Supporting materials

Four-component reaction between naphthols, substituted *β*-nitrostyrenes, substituted benzaldehydes and ammonium acetate in water-PEG 400: approach to construct polysubstituted naphthofuranamines

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Experimental section

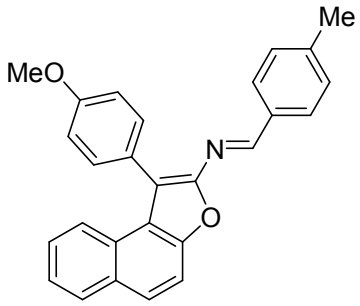
All melting points were determined in a Yanaco melting point apparatus and are uncorrected. IR spectra were recorded in a Nicolet FT-IR 5DX spectrometer. The ^{1}H NMR (400 or 600 MHz) and ^{13}C NMR (100 or 150 MHz) spectra were recorded in a Bruker AV-600 spectrometer with TMS as internal reference in $CDCl_3$ solutions. The *J* values are given in hertz. Only discrete or characteristic signals for the ^{1}H NMR are reported. The MS spectra were obtained on a ZAB-HS mass spectrometer with 70 eV. X-ray crystallographic analysis was performed with a SMART APEX-Ⅱ diffractometer. Flash chromatography was performed on silica gel (230-400 mesh) eluting with ethyl acetate-hexanes mixture. All reactions were monitored by thin layer chromatography (TLC). All reagents and solvents were purchased from commercial sources and purified commonly before used.

General procedure for preparation of polysubstituted naphthofuranamines via four-component reaction

The standard procedure for the synthesis of polysubstituted naphthofuranamines via four-component reaction between substituted *β*-nitrostyrenes, *β*-naphthols or *a*-naphthol, substituted benzaldehydes and ammonium acetate is as follows. To the mixture of substituted *β*-nitrostyrenes (3 mmol), *β*-naphthols or *a*-naphthol (4.5 mmol) and sodium hydroxide (6 mmol, 0.24g) in water (13 mL) and PEG-400 (2 mL) was added corresponding imines generated firstly from substituted benzaldehydes (3 mmol) and ammonium acetate (6.0 mmol, 0.462g). The resulting mixture was stirred at 80 ^{o}C for 8 h for *β*-naphthols or 12 h for *a*-naphthol, and the completion of reaction was confirmed by TLC (Hexanes/EtOAc, 5:1). Subsequently, the reaction mixture was extracted with dichloromethane (10 mL X 2). The organic phase was washed with 3% HCl (10 mL), water (10 mL) and brine (5 mL), and dried over anhydrate sodium sulfate. After removal of dichloromethane, the crude product was purified by flash chromatography (silica gel, EtOAc/hexanes, 1/8) to give the desirable products **4a-x**.

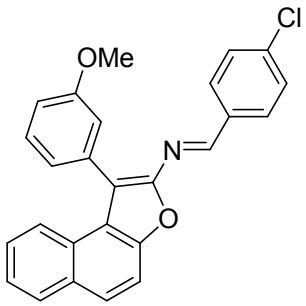
Spectroscopic data of the products 4a-4x

(E)-N-(1-(4-methoxyphenyl)naphtho[2,1-b]furan-2-yl)-1-(p-tolyl)methanimine (**4a**)



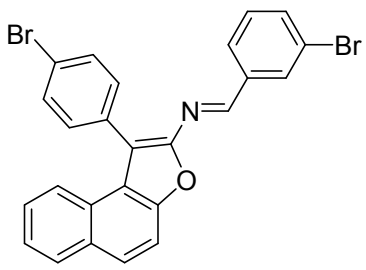
Yellow solid, yield 86%, m.p. 168.1 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (*ppm*): 8.90 (s, 1 H), 8.07 (d, *J* = 8.4 Hz, 1 H), 7.90 (d, *J* = 8.0 Hz, 1 H), 7.76 (d, *J* = 8.8 Hz, 1 H), 7.75 (d, *J* = 8.4 Hz, 2 H), 7.62 (d, *J* = 8.8 Hz, 3 H), 7.42 (dd, *J* = 7.2 Hz, 1 H), 7.35 (dd, *J* = 8.4 Hz, 1 H), 7.21 (d, *J* = 8. 0 Hz, 2 H), 7.08 (d, *J* = 8.8 Hz, 2 H), 3.94 (s, 3 H), 2.39 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ (*ppm*): 159.1, 155.3, 152.8, 149.1, 141.7, 134.1, 132.2, 130.8, 129.4, 129.0, 128. 8, 128.2, 126.6, 125.9, 125.2, 124.3, 123.7, 122.9, 113.6, 111.9, 55.3, 21.7; IR (KBr, cm^{-1}): 2932, 1640, 1526, 1439, 1379, 1180, 1045, 832, 810; MS (EI) (m/z): 392.7 [$(M+1)^{+}$] .

(E)-1-(4-chlorophenyl)-N-(1-(3-methoxyphenyl)naphtho[2,1-b]furan-2-yl)methanimine (**4b**)



Yellow solid, yield, 83%, m.p. 162.5 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (*ppm*): 8.87 (d, *J* = 4.0 Hz, 1 H), 8.06 (d, J = 8.0 Hz, 1 H), 7.91 (d, *J* = 8.0 Hz, 1 H), 7.81-7.76 (m, 3 H), 7.62 (d, *J* = 9.2 Hz, 1 H), 7.49-7.43 (m, 2 H), 7.42-7.35 (m, 3H), 7.28 (d, *J* = 7.6 Hz, 1 H), 7.25-7.24 (m, 1 H), 7.06 (dd, J_1 = 1.2 Hz, J_2 = 8.4 Hz, 1 H), 3.87 (s, 1 H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ (*ppm*): 159.3, 154.0, 149.32, 137.10, 135.0, 134.1, 130.8, 129.9, 129.1, 129.0, 128.9, 128.1, 126.2, 124.6, 123.8, 123.5, 122.7, 118.3, 116.1, 113.9, 111.9, 55.3; IR (KBr, cm^{-1}): 2930, 1603, 1592, 1488, 1460, 1388, 1243, 1037, 834, 797. MS (EI) (m/z): 412.6 [$(M+1)^{+}$].

(E)-1-(3-bromophenyl)-N-(1-(4-bromophenyl)naphtho[2,1-b]furan-2-yl)methanimine (**4c**)

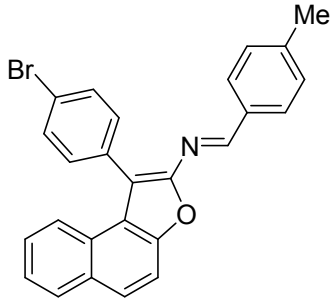


Yellow solid, yield 50%, m.p. 202.3 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (*ppm*): 8.84 (s, 1 H), 8.00-7. 96 (m, 2 H), 7.92 (d, *J* = 8.4 Hz, 1 H), 7.80 (d, *J* = 8.4 Hz, 1 H), 7.74 (d, *J* = 7.2 Hz, 1 H), 7.6 8 (d, *J* = 8.0 Hz, 2 H), 7.62 (d, *J* = 8.8 Hz, 1 H), 7.58-7.54 (m, 3 H), 7.47-7.37 (m, 2 H), 7.30 (dd, *J* = 8.0 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(*ppm*): 154.0, 152.2, 149.5, 138.4, 134.0, 132.6, 131.8, 131.4, 130.9, 130.2, 129. 2, 128.0, 127.6, 127.4, 126.4, 124.7, 123.4, 123.0, 122.3, 122.1, 111.9; IR (KB r, cm^{-1}): 2921, 1642, 1578, 1482, 1379, 1251, 1072, 1035, 853, 802; MS (EI) (m/z): 506.6 [$(M+3)^{+}$].

(E)-N-(1-(4-bromophenyl)naphtho[2,1-b]furan-2-yl)-1-(p-tolyl)methanimine (**4d**)

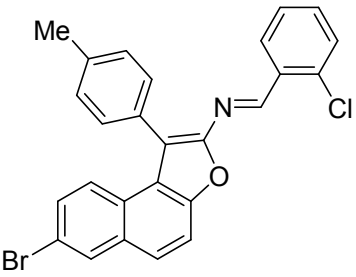
Yellow solid, yield 77%, m.p. 196.8 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (*ppm*):

8.90 (s, 1 H), 8.01 (d, *J* = 8.4 Hz, 1 H), 7.91 (d, *J* = 8.0 Hz, 1 H), 7.77 (d, *J* = 8.8 Hz, 1 H), 7.73 (d, *J* = 8.0 Hz, 2H), 7.69-7.67 (m, 2 H), 7.64-7.58 (



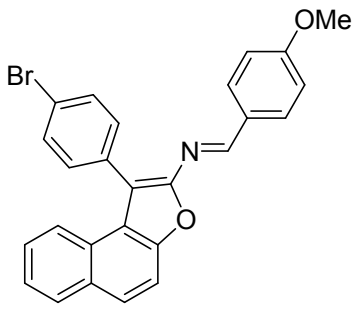
m, 3 H), 7.44 (dd, *J* = 7.6Hz, 1 H), 7.38 (d, *J* = 6.8 Hz, 1 H), 7.22 (d, *J* = 8.0 Hz, 2 H), 2.40 (s, 3 H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ (*ppm*): 156.0, 149. 2, 142.1, 133.9, 132.7, 132.1, 131.3, 130.9, 129.5, 1 29.2, 128.9, 127.9, 126.9, 126.1, 124.5, 123.5, 122.4, 121.7, 111.9, 21.7; IR (KBr, cm^{-1}): 3049, 1589, 156 3, 1486, 1390, 1272, 1193,1069, 803,747; MS (EI) (m/z): 442.6 [$(M+3)^+$]).

(E)-N-(7-bromo-1-(*p*-tolyl)naphtho[2,1-*b*]furan-2-yl)-1-(2-chlorophenyl)methanimine (**4e**)



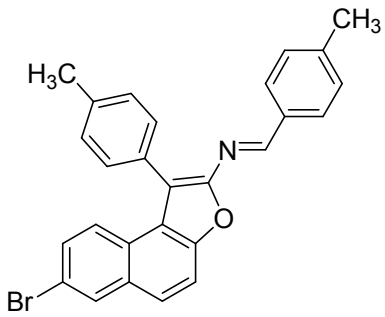
Yellow solid, yield 76%, m.p. 219.9 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (*ppm*): 9.31 (s, 1 H), 8.10 (d, *J* = 7.6 Hz, 1 H), 8.06-8.05 (m, 1H), 7.93 (d, *J* = 8.8 Hz, 1 H), 7.69 (s, 2H), 7.54 (d, *J* = 7.6 Hz, 2 H), 7.44-7.39 (m, 2H), 7.35 (d, *J* = 7.6 Hz, 2 H), 7.31 (d, *J* = 7.6 Hz, 1 H), 7.27 (d, *J* = 7.6 Hz, 1 H), 2.50 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ (*ppm*): 152.8, 151.9, 149.4, 137.6, 136.2, 133.5, 132.1, 131.9, 131.0, 130.7, 129. 9, 129.4, 129.2, 129.0, 128.4, 126.9, 126.6, 126.2, 125.3, 122.9, 118.7, 118.2, 113.1, 21.5; IR (KBr, cm^{-1}): 2921, 1630, 1492, 1395, 1200, 1119, 962, 873, 7 55; MS (EI) (m/z): 476.6 [$(M+3)^+$].

(E)-N-(1-(4-bromophenyl)naphtho[2,1-*b*]furan-2-yl)-1-(4-methoxyphenyl)methanimi ne (**4f**)



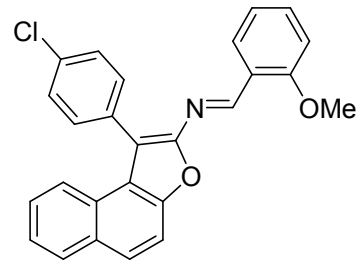
Yellow solid, yield 80%, m.p. 178.8 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (*ppm*): 8.96 (s, 1 H), 8.01 (d, *J* = 8.0 Hz, 1 H), 7.92 (d, *J* = 8.0 Hz, 1 H), 7.80 (dd, *J* = 10.8 Hz, 3 H), 7.67 (dd, J = 8.8 Hz, 3 H), 7.61 (dd, *J* = 7.6 Hz, 3 H), 7.44 (dd, *J* = 7.6 Hz, 1 H), 7.39 (dd, *J* = 7.2 Hz, 1 H), 6.95 (d, *J* = 8.4 Hz, 2 H), 3.87 (s, 3 H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ (*ppm*): 162.4, 155.5, 149.1, 132.7, 132.2 , 131.2, 130.8, 130.7, 129.5,129.1, 127.9, 126.6, 126.1, 124.5, 123.5, 122.4, 12 1.6, 114.3, 111.9, 55.4; IR (KBr, cm^{-1}): 2953, 1630, 1556, 1407, 1379, 1291, 1162, 1042, 824, 775; MS (EI) (m/z): 458.6 [$(M+3)^+$].

(E)-N-(7-bromo-1-(p-tolyl)naphtho[2,1-b]furan-2-yl)-1-(p-tolyl)methanimine (**4g**)
Yellow solid, yield 55%, m.p. 170.1 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (*ppm*): 8.88 (s, 1 H), 8.05 (s, 1 H), 7.95 (d, *J* = 9.2 Hz, 1 H), 7.73 (d, *J* = 8.0 Hz, 2 H), 7.64 (s, 2H), 7.56 (d, *J* = 8.0 Hz, 2 H), 7.40 (dd, J_1 = 8.8 Hz, J_2 = 1.



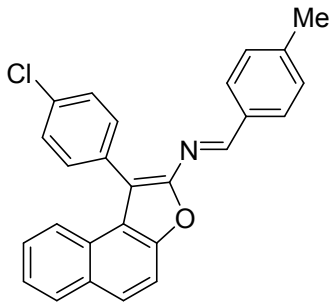
6 Hz, 1H), 7.35 (d, *J* = 8.0 Hz, 2 H), 7.21 (d, *J* = 7.6 Hz, 2 H), 2.52 (s, 3 H), 2.39 (s, 3 H); ^{1} ^{3}C NMR ($CDCl_3$, 100 MHz) δ (*ppm*): 156.0, 153.1 , 149.1, 141.9, 137.5, 133.9,132.1, 130.9, 130.8, 1 30.8, 129.6, 129.5, 129.0, 128.9, 126.6, 125.5, 12 5.4, 123.0, 118.1, 116.9, 113.0, 21.8, 21.5; IR (K Br, cm^{-1}): 2931, 1643, 1500, 1400, 1198, 1119, 8 67, 745; MS (EI) (m/z): 454.0 [$(M+1)^+$].

(E)-N-(1-(4-chlorophenyl)naphtho[2,1-b]furan-2-yl)-1-(2-methoxyphenyl)methanimi ne (**4h**)



Yellow solid, yield 78%, m.p. 203.3 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (*ppm*): 9.37 (s, 1 H), 8.02 (t, *J* = 7.2 Hz, 2 H), 7.91 (d, *J* = 7.6 Hz, 1 H), 7.77 (d, *J* = 8.0 Hz, 1 H), 7.66 (s, 1 H), 7.64 (s, 1 H), 7.52 (s, 1 H), 7.50 (s, 1 H), 7.43 (dd, *J* = 6.8 Hz, 1 H), 7.39-7.35 (m, 2 H), 6.98 (dd, *J* = 7.6 Hz, 1 H), 6.92 (d, *J* = 8.4 Hz, 1 H), 3.95 (s, 3 H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ (*ppm*): 159.7, 153.6, 151.9, 149.2, 133.4, 132.8, 13 2.4, 131.7, 130.8, 129.1, 128.3, 127.9, 127.4, 126.8, 126.1, 125.0, 124.5, 123.5, 122.5, 120.9, 116.0, 112.0, 111.1, 55.6; IR (KBr, cm^{-1}): 2923, 1603, 1521, 141 6, 1390, 1247, 1160, 1037, 813, 773; MS (EI) (m/z): 412.7 [$(M+1)^+$].

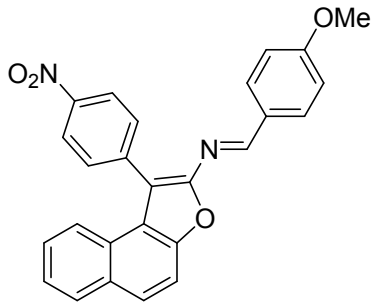
(E)-N-(1-(4-chlorophenyl)naphtho[2,1-b]furan-2-yl)-1-(4-methylphenyl)methanimine (**4i**)



Yellow solid, yield 82%, m.p. 175.7 ^{o}C; ^{1}H NMR (4 00 MHz, $CDCl_3$) δ (*ppm*): 8.91 (s, 1 H), 8.00 (d, *J* = 8.0 Hz, 1 H), 7.91 (d, *J* = 8.0 Hz, 1 H), 7.77 (d, *J* = 8.8 Hz, 1 H), 7.73 (d, *J* = 8.0 Hz, 2 H), 7.66-7.6 3 (m, 3 H), 7.53 (s, 1 H), 7.51 (s, 1 H), 7.44 (dd, *J* = 7.2 Hz, 1 H), 7.41-7.36 (m, 1 H), 7.25-7.22 (m, 2 H), 2.40 (s, 3 H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ (*ppm*): 156.1, 152.9, 149.2, 142.0, 133.9, 133.5, 132.4, 131.6, 130.9, 129.5, 129.2, 128.9, 128.3, 127.9, 126.9, 126.1, 124.5, 123.5, 111.9 , 21.7; IR (KBr, cm^{-1}): 2931, 1621, 1489, 1390, 1149, 1100, 912, 749; MS (E I) (m/z): 396.6 [$(M+1)^+$].

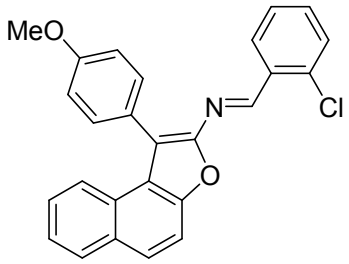
(E)-1-(4-methoxyphenyl)-N-(1-(4-nitrophenyl)naphtho[2,1-b]furan-2-yl)methanimine (**4j**)

Yellow solid, yield 56%, m.p. 201.6 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (*ppm*): 8.93 (s, 1 H), 8.42-8.41 (m, 1 H), 8.40-8.38 (m, 1 H), 7.96 (s, 1 H), 7.94 (s, 1 H), 7.93-7.92 (m, 1 H), 7.91-7.90 (m, 1 H), 7.83-7.79 (m, 3 H), 7.65 (d, *J* = 8.8 Hz, 1 H), 7.48-7.44 (m, 1 H), 7.42-7.38 (m, 1 H), 6.98 (s, 1 H), 6.95



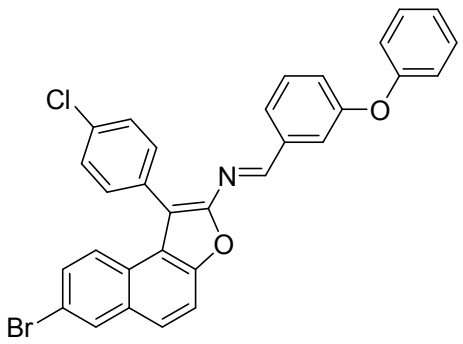
(s, 1 H), 3.87 (s, 3 H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ (*ppm*): 162.8, 156.6, 153.6, 149.3, 147.1, 140.6, 131.9, 130.9, 130.9, 129.4, 129.2, 127.6, 1 27.1, 126.3, 124.7, 123.3, 121.9, 114.4, 111.9, 55. 5; IR (KBr, cm^{-1}): 2949, 1597, 1523, 1448, 1370, 1126, 1091, 823, 737; MS (EI) (m/z): 423.6 [$(M+1)^+$].

(E)-1-(2-chlorophenyl)-N-(1-(4-methoxyphenyl)naphtho[2,1-b]furan-2-yl)methanimi ne (**4k**)



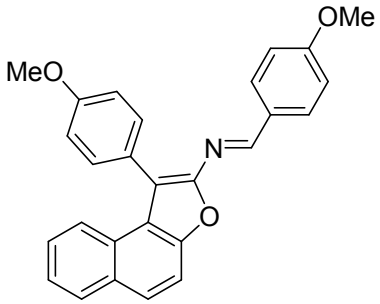
Yellow solid, yield 75%, m.p. 178.3 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (*ppm*): 9.31 (s, 1 H), 8.13 (dd, J_1 = 7.6 Hz, J_2 = 14 Hz, 2 H), 7.91 (d, J = 8.0 H z,1 H), 7.79 (d, J = 8.8 Hz, 1 H), 7.65 (d, J = 8.8 Hz, 1 H), 7.61 (d, J = 8.4 Hz, 2 H), 7.45-7.36 (m, 3 H), 7.35-7.32 (m, 1 H), 7.30-7.27 (m, 1 H), 7.08 (d, J = 8.4 Hz, 2 H), 3.94 (s, 3 H); ^{13}C NMR (CD Cl_3, 100 MHz) δ (*ppm*): 159.3, 152.6, 151.3, 149.5, 136.0, 133.7, 132.1, 131.7, 130.8, 129.9, 129.1, 128.4, 128.3, 127.4, 126.9, 126.1, 125.0, 124.5, 123.6, 122.8 , 118.9, 113.6, 112.1, 55.3; IR (KBr, cm^{-1}): 2963, 1630, 1511, 1406, 1392, 12 52, 1163, 1029, 823, 780; MS (EI) (m/z): 412.6 [$(M+1)^+$].

(E)-N-(7-bromo-1-(4-chlorophenyl)naphtho[2,1-b]furan-2-yl)-1-(3-phenoxyphenyl)m ethanimine (**4l**)



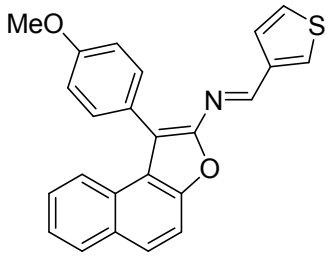
Yellow solid, yield 83%, m.p. 163.3 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (*ppm*): 8.82 (s, 1 H), 8.05 (d, J = 1.6 Hz, 1 H), 7.86 (d, J = 8.8 Hz, 1 H), 7.65 (d, J = 8.8 Hz, 2H), 7.55-7.50 (m, 3 H), 7.46-7.42 (m, 4 H), 7.3 8 (dd, J = 8.0 Hz, 3 H), 7.20 (dd, J = 7.2 Hz, 1 H), 7.11 (dd, J_1 = 8.0 Hz, J_2 = 2.0 Hz, 1 H), 7.03 (d, J = 7.6 Hz, 2 H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ (*ppm*): 158.1, 1 56.3, 155.5, 152.7, 149.3, 138.1, 133.8, 132.1, 132.1, 131.1, 130.9, 130.1, 129. 9, 129.4, 128.5, 126.4, 126.2, 125.1, 124.0, 123.9, 122.4, 121.7, 119.6, 118.4, 117.3, 116.9, 113.0; IR (KBr, cm^{-1}): 3060, 2912, 1580, 1489, 1438, 1349, 124 6,1211, 1089, 857, 785; MS (EI) (m/z): 554.3 [$(M+2)^+$].

(E)-1-(4-methoxyphenyl)-N-(1-(4-methoxyphenyl)naphtho[2,1-b]furan-2-yl)methani mine (**4m**)



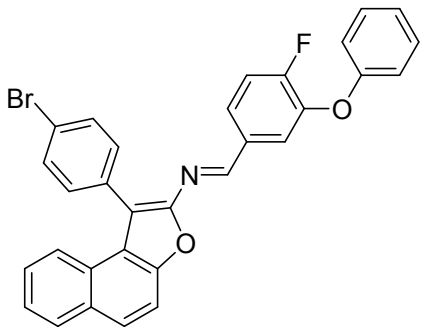
Yellow solid, yield 88%, m.p. 197.3 ^{o}C; ^{1}H NM R (400 MHz, $CDCl_3$) δ(*ppm*): 8.87 (s, 1 H), 8.0 7 (d, *J* = 8.4 Hz, 1 H), 7.90 (d, *J* = 7.6 Hz, 1 H), 7.79 (d, *J* = 8.8 Hz, 2 H), 7.74 (d, *J* = 8.8 Hz,1 H), 7.61 (d, *J* = 8.4 Hz, 3 H), 7.41 (dd, J_1 = 1.2 Hz, J_2 = 7.2 Hz, 1 H), 7.34 (dd, J_1 = 1.2 Hz, J_2 = 8.0 Hz, 1 H), 7.07 (d, *J* = 8.4 Hz, 2H), 6.92 (d, *J* = 8.8 Hz, 2H), 3.94 (s, 3H), 3.85 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ (*ppm*): 162.2, 159.1, 154.8, 152.9, 148.9, 132.2, 130.8, 130.6, 129.7, 129.0, 128.2, 126.4, 125.9, 125.3, 124.3, 123.7, 122.9 , 116.3, 114.2, 113.6, 111.9, 55.4, 55.3; IR (KBr, cm^{-1}): 2943, 1610, 1572, 14 80, 1253, 1176, 1035, 825, 813; MS(EI) (m/z): 408.7 [(M+1)$^{+}$].

(E)-N-(1-(4-methoxyphenyl)naphtho[2,1-b]furan-2-yl)-1-(thiophen-3-yl)methanimine (**4n**)



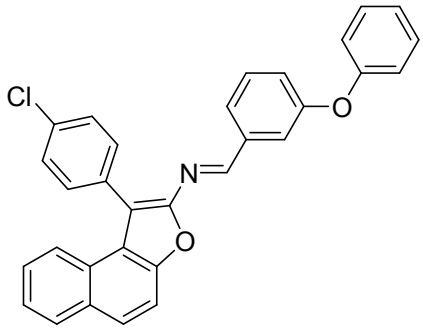
Yellow solid, yield 76%, m.p.150.1 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (*ppm*): 8.92 (s, 1 H), 8.06 (d, *J* = 8.0 Hz, 1 H), 7.89 (d, *J* = 8.0 Hz, 1 H), 7.77-7.75 (m, 2 H), 7.62-7.58 (m, 4 H), 7.42 (dd, *J* = 8.0 Hz, 1 H), 7.35 (dd, *J* = 7.2 Hz, 1 H), 7.31-7.29 (m, 1 H), 7. 06 (d, *J* = 8.4 Hz, 2 H), 3.93 (s, 3 H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ (*ppm*): 159.2, 152.6, 149.5, 149. 1, 141.4, 132.1, 130.8, 129.9, 129.0, 128.2, 126.7, 126.4, 126.1, 125.9, 125.1, 124.4, 123.6, 122.9, 117.1, 113.6, 111.9, 55.3; IR (KBr, cm^{-1}): 2924, 1624, 13 89, 1231, 1159, 1072, 859, 827; MS (EI) (m/z): 384.5[(M+1)$^{+}$] (100%).

(E)-N-(1-(4-bromophenyl)naphtho[2,1-b]furan-2-yl)-1-(4-fluoro-3-phenoxyphenyl)m ethanimine (**4o**)



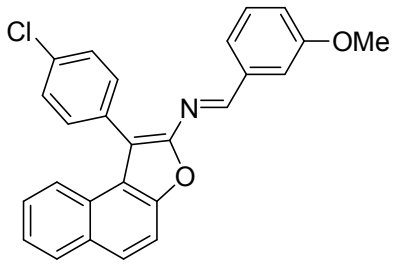
Yellow solid, yield 87%, m.p. 173.5 ^{o}C ^{1}H N MR (400 MHz, $CDCl_3$) δ (*ppm*): 8.78 (s, 1 H), 7.99 (d, *J* = 8.4 Hz, 1 H), 7.90 (d, *J* = 8.0 Hz, 1 H), 7.78 (d, *J* = 8.8 Hz, 1 H), 7.60 (d, *J* = 3.6 Hz, 1 H), 7.58 (d, *J* = 3.2 Hz, 2H), 7.54-7.49 (m, 4H), 7.44 (dd, *J* = 7.6 Hz, 1 H), 7.38 (dd, *J* = 7.6Hz, 3 H), 7.22 (s, 1 H), 7.20 (s, 1 H), 7.03 (d, *J* = 8.0 Hz, 2 H); ^{13}C NM R ($CDCl_3$, 100 MHz) δ (*ppm*): 156.2, 154.5, 1 53.6, 153.6, 152.5 (d, *J* = 243.5 Hz), 151.1, 150.5, 149.9, 147.4, 145.2, 145.1, 133.6, 133.6, 133.7, 132.5, 131.3, 130.8, 129.9, 129.2, 127.9, 127.4, 126.3, 125.3 , 125.2, 124.9 (d, *J* = 7.5 Hz), 123.5, 122.2, 121.8, 119.7 (d, *J* = 6.9 Hz), 11 8.4, 117.4, 117.2 (*J* = 18.9 Hz), 111.9, 77.2; IR (KBr, cm^{-1}): 3049, 2923, 158 4, 1508, 1488, 1366, 1279, 1214, 1068, 801, 741; MS (EI) (m/z): 540.0 [(M+ 1)$^{+}$].

(E)-N-(1-(4-chlorophenyl)naphtho[2,1-b]furan-2-yl)-1-(3-phenoxyphenyl)methanimin e (**4p**)



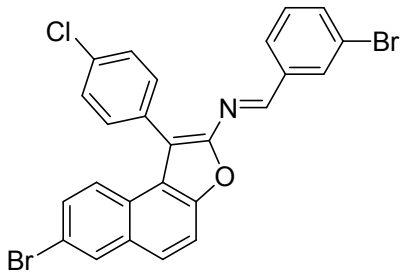
Yellow solid, yield 86%, m.p. 155.0 °C; ^{1}H N MR (400 MHz, $CDCl_3$) δ (*ppm*): 8.85 (d, *J* = 7.2 Hz, 1 H), 8.00 (dd, *J* = 8.8 Hz, 1 H), 7.9 1 (d, *J* = 8.0 Hz, 1 H), 7.81-7.75 (m, 2 H), 7.6 9-7.58 (m, 3 H), 7.52 (d, *J* = 7.6 Hz, 2 H), 7.4 9-7.42 (m, 3 H), 7.38 (dd, *J* = 8.4 Hz, 4 H), 7.19 (dd, *J* = 7.2 Hz, 1 H), 7.08 (d, *J* = 8.0 Hz, 1 H), 7.03 (d, *J* = 8.0 Hz, 1 H); ^{13}CNM R ($CDCl_3$, 100 MHz) δ (*ppm*): 158.1, 156.4, 1 54.9, 154.3, 152.4, 149.4, 149.4, 138.3, 137.3, 134.9, 133.7, 133.6, 132.3, 132. 3, 131.4, 131.3, 131.1, 130.8, 130.8, 130.1, 129.9, 129.9, 129.2, 129.0, 128.8, 128.4, 128.3, 128.0, 127.4, 127.3, 126.3, 126.2, 124.7, 124.6, 123.9, 123.9, 123.5 , 123.4, 122.4, 122.3, 121.5, 119.5, 119.1, 117.3, 111.9; IR (KBr, cm^{-1}): 3055, 2922, 1587, 1486, 1444, 1365, 1245, 1210, 1086, 1005, 802, 742; MS (EI) (m /z): 474.6 [$(M+1)^+$].

(E)-N-(1-(4-chlorophenyl)naphtho[2,1-b]furan-2-yl)-1-(3-methoxyphenyl)methanimi ne (**4q**)



Yellow solid, yield 58%, m.p.185.4 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (*ppm*): 8.88 (s, 1 H), 8.01 (d, *J* = 8.0 Hz, 1 H), 7.91 (d, *J* = 8.0 Hz, 1 H), 7.78 (d, *J* = 9.2 Hz, 1 H), 7.64 (dd, *J* = 8.8 Hz, 3 H), 7.51 (d, *J* = 8.4 Hz, 2H), 7.46-7.38(m, 4 H), 7.34 (dd, *J* = 8.0 Hz, 1 H), 6.98 (d, *J* = 7.6 Hz, 1 H), 3.84 (s, 3 H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ (*ppm*): 159.9, 155.8, 152.6, 149.3, 137.9, 133.6, 132.4, 131.5, 130.9 , 129.7, 129.2, 128.3, 127.9, 127.2, 126.2, 124.6, 123.5, 122.2, 117.7, 112.6, 1 11.9, 55.3; IR (KBr, cm^{-1}): 2933, 1615, 1601, 1492, 1393, 1250, 1035, 840, 7 83; MS (EI) (m/z): 412.6 [$(M+1)^+$].

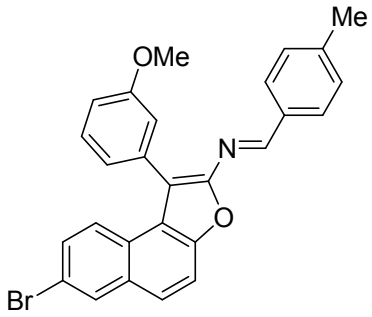
(E)-N-(7-bromo-1-(4-chlorophenyl)naphtho[2,1-b]furan-2-yl)-1-(3-bromophenyl)met hanimine (**4r**)



Yellow solid, yield 54%, m.p. 210.1 °C; ^{1}H NM R (400 MHz, $CDCl_3$) δ (*ppm*): 8.82 (s, 1 H), 8. 07 (s, 1 H), 7.98 (s, 1 H), 7.87-7.84 (m, 2 H), 7.75-7.70 (m, 2 H), 7.64 (d, *J* = 9.2 Hz, 2 H), 7.59 (d, *J* = 7.6 Hz, 1 H), 7.55 (d, *J* = 7.6 Hz, 1 H), 7.50-7.45 (m, 2 H), 7.31 (dd, *J* = 7.6 Hz, 1 H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ (*ppm*):154.7 , 149.8, 138.2, 134.5, 134.3, 133.8, 132.2, 131.5, 131.2, 131.1, 130.3, 129.8, 1 29.6, 129.4, 127.6, 126.5, 126.3, 125.1, 123.1, 122.3, 118.5, 113.2; IR (KBr, c m^{-1}): 2930, 1647, 1546, 1489, 1400, 1256, 1246, 857, 820; MS (EI) (m/z):538.

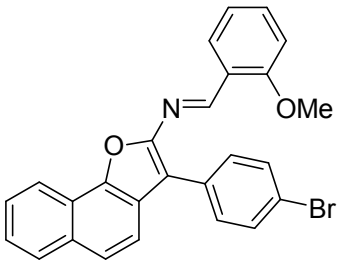
9 [(M+2)$^+$].

(E)-N-(7-bromo-1-(3-methoxyphenyl)naphtho[2,1-b]furan-2-yl)-1-(p-tolyl)methanimine (**4s**)



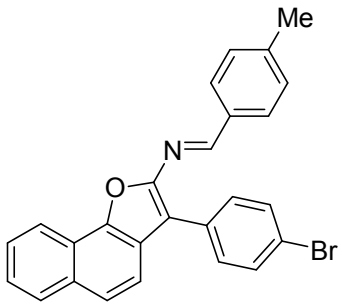
Yellow solid, yield 65%, m.p. 176.1 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (*ppm*): 8.89 (s, 1 H), 8.03 (d, *J* = 1.6 Hz, 1 H), 7.71 (d, *J* = 8.0 Hz, 2 H), 7.65 (s, 2 H), 7.58 (d, *J* = 9.2 Hz, 1 H), 7.54-7.49 (m, 2 H), 7.38-7.36 (m, 1 H), 7.19 (d, *J* = 8.0 Hz, 2 H), 7.15 (d, *J* = 7.2 Hz, 1 H), 7.07 (d, *J* = 8.0 Hz, 1 H), 3.67 (s, 3 H), 2.34 (s, 3 H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ (*ppm*): 157.8, 156.1, 153.3, 148.9, 141.9, 133.9, 133.3, 131.9, 130.5, 129.6, 129.4, 129.0, 128.8, 127.1, 125.5, 125.2, 123.9, 121.8, 120.5, 117.9, 113.4, 113.1, 110.8, 55.2, 22.2; IR (KBr, cm^{-1}): 2945, 1640, 1532, 1458, 1398, 1254, 1267, 857, 827; MS (EI) (m/z): 471.1[(M+1)$^+$]

(E)-N-(3-(4-bromophenyl)naphtho[1,2-b]furan-2-yl)-1-(2-methoxyphenyl)methanimine (**4t**)



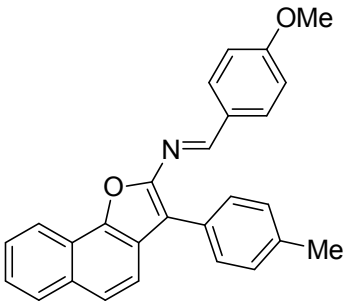
Yellow solid, yield 38%, m.p. 230.0 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (*ppm*): 9.50 (s, 1 H), 8.40 (d, *J* = 8.0 Hz, 1 H), 8.91 (dd, J_1 = 1.2 Hz, J_2 = 7.6 Hz, 1 H), 7.92 (d, *J* = 8.0 Hz, 1 H), 7.83 (dd, *J* = 8.4 Hz, 3 H), 7.71-7.65 (m, 3 H), 7.61 (dd, *J* = 7.6 Hz, 1 H), 7.51 (dd, *J* = 8.4 Hz, 1 H), 7.45 (d d, J_1 = 1.6 Hz, J_2 = 8.8 Hz, 1 H), 7.04 (dd, *J* = 7.6 Hz, 1 H), 6.97 (d, *J* = 8.0 Hz, 1 H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ (*ppm*): 159.8, 152.0, 147.2, 132.9, 132.1, 131.6, 131.5, 131.2, 130.9, 128.5, 127.5, 126.5, 125.5, 125.1, 123.7, 123.7, 121.2, 121.1, 120.9, 120.4, 118.5, 111.5, 102.7, 55.7; IR (KBr, cm^{-1}): 2931, 1642, 1562, 1433, 1380, 1299, 1179, 1062, 857, 773; MS (EI) (m/z): 458.7 [(M+2)$^+$].

(E)-N-(3-(4-bromophenyl)naphtho[1,2-b]furan-2-yl)-1-(p-tolyl)methanimine (**4u**)



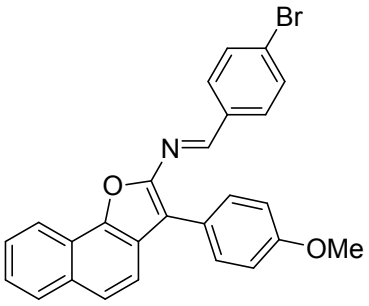
Yellow solid, yield 45%, m.p. 202.9 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (*ppm*): 9.06 (s, 1 H), 8.36 (d, *J* = 7.6 Hz, 1 H), 7.92 (d, *J* = 8.4 Hz, 1 H), 7.86 (s, 1 H), 7.84-7.79 (m, 5 H), 7.71 (s, 1 H), 7.68 (dd, *J* = 2.8 Hz, 1 H), 7.65 (dd, *J* = 2.8 Hz, 1 H), 7.63-7.59 (m, 1 H), 7.55-7.47 (m, 1H), 7.28 (d, *J* = 8.0 Hz, 2 H), 2.43 (s, 3 H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ (*ppm*): 156.2, 152.1, 147.1, 142.2, 134.0, 132.1, 131.6, 131.4, 131.2, 129.6, 129.0, 128.5, 126.5, 125.6, 123.8, 123.7, 121.3, 121.0, 120.2, 118.5, 114.6, 21.7; IR (KBr, cm^{-1}): 2928, 1590, 1490, 1394, 1275, 1200, 1171, 820, 779; MS (EI) (m/z): 440.6 [(M+1)$^+$].

(E)-1-(4-methoxyphenyl)-N-(3-(p-tolyl)naphtho[1,2-b]furan-2-yl)methanimine (**4v**)



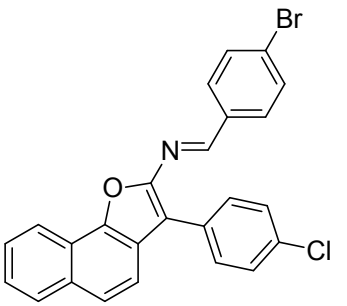
Yellow solid, yield 55%, m.p. 152.1 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ(*ppm*): 9.03 (s, 1 H), 8.36 (d, *J* = 8.4 Hz, 1 H), 7.91 (d, *J* = 8.8 Hz, 3 H), 7.86(d d, *J* = 8.4 Hz, 3 H), 7.69 (d, *J* = 8.4 Hz, 1 H), 7. 60 (dd, *J* = 7.2 Hz, 1 H), 7.49 (dd, *J* = 7.2 Hz, 1 H), 6.98 (d, *J* = 8.8 Hz, 2 H), 3.88 (s, 3 H), 2.45 (s, 3 H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ (*ppm*): 16 2.3, 154.8, 152.1, 146.9, 136.9, 132.0, 130.7, 129.8, 129.5, 129.2, 128.4, 126.3, 125.3, 124.3, 123.4, 121.1, 120.2, 119.0, 115.0, 114.3 , 110.0, 55.4, 21.3; IR (KBr, cm^{-1}): 2936, 1652, 1539, 1460, 1389, 1200, 1100, 846, 829; MS (EI) (m/z): 392.7 [(M+1)$^{+}$].

(E)-1-(4-bromophenyl)-N-(3-(4-methoxyphenyl)naphtho[1,2-b]furan-2-yl)methanimi ne (**4w**)



Yellow solid, yield 50%, m.p. 218.3 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (*ppm*): 8.99 (s, 1 H), 8.35 (d, *J* = 8.0 Hz, 1 H), 7.92 (d, *J* = 8.0 Hz, 1 H), 7.87 (d, *J* = 8.4 Hz, 1 H), 7.86 (d, *J* = 8.4 Hz, 2 H), 7.80 (d, *J* = 8.4 Hz, 2 H), 7.68 (d, *J* = 8.8 Hz, 1 H), 7.63-7.59 (m, 3H), 7.51 (dd, *J* = 8.0 H z, 1 H), 7.09 (d, *J* = 8.8 Hz, 2 H), 3.91 (s, 3 H); ^{13}C NMR (DMSO-d_6, 100 MHz) δ (*ppm*): 159.3, 1 55.3, 151.2, 146.9, 135.9, 132.6, 132.3, 131.0, 130.9, 129.1, 127.4, 126.5, 125. 6, 124.5, 124.0, 123.9, 120.7, 120.4, 119.2, 116.2, 114.7, 55.7; IR (KBr, cm^{-1}): 2921, 1645, 1550, 1416, 1382, 1290, 1178, 1100, 827, 778; MS (EI) (m/z): 45 8.6 [(M+2)$^{+}$].

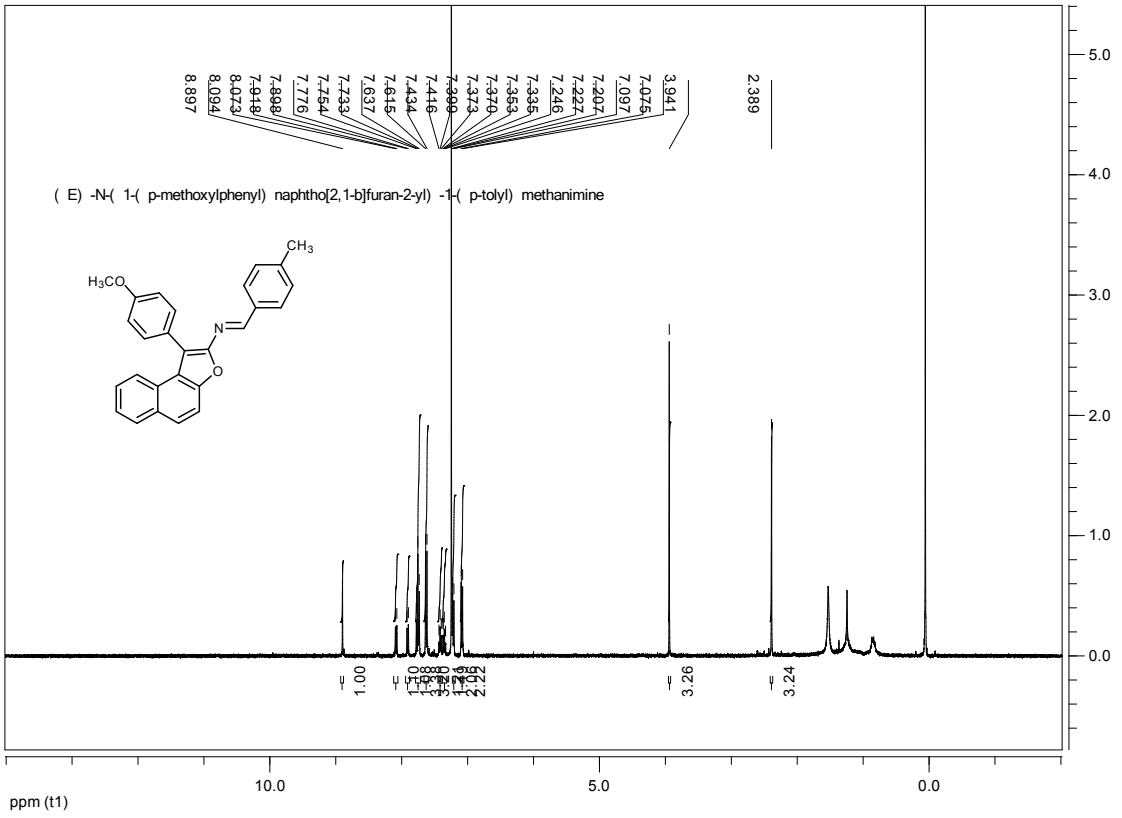
(E)-1-(4-bromophenyl)-N-(3-(4-chlorophenyl)naphtho[1,2-b]furan-2-yl)methanimine (**4x**)

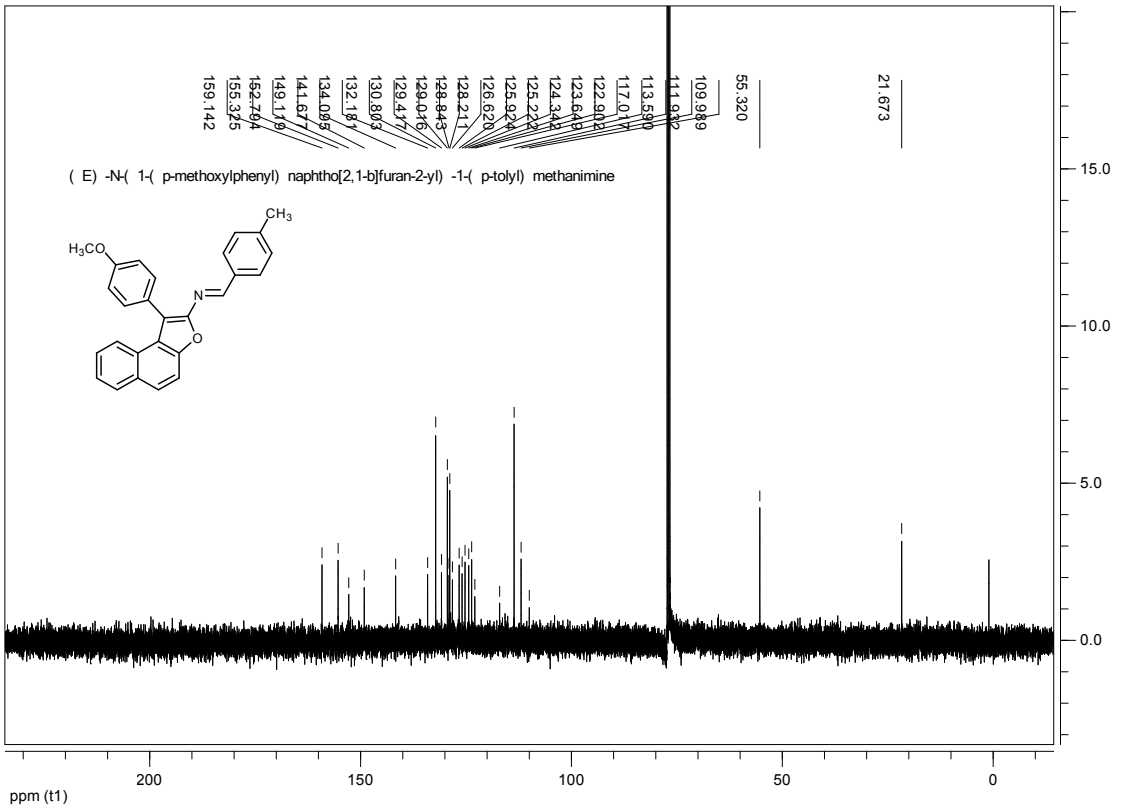


Yellow solid, yield 44%, m.p. 209.3 ^{o}C; ^{1}H NMR (4 00 MHz, $CDCl_3$) δ (*ppm*): 9.04 (s, 1 H), 8.36 (d, *J* = 8.0 Hz, 1 H), 7.94 (d, *J* = 8.4 Hz, 1 H), 7.88 (d, *J* = 8.4 Hz, 2 H), 7.81 (d, *J* = 8.0 Hz, 2 H), 7.71 (d, *J* = 8.4 Hz, 1 H), 7.70 (d, *J* = 8.4 Hz, 2 H), 7. 63 (d, *J* = 7.2 Hz, 1 H), 7.55 (d, *J* = 7.2 Hz, 1 H), 7.54 (d, *J* = 7.2 Hz, 1 H), 7.45 (d, *J* = 8.4 Hz, 2 H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ (*ppm*): 154.4, 15 1.6, 137.4, 134.9, 132.3, 131.7, 131.2, 131.1, 130.0, 129.2, 128.9, 126.6, 125.8, 123.9, 123.6, 121.5, 120.9, 120.2, 118.5, 115.8; IR (KBr, cm^{-1}): 2925, 1645, 1 500, 1419, 1256, 1200, 967, 879, 768; MS (EI) (m/z): 461.0 [(M+2)$^{+}$].

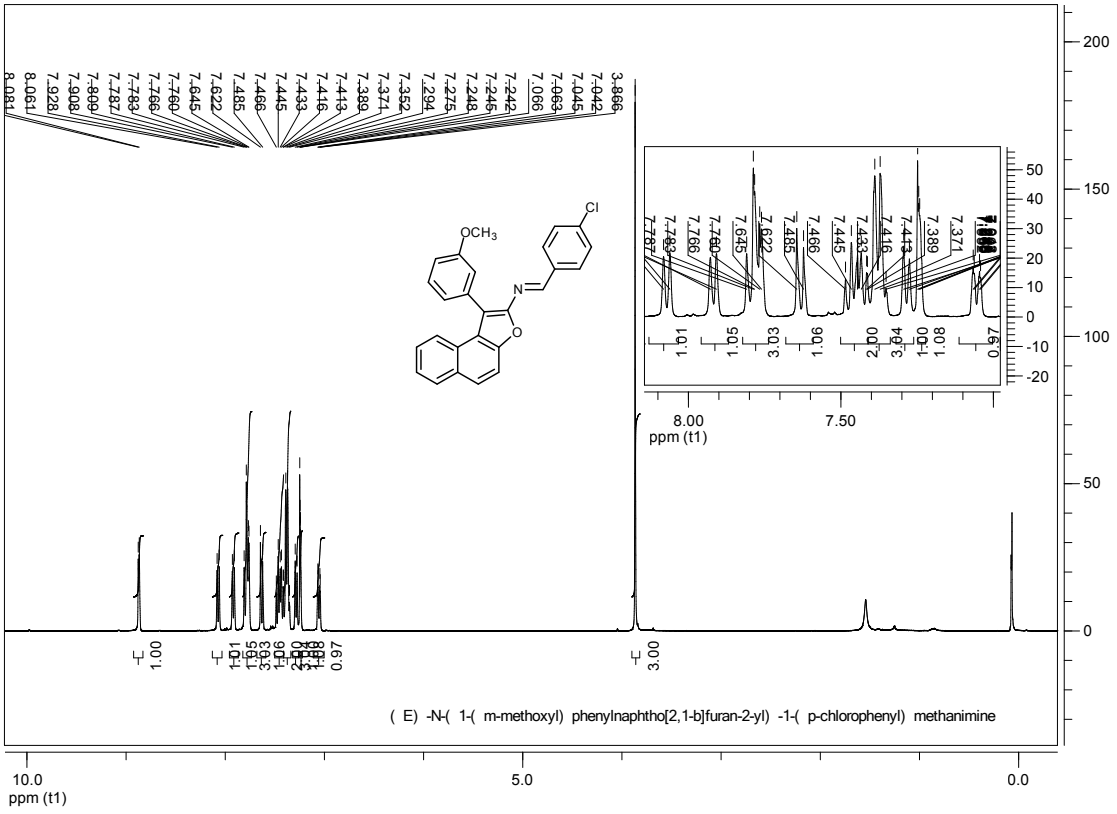
Copies of NMR Spectroscopies

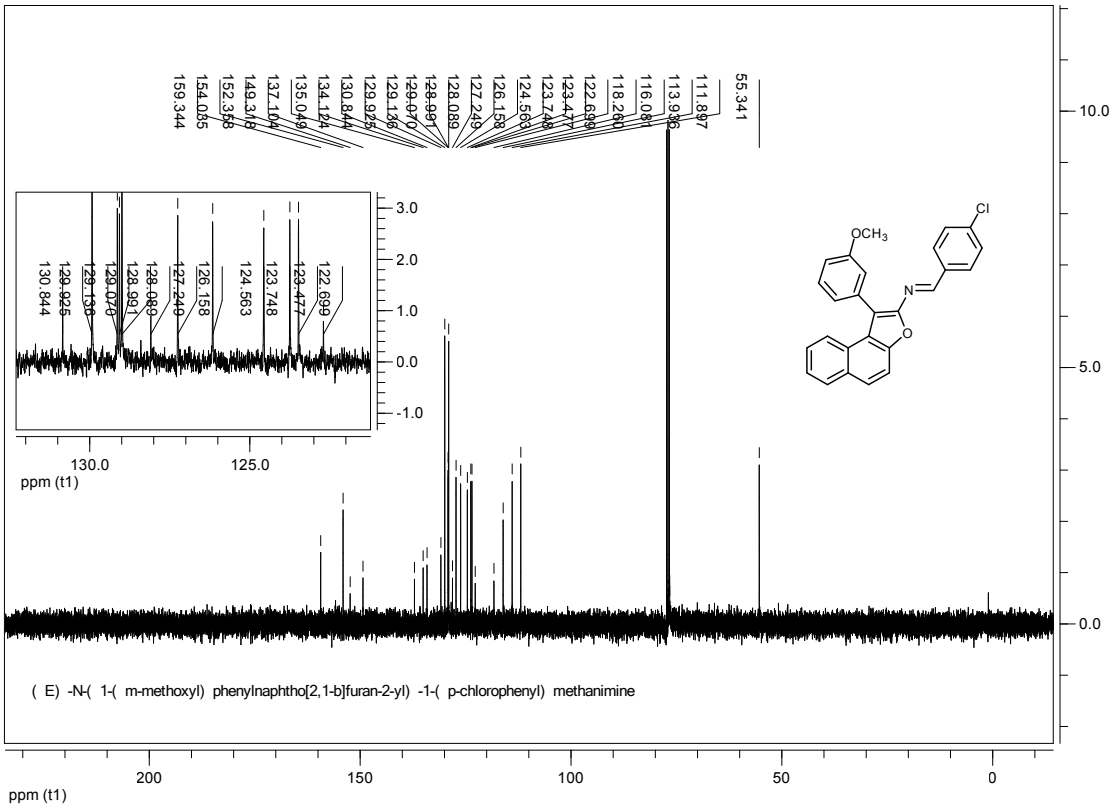
(E)-N-(1-(p-methoxylphenyl)naphtho[2,1-b]furan-2-yl)-1-(p-tolyl)methanimine (**4a**)



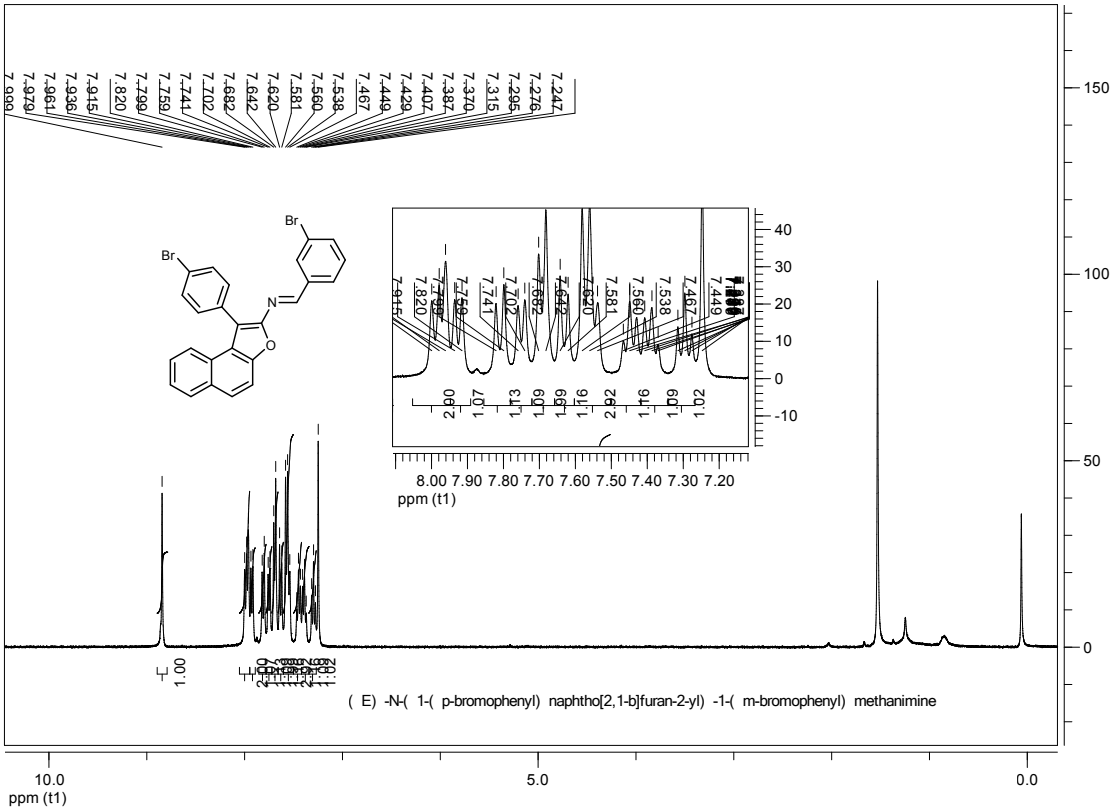


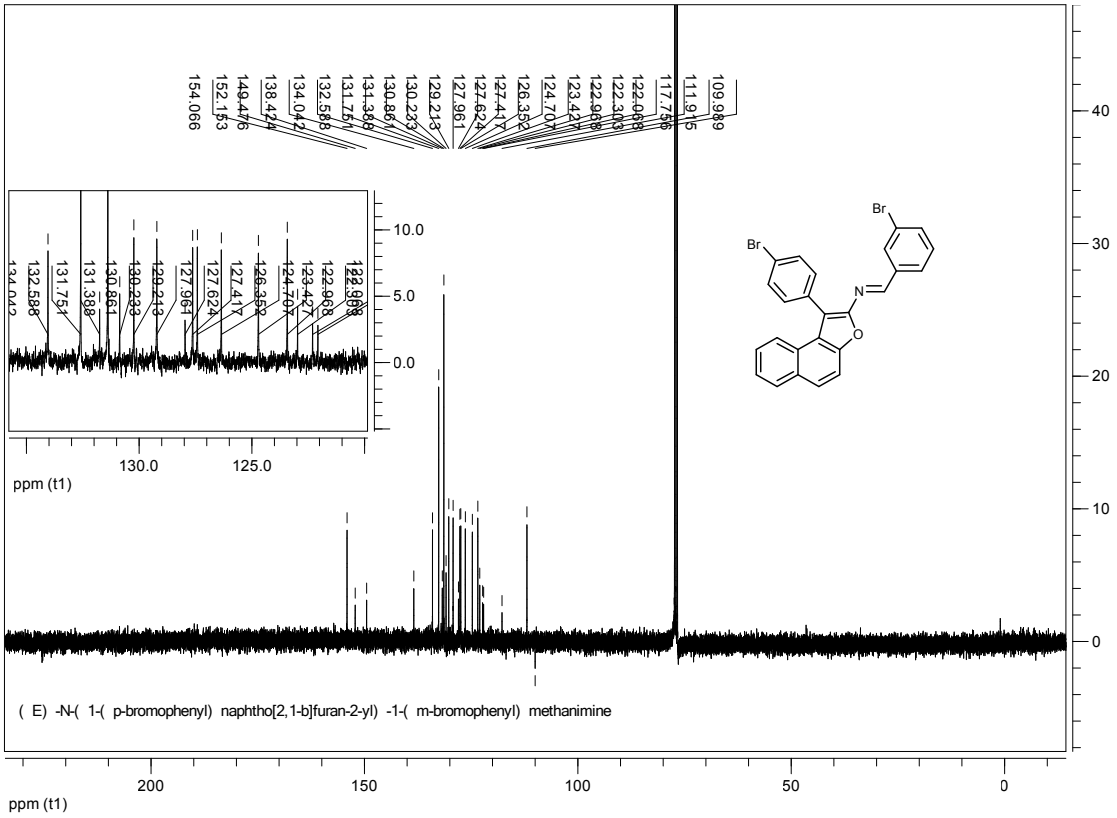
(E)-1-(4-chlorophenyl)-N-(1-(3-methoxyphenyl)naphtho[2,1-b]furan-2-yl)methanimine (**4b**)



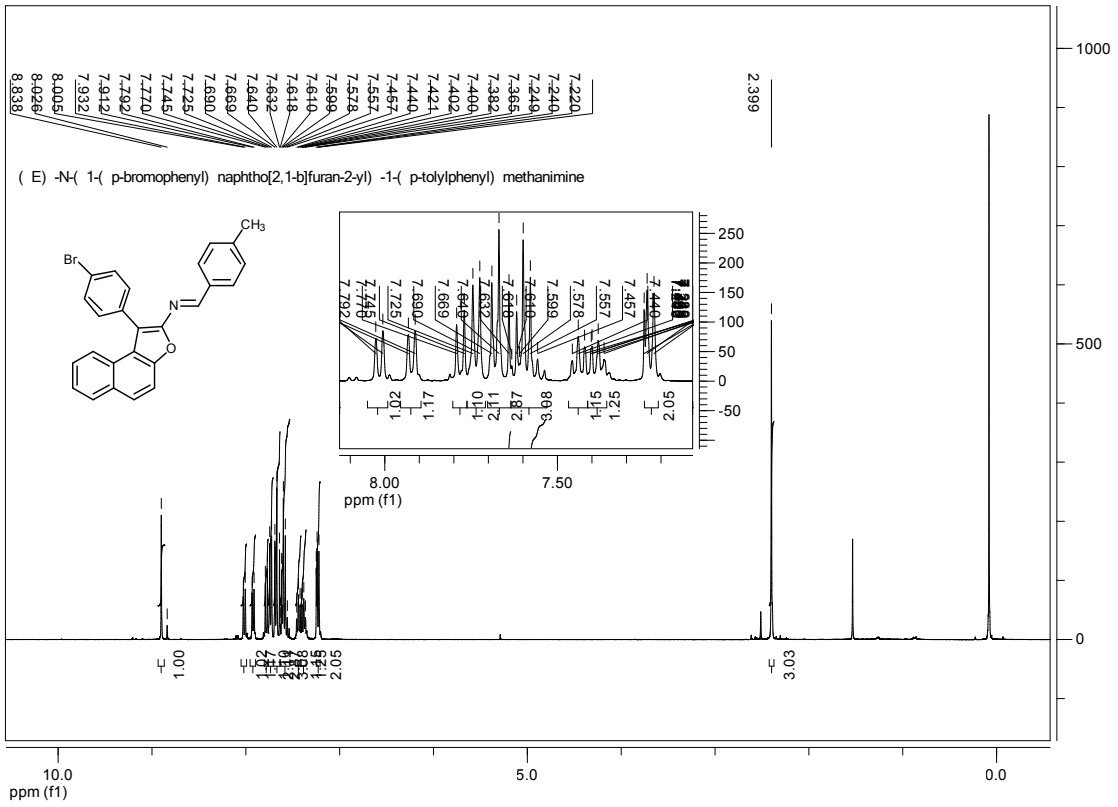


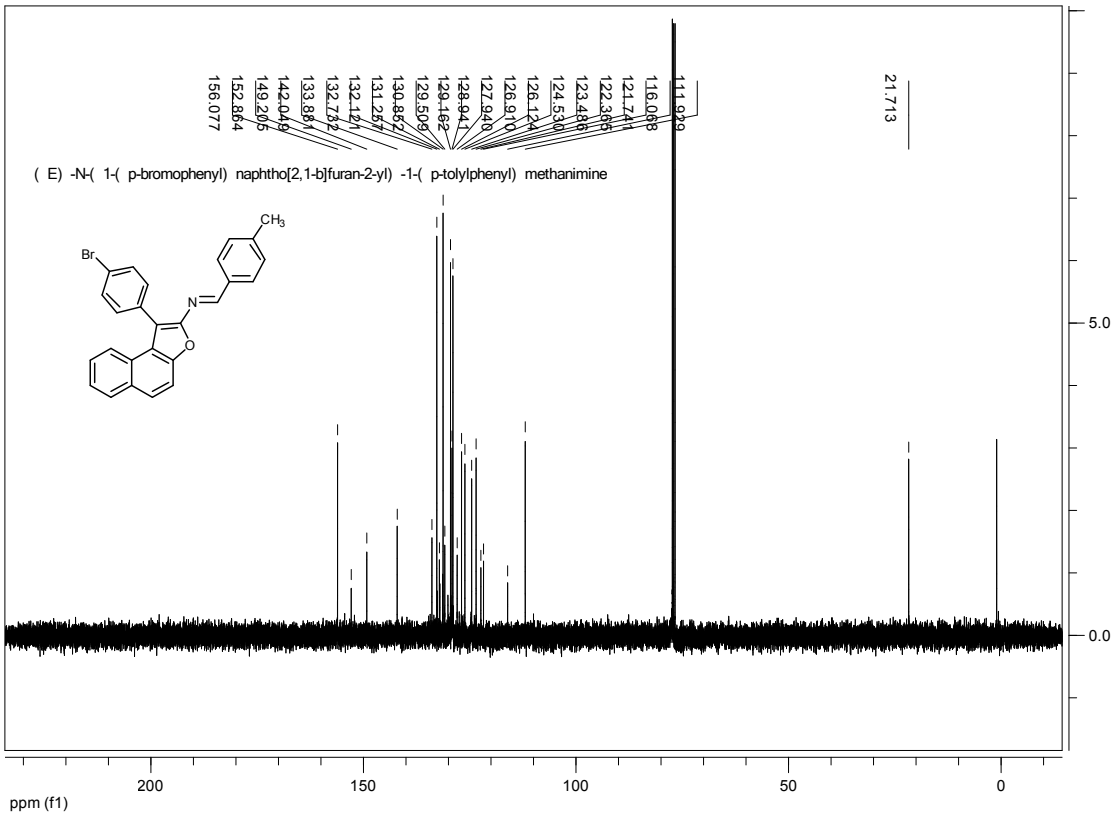
(E)-1-(3-bromophenyl)-N-(1-(4-bromophenyl)naphtho[2,1-b]furan-2-yl)methanimine (**4c**)



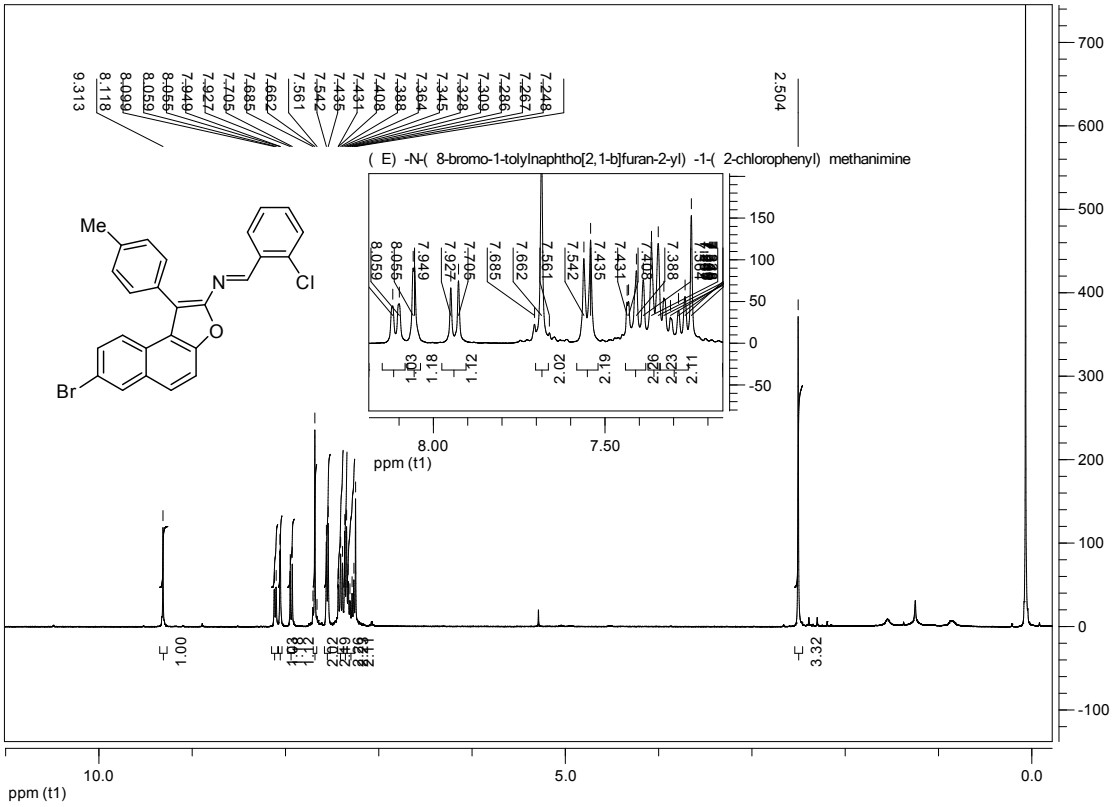


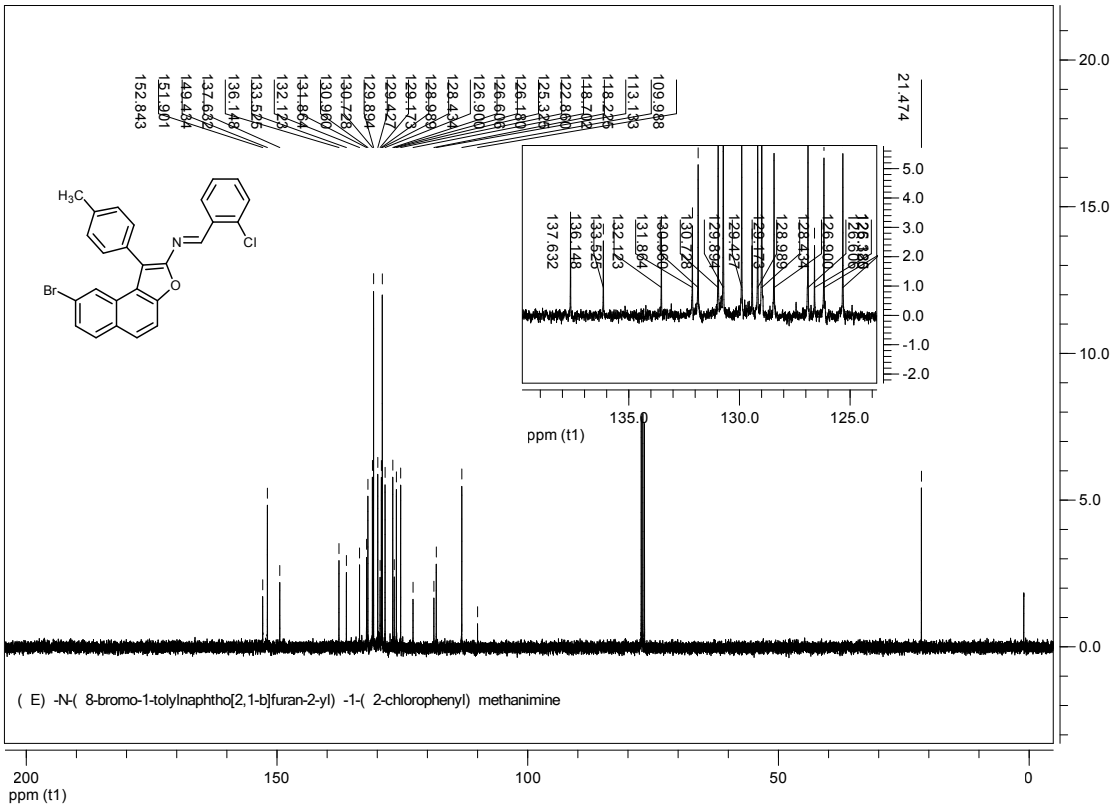
(E)-N-(1-(p-bromophenyl)naphtho[2,1-b]furan-2-yl)-1-(p-tolyl)methanimine (**4d**)



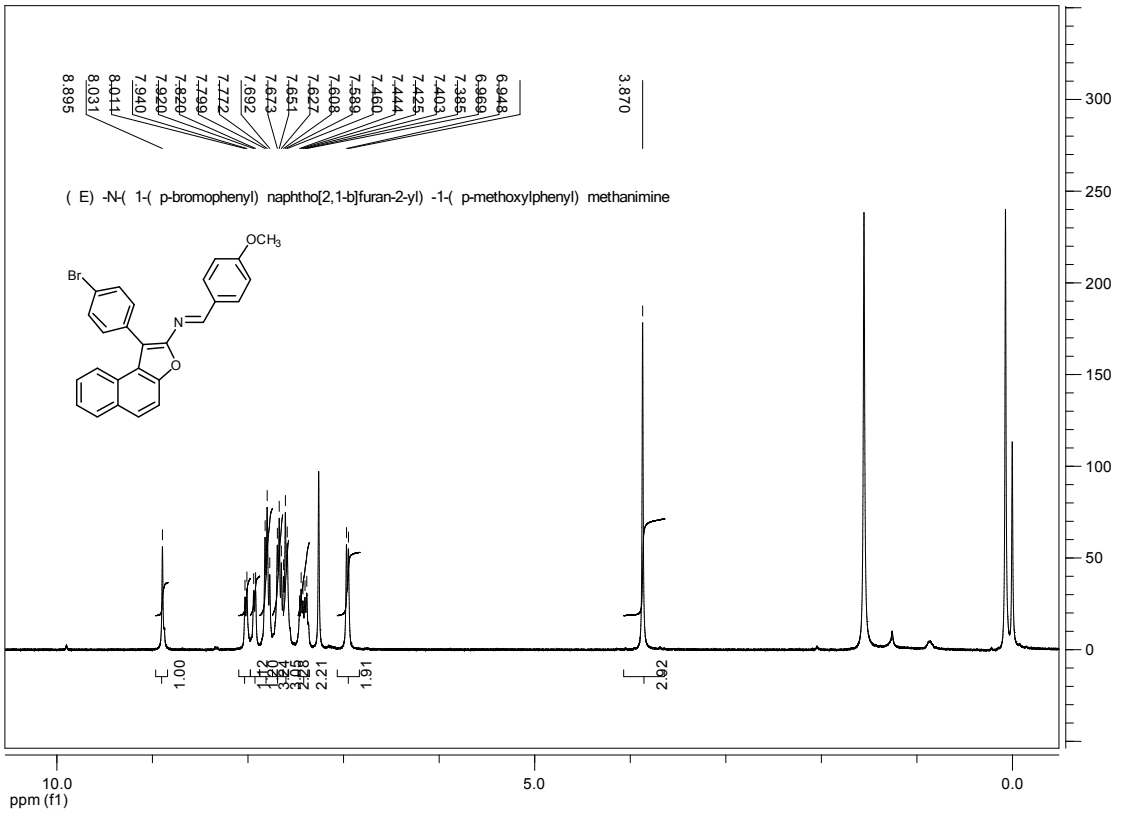


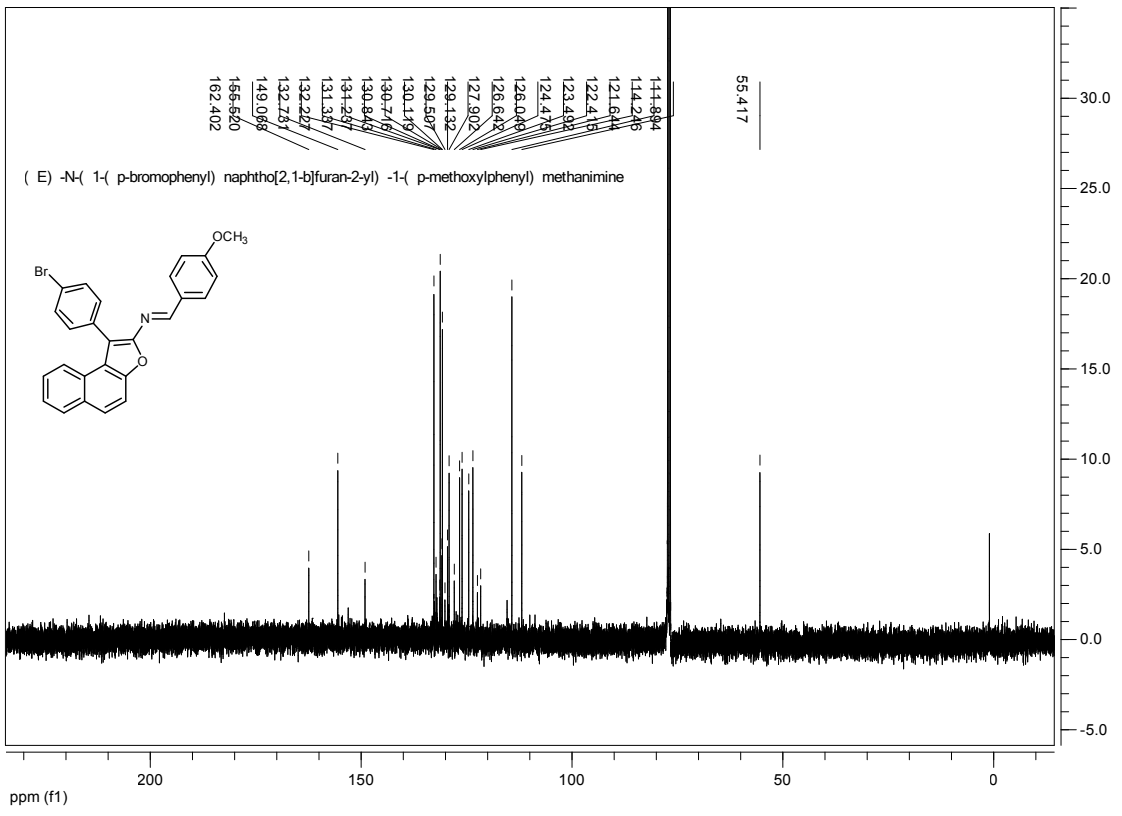
(E)-N-(7-bromo-1-(*p*-tolyl)naphtho[2,1-*b*]furan-2-yl)-1-(2-chlorophenyl)methanimine (**4e**)



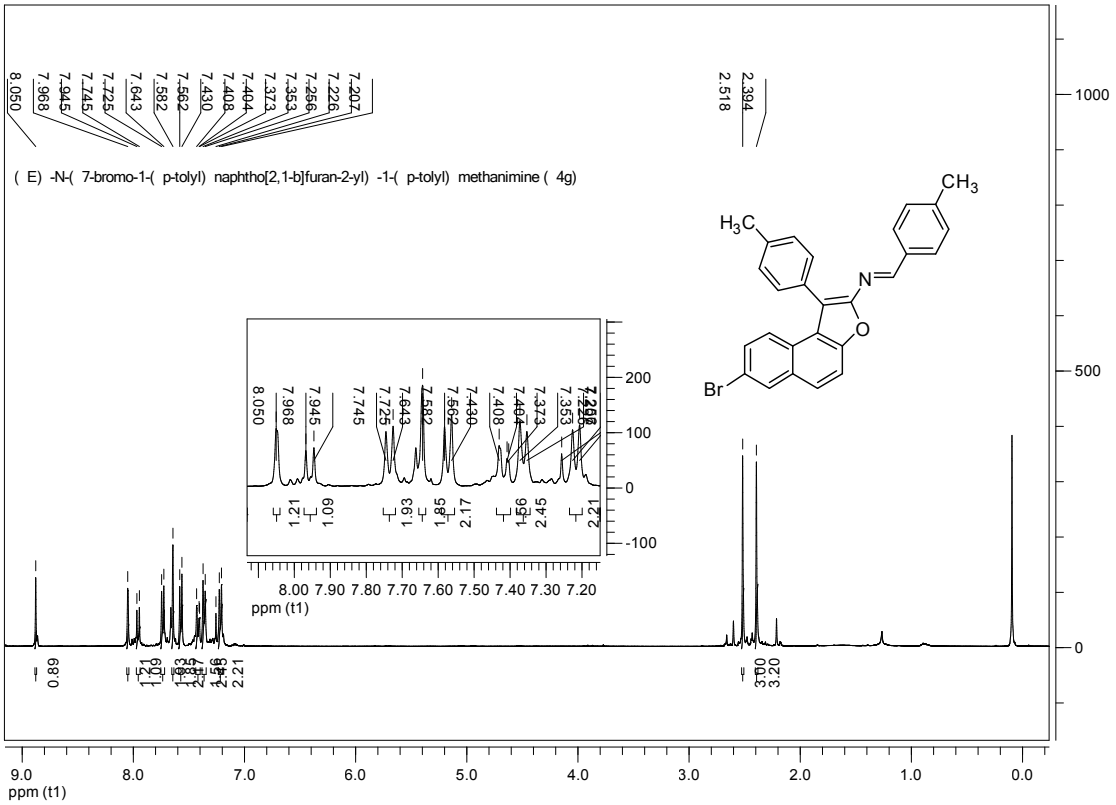


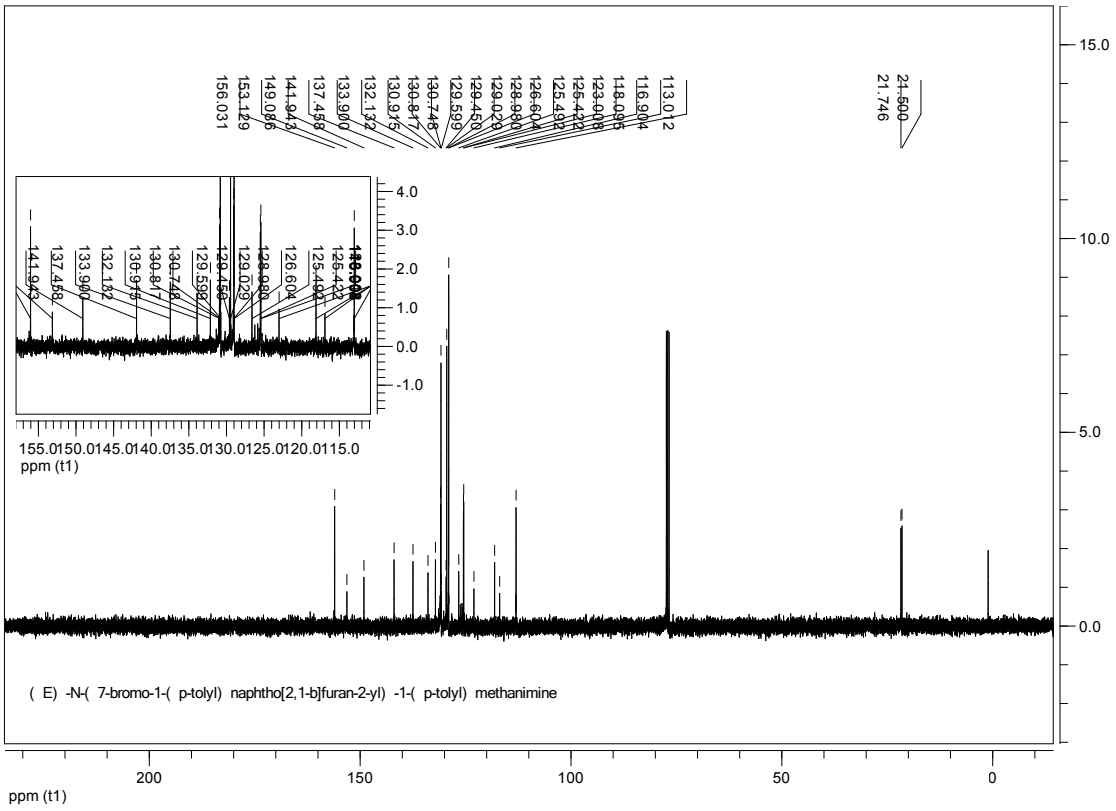
(E)-N-(1-(p-bromophenyl)naphtho[2,1-b]furan-2-yl)-1-(p-methoxylphenyl)methanimine (**4f**)



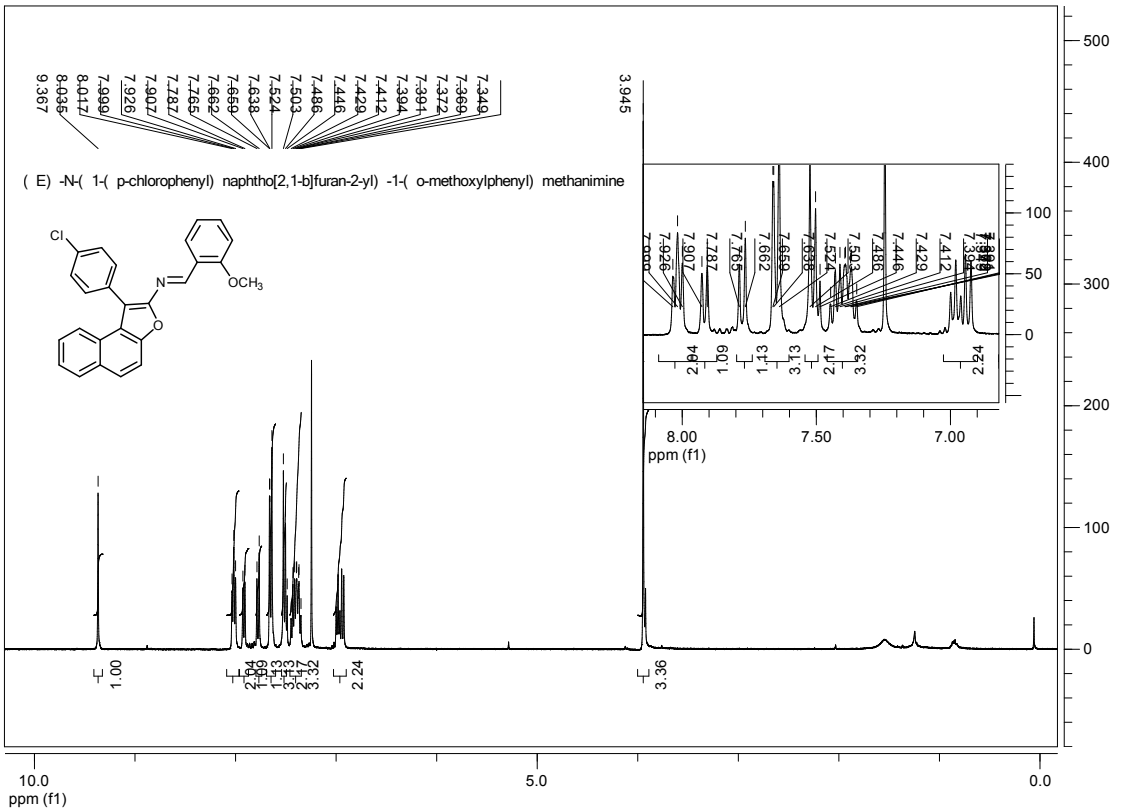


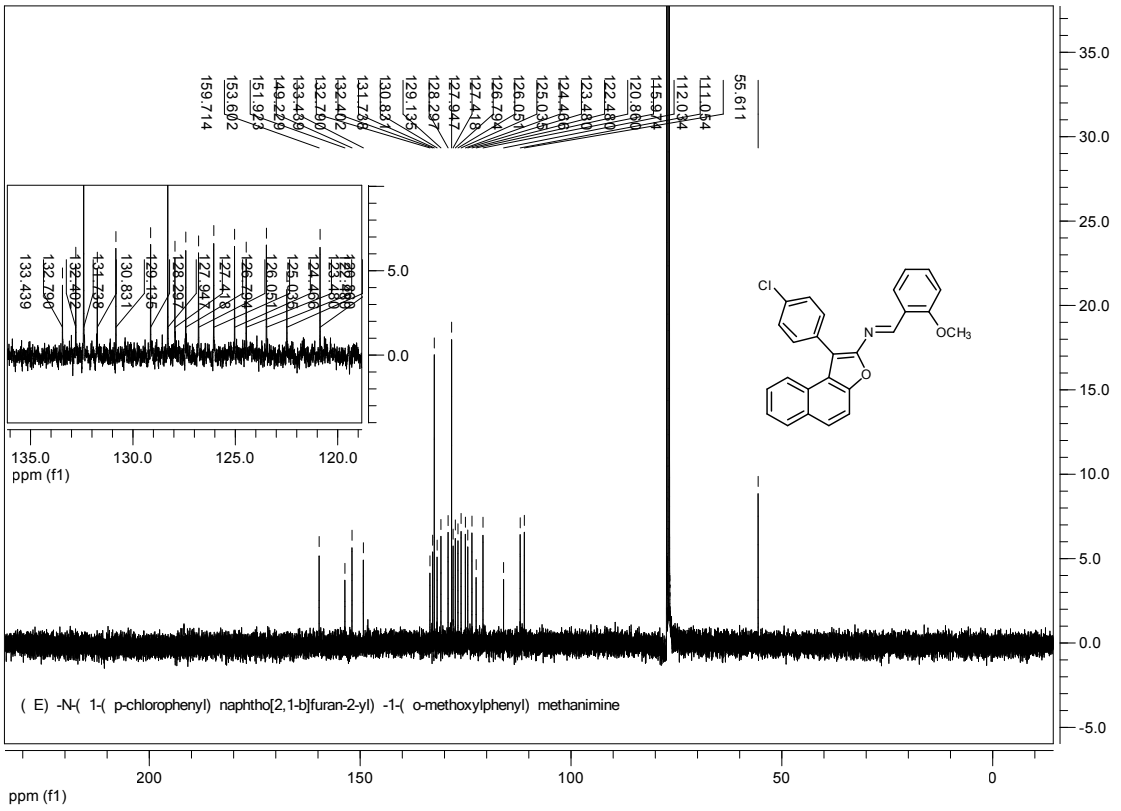
(E)-N-(7-bromo-1-(p-tolyl)naphtho[2,1-b]furan-2-yl)-1-(p-tolyl)methanimine (**4g**)



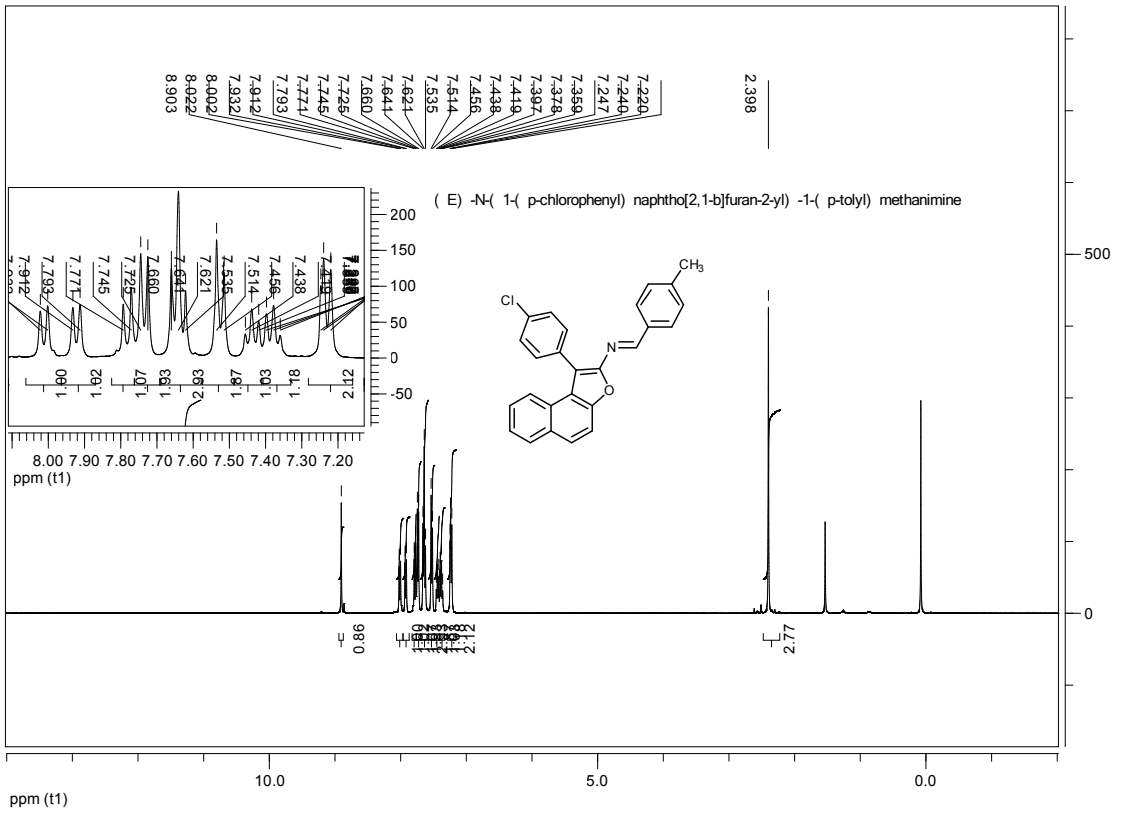


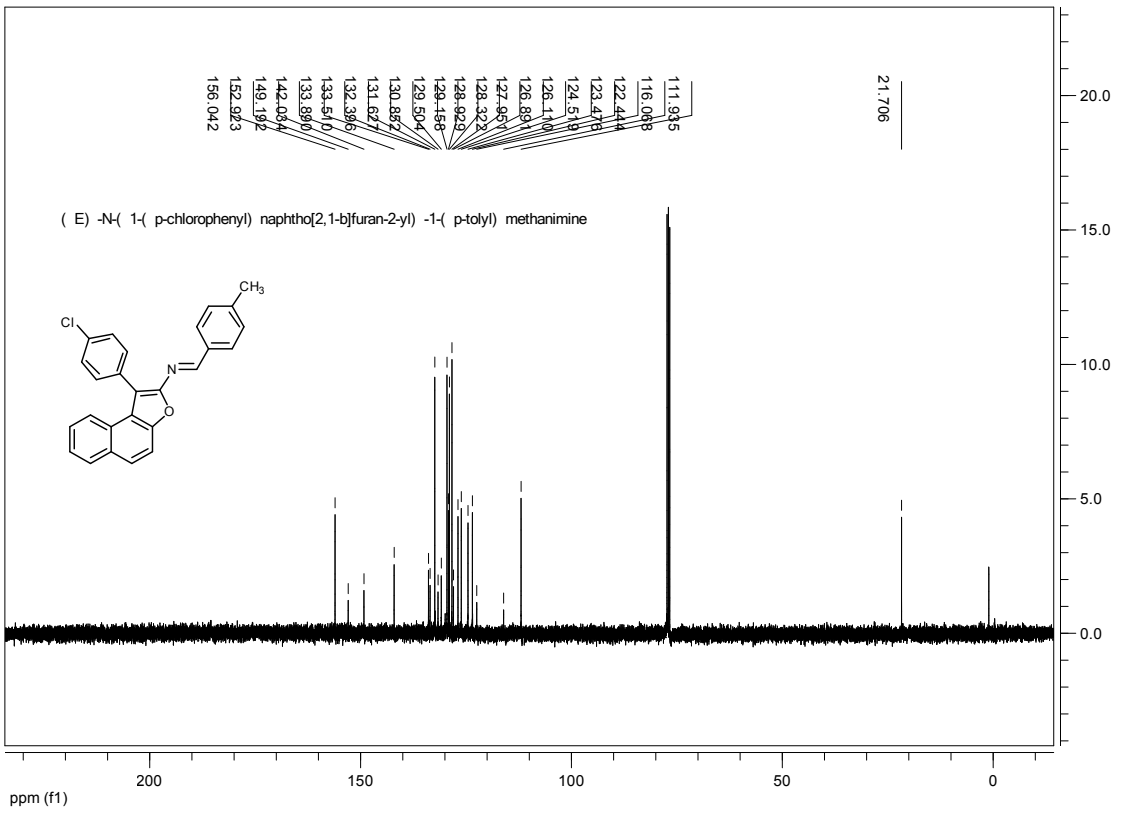
(E)-N-(1-(p-chlorophenyl)naphtho[2,1-b]furan-2-yl)-1-(o-methoxylphenyl)methanimine (**4h**)



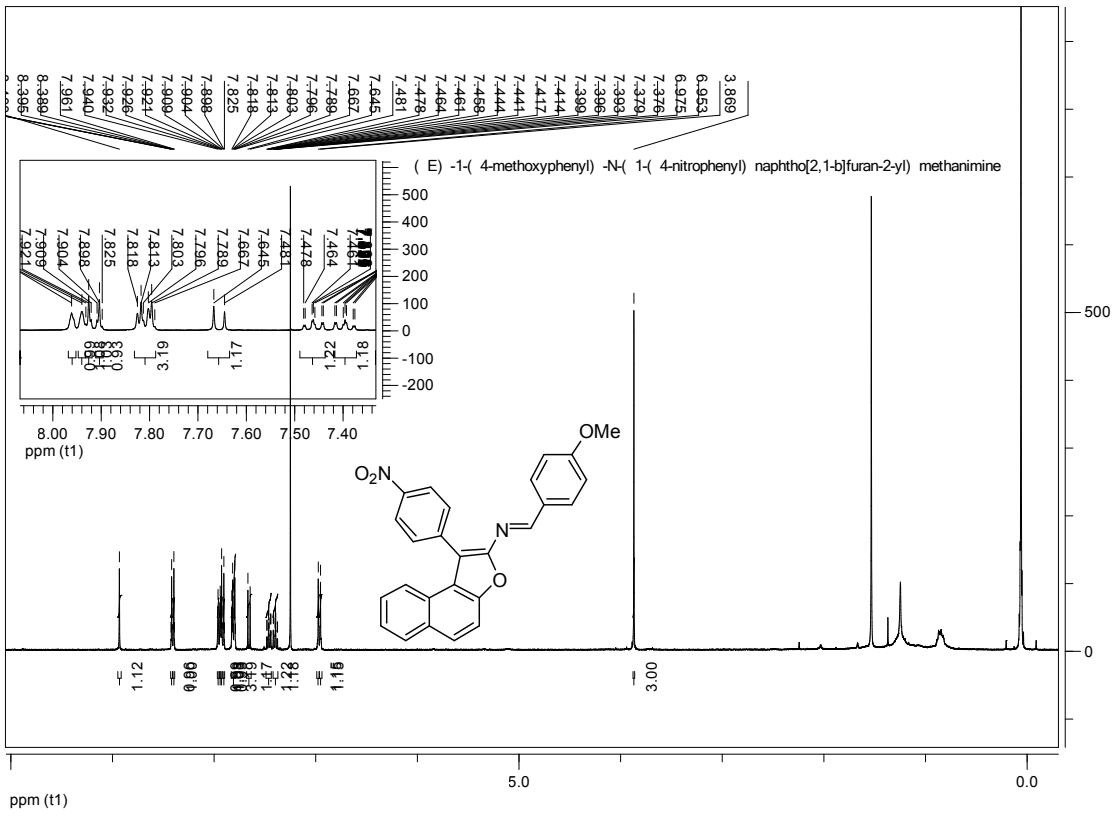


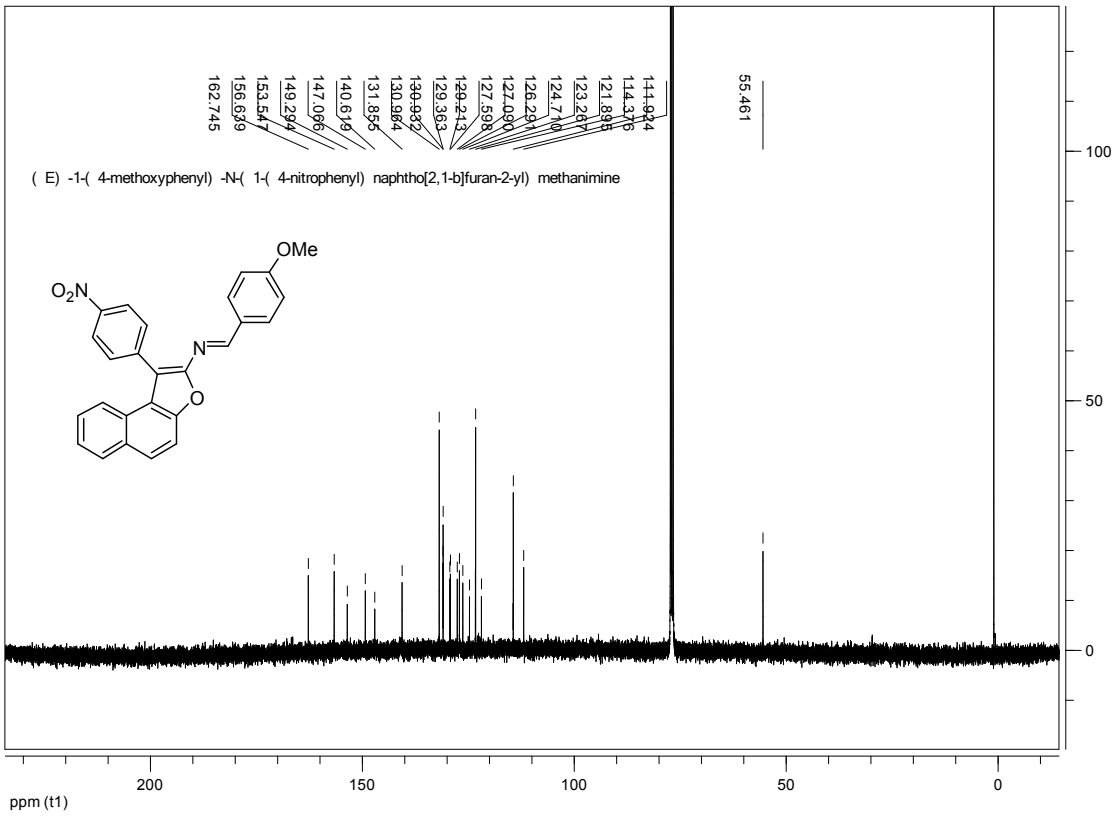
(E)-N-(1-(p-chlorophenyl)naphtho[2,1-b]furan-2-yl)-1-(p-tolyl)methanimine (**4i**)



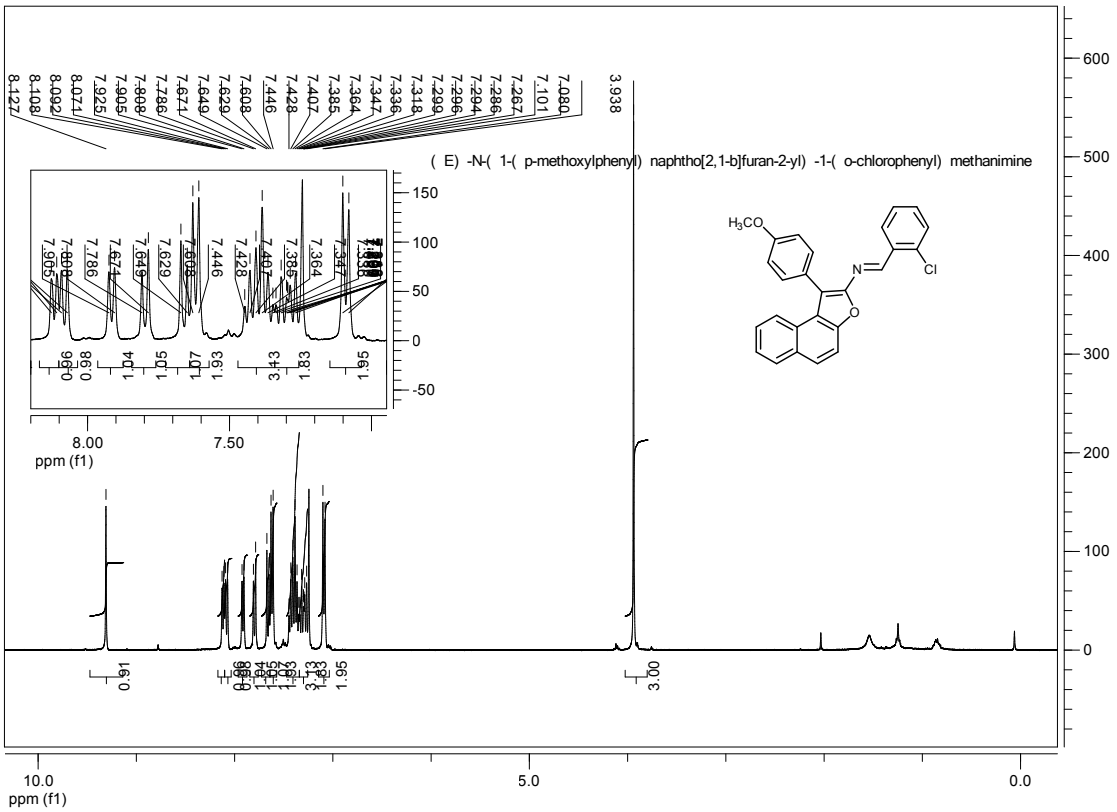


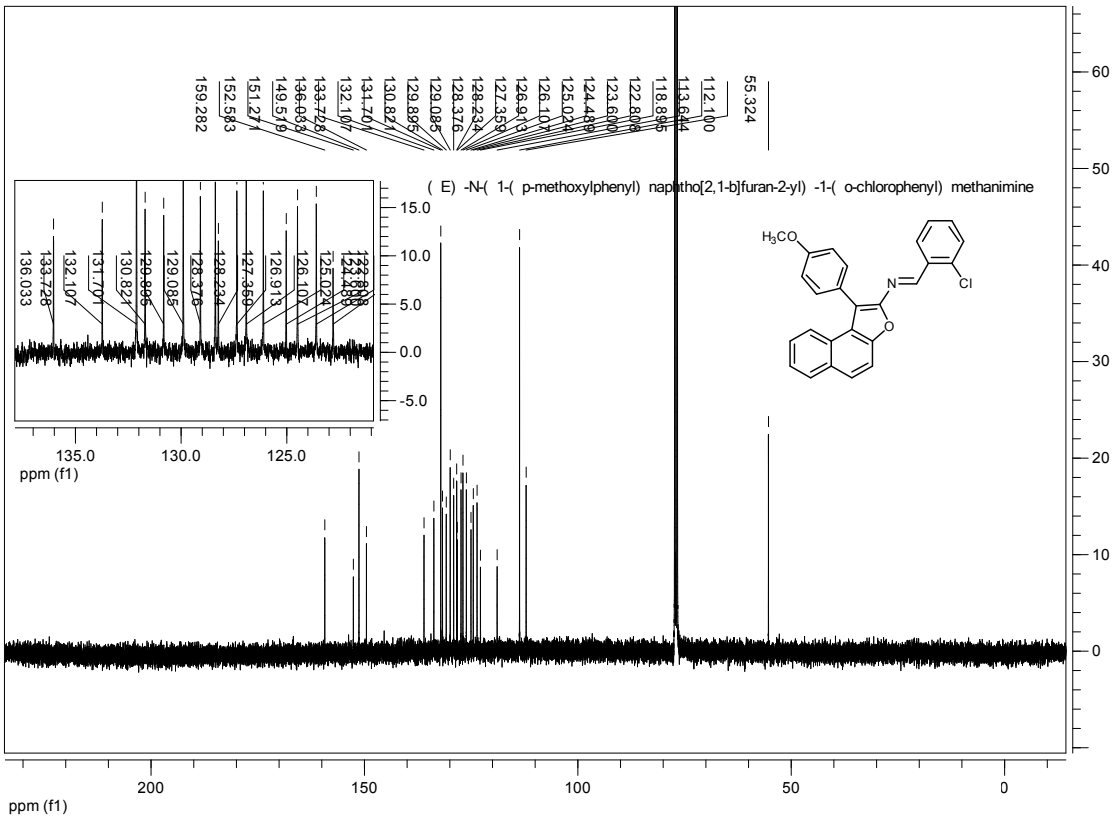
(E)-1-(4-methoxyphenyl)-N-(1-(4-nitrophenyl)naphtho[2,1-b]furan-2-yl)methanimine (**4j**)



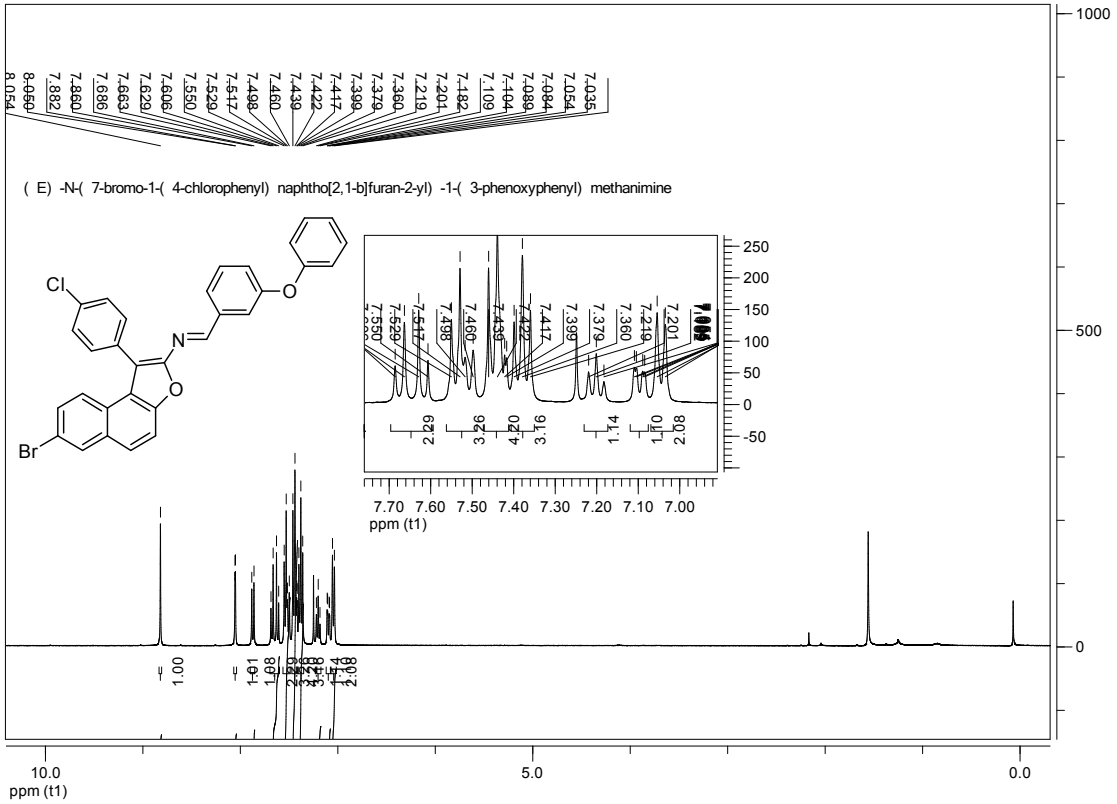


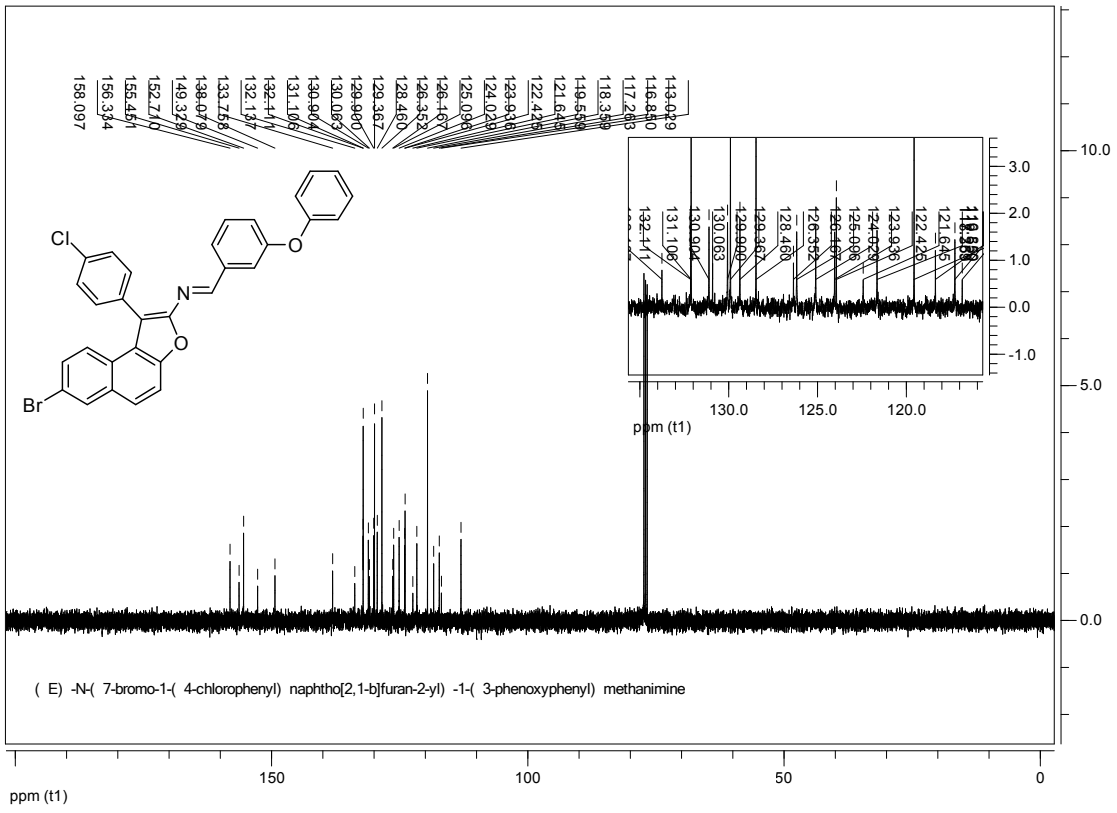
(E)-N-(1-(p-methoxylphenyl)naphtho[2,1-b]furan-2-yl)-1-(o-chlorophenyl)methanimine (**4k**)



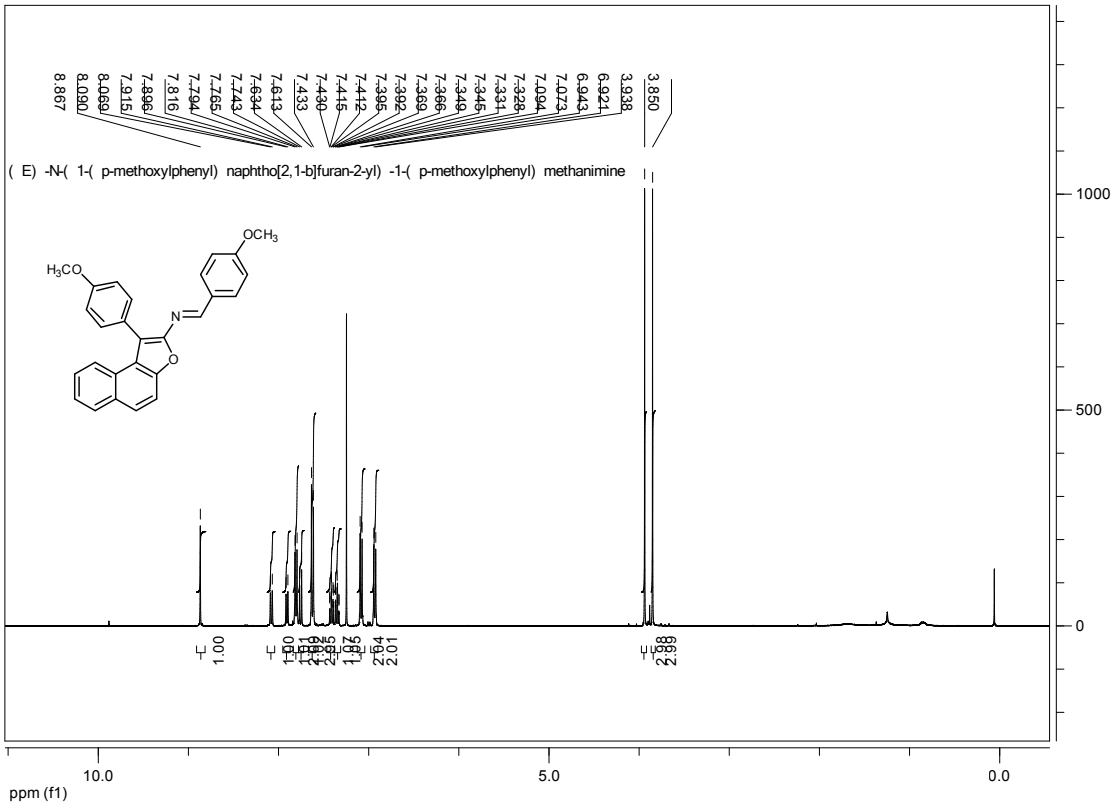


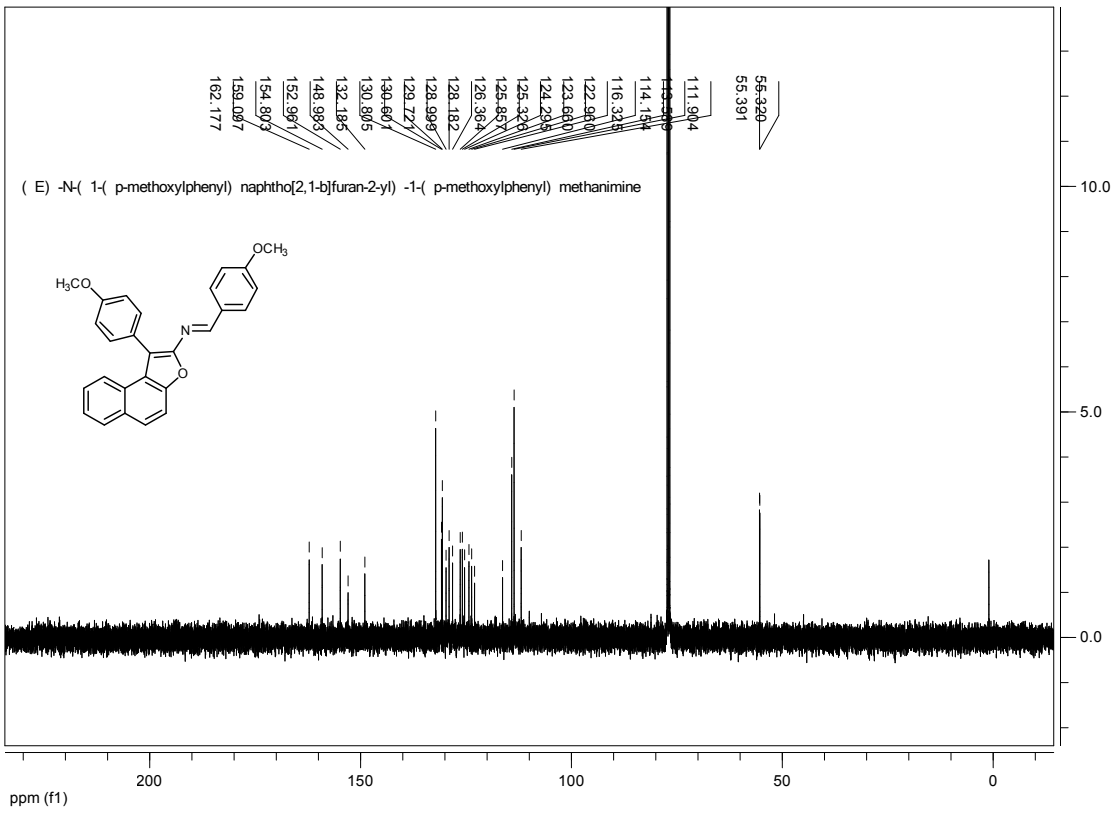
(E)-N-(7-bromo-1-(4-chlorophenyl)naphtho[2,1-b]furan-2-yl)-1-(3-phenoxyphenyl)methanimine (**4l**)



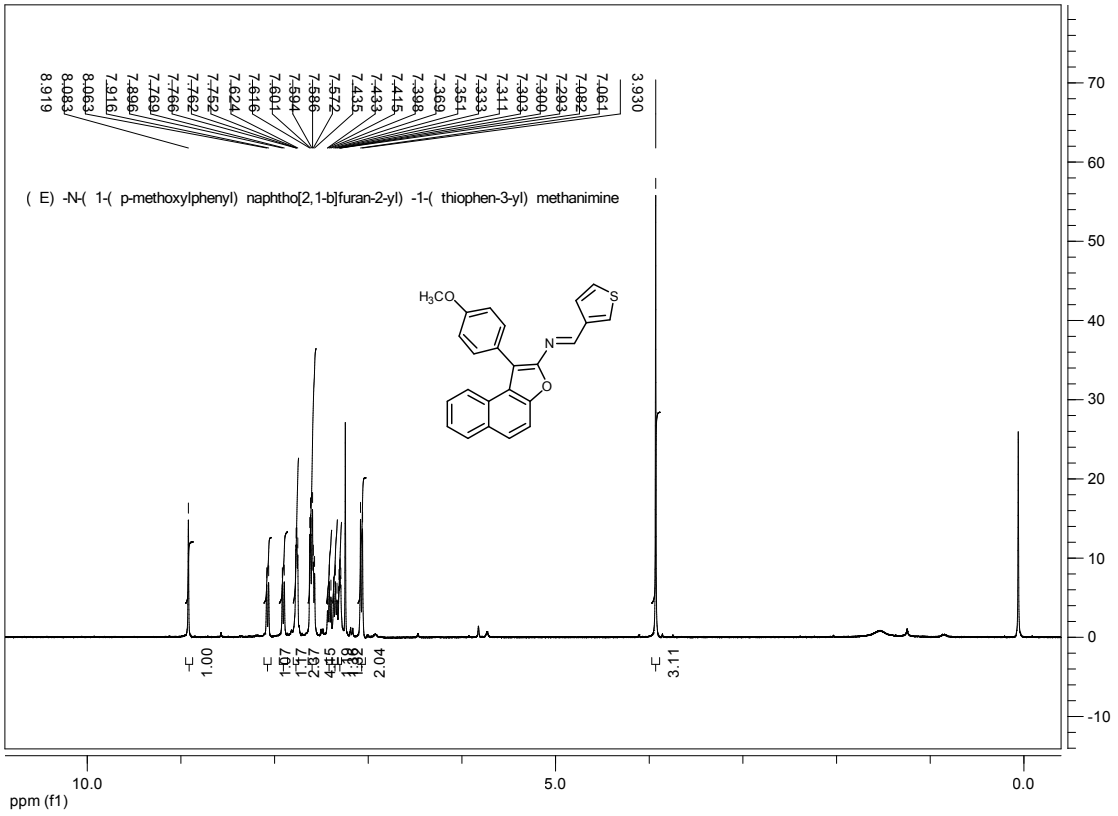


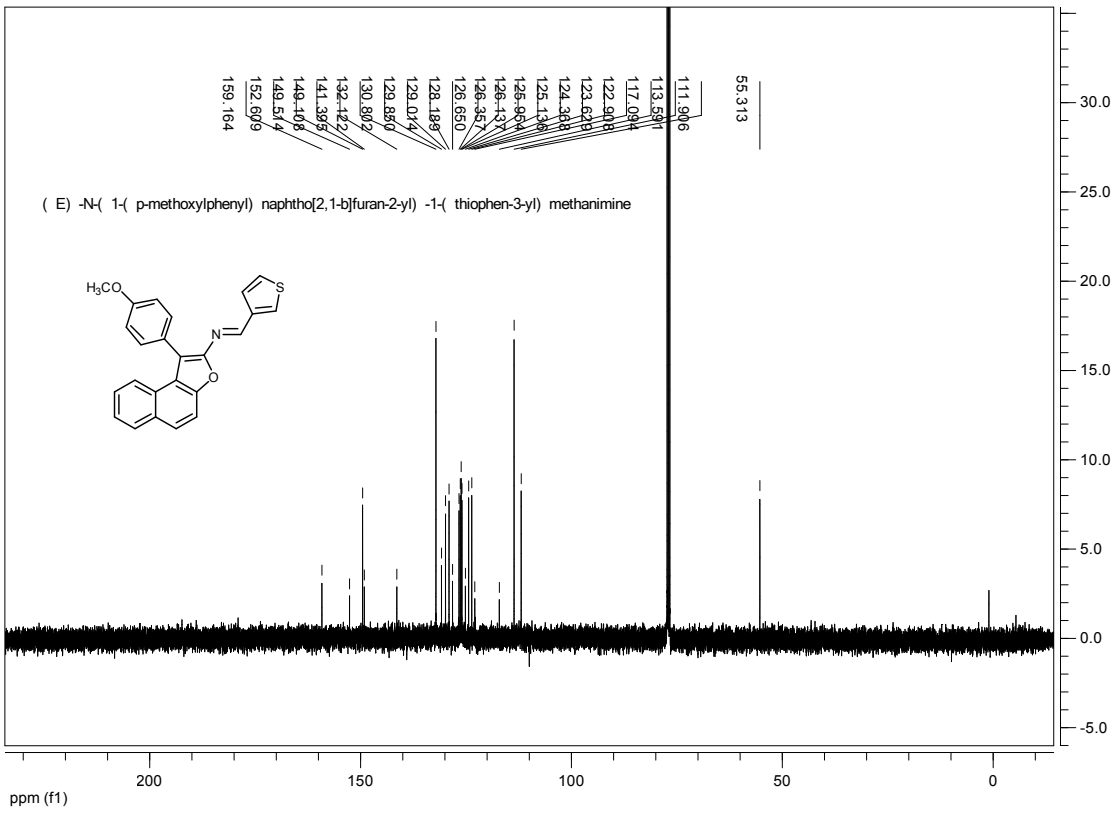
(E)-N-(1-(p-methoxylphenyl)naphtho[2,1-b]furan-2-yl)-1-(p-methoxylphenyl)methanimine (**4m**)



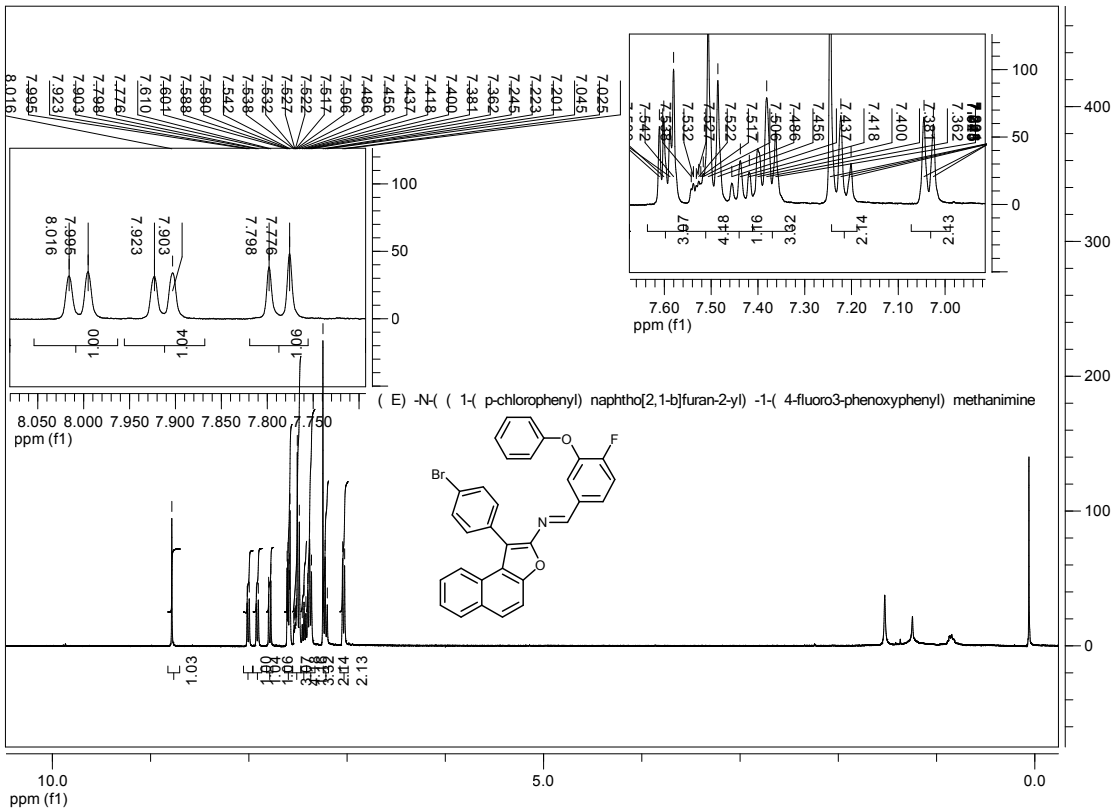


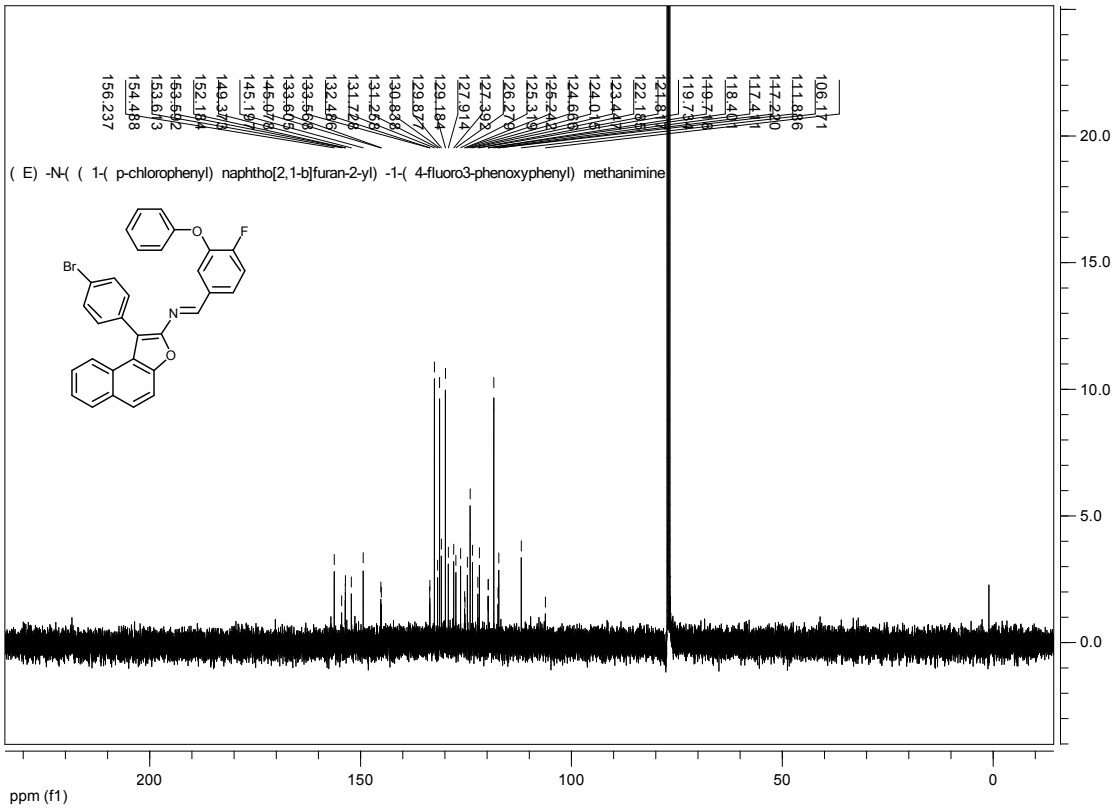
(E)-N-(1-(p-methoxylphenyl)naphtho[2,1-b]furan-2-yl)-1-(thiophen-3-yl)methanimine (**4n**)



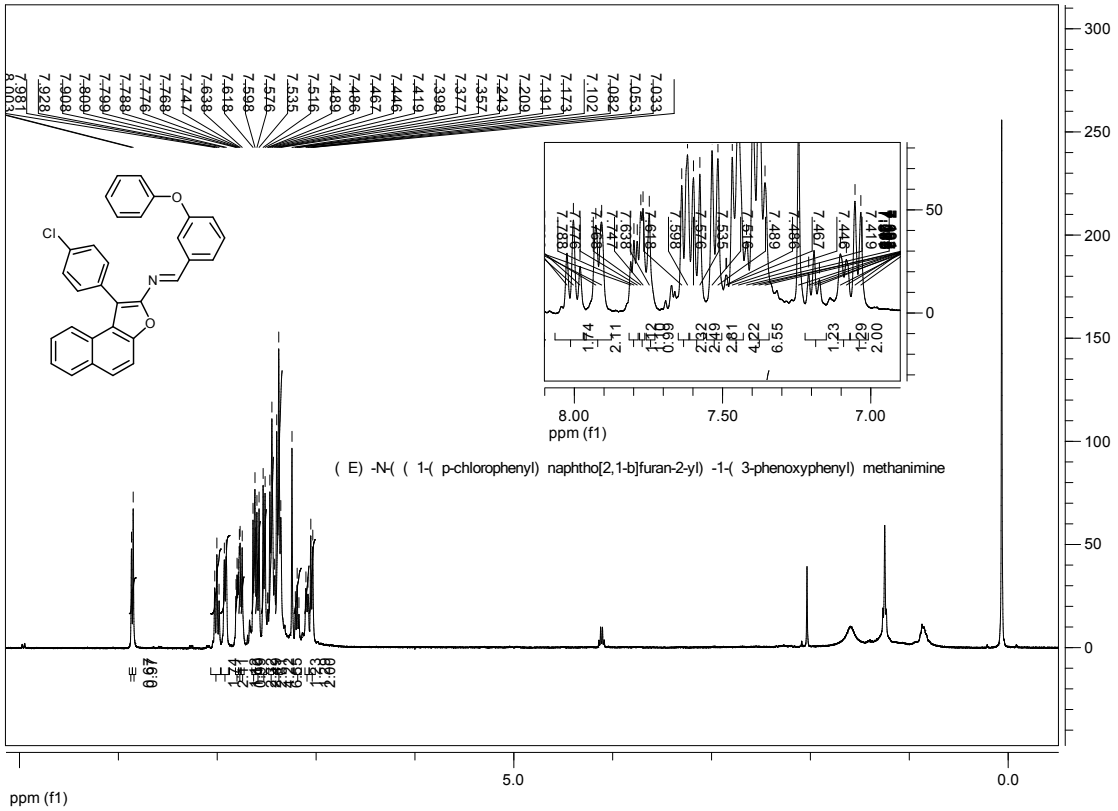


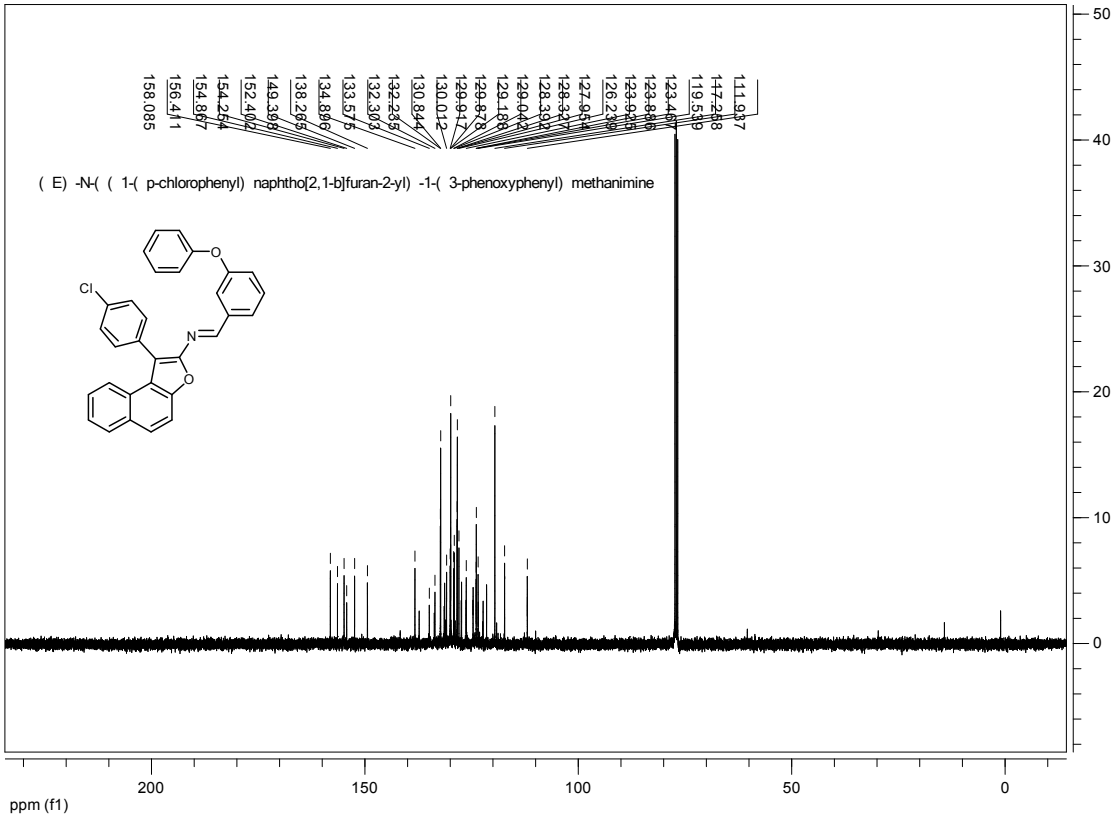
(E)-N-((1-(p-chlorophenyl)naphtho[2,1-b]furan-2-yl)-1-(4-fluoro3-phenoxyphenyl)methanimine (**4o**)



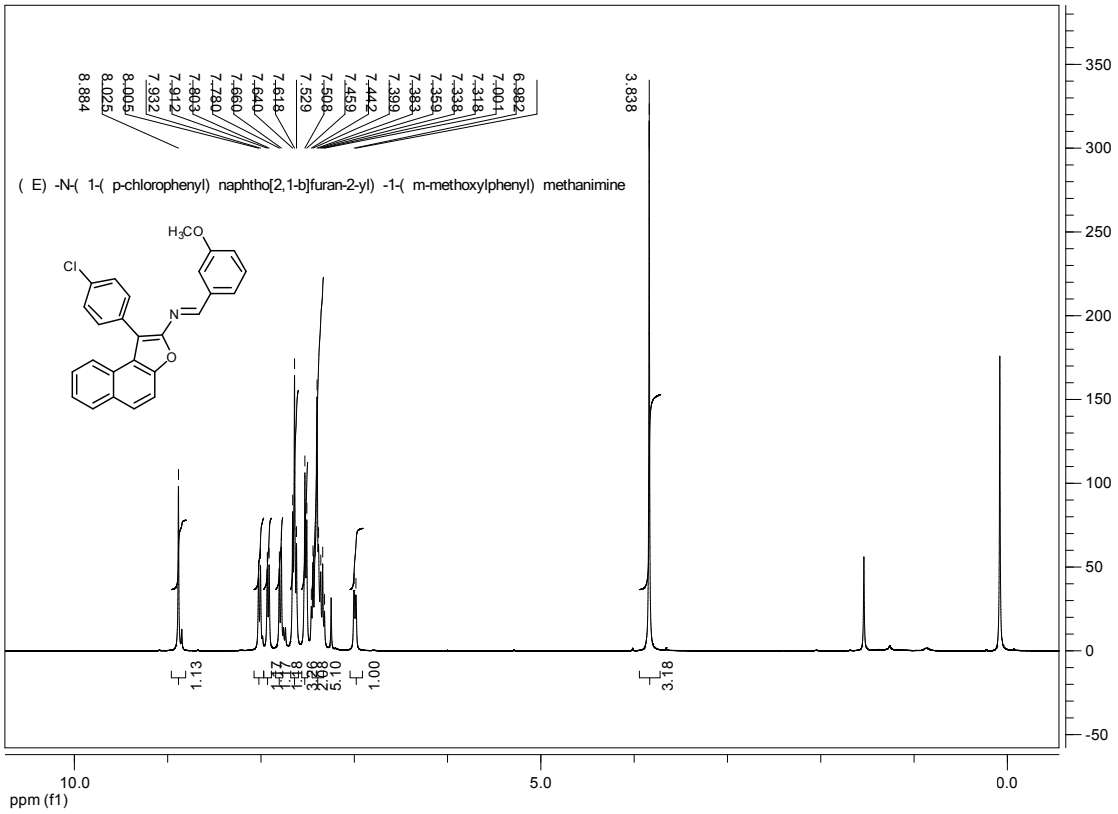


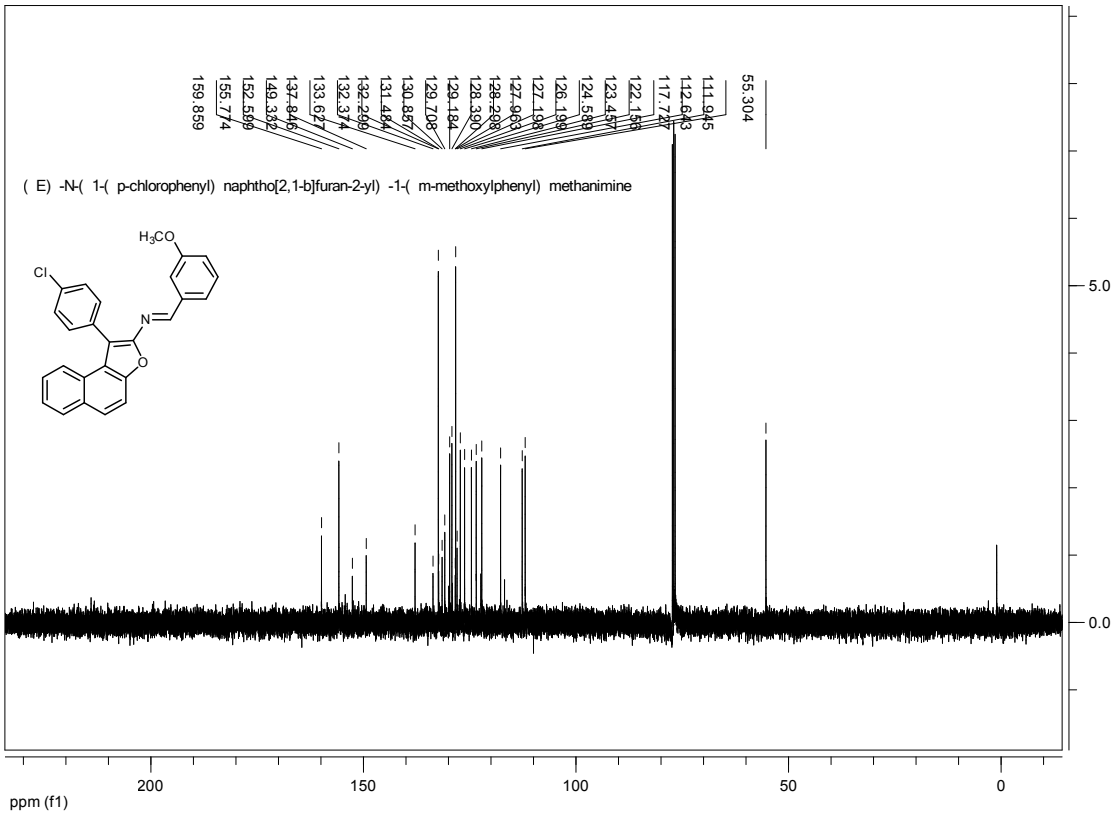
(E)-N-((1-(p-chlorophenyl)naphtho[2,1-b]furan-2-yl)-1-(3-phenoxyphenyl)methanimine (**4p**)



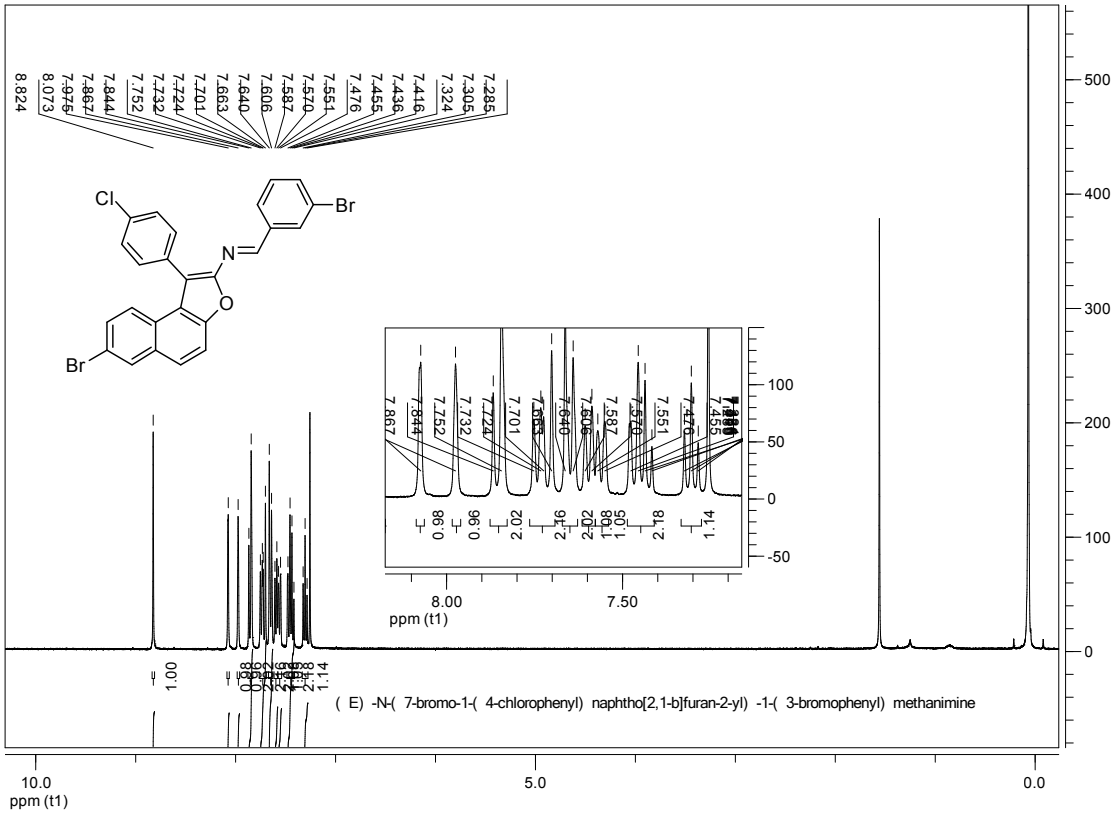


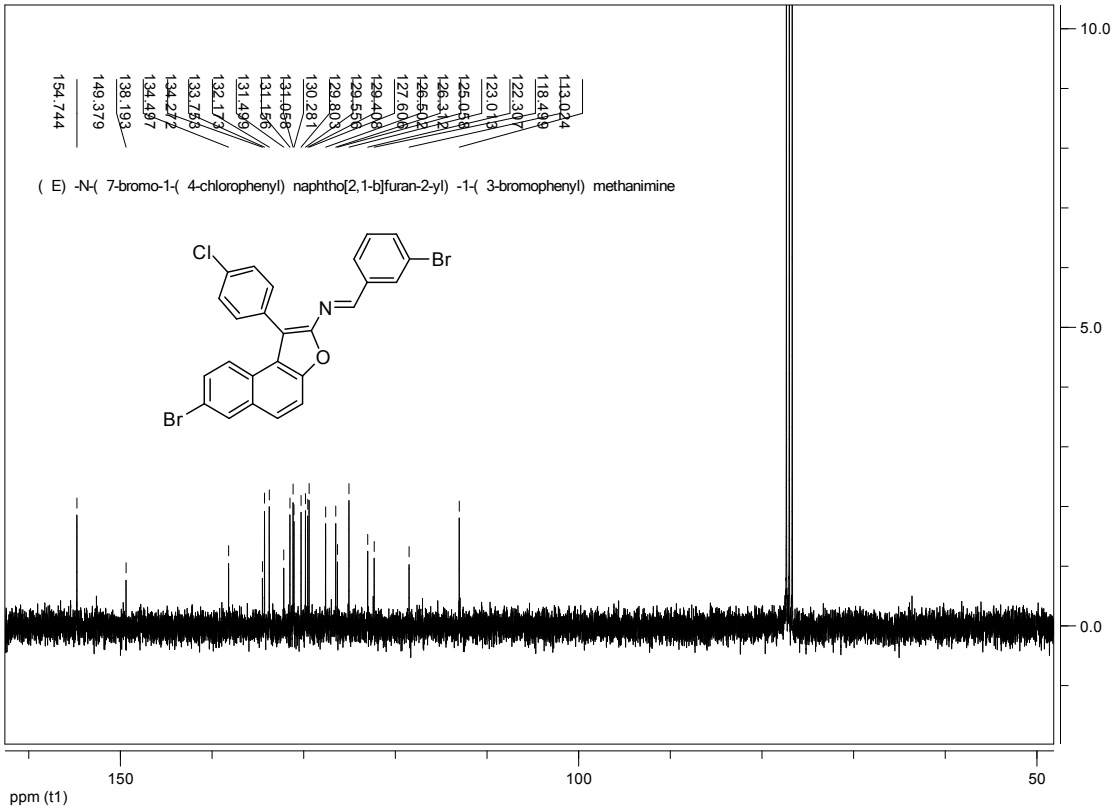
(E)-N-(1-(p-chlorophenyl)naphtho[2,1-b]furan-2-yl)-1-(m-methoxylphenyl)methanimine (**4q**)



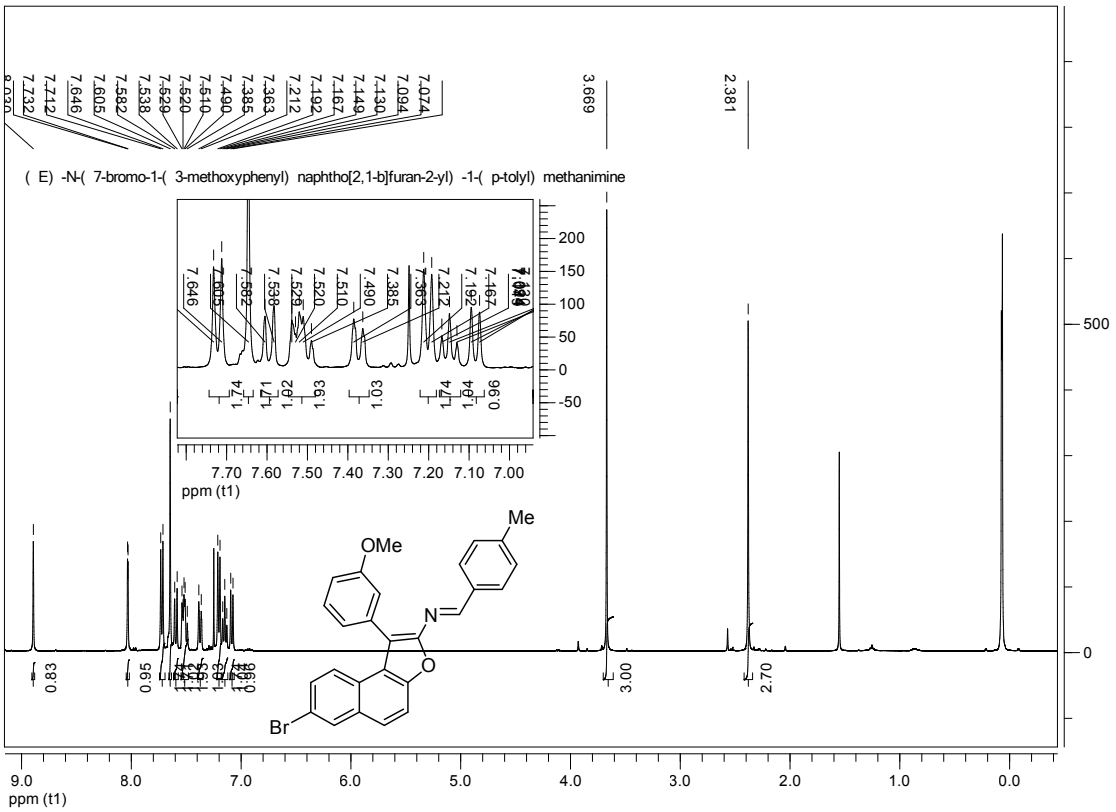


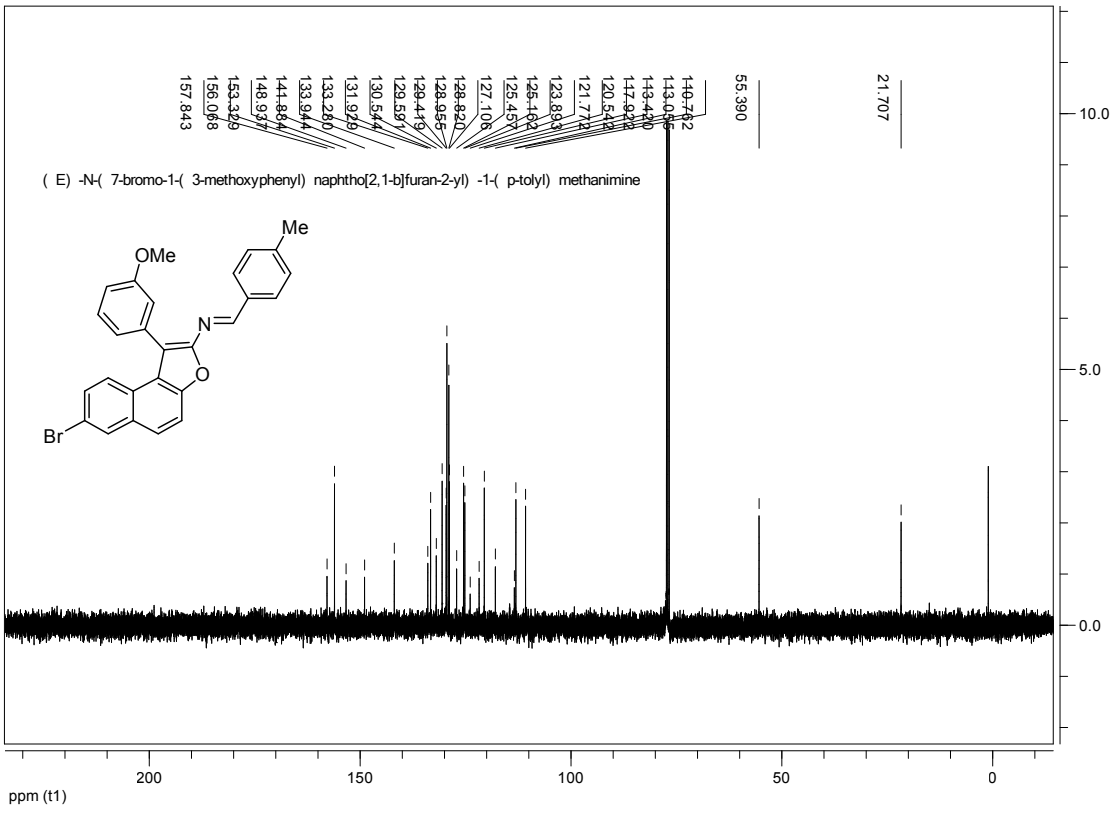
(E)-N-(7-bromo-1-(4-chlorophenyl)naphtho[2,1-b]furan-2-yl)-1-(3-bromophenyl)methanimine (**4r**)



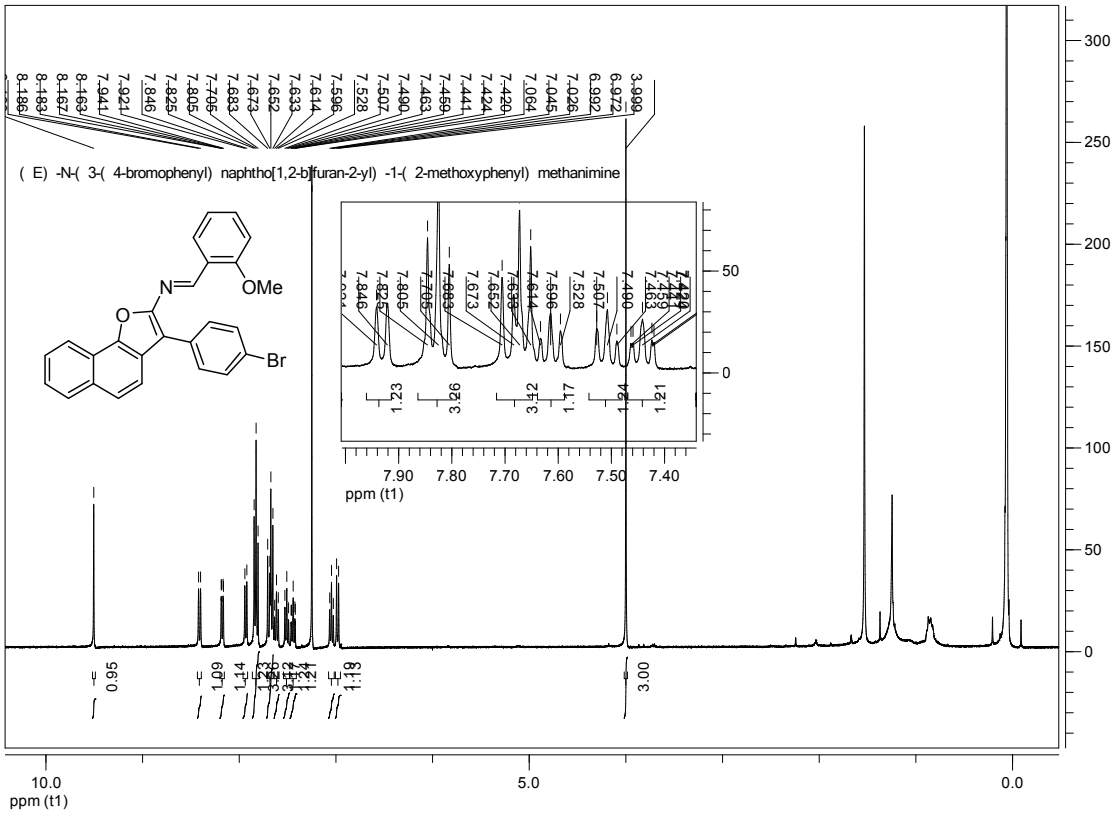


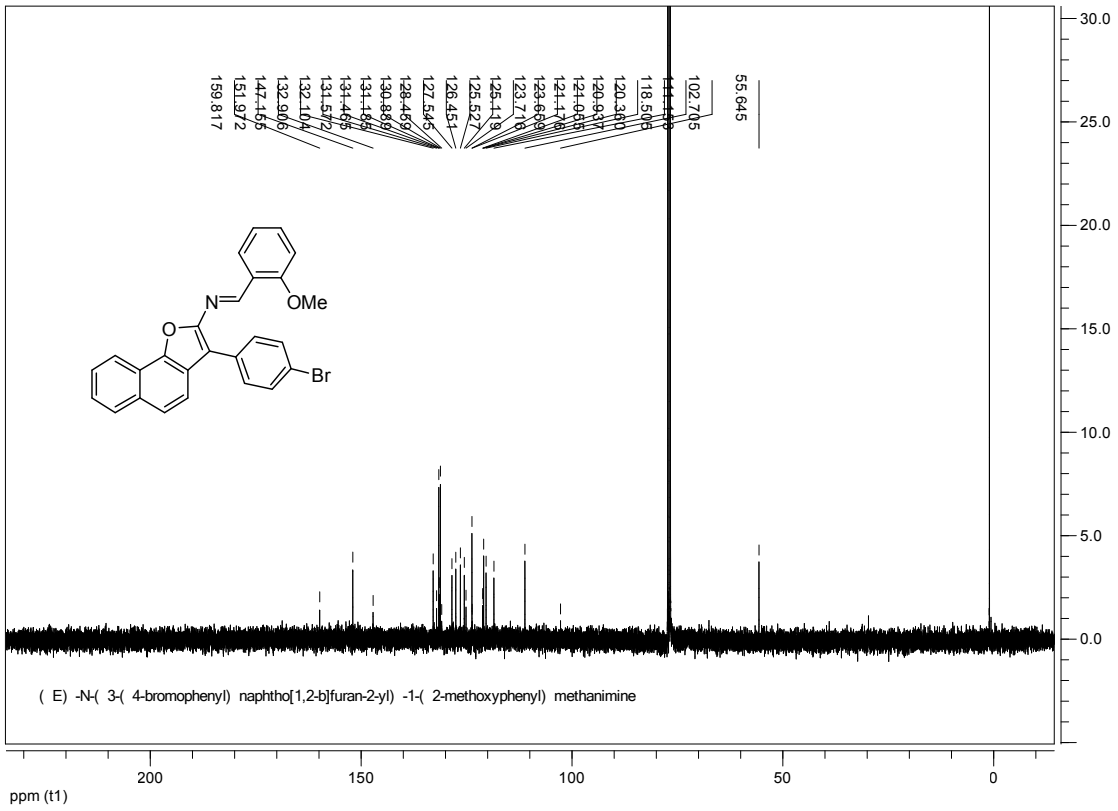
(E)-N-(7-bromo-1-(3-methoxyphenyl)naphtho[2,1-b]furan-2-yl)-1-(p-tolyl)methanimine (**4s**)



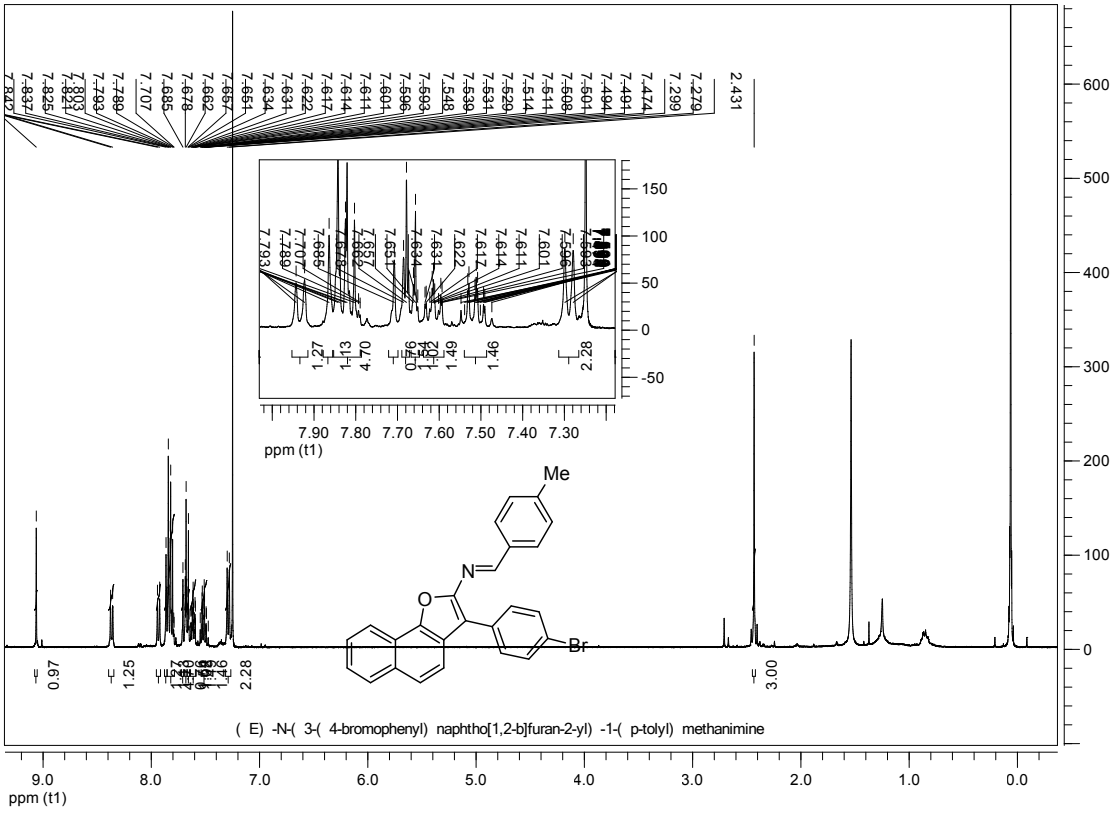


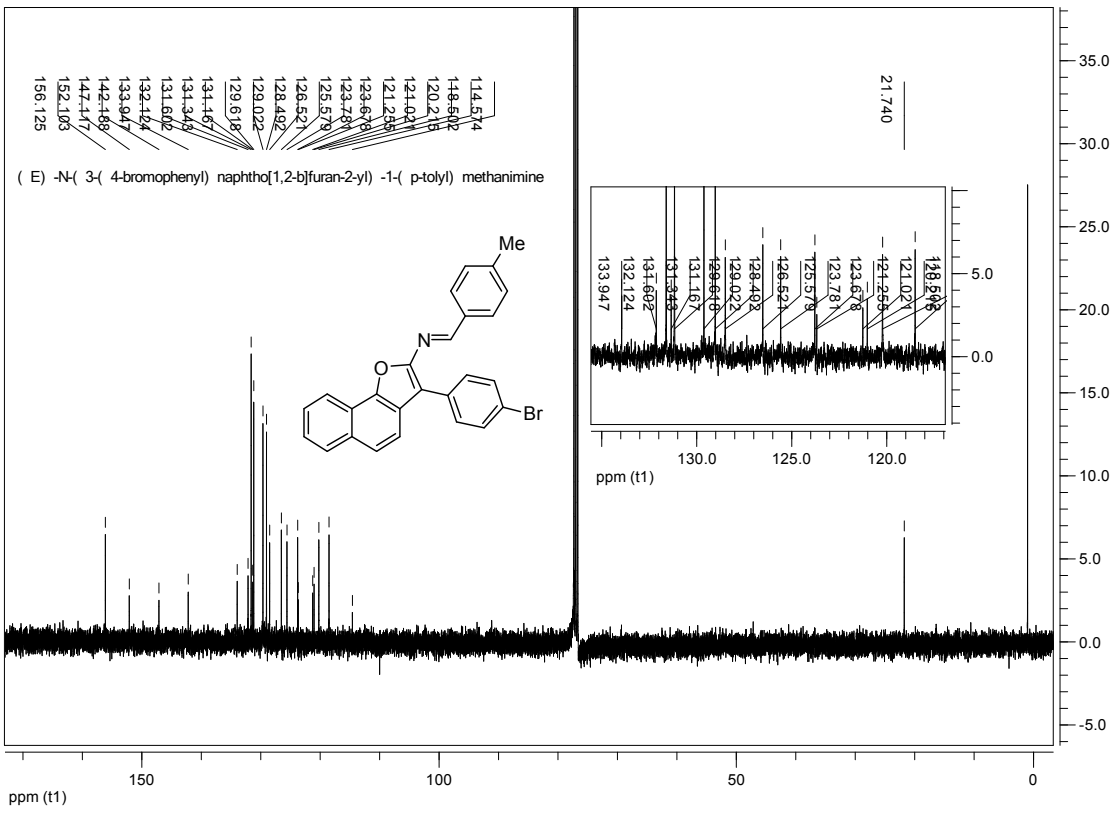
(E)-N-(3-(4-bromophenyl)naphtho[1,2-b]furan-2-yl)-1-(2-methoxyphenyl)methanimine (**4t**)



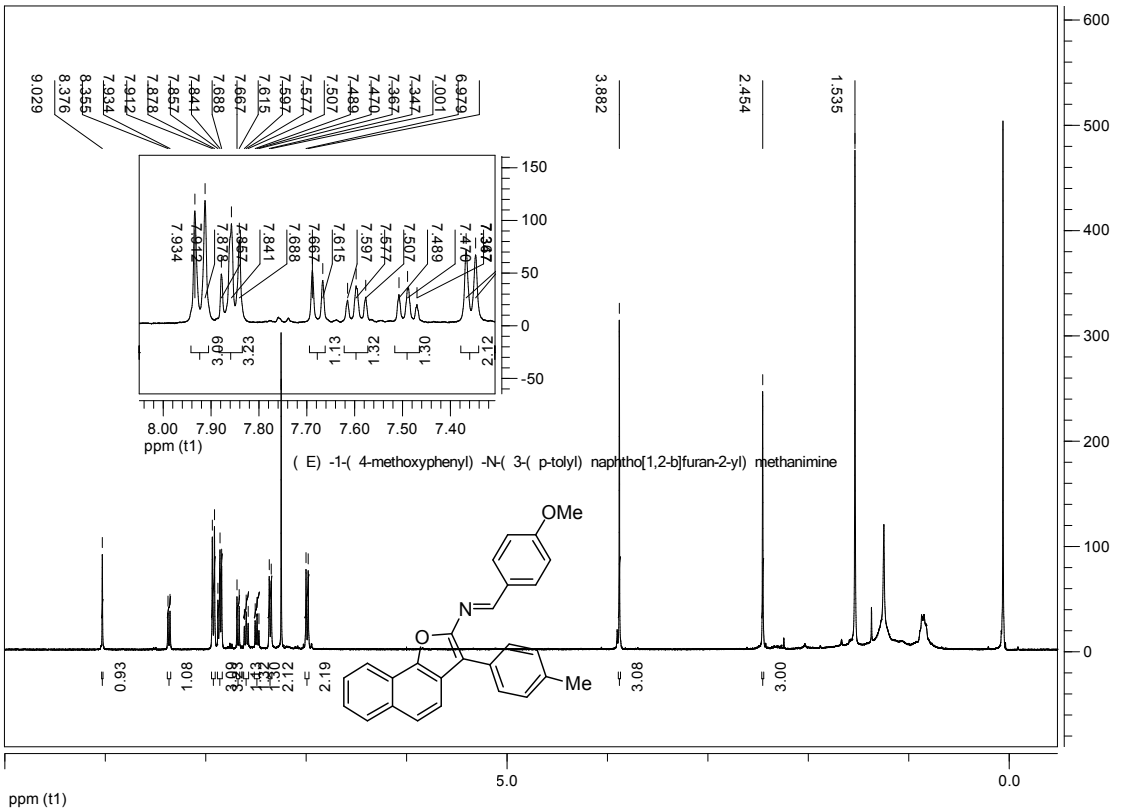


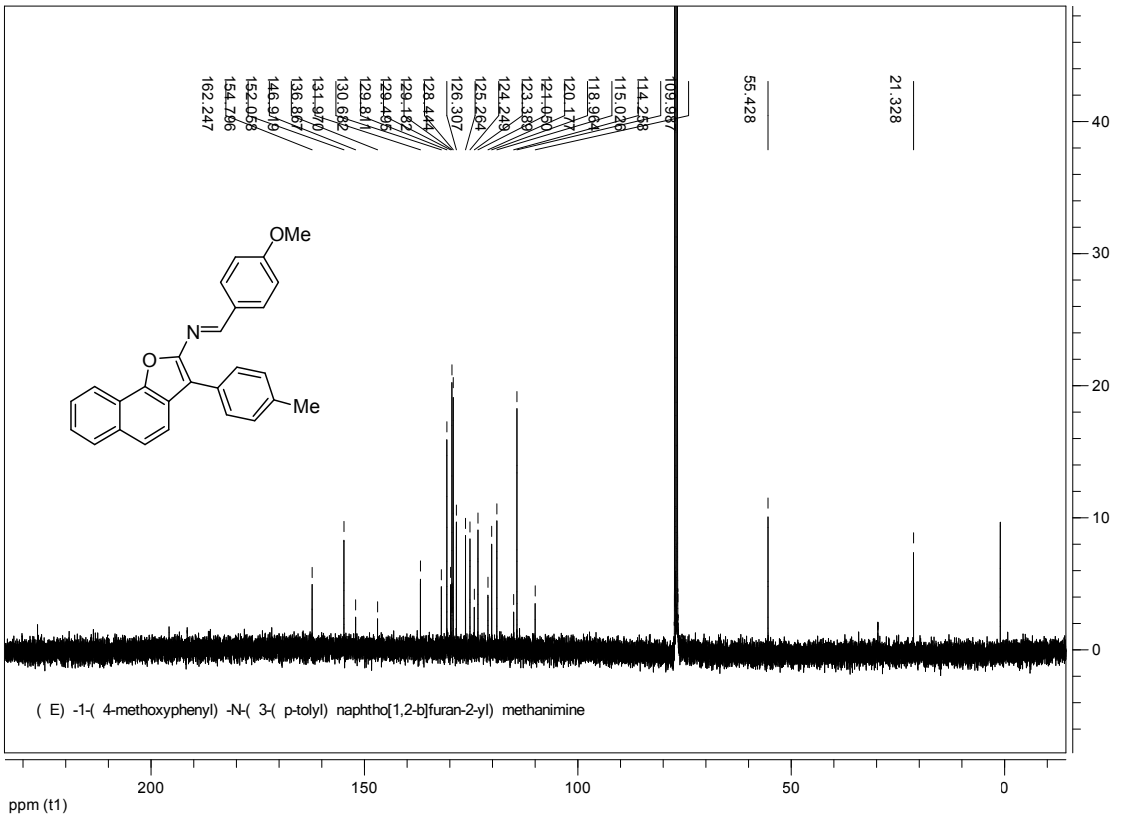
(E)-N-(3-(4-bromophenyl)naphtho[1,2-b]furan-2-yl)-1-(p-tolyl)methanimine (**4u**)



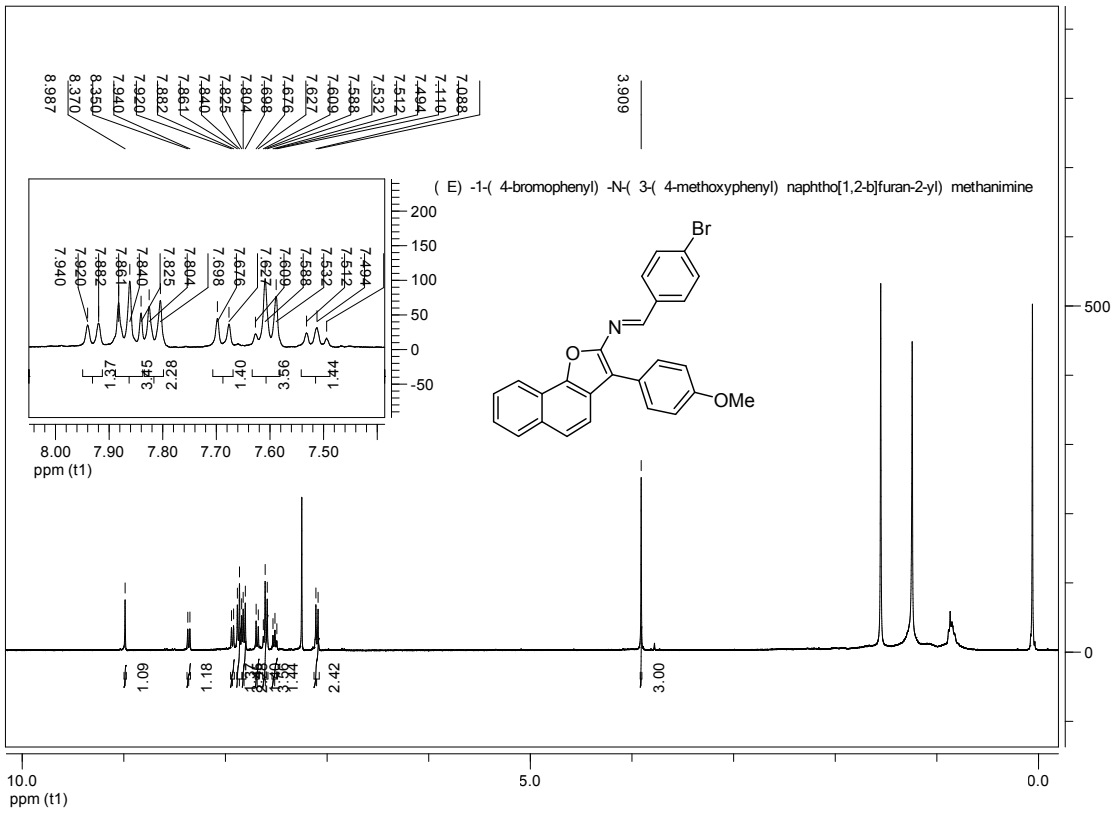


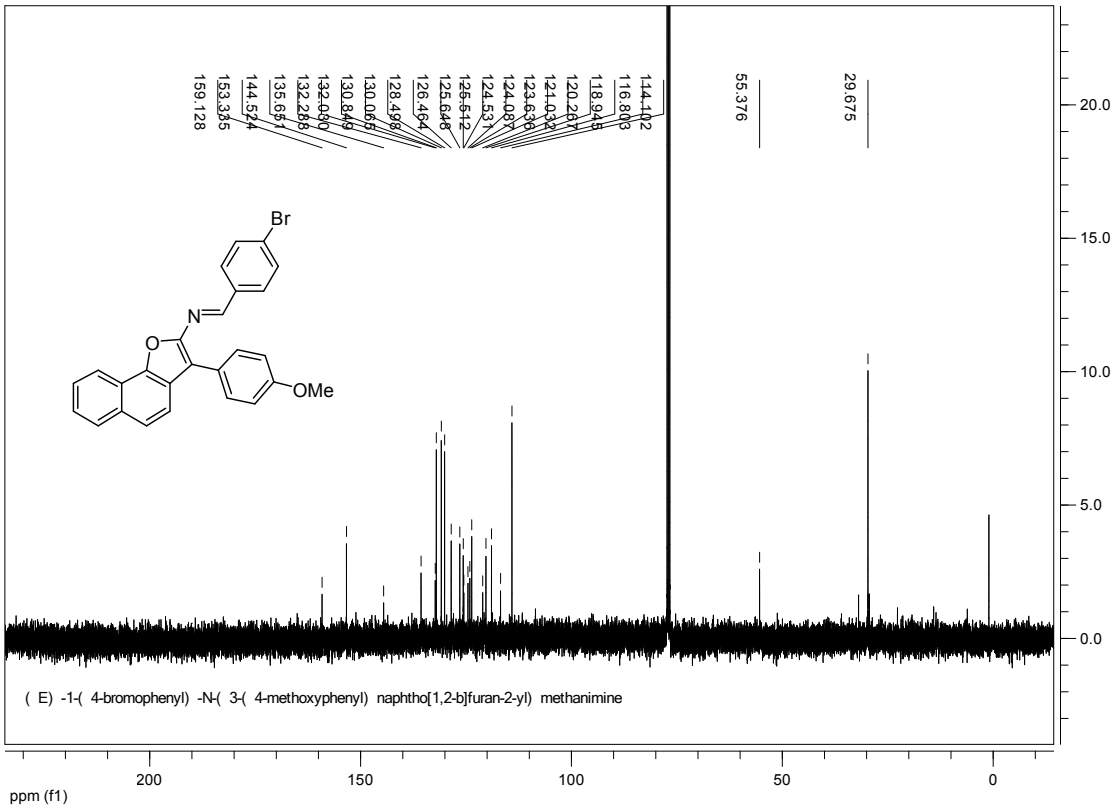
(E)-1-(4-methoxyphenyl)-N-(3-(p-tolyl)naphtho[1,2-b]furan-2-yl)methanimine (**4v**)



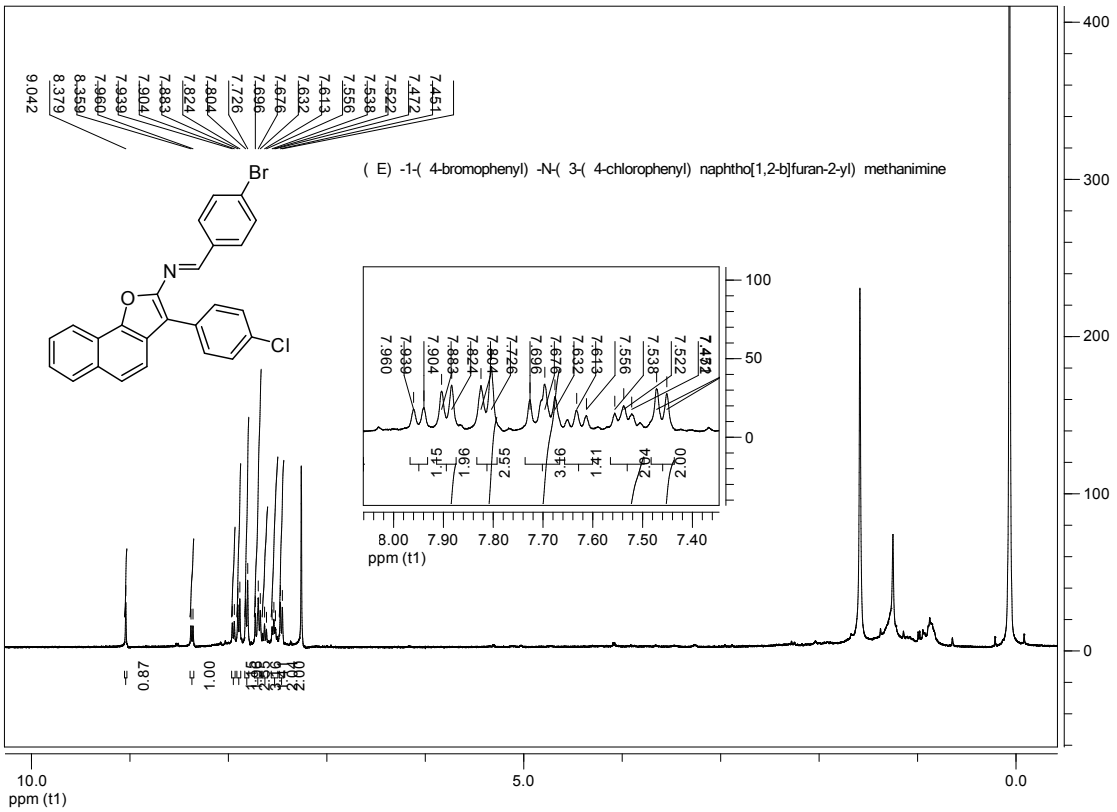


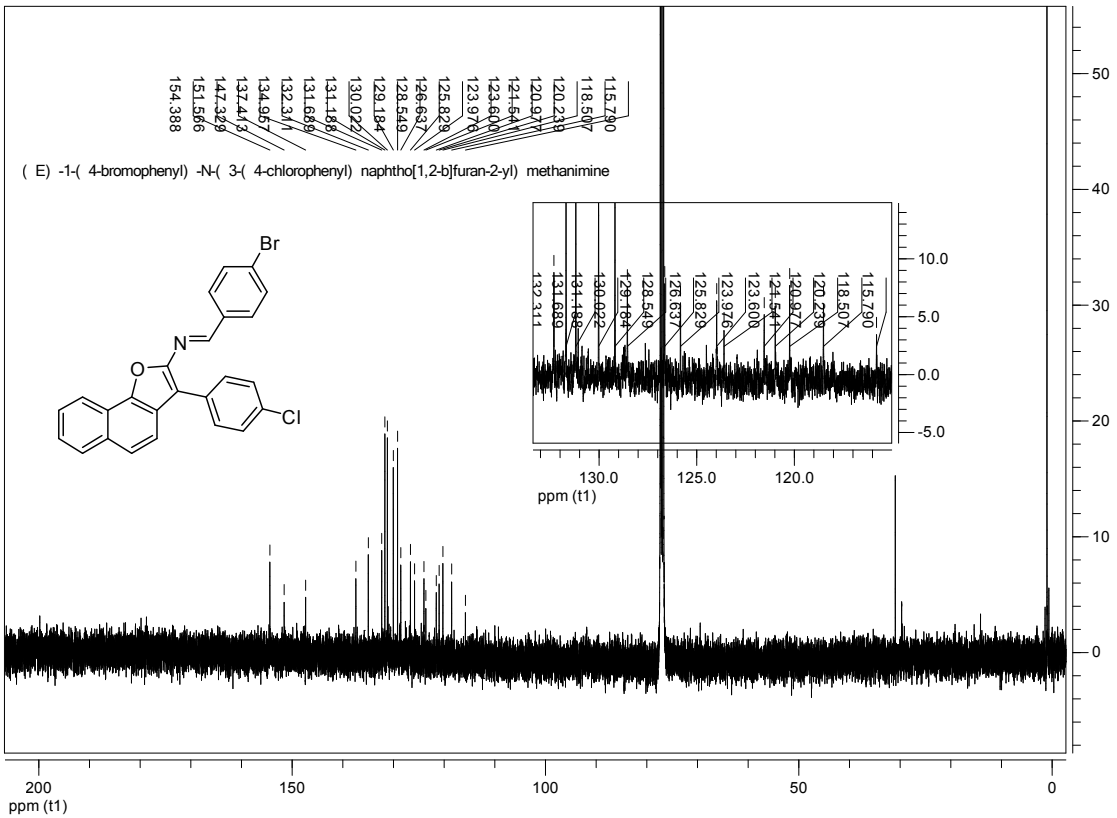
(E)-1-(4-bromophenyl)-N-(3-(4-methoxyphenyl)naphtho[1,2-b]furan-2-yl)methanimi
ne (**4w**)





(E)-1-(4-bromophenyl)-N-(3-(4-chlorophenyl)naphtho[1,2-b]furan-2-yl)methanimine (**4x**)





X-ray Structure of 4b and 4f

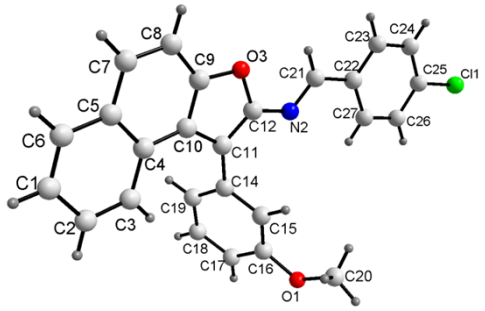


Figure 1 Molecular structure of naphtho[2,1‑*b*]furan derivative **4b**

Table 1-1. Crystal data and structure refinement for naphtho[2,1‑*b*]furan derivative **4b**.

Identification code	**4b**
Empirical formula	C_{26} H_{18} Cl N O_2
Formula weight	411.86
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P b c a
Unit cell dimensions	a = 7.7340(10) A alpha = 90 deg.
	b = 20.297(3) A beta = 90 deg.
	c = 26.738(3) A gamma = 90 deg.
Volume	4197.3(9) A^3
Z, Calculated density	8, 1.304 Mg/m^3
Absorption coefficient	0.204 mm^-1
F(000)	1712
Crystal size	0.35 x 0.33 x 0.3 mm
Theta range for data collection	1.52 to 27.58 deg.
Limiting indices	-9<=h<=10, -21<=k<=26, -34<=l<=31
Reflections collected / unique	32851 / 4854 [R(int) = 0.0799]
Completeness to theta = 27.58	98.2 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4766 / 0 / 272
Goodness-of-fit on F^2	1.249
Final R indices [I>2sigma(I)]	R1 = 0.0792, wR2 = 0.1959
R indices (all data)	R1 = 0.1836, wR2 = 0.2321
Largest diff. peak and hole	0.269 and -0.255 e.A^-3

Table 1-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for naphtho[2,1-*b*]furan derivative **4b**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Cl(1)	13126(2)	1063(1)	-2388(1)	125(1)
O(1)	9691(3)	3476(1)	170(1)	75(1)
O(3)	7211(3)	279(1)	288(1)	53(1)
N(2)	9173(3)	958(1)	-159(1)	50(1)
C(1)	3806(7)	1325(4)	2248(2)	115(2)
C(2)	4943(6)	1821(3)	2066(2)	102(2)
C(3)	5930(5)	1686(2)	1656(1)	75(1)
C(4)	5799(4)	1071(2)	1406(1)	59(1)
C(5)	4608(4)	590(2)	1593(1)	71(1)
C(6)	3648(6)	739(3)	2018(2)	106(2)
C(7)	4390(5)	-12(2)	1334(2)	82(1)
C(8)	5211(4)	-144(2)	901(1)	70(1)
C(9)	6337(4)	329(2)	726(1)	52(1)
C(10)	6733(4)	914(2)	968(1)	49(1)
C(11)	7993(4)	1241(1)	661(1)	46(1)
C(12)	8210(4)	845(1)	255(1)	48(1)
C(14)	8965(4)	1855(1)	747(1)	47(1)
C(15)	8812(4)	2375(1)	413(1)	49(1)
C(16)	9783(4)	2935(2)	481(1)	56(1)
C(17)	10917(4)	2988(2)	878(1)	72(1)
C(18)	11031(5)	2477(2)	1211(1)	77(1)
C(19)	10061(4)	1914(2)	1152(1)	67(1)
C(20)	8473(5)	3463(2)	-229(1)	82(1)
C(21)	9210(4)	551(1)	-521(1)	50(1)
C(22)	10161(4)	683(1)	-978(1)	50(1)
C(23)	10238(4)	214(2)	-1352(1)	60(1)
C(24)	11143(5)	330(2)	-1786(1)	70(1)
C(25)	11975(5)	915(2)	-1850(1)	72(1)
C(26)	11902(4)	1398(2)	-1485(1)	75(1)
C(27)	11014(4)	1280(2)	-1051(1)	63(1)

Table 1-3. Bond lengths [A] and angles [deg]
for naphtho[2,1‑*b*]furan derivative **4b**.

Cl(1)-C(25)	1.719(4)	O(1)-C(16)	1.377(4)
O(1)-C(20)	1.424(4)	O(3)-C(9)	1.354(4)
O(3)-C(12)	1.386(3)	N(2)-C(21)	1.274(3)
N(2)-C(12)	1.353(4)	C(1)-C(6)	1.344(7)
C(1)-C(2)	1.423(7)	C(1)-H(1)	0.9300
C(2)-C(3)	1.363(5)	C(2)-H(2)	0.9300
C(3)-C(4)	1.419(5)	C(3)-H(3)	0.9300
C(4)-C(10)	1.414(4)	C(4)-C(5)	1.432(5)
C(5)-C(6)	1.391(6)	C(5)-C(7)	1.415(5)
C(6)-H(6)	0.9300	C(7)-C(8)	1.346(5)
C(7)-H(7)	0.9300	C(8)-C(9)	1.378(4)
C(8)-H(8)	0.9300	C(9)-C(10)	1.386(4)
C(10)-C(11)	1.435(4)	C(11)-C(12)	1.363(4)
C(11)-C(14)	1.474(4)	C(14)-C(19)	1.380(4)
C(14)-C(15)	1.388(4)	C(15)-C(16)	1.375(4)
C(15)-H(15)	0.9300	C(16)-C(17)	1.381(4)
C(17)-C(18)	1.370(5)	C(17)-H(17)	0.9300
C(18)-C(19)	1.376(5)	C(18)-H(18)	0.9300
C(19)-H(19)	0.9300	C(20)-H(20A)	0.9600
C(20)-H(20B)	0.9600	C(20)-H(20C)	0.9600
C(21)-C(22)	1.451(4)	C(21)-H(21)	0.9300
C(22)-C(23)	1.381(4)	C(22)-C(27)	1.394(4)
C(23)-C(24)	1.377(4)	C(23)-H(23)	0.9300
C(24)-C(25)	1.362(5)	C(24)-H(24)	0.9300
C(25)-C(26)	1.385(5)	C(26)-C(27)	1.369(5)
C(26)-H(26)	0.9300	C(27)-H(27)	0.9300
C(16)-O(1)-C(20)	118.1(2)	C(9)-O(3)-C(12)	105.8(2)
C(21)-N(2)-C(12)	121.5(3)	C(6)-C(1)-C(2)	121.7(4)
C(6)-C(1)-H(1)	119.1	C(2)-C(1)-H(1)	119.1
C(3)-C(2)-C(1)	118.6(5)	C(3)-C(2)-H(2)	120.7
C(1)-C(2)-H(2)	120.7	C(2)-C(3)-C(4)	121.0(4)
C(2)-C(3)-H(3)	119.5	C(4)-C(3)-H(3)	119.5
C(3)-C(4)-C(10)	123.5(3)	C(3)-C(4)-C(5)	118.8(3)
C(10)-C(4)-C(5)	117.6(3)	C(6)-C(5)-C(7)	121.7(4)
C(6)-C(5)-C(4)	118.7(5)	C(7)-C(5)-C(4)	119.6(3)
C(1)-C(6)-C(5)	121.2(5)	C(1)-C(6)-H(6)	119.4
C(5)-C(6)-H(6)	119.4	C(8)-C(7)-C(5)	122.5(3)
C(8)-C(7)-H(7)	118.7	C(5)-C(7)-H(7)	118.7
C(7)-C(8)-C(9)	116.8(4)	C(7)-C(8)-H(8)	121.6

C(9)-C(8)-H(8)	121.6	O(3)-C(9)-C(8)	123.8(3)
O(3)-C(9)-C(10)	110.9(2)	C(8)-C(9)-C(10)	125.3(3)
C(9)-C(10)-C(4)	117.9(3)	C(9)-C(10)-C(11)	106.2(3)
C(4)-C(10)-C(11)	135.7(3)	C(12)-C(11)-C(10)	105.4(3)
C(12)-C(11)-C(14)	124.1(3)	C(10)-C(11)-C(14)	130.5(3)
N(2)-C(12)-C(11)	128.3(3)	N(2)-C(12)-O(3)	120.1(2)
C(11)-C(12)-O(3)	111.6(3)	C(19)-C(14)-C(15)	119.4(3)
C(19)-C(14)-C(11)	120.5(3)	C(15)-C(14)-C(11)	120.0(3)
C(16)-C(15)-C(14)	119.8(3)	C(16)-C(15)-H(15)	120.1
C(14)-C(15)-H(15)	120.1	C(15)-C(16)-O(1)	123.4(3)
C(15)-C(16)-C(17)	120.8(3)	O(1)-C(16)-C(17)	115.8(3)
C(18)-C(17)-C(16)	118.9(3)	C(18)-C(17)-H(17)	120.6
C(16)-C(17)-H(17)	120.6	C(17)-C(18)-C(19)	121.2(3)
C(17)-C(18)-H(18)	119.4	C(19)-C(18)-H(18)	119.4
C(18)-C(19)-C(14)	119.8(3)	C(18)-C(19)-H(19)	120.1
C(14)-C(19)-H(19)	120.1	O(1)-C(20)-H(20A)	109.5
O(1)-C(20)-H(20B)	109.5	H(20A)-C(20)-H(20B)	109.5
O(1)-C(20)-H(20C)	109.5	H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5	N(2)-C(21)-C(22)	122.1(3)
N(2)-C(21)-H(21)	119.0	C(22)-C(21)-H(21)	119.0
C(23)-C(22)-C(27)	118.6(3)	C(23)-C(22)-C(21)	120.2(3)
C(27)-C(22)-C(21)	121.3(3)	C(24)-C(23)-C(22)	120.9(3)
C(24)-C(23)-H(23)	119.5	C(22)-C(23)-H(23)	119.5
C(25)-C(24)-C(23)	119.7(3)	C(25)-C(24)-H(24)	120.2
C(23)-C(24)-H(24)	120.2	C(24)-C(25)-C(26)	120.7(3)
C(24)-C(25)-Cl(1)	120.2(3)	C(26)-C(25)-Cl(1)	119.1(3)
C(27)-C(26)-C(25)	119.6(3)	C(27)-C(26)-H(26)	120.2
C(25)-C(26)-H(26)	120.2	C(26)-C(27)-C(22)	120.5(3)
C(26)-C(27)-H(27)	119.7	C(22)-C(27)-H(27)	119.7

Symmetry transformations used to generate equivalent atoms:

Table 1-4. Anisotropic displacement parameters (A^2 x 10^3) for naphtho[2,1-*b*]furan derivative **4b**. The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Cl(1)	107(1)	187(1)	80(1)	-9(1)	35(1)	-15(1)
O(1)	69(2)	51(1)	106(2)	14(1)	-1(2)	-15(1)
O(3)	50(1)	43(1)	67(1)	2(1)	1(1)	-3(1)
N(2)	49(2)	43(1)	56(2)	-4(1)	1(1)	3(1)
C(1)	77(3)	214(6)	54(3)	22(3)	16(2)	40(4)
C(2)	89(3)	148(4)	69(3)	-16(3)	-5(3)	43(3)
C(3)	65(2)	110(3)	50(2)	1(2)	-2(2)	26(2)
C(4)	47(2)	80(2)	48(2)	12(2)	-2(2)	17(2)
C(5)	43(2)	120(3)	51(2)	31(2)	1(2)	9(2)
C(6)	71(3)	183(5)	63(3)	35(3)	5(3)	11(3)
C(7)	57(2)	103(3)	86(3)	37(3)	-6(2)	-10(2)
C(8)	54(2)	65(2)	91(3)	22(2)	-6(2)	-9(2)
C(9)	38(2)	52(2)	65(2)	12(2)	-4(2)	2(2)
C(10)	40(2)	57(2)	50(2)	17(2)	-3(2)	9(2)
C(11)	48(2)	45(2)	47(2)	3(1)	0(1)	8(1)
C(12)	44(2)	43(2)	57(2)	3(2)	1(2)	3(2)
C(14)	47(2)	43(2)	50(2)	-5(1)	3(2)	5(2)
C(15)	45(2)	48(2)	54(2)	-2(2)	3(2)	0(2)
C(16)	45(2)	47(2)	77(2)	-5(2)	6(2)	2(2)
C(17)	53(2)	54(2)	109(3)	-17(2)	-18(2)	-2(2)
C(18)	72(3)	74(2)	85(2)	-19(2)	-28(2)	2(2)
C(19)	76(2)	58(2)	66(2)	-3(2)	-19(2)	8(2)
C(20)	76(3)	72(2)	99(3)	38(2)	-2(2)	-11(2)
C(21)	46(2)	40(2)	62(2)	-3(2)	-6(2)	3(1)
C(22)	43(2)	54(2)	51(2)	-8(2)	-6(2)	9(2)
C(23)	55(2)	59(2)	66(2)	-12(2)	-10(2)	9(2)
C(24)	60(2)	96(3)	56(2)	-23(2)	-1(2)	15(2)
C(25)	56(2)	105(3)	56(2)	-8(2)	8(2)	8(2)
C(26)	64(2)	80(2)	79(3)	0(2)	7(2)	-16(2)
C(27)	56(2)	66(2)	65(2)	-15(2)	4(2)	-4(2)

Table 1-5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for naphtho[2,1-*b*]furan derivative **4b**.

	x	y	z	U(eq)
H(1)	3156	1408	2534	138
H(2)	5011	2229	2223	122
H(3)	6701	2001	1538	90
H(6)	2883	428	2146	127
H(7)	3652	-328	1467	98
H(8)	5027	-536	729	84
H(15)	8055	2345	143	59
H(17)	11592	3363	918	87
H(18)	11778	2511	1482	92
H(19)	10144	1574	1383	80
H(20A)	7339	3377	-98	124
H(20B)	8781	3121	-461	124
H(20C)	8476	3880	-398	124
H(21)	8608	156	-492	60
H(23)	9672	-187	-1309	72
H(24)	11185	10	-2035	84
H(26)	12453	1800	-1534	89
H(27)	10981	1601	-803	75

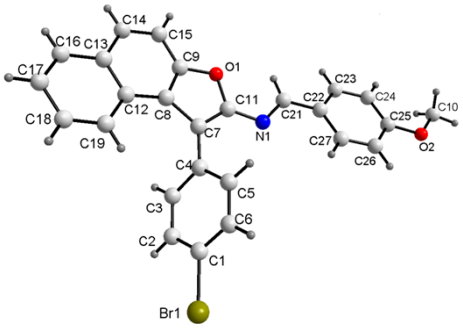


Figure 2 Molecular structure of naphtho[2,1‑*b*]furan derivative **4f**

Table 2-1. Crystal data and structure refinement for naphtho[2,1‑*b*]furan derivative **4f**.

Identification code	**4f**
Empirical formula	C_{26} H_{18} Br N O_2
Formula weight	456.31
Temperature	296(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, Pca2(1)
Unit cell dimensions	a = 15.285(3) A alpha = 90 deg.
	b = 18.355(4) A beta = 90 deg.
	c = 7.5960(16) A gamma = 90 deg.
Volume	2131.1(8) A^3
Z, Calculated density	4, 1.422 Mg/m^3
Absorption coefficient	1.951 mm^-1
F(000)	928.0
Crystal size	0.35 x 0.33 x 0.3 mm
Theta range for data collection	1.11 to 27.50 deg.
Limiting indices	-19<=h<=19, -17<=k<=23, -9<=l<=8
Reflections collected / unique	10325 / 4870 [R(int) = 0.0574]
Completeness to theta = 27.50	99.0 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4411 / 1 / 272
Goodness-of-fit on F^2	1.023
Final R indices [I>2sigma(I)]	R1 = 0.0888, wR2 = 0.2049
R indices (all data)	R1 = 0.1696, wR2 = 0.2461
Absolute structure parameter	0.90(3)
Largest diff. peak and hole	0.447 and -0.367 e.A^-3

Table 2-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for naphtho[2,1-*b*]furan derivative **4f**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Br(1)	2893(1)	1730(1)	528(2)	96(1)
O(1)	6859(4)	3182(3)	7142(9)	46(1)
C(22)	8272(5)	1653(4)	4451(11)	39(2)
C(8)	5424(5)	3469(3)	7162(11)	35(2)
C(7)	5576(4)	2934(3)	5781(10)	33(2)
C(11)	6447(5)	2767(4)	5860(10)	39(2)
O(2)	9927(5)	116(3)	2029(9)	61(2)
C(25)	9394(6)	647(5)	2909(11)	50(2)
N(1)	6904(4)	2269(3)	4927(8)	43(2)
C(4)	4956(5)	2632(4)	4491(10)	39(2)
C(23)	9178(6)	1694(4)	4676(13)	51(2)
C(12)	4678(5)	3824(4)	7886(11)	41(2)
C(5)	4783(5)	1894(4)	4355(11)	44(2)
C(9)	6228(5)	3599(4)	7902(12)	44(2)
C(24)	9732(5)	1197(5)	3900(11)	48(2)
C(3)	4509(6)	3085(5)	3330(12)	52(2)
C(21)	7732(5)	2195(4)	5288(12)	43(2)
C(27)	7951(5)	1090(4)	3432(12)	47(2)
C(1)	3746(5)	2099(6)	2094(11)	53(2)
C(17)	3281(7)	4562(6)	9526(15)	68(3)
C(13)	4837(5)	4324(4)	9298(12)	47(2)
C(26)	8495(6)	594(4)	2670(12)	54(2)
C(6)	4179(6)	1625(5)	3186(13)	59(2)
C(19)	3801(5)	3694(4)	7397(12)	48(2)
C(15)	6383(6)	4076(4)	9323(13)	56(2)
C(2)	3920(6)	2825(5)	2115(12)	58(2)
C(18)	3129(6)	4045(6)	8155(14)	62(3)
C(16)	4105(6)	4696(4)	10044(13)	60(3)
C(14)	5685(6)	4430(5)	9978(13)	62(3)
C(10)	10710(9)	109(6)	2369(17)	82(3)

Table 2-3. Bond lengths [A] and angles [deg] for naphtho[2,1-*b*]furan derivative **4f**.

Br(1)-C(1)	1.890(8)	O(1)-C(9)	1.360(10)
O(1)-C(11)	1.387(9)	C(22)-C(27)	1.382(12)
C(22)-C(23)	1.396(12)	C(22)-C(21)	1.441(11)
C(8)-C(9)	1.372(11)	C(8)-C(12)	1.424(11)
C(8)-C(7)	1.454(11)	C(7)-C(11)	1.368(10)
C(7)-C(4)	1.472(10)	C(11)-N(1)	1.351(10)
O(2)-C(10)	1.224(13)	O(2)-C(25)	1.435(11)
C(25)-C(24)	1.362(12)	C(25)-C(26)	1.390(13)
N(1)-C(21)	1.302(9)	C(4)-C(5)	1.384(11)
C(4)-C(3)	1.391(11)	C(23)-C(24)	1.377(12)
C(12)-C(19)	1.411(11)	C(12)-C(13)	1.433(11)
C(5)-C(6)	1.373(12)	C(9)-C(15)	1.409(12)
C(3)-C(2)	1.375(13)	C(27)-C(26)	1.361(12)
C(1)-C(2)	1.359(13)	C(1)-C(6)	1.372(13)
C(17)-C(16)	1.342(13)	C(17)-C(18)	1.428(15)
C(13)-C(14)	1.409(12)	C(13)-C(16)	1.428(11)
C(19)-C(18)	1.342(12)	C(15)-C(14)	1.345(13)
C(9)-O(1)-C(11)	106.6(6)	C(27)-C(22)-C(23)	117.5(7)
C(27)-C(22)-C(21)	124.0(7)	C(23)-C(22)-C(21)	118.5(7)
C(9)-C(8)-C(12)	118.6(7)	C(9)-C(8)-C(7)	105.7(6)
C(12)-C(8)-C(7)	135.6(7)	C(11)-C(7)-C(8)	106.0(6)
C(11)-C(7)-C(4)	124.9(7)	C(8)-C(7)-C(4)	129.1(6)
N(1)-C(11)-C(7)	129.1(7)	N(1)-C(11)-O(1)	120.4(6)
C(7)-C(11)-O(1)	110.4(6)	C(10)-O(2)-C(25)	117.7(8)
C(24)-C(25)-C(26)	119.9(8)	C(24)-C(25)-O(2)	123.1(8)
C(26)-C(25)-O(2)	117.0(8)	C(21)-N(1)-C(11)	117.5(7)
C(5)-C(4)-C(3)	116.4(8)	C(5)-C(4)-C(7)	122.7(7)
C(3)-C(4)-C(7)	120.9(7)	C(24)-C(23)-C(22)	121.4(8)
C(19)-C(12)-C(8)	125.6(7)	C(19)-C(12)-C(13)	117.8(7)
C(8)-C(12)-C(13)	116.5(7)	C(6)-C(5)-C(4)	121.9(8)
O(1)-C(9)-C(8)	111.2(7)	O(1)-C(9)-C(15)	123.7(7)
C(8)-C(9)-C(15)	125.0(8)	C(25)-C(24)-C(23)	119.6(8)
C(2)-C(3)-C(4)	122.7(9)	N(1)-C(21)-C(22)	122.5(8)
C(26)-C(27)-C(22)	121.4(8)	C(2)-C(1)-C(6)	121.3(8)
C(2)-C(1)-Br(1)	119.6(7)	C(6)-C(1)-Br(1)	119.1(8)
C(16)-C(17)-C(18)	119.2(8)	C(14)-C(13)-C(16)	120.6(8)
C(14)-C(13)-C(12)	121.3(7)	C(16)-C(13)-C(12)	118.1(8)
C(27)-C(26)-C(25)	120.2(8)	C(5)-C(6)-C(1)	119.2(8)
C(18)-C(19)-C(12)	122.2(8)	C(14)-C(15)-C(9)	116.8(8)

C(1)-C(2)-C(3)	118.5(8)	C(19)-C(18)-C(17)	120.5(9)
C(17)-C(16)-C(13)	122.1(9)	C(15)-C(14)-C(13)	121.8(8)

Symmetry transformations used to generate equivalent atoms:

Table 2-4. Anisotropic displacement parameters (A^2 x 10^3) for naphtho[2,1-*b*]furan derivative **4f**.

The anisotropic displacement factor exponent takes the form:

-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Br(1)	61(1)	153(1)	73(1)	-35(1)	-25(1)	-6(1)
O(1)	38(3)	41(3)	59(4)	-4(3)	-6(3)	3(2)
C(22)	45(4)	39(4)	31(4)	7(4)	-1(4)	9(3)
C(8)	37(4)	23(3)	44(5)	4(3)	-8(4)	0(3)
C(7)	44(4)	23(3)	32(4)	5(3)	-2(4)	2(3)
C(11)	41(4)	35(4)	40(5)	5(4)	-3(4)	4(4)
O(2)	81(4)	48(3)	54(4)	-14(3)	-6(4)	9(3)
C(25)	58(5)	53(5)	38(5)	1(4)	3(4)	11(4)
N(1)	38(4)	47(4)	44(4)	10(3)	-3(3)	9(3)
C(4)	40(4)	47(5)	31(4)	-2(4)	2(4)	9(3)
C(23)	51(5)	47(5)	56(5)	1(4)	-6(5)	8(4)
C(12)	43(4)	27(4)	52(5)	7(4)	3(4)	-3(3)
C(5)	44(4)	42(5)	44(5)	0(4)	-13(4)	5(4)
C(9)	47(5)	33(4)	52(5)	1(4)	-2(4)	-4(4)
C(24)	38(4)	60(5)	46(5)	1(4)	3(4)	6(4)
C(3)	60(6)	52(5)	44(5)	7(4)	-6(5)	15(4)
C(21)	52(5)	37(4)	40(5)	5(4)	-3(5)	5(3)
C(27)	41(4)	44(5)	56(5)	5(4)	-2(4)	9(4)
C(1)	35(5)	92(7)	31(4)	-12(5)	-3(4)	12(4)
C(17)	66(6)	72(6)	66(6)	0(6)	22(6)	27(5)
C(13)	57(5)	36(4)	48(5)	0(4)	-1(4)	6(4)
C(26)	66(6)	44(4)	52(5)	-7(4)	-7(5)	6(4)
C(6)	59(5)	58(6)	60(6)	-11(5)	4(5)	-1(5)
C(19)	52(5)	48(5)	44(5)	-1(4)	-6(4)	-3(4)
C(15)	51(5)	41(5)	76(6)	-12(5)	-14(5)	-1(4)
C(2)	62(6)	71(7)	42(5)	4(5)	-14(5)	22(5)
C(18)	44(5)	78(7)	63(7)	4(5)	7(5)	15(5)
C(16)	75(6)	35(4)	70(8)	-8(4)	17(5)	14(4)
C(14)	78(6)	43(5)	66(7)	-18(5)	-8(5)	-6(5)
C(10)	114(9)	64(6)	69(8)	-22(6)	10(8)	38(6)

Table 2-5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for naphtho[2,1-*b*]furan derivative **4f**.

	x	y	z	U(eq)
H(23)	9411	2065	5365	62
H(5)	5086	1571	5076	52
H(24)	10334	1237	4052	58
H(3)	4613	3584	3378	62
H(21)	7983	2503	6117	52
H(27)	7350	1048	3264	56
H(17)	2815	4803	10054	81
H(26)	8264	220	1988	65
H(6)	4064	1128	3136	71
H(19)	3684	3353	6521	58
H(15)	6941	4142	9785	67
H(2)	3648	3139	1325	70
H(18)	2561	3951	7785	74
H(16)	4203	5043	10915	72
H(14)	5765	4754	10905	75
H(10A)	10968	562	2012	123
H(10B)	10985	-285	1748	123
H(10C)	10790	43	3612	123