Supporting Information

For

A general synthesis of arylindoles and (1-arylvinyl)carbazoles *via* a one-pot reaction from *N*-tosylhydrazones and 2-nitro-haloarenes and theirpotentialapplication to colon cancer

Tourin Bzeih, Timothée Naret, Ali Hachem, Nada Jaber, Ali Khalaf, Jerome Bignon, Jean-Daniel Brion, Mouad Alami,* and Abdallah Hamze*

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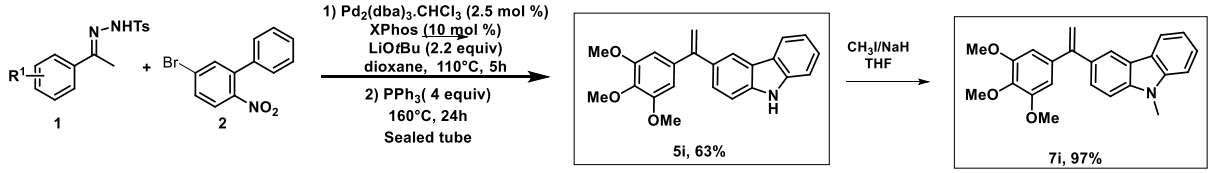
I. Comparative synthesis of compound **7i**by:

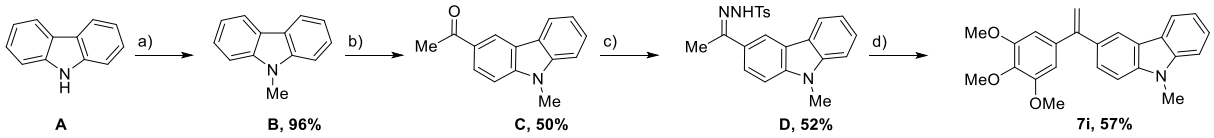
a) the one-pot approach from *N*-tosylhydrazones and *ortho*-nitro-haloarenes, followed by reduction.



- **Overall yield = 61%**
- **Access to the free amine carbazole**

b) functionalization of carbazole and coupling with *N*-tosylhydrazones.

For comparison, compound **7i** was prepared from commercial carbazole (Scheme 1, SI). After methylation of the free amine, Friedel-Craft acylation which constitutes the limiting step leads to the corresponding (carbzol-3-yl)ethanone. This latter was converted to hydrazone and then, the coupling with 5-iodo-3,4,5-trimethoxybenzene afforded compound **7i** in a 14% overall yield.



- **Overall yield = 14%**
- **Difficulty to access to the free amine carbazole**

Scheme 1**.** a) NaH, CH_3I, DMF, 0°C to RT (96%); b) AcCl, $AlCl_3$, DCM, RT to reflux, 2h (50%); c) $TsNHNH_2$, APTS cat., MeOH, reflux, 4h (52%); 5-iodo-1,2,3-trimethoxybenzene, $Pd_2(dba)_3.CHCl_3$, XPhos, LiO*t*Bu, dioxane, sealed tube, 100°C, 3h (57%).

II. General methods

Melting points (mp) were recorded on a Büchi B-450 apparatus and were uncorrected. NMR spectra were performed on a Bruker AMX 200 (^{1}H, 200 MHz; ^{13}C, 50 MHz; ^{19}F, 88 MHz), Bruker AVANCE 300 or Bruker AVANCE 400 (^{1}H, 300 MHz or 400 MHz; ^{13}C, 75 MHz or 100 MHz). Solvent peaks were used as reference values with $CDCl_3$ at 7.26 ppm for ^{1}H NMR and 77.16 ppm for ^{13}C NMR, with DMSO at 2.50 ppm for ^{1}H NMR and 39.52 ppm for ^{13}C NMR,

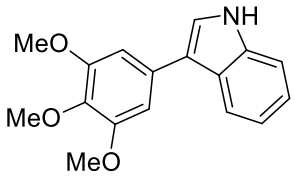
with CD_3CN at 1.94 ppm for ^1H NMR and 1.32 and 118.26 ppm for ^{13}C NMR, and with $(CD_3)_2CO$ at 2.05 ppm for ^1H NMR and 29.84 and 206.26 ppm for ^{13}C NMR. Chemical shifts δ are given in ppm, and the following abbreviations are used: singlet (s), doublet (d), doublet of doublet (dd), triplet (t), quadruplet (q) and multiplet (m). Infrared spectra (IR) were measured on a Bruker Vector 22 spectrophotometer and were recorded in film (film, cm^{-1}). High resolution mass spectra were recorded on a MicrotofQ Bruker Daltonics. Reaction courses and product mixtures were routinely monitored by TLC on silica gel (precoated F254 Merck plates), and compounds were visualized under a UVP Mineralight UVGL-58 lamp (254 nm) and with phosphomolybdic acid/Δ, or vanillin/Δ. Flash chromatography was performed using silica gel 60 (40−63 mm, 230−400 mesh) at medium pressure (200 mbar). Dioxane was distilled over CaH_2. Others solvents were used as received. *N*-Tosylhydrazones were prepared according to literature procedure. $Pd_2(dba)_3.CHCl_3$ was prepared according to literature procedure (*Organometal. Chem.* **1974**, *65*, 253).XPhos was purchased from Sigma-Aldrich. Others reagent were purchased from Sigma-Aldrich, Alfa Aesar and Acros. All products reported showed ^1H and ^{13}C NMR spectra in agreement with the assigned structures.

III. General procedure for one-pot synthesis of indoles and carbazoles

A 5 mLsealed tube under argon atmosphere was charged with *N*-tosylhydrazone (0.5 mmol, 1.0eq), 1-bromo-2-nitroarene (0.5 mmol, 1.0eq), $Pd_2dba_3{\cdot}CHCl_3$ (5 mol %), and XPhos (10 mol %). Then dioxane (2mL) was added via syringe and the mixture was stirred at room temperature for 1 min before the addition of LiO-*t*-Bu (1.1 mmol, 2.2 eq). Then the flask was put into a preheated oil bath (110 ^oC) and stirred. After 5h, PPh_3 (2 mmol, 4.0eq) was added to the same reaction mixture which was stirred at 160 $^\circ C$ for 24-30 h. The crude reaction mixture was allowed to cool to room temperature. EtOAc was added to the mixture, which was filtered through Celite®. The solvents were evaporated under reduced pressure, and the crude residue was purified by column chromatography on silica gel.

IV. Product characterizations

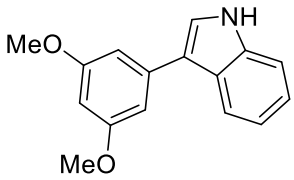
3-(3,4,5-trimethoxyphenyl)-1H-indole (4a)



Column chromatography on silica gel afforded 123 mg of the desired indole **4a** (0.44 mmol, yield 87%), white solid, m.p.: 140-141 °C. TLC: Rf= 0.15 (cyclohexane/EtOAc 8/2). IR (film, cm^{-1}):2936, 2834, 2360, 1735, 1585, 1547, 1502, 1459, 1409, 1362, 1335, 1285, 1237, 1222, 1175, 1123, 1098, 1045. ^1H NMR (300 MHz, $CDCl_3$) δ (ppm) 8.55(s, 1H), 7.95 (d, *J*=7.8 Hz,

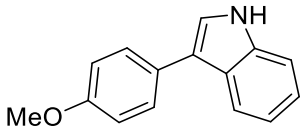
1H), 7.45 (d, *J* = 7.8 Hz, 1H), 7.35 (s, 1H), 7.32-7.19 (m, 2H), 6.92 (s, 2H); 3.96(s, 9H). ^{13}C NMR (75 MHz, CDCl3) δ (ppm) 153.7 (3C), 136.8 (C), 131.5 (C), 125.8 (C), 122.6 (CH), 121.8 (CH), 120.5 (CH), 119.8 (CH), 118.6 (C), 111.6 (CH), 105.0 (2CH), 60.8 (CH_3), 56.3 ($2CH_3$). HRMS (ESI): for $C_{17}H_{17}NO_3Na$ $(M+Na)^+$: *m/z* calcd 306.1106, found 306.1105.

3-(3,5-dimethoxyphenyl)-1H-indole (4b)



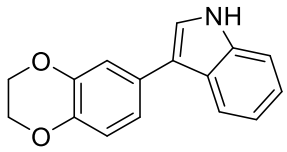
Column chromatography on silica gel afforded 117 mg of the desired indole **4b** (0.46 mmol, yield 92%). Yellowish-brown oil. TLC: Rf= 0.43 (cyclohexane/EtOAc 8/2). IR (film, cm^{-1}):2960, 2926, 2361, 2340, 1605,1590, 1527, 1454, 1424, 1351, 1278, 1205, 1157, 1065, 1049, 909.^{1}H NMR (300 MHz, $CDCl_3$)δ (ppm) 8.19 (s, 1H), 7.90 (d, *J* = 7.6 Hz, 1H), 7.33(d, *J* = 7.5 Hz 1H), 7.26 (d, *J* = 2.4 Hz, 1H), 7.22 – 7.09 (m, 2H), 6.78 (d, *J* = 2.1 Hz, 2H), 6.38 (t, *J* = 2.1 Hz, 1H), 3.82 (s, 6H). ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm) 161.2 (2C), 137.6 (C), 136.8 (C), 125.8 (C), 122.6 (CH), 122.2 (CH), 120.5 (CH), 120.0 (CH), 118.3 (C), 111.6 (CH), 106.8 (2CH), 98.3 (CH), 55.5 ($2CH_3$). HRMS (ESI): for $C_{16}H_{16}NO_2$ $(M+H)^+$: *m/z* calcd 254.1181, found 254.1177.

3-(4-methoxyphenyl)-1H-indole (4c)



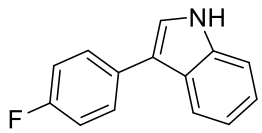
Column chromatography on silica gel afforded 84 mg of the desired indole **4c** (0.38 mmol, yield 75%). Off-white solid, m.p.= 133-135°C. TLC: Rf= 0.43 (cyclohexane/EtOAc 8/2). IR (film, cm^{-1}):3403, 2835, 1612, 1549, 1502, 1456, 1408, 1332, 1303, 1281, 1246, 1179, 1110, 1032. ^{1}H NMR (300 MHz, $CDCl_3$)δ (ppm) 8.18 (s, 1H), 7.92 (d, *J* = 7.8 Hz, 1H), 7.61 (d, *J* = 8.3 Hz, 2H), 7.42 (d, *J* = 8.1 Hz, 1H), 7.29 (d, *J* = 2.4 Hz, 1H), 7.3– 7.17 (m, 2H), 7.02 (d, *J* = 8.3 Hz, 2H), 3.88 (s, 3H).^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm) 158.2 (C), 136.7 (C), 128.8 (2CH), 128.3 (C), 126.1 (C), 122.4 (CH), 121.3 (CH), 120.3 (CH), 119.9 (CH), 118.2 (C), 114.4 (2CH), 111.5 (CH), 55.5 (CH_3). HRMS (ESI): for $C_{15}H_{14}NO$ $(M+H)^+$: *m/z* calcd 224.1075, found 224.1075.

3-(2,3-dihydrobenzo[b][1,4]dioxin-6-yl)-1H-indole (4d)



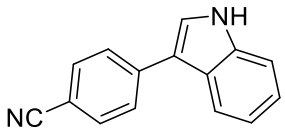
Column chromatography on silica gel afforded 92 mg of the desired indole **4d** (0.365 mmol, yield 73%). Light brown solid, m.p.= 101-103°C. TLC: Rf= 0.46 (cyclohexane/EtOAc 8/2). IR (film, cm^{-1}):3407, 2977, 2927, 2874, 2360, 1617, 1586, 1552, 1500, 1456, 1411, 1348, 1330, 1317, 1298, 1281, 1260, 1244, 1228, 1189, 1124, 1096, 1067, 1048, 1014. ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm) 8.10 (s, 1H), 8.07 (d, *J* = 6.7 Hz, 1H), 7.41 – 7.34 (m, 3H), 7.32 (dd, *J* = 7.2, 2.0 Hz, 1H), 7.28 (dd, *J* = 8.3, 2.0 Hz, 1H), 7.23 (d, *J* = 2.2 Hz, 1H), 7.10 (d, *J* = 8.3 Hz, 1H), 4.34 (s, 4H).^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm)143.8 (C), 142.1 (C), 136.7 (2C), 129.3 (C), 125.8 (C), 122.4 (CH), 121.5 (CH), 120.8 (CH), 120.2 (CH), 119.8 (CH), 117.6 (CH), 116.2 (CH), 111.5 (CH), 64.6 (CH_2), 64.5 (CH_2). HRMS (ESI): for $C_{16}H_{14}NO_2$ $(M+H)^+$: *m/z* calcd 252.1025, found 252. 1020.

3-(4-fluorophenyl)-1H-indole (4e)



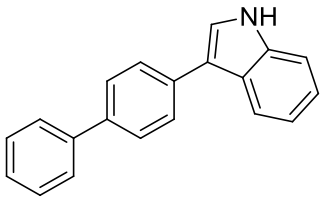
Column chromatography on silica gel afforded 85 mg of the desired indole **4e** (0.4 mmol, yield 80%). Off-white solid, m.p.= 102-103°C. TLC: Rf= 0.56 (cyclohexane/EtOAc 8/2). IR (film, cm^{-1}): 3407, 3059, 2926, 2360, 1595, 1551, 1500, 1456, 1424, 1403, 1331, 1296. 1258, 1236, 1216, 1157, 1096, 1014.^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm) 8.21 (s, 1H), 7.90 (d, *J* = 7.2 Hz, 1H), 7.69-7.59 (m, 2H), 7.45 (d, *J* = 7.6 Hz, 1H), 7.32 (s, 1H), 7.30-7.20 (m, 2H), 7.20-7.12 (m, 2H). ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm) 161.6 (d, *J* = 244.7 Hz, CF), 136.7 (C), 131.7 (d, *J* = 3.0 Hz, C), 129.1 (d, *J* = 7.7 Hz, 2CH) 125.9 (C), 122.7 (CH), 121.7 (CH), 120.5 (CH), 119.7 (CH), 117.6 (C), 115.7 (d, *J* = 21.3 Hz, 2CH), 111.6 (CH). ^{19}F NMR (188 MHz, $CDCl_3$) δ (ppm) -115.1 (s). HRMS (ESI): for $C_{14}H_{11}NF$ $(M+H)^+$: *m/z* calcd 212.0876, found 212.0872.

4-(1H-indol-3-yl)benzonitrile (4f)



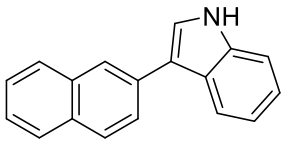
Column chromatography on silica gel afforded 87 mg of the desired indole **4f** (0.4 mmol, yield 80%). White-yellowish solid, m.p.= 168-169°C. TLC: Rf= 0.38 (cyclohexane/EtOAc 8/2). IR (film, cm^{-1}):3357, 2963, 2927, 2854, 2362, 2224, 1604, 1554, 1540, 1491, 1430, 1407, 1335, 1261, 1239, 1179, 1114, 1016, 961. ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm) 8.46 (s, 1H), 7.91 (d, *J* = 7.7 Hz, 1H), 7.76 (d, *J* = 8.2 Hz, 2H), 7.69 (d, *J* = 8.5 Hz, 2H), 7.47-7.44 (m, 2H), 7.31 – 7.21 (m, 2H). ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm) 140.8 (C), 136.9 (C), 132.7 (2CH), 127.5 (2CH), 125.2 (C), 123.3 (CH), 123.1 (CH), 121.2 (CH), 119.6 (CH), 116.8 (C), 111.9 (CH), 108.9 (C). HRMS (ESI): for $C_{15}H_{11}N_2$ $(M+H)^+$: *m/z* calcd 219.0922, found 219.0915.

3-([1,1'-biphenyl]-4-yl)-1H-indole (4g)



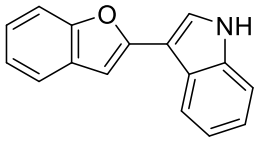
Column chromatography on silica gel afforded 123 mg of the desired indole **4g** (0.455 mmol, yield 91%). Off-white solid,m.p.= 181-183°C. TLC: Rf= 0.6 (cyclohexane/ Ethyl acetate 8/2). IR (film, cm^{-1}): 3429, 3057. 3029, 1485, 1456, 1425, 1403, 1256, 1236, 1119.^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm) 8.15 (s, 1H), 7.93 (d, *J* = 7.5 Hz, 1H), 7.69(d, *J*= 8.3 Hz, 2H), 7.64-7.58 (m, 4H), 7.42-7.32 (m, 4H), 7.30 (d, *J* = 7.2 Hz, 1H), 7.24 – 7.11 (m, 2H).^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm) 141.2 (C), 138.9 (C), 136.9 (C), 134.8 (C), 128.9 (2CH), 127.9 (2CH), 127.6 (2CH), 127.2 (CH), 127.1 (2CH), 125.9 (C), 122.6 (CH), 122.0 (CH), 120.5 (CH), 120.0 (CH), 118.0 (C), 111.6 (CH). HRMS (ESI): for $C_{20}H_{16}N$ $(M+H)^+$: *m/z* calcd 270.1283, found 270.1275.

3-(naphthalen-2-yl)-1H-indole (4h)



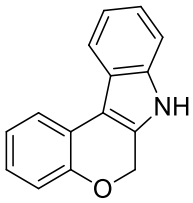
Column chromatography on silica gel afforded 103 mg of the desired indole **4h** (0.425 mmol, yield 85%). Light brown solid, m.p.= 139-140°C. TLC: Rf= 0.41 (cyclohexane/EtOAc 8/2). IR (film, cm^{-1}): 3423, 3393, 3056, 1626, 1596, 1541, 1455, 1416, 1336, 1264, 1238, 1199, 1130, 1112, 1015. ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm) 8.26 (s, 1H), 8.16 (s, 1H), 8.09 (d, *J* = 7.3 Hz, 1H), 7.95 -7.81(m, 4H), 7.52-7.45 (m, 4H), 7.34 – 7.23 (m, 2H). ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm) 136.9 (C), 134.1 (C), 133.2 (C), 132.2 (C), 128.4 (CH), 127.9 (CH), 127.8 (CH), 126.6 (CH), 126.3 (CH), 126.0 (C), 125.4 (2CH), 122.7 (CH), 122.3 (CH), 120.6 (CH), 120.1 (CH), 118.4 (C), 111.6 (CH). HRMS (ESI): for $C_{18}H_{14}N$ $(M+H)^+$: *m/z* calcd 244.1126, found 244.1121.

3-(benzofuran-2-yl)-1H-indole (4i)



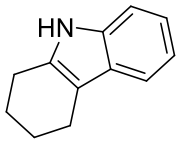
Column chromatography on silica gel afforded 64 mg of the desired indole **4i** (0.275 mmol, yield 55%). White solid, m.p.= 165-166 °C. TLC: Rf= 0.34 (cyclohexane/EtOAc 8/2). IR (film, cm^{-1}): 3405, 3056, 2923, 2853, 2360, 2341, 1626, 1611, 1453, 1426, 1360, 1334, 1308, 1251, 1172, 1102, 1011. ^{1}H NMR (300 MHz, CD_3CN) δ (ppm) 9.55 (s, 1H), 7.90 (dd, *J* = 6.1, 2.3 Hz, 1H), 7.67 (d, *J* = 2.7 Hz, 1H), 7.47 – 7.43 (m, 1H), 7.41 – 7.36 (m, 2H), 7.14 – 7.07 (m, 4H), 6.86 (d, *J* = 0.7 Hz, 1H). ^{13}C NMR (75 MHz, CD_3CN) δ (ppm) 154.7 (C), 154.4 (C), 137.8 (C), 130.8 (C), 125.2 (C), 125.0 (CH), 124.2 (CH), 123.8 (CH), 123.6 (CH), 121.6 (CH), 121.1 (CH), 120.8 (CH), 113.0 (CH), 111.4 (CH), 108.1 (C), 99.9 (CH). HRMS (ESI): for $C_{16}H_{12}NO$ $(M+H)^+$: *m/z* calcd 234.0919, found 234.0912.

6,11-dihydrochromeno[4,3-b]indole (4j)



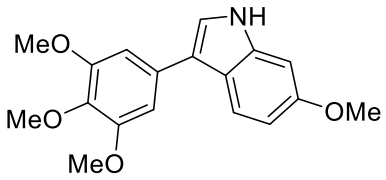
Column chromatography on silica gel afforded 47 mg of the desired indole **4j** (0.21 mmol, yield 42%). Yellowish oil. TLC: Rf= 0.16 (cyclohexane/EtOAc 9/1). IR (film, cm^{-1}): 3399, 3071, 2360, 1560, 1504, 1455, 1391, 1365, 1334, 1277, 1254, 1223, 1195, 1150, 1104, 1034, 1012, 928. ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm) 8.05 (s, 1H), 8.03 – 7.96 (m, 1H), 7.82 – 7.77 (m, 1H), 7.45 – 7.39 (m, 1H), 7.29 – 7.25 (m, 2H), 7.11 – 7.08 (m, 2H), 7.02 – 6.98 (m, 1H), 5.48 (s, 2H).^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm) 151.4(C), 136.8 (C), 130.1 (C), 126.1 (CH), 124.7 (C), 124.1(C), 122.8 (CH), 122.5 (CH), 122.3 (CH), 121.2 (CH), 119.8 (CH), 116.4 (CH), 111.7 (CH), 107.2 (C), 63.9(CH_2). HRMS (ESI): for $C_{15}H_{12}NO$ $(M+H)^+$: *m/z* calcd 222.0919, found 222.0921.

2,3,4,9-tetrahydro-1H-carbazole (4k)



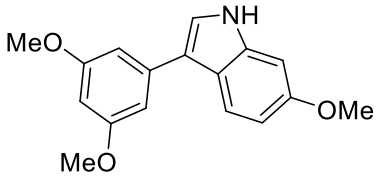
Column chromatography on silica gel afforded 46 mg of the desired indole **4k** (0.27 mmol, yield 54%). Yellowish solid,m.p.=108-110 °C. TLC: Rf= 0.44 (cyclohexane/EtOAc 9/1). IR (film, cm^{-1}):3399, 3051, 2929, 2852, 2360, 1621, 1589, 1469, 1440, 1364, 1326, 1304, 1235, 1010.^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm) 7.64 (s, 1H), 7.47 (d, *J* = 6.9 Hz, 1H), 7.30 – 7.24 (m, 1H), 7.16 – 7.05 (m, 2H), 2.75 – 2.71 (m, 4H), 1.94 – 1.87 (m, 4H). ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm) 135.8 (C), 134.2 (C), 127.9 (C), 121.1 (CH), 119.2 (CH), 117.8 (CH), 110.5 (CH), 110.3 (C), 23.4 ($2CH_2$), 23.3 (CH_2), 21.0 (CH_2). HRMS (ESI): for $C_{12}H_{14}N$ $(M+H)^+$: *m/z* calcd 172.1126, found 172.1123.

6-methoxy-3-(3,4,5-trimethoxyphenyl)-1H-indole (4l)



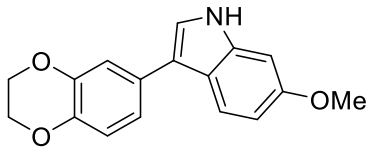
Column chromatography on silica gel afforded 102 mg of the desired indole **4l** (0.325 mmol, yield 65%). White solid, m.p.: 111-113 °C. TLC: Rf= 0.11 (cyclohexane/EtOAc 8/2). IR (film, cm^{-1}):2833, 1629, 1586, 1547, 1502, 1453, 1395, 1363, 1337, 1251, 1234, 1199, 1161, 1124, 1029. 1H NMR (300 MHz, $CDCl_3$) δ (ppm) 8.36 (s, 1H), 7.78 (d, *J*=8.5 Hz, 1H), 7.22 (d, *J* =2.3 Hz, 1H), 6.90 (s, 2H), 6.87 (s, 2H), 3.93 (s, 6H), 3.92 (s, 3H), 3.86 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm) 156.9 (C), 153.7 (3C), 137.6 (C), 131.5 (C), 120.5 (CH), 120.4 (CH), 120.3 (C), 118.6 (C), 110.5 (CH), 104.8 (2CH), 95.0 (CH), 61.1 (CH_3), 56.3 ($2CH_3$), 55.8 (CH_3). HRMS (ESI): for $C_{18}H_{19}NO_4Na$ $(M+Na)^+$: *m/z* calcd 336.1212, found 336.1205.

3-(3,5-dimethoxyphenyl)-6-methoxy-1H-indole (4m)



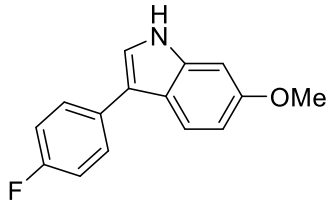
Column chromatography on silica gel afforded 130 mg of the desired indole **4m** (0.46 mmol, yield 92%). White solid, m.p.= 105-107°C. TLC: Rf= 0.23 (cyclohexane/EtOAc 8/2). IR (film, cm^{-1}): 3407, 2998, 2835, 1631, 1605, 1590, 1572, 1546, 1502, 1454, 1425, 1394, 1394, 1360, 1338, 1300, 1252, 1201, 1151, 1113, 1065, 1057, 1029, 1007. ^1H NMR (300 MHz, $CDCl_3$) δ (ppm) 8.52 (s, 1H), 8.23 (d, *J* = 8.6 Hz, 1H), 7.67 (d, *J* = 2.1 Hz, 1H), 7.30-7.25 (m, 2H), 7.23 (d, *J* = 2.2 Hz, 2H), 6.84 (t, *J* = 2.1 Hz, 1H), 4.27 (s, 9H). ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm) 161.2 (3C), 156.8 (C), 137.6 (C), 120.9 (CH), 120.7 (CH), 120.1 (C), 118.5 (C), 110.5 (CH), 106.6 (2CH), 98.3 (CH), 94.9 (CH), 55.8 (CH_3), 55.5 ($2CH_3$). HRMS (ESI): for $C_{17}H_{18}NO_3$ $(M+H)^+$: *m/z* calcd 284.1287, found 284.1283.

3-(2,3-dihydrobenzo[b][1,4]dioxin-6-yl)-6-methoxy-1H-indole (4n)



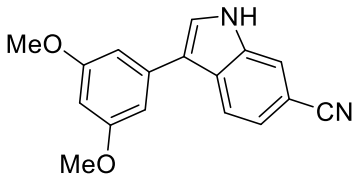
Column chromatography on silica gel afforded 110 mg of the desired indole **4n** (0.4 mmol, yield 78%). White solid, m.p.= 146-147°C. TLC: Rf= 0.19 (cyclohexane/EtOAc 8/2). IR (film, cm^{-1}): 3362, 3347, 2990, 2928, 2883, 2363, 1623, 1552, 1495, 1453, 1435, 1388, 1358, 1324, 1296, 1280, 1260, 1243, 1230, 1201, 1163, 1126, 1105, 1064, 1028. ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm) 8.04 (s, 1H), 7.78 (d, *J* = 8.6 Hz, 1H), 7.17 (s, 2H), 7.14 (dd, *J* = 8.4, 1.3 Hz, 1H), 6.95 (d, *J* = 8.3 Hz, 1H), 6.89 (s, 1H), 6.85 (d, *J* = 8.6 Hz, 1H), 4.31 (s, 4H), 3.86 (s, 3H).^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm) 156.8 (C), 143.8 (C), 142.1 (C), 137.5 (C), 129.3 (C), 120.7 (CH), 120.6 (CH), 120.3 (C), 120.1 (CH), 117.9 (C), 117.6 (CH), 116.1 (CH), 110.3 (CH), 94.9 (CH), 64.6 ($2CH_2$), 55.8 (CH_3). HRMS (ESI): for $C_{17}H_{16}NO_3$ $(M+H)^+$: *m/z* calcd 282.1130, found 282.1127.

3-(4-fluorophenyl)-6-methoxy-1H-indole (4o)



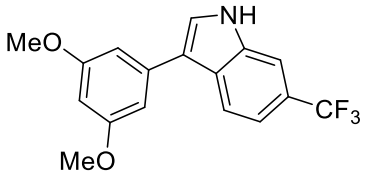
Column chromatography on silica gel afforded 98 mg of the desired indole **4o** (0.41 mmol, yield 82%). Light brown solid, m.p.= 100-101°C. TLC: Rf= 0.3 (cyclohexane/EtOAc 8/2). IR (film, cm^{-1}): 3414, 3383, 2927, 1625, 1546, 1499, 1455, 1390, 1355, 1329, 1306, 1281, 1265, 1247, 1221, 1198, 1164, 1111, 1024. ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm) 8.08 (s, 1H), 7.78 (d, *J* = 8.6 Hz, 1H), 7.68 – 7.56 (m, 2H), 7.24 – 7.10 (m, 3H), 6.97 – 6.83 (m, 2H), 3.87 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm) 161.6 (d, *J* = 244.5 Hz, CF), 156.8 (C), 152.6 (C), 137.5 (C), 131.7 (C), 128.8 (d, *J* = 7.7 Hz, 2CH), 120.5 (CH), 120.3 (CH), 117.4 (C), 115.7 (d, *J* = 21.3 Hz, 2CH), 110.5 (CH), 94.9 (CH), 55.8 (CH_3).^{19}F NMR (188 MHz, $CDCl_3$) δ (ppm) -115.2 (s). HRMS (ESI): for $C_{15}H_{13}NOF$ $(M+H)^+$: *m/z* calcd 242.0981, found 242.0975.

3-(3,5-dimethoxyphenyl)-1H-indole-6-carbonitrile (4p)



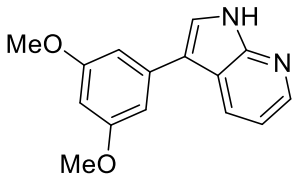
Column chromatography on silica gel afforded 75mg of the desired indole **4p** (0.27 mmol, yield 54%). Off-white solid, m.p.= 172-173 °C. TLC: Rf= 0.28 (cyclohexane/EtOAc 8/2). IR (film, cm^{-1}): 2959, 2926, 2854, 2219, 1725, 1606, 1593, 1459, 1361, 1340, 1287, 1205, 1156, 1121, 1070, 1012. ^{1}H NMR (300 MHz, CD_3CN) δ (ppm) 9.76 (s, 1H), 7.85 (d, *J* = 8.3 Hz, 1H), 7.74 (s, 1H), 7.60 (s, 1H), 7.24 (d, *J* = 9.1 Hz, 1H), 6.65 (s, 2H), 6.30 (s, 1H), 3.69 (s, 6H).^{13}C NMR (75 MHz, CD_3CN) δ (ppm) 162.3 (2C), 137.5 (C), 136.6 (C), 129.3 (C), 128.2 (CH), 123.6 (CH), 121.4 (CH), 121.2 (C), 118.6 (C), 117.8 (CH), 106.3 (2CH), 106.0 (C), 99.3 (CH), 56.0 ($2CH_3$). HRMS (ESI): for $C_{17}H_{15}N_2O_2$ $(M+H)^+$: *m/z* calcd 279.1134, found 279.1141.

3-(3,5-dimethoxyphenyl)-6-(trifluoromethyl)-1H-indole (4q)



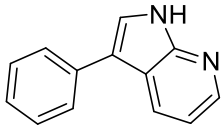
Column chromatography on silica gel afforded 112 mg of the desired indole **4q** (0.35 mmol, yield 70%). Off-white solid, m.p.= 151-153°C. TLC: Rf= 0.33 (cyclohexane/EtOAc 8/2). IR (film, cm^{-1}): 3344, 2925, 1724, 1609, 1593, 1512, 1457, 1430, 1333, 1302, 1266, 1223, 1204, 1154, 1145, 1113, 1084, 1053, 1007. ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm) 8.45 (s, 1H), 8.02 (d, *J* = 8.2 Hz, 1H), 7.71 (s, 1H), 7.51 (s, 1H), 7.43 (d, *J* = 8.6 Hz, 1H), 6.80 (s, 2H), 6.47 (s, 1H), 3.87 (s, 6H). ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm) 161.3 (2C), 136.7 (C), 135.6 (C), 128.1 (C), 124.6 (CH), 124.0 (q, *J*= 153.8 Hz, C), 120.4 (CH), 119.8 (C), 118.9 (C), 117.6 (d, *J*= 3.0 Hz, CH), 109.14 (d, *J*= 3.8 Hz, CH), 106.9 (2CH), 98.6 (CH), 55.6 ($2CH_3$). ^{19}F NMR (188 MHz, $CDCl_3$) δ (ppm) -58.7 (s). HRMS (ESI): for $C_{17}H_{15}NO_2F_3$ $(M+H)^+$: *m/z* calcd 322.1055, found 322.1058.

3-(3,5-dimethoxyphenyl)-1H-pyrrolo[2,3-b]pyridine (4r)



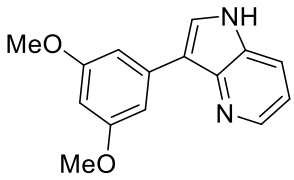
Column chromatography on silica gel afforded 64 mg of the desired indole **4r** (0.25 mmol, yield 50%). Light brown solid, m.p.= 156-158°C. TLC: Rf= 0.42 (cyclohexane/EtOAc 5/5). IR (film, cm^{-1}): 2959, 2925, 2854, 2359, 1729, 1596, 1538, 1461, 1356, 1283, 1204, 1155, 1110, 1068, 1012. ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm) 11.29 (s, 1H), 8.41 (s, 1H), 8.30 (d, *J* = 7.4 Hz, 1H), 7.59 (s, 1H), 7.19 (s, 1H), 6.82 (d, *J* = 2.2 Hz, 2H), 6.45 (t, *J* = 2.2 Hz, 1H), 3.87 (s, 6H). ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm) 161.4 (2C), 149.3 (C), 142.9 (CH), 137.1 (C), 128.7 (CH), 122.8 (CH), 119.0 (C), 116.4 (CH), 113.0 (C), 106.5 (2CH), 98.4 (CH), 55.5 ($2CH_3$). HRMS (ESI): for $C_{15}H_{15}N_2O_2$ $(M+H)^+$: *m/z* calcd 255.1134, found 255.1128.

3-phenyl-1H-pyrrolo[2,3-b]pyridine (4s)



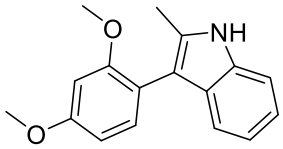
Column chromatography on silica gel afforded 53 mg of the desired indole **4s** (0.275 mmol, yield 55%). White solid, m.p.= 194-196ºC. TLC: Rf= 0.23 (cyclohexane/EtOAc 7/3). IR (film, cm^{-1}): 2961, 2923, 2852, 2360, 1736, 1601, 1536, 1495, 1463, 1437, 1417, 1260, 1202, 1161, 1075, 1029, 1015. ^{1}H NMR (300 MHz, DMSO) δ (ppm) 11.88 (s, 1H), 8.25 (d, *J* = 6.3 Hz, 2H), 7.83 (d, *J* = 1.8 Hz, 1H), 7.69 (d, *J* = 7.8 Hz, 2H), 7.41 (t, *J* = 7.6 Hz, 2H), 7.22 (t, *J* = 7.3 Hz, 1H), 7.15 – 7.09 (m, 1H).^{13}C NMR (75 MHz, DMSO) δ (ppm) 149.1 (C), 142.9 (CH), 135.1 (C), 128.9 (2CH), 127.4 (CH), 126.2 (2CH), 12.6 (CH), 123.7 (CH), 117.3 (C), 116.0 (CH), 114.3(C). HRMS (ESI): for $C_{13}H_{11}N_2$ $(M+H)^+$: *m/z* calcd 195.0922, found 195.0918.

3-(3,5-dimethoxyphenyl)-1H-pyrrolo[3,2-b]pyridine (4t)



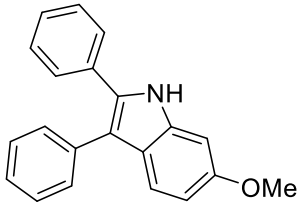
Column chromatography on silica gel afforded 58 mg of the desired indole **4t** (0.23 mmol, yield 46%). White solid, m.p.= 218-220ºC. TLC: Rf= 0.5 (cyclohexane/EtOAc 5/5). IR (film, cm^{-1}): 3114, 2942, 2814, 2360, 1606, 1587, 1451, 1409, 1354, 1333, 1282, 1246, 1204, 1154, 1124, 1106, 1062, 1020.^{1}H NMR (300 MHz, DMSO-d_6) δ (ppm) 11.57 (s, 1H), 8.44 (d, *J* = 4.0 Hz, 1H), 8.20 (d, *J* = 2.5 Hz, 1H), 7.81 (d, *J* = 8.0 Hz, 1H), 7.53 (s, 2H), 7.16 (dd, *J* = 8.1, 4.5 Hz, 1H), 6.35 (s, 1H), 3.80 (s, 6H). ^{13}C NMR (300 MHz, DMSO-d_6) δ (ppm) 160.5 (2C), 143.5 (C), 142.7 (CH), 136.5 (C), 129.5 (C), 127.1(CH), 118.9 (CH), 116.5 (CH), 114.0 (C), 104.1(2CH), 97.2 (CH), 55.1 ($2CH_3$). HRMS (ESI): for $C_{15}H_{15}N_2O_2$ $(M+H)^+$: *m/z* calcd 255.1134, found 255.1128.

3-(2,4-dimethoxyphenyl)-2-methyl-1H-indole (4u)



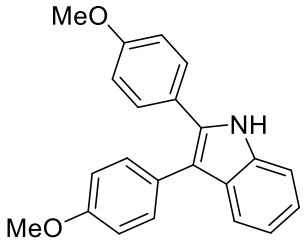
Column chromatography on silica gel afforded 87 mg of the desired indole **4u** (0.325 mmol, yield 65%). Off-white solid, m.p.= 198-200°C. TLC: Rf= 0.42 (cyclohexane/EtOAc 8/2). IR (film, cm^{-1}): 3385, 2958, 1611, 1563, 1502, 1461, 1437, 1414, 1332, 1302, 1278, 1258, 1209, 1186, 1157, 1136, 1049, 1032. ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm) 7.87 (s, 1H), 7.35 (d, *J* = 7.6 Hz, 1H), 7.24 (d, *J* = 2.8 Hz, 1H), 7.21 (d, *J* = 2.3 Hz, 1H),7.08 (t, *J* = 7.2 Hz, 1H), 7.01 (t, *J* = 7.4 Hz, 1H), 6.59 – 6.53 (m, 2H), 3.84 (s, 3H), 3.73 (s, 3H), 2.31 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm) 159.9 (C), 158.4 (C), 135.3 (C), 132.6 (CH), 132.5 (C), 128.8 (C), 128.0 (C), 121.1 (CH), 119.6 (CH), 119.4 (CH), 116.6 (C), 110.3 (CH), 104.4 (CH), 99.1 (CH), 55.5 ($2CH_3$), 12.9 (CH_3). HRMS (ESI): for $C_{17}H_{18}NO_2$ $(M+H)^+$: *m/z* calcd 268.1338, found 268.1330.

6-methoxy-2,3-diphenyl-1H-indole (4v)



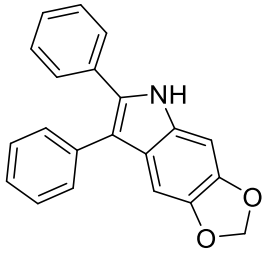
Column chromatography on silica gel afforded 116 mg of the desired indole **4v** (0.385 mmol, yield 77%). White solid,m.p.= 207-208°C. TLC: Rf= 0.45 (cyclohexane/EtOAc 8/2). IR (film, cm^{-1}): 3336, 2959, 2923, 2853, 1736, 1622, 1603, 1556, 1499, 1459, 1436, 1378, 1327, 1260, 1195, 1157, 1120, 1094, 1071, 1017. ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm) 8.13 (s, 1H), 7.56 (d, *J* = 8.7 Hz, 1H), 7.47 – 7.37 (m, 5H), 7.37-7.27 (m, 5H), 6.93 (s, 1H), 6.83 (d, *J* = 8.7 Hz, 1H), 3.88 (s, 3H).^{13}C NMR (75 MHz, $(CD_3)_2CO$) δ (ppm) 158.0 (C), 138.4 (C), 136.9 (C), 134.2 (C), 133.9 (C), 131.0 (2CH), 129.5 (2CH), 129.4 (2CH), 129.0 (2CH), 128.1 (CH), 127.1 (CH), 124.2 (C), 120.7 (CH), 115.2 (C), 111.1 (CH), 95.4 (CH), 55.9 (CH_3).HRMS (ESI): for $C_{21}H_{18}NO$ $(M+H)^+$: *m/z* calcd 300.1388, found 300.1393.

2,3-bis(4-methoxyphenyl)-1H-indole (4w)



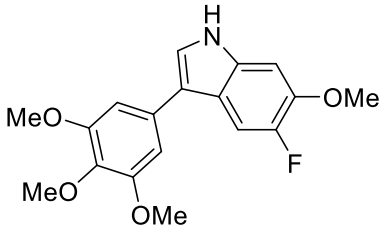
Column chromatography on silica gel afforded 135 mg of the desired indole **4w** (0.41 mmol, yield 82%). White solid, m.p.= 92-93 °C. TLC: Rf= 0.38 (cyclohexane/EtOAc 8/2). IR (film, cm^{-1}): 3405, 2835, 1611, 1556, 1519, 1496, 1455, 1438, 1369, 1330, 1304, 1283, 1242, 1175, 1109, 1031.^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm)8.15 (s, 1H), 7.66 (d, *J* = 7.8 Hz, 1H),7.41 (d, *J* = 8.3 Hz, 1H), 7.36 (d, *J* = 8.6 Hz, 4H), 7.25 – 7.11 (m, 2H), 6.96 (d, *J* = 8.6 Hz, 2H), 6.89 (d, *J* = 8.7 Hz, 2H), 3.86 (s, 3H), 3.82 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ(ppm) 159.3 (C), 158.2 (C), 135.9 (C), 133.9 (C), 131.3 (2CH), 130.1 (C), 129.5 (2CH), 129.18 (C), 127.7 (C), 125.5 (C), 122.4 (CH), 120.4 (CH), 119.6 (CH), 114.3 (2CH), 114.2 (2CH), 110.8 (CH), 55.4 ($2CH_3$). HRMS (ESI): for $C_{22}H_{20}NO_2$ $(M+H)^+$: *m/z* calcd 330.1494, found 330.1496.

6,7-diphenyl-5H-[1,3]dioxolo[4,5-f]indole (4x)



Column chromatography on silica gel afforded 118 mg of the desired indole **4x** (0.375 mmol, yield 75%). White solid, m.p.= 188-189°C. TLC: Rf= 0.49 (cyclohexane/EtOAc 8/2). IR (film, cm^{-1}): 3400, 3043, 1601, 1503, 1464, 1437, 1357, 1336, 1245, 1200, 1163, 1119, 1072, 1039.^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm) 8.10 (s, 1H), 7.41 – 7.37 (m, 6H), 7.35 – 7.27 (m, 4H), 7.06 (s, 1H), 6.90 (s, 1H), 5.96 (s, 2H). ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm) 145.5 (C), 143.7 (C), 135.2 (C), 132.9 (C), 131.0 (C), 130.1 (2CH), 128.8 (CH), 128.7 (2CH), 127.8 (2CH), 127.3 (CH), 126.4 (2CH), 124.5 (C), 123.0 (C), 115.5 (C), 100.8 (CH_2), 98.4 (CH), 91.9 (CH). HRMS (ESI): for $C_{21}H_{16}NO_2$ $(M+H)^+$: *m/z* calcd 314.1181, found 314.1180.

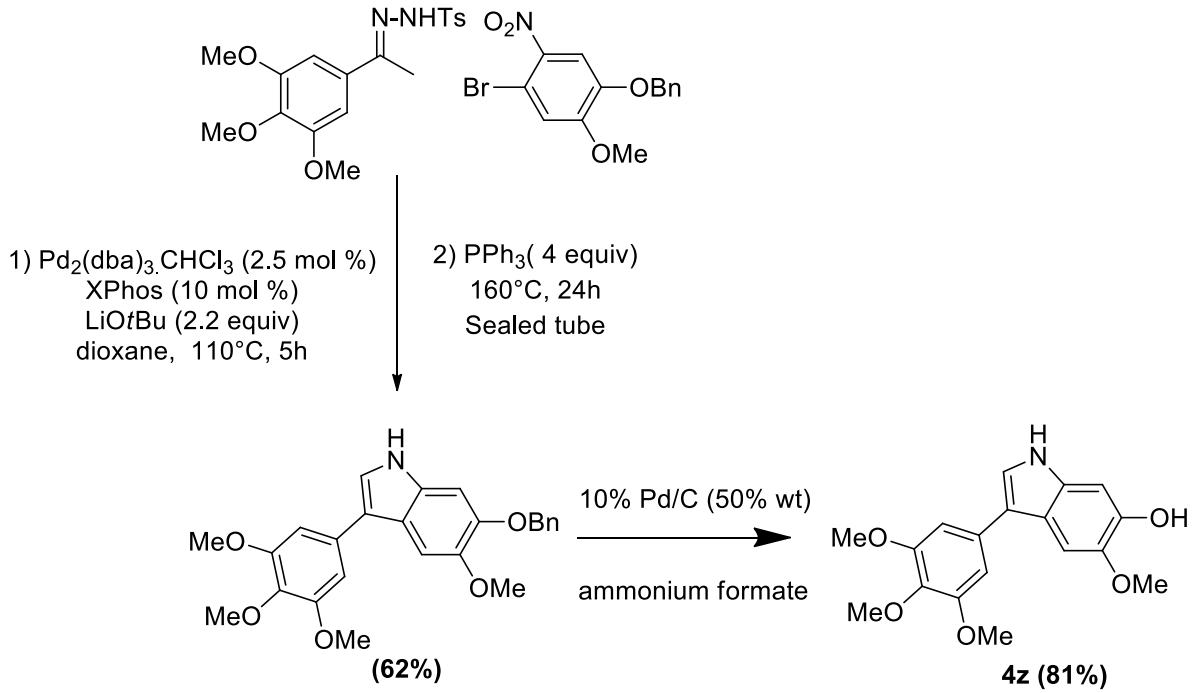
5-fluoro-6-methoxy-3-(3,4,5-trimethoxyphenyl)-1H-indole (4y)



Column chromatography on silica gel afforded 99 mg of the desired indole **4y** (0.3 mmol, yield 60%). White solid, m.p.= 126-127°C.TLC: Rf= 0.15 (cyclohexane/EtOAc 7/3). IR (film, cm^{-1}): 3328, 2926, 2360, 1588, 1552, 1505, 1481, 1462, 1402, 1368, 1324, 1255, 1223, 1199, 1162, 1126, 1027, 1000. ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm) 8.27 (s, 1H), 7.54 (d, *J* = 11.9 Hz, 1H), 7.25 (s, 1H), 6.97 (d, *J* = 7.2 Hz, 1H), 6.79 (s, 2H), 3.92 (s, 9H), 3.90 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm) 153.7 (2C), 149.6 (d, *J*= 234.8 Hz, CF), 145.5 (d, *J* = 14.0 Hz, C), 136.8 (C), 132.7 (C), 131.2 (C), 121.3 (CH), 118.7 (d, *J* = 7.7 Hz, C), 118.6 (d, *J* = 8.8 Hz, C). 105.70 (d, *J* = 21.2 Hz, CH), 104.7 (2CH), 96.1 (CH), 61.1 (CH_3), 56.8 (CH_3), 56.4 ($2CH_3$). ^{19}F NMR (188 MHz, $CDCl_3$) δ (ppm) -143.2 (s). (HRMS (ESI): for $C_{18}H_{19}NO_4F$ $(M+H)^+$: *m/z* calcd 332.1298, found 332.1294.

From 6-(benzyloxy)-5-methoxy-3-(3,4,5-trimethoxyphenyl)-1H-indole

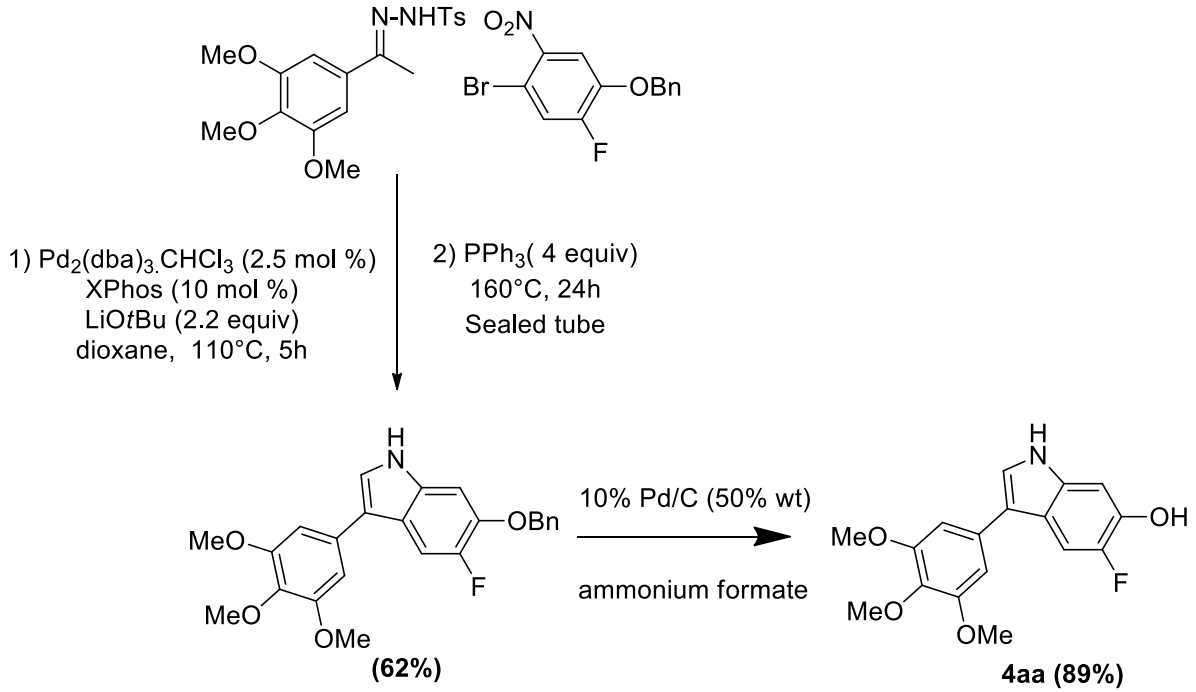
to 5-methoxy-3-(3,4,5-trimethoxyphenyl)-1H-indol-6-ol (4z)



Column chromatography on silica gel afforded 130 mg of 6-(benzyloxy)-5-methoxy-3-(3,4,5-trimethoxyphenyl)-1H-indole (0.31 mmol, yield 62%). TLC: Rf= 0.25 (cyclohexane/EtOAc 7/3).

Then a stirred solution of 6-(benzyloxy)-5-methoxy-3-(3,4,5-trimethoxyphenyl)-1H-indole (0.19 mmol, 80 mg) and ammonium formate (0.95 mmol) in a anhydrous MeOH was degassed and then 10% Pd/C (50% wt) was added under argon. The mixture was stirred at r.t. overnight. The catalyst was filtered through celite® and the filtrate was concentrated under vacuum. The crude residue was purified by column chromatography on silica gel to afford 51 mg of the title compound **4z** as dark red oil (yield 81%). TLC: Rf= 0.28 (cyclohexane/EtOAc 5/5). IR (film, cm^{-1}): 3329, 2960, 2854, 2360, 2341, 1580, 1546, 1505, 1481, 1463, 1411, 1341, 1320, 155, 1238, 1159, 1126, 1001. ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm) 8.17 (s, 1H), 7.30 (t, *J* = 5.7 Hz, 1H), 7.18 (d, *J* = 2.3 Hz, 1H), 6.99 (t, *J* = 5.9 Hz, 1H), 6.83 (t, *J* = 5.9 Hz, 2H), 3.94 (s, 3H), 3.93 (s, 6H), 3.92 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm) 153.7 (3C), 143.7 (C), 143.3 (C), 131.8 (C), 131.5 (C), 120.3 (CH), 118.6 (C), 118.4 (C), 104.9 (2CH), 100.5 (CH), 96.9 (CH), 61.1 (CH_3), 56.6 (CH_3), 56.3 ($2CH_3$). HRMS (ESI): for $C_{18}H_{20}NO_5$ $(M + H)^+$: *m/z* calcd 330.1341, found 330.1341.

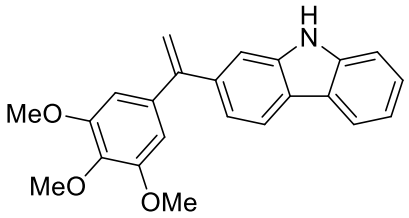
From 6-(benzyloxy)-5-fluoro-3-(3,4,5-trimethoxyphenyl)-1H-indole to 5-fluoro-3-(3,4,5-trimethoxyphenyl)-1H-indol-6-ol (4aa)



Column chromatography on silica gel afforded 126 mg of 6-(benzyloxy)-5-fluoro-3-(3,4,5-trimethoxyphenyl)-1H-indole (0.31 mmol, yield 62%). TLC: Rf= 0.22 (cyclohexane/EtOAc 7/3).

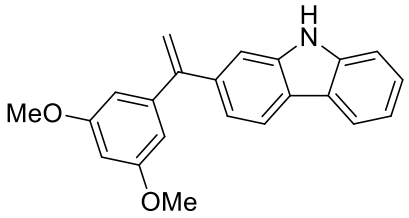
Then a stirred solution of 6-(benzyloxy)-5-fluoro-3-(3,4,5-trimethoxyphenyl)-1H-indole (0.23 mmol, 100 mg) and ammonium formate (1.16 mmol) in anhydrous MeOH was degassed and then 10% Pd/C (50% wt) was added under argon. The mixture was stirred at r.t. overnight. The catalyst was filtered through celite® and the filtrate was concentrated under vacuum. The crude residue was purified by column chromatography on silica gel to afford 66mg of the title compound **4aa** as dark red oil (yield 89%), TLC: Rf= 0.37 (cyclohexane/EtOAc 5/5).IR (film, cm^{-1}): 2961, 2924, 2853, 2360, 1738, 1554, 1506, 1469, 1412, 1332, 1261, 1235, 1160, 1126, 1102, 1010.^{1}H NMR (400 MHz, $CDCl_3$) δ 8.44 (s, 1H), 7.54 (d, *J* = 11.1 Hz, 1H), 7.25 (s, 1H), 7.03 (d, *J* = 5.6 Hz, 1H), 5.63(s, 1H), 6.80 (s, 2H), 3.92 (s, 9H).^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 153.7 (2C), 148.5 (d, *J* = 229.4 Hz, CF), 141.10 (d, *J* = 17.6 Hz, C), 136.8 (C), 133.2 (C), 131.19 (C), 121.6 (CH), 118.8 (d, *J* = 8.3 Hz, C), 118.4 (d, *J* = 3.0 Hz, C), 104.9 (d, *J* = 26.1 Hz, CH), 104.7 (2CH), 98.8 (CH), 61.1 (CH_3), 56.3 ($2CH_3$). ^{19}F NMR (188 MHz, $CDCl_3$) δ (ppm) -146.8 (s).HRMS (ESI): for $C_{17}H_{17}NO_4F$ $(M+H)^+$: *m/z* calcd 318.1142, found 318.1140.

2-(1-(3,4,5-trimethoxyphenyl)vinyl)-9H-carbazole (5a)



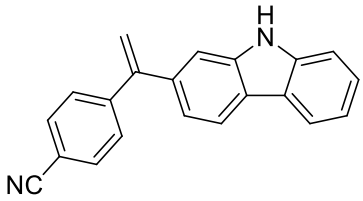
Column chromatography on silica gel afforded 108 mg of the desired carbazole **5a** (0.3 mmol, yield 60%). Brownish solid, m.p.=167-168 °C. TLC: Rf= 0.47 (cyclohexane/EtOAc 8/2). IR (film, cm^{-1}): 3409, 2936, 1610, 1580, 1503, 1461, 1440, 1412, 1347, 1327, 1238, 1175, 1125, 1001.^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm) 8.08 (d, *J* = 7.2 Hz, 2H), 8.03 (d, *J* = 8.1 Hz, 1H), 7.42 (d, *J* = 3.4 Hz, 2H), 7.39 (s, 1H), 7.31 – 7.24 (m, 2H), 6.62 (s, 2H), 5.55 (s, 1H), 5.47 (s, 1H), 3.90 (s, 3H), 3.80 (s, 6H). ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm) 153.0 (2C), 150.9 (C), 140.1 (C), 139.6 (C), 139.3 (C), 138.5 (C), 137.9 (C), 126.1 (CH), 123.2 (C), 120.5 (CH), 120.3 (CH), 120.0 (CH), 119.8 (CH), 114.0 (CH_2), 110.8 (CH), 110.7 (CH), 107.0 (2CH), 61.1 (CH_3), 56.3 ($2CH_3$). HRMS (ESI): for $C_{23}H_{22}NO_3$ $(M+H)^+$: *m/z* calcd 360.1600, found 360.1599.

2-(1-(3,5-dimethoxyphenyl)vinyl)-9H-carbazole (5b)



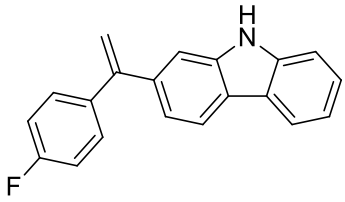
Column chromatography on silica gel afforded 115 mg of the desired carbazole **5b** (0.35 mmol, yield 70%). White solid, m.p.=127-128°C. TLC: Rf= 0.67 (cyclohexane/EtOAc 8/2). IR (film, cm^{-1}): 3406, 3000, 2837, 2359, 1604, 1583, 1458, 1439, 1421, 1351, 1328, 1283, 1239, 1204, 1154, 1064, 1048. ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm) 8.07 (d, *J* = 7.8 Hz, 1H), 8.02 (d, *J* = 7.8 Hz, 1H), 7.98 (s, 1H), 7.41 (d, *J* = 3.7 Hz, 2H), 7.37 (s, 1H), 7.30 – 7.23 (m, 2H), 6.56 (d, *J* = 2.0 Hz, 2H), 6.48 (t, *J* = 2.3 Hz, 1H), 5.56 (s, 1H), 5.50 (s, 1H), 3.77 (s, 6H). ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm) 160.6 (2C), 150.7 (C), 144.4 (C), 140.1 (C), 139.6 (C), 139.2 (C), 126.0 (CH), 123.3 (C), 123.1 (C), 120.5 (CH), 120.2 (CH), 120.0 (CH), 119.7 (CH), 114.5 (CH_2), 110.7 (CH), 110.6 (CH), 106.9 (2CH), 100.1 (CH), 55.5 ($2CH_3$). HRMS (ESI): for $C_{22}H_{20}NO_2$ $(M+H)^+$: *m/z* calcd 330.1494, found 330.1497.

4-(1-(9H-carbazol-2-yl)vinyl)benzonitrile (5c)



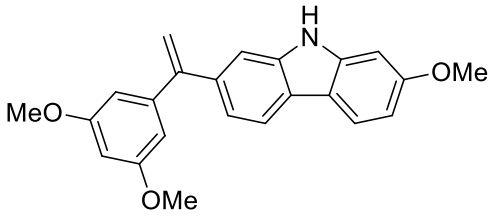
Column chromatography on silica gel afforded 70 mg of the desired carbazole **5c** (0.235 mmol, yield 47%). Off-white solid, m.p.=202-203°C. TLC: Rf= 0.39 (cyclohexane/EtOAc 8/2). IR (film, cm^{-1}): 3407, 2361, 2341, 2227, 1605, 1563, 1492, 1460, 1441, 1399, 1327, 1241, 1205, 1066, 1017, 1000.^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm) 8.09- 8.02 (m, 3H), 7.64 (d, *J* = 8.2 Hz, 2H), 7.50 (d, *J* = 8.2 Hz, 2H), 7.44 (d, *J* = 3.8 Hz, 2H), 7.32 (s, 1H), 7.26 (s, 1H), 7.18 (d, *J* = 8.1 Hz, 1H), 5.68 (s, 1H), 5.58 (s, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm) 149.5 (C), 146.8 (C), 140.1 (C), 139.6 (C), 138.2 (C), 132.2 (2CH), 129.2 (2CH), 126.3 (CH), 123.5 (C), 123.1 (C), 120.6 (CH), 120.3 (CH), 120.1 (CH), 119.9 (CH), 119.1 (C), 116.7 (CH_2), 111.4 (C), 110.8 (CH), 110.5 (CH). HRMS (ESI): for $C_{21}H_{15}N_2$ $(M+H)^+$: *m/z* calcd 295.1235, found 295.1245.

2-(1-(4-fluorophenyl)vinyl)-9H-carbazole (5d)



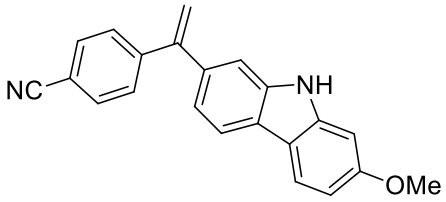
Column chromatography on silica gel afforded 108mg of the desired carbazole **5d** (0.375 mmol, yield 75%). Off-white solid, m.p.=212-213°C. TLC: Rf= 0.48 (cyclohexane/EtOAc 8/2). IR (film, cm^{-1}): 3412, 2363, 1600, 1504, 1460, 1440, 1370, 1328, 1243, 1217, 1156, 1014. ^{1}H NMR (300 MHz, $(CD_3)_2CO$) δ (ppm) 10.32 (s, 1H), 8.12 (t, *J* = 8.0 Hz, 2H), 7.52 (d, *J* = 7.9 Hz, 1H), 7.47 – 7.38 (m, 4H), 7.23 – 7.13 (m, 4H), 5.57 (s, 1H), 5.49 (s, 1H). ^{13}C NMR (75 MHz, $(CD_3)_2CO$) δ (ppm) 162.5 (d, *J* = 244.6 Hz, CF), 150.0 (C), 145.9 (C), 140.6 (C), 140.1 (C), 138.9 (C), 138.4 (C), 130.2 (2CH, d, *J* = 8.5 Hz), 125.7 (CH), 122.9 (C), 120.1 (CH), 119.8 (CH), 119.3 (CH), 119.0 (CH), 114.8 (2CH, d, *J* = 21.8 Hz), 113.5 (CH_2), 110.9 (CH), 110.5 (CH). ^{19}F NMR (188 MHz, $CDCl_3$) δ (ppm) -114.5 (s). HRMS (ESI): for $C_{20}H_{15}NF$ $(M+H)^+$: *m/z* calcd 288.1189, found 288.1183.

2-(1-(3,5-dimethoxyphenyl)vinyl)-6-methoxy-9H-carbazole (5e)



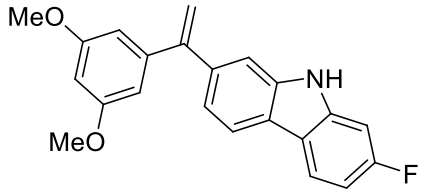
Column chromatography on silica gel afforded 144 mg of the desired carbazole **5e** (0.4 mmol, yield 80%). White solid, m.p.=170-171 °C. TLC: Rf= 0.41 (cyclohexane/EtOAc 8/2). IR (film,cm^{-1}): 3413, 3006, 2361, 1630, 1606, 1582, 1503, 1462, 1441, 1425, 1339, 1325, 1284, 1268, 1239, 1200, 1161, 1109, 1062, 1050, 1032. ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm)7.92 (d, *J* = 4.6 Hz, 1H), 7.90 (d, *J* = 4.3 Hz, 1H), 7.88 (s, 1H), 7.31 (s, 1H), 7.25 (d, *J*= 6.2 Hz, 1H), 6.89 – 6.83 (m, 2H), 6.56 (d, *J* = 2.1 Hz, 2H), 6.48 (t, *J* = 2.1 Hz, 1H), 5.54 (s, 1H), 5.47 (s, 1H), 3.90 (s, 3H), 3.77 (s, 6H). ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm) 160.6 (2C), 159.2 (C), 150.8 (C), 144.5 (C), 141.5 (C), 139.6 (C), 137.9 (C), 123.4 (C), 121.2 (CH), 120.3 (CH), 119.1 (CH), 117.2 (C), 114.2 (CH_2), 110.4 (CH), 108.5 (CH), 106.9 (2CH), 100.1 (CH), 94.8 (CH), 55.8 (CH_3), 55.5 ($2CH_3$). HRMS (ESI): for $C_{23}H_{22}NO_3$ $(M+H)^+$: *m/z* calcd 360.1600, found 360.1602

4-(1-(6-methoxy-9H-carbazol-2-yl)vinyl)benzonitrile (5f)



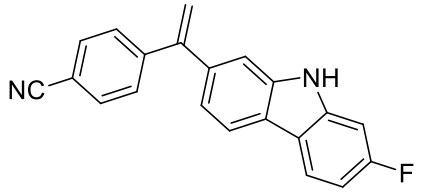
Column chromatography on silica gel afforded 114 mg of the desired carbazole **5f** (0.35 mmol, yield 70%). White solid, m.p.=230-231 °C. TLC: Rf= 0.40 (cyclohexane/EtOAc 8/2). IR (film, cm^{-1}): 3426, 2963, 2924, 2361, 2224, 1613, 1503, 1463, 1431, 1397, 1334, 1306, 1224, 1030. ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm) 7.87 (s, 1H), 7.86 (d, *J* = 8.6 Hz, 1H), 7.57 (d, *J* = 8.4 Hz, 2H), 7.43 (d, *J* = 8.4 Hz, 2H), 7.19 (s, 2H), 7.07 (d, *J* = 7.2 Hz, 1H), 6.84 (s, 1H), 6.80 (d, *J* = 8.1 Hz, 1H), 5.59 (s, 1H), 5.48 (s, 1H), 3.84 (s, 3H). ^{13}C NMR (75 MHz, DMSO-d_6) δ (ppm) 158.7 (C), 148.8 (C), 146.3 (C), 141.7 (C), 139.7 (C), 135.7 (C), 132.3 (2CH), 129.0 (2CH), 122.7 (C), 121.1 (CH), 119.2 (CH), 118.8 (C), 118.7 (CH), 116.4 (CH_2), 115.9 (C), 110.3 (C), 110.1 (CH), 108.1 (CH), 94.5 (CH), 55.3 (CH_3). HRMS (ESI): for $C_{22}H_{17}N_2O$ $(M+H)^+$: *m/z* calcd 325.1341, found 325.1343.

2-(1-(3,5-dimethoxyphenyl)vinyl)-6-fluoro-9H-carbazole (5g)



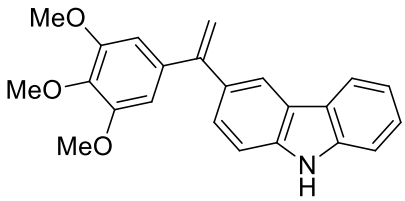
Column chromatography on silica gel afforded 127 mg of the desired carbazole **5g** (0.365 mmol, yield 73%). White solid, m.p.=132-133 °C. TLC: Rf= 0.44 (cyclohexane/EtOAc 8/2). IR (film, cm^{-1}): 3410, 2837, 1635, 1582, 1562, 1500, 1454, 1421, 1357, 1317, 1282, 1266, 1230, 1203, 1155, 1130, 1105, 1063, 1045.^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm) 8.02 – 7.91 (m, 3H), 7.33 (s, 1H), 7.29 (d, *J* = 8.1 Hz, 1H), 7.06 (dd, *J* = 9.5, 2.1 Hz, 1H), 6.97 (td, *J* = 9.1, 2.2 Hz, 1H), 6.57 (d, *J*= 2.2 Hz, 2H), 6.49 (t, *J* = 2.2 Hz, 1H), 5.55 (s, 1H), 5.51 (s, 1H), 3.77 (s, 6H). ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm) 162.1 (d, *J*= 240 Hz, C), 160.7 (2C), 150.6 (C), 144. 3 (C), 140.6 (d, *J*= 12.8 Hz, C), 140.0 (C), 138.9 (C), 122.7 (C), 121.3 (d, *J*= 10.5 Hz, CH), 120.6 (CH), 119.7 (C), 119.6 (CH), 114.6 (CH_2), 110.6 (CH), 107.9 (d, *J*= 24 Hz, CH), 106.9 (2CH), 100.1 (CH), 97.6 (d, *J*= 26. 3 Hz, CH), 55.5 ($2CH_3$). ^{19}F NMR (188 MHz, $CDCl_3$) δ (ppm) -113.4 (s). HRMS (ESI): for $C_{22}H_{19}NO_2F$ $(M+H)^+$: *m/z* calcd 348.1400, found 348.1404.

4-(1-(6-fluoro-9H-carbazol-2-yl)vinyl)benzonitrile (5h)



Column chromatography on silica gel afforded 81 mg of the desired carbazole **5h** (0.26 mmol, yield 52%). White solid, m.p.=214-215 °C. TLC: Rf= 0.52 (cyclohexane/EtOAc 8/2). IR (film, cm^{-1}): 3406, 2358, 2228, 1613, 1564, 1503, 1458, 1433, 1359, 1319, 1271, 1222, 1144, 1105, 1069. ^{1}H NMR (300 MHz, DMSO-d_6) δ (ppm)11.36 (s, 1H), 8.16 – 8.06 (m, 2H), 7.86 (d, *J* = 7.9 Hz, 2H), 7.54 (d, *J* = 8.0 Hz, 2H), 7.33 (s, 1H), 7.27 (dd, *J* = 10.1, 1.8 Hz, 1H), 7.11 (d, *J* = 8.1 Hz, 1H), 7.04 – 6.95 (m, 1H), 5.72 (s, 1H), 5.65 (s, 1H).^{13}C NMR (75 MHz, DMSO-d_6) δ (ppm) 161.3 (d, *J* = 239.1 Hz, C), 148.6 (C), 146.1 (C), 140.9 (d, *J* = 13.0 Hz, C), 140.3 (C), 136.9 (C), 132.3 (2CH), 128.9 (2CH), 122.0 (C), 121.6 (d, *J* = 9.8 Hz, CH), 120.0 (CH), 119.2 (CH), 118.9 (C), 118.8 (C), 117.0 (CH_2), 110.4 (CH), 106.8 (d, *J* = 24.8 Hz, CH), 97.4 (d, *J* = 26.2 Hz, CH). ^{19}F NMR (188 MHz, $CDCl_3$) δ (ppm) -115.1 (s). HRMS (ESI): for $C_{21}H_{14}N_2F$ $(M+H)^+$: *m/z* calcd 313.1141, found 313.1144.

3-(1-(3,4,5-trimethoxyphenyl)vinyl)-9H-carbazole (5i)



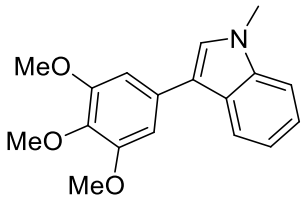
Column chromatography on silica gel afforded 113 mg of the desired carbazole **5i** (0.315 mmol, yield 63%). Yellowish oil. TLC: Rf= 0.39 (cyclohexane/EtOAc 8/2). IR (film, cm^{-1}): 3410, 2936, 1607, 1580, 1504, 1462, 1411, 1345, 1237, 1176, 1125, 1005. ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm) 8.26 (s, 1H), 8.12 – 8.04 (m, 2H), 7.47 – 7.41 (m, 3H), 7.36 (d, *J* = 8.4 Hz, 1H), 7.27 – 7.21 (m, 1H), 6.67 (s, 2H), 5.53 (s, 1H), 5.45 (s, 1H), 3.94 (s, 3H), 3.81 (s, 6H). ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm) 153.0 (2C), 150.9 (C), 140.1 (C), 139.4 (C), 138.3 (C), 137.8 (C), 132.9 (C), 126.7 (CH), 126.1 (CH), 123.4 (C), 123.3 (C), 120.5 (CH), 120.2 (CH), 119.7 (CH), 112.9 (CH_2), 110.9 (CH), 110.3 (CH), 106.9 (2CH), 61.1 (CH_3), 56.2 ($2CH_3$). HRMS (ESI): for $C_{23}H_{22}NO_3$ $(M+H)^+$: *m/z* calcd 360.1600, found 360.1599.

V. General procedure for the methylation reaction

The carbazole or indole (0.3 mmol, 1equiv) was dissolved in freshly distilled THF, and at 0°C NaH (60 % dispersion in oil, 0.75 mmol, 2.5 eq) was added. After 15 min, MeI (0.4 mmol, 1.34 eq) was added slowly and the reaction mixture was allowed to stir at room temperature for 60 min, then it was cooled to 0°C and ammonium chloride solution was added. The mixture was extracted with Et_2O. The combined organic layers were washed with saturated aqueous $NaHCO_3$ and brine. The organic phase was dried on $MgSO_4$, evaporated to dryness and the crude product was purified by column chromatography on silica gel.

VI. N-methylated product characterizations

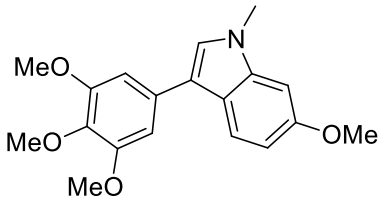
1-methyl-3-(3,4,5-trimethoxyphenyl)-1H-indole (6a)



Column chromatography on silica gel and afforded 82 mg of the desired methylated indole **6a** (0.28 mmol, yield 92%).White solid, m.p.: 117-118 °C. TLC: Rf= 0.27 (cyclohexane/EtOAc 8/2). IR (film, cm^{-1}):2936, 2360, 1582, 1547, 1503, 1449, 1415, 1384, 1332, 1305, 1234, 1158, 1123, 1055, 1006. ^{1}H NMR (300 MHz, CDCl3) δ (ppm) 7.93 (d, *J*=7.9 Hz, 1H), 7.38 (d, *J* = 8.1 Hz, 1H), 7.32 (t, *J* = 7.4 Hz, 1H),7.26 – 7.18 (m, 2H), 6.87 (s, 2H), 3.94 (s, 6H), 3.93 (s, 3H), 3.84 (s, 3H).^{13}C NMR (75 MHz, CDCl3) δ (ppm) 153.7 (3C), 137.6 (C), 131.5 (C), 126.5

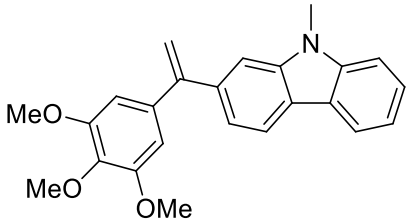
(CH),126.3 (C), 122.2 (CH), 120.1 (CH), 119.8 (CH), 117.0 (C), 109.8 (CH), 104.8(2CH), 61.1 (CH_3), 56.3 ($2CH_3$), 32.9 (CH3). HRMS (ESI): for $C_{18}H_{19}NO_3Na$ $(M+Na)^+$: *m/z* calcd 320.1263, found 320.1264.

6-methoxy-1-methyl-3-(3,4,5-trimethoxyphenyl)-1H-indole (6l)



Column chromatography on silica gel and afforded 89 mg of the desired methylated indole **6l** (0.27 mmol, yield 91%)**.**White solid, m.p.: 135-136 °C. TLC: Rf= 0.18 (cyclohexane/EtOAc 8/2). IR (film, cm^{-1}): 2936, 2828, 2360, 1623, 1602, 1583, 1552, 1505, 1463, 1416, 1391, 1336, 1241, 1199, 1172, 1126, 1091, 1031, 1008. ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm) 7.92 (dd, *J* = 8.7, 0.8 Hz, 1H), 7.25 (d, *J* = 1.2 Hz, 1H), 7.04 – 7.00 (m, 1H), 6.99 (d, *J* = 1.3 Hz, 2H), 6.97 – 6.94 (m, 1H), 4.08 (s, 3H), 4.07 (s, 3H), 4.06 (s, 6H),3.91 (d, *J* = 1.2 Hz, 3H).^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm) 156.7 (C), 153.5 (3C), 138.3 (C), 136.5 (C), 131.5 (C), 125.3 (CH), 120.5 (CH), 116.9 (C), 109.9 (CH), 104.5 (2CH), 93.1 (CH), 61.0 (CH_3), 56.2 ($2CH_3$),55.8 (CH_3), 32.9 (CH_3). HRMS (ESI): for $C_{19}H_{21}NO_4Na$ $(M+Na)^+$: *m/z* calcd 350.1368, found 350.1375.

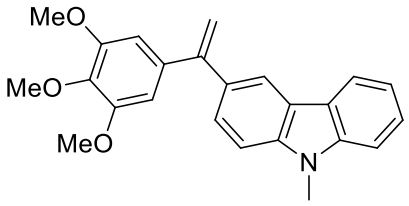
9-methyl-2-(1-(3,4,5-trimethoxyphenyl)vinyl)-9H-carbazole (7a)



Column chromatography on silica gel afforded 109mg of the desired methylated carbazole **7a** (0.29 mmol, yield 98%). Yellowish oil. TLC: Rf= 0.61 (cyclohexane/EtOAc 8/2).IR (film, cm^{-1}): 2936, 2834, 1601, 1578, 1503, 1450, 1411, 1362, 1338, 1322, 1246, 1232, 1180, 1124, 1001. ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm) 8.13 (d, *J* = 7.7 Hz, 1H), 8.09 (d, *J* = 8.1 Hz, 1H), 7.55 – 7.49 (m, 1H), 7.44 (s, 1H), 7.42 (d, *J* = 8.6 Hz, 1H), 7.33 – 7.28 (m, 2H), 6.70 (s, 2H), 5.62 (s, 1H), 5.56 (s, 1H), 3.96 (s, 3H), 3.85 (s, 9H). ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm) 153.0 (3C), 151.1 (C), 141.6 (C), 141.1 (C), 139.2 (C), 137.9 (C), 125.9 (CH), 122.6 (2C), 120.4 (CH), 119.9

(2CH), 119.1 (CH), 114.0 (CH_2), 108.6 (CH), 108.5 (CH), 106.9 (2CH), 61.0 (CH_3), 56.2 ($2CH_3$), 29.2 (CH_3).HRMS (ESI): for $C_{24}H_{24}NO_3$ $(M+H)^+$: *m/z* calcd 374.1756, found 374.1760.

9-methyl-3-(1-(3,4,5-trimethoxyphenyl)vinyl)-9H-carbazole (7i)

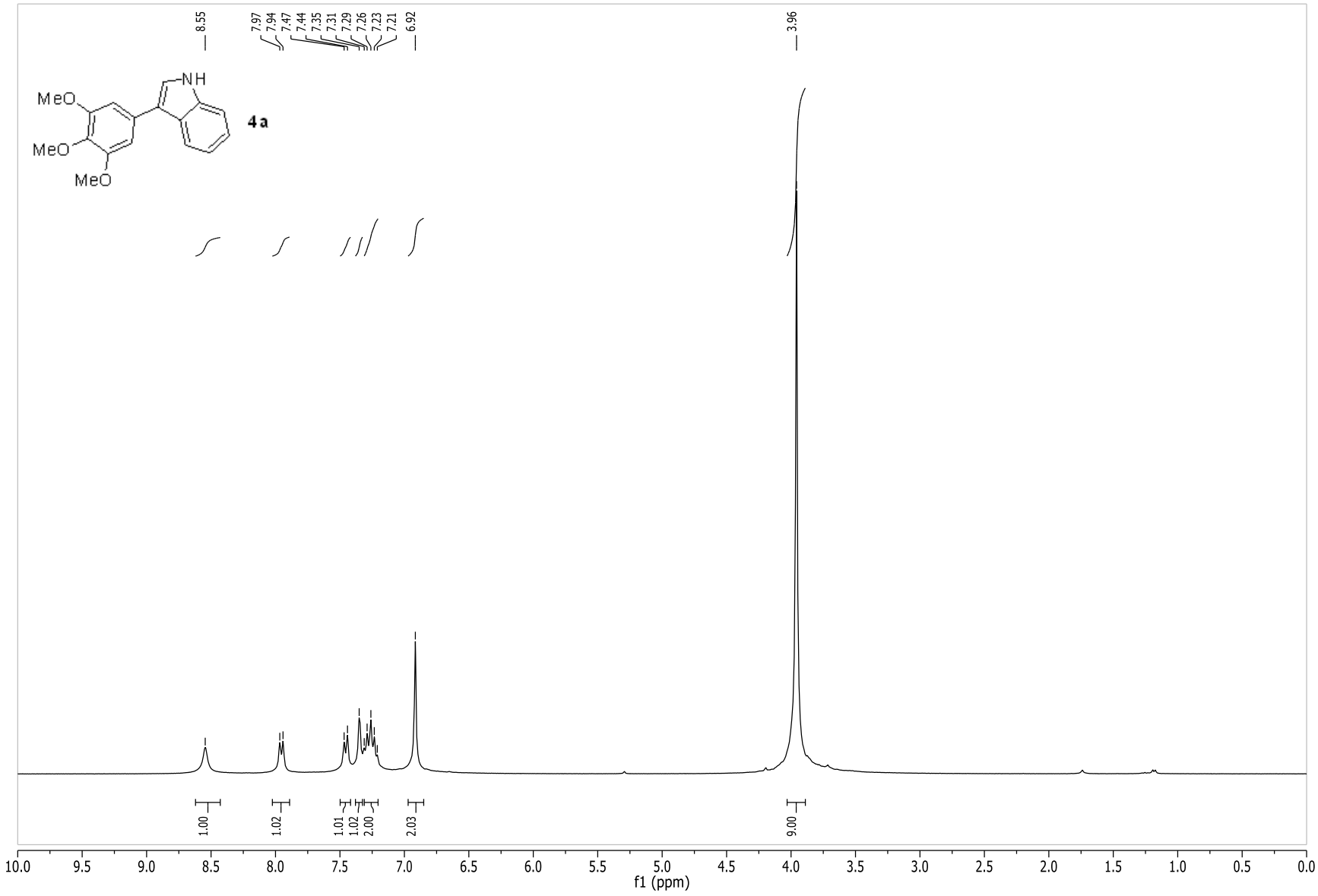


Column chromatography on silica gel afforded 108 mg of the desired methylated carbazole **7i** (0.29 mmol, yield 97%). Yellowish oil. TLC: Rf= 0.36 (cyclohexane/EtOAc 8/2). IR (film, cm^{-1}): 2936, 2833, 2360, 1600, 1579, 1503, 1450, 1411, 1362, 1343, 1247, 1234, 1180, 1126, 1007. ^1H NMR (300 MHz, $CDCl_3$) δ (ppm) 8.14 (s, 1H), 8.11 (d, *J* = 7.8 Hz, 1H), 7.54 – 7.47 (m, 2H), 7.43 (d, *J* = 7.9 Hz, 1H), 7.37 (d, *J* = 8.5 Hz, 1H), 7.28-7.23 (m, 1H), 6.68 (s, 2H), 5.54 (s, 1H), 5.47 (s, 1H), 3.94 (s, 3H), 3.87 (s, 3H), 3.83 (s, 6H). ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm) 153.0 (2C), 150.9 (C), 141.5 (C), 140.9 (C), 138.3 (C), 137.9 (C), 132.4 (C), 126.5 (CH), 126.0 (CH), 122.9 (C), 122.7 (C), 120.5 (CH), 120.3 (CH), 119.2 (CH), 112.7 (CH_2), 108.7 (CH), 108.1 (CH), 106.9 (2CH), 61.0 (CH_3), 56.2 ($2CH_3$), 29.3 (CH_3).HRMS (ESI): for $C_{24}H_{24}NO_3$ $(M+H)^+$: *m/z* calcd 374.1756, found 374.1752.

VII. Biology

Cancer cell lines were obtained from the American type Culture Collection (Rockville, MD) and were cultured according to the supplier's instructions. HCT116 colorectal carcinoma cells were grown in RPMI 1640 containing 10% FCS and 1% glutamine. All cell lines were maintained at 37°C in a humidified atmosphere containing 5% CO_2. Cell viability was assessed using Promega CellTiter-Blue TM reagent according to the manufacturer's instructions. Cells were seeded in 96-well plates (5 × 103 cells/well) containing 50 µL growth medium. After 24 h of culture, the cells were supplemented with 50 µL of the tested compound dissolved in DMSO (less than 0.1% in each preparation). After 72 h of incubation, 20 µL of resazurin was added for 2 h before recording fluorescence (λex = 560 nm, λem = 590 nm) using a Victor microtiter plate fluorimeter (Perkin-Elmer,USA). The GI_{50} corresponds to the concentration of the tested compound that caused a decrease of 50% in fluorescence of drug treated cells compared with untreated cells. Experiments were performed in triplicate. The GI_{50} values for all compounds were compared to the GI_{50} of *iso*CA-4 and measured the same day under the same conditions.

VIII. ^{1}H, ^{13}C NMR Spectra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7.94
7.47
7.44
7.35
7.31
7.29
7.26
7.23
7.21
6.92
3.96
NH
MeO
MeO
MeO
4a
1.00
1.02
1.01
1.02
2.00
2.03
9.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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2.5
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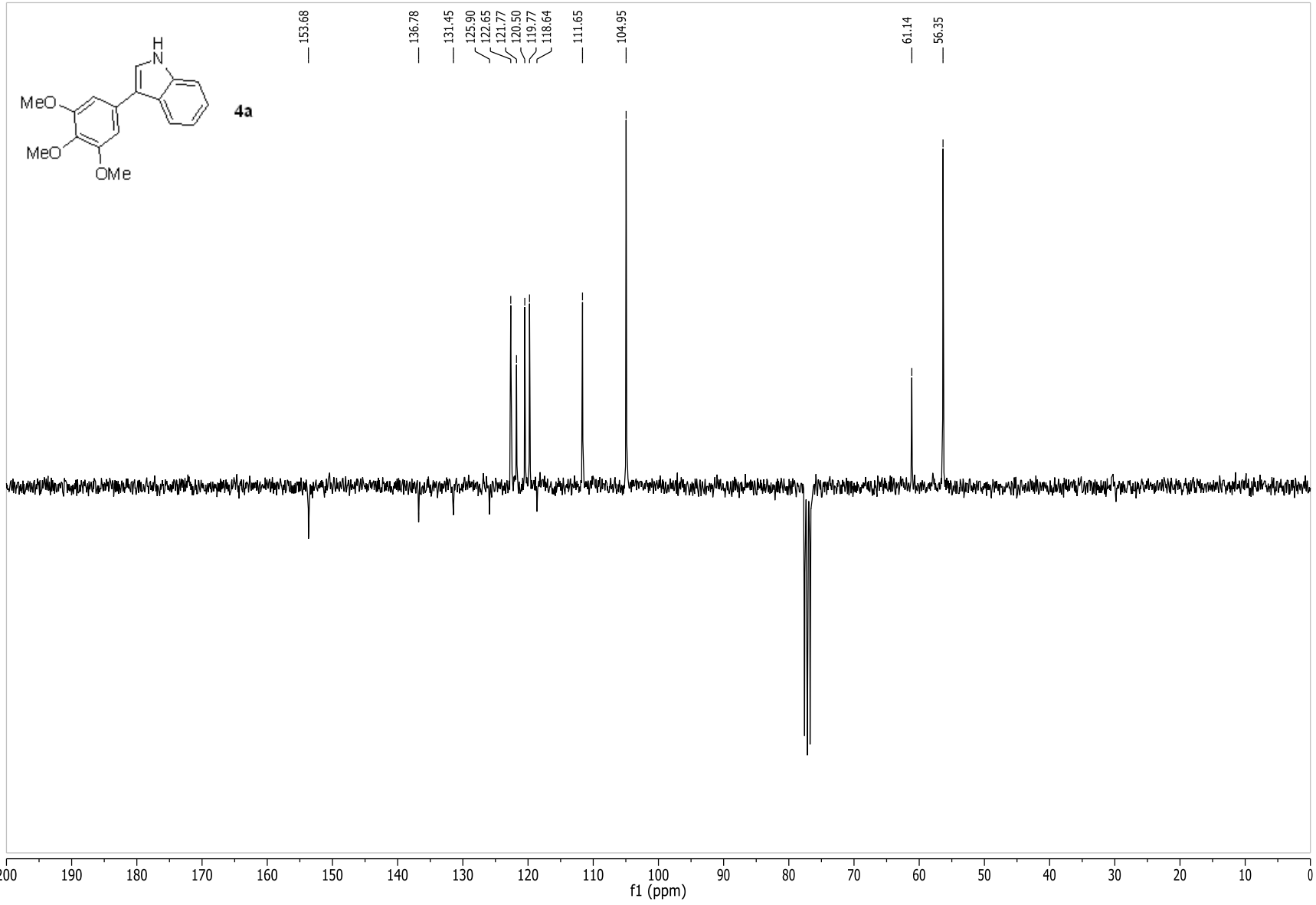
1.0
0.5
0.0
f1 (ppm)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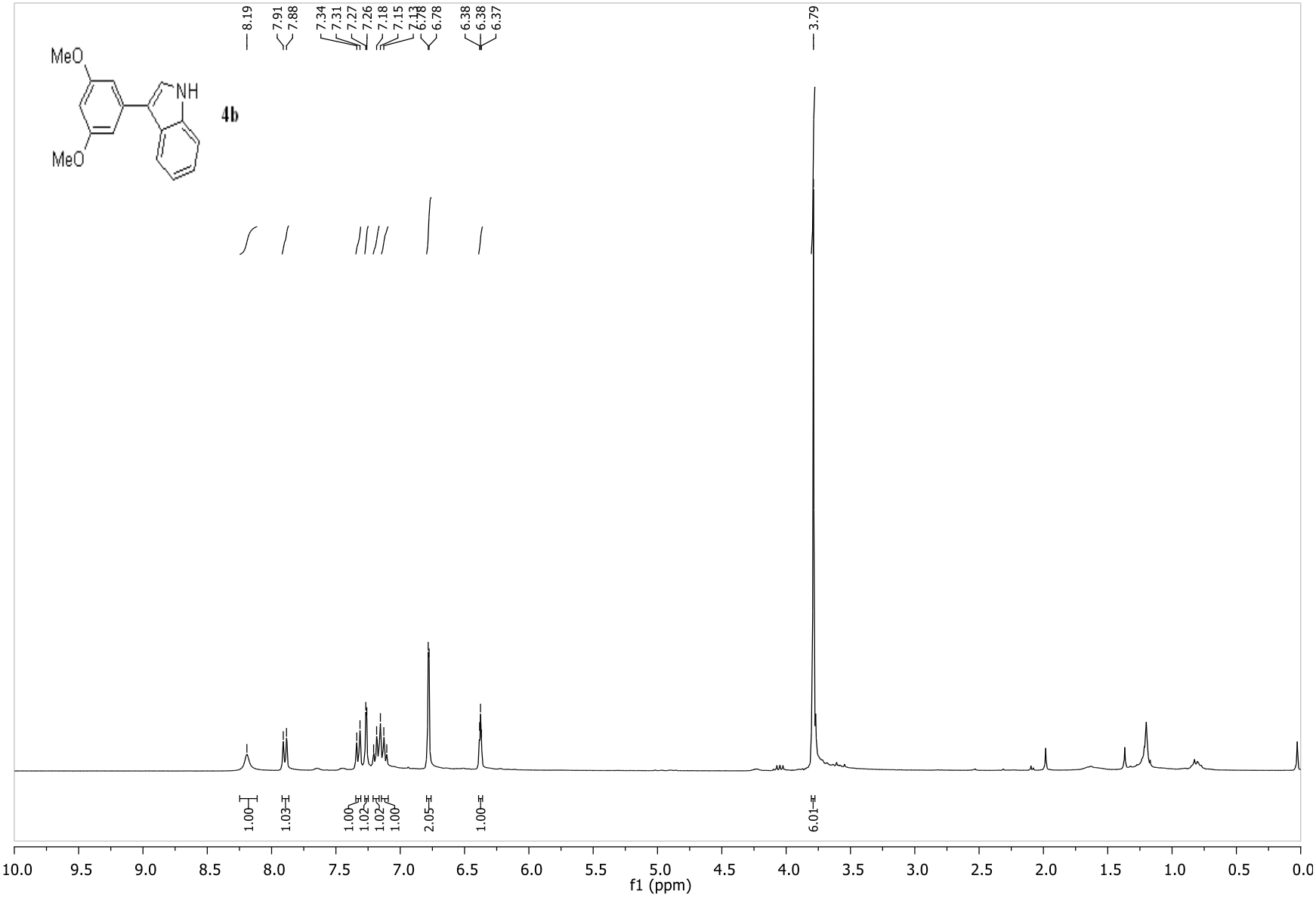
136.78
131.45
125.90
122.65
121.77
120.50
119.77
118.64
111.65
104.95
61.14
56.35
MeO
MeO
OMe
H
N
4a
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.34
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7.27
7.26
7.18
7.15
7.13
6.78
6.38
6.38
6.37
3.79
MeO
MeO
NH
4b
1.00
1.03
1.00
1.02
1.02
1.00
2.05
1.00
6.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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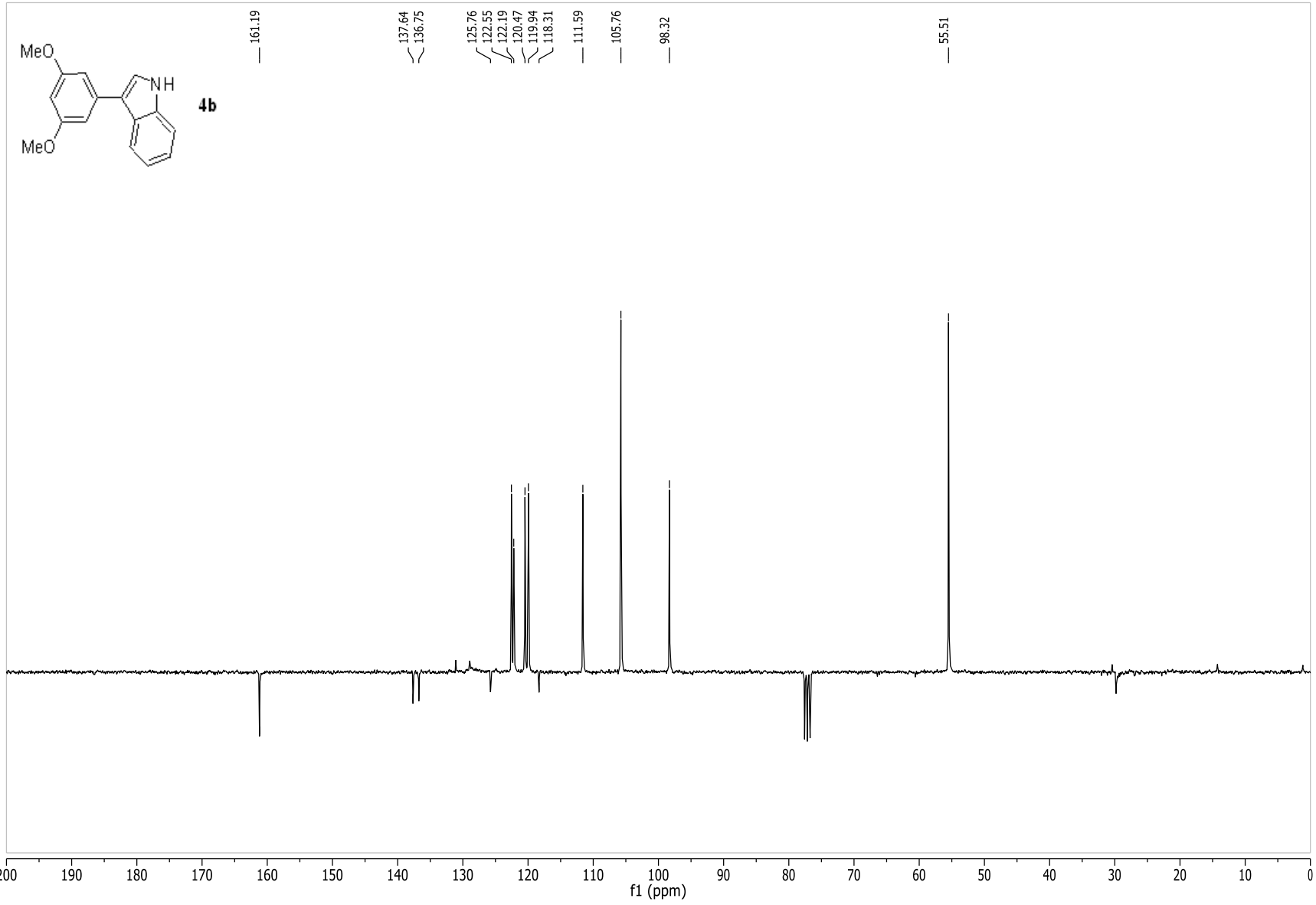
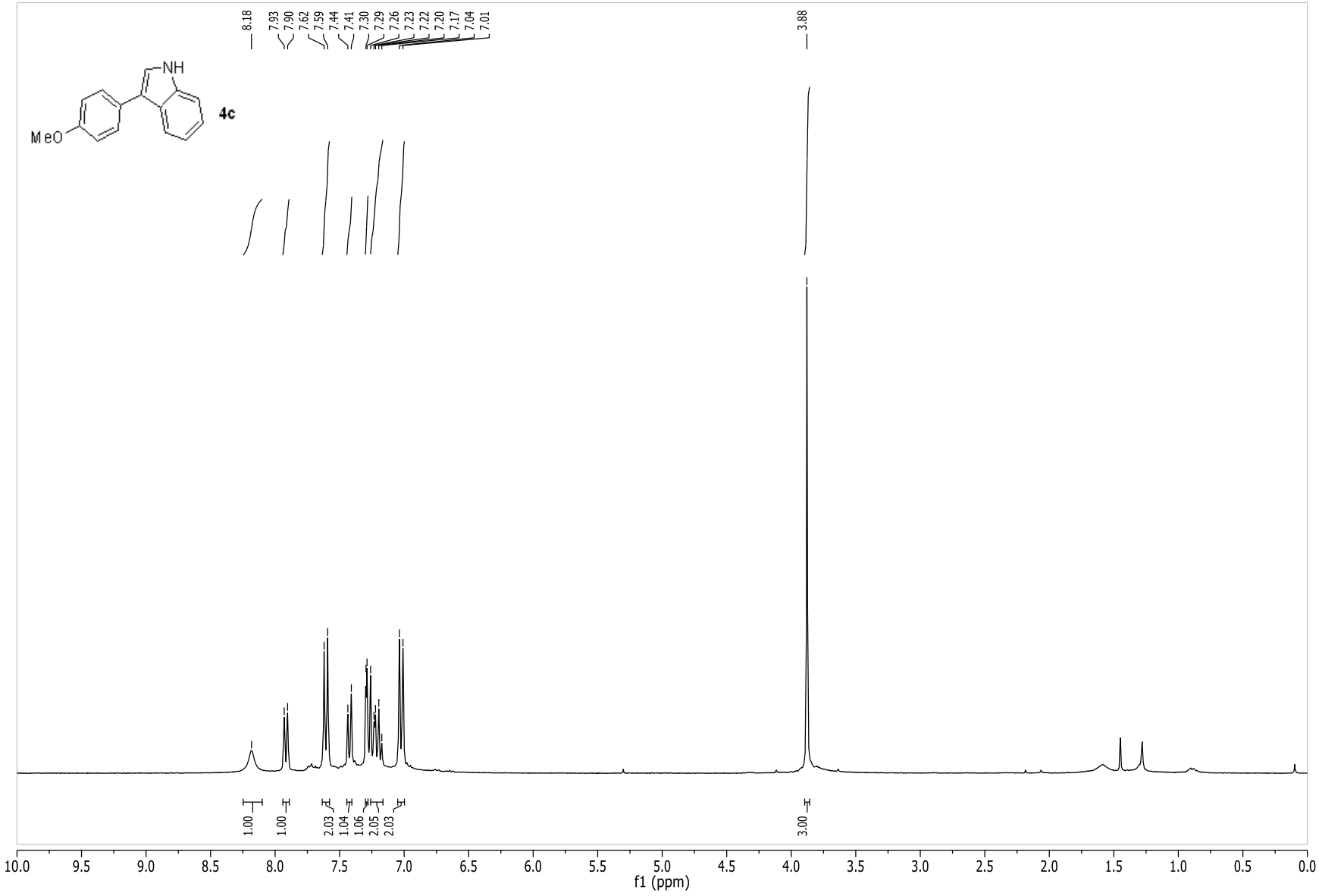
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


MeO
MeO
NH
4b
161.19
137.64
136.75
125.76
122.55
122.19
120.47
119.94
118.31
111.59
105.76
98.32
55.51
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.93
7.90
7.62
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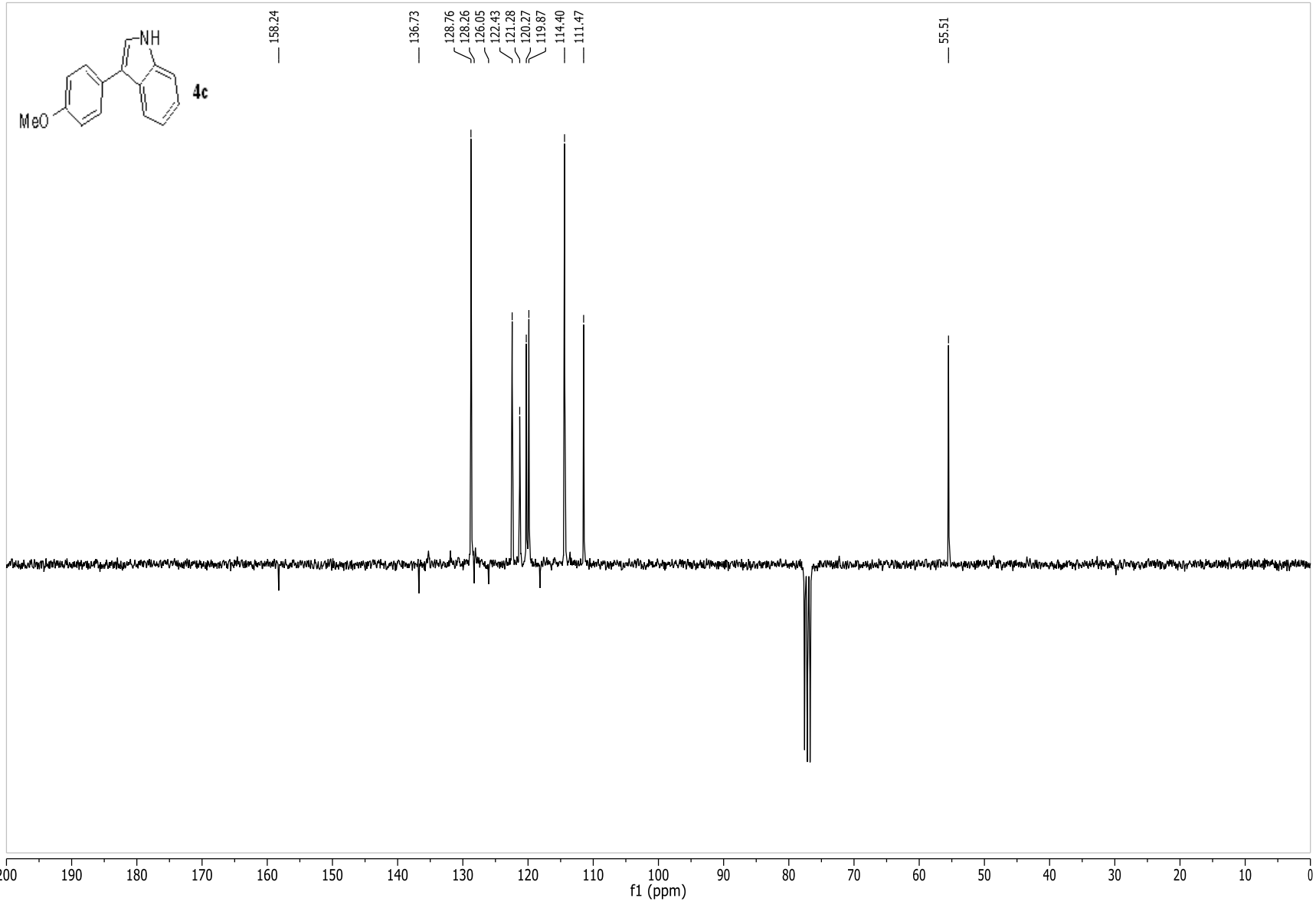
7.44
7.41
7.30
7.29
7.26
7.23
7.22
7.20
7.17
7.04
7.01
3.88
NH
MeO
4c
1.00
1.00
2.03
1.04
1.06
2.05
2.03
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


NH
MeO
4c
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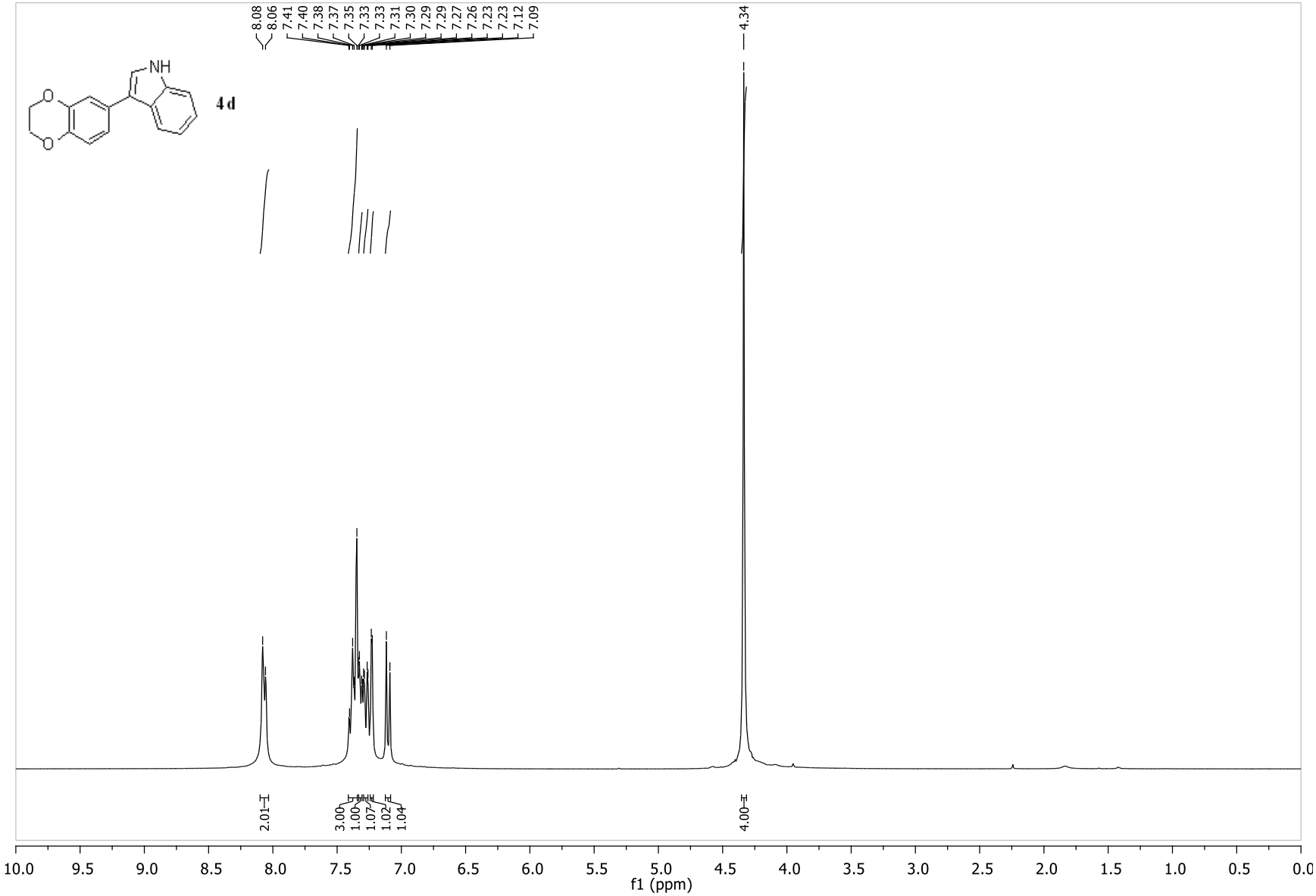
128.76
128.26
126.05
122.43
121.28
120.27
119.87
114.40
111.47
55.51
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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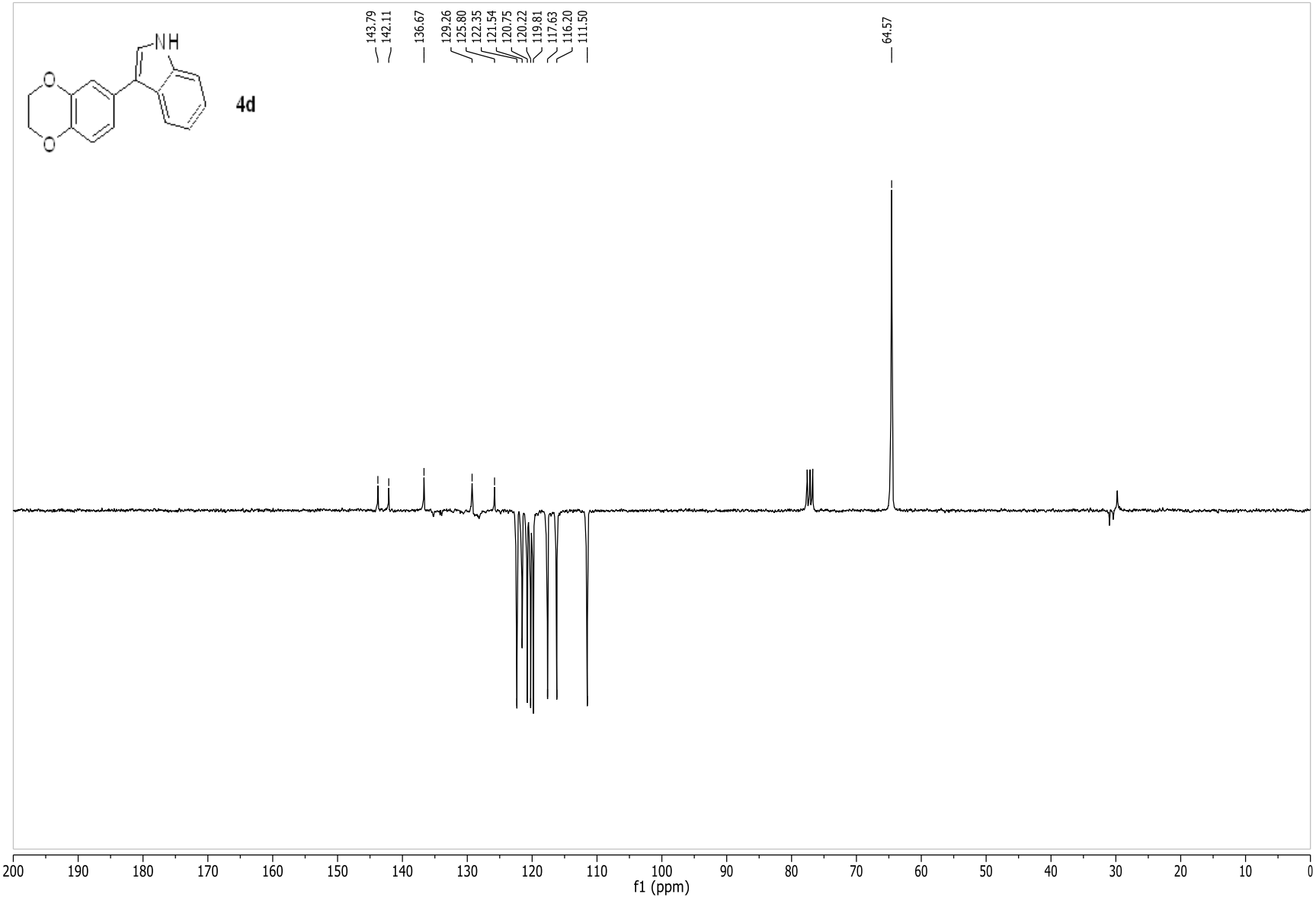
7.37
7.35
7.33
7.33
7.31
7.30
7.29
7.29
7.27
7.26
7.23
7.23
7.12
7.09
4.34
NH
O
O
4 d
2.01
3.00
1.00
1.07
1.02
1.04
4.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


NH
O
O
4d
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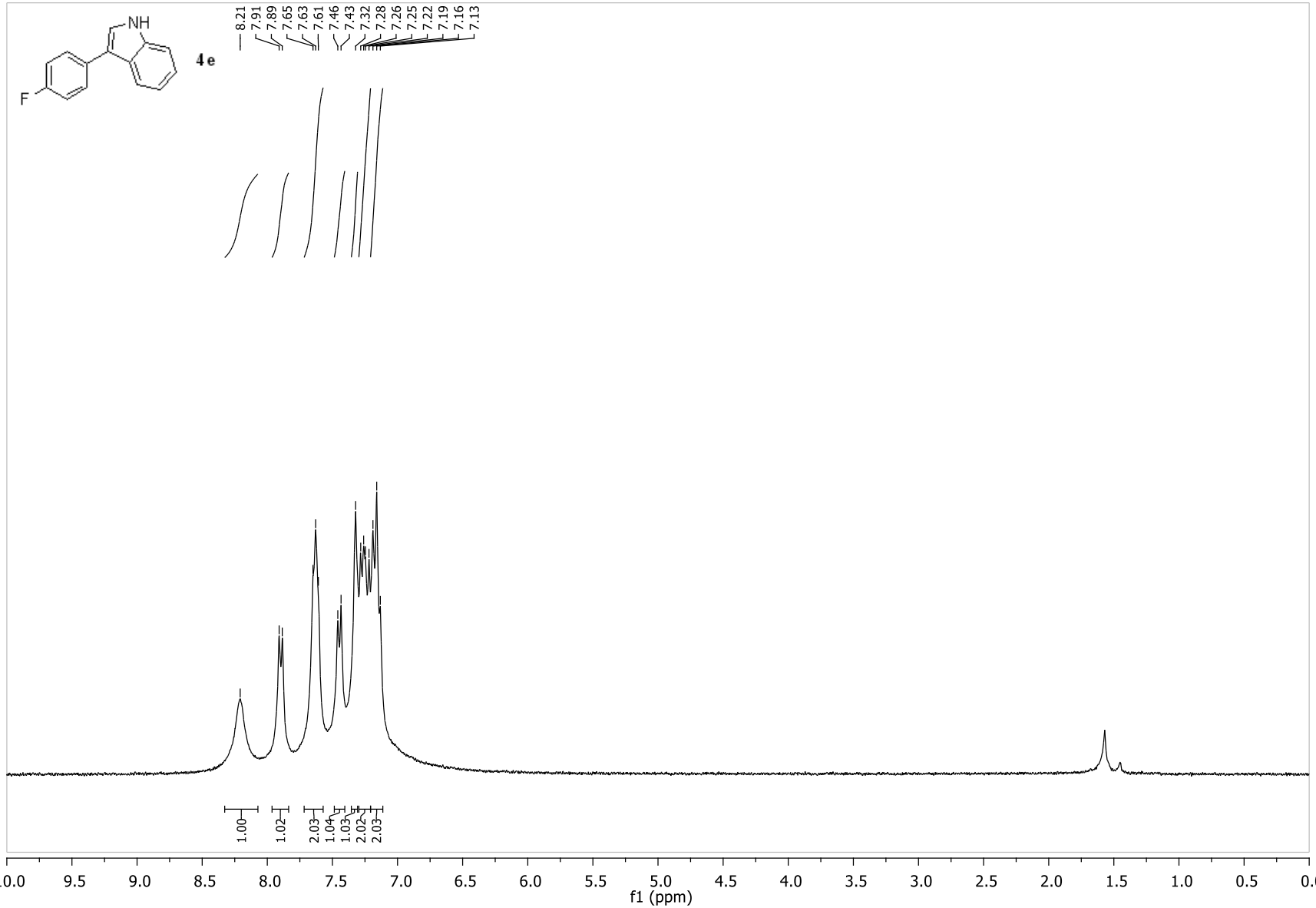
142.11
136.67
129.26
125.80
122.35
121.54
120.75
120.22
119.81
117.63
116.20
111.50
64.57
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


NH
F
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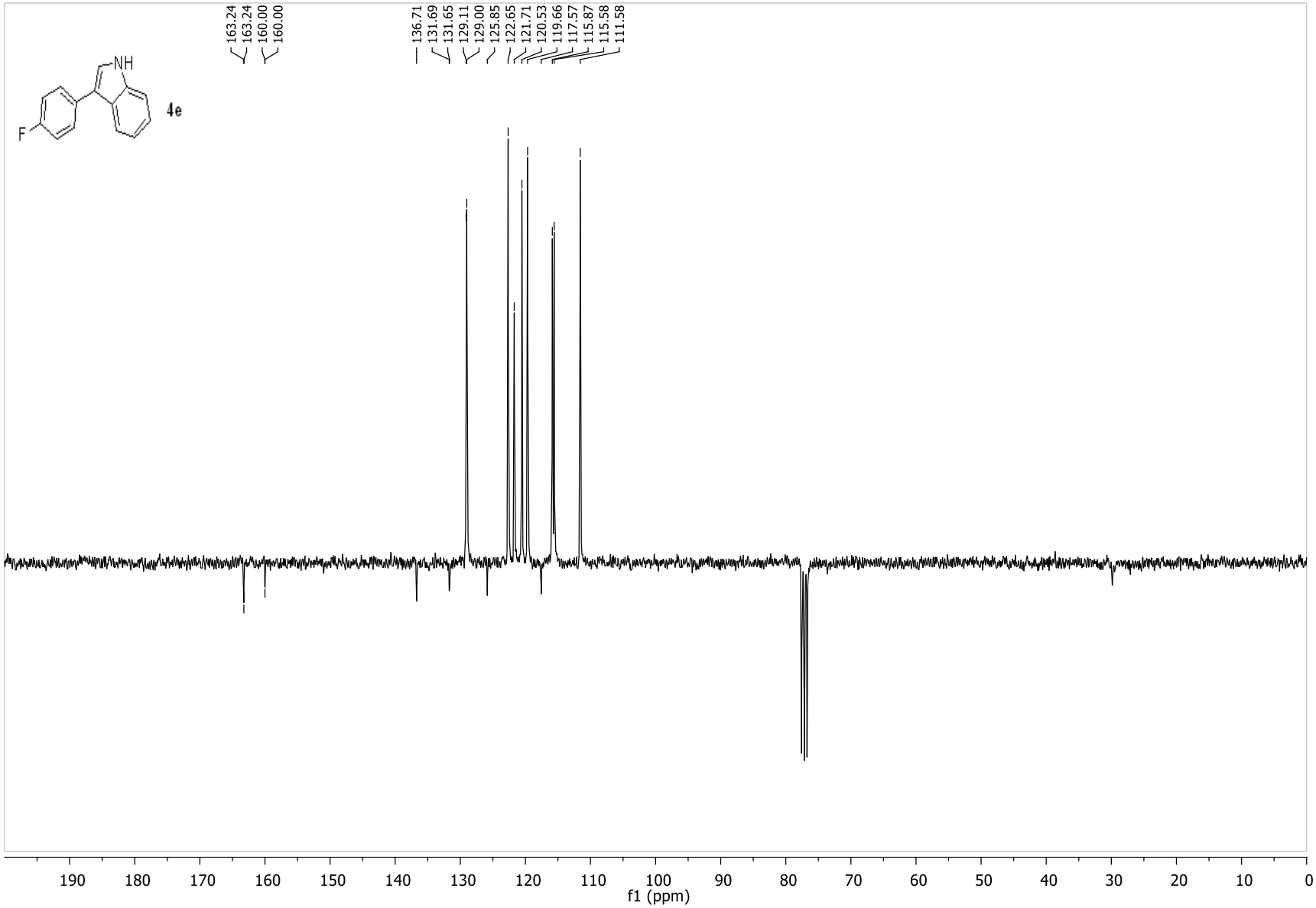
7.65
7.63
7.61
7.46
7.43
7.32
7.28
7.26
7.25
7.22
7.19
7.16
7.13
1.00
1.02
2.03
1.04
1.03
2.02
2.03
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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163.24
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160.00
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131.69
131.65
129.11
129.00
125.85
122.65
121.71
120.53
119.66
117.57
115.87
115.58
111.58
NH
F
4e
190
180
170
160
150
140
130
120
110
100
90
80
70
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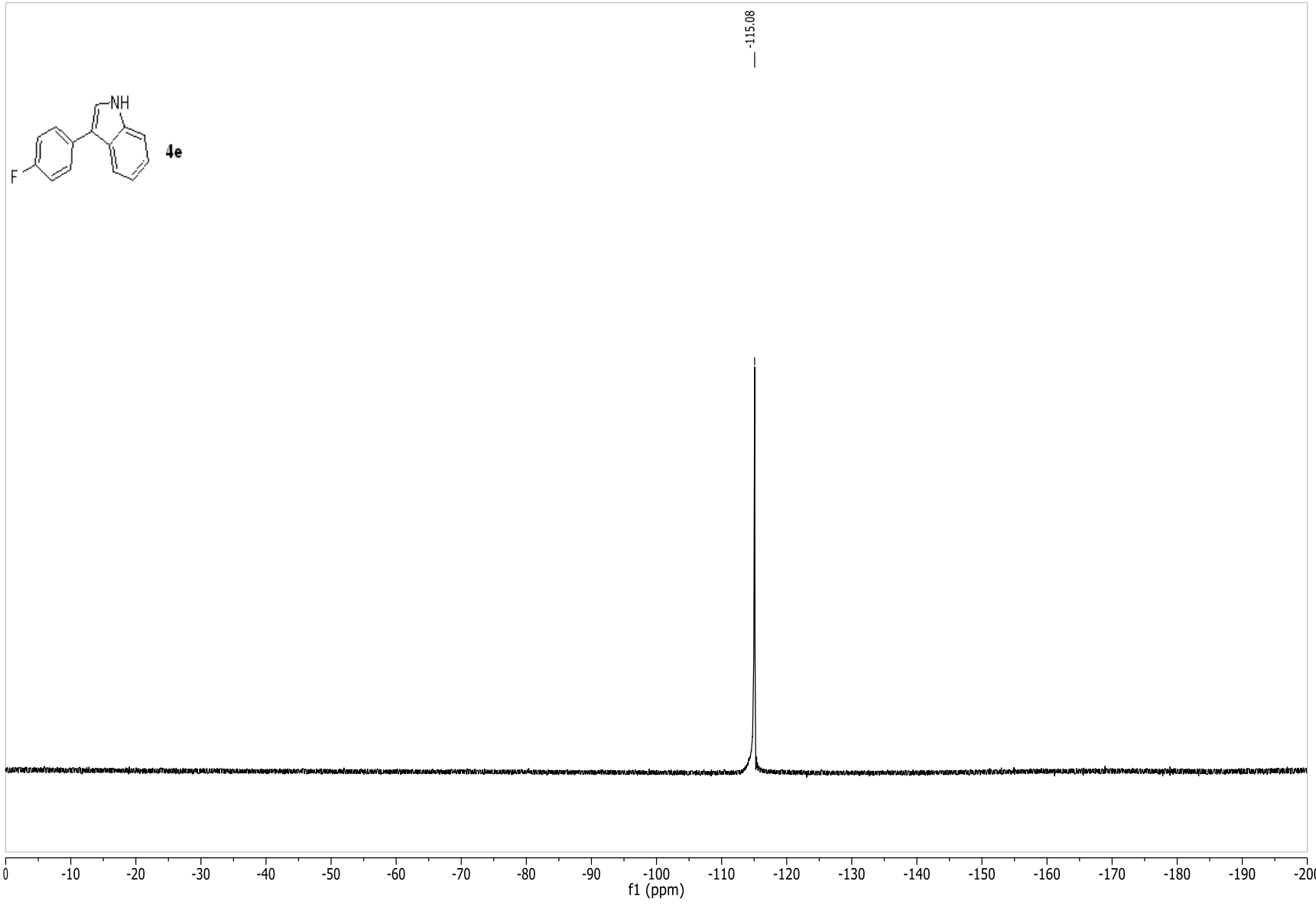
50
40
30
20
10
0
f1 (ppm)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-20
-30
-40
-50
-60
-70
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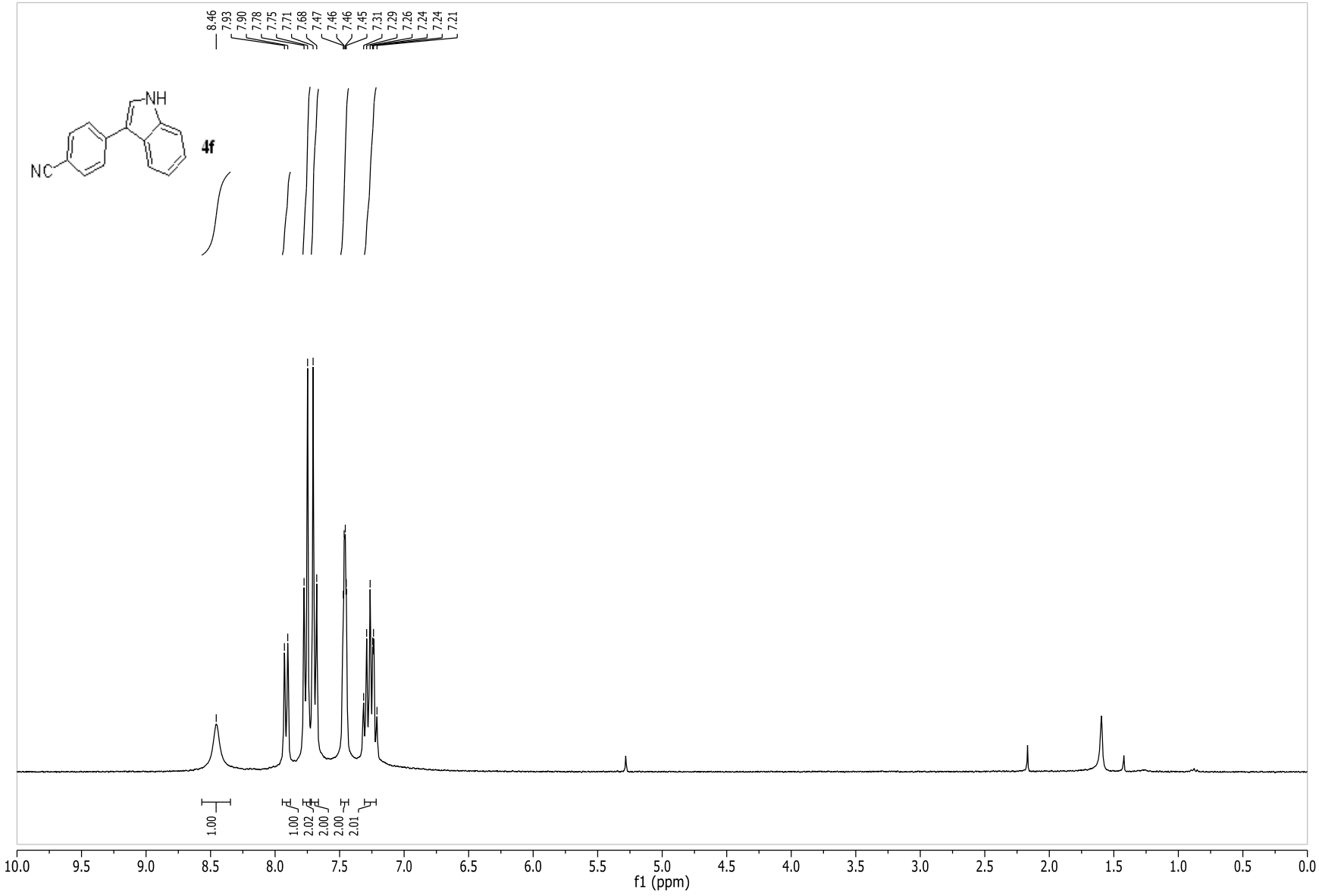
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
f1 (ppm)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7.71
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7.47
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7.45
7.31
7.29
7.26
7.24
7.24
7.21
NH
NC
4f
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1.00
2.02
2.00
2.00
2.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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3.5
3.0
2.5
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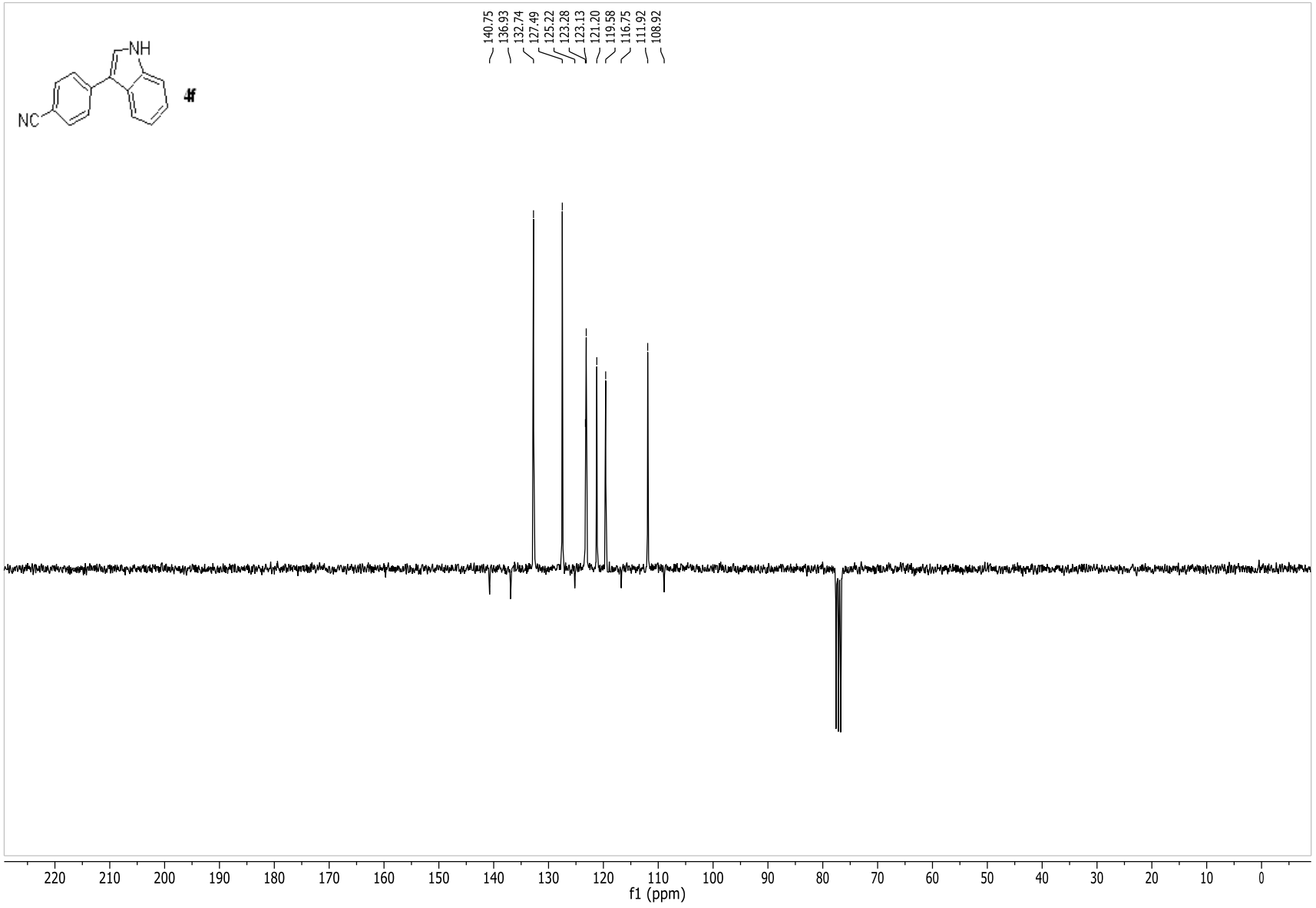
0.0
f1 (ppm)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NC
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127.49
125.22
123.28
123.13
121.20
119.58
116.75
111.92
108.92
220
210
200
190
180
170
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120
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90
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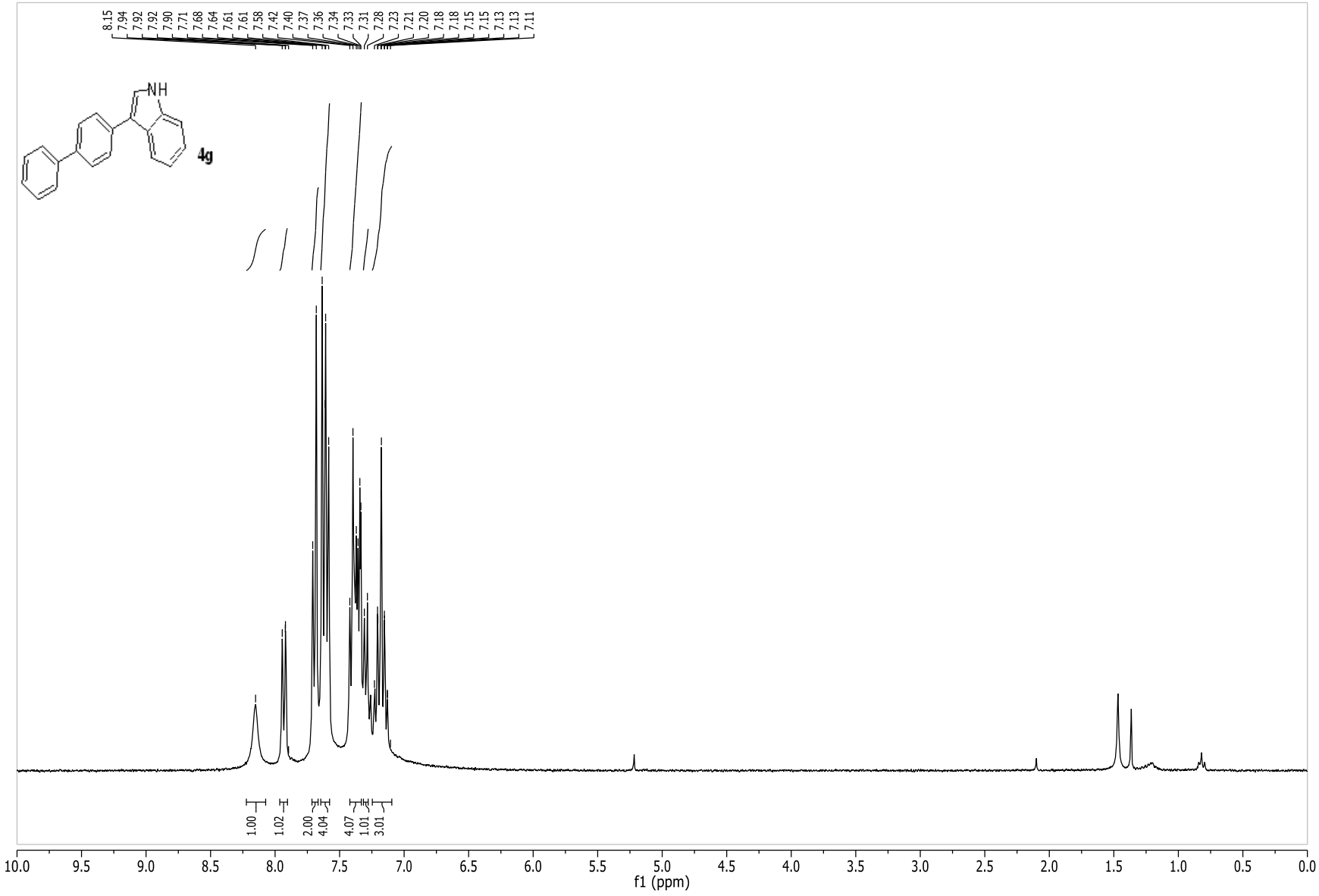
50
40
30
20
10
0
f1 (ppm)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7.68
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7.40
7.37
7.36
7.34
7.33
7.31
7.28
7.23
7.21
7.20
7.18
7.18
7.15
7.15
7.13
7.13
7.11
NH
4g
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1.02
2.00
4.04
4.07
1.01
3.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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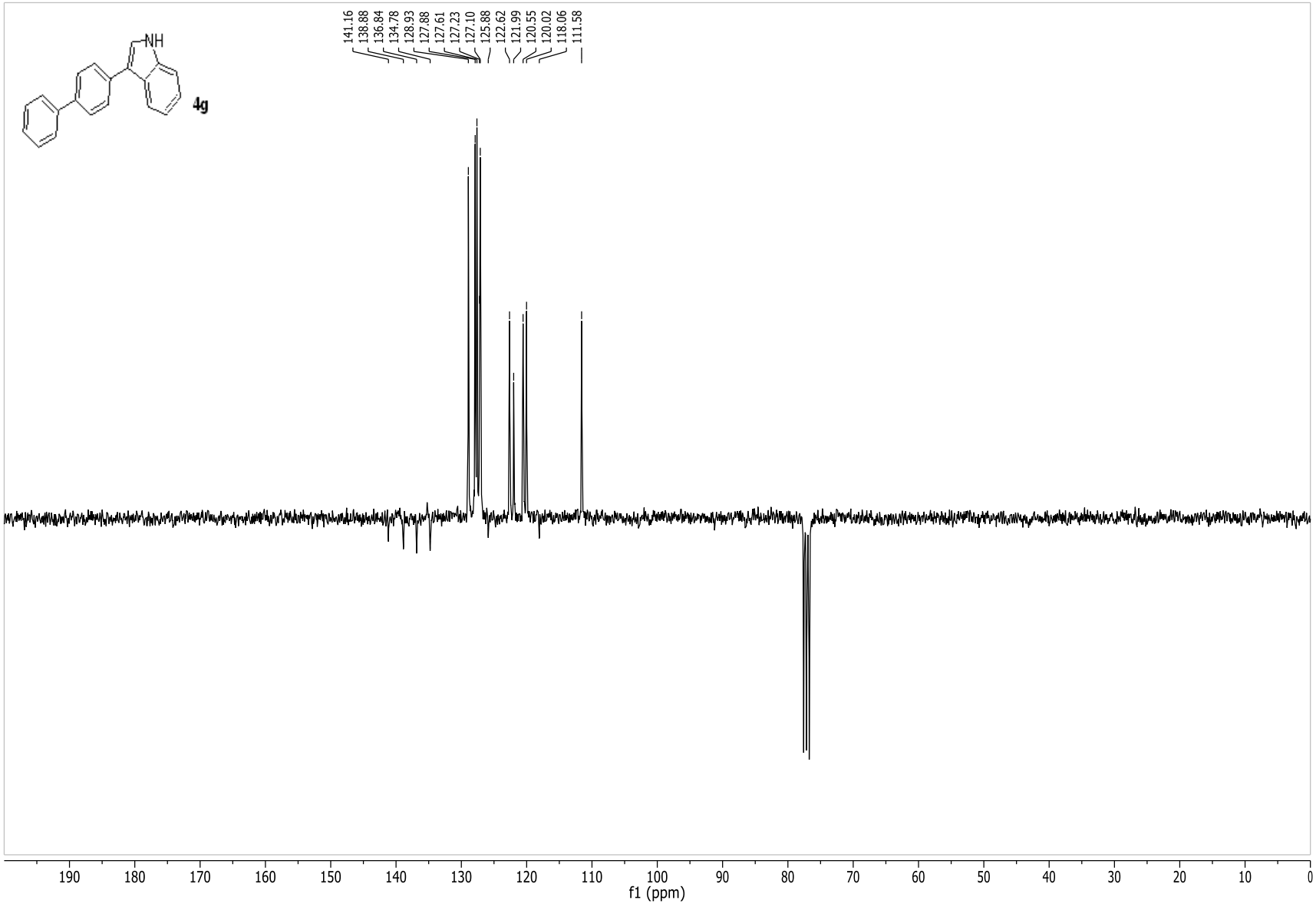
f1 (ppm)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134.78
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127.88
127.61
127.23
127.10
125.88
122.62
121.99
120.55
120.02
118.06
111.58
NH
4g
190
180
170
160
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130
120
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90
80
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50
40
30
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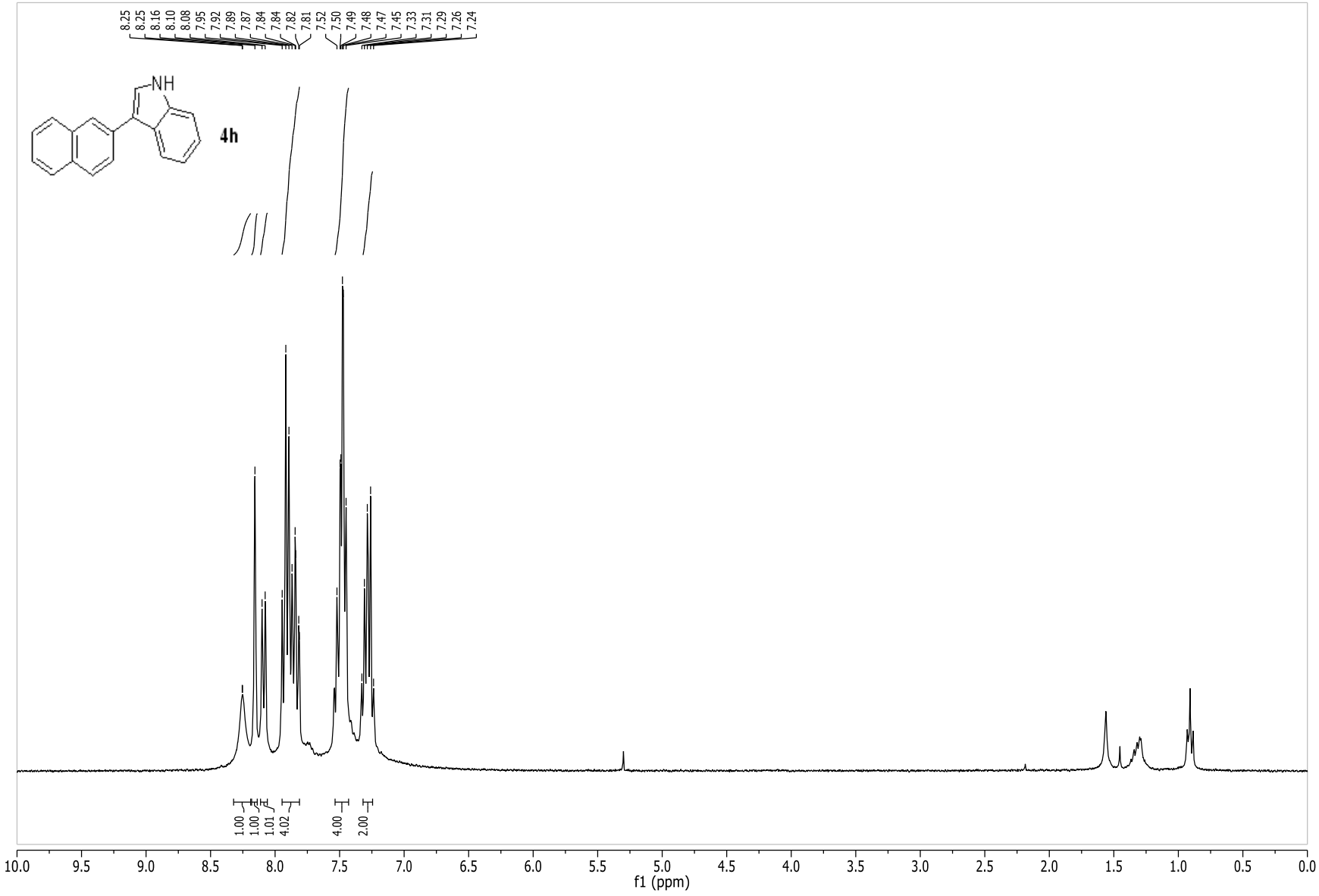
0
f1 (ppm)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7.31
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7.26
7.24
NH
4h
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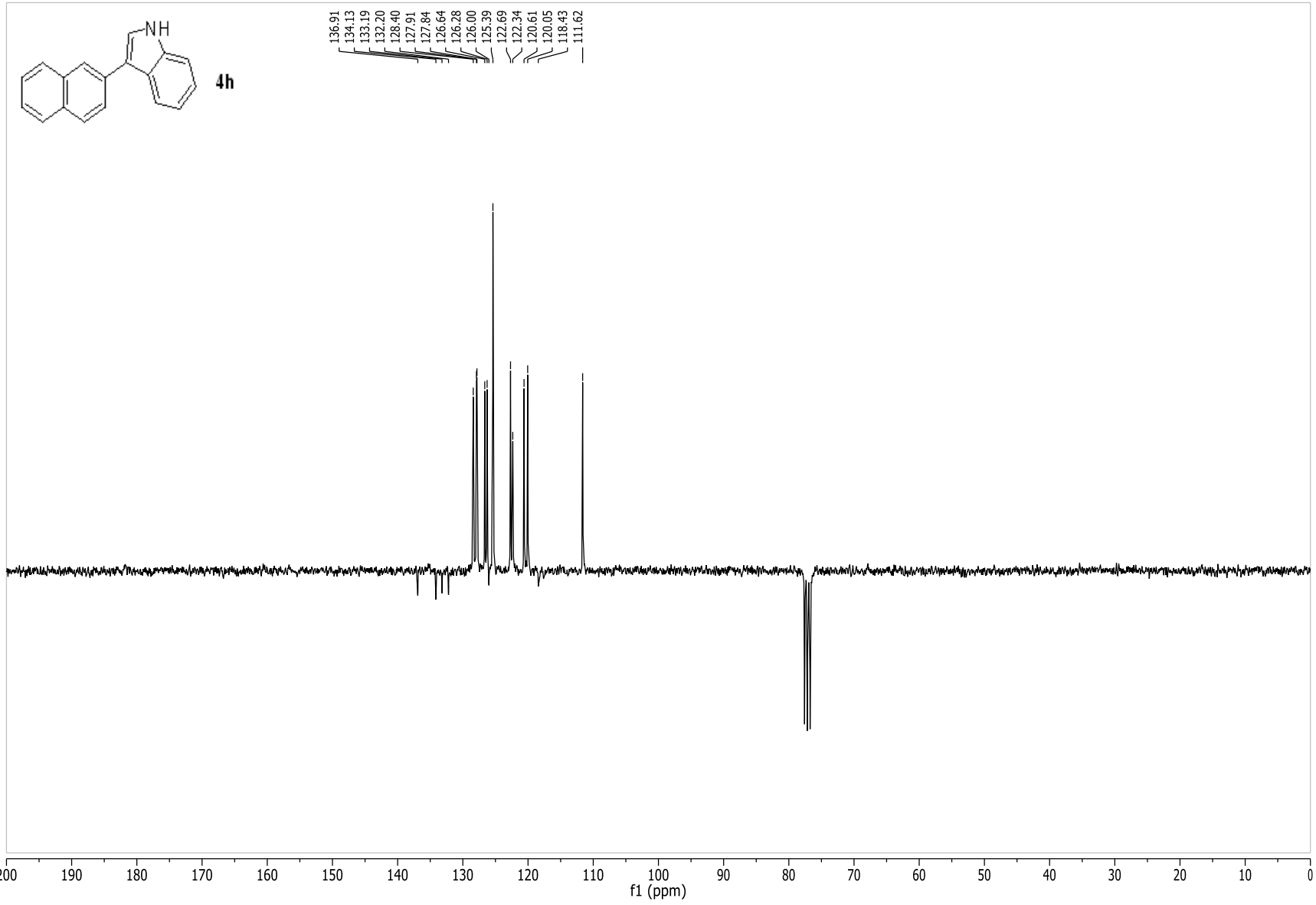
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122.69
122.34
120.61
120.05
118.43
111.62
200
190
180
170
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90
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50
40
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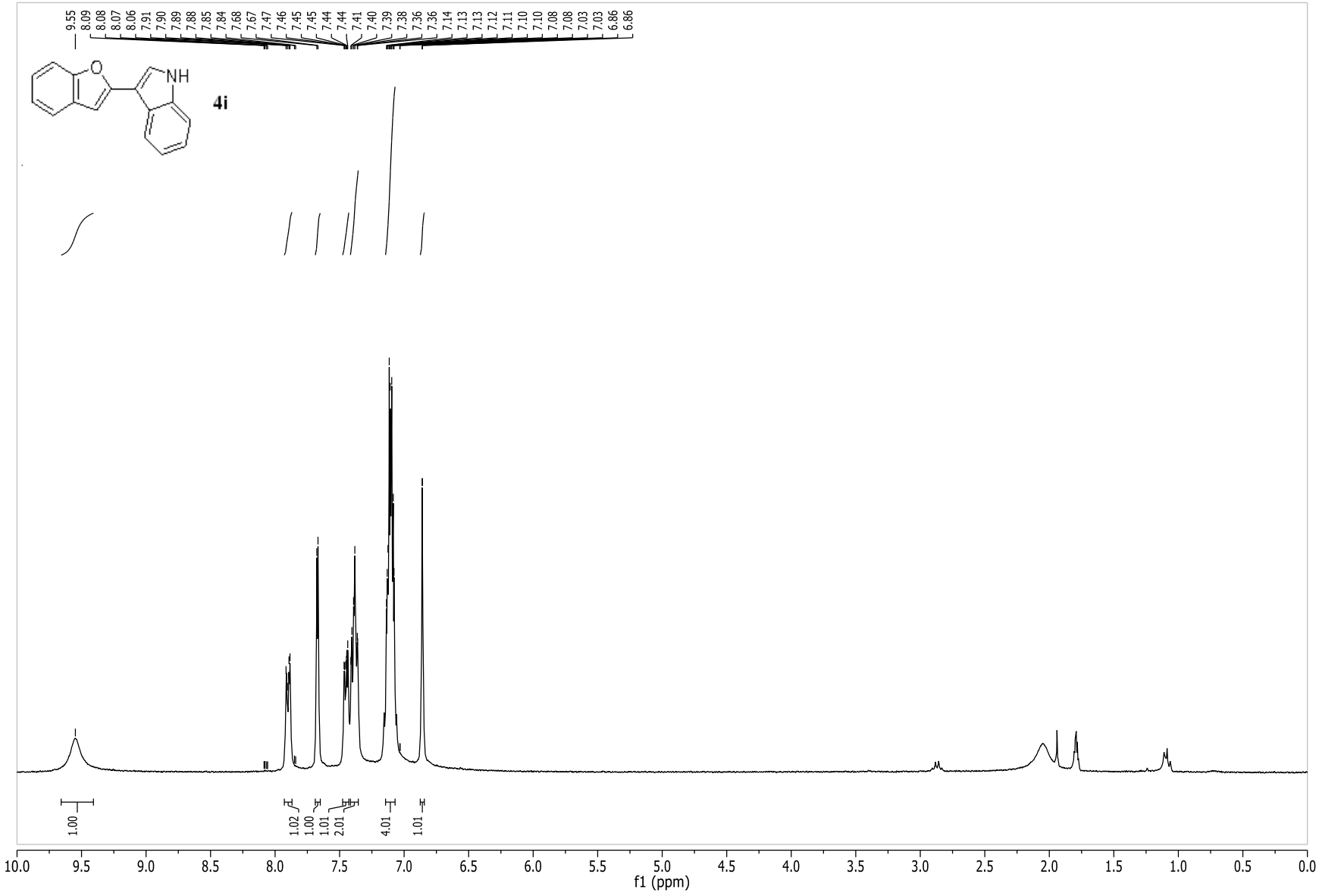
f1 (ppm)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7.03
6.86
6.86
O
NH
4i
1.00
1.02
1.00
1.01
2.01
4.01
1.01
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9.0
8.5
8.0
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7.0
6.5
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2.5
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1.0
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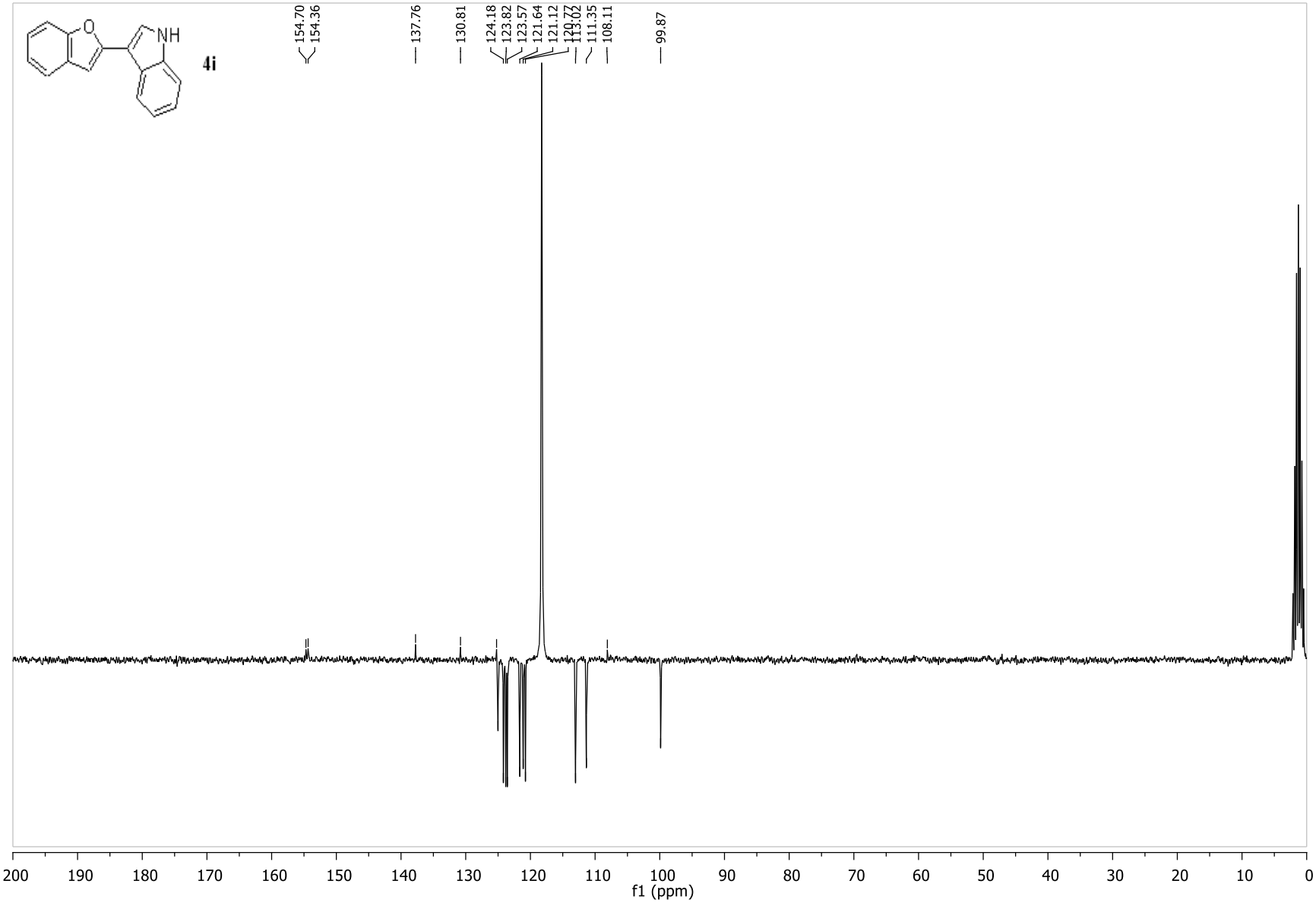
0.0
f1 (ppm)


4i
154.70
154.36
137.76
130.81
124.18
123.82
123.57
121.64
121.12
120.77
111.35
108.11
99.87
200
190
180
170
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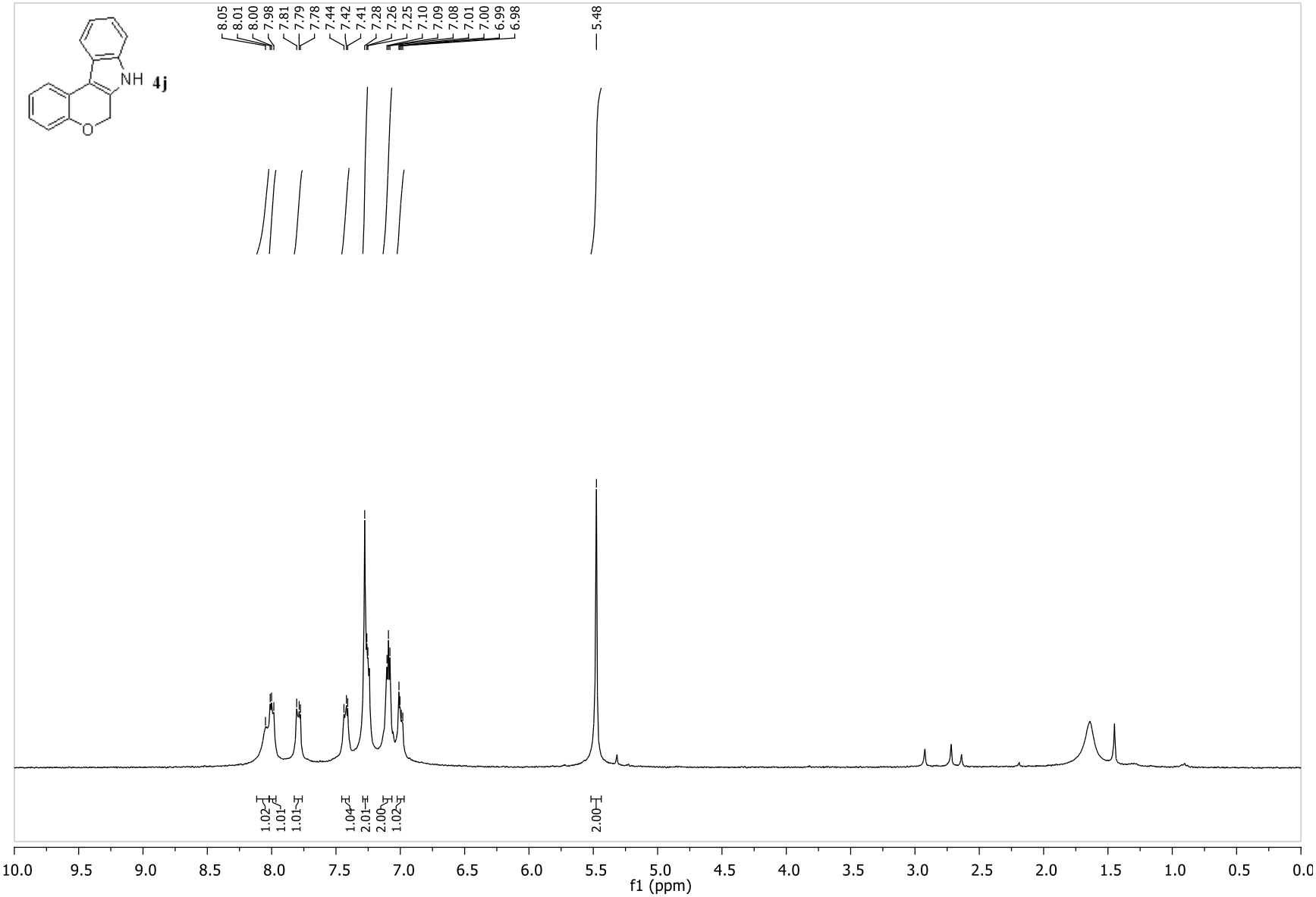
f1 (ppm)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O
4j
8.05
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8.00
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7.81
7.79
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7.44
7.42
7.41
7.28
7.26
7.25
7.10
7.09
7.08
7.01
7.00
6.99
6.98
5.48
1.02
1.01
1.01
1.04
2.01
2.00
1.02
2.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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3.5
3.0
2.5
2.0
1.5
1.0
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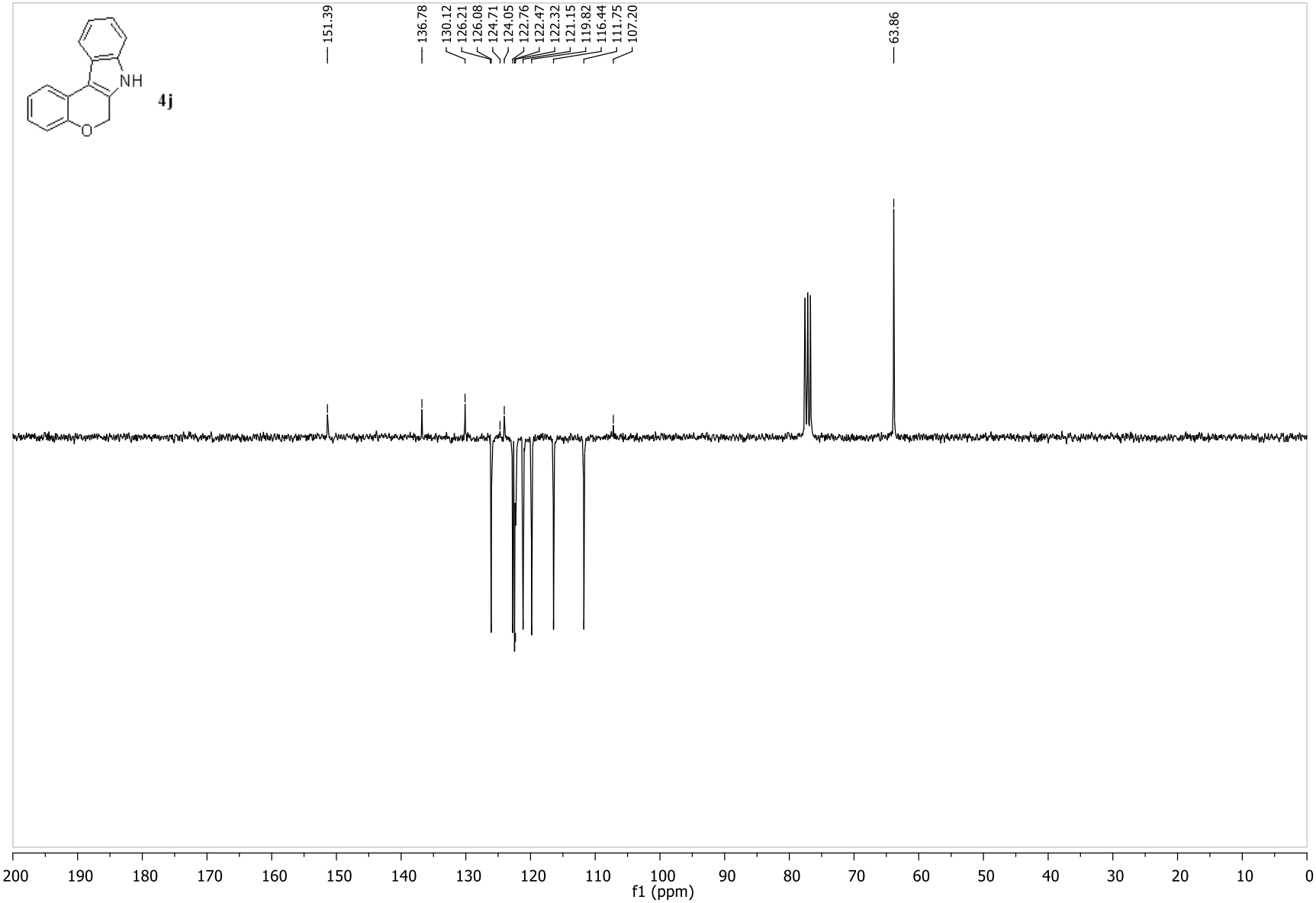
0.0
f1 (ppm)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O
4j
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136.78
130.12
126.21
126.08
124.71
124.05
122.76
122.47
122.32
121.15
119.82
116.44
111.75
107.20
63.86
200
190
180
170
160
150
140
130
120
110
100
90
80
70
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50
40
30
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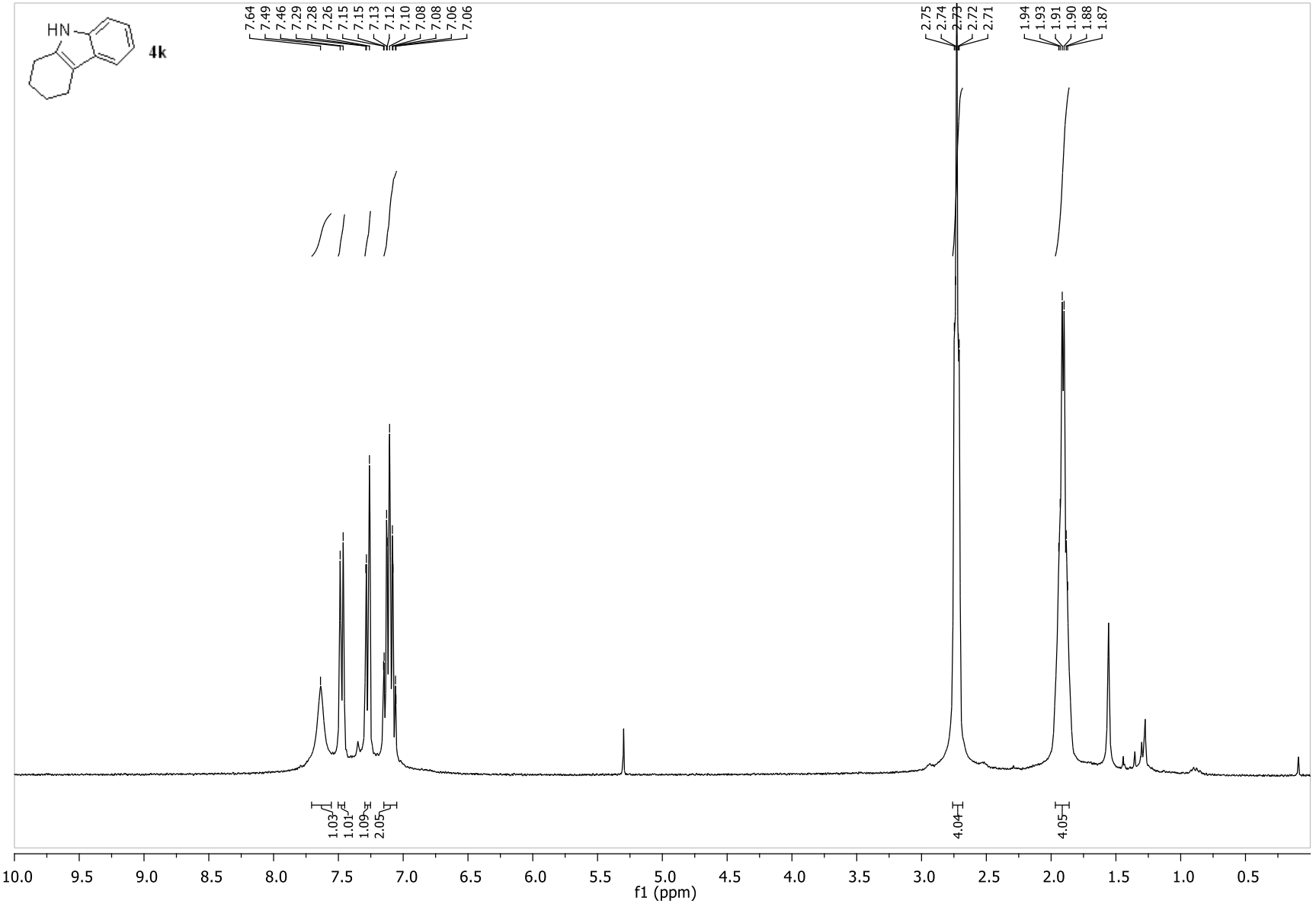
10
0
f1 (ppm)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4k
7.64
7.49
7.46
7.29
7.28
7.26
7.15
7.15
7.13
7.12
7.10
7.08
7.08
7.06
7.06
2.75
2.74
2.73
2.72
2.71
1.94
1.93
1.91
1.90
1.88
1.87
1.03
1.01
1.09
2.05
4.04
4.05
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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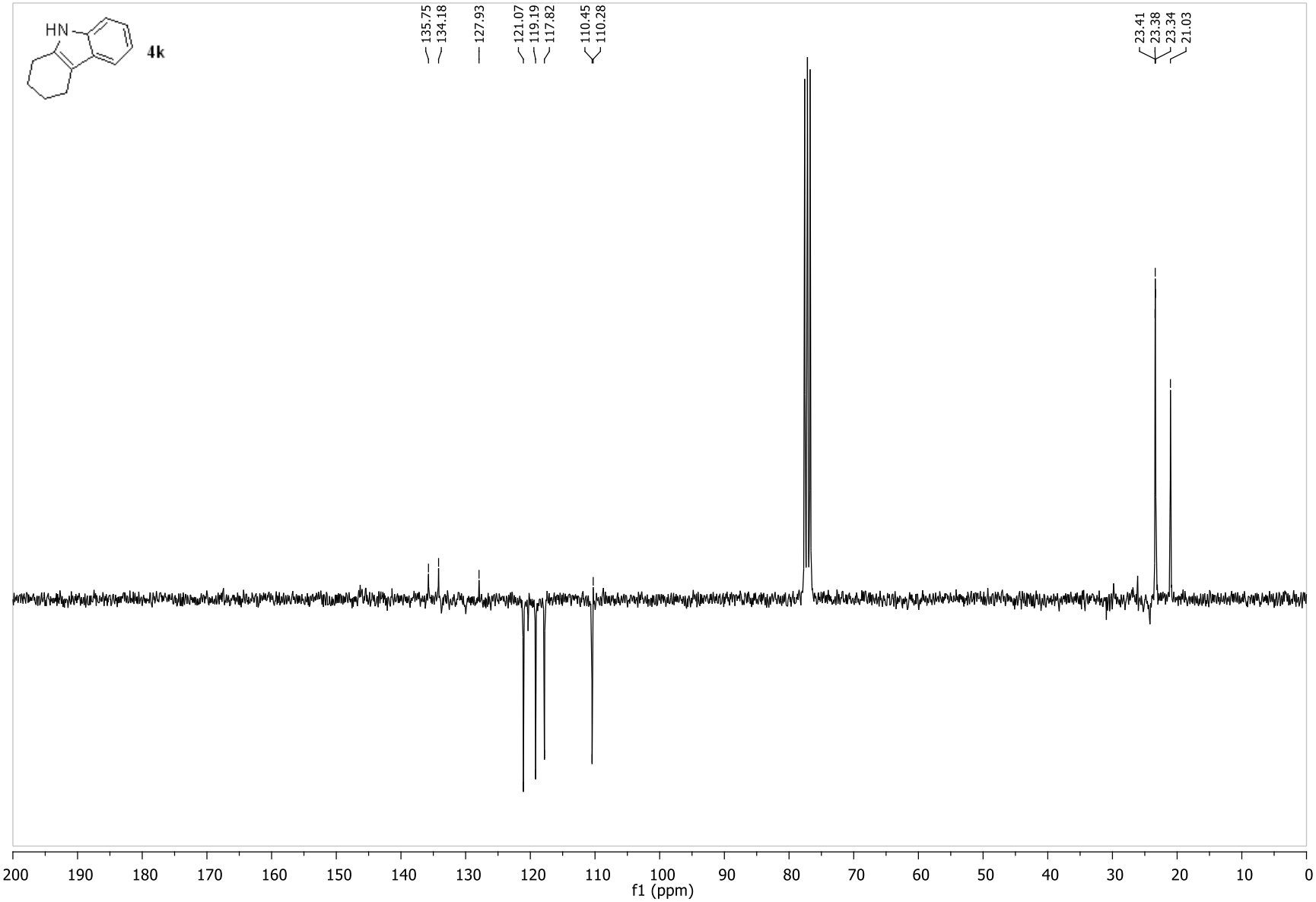
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


HN
4k
135.75
134.18
127.93
121.07
119.19
117.82
110.45
110.28
23.41
23.38
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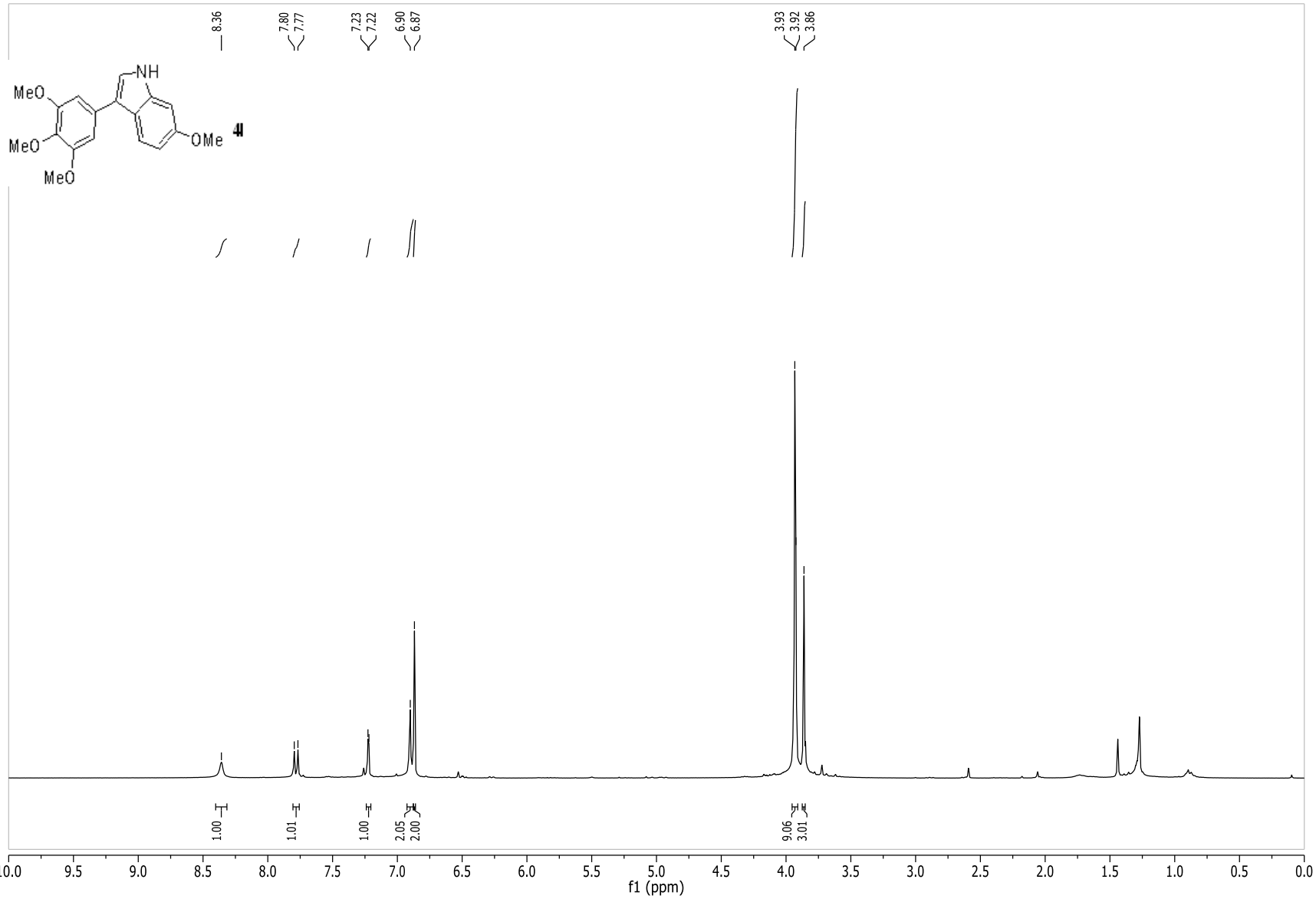
21.03
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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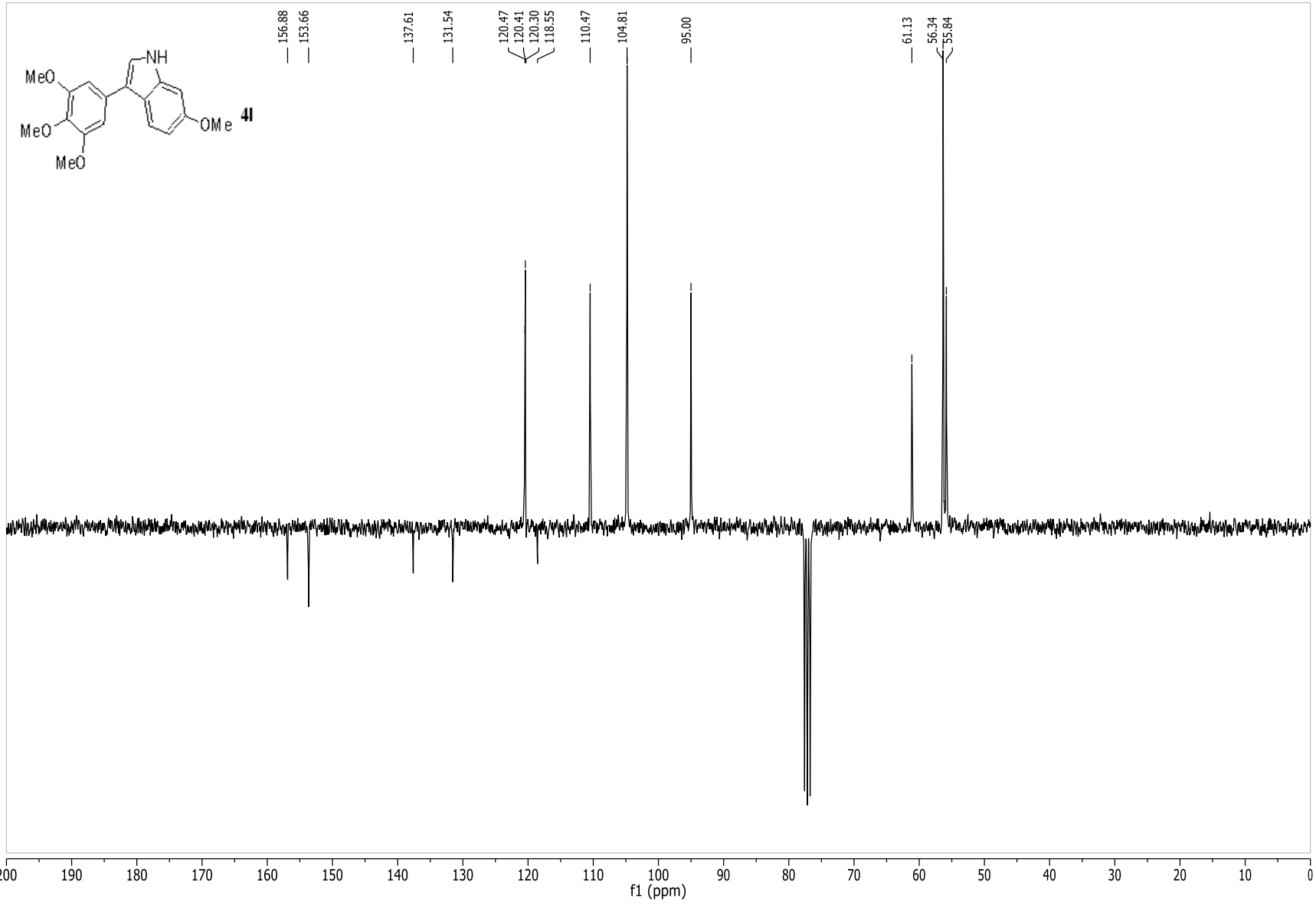
7.80
7.77
7.23
7.22
6.90
6.87
3.93
3.92
3.86
NH
MeO
MeO
MeO
OMe
4l
1.00
1.01
1.00
2.05
2.00
9.06
3.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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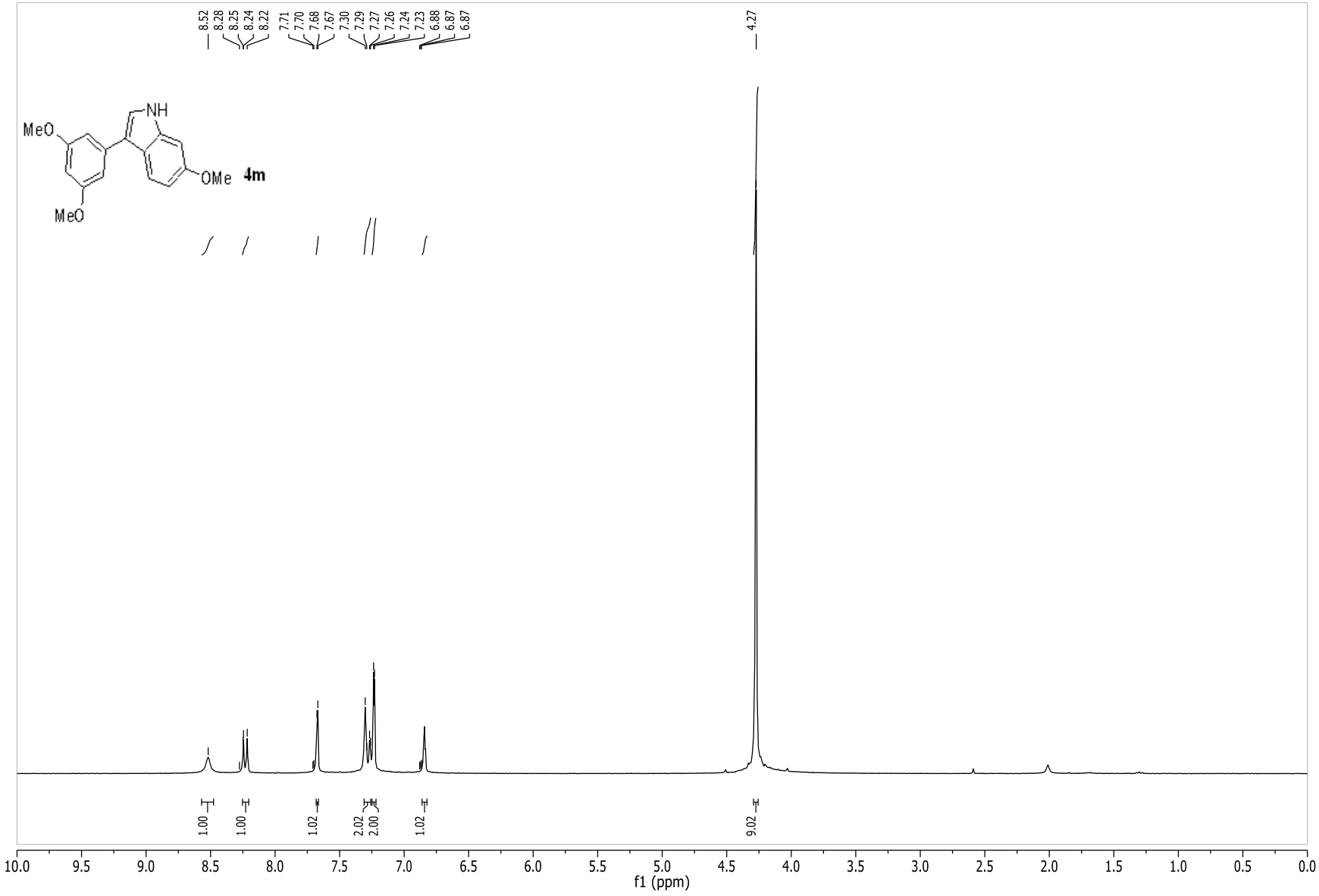
153.66
137.61
131.54
120.47
120.41
120.30
118.55
110.47
104.81
95.00
61.13
56.34
55.84
MeO
MeO
MeO
NH
OMe
4l
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.52
8.28
8.25
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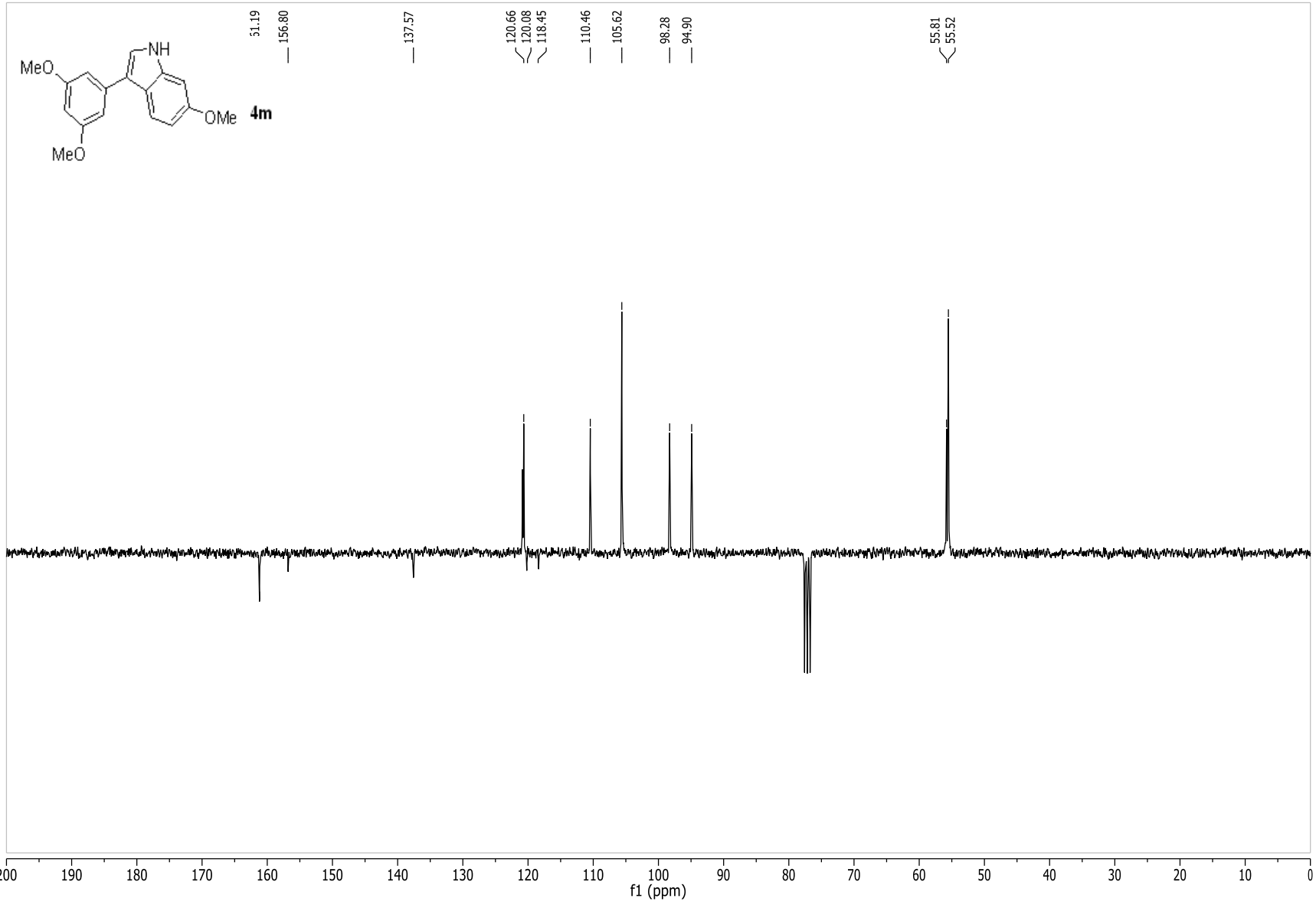
7.71
7.70
7.68
7.67
7.30
7.29
7.27
7.26
7.24
7.23
6.88
6.87
6.87
4.27
NH
MeO
OMe
MeO
4m
1.00
1.00
1.02
2.02
2.00
1.02
9.02
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


51.19
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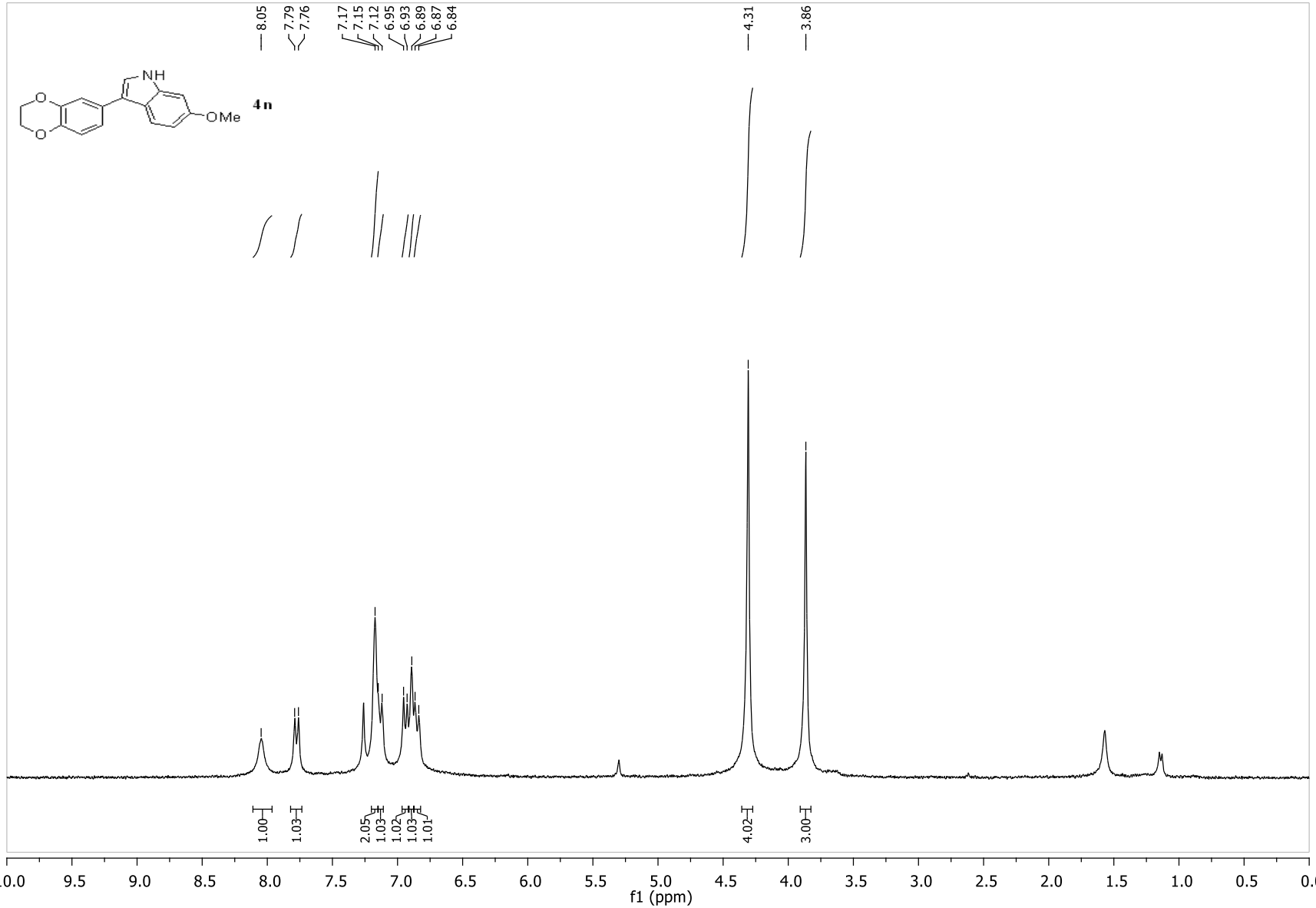
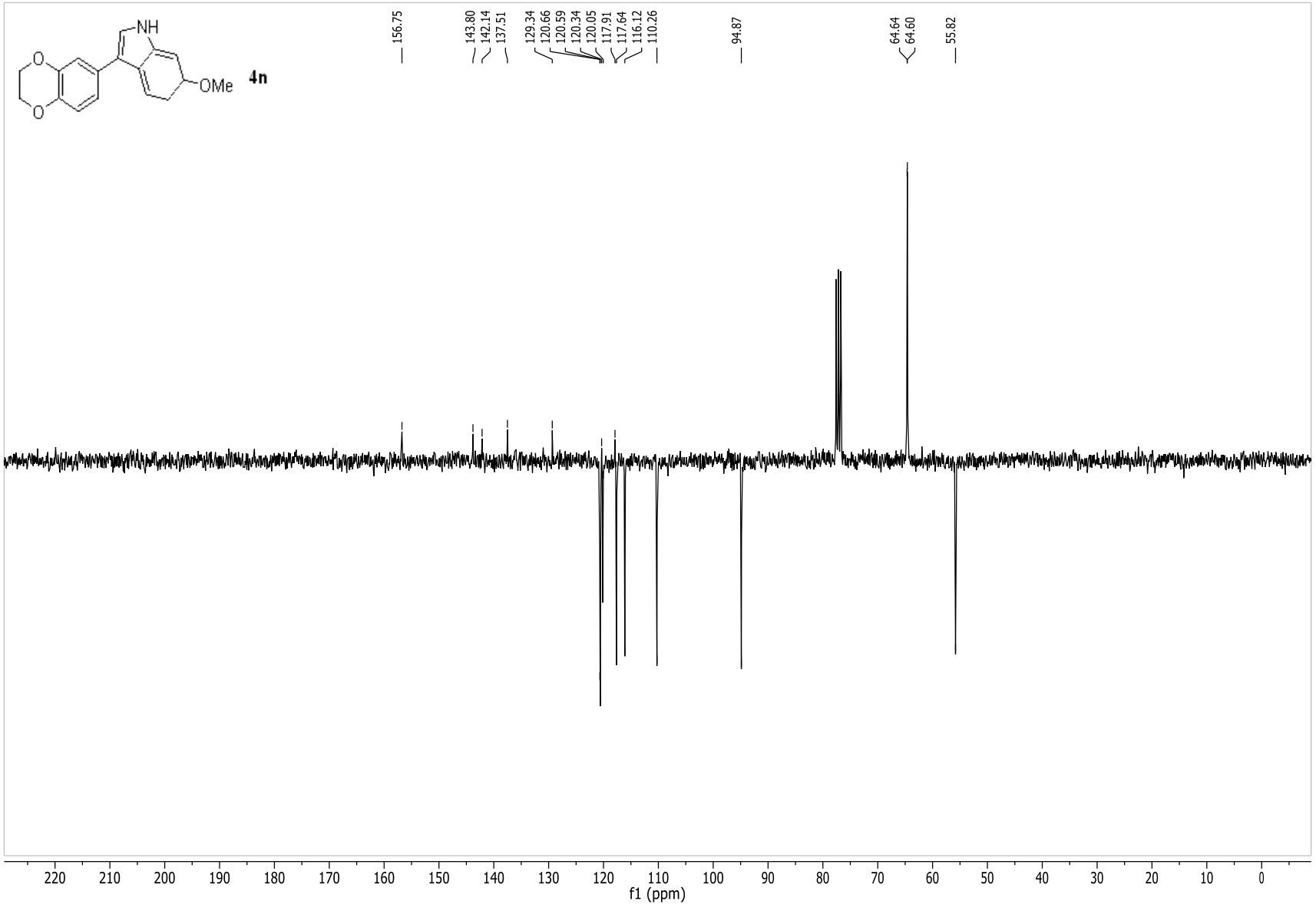
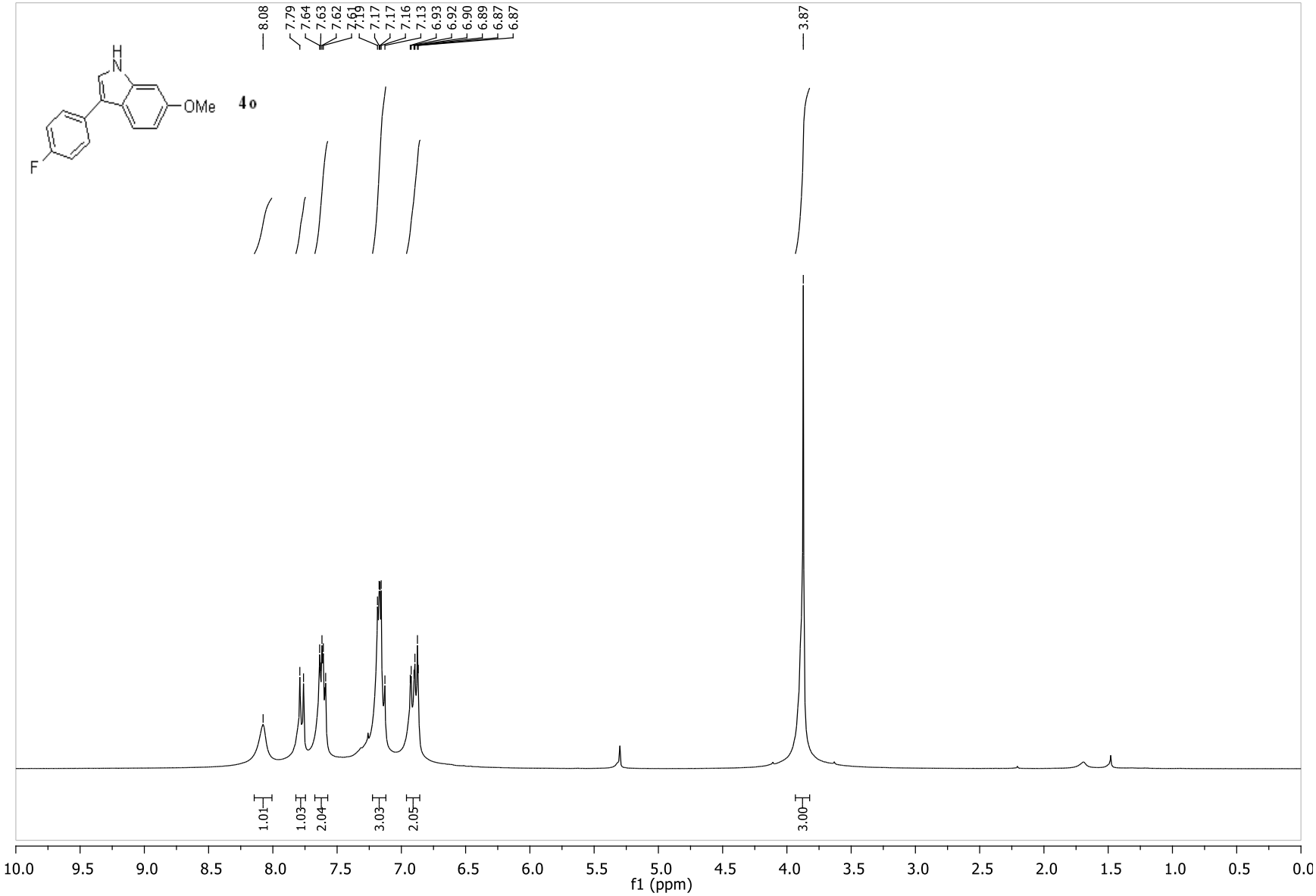
137.57
120.66
120.08
118.45
110.46
105.62
98.28
94.90
55.81
55.52
NH
MeO
OMe
MeO
4m
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.05
7.79
7.76
7.17
7.15
7.12
6.95
6.93
6.89
6.87
6.84
4.31
3.86
NH
O
O
OMe
4n
1.00
1.03
2.05
1.03
1.02
1.03
1.01
4.02
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


NH
OMe
4n
156.75
143.80
142.14
137.51
129.34
120.66
120.59
120.34
120.05
117.91
117.64
116.12
110.26
94.87
64.64
64.60
55.82
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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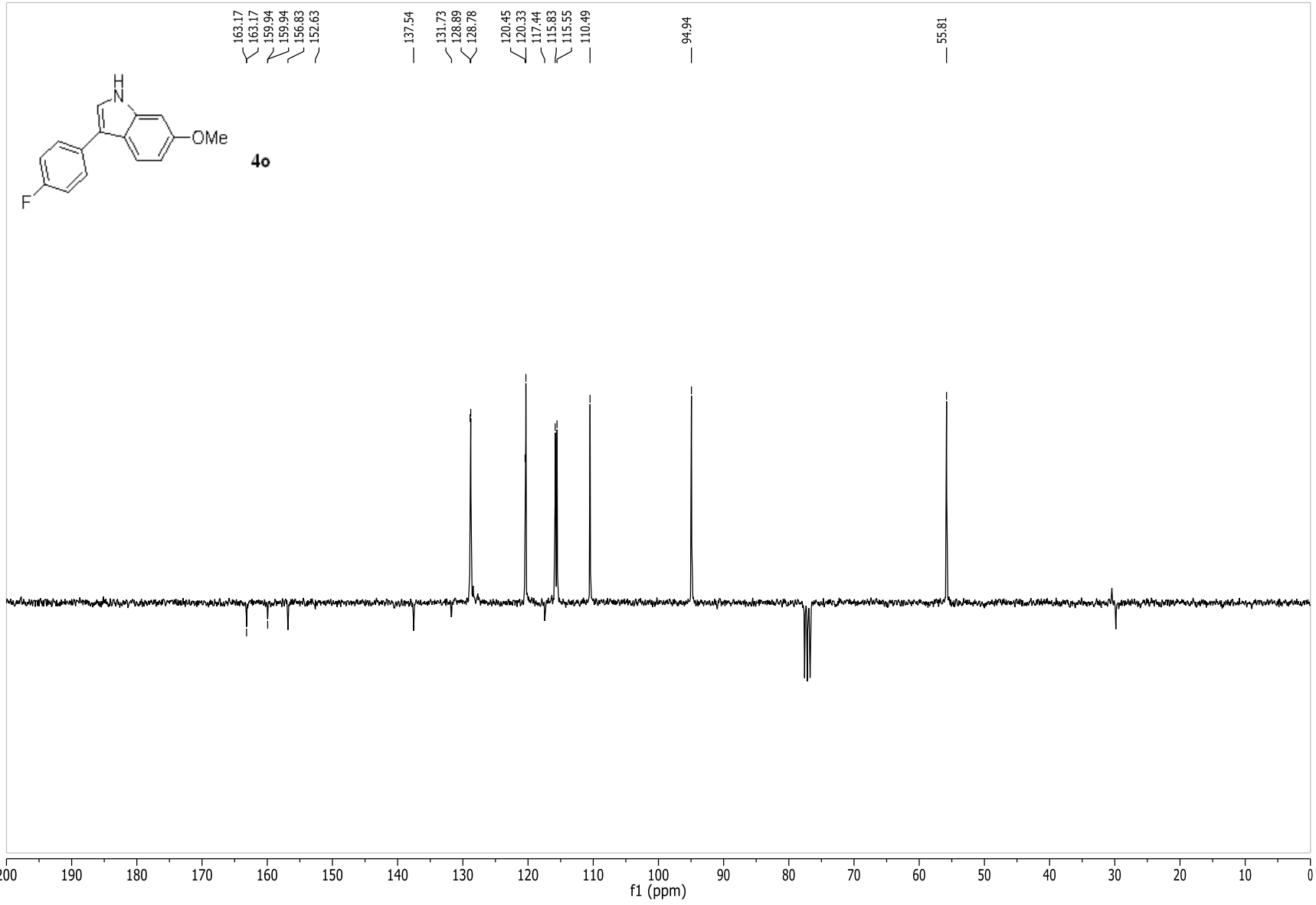
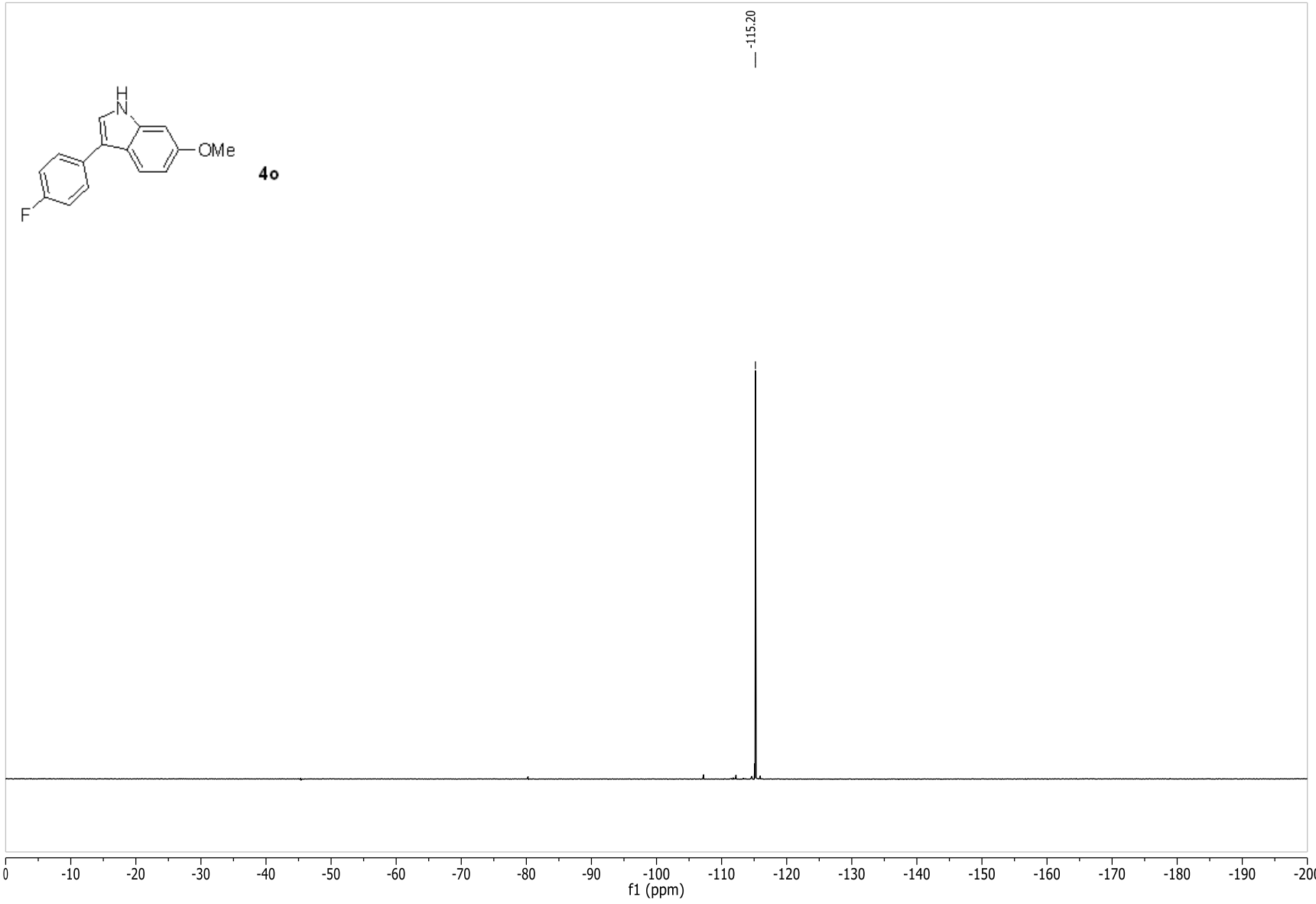
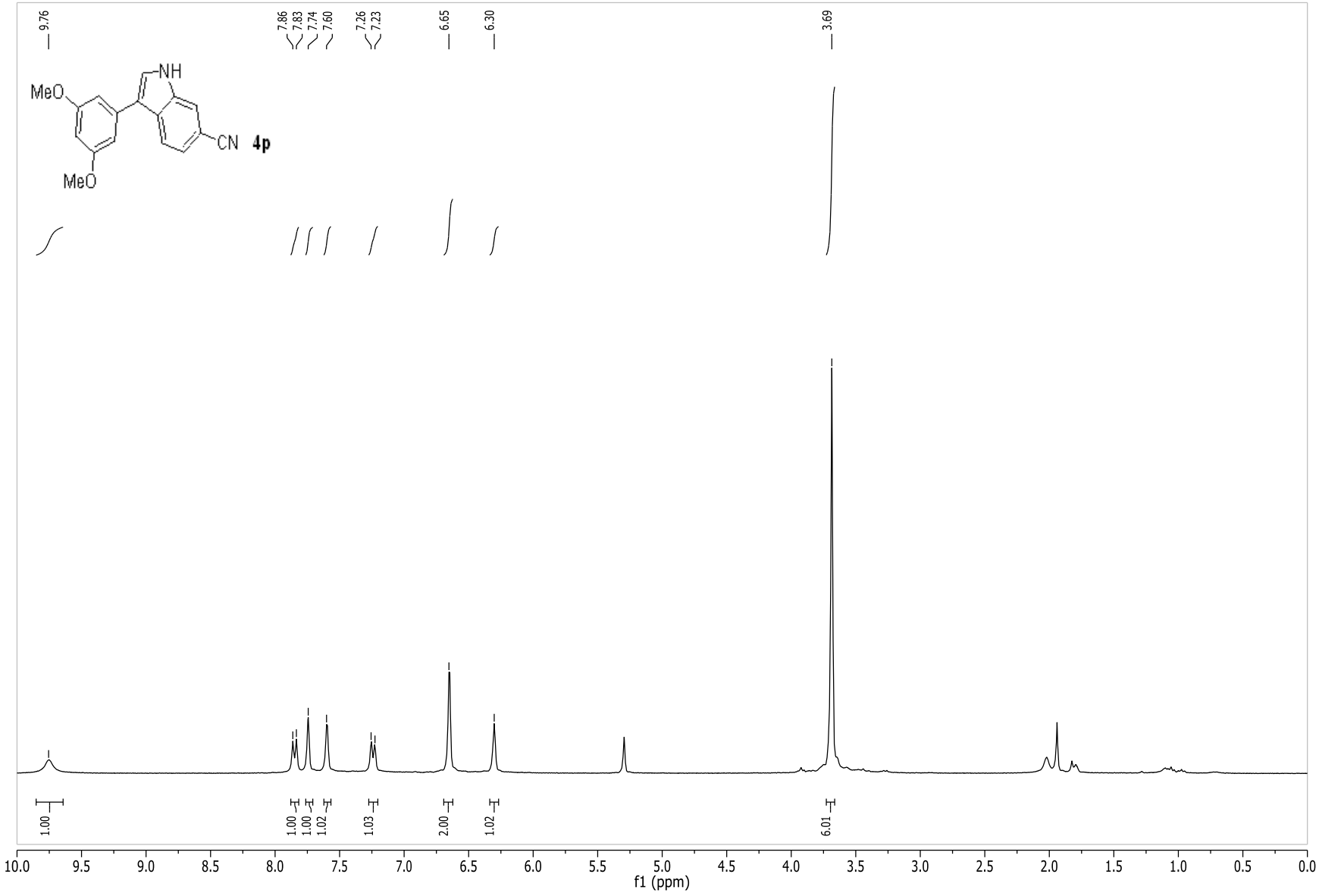
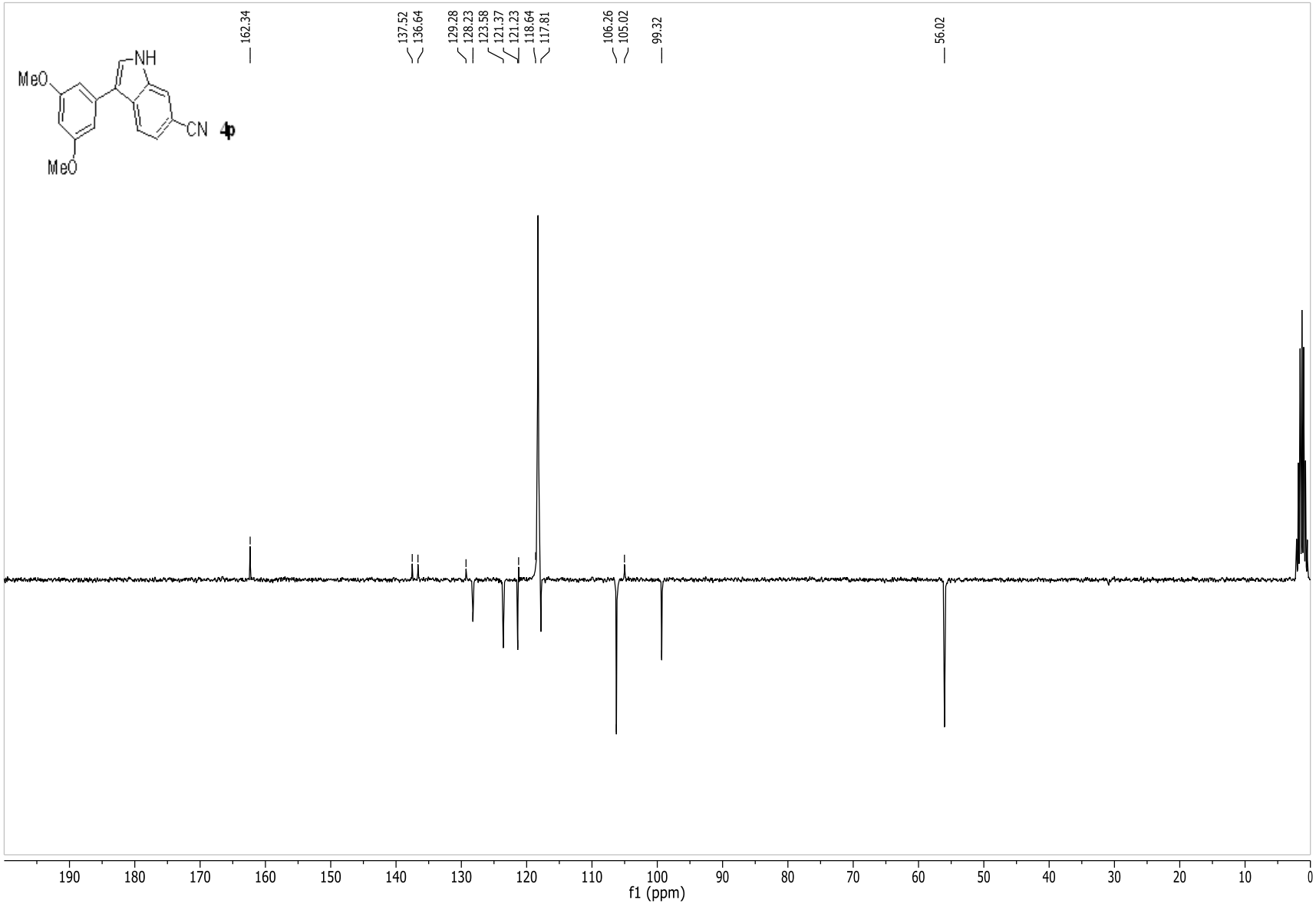
7.79
7.64
7.63
7.62
7.61
7.19
7.17
7.17
7.16
7.13
6.93
6.92
6.90
6.89
6.87
6.87
3.87
OMe
4o
F
1.01
1.03
2.04
3.03
2.05
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


163.17
163.17
159.94
159.94
156.83
152.63
137.54
131.73
128.89
128.78
120.45
120.33
117.44
115.83
115.55
110.49
94.94
55.81
OMe
F
4o
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


-115.20
H
N
OMe
F
4o
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
f1 (ppm)


9.76
7.86
7.83
7.74
7.60
7.26
7.23
6.65
6.30
3.69
NH
MeO
MeO
CN
4p
1.00
1.00
1.00
1.02
1.03
2.00
1.02
6.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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136.64
129.28
128.23
123.58
121.37
121.23
118.64
117.81
106.26
105.02
99.32
56.02
NH
MeO
MeO
CN
4p
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
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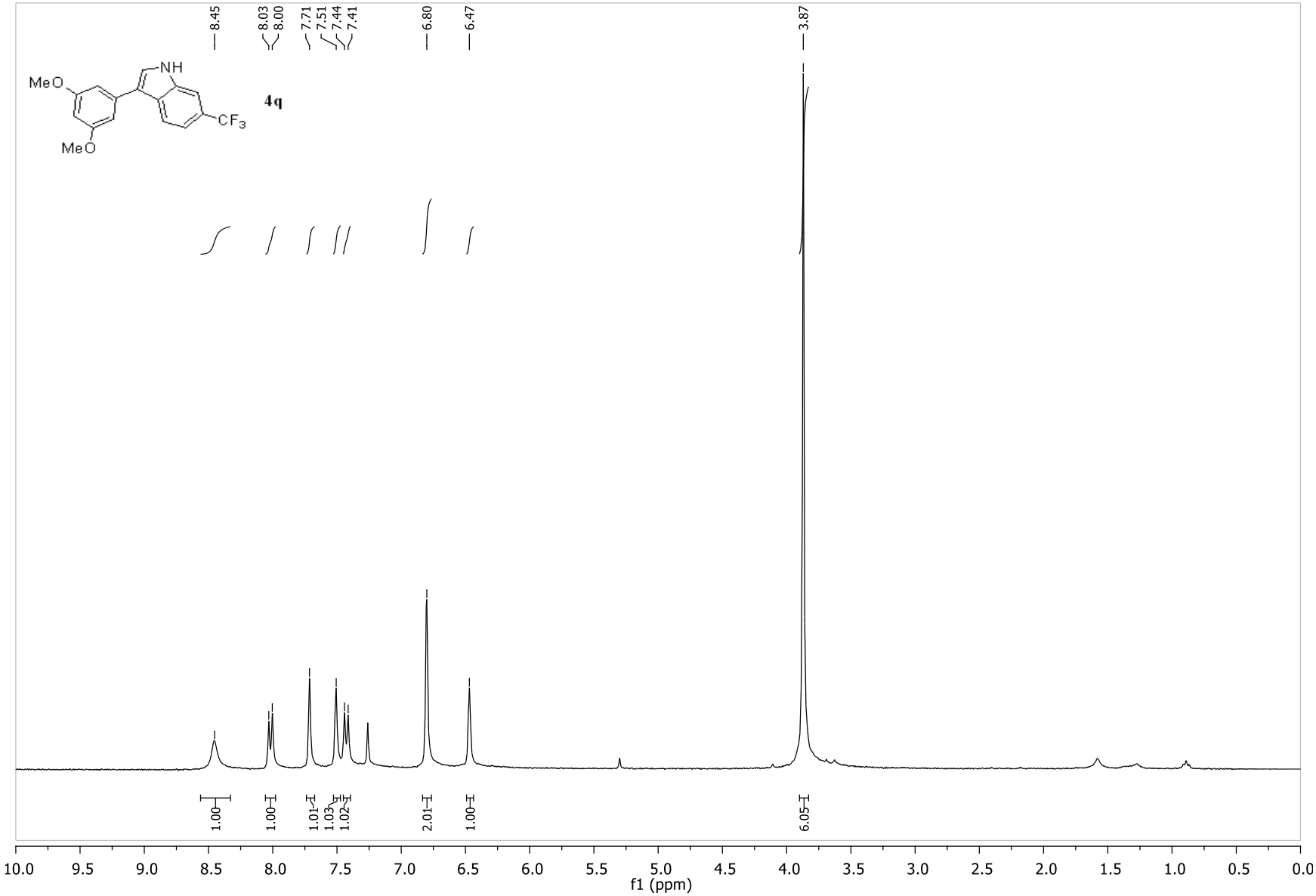
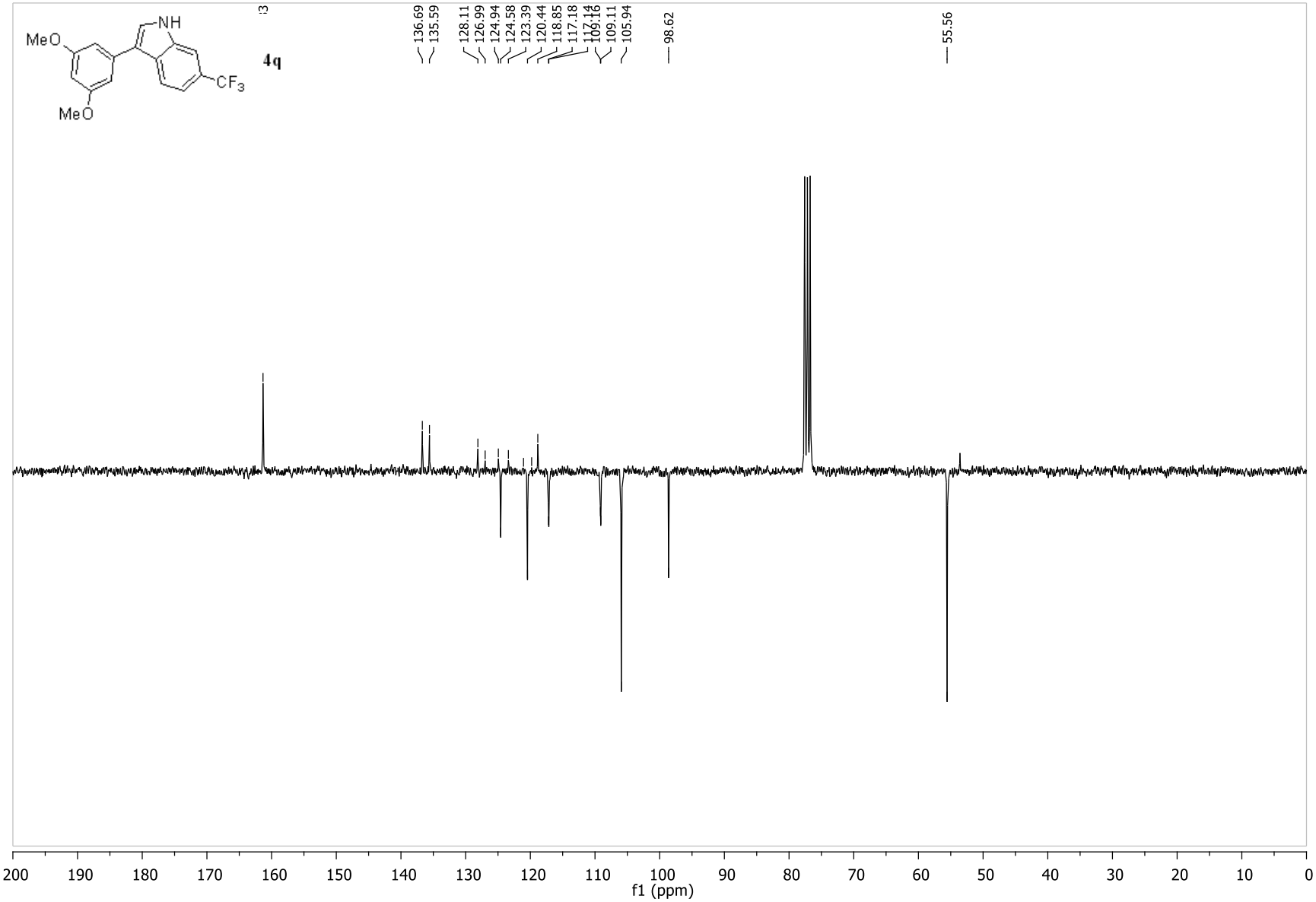
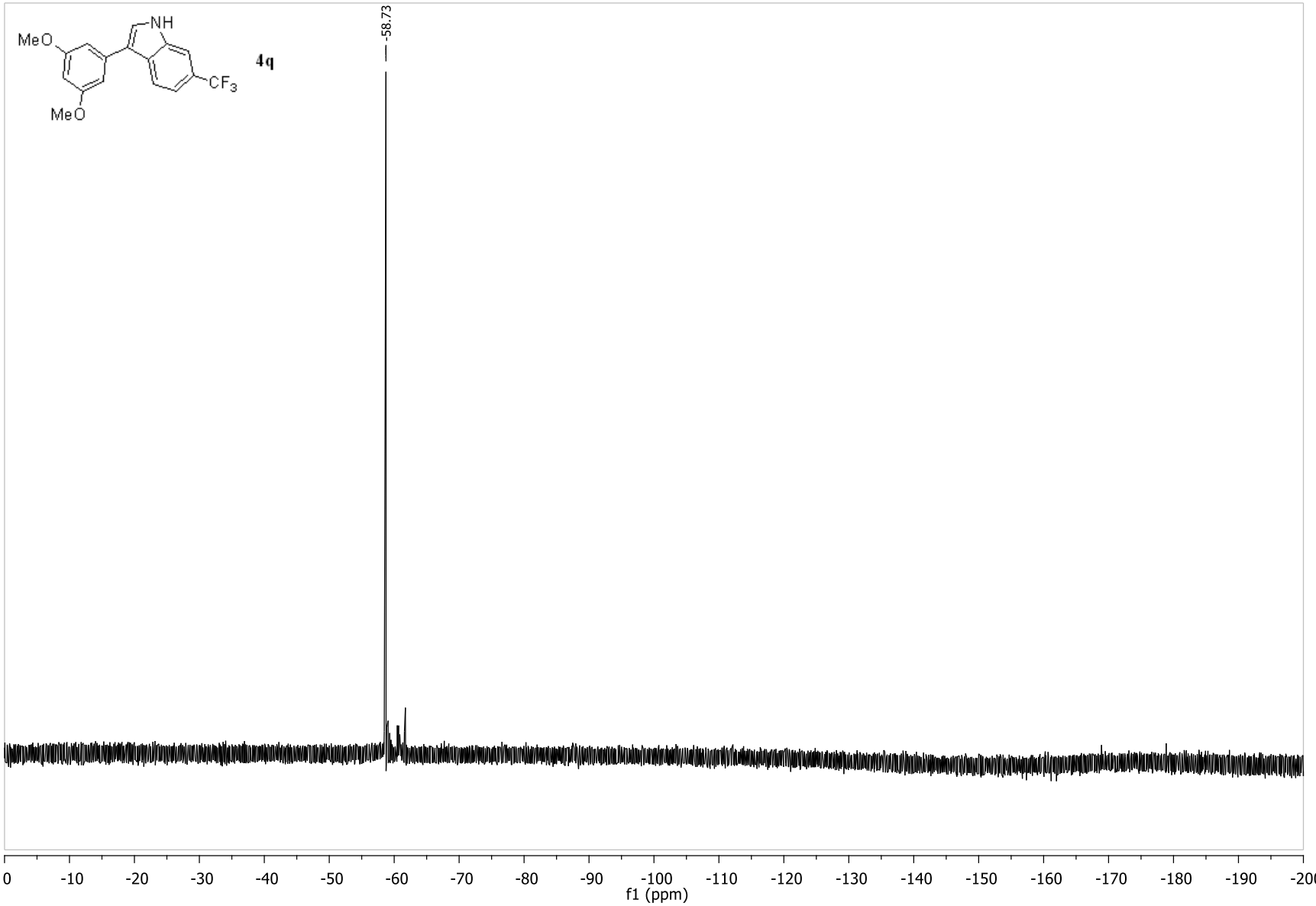
f1 (ppm)


8.45
8.03
8.00
7.71
7.51
7.44
7.41
6.80
6.47
3.87
NH
MeO
MeO
CF3
4q
1.00
1.00
1.01
1.03
1.02
2.01
1.00
6.05
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


MeO
NH
MeO
CF3
4q
136.69
135.59
128.11
126.99
124.94
124.58
123.39
120.44
118.85
117.18
109.16
109.11
105.94
98.62
55.56
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


MeO
NH
CF3
MeO
4q
-58.73
0
-10
-20
-30
-40
-50
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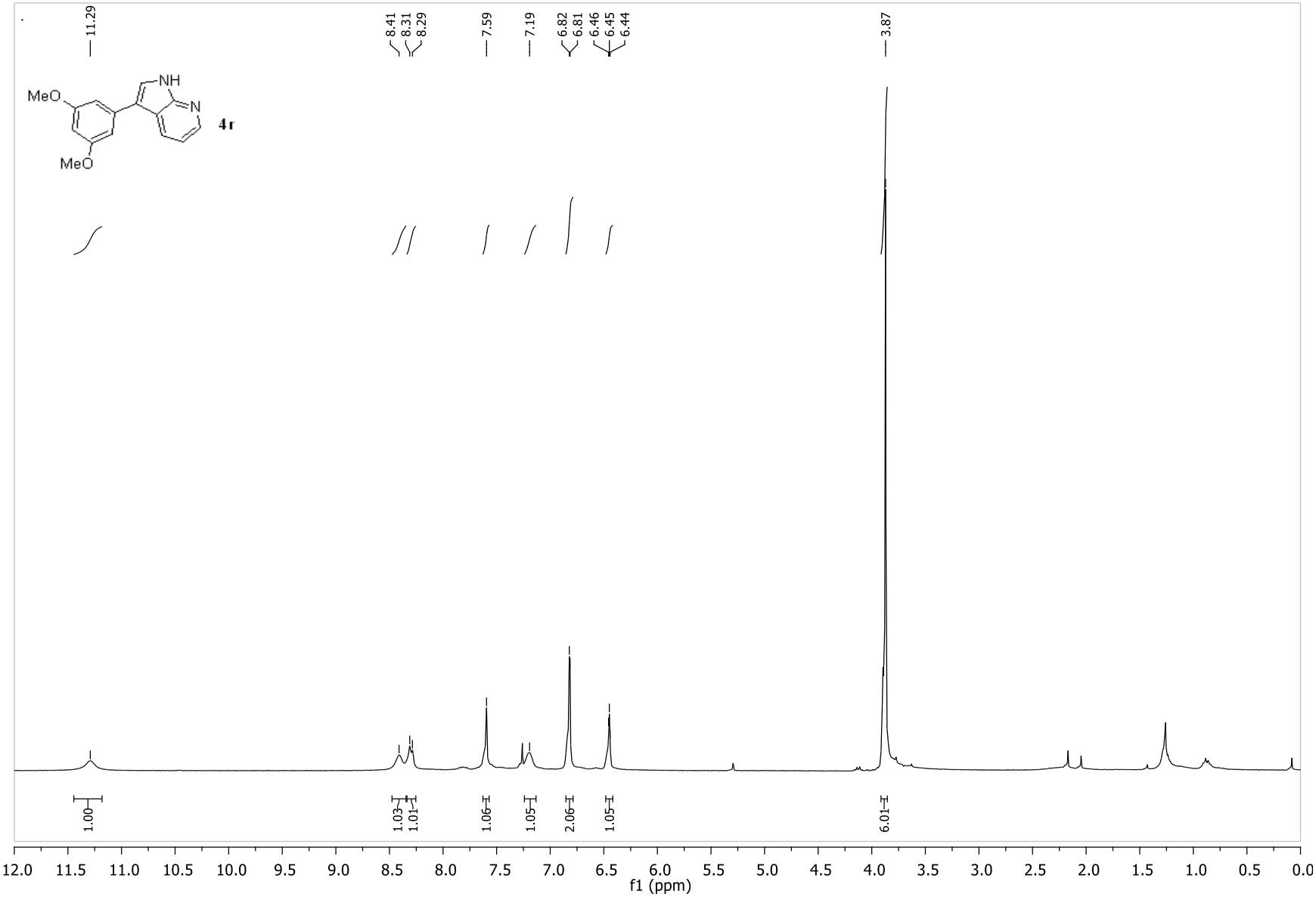
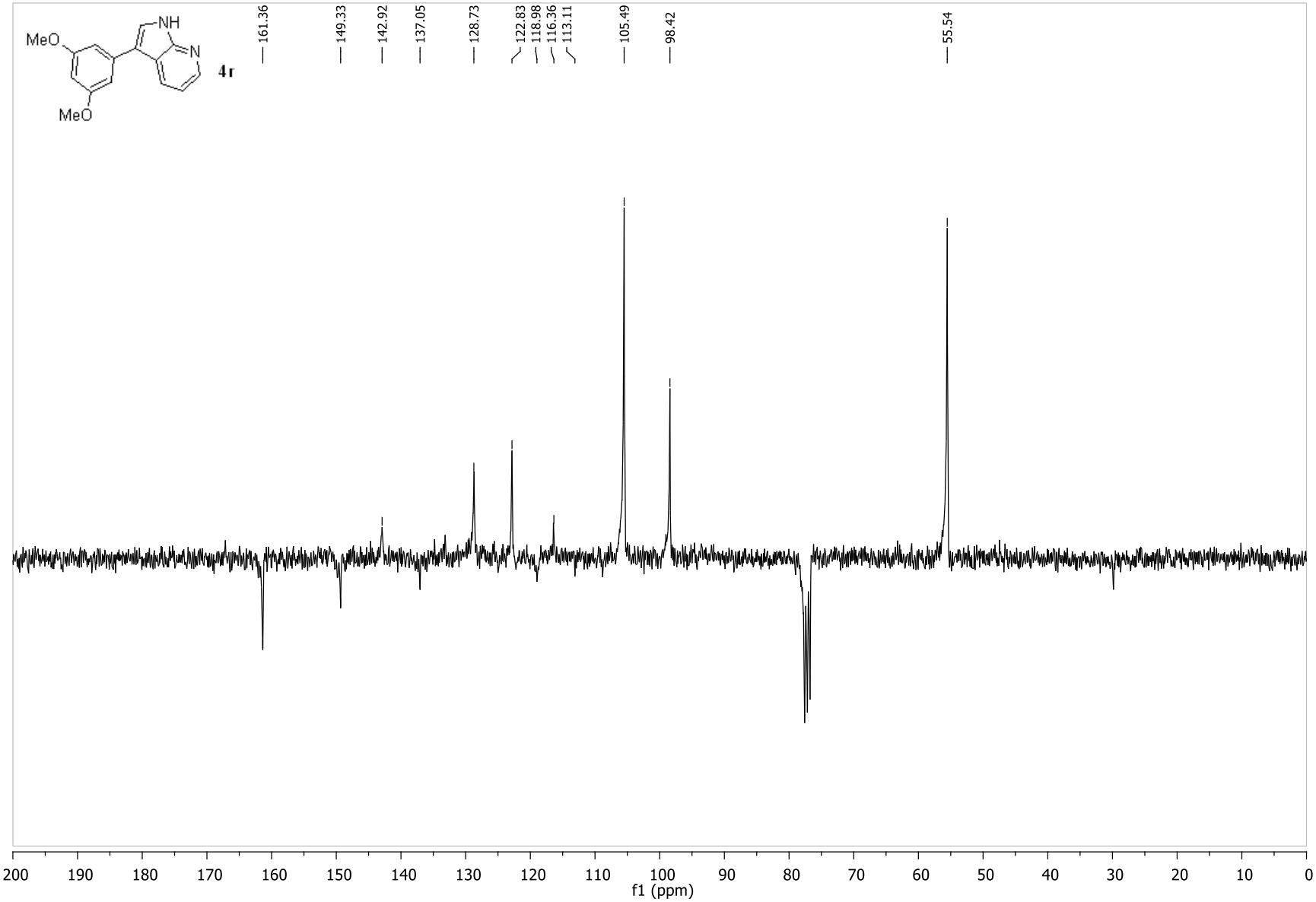
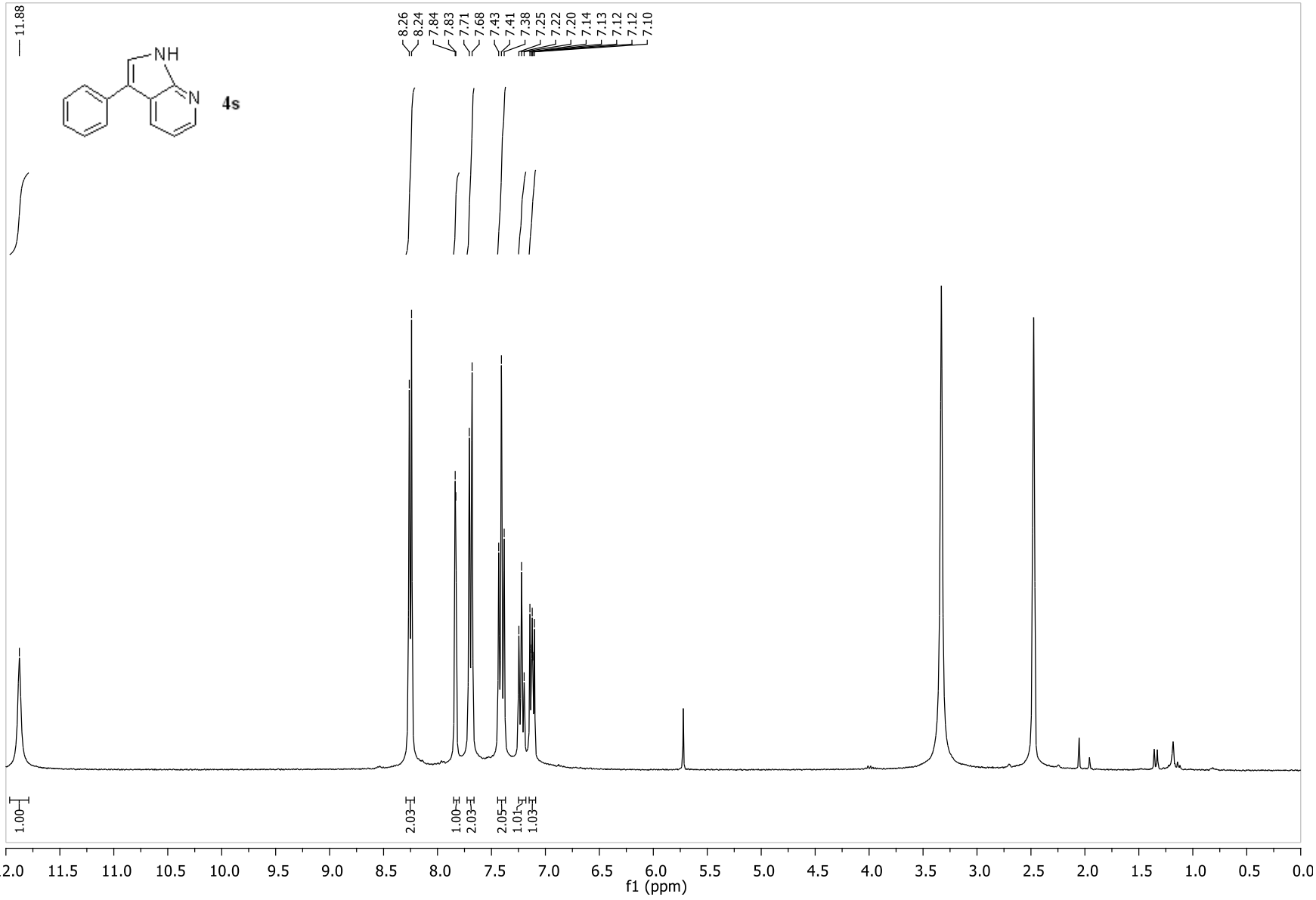
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
f1 (ppm)


11.29
8.41
8.31
8.29
7.59
7.19
6.82
6.81
6.46
6.45
6.44
3.87
MeO
MeO
NH
N
4r
1.00
1.03
1.01
1.06
1.05
2.06
1.05
6.01
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


MeO
MeO
NH
N
4r
161.36
149.33
142.92
137.05
128.73
122.83
118.98
116.36
113.11
105.49
98.42
55.54
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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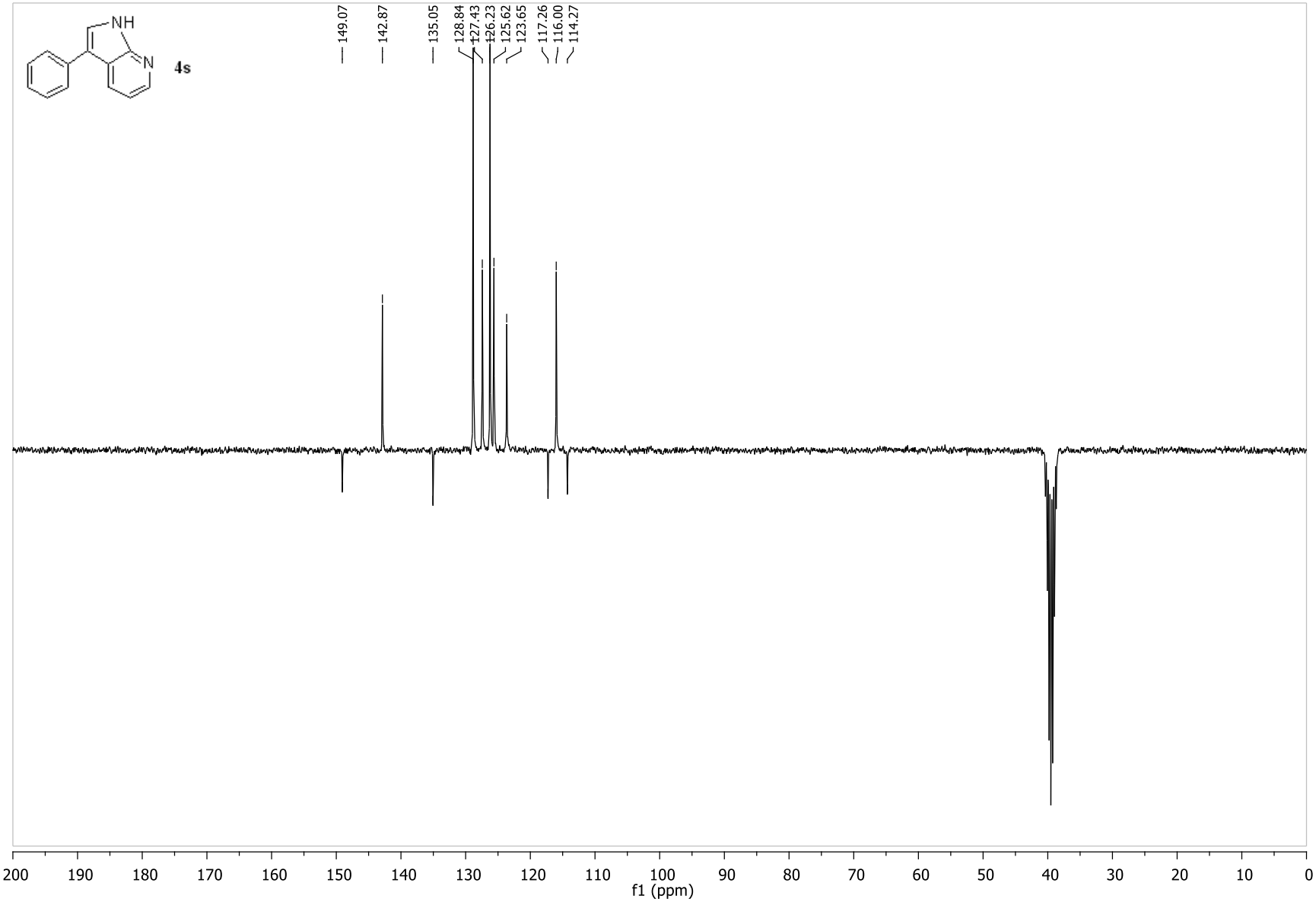
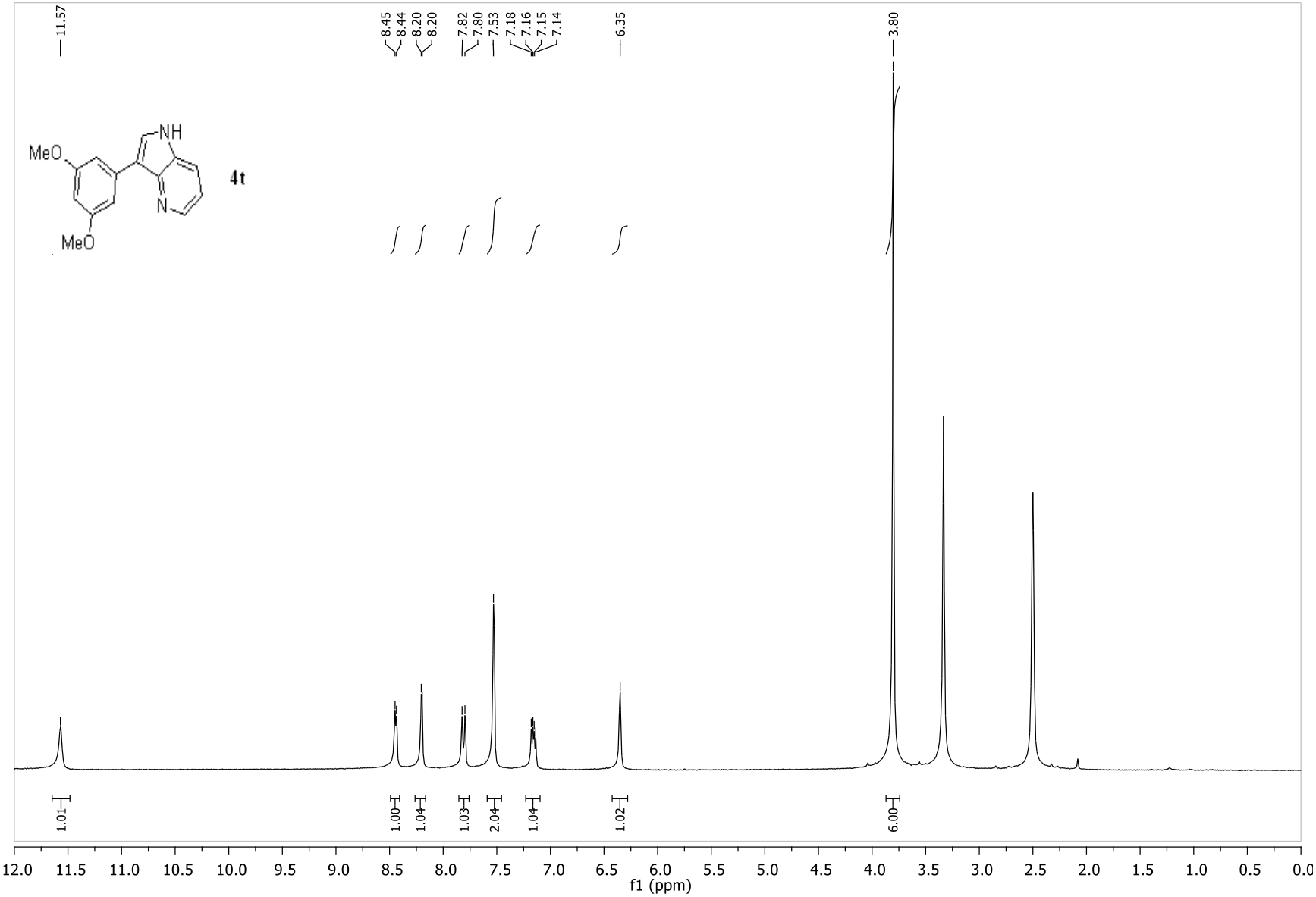
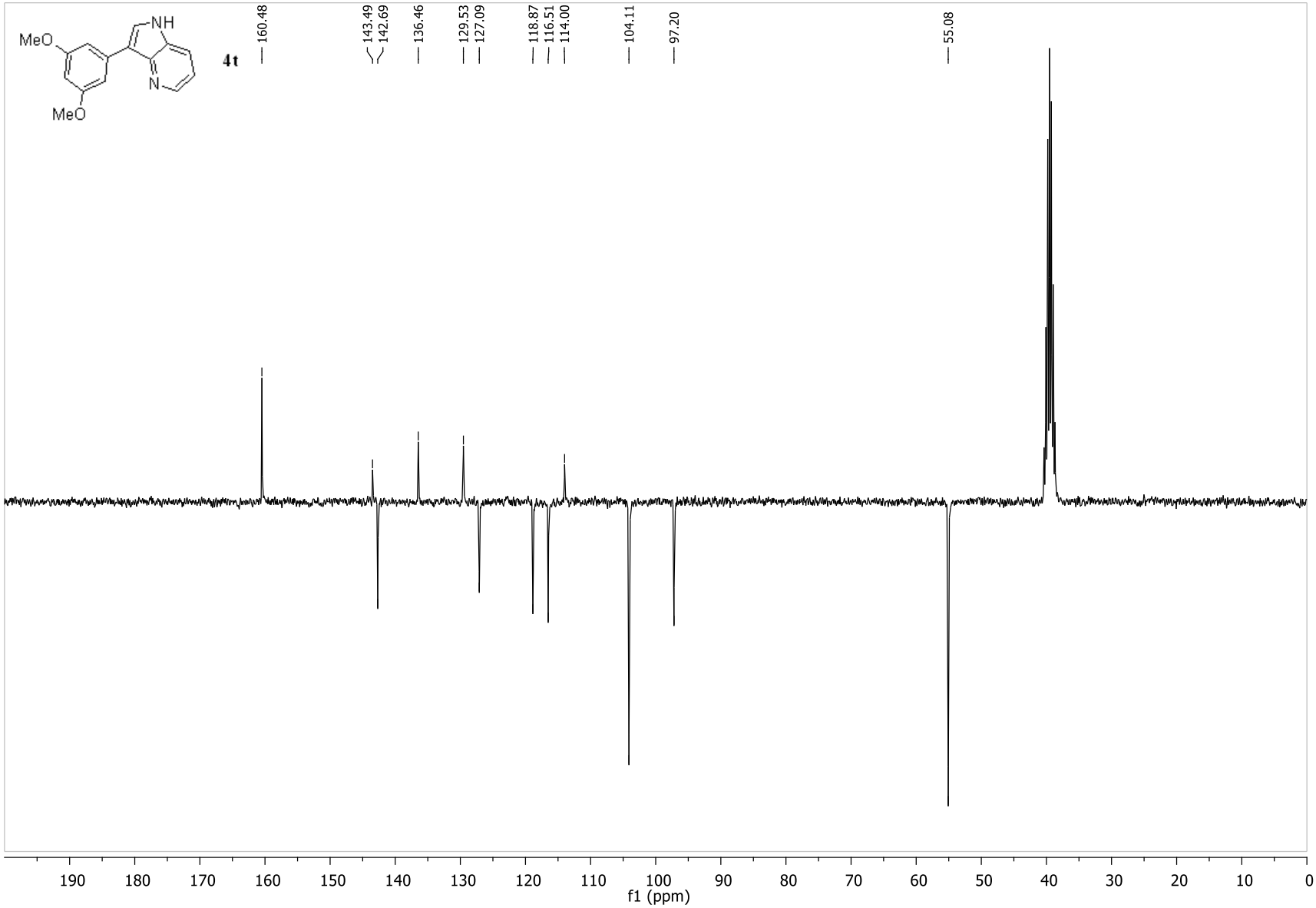
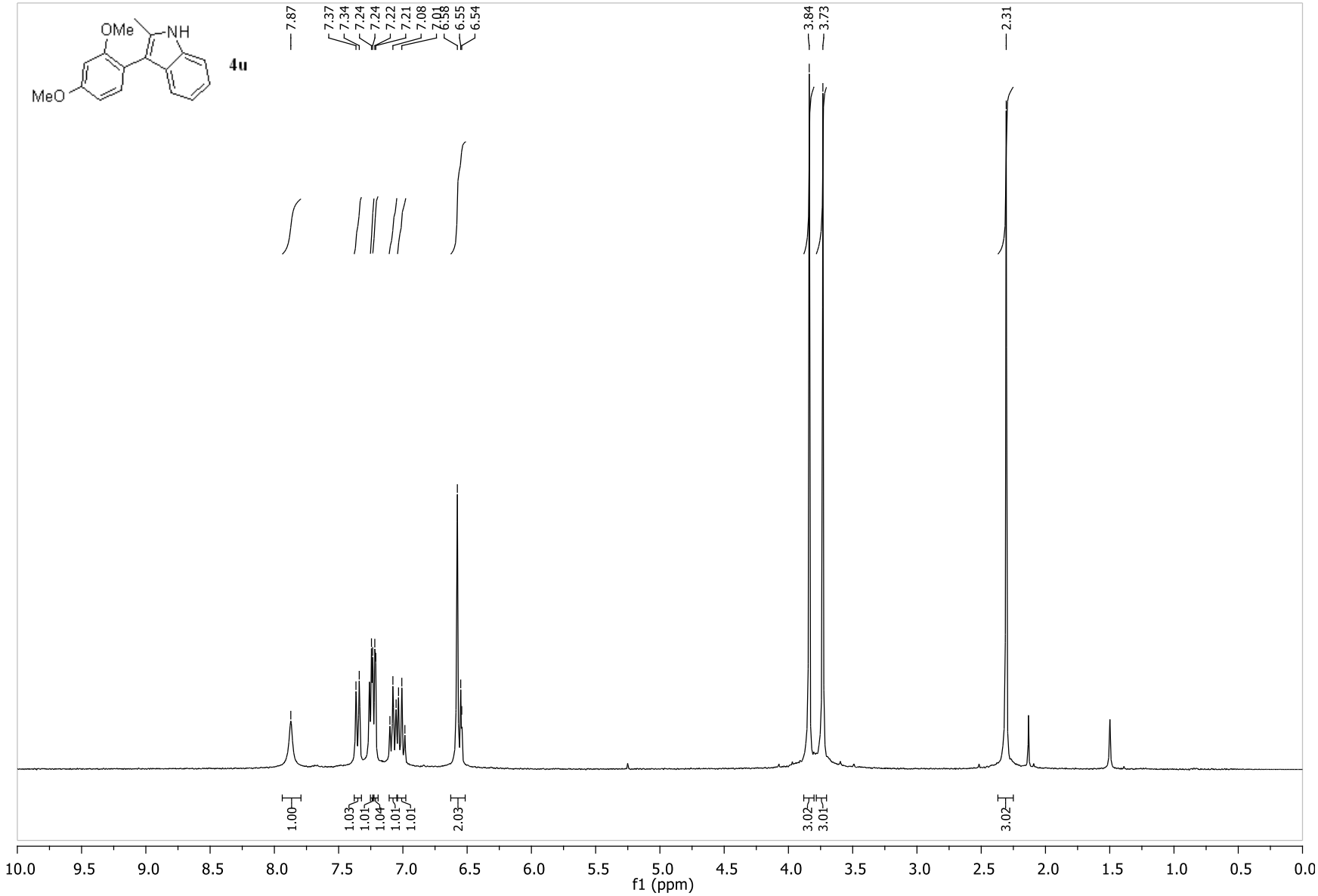
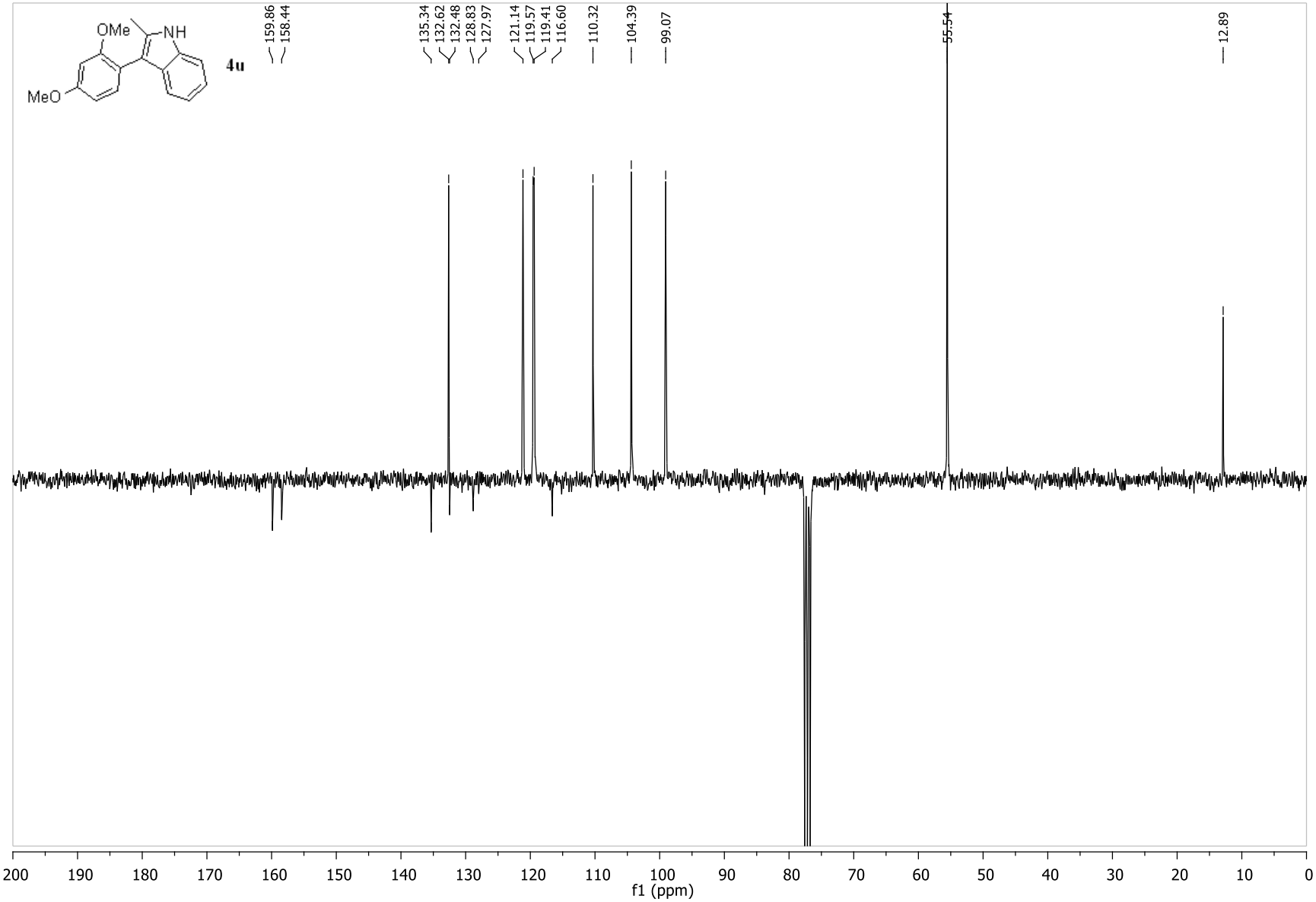
8.24
7.84
7.83
7.71
7.68
7.43
7.41
7.38
7.25
7.22
7.20
7.14
7.13
7.12
7.12
7.10
NH
N
4s
1.00
2.03
1.00
2.03
2.05
1.01
1.03
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

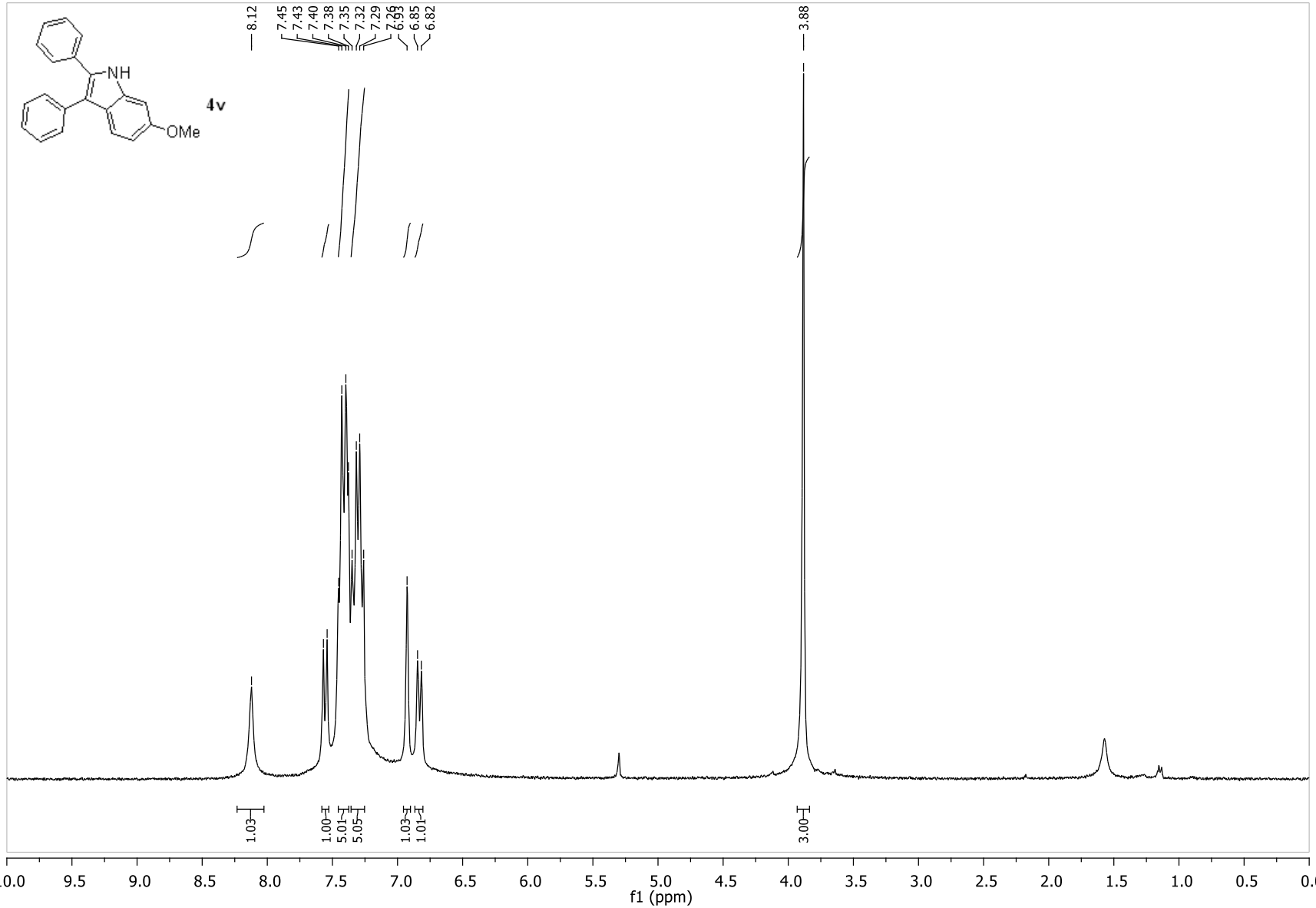

NH
N
4s
149.07
142.87
135.05
128.84
127.43
126.23
125.62
123.65
117.26
116.00
114.27
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

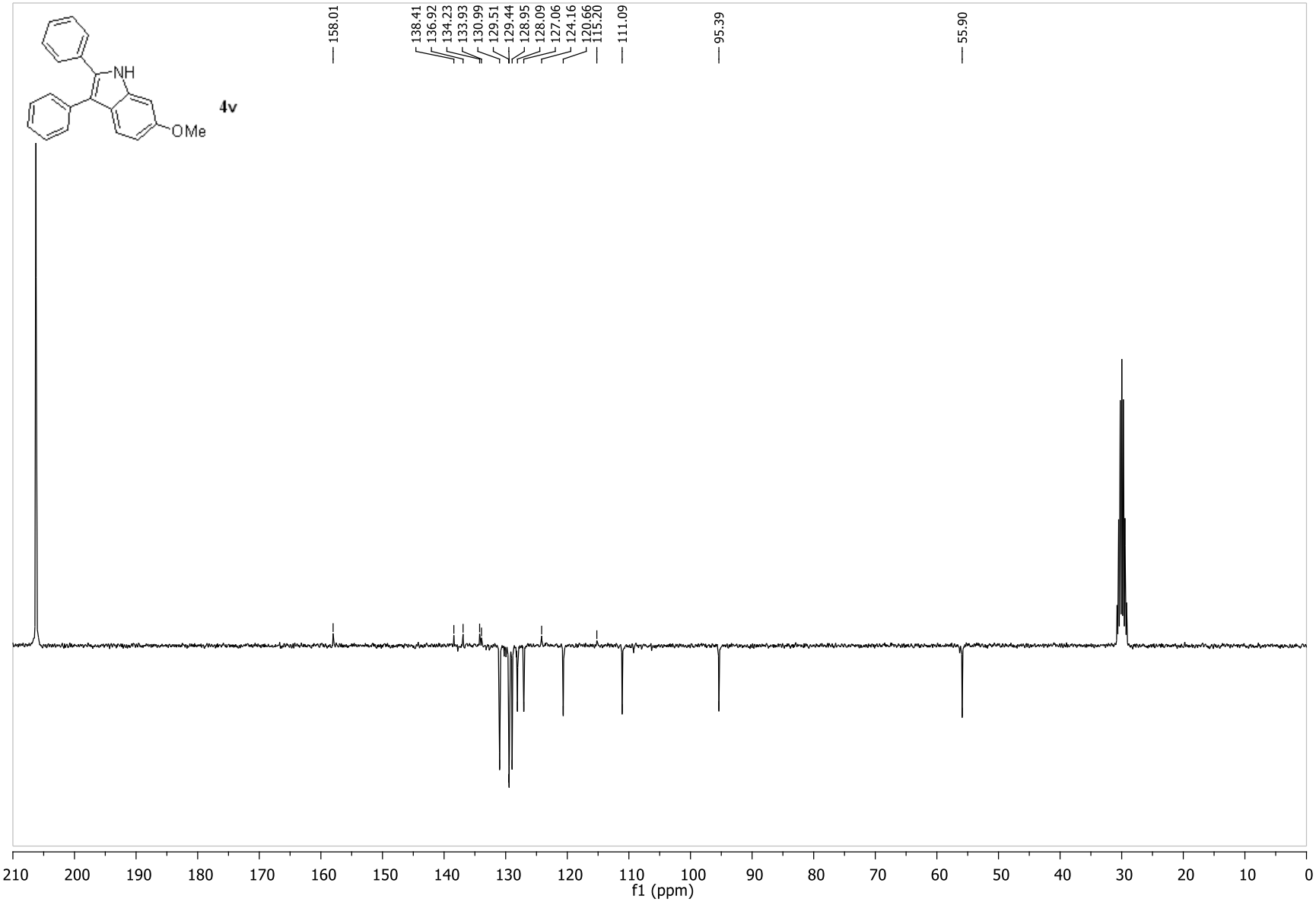

11.57
8.45
8.44
8.20
8.20
7.82
7.80
7.53
7.18
7.16
7.15
7.14
6.35
3.80
NH
MeO
MeO
N
4t
1.01
1.00
1.04
1.03
2.04
1.04
1.02
6.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

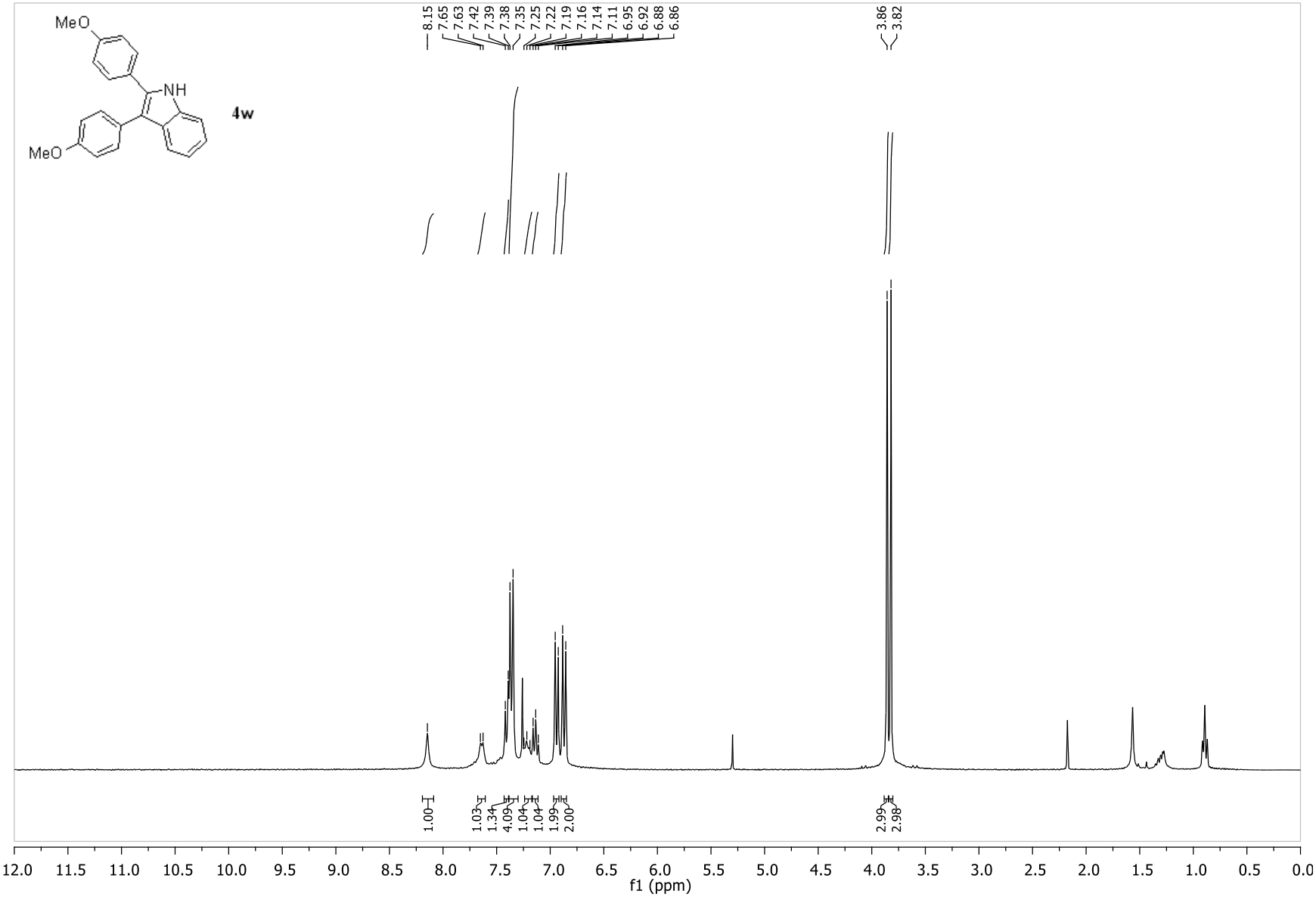

MeO
MeO
NH
N
4t
160.48
143.49
142.69
136.46
129.53
127.09
118.87
116.51
114.00
104.11
97.20
55.08
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

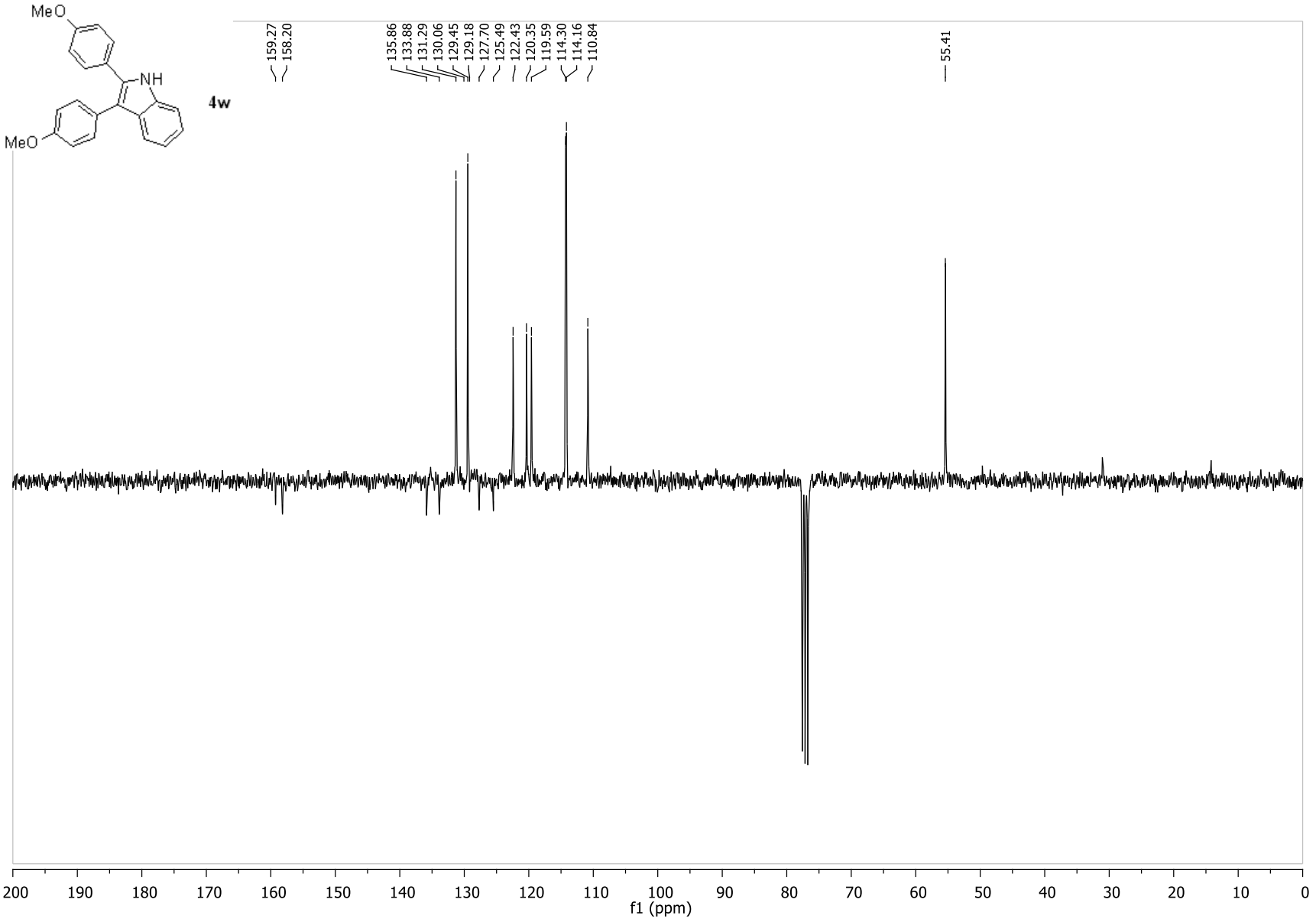

OMe
NH
MeO
4u
7.87
7.37
7.34
7.24
7.24
7.22
7.21
7.08
7.01
6.58
6.55
6.54
3.84
3.73
2.31
1.00
1.03
1.01
1.04
1.01
1.01
2.03
3.02
3.01
3.02
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

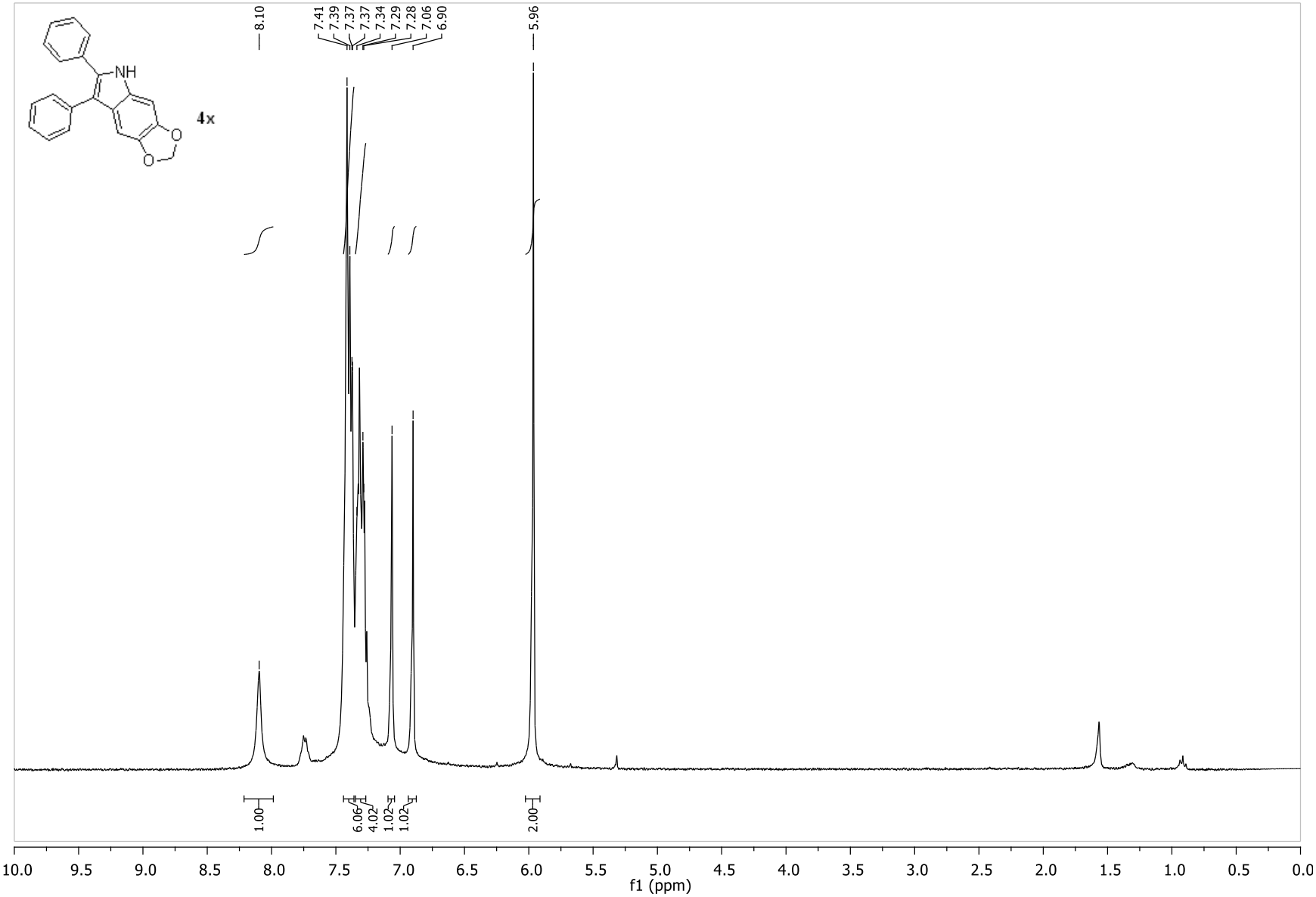

OMe
NH
MeO
4u
159.86
158.44
135.34
132.62
132.48
128.83
127.97
121.14
119.57
119.41
116.60
110.32
104.39
99.07
55.54
12.89
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

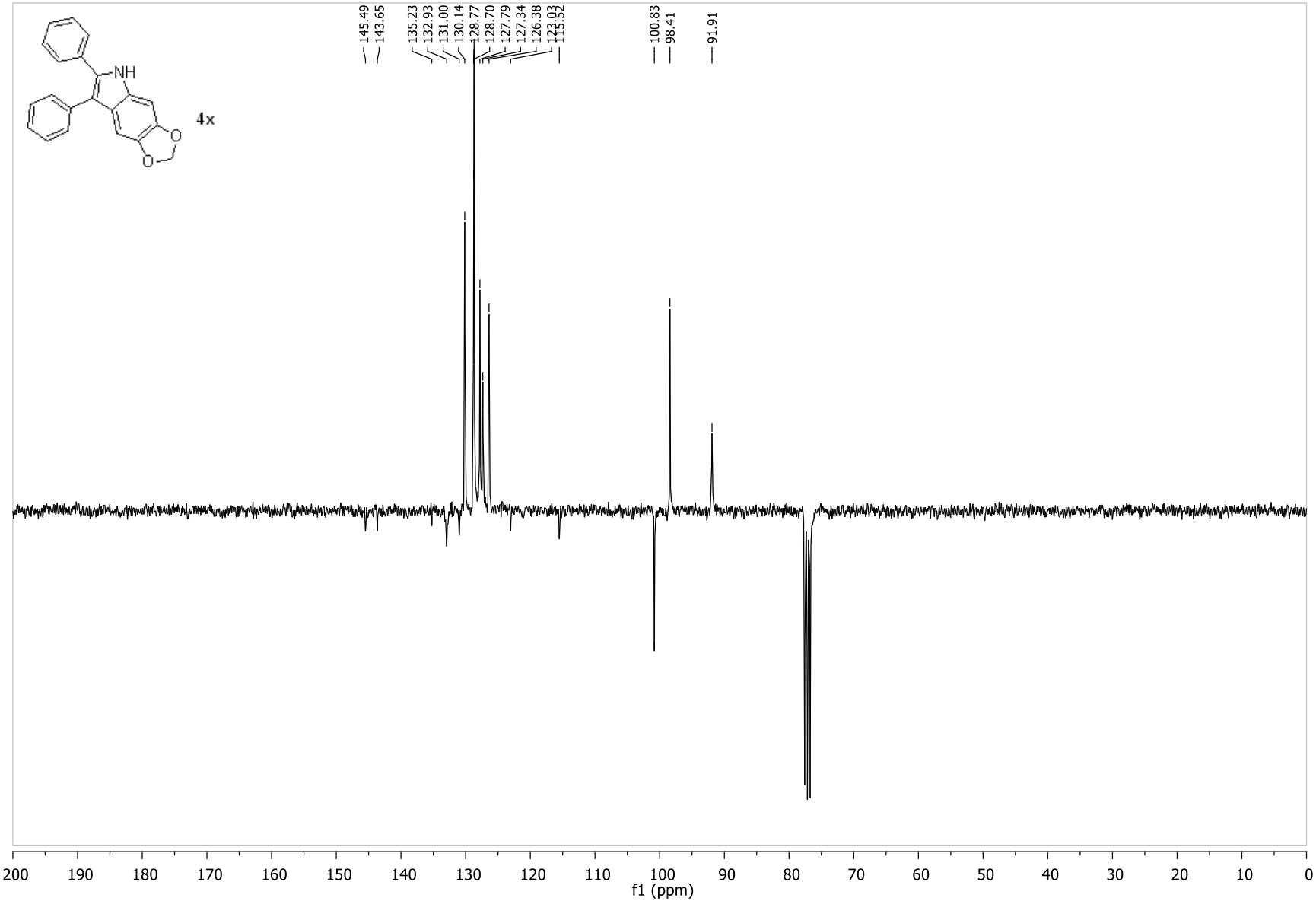

NH
OMe
4v
8.12
7.45
7.43
7.40
7.38
7.35
7.32
7.29
7.26
6.93
6.85
6.82
3.88
1.03
1.00
5.01
5.05
1.03
1.01
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

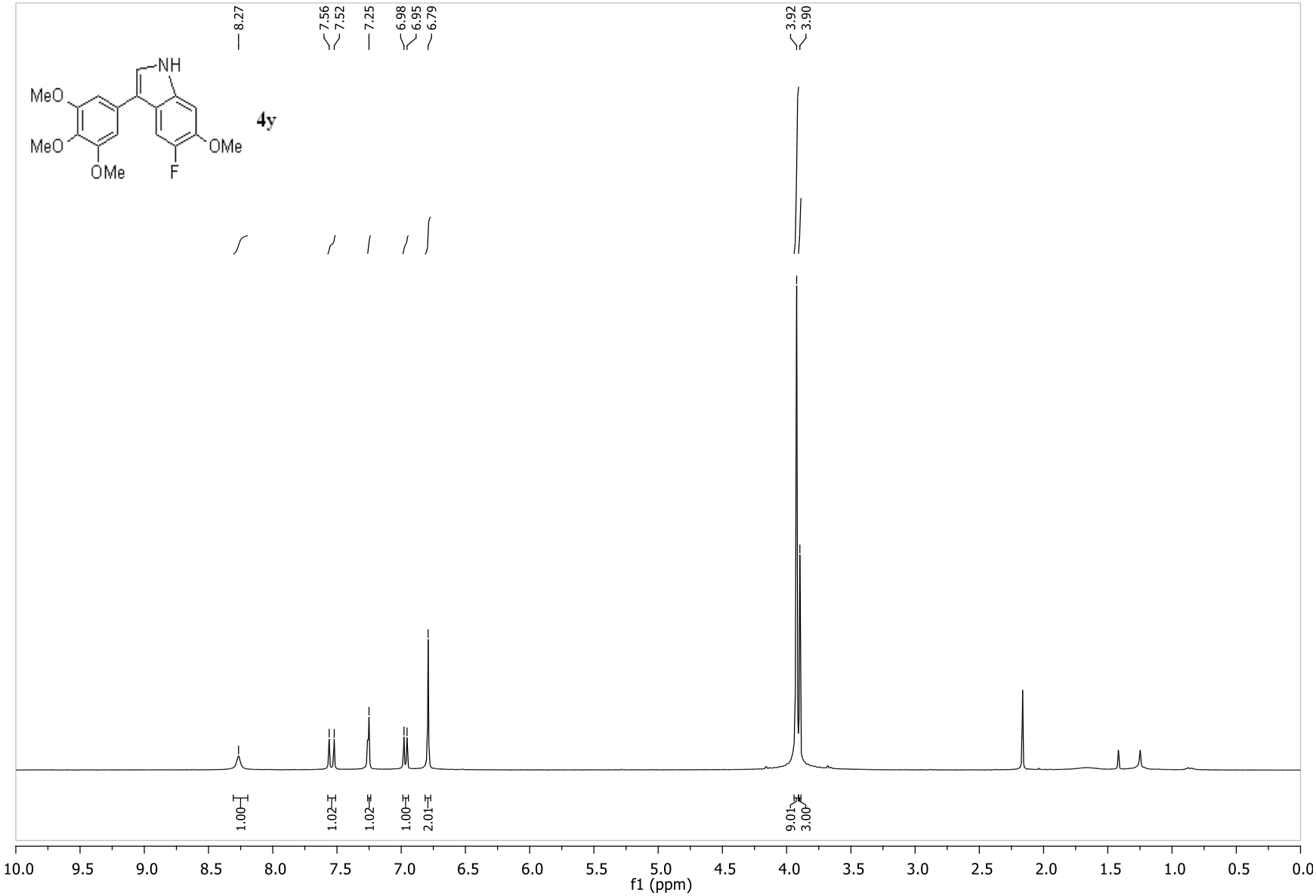

158.01
138.41
136.92
134.23
133.93
130.99
129.51
129.44
128.95
128.09
127.06
124.16
120.66
115.20
111.09
95.39
55.90
NH
OMe
4v
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

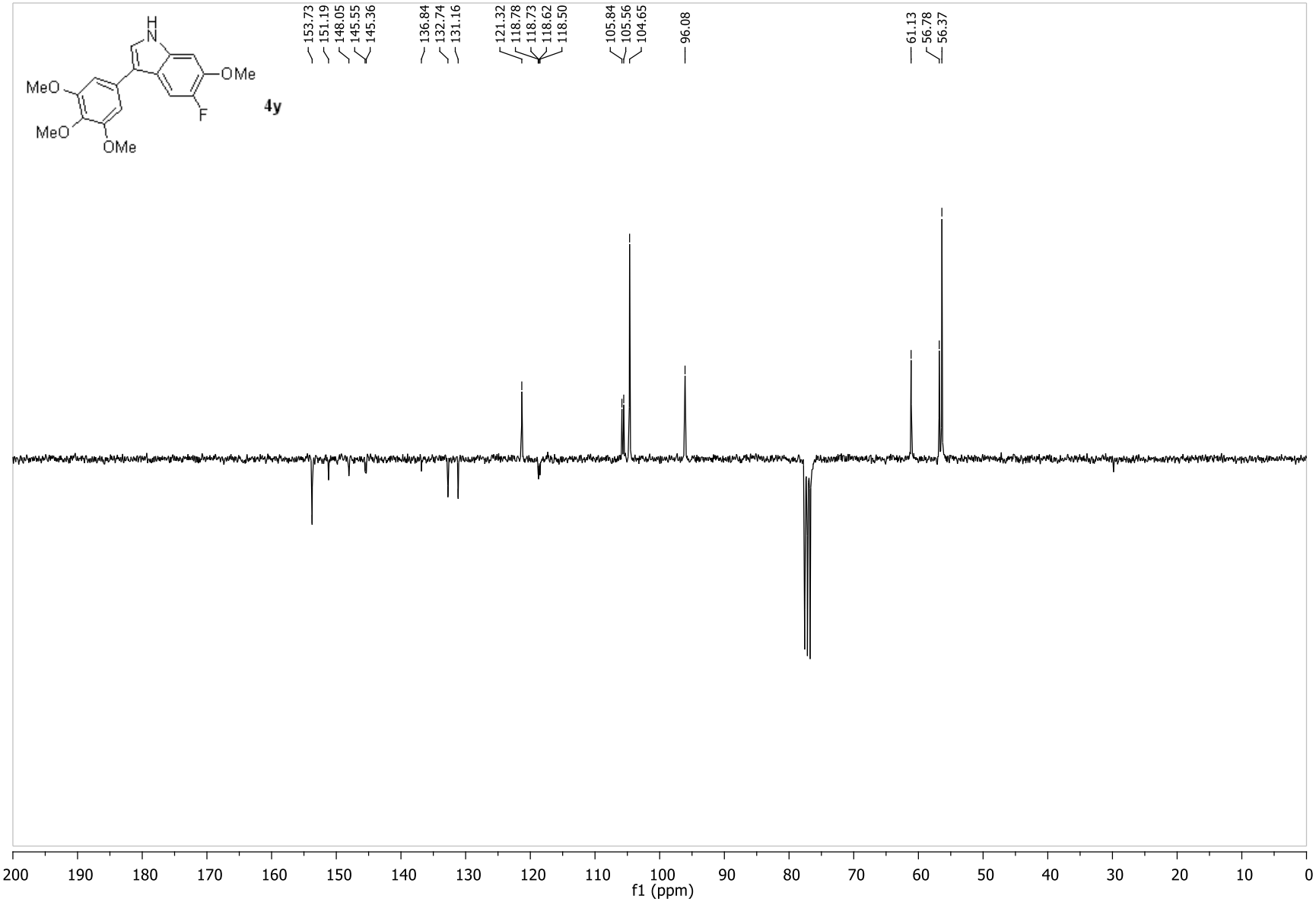

MeO
NH
MeO
4w
8.15
7.65
7.63
7.42
7.39
7.38
7.35
7.25
7.22
7.19
7.16
7.14
7.11
6.95
6.92
6.88
6.86
3.86
3.82
1.00
1.03
1.34
4.09
1.04
1.99
2.00
2.99
2.98
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

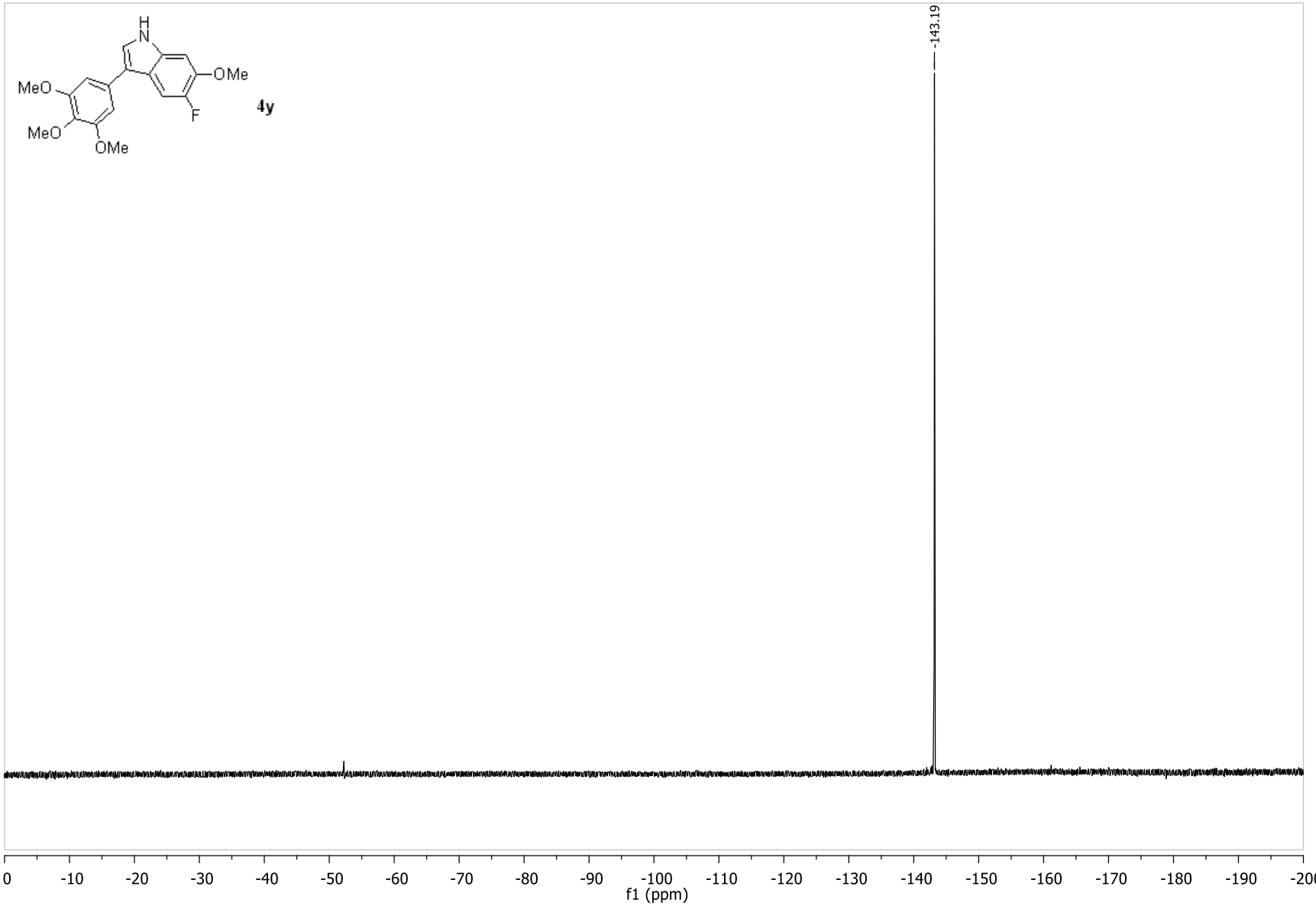

MeO
NH
MeO
4w
159.27
158.20
135.86
133.88
131.29
130.06
129.45
129.18
127.70
125.49
122.43
120.35
119.59
114.30
114.16
110.84
55.41
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

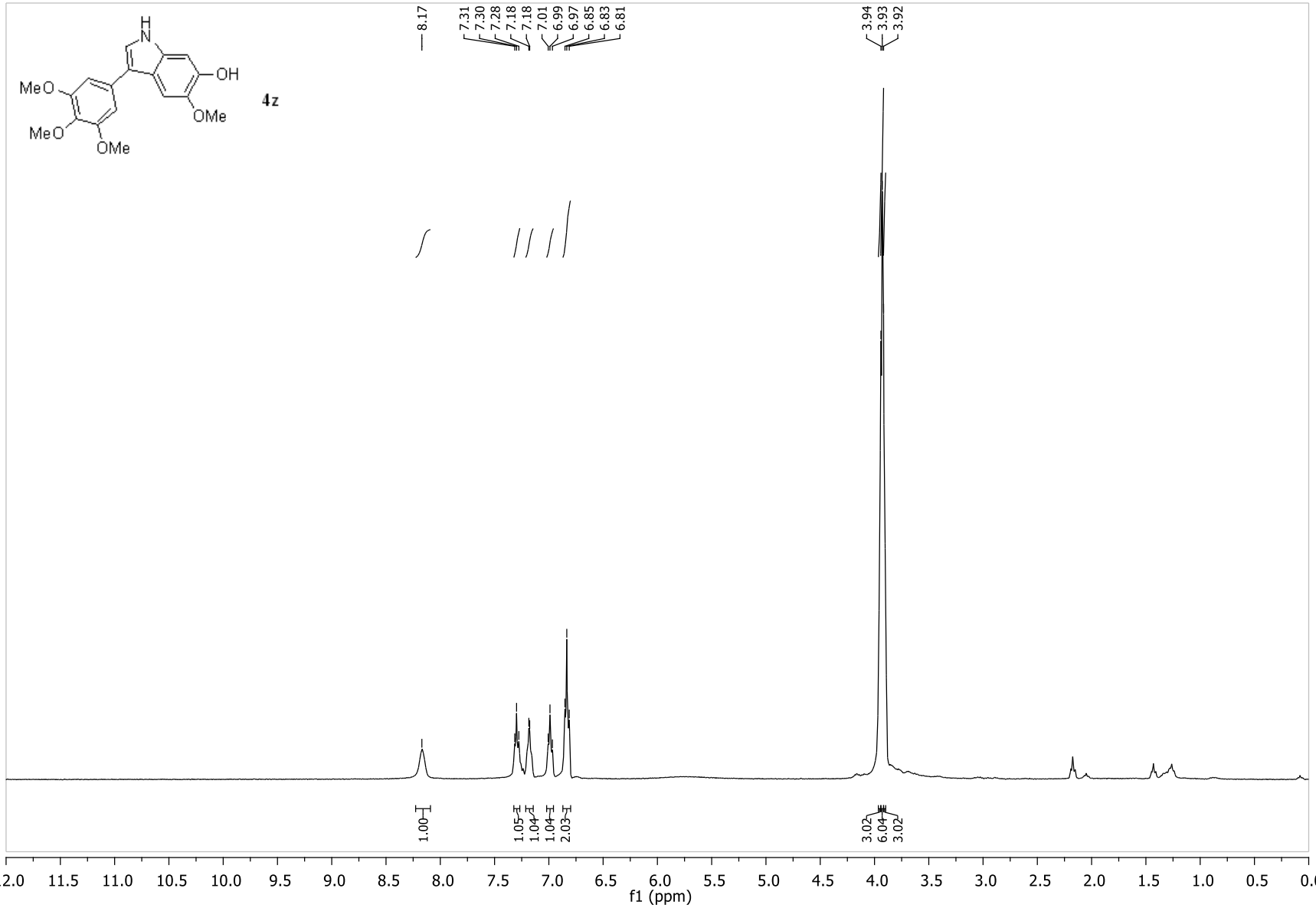

NH
O
O
4x
8.10
7.41
7.39
7.37
7.37
7.34
7.29
7.28
7.06
6.90
5.96
1.00
6.06
4.02
1.02
1.02
2.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

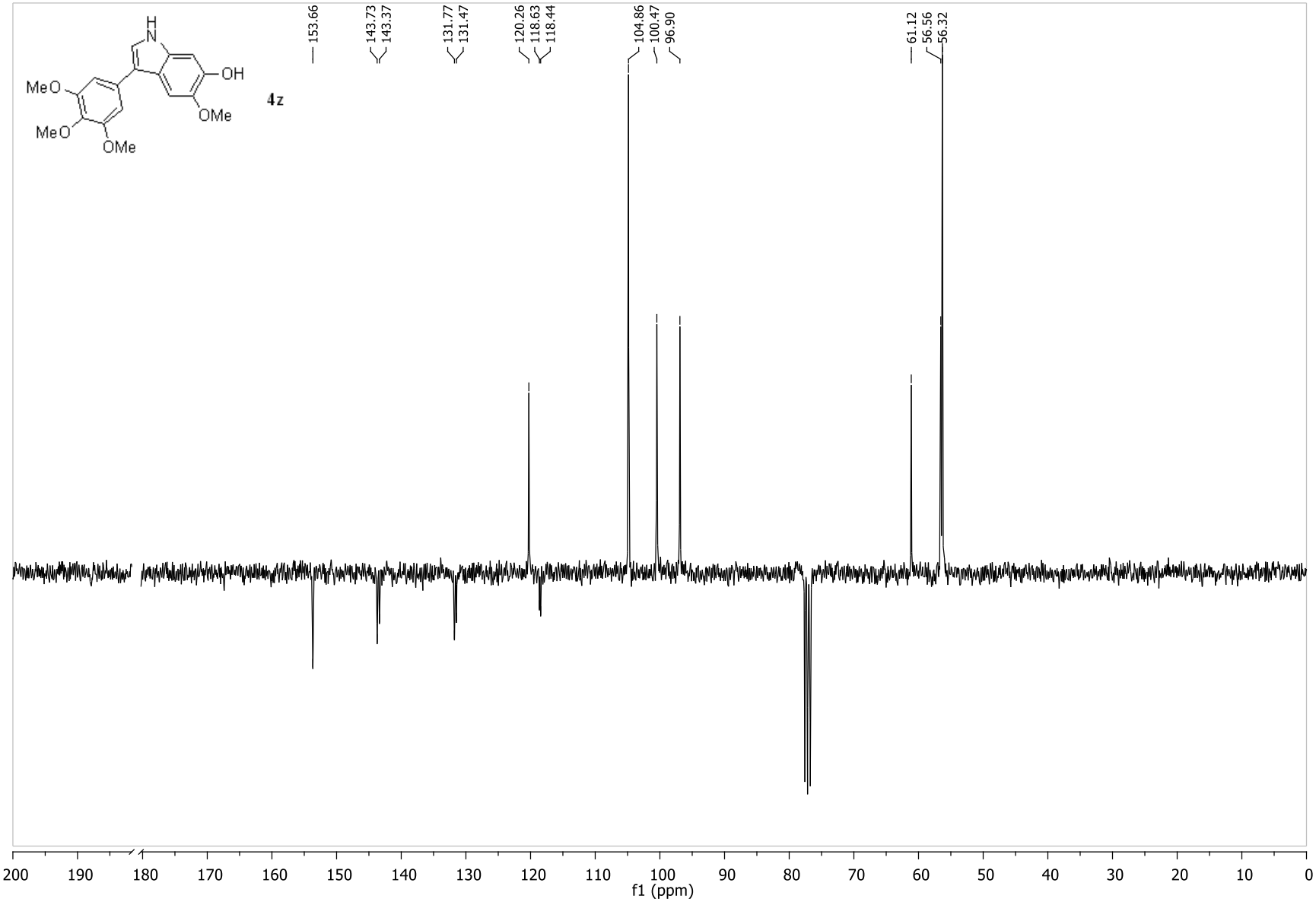

NH
O
O
4x
145.49
143.65
135.23
132.93
131.00
130.14
128.77
128.70
127.79
127.34
126.38
123.03
115.52
100.83
98.41
91.91
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

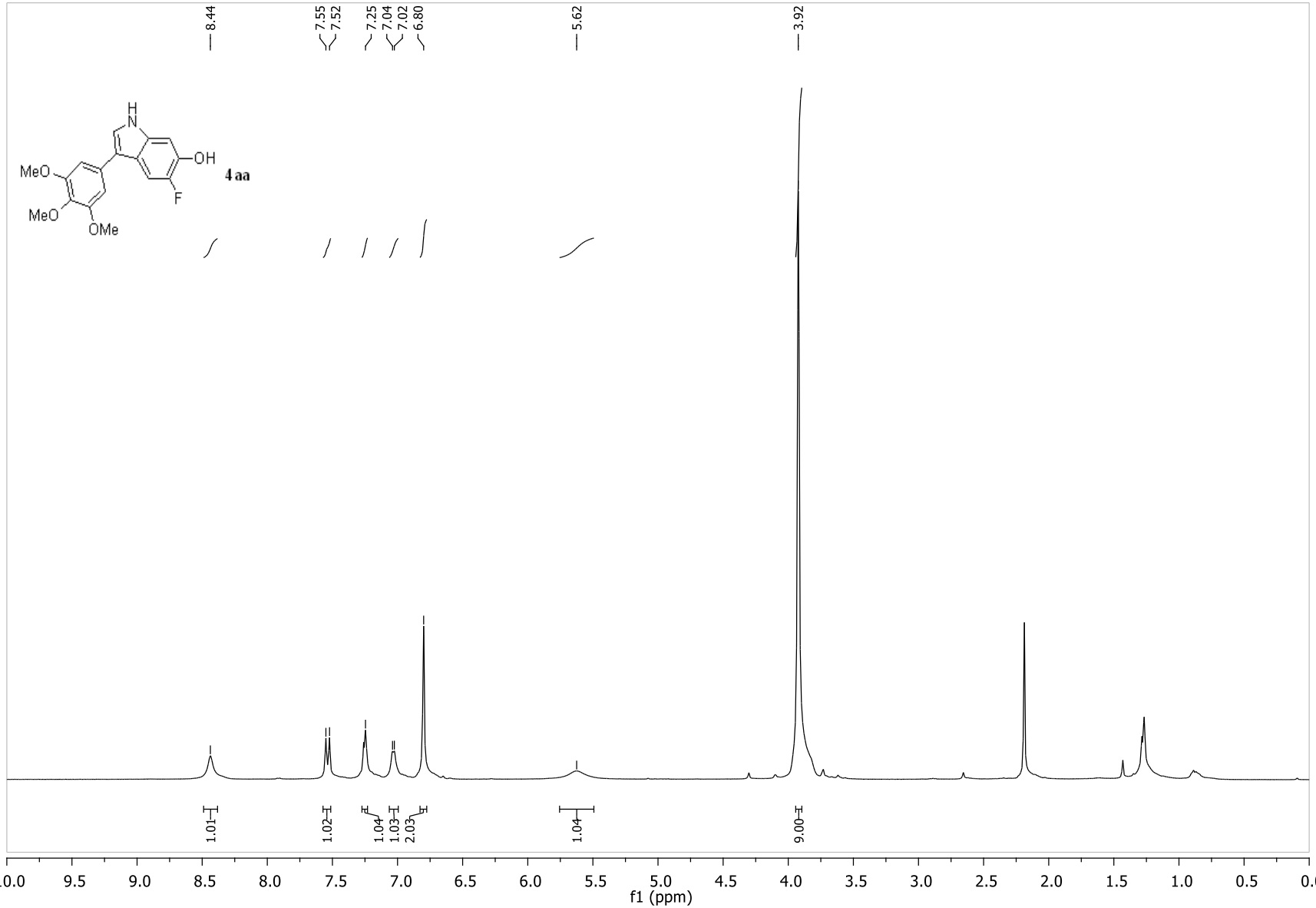

8.27
7.56
7.52
7.25
6.98
6.95
6.79
3.92
3.90
NH
MeO
MeO
OMe
OMe
F
4y
1.00
1.02
1.02
1.00
2.01
9.01
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

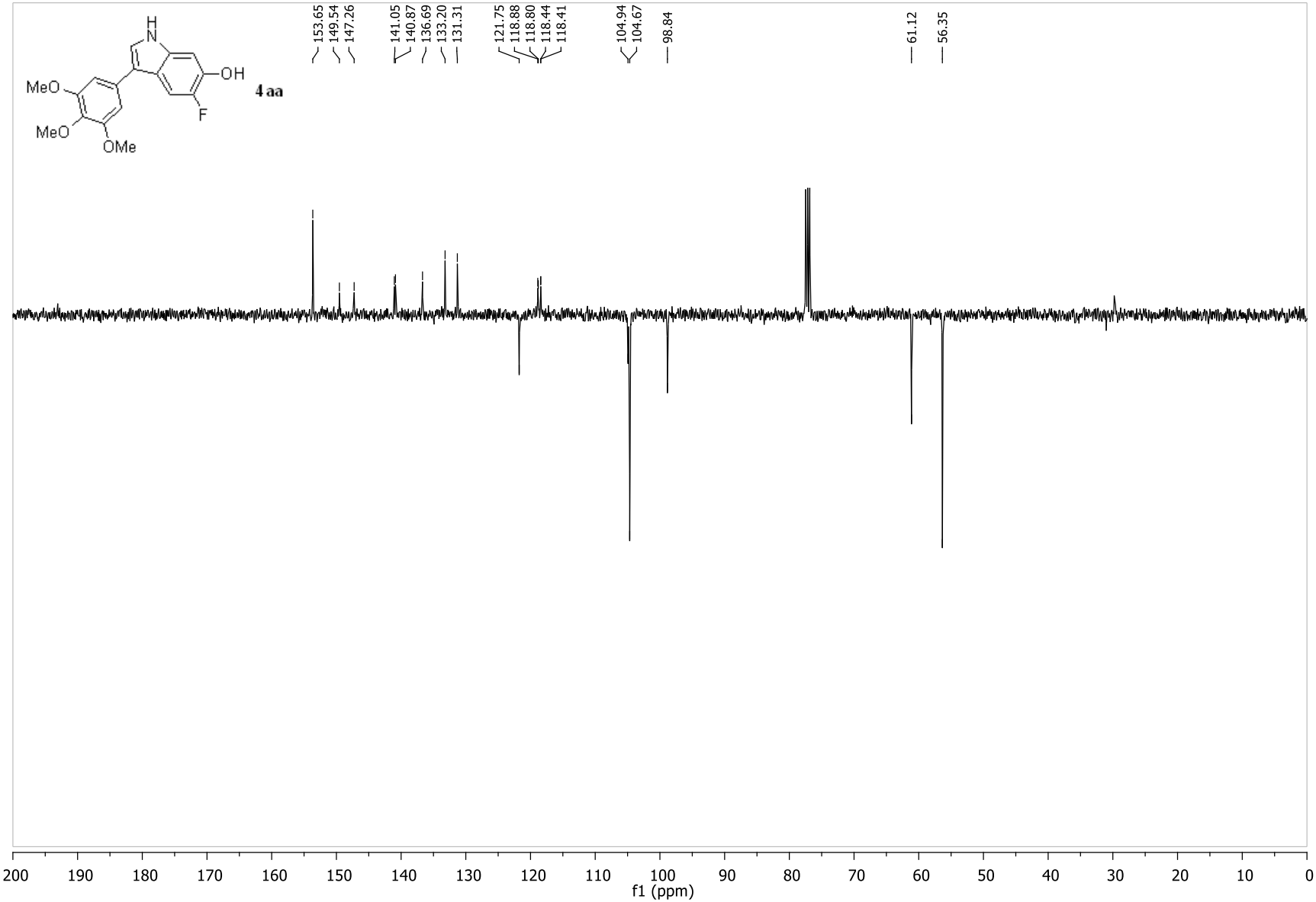

153.73
151.19
148.05
145.55
145.36
136.84
132.74
131.16
121.32
118.78
118.73
118.62
118.50
105.84
105.56
104.65
96.08
61.13
56.78
56.37
MeO
MeO
OMe
OMe
F
4y
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

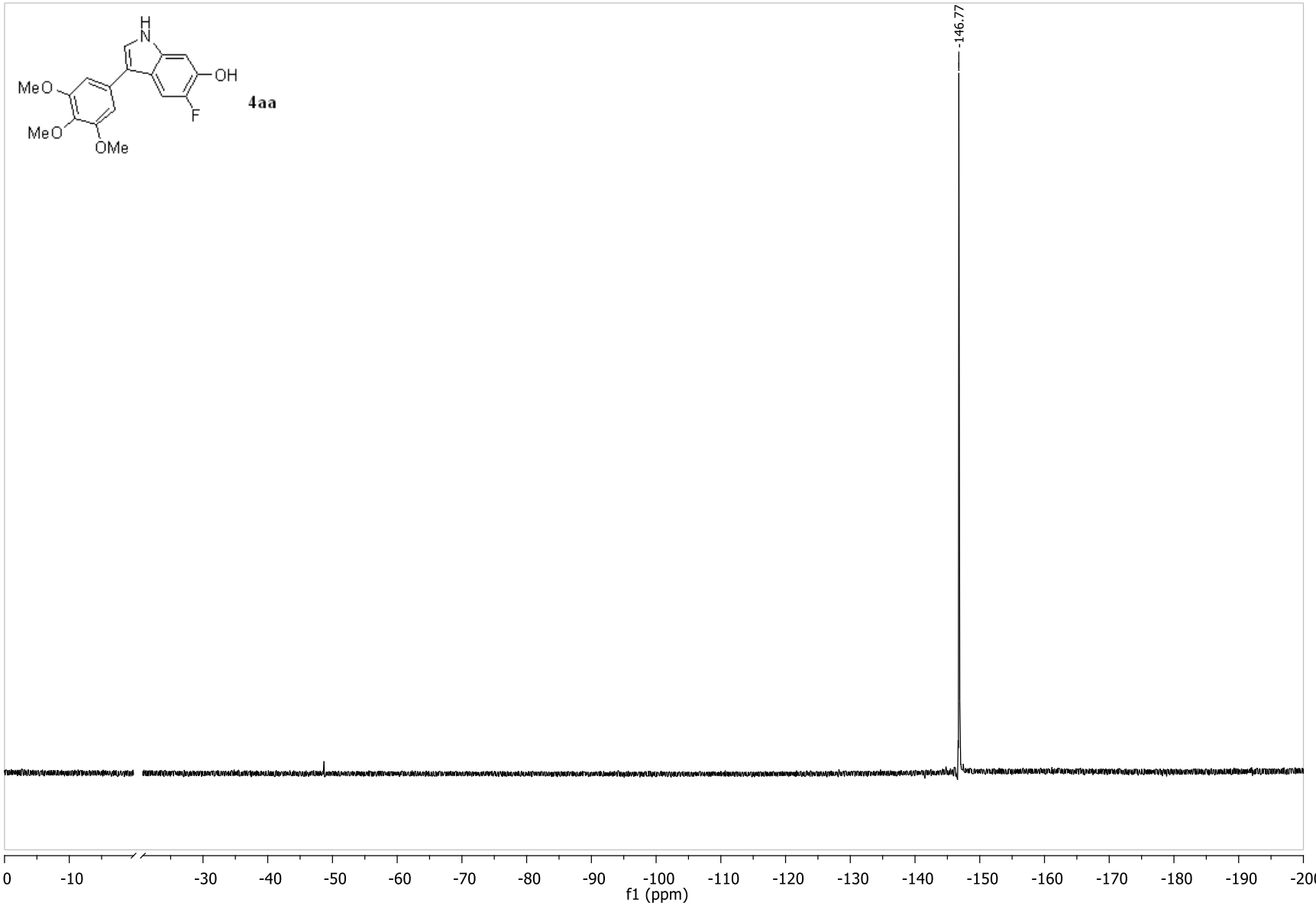

H
N
OMe
MeO
F
MeO
OMe
4y
-143.19
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
f1 (ppm)

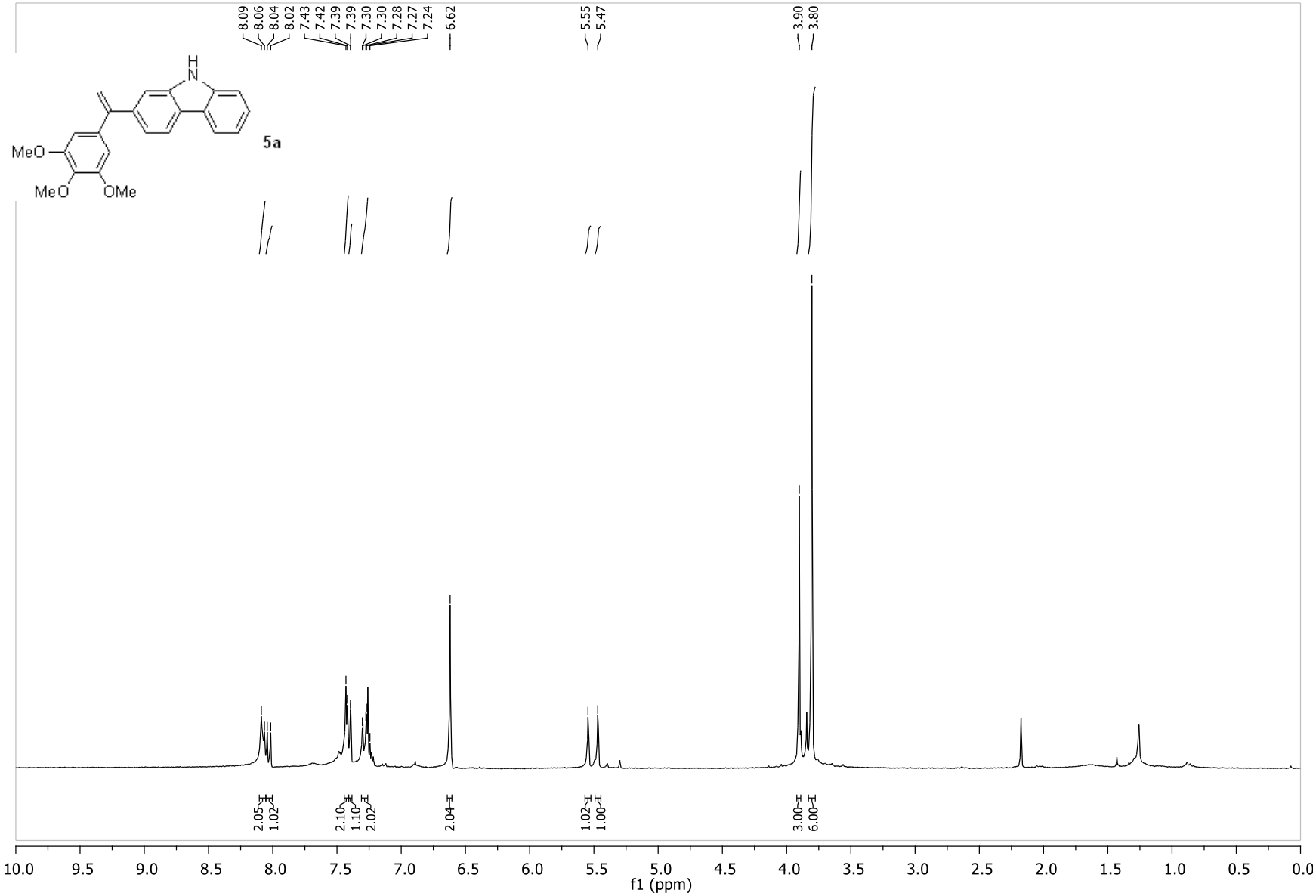

8.17
7.31
7.30
7.28
7.18
7.18
7.01
6.99
6.97
6.85
6.83
6.81
3.94
3.93
3.92
MeO
MeO
OMe
OMe
OH
4z
1.00
1.05
1.04
1.04
2.03
3.02
6.04
3.02
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

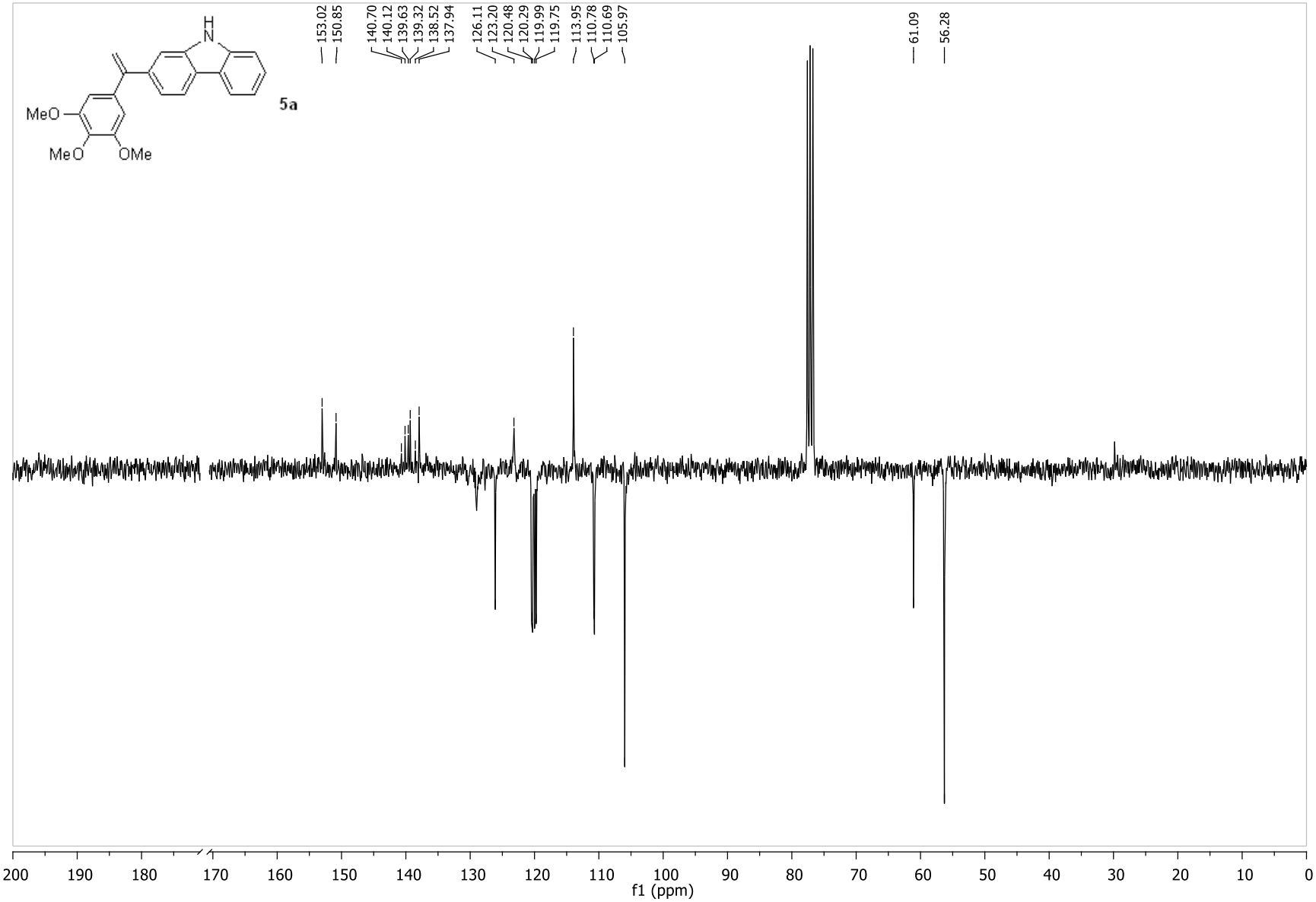

153.66
143.73
143.37
131.77
131.47
120.26
118.63
118.44
104.86
100.47
96.90
61.12
56.56
56.32
MeO
MeO
OMe
OMe
OH
4z
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

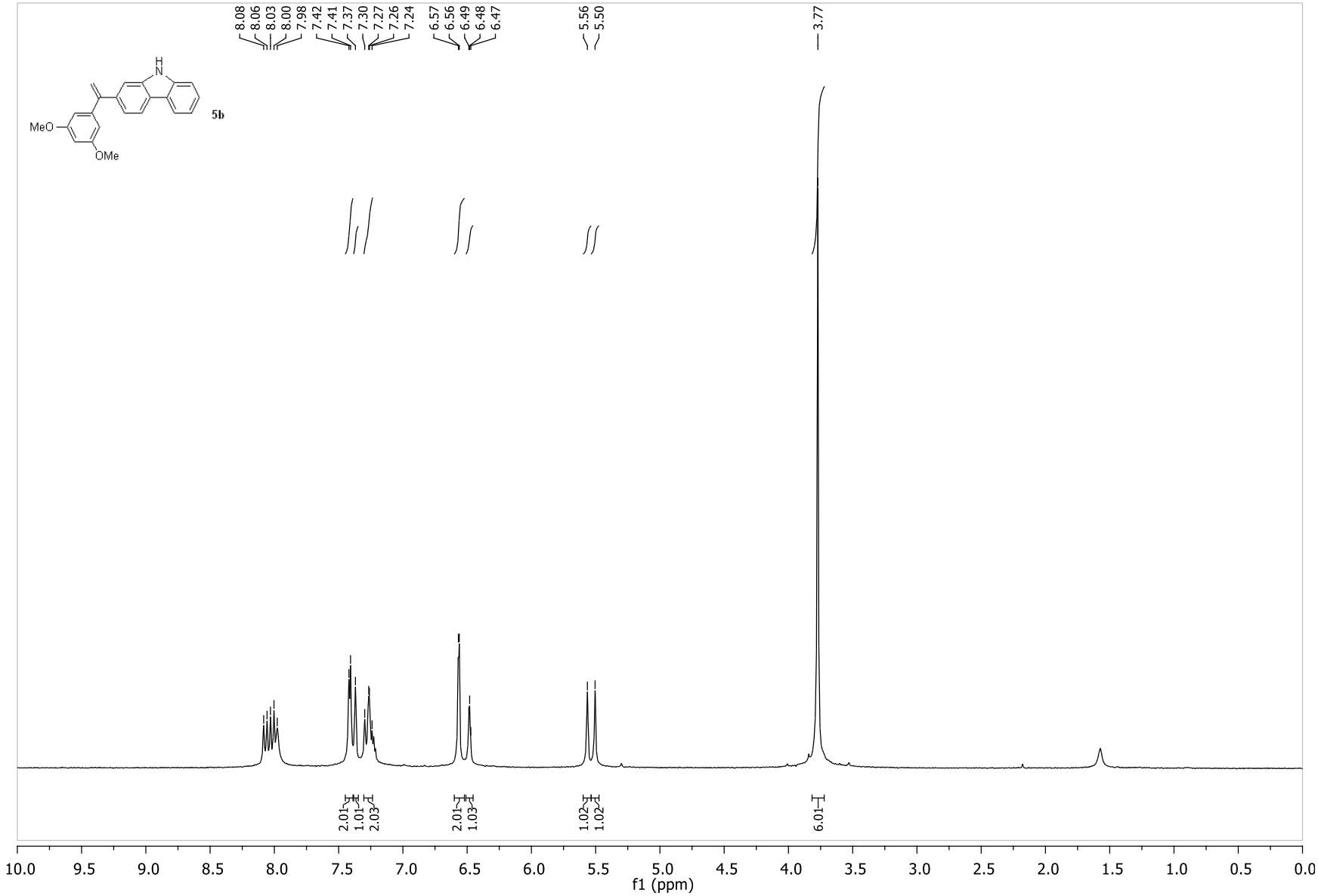

8.44
7.55
7.52
7.25
7.04
7.02
6.80
5.62
3.92
MeO
MeO
OMe
OH
F
H
N
4aa
1.01
1.02
1.04
1.03
2.03
1.04
9.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

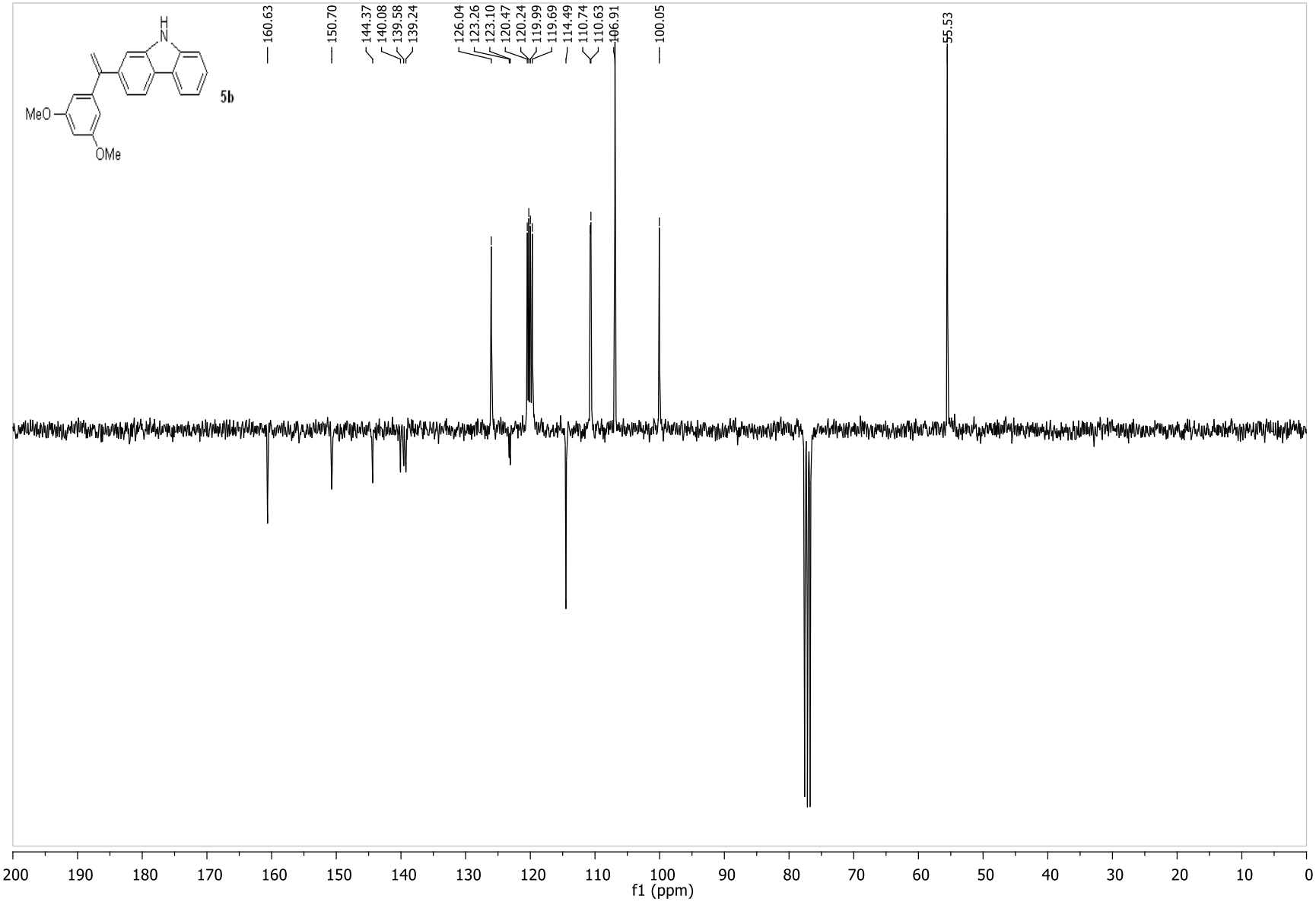

153.65
149.54
147.26
141.05
140.87
136.69
133.20
131.31
121.75
118.88
118.80
118.44
118.41
104.94
104.67
98.84
61.12
56.35
MeO
MeO
OMe
OH
F
H
N
4aa
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

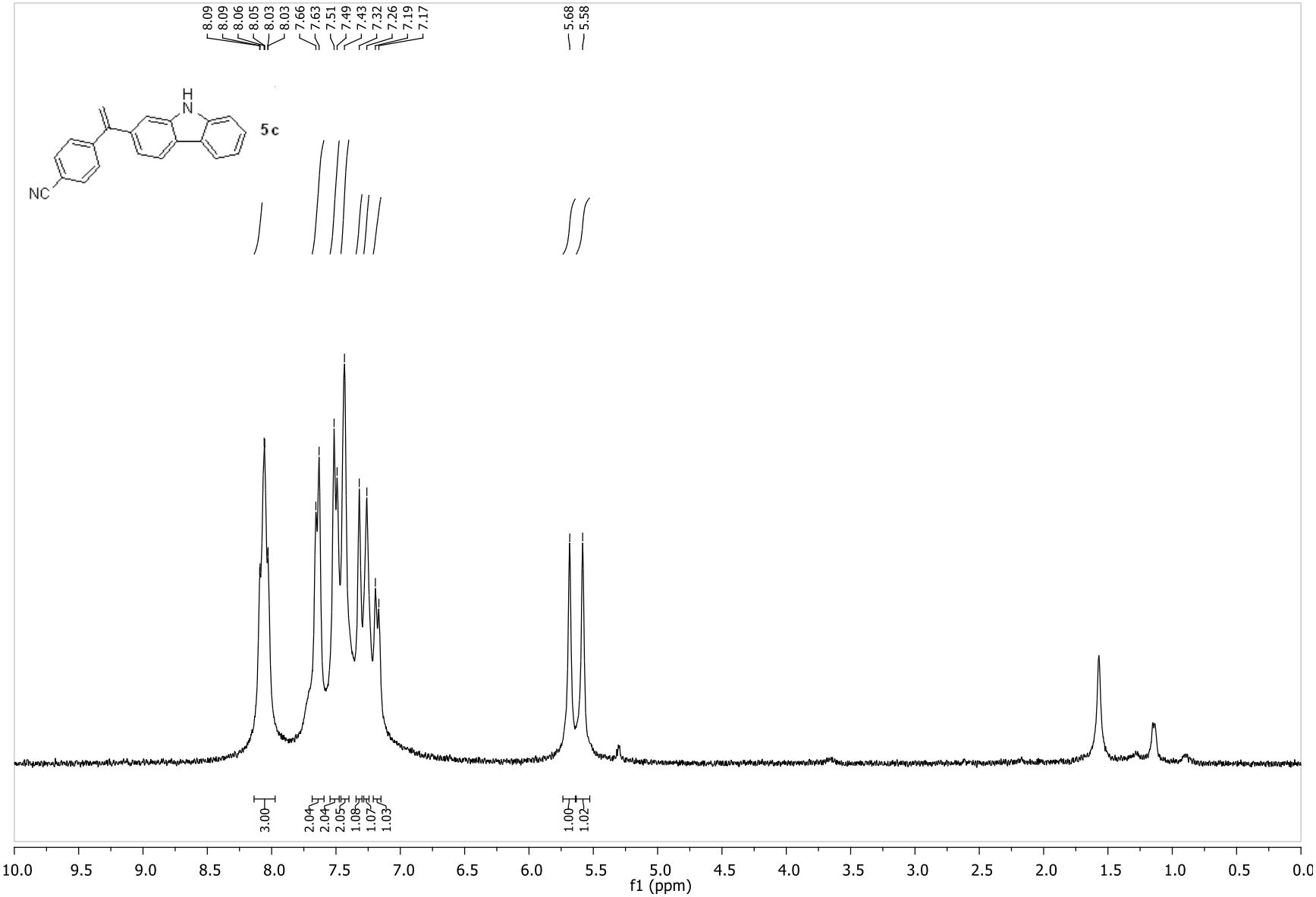

H
N
OH
F
MeO
MeO
OMe
4aa
-146.77
0
-10
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
f1 (ppm)

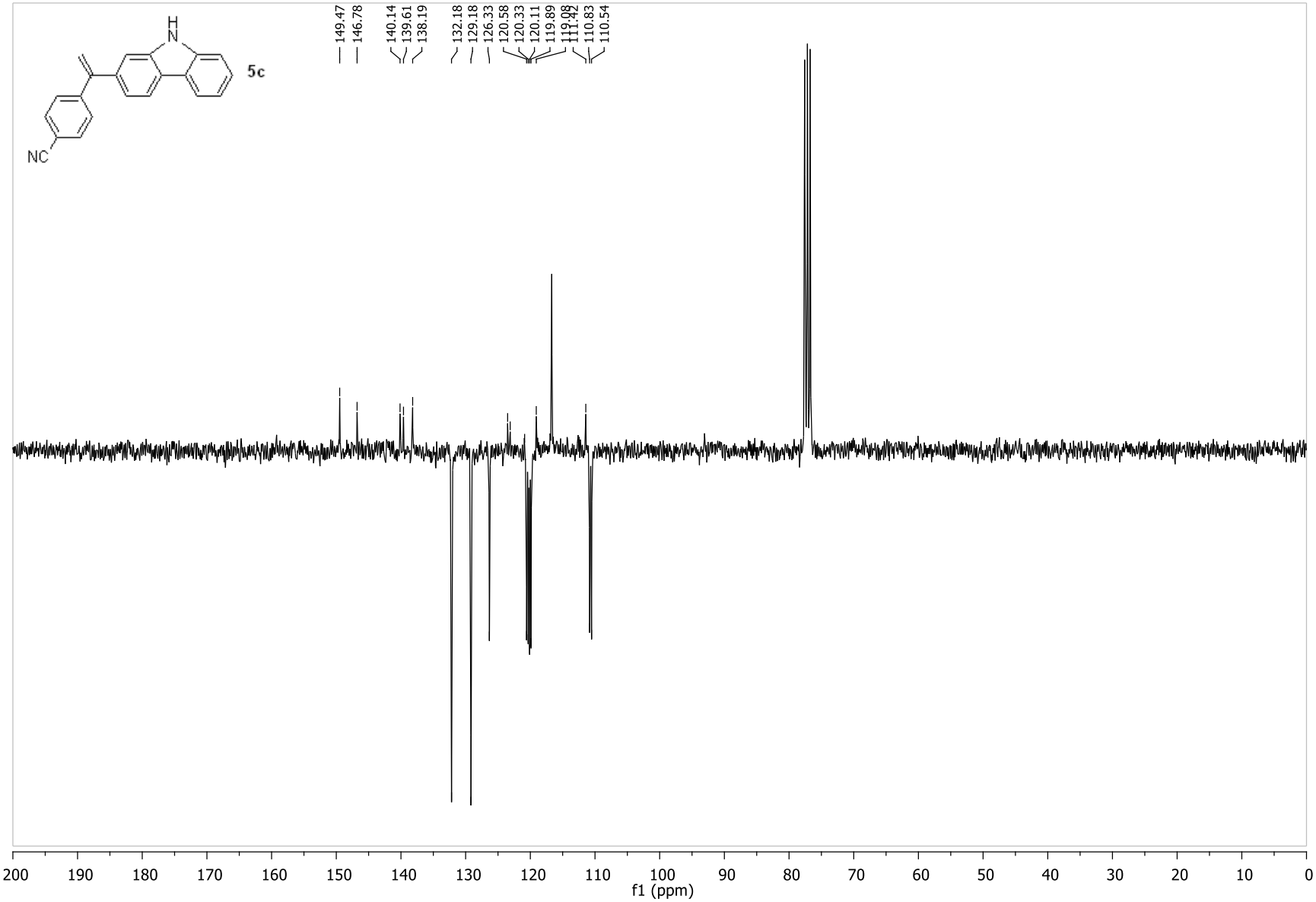

8.09
8.06
8.04
8.02
7.43
7.42
7.39
7.39
7.30
7.30
7.28
7.27
7.24
6.62
5.55
5.47
3.90
3.80
MeO
MeO
OMe
5a
2.05
1.02
2.10
1.10
2.02
2.04
1.02
1.00
3.00
6.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


153.02
150.85
140.70
140.12
139.63
139.32
138.52
137.94
126.11
123.20
120.48
120.29
119.99
119.75
113.95
110.78
110.69
105.97
61.09
56.28
5a
MeO
MeO
OMe
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.08
8.06
8.03
8.00
7.98
7.42
7.41
7.37
7.30
7.27
7.26
7.24
6.57
6.56
6.49
6.48
6.47
5.56
5.50
3.77
MeO
OMe
5b
2.01
1.01
2.03
2.01
1.03
1.02
1.02
6.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


160.63
150.70
144.37
140.08
139.58
139.24
126.04
123.26
123.10
120.47
120.24
119.99
119.69
114.49
110.74
110.63
106.91
100.05
55.53
5b
MeO
OMe
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.09
8.09
8.06
8.05
8.03
8.03
7.66
7.63
7.51
7.49
7.43
7.32
7.26
7.19
7.17
5.68
5.58
H
N
NC
5c
3.00
2.04
2.04
2.05
1.08
1.07
1.03
1.00
1.02
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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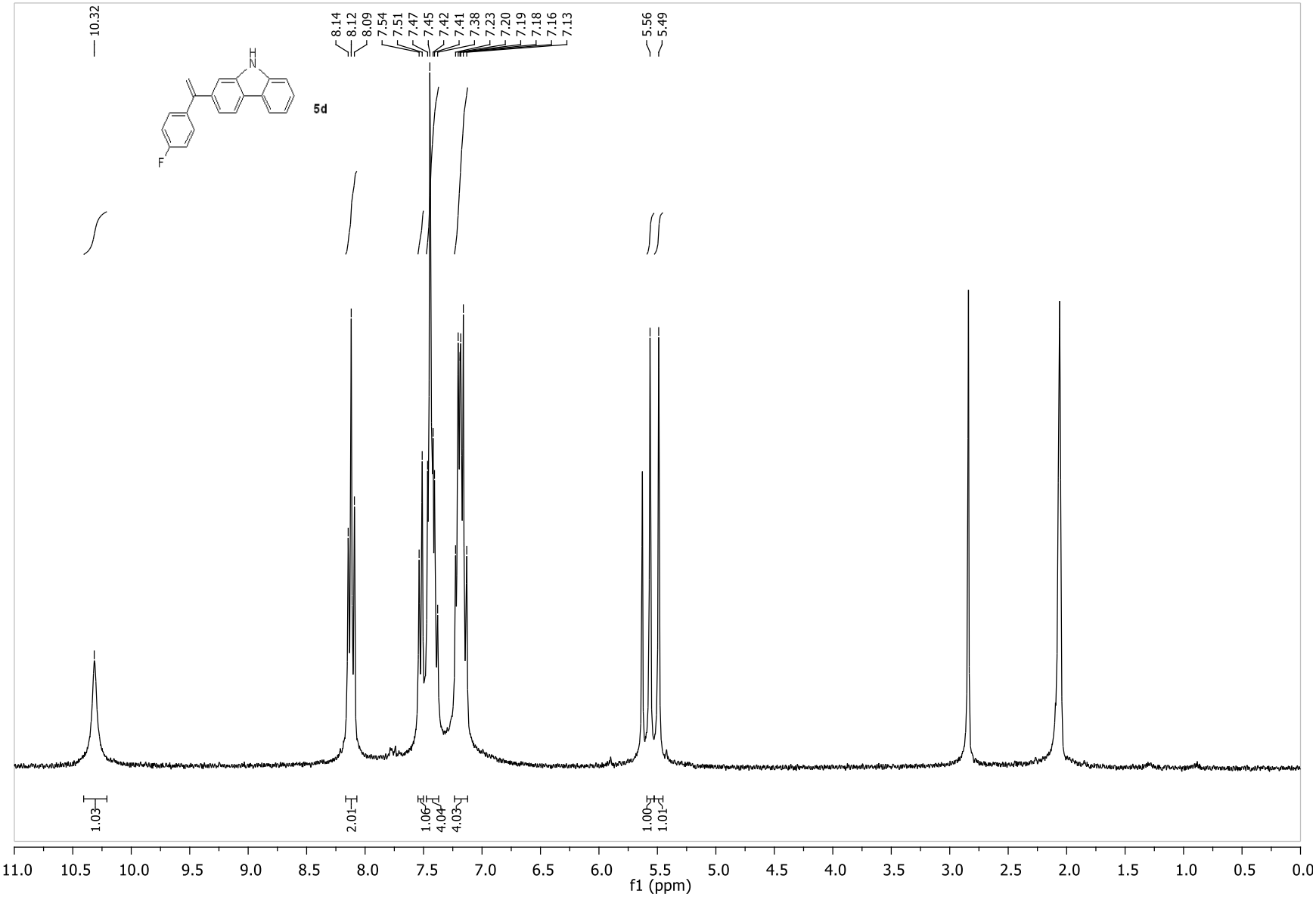
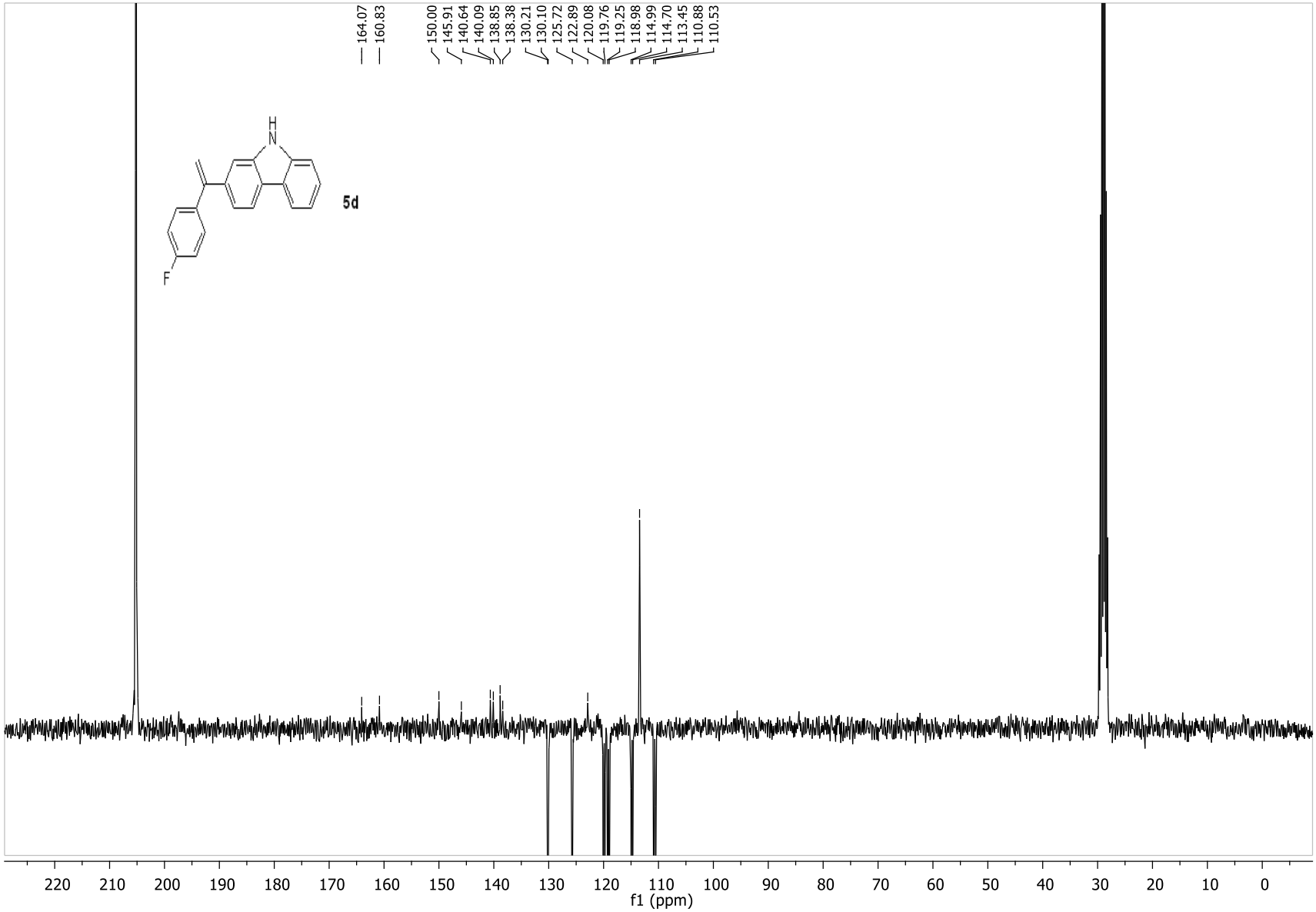
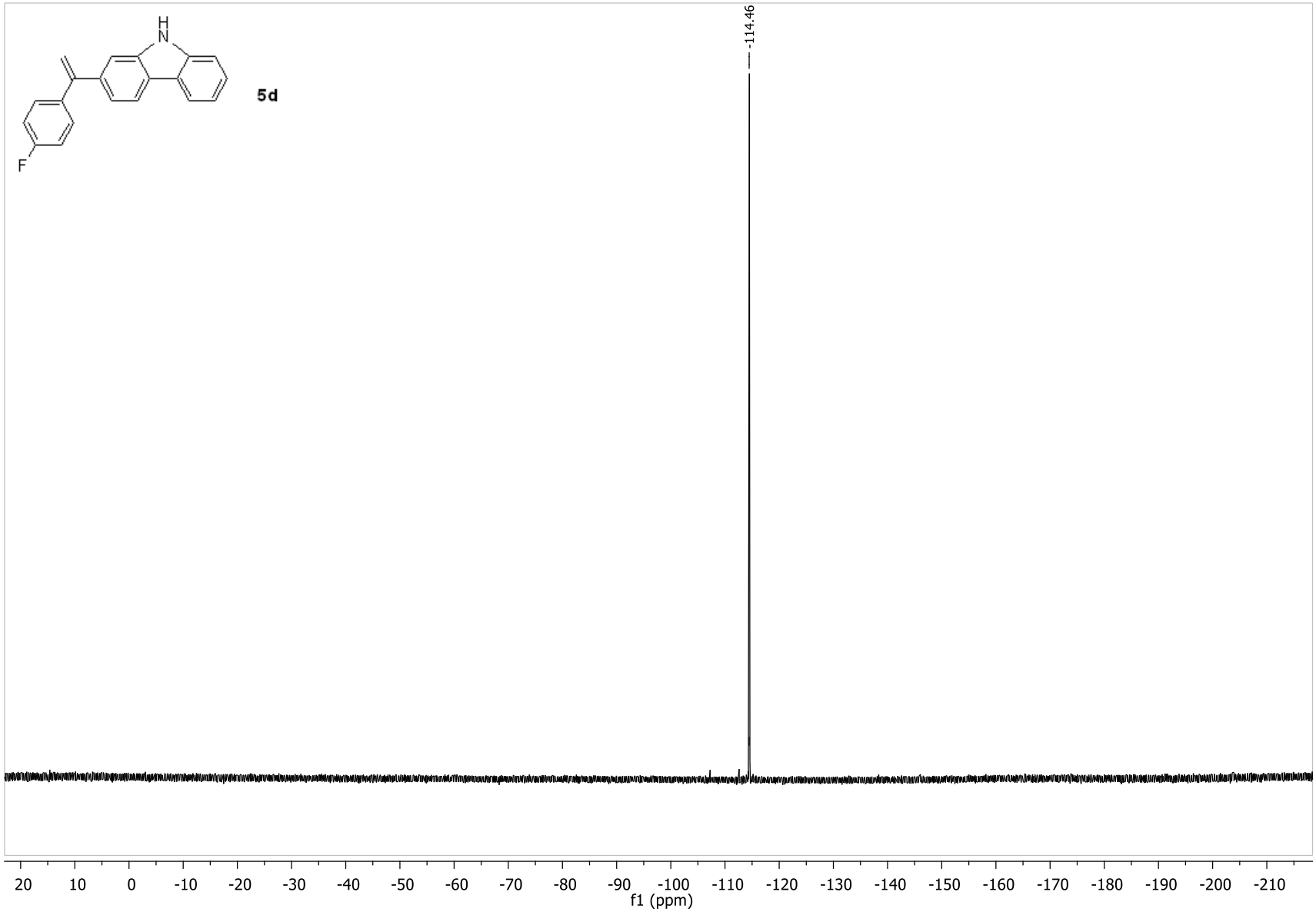
146.78
140.14
139.61
138.19
132.18
129.18
126.33
120.58
120.33
120.11
119.89
119.08
111.42
110.83
110.54
5c
NC
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


10.32
8.14
8.12
8.09
7.54
7.51
7.47
7.45
7.42
7.41
7.38
7.23
7.20
7.19
7.18
7.16
7.13
5.56
5.49
5d
F
1.03
2.01
1.06
4.04
4.03
1.00
1.01
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


164.07
160.83
150.00
145.91
140.64
140.09
138.85
138.38
130.21
130.10
125.72
122.89
120.08
119.76
119.25
118.98
114.99
114.70
113.45
110.88
110.53
5d
F
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


H
N
F
5d
-114.46
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
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-110
-120
-130
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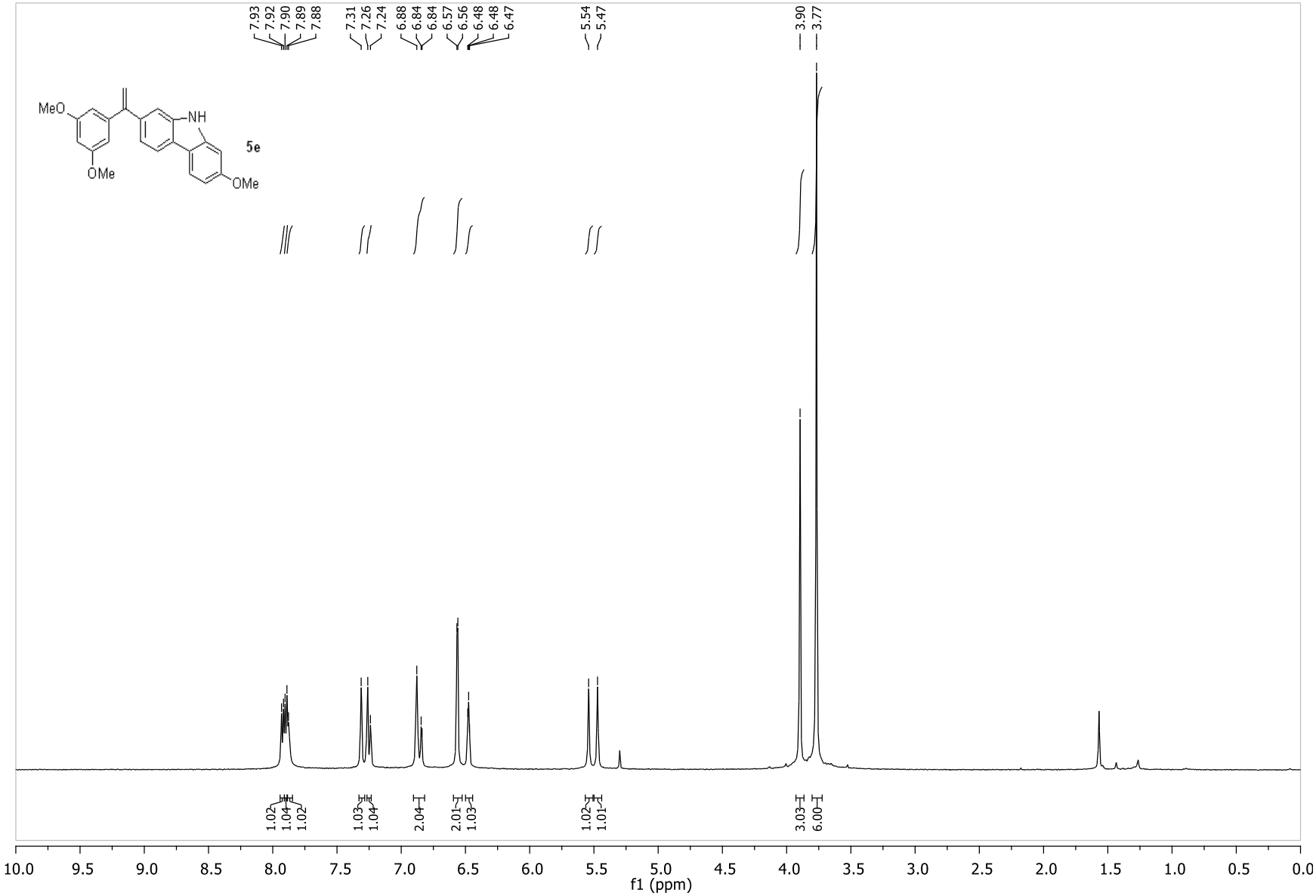
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


7.93
7.92
7.90
7.89
7.88
7.31
7.26
7.24
6.88
6.84
6.84
6.57
6.56
6.48
6.48
6.47
5.54
5.47
3.90
3.77
MeO
NH
OMe
OMe
5e
1.02
1.04
1.02
1.03
1.04
2.04
2.01
1.03
1.02
1.01
3.03
6.00
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9.0
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8.0
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6.5
6.0
5.5
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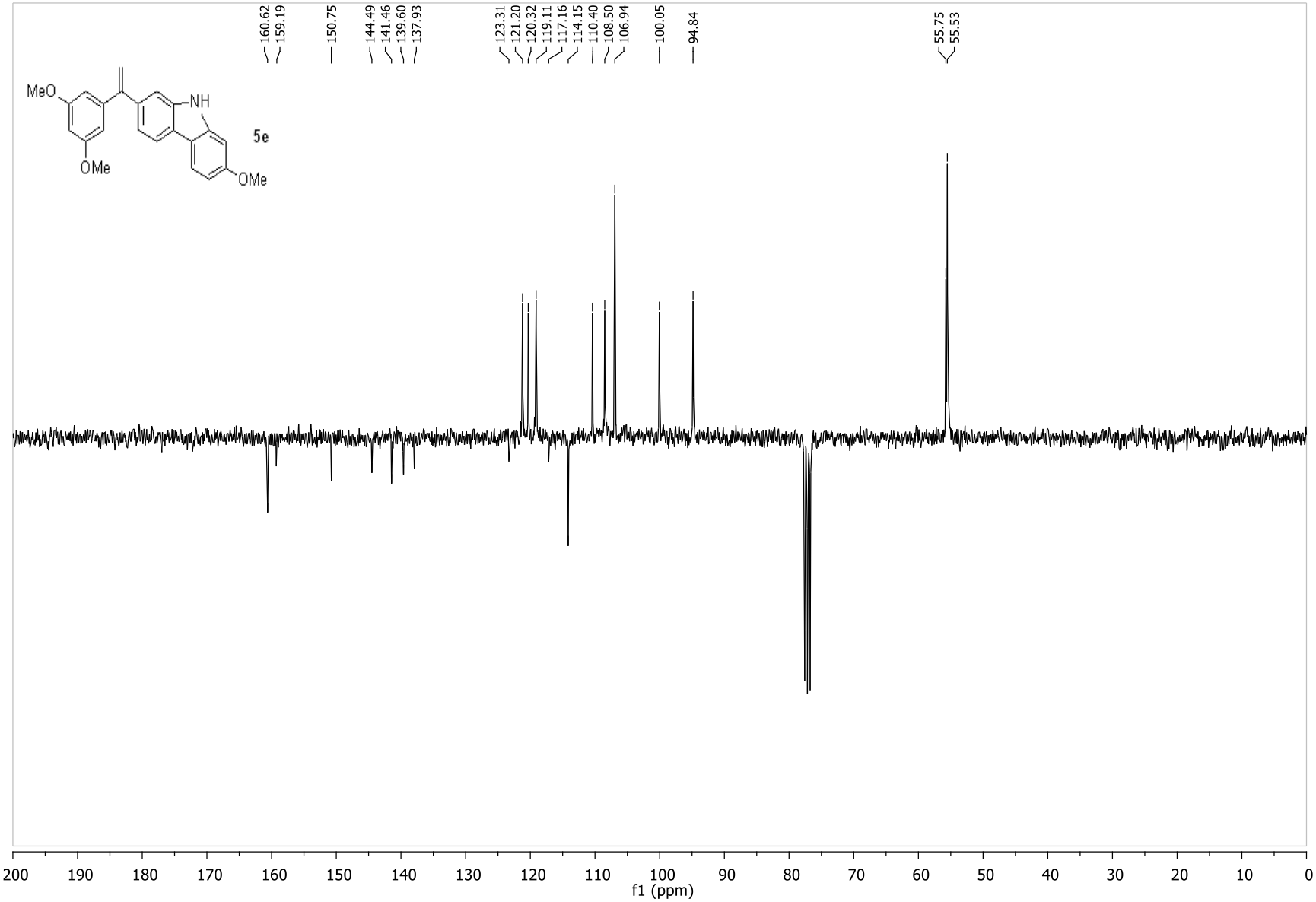
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139.60
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123.31
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120.32
119.11
117.16
114.15
110.40
108.50
106.94
100.05
94.84
55.75
55.53
MeO
NH
OMe
OMe
5e
200
190
180
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150
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130
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50
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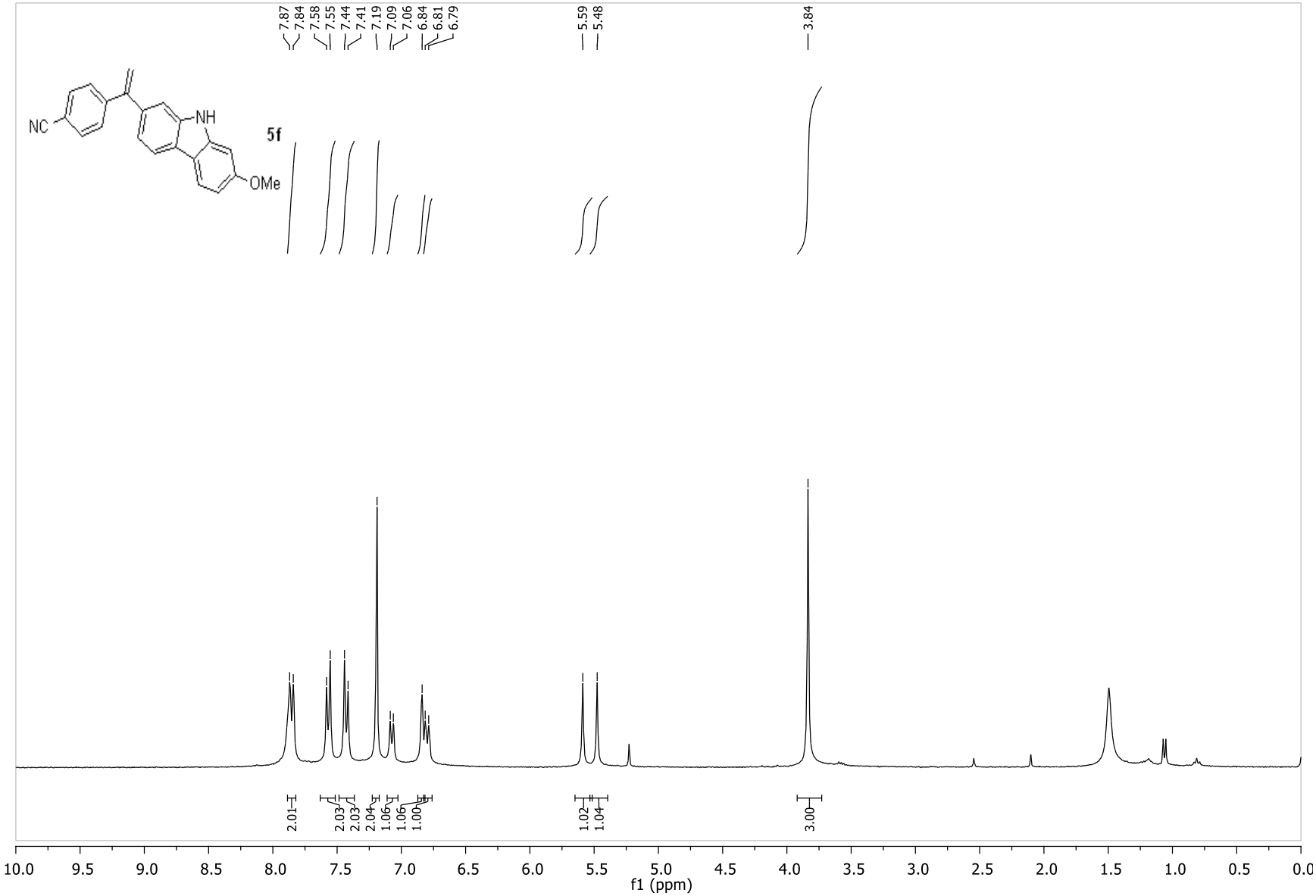
f1 (ppm)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7.19
7.09
7.06
6.84
6.81
6.79
5.59
5.48
3.84
NC
NH
OMe
5f
2.01
2.03
2.03
2.04
1.06
1.06
1.00
1.02
1.04
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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3.0
2.5
2.0
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1.0
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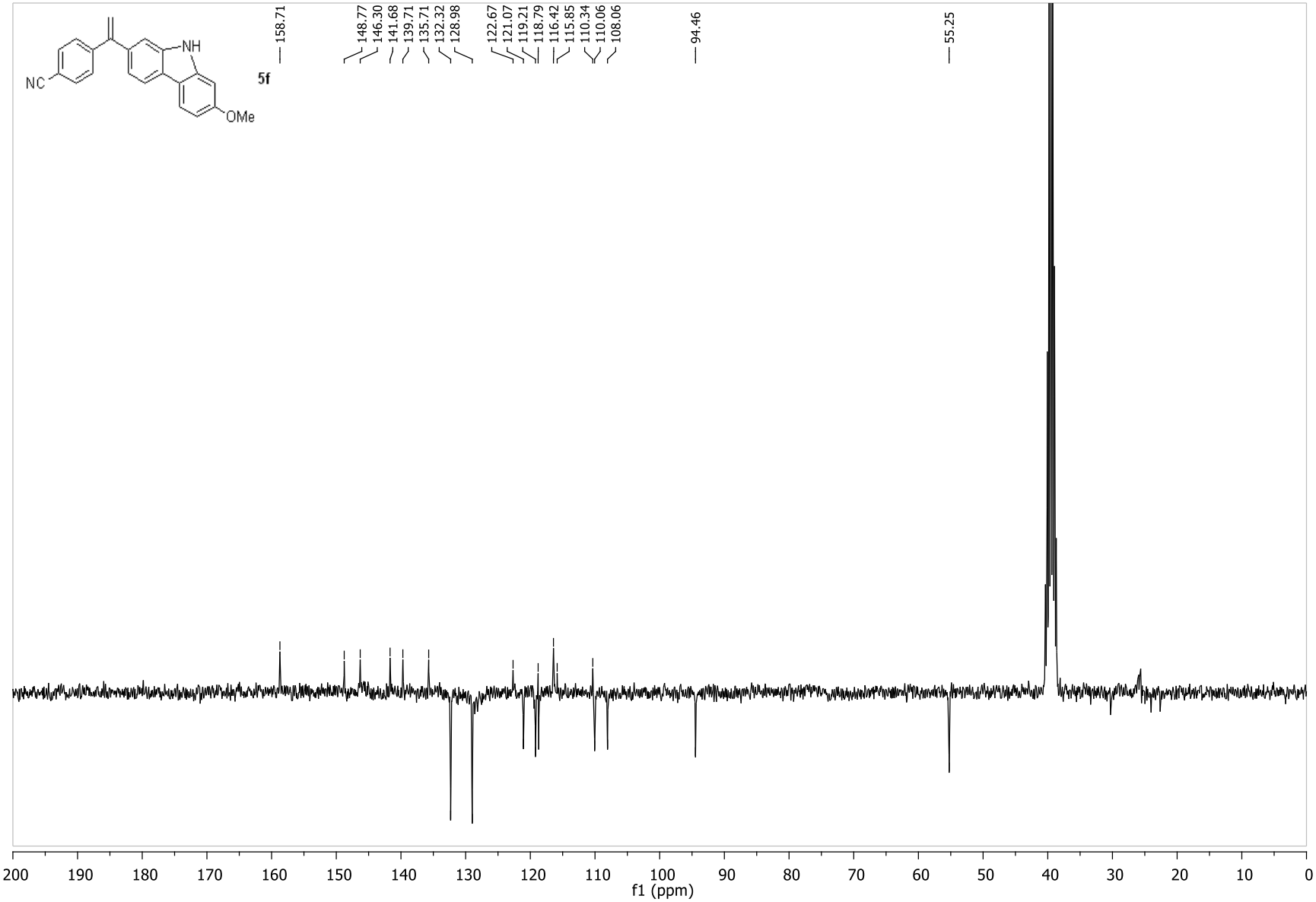
0.0
f1 (ppm)


NC
NH
OMe
5f
158.71
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146.30
141.68
139.71
135.71
132.32
128.98
122.67
121.07
119.21
118.79
116.42
115.85
110.34
110.06
108.06
94.46
55.25
200
190
180
170
160
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130
120
110
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90
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50
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10
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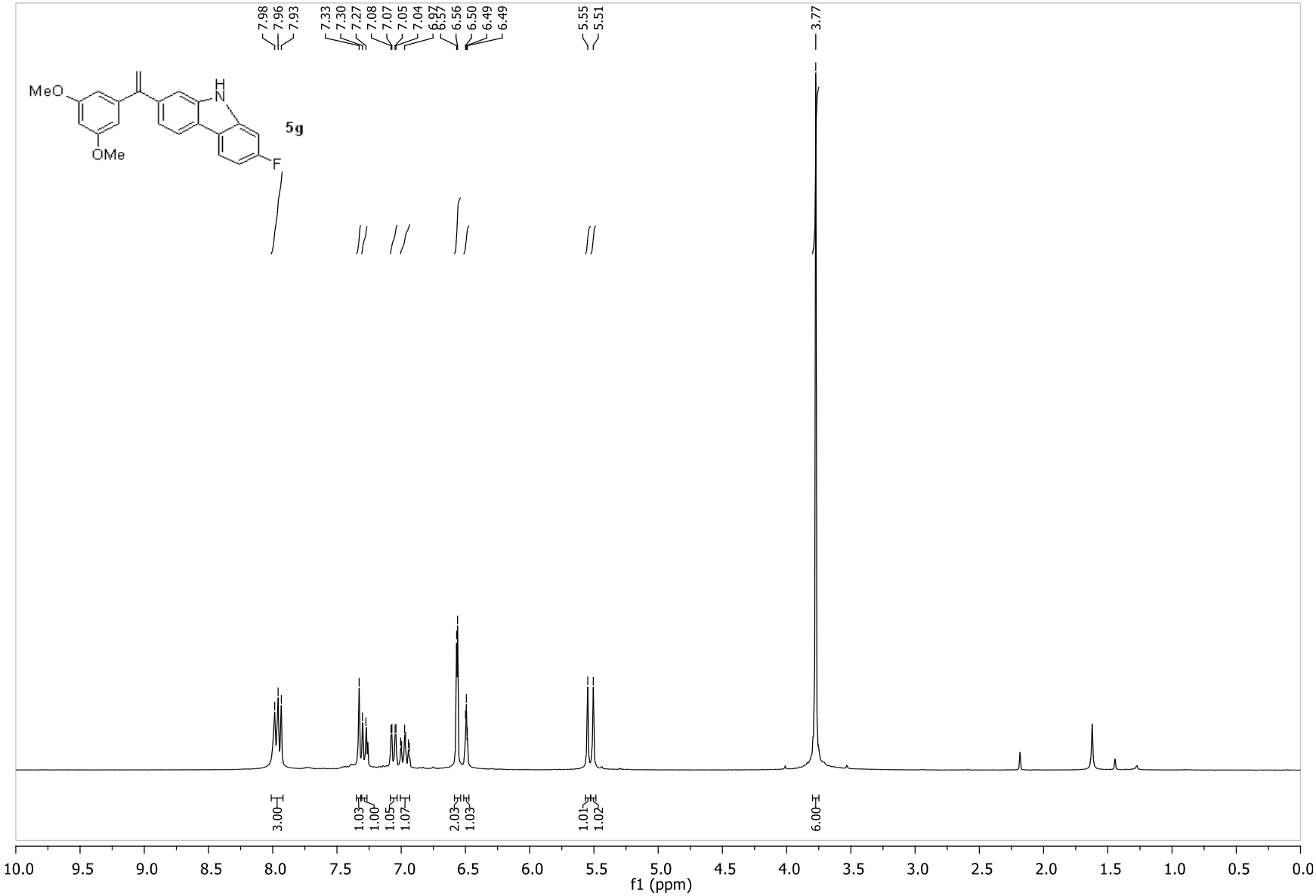
f1 (ppm)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7.93
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7.27
7.08
7.07
7.05
7.04
6.57
6.56
6.50
6.49
6.49
5.55
5.51
3.77
MeO
OMe
H
N
F
5g
3.00
1.03
1.00
1.05
1.07
2.03
1.03
1.01
1.02
6.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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2.0
1.5
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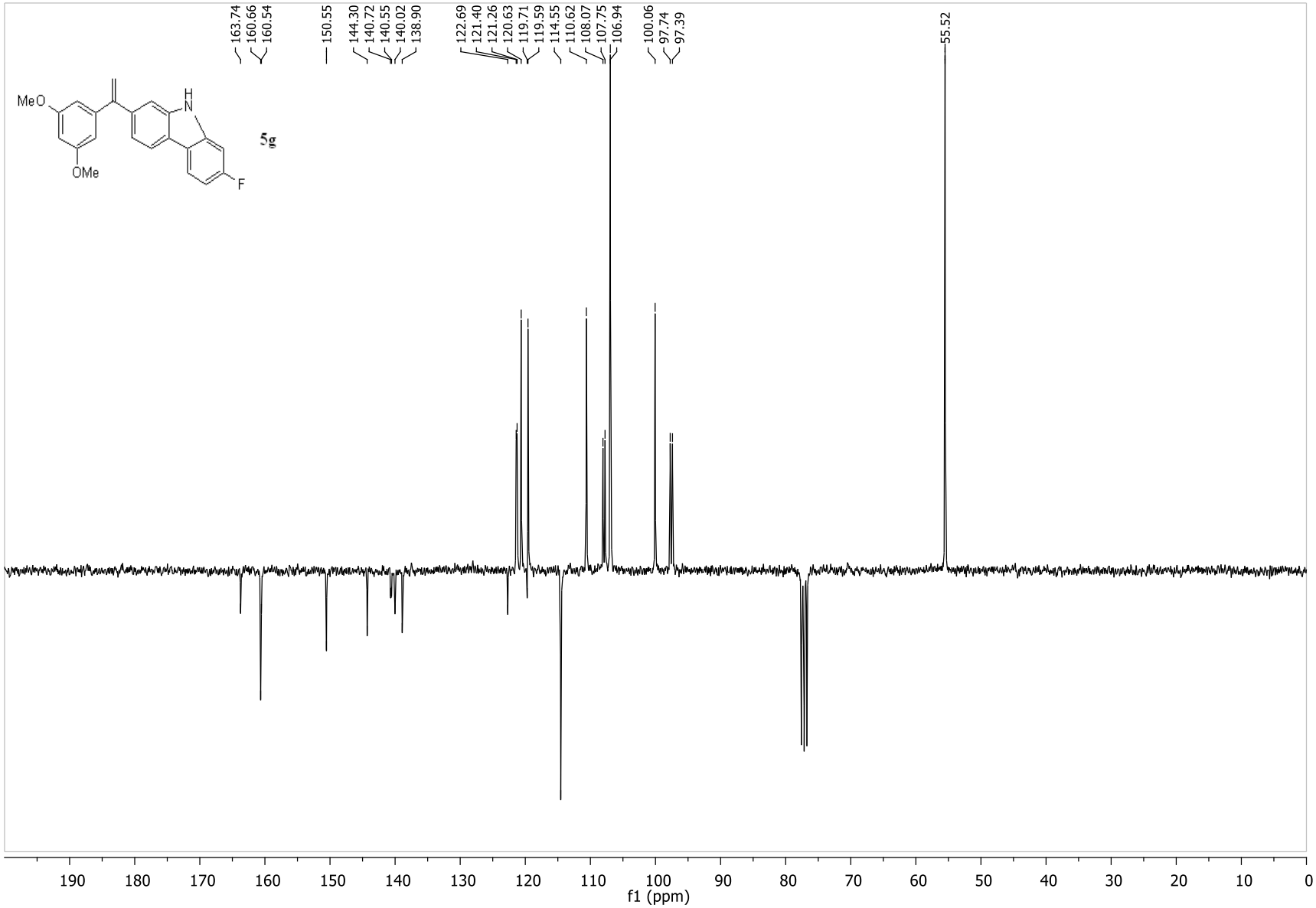
0.0
f1 (ppm)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160.66
160.54
150.55
144.30
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140.02
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121.40
121.26
120.63
119.71
119.59
114.55
110.62
108.07
107.75
106.94
100.06
97.74
97.39
55.52
MeO
OMe
H
N
F
5g
190
180
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90
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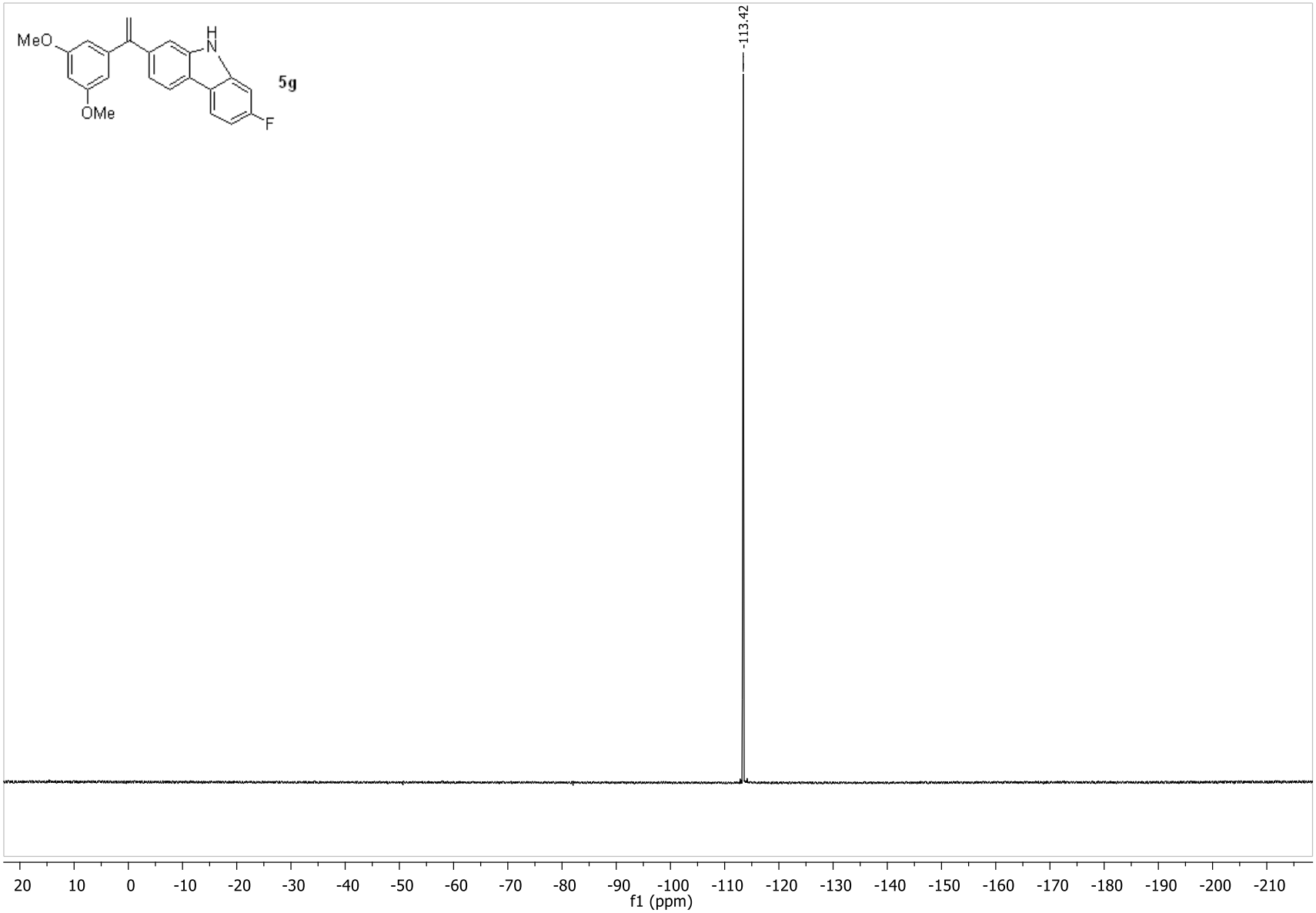
f1 (ppm)


MeO
OMe
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N
F
5g
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-10
-20
-30
-40
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-60
-70
-80
-90
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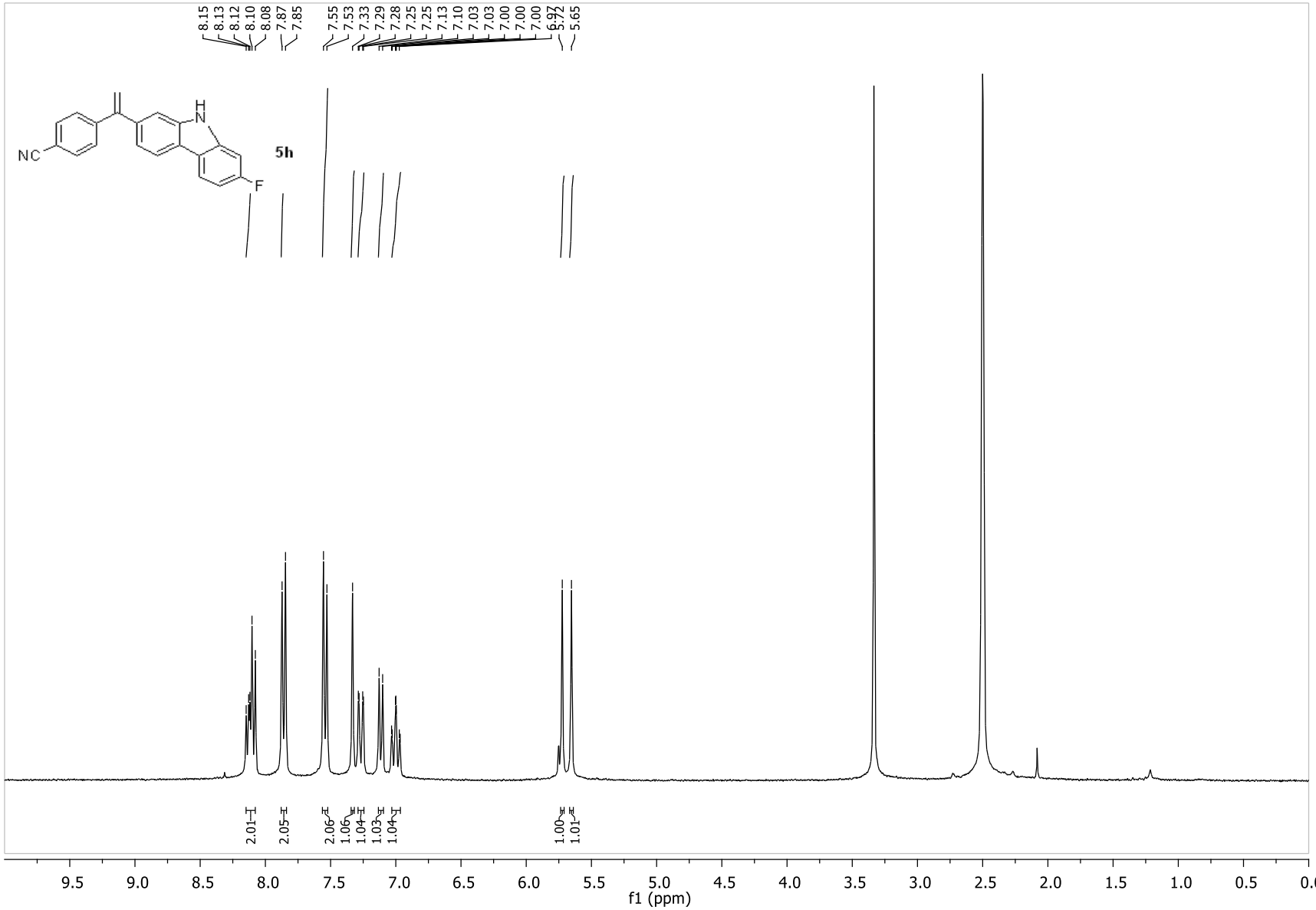
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)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8.13
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8.08
7.87
7.85
7.55
7.53
7.33
7.29
7.28
7.25
7.25
7.13
7.10
7.03
7.03
7.00
7.00
7.00
6.97
5.72
5.65
NC
5h
F
H
N
2.01
2.05
2.06
1.06
1.04
1.03
1.04
1.00
1.01
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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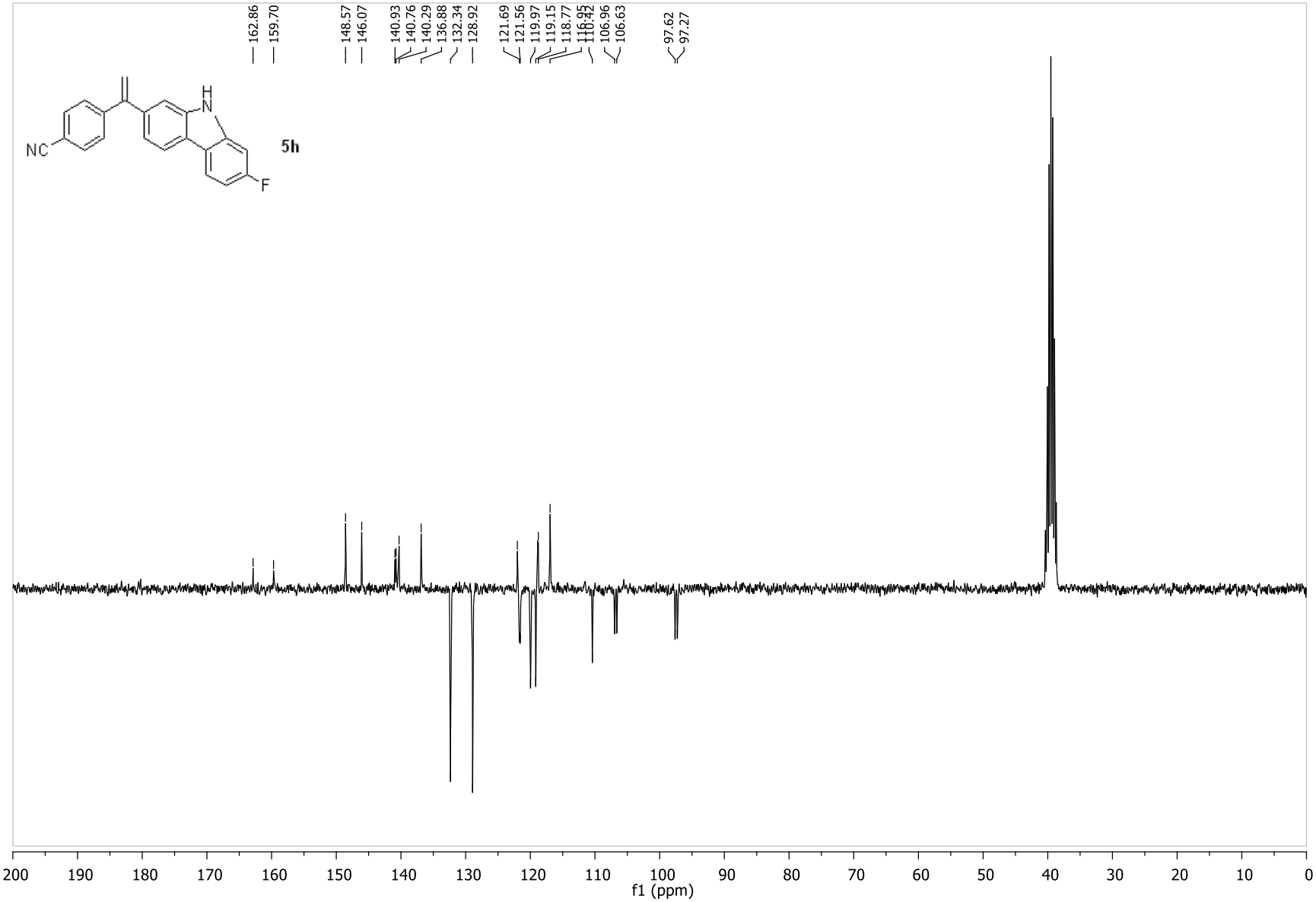
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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140.76
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136.88
132.34
128.92
121.69
121.56
119.97
119.15
118.77
106.96
106.63
97.62
97.27
NC
H
N
F
5h
200
190
180
170
160
150
140
130
120
110
100
90
80
70
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50
40
30
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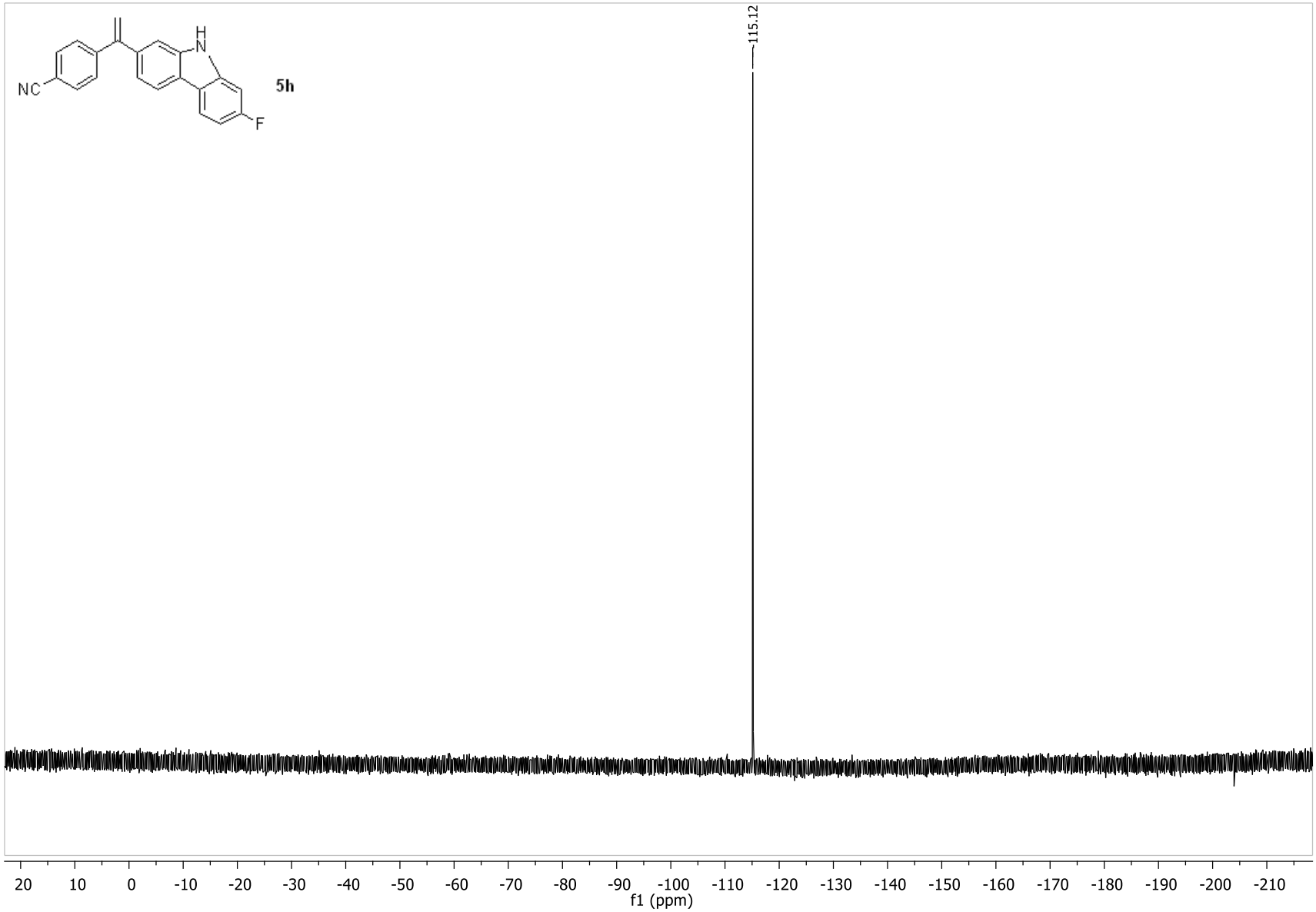
10
0
f1 (ppm)


NC
H
N
F
5h
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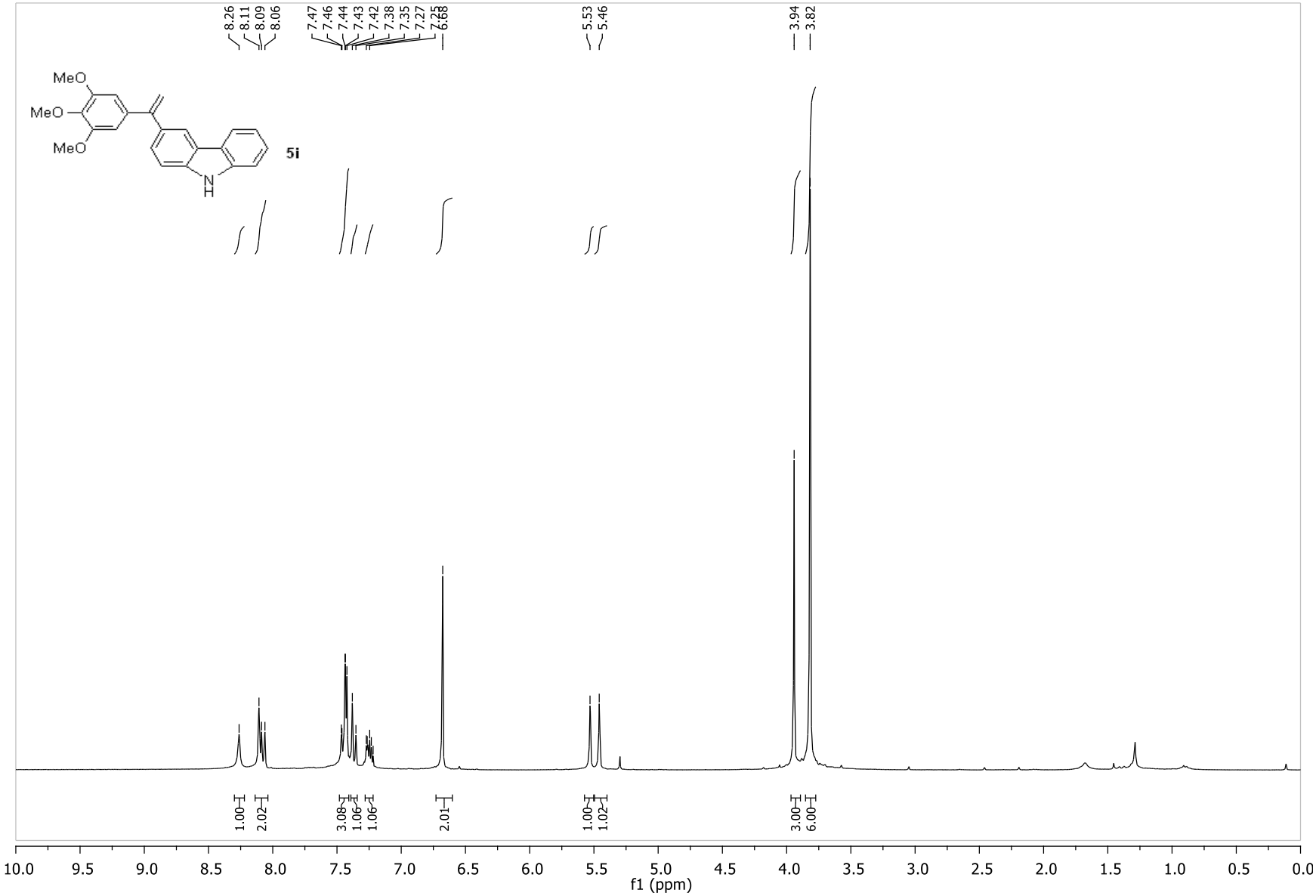
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)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8.06
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7.46
7.44
7.43
7.42
7.38
7.35
7.27
7.25
6.68
5.53
5.46
3.94
3.82
MeO
MeO
MeO
N
H
5i
1.00
2.02
3.08
1.06
1.06
2.01
1.00
1.02
3.00
6.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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4.5
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3.5
3.0
2.5
2.0
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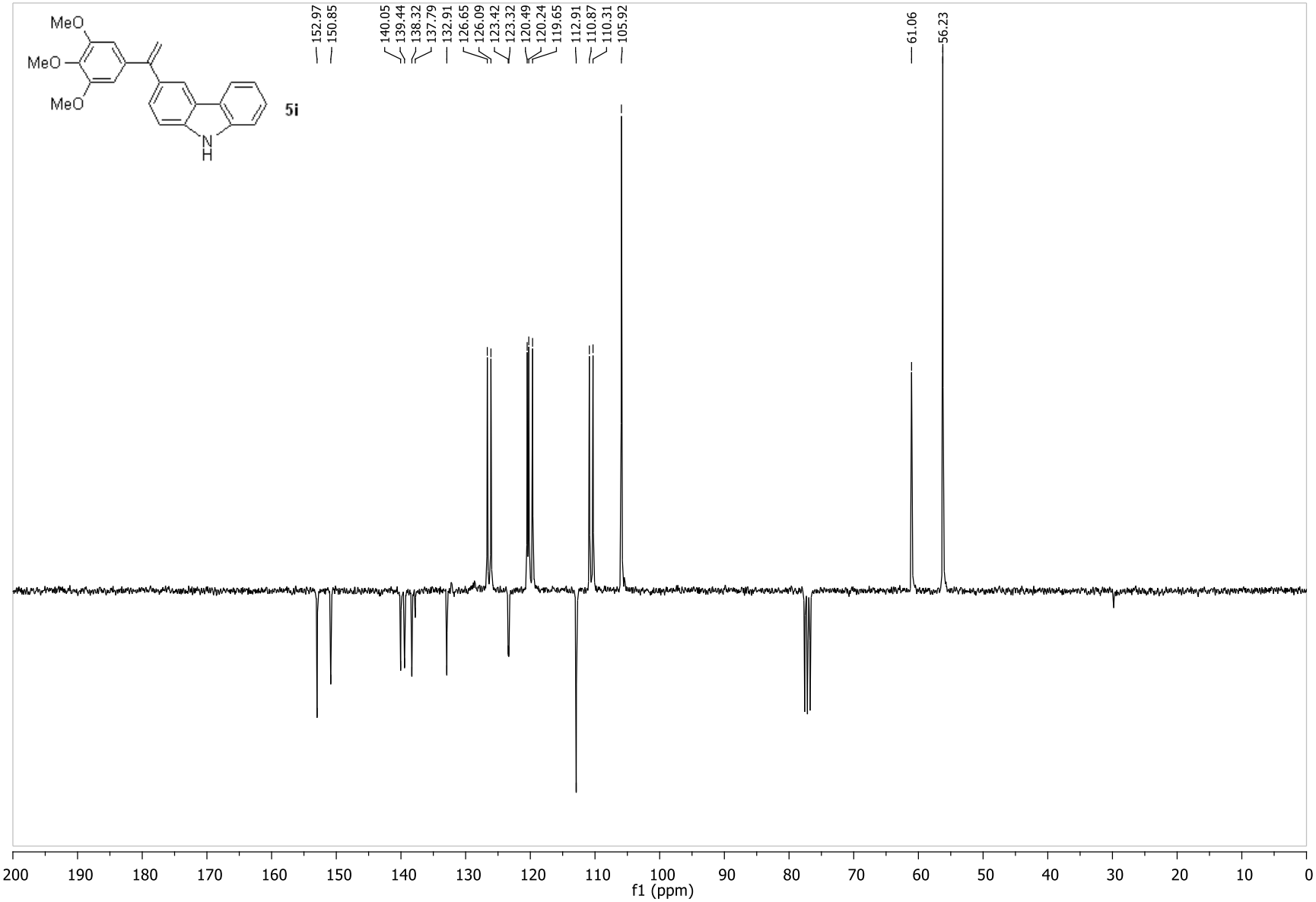
0.0
f1 (ppm)


MeO
MeO
MeO
N
H
5i
152.97
150.85
140.05
139.44
138.32
137.79
132.91
126.65
126.09
123.42
123.32
120.49
120.24
119.65
112.91
110.87
110.31
105.92
61.06
56.23
200
190
180
170
160
150
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130
120
110
100
90
80
70
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50
40
30
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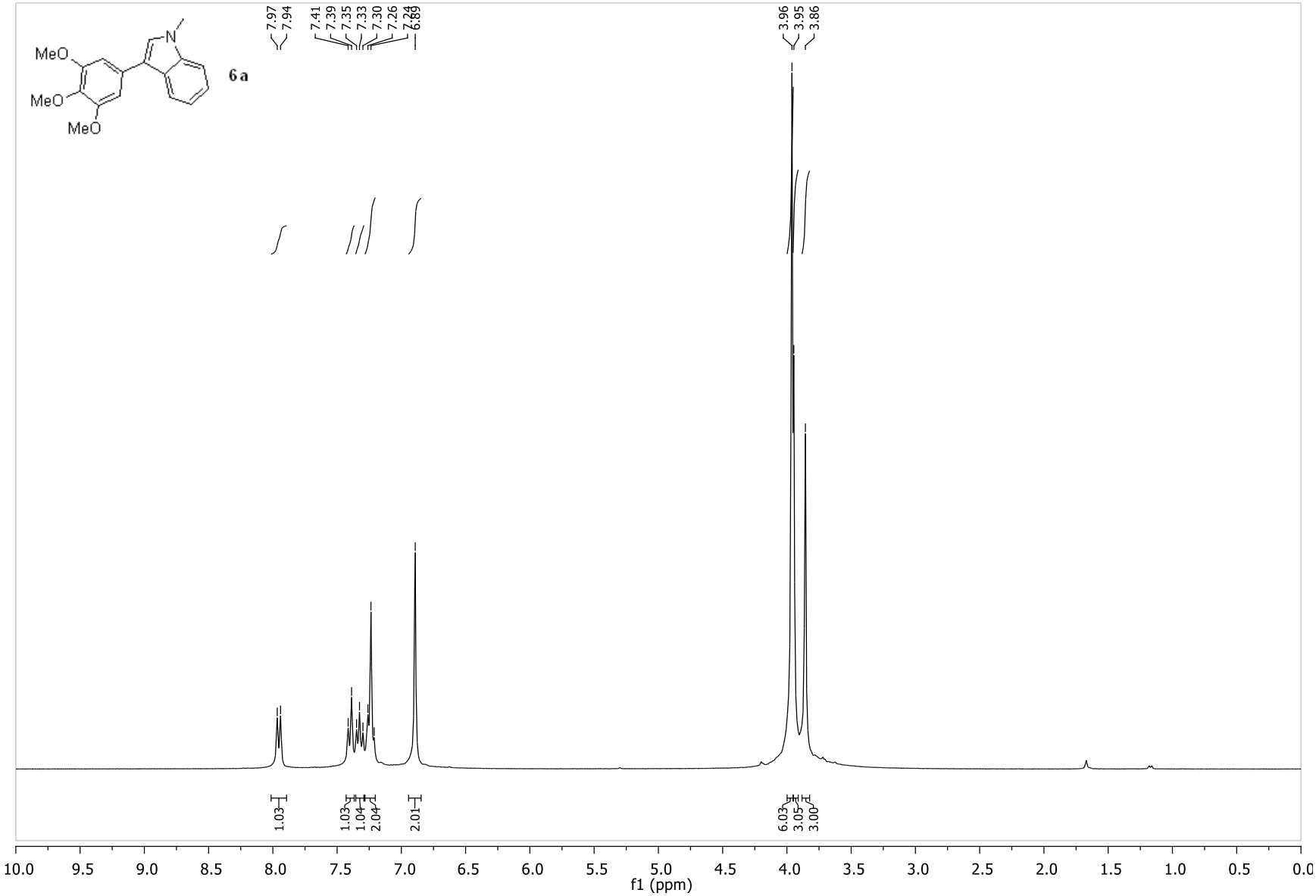
10
0
f1 (ppm)


MeO
MeO
MeO
N
6a
7.97
7.94
7.41
7.39
7.35
7.33
7.30
7.26
7.24
6.89
3.96
3.95
3.86
1.03
1.03
1.04
2.04
2.01
6.03
3.05
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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3.5
3.0
2.5
2.0
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1.0
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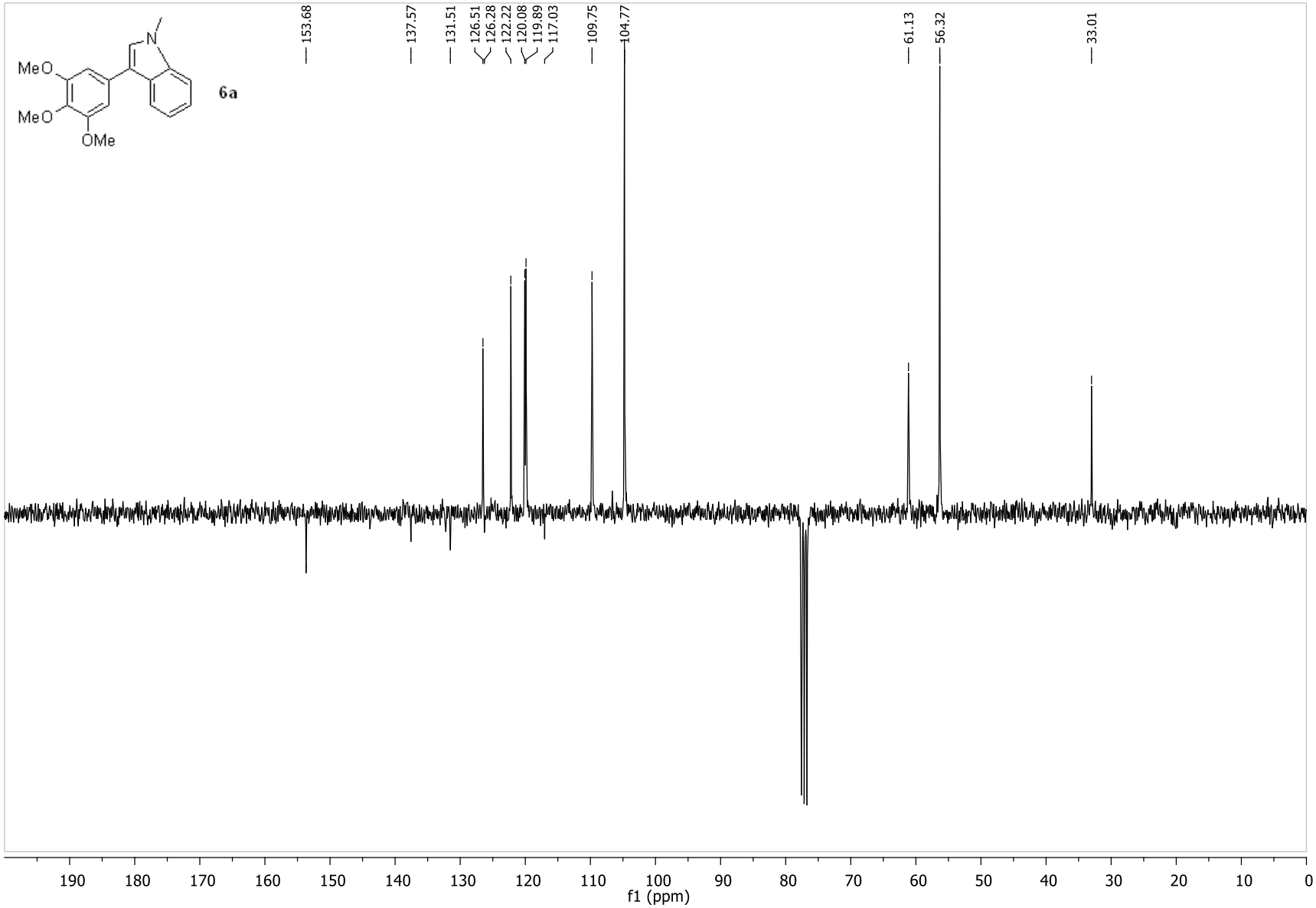
0.0
f1 (ppm)


MeO
MeO
OMe
N
6a
153.68
137.57
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126.51
126.28
122.22
120.08
119.89
117.03
109.75
104.77
61.13
56.32
33.01
190
180
170
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150
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130
120
110
100
90
80
70
60
50
40
30
20
10
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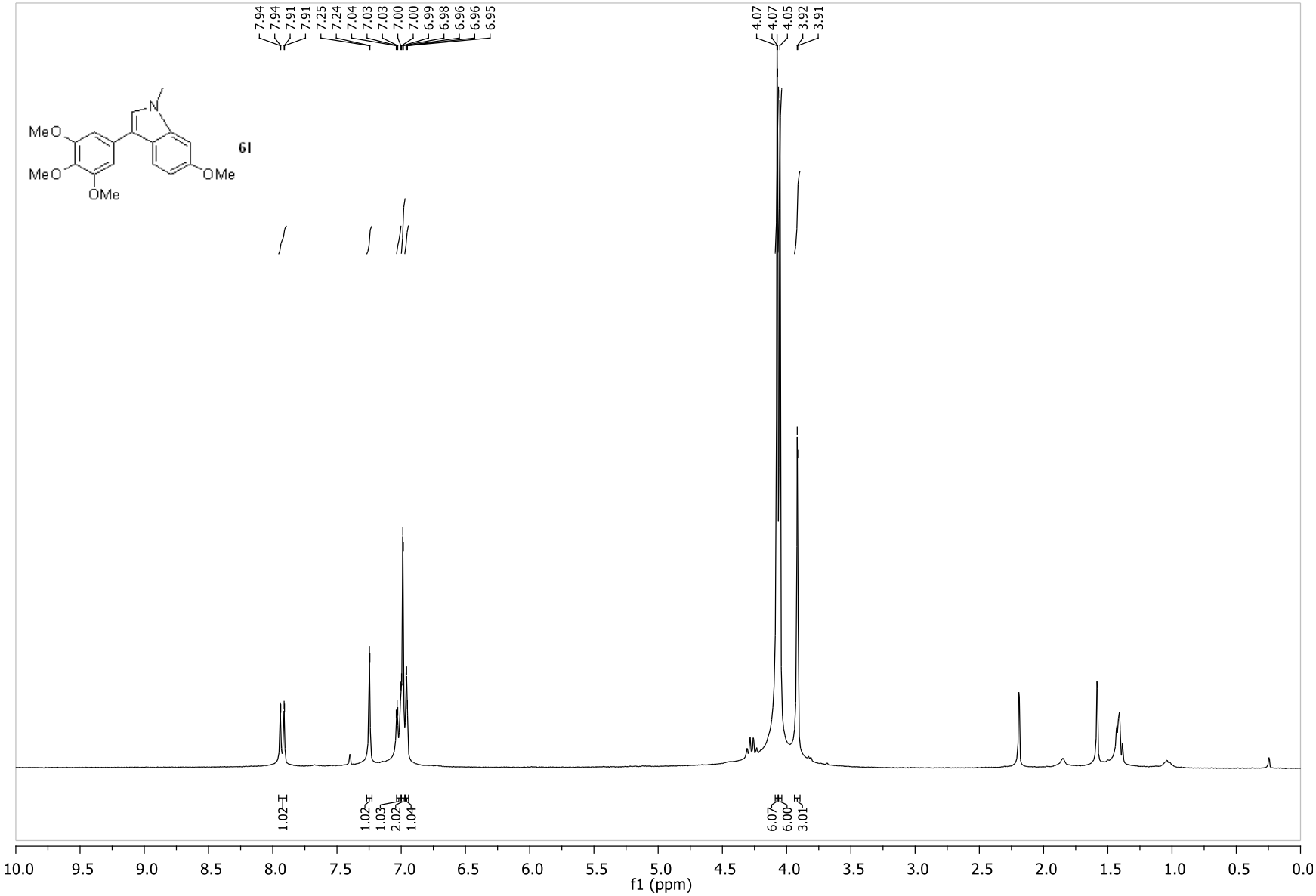
f1 (ppm)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7.91
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7.03
7.03
7.00
7.00
6.99
6.98
6.96
6.96
6.95
4.07
4.07
4.05
3.92
3.91
MeO
MeO
OMe
OMe
N
6l
1.02
1.02
1.03
2.02
1.04
6.07
6.00
3.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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2.5
2.0
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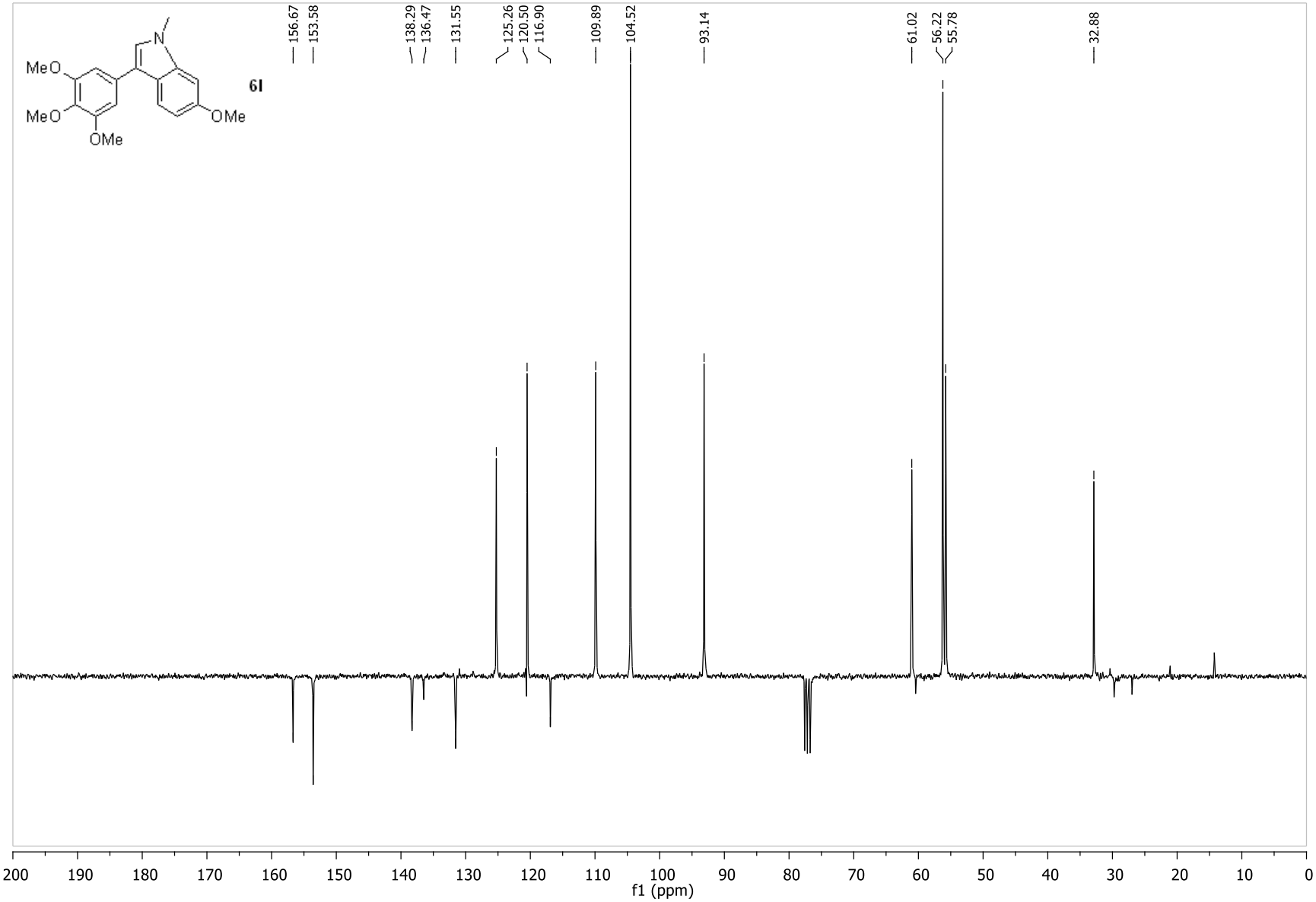
0.0
f1 (ppm)


MeO
MeO
OMe
OMe
N
6l
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136.47
131.55
125.26
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116.90
109.89
104.52
93.14
61.02
56.22
55.78
32.88
200
190
180
170
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150
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130
120
110
100
90
80
70
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50
40
30
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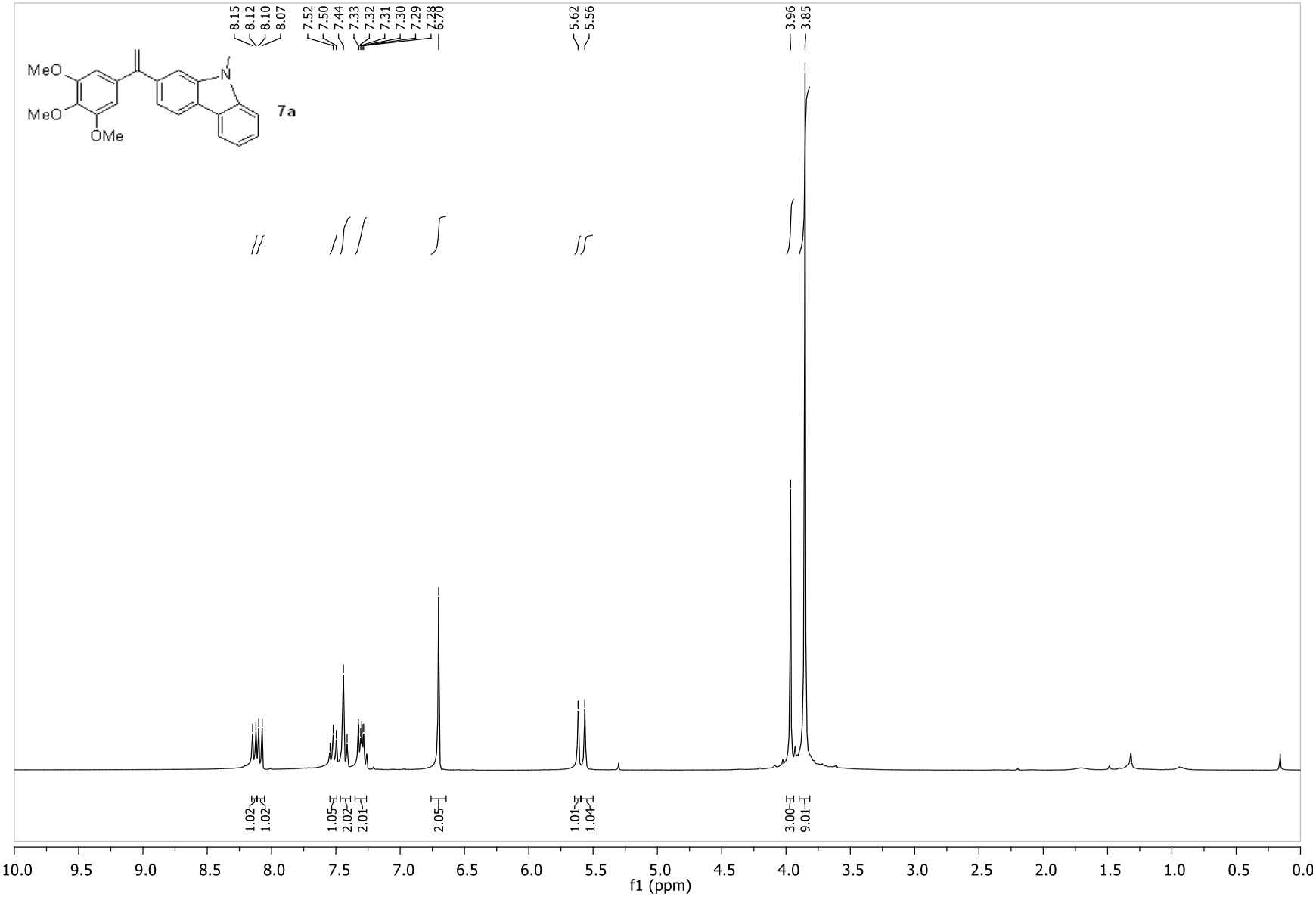
10
0
f1 (ppm)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7.32
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7.30
7.29
7.28
6.70
5.62
5.56
3.96
3.85
MeO
MeO
OMe
N
7a
1.02
1.02
1.05
2.02
2.01
2.05
1.01
1.04
3.00
9.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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2.0
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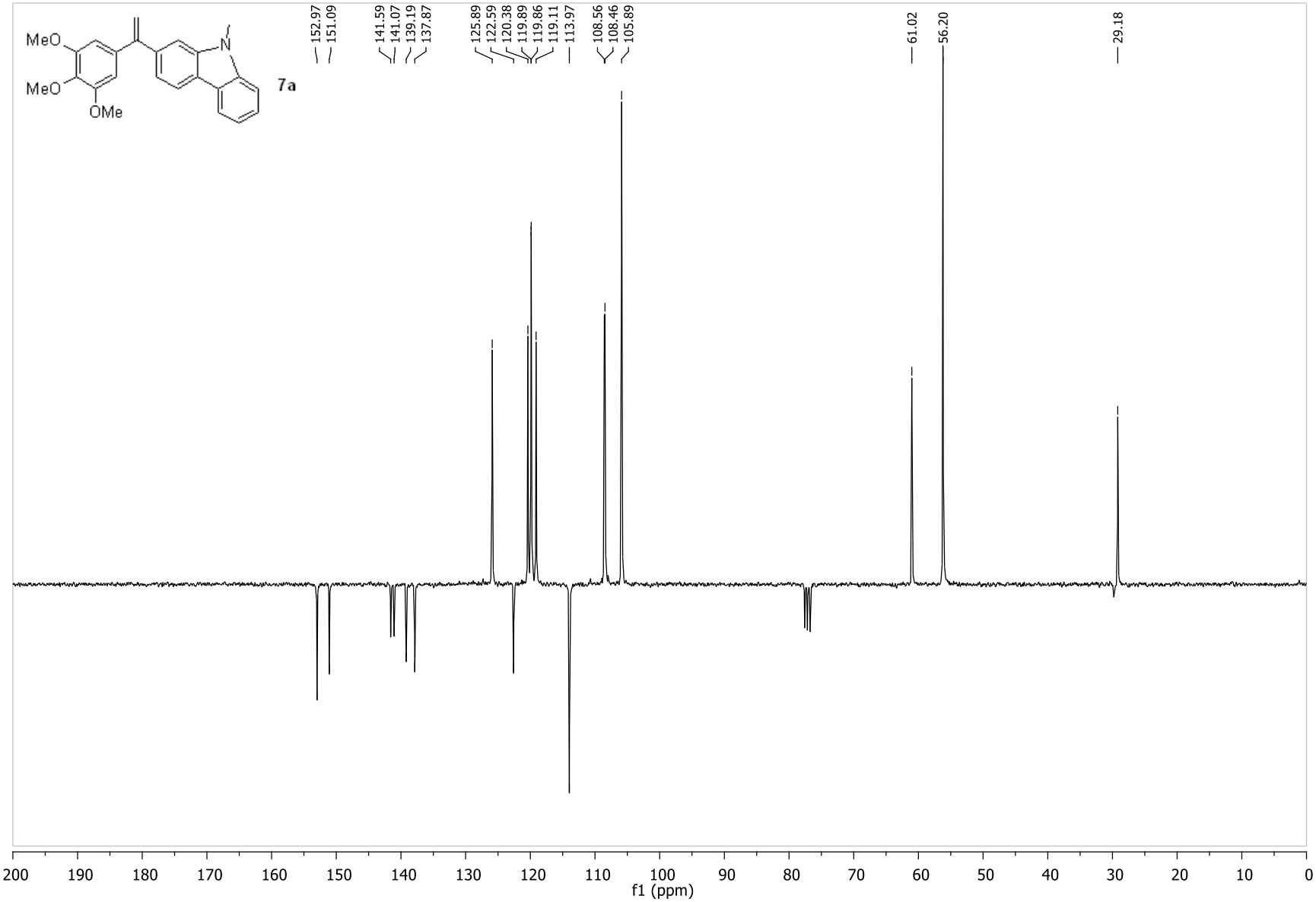
0.0
f1 (ppm)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MeO
OMe
N
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151.09
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137.87
125.89
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120.38
119.89
119.86
119.11
113.97
108.56
108.46
105.89
61.02
56.20
29.18
200
190
180
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150
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130
120
110
100
90
80
70
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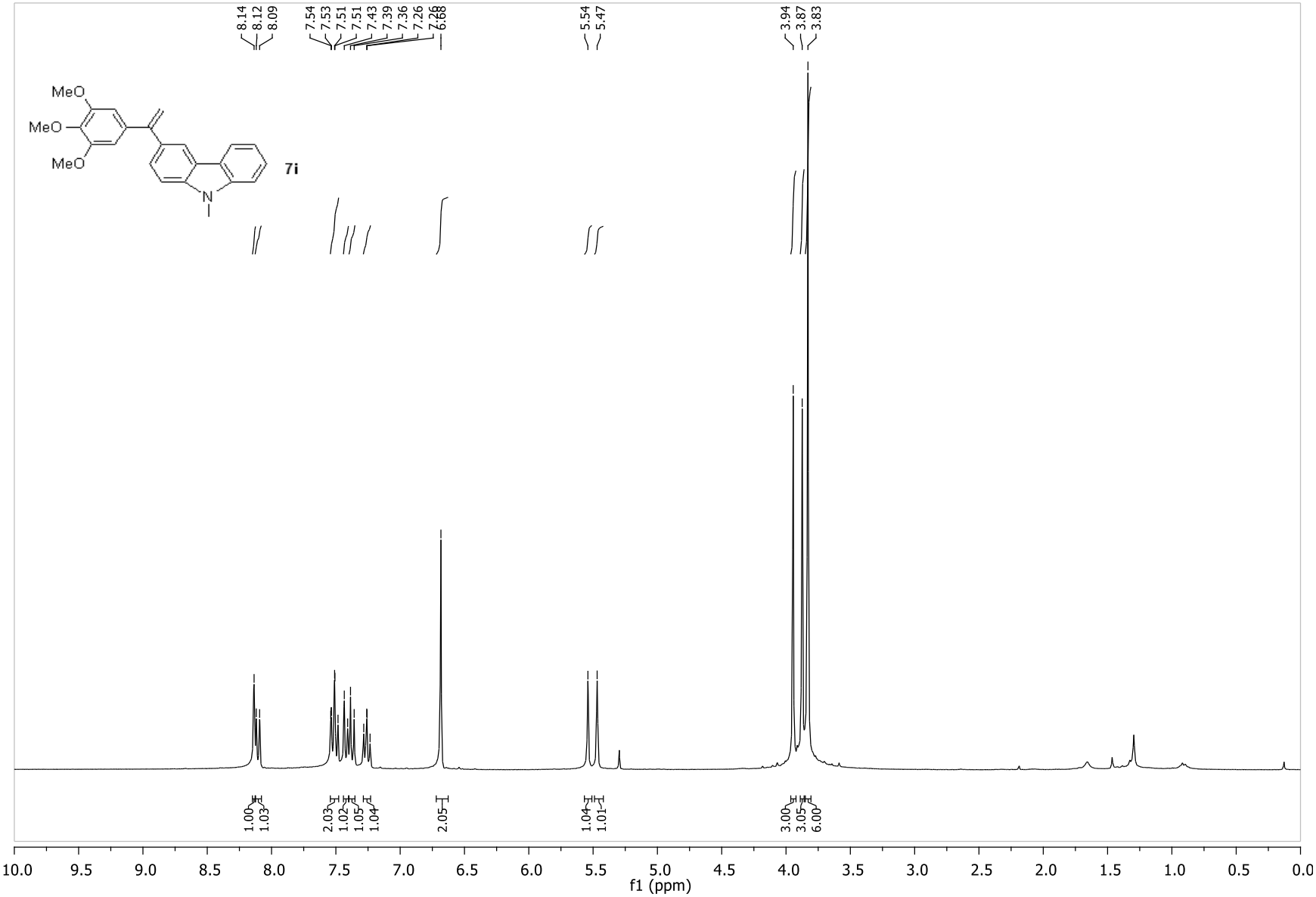
50
40
30
20
10
0
f1 (ppm)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7.51
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7.43
7.39
7.36
7.26
6.68
5.54
5.47
3.94
3.87
3.83
MeO
MeO
MeO
N
7i
1.00
1.03
2.03
1.02
1.05
1.04
2.05
1.04
1.01
3.00
3.05
6.00
10.0
9.5
9.0
8.5
8.0
7.5
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6.5
6.0
5.5
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3.5
3.0
2.5
2.0
1.5
1.0
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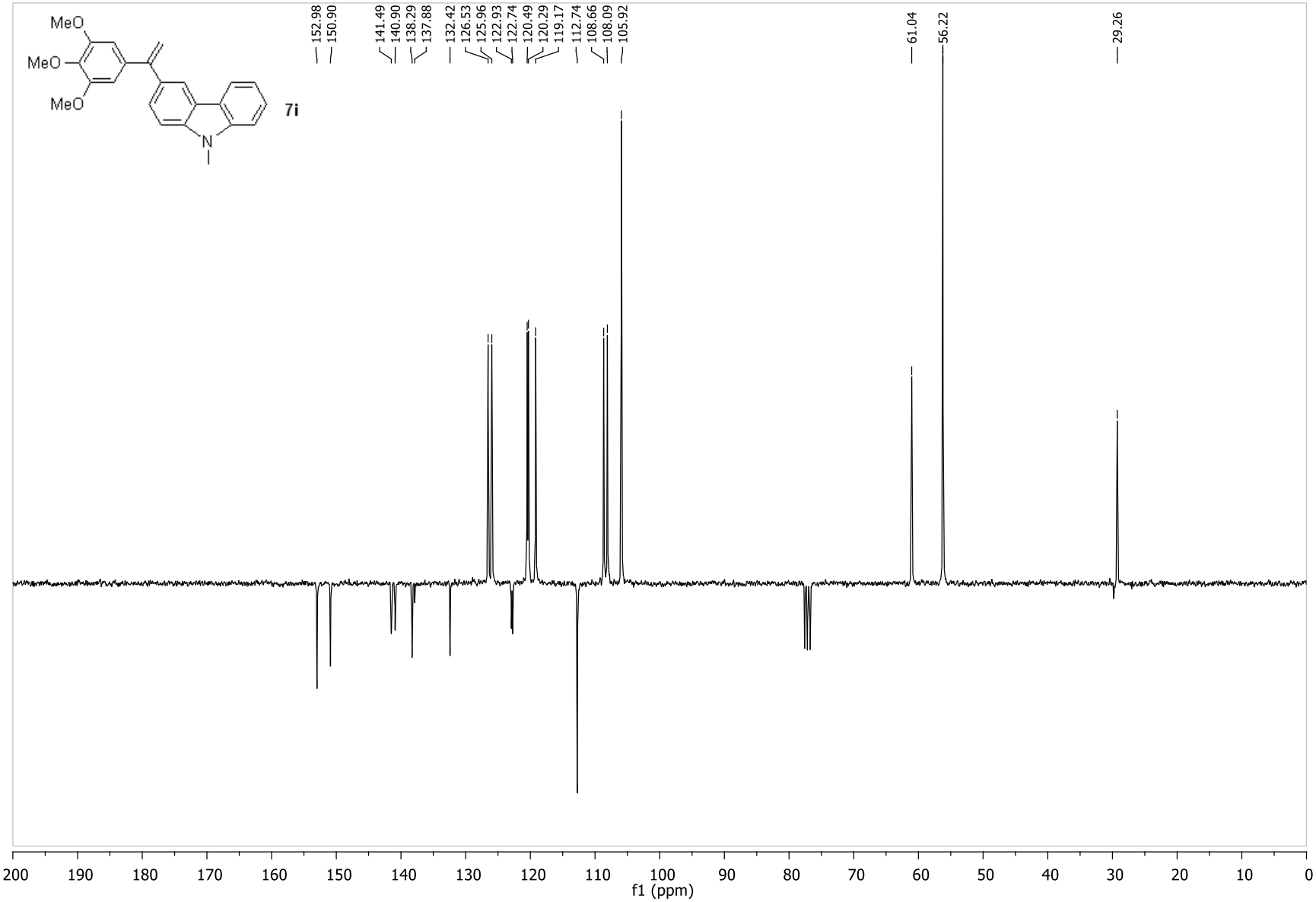
0.0
f1 (ppm)


MeO
MeO
MeO
N
7i
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150.90
141.49
140.90
138.29
137.88
132.42
126.53
125.96
122.93
122.74
120.49
120.29
119.17
112.74
108.66
108.09
105.92
61.04
56.22
29.26
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)