Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Copper catalyzed C(sp^3)−H functionalization of ketones with vinyl azides: Synthesis of substituted−1H−pyrroles

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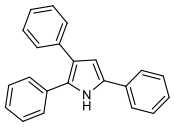
EXPERIMENTAL SECTION:

General Methods: All commercially available chemicals and reagents were used without any further purification unless otherwise indicated. ^{1}H and ^{13}C NMR spectra were recorded at 500, and 125 MHz, respectively. The spectra were recorded in DMSO as a solvent. Multiplicity was indicated as follows: s (singlet); d (doublet); t (triplet); m (multiplet); dd (doublet of doublets), etc. Coupling constants (*J*) were given in Hz. Chemical shifts are reported in δ relative to TMS as an internal standard. The peaks around δ values of 2.50 (^{1}H NMR), 39.9 (^{13}C NMR) are corresponding to DMSO. The peak around δ values of 3.35 (^{1}H NMR) is corresponding to the H_2O present in DMSO solvent. Silica gel 100 – 200 or 200 – 400 mesh sizes was used for column chromatography. Starting substrates vinyl azides were synthesized by reported methods[1]

Typical procedure for the synthesis of 2,3,5-triphenyl-1H-pyrrole 3a[2]: 88.2 mg (0.45 mmol) of 1,2-diphenylethanone **1a,** 43.5 mg (0.3 mmol) of (1-azidovinyl)benzene **2a,** and 6 mg of (0.03mmol) of $CuAco_2.H_2O$ were taken in a 10 ml tube, added 1 ml of DMF to the reaction mixture then sealed with a rubber septum. The system was purged with argon gas for 2 to 3 minutes. After placing the reaction tube in a preheated oil bath at 40 ^{0}C for 24h, the reaction mixture was allowed to attain room temperature, added 10-15 ml of brine solution and extracted with 3x15 ml of ethyl acetate. Extracted solution was washed with water 3 x10 ml. After removing of volatiles, crude mixture is subjected to column chromatography. 78 % of the product 2,3,5-triphenyl-1H-pyrrole **3a** was isolated.

2,3,5-triphenyl-1H-pyrrole (3a)[2]:

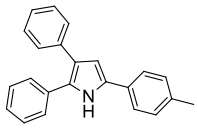
Silica gel 100 – 200 mesh size neutralised with 5% triethyl amine solution in hexane was used for column chromatography. 5% ethyl acetate in hexane used as an eluent.



White solid, yield 78% (69 mg). ^{1}H NMR (500 MHz, DMSO): δ 6.76 (d, *J* = 2.5 Hz, 1H), 7.15 – 7.21 (m, 2H),7.24 – 7.30 (m, 5H), 7.32 – 7.42 (m, 6H), 7.79 (d, *J* = 8.0 Hz , 2H), 11.39 (s, 1H); ^{13}C NMR (125 MHz, DMSO): 107.9, 122.6, 123.8, 125.5, 125.8, 126.6, 127.8, 128.0, 128.2, 128.5, 129.3, 131.9, 132.2, 132.8, 136.5. HRMS calcd for $C_{22}H_{18}N$: 296.1439 found: 296.1436.

2,3-diphenyl-5-(p-tolyl)-1H-pyrrole (3b)[2]:

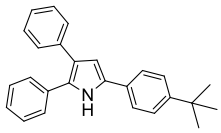
Silica gel 100 – 200 mesh size neutralised with 5% triethyl amine solution in hexane was used for column chromatography. 5% ethyl acetate in hexane used as an eluent.



White solid, yield 66 % (61.2 mg). ^{1}H NMR (500 MHz, DMSO): δ 2.30 (s, 3H), 6.68 (d, *J* = 2 Hz, 1H), 7.15 – 7.19 (m, 3H), 7.23 – 7.34 (m, 8H), 7.39 (d, *J* = 8.0 Hz, 2H), 7.67 (d, *J* = 8.0 Hz, 2H), 11.31 (s, 1H); ^{13}C NMR (125 MHz, DMSO): 20.6, 107.4, 122.4, 123.8, 125.4, 126.4, 127.8, 127.9, 128.1, 128.8, 129.1, 129.5, 132.0, 132.9, 134.9, 136.6. HRMS calcd for $C_{23}H_{20}N$: 310.1596 found: 310.1602.

5-(4-(tert-butyl)phenyl)-2,3-diphenyl-1H-pyrrole (3c)

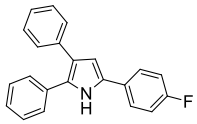
Silica gel 100 – 200 mesh size neutralised with 5% triethyl amine solution in hexane was used for column chromatography. 5% ethyl acetate in hexane used as an eluent.



White solid, observed melting point 136.3 °C yield 70% (73.8 mg). ^{1}H NMR (500 MHz, DMSO): δ 1.30 (s, 9H), 6.68 (d, *J* = 2 Hz, 1H), 7.16 (t, *J* = 6.0 Hz 1H), 7.23 – 7.29 (m, 5H), 7.33 (t, *J* = 7.5 Hz, 2H), 7.38 – 7.41 (m, 4H), 7.70 (d, *J* = 8.5 Hz, 2H), 11.33 (s, 1H); ^{13}C NMR (125 MHz, DMSO): 31.6, 34.6, 108.0, 123.0, 124.2, 125.8, 126.0, 127.0, 128.3, 128.5, 128.7, 129.4, 130.0, 132.5, 133.4, 137.1, 148.7. IR: 3461, 2957, 1607, 1495, 1261, 1178, 1024, 955, 808, 763, 697. HRMS calcd for $C_{26}H_{26}N$: 352.2065 found: 352.2068.

5-(4-fluorophenyl)-2,3-diphenyl-1H-pyrrole (3d)[3]:

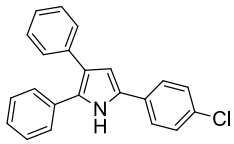
Silica gel 100 – 200 mesh size neutralised with 5% triethyl amine solution in hexane was used for column chromatography. 5% ethyl acetate in hexane used as an eluent.



White solid yield 57 % (53.5 mg). ^{1}H NMR (500 MHz, DMSO): δ 6.73 (s, 1H), 7.17 – 7.41 (m, 12H), 7.82 (d, *J* = 7.0 Hz , 2H), 11.38 (s, 1H) ; ^{13}C NMR (125 MHz, DMSO): 108.0, 115.4 (d, *J* = 21.0 Hz), 122.7, 125.6, 125.8 (d, *J* = 7.0 Hz), 126.7, 127.9, 128.1, 128.3, 129.0, 129.3, 131.1, 132.9, 136.6, 159.7(d, *J* = 241.7 Hz). HRMS calcd for $C_{22}H_{17}NF$: 314.1345 found: 314.1341.

5-(4-chlorophenyl)-2,3-diphenyl-1H-pyrrole (3e)[2]:

Silica gel 100 – 200 mesh size neutralised with 5% triethyl amine solution in hexane was used for column chromatography. 5% ethyl acetate in hexane used as an eluent.

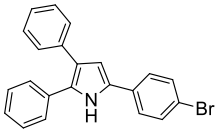


White solid yield 60 % (59.2 mg). ^{1}H NMR (500 MHz, DMSO): δ 6.80 (d, *J* = 1 Hz, 1H), 7.17 – 7.18 (m, 1H), 7.25 – 7.28 (m, 5H), 7.33 (t, *J* = 7.5Hz , 2H), 7.40 – 7.43 (m, 4H), 7.81 (d, *J* = 8.0

Hz, 2H), 11.45 (s, 1H); ^{13}C NMR (125 MHz, DMSO); 109.1, 123.3, 125.9, 126.1, 127.2, 128.3, 128.5, 128.7, 129.0, 130.3, 130.6, 131.2, 131.6, 133.1, 136.8. HRMS calcd for $C_{22}H_{17}NCl$: 330.1050 found: 330.1056.

5-(4-bromophenyl)-2,3-diphenyl-1H-pyrrole (3f)[2]:

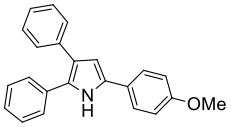
Silica gel 100 – 200 mesh size neutralised with 5% triethyl amine solution in hexane was used for column chromatography. 5% ethyl acetate in hexane used as an eluent. Due to impurities present in the product column chromatography was repeated with silica gel 100 – 200 mesh size and 5 % ethyl acetate in hexane solution used as an eluent.



White solid yield 62 % (69.6 mg). ^{1}H NMR (500 MHz, DMSO): δ 6.81 (d, *J* = 2.5 Hz, 1H), 7.15 – 7.20 (m, 1H), 7.25 – 7.28 (m, 5H), 7.34 (t, *J* = 8.0 Hz, 2H), 7.39 (d, *J* = 7. 5 Hz, 2H) 7.55 (d, *J* = 8.5 Hz, 2H) 7.74 (d, *J* = 8.5 Hz, 2H) 11.45 (s, 1H); ^{13}C NMR (125 MHz, DMSO): 108.6, 118.4, 122.7, 125.6, 125.7, 126.7, 127.8, 128.0, 128.2, 129.8, 130.6, 131.3, 131.4, 132.6, 136.3. HRMS calcd for $C_{22}H_{17}NBr$: 374.0544 found: 374.0553.

5-(4-methoxyphenyl)-2,3-diphenyl-1H-pyrrole (3g)[2]:

Silica gel 200 – 400 mesh size used for column chromatography. 1: 5 : 94 tri ethyl amine, ethyl acetate and hexane solution used as an eluent. After removing the impurities, 10 % ethyl acetate in hexane used as an eluent to obtain the product.

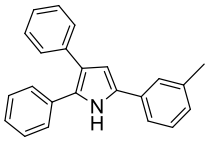


White solid yield 51 % (49.7 mg). ^{1}H NMR (500 MHz, DMSO): δ 3.77 (s, 3H), 6.61 (s, 1H), 6.95 (d, *J* = 8.0 Hz, 2H), 7.14 – 7.17 (m, 1H), 7.22 – 7.34 (m, 7H), 7.38 (d , *J* = 8.0 Hz, 2H), 7.71 (d, *J* = 8.5Hz, 2H), 11.25 (s, 1H) ;^{13}C NMR (125 MHz, DMSO): 55.5, 107.3, 114.5, 122.9,

125.6, 125.8, 125.9, 126.9, 128.3, 128.4, 128.7, 129.0, 132.5, 133.5, 137.2, 158.2. HRMS calcd for $C_{23}H_{20}NO$: 326.1545 found: 326.1545.

2,3-diphenyl-5-(m-tolyl)-1H-pyrrole (3h)[2]:

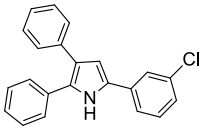
Silica gel 100 – 200 mesh size neutralised with 5% triethyl amine solution in hexane was used for column chromatography. 5% ethyl acetate in hexane used as an eluent. Due to impurities present in the product column was repeated with silica gel 100 – 200 mesh size and 5 % ethyl acetate in hexane solution used as an eluent.



White solid, yield 57 % (52.9 mg). ^{1}H NMR (500 MHz, DMSO): δ 2.34 (s, 3H), 6.74 (d, *J* = 2.5 Hz, 1H), 7.00 (d, *J* = 7.5 Hz, 1H), 7.16 (t, *J* = 7.0 Hz, 1H), 7.24 – 7.35 (m, 8H), 7.41 (d, *J* = 7.0 Hz, 2H), 7.58 (d, *J* = 8.0 Hz, 1H), 7.66 (s, 1H), 11.36 (s, 1H); ^{13}C NMR (125 MHz, DMSO): 21.6, 108.4, 121.6, 123.0, 124.9, 126.0, 127.0, 128.3, 128.5, 128.7, 128.9, 129.7, 132.5, 132.6, 133.4, 137.1, 138.1. HRMS calcd for $C_{23}H_{20}N$: 310.1596 found: 310.1577.

5-(3-chlorophenyl)-2,3-diphenyl-1H-pyrrole (3i):

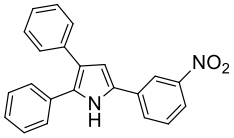
Silica gel 100 – 200 mesh size neutralised with 5% triethyl amine solution in hexane was used for column chromatography. 5% ethyl acetate in hexane used as an eluent. Due to present of impurities in the product column was repeated with silica gel 100 – 200 mesh size and 5 % ethyl acetate in hexane solution used as an eluent.



Light yellow viscus liquid, yield 56 % (55.4 mg). ^{1}H NMR (500 MHz, DMSO): δ 6.88 (d, *J* = 2.5 Hz, 1H), 7.16 – 7.30 (m, 7H), 7.33 – 7.42 (m, 5H), 7.74 (d, *J* = 8.0 Hz, 1H), 7.94 (s, 1H), 11.50 (s, 1H); ^{13}C NMR (125 MHz, DMSO): 109.6, 122.8, 123.3, 123.7, 125.8, 126.1, 127.3, 128.4, 128.6, 128.7, 130.6, 130.8, 130.9, 133.1, 134.1, 134.8, 136.8. IR: 3425, 2362, 1638, 1474, 1175, 1097, 951, 761, 691, 516. HRMS calcd for $C_{22}H_{17}ClN$: 330.1050 found: 330.1054.

5-(3-nitrophenyl)-2,3-diphenyl-1H-pyrrole (3j)[2]:

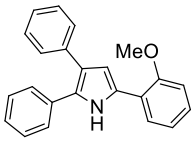
Silica gel 100 – 200 mesh size used for column chromatography. 5 % ethyl acetate in hexane solution was used as an eluent.



Red colour solid, yield 65 % (66.3 mg). ^{1}H NMR (500 MHz, DMSO): δ 7.02 (d, *J* = 2.5 Hz, 1H), 7.19 (t, *J* = 6.5 Hz, 1H), 7.27 – 7.32 (m, 5H), 7.37 (t, *J* = 7.5Hz, 2H); 7.43(d, *J* = 7.5 Hz, 2H) 7.65(t, *J* = 8.0 Hz, 1H), 8.00 (d, *J* = 8.0 Hz, 1H), 8.21 (d, *J* = 8.0 Hz, 1H), 8.72 (s, 1H), 11.77 (s, 1H); ^{13}C NMR (125 MHz, DMSO): 110.4, 118.1, 120.5, 123.5, 126.2, 127.5, 128.4, 128.7, 128.8, 130.1, 130.5, 131.3, 132.9, 134.4, 136.6, 149.0. HRMS calcd for $C_{22}H_{17}N_2O_2$: 341.1290 found: 341.1305.

5-(2-methoxyphenyl)-2,3-diphenyl-1H-pyrrole (3k):

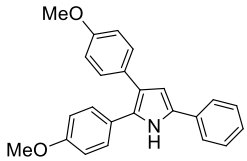
Silica gel 200 – 400 mesh size used for column chromatography. 1: 5: 94 triethyl amine ethyl acetate and hexane solution used as an eluent.



White solid, observed melting point 121.8 °C yield 50 % (48.8 mg). ^{1}H NMR (500 MHz, DMSO): δ 3.89 (s, 3H), 6.76 (d, *J* = 2.5 Hz, 1H), 6.99 (t, *J* = 7.5Hz, 1H); 7.08 (d, *J* = 6.5Hz, 1H), 7.15 – 7.18 (m, 1H), 7.20 – 7.27 (m, 6H), 7.32 (t, *J* = 8.0 Hz, 2H), 7.38 (d, *J* = 7.0 Hz, 2H), 7.73 (dd, J_1 = 9.0 Hz, J_2 = 1.5Hz, 1H), 11.00 (s, 1H); ^{13}C NMR (125 MHz, DMSO): 55.5, 111.3, 111.7, 120.6, 121.0, 122.1, 125.6, 126.6, 126.8, 127.3, 128.0, 128.1, 128.4, 128.7, 133.0, 136.9, 155.4.IR: 3418, 3061, 2836, 1638, 1600, 1472, 1238, 1167, 1122, 1022, 762, 732, 696, 612. HRMS calcd for $C_{23}H_{20}NO$: 326.1545 found: 326.1548.

2,3-bis(4-methoxyphenyl)-5-phenyl-1H-pyrrole (3l):

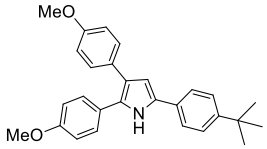
Silica gel 200 – 400 mesh size used for column chromatography. 10: 2: 88 dichloromethane, ethyl acetate and hexane solution used as an eluent.



White solid, observed melting point 128.3 °C yield 69 % (73.5 mg). ^{1}H NMR (500 MHz, DMSO): δ 3.73 (s, 3H), δ 3.76 (s, 3H), 6.67 (s, 1H), 6.84 (d, *J* = 8.5 Hz, 2H), 6.91 (d, *J* = 8.5 Hz, 2H), 7.15 – 7.20, (m, 3H), 7.32 – 7.37 (m, 4H), 7.75 (d, *J* = 7.5 Hz, 2H), 11.21 (s, 1H); ^{13}C NMR (125 MHz, DMSO): 55.4, 55.5, 108.1, 114.2, 122.0, 124.1, 126.0, 126.1, 129.0, 129.3, 129.5, 129.7, 131.6, 132.9, 157.7, 158.5. IR: 3416, 2367, 2341, 1605, 1520, 1492, 1241, 1177, 1024, 832, 761, 692, 520. HRMS calcd for $C_{24}H_{22}NO_2$: 356.1651 found: 356.1635.

5-(4-(tert-butyl)phenyl)-2,3-bis(4-methoxyphenyl)-1H-pyrrole (3m):

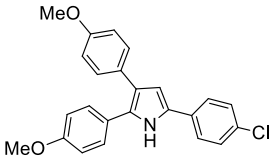
Silica gel 200 – 400 mesh size used for column chromatography. 10 : 2 : 88 dichloromethane, ethyl acetate and hexane solution used as an eluent.



White solid, observed melting point 69.5 °C yield 65 % (80.2 mg). ^{1}H NMR (500 MHz, DMSO): δ 1.29 (s, 9H), 3.73 (s, 3H), 3.76 (s, 3H), 6.59 (d, *J* = 2.0 Hz, 1H), 6.83 (d, *J* = 9.0 Hz, 2H), 6.90 (d, *J* = 8.5 Hz, 2H), 7.18(d, *J* = 8.5 Hz, 2H), 7.30 (d, *J* = 7.0 Hz, 2H), 7.36 (d, *J* = 7.0 Hz, 2H), 7.66 (d, *J* = 8.5 Hz, 2H), 11.13 (s, 1H); ^{13}C NMR (125 MHz, DMSO): 31.5, 34.6, 55.4, 55.5, 107.6, 114.2, 121.9, 124.0, 125.7, 126.0, 128.8, 129.3, 129.6, 129.7, 130.2, 131.7, 148.5, 157.6, 158.4. IR: 3484, 2958, 2371, 1637, 1508, 1246, 1175, 1030, 833, 529. HRMS calcd for $C_{28}H_{30}NO_2$: 412.2277 found: 412.2289.

5-(4-chlorophenyl)-2,3-bis(4-methoxyphenyl)-1H-pyrrole (3n):

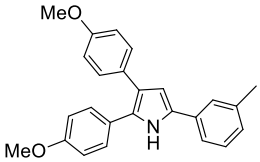
Silica gel 200 – 400 mesh size used for column chromatography. 10 : 2 : 88 dichloromethane, ethyl acetate and hexane solution used as an eluent.



White solid, observed melting point 133.6 °C yield 64 % (74.8 mg). ^{1}H NMR (500 MHz, DMSO): δ 3.73 (s, 3H), 3.76 (s, 3H), 6.70 (d, *J* = 2.5 Hz, 1H), 6.84 (d, *J* = 8.5 Hz, 2H), 6.91 (d, *J* = 9.0 Hz, 2H), 7.17 (d, *J* = 8.5 Hz, 2H), 7.30 (d, *J* = 8.5 Hz, 2H), 7.39 (d, *J* = 8.0 Hz, 2H), 7.77 (d, *J* = 8.5 Hz, 2H), 11.26 (s, 1H); ^{13}C NMR (125 MHz, DMSO): 54.5, 54.6, 107.9, 113.3, 121.4, 124.8, 124.9, 128.1, 128.5, 128.9, 129.3, 129.5, 131.0, 156.9. 157.7. IR: 3461, 2365, 1891, 1605, 1519, 1488, 1247, 1175, 1093, 1021, 954, 831, 801, 692. HRMS calcd for $C_{24}H_{21}ClNO_2$: 390.1261 found: 390.1278.

2,3-bis(4-methoxyphenyl)-5-(m-tolyl)-1H-pyrrole (3o):

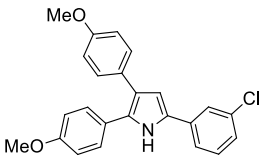
Silica gel 200 – 400 mesh size used for column chromatography. 10 : 2 : 88 dichloromethane, ethyl acetate and hexane solution used as an eluent.



Light yellow solid, observed melting point 162.6 °C yield 65 % (72 mg). ^{1}H NMR (500 MHz, DMSO): δ 2.33 (s, 3H), 3.73 (s, 3H), 3.76 (s, 3H), 6. 64 (d, *J* = 2.5 Hz, 1H), 6.83 (d, *J* = 8.5 Hz, 2H), 6.90 (d, *J* = 8.5 Hz, 2H), 6.97 (d, *J* = 7.5 Hz, 1H), 7.18 (d, *J* = 8.5 Hz, 2H), 7.23 (t, *J* = 7.5 Hz, 1H), 7.31 (d, *J* = 8.5 Hz, 2H), 7.54(d, *J* = 8.0 Hz, 1H), 7.61(s, 1H) 11.15 (s, 1H); ^{13}C NMR (125 MHz, DMSO): 21.0, 54.8, 55.0, 107.5, 113.6, 120.8, 121.4, 124.2, 125.5, 128.3, 128.6, 128.8, 129.1, 129.2, 131.2, 132.3, 137.4, 157.1, 157.9.IR: 3384, 2368, 1606, 1519, 1486, 1458, 1287, 1172, 1026, 827, 784, 691, 528. HRMS calcd for $C_{25}H_{24}NO_2$: 370.1807 found: 370.1805.

5-(3-chlorophenyl)-2,3-bis(4-methoxyphenyl)-1H-pyrrole (3p):

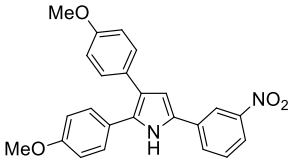
Silica gel 200 – 400 mesh size used for column chromatography. 10 : 2 : 88 dichloromethane, ethyl acetate and hexane solution used as an eluent.



Light yellow solid, observed melting point 126.4 °C yield 68 % (79.5 mg). ^{1}H NMR (500 MHz, DMSO): 3.73 (s, 3H), 3.77 (s, 3H), 6.78 (d, *J* = 2.5 Hz, 1H), 6.84 (d, *J* = 9 Hz, 2H), 6.92 (d, *J* = 8.5 Hz, 2H), 7.18 – 7.20 (m, 3H), 7.31 – 7.38 (m, 3H), 7.70 (d, *J* = 7.5 Hz, 1H), 7.89 (s, *J* = 1H), 11.30 (s, 1H); ^{13}C NMR (125 MHz, DMSO): 54.8, 55.0, 108.8, 113.6, 121.7, 122.1, 122.9, 124.9, 125.2, 128.8, 129.2, 129.4, 129.5, 130.2, 133.5, 134.4, 157.2, 158.1. IR: 3413, 2363, 1646, 1601, 1519, 1482, 1241, 1174, 1101, 1023, 828, 781, 761, 680, 587, 529. HRMS calcd for $C_{24}H_{21}ClNO_2$: 390.1261 found: 390.1243

2,3-bis(4-methoxyphenyl)-5-(3-nitrophenyl)-1H-pyrrole (3q):

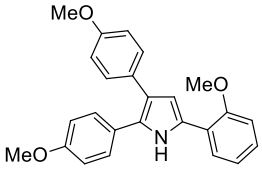
Silica gel 100 – 200 mesh size used for column chromatography. 10 % ethyl acetate in hexane solution was used as an eluent.



Red colour solid, observed melting point 148.1 °C yield 66 % (79.2 mg). ^{1}H NMR (500 MHz, DMSO): δ 3.74 (s, 3H), 3.78 (s, 3H), 6. 85 (d, *J* = 8.5 Hz, 2H), 6.93 (d, *J* = 9 Hz, 3H), 7.20 (d, *J* = 8.5 Hz, 2H), 7.34 (d, *J* = 8.0 Hz, 2H), 7.62 (t, *J* = 8.0 Hz, 1H), 7.97 (d, *J* = 8.0 Hz, 1H), 8.18 (d, *J* = 8.0 Hz, 1H), 8.68 (s, 1H), 11.58 (s, 1H); ^{13}C NMR (125 MHz, DMSO): 54.8, 55.0, 109.6, 113.7, 117.3, 119.6, 122.0, 125.0, 128.5, 128.7, 128.8, 129.3, 129.7, 129.9, 130.2, 134.1, 148.5, 157.3, 158.2. IR: 3397, 2937, 2367, 1616, 1518, 1347, 1244, 1176, 1029, 832, 800, 736. HRMS calcd for $C_{24}H_{21}N_2O_4$: 401.1501 found: 401.1531.

5-(2-methoxyphenyl)-2,3-bis(4-methoxyphenyl)-1H-pyrrole (3r):

Silica gel 200 – 400 mesh size used for column chromatography. 10: 2: 88 dichloromethane, ethyl acetate and hexane solution used as an eluent.

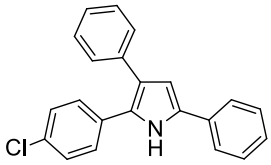


White colour solid, observed melting point 116.0 °C yield 67 % (77.4 mg). ^{1}H NMR (500 MHz, DMSO): 3.73 (s, 3H), 3.76 (s, 3H), 3.88 (s, 3H), 6. 69 (d, *J* = 2.5 Hz, 1H), 6.84 (d, *J* = 8.5 Hz, 2H), 6.90 (d, *J* = 8.5 Hz, 2H), 6.97 (t, *J* = 7.5 Hz, 1H), 7.06 (d, *J* = 8.5 Hz, 1H), 7.17 – 7.20 (m,

3H), 7.30 (d, *J* = 8.5 Hz, 2H), 7.72 (d, *J* = 7.5 Hz, 1H), 10.82 (s, 1H); ^{13}C NMR (125 MHz, DMSO): 55.4, 55.5, 55.9, 111.4, 112.1, 114.2, 121.0, 121.4, 121.5, 126.1, 126.9, 127.3, 128.2, 128.3, 129.4, 129.5, 129.8, 155.7, 157.7, 158.4. IR: 3418, 2365, 1638, 1521, 1489, 1458, 1289, 1241, 1172, 1124, 1027, 827, 792, 755, 674. HRMS calcd for $C_{25}H_{24}NO_3$: 386.1756 found: 386.1747.

2-(4-chlorophenyl)-3,5-diphenyl-1H-pyrrole (3s)[3]:

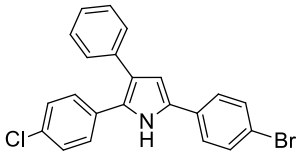
Silica gel 100 – 200 mesh size neutralised with 5% triethyl amine solution in hexane was used for column chromatography. 5% ethyl acetate in hexane used as an eluent. Due to impurities present in the product, column chromatography was repeated with silica gel 100 – 200 mesh size and 5 % ethyl acetate in hexane solution used as an eluent.



White colour solid, yield 65 % (64.3 mg). ^{1}H NMR (500 MHz, DMSO): δ 6. 77 (d, *J* = 2.0 Hz, 1H), 7.20 – 7.24 (m, 2H), 7.31 (d, *J* = 4.5 Hz, 4H), 7.39 – 7.44 (m, 6H), 7.81(d, *J* = 8.0 Hz, 2H), 11.47 (s, 1H); ^{13}C NMR (125 MHz, DMSO): 108.7, 123.7, 124.5, 126.3, 126.5, 128.4, 128.5, 128.7, 128.8, 129.1, 130.0, 131.5, 132.1, 132.6, 132.9, 136.8. HRMS calcd for $C_{22}H_{17}NCl$: 330.1050 found: 330.1056.

5-(4-bromophenyl)-2-(4-chlorophenyl)-3-phenyl-1H-pyrrole (3t):

Silica gel 100 – 200 mesh size neutralised with 5% triethyl amine solution in was used for column chromatography. 5% ethyl acetate in hexane used as an eluent. Due to impurities present in the product column chromatography was repeated with silica gel 100 – 200 mesh size and 5 % ethyl acetate in hexane solution used as an eluent.

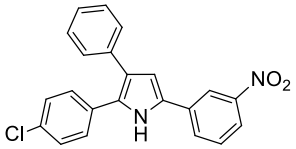


White colour solid, observed melting point 171.8 °C yield 72 % (88.2 mg). ^{1}H NMR (500 MHz, DMSO): δ 6. 80 (d, *J* = 2.5 Hz, 1H), 7.18 – 7.21 (m, 1H), 7.27 – 7.31 (m, 4H), 7.40 (s, 4H), 7.56

(d, *J* = 8.5 Hz, 2H), 7.74 (d, *J* = 8.5 Hz, 2H), 11.49 (s, 1H); ^{13}C NMR (125 MHz, DMSO): 108.8, 118.6, 123.3, 125.8, 127.9, 128.2, 128.3, 129.5, 131.0, 131.1, 131.3, 131.4, 136.0. IR: 3449, 2370, 1638, 1479, 1282, 1077, 824, 765, 699, 549, 520. HRMS calcd for $C_{22}H_{16}BrClN$: 408.0155 found: 408.0129.

2-(4-chlorophenyl)-5-(3-nitrophenyl)-3-phenyl-1H-pyrrole (3u):

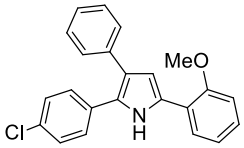
Silica gel 100 – 200 mesh size used for column chromatography. 5 % ethyl acetate in hexane solution was used as an eluent.



Red colour solid, observed melting point 158.5 °C yield 80 % (90 mg). ^{1}H NMR (500 MHz, DMSO): 7. 02 (d, *J* = 2.5 Hz, 1H), 7.20 – 7.22 (m, 1H), 7.30 (d, *J* = 5.5 Hz, 4H), 7.43 (s, 4H), 7.66 (t, *J* = 8.0 Hz, 1H), 8.01 (d, *J* = 7.5 Hz, 1H), 8.21 (d, *J* = 7.5 Hz, 1H), 8.71(s, 1H), 11.79 (s, 1H); ^{13}C NMR (125 MHz, DMSO): 110.6, 118.2, 120.7, 124.1, 126.4, 128.5, 128.8, 128.9, 129.8, 130.2, 130.5, 130.6, 131.7, 132.0, 134.3, 136.3, 149.0. IR: 3409, 2367, 1614, 1340, 1285, 1095, 825, 765, 732, 699. HRMS calcd for $C_{22}H_{16}ClN_2O_2$: 375.0900 found: 375.0918.

2-(4-chlorophenyl)-5-(2-methoxyphenyl)-3-phenyl-1H-pyrrole (3v):

Silica gel 200 – 400 mesh size used for column chromatography. 1: 5: 94 triethyl amine ethyl acetate and hexane solution used as an eluent.

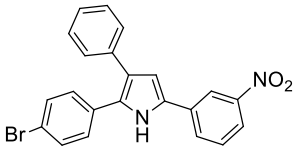


White colour solid, observed melting point 132.8 °C yield 72 % (77.5 mg). ^{1}H NMR (500 MHz, DMSO): 3.89 (s, 3H), 6.75 (d, *J* = 2.5 Hz, 1H), 7.00 (t, *J* = 7.0 Hz, 1H), 7.09 (d, *J* = 8.0 Hz, 1H), 7.18 – 7.31 (m, 6H), 7.37 – 7.41 (m, 4H), 7.73 (dd, J_1 = 9.0 Hz, J_2 = 1.5 Hz, 1H), 11.08 (s, 1H); ^{13}C NMR (125 MHz, DMSO): 54.6, 110.5, 110.7, 110.8, 119.7, 119.9, 121.8, 124.8, 126.0, 126.5, 127.2, 127.4, 127.5, 128.2, 128.6, 130.0, 130.9, 135.7, 154.6. IR: 3442, 2372, 1637, 1476,

1240, 1171, 1122, 1090, 1020, 823, 764, 740, 615. HRMS calcd for $C_{23}H_{19}ClNO$: 360.1155 found: 360.1173.

2-(4-bromophenyl)-5-(3-nitrophenyl)-3-phenyl-1H-pyrrole (3w):

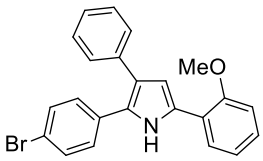
Silica gel 100 – 200 mesh size used for column chromatography. 5 % ethyl acetate in hexane solution was used as an eluent.



Red colour solid, observed melting point 160.5 °C yield 80 % (88 mg). ^{1}H NMR (500 MHz, DMSO): 7.02 (d, *J* = 2.5 Hz, 1H), 7.20 – 7.23 (m, 1H), 7.30 (d, *J* = 5.5 Hz, 4H), 7.36 (d, *J* = 8.5 Hz, 2H), 7.55 (d, *J* = 8.5 Hz, 2H), 7.66 (t, *J* = 8.0 Hz, 1H), 8.02 (d, *J* = 8.0 Hz, 1H), 8.21(d, *J* = 8.0 Hz, 1H), 8.71 (s 1H), 11.79 (s, 1H); ^{13}C NMR (125 MHz, DMSO): 110.3, 117.9, 120.1, 120.3, 123.7, 126.1, 128.1, 128.5, 129.4, 130.1, 131.3, 131.7, 133.9, 135.9, 148.6. IR: 3416, 2367, 1737, 1617, 1504, 1349, 1284, 1236, 1066, 822, 766, 741, 701. HRMS calcd for $C_{22}H_{16}BrN_2O_2$: 419.0395 found: 419.0369.

2-(4-bromophenyl)-5-(2-methoxyphenyl)-3-phenyl-1H-pyrrole (3x):

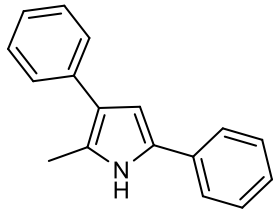
Silica gel 200 – 400 mesh size used for column chromatography. 1: 5: 94 triethyl amine, ethyl acetate and hexane solution used as an eluent.



White colour solid, observed melting point 162.3 °C yield 70 % (84.5 mg). ^{1}H NMR (500 MHz, DMSO): δ 3.88 (s, 3H), 6. 75 (d, *J* = 2.0 Hz, 1H), 7.00 (t, *J* = 7.5 Hz, 1H), 7.08 (d, *J* = 8.0 Hz, 1H), 7.18 – 7.34 (m, 9H), 7.50 (d, *J* = 8.5 Hz, 2H), 7.73 (d, *J* = 7.5 Hz, 1H), 11.08 (s, 1H); ^{13}C NMR (125 MHz, DMSO): 55.1, 111.2, 111.4, 119.1, 120.2, 120.5, 122.4, 125.4, 126.6, 127.1, 127.8, 128.1, 128.9, 129.5, 130.9, 131.8, 136.3, 155.1. IR: 3438, 2367, 1638, 1600, 1475, 1239, 1171, 1122, 1018, 764, 740, 699. HRMS calcd for $C_{23}H_{19}BrNO$: 404.0650 found: 404.0642.

2-methyl-3,5-diphenyl-1H-pyrrole (3y):

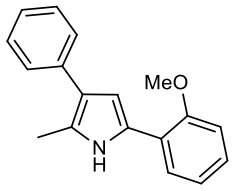
Silica gel 100 – 200 mesh size neutralised with 5% triethyl amine solution in hexane was used for column chromatography. 5% ethyl acetate in hexane used as an eluent



Light yellow oil, yield 83 % (58.0 mg). ^{1}H NMR (500 MHz, $CDCl_3$): δ 2.43 (s, 3H), 6. 62 (s, 1H), 7.16 – 7.22 (m, 2H), 7.32 – 7.39 (m, 4H), 7.44 (d, *J* = 8.0 Hz, 4H), 8.18 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$):12.3, 105.8, 122.4, 122.9, 124.9, 125.4, 127.0, 127.9, 128.4, 129.6, 132.1, 136.3: IR: 3401, 3072, 2360, 2338, 1606, 1496, 1450, 1157, 1070, 814, 759, 696, 581, 532. HRMS calcd for $C_{17}H_{16}N$: 234.1283 found: 234.1288.

5-(2-methoxyphenyl)-2-methyl-3-phenyl-1H-pyrrole (3z):

Silica gel 100 – 200 mesh size neutralised with 5% triethyl amine solution in hexane was used for column chromatography. 5% ethyl acetate in hexane used as an eluent

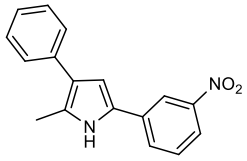


Light yellow oil, yield 81 % (63.9 mg). ^{1}H NMR (500 MHz, $CDCl_3$): δ 2.46 (s, 3H), 3.94 (s, 3H), 6.71 (d, *J* = 2.5 Hz, 1H),6.93 – 6.99 (m, 2H), 7.11 – 7.14 (m, 1H), 7.18 – 7.21 (m, 1H), 7.37 (t, *J* = 8.0 Hz, 2H), 7.45 – 7.47 (m, 2H) 7.64 (dd, J_1 = 9.0 Hz, J_2 = 1.5 Hz, 1H) 9.45 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$):12.5, 55.23, 106.1, 111.1, 120.4, 121.0. 121.3, 123.8, 124.6, 125.8, 125.9, 127.1, 127.3, 127.8, 136.6, 154.2. IR: 3446, 3059, 2938, 2841, 2361, 2337, 1709, 1600,

1493, 1242, 1156, 1123, 1024, 798, 751, 699, 667, 590. HRMS calcd for $C_{18}H_{18}NO$: 264.1388 found: 264.1381.

2-methyl-5-(3-nitrophenyl)-3-phenyl-1H-pyrrole (3aa):

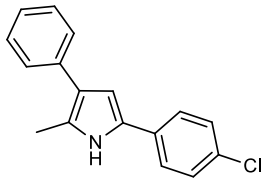
Silica gel 100 – 200 mesh size used for column chromatography. 10% ethyl acetate in hexane solution used as an eluent



Red colour solid, yield 93 % (77.5 mg). ^{1}H NMR (500 MHz, DMSO): δ 2.43 (s, 3H), 6. 97 (d, *J* = 3.0 Hz, 1H), 7.19 (t, *J* = 7.5 Hz, 1H), 7.38 (t, *J* = 7.5 Hz, 2H), 7.46 (d, *J* = 7.0 Hz, 2H), 7.61 (t, *J* = 8.0 Hz, 1H), 7.94 (dd, J_1 = 9.5 Hz, J_2 = 1.5 Hz, 1H), 8.07 (d, *J* = 8.0 Hz, 1H), 8.50 (s, 1H), 11.50 (s, 1H) ^{13}C NMR (125 MHz, DMSO):13.11, 108.0, 117.1, 119.8, 122.3, 125.4, 127.2, 127.5, 128.1, 128.9, 129.6, 130.6, 134.8, 136.8, 149.0. IR: 3441, 3373, 2361, 2338, 1638, 1524, 1350, 739, 669. HRMS calcd for $C_{17}H_{16}N_2O_2$: 279.1134 found: 279.1130.

5-(4-chlorophenyl)-2-methyl-3-phenyl-1H-pyrrole (3ab):

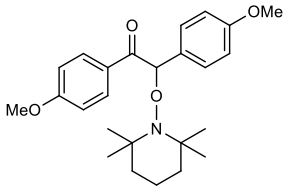
Silica gel 100 – 200 mesh size neutralised with 5% triethyl amine solution in hexane was used for column chromatography. 5% ethyl acetate in hexane used as an eluent.



Light yellow oil, yield 80 % (64.0 mg). ^{1}H NMR (500 MHz, $CDCl_3$): δ 2.42 (s, 3H), 6. 58 (d, *J* = 3.0 Hz, 1H), 7.20 (t, *J* = 7.5 Hz, 1H), 7.28 (d, *J* = 8.5 Hz, 2H), 7.35 – 7.39 (m, 4H), 7.42 – 7.44 (d, *J* = 7 Hz, 2H), 8.14 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$):12.2, 106.2, 122.6, 124.0, 125.0, 125.3, 127.0, 127.9, 128.5, 130.5, 130.9, 136.0. IR: 3432, 3057, 2920, 2362, 2338, 1604, 1495, 1444, 1259, 1154, 1093, 827, 802, 765, 700, 658, 510. HRMS calcd for $C_{17}H_{15}NCl$: 268.0893 found: 268.088

1,2-bis(4-methoxyphenyl)-2-((2,2,6,6-tetramethylpiperidin-1-yl)oxy)ethanone (4):

Silica gel 100 – 200 mesh size used for column chromatography. 5% ethyl acetate in hexane used as an eluent



Colourless oil, yield 70 % (129 mg). ^{1}H NMR (500 MHz, $CDCl_3$): δ 0.81 (s, 3H), 0.98 (s, 3H), 1.17 (s, 6H), 1.25 – 1.44 (m, 6H), 3.73 (s, 3H), 3.82 (s, 3H), 5.88 (s, 1H), 6.80 (d, *J* = 8.5 Hz, 2H), 6.86 (d, *J* = 8.5 Hz, 2H), 7.39 (d, *J* = 8.5 Hz, 2H), 8.06 (d, *J* = 8.5 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): 17.1, 20.3, 20.4, 33.3, 33.8, 55.2, 55.4, 59.7, 60.0, 92.7, 113.6, 113.8, 128.3, 128.5, 130.4, 131.6, 159.0, 163.3, 197.0. HRMS calcd for $C_{25}H_{34}NO_4$: 412.2488 found: 412.2491.

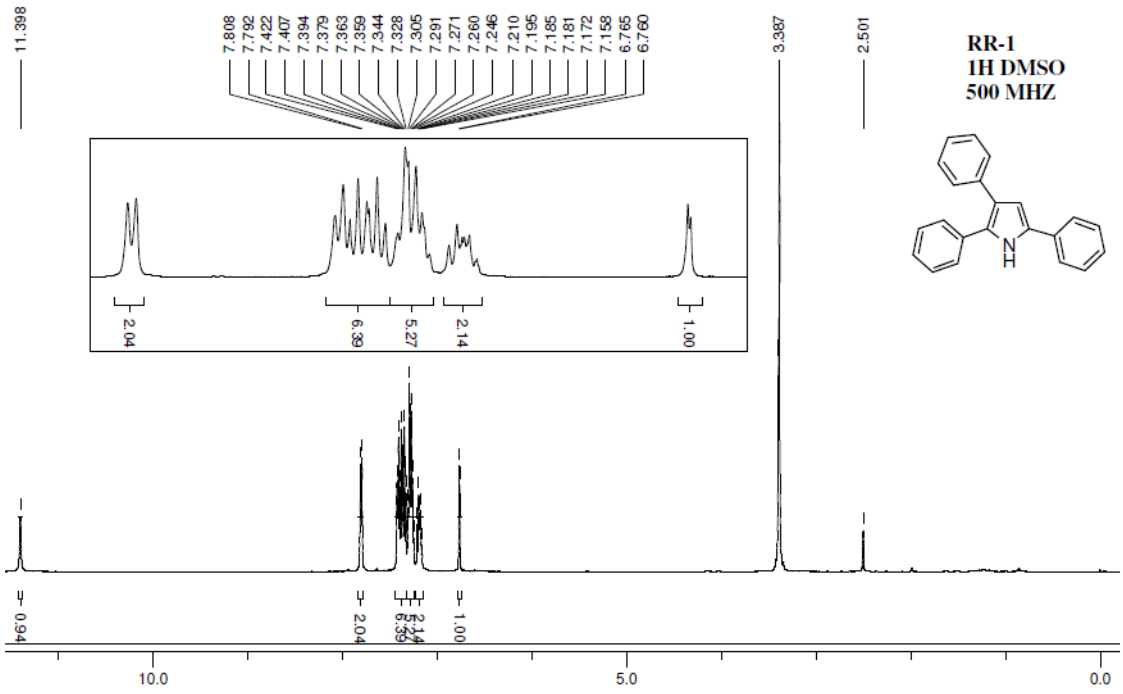
Refferences:

1) (a) Donthiri, R. R.; Pappula, V.; Reddy, N. N. K.; Bairagi, D.; Adimurthy, S.; *J. Org. Chem*. **2014**, *79* ,11277. (b) Gu, P.; Su, Y.; Wu, X.-P.; Sun, J.; Liu, W.-Y.; Xue, P.; Li, R. Org. Lett. **2012**, *14*, 2246.

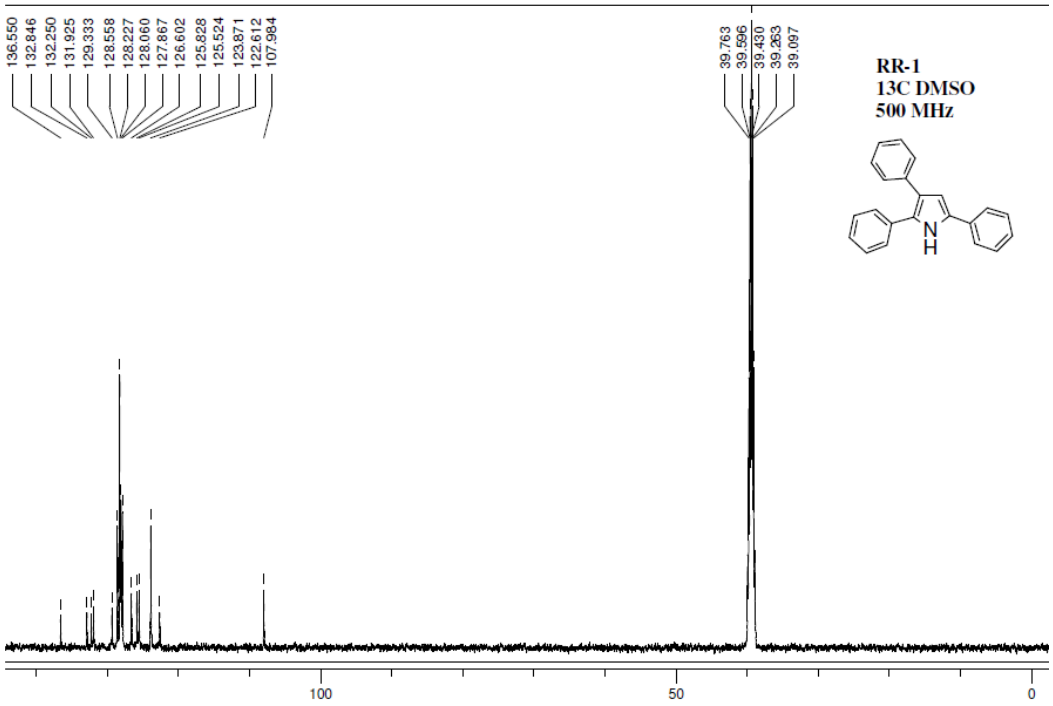
2) Xu, Y.-H.; He, T.; Zhang, Q.-C.; Loh, T.-P. *Chem. Commun*. **2014**, *50*, 2784.

3) Shen, J.; Cheng, G.; Cui, X. *Chem. Commun.* **2013**, *49*, 10641.

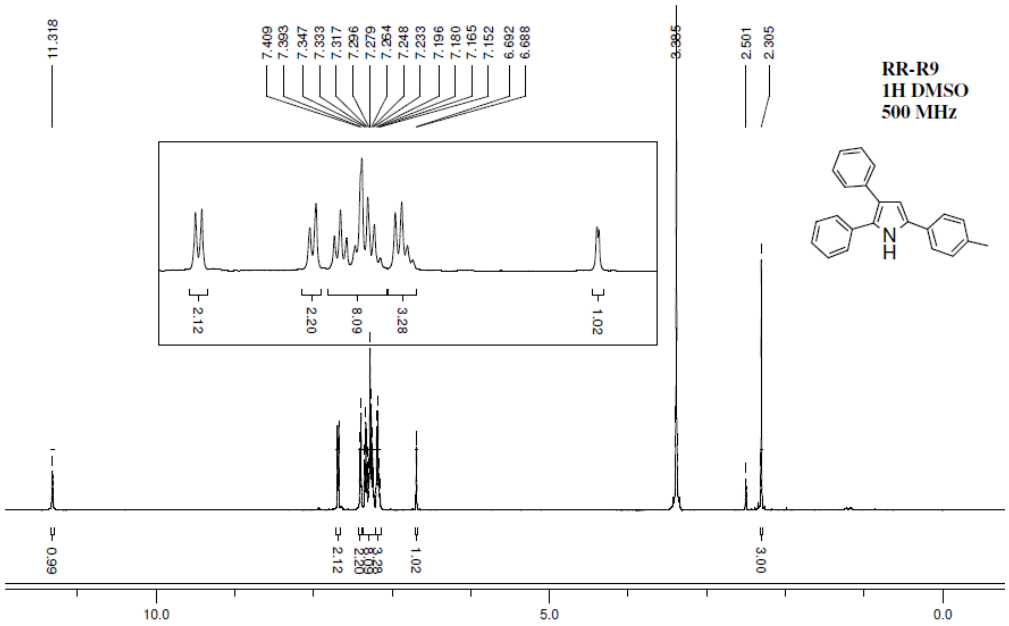
Copies of ^{1}H and ^{13}C NMR spectra



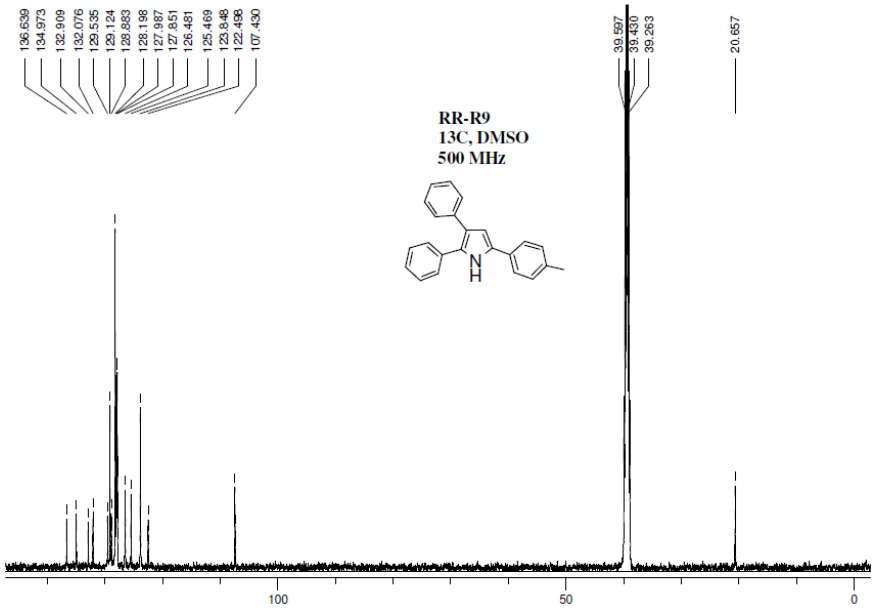
^{1}H NMR (Table 2, **3a**)



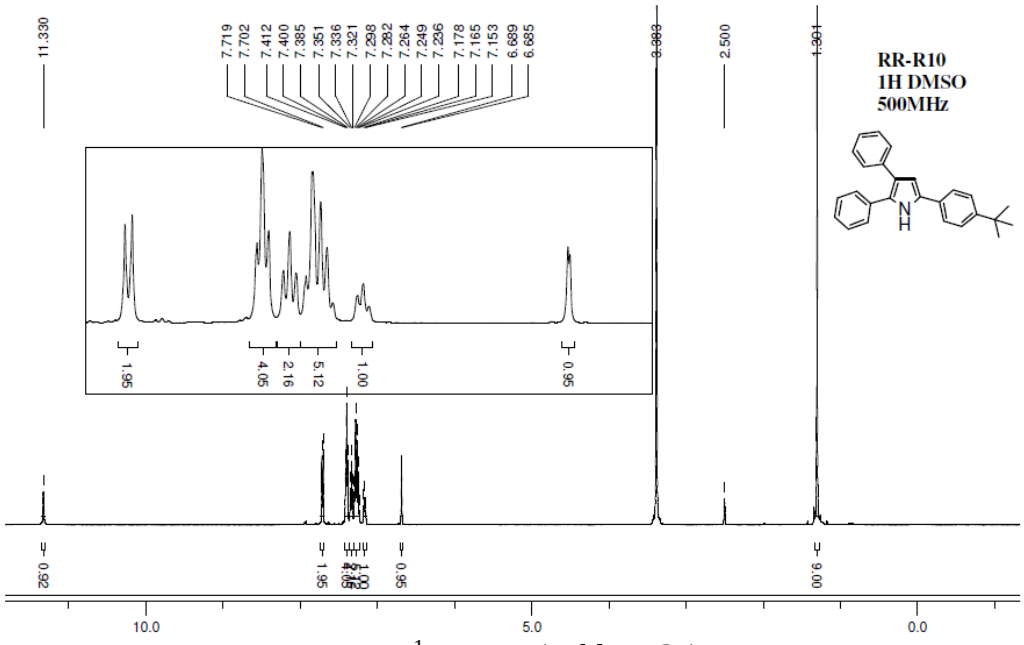
^{13}C NMR (Table 2, **3a**)



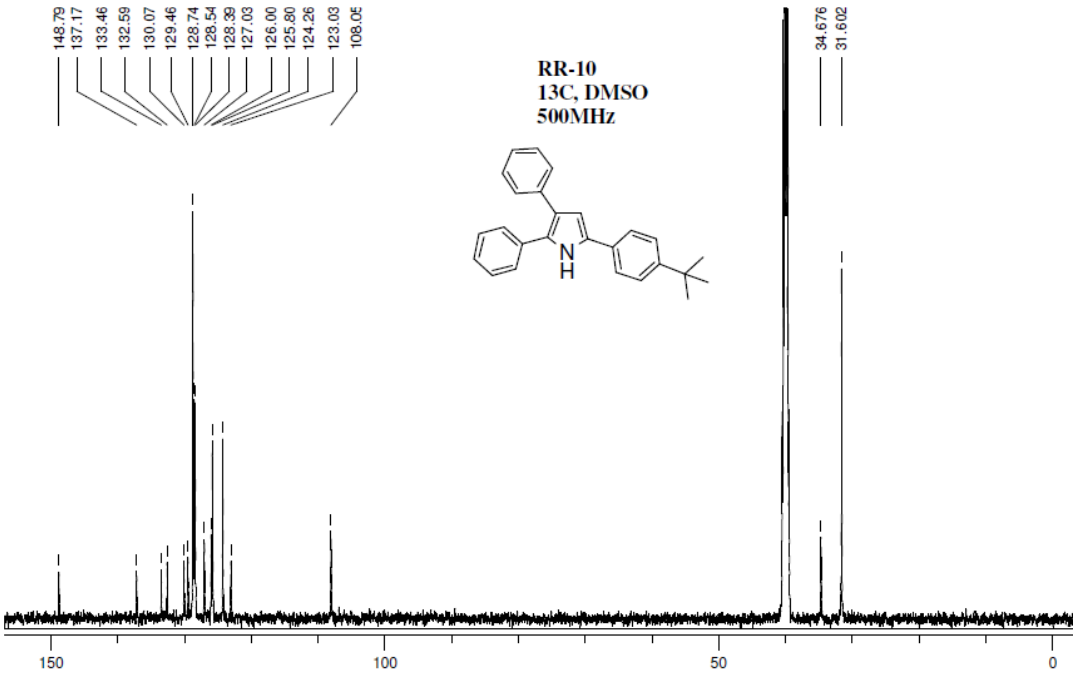
^{1}H NMR (Table 2, **3b**)



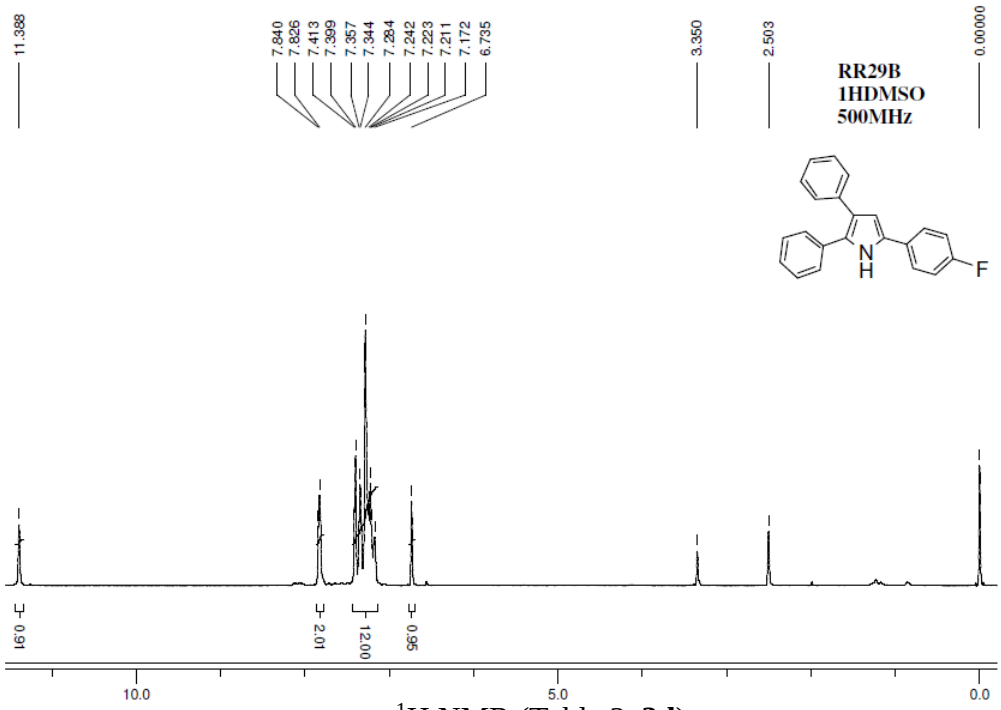
^{13}C NMR (Table 2, **3b**)



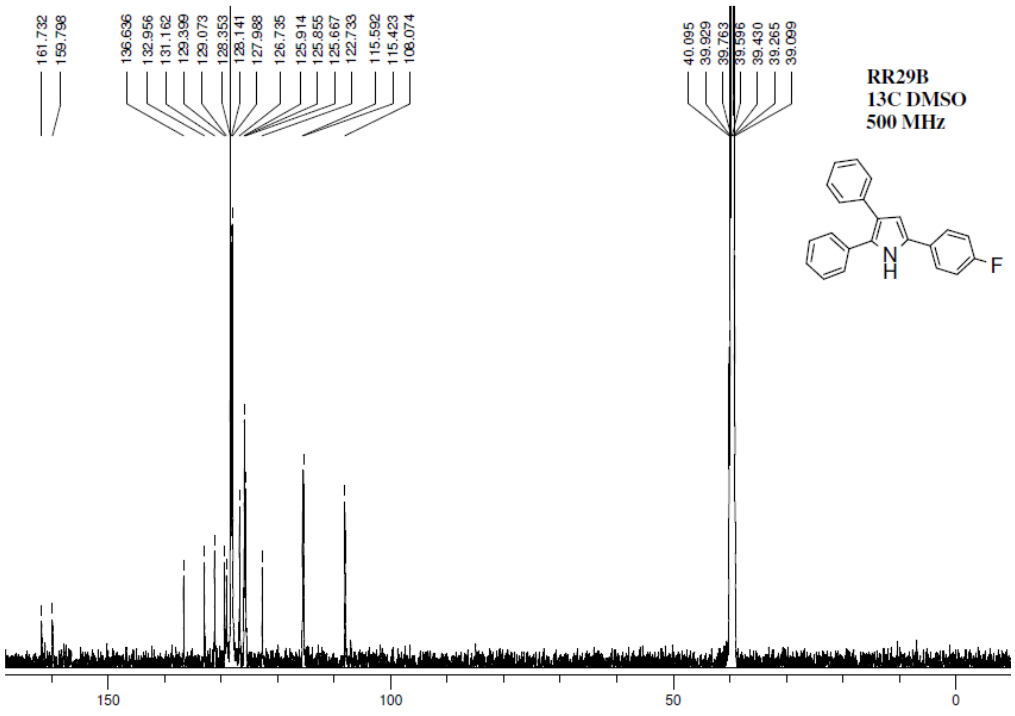
^{1}H NMR (Table 2, **3c**)



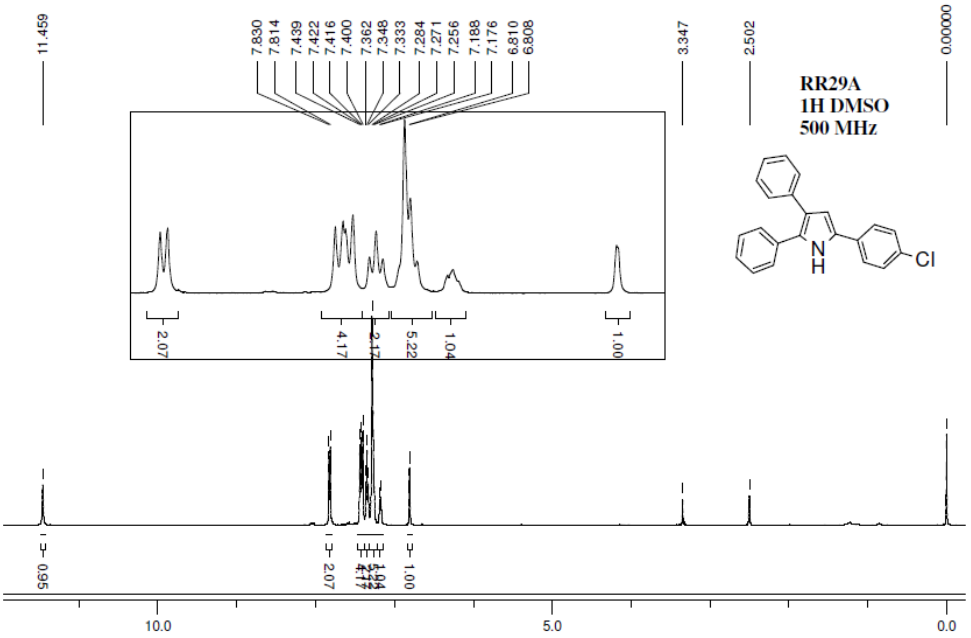
^{13}C NMR (Table 2, **3c**)



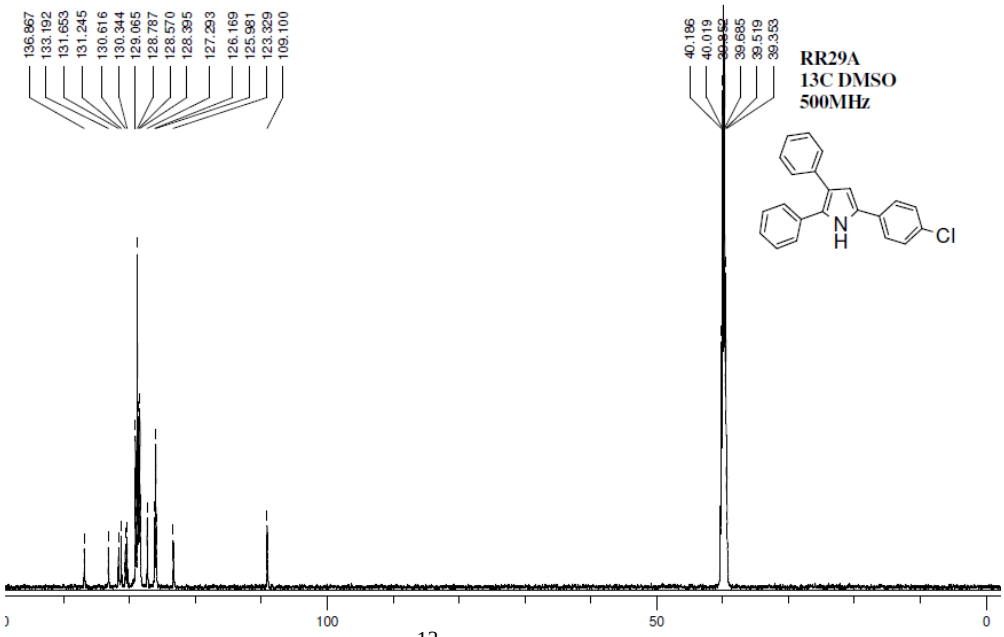
^{1}H NMR (Table 2, **3d**)



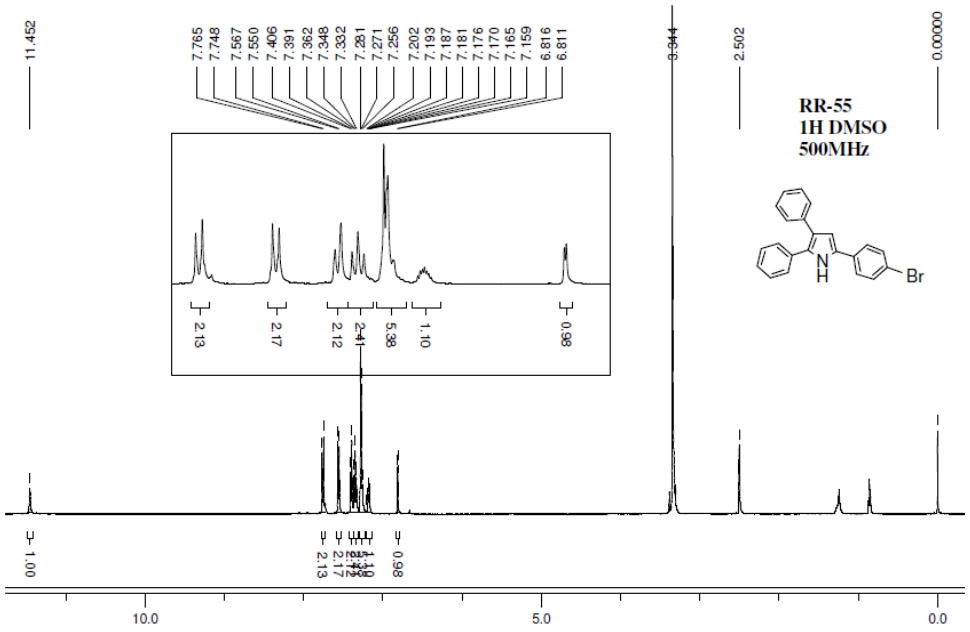
^{13}C NMR (Table 2, **3d**)



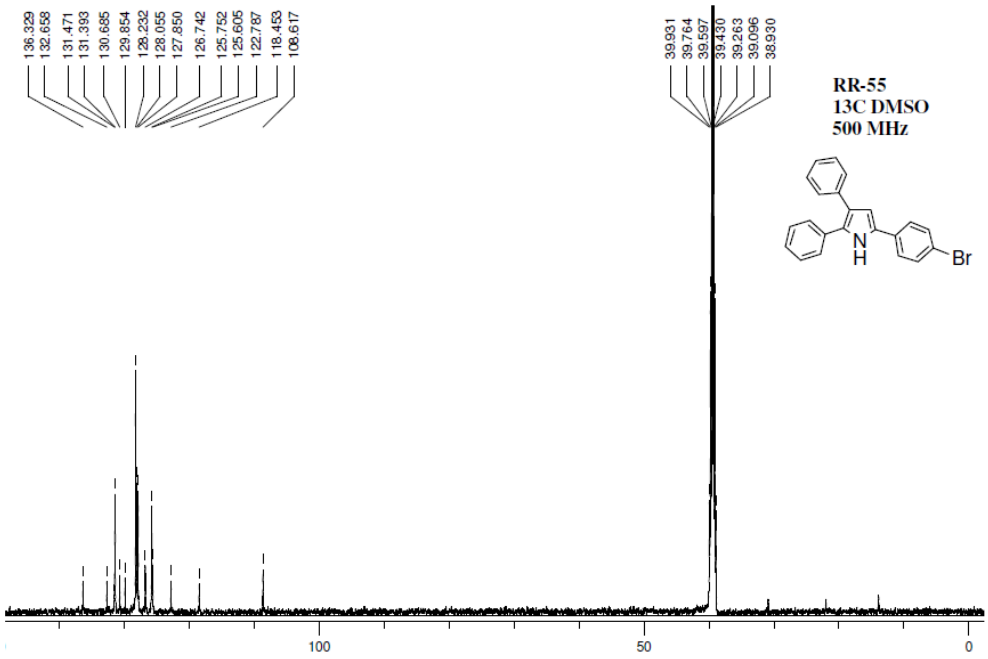
^{1}H NMR (Table 2, **3e**)



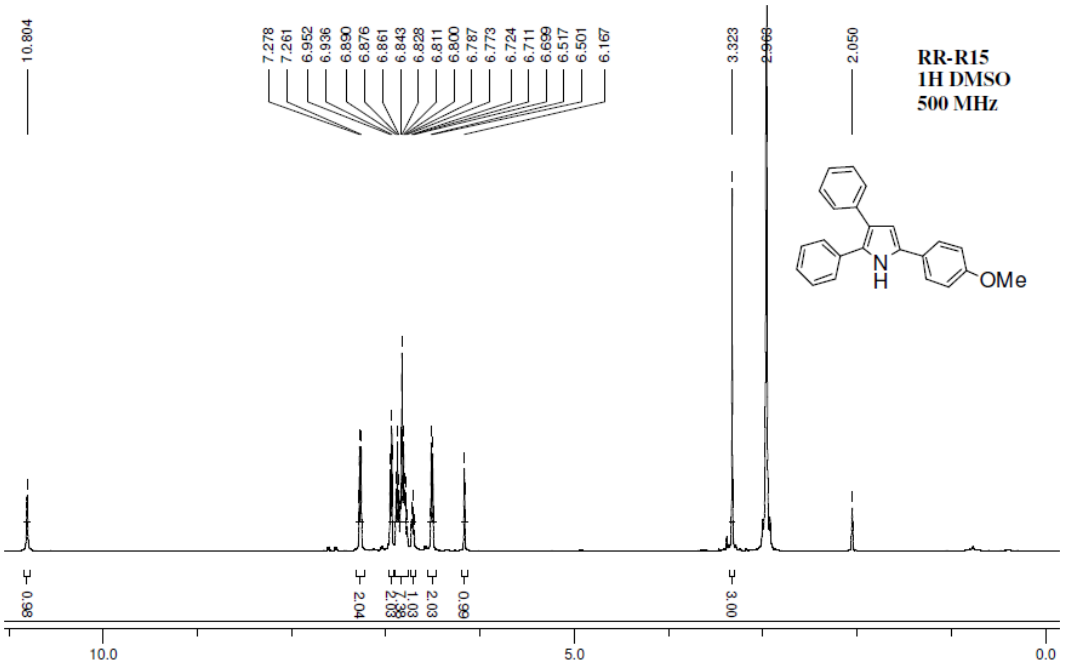
^{13}C NMR (Table 2, **3e**)



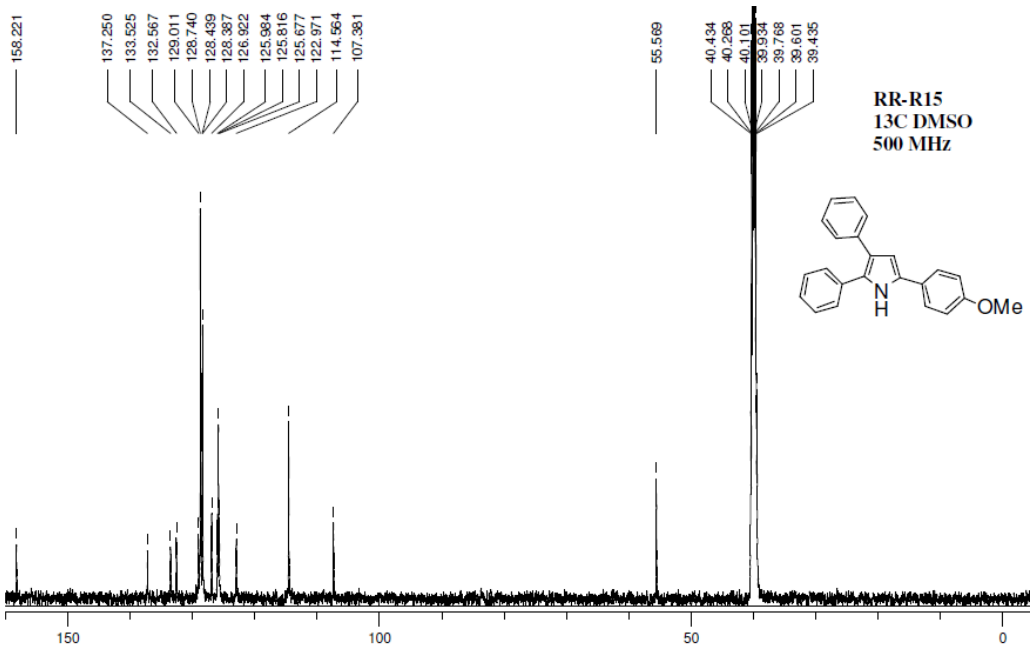
^{1}H NMR (Table 2, **3f**)



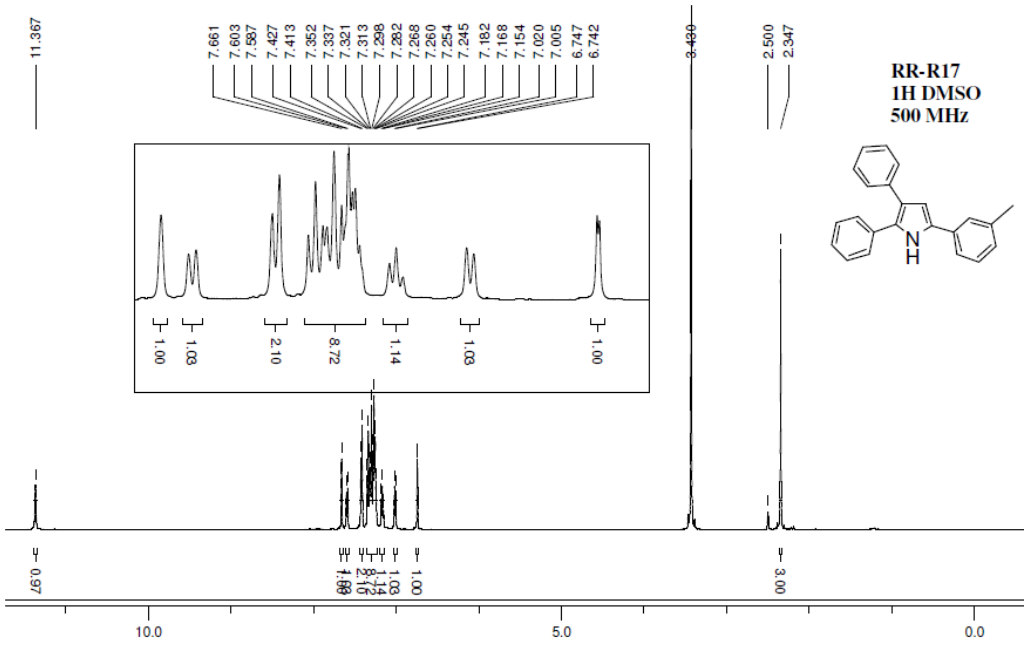
^{13}C NMR (Table 2, **3f**)



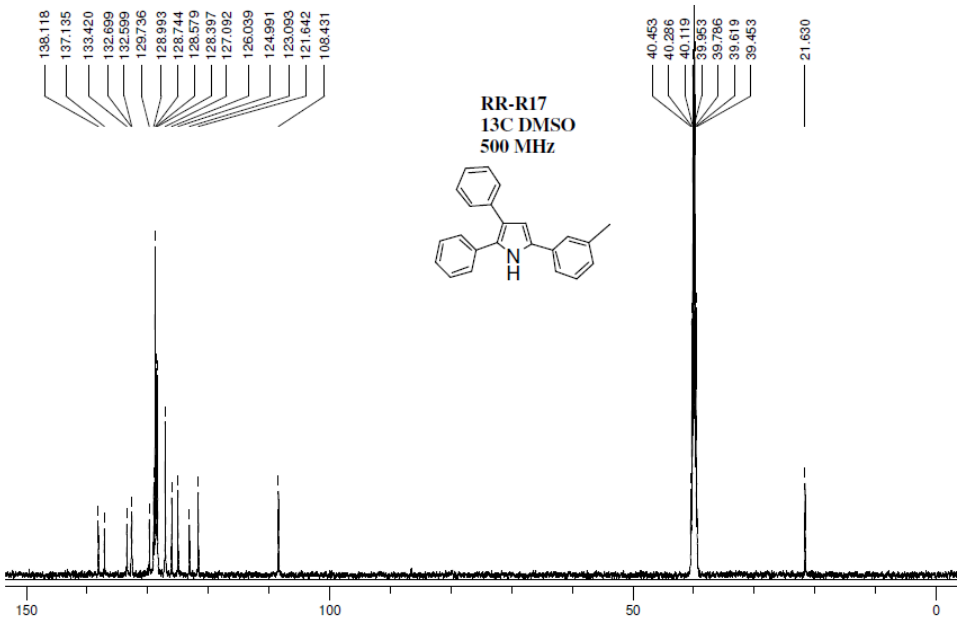
^{1}H NMR (Table 2, **3g**)



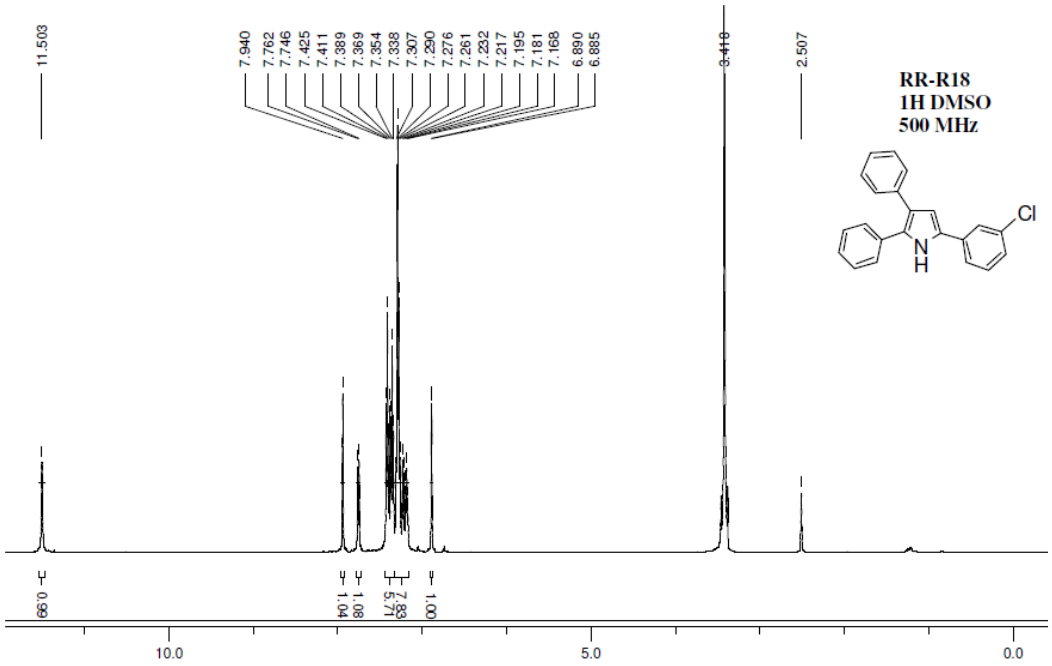
^{13}C NMR (Table 2, **3g**)



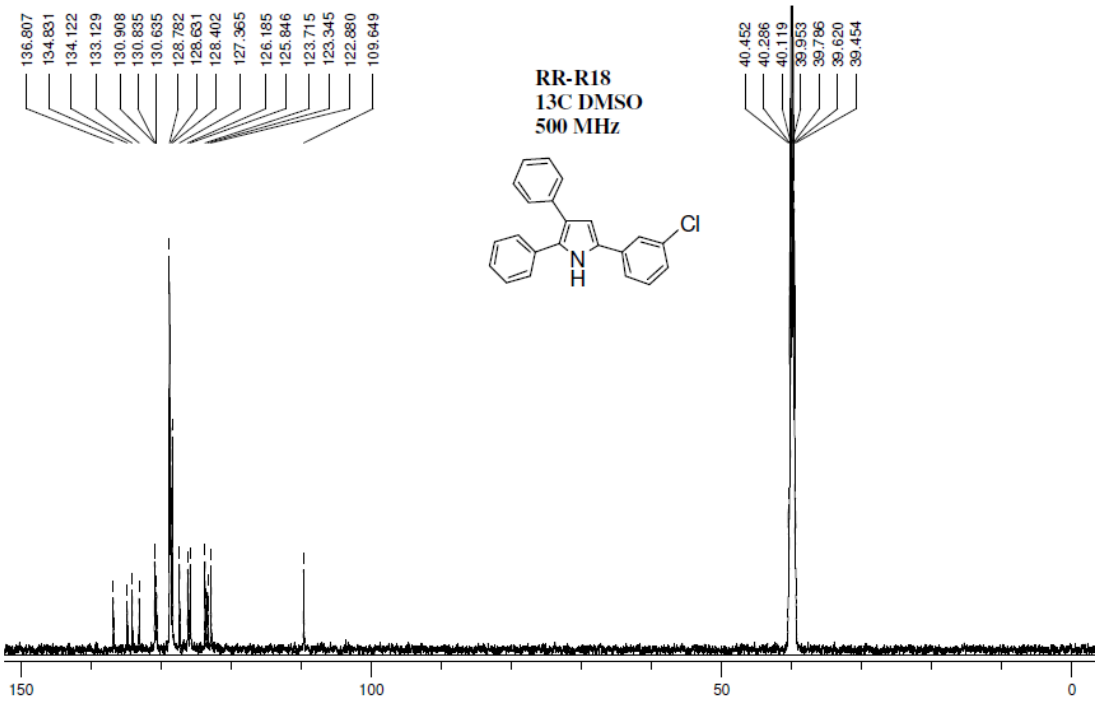
^{1}H NMR (Table 2, **3h**)



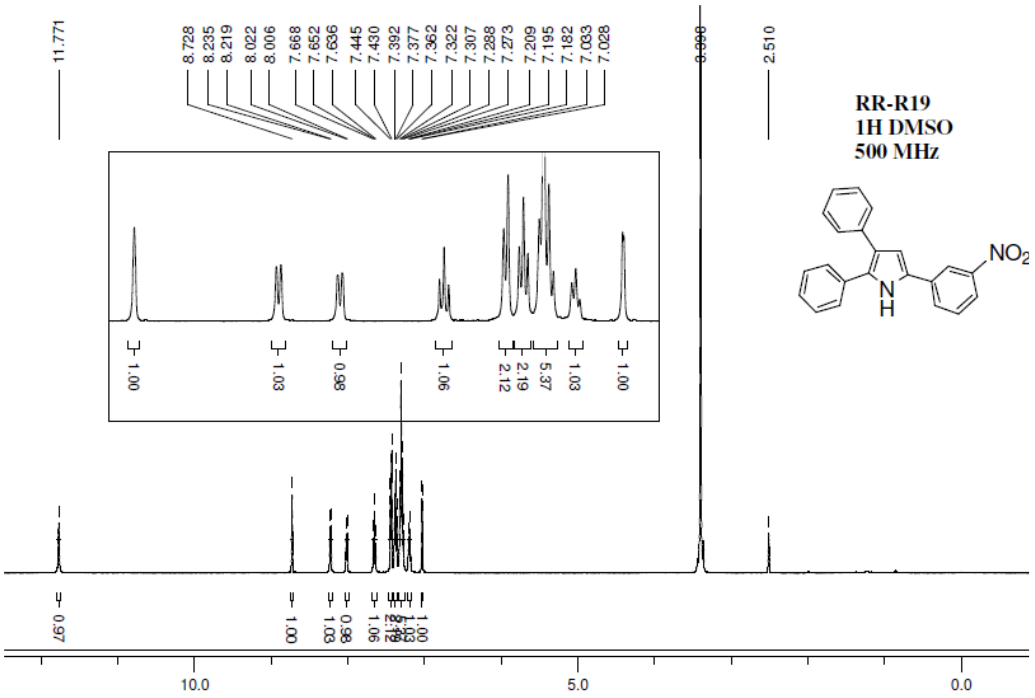
^{13}C NMR (Table 2, **3h**)



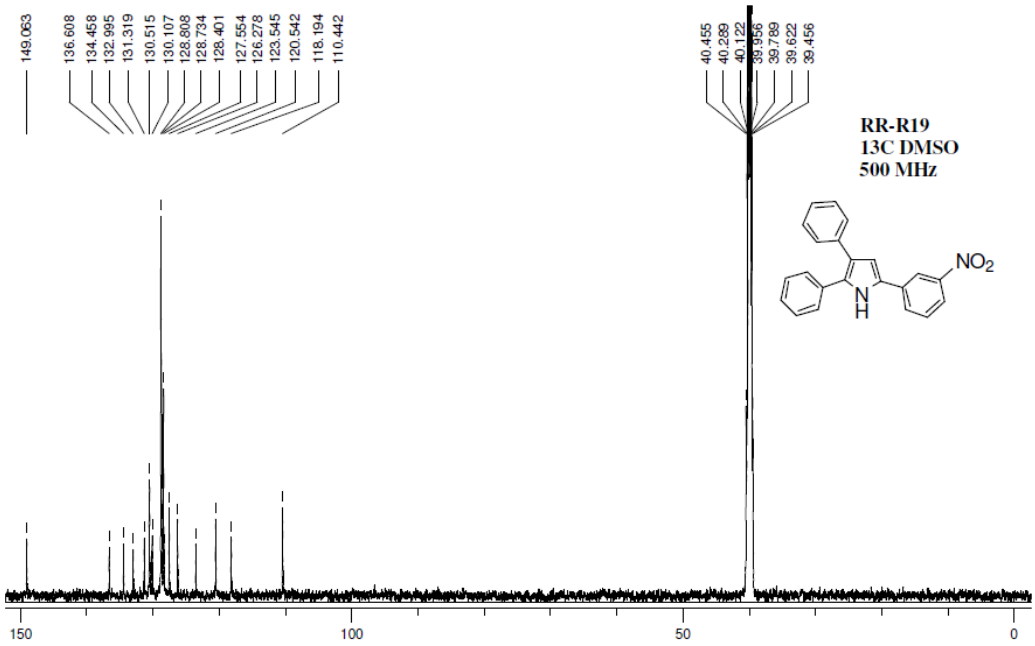
^{1}H NMR (Table 2, **3i**)



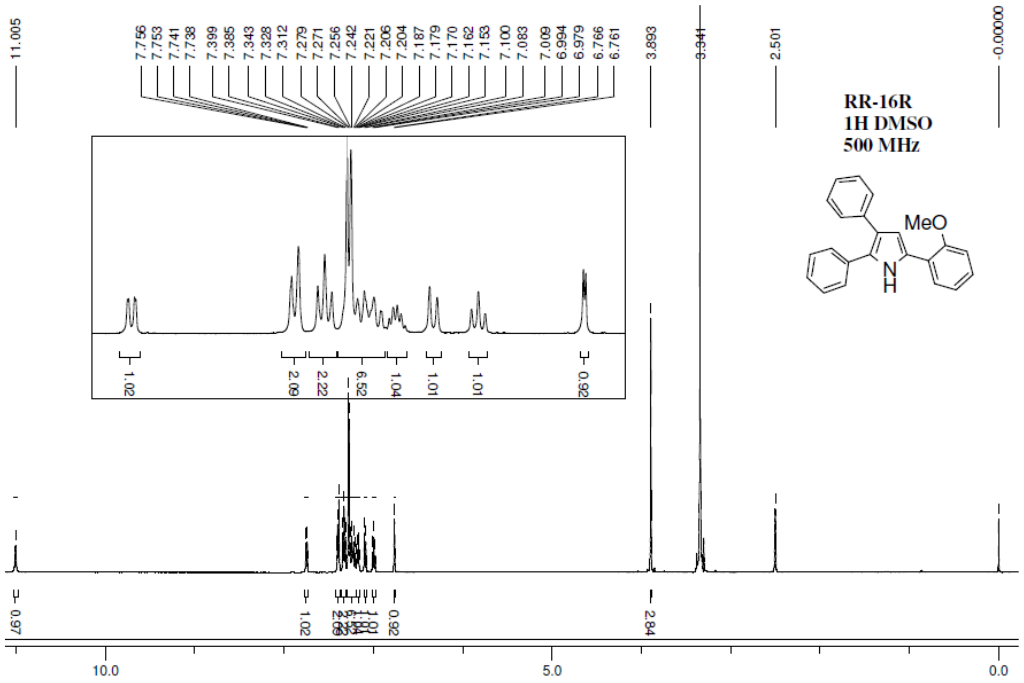
^{13}C NMR (Table 2, **3i**)



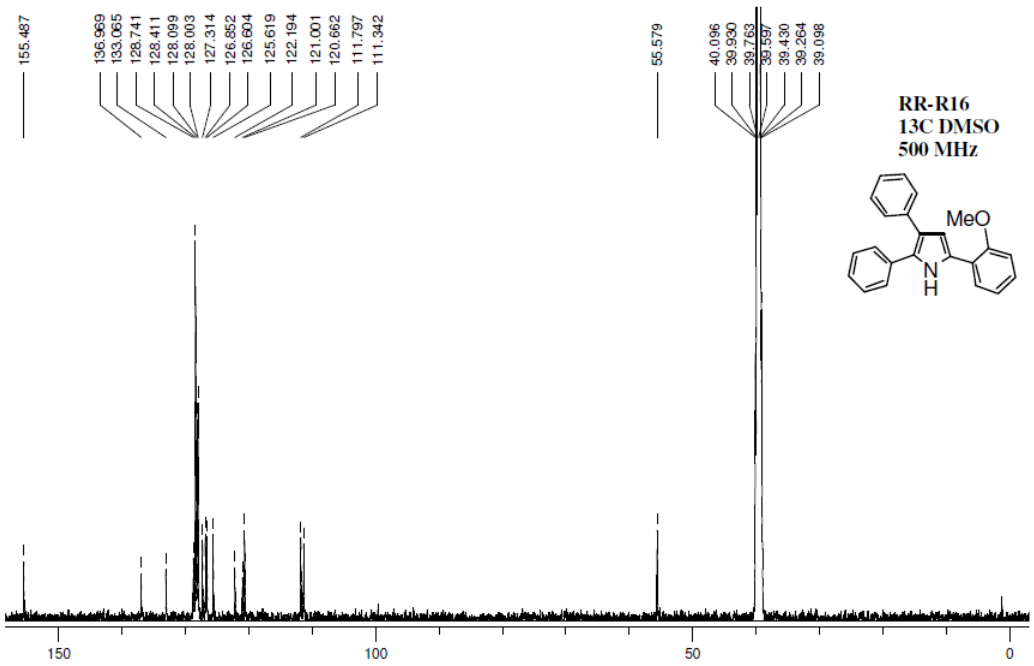
^{1}H NMR (Table 2, **3j**)



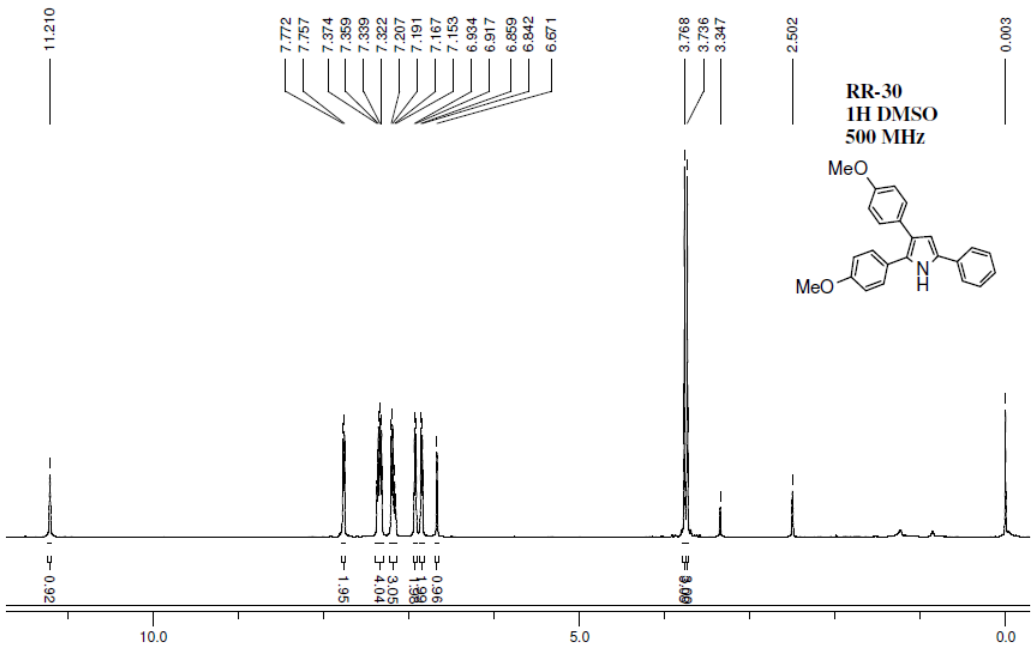
^{13}C NMR (Table 2, **3j**)



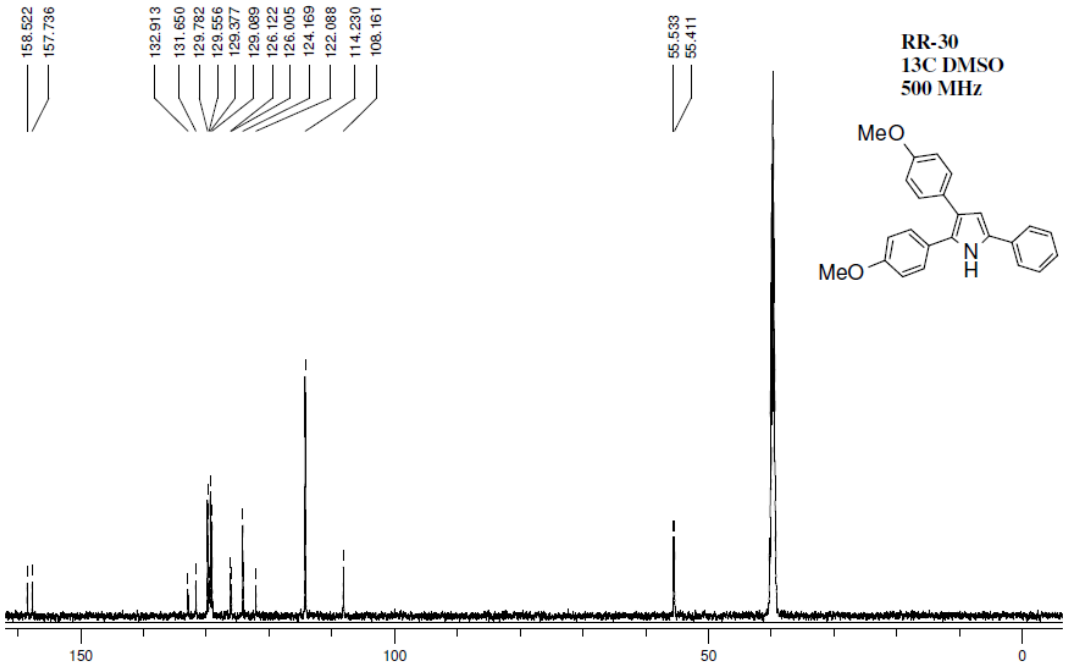
^{1}H NMR (Table 2, **3k**)



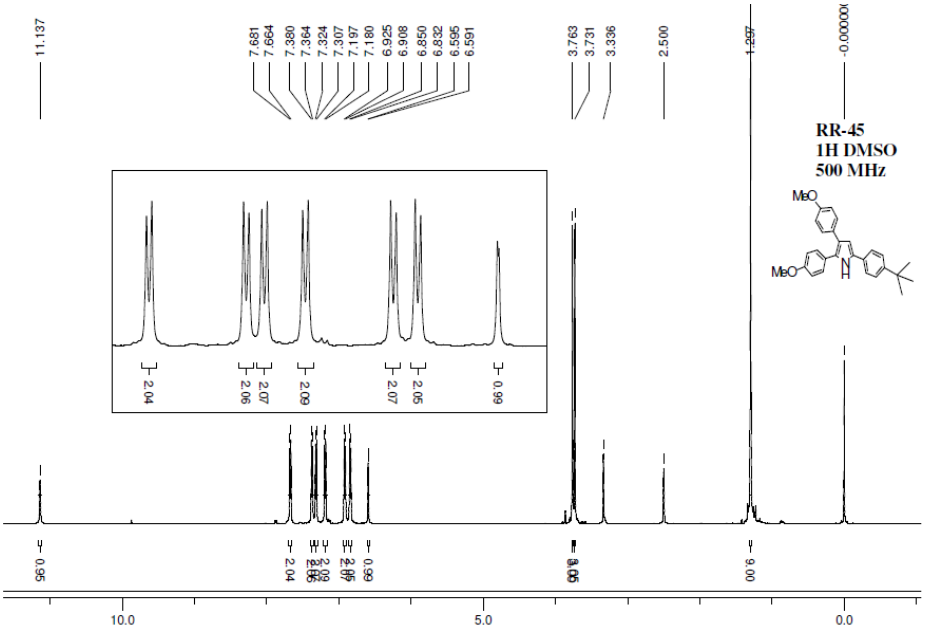
^{13}C NMR (Table 2, **3k**)



^{1}H NMR (Table 2, **3l**)



^{13}C NMR (Table 2, **3l**)



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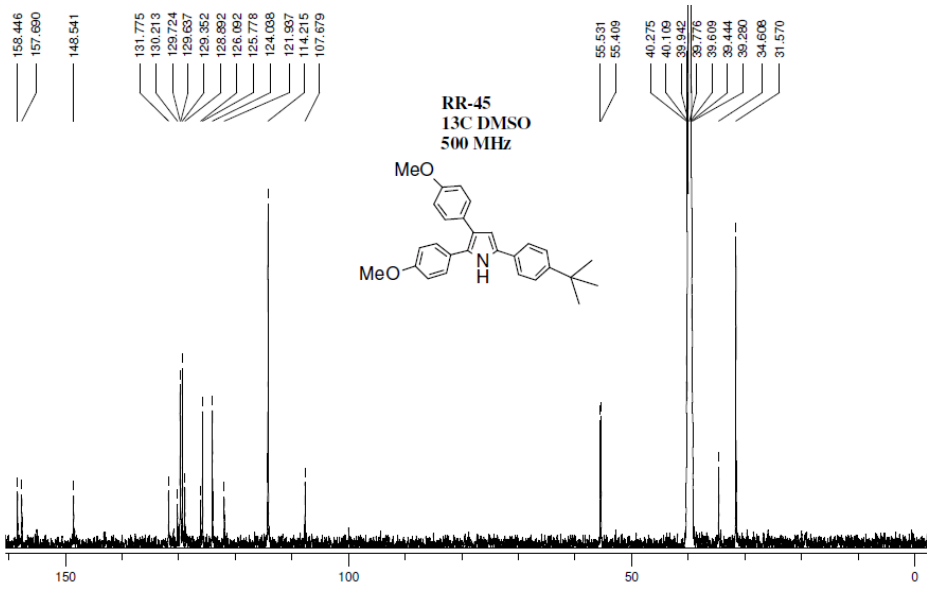
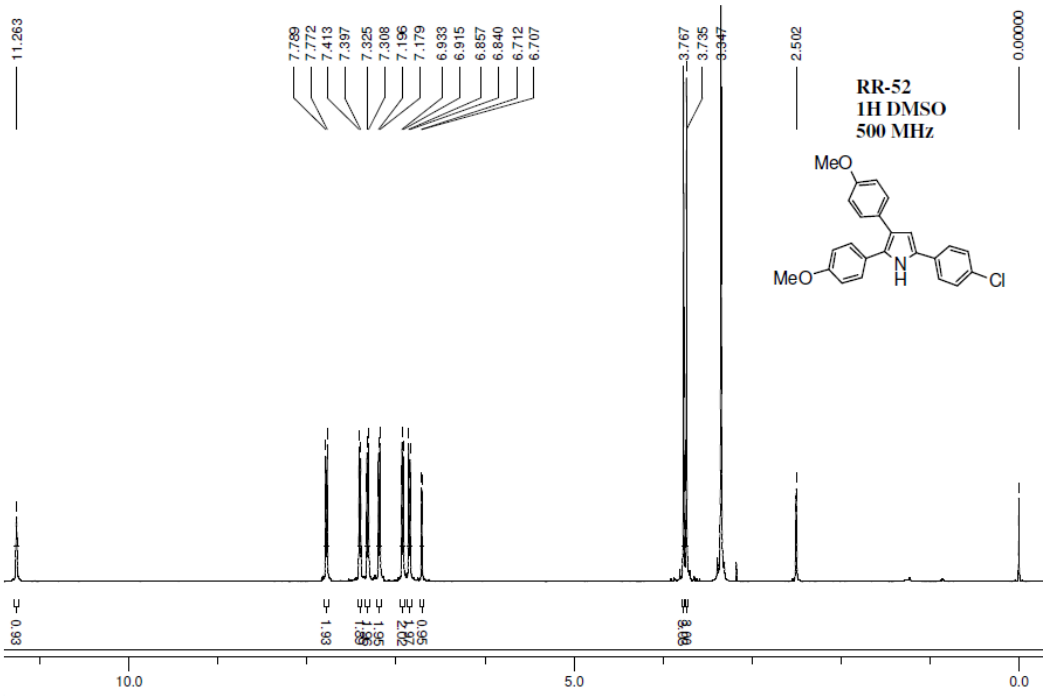
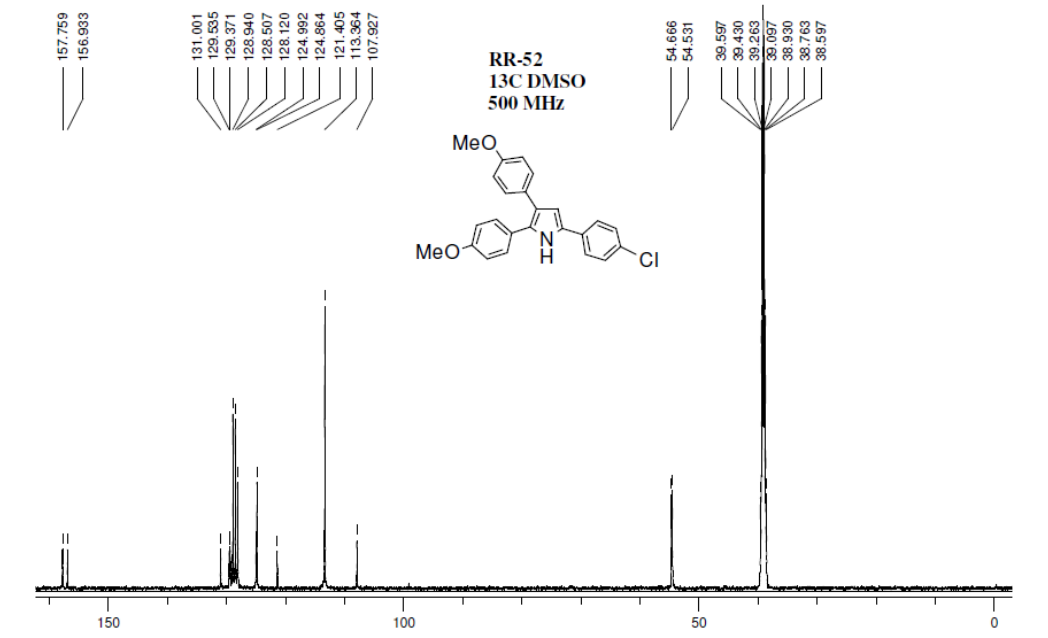


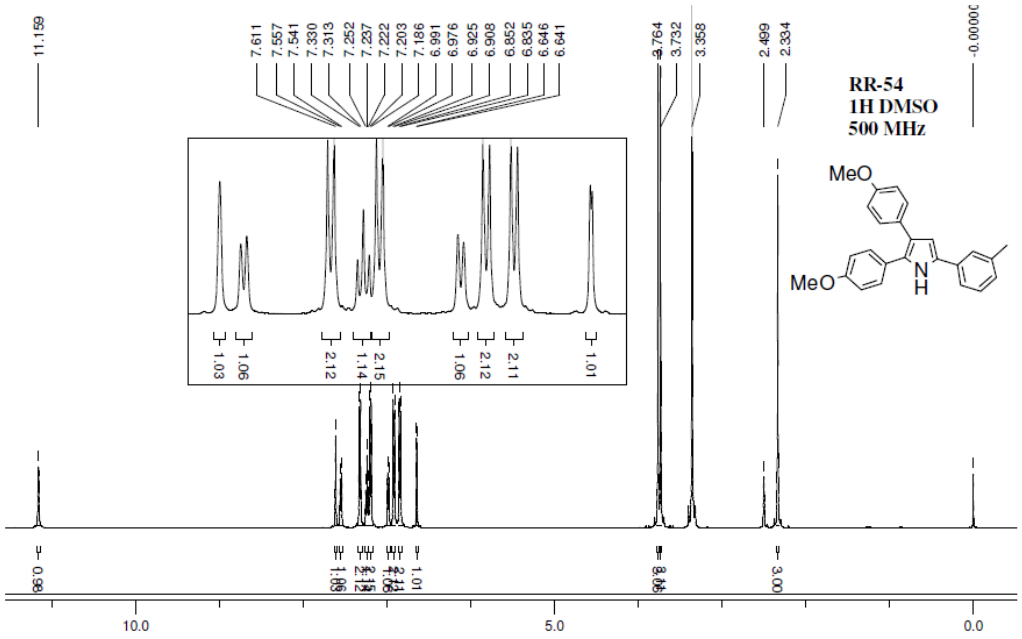
^{13}C NMR (Table 2, **3m**)



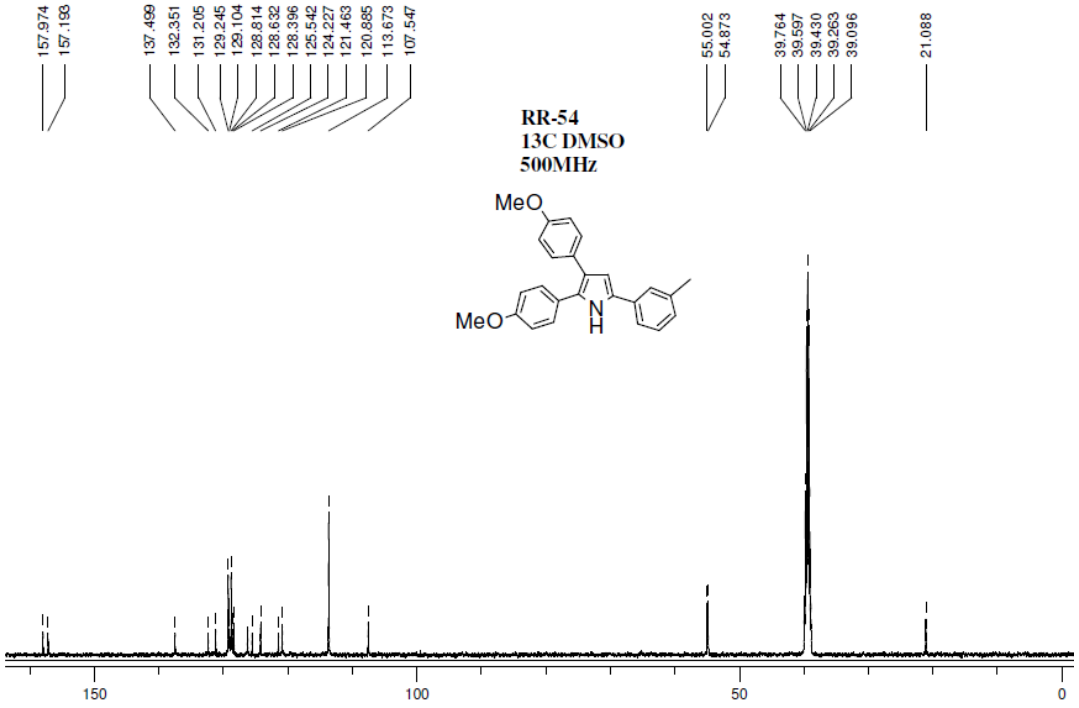
^{1}H NMR (Table 2, **3n**)



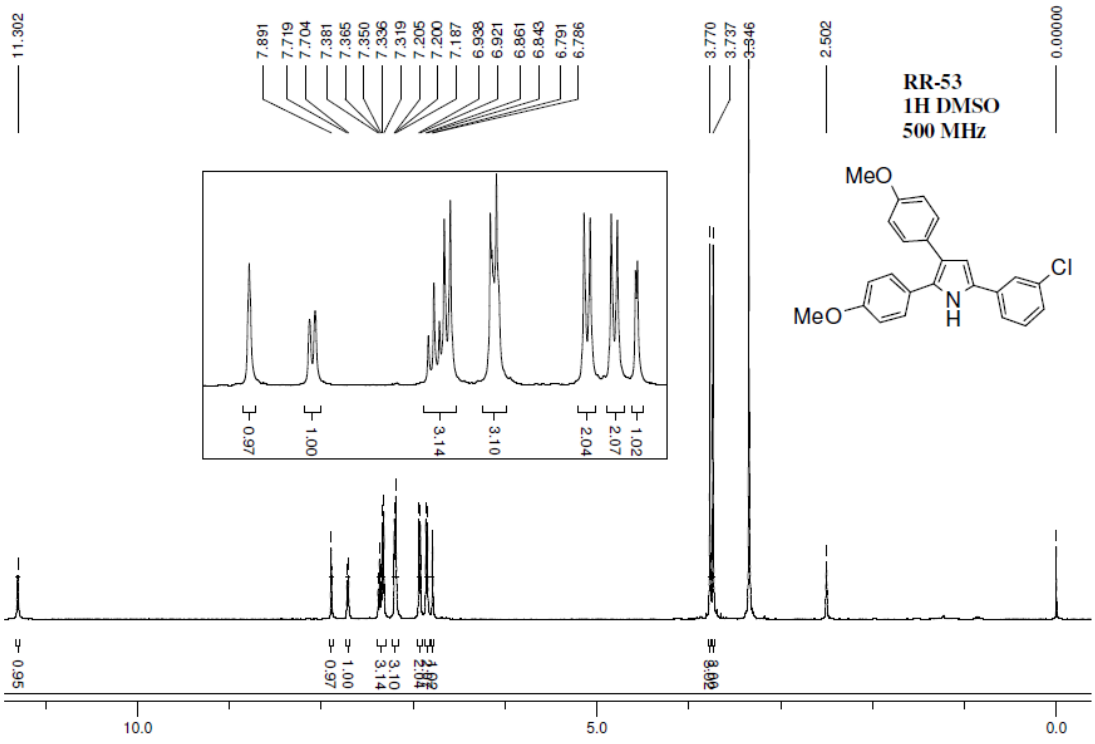
^{13}C NMR (Table 2, **3n**)



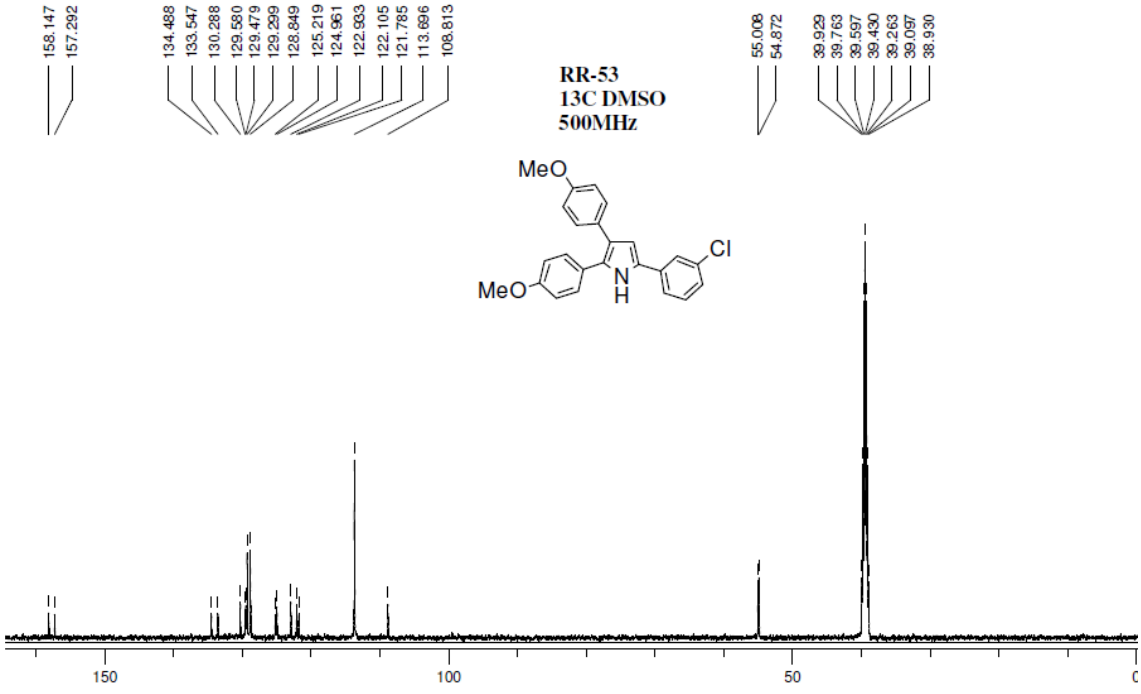
^{1}H NMR (Table 2, **3o**)



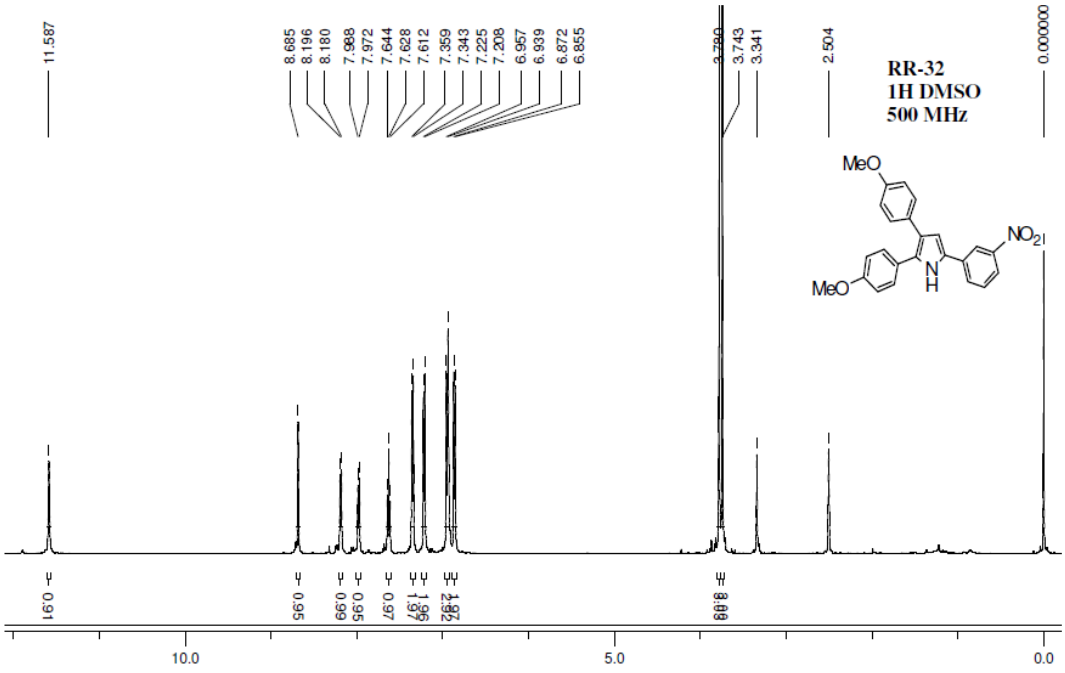
^{13}C NMR (Table 2, **3o**)



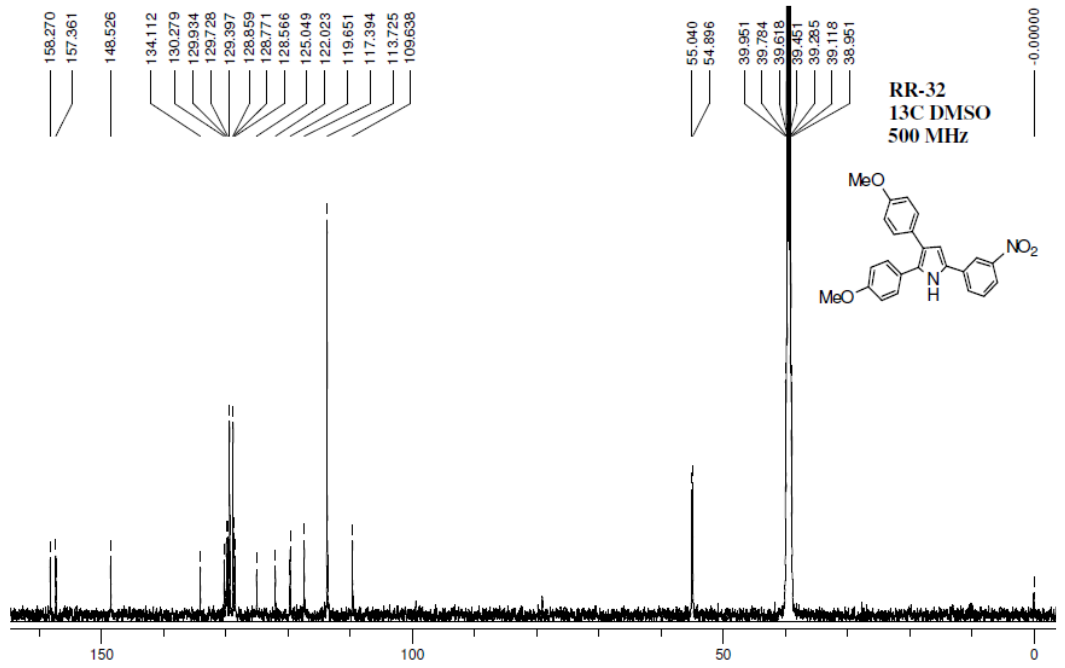
^{1}H NMR (Table 2, **3p**)



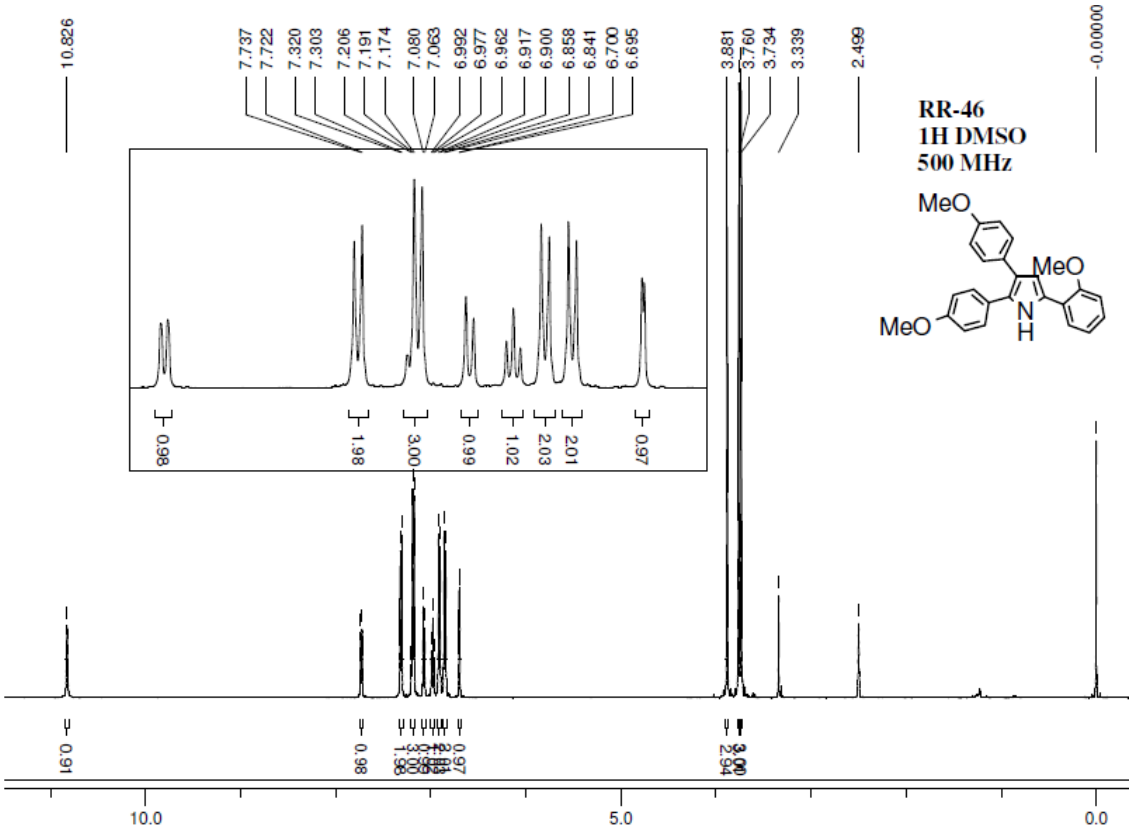
^{13}C NMR (Table 2, **3p**)



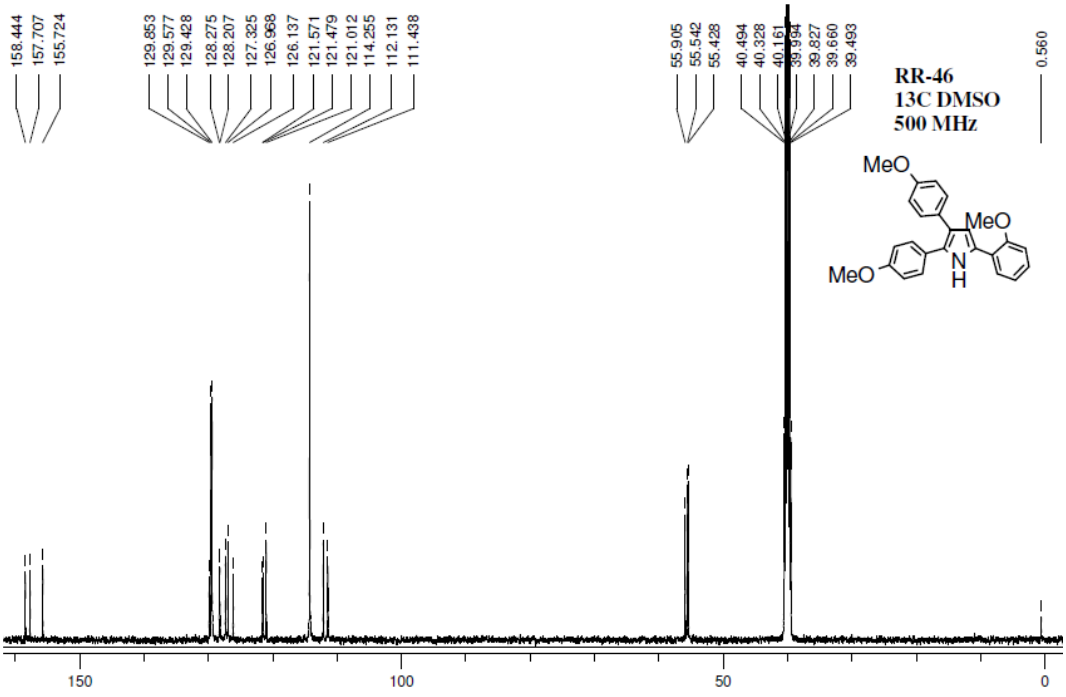
^{1}H NMR (Table 2, **3q**)



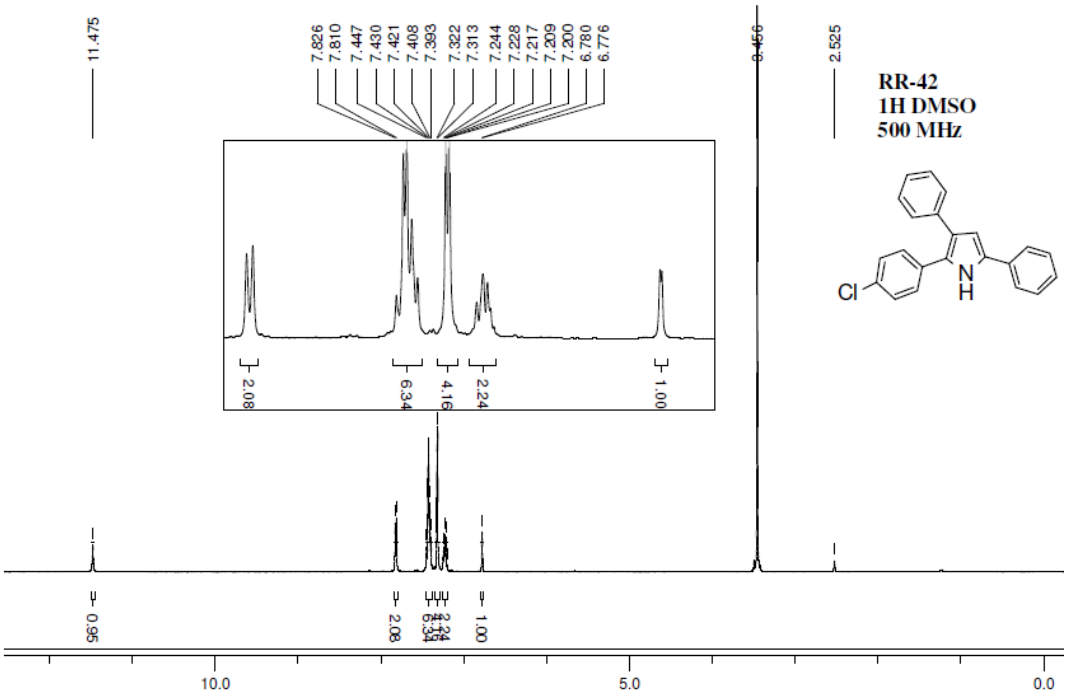
^{13}C NMR (Table 3, **3q**)



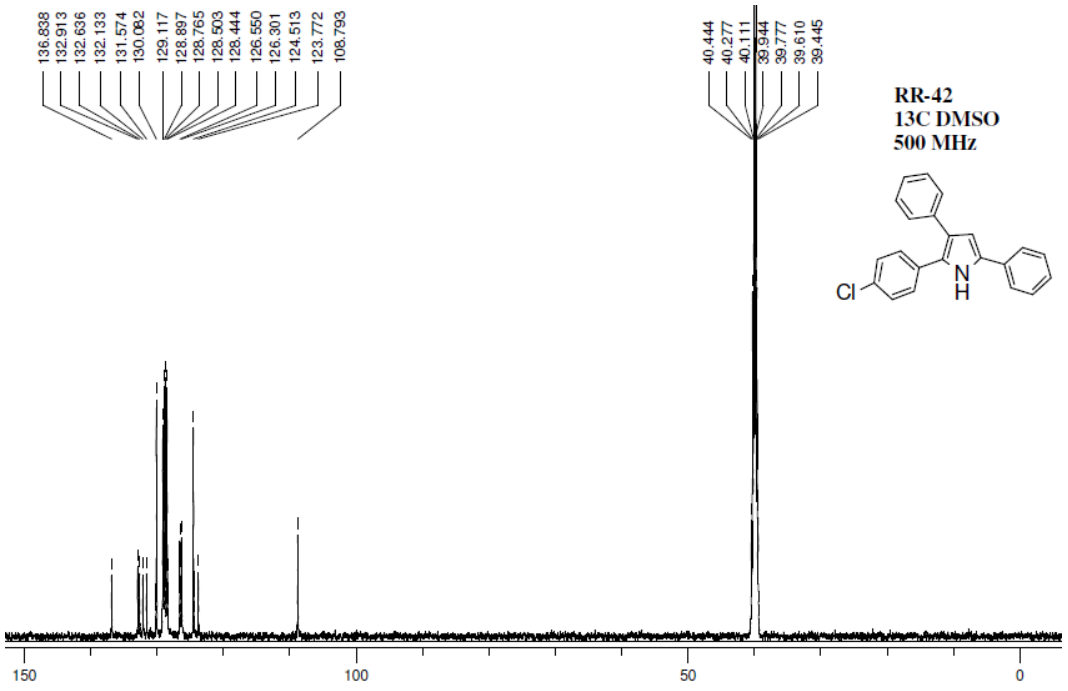
^{1}H NMR (Table 2, **3r**)



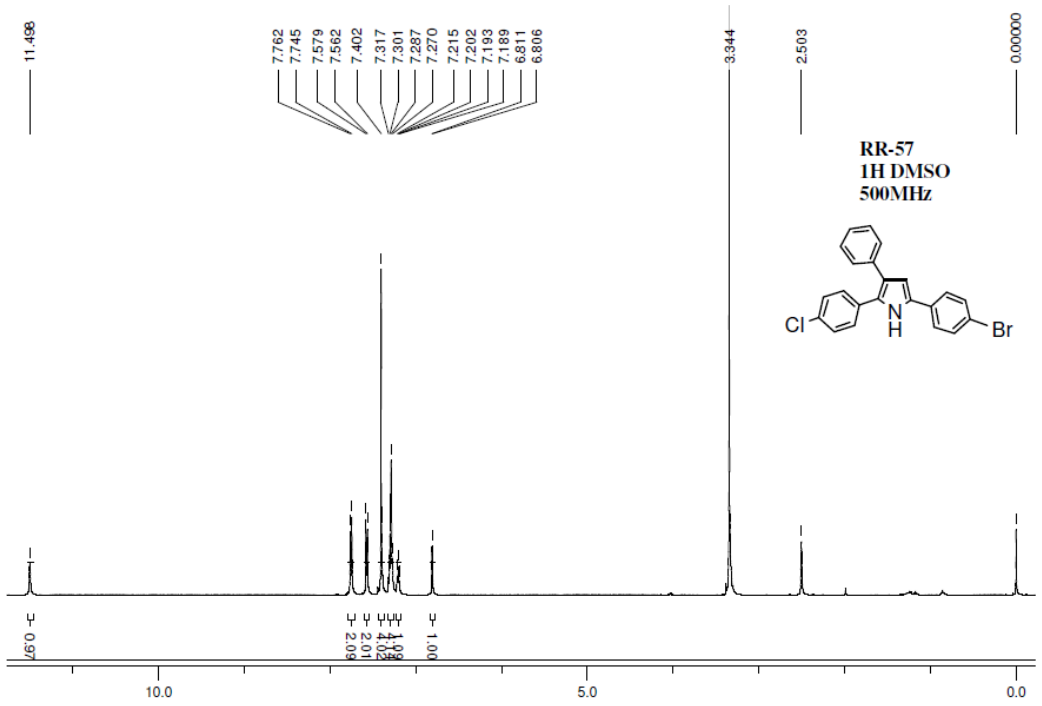
^{13}C NMR (Table 2, **3r**)



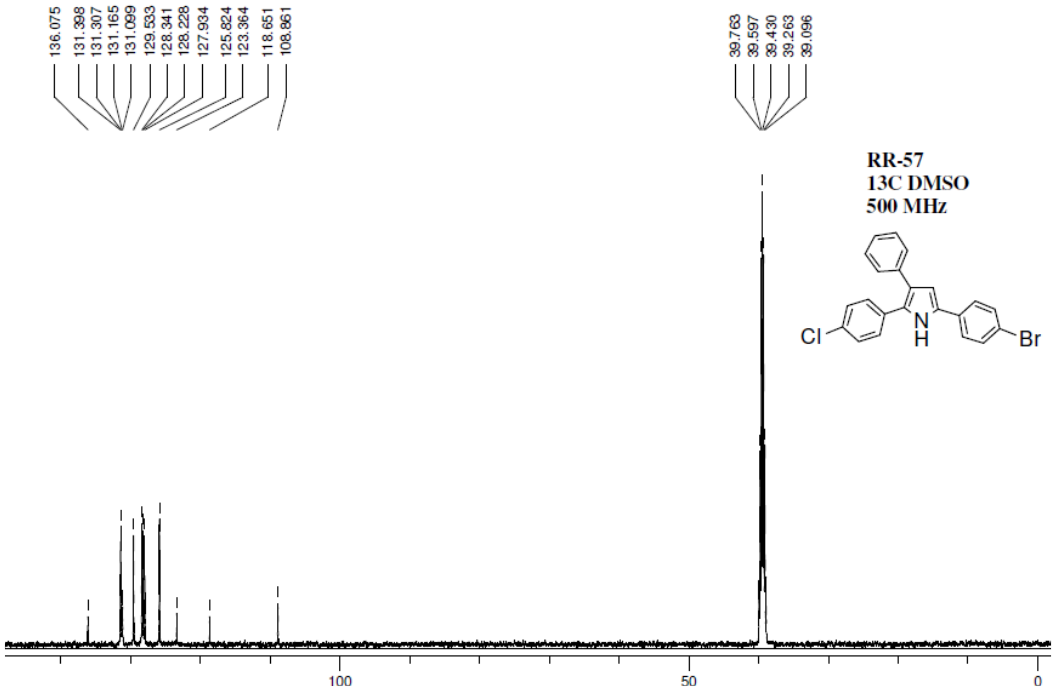
^{1}H NMR (Table 2, **3s**)



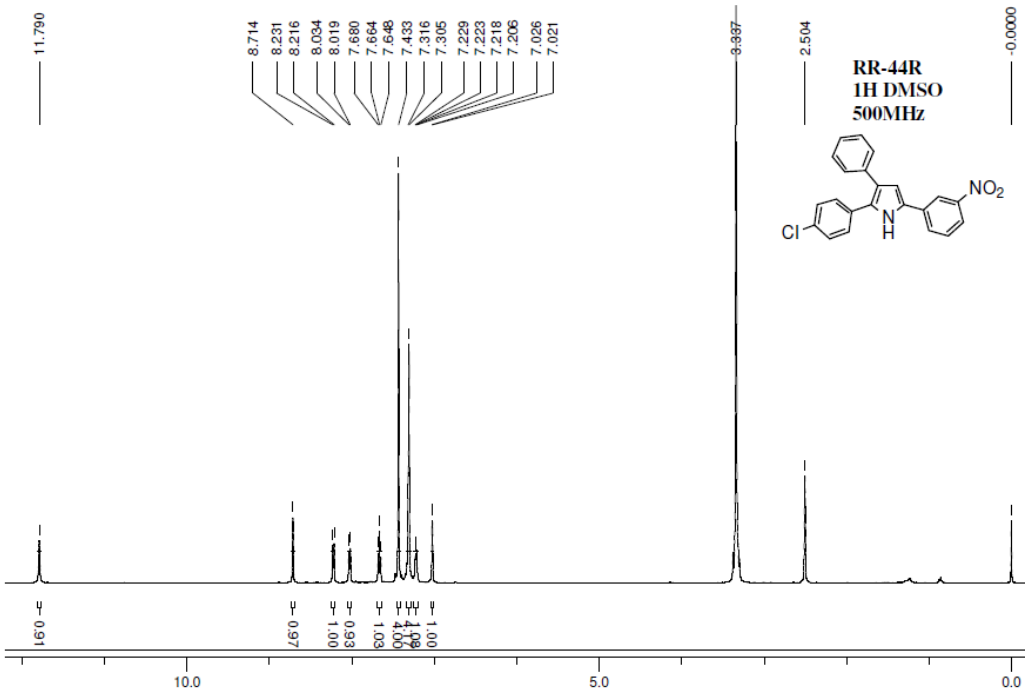
^{13}C NMR (Table 2, **3s**)



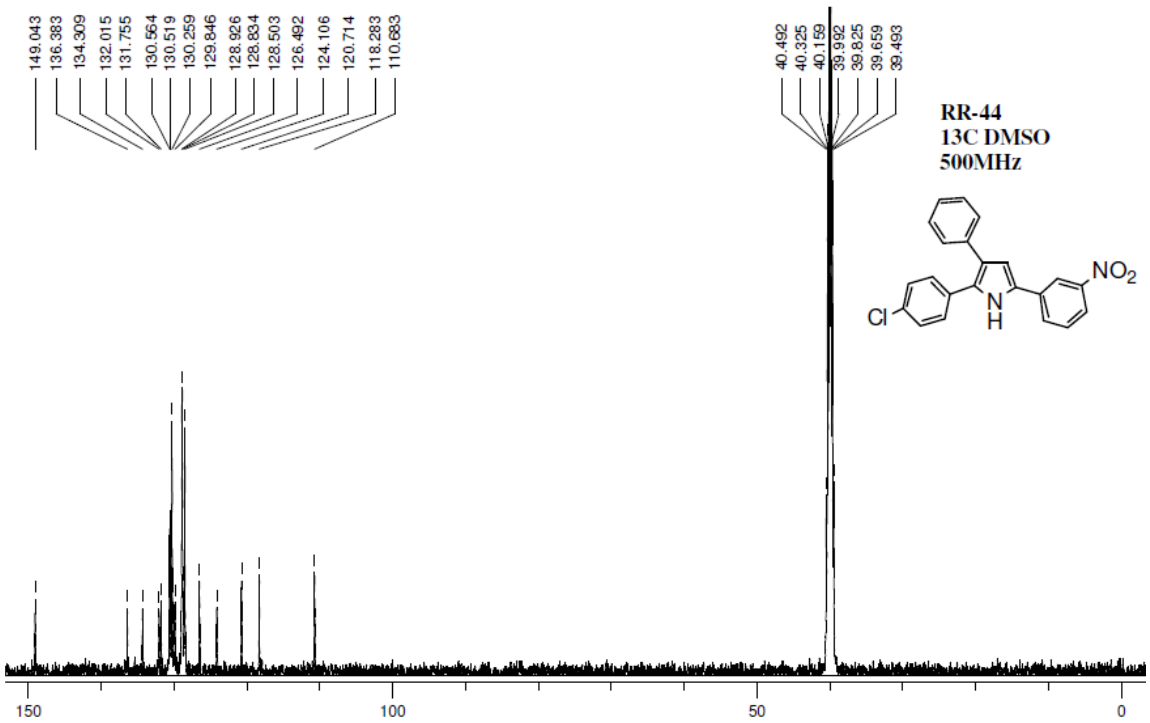
^{1}H NMR (Table 2, **3t**)



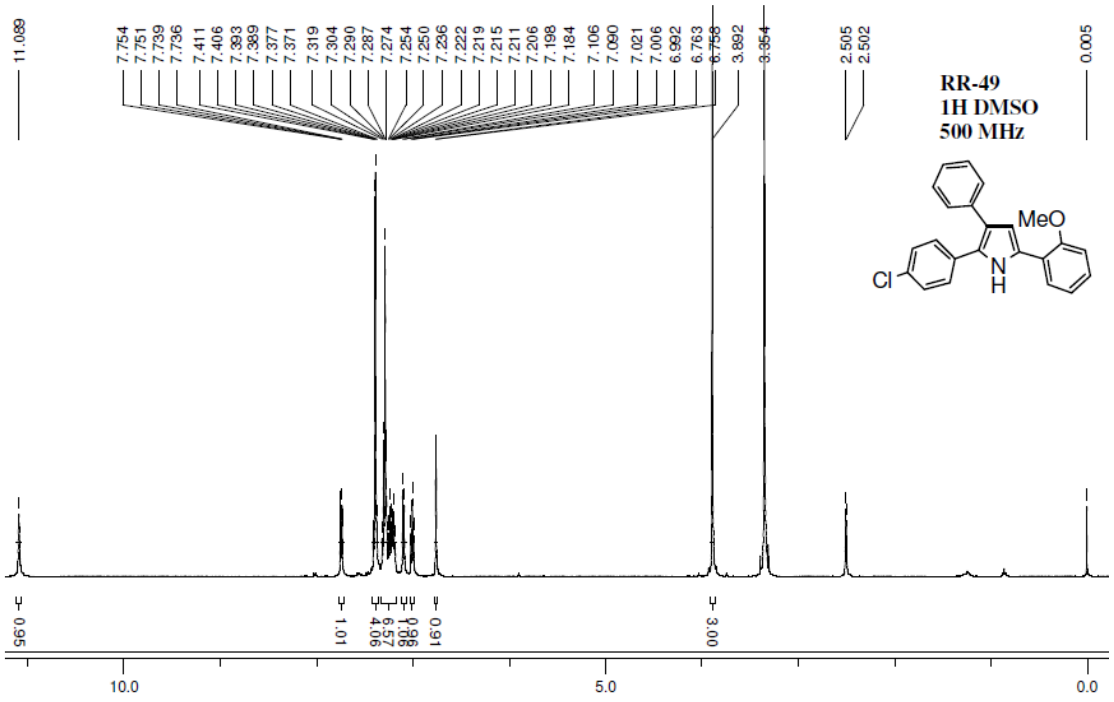
^{13}C NMR (Table 2, **3t**)



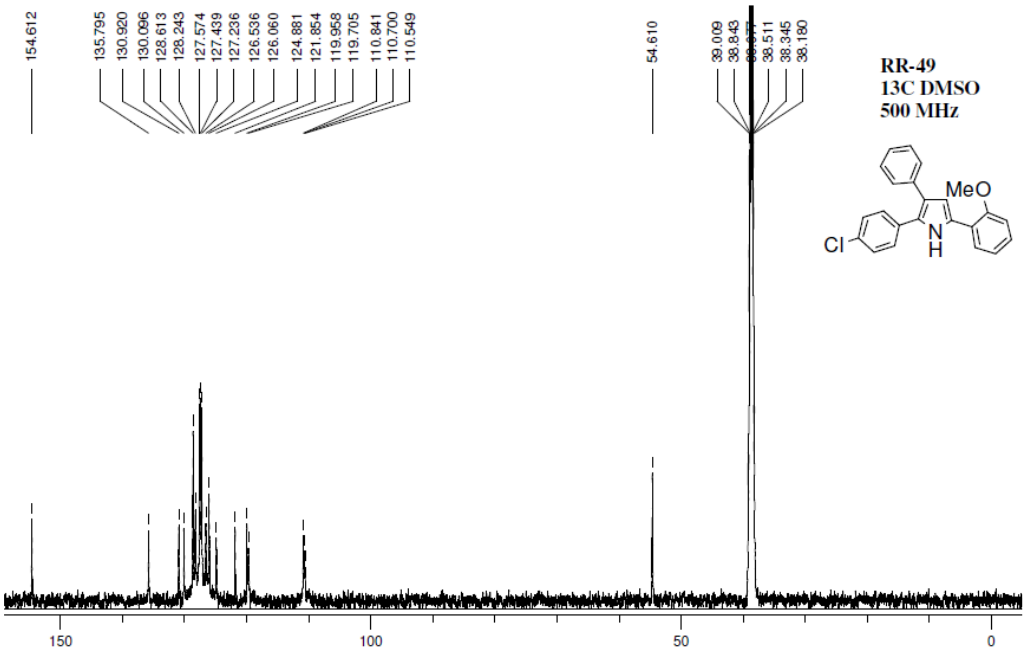
^{1}H NMR (Table 2, **3u**)



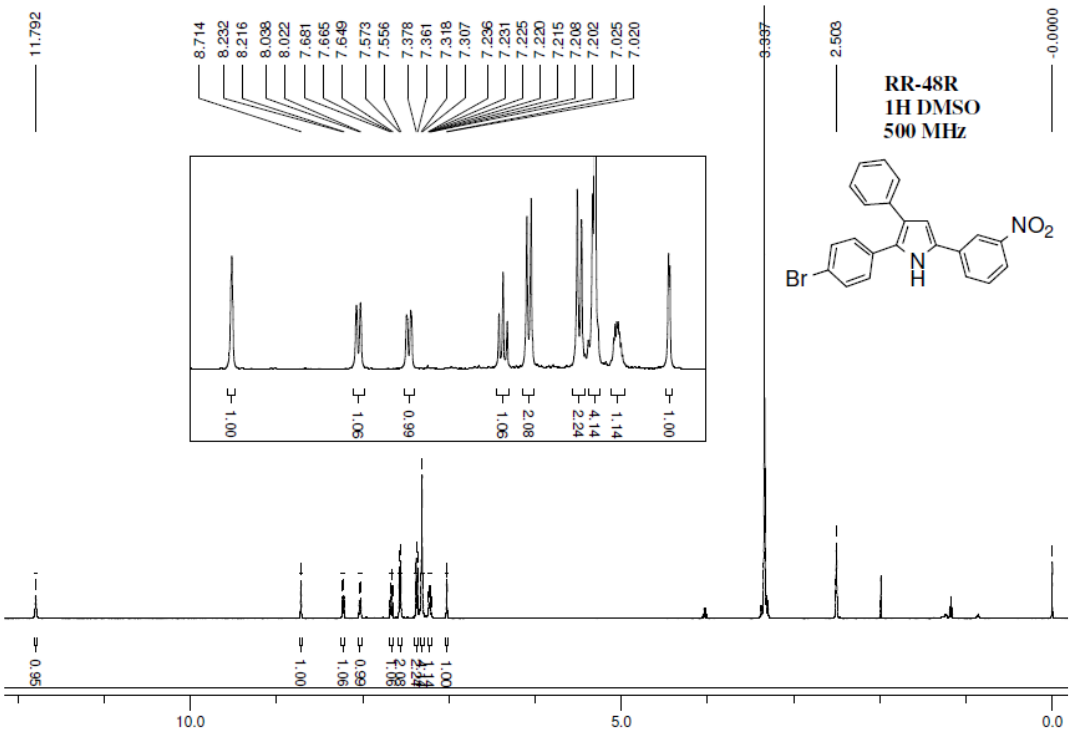
^{13}C NMR (Table 2, **3u**)



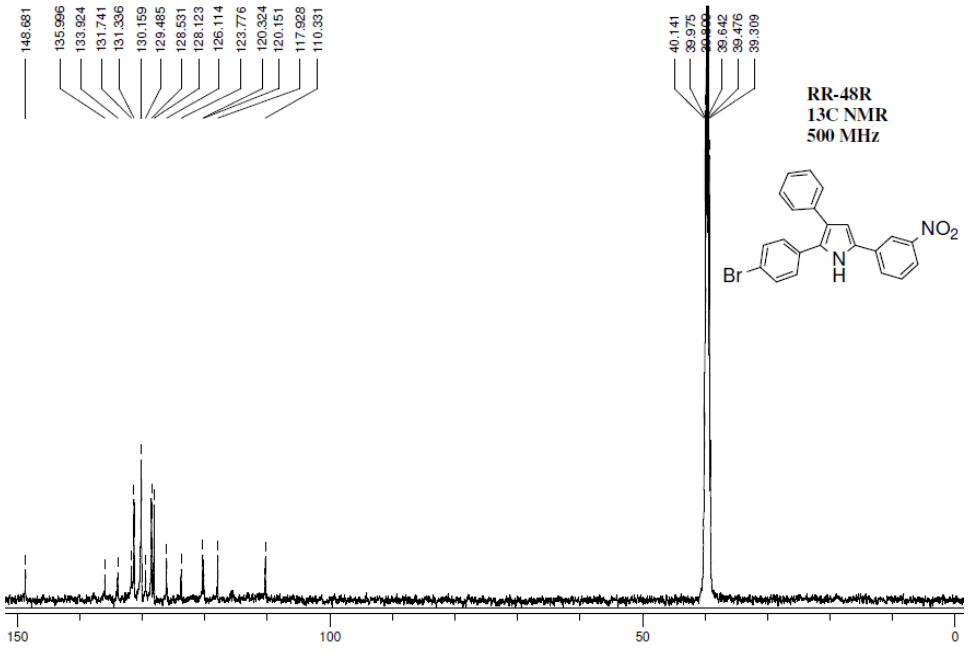
^{1}H NMR (Table 2, **3v**)



^{13}C NMR (Table 2, **3v**)



^{1}H NMR (Table 2, **3w**)



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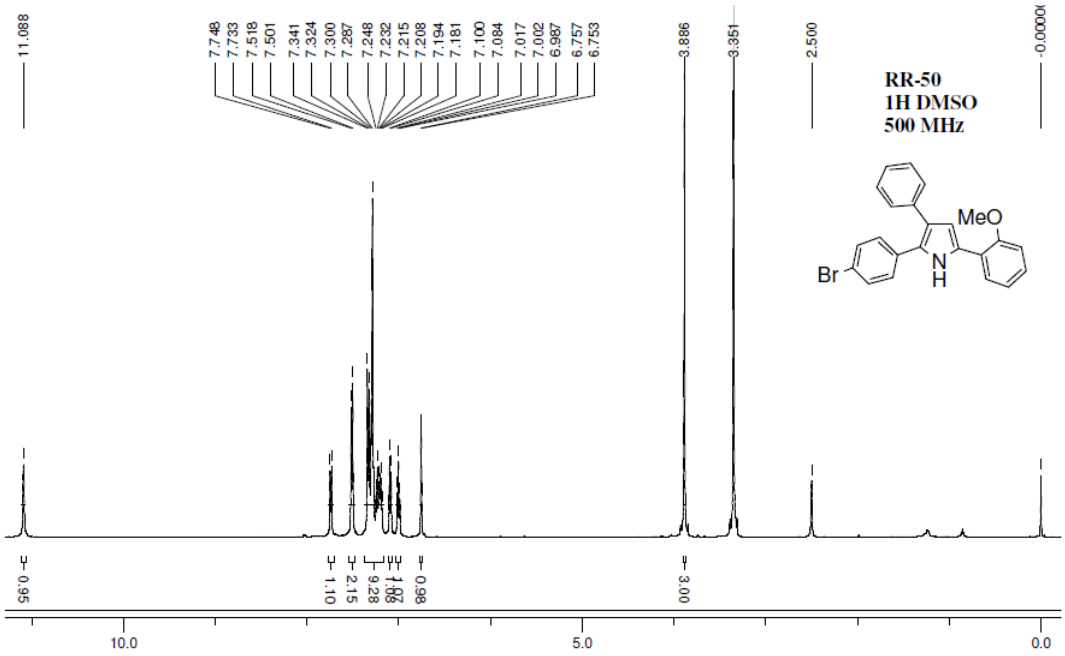
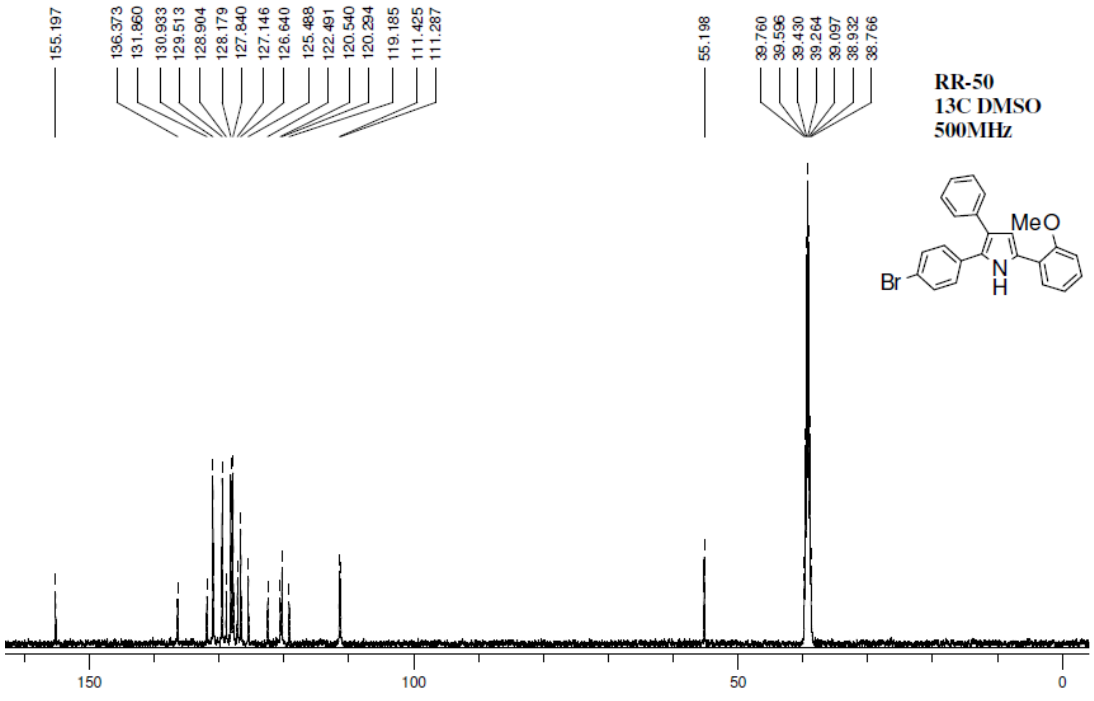
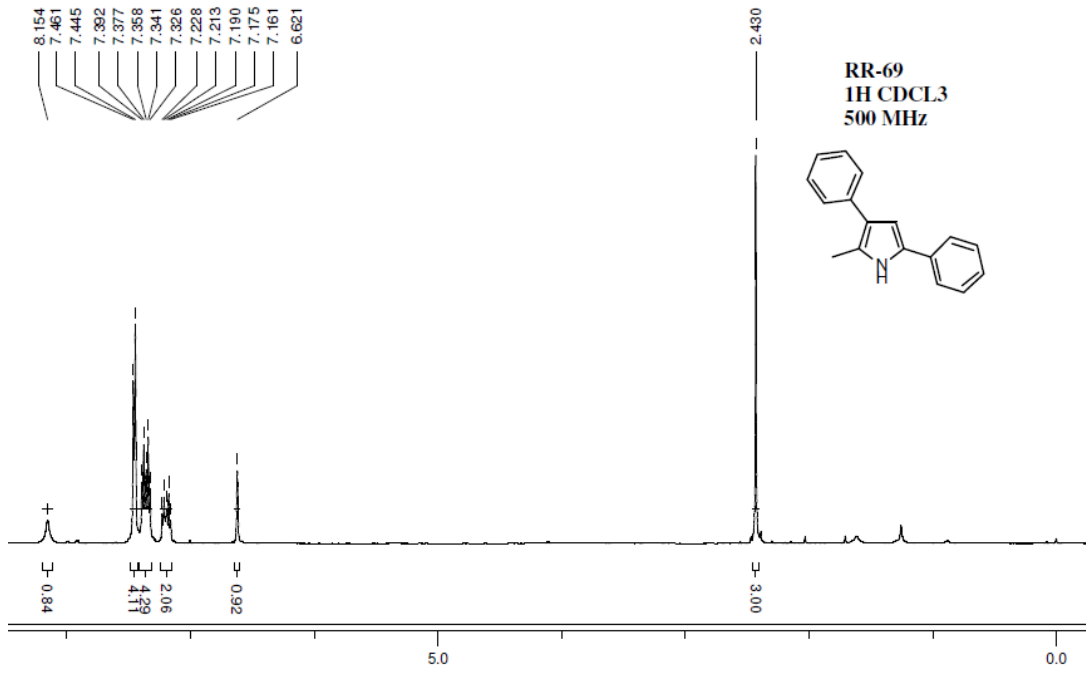


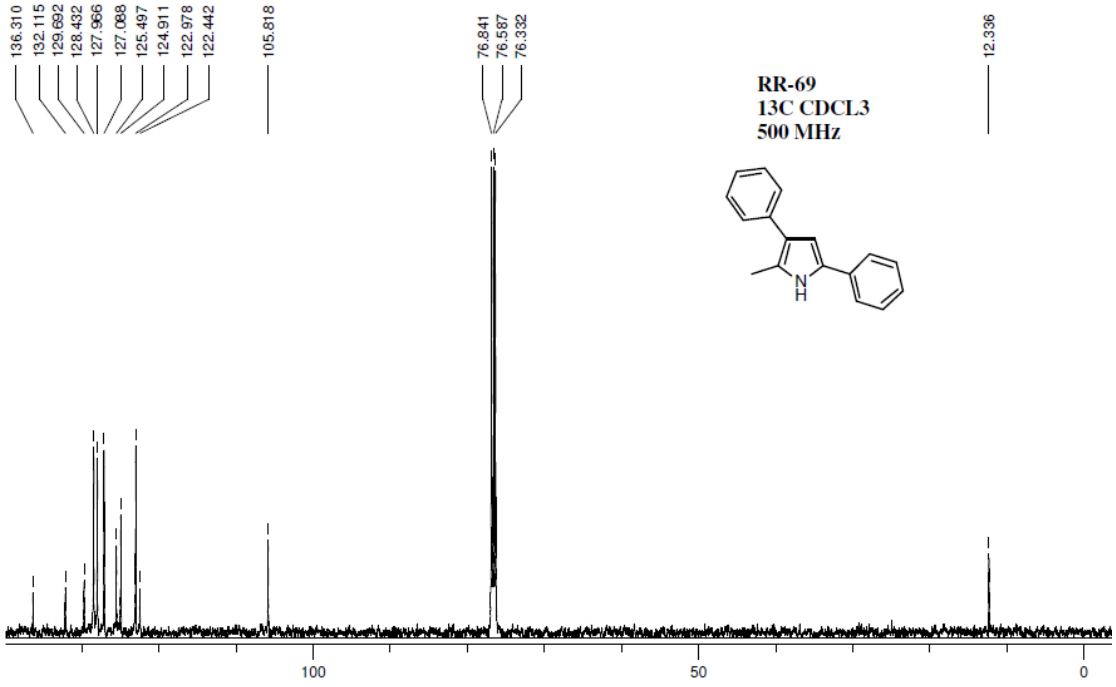
^{1}H NMR (Table 2, **3x**)



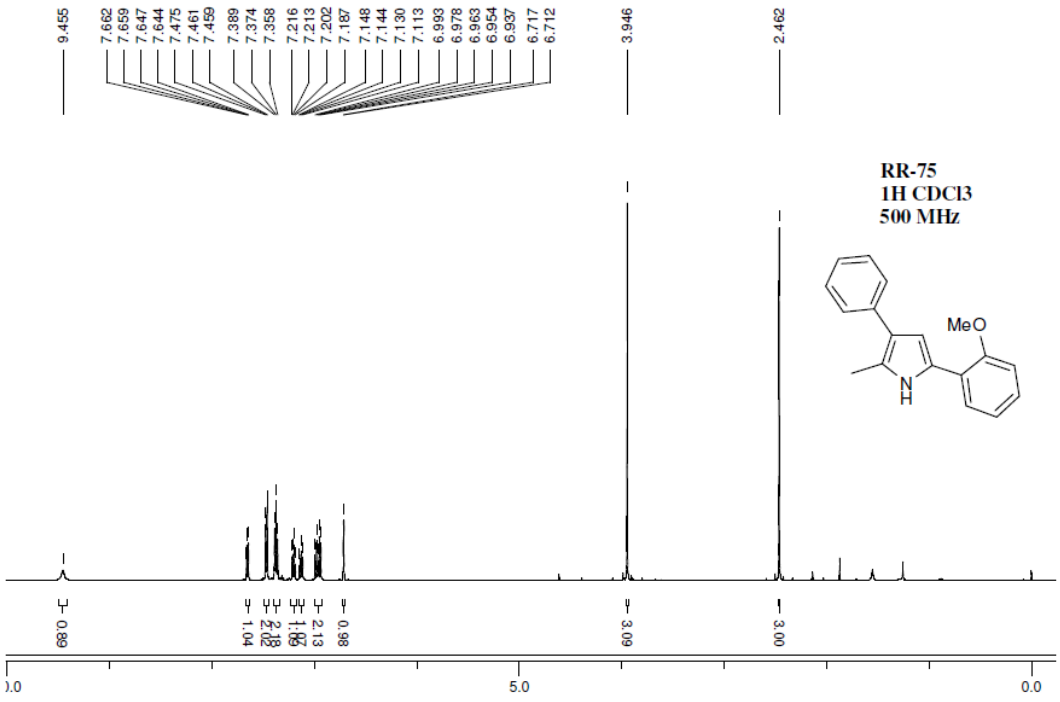
^{13}C NMR (Table 2, **3x**)



^{1}H NMR (Table 2, **3y**)



^{13}C NMR (Table 2, **3y**)



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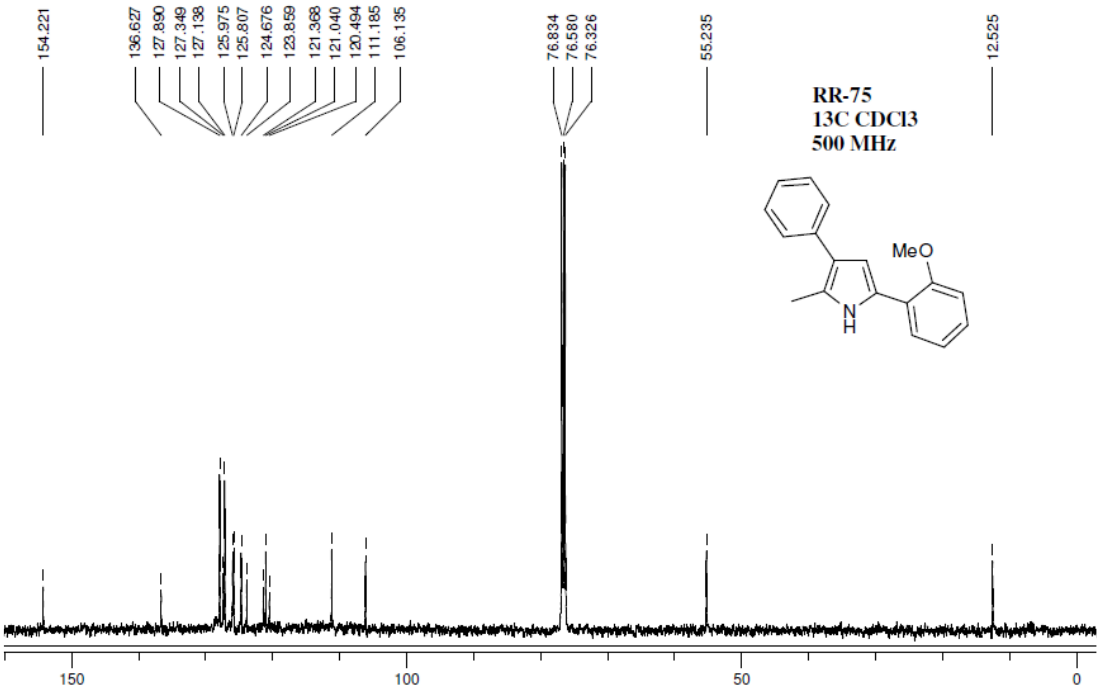

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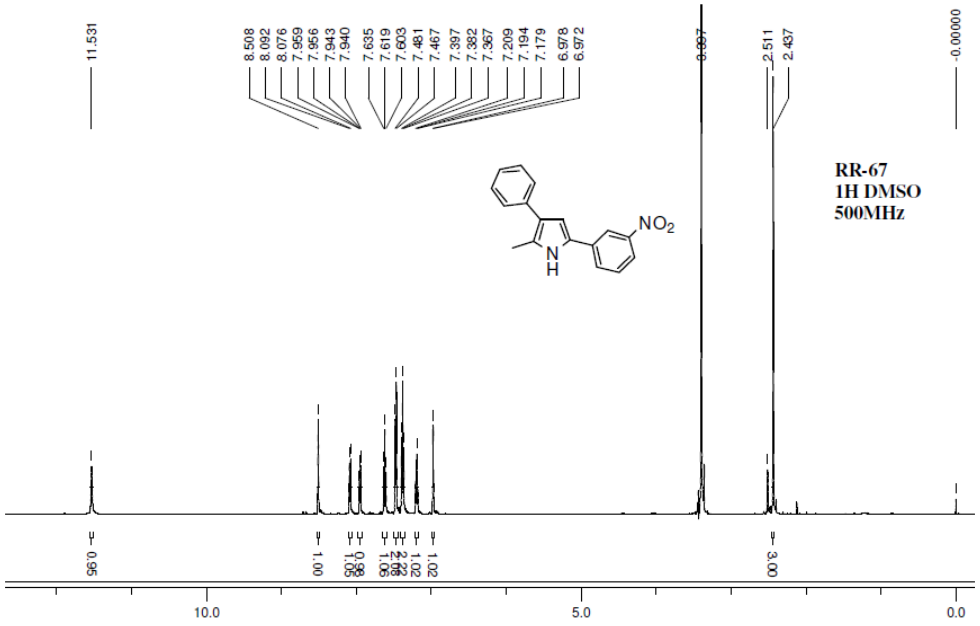
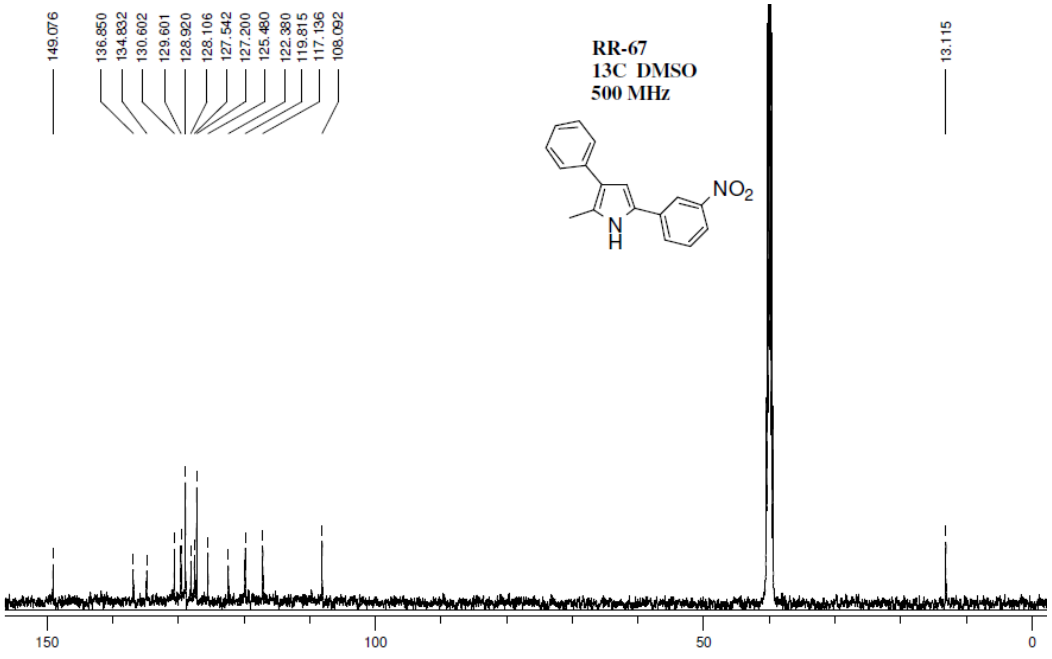
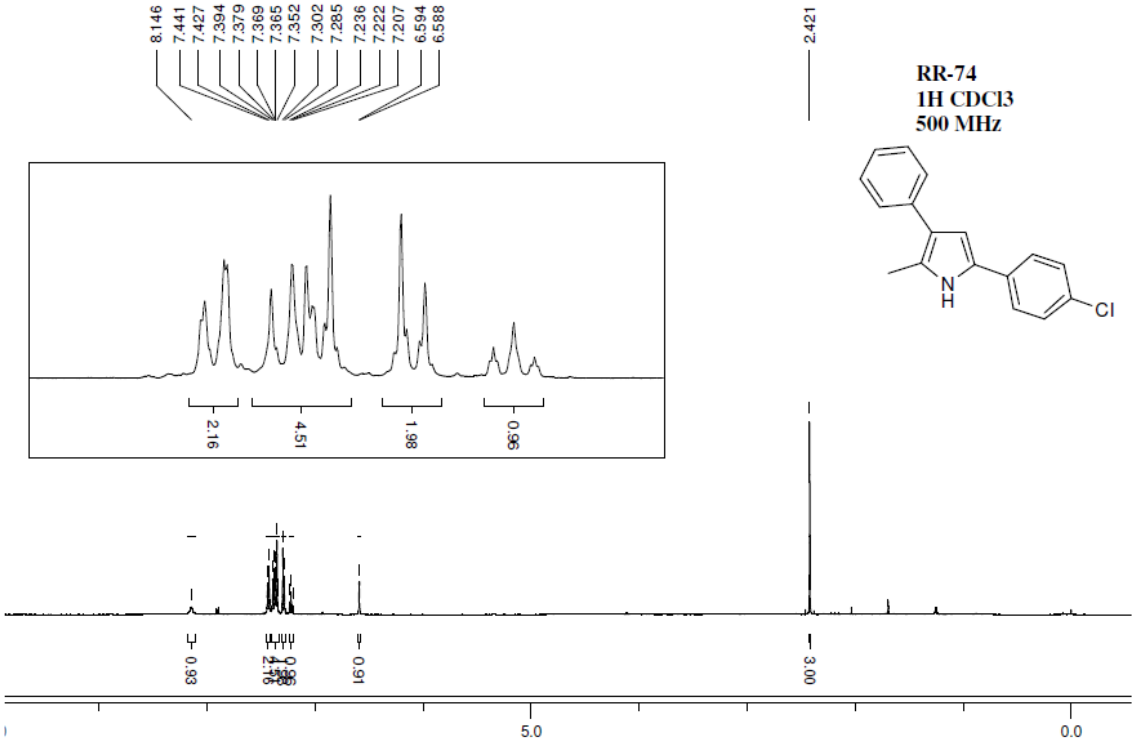


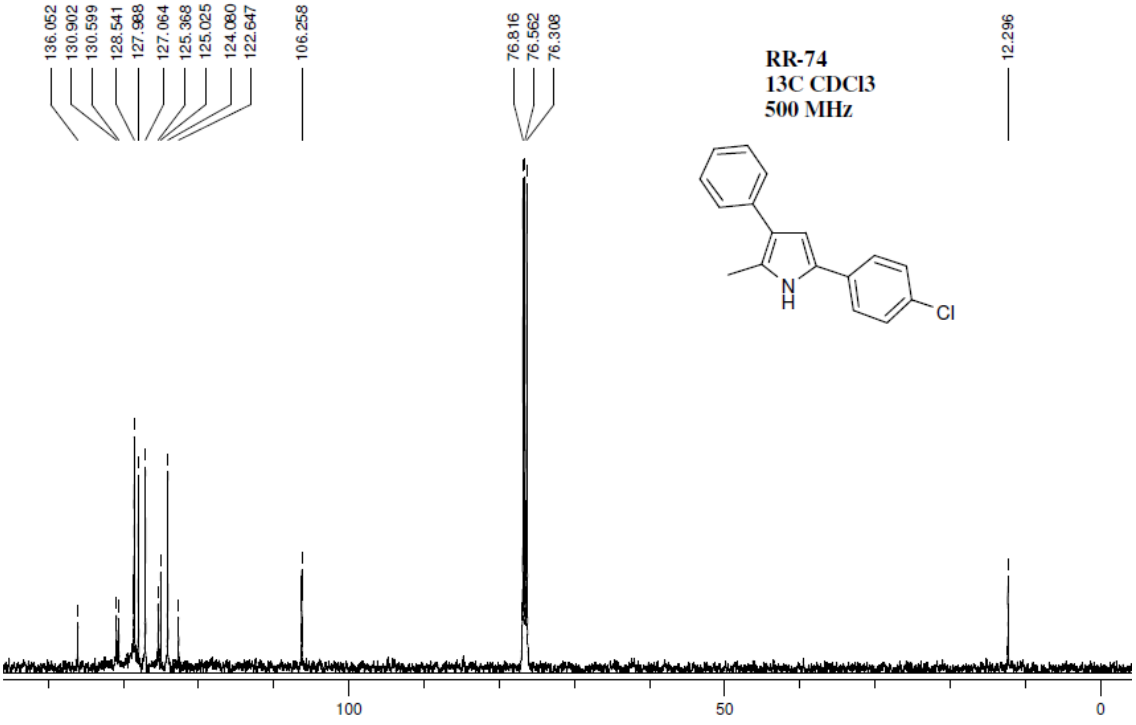
^{1}H NMR (Table 2, **3aa**)



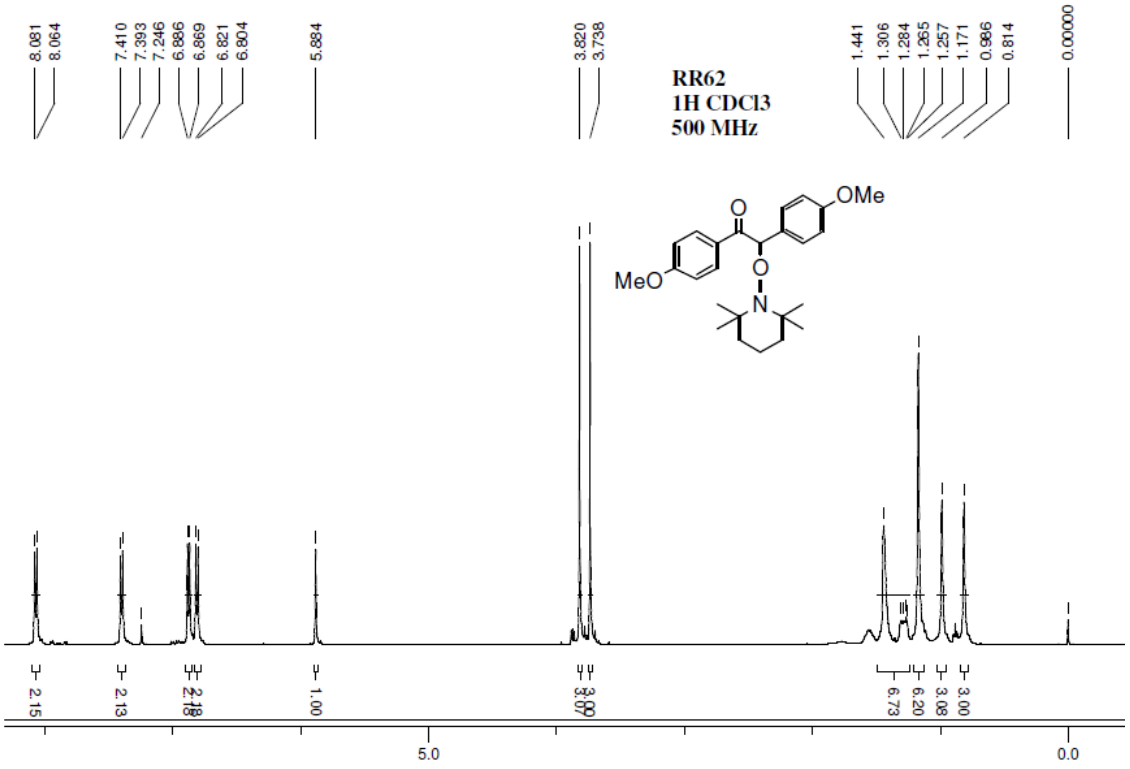
^{13}C NMR (Table 2, **3aa**)



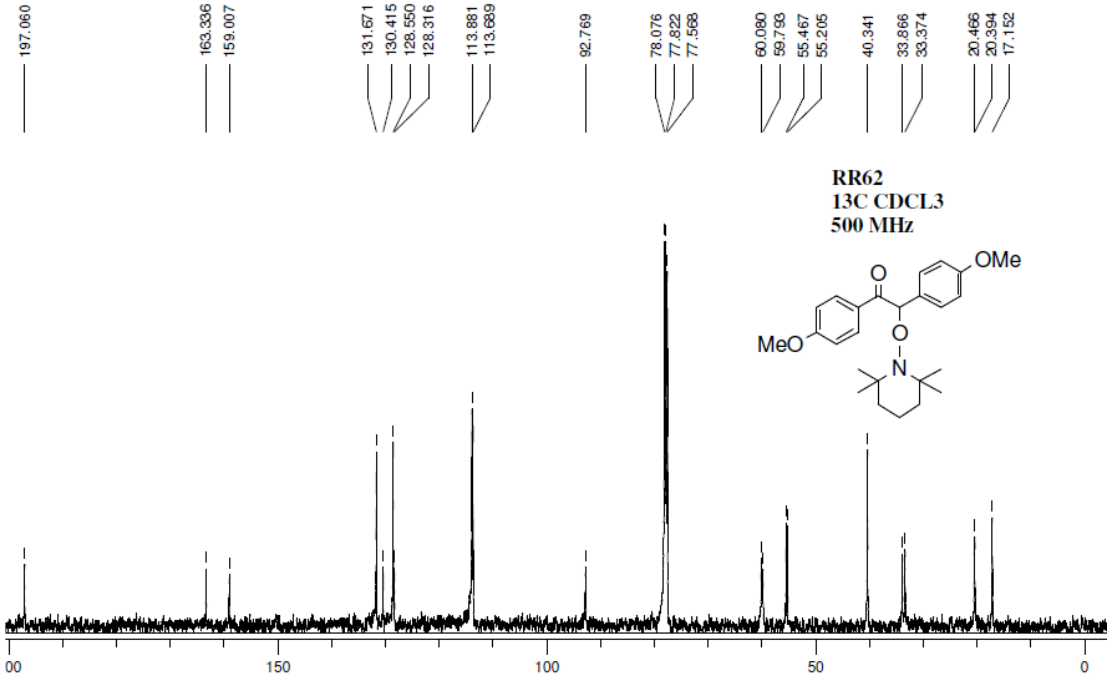
^{1}H NMR (Table 2, **3ab**)



^{13}C NMR (Table 2, **3ab**)



^{1}H NMR (Scheme 2, **4**)

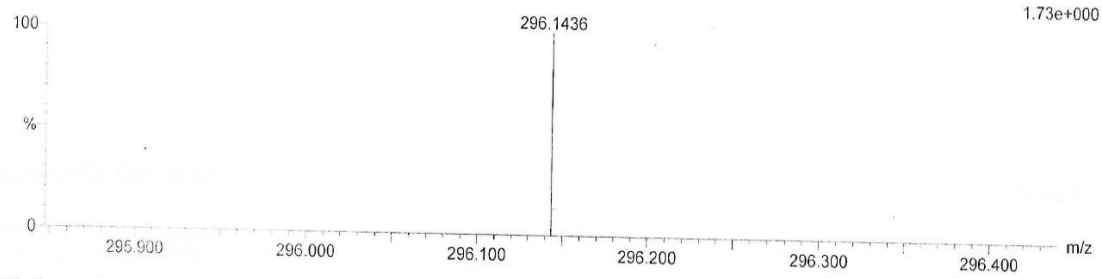


^{13}C NMR (Scheme 2, **4**)

HRMS spectral Copies

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
2 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-23 H: 0-18 N: 0-1
RR 3A HR 26 (0.309)
1: TOF MS ES+

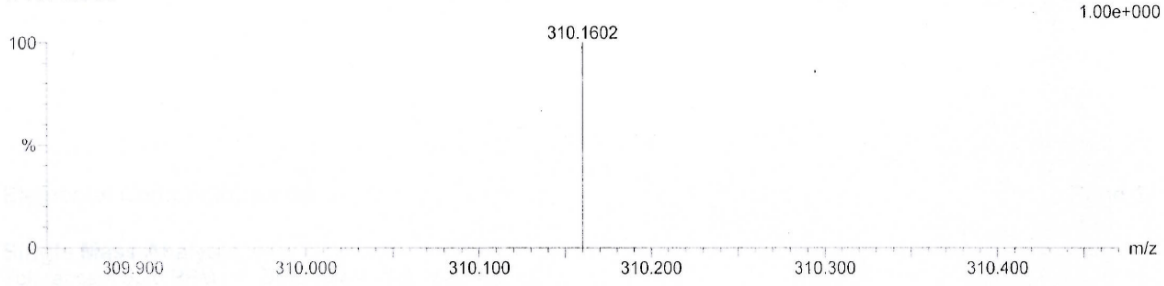


Minimum:				-1.5		
Maximum:		5.0	50.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
296.1436	296.1439	-0.3	-1.0	14.5	n/a	C22 H18 N

(Table 2, **3a**)

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
2 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-24 H: 0-20 N: 0-1
RR 3B HR 13 (0.155)
1: TOF MS ES+



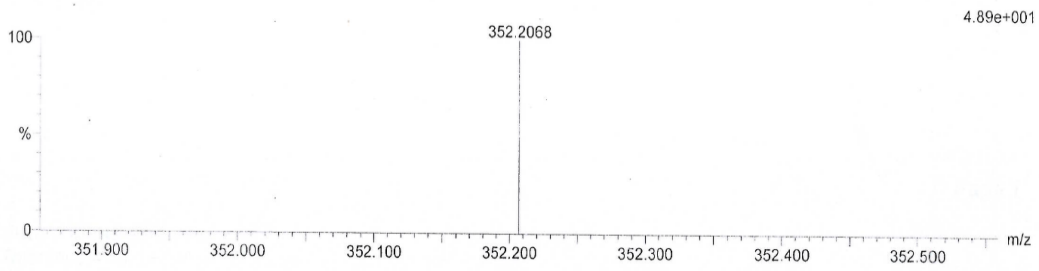
Minimum:				-1.5		
Maximum:		5.0	50.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
310.1602	310.1596	0.6	1.9	14.5	n/a	C23 H20 N

(Table 2, **3b**)

Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
2 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-27 H: 0-26 N: 0-1
RR 110 HR1 8 (0.095)
1: TOF MS ES+

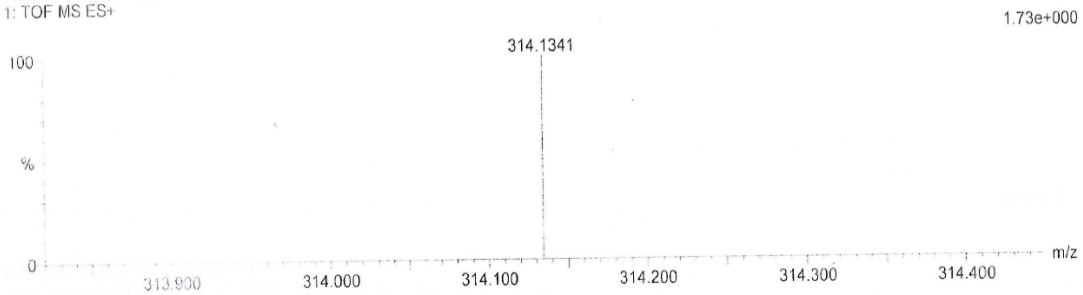


Minimum:				-1.5		
Maximum:		5.0	50.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
352.2068	352.2065	0.3	0.9	14.5	n/a	C26 H26 N

(Table 2, **3c**)

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions
2 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-23 H: 0-17 N: 0-1 F: 0-1
RR 3D HR 73 (0.867)
1: TOF MS ES+

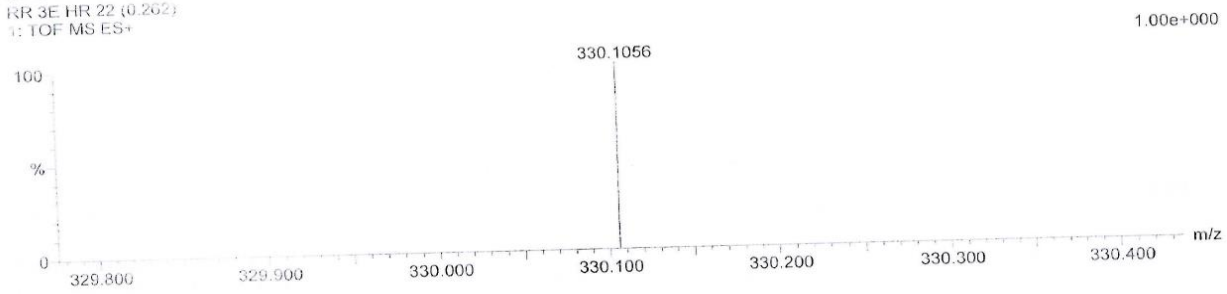


Minimum:		5.0	50.0	-1.5		
Maximum:				50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
314.1341	314.1345	-0.4	-1.3	14.5	n/a	C22 H17 N F

(Table 2, **3d**)

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions
2 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-23 H: 0-17 N: 0-1 Cl: 0-1
RR 3E HR 22 (0.262)
1: TOF MS ES+



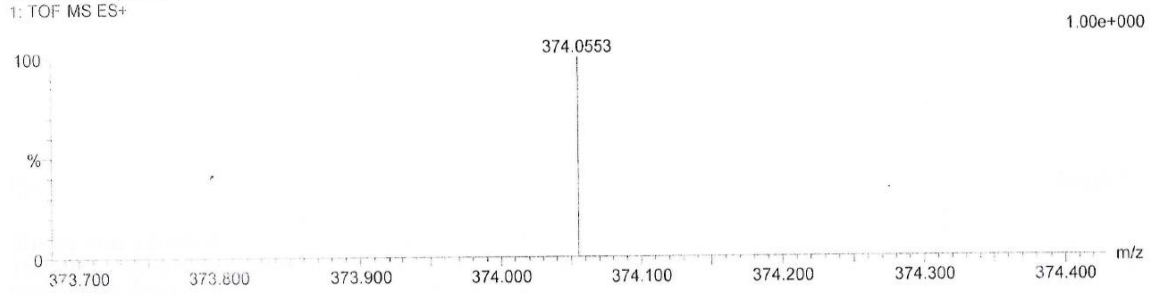
Minimum:		5.0	50.0	-1.5		
Maximum:				50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
330.1056	330.1056	0.6	1.8	14.5	n/a	C22 H17 N Cl

(Table 2, **3e**)

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
4 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-23 H: 0-17 N: 0-1 Br: 0-1

RR 3F HR 63 (0.748)
1: TOF MS ES+



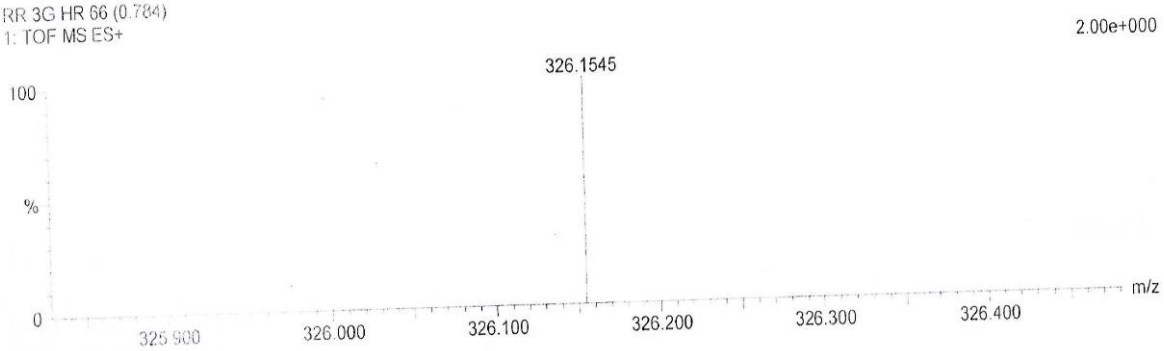
Minimum:		5.0	50.0	-1.5		
Maximum:				50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
374.0553	374.0544	0.9	2.4	14.5	n/a	C22 H17 N Br

(Table 2, **3f**)

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
2 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-24 H: 0-20 N: 0-1 O: 0-1

RR 3G HR 66 (0.784)
1: TOF MS ES+

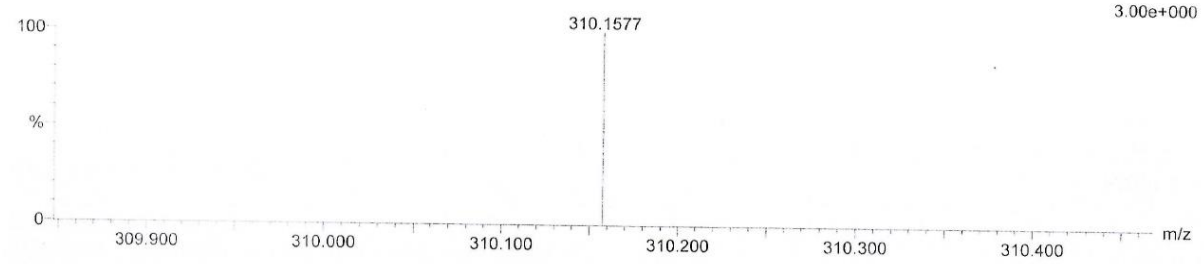


Minimum:		5.0	50.0	-1.5		
Maximum:				50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
326.1545	326.1545	0.0	0.0	14.5	n/a	C23 H20 N O

(Table 2, **3g**)

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions
2 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-24 H: 0-20 N: 0-1
RR 3H HR 28 (0.332)
1: TOF MS ES+



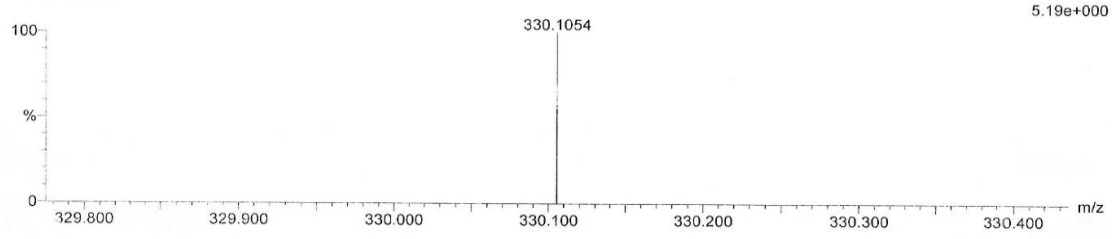
Minimum:				-1.5		
Maximum:		5.0	50.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
310.1577	310.1596	-1.9	-6.1	14.5	n/a	C23 H20 N

(Table 2, **3h**)

Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
4 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-23 H: 0-17 N: 0-2 Cl: 0-1
RR K18 HR 47 (0.558)
1: TOF MS ES+

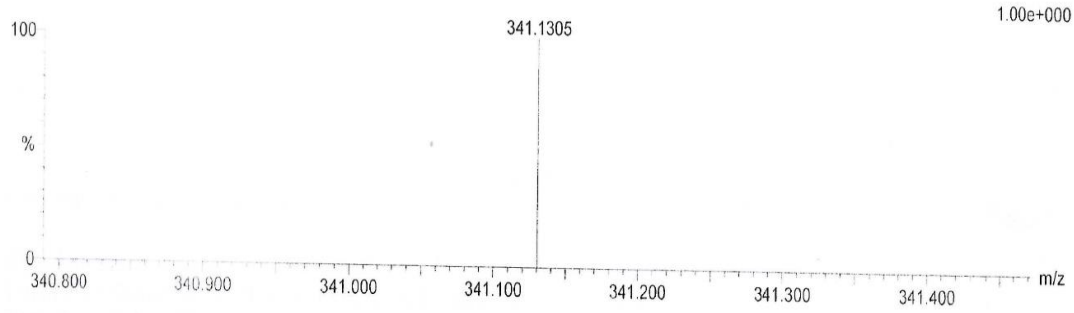


Minimum:				-1.5		
Maximum:		5.0	50.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
330.1054	330.1050	0.4	1.2	14.5	n/a	C22 H17 N Cl

(Table 2, **3i**)

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions
3 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-23 H: 0-17 N: 0-2 O: 0-2
RR 3J HR 5 (0.060)
1: TOF MS ES+



Minimum:				-1.5		
Maximum:		5.0	50.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
341.1305	341.1290	1.5	4.4	15.5	n/a	C22 H17 N2 O2

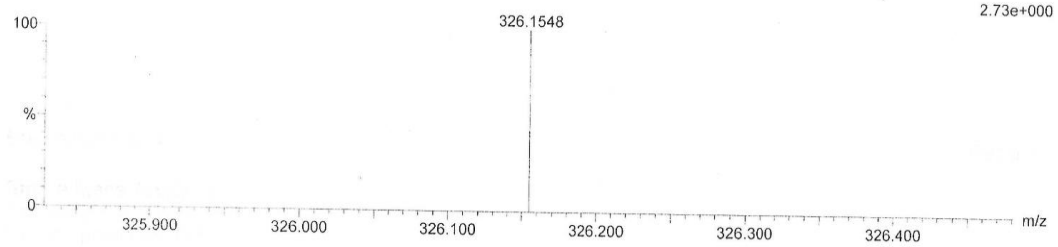
(Table 2, **3j**)

Elemental Composition Report

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions
447 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-24 H: 0-20 B: 0-1 N: 0-1 O: 0-1 Si: 0-1 P: 0-1 Cu: 0-1 Br: 0-1 Ru: 0-1

RR K 16 HR 64 (0.760)
1: TOF MS ES+



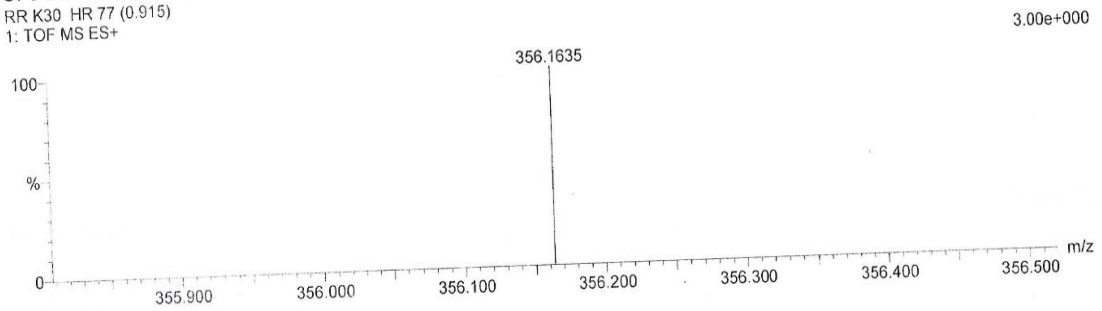
Minimum:				-1.5		
Maximum:		5.0	50.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
326.1548	326.1545	0.3	0.9	14.5	n/a	C23 H20 N O
	326.1396	15.2	46.6	14.0	n/a	C22 H20 B P

(Table 2, **3k**)

Elemental Composition Report

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions
2 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-25 H: 0-22 N: 0-1 O: 0-2
RR K30 HR 77 (0.915)
1: TOF MS ES+



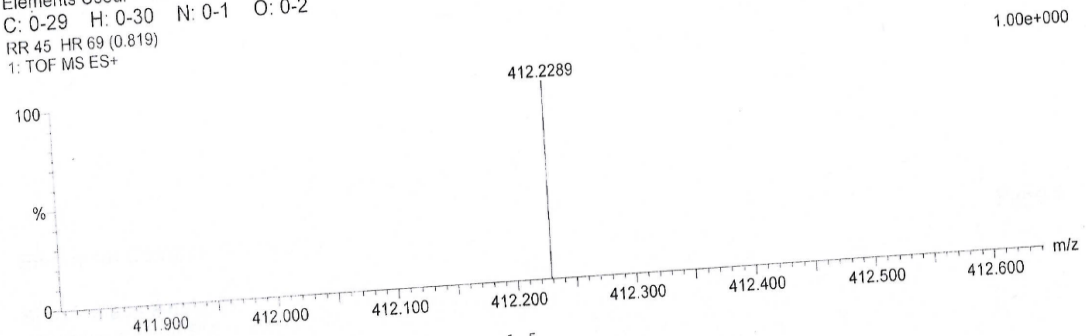
Minimum:		5.0	50.0	-1.5		
Maximum:				50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
356.1635	356.1651	-1.6	-4.5	14.5	n/a	C24 H22 N O2

(Table 2, **3l**)

Elemental Composition Report

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions
2 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-29 H: 0-30 N: 0-1 O: 0-2
RR 45 HR 69 (0.819)
1: TOF MS ES+



Minimum:		5.0	50.0	-1.5		
Maximum:				50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
412.2289	412.2277	1.2	2.9	14.5	n/a	C28 H30 N O2

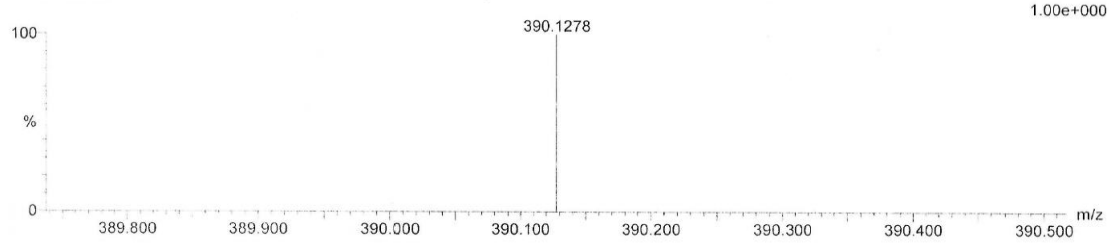
(Table 2, **3m**)

Elemental Composition Report

Page 1

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
5 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-25 H: 0-21 N: 0-1 O: 0-2 Cl: 0-1
RR 52 HR 58 (0.688)
1: TOF MS ES+



Minimum:				-1.5		
Maximum:		5.0	50.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
390.1278	390.1261	1.7	4.4	14.5	n/a	C24 H21 N O2 Cl

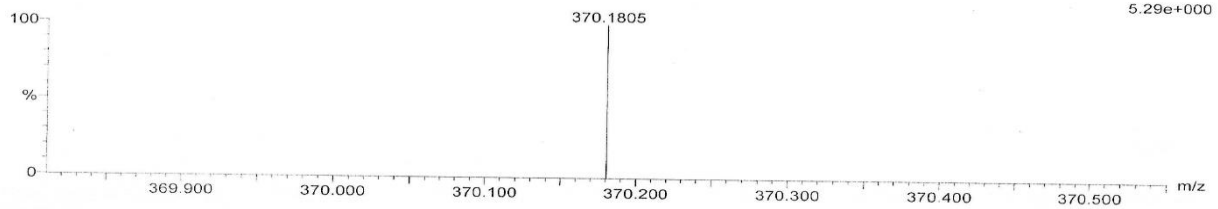
(Table 2, **3n**)

Elemental Composition Report

Page 1

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
2 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-26 H: 0-24 N: 0-1 O: 0-2
RR 54 HR 57 (0.677)
1: TOF MS ES+



Minimum:				-1.5		
Maximum:		5.0	50.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
370.1805	370.1807	-0.2	-0.5	14.5	n/a	C25 H24 N O2

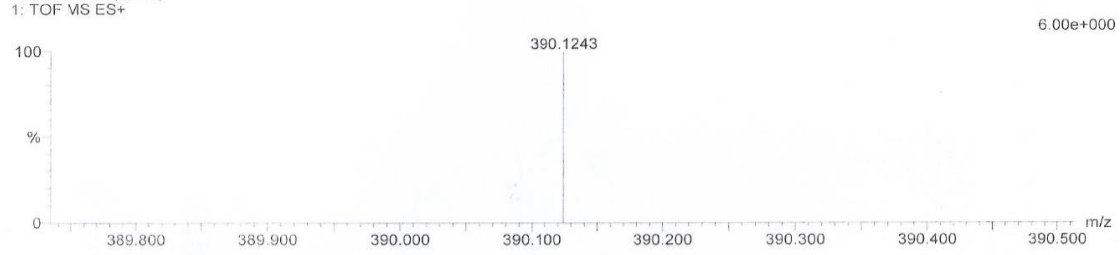
(Table 2, **3o**)

Elemental Composition Report

Page 1

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions
5 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-25 H: 0-21 N: 0-1 O: 0-2 Cl: 0-1
RR 53 HR 10 (0.119)
1: TOF MS ES+



Minimum:				-1.5		
Maximum:		5.0	50.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
390.1243	390.1261	-1.8	-4.6	14.5	n/a	C24 H21 N O2 Cl

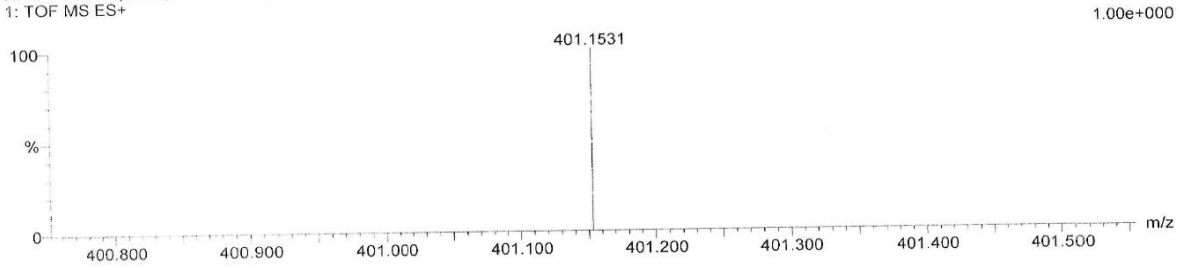
(Table 2, **3p**)

Elemental Composition Report

Page 1

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions
8 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-25 H: 0-21 N: 0-2 O: 0-4
RR 32 HR 27 (0.320)
1: TOF MS ES+



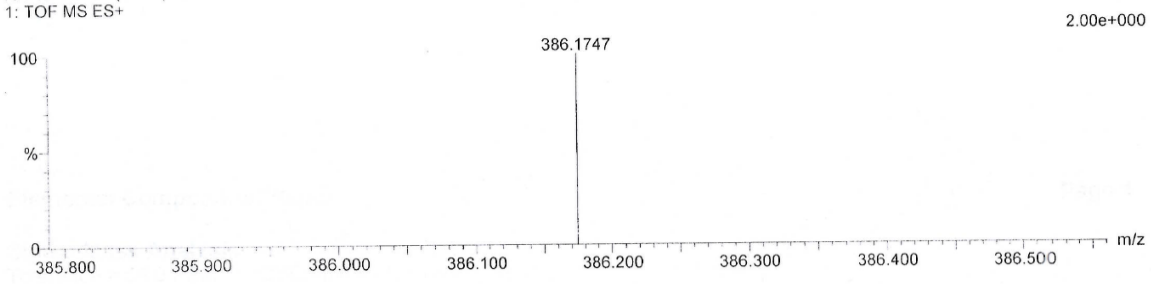
Minimum:				-1.5		
Maximum:		5.0	50.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
401.1531	401.1501	3.0	7.5	15.5	n/a	C24 H21 N2 O4

(Table 2, **3q**)

Elemental Composition Report

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions
3 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-26 H: 0-24 N: 0-1 O: 0-3
RR 46 HR 54 (0.641)
1: TOF MS ES+

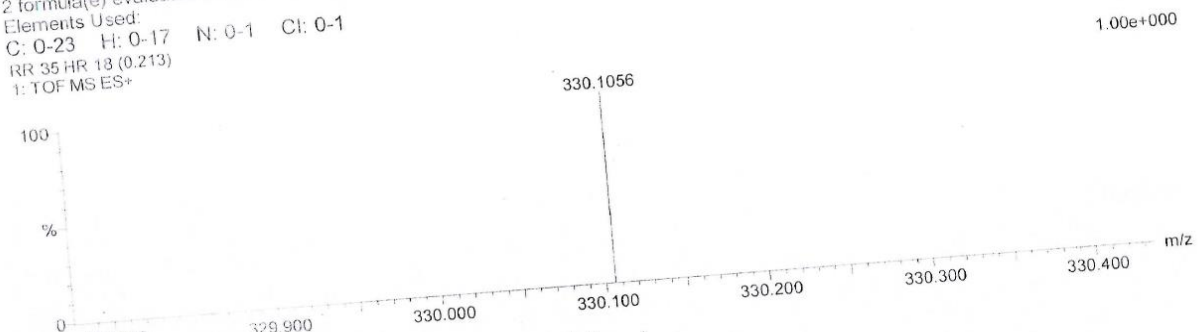


Minimum:				-1.5		
Maximum:		5.0	50.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
386.1747	386.1756	-0.9	-2.3	14.5	n/a	C25 H24 N O3

(Table 2, **3r**)

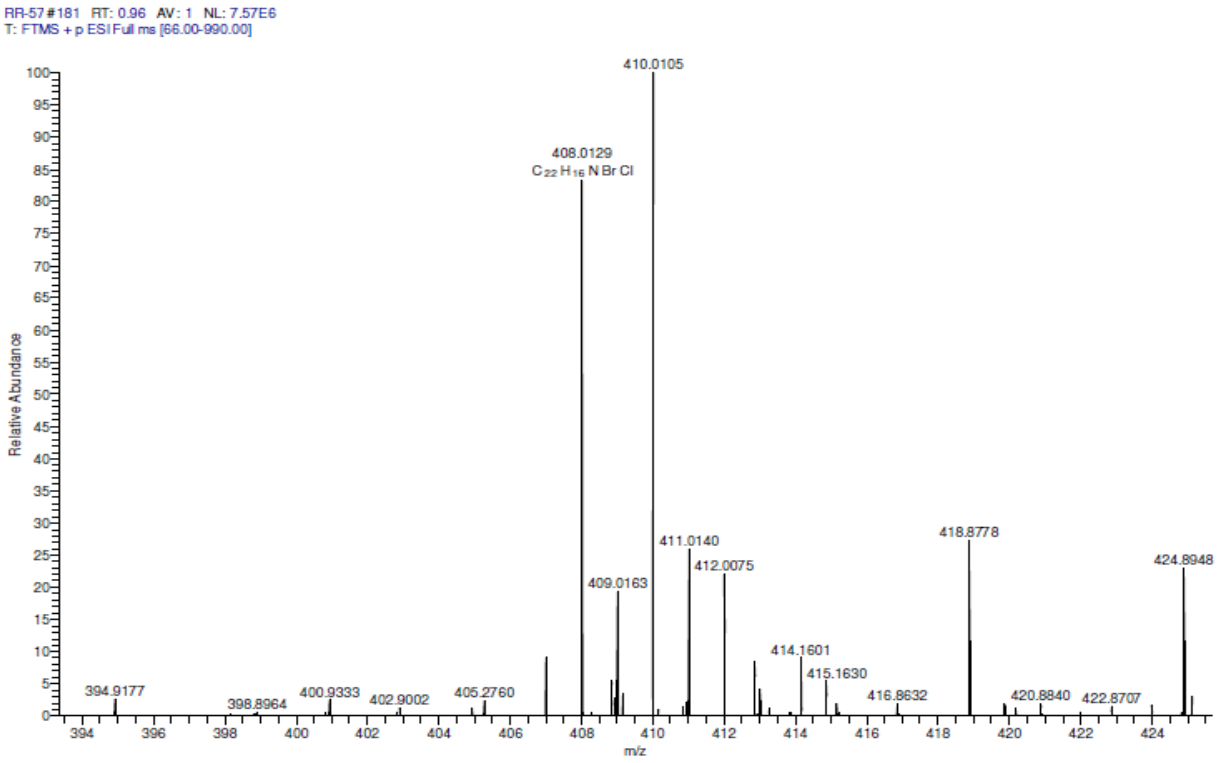
Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions
2 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-23 H: 0-17 N: 0-1 Cl: 0-1
RR 35 HR 18 (0.213)
1: TOF MS ES+

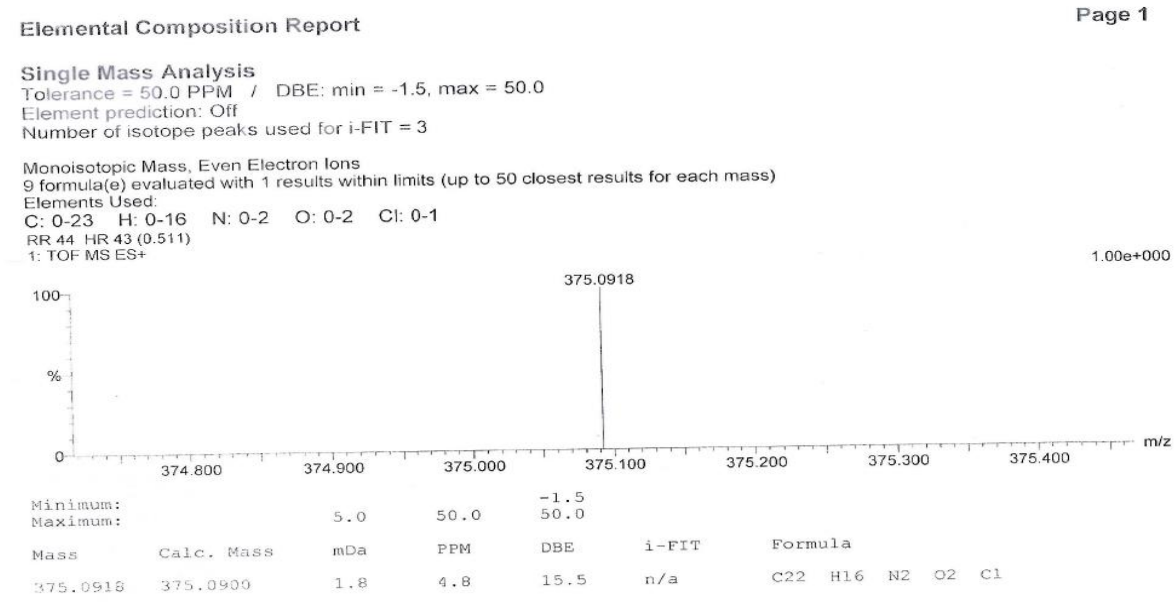


Minimum:				-1.5		
Maximum:		5.0	50.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
330.1056	330.1050	0.6	1.8	14.5	n/a	C22 H17 N Cl

(Table 2, **3s**)



(Table 2, **3t**)



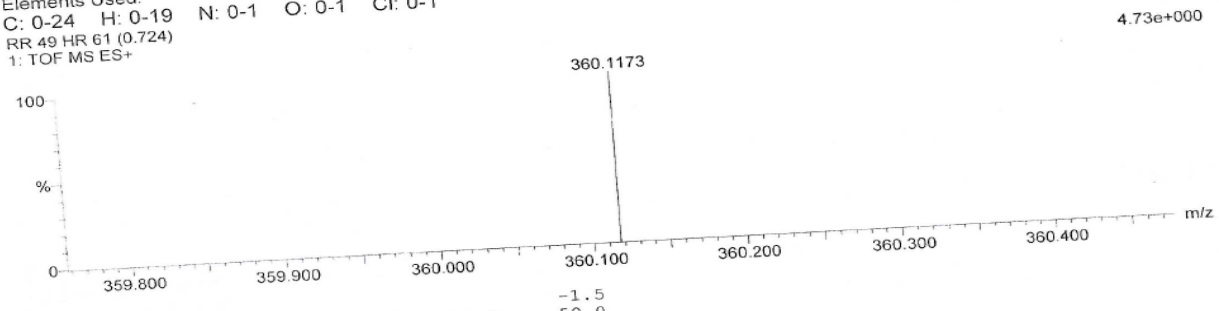
(Table 2, **3u**)

Elemental Composition Report

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

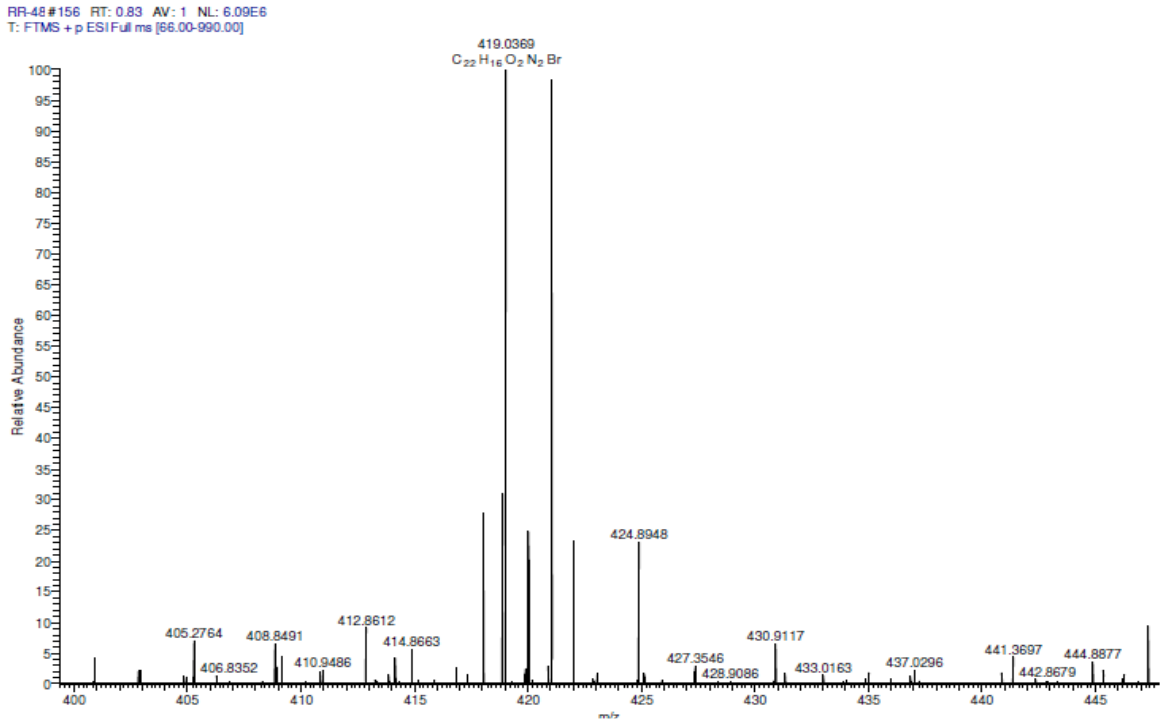
Monoisotopic Mass, Even Electron Ions
3 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-24 H: 0-19 N: 0-1 O: 0-1 Cl: 0-1

RR 49 HR 61 (0.724)
1: TOF MS ES+



Minimum:		5.0	50.0	-1.5		
Maximum:				50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
360.1173	360.1155	1.8	5.0	14.5	n/a	C23 H19 N O Cl

(Table 2, **3v**)



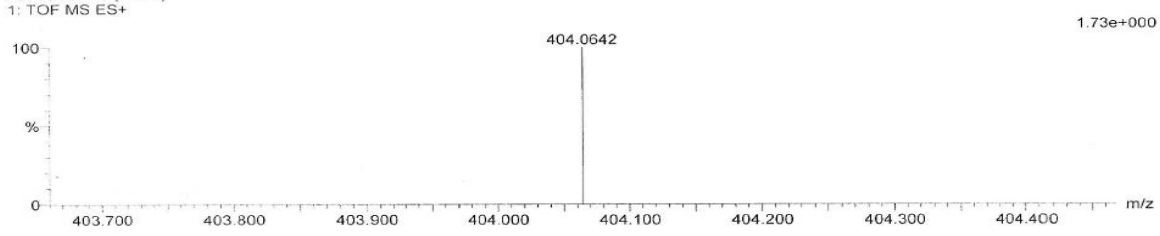
(Table 2, **3w**)

Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions
6 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-24 H: 0-19 N: 0-1 O: 0-1 Br: 0-1

RR 50 HR 71 (0.843)
1: TOF MS ES+



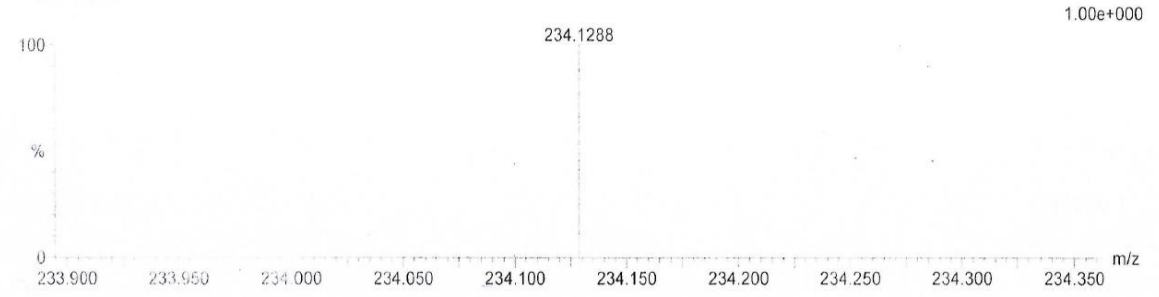
Minimum:				-1.5		
Maximum:		5.0	50.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
404.0642	404.0650	-0.8	-2.0	14.5	n/a	C23 H19 N O Br

(Table 2, **3x**)

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
2 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-18 H: 0-16 N: 0-1

RR69 HR 88 (0.910)
1: TOF MS ES+

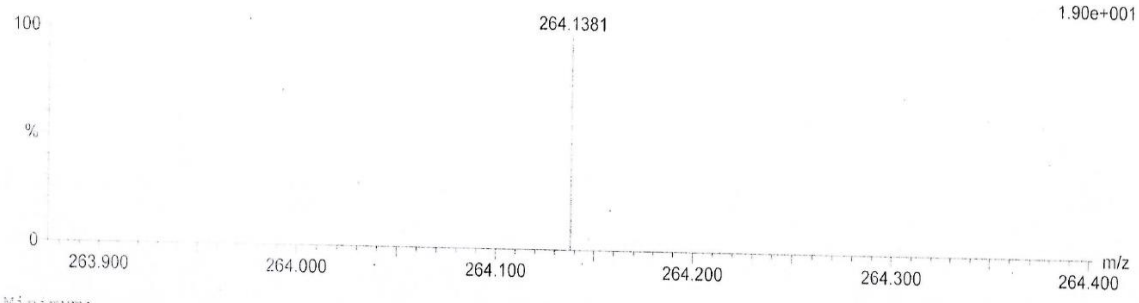


Minimum:				-1.5		
Maximum:		5.0	50.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
234.1288	234.1283	0.5	2.1	10.5	n/a	C17 H16 N

(Table 2, **3y**)

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions
2 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-19 H: 0-18 N: 0-1 O: 0-1
RR 75 HR 57 (0.592)
1: TOF MS ES+

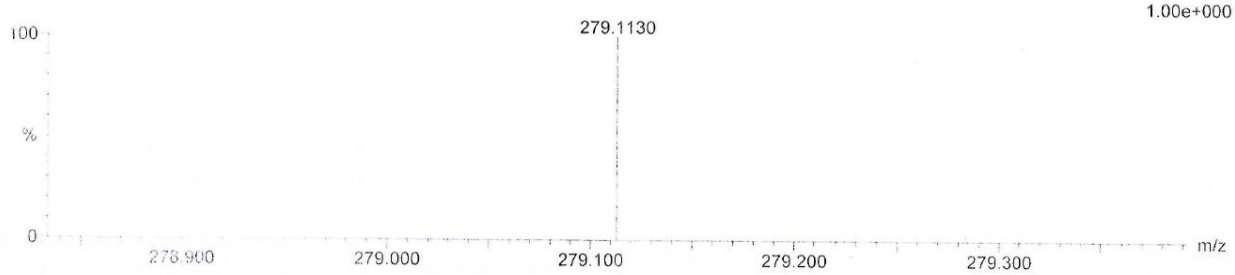


Minimum:		5.0	50.0	-1.5		
Maximum:				50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
264.1381	264.1386	-0.7	-2.7	10.5	n/a	C18 H18 N O

(Table 2, **3z**)

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions
3 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-18 H: 0-15 N: 0-2 O: 0-2
RR 67 HR 15 (0.154)
1: TOF MS ES+

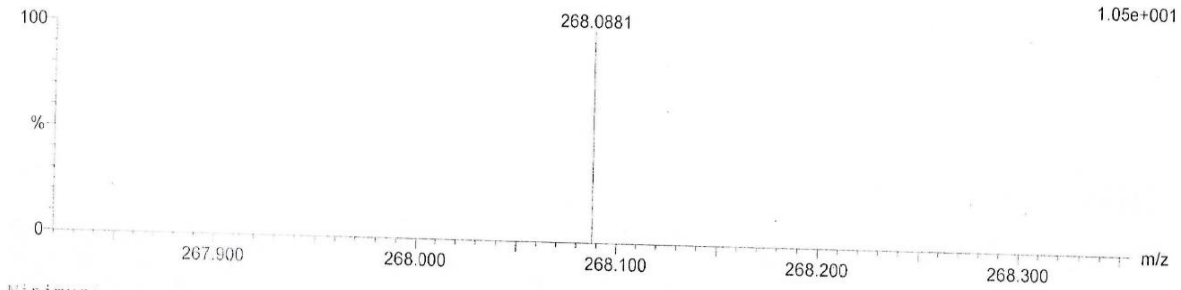


Minimum:		5.0	50.0	-1.5		
Maximum:				50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
279.1130	279.1134	-0.4	-1.4	11.5	n/a	C17 H15 N2 O2

(Table 2, **3aa**)

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions
3 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-18 H: 0-15 N: 0-1 Cl: 0-1
RR70 HR 27 (0.284)
1: TOF MS ES+



Minimum:				-1.5		
Maximum:		5.0	50.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
268.0881	268.0893	-1.2	-4.5	10.5	n/a	C17 H15 N Cl

(Table 2, **3ab**)

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions
7 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-26 H: 0-34 N: 0-1 O: 0-4
RR 62 HR 85 (1.009)
1: TOF MS ES+

Minimum:				-1.5		
Maximum:		5.0	50.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
412.2491	412.2488	0.3	0.7	9.5	n/a	C25 H34 N O4

(Scheme 2, **4**)