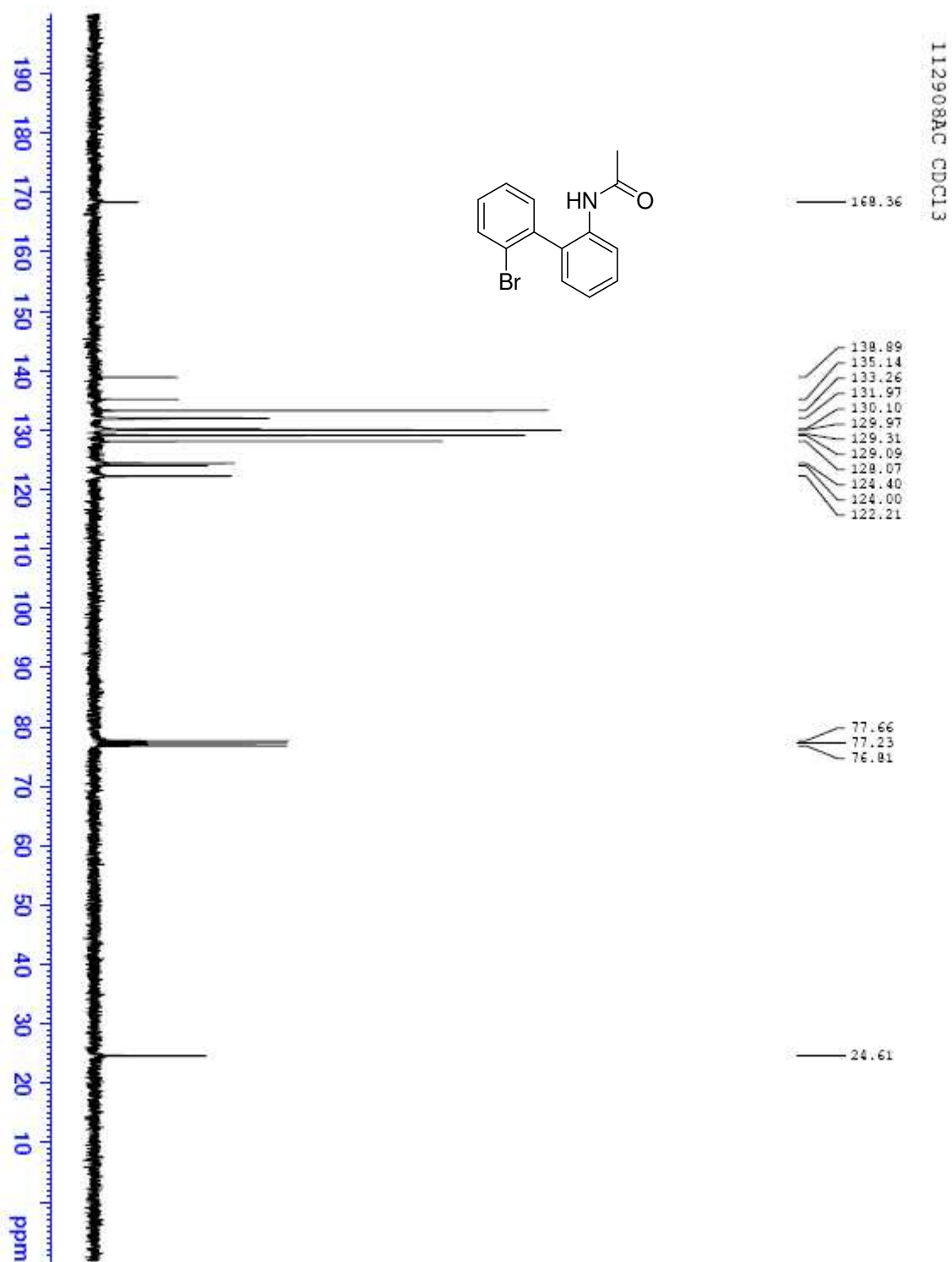
scale (δ) using deuterated solvents as internal standards (CDCl_3 , 77.23), and the coupling constant values (J) are in Hertz. Abbreviations for NMR data: s = singlet; d = doublet; t = triplet; q = quartet; dd = doublet of doublets; dt = doublet of triples; dq = doublet of quartets; tt = triplet of triplets; m = multiplet; br = broad. High resolution and low resolution mass spectra were recorded of a VG 7070 spectrometer. Infrared (IR) spectra were collected on an Avatar 360 Nicolet FT-IR spectrometer. Samples for IR were prepared as a thin film on a NaBr plate by dissolving the sample in CH_2Cl_2 and then evaporating the CH_2Cl_2 .

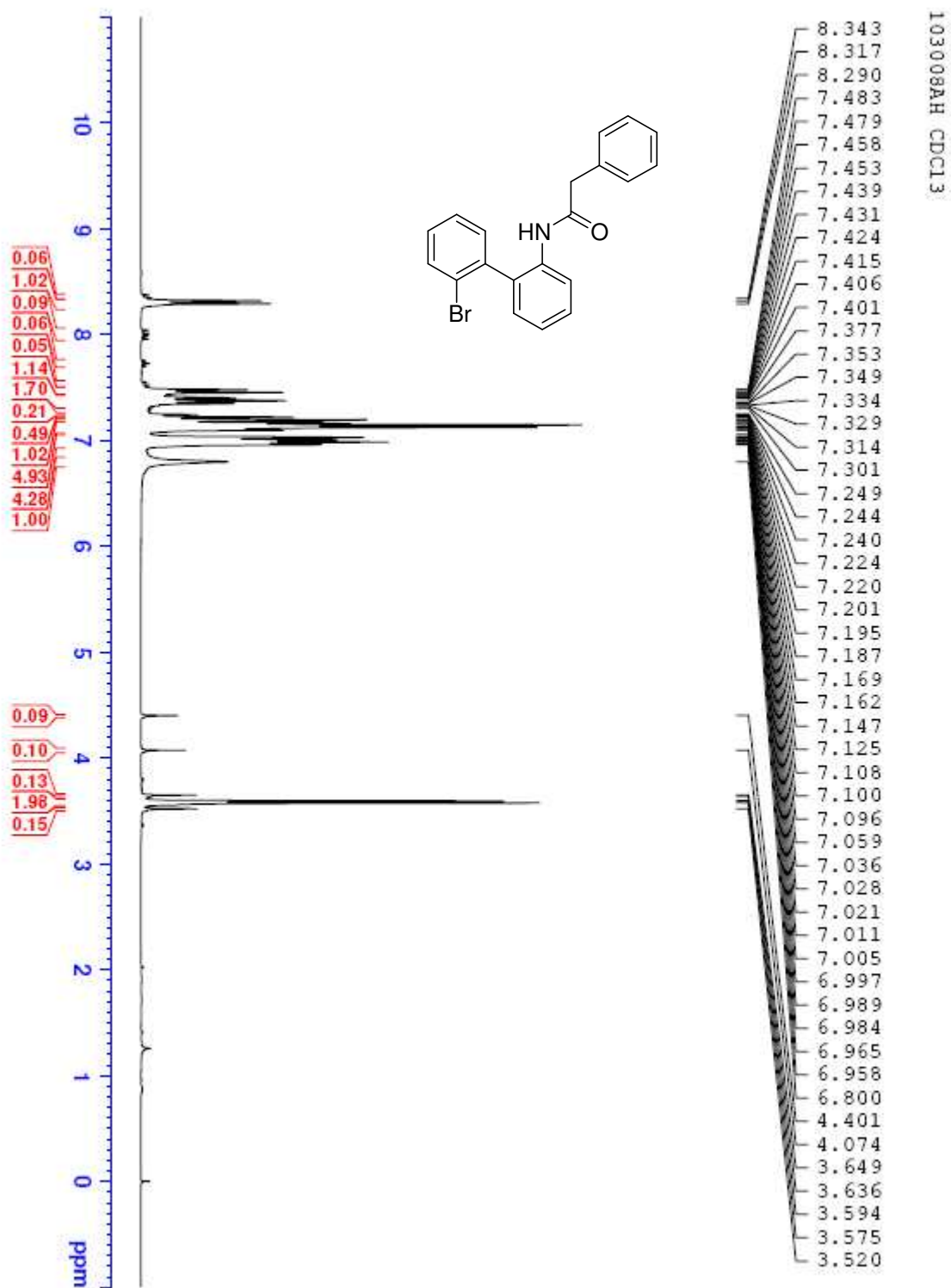
5-Amino-N-methyl-dibenzazepin-6-one (1).

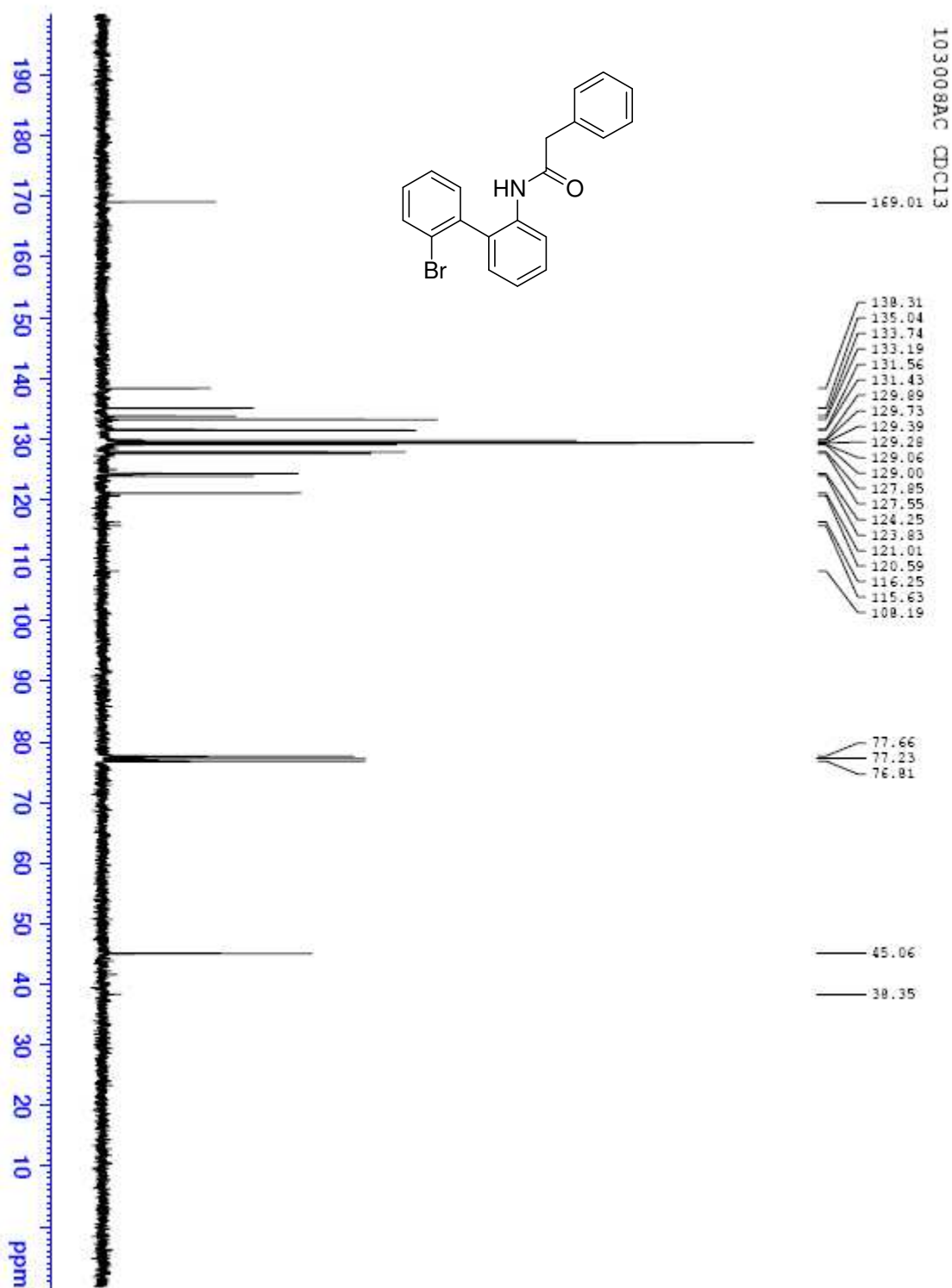
[1,1'-Biphenyl]-2-amine, 2'-bromo- (2).

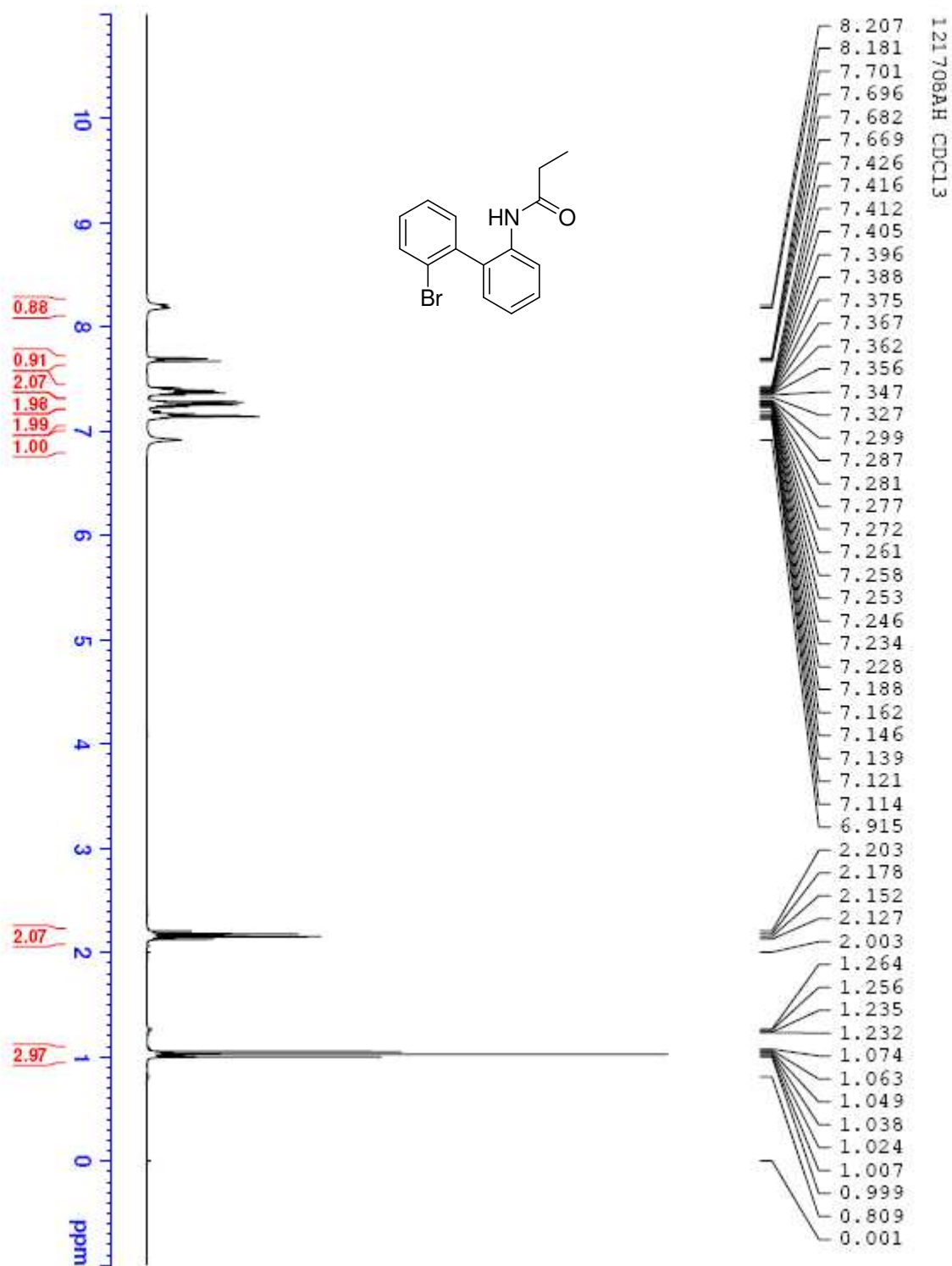
[1,1'-Biphenyl]-2-amine, 2'-bromo- (2).

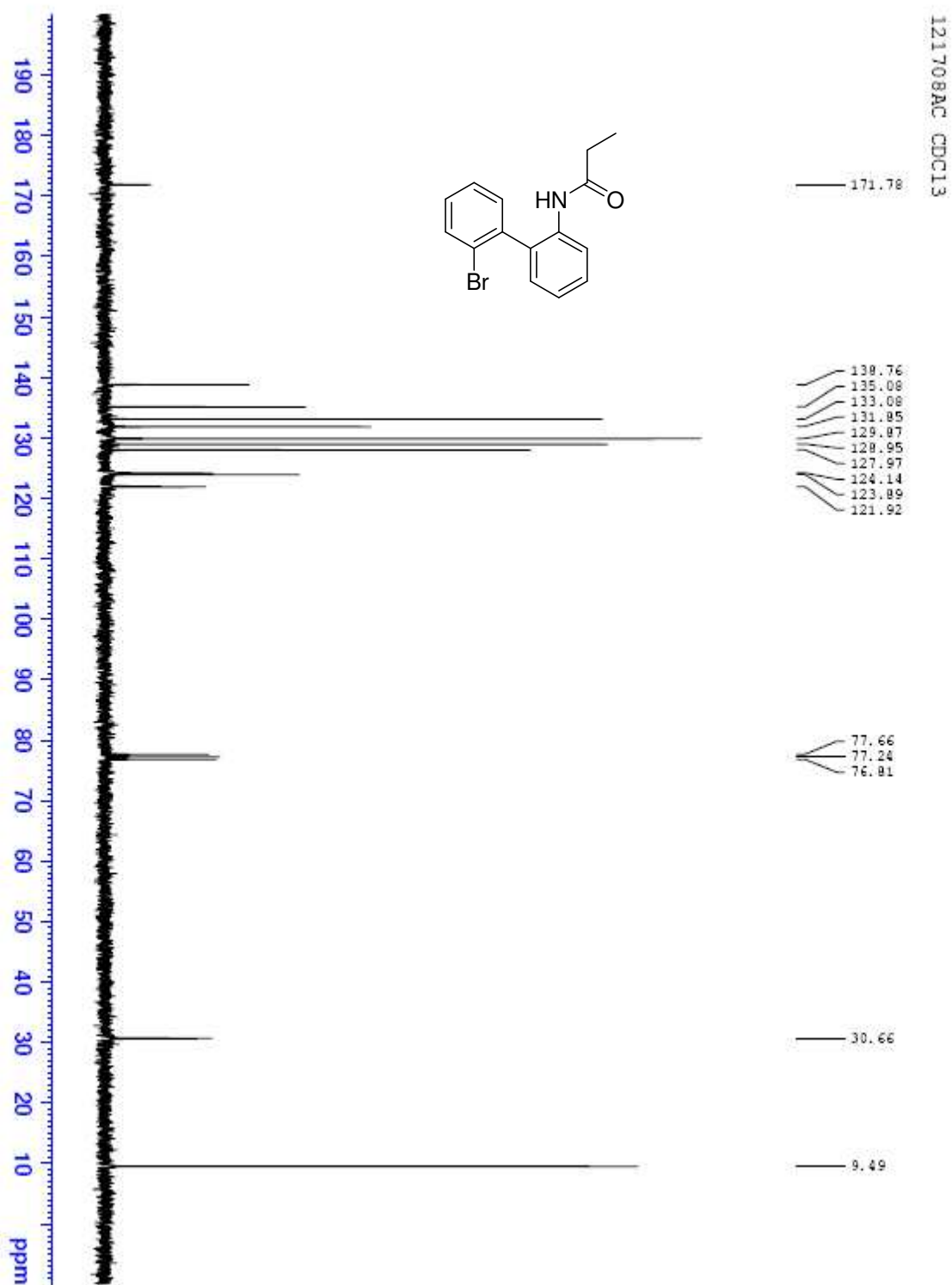
[1,1'-Biphenyl]-2-acetamide, 2'-bromo- (3).

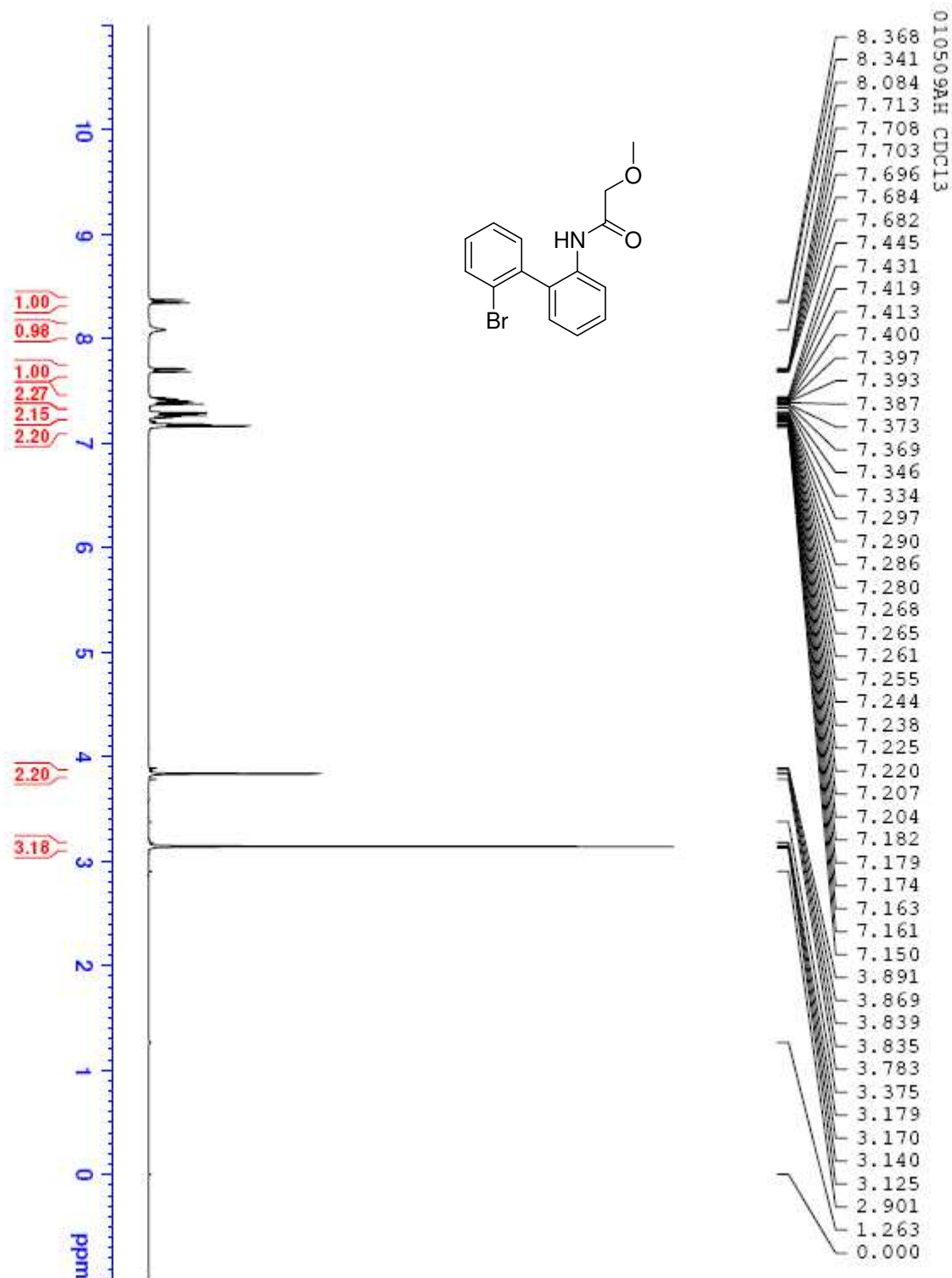
[1,1'-Biphenyl]-2-acetamide, 2'-bromo- (3).

[1,1'-Biphenyl]-2-phenylacetamide, 2'-bromo- (4).

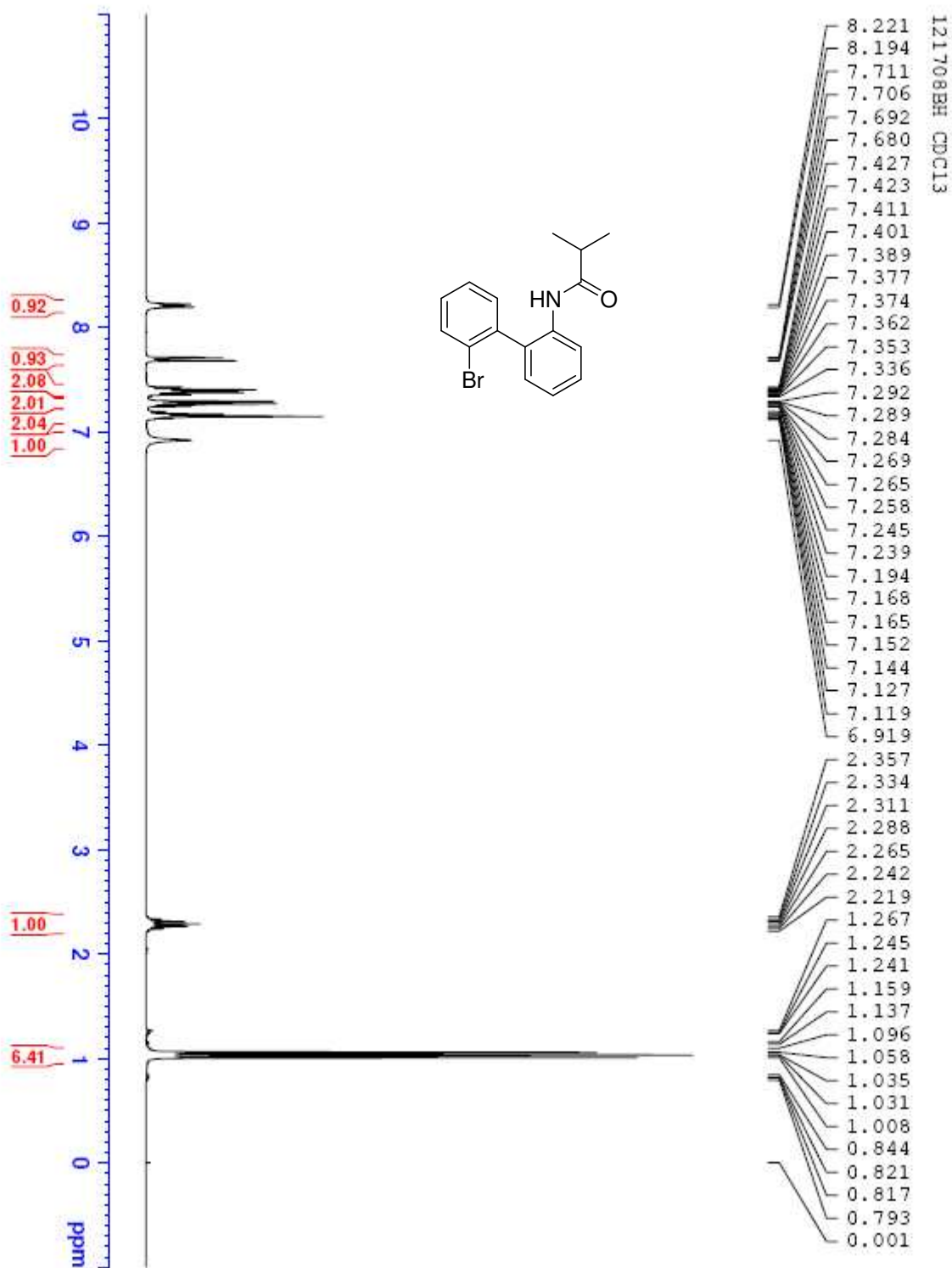
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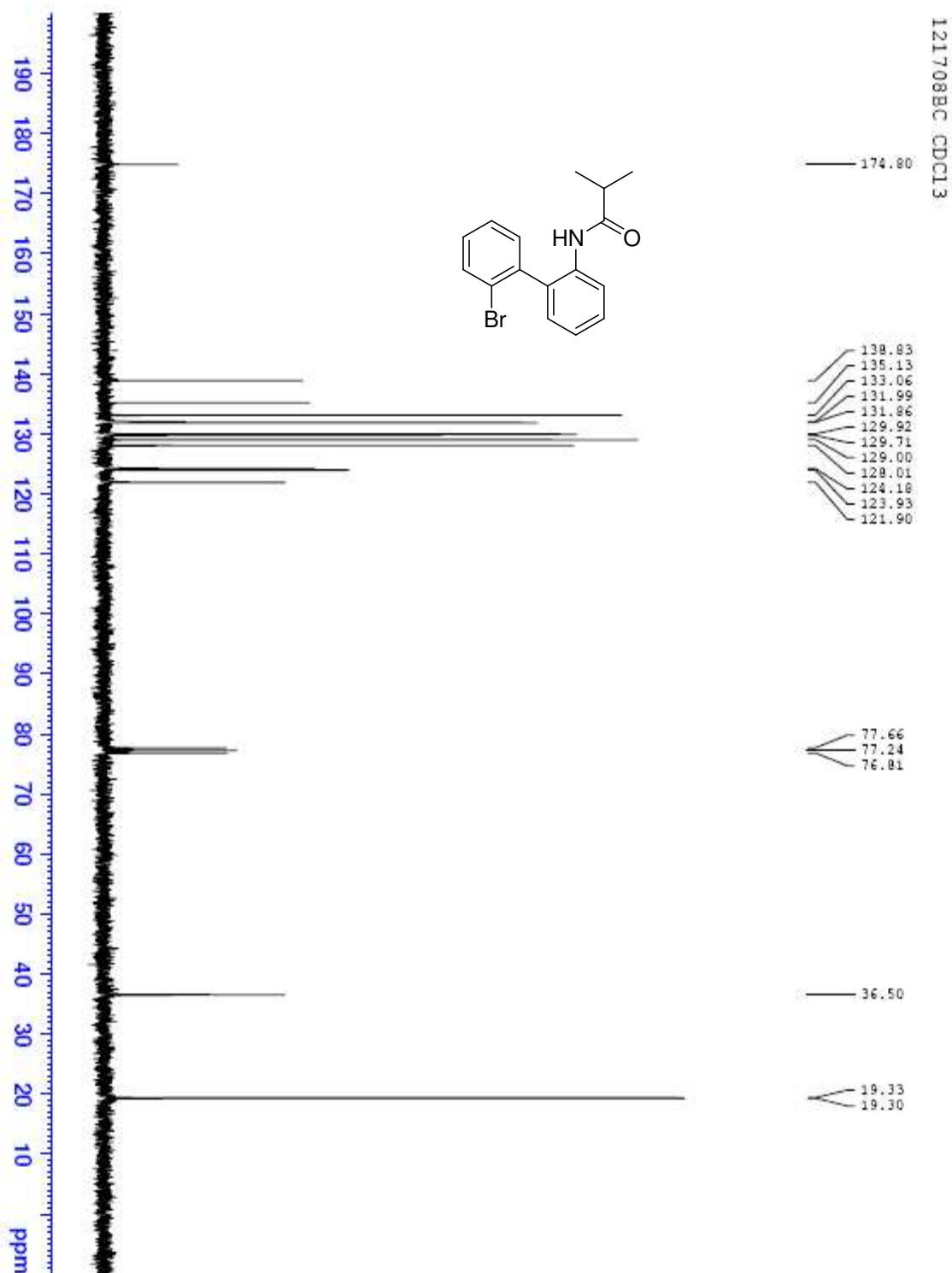
[1,1'-Biphenyl]-2-propionamide, 2'-bromo- (5).

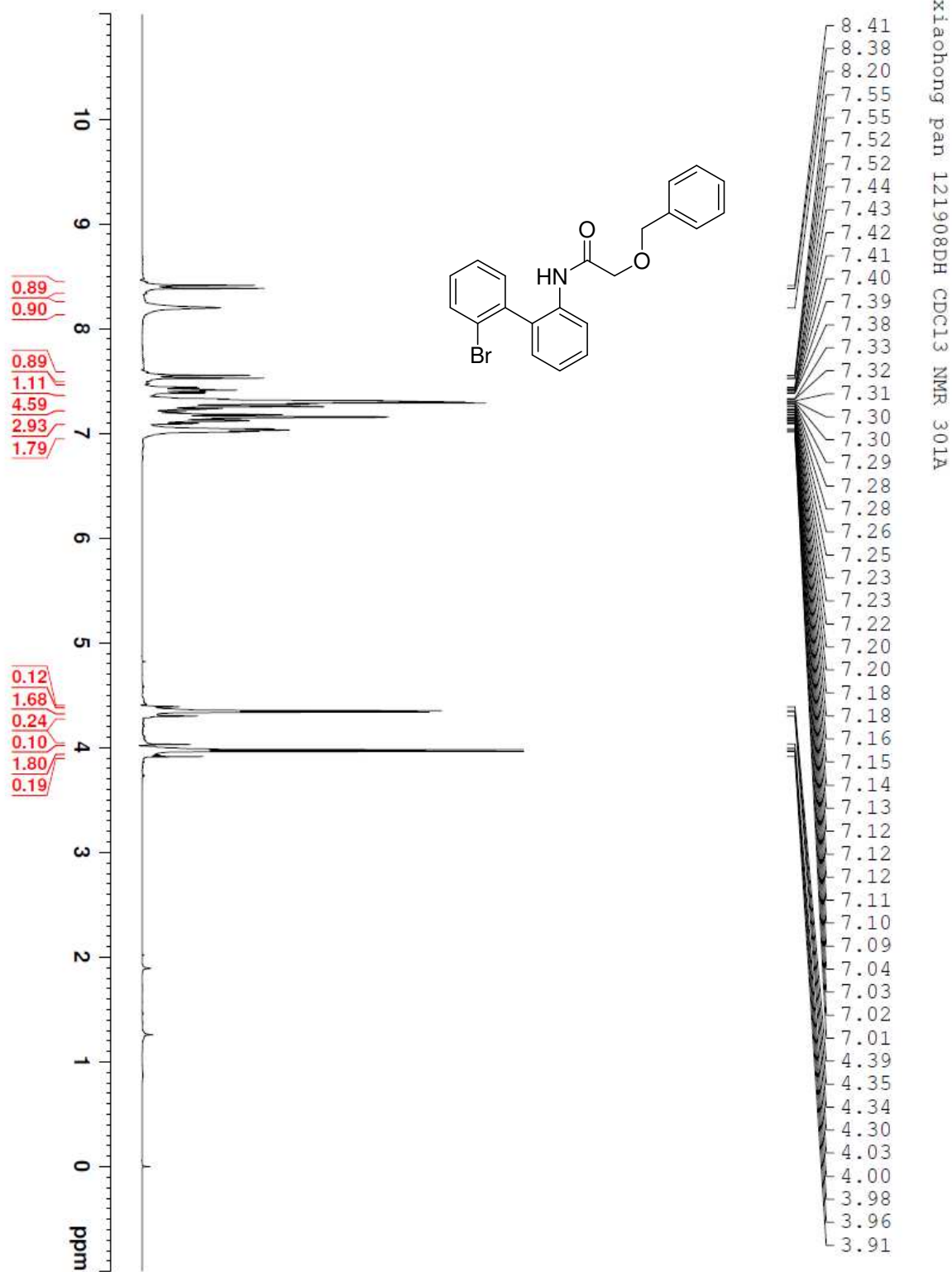
[1,1'-Biphenyl]-2-propionamide, 2'-bromo- (5).

[1,1'-Biphenyl]-2-methoxyacetamide, 2'-bromo- (6).

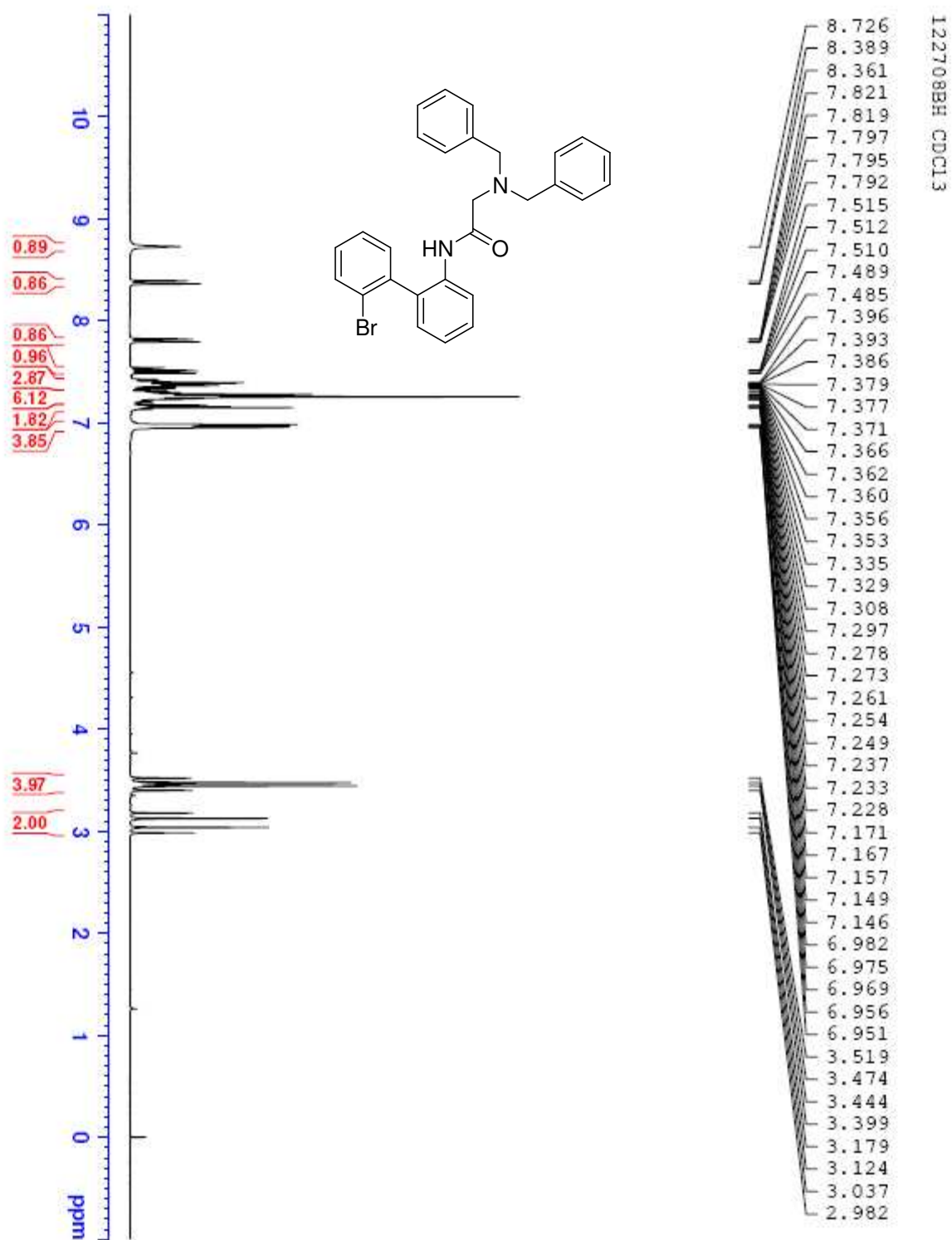
[1,1'-Biphenyl]-2-methoxyacetamide, 2'-bromo- (6).

[1,1'-Biphenyl]-2-isobutyramide, 2'-bromo- (7).

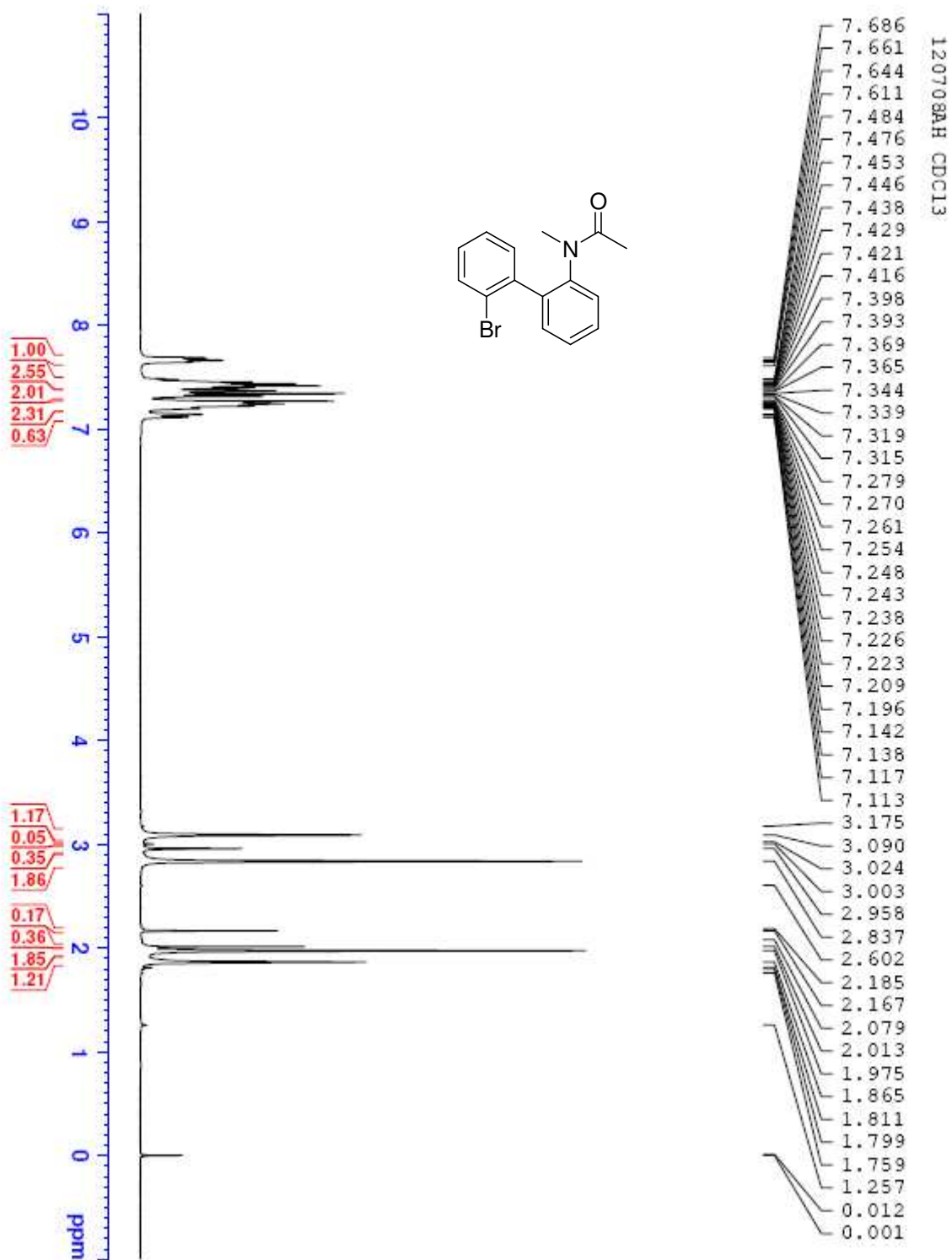
[1,1'-Biphenyl]-2-isobutyramide, 2'-bromo- (7).

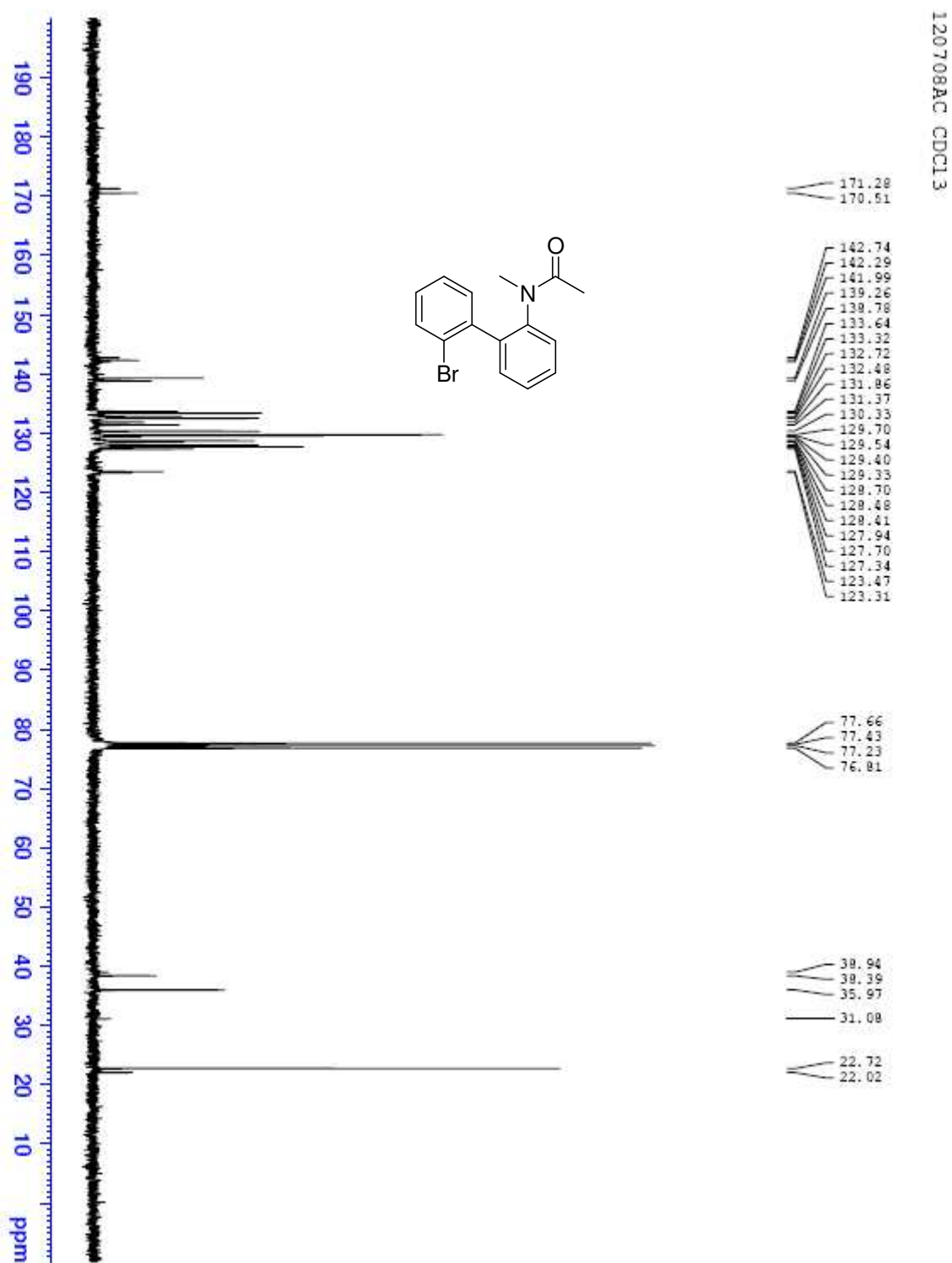
[1,1'-Biphenyl]-2-benzyloxyacetamide, 2'-bromo- (8).

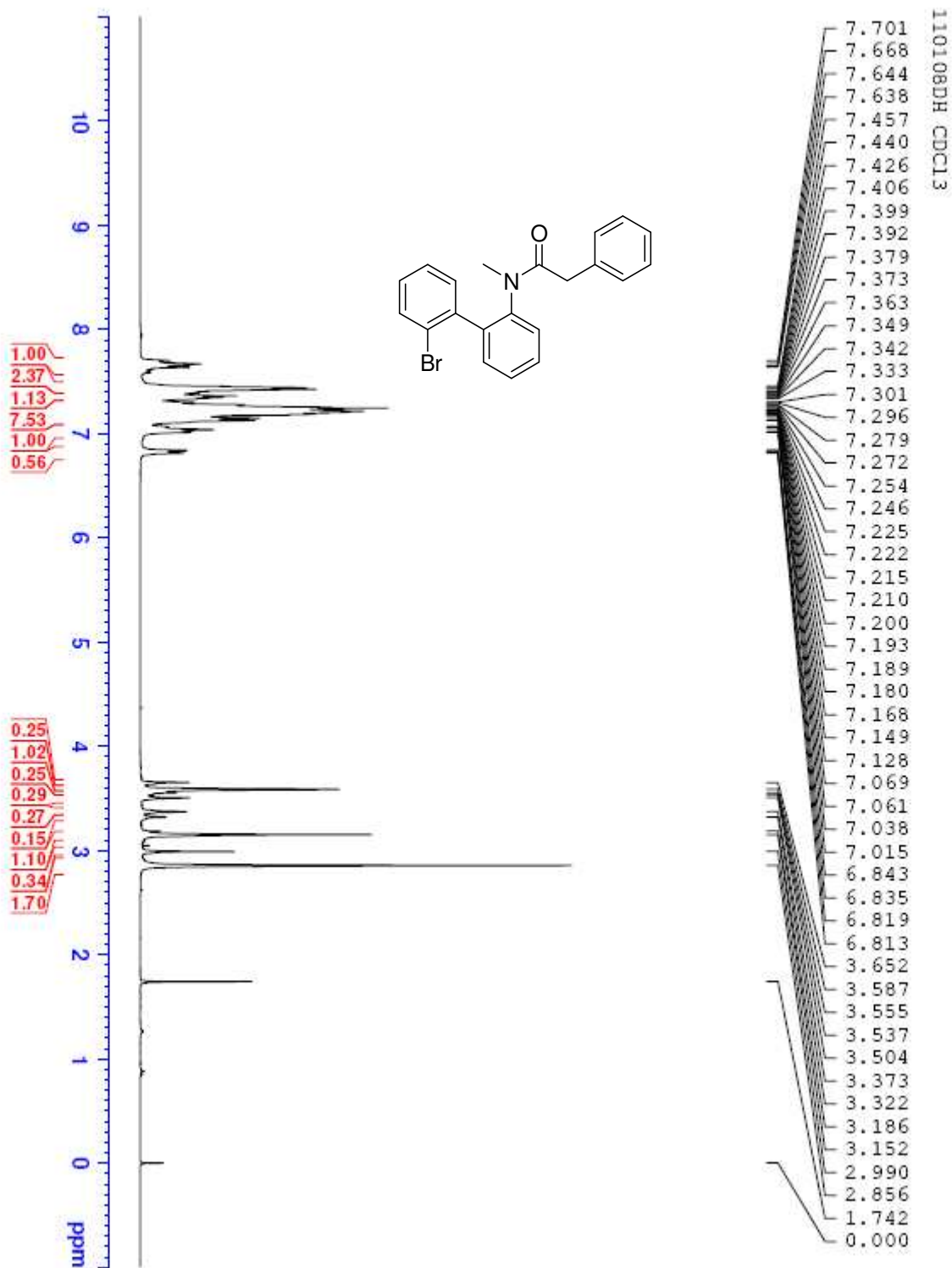
[1,1'-Biphenyl]-2-benzyloxyacetamide, 2'-bromo- (8).

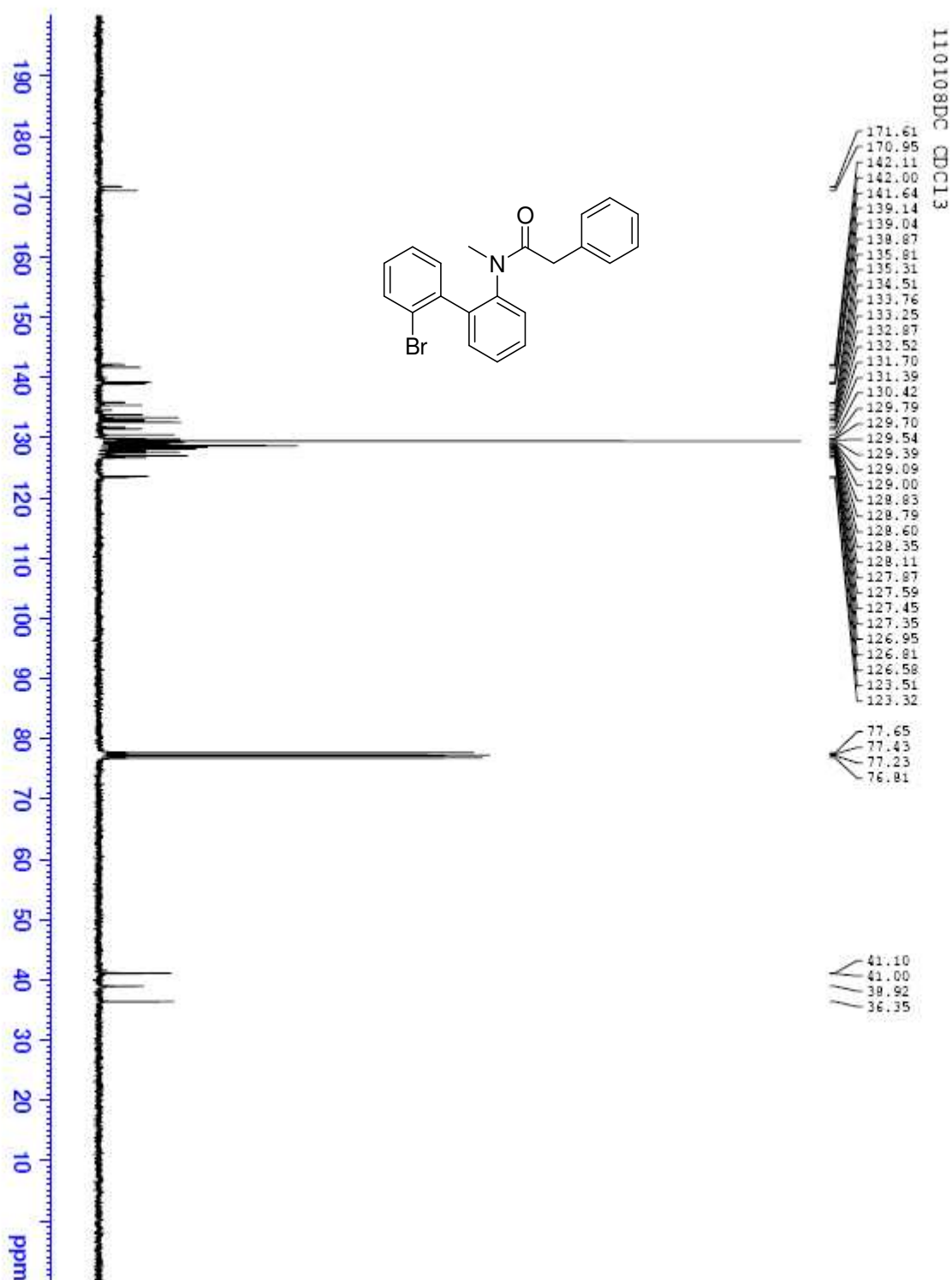
[1,1'-Biphenyl]-2-dibenzylaminoacetamide, 2'-bromo- (9).

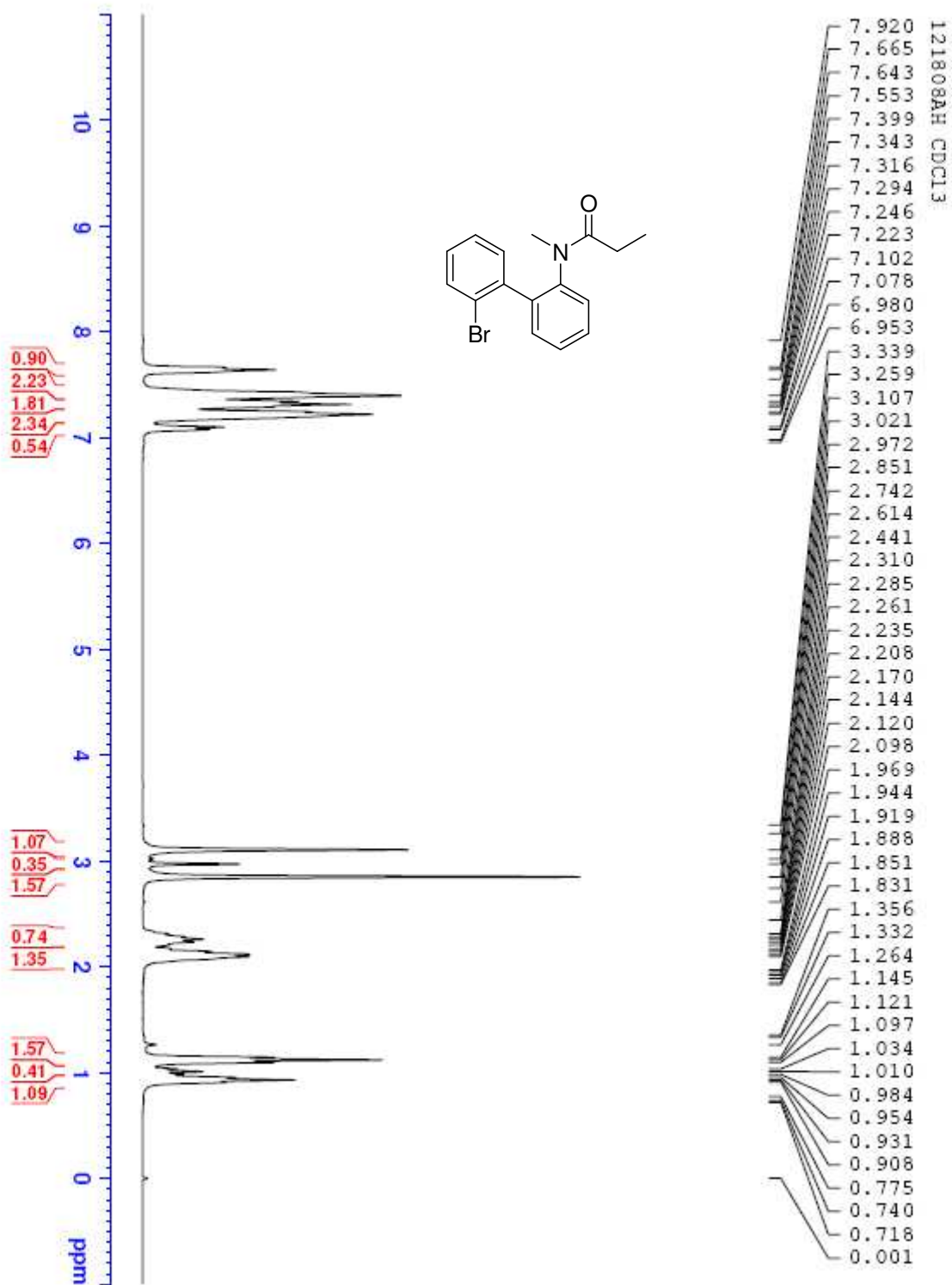
[1,1'-Biphenyl]-2-dibenzylaminoacetamide, 2'-bromo- (9).

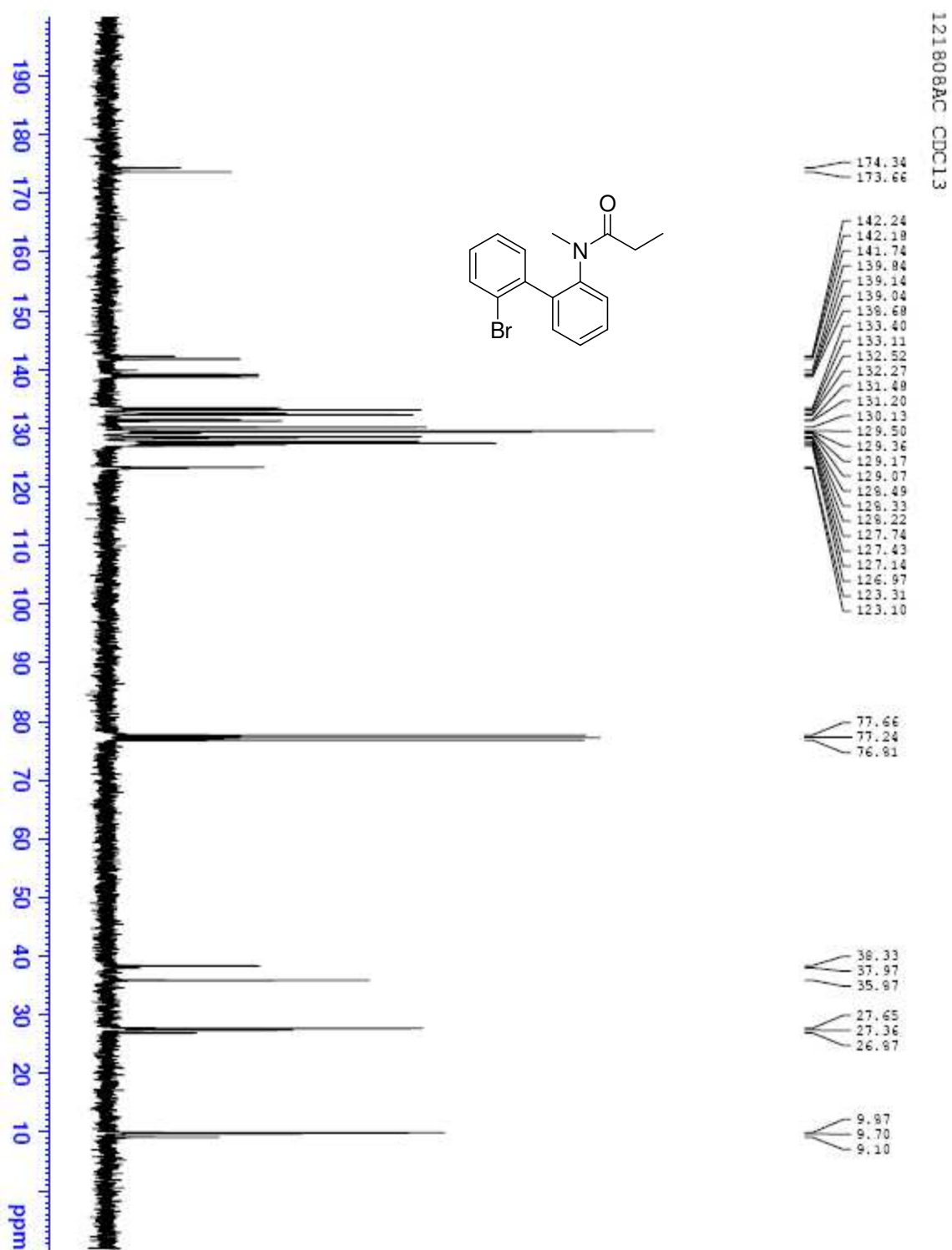
[1,1'-Biphenyl]-2-(N-methyl-acetamide), 2'-bromo- (10).

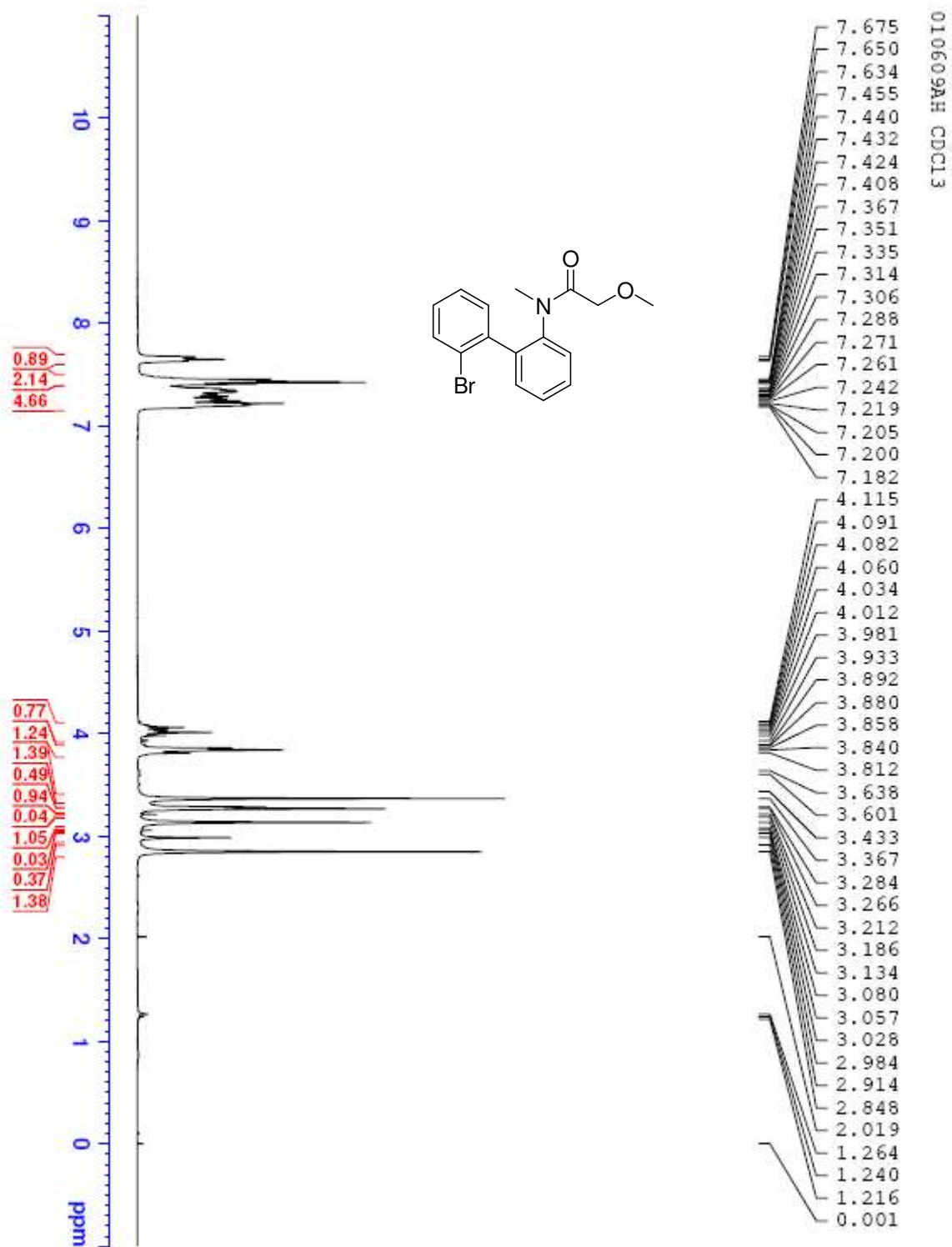
[1,1'-Biphenyl]-2-(N-methyl-acetamide), 2'-bromo- (10).

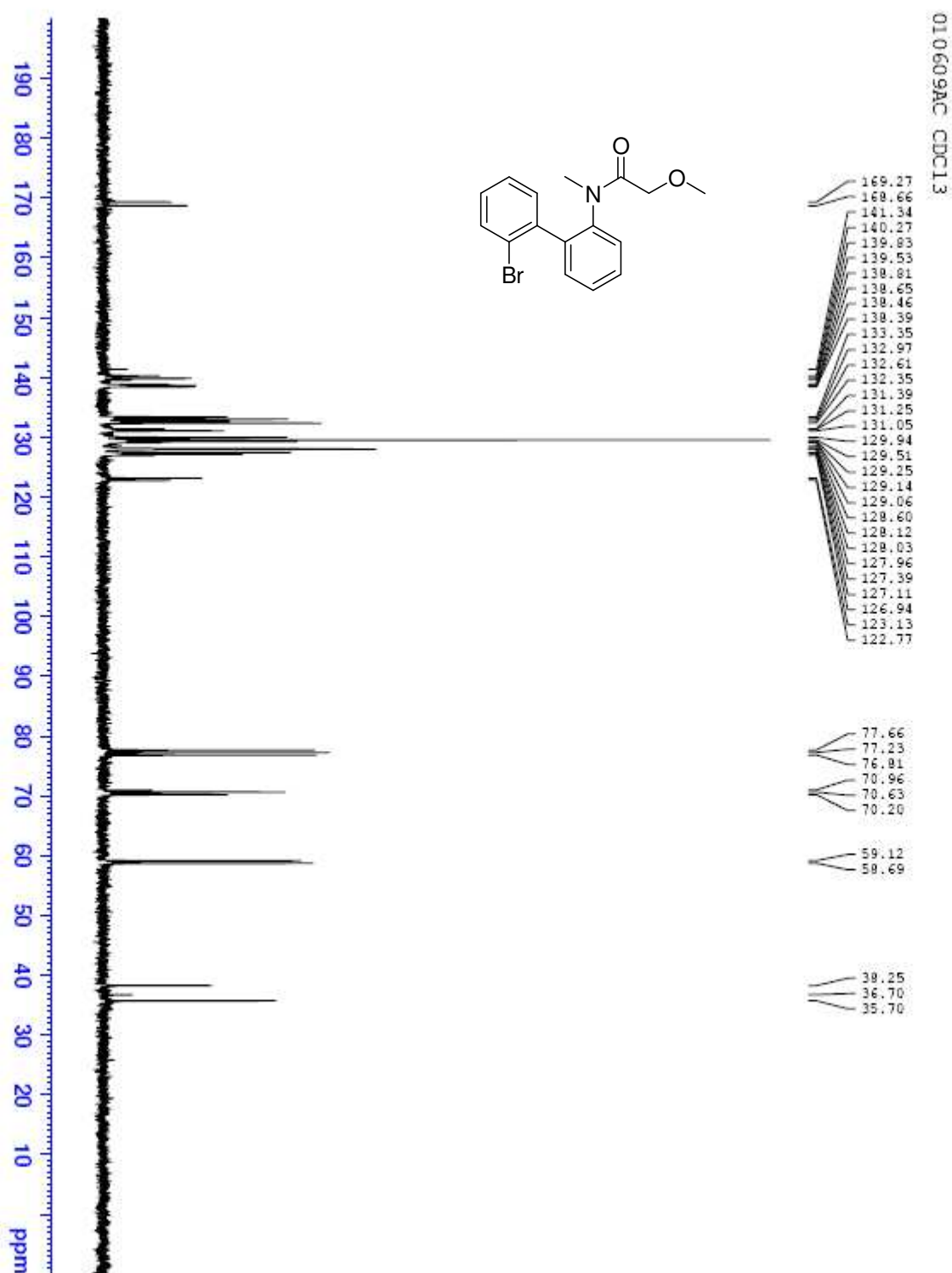
[1,1'-Biphenyl]-2-(N-methyl-phenylacetamide), 2'-bromo- (11).

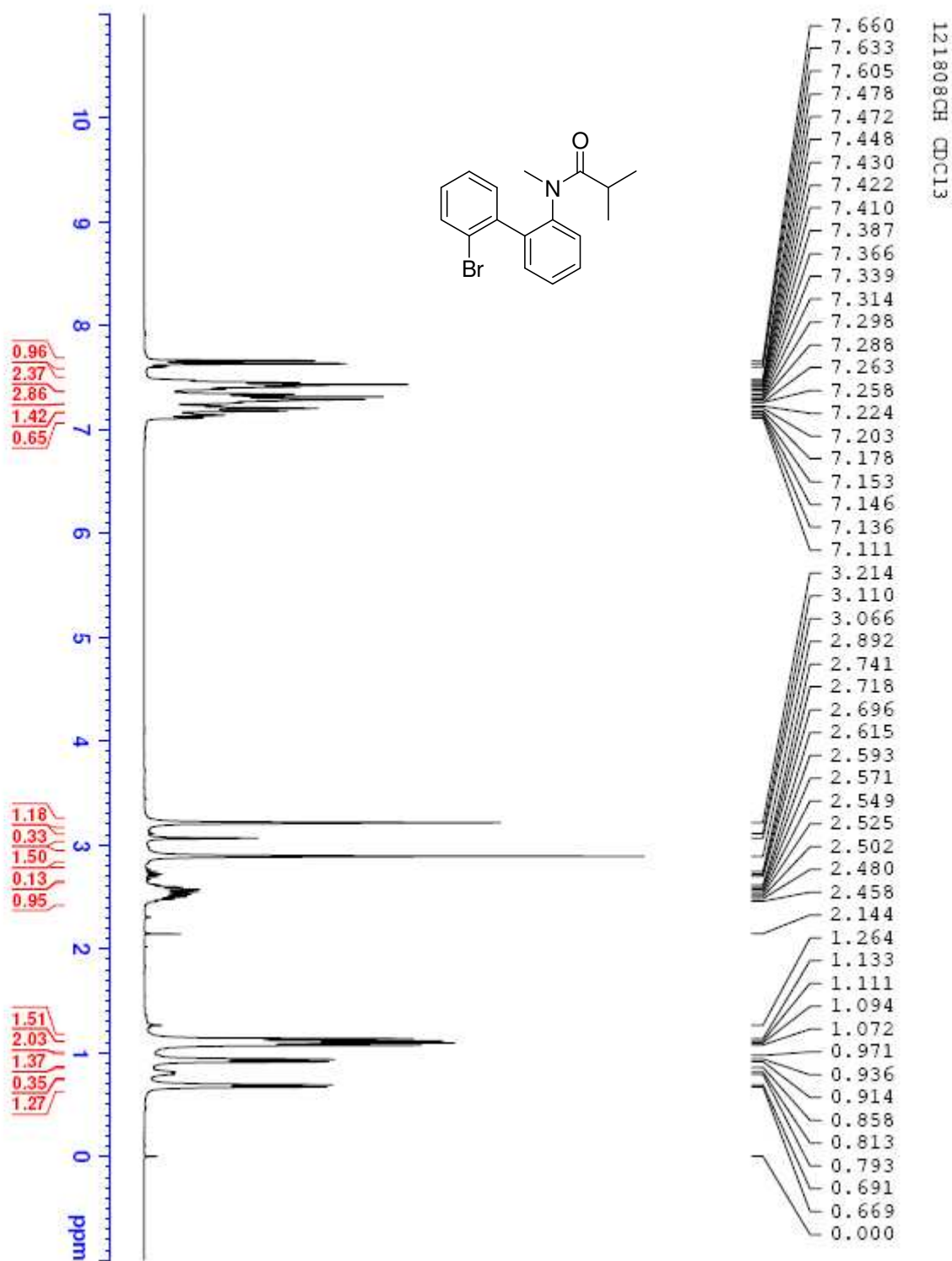
[1,1'-Biphenyl]-2-(N-methyl-phenylacetamide), 2'-bromo- (11).

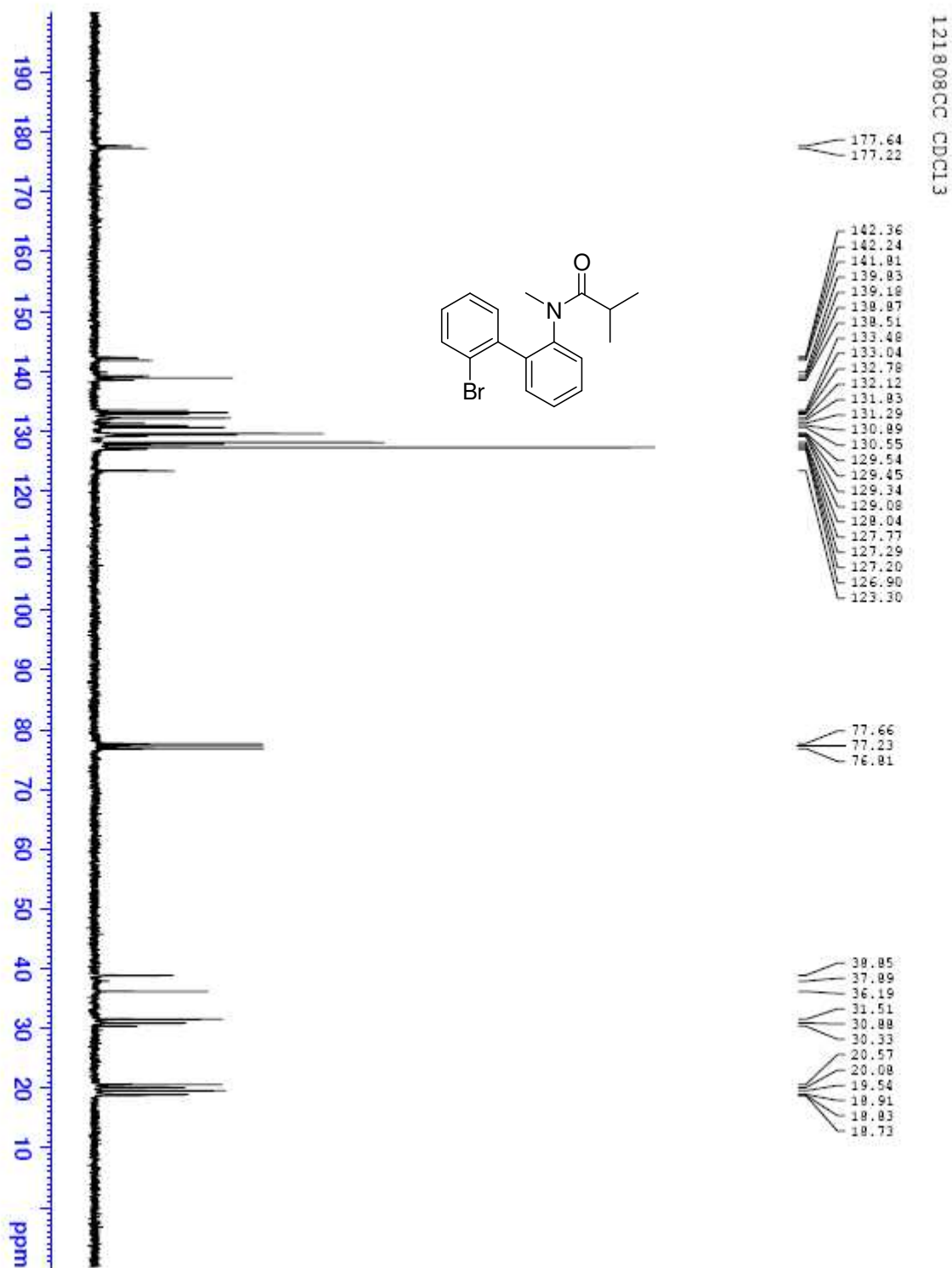
[1,1'-Biphenyl]-2-(N-methyl-propionamide), 2'-bromo- (12).

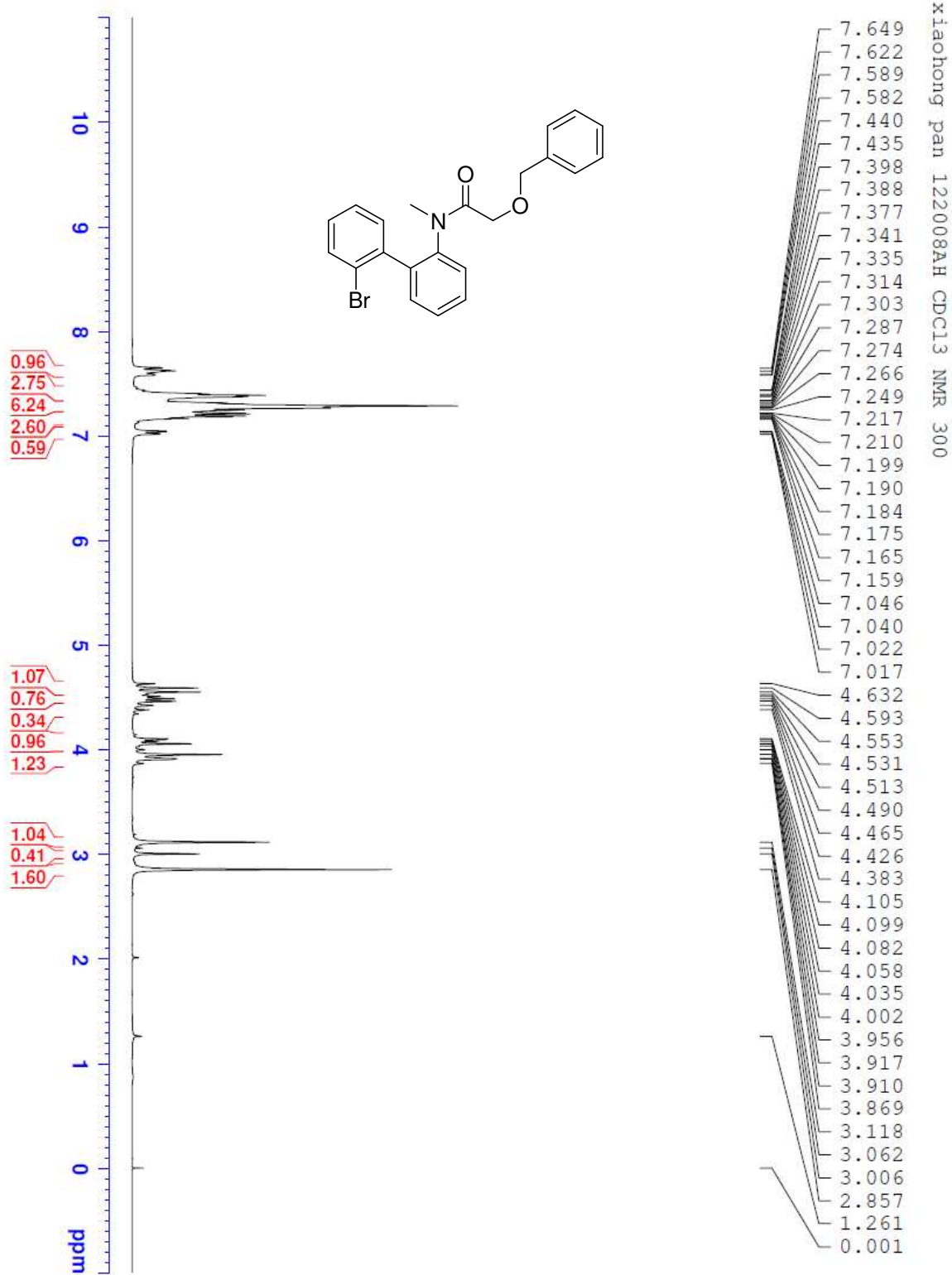
[1,1'-Biphenyl]-2-(N-methyl-propionamide), 2'-bromo- (12).

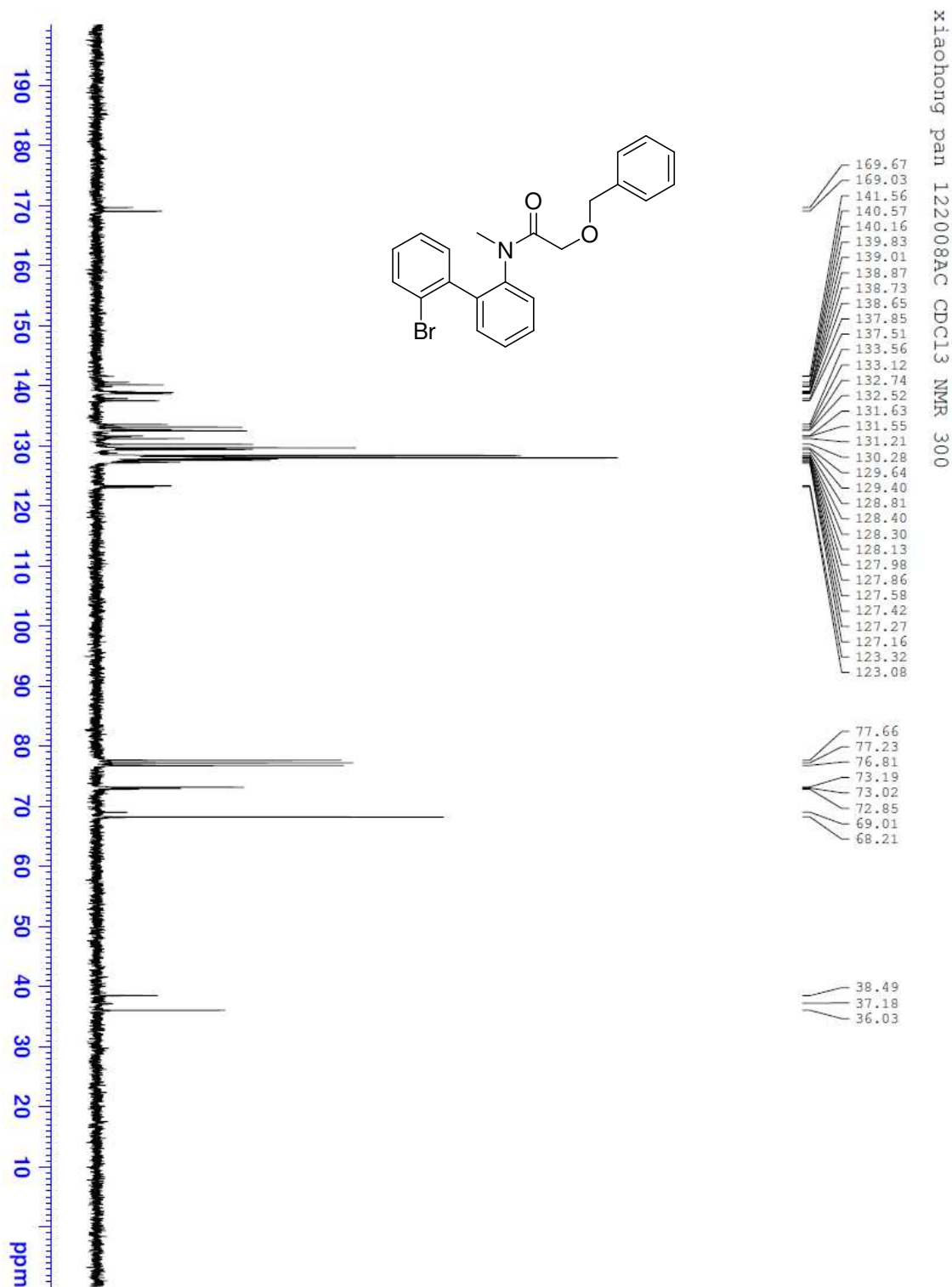
[1,1'-Biphenyl]-2-(N-methyl-methoxyacetamide), 2'-bromo- (13).

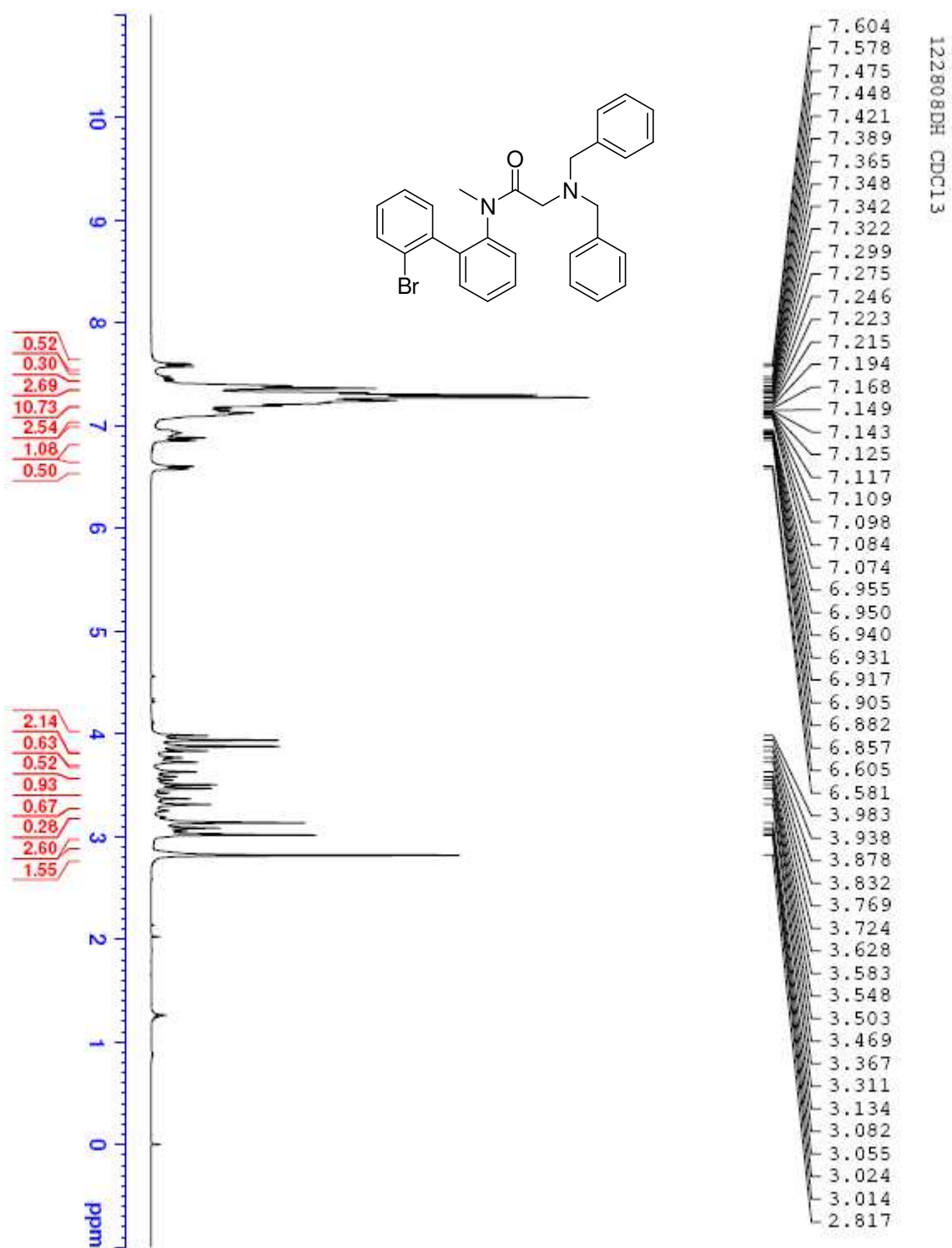
[1,1'-Biphenyl]-2-(*N*-methyl-methoxyacetamide), 2'-bromo- (13).

[1,1'-Biphenyl]-2-(N-methyl-isobutyramide), 2'-bromo- (14).

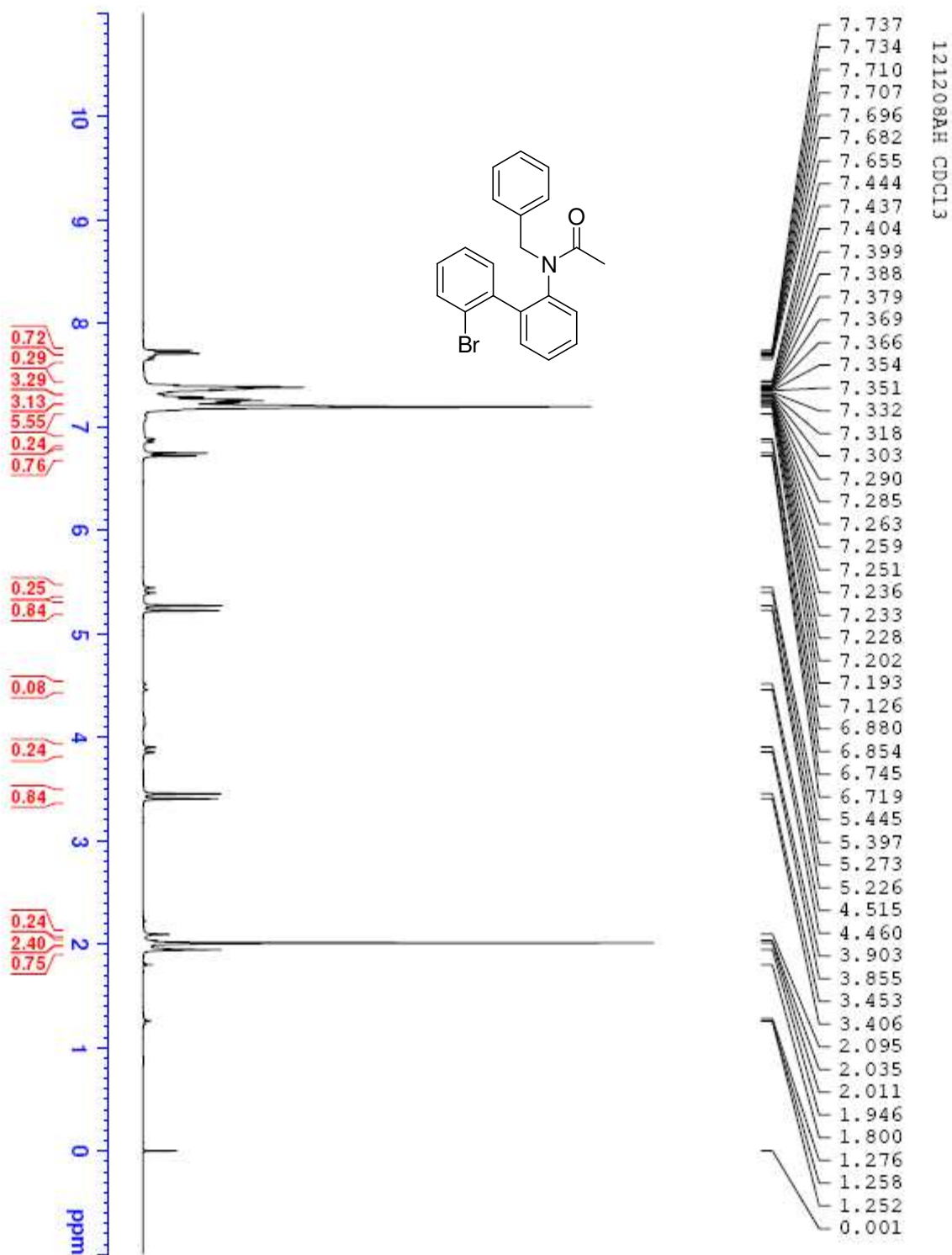
[1,1'-Biphenyl]-2-(N-methyl-isobutyramide), 2'-bromo- (14).

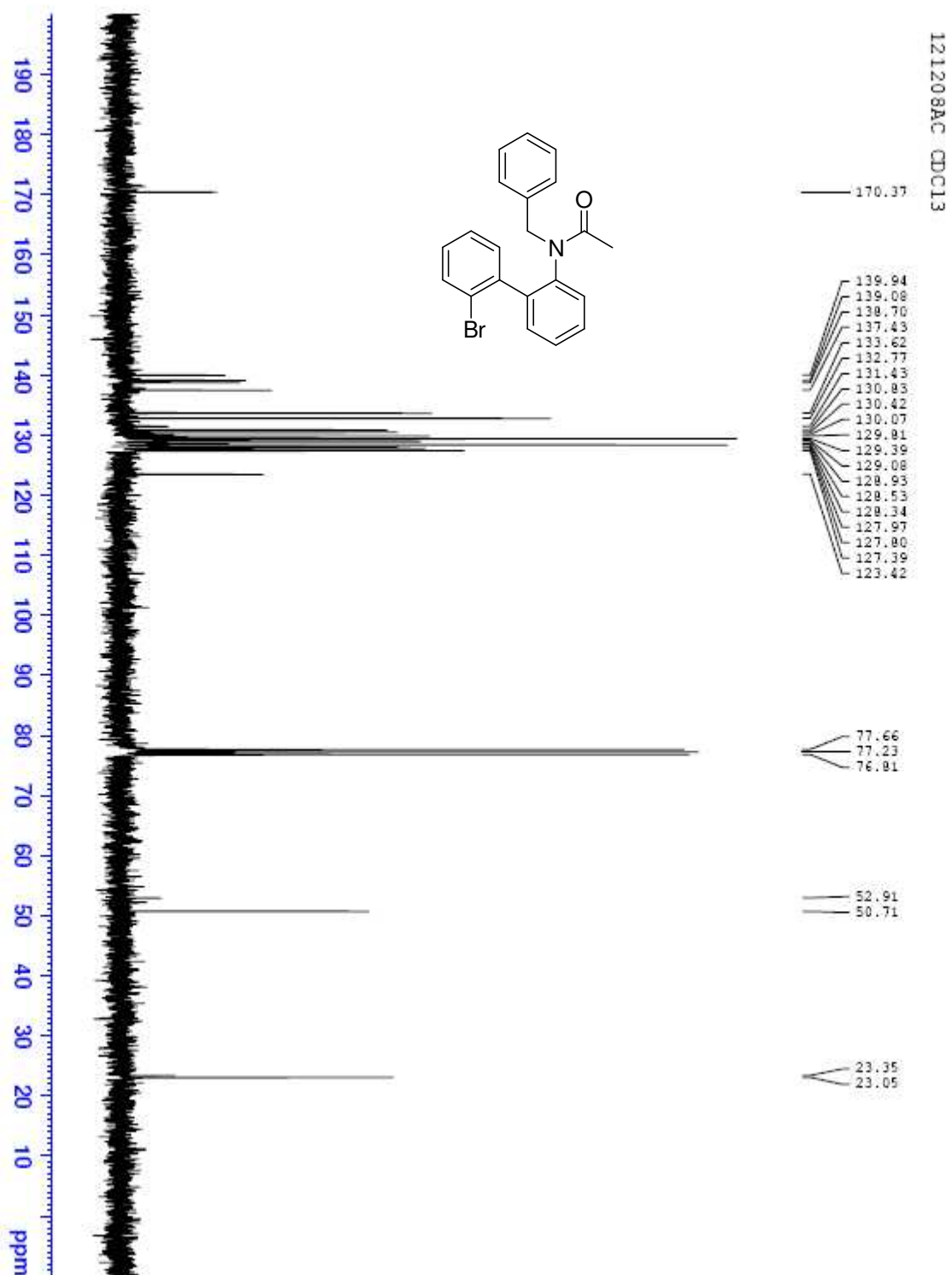
[1,1'-Biphenyl]-2-(N-methyl-benzyloxyacetamide), 2'-bromo- (15).

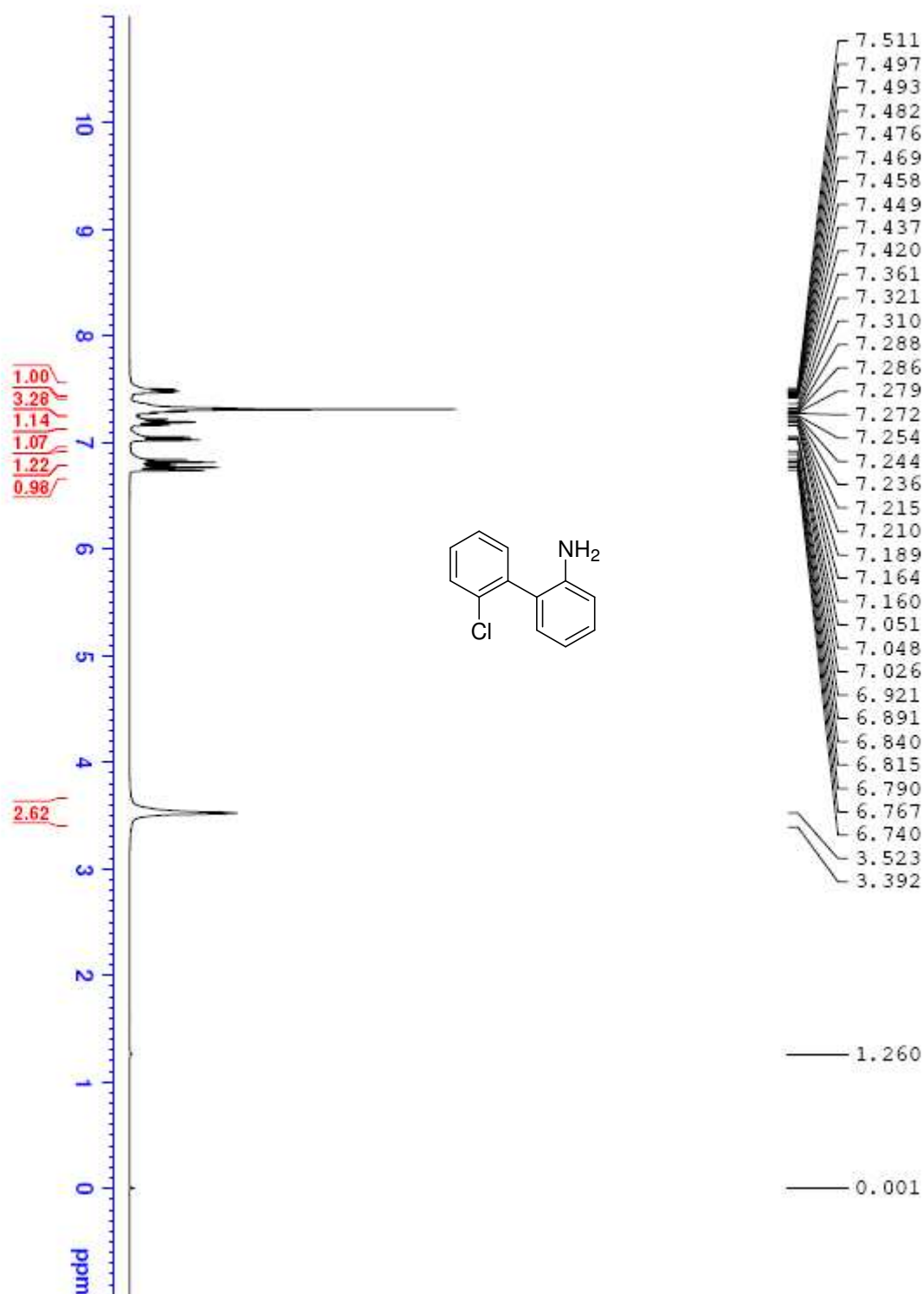
[1,1'-Biphenyl]-2-(N-methyl-benzyloxyacetamide), 2'-bromo- (15).

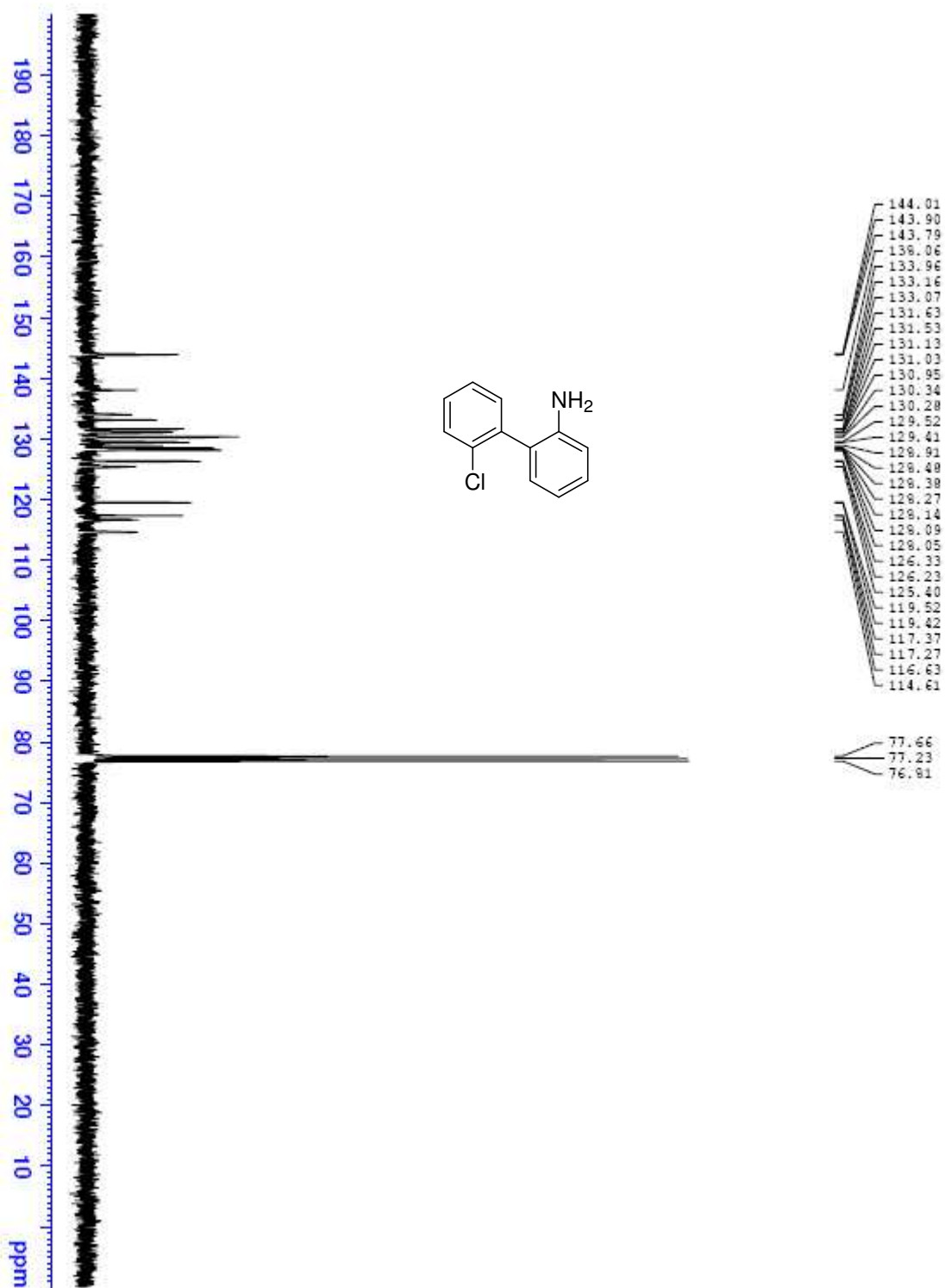
[1,1'-Biphenyl]-2-(N-methyl-dibenzylaminoacetamide), 2'-bromo- (16).

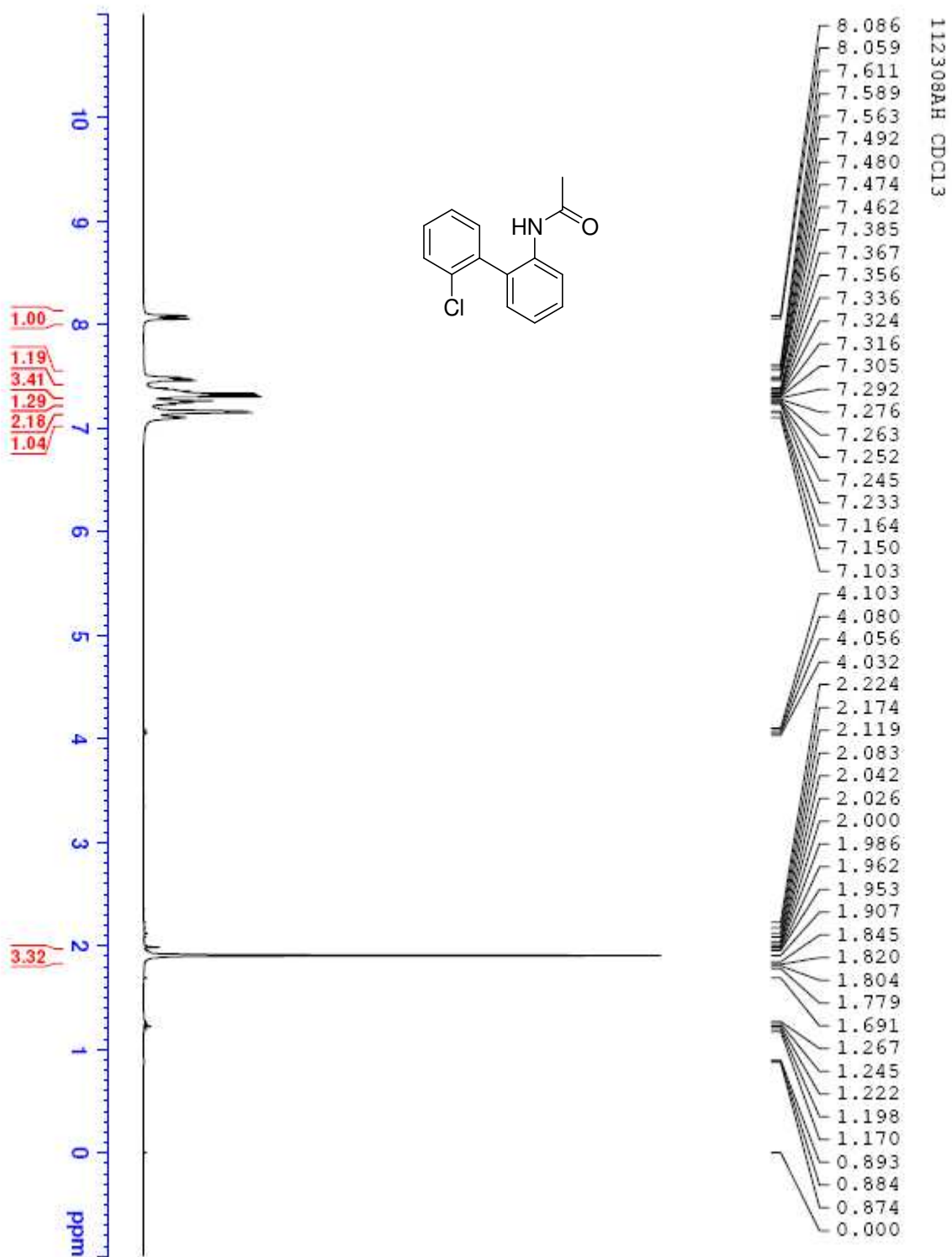
[1,1'-Biphenyl]-2-(N-methyl-dibenzylaminoacetamide), 2'-bromo- (16).

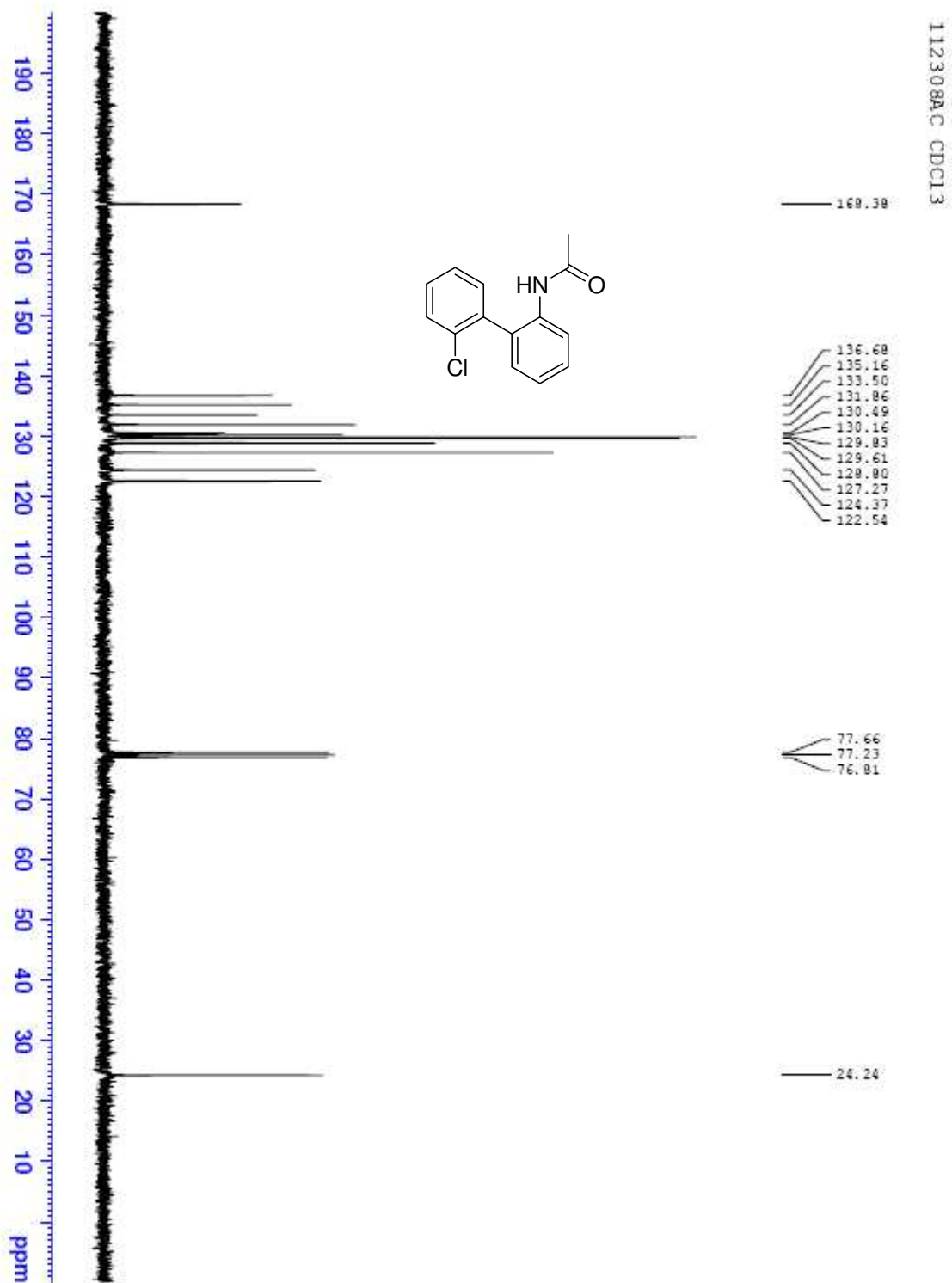
[1,1'-Biphenyl]-2-(N-benzyl-acetamide), 2'-bromo- (17).

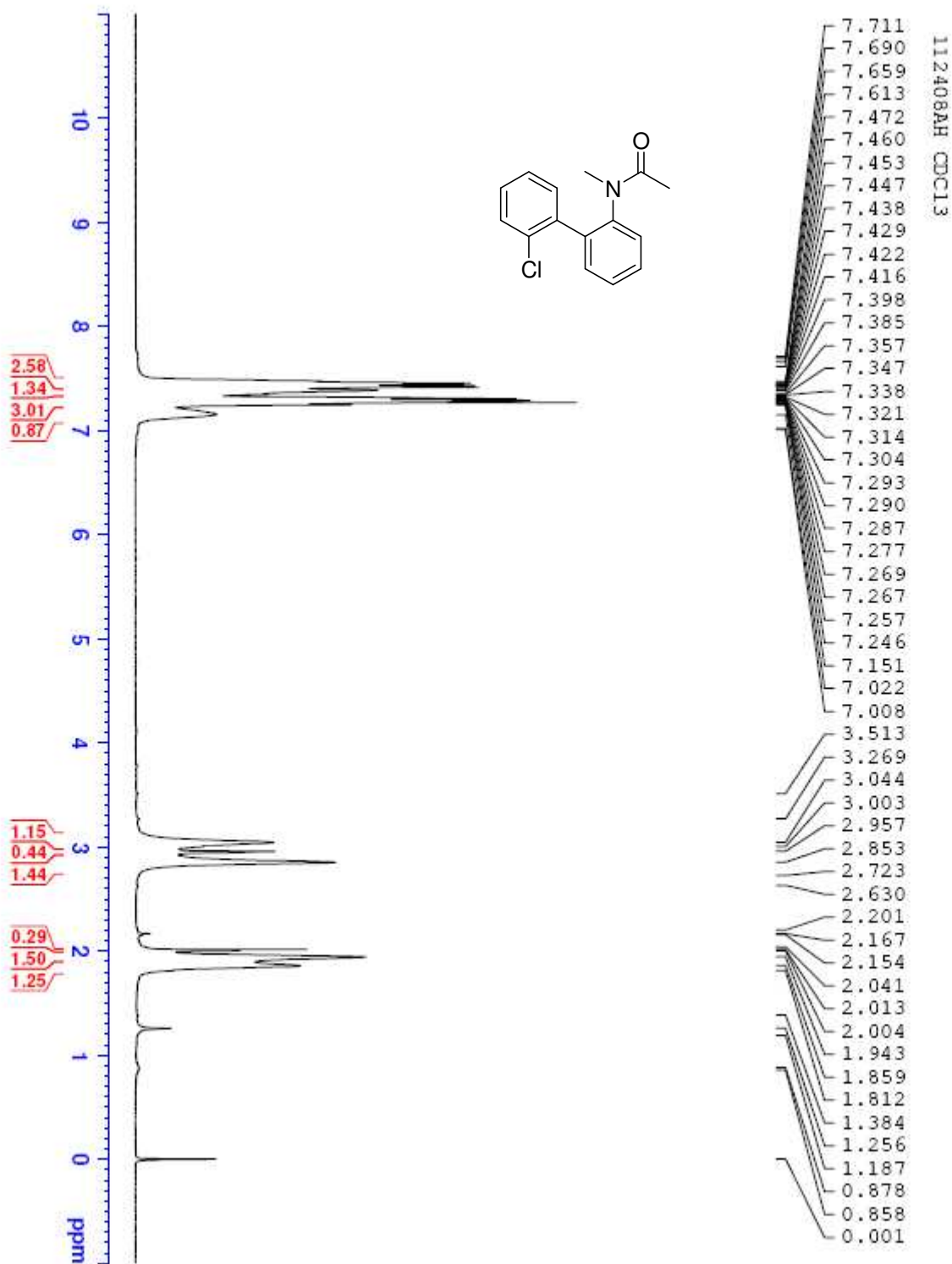
[1,1'-Biphenyl]-2-(N-benzyl-acetamide), 2'-bromo- (17).

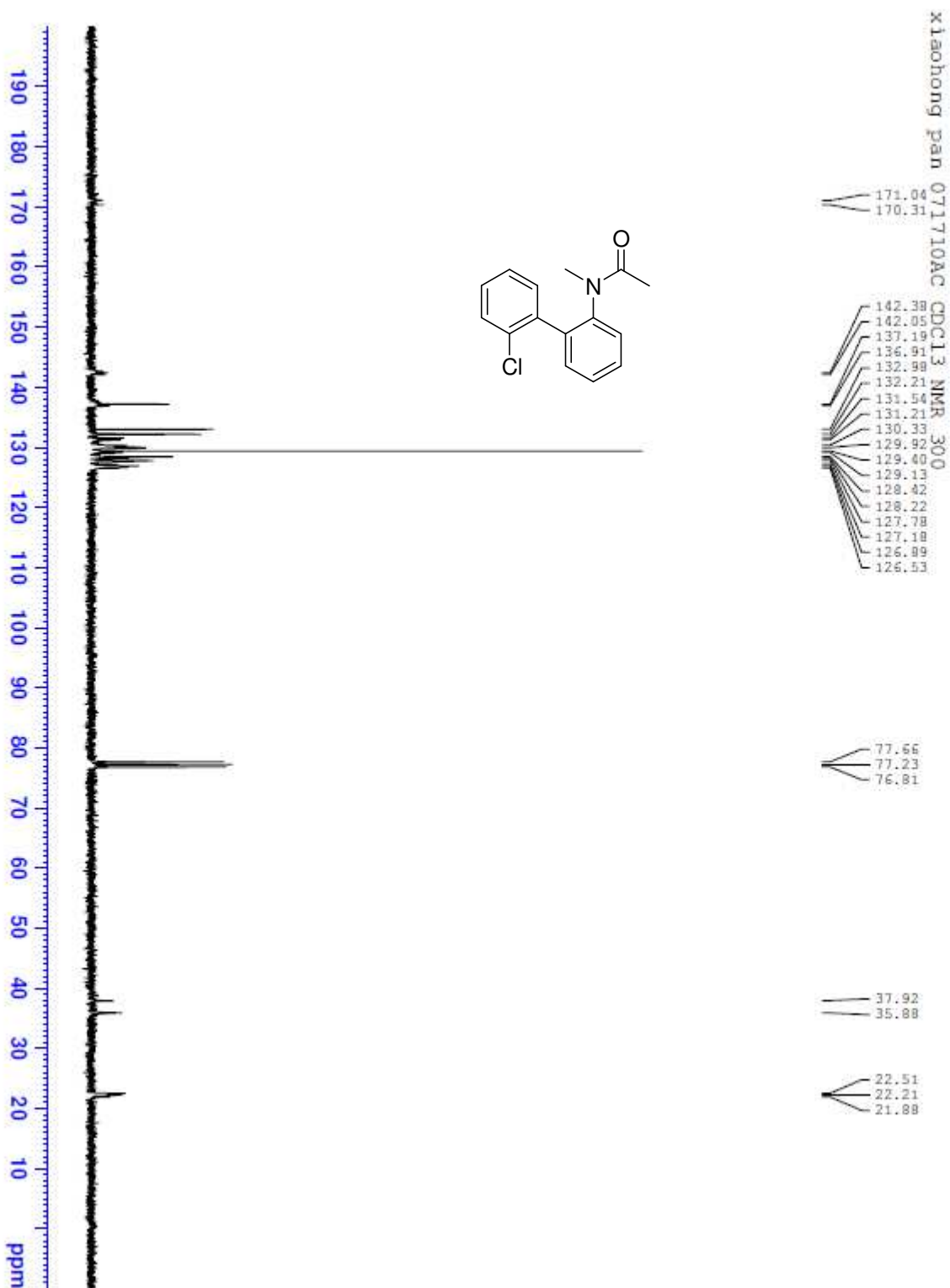
[1,1'-Biphenyl]-2-amine, 2'-chloro- (21).

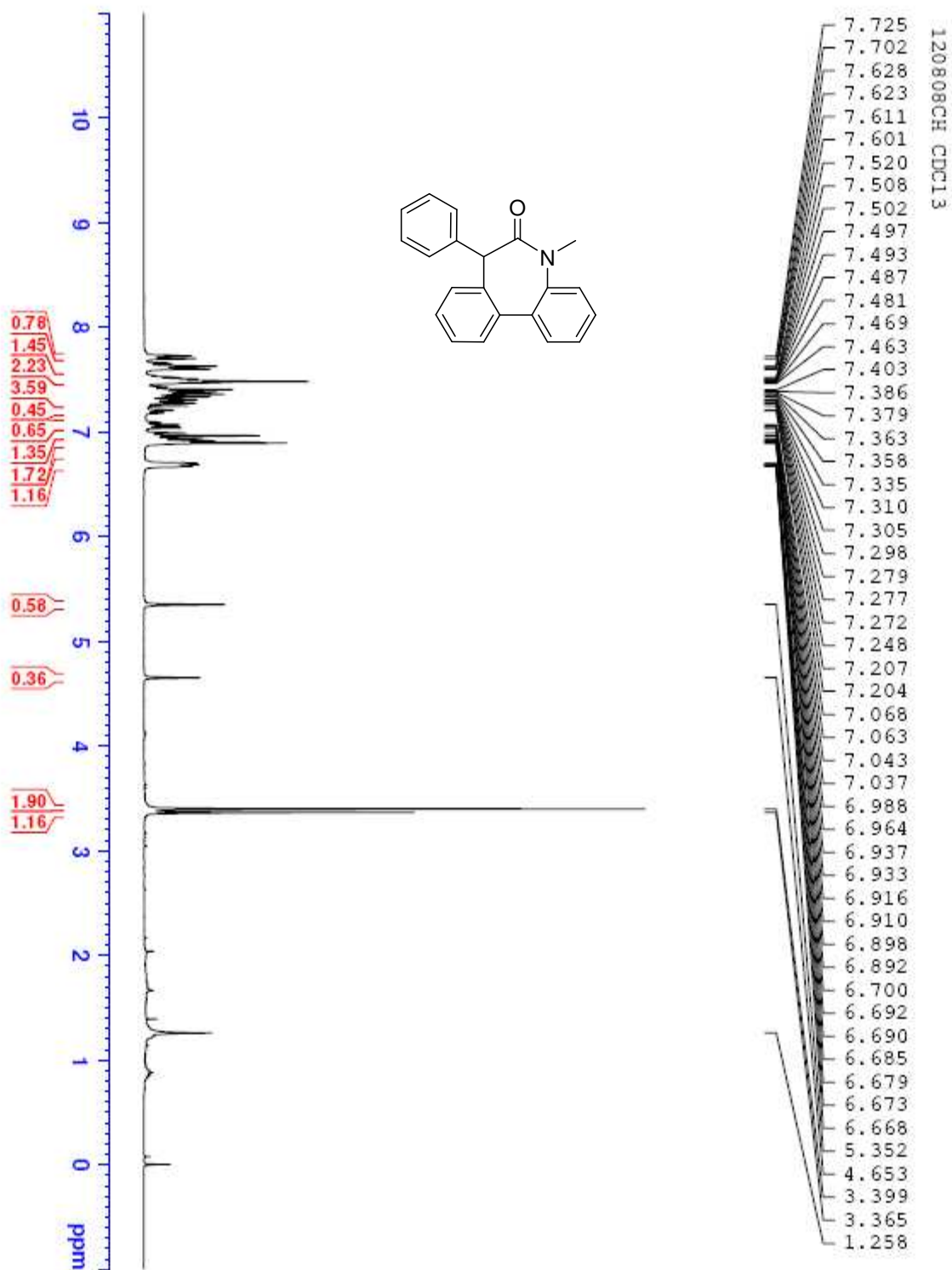
[1,1'-Biphenyl]-2-amine, 2'-chloro- (21).

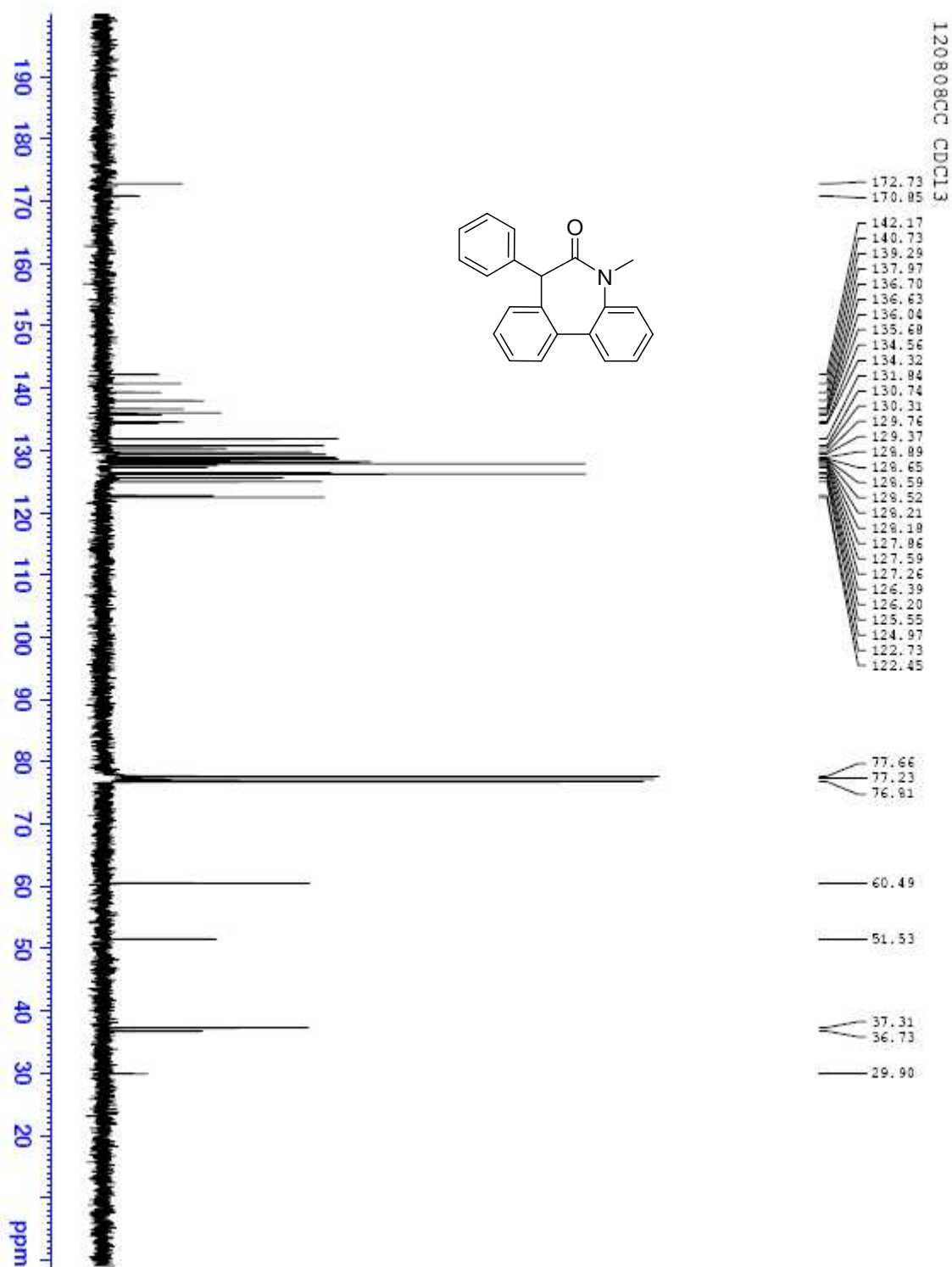
[1,1'-Biphenyl]-2-acetamide, 2'-chloro- (22).

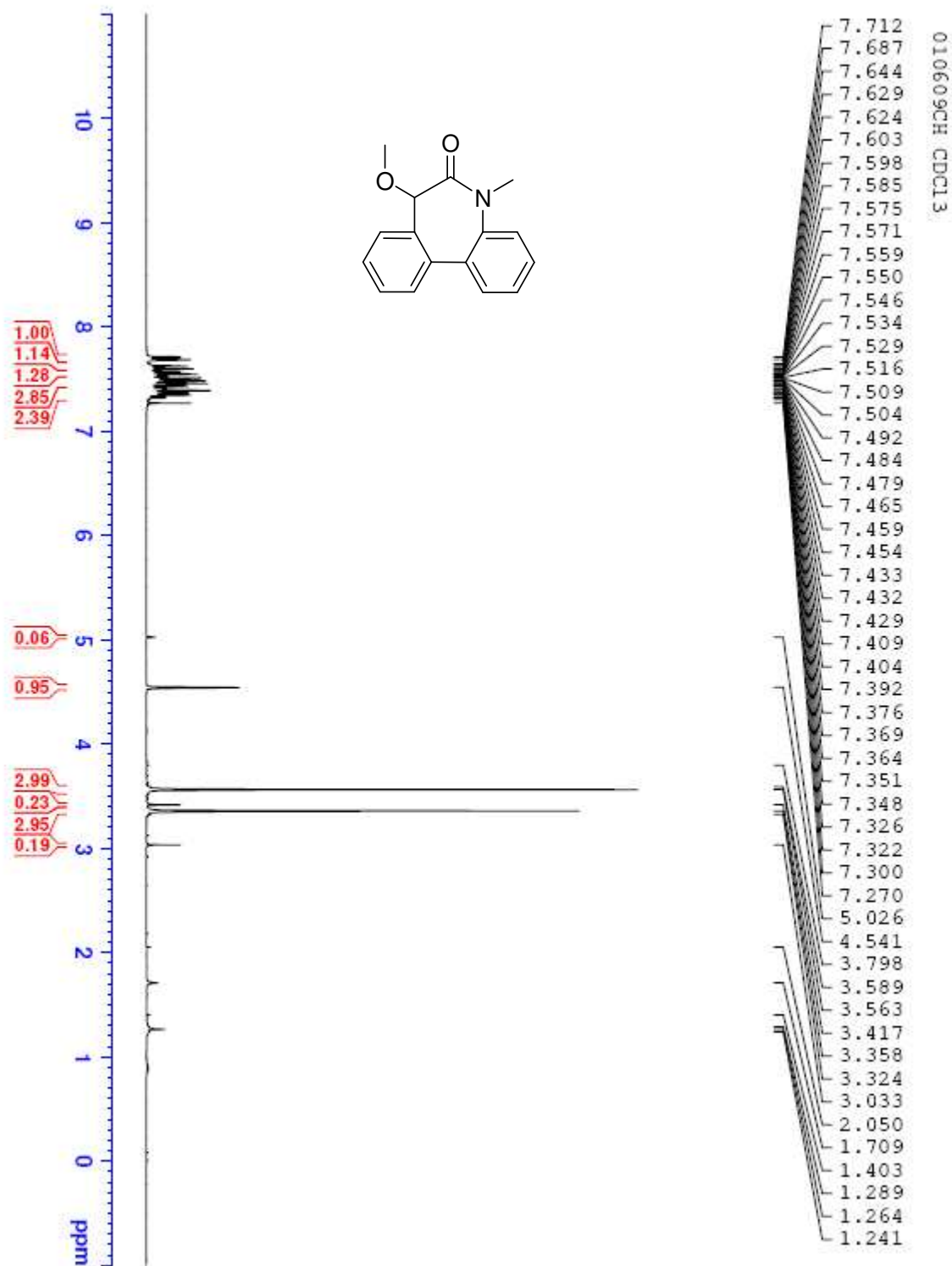
[1,1'-Biphenyl]-2-acetamide, 2'-chloro- (22).

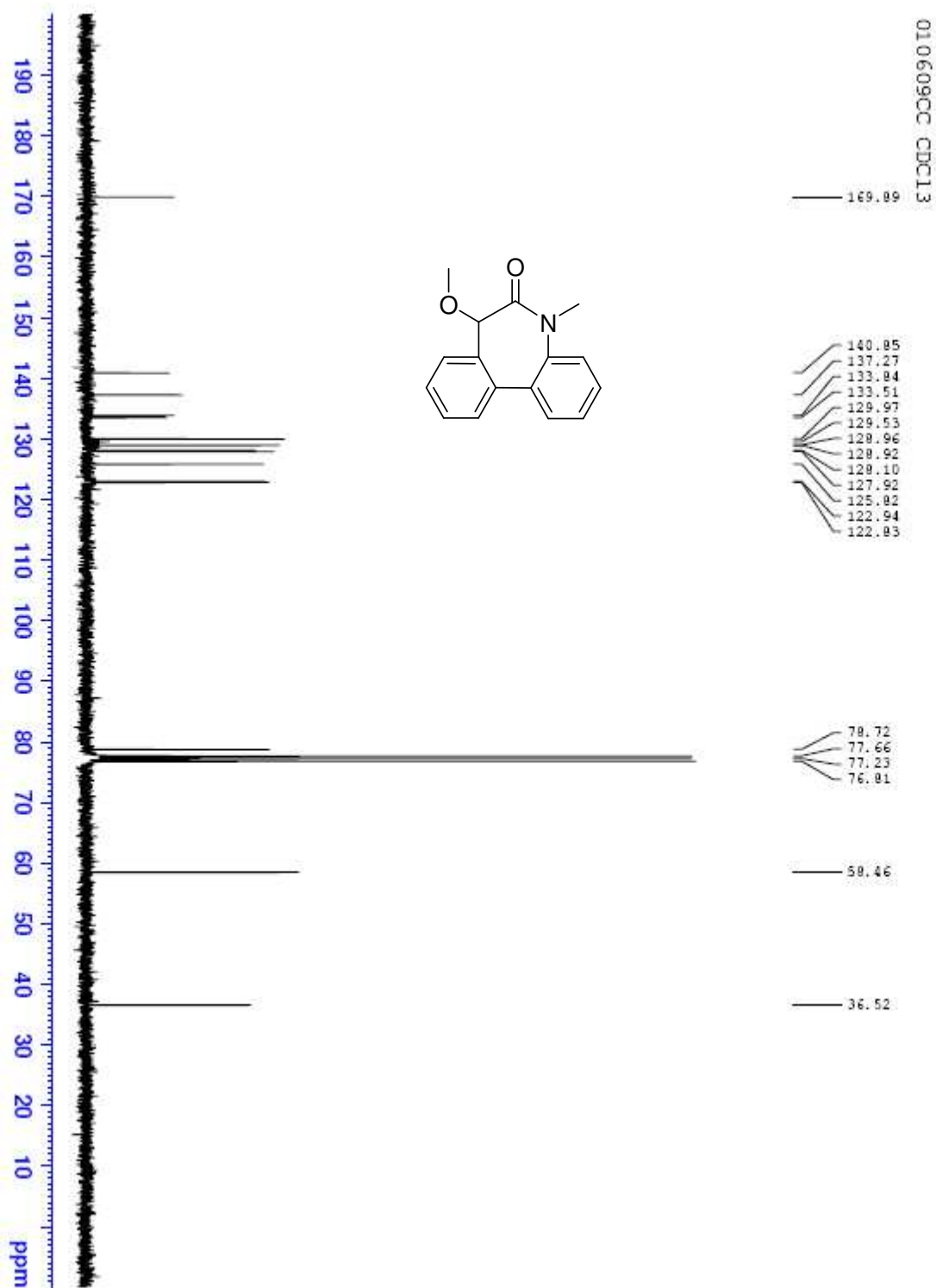
[1,1'-Biphenyl]-2-(*N*-methyl-acetamide), 2'-chloro- (23).

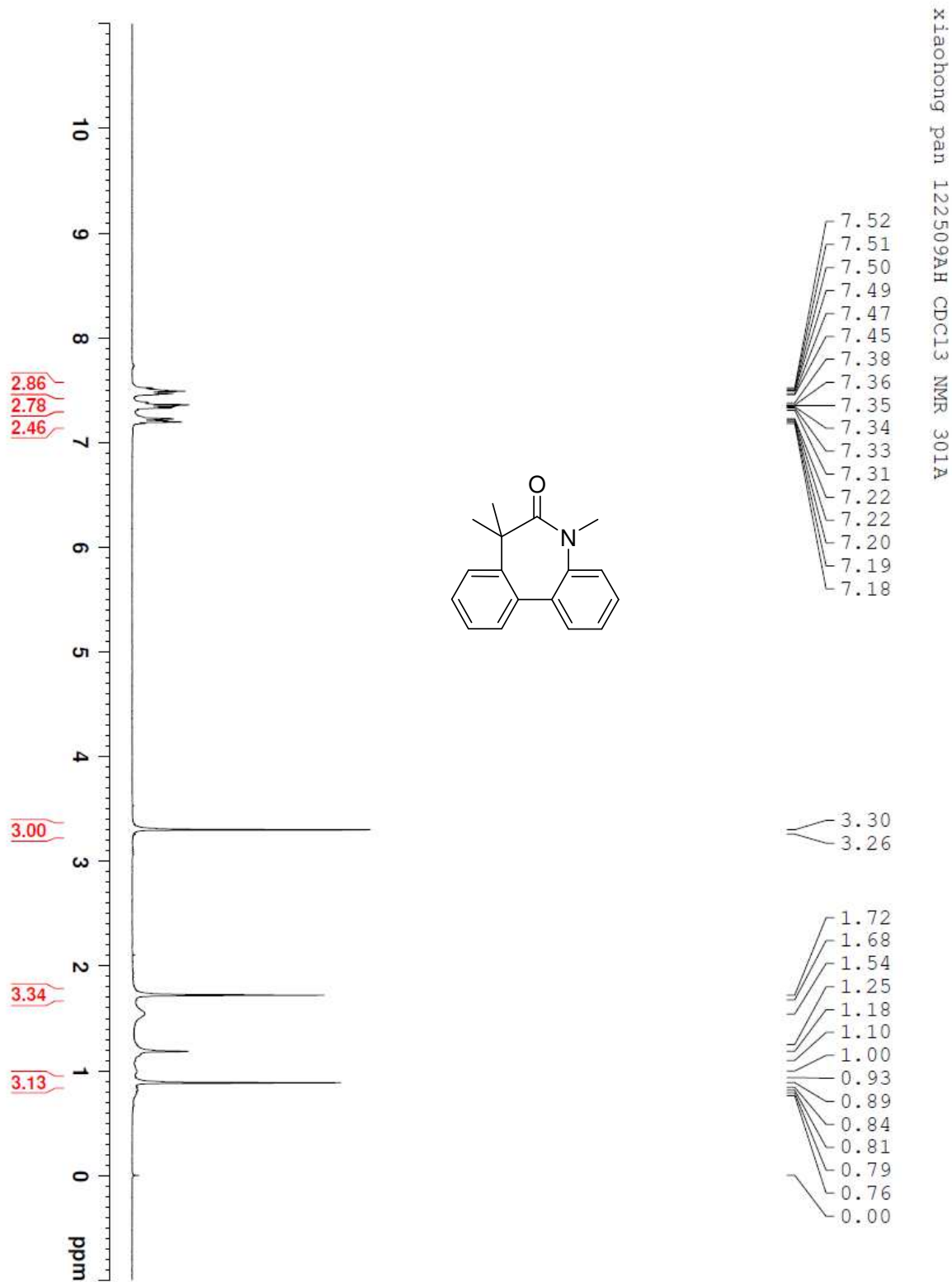
[1,1'-Biphenyl]-2-(N-methyl-acetamide), 2'-chloro- (23).

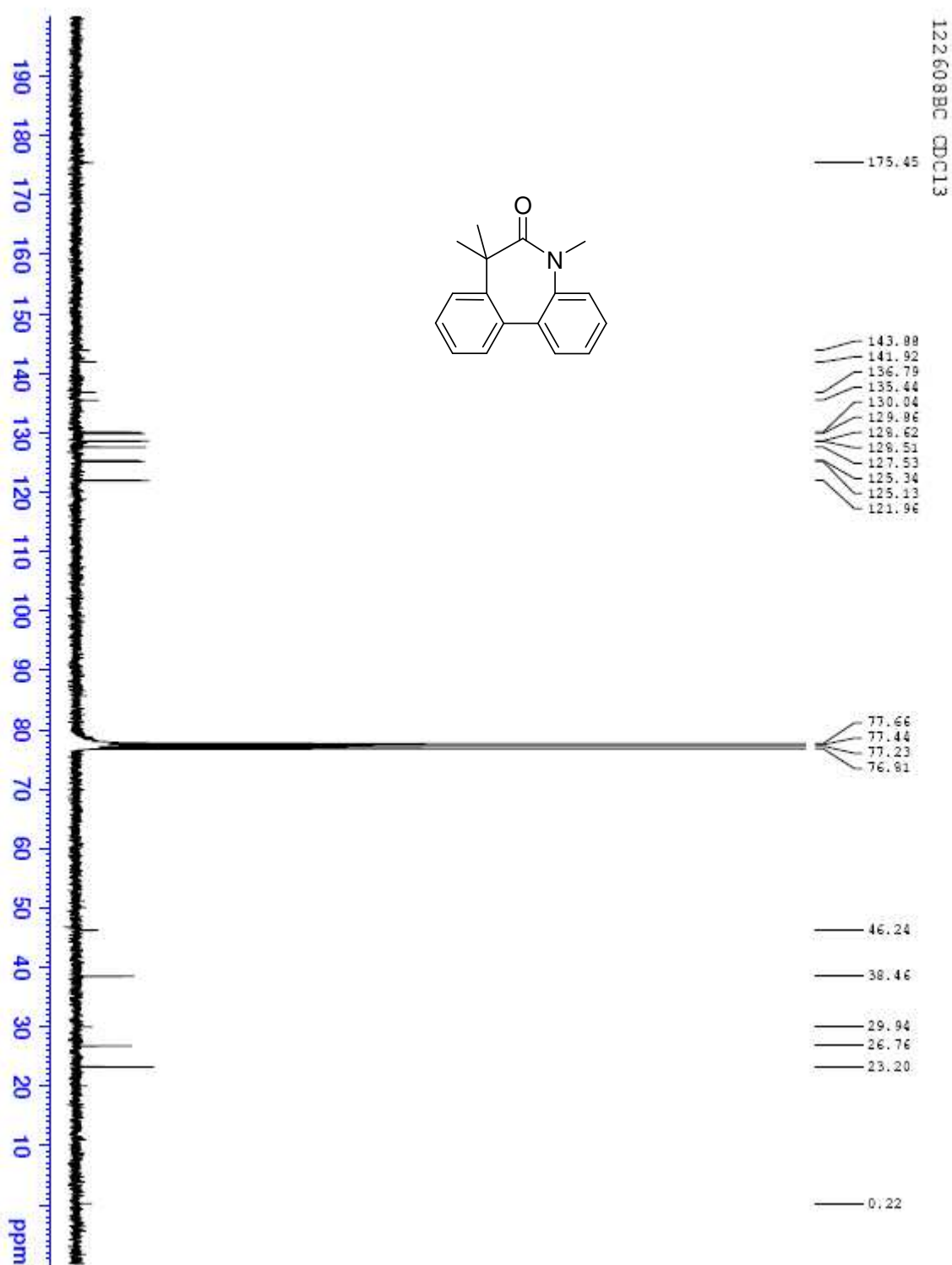
5-Phenyl-N-methyl-dibenzazepin-6-one (24).

5-Phenyl-N-methyl-dibenzazepin-6-one (24).

5-Methoxy-*N*-methyl-dibenzazepin-6-one (26).

5-Methoxy-*N*-methyl-dibenzazepin-6-one (26).

5,5-Dimethyl-N-methyl-dibenzazepin-6-one (27).

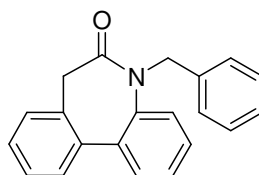
5,5-Dimethyl-*N*-methyl-dibenzazepin-6-one (27).

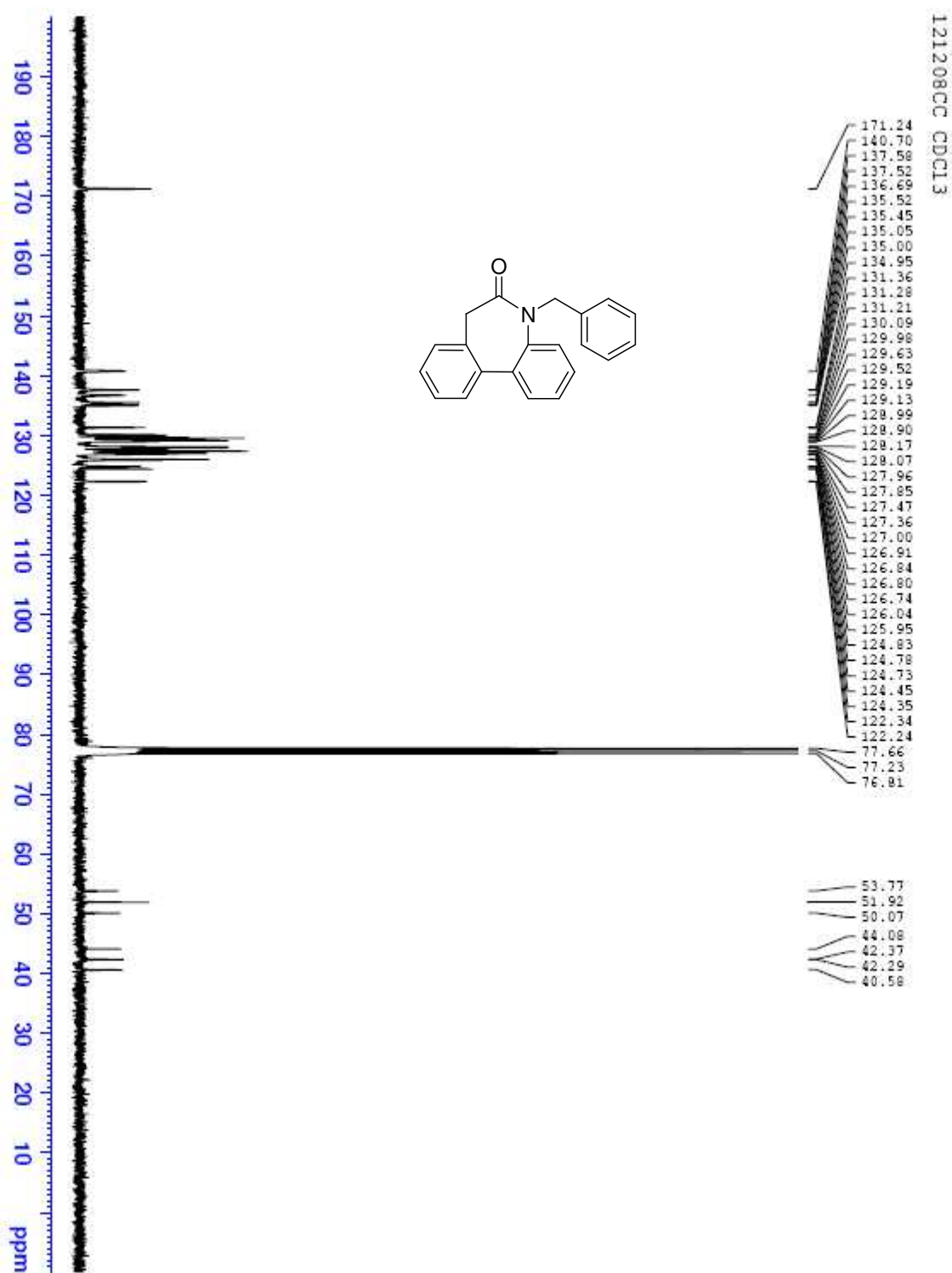
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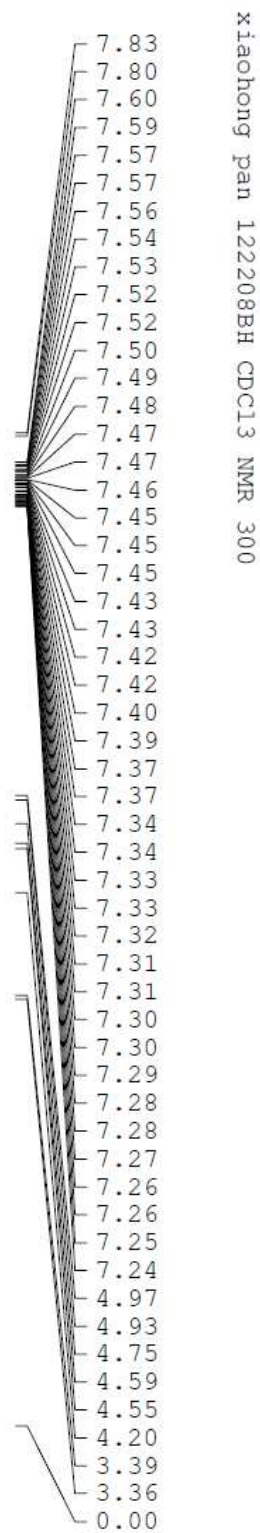
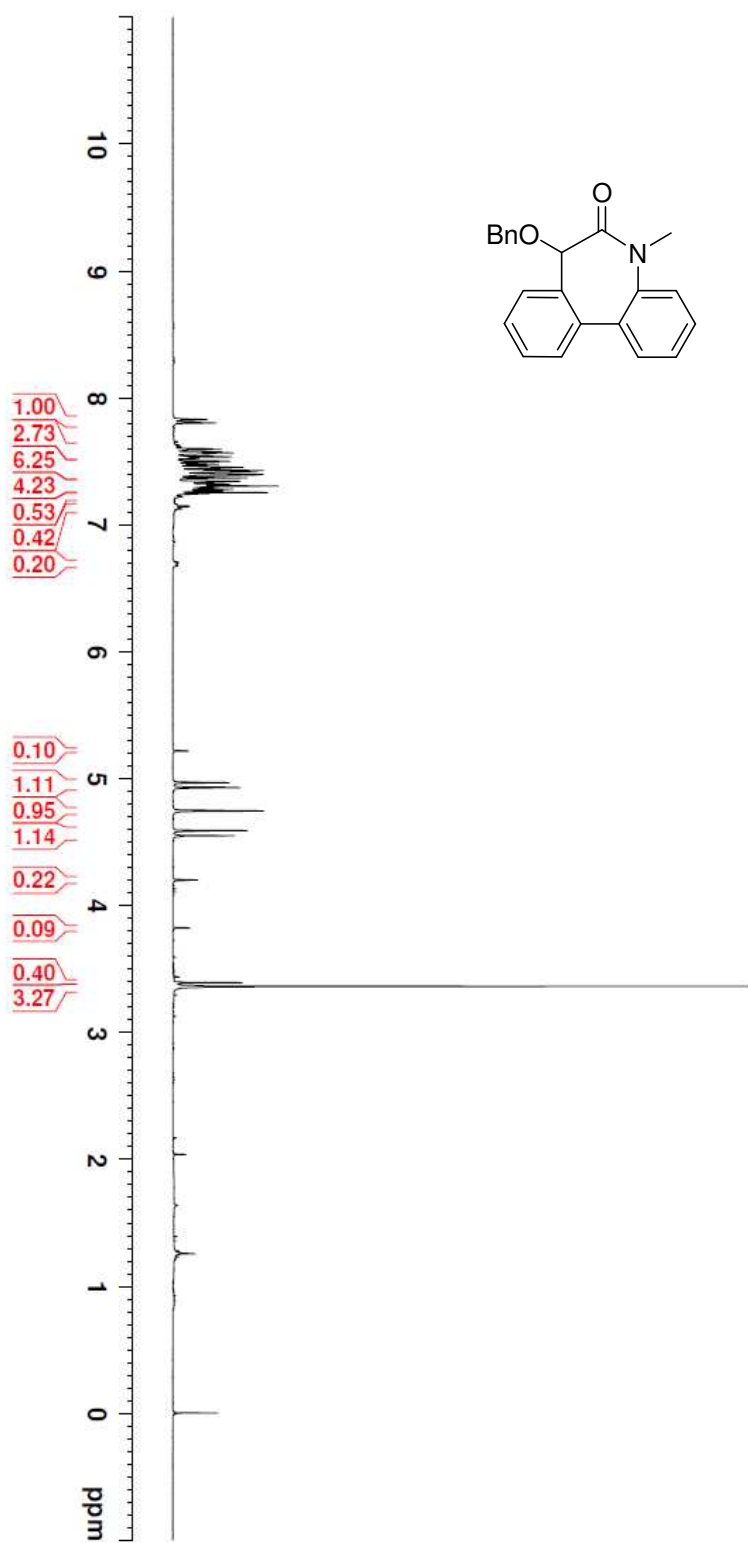
Chemical structure: O=C1Cc2ccccc2N(Cc3ccccc3)c4ccccc14

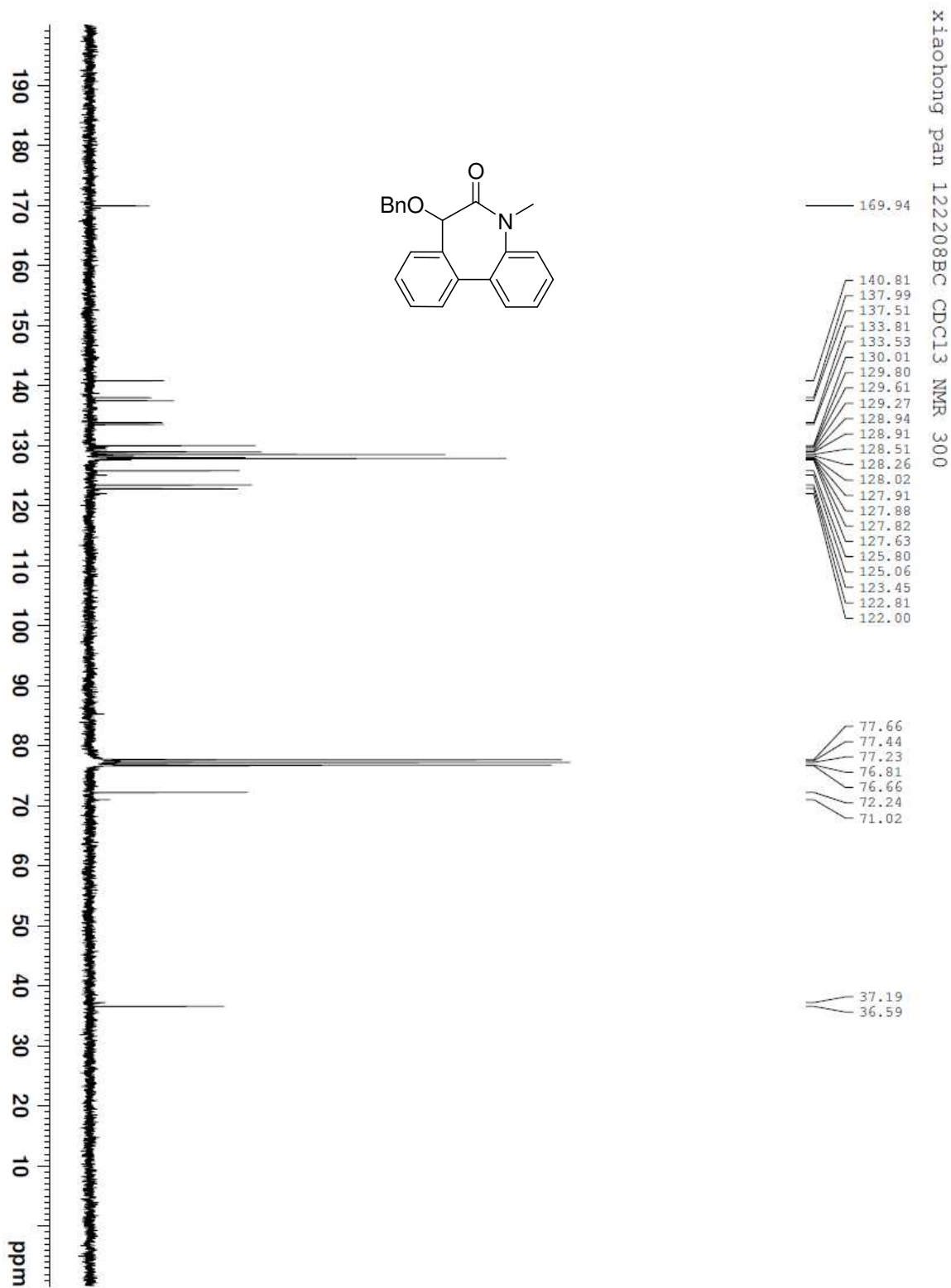
Integration values (left): 1.95, 2.82, 1.77, 1.28, 2.71, 1.76, 0.99, 1.00, 1.02, 1.00

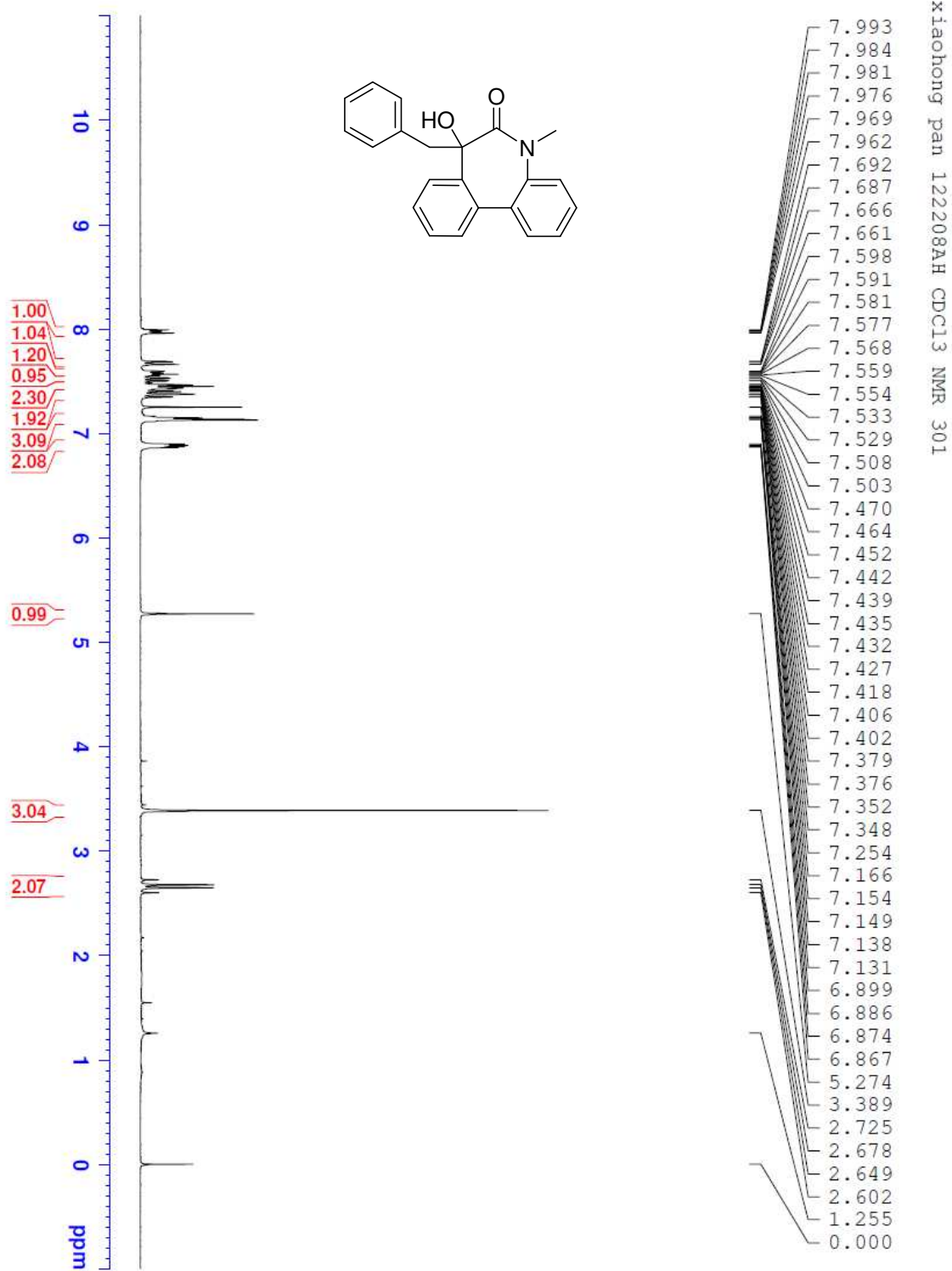
Chemical shifts (right): 7.515, 7.513, 7.502, 7.500, 7.492, 7.487, 7.472, 7.455, 7.436, 7.419, 7.408, 7.379, 7.357, 7.351, 7.331, 7.325, 7.303, 7.298, 7.288, 7.277, 7.271, 7.261, 7.254, 7.244, 7.236, 7.230, 7.213, 7.207, 7.171, 7.156, 7.150, 7.125, 7.111, 7.103, 7.090, 7.070, 6.908, 6.896, 6.884, 6.877, 5.191, 5.169, 5.139, 4.939, 4.887, 3.675, 3.634, 3.601, 3.553, 3.512, 1.963, 1.736, 1.256, 0.001

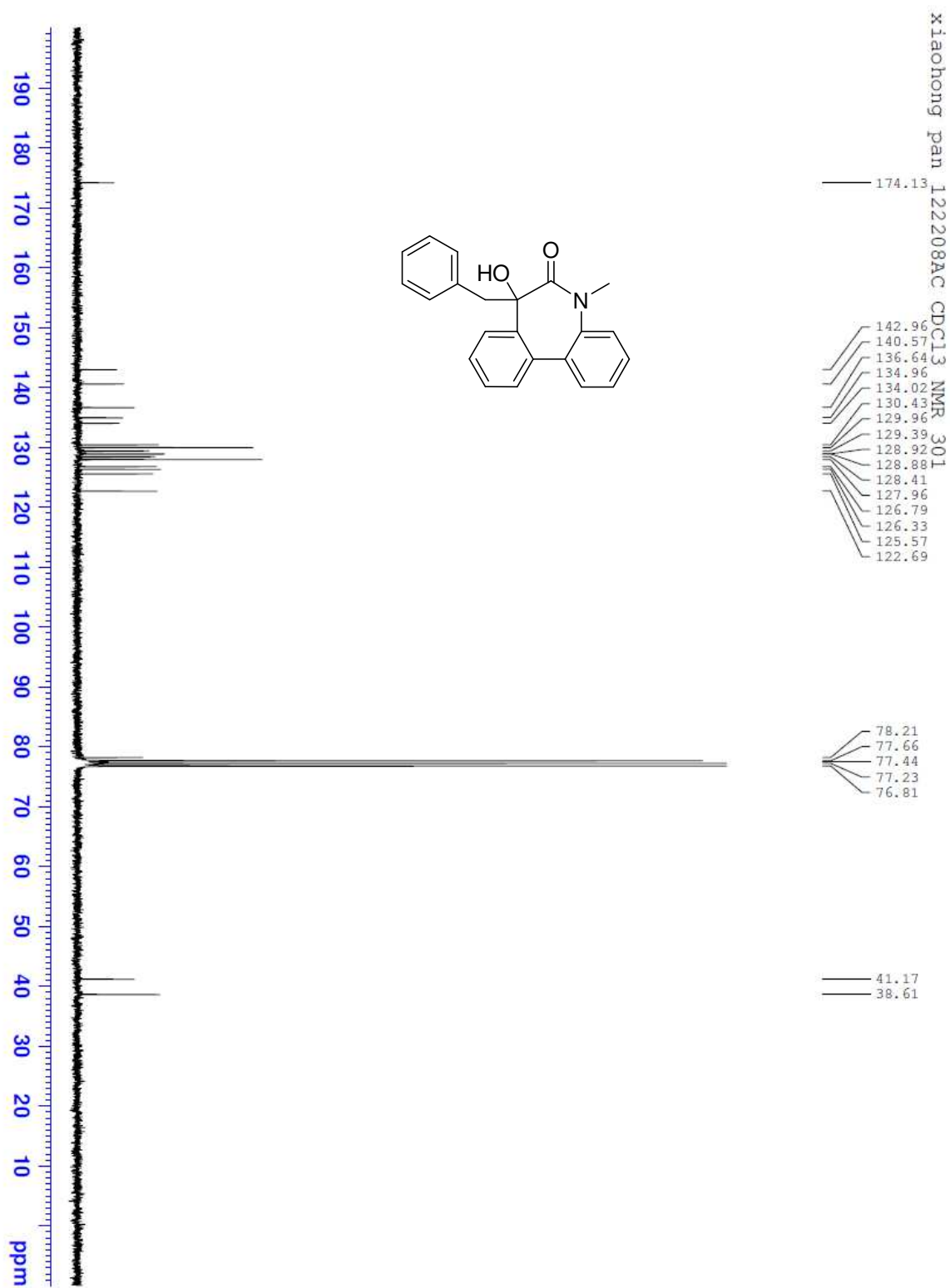


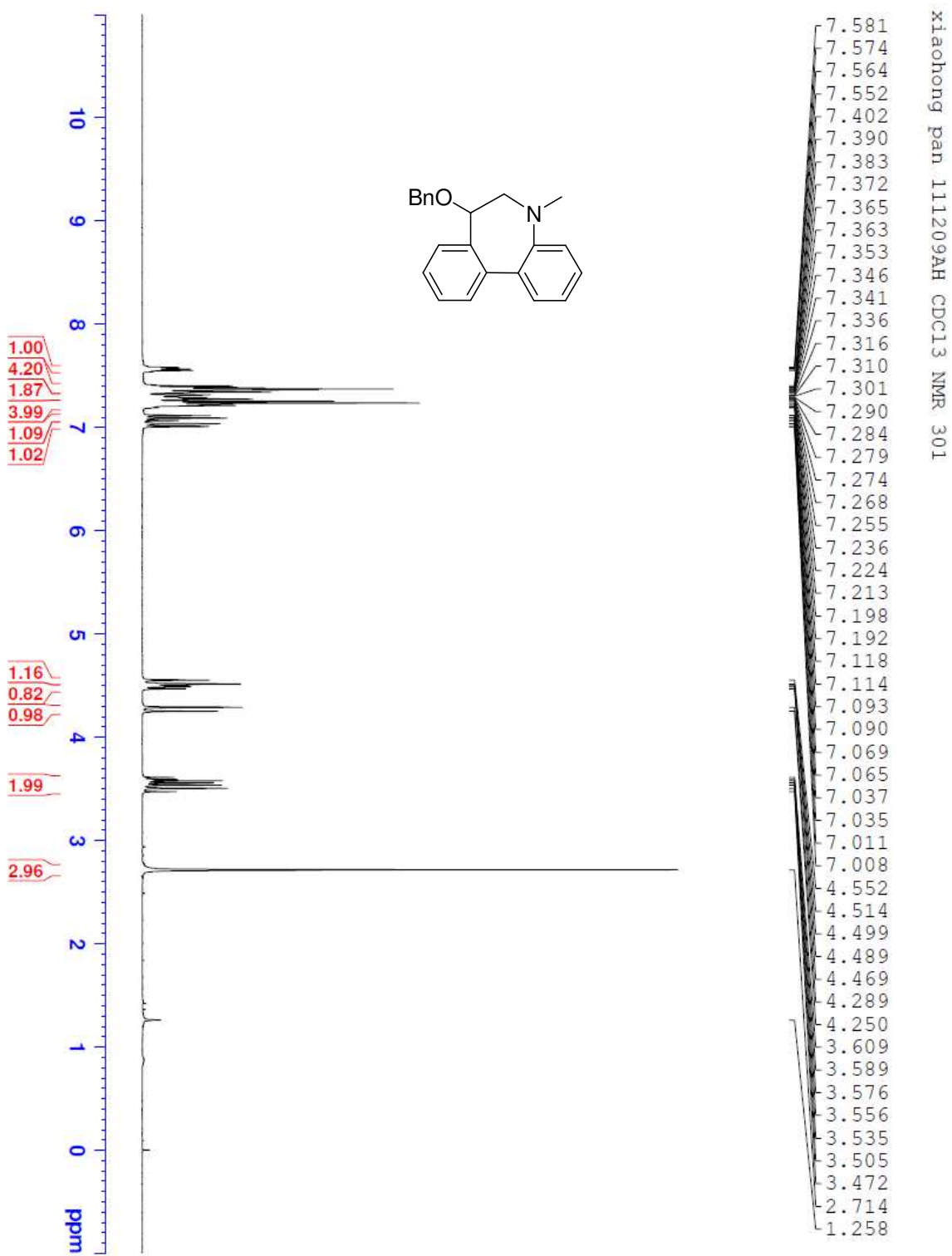
***N*-Benzyl-dibenzazepin-6-one (28).**

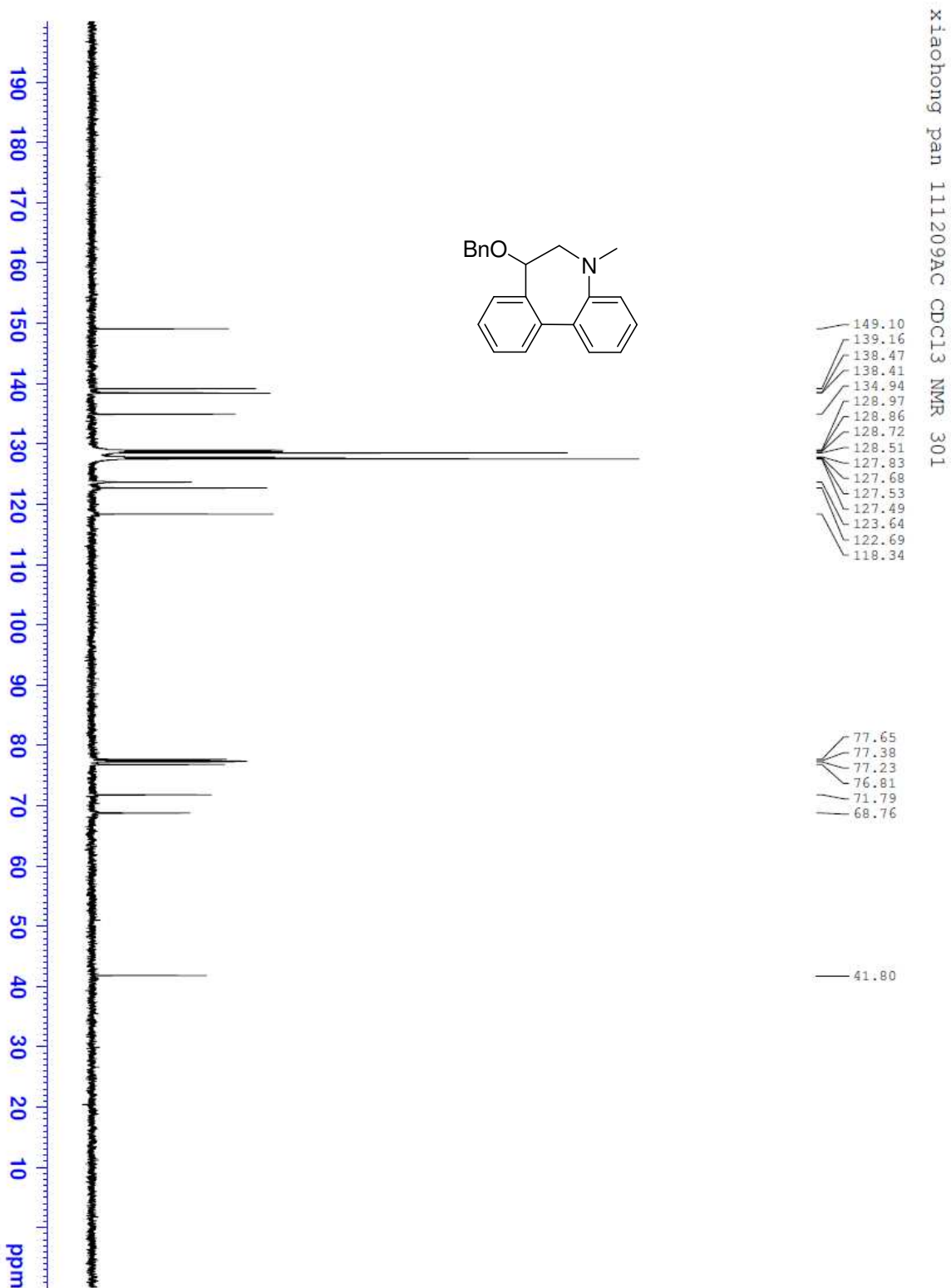
5-Benzyloxy-N-methyl-dibenzazepin-6-one (29).

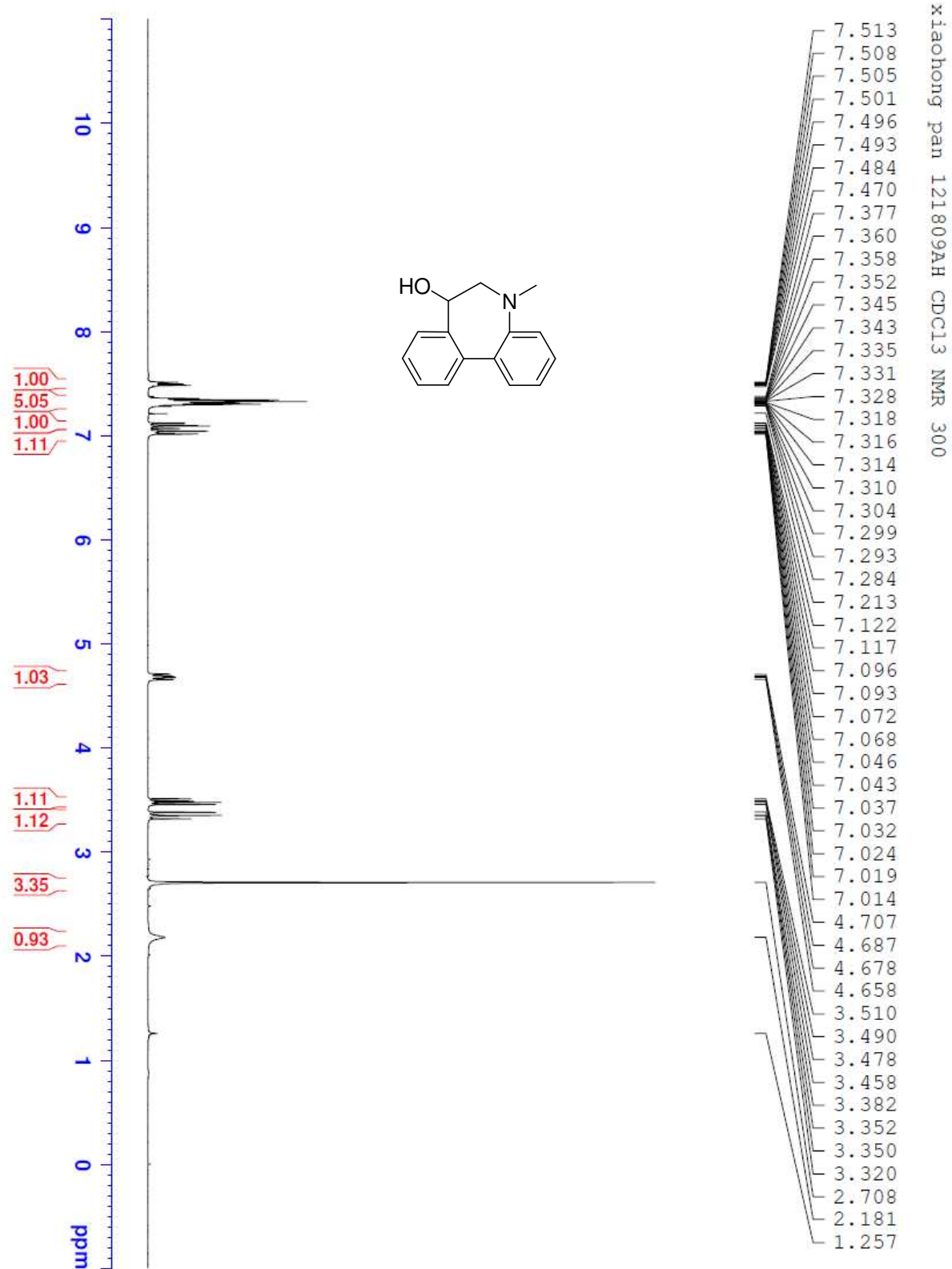
5-Benzyloxy-N-methyl-dibenzazepin-6-one (29).

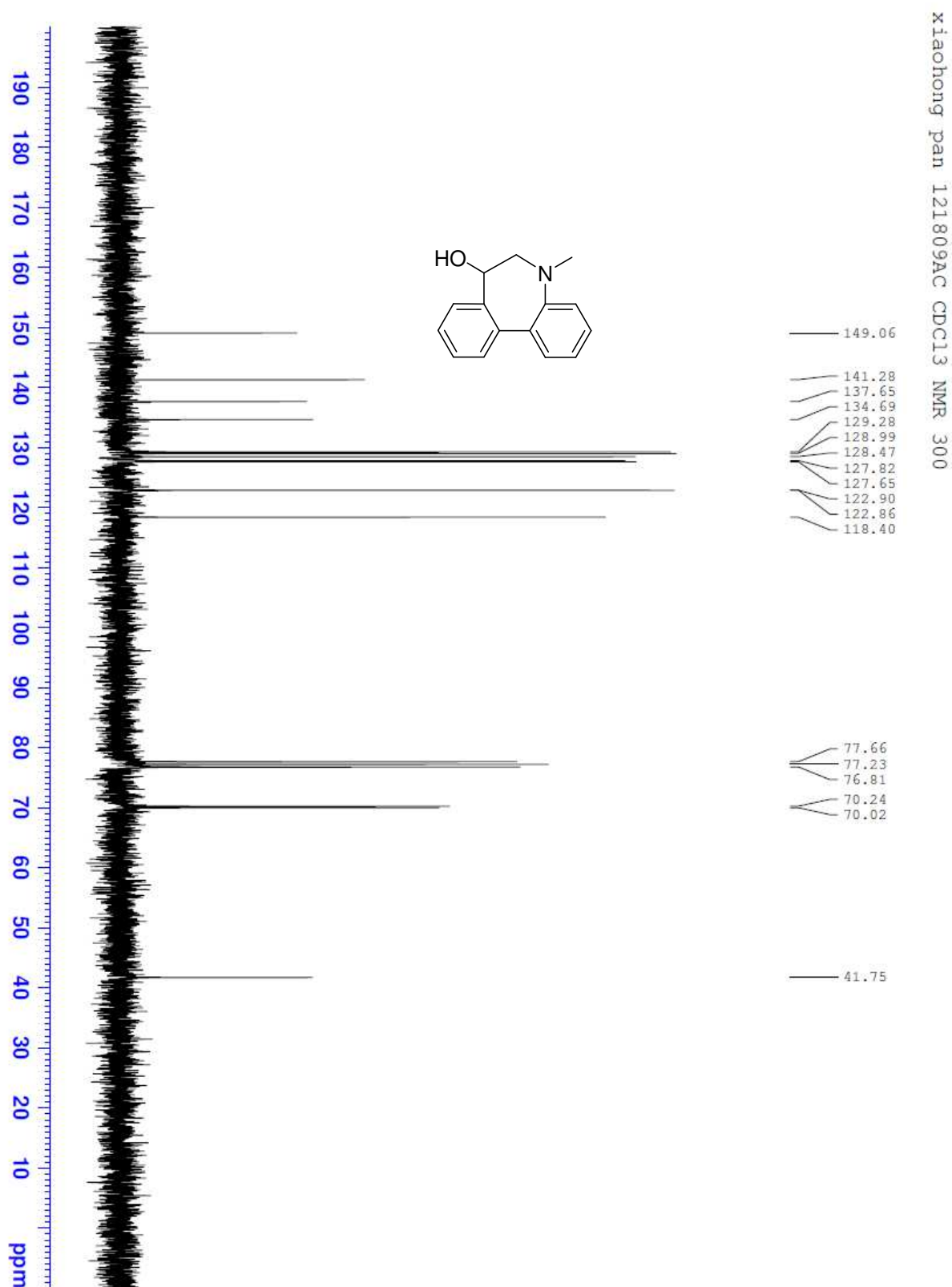
5-Benzyl-5-hydroxy-*N*-methyl-dibenzazepin-6-one (30).

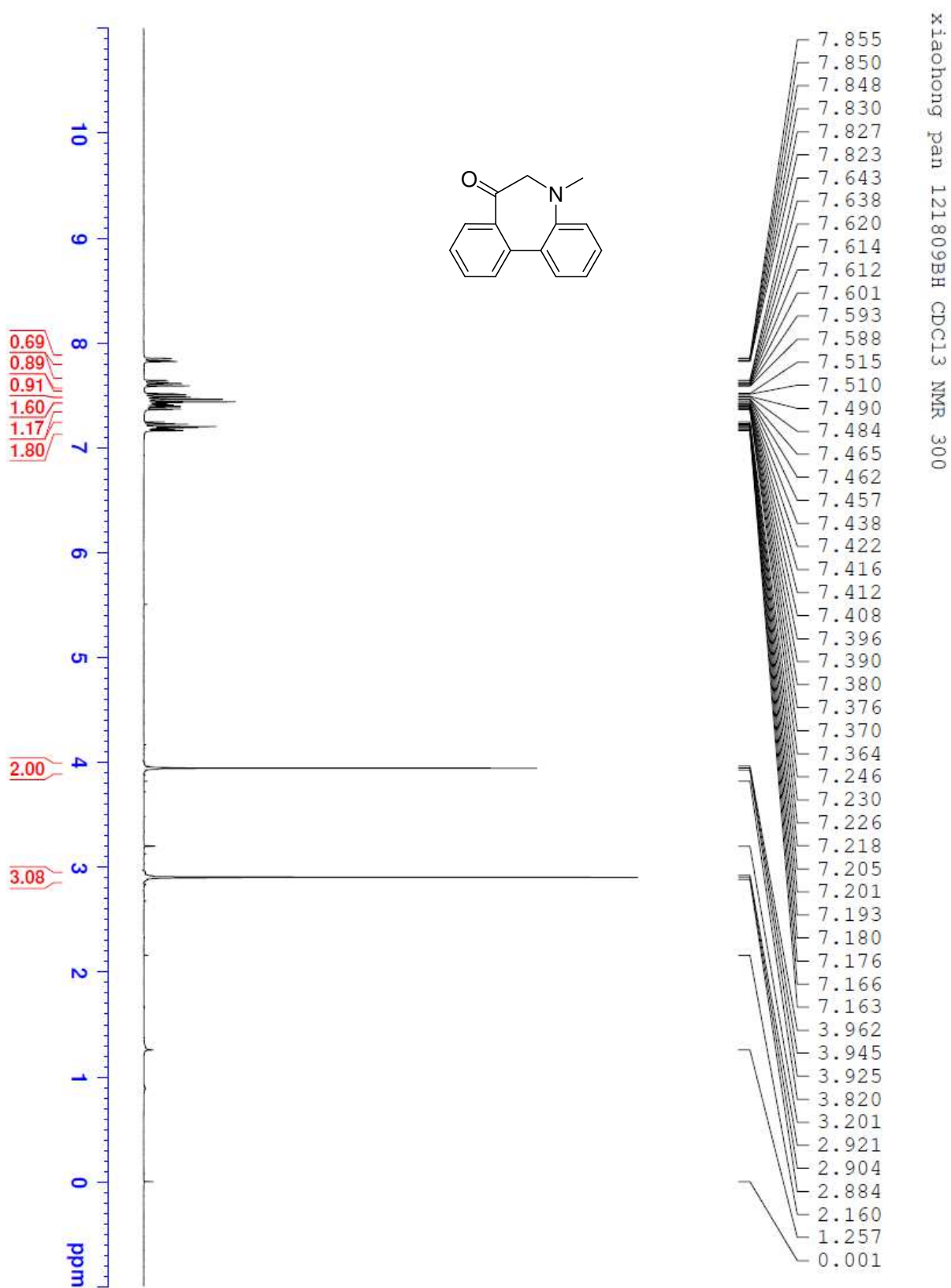
5-Benzyl-5-hydroxy-*N*-methyl-dibenzazepin-6-one (30).

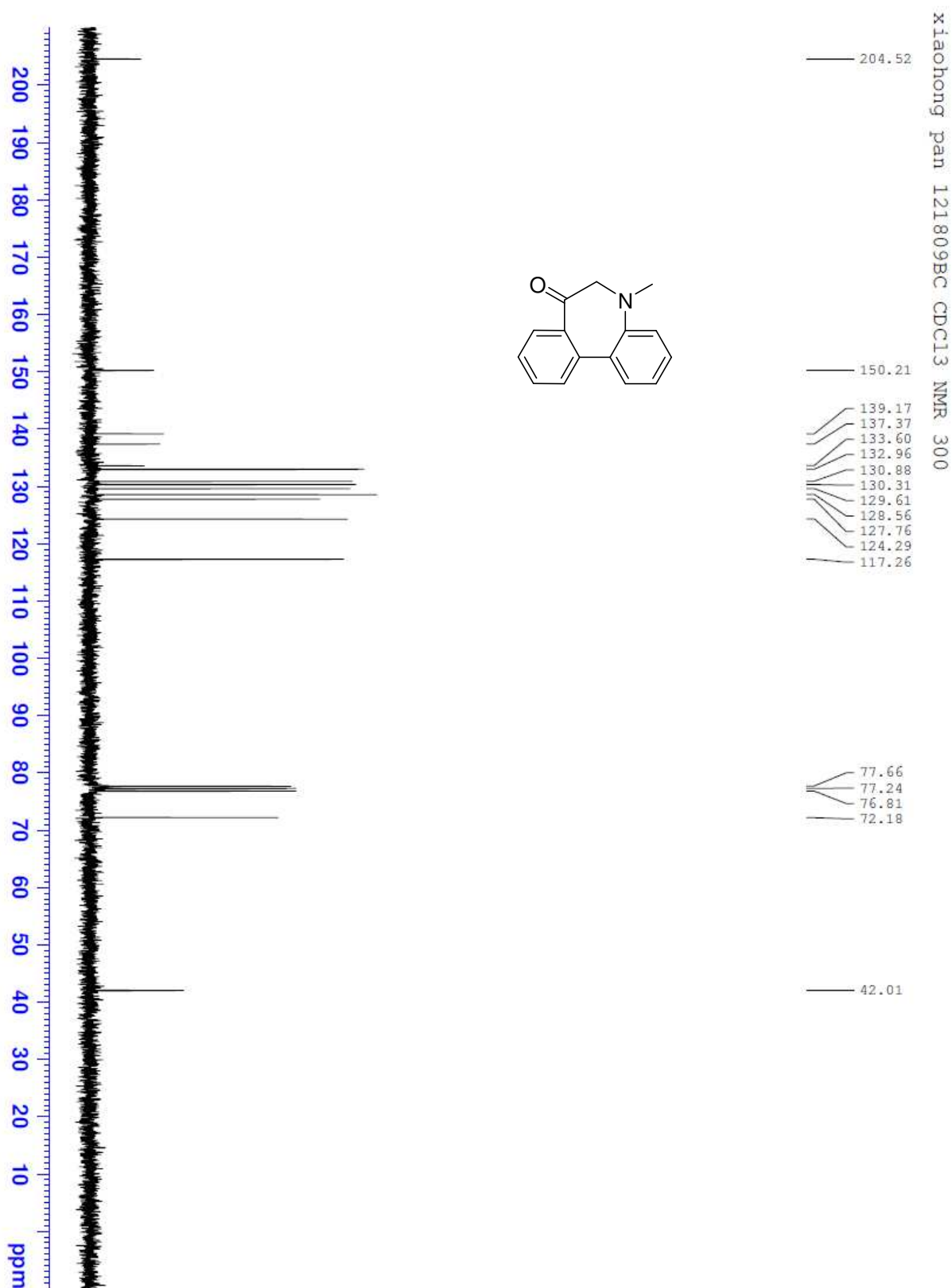
5-Benzyloxy-N-methyl-dihydrodibenzazepine (31).

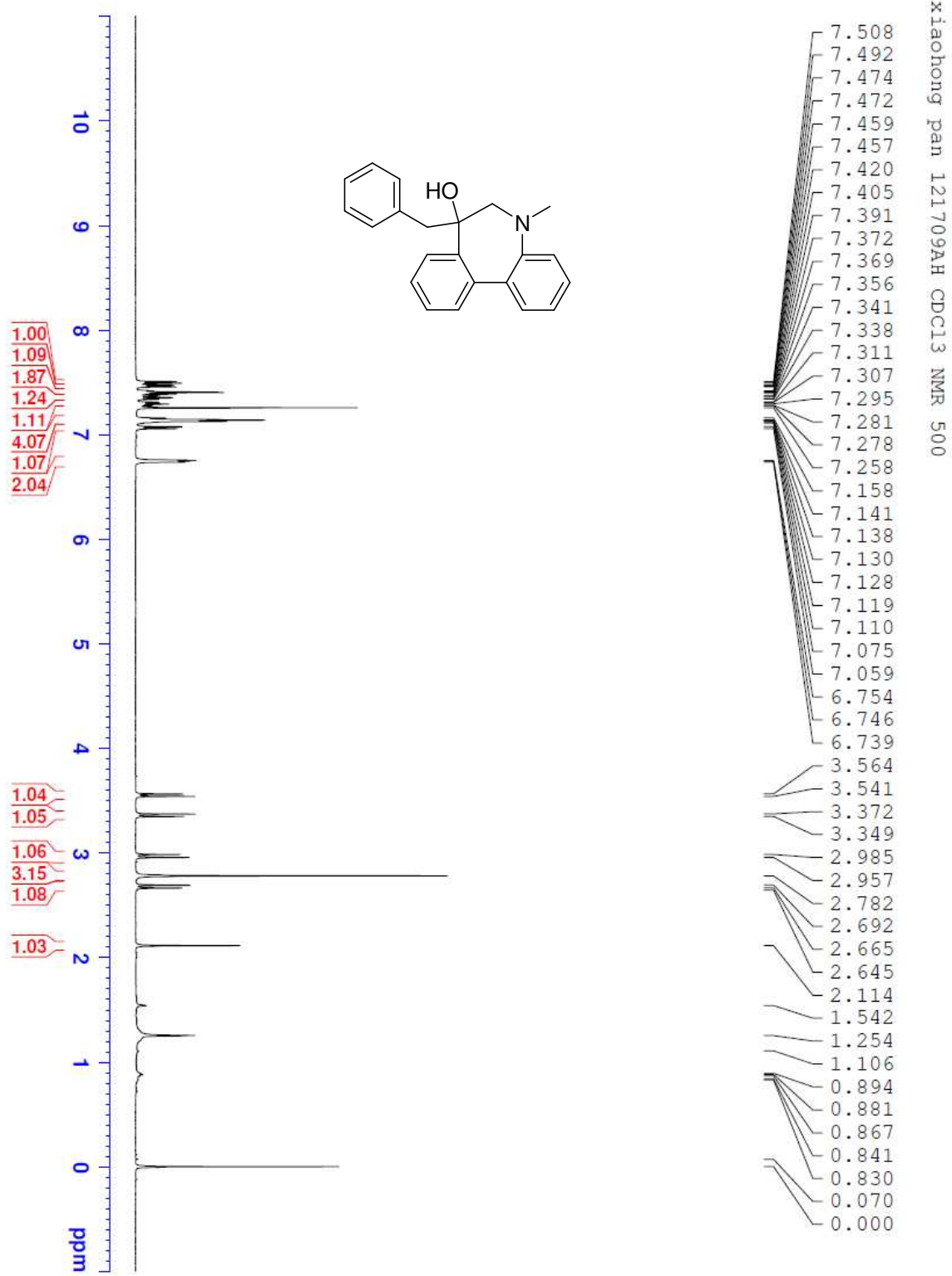
5-Benzyloxy-*N*-methyl-dihydrodibenzazepine (31).

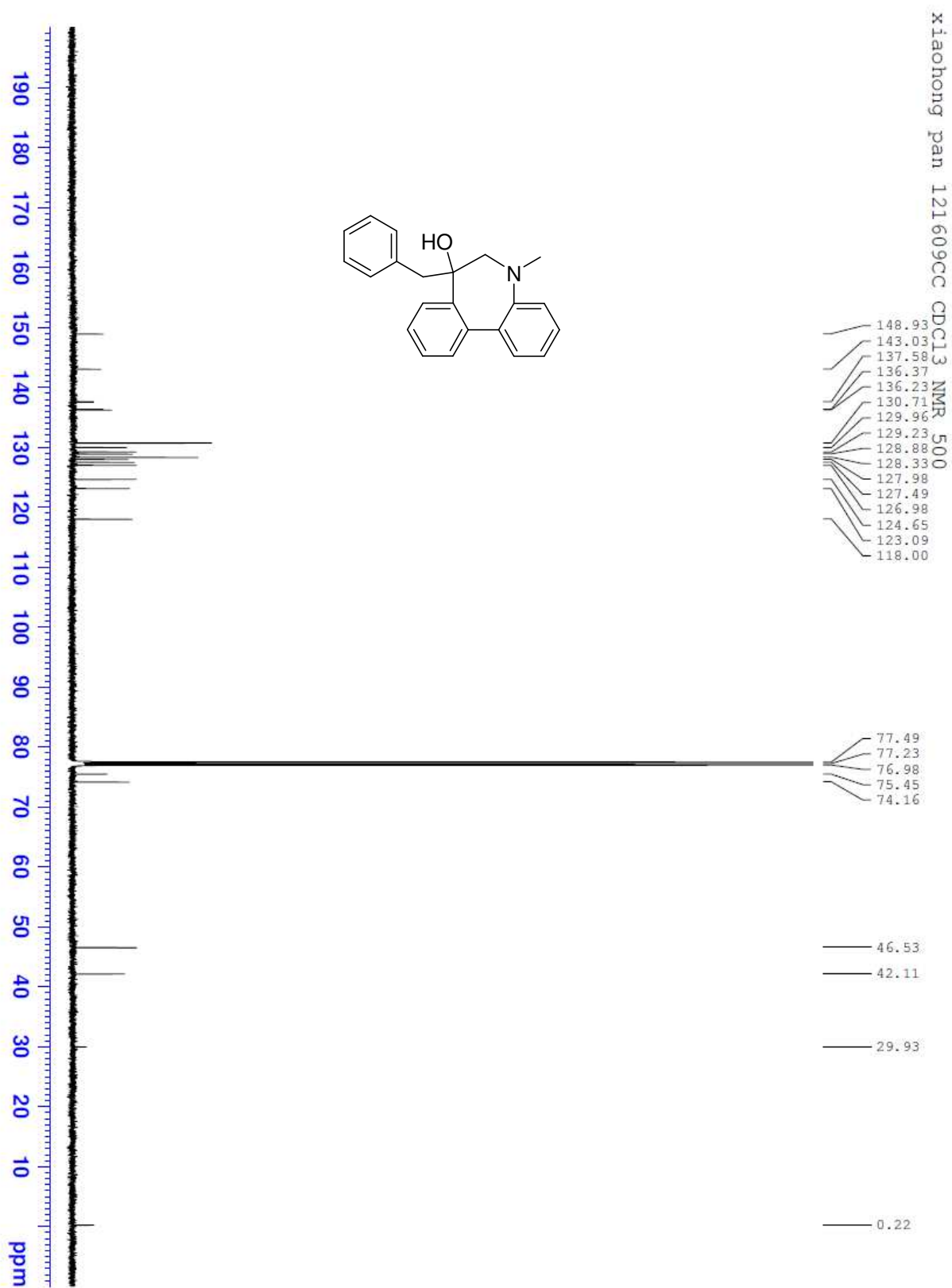
5-Hydroxy-*N*-methyl-dihydrodibenzazepine (32).

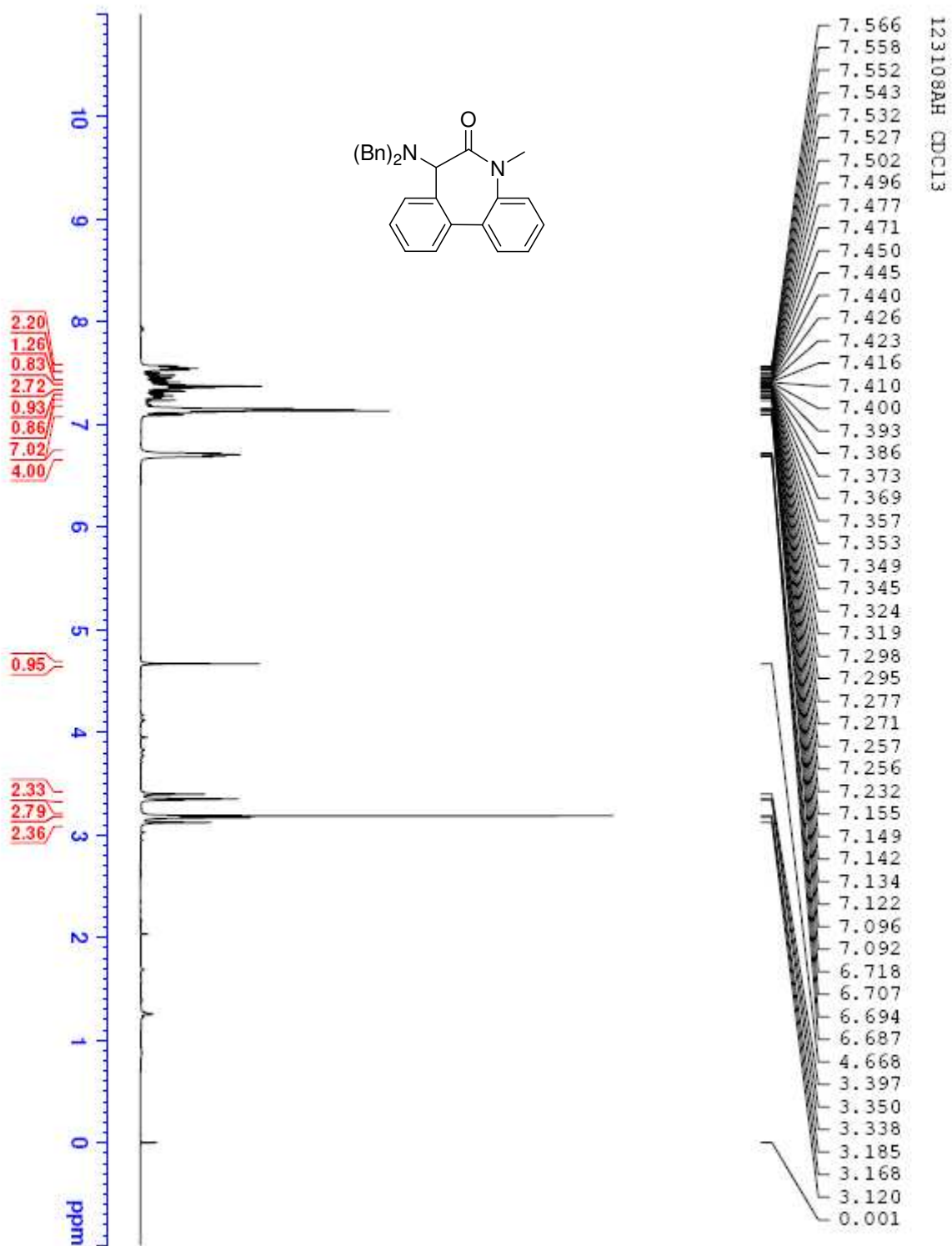
5-Hydroxy-*N*-methyl-dihydrodibenzazepine (32).

***N*-Methyl-dibenzazepin-5-one (33).**

N-Methyl-dibenzazepin-5-one (33).

5-Benzyl-5-hydroxy-*N*-methyl-dihydrodibenzazepine (34).

5-Benzyl-5-hydroxy-*N*-methyl-dihydrodibenzazepine (34).

5-Dibenzylamino-*N*-methyl-dibenzazepin-6-one (35).

5-Dibenzylamino-*N*-methyl-dibenzazepin-6-one (35).