Supporting Information

Construction of a Library of Bicyclic β-Benzyloxy and β-Hydroxy Amides from Nitriles through a Multicomponent Cyclization Reaction

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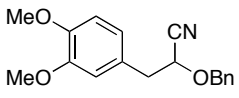
General Information

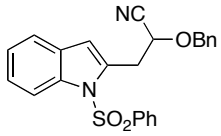
All air and moisture sensitive reactions were performed under an argon atmosphere. Proton (^{1}H NMR) and carbon (^{13}C NMR) nuclear magnetic resonance spectra were recorded on Bruker Avance 300 spectrometer at 300 MHz and 75 MHz, respectively. Chemical shifts (δ) are reported in parts per million (ppm). Chloroform-*d* was used as an internal standard. Data are reported as follows: (s = singlet; d = doublet; t = triplet; q = quartet; m = multiplet, sept = septet; dd = doublet of doublets; ddd = doublet of doublet of doublets; br = broad). High resolution and low resolution mass spectra were recorded on a VG 7070 spectrometer. Infrared (IR) spectra were obtained on a Smiths Detection IdentifyIR FT-IR spectrometer. Analytical TLC was performed on E. Merck pre-coated (25 mm) silica gel 60F-254 plates. Visualization was done under UV (254 nm). Flash chromatography was done using Merck silica gel 60 (230-400 mesh) or CombiFlash Companion (Teledyne Isco). Diastereoisomers were purified on a Waters micromass ZQ ESCI multimode. A Varian DYNAMAX C18 column (250 × 21.4 mm) was used. H-Cube (Thales Nanotechnology, Inc.) was used for continuous-flow hydrogenation. Melting points were obtained on a MelTemp melting point apparatus with digital temperature reading and are reported uncorrected. Nitrile **7** was prepared as previously reported.[1]

[1] Xiao, Q.; Floreancig, P. E. *Org. Lett*. **2008**, *10*, 1139-1142.



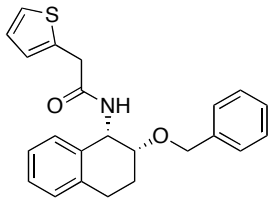
2-benzyloxy-3-(3,4-dimethoxyphenyl)-propionitrile (8)

To a suspension of $BiBr_3$ (0.22 g, 0.5mmol) and BnOTMS (4.3 g, 24 mmol) in CH_2Cl_2 (15 ml), was added 3,4-dimethoxyphenylacetaldehyde[1] (1.8 g, 10 mmol) at rt under argon atmosphere. The mixture was heated to reflux and stirred overnight. After cooling to rt, TMSCN (2.0 g, 20 mmol) and $BiBr_3$ (0.22 g, 0.5 mmol) were added. The mixture was heated to reflux and stirred overnight. The reaction mixture was diluted with EtOAc and quenched with saturated $NaHCO_3$. The mixture was extracted with ethyl acetate and the combined organic layer was washed with brine. The organic layer was dried over Na_2SO_4. The solvent was removed and the residue was purified by flash chromatography (hexane: ethyl acetate = 100:1 → 5:1) to give the product as a colorless oil (1.07 g, 36%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.37-7.33 (m, 3H), 7.28-7.25 (m, 2H), 6.82-6.81 (m, 2H), 6.77 (s, 1H), 4.86 (d, 1H, J = 11.4 Hz), 4.52 (d, 1H, J = 11.7 Hz), 4.29 (t, 1H, J = 6.9 Hz), 3.89 (s, 3H), 3.84 (s, 3H), 3.10 (d, 2H, J = 6.9 Hz). ^{13}C NMR (75 MHz, $CDCl_3$) δ 149.1, 148.7, 136.1, 128.8, 128.6, 128.4, 127.3, 122.0, 118.2, 113.0, 111.5, 72.6, 69.2, 56.1, 39.7; IR (neat) 2933, 1590, 1513, 1237, 1141, 1090, 1025, 738, 699 cm^{-1}; HRMS (EI) *m/z* calcd for $C_{18}H_{19}NO_3$ (M^+) 297.1365, found 297.1351.



3-(1-benzenesulfonyl-1H-indol-2-yl)-2-benzyloxypropionitrile (9)

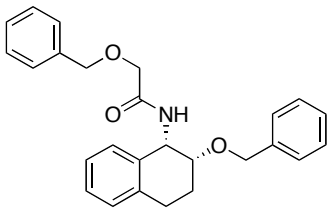
To a suspension of $BiBr_3$ (135 mg, 0.3 mmol) and (1-benzenesulfonyl-1H-indol-2-yl)acetaldehyde[1] (1.8 g, 6 mmol) in Dichloromethane (10 ml), was added BnOTMS (2.6 g, 14.4 mmol) at 0 °C under argon atmosphere. The mixture was warmed to rt and stirred overnight. TMSCN (1.68 ml, 12.6 mmol) was added at 0 °C. Then the mixture was stirred at rt overnight. $BiBr_3$(135 mg, 0.3 mmol) was added to the above solution, continued to stir at rt for 24 h. The reaction mixture was diluted with EtOAc and quenched with saturated $NaHCO_3$. The mixture was extracted with ethyl acetate and the combined organic layer was washed with brine. The organic layer was dried over Na_2SO_4. The solvent was removed and the residue was purified by flash chromatography (hexane: ethyl acetate = 9:1 → 4:1 → 3:1) to give the product as a yellow oil (0.75 g, 30%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.15 (d, 1H, J = 8.4 Hz), 7.68 (d, 2H, J = 7.5 Hz), 7.56-7.24 (m, 11H), 6.64 (s, 1H), 4.85 (d, 1H, J = 11.4 Hz), 4.75 (t, 1H, J = 6.9 Hz), 4.58 (d, 1H, J = 11.4 Hz), 3.66-3.49 (m, 2H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 138.3, 137.4, 135.7, 134.0, 133.5, 129.4, 128.6, 128.5, 128.2, 126.1, 125.1, 124.1, 121.0, 117.9, 115.0, 113.7, 72.7, 67.5, 33.9; IR (neat) 3062, 1446, 1364, 1172, 1148, 1088, 727 cm^{-1}; HRMS (ESI) *m/z* calcd for $C_{24}H_{20}N_2O_3NaS$ ($[M+Na]^+$) 439.1092, found 439.1076.



***cis-N*-(2-benzyloxy-1,2,3,4-tetrahydronaphthalen-1-yl)-2-thioph en-2-yl acetamide (23i)**

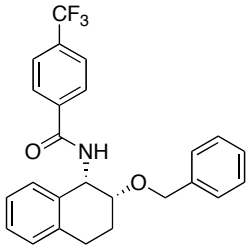
To **7** (200 mg, 0.80 mmol) in dichloromethane (15 mL) was added $Cp_2Zr(H)Cl$ (348 mg, 1.35 mmol). The reaction mixture was stirred for 20 min at room temperature. 2-Thiopheneacetyl chloride (150 μL, 1.2 mmol) was added and the mixture was stirred for another 20 min at room temperature. $ZnCl_2$ in Et_2O (840 μL, 0.84 mmol) was added and the mixture was stirred overnight at room temperature. The reaction was quenched with saturated $NaHCO_3$. The mixture was extracted with ethyl acetate and the

combined organic layer was washed with brine. The organic layer was dried over Na_2SO_4. The solvent was removed and the residue was purified by flash chromatography (hexane: ethyl acetate = 9:1 → 4:1 → 2:1) to give product as two diasteromers (dr 9: 1) (154 mg, 51%). The major (faster eluting) diasteromer was isolated by Semi Waters micromass ZQ ESCI multimode (Varian DYNAMAX C18 column (250 × 21.4 mm)). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.36-7.29 (m, 3H), 7.23-7.12 (m, 6H), 7.09-7.05 (m, 1H), 6.92 (d, 2H, *J* = 3.6 Hz), 6.38 (d, 1H, *J* = 9.3 Hz), 5.34 (dd, 1H, *J* = 3.9, 9.3 Hz), 4.58 (d, 1H, *J* = 11.7 Hz), 4.41 (d, 1H, *J* = 11.7 Hz), 3.93-3.90 (m, 1H), 3.86 (d, 2H, *J* = 4.2 Hz), 2.99 (ddd, 1H, *J* = 5.4, 11.7, 16.8 Hz), 2.68 (ddd, 1H, *J* = 3.0, 5.4, 16.5 Hz), 2.25-2.15 (m, 1H), 1.91-1.80 (m, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 170.0, 138.2, 136.6, 136.2, 135.2, 128.7, 128.6, 128.1, 127.9, 127.6, 127.5, 127.2, 126.6, 125.8, 74.1, 71.0, 50.3, 38.0, 24.9, 24.5; IR (neat) 3405, 3308, 3060, 3041, 2928, 1646, 1510, 1452, 1079, 745, 697 cm^{-1}; HRMS (ESI) *m/z* calcd for $C_{23}H_{23}NO_2NaS$ ($[M+Na]^+$) 400.1347, found 400.1326.



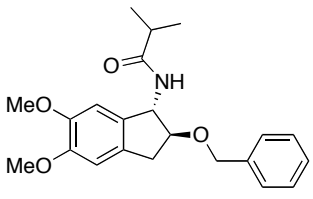
***cis*-2-benzyloxy-*N*-(2-benzyloxy-1,2,3,4-tetrahydronaphthalen-1-yl)acetamide (23e)**

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.40-7.27 (m, 11H), 7.22-7.17 (m, 2H), 7.15-7.11 (m, 1H), 5.44 (dd, 1H, *J* = 3.9, 9.6 Hz), 4.70 (d, 1H, *J* = 11.7 Hz), 4.60 (s, 2H), 4.57 (d, 1H, *J* = 12.0 Hz), 4.14 (d, 1H, *J* = 15.0 Hz), 4.07 (d, 1H, *J* = 15.3 Hz), 4.02-3.96 (m, 1H), 3.07 (ddd, 1H, *J* = 5.4, 10.8, 16.5 Hz), 2.75 (ddd, 1H, *J* = 4.5, 9.6, 16.8 Hz), 2.30-2.21 (m, 1H), 1.98-1.93 (m, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 169.6, 138.2, 136.9, 136.5, 135.1, 128.6, 128.5, 128.4, 128.1, 127.9, 127.7, 127.1, 126.4, 74.0, 73.6, 70.7, 69.6, 49.3, 24.8; IR (neat) 3416, 3060, 3027, 2924, 1675, 1513, 1452, 1100, 745, 697 cm^{-1}; HRMS (ESI) *m/z* calcd for $C_{26}H_{27}NO_3Na$ ($[M+Na]^+$) 424.1889, found 424.1872.



***cis*-*N*-(2-benzyloxy-1,2,3,4-tetrahydronaphthalen-1-yl)-4-trifluoromethylbenzamide (23l)**

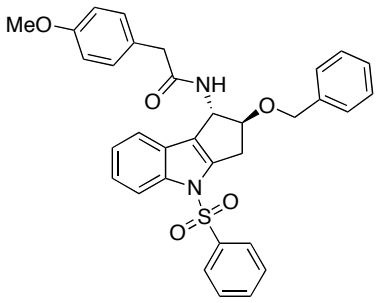
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.83 (d, 2H, *J* = 8.1 Hz), 7.69 (d, 2H, *J* = 8.4 Hz), 7.33-7.26 (m, 6H), 7.19-7.16 (m, 3H), 6.91 (d, 1H, *J* = 9.0 Hz), 5.57 (dd, 1H, *J* = 3.6, 9.3 Hz), 4.74 (d, 1H, *J* = 11.4 Hz), 4.51 (d, 1H, *J* = 11.7 Hz), 4.11-4.08 (m, 1H), 3.11 (ddd, 1H, *J* = 5.4, 12.0, 16.8 Hz), 2.81-2.76 (m, 1H), 2.40-2.32 (m, 1H), 2.02-1.94 (m, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 166.2, 138.2, 138.0, 136.7, 135.1, 128.8, 128.3, 128.2, 127.8 (q, J_{C-F} = 52.5 Hz), 127.7, 125.8 (d, *J*C-F = 3.8 Hz), 74.3, 71.1, 50.7, 25.0, 24.6; IR (neat) 3315, 3306, 2928, 1640, 1532, 1495, 1323, 1165, 1124, 1064, 857 cm^{-1}; HRMS (ESI) *m/z* calcd for $C_{25}H_{22}NO_2F_3Na$ ($[M+Na]^+$) 448.1500, found 448.1545.



***trans*-*N*-(2-benzyloxy-5,6-dimethoxyindan-1-yl)isobutyramide (26a)**

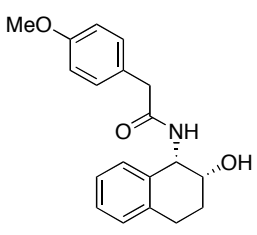
To **8** (200 mg, 0.67 mmol) in dichloromethane (15.0 mL) was added $Cp_2Zr(H)Cl$ (242 mg, 0.94 mmol). The reaction mixture was stirred for 20 min at room temperature. Isobutyryl chloride (0.1 ml, 1.0 mmol) was added and the mixture was stirred for

30 min at room temperature. $ZnCl_2$ in Et_2O (0.70 ml, 0.70 mmol) was added and the mixture was stirred overnight at room temperature. The reaction was quenched with saturated $NaHCO_3$. The mixture was extracted with ethyl acetate and the combined organic layer was washed with brine. The organic layer was dried over Na_2SO_4. The solvent was removed and the residue was purified by flash chromatography (hexane: ethyl acetate = 4:1 → 2:1 → 1:1) to give product as two diasteromers (dr 10:1) (98 mg, 40%). Recrystallization from hexane and ethyl acetate (3:1) gave the major product as a white solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.39-7.21 (m, 5H), 6.76 (s, 1H), 6.74 (s, 1H), 5.48-5.46 (m, 1H), 4.83 (d, 1H, *J* = 12.0 Hz), 4.71 (d, 1H, *J* = 12.0 Hz), 4.15-4.10 (m, 1H), 3.87 (s, 3H), 3.85 (s, 3H), 3.26 (dd, 1H, *J* = 6.9, 16.2 Hz), 2.91 (dd, 1H, *J* = 4.5, 16.2 Hz), 2.38 (sept, 1H, *J* = 6.9 Hz), 1.22 (d, 3H, *J* = 6.9 Hz), 1.21 (d, 3H, *J* = 6.9 Hz). ^{13}C NMR (75 MHz, $CDCl_3$) δ 176.6, 149.9, 148.9, 138.5, 132.8, 132.1, 128.3, 128.0, 127.8, 127.5, 107.8, 107.6, 85.8, 71.3, 59.8, 56.1, 56.0, 37.5, 35.7, 19.7; IR (neat) 3284, 2961, 2932, 1642, 1534, 1502, 1305, 1221, 1100, 699 cm^{-1}; HRMS (ESI) *m/z* calcd for $C_{22}H_{27}NO_4Na$ ([M+Na]$^+$) 392.1838, found 392.1803.



trans-N-(4-benzenesulfonyl-2-benzyloxy-1,2,3,4-tetrahydrocyclopenta[b]indol-1-yl)-2-(4-methoxyphenyl)acetamide (28b)

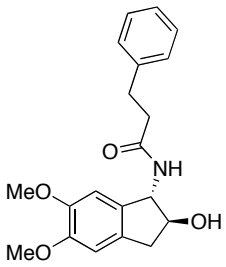
To a solution of **9** (200 mg, 0.48 mmol) in dichloromethane (15 ml) was added $Cp_2Zr(H)Cl$ (173 mg, 0.67 mmol). The mixture was stirred at rt for 20 min. 4-Methoxyphenylacetyl chloride (0.11 ml, 0.72 mmol) was added therein. The mixture was stirred for 20 min then $ZnCl_2$ in Et_2O (0.5 ml, 0.5 mmol) was added at rt, then stirred overnight. The mixture was quenched with saturated $NaHCO_3$. The mixture was extracted with ethyl acetate and the combined organic layer was washed with brine. The organic layer was dried over Na_2SO_4. The solvent was removed and the residue was purified by flash chromatography (hexane: ethyl acetate = 9:1 → 3:1 → 1:1) to give the desired product (51 mg, 19%) as a white solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.98 (d, 1H, *J* = 7.8 Hz), 7.85 (d, 2H, *J* = 7.5 Hz), 7.59-7.54 (m, 1H), 7.47-7.42 (m, 2H), 7.38-7.13 (m, 10H), 6.85-6.82 (m, 2H), 5.54 (d, 1H, *J* = 8.4 Hz), 5.49 (d, 1H, *J* = 8.4 Hz), 4.86 (d, 1H, *J* = 12.0 Hz), 4.71 (d, 1H, *J* = 12.3 Hz), 4.37-4.33 (m, 1H), 3.79 (s, 3H), 3.67 (dd, 1H, *J* = 6.9, 17.4 Hz), 3.57 (s, 2H), 3.14 (dd, 1H, *J* = 3.3, 17.7 Hz). ^{13}C NMR (75 MHz, $CDCl_3$) δ 171.2, 159.1, 142.1, 139.9, 138.6, 138.2, 134.2, 130.5, 129.6, 128.6, 128.0, 127.9, 126.9, 125.9, 124.3, 124.0, 122.8, 119.4, 114.7, 114.5, 89.7, 71.6, 55.5, 43.3, 35.2; IR (neat) 3386, 3302, 2948, 1640, 1510, 1446, 1245, 1174, 1088, 747 cm^{-1}; HRMS (ESI) *m/z* calcd for $C_{33}H_{30}N_2O_5NaS$ ([M+Na]$^+$) 589.1773, found 589.1728.



cis-N-(2-hydroxy-1,2,3,4-tetrahydronaphthalen-1-yl)-2-(4-methoxyphenyl)acetamide (29c)

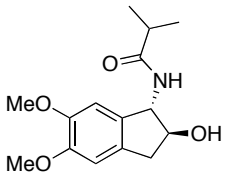
Catalytic hydrogenolysis of **23f** (60 mg, 0.15 mmol) in EtOH/EtOAc (1:1, 15 mL) was carried over 10% Pd-C using the H-cube flow reactor (temperature = 45 °C, flow rate = 1 mL/min), followed by removal of excess solvent under reduced pressure to give the desired alcohol (43 mg, 92%) as a white solid. ^{1}H NMR

(300 MHz, $CDCl_3$) δ 7.24-7.05 (m, 6H), 6.91-6.85 (m, 2H), 5.84 (d, 1H, *J* = 8.4 Hz), 5.24 (dd, 1H, *J* = 4.2, 8.1 Hz), 4.20-4.15 (m, 1H), 3.79 (s, 3H), 3.62 (s, 2H), 2.96-2.88 (m, 1H), 2.82-2.72 (m, 1H), 2.01-1.94 (m, 1H), 1.89-1.77 (m, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 173.1, 159.2, 136.6, 134.4, 130.6, 129.2, 129.0, 127.9, 126.8, 114.7, 69.4, 55.5, 52.2, 43.1, 27.1, 26.0; IR (neat) 3401, 3300, 2926, 1636, 1508, 1452, 1243, 1176, 742 cm^{-1}; HRMS (ESI) *m/z* calcd for $C_{19}H_{21}NO_3Na$ ([M+Na]$^+$) 334.1419, found 334.1422.



***trans*-*N*-(2-hydroxy-5,6-dimethoxyindan-1-yl)-3-phenylpropionamide (30d)**

Catalytic hydrogenolysis of **26g** (60 mg, 0.14 mmol) in EtOH (25 mL) was carried over 10% Pd-C using the H-cube flow reactor (pressure = 20 bar, temperature = 45 °C, flow rate = 1 mL/min), followed by removal of excess solvent under reduced pressure and subsequent purification of the residue by Waters micromass ZQ ESCI multimode (Varian DYNAMAX C18 column (250 × 21.4 mm)) to give two products. The major product 30d (20 mg, 42.1%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.33-7.28 (m, 2H), 7.24-7.19 (m, 3H), 6.71 (s, 1H), 6.44 (s, 1H), 5.00 (t, 1H, *J* = 5.4 Hz), 4.44 (s,1H), 4.30-4.23 (m, 1H), 3.84 (s, 3H), 3.81 (s, 3H), 3.18 (dd, 1H, *J* = 7.8, 15.6 Hz), 3.02 (t, 2H, *J* = 7.5 Hz), 2.81 (dd, 1H, *J* = 7.5, 15.6 Hz), 2.60 (t, 2H, *J* = 7.5 Hz). ^{13}C NMR (75 MHz, $CDCl_3$) δ 174.4, 149.8, 148.8, 140.5, 132.7, 129.9, 128.6, 128.4, 126.5, 108.1, 106.0, 82.0, 64.4, 56.3, 56.0, 38.3, 38.2, 31.8; IR (neat) 3349, 3340, 2933, 1644, 1539, 1500, 1454, 1303, 1219, 1088, 701 cm^{-1}; HRMS (ESI) *m/z* calcd for $C_{20}H_{21}NO_3$ ([M-H_2O]$^+$) 323.1521, found 323.1506.



***trans*-*N*-(2-hydroxy-5,6-dimethoxyindan-1-yl)isobutyramide (30a)**

^{1}H NMR (300 MHz, $CDCl_3$) δ 6.77 (s, 1H), 6.69 (s, 1H), 5.90 (brs, 1H), 5.07 (t, 1H, *J* = 5.4 Hz), 4.54 (s, 1H), 4.39 (m, 1H), 3.89 (s, 3H), 3.88 (s, 3H), 3.27 (dd, 1H, *J* = 8.1, 15.9 Hz), 2.89 (dd, 1H, *J* = 7.8, 15.6 Hz), 2.50 (sept, 1H, *J* = 6.9 Hz), 1.25 (d, 3H, *J* = 6.9 Hz), 1.23 (d, 3H, *J* = 6.6 Hz). ^{13}C NMR (75 MHz, $CDCl_3$) δ 179.4, 150.0, 148.9, 132.9, 130.2, 108.3, 106.1, 82.3, 64.5, 56.3, 56.1, 38.4, 35.3, 19.7, 19.5; IR (neat) 3342, 3336, 2962, 2930, 1640, 1532, 1500, 1299, 1217, 1094, 1073, 991, 680 cm^{-1}; HRMS (ESI) *m/z* calcd for $C_{15}H_{21}NO_4Na$ ([M+Na]$^+$) 302.1368, found 302.1368.

Computational protocols

All computational analyses were performed using a Linux PC/dual-core dual-CPU Xeon-based HPCC 30-processor Dell cluster, loaded with Tripos Sybyl molecular modeling package (version 8.0). The 330,000 compound SMR compound library was downloaded from the NIH Small Molecular Repository.[2] The 57,000 compound Maybridge screening collection was downloaded from the Maybridge website.[3] Tripos CONCORD[4] was used to generate the 3D conformation for each member of the library.

[2] http://pubchem.ncbi.nlm.nih.gov/sources/sources.cgi?mode=contact&dsn=MLSMR.
[3] http://www.maybridge.com/FTP/Downloads//screening/Screening+Fragments_db.zip.
[4] CONCORD software; Tripos Inc.: 1699 S. Hanley Road, St. Louis, MO 63144.

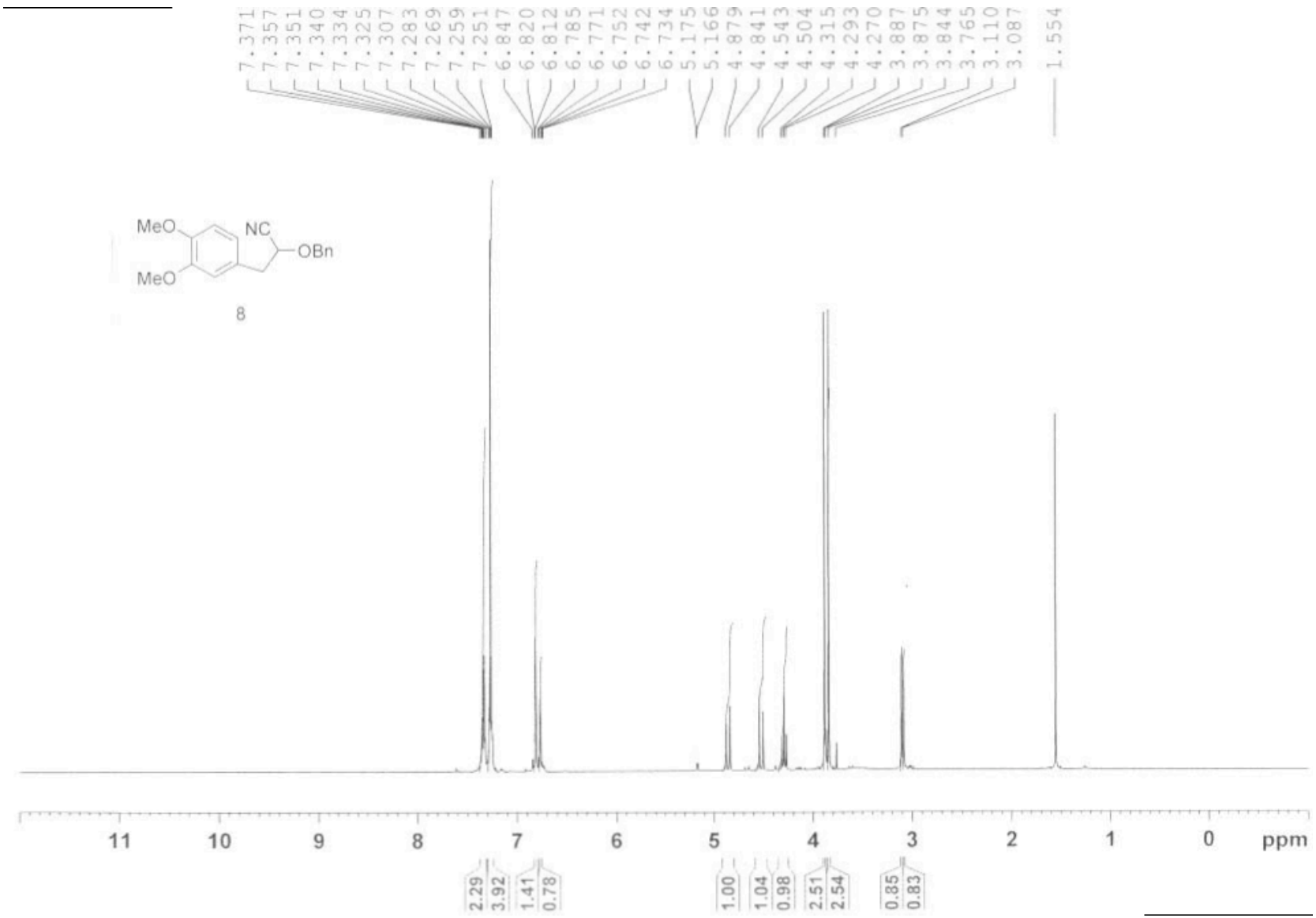
Multi-dimensional chemistry space coordinates were calculated for each compound in the library according to four main classes of atomic properties including atomic Gasteiger-Hückel charge, polarity, H-bond donor (HBD) and H-bond acceptor (HBA) attributes. BCUT matrices[5] incorporated molecule physical properties, topology and conformation information by filling the diagonal elements by those atomic properties and off-diagonal elements by distance-related information. All the molecular information was condensed into a set of real numbers by taking the lowest or highest Eigen values of series of BCUT matrices. BCUT descriptors were generated for both SMR and Maybridge libraries using DiverseSolutions. For visualization and dimension reduction purpose, the chemistry space was defined by the best three BCUT descriptors and raw descriptor values were rescaled to range from 0 to 10. A diversity analysis was performed by cell statistics under the chemistry space.

Pair wise Tanimoto coefficient (Tc) calculations based on 2D molecular fingerprints were conducted to compare the library to the SMR.[6] The comparison of was done using the Tripos SELECTOR program. Molecular fingerprints were calculated using the standard Tripos UNITY 2D fingerprints and the data processes were carried out using Sybyl Molecular Spreadsheet.[7]

[5] Menard, P. R.; Morize, I.; Bauerschmidt, S. *J. Chem. Inf. Comput. Sci.* **1998**, *38*, 1204-1213.

[6] Wild, D. J.; Blankley, C. J. *J. Chem. Inf. Comput. Sci.* **2000**, *40* 155-162.

[7] Tripos-vn.7.6, *Tripos Sybyl (version 7.2) molecular modeling software packages.* www.tripos.com, TRIPOS, Associates, Inc.: St. Louis, Mo. 63144.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3.765
3.110
3.087
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NC
OBn
MeO
8
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10
9
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5
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1
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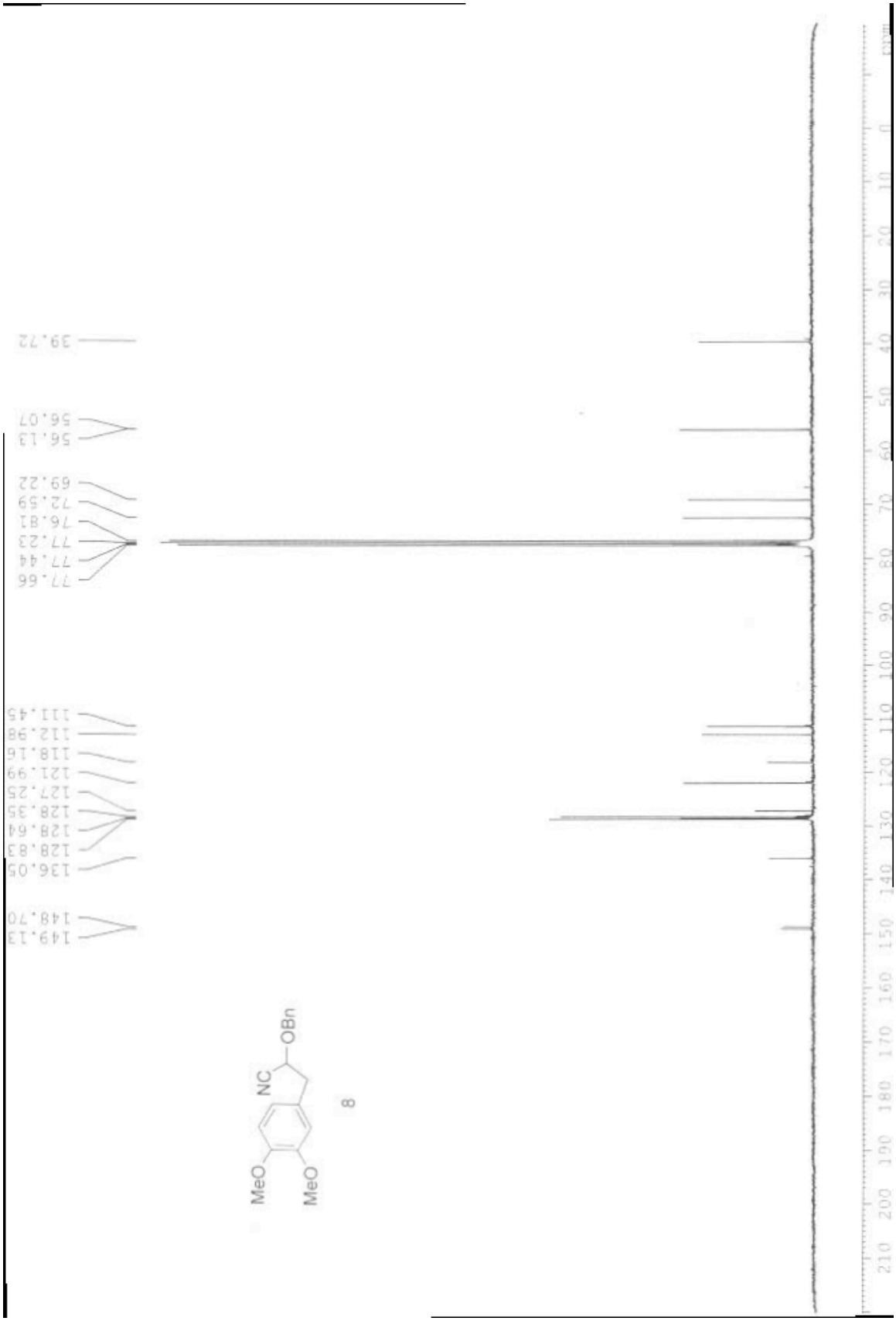
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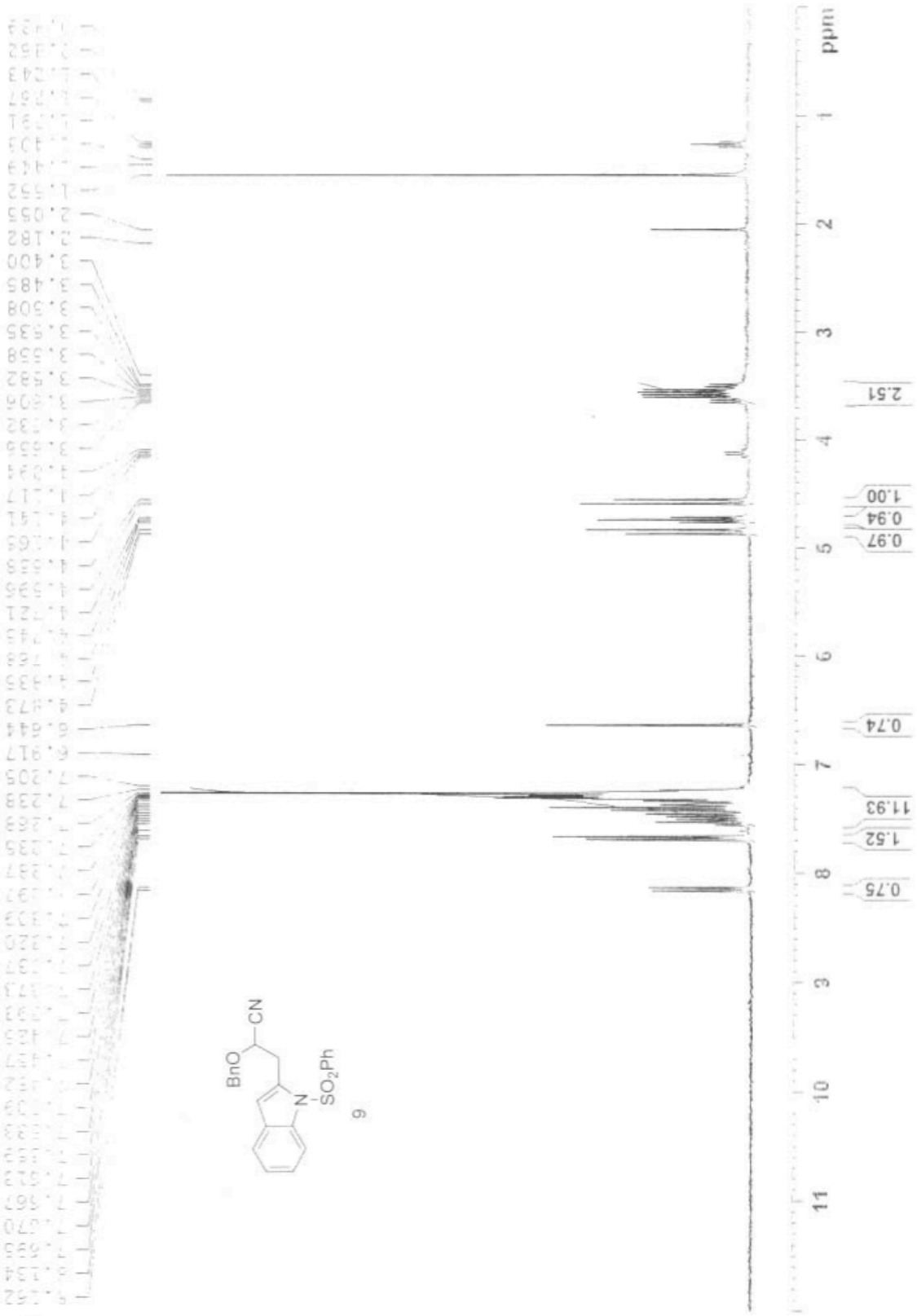
OBn
MeO
MeO
8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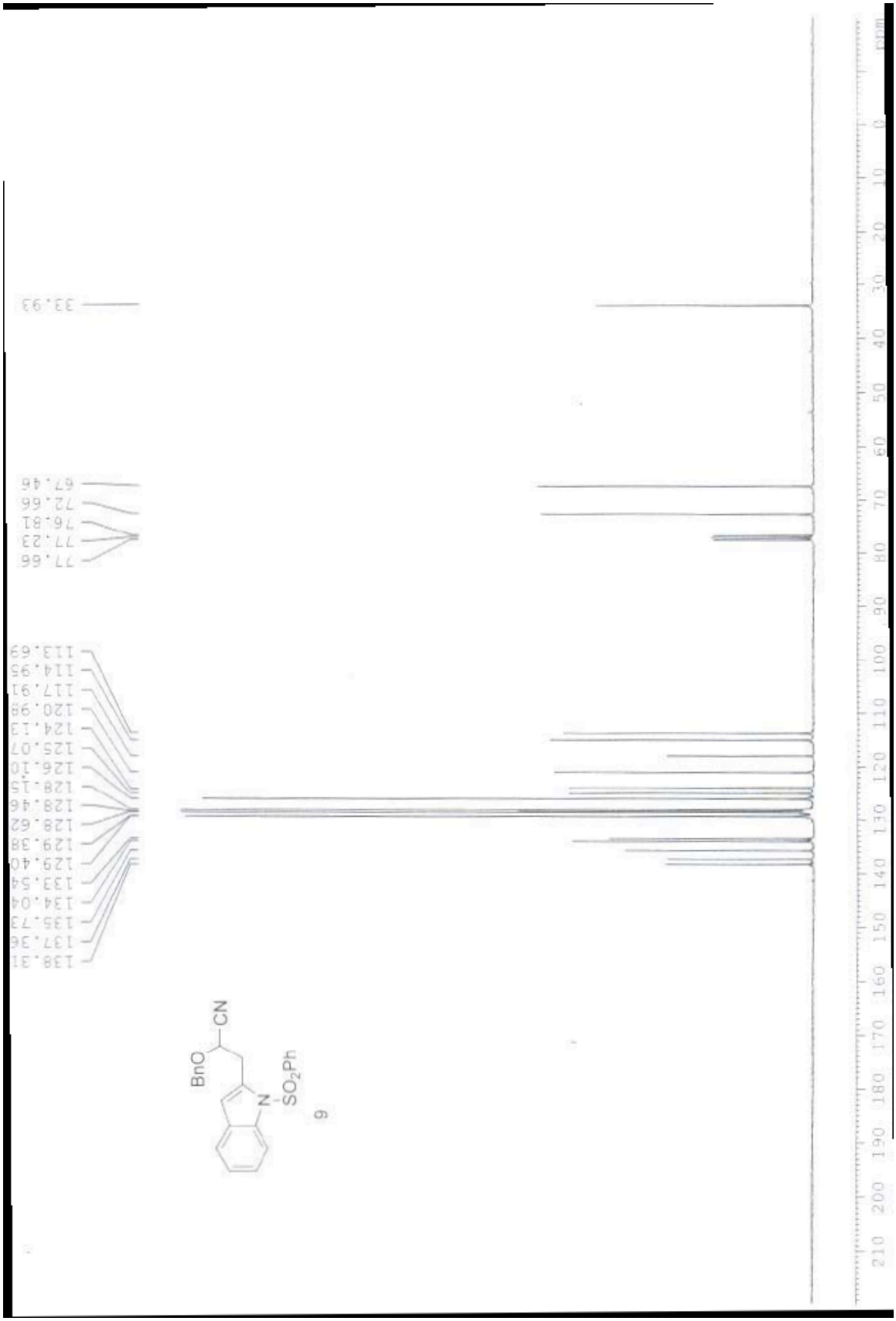
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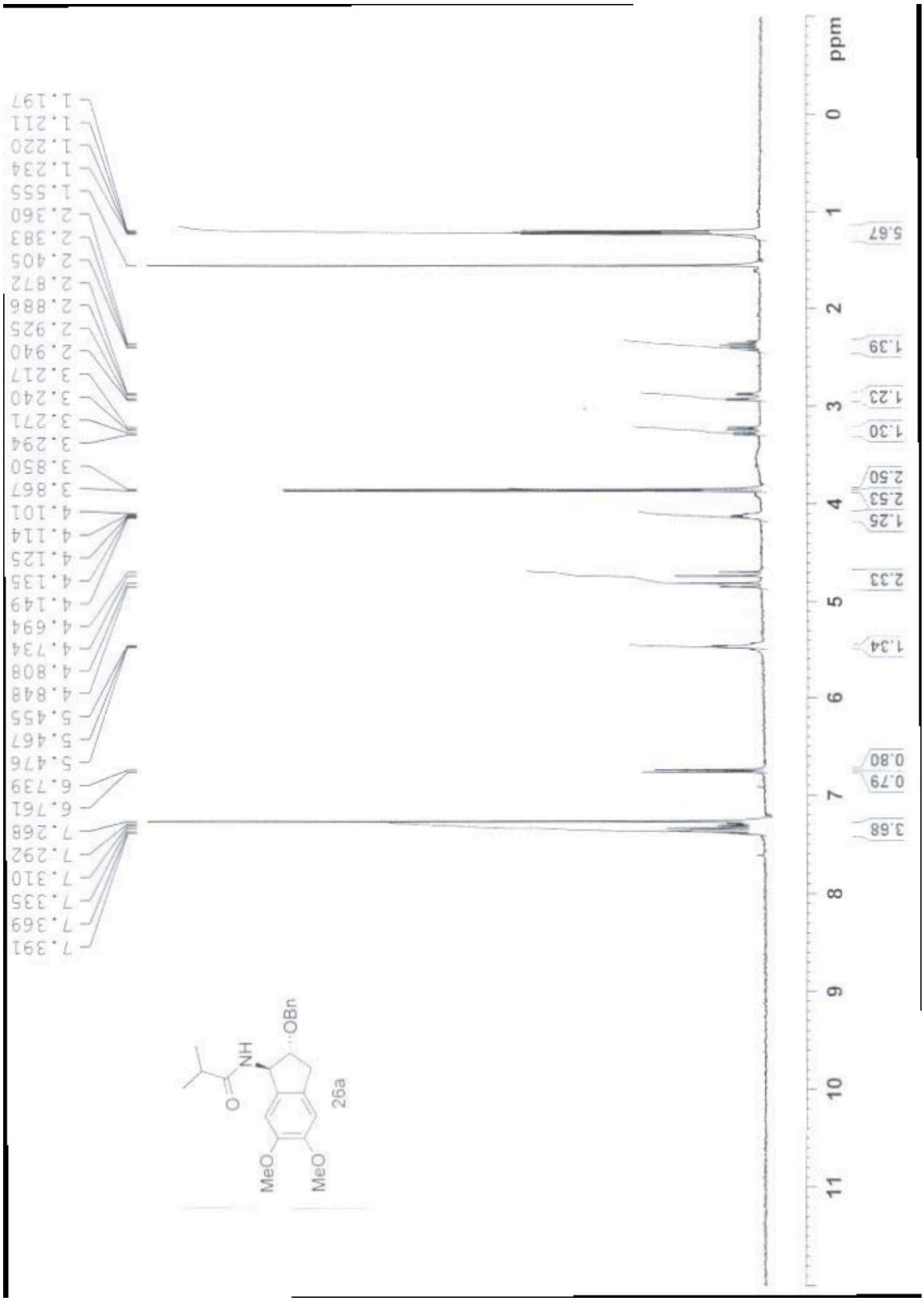
BnO
CN
N
SO2Ph
9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1.25
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2.405
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3.240
3.271
3.294
3.850
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4.101
4.114
4.125
4.135
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4.734
4.808
4.848
5.455
5.467
5.476
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MeO
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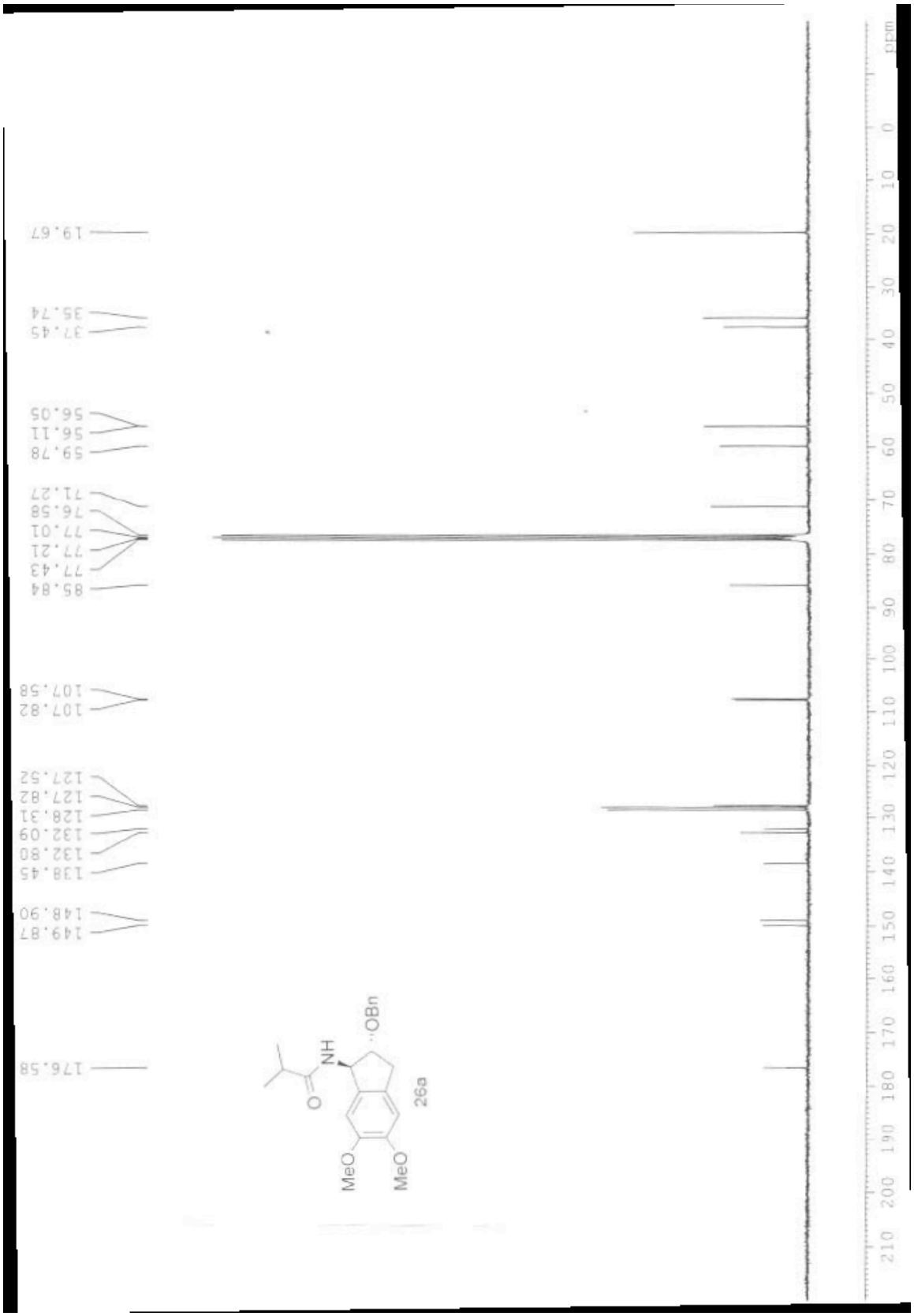
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149.87
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NH
OBn
O
MeO
MeO
26a
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30
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90
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150
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170
180
190
200
210

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2.704
2.712
2.722
2.986
3.796
3.852
3.866
3.902
3.915
3.922
3.928
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5.333
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7.348
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8
9
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1.21
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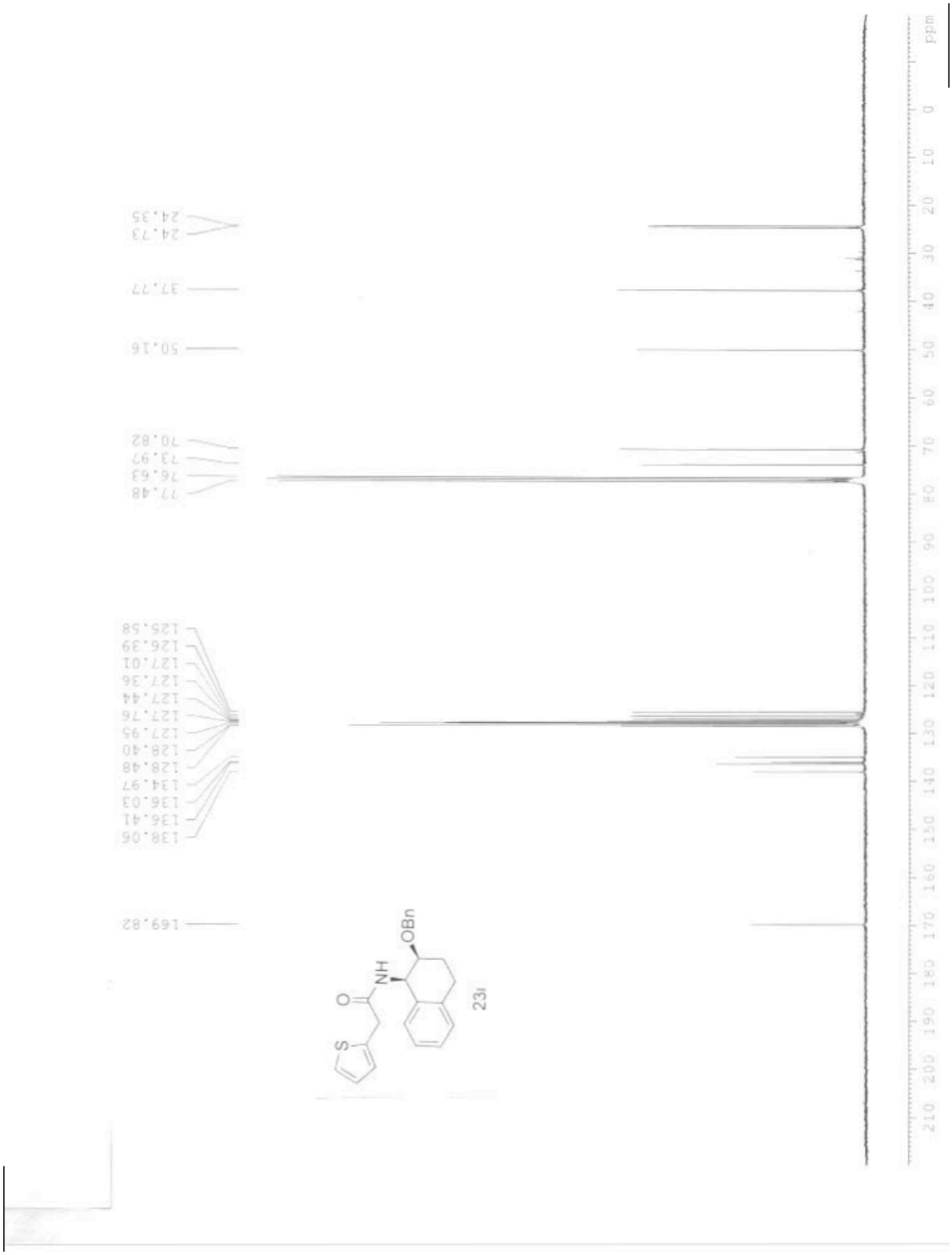
NH
OBn
S
23i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ppm
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20
30
40
50
60
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120
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200
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OBn
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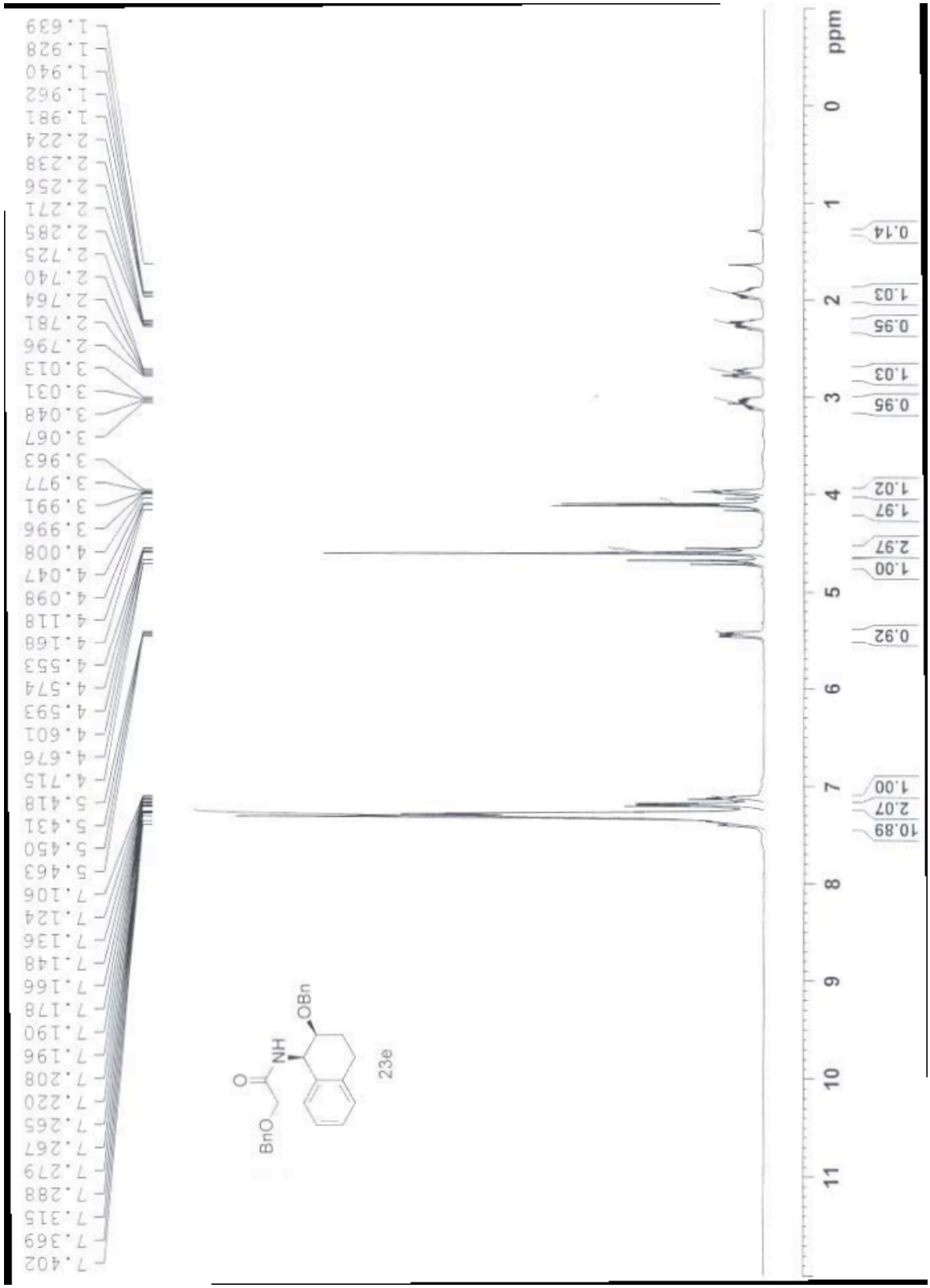
O
S
23i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0.92
1.00
2.07
10.89
1.639 1.928 1.940 1.962 1.981 2.224 2.238 2.256 2.271 2.285 2.725 2.740 2.764 2.781 2.796 3.013 3.031 3.048 3.067 3.963 3.977 3.991 3.996 4.008 4.047 4.098 4.118 4.168 4.553 4.574 4.593 4.601 4.676 4.715 5.418 5.431 5.450 5.463 7.106 7.124 7.136 7.148 7.166 7.178 7.190 7.196 7.208 7.220 7.265 7.267 7.279 7.288 7.315 7.369 7.402
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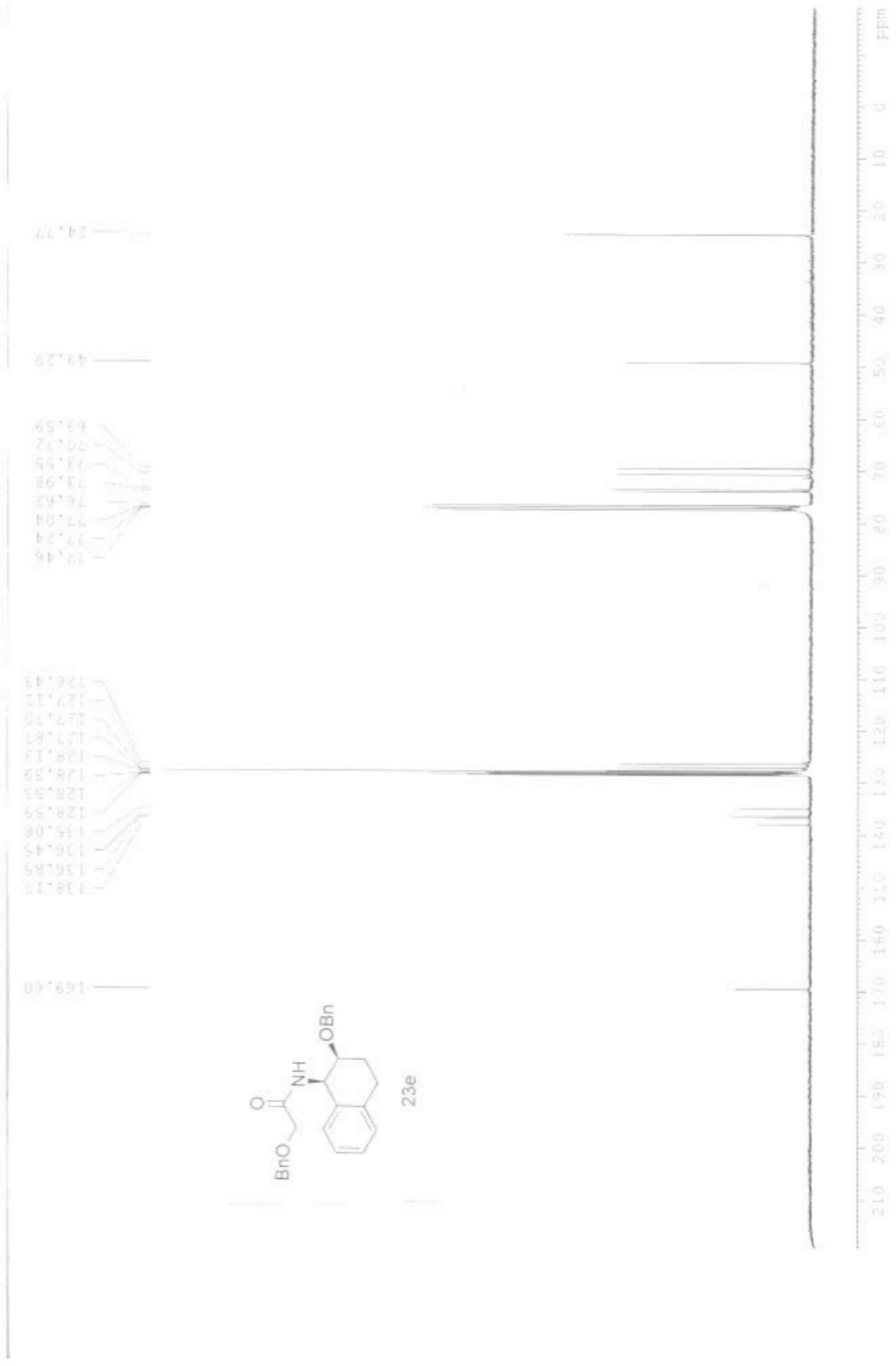
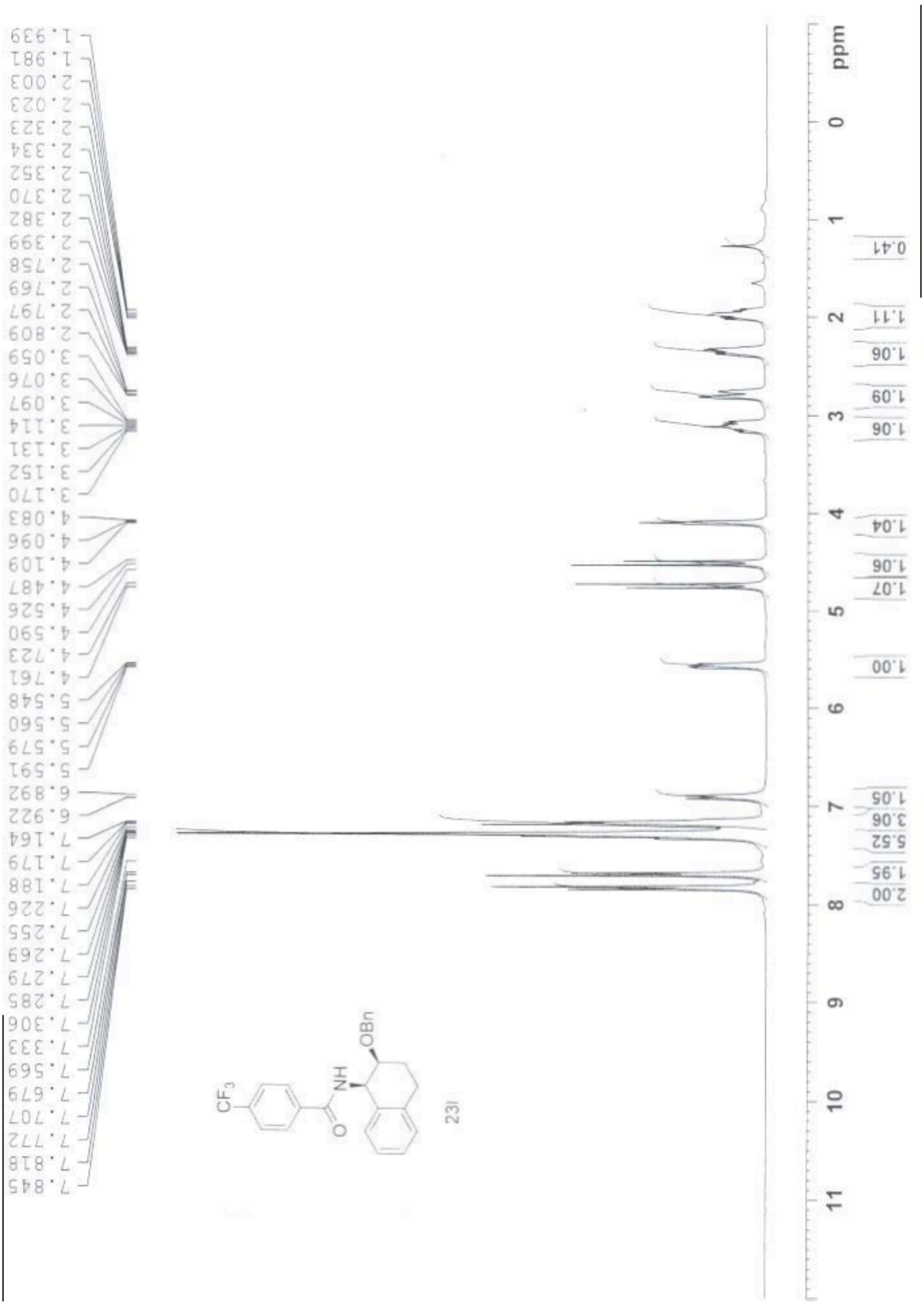
NH
OBn
BnO
23e


OBn
NH
O
BnO
23e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3.097
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3.131
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4.083
4.096
4.109
4.487
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4.590
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6.922
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7.188
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7.255
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7.279
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23l
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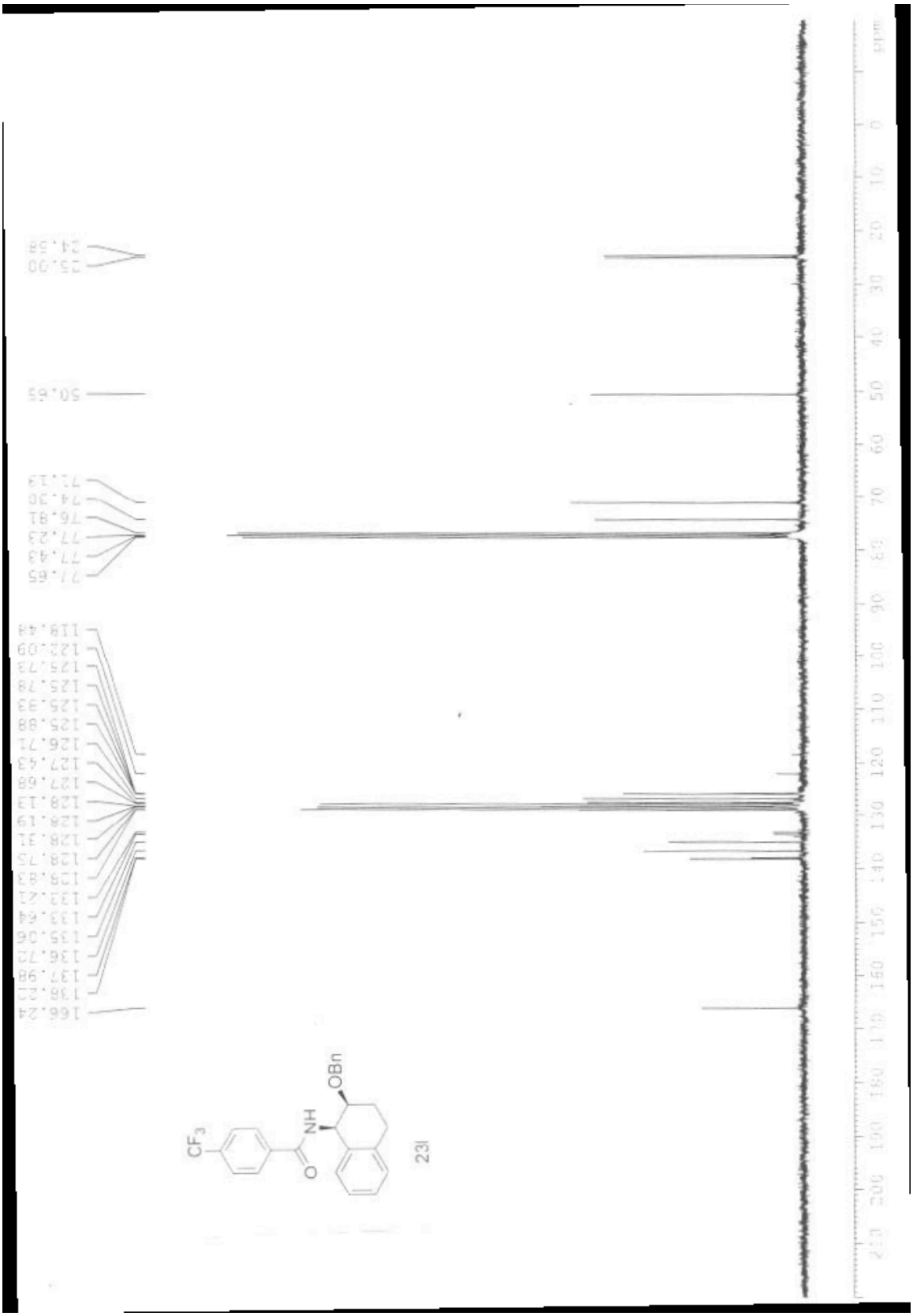
2.00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128.19
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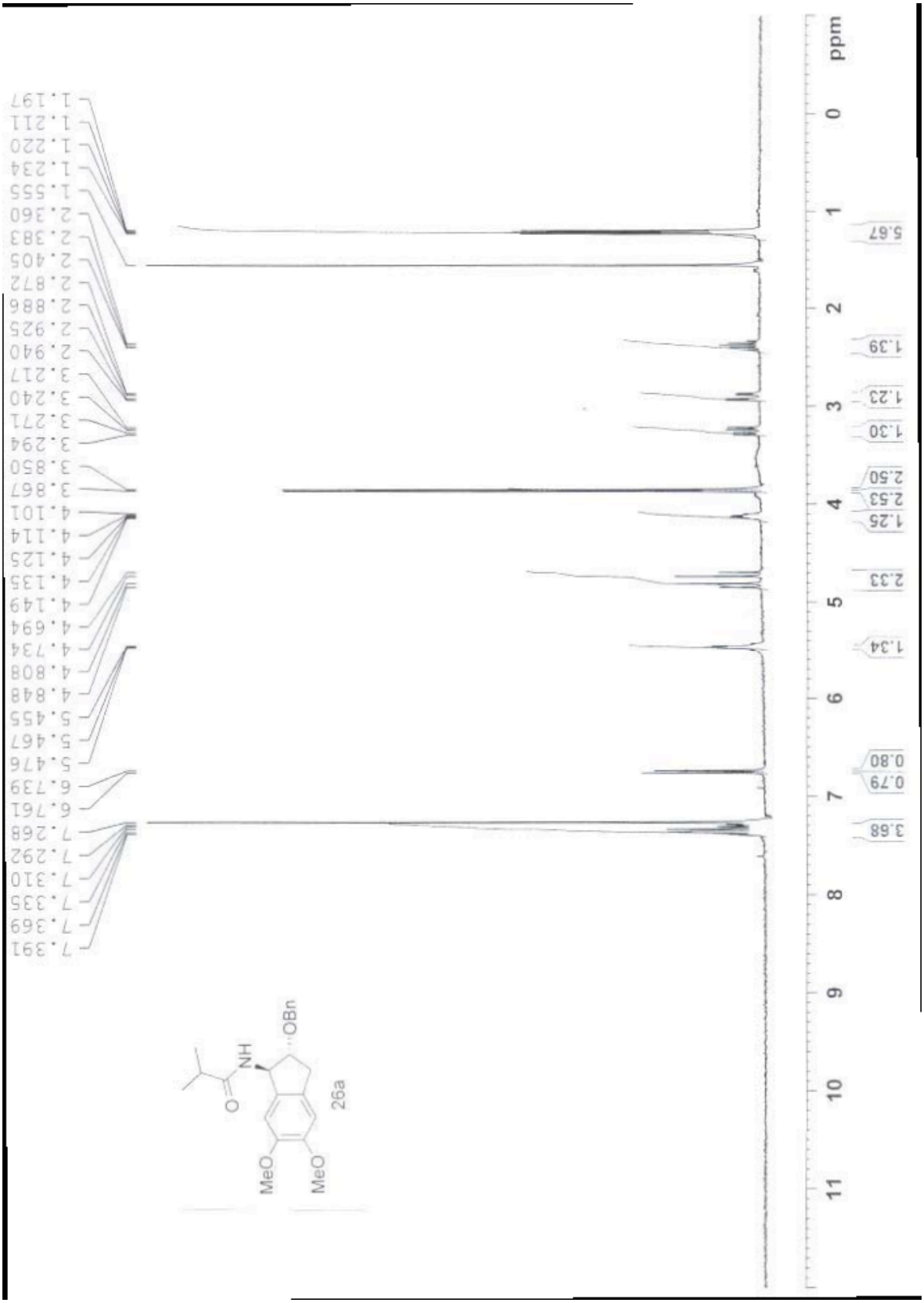
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2.53
1.25
2.33
1.34
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0.80
3.68
1.197
1.211
1.220
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2.940
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3.271
3.294
3.850
3.867
4.101
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4.734
4.808
4.848
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7.310
7.335
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NH
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MeO
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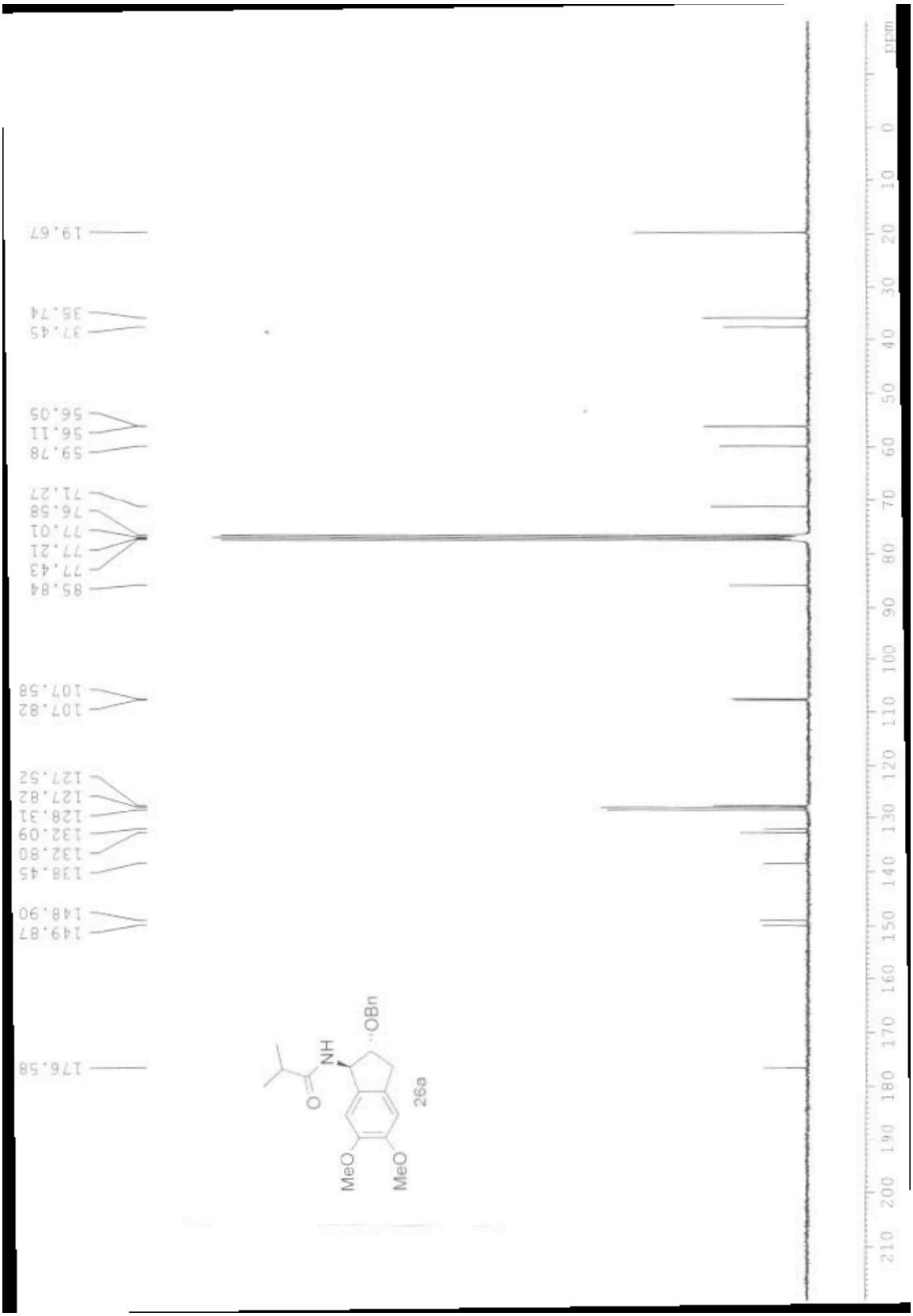
26a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71.27
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77.21
77.43
85.84
107.58
107.82
127.52
127.82
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149.87
176.58
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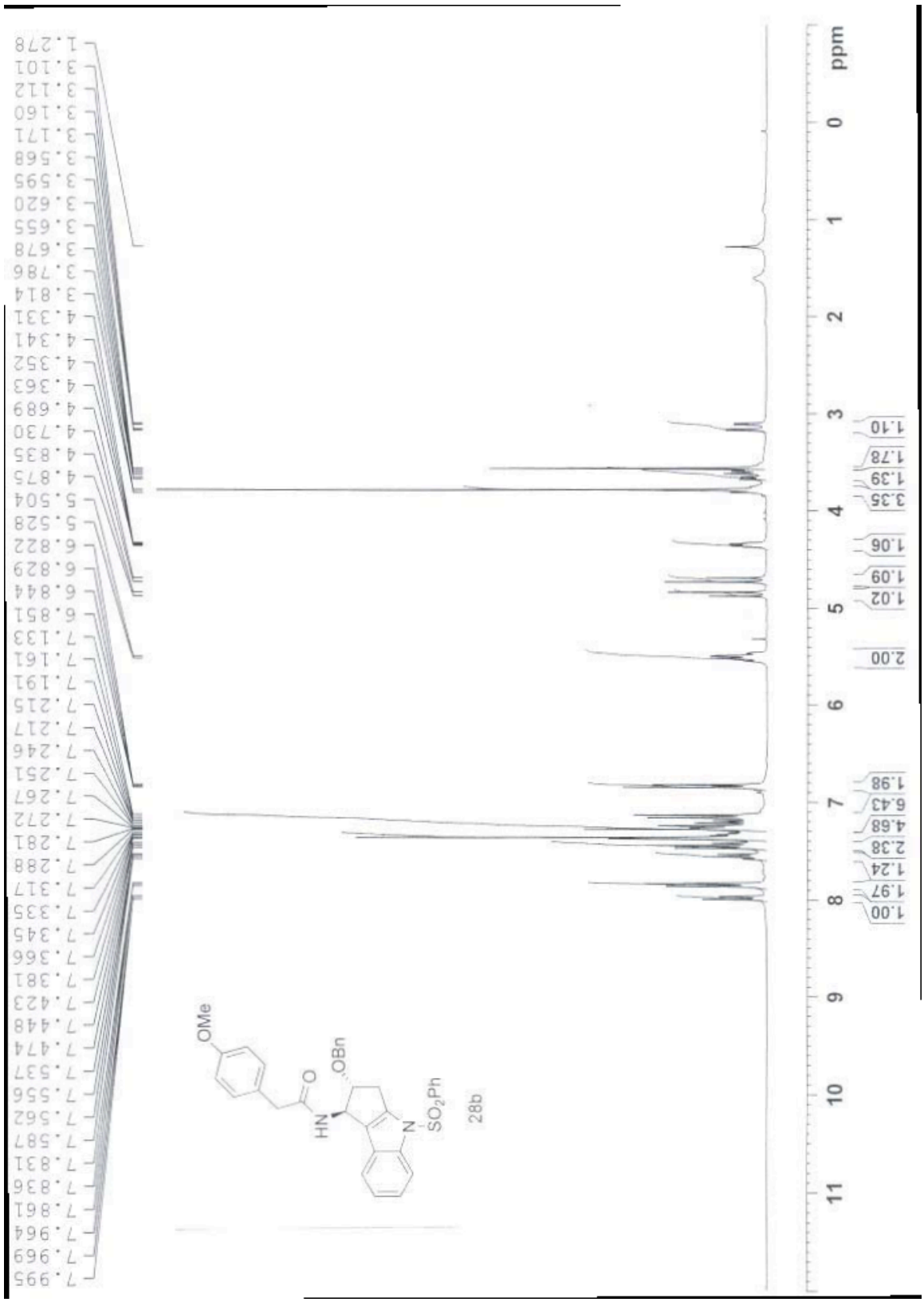
OBn
O
MeO
MeO
26a
ppm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10
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4.68
6.43
1.98
2.00
1.02
1.09
1.06
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1.78
1.10
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7.317
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7.267
7.251
7.246
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7.215
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7.161
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6.822
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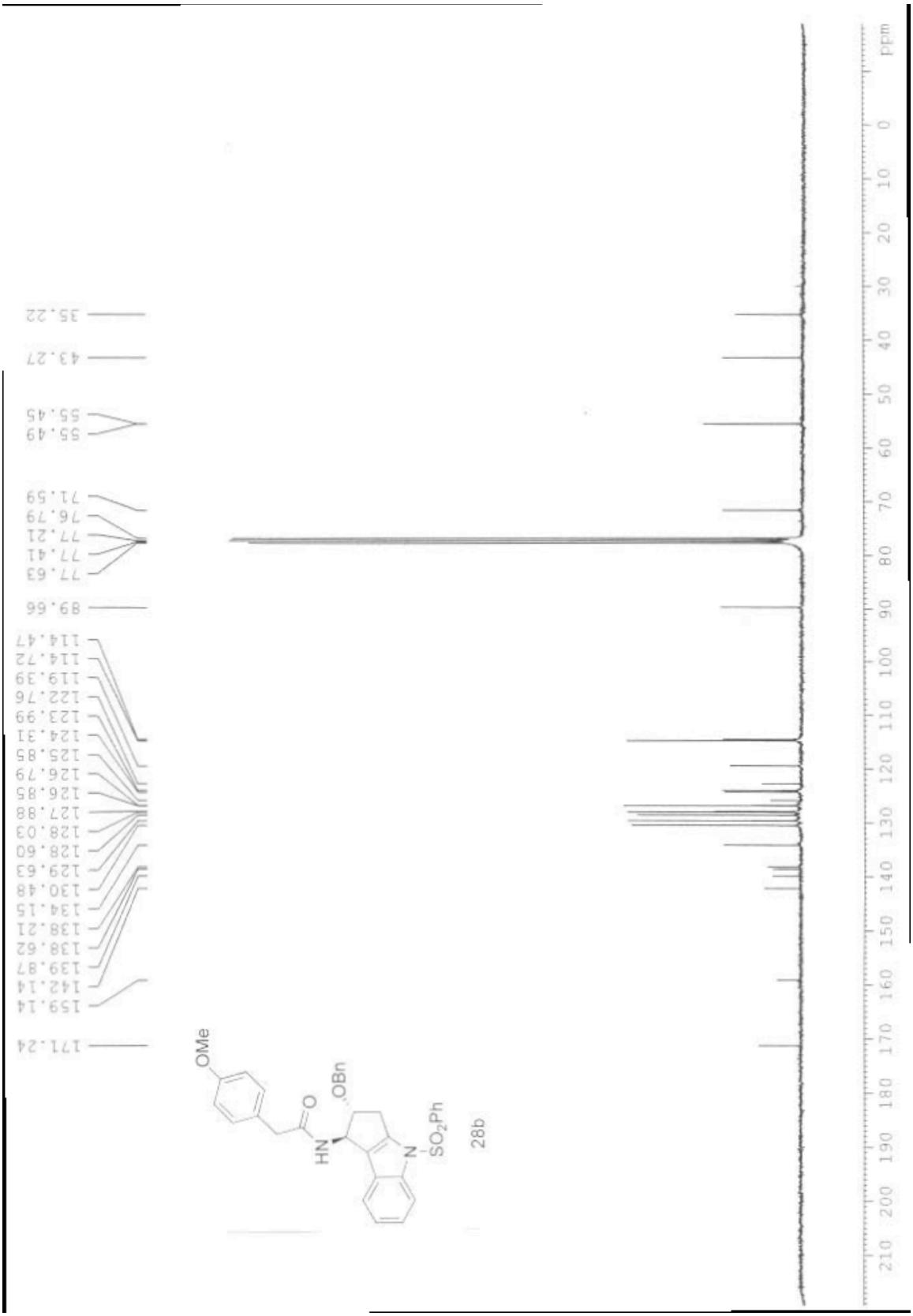
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125.85
124.31
123.99
122.76
119.39
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114.47
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77.41
77.21
76.79
71.59
55.49
55.45
43.27
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20
30
40
50
60
70
80
90
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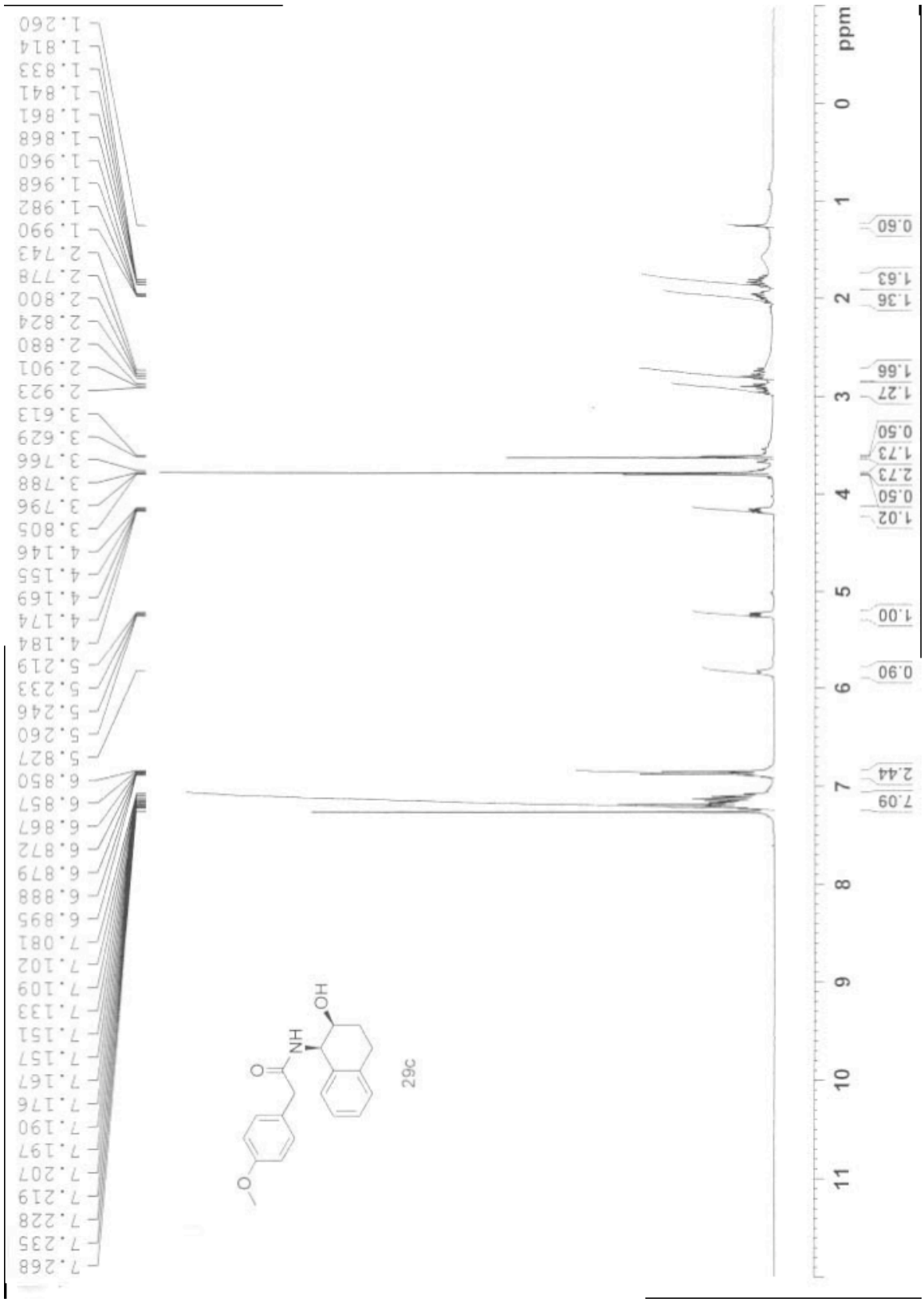
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1.02
1.00
0.90
2.44
7.09
1.260 1.814 1.833 1.841 1.861 1.868 1.960 1.968 1.982 1.990 2.743 2.778 2.800 2.824 2.880 2.901 2.923 3.613 3.629 3.766 3.788 3.796 3.805 4.146 4.155 4.169 4.174 4.184 5.219 5.233 5.246 5.260 5.827 6.850 6.857 6.867 6.872 6.879 6.888 6.895 7.081 7.102 7.109 7.133 7.151 7.157 7.167 7.176 7.190 7.197 7.207 7.219 7.228 7.235 7.268
HO
NH
O
O
29c

25.95
27.18
43.11
52.23
55.48
69.39
76.81
77.23
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114.88
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127.89
128.58
128.99
129.16
130.63
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136.62
159.16
173.05
OH
NH
O
O
29c
ppm
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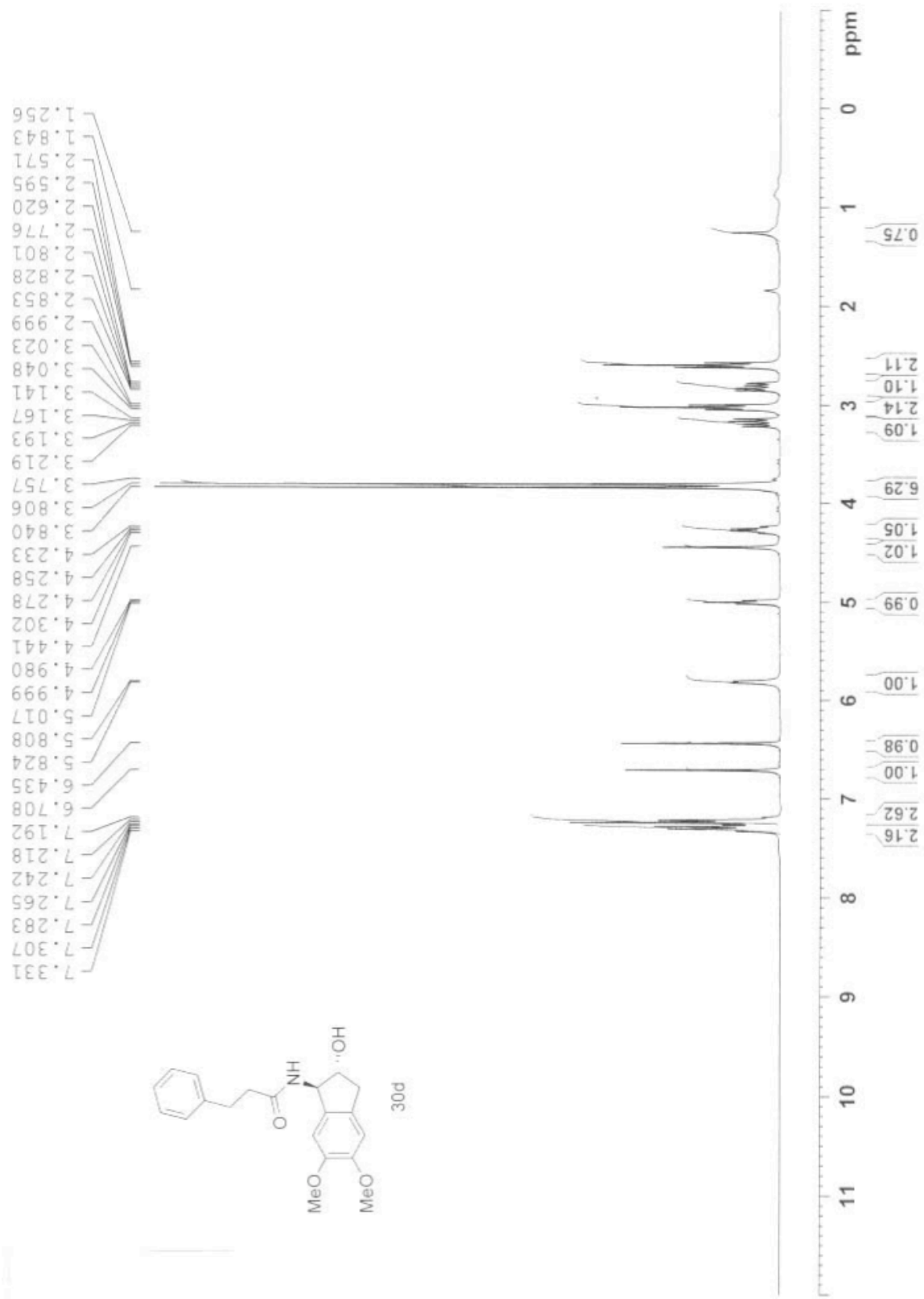
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1.00
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2.16
7.331
7.307
7.283
7.265
7.242
7.218
7.192
6.708
6.435
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5.808
5.017
4.999
4.980
4.441
4.302
4.278
4.258
4.233
3.840
3.806
3.757
3.219
3.193
3.167
3.141
3.048
3.023
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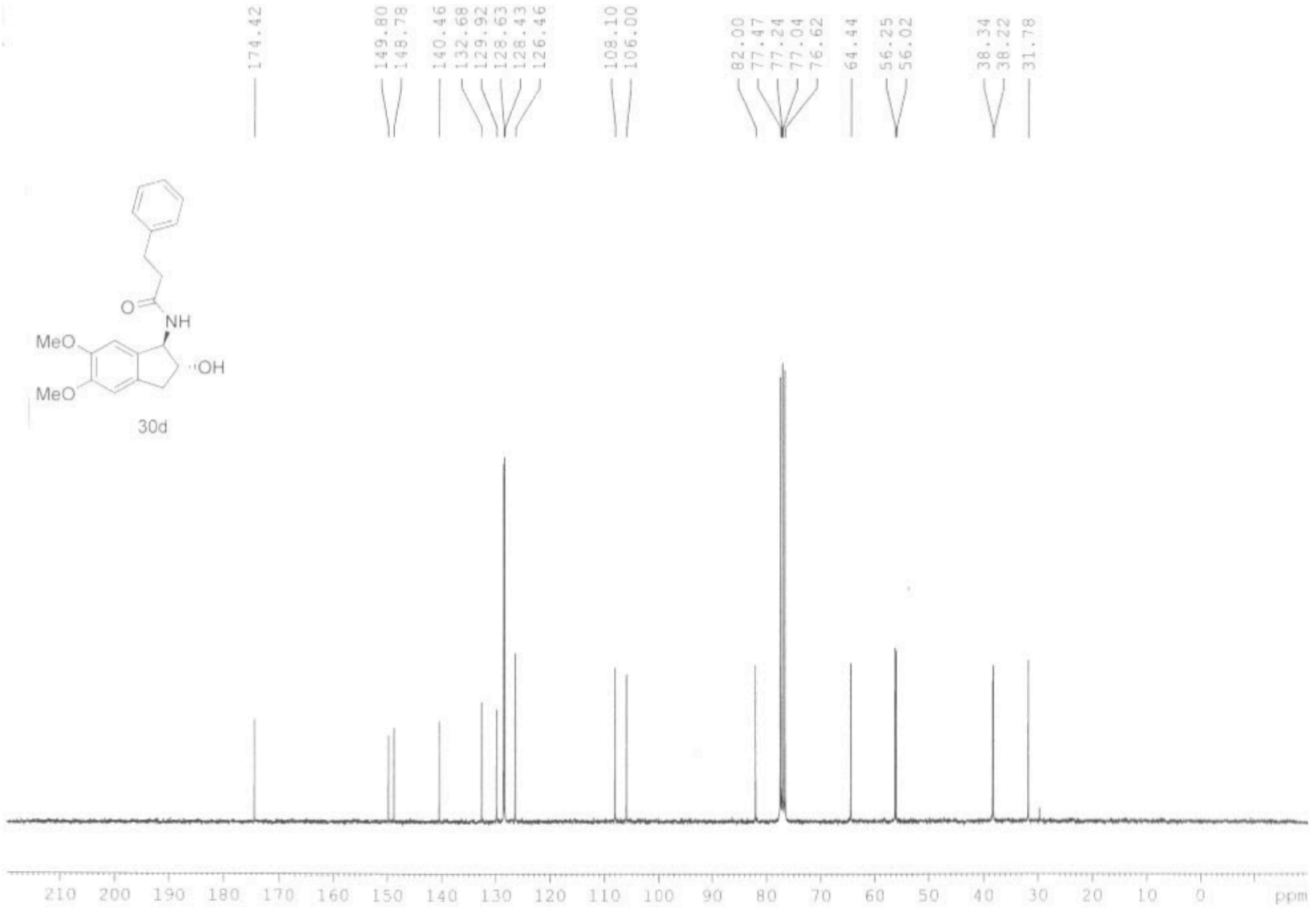
MeO
MeO
30d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82.00
77.47
77.24
77.04
76.62
64.44
56.25
56.02
38.34
38.22
31.78
O
NH
MeO
MeO
OH
30d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

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1.263
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2.475
2.498
2.521
2.544
2.848
2.874
2.900
2.926
3.235
3.261
3.287
3.314
3.846
3.874
3.884
3.894
4.357
4.382
4.405
4.427
4.537
5.051
5.069
5.087
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6.687
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7.259
7.269
ppm
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1.19
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1.02
1.01
1.10
0.99
1.00
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NH
O
MeO
MeO
30a


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77.43
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