Electronic Supplementary Material (ESI) for RSC Advances.

Fe-promoted oxidative cyclization of *α*-benzoylthioformanilides for the synthesis of 2-benzoylbenzothiazoles

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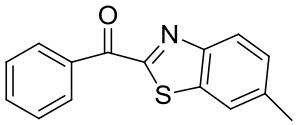
1.Experimental section

The melting points were determined on a XT-5 melting point apparatus and are uncorrected. IR spectra were recorded on a Varian F-1000 spectrometer in KBr with absorptions in cm^{-1}. ^1H NMR (400 MHz or 300 MHz) and ^{13}C NMR (100 MHz or 75 MHz) spectra were recorded on a Varian Inova-300 MHz and Varian Inova-400 MHz in in DMSO-d_6 or $CDCl_3$ solution. *J* values are in hertz. Chemical shifts are expressed in parts per million downfield from internal standard TMS. High-resolution mass spectra (HRMS) for all the compounds were determined on Bruker MicrOTOF-QII mass spectrometer with ESI resource. Dimethyl sulfoxide (DMSO) was dried and distilled from calcium hydride. Toluene was dried and distilled from sodium. All chemicals and solvents were used without further purification unless otherwise stated.

2.General procedure

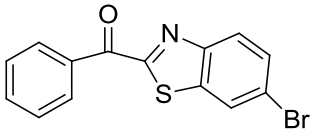
A Schlenk tube equipped with a stir-bar was charged with $FeCl_3$ (0.05 mmol), *α*-benzoylthioformanilides **1** (0.50 mmol) and $K_2S_2O_8$ (134.9 mg, 0.50 mmol). After that, the reaction tube was purged with nitrogen. Then pyridine (1.0 mmol) and 2 mL of DMSO was added to the reaction tube via a syringe. Finally, the Schlenk tube was warmed to 80 ^oC and stirred for 1 h. Then the reaction mixture was quenched with water and extracted with ethyl acetate (20 mL × 2). The organic layers were combined, dried over anhydrous Na_2SO_4 and concentrated under reduced pressure, the crude products were purified by recrystallization from 95% ethanol to give pure product **2** with a yield of 80-96%. The products were further identified by FTIR, NMR and HRMS.

3. Analytical Data of 2- benzoyl benzothiazole



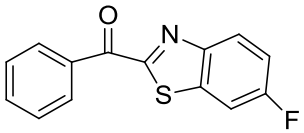
2-Benzoyl-6-methylbenzothiazole (2a)

Purified by recrystallization from 95% ethanol yield **2a** (108.8 mg, 86%) as a white solid. m.p. 100-102 ℃(Lit.[1] 104-108 ℃). IR (KBr, cm^{-1}) *v*: 3059, 1640, 1597, 1570, 1493, 1292, 1118, 909, 852, 704. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 (d, *J* = 7.6 Hz, 2H, ArH), 8.07 (d, *J* = 8.4 Hz, 1H, ArH), 7.75 (s, 1H, ArH), 7.62 (t, *J* = 7.2 Hz, 1H, ArH), 7.51 (t, *J* = 7.2 Hz, 2H, ArH), 7.35 (d, *J* = 8.4 Hz, 1H, ArH), 2.49 (s, 3H, CH_3). ^{13}C NMR (75 MHz, $CDCl_3$) δ 185.4, 166.1, 152.1, 138.3, 137.3, 135.1, 133.8, 131.2, 128.8, 128.5, 125.2, 121.7, 21.8. HRMS (ESI): *m/z* calcd for $C_{15}H_{11}NNaOS$ [$(M+Na)^+$], 276.0459; found, 276.0459.



2-Benzoyl-6-bromobenzothiazole (2b)

Purified by recrystallization from 95% ethanol yield **2b** (141.0 mg, 89%) as a white solid. m.p. 121-123 ℃ (Lit.[2] 123-125 ℃). IR (KBr, cm^{-1}) *v*: 3099, 1642, 1594, 1535, 1478, 1287, 1123, 893, 703. ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.56 (s, 1H, ArH), 8.42 (d, *J* = 6.6 Hz, 2H, ArH), 8.19 (d, *J* = 8.4 Hz, 1H, ArH), 7.80-7.75 (m, 2H, ArH), 7.65-7.59 (m, 2H, ArH). ^{13}C NMR (100 MHz, $CDCl_3$) δ 184.9, 167.7, 152.7, 138.5, 134.7, 134.1, 131.3, 130.7, 128.6, 126.8, 124.8, 122.0.

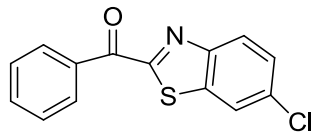


2-Benzoyl-6-fluorobenzothiazole (2c)

Purified by recrystallization from 95% ethanol yield **2c** (119.5 mg, 93%) as a light grey solid. m.p. 96-97 ℃(Lit.[1] 92-97 ℃). IR (KBr, cm^{-1}) *v*: 3086, 1641, 1598, 1563, 1497, 1440, 1248, 863, 704. ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.42 (d, *J* = 6.9 Hz, 2H, ArH), 8.29-8.26 (m, 1H, ArH), 8.13 (d, *J* = 8.1 Hz, 1H, ArH), 7.76-7.73 (m, 1H, ArH), 7.64-7.60 (m, 2H, ArH), 7.54-7.50(m, 1H, ArH). ^{13}C NMR (75 MHz, DMSO-d_6) δ 185.0, 167.4, 161.8 (d, J_{CF} = 245.8 Hz), 150.6, 138.3, 138.1, 134.7 (d, J_{CF} = 9.5 Hz), 131.2, 129.1, 127.6 (d, J_{CF} = 9.9 Hz), 116.9 (d, J_{CF} = 25.4 Hz), 109.4 (d, J_{CF} = 25.9 Hz). HRMS (ESI): *m/z* calcd

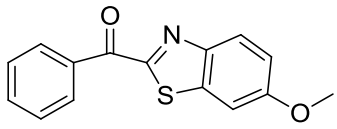
for $C_{14}H_8FNNaOS$ [$(M+Na)^+$], 280.0208; found, 280.0200.

6-Chloro-2-Benzoylbenzothiazole (2d)



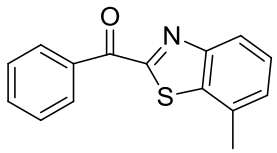
Purified by recrystallization from 95% ethanol yield **2d** (122.8 mg, 90 %) as a white solid. m.p. 105-106 ℃(Lit.[1] 103-106 ℃). IR (KBr, cm^{-1}) *v*: 3126, 1657, 1588, 1533, 1483, 1292, 1095, 844, 712. ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.44-8.40 (m, 3H, ArH), 8.26 (d, *J* = 8.4 Hz, 1H, ArH), 7.76 (d, *J* = 6.3 Hz, 1H, ArH), 7.68-7.63 (m, 3H, ArH). ^{13}C NMR (75 MHz, DMSO-d_6) δ 185.1, 168.1, 152.4, 138.1, 134.7, 133.2, 131.3, 129.1, 128.5, 127.1, 122.9. HRMS (ESI): *m/z* calcd for $C_{14}H_8ClNNaOS$ [$(M+Na)^+$], 295.9913; found, 295.9904.

2-Benzoyl-6-methoxybenzothiazole (2e)

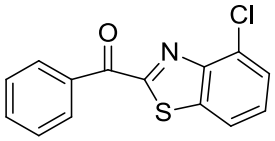


Purified by recrystallization from 95% ethanol yield **2e** (117.0 mg, 87 %) as a white solid. m.p. 168-169 ℃(Lit.[2] 171-173 ℃). IR (KBr, cm^{-1}) *v*: 3095, 1640, 1607, 1494, 1452, 1258, 1229, 1017, 860, 708. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.54 (d, *J* = 7.2 Hz, 2H, ArH), 8.11 (d, *J* = 9.2 Hz, 1H, ArH), 7.66 (t, *J* = 7.6 Hz, 1H, ArH), 7.56 (t, *J* = 7.6 Hz, 2H, ArH), 7.43-7.42 (m, 1H, ArH), 7.26-7.18 (m, 1H, ArH), 3.93 (s, 3H, OCH_3). ^{13}C NMR (100 MHz, $CDCl_3$) δ 185.2, 164.6, 159.8, 148.5, 139.1, 135.2, 133.7, 131.2, 128.5, 126.5, 117.7, 103.4, 55.9.

2-Benzoyl-7-methylbenzothiazole (2f)

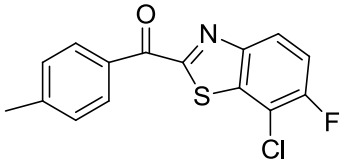


Purified by recrystallization from 95% ethanol yield **2f** (105.0 mg, 83 %) as a light yellow solid. m.p. 96-98 ℃. IR (KBr, cm^{-1}) *v*: 3121, 1642, 1597, 1480, 1440, 1291, 1123, 861, 784, 720. ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.43 (d, *J* = 5.1 Hz, 2H, ArH), 8.10 (d, *J* = 7.2 Hz, 1H, ArH), 7.75 (d, *J* = 6.3 Hz, 1H, ArH), 7.65-7.55 (m, 3H, ArH), 7.47-7.44 (m, 1H, ArH), 2.59 (s, 3H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$) δ 185.4, 166.6, 153.8, 137.7, 135.0, 133.9, 132.2, 131.3, 128.5, 127.6, 127.2, 123.2, 21.4. HRMS (ESI): *m/z* calcd for $C_{15}H_{11}NNaOS$ [$(M+Na)^+$], 276.0459; found, 276.0472.



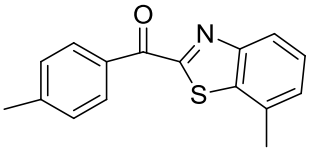
4-Chloro-2-Benzoylbenzothiazole (2g)

Purified by recrystallization from 95% ethanol yield **2g** (113.3 mg, 83 %) as a white solid. m.p. 110-111 ℃(Lit. 110-112 ℃)[3]. IR (KBr, cm^{-1}) *v*: 3057, 1650, 1599, 1482, 1442, 1291, 1100, 888, 769. ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.52-8.46 (m, 2H, ArH), 8.25-8.21 (m, 1H, ArH), 7.77-7.74 (m, 2H, ArH), 7.65-7.61 (m, 3H, ArH). ^{13}C NMR (100 MHz, $CDCl_3$) δ 184.3, 167.8, 150.9, 138.4, 134.5, 134.2, 131.6, 130.5, 128.6, 128.1, 127.1, 120.7.



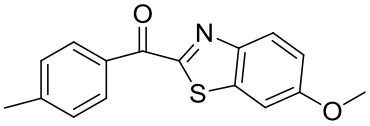
7-Chloro-6-fluoro-2-(4-methylbenzoyl)benzothiazole (2h)

Purified by recrystallization from 95% ethanol yield **2h** (137.2 mg, 90 %) as a light grey solid. m.p. 150-152 ℃. IR (KBr, cm^{-1}) *v*: 3122, 1633, 1601, 1494, 1452, 1390, 1294, 1268, 1253,1184, 1093, 968, 891. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46 (d, J = 8.0 Hz, 2H, ArH), 8.11-8.08 (m, 1H, ArH), 7.41 (d, J = 9.2 Hz, 1H, ArH), 7.38-7.34 (m, 2H, ArH), 2.47 (s, 3H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$) δ 183.7, 168.3, 157.3 (d, J_{CF} = 250.8 Hz), 150.1, 145.4, 139.1, 131.8, 131.4, 129.3, 126.8, 125.0 (d, J_{CF} = 8.4 Hz), 116.6 (d, J_{CF} = 24.3 Hz), 113.8 (d, J_{CF} = 22.7 Hz), 109.0, 108.8, 21.9. HRMS (ESI): *m/z* calcd for $C_{15}H_9ClFNNaOS$ [$(M+Na)^+$], 327.9975; found, 327.9974.



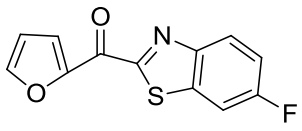
7-Methyl-2-(4-methylbenzoyl)benzothiazole (2i)

Purified by recrystallization from 95% ethanol yield **2i** (106.8 mg, 80 %) as a white solid. m.p. 112-114 ℃. IR (KBr, cm^{-1}) *v*: 3095, 1639, 1600, 1560, 1479, 1286, 1180, 1121, 864, 789. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.47 (d, J = 8.0 Hz, 2H, ArH), 8.08 (d, J = 8.4 Hz, 1H, ArH), 7.50 (t, J = 7.6 Hz, 1H, ArH), 7.32-7.37 (m, 3H, ArH), 2.65 (s, 3H, CH_3), 2.47 (s, 3H, CH_3). ^{13}C NMR (75 MHz, $CDCl_3$) δ 185.0, 166.9, 153.8, 144.9, 137.6, 132.5, 132.3, 131.4, 129.3, 127.4, 127.1, 123.1, 21.9, 21.4. HRMS (ESI): *m/z* calcd for $C_{16}H_{13}NNaOS$ [$(M+Na)^+$], 290.0616; found, 290.0606.



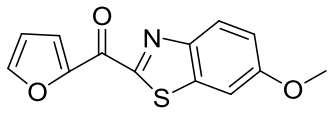
2-(4-Methylbenzoyl)-6-methoxybenzothiazole (2j)

Purified by recrystallization from 95% ethanol yield **2j** (124.5 mg, 88 %) as a light grey solid. m.p. 148-150 ℃. IR (KBr, cm^{-1}) *v*: 3094, 1634, 1604, 1492, 1450, 1255, 1229, 1180, 1020, 865, 830, 741.^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 (d, *J* = 7.6 Hz, 2H, ArH), 8.09 (d, *J* = 9.2 Hz, 1H, ArH), 7.40 (s, 1H, ArH), 7.34 (d, *J* = 7.6 Hz, 2H, ArH), 7.17 (d, *J* = 8.8 Hz, 1H, ArH), 3.91 (s, 3H, OCH_3), 2.46 (s, 3H, CH_3). ^{13}C NMR (75 MHz, $CDCl_3$) δ 184.7, 164.9, 159.6, 148.5, 144.7, 139.0, 132.6, 131.3, 129.2, 126.4, 117.5, 103.4, 55.8, 21.8. HRMS (ESI): *m/z* calcd for $C_{16}H_{13}NNaO_2$ [$(M+Na)^+$], 306.0565; found, 306.0570.



(6-Fluorobenzo[*d*]thiazol-2-yl)(furan-2-yl)methanone (2k)

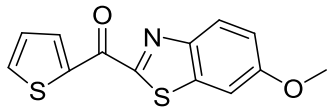
Purified by recrystallization from 95% ethanol yield **2k** (118.6 mg, 96 %) as a grey solid. m.p. 144-146 ℃. IR (KBr, cm^{-1}) *v*: 3126, 1636, 1597, 1497, 1461, 1393, 1247, 1015, 840. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (s, 1H, ArH), 8.17-8.14 (m, 1H, ArH), 7.83 (s, 1H, ArH), 7.66 (d, *J* = 7.6 Hz, 1H, ArH), 7.34-7.28 (m, 1H, ArH), 6.69 (s, 1H, ArH). ^{13}C NMR (75 MHz, DMSO-d_6) δ 173.5, 168.6, 163.8 (d, J_{CF} = 245.6 Hz), 153.2, 152.7, 151.4, 140.1 (d, J_{CF} = 11.8 Hz), 129.6 (d, J_{CF} = 9.4 Hz), 128.0, 119.2 (d, J_{CF} = 25.3 Hz), 116.1, 111.7 (d, J_{CF} = 27.2 Hz). HRMS (ESI): *m/z* calcd for $C_{12}H_6FNNaO_2S$ [$(M+Na)^+$], 270.0001; found, 270.0012.



(Furan-2-yl)(6-methoxybenzo[*d*]thiazol-2-yl)methanone (2l)

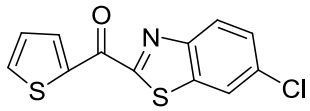
Purified by recrystallization from 95% ethanol yield **2l** (117.8 mg, 91 %) as a light yellow solid. m.p. 208-210 ℃. IR (KBr, cm^{-1}) *v*: 3086, 1629, 1603, 1495, 1465, 1399, 1259, 1230, 1024, 839, 797, 755. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.29-8.24 (m, 2H, ArH), 8.15 (d, *J* = 8.4 Hz, 1H, ArH), 7.81 (s, 1H, ArH), 7.27 (d, *J* = 8.4 Hz, 1H, ArH), 6.88 (s, 1H, ArH), 3.89 (s, 3H, OCH_3). ^{13}C NMR (75 MHz, $CDCl_3$) δ 172.1, 163.4, 159.7, 149.9, 148.6, 148.4, 138.9, 126.2, 124.5,

117.7, 112.8, 103.4, 55.9. HRMS (ESI): *m/z* calcd for $C_{13}H_9NNaO_3S$ [$(M+Na)^+$], 282.0201; found, 282.0200.



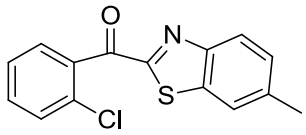
(6-Methoxybenzo[*d*]thiazol-2-yl)(thiophen-2-yl)methanone (2m)

Purified by recrystallization from 95% ethanol yield **2m** (127.9 mg, 93 %) as a light yellow solid. m.p. 162-164 ℃. IR (KBr, cm^{-1}) *v*: 3065, 1621, 1605, 1495, 1410, 1256, 1230, 1038, 833. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.71 (s, 1H, ArH), 8.09 (s, 1H, ArH), 7.80 (s, 1H, ArH), 7.38 (s, 1H, ArH), 7.18 (s, 2H, ArH), 3.91 (s, 3H, OCH_3). ^{13}C NMR (75 MHz, $CDCl_3$) δ 176.9, 164.0, 159.7, 148.3, 139.8, 139.1, 137.0, 136.4, 128.4, 126.3, 117.7, 103.5, 55.9. HRMS (ESI): *m/z* calcd for $C_{13}H_9NNaO_2S_2$ [$(M+Na)^+$], 297.9972; found, 297.9986.



(6-Chlorobenzo[*d*]thiazol-2-yl)(thiophen-2-yl)methanone (2n)

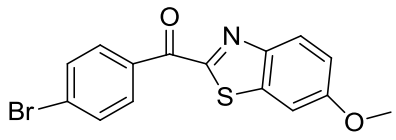
Purified by recrystallization from 95% ethanol yield **2n** (131.6 mg, 94 %) as a light grey solid. m.p. 140-142 ℃. IR (KBr, cm^{-1}) *v*: 3088, 1630, 1485,1410, 1294, 1124, 1087, 1038, 813, 785, 718. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.74 (s, 1H, ArH), 8.13 (d, *J* = 8.4 Hz, 1H, ArH), 7.97 (s, 1H, ArH), 7.85-7.84 (m, 1H, ArH), 7.54 (d, *J* = 8.8 Hz, 1H, ArH), 7.26 (s, 1H, ArH). ^{13}C NMR (75 MHz, $CDCl_3$) δ 176.6, 167.1, 152.2, 139.5, 138.1, 137.5, 137.0, 133.9, 128.5, 128.0, 126.3, 121.8. HRMS (ESI): *m/z* calcd for $C_{12}H_6ClNNaOS_2$ [$(M+Na)^+$], 301.9477; found, 301.9455.



2-(2-Chlorobenzoyl)-6-methylbenzothiazole (2o)

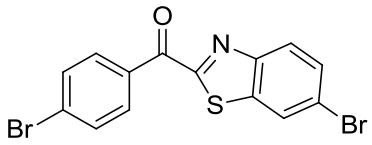
Purified by recrystallization from 95% ethanol yield **2o** (124.8 mg, 87 %) as a light yellow solid. m.p. 164-166 ℃. IR (KBr, cm^{-1}) *v*: 3079, 1658, 1588, 1485, 1433, 1297, 1267, 909, 857, 813, 744. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 8.4 Hz, 1H, ArH), 7.79 (s, 1H, ArH), 7.77 – 7.73 (m, 1H, ArH), 7.53-7.46 (m, 2H, ArH), 7.43-7.39 (m, 1H, ArH), 7.38-7.36 (m, 1H, ArH), 2.52 (s, 3H, CH_3). ^{13}C NMR (75 MHz, $CDCl_3$) δ 187.7, 164.9, 152.0, 138.8, 137.8, 136.1, 132.6, 132.3, 130.8, 130.5, 129.0, 126.5, 125.5, 121.9, 21.9. HRMS

(ESI): *m/z* calcd for $C_{15}H_{10}ClNNaOS$ [$(M+Na)^+$], 310.0069; found, 310.0057.



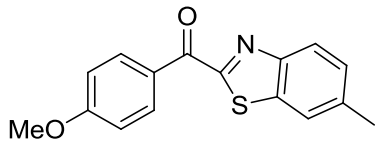
2-(4-Bromobenzoyl)-6-methoxybenzothiazole (2p)

Purified by recrystallization from 95% ethanol yield **2p** (147.4 mg, 85 %) as a light yellow solid. m.p. 192-195 ℃(Lit.[4] 197-199 ℃). IR (KBr, cm^{-1}) *v*: 3090, 1637, 1604, 1496, 1448, 1257, 1114, 1016, 910, 863, 832, 747. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.44 (s, 2H, ArH), 8.08 (s, 1H, ArH), 7.69 (s, 2H, ArH), 7.40 (s, 1H, ArH), 7.19 (s, 1H, ArH), 3.93 (s, 3H, OCH_3). ^{13}C NMR (75 MHz, $CDCl_3$) δ 184.0, 164.2, 159.9, 148.5, 139.2, 133.9, 132.7, 131.8, 129.2, 126.5, 117.8, 103.4, 55.9. HRMS (ESI): *m/z* calcd for $C_{15}H_{10}BrNNaO_2S$ [$(M+Na)^+$], 369.9513; found, 369.9493.



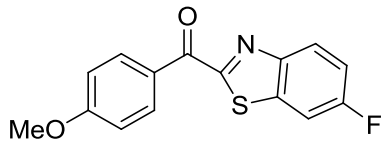
2-(4-Bromobenzoyl)-6-bromobenzothiazole (2q)

Purified by recrystallization from 95% ethanol yield **2q** (172.7 mg, 87 %) as a light yellow solid. m.p. 160-161 ℃. IR (KBr, cm^{-1}) *v*: 3092, 1642, 1584, 1477, 1397, 1289, 1124, 1075, 891, 836, 751. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.44 (d, *J* = 7.6 Hz, 2H, ArH), 8.16 (s, 1H, ArH), 8.08 (d, *J* = 8.8 Hz, 1H, ArH), 7.70 (d, *J* = 6.8 Hz, 3H, ArH). ^{13}C NMR (75 MHz, $CDCl_3$) δ 182.7, 166.2, 151.5, 137.5, 132.3, 131.7, 130.9, 129.8, 128.7, 125.7, 123.7, 121.2. HRMS (ESI): *m/z* calcd for $C_{14}H_7Br_2NNaOS$ [$(M+Na)^+$], 417.8513; found, 417.8509.



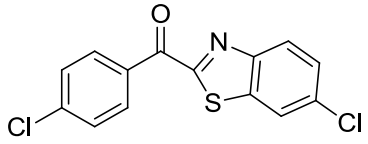
2-(4-Methoxybenzoyl)-6-methylbenzothiazole (2r)

Purified by recrystallization from 95% ethanol yield **2r** (125.9 mg, 89 %) as a light yellow solid. m.p. 138-139 ℃ (Lit.[3] 137-139 ℃). IR (KBr, cm^{-1}) *v*: 3033, 2913, 1632, 1603, 1494, 1301, 1267, 1118, 1031, 911, 860, 814, 760. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.63 (d, *J* = 8.4 Hz, 2H, ArH), 8.09 (d, *J* = 8.4 Hz, 1H, ArH), 7.77 (s, 1H, ArH), 7.37 (d, *J* = 8.4 Hz, 1H, ArH), 7.03 (d, *J* = 8.4 Hz, 1H, ArH), 3.91 (s, 3H, OCH_3), 2.52 (s, 3H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$) δ 183.7, 167.2, 164.6, 152.4, 138.4, 137.5, 134.1, 129.0, 128.2, 125.4, 122.0, 114.2, 55.9, 22.2. HRMS (ESI): *m/z* calcd for $C_{16}H_{13}NNaO_2S$ [$(M+Na)^+$], 306.0565; found, 306.0575.



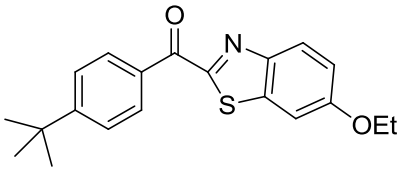
6-Fluoro-2-(4-Methoxybenzoyl)benzothiazole (2s)

Purified by recrystallization from 95% ethanol yield **2s** (127.7 mg, 89 %) asd a light yellow solid. m.p. 146-148 ℃. IR (KBr, cm^{-1}) *v*: 3097, 1632, 1603, 1564, 1501, 1448, 1304, 1250, 1177, 1111, 869, 840, 760. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.56 (d, *J* = 8.4 Hz, 2H, ArH), 8.18-8.17 (m, 1H, ArH), 7.66 (d, *J* = 8.0 Hz, 1H, ArH), 7.33-7.29 (m, 1H, ArH), 7.14 (d, *J* = 8.4 Hz, 1H, ArH), 3.91 (s, 3H, OCH_3). ^{13}C NMR (75 MHz, $CDCl_3$) δ 181.8, 166.8, 163.4, 160.8 (d, J_{CF} = 248.2 Hz), 149.5, 137.1 (d, J_{CF} = 11.2 Hz), 132.8, 126.5, 125.8 (d, J_{CF} = 9.6 Hz), 115.0 (d, J_{CF} = 25.1 Hz), 112.9, 107.1 (d, J_{CF} = 26.5 Hz), 54.6. HRMS (ESI): *m/z* calcd for $C_{15}H_{11}FNO_2S$ [$(M+Na)^+$], 288.0495; found, 288.0471.



6-Chloro-2-(4-chlorobenzoyl)benzothiazole (2t)

Purified by recrystallization from 95% ethanol yield **2t** (130.9 mg, 85 %) as a light yellow solid. m.p. 136-138 ℃. IR (KBr, cm^{-1}) *v*: 3089, 1638, 1586, 1479, 1294, 1134, 1095, 898, 842, 810, 750. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.54 (d, *J* = 8.8 Hz, 2H, ArH), 8.14 d, *J* = 8.8 Hz, 1H, ArH), 7.99 (s, 1H, ArH), 7.56-7.52 (m, 3H, ArH). ^{13}C NMR (75 MHz, $CDCl_3$) δ 184.5, 167.3, 152.3, 140.8, 138.1, 134.2, 132.9, 132.7, 128.9, 128.1, 126.5, 121.8. HRMS (ESI): *m/z* calcd for $C_{14}H_7Cl_2NNaOS$ [$(M+Na)^+$], 329.9523; found, 329.9499.



2-(4-*tert*-butylbenzoyl)-6-ethoxybenzothiazole (2u)

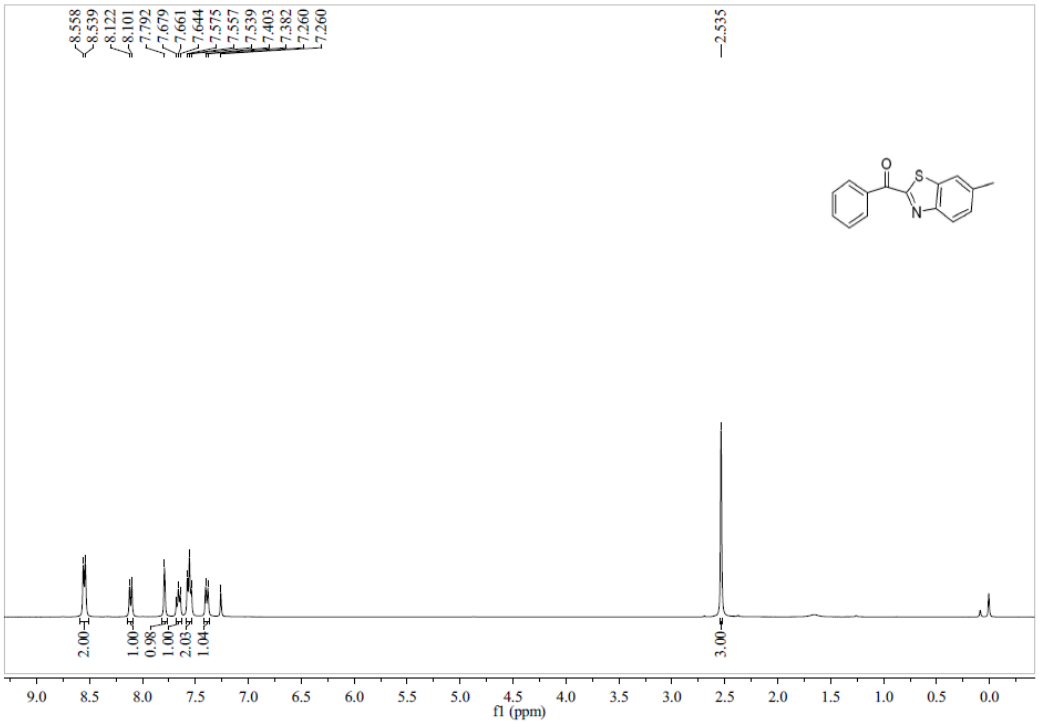
Purified by recrystallization from 95% ethanol yield **2u** (152.5 mg, 90 %) as a light yellow solid. m.p. 108-110 ℃. IR (KBr, cm^{-1}) *v*: 3080, 2970, 1633, 1601, 1492, 1250, 1223, 1191, 1054, 899, 861, 726. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (d, *J* = 8.8 Hz, 2H, ArH), 8.07 (d, *J* = 9.2 Hz, 1H, ArH), 7.56 (d, *J* = 8.8 Hz, 2H, ArH), 7.37 (s, 1H, ArH), 7.16-7.14 (m, 1H, ArH), 4.14-4.09 (m, 2H, CH_2), 1.47 (t, *J* = 6.8 Hz, 3H, CH_3), 1.37 (s, 9H, 3× CH_3),. ^{13}C NMR (75 MHz, $CDCl_3$) δ 183.7, 163.8, 158.0, 156.4, 147.4, 138.0, 131.5, 130.1, 125.3, 124.5, 116.8, 102.9, 63.1, 34.2, 30.1, 13.7. HRMS (ESI): *m/z* calcd for $C_{20}H_{21}NNaO_2S$ [$(M+Na)^+$], 362.1191; found, 362.1202.

4.Reference

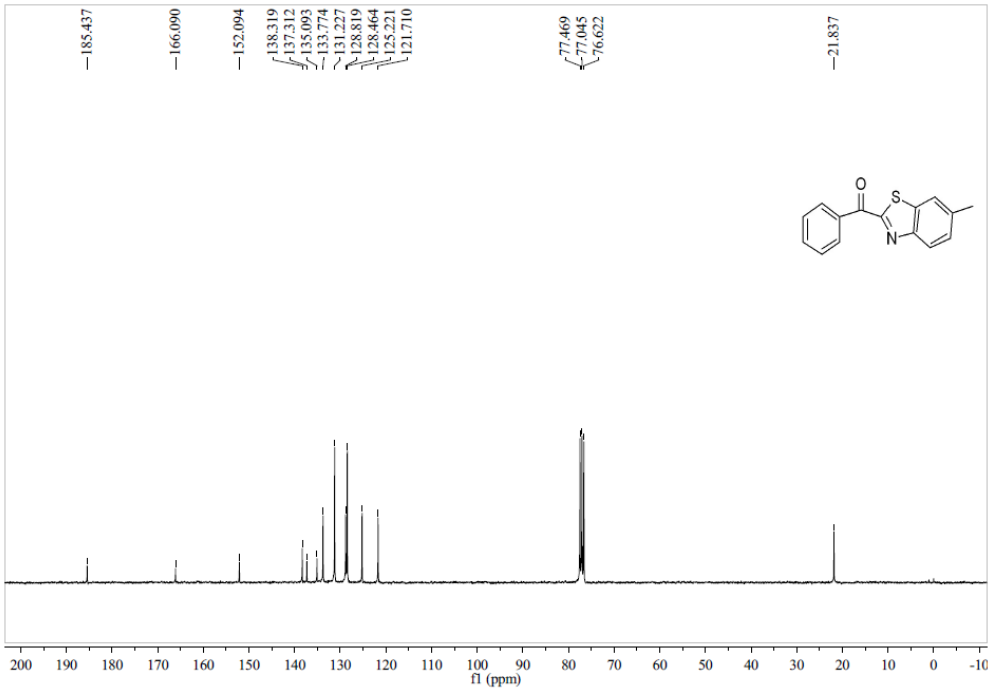
1. Gao, F. F.; Guo, Y. Q.; Li, H. Z.; Wu, A. X.; Xue, W. J. *Org. Lett.* **2013**, *15(4)*, 890-893.
2. Jakub, H.; Jiri, S.; *Eur. J. Org. Chem.* **2010**, *(15)*, 2849-2851.
3. Fan, X. S.; He, Y.; Zhang, X. Y.; Guo, S. H.; Wang, Y. Y.; *Tetrahedron* **2011**, *67(34)*, 6369-6374.
4. Cai, Q.; Gao, Q.; Jia, F.; Liu, M.; Wu, A.; Wu, X.; Zhu, Y. P. *J. Org. Chem.*, **2013**, *(6)*, 2792 – 2797.

5.NMR Spectra of Products

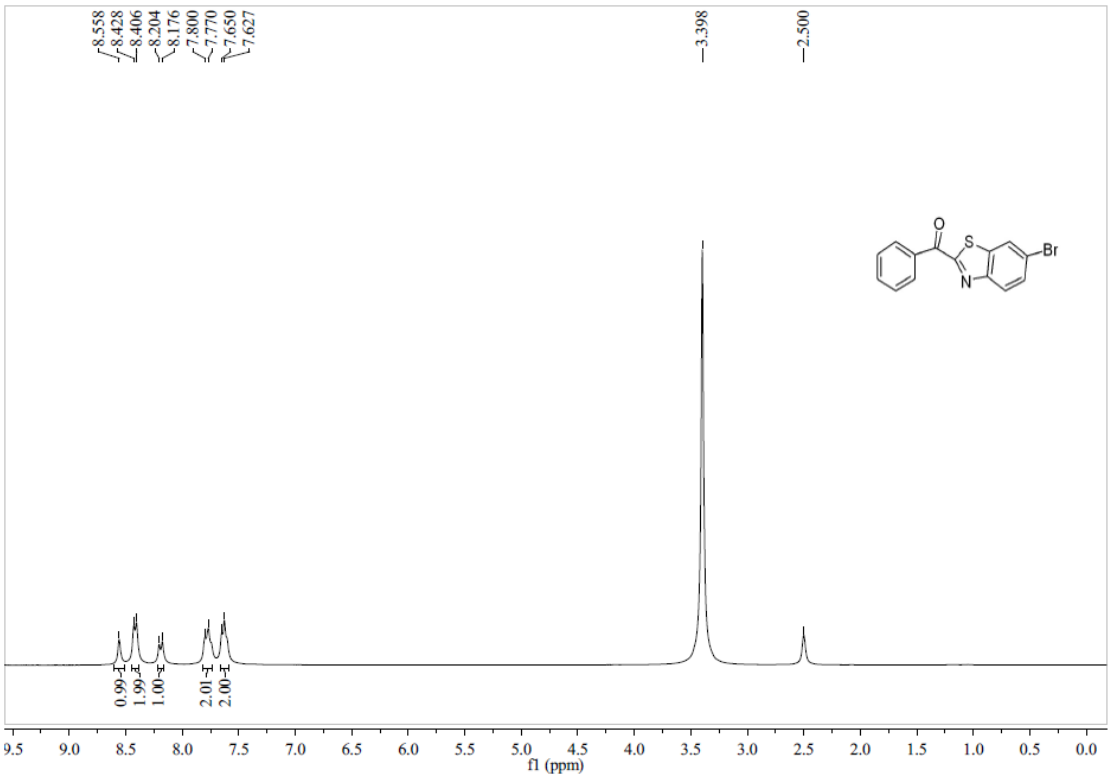
^{1}H NMR of compounds **2a**



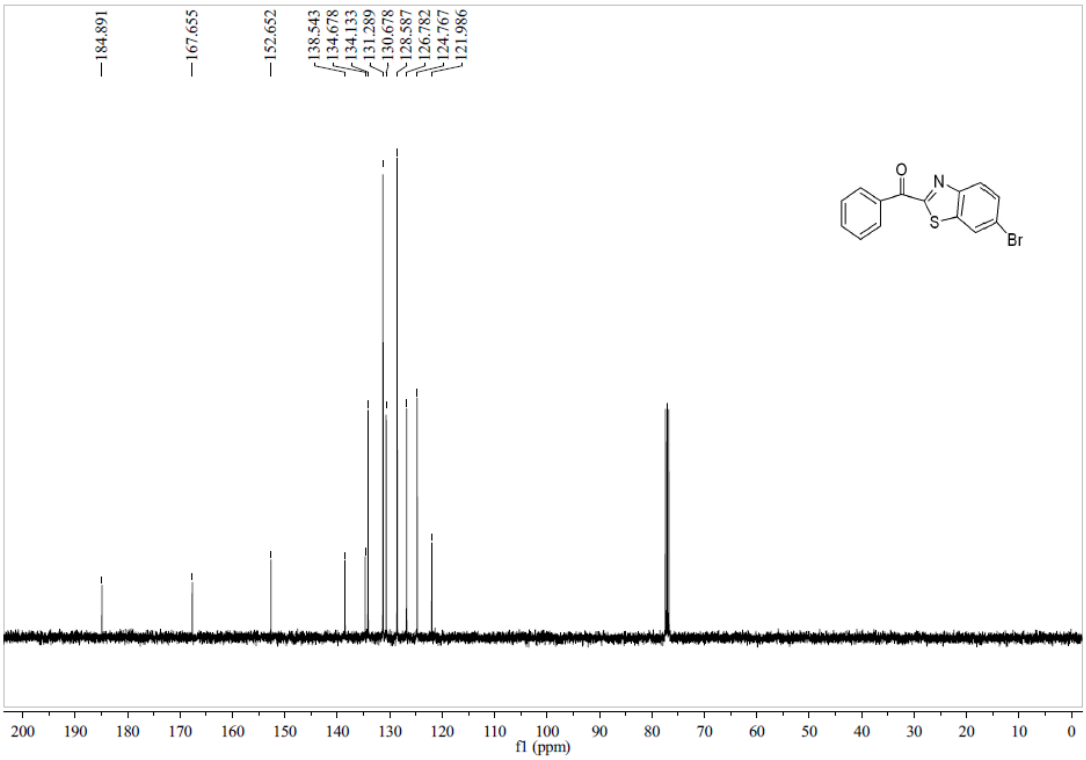
^{13}C NMR of compounds **2a**



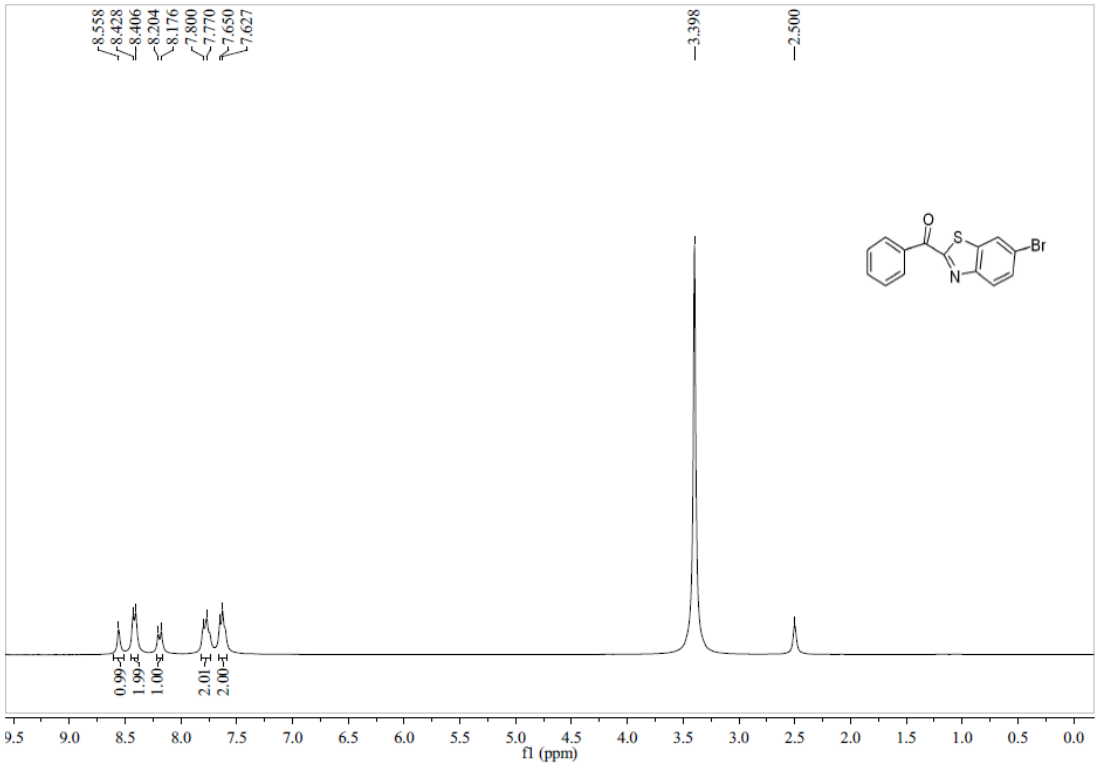
^{1}H NMR of compounds **2b**



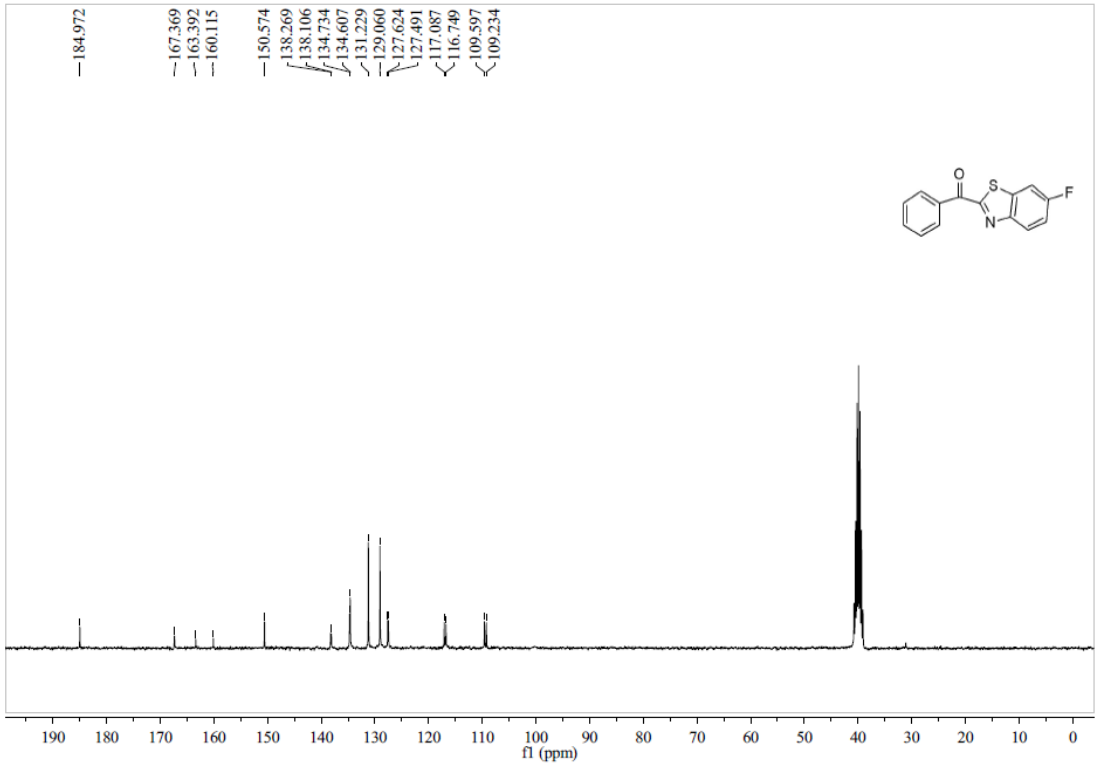
^{13}C NMR of compounds **2b**



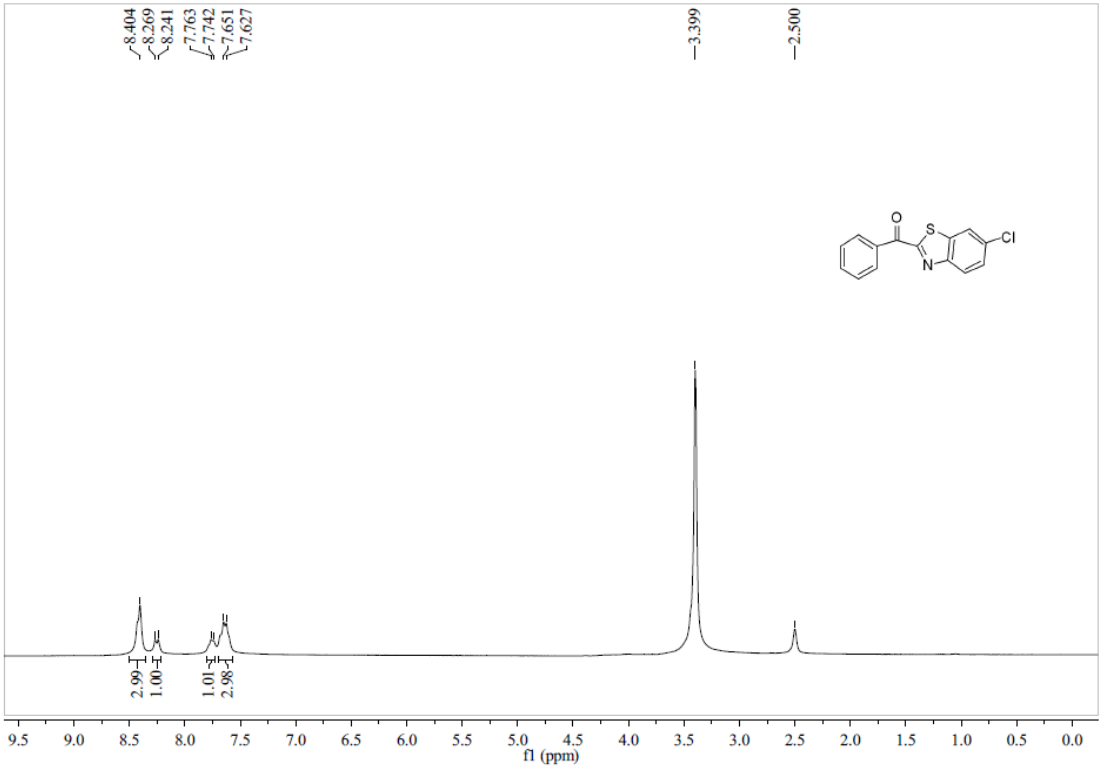
^{1}H NMR of compounds **2c**



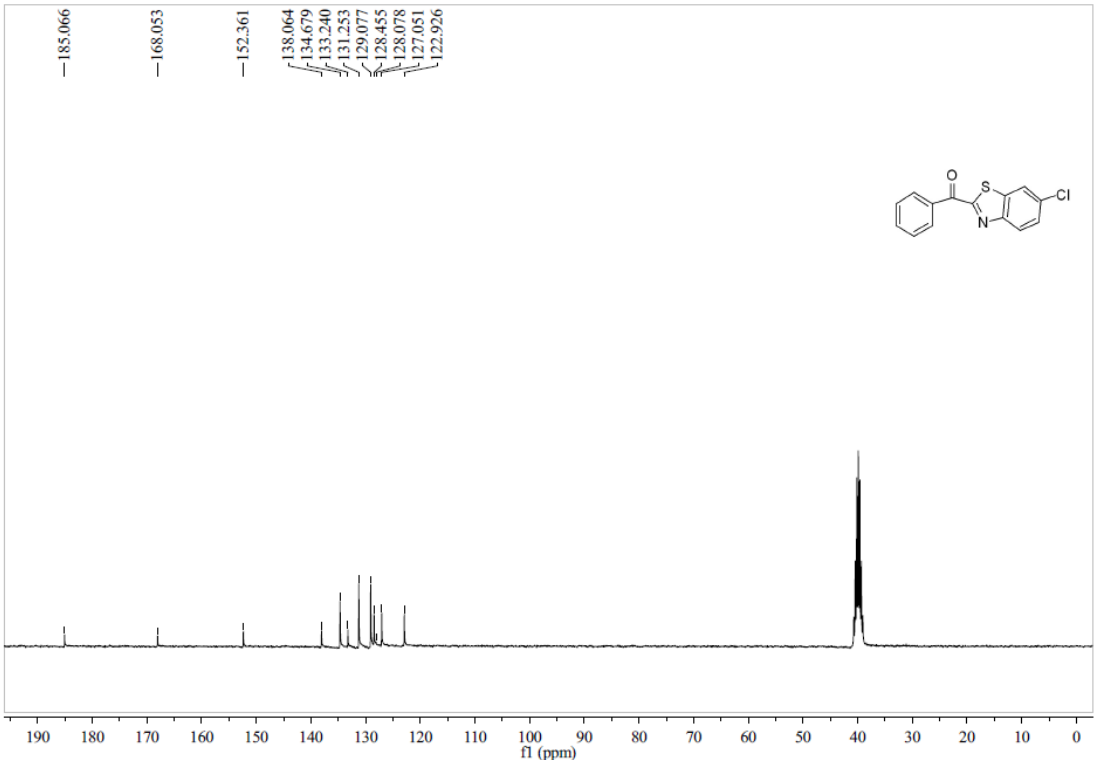
^{13}C NMR of compounds **2c**



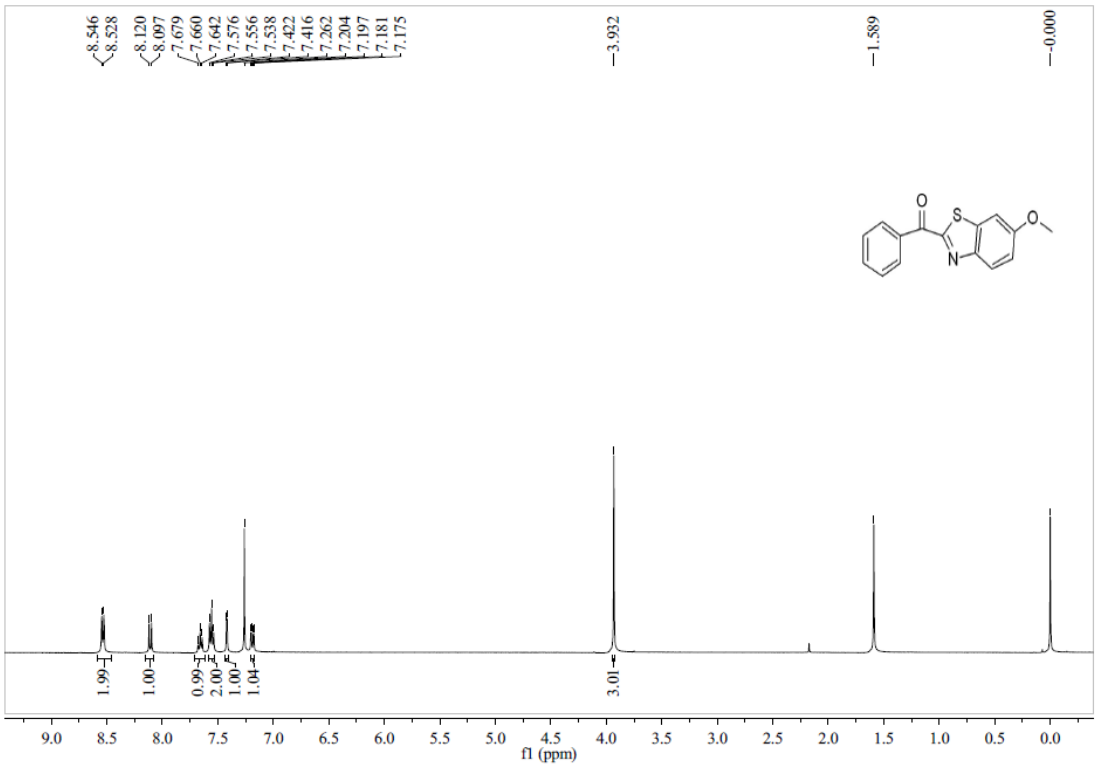
^{1}H NMR of compounds **2d**



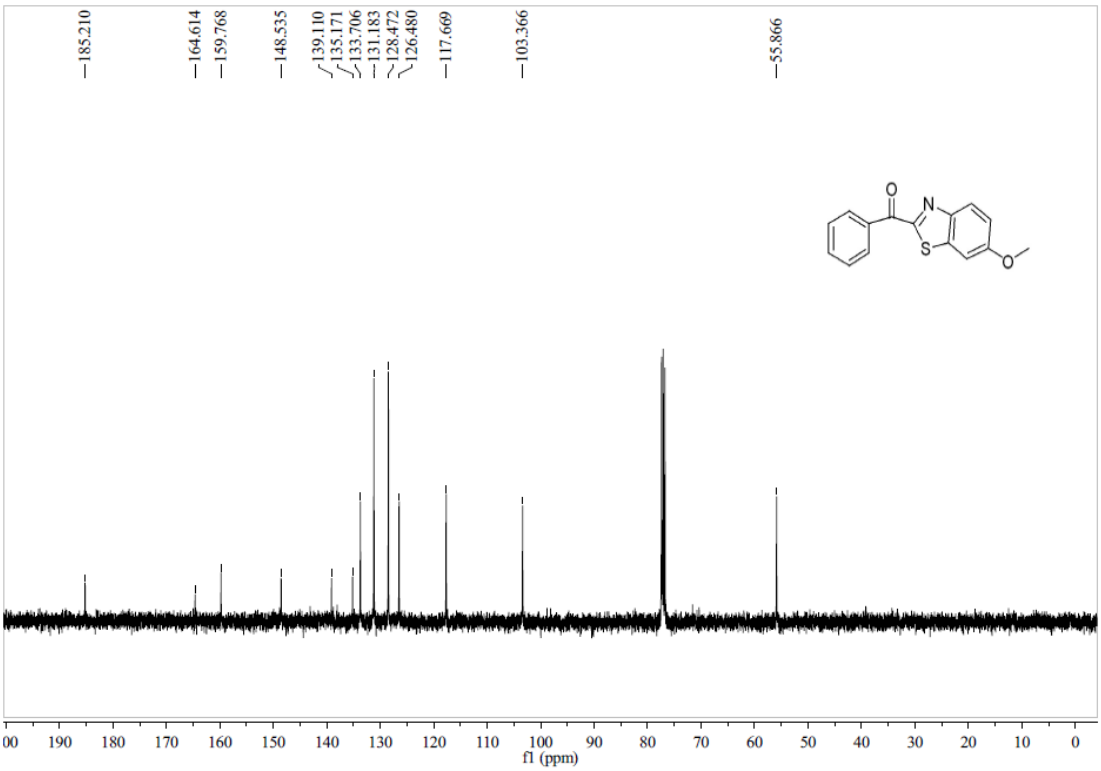
^{13}C NMR of compounds **2d**



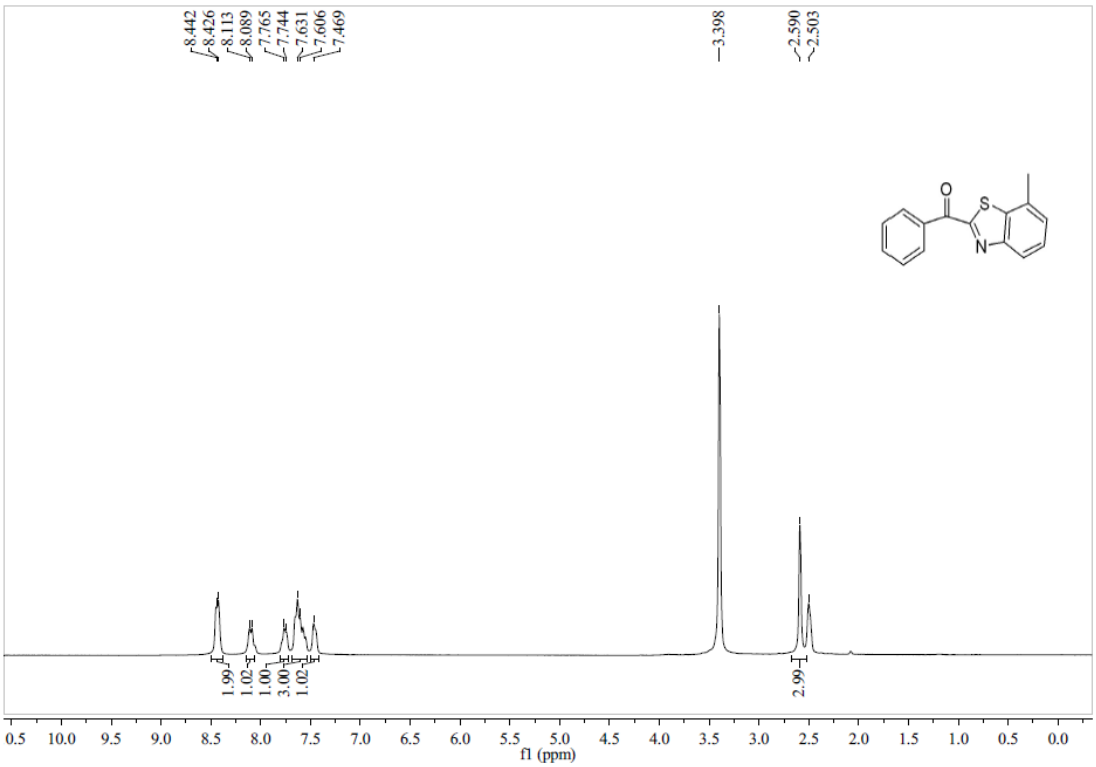
^{1}H NMR of compounds **2e**



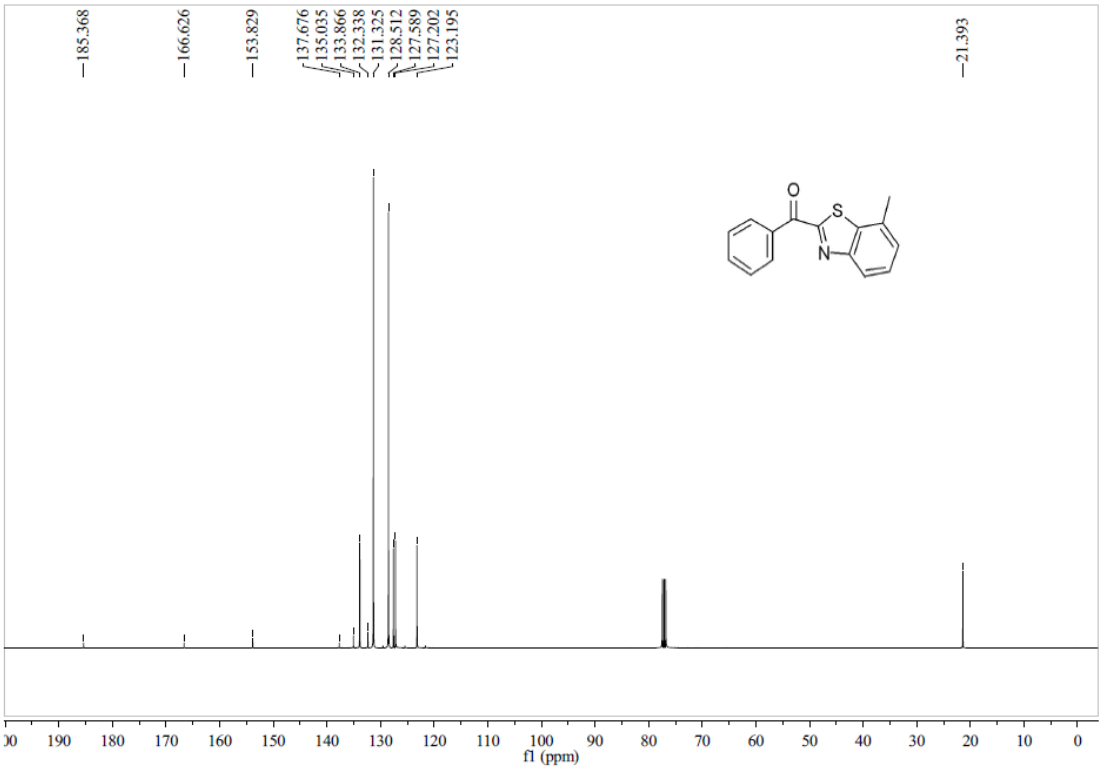
^{13}C NMR of compounds **2e**



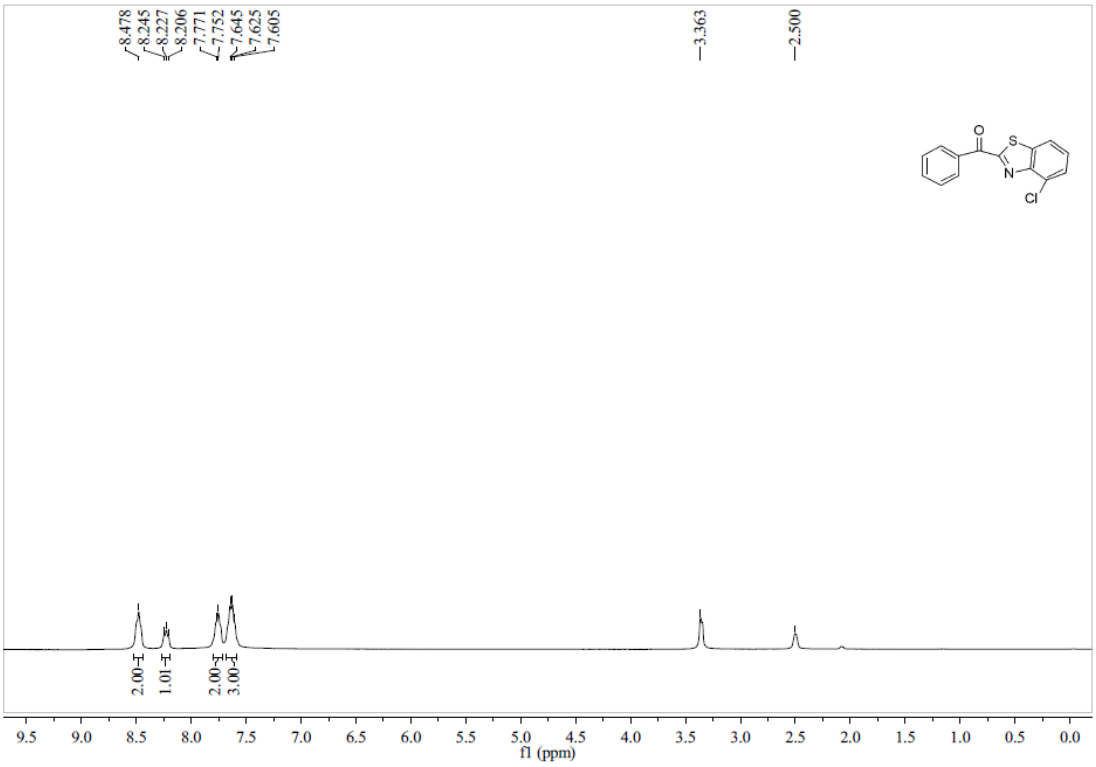
^{1}H NMR of compounds **2f**



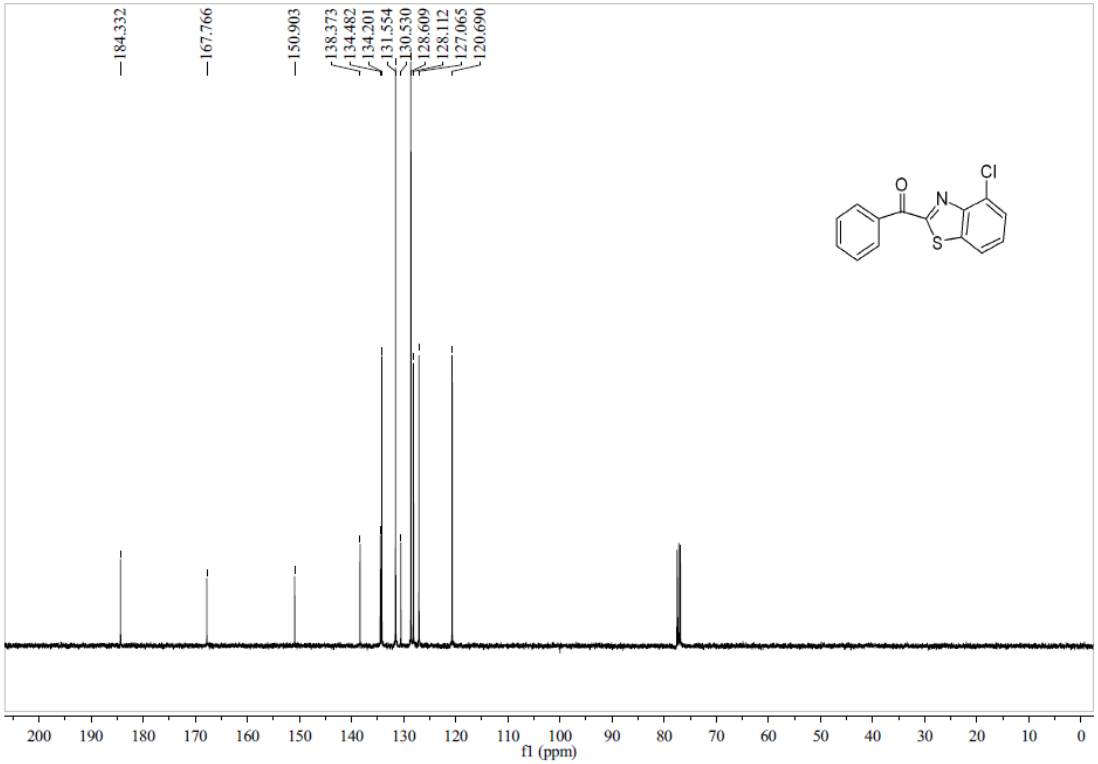
^{13}C NMR of compounds **2f**



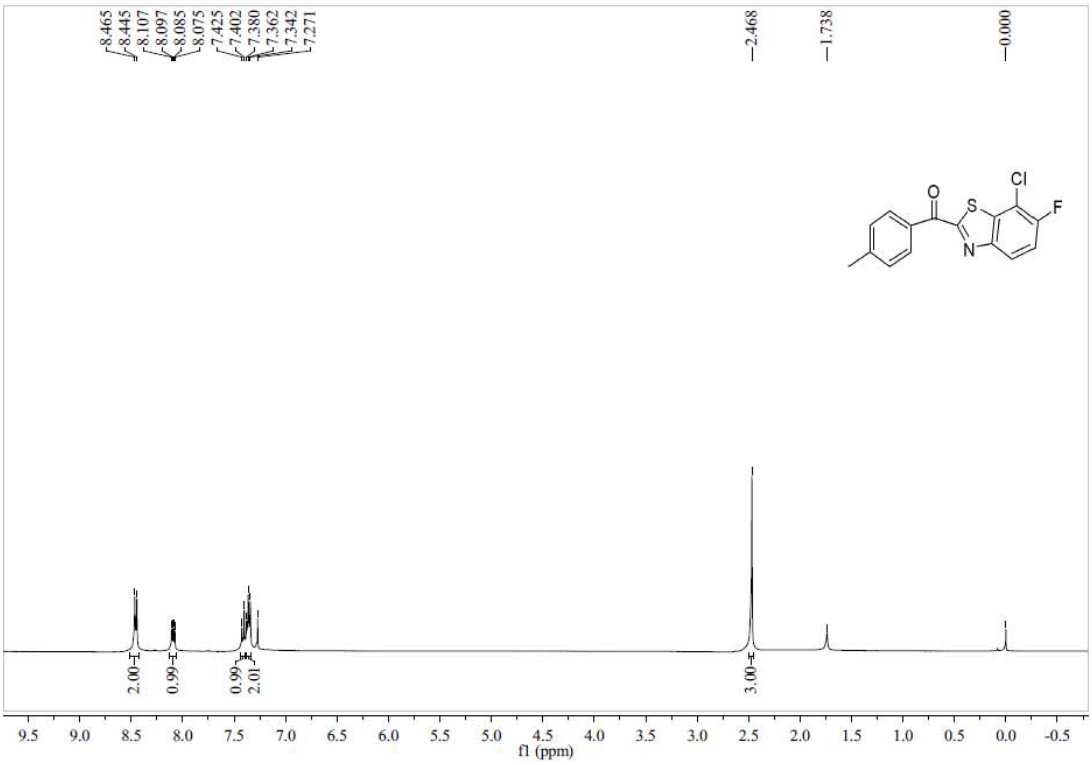
^{1}H NMR of compounds **2g**



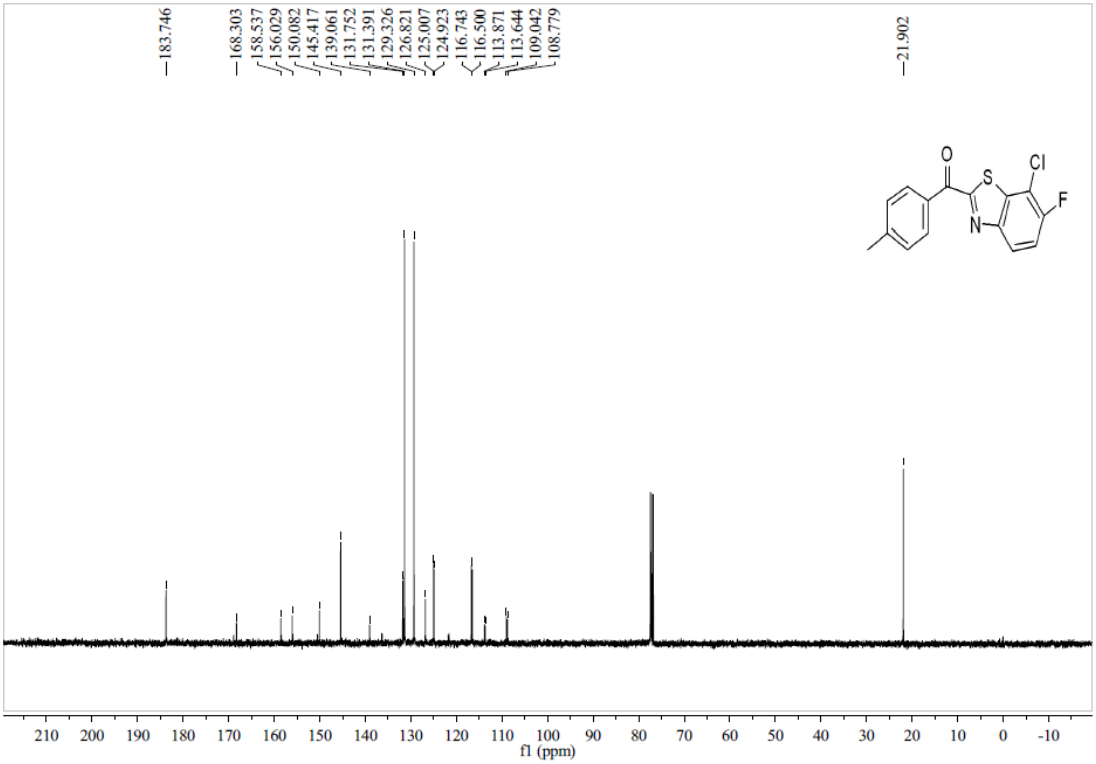
^{13}C NMR of compounds **2g**



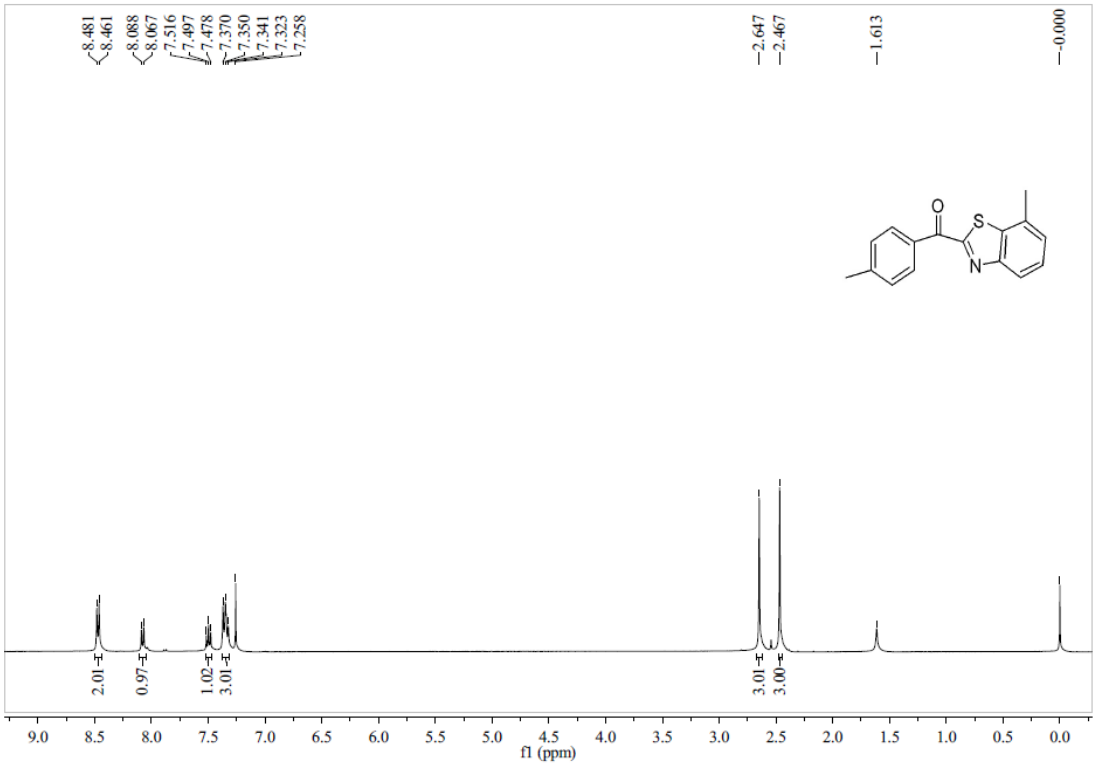
^{1}H NMR of compounds **2h**



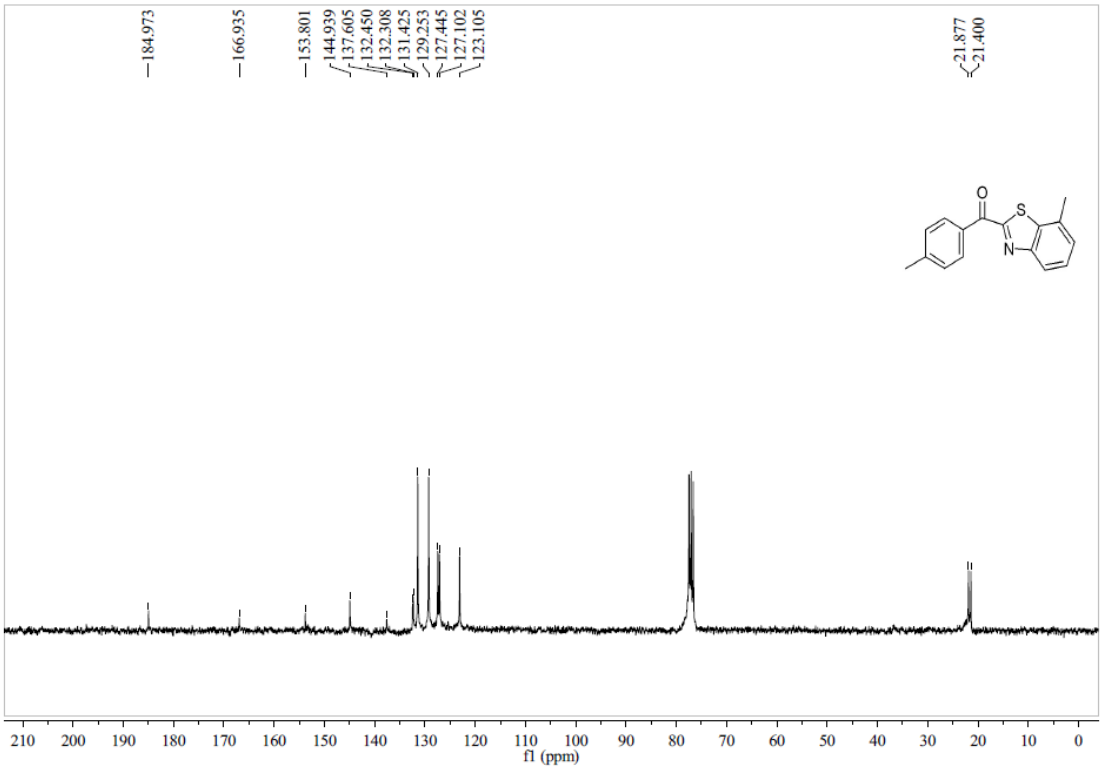
^{13}C NMR of compounds **2h**



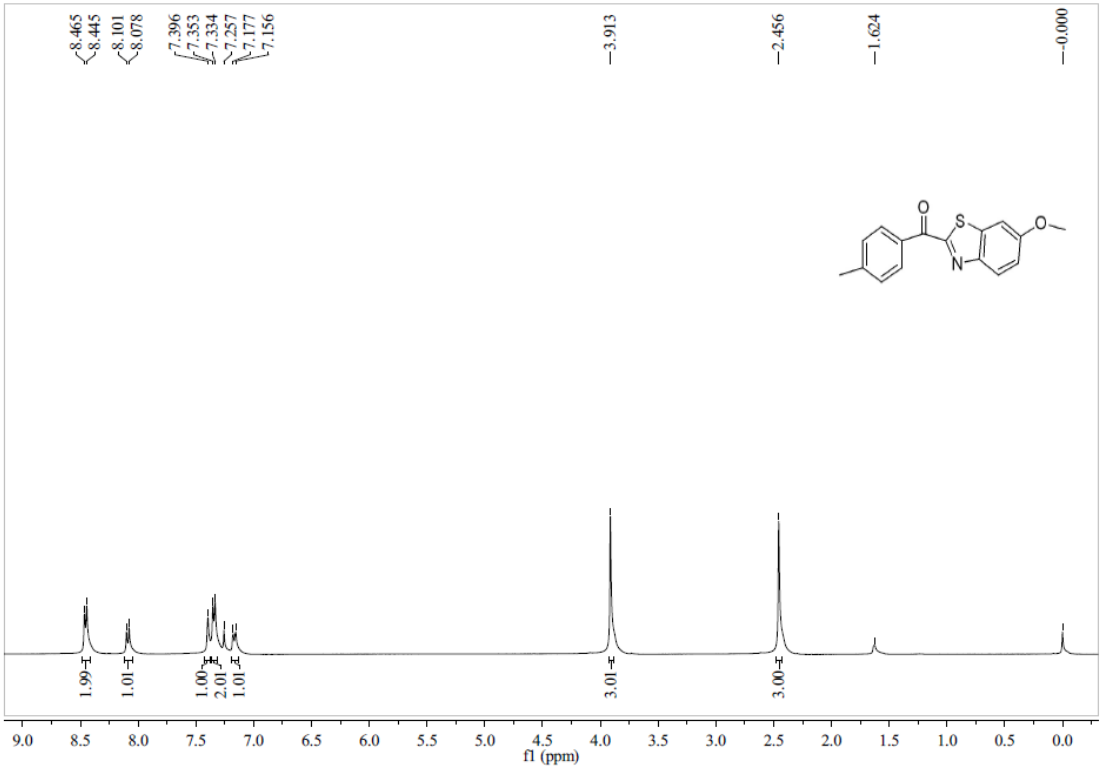
^{1}H NMR of compounds **2i**



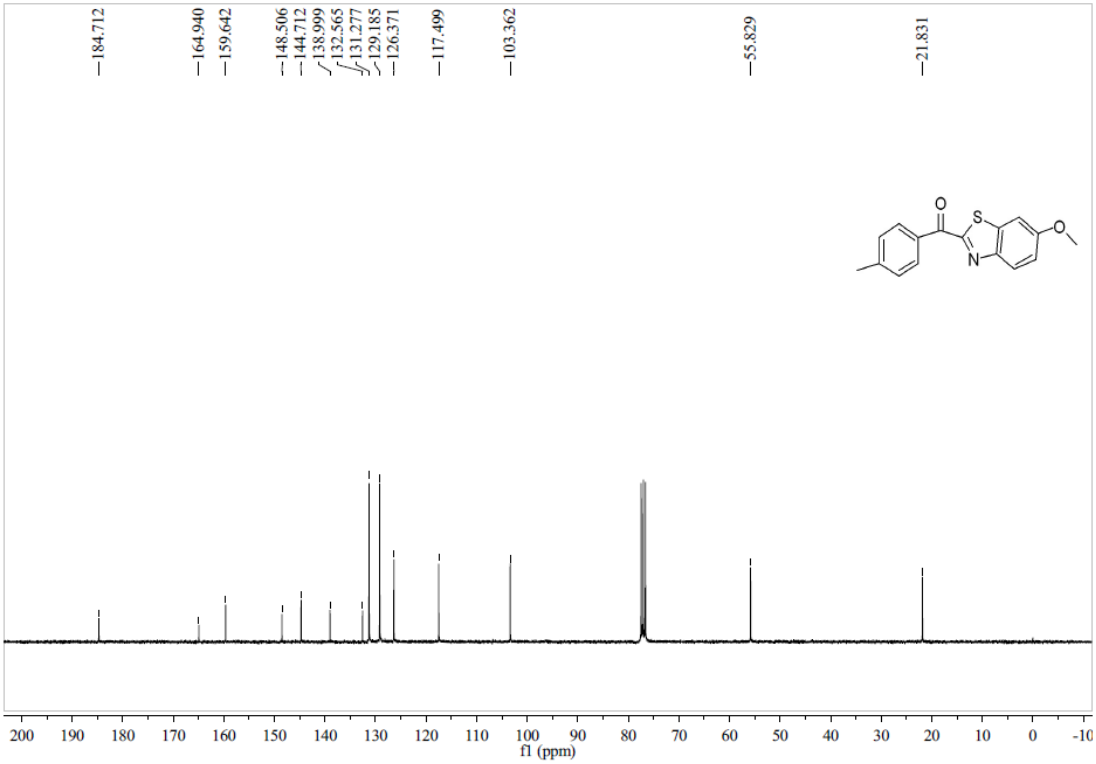
^{13}C NMR of compounds **2i**



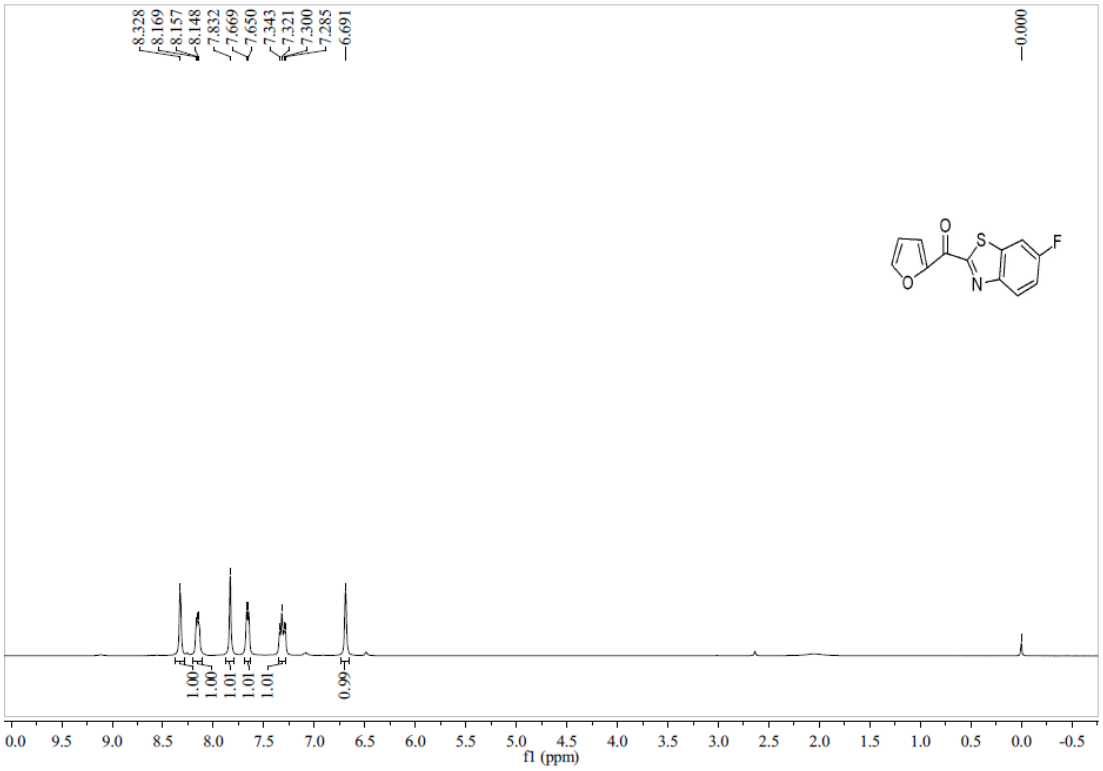
^{1}H NMR of compounds **2j**



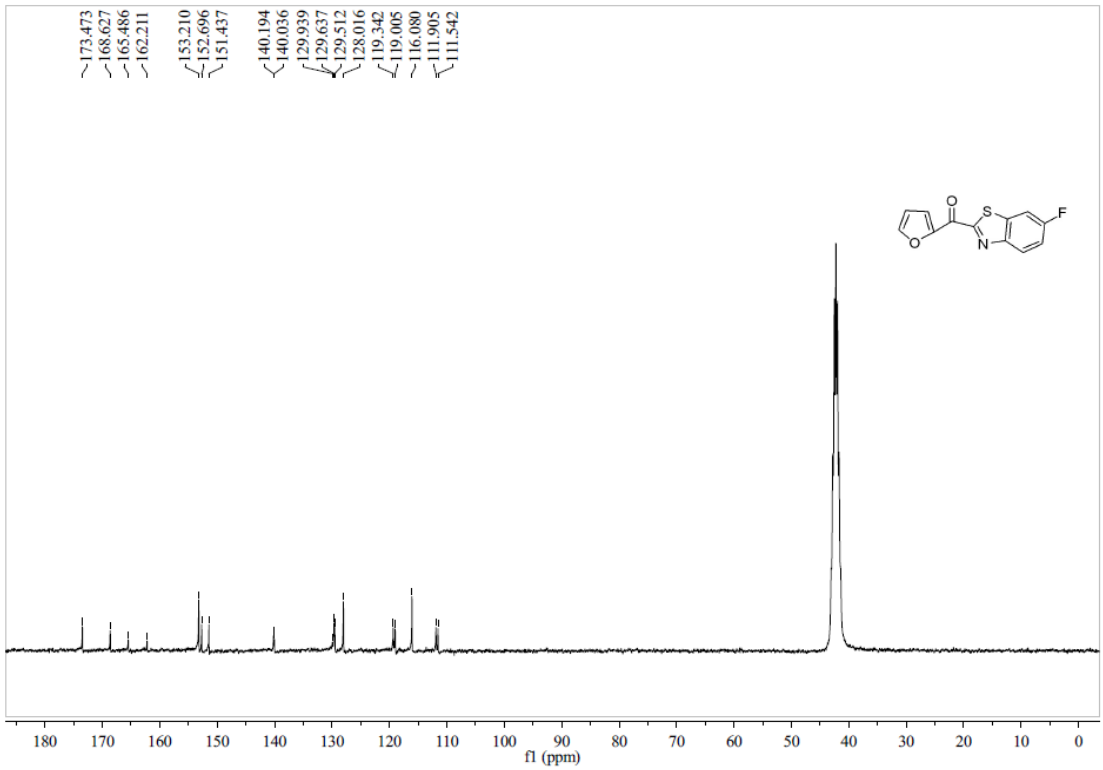
^{13}C NMR of compounds **2j**



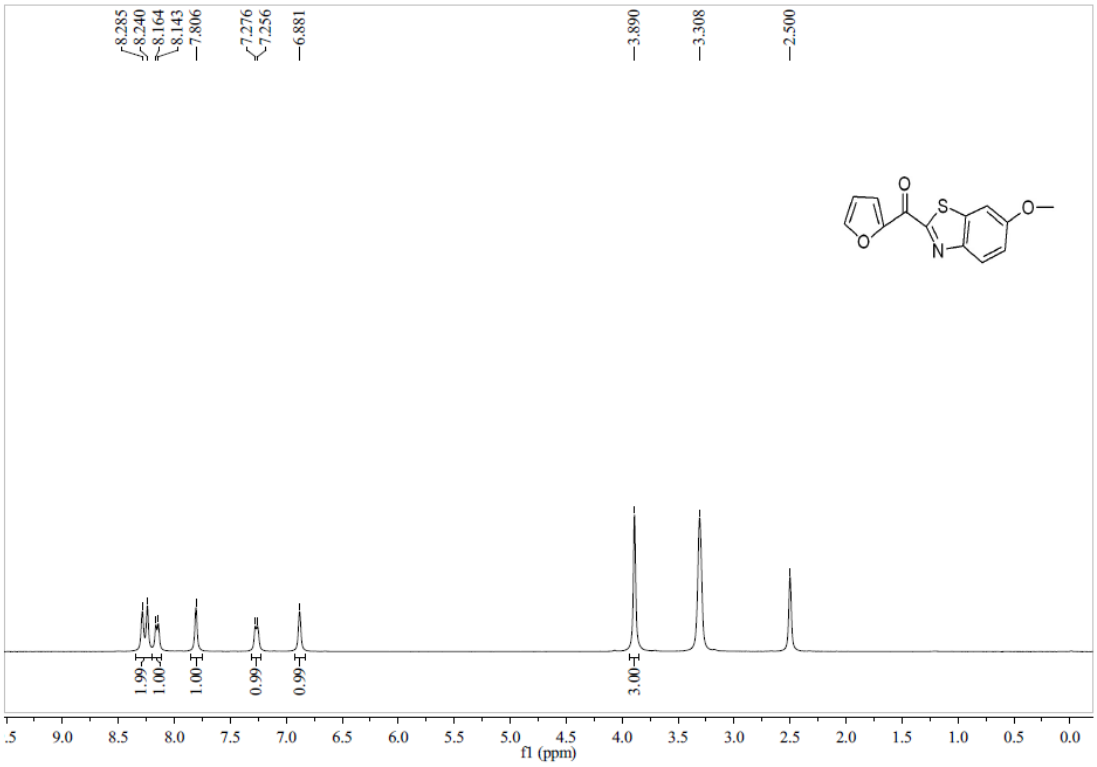
^{1}H NMR of compounds **2k**



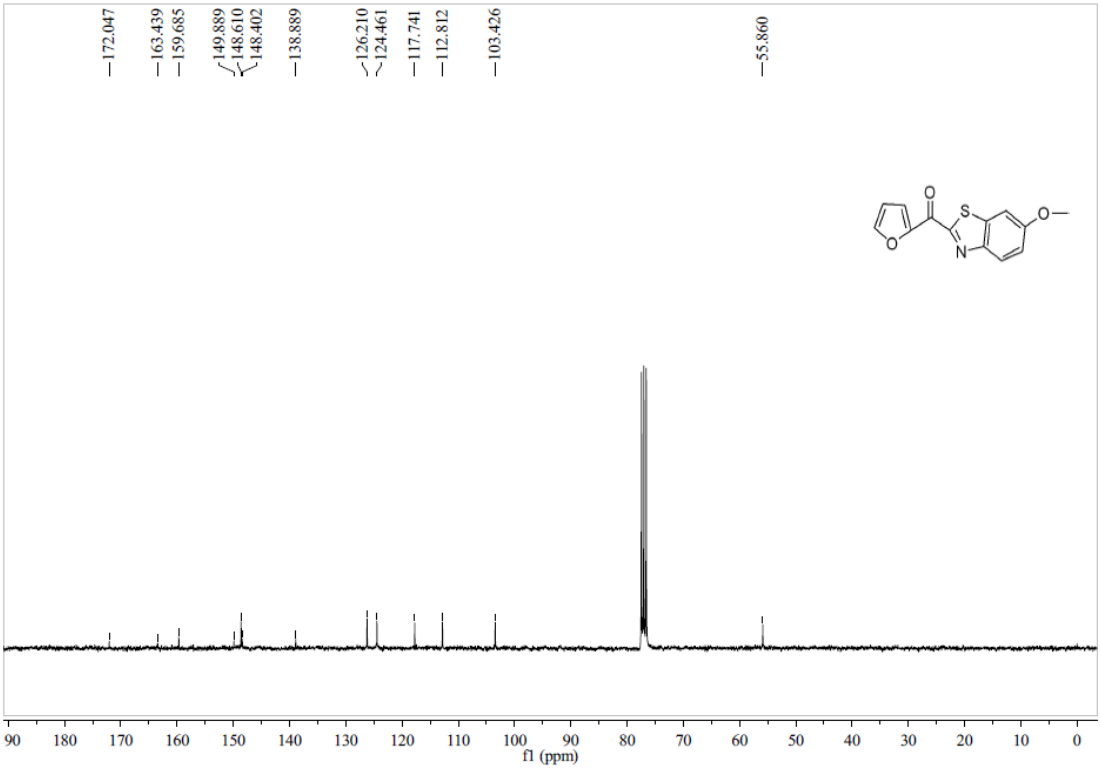
^{13}C NMR of compounds **2k**



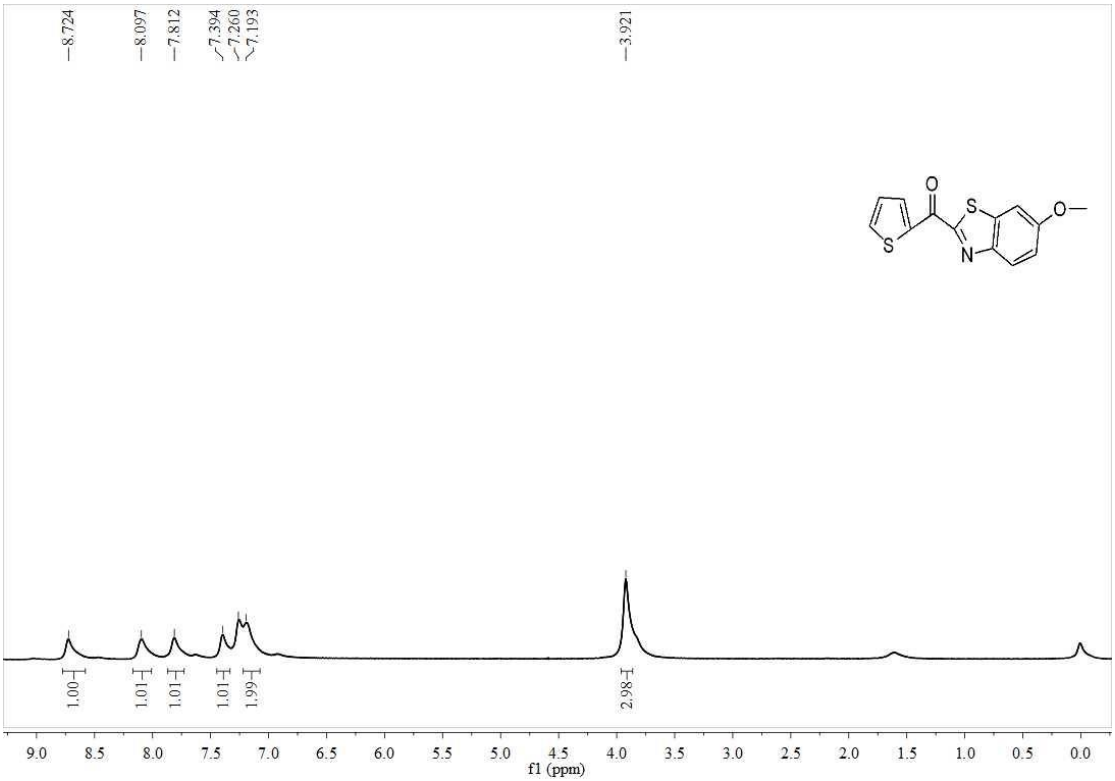
^{1}H NMR of compounds **2l**



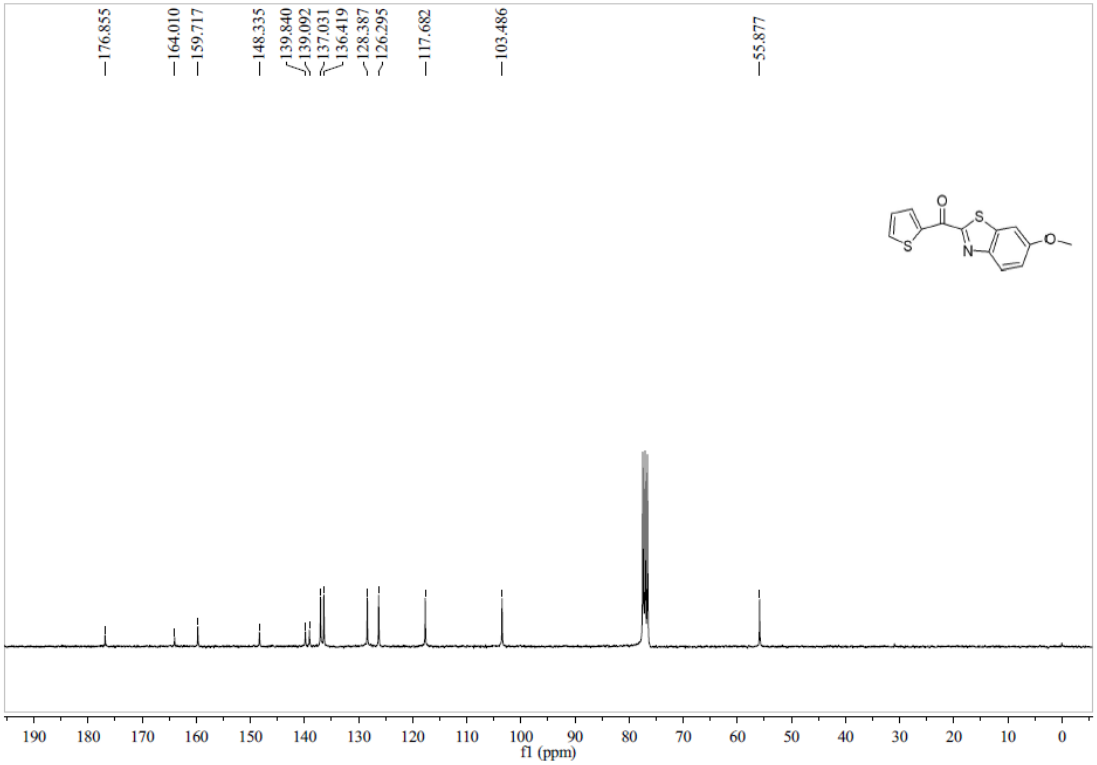
^{13}C NMR of compounds **2l**



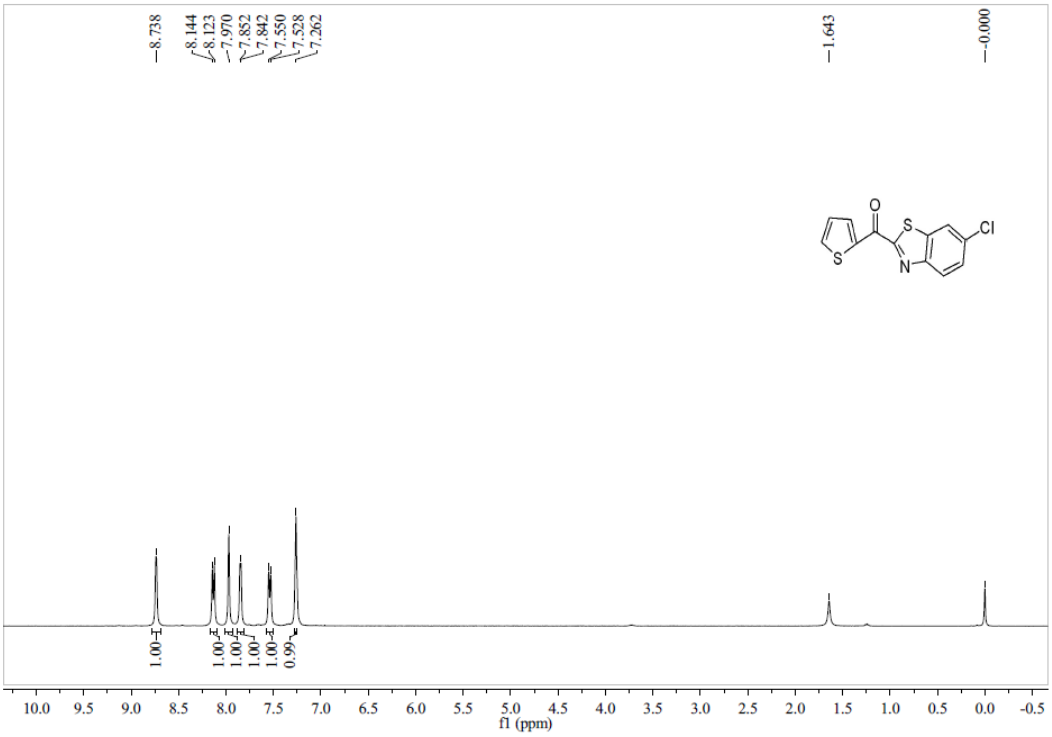
^{1}H NMR of compounds **2m**



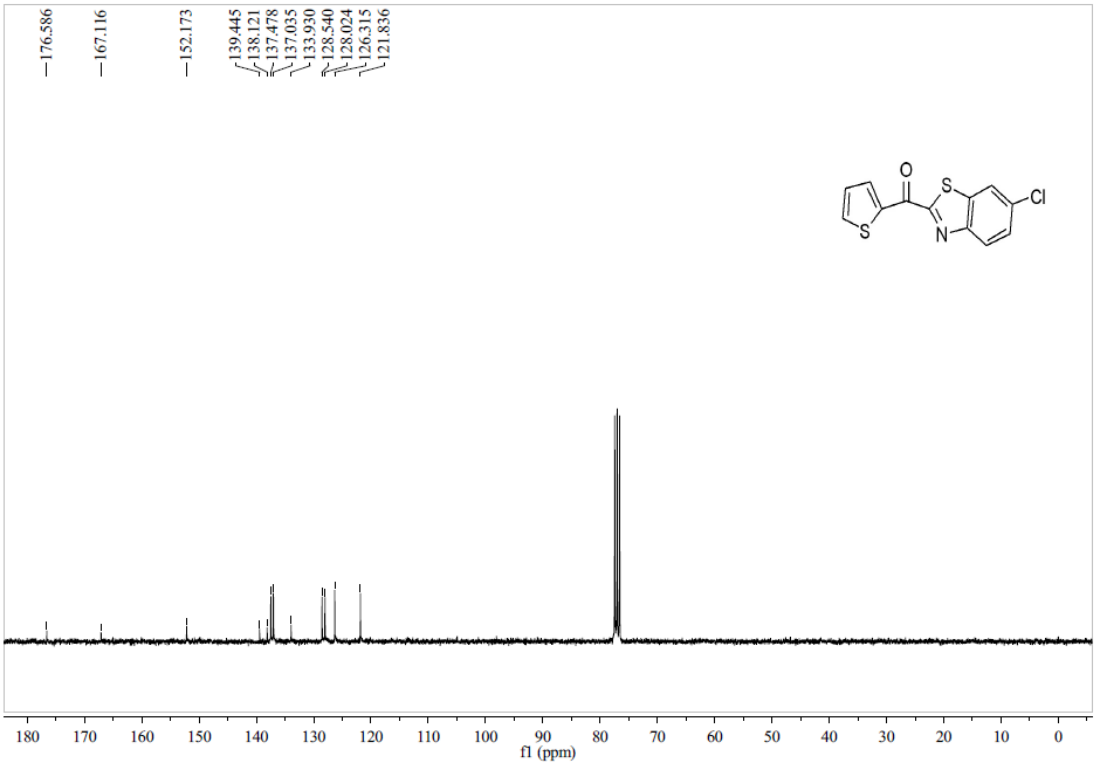
^{13}C NMR of compounds **2m**



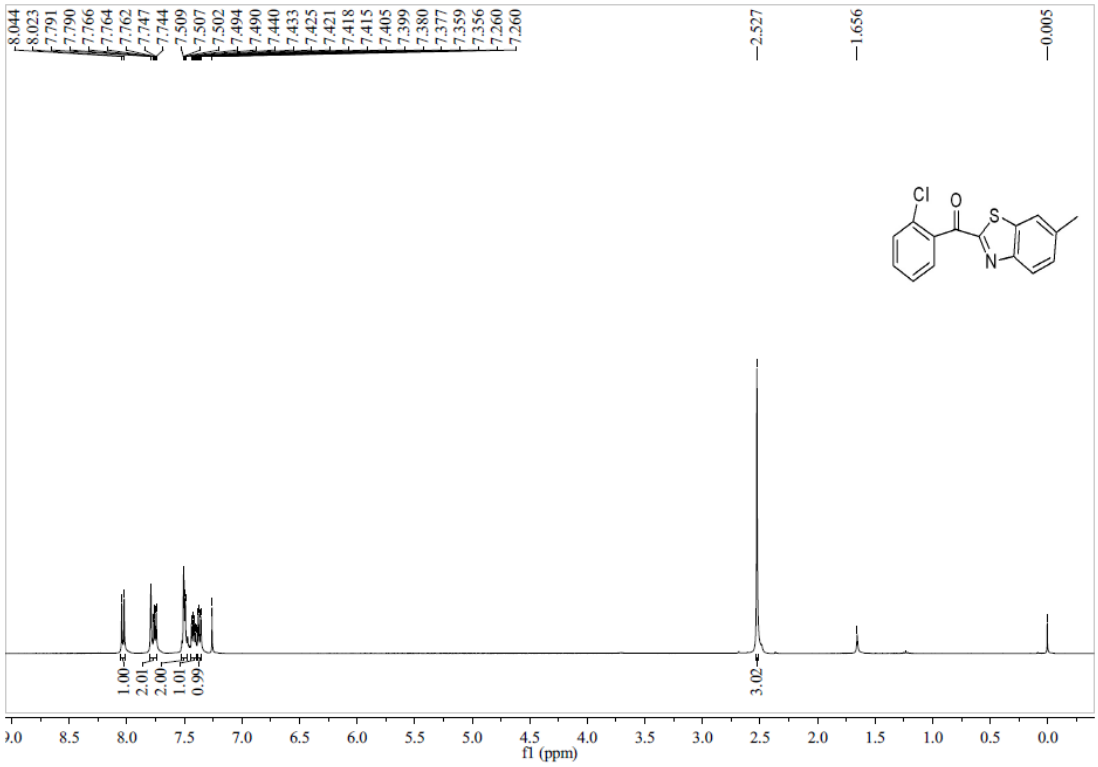
^{1}H NMR of compounds **2n**



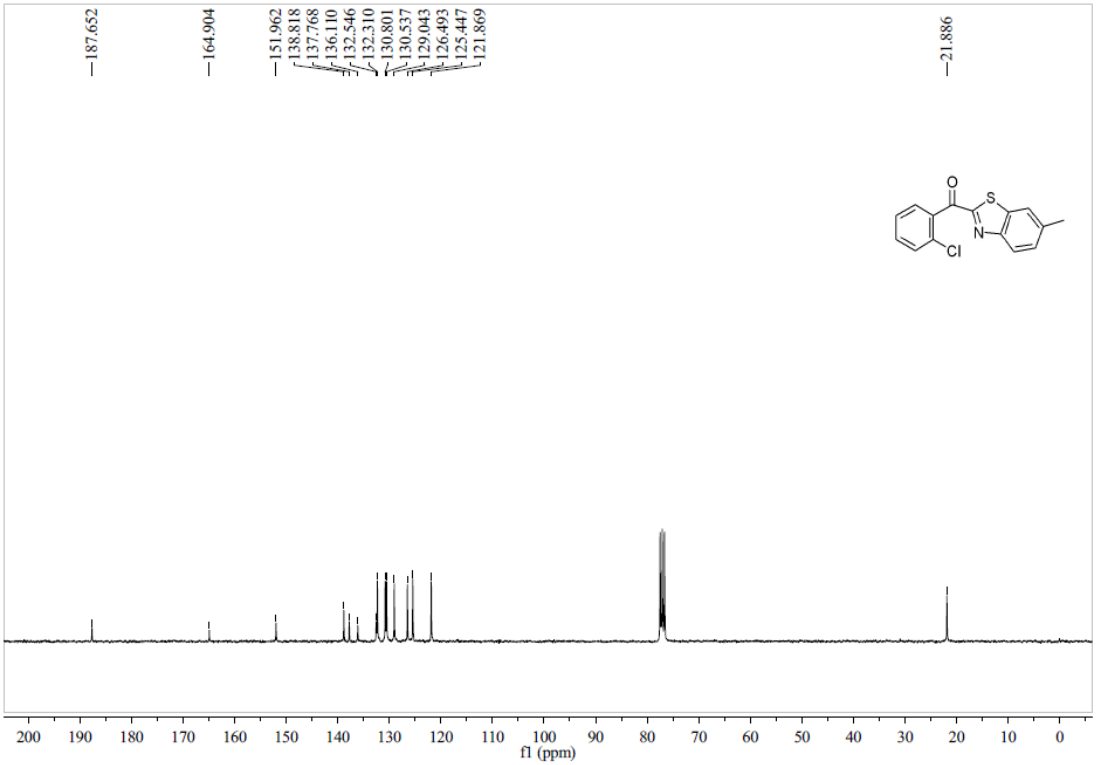
^{13}C NMR of compounds **2n**



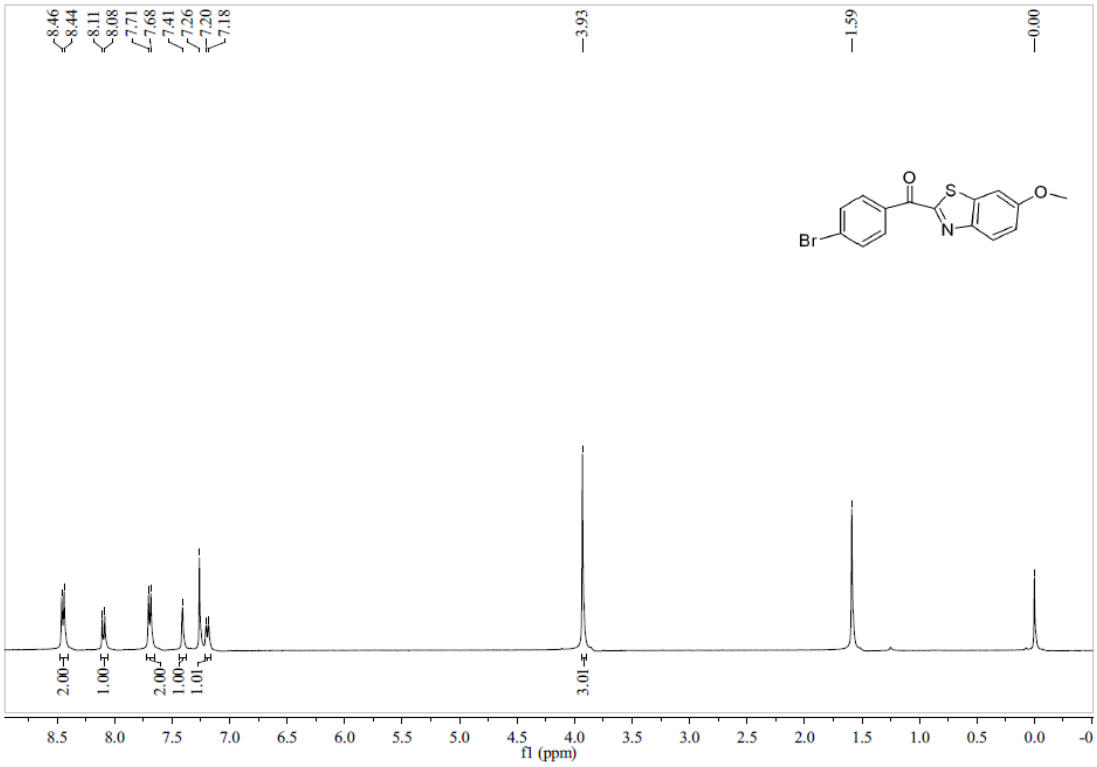
^{1}H NMR of compounds **2o**



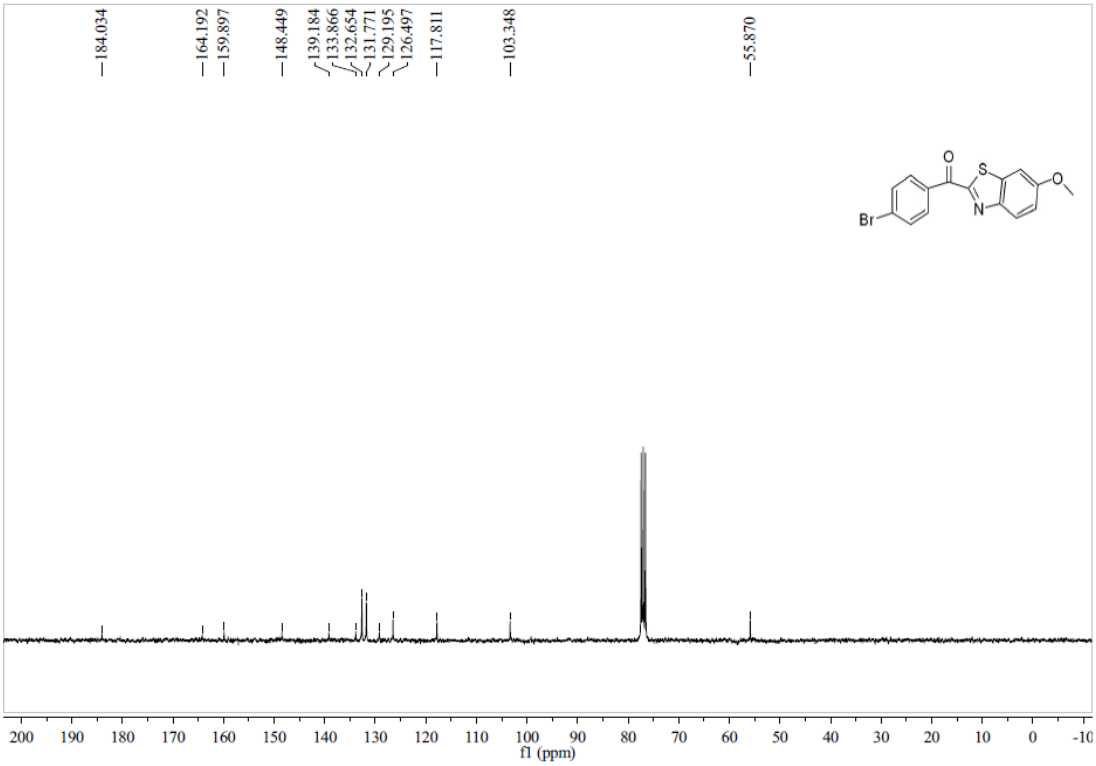
^{13}C NMR of compounds **2o**



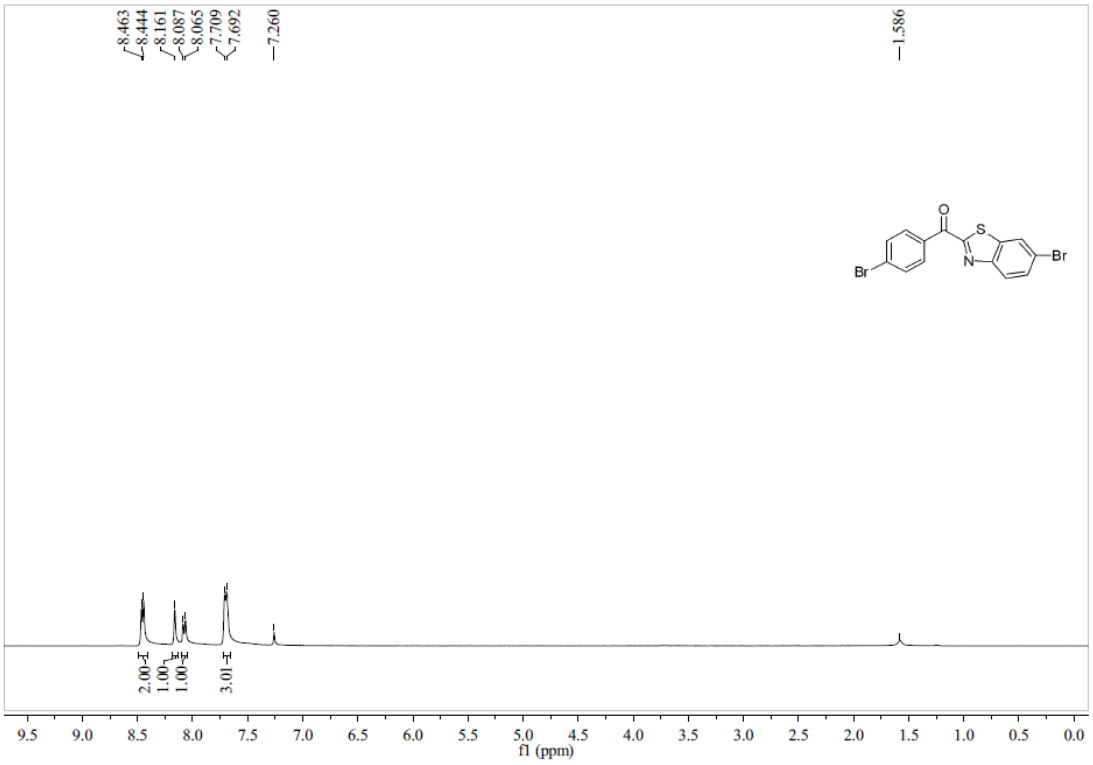
^{1}H NMR of compounds **2p**



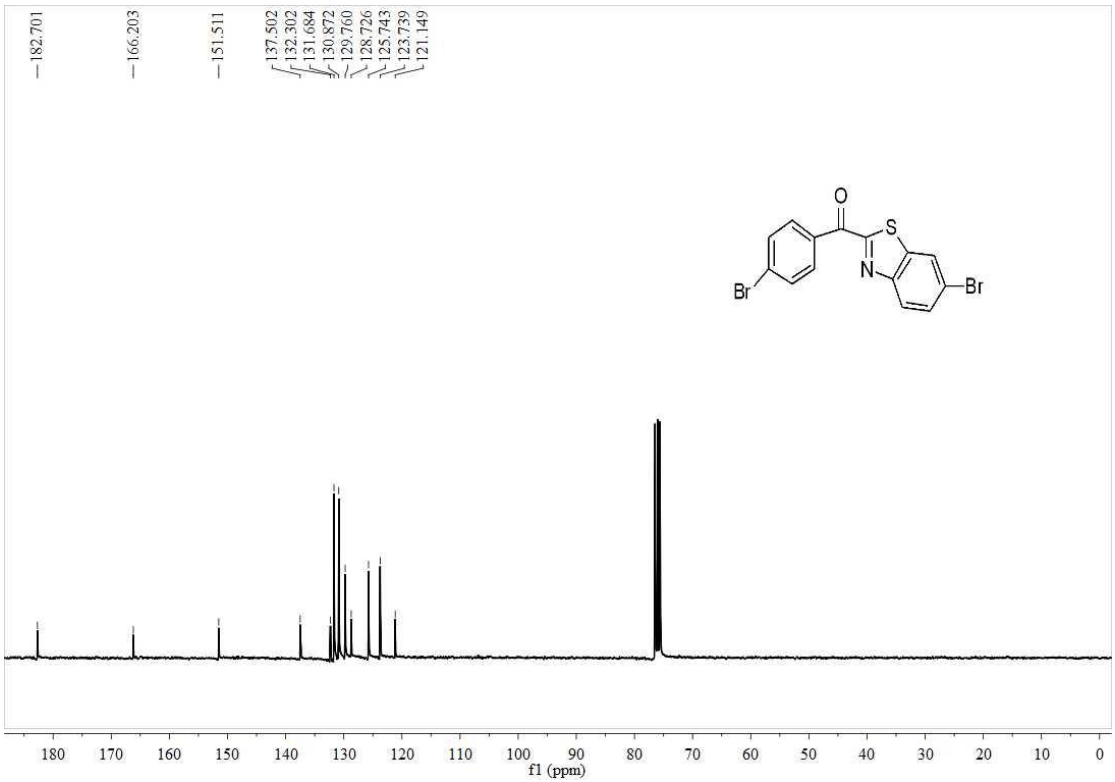
^{13}C NMR of compounds **2p**



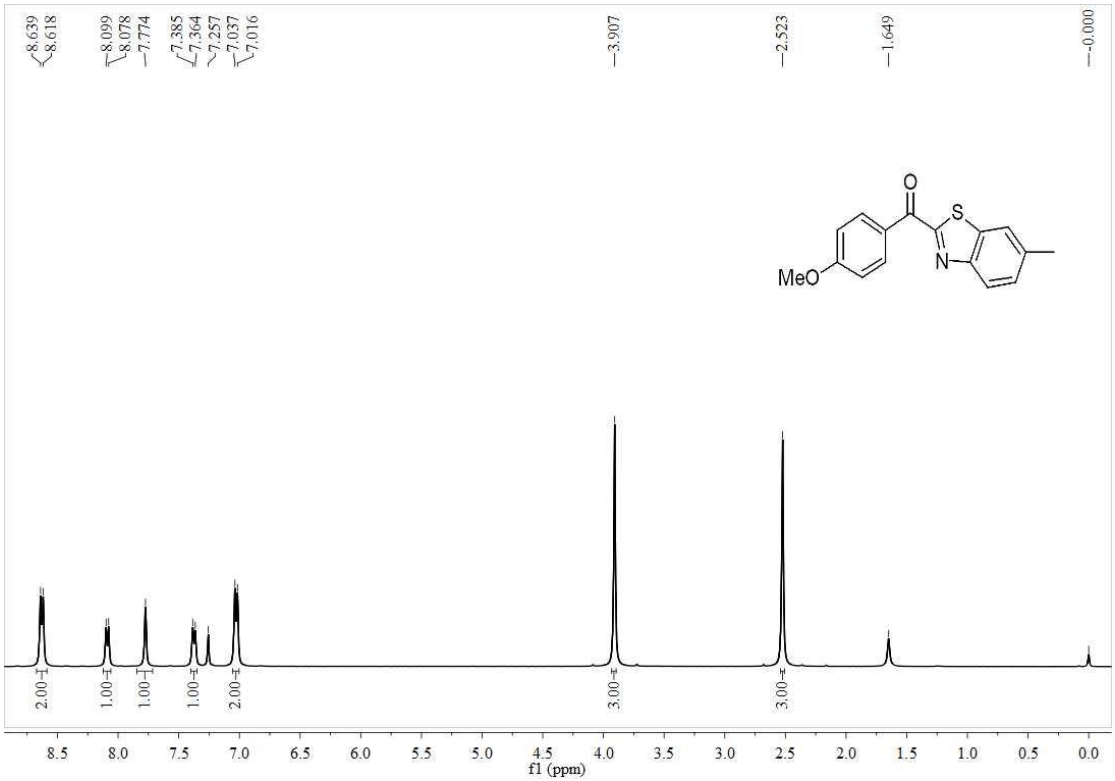
^{1}H NMR of compounds **2q**



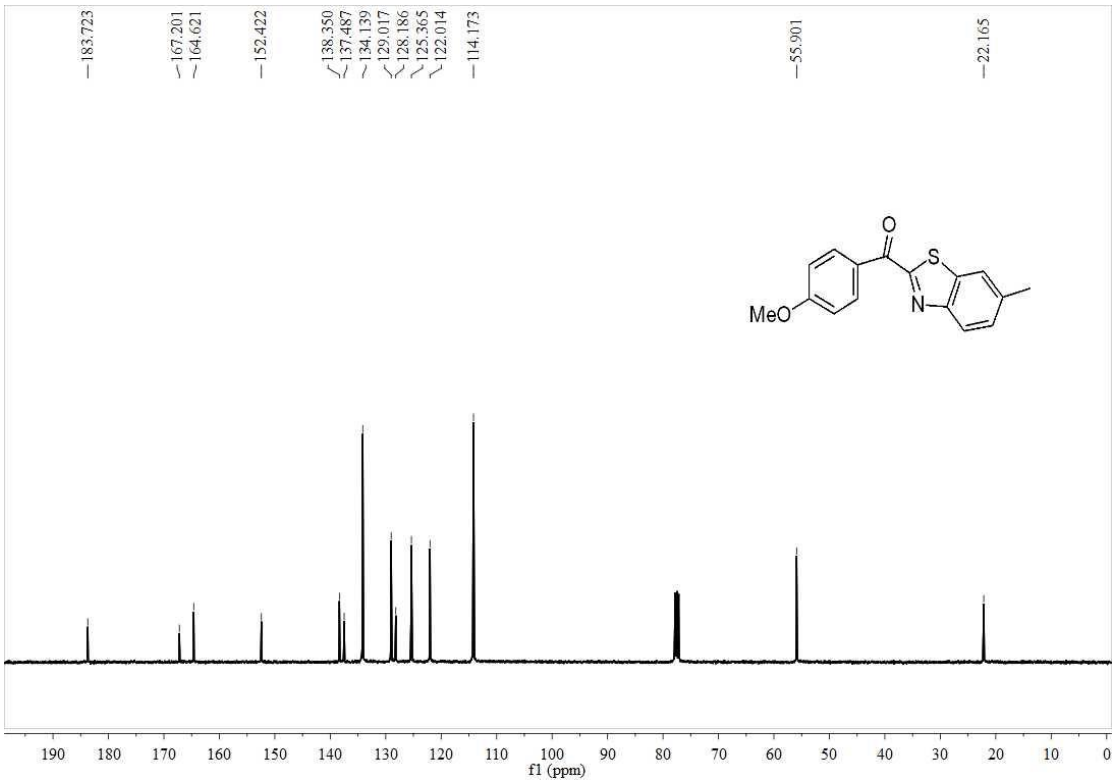
^{13}C NMR of compounds **2q**



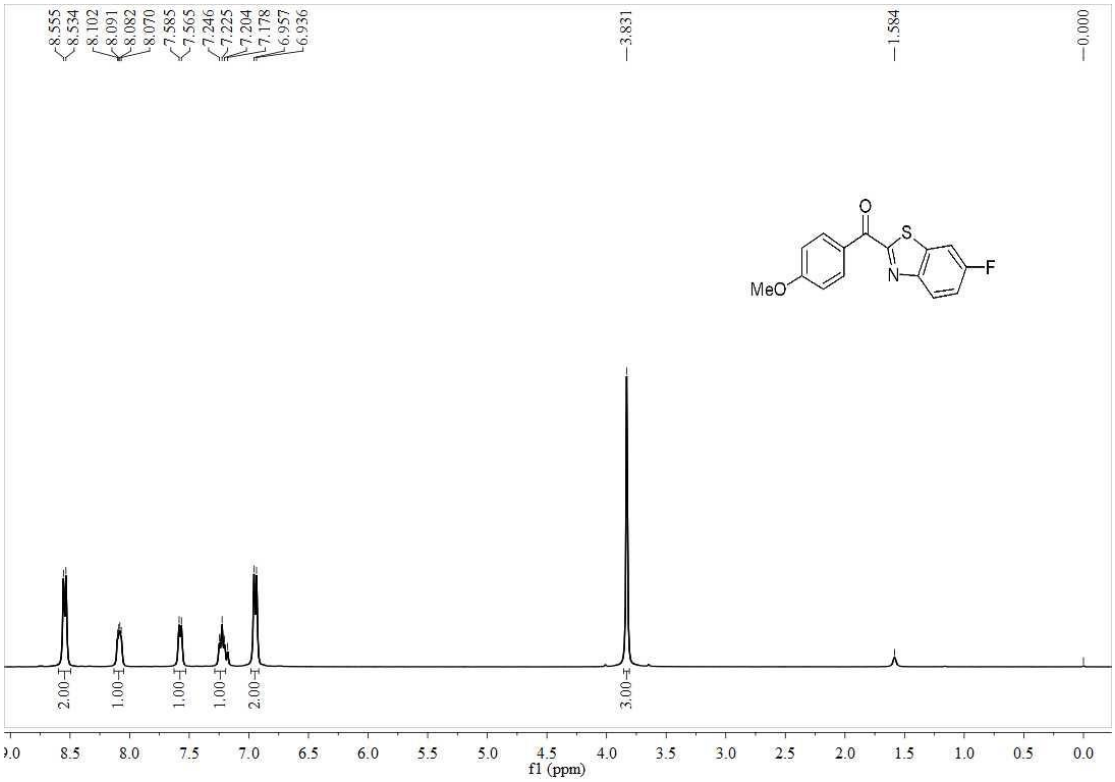
^{1}H NMR of compounds **2r**



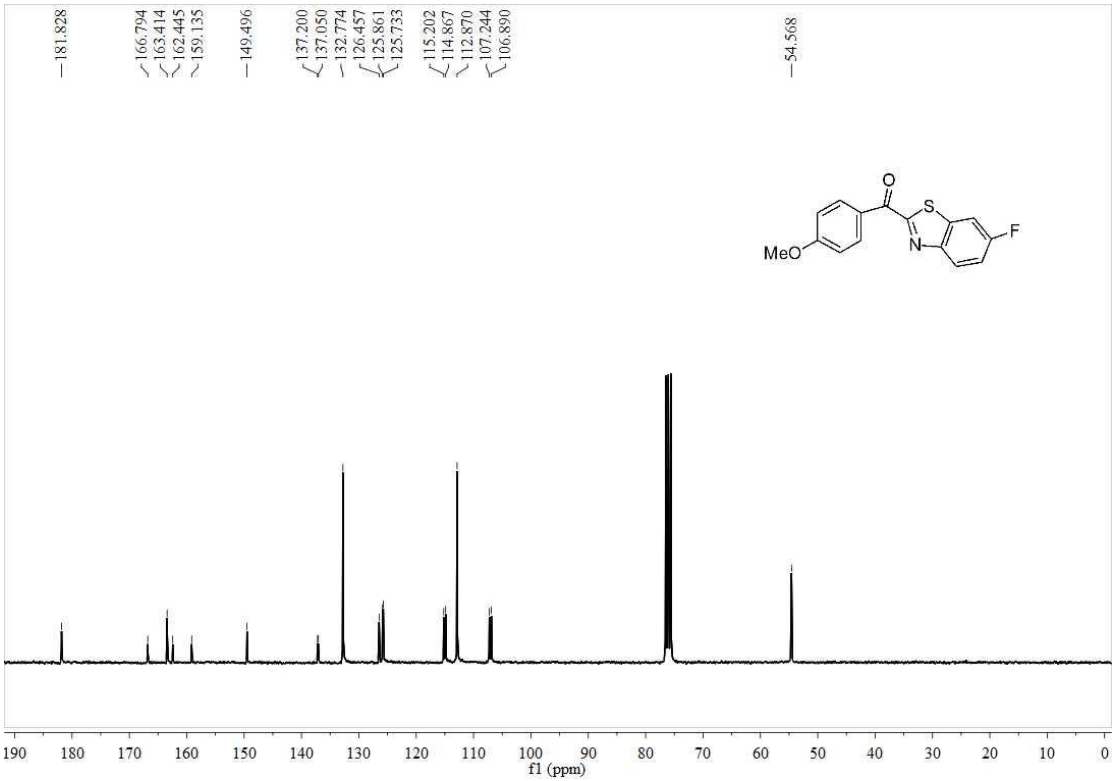
^{13}C NMR of compounds **2r**



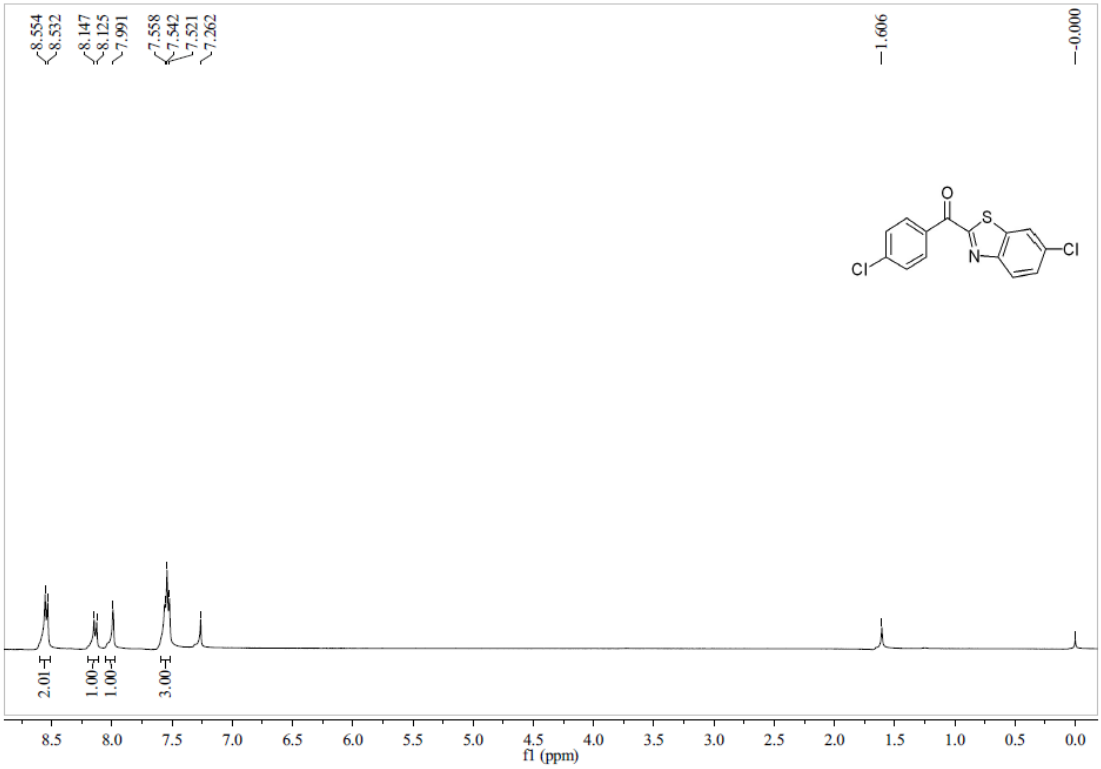
^{1}H NMR of compounds **2s**



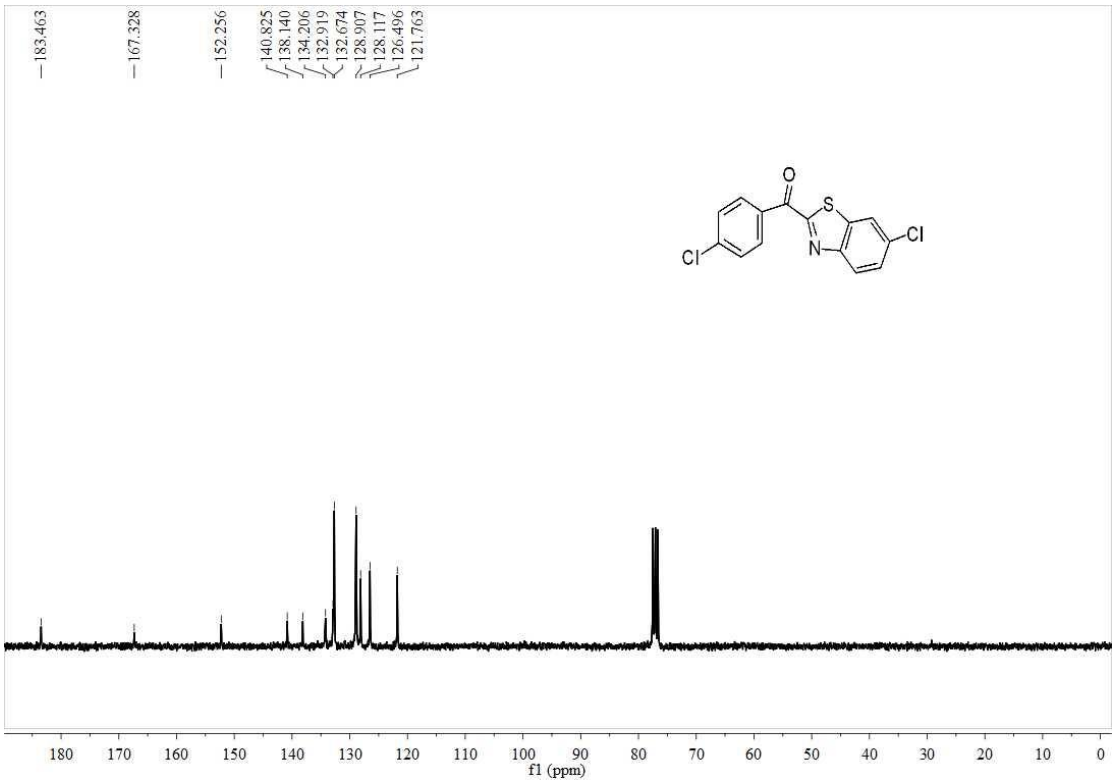
^{13}C NMR of compounds **2s**



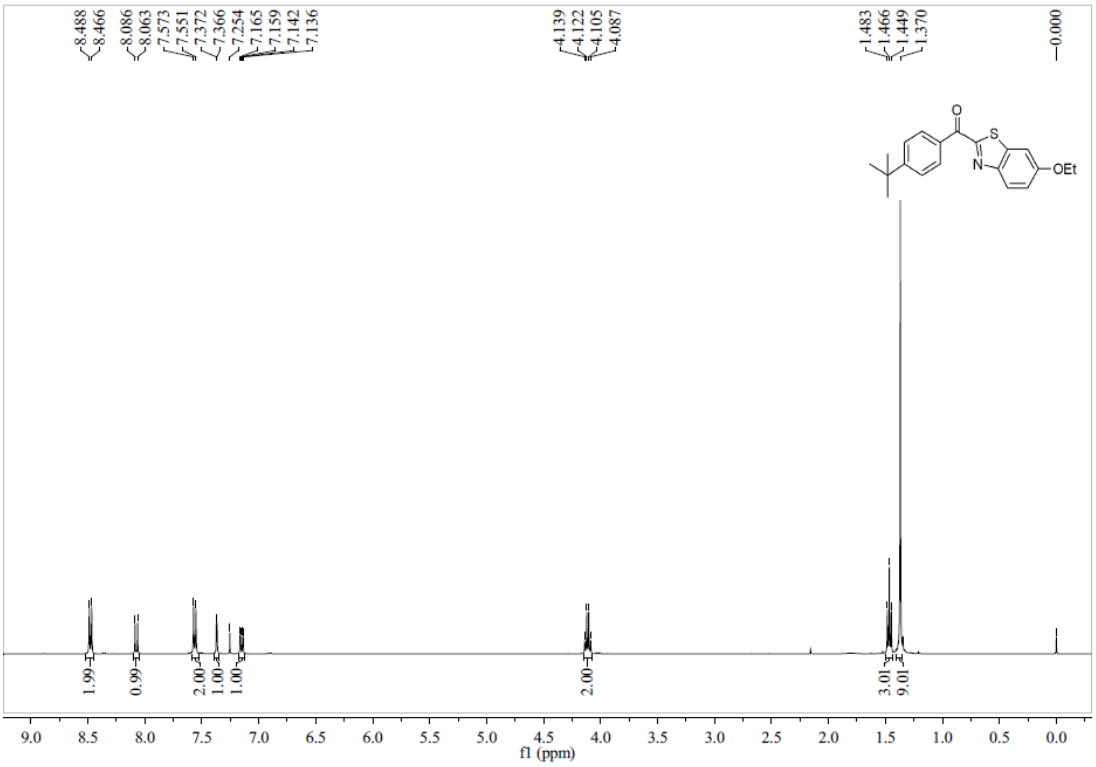
^{1}H NMR of compounds **2t**



^{13}C NMR of compounds **2t**



^{1}H NMR of compounds **2u**



^{13}C NMR of compounds **2u**