Electronic Supplementary Material (ESI) for ChemComm.

Synthesis of highly substituted isoquinolines/isoquinolones by Ruthenium (II) catalyzed reaction of benzyl/α-methyl benzyl/benzoyl isocyanates with diaryl Alkynes

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1. General Information

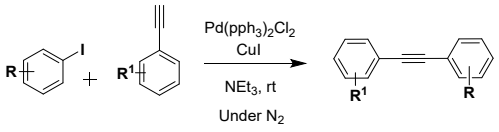
All reagents and solvents were purchased from commercial sources and used as received. The progress of the reaction was monitored by analytical TLC on silica gel G/GF 254 plates. The column chromatography was performed with silica gel 100-200 mesh. ^{1}H and ^{13}C NMR spectra were recorded on a 300 MHz or 400 MHz or 100MHz instrument respectively using TMS as an internal standard and chemical shifts are presented in δ ppm. Melting points are uncorrected were determined in capillary tubes on a hot stage melting point apparatus containing silicon oil. High resolution mass spectra were taken with a 3000 massspectrometer and Q-TOF Analyzer. IR spectra were recorded using a FTIR spectrophotometer**.**

2. Procedure for synthesis of substituted isoquinolines:

In an oven dried 50 ml R.B flask charged with stir bar, beznylisocyanate (0.75 mmol), diarylalkyne (0.75 mmol), $[RuCl_2(pcymene)_2]$ (5 mol%), $Cu(OTf)_2$ (0.5 equiv.) and $CsCO_3$ (1.0 equvi.) in 2ml DCE, resulting mixture was stirred at 120 °C for 1 h. Completion of reaction was monitored by TLC (1:8 Ethyl acetate and Hexane). Reaction mixture was cooled down to room temperature and diluted with 10 mL of H_2O. The resultant mixture was extracted with ethyl acetate (3 × 15 mL). The combined organic phase was dried over anhydrous Na_2SO_4. After removal of the solvent under reduced pressure, the crude product was purified by column chromatography on silica gel (100-200 mesh) by using hexane/ethylacetate solvent system to give desired poly substituted indole compounds.

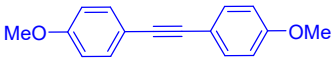
3. General procedure for the preparation of alkynes

$[Pd(PPh_3)Cl_2]_2$ (2 mol%), CuI (4 mol%), Et_3N (2.0 equiv.) and iodobenzene (1.1 equiv.) were dissolved in 10.0 mL NEt_3 at room temperature. Subsequently, phenylacetylene (1.0 equiv.) was added to the resulting mixture by syringe, and the reaction was stirred under argon atmosphere for 10 h. After this solvent was removed and extracted with CH_2Cl_2 (4×50 mL). The combined organic layer was washed with brine, dried over Na_2SO_4, concentrated under reduced pressure to give crude alkyne. The residue was purified by silica gel flash chromatography using petroleum ether to afford the desired product**.**



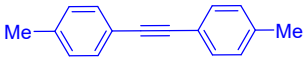
4. Spectral data of internal alkynes

1,2-bis(4-methoxyphenyl)ethyne(2b)



Yield 81%(192 mg); white solid; mp 171-173 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.45-7.46 (m, 4H), 6.86-6.88 (d, 4H), 3.83 (s, 6H); ^{13}C NMR (400 MHz, $CDCl_3$): δ159.4, 132.8, 115.7, 113.9, 87.9, 77.0, 55.2; mass (ES+) m/z = 239.1072 (M+H)+; HRMS (ESI-TOF) calcd for $C_{16}H_{15}O_2$239.1072 Found 239.1070.

1,2-di-p-tolylethyne(2c)



Yield 88%(181 mg);white solid; mp 125-128 °C; ^{1}H NMR (400 MHz, $CDCl_3$): 7.40 (d, *J* = 8.0 Hz, 4H), 7.12 (d, *J* = 7.8 Hz, 4H), 2.34 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 138.1, 132.4, 129.1, 120.4, 88.9, 21.5; mass (ES+) m/z = 207.2 (M+H)+; HRMS (ESI-TOF) calcd for $C_{22}H_{27}$ 207.1168 Found 207.1173.

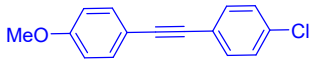
1,2-bis(4-(tert-butyl)phenyl)ethyne(2d)

Yield 89%(258 mg); white solid; mp 171-173 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.46-7.43 (m, 4H), 7.36-7.32 (m, 4H), 1.31 (s, 9H), 1.30 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.3, 137.1, 132.2, 127.6, 125.5, 120.5, 88.9, 34.9, 34.8, 31.2; mass (ES+) m/z = 291.2 (M+H)+; HRMS (ESI-TOF) calcd for $C_{22}H_{27}$ 291.2107 Found 291.2146.

1,2-bis(4-fluorophenyl)ethyne(2e)

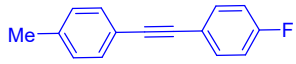
Yield 72%(154 mg); white solid; mp 132-133 °C; ^{1}H NMR (400 MHz, $CDCl_3$): 7.49-7.45 (m, 4H), 7.04-6.99 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.8, 161.3, 134.6, 134.5, 133.5, 133.4, 119.2,115.8, 115.5, 88.0; mass (ES+) m/z = 215.3 (M+H)+; HRMS (ESI-TOF) calcd for $C_{14}H_9F_2$ 215.0667 Found 215.0687.

1-chloro-4-((4-methoxyphenyl)ethynyl)benzene (2f)



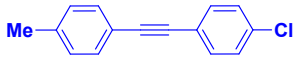
Yield 74% (117 mg); white solid; mp 123-128 °C; (KBr) cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ 7.44-7.46 (d, *J* = 8.8 Hz, 2H), 7.41-7.43 (d, *J* = 8.6 Hz. 2H), 7.29-7.31 (d, *J* = 8.6 Hz, 2H), 7.25 (s), 6.86-6.88 (d, *J* = 8.8 Hz, 2H), 3.82 (s, 3H) ; ^{13}C NMR (100 MHz, $CDCl_3$): *δ* 159.8, 133.8, 133.0, 132.6, 128.6, 122.1, 115.0, 114.0, 90.3, 87.0, 55.3.

1-fluoro-4-(p-tolylethynyl)benzene (2g)



Yield 79% (181 mg);white solid;mp 123-128 °C; (KBr) cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ 7.48-7.51 (m, 2H), 7.40-7.43 (d, *J* = 8.16Hz. 2H), 7.26(s), 7.15-7.17 (d, *J* = 7.98 Hz, 2H), 7.01-7.06 (t, *J* = 8.8 Hz, 2H), 2.37 (s, 3H) ; ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.4, 138.4, 133.4131.4, 129.1, 120.0, 119.5, 115.5, 89.2, 87.6, 21.5.

1-chloro-4-(p-tolylethynyl)benzene (2h)



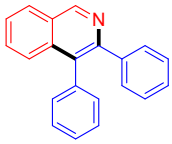
Yield 82% (185 mg); white solid; mp 138-140 °C; ^{1}H NMR (400 MHz, $CDCl_3$): 7.51-7.47 (m, 2H), 7.42-7.44 (d, *J* = 8.64 Hz, 2H), 7.30-7.32 (d, *J* = 8.59 Hz, 2H), 7.25 (s), 7.02-7.06 (t, *J* = 8.76 Hz, 2H) ; ^{13}C NMR (100 MHz, $CDCl_3$): δ 138.6, 134.0, 132.7, 131.4, 129.1, 128.6, 122.0, 119.8, 90.5, 87.6, 21.5; mass (ES+) m/z = 227.06 $(M+H)^+$; HRMS (ESI-TOF) calcd for $C_{15}H_{12}Cl$ 227.0628 Found 227.0815.

5. Reference

1 Doucet, H.; Hierso, J. C.; *Angew. Chem., Int. Ed*., **2007**, *46*, 834.

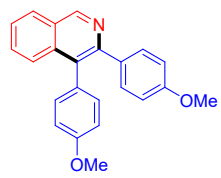
6. Spectral data of the obtained compounds

3,4-diphenylisoquinoline(3aa)



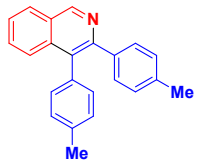
Yield 88% (185 mg); white solid;mp 122-127 °C; (KBr) cm^{-1}: 645, 666, 746, 808, 969, 1030, 1073, 1122, 1183, 1285, 1362, 1378, 1454, 1494, 1540, 1557, 1580, 1600, 1684, 1730, 2337, 2356, 2853, 2923, 2954, 3648, 3688, 3734 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ 9.38 (s, 1H), 8.03-8.01 (m, 1H), 8.03-8.01 (m, 1H), 7.68-7.58 (m, 3H), 7.38-7.333 (m, 5H), 7.26-7.23 (m, 2H), 7.20-7.19 (m, 2H); ^{13}C NMR (400MHz, $CDCl_3$): δ 151.8, 150.6, 140.8, 137.3, 135.9, 131.3, 130.7, 130.5, 130.3, 126.4, 127.7, 127.6, 127.5, 127.4, 127.0, 126.9, 125.7; mass (ES+) m/z = 282.12 $(M+H)^+$; HRMS (ESI-TOF) calcd for $C_{21}H_{16}N$282.1283Found 282.1268.

3,4-bis(4-methoxyphenyl)isoquinoline(3ab)



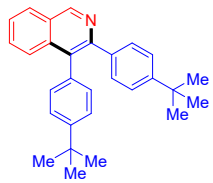
Yield 83% (212 mg); brown solid; mp 143-148 °C; (KBr) cm^{-1}: 700, 792, 864, 1017, 1083, 1258, 2926, 2962 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ 9.26 (s, 1H), 7.95-7.93 (m, 1H), 7.62-7.60 (m, 1H), 7.54-7.47 (m, 2H), 6.85 (d, *J* = 8.6 Hz, 2H), 7.09 (d, *J* = 8.6 Hz, 2H), 6.85 (d, *J* = 8.6 Hz, 2H), 6.69 (d, *J* = 8.9 Hz, 2H), 3.78 (s, 3H), 3.70 (s, 3H); ^{13}C NMR (400MHz, $CDCl_3$): δ 158.9, 158.7, 151.5, 150.4, 136.4, 133.5, 132.2, 131.6, 130.5, 129.8, 129.7, 127.6, 127.3, 126.6, 125.6, 113.9, 113.2, 113.0, 55.3, 55.2; mass (ES+) m/z = 342.14 $(M+H)^+$; HRMS (ESI-TOF) calcd for $C_{23}H_{20}NO_2$342.1494Found 342.1483.\

3,4-di-p-tolylisoquinoline(3ac)



Yield 81% (188 mg); light green solid; mp98-103 °C; (KBr) cm^{-1}: 642, 699, 731, 794, 813, 926, 963, 1023, 1110, 1184, 1212, 1265, 1333, 1371, 1417, 1448, 1490, 1513, 1574, 1615, 1693, 2854, 2920, 3027 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ 9.34 (s, 1H), 8.01-7.99 (m, 1H), 7.67-7.64 (m, 1H), 7.59-7.53 (m, 2H), 7.29-7.27 (m, 2H), 7.18-7.11 (m, 4H), 7.00 (d, J = 7.7 Hz, 2H); ^{13}C NMR (400MHz, $CDCl_3$): δ 151.6, 150.6, 138.0, 136.8, 136.7, 136.3, 134.4, 131.0, 130.4, 130.4, 130.2, 129.0, 128.7, 128.5, 127.6, 127.4, 126.7, 125.7, 21.4, 21.3; mass (ES+) m/z = 310.16 $(M+H)^+$; HRMS (ESI-TOF) calcd for $C_{23}H_{20}N$310.1596Found 310.1584.

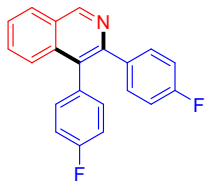
3,4-bis(4-(tert-butyl)phenyl)isoquinoline(3ad)



Yield 79% (233 mg); light yellow oil; (KBr) cm^{-1}: 625, 631, 732, 768, 801, 816, 877, 926, 981, 1027, 1079, 1141, 1156, 1191, 1220, 1301, 1337, 1359, 1453, 1494, 1506, 1585, 1606, 1644, 1684, 1732, 2963, 3031, 3063, 3275, 3648, 3734, 3746 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ 9.34 (s, 1H), 8.03-8.01 (m, 1H), 7.73-7.70 (m, 1H), 7.61-7.57 (m, 2H), 7.38-7.36 (m, 2H), 7.30-7.27 (m, 2H), 7.20-7.16 (m, 4H), 1.35 (s, 9H), 1.26 (m, 9H); ^{13}C NMR (400MHz, $CDCl_3$): δ 151.5, 150.7, 150.3, 149.9, 137.9, 136.3, 134.3, 130.8, 130.5, 130.3, 129.9, 129.0, 128.7, 127.5, 127.6, 126.7, 125.8, 125.0,

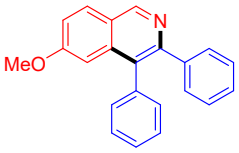
124.5, 34.6, 34.5, 31.4, 31.3; mass (ES+) m/z = 394.16 $(M+H)^+$; HRMS (ESI-TOF) calcd for $C_{29}H_{32}N$394.2535Found 394.2520.

3,4-bis(4-fluorophenyl)isoquinoline(3ae)



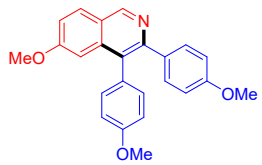
Yield 73% (173 mg); light green solid; mp 123-128 °C; (KBr) cm^{-1}: 632, 692, 727, 757, 795, 819, 840, 850, 935, 959, 978, 1013, 1088, 1104, 1155, 1216, 1300, 1332, 1395, 1413, 1455, 1487, 1505, 1556, 1595, 1682, 1697, 1714, 1731, 1747, 1908, 2328, 2352, 2848, 2916, 2956 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ 9.36 (s, 1H), 8.07-8.04 (m, 1H), 7.64-7.62 (m, 3H), 7.34-7.30 (m, 2H), 7.22-7.18 (m, 2H), 7.09 (t, *J* = 7.0 Hz, 2H), 6.92 (t, *J* = 6.9 Hz, 2H); ^{13}C NMR (400MHz, $CDCl_3$): δ 163.135.9, 132.9, 132.9, 132.8, 132.0, 131.9, 130.8, 129.9, 127.7, 127.5, 127.0, 125.3, 115.8, 115.5, 115.4, 114.7, 114.0; mass (ES+) m/z = 318.10 $(M+H)^+$; HRMS (ESI-TOF) calcd for $C_{21}H_{14}F_2N$318.1094Found 318.1081.

6-methoxy-3,4-diphenylisoquinoline(3ba)



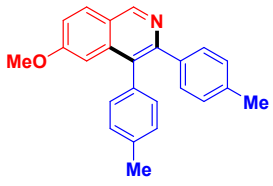
Yield 83% (193 mg); light grey solid; mp 147-152 °C; (KBr) cm^{-1}: 696,741, 850, 928, 966, 1023, 1070, 1113, 1223, 1249, 1326, 1393, 1410, 1452, 1486, 1576, 16144, 1688, 2584, 2922, 2963 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ 9.22 (s, 1H), 7.94 (d, *J* = 9.0 Hz, 1H), 7.36-7.32 (m, 5H), 7.25-7.17 (m, 6H), 6.90 (d, *J* = 2.3 Hz, 1H), 3.74 (s, 3H); ^{13}C NMR (400MHz, $CDCl_3$): δ 161.2, 151.2, 150.9, 140.9, 137.6, 131.2, 130.3, 129.9, 129.4, 128.4, 127.6, 127.3, 127.0, 123.3, 119.6, 103.8, 55.3; mass (ES+) m/z = 312.13$(M+H)^+$; HRMS (ESI-TOF) calcd for $C_{22}H_{18}NO$312.1388Found 312.1373.

6-methoxy-3,4-bis(4-methoxyphenyl)isoquinoline(3bb)



Yield 81% (225 mg); light yellow solid; mp 133-168 °C; (KBr) cm^{-1}: 650, 689, 732, 794, 833, 928, 968, 1031, 1069, 1123, 1175, 1245, 1289, 1334, 1398, 1421, 1461, 1493, 1511, 1578, 1611, 2835, 2957, 3002 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ 9.18 (s, 1H), 7.91(d, *J* = 8.9 Hz, 1H), 7.30 (d, *J* = 8.9 Hz, 2H), 7.20 (dd, *J* = 2.3, 2.3 Hz, 1H), 7,12 (d, *J* = 8.9 Hz, 2H), 6.92 (d, *J* = 8.7 Hz, 3H), 6.73 (d, *J* = 8.8 Hz, 2H), 7.163.85 (s, 3H), 3.78 (s, 3H), 3.76 (s, 3H); ^{13}C NMR (400MHz, $CDCl_3$): δ 161.0, 158.7, 158.6, 150.9, 138.4, 133.7, 132.2, 131.5, 129.9, 129.4, 128.9, 123.2, 119.3, 113.2, 103.7, 55.4, 55.3, 55.2; mass (ES+) m/z = 372.16$(M+H)^+$; HRMS (ESI-TOF) calcd for $C_{24}H_{22}NO_3$ 372.1600Found 372.1588.

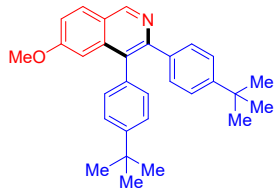
6-methoxy-3,4-di-p-tolylisoquinoline(3bc)



Yield 78% (198 mg); light yellow solid; mp 123-128 °C; (KBr) cm^{-1}: 612, 623, 970, 1339, 1376, 1489, 1520, 1558, 1616, 1652, 1683, 1716, 1748, 1792, 2364, 2850, 2920, 2952, 3648, 3749 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ 9.19 (s, 1H), 7.91 (d, *J* = 8.9 Hz, 1H), 7.25 (d, *J* = 7.0 Hz. 2H), 7.22-7.11 (m, 5H), 7.00 (d, *J* = 7.9 Hz, 2H), 6.91 (d, *J* = 2.3 Hz, 1H), 3.74 (s, 3H), 2.39 (s, 3H), 2.28 (s, 3H); ^{13}C NMR (100MHz, $CDCl_3$): δ

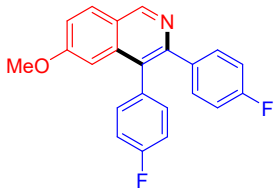
161.0, 151.0, 138.2, 138.2, 136.8, 136.6, 134.6, 130.9, 130.2, 129.4, 129.2, 128.4, 123.3, 119.3, 103.8, 55.4, 21.4, 21.2; mass (ES+) m/z = 340.17 $(M+H)^+$; HRMS (ESI-TOF) calcd for $C_{24}H_{22}NO$340.1701Found 404.1048.

3,4-bis(4-(tert-butyl)phenyl)-6-methoxyisoquinoline(3bd)



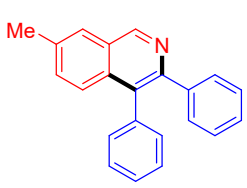
Yield 75% (238 mg); light green solid; mp 120-125 °C; (KBr) cm^{-1}: 1710, 1790, 836, 927, 970, 1029, 1068, 1121, 1174, 1200, 1266, 1334, 1394, 1417, 1462, 1494, 1581, 1618, 1731, 2867, 2958 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ 9.20 (s, 1H), 7.92 (d, *J* = 8.8 Hz, 1H), 7.36 (d, *J* = 8.2 Hz, 2H), 7.25 - 7.15 (m, 7H), 6.98 (d, *J* = 1.8 Hz, 1H), 3.76 (s, 3H), 1.34 (s, 9H), 1.25 (s, 9H) ; ^{13}C NMR (400MHz, $CDCl_3$): δ 161.3, 150.9, 150.3, 149.9, 134.4, 130.8, 129.9, 129.5, 124.5, 123.2, 119.3, 104.0, 55.4, 34.5, 34.5, 31.4, 31.3; mass (ES+) m/z = 424.26 $(M+H)^+$; HRMS (ESI-TOF) calcd for $C_{30}H_{34}NO$ 424.2640Found 424.2628.

3,4-bis(4-fluorophenyl)-6-methoxyisoquinoline(3be)



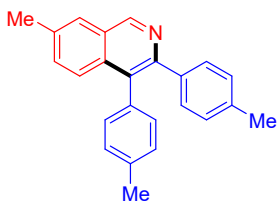
Yield 68% (177 mg); light brown solid;mp 128-133 °C; (KBr) cm^{-1}: 690, 751, 815, 839, 1030, 1095, 1124, 1158, 1227, 1257, 1333, 1396, 1421, 1460, 1508, 1618, 1691, 2852, 2923 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ 9.20 (s, 1H), 7.95 (d, *J* = 8.9 Hz, 1H), 7.32-7.28 (m, 2H), 7.25-7.18 (m, 3H), 7.08 (t, *J* = 7.0 Hz, 2H), 6.93-6.85 (m, 3H), 3.76 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$): δ 163.4, 163.3, 161.6, 160.9, 160.8, 150.9, 150.3, 138.0, 136.7, 132.8, 132.7, 131.9, 131.9, 129.6, 128.9, 123.3, 119.8, 115.8, 115.6, 114.9, 114.6, 103.5, 55.4 ; mass (ES+) m/z = 348.12 $(M+H)^+$; HRMS (ESI-TOF) calcd for $C_{22}H_{16}F_2NO$ 348.1200Found 348.1198

7-methyl-3,4-diphenylisoquinoline(3ca)



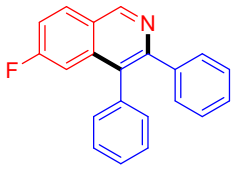
Yield 80% (177 mg); light yellow solid; mp 141-146 °C; (KBr) cm^{-1}: 621, 654, 718, 739, 774, 814, 836, 892, 920, 950, 980, 1039, 1061, 1079, 1125, 1150, 1181, 1243, 1260, 1279, 1339, 1374, 1396, 1436, 1473, 1488, 1521, 1541, 1557, 1569, 1615, 1636, 1670, 1682, 1700, 1715, 1748, 1770, 1800, 1827 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ 9.28 (s, 1H), 7.81 (s, 1H), 7.56 (d, *J* = 8.7 Hz, 1H), 7.44 (dd, *J* = 1.8, 1.7 Hz, 1H), 7.37-7.33 (m, 5H), 7.25-7.22 (m, 2H), 7.19-7.18 (m, 3H), 2.56 (s, 3H); ^{13}C NMR (400MHz, $CDCl_3$): δ 152.2, 149.9, 140.9, 137.4, 136.9, 134.3, 132.8, 131.3, 130.6, 130.3, 128.3, 127.6, 127.3, 126.9, 126.6, 125.5, 21.6; mass (ES+) m/z = 296.14 $(M+H)^+$; HRMS (ESI-TOF) calcd for $C_{22}H_{18}N$296.1439Found 296.1426.

7-methyl-3,4-di-p-tolylisoquinoline(3cc)



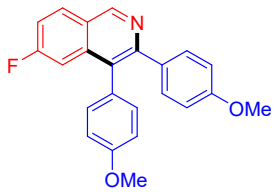
Yield 76% (184 mg); light grey solid; mp 133-138 °C; (KBr) cm^{-1}: 699, 730, 789, 816, 876, 931, 969, 1022, 1038, 1110, 1183, 1244, 1267, 1339, 1368, 1426, 1490, 1513, 1574, 1610, 1694, 2863, 2919, 3021 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ 9.26 (s, 1H), 7.79 (s, 1H), 7.56 (d, *J* = 8.7 Hz, 1H), 7.41 (dd, *J* = 1.7, 1.7 Hz, 1H), 7.27 (d, *J* = 8.0 Hz, 2H), 7.17 (d, *J* = 7.8 Hz, 2H), 7.12 ((d, *J* = 8.0 Hz, 2H), 7.01 (d, *J* = 7.8 Hz, 2H), 2.54 (s, 3H), 2.39 (s, 3H), 2.28 (s, 3H); ^{13}C NMR (100MHz, $CDCl_3$): δ 150.9, 149.9, 138.0, 136.8, 136.6, 136.6, 134.6, 132.6, 131.0, 130.3, 130.1, 129.0, 128.4, 127.6, 126.3, 125.6, 21.6, 21.4, 21.2; mass (ES+) m/z = 324.17 $(M+H)^+$; HRMS (ESI-TOF) calcd for $C_{24}H_{22}N$324.1772Found 324.1757.

6-fluoro-3,4-diphenylisoquinoline(3da)



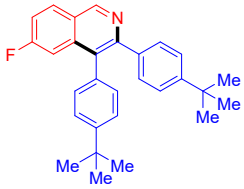
Yield 67% (150 mg); light green solid; mp 103-108 °C; (KBr) cm^{-1}: 697, 721, 746, 977, 1078, 1246, 1276, 1362, 1377, 1459, 2851, 2920, 2952 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ 9.34 (s, 1H), 8.07 (dd, *J* =7.28 (dd, *J* = 2.4, 2.6 Hz, 1H), 7.38-7.33 (m, 6H), 7.28 (dd, *J* = 2.4, 2.6 Hz, 1H), 7.23-7.19 (m, 5H); ^{13}C NMR (400MHz, $CDCl_3$): δ 164.7, 162.7, 151.5, 151.3, 140.5, 137.9, 137.8, 136.9, 131.0, 130.7, 130.6, 130.6, 130.4, 130.3, 128.6, 127.7, 127.7, 127.4, 124.7, 117.6, 117.4, 109.5, 109.3; mass (ES+) m/z = 300.11 $(M+H)^+$; HRMS (ESI-TOF) calcd for $C_{21}H_{15}FN$300.1189Found 300.1175.

6-fluoro-3,4-bis(4-methoxyphenyl)isoquinoline(3db)



Yield 63% (169 mg); light yellow solid; mp 122-127 °C; (KBr) cm^{-1}: 662, 679, 731, 786, 842, 895, 965, 1027, 1109, 1175, 1244, 1336, 1395, 1420, 1472, 1491, 1513, 1540, 1558, 1619, 1650, 1679, 1699, 1740, 1771, 1795, 1827, 1866, 1889, 1916, 1941, 1962, 1991, 2202, 2313, 2352, 2375, 2641, 2703, 2791, 3626, 3649, 3672 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ 9.29 (s, 1H), 8.04-8.00 (m, 1H), 7.34-7.29 (m, 4H), 7.15-7.13 (m, 2H), 6.94-6.92 (m, 2H), 6.77-6.75 (m, 2H), 3.85 (s, 3H), 3.78 (s, 3H); ^{13}C NMR (400MHz, $CDCl_3$): δ 164.5, 162.4, 158.9, 158.9, 151.2, 150.9, 138.3, 138.2, 133.0, 132.2, 131.6, 130.6, 129.2, 127.8, 124.5, 117.3, 116.9, 114.2, 114.0, 113.2, 109.4, 109.3, 55.3, 55.2; mass (ES+) m/z = 360.14$(M+H)^+$; HRMS (ESI-TOF) calcd for $C_{23}H_{19}FNO_2$360.1400Found 360.1401.

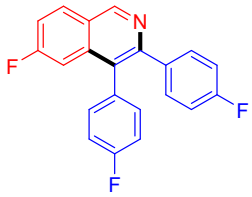
3,4-bis(4-(tert-butyl)phenyl)-6-fluoroisoquinoline(3dd)



Yield 59% (182 mg); light brown solid; mp 103-108 °C; (KBr) cm^{-1}: 632, 697, 738, 782, 836, 871, 925, 978, 1019, 1116, 1172, 1201, 1268, 1333, 1361, 1395, 1426, 1455, 1493, 1576, 1625, 1692, 2867, 2927, 2960, 2032 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ 9.30 (s, 1H), 8.05-8.01 (m, 1H), 7.38 (d, *J* = 8.2 Hz, 2H), 7.33 (s, 1H), 7.30-7.27 9 (m, 3H), 7.19 (d, *J* = 8.5 Hz, 2H), 7.14 (d, *J* = 8.2 Hz, 2H), 1.35 (s, 9H), 1.26 (s, 9H); ^{13}C NMR (400

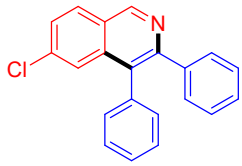
MHz, $CDCl_3$): δ 164.8, 162.3, 151.4, 150.9, 150.6, 150.2, 138.0, 137.9, 137.6, 133.9, 130.7, 130.6, 130.5, 130.2, 130.2, 129.9, 128.7, 125.4, 124.6, 124.5, 117.3, 117.0, 109.6, 109.4, 34.7, 34.5, 31.9, 31.4; mass (ES+) m/z = 412.24 $(M+H)^+$; HRMS (ESI-TOF) calcd for $C_{29}H_{31}FN$ 412.2441Found 412.2441.

6-fluoro-3,4-bis(4-fluorophenyl)isoquinoline(3de)



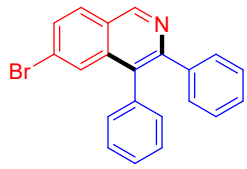
Yield 54% (135 mg); light yellow solid; mp 123-128 °C; (KBr) cm^{-1}: 651, 734, 788, 814, 872, 929, 976, 1015, 1094, 1117, 1158, 1226, 1265, 1334, 1359, 1428, 1510, 1576, 1603, 1625, 1731, 2853, 2923 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ 9.31 (s, 1H), 8.08 (dd, *J* = 5.7, 5.6 Hz, 1H), 7.40-7.30 (m, 3H), 7.24-7.17 (m, 3H), 7.10 (t, *J* = 7.1 Hz, 2H), 6.92 (t, *J* = 6.9 Hz, 2H) ; ^{13}C NMR (400 MHz, $CDCl_3$): δ 164.8, 163.4, 163.2, 162.8, 161.4, 161.3, 151.5, 150.7, 139.3, 136.3, 132.7, 132.7, 131.9, 131.9, 130.7, 124.7, 117.8, 117.5, 115.9, 115.8, 114.9, 114.8, 114.0, 109.3, 109.0; mass (ES+) m/z = 336.10 $(M+H)^+$; HRMS (ESI-TOF) calcd for $C_{21}H_{13}F_3N$ 336.1000Found 336.1005

6-chloro-3,4-diphenylisoquinoline(3ea)



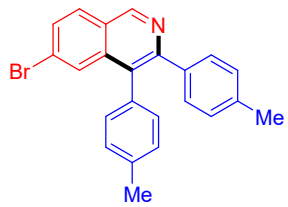
Yield 71% (168 mg); light yellow solid; mp 123-128 °C; (KBr) cm^{-1}: 622, 699, 763, 798, 819, 964, 1079, 1357, 1375, 1409, 1453, 1610, 1689, 2852, 2921, 3270 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ 9.35 (s, 1H), 7.99 (d, *J* = 8.7 Hz, 1H), 7.64-7.64 (m, 1H), 7.55 (dd, *J* = 1.9, 1.9 Hz, 1H), 7.39-7.33 (m, 5H), 7.28 (d, *J* = 8.5 Hz, 1H), 7.23-7.19 (m, 4H); ^{13}C NMR (400MHz, $CDCl_3$): δ 151.8, 151.4, 148.9, 140.4, 137.0, 136.9, 136.6, 134.4, 133.9, 131.2, 130.7, 130.3, 129.9, 129.3, 128.9, 128.6, 128.0, 127.7, 127.4, 125.6, 124.7; mass (ES+) m/z = 316.08$(M+H)^+$; HRMS (ESI-TOF) calcd for $C_{21}H_{15}ClN$316.0893Found 316.0881.

6-bromo-3,4-diphenylisoquinoline(3fa)



Yield 73% (196 mg); light yellow solid; mp 123-128 °C; (KBr) cm^{-1}: 759, 956, 1101, 1220, 1399, 1469, 1615, 2960, 3020, 3582 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ 9.33 (s, 1H), 7.91 (d, *J* = 8.8 Hz, 1H), 7.82-7.82 (m, 1H), 7.69 (dd, *J* = 1.7,1.7 Hz, 1H), 7.38-7.32 (m, 5H), 7.23-7.19 (m, 5H); ^{13}C NMR (400MHz, $CDCl_3$): δ 151.8, 151.6, 140.4, 137.2, 136.5, 131.9, 131.2, 130.9, 130.6, 130.3, 129.8, 129.2, 128.6, 127.9, 127.7, 127.4, 125.8; mass (ES+) m/z = 360.03 $(M+H)^+$; HRMS (ESI-TOF) calcd for $C_{21}H_{15}BrN$360.0388Found 360.0376.

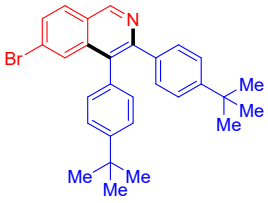
6-bromo-3,4-di-p-tolylisoquinoline (3fc)



Yield 65% (189 mg); white solid; mp 138-143 °C; (KBr) cm^{-1}: 653, 695, 725, 787, 815, 881,926, 963, 1020, 1065, 1112, 1185, 1215, 1268, 1351, 1377, 1409, 1475, 1512, 1568, 1604, 1692, 2856, 2920, 3025 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): *δ* 9.29 (s, 1H), 7.87(d, *J* = 8.5 Hz, 1H), 7.82-7.82 (m, 1H), 7.64 (dd, *J* = 1.8, 1.8 Hz, 1H), 7.27-7.24 (m, 2H), 7.19 (d, *J* = 7.7 Hz, 2H), 7.10 (d, *J* = 8.0 Hz, 2H), 7.01 (d, *J* = 8.0 Hz, 2H), 2.40 (s, 3H), 2.29 (s, 3H); ^{13}C NMR (400MHz, $CDCl_3$): δ 151.7, 151.3, 137.7, 137.5, 137.3, 137.0, 133.6,

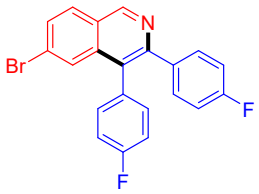
130.9, 130.3, 130.2, 129.5, 129.4, 129.2, 128.5, 127.9, 125.7, 125.5, 21.4, 21.4; mass (ES+) m/z = 388.07$(M+H)^+$; HRMS (ESI-TOF) calcd for $C_{23}H_{19}BrN$388.0701Found 388.0701.

6-bromo-3,4-bis(4-(tert-butyl)phenyl)isoquinoline(3fd)



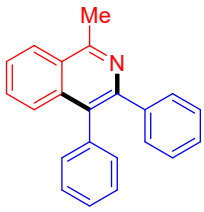
Yield 63% (222 mg); white solid; mp 168-173 °C; (KBr) cm^{-1}: 633, 790, 833, 965, 1019, 1065, 1112, 1269, 1359, 1397, 1475, 1511, 1569, 1605, 2867, 2960, 3037 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ 9.29 (s, 1H), 7.89-7.87 (m, 2H), 7.66 (dd, *J* = 1.8,1.8 Hz, 1H),7.38 (d, *J* = 8.2 Hz, 2H), 7.24 (d, *J* = 5.2 Hz, 2H), 7.18 (d, *J* = 8.6 Hz, 2H), 7.14 (d, *J* = 8.4 Hz, 2H), 1.37 (s, 9H), 1.26 (s, 9H); ^{13}C NMR (400 MHz, $CDCl_3$): δ 151.9,151.2, 150.6, 150.2, 137.5, 137.4, 133.8, 130.3, 129.9, 129.6, 129.2, 127.9, 125.7, 125.5, 125.4, 124.5, 34.7, 34.5, 31.4, 31.3; mass (ES+) m/z = 472.16 $(M+H)^+$; HRMS (ESI-TOF) calcd for $C_{29}H_{31}BrN$ 472.1640Found 472.1640.

6-bromo-3,4-bis(4-fluorophenyl)isoquinoline(3fe)



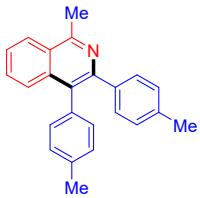
Yield 58% (172 mg); grey solid; mp 118-123 °C; (KBr) cm^{-1}: 658, 734, 836, 881, 929, 964, 1014, 1095, 1157, 1191, 1269, 1296, 1331, 1352, 1414, 1477, 1508, 1569, 1602, 1698, 1896, 2854, 2925, 3050 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ 9.32 (s, 1H), 7.92 (d, *J* = 8.8 Hz, 1H), 7.78 (d, *J* = 1.4 Hz, 1H), 7.70 (dd, *J* = 1.7, 1.7 Hz, 1H), 7.37 - 7.29 (m, 2H), 7.20-7.16 (m, 2H), 7.11 (t, *J* = 7.1 Hz, 2H), 6.92 (t,*J* = 6.9 Hz, 2H); ^{13}C NMR (400 MHz, $CDCl_3$): δ 163.4, 163.2, 161.4, 161.3, 151.8, 150.9, 137.2, 136.3, 132.8, 132.7, 132.3, 131.9, 131.9, 130.8, 129.3, 128.7, 127.7, 126.0, 125.8, 115.9, 115.9, 114.9, 114.8; mass (ES+) m/z = 396.01 $(M+H)^+$; HRMS (ESI-TOF) calcd for $C_{21}H_{13}BrF_2N$ 396.0199 Found 396.0200

1-methyl-3,4-diphenylisoquinoline (3ga)



Yield 85% (188 mg); brown solid; mp 128-133 °C; (KBr) cm^{-1}: 700, 729, 800, 1029, 1073, 1184, 1274, 1334, 1359, 1441, 1502, 1555, 1610, 1665, 1736, 2690, 2851, 2920, 3059 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ8.21-8.24 (m, 1H), 7.66-7.88 (m, 1H), 7.60-7.64 (m, 2H), 7.31-7.39 (m, 5H), 7.17-7.23 (m, 5H), 3.13 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$): δ157.8, 148.6, 139.9, 137.1, 136.2, 131.3, 130.5, 130.3, 129.7, 128.2, 127.7, 127.3, 127.2, 126.8, 126.3, 126.1, 125.7, 22.3 ; mass (ES+) m/z = 296.14 $(M+H)^+$; HRMS (ESI-TOF) calcd for $C_{22}H_{18}N$296.1439Found 296.1442.

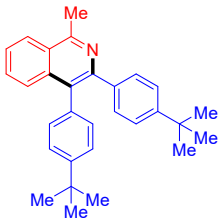
1-methyl-3,4-di-p-tolylisoquinoline (3gc)



Yield 82% (199 mg); light yellow oil; mp137-142°C; (KBr) cm^{-1}: 627, 735, 799, 830, 954, 981, 1023, 1112, 1197, 1266, 1333, 1363, 1391, 1438, 1461, 1513, 1569, 1611, 1742, 2859, 2952, 2925, 2958, 3066 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): 8.15-8.18 (m, 1H), 7.63-7.66 (m, 1H), 7.53-7.56 (m, 2H), 7.26-7.28 (d, 2H), 7.25 (s), 7.15-7.16 (d, 2H), 7.10-7.11(d, 2H), 6.99-7.01

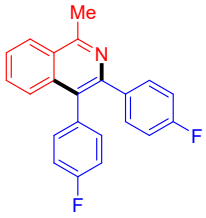
(d, 2H), 3.05 (s, 3H), 2.38 (s, 3H), 2.27 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$): δ157.42, 149.38, 138.28, 136.62, 136.46, 136.29, 134.70, 131.23, 130.16, 129.71, 128.97, 128.86, 128.36, 126.28, 126.06, 125.47, 22.72, 21.31, 21.19 ; mass (ES+) m/z = 324.17 $(M+H)^+$; HRMS (ESI-TOF)calcdfor $C_{24}H_{21}N$ 324.1752 Found 324.1755.

3,4-bis(4-(tert-butyl)phenyl)-1-methylisoquinoline (3gd)



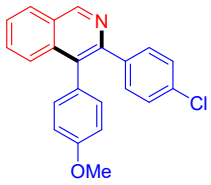
Yield 79% (241 mg); light yellow oil; mp 129-134 °C; (KBr) cm^{-1}: 627, 735, 799, 830, 954, 981, 1023, 1112, 1197, 1266, 1333, 1363, 1391, 1438, 1461, 1513, 1569, 1611, 1742, 2859, 2952, 2925, 2958, 3066 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): 8.19-8.21 (m, 1H), 7171-7.73 (m, 2H), 7.35 (d, *J* = 8.48 Hz, 2H), 7.30 (d, *J* = 8.48 Hz, 2H), 7.20 (d, *J* = 8.60 Hz, 2H), 7.15 (d, *J* = 8.49 Hz, 2H), 3.126 (s, 3H), 1.34 (s, 9H), 1.24 (s, 9H) ; ^{13}C NMR (400 MHz, $CDCl_3$): δ157.4,150.1, 149.9, 148.7, 137.1, 136.4, 134.2, 131.0, 130.2, 129.9, 129.5, 126.6, 126.4, 126.0, 125.6, 125.0, 124.5, 34.5, 34.4, 31.3, 31.2, 22.3; mass (ES+) m/z = 408.26 $(M+H)^+$; HRMS (ESI-TOF)calcdfor $C_{30}H_{34}N$408.2991Found 408.2689.

3,4-bis(4-fluorophenyl)-1-methylisoquinoline(3ge)



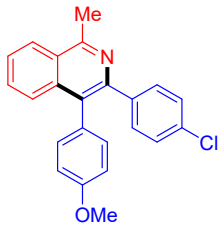
Yield 71% (176 mg); brown solid; mp 113-118 °C; (KBr) cm^{-1}: 667, 730, 762, 812, 876, 954, 983, 1020, 1094, 1156, 1225, 1296, 1333, 1391, 1438, 1510, 1572, 1603, 1740, 2854, 2924, 3069 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ8.20-8.22, (m, 1H), 7.61-7.62 (m, 3H), 7.30-7.34 (m, 2H), 7.15-7.19 (m, 2H), 7.04-7.09(m, 2H), 6.88-6.93 (m, 2H), 3.08 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$): δ163.1, 163.0, 161.1,161.0, 158.1, 148.4, 136.6, 136.0, 133.3, 133.2, 132.9, 132.8, 132.0, 131.9, 130.3, 128.2, 126.8, 126.2, 125.9, 125.7, 115.5, 115.4, 114.8, 114.6, 22.6; mass (ES+) m/z = 332.12 $(M+H)^+$; HRMS (ESI-TOF) calcd for $C_{22}H_{16}F_2N$332.1251Found 332.1250.

1-methyl-3,4-di-p-tolylisoquinoline (3af)



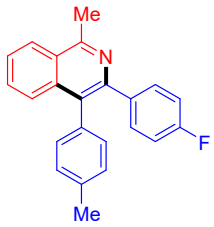
Yield 77% (199 mg); light yellow solid; mp 195 °C; (KBr) cm^{-1}: 668, 750, 907, 1214, 1514, 2363, 3020, 3656, 3778, 3839 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): 9.33 (s,1H), 8.03-8.05 (m, 1H), 7.69-7.72 (m, 1H), 7.59-7.65 (m, 2H), 7.31-7.33 (d,*J*= 8.6 Hz, 2H), 7.26 (s), 7.18-7.20 (d, *J*= 8.6 Hz, 2H), 7.13-7.15 (d, *J*= 8.7 Hz, 2H), 6.91-6.94 (d, *J*= 8.7 Hz, 2H), 3.86 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$): 159.02, 151.60, 149.4, 139.3, 136.2, 133.1, 132.2, 131.6, 130.6, 128.94, 127.9, 127.5, 127.0, 125.6, 114.0, 55.2; mass (ES+) m/z = 346.09 $(M+H)^+$; HRMS (ESI-TOF) calcd for $C_{22}H_{17}ClNO$ 346.0999 Found 346.0995.

1-methyl-3,4-di-p-tolylisoquinoline (3gf)



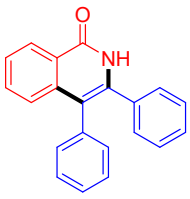
Yield 73% (196 mg); light brown; mp 102°C; (KBr) cm^{-1}: 759, 797, 1033, 1091, 1176, 1245, 1390, 1437, 1492, 1512, 1572, 1608, 2952, 2955, 3480, 3594, 3615, 3654 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): 8.16-8.21 (m, 1H), 7.66-7.70 (m, 1H), 7.57-7.61 (m, 2H),7.30-7.33(d, 2H), 7.26 (s), 7.17-7.19 (d, 2H), 7.09-7.13 (d, 2H), 6.89-6.92 (d, 2H), 3.85 (s, 3H), 3.05 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$): δ158.8, 157.7, 148.2, 139.69, 136.3, 132.9, 132.3, 132.6, 129.9, 129.3, 128.9, 128.7,127.8, 127.3, 126.6, 126.3, 125.5, 113.9, 55.2, 22.6; mass (ES+) m/z = 360.11 $(M+H)^+$; HRMS (ESI-TOF) calcd for $C_{23}H_{18}ClNO$ 360.1155 Found 360.1158.

1-methyl-3,4-di-p-tolylisoquinoline (gg)



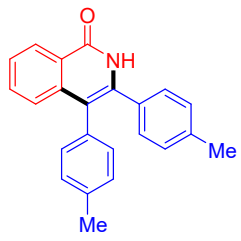
Yield 71%(174 mg); brown solid; mp 98°C; (KBr) cm^{-1}:761, 818, 840, 1157, 1225, 1390, 1437, 1510, 1570, 1604, 2857, 2923, 3068, 3527, 3634, 3696, 3754, 3831 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): 8.15-8.20 (m, 1H), 7.69-7.67 (m, 1H), 7.55-7.59 (m, 2H), 7.33-7.36 (d, 2H), 7.25 (s), 7.15-7.17 (m, 2H), 7.07-7.09 (d, 2H), 6.86-6.90 (t, 2H), 3.05 (s, 3H), 2.39 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$): δ 161.9 157.6, 148.3, 137.2, 136.9, 136.1, 134.3,131.9, 131.1, 129.9, 129.1, 129.0, 126.5, 126.3, 126.2, 125.5, 114.5, 22.6, 21.2; mass (ES+) m/z = 328.15 $(M+H)^+$; HRMS (ESI-TOF) calcd for $C_{23}H_{18}FN$ 328.1502 Found 328.1503.

3,4-diphenylisoquinolin-1(2H)-one(3ha)



Yield 73% (162 mg); white solid; mp243-248 °C; (KBr) cm^{-1}: 687, 1074, 1116, 1288, 1339, 1374, 1396, 1436, 1473, 1489, 1507,1540, 1568, 1594, 1616, 1635, 1647, 1662, 1683, 1698, 1716, 1733, 1760, 1771, 1792, 1800, 1828, 1868, 1889, 1908, 1919, 1942, 1966, 1990, 2016, 2041, 2064, 2319, 2373, 3545, 3566, 3617, 3689 cm^{-1};^1H NMR (400 MHz, $CDCl_3$): δ 9.36 (s,1H), 8.47 (dd, J = 1.0, 1.1 Hz, 1H), 7.60-7.55 (m, 1H), 7.51-7.47 (m, 1H), 7.35 (d, J = 8.1 Hz, 1H), 7.31-7.22 (m, 8H), 7.19-7.17 (m, 2H); ^{13}C NMR (400 MHz, $CDCl_3$): δ 162.7, 138.7, 136.9, 135.8, 135.2, 133.0, 132.8, 131.9, 129.2, 128.9, 128.7, 128.5, 128.0, 127.6, 127.4, 126.7, 125.8, 117.3; mass (ES+) m/z = 298.12 $(M+H)^+$; HRMS (ESI-TOF) calcd for $C_{21}H_{16}NO$ 298.1232Found 298.1230.

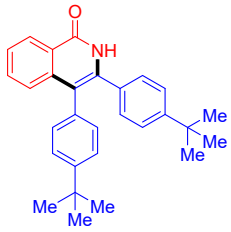
3,4-di-p-tolylisoquinolin-1(2H)-one(3hc)



Yield 69% (168 mg); light green solid; mp 208-213 °C; (KBr) cm^{-1}: 656, 768, 816, 1149, 1330, 1399, 1433, 1463, 1491, 1511, 1541, 1574, 1645, 1678, 1700, 1739, 2847, 2914, 2952, 3624, 3672, 3742, 3869 cm^{-1};^1H NMR (400 MHz, $CDCl_3$): δ 9.16 (s,1H), 8.47-8.45 (m, 1H), 7.57-7.53 (1H), 7.49-7.45 (m, 1H), 7.35-7.33 (m, 1H), 7.12 (d, J = 8.5 Hz, 4H), 7.06-7.03 (m, 4H), 2.35 (s, 3H), 2.29 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$): δ 162.8, 138.9, 138.6, 136.9, 136.9, 132.8, 132.6, 132.4, 131.7, 131.0, 129.3, 129.2, 129.0, 129.0,

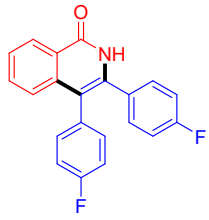
128.8, 127.5, 126.4, 125.7, 125.0, 116.9, 21.6, 21.3; mass (ES+) m/z = 326.16 $(M+H)^+$; HRMS (ESI-TOF) calcd for $C_{23}H_{20}NO$ 326.1539 Found 326.1538.

3,4-bis(4-(tert-butyl)phenyl)isoquinolin-1(2H)-one(3hd)



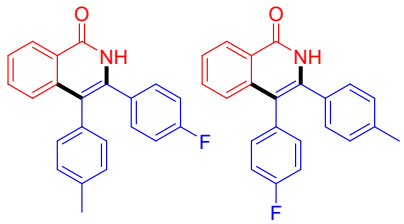
Yield 66% (202 mg); white solid; mp 123-128 °C; (KBr) cm^{-1}: 648, 733, 774, 836, 872, 910, 966, 1025, 1117, 1270, 1310, 1359, 1467, 1510, 1551, 1647, 1741, 2321, 2961, 3034, 3162 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ 8.75 (s,1H), 8.49-8.48 (m, 1H), 7.60-7.55 (1H), 7.50-7.46 (m, 1H), 7.39 (d, *J* = 8.4 Hz, 2H), 7.23 (t, *J* = 7.2 Hz, 2H), 7.09 (t, *J* = 7.1 Hz, 4H), 1.33 (s, 9H), 1.26 (s, 9H); ^{13}C NMR (400 MHz, $CDCl_3$): δ 162.6, 151.7, 150.3, 138.9, 136.8, 132.7, 132.6, 132.4, 131.5, 128.8, 127.5, 126.5, 125.9, 125.3, 125.2, 125.0, 117.0, 34.7, 34.6, 31.4, 31.2; mass (ES+) m/z = 410.24 $(M+H)^+$; HRMS (ESI-TOF) calcd for $C_{29}H_{32}NO$ 410.2484Found 410.2477.

3,4-bis(4-fluorophenyl)isoquinolin-1(2H)-one(3he)



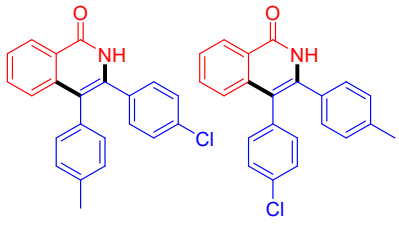
Yield 61% (152 mg); white solid; mp273-278 °C; (KBr) cm^{-1}: 658, 711, 768, 803, 868, 954, 1025, 1081, 1137, 1188, 1246, 1316, 1338, 1395, 1420, 1455, 1514, 1539, 1616, 1699, 1747, 1767, 1794, 1827, 1867, 1918, 1941, 2021, 2239, 2320, 2375, 2730, 2807, 2922, 3031, 3230, 3590, 3648, 3672, 3800 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ 9.32 (s, 1H), 7.92 (d, *J*= 8.8 Hz, 1H), 7.78 (d, *J* = 1.4 Hz, 1H), 7.70(dd, *J* = 1.7, 1.7 Hz, 1H), 7.37 - 7.29 (m, 2H), 7.20 – 7.16 (m, 2H), 7.11 (t, *J* = 7.1 Hz, 2H), 6.92 (t *J*= 6.9 Hz, 2H);^{13}C NMR (400 MHz, $CDCl_3$): δ 163.9, 163.4, 163.0, 161.6, 160.9, 138.6, 136.7, 133.5, 133.4, 132.9, 131.6, 131.4, 131.4, 130.8, 127.6, 126.9, 125.4, 125.2, 116.4, 115.8, 115.7, 115.6, 115.5; mass (ES+) m/z = 334.05 $(M+H)^+$; HRMS (ESI-TOF) calcd for $C_{21}H_{14}F_2NO$ 334.1038 Found 334.1039

4-(4-fluorophenyl)-3-(p-tolyl)isoquinolin-1(2H)-one (3hg)



Yield 61% (136 mg); brown solid; mp 148-152 °C; (KBr) cm^{-1}: 697, 1959, 1970, 3362, 3403, 3424, 3491, 3509, 3566 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.23-9.66 (broad s, 1H), 8.43-8.47 (m, 1H), 7.55-7.61 (m, 1H), 7.47-7.51 (m, 1H), 7.29-7.36 (m, 1H), 7.26 (s), 7.22-7.24 (m, 1H), 7.11-7.16 (m, 2H), 7.04-7.09 (m, 2H), 6.92-7.01(m, 2H), 2.31-2.36 (s,3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.2, 162.8, 162.7, 160.84, 160.80, 138.8, 138.7, 137.5, 137.1, 136.1, 133.4, 133.3, 132.7, 132.6, 132.4, 131.9, 131.83, 131.79, 131.6, 131.3, 131.2, 129.2, 129.0, 127.6, 127.4, 126.6, 126.5, 125.7, 125.3, 125.1, 125.0, 115.8, 115.6, 115.5, 115.4, 115.3, 21.2; mass (ES+) m/z = 330.13 $(M+H)^+$; HRMS (ESI-TOF) calcd for $C_{22}H_{17}FNO$ 330.1294 Found 330.1289.

4-(4-chlorophenyl)-3-(p-tolyl)isoquinolin-1(2H)-one (3hh)



Yield 64% (150 mg); grey solid; mp 145-150 °C; (KBr) cm^{-1}: 658, 1638, 1654, 2850, 2919, 3395, 3452, 3509 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.36-9.81 (broad s,1H), 8.43-8.47 (t, J=7.89 Hz, 1H), 7.48-7.58 (m, 2H), 7.29-7.31 (m, 2H), 7.26 (s), 7.20-7.22 (m, 2H), 7.03-7.12 (m, 2H), 2.31-2.36 (s,3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.9, 162.7, 138.9, 138.7, 138.4, 137.4, 137.2, 135.8, 134.6, 134.4, 133.5, 133.2, 133.1, 132.8, 132.7, 132.3, 131.8, 131.5, 130.7, 129.3, 129.2, 129.0, 128.7, 128.6, 127.6, 127.4, 126.7, 126.6, 125.8, 125.2, 124.9, 117.6, 115.7, 21.2; mass (ES+) m/z = 346.09 $(M+H)^+$; HRMS (ESI-TOF) calcd for $C_{22}H_{17}ClNO$ 346.0999 Found 346.1002.

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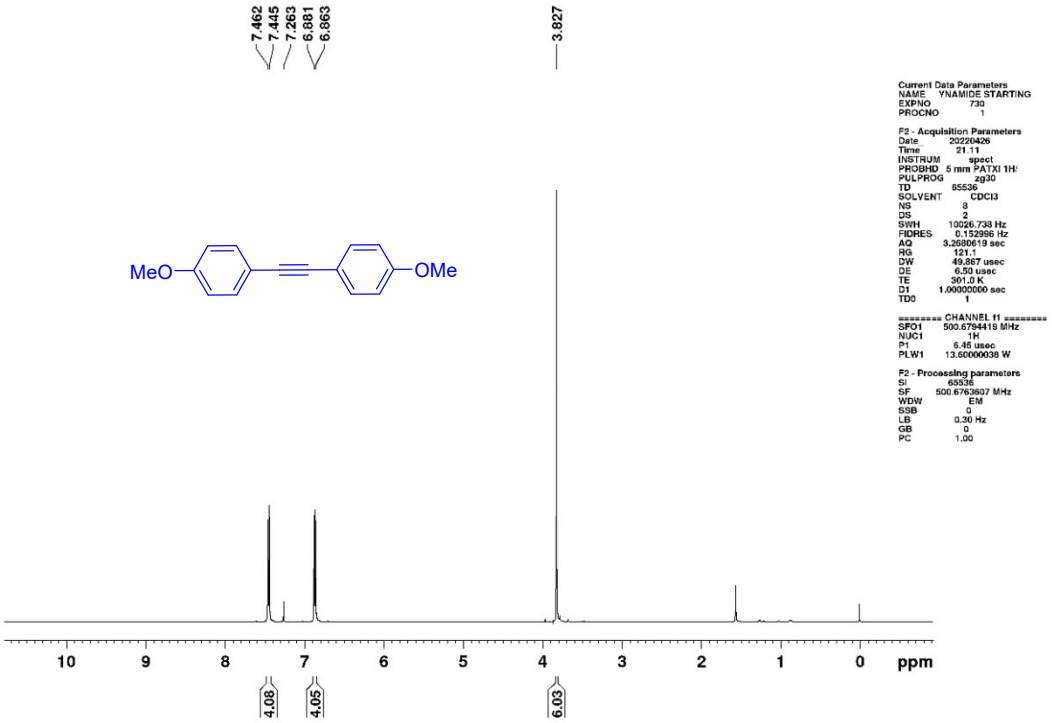
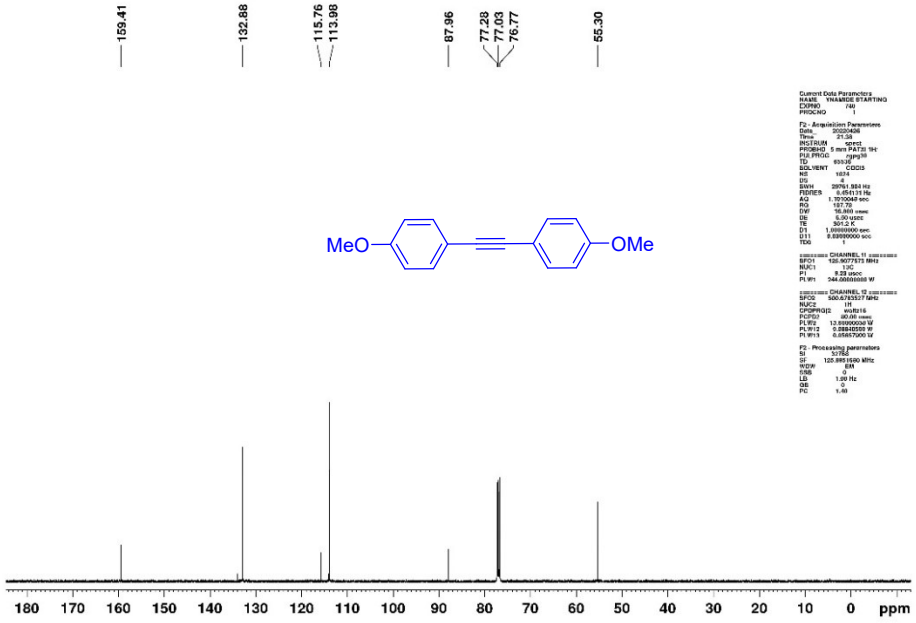
7. Copies of NMR Spectra

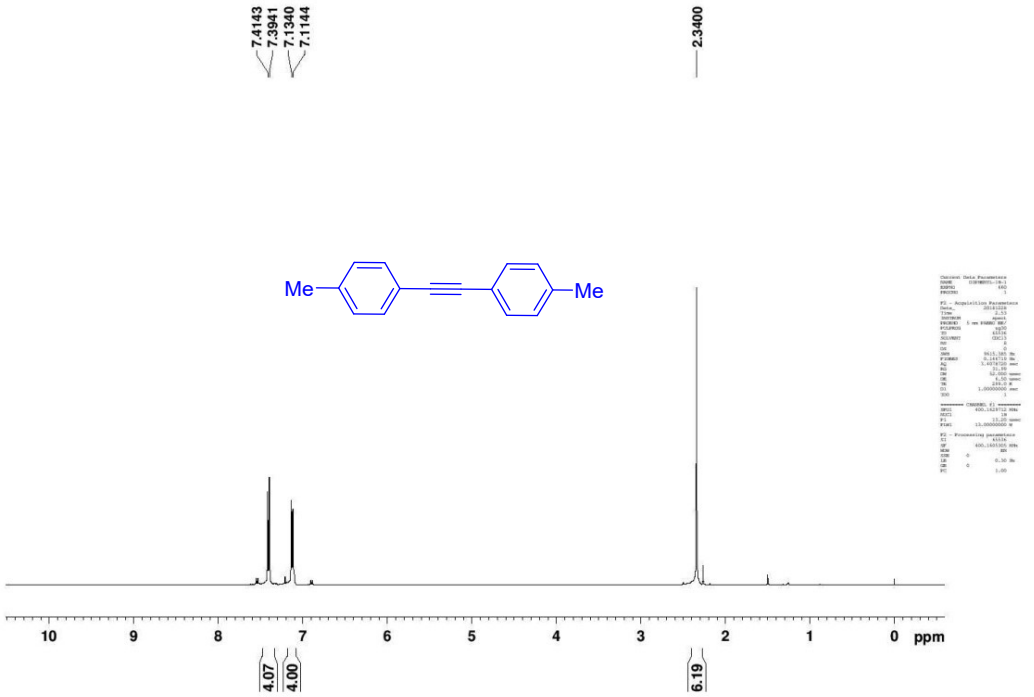
^{1}H NMR spectrum of compound- 2b (400 MHz, $CDCl_3$)



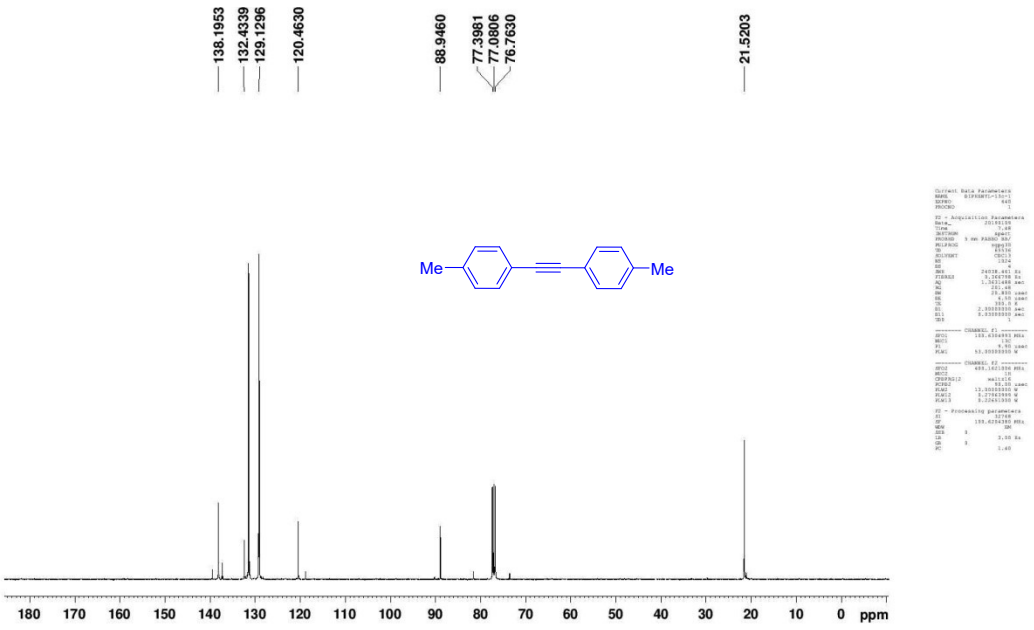
^{13}C NMR spectrum of compound-2b (100 MHz, $CDCl_3$)



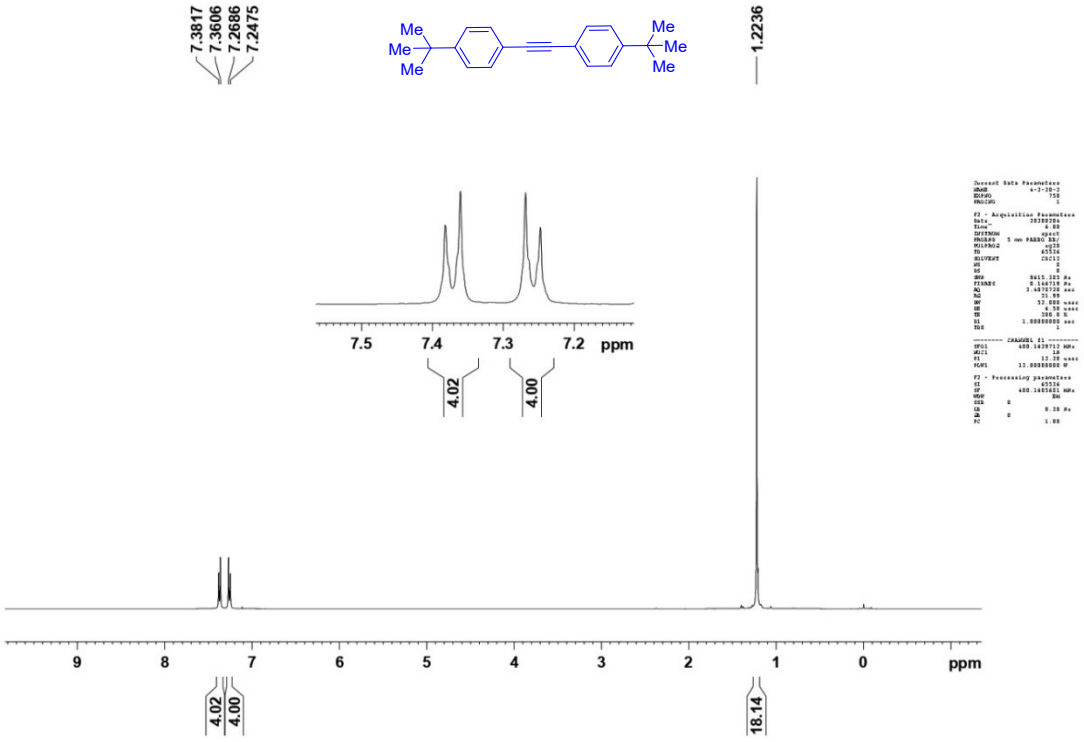
^{1}H NMR spectrum of compound- 2c (400 MHz, $CDCl_3$)



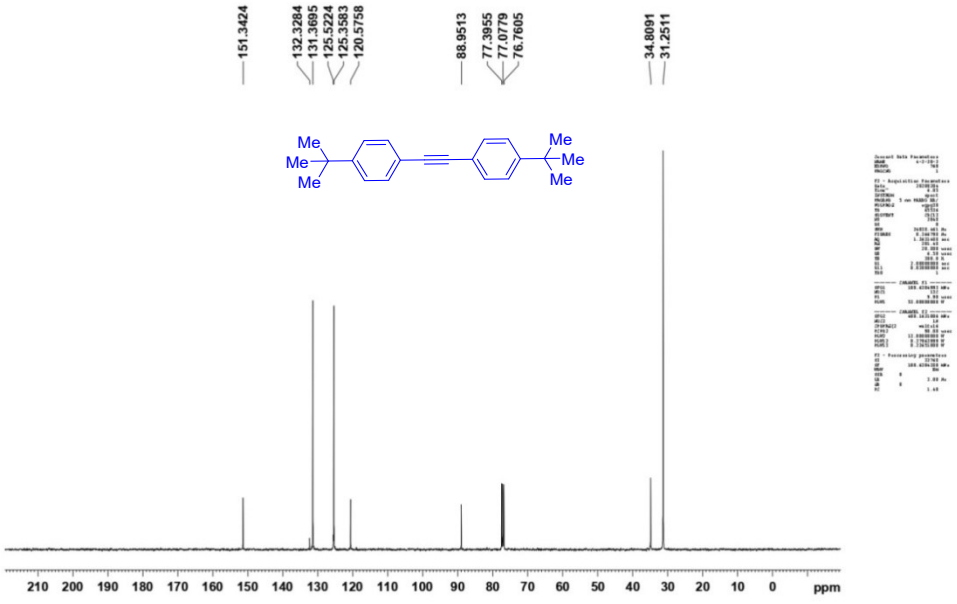
^{13}C NMR spectrum of compound-2c (100 MHz, $CDCl_3$)



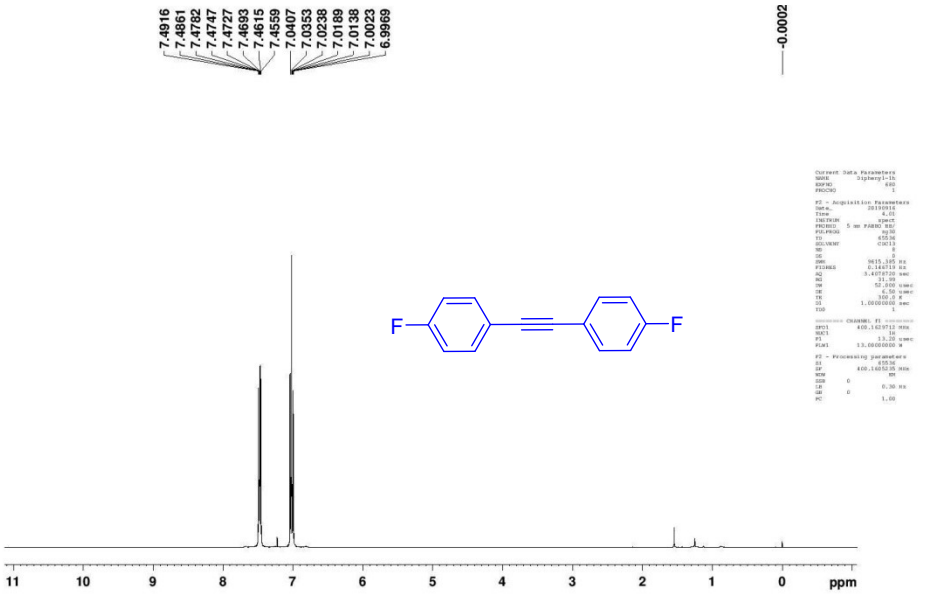
^{1}H NMR spectrum of compound -2d (400 MHz, $CDCl_3$)



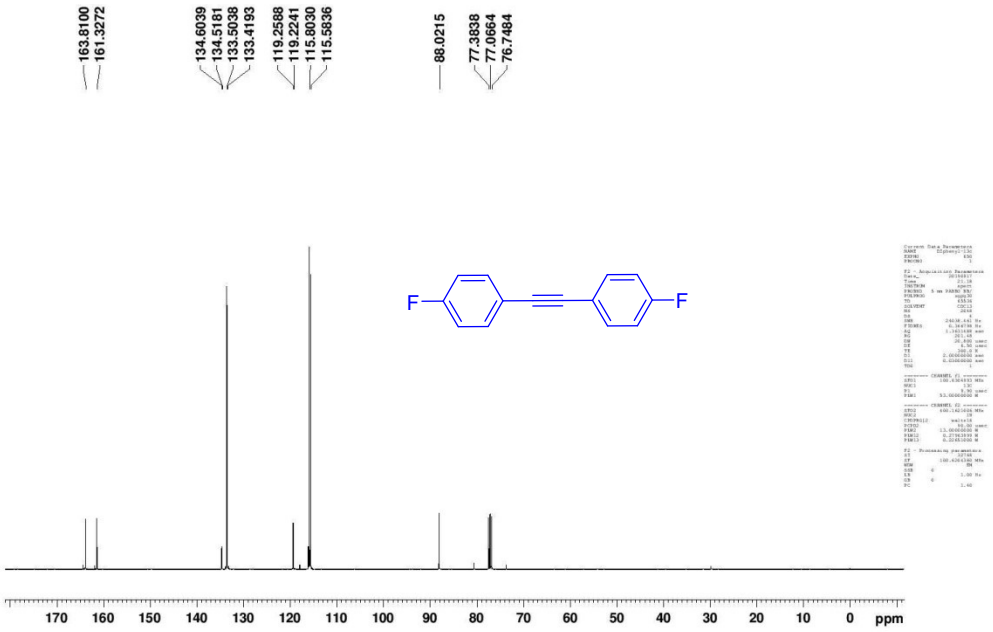
^{13}C NMR spectrum of compound -2d (100 MHz, $CDCl_3$)



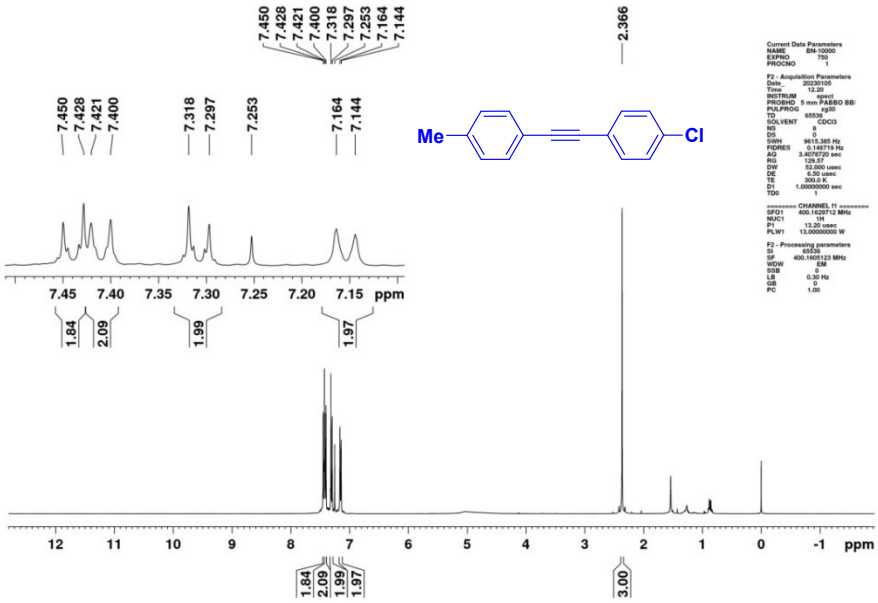
^{1}H NMR spectrum of compound- 2e (400 MHz, $CDCl_3$)



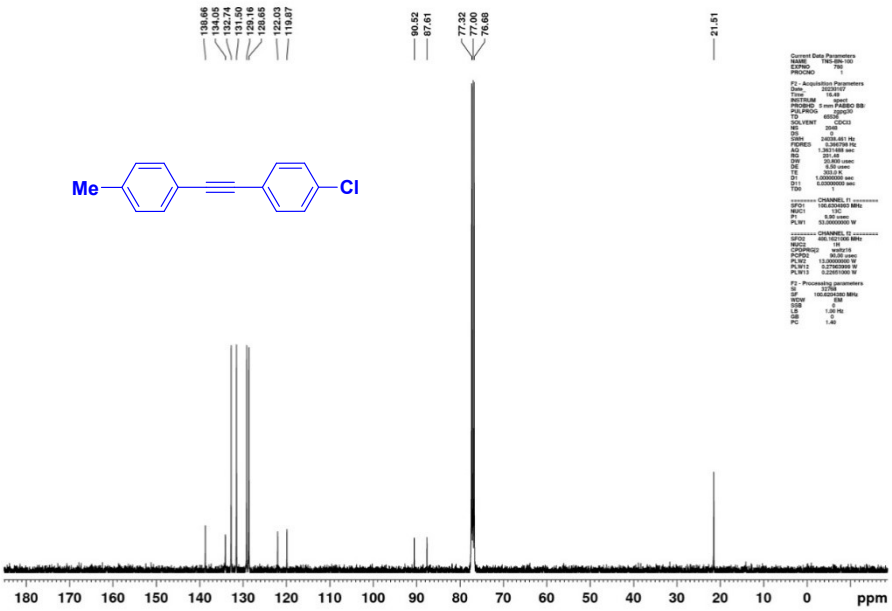
^{13}C NMR spectrum of compound- 2e (100 MHz, $CDCl_3$)



^{1}H NMR spectrum of compound- 2h (400 MHz, $CDCl_3$)

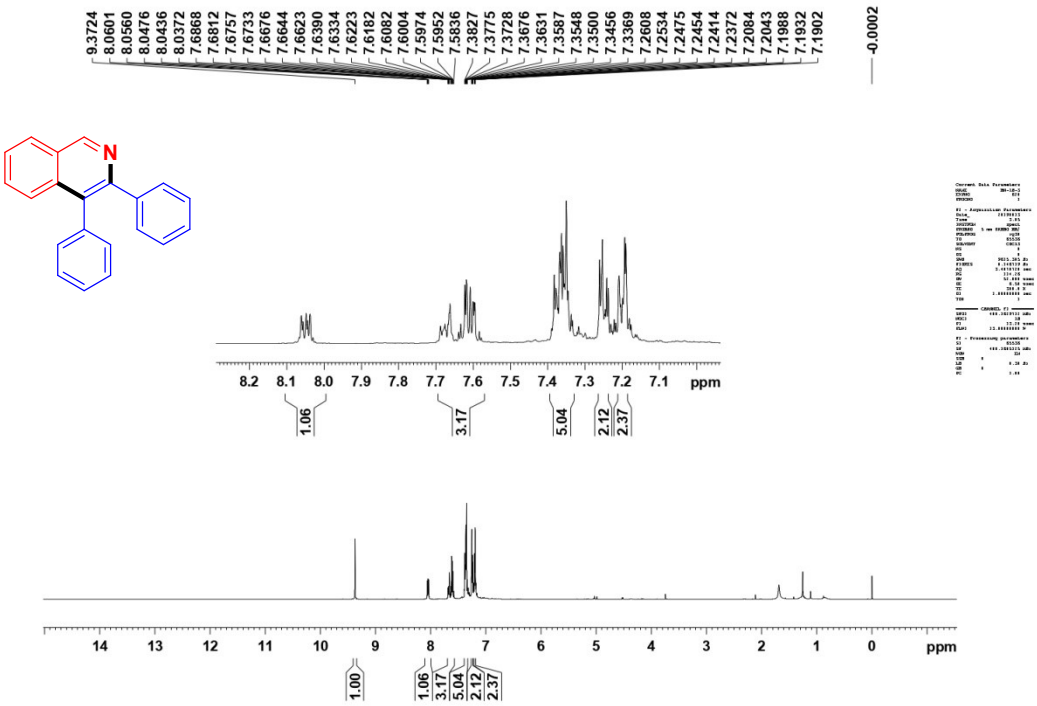


^{13}C NMR spectrum of compound- 2h (100 MHz, $CDCl_3$)

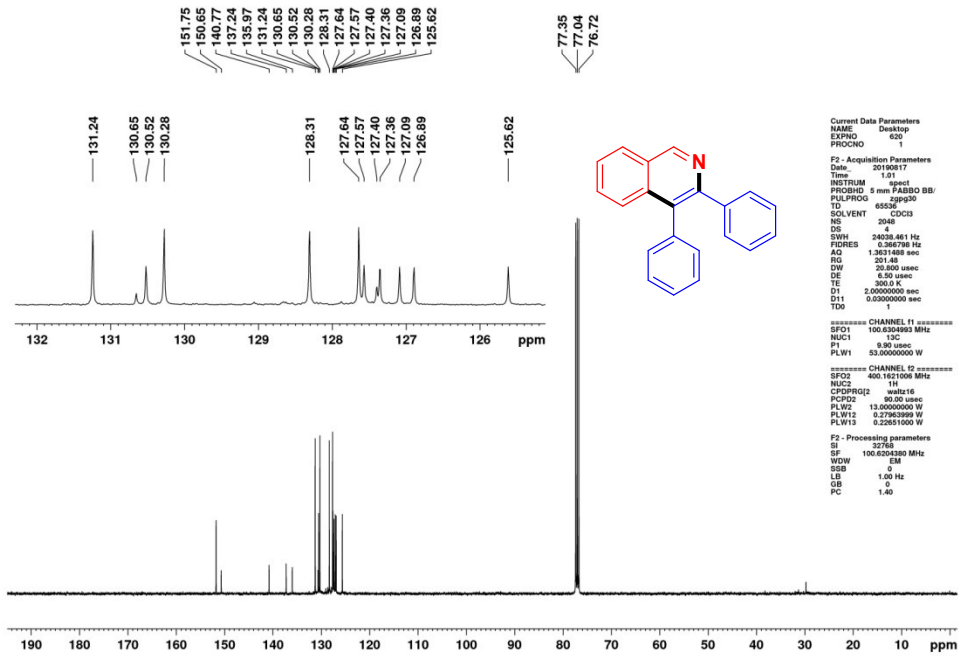


5. Copies of NMR Spectra

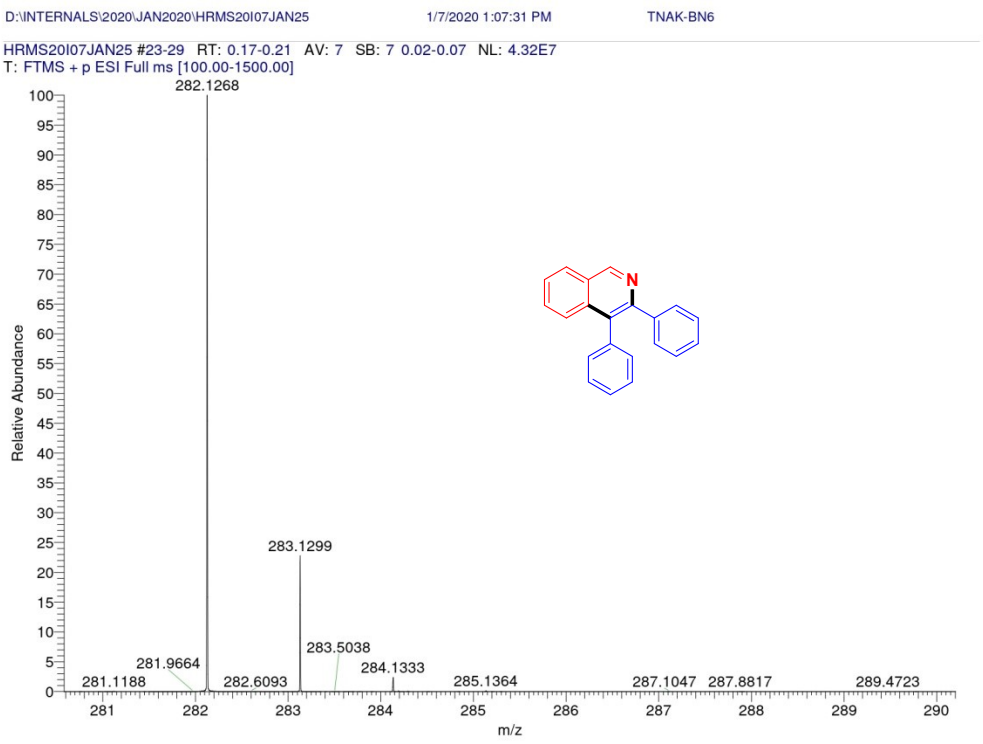
^{1}H NMR spectrum of compound- 3aa (400 MHz, $CDCl_3$)



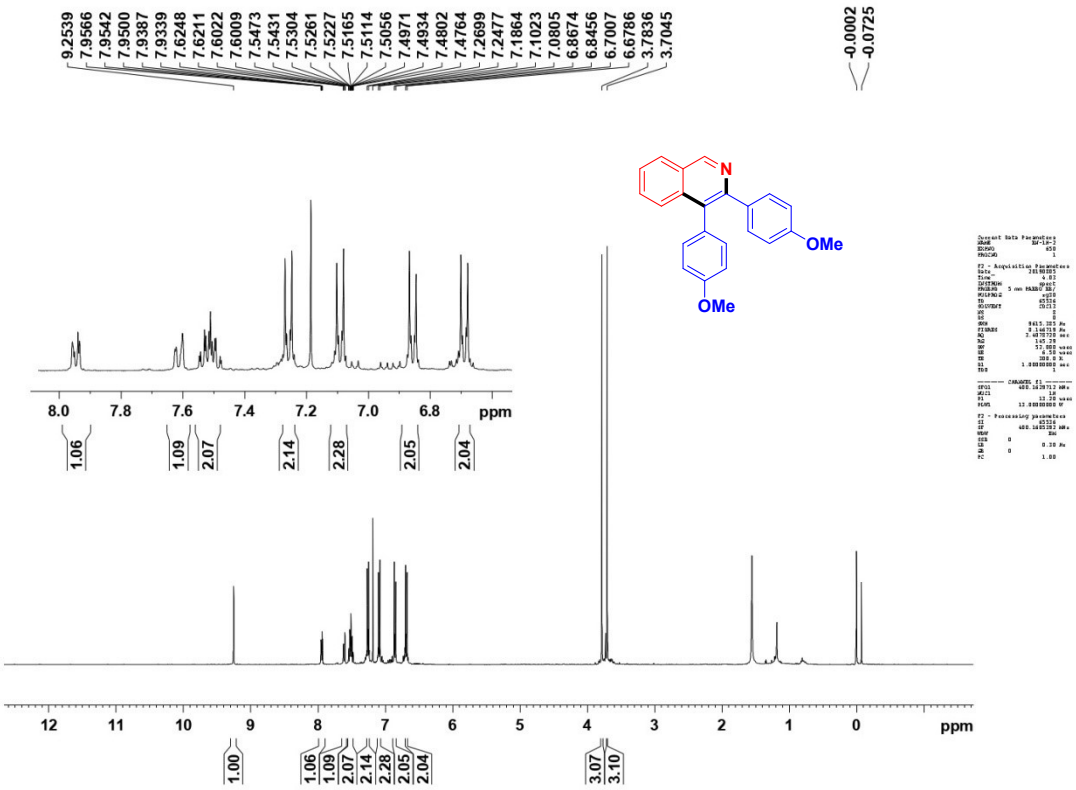
^{13}C NMR spectrum of compound- 3aa (100 MHz, $CDCl_3$)



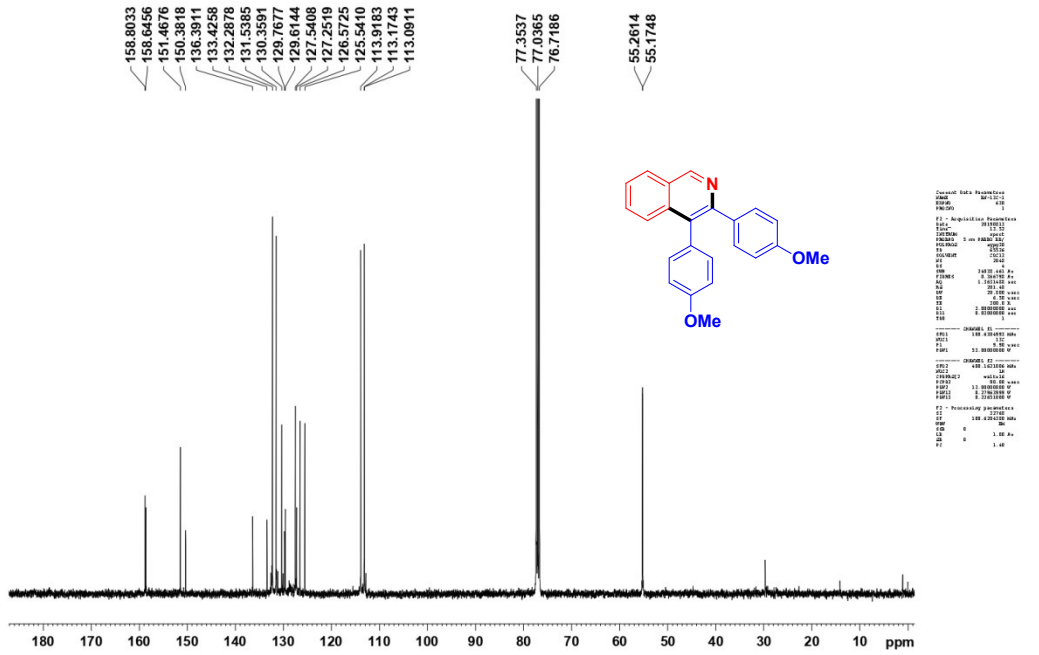
HRMS spectrum of compound- 3aa



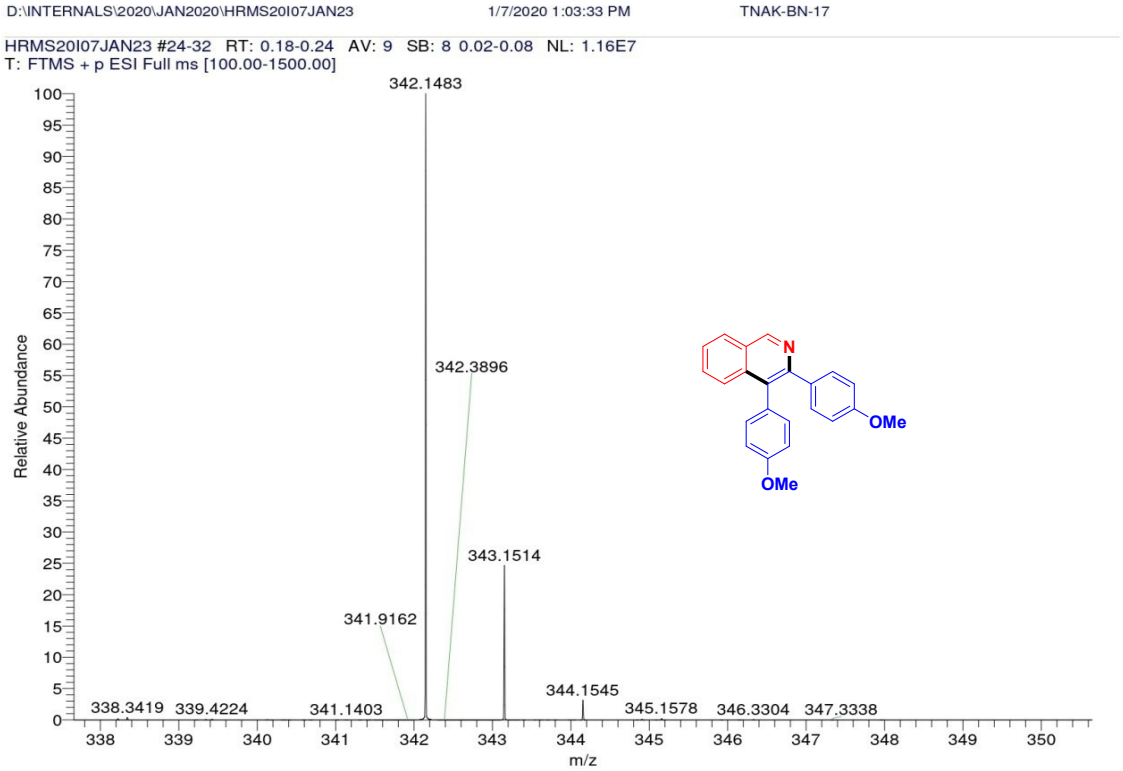
^{1}H NMR spectrum of compound- 3ab (400 MHz, $CDCl_3$)



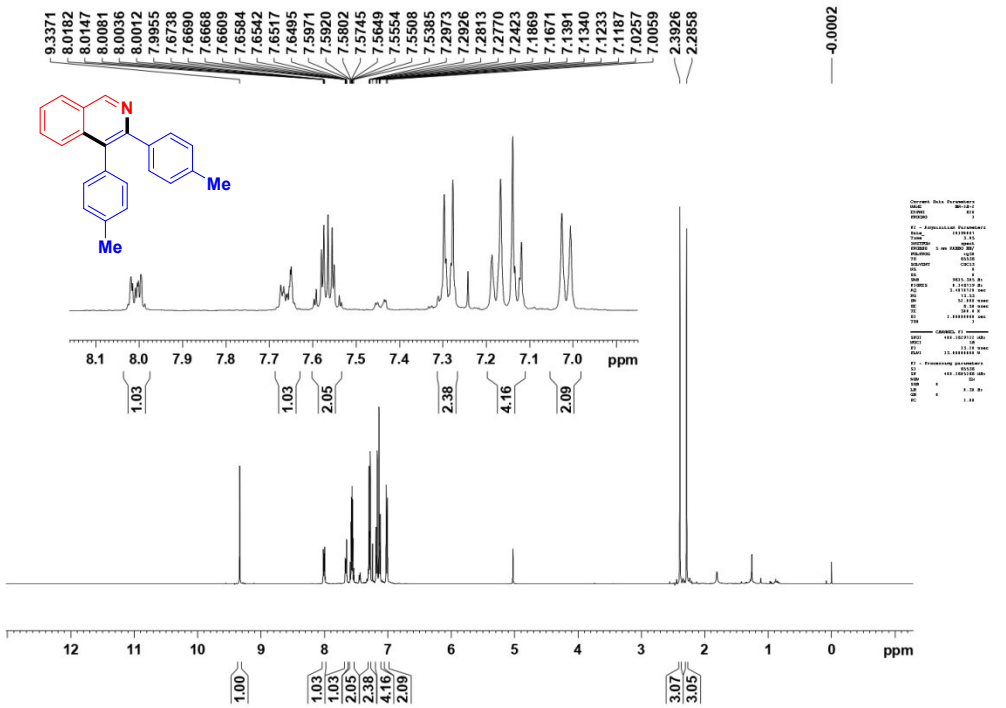
^{13}C NMR spectrum of compound- 3ab (100 MHz, $CDCl_3$)



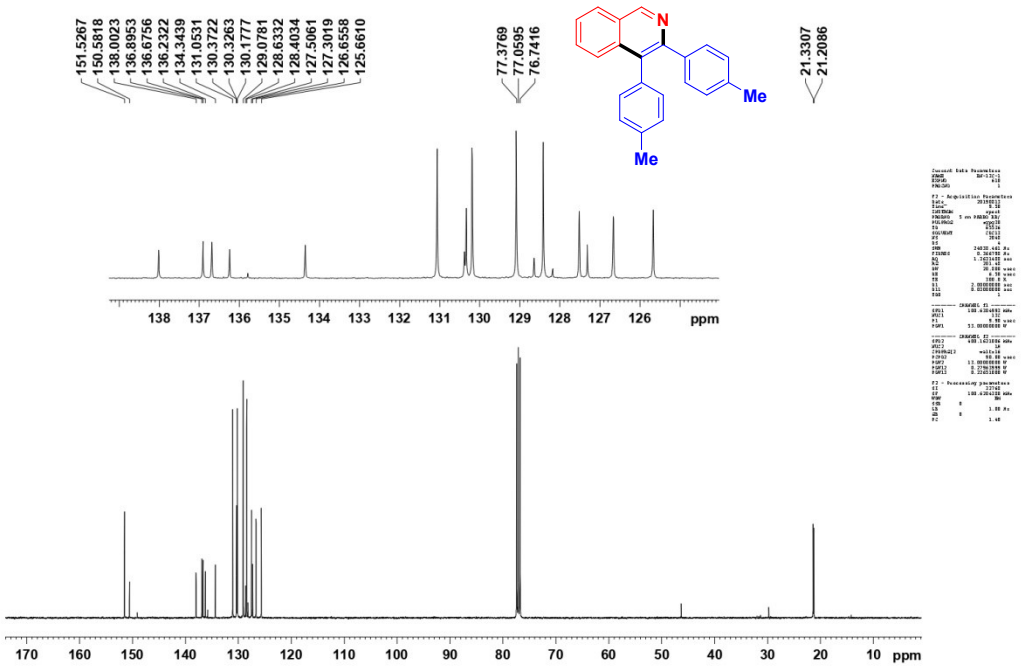
HRMS spectrum of compound- 3ab



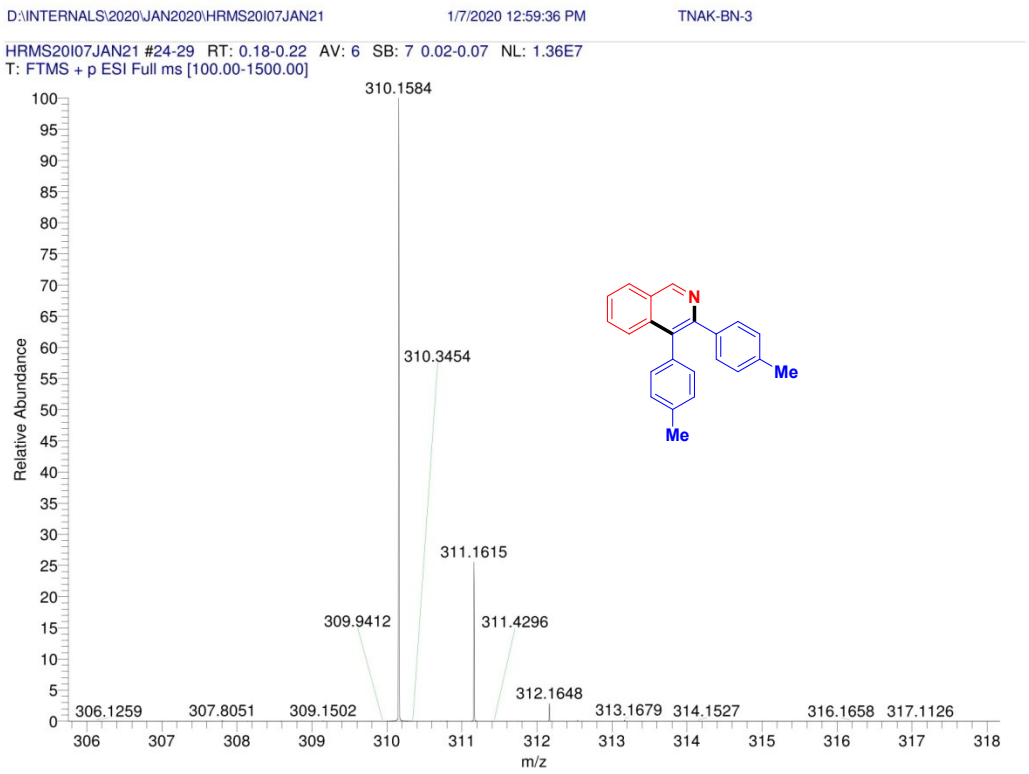
^{1}H NMR spectrum of compound- 3ac (400 MHz, $CDCl_3$)



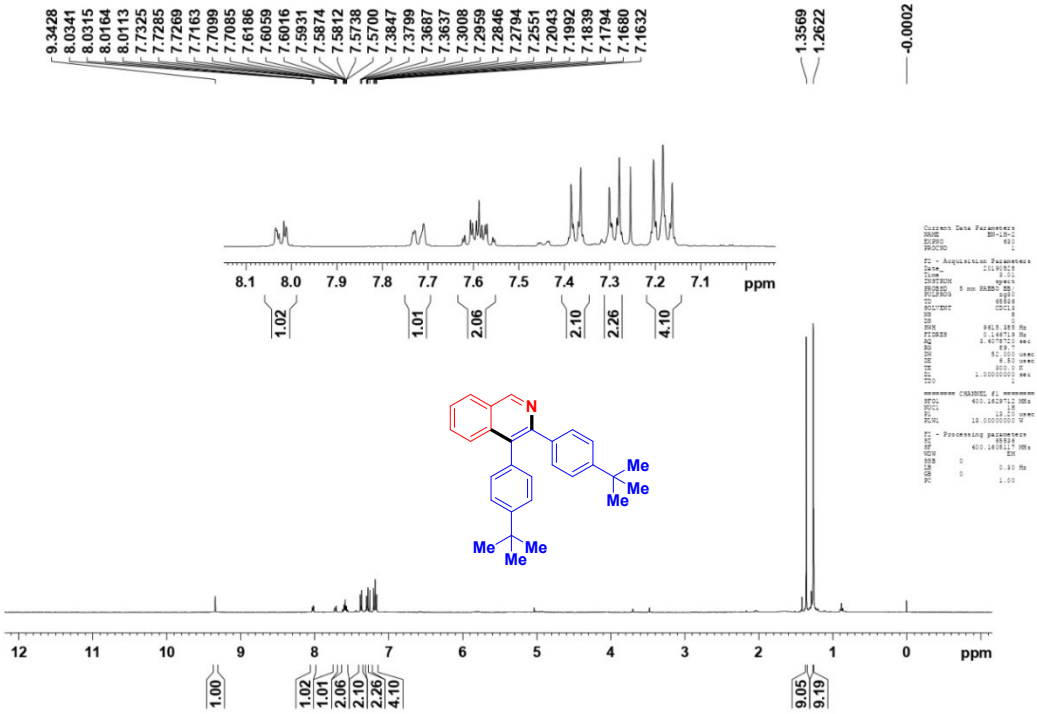
^{13}C NMR spectrum of compound- 3ac (100 MHz, $CDCl_3$)



HRMS spectrum of compound- 3ac

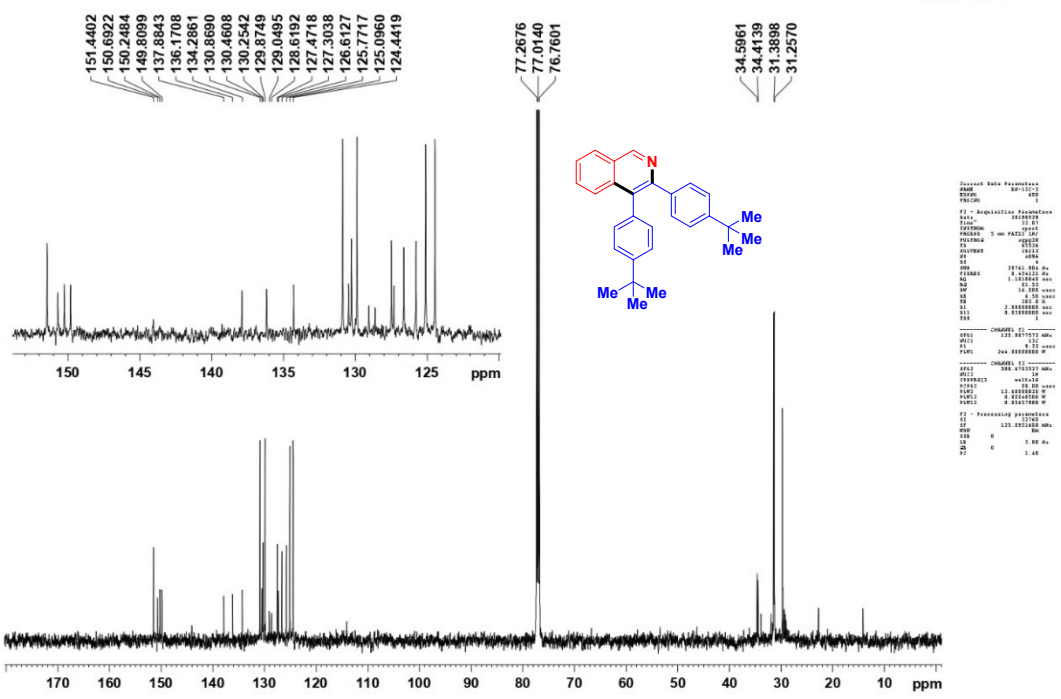


^{1}H NMR spectrum of compound- 3ad (400 MHz, CDC

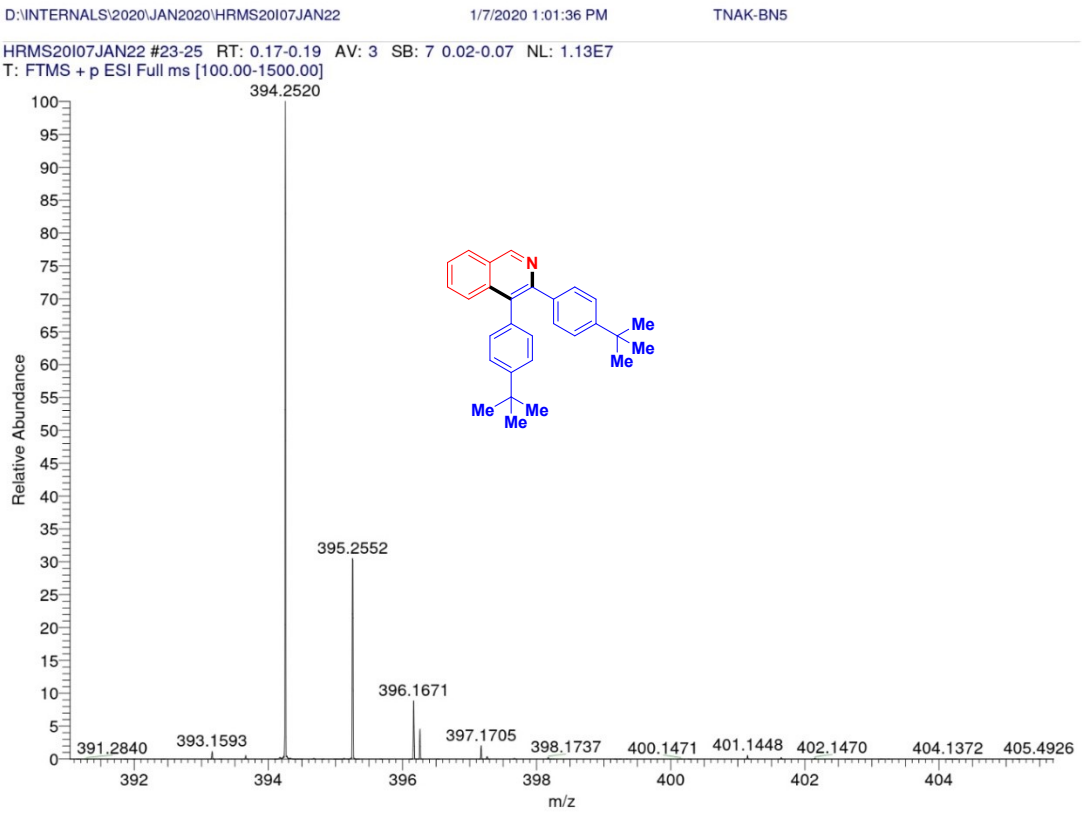


l_3)

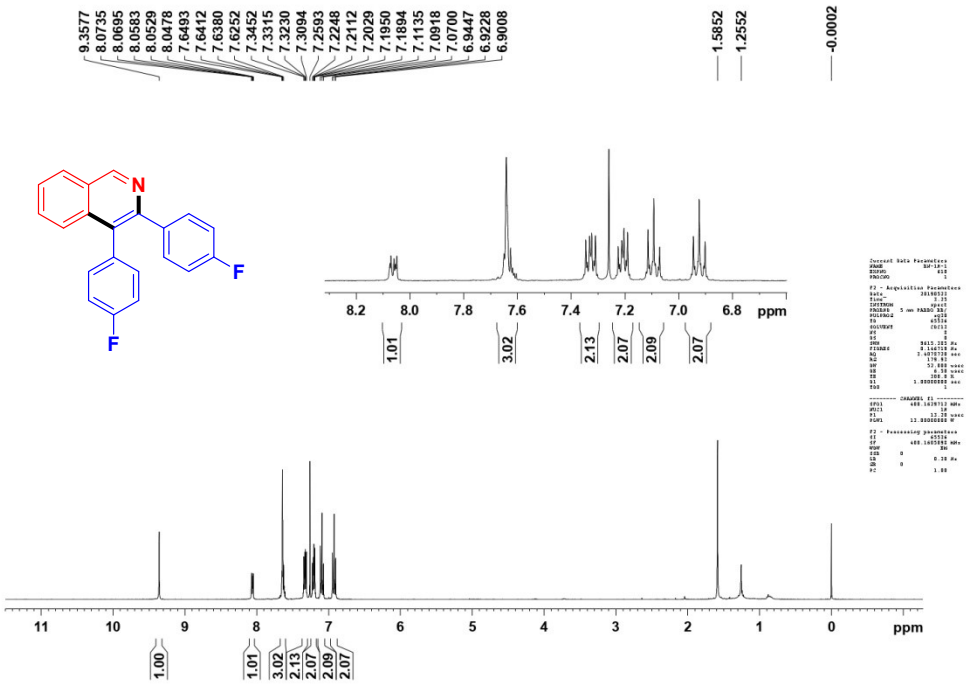
^{13}C NMR spectrum of compound- 3ad (100 MHz, $CDCl_3$)



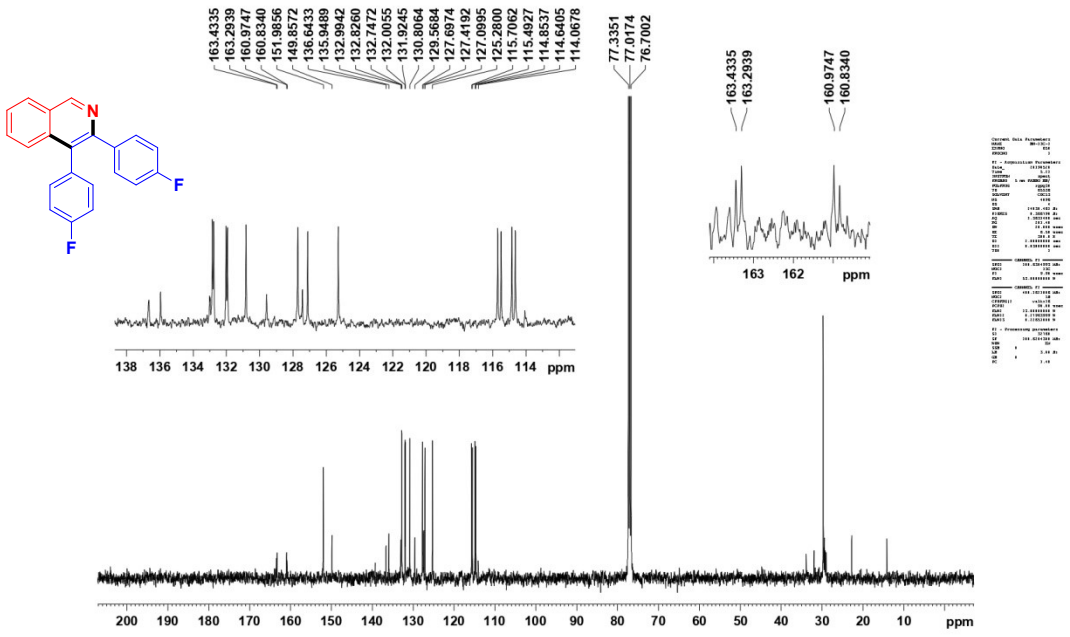
HRMS spectrum of compound- 3ad



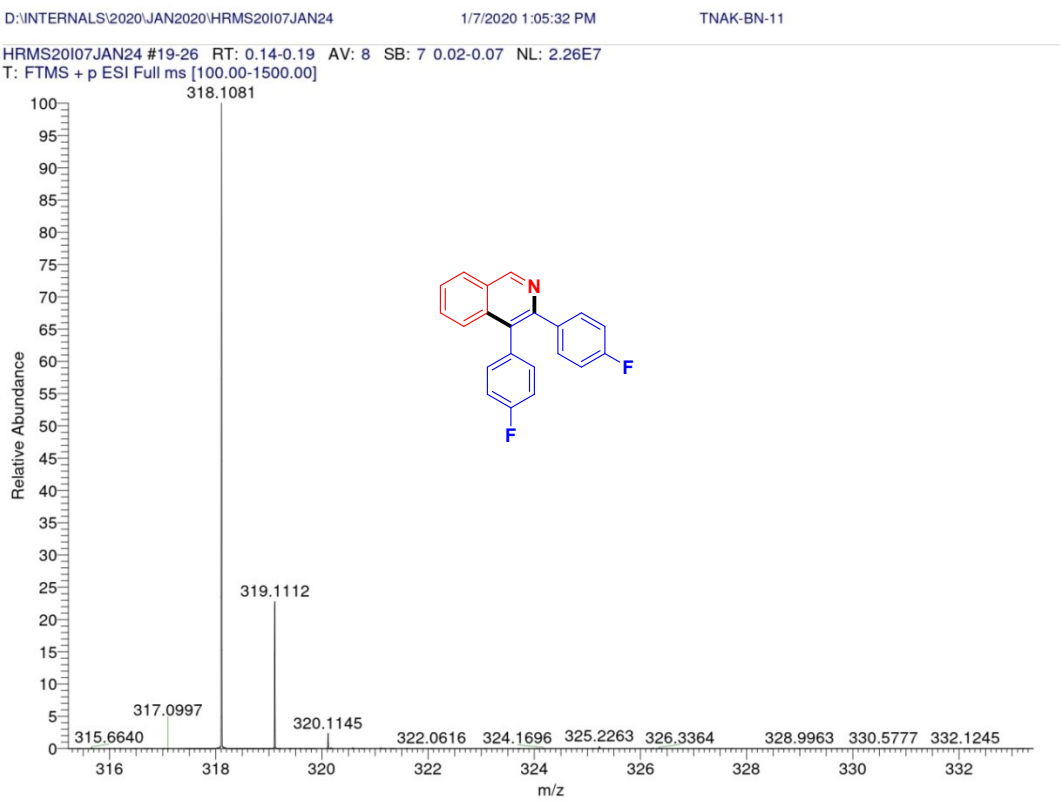
^{1}H NMR spectrum of compound- 3ae (400 MHz, $CDCl_3$)



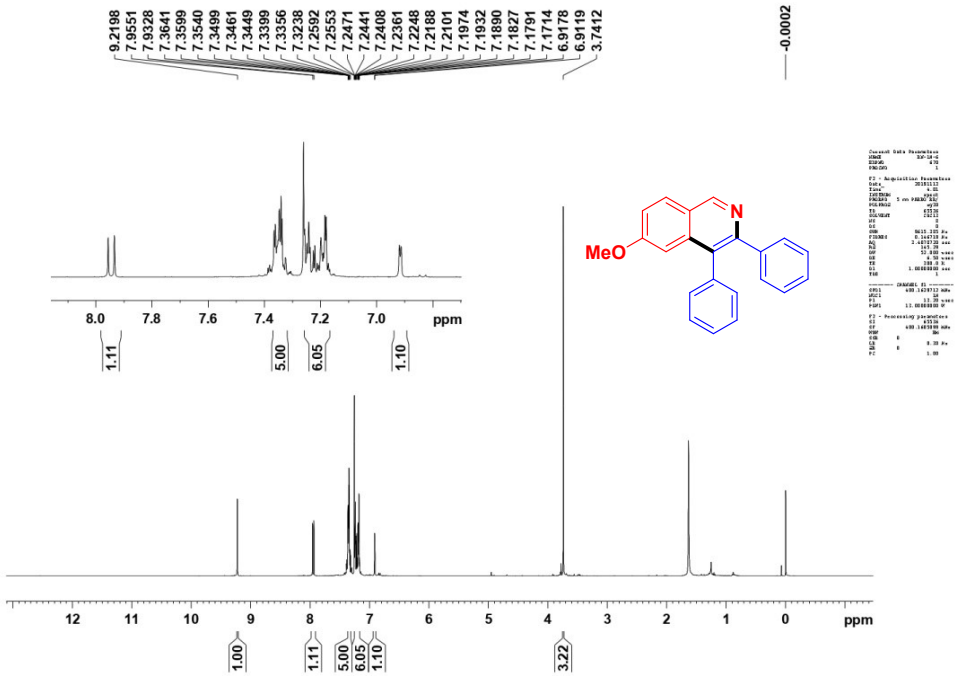
^{13}C NMR spectrum of compound- 3ae (100 MHz, $CDCl_3$)



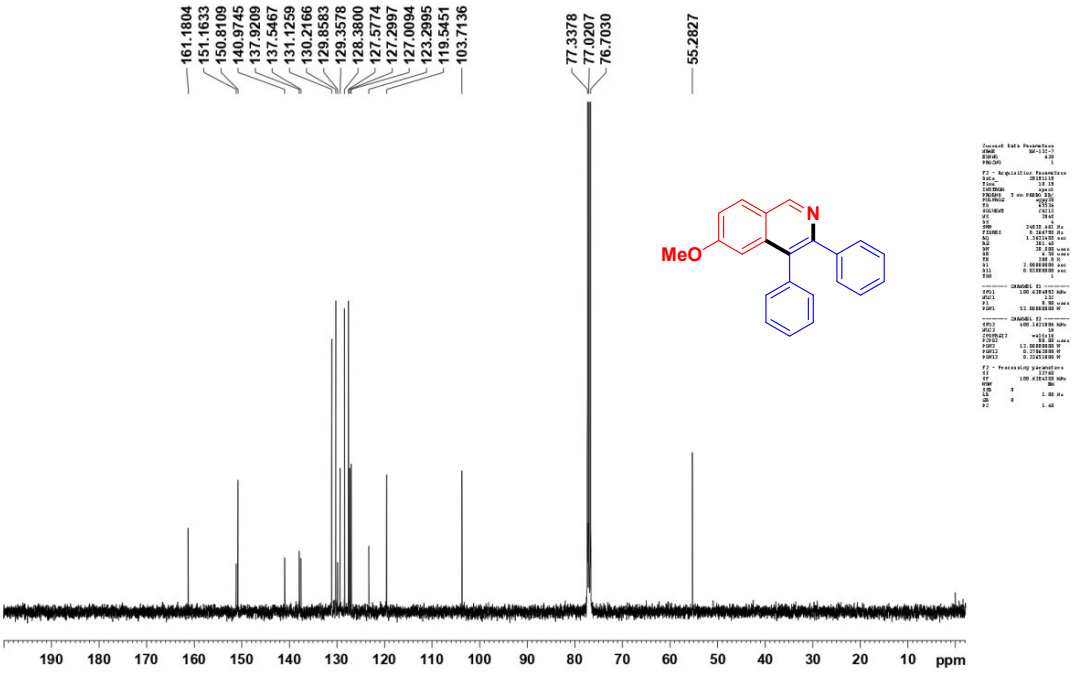
HRMS spectrum of compound- 3ae



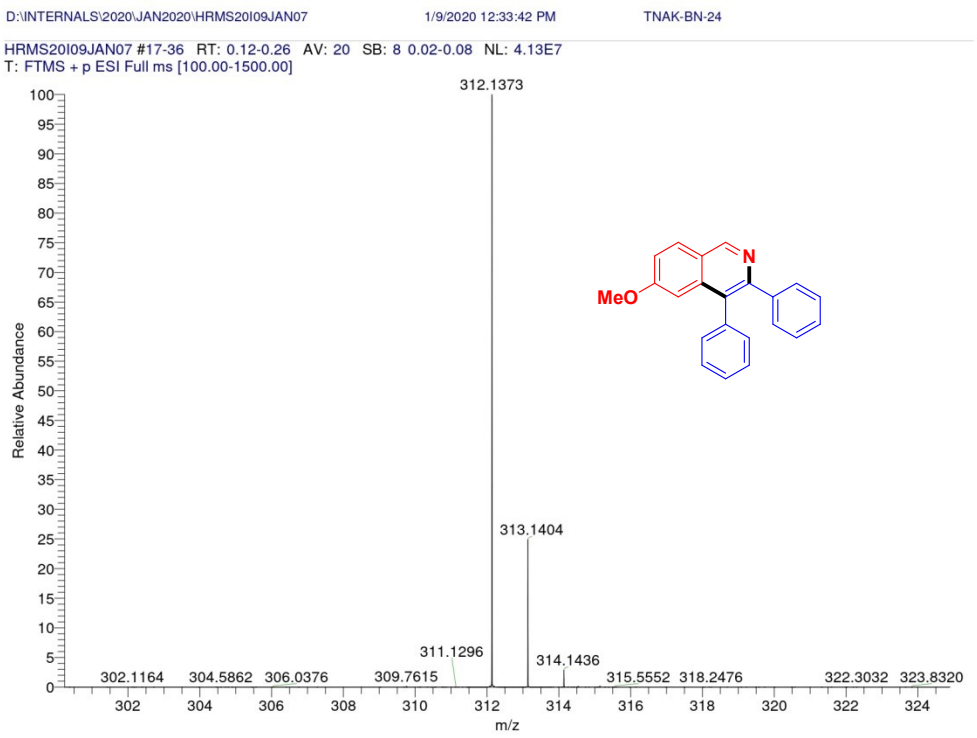
^{1}H NMR spectrum of compound- 3ba (400 MHz, $CDCl_3$)



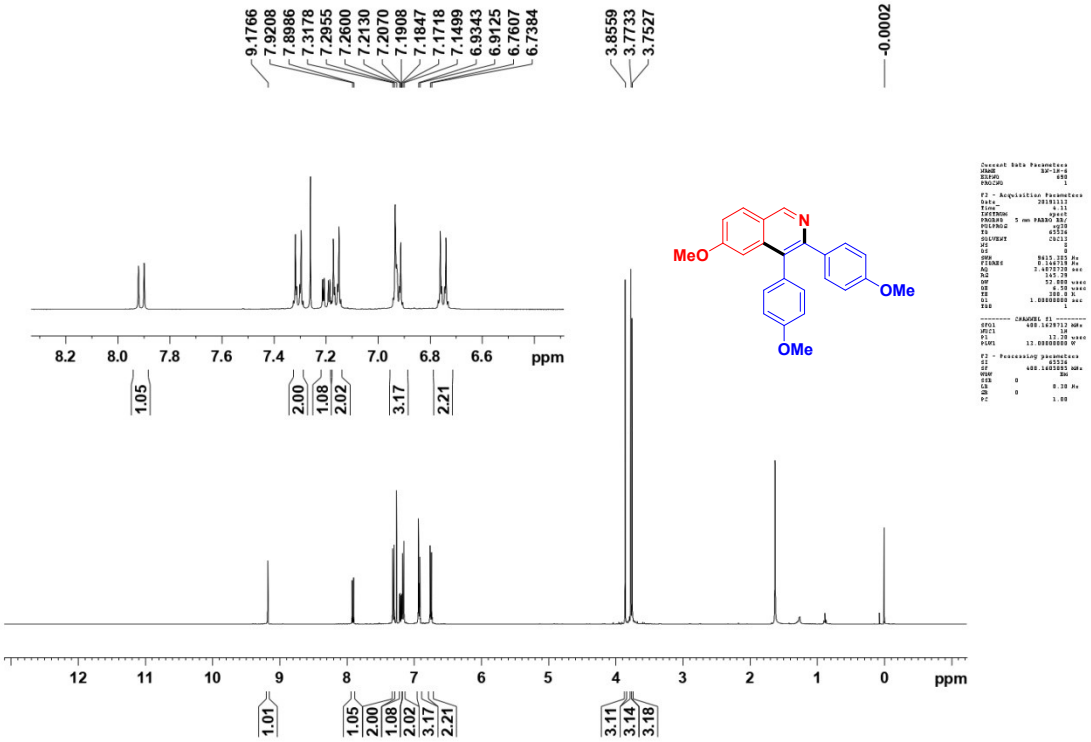
^{13}C NMR spectrum of compound- 3ba (100 MHz, $CDCl_3$)



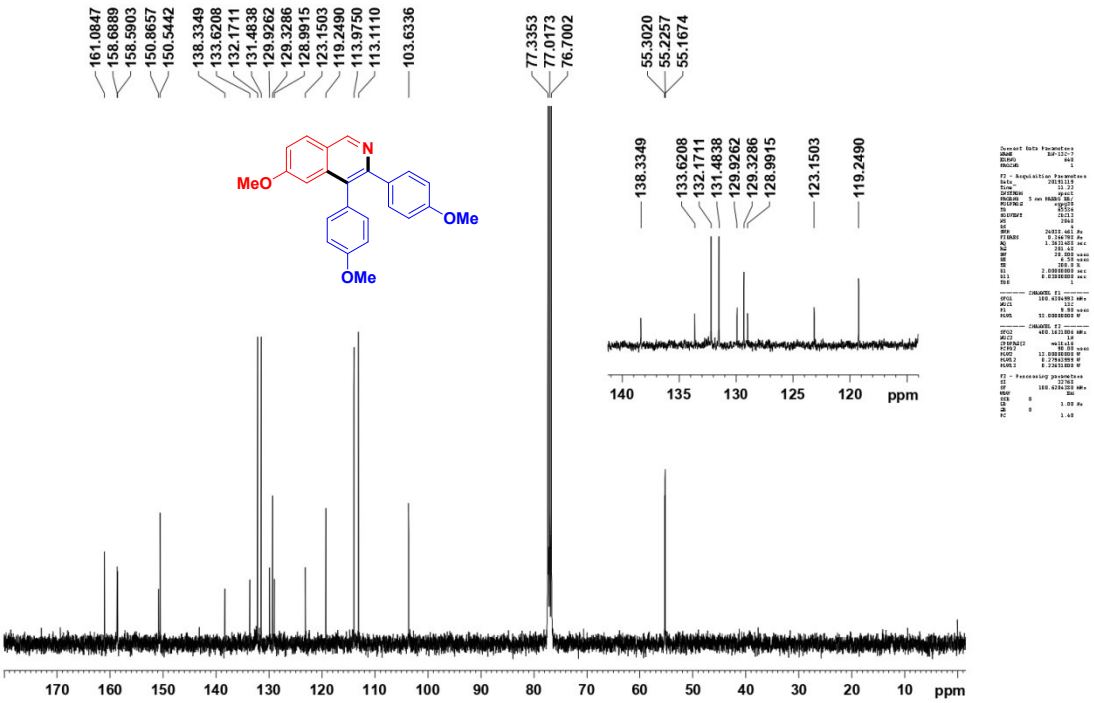
HRMS spectrum of compound- 3ba



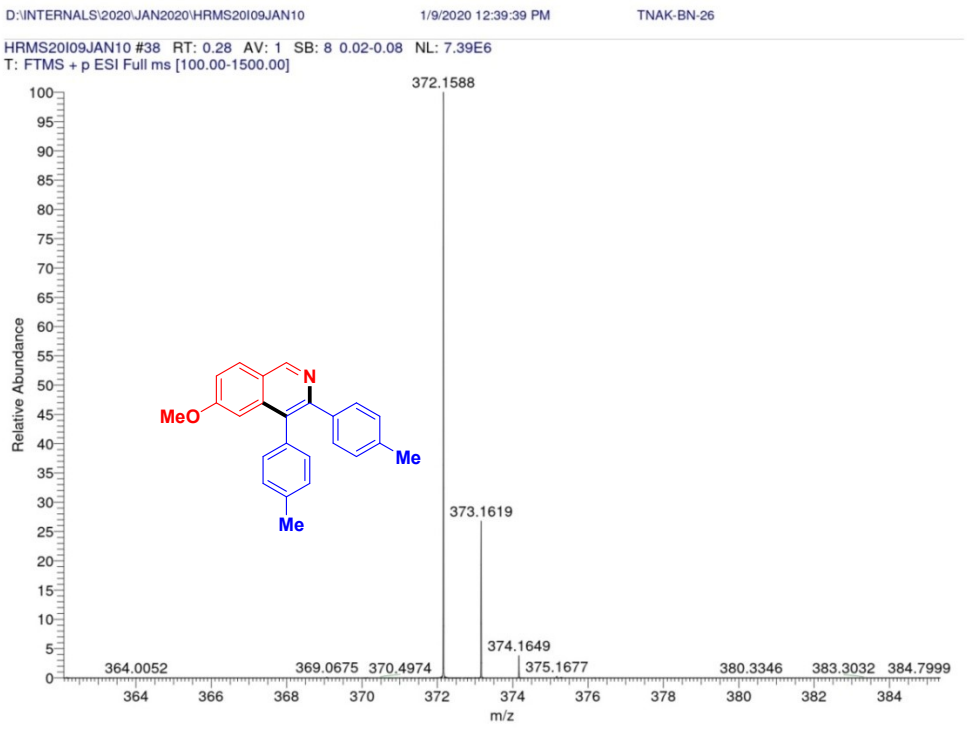
^{1}H NMR spectrum of compound- 3bb (400 MHz, $CDCl_3$)



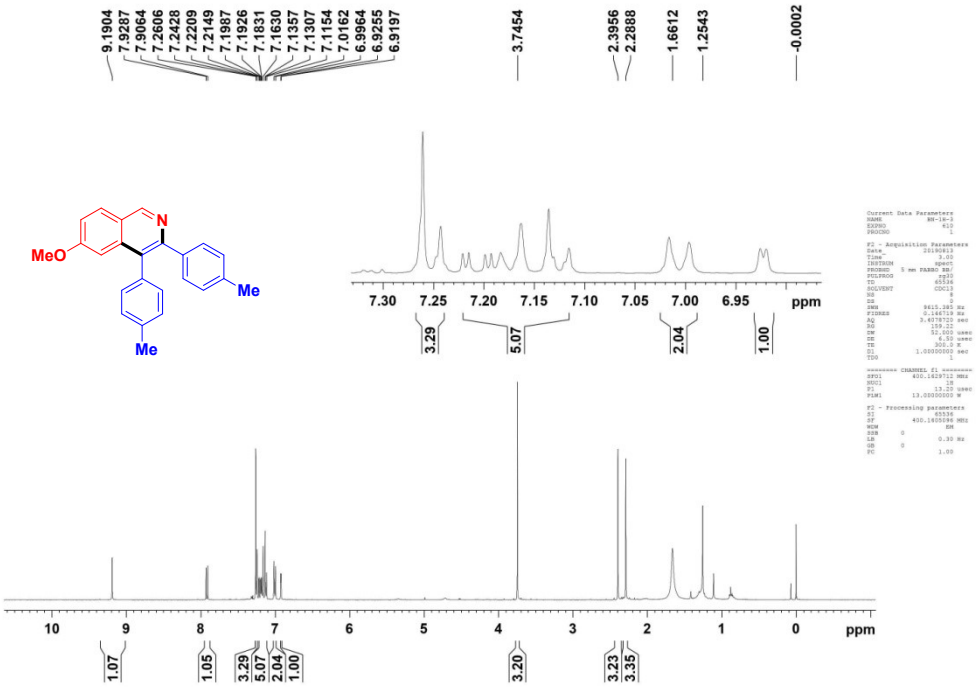
^{13}C NMR spectrum of compound- 3bb (100 MHz, $CDCl_3$)



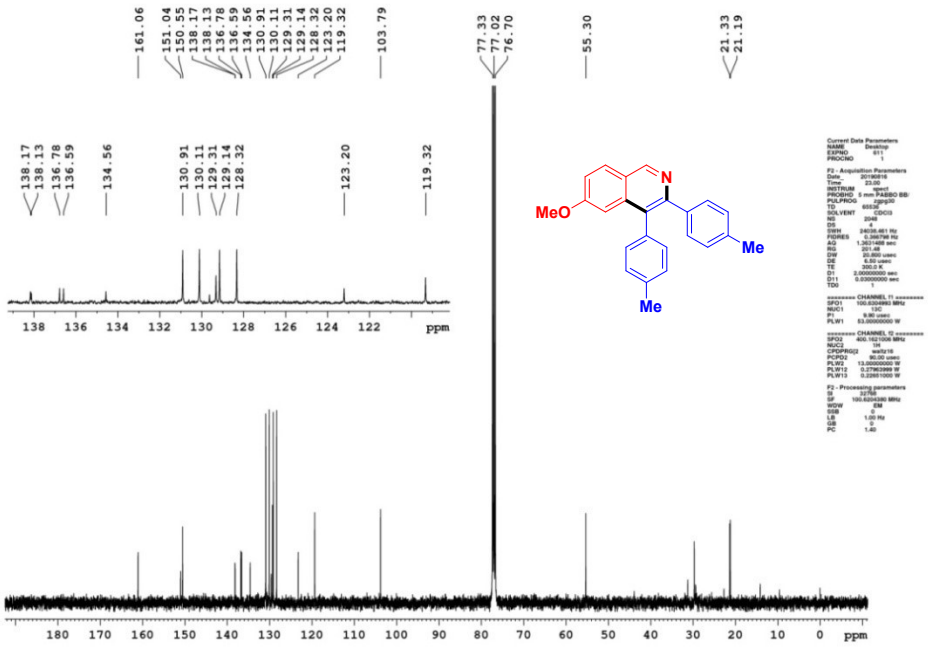
HRMS spectrum of compound- 3bb



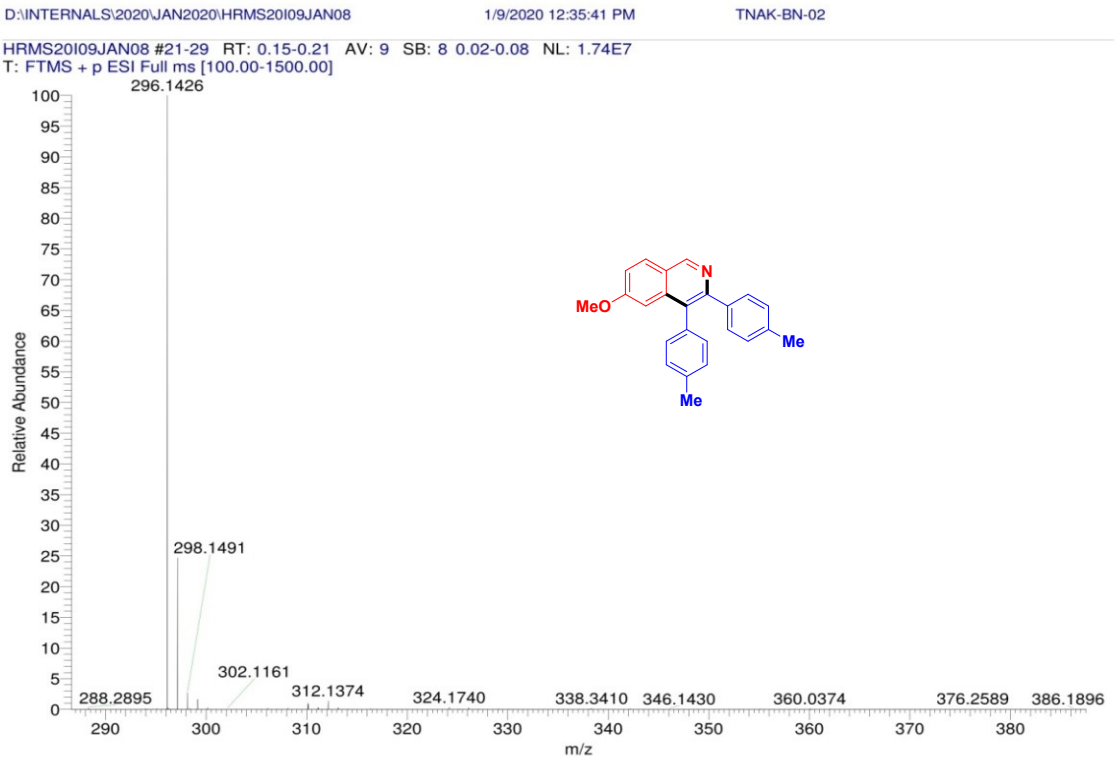
^{1}H NMR spectrum of compound- 3bc (400 MHz, $CDCl_3$)



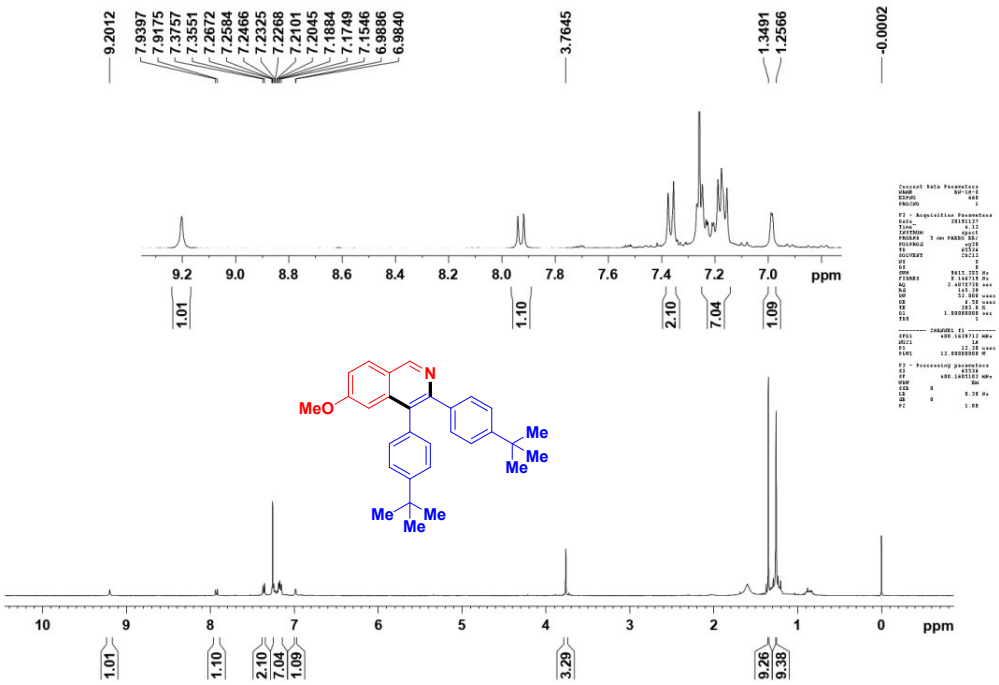
^{13}C NMR spectrum of compound- 3bc (100 MHz, $CDCl_3$)



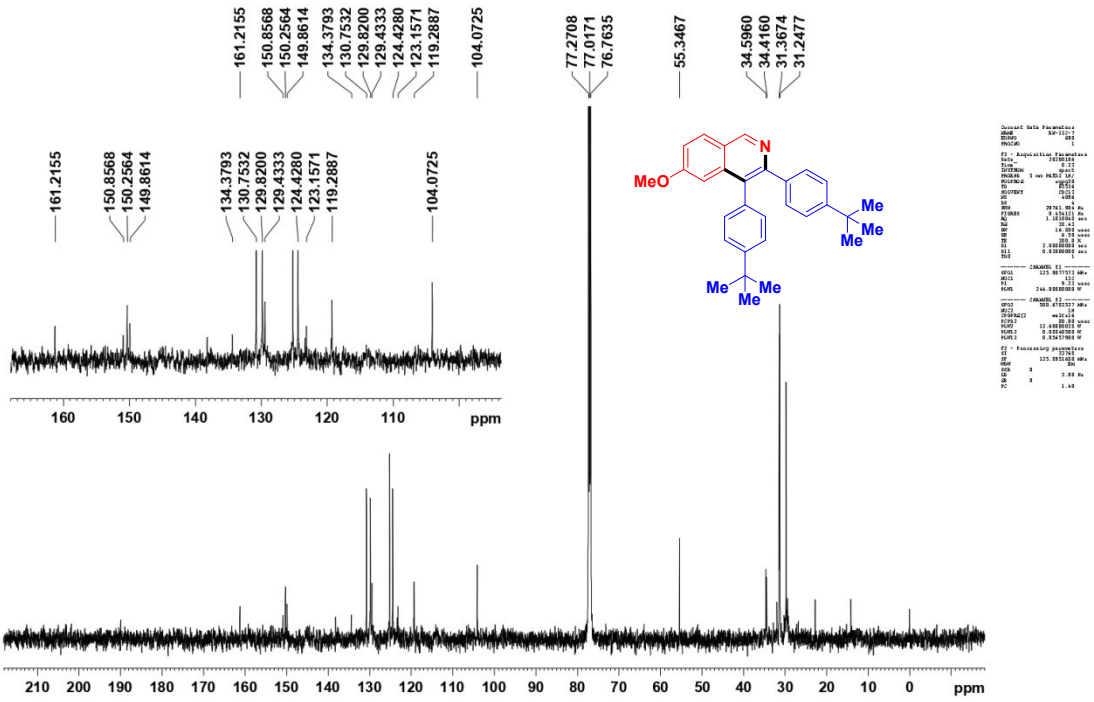
HRMS spectrum of compound- 3bc



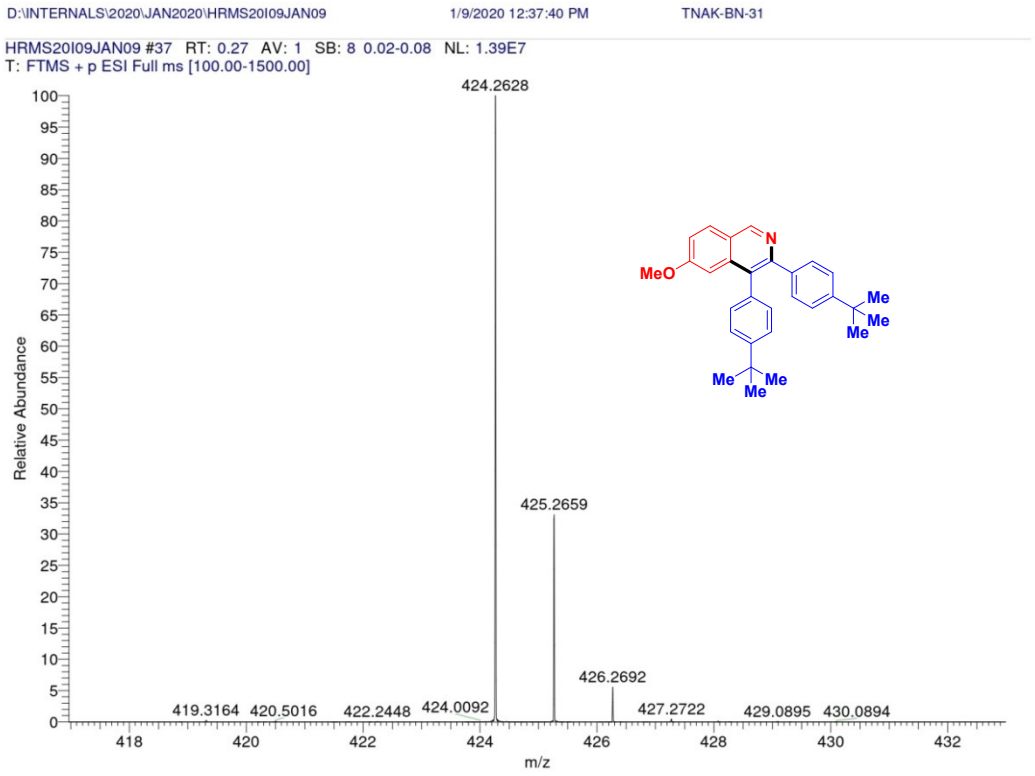
^{1}H NMR spectrum of compound- 3bd (400 MHz, $CDCl_3$)



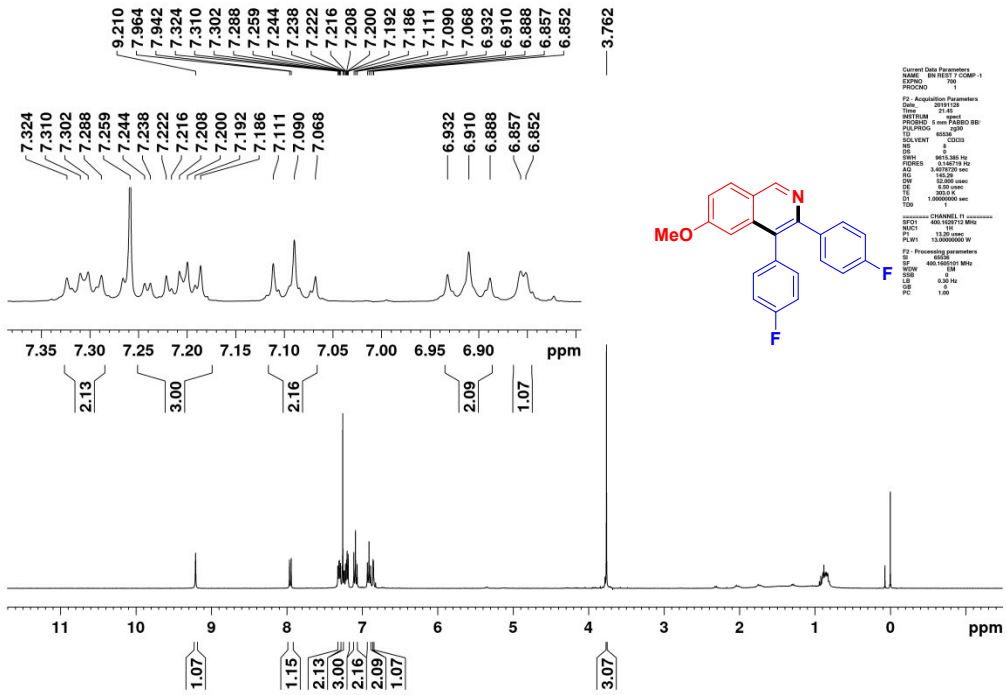
^{13}C NMR spectrum of compound- 3bd (100 MHz, $CDCl_3$)



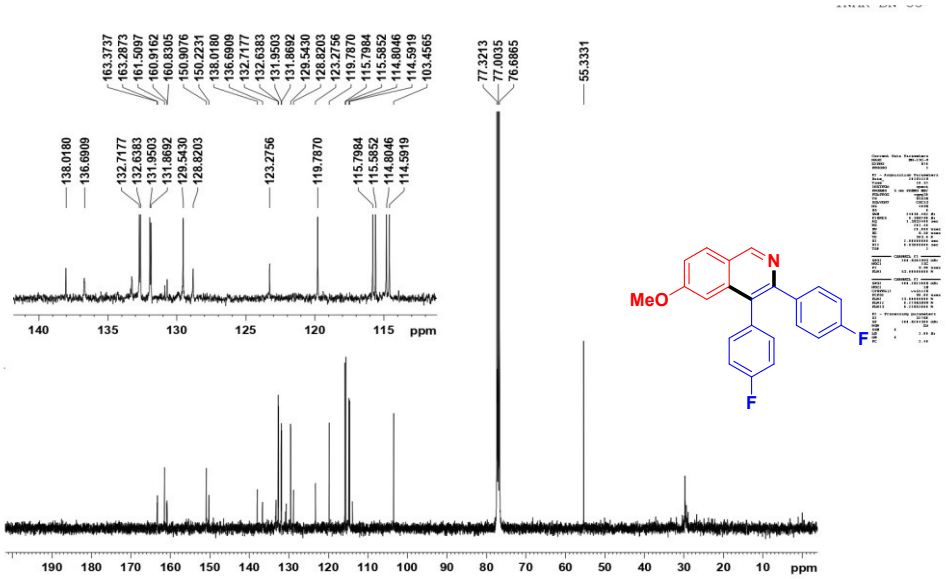
HRMS spectrum of compound- 3bd



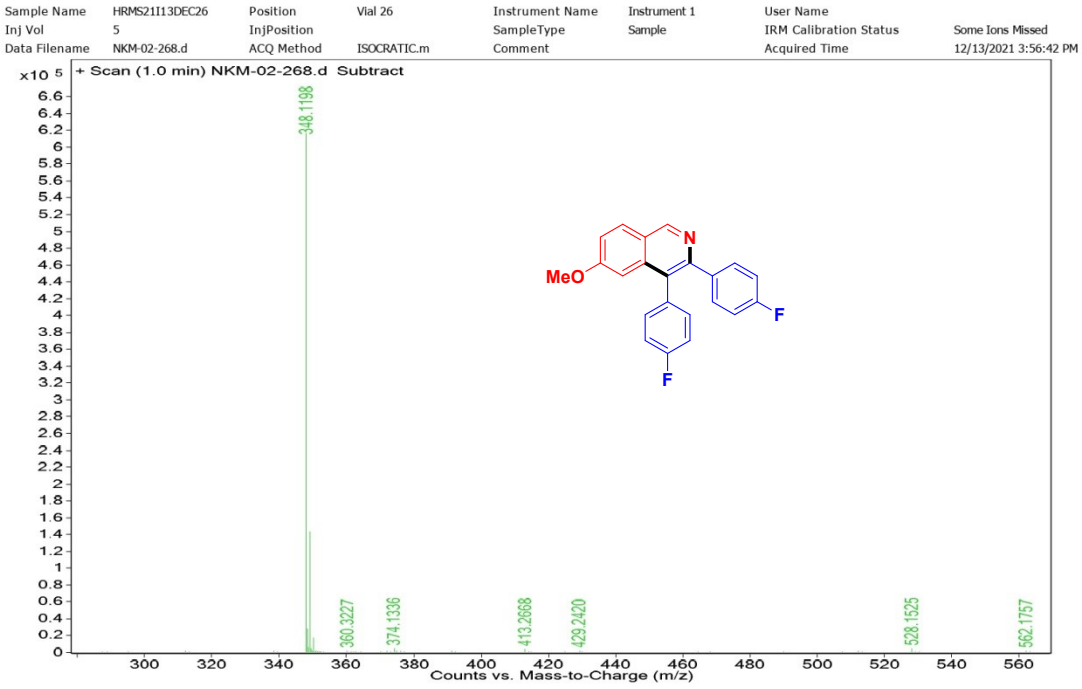
^{1}H NMR spectrum of compound- 3be (400 MHz, $CDCl_3$)



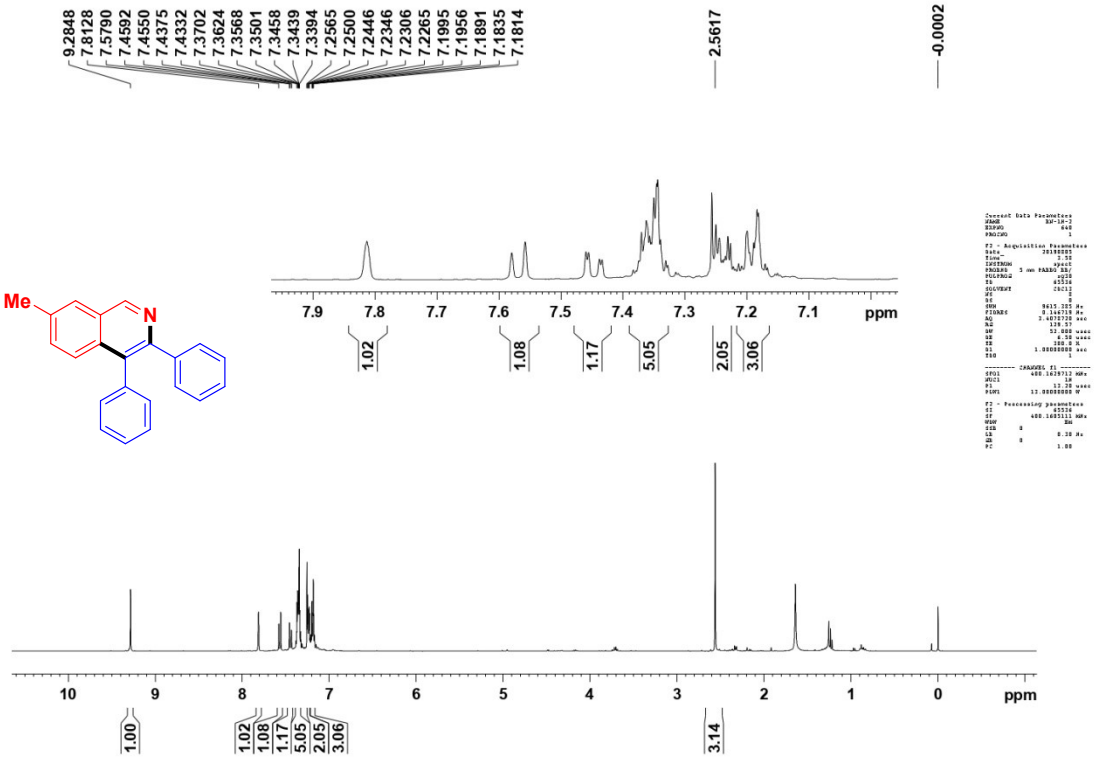
^{13}C NMR spectrum of compound- 3be (100 MHz, $CDCl_3$)



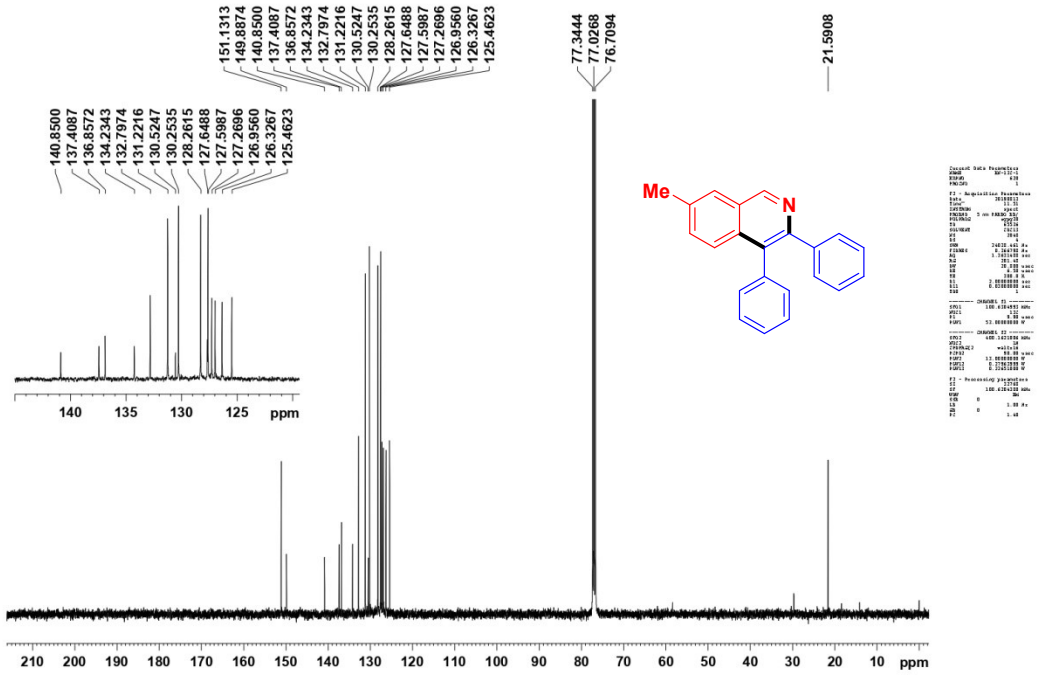
HRMS spectrum of compound- 3be



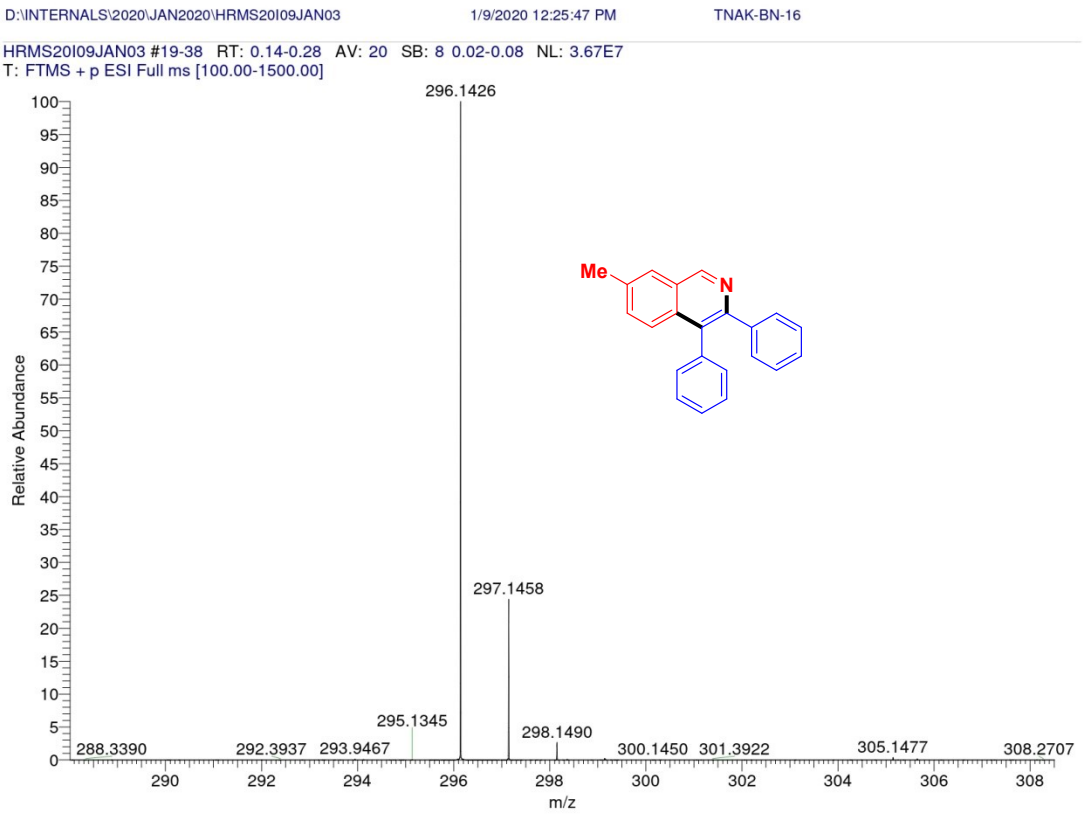
^{1}H NMR spectrum of compound- 3ca (400 MHz, $CDCl_3$)



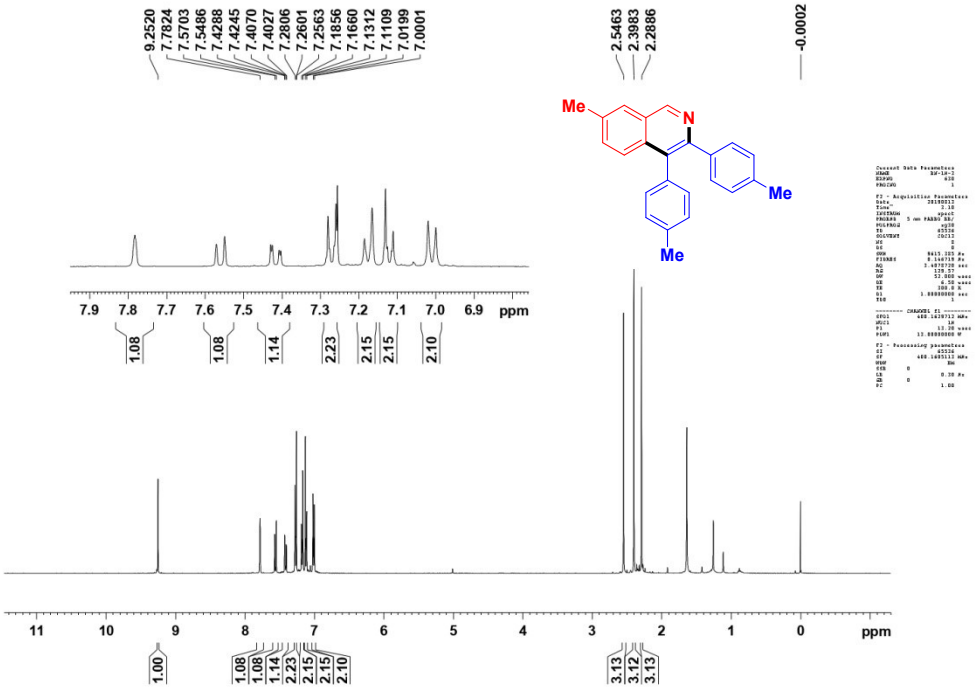
^{13}C NMR spectrum of compound- 3ca (100 MHz, $CDCl_3$)



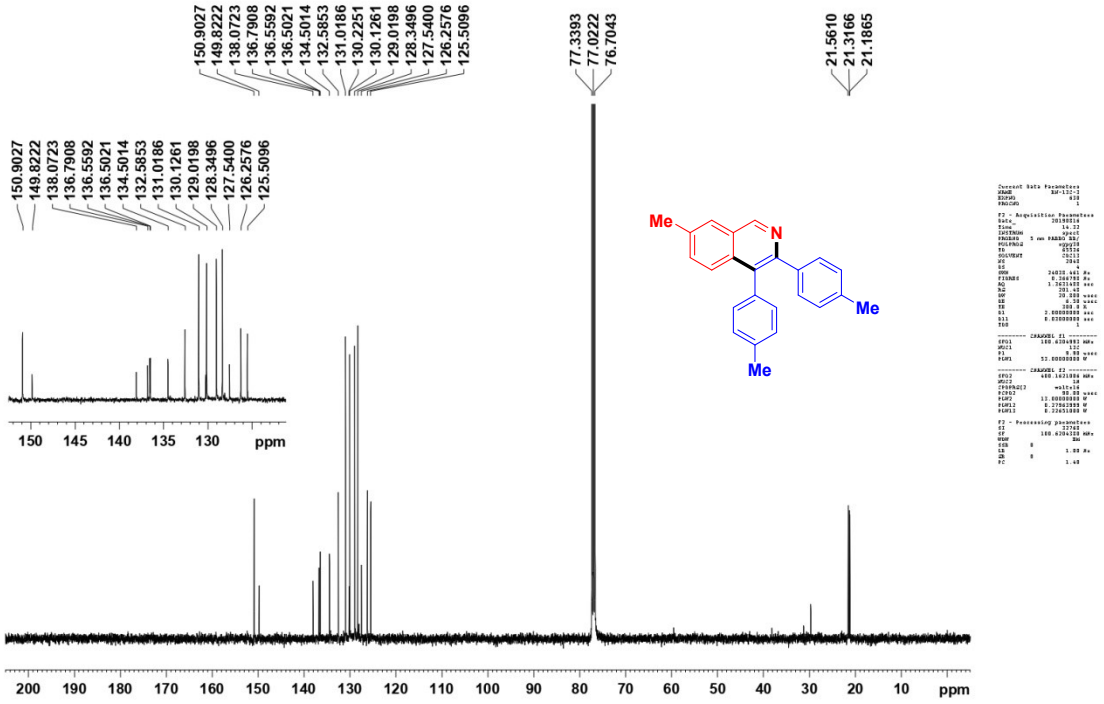
HRMS spectrum of compound- 3ca



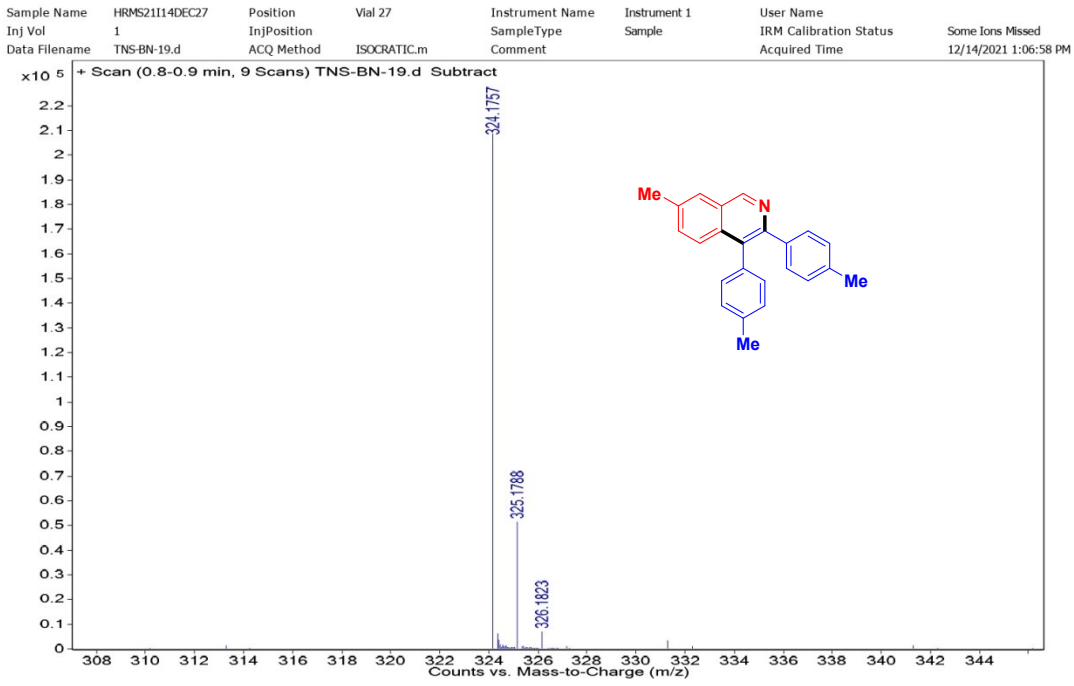
^{1}H NMR spectrum of compound- 3cc (400 MHz, $CDCl_3$)



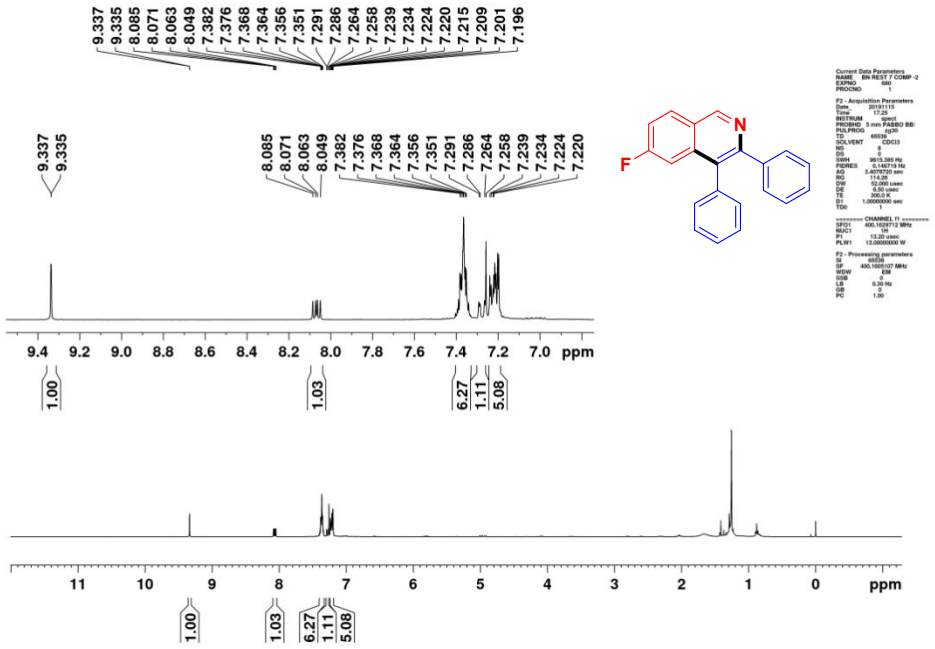
^{13}C NMR spectrum of compound- 3cc (100 MHz, $CDCl_3$)



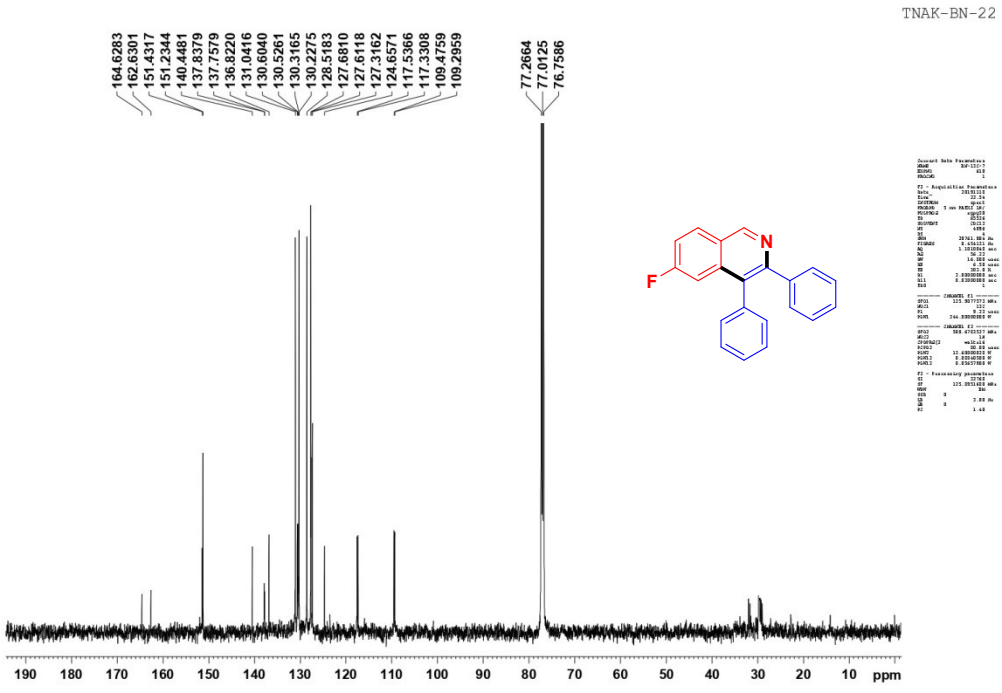
HRMS spectrum of compound- 3cc



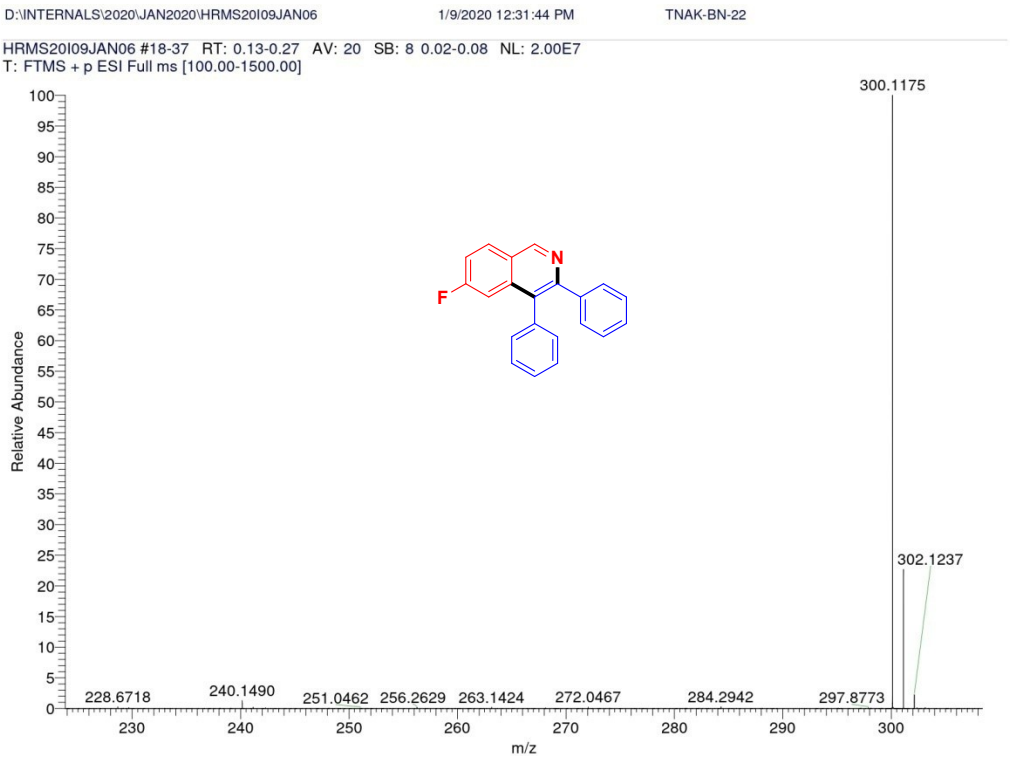
^{1}H NMR spectrum of compound- 3da (400 MHz, $CDCl_3$)



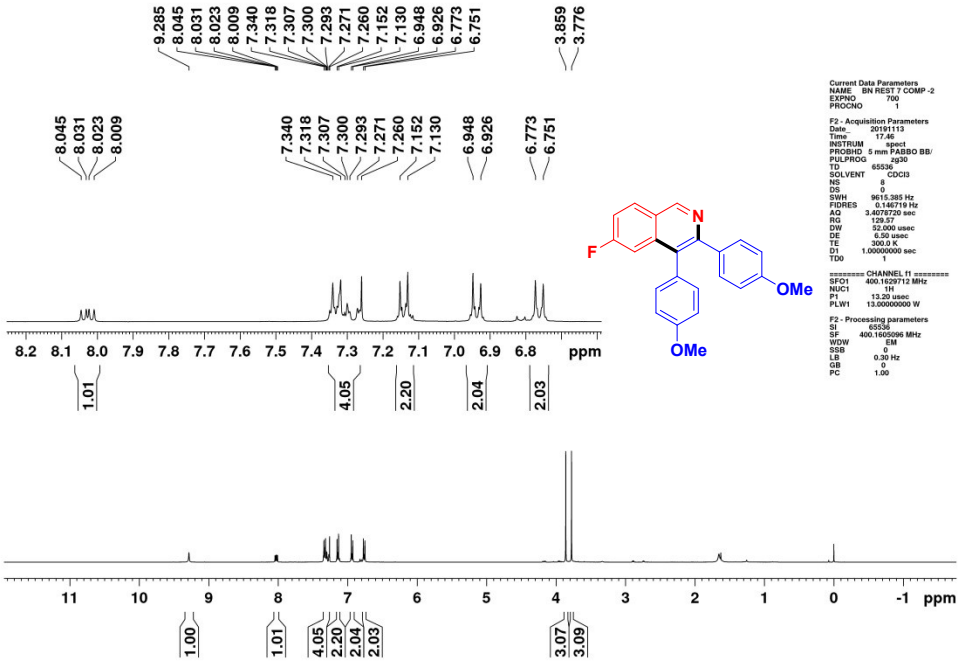
^{13}C NMR spectrum of compound- 3da (400 MHz, $CDCl_3$)



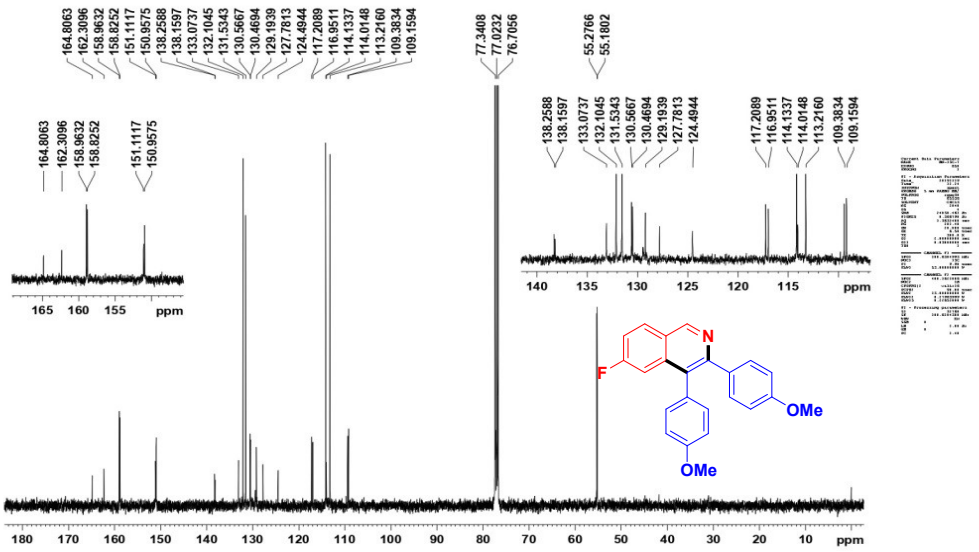
HRMS spectrum of compound- 3da



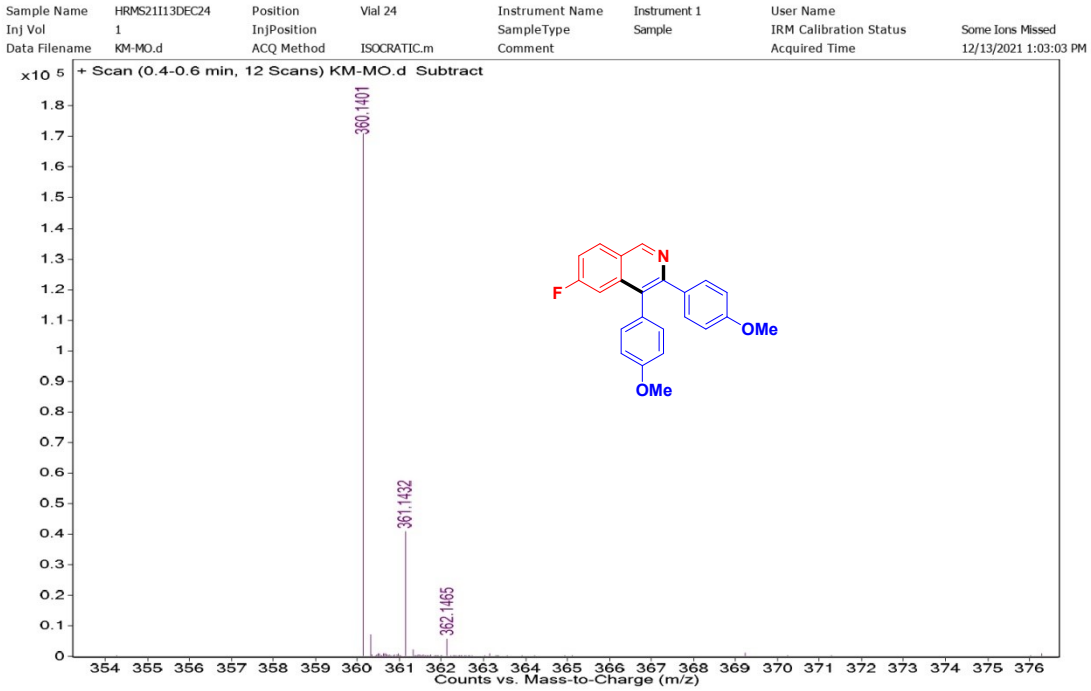
^{1}H NMR spectrum of compound- 3db (400 MHz, $CDCl_3$)



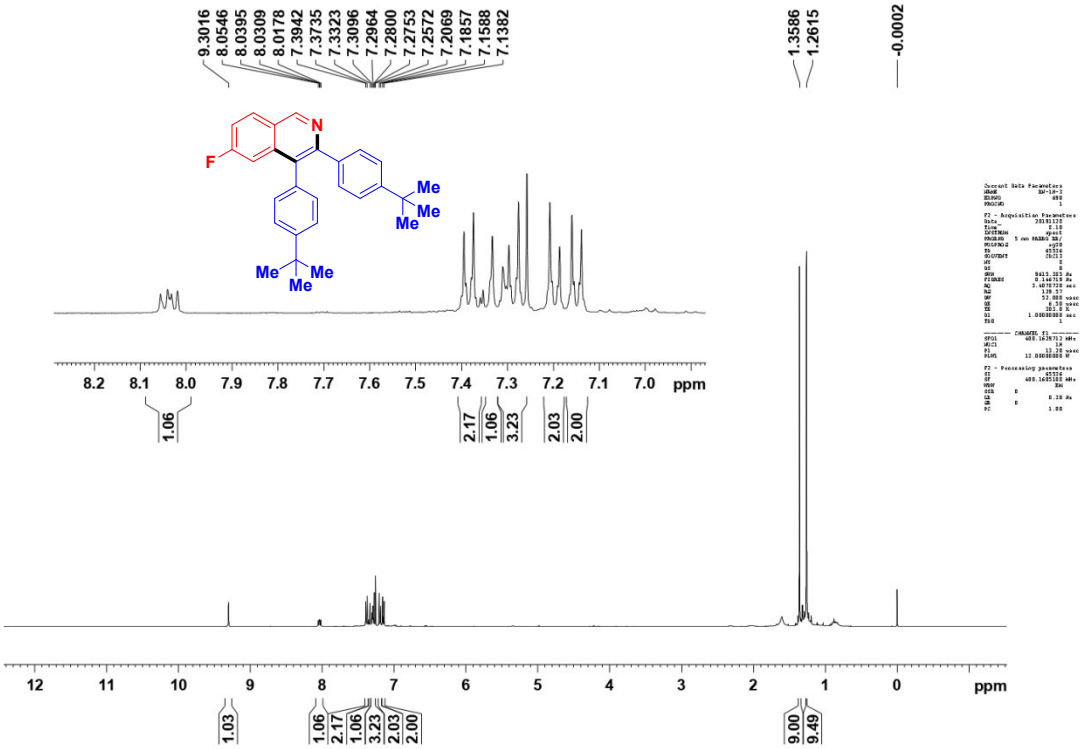
^{13}C NMR spectrum of compound- 3db (400 MHz, $CDCl_3$)



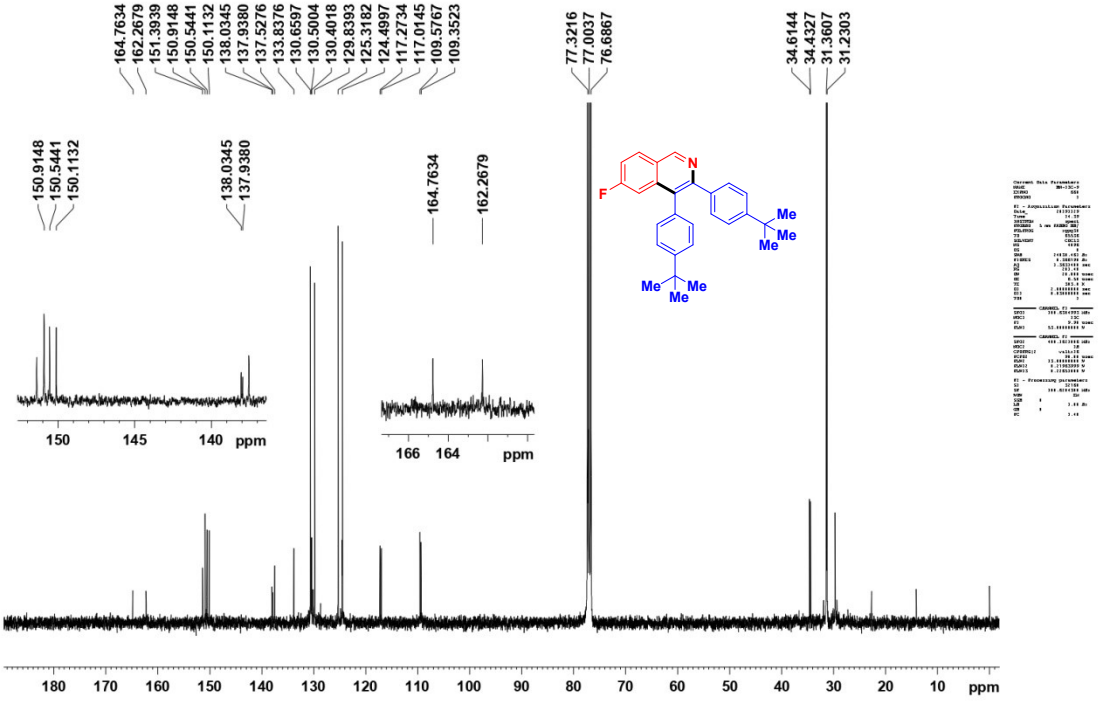
HRMS spectrum of compound- 3db



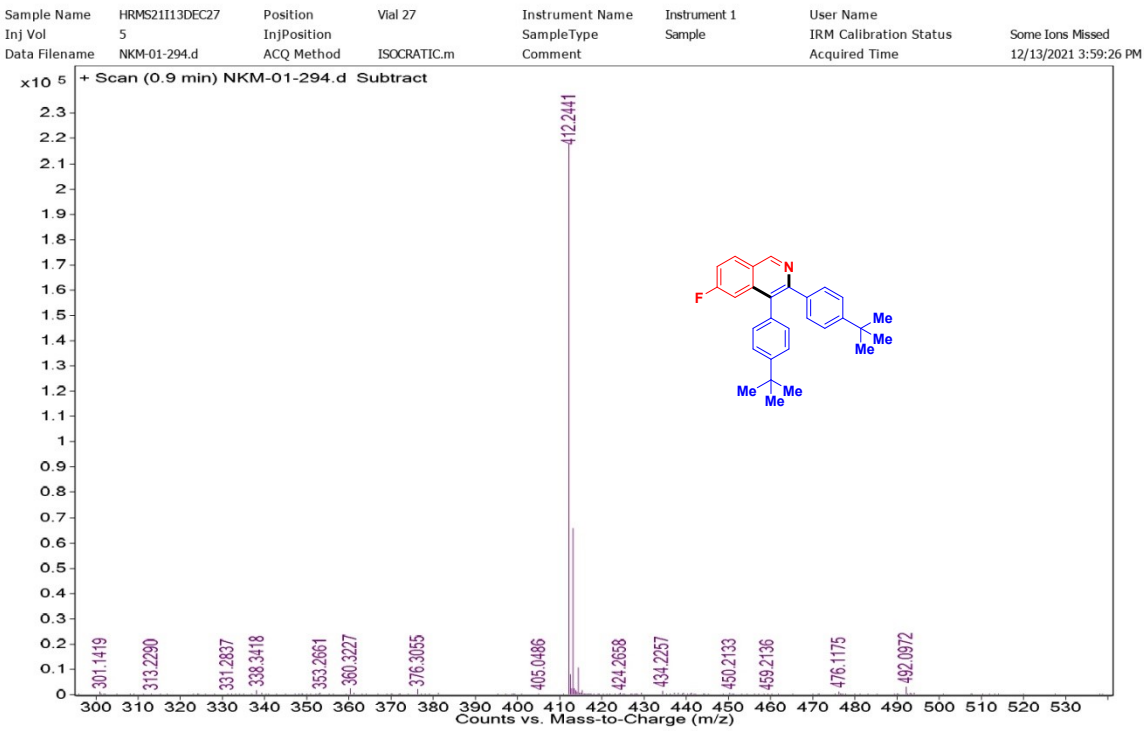
^{1}H NMR spectrum of compound- 3dd (400 MHz, $CDCl_3$)



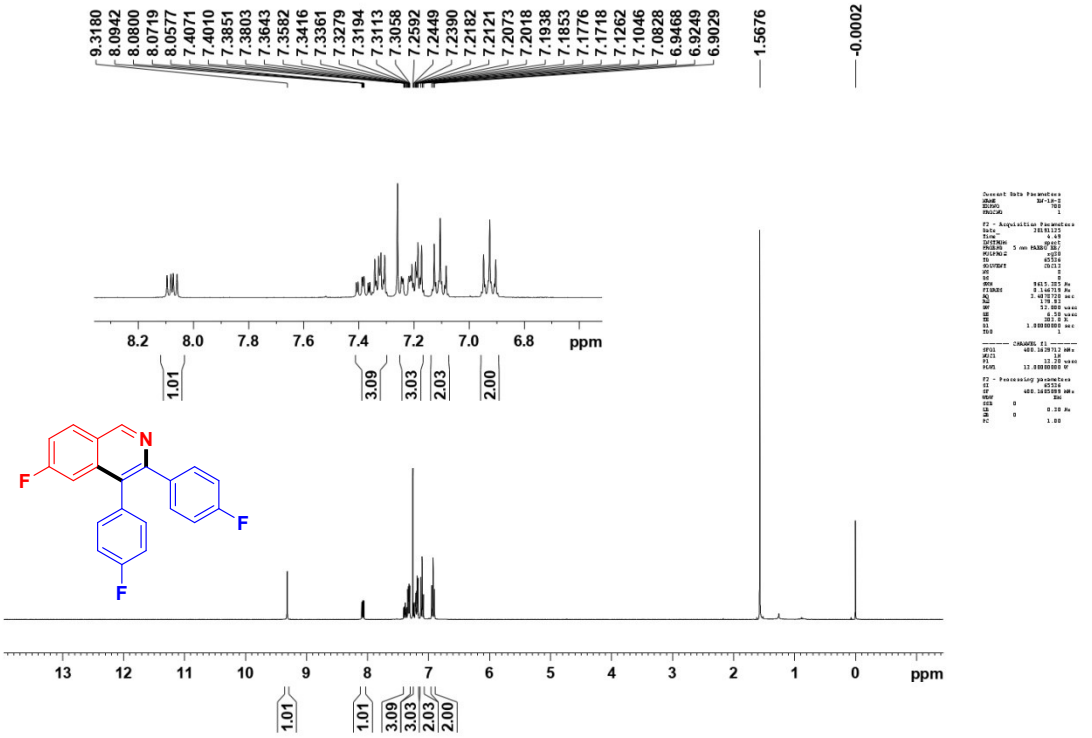
^{13}C NMR spectrum of compound- 3dd (400 MHz, $CDCl_3$)



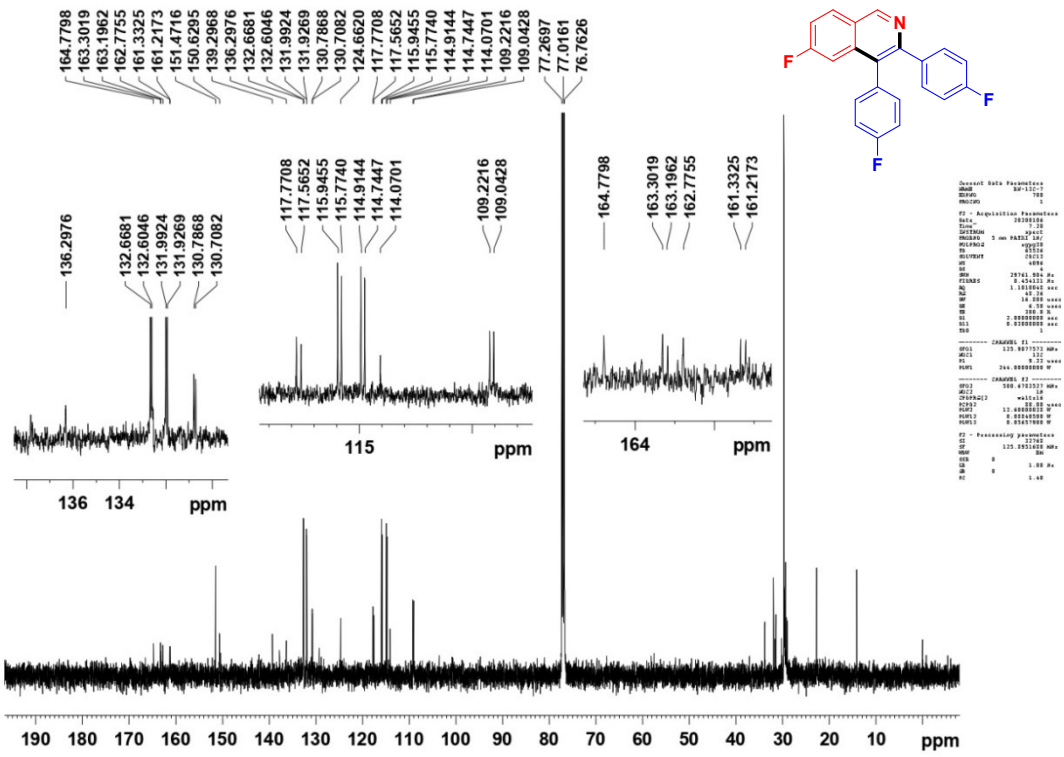
HRMS spectrum of compound- 3dd



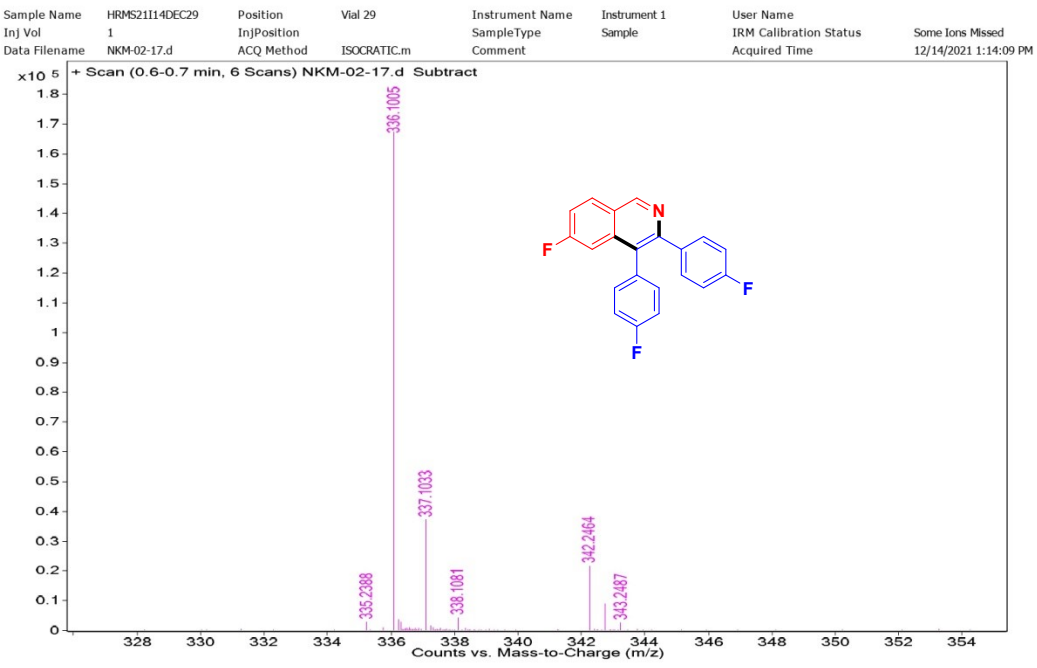
^{1}H NMR spectrum of compound- 3de (400 MHz, $CDCl_3$)



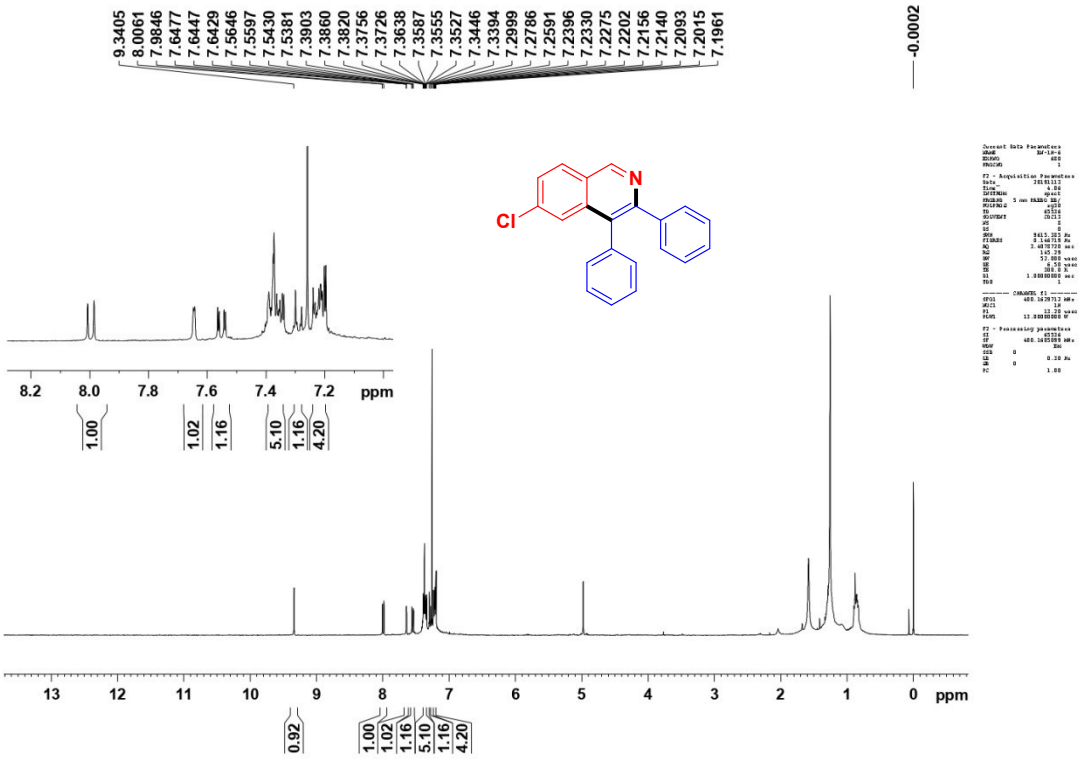
^{13}C NMR spectrum of compound- 3de (400 MHz, $CDCl_3$)



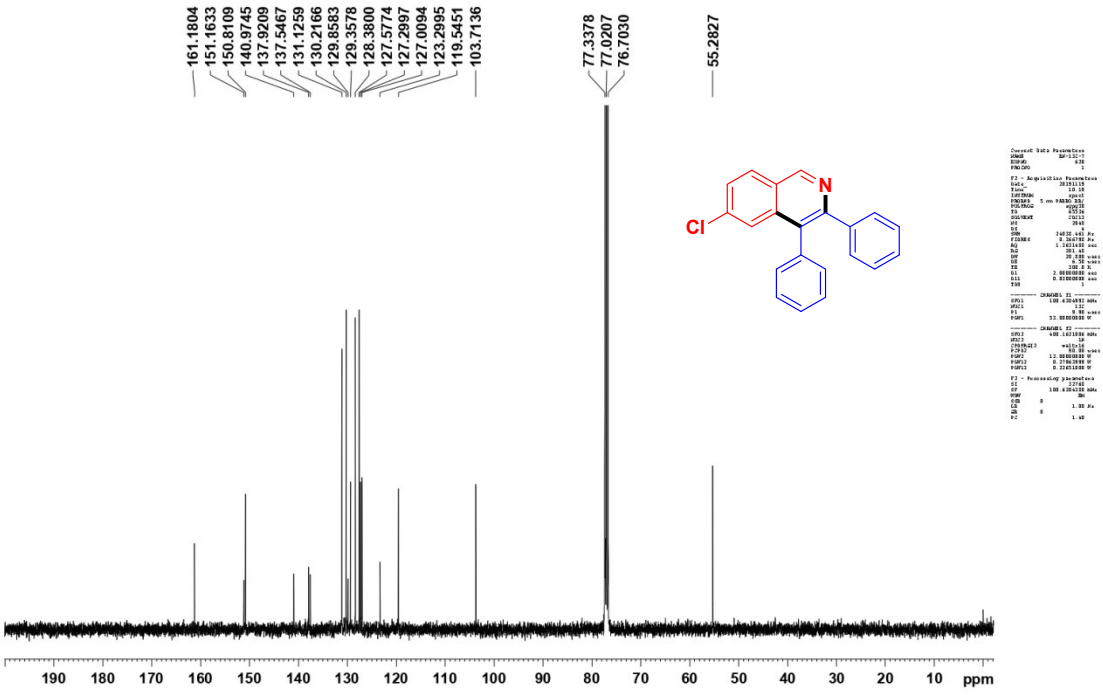
HRMS spectrum of compound- 3de



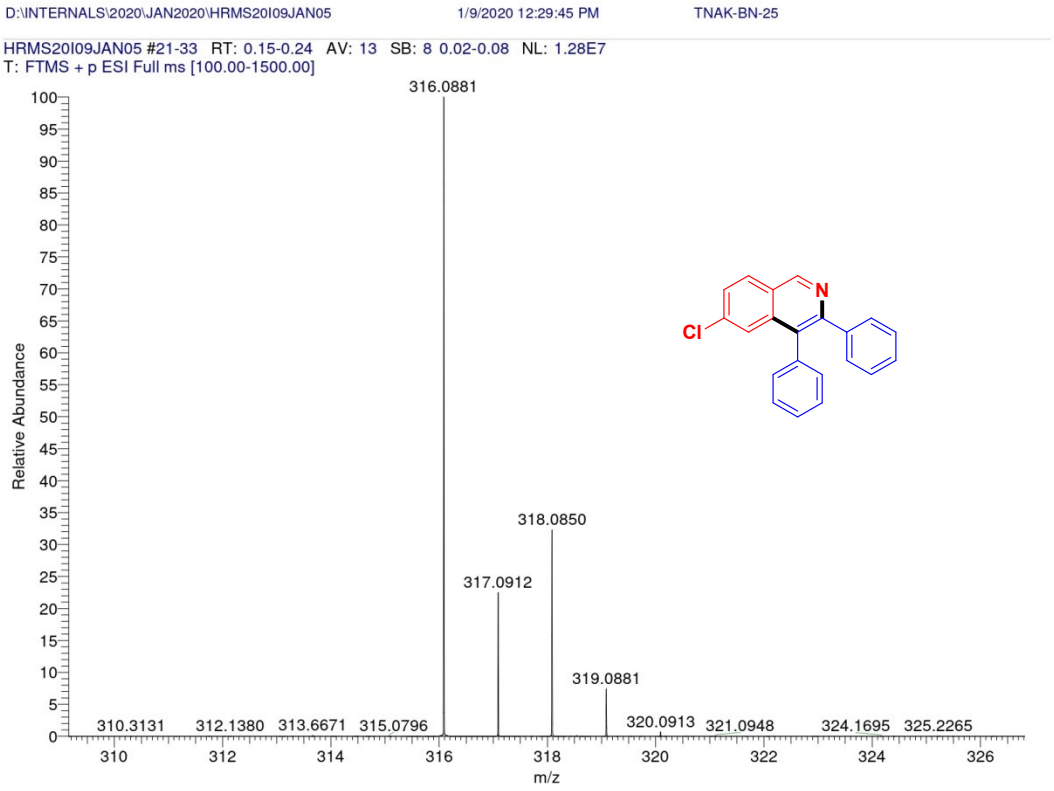
^{1}H NMR spectrum of compound- 3ea (400 MHz, $CDCl_3$)



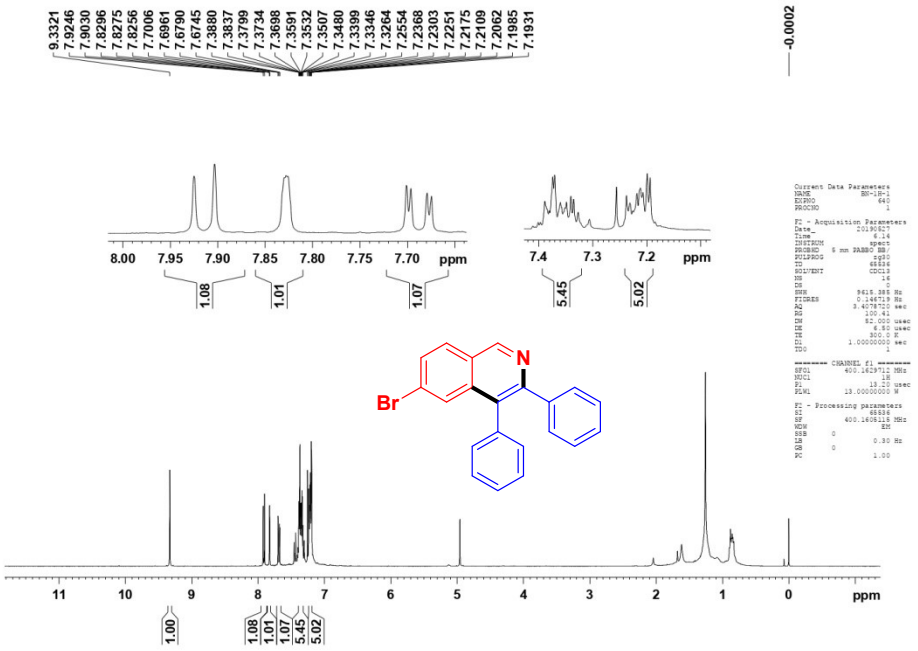
^{13}C NMR spectrum of compound- 3ea (400 MHz, $CDCl_3$)



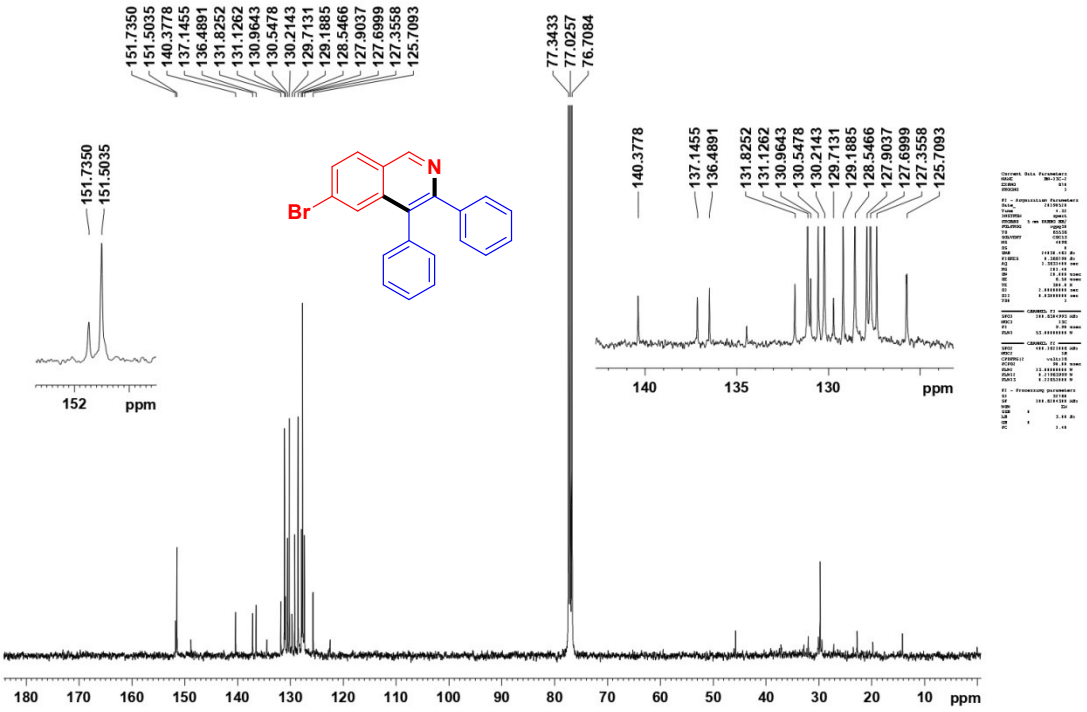
HRMS spectrum of compound- 3ea



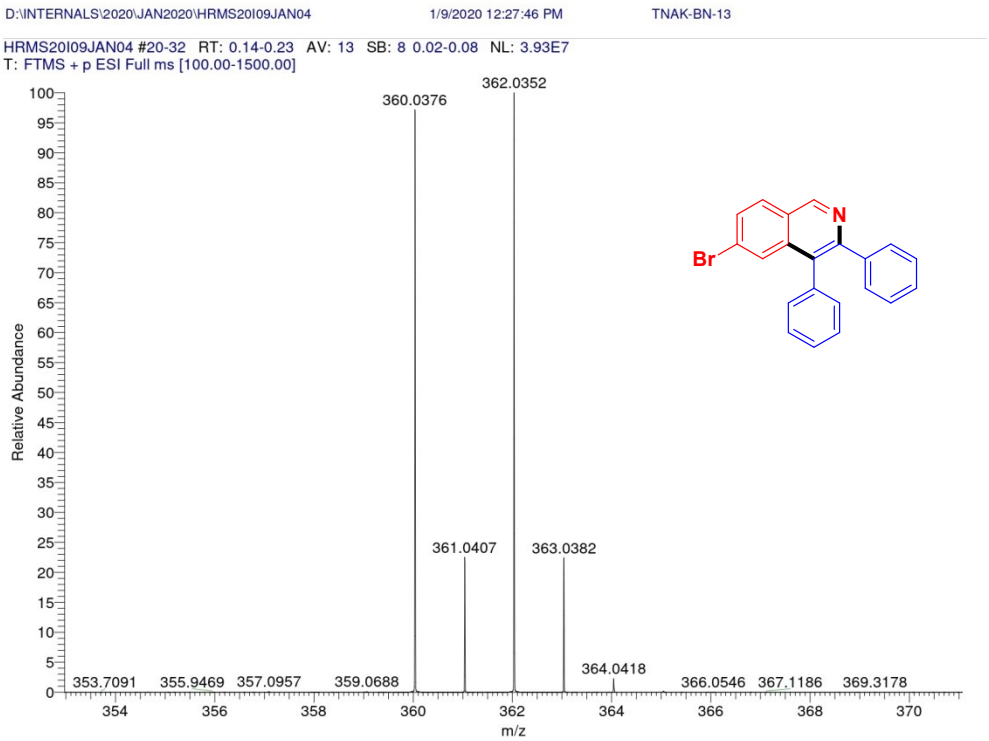
^{1}H NMR spectrum of compound- 3fa (400 MHz, $CDCl_3$)



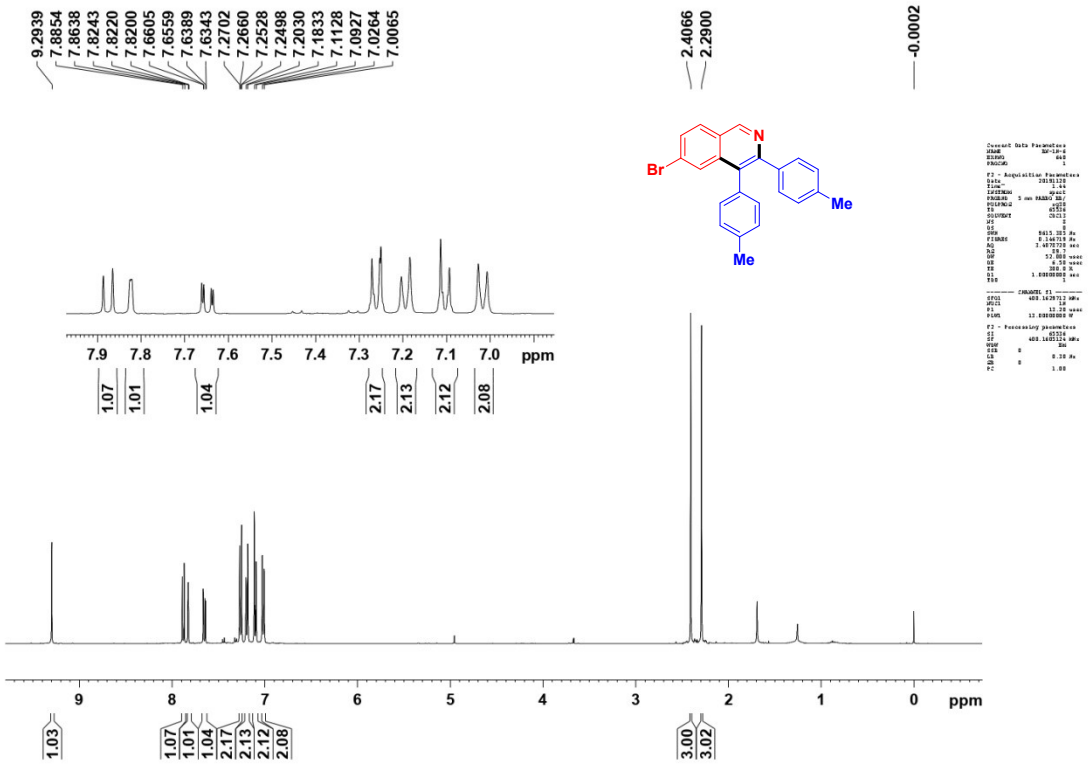
^{13}C NMR spectrum of compound- 3fa (400 MHz, $CDCl_3$)



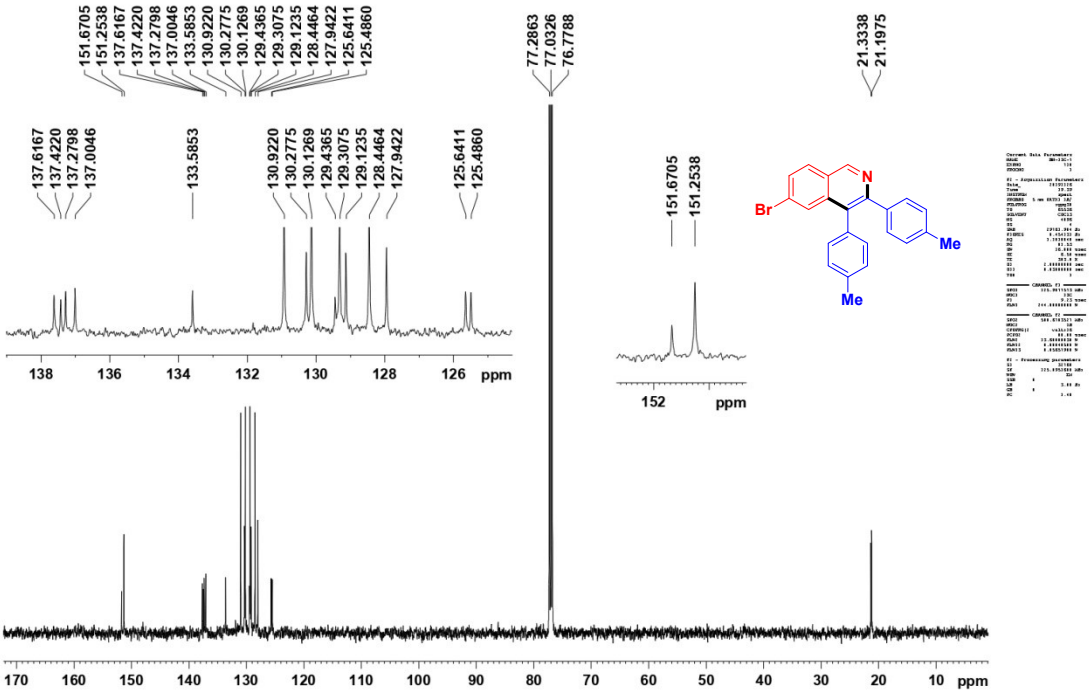
HRMS spectrum of compound- 3fa



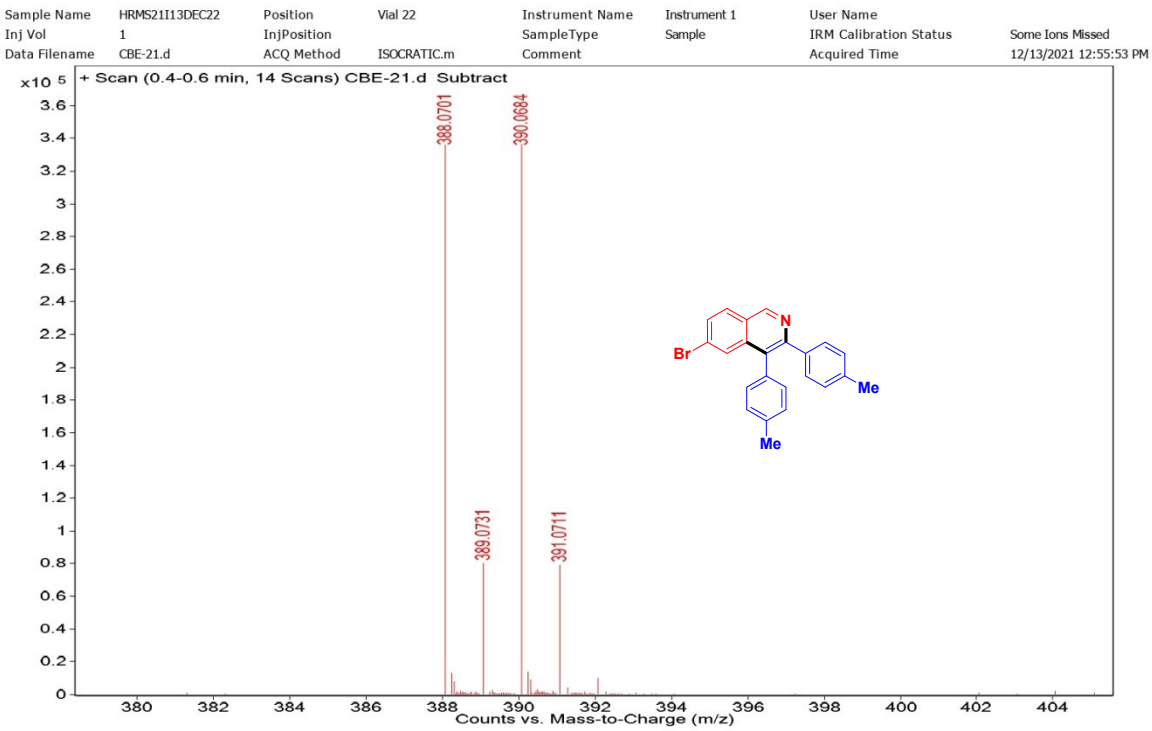
^{1}H NMR spectrum of compound- 3fc (400 MHz, $CDCl_3$)



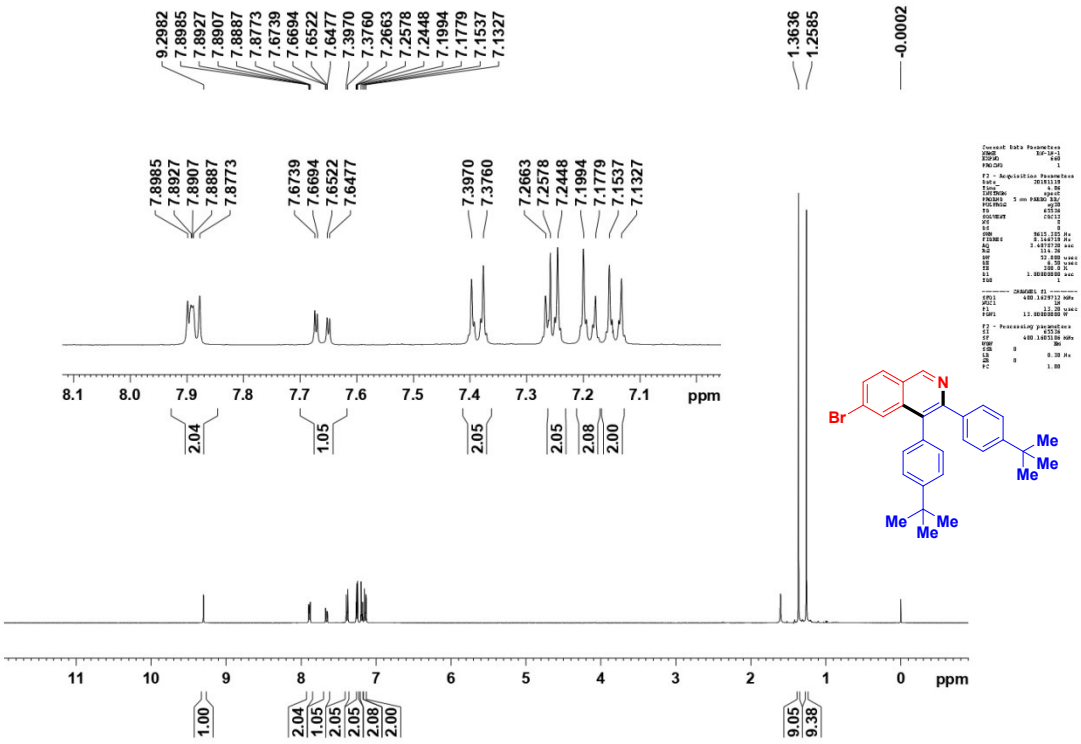
^{13}C NMR spectrum of compound- 3fc (400 MHz, $CDCl_3$)



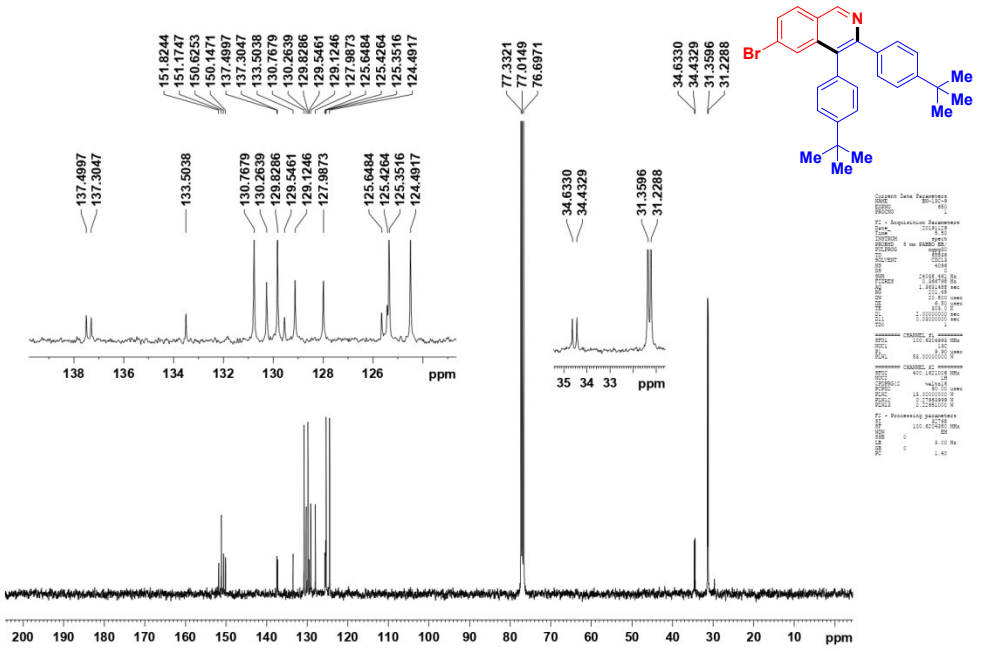
HRMS spectrum of compound- 3fc



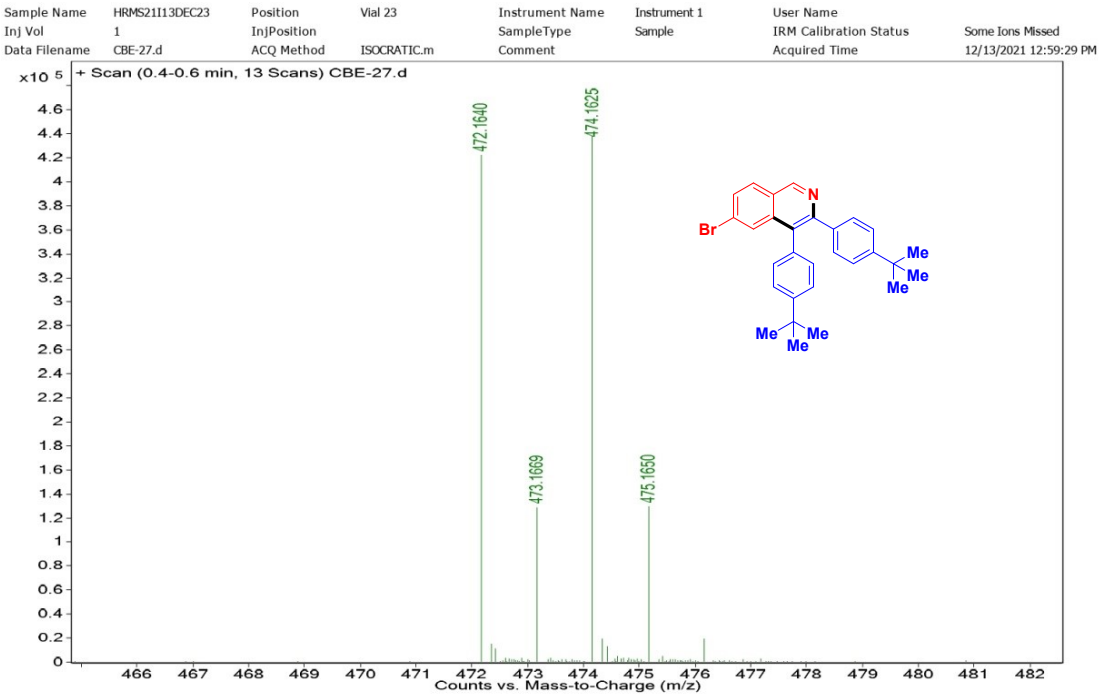
^{1}H NMR spectrum of compound- 3fd (400 MHz, $CDCl_3$)



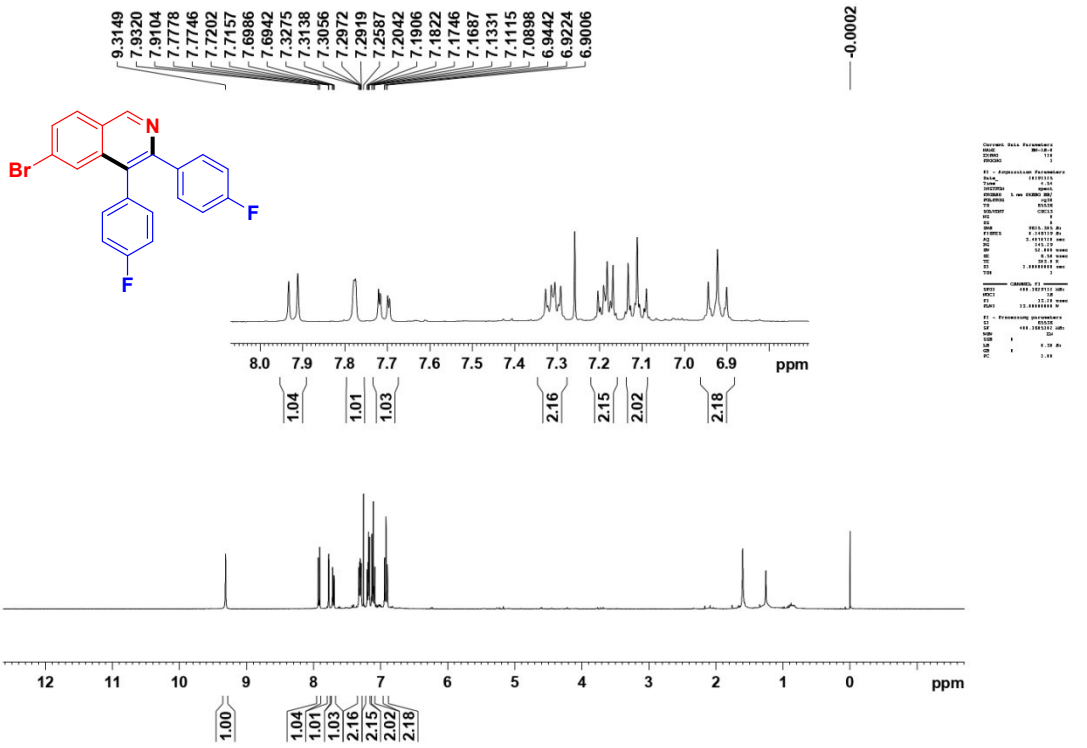
^{13}C NMR spectrum of compound- 3fd (400 MHz, $CDCl_3$)



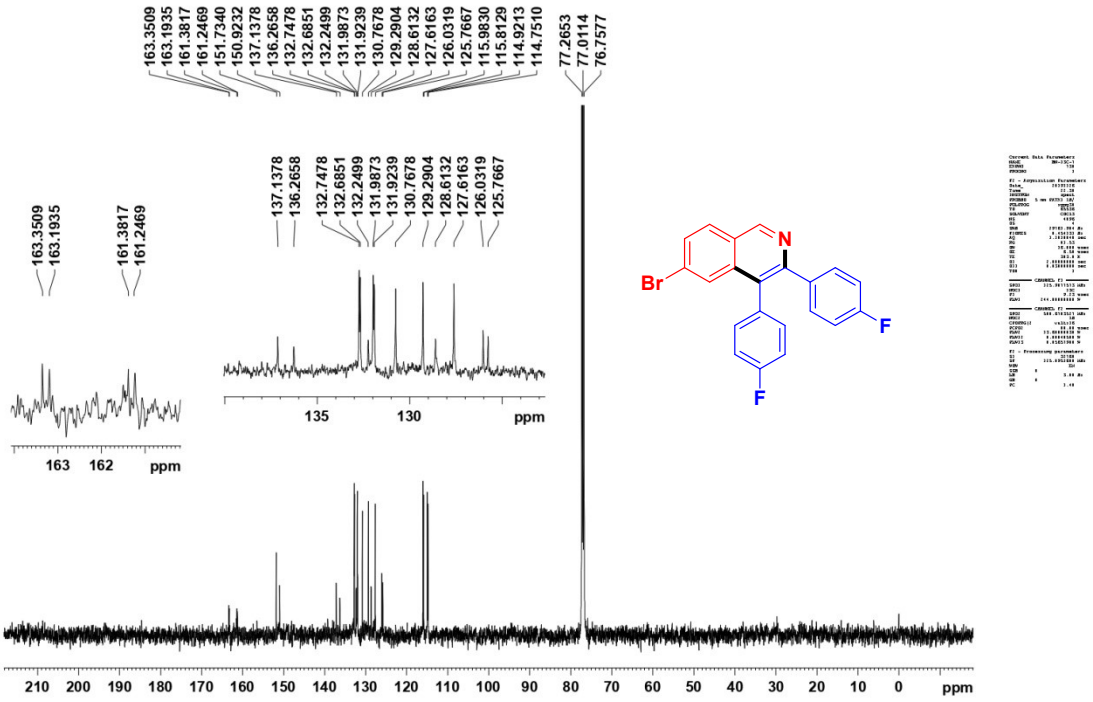
HRMS spectrum of compound- 3fd



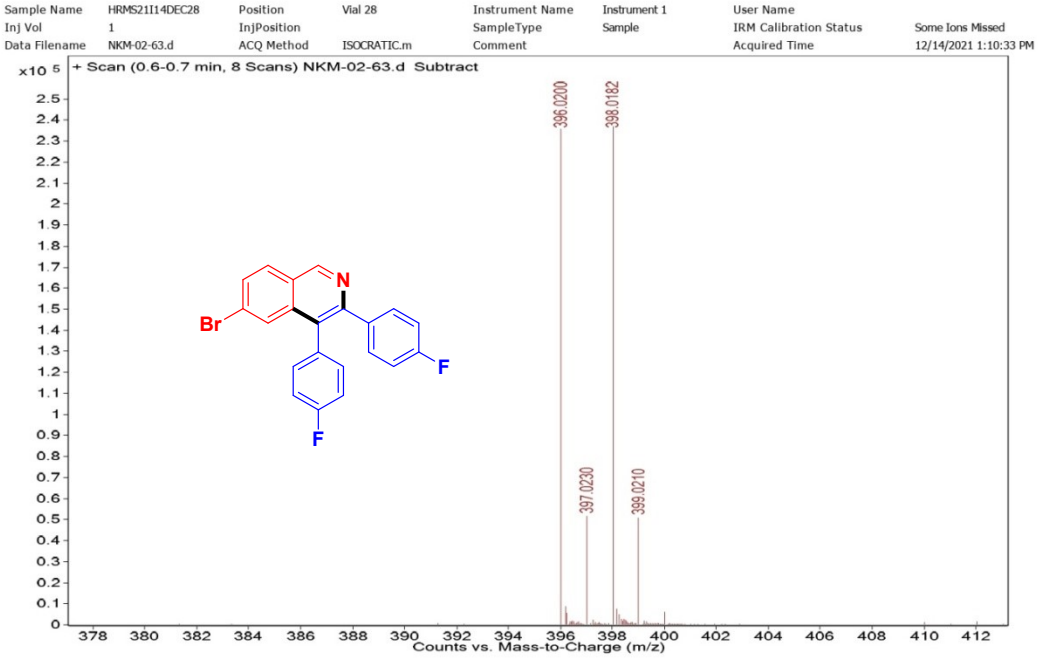
^{1}H NMR spectrum of compound- 3fe (400 MHz, $CDCl_3$)



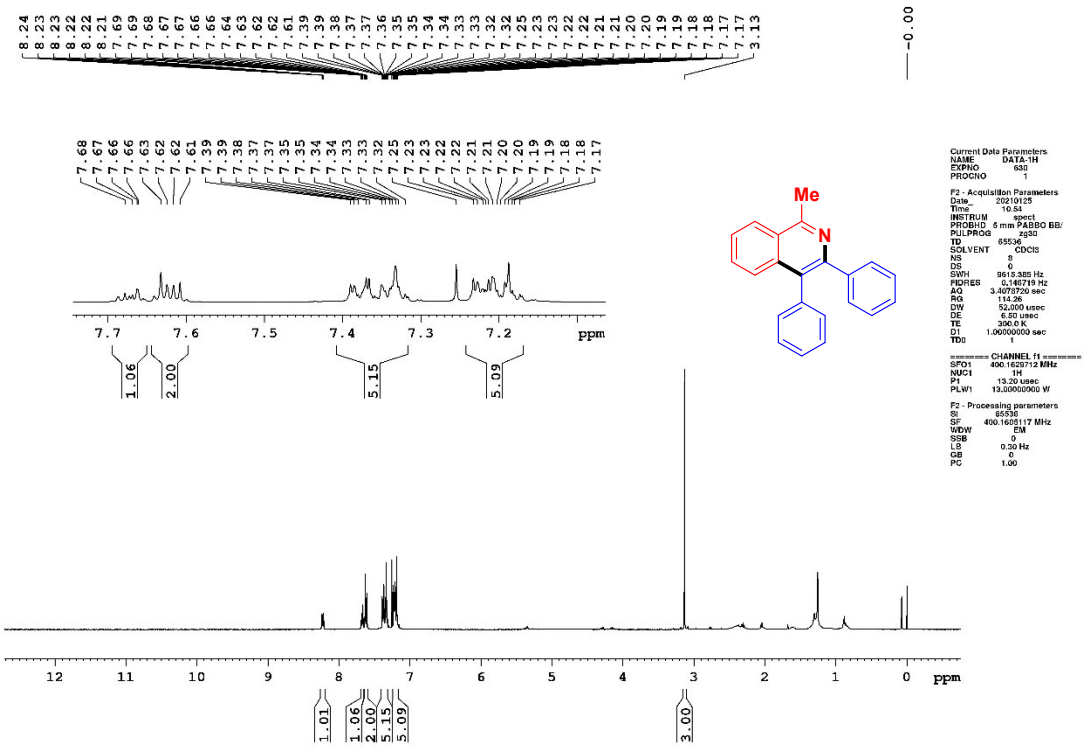
^{13}C NMR spectrum of compound- 3fe (400 MHz, $CDCl_3$)



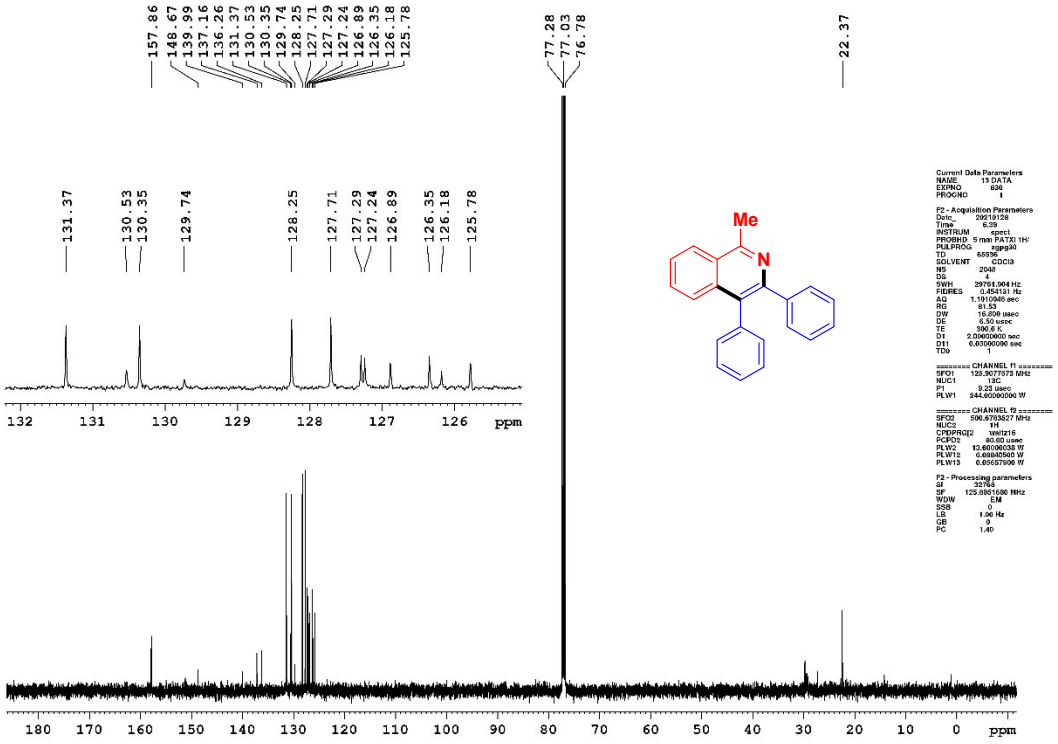
HRMS spectrum of compound- 3fe



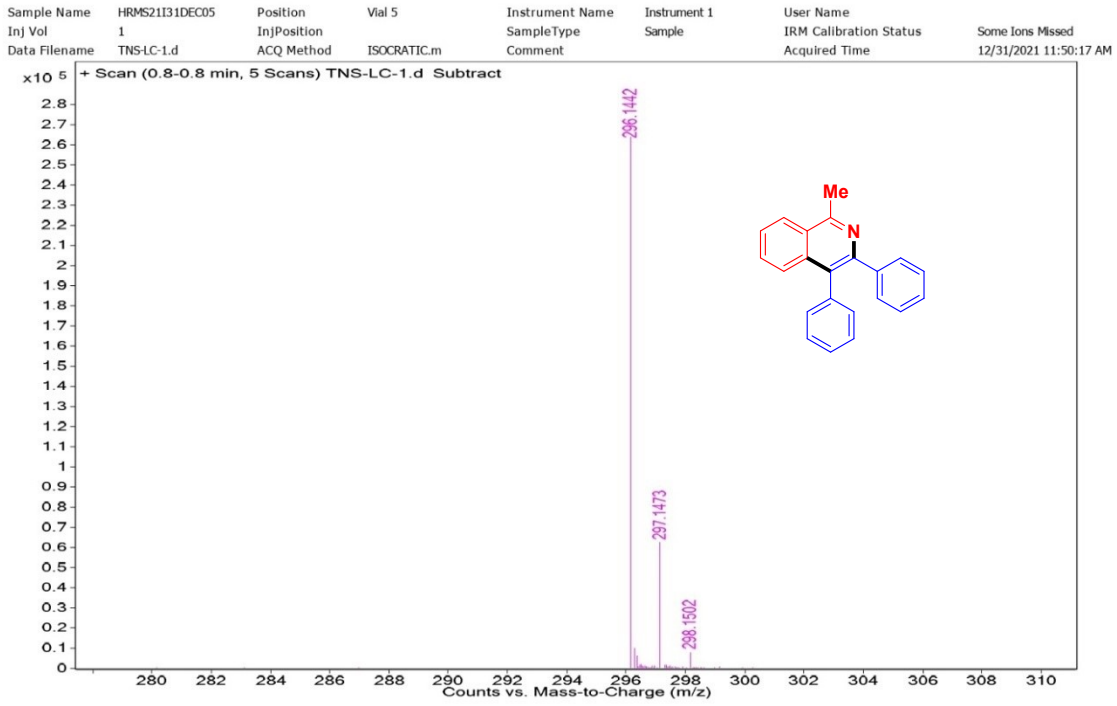
^{1}H NMR spectrum of compound- 3ga (400 MHz, $CDCl_3$)



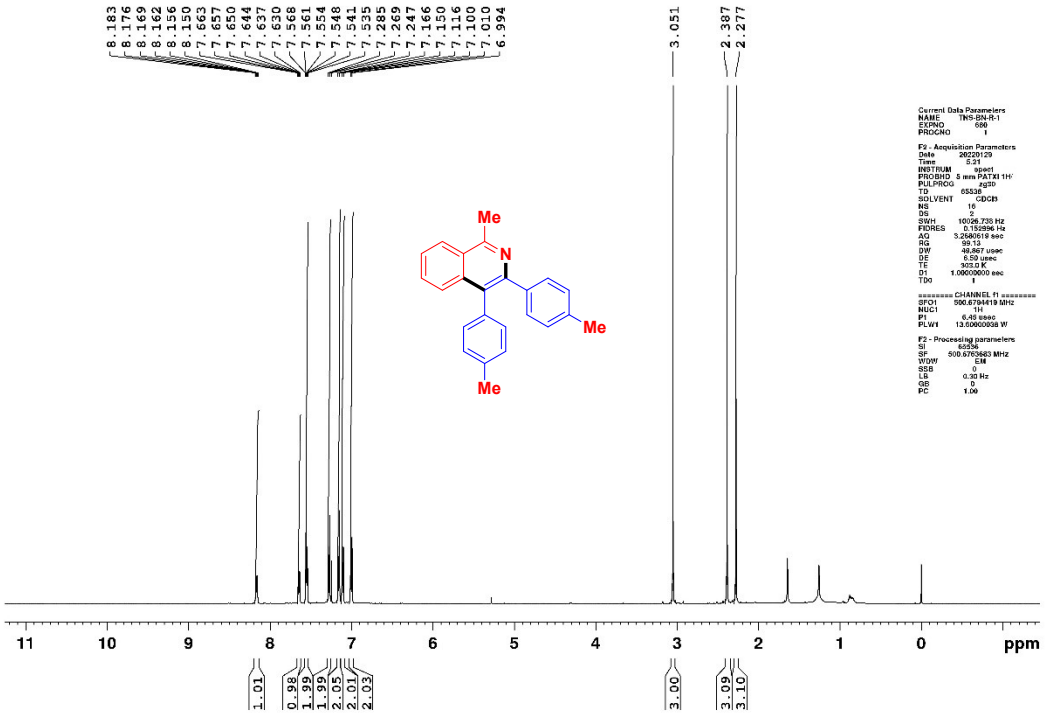
^{13}C NMR spectrum of compound- 3ga (400 MHz, $CDCl_3$)



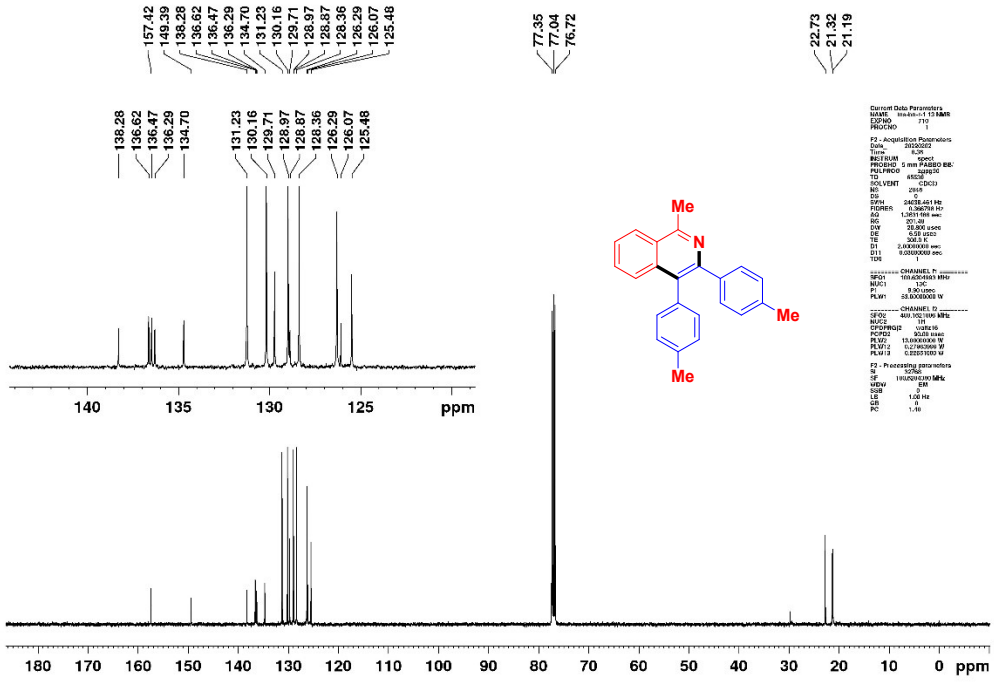
HRMS spectrum of compound- 3ga



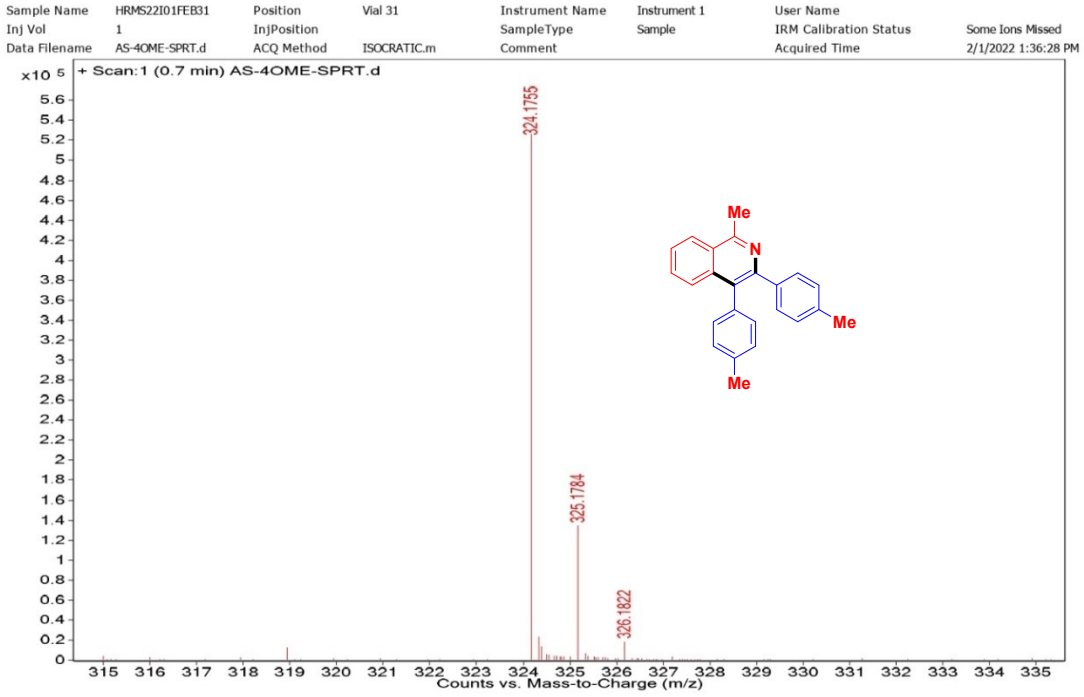
^{1}H NMR spectrum of compound- 3gc (400 MHz, $CDCl_3$)



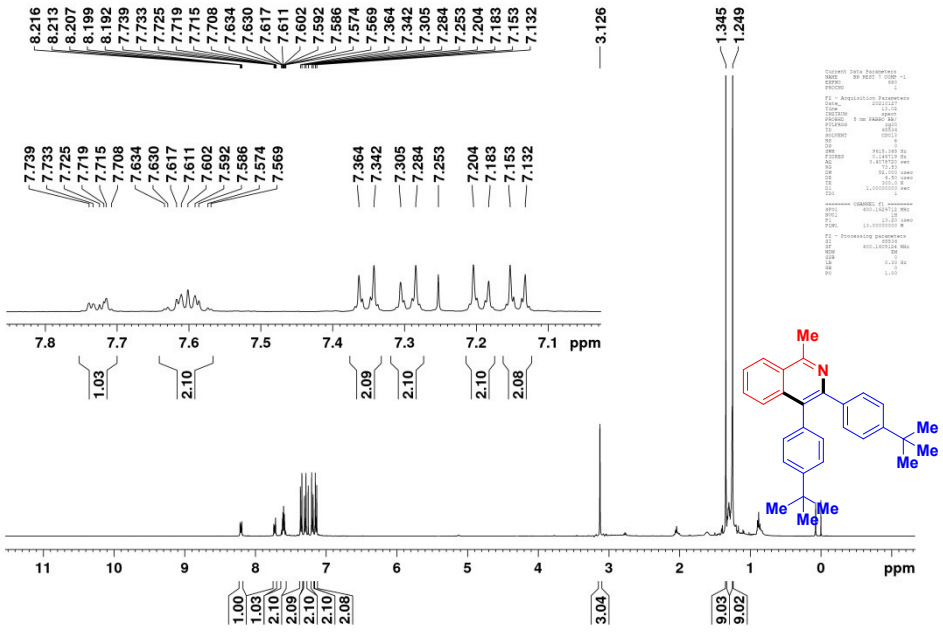
^{13}C NMR spectrum of compound- 3gc (400 MHz, $CDCl_3$)



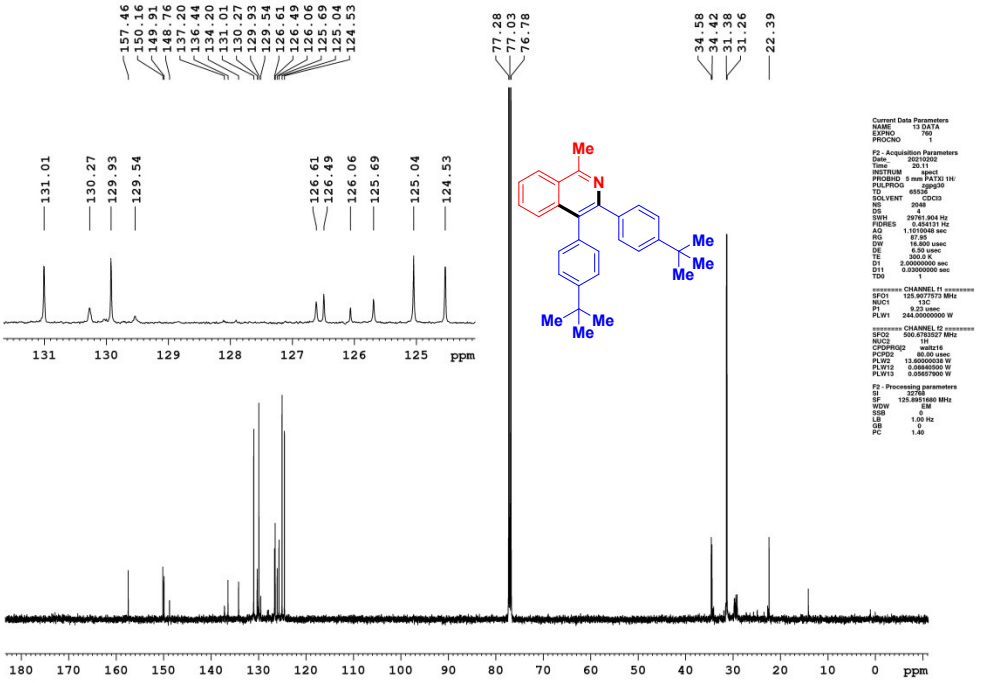
HRMS spectrum of compound- 3gc



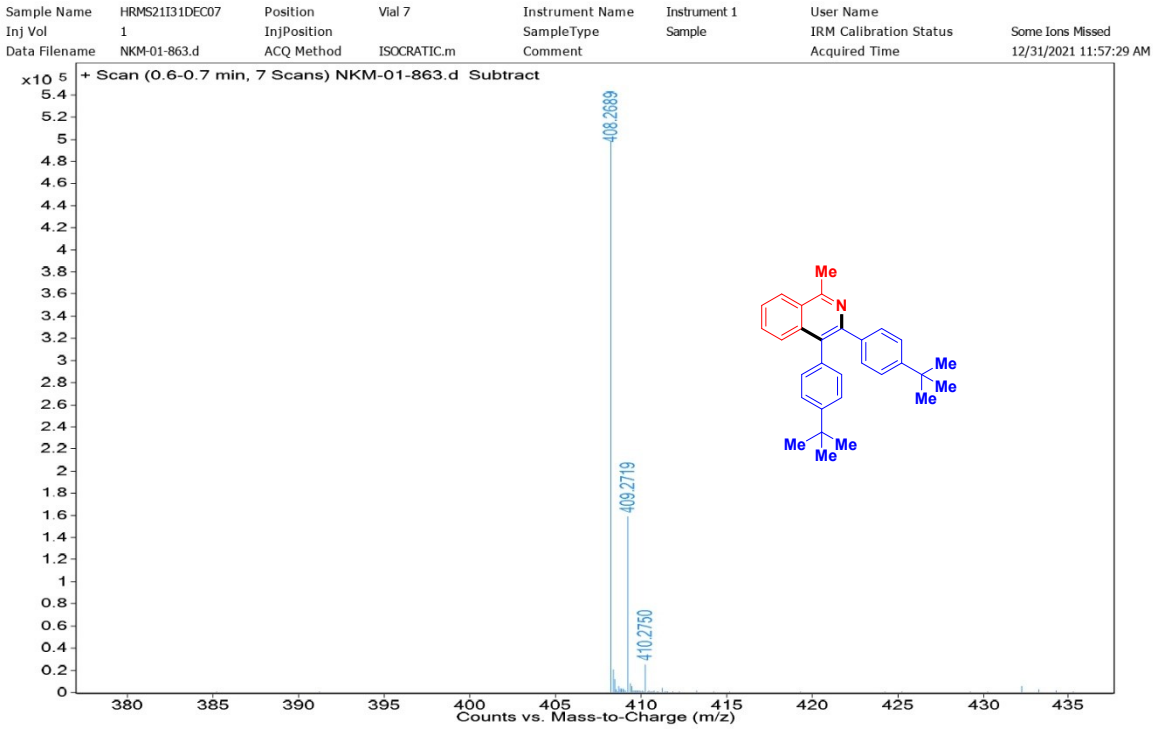
^{1}H NMR spectrum of compound- 3gd (400 MHz, $CDCl_3$)



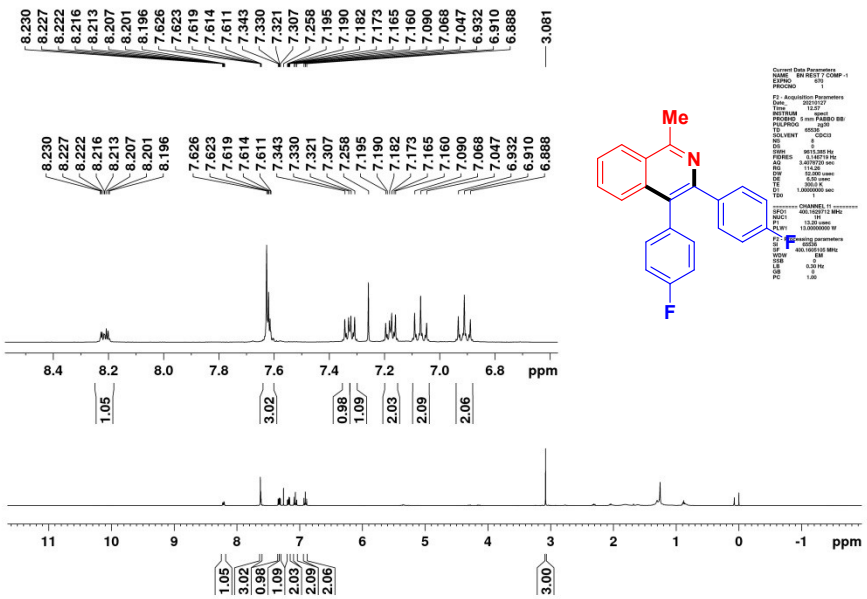
^{13}C NMR spectrum of compound- 3gd (400 MHz, $CDCl_3$)



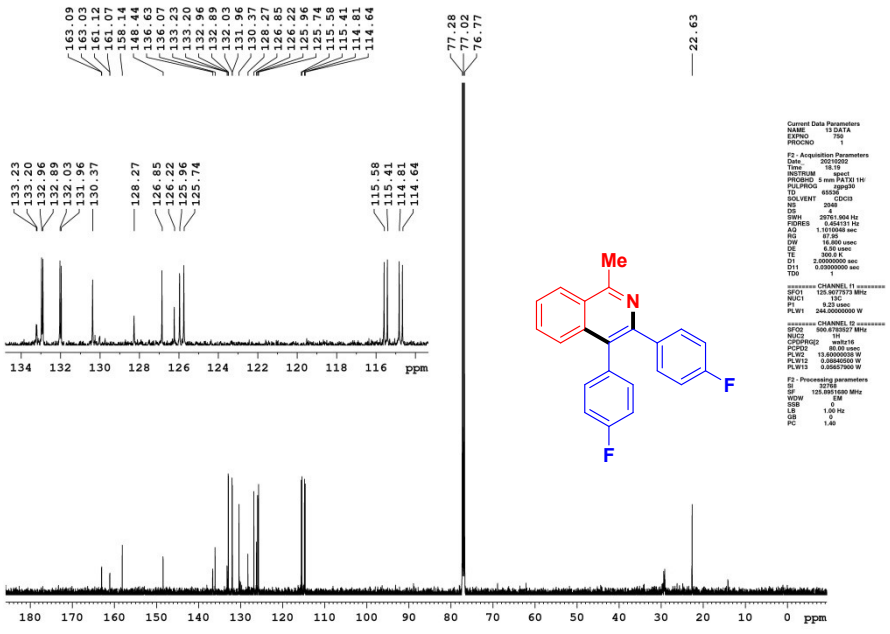
HRMS spectrum of compound- 3gd



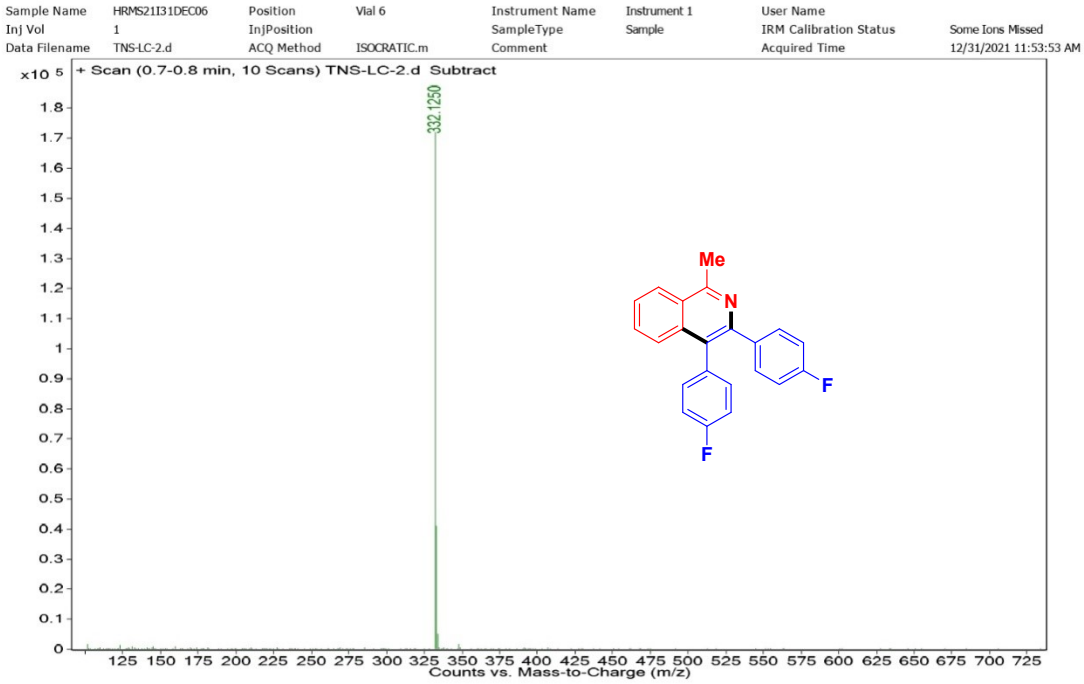
^{1}H NMR spectrum of compound- 3ge (400 MHz, $CDCl_3$)



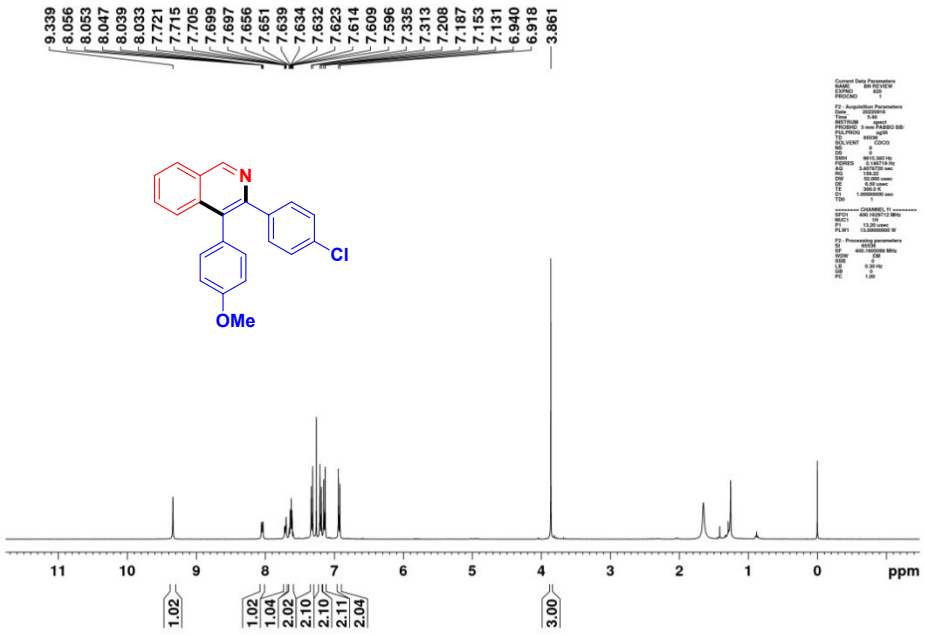
^{13}C NMR spectrum of compound- 3ge (400 MHz, $CDCl_3$)



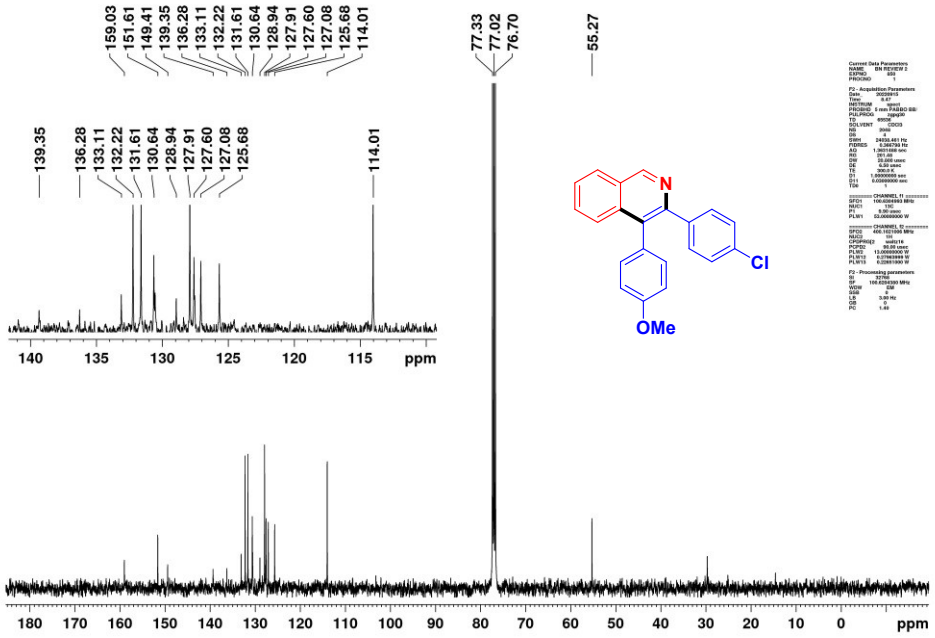
HRMS spectrum of compound- 3ge



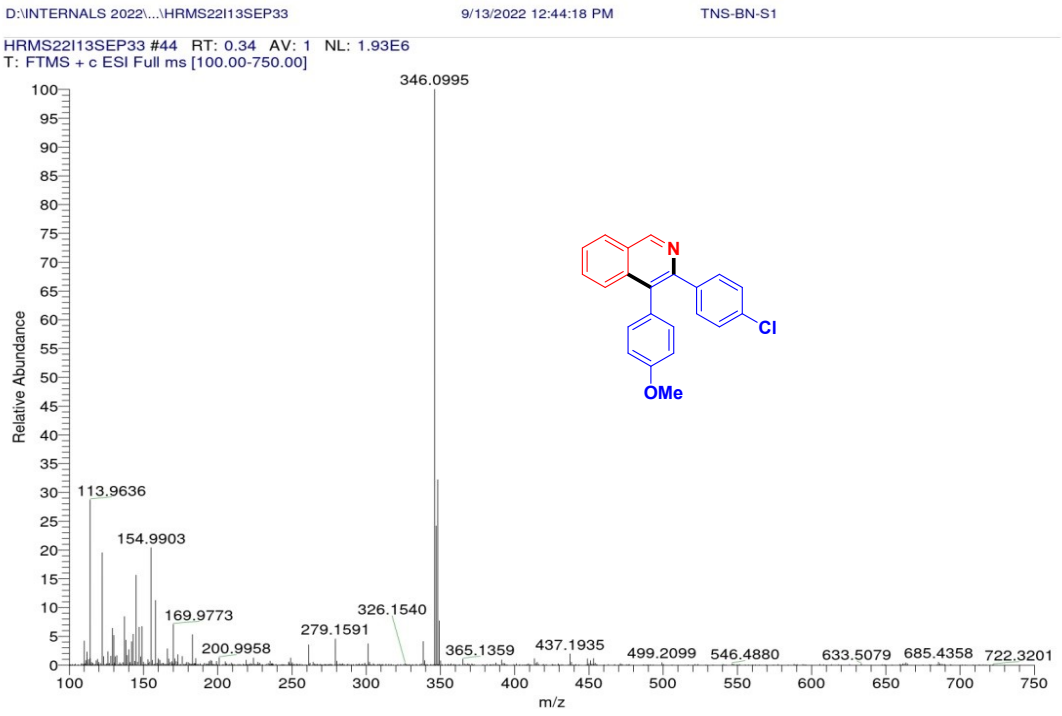
^{1}H NMR spectrum of compound –3af (400 MHz, $CDCl_3$)



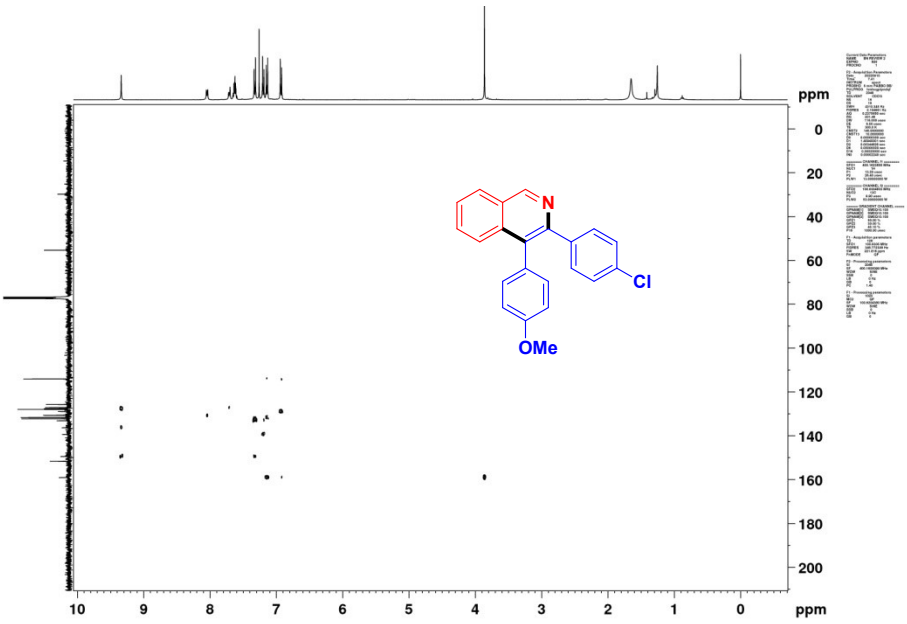
^{13}C NMR spectrum of compound- 3af (100 MHz, $CDCl_3$)



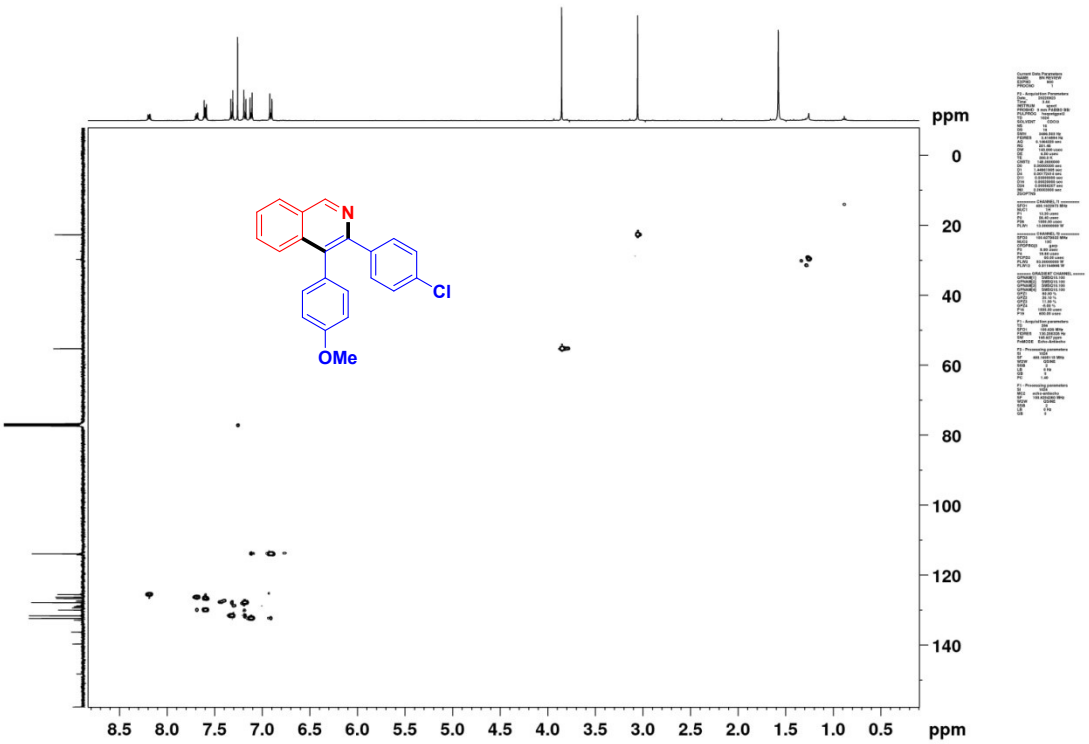
HRMS spectrum of compound- 3af



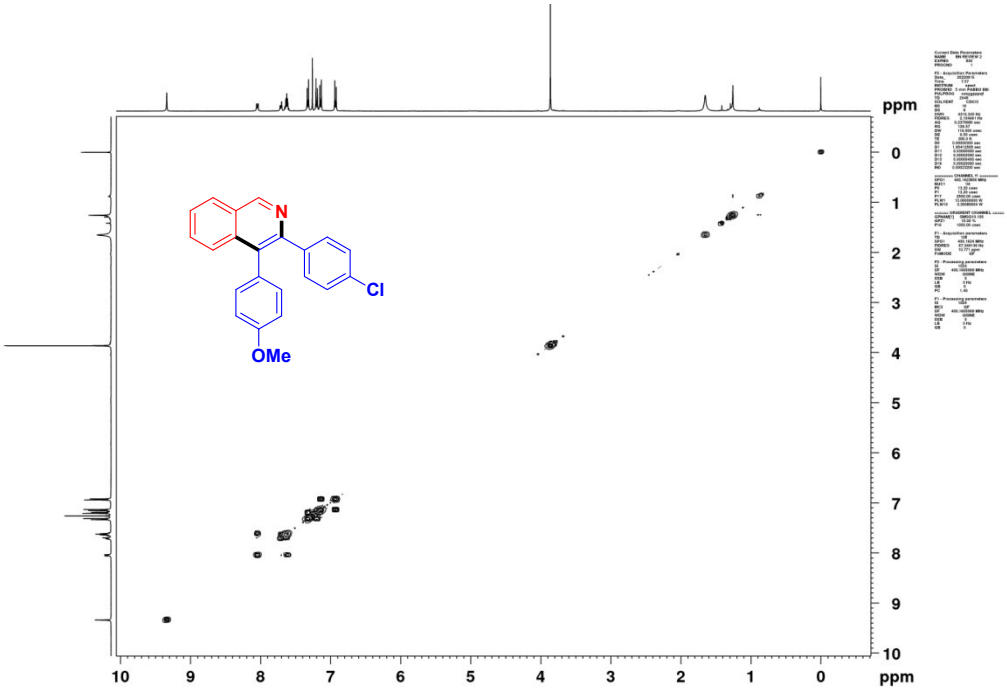
HMBC spectrum of compound- 3af



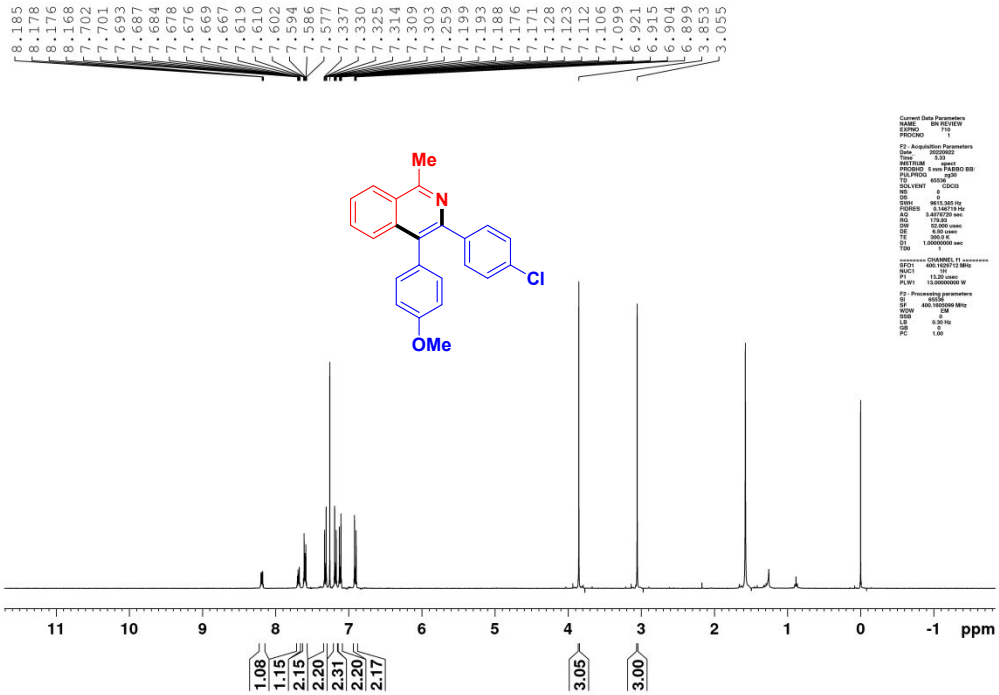
HSQC spectrum of compound- 3af



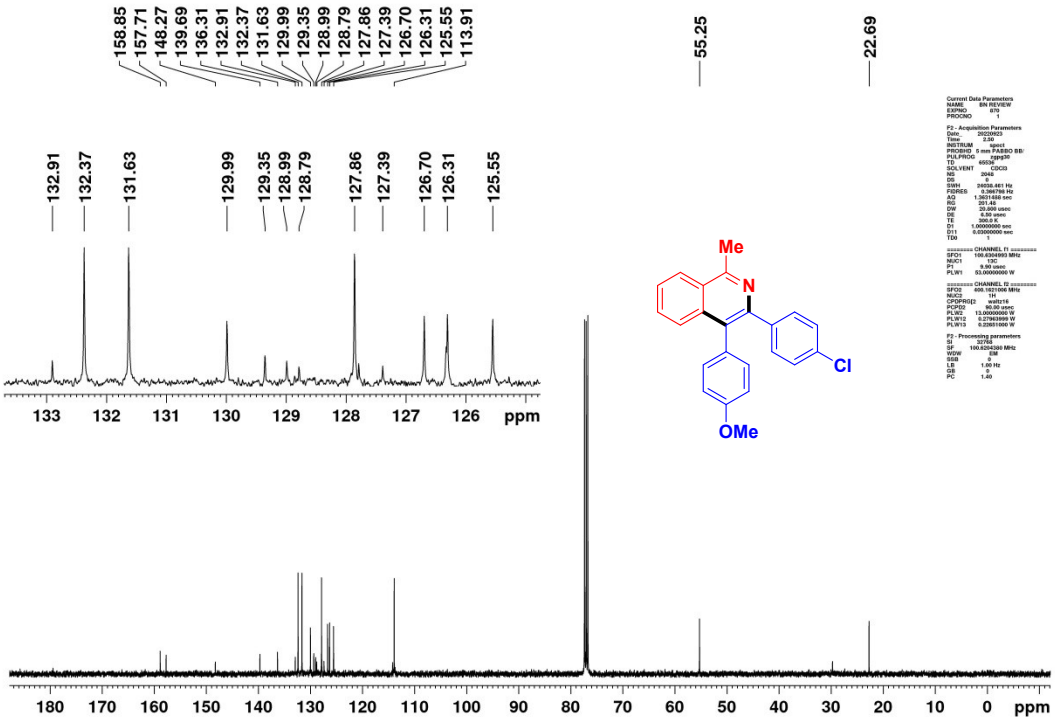
COSY spectrum of compound- 3af



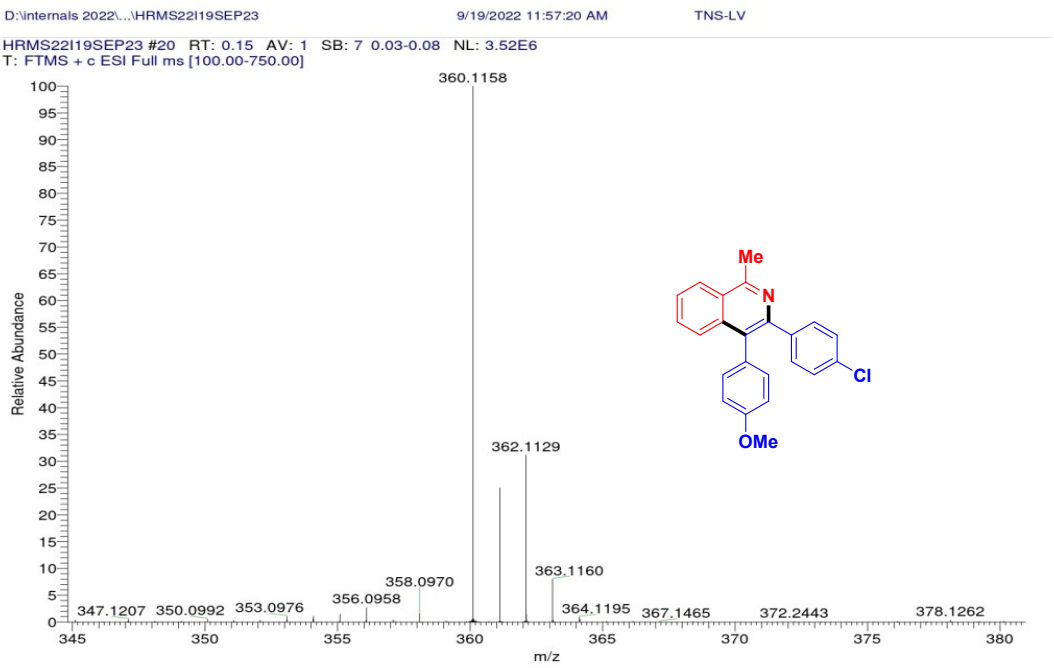
^{1}H NMR spectrum of compound –3gf (400 MHz, $CDCl_3$)



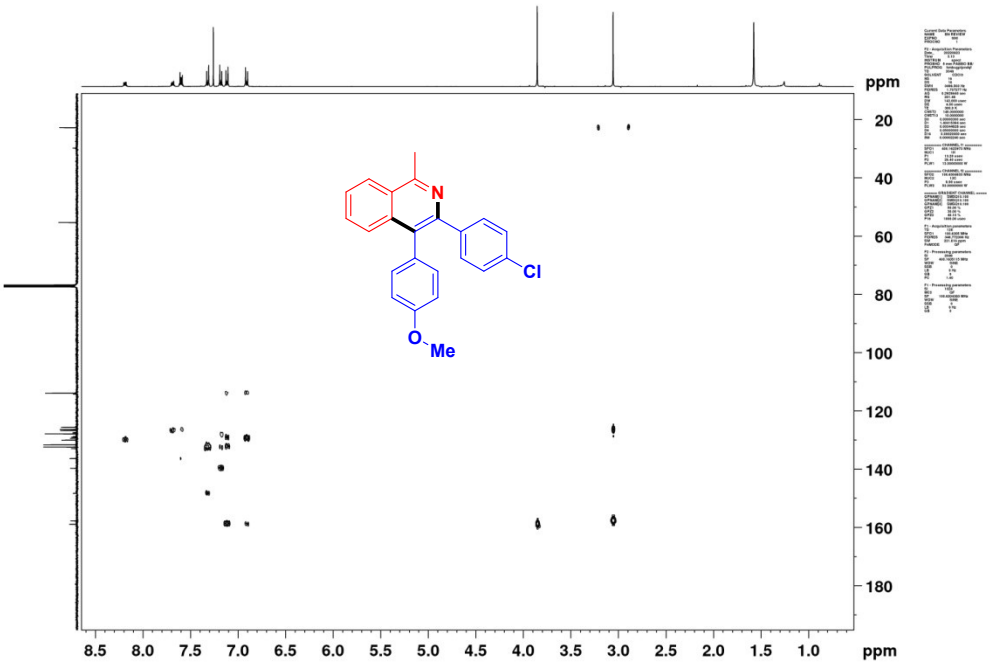
^{13}C NMR spectrum of compound- 3gf (100 MHz, $CDCl_3$)



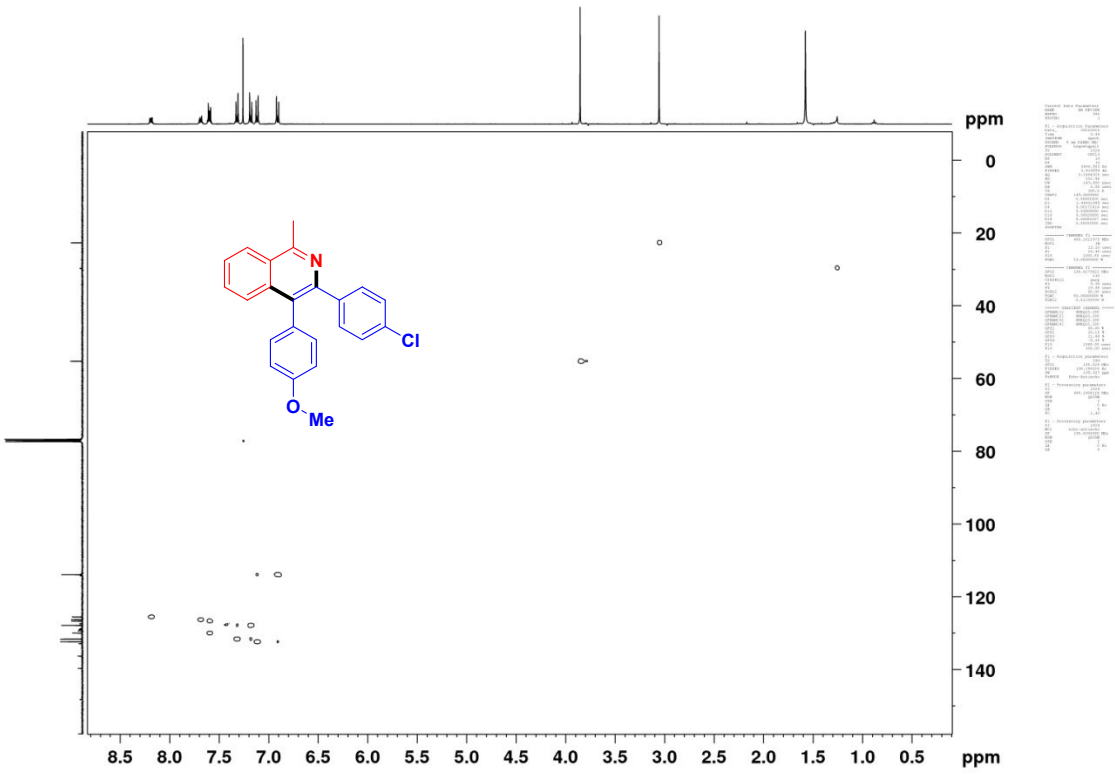
HRMS spectrum of compound- 3gf



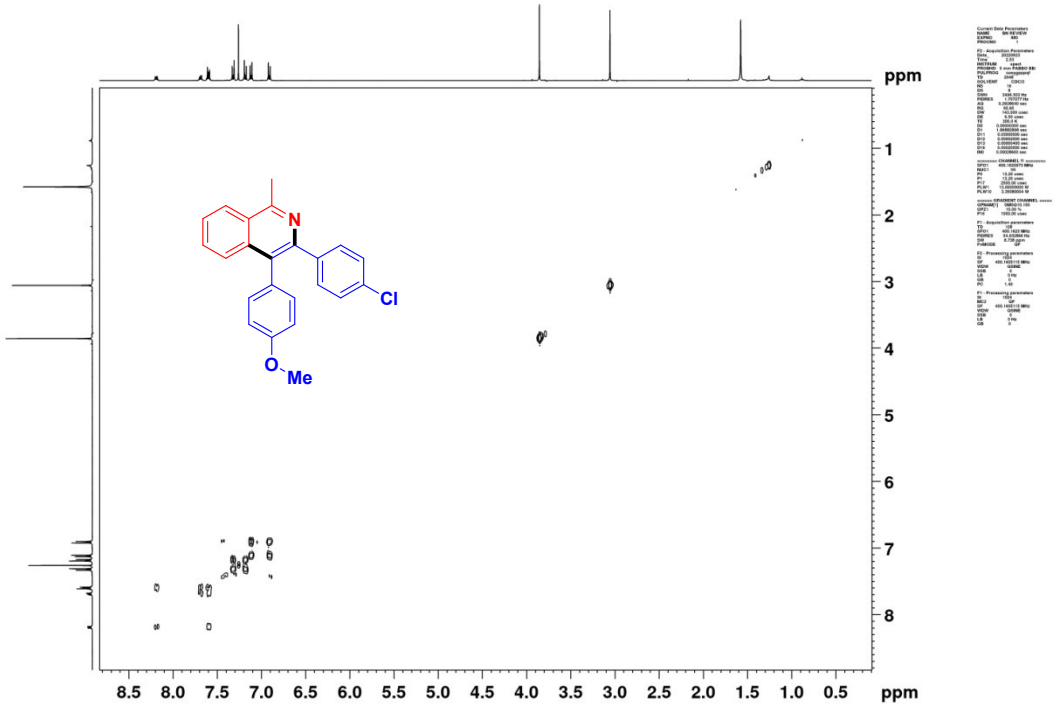
HMBC spectrum of compound- 3gf



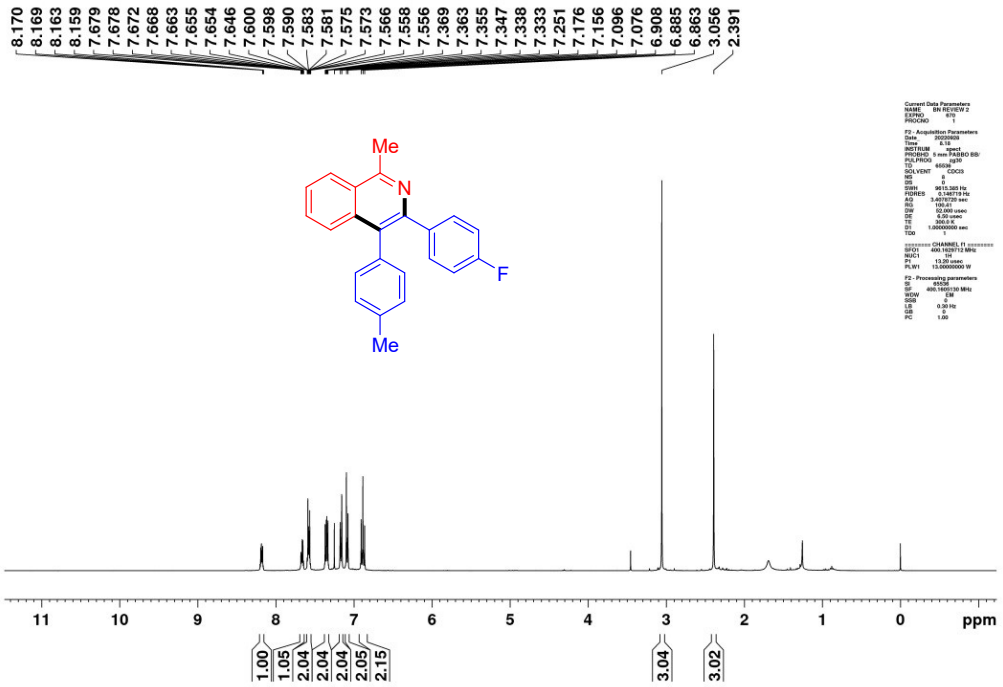
HSQC spectrum of compound- 3gf



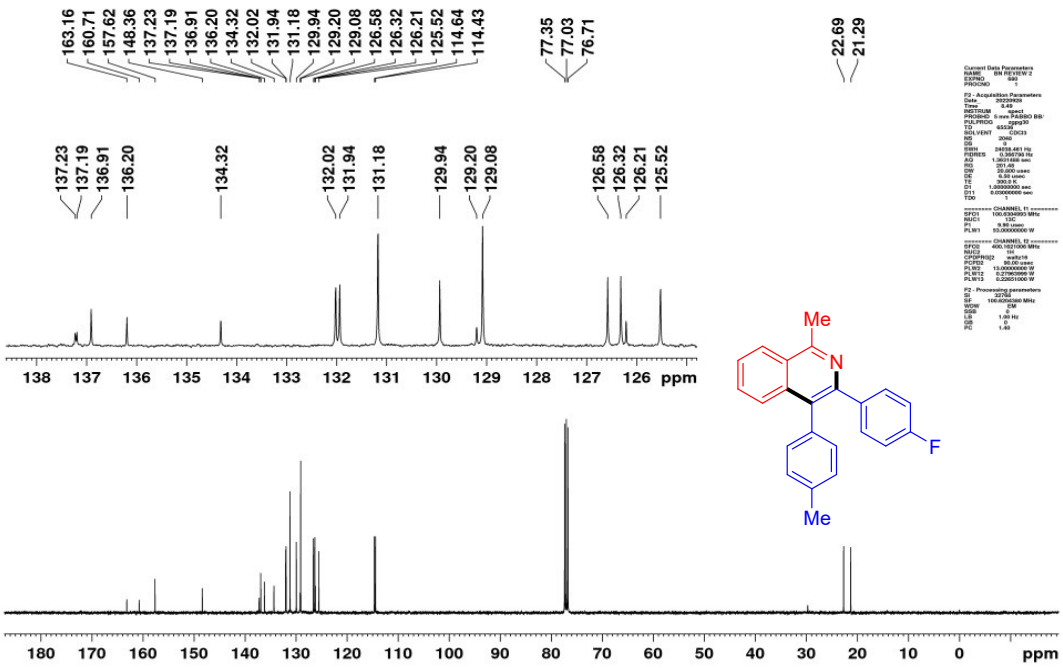
COSY spectrum of compound- 3gf



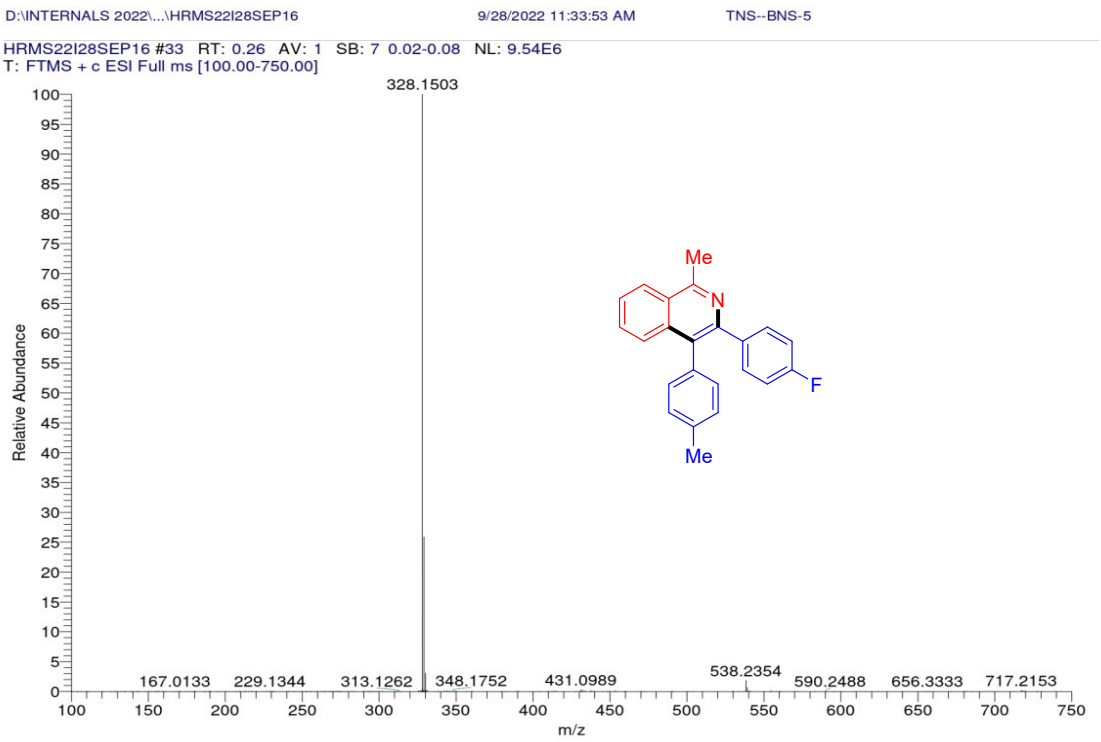
^{1}H NMR spectrum of compound –3gg (400 MHz, $CDCl_3$)



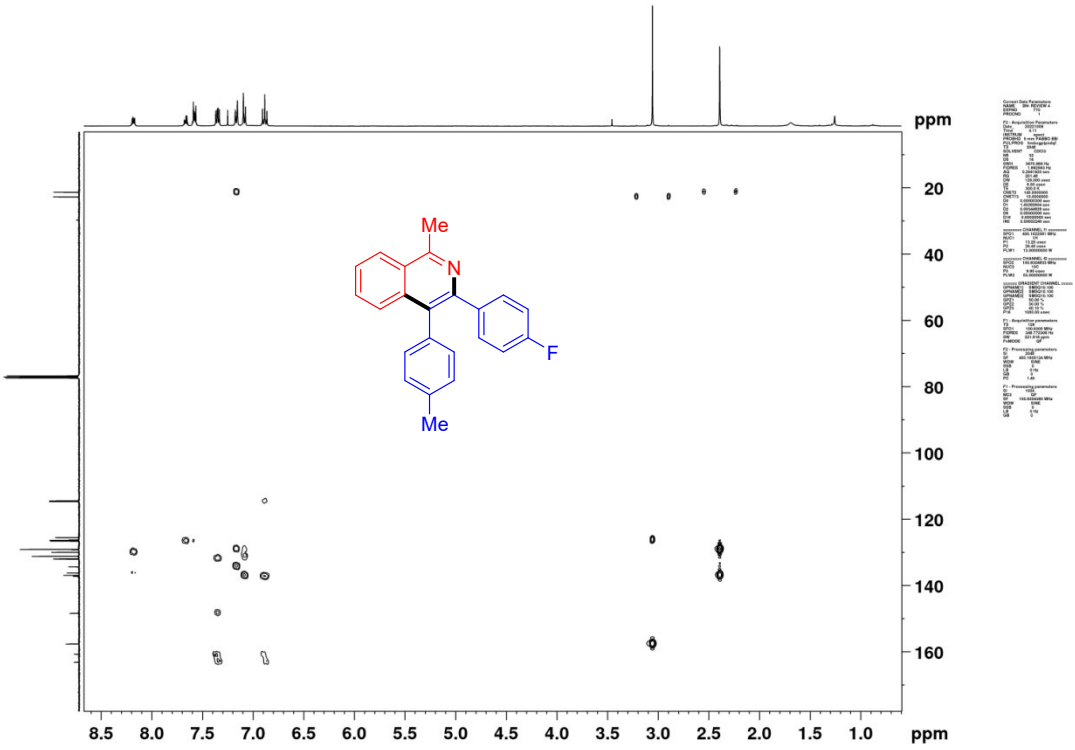
^{13}C NMR spectrum of compound- 3gg (100 MHz, $CDCl_3$)



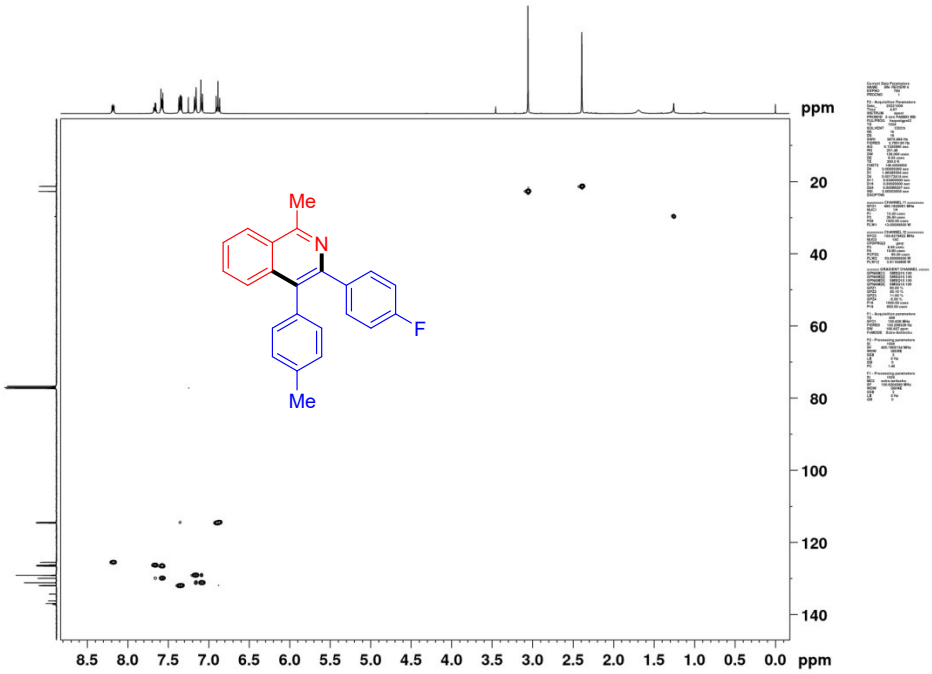
HRMS spectrum of compound- 3gg



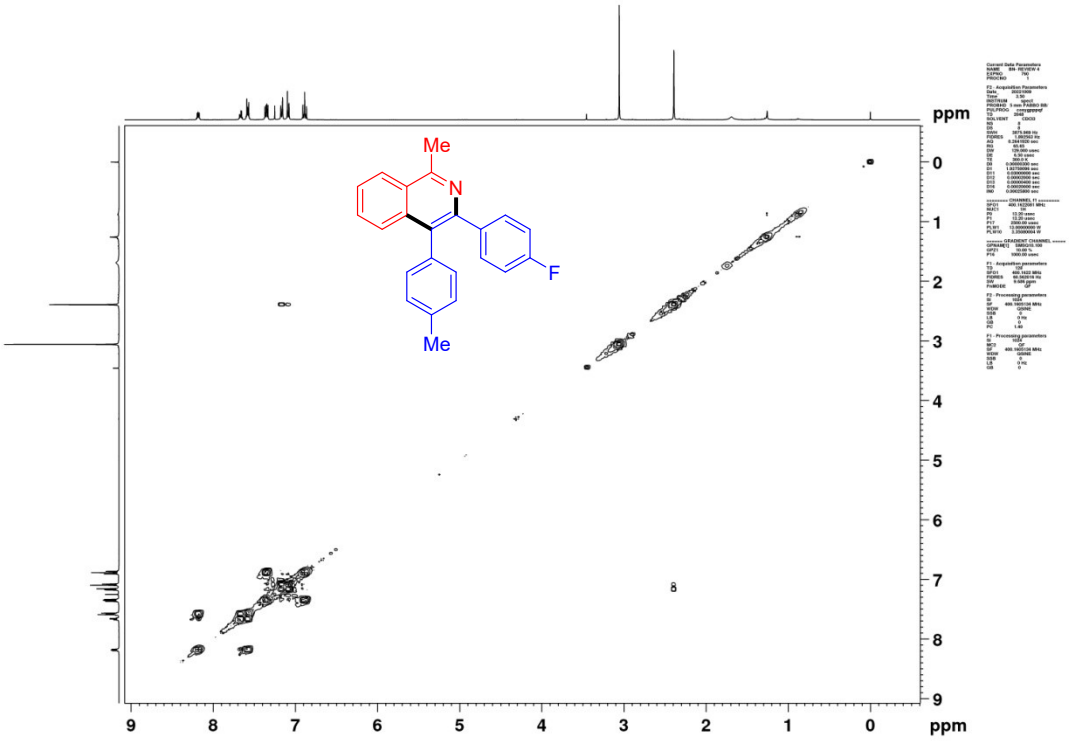
HMBC spectrum of compound- 3gg



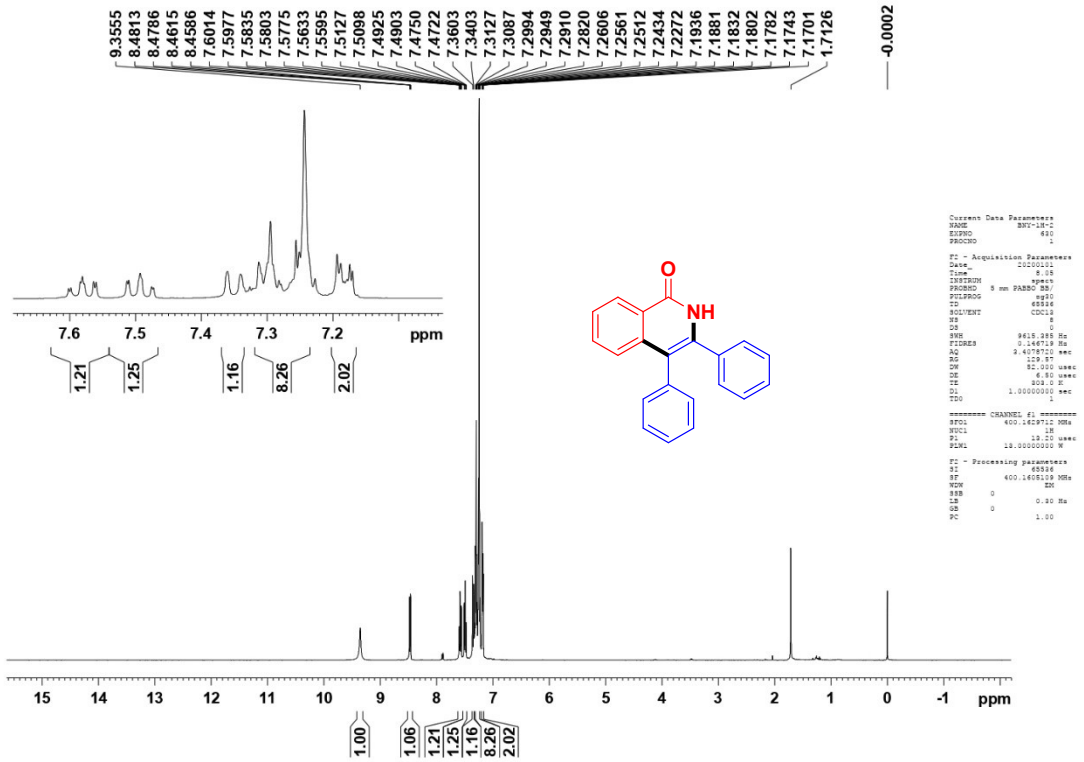
HSQC spectrum of compound- 3 gg



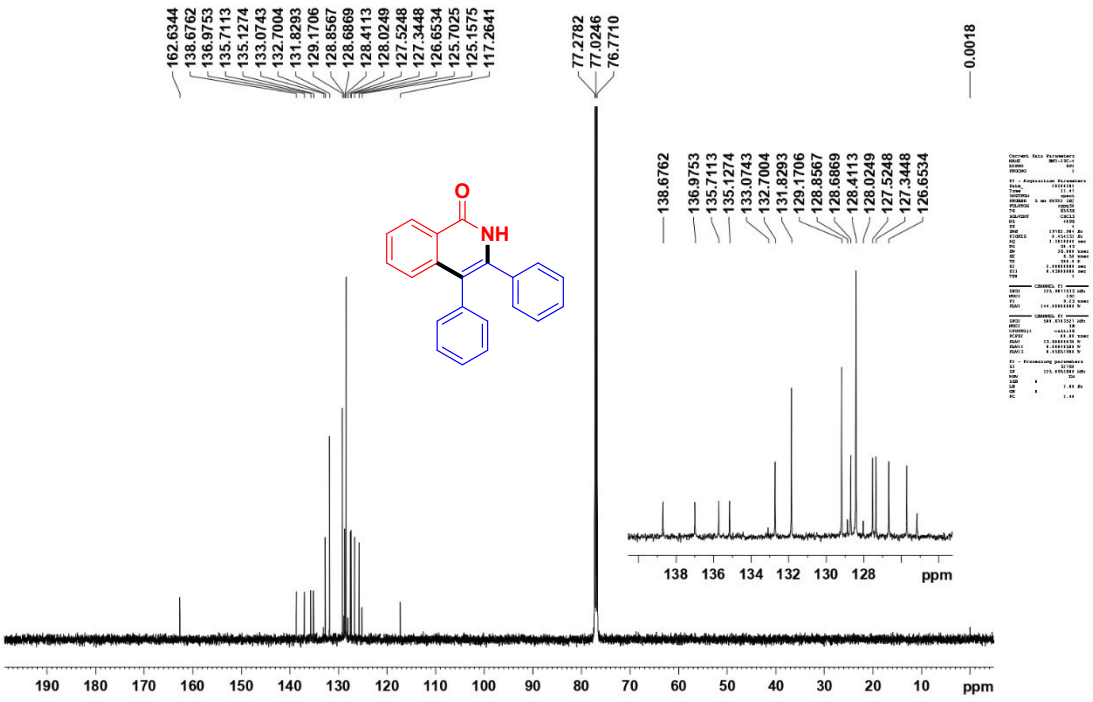
COSY spectrum of compound- 3gg



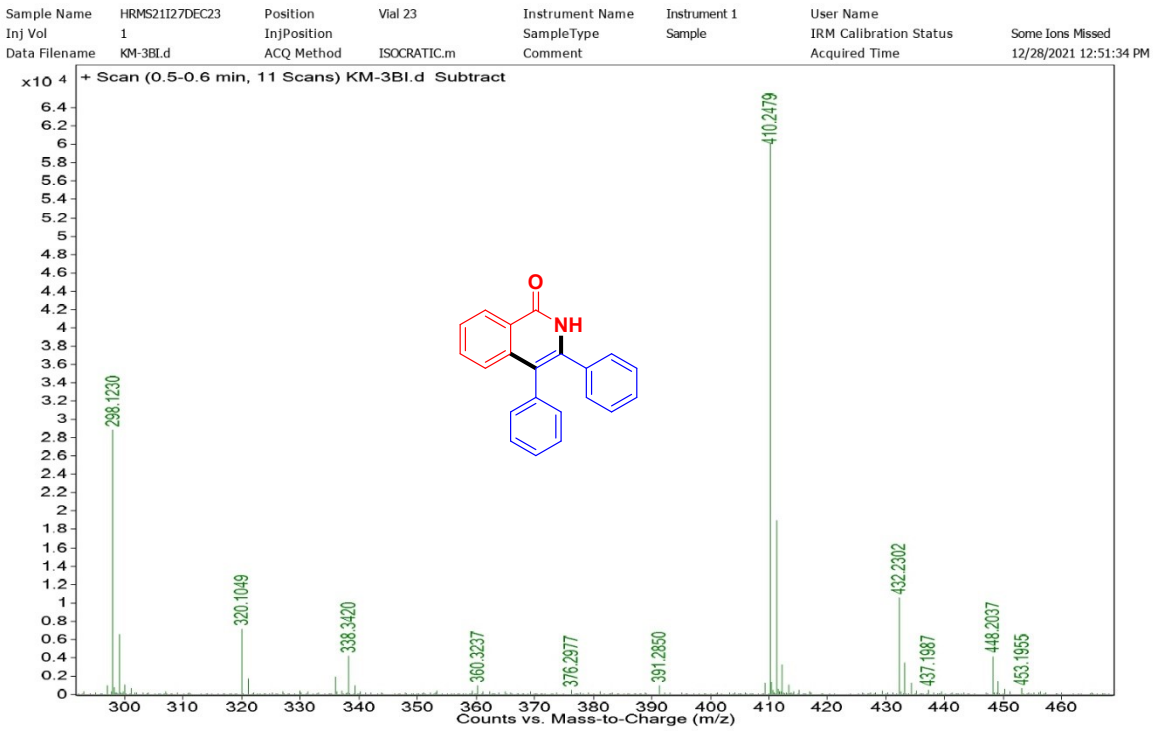
^{1}H NMR spectrum of compound- 3ha (400 MHz, $CDCl_3$)



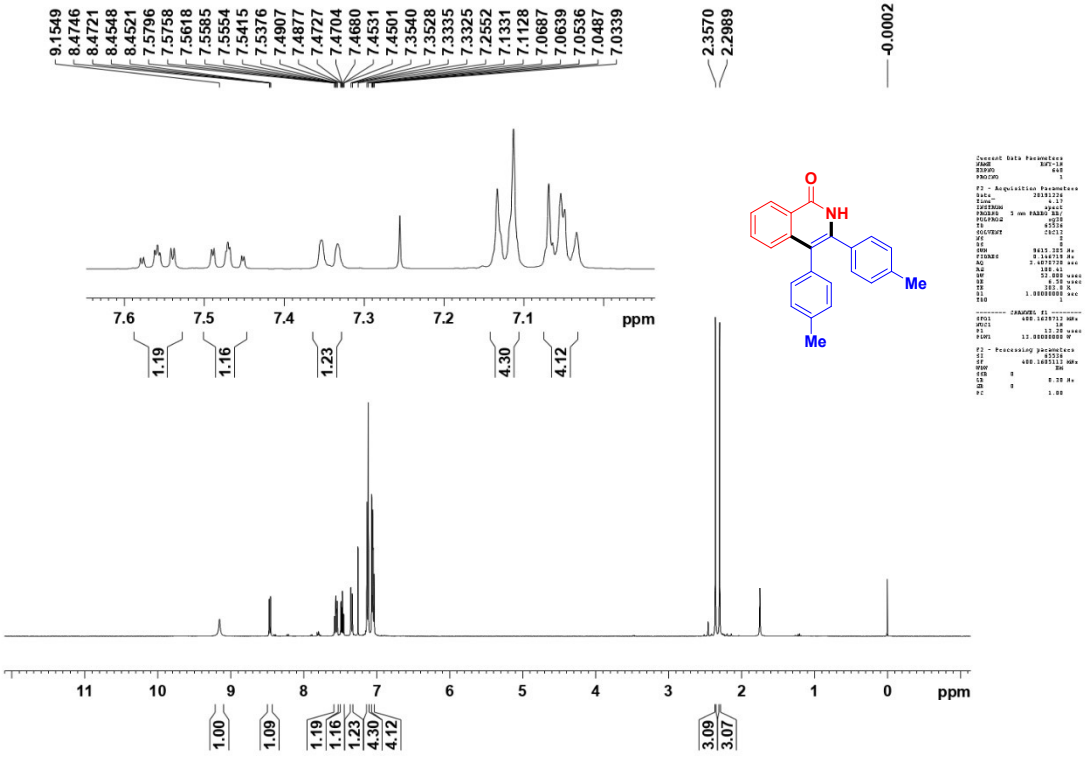
^{13}C NMR spectrum of compound- 3ha (400 MHz, $CDCl_3$)



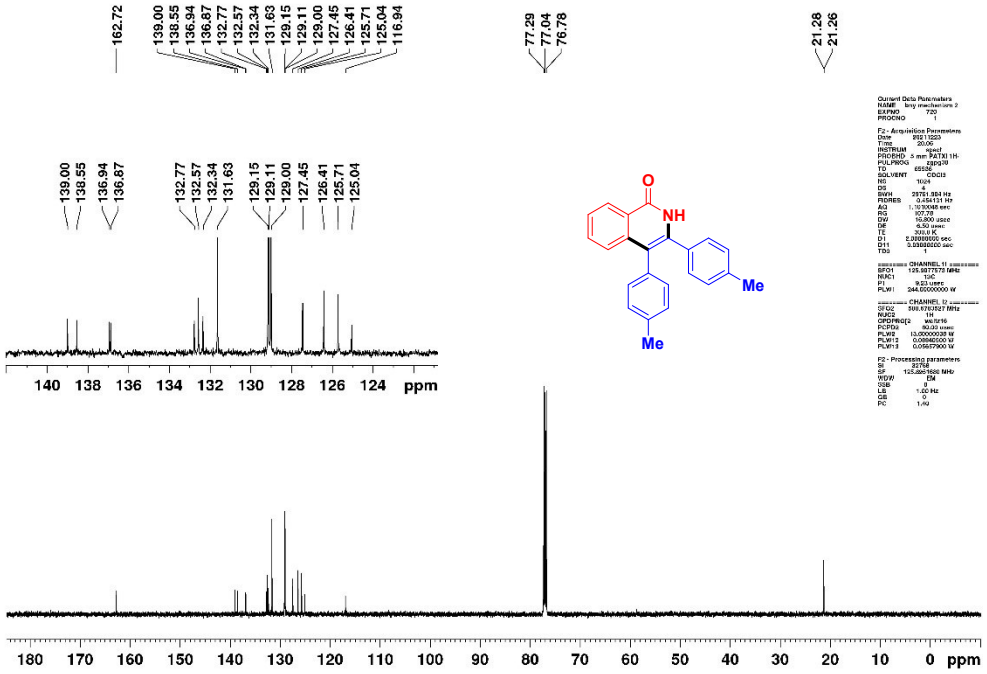
HRMS spectrum of compound- 3ha



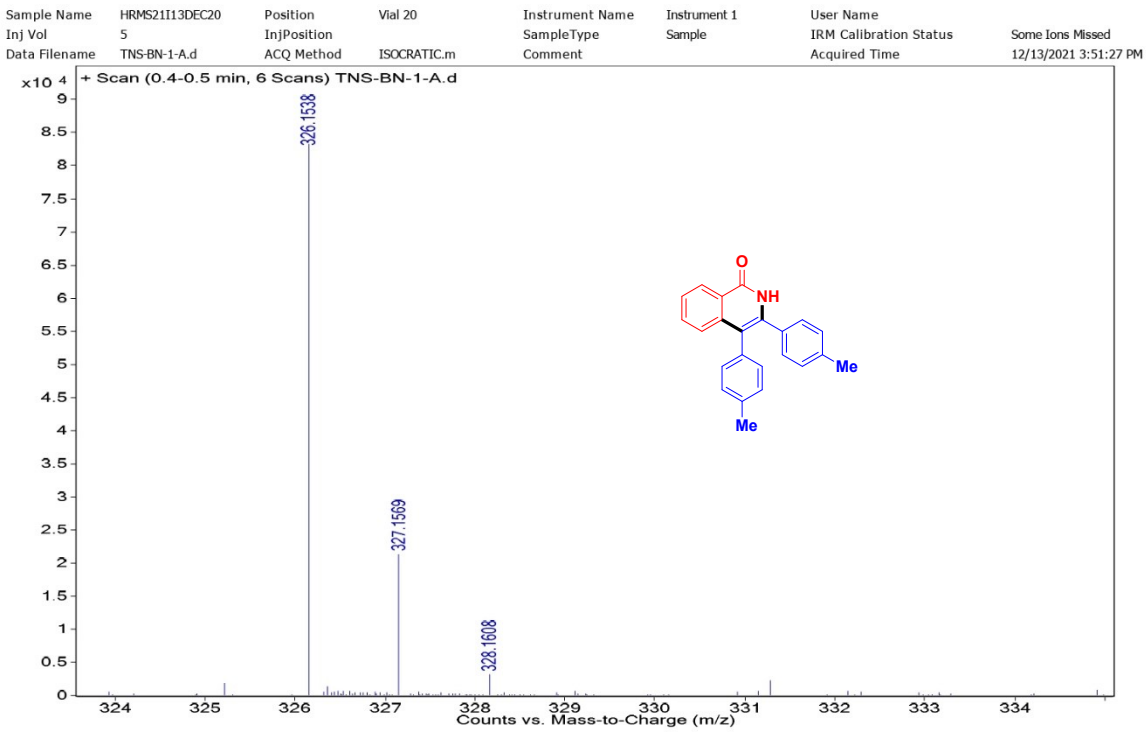
^{1}H NMR spectrum of compound- 3hc (400 MHz, $CDCl_3$)



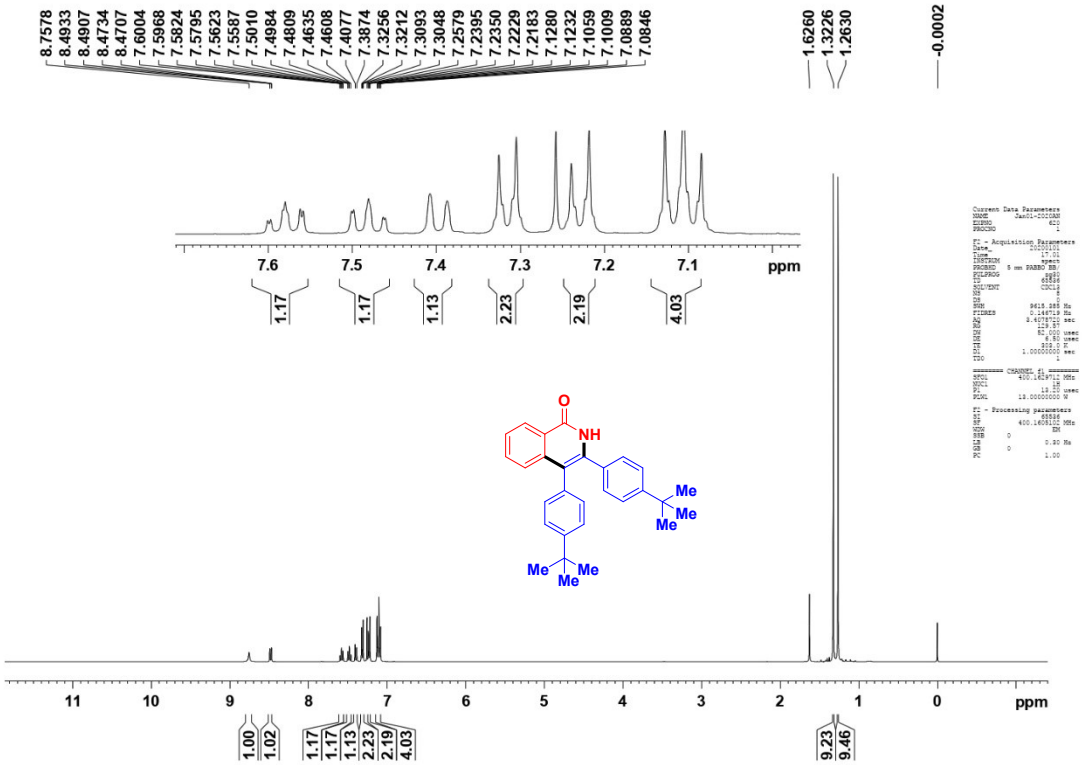
^{13}C NMR spectrum of compound- 3hc (400 MHz, $CDCl_3$)



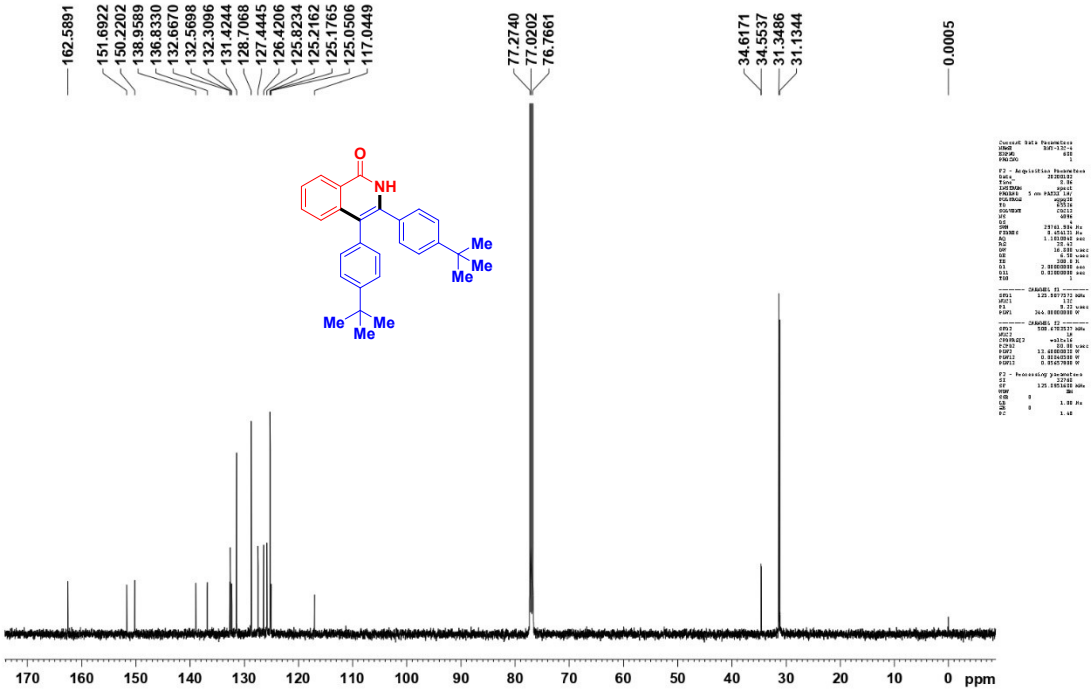
HRMS spectrum of compound- 3hc



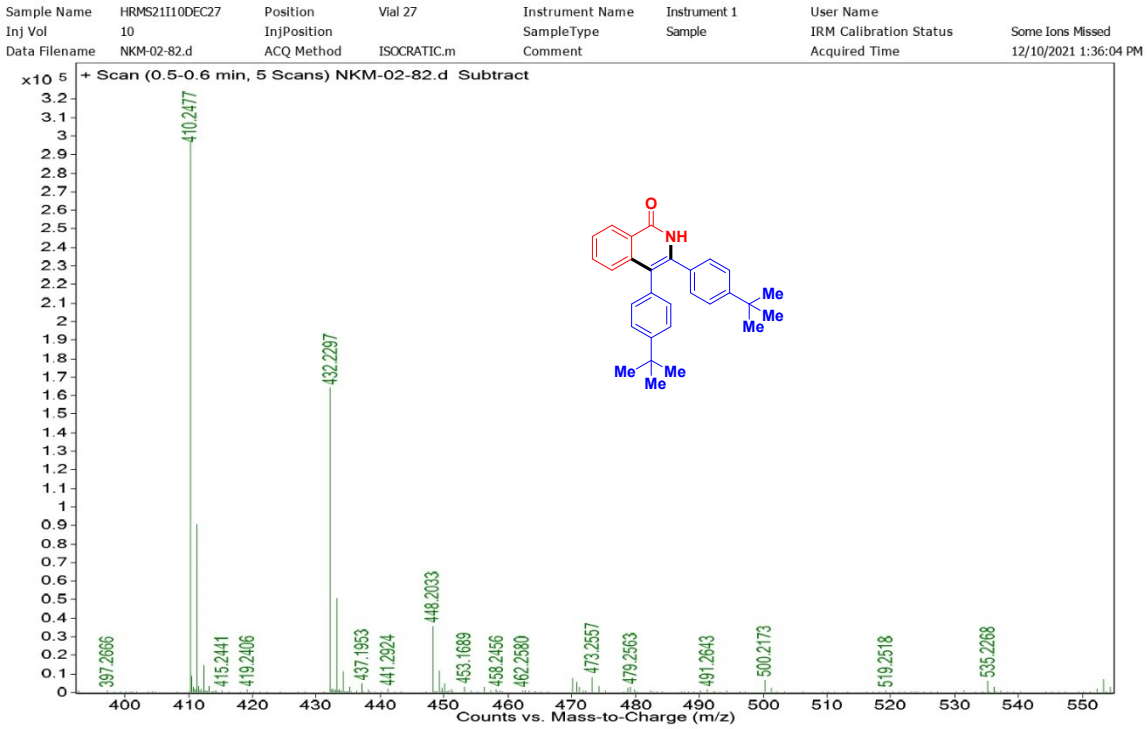
^{1}H NMR spectrum of compound- 3hd (400 MHz, $CDCl_3$)



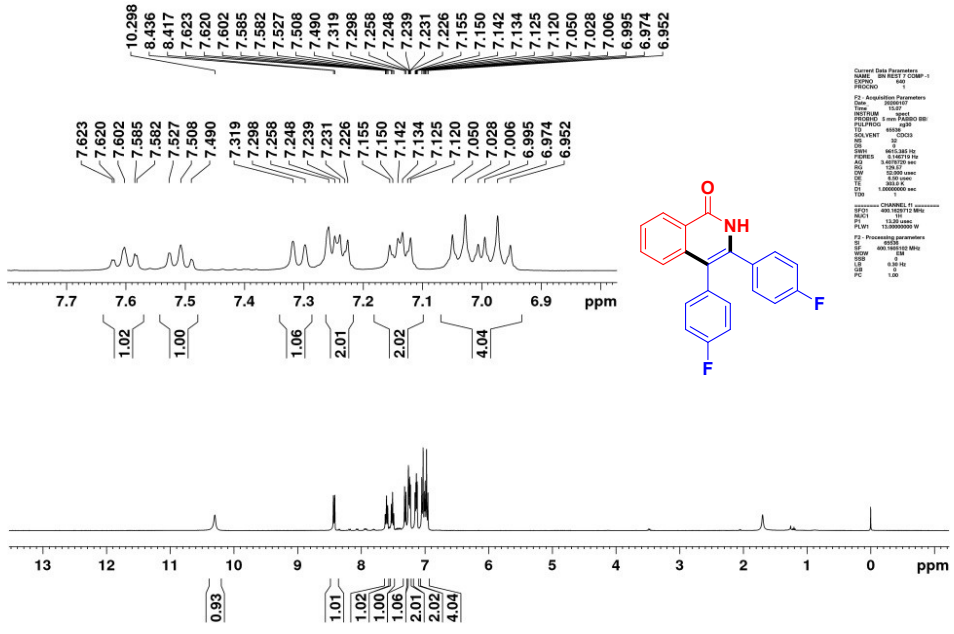
^{13}C NMR spectrum of compound- 3hd (400 MHz, $CDCl_3$)



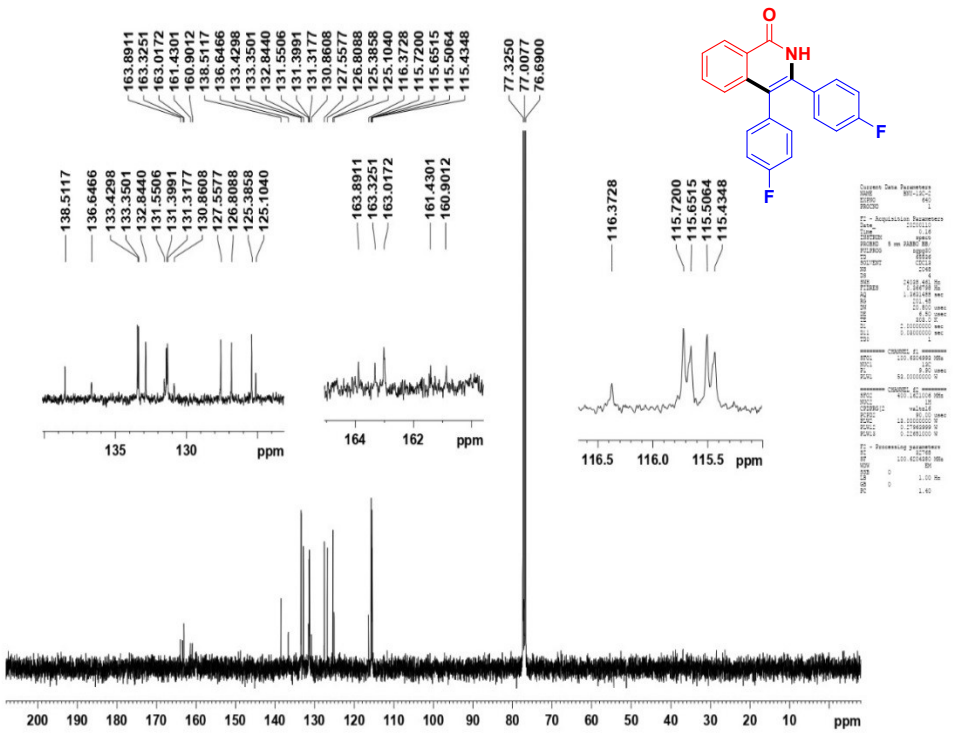
HRMS spectrum of compound- 3hd



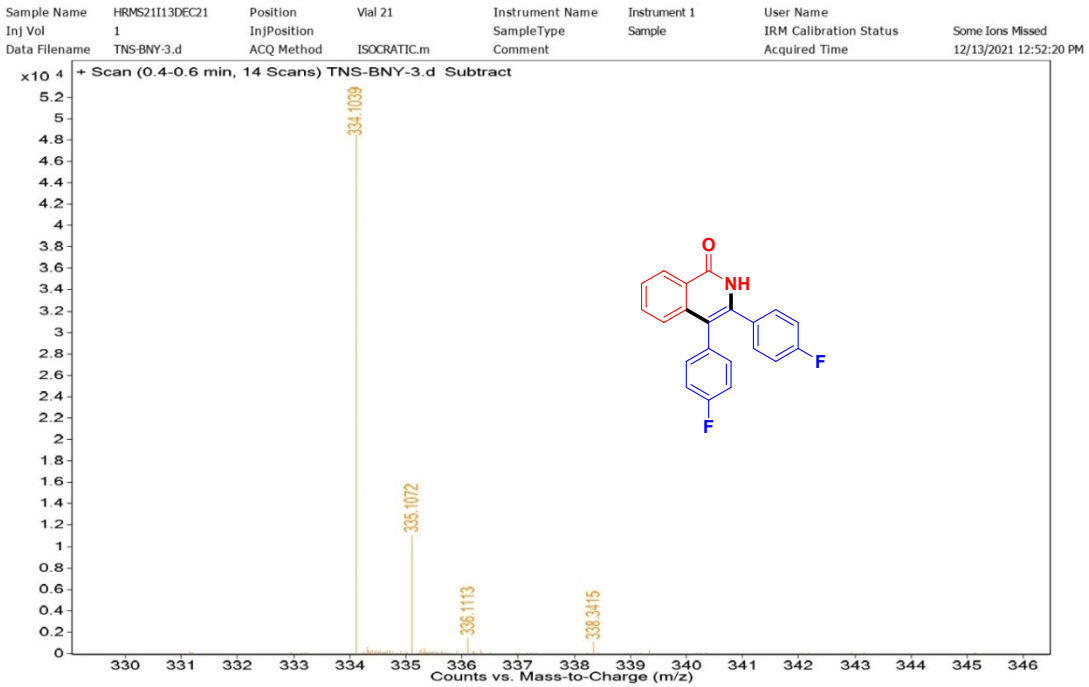
^{1}H NMR spectrum of compound- 3he (400 MHz, $CDCl_3$)



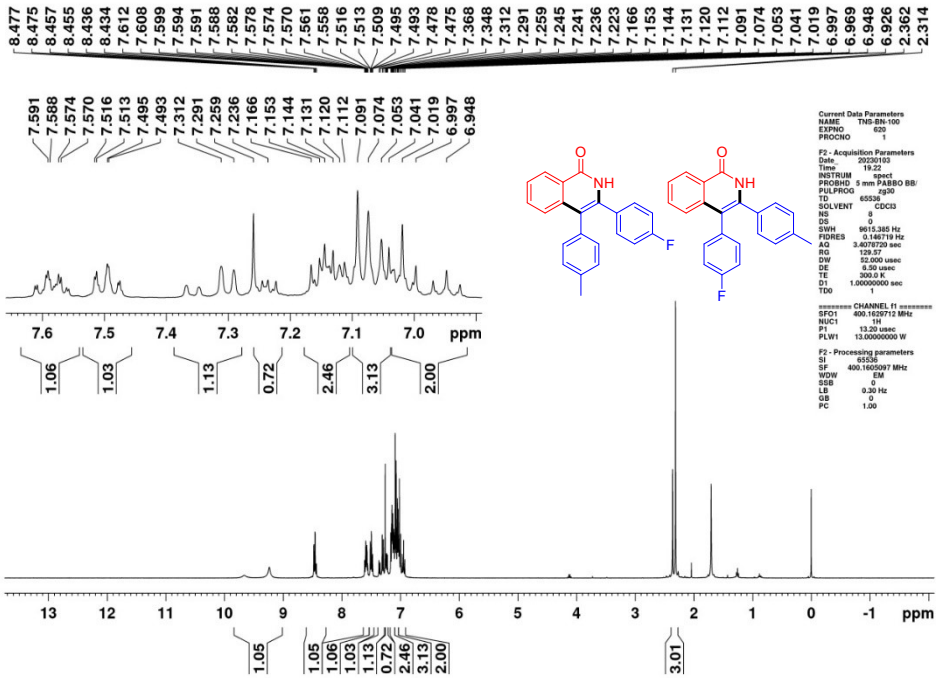
^{13}C NMR spectrum of compound- 3he (400 MHz, $CDCl_3$)



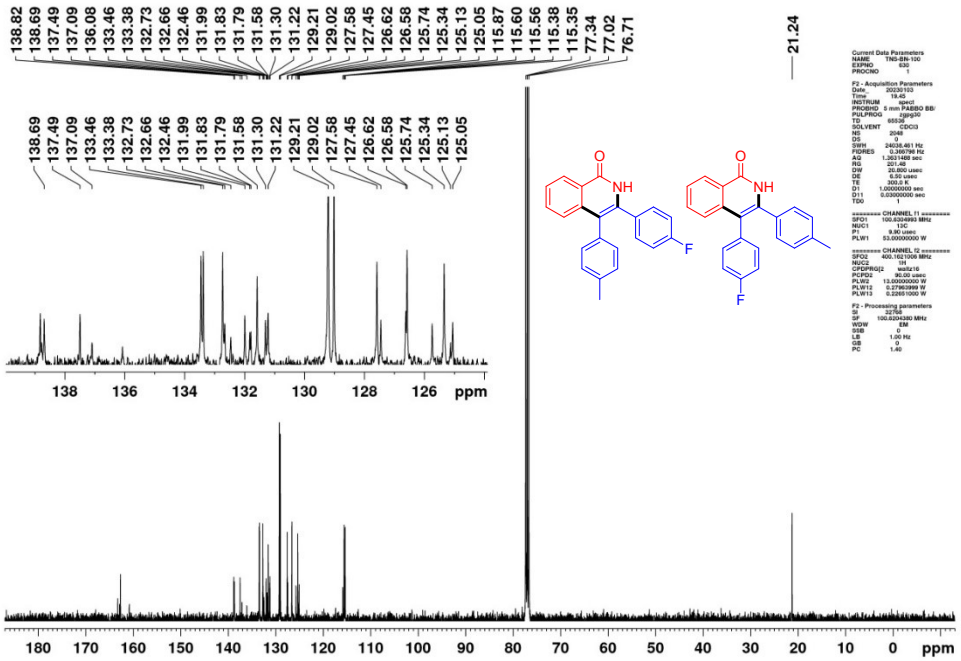
HRMS spectrum of compound- 3he



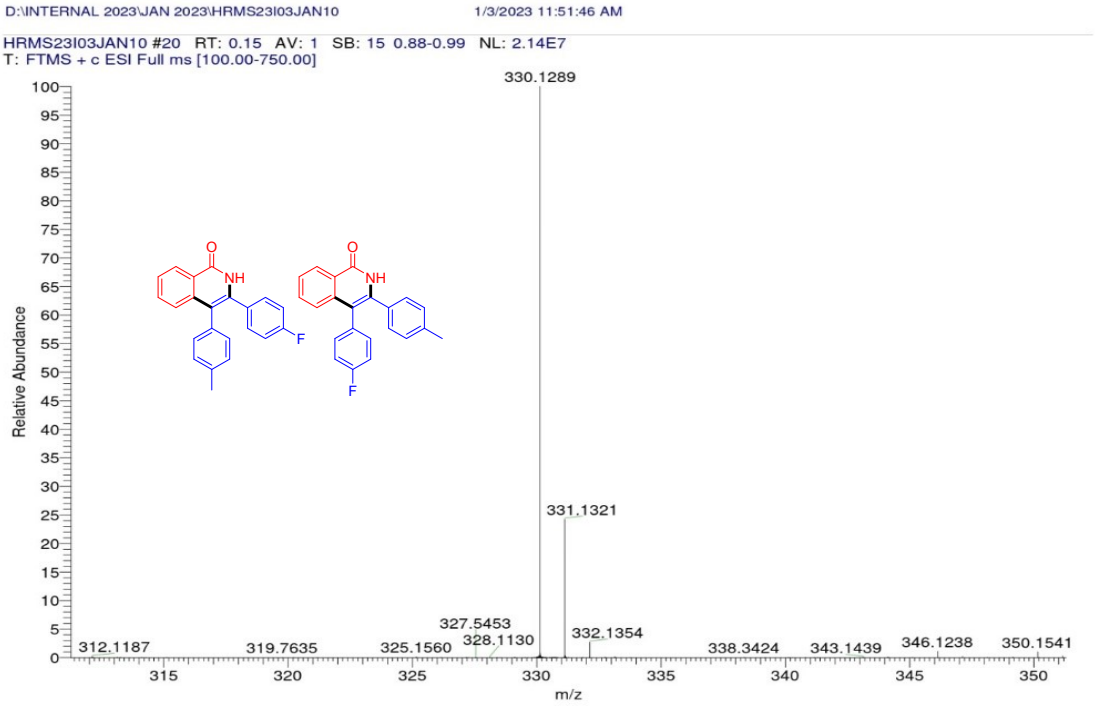
^{1}H NMR spectrum of compound- 3hg (400 MHz, $CDCl_3$)



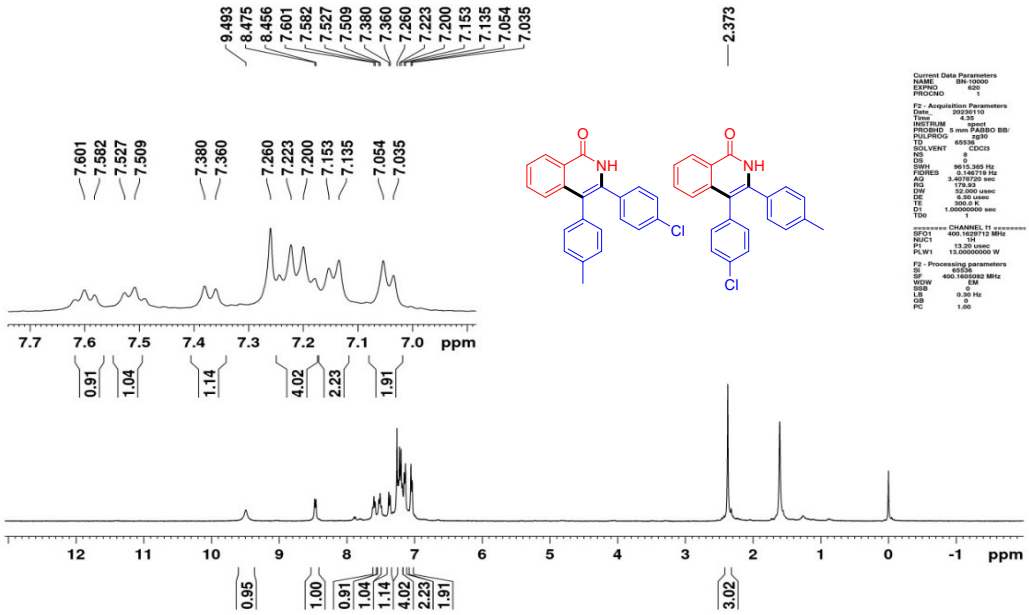
^{13}C NMR spectrum of compound- 3hg (400 MHz, $CDCl_3$)



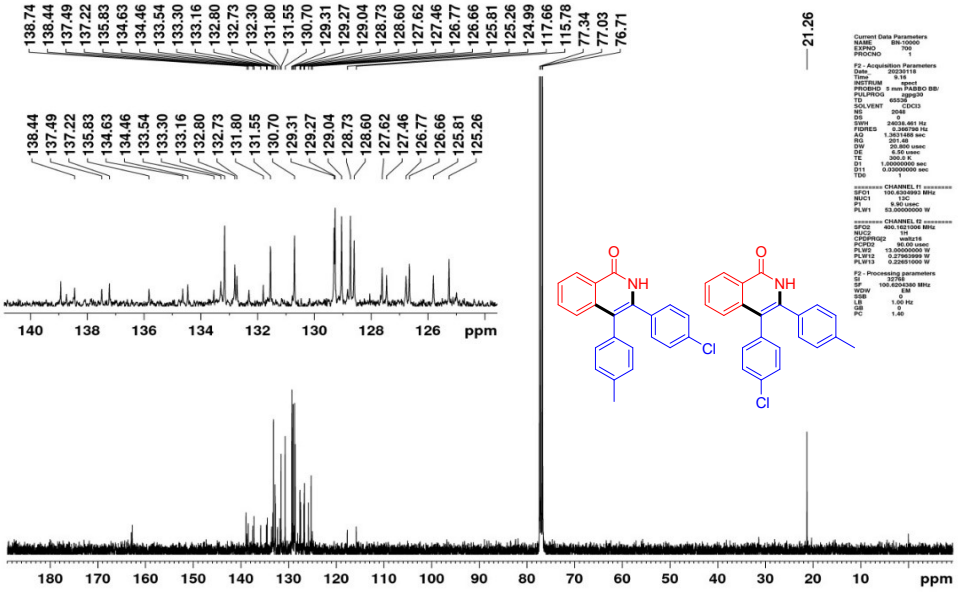
HRMS spectrum of compound-3hg



^{1}H NMR spectrum of compound- 3hh (400 MHz, $CDCl_3$)



^{13}C NMR spectrum of compound- 3hh (400 MHz, $CDCl_3$)



HRMS spectrum of compound-3hh