

**Gold(III)-Catalyzed Three-Component Coupling Reaction (TCC) Selective
towards Furans**

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Supporting Information

Contents:	Pages
General Remarks	S2
General Procedure for Au-catalyzed Three-component Reactions	S2
Characterization of furans 4a-4m	S3-S8
NMR spectrum of all new compounds 4a-4m	S9-S21

General Remarks.

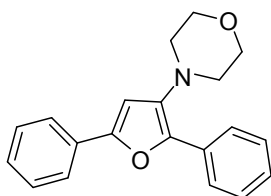
All reactions were carried out under an air atmosphere condition. Various reagents were purchased from Aldrich, Acros or Alfa. The compounds **1** were prepared according literature from acetophenone. Flash column chromatography was performed using silica gel (200–300 mesh). Analytical thin-layer chromatography was performed using glass plates pre-coated with 200–300 mesh silica gel impregnated with a fluorescent indicator (254 nm). NMR spectra were recorded in CDCl₃ on Bruker NMR-300 (300MHz), NMR-400 (400MHz) and NMR-500 (500MHz) with TMS as an internal reference. The model of HRMS is Bruker maXis UHR-TOF.

General Procedure for Au-catalyzed Three-component Reactions.

A solution of phenylglyoxal derivatives **1** (1 mmol), amine **2** (1.5 mmol), AuBr₃ (8.7 mg, 0.02 mmol) and alkyne **3** (2 mmol) in anhydrous menthol (1 mL) was stirred at 60 °C for 12 h under N₂ atmosphere. After completion of the reaction (observed on TLC), the solvent was evaporated under reduced pressure to obtain the crude mixture. The residues was purified by silica-gel column chromatography (Ethyl acetate / Petroleum ether = 1/10 - 1/4) to afford the pure product **4**. The obtained product was analyzed by ¹H NMR, ¹³C NMR and HRMS.

Characterization of furans 4a-4m

4-(2, 5-diphenylfuran-3-yl)morpholine (4a)

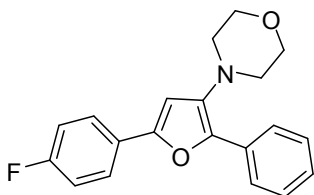


4a

^1H NMR (400 MHz, CDCl_3) 7.99 (d, $J = 7.3$ Hz, 2H), 7.70 (d, $J = 7.3$ Hz, 2H), 7.39 (q, $J = 7.7$ Hz, 4H), 7.24 (q, $J = 8.6$ Hz, 2H), 6.76 (s, 1H), 3.86 (t, $J = 4.4$ Hz, 4H), 2.95 (t, $J = 4.4$ Hz, 4H).

^{13}C NMR (75 MHz, CDCl_3) 151.39, 141.39, 138.32, 131.27, 130.65, 128.74, 128.54, 127.49, 126.40, 124.11, 123.62, 101.79, 67.23, 52.43. MS (m/z): HRMS (ESI) calcd for $\text{C}_{20}\text{H}_{19}\text{NO}_2$ ($[\text{M}+\text{H}]$): 306.1494 found 306.1492.

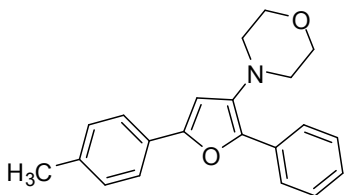
4-[5-(4-fluorophenyl)2-phenylfuran-3-yl]morpholine (4b)



4b

^1H NMR (400 MHz, CDCl_3) δ 7.98 (d, $J = 7.5$ Hz, 2H), 7.68-7.66 (m, 2H), 7.40 (t, $J = 7.6$ Hz, 2H), 7.24-7.22 (m, 1H), 7.08 (t, $J = 7.6$ Hz, 2H), 6.68 (s, 1H), 3.87 (t, $J = 4.4$ Hz, 4H), 2.95 (t, $J = 4.4$ Hz, 4H). ^{13}C NMR (125 MHz, CDCl_3) δ 163.25, 161.28, 150.61, 141.44, 138.31, 131.21, 128.97, 128.59, 127.10, 126.49, 125.43, 125.37, 124.12, 115.91, 115.74, 101.51, 67.25, 52.46. MS (m/z): HRMS (ESI) calcd for $\text{C}_{20}\text{H}_{18}\text{FNO}_2$ ($[\text{M}+\text{H}]$): 324.1400 found 324.1394.

4-(2-phenyl-5-p-tolylfuran-3-yl)morpholine (4c)

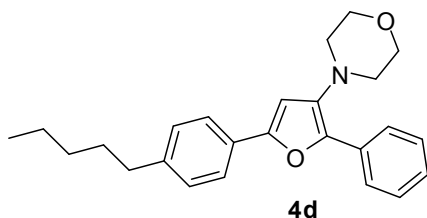


4c

^1H NMR (400 MHz, CDCl_3) δ 7.99 (d, $J = 7.8$ Hz, 2H), 7.60 (d, $J = 8.0$ Hz, 2H), 7.39 (t, $J = 7.6$

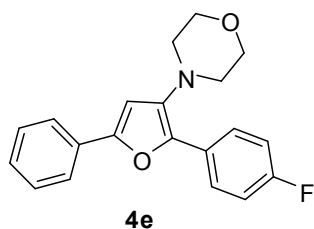
Hz, 2H), 7.24-7.22 (m, 3H), 6.68 (s, 1H), 3.86 (t, $J = 4.4$ Hz, 4H), 2.95 (t, $J = 4.4$ Hz, 4H), 2.36 (s, 3H). ^{13}C NMR (125 MHz, CDCl_3) δ 151.63, 140.94, 138.26, 137.35, 131.67, 131.33, 129.38, 128.92, 128.66, 128.47, 128.07, 127.96, 126.21, 123.99, 123.66, 101.04, 67.21, 52.41, 21.31. MS (m/z): HRMS (ESI) calcd for $\text{C}_{21}\text{H}_{21}\text{NO}_2$ ($[\text{M}+\text{H}]$): 320.1650 found 320.1643.

4-[5-(4-pentylphenyl)-2-phenylfuran-3-yl]morpholine (4d)



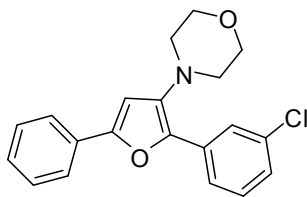
^1H NMR (400 MHz, CDCl_3) δ 7.98 (d, $J = 8.0$ Hz, 2H), 7.62 (d, $J = 8.0$ Hz, 2H), 7.40 (t, $J = 7.8$ Hz, 2H), 7.20 (d, $J = 7.8$ Hz, 3H), 6.7 (s, 1H), 3.87 (t, $J = 4.4$ Hz, 4H), 2.96 (t, $J = 4.4$ Hz, 4H), 2.61 (t, $J = 7.6$ Hz, 2H), 1.62 (t, $J = 7.1$ Hz, 2H), 1.33-1.31 (m, 4H), 0.89 (t, $J = 6.0$ Hz, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 151.73, 142.51, 141.03, 138.28, 131.37, 128.97, 128.77, 128.48, 128.19, 126.22, 124.02, 123.61, 101.08, 67.24, 52.45, 35.74, 31.47, 31.06, 22.55, 14.04. MS (m/z): HRMS (ESI) calcd for $\text{C}_{25}\text{H}_{29}\text{NO}_2$ ($[\text{M}+\text{H}]$): 376.2276 found 376.2270.

4-[2-(4-fluorophenyl)-5-phenylfuran-3-yl]morpholine (4e)



^1H NMR (400 MHz, CDCl_3) δ 7.98 (t, $J = 6.2$ Hz, 2H), 7.69 (d, $J = 7.7$ Hz, 2H), 7.39 (t, $J = 7.6$ Hz, 2H), 7.27-7.25 (m, 1H), 7.10 (t, $J = 8.6$ Hz, 2H), 6.7 (s, 1H), 3.86 (s, 4H), 2.94 (s, 4H). ^{13}C NMR (75 MHz, CDCl_3) δ 162.98, 159.71, 151.35, 140.88, 137.72, 130.54, 128.74, 127.53, 125.87, 125.77, 123.57, 115.66, 115.37, 101.81, 67.22, 52.47. MS (m/z): HRMS (ESI) calcd for $\text{C}_{20}\text{H}_{18}\text{FNO}_2$ ($[\text{M}+\text{H}]$): 324.1400 found 324.1396.

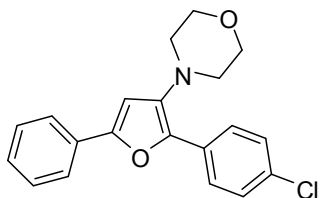
4-[2-(3-chlorophenyl)-5-phenylfuran-3-yl]morpholine (4f)



4f

^1H NMR (400 MHz, CDCl_3) δ 8.01(s, 1H), 7.86 (d, $J = 7.8$ Hz, 1H), 7.71 (d, $J = 7.6$ Hz, 2H), 7.40 (t, $J = 7.6$ Hz, 2H), 7.32-7.28 (m, 2H), 7.18-7.16 (m, 1H), 6.75 (s, 1H), 3.88 (t, $J = 4.2$ Hz, 4H), 2.96 (t, $J = 4.2$ Hz, 4H). ^{13}C NMR (75 MHz, CDCl_3) δ 152.03, 139.97, 139.33, 134.56, 132.77, 131.84, 130.33, 129.79, 128.77, 127.79, 126.13, 123.90, 123.74, 121.87, 101.84, 67.15, 52.39. MS (m/z): HRMS (EI) calcd for $\text{C}_{20}\text{H}_{18}\text{ClNO}_2$ ($[\text{M}+\text{H}]$): 340.1104 found 340.1105.

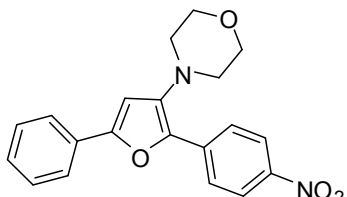
4-[2-(4-chlorophenyl)-5-phenylfuran-3-yl]morpholine (4g)



4g

^1H NMR (400 MHz, CDCl_3) δ 7.93 (d, $J = 8.5$ Hz, 2H), 7.70 (d, $J = 7.6$ Hz, 2H), 7.38 (t, $J = 7.6$ Hz, 4H), 7.25-7.22 (m, 1H), 6.75 (s, 1H), 3.86 (t, $J = 4.2$ Hz, 4H), 2.94 (t, $J = 4.2$ Hz, 4H). ^{13}C NMR (75 MHz, CDCl_3) δ 153.90, 145.01, 142.51, 139.31, 136.81, 129.84, 128.90, 124.27, 124.08, 123.66, 102.22, 67.02, 52.41. MS (m/z): HRMS (ESI) calcd for $\text{C}_{20}\text{H}_{18}\text{ClNO}_2$ ($[\text{M}+\text{H}]$): 340.1104 found 340.1098.

4-[2-(4-nitrophenyl)-5-phenylfuran-3-yl]morpholine (4h)

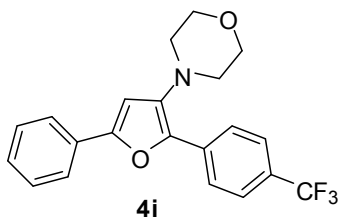


4h

^1H NMR (400 MHz, CDCl_3) δ 8.26 (d, $J = 8.8$ Hz, 2H), 8.08 (d, $J = 8.8$ Hz, 2H), 7.74 (d, $J = 7.7$ Hz, 2H), 7.43 (t, $J = 7.7$ Hz, 2H), 7.33-7.32 (m, 1H), 6.80 (s, 1H), 3.90 (t, $J = 4.2$ Hz, 4H), 2.98 (t, $J = 4.2$ Hz, 4H). ^{13}C NMR (75 MHz, CDCl_3) δ 153.90, 145.01, 142.51, 139.31, 136.81, 129.84,

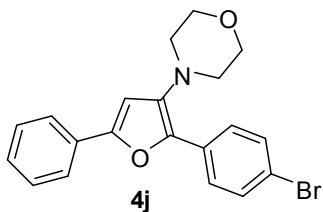
128.90, 128.50, 124.27, 124.08, 123.66, 102.22, 67.02, 52.40. MS (*m/z*): HRMS (ESI) calcd for C₂₀H₁₈N₂O₄ ([M+H]): 351.1345 found 351.1340.

4-[5-phenyl-2-(4-trifluoromethyl-phenyl)furan-3-yl]morpholine (4i)



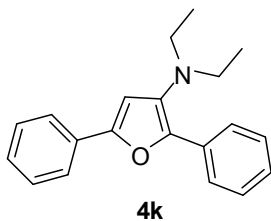
¹H NMR (400 MHz, CDCl₃) δ 8.08 (d, *J* = 8.1 Hz, 2H), 7.72 (d, *J* = 7.6 Hz, 2H), 7.64 (d, *J* = 8.1 Hz, 2H), 7.42 (t, *J* = 7.6 Hz, 2H), 7.32-7.30 (m, 1H), 6.78 (s, 1H), 3.88 (t, *J* = 4.2 Hz, 4H), 2.97 (t, *J* = 4.2 Hz, 4H). ¹³C NMR (75 MHz, CDCl₃) δ 152.56, 140.29, 139.99, 134.31, 131.82, 130.23, 128.81, 127.99, 125.47, 123.83, 101.93, 67.13, 52.41. MS (*m/z*): HRMS (ESI) calcd for C₂₁H₁₈F₃NO₂ ([M+H]): 374.1368 found 374.1363.

4-[2-(4-bromophenyl)-5-phenylfuran-3-yl]morpholine (4j)



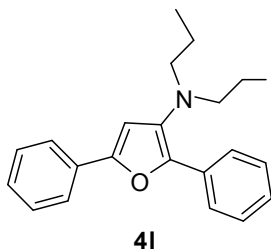
¹H NMR (400 MHz, CDCl₃) δ 7.86 (d, *J* = 8.5 Hz, 2H), 7.70 (d, *J* = 7.6 Hz, 2H), 7.52 (d, *J* = 8.5 Hz, 2H), 7.40 (t, *J* = 7.6 Hz, 2H), 7.28-7.25 (m, 1H), 6.75 (s, 1H), 3.86 (t, *J* = 4.4 Hz, 4H), 2.94 (t, *J* = 4.4 Hz, 4H). ¹³C NMR (75 MHz, CDCl₃) δ 151.78, 140.47, 138.85, 131.64, 130.40, 128.77, 125.51, 123.66, 119.90, 101.86, 67.17, 52.38. MS (*m/z*): HRMS (ESI) calcd for C₂₀H₁₈BrNO₂ ([M+H]): 383.0521 found 383.0517.

***N,N*-diethyl-2,5-diphenylfuran-3-amine (4k)**



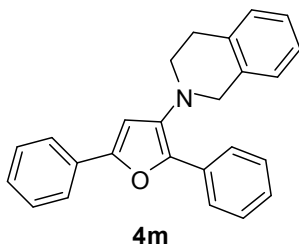
^1H NMR (400 MHz, CDCl_3) δ 8.15 (d, $J = 7.7$ Hz, 2H), 7.72 (d, $J = 7.7$ Hz, 2H), 7.38 (t, $J = 7.5$ Hz, 4H), 7.24-7.20 (m, 2H), 6.78 (s, 1H), 2.96 (q, $J = 7.1$ Hz, 4H), 1.05 (t, $J = 7.1$ Hz, 6H). ^{13}C NMR (75 MHz, CDCl_3) δ 151.14, 144.42, 136.17, 131.54, 130.91, 128.70, 128.28, 127.28, 126.27, 124.30, 123.56, 103.96, 48.93, 12.77. MS (m/z): HRMS (ESI) calcd for $\text{C}_{20}\text{H}_{21}\text{NO}$ ($[\text{M}+\text{H}]$): 292.1701 found 292.1703.

2, 5-diphenyl-*N,N*-dipropylfuran-3-amine (4l)



^1H NMR (400 MHz, CDCl_3) δ 8.12 (d, $J = 7.8$ Hz, 2H), 7.71 (d, $J = 7.8$ Hz, 2H), 7.38 (t, $J = 7.6$ Hz, 4H), 7.24-7.20 (m, 2H), 6.78 (s, 1H), 2.87 (t, $J = 7.4$ Hz, 4H), 1.52 (q, $J = 7.4$ Hz, 4H), 0.85 (t, $J = 7.4$ Hz, 6H). ^{13}C NMR (75 MHz, CDCl_3) δ 151.06, 143.90, 136.87, 133.18, 131.47, 130.89, 128.89, 128.67, 128.27, 127.69, 127.26, 126.20, 124.27, 123.55, 103.98, 57.15, 20.64, 11.82. MS (m/z): HRMS (ESI) calcd for $\text{C}_{22}\text{H}_{25}\text{NO}$ ($[\text{M}+\text{H}]$): 320.2014 found 320.2014.

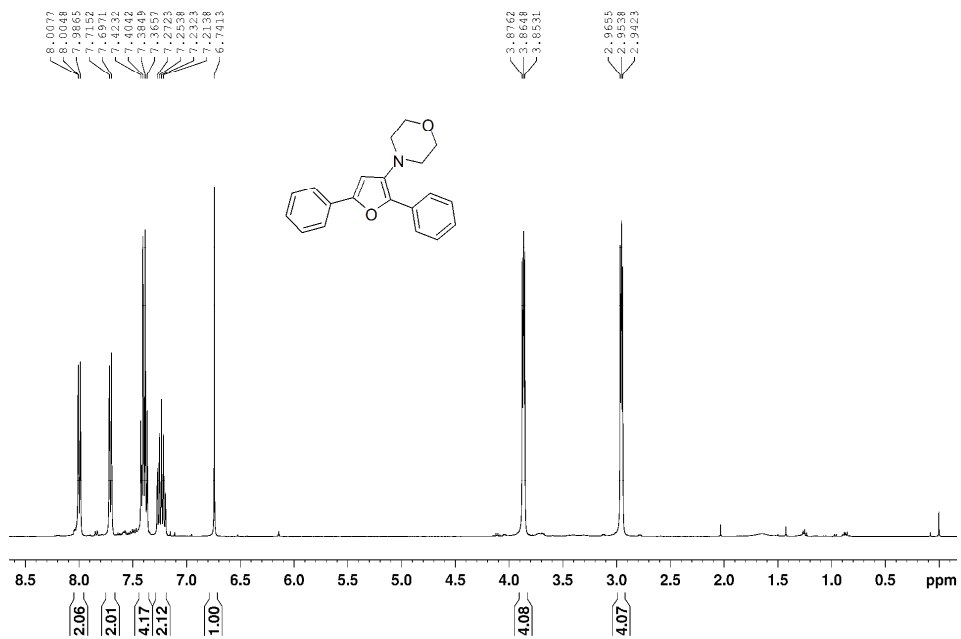
2-(2, 5-diphenylfuran-3-yl)-1, 2, 3, 4-tetrahydroisoquinoline (4m)



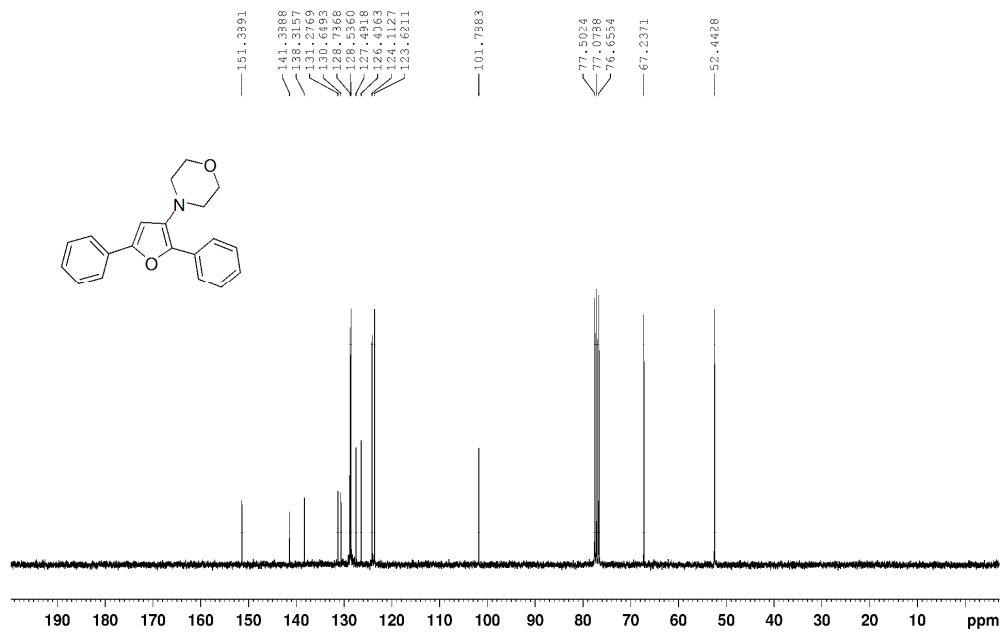
^1H NMR (400 MHz, CDCl_3) δ 8.02 (d, $J = 7.8$ Hz, 2H), 7.73 (d, $J = 7.8$ Hz, 2H), 7.40-7.36 (m, 5H), 7.23-7.19 (m, 4H), 7.08-7.06 (m, 1H), 6.78 (s, 1H), 4.16 (s, 2H), 3.26 (t, $J = 5.6$ Hz, 2H),

3.03 (t, $J = 5.6$ Hz, 2H). ^{13}C NMR (125 MHz, CDCl_3) δ 151.19, 141.41, 138.36, 134.75, 134.24, 132.48, 131.36, 130.69, 128.89, 128.67, 128.48, 128.15, 127.76, 127.36, 126.45, 126.31, 126.24, 125.80, 124.04, 123.57, 102.38, 54.26, 50.48, 29.26. MS (m/z): HRMS (EI) calcd for $\text{C}_{25}\text{H}_{21}\text{NO}$ ($[\text{M}+\text{H}]$): 352.1701 found 352.1695.

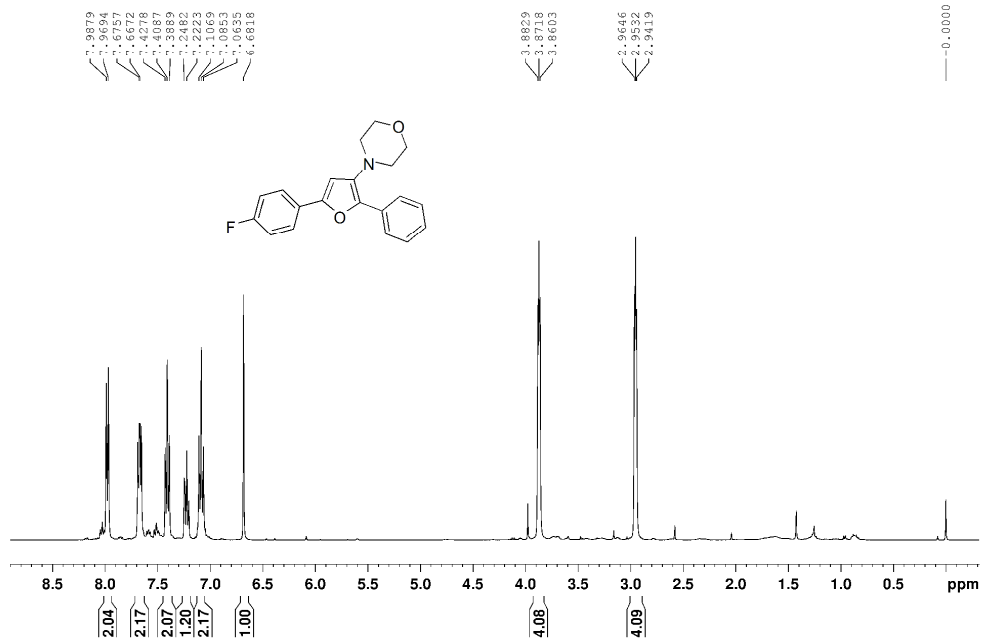
NMR spectrum of all new compounds 4a-4m



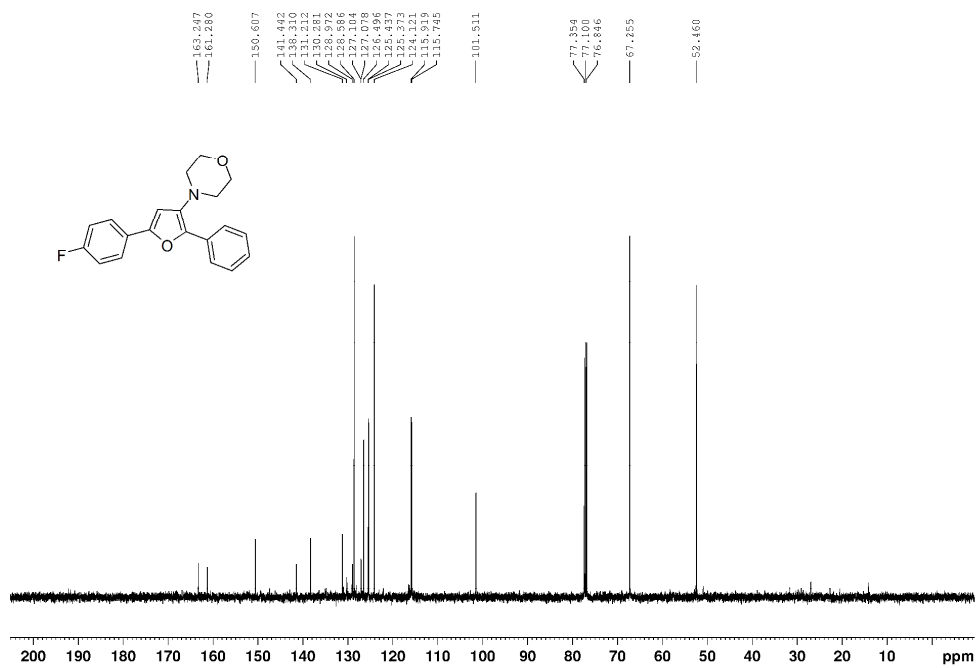
¹H NMR spectrum of compounds 4a



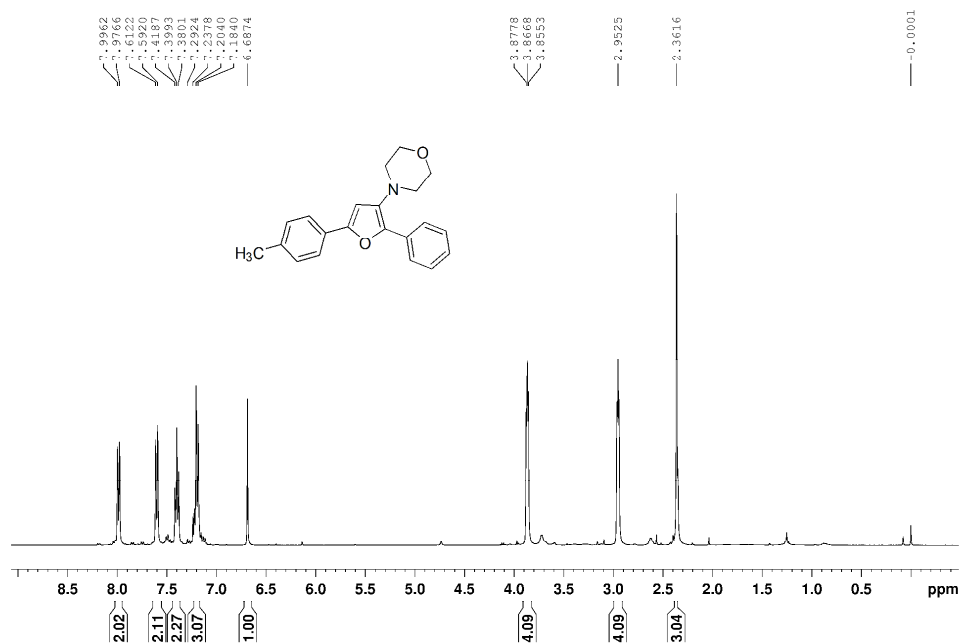
¹³C NMR spectrum of compounds 4a



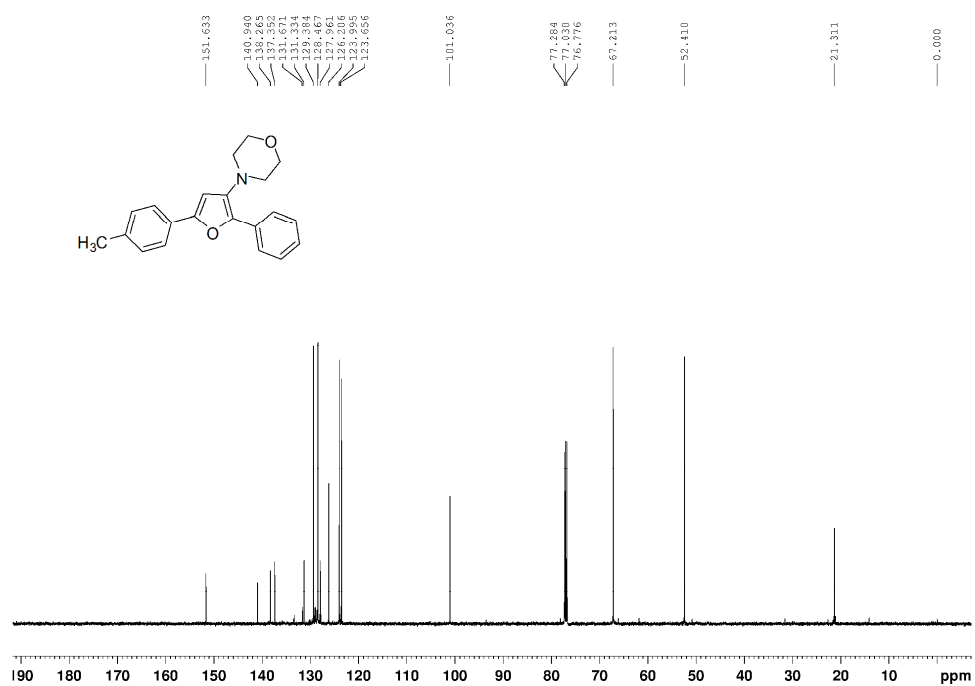
¹H NMR spectrum of compounds 4b



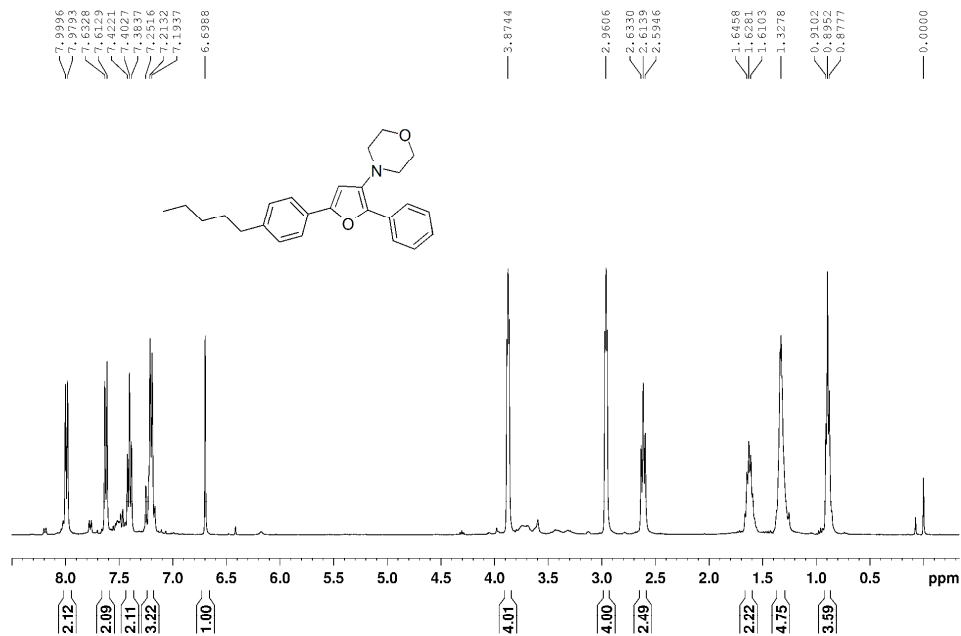
¹³C NMR spectrum of compounds 4b



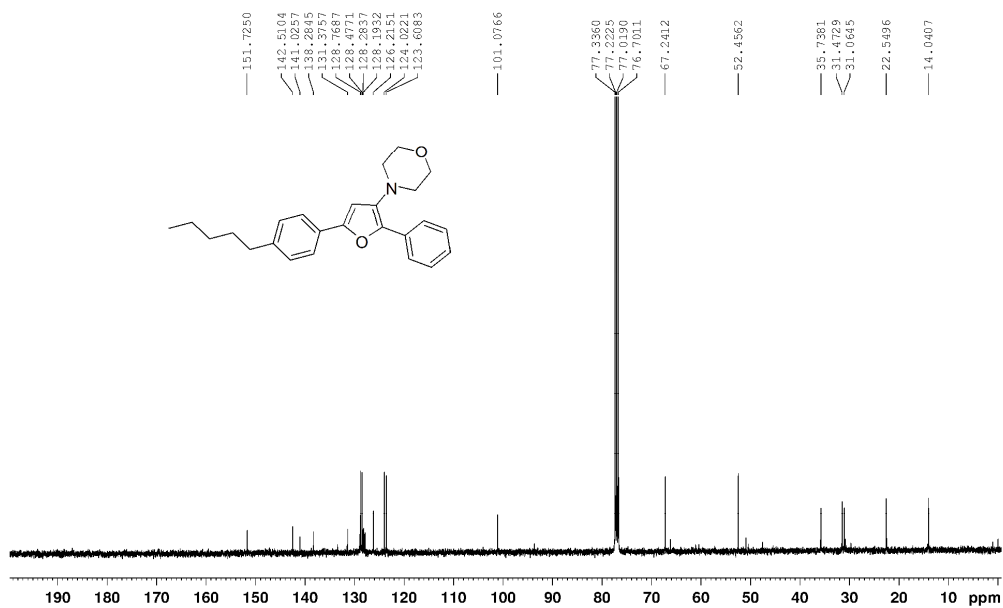
¹H NMR spectrum of compounds 4c



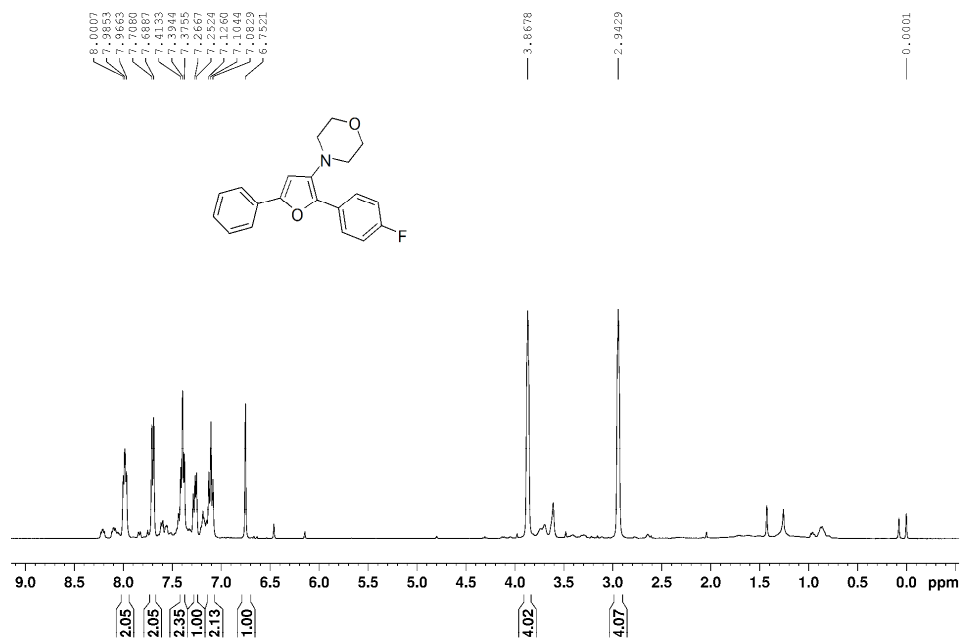
¹³C NMR spectrum of compounds 4c



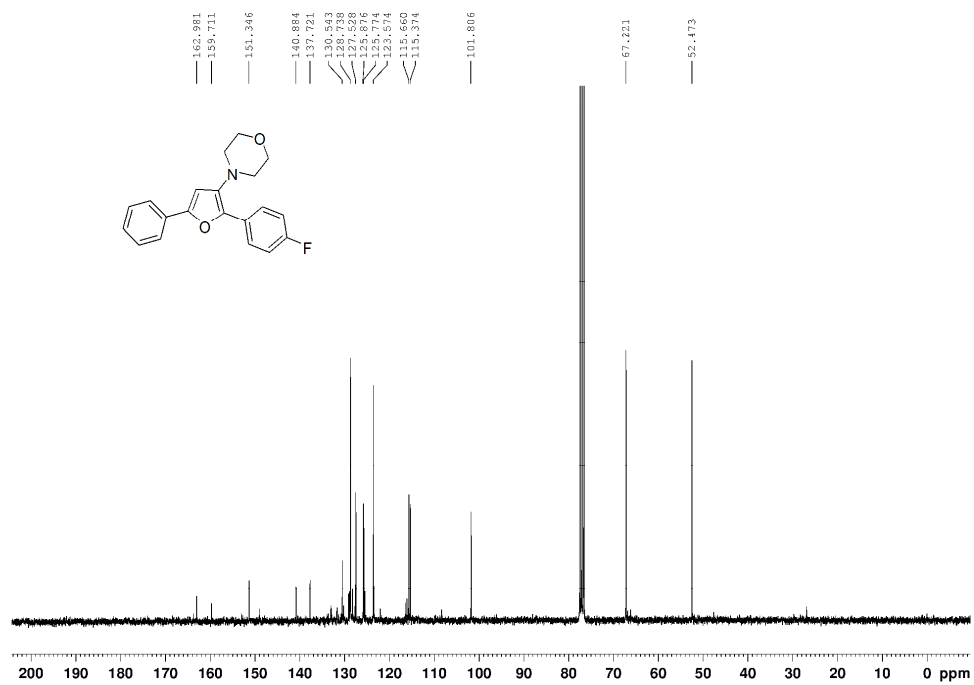
¹H NMR spectrum of compounds 4d



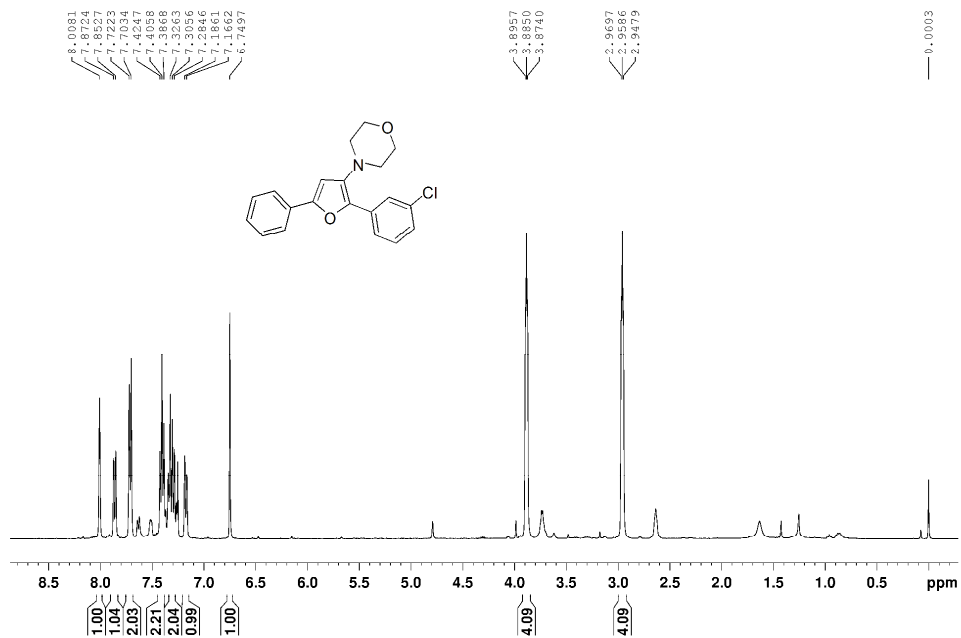
¹³C NMR spectrum of compounds 4d



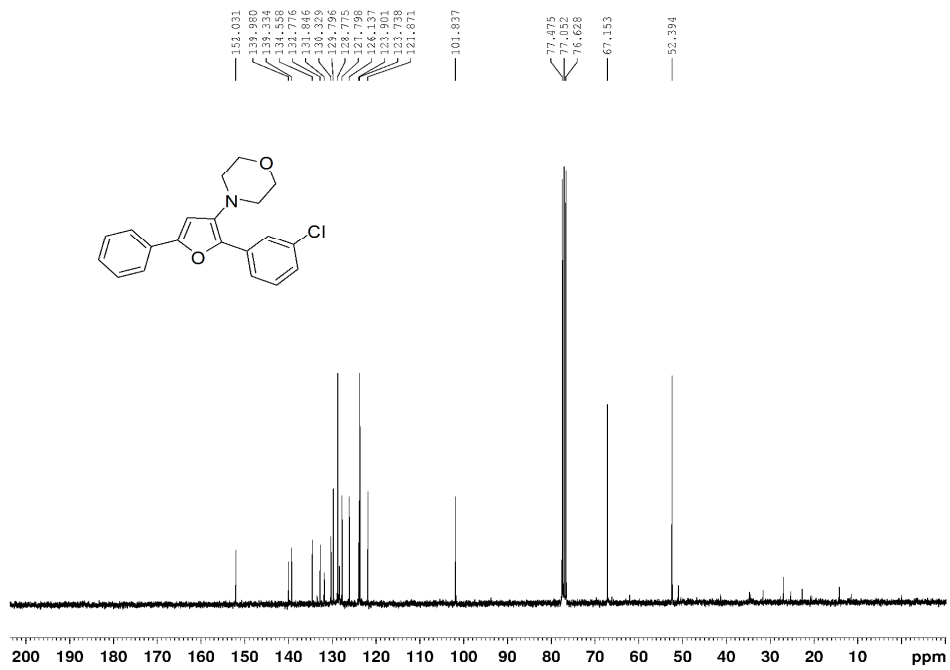
¹H NMR spectrum of compounds 4e



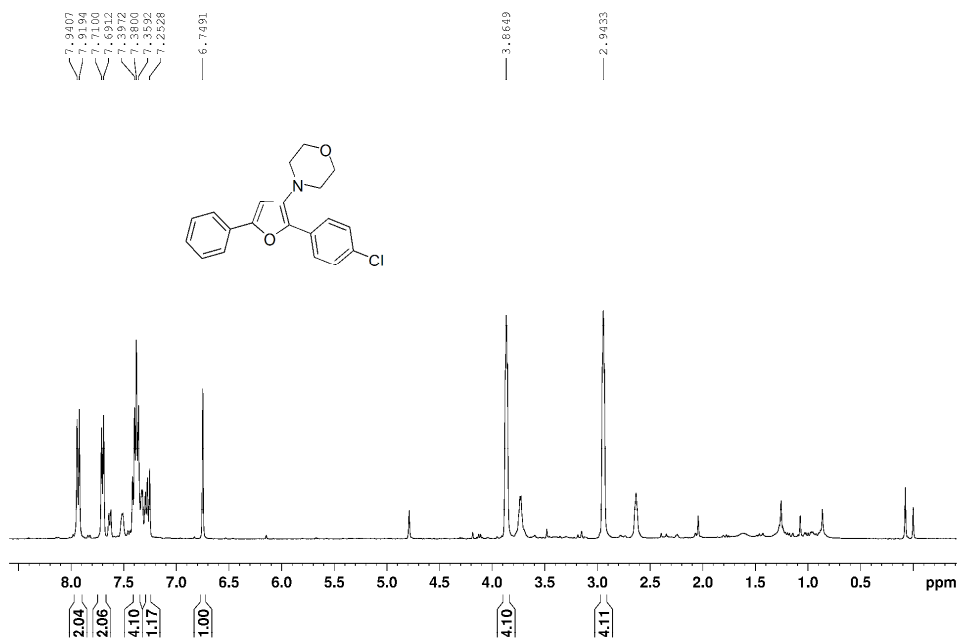
¹³C NMR spectrum of compounds 4e



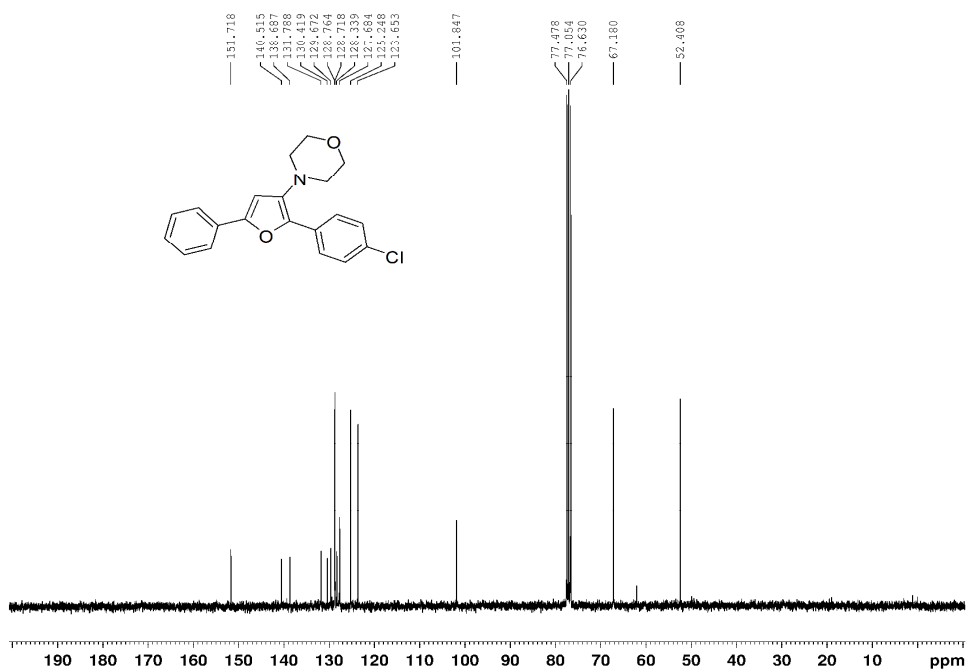
¹H NMR spectrum of compounds 4f



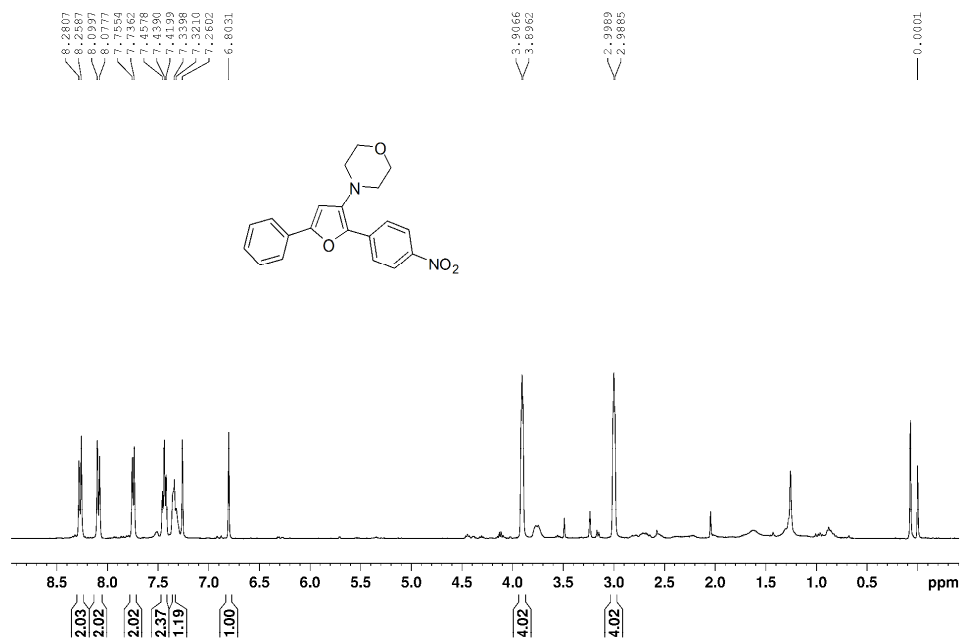
¹³C NMR spectrum of compounds 4f



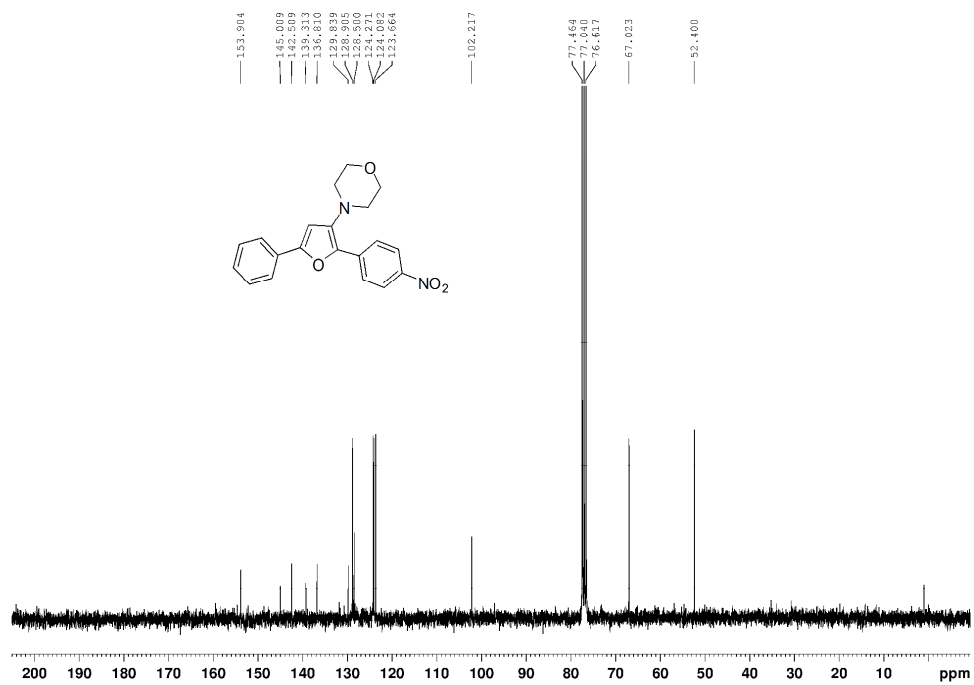
¹H NMR spectrum of compounds 4g



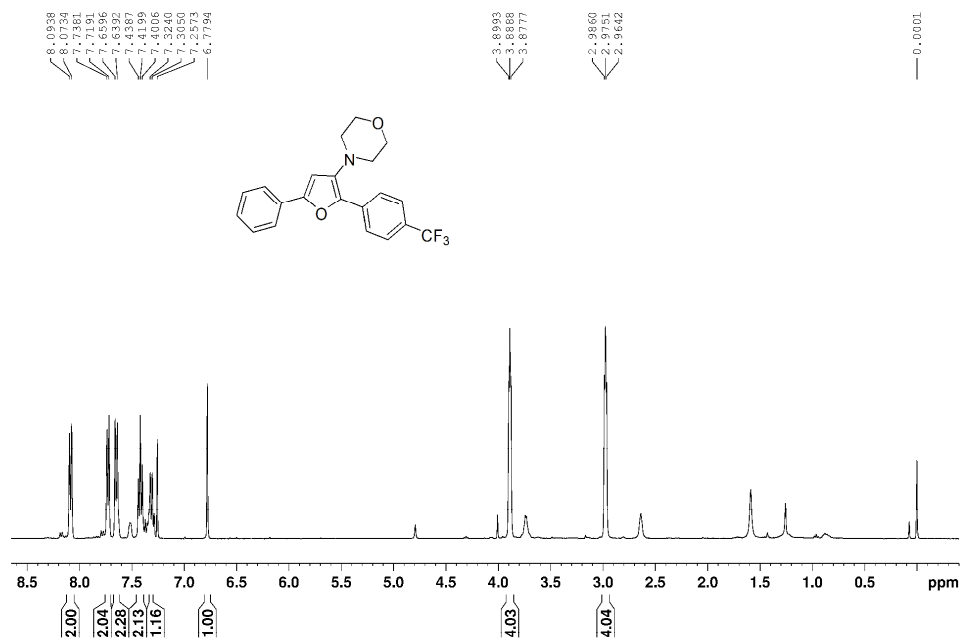
¹³C NMR spectrum of compounds 4g



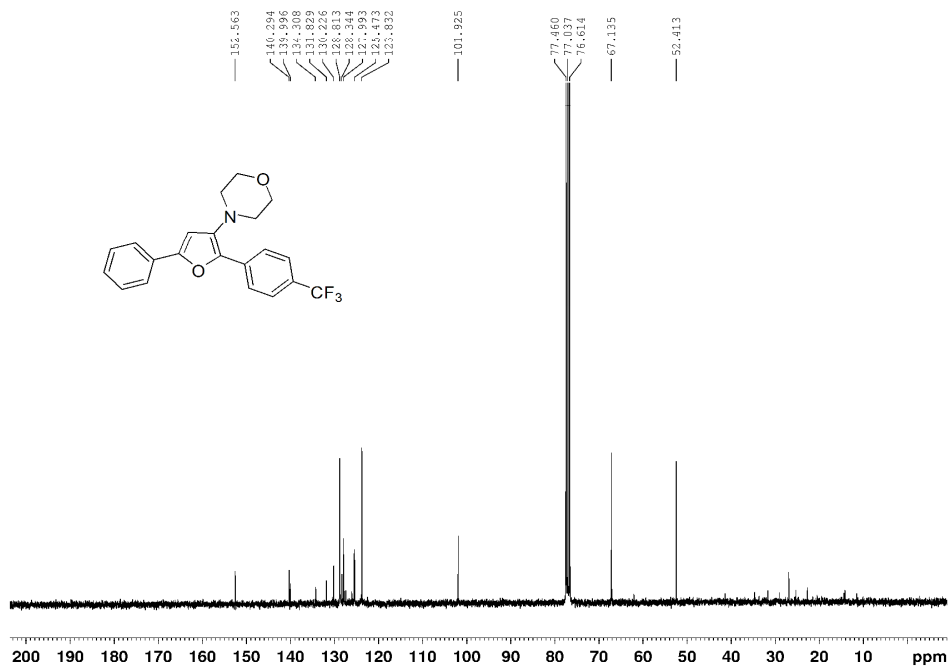
¹H NMR spectrum of compounds 4h



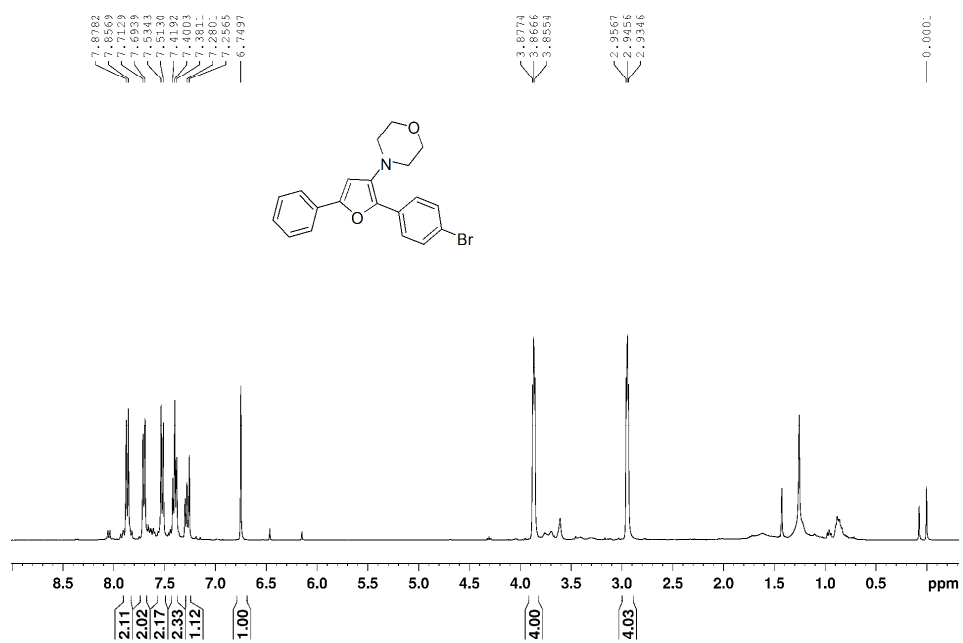
¹³C NMR spectrum of compounds 4h



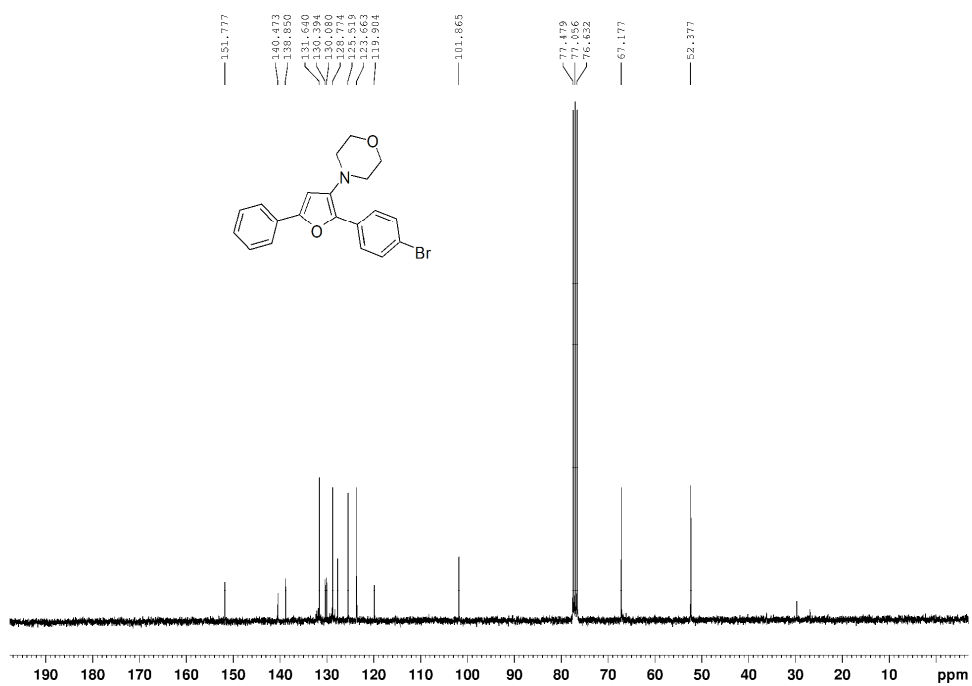
¹H NMR spectrum of compounds 4i



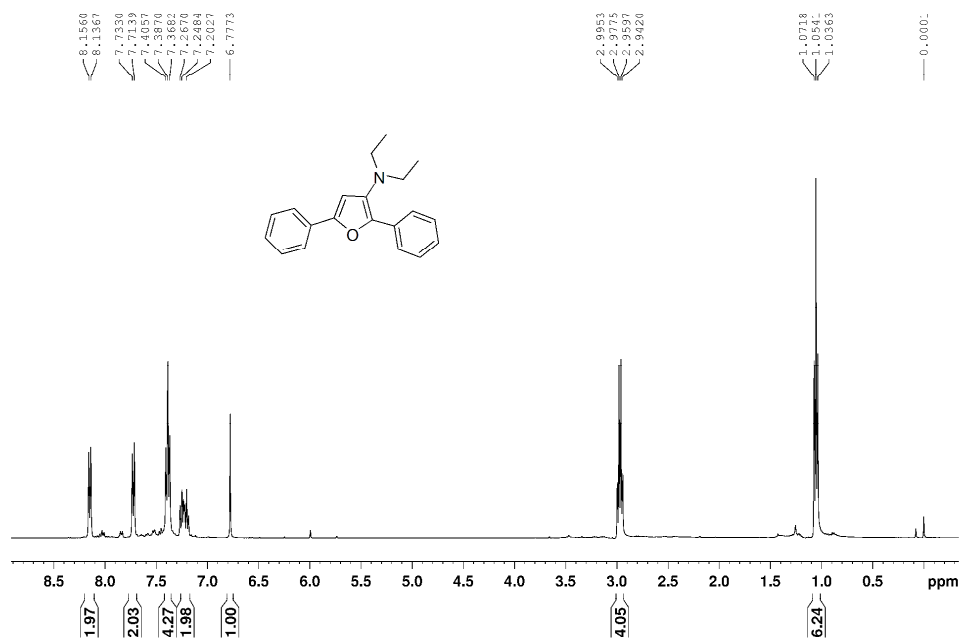
¹³C NMR spectrum of compounds 4i



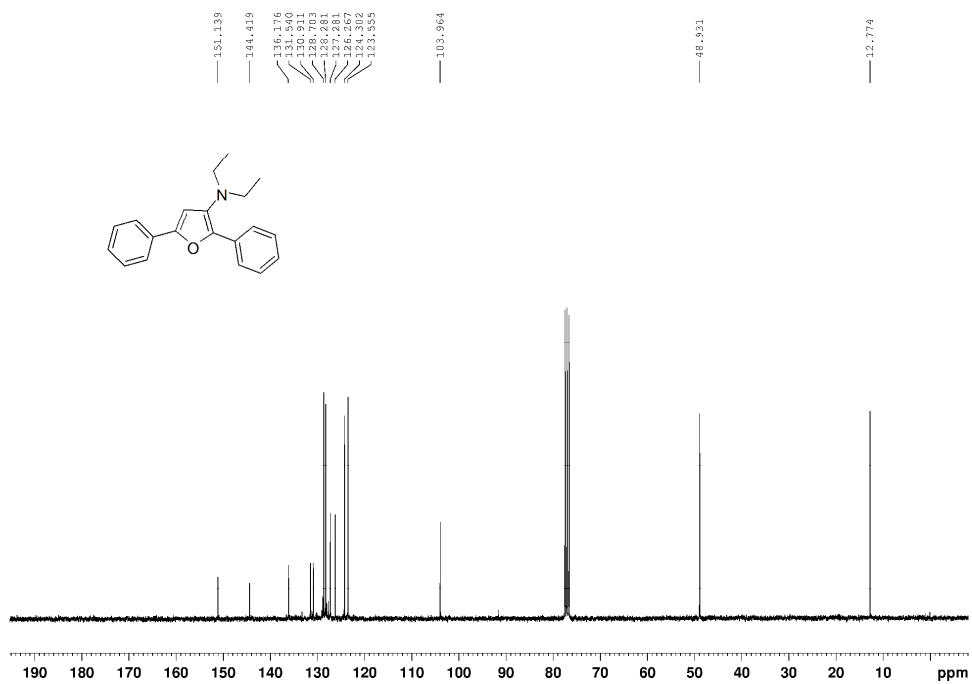
¹H NMR spectrum of compounds 4j



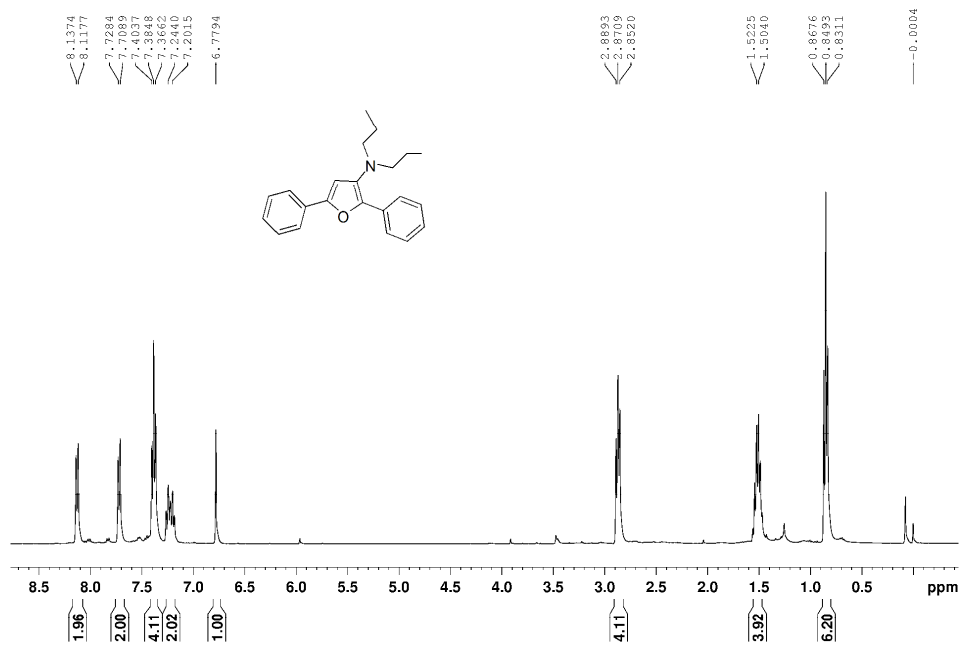
¹³C NMR spectrum of compounds 4j



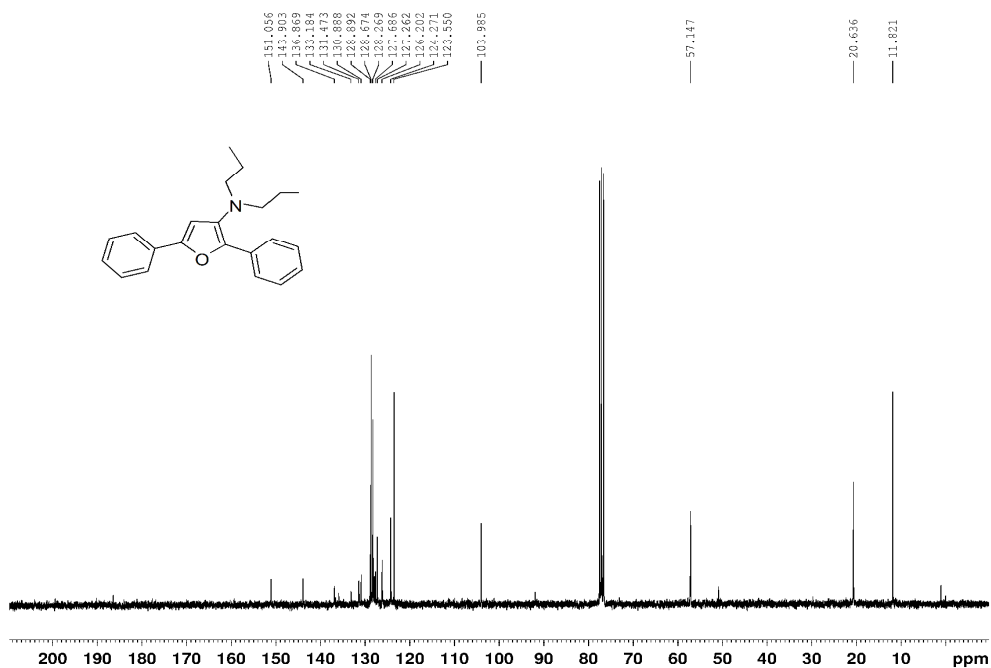
¹H NMR spectrum of compounds 4k



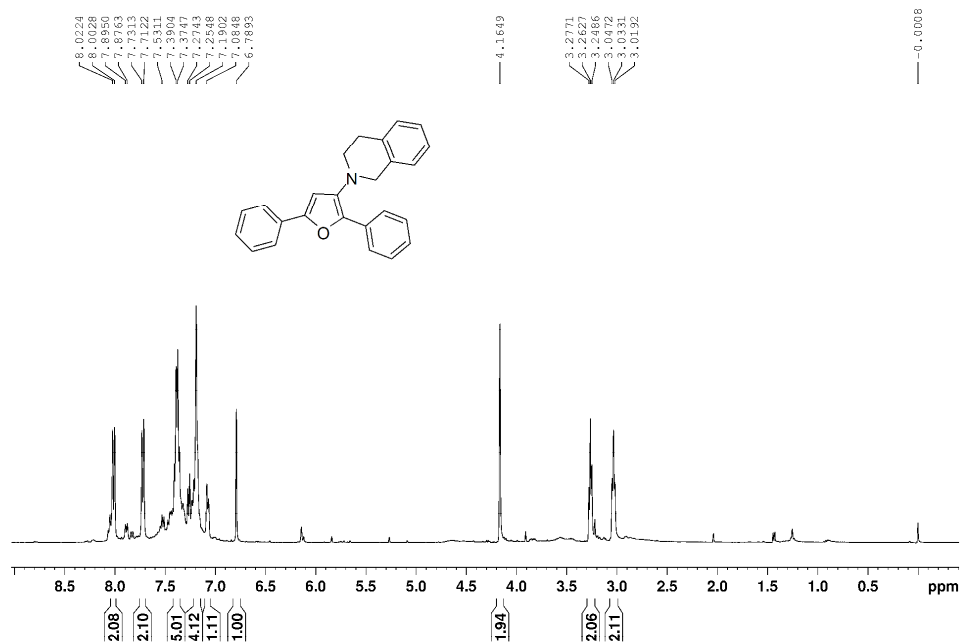
¹³C NMR spectrum of compounds 4k



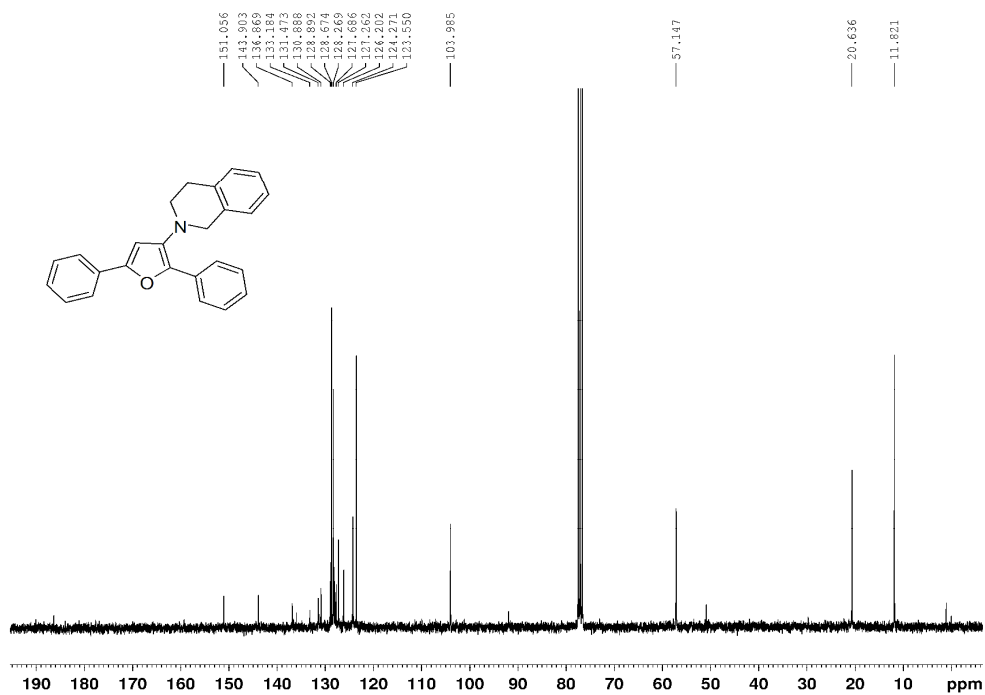
¹H NMR spectrum of compounds 41



¹³C NMR spectrum of compounds 41



¹H NMR spectrum of compounds 4m



¹³C NMR spectrum of compounds 4m