Electronic Supplementary Information

An Iodine/DMSO-catalyzed sequential one-pot approach to 2, 4, 5-trisubstituted-1*H*-imidazoles from α-methylene ketones

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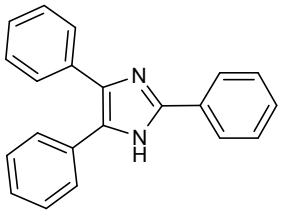
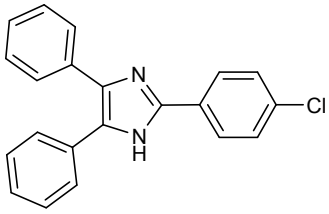
I. General Information

All reagents were purchased without further purification. All ^{1}H and ^{13}C Nuclear Magnetic Resonance (NMR) spectra were recorded on a Bruker Advance III spectrometer operating at either 400 or 500 MHz. Chemical shifts (δ) were reported in ppm using the Dimethyl Sulfoxide-d_6 (DMSO-d_6) residual peak (δ 2.50) for ^{1}H NMR. Chemical shifts of ^{13}C NMR were reported relative to DMSO-d_6 (δ 39.51). The following abbreviations were used to describe peak splitting patterns when appropriate: br = broad, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. Coupling constants, J, were reported in Hertz unit (Hz). High-resolution electron-spray ionization (ESI) mass spectra were recorded on a time-of-flight (TOF) micromass spectrometer. Infra-Red (IR) spectra were recorded on Carey 630 FTIR. Absorption maxima are expressed in wavenumbers (cm^{-1}). Melting points were determined using Kofler hot-stage melting apparatus.

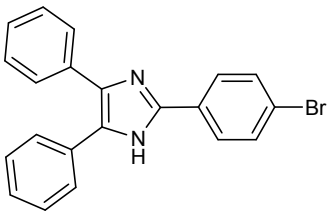
II. Characterization of Imidazole Derivatives



2,4,5-Triphenyl-1*H*-imidazole (3a, $C_{21}H_{16}N_2$, 3a, 82%)[1, 2]: white solid. **Mp** 271-273 °C; **υ_{max} (neat, cm^{-1})**: 3037, 2852, 1586, 1488, 1322; **^{1}H NMR (400 MHz, DMSO-D$_6$)**: 12.69(s, 1H), 8.12-8.10 (d, *J* = 7.64, 2H,), 7.58-7.56 (m, 2H), 7.53-7.50 (m, 2H), 7.48-7.43 (m, 4H), 7.39-7.36 (m, 2H), 7.32-7.29 (m, 2H), 7.24-7.22 (m, 1H); **^{13}C (100 MHz, DMSO-D$_6$)**: 145.5, 137.1, 135.2, 131.1, 130.3, 128.6, 128.4, 128.2, 128.1, 127.7, 127.1, 126.5, 125.2; **ESI-MS (*m/z*)**: 297.1396 (100) $[M+H]^+$, 298.1432 (25).

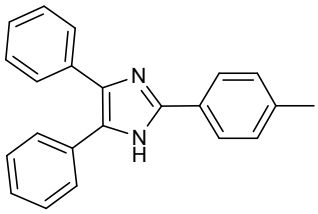


2-(4-Chlorophenyl)-4,5-diphenyl-1*H*-imidazole (3b, $C_{21}H_{15}ClN_2$, 86%)[3, 4]: white solid. **Mp** 262-263 °C; **υ_{max} (neat, cm^{-1})**: 3057, 2961, 1599, 1483, 1323, 764; **^{1}H NMR (400 MHz, DMSO-D$_6$)**: 12.76 (s, 1H), 8.11-8.09 (d, *J* = 6.47 Hz, 2H), 7.55-7.53 (m, 6H), 7.43-7.32 (m, 6H); **^{13}C (100 MHz, DMSO-D$_6$)**: 144.4, 137.3, 135.0, 132.7, 131.0, 129.2, 128.7, 128.6, 128.4, 127.1, 126.8; **ESI-MS (*m/z*)**: 331.1011 (100) $[M+H]^+$, 333.0989 (41).

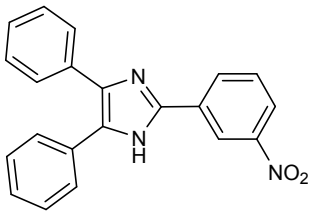


2-(4-Bromophenyl)-4,5-diphenyl-1*H*-imidazole (3c, $C_{21}H_{15}BrN_2$, 82%)[3, 4] : white solid. **Mp** 250-251 °C; **υ_{max} (neat, cm^{-1})**: 3057, 1587, 1491, 1382, 724; **^{1}H NMR (400 MHz, DMSO-D$_6$)**: 12.77 (s, 1H), 8.05-8.03 (d, *J* = 6.18 Hz, 2H), 7.69-7.67 (d, *J*

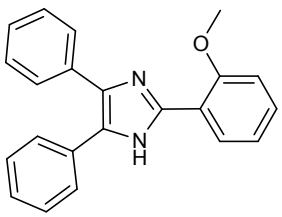
= 6.38 Hz, 2H), 7.53 (m, 4H), 7.44-7.24 (m, 6H); **^{13}C (100 MHz, DMSO-D$_6$)**: 144.4, 137.3, 135.0, 131.6, 130.9, 129.5, 128.6, 128.4, 128.2, 127.8, 127.1, 126.6, 121.4; **ESI-MS (*m/z*)**: 375.0503 (100) $[M+H]^+$, 376.0532 (25), 377.0487 (96), 378.0519 (23).



4,5-diphenyl-2-(*p*-tolyl)-1*H*-imidazole (3d, $C_{22}H_{18}N_2$, 80%)[5] : white solid. **Mp** 231-233 °C; **υ_{max} (neat, cm^{-1})**: 3036, 2870, 1602, 1493, 1449; **^{1}H NMR (400 MHz, DMSO-D$_6$)**: 12.61 (s, 1H), 799-7.97 (m, 2H), 7.53-7.23 (m, 12H), 2.35 (s, 3H); **^{13}C (100 MHz, DMSO-D$_6$)**: 145.7, 137.7, 137.0, 135.3, 131.2, 129.3, 128.7, 128.5, 128.2, 128.0, 127.7, 127.1, 126.5, 125.2, 20.9; **ESI-MS (*m/z*)**: 310.1429 (25) $[M]^+$, 309.1393 (100) $[M-H]^+$, 311.1581 (10).

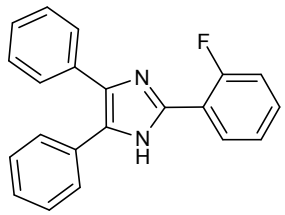


2-(3-Nitrophenyl)-4,5-diphenyl-1*H*-imidazole (3e, $C_{21}H_{15}N_3O_2$, 75%)[3, 4] : yellow solid. **Mp** 315-317 °C; **υ_{max} (neat, cm^{-1})**: 3059, 2861, 1584, 1522, 1480, 1347; **^{1}H NMR (400 MHz, DMSO-D$_6$)**: 13.08 (s, 1H), 8.95 (s, 1H), 8.52-8.50 (d, *J* = 6.31 Hz, 1H), 8.21-8.19 (d, *J* = 8.14 Hz, 1H), 7.79-7.75 (t, *J* = 8.00 Hz, 1H), 7.55-7.54 (d, *J* = 7.09 Hz, 4H), 7.39-7.37 (m, 6H); **^{13}C (100 MHz, DMSO-D$_6$)**: 148.4, 143.4, 131.8, 131.1, 130.4, 128.5, 127.6, 122.5, 119.4; **ESI-MS (*m/z*)**: 342.1248 (100) $[M+H]^+$, 343.1281 (25).

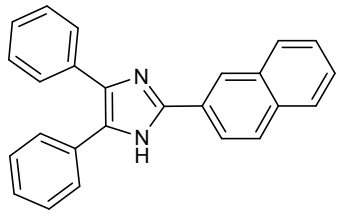


2-(2-Methoxyphenyl)-4,5-diphenyl-1*H*-imidazole (3f, $C_{22}H_{18}N_2O$, 63%)[2] : white solid. **Mp** 224-226 °C; **υ_{max} (neat, cm^{-1})**: 3059, 2834, 1583, 1468, 1249, 1016;

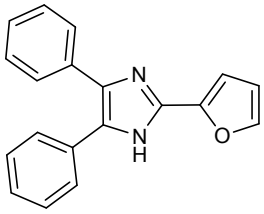
^{1}H NMR (400 MHz, DMSO-D_6): 11.87 (s, 1H), 8.07-8.05 (d, *J* = 6.35 Hz, 1H), 7.55-7.53 (d, *J* = 7.56 Hz, 2H), 7.49-7.47 (m, 2H), 7.45-7.41 (t, *J* = 7.50 Hz, 2H), 7.38-7.37 (m, 2H), 7.31-7.27 (t, *J* = 7.36 Hz, 2H), 7.23-7.19 (m, 1H), 7.17-7.15 (m, 1H), 7.09-7.05 (t, *J* = 7.40 Hz, 1H), 3.93 (s, 3H); **^{13}C (100 MHz, DMSO-D_6)**: 156.0, 143.1, 136.4, 135.3, 131.2, 129.7, 128.8, 128.6, 128.5, 128.1, 127.6, 127.4, 127.0, 126.4, 120.6, 118.9, 111.6, 55.5; **ESI-MS (*m/z*)**: 327.1503 (100) $[M+H]^+$, 328.1535 (30).



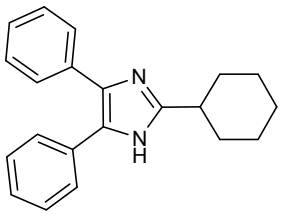
2-(2-Fluorophenyl)-4,5-diphenyl-1*H*-imidazole (3g, $C_{21}H_{15}FN_2$, 68%)[6]: white solid. **Mp** 239-240 °C; **υ_{max} (neat, cm^{-1})**: 3028, 2777, 1577, 1483, 1252, 1100; **^{1}H NMR (400 MHz, DMSO-D_6)**: 12.57 (s, 1H), 8.03-7.99 (m, 1H), 7.56-7.54 (d, *J* = 7.32 Hz, 2H), 7.51-7.41 (m, 5H), 7.39-7.29 (m, 5H), 7.24-7.21 (m, 1H); **^{13}C (100 MHz, DMSO-D_6)**: 160.1, 157.6, 140.8, 140.8, 137.2, 135.0, 130.9, 130.4, 130.3, 129.6, 129.6, 128.5, 128.2, 127.8, 127.1, 126.6, 124.7, 124.6, 118.7, 118.6, 116.3, 116.1; **ESI-MS (*m/z*)**: 315.1305 (100) $[M+H]^+$, 316.1337 (26).



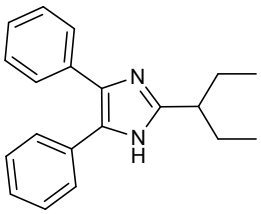
2-(naphthalen-2-yl)-4,5-diphenyl-1*H*-imidazole (3h, $C_{25}H_{18}N_2$, 74%)[7]: white solid. **Mp** 274-275 °C; **υ_{max} (neat, cm^{-1})**: 3057, 2970, 1582, 1500, 1341; **^{1}H NMR (400 MHz, DMSO-D_6)**: 12.86 (s, 1H), 8.63 (s, 1H), 8.29-8.26 (d, *J* = 6.10 Hz, 1H), 8.02-7.93 (m, 3H), 7.59-7.51 (m, 6H), 7.39 (m, 6H); **^{13}C (100 MHz, DMSO-D_6)**: 145.5, 133.0, 132.7, 128.4, 128.2, 128.1, 127.8, 127.7, 126.7, 126.3, 123.7, 123.5; **ESI-MS (*m/z*)**: 347.1553 (100) $[M+H]^+$, 348.1586 (30).



2-(2-Furan-2-yl)-4,5-diphenyl-1*H*-imidazole (3i, $C_{19}H_{14}N_2O$, 42%)[8]: brown solid. **Mp** 229-231 °C; **υ_{max} (neat, cm^{-1})**: 3056, 2726, 1602, 1485, 1014; **^{1}H NMR (400 MHz, DMSO-D_6)**: 12.80 (s, 1H), 7.80 (m, 1H), 7.53-7.47 (m, 4H), 7.44-7.40 (m, 2H), 7.38-7.34 (m, 1H), 7.31-7.28 (m, 2H), 7.24-7.21 (m, 1H), 6.98-6.97 (d, *J* = 3.10 Hz, 1H), 6.64 (m, 1H); **^{13}C (100 MHz, DMSO-D_6)**: 145.7, 143.0, 138.5, 137.0, 135.0, 130.8, 128.6, 128.3, 128.2, 127.8, 127.5, 127.1, 126.6, 111.8, 107.4; **ESI-MS (*m/z*)**: 287.1189 (100) $[M+H]^+$, 288.1223 (24).

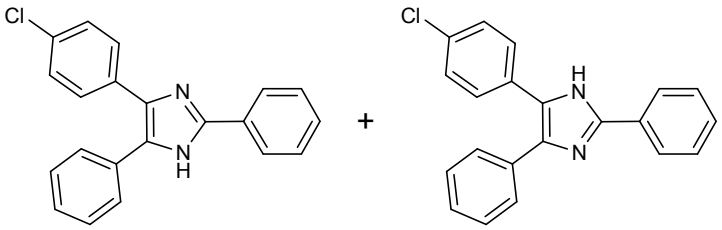


2-(Cyclohexyl)-4,5-diphenyl-1*H*-imidazole (3j, $C_{21}H_{22}N_2$, 51%)[2]: pale brown solid. **Mp** 242-244 °C; **υ_{max} (neat, cm^{-1})**: 3032, 2926, 2848, 1602, 1534, 1499, 1447; **^{1}H NMR (400 MHz, DMSO-D_6)**: 11.90 (s, 1H), 7.48-7.46 (m, 2H), 7.39-7.35 (m, 4H), 7.31-7.23 (m, 3H), 7.18-7.14 (m, 1H), 2.73-2.66 (m, 1H), 1.98-1.95 (m, 2H), 1.81-1.78 (m, 2H), 1.70-1.67 (m, 1H), 1.64-1.54 (m, 2H), 1.40-1.20 (m, 3H); **^{13}C (100 MHz, DMSO-D_6)**: 152.3, 135.8, 135.0, 131.6, 128.5, 128.0, 127.8, 127.1, 127.0, 126.0, 125.7, 37.2, 31.5, 25.7, 25.6; **ESI-MS (*m/z*)**: 303.1862 (100) $[M+H]^+$, 304.1895 (25).

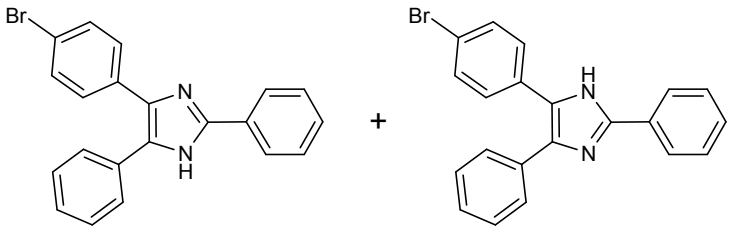


2-(pentan-3-yl)-4,5-diphenyl-1*H*-imidazole (3k, $C_{20}H_{22}N_2$, 35%)[9]: white solid. **Mp** 240-242 °C; **υ_{max} (neat, cm^{-1})**: 3064, 3030, 2957, 2925, 2869, 1601, 1498,

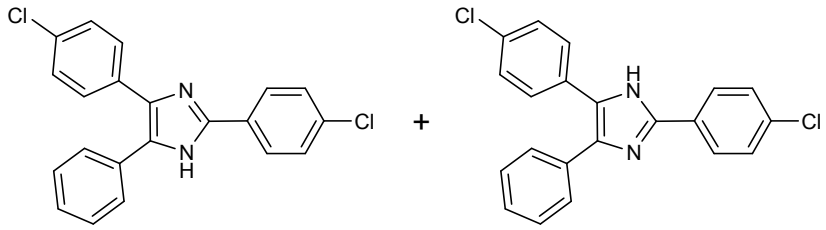
1333; **^{1}H NMR (400 MHz, DMSO-D$_6$)**: 11.92 (s, 1H), 7.51-7.49 (m, 2H), 7.42-7.36 (m, 4H), 7.31-7.23 (m, 3H), 7.18-7.16 (m, 1H), 2.62-2.55 (m, 1H), 1.79-1.62 (m, 4H), 0.86-0.82 (m, 6H); **^{13}C (100 MHz, DMSO-D$_6$)**: 151.2, 135.8, 135.2, 131.7, 129.5, 129.4, 128.5, 128.0, 127.8, 127.0, 126.9, 126.0, 125.6, 42.2, 26.6, 12.0; **ESI-MS (*m/z*)**: 289.1707 (100) $[M-H]^+$, 290.1738 (25) $[M]^+$.



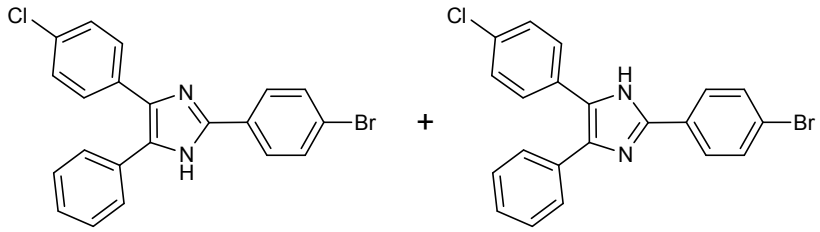
5-(4-Chlorophenyl)-4,5-diphenyl-1*H*-imidazole (3n, $C_{21}H_{15}ClN_2$, 84%)[10]: white solid. **Mp** 241-243 °C; **υ_{max} (neat, cm^{-1})**: 3038, 2969, 1541, 1485, 1091, 768; **^{1}H NMR (400 MHz, DMSO-D$_6$)**: 12.74-12.71 (s, 1H), 8.09-8.07 (d, *J* = 6.16 Hz, 2H), 7.57-7.25 (m, 12H); **^{13}C (100 MHz, DMSO-D$_6$)**: 145.9, 145.7, 137.7, 135.8, 135.0, 134.0, 132.3, 131.0, 130.8, 130.2, 130.2, 130.0, 129.9, 128.8, 128.7, 128.6, 128.6, 128.4, 128.4, 128.3, 128.1, 127.3, 127.0, 126.8, 125.3, 125.2; **ESI-MS (*m/z*)**: 331.1010 $[M+H]^+$, 332.1042 (25).



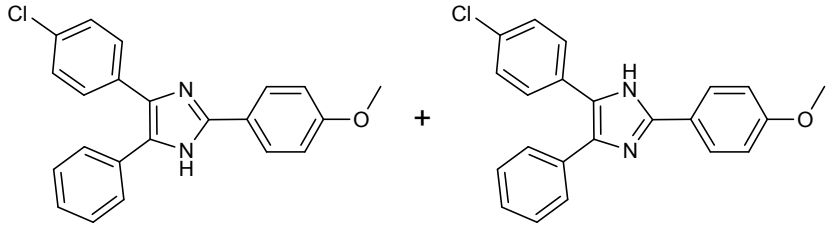
5-(4-Bromophenyl)-4,5-diphenyl-1*H*-imidazole (3o, $C_{21}H_{15}BrN_2$, 78%)[10]: white solid. **Mp** 253-255 °C; **υ_{max} (neat, cm^{-1})**: 3049, 2845, 1596, 1482, 1010, 767; **^{1}H NMR (400 MHz, DMSO-D$_6$)**: 12.77 (s, 1H), 8.10-8.08 (d, *J* = 618 Hz, 2H), 7.62-7.27 (m, 12H); **^{13}C (100 MHz, DMSO-D$_6$)**: 145.9, 145.7, 137.8, 135.8, 135.0, 134.4, 131.6, 131.2, 130.8, 130.2, 128.9, 128.8, 128.7, 128.6, 128.4, 128.1, 127.3, 127.0, 126.8, 125.3, 120.8, 119.5; **ESI-MS (*m/z*)**: 373.0344 (100) $[M-H]^+$, 374.0378 (24), 375.0326 (100) $[M+H]^+$.



2,5-Bis-(4-chlorophenyl)-4-phenyl-1*H*-imidazole (3p, $C_{21}H_{14}Cl_2N_2$, 76%)[10]: white solid. **Mp** 250-252 °C; **υ_{max} (neat, cm^{-1})**: 3060, 2835, 1599, 1500, 1478, 1445, 1087, 830; **^{1}H NMR (400 MHz, DMSO-D_6)**: 12.81 (s, 1H), 8.11-8.09 (d, *J* = 8.24 Hz, 2H), 7.55-7.41 (m, 11H); **^{13}C (100 MHz, DMSO-D_6)**: 144.6, 132.8, 129.0, 128.7, 128.6, 128.4, 126.9; **ESI-MS (*m/z*)**: 363.0455 (100) $[M-H]^+$, 364.0493 (24) $[M]^+$, 365.0426 (67) $[M+H]^+$.

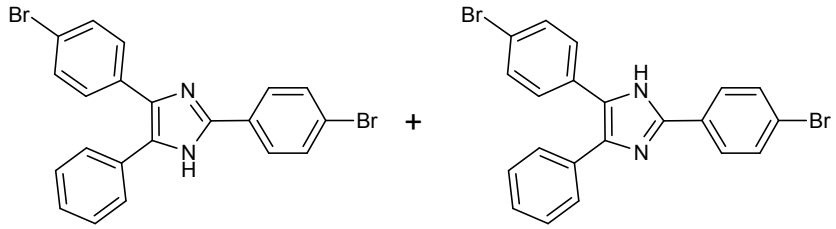


2-(4-Bromophenyl)-5-(4-chlorophenyl)-4-phenyl-1*H*-imidazole (3q, $C_{21}H_{14}BrClN_2$, 72%)[10]: white solid. **Mp** 251-253 °C; **υ_{max} (neat, cm^{-1})**: 3067, 2829, 1480, 1446, 1091, 830, 729; **^{1}H NMR (400 MHz, DMSO-D_6)**: 12.82 (s, 1H), 8.03-8.01 (m, 2H), 7.69-7.67 (m, 2H), 7.52-7.41 (m, 9H); **^{13}C (100 MHz, DMSO-D_6)**: 144.7, 131.8, 129.4, 129.0, 128.6, 128.2, 127.2, 125..4, 121.6; **ESI-MS (*m/z*)**: 406.9953 (80) $[M-H]^+$, 408.9936 (100) $[M]^+$, 409.9964 (32) $[M+H]^+$.

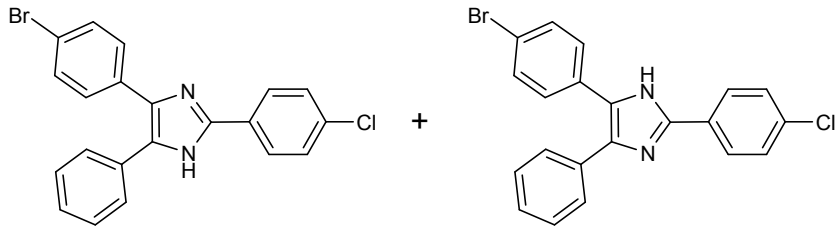


5-(4-Chlorophenyl)-2-(4-methoxyphenyl)-4-phenyl-1*H*-imidazole (3r, $C_{22}H_{17}ClN_2O$, 66%): pale yellow solid. **Mp** 253-255 °C; **υ_{max} (neat, cm^{-1})**: 3067, 2829, 1480, 1446, 1091, 830, 729; **^{1}H NMR (400 MHz, DMSO-D_6)**: 12.55 (s, 1H), 8.02-8.00 (m, 2H), 7.52-7.38 (m, 9H), 7.05-7.03 (m, 2H), 3.82 (s,

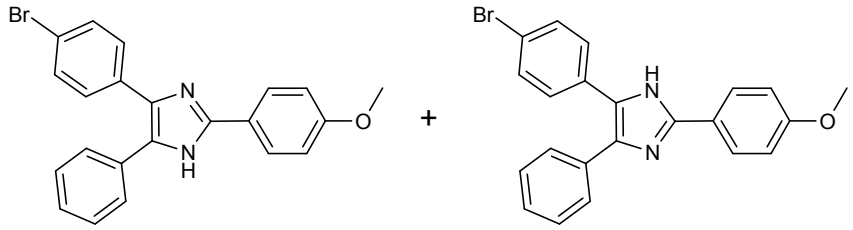
3H); **^{13}C (100 MHz, DMSO-D$_6$)**:; **ESI-MS (*m/z*)**: 159.5, 145.8, 128.4, 126.7, 123.0, 114.1, 55.2; calcd for $C_{22}H_{17}ClN_2O$ 360.1029, found 361.1116 $[M+H]^+$.



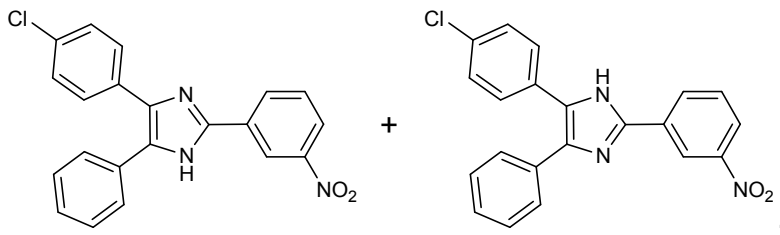
2,5-Bis-(4-bromophenyl)-4-phenyl-1*H*-imidazole (3s, $C_{21}H_{14}Br_2N_2$, 81%): white solid. **Mp** 252-255 °C; **υ_{max} (neat, cm^{-1})**: 3060, 2826, 1598, 1479, 1067, 826, 730; **^{1}H NMR (400 MHz, DMSO-D$_6$)**: 12.84 (s, 1H), 8.04-8.02 (d, *J* = 8.20 Hz, 2H), 7.70-7.68 (d, *J* = 8.20 Hz, 2H), 7.53-7.42 (m, 9H); **^{13}C (100 MHz, DMSO-D$_6$)**: 144.7, 131.7, 131.3, 129.4, 128.6, 127.1, 121.5; **ESI-MS (*m/z*)**: calcd for $C_{21}H_{14}Br_2N_2$ 451.9524, found 450.9443 $[M-H]^+$.



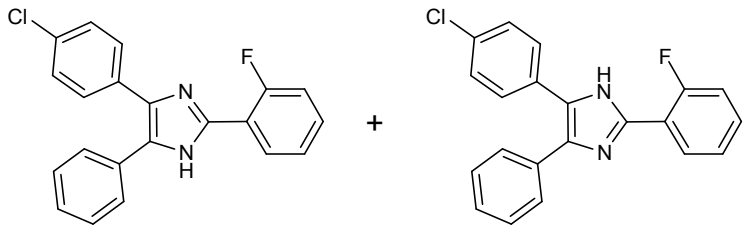
2-(4-Chlorophenyl)-5-(4-bromophenyl)-4-phenyl-1*H*-imidazole (3t, $C_{21}H_{14}BrClN_2$, 75%): white solid. **Mp** 249-251 °C; **υ_{max} (neat, cm^{-1})**: 3059, 2826, 1476, 1080, 823, 732; **^{1}H NMR (400 MHz, DMSO-D$_6$)**: 12.84 (s, 1H), 8.12-8.10 (d, *J* = 7.72 Hz, 2H), 7.56-7.50 (m, 11H); **^{13}C (100 MHz, DMSO-D$_6$)**: 144.8, 144.7, 137.9, 136.0, 134.8, 134.2, 132.9, 131.6, 131.1, 130.6, 130.2, 130.0, 129.0, 128.9, 1288, 128.5, 128.3, 128.1, 127.3, 126.9, 120.9, 119.6; **ESI-MS (*m/z*)**: calcd for $C_{21}H_{14}BrClN_2$ 408.0029, found 406.9941 $[M-H]^+$.



5-(4-Bromophenyl)-2-(4-methoxyphenyl)-4-phenyl-1*H*-imidazole (3u, $C_{22}H_{17}BrN_2O$, 68%): pale yellow solid. **Mp** 251-253 °C; **υ_{max} (neat, cm^{-1})**: 2960, 2832, 1607, 1481, 1246, 1173; **^{1}H NMR (400 MHz, DMSO-D_6)**: 12.56 (s, 1H), 8.03-8.01 (m, 2H), 7.53-7.38 (m, 9H), 7.06-7.04 (m, 2H), 3.83 (s, 3H); **^{13}C (100 MHz, DMSO-D_6)**: 159.5, 145.9, 131.2, 128.5, 128.4, 126.8, 123.0, 114.1, 55.2; **ESI-MS (*m/z*)**: calcd for $C_{22}H_{17}BrN_2O$ 404.0524, found 403.0441 $[M-H]^+$.

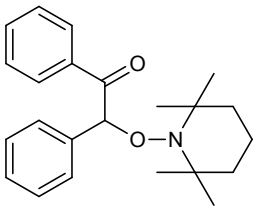


4-(4-Chlorophenyl)-2-(3-nitrophenyl)-5-phenyl-1*H*-imidazole (3v, $C_{21}H_{14}ClN_3O_2$, 85%): yellow solid. **Mp** 247-249 °C; **υ_{max} (neat, cm^{-1})**: 3070, 2858, 1518, 1476, 1345; **^{1}H NMR (400 MHz, DMSO-D_6)**: 13.11 (s, 1H), 8.94 (s, 1H), 8.51-8.49 (d, *J* = 7.76 Hz, 1H), 8.21-8.19 (d, *J* = 8.08 Hz, 1H), 778.-7.74 (t, *J* = 8.00 Hz, 1H), 7.57-7.53 (t, *J* = 8.08 Hz, 4H), 7.43 (m, 5H); **^{13}C (100 MHz, DMSO-D_6)**: 148.3, 143.6, 131.7, 131.2, 130.3, 128.6, 128.4, 122.6, 119.4; **ESI-MS (*m/z*)**: calcd for $C_{21}H_{14}ClN_3O_2$ 375.0775, found 374.0701 $[M-H]^+$.



4-(4-Chlorophenyl)-2-(2-fluorophenyl)-5-phenyl-1*H*-imidazole (3w, $C_{21}H_{14}ClFN_2$, 53%): white solid. **Mp** 248-250 °C; **υ_{max} (neat, cm^{-1})**: 2963, 2728, 1500, 1483, 1223, 1090; **^{1}H NMR (400 MHz, DMSO-D_6)**: 12.61-12.60 (s, 1H), 8.02-7.99 (t, *J* = 7.48 Hz, 1H), 7.57-7.44 (m, 7H), 7.42-7.24 (m,

5H); **^{13}C (100 MHz, DMSO-D$_6$)**: 160.1, 157.6, 141.1, 141.0, 137.8, 135.9, 134.7, 133.8, 132.3, 131.1, 130.6, 130.5, 130.4, 130.2, 129.6, 129.6, 129.0, 128.7, 128.6, 128.3, 128.2, 128.1, 127.3, 126.8, 124.7, 124.7, 118.6, 118.4, 116.3, 116.1; **ESI-MS (*m/z*)**: calcd for $C_{21}H_{14}ClFN_2$ 348.0830, found 347.0760 $[M-H]^+$.



1,2-diphenyl-2-((2,2,6,6-tetramethylpiperidin-1-yl)oxy)ethanone (6a, C$_{23}$H$_{29}$NO$_2$, 46%)[11]: white solid. **Mp** 229-231 °C; **υ_{max} (neat, cm^{-1})**: 3068, 2922, 2852, 1667, 1596, 1446, 1262, 1042; **^{1}H NMR (400 MHz, DMSO-D$_6$)**: 8.01-7.99 (m, 2H), 7.43-7.39 (m, 3H), 7.34-7.30 (m, 2H), 7.22-7.18 (m, 2H), 7.14-7.10 (m, 1H), 5.92 (s, 1H), 1.38-1.37 (m, 6H), 1.24-1.11 (m, 6H), 0.92 (m, 3H), 0.73 (m, 3H); **^{13}C (100 MHz, DMSO-D$_6$)**: 198.3, 137.8, 135.3, 132.9, 129.3, 128.3, 127.5, 127.2, 93.5, 60.0, 59.8, 40.3, 33.6, 33.3, 20.3, 20.2, 17.0; **ESI-MS (*m/z*)**: 352.2287 (100) $[M+H]^+$, 353.232. (27) [M+2H].

III. References

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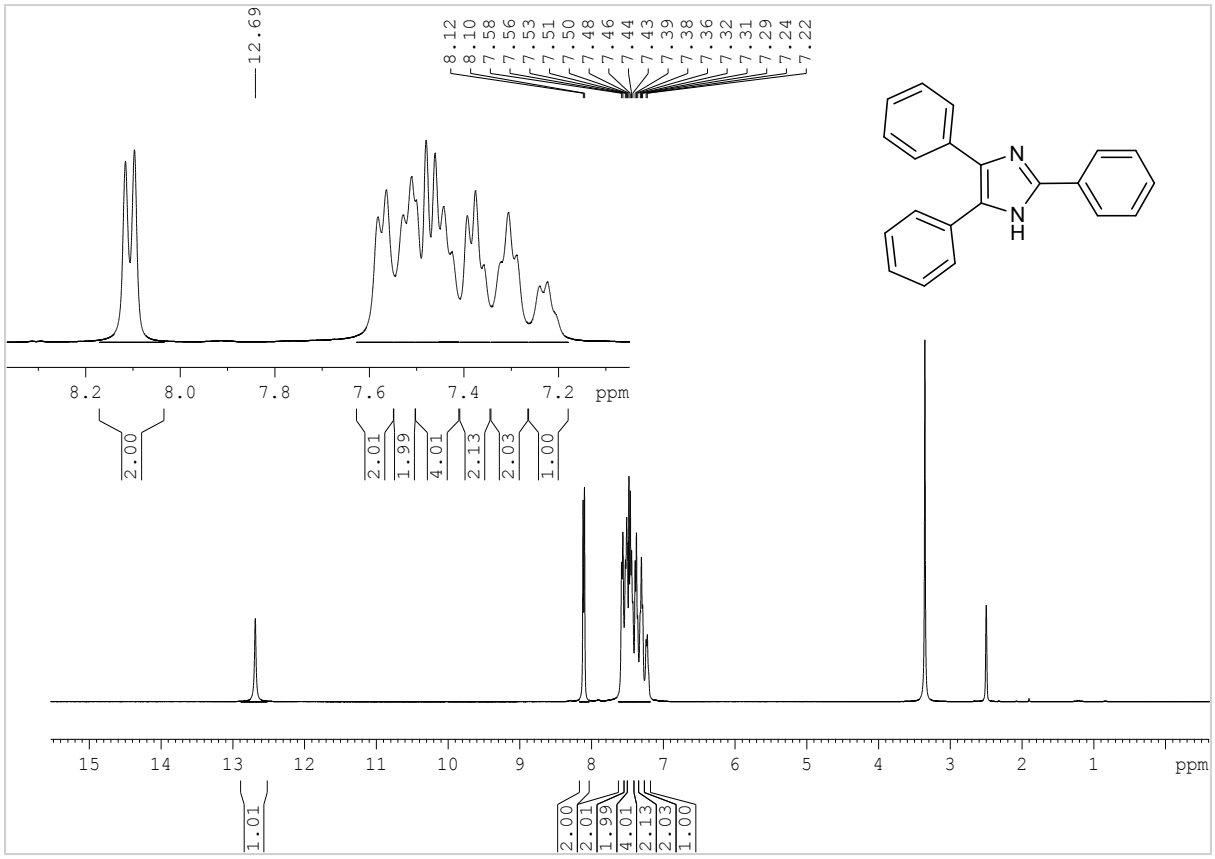
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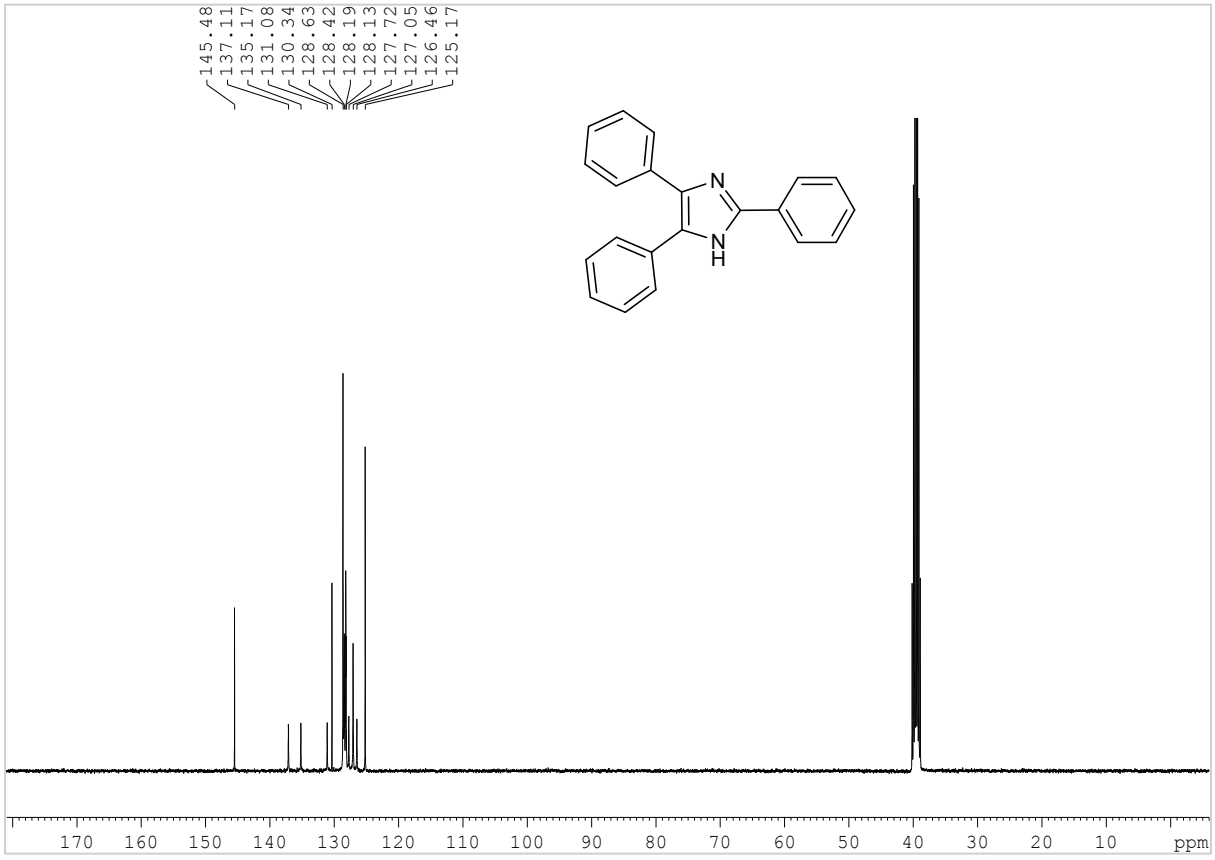
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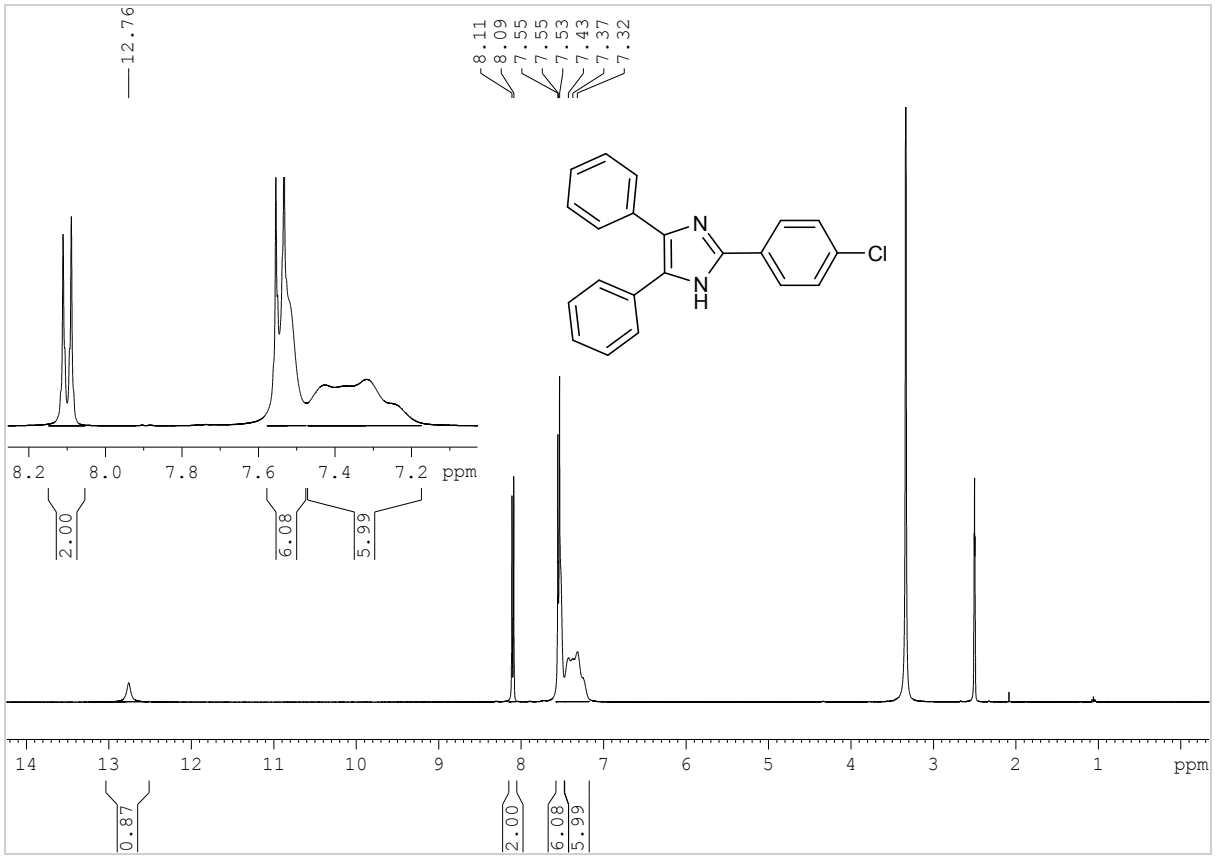
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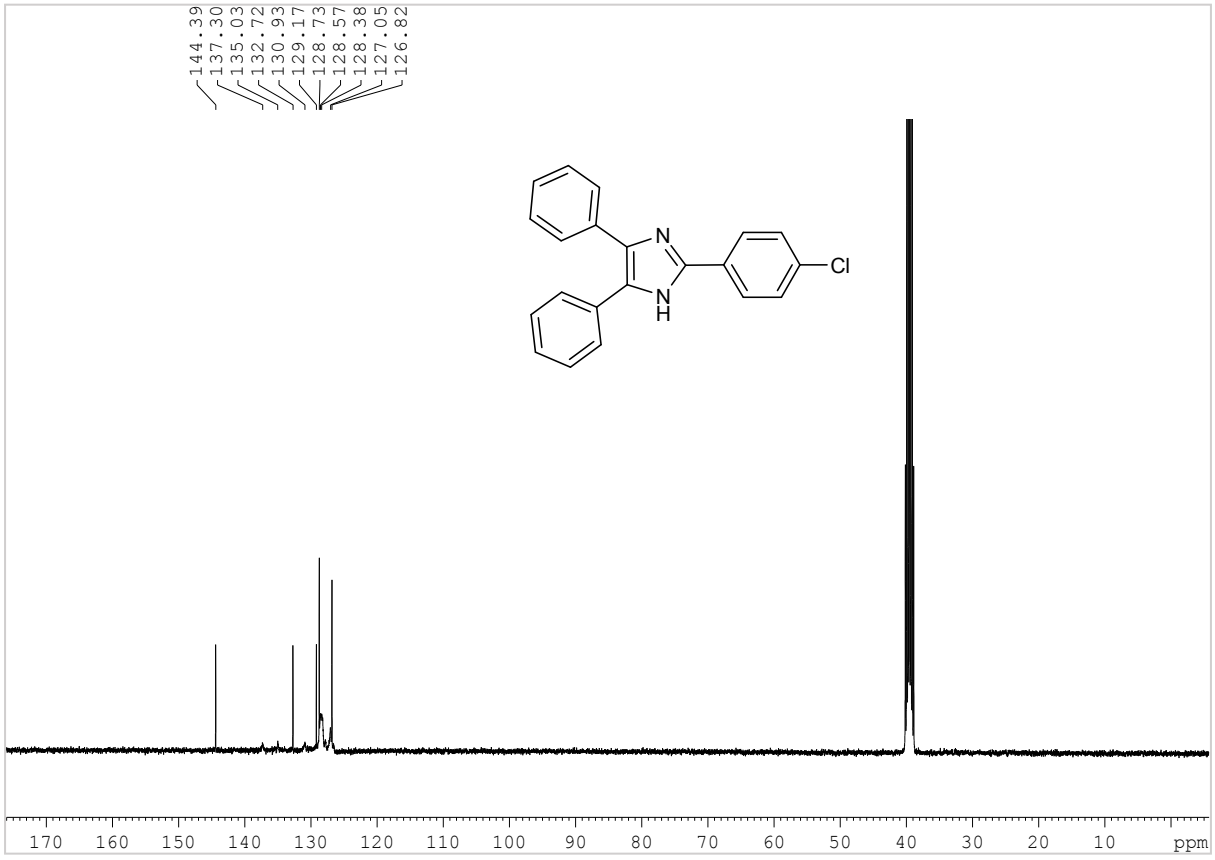
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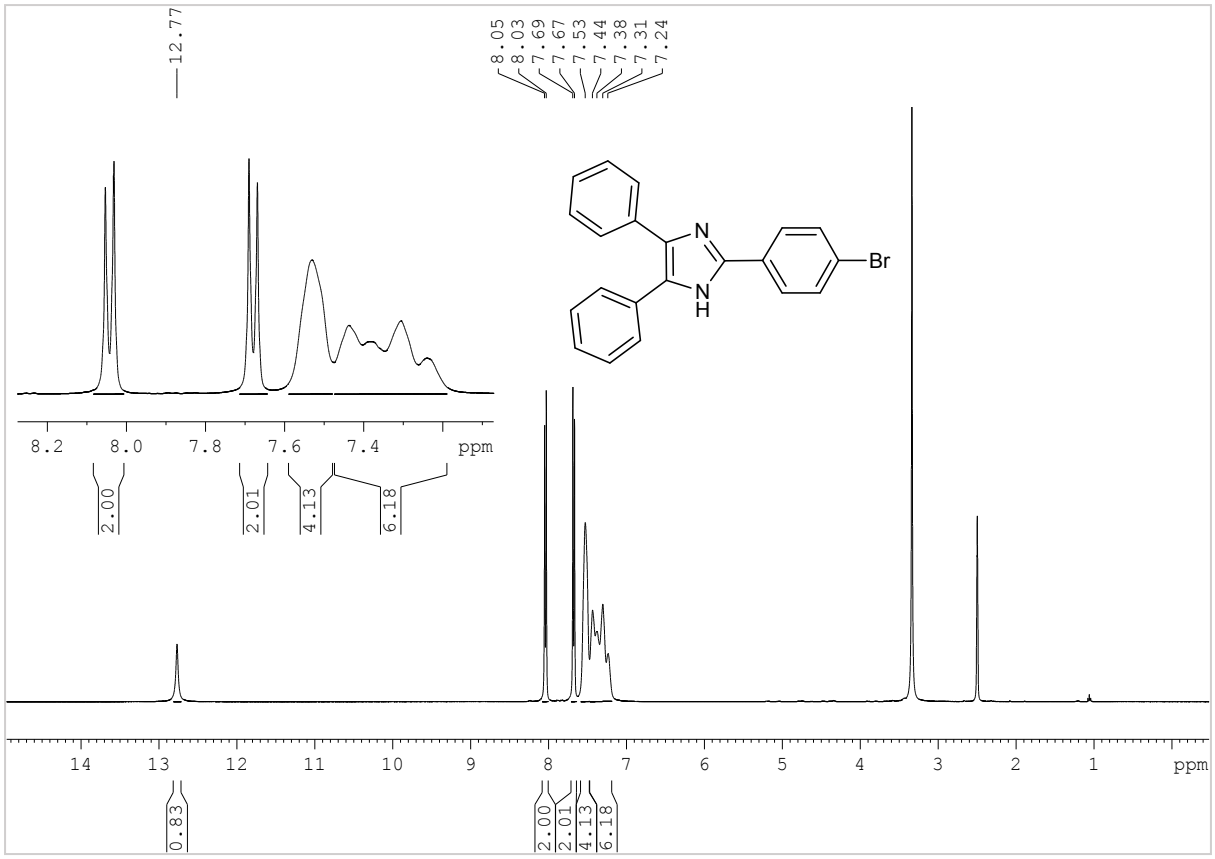
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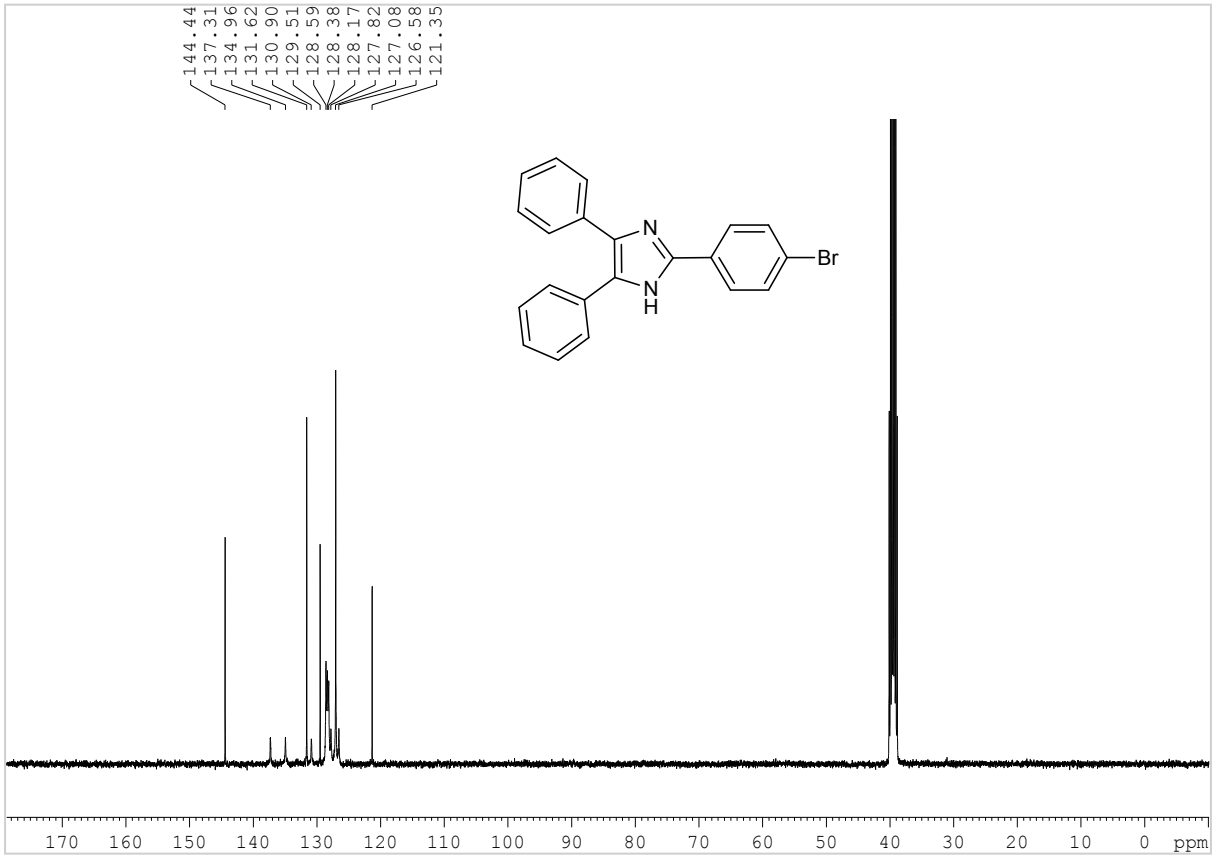
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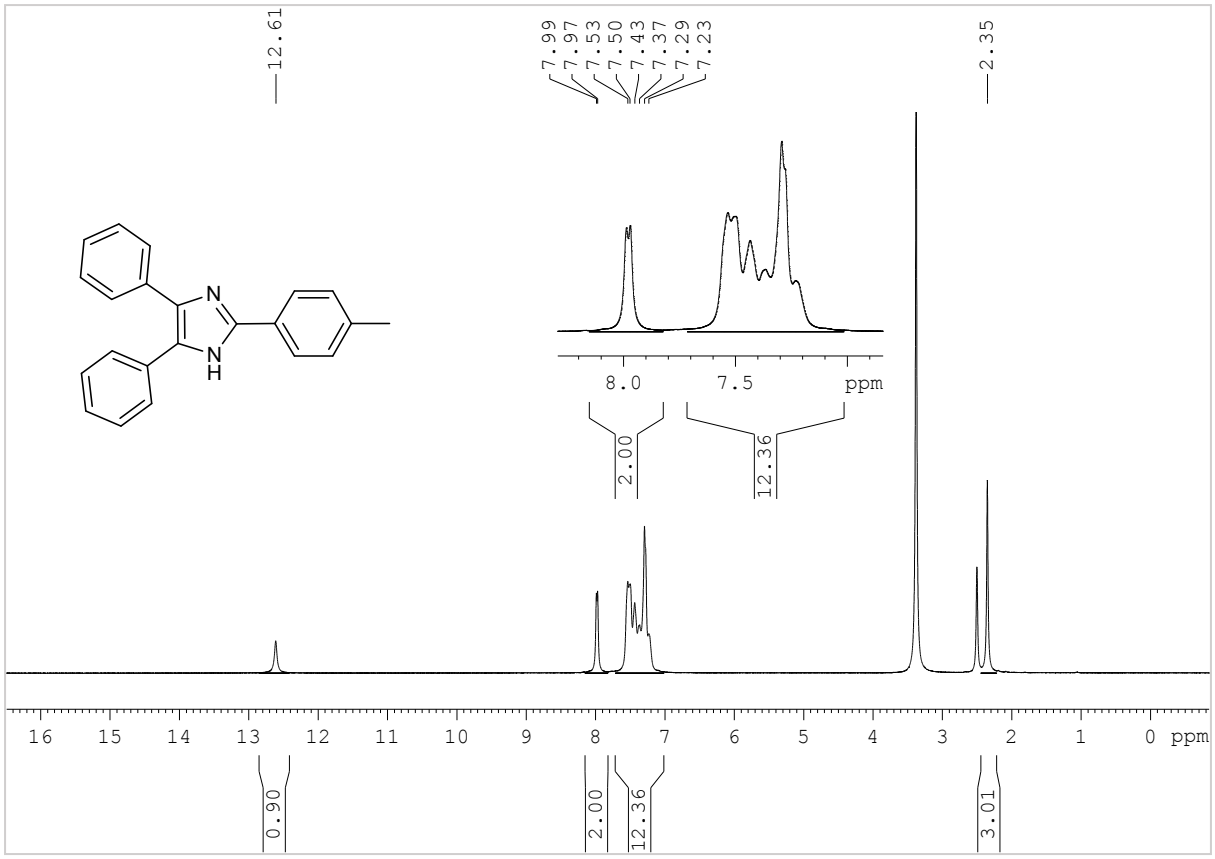
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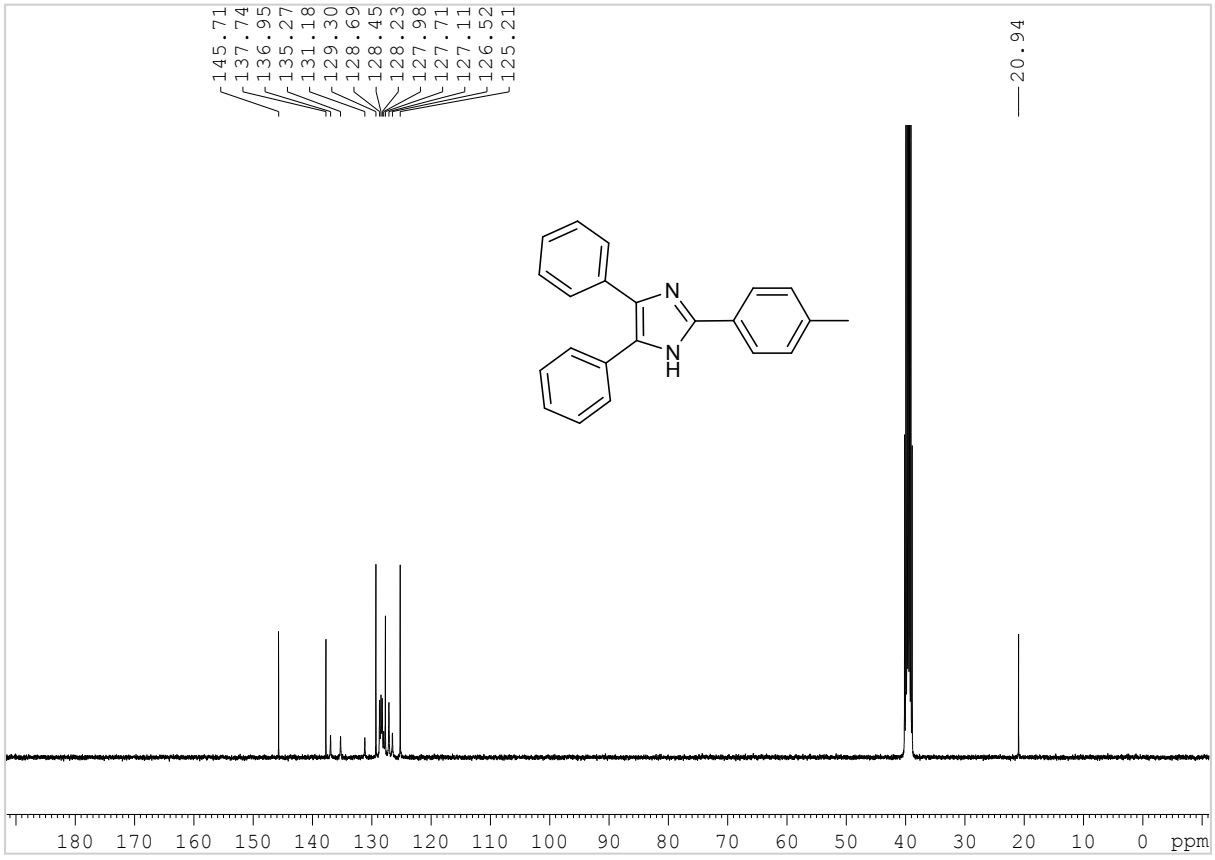
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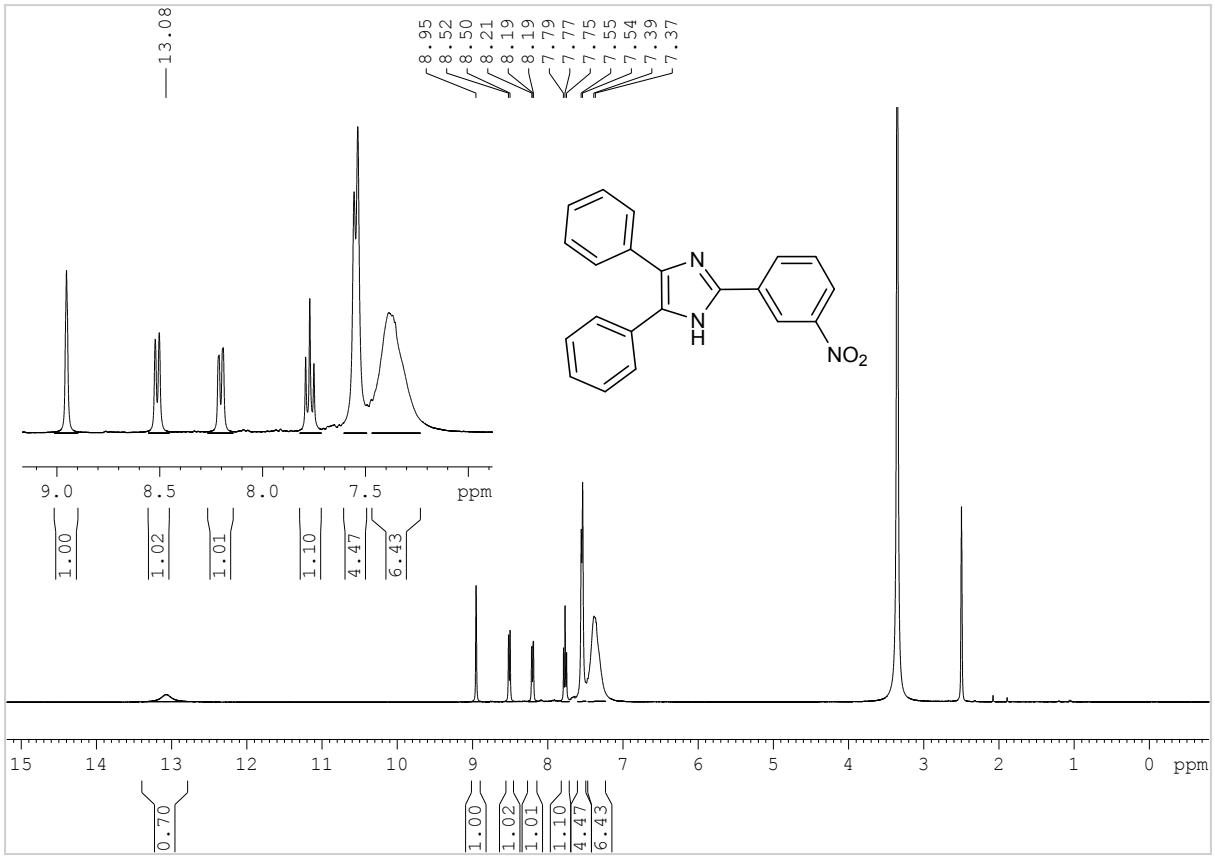
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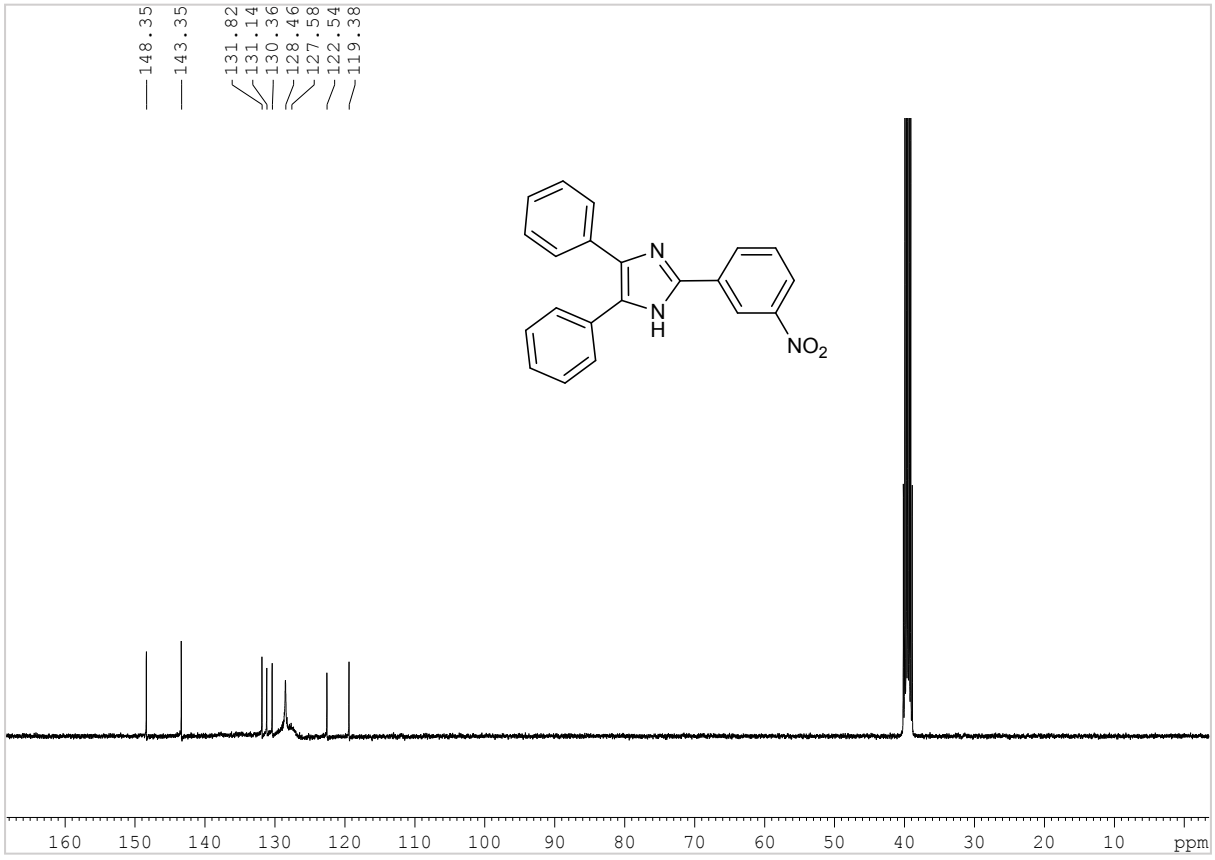
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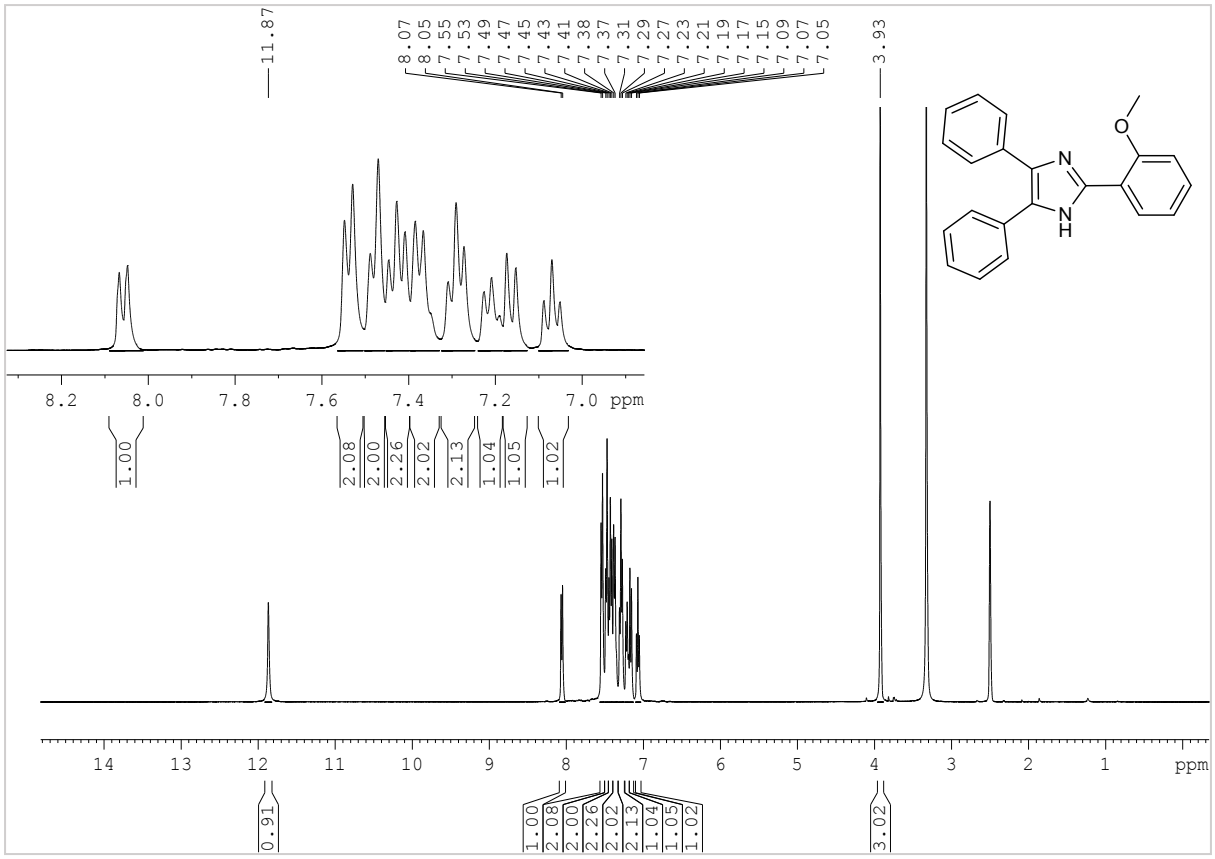
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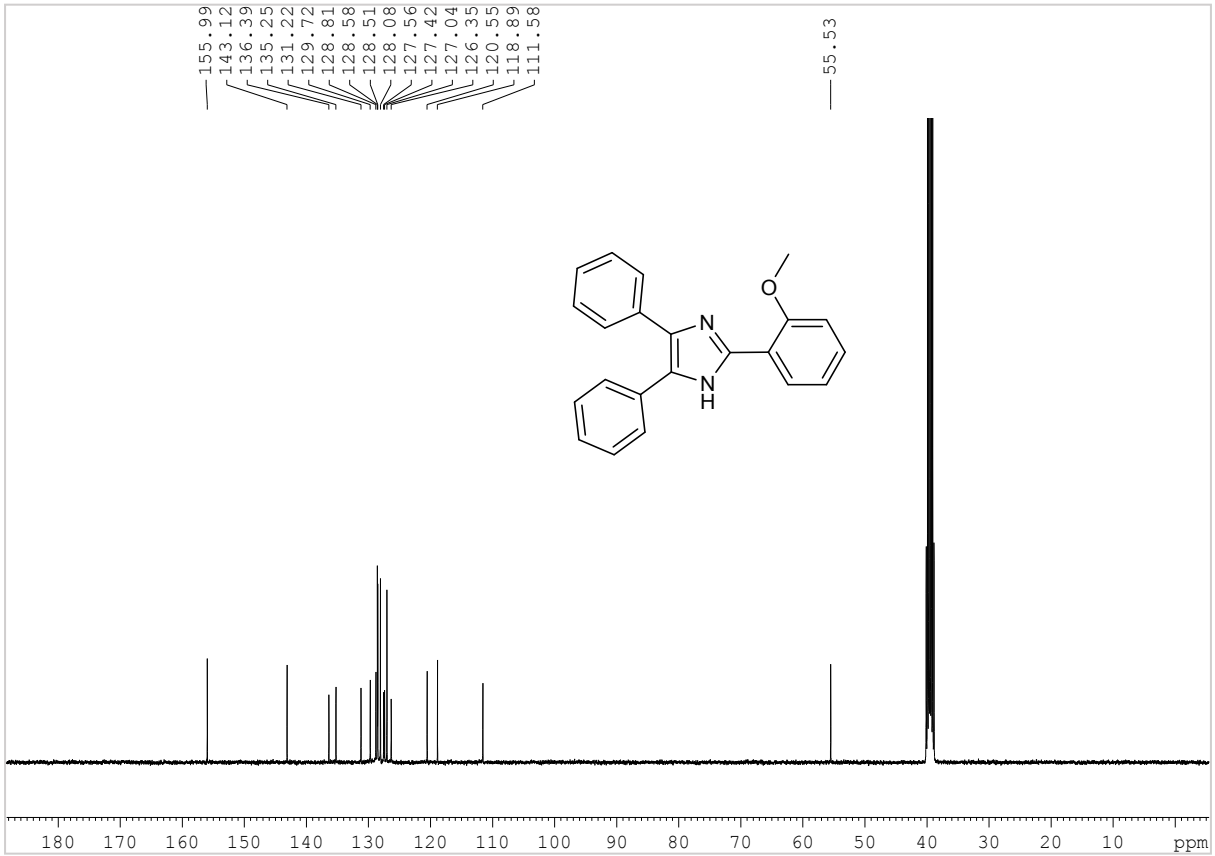
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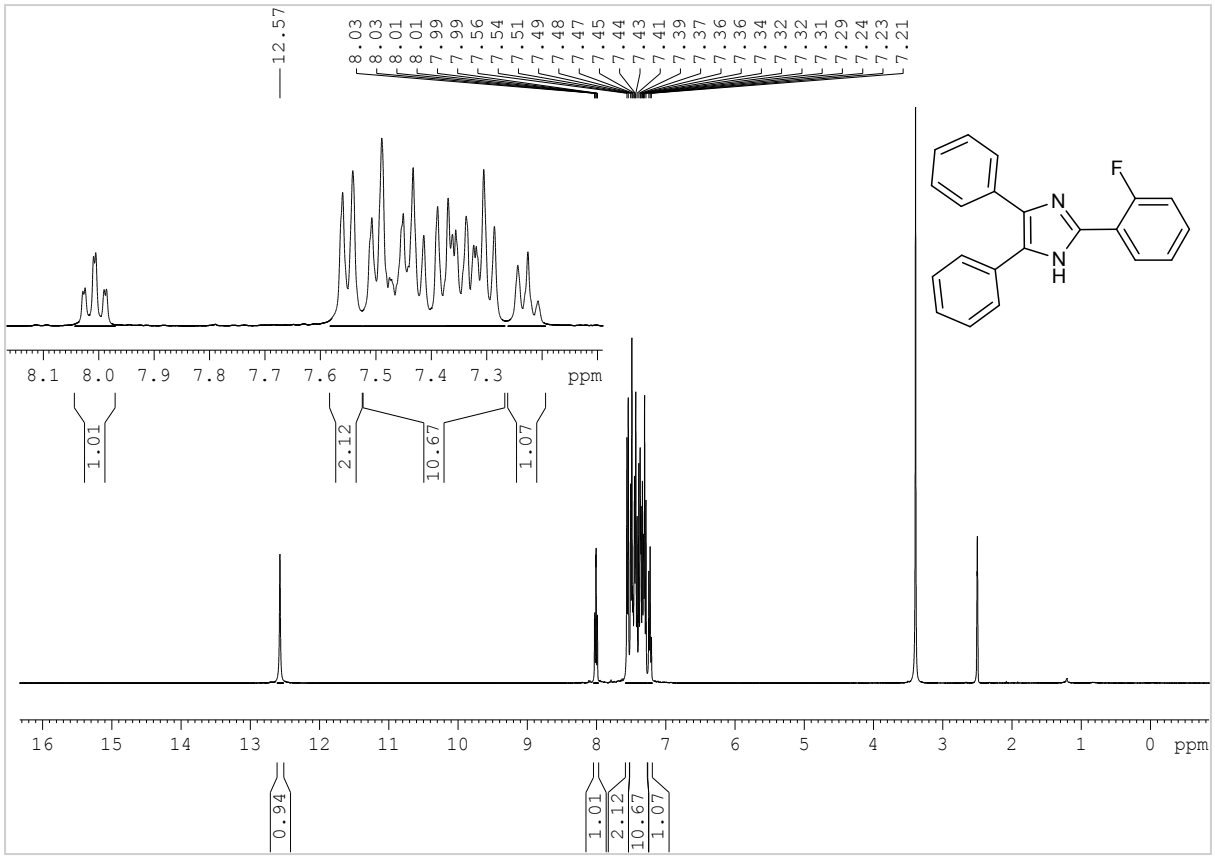
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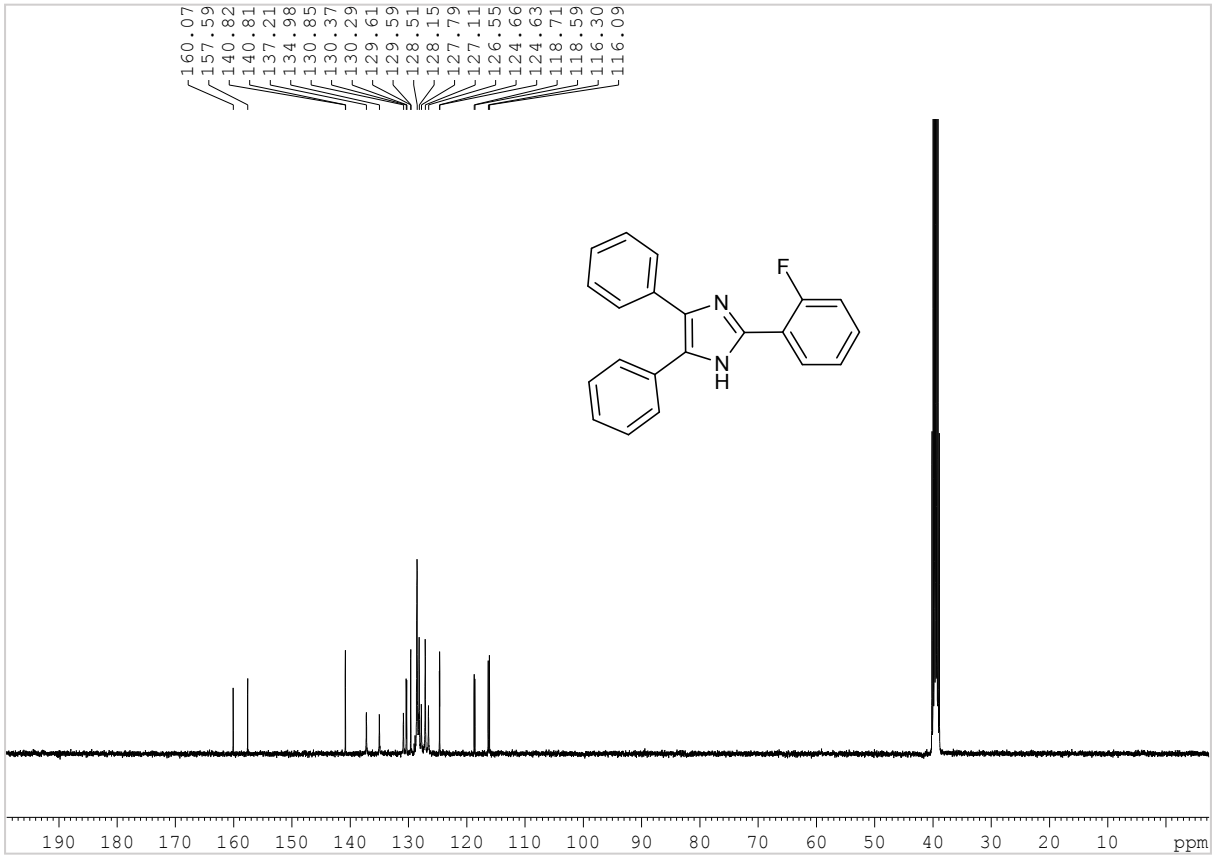
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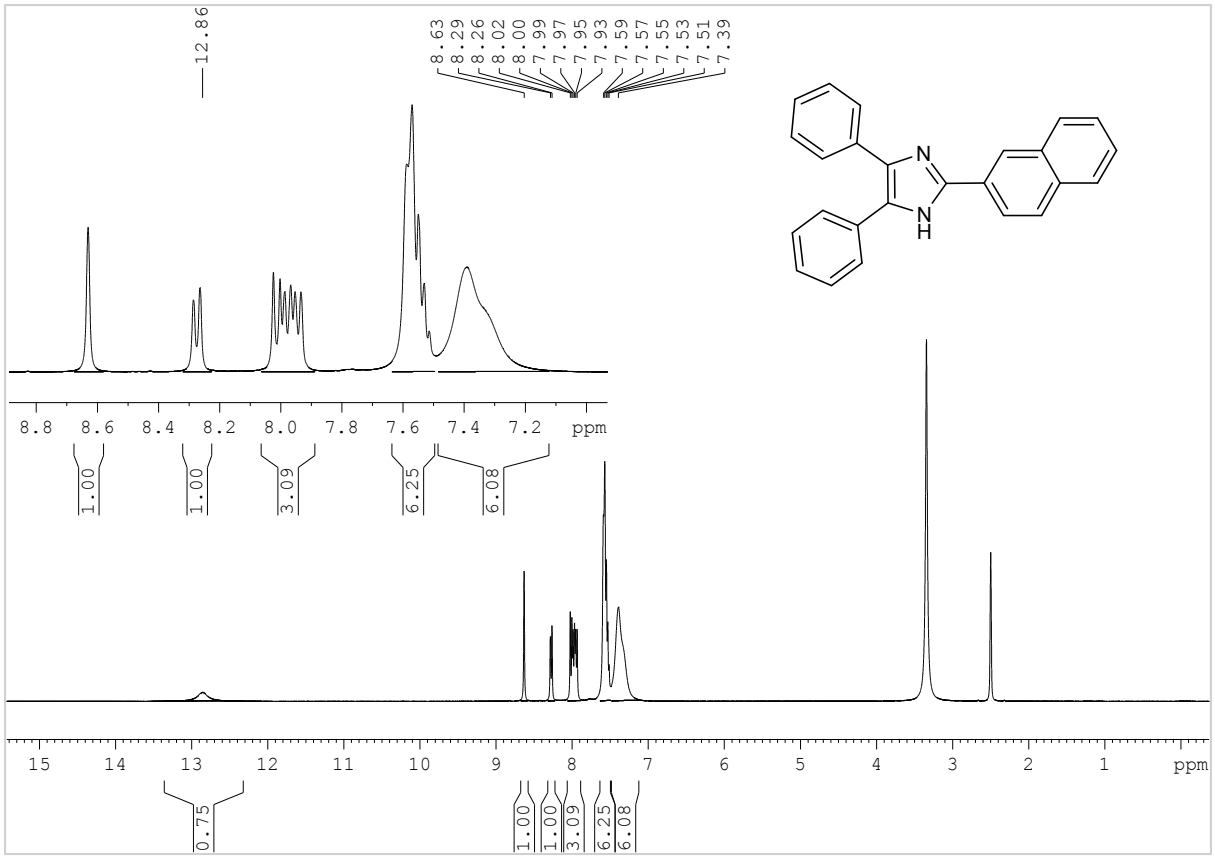
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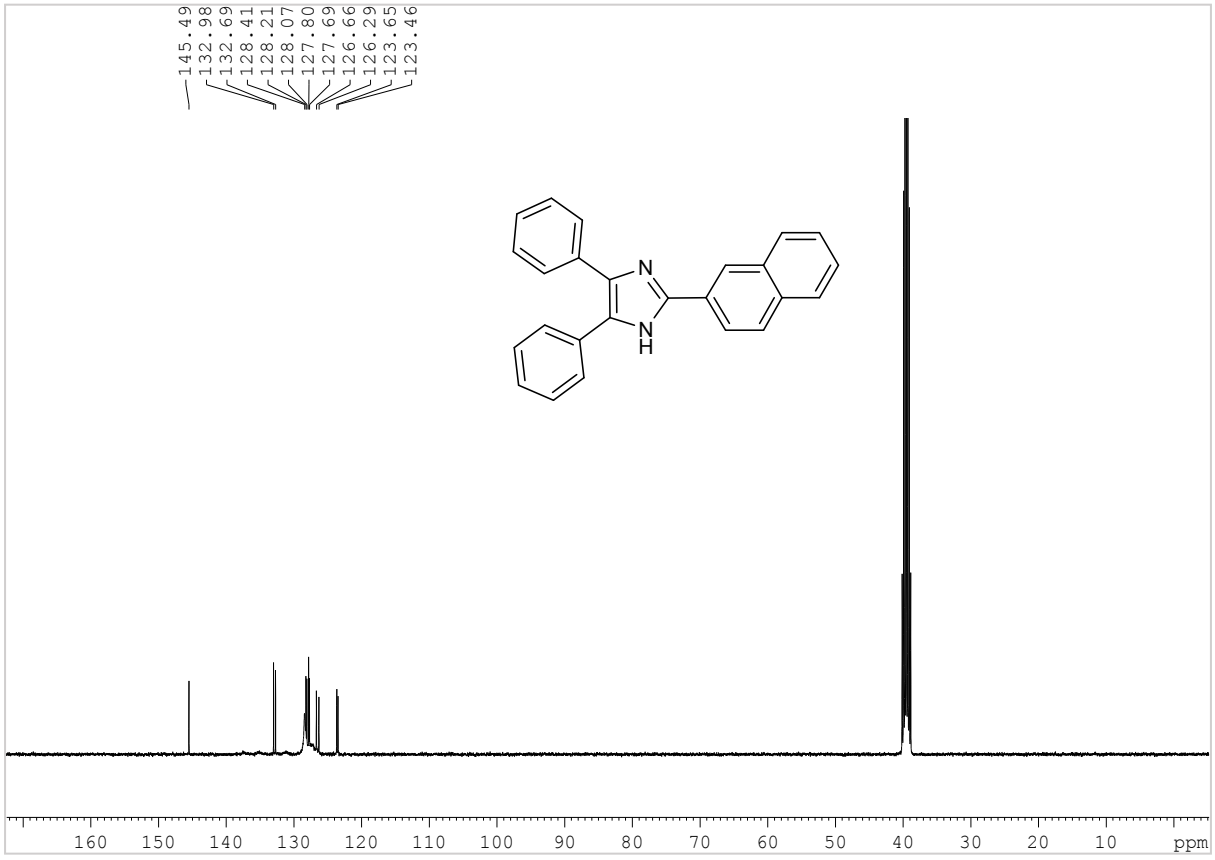
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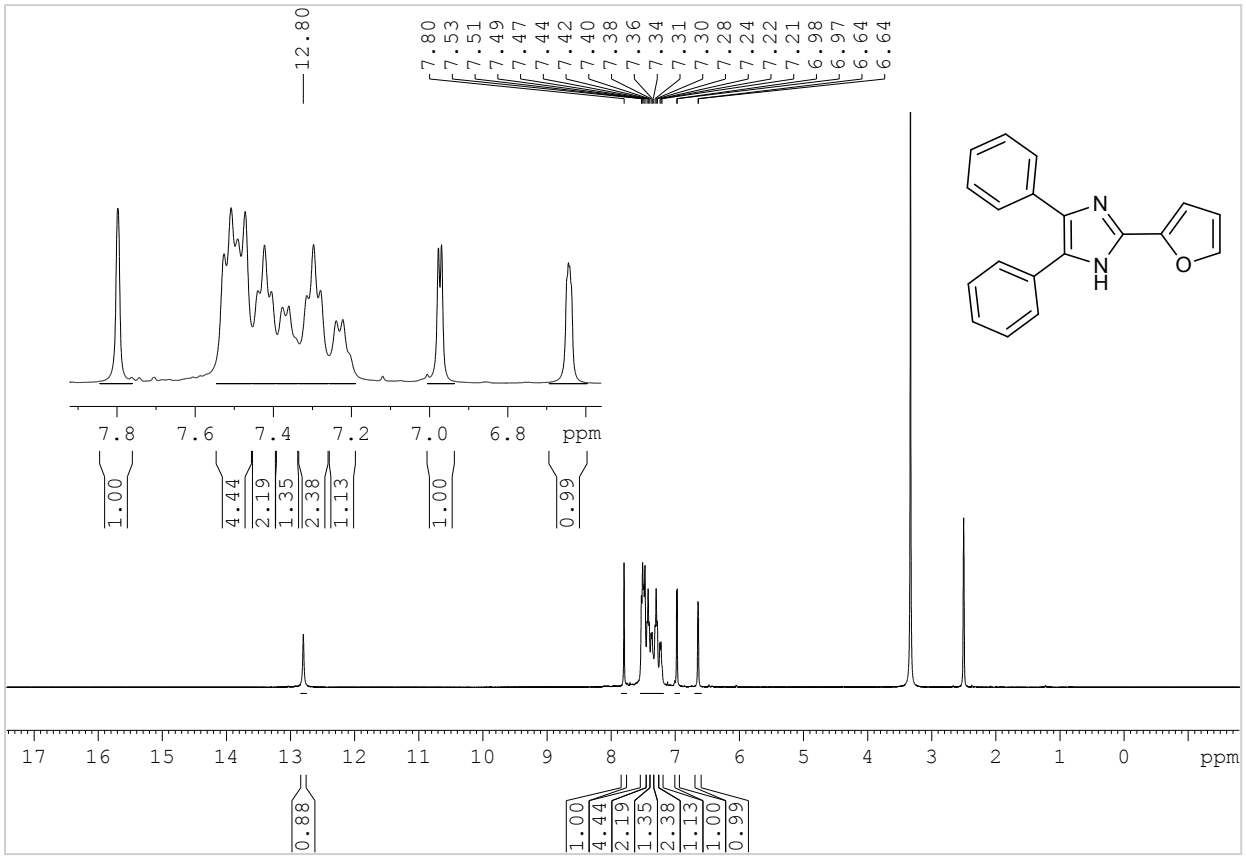
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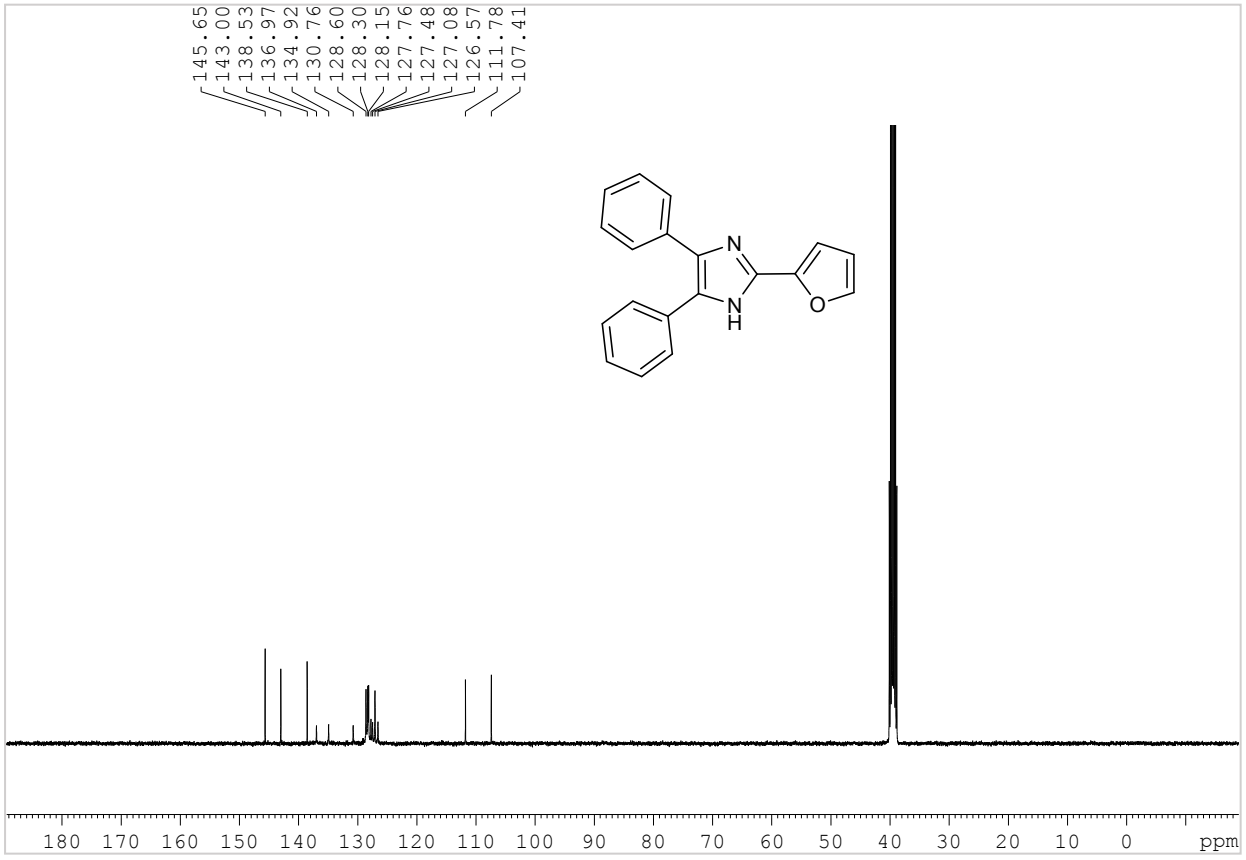
1.35
2.38
1.13
1.00
0.99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143.00
138.53
136.97
134.92
130.76
128.60
128.30
128.15
127.76
127.48
127.08
126.57
111.78
107.41
N
N
H
O
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


11.90
7.48
7.46
7.39
7.37
7.35
7.31
7.29
7.27
7.25
7.23
7.18
7.16
7.14
1.98
1.95
1.81
1.78
1.70
1.67
1.64
1.63
1.61
1.60
1.58
1.57
1.55
1.54
1.40
1.37
1.34
1.31
1.29
1.26
1.23
1.20
2.73
2.72
2.71
2.70
2.69
2.68
2.67
2.66
7.4
7.2 ppm
2.7 ppm
2.0
1.8
1.6
1.4
1.2 ppm
2.00
4.03
3.14
1.14
0.95
1.96
2.15
1.30
2.34
3.49
N
N
H
14
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm
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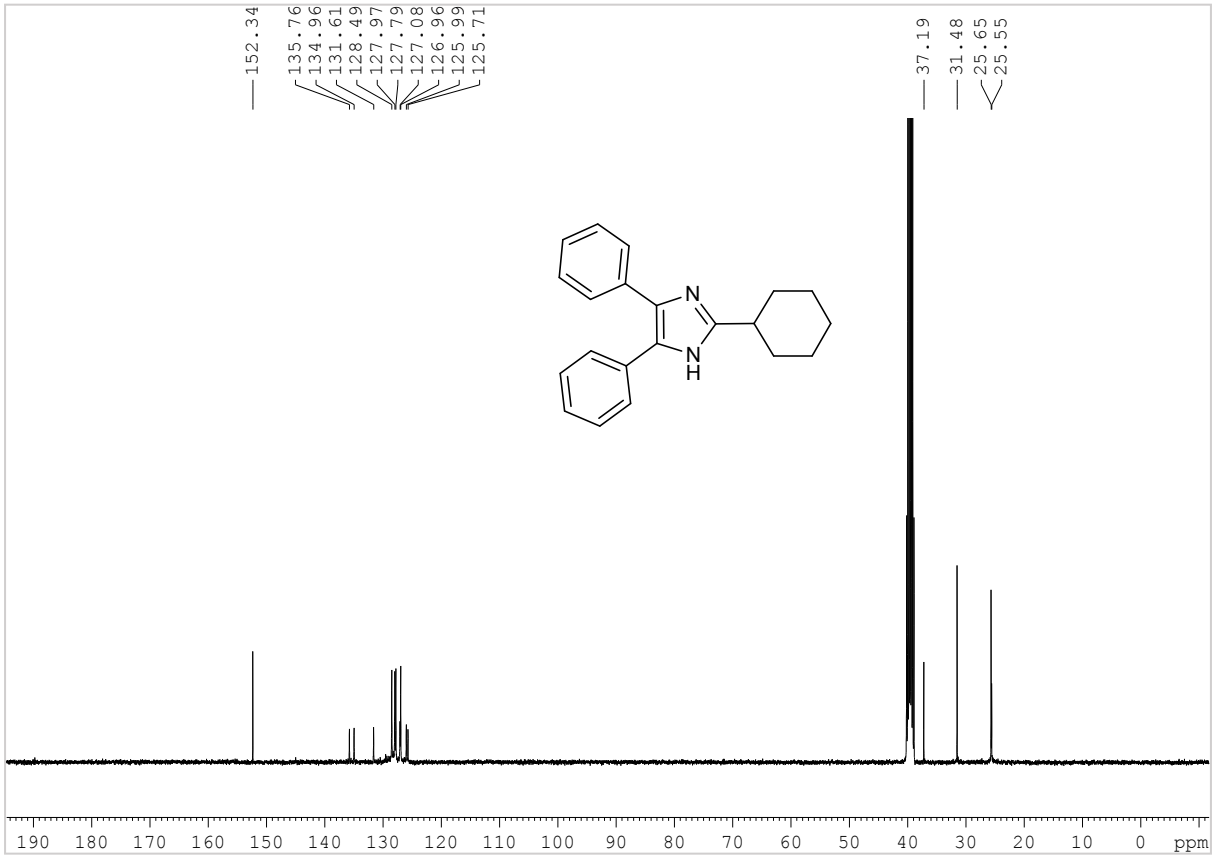
0.95
1.96
2.15
1.30
2.34
3.49


152.34
135.76
134.96
131.61
128.49
127.97
127.79
127.08
126.96
125.99
125.71
37.19
31.48
25.65
25.55
N
N
H
190
180
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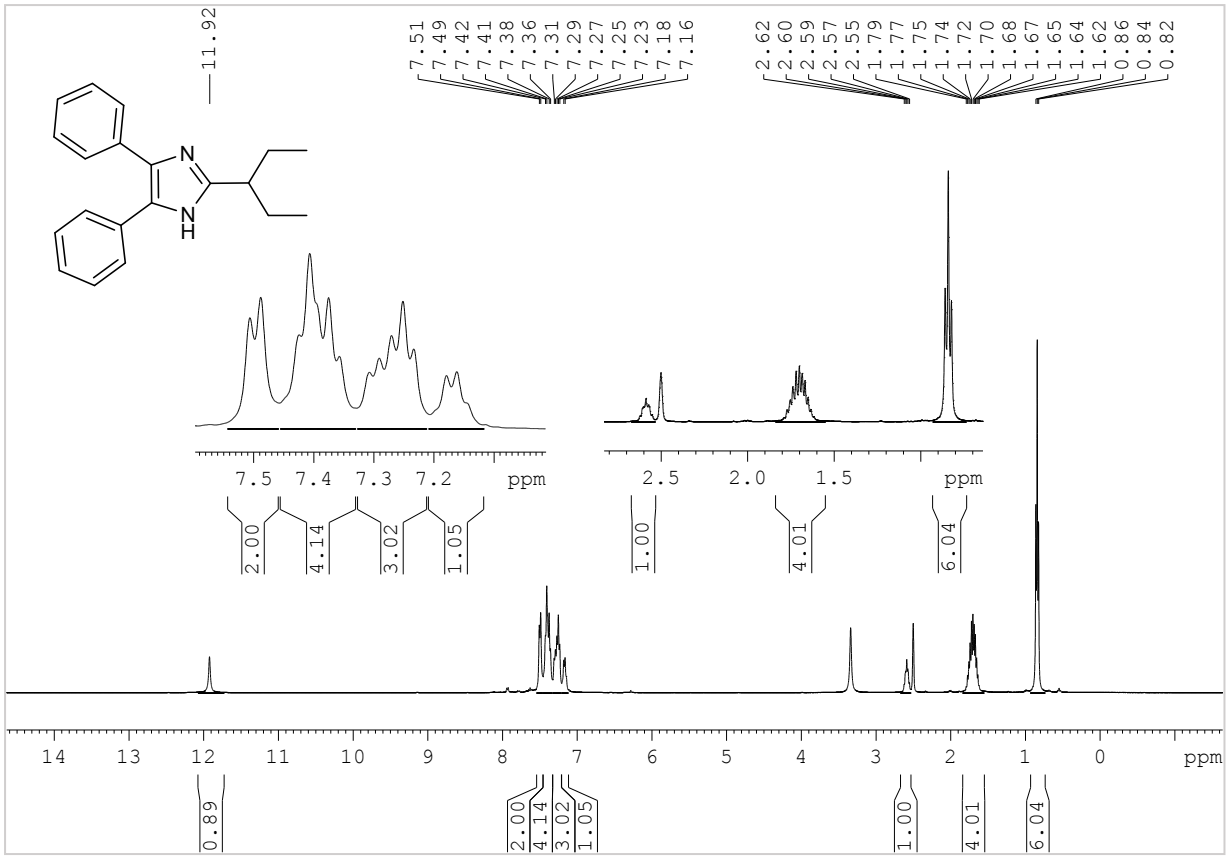
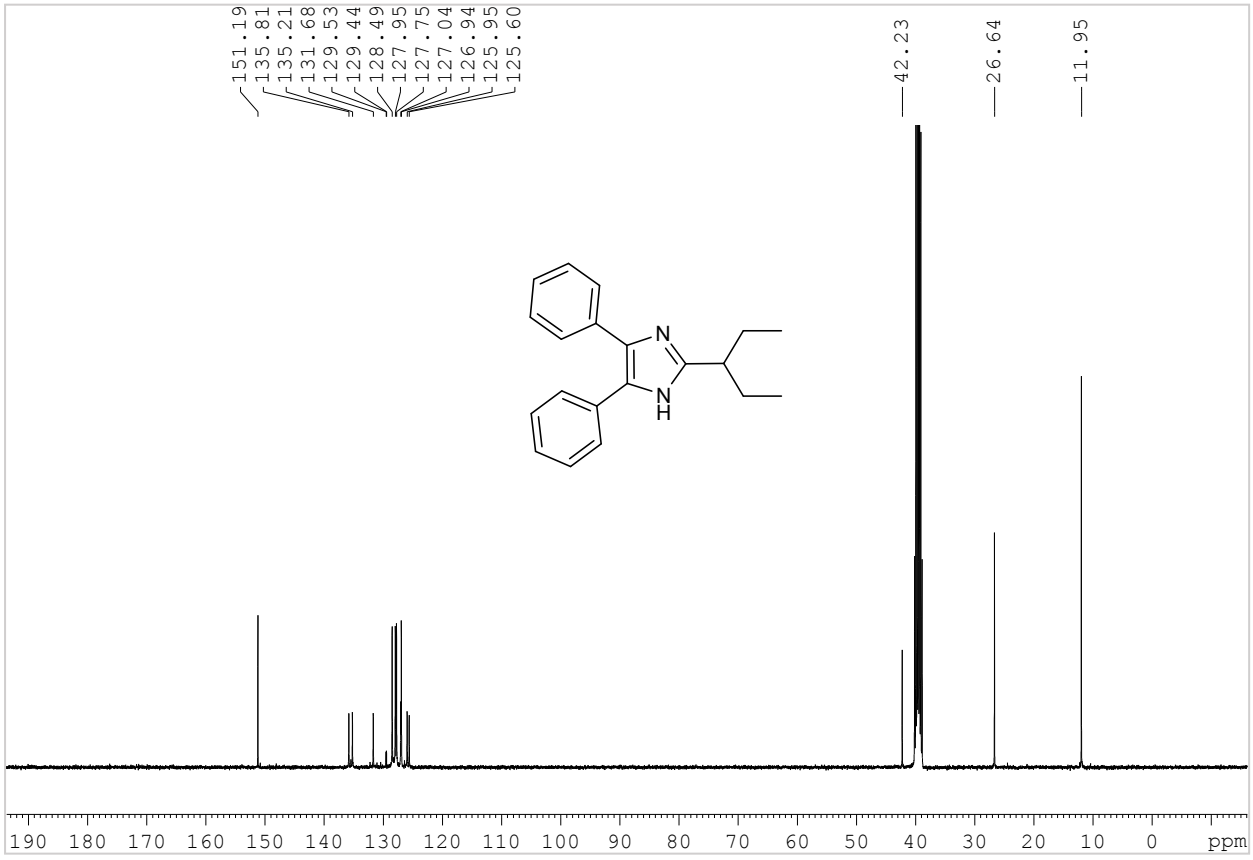
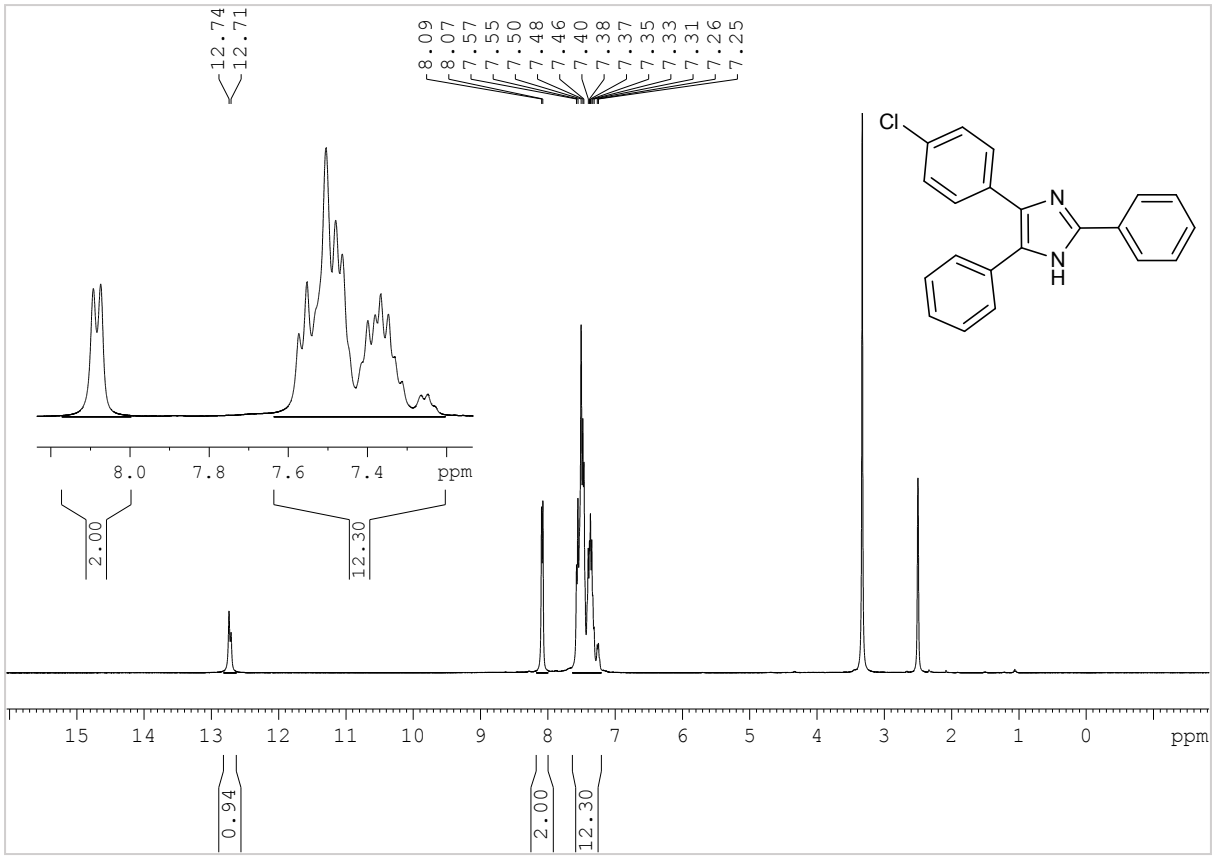
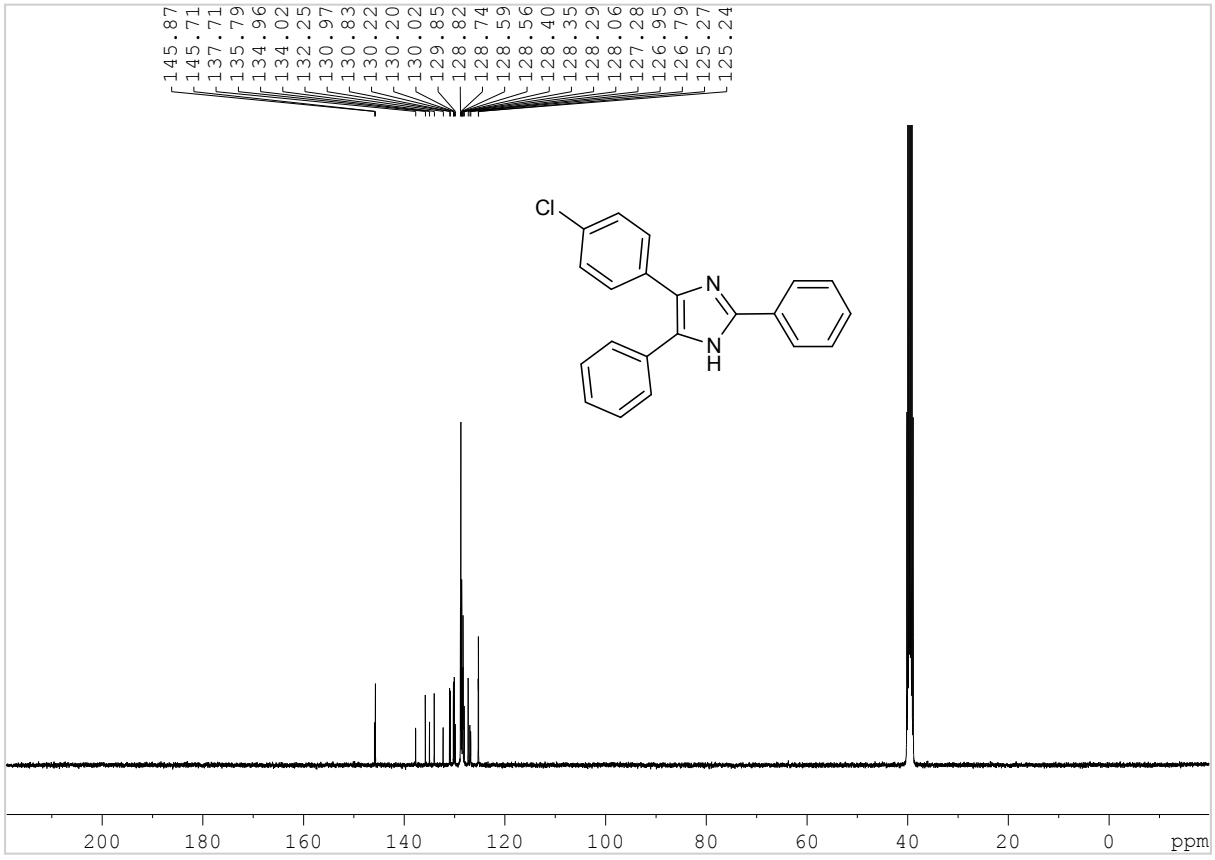
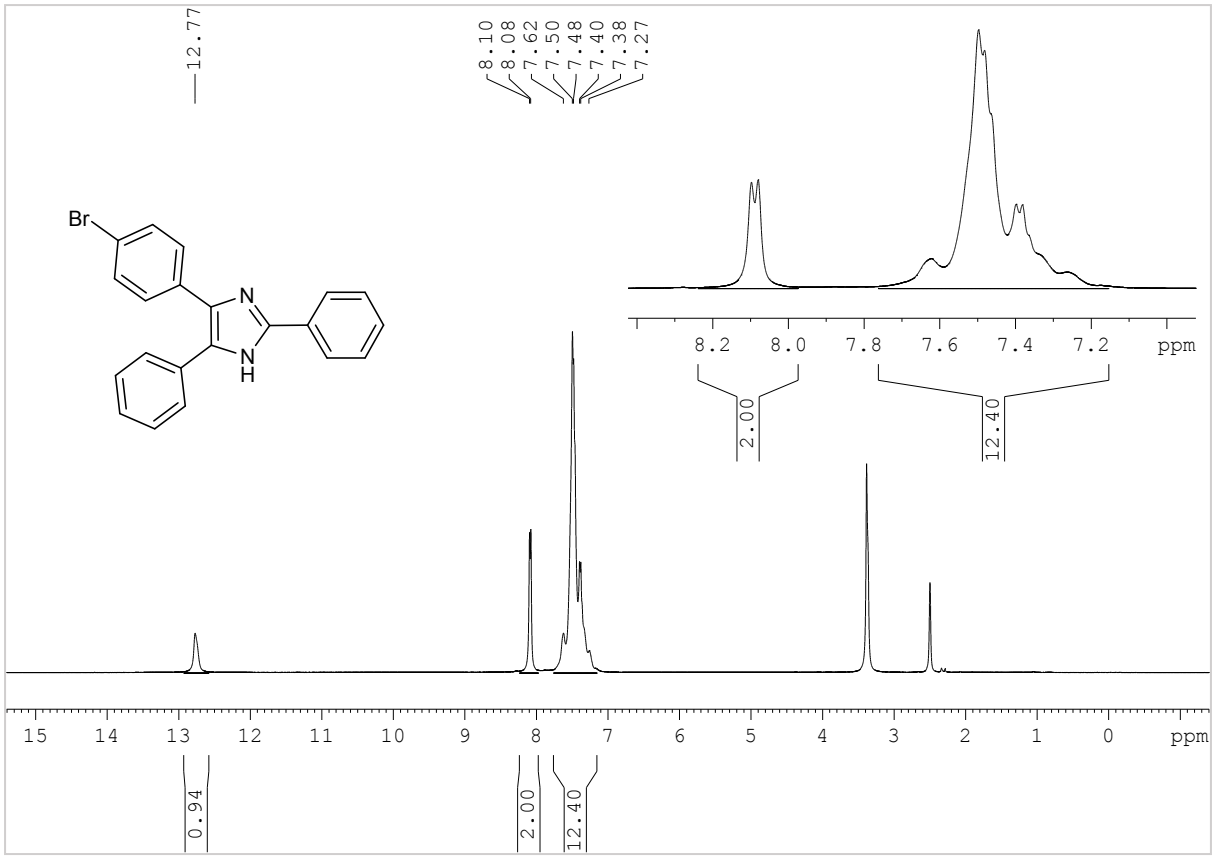
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

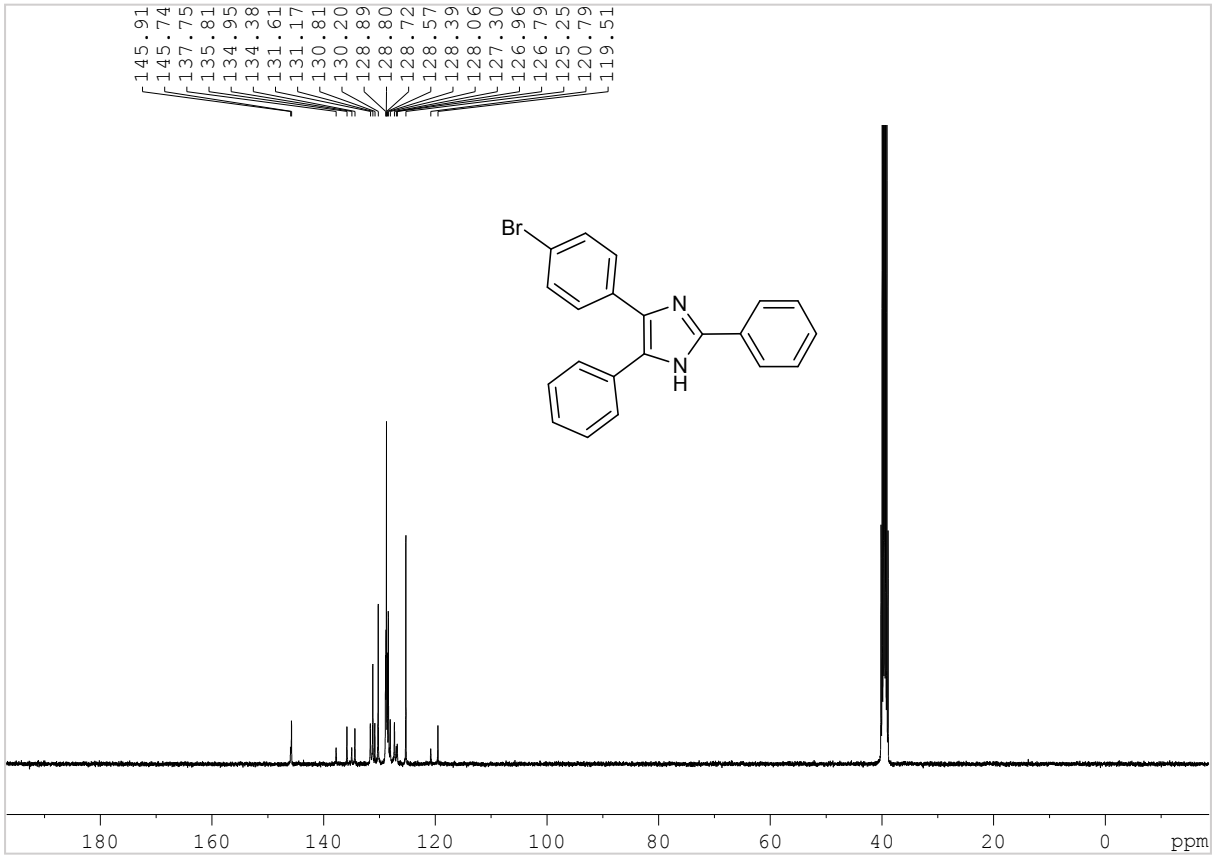

11.92
7.51
7.49
7.42
7.41
7.38
7.36
7.31
7.29
7.27
7.25
7.23
7.18
7.16
2.62
2.60
2.59
2.57
2.55
1.79
1.77
1.75
1.74
1.72
1.70
1.68
1.67
1.65
1.64
1.62
0.86
0.84
0.82
N
N
H
7.5 7.4 7.3 7.2 ppm
2.5 2.0 1.5 ppm
2.00
4.14
3.02
1.05
1.00
4.01
6.04
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.89
2.00
4.14
3.02
1.05
1.00
4.01
6.04


151.19
135.81
135.21
131.68
129.53
129.44
128.49
127.95
127.75
127.04
126.94
125.95
125.60
42.23
26.64
11.95
N
N
H
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


12.74
12.71
8.09
8.07
7.57
7.55
7.50
7.48
7.46
7.40
7.38
7.37
7.35
7.33
7.31
7.26
7.25
Cl
N
N
H
8.0
7.8
7.6
7.4
ppm
2.00
12.30
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.94
2.00
12.30


145.87
145.71
137.71
135.79
134.96
134.02
132.25
130.97
130.83
130.22
130.20
130.02
129.85
128.82
128.74
128.59
128.56
128.40
128.35
128.29
128.06
127.28
126.95
126.79
125.27
125.24
Cl
N
N
H
200
180
160
140
120
100
80
60
40
20
0
ppm


12.77
8.10
8.08
7.62
7.50
7.48
7.40
7.38
7.27
Br
N
N
H
8.2
8.0
7.8
7.6
7.4
7.2
ppm
2.00
12.40
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.94
2.00
12.40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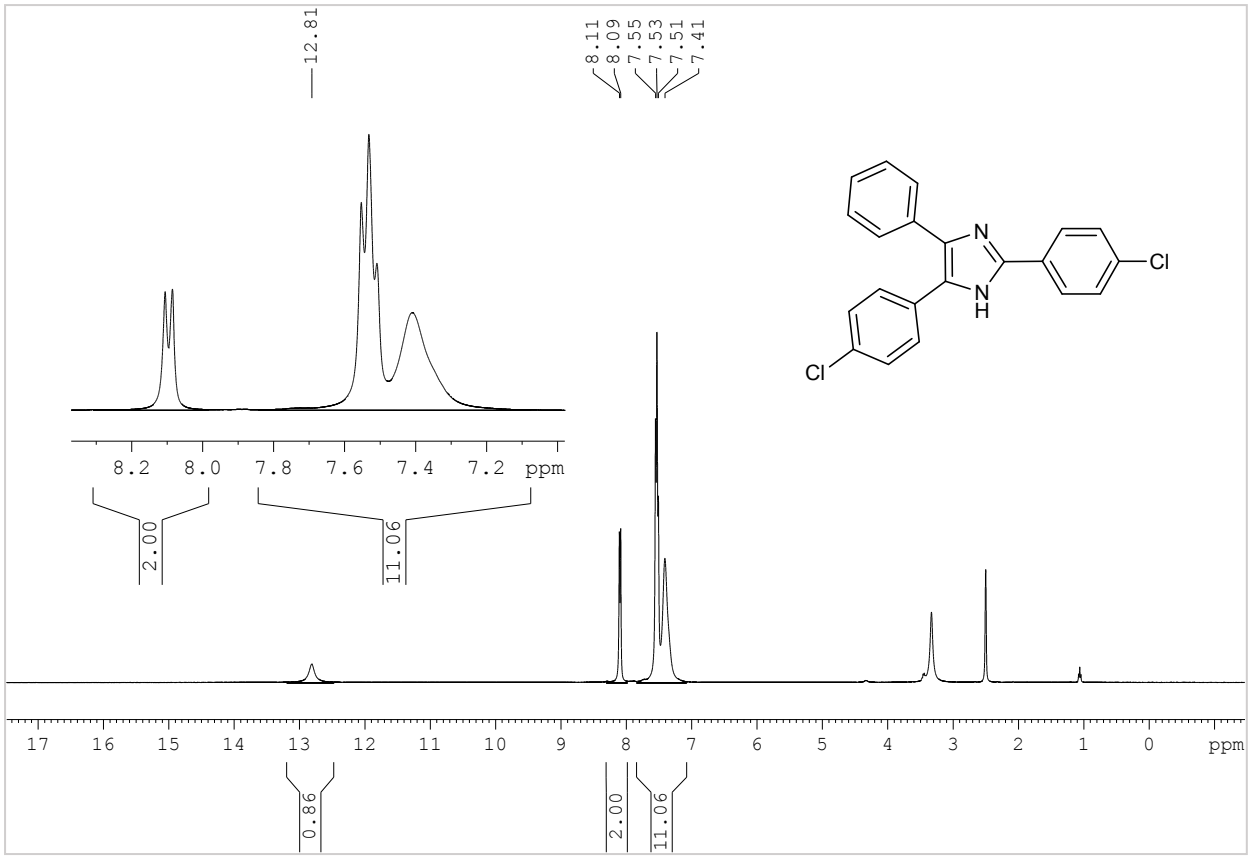
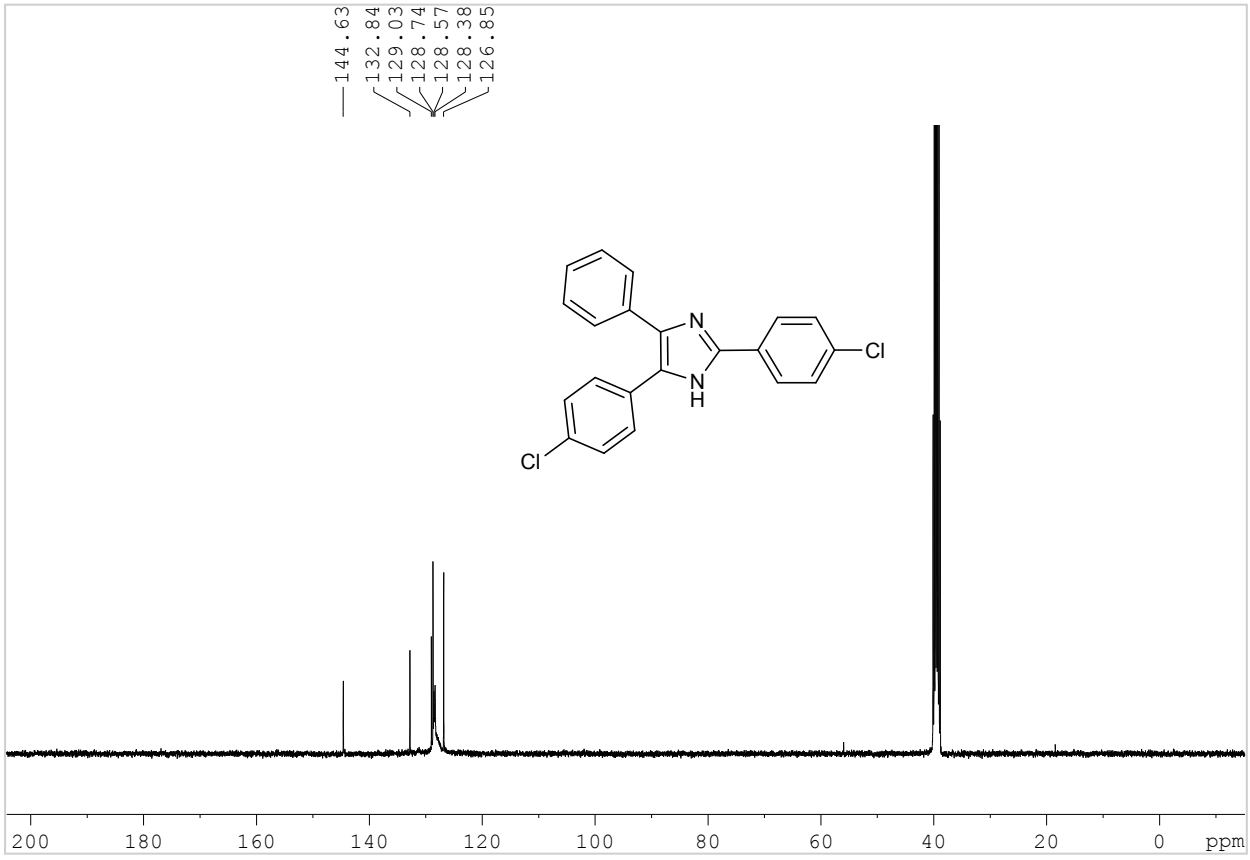
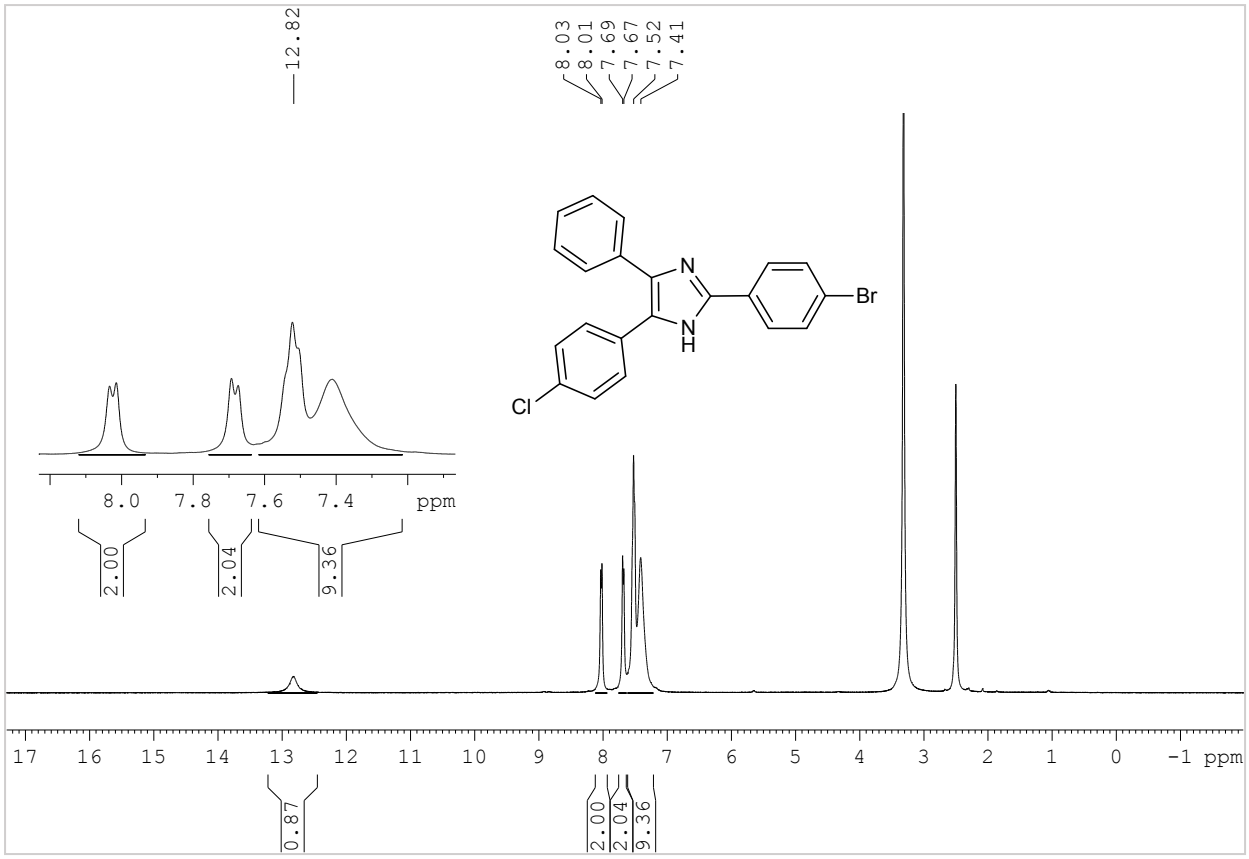
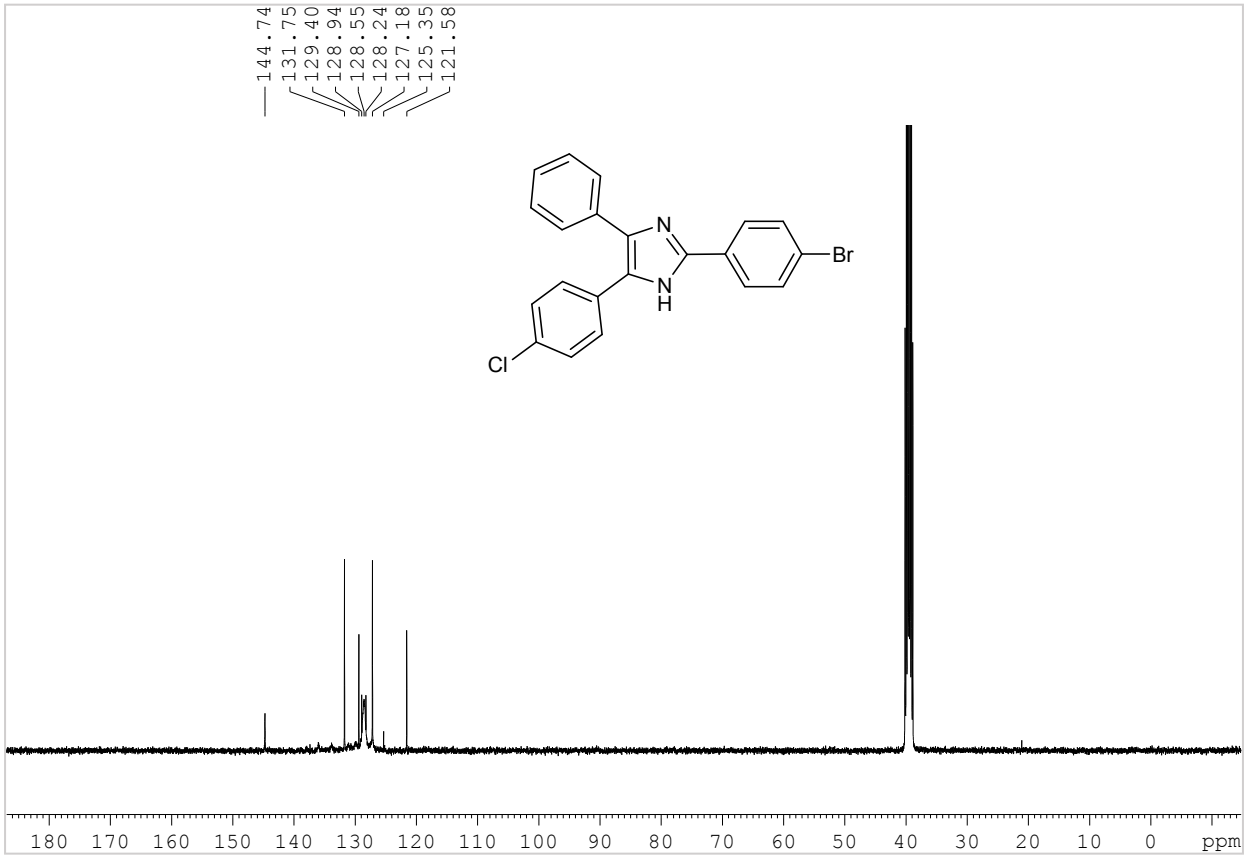
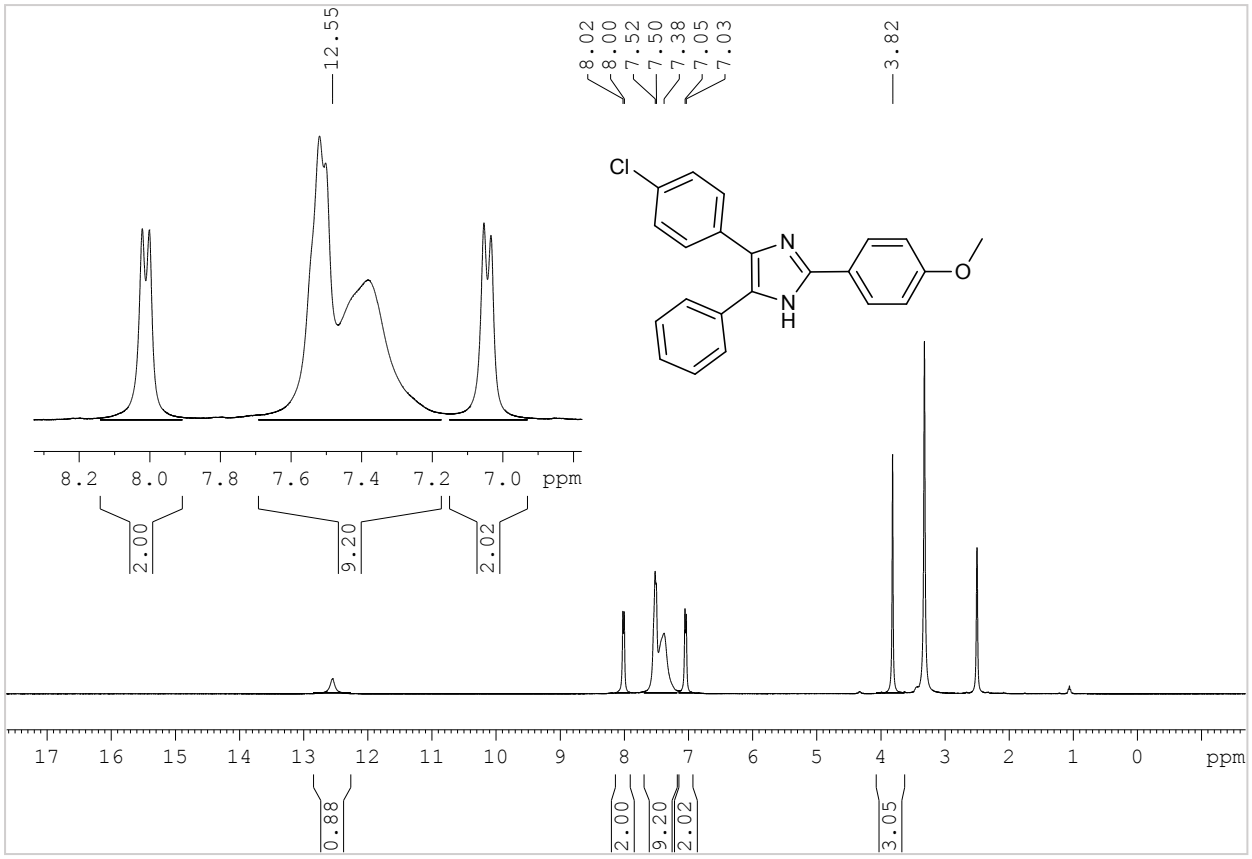
145.74
137.75
135.81
134.95
134.38
131.61
131.17
130.81
130.20
128.89
128.80
128.72
128.57
128.39
128.06
127.30
126.96
126.79
125.25
120.79
119.51
Br
N
N
H
180
160
140
120
100
80
60
40
20
0
ppm

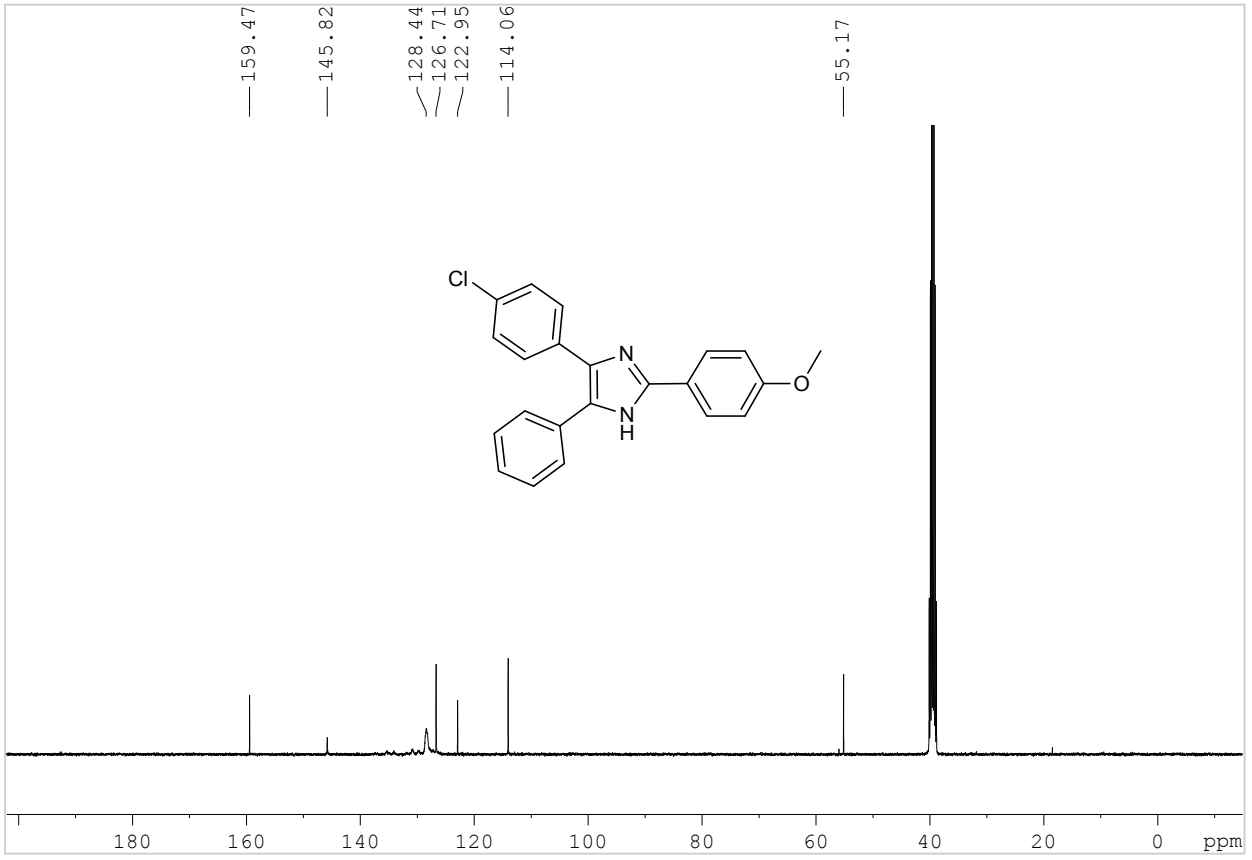

12.81
8.11
8.09
7.55
7.53
7.51
7.41
N
N
H
Cl
Cl
8.2
8.0
7.8
7.6
7.4
7.2
ppm
2.00
11.06
17
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.86
2.00
11.06


144.63
132.84
129.03
128.74
128.57
128.38
126.85
N
N
H
Cl
Cl
200
180
160
140
120
100
80
60
40
20
0
ppm


12.82
8.03
8.01
7.69
7.67
7.52
7.41
N
N
H
Br
Cl
8.0
7.8
7.6
7.4
ppm
2.00
2.04
9.36
17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 ppm
0.87
2.00
2.04
9.36


144.74
131.75
129.40
128.94
128.55
128.24
127.18
125.35
121.58
N
N
H
Br
Cl
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


12.55
8.02
8.00
7.52
7.50
7.38
7.05
7.03
3.82
Cl
N
N
H
O
8.2 8.0 7.8 7.6 7.4 7.2 7.0 ppm
2.00
9.20
2.02
17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.88
2.00
9.20
2.02
3.05


159.47
145.82
128.44
126.71
122.95
114.06
55.17
Cl
N
N
H
O
180 160 140 120 100 80 60 40 20 0 ppm

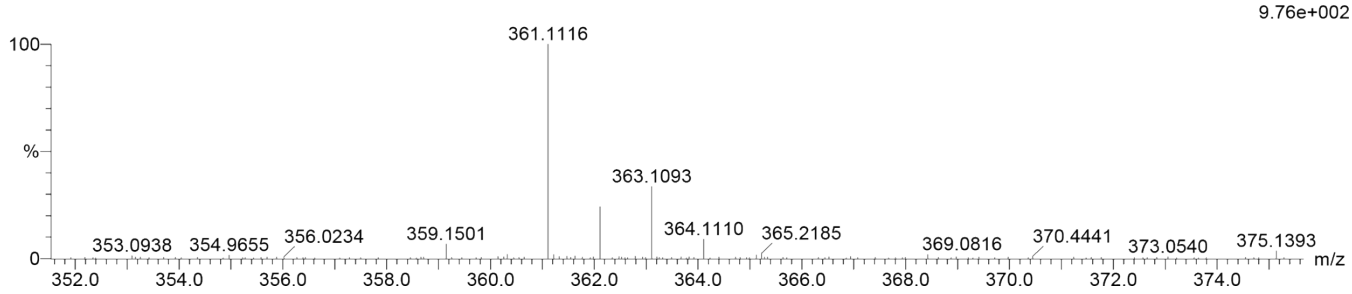
Elemental Composition Report
Page 1

Single Mass Analysis

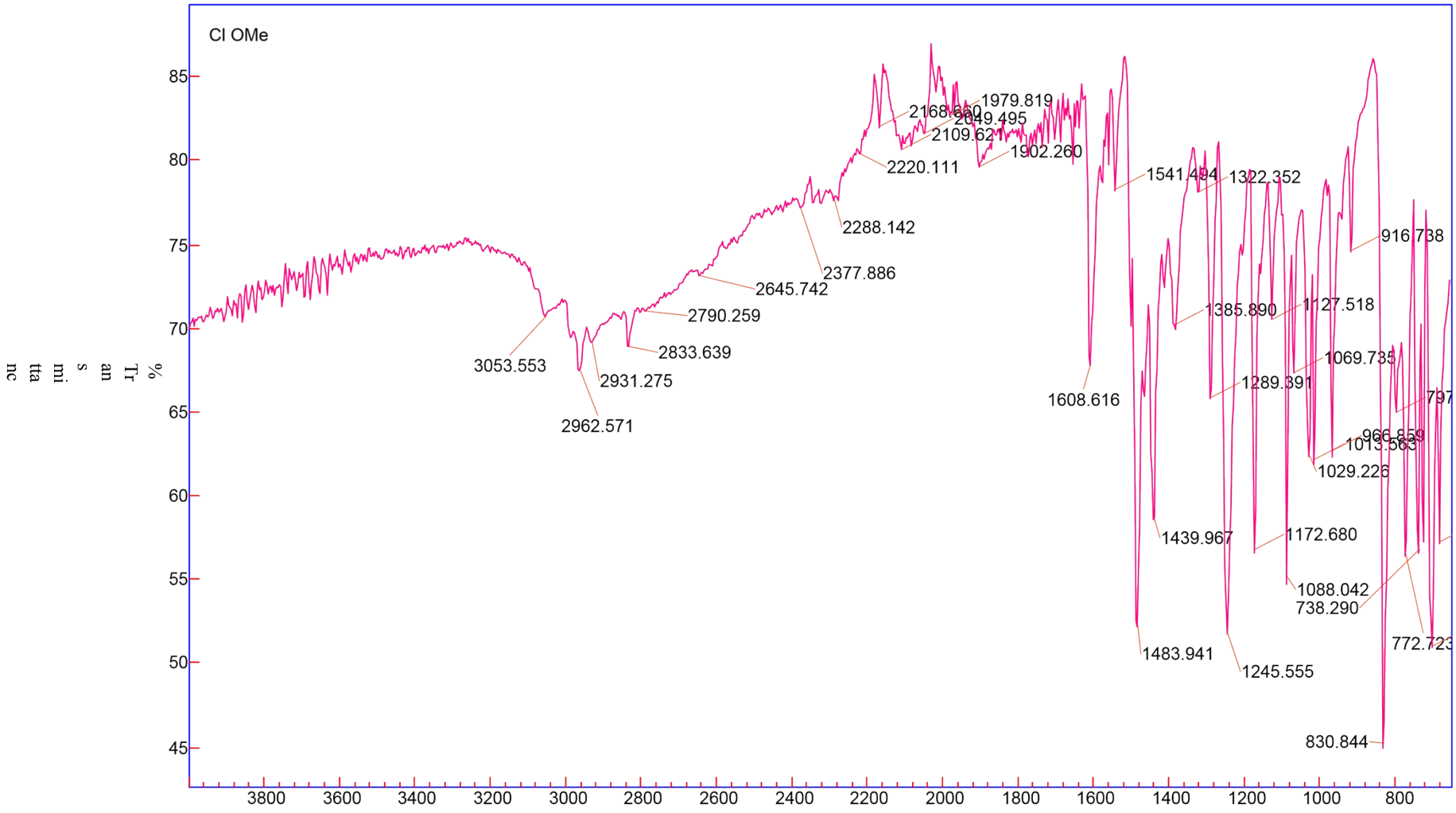
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

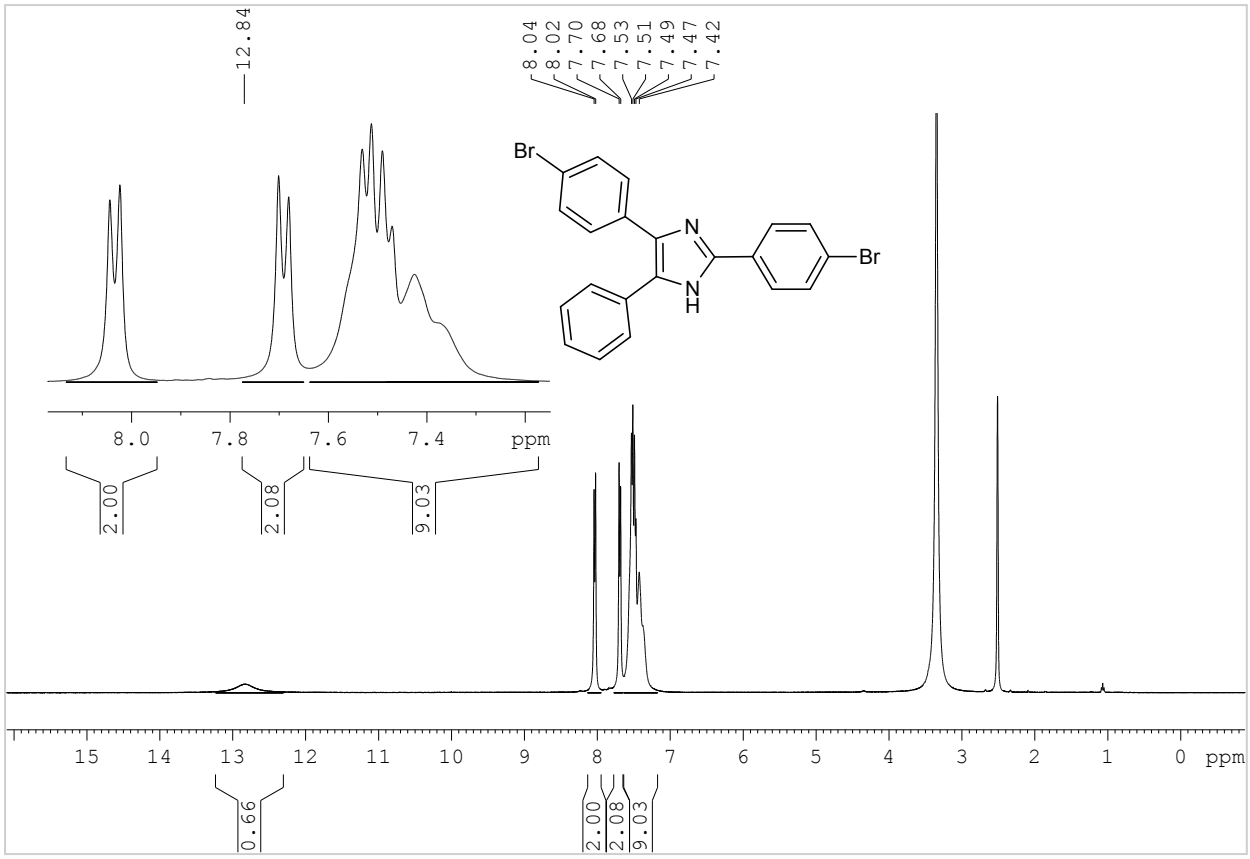
Monoisotopic Mass, Even Electron Ions
36 formula(e) evaluated with 1 results within limits (up to 20 best isotopic matches for each mass) Elements Used:
C: 20-25 H: 15-20 N: 0-5 O: 0-5 Cl: 0-1

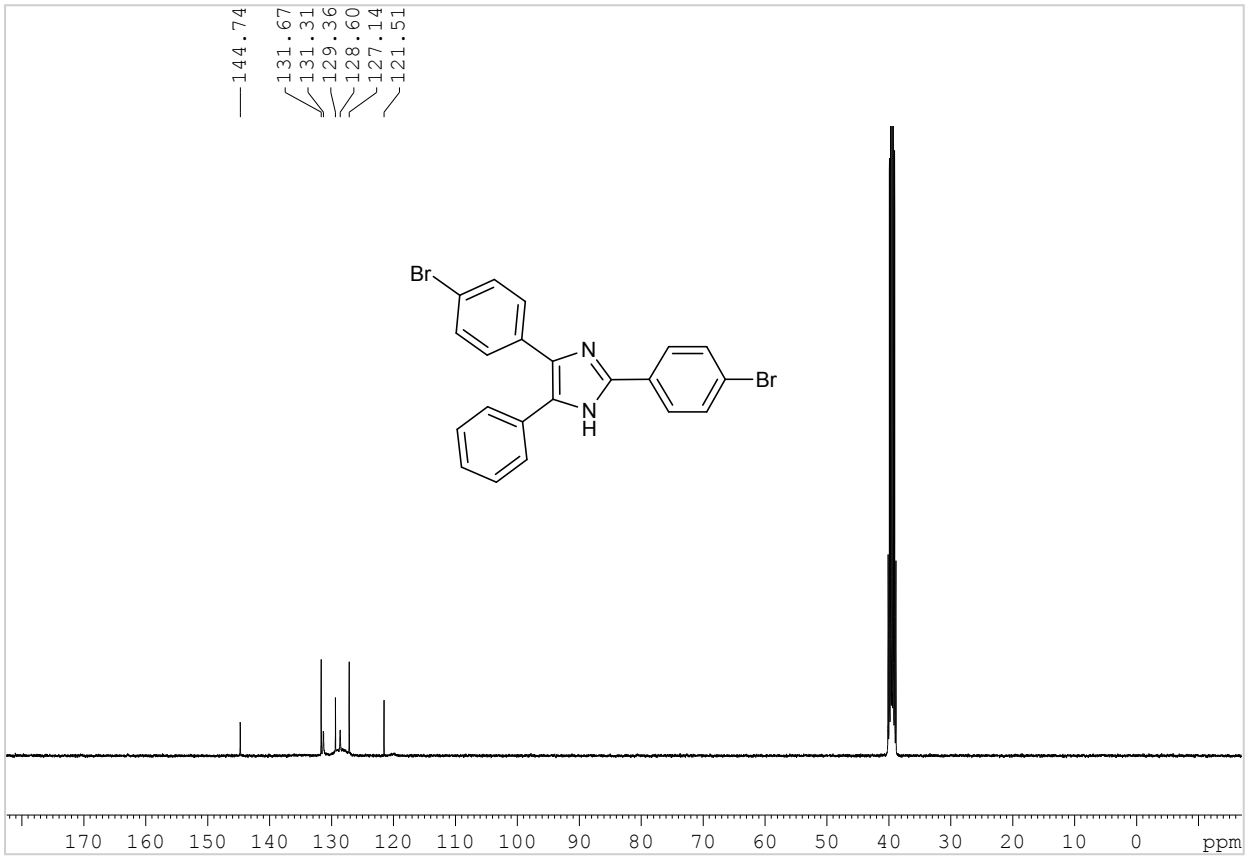
Chloro-methoxy Imid 60 (1.005)
TOF MS ES+



Minimum:				-1.5			
Maximum:		5.0	5.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
361.1116	361.1108	0.8	2.2	14.5	58.1	0.0	C22 H18 N2 O Cl


Cl OMe
% Transmittance
85
80
75
70
65
60
55
50
45
3800
3600
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
3053.553
2962.571
2931.275
2833.639
2790.259
2645.742
2377.886
2288.142
2220.111
2168.660
2109.621
2049.495
1979.819
1902.260
1608.616
1541.494
1483.941
1439.967
1385.890
1322.352
1289.391
1245.555
1172.680
1127.518
1088.042
1069.735
1029.226
1013.563
966.859
916.738
830.844
797
772.723
738.290


12.84
8.04
8.02
7.70
7.68
7.53
7.51
7.49
7.47
7.42
Br
N
N
H
Br
8.0
7.8
7.6
7.4
ppm
2.00
2.08
9.03
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.66
2.00
2.08
9.03


144.74
131.67
131.31
129.36
128.60
127.14
121.51
Br
N
N
H
Br
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

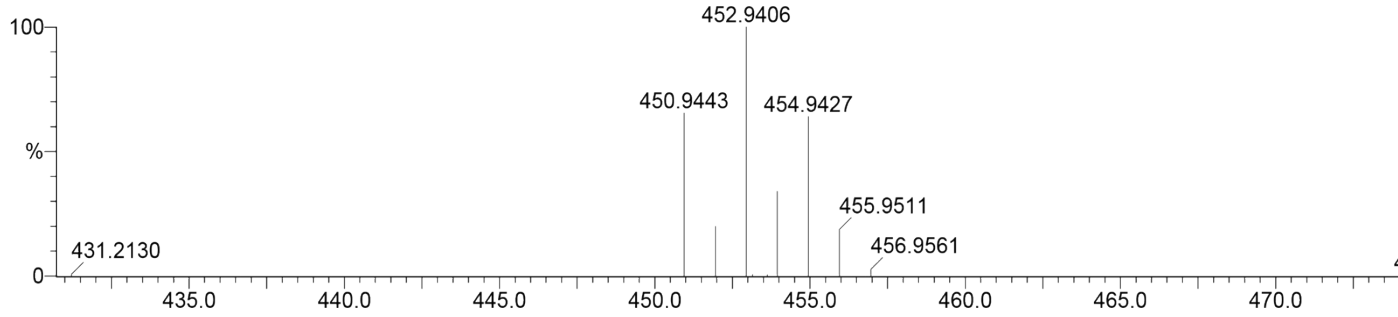
Elemental Composition Report
Page 1

Single Mass Analysis

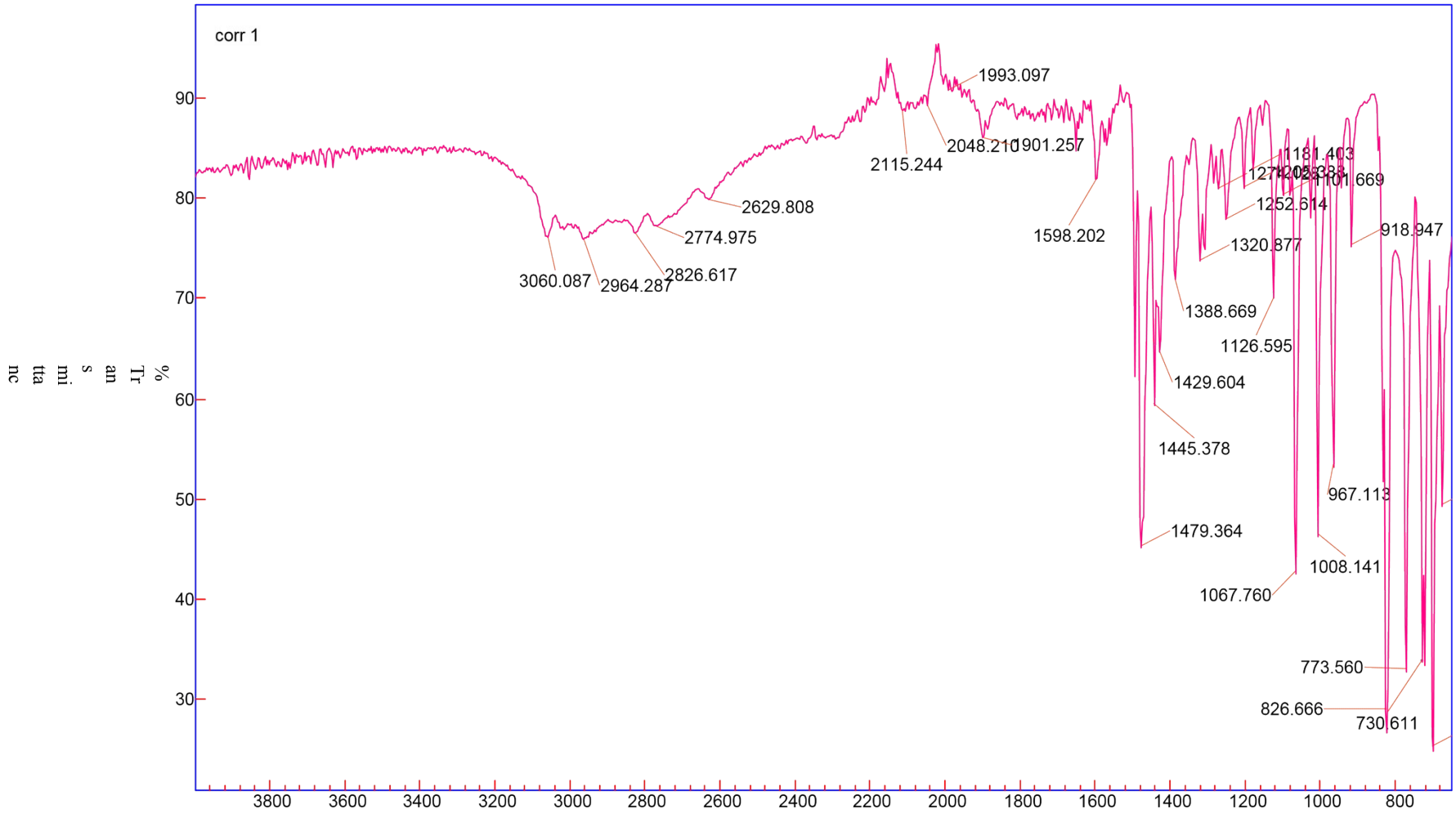
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

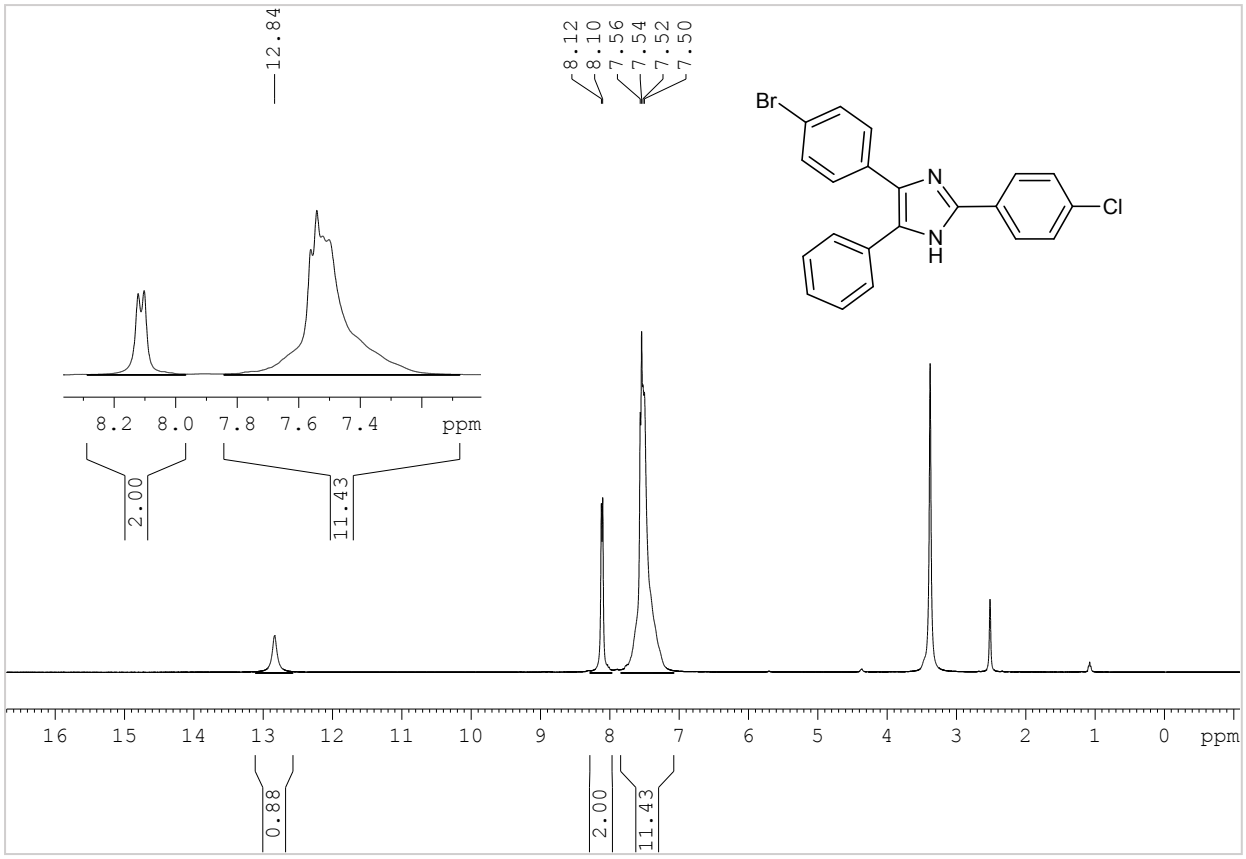
Monoisotopic Mass, Even Electron Ions
12 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass) Elements Used:
C: 20-25 H: 10-15 N: 0-5 Br: 0-2

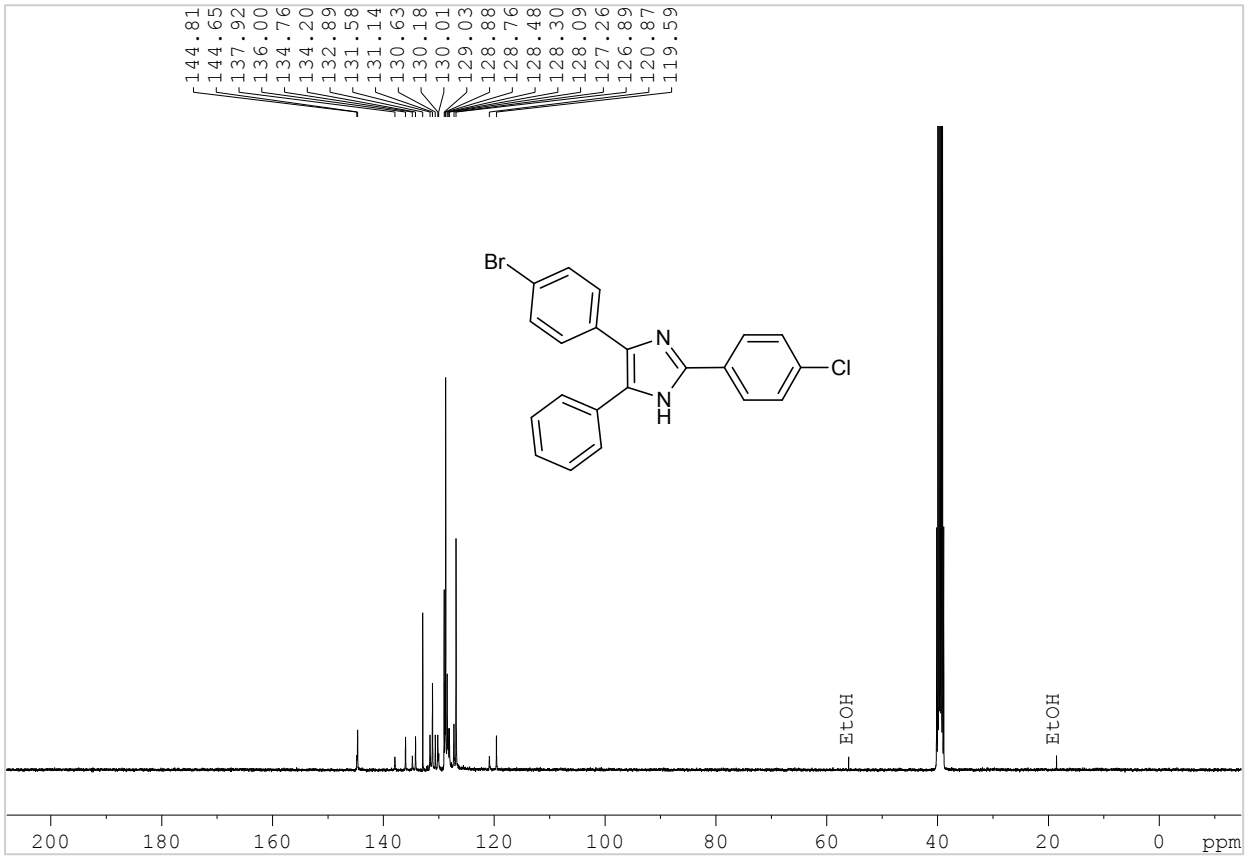
Corr 1 50 (1.653) Cm (1:61)
TOF MS ES-



Minimum:				-1.5			
Maximum:		5.0	5.0	500.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
450.9443	450.9445	-0.2	-0.4	15.5	28.8	0.0	C21 H13 N2 Br2


corr 1
%Transmittance
90
80
70
60
50
40
30
3800
3600
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
3060.087
2964.287
2826.617
2774.975
2629.808
2115.244
2048.210
1993.097
1901.257
1598.202
1429.604
1445.378
1479.364
1388.669
1320.877
1252.614
1181.403
1126.595
1067.760
1008.141
967.113
918.947
773.560
826.666
730.611


12.84
8.12
8.10
7.56
7.54
7.52
7.50
Br
N
N
H
Cl
8.2 8.0 7.8 7.6 7.4 ppm
2.00
11.43
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.88
2.00
11.43


144.81
144.65
137.92
136.00
134.76
134.20
132.89
131.58
131.14
130.63
130.18
130.01
129.03
128.88
128.76
128.48
128.30
128.09
127.26
126.89
120.87
119.59
Br
N
N
H
Cl
EtOH
EtOH
200 180 160 140 120 100 80 60 40 20 0 ppm

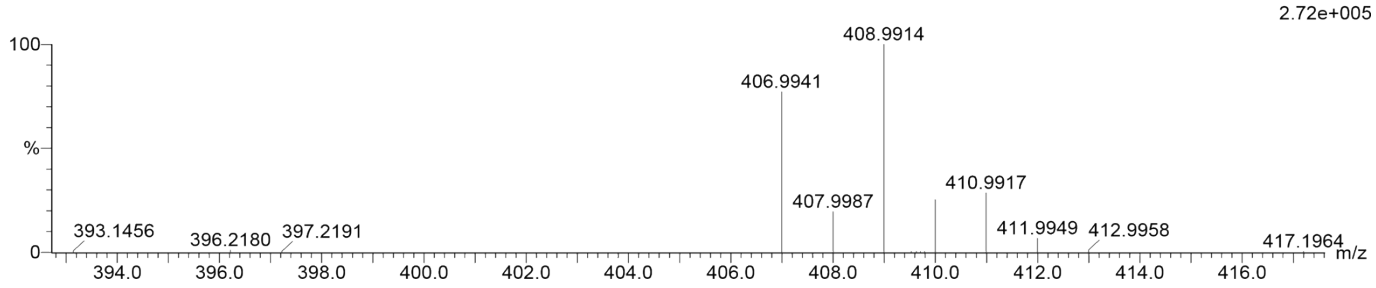
Elemental Composition Report
Page 1

Single Mass Analysis

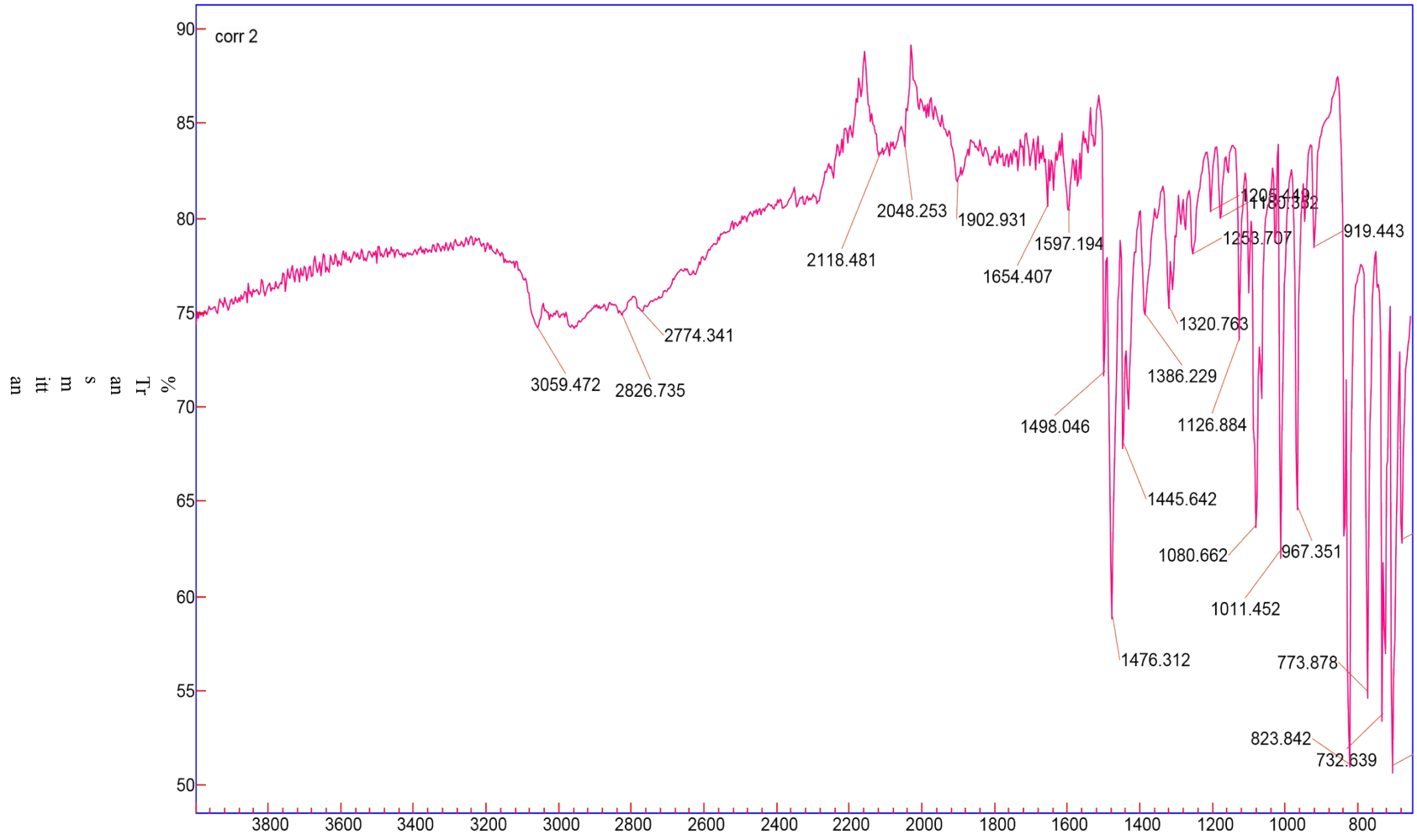
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

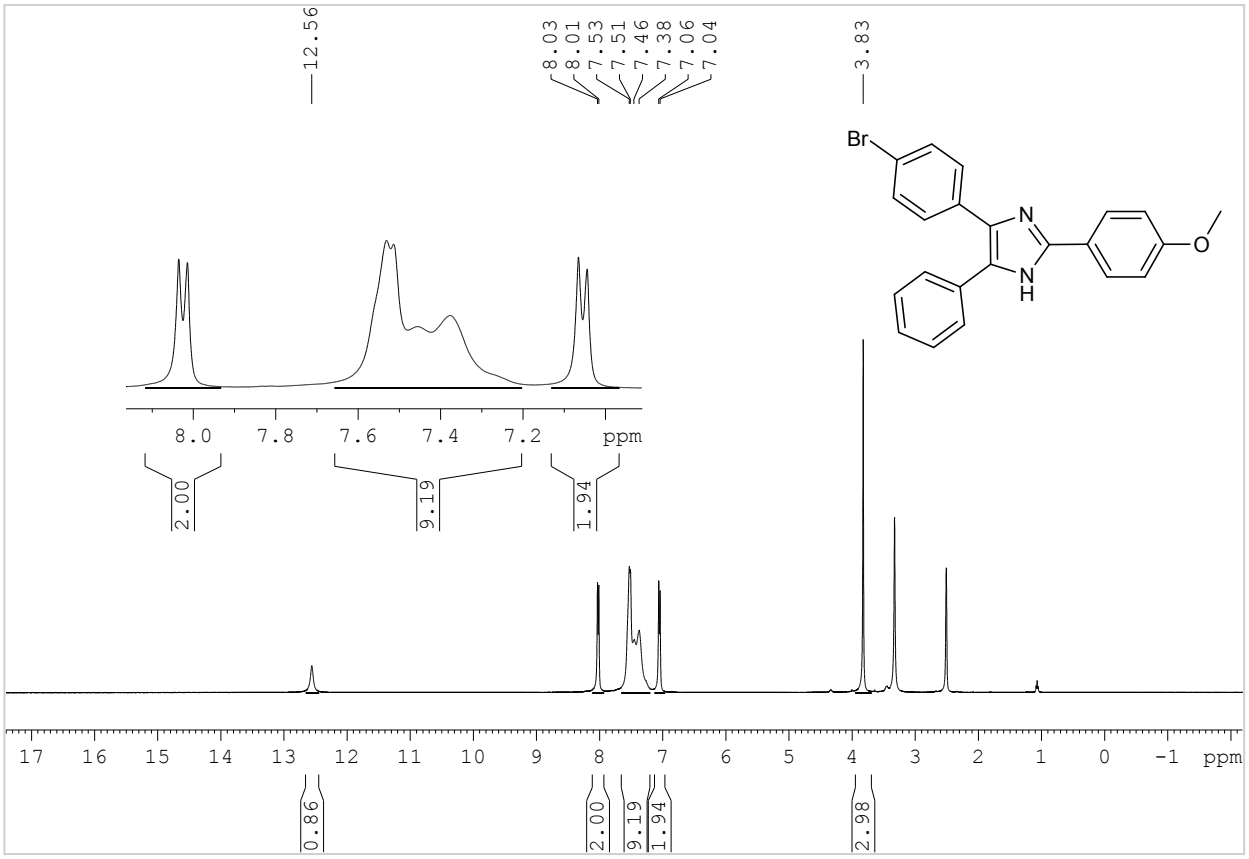
Monoisotopic Mass, Even Electron Ions
12 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass) Elements Used:
C: 20-25 H: 10-15 N: 0-5 Cl: 0-1 Br: 0-1

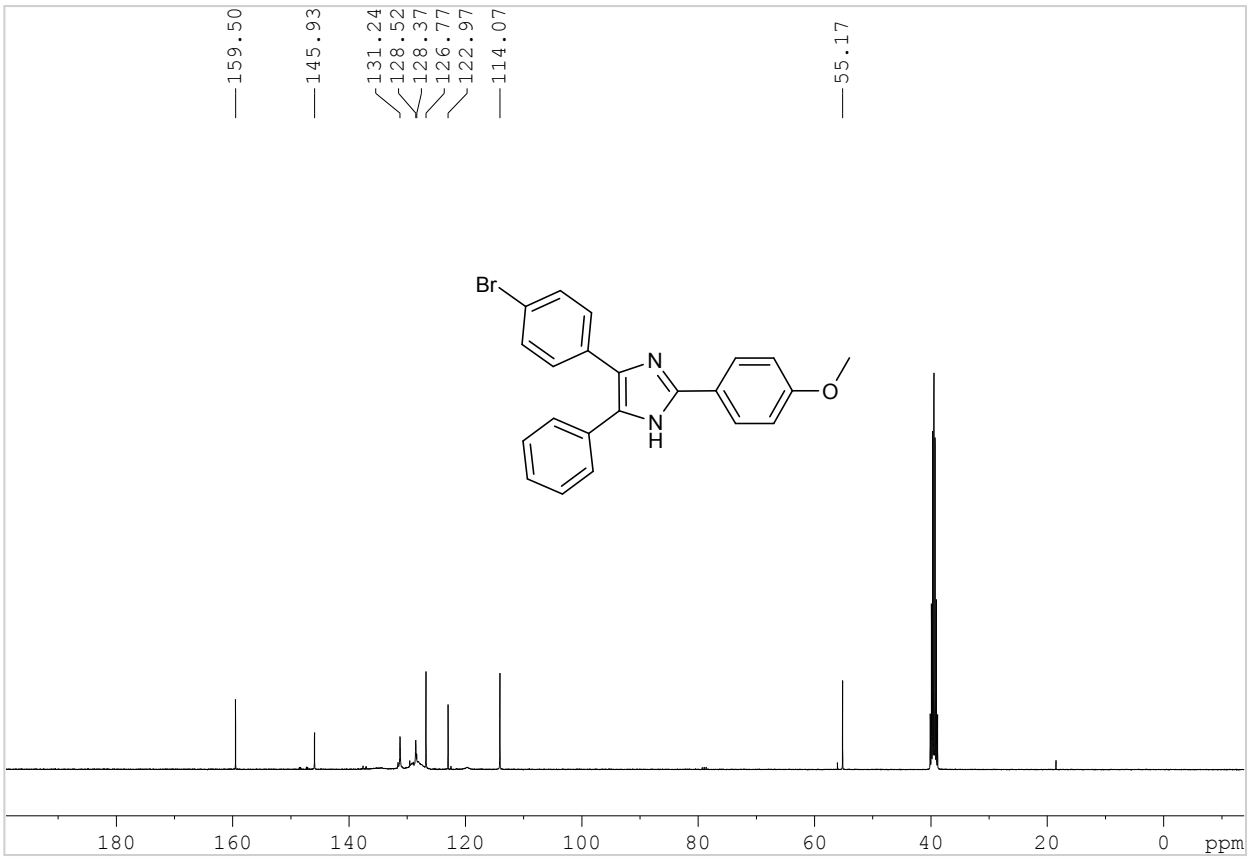
Corr 2 58 (1.923) Cm (1:61)
TOF MS ES-



Minimum:				-1.5			
Maximum:		5.0	5.0	500.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
406.9941	406.9951	-1.0	-2.5	15.5	15.4	0.0	C21 H13 N2 Cl Br


corr 2
Transmittance %
90
85
80
75
70
65
60
55
50
3800
3600
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
3059.472
2826.735
2774.341
2118.481
2048.253
1902.931
1654.407
1597.194
1498.046
1476.312
1445.642
1386.229
1320.763
1253.707
1126.884
1080.662
1011.452
967.351
919.443
773.878
823.842
732.639


12.56
8.03
8.01
7.53
7.51
7.46
7.38
7.06
7.04
3.83
Br
N
O
N
H
8.0
7.8
7.6
7.4
7.2
ppm
2.00
9.19
1.94
17
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
ppm
0.86
2.00
9.19
1.94
2.98


159.50
145.93
131.24
128.52
128.37
126.77
122.97
114.07
55.17
Br
N
O
N
H
180
160
140
120
100
80
60
40
20
0
ppm

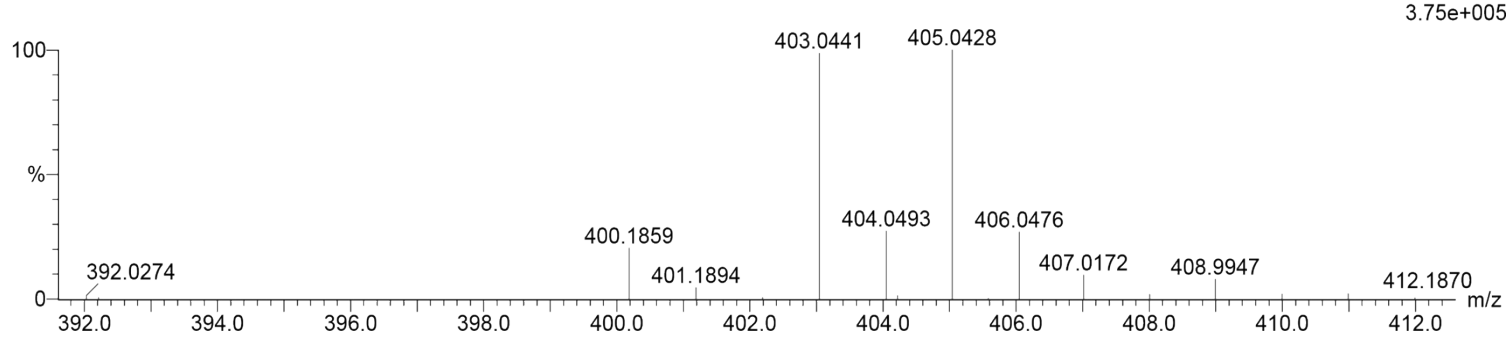
Elemental Composition Report
Page 1

Single Mass Analysis

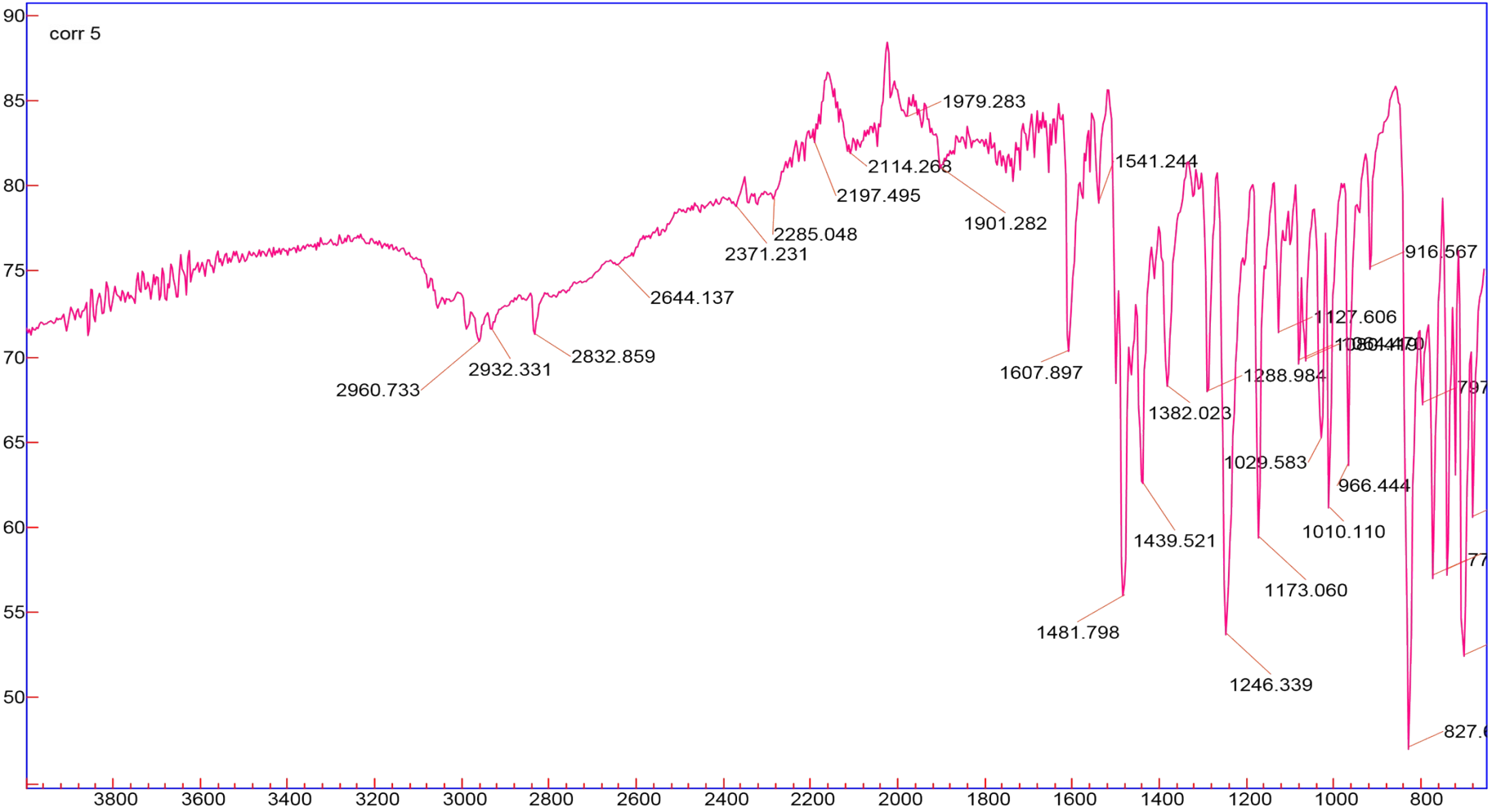
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

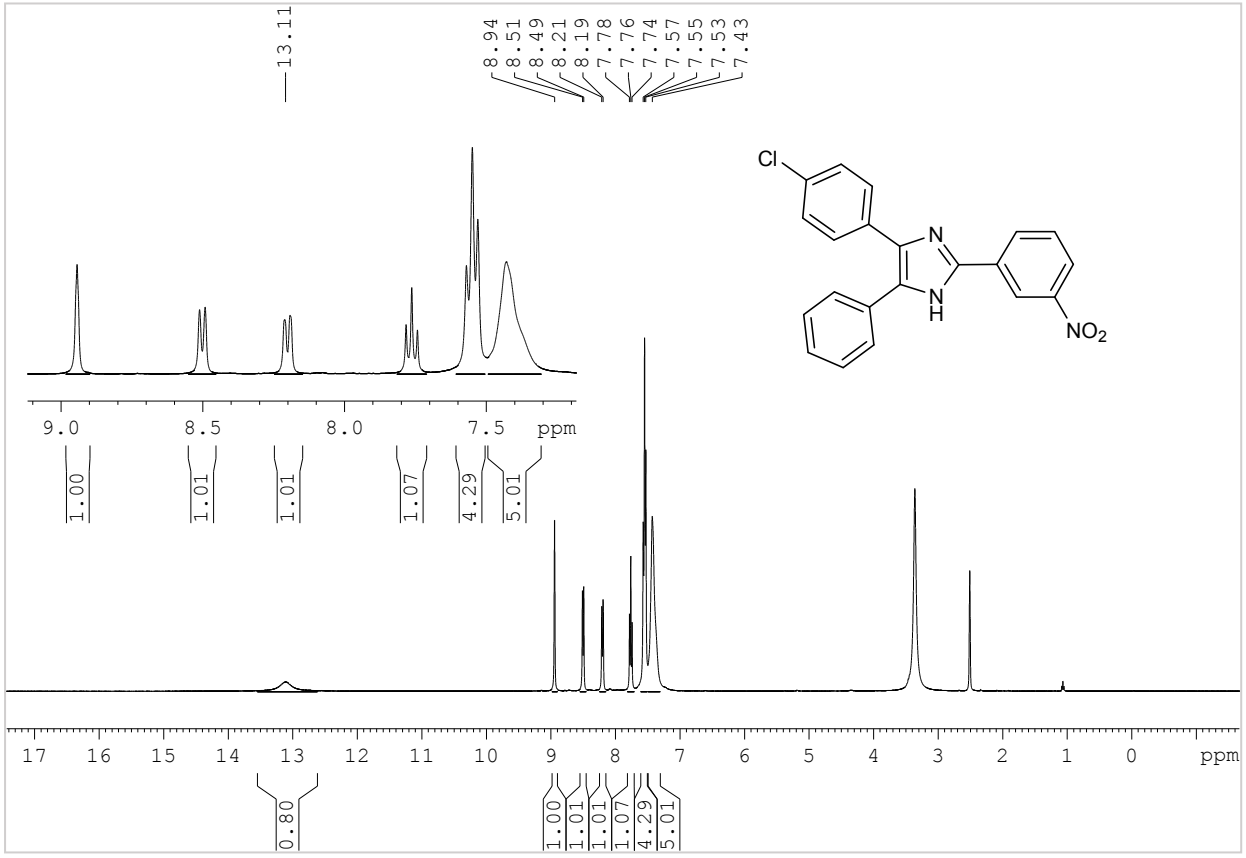
Monoisotopic Mass, Even Electron Ions
32 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 20-25 H: 15-20 N: 0-5 O: 0-5 Br: 0-1

Corr 5 39 (1.281) Cm (1:61)
TOF MS ES-



Minimum:				-1.5			
Maximum:		5.0	5.0	500.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
403.0441	403.0446	-0.5	-1.2	15.5	37.1	0.0	C22 H16 N2 O Br


corr 5
90
85
80
75
70
65
60
55
50
3800
3600
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
2960.733
2932.331
2832.859
2644.137
2371.231
2285.048
2197.495
2114.268
1979.283
1901.282
1607.897
1541.244
1382.023
1288.984
1127.606
1029.583
966.444
916.567
1010.110
1439.521
1173.060
1481.798
1246.339

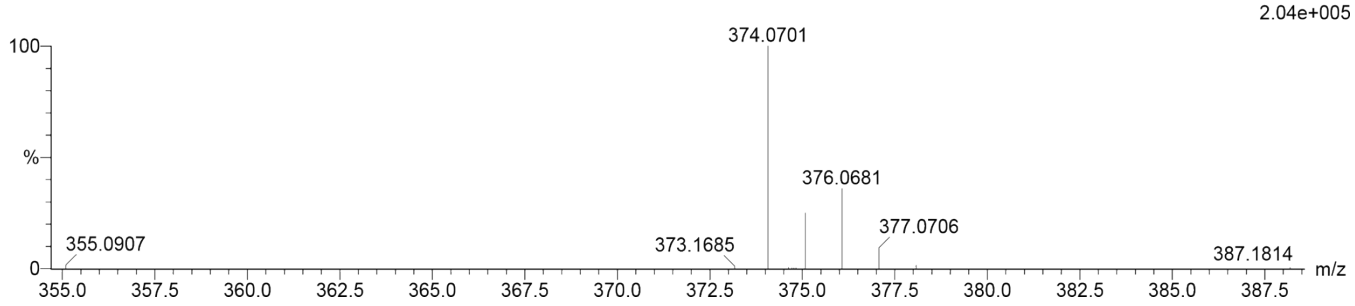

13.11
8.94
8.51
8.49
8.21
8.19
7.78
7.76
7.74
7.57
7.55
7.53
7.43
Cl
N
N
H
NO2
9.0
8.5
8.0
7.5
ppm
1.00
1.01
1.01
1.07
4.29
5.01
17
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.80
1.00
1.01
1.01
1.07
4.29
5.01

Elemental Composition Report
Page 1

Single Mass Analysis

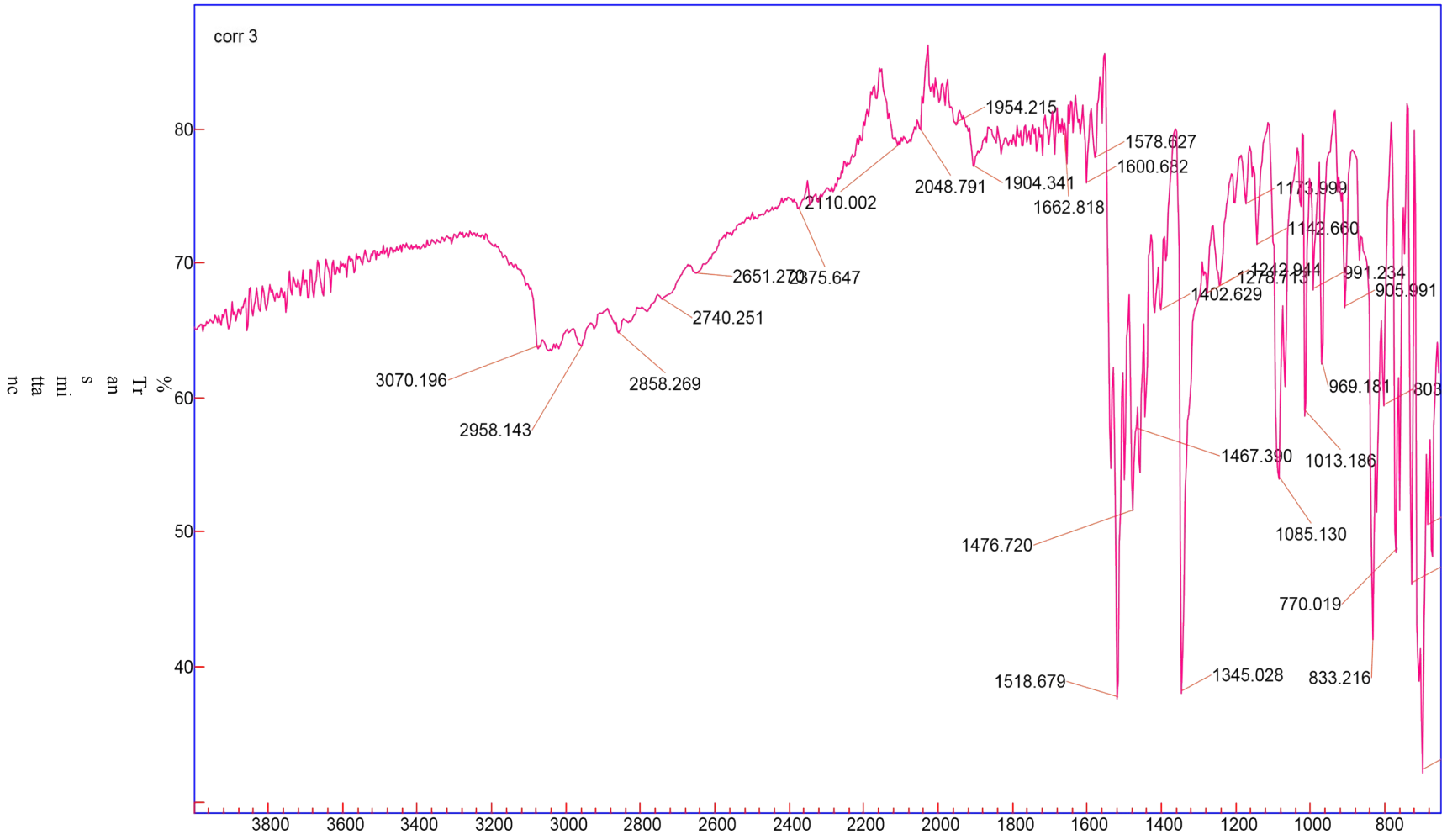
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

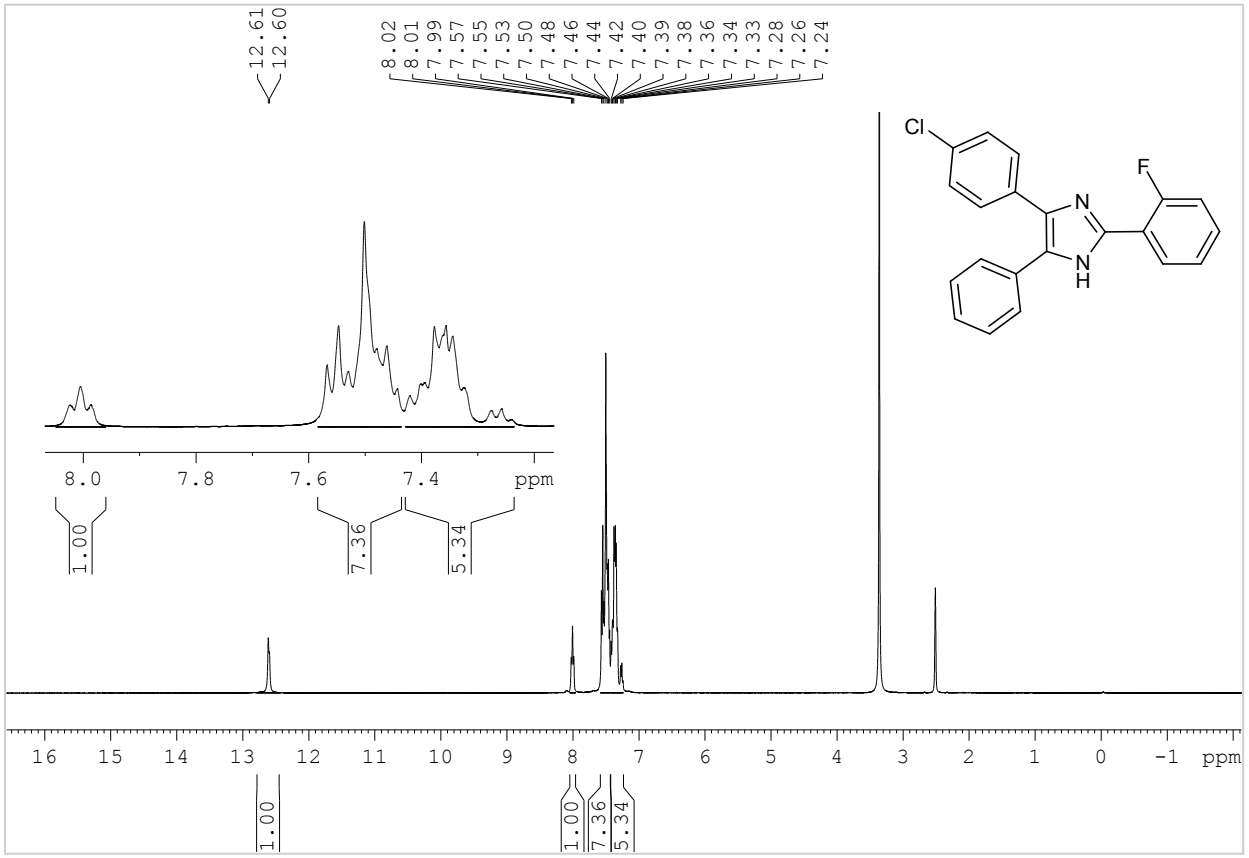
Monoisotopic Mass, Even Electron Ions
31 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass) Elements Used:
C: 20-25 H: 10-15 N: 0-5
O: 0-5 Cl: 0-1 Corr 3 58
(1.922) Cm (1:61)
TOF MS ES-

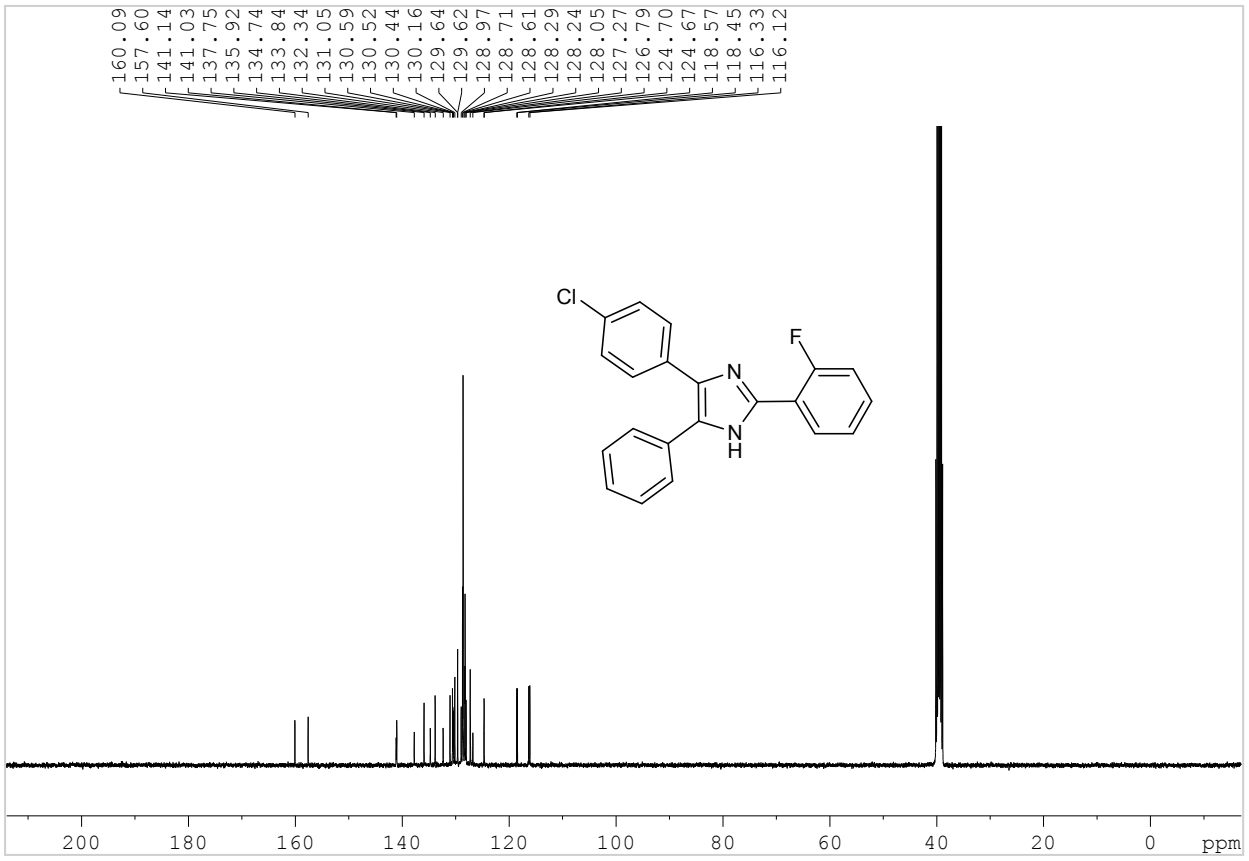


Minimum:			-1.5
Maximum:	5.0	5.0	500.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
374.0701	374.0696	0.5	1.3	16.5	61.2	0.0	C21 H13 N3 O2 Cl


corr 3
%Transmittance
80
70
60
50
40
3800
3600
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
3070.196
2958.143
2858.269
2740.251
2651.270
2375.647
2110.002
2048.791
1954.215
1904.341
1662.818
1600.682
1578.627
1518.679
1476.720
1467.390
1402.629
1345.028
1278.713
1242.944
1173.999
1142.660
1085.130
1013.186
991.234
969.181
905.991
833.216
770.019
803


12.61
12.60
8.02
8.01
7.99
7.57
7.55
7.53
7.50
7.48
7.46
7.44
7.42
7.40
7.39
7.38
7.36
7.34
7.33
7.28
7.26
7.24
Cl
F
N
N
H
8.0
7.8
7.6
7.4
ppm
1.00
7.36
5.34
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
ppm
1.00
1.00
7.36
5.34


160.09
157.60
141.14
141.03
137.75
135.92
134.74
133.84
132.34
131.05
130.59
130.52
130.44
130.16
129.64
129.62
128.97
128.71
128.61
128.29
128.24
128.05
127.27
126.79
124.70
124.67
118.57
118.45
116.33
116.12
Cl
F
N
N
H
200
180
160
140
120
100
80
60
40
20
0
ppm

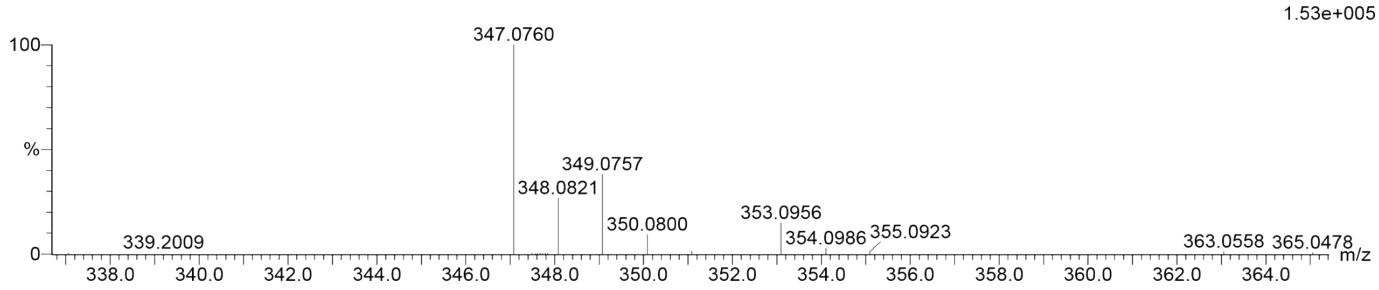
Elemental Composition Report
Page 1

Single Mass Analysis

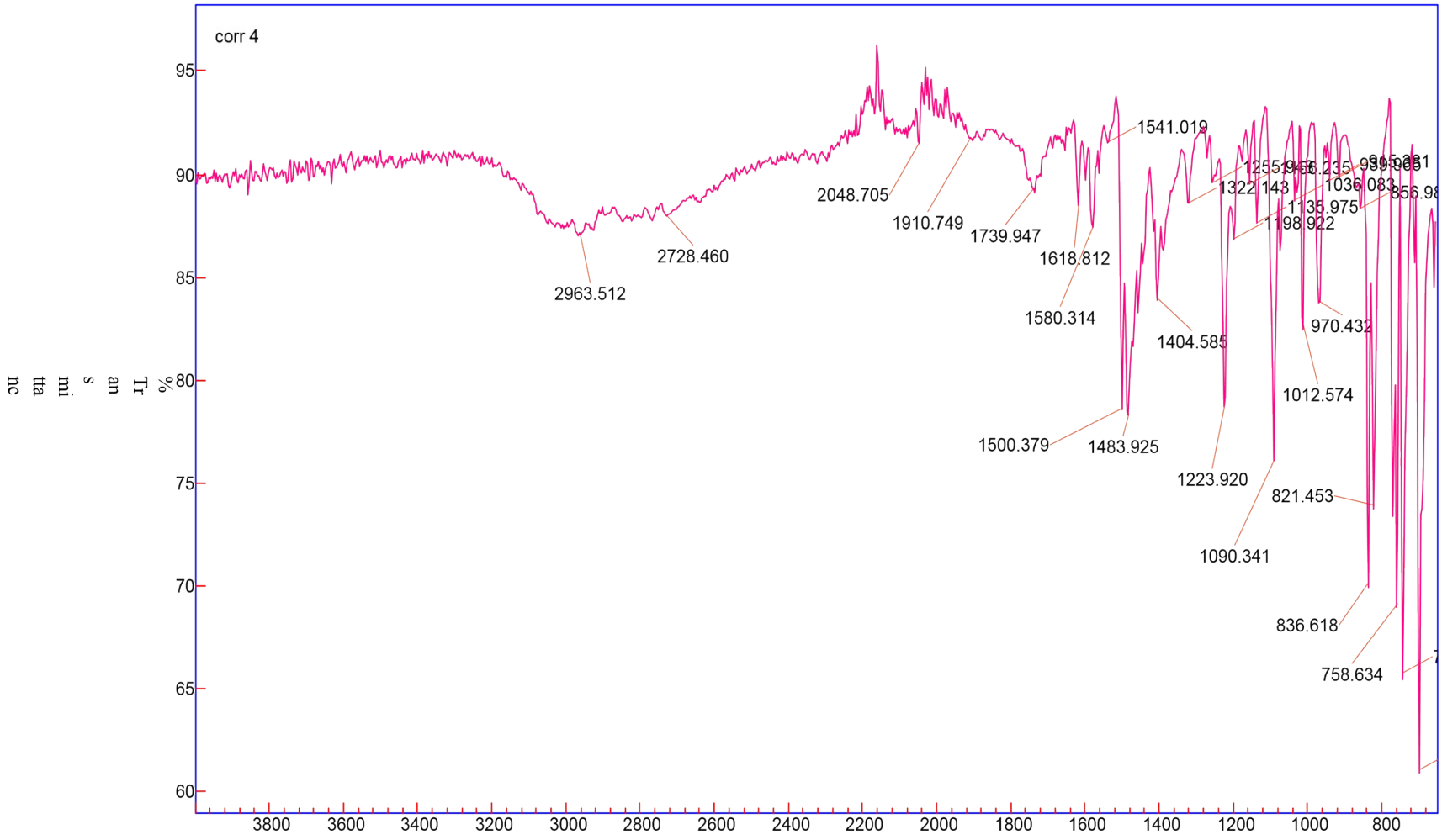
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

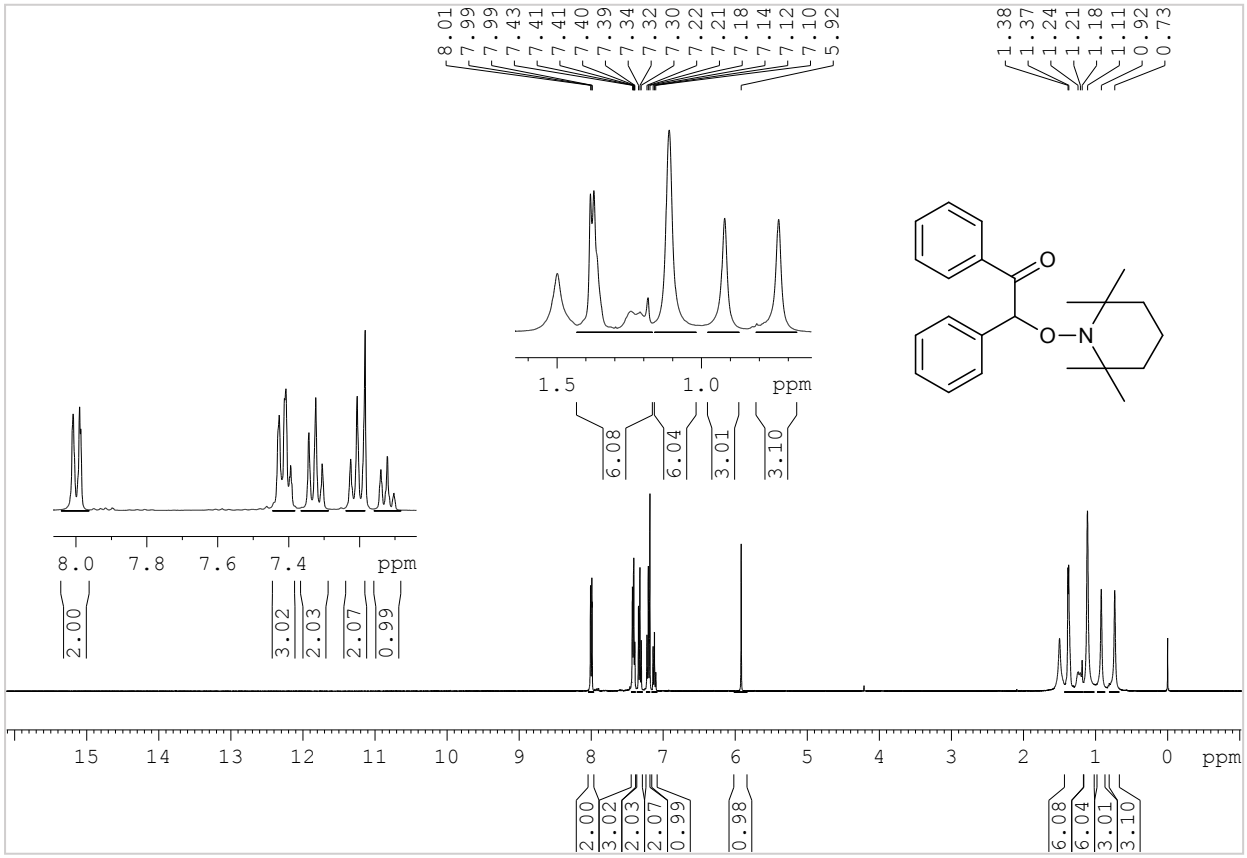
Monoisotopic Mass, Even Electron Ions
11 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass) Elements Used:
C: 20-25 H: 10-15 N: 0-5 Cl: 0-1 F: 0-1

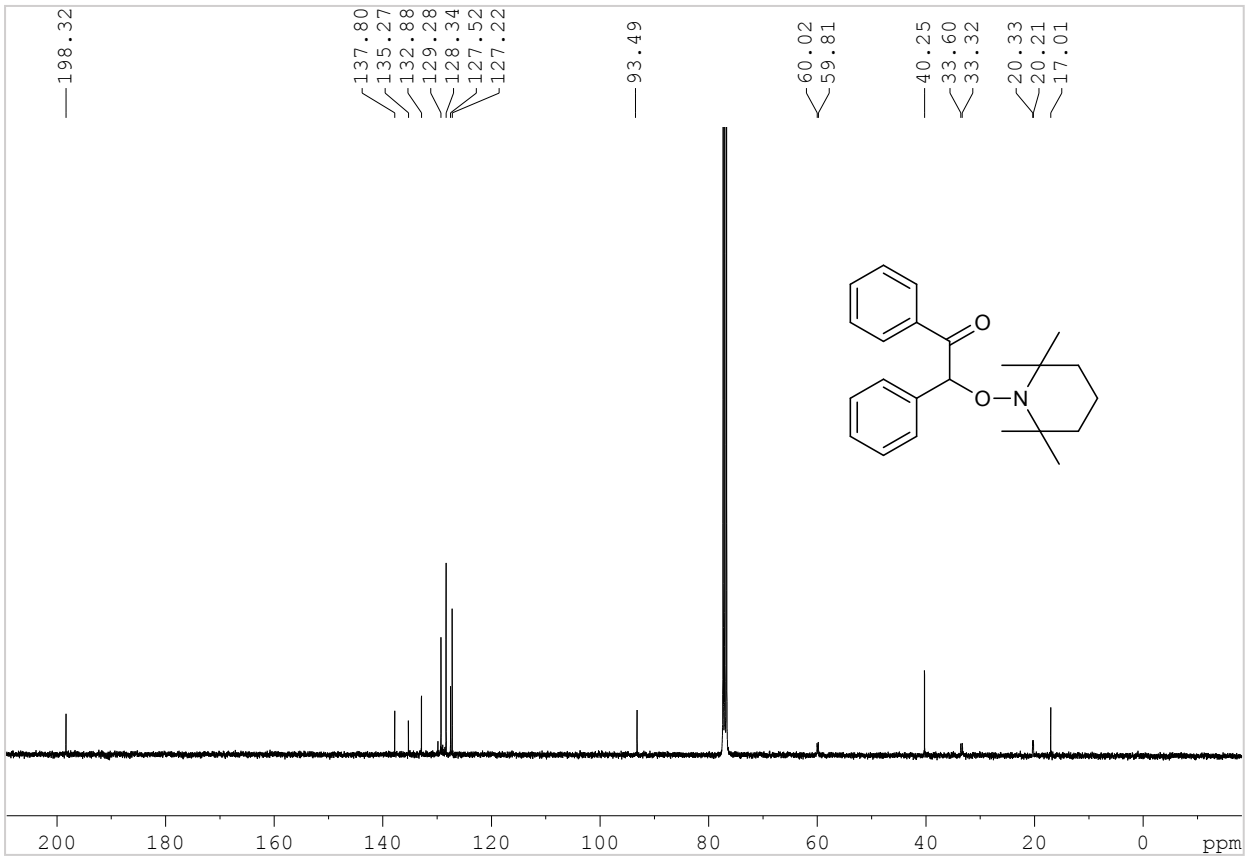
Corr 4 58 (1.922) Cm (1:61)
TOF MS ES-



Minimum:				-1.5			
Maximum:		5.0	5.0	500.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
347.0760	347.0751	0.9	2.6	15.5	108.7	0.0	C21 H13 N2 Cl F


corr 4
Transmittance %
95
90
85
80
75
70
65
60
3800
3600
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
2963.512
2728.460
2048.705
1910.749
1739.947
1618.812
1580.314
1541.019
1500.379
1483.925
1404.585
1322.143
1223.920
1198.922
1135.975
1090.341
1036.083
1012.574
970.432
821.453
836.618
758.634


8.01
7.99
7.99
7.43
7.41
7.41
7.40
7.39
7.34
7.32
7.30
7.22
7.21
7.18
7.14
7.12
7.10
5.92
1.38
1.37
1.24
1.21
1.18
1.11
0.92
0.73
O
O—N
1.5
1.0
ppm
6.08
6.04
3.01
3.10
8.0
7.8
7.6
7.4
ppm
2.00
3.02
2.03
2.07
0.99
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
3.02
2.03
2.07
0.99
0.98
6.08
6.04
3.01
3.10


198.32
137.80
135.27
132.88
129.28
128.34
127.52
127.22
93.49
60.02
59.81
40.25
33.60
33.32
20.33
20.21
17.01
O
O—N
200
180
160
140
120
100
80
60
40
20
0
ppm