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An efficient synthesis of 4-phenoxy-quinazoline, 2-phenoxy-quinoxaline, 2-phenoxy-pyridine derivatives by aryne chemistry,

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General procedure for the preparation of 4-Phenoxy-2-arylquinazoline(3a-e) with aryne

4-Phenoxy-2-phenylquinazoline (3a)

4-Phenoxy-2-(3,4,5-trimethoxyphenyl)quinazoline (3b)

2-(4-(Methylthio)phenyl)-4-phenoxyquinazoline (3c)

4-Phenoxy-2-(4-(trifluoromethoxy)phenyl)quinazoline (3d)

4-Phenoxy-2-(4-(trifluoromethyl)phenyl)quinazoline (3e)

General procedure for the preparation of (*E*)-2-Phenoxy-3-styrylquinoxaline (5a-e) with aryne

(*E*)-2-(4-Methoxystyryl)-3-phenoxyquinoxaline (5a)

(*E*)-3-(4-Methoxystyryl)-1-phenylquinoxalin-2(1*H*)-one (6a)

(*E*)-2-Phenoxy-3-(3,4,5-trimethoxystyryl)quinoxaline (5b)

(*E*)-1-Phenyl-3-(3,4,5-trimethoxystyryl)quinoxalin-2(1*H*)-one (6b)

2-((*E*)-2-(Benzo[*d*][1,3]dioxol-5-yl)vinyl)-3-phenoxyquinoxaline (5c)

(*E*)-3-(2-(Benzo[d][1,3]dioxol-5-yl)vinyl)-1-phenylquinoxalin-2(1*H*)-one (6c)

(*E*)-2-Phenoxy-3-(4-(trifluoromethyl)styryl)quinoxaline (5d)

(*E*)-1-Phenyl-3-(4-(trifluoromethyl)styryl)quinoxalin-2(1*H*)-one (6d)

(*E*)-2-(2-Chlorostyryl)-3-phenoxyquinoxaline (5e)

(*E*)-3-(2-Chlorostyryl)-1-phenylquinoxalin-2(1*H*)-one (6e)

General procedure for the preparation of 2-phenoxy pyridine derivatives (8a-f) with aryne

2-Phenoxy-6-phenyl-4-(3,4,5-trimethoxyphenyl)pyridine (8a)

2-(4-Methoxyphenyl)-6-phenoxy-4-(3,4,5-trimethoxyphenyl)pyridine (8b)

4-(3-Nitrophenyl)-2-phenoxy-6-phenylpyridine (8c)

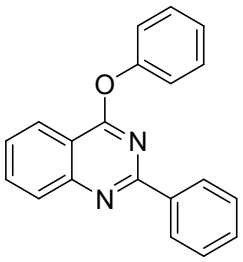
4-(4-Bromophenyl)-2-(4-chlorophenyl)-6-phenoxypyridine (8d)

6-Phenoxy-4-phenyl-2, 2′-bipyridine (8e)

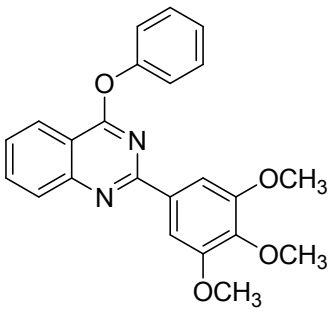
4-(Furan-2-yl)-2-phenoxy-6-phenylpyridine (8f)

General procedure for the preparation of 4-Phenoxy-2-arylquinazoline(3a-e) with aryne:

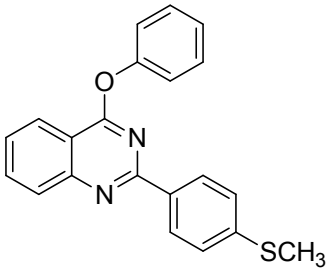
To a stirred solution of 2-phenylquinazolin-4(3*H*)-one (**1a-e**) (0.45mmol, 1.0 equiv) and trimethylsilyl phenyl triflate (**2**) (0.54mmol, 1.2 equiv) in acetonitrile as solvent, was added cesium fluoride (1.35mmol, 3.0 equiv) at room temperature. The mixture was stirred at room temperature for 4hr, after completing the reaction, reaction mixture was concentrated in vacuo. To the resulting residue, water was added, and the mixture was extracted with ethyl acetate three times. The combined organic phase was dried over sodium sulphate, and concentrated in vacuo. The crude product was purified by column chromatography (EtOAc in Hexane) resulting the product.



4-Phenoxy-2-phenylquinazoline (3a). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.25 (d, *J* = 7.7 Hz, 3H), 7.94 (d, *J* = 8.4 Hz, 1H), 7.75 (dd, *J* = 11.3, 4.0 Hz, 1H), 7.47 (t, *J* = 7.6 Hz, 1H), 7.39 (t, *J* = 7.8 Hz, 2H), 7.26 (ddd, *J* = 19.9, 10.0, 4.5 Hz, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.51, 160.71, 153.53, 153.49, 138.51, 134.77, 131.38, 130.25, 129.28, 129.19, 128.97, 127.64, 126.35, 124.39, 122.85, 115.94; IR: 3387, 3064, 2850, 1622, 1573, 1484, 1347, 1210, 933, 770 cm^{-1}; HRMS-ESI $[M+H]^+$*m/z* calcd for $C_{20}H_{15}N_2O$: 299.1179, found 299.1176.



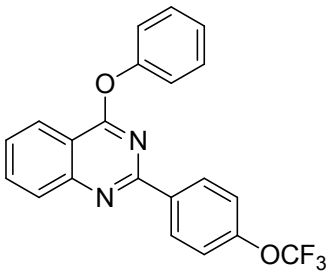
4-Phenoxy-2-(3,4,5-trimethoxyphenyl)quinazoline (3b). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.25 (d, *J* = 7.9 Hz, 1H), 7.95 (d, *J* = 8.4 Hz, 1H), 7.79 (dd, *J* = 11.2, 4.1 Hz, 1H), 7.55 (s, 2H), 7.49 (t, *J* = 7.5 Hz, 1H), 7.39 (t, *J* = 7.8 Hz, 2H), 7.28 (d, *J* = 7.7 Hz, 2H), 7.22 (t, *J* = 7.3 Hz, 1H), 3.79 (s, 3H), 3.76 (s, 6H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 166.61, 159.11, 153.07, 152.84, 152.74, 140.40, 133.97, 132.90, 129.21, 128.05, 126.74, 125.50, 123.53, 122.40, 114.81, 105.49, 60.88, 55.91; IR: 3352, 2581, 1622, 1575, 1398, 1268, 1165, 1126, 767 cm^{-1}; HRMS-ESI $[M+H]^+$*m/z* calcd for $C_{23}H_{21}N_2O_4$: 389.1496, found 389.1506.



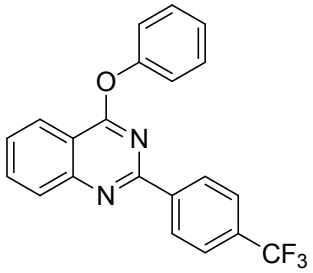
2-(4-(Methylthio)phenyl)-4-phenoxyquinazoline (3c). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.41 (d, *J* = 8.4 Hz, 2H), 8.03 (d, *J* = 8.1 Hz, 1H), 7.86 (d, *J* = 8.4 Hz, 1H), 7.70 (t, *J* = 7.4 Hz, 1H), 7.43 – 7.29 (m, 5H), 7.28 – 7.17 (m, 3H), 4.15 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 167.05, 159.44, 151.81, 139.46, 136.62, 134.81, 133.50, 132.00, 129.84, 129.34, 129.16, 127.92, 127.58, 126.43, 123.46, 115.29, 54.05; IR:

3361, 2922, 1621, 1576, 1502, 1452, 1348, 1175, 799, 690 cm^{-1}; HRMS-ESI $[M+H]^+$*m/z* calcd for $C_{21}H_{17}N_2OS$: 355.1624, found 355.1628.

4-Phenoxy-2-(4-(trifluoromethoxy)phenyl)quinazoline (3d). ^1H NMR (400 MHz, $CDCl_3$): δ 8.24 (t, *J* = 7.5 Hz, 3H), 7.91 (d, *J* = 8.4 Hz, 1H), 7.76 (dd, *J* = 11.2, 4.0 Hz, 1H), 7.47 (t, *J* = 7.5 Hz, 1H), 7.42 – 7.36 (m, 2H), 7.28 – 7.19 (m, 3H), 7.11 (d, *J* = 8.5 Hz, 2H): ^{13}C NMR (101 MHz, $CDCl_3$): δ 166.83, 158.56, 152.66, 152.57, 151.07, 136.26, 134.10, 130.10, 129.51, 128.17, 127.09, 125.70, 123.62, 122.03, 120.47, 115.10; IR: 3392, 2921, 1607, 1562, 1486, 1162, 861, 742 cm^{-1};HRMS-ESI $[M+H]^+$*m/z* calcd for $C_{21}H_{14}F_3N_2O_2$: 383.1002, found 383.1004.



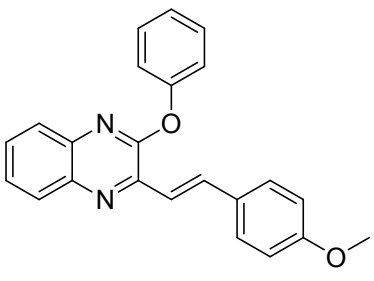
4-Phenoxy-2-(4-(trifluoromethyl)phenyl)quinazoline (3e). ^1H NMR (400 MHz, $CDCl_3$): δ 8.34 (d, *J* = 8.1 Hz, 2H), 8.28 (d, *J* = 8.1 Hz, 1H), 7.96 (d, *J* = 8.4 Hz, 1H), 7.81 (t, *J* = 7.7 Hz, 1H), 7.54 (t, *J* = 7.8 Hz, 3H), 7.42 (t, *J* = 7.8 Hz, 2H), 7.30 – 7.24 (m, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 167.76, 159.26, 153.46, 153.36, 141.82, 135.04, 130.35, 129.52, 129.15, 128.26, 126.58, 126.13, 126.10, 124.49, 122.83, 116.16; IR: 3387, 2921, 2350, 1744, 1622, 1324, 1111, 690 cm^{-1};HRMS-ESI $[M+H]^+$*m/z* calcd for $C_{21}H_{14}F_3N_2O$: 367.1053, found 367.1055.



General procedure for the preparation of (*E*)-2-Phenoxy-3-styrylquinoxaline(5a-e) with aryne:

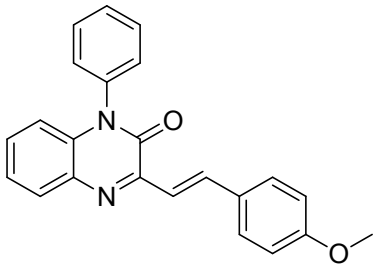
To a stirred solution of (*E*)-3-styrylquinoxalin-2(1*H*)-one(**4a-e**) (0.28mmol, 1.0 equiv) and trimethylsilyl phenyl triflate (**2)** (0.33mmol, 1.2 equiv) in acetonitrile as solvent, was added Cesium fluoride (1.35mmol, 3.0 equiv) at room temperature. The mixture was stirred at room temperature for 4hr, after completing the reaction, reaction mixture was concentrated in vacuo. To the resulting residue, water was added, and the mixture was extracted with ethyl acetate three times. The combined organic phase was dried over sodium sulphate, and concentrated in vacuo. The crude product was purified by column chromatography (EtoAc in Hexane), resulting the product.

(*E*)-2-(4-Methoxystyryl)-3-phenoxyquinoxaline (5a).^1H NMR (400 MHz, $CDCl_3$): δ 8.04 (d, *J* = 16.0 Hz, 1H), 7.96 – 7.91 (m,



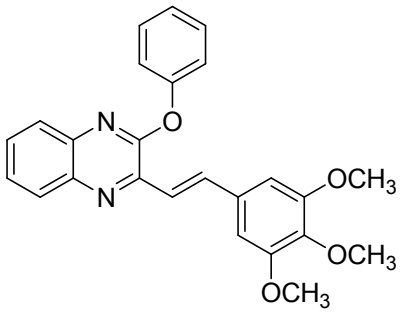
1H), 7.62 – 7.54 (m, 4H), 7.52 – 7.44 (m, 2H), 7.40 (t, *J* = 7.8 Hz, 2H), 7.21 (dd, *J* = 13.1, 11.1 Hz, 3H), 6.86 (d, *J* = 8.6 Hz, 2H), 3.77 (s, 3H).^{13}C NMR (101 MHz, $CDCl_3$): δ 160.58, 155.15, 153.11, 144.33, 139.95, 139.30, 137.27, 129.59, 129.37, 129.29, 129.04, 128.38, 127.52, 127.28, 125.28, 121.86, 118.65, 114.30, 55.38.IR: 3361, 2922, 1621, 1576, 1502, 1452, 1348, 1175, 799, 690 cm^{-1}; HRMS-ESI $[M+H]^+$*m/z* calcd for $C_{23}H_{19}N_2O_2$: 355.1441, found 355.1447.

(*E*)-3-(4-Methoxystyryl)-1-phenylquinoxalin-2(1*H*)-one



(6a).^{1}H NMR (400 MHz, $CDCl_3$): δ 8.13 (d, *J* = 16.2 Hz, 1H), 7.84 – 7.78 (m, 1H), 7.59 – 7.45 (m, 6H), 7.28 – 7.16 (m, 4H), 6.84 (d, *J* = 8.6 Hz, 2H), 6.57 (d, *J* = 8.1 Hz, 1H), 3.76 (s, 3H).^{13}C NMR (101 MHz, $CDCl_3$): δ 160.73, 154.93, 153.36, 138.57, 136.13, 133.64, 133.43, 130.31, 129.50, 129.41, 129.40, 129.32, 129.07, 128.30, 124.00, 120.27, 115.40, 114.31, 55.37.IR: 3361, 2922, 1621, 1576, 1502, 1452, 1348, 1175, 799, 690 cm^{-1};HRMS-ESI $[M+H]^+$*m/z* calcd for $C_{23}H_{19}N_2O_2$: 355.1441, found 355.1435.

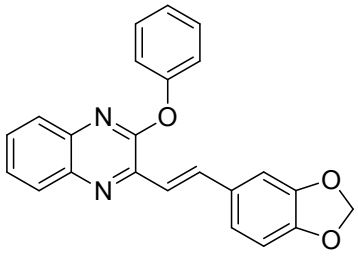
(*E*)-2-Phenoxy-3-(3,4,5-trimethoxystyryl)quinoxaline



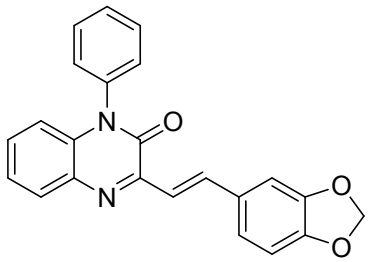
(5b).^{1}H NMR (400 MHz, $CDCl_3$): δ 8.11 (d, *J* = 16.0 Hz, 1H), 8.02 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.70 – 7.62 (m, 2H), 7.57 (ddd, *J* = 7.6, 5.2, 1.8 Hz, 2H), 7.52 – 7.47 (m, 2H), 7.35 – 7.29 (m, 3H), 6.94 (s, 2H), 3.94 (s, 6H), 3.91 (s, 3H).^{13}C NMR (126 MHz, $CDCl_3$): δ 155.25, 153.46, 152.99, 143.81, 139.87, 139.40, 139.22, 137.73, 132.13, 129.68, 129.37, 128.41, 127.65, 127.30, 125.45, 122.01, 120.37, 104.83, 61.04, 56.23.IR: 3361, 2922, 1621, 1576, 1502, 1452, 1348, 1175, 799, 690 cm^{-1};HRMS-ESI $[M+H]^+$*m/z* calcd for $C_{25}H_{23}N_2O_4$: 415.1652, found 415.1653.

(*E*)-1-Phenyl-3-(3,4,5-trimethoxystyryl)quinoxalin-2(1*H*)-one (6b).^{1}H NMR (400 MHz, $CDCl_3$): δ 8.21 (d, *J* = 16.1 Hz, 1H), 7.92 – 7.87 (m, 1H), 7.67 – 7.54 (m, 4H), 7.36 – 7.27 (m, 4H), 6.90 (s, 2H), 6.67 (dd, *J* = 7.8, 1.8 Hz, 1H), 3.90 (s, 6H), 3.89 (s, 3H).^{13}C NMR (126 MHz, $CDCl_3$): δ 154.92, 153.38, 152.89, 139.28, 139.01, 135.98, 133.62, 133.37, 132.14, 130.34, 129.49, 129.46, 129.40, 128.23, 124.16, 122.00, 115.49, 104.88, 61.01, 56.11.IR: 3361, 2922, 1621, 1576, 1502, 1452, 1348, 1175, 799, 690 cm^{-1};HRMS-ESI $[M+H]^+$*m/z* calcd for $C_{25}H_{23}N_2O_4$: 415.1652, found 415.1606.

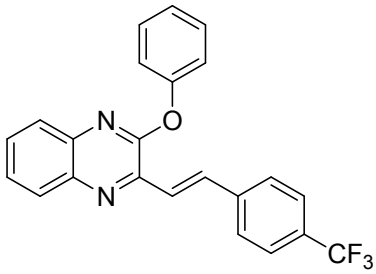
2-((*E*)-2-(Benzo[*d*][1,3]dioxol-5-yl)vinyl)-3-phenoxyquinoxaline (5c). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.11 (d, *J* = 15.9 Hz, 1H), 8.05 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.70 (dd, *J* = 7.8, 1.5 Hz, 1H), 7.64 (d, *J* = 16.0 Hz, 1H), 7.59 (td, *J* = 7.3, 1.6 Hz, 2H), 7.52 (t, *J* = 7.9 Hz, 2H), 7.36 – 7.31 (m, 3H), 7.29 (s, 1H), 7.20 (d, *J* = 8.0 Hz, 1H), 6.88 (d, *J* = 8.0 Hz, 1H), 6.03 (s, 2H).^{13}C NMR (101 MHz, $CDCl_3$): δ 155.14, 153.04, 148.72, 148.33, 144.09, 139.91, 139.35, 137.29, 131.08, 129.62, 129.16, 128.41, 127.58, 127.29, 125.33, 123.73, 121.87, 119.02, 108.58, 106.40, 101.42.IR: 3361, 2922, 1621, 1576, 1502, 1452, 1348, 1175, 799, 690 cm^{-1};HRMS-ESI $[M+H]^+$*m/z* calcd for $C_{23}H_{17}N_2O_3$: 369.1234, found 369.1243.



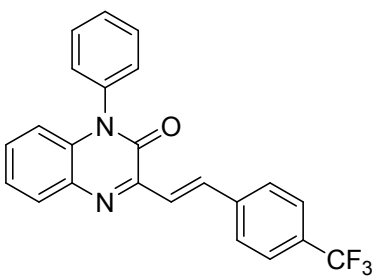
(*E*)-3-(2-(Benzo[d][1,3]dioxol-5-yl)vinyl)-1-phenylquinoxalin-2(1*H*)-one (6c). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.19 (d, *J* = 16.1 Hz, 1H), 7.94 – 7.88 (m, 1H), 7.66 (t, *J* = 7.4 Hz, 2H), 7.59 (t, *J* = 12.0 Hz, 2H), 7.33 (t, *J* = 7.1 Hz, 3H), 7.26 (d, *J* = 20.9 Hz, 2H), 7.15 (d, *J* = 8.1 Hz, 1H), 6.85 (d, *J* = 8.0 Hz, 1H), 6.68 (d, *J* = 7.7 Hz, 1H), 6.03 (s, 2H).^{13}C NMR (101 MHz, $CDCl_3$): δ 154.91, 153.17, 148.87, 148.29, 138.61, 136.07, 133.65, 133.39, 131.14, 130.34, 129.46, 129.36, 129.20, 128.27, 124.07, 124.05, 120.70, 115.42, 108.56, 106.44, 101.40.IR: 3361, 2922, 1621, 1576, 1502, 1452, 1348, 1175, 799, 690 cm^{-1};HRMS-ESI $[M+H]^+$*m/z* calcd for $C_{23}H_{17}N_2O_3$: 369.1234, found 369.1237.



(*E*)-2-Phenoxy-3-(4-(trifluoromethyl)styryl)quinoxaline(5d). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.10 (d, *J* = 16.1 Hz, 1H), 8.01 – 7.96 (m, 1H), 7.77 (dd, *J* = 21.8, 12.1 Hz, 3H), 7.63 (ddd, *J* = 15.1, 8.5, 5.1 Hz, 3H), 7.56 – 7.50 (m, 2H), 7.46 – 7.40 (m, 2H), 7.29 – 7.18 (m, 3H).^{13}C NMR (126 MHz, $CDCl_3$): δ 155.26, 152.88, 143.17, 139.88, 139.83, 139.74, 135.70, 129.84, 129.68, 128.66, 127.83, 127.79, 127.37, 125.80, 125.77, 125.49, 123.38, 121.87.IR: 3361, 2922, 1621, 1576, 1502, 1452, 1348, 1175, 799, 690 cm^{-1};HRMS-ESI $[M+H]^+$*m/z* calcd for $C_{23}H_{16}F_3N_2O$: 393.1209, found 393.1225.

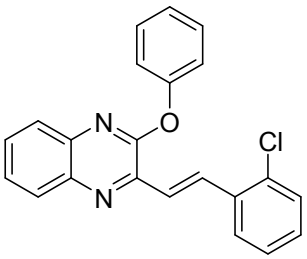


(*E*)-1-Phenyl-3-(4-(trifluoromethyl)styryl)quinoxalin-2(1*H*)-one (6d). ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.17 (d, *J* = 16.2 Hz, 1H), 7.87 – 7.82 (m, 1H), 7.68 (dd, *J* = 14.2, 12.3 Hz, 3H), 7.56 (dd, *J* = 10.1, 4.7 Hz, 4H), 7.51 (d, *J*= 7.5 Hz, 1H), 7.28 – 7.21

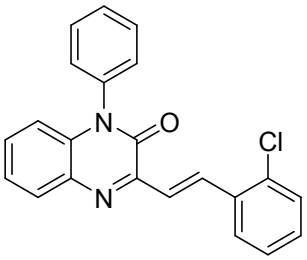


(m, 4H), 6.62 – 6.57 (m, 1H).^{13}C NMR (126 MHz, $CDCl_3$): δ 154.82, 152.55, 139.91, 136.95, 135.87, 133.88, 133.25, 130.42, 130.00, 129.74, 129.60, 128.21, 127.94, 125.79, 125.76, 124.99, 124.23, 115.55.IR: 3361, 2922, 1621, 1576, 1502, 1452, 1348, 1175, 799, 690 cm^{-1};HRMS-ESI $[M+H]^+$*m/z* calcd for $C_{23}H_{16}F_3N_2O$: 393.1209, found 393.1218.

(*E*)-2-(2-Chlorostyryl)-3-phenoxyquinoxaline (5e).^{1}HNMR (500 MHz, $CDCl_3$): δ 8.02 (d, *J* = 16.0 Hz, 1H), 7.94 (dd, *J* = 8.0, 1.8 Hz, 1H), 7.67 (d, *J* = 16.0 Hz, 1H), 7.62 – 7.58 (m, 1H), 7.56 (d, *J* = 8.6 Hz, 2H), 7.51 – 7.48 (m, 2H), 7.40 (t, *J* = 7.9 Hz, 2H), 7.30 (d, *J* = 8.5 Hz, 2H), 7.22 (dd, *J* = 5.9, 4.9 Hz, 2H), 7.18 – 7.16 (m, 1H).^{13}C NMR (126 MHz, $CDCl_3$): δ 154.15, 151.90, 142.55, 138.82, 138.53, 135.08, 133.96, 133.83, 128.59, 128.50, 128.03, 127.88, 127.51, 126.64, 126.30, 124.36, 120.80, 120.44, 28.68.IR: 3361, 2922, 1621, 1576, 1502, 1452, 1348, 1175, 799, 690 cm^{-1};HRMS-ESI $[M+H]^+$*m/z* calcd for $C_{22}H_{16}ClN_2O$: 359.0946, found 359.0951.

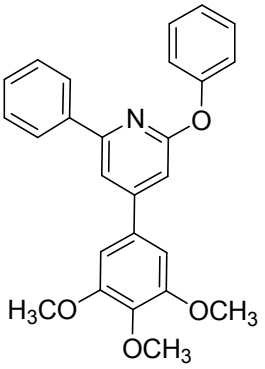


(*E*)-3-(2-Chlorostyryl)-1-phenylquinoxalin-2(1*H*)-one (6e).^{1}H NMR (400 MHz, $CDCl_3$): δ 8.12 (d, *J* = 16.2 Hz, 1H), 7.87 – 7.81 (m, 1H), 7.65 – 7.49 (m, 5H), 7.27 (ddd, *J* = 8.9, 7.2, 5.3 Hz, 6H), 7.19 (s, 1H), 6.60 (dd, *J* = 7.6, 2.0 Hz, 1H).^{13}C NMR (126 MHz, MeOD): δ 154.95, 152.42, 136.68, 136.01, 135.07, 134.79, 133.74, 133.23, 130.08, 129.70, 129.35, 129.07, 128.85, 128.76, 128.12, 124.12, 122.03, 115.36.IR: 3361, 2922, 1621, 1576, 1502, 1452, 1348, 1175, 799, 690 cm^{-1};HRMS-ESI $[M+H]^+$*m/z* calcd for $C_{22}H_{16}ClN_2O$: 359.0946, found 359.0952.



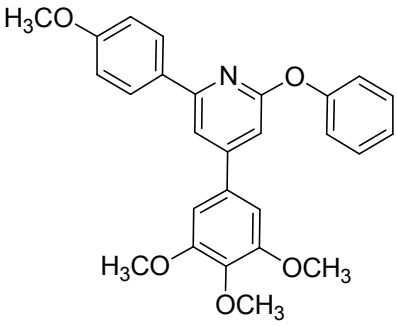
General procedure for the preparation of 2-phenoxy pyridine derivatives(8a-f) with aryne

To a stirred solution of 4, 6-diphenylpyridin-2(1*H*)-one (**7a-f**) (0.24mmol, 1.0 equiv) and trimethylsilyl phenyl triflate (**2**) (0.29mmol, 1.2 equiv) in acetonitrile as solvent, was added Cesium fluoride (0.72mmol, 3.0 equiv) at room temperature. The mixture was stirred at room temperature for 4hr, after completing the reaction, reaction mixture was concentrated in vacuo. To the resulting residue, water was added, and the mixture was extracted with ethyl acetate three times. The combined organic phase was dried over sodium sulphate, and concentrated in vacuo. The crude product was purified by column chromatography (EtoAc in Hexane), resulting the product.

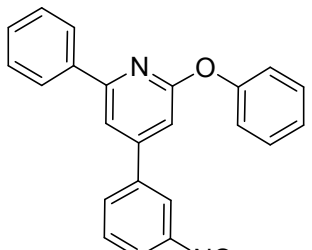


2-Phenoxy-6-phenyl-4-(3,4,5-trimethoxyphenyl)pyridine (8a). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.87 (dd, *J* = 8.0, 1.4 Hz, 2H), 7.54 (d, *J*= 1.1 Hz, 1H), 7.36 – 7.27 (m, 5H), 7.17 (dd, *J* = 8.6, 0.9 Hz, 2H), 7.12 (dd, *J* = 11.5, 4.2 Hz, 1H), 6.89 (d, *J* = 1.0 Hz, 1H), 6.75 (s, 2H), 3.84 (s, 6H), 3.82 (s, 3H).^{13}C NMR (126 MHz, $CDCl_3$): δ 163.92, 156.01, 154.38, 153.73, 153.26, 139.05, 138.49, 134.35, 129.54, 129.26, 128.70, 126.92, 124.45, 121.12, 113.54, 107.61, 104.44, 61.04, 56.36. IR: 3345, 2922, 1592, 1649, 1489, 1370, 1306, 1127, 1017, 773, 694 cm^{-1}; HRMS-ESI $[M+H]^+$*m/z* calcd for $C_{26}H_{24}NO_4$: 414.17, found 414.1687.

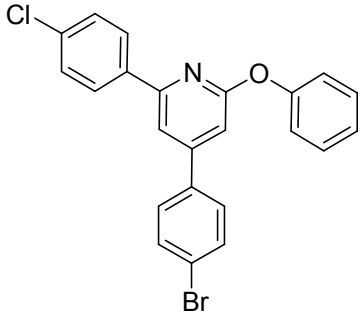
2-(4-Methoxyphenyl)-6-phenoxy-4-(3,4,5-trimethoxyphenyl)pyridine (8b). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.95 (d, *J* = 8.9 Hz, 2H), 7.59 (d, *J* = 1.2 Hz, 1H), 7.45 (dd, *J* = 8.5, 7.4 Hz, 2H), 7.28 (dd, *J* = 8.6, 1.0 Hz, 2H), 7.24 (dd, *J* = 11.5, 4.2 Hz, 1H), 6.95 (dd, *J* = 9.0, 5.0 Hz, 3H), 6.87 (s, 2H), 3.97 (s, 6H), 3.94 (s, 3H), 3.86 (s, 3H).^{13}C NMR (101 MHz, $CDCl_3$): δ 163.83, 160.68, 155.73, 154.50, 153.72, 153.15, 139.14, 134.48, 131.13, 129.47, 128.23, 124.32, 121.09, 114.04, 112.63, 106.76, 104.57, 60.98, 56.37, 55.34.IR: 3361, 2922, 1621, 1576, 1502, 1452, 1348, 1175, 799, 690 cm^{-1};HRMS-ESI $[M+H]^+$*m/z* calcd for $C_{27}H_{26}NO_5$: 444.1805, found 444.1799.



4-(3-Nitrophenyl)-2-phenoxy-6-phenylpyridine (8c). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.40 (t, *J* = 1.9 Hz, 1H), 8.19 (ddd, *J* = 8.2, 2.2, 1.0 Hz, 1H), 7.86 (ddd, *J* = 4.6, 2.4, 1.4 Hz, 3H), 7.56 (dd, *J* = 11.3, 4.6 Hz, 2H), 7.32 (ddd, *J* = 8.1, 6.2, 4.6 Hz, 5H), 7.19 – 7.11 (m, 3H), 6.91 (d, *J* = 1.2 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$): δ 164.20, 156.60, 154.08, 150.45, 148.79, 140.18, 137.99, 133.09, 130.21, 129.63, 129.56, 128.77, 126.93, 124.74, 123.82, 122.09, 121.27, 113.10, 107.50. IR: 3398, 2921, 1551, 1489, 1390, 1214, 772, 693 cm^{-1};HRMS-ESI $[M+H]^+$*m/z* calcd for $C_{23}H_{17}N_2O_3$: 369.1234, found 369.1232.

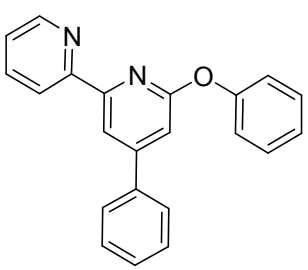


4-(4-Bromophenyl)-2-(4-chlorophenyl)-6-phenoxypyridine (8d). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.80 (d, *J* = 8.7 Hz, 2H), 7.51 (dd, *J*= 12.8, 4.9 Hz, 3H), 7.44 – 7.39 (m, 2H), 7.37 – 7.31 (m, 2H), 7.29 (d, *J* = 8.7 Hz, 2H), 7.18 – 7.12 (m, 3H), 6.87 (d, *J* = 1.2 Hz, 1H).^{13}C NMR (126 MHz, $CDCl_3$): δ 164.18, 154.98, 154.12, 151.97, 137.17, 136.73, 135.40, 132.32, 129.64, 128.89, 128.68,

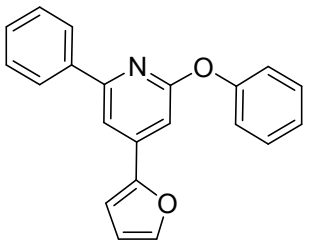


128.16, 124.71, 123.74, 121.24, 112.87, 107.39. IR: 3389, 2921, 1649, 1594, 1488, 1377, 1182, 1011, 763 cm^{-1};HRMS-ESI $[M+H]^+$*m/z* calcd for $C_{23}H_{16}BrClNO$: 436.0098, found 436.0095.

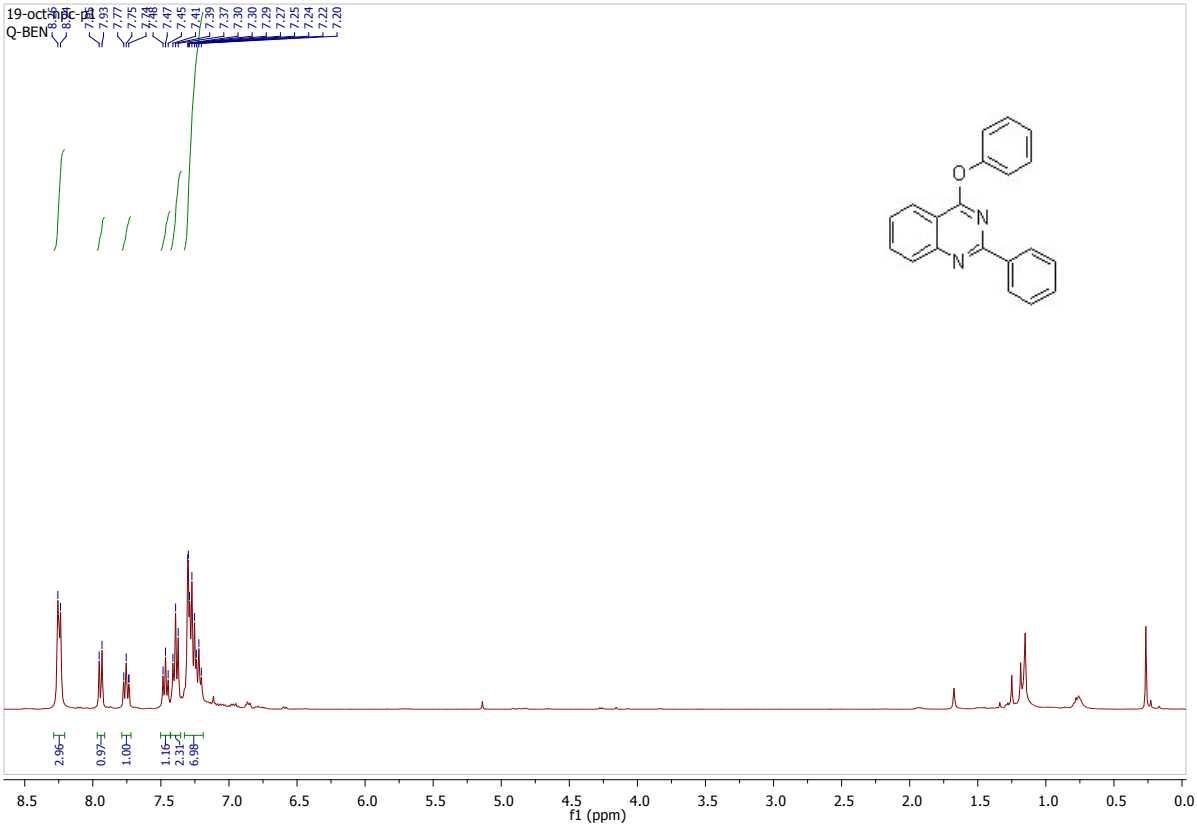
6-Phenoxy-4-phenyl-2,2′-bipyridine (8e). ^1H NMR (500 MHz, $CDCl_3$): δ 8.73 – 8.70 (m, 1H), 8.51 (d, *J* = 1.3 Hz, 1H), 8.25 (d, *J* = 8.0 Hz, 1H), 7.81 – 7.75 (m, 3H), 7.55 – 7.46 (m, 5H), 7.31 (dt, *J* = 15.8, 4.2 Hz, 4H), 7.16 (d, *J* = 1.3 Hz, 1H).^{13}C NMR (126 MHz, $CDCl_3$): δ 163.89, 155.46, 154.69, 154.42, 153.27, 149.04, 138.14, 136.96, 129.62, 129.24, 129.02, 127.23, 124.53, 123.89, 121.45, 121.21, 114.18, 108.91.IR: 3345,2921,2851, 1584, 1551, 1490, 1393, 1358, 1214, 949, 763 cm^{-1};HRMS-ESI $[M+H]^+$*m/z* calcd for $C_{22}H_{17}N_2O$: 325.1335, found 325.1337.



4-(Furan-2-yl)-2-phenoxy-6-phenylpyridine (8f). ^1H NMR (400 MHz, $CDCl_3$): δ 7.89 (dd, *J* = 8.1, 1.5 Hz, 2H), 7.66 (d, *J* = 1.1 Hz, 1H), 7.48 – 7.45 (m, 1H), 7.38 – 7.28 (m, 5H), 7.19 – 7.11 (m, 3H), 6.94 (d, *J* = 1.1 Hz, 1H), 6.81 (dd, *J* = 3.4, 0.5 Hz, 1H), 6.46 (dd, *J* = 3.4, 1.8 Hz, 1H).^{13}C NMR (101 MHz, $CDCl_3$): δ 164.13, 156.25, 154.40, 151.49, 143.77, 141.75, 138.36, 129.56, 129.24, 128.64, 126.87, 124.46, 121.12, 112.10, 109.73, 108.95, 103.37.IR: 3398, 2921, 1594, 1559, 1489, 1397, 1215, 1020, 772 cm^{-1};HRMS-ESI $[M+H]^+$*m/z* calcd for $C_{21}H_{16}NO_2$: 314.1176, found 314.118.



^1H &^{13}C NMR of 4-Phenoxy-2-phenylquinazoline (3a)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8.25
7.93
7.77
7.75
7.74
7.48
7.47
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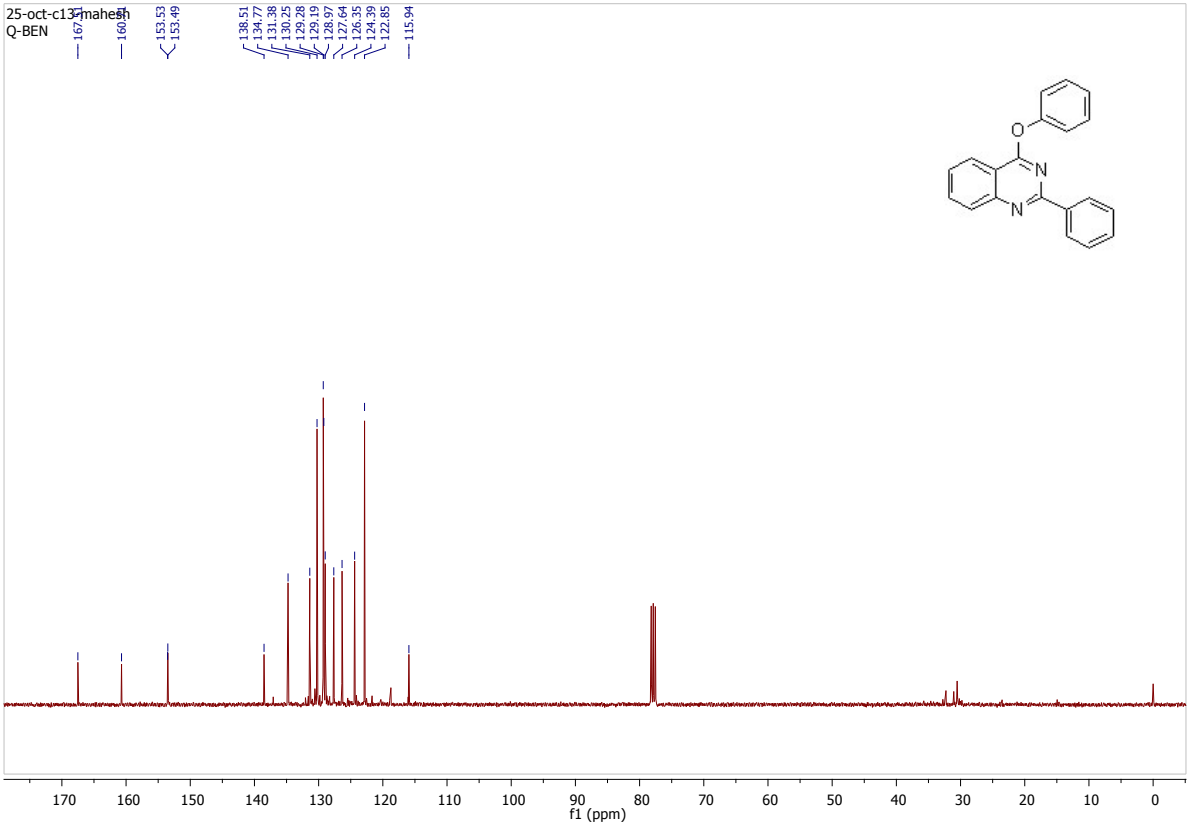
7.41
7.39
7.37
7.30
7.30
7.29
7.27
7.25
7.24
7.22
7.20
O
N
N
2.96
0.97
1.00
1.16
2.31
6.98
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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Q-BEN
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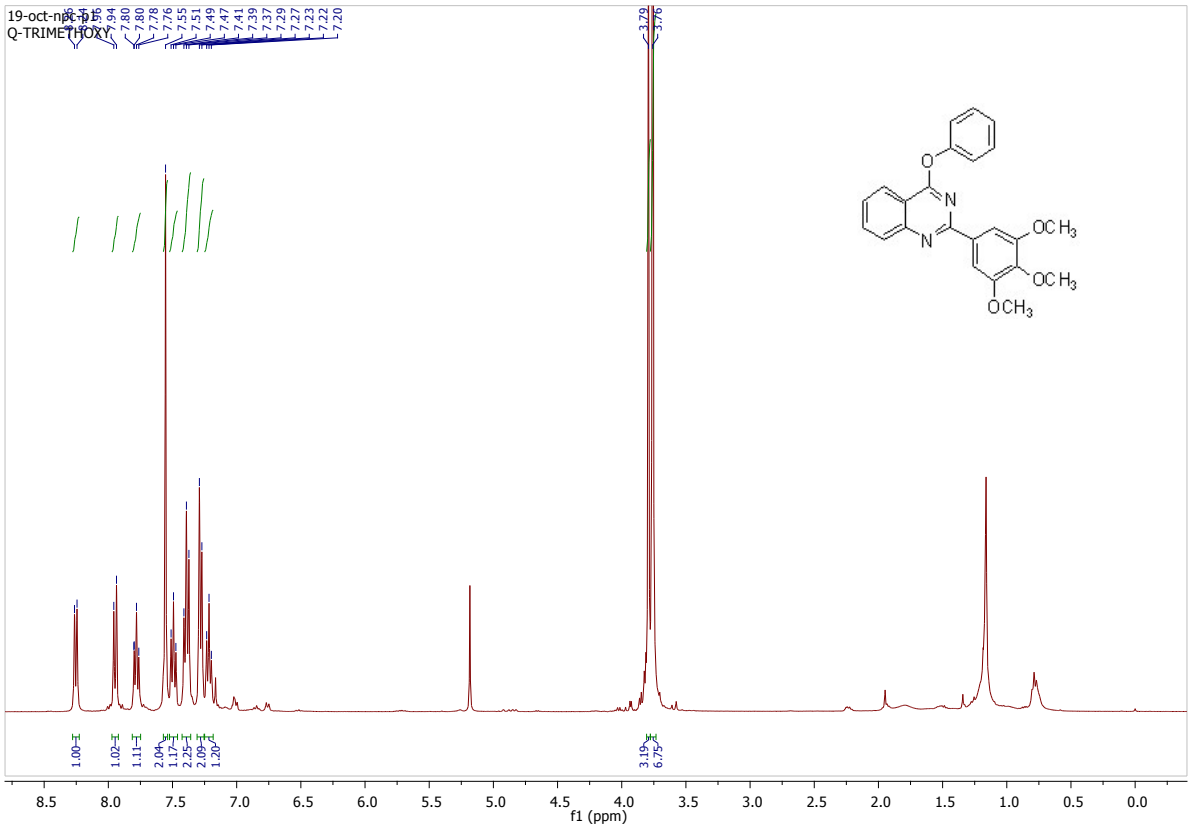
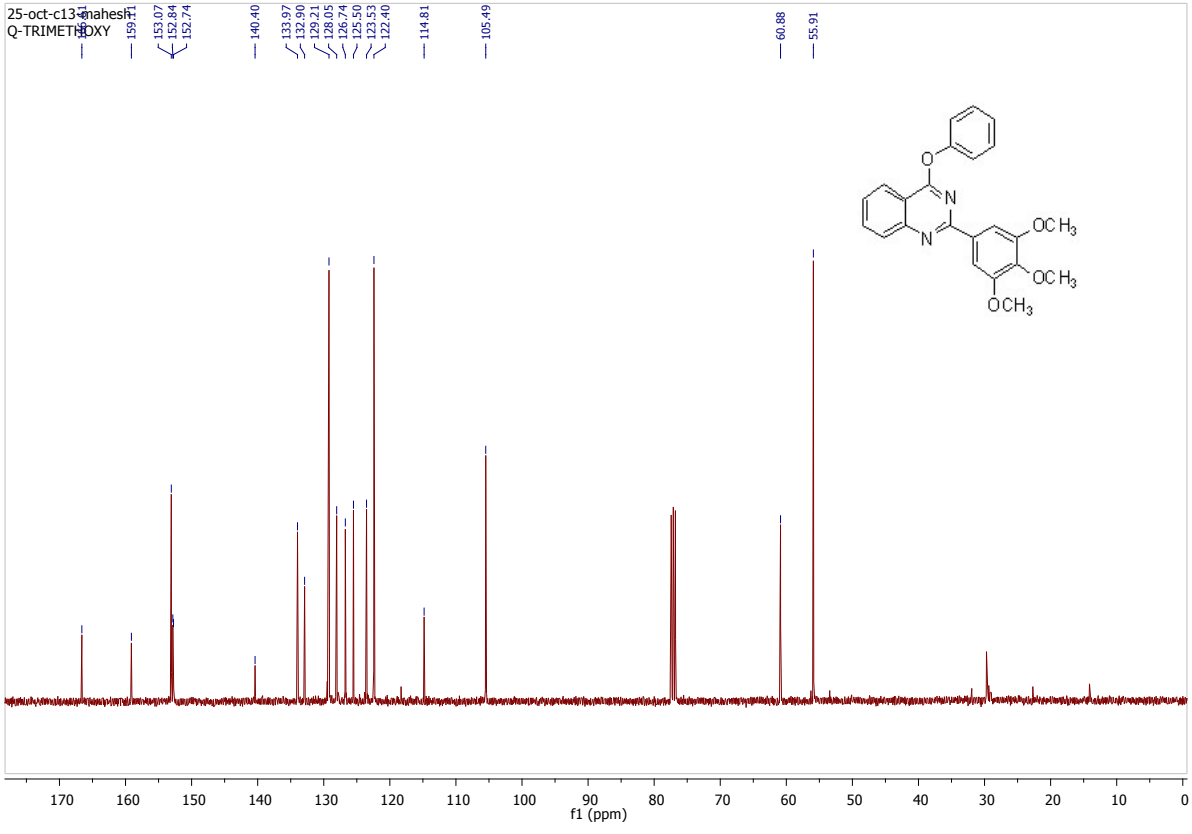
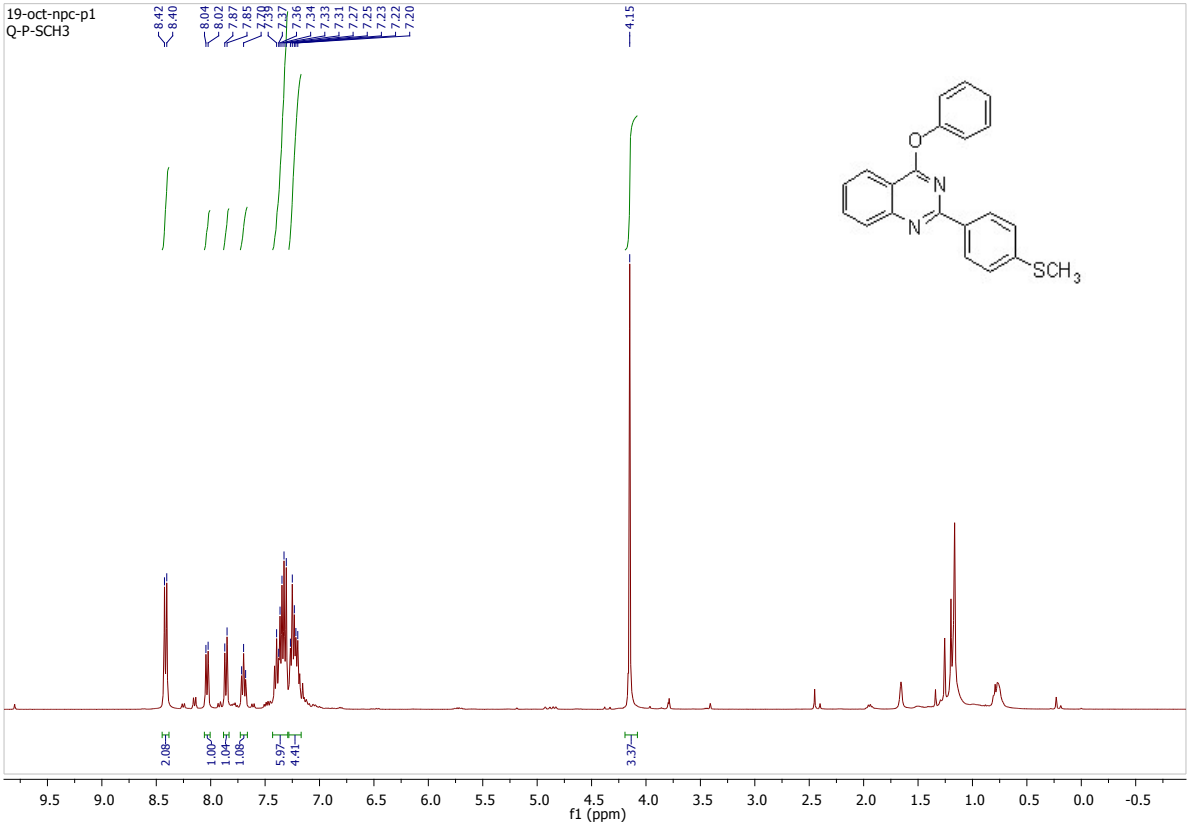
160.
153.53
153.49
138.51
134.77
131.38
130.25
129.28
129.19
128.97
127.64
126.35
124.39
122.85
115.94
O
N
N
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

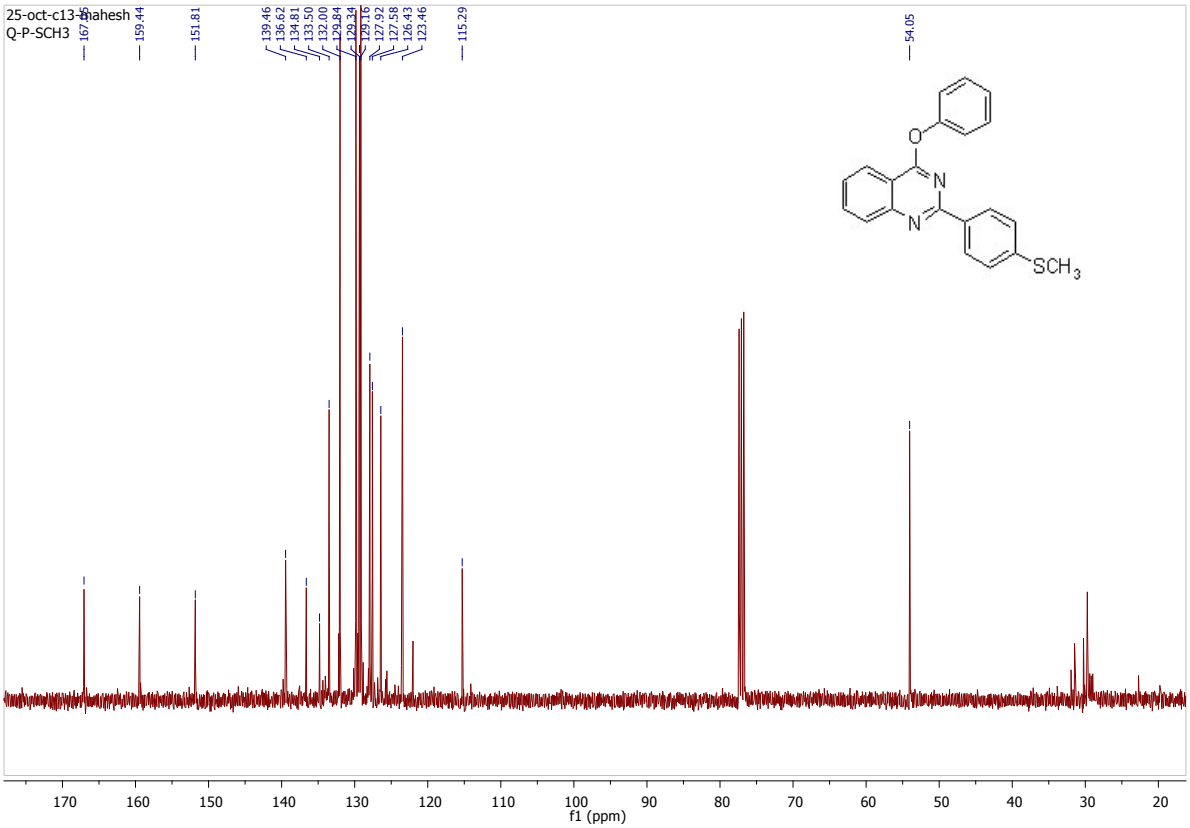
^{1}H &^{13}C NMR of 4-Phenoxy-2-(3,4,5-trimethoxyphenyl)quinazoline (3b)



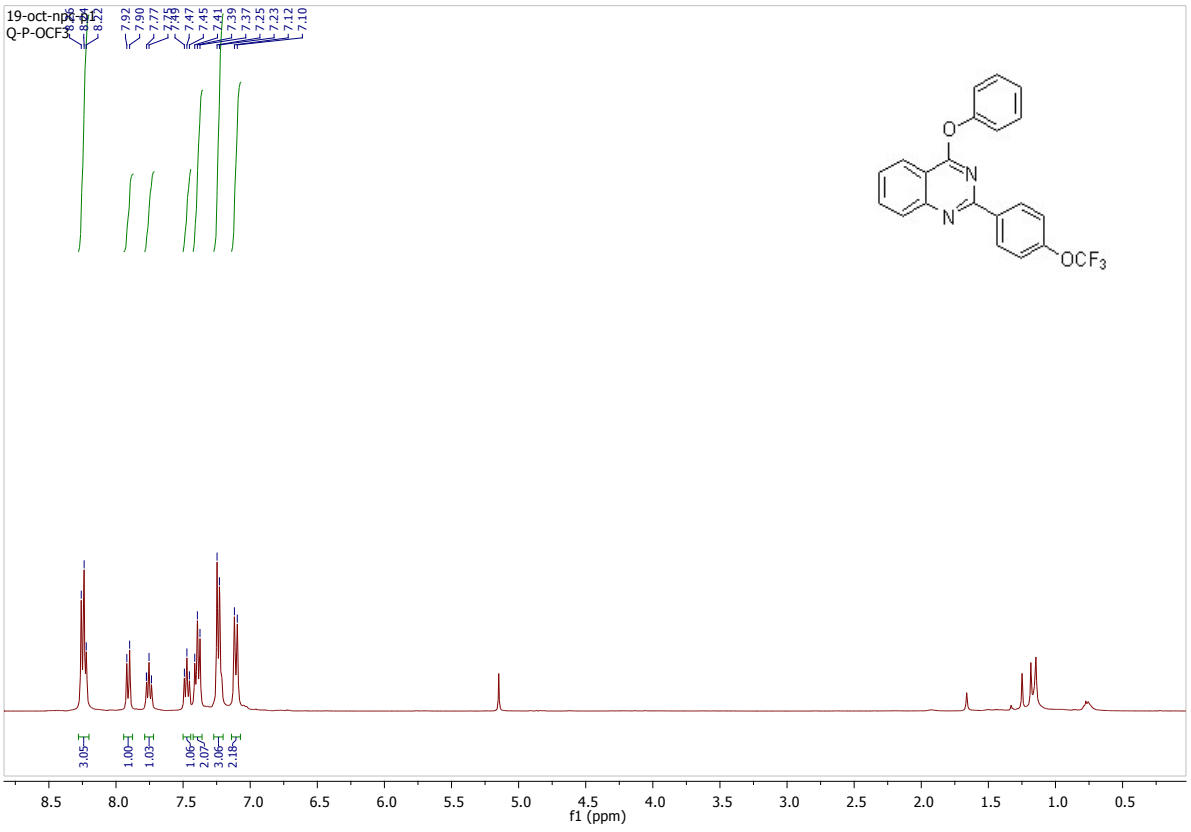


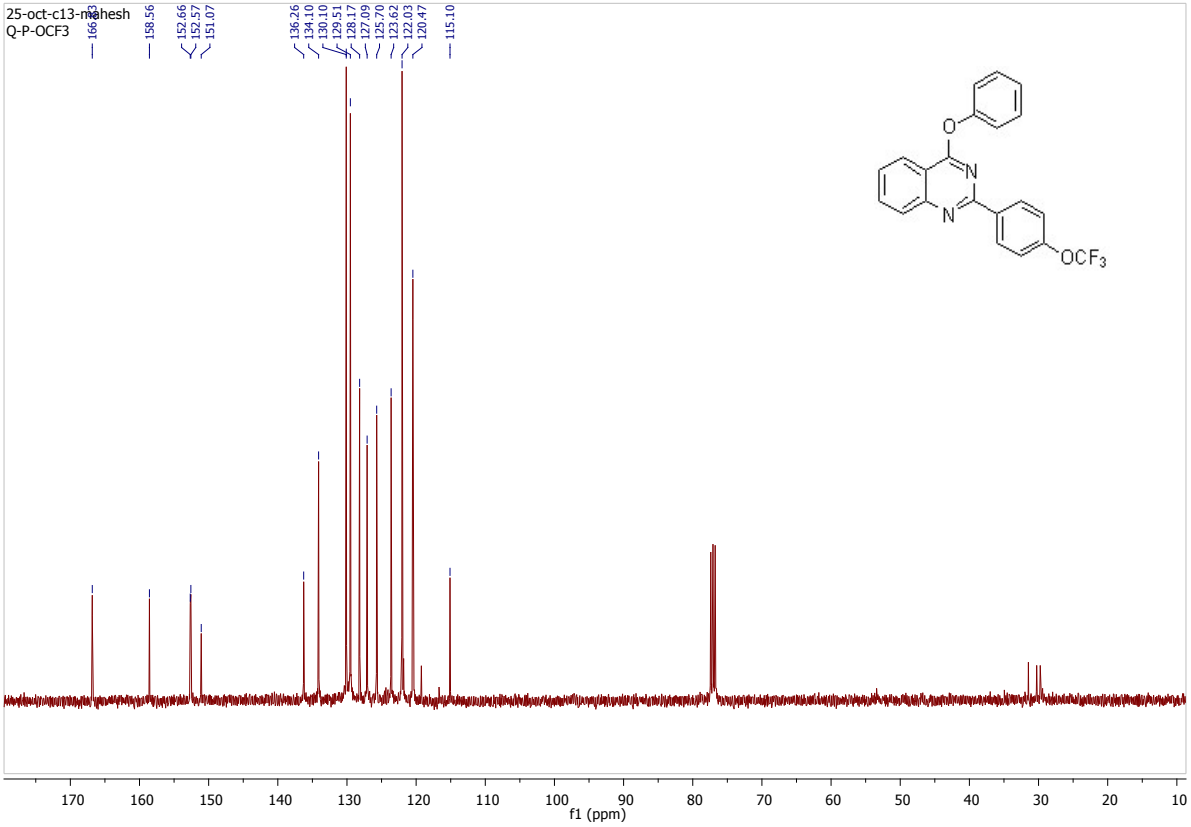
^{1}H &^{13}C NMR of 2-(4-(Methylthio)phenyl)-4-phenoxyquinazoline(3c)



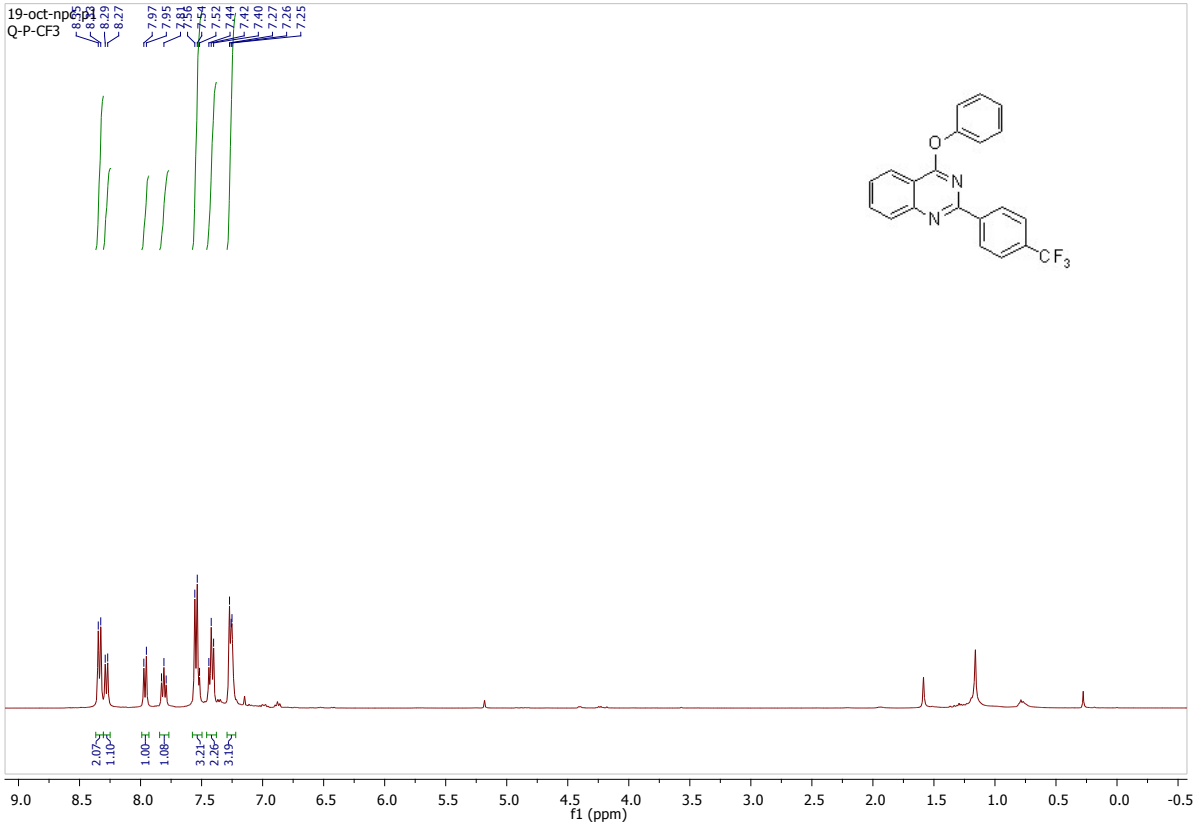


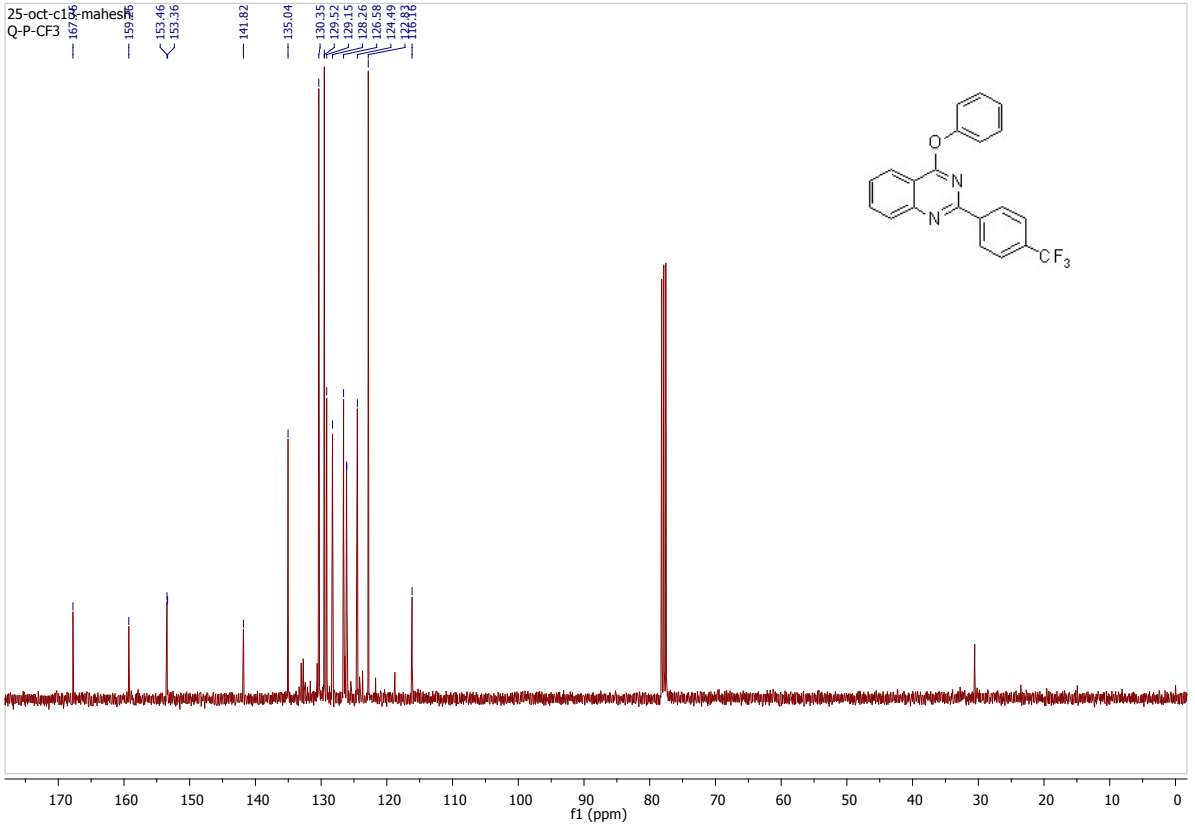
^{1}H &^{13}C NMR of 4-Phenoxy-2-(4-(trifluoromethoxy)phenyl)quinazoline (3d)



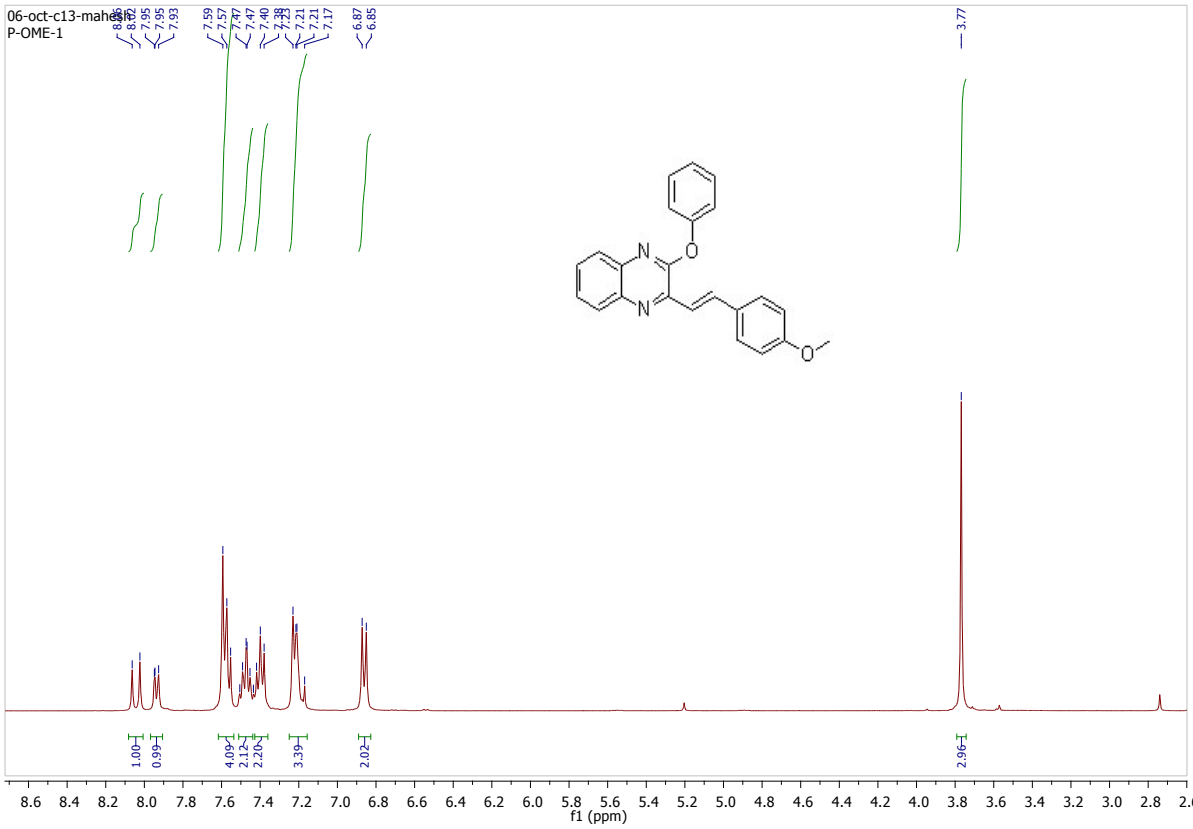


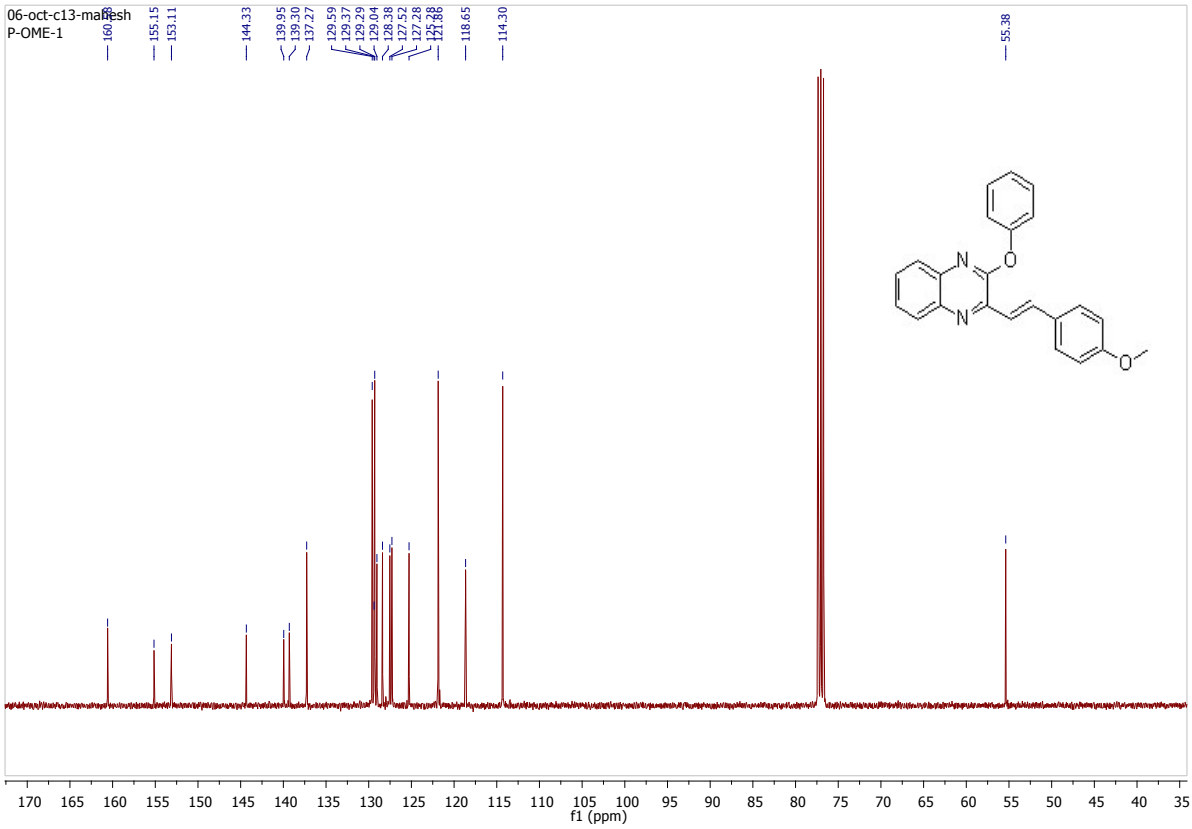
^{1}H &^{13}C NMR of 4-Phenoxy-2-(4-(trifluoromethyl)phenyl)quinazoline (3e)



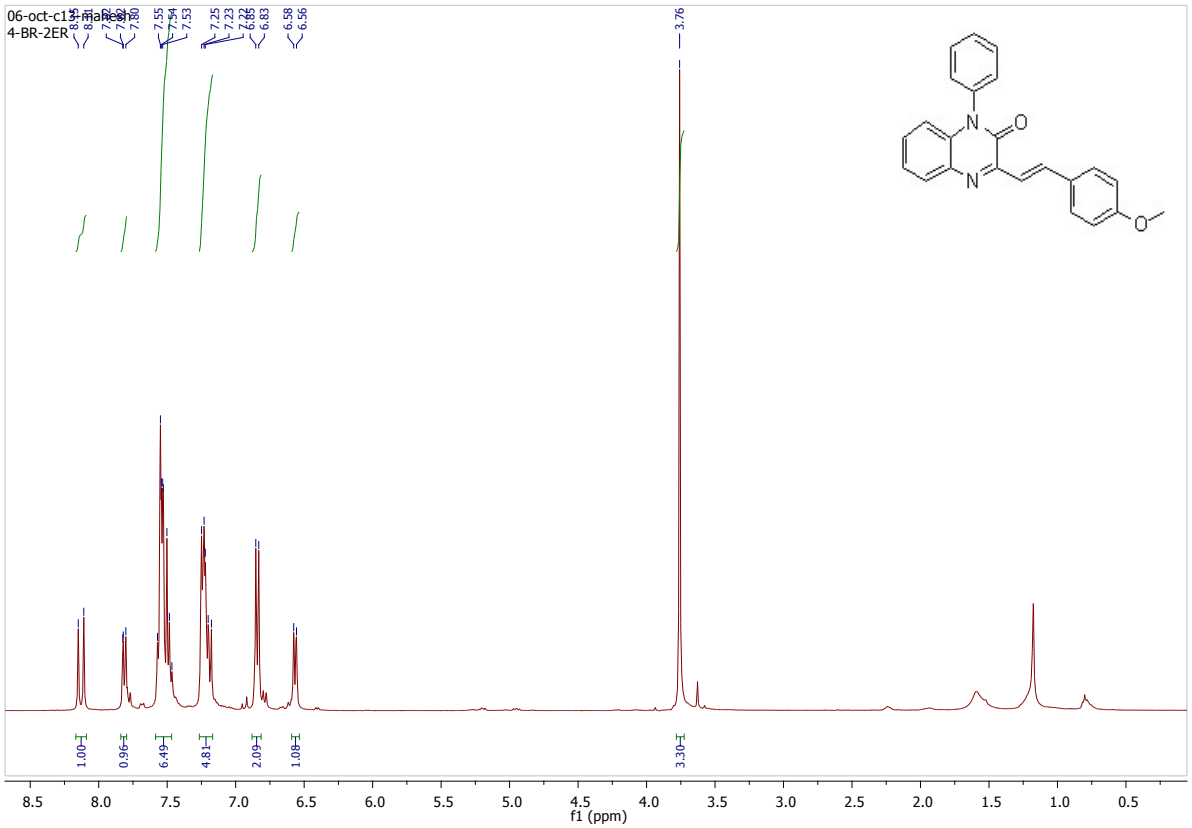


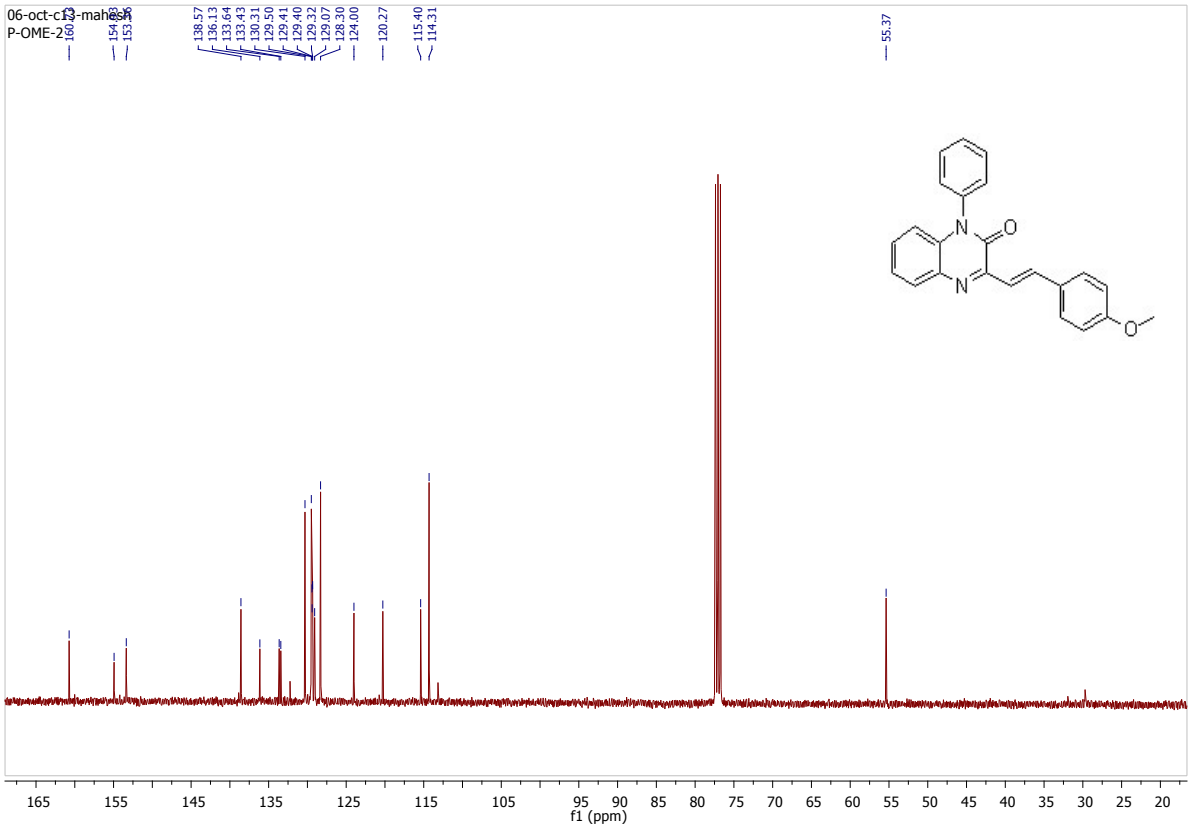
^{1}H &^{13}C NMR of (*E*)-2-(4-Methoxystyryl)-3-phenoxyquinoxaline(5a)



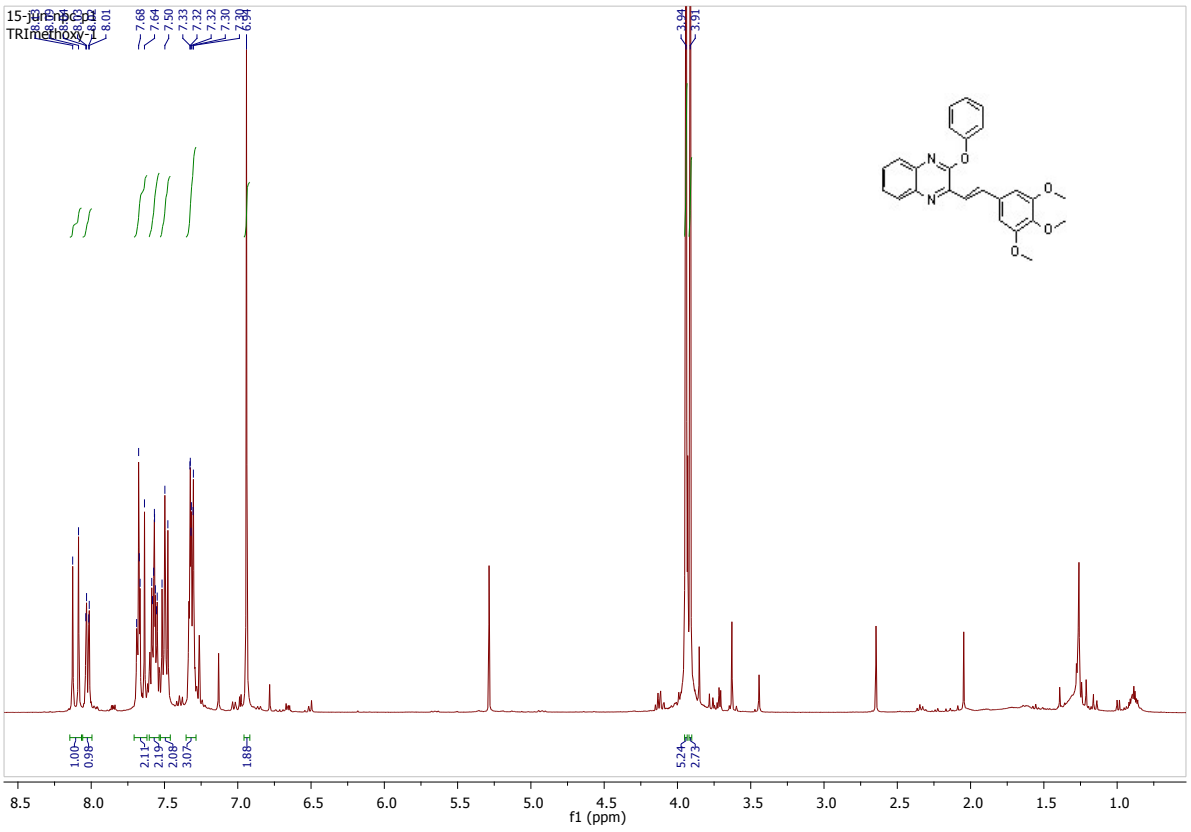


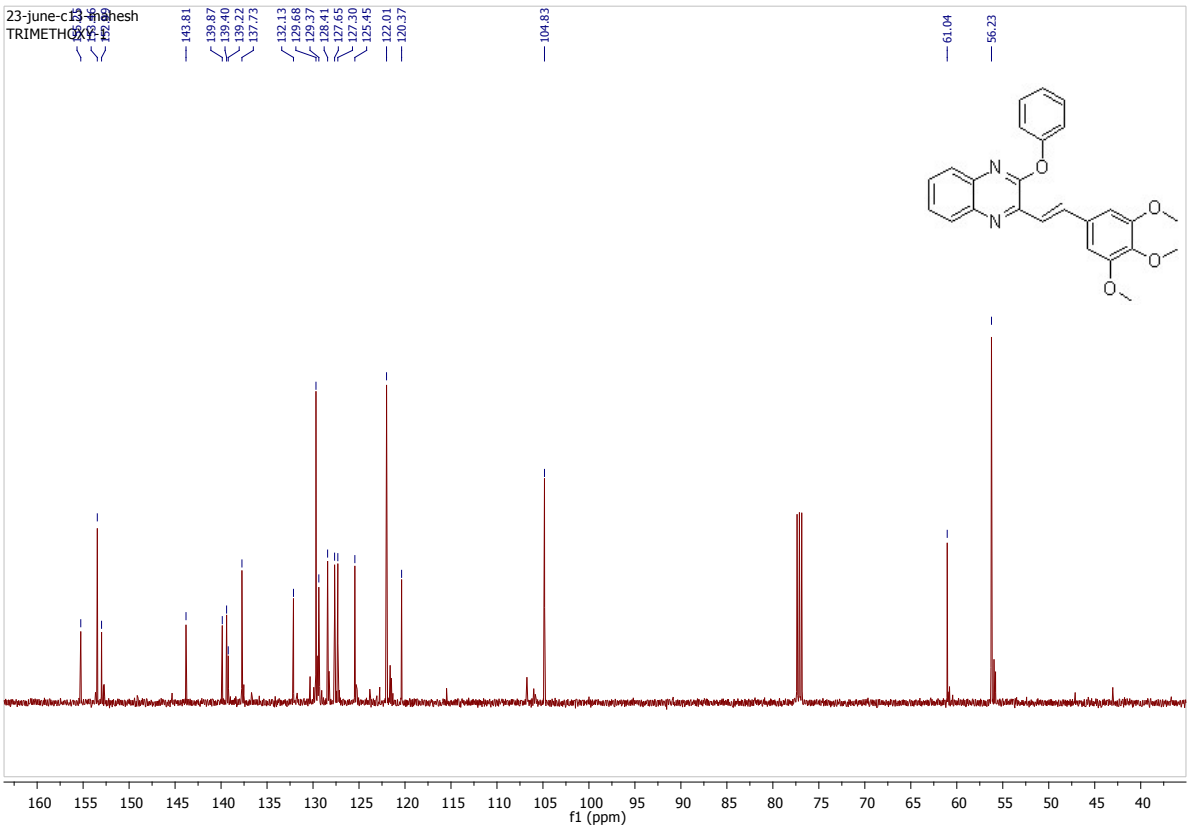
^{1}H &^{13}C NMR of (*E*)-3-(4-Methoxystyryl)-1-phenylquinoxalin-2(1*H*)-one(6a)



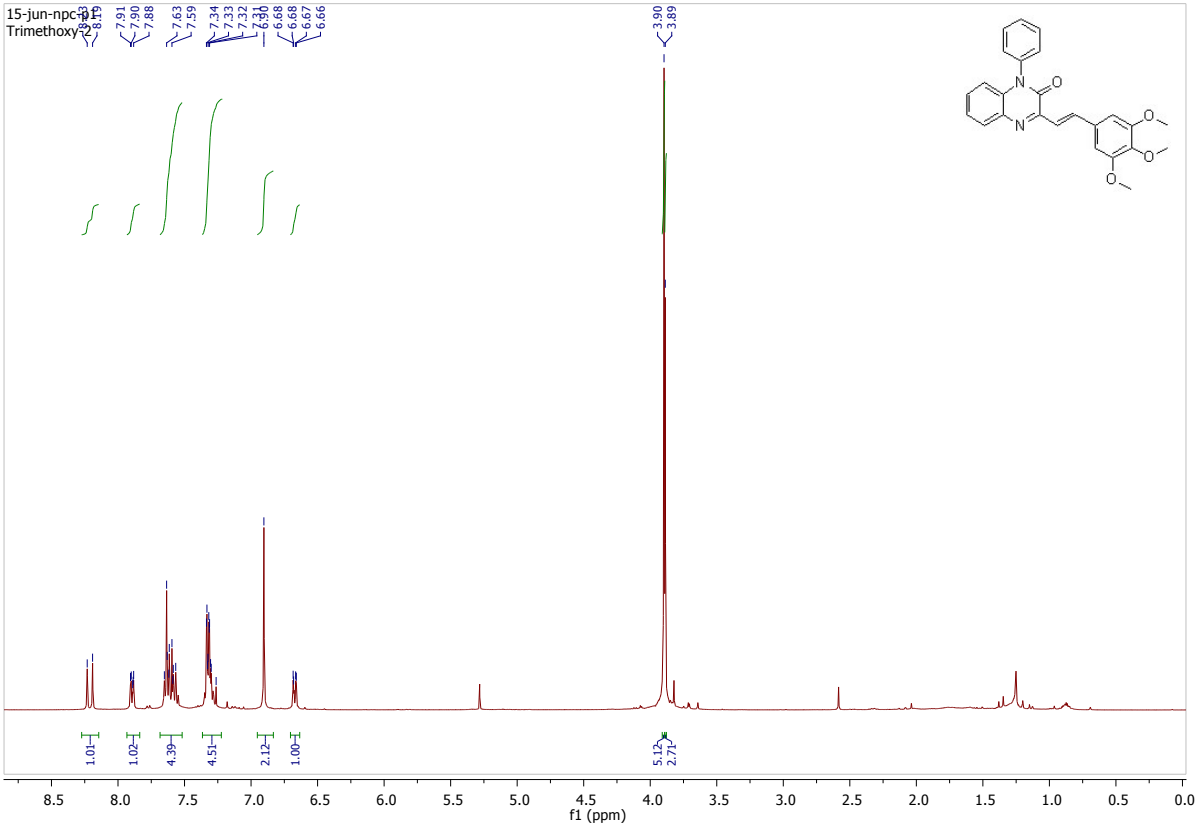


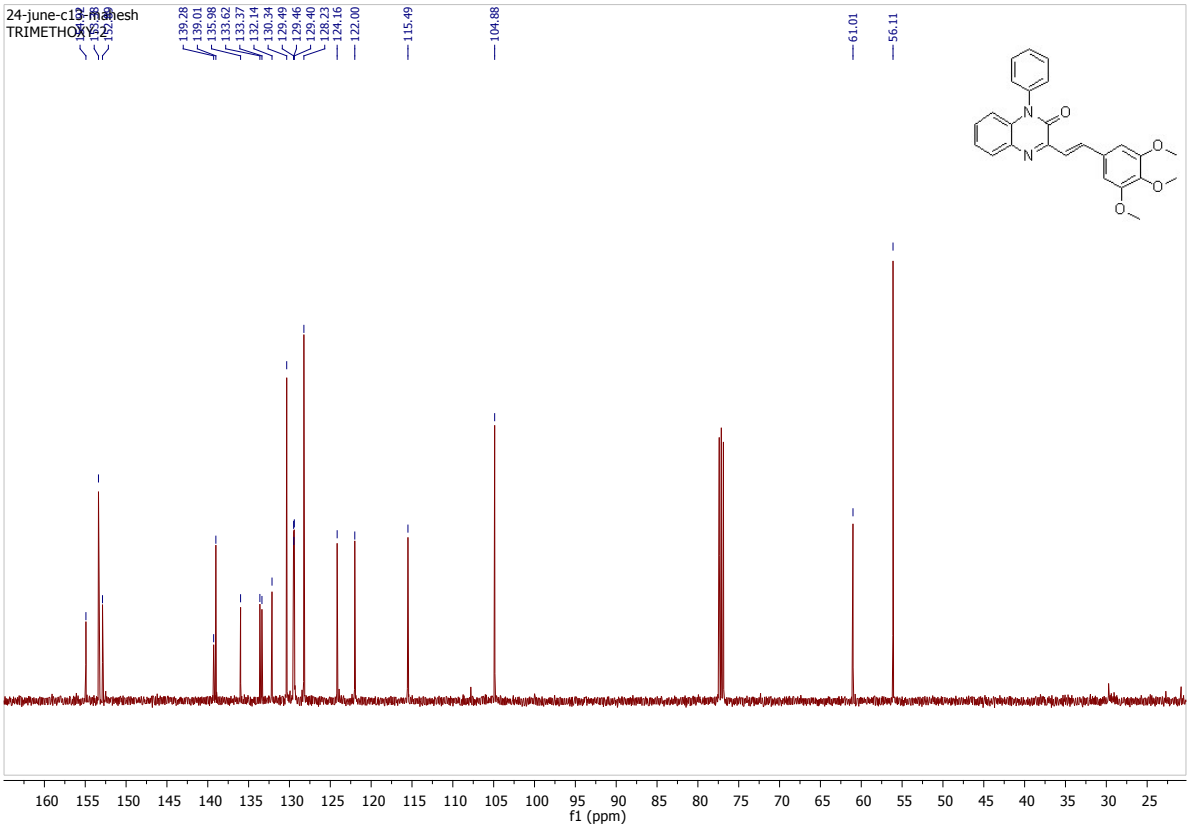
^{1}H &^{13}C NMR of (*E*)-2-Phenoxy-3-(3,4,5-trimethoxystyryl)quinoxaline(5b)



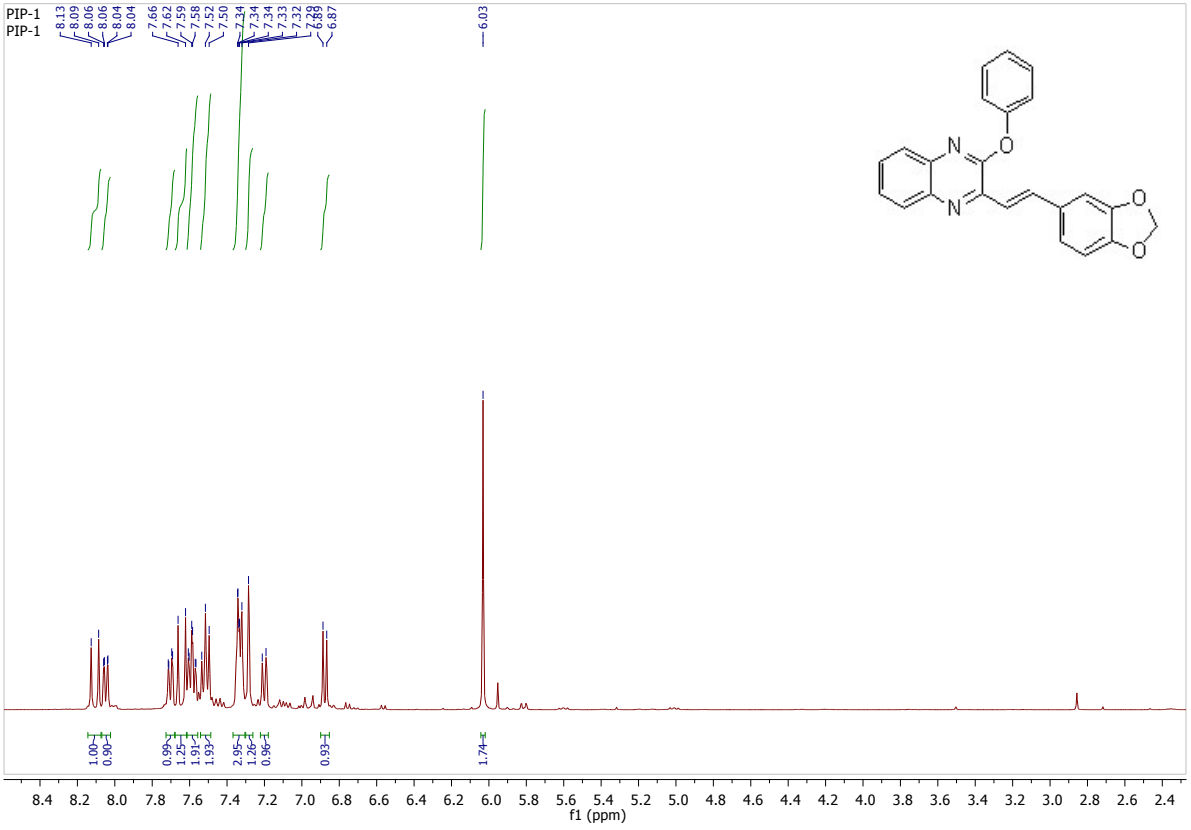


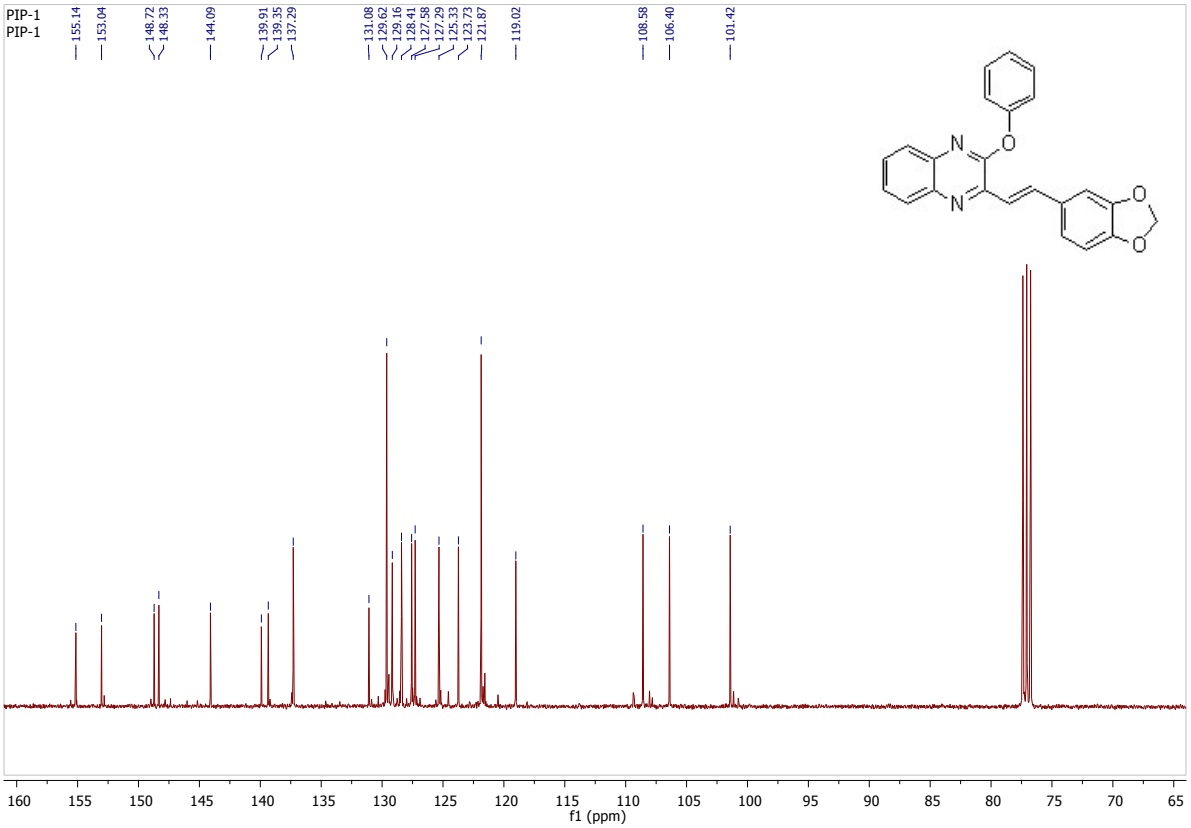
^{1}H &^{13}C NMR of (*E*)-1-Phenyl-3-(3,4,5-trimethoxystyryl)quinoxalin-2(1*H*)-one(6b)



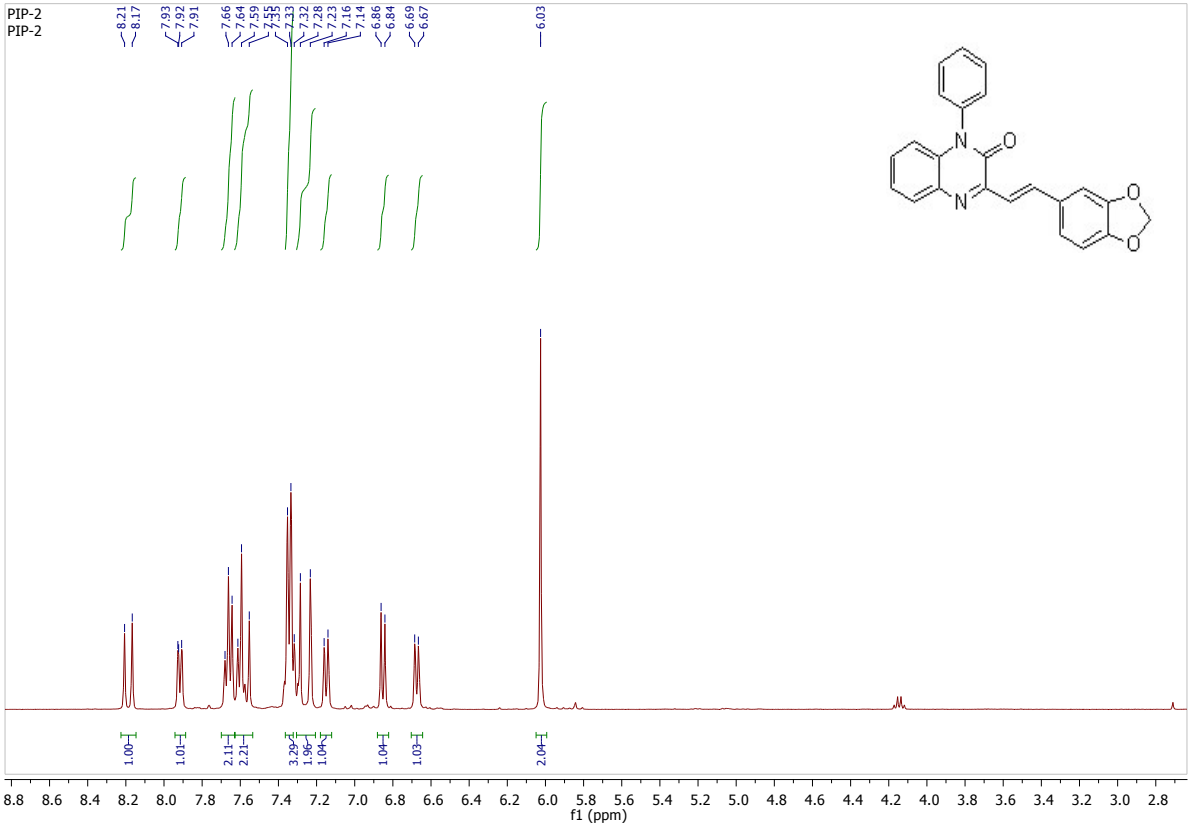


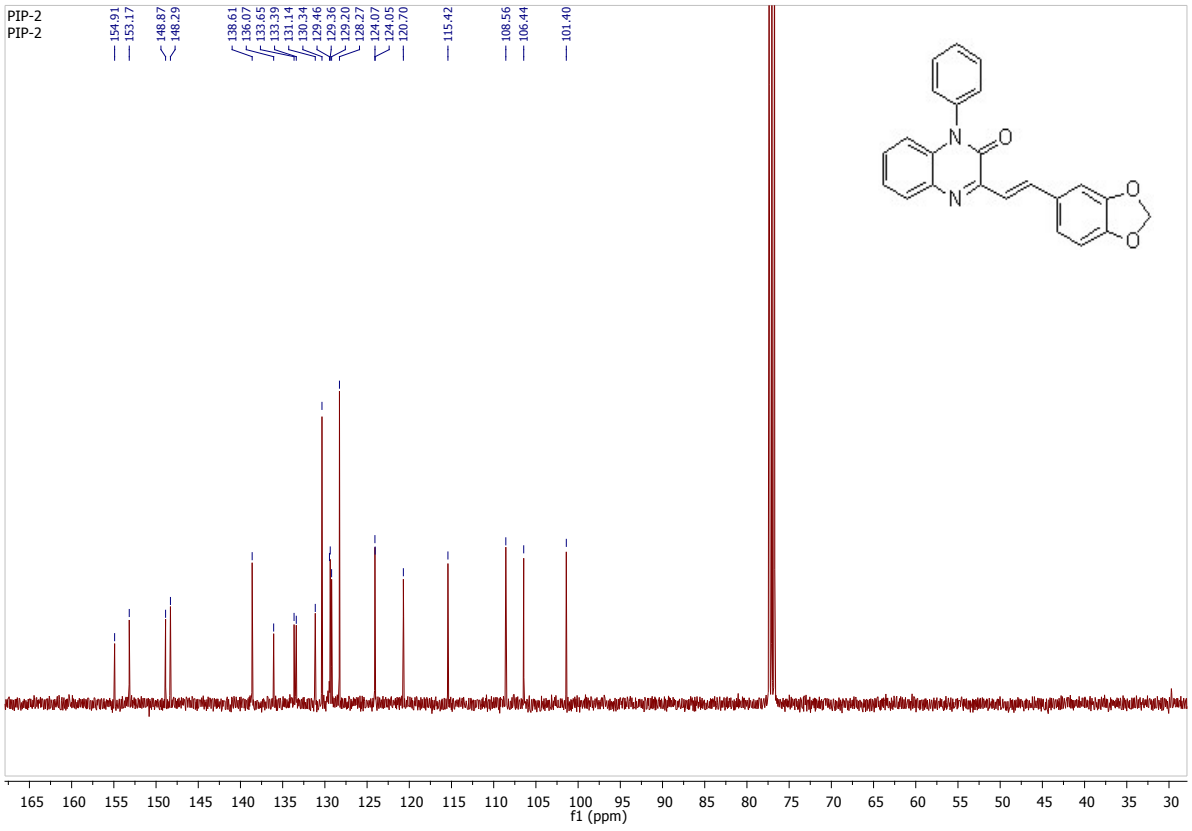
^{1}H &^{13}C NMR of 2-((*E*)-2-(Benzo[d][1,3]dioxol-5-yl)vinyl)-3-phenoxyquinoxaline(5c)



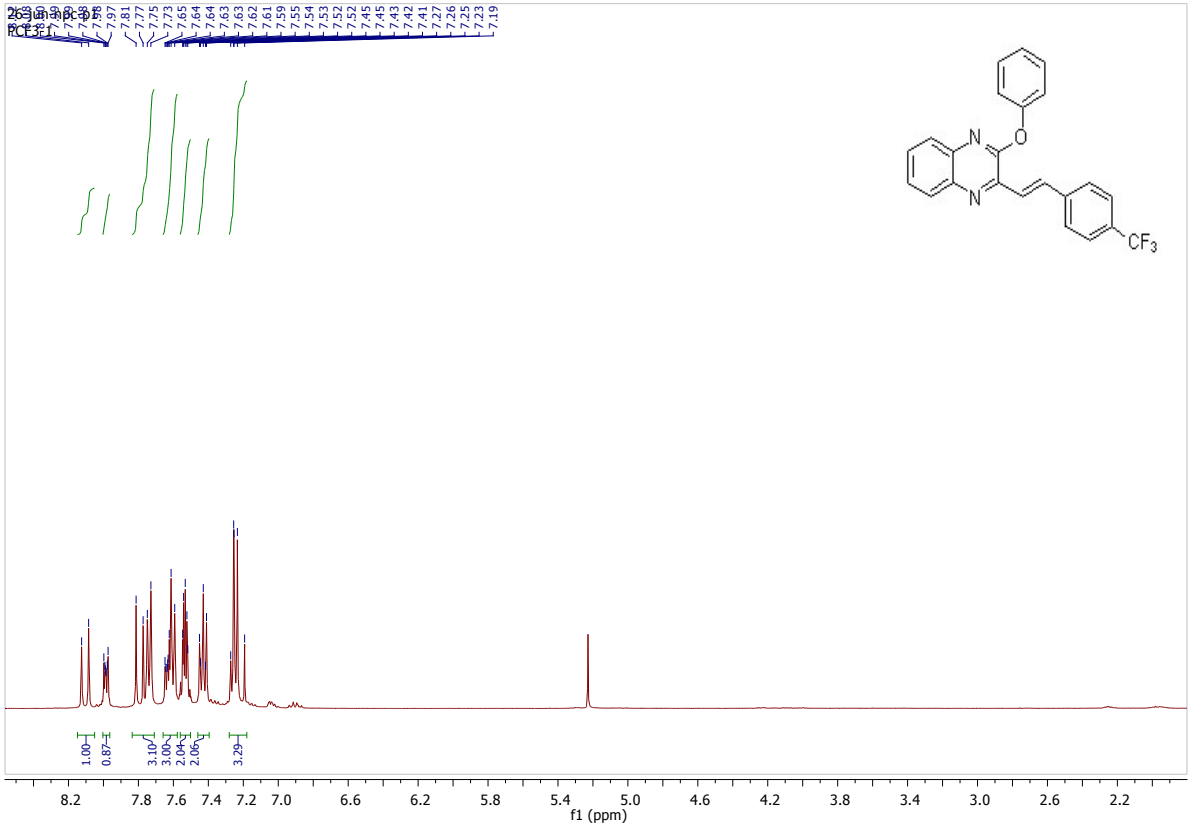


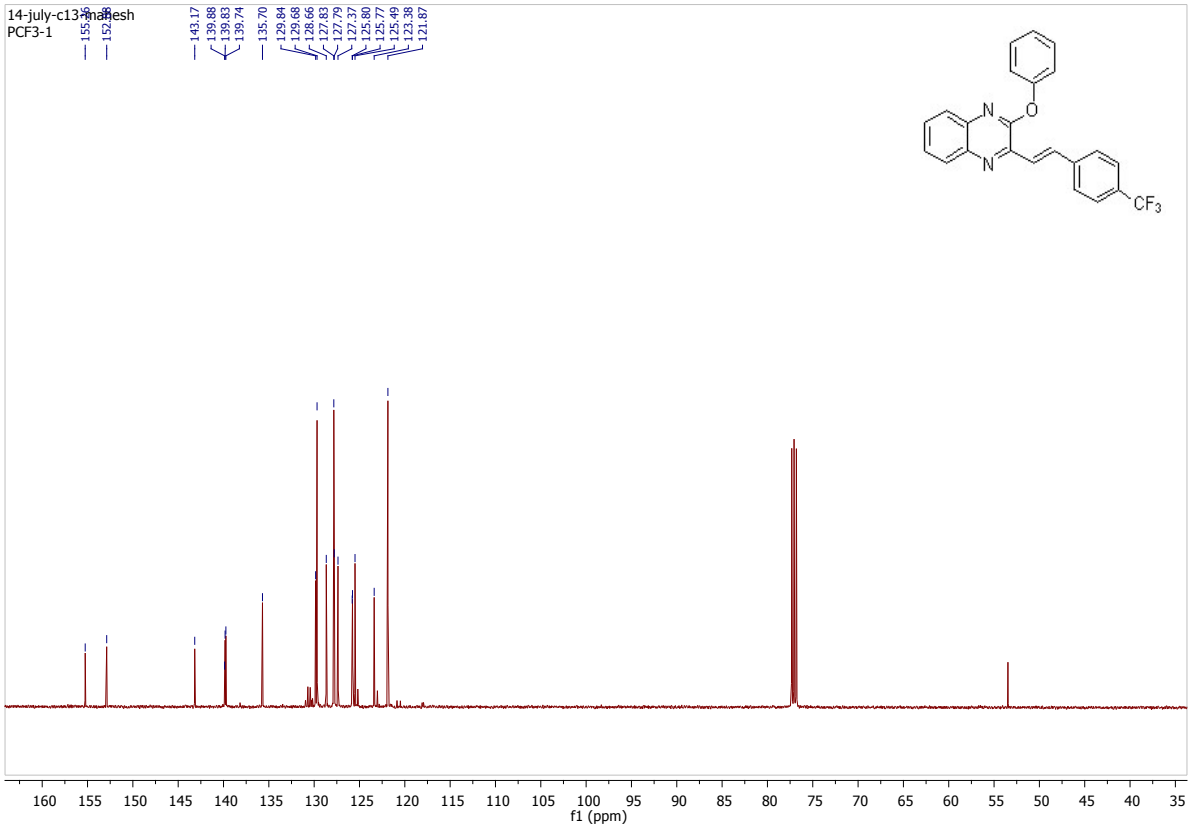
^{1}H &^{13}C NMR of (*E*)-3-(2-(Benzo[d][1,3]dioxol-5-yl)vinyl)-1-phenylquinoxalin-2(1*H*)-one(6c)



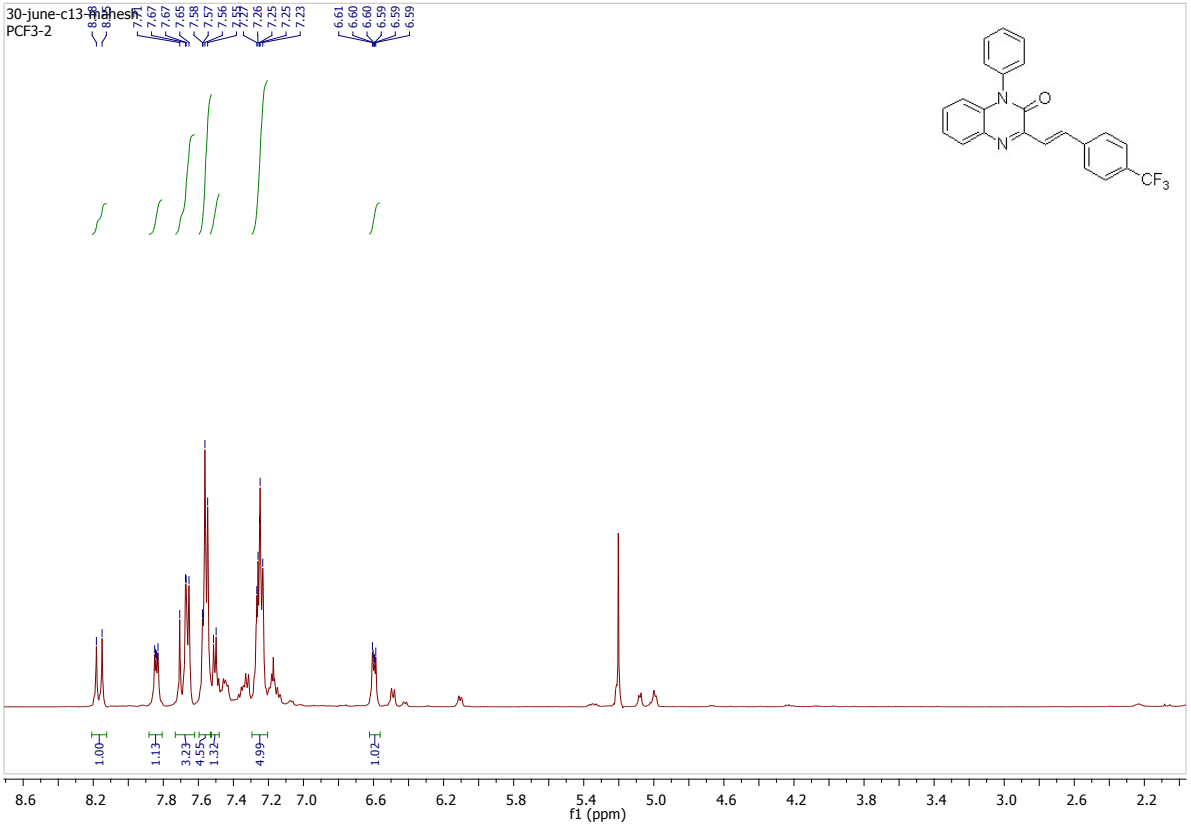


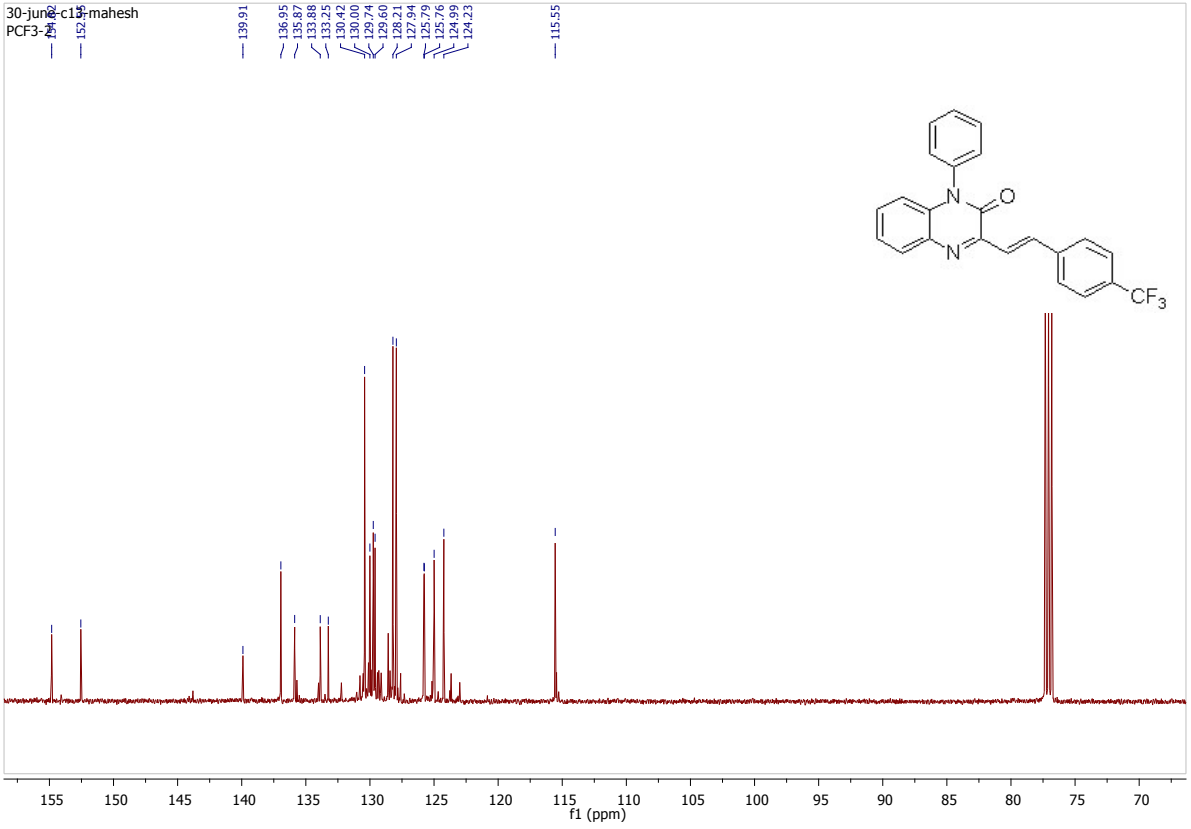
^{1}H &^{13}C NMR of (*E*)-2-Phenoxy-3-(4-(trifluoromethyl)styryl)quinoxaline(5d)



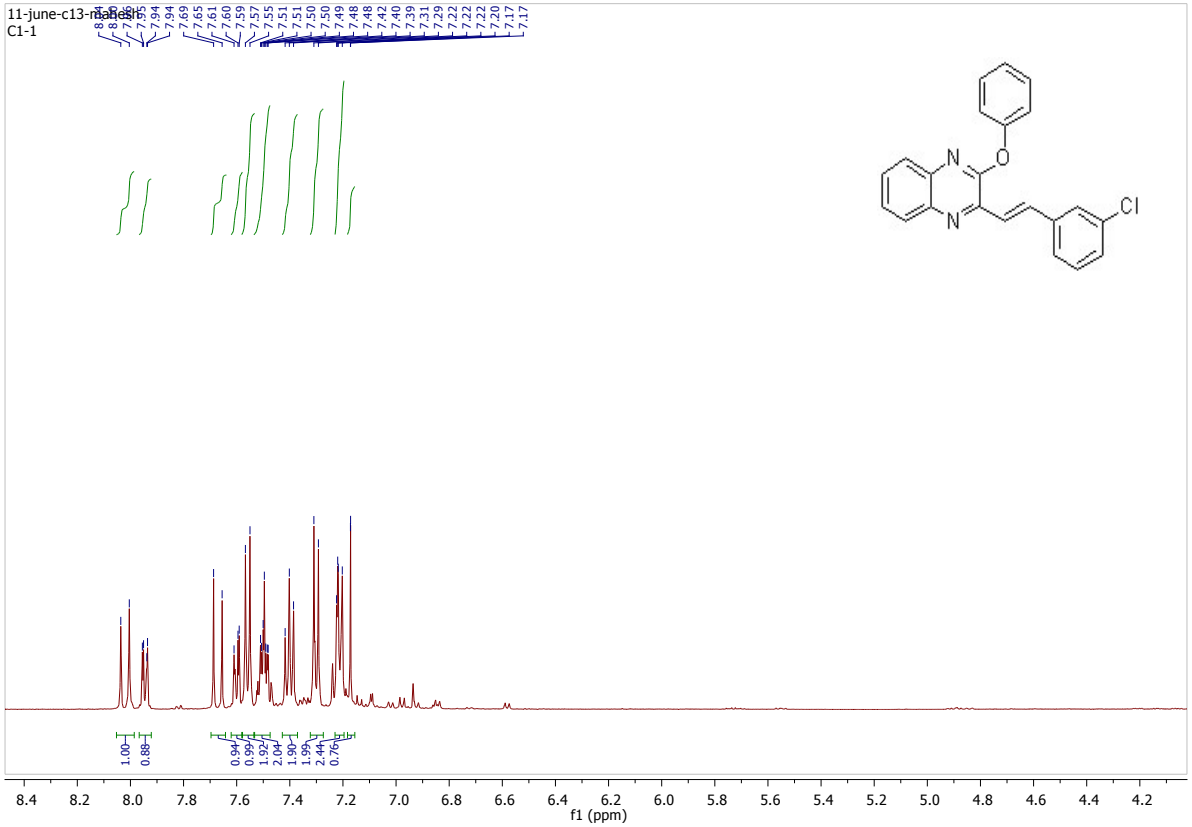


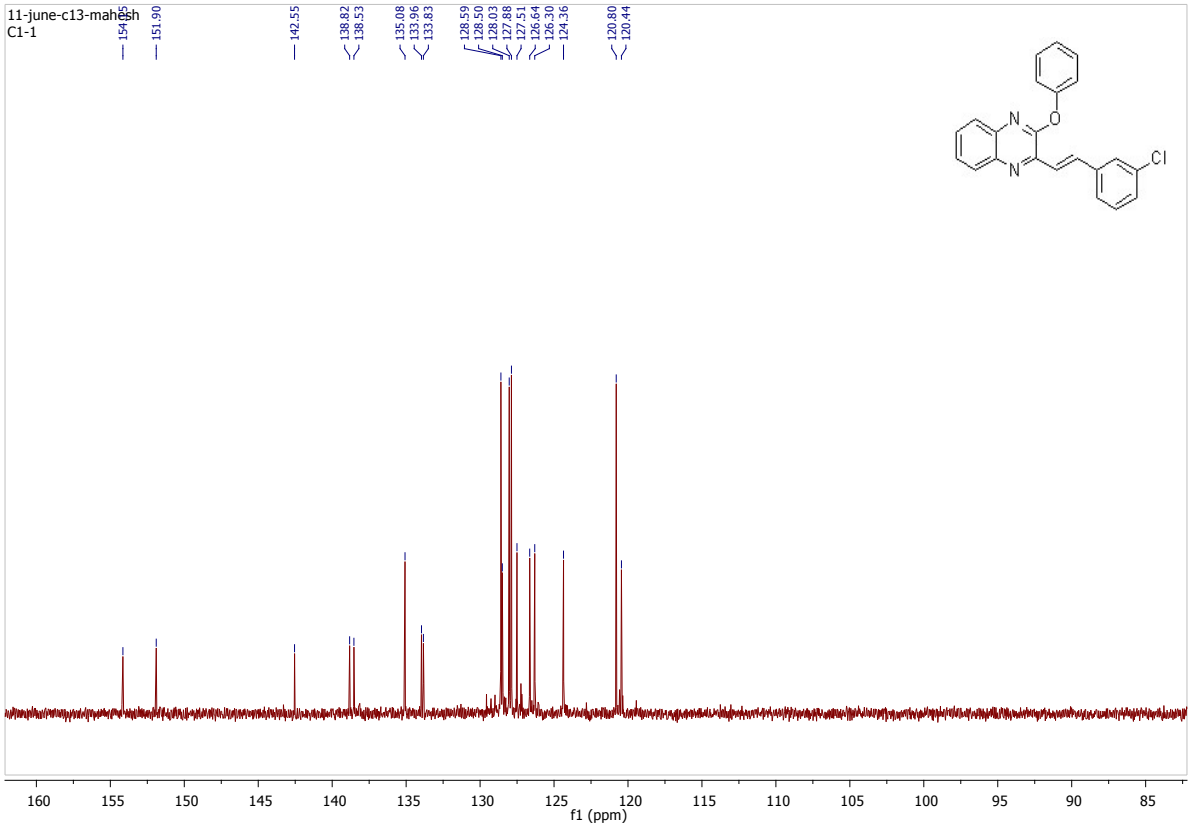
^{1}H &^{13}C NMR of (*E*)-1-Phenyl-3-(4-(trifluoromethyl)styryl)quinoxalin-2(1*H*)-one(6d)



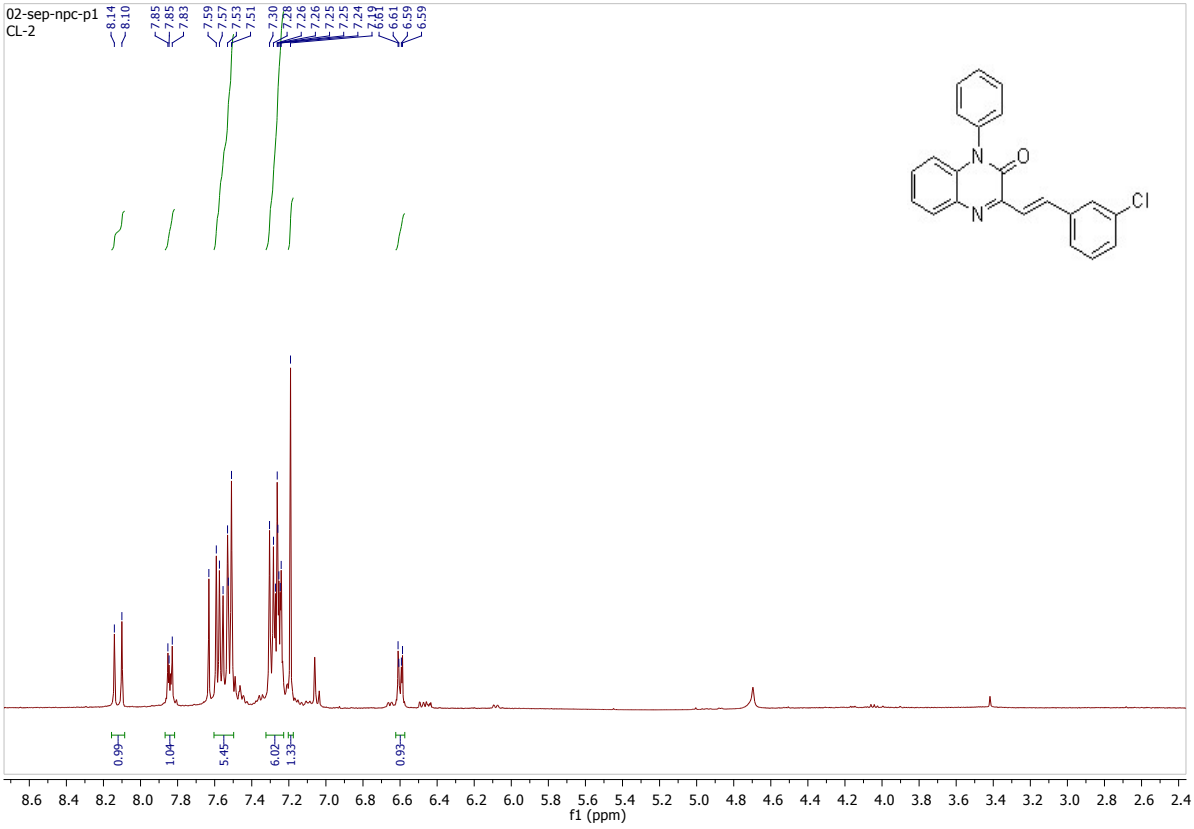


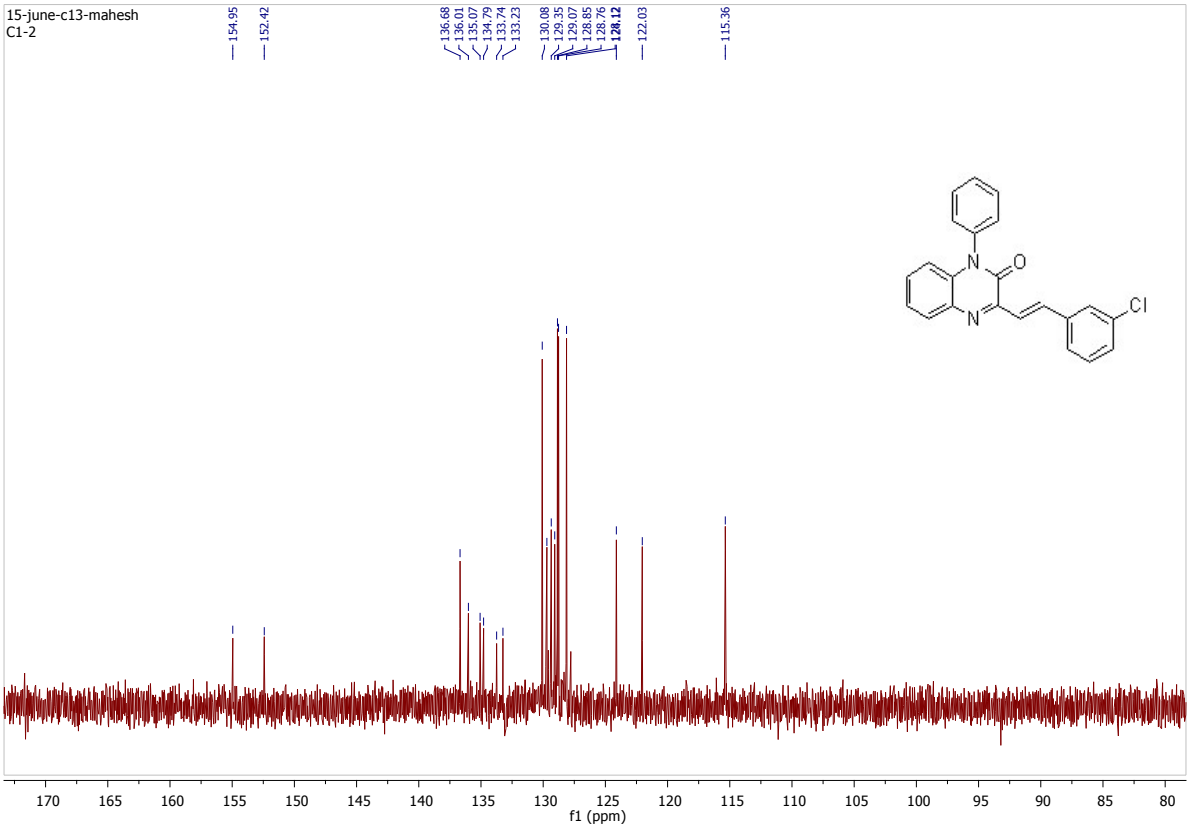
^{1}H &^{13}C NMR of (*E*)-2-(2-Chlorostyryl)-3-phenoxyquinoxaline(5e)



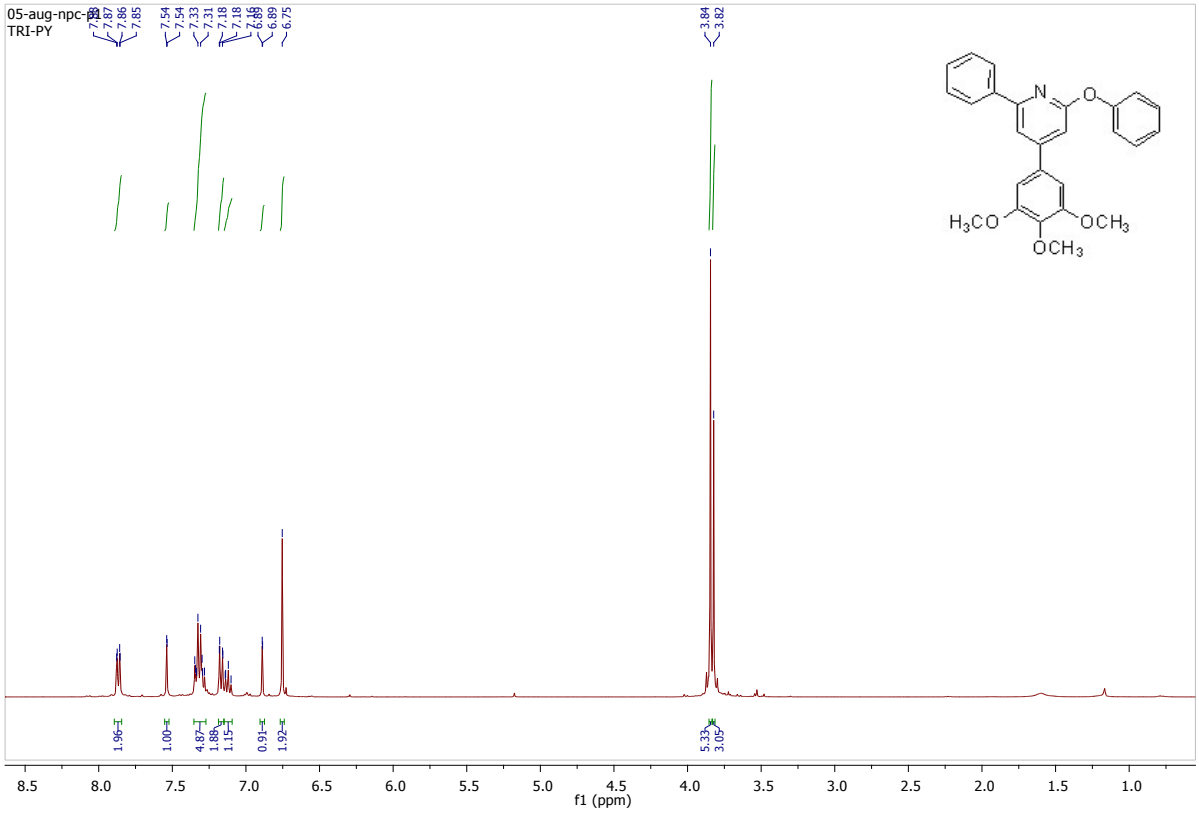


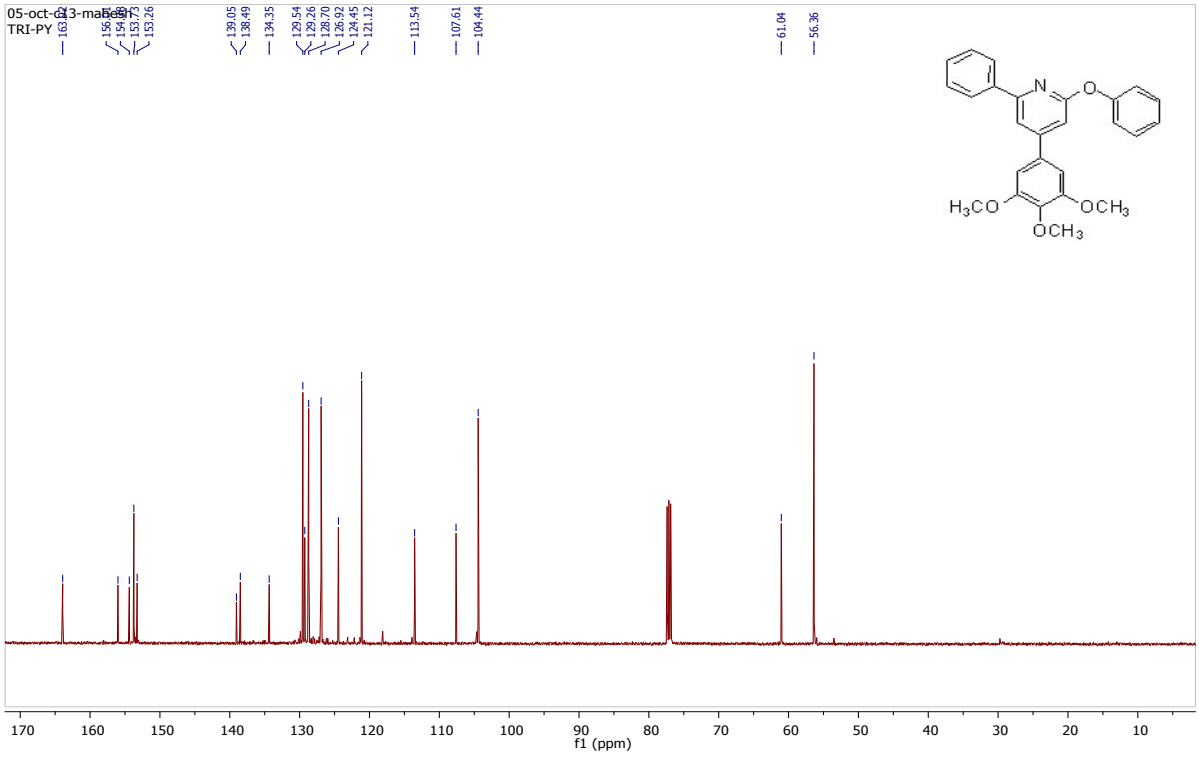
^{1}H &^{13}C NMR of (*E*)-3-(2-Chlorostyryl)-1-phenylquinoxalin-2(1*H*)-one(6e)



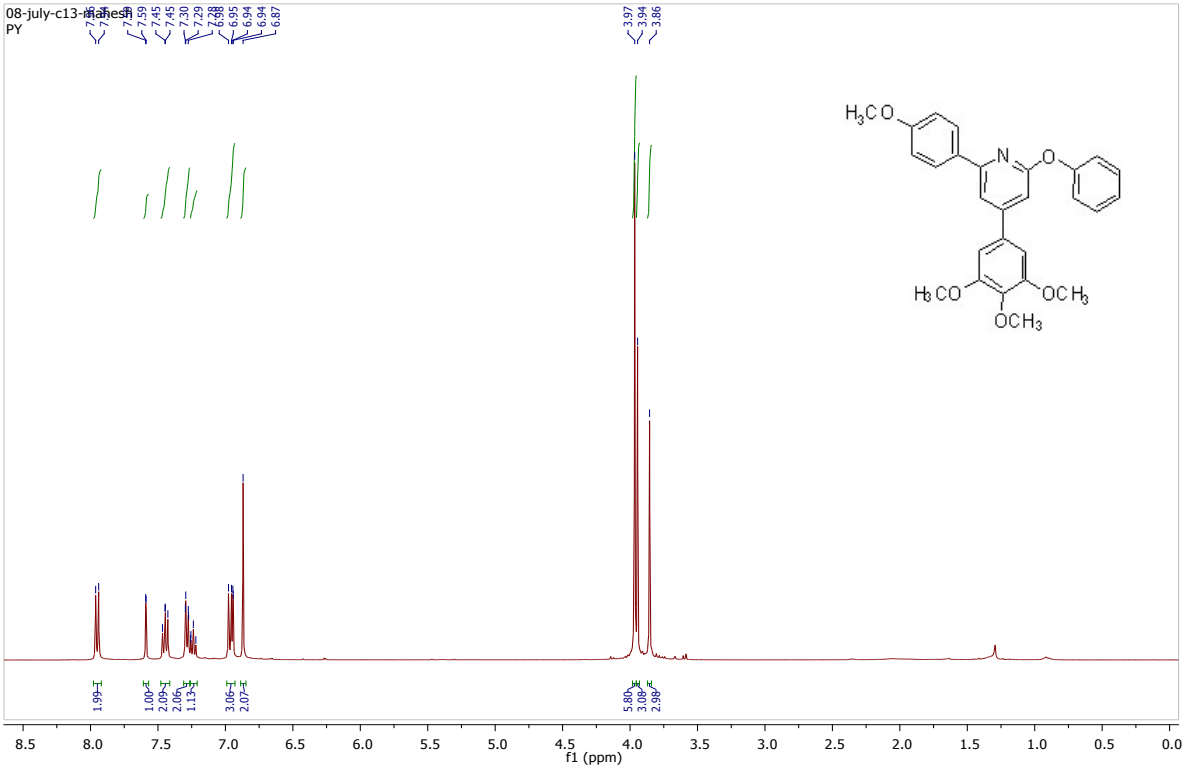


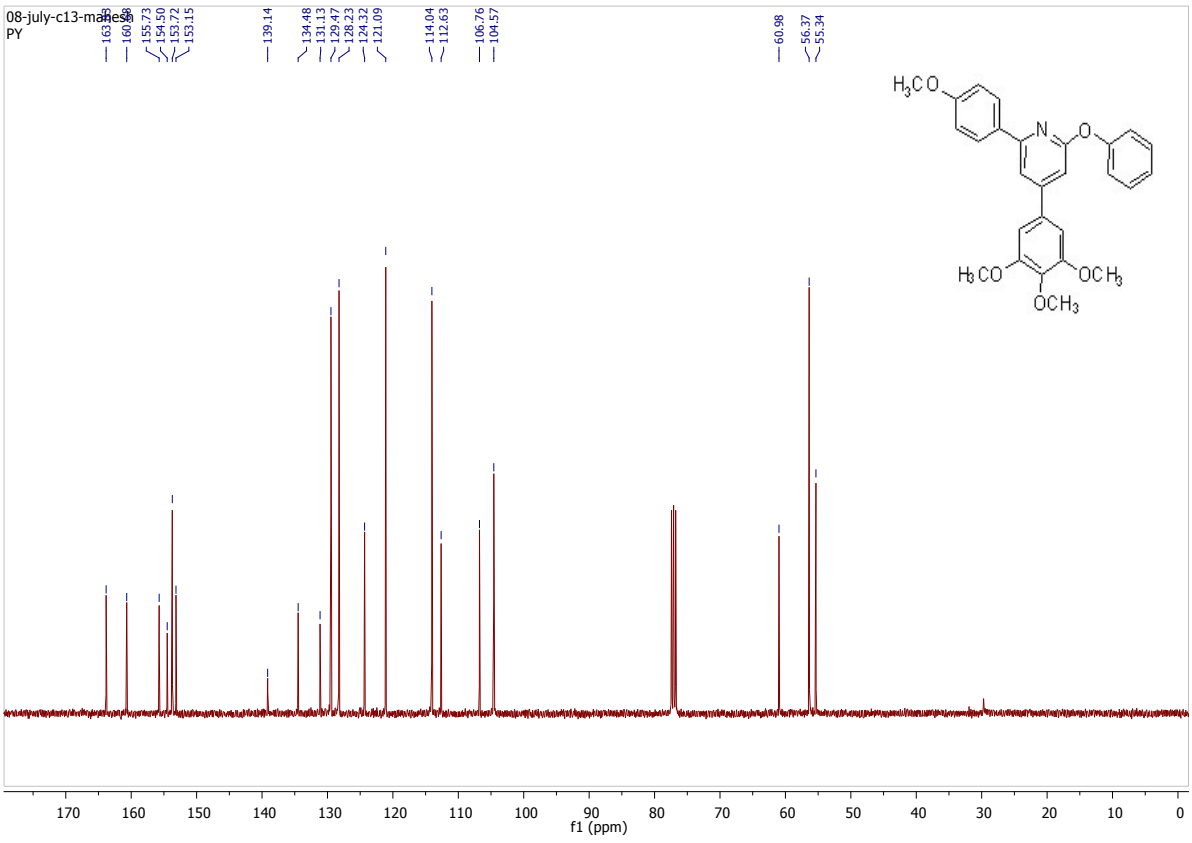
^{1}H &^{13}C NMR of 2-Phenoxy-6-phenyl-4-(3,4,5-trimethoxyphenyl)pyridine (8a)



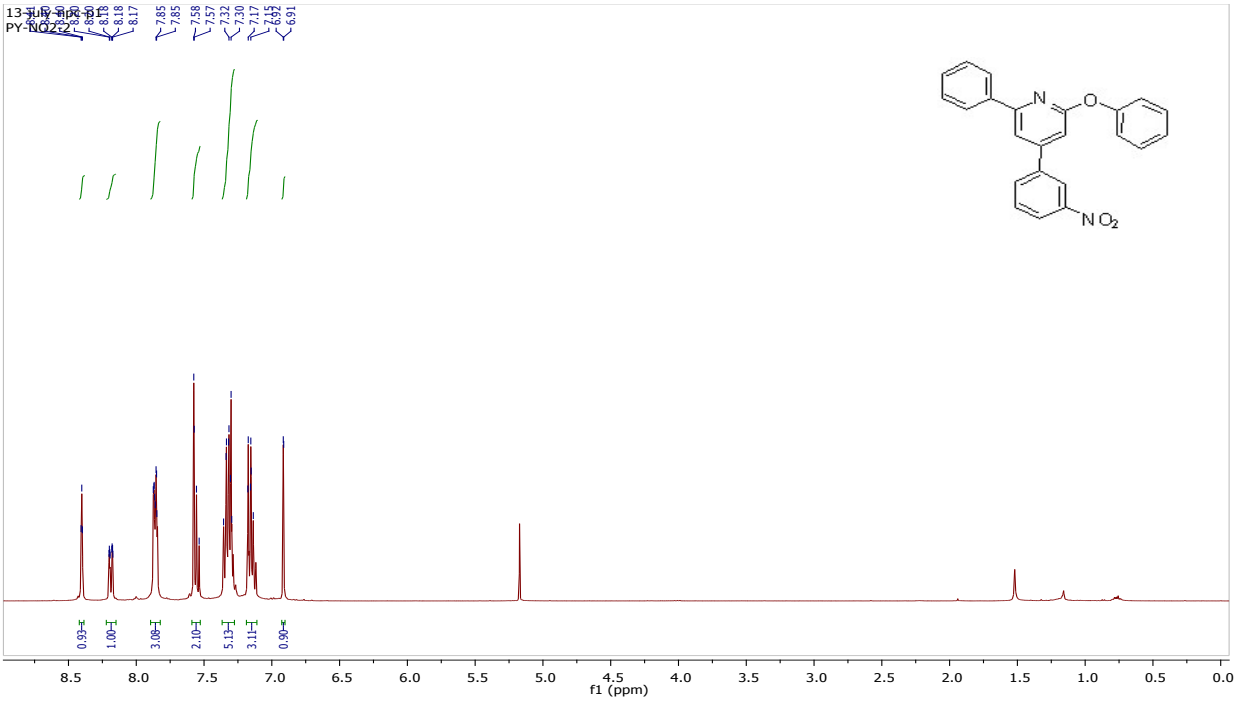


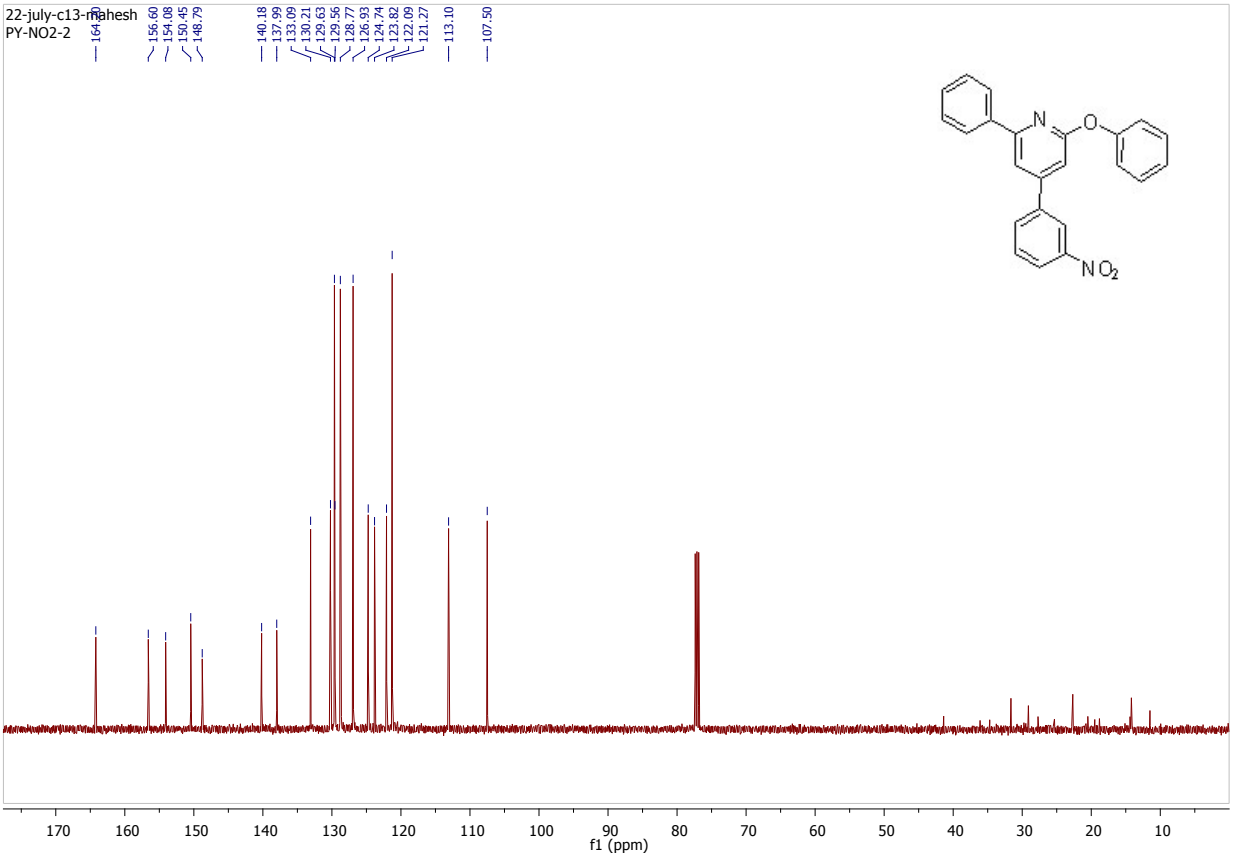
^{1}H &^{13}C NMR of 2-(4-Methoxyphenyl)-6-phenoxy-4-(3,4,5-trimethoxyphenyl)pyridine(8b)



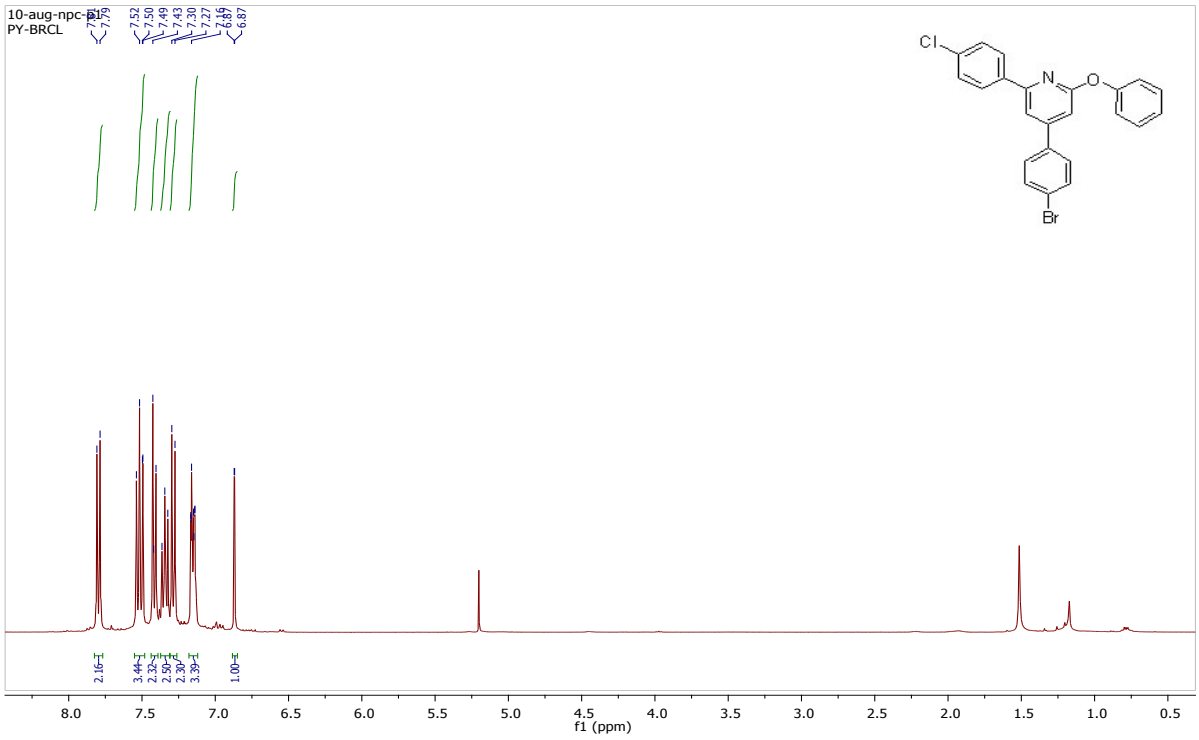


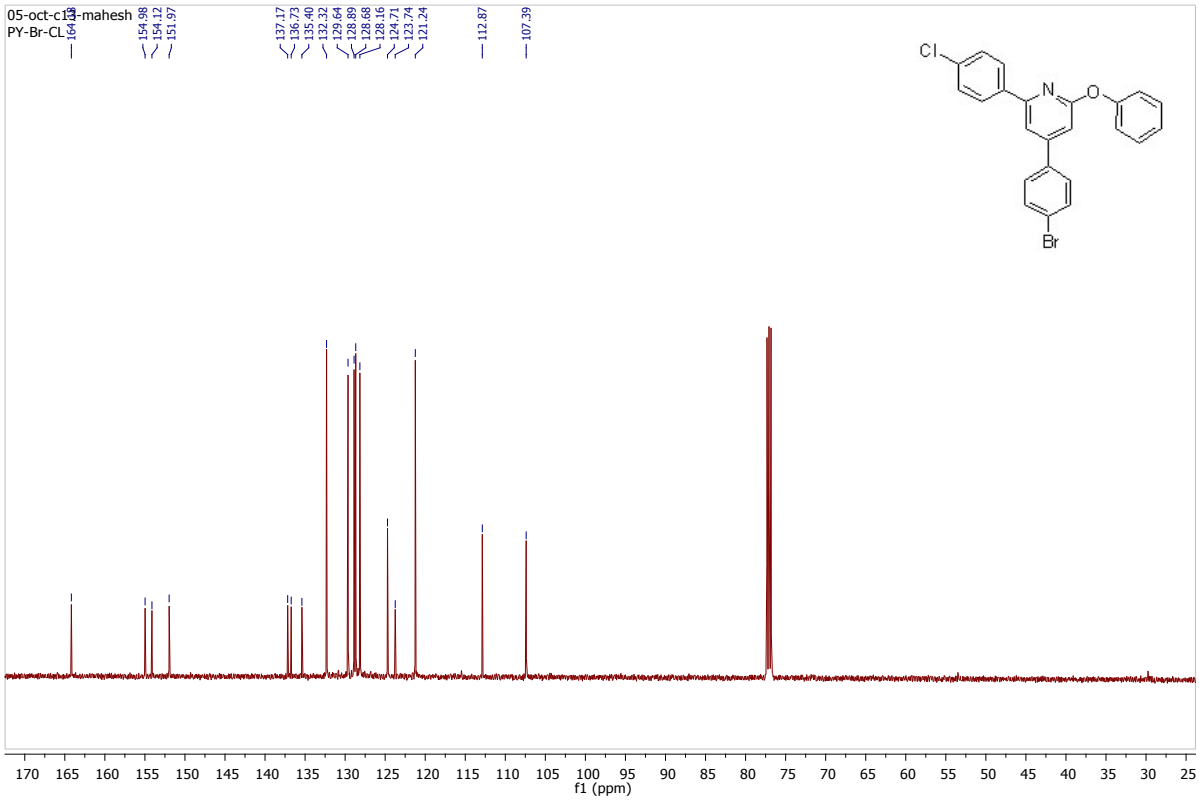
^{1}H &^{13}C NMR of 4-(3-Nitrophenyl)-2-phenoxy-6-phenylpyridine(8c)



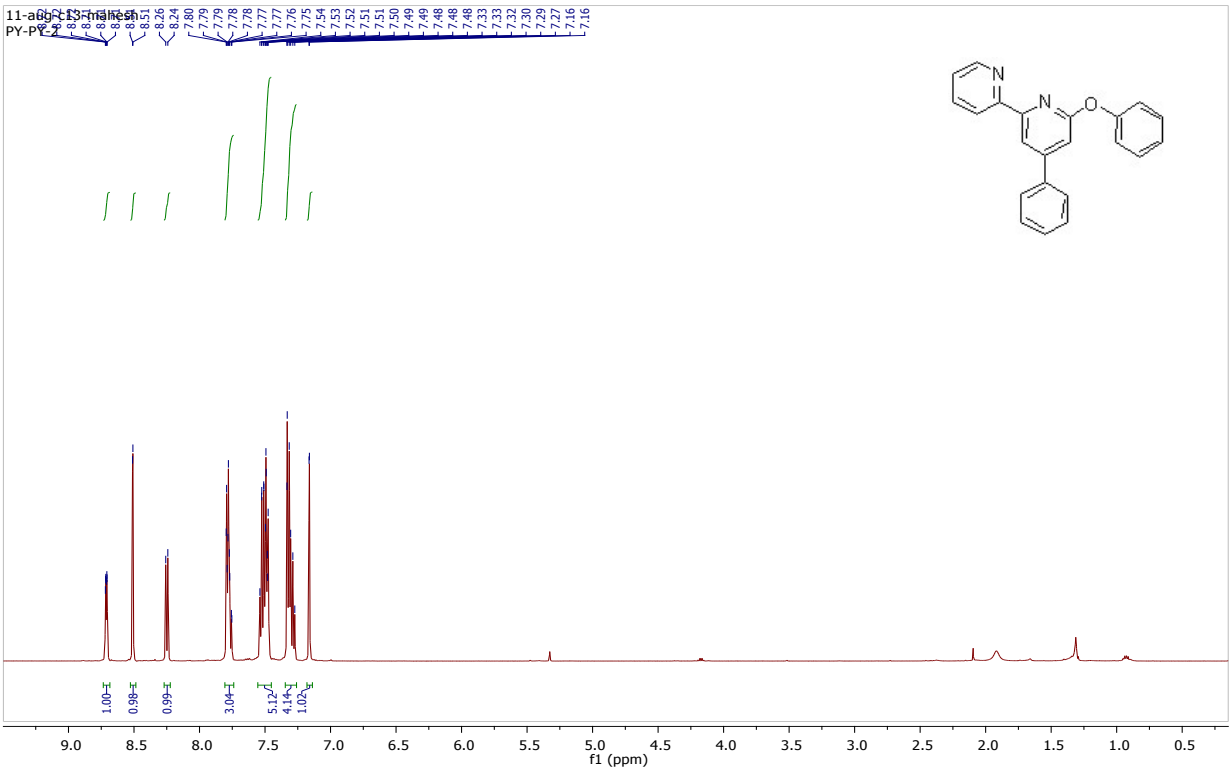


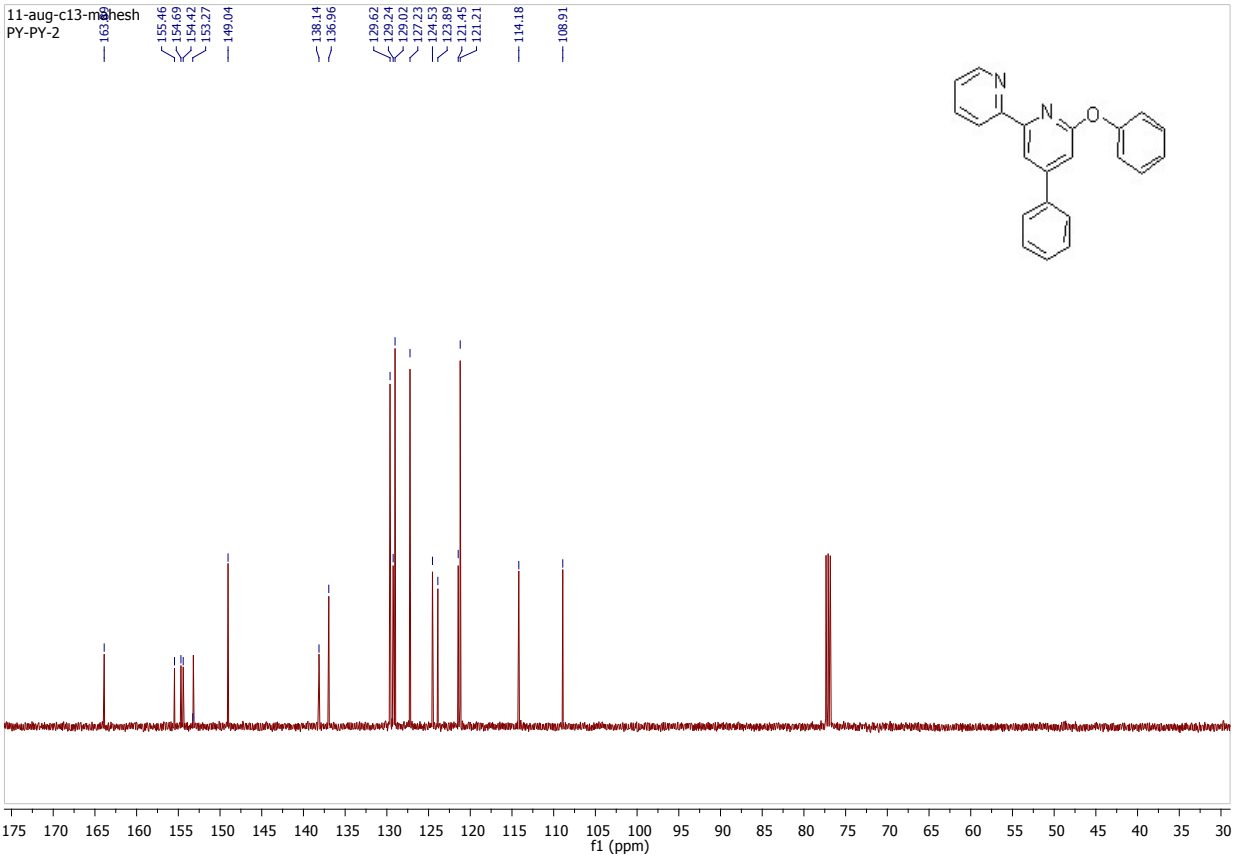
^{1}H &^{13}C NMR of 4-(4-Bromophenyl)-2-(4-chlorophenyl)-6-phenoxypyridine (8d)



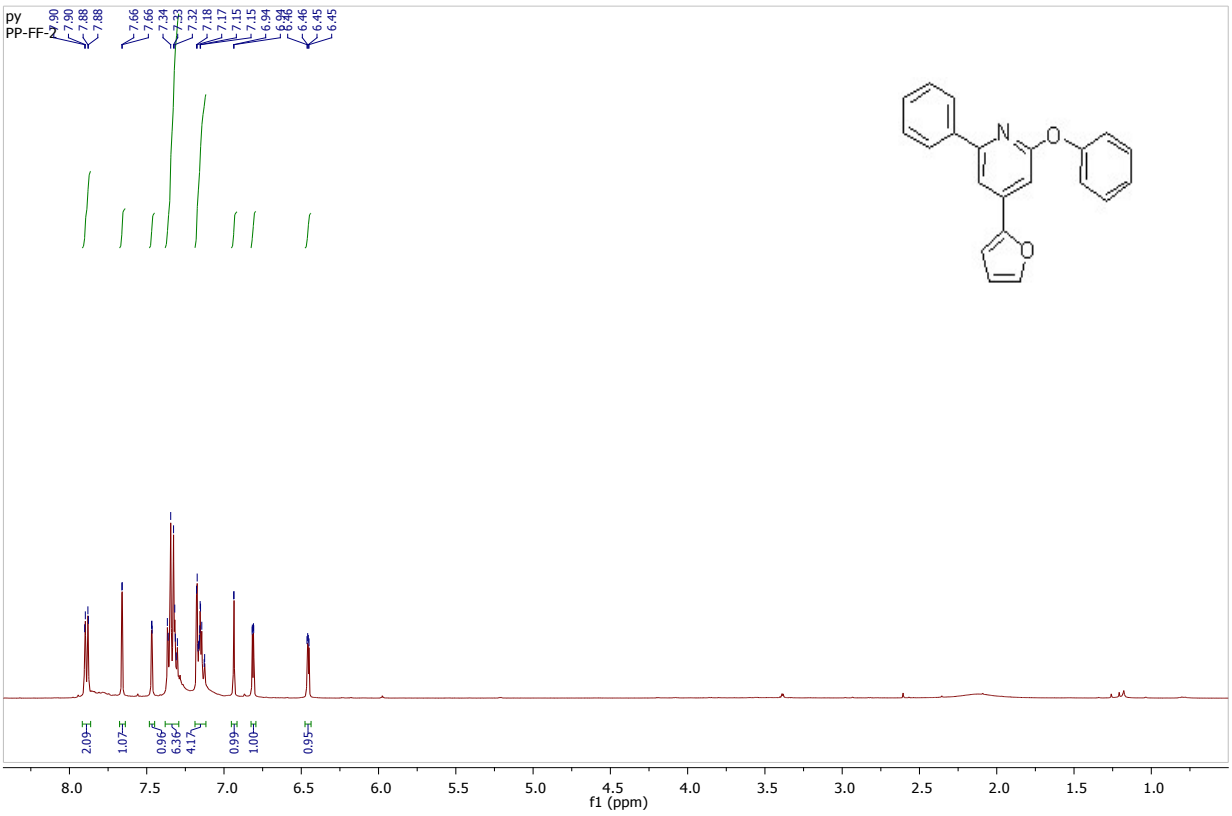


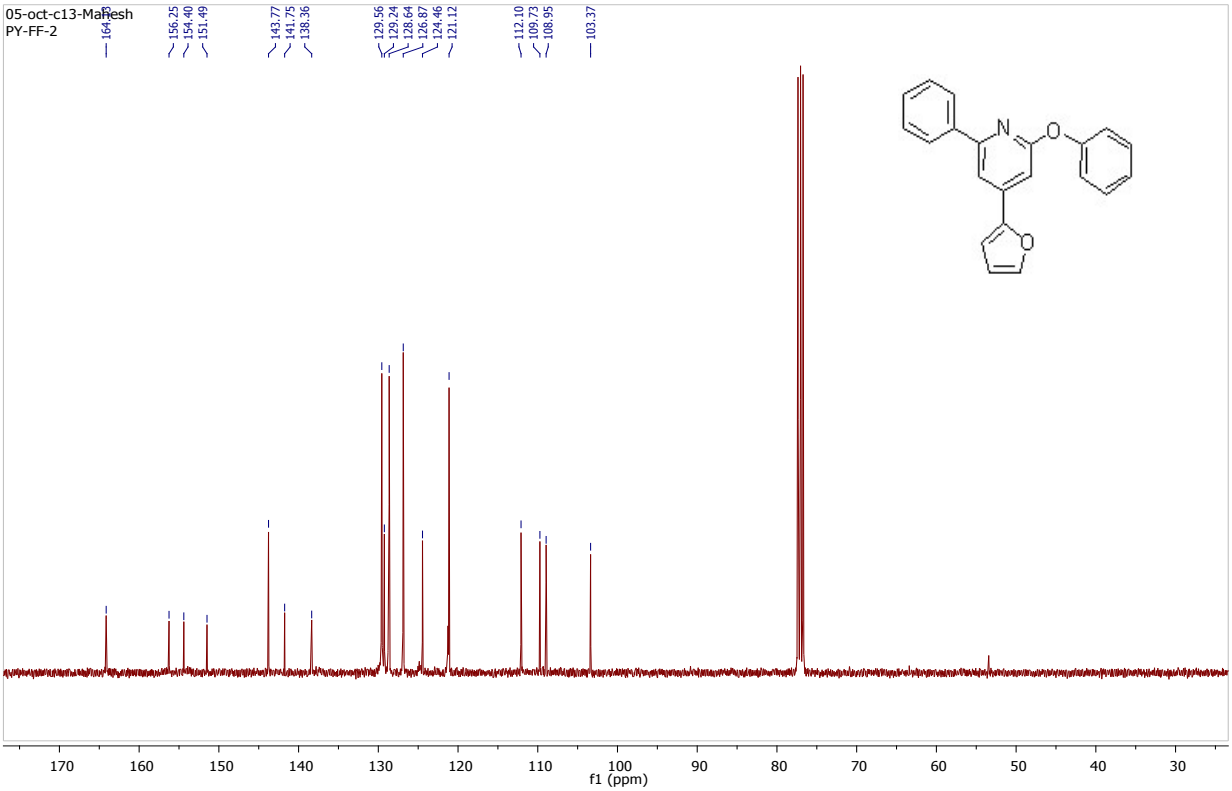
^{1}H &^{13}C NMR of 6-Phenoxy-4-phenyl-2,2-bipyridine(8e)





^{1}H &^{13}C NMR of 4-(Furan-2-yl)-2-phenoxy-6-phenylpyridine(8f)





X-ray crystallographic data ofcompound 8c:

X-ray intensity data of 7234 reflections (of which 3530 unique) were collected on *X'calibur* CCD area-detector diffractometer equipped with graphite monochromated MoKα radiation (λ = 0.71073 Å). The crystal used for data collection was of dimensions 0.30 x 0.20 x 0.20 mm. The cell dimensions were determined by least-squares fit of angular settings of 1788 reflections in the θ range 3.93 to 27.57^o**.** The intensities were measured by ω scan mode for θ ranges 3.53 to 26.00^o. 2176 reflections were treated as observed (I > 2σ(I)). Data were corrected for Lorentz, polarisation and absorption factors. The structure was solved by direct methods using SHELXS97 [1]. All non-hydrogen atoms of the molecule were located in the best E-map. Full-matrix least-squares refinement was carried out using SHELXL97 [1]. The final refinement cycles converged to an R = 0.0445 and wR (F^2) = 0.0911 for the observed data. Residual electron densities ranged from -0.126 < $\Delta\rho$<0.158 eÅ^{-3}. Atomic scattering factors were taken from International Tables for X-ray Crystallography (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4). The crystallographic data are summarized in Table 1. An ORTEP view of the compound with atomic labelling is shown in Fig.1 [2]. The geometry of the molecule was calculated using the WinGX [3], PARST [4] and PLATON [5] software's. The compound 4-(3-Nitrophenyl)-2-phenoxy-6-phenylpyridine $C_{23}H_{17}N_2O_3$(**8c**), crystallizes in the monoclinic space group C2/c with the unit-cell parameters: a,b,c as 22.076 (2), 10.1079 (8), 16.921 (2)Å,β = 107.250 (11)^o and Z = 8. The crystal structure was solved by direct methods using single-crystal X-ray diffraction data collected at room temperature and refined by full-matrix least-squares procedures to a final R-value of 0.0445 for 2176 observed reflections.

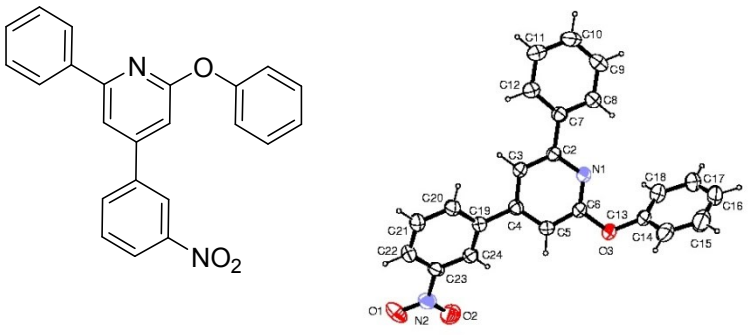


Fig. 1: ORTEP of (CCDC No. 1451640) compound **8c** whichcrystallized in monoclinic space group C2/cUnit Cell Parameters: a = 22.076 (2)Å,b = 10.1079 (8)Å, c = 16.921(2) Åfor 8c.

Table S1: Crystal and diffraction parameters of **8c**

Chemical formula	$C_{23}H_{16}N_2O_3$
M_r	368.38
Crystal system, space group	MONOCLINIC, *C*2/*c*
Temperature (K)	293
a, *b*, *c* (Å)	22.076 (2), 10.1079 (8), 16.921 (2)
β (°)	107.250 (11)
V (Å^3)	3605.9 (6)
Z	8
F(000)	1536
D_x (Mg m^{-3})	1.357
Radiation type	Mo *K*α
No. of reflections for cell measurement	1788
θ range (°) for cell measurement	3.9–27.6
μ (mm^{-1})	0.09
Crystal shape	BLOCK
Colour	White
Crystal size (mm)	0.30 × 0.20 × 0.20
Scan method	ω scans
Absorption correction	Multi-scan
T_{min}, T_{max}	0.893, 1.000
No. of measured, independent and observed [I> 2σ(I)] reflections	7234, 3530, 2176
R_{int}	0.028
θ values (°)	θ_{max} = 26.0, θ_{min} = 3.5
(sin θ/λ)$_{max}$ (Å^{-1})	0.617
Range of *h*, *k*, *l*	*h* = −27→17, *k* = −12→8, *l* = −20→20
Refinement on	F^2
$R[F^2> 2\sigma(F^2)]$, $wR(F^2)$, S	0.0445, 0.1090, 0.993
No. of reflections	3530
No. of parameters	254
No. of restraints	0
H-atom treatment	H-atom parameters constrained
Weighting scheme	$w = 1/[\sigma^2(F_o^2) + (0.0433P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
(Δ/σ)$_{max}$	< 0.001
Δρ$_{max}$, Δρ$_{min}$ (e Å^{-3})	0.16, −0.13

X-ray crystallographic data ofcompound 8e:

X-ray intensity data of 5807 reflections (of which 3223 unique) were collected on *X'calibur* CCD area-detector diffractometer equipped with graphite monochromated MoKα radiation (λ = 0.71073 Å). The crystal used for data collection was of dimensions 0.30 x 0.20 x 0.20

mm. The cell dimensions were determined by least-squares fit of angular settings of 1471 reflections in the θ range 4.12 to 26.09°**.** The intensities were measured by ω scan mode for θ ranges 3.52 to 26.00°. 1919 reflections were treated as observed ($I > 2\sigma(I)$). Data were corrected for Lorentz, polarisation and absorption factors. The structure was solved by direct methods using SHELXS97. [23] All non-hydrogen atoms of the molecule were located in the best E-map. Full-matrix least-squares refinement was carried out using SHELXL97. [23]The final refinement cycles converged to an R = 0.0533 and wR (F^2) = 0.1235 for the observed data. Residual electron densities ranged from $-0.162 < \Delta\rho < 0.172$ eÅ^{-3}. Atomic scattering factors were taken from International Tables for X-ray Crystallography (1992, Vol. C, Tables **4.2.6.8** and **6.1.1.4**). The crystallographic data are summarized in Table 2.Compound 6-phenoxy-4-phenyl-2, 2′-bipyridine $C_{22}H_{16}N_2O$ (**8e**), crystallizes in the triclinic space group *P-1* with the unit-cell parameters: a,b,c,α, β, γ as 8.1694 (12), 9.7524 (16), 11.8980 (18)Å,73.012 (14), 75.211 (13), 67.352 (15)° and Z = 2. The crystal structures **8e** was solved by direct methods using single-crystal X-ray diffraction data collected at room temperature and refined by full-matrix least-squares procedures to final R-values of 0.0579 for 1636 observed reflections and 0.0533 for 1919 observed reflections respectively.

Crystal structure of 6-phenoxy-4-phenyl-2, 2′-bipyridine (8e)

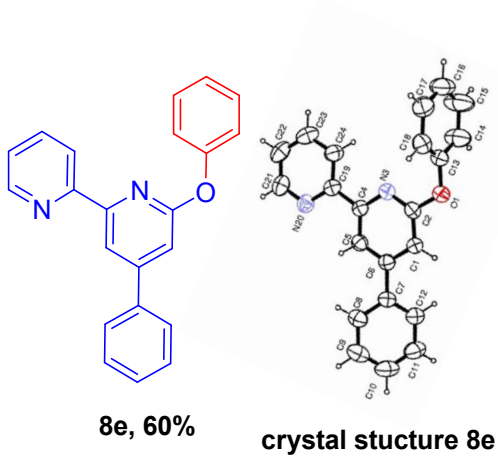


Fig. 2: ORTEP of (CCDC No. 1451639) compound **8e**whichcrystallized in triclinic space group *P-1*Unit Cell Parameters: a = 8.1694 (12) Å, b = 9.7524 (16) Å, c = 11.8980 (18) Å.

Table S2: Crystal and diffraction parameters of **8e.**

Chemical formula	$C_{22}H_{16}N_2O$
M_r	324.37
Crystal system, space group	TRICLINIC, *P*1
Temperature (K)	293
a, *b*, *c* (Å)	8.1694 (12), 9.7524 (16), 11.8980 (18)
α, β, γ (°)	73.012 (14), 75.211 (13), 67.352 (15)
V (Å^3)	825.6 (2)
Z	2
F(000)	340
D_x (Mg m^{-3})	1.305
Radiation type	Mo *K*α
No. of reflections for cell measurement	1471
θ range (°) for cell measurement	4.1–26.1
μ (mm^{-1})	0.08
Crystal shape	BLOCK
Colour	White
Crystal size (mm)	0.30 × 0.20 × 0.20
Diffractometer	Xcalibur, Sapphire3 diffractometer
Scan method	ω Scan scans
Absorption correction	Multi-scan
T_{min}, T_{max}	0.868, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	5807, 3223, 1919
R_{int}	0.028
θ values (°)	θ_{max} = 26.0, θ_{min} = 3.5
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.617
Range of *h*, *k*, *l*	*h* = −10→10, *k* = −12→5, *l* = −14→14
Refinement on	F^2
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.0533, 0.1519, 1.042
No. of reflections	3223
No. of parameters	227
No. of restraints	0
H-atom treatment	H-atom parameters constrained
Weighting scheme	$w = 1/[\sigma^2(F_o^2) + (0.058P)^2 + 0.0032P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$	< 0.001
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.17, −0.16

References

1. Sheldrick GM (2008) Acta Cryst A64: 112
2. Farrugia LJ (1997) J Appl Cryst30:565
3. Farrugia LJ (1999) J Appl Cryst32:837
4. Nardelli M (1995) J Appl Cryst 28:659

5. Spek AL (2009) Acta Cryst D65: 148–155