Supporting Information

Synthesis of Spiroindolenine-3,3'-pyrrolo[2,1-b]-quinazolinones through Gold(I)-Catalyzed Dearomative Cyclization of *N*-Alkynyl Quinazolinone-Tethered Indoles

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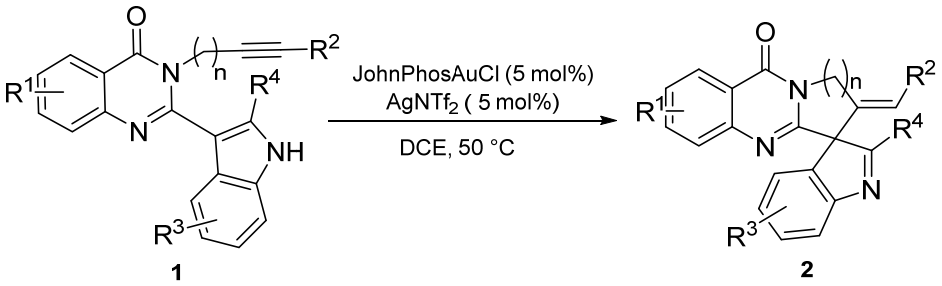
1. General experimental information

^{1}H NMR and ^{13}C NMR spectra were recorded at ambient temperature using 400 spectrometers. The data are reported as follows: chemical shift in ppm from internal tetramethylsilane on the δ scale, multiplicity (br = broad, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constants (Hz), and integration. IR spectra were recorded on FT-IR spectrometer, and only major peaks are reported in cm^{-1}. High resolution mass spectra (HRMS) were measured in ESI mode, and the mass analyzer of the HRMS was TOF. Analytical thin layer chromatography was performed on 0.25 mm extra hard silica gel plates with UV254 fluorescent indicator. Chromatography was performed using with 300-400 mesh silica gel (SiO_2). Unless otherwise noted, all reagents and solvents were obtained from commercial sources and, where appropriate, purified prior to use.

2. Synthesis of spiroindolenine-3,3'-pyrrolo[2,1-b]quinazolinones 2

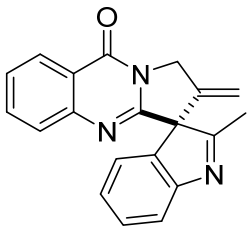


1 2

General procedure A: In a Schlenk flask was charged with JohnPhosAuCl (8.0 mg, 5 mol%), $AgNTf_2$ (5.8 mg, 5 mol%) and DCE (3.0 mL). The mixture was stirred vigorously at room temperature under dark for 15 min. Then, compound **1** (0.3 mmol) was added. The mixture was stirred vigorously at 50 °C for 3-5 h until compound **1** was completely consumed (monitored by TLC). At this time, the solvent was removed under reduced pressure and the crude product was purified by flash column chromatography (the crude residue was dry loaded with silica gel, 1/6 to 1/1, ethyl acetate/petroleum ether) to provide compounds **2a**-**2p** and **2aa**-**2aq**.

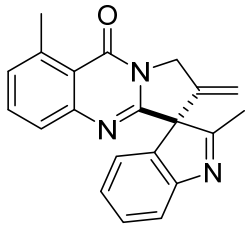
General procedure B: In a Schlenk flask was charged with JohnPhosAuCl (8.0 mg, 5 mol%), $AgNTf_2$ (5.8 mg, 5 mol%) and DCE (3.0 mL). The mixture was stirred

vigorously at room temperature under dark for 15 min. Then compound **1** (0.3 mmol) was added. The mixture was stirred vigorously at 80 °C or 100 °C for 10 to 36 h until compound **1** was completely consumed (monitored by TLC). At this time, the solvent was removed under reduced pressure and the crude product was purified by flash column chromatography (the crude residue was dry loaded with silica gel, 1/10 to 1/4, ethyl acetate/petroleum ether) to provide compounds **2q**-**2t**.



2a

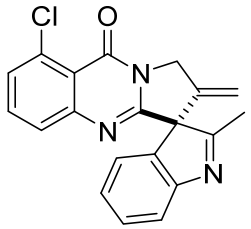
2-Methyl-2'-methylene-1',2'-dihydro-*9'H*-spiro[indole-3,3'-pyrrolo[2,1-b]quinazolin]-9'-one (**2a**). A white solid, 0.085 g, 90% yield; mp: 282–283 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.20 (dd, J = 7.9, 1.0 Hz, 1H), 7.79 – 7.72 (m, 1H), 7.59 – 7.49 (m, 3H), 7.46 (d, J = 7.3 Hz, 1H), 7.39 (td, J = 7.6, 1.2 Hz, 1H), 7.19 (dt, J = 7.5, 0.9 Hz, 1H), 5.39 – 5.38 (m, 1H), 5.20 – 5.00 (m, 2H), 4.67 – 4.66 (m, 1H), 2.18 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6): δ 179.8, 160.3, 157.6, 156.4, 149.3, 143.5, 139.1, 134.9, 129.5, 127.6, 127.3, 126.6, 126.3, 123.9, 121.4, 120.2, 111.8, 72.9, 51.4, 16.7. IR (thin film) 3295, 3233, 3138, 3039, 2125, 1679, 1559, 946, 755 cm^{-1}; HRMS (ESI) m/z calcd for $C_{20}H_{16}N_3O$ $(M+H)^+$: 314.1288 found 314.1276.



2b

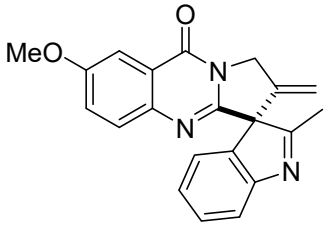
2,8'-Dimethyl-2'-methylene-1',2'-dihydro-*9'H*-spiro[indole-3,3'-pyrrolo[2,1-b]quinazolin]-9'-one (**2b**). A white solid, 0.049 g, 50% yield; mp: 122–123 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.59 – 7.53 (m, 2H), 7.46 (d, J = 7.4 Hz, 1H), 7.39 (td, J = 7.6, 1.1 Hz, 1H), 7.31 (d, J = 8.1 Hz, 1H), 7.27 (d, J = 7.3 Hz, 1H), 7.19 (dt, J = 7.5, 0.9 Hz, 1H), 5.42 – 5.32 (m, 1H), 5.15 – 4.96 (m, 2H), 4.70 – 4.61 (m, 1H), 2.83 (s,

3H), 2.18 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 179.8, 160.9, 157.2, 156.4, 150.9, 143.4, 140.5, 139.2, 133.9, 129.5, 129.4, 126.6, 125.8, 123.8, 120.2, 119.7, 111.7, 72.8, 51.4, 23.1, 16.6. IR (thin film) 3450, 3150, 2847, 2040, 1684, 1551, 1382, 1021, 764 cm^{-1}; HRMS (ESI) m/z calcd for $C_{21}H_{18}N_3O$ $(M+H)^+$ 328.1444 found 328.1418.



2c

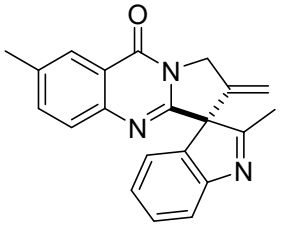
8'-Chloro-2-methyl-2'-methylene-1',2'-dihydro-*9'H*-spiro[indole-3,3'-pyrrolo[2,1-b]quinazolin]-9'-one (**2c**). A white solid, 0.094 g, 90% yield; mp: 236–237 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.67 – 7.61 (m, 1H), 7.56 – 7.50 (m, 2H), 7.49 – 7.46 (m, 1H), 7.44 (dd, J = 8.2, 1.2 Hz, 1H), 7.39 (td, J = 7.6, 1.2 Hz, 1H), 7.19 (dt, J = 7.5, 0.9 Hz, 1H), 5.42 – 5.30 (m, 1H), 5.17 – 4.95 (m, 2H), 4.68 – 4.56 (m, 1H), 2.19 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 179.6, 158.3, 156.4, 151.9, 143.3, 138.9, 134.6, 132.9, 129.5, 129.5, 127.2, 126.6, 124.0, 120.2, 118.4, 111.8, 72.9, 51.7, 16.6. IR (thin film) 3352, 3086, 2953, 1679, 1626, 1458, 1308, 123, 904, 690 cm^{-1}; HRMS (ESI) m/z calcd for $C_{20}H_{15}ClN_3O$ $(M+H)^+$ 348.0898 found 348.0887.



2d

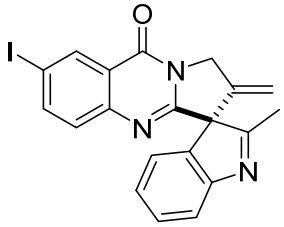
7'-Methoxy-2-methyl-2'-methylene-1',2'-dihydro-*9'H*-spiro[indole-3,3'-pyrrolo[2,1-b]quinazolin]-9'-one (**2d**). A white solid, 0.084 g, 82% yield; mp: 176–177 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.57 – 7.51 (m, 2H), 7.46 (dd, J = 8.0, 3.0 Hz, 2H), 7.41 – 7.32 (m, 2H), 7.18 (t, J = 7.4 Hz, 1H), 5.37 (s, 1H), 5.18 – 5.01 (m, 2H), 4.66 (s, 1H), 3.85 (s, 3H), 2.16 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 179.9, 160.0, 158.3, 156.3, 155.2, 143.7, 143.6, 139.3, 129.4, 129.3, 126.6, 124.1, 123.8, 122.2,

120.2, 111.7, 106.4, 72.6, 56.2, 51.3, 16.6. IR (thin film) 3072, 2916, 2849, 2440, 1665, 1517, 1489, 1358, 1283, 1028, 752 cm^{-1}; HRMS (ESI) m/z calcd for $C_{21}H_{18}N_3O_2$ $(M+H)^+$ 344.1394 found 344.1376.



2e

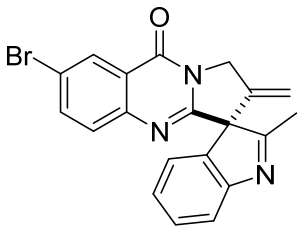
2,7'-Dimethyl-2'-methylene-1',2'-dihydro-*9'H*-spiro[indole-3,3'-pyrrolo[2,1-b]quinazolin]-9'-one (**2e**). A white solid, 0.087 g, 89% yield; mp: 168–169 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.99 (s, 1H), 7.60 – 7.53 (m, 2H), 7.46 (d, J = 7.3 Hz, 1H), 7.43 – 7.36 (m, 2H), 7.19 (t, J = 7.2 Hz, 1H), 5.37 (s, 1H), 5.20 – 5.00 (m, 2H), 4.66 (s, 1H), 2.44 (s, 3H), 2.16 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 179.8, 160.2, 156.7, 156.3, 147.3, 143.5, 139.2, 137.0, 136.1, 129.4, 127.5, 126.6, 125.6, 123.8, 121.1, 120.2, 111.7, 72.7, 51.3, 21.3, 16.6. IR (thin film) 3400, 2922, 1665, 1510, 1486, 1374, 1014, 913, 782 cm^{-1}; HRMS (ESI) m/z calcd for $C_{21}H_{18}N_3O$ $(M+H)^+$ 328.1444 found 328.1433.



2f

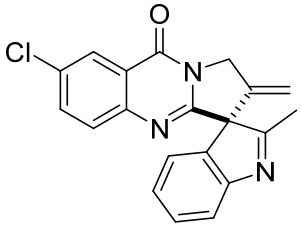
7'-Iodo-2-methyl-2'-methylene-1',2'-dihydro-*9'H*-spiro[indole-3,3'-pyrrolo[2,1-b]quinazolin]-9'-one (**2f**). A white solid, 0.115 g, 88% yield; mp: 140–141 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.44 (d, J = 2.0 Hz, 1H), 8.02 (dd, J = 8.6, 2.1 Hz, 1H), 7.54 (d, J = 7.7 Hz, 1H), 7.46 (d, J = 7.4 Hz, 1H), 7.39 (td, J = 7.6, 1.1 Hz, 1H), 7.30 (d, J = 8.6 Hz, 1H), 7.19 (td, J = 7.5, 0.9 Hz, 1H), 5.37 (s, 1H), 5.23 – 5.02 (m, 2H), 4.66 (s, 1H), 2.17 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 179.7, 159.0, 158.3, 156.3, 148.6, 143.3, 143.1, 138.9, 134.5, 129.8, 129.5, 126.6, 123.9, 123.2, 120.2, 111.9, 92.2, 72.9, 51.5, 16.7. IR (thin film) 3435, 3059, 2927, 1677, 1512, 1461, 1329,

909, 750 cm^{-1}; HRMS (ESI) m/z calcd for $C_{20}H_{15}IN_3O$ $(M+H)^+$ 440.0254 found 440.0263.



2g

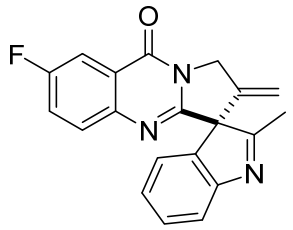
7'-Bromo-2-methyl-2'-methylene-1',2'-dihydro-*9'H*-spiro[indole-3,3'-pyrrolo[2,1-b]quinazolin]-9'-one (**2g**). A white solid, 0.112 g, 96% yield; mp: 122–123 °C; ^1H NMR (400 MHz, DMSO-d_6) δ 8.25 (d, J = 2.3 Hz, 1H), 7.89 (dd, J = 8.7, 2.4 Hz, 1H), 7.55 (d, J = 7.7 Hz, 1H), 7.50 – 7.44 (m, 2H), 7.39 (dt, J = 7.6, 1.1 Hz, 1H), 7.19 (dt, J = 7.5, 0.7 Hz, 1H), 5.38 (s, 1H), 5.16 – 5.00 (m, 2H), 4.66 (s, 1H), 2.17 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 179.7, 159.1, 158.3, 156.4, 148.3, 143.3, 138.9, 137.6, 130.0, 129.5, 128.3, 126.6, 124.0, 123.1, 120.2, 119.6, 111.9, 72.8, 51.5, 16.7. IR (thin film) 3410, 3059, 2929, 1675, 1465, 1335, 1122, 920, 780 cm^{-1}; HRMS (ESI) m/z calcd for $C_{20}H_{15}BrN_3O$ $(M+H)^+$ 392.0393 found 392.0388.



2h

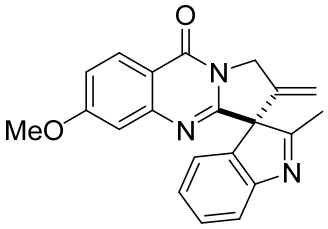
7'-Chloro-2-methyl-2'-methylene-1',2'-dihydro-*9'H*-spiro[indole-3,3'-pyrrolo[2,1-b]quinazolin]-9'-one (**2h**). A white solid, 0.101 g, 97% yield; mp: 197–198 °C; ^1H NMR (400 MHz, DMSO-d_6) δ 8.11 (d, J = 2.5 Hz, 1H), 7.78 (dd, J = 8.8, 2.5 Hz, 1H), 7.56 (d, J = 8.6 Hz, 2H), 7.48 (d, J = 7.3 Hz, 1H), 7.40 (dt, J = 7.6, 1.1 Hz, 1H), 7.20 (td, J = 7.5, 0.9 Hz, 1H), 5.41 – 5.38 (m, 1H), 5.26 – 4.94 (m, 2H), 4.84 – 4.62 (m, 1H), 2.19 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 179.7, 159.3, 158.2, 156.4, 148.0, 143.4, 138.8, 134.8, 131.5, 129.9, 129.5, 126.6, 125.2, 123.9, 122.7, 120.2, 111.9, 72.8, 51.5, 16.7. IR (thin film) 3529, 3402, 3057, 2993, 1680, 1509, 1458,

1375, 1237, 927, 841 cm^{-1}; HRMS (ESI) m/z calcd for $C_{20}H_{15}ClN_3O$ $(M+H)^+$ 348.0898 found 348.0889.



2i

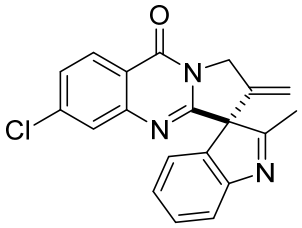
7'-Fluoro-2-methyl-2'-methylene-1',2'-dihydro-9'H-spiro[indole-3,3'-pyrrolo[2,1-b]quinazolin]-9'-one (**2i**). A white solid, 0.088 g, 89% yield; mp: 164–165 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.87 (d, J = 7.2 Hz, 1H), 7.72 – 7.52 (m, 3H), 7.51 – 7.32 (m, 2H), 7.28 – 7.07 (m, 1H), 5.39 (s, 1H), 5.11 (s, 2H), 4.67 (s, 1H), 2.18 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 179.8, 160.5 (d, J = 245 Hz), 159.6 (d, J = 3.4 Hz), 157.2 (d, J = 2.0 Hz), 156.3, 146.1 (d, J = 1.7 Hz), 143.5, 139.0, 130.4 (d, J = 8.4 Hz), 129.5, 126.6, 123.9, 123.2 (d, J = 23.9 Hz), 122.7 (d, J = 8.4 Hz), 120.2, 111.8, 111.0 (d, J = 23.4 Hz), 72.7, 51.4, 16.6. IR (thin film) 3410, 3082, 2919, 1676, 1515, 1483, 1346, 1135, 918, 784 cm^{-1}; HRMS (ESI) m/z calcd for $C_{20}H_{15}FN_3O$ $(M+H)^+$ 332.1194 found 332.1186.



2j

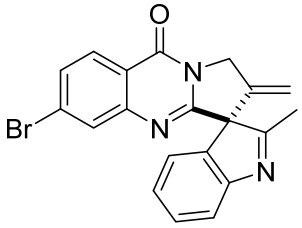
6'-Methoxy-2-methyl-2'-methylene-1',2'-dihydro-*9'H*-spiro[indole-3,3'-pyrrolo[2,1-b]quinazolin]-9'-one (**2j**). A white solid, 0.087 g, 85% yield; mp: 187–188 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.07 (d, J = 8.8 Hz, 1H), 7.56 (d, J = 7.7 Hz, 1H), 7.47 (d, J = 7.3 Hz, 1H), 7.40 (td, J = 7.6, 1.0 Hz, 1H), 7.21 (dd, J = 10.9, 4.0 Hz, 1H), 7.08 (dd, J = 8.8, 2.5 Hz, 1H), 7.01 (d, J = 2.4 Hz, 1H), 5.38 (s, 1H), 5.23 – 4.96 (m, 2H), 4.67 (s, 1H), 3.81 (s, 3H), 2.18 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 179.7, 164.5, 159.8, 158.2, 156.4, 151.6, 143.5, 139.2, 129.4, 127.7, 126.6, 123.9, 120.2, 117.1, 114.7, 111.8, 108.7, 72.9, 56.2, 51.3, 16.6. IR (thin film) 3438, 3079, 2981,

2849, 1671, 1614, 1487, 1213, 1027, 774 cm^{-1}; HRMS (ESI) m/z calcd for $C_{21}H_{18}N_3O_2$ $(M+H)^+$ 344.1394 found 344.1389.



2k

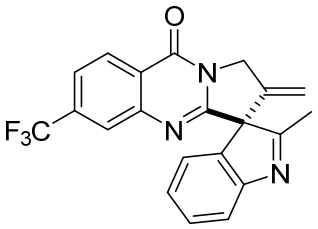
6'-Chloro-2-methyl-2'-methylene-1',2'-dihydro-*9'H*-spiro[indole-3,3'-pyrrolo[2,1-b]quinazolin]-9'-one (**2k**). A white solid, 0.087 g, 84% yield; mp: 202–203 °C; ^1H NMR (400 MHz, DMSO-d_6) δ 8.18 (d, J = 8.6 Hz, 1H), 7.64 (d, J = 1.9 Hz, 1H), 7.57 – 7.55 (m, 2H), 7.48 (d, J = 7.4 Hz, 1H), 7.40 (td, J = 7.6, 1.0 Hz, 1H), 7.22 – 7.18 (m, 1H), 5.39 (s, 1H), 5.22 – 4.98 (m, 2H), 4.67 (s, 1H), 2.19 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 179.6, 159.7, 159.2, 156.4, 150.4, 143.4, 139.5, 138.9, 129.5, 128.3, 127.5, 126.9, 126.6, 124.0, 120.2, 111.9, 72.9, 51.5, 16.6. IR (thin film) 3436, 3089, 3009, 2926, 1677, 1601, 1462, 1076, 907, 778 cm^{-1}; HRMS (ESI) m/z calcd for $C_{20}H_{15}ClN_3O$ $(M+H)^+$ 348.0898 found 348.0882.



2l

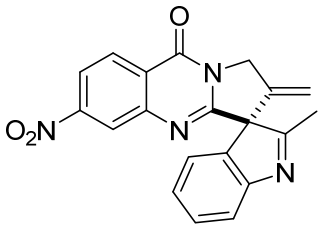
6'-Bromo-2-methyl-2'-methylene-1',2'-dihydro-*9'H*-spiro[indole-3,3'-pyrrolo[2,1-b]quinazolin]-9'-one (**2l**). A white solid, 0.095 g, 81% yield; mp: 231–232 °C; ^1H NMR (400 MHz, DMSO-d_6) δ 8.09 (d, J = 8.5 Hz, 1H), 7.77 (d, J = 1.8 Hz, 1H), 7.68 (dd, J = 8.5, 1.9 Hz, 1H), 7.55 (d, J = 7.7 Hz, 1H), 7.47 (d, J = 7.3 Hz, 1H), 7.41 – 7.37 (m, 1H), 7.19 (t, J = 7.4 Hz, 1H), 5.38 (s, 1H), 5.17 – 4.97 (m, 2H), 4.66 (s, 1H), 2.18 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 179.6, 159.8, 159.1, 156.4, 150.4, 143.4, 138.9, 130.3, 130.0, 129.5, 128.5, 128.3, 126.6, 124.0, 120.5, 120.2, 111.9, 72.9, 51.5, 16.6. IR (thin film) 3435, 3075, 2924, 2856, 1737, 1675, 1457, 1224, 1182, 1052, 749 cm^{-1}; HRMS (ESI) m/z calcd for $C_{20}H_{15}BrN_3O$ $(M+H)^+$ 392.0393 found

392.0398.



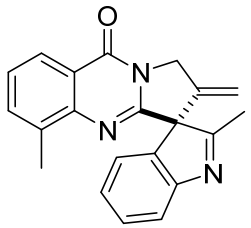
2m

2-Methyl-2'-methylene-6'-(trifluoromethyl)-1',2'-dihydro-*9'H*-spiro[indole-3,3'-pyrrolo[2,1-b]quinazolin]-9'-one (**2m**). A white solid, 0.093 g, 82% yield; mp: 198–199 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.37 (d, J = 8.3 Hz, 1H), 7.90 (s, 1H), 7.81 (dd, J = 8.4, 1.5 Hz, 1H), 7.56 (d, J = 7.7 Hz, 1H), 7.48 (d, J = 7.4 Hz, 1H), 7.40 (dt, J = 7.6, 1.1 Hz, 1H), 7.20 (dt, J = 7.5, 0.8 Hz, 1H), 5.40 (s, 1H), 5.19 – 5.06 (m, 2H), 4.68 (s, 1H), 2.20 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 179.6, 159.5 (q, J = 13.5 Hz), 156.4, 149.3, 143.3, 138.8, 134.3 (q, J = 31.9 Hz), 129.5, 128.1, 126.7, 124.3, 124.0, 123.9 (q, J = 203.4 Hz), 122.5, 120.2, 112.0, 72.9, 51.6, 16.7. IR (thin film) 3427, 3083, 1689, 1519, 1437, 1322, 1134, 1051, 920, 773 cm^{-1}; HRMS (ESI) m/z calcd for $C_{21}H_{15}FN_3O$ $(M+H)^+$ 382.1162 found 382.1156.



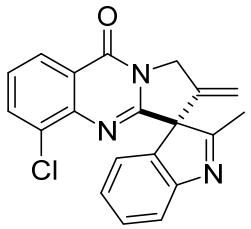
2n

2-Methyl-2'-methylene-6'-nitro-1',2'-dihydro-*9'H*-spiro[indole-3,3'-pyrrolo[2,1-b]quinazolin]-9'-one (**2n**). A yellow solid, 0.092 g, 86% yield; mp: 252–253 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.41 (dd, J = 8.3, 0.8 Hz, 1H), 8.27 – 8.21 (m, 2H), 7.57 (d, J = 7.7 Hz, 1H), 7.50 (d, J = 7.3 Hz, 1H), 7.41 (dt, J = 7.6, 1.1 Hz, 1H), 7.21 (dt, J = 7.5, 0.7 Hz, 1H), 5.41 (s, 1H), 5.22 – 5.05 (m, 2H), 4.69 (s, 1H), 2.22 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 179.5, 160.1, 159.4, 156.4, 151.5, 149.6, 143.3, 138.7, 129.6, 128.5, 126.7, 125.8, 124.0, 122.7, 120.8, 120.3, 112.0, 72.9, 51.7, 16.7. IR (thin film) 3429, 3086, 2922, 1974, 1687, 1611, 1529, 1344, 1167, 770 cm^{-1}; HRMS (ESI) m/z calcd for $C_{20}H_{15}N_4O_3$ $(M+H)^+$ 359.1139 found 359.1128.



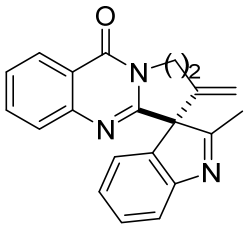
2o

2,5'-Dimethyl-2'-methylene-1',2'-dihydro-*9'H*-spiro[indole-3,3'-pyrrolo[2,1-b]quinazolin]-9'-one (**2o**). A white solid, 0.085 g, 87% yield; mp: 179–180 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.58 – 7.54 (m, 2H), 7.45 (d, J = 7.3 Hz, 1H), 7.39 (dt, J = 7.6, 1.0 Hz, 1H), 7.30 (d, J = 8.1 Hz, 1H), 7.26 (d, J = 7.3 Hz, 1H), 7.20 – 7.17 (m, 3.7 Hz, 1H), 5.37 (s, 1H), 5.16 – 4.90 (m, 2H), 4.65 (s, 1H), 2.83 (s, 3H), 2.17 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 179.7, 160.9, 157.1, 156.3, 150.9, 143.4, 140.4, 139.2, 133.9, 129.5, 129.4, 126.6, 125.8, 123.8, 120.2, 119.6, 111.7, 72.8, 51.4, 23.1, 16.6. IR (thin film) 3435, 3052, 2927, 1671, 1626, 1595, 1459, 1315, 1231, 810 cm^{-1}; HRMS (ESI) m/z calcd for $C_{21}H_{18}N_3O$ $(M+H)^+$ 328.1444 found 328.1442.



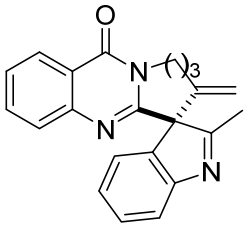
2p

5'-Chloro-2-methyl-2'-methylene-1',2'-dihydro-*9'H*-spiro[indole-3,3'-pyrrolo[2,1-b]quinazolin]-9'-one (**2p**). A white solid, 0.094 g, 90% yield; mp: 244–245 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.16 (dd, J = 8.0, 1.3 Hz, 1H), 7.92 (dd, J = 7.7, 1.3 Hz, 1H), 7.57 (d, J = 7.7 Hz, 1H), 7.53 – 7.46 (m, 2H), 7.41 (dt, J = 7.6, 0.8 Hz, 1H), 7.20 (t, J = 7.4 Hz, 1H), 5.38 (s, 1H), 5.26 – 4.97 (m, 2H), 4.66 (s, 1H), 2.20 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 179.6, 159.7, 158.6, 156.2, 145.8, 143.5, 139.0, 135.0, 131.0, 129.5, 127.6, 126.6, 125.5, 123.9, 123.2, 120.3, 111.8, 73.0, 51.5, 16.7. IR (thin film) 3054, 2989, 1736, 1680, 1513, 1370, 1188, 940, 770 cm^{-1}; HRMS (ESI) m/z calcd for $C_{20}H_{15}ClN_3O$ $(M+H)^+$ 348.0896 found 348.0888.



2q

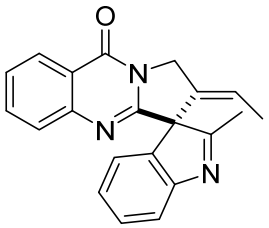
2-Methyl-7'-methylene-8',9'-dihydro-*7'H*,*11'H*-spiro[indole-3,6'-pyrido[2,1-b]quinazolin]-11'-one (**2q**). A white solid, 0.086 g, 88% yield; mp: 186-187 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.15 (dd, J = 8.0, 1.2 Hz, 1H), 7.71 (ddd, J = 8.4, 7.2, 1.5 Hz, 1H), 7.54 – 7.46 (m, 2H), 7.43 (d, J = 7.4 Hz, 1H), 7.37 (d, J = 7.9 Hz, 1H), 7.32 (dt, J = 7.6, 1.1 Hz, 1H), 7.10 (dt, J = 7.5, 0.9 Hz, 1H), 5.00 (s, 1H), 4.43 (ddd, J = 13.5, 6.9, 4.5 Hz, 1H), 4.34 (s, 1H), 4.30 – 4.19 (m, 1H), 3.04 (ddd, J = 14.4, 6.6, 4.0 Hz, 1H), 2.94 – 2.80 (m, 1H), 2.21 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 182.3, 161.5, 155.9, 152.6, 147.6, 147.4, 140.9, 134.9, 128.8, 127.3, 127.3, 126.6, 126.1, 122.4, 120.6, 120.5, 111.4, 69.8, 42.4, 30.8, 17.2. IR (thin film) 3438, 3062, 2918, 1671, 1585, 1562, 1472, 1393, 1315, 775 cm^{-1}; HRMS (ESI) m/z calcd for $C_{21}H_{18}N_3O$ $(M+H)^+$ 328.1444 found 328.1434.



2r

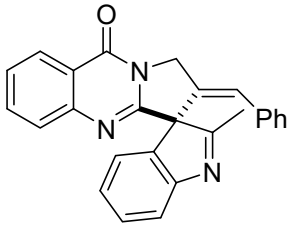
2'-Methyl-7-methylene-7,8,9,10-tetrahydro-*12H*-spiro[azepino[2,1-b]quinazoline-6,3'-indol]-12-one (**2r**). A white solid, 0.043 g, 42% yield; mp: 171-172 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.13 (dd, J = 8.0, 1.2 Hz, 1H), 7.76 – 7.70 (m, 1H), 7.58 (d, J = 7.5 Hz, 1H), 7.53 – 7.47 (m, 2H), 7.45 – 7.36 (m, 2H), 7.18 (dt, J = 7.5, 1.0 Hz, 1H), 5.12 (d, J = 12.3 Hz, 1H), 4.88 (s, 1H), 4.24 (s, 1H), 4.22 – 4.09 (m, 1H), 2.79 – 2.66 (m, 1H), 2.59 – 2.51 (m, 2H), 2.30 (s, 3H), 2.13 – 1.98 (m, 1H), 1.96 – 1.81 (m, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 183.0, 161.5, 156.8, 154.8, 147.2, 144.7, 135.0, 129.7, 129.5, 128.9, 127.5, 126.8, 126.4, 123.1, 121.0, 120.5, 112.0, 74.7, 30.7, 27.5,

17.7. IR (thin film) 3210, 3002, 2702, 2010, 1768, 1655, 1400, 1210, 1071, 732 cm^{-1}; HRMS (ESI) m/z calcd for $C_{22}H_{20}N_3O$ $(M+H)^+$ 342.1601 found 342.1593.



2s

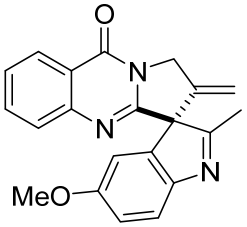
2'-Ethylidene-2-methyl-1',2'-dihydro-*9'H*-spiro[indole-3,3'-pyrrolo[2,1-b]quinazolin]-9'-one (**2aj**). A white solid, 0.069 g, 70% yield; mp: 190-191 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.15 (dd, J = 8.0, 1.2 Hz, 1H), 7.75 – 7.65 (m, 1H), 7.56 – 7.43 (m, 2H), 7.40 – 7.31 (m, 3H), 7.14 (dt, J = 7.5, 0.9 Hz, 1H), 6.24 – 6.14 (m, 1H), 4.81 – 4.67 (m, 2H), 2.19 (s, 3H), 1.23 (d, J = 1.5 Hz, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 182.0, 161.3, 156.3, 151.2, 147.7, 144.2, 134.9, 129.3, 128.7, 127.3, 127.2, 126.4, 126.2, 122.9, 120.6, 120.5, 120.2, 68.3, 44.4, 17.4, 17.2. IR (thin film) 3075, 2922, 2886, 1674, 1584, 1561, 1475, 1402, 1325, 773 cm^{-1}; HRMS (ESI) m/z calcd for $C_{21}H_{18}N_3O$ $(M+H)^+$ 328.1444 found 328.1439.



2t

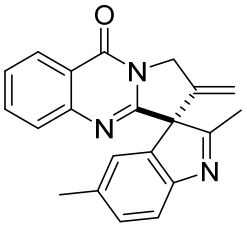
2'-Benzylidene-2-methyl-1',2'-dihydro-*9'H*-spiro[indole-3,3'-pyrrolo[2,1-b]quinazolin]-9'-one (**2t**). A white solid, 0.115 g, 99% yield; mp: 231-232 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.16 (dd, J = 8.0, 1.2 Hz, 1H), 7.77 – 7.70 (m, 1H), 7.56 (d, J = 7.3 Hz, 1H), 7.54 – 7.47 (m, 2H), 7.43 – 7.37 (m, 2H), 7.24 – 7.20 (m, 1H), 7.19 – 7.10 (m, 3H), 6.71 – 6.62 (m, 2H), 6.52 (t, J = 3.5 Hz, 1H), 5.07 – 4.92 (m, 2H), 2.02 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 181.9, 161.3, 156.2, 151.5, 147.7, 144.7, 138.5, 135.1, 134.1, 129.7, 129.5, 128.9, 128.7, 128.6, 127.4, 127.4, 126.8, 126.5, 126.4, 125.1, 123.2, 120.7, 120.5, 67.8, 44.6, 17.9. IR (thin film) 3437, 3062, 2952,

1683, 1586, 1554, 1473, 1177, 1022, 771 cm^{-1}; HRMS (ESI) m/z calcd for $C_{26}H_{20}N_3O$ $(M+H)^+$ 390.1601 found 390.1572.



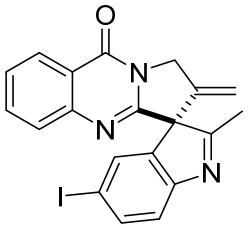
2aa

5-Methoxy-2-methyl-2'-methylene-1',2'-dihydro-*9'H*-spiro[indole-3,3'-pyrrolo[2,1-b]quinazolin]-9'-one (**2aa**). A white solid, 0.097 g, 94% yield; mp: 130–131 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.20 (dd, J = 8.1, 1.3 Hz, 1H), 7.80 – 7.72 (m, 1H), 7.60 – 7.49 (m, 2H), 7.45 (d, J = 8.5 Hz, 1H), 7.16 (d, J = 2.5 Hz, 1H), 6.92 (dd, J = 8.5, 2.5 Hz, 1H), 5.38 (s, 1H), 5.17 – 5.00 (m, 2H), 4.68 (s, 1H), 3.70 (s, 3H), 2.13 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 177.5, 160.3, 158.6, 157.8, 149.7, 149.3, 145.1, 139.4, 134.8, 127.6, 127.2, 126.3, 121.4, 120.5, 114.3, 111.7, 110.3, 72.9, 56.0, 51.4, 16.5. IR (thin film) 3436, 2941, 2839, 1771, 1678, 1610, 1468, 1335, 1031, 775 cm^{-1}; HRMS (ESI) m/z calcd for $C_{21}H_{18}N_3O_2$ $(M+H)^+$ 344.1394 found 344.1386.



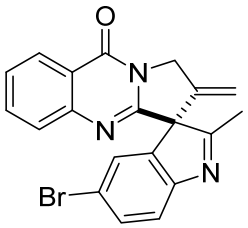
2ab

2,5-Dimethyl-2'-methylene-1',2'-dihydro-*9'H*-spiro[indole-3,3'-pyrrolo[2,1-b]quinazolin]-9'-one (**2ab**). A white solid, 0.095 g, 97% yield; mp: 157–158 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.25 – 8.13 (m, 1H), 7.85 – 7.69 (m, 1H), 7.55 – 7.49 (m, 2H), 7.42 (d, J = 7.9 Hz, 1H), 7.31 – 7.27 (m, 1H), 7.23 – 7.14 (m, 1H), 5.41 – 5.33 (m, 1H), 5.22 – 4.95 (m, 2H), 4.68 – 4.65 (m, 1H), 2.26 (s, 3H), 2.15 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 178.7, 160.2, 157.8, 154.0, 149.3, 143.8, 139.3, 136.1, 134.8, 129.8, 127.6, 127.2, 126.3, 124.3, 121.3, 119.8, 111.9, 72.6, 51.4, 21.3, 16.6. IR (thin film) 3409, 3125, 3086, 2989, 2926, 1677, 1512, 1469, 1375, 1037, 771 cm^{-1}; HRMS (ESI) m/z calcd for $C_{21}H_{18}N_3O$ $(M+H)^+$ 328.1444 found 328.1439.



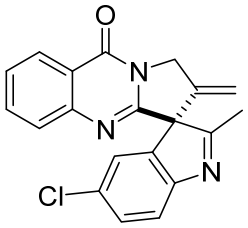
2ac

5-Iodo-2-methyl-2'-methylene-1',2'-dihydro-*9'H*-spiro[indole-3,3'-pyrrolo[2,1-b] quinazolin]-9'-one (**2ac**). A white solid, 0.121 g, 92% yield; mp: 193–194 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.21 (dd, J = 8.2, 1.4 Hz, 1H), 7.97 (d, J = 1.6 Hz, 1H), 7.80 – 7.73 (m, 2H), 7.57 – 7.50 (m, 2H), 7.39 (d, J = 8.1 Hz, 1H), 5.41 (s, 1H), 5.16 – 4.99 (m, 2H), 4.71 (s, 1H), 2.17 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 180.6, 160.2, 157.1, 156.1, 149.2, 145.8, 138.6, 138.2, 134.8, 132.7, 127.6, 127.3, 126.3, 122.4, 121.5, 112.2, 91.9, 72.8, 51.4, 16.6. IR (thin film) 3428, 2925, 2855, 1672, 1610, 1466, 1373, 1219, 774 cm^{-1}; HRMS (ESI) m/z calcd for $C_{20}H_{15}IN_3O$ $(M+H)^+$ 440.0254 found 440.0227.



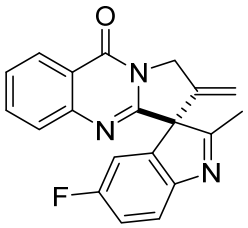
2ad

5-Bromo-2-methyl-2'-methylene-1',2'-dihydro-*9'H*-spiro[indole-3,3'-pyrrolo[2,1-b]quinazolin]-9'-one (**2ad**). A white solid, 0.102 g, 87% yield; mp: 200–201 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.23 – 8.16 (m, 1H), 7.83 (d, J = 1.9 Hz, 1H), 7.79 – 7.71 (m, 1H), 7.62 – 7.56 (m, 1H), 7.56 – 7.47 (m, 3H), 5.45 – 5.34 (m, 1H), 5.16 – 4.98 (m, 2H), 4.76 – 4.64 (m, 1H), 2.17 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 180.9, 160.2, 157.0, 155.6, 149.2, 145.7, 138.5, 134.8, 132.3, 127.6, 127.3, 127.3, 126.3, 122.0, 121.5, 119.3, 112.3, 73.0, 51.4, 16.6. IR (thin film) 3340, 3212, 2986, 2074, 1684, 1544, 1328, 1120, 751 cm^{-1}; HRMS (ESI) m/z calcd for $C_{20}H_{15}BrN_3O$ $(M+H)^+$ 392.0393 found 392.0375.



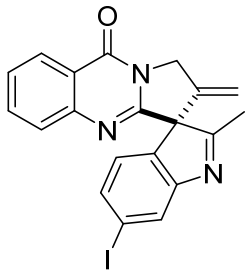
2ae

5-Chloro-2-methyl-2'-methylene-1',2'-dihydro-*9'H*-spiro[indole-3,3'-pyrrolo[2,1-b]quinazolin]-9'-one (**2ae**). A white solid, 0.094 g, 90% yield; mp: 208–209 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.21 (dd, J = 8.3, 1.4 Hz, 1H), 7.80 – 7.73 (m, 1H), 7.71 (d, J = 2.0 Hz, 1H), 7.60 – 7.50 (m, 3H), 7.46 (dd, J = 8.3, 2.1 Hz, 1H), 5.42 (s, 1H), 5.17 – 5.02 (m, 2H), 4.71 (s, 1H), 2.19 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 180.9, 160.2, 157.0, 155.2, 149.2, 145.3, 138.5, 134.8, 131.0, 129.5, 127.6, 127.3, 126.3, 124.5, 121.5, 121.5, 112.3, 73.0, 51.4, 16.6. IR (thin film) 3443, 3072, 2999, 1680, 1613, 1458, 1376, 1054, 777 cm^{-1}; HRMS (ESI) m/z calcd for $C_{20}H_{15}ClN_3O$ $(M+H)^+$ 348.0898 found 348.0900.



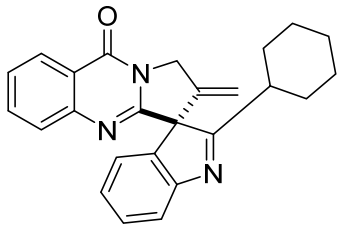
2af

5-Fluoro-2-methyl-2'-methylene-1',2'-dihydro-*9'H*-spiro[indole-3,3'-pyrrolo[2,1-b]quinazolin]-9'-one (**2af**). A white solid, 0.077 g, 78% yield; mp: 144–145 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.23 – 8.16 (m, 1H), 7.79 – 7.70 (m, 1H), 7.60 – 7.50 (m, 3H), 7.47 (dd, J = 8.4, 2.5 Hz, 1H), 7.22 (td, J = 9.2, 2.5 Hz, 1H), 5.41 (s, 1H), 5.17 – 5.02 (m, 2H), 4.70 (s, 1H), 2.16 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 180.0 (d, J = 3.5 Hz), 161.3 (d, J = 240.8 Hz), 160.2, 157.1, 152.6 (d, J = 2.1 Hz), 149.2, 145.2 (d, J = 9.6 Hz), 138.7, 134.8, 127.6, 127.3, 126.3, 121.4, 121.1 (J = 8.9 Hz), 115.8 (d, J = 23.4 Hz), 112.1, 112.0 (d, J = 25.7 Hz), 73.1 (d, J = 2.12 Hz), 51.4, 16.6. IR (thin film) 3297, 2925, 2855, 1772, 1684, 1605, 1525, 1419, 1180, 775 cm^{-1}; HRMS (ESI) m/z calcd for $C_{20}H_{15}FN_3O$ $(M+H)^+$ 332.1194 found 332.1181.



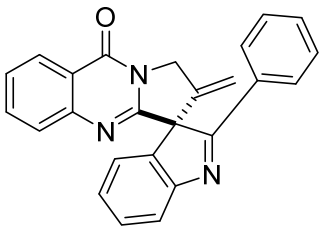
2ag

6-Iodo-2-methyl-2'-methylene-1',2'-dihydro-*9'H*-spiro[indole-3,3'-pyrrolo[2,1-b] quinazolin]-9'-one (**2ag**). A white solid, 0.110 g, 84% yield; mp: 223–224 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.19 (d, J = 7.7 Hz, 1H), 7.93 (s, 1H), 7.76 (t, J = 7.3 Hz, 1H), 7.61 – 7.46 (m, 3H), 7.32 (d, J = 7.8 Hz, 1H), 5.40 (s, 1H), 5.16 – 4.99 (m, 2H), 4.71 (s, 1H), 2.19 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 181.6, 160.2, 158.1, 157.0, 149.2, 143.1, 138.4, 135.2, 134.8, 128.9, 127.6, 127.3, 126.3, 126.0, 121.4, 112.3, 95.2, 72.8, 51.4, 16.7. IR (thin film) 3446, 3059, 3012, 2932, 1668, 1509, 1454, 1454, 1372, 771 cm^{-1}; HRMS (ESI) m/z calcd for $C_{20}H_{15}IN_3O$ $(M+H)^+$ 440.0254 found 440.0259.



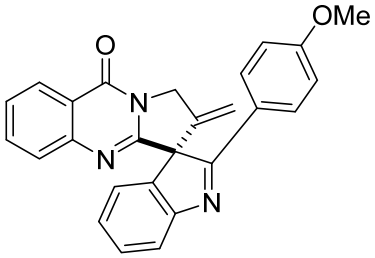
2ah

2-Cyclohexyl-2'-methylene-1',2'-dihydro-*9'H*-spiro[indole-3,3'-pyrrolo[2,1-b]qui nazolin]-9'-one (**2ah**). A white solid, 0.090 g, 79% yield; mp:111-112 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.20 (dd, J = 8.0, 1.1 Hz, 1H), 7.78 – 7.72 (m, 1H), 7.60 – 7.48 (m, 3H), 7.44 – 7.35 (m, 2H), 7.21 – 7.14 (m, 1H), 5.37 (s, 1H), 5.14 (s, 2H), 4.67 (s, 1H), 1.88 – 1.78 (m, 1H), 1.75 – 1.66 (m, 1H), 1.64 – 1.47 (m, 4H), 1.38 – 1.32 (m, 1H), 1.31 – 1.19 (m, 2H), 1.19 – 1.03 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 186.47, 160.22, 157.54, 156.26, 149.14, 143.41, 138.50, 134.94, 129.33, 127.61, 127.28, 126.71, 126.30, 123.63, 121.19, 120.40, 111.91, 73.06, 51.59, 32.52, 32.21, 25.89, 25.81. IR (thin film) 3341, 2975, 2840, 1681, 1472, 1124, 980, 881, 773 cm^{-1}; HRMS (ESI) m/z calcd for $C_{25}H_{24}N_3O$ $(M+H)^+$ 382.1914 found 382.1898.



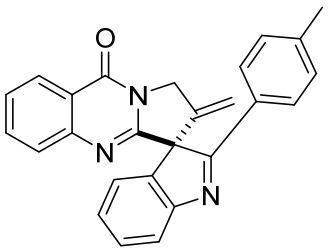
2ai

2'-Methylene-2-phenyl-1',2'-dihydro-9'*H*-spiro[indole-3,3'-pyrrolo[2,1-b]quinazolin]-9'-one (**2ai**). A white solid, 0.105 g, 93% yield; mp: 276–277 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.22 (dd, J = 8.0, 1.1 Hz, 1H), 7.82 – 7.74 (m, 3H), 7.73 – 7.66 (m, 1H), 7.59 (d, J = 7.4 Hz, 1H), 7.55 – 7.48 (m, 1H), 7.48 – 7.38 (m, 5H), 7.22 (t, J = 7.5 Hz, 1H), 5.35 (s, 2H), 5.32 (s, 1H), 4.68 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 176.0, 160.2, 158.3, 154.3, 149.1, 145.4, 139.7, 134.9, 131.9, 131.1, 129.6, 129.6, 128.9, 127.6, 127.4, 126.4, 122.8, 121.5, 121.3, 111.9, 70.5, 51.3. IR (thin film) 3789, 3050, 2979, 2939, 2323, 1736, 1677, 1520, 1455, 1337, 1046, 773 cm^{-1}; HRMS (ESI) m/z calcd for $C_{25}H_{18}N_3O$ $(M+H)^+$ 376.1444 found 376.1451.



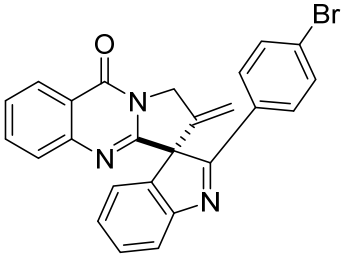
2aj

2-(4-Methoxyphenyl)-2'-methylene-1',2'-dihydro-9'*H*-spiro[indole-3,3'-pyrrolo[2,1-b]quinazolin]-9'-one (**2aj**). A white solid, 0.104 g, 86% yield; mp: 230–231 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.22 (dd, J = 8.0, 1.3 Hz, 1H), 7.78 – 7.67 (m, 4H), 7.58 – 7.47 (m, 2H), 7.45 – 7.38 (m, 2H), 7.18 (td, J = 7.5, 0.9 Hz, 1H), 7.03 – 6.92 (m, 2H), 5.39 – 5.25 (m, 3H), 4.73 – 4.62 (m, 1H), 3.75 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 175.6, 162.2, 160.2, 158.6, 154.7, 149.1, 145.3, 140.1, 134.9, 130.8, 129.5, 127.6, 127.4, 126.8, 126.4, 123.7, 122.7, 121.2, 121.0, 115.0, 111.8, 70.3, 55.8, 51.3. IR (thin film) 3442, 3051, 2929, 2835, 1679, 1610, 1507, 1454, 1418, 772 cm^{-1}; HRMS (ESI) m/z calcd for $C_{26}H_{20}N_3O_2$ $(M+H)^+$ 406.1550 found 406.1535.



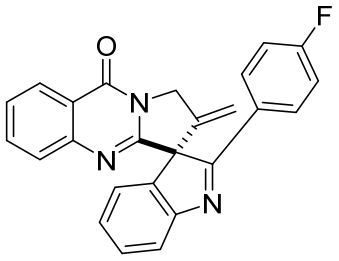
2ak

2'-Methylene-2-(p-tolyl)-1',2'-dihydro-*9'H*-spiro[indole-3,3'-pyrrolo[2,1-b]quinazolin]-9'-one (**2ak**). A white solid, 0.106 g, 91% yield; mp: 227–228 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.22 (dd, J = 8.0, 1.2 Hz, 1H), 7.75 – 7.65 (m, 4H), 7.59 – 7.55 (m, 1H), 7.54 – 7.49 (m, 1H), 7.47 – 7.38 (m, 2H), 7.24 – 7.19 (m, 3H), 5.38 – 5.29 (m, 3H), 4.70 – 4.65 (m, 1H), 2.28 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 176.0, 160.2, 158.4, 154.5, 149.1, 145.3, 142.0, 139.8, 134.9, 130.2, 129.6, 128.9, 128.5, 127.6, 127.4, 127.1, 126.4, 122.7, 121.3, 121.2, 111.8, 70.4, 51.3, 21.5. IR (thin film) 3442, 3062, 2916, 1682, 1616, 1532, 1466, 1377, 1336, 772 cm^{-1}; HRMS (ESI) m/z calcd for $C_{26}H_{20}N_3O$ $(M+H)^+$ 390.1601 found 390.1597.



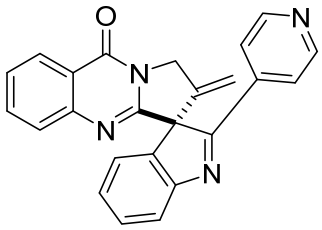
2al

2-(4-Bromophenyl)-2'-methylene-1',2'-dihydro-*9'H*-spiro[indole-3,3'-pyrrolo[2,1-b]quinazolin]-9'-one (**2al**). A white solid, 0.126 g, 93% yield; mp: 271–272 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.22 (dd, J = 8.0, 1.2 Hz, 1H), 7.80 – 7.68 (m, 4H), 7.66 – 7.58 (m, 3H), 7.56 – 7.50 (m, 1H), 7.49 – 7.39 (m, 2H), 7.25 (td, J = 7.5, 1.0 Hz, 1H), 5.42 – 5.28 (m, 3H), 4.74 – 4.67 (m, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 175.0, 160.2, 157.9, 154.1, 149.1, 145.3, 139.4, 134.9, 132.7, 130.8, 130.2, 129.7, 127.7, 127.6, 127.4, 126.4, 125.7, 122.8, 121.7, 121.3, 112.1, 70.4, 51.3. IR (thin film) 3443, 3059, 1681, 1615, 1530, 1455, 1375, 1335, 1271, 770 cm^{-1}; HRMS (ESI) m/z calcd for $C_{25}H_{17}BrN_3O$ $(M+H)^+$ 454.0550 found 454.0543.



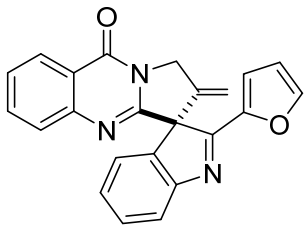
2am

2-(4-Fluorophenyl)-2'-methylene-1',2'-dihydro-*9'H*-spiro[indole-3,3'-pyrrolo[2,1-b]quinazolin]-9'-one (**2am**). A white solid, 0.116 g, 99% yield; mp: 269–270 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.22 (dd, J = 8.0, 1.2 Hz, 1H), 7.90 – 7.83 (m, 2H), 7.76 (d, J = 7.6 Hz, 1H), 7.74 – 7.68 (m, 1H), 7.60 (d, J = 7.2 Hz, 1H), 7.56 – 7.49 (m, 1H), 7.48 – 7.39 (m, 2H), 7.31 – 7.19 (m, 3H), 5.41 – 5.28 (m, 3H), 4.73 – 4.66 (m, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 174.9, 165.5, 163.0, 159.1 (d, J = 210.7 Hz), 154.2, 149.1, 145.3, 139.6, 134.9, 131.5 (d, J = 8.9 Hz), 129.7, 127.7 (d, J = 3.0 Hz), 127.6, 127.4, 126.4, 122.8, 121.5, 121.3, 116.7 (d, J = 21.8 Hz), 112.1, 70.4, 51.3. IR (thin film) 3431, 3062, 1912, 1684, 1612, 1538, 1504, 1455, 1405, 772 cm^{-1}; HRMS (ESI) m/z calcd for $C_{25}H_{17}FN_3O$ $(M+H)^+$ 394.1350 found 394.1342.



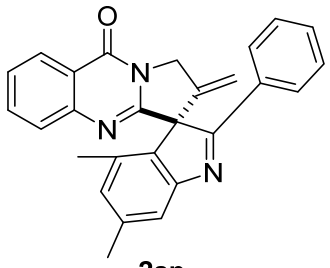
2an

2'-Methylene-2-(pyridin-4-yl)-1',2'-dihydro-*9'H*-spiro[indole-3,3'-pyrrolo[2,1-b]quinazolin]-9'-one (**2an**). A white solid, 0.112 g, 99% yield; mp: 231-232 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.67 (d, J = 5.0 Hz, 2H), 8.23 (d, J = 7.7 Hz, 1H), 7.86 (d, J = 7.6 Hz, 1H), 7.77 – 7.62 (m, 4H), 7.52 (dd, J = 15.7, 7.9 Hz, 2H), 7.42 (d, J = 8.1 Hz, 1H), 7.31 (t, J = 7.4 Hz, 1H), 5.48 – 5.27 (m, 3H), 4.73 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 174.5, 160.2, 157.5, 153.7, 151.2, 149.0, 145.4, 138.7, 137.7, 134.9, 129.9, 128.5, 127.6, 127.5, 126.4, 123.0, 122.3, 121.4, 112.3, 70.5, 51.3. IR (thin film) 3433, 3229, 3066, 1678, 1618, 1527, 1467, 1410, 1374, 774 cm^{-1}; HRMS (ESI) m/z calcd for $C_{24}H_{17}N_4O$ $(M+H)^+$ 377.1397 found 377.1380.



2ao

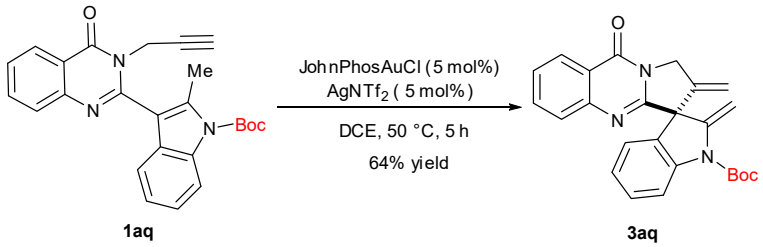
2-(Furan-2-yl)-2'-methylene-1',2'-dihydro-*9'H*-spiro[indole-3,3'-pyrrolo[2,1-b]quinazolin]-9'-one (**2ao**). A white solid, 0.104 g, 95% yield; mp: 195-196 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.21 (dd, J = 8.0, 1.2 Hz, 1H), 7.87 (dd, J = 1.7, 0.6 Hz, 1H), 7.76 – 7.70 (m, 1H), 7.68 (d, J = 7.7 Hz, 1H), 7.58 – 7.50 (m, 2H), 7.48 – 7.40 (m, 2H), 7.23 (td, J = 7.5, 1.0 Hz, 1H), 7.19 – 7.16 (m, 1H), 6.63 (dd, J = 3.6, 1.7 Hz, 1H), 5.38 – 5.32 (m, 1H), 5.31 – 5.17 (m, 2H), 4.73 – 4.65 (m, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 167.4, 160.2, 157.9, 155.7, 149.1, 147.9, 147.7, 143.7, 139.4, 134.9, 129.8, 127.6, 127.4, 127.2, 126.3, 123.5, 121.1, 121.1, 115.9, 113.5, 112.0, 70.6, 51.5. IR (thin film) 3435, 3265, 3104, 1678, 1616, 1577, 1533, 1471, 1380, 773 cm^{-1}; HRMS (ESI) m/z calcd for $C_{23}H_{16}N_3O_2$ $(M+H)^+$ 366.1237 found 366.1228.



2ap

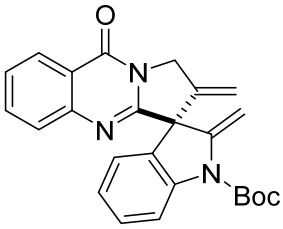
4,6-Dimethyl-2'-methylene-2-phenyl-1',2'-dihydro-*9'H*-spiro[indole-3,3'-pyrrolo[2,1-b]quinazolin]-9'-one (**2ap**). A white solid, 0.111 g, 92% yield; mp: 262–263 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.23 (dd, J = 8.0, 1.2 Hz, 1H), 7.77 – 7.66 (m, 3H), 7.57 – 7.51 (m, 1H), 7.48 – 7.37 (m, 5H), 6.87 (s, 1H), 5.50 – 5.25 (m, 3H), 4.76 (s, 1H), 2.37 (s, 3H), 1.94 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 176.6, 160.0, 157.5, 155.6, 149.0, 141.0, 139.5, 137.2, 135.2, 132.3, 131.7, 131.5, 129.7, 128.3, 127.7, 127.6, 126.5, 120.7, 119.9, 112.6, 70.2, 51.6, 21.4, 17.8. IR (thin film) 3442, 3062, 2916, 1682, 1616, 1532, 1466, 1377, 1326, 778 cm^{-1}; HRMS (ESI) m/z calcd for $C_{27}H_{22}N_3O$ $(M+H)^+$ 404.1757 found 404.1729.

3. Synthesis of spiroindolenine-3,3'-pyrrolo[2,1-b]quinazolinone 3aq



1aq 3aq

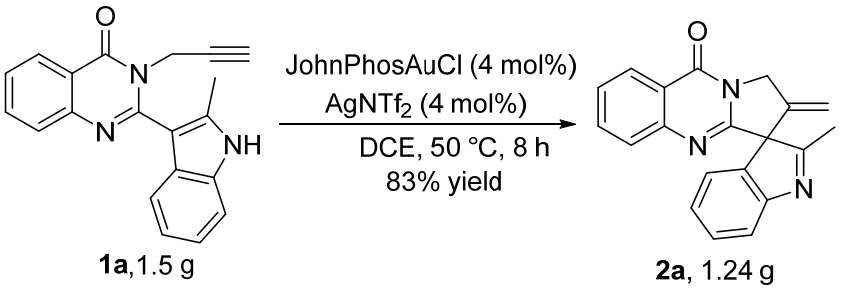
General procedure C: In a Schlenk flask was charged with JohnPhosAuCl (8.0 mg, 5 mol%), $AgNTf_2$ (5.8 mg, 5 mol%) and DCE (3.0 mL). The mixture was stirred vigorously at room temperature under dark for 15 min. Then, compound **1aq** (0.3 mmol) was added. The mixture was stirred vigorously at 50 °C for 4-5 h until compound **1aq** was completely consumed (monitored by TLC). At this time, the solvent was removed under reduced pressure and the crude product was purified by flash column chromatography (the crude residue was dry loaded with silica gel, 1/10 to 1/4, ethyl acetate/petroleum ether) to provide compounds **3aq**.



3aq

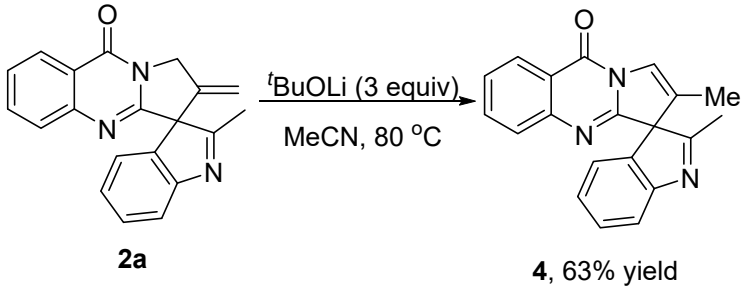
Tert-butyl 2,2'-dimethylene-9'-oxo-1',2'-dihydro-9'*H*-spiro[indoline-3,3'-pyrrolo [2,1-b] quinazoline]-1-carboxylate (3aq). A white solid, 0.079 g, 64% yield; mp: 188-189 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.19 (d, J = 7.9 Hz, 1H), 7.83 (d, J = 8.3 Hz, 1H), 7.80 – 7.71 (m, 1H), 7.53 (dd, J = 16.2, 7.9 Hz, 2H), 7.38 – 7.32 (m, 1H), 7.23 (d, J = 7.5 Hz, 1H), 7.06 (t, J = 7.5 Hz, 1H), 5.68 (s, 1H), 5.50 (s, 1H), 5.04 (s, 2H), 4.92 – 4.84 (m, 1H), 4.70 – 4.62 (m, 1H), 1.62 (s, 9H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.6, 156.0, 151.0, 150.9, 149.6, 147.0, 142.1, 134.8, 132.9, 129.6, 127.6, 127.2, 126.3, 125.2, 124.7, 121.2, 115.8, 113.1, 97.6, 83.7, 63.7, 50.8, 28.3. IR (thin film) 3426, 2973, 2929, 1711, 1677, 1519, 1344, 1155, 849, 765 cm^{-1}; HRMS (ESI) m/z calcd for $C_{25}H_{24}N_3O_3$ $(M+H)^+$ 414.1812 found 414.1831.

4. Gram scalable preparation of 2a



In a 150 mL round bottom flask was charged with JohnPhosAuCl (101.6 mg, 0.19 mmol, 4 mol%), $AgNTf_2$ (73.7 mg, 0.19 mmol, 4 mol%) and DCE (60 mL). The mixture was stirred vigorously at room temperature under dark for 15 min. Then, compound **1a** (1.500 g, 4.79 mmol) was added. The mixture was stirred vigorously at room temperature for 8 hours until compounds **1a** were completely consumed (monitored by TLC). At this time, the solvent was removed under reduced pressure and the crude product was purified by flash column chromatography (the crude residue was dry loaded with silica gel, 1/10 to 1/4, ethyl acetate/petroleum ether) to provide compound **2a** (1.240 g, 83% yield) **.**

5. Synthesis of compound 4.

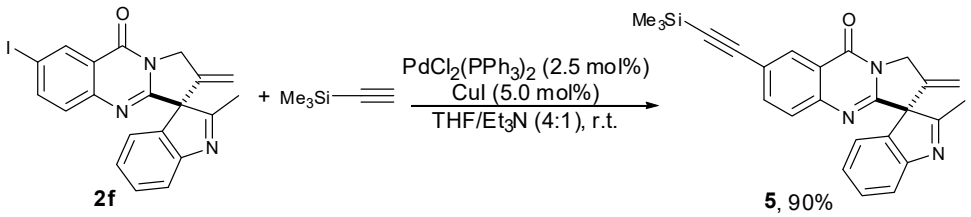


In a Schlenk flask was charged with **2a** (80 mg, 0.26 mmol), CH_3CN (3.0 mL) and ^{t}BuOLi (61 mg, 0.77 mmol). The reaction vessel was stirred vigorously at 80 °C for 3 h until the substrate **2a** disappeared (monitored by TLC). The mixture was concentrated under reduced pressure. The crude product was purified by silica gel column chromatography (PE/EtOAc = 10/1 to 2/1) to afford compound **4**.

2,2'-Dimethyl-*9'H*-spiro[indole-3,3'-pyrrolo[2,1-b]quinazolin]-9'-one (**4**). A white solid, 0.050 g, 63% yield; mp: 276−277°C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.27 –

8.21 (m, 1H), 7.86 – 7.82 (m, 1H), 7.81 – 7.74 (m, 1H), 7.63 (d, *J* = 7.7 Hz, 1H), 7.60 – 7.53 (m, 2H), 7.46 (td, *J* = 7.6, 1.4 Hz, 1H), 7.32 – 7.27 (m, 1H), 7.23 (td, *J* = 7.4, 0.9 Hz, 1H), 2.08 (s, 3H), 1.46 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 177.3, 157.5, 157.0, 147.8, 137.1, 134.8, 130.0, 127.9, 127.5, 126.8, 126.7, 126.0, 125.9, 123.8, 121.3, 120.4, 75.9, 16.4, 10.0. IR (thin film) 3451, 3244, 3011, 1684, 1588, 1476, 1211, 1056, 911, 743 cm^{-1}; HRMS (ESI) m/z calcd for $C_{20}H_{16}N_3O$ $(M+H)^+$ 314.1288 found 314.1279.

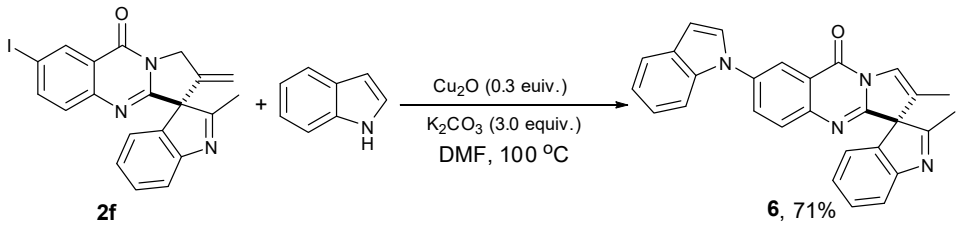
6. Synthesis of compound 5



To a solution of **2f** (89 mg, 0.2 mmol) and ethynyltrimethylsilane (29 mg, 0.3 mmol) in 3 mL of THF was charged CuI (2.0 mg, 0.01 mmol) and $PdCl_2(PPh_3)_2$ (3.5 mg, 0.005 mmol), then charged 1.5 mL of TEA under a N_2 atmosphere at room temperature. The reaction mixture was stirred for 4 h. Upon completion the reaction was quenched with water, extracted with EA, and dried over anhydrous Na_2SO_4. The crude product was purified by silica gel column chromatography (PE/EtOAc = 6/1 to 4/1) to afford **5**.

2-Methyl-2'-methylene-7'-((trimethylsilyl)ethynyl)-1',2'-dihydro-*9'H*-spiro[indole-3,3'-pyrrolo[2,1-b]quinazolin]-9'-one (**5**). A white solid, 0.074 g, 90% yield; mp: 261–262 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.20 – 8.13 (m, 1H), 7.75 (dd, *J* = 8.5, 2.0 Hz, 1H), 7.55 (d, *J* = 7.7 Hz, 1H), 7.51 – 7.44 (m, 2H), 7.40 (td, *J* = 7.6, 1.2 Hz, 1H), 7.19 (td, *J* = 7.5, 1.0 Hz, 1H), 5.39 – 5.37 (m, 1H), 5.18 – 5.02 (m, 2H), 4.68 – 4.65 (m, 1H), 2.18 (s, 3H), 0.26 (s, 9H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 179.6, 159.4, 158.7, 156.3, 149.2, 143.4, 138.9, 137.1, 129.5, 128.2, 126.6, 124.0, 121.5, 120.7, 120.2, 111.9, 104.4, 96.4, 72.9, 55.4, 51.5, 16.7, 0.3. IR (thin film) 3182, 2966, 2859, 2570, 1765, 1617, 1470, 1308, 1203, 1018, 712 cm^{-1}; HRMS (ESI) m/z calcd for $C_{25}H_{23}N_3OSi$ $(M+H)^+$: 410.1683 found 410.1683.

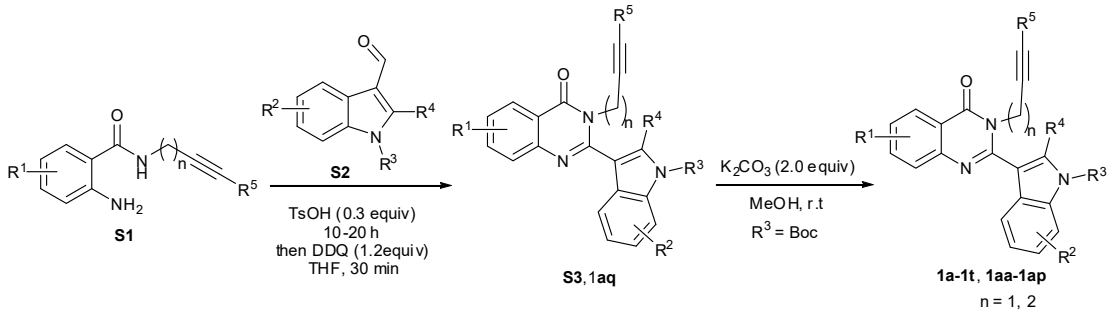
7. Synthesis of compound 6



In a Schlenk flask was charged with **2f** (89 mg, 0.2 mmol), Indole (35 mg, 0.3 mmol), Cu_2O(9 mg, 0.06 mmol), K_2CO_3 (83 mg, 0.6 mmol) and DMF (3.0 mL). The reaction vessel was stirred vigorously at 100 °C for 12 h until the substrate **2f** disappeared (monitored by TLC). The mixture was concentrated under reduced pressure. The crude product was purified by silica gel column chromatography (PE/EtOAc = 10/1 to 4/1) to afford **6**.

7'-(1H-indol-1-yl)-2,2'-dimethyl-9'*H*-spiro[indole-3,3'-pyrrolo[2,1-b]quinazolin]-9'-one (**6**). A white solid, 0.061 g, 71% yield; mp: 273–274 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.31 (d, J = 2.6 Hz, 1H), 8.03 (dd, J = 8.7, 2.6 Hz, 1H), 7.88 (d, J = 1.7 Hz, 1H), 7.81 – 7.76 (m, 2H), 7.70 (d, J = 7.7 Hz, 1H), 7.63 (t, J = 8.8 Hz, 2H), 7.50 – 7.46 (m, 1H), 7.33 (d, J = 6.9 Hz, 1H), 7.27 – 7.24 (m, 2H), 7.18 (t, J = 7.1 Hz, 1H), 6.78 (d, J = 3.2 Hz, 1H), 2.11 (s, 3H), 1.48 – 1.47 (m, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 177.3, 157.5, 157.0, 156.6, 145.8, 138.0, 137.1, 135.4, 130.3, 130.1, 129.8, 129.8, 129.0, 126.9, 126.5, 125.9, 123.9, 123.2, 122.3, 121.7, 121.2, 120.5, 120.0, 110.5, 104.9, 75.9, 16.4, 10.0. IR (thin film) 3394, 3123, 3100, 3039, 2025, 1685, 1569, 956, 745 cm−1; HRMS (ESI) m/z calcd for $C_{28}H_{20}N_4O$ $(M+H)^+$: 429.1715 found 429.1710.

8. Synthesis of N-alkynyl quinazolinone-tethered indoles 1.

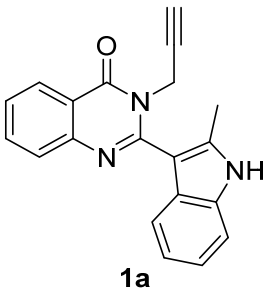


Synthesis of N-alkynyl quinazolinone-tethered indoles 1:

Alkynyl anilines derivatives **S1** was prepared according to literature method.[1] Heteroaryl formaldehydes **S2** was prepared according to literaure method[2] or were purchased from Sigma Alderich.

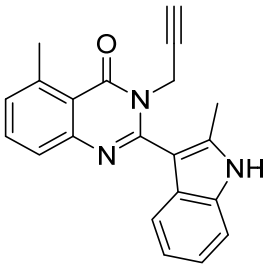
To a stirred mixture of N-alkynyl anilines **S1** (5.0 mmol, 1.0 equiv.), heteroaryl formaldehyde **S2** (5.0 mmol, 1.0 equiv.) and anhydrous magnesium sulfate (1800 mg, 3.0 equiv) in THF (0.2 M) was added *p*-toluene sulfonic acid (258 mg, 0.3 equiv) at 25 °C under nitrogen. The resulting mixture was stirred at 25 °C for 10−20 h. After completion indicated by TLC, 2,3-dicyano-5,6-dichlorobenzoquinone (DDQ, 1362 mg, 1.2 equiv.) was added. The resultant reaction mixture was stirred at room temperature for an additional 0.5 h (monitored by TLC). The mixture was concentrated under reduced pressure. The crude product was purified by silica gel column chromatography (PE/EtOAc = 20/1 to 6/1) to afford **S3** or **1aq.**

A 150 mL round bottom flask was charged with **S3** (2.0 mmol), K_2CO_3 (552 mg, 2.0 equiv) and MeOH (15 mL). The mixture was stirred vigorously at room temperature under dark for 15-20 h until compounds **S3** were completely consumed (monitored by TLC). At this time, the reaction was removed under reduced pressure, then, water was added, ultrasound was performed, and solids were separated out. The reaction was filtered and washed with water. The crude product was purified by flash column chromatography (the crude residue was dry loaded with silica gel, 1/6 to 1/2, ethyl acetate/petroleum ether) to provide compounds **1a-1t** or **1aa-1ap**.



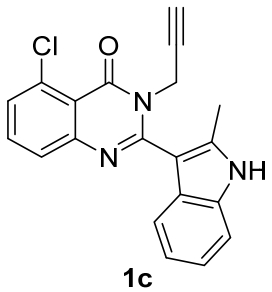
1a

2-(2-Methyl-*1H*-indol-3-yl)-3-(prop-2-yn-1-yl)quinazolin-4(*3H*)-one (**1a**). A white solid, 0.470 g, 75% yield; mp: 224−225 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ 11.61 (s, 1H), 8.23 (dd, J = 8.0, 1.1 Hz, 1H), 7.90 – 7.80 (m, 1H), 7.69 (d, J = 7.9 Hz, 1H), 7.63 – 7.54 (m, 1H), 7.44 – 7.38 (m, 2H), 7.18 – 7.10 (m, 1H), 7.09 – 7.01 (m, 1H), 5.06 – 5.02 (m, 1H), 4.52 – 4.48 (m, 1H), 3.14 (t, J = 2.3 Hz, 1H), 2.45 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6): δ 161.6, 152.1, 147.9, 137.7, 135.2, 135.1, 127.7, 127.4, 126.8, 126.7, 121.8, 120.6, 120.6, 118.4, 111.8, 107.6, 79.3, 74.4, 35.0, 12.7. IR (thin film) 3469, 3302, 3146, 3103, 3019, 1685, 1587, 1331, 1241, 743 cm^{-1}; HRMS (ESI) m/z calcd for $C_{20}H_{14}N_3O$ $(M–H)^-$ 312.1137, found 312.1134.



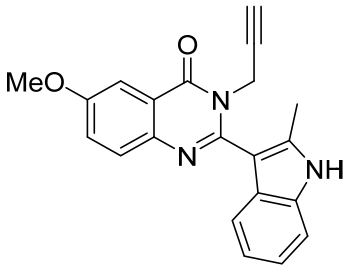
1b

5-Methyl-2-(2-methyl-1H-indol-3-yl)-3-(prop-2-yn-1-yl)quinazolin-4(*3H*)-one (**1b**). A white solid, 0.523 g, 80% yield; mp: 223−224 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.59 (s, 1H), 7.67 (t, J = 7.7 Hz, 1H), 7.49 (d, J = 8.0 Hz, 1H), 7.43 (d, J = 8.1 Hz, 1H), 7.38 (d, J = 7.8 Hz, 1H), 7.32 (d, J = 7.3 Hz, 1H), 7.18 – 7.11 (m, 1H), 7.05 (t, J = 7.4 Hz, 1H), 4.97 (d, J = 15.3 Hz, 1H), 4.46 (d, J = 14.9 Hz, 1H), 3.12 (t, J = 2.3 Hz, 1H), 2.86 (s, 3H), 2.44 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.1, 151.8, 149.4, 140.6, 137.5, 135.3, 134.2, 129.7, 126.8, 125.9, 121.8, 120.6, 119.0, 118.4, 111.7, 107.6, 79.6, 74.2, 34.9, 23.2, 12.7. IR (thin film) 3247, 2925, 2117, 1668, 1581, 1457, 1363, 1158, 749 cm^{-1}; HRMS (ESI) m/z calcd for $C_{21}H_{18}N_3O$ $(M+H)^+$ 328.1444, found 328.1440.



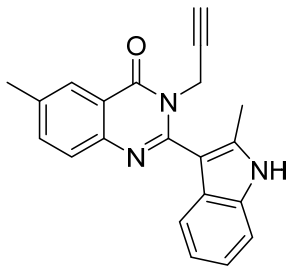
1c

5-Chloro-2-(2-methyl-1H-indol-3-yl)-3-(prop-2-yn-1-yl)quinazolin-4(*3H*)-one (**1c**). A white solid, 0.521 g, 75% yield; mp: 240−241 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.65 (s, 1H), 7.76 (t, J = 8.0 Hz, 1H), 7.65 – 7.56 (m, 2H), 7.43 (d, J = 8.7 Hz, 2H), 7.18 – 7.12 (m, 1H), 7.09 – 7.02 (m, 1H), 4.95 (d, J = 11.9 Hz, 1H), 4.50 (d, J = 12.5 Hz, 1H), 3.15 (t, J = 2.3 Hz, 1H), 2.46 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 159.6, 153.0, 150.3, 138.0, 135.3, 134.9, 133.1, 129.6, 127.3, 126.6, 121.9, 120.7, 118.5, 117.5, 111.8, 107.3, 79.3, 74.5, 35.4, 12.7. IR (thin film) 3388, 3242, 2123, 1678, 1570, 1441, 1384, 1273, 1155, 958, 751 cm^{-1}; HRMS (ESI) m/z calcd for $C_{20}H_{15}ClN_3O$ $(M+H)^+$ 348.0898, found 348.0887.



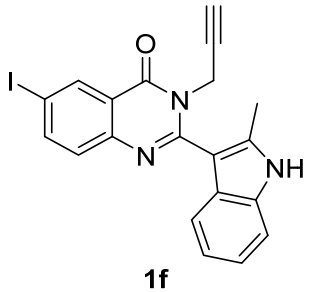
1d

6-Methoxy-2-(2-methyl-1H-indol-3-yl)-3-(prop-2-yn-1-yl)quinazolin-4(*3H*)-one (**3d**). A white solid, 0.624 g, 91% yield; mp: 138−139 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.56 (s, 1H), 7.63 (d, J = 8.9 Hz, 1H), 7.60 (d, J = 2.9 Hz, 1H), 7.46 (dd, J = 8.9, 3.0 Hz, 1H), 7.41 (d, J = 8.1 Hz, 1H), 7.36 (d, J = 7.9 Hz, 1H), 7.16 – 7.10 (m, 1H), 7.06 – 6.99 (m, 1H), 5.02 (d, J = 16.4 Hz, 1H), 4.47 (d, J = 16.8 Hz, 1H), 3.91 (s, 3H), 3.11 (s, 1H), 2.41 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.4, 158.4, 149.7, 142.4, 137.5, 135.3, 129.4, 126.9, 124.7, 121.8, 121.4, 120.5, 118.3, 111.7, 107.5, 106.7, 79.4, 74.4, 56.2, 35.0, 12.7. IR (thin film) 3574, 3292, 3181, 2140, 1970, 1619, 1558, 1491, 1369, 1228, 1025, 752 cm^{-1}; HRMS (ESI) m/z calcd for $C_{21}H_{18}N_3O_2$ $(M+H)^+$ 344.1394, found 344.1399.



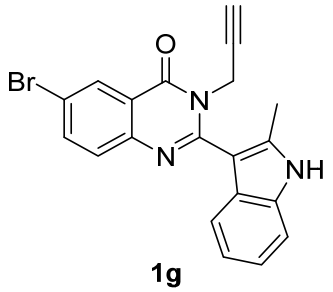
1e

6-Methyl-2-(2-methyl-1H-indol-3-yl)-3-(prop-2-yn-1-yl)quinazolin-4(*3H*)-one (**1e**). A white solid, 0.530 g, 81% yield; mp: 155−156 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.57 (s, 1H), 8.01 (s, 1H), 7.67 (dd, J = 8.4, 1.9 Hz, 1H), 7.58 (d, J = 8.3 Hz, 1H), 7.41 (d, J = 8.1 Hz, 1H), 7.36 (d, J = 7.8 Hz, 1H), 7.16 – 7.10 (m, 1H), 7.06 – 7.00 (m, 1H), 5.02 (d, J = 16.1 Hz, 1H), 4.47 (d, J = 16.2 Hz, 1H), 3.11 (t, J = 2.4 Hz, 1H), 2.48 (s, 3H), 2.42 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.5, 151.2, 146.0, 137.6, 137.1, 136.4, 135.3, 127.6, 126.8, 126.0, 121.8, 120.6, 120.3, 118.3, 111.7, 107.6, 79.4, 74.3, 34.9, 21.4, 12.7. IR (thin film) 3290, 2126, 1674, 1585, 1489, 1459, 1334, 1195, 955, 746 cm^{-1}; HRMS (ESI) m/z calcd for $C_{21}H_{18}N_3O_2$ $(M+H)^+$ 328.1444, found 328.1429.



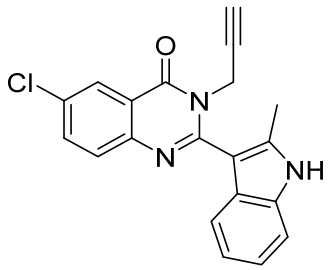
1f

6-Iodo-2-(2-methyl-1H-indol-3-yl)-3-(prop-2-yn-1-yl)quinazolin-4(*3H*)-one (**1f**). A white solid, 0.790 g, 90% yield; mp: 249-250 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.64 (s, 1H), 8.49 (d, J = 2.0 Hz, 1H), 8.14 (dd, J = 8.5, 2.1 Hz, 1H), 7.47 (d, J = 8.5 Hz, 1H), 7.41 (t, J = 8.0 Hz, 2H), 7.17 – 7.12 (m, 1H), 7.09 – 7.01 (m, 1H), 5.01 (d, J = 14.6 Hz, 1H), 4.50 (d, J = 14.8 Hz, 1H), 3.15 (t, J = 2.4 Hz, 1H), 2.44 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 160.4, 152.8, 147.1, 143.5, 138.0, 135.3, 135.0, 130.0, 126.6, 122.3, 121.9, 120.8, 118.5, 111.8, 107.4, 92.2, 79.1, 74.6, 35.3, 12.8. IR (thin film) 3649, 3274, 2133, 1658, 1571, 1458, 1273, 1195, 1000, 755 cm^{-1}; HRMS (ESI) m/z calcd for $C_{20}H_{15}IN_3O$ $(M+H)^+$ 440.0254, found 440.0237.



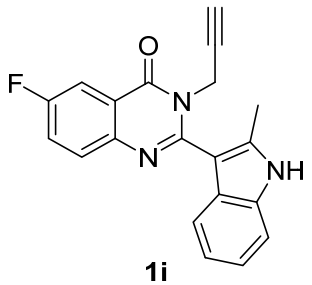
1g

6-Bromo-2-(2-methyl-1H-indol-3-yl)-3-(prop-2-yn-1-yl)quinazolin-4(*3H*)-one (1g). A white solid, 0.633 g, 81% yield; mp: 273-274 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.64 (s, 1H), 8.30 (d, J = 2.3 Hz, 1H), 8.00 (dd, J = 8.7, 2.4 Hz, 1H), 7.64 (d, J = 8.7 Hz, 1H), 7.42 (t, J = 7.2 Hz, 2H), 7.18 – 7.11 (m, 1H), 7.09 – 7.00 (m, 1H), 5.01 (d, J = 14.7 Hz, 1H), 4.51 (d, J = 14.2 Hz, 1H), 3.15 (t, J = 2.4 Hz, 1H), 2.44 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 160.6, 152.7, 146.9, 138.0, 135.0, 130.1, 128.8, 126.6, 122.1, 121.9, 120.7, 119.7, 118.5, 111.8, 107.3, 79.1, 74.7, 49.1, 35.3, 12.7. IR (thin film) 3271, 2123, 1662, 1577, 1450, 1273, 1195, 1021, 754 cm^{-1}; HRMS (ESI) m/z calcd for $C_{20}H_{15}BrN_3O$ $(M+H)^+$ 392.0393, found 392.0392.



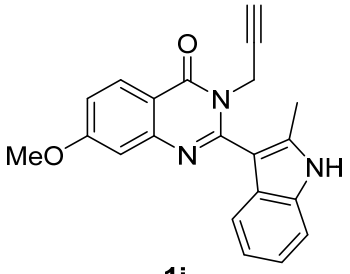
1h

6-Chloro-2-(2-methyl-1H-indol-3-yl)-3-(prop-2-yn-1-yl)quinazolin-4(*3H*)-one (**1h**). A white solid, 0.584 g, 84% yield; mp: 271-272 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.64 (s, 1H), 8.16 (d, J = 2.5 Hz, 1H), 7.88 (dd, J = 8.7, 2.5 Hz, 1H), 7.71 (d, J = 8.7 Hz, 1H), 7.42 (t, J = 7.4 Hz, 2H), 7.20 – 7.11 (m, 1H), 7.10 – 7.00 (m, 1H), 5.03 (d, J = 15.2 Hz, 1H), 4.52 (d, J = 15.3 Hz, 1H), 3.15 (t, J = 2.4 Hz, 1H), 2.45 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 160.7, 152.6, 146.6, 138.0, 135.3, 131.5, 123.0, 126.7, 125.7, 121.9, 121.8, 120.7, 118.5, 111.8, 107.3, 79.1, 74.7, 49.1, 12.7. IR (thin film) 3650, 3270, 2113, 1661, 1576, 1450, 1414, 1271, 1195, 1121, 755 cm^{-1}; HRMS (ESI) m/z calcd for $C_{20}H_{15}ClN_3O$ $(M+H)^+$ 348.0898, found 348.0883.



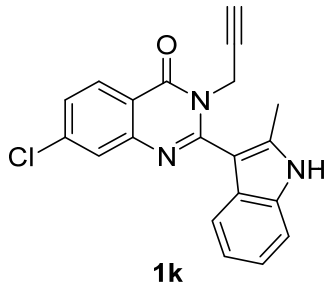
1i

6-Fluoro-2-(2-methyl-1H-indol-3-yl)-3-(prop-2-yn-1-yl)quinazolin-4(*3H*)-one (**2i**). A white solid, 0.622 g, 94% yield; mp: 230-231 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.63 (s, 1H), 7.94 – 7.87 (m, 1H), 7.81 – 7.71 (m, 2H), 7.47 – 7.39 (m, 2H), 7.19 – 7.12 (m, 1H), 7.10 – 7.02 (m, 1H), 5.04 (d, J = 16.5 Hz, 1H), 4.51 (d, J = 16.5 Hz, 1H), 3.16 (t, J = 2.4 Hz, 1H), 2.45 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.0 (d, J = 3.4 Hz), 160.6 (d, J = 244.2 Hz), 151.5 (d, J = 2.1 Hz), 144.8 (d, J = 1.6 Hz), 137.8, 135.3, 130.7 (d, J = 8.4 Hz), 126.7, 123.6 (d, J = 24.0 Hz), 121.9, 121.7 (d, J = 8.6 Hz), 120.6, 118.4, 111.8, 111.3 (d, J = 23.3 Hz), 107.3, 79.1, 74.6, 35.2, 12.7. IR (thin film) 3290, 2984, 2127, 1657, 1562, 1483, 1272, 1130, 1011, 833, 688 cm^{-1}; HRMS (ESI) m/z calcd for $C_{20}H_{15}FN_3O$ $(M+H)^+$ 332.1194, found 332.1181.



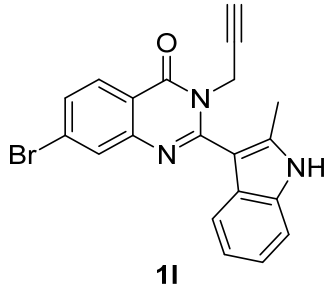
1j

7-Methoxy-2-(2-methyl-1H-indol-3-yl)-3-(prop-2-yn-1-yl)quinazolin-4(*3H*)-one (**1j**). A white solid, 0.604 g, 88% yield; mp: 230-231 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.60 (s, 1H), 8.12 (d, J = 8.7 Hz, 1H), 7.43 (d, J = 8.0 Hz, 1H), 7.37 (d, J = 7.8 Hz, 1H), 7.19 – 7.11 (m, 3H), 7.05 (t, J = 7.3 Hz, 1H), 5.02 (d, J = 16.6 Hz, 1H), 4.46 (d, J = 16.6 Hz, 1H), 3.91 (s, 3H), 3.12 (t, J = 2.2 Hz, 1H), 2.44 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 164.7, 161.1, 152.7, 150.1, 137.6, 135.3, 128.4, 126.7, 121.8, 120.6, 118.3, 117.1, 114.0, 111.8, 108.7, 107.7, 79.5, 74.3, 56.2, 34.8, 12.8. IR (thin film) 3574, 3292, 3181, 2140, 1970, 1619, 1558, 1491, 1369, 1228, 1025, 752 cm^{-1}; HRMS (ESI) m/z calcd for $C_{21}H_{18}N_3O_2$ $(M+H)^+$ 344.1394, found 344.1376.



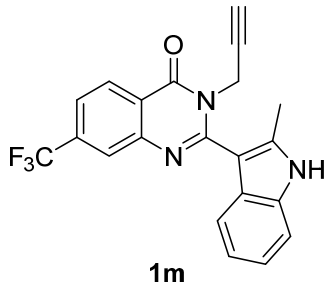
1k

7-Chloro-2-(2-methyl-1H-indol-3-yl)-3-(prop-2-yn-1-yl)quinazolin-4(*3H*)-one (**1k**). A white solid, 0.597 g, 86% yield; mp: 268-269 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.69 (s, 1H), 8.21 (d, J = 8.5 Hz, 1H), 7.74 (s, 1H), 7.61 (d, J = 8.3 Hz, 1H), 7.42 (t, J = 7.1 Hz, 2H), 7.14 (t, J = 7.4 Hz, 1H), 7.05 (t, J = 7.4 Hz, 1H), 5.01 (d, J = 11.6 Hz, 1H), 4.50 (d, J = 13.3 Hz, 1H), 3.24 – 3.01 (m, 1H), 2.44 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.1, 153.7, 148.9, 139.7, 138.1, 135.2, 128.9, 127.6, 126.8, 126.6, 121.9, 120.7, 119.4, 118.4, 111.8, 107.3, 79.1, 74.6, 35.2, 12.7. IR (thin film) 3559, 3285, 2130, 1661, 1553, 1463, 1243, 956, 751 cm^{-1}; HRMS (ESI) m/z calcd for $C_{20}H_{15}ClN_3O$ $(M+H)^+$ 348.0898, found 348.0869.



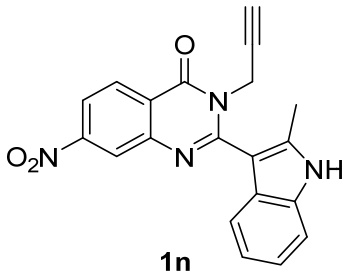
1l

7-Bromo-2-(2-methyl-1H-indol-3-yl)-3-(prop-2-yn-1-yl)quinazolin-4(*3H*)-one (**1l**). A white solid, 0.633 g, 81% yield; mp: 217-218 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.65 (s, 1H), 8.13 (d, J = 8.5 Hz, 1H), 7.90 (d, J = 1.8 Hz, 1H), 7.73 (dd, J = 8.5, 1.9 Hz, 1H), 7.47 – 7.38 (m, 2H), 7.19 – 7.12 (m, 1H), 7.06 (td, J = 7.5, 0.9 Hz, 1H), 5.02 (d, J = 13.4 Hz, 1H), 4.51 (d, J = 13.4 Hz, 1H), 3.15 (t, J = 2.4 Hz, 1H), 2.45 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.2, 153.6, 149.0, 138.1, 135.3, 130.3, 129.9, 128.9, 128.7, 126.6, 121.9, 120.7, 119.7, 118.5, 111.8, 107.3, 79.1, 74.6, 35.2, 12.7. IR (thin film) 3223, 3150, 2950, 1687, 1640, 1387, 1120, 902, 745 cm^{-1}; HRMS (ESI) m/z calcd for $C_{20}H_{15}BrN_3O$ $(M+H)^+$ 392.0393, found 392.0382.



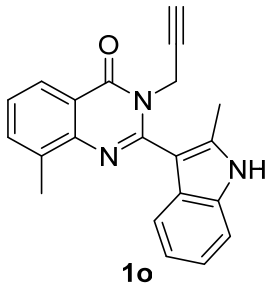
1m

2-(2-Methyl-1H-indol-3-yl)-3-(prop-2-yn-1-yl)-7-(trifluoromethyl)quinazolin-4(*3H*)-one (**1m**). A white solid, 0.625 g, 82% yield; mp: 263-264 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.69 (s, 1H), 8.43 (d, J = 8.3 Hz, 1H), 8.02 (s, 1H), 7.91 – 7.80 (m, 1H), 7.45 (dd, J = 7.9, 3.2 Hz, 2H), 7.16 (t, J = 7.3 Hz, 1H), 7.07 (t, J = 7.3 Hz, 1H), 5.04 (s, 1H), 4.58 (s, 1H), 3.18 (t, J = 2.0 Hz, 1H), 2.47 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.0, 153.9, 147.9, 138.2, 135.3, 134.8 (q, J = 32.0 Hz), 128.6, 126.6, 124.9 (q, J = 7.6 Hz), 124.0 (q, J = 271.4 Hz), 123.3, 123.0 (q, J = 7.5 Hz), 121.9, 120.7, 118.5, 111.8, 107.2, 78.9, 74.7, 35.4, 12.7. IR (thin film) 3289, 2983, 2130, 1663, 1563, 1420, 1320, 1157, 1122, 749 cm^{-1}; HRMS (ESI) m/z calcd for $C_{21}H_{15}F_3N_3O$ $(M+H)^+$ 382.1162, found 382.1139.



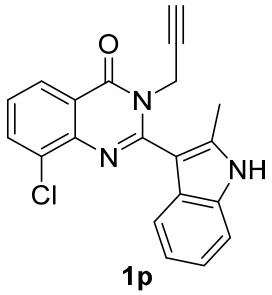
1n

2-(2-Methyl-1H-indol-3-yl)-7-nitro-3-(prop-2-yn-1-yl)quinazolin-4(*3H*)-one (**1n**). A yellow solid, 0.573 g, 80% yield; mp: 273-274 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.71 (s, 1H), 8.46 – 8.41 (m, 1H), 8.39 (d, J = 2.0 Hz, 1H), 8.27 (dd, J = 8.7, 2.3 Hz, 1H), 7.51 – 7.39 (m, 2H), 7.21 – 7.12 (m, 1H), 7.11 – 7.04 (m, 1H), 5.15 – 4.90 (m, 1H), 4.70 – 4.41 (m, 1H), 3.18 (t, J = 2.4 Hz, 1H), 2.48 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 160.8, 154.4, 151.8, 148.2, 138.5, 135.3, 129.1, 126.6, 124.8, 122.7, 122.0, 120.8, 118.5, 111.8, 107.0, 78.8, 74.9, 35.6, 12.8. IR (thin film) 3289, 3316, 3101, 2983, 2127, 1651, 1550, 1527, 1354, 1255, 1194, 746 cm^{-1}; HRMS (ESI) m/z calcd for $C_{20}H_{15}N_4O_3$ $(M+H)^+$ 359.1139, found 359.1170.



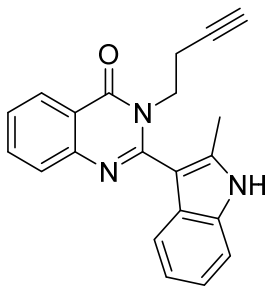
1o

8-Methyl-2-(2-methyl-1H-indol-3-yl)-3-(prop-2-yn-1-yl)quinazolin-4(*3H*)-one (**1o**). A white solid, 0.543 g, 83% yield; mp: 221-222 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.60 (s, 1H), 7.67 (t, J = 7.7 Hz, 1H), 7.49 (d, J = 7.9 Hz, 1H), 7.43 (d, J = 8.0 Hz, 1H), 7.39 (d, J = 7.8 Hz, 1H), 7.32 (d, J = 7.3 Hz, 1H), 7.18 – 7.12 (m, 1H), 7.08 – 7.02 (m, 1H), 4.99 (d, J = 15.0 Hz, 1H), 4.47 (d, J = 15.7 Hz, 1H), 3.12 (t, J = 2.3 Hz, 1H), 2.86 (s, 3H), 2.45 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.1, 151.8, 149.4, 140.6, 137.6, 135.3, 134.2, 129.6, 126.8, 125.9, 121.8, 120.6, 119.0, 118.4, 111.7, 107.6, 79.6, 74.2, 34.9, 23.2, 12.7. IR (thin film) 3435, 3052, 2927, 1671, 1626, 1595, 1459, 1315, 1231, 810 cm^{-1}; HRMS (ESI) m/z calcd for $C_{21}H_{18}N_3O$ $(M+H)^+$ 328.1444, found 328.1444.



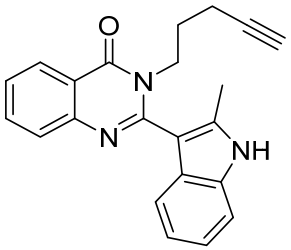
1p

8-Chloro-2-(2-methyl-1H-indol-3-yl)-3-(prop-2-yn-1-yl)quinazolin-4(*3H*)-one (**1q**). A white solid, 0.555 g, 80% yield; mp: 234-235 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.72 (s, 1H), 8.18 (dd, J = 8.0, 1.3 Hz, 1H), 8.01 (dd, J = 7.8, 1.3 Hz, 1H), 7.54 (t, J = 7.9 Hz, 1H), 7.49 – 7.40 (m, 2H), 7.23 – 7.11 (m, 1H), 7.11 – 6.99 (m, 1H), 5.16 – 4.87 (m, 1H), 4.76 – 4.42 (m, 1H), 3.17 (t, J = 2.3 Hz, 1H), 2.50 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.2, 152.9, 144.3, 138.7, 135.2, 135.2, 131.2, 127.6, 126.6, 126.0, 122.2, 122.0, 120.8, 118.6, 111.9, 107.4, 79.0, 74.7, 35.5, 12.8. IR (thin film) 3289, 2984, 2123, 1658, 1564, 1423, 1326, 960, 755 cm^{-1}; HRMS (ESI) m/z calcd for $C_{20}H_{15}ClN_3O$ $(M+H)^+$ 348.0896, found 348.0916.



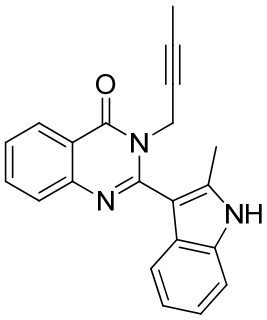
1q

3-(But-3-yn-1-yl)-2-(2-methyl-*1H*-indol-3-yl)quinazolin-4(*3H*)-one (**1q**). A white solid, 0.549 g, 84% yield; mp: 208-209 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.59 (s, 1H), 8.21 (dd, J = 8.0, 1.2 Hz, 1H), 7.86 – 7.76 (m, 1H), 7.64 (d, J = 7.8 Hz, 1H), 7.56 – 7.50 (m, 1H), 7.41 (d, J = 8.0 Hz, 1H), 7.35 (d, J = 7.8 Hz, 1H), 7.17 – 7.10 (m, 1H), 7.09 – 7.02 (m, 1H), 4.44 – 4.28 (m, 1H), 4.19 – 3.99 (m, 1H), 2.73 (t, J = 2.6 Hz, 1H), 2.49 (s, 3H), 2.48 – 2.32 (m, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.2, 152.7, 148.0, 138.0, 135.2, 134.9, 127.5, 126.9, 126.9, 126.7, 121.7, 120.7, 120.6, 118.5, 111.8, 107.9, 81.0, 73.4, 44.3, 17.6, 12.8. IR (thin film) 3300, 3149, 3057, 2975, 2757, 2120, 1676, 1550, 1471, 743 cm^{-1}; HRMS (ESI) m/z calcd for $C_{21}H_{18}N_3O$ $(M+H)^+$ 328.1444, found 328.1429.



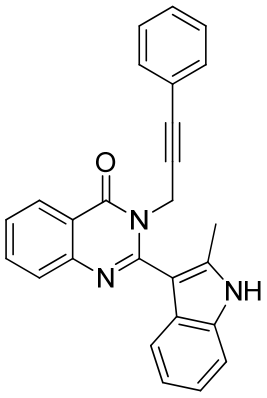
1r

2-(2-Methyl-*1H*-indol-3-yl)-3-(pent-4-yn-1-yl)quinazolin-4(*3H*)-one (**1r**). A white solid, 0.590 g, 85% yield; mp: 188-189 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.52 (s, 1H), 8.21 (dd, J = 8.0, 1.1 Hz, 1H), 7.87 – 7.76 (m, 1H), 7.65 (d, J = 8.0 Hz, 1H), 7.59 – 7.51 (m, 1H), 7.41 (d, J = 8.0 Hz, 1H), 7.33 (d, J = 7.8 Hz, 1H), 7.17 – 7.08 (m, 1H), 7.09 – 7.00 (m, 1H), 4.35 – 4.20 (m, 1H), 4.18 – 3.89 (m, 1H), 2.46 (s, 3H), 2.37 (t, J = 2.6 Hz, 1H), 1.95 – 1.85 (m, 2H), 1.68 – 1.48 (m, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.3, 152.6, 148.0, 137.1, 135.3, 134.7, 127.5, 127.1, 126.9, 126.7, 121.7, 120.8, 120.5, 118.4, 111.7, 108.1, 83.3, 71.5, 44.6, 27.5, 15.7, 12.6. IR (thin film) 3151, 2987, 2810, 2231, 1689, 1578, 1450, 1320, 1021, 750 cm^{-1}; HRMS (ESI) m/z calcd for $C_{22}H_{20}N_3O$ $(M+H)^+$ 342.1601, found 342.1590.



1s

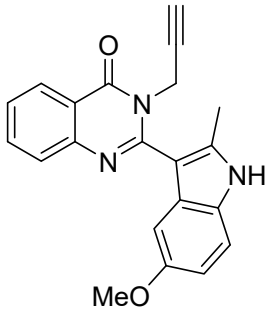
3-(But-2-yn-1-yl)-2-(2-methyl-*1H*-indol-3-yl)quinazolin-4(*3H*)-one (**1s**). A white solid, 0.576 g, 88% yield; mp: 246-247 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.57 (s, 1H), 8.21 (dd, J = 8.0, 1.2 Hz, 1H), 7.87 – 7.80 (m, 1H), 7.67 (d, J = 7.8 Hz, 1H), 7.60 – 7.51 (m, 1H), 7.41 (d, J = 8.0 Hz, 1H), 7.36 (d, J = 7.9 Hz, 1H), 7.16 – 7.09 (m, 1H), 7.06 – 6.98 (m, 1H), 4.95 (d, J = 15.7 Hz, 1H), 4.46 (d, J = 15.9 Hz, 1H), 2.43 (s, 3H), 1.63 (t, J = 2.2 Hz, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.6, 152.3, 147.9, 137.5, 135.2, 135.1, 127.7, 127.3, 126.9, 126.8, 121.8, 120.7, 120.5, 118.4, 111.7, 107.7, 79.6, 74.9, 35.3, 12.6, 3.4. IR (thin film) 3327, 3058, 2977, 2921,2756, 2238, 1681, 1586, 1470, 749 cm^{-1}; HRMS (ESI) m/z calcd for $C_{21}H_{18}N_3O$ $(M+H)^+$ 328.1444, found 328.1437.



1t

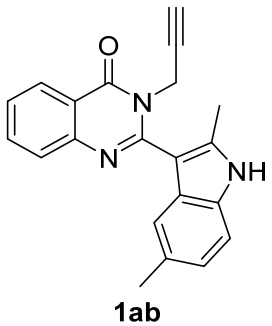
2-(2-Methyl-*1H*-indol-3-yl)-3-(3-phenylprop-2-yn-1-yl)quinazolin-4(*3H*)-one (**1t**). A white solid, 0.622 g, 80% yield; mp: 195-196 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.65 (s, 1H), 8.31 – 8.25 (m, 1H), 7.91 – 7.84 (m, 1H), 7.72 (d, J = 8.0 Hz, 1H), 7.64 – 7.55 (m, 1H), 7.48 (t, J = 8.4 Hz, 2H), 7.38 – 7.24 (m, 5H), 7.20 – 7.14 (m, 1H), 7.08 (t, J = 7.5 Hz, 1H), 5.28 (d, J = 17.3 Hz, 1H), 4.80 (d, J = 17.2 Hz, 1H), 2.48 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.7, 152.2, 148.0, 137.6, 135.3, 135.1,

131.8, 129.2, 129.1, 127.8, 127.4, 126.9, 126.8, 122.1, 121.8, 120.7, 120.5, 118.6, 111.8, 107.8, 85.4, 82.8, 35.6, 12.7. IR (thin film) 3428, 3052, 2343, 1679, 1584, 1329, 1167, 958, 751 cm^{-1}; HRMS (ESI) m/z calcd for $C_{26}H_{20}N_3O$ $(M+H)^+$ 390.1601, found 390.1579.



1aa

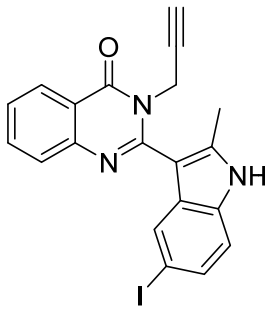
2-(5-Methoxy-2-methyl-*1H*-indol-3-yl)-3-(prop-2-yn-1-yl)quinazolin-4(*3H*)-one (**1aa**). A white solid, 0.487 g, 71% yield; mp: 240-241 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.44 (s, 1H), 8.22 (dd, J = 8.0, 1.2 Hz, 1H), 7.89 – 7.82 (m, 1H), 7.68 (d, J = 7.9 Hz, 1H), 7.59 – 7.53 (m, 1H), 7.31 (d, J = 8.8 Hz, 1H), 6.93 (d, J = 2.3 Hz, 1H), 6.76 (dd, J = 8.8, 2.4 Hz, 1H), 5.04 (d, J = 16.8 Hz, 1H), 4.50 (d, J = 16.7 Hz, 1H), 3.70 (s, 3H), 3.16 (t, J = 2.3 Hz, 1H), 2.40 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.7, 154.7, 152.2, 148.0, 138.1, 135.0, 130.0, 127.7, 127.3, 127.1, 126.7, 120.6, 112.5, 111.7, 107.6, 100.4, 79.5, 74.5, 55.8, 35.1, 12.8. IR (thin film) 3301, 3159, 3058, 2964, 2130, 1678, 1583, 1479, 1303, 1035, 776 cm^{-1}; HRMS (ESI) m/z calcd for $C_{21}H_{18}N_3O_2$ $(M+H)^+$ 344.1394, found 344.1383.



1ab

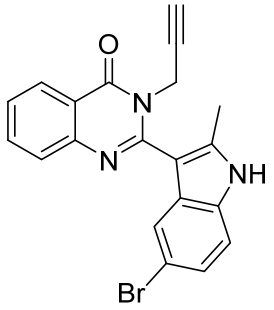
2-(2,5-Dimethyl-*1H*-indol-3-yl)-3-(prop-2-yn-1-yl)quinazolin-4(*3H*)-one (**1ab**). A white solid, 0.530 g, 81% yield; mp: 279-280 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.47 (s, 1H), 8.22 (dd, J = 8.0, 1.3 Hz, 1H), 7.88 – 7.81 (m, 1H), 7.68 (d, J = 7.8 Hz, 1H), 7.61 – 7.50 (m, 1H), 7.30 (d, J = 8.2 Hz, 1H), 7.19 (s, 1H), 6.95 (dd, J = 8.3, 1.2

Hz, 1H), 5.04 (d, J = 17.0 Hz, 1H), 4.49 (d, J = 17.0 Hz, 1H), 3.15 (t, J = 2.4 Hz, 1H), 2.42 (s, 3H), 2.33 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.6, 152.2, 147.9, 137.6, 135.1, 133.5, 129.3, 127.7, 127.3, 127.0, 126.7, 123.3, 120.5, 118.1, 111.4, 107.1, 79.4, 74.4, 35.1, 21.6, 12.7. IR (thin film) 3281, 3162, 3056, 2917, 2735, 2123, 1684, 1586, 1471, 1337, 1158, 777 cm^{-1}; HRMS (ESI) m/z calcd for $C_{21}H_{18}N_3O$ $(M+H)^+$ 328.1444, found 328.1459.



1ac

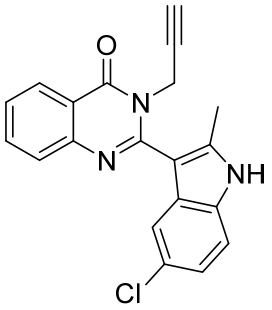
2-(5-Iodo-2-methyl-*1H*-indol-3-yl)-3-(prop-2-yn-1-yl)quinazolin-4(*3H*)-one (**1ac**). A white solid, 0.773 g, 88% yield; mp: 258-259 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.77 (s, 1H), 8.23 (dd, J = 8.0, 1.2 Hz, 1H), 7.90 – 7.80 (m, 2H), 7.69 (d, J = 7.8 Hz, 1H), 7.62 – 7.55 (m, 1H), 7.41 (dd, J = 8.5, 1.6 Hz, 1H), 7.28 (d, J = 8.5 Hz, 1H), 4.97 (d, J = 16.6 Hz, 1H), 4.42 (d, J = 16.5 Hz, 1H), 3.16 (t, J = 2.4 Hz, 1H), 2.42 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.6, 151.5, 147.8, 138.6, 135.1, 134.4, 129.8, 129.4, 127.7, 127.5, 126.8, 126.7, 120.8, 114.1, 107.1, 84.5, 79.4, 74.5, 35.2, 12.7. IR (thin film) 3650, 3279, 2130, 1658, 1555, 1467, 1302, 955, 768 cm^{-1}; HRMS (ESI) m/z calcd for $C_{20}H_{15}IN_3O$ $(M+H)^+$ 440.0254, found 440.0245.



1ad

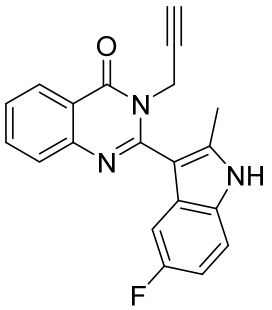
2-(5-Bromo-2-methyl-*1H*-indol-3-yl)-3-(prop-2-yn-1-yl)quinazolin-4(*3H*)-one (**1ad**). A white solid, 0.579 g, 74% yield; mp: 263-264 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.81 (s, 1H), 8.24 (dd, J = 8.0, 1.2 Hz, 1H), 7.90 – 7.82 (m, 1H), 7.71 –

7.66 (m, 2H), 7.63 – 7.55 (m, 1H), 7.40 (d, J = 8.6 Hz, 1H), 7.26 (dd, J = 8.6, 1.9 Hz, 1H), 4.99 (d, J = 16.5 Hz, 1H), 4.44 (d, J = 16.5 Hz, 1H), 3.17 (t, J = 2.4 Hz, 1H), 2.44 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.6, 151.4, 147.8, 139.1, 135.1, 134.0, 128.6, 127.7, 127.5, 126.7, 124.3, 120.8, 120.8, 113.6, 113.2, 107.5, 79.4, 74.5, 35.1, 12.8. IR (thin film) 3282, 2985, 2137, 1655, 1554, 1468, 1303, 1191, 954, 690 cm^{-1}; HRMS (ESI) m/z calcd for $C_{20}H_{15}BrN_3O$ $(M+H)^+$ 392.0393, found 392.0396.



1ae

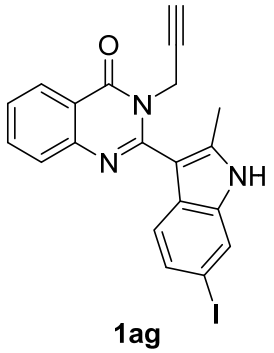
2-(5-Chloro-2-methyl-*1H*-indol-3-yl)-3-(prop-2-yn-1-yl)quinazolin-4(*3H*)-one (**1ae**). A white solid, 0.590 g, 85% yield; mp: 265-266 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.81 (s, 1H), 8.25 (d, J = 7.3 Hz, 1H), 7.90 – 7.83 (m, 1H), 7.70 (d, J = 8.1 Hz, 1H), 7.60 (t, J = 7.4 Hz, 1H), 7.54 (d, J = 1.4 Hz, 1H), 7.45 (d, J = 8.6 Hz, 1H), 7.16 (dd, J = 8.6, 1.8 Hz, 1H), 5.00 (d, J = 16.1 Hz, 1H), 4.47 (d, J = 16.0 Hz, 1H), 3.18 (s, 1H), 2.45 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.6, 151.4, 147.8, 139.3, 135.1, 133.8, 128.0, 127.7, 127.5, 126.8, 125.2, 121.8, 120.8, 117.9, 113.2, 107.6, 79.4, 74.5, 35.1, 12.8. IR (thin film) 3286, 3053, 2986, 2727, 2127, 1667, 1555, 1469, 1304, 955, 766, 691 cm^{-1}; HRMS (ESI) m/z calcd for $C_{20}H_{15}ClN_3O$ $(M+H)^+$ 348.0898, found 348.0889.



1af

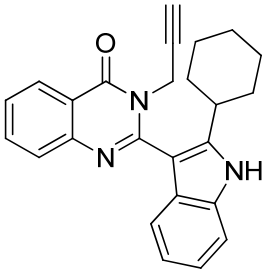
2-(5-Fluoro-2-methyl-*1H*-indol-3-yl)-3-(prop-2-yn-1-yl)quinazolin-4(*3H*)-one (**1af**). A white solid, 0.583 g, 88% yield; mp: 268-269 °C; ^{1}H NMR (400 MHz,

DMSO-d_6) δ 11.74 (s, 1H), 8.22 (dd, J = 8.0, 1.1 Hz, 1H), 7.91 – 7.82 (m, 1H), 7.68 (d, J = 7.8 Hz, 1H), 7.64 – 7.55 (m, 1H), 7.42 (dd, J = 8.8, 4.5 Hz, 1H), 7.23 (dd, J = 9.9, 2.4 Hz, 1H), 6.97 (td, J = 9.3, 2.5 Hz, 1H), 5.00 (d, J = 13.6 Hz, 1H), 4.46 (d, J = 15.9 Hz, 1H), 3.15 (t, J = 2.3 Hz, 1H), 2.42 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.6, 158..0 (d, J = 231.4Hz), 151.6, 147.8, 139.7, 135.1, 132.0, 127.7, 127.4, 127.1 (d, J = 10.4 Hz), 126.7, 120.7, 112.8 (d, J = 9.6 Hz), 109.7 (d, J = 25.7 Hz), 108.0 (d, J = 4.2 Hz), 103.6 (d, J = 24.3 Hz), 79.4, 74.5, 35.0, 12.9. IR (thin film) 3294, 2136, 1659, 1550, 1473, 1313, 1161, 958, 768 cm^{-1}; HRMS (ESI) m/z calcd for $C_{20}H_{15}FN_3O$ $(M+H)^+$ 332.1194, found 332.1218.



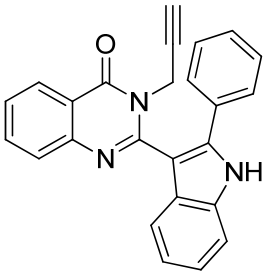
1ag

2-(6-Iodo-2-methyl-*1H*-indol-3-yl)-3-(prop-2-yn-1-yl)quinazolin-4(*3H*)-one (**1ag**). A white solid, 0.711 g, 81% yield; mp: 276-277 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.71 (s, 1H), 8.22 (dd, J = 8.0, 1.1 Hz, 1H), 7.90 – 7.84 (m, 1H), 7.77 (d, J = 1.2 Hz, 1H), 7.68 (d, J = 7.7 Hz, 1H), 7.63 – 7.56 (m, 1H), 7.32 (dd, J = 8.3, 1.5 Hz, 1H), 7.25 (d, J = 8.3 Hz, 1H), 4.96 (d, J = 16.6 Hz, 1H), 4.44 (d, J = 15.8 Hz, 1H), 3.13 (t, J = 2.4 Hz, 1H), 2.42 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.5, 151.5, 147.8, 138.3, 136.8, 135.2, 128.9, 127.8, 127.5, 126.8, 126.2, 120.7, 120.1, 107.9, 85.7, 79.2, 74.5, 35.0, 12.7. IR (thin film) 3281, 2983, 2386, 1657, 1614, 1557, 1469, 1417, 1359, 765 cm^{-1}; HRMS (ESI) m/z calcd for $C_{20}H_{15}IN_3O$ $(M+H)^+$ 440.0254, found 440.0236.



1ah

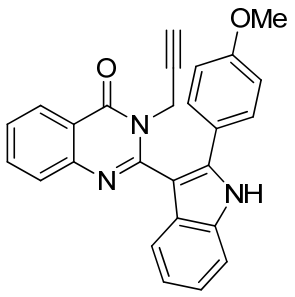
2-(2-Cyclohexyl-*1H*-indol-3-yl)-3-(prop-2-yn-1-yl)quinazolin-4(*3H*)-one (**1ah**). A white solid, 0.587 g, 77% yield; mp: 102-103 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.53 (s, 1H), 8.23 (dd, J = 8.0, 1.2 Hz, 1H), 7.92 – 7.80 (m, 1H), 7.66 (d, J = 7.7 Hz, 1H), 7.62 – 7.54 (m, 1H), 7.45 (d, J = 8.1 Hz, 1H), 7.34 (d, J = 7.9 Hz, 1H), 7.19 – 7.10 (m, 1H), 7.08 – 6.99 (m, 1H), 5.01 (dd, J = 17.1, 2.4 Hz, 1H), 4.51 (dd, J = 17.1, 2.4 Hz, 1H), 3.14 (t, J = 2.4 Hz, 1H), 2.96 – 2.84 (m, 1H), 2.11 – 2.01 (m, 1H), 1.97 – 1.87 (m, 1H), 1.82 – 1.53 (m, 5H), 1.31 – 1.19 (m, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.6, 152.1, 147.9, 146.2, 135.4, 135.2, 127.8, 127.4, 126.7, 126.4, 121.9, 120.6, 120.6, 118.5, 112.0, 105.9, 79.3, 74.5, 36.8, 35.2, 32.7, 32.1, 26.5, 26.4, 26.0. IR (thin film) 3244, 2988, 2120, 1677, 1532, 1411, 1306, 980, 700 cm^{-1}; HRMS (ESI) m/z calcd for $C_{25}H_{24}N_3O$ $(M+H)^+$ 382.1914, found 382.1898.



1ai

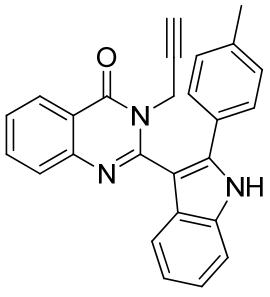
2-(2-Phenyl-*1H*-indol-3-yl)-3-(prop-2-yn-1-yl)quinazolin-4(*3H*)-one (**1ai**). A white solid, 0.713 g, 95% yield; mp: 291-292 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.07 (s, 1H), 8.26 (dd, J = 7.9, 1.0 Hz, 1H), 7.88 – 7.81 (m, 1H), 7.66 – 7.53 (m, 5H), 7.48 (d, J = 7.9 Hz, 1H), 7.41 (t, J = 7.5 Hz, 2H), 7.33 (t, J = 7.3 Hz, 1H), 7.29 – 7.22 (m, 1H), 7.11 (t, J = 7.3 Hz, 1H), 4.84 (dd, J = 17.2, 2.3 Hz, 1H), 4.57 (dd, J = 17.2, 2.3 Hz, 1H), 2.99 (t, J = 2.3 Hz, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.5, 152.0, 147.8, 137.6, 136.2, 135.3, 131.6, 129.3, 128.9, 127.9, 127.8, 127.7, 126.9, 123.2, 121.1,

120.8, 119.3, 112.4, 107.3, 78.8, 74.8, 34.9. IR (thin film) 3451, 3303, 2127, 1674, 1658, 1580, 1239, 948, 777, 750 cm^{-1}; HRMS (ESI) m/z calcd for $C_{25}H_{18}N_3O$ $(M+H)^+$ 376.1444, found 376.1431.



1aj

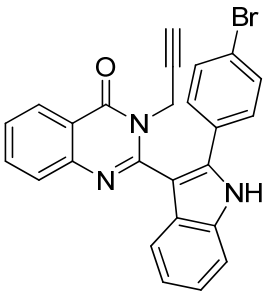
2-(2-(4-Methoxyphenyl)-*1H*-indol-3-yl)-3-(prop-2-yn-1-yl)quinazolin-4(*3H*)-one (**1aj**). A white solid, 0.778 g, 96% yield; mp: 252-253 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.94 (s, 1H), 8.25 (dd, J = 8.0, 1.1 Hz, 1H), 7.90 – 7.79 (m, 1H), 7.66 – 7.56 (m, 2H), 7.57 – 7.49 (m, 3H), 7.44 (d, J = 8.0 Hz, 1H), 7.25 – 7.19 (m, 1H), 7.11 – 7.04 (m, 1H), 7.03 – 6.94 (m, 2H), 4.81 (dd, J = 17.2, 2.4 Hz, 1H), 4.57 (dd, J = 17.2, 2.4 Hz, 1H), 3.74 (s, 3H), 2.98 (t, J = 2.4 Hz, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.5, 159.9, 152.2, 147.9, 137.7, 136.0, 135.3, 129.2, 128.0, 127.9, 127.7, 126.9, 124.0, 122.8, 121.0, 120.8, 119.0, 114.9, 112.1, 106.3, 78.8, 74.8, 55.7, 34.9. IR (thin film) 3291, 2130, 1682, 1584, 1505, 1447, 1333, 1290, 1251, 773 cm^{-1}; HRMS (ESI) m/z calcd for $C_{26}H_{20}N_3O_2$ $(M+H)^+$ 406.1550, found 406.1532.



1ak

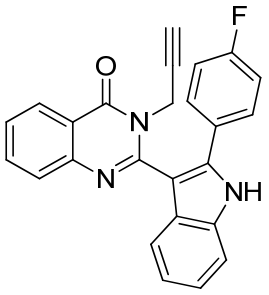
3-(Prop-2-yn-1-yl)-2-(2-(p-tolyl)-*1H*-indol-3-yl)quinazolin-4(*3H*)-one (**1ak**). A white solid, 0.537 g, 69% yield; mp: 271-272 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.00 (s, 1H), 8.25 (dd, J = 8.0, 1.1 Hz, 1H), 7.88 – 7.81 (m, 1H), 7.65 – 7.57 (m, 2H), 7.54 (d, J = 8.1 Hz, 1H), 7.51 – 7.42 (m, 3H), 7.28 – 7.18 (m, 3H), 7.13 – 7.05 (m, 1H), 4.81 (dd, J = 17.2, 2.4 Hz, 1H), 4.58 (dd, J = 17.2, 2.4 Hz, 1H), 2.98 (t, J = 2.4

Hz, 1H), 2.28 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.5, 152.1, 147.9, 138.5, 137.8, 136.1, 135.3, 129.9, 128.7, 127.9, 127.9, 127.7, 126.9, 123.0, 121.0, 120.8, 119.2, 112.3, 106.9, 78.8, 74.8, 34.9, 21.2. IR (thin film) 3297, 2126, 1683, 1656, 1559, 1445, 1334, 1240, 1154, 744 cm^{-1}; HRMS (ESI) m/z calcd for $C_{26}H_{20}N_3O$ $(M+H)^+$ 390.1601, found 390.1592.



1al

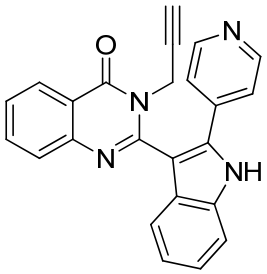
2-(2-(4-Bromophenyl)-*1H*-indol-3-yl)-3-(prop-2-yn-1-yl)quinazolin-4(*3H*)-one (**1al**). A white solid, 0.797 g, 88% yield; mp: 260-261 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.13 (s, 1H), 8.28 – 8.22 (m, 1H), 7.88 – 7.81 (m, 1H), 7.65 – 7.58 (m, 4H), 7.58 – 7.52 (m, 3H), 7.48 (d, J = 8.0 Hz, 1H), 7.29 – 7.22 (m, 1H), 7.15 – 7.08 (m, 1H), 4.90 (dd, J = 17.3, 2.4 Hz, 1H), 4.52 (dd, J = 17.3, 2.4 Hz, 1H), 2.99 (t, J = 2.4 Hz, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.4, 151.8, 147.8, 136.4, 136.2, 135.3, 132.3, 130.8, 129.8, 127.9, 127.8, 127.7, 126.9, 123.5, 122.2, 121.3, 120.9, 119.4, 112.5, 107.8, 78.8, 74.9, 34.9. IR (thin film) 3291, 3055, 2130, 1682, 1652, 1581, 1472, 1443, 1380, 745 cm^{-1}; HRMS (ESI) m/z calcd for $C_{25}H_{17}BrN_3O$ $(M+H)^+$ 454.0550, found 454.0511.



1am

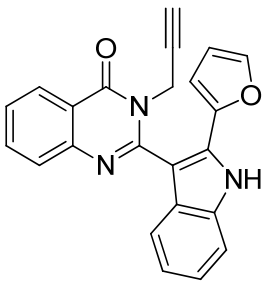
2-(2-(4-Fluorophenyl)-*1H*-indol-3-yl)-3-(prop-2-yn-1-yl)quinazolin-4(*3H*)-one

(**1am**). A white solid, 0.637 g, 81% yield; mp: 265-266 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.09 (s, 1H), 8.26 (dd, J = 8.0, 1.1 Hz, 1H), 7.89 – 7.79 (m, 1H), 7.69 – 7.53 (m, 5H), 7.48 (d, J = 8.0 Hz, 1H), 7.34 – 7.22 (m, 3H), 7.17 – 7.07 (m, 1H), 4.89 (dd, J = 17.2, 2.4 Hz, 1H), 4.54 (dd, J = 3.1 Hz, 1H), 2.99 (t, J = 2.4 Hz, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.5 (d, J = 244.9 Hz), 161.5, 151.9, 147.8, 136.7, 136.1, 135.3, 130.0 (d, J = 8.4 Hz), 123.0, 128.2 (d, J = 3.1 Hz), 127.9, 127.7, 126.9, 123.3, 121.2, 120.8, 119.3, 116.4 (d, J = 21.7 Hz), 112.4, 107.3, 78.8, 74.8, 35.0. IR (thin film) 3650, 3280, 3053, 2130, 1678, 1654, 1632, 1603, 1471, 751 cm^{-1}; HRMS (ESI) m/z calcd for $C_{25}H_{17}FN_3O$ $(M+H)^+$ 394.1350, found 394.1323.



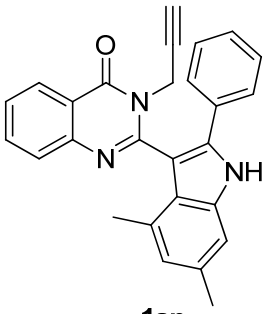
1an

3-(Prop-2-yn-1-yl)-2-(2-(pyridin-4-yl)-*1H*-indol-3-yl)quinazolin-4(*3H*)-one (**1an**). A white solid, 0.481 g, 64% yield; mp: 272-273 °C; 1H NMR (400 MHz, DMSO-d_6) δ 12.33 (s, 1H), 8.57 (d, J = 5.9 Hz, 2H), 8.27 (d, J = 7.4 Hz, 1H), 7.90 – 7.80 (m, 1H), 7.69 – 7.57 (m, 3H), 7.57 – 7.46 (m, 3H), 7.32 (t, J = 7.5 Hz, 1H), 7.14 (t, J = 7.5 Hz, 1H), 4.94 (dd, J = 17.3, 2.0 Hz, 1H), 4.48 (dd, J = 17.3, 2.0 Hz, 1H), 2.98 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.4, 151.4, 150.6, 147.7, 138.6, 136.5, 135.3, 134.3, 128.0, 127.9, 127.5, 126.9, 124.3, 121.7, 121.6, 121.0, 119.8, 112.7, 109.6, 78.7, 75.0, 35.0. IR (thin film) 3282, 2126, 1940, 1685, 1652, 1599, 1473, 1445, 1418, 752 cm^{-1}; HRMS (ESI) m/z calcd for $C_{24}H_{17}N_4O$ $(M+H)^+$ 377.1397, found 377.1381.



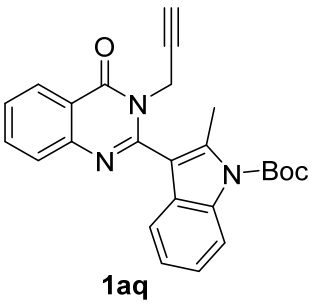
1ao

2-**(2-(Furan-2-yl)-*1H*-indol-3-yl)-3-(prop-2-yn-1-yl)quinazolin-4(*3H*)-one** (**1ao**). A white solid, 0.438 g, 60% yield; mp: 232-233 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.14 (s, 1H), 8.27 (d, J = 7.5 Hz, 1H), 7.88 (d, J = 7.0 Hz, 1H), 7.80 – 7.58 (m, 3H), 7.52 (d, J = 7.8 Hz, 1H), 7.44 (d, J = 7.5 Hz, 1H), 7.24 (t, J = 6.9 Hz, 1H), 7.09 (t, J = 6.8 Hz, 1H), 6.79 – 6.65 (m, 1H), 6.61 – 6.46 (m, 1H), 4.75 (d, J = 16.9 Hz, 1H), 4.56 (d, J = 17.0 Hz, 1H), 2.90 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.4, 151.4, 147.8, 146.3, 144.3, 136.1, 135.3, 128.4, 127.9, 127.8, 127.5, 126.8, 123.4, 121.1, 120.9, 119.3, 112.5, 112.2, 109.1, 106.1, 78.7, 74.4, 35.0. IR (thin film) 3436, 3245, 2925, 1678, 1605, 1529, 1465, 1369, 1333, 767 cm^{-1}; HRMS (ESI) m/z calcd for $C_{23}H_{16}N_3O_2$ $(M+H)^+$ 366.1237, found 366.1234.



1ap

2-(4,6-Dimethyl-2-phenyl-*1H*-indol-3-yl)-3-(prop-2-yn-1-yl)quinazolin-4(*3H*)-one (**1ap**). A white solid, 0.661 g, 82% yield; mp: 207-208 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.85 (s, 1H), 8.26 (d, J = 7.6 Hz, 1H), 7.89 (t, J = 7.2 Hz, 1H), 7.72 (d, J = 8.0 Hz, 1H), 7.63 (t, J = 7.5 Hz, 1H), 7.55 (d, J = 7.5 Hz, 2H), 7.37 (t, J = 7.5 Hz, 2H), 7.29 (t, J = 7.3 Hz, 1H), 7.18 (s, 1H), 6.70 (s, 1H), 4.67 (dd, J = 17.1, 2.0 Hz, 1H), 4.53 (dd, J = 17.1, 2.0 Hz, 1H), 2.95 (s, 1H), 2.40 (s, 3H), 2.09 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.1, 153.2, 147.3, 136.9, 135.5, 132.5, 131.8, 129.4, 129.1, 128.5, 128.0, 127.3, 126.9, 124.8, 124.1, 120.7, 109.9, 107.2, 78.2, 74.8, 35.2, 21.8, 19.1. IR (thin film) 3303, 3012, 2987, 2369, 1685, 1586, 1469, 1334, 1239, 774 cm^{-1}; HRMS (ESI) m/z calcd for $C_{27}H_{22}N_3O$ $(M+H)^+$ 404.1757, found 404.1755.



1aq

***Tert*-butyl 2-methyl-3-(4-oxo-3-(prop-2-yn-1-yl)-3,4-dihydroquinazolin-2-yl)-*1H*-Ind -ole-1-carboxylate** (**1aq**). A white solid, 1.673 g, 81% yield; mp: 207-208 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.26 (dd, J = 8.0, 1.1 Hz, 1H), 8.16 (d, J = 8.4 Hz, 1H), 7.93 – 7.86 (m, 1H), 7.72 (d, J = 7.7 Hz, 1H), 7.67 – 7.60 (m, 1H), 7.44 (d, J = 7.7 Hz, 1H), 7.41 – 7.33 (m, 1H), 7.29 – 7.21 (m, 1H), 4.92 (dd, J = 17.4, 2.4 Hz, 1H), 4.39 (dd, J = 17.5, 2.4 Hz, 1H), 3.19 (t, J = 2.4 Hz, 1H), 2.55 (s, 3H), 1.68 (s, 9H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.2, 150.3, 150.1, 147.5, 137.9, 135.3, 135.2, 128.1, 127.9, 127.5, 126.9, 124.9, 123.9, 121.0, 119.2, 115.8, 115.1, 85.3, 79.0, 74.9, 34.9, 28.2, 15.8. IR (thin film) 3441, 3284, 2982, 2123, 1731, 1684, 1591, 1324, 1157, 773 cm^{-1}; HRMS (ESI) m/z calcd for $C_{25}H_{24}N_3O_3$ $(M+H)^+$ 414.1812, found 414.1796.

9. Biological activity studies of compounds 2.

Cell Cuture: Murine monocyte-macrophage RAW264.7 cells maintained in DMEM(Giboc, USA) incubated at 37 °C in a humidified atmosphere containing 5% CO_2. Mouse peritoneal macrophages purchased from Procell Life Science& Technology Co., Ltd.

Cell Viability assay: Cell cytotoxicity was evaluated by MTT. The MTT solution was added into each well and after incubation at 37 °C for 4 h, the culture media containing MTT were removed, and then DMSO was added into each well and the absorbance at 570 nm was measured by a microplate reader.[3]

Assay for NO production: NO production was quantified by nitrite accumulation in the culture medium using the Griess reaction. Briefly, Raw264.7 cells were pretreated with compounds for 1h, and then stimulated with or without LPS (1 mg/mL) for 24 h. The isolated supernatants were mixed with an equal volume of Griess

reagent (Beyotime Biotechnology, China). $NaNO_2$ was used togenerate a standard curve, and nitrite production was determined by measuring the optical density at 540 nm by a microplate reader.[3]

Table S1. The effects of the target compounds on the cell viability of RAW 264.7 at the concentration of 50 μM. (the MTT assay).

Compounds	Cell survual (% of normal)	Compounds	Cell survual (% of normal)
2c	85.91±2.44	**2m**	75.32±6.32
2d	99.4±3.57	**2n**	77.73±7.11
2e	122.81±3.11	**2o**	94.94±3.22
2f	97.82±7.21	**2aa**	101.35±6.15
2j	103.75±5.11	**2ab**	109.28±3.14
2k	79.17±5.56	**2ai**	105.78±5.12
2l	107.00±1.14	**Indometacin**	93.33±5.69

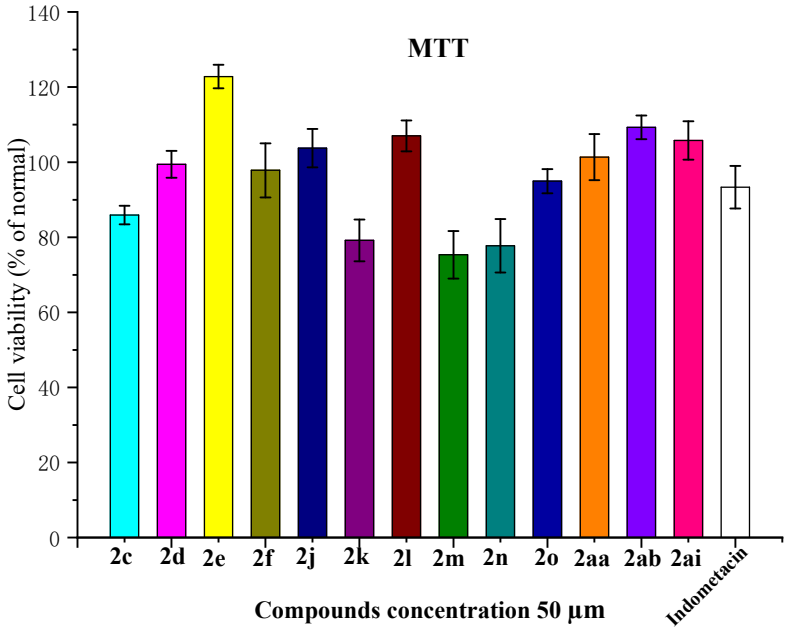
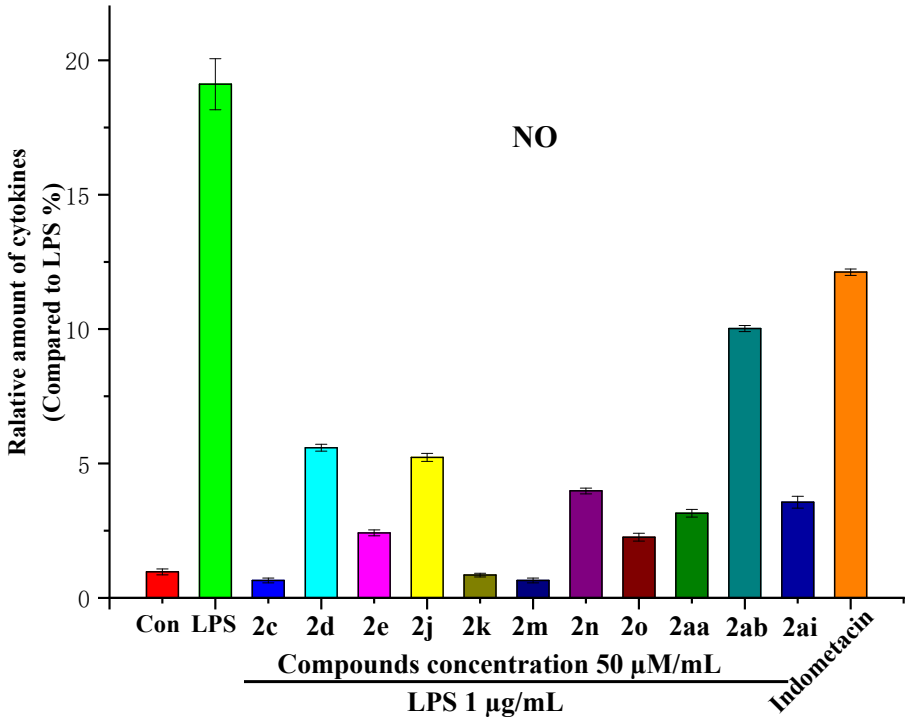
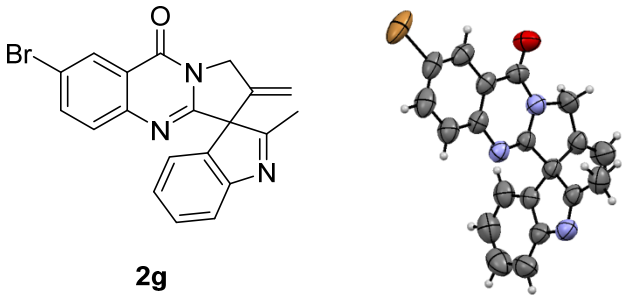


Table S2 The Effect of the compounds **2c**、**2d**、**2e**、**2j**、**2k**、**2m**、**2n**、**2o**、**2aa**、**2ab**、**2ai** on the inhibition of NO produced by RAW 264.7 cell induced by LPS. In the 50 μM compound concentration, LPS comcentration 1μg/mL.

Compounds	Concentration of NO (μmol/L)	Compounds	Concentration of NO (μmol/L)
con	0.97±0.11	**2m**	0.85±0.07
LPS	19.11±0.95	**2n**	3.98±0.11
2c	0.65±0.09	**2o**	2.26±0.15
2d	5.59±0.13	**2aa**	3.15±0.14
2e	2.42±0.11	**2ab**	10.02±0.11
2j	5.23±0.15	**2ai**	3.56±0.22
2k	0.65±0.09	**Indometacin**	12.12±0.12



10. X-ray structure of compound 2g



2g

Figure S2: ORTEP diagram of **2g** at 50% ellipsoid probability

Table S3. Crystal data and structure refinement details for compound **2g**.

Compound	**2g**
Empirical formula	$C_{20}H_{14}BrN_3O$
Formula weight	392.25
Crystal system	orthorhombic
Space group	Pdcn
a(Å)	19.5352 (5)
b (Å)	14.0585 (4)
c (Å)	13.97781 (5)
α(°)	90
b(°)	90
γ(°)	90
V(Å^3)	3838.8(2)
Z	8
T(k)	295.48(10)
D_x (mg/ m^3)	1.357
F(000)	1584.0
μ(mm^{-1})	3.007
Measured reflections	10503
Independent reflections	3012
Parameters	227

R_{int}	0.0514
$wR(F^2)$	1.123
CCDC No.	2114483

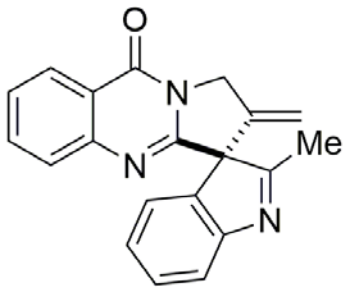
11. References

[1] X.-F. Kong, F. Zhan, G.-X. He, C.-X. Pan, C.-X. Gu, K. Lu, D.-L. Mo, and G.-F. Su. *J. Org. Chem.* 2018, **83**, 2006.

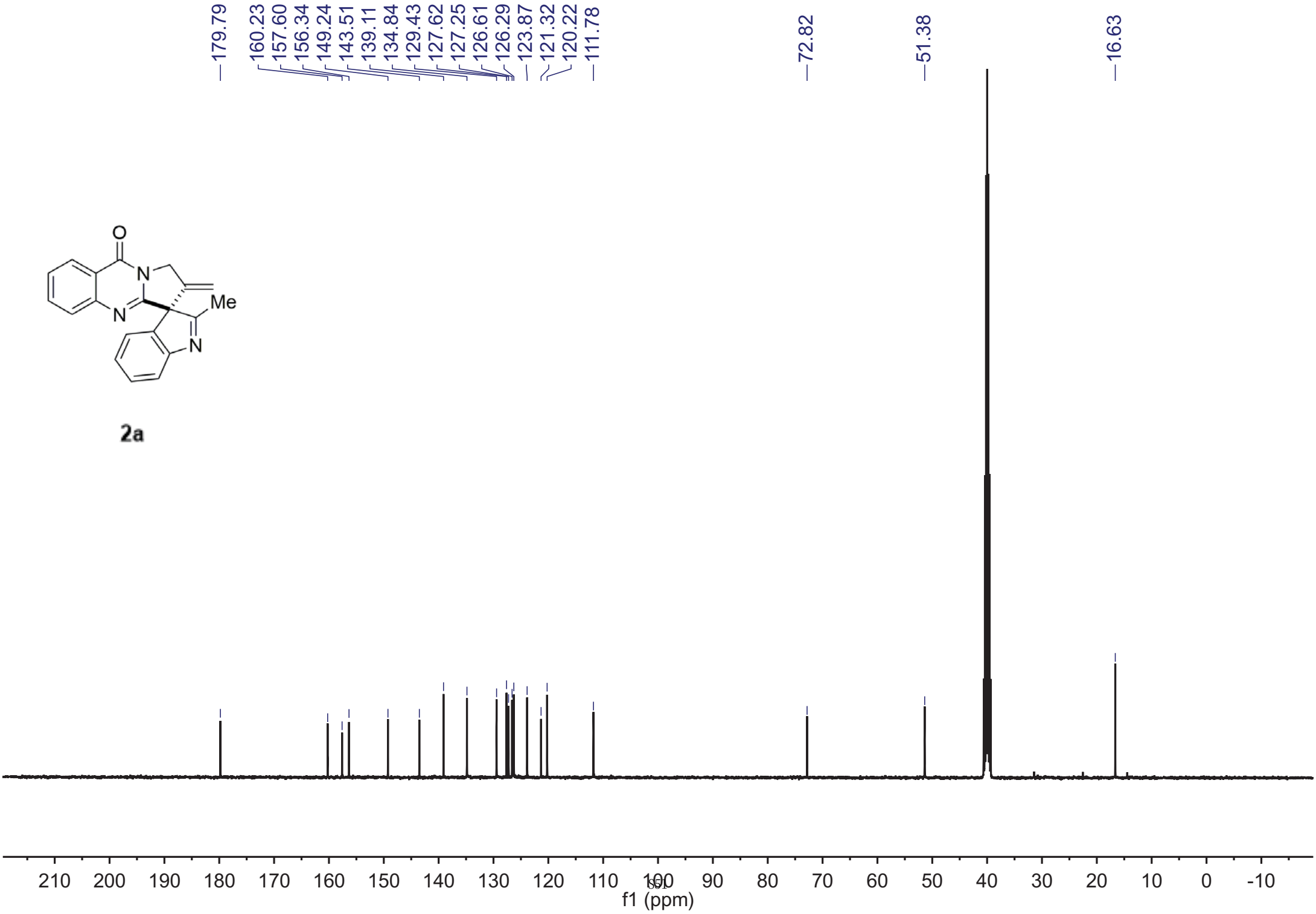
[2] H. C. Chung, J. Kim, G. A. González-Montiel, P. H-.Y. Cheong, and H. G. Lee, *Org. Lett.* 2021, **23**, 1096.

[3] S.-Y. Liu, P. Xu, X.-L. Luo, J.-F. Hu, and X.-H. Liu, *Neurochem. Res.* 2016, **41**, 1570.

12. NMR spectra for compounds 2, 3, 4, 5, 6, and 1.



2a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126.29
123.87
121.32
120.22
111.78
72.82
51.38
16.63
O
N
N
Me
N
2a
210
200
190
180
170
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150
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120
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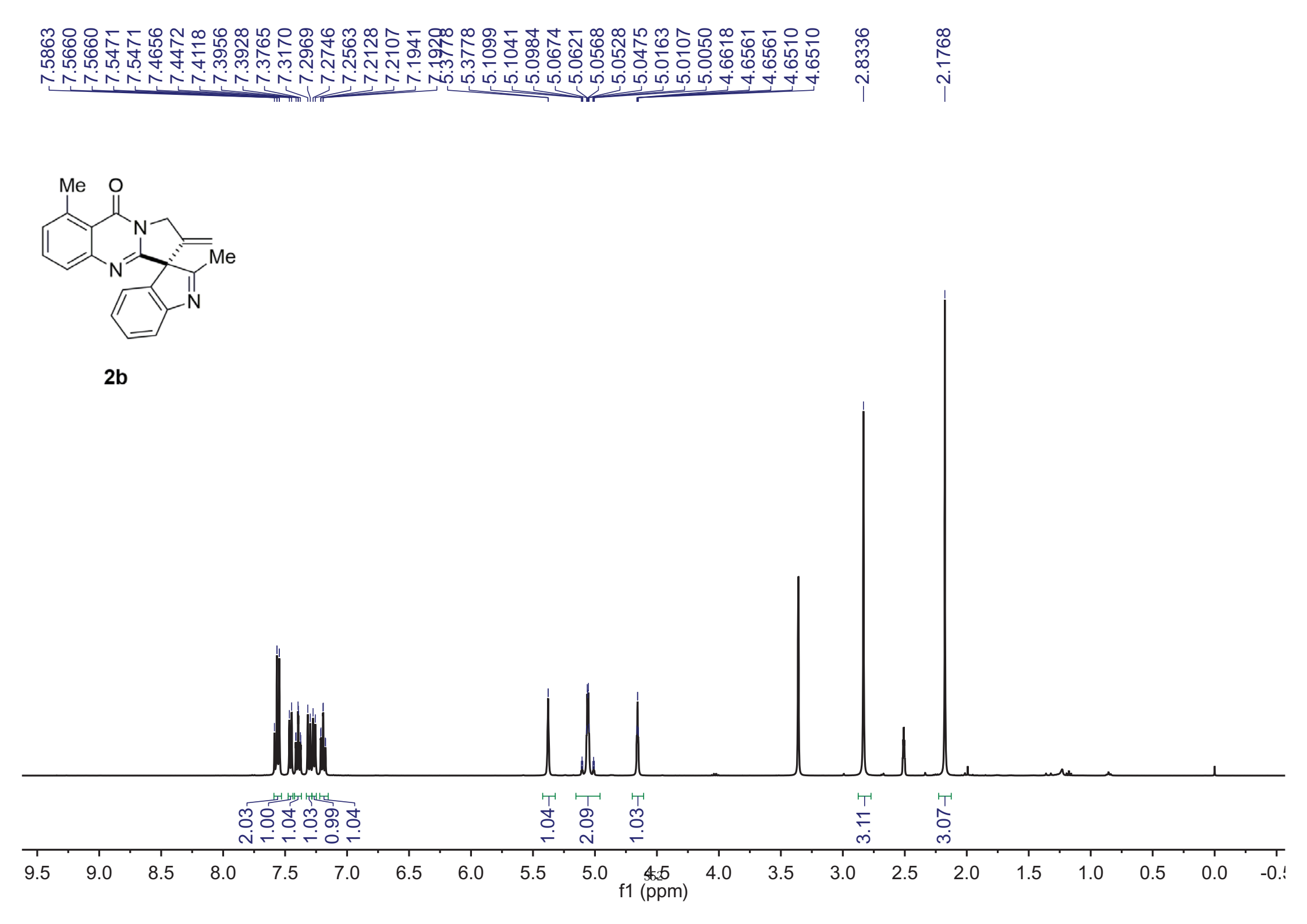
f1 (ppm)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7.3170
7.2969
7.2746
7.2563
7.2128
7.2107
7.1941
7.1920
5.3778
5.3778
5.1099
5.1041
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5.0674
5.0621
5.0568
5.0528
5.0475
5.0163
5.0107
5.0050
4.6618
4.6561
4.6561
4.6510
4.6510
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2.1768
Me
O
N
N
Me
N
2b
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1.00
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1.03
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1.04
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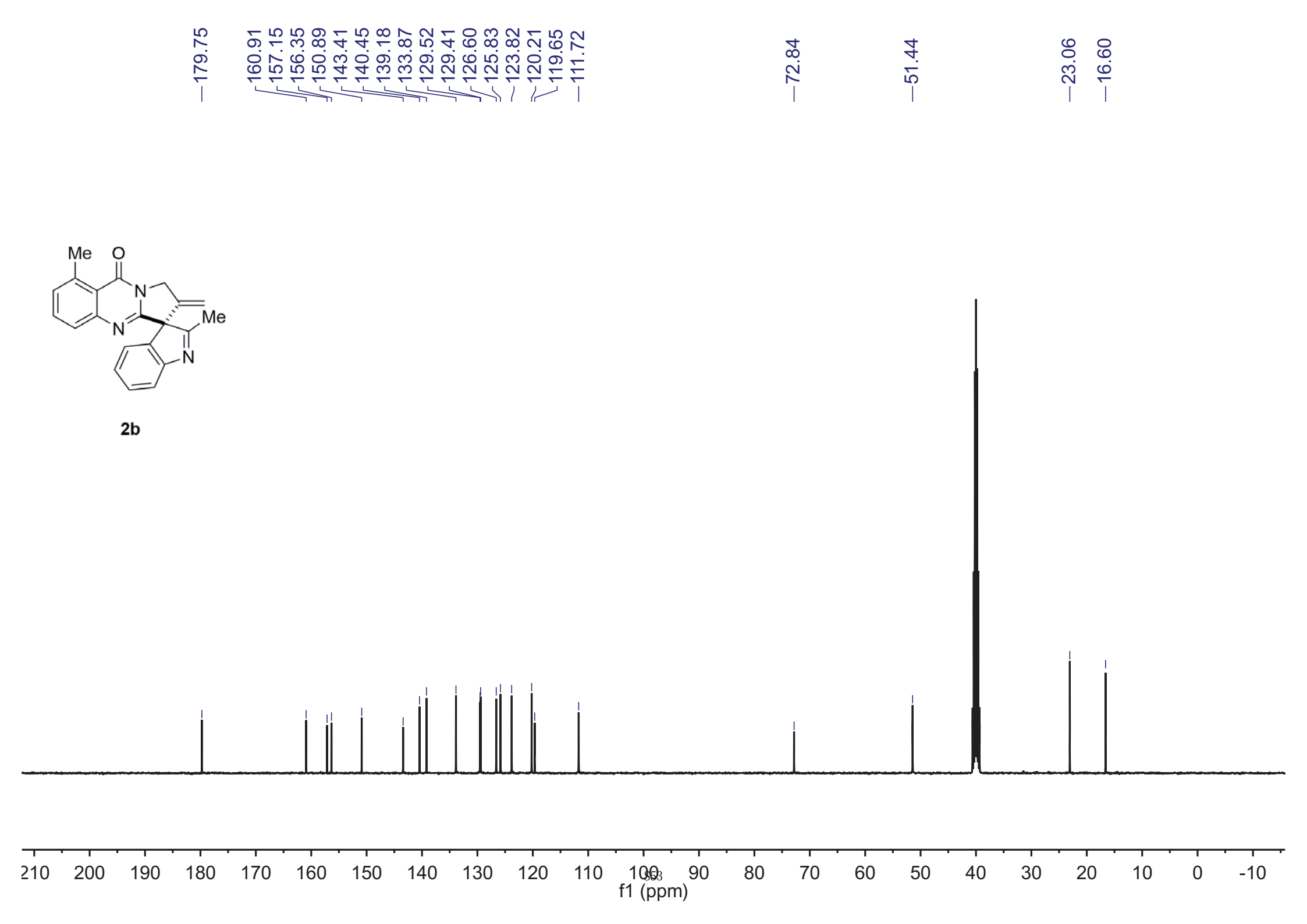
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23.06
16.60
Me
O
N
N
Me
N
2b
210
200
190
180
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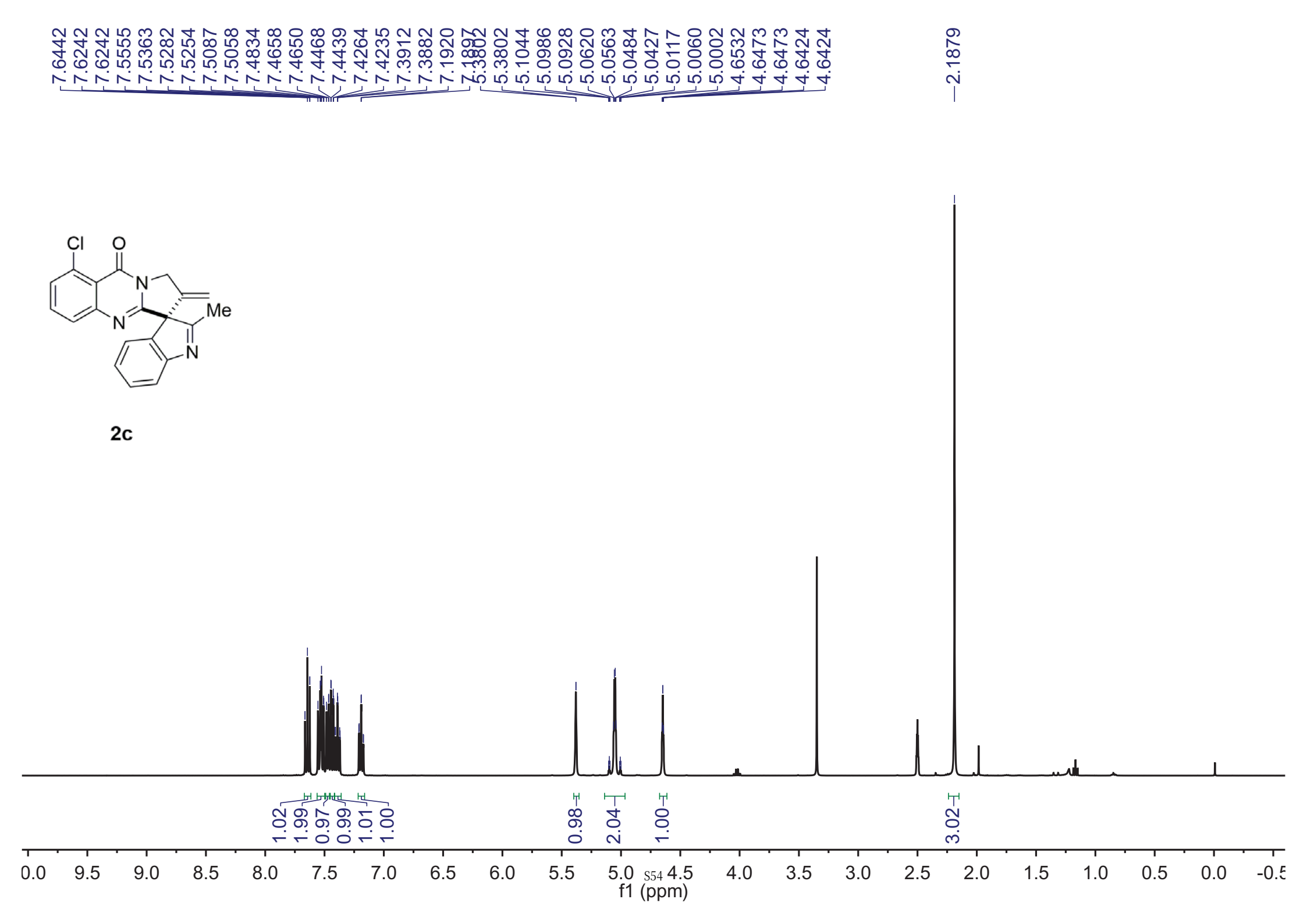
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1.00
3.02
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9.0
8.5
8.0
7.5
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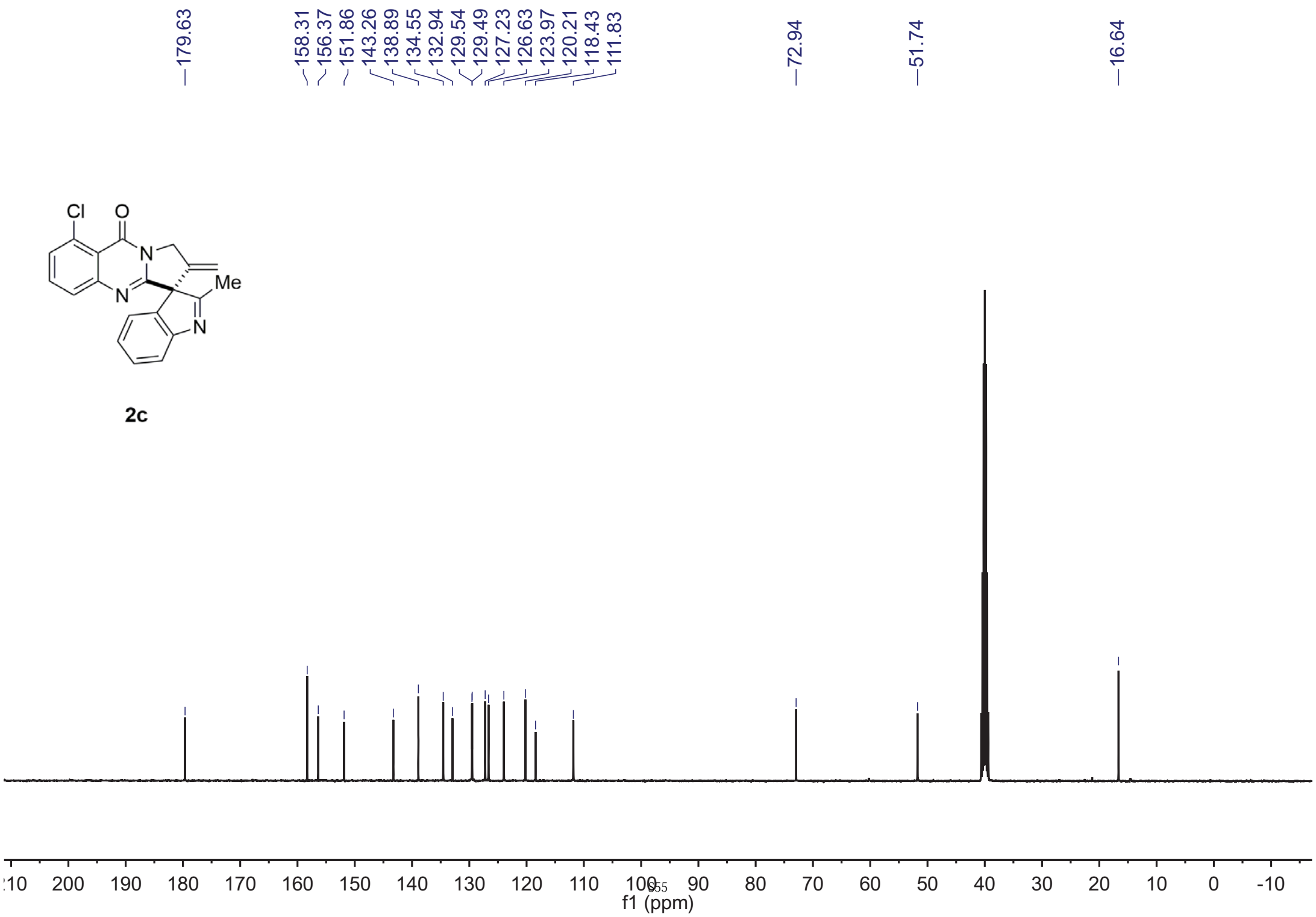
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Me
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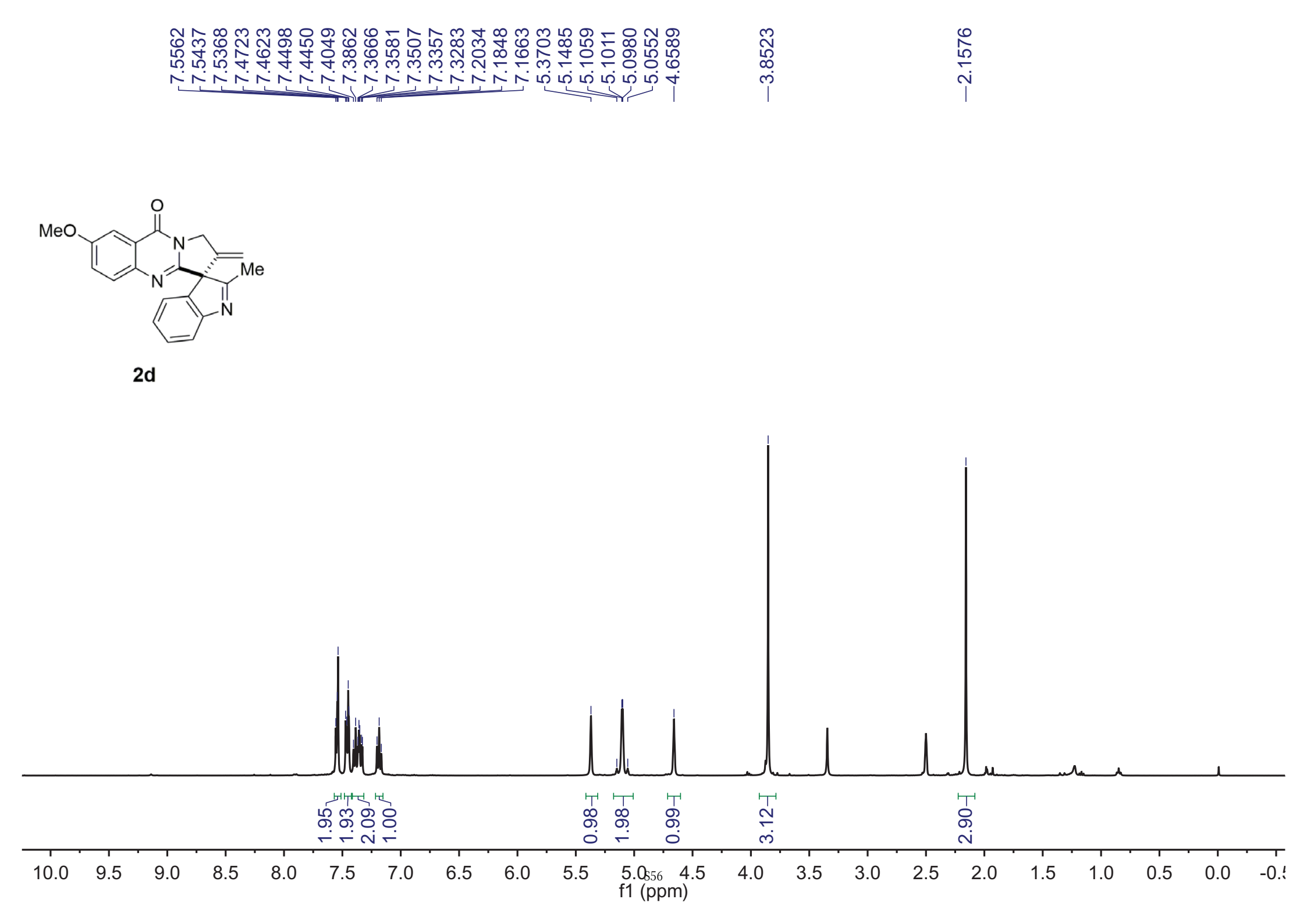
2c
f1 (ppm)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5.0980
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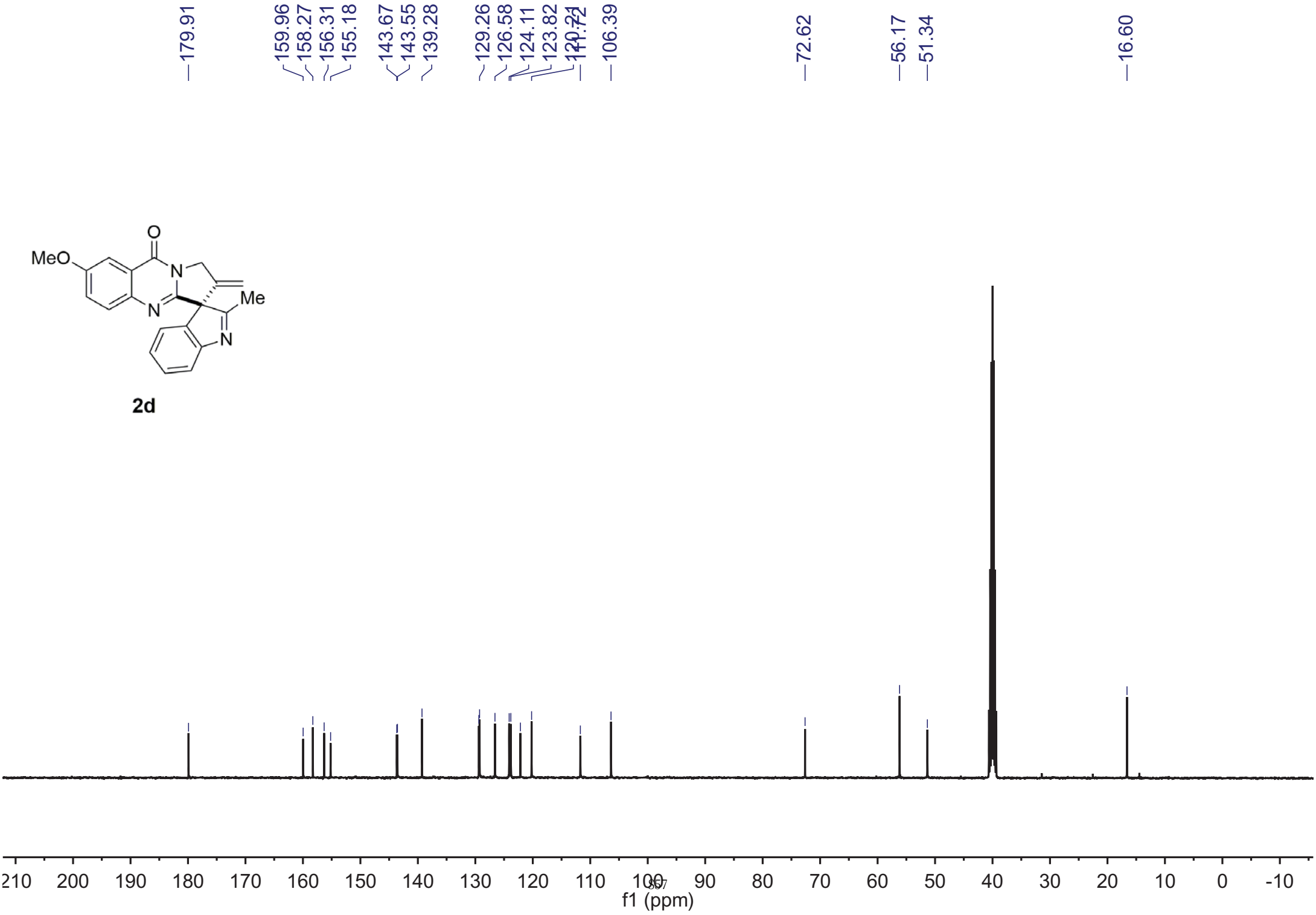
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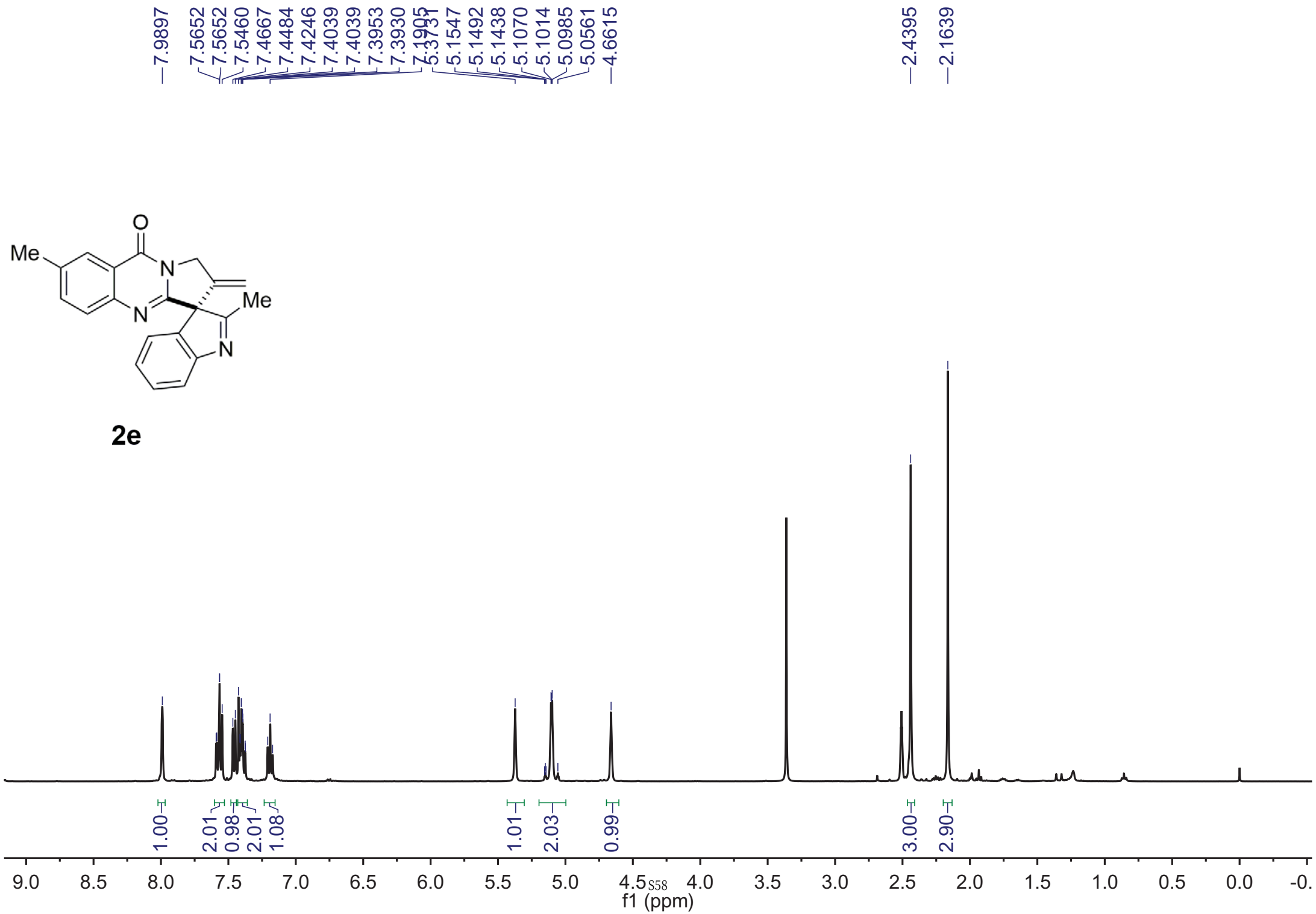
f1 (ppm)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Me
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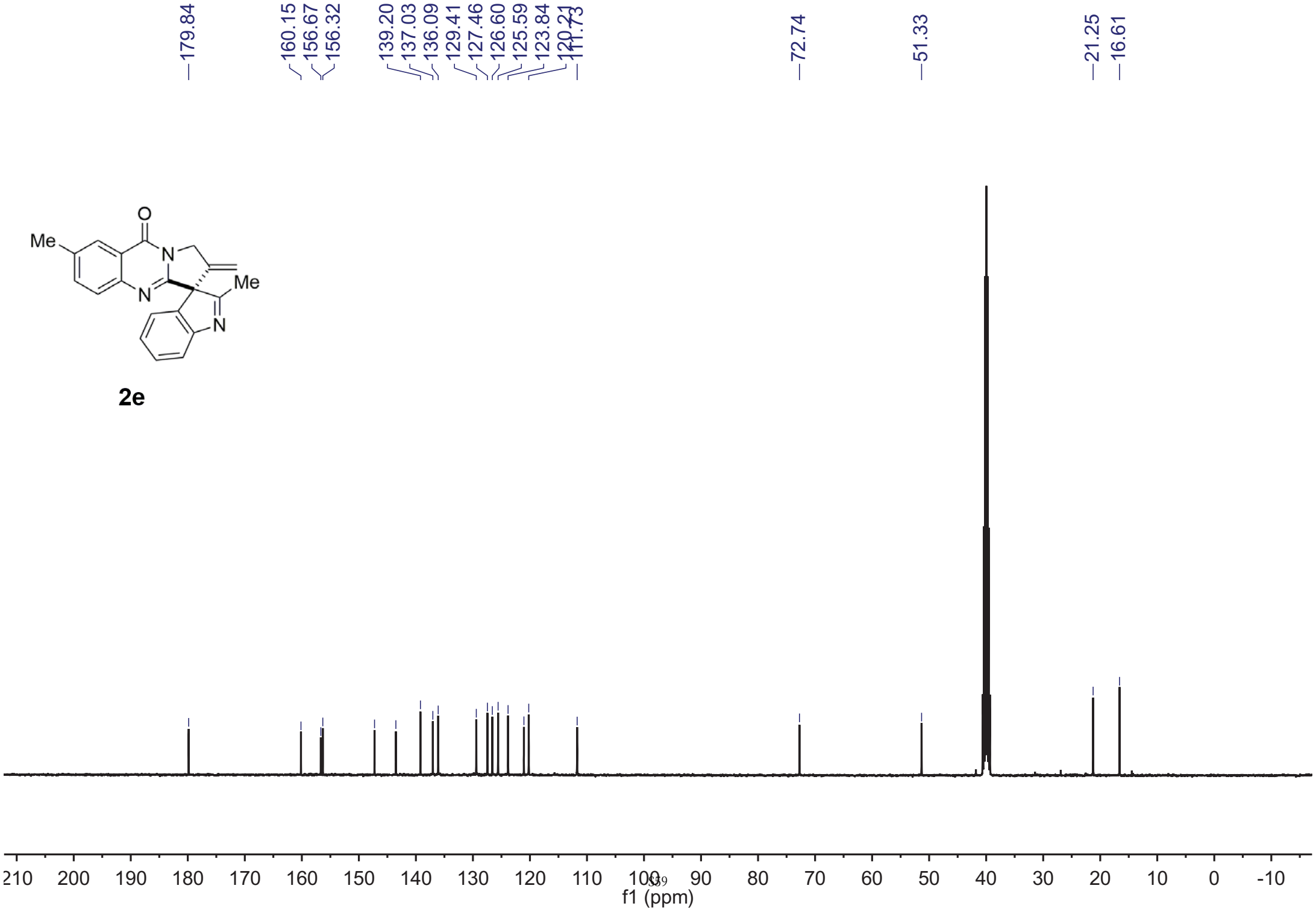
2e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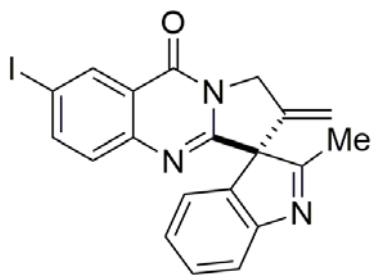
f1 (ppm)



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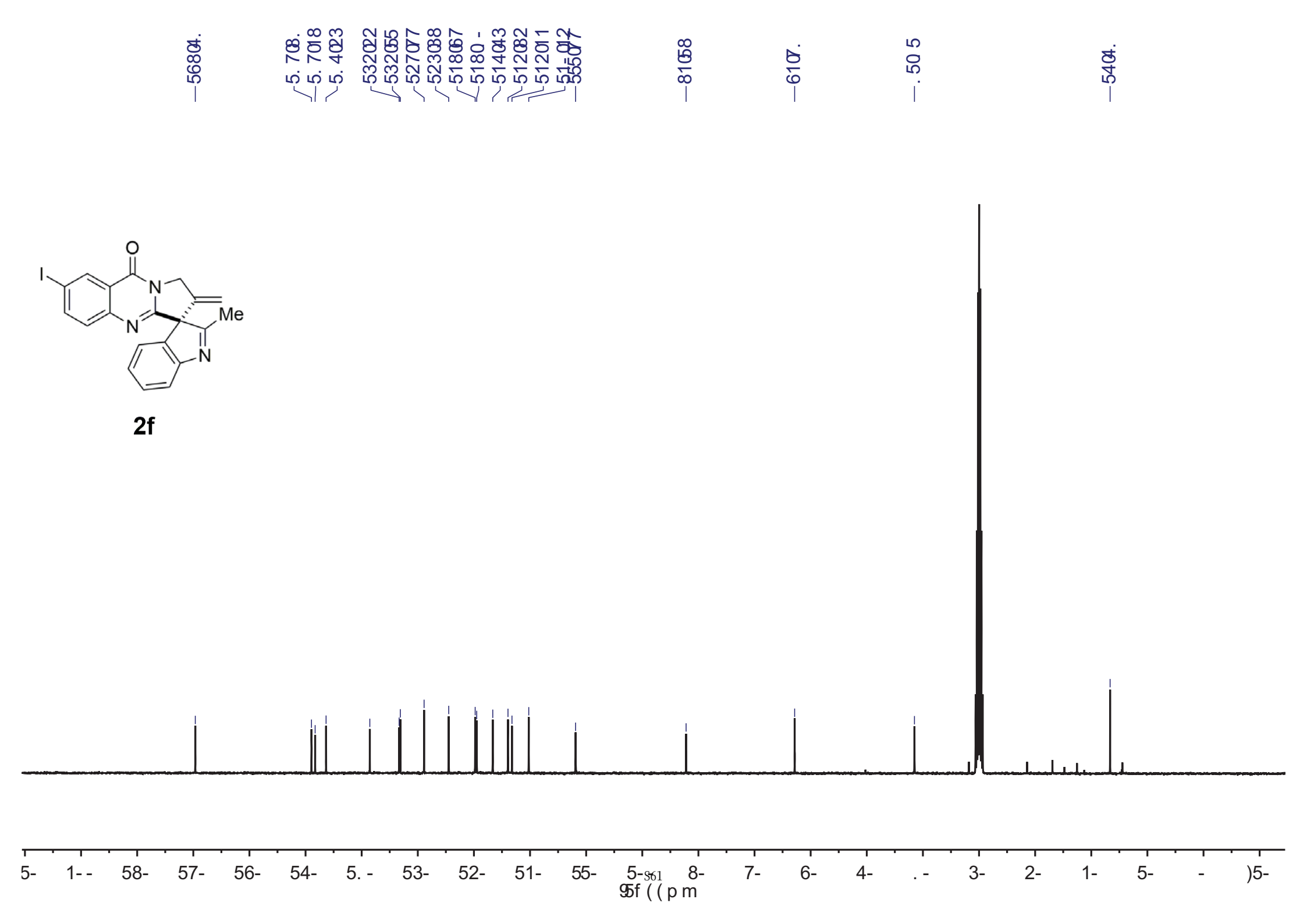
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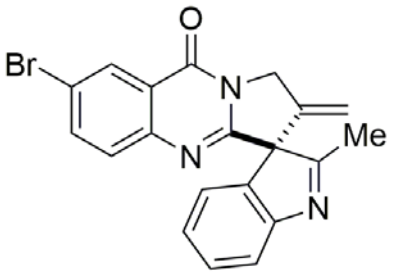

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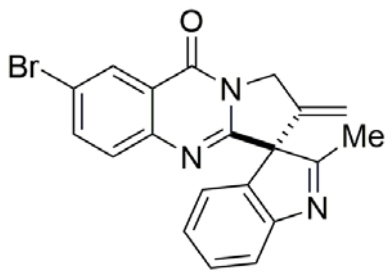

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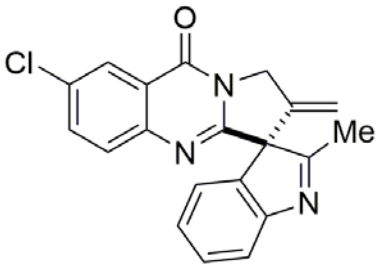

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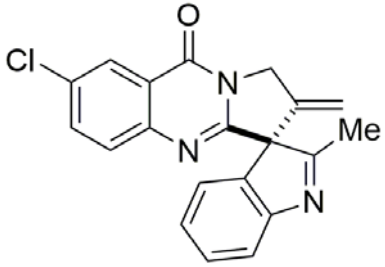
O
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2h

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129.50
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122.68
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16.65
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
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40
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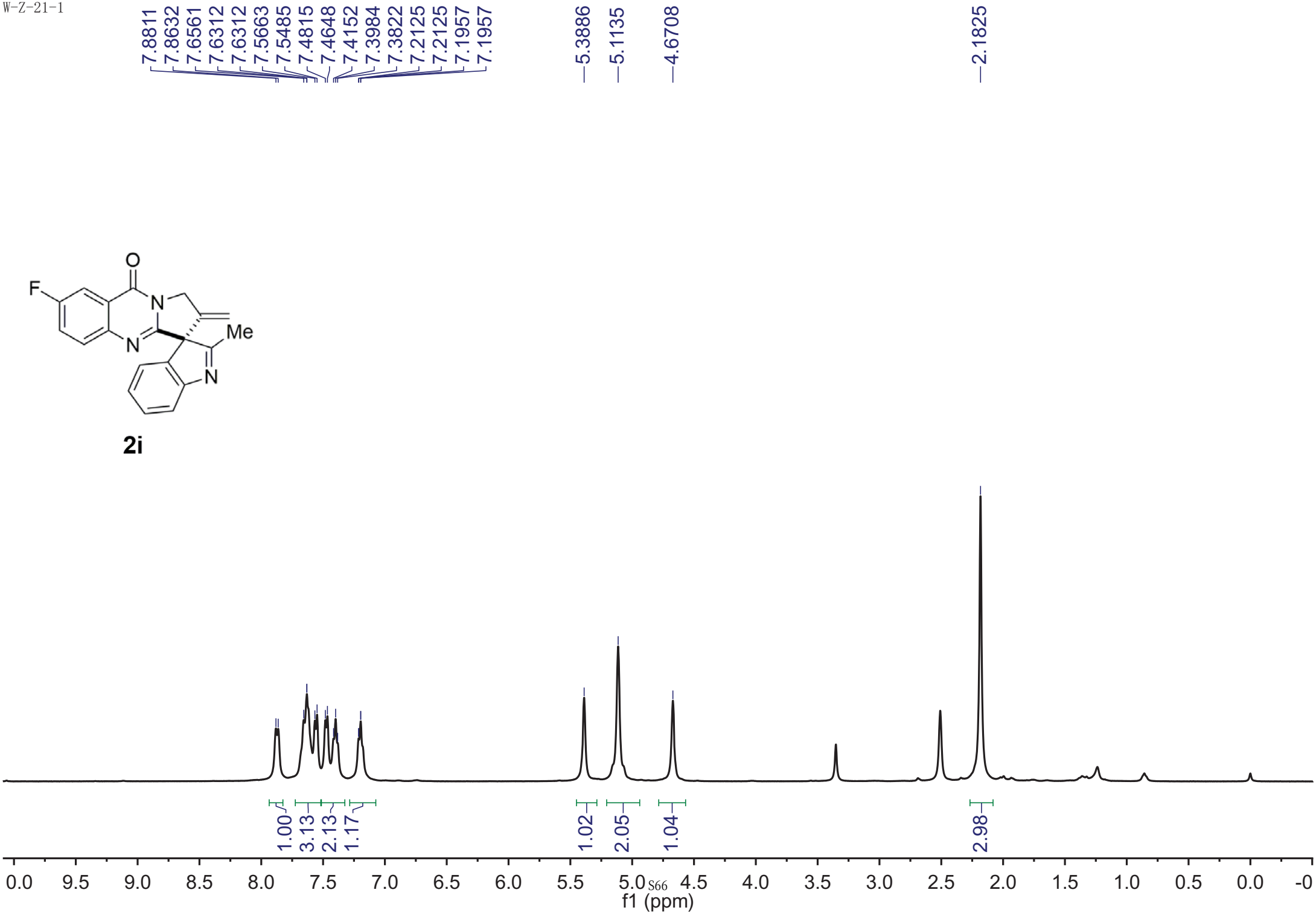
20
10
0
-10
f1 (ppm)

W-Z-21-1

O
F
N
N
Me
N

2i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7.2125
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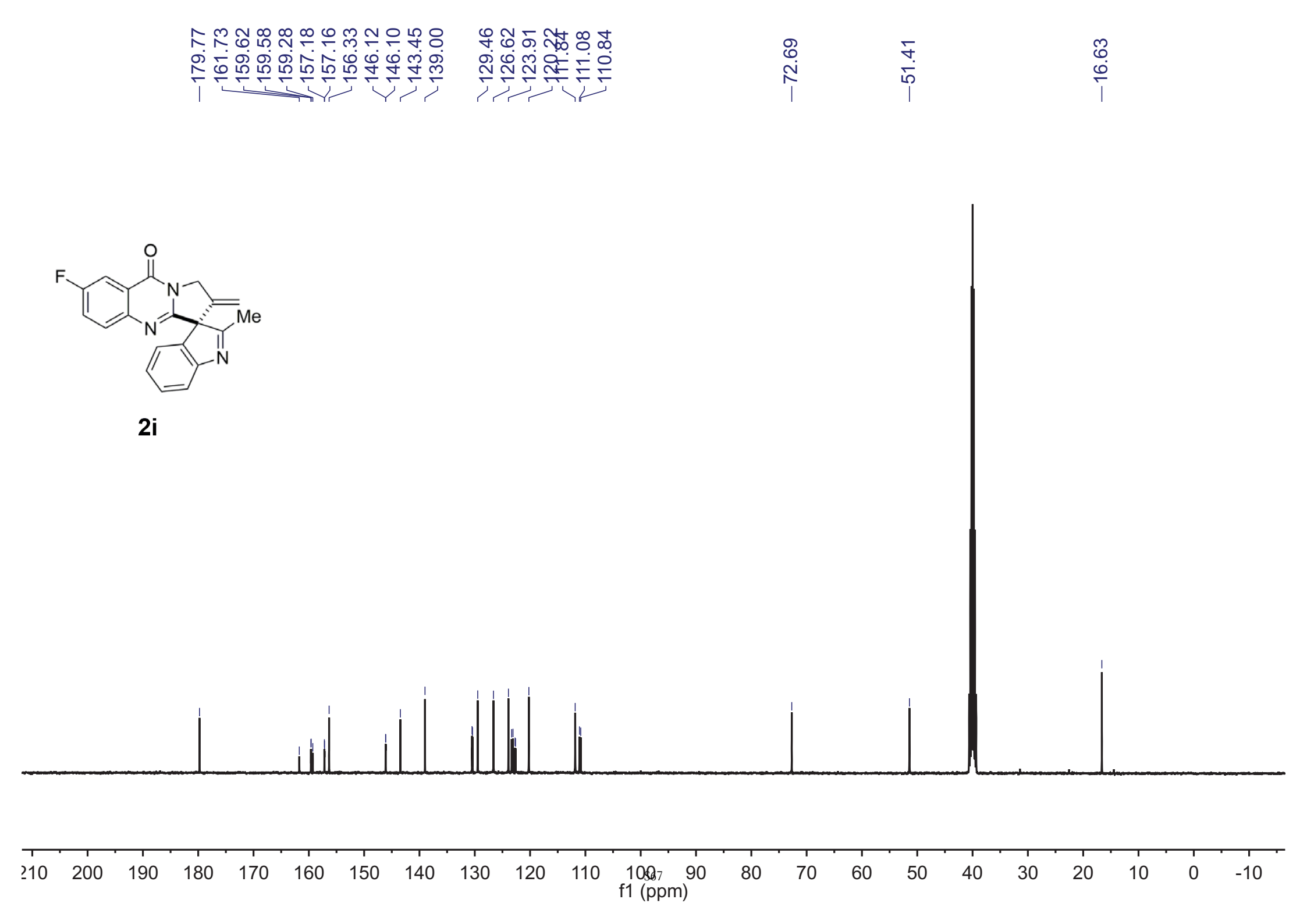
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F
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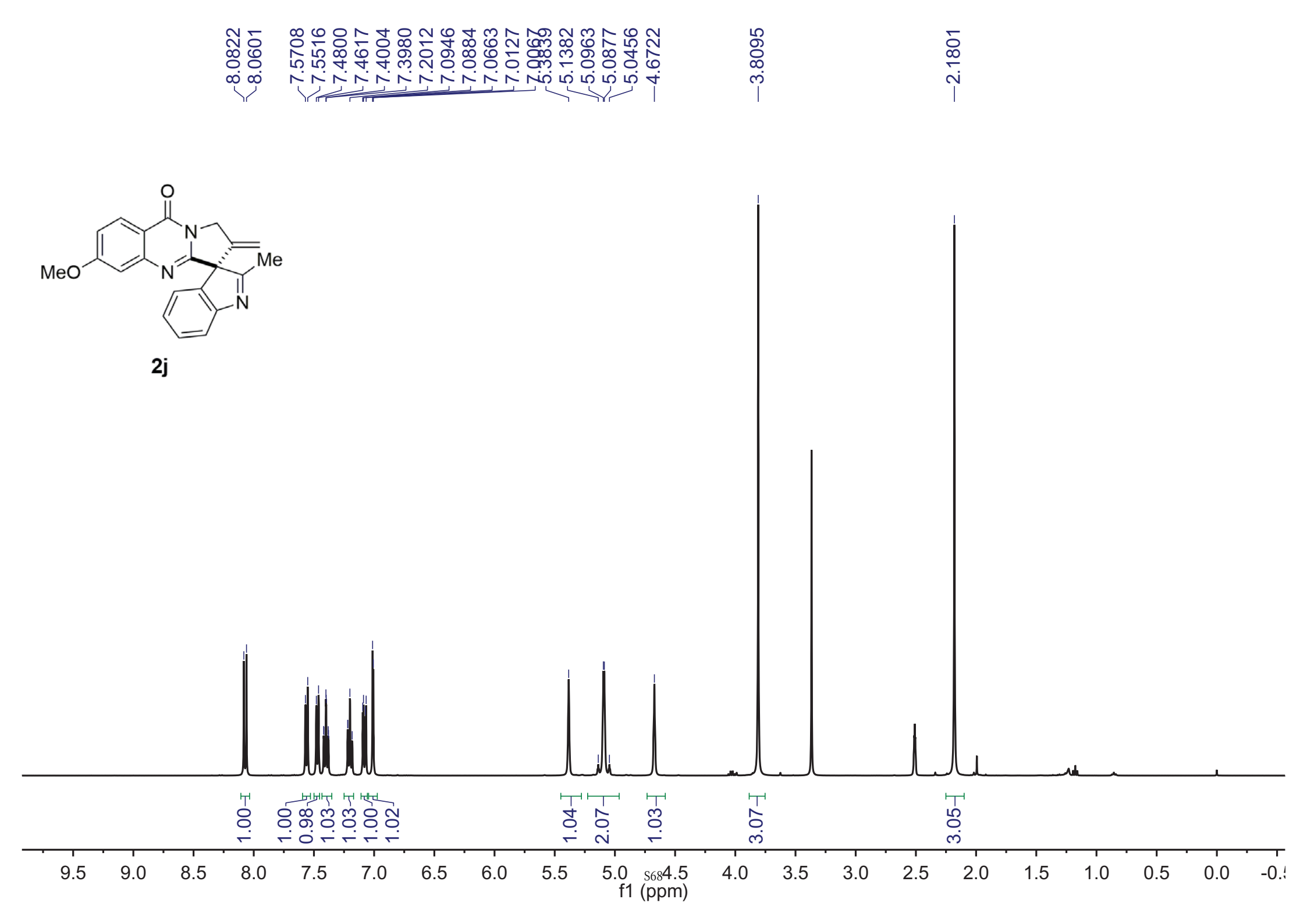
Me
N
2i
f1 (ppm)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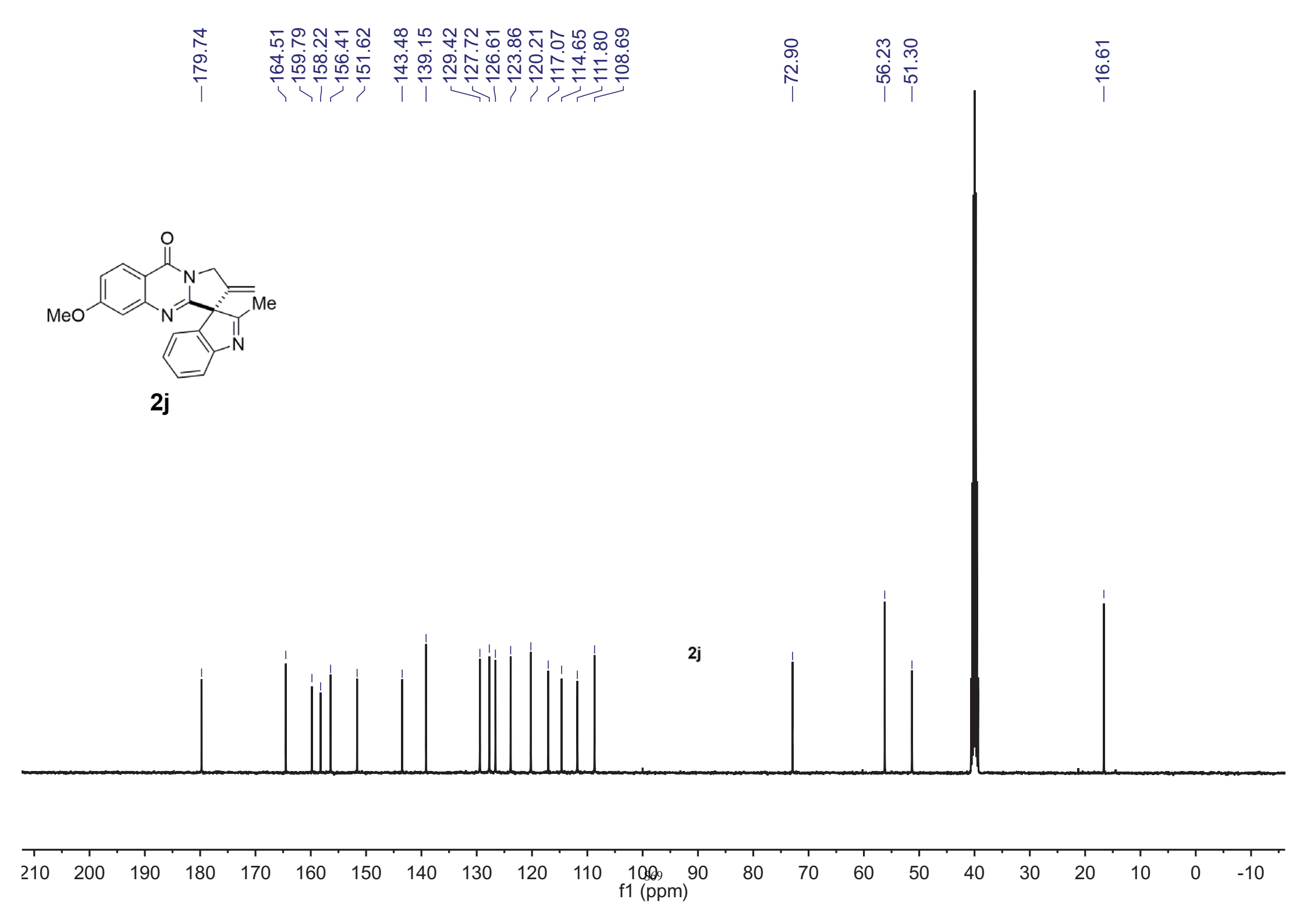
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16.61
O
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MeO
N
Me
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2j
2j
210
200
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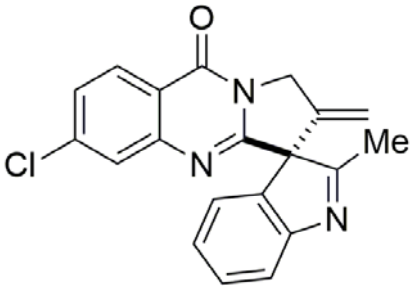
f1 (ppm)



2k

O
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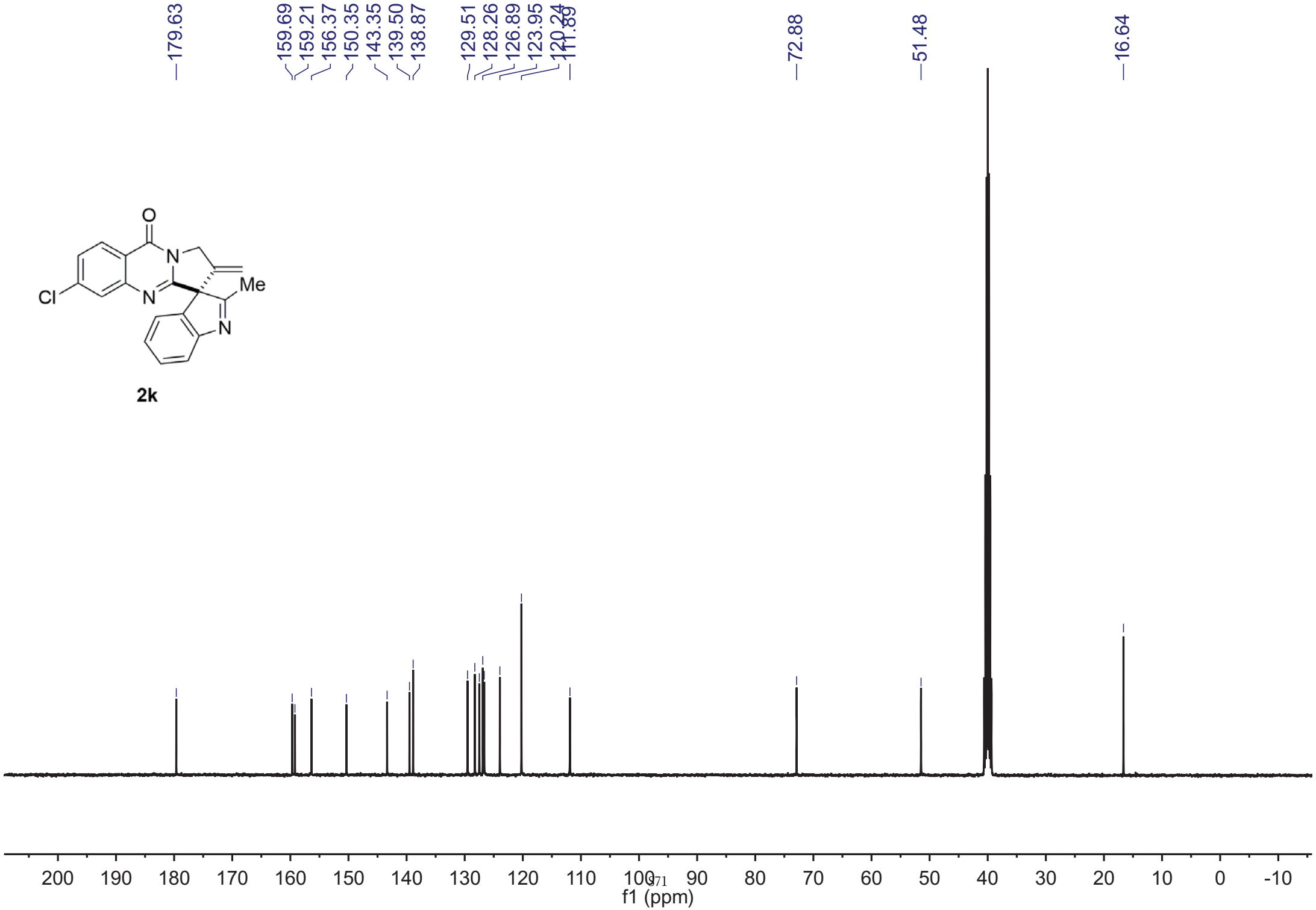
Cl
N
Me
N

2k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30
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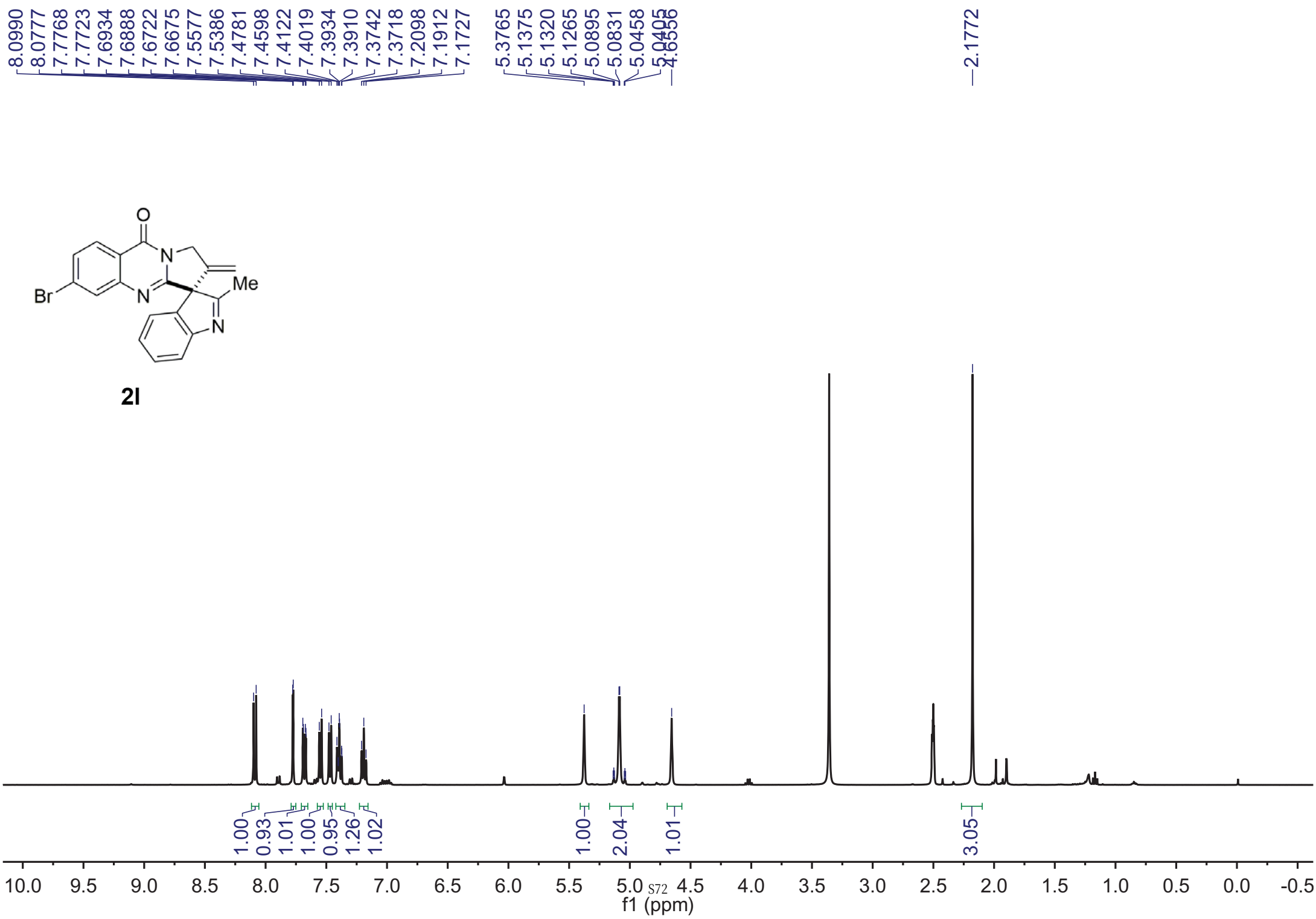
0
-10
f1 (ppm)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5.1320
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5.0831
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Br
Me
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2l
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1.00
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1.00
2.04
1.01
3.05
10.0
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9.0
8.5
8.0
7.5
7.0
6.5
6.0
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2.0
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0.5
0.0
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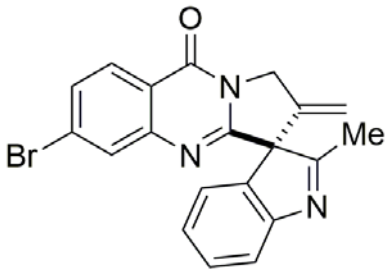
f1 (ppm)



2l

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129.51
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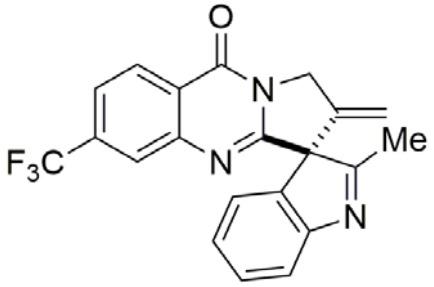
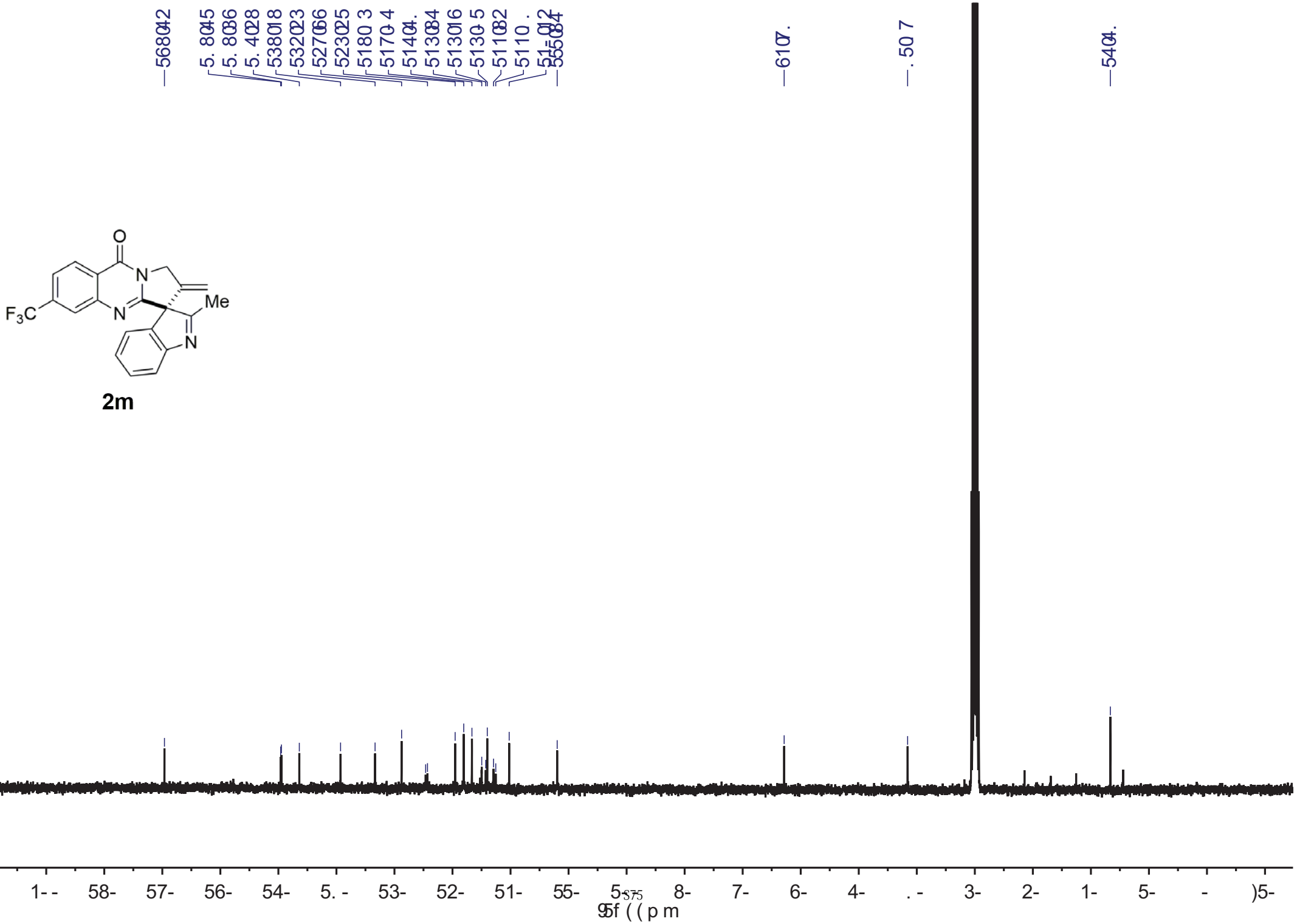
123.95
120.23
111.89
72.87
51.49
16.64

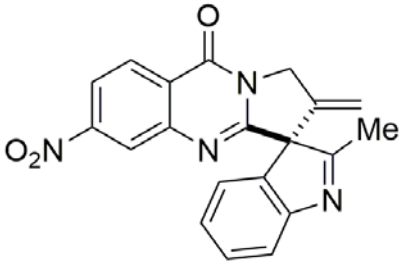
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

f1 (ppm)

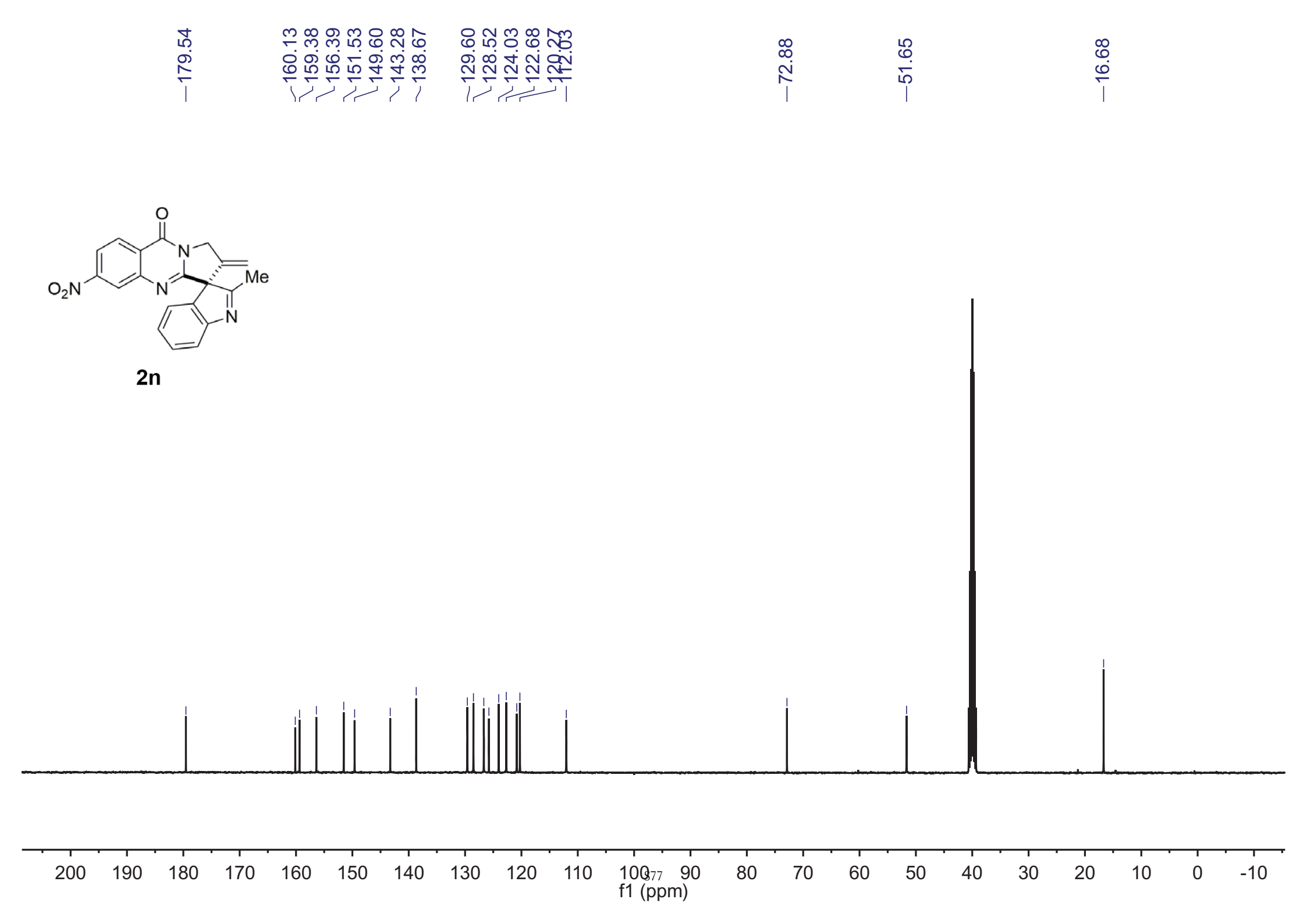


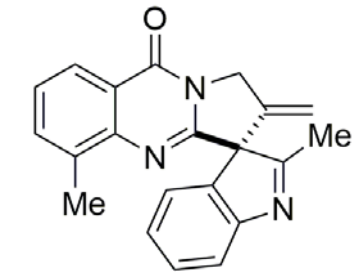
2m


O
N
N
F3C
Me
N
2m

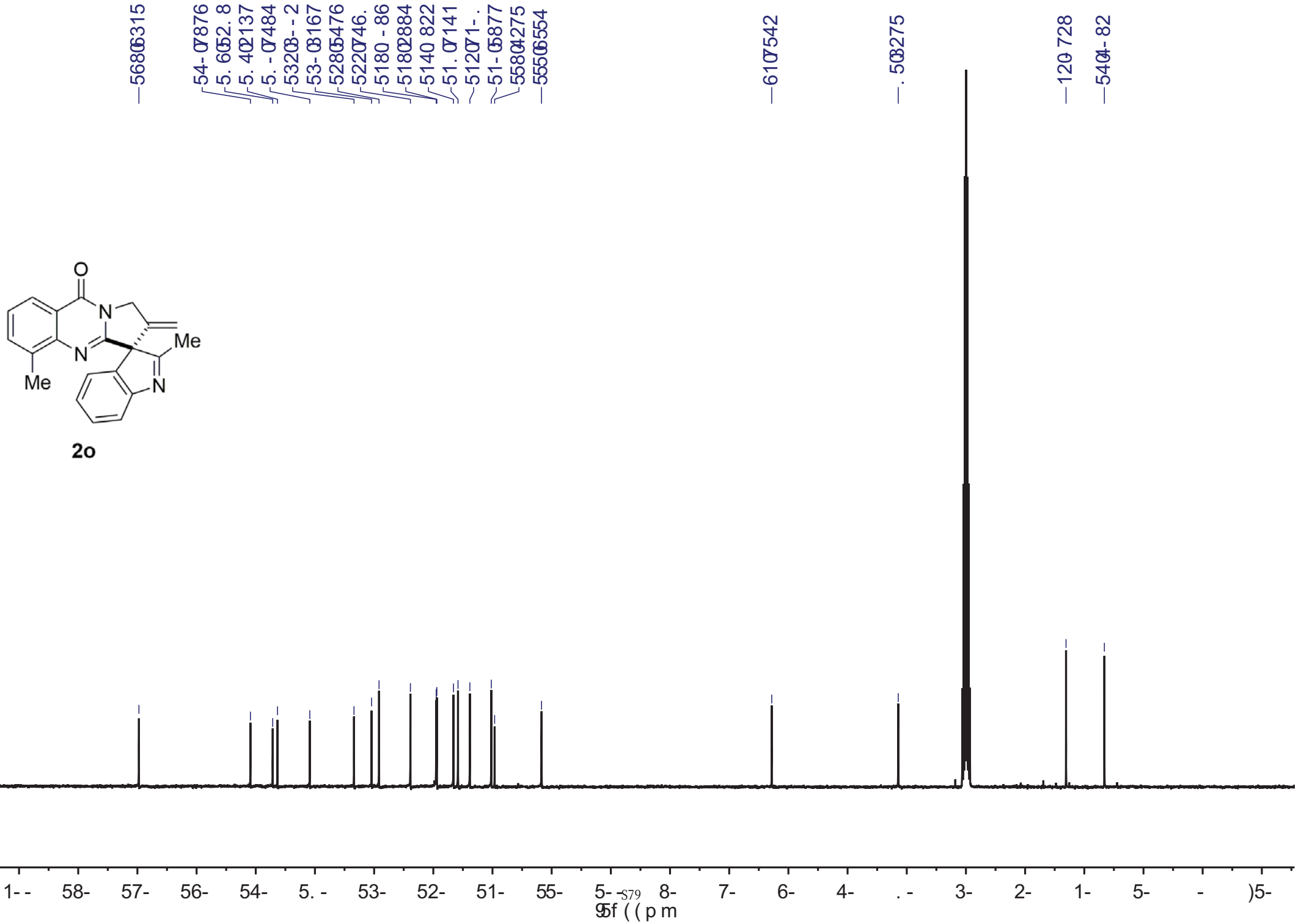


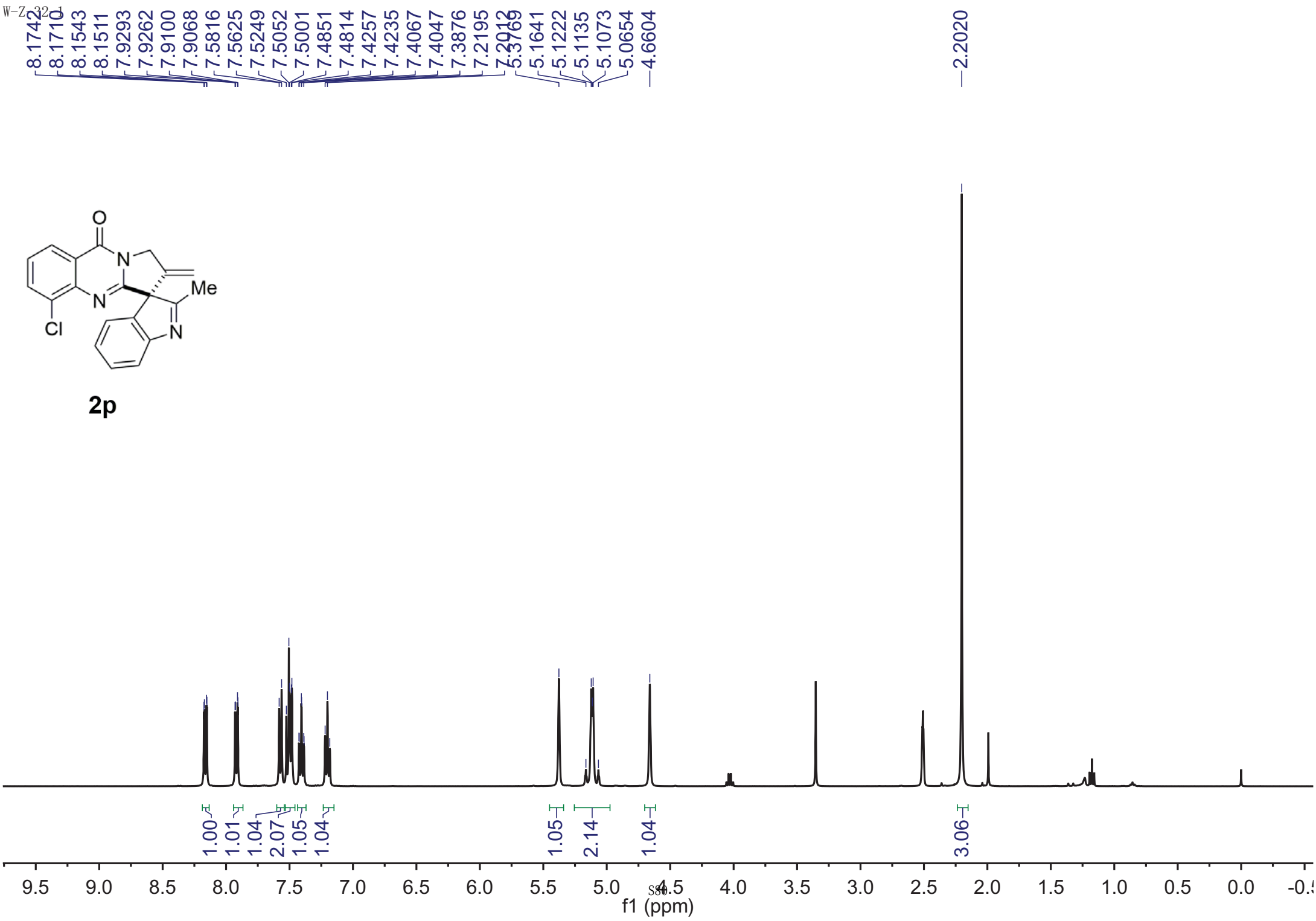
2n


179.54
160.13
159.38
156.39
151.53
149.60
143.28
138.67
129.60
128.52
124.03
122.68
120.27
112.03
72.88
51.65
16.68
O
N
N
N
Me
O_2N
2n
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

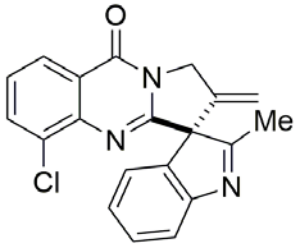


2o


O
N
N
Me
Me
N
2o

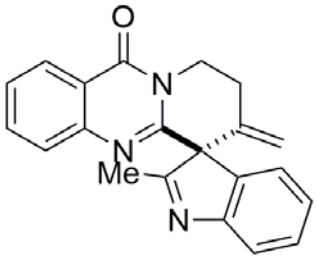

W-Z-32-1
8.1742
8.1710
8.1543
8.1511
7.9293
7.9262
7.9100
7.9068
7.5816
7.5625
7.5249
7.5052
7.5001
7.4851
7.4814
7.4257
7.4235
7.4067
7.4047
7.3876
7.2195
5.1641
5.1222
5.1135
5.1073
5.0654
4.6604
2.2020
O
N
N
Me
Cl
N
2p
1.00
1.01
1.04
2.07
1.05
1.04
1.05
2.14
1.04
3.06
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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)

W-Z-32-1

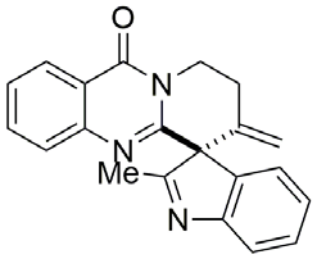

O
N
N
Me
Cl
N

2p

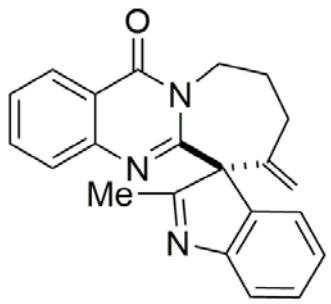
179.58
159.74
158.57
156.18
139.00
135.03
131.01
129.48
127.59
126.61
125.49
123.85
123.22
120.30
111.67
73.01
51.48
16.69
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)



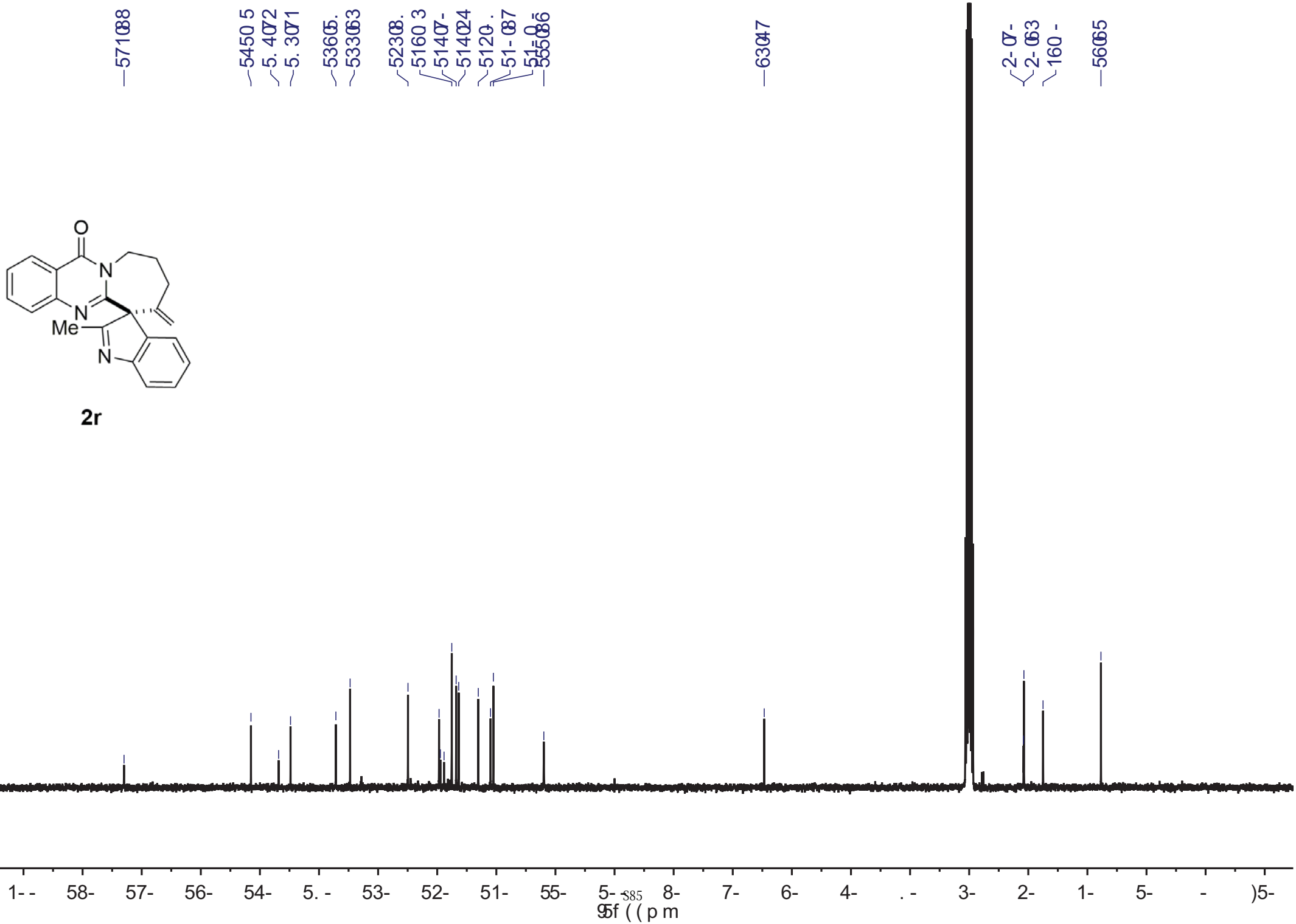
2q

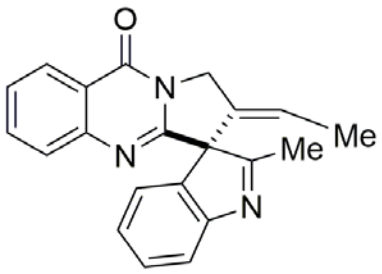


2q

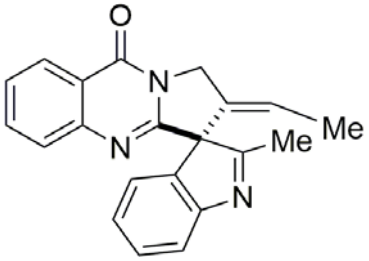


2r

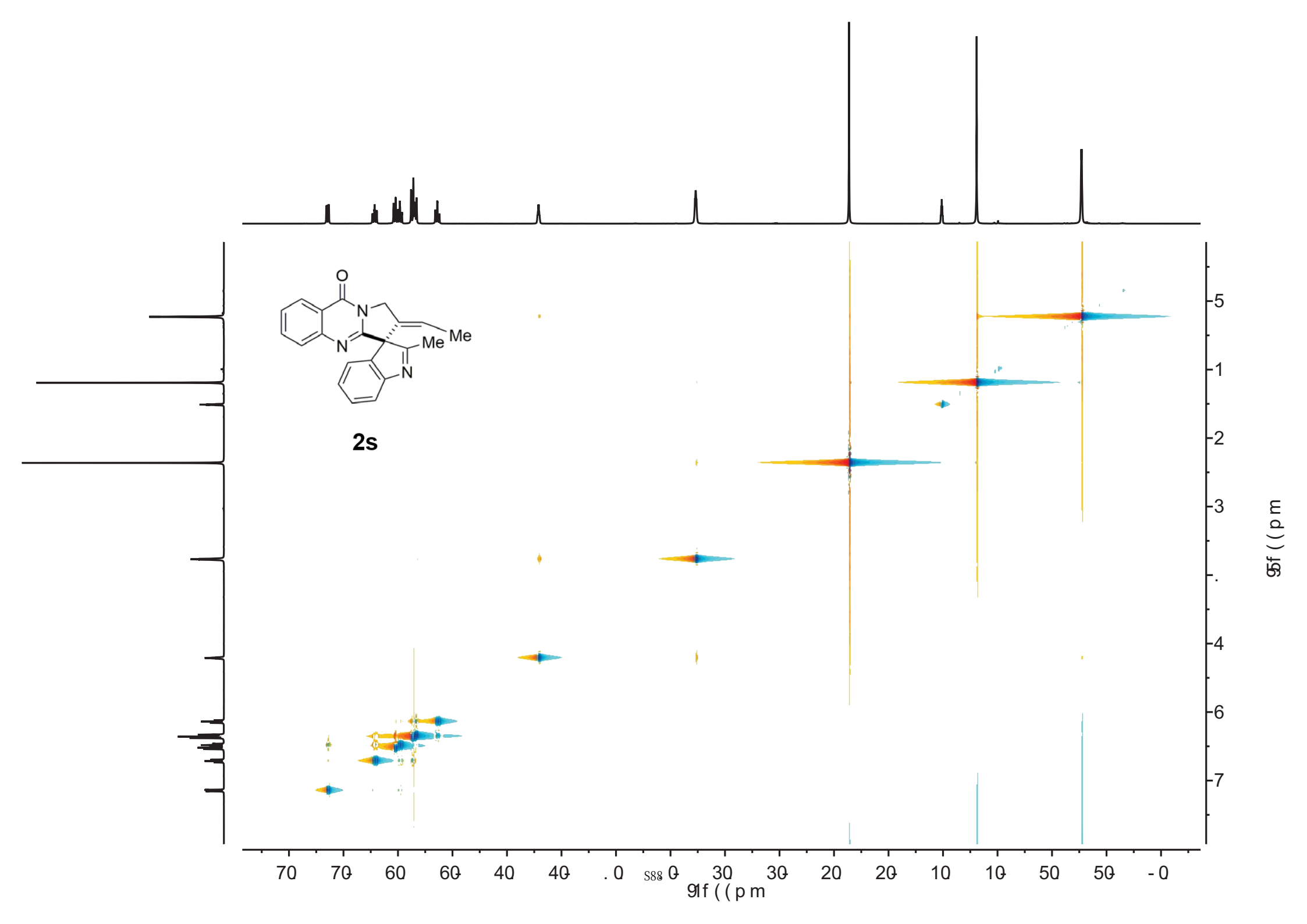

O
N
N
Me
N
2r

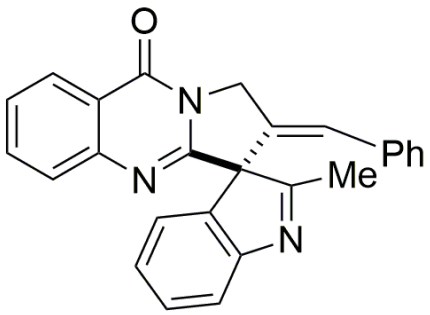


2s

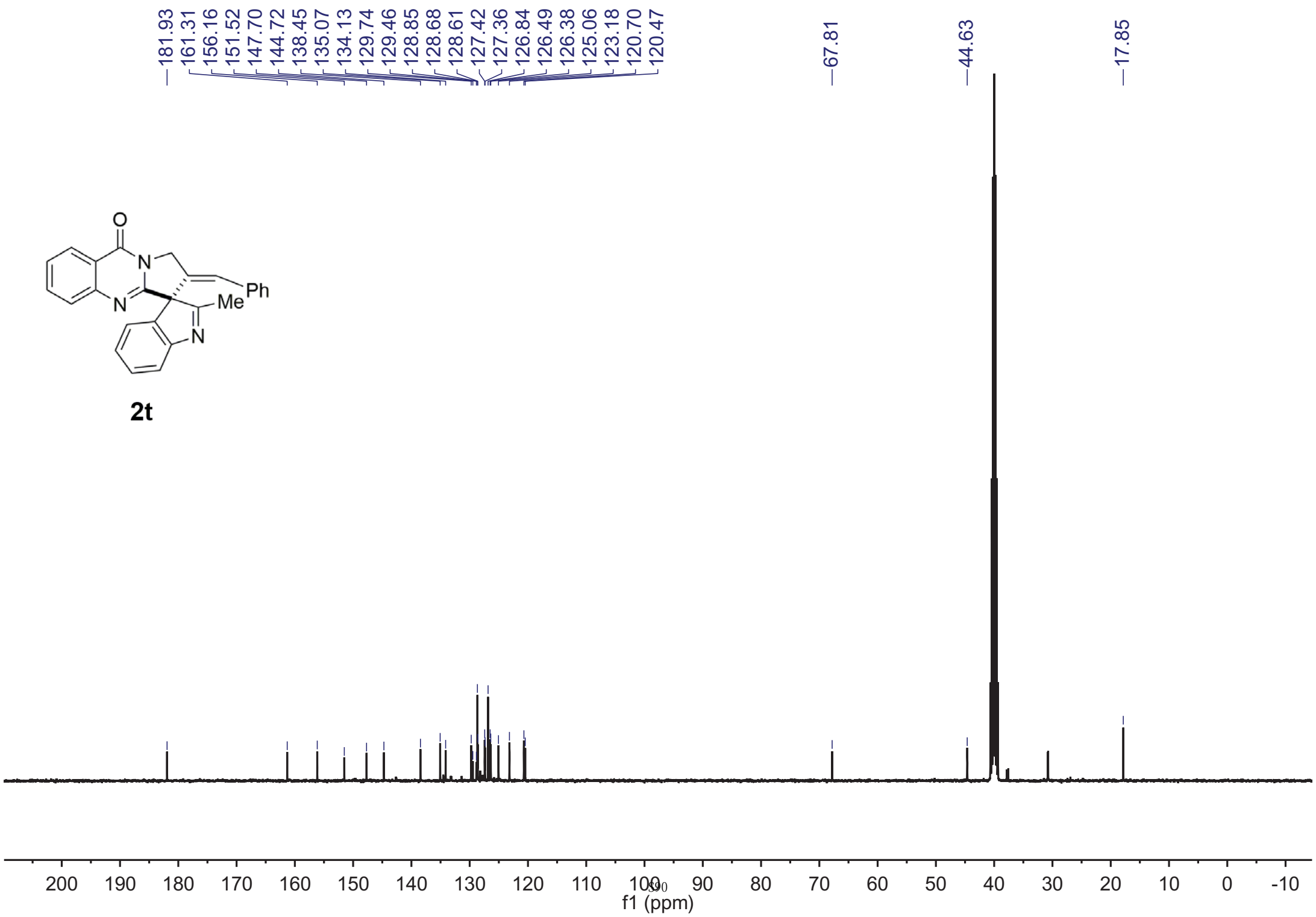


2s


O
N
N
Me
Me
N
2s

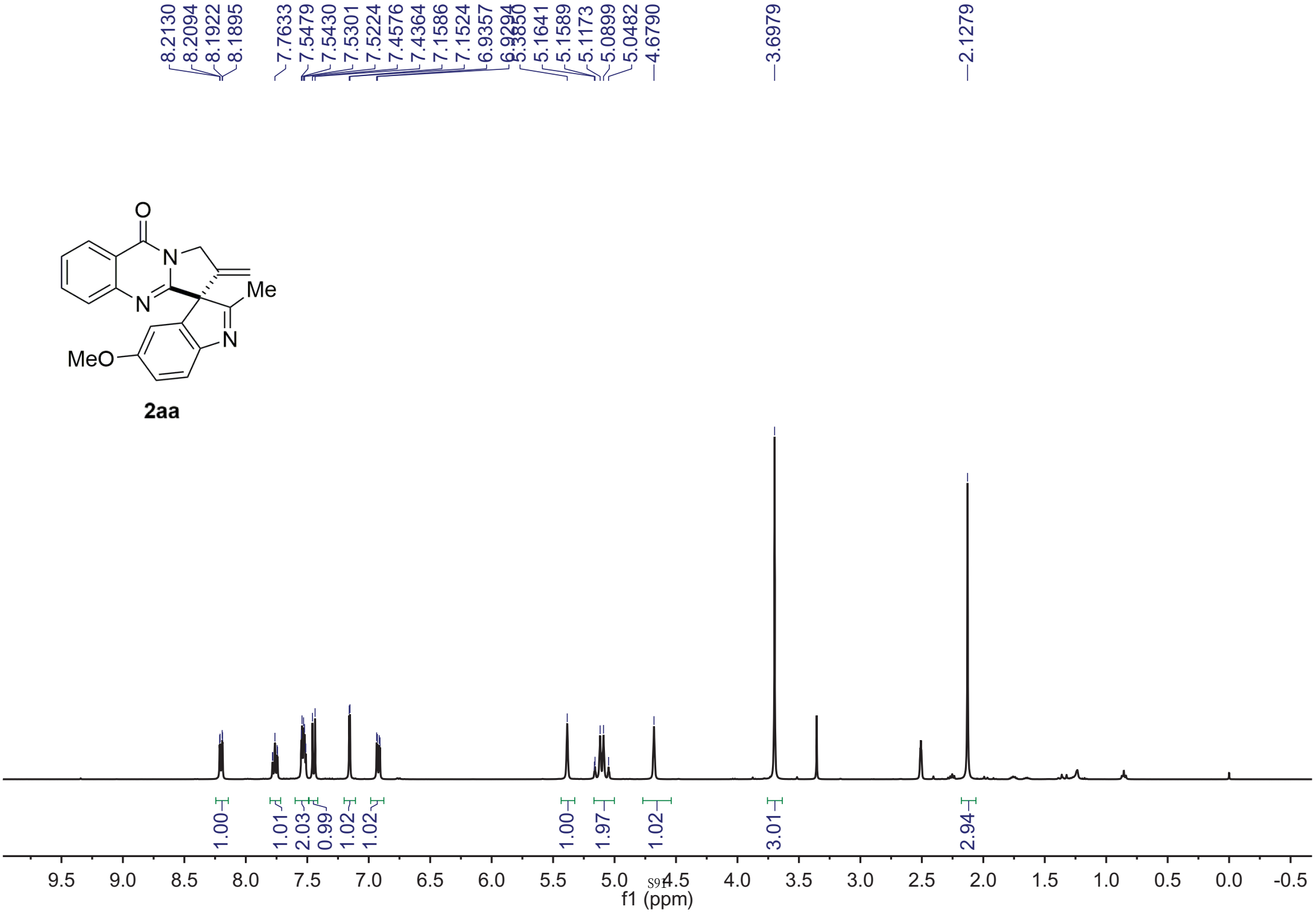


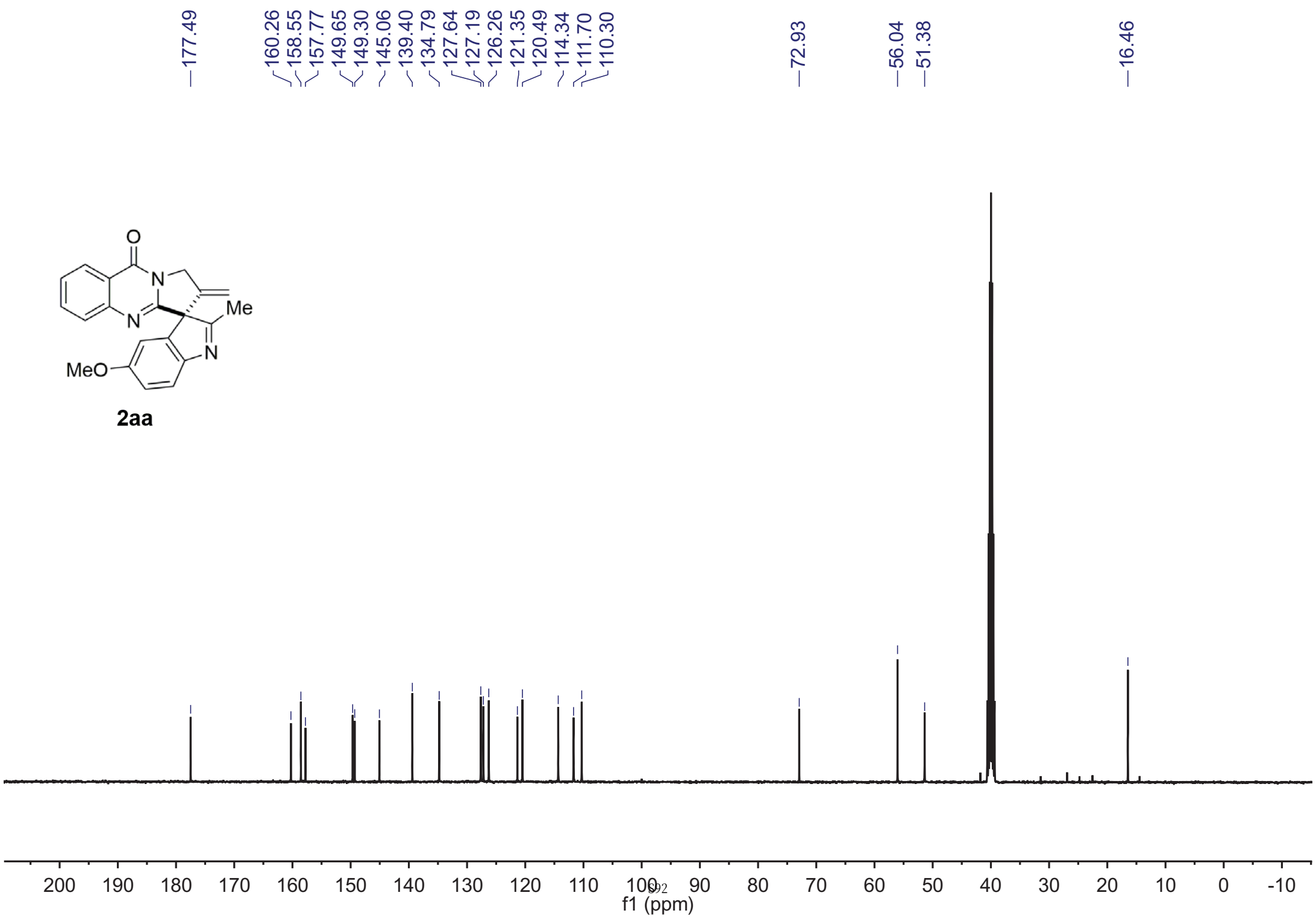
2t

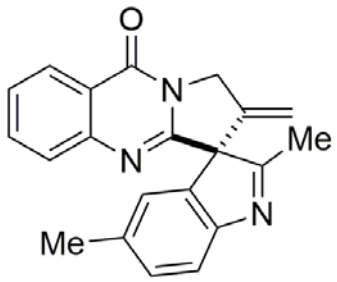

181.93
161.31
156.16
151.52
147.70
144.72
138.45
135.07
134.13
129.74
129.46
128.85
128.68
128.61
127.42
127.36
126.84
126.49
126.38
125.06
123.18
120.70
120.47
67.81
44.63
17.85
O
N
N
Me
Ph
N
2t
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

O
N
N
Me
N
MeO

2aa


8.2130
8.2094
8.1922
8.1895
7.7633
7.5479
7.5430
7.5301
7.5224
7.4576
7.4364
7.1586
7.1524
6.9357
6.9294
5.3850
5.1641
5.1589
5.1173
5.0899
5.0482
4.6790
3.6979
2.1279
1.00
1.01
2.03
0.99
1.02
1.02
1.00
1.97
1.02
3.01
2.94
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
-0.5
f1 (ppm)

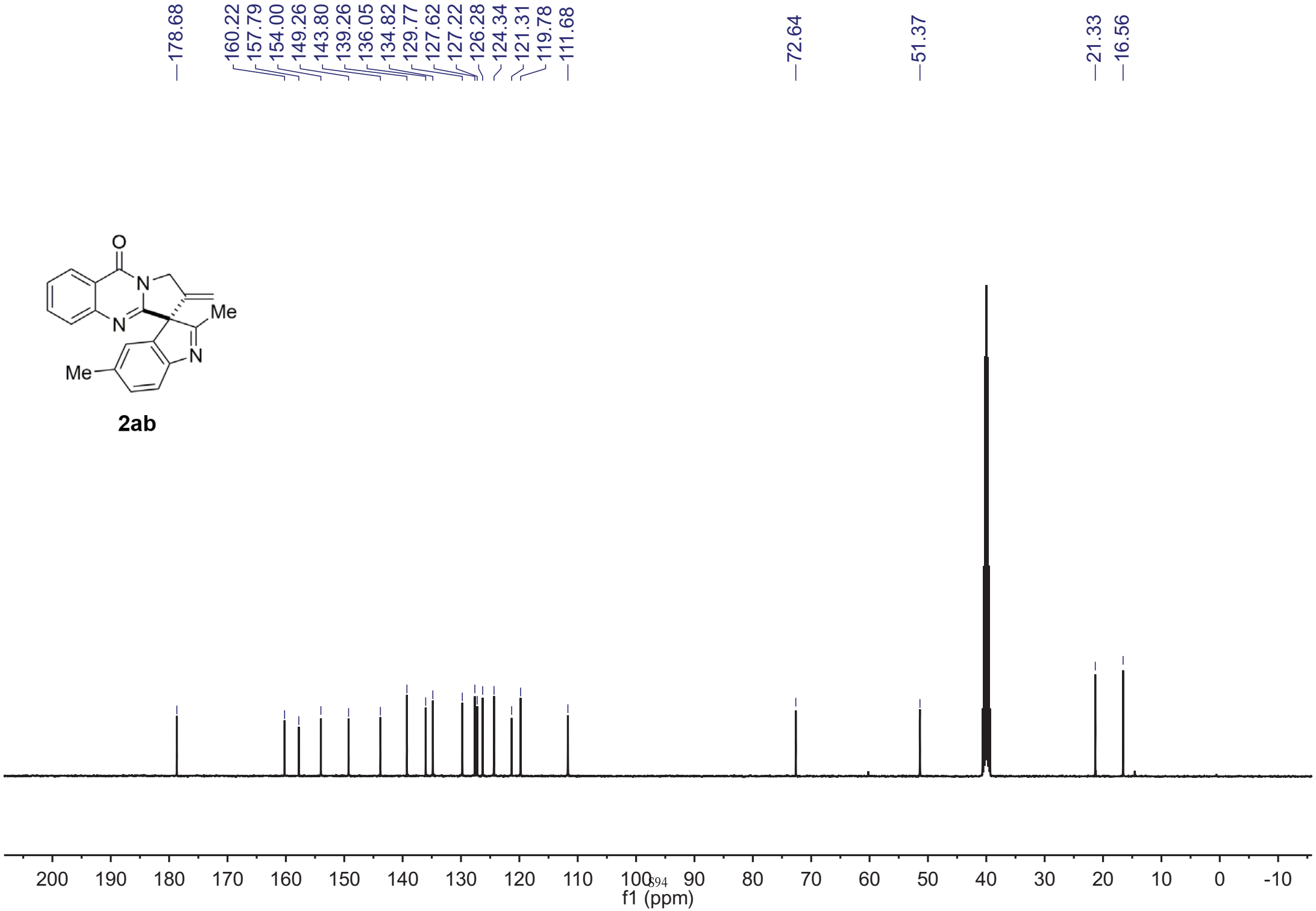

177.49
160.26
158.55
157.77
149.65
149.30
145.06
139.40
134.79
127.64
127.19
126.26
121.35
120.49
114.34
111.70
110.30
72.93
56.04
51.38
16.46
O
N
N
Me
N
MeO
2aa
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

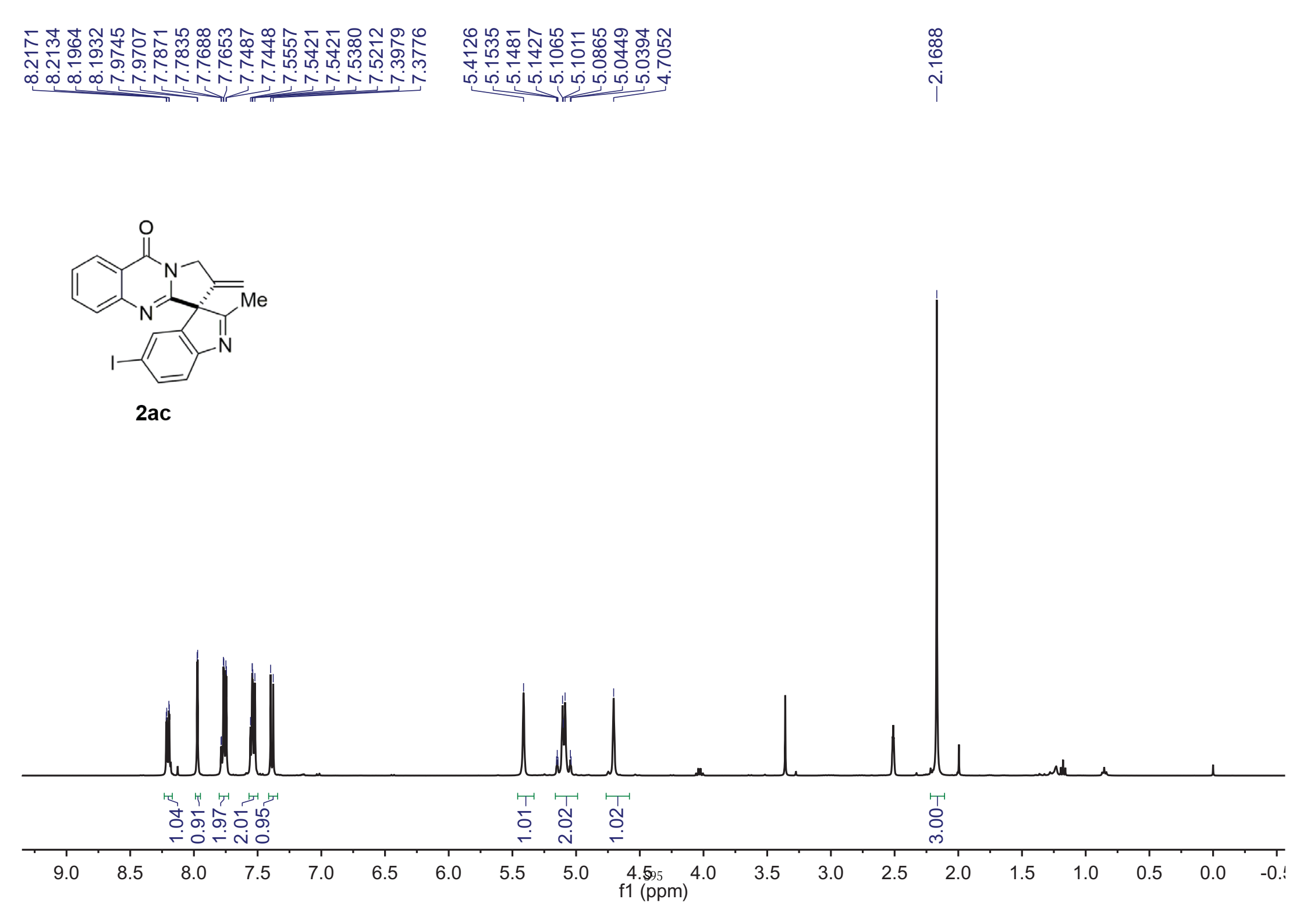


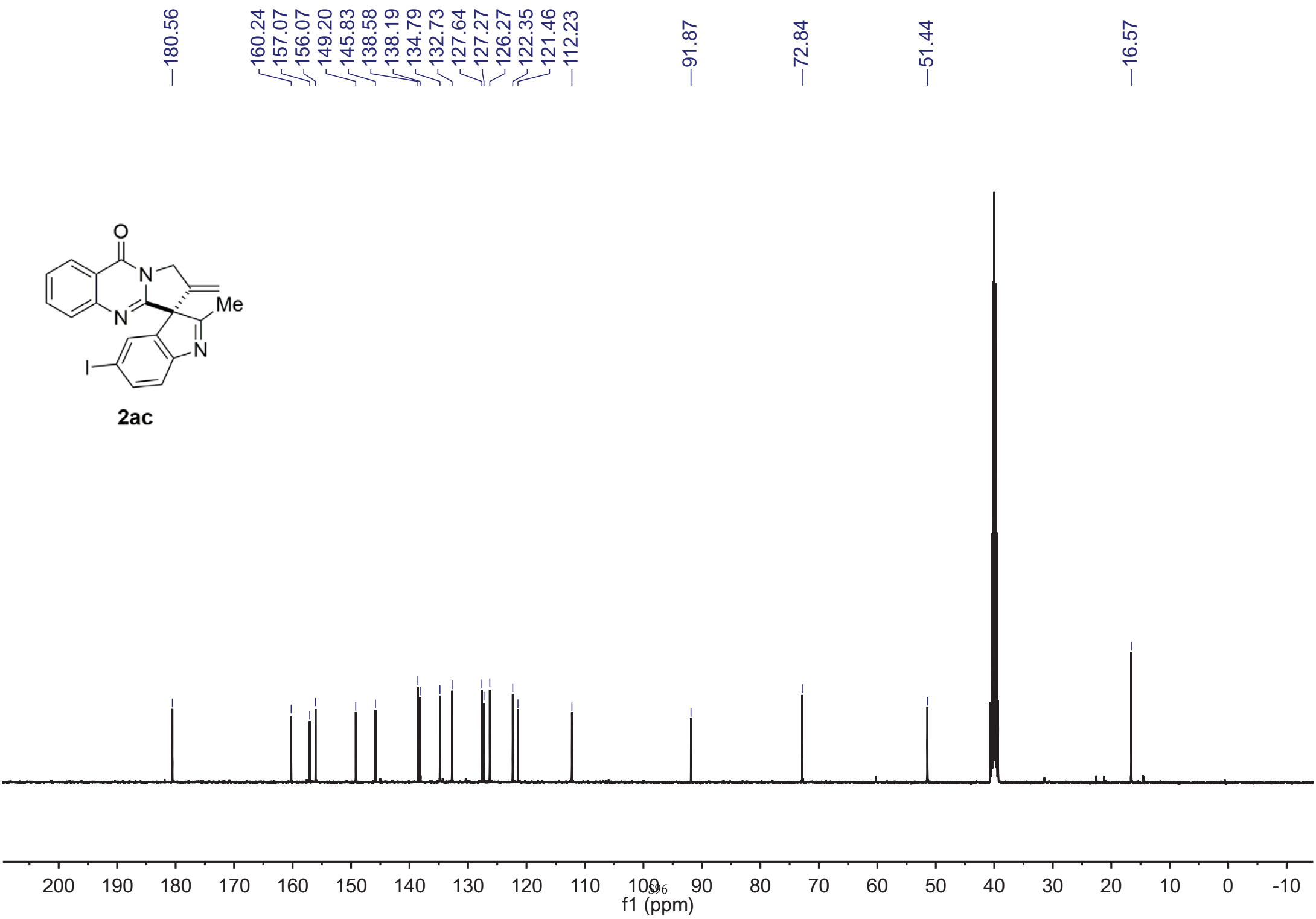
2ab

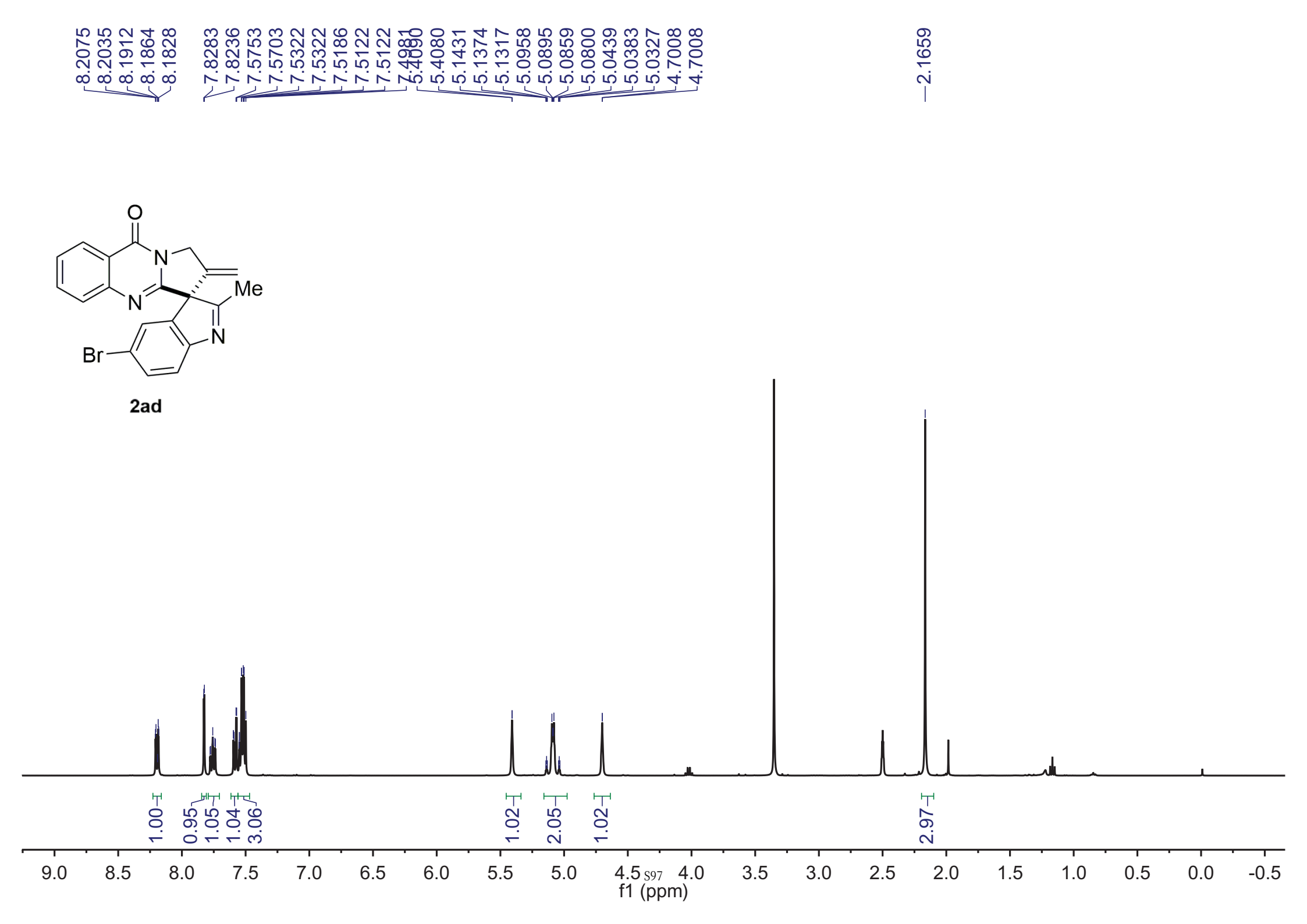
O
N
N
Me
N
Me

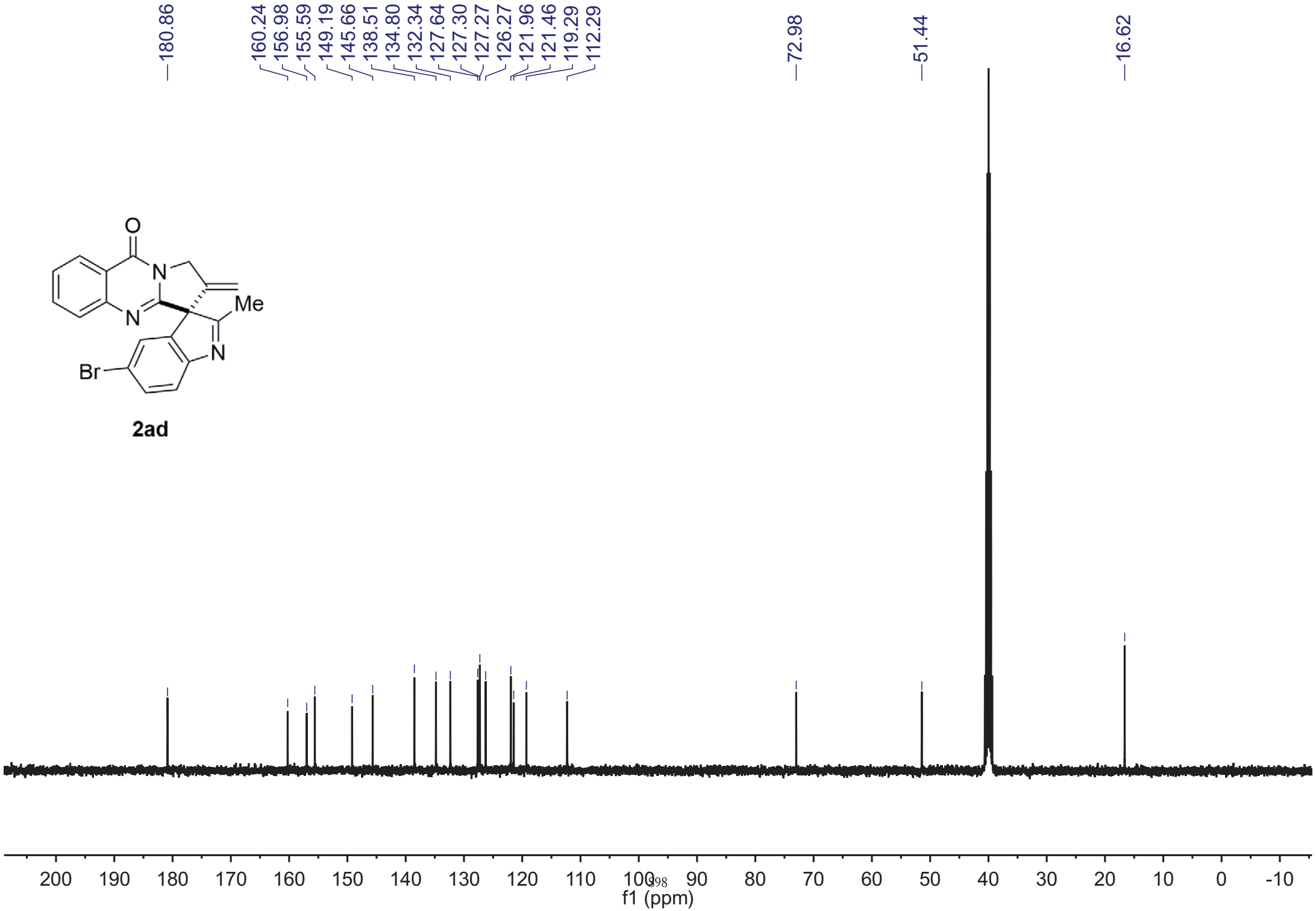
2ab


178.68
160.22
157.79
154.00
149.26
143.80
139.26
136.05
134.82
129.77
127.62
127.22
126.28
124.34
121.31
119.78
111.68
72.64
51.37
21.33
16.56
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


8.2171
8.2134
8.1964
8.1932
7.9745
7.9707
7.7871
7.7835
7.7688
7.7653
7.7487
7.7448
7.5557
7.5421
7.5421
7.5380
7.5212
7.3979
7.3776
5.4126
5.1535
5.1481
5.1427
5.1065
5.1011
5.0865
5.0449
5.0394
4.7052
2.1688
O
N
N
Me
N
I
2ac
1.04
0.91
1.97
2.01
0.95
1.01
2.02
1.02
3.00
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)


180.56
160.24
157.07
156.07
149.20
145.83
138.58
138.19
134.79
132.73
127.64
127.27
126.27
122.35
121.46
112.23
91.87
72.84
51.44
16.57
O
N
N
Me
N
I
2ac
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


8.2075
8.2035
8.1912
8.1864
8.1828
7.8283
7.8236
7.5753
7.5703
7.5322
7.5322
7.5186
7.5122
7.5122
7.4981
5.4080
5.4080
5.1431
5.1374
5.1317
5.0958
5.0895
5.0859
5.0800
5.0439
5.0383
5.0327
4.7008
4.7008
2.1659
O
N
N
Me
N
Br
2ad
1.00
0.95
1.05
1.04
3.06
1.02
2.05
1.02
2.97
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
-0.5
f1 (ppm)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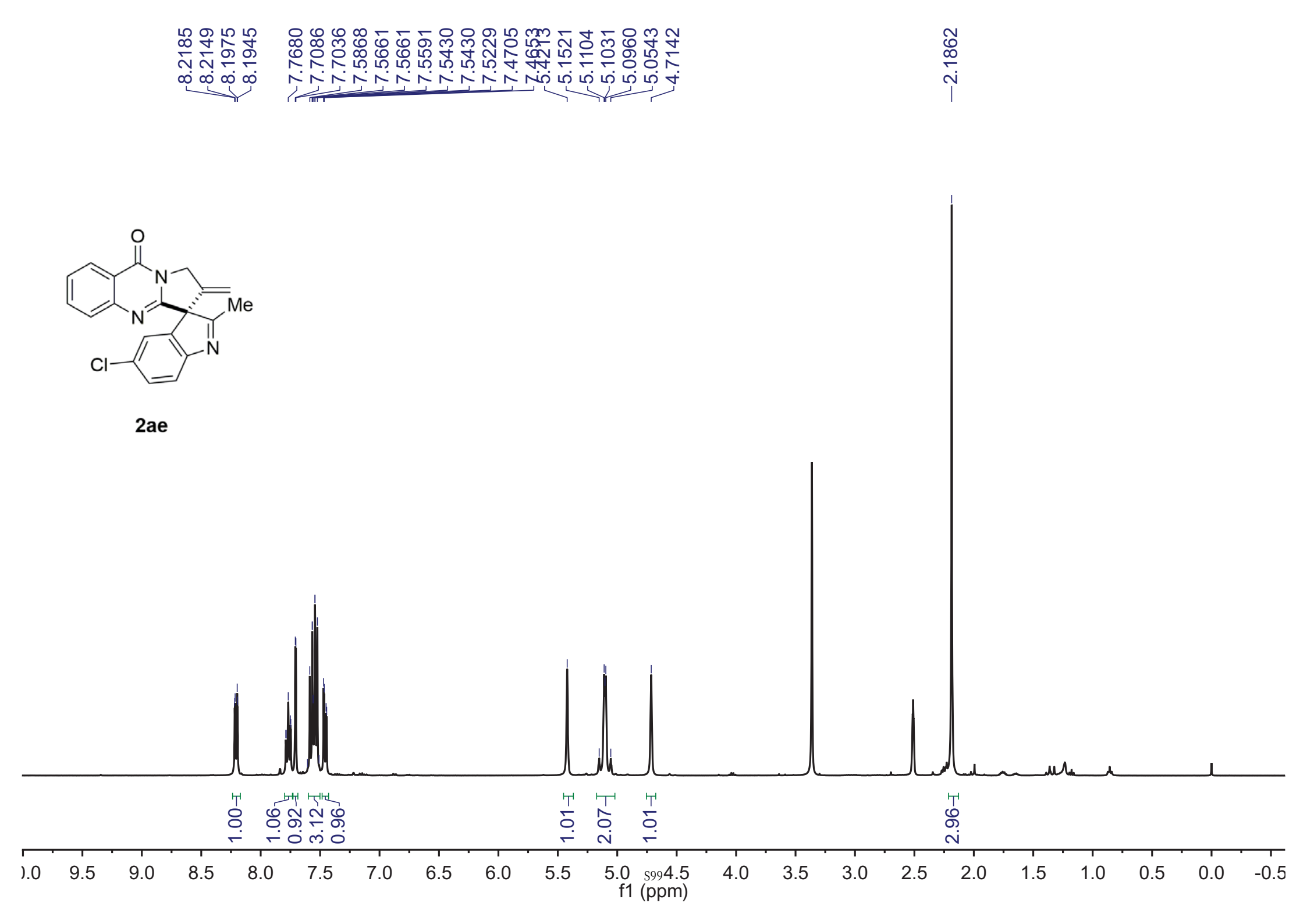
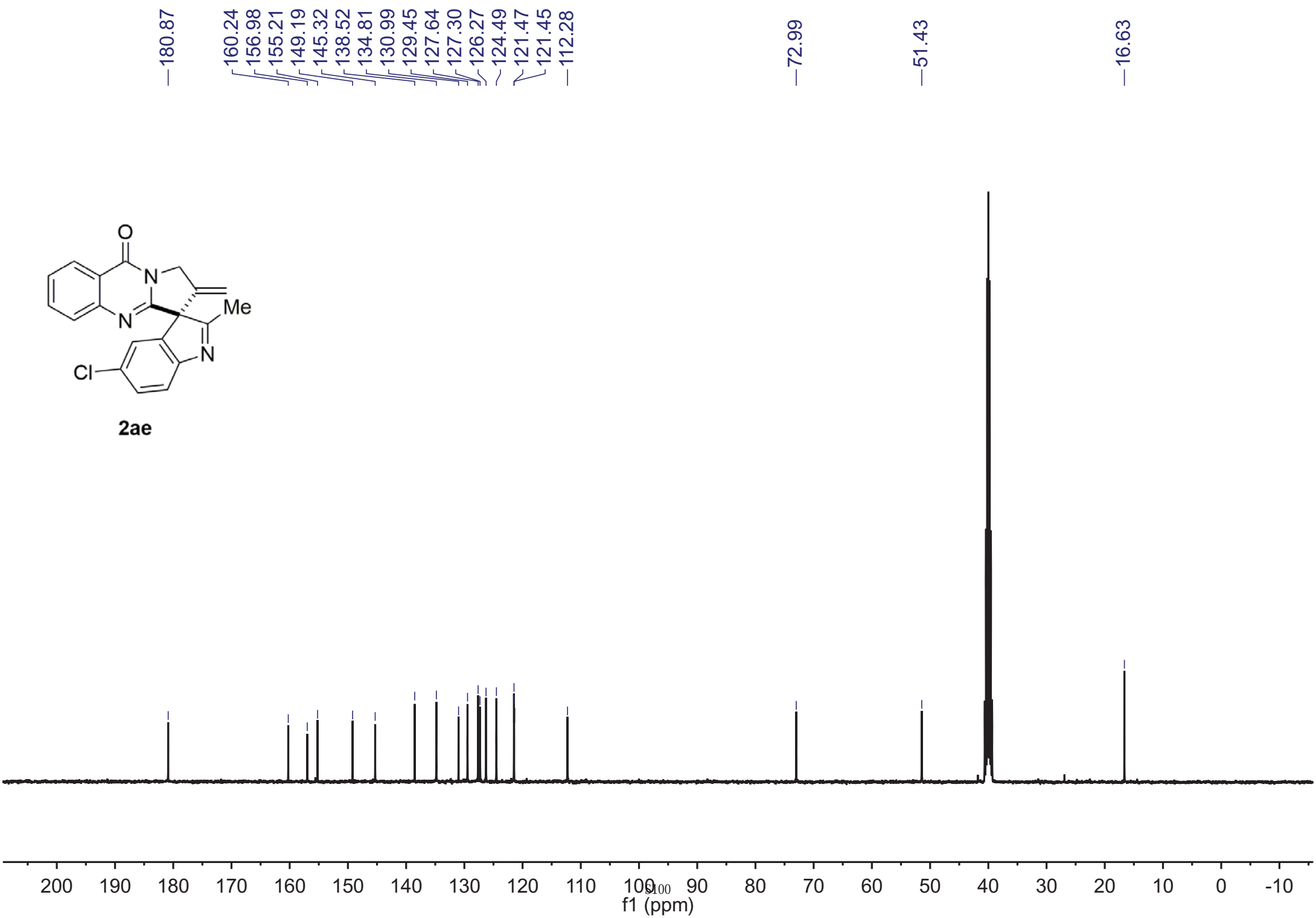
160.24
156.98
155.59
149.19
145.66
138.51
134.80
132.34
127.64
127.30
127.27
126.27
121.96
121.46
119.29
112.29
72.98
51.44
16.62
O
N
N
Me
N
Br
2ad
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


8.2185
8.2149
8.1975
8.1945
7.7680
7.7086
7.7036
7.5868
7.5661
7.5661
7.5591
7.5430
7.5430
7.5229
7.4705
5.1521
5.1104
5.1031
5.0960
5.0543
4.7142
2.1862
O
N
N
Me
N
Cl
2ae
1.00
1.06
0.92
3.12
0.96
1.01
2.07
1.01
2.96
f1 (ppm)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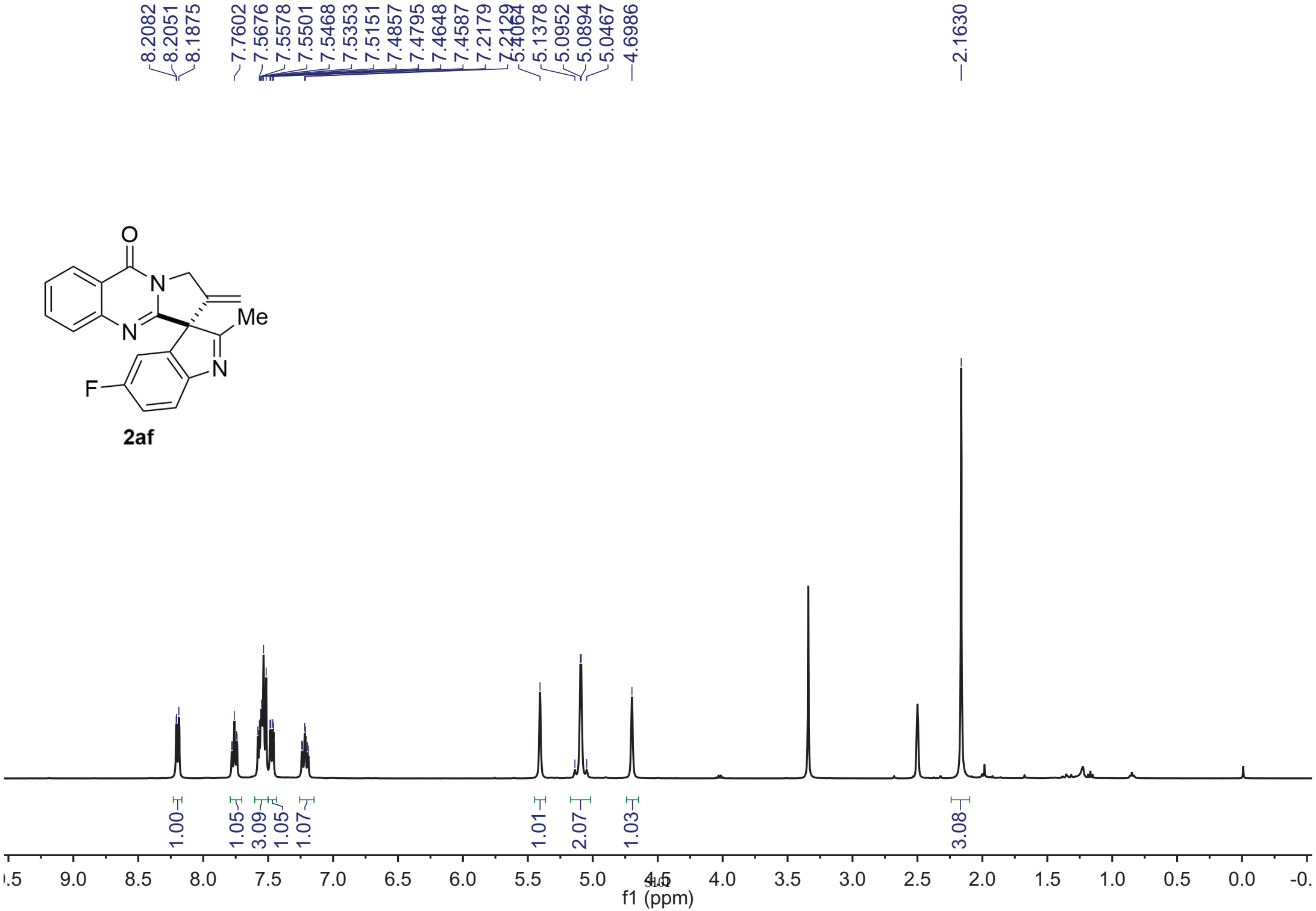
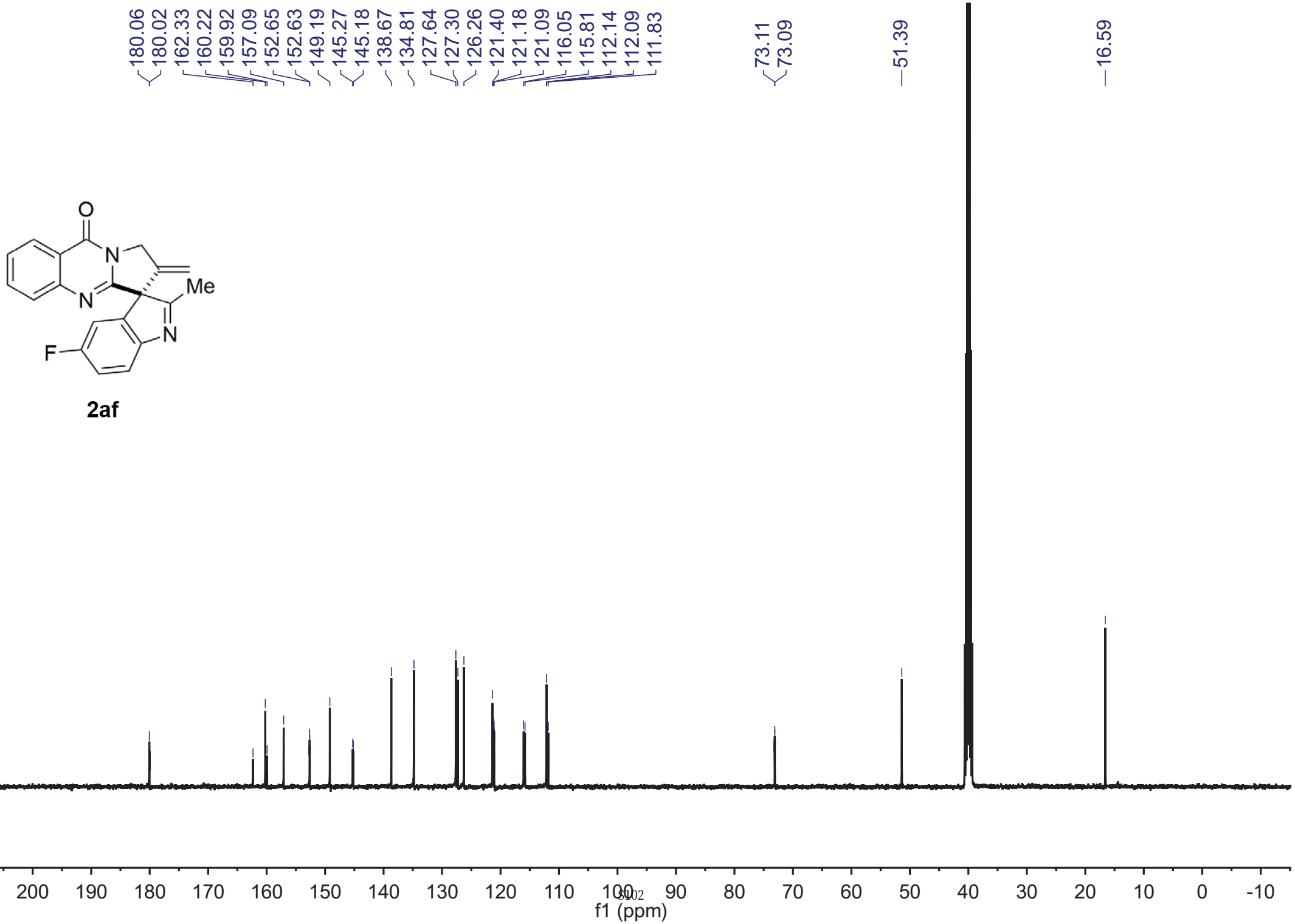
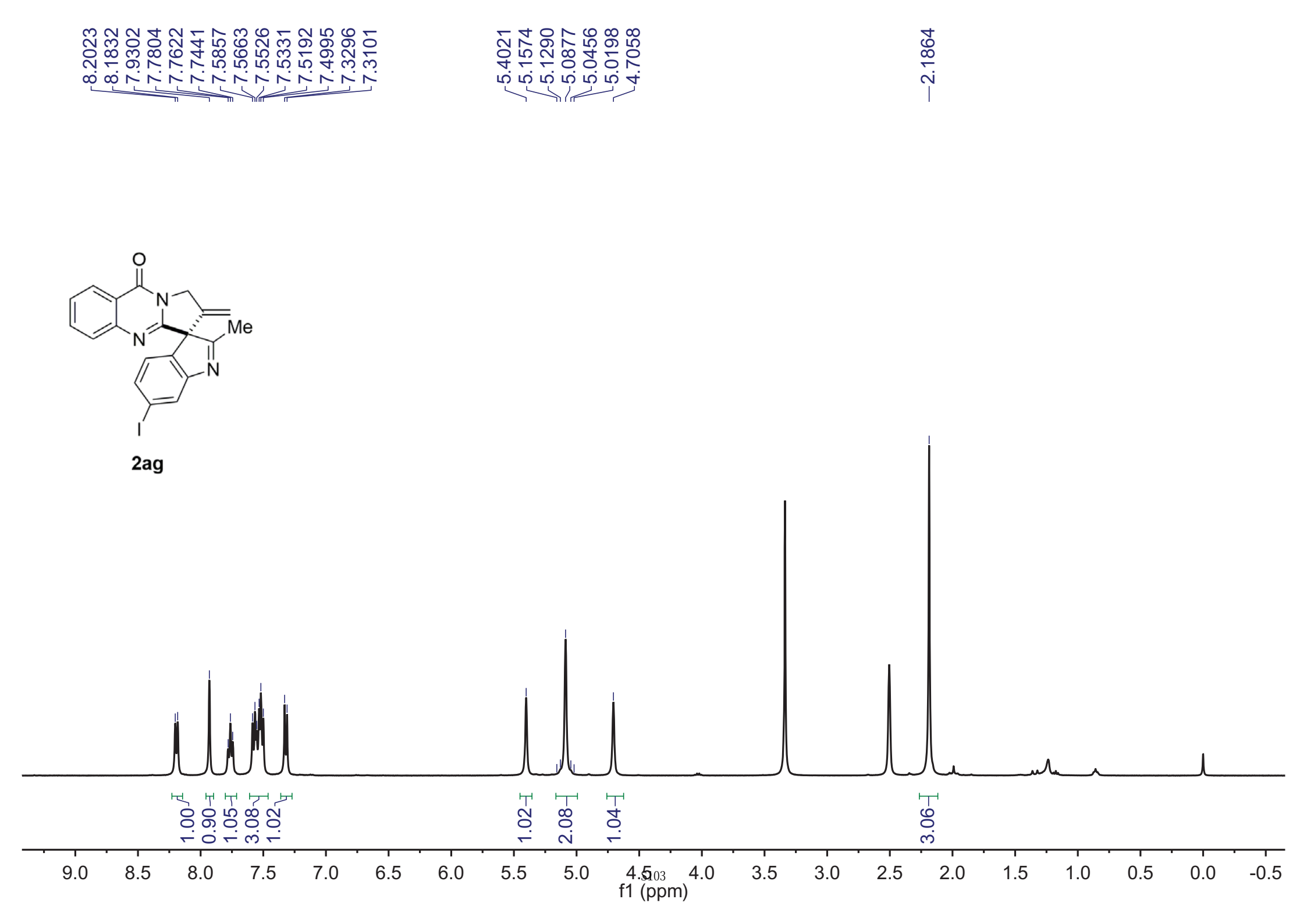
160.24
156.98
155.21
149.19
145.32
138.52
134.81
130.99
129.45
127.64
127.30
126.27
124.49
121.47
121.45
112.28
72.99
51.43
16.63
O
N
N
Me
N
Cl
2ae
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

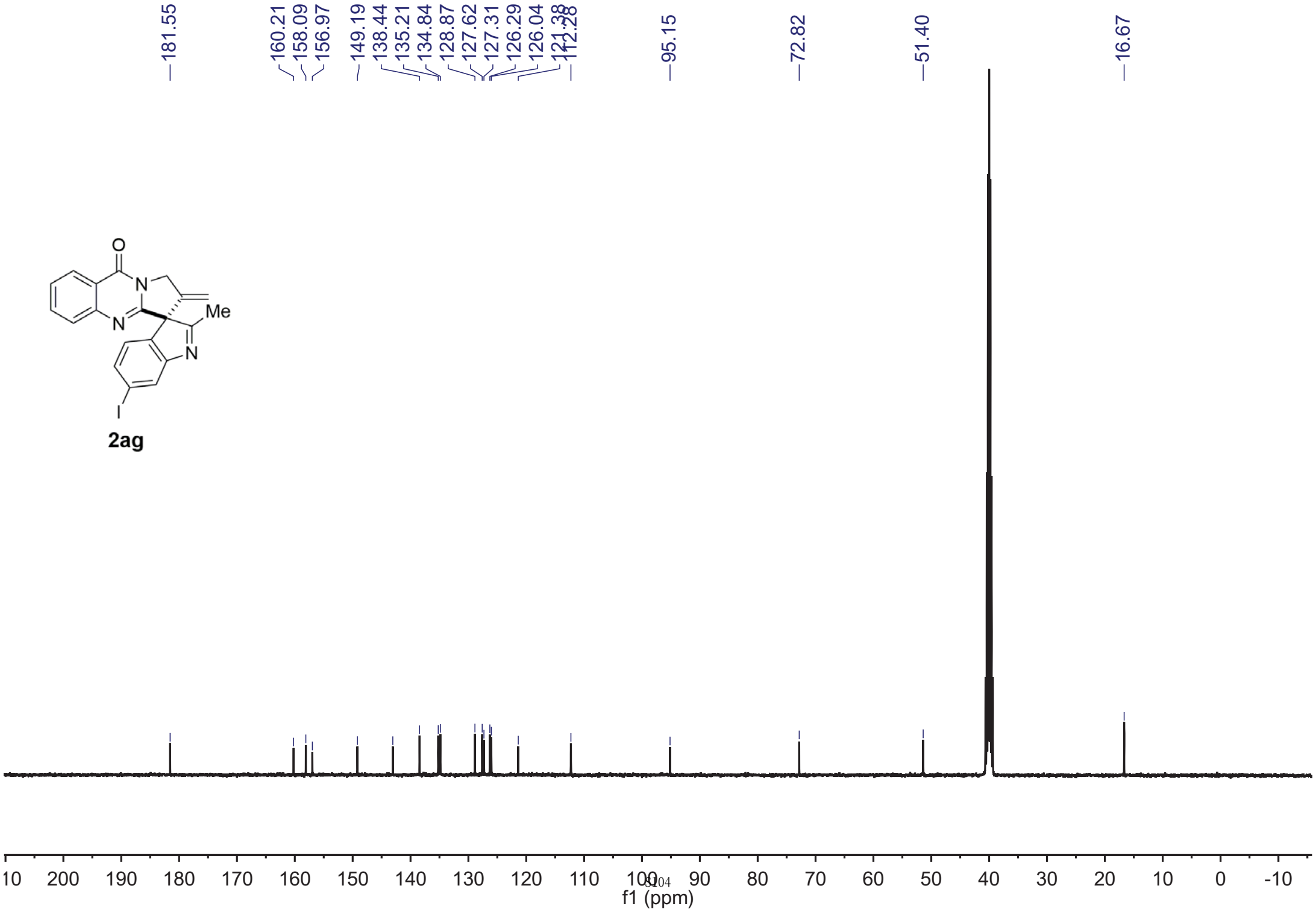
O
N
N
Me
N
F

2af


8.2082
8.2051
8.1875
7.7602
7.5676
7.5578
7.5501
7.5468
7.5353
7.5151
7.4857
7.4795
7.4648
7.4587
7.2179
7.2129
7.2064
5.1378
5.0952
5.0894
5.0467
4.6986
2.1630
1.00
1.05
3.09
1.05
1.07
1.01
2.07
1.03
3.08
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)


180.06
180.02
162.33
160.22
159.92
157.09
152.65
152.63
149.19
145.27
145.18
138.67
134.81
127.64
127.30
126.26
121.40
121.18
121.09
116.05
115.81
112.14
112.09
111.83
73.11
73.09
51.39
16.59
O
N
N
Me
N
F
2af
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


8.2023
8.1832
7.9302
7.7804
7.7622
7.7441
7.5857
7.5663
7.5526
7.5331
7.5192
7.4995
7.3296
7.3101
5.4021
5.1574
5.1290
5.0877
5.0456
5.0198
4.7058
2.1864
O
N
N
Me
N
I
2ag
1.00
0.90
1.05
3.08
1.02
1.02
2.08
1.04
3.06
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
-0.5
f1 (ppm)


181.55
160.21
158.09
156.97
149.19
138.44
135.21
134.84
128.87
127.62
127.31
126.29
126.04
121.38
112.28
95.15
72.82
51.40
16.67
O
N
N
Me
N
I
2ag
10
200
190
180
170
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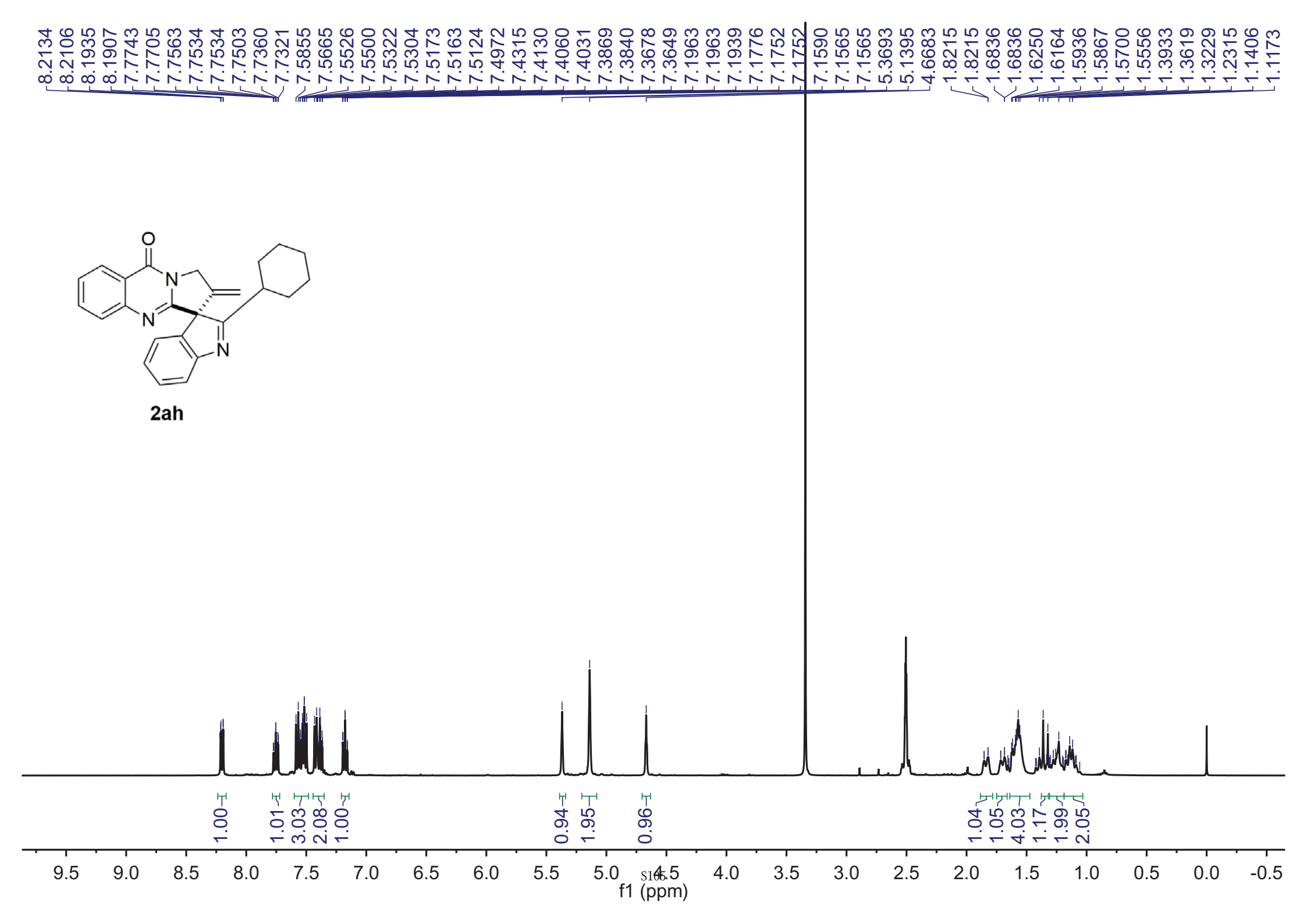
f1 (ppm)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7.7321
7.5855
7.5665
7.5526
7.5500
7.5322
7.5304
7.5173
7.5163
7.5124
7.4972
7.4315
7.4130
7.4060
7.4031
7.3869
7.3840
7.3678
7.3649
7.1963
7.1963
7.1939
7.1776
7.1752
7.1752
7.1590
7.1565
7.1565
5.3693
5.1395
4.6683
1.8215
1.8215
1.6836
1.6836
1.6250
1.6164
1.5936
1.5867
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1.5556
1.3933
1.3619
1.3229
1.2315
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1.1173
O
N
N
N
2ah
1.00
1.01
3.03
2.08
1.00
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1.95
0.96
1.04
1.05
4.03
1.17
1.99
2.05
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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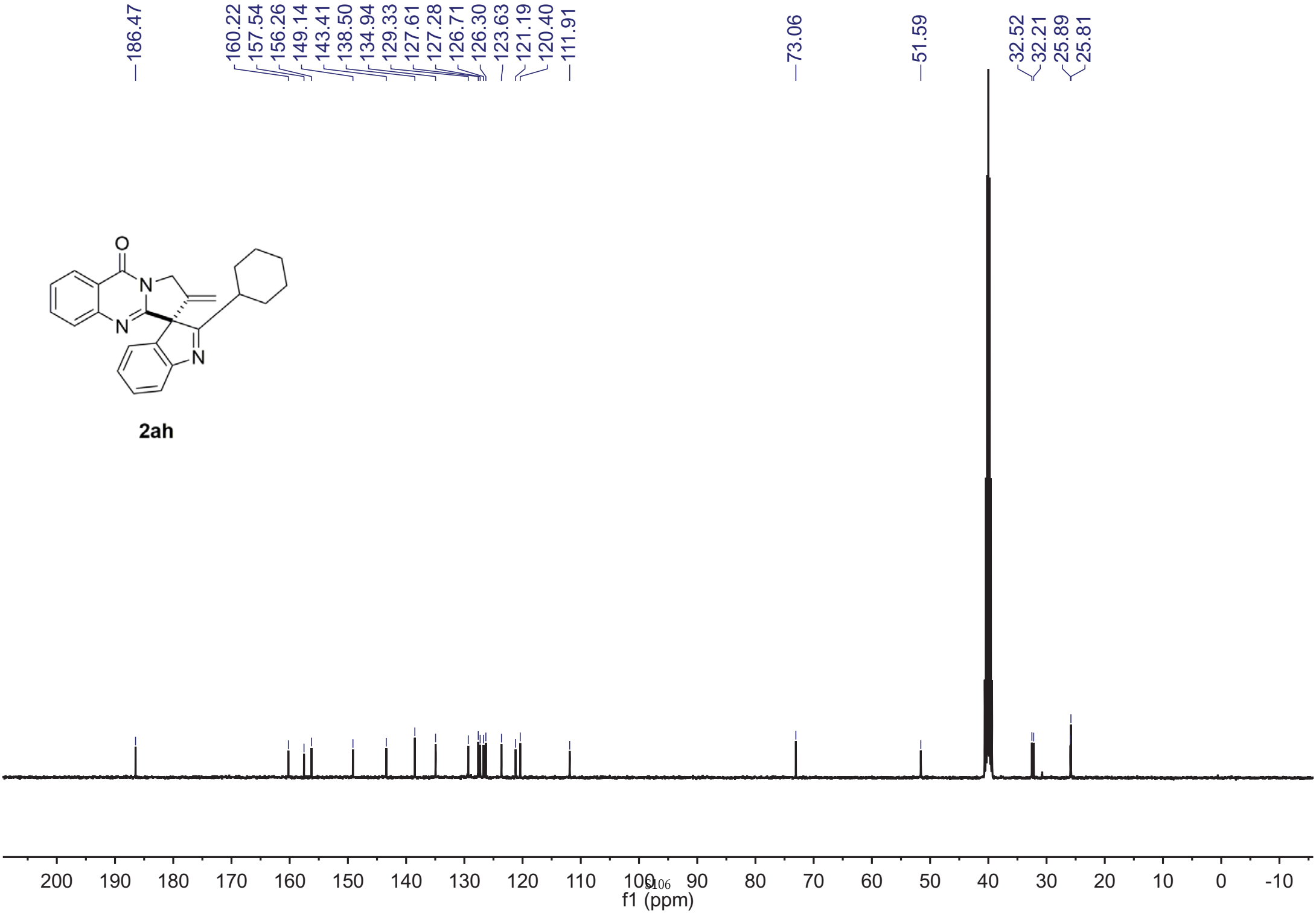
f1 (ppm)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134.94
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126.71
126.30
123.63
121.19
120.40
111.91
73.06
51.59
32.52
32.21
25.89
25.81
O
N
N
N
2ah
200
190
180
170
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120
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100
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80
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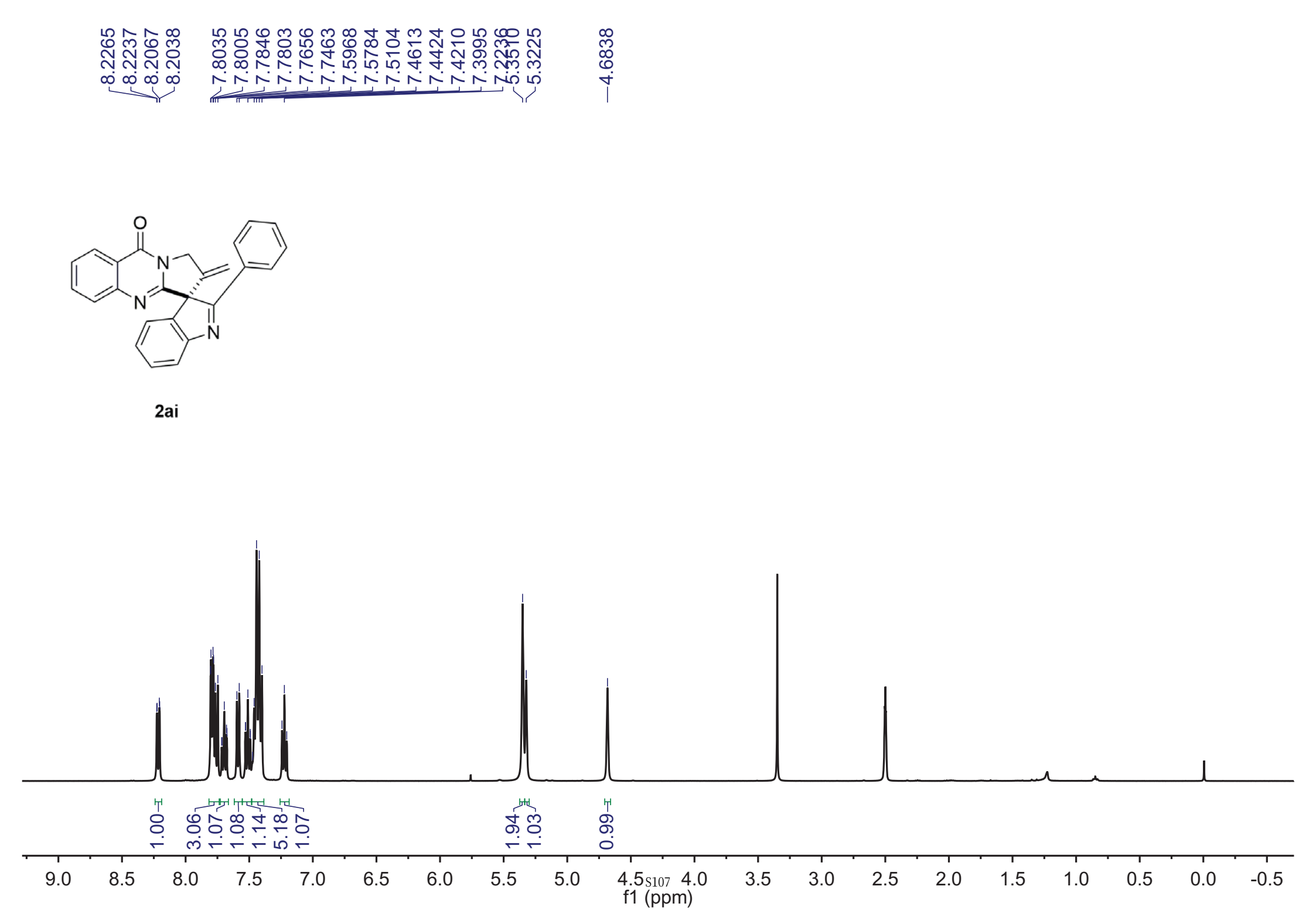
f1 (ppm)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7.7656
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7.5968
7.5784
7.5104
7.4613
7.4424
7.4210
7.3995
7.2236
5.3510
5.3225
4.6838
O
N
N
N
2ai
1.00
3.06
1.07
1.08
1.14
5.18
1.07
1.94
1.03
0.99
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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3.0
2.5
2.0
1.5
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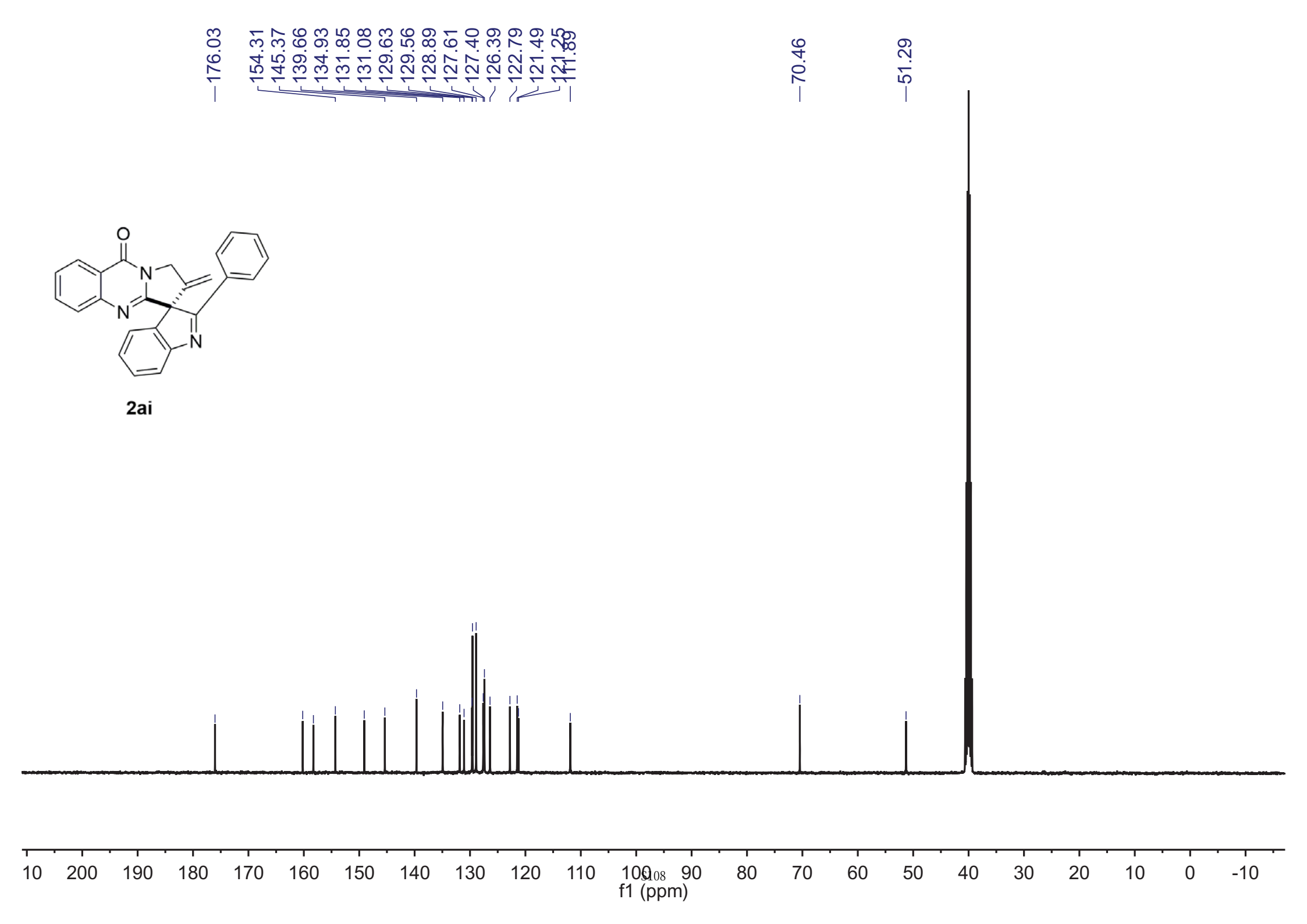
0.0
-0.5
f1 (ppm)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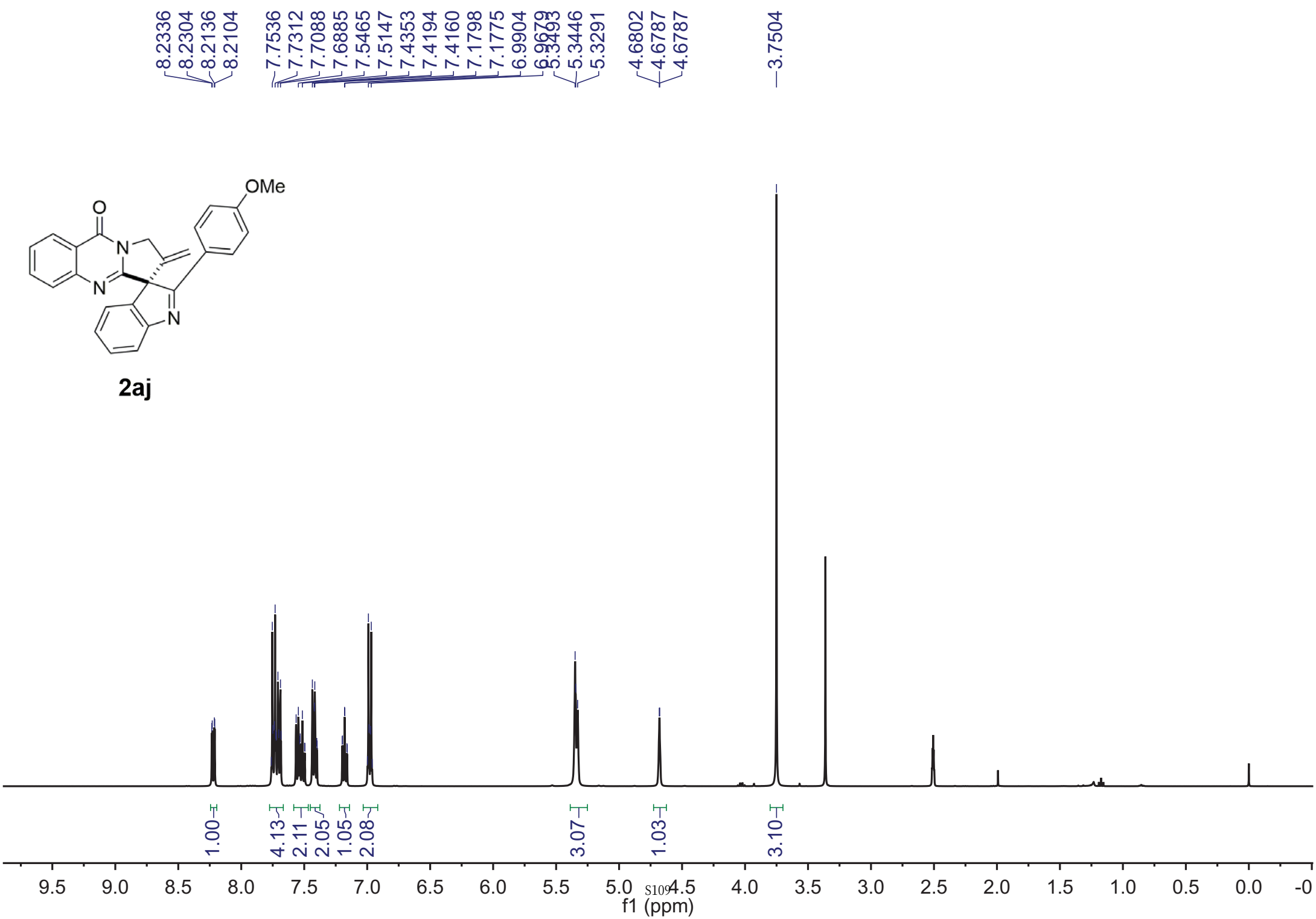
154.31
145.37
139.66
134.93
131.85
131.08
129.63
129.56
128.89
127.61
127.40
126.39
122.79
121.49
121.25
111.89
70.46
51.29
O
N
N
N
2ai
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.5147
7.4353
7.4194
7.4160
7.1798
7.1775
6.9904
5.3446
5.3291
4.6802
4.6787
4.6787
3.7504
OMe
O
N
N
N
2aj
1.00
4.13
2.11
2.05
1.05
2.08
3.07
1.03
3.10
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
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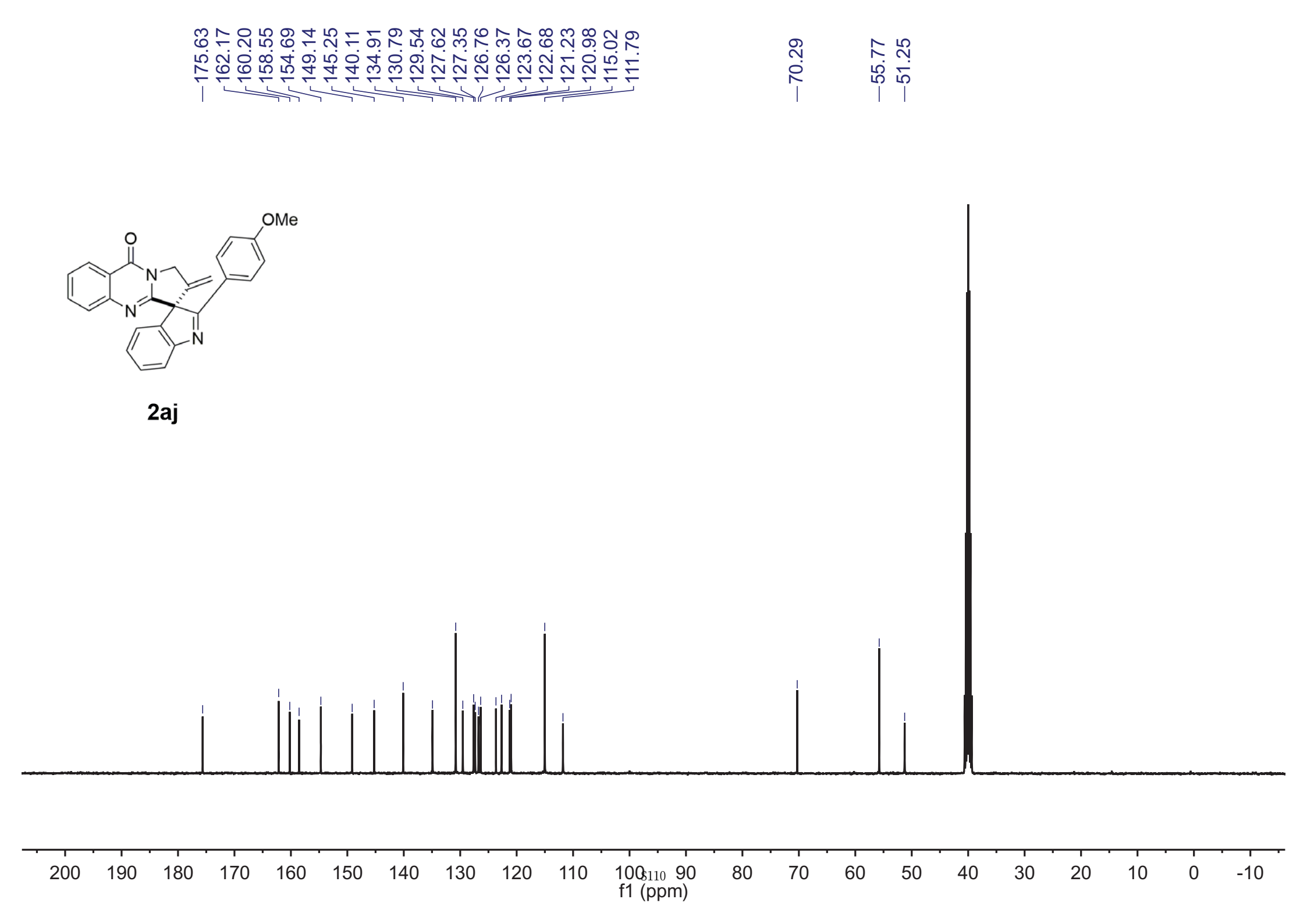
-0
f1 (ppm)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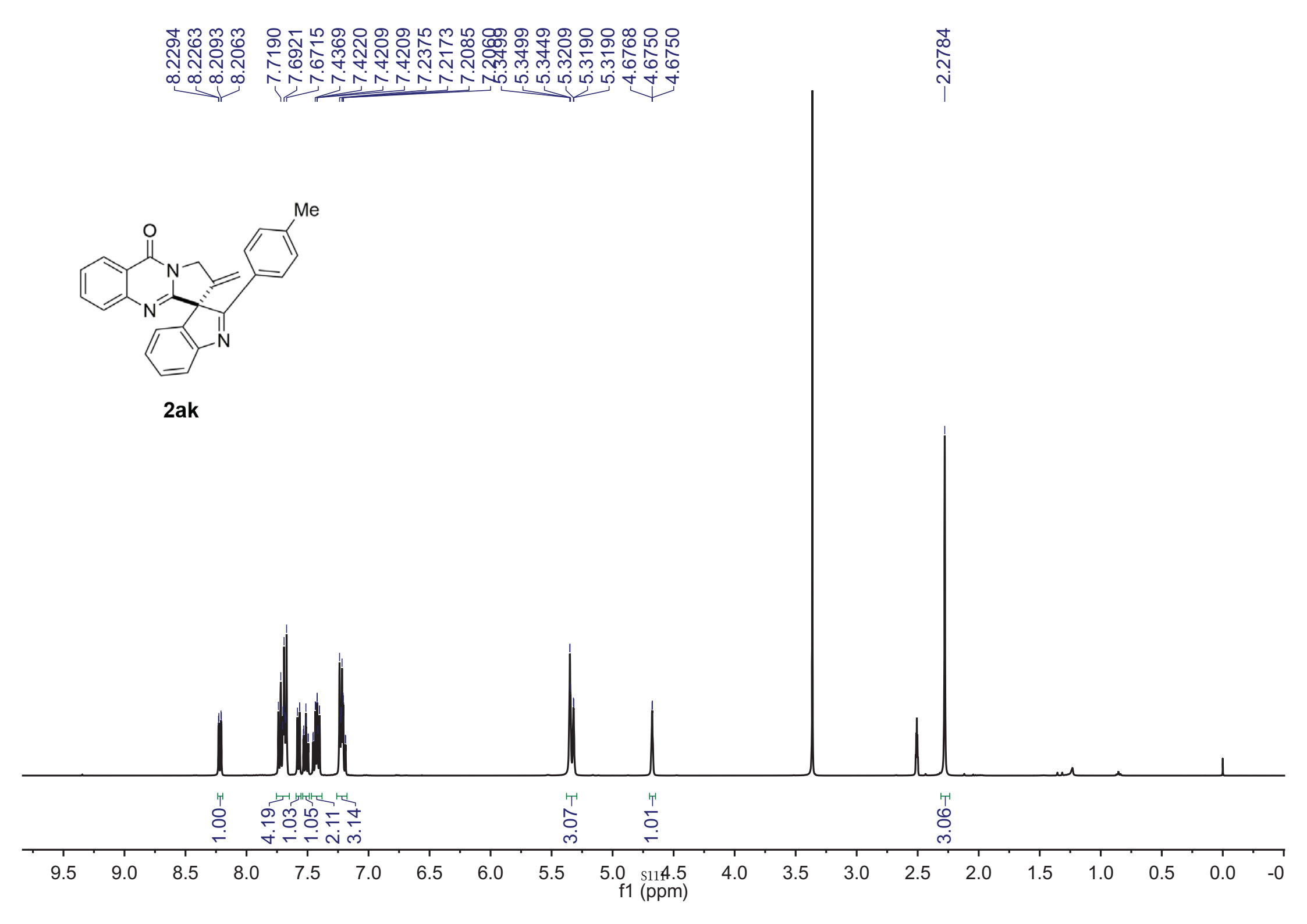
158.55
154.69
149.14
145.25
140.11
134.91
130.79
129.54
127.62
127.35
126.76
126.37
123.67
122.68
121.23
120.98
115.02
111.79
70.29
55.77
51.25
OMe
O
N
N
N
2aj
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.4220
7.4209
7.4209
7.2375
7.2173
7.2085
5.3499
5.3449
5.3209
5.3190
5.3190
4.6768
4.6750
4.6750
2.2784
Me
O
N
N
N
2ak
1.00
4.19
1.03
1.05
2.11
3.14
3.07
1.01
3.06
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
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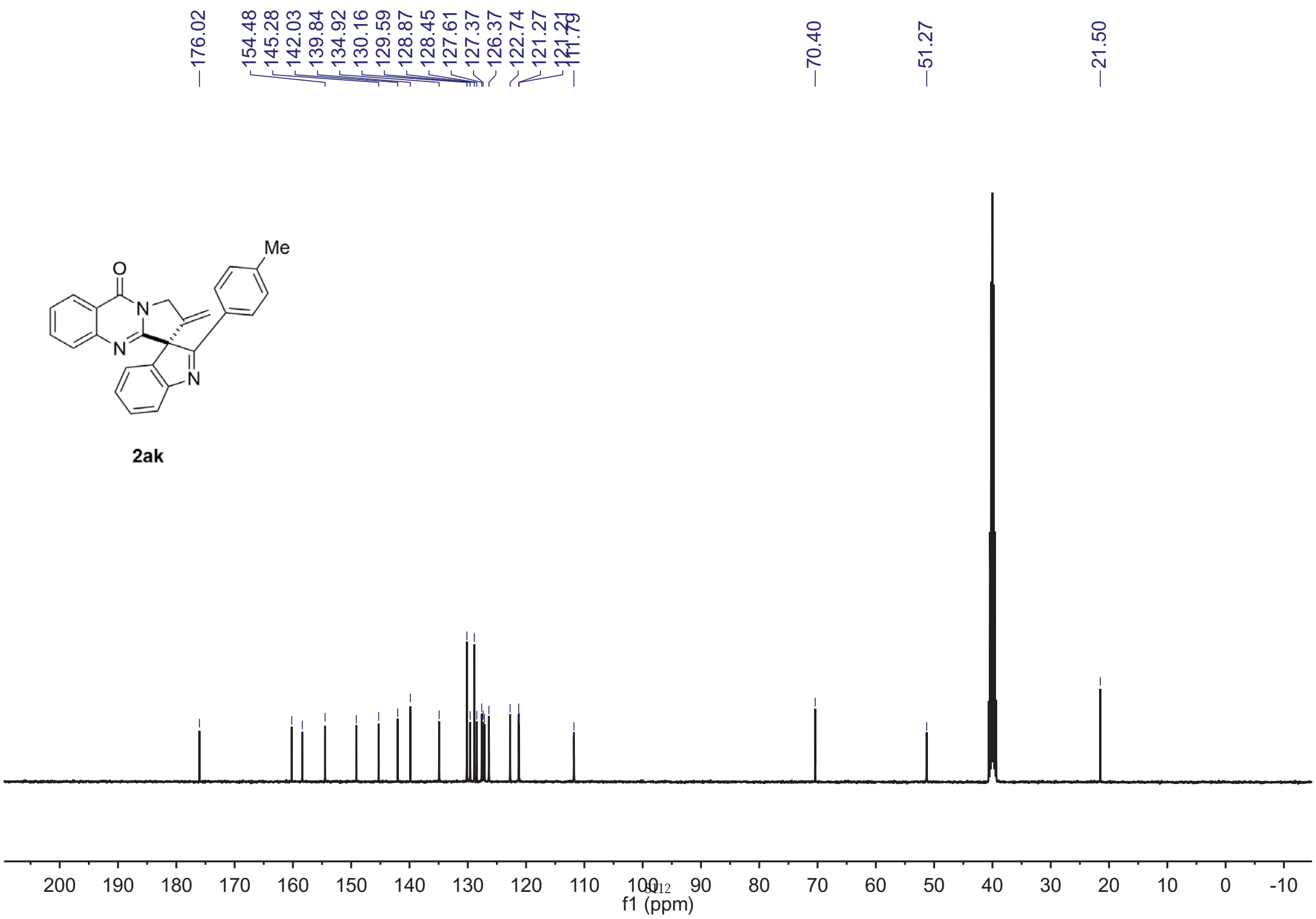
-0
f1 (ppm)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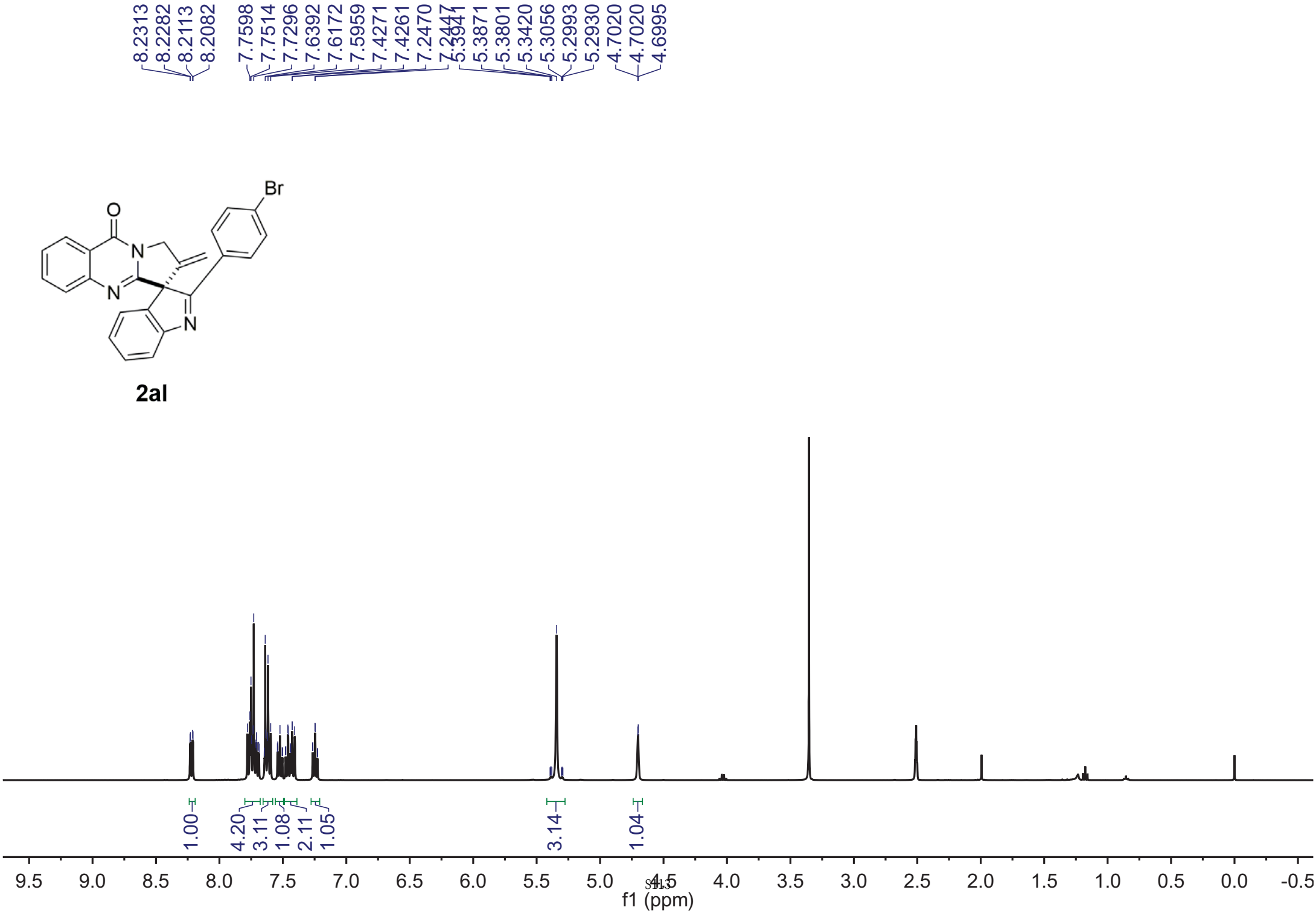
142.03
139.84
134.92
130.16
129.59
128.87
128.45
127.61
127.37
126.37
122.74
121.27
121.21
111.79
70.40
51.27
21.50
Me
O
N
N
N
2ak
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

O
N
N
N
Br

2al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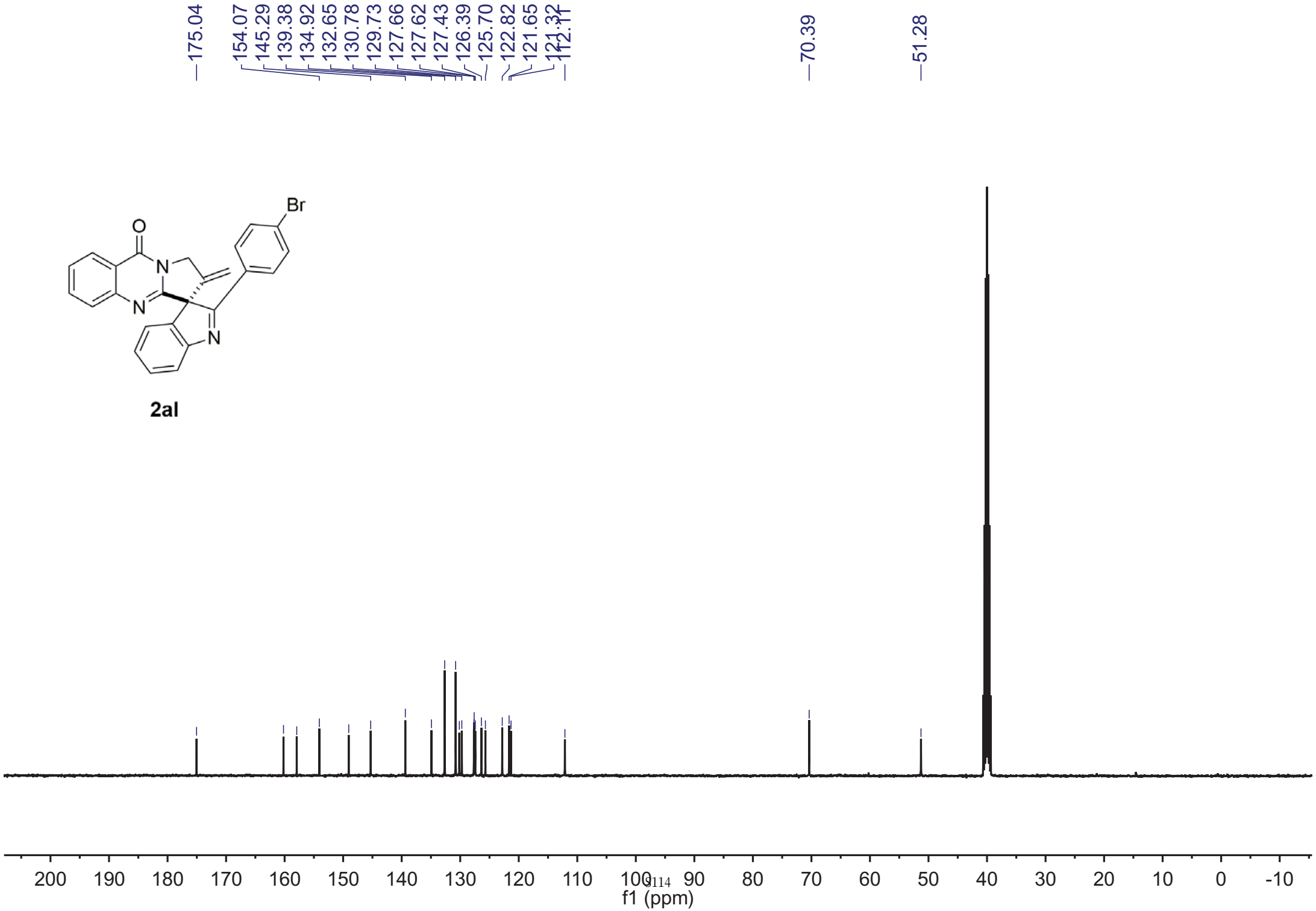
7.4261
7.2470
7.2447
7.2441
5.3941
5.3871
5.3801
5.3420
5.3056
5.2993
5.2930
4.7020
4.7020
4.6995
1.00
4.20
3.11
1.08
2.11
1.05
3.14
1.04
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

Br
O
N
N
N

2al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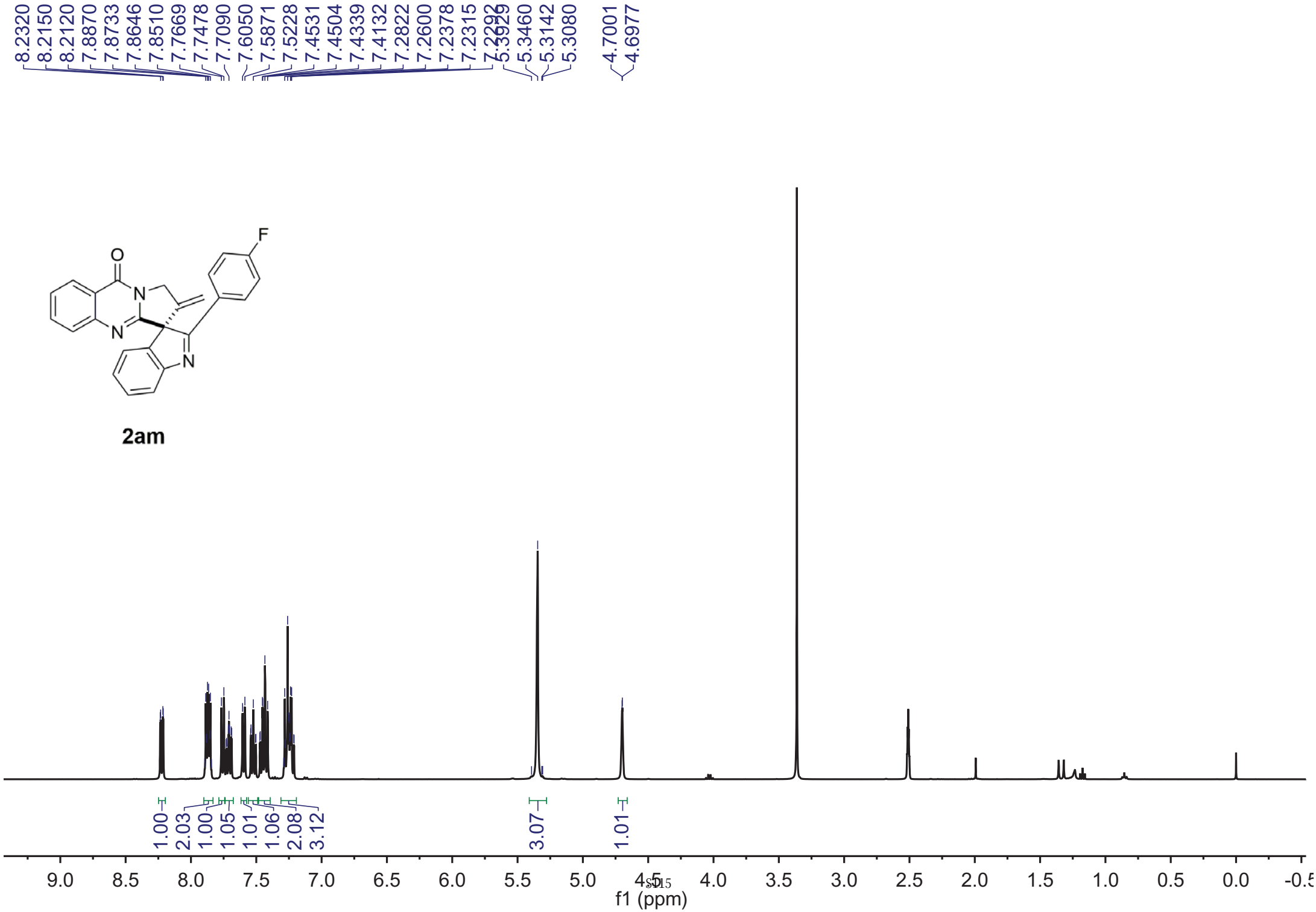
129.73
127.66
127.62
127.43
126.39
125.70
122.82
121.65
121.32
112.11
70.39
51.28
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.8733
7.8646
7.8510
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7.7478
7.7090
7.6050
7.5871
7.5228
7.4531
7.4504
7.4339
7.4132
7.2822
7.2600
7.2378
7.2315
5.3460
5.3142
5.3080
4.7001
4.6977
O
N
N
N
F
2am
1.00
2.03
1.00
1.05
1.01
1.06
2.08
3.12
3.07
1.01
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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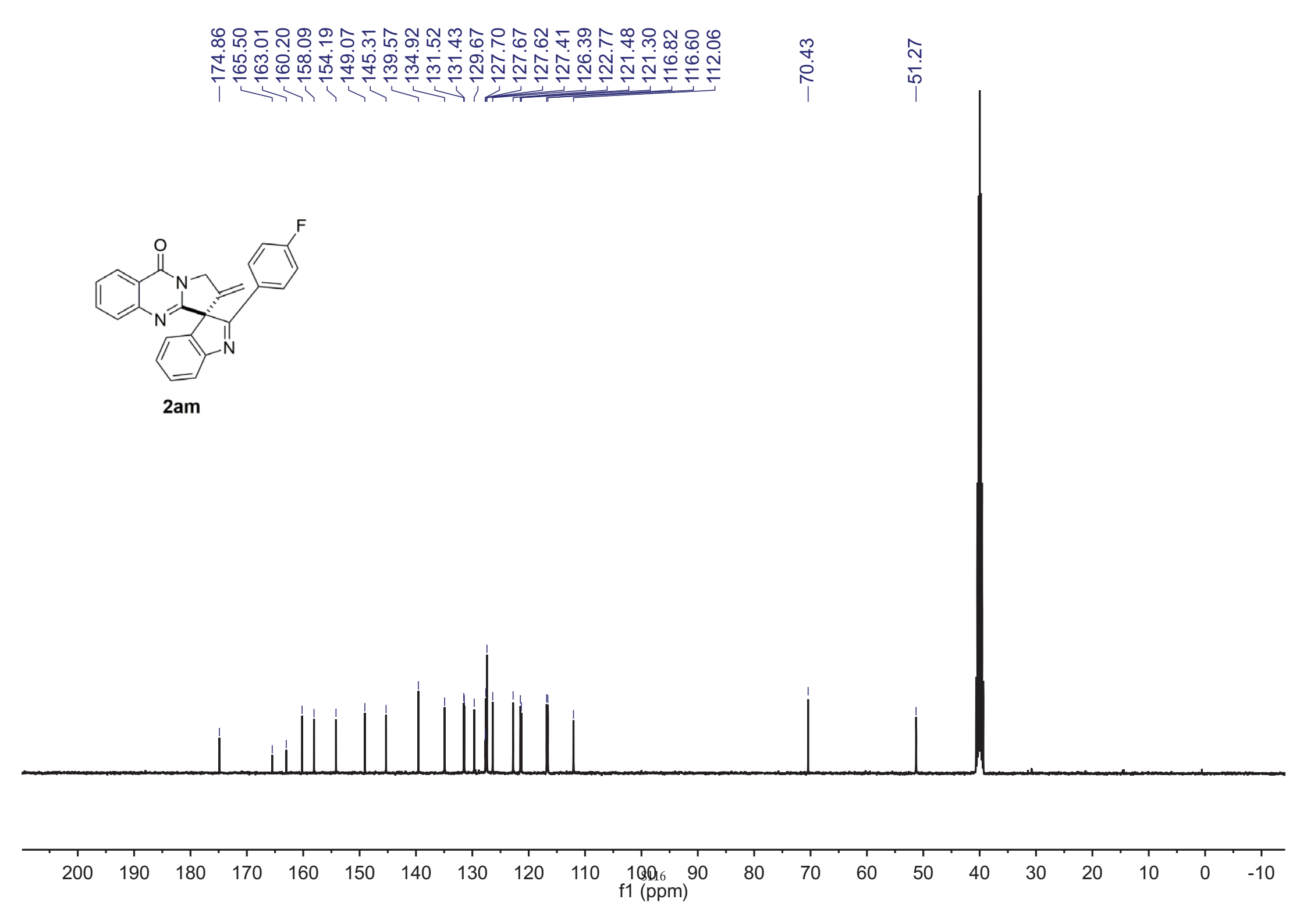
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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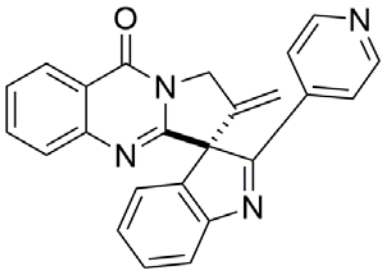
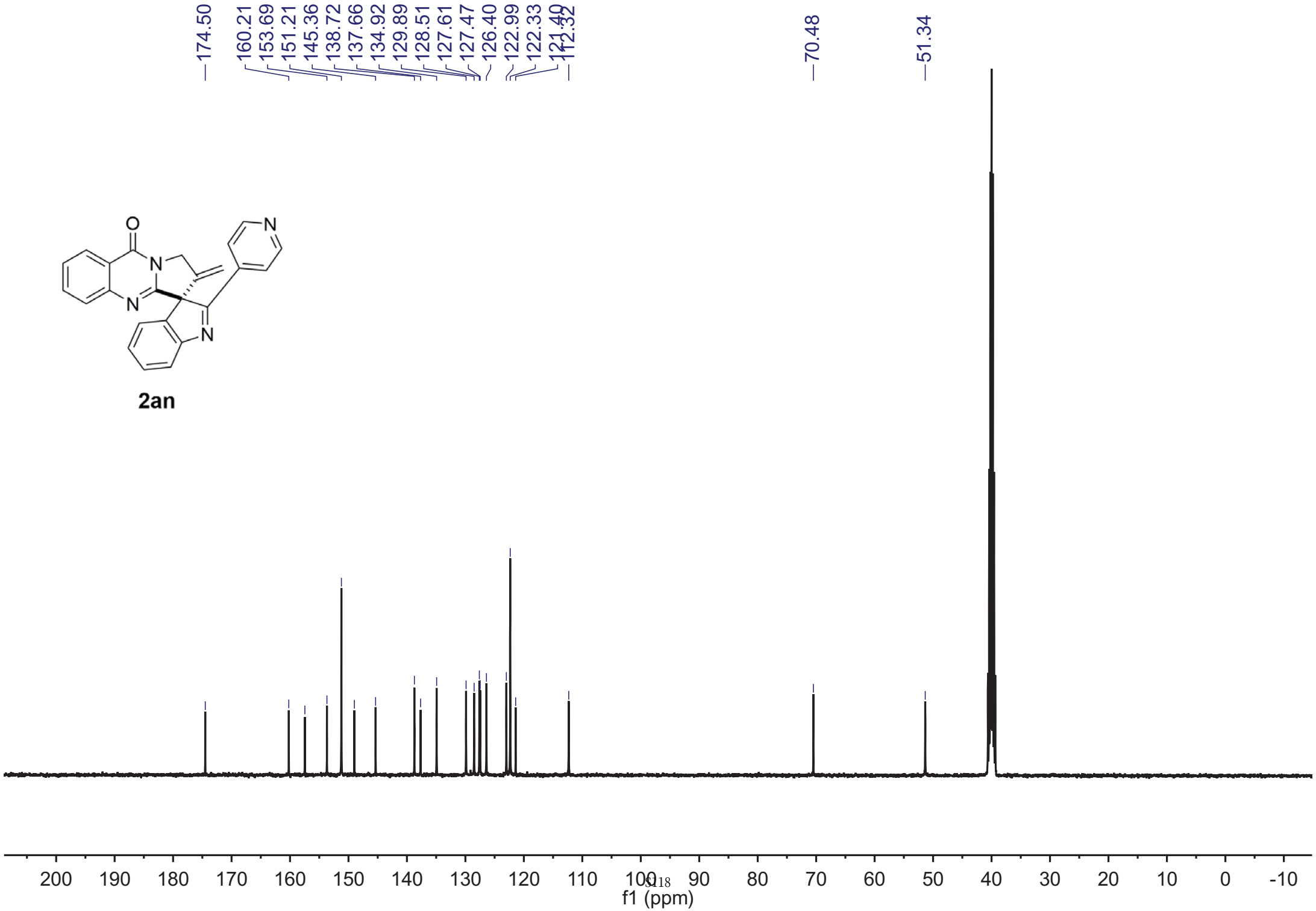
145.31
139.57
134.92
131.52
131.43
129.67
127.70
127.67
127.62
127.41
126.39
122.77
121.48
121.30
116.82
116.60
112.06
70.43
51.27
O
N
N
N
F
2am
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)



2an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134.92
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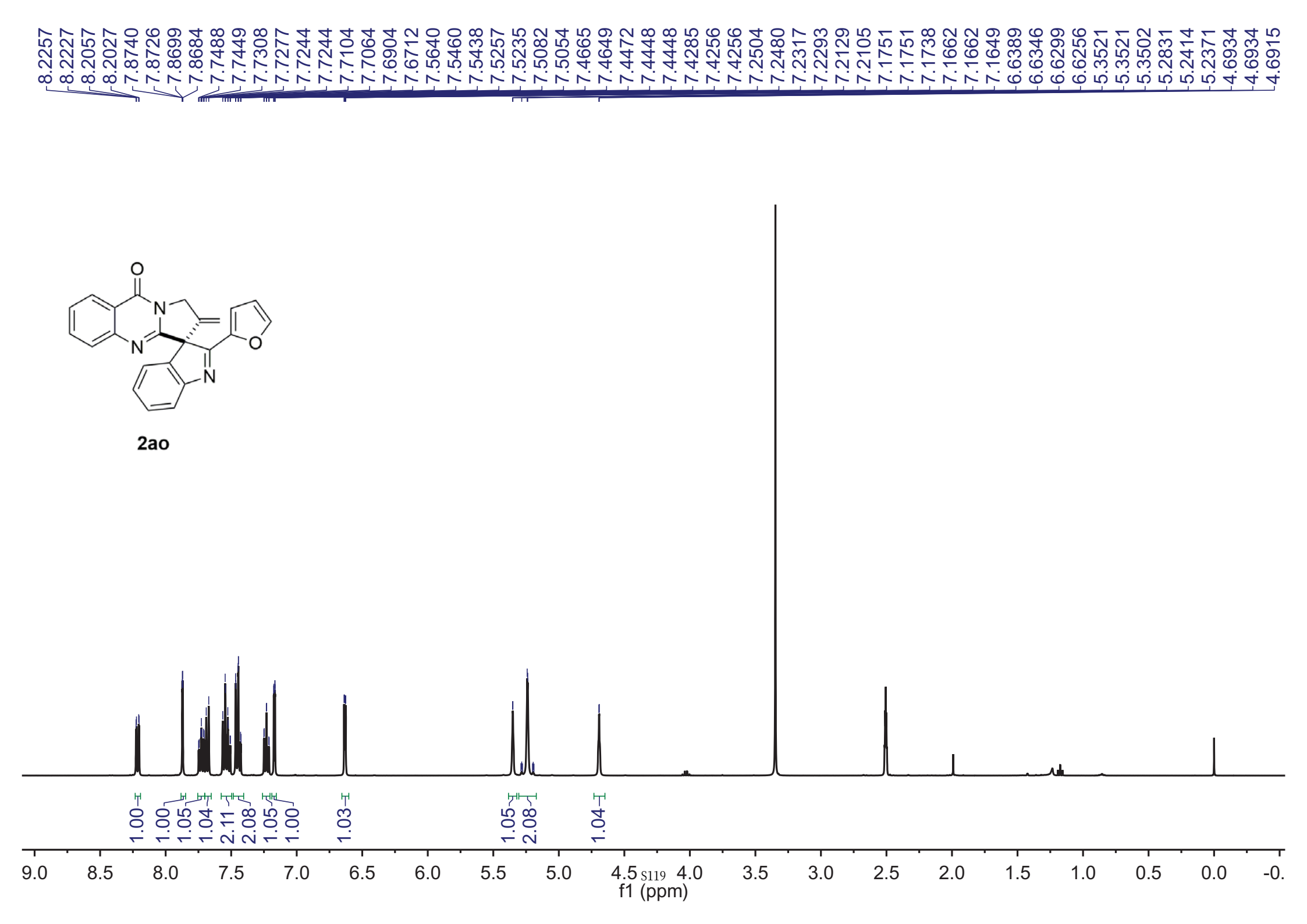
128.51
127.61
127.47
126.40
122.99
122.33
121.40
112.32
70.48
51.34
O
N
N
N
N
2an
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.7308
7.7277
7.7244
7.7244
7.7104
7.7064
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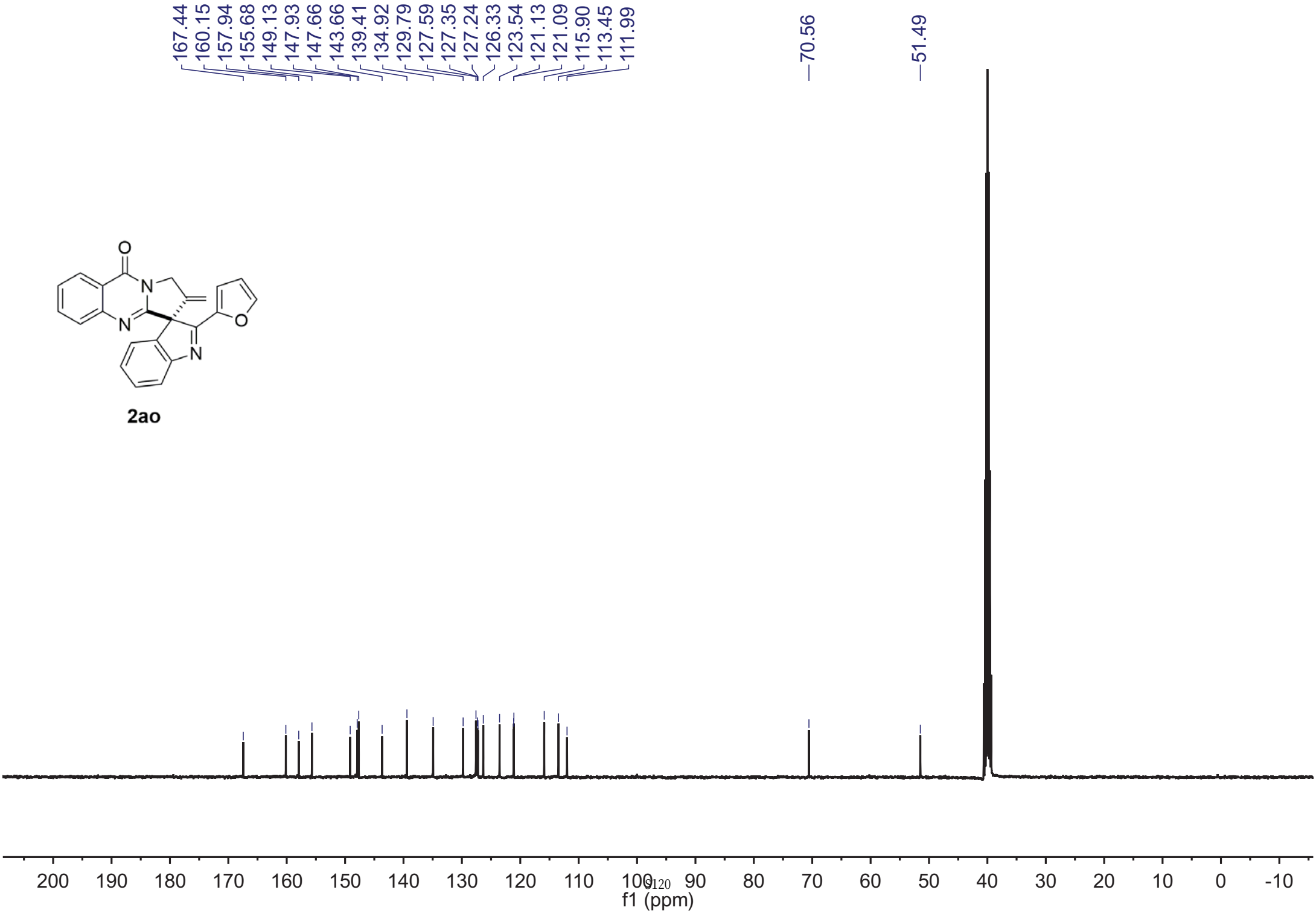
7.6712
7.5640
7.5460
7.5438
7.5257
7.5235
7.5082
7.5054
7.4665
7.4649
7.4472
7.4448
7.4448
7.4285
7.4256
7.4256
7.2504
7.2480
7.2317
7.2293
7.2129
7.2105
7.1751
7.1751
7.1738
7.1662
7.1662
7.1649
6.6389
6.6346
6.6299
6.6256
5.3521
5.3521
5.3502
5.2831
5.2414
5.2371
4.6934
4.6934
4.6915
O
N
N
O
N
2ao
1.00
1.00
1.05
1.04
2.11
2.08
1.05
1.00
1.03
1.05
2.08
1.04
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
-0.
f1 (ppm)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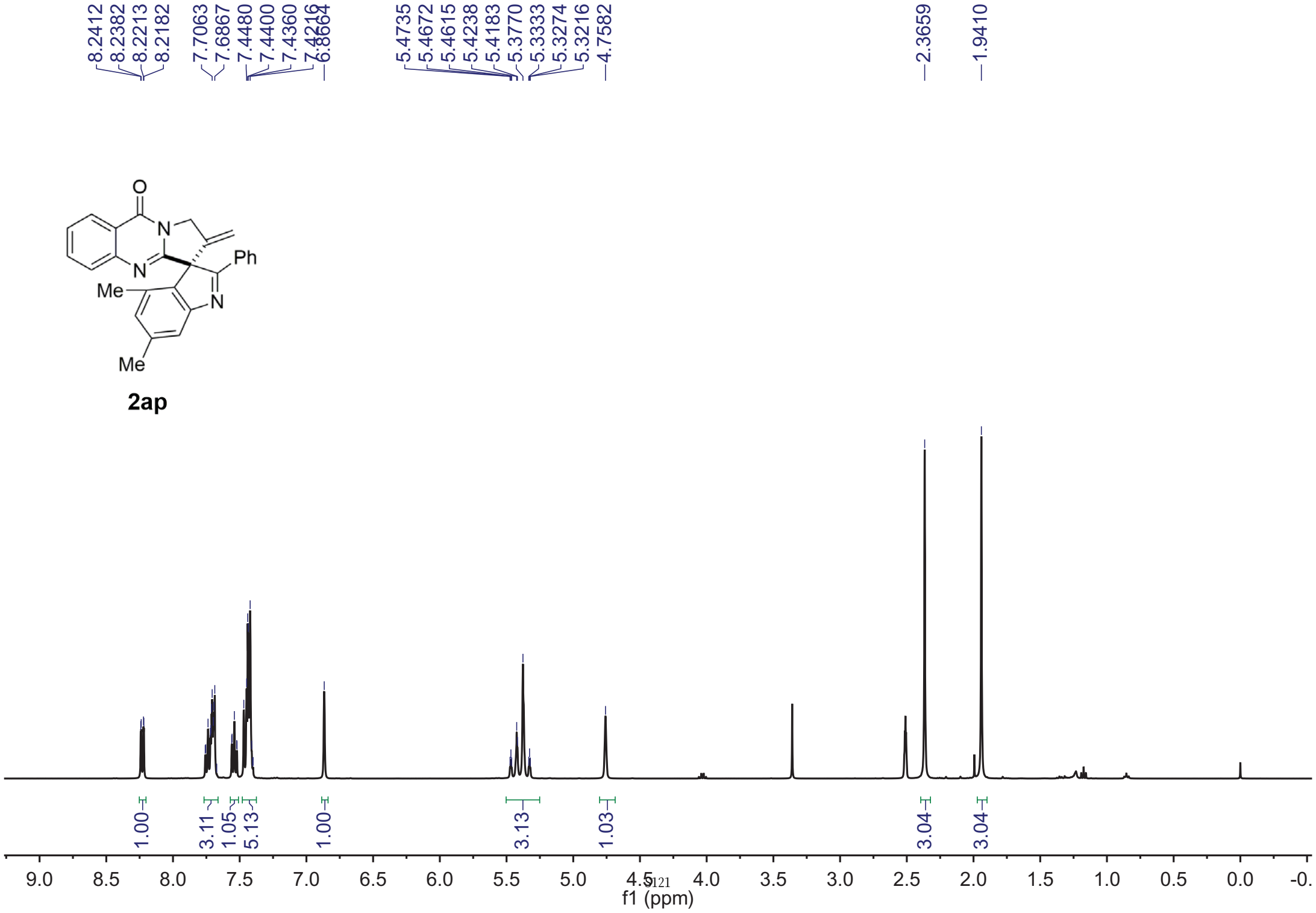
139.41
134.92
129.79
127.59
127.35
127.24
126.33
123.54
121.13
121.09
115.90
113.45
111.99
70.56
51.49
O
N
N
O
N
2ao
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

O
N
N
Ph
Me
N
Me

2ap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7.4360
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5.4735
5.4672
5.4615
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5.4183
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5.3333
5.3274
5.3216
4.7582
2.3659
1.9410
1.00
3.11
1.05
5.13
1.00
3.13
1.03
3.04
3.04
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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4.0
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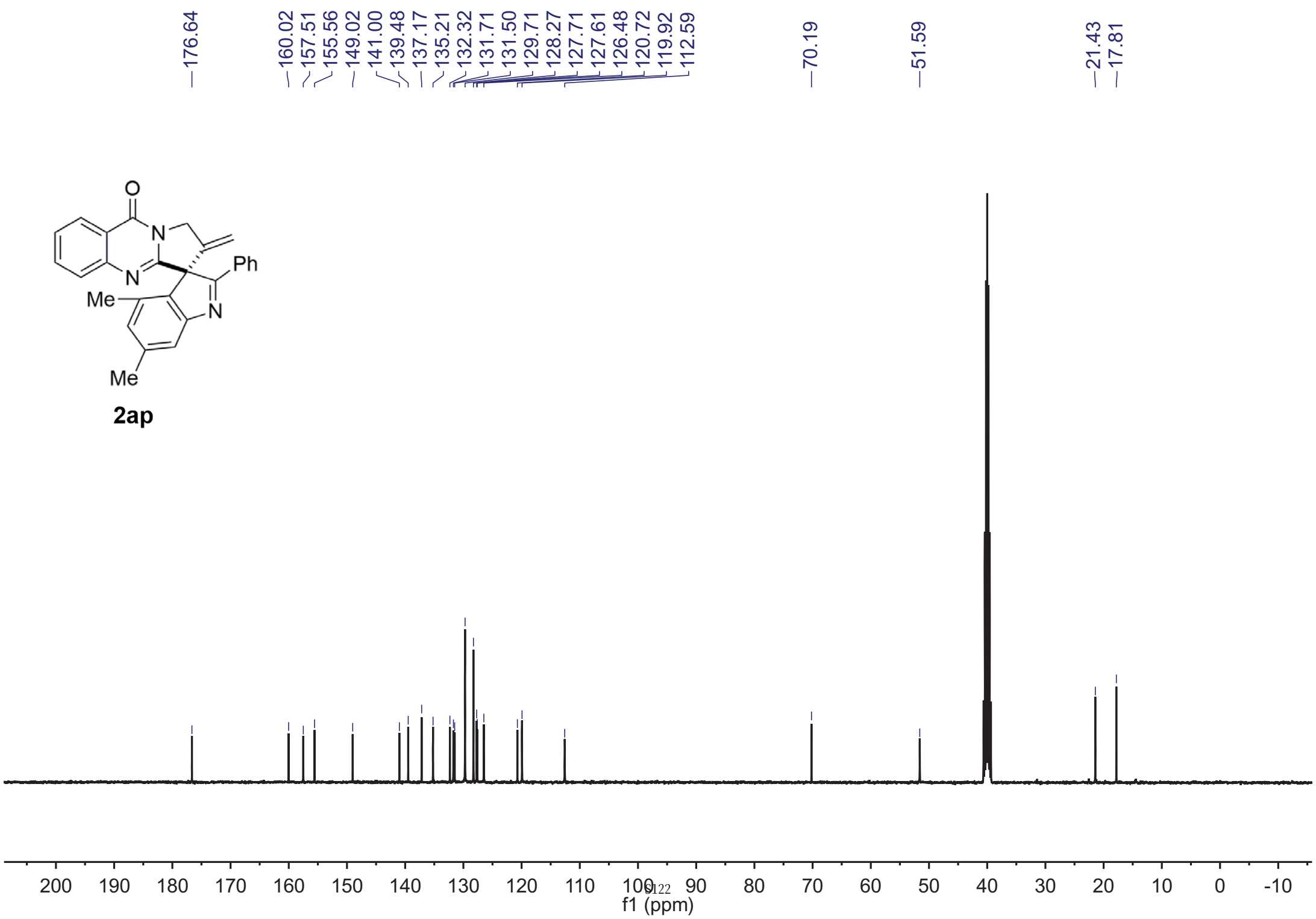
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.
f1 (ppm)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131.50
129.71
128.27
127.71
127.61
126.48
120.72
119.92
112.59
70.19
51.59
21.43
17.81
O
N
N
Ph
Me
N
Me
2ap
200
190
180
170
160
150
140
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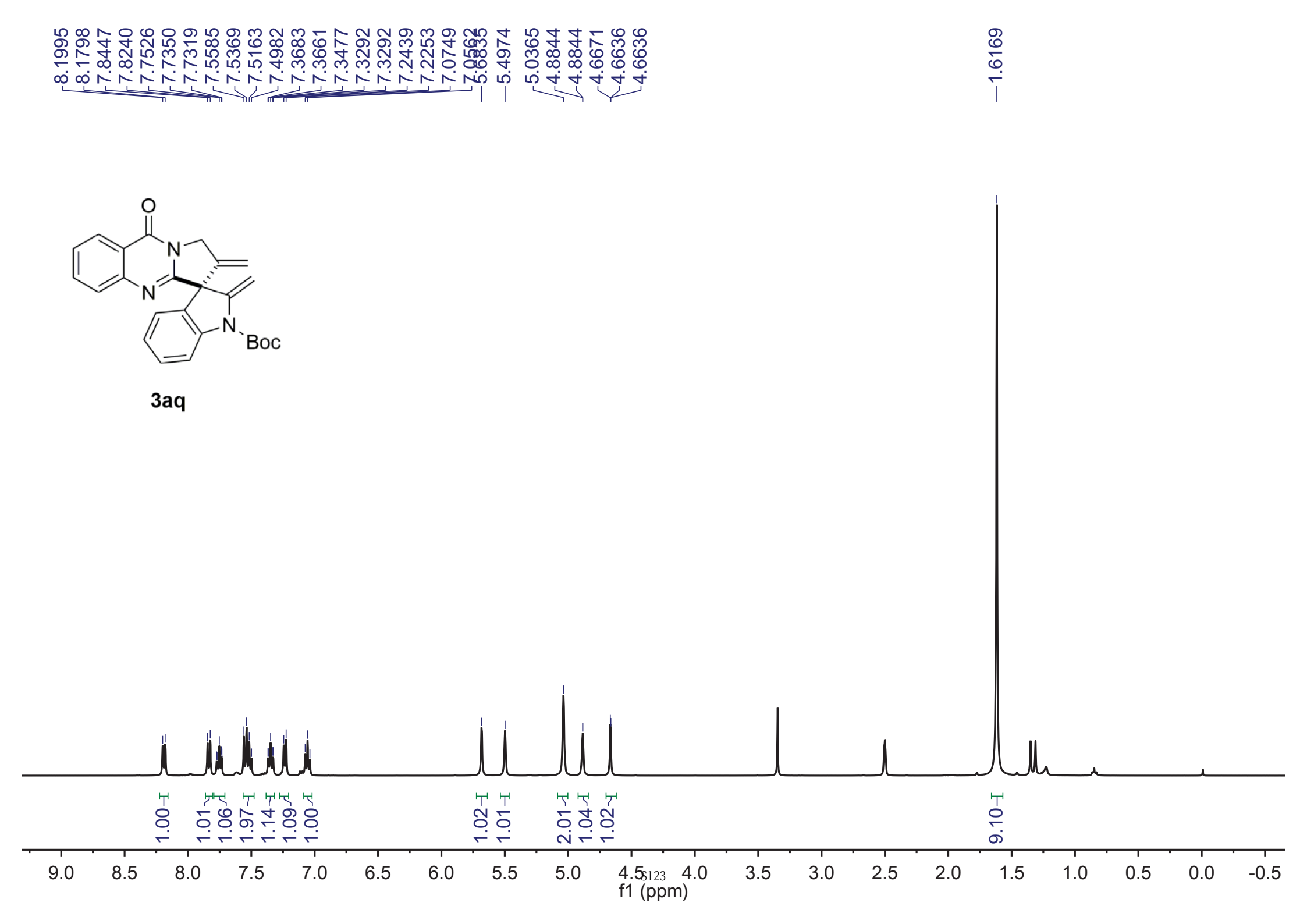
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.3683
7.3661
7.3477
7.3292
7.3292
7.2439
7.2253
7.0749
5.8835
5.4974
5.0365
4.8844
4.8844
4.6671
4.6636
4.6636
1.6169
O
N
N
N
Boc
1.00
1.01
1.06
1.97
1.14
1.09
1.00
1.02
1.01
2.01
1.04
1.02
9.10
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
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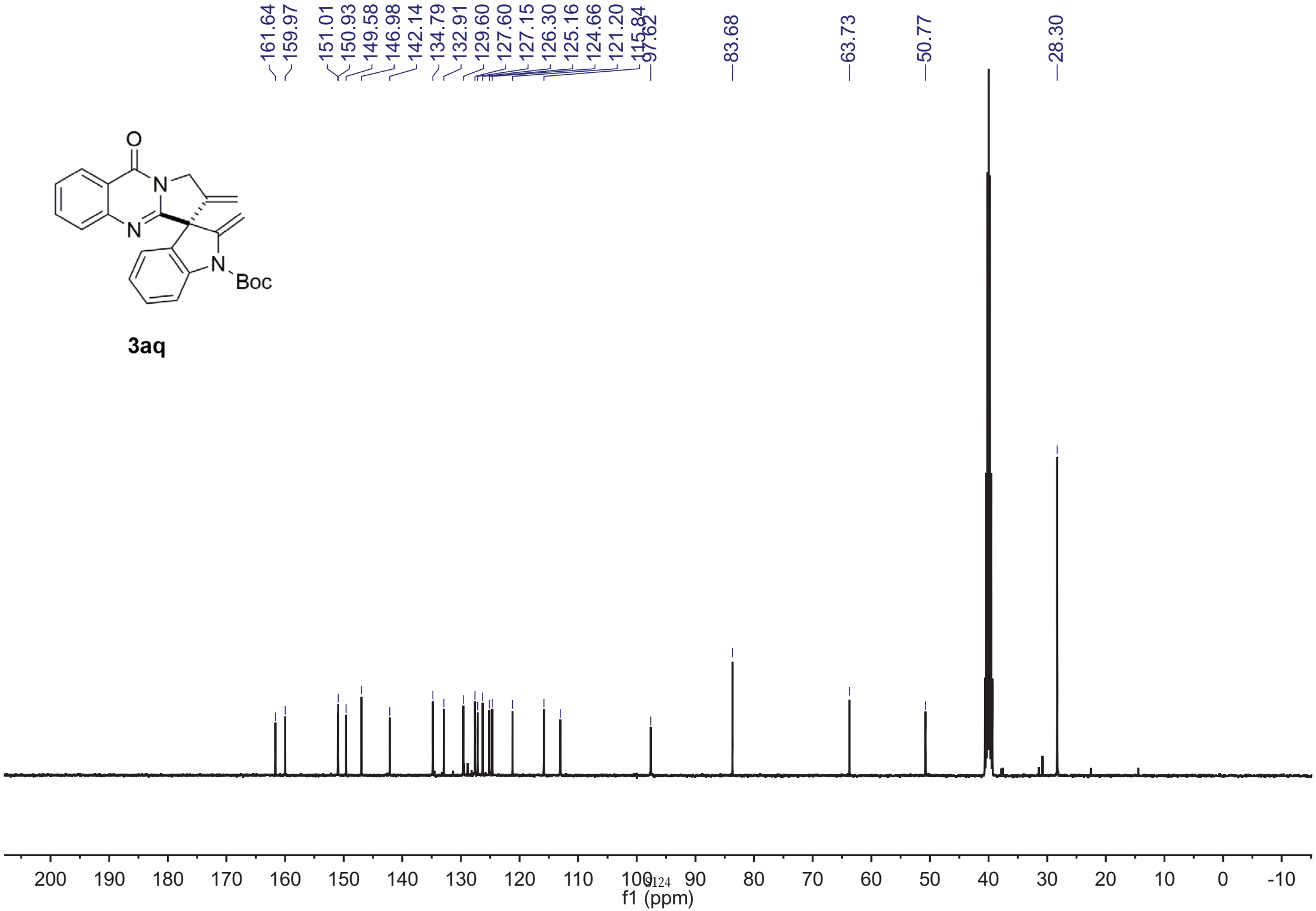
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

3aq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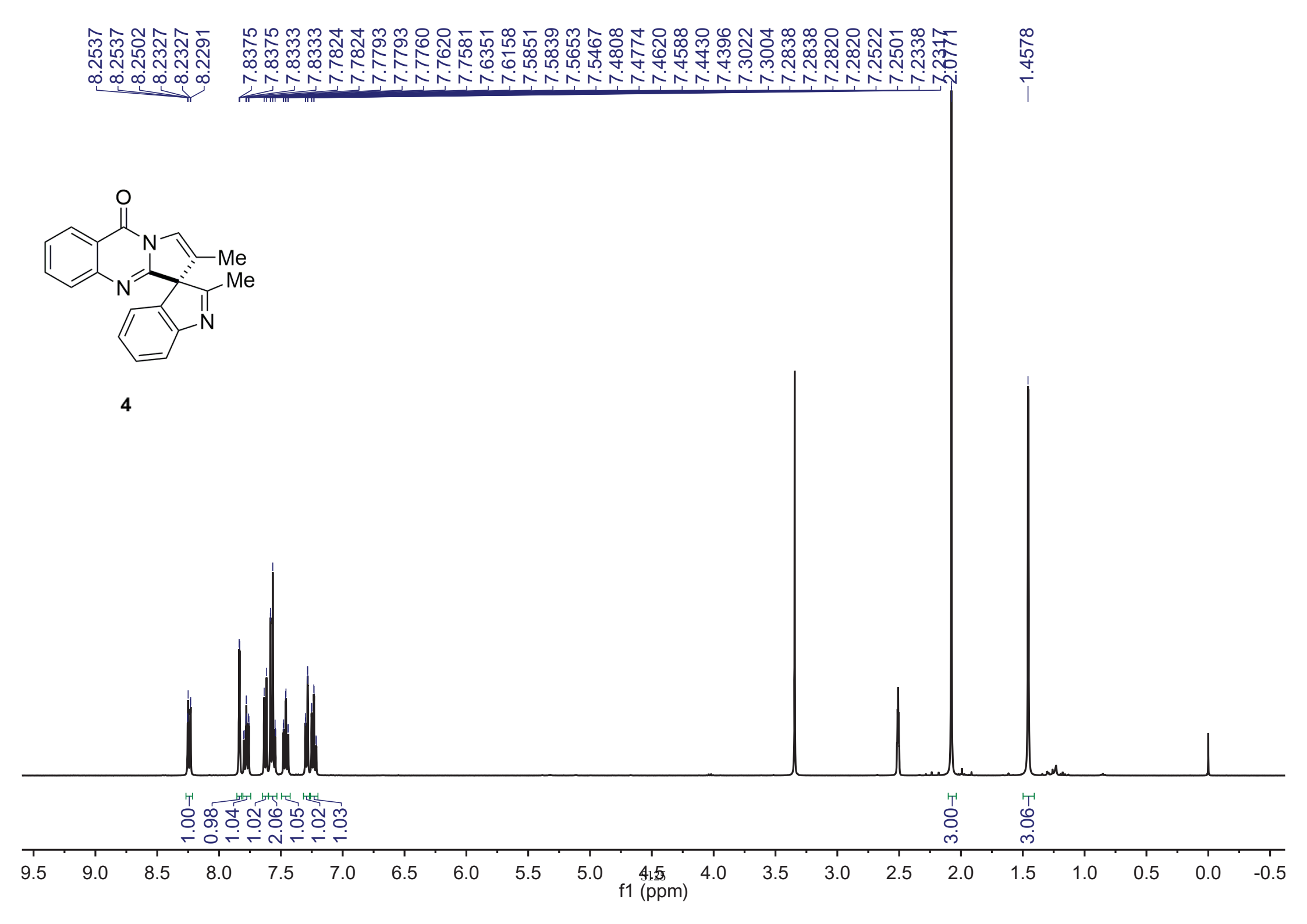
150.93
149.58
146.98
142.14
134.79
132.91
129.60
127.60
127.15
126.30
125.16
124.66
121.20
115.84
97.62
83.68
63.73
50.77
28.30
O
N
N
N
Boc
3aq
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.7824
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7.7760
7.7620
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7.6158
7.5851
7.5839
7.5653
7.5467
7.4808
7.4774
7.4620
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7.4430
7.4396
7.3022
7.3004
7.2838
7.2838
7.2820
7.2820
7.2522
7.2501
7.2338
7.2317
2.0771
1.4578
O
N
N
N
Me
Me
4
1.00
0.98
1.04
1.02
2.06
1.05
1.02
1.03
3.00
3.06
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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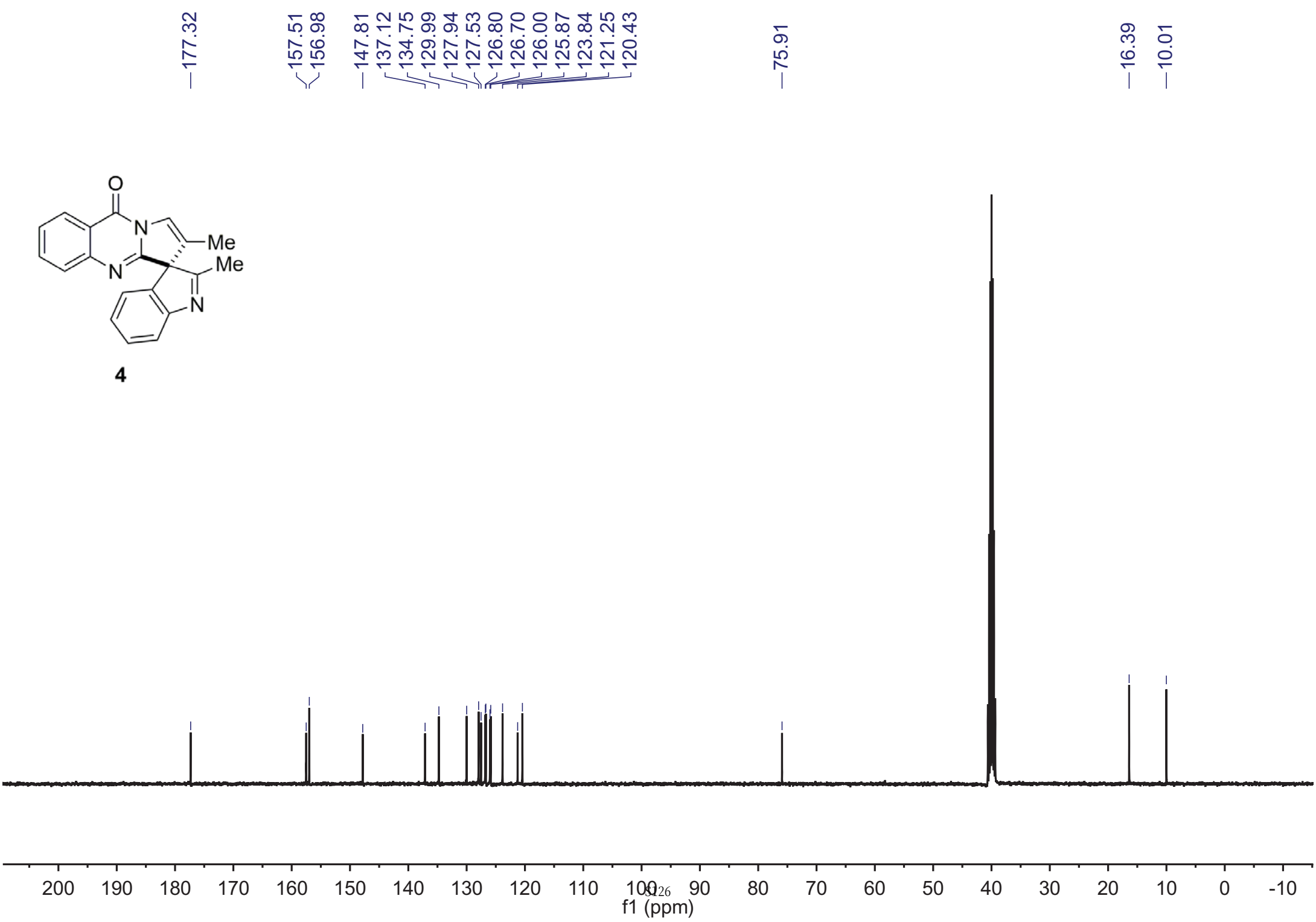
f1 (ppm)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121.25
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75.91
16.39
10.01
O
N
N
N
Me
Me
4
200
190
180
170
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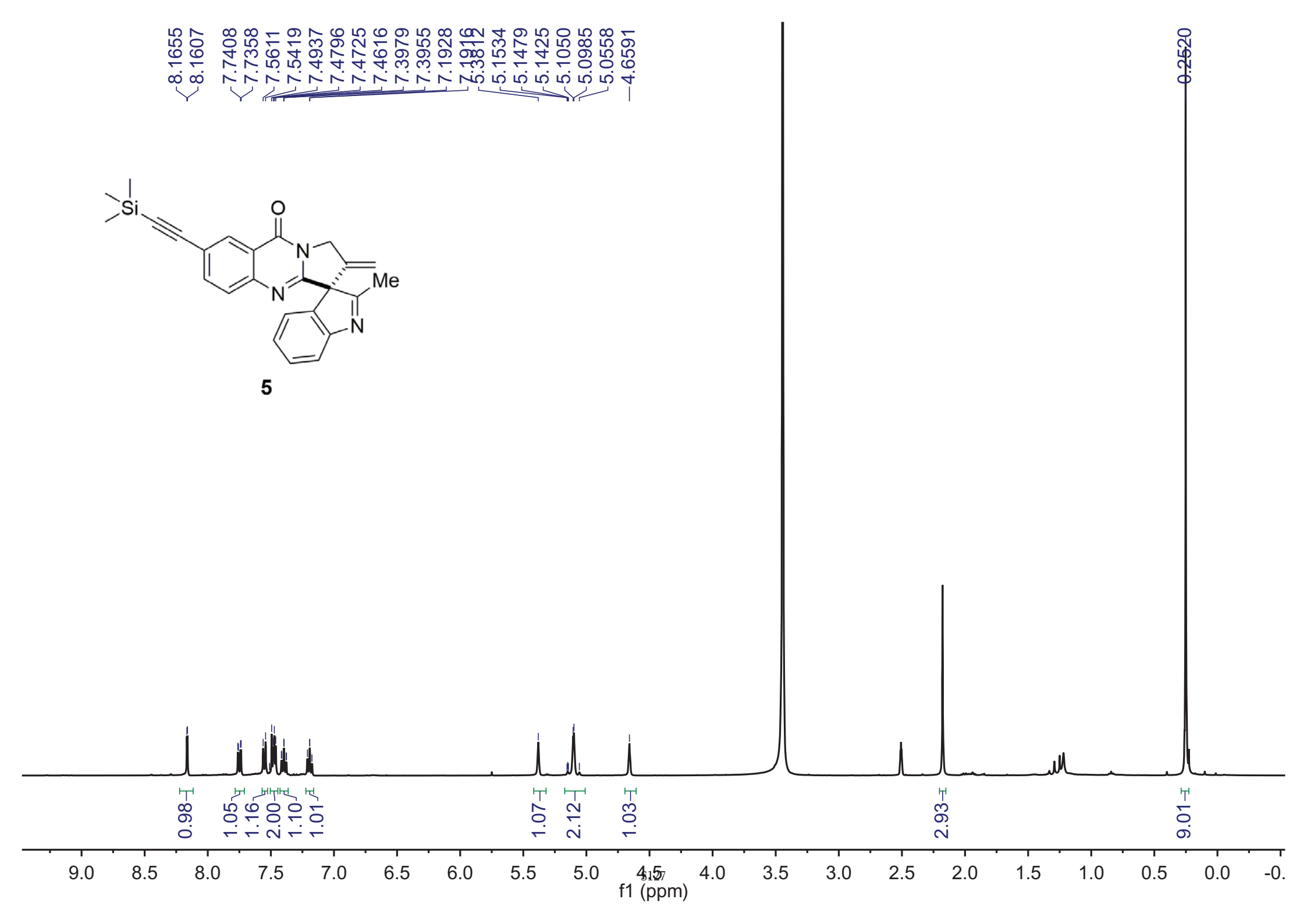
f1 (ppm)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7.1928
7.1916
5.3812
5.1534
5.1479
5.1425
5.1050
5.0985
5.0558
4.6591
0.2520
Si
O
N
N
Me
N
5
0.98
1.05
1.16
2.00
1.10
1.01
1.07
2.12
1.03
2.93
9.01
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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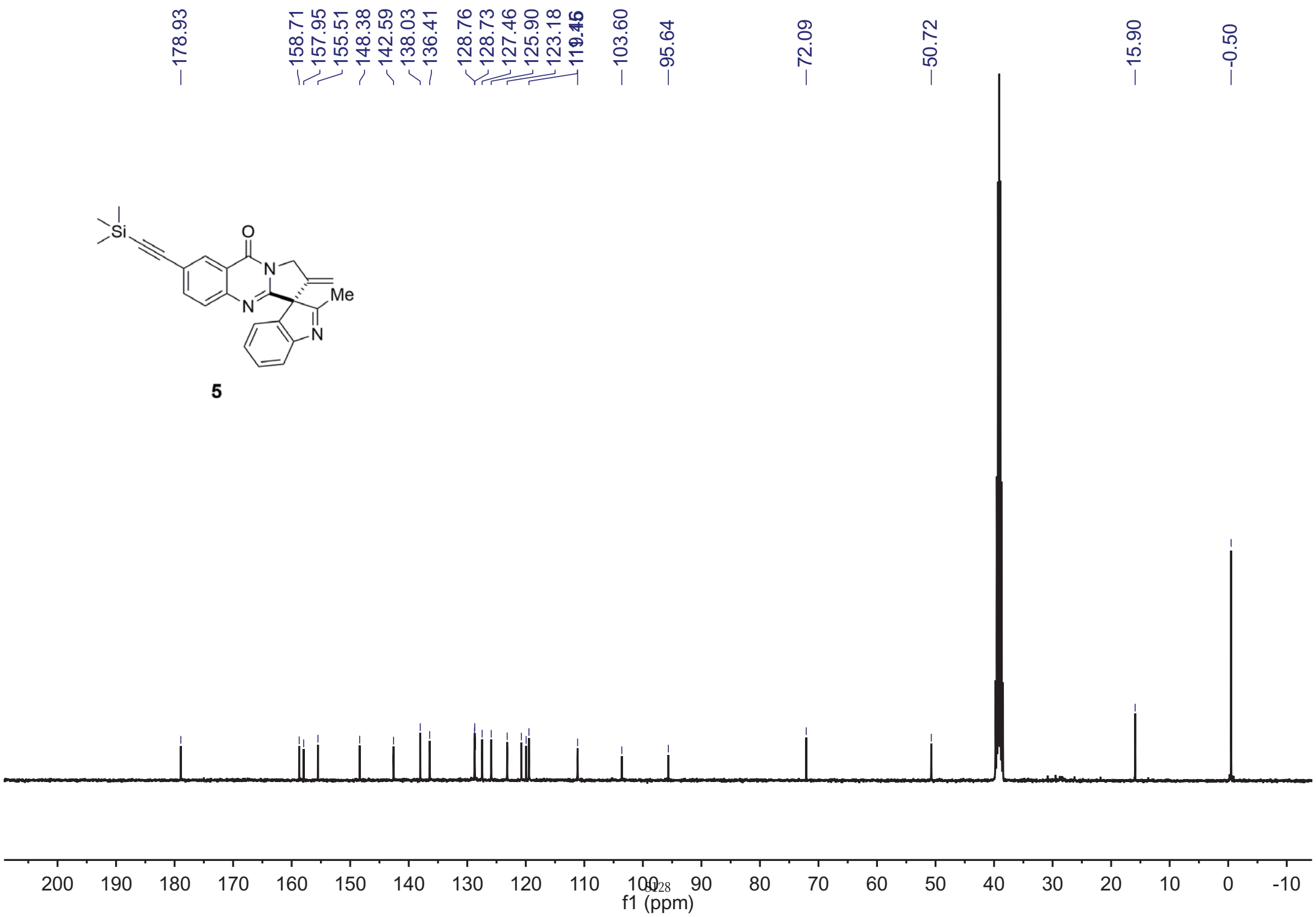
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.
f1 (ppm)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136.41
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128.73
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125.90
123.18
103.60
95.64
72.09
50.72
15.90
-0.50
Si
O
N
N
Me
N
5
200
190
180
170
160
150
140
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120
110
100
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80
70
60
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40
30
20
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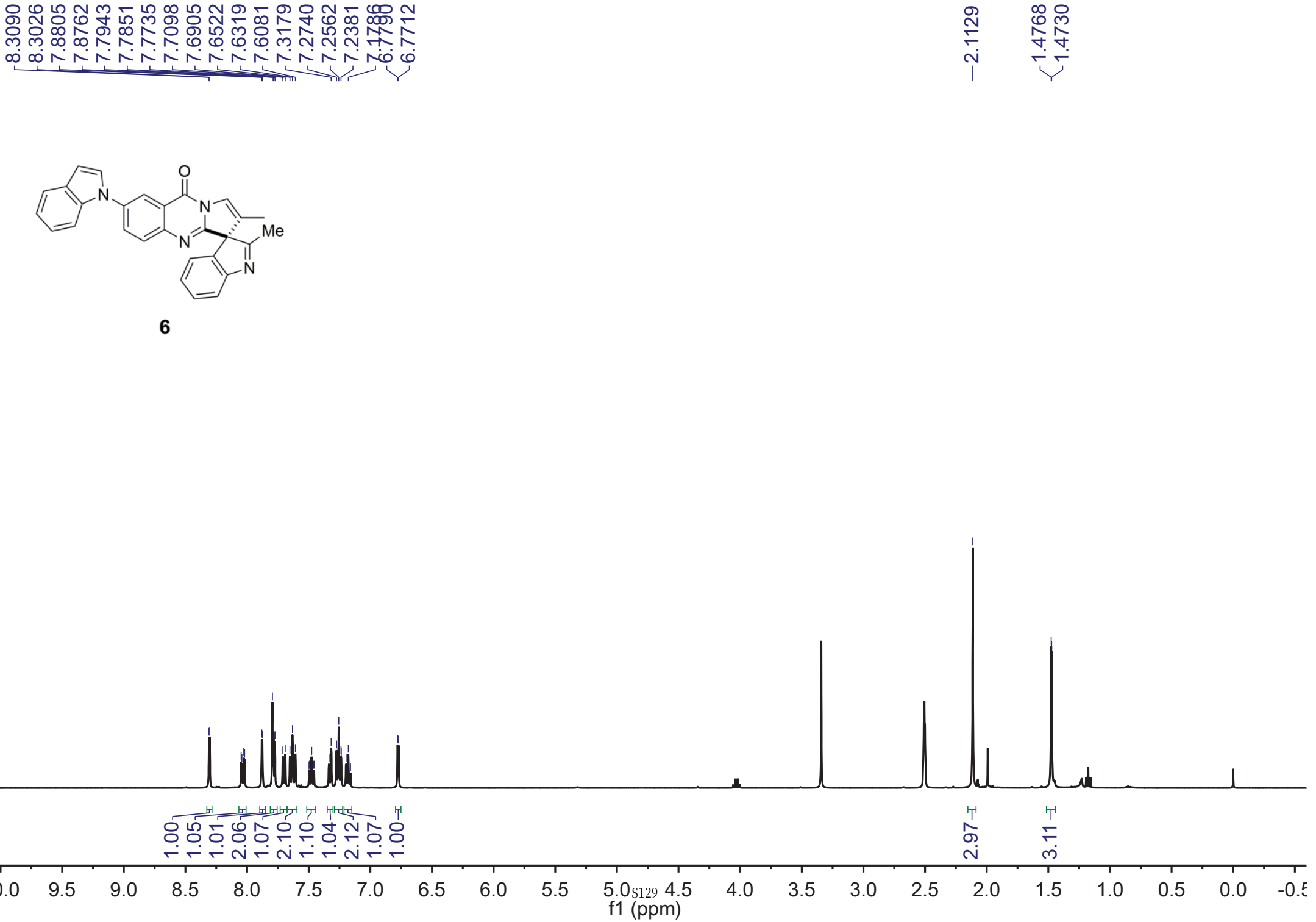
-10
f1 (ppm)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7.6081
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7.2740
7.2562
7.2381
7.1786
6.7790
6.7712
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1.4768
1.4730
O
N
N
N
N
Me
1.00
1.05
1.01
2.06
1.07
2.10
1.10
1.04
2.12
1.07
1.00
2.97
3.11
10.0
9.5
9.0
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8.0
7.5
7.0
6.5
6.0
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4.0
3.5
3.0
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1.0
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0.0
f1 (ppm)

6

O
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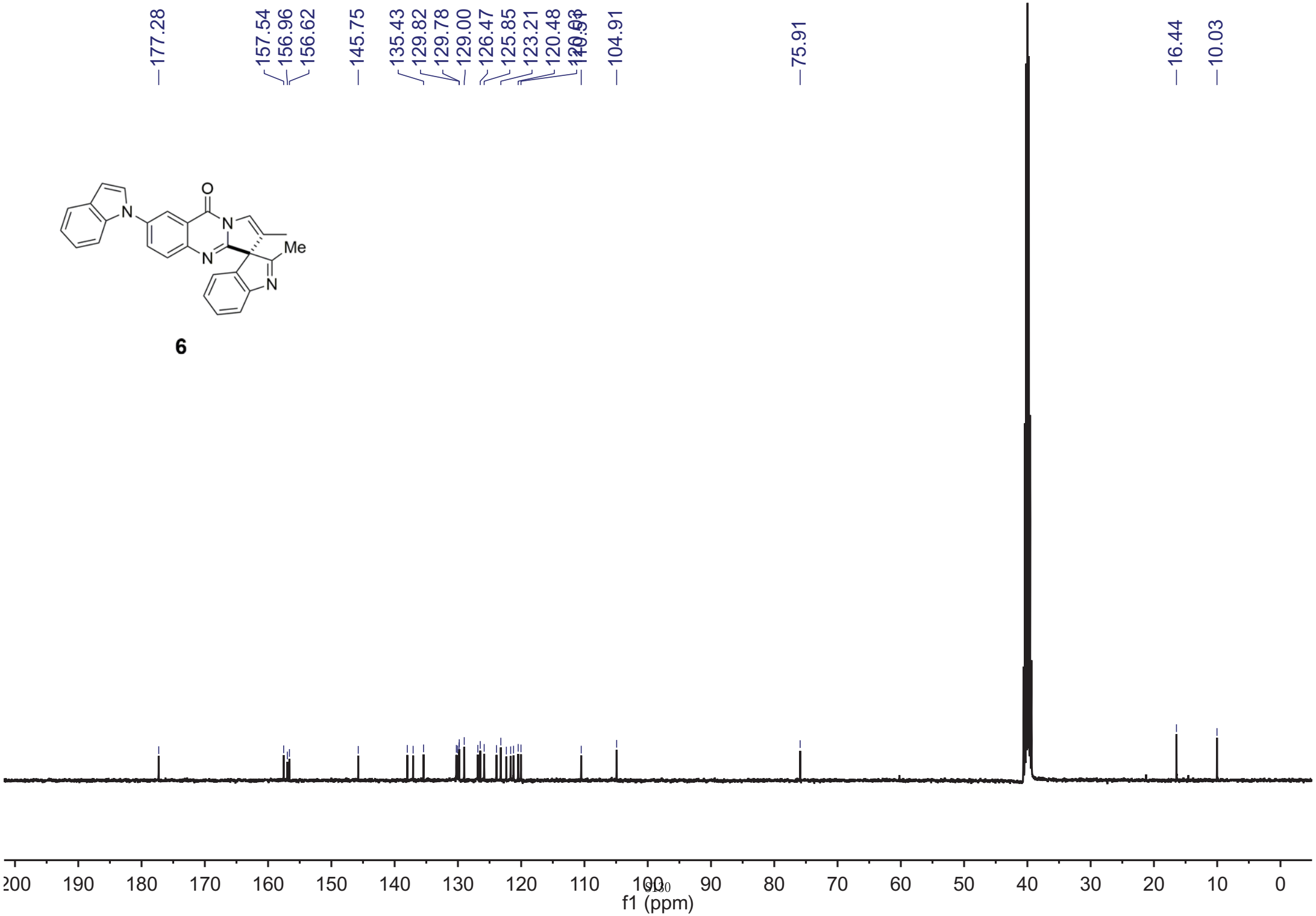
N
N
Me
N

6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129.78
129.00
126.47
125.85
123.21
120.48
104.91
75.91
16.44
10.03
200
190
180
170
160
150
140
130
120
110
100
90
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70
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50
40
30
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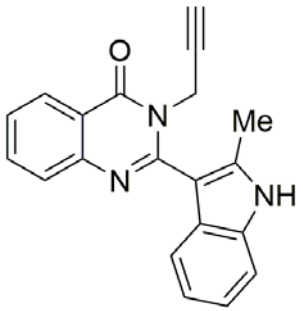
10
0
f1 (ppm)



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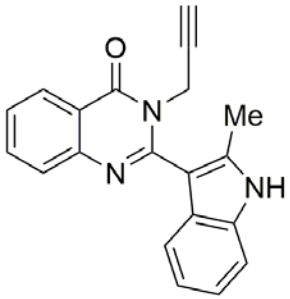

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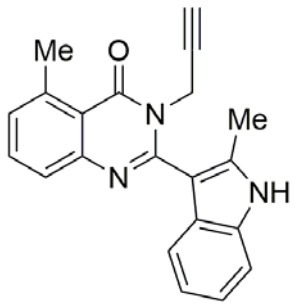

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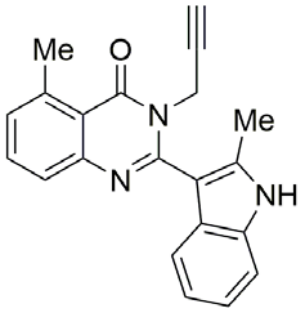

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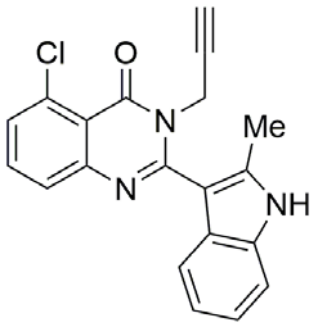

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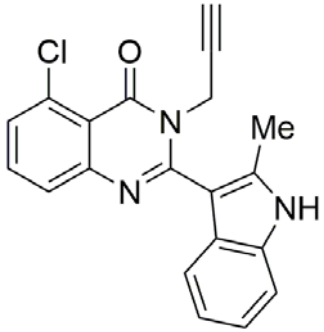

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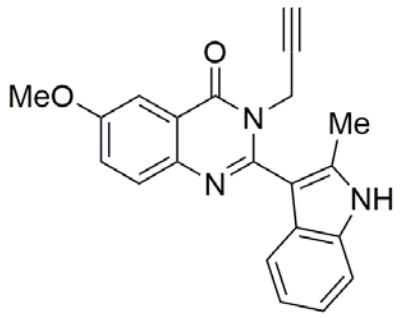

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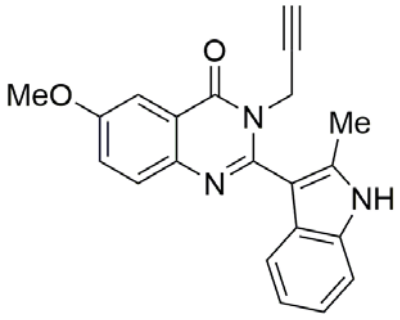

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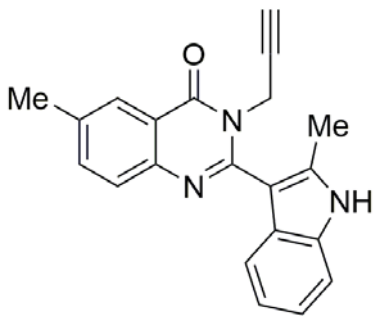

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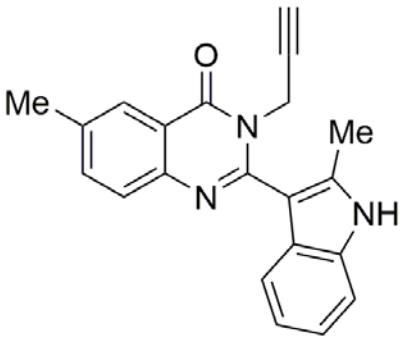

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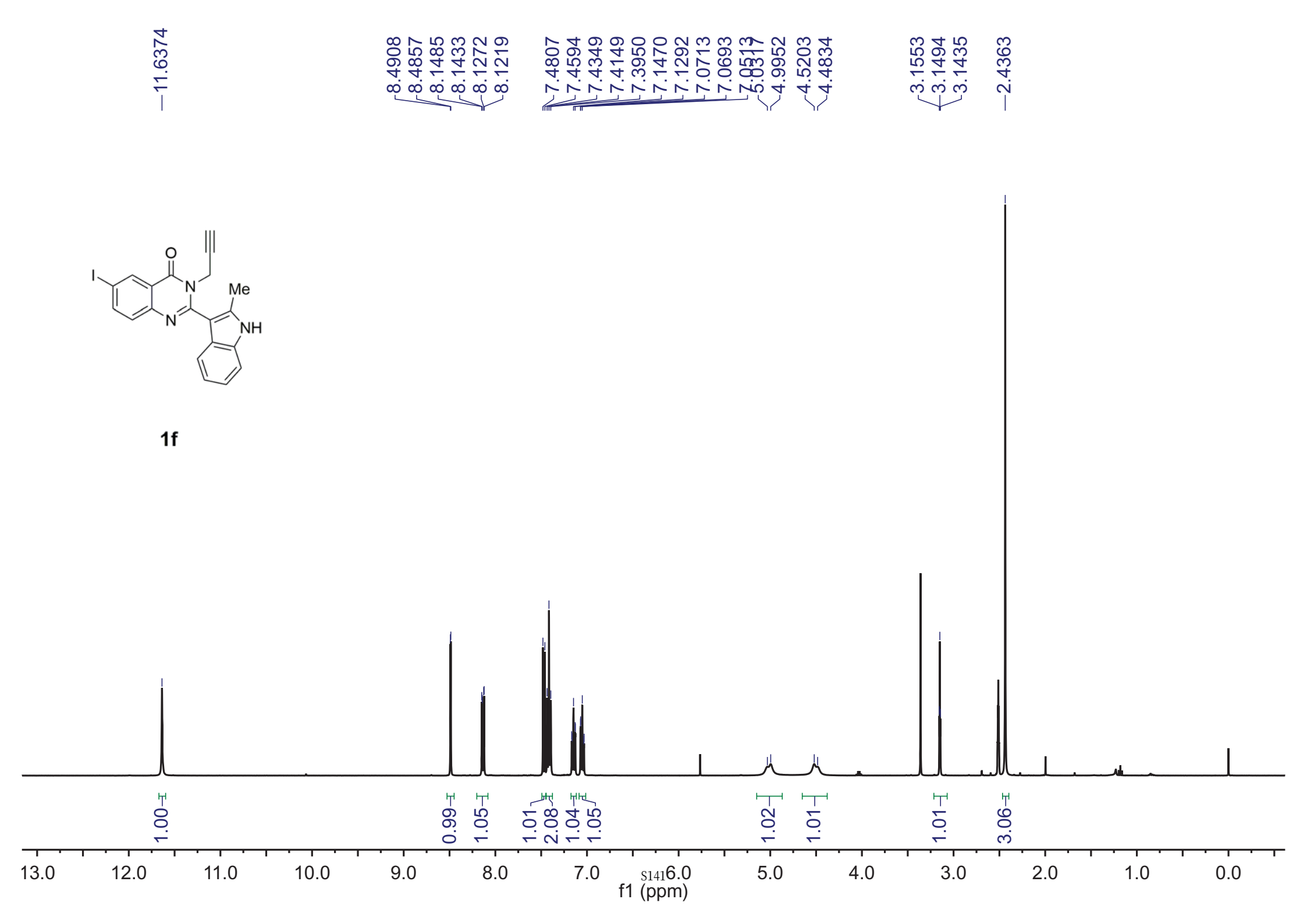
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8.1219
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7.4149
7.3950
7.1470
7.1292
7.0713
7.0693
7.0513
7.0317
4.9952
4.5203
4.4834
3.1553
3.1494
3.1435
2.4363
O
I
N
N
Me
NH
1.00
0.99
1.05
1.01
2.08
1.04
1.05
1.02
1.01
1.01
3.06
13.0
12.0
11.0
10.0
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8.0
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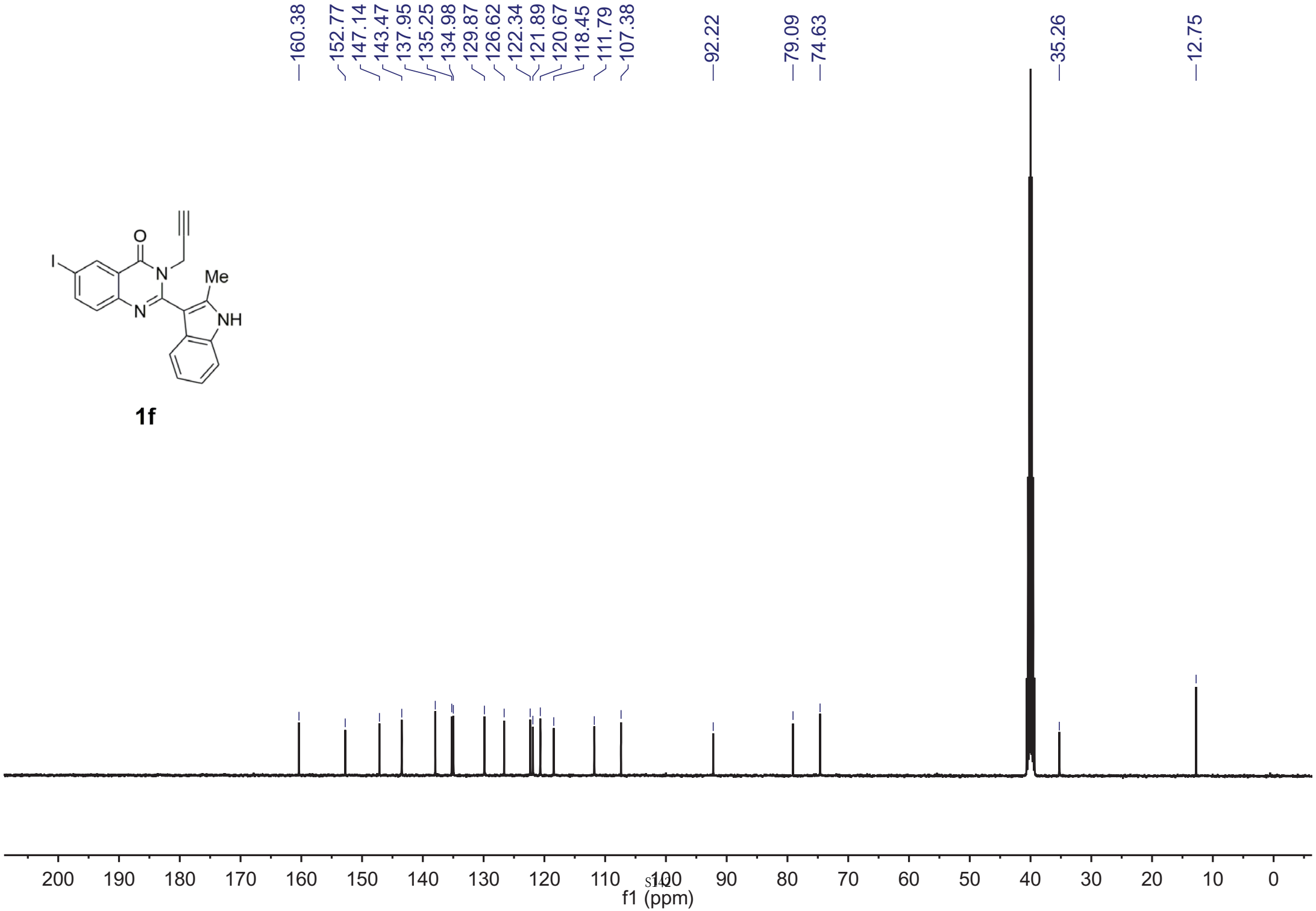
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

1f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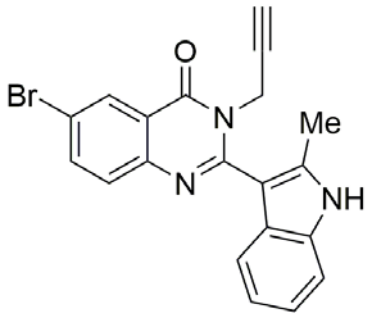
152.77
147.14
143.47
137.95
135.25
134.98
129.87
126.62
122.34
121.89
120.67
118.45
111.79
107.38
92.22
79.09
74.63
35.26
12.75
O
I
N
N
Me
NH
1f
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



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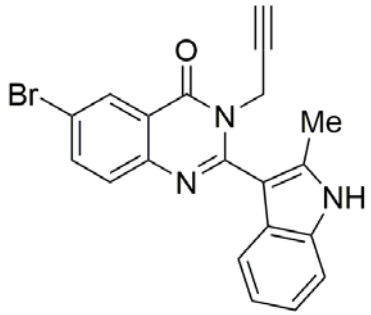
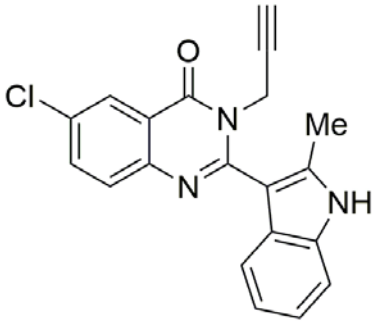


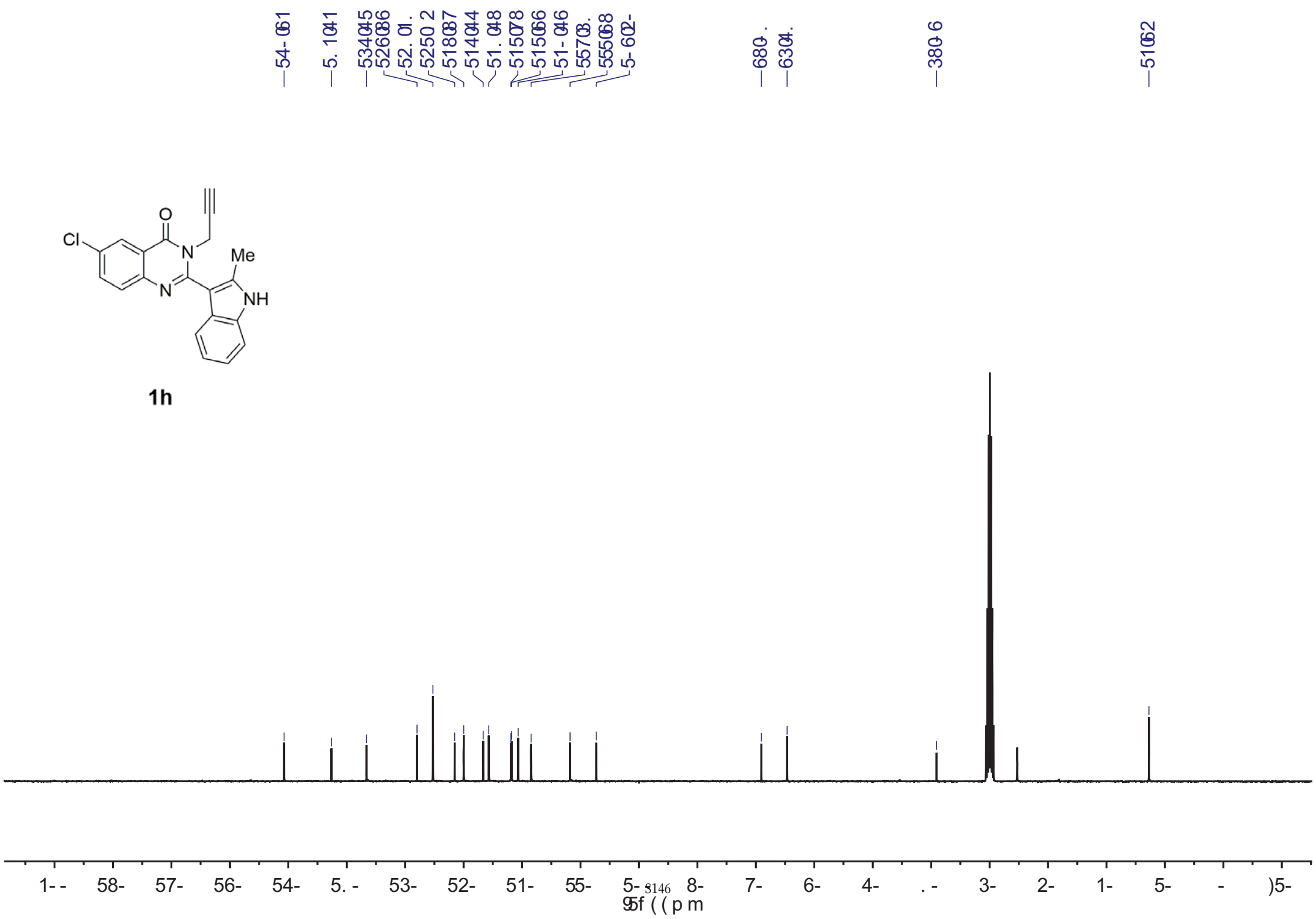
1g



1h

O
Cl
N
Me
N
NH

1h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525022
518087
514044
51.048
515078
515066
51-046
55708.
555068
5-602-
680.
6304.
3806
51062
1--
58-
57-
56-
54-
5.-
53-
52-
51-
55-
5-
8-
7-
6-
4-
.-
3-
2-
1-
5-
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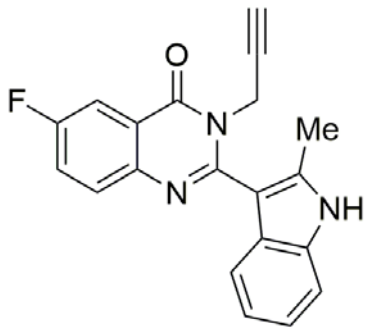
)5-
95f ((pm



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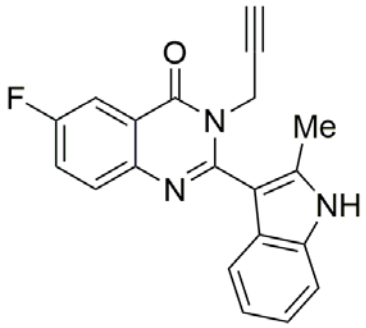
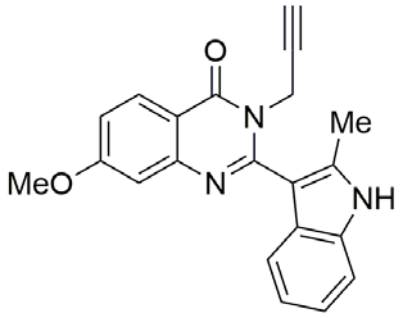
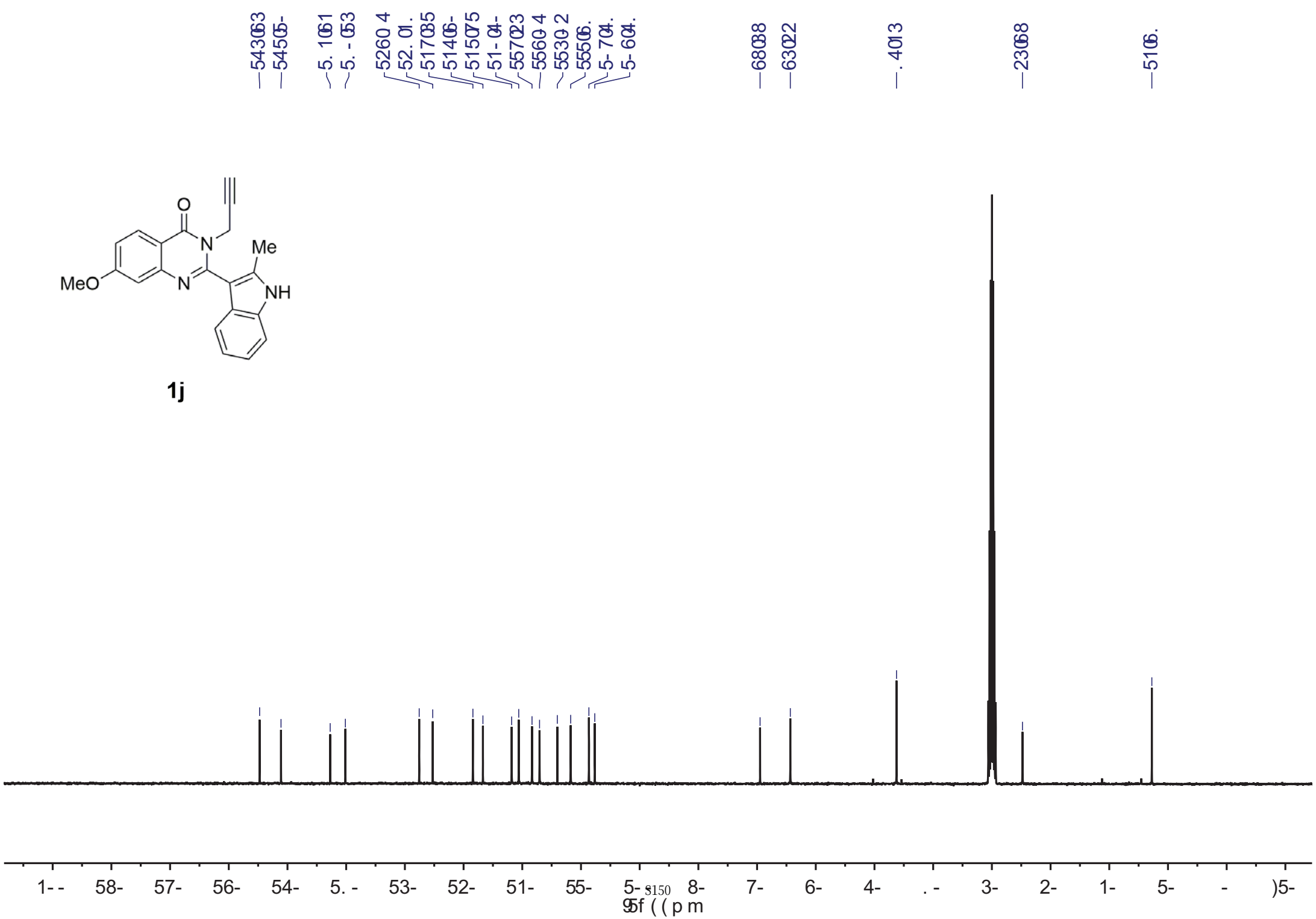


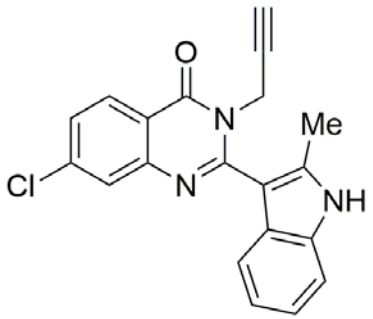
1i



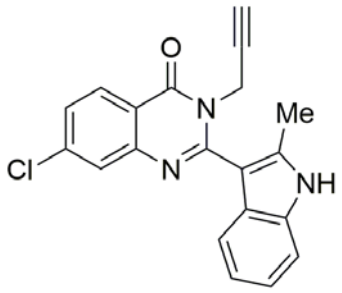
1j

1j

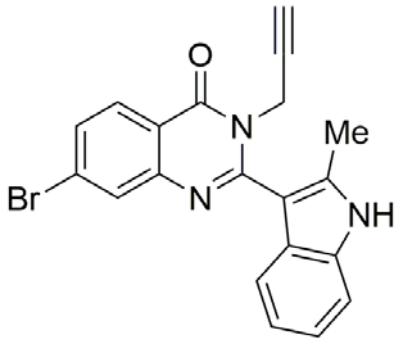




1k



1k



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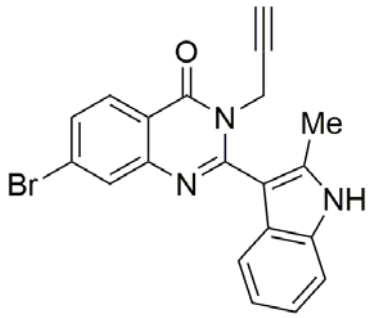
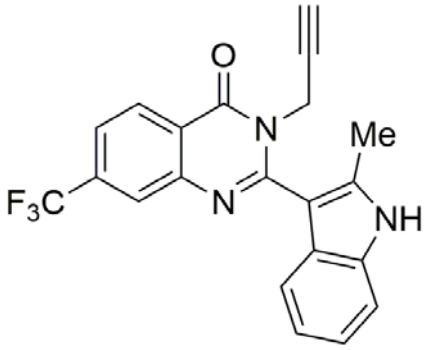
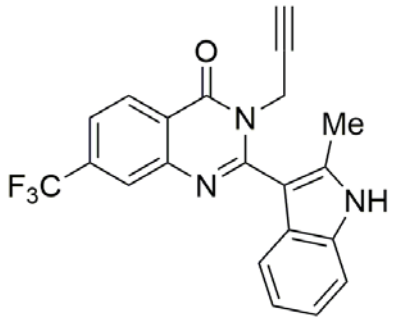


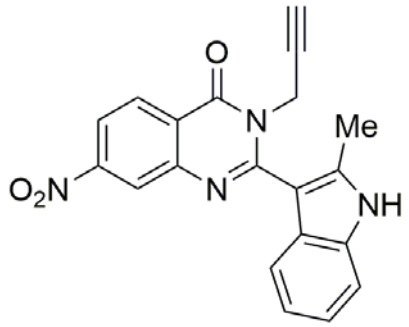
1l



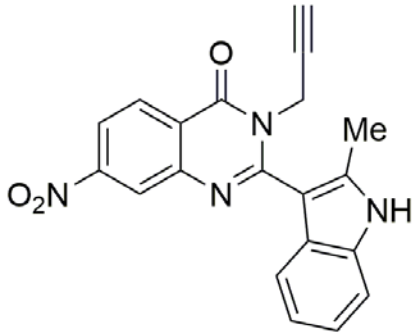
1m



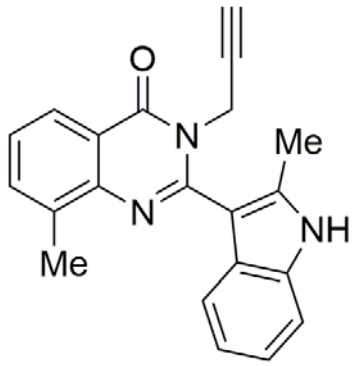
1m



1n



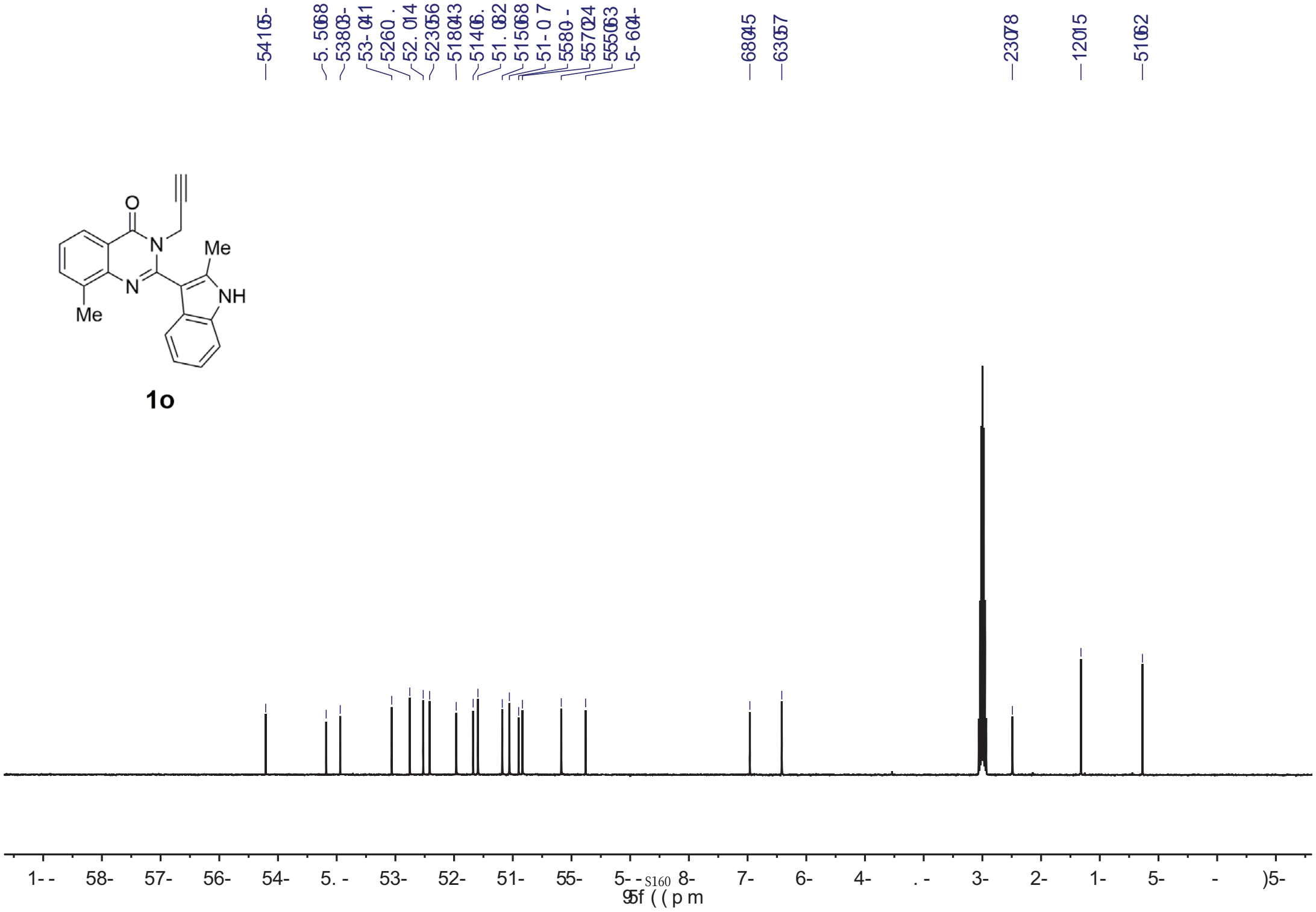
1n



1o

O
N
Me
N
NH
Me

1o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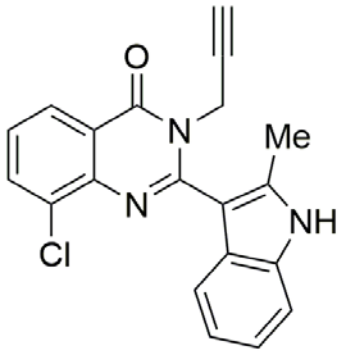
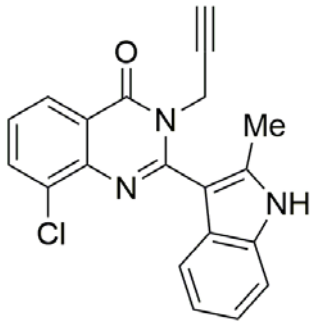
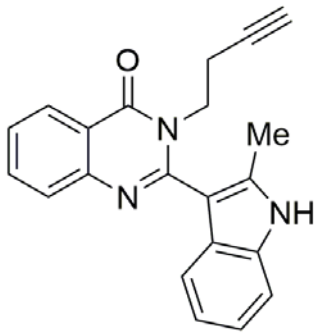
51804
51406.
51.082
51568
51-07
5580-
55702
55563
5-604-
68045
63057
23078
12015
51062
1--
58-
57-
56-
54-
5.-
53-
52-
51-
55-
5--
8-
7-
6-
4-
.-
3-
2-
1-
5-
-
)5-
95f ((pm



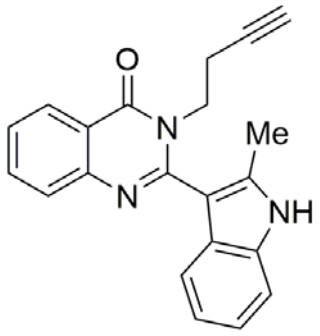
1p



1p



1q



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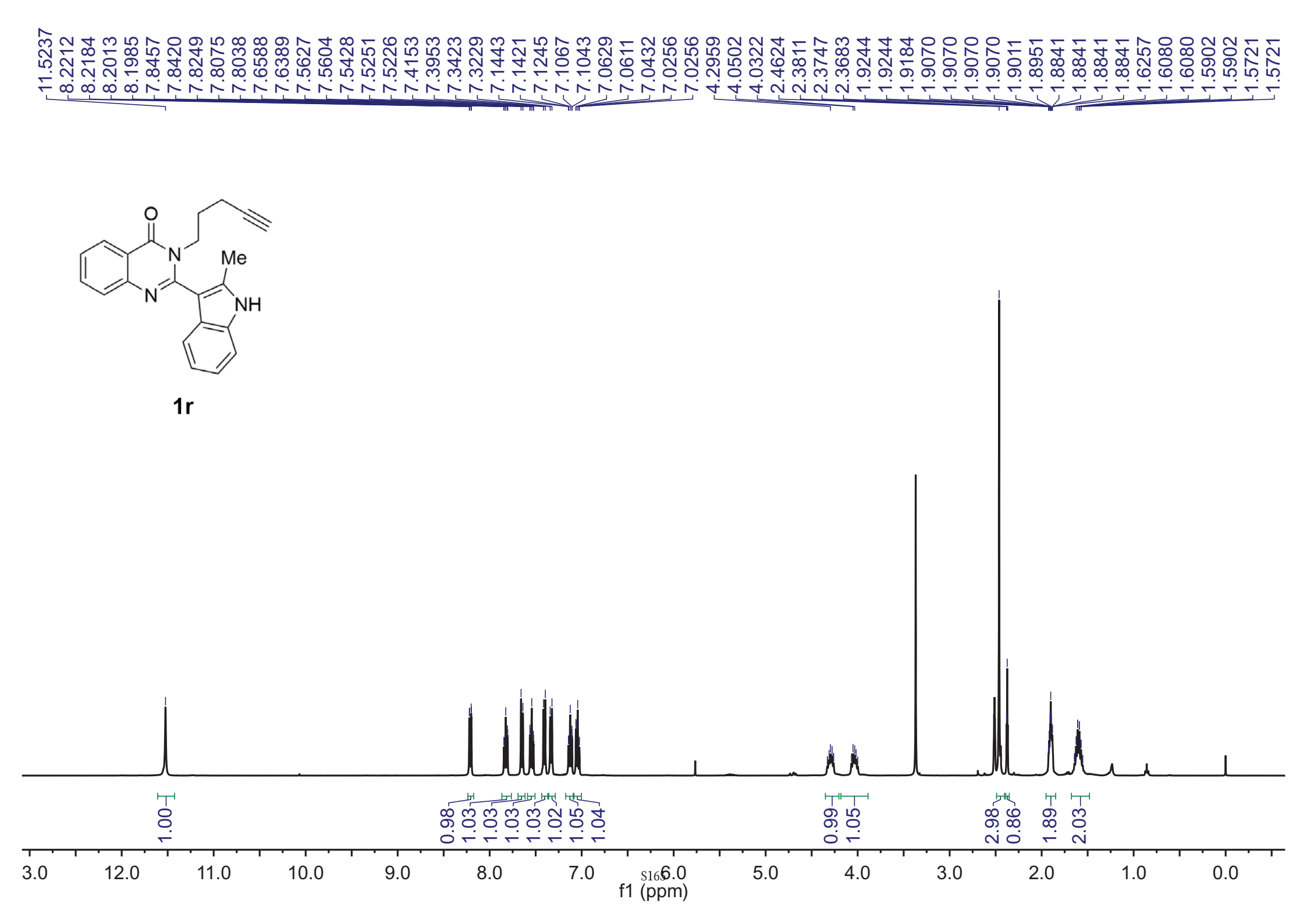
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O
N
Me
N
NH
1r
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0.98
1.03
1.03
1.03
1.03
1.02
1.05
1.04
0.99
1.05
2.98
0.86
1.89
2.03
3.0
12.0
11.0
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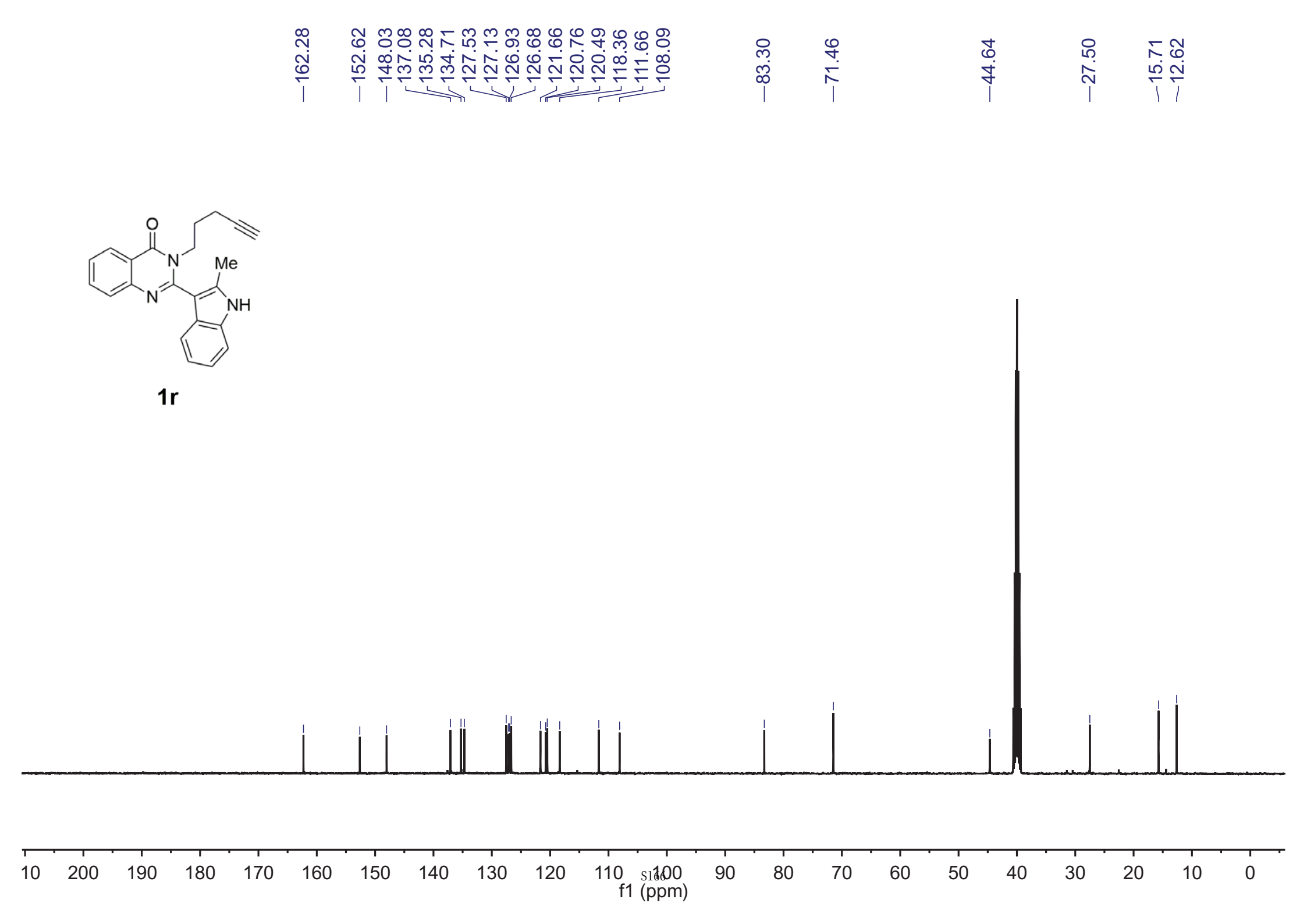
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)


162.28
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127.13
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126.68
121.66
120.76
120.49
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111.66
108.09
83.30
71.46
44.64
27.50
15.71
12.62
O
N
Me
N
NH
1r
10
200
190
180
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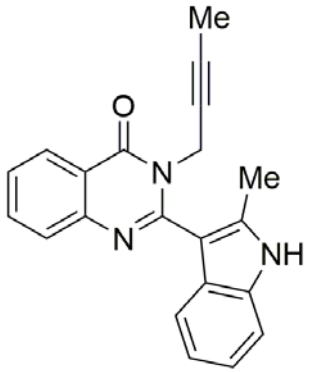
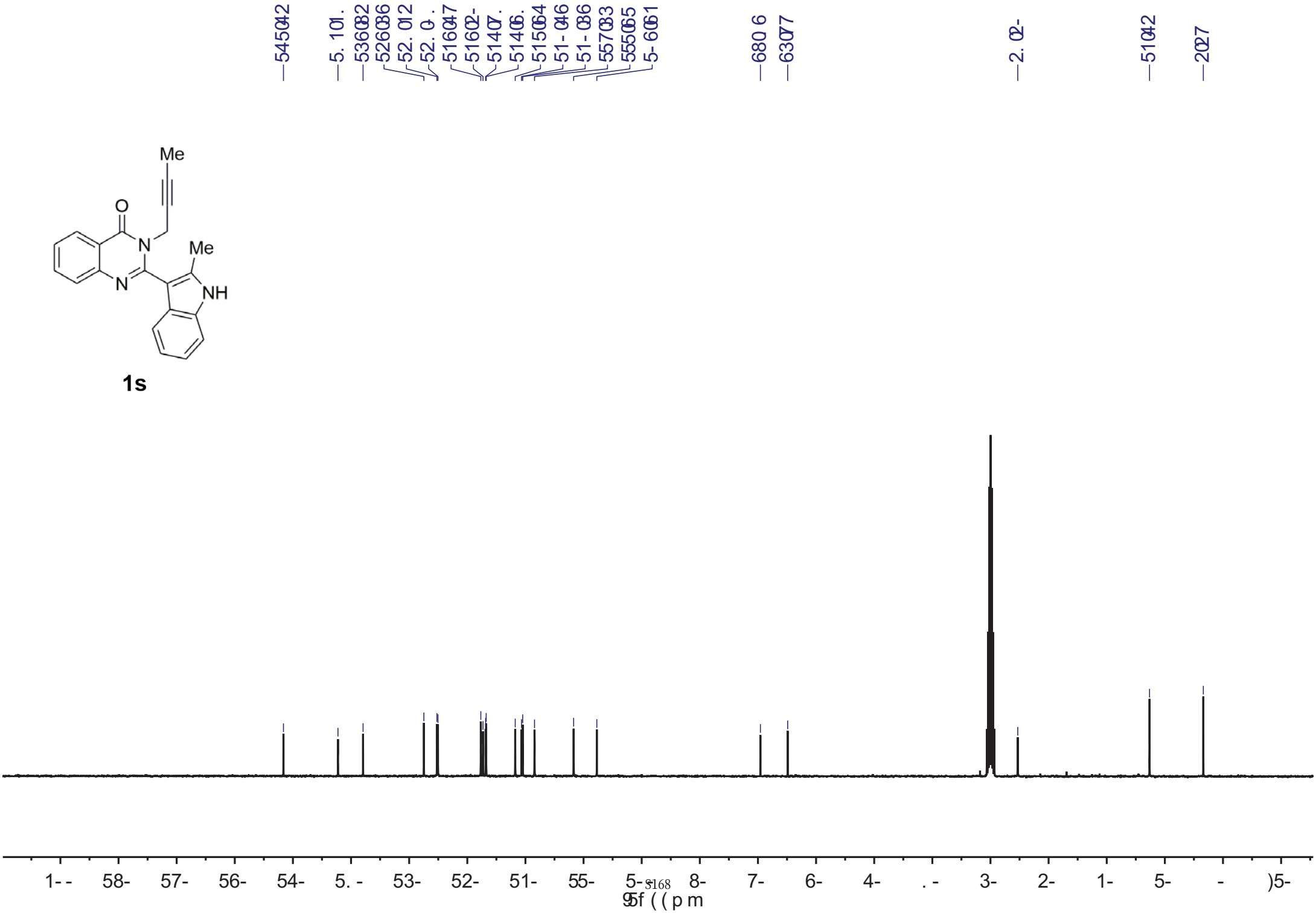
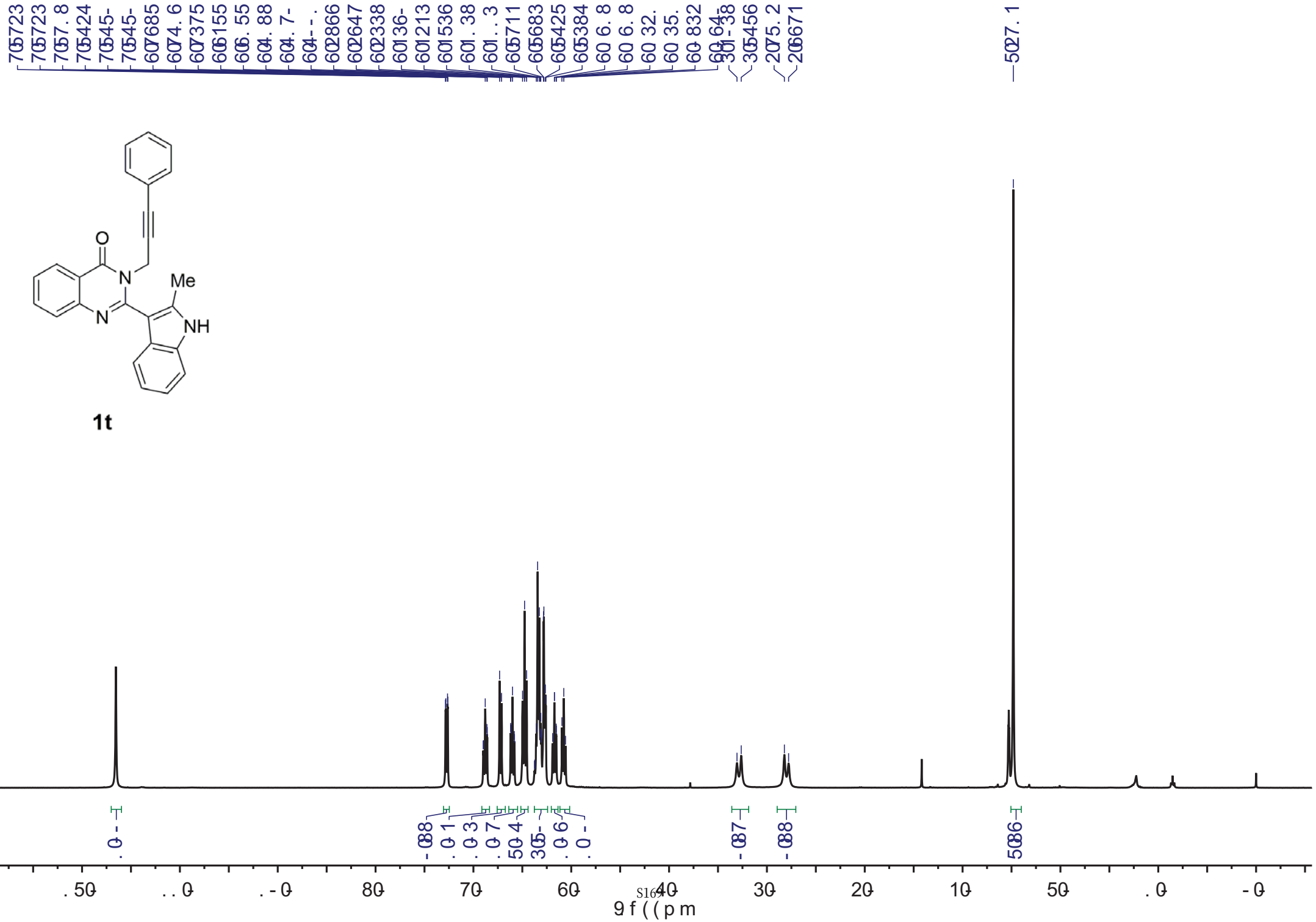
f1 (ppm)



1s

1s

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NH
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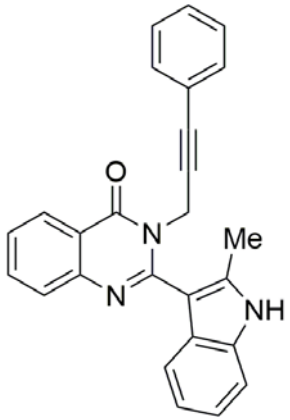

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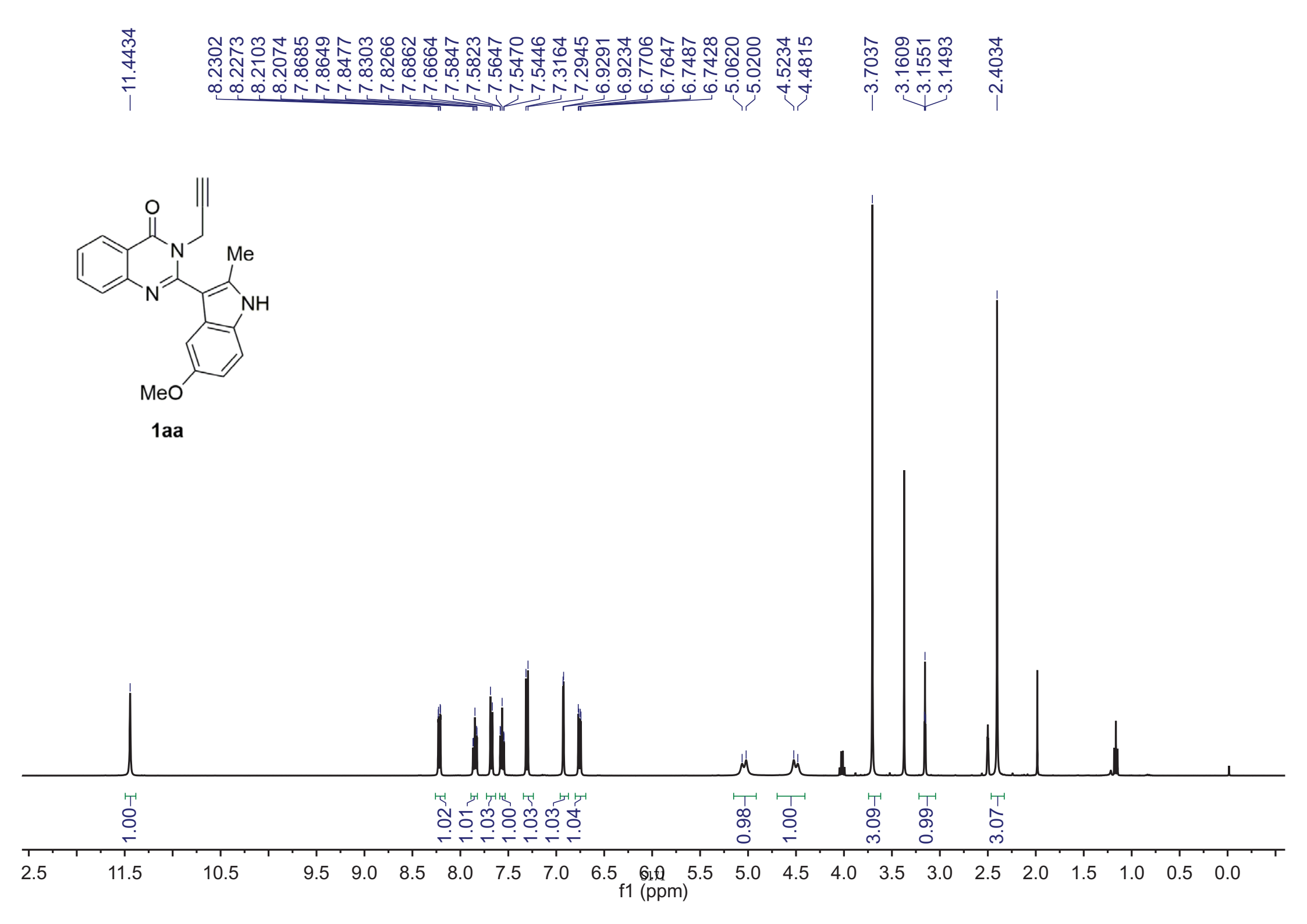
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7.6862
7.6664
7.5847
7.5823
7.5647
7.5470
7.5446
7.3164
7.2945
6.9291
6.9234
6.7706
6.7647
6.7487
6.7428
5.0620
5.0200
4.5234
4.4815
3.7037
3.1609
3.1551
3.1493
2.4034
O
N
Me
N
NH
MeO
1aa
1.00
1.02
1.01
1.03
1.00
1.03
1.03
1.04
0.98
1.00
3.09
0.99
3.07
2.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
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6.5
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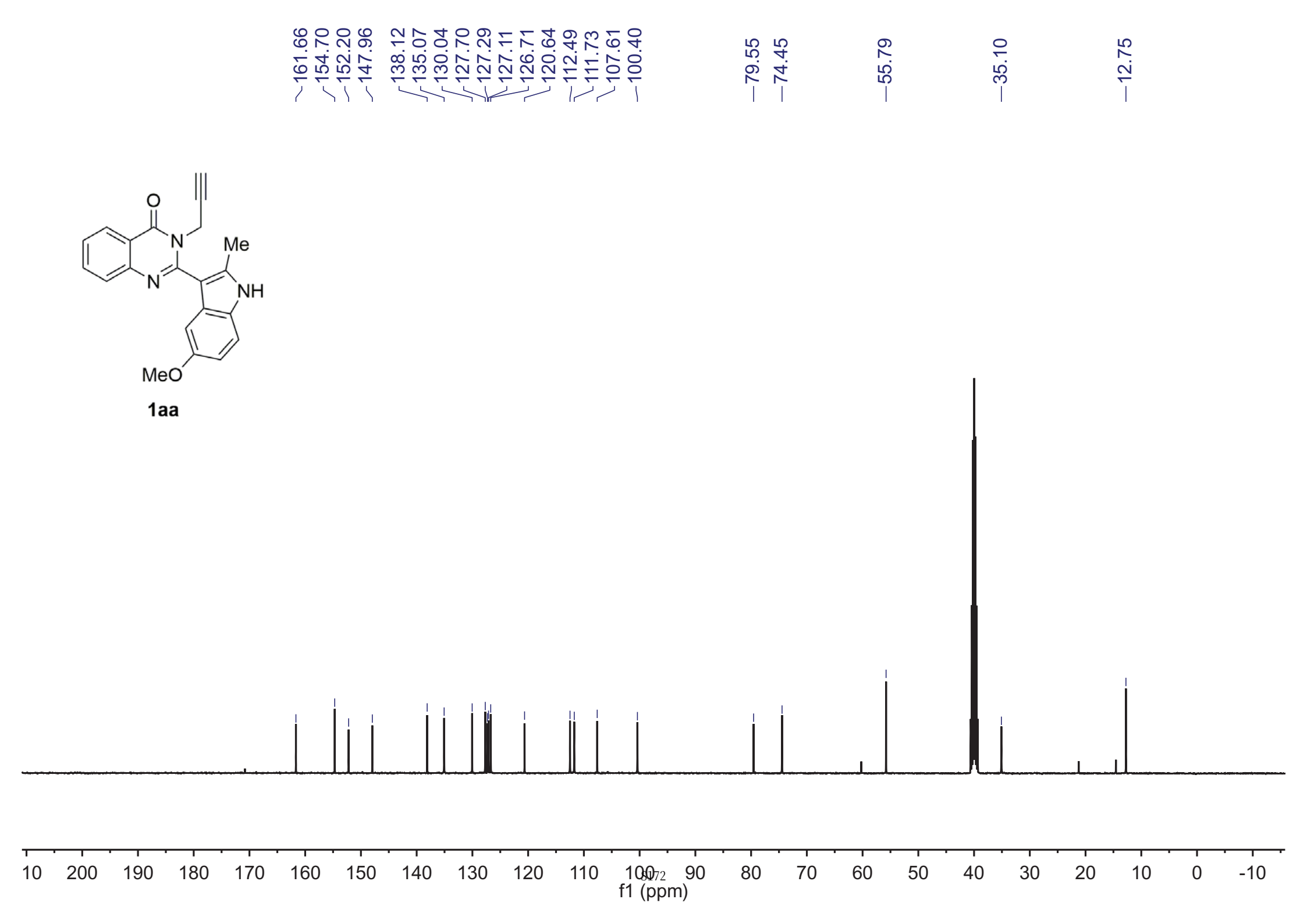
0.0
f1 (ppm)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135.07
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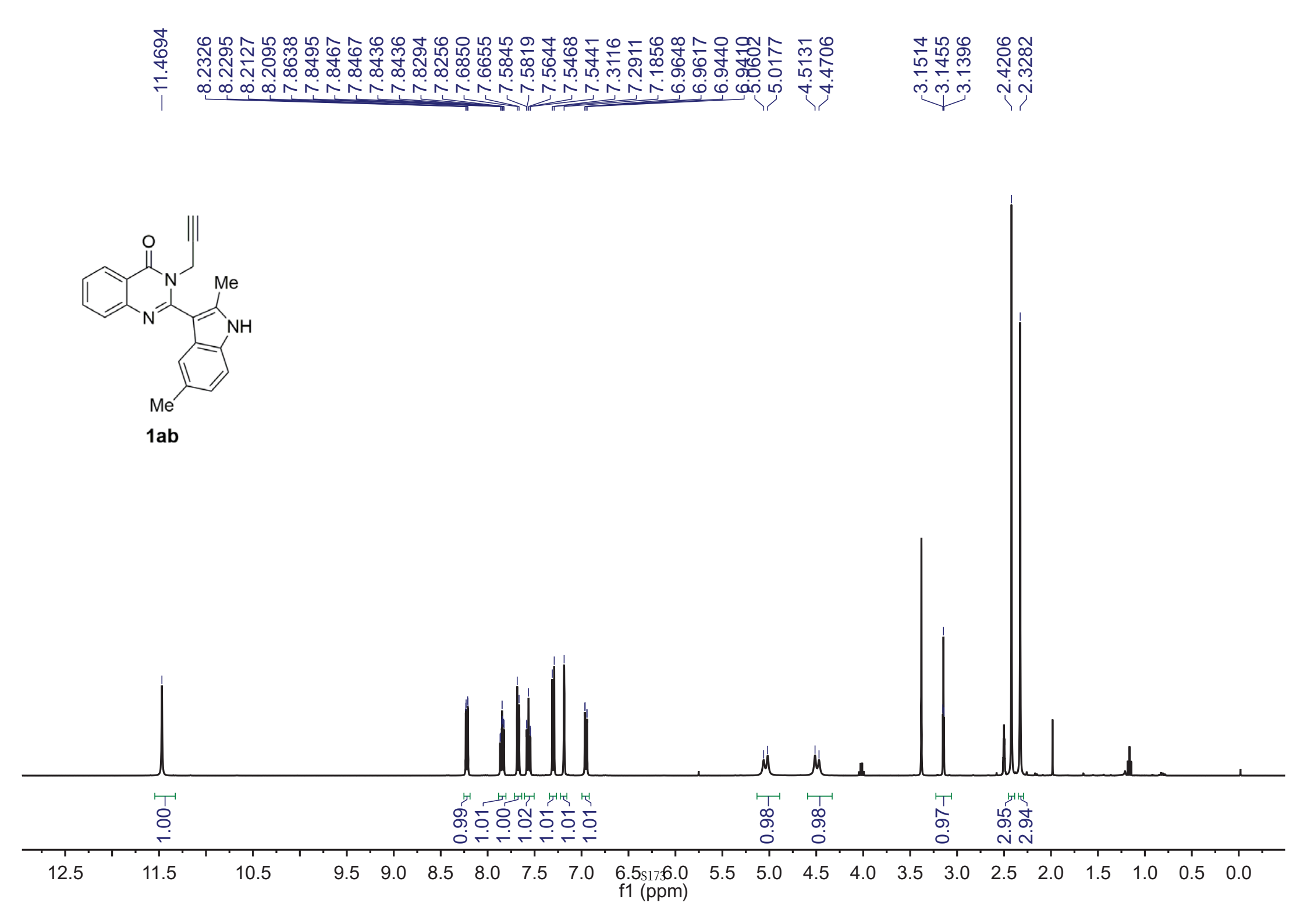
127.70
127.29
127.11
126.71
120.64
112.49
111.73
107.61
100.40
79.55
74.45
55.79
35.10
12.75
O
N
N
Me
NH
MeO
1aa
10 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.8256
7.6850
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7.5845
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7.5644
7.5468
7.5441
7.3116
7.2911
7.1856
6.9648
6.9617
6.9440
6.9410
5.0602
5.0177
4.5131
4.4706
3.1514
3.1455
3.1396
2.4206
2.3282
O
N
N
Me
NH
Me
1ab
1.00
0.99
1.01
1.00
1.02
1.01
1.01
1.01
0.98
0.98
0.97
2.95
2.94
12.5
11.5
10.5
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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1.0
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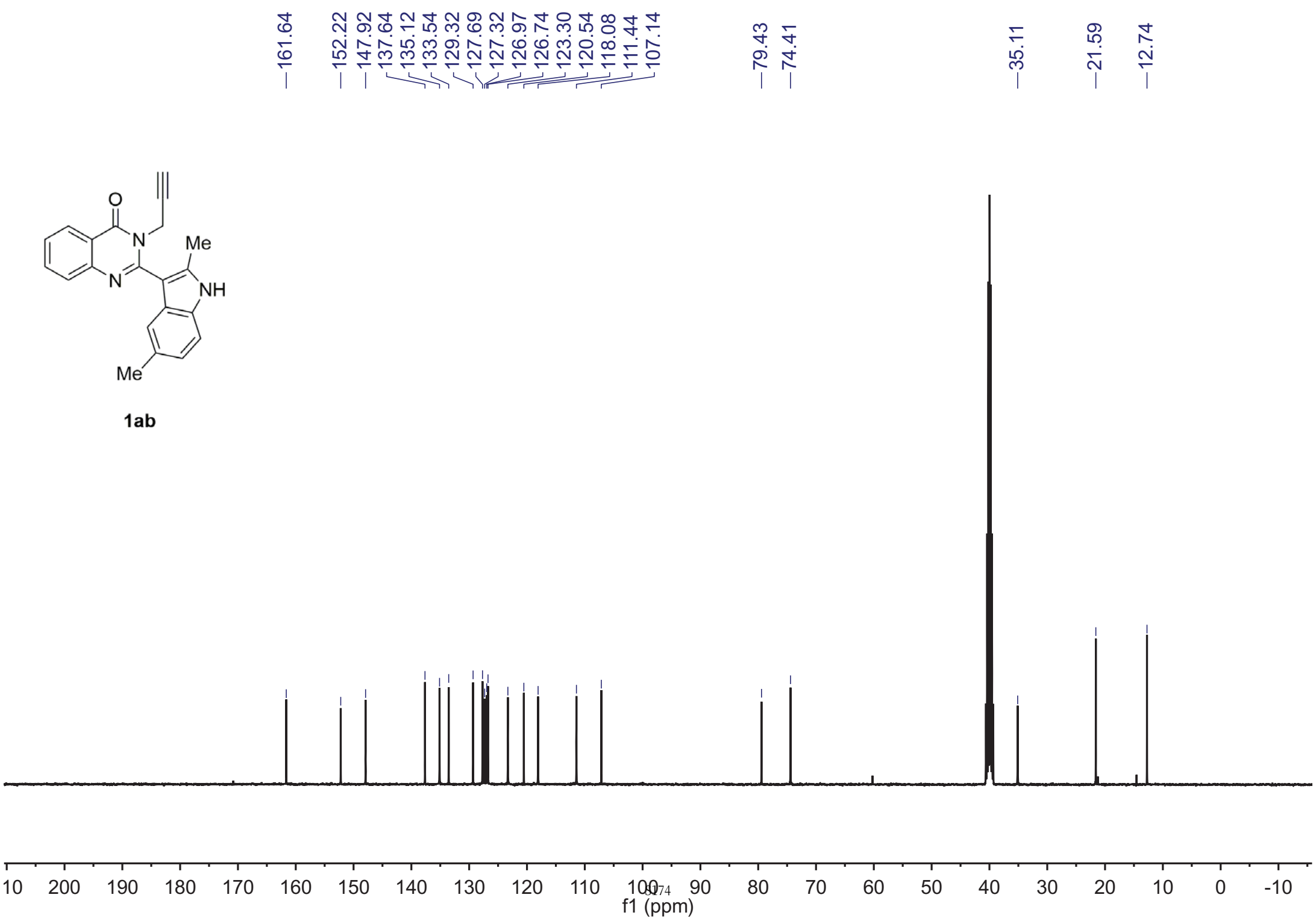
0.0
f1 (ppm)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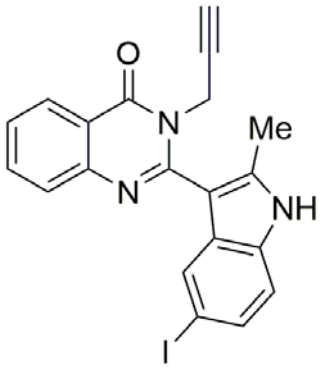
126.97
126.74
123.30
120.54
118.08
111.44
107.14
79.43
74.41
35.11
21.59
12.74
O
N
N
Me
NH
Me
1ab
f1 (ppm)



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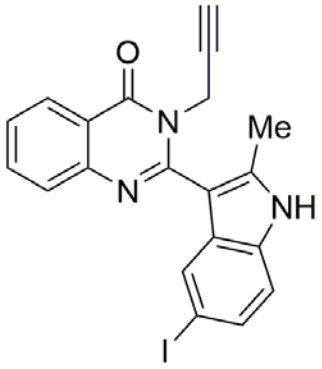

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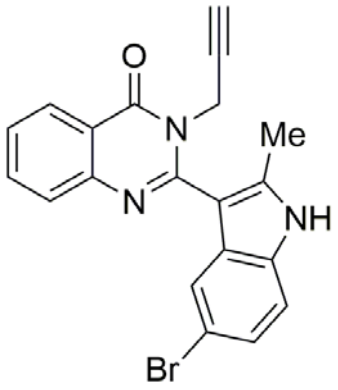

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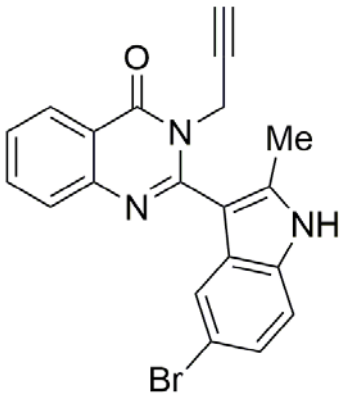

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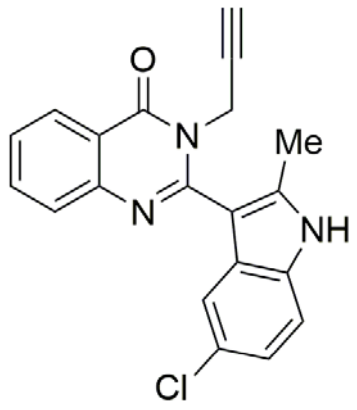

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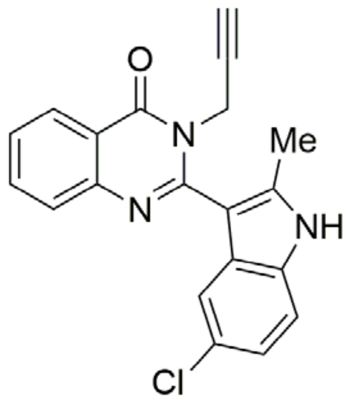

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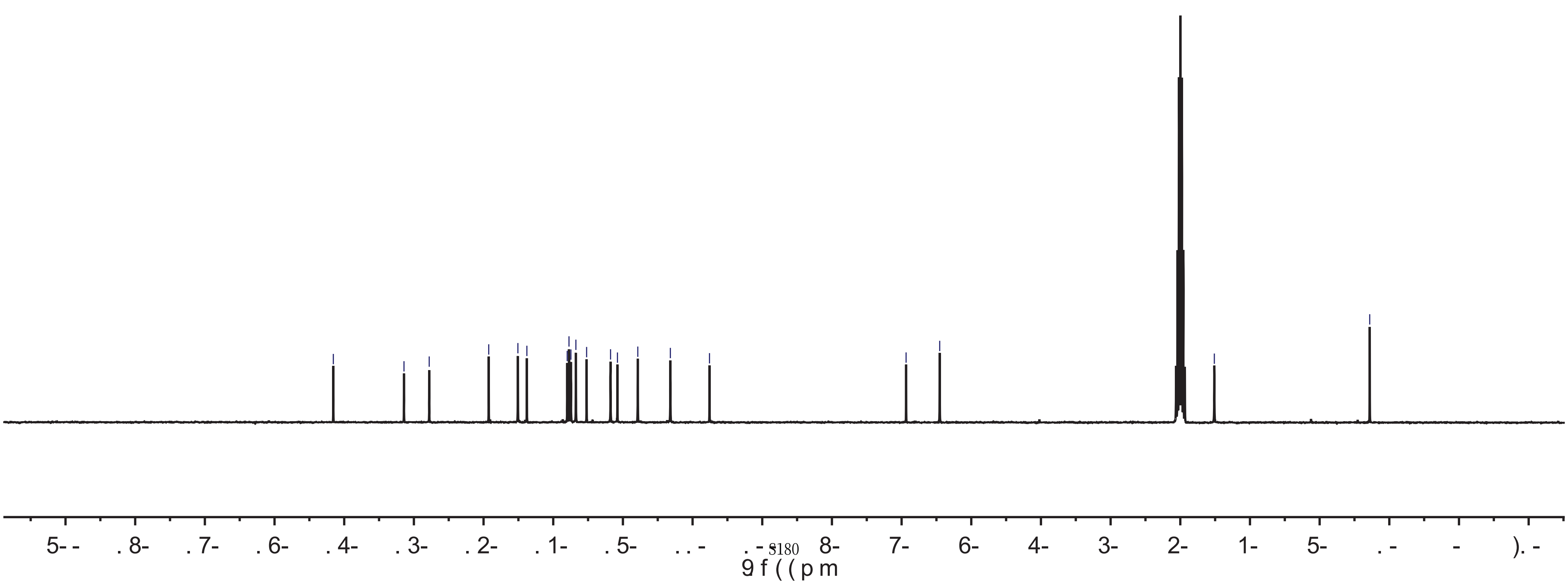

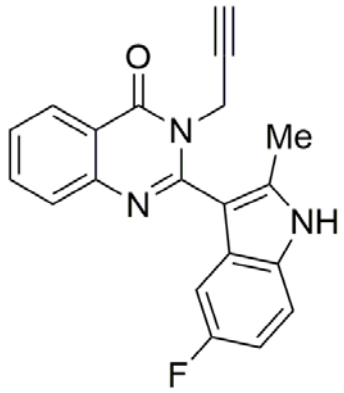

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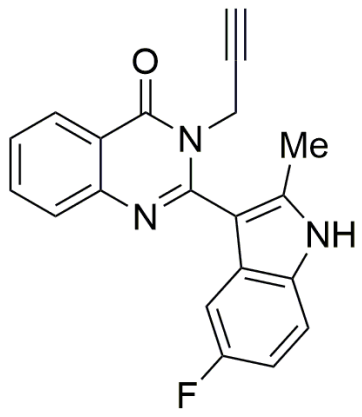

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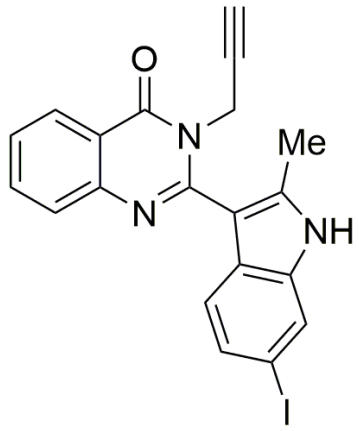

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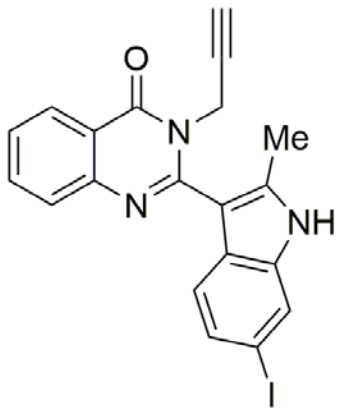

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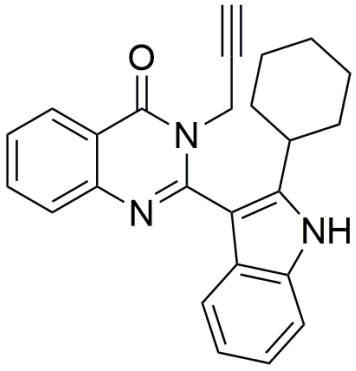

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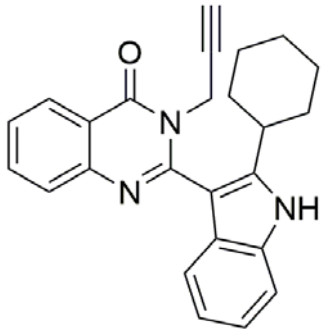

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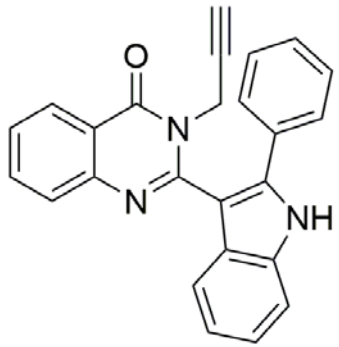
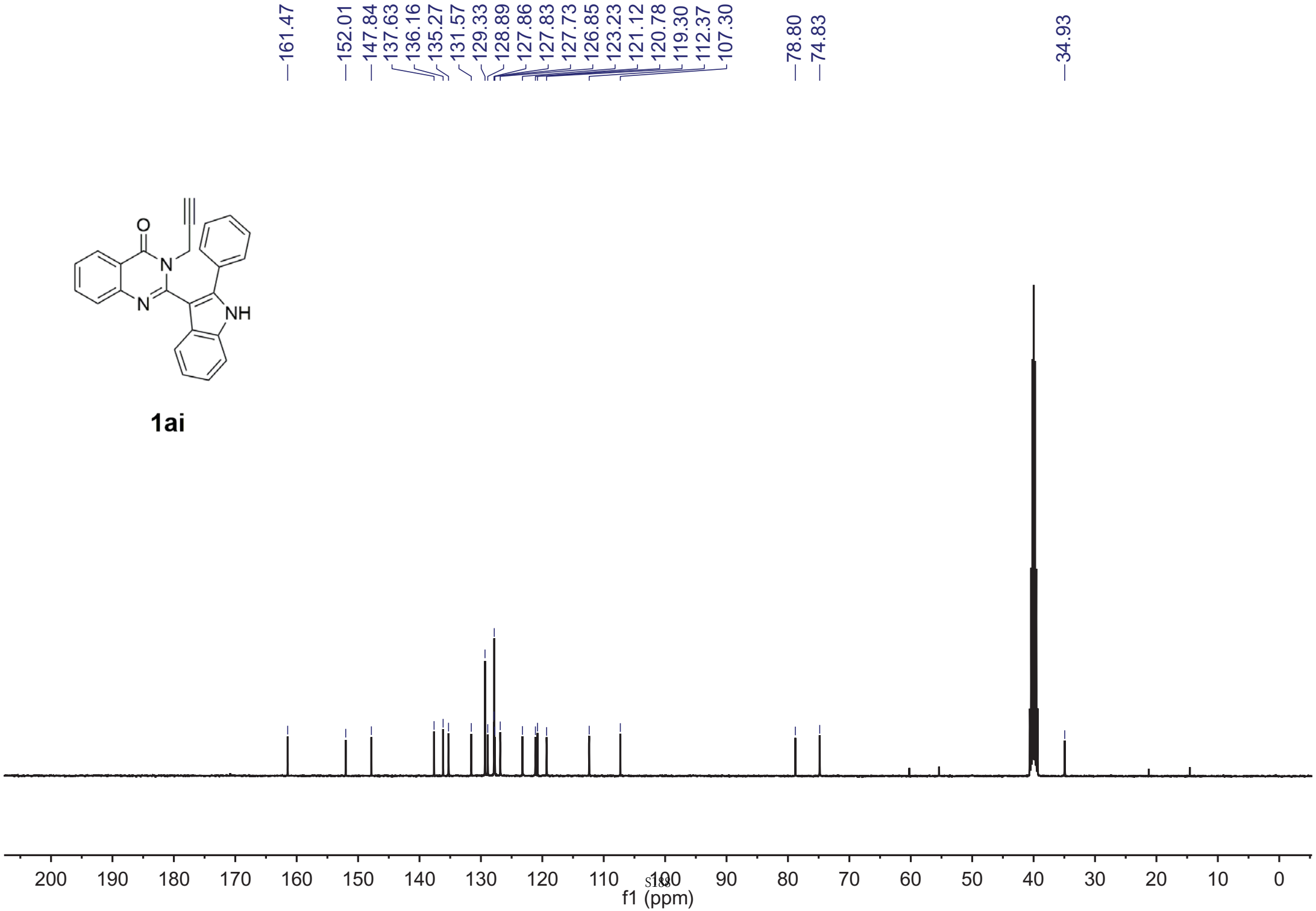


1ai

O
N
N
NH

1ai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127.73
126.85
123.23
121.12
120.78
119.30
112.37
107.30
78.80
74.83
34.93
200
190
180
170
160
150
140
130
120
110
100
90
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70
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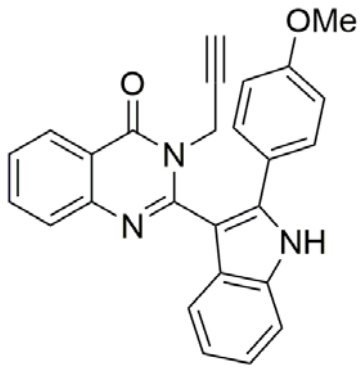
50
40
30
20
10
0
f1 (ppm)



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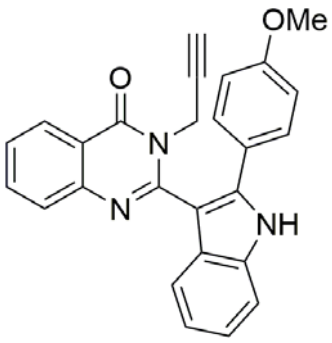

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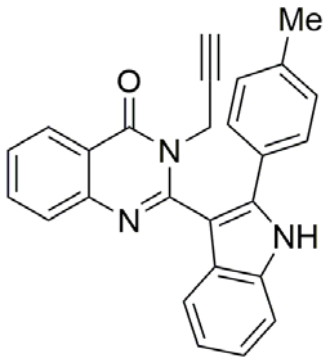

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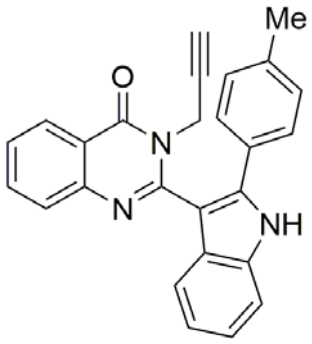

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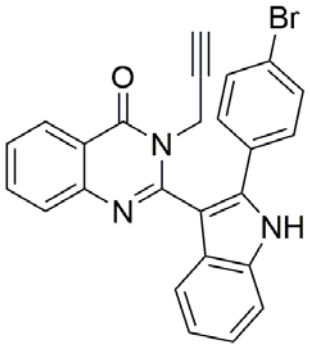

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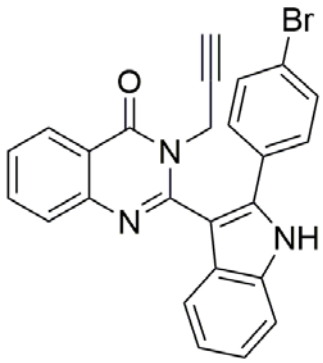

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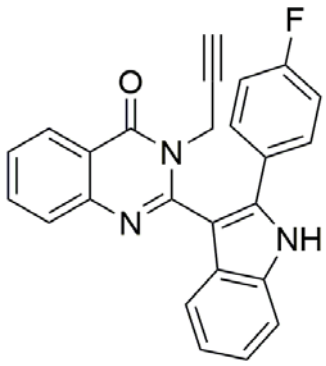

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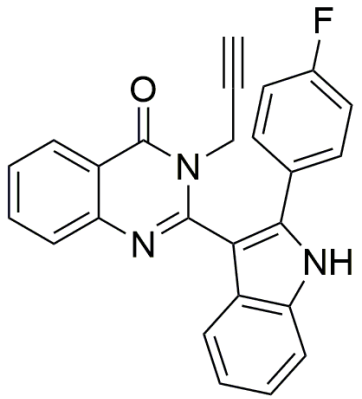

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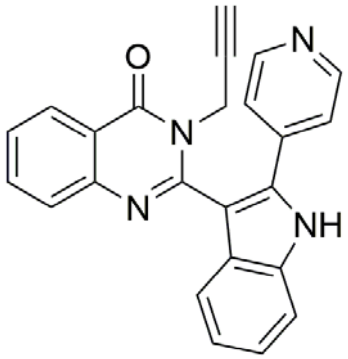

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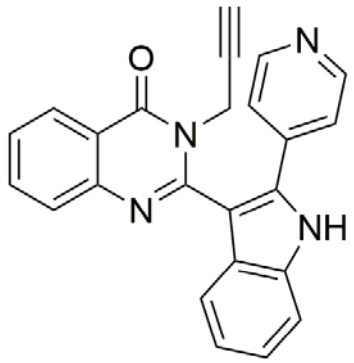

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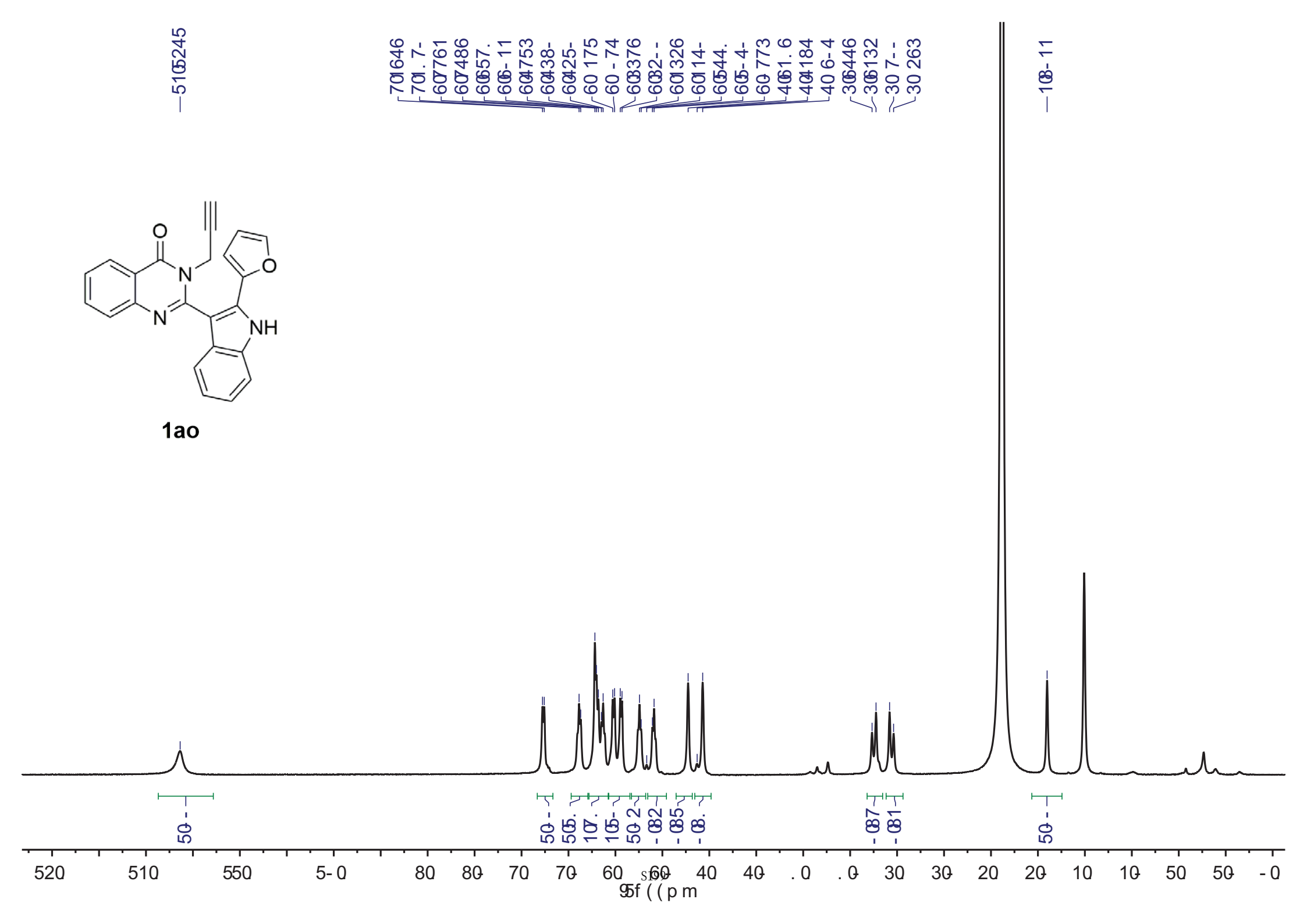

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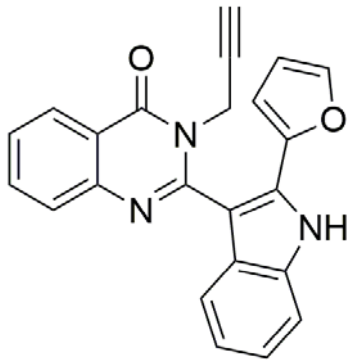

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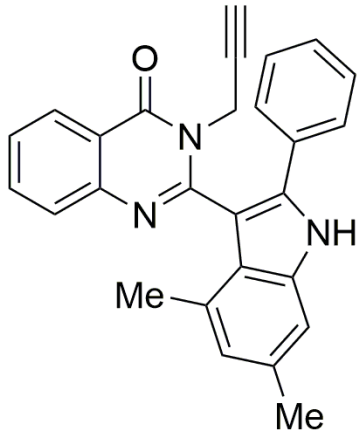

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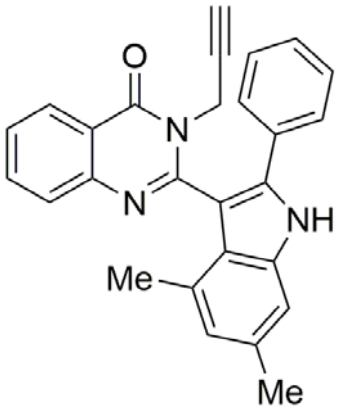

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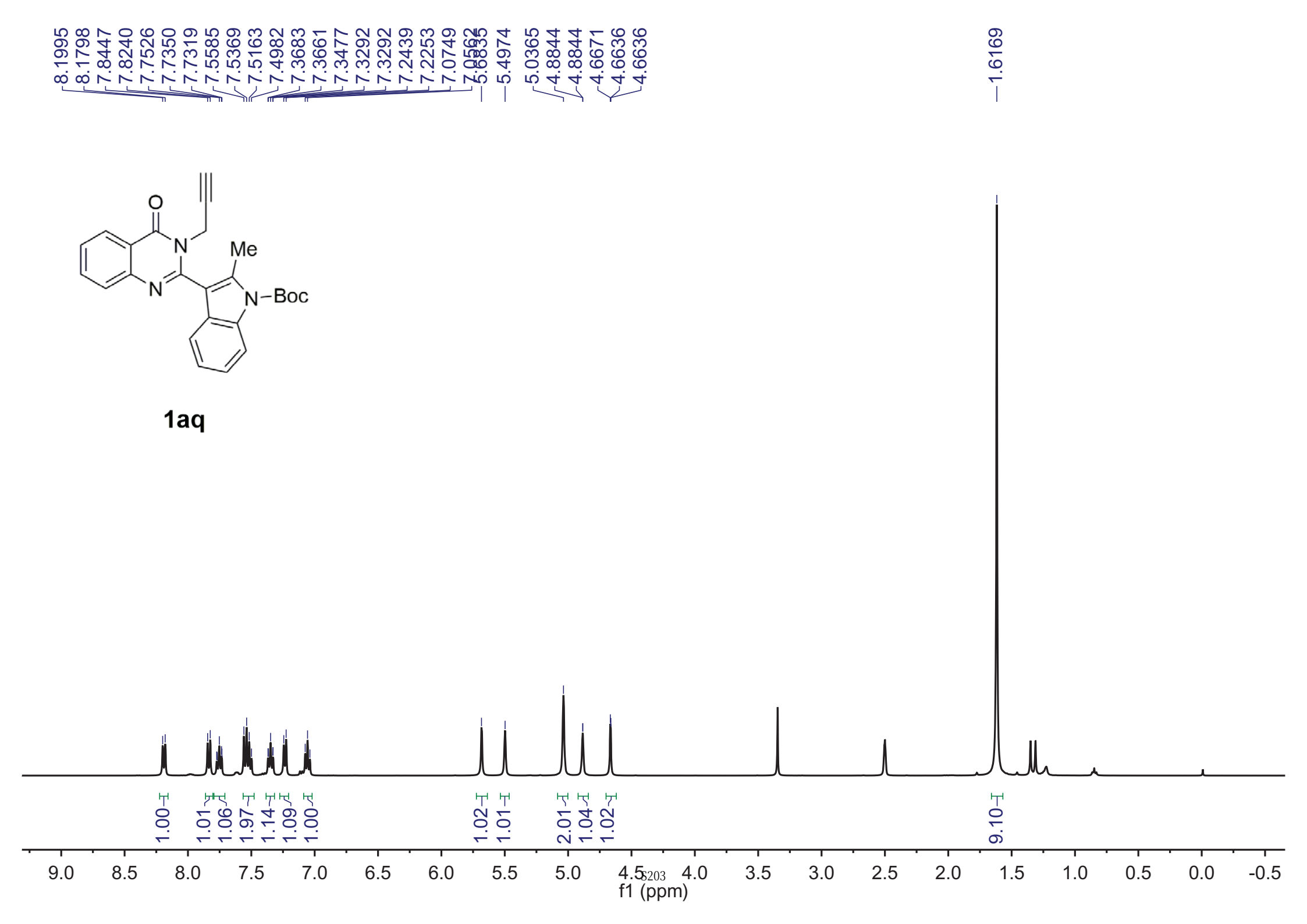
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5.0365
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4.8844
4.6671
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4.6636
1.6169
O
N
N
Me
N–Boc
1aq
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1.01
1.06
1.97
1.14
1.09
1.00
1.02
1.01
2.01
1.04
1.02
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4.5
4.0
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3.0
2.5
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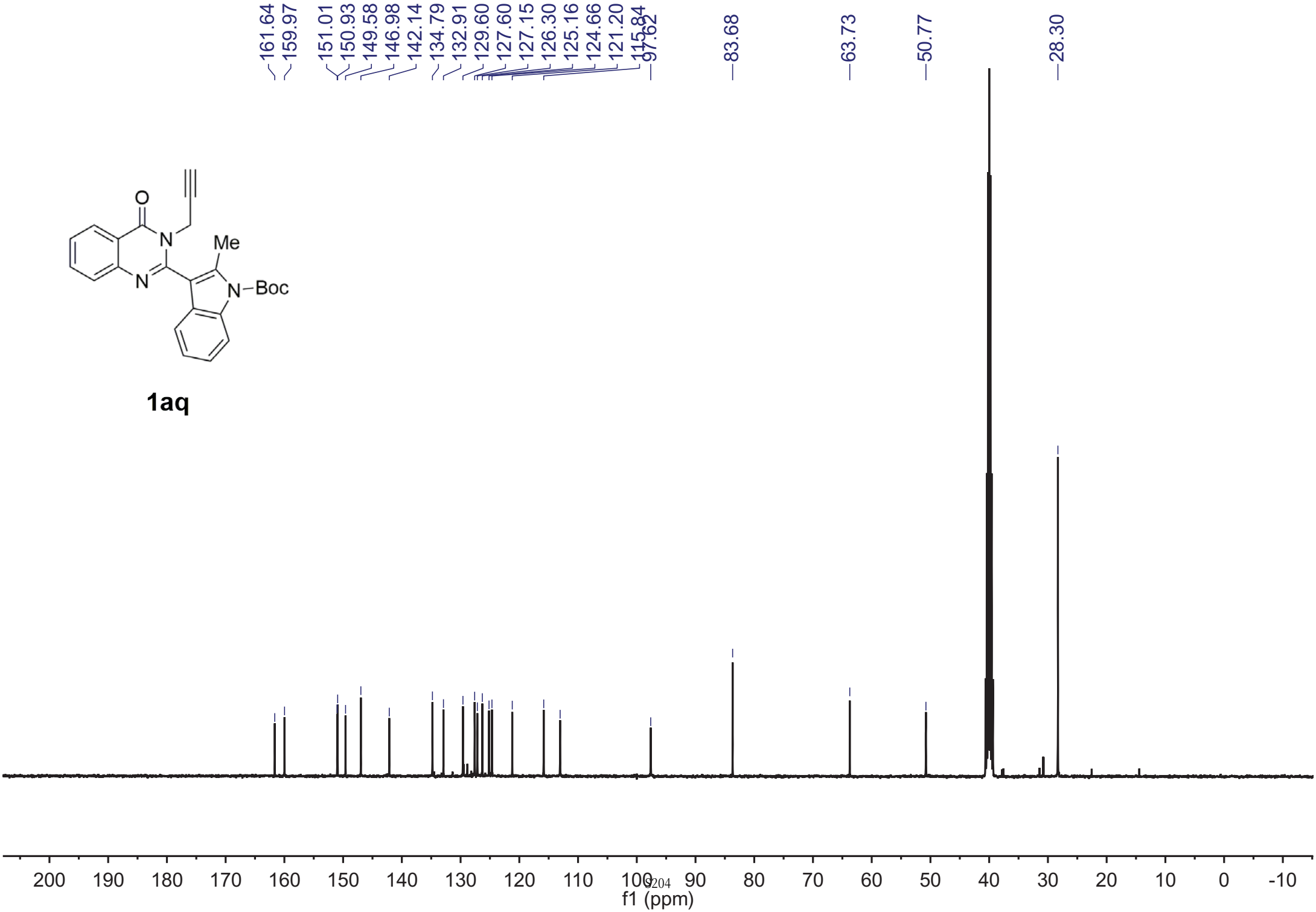
f1 (ppm)

O
N
Me
N
N–Boc

1aq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63.73
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28.30
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180
170
160
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130
120
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100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)