

Supporting information

A general and straightforward method for the synthesis of 2-trifluoromethylbenzothiazoles

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General:

Melting points were uncorrected. ^1H NMR spectra were recorded on a Bruker AM-300 spectrometer (300 MHz) with TMS as internal standard. ^{19}F NMR spectra were taken on a Bruker AM-300 (282 MHz) spectrometer using CFCl_3 as external standard. ^{13}C NMR spectra were taken on a Bruker AM-400 (100 MHz) spectrometer. IR spectra were obtained with a Nicolet AV-360 spectrophotometer. All reagents were used as received from commercial sources. Column chromatography over silica gel (mesh 300-400) and petroleum ether/ethyl acetate combination was used as the eluent.

General procedure for the synthesis of trifluoromethylbenzothiazoles.

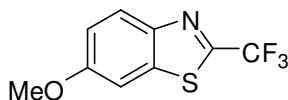
Condition a: using trifluoromethylimidoyl chlorides **1** as the substrates.

To a mixture of the trifluoromethylimidoyl chlorides **1** (1.0 mmol) in DMSO (3 ml) was added sodium hydrosulfide hydrate (80 mg, 1.0 mmol), then was stirred at 50 °C for half an hour, followed by addition of PdCl_2 (9 mg, 0.05 mmol). The mixture was warmed at 110 °C for 3h and then the reaction was stopped. Water (10 ml) was added to the solvent. The mixture was extracted with ethyl acetate (15 ml \times 2). The organic layer was washed with brine, dried over MgSO_4 , and concentrated under vacuo. The residue was purified by column chromatography on silica gel to provide the desired product.

Condition b: using trifluoromethylthiobenzamides **2** as the substrates

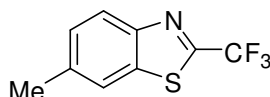
The mixture of trifluoromethylthiobenzamides **2** (1.0 mmol) and PdCl_2 (9 mg, 0.04 mmol) in DMSO (3 ml) was stirred at 110 °C for 3h. Then water (10 ml) was added and the mixture was extracted with ethyl acetate (15 ml \times 2). The organic layer was washed with brine, dried over MgSO_4 , and concentrated under vacuo. The residue was purified by column chromatography on silica gel to provide the desired product.

6-methoxy-2-(trifluoromethyl)benzo[*d*]thiazole (**3b**)



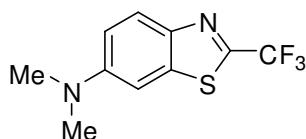
White solid, mp 34 °C; ^1H NMR (300 MHz, CDCl_3): δ 8.06 (d, $J = 9.1$ Hz, 1H), 7.37 (s, 1H), 7.20 (d, $J = 9.1$ Hz, 1H); ^{19}F NMR (282 MHz, CDCl_3): δ -61.83 (s, 3F); ^{13}C NMR (100 MHz, CDCl_3): δ 159.4, 152.9 (q, $J = 41.0$ Hz), 146.6, 136.7, 125.5, 119.9 (q, $J = 272.9$ Hz), 117.4, 103.6, 55.8; IR (film): ν 2952, 1608, 1519, 1334, 1253, 1224, 1179, 1153, 1008, 828 cm^{-1} ; MS (EI): m/z (%): 233 (100.00) [M^+]; Anal. Calcd. For $\text{C}_9\text{H}_6\text{F}_3\text{NOS}$: C, 46.35, H, 2.59, N, 6.01; Found: C, 46.58, H, 2.74, N, 5.88.

6-methyl-2-(trifluoromethyl)benzo[*d*]thiazole (**3c**)



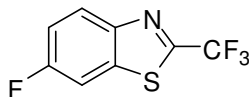
White solid, mp 86 °C; ^1H NMR (300 MHz, CDCl_3): δ 8.04 (d, $J = 7.9$ Hz, 1H), 7.72 (s, 1H), 7.39 (d, $J = 7.9$ Hz, 1H), 2.51 (s, 3H); ^{19}F NMR (282 MHz, CDCl_3): δ -62.00 (s, 3F); ^{13}C NMR (100 MHz, CDCl_3): 154.7 (q, $J = 40.3$ Hz), 150.3, 138.1, 135.2, 129.1, 124.4, 121.3, 119.9 (q, $J = 273.6$ Hz), 21.6; IR (film): ν 3074, 3056, 1520, 1331, 1189, 1133, 1008, 828 cm^{-1} ; MS(EI): m/z (%): 217 (100.00) [M^+]; Anal. Calcd. For $\text{C}_9\text{H}_6\text{F}_3\text{NS}$: C, 49.77, H, 2.78, N, 6.45; Found: C, 49.59, H, 2.80, N, 6.32.

N,N-dimethyl-2-(trifluoromethyl)benzo[*d*]thiazol-6-amine (**3d**)



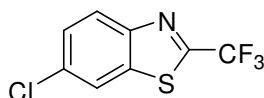
White solid, mp 76 °C; ^1H NMR (300 MHz, CDCl_3): δ 8.18 (d, $J = 9.1$ Hz, 1H), 7.05-7.00 (m, 2H), 3.05 (s, 6H); ^{19}F NMR (282 MHz, CDCl_3): δ -61.53 (s, 3F); ^{13}C NMR (100 MHz, CDCl_3): δ 150.0, 149.8 (q, $J = 40.3$ Hz), 143.6, 137.7, 124.8, 120.2 (q, $J = 272.2$ Hz); IR (film): ν 2914, 2817, 1607, 1514, 1335, 1179, 1137, 1004, 810 cm^{-1} ; MS (EI): m/z (%): 245 (100.00) [M^+]; Anal. Calcd. For $\text{C}_{10}\text{H}_9\text{F}_3\text{N}_2\text{S}$: C, 48.77, H, 3.68, N, 11.38; Found: C, 48.64, H, 3.83, N, 11.21.

6-fluoro-2-(trifluoromethyl)benzo[*d*]thiazole (**3e**)



White solid, mp 80 °C; ^1H NMR (300 MHz, CDCl_3): δ 8.18-8.14 (m, 1H), 7.66 (dd, $J_1 = 2.3$ Hz, $J_2 = 7.8$ Hz, 1H), 7.39-7.33 (m, 1H); ^{19}F NMR (282 MHz, CDCl_3): δ -62.19 (s, 3F), -111.94 (m, 1F); ^{13}C NMR (100 MHz, CDCl_3): δ 161.7 (d, $J = 249.4$ Hz), 155.6 (qd, $J_1 = 41.1$ Hz, $J_2 = 3.7$ Hz), 148.8, 136.2 (d, $J = 11.0$ Hz), 126.3 (d, $J = 9.5$ Hz), 119.5 (q, $J = 273.6$ Hz), 116.6 (d, $J = 24.9$ Hz), 108.1 (d, $J = 27.2$ Hz); IR (film): ν 3063, 1566, 1522, 1454, 1338, 1031, 1185, 1154, 1011, 820 cm^{-1} ; MS (EI): m/z (%): 221 (100.00) [M^+]; Anal. Calcd. For $\text{C}_8\text{H}_3\text{F}_4\text{NS}$: C, 43.44, H, 1.37, N, 6.33; Found: C, 43.28, H, 1.52, N, 6.27.

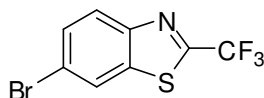
6-chloro-2-(trifluoromethyl)benzo[*d*]thiazole (**3f**)



White solid, mp 102 °C; ^1H NMR (300 MHz, CDCl_3): δ 8.12 (d, $J = 8.7$ Hz, 1H), 7.98 (d, $J = 1.8$ Hz, 1H), 7.58 (dd, $J_1 = 8.7$ Hz, $J_2 = 1.8$ Hz, 1H); ^{19}F NMR (282 MHz, CDCl_3): δ -61.71 (s, 3F); ^{13}C NMR (100 MHz, CDCl_3): δ 156.3 (q, $J = 40.3$ Hz), 150.6, 136.1, 133.8, 128.4, 125.8, 121.6, 119.5 (q, $J = 272.9$ Hz); IR (film): ν 3086, 1547, 1519, 1294, 1179, 1133, 1105, 1012, 830 cm^{-1} ; MS (EI): m/z (%): 237 (100.00)

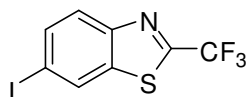
[M⁺]; Anal. Calcd. For C₈H₃ClF₃NS: C, 40.44, H, 1.27, N, 5.89; Found: C, 40.34, H, 1.53, N, 5.83.

6-bromo-2-(trifluoromethyl)benzo[d]thiazole (**3g**)



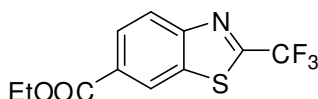
White solid, mp 96 °C; ¹H NMR (300 MHz, CDCl₃): δ 8.13 (d, *J* = 2.1 Hz, 1H), 8.05 (d, *J* = 8.7 Hz, 1H), 7.71 (dd, *J*₁ = 2.1 Hz, *J*₂ = 8.7 Hz, 1H); ¹⁹F NMR (282 MHz, CDCl₃): δ -62.17 (s, 3F); ¹³C NMR (100 MHz, CDCl₃): δ 156.4 (q, *J* = 41.0 Hz), 150.9, 136.5, 131.1, 126.1, 124.6, 121.5, 119.5 (q, *J* = 272.9 Hz); IR (film): ν 3056, 1543, 1520, 1326, 1292, 1326, 1292, 1181, 1133, 1093, 1010, 828 cm⁻¹; MS (EI): *m/z* (%): 283 (100.00) [M⁺]; Anal. Calcd. For C₈H₃F₃BrNS: C, 34.06, H, 1.07, N, 4.97; Found: C, 33.80, H, 1.41, N, 4.83.

6-iodo-2-(trifluoromethyl)benzo[d]thiazole (**3h**)



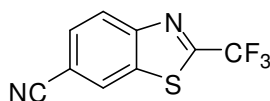
White solid, mp 75 °C; ¹H NMR (300 MHz, CDCl₃): δ 8.33 (s, 1H), 7.92-7.89 (m, 2H); ¹⁹F NMR (282 MHz, CDCl₃): δ -62.14 (s, 3F); ¹³C NMR (100 MHz, CDCl₃): δ 156.3 (q, *J* = 41.1 Hz), 151.4, 136.9, 136.7, 130.6, 126.3, 119.5 (q, *J* = 273.7 Hz), 92.5; IR (film): ν 3050, 1537, 1516, 1323, 1288, 1187, 1128, 1084, 1010, 825 cm⁻¹; MS (EI): *m/z* (%): 329 (100.00) [M⁺]; Anal. Calcd. For C₈H₃F₃INS: C, 29.20, H, 0.92, N, 4.26; Found: C, 29.41, H, 1.08, N, 4.23.

ethyl 2-(trifluoromethyl)benzo[d]thiazole-6-carboxylate (**3i**)



White solid, mp 87 °C; ¹H NMR (300 MHz, CDCl₃): δ 8.73 (d, *J* = 1.5 Hz, 1H), 8.31-8.22 (m, 2H), 4.46 (q, *J* = 7.1 Hz, 2H), 1.45 (t, *J* = 7.1 Hz, 3H); ¹⁹F NMR (282 MHz, CDCl₃): δ -62.37 (s, 3F); ¹³C NMR (100 MHz, CDCl₃): δ 165.4, 158.9 (q, *J* = 41.1 Hz), 154.7, 134.9, 129.7, 128.3, 124.8, 124.2, 119.5, (q, *J* = 273.7 Hz), 61.6, 14.2; IR (film): ν 3093, 2994, 1713, 1603, 1519, 1317, 1176, 1127, 1015, 771 cm⁻¹; MS (EI): *m/z* (%): 275 (30.03) [M⁺], 230 (100.00); Anal. Calcd. For C₁₁H₈F₃NO₂S: C, 48.00, H, 2.93, N, 5.09; Found: C, 48.01, H, 2.86, N, 5.15.

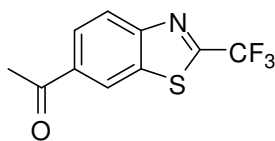
2-(trifluoromethyl)benzo[d]thiazole-6-carbonitrile (**3j**)



White solid, mp 146 °C; ¹H NMR (300 MHz, CDCl₃): δ 8.40 (s, 1H), 8.33 (d, *J* = 8.5 Hz, 1H), 7.90 (d, *J* = 8.5 Hz, 1H); ¹⁹F NMR (282 MHz, CDCl₃): δ -62.37 (s, 3F); ¹³C NMR (100 MHz, CDCl₃): δ 160.0 (q, *J* = 41.1 Hz), 154.2, 135.4, 130.3, 127.2, 126.0,

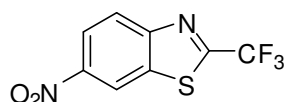
119.3 (q, $J = 274.4$ Hz), 117.7, 111.4; IR (film): ν 3080, 3062, 2231, 1520, 1400, 1334, 1297, 1189, 1142, 1015, 842 cm^{-1} ; MS (EI): m/z (%): 228 (100.00) [M^+]; Anal. Calcd. For $\text{C}_9\text{H}_3\text{F}_3\text{N}_2\text{S}$: C, 47.37, H, 1.33, N, 12.28; Found: C, 47.30, H, 1.41, N, 12.27.

1-(2-(trifluoromethyl)benzo[*d*]thiazol-6-yl)ethanone (**3k**)



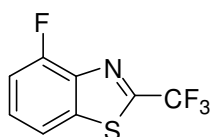
White solid, mp 97 °C; ^1H NMR (300 MHz, CDCl_3): δ 8.64 (s, 1H), 8.28-8.19 (m, 2H), 2.74 (s, 3H); ^{19}F NMR (282 MHz, CDCl_3): δ -62.38 (s, 3F); ^{13}C NMR (100 MHz, CDCl_3): δ 196.5, 159.3 (q, $J = 40.5$ Hz), 154.7, 135.9, 135.3, 127.2, 125.1, 123.0, 119.4 (q, $J = 273.4$ Hz), 26.8; IR (film): ν 3080, 1682, 1593, 1518, 1337, 1302, 1259, 1188, 1143, 1013, 835 cm^{-1} ; MS (EI): m/z (%): 245 (34.48) [M^+], 230 (100.00); Anal. Calcd. For $\text{C}_{10}\text{H}_6\text{F}_3\text{NOS}$: C, 48.98, H, 2.47, N, 5.71; Found: C, 49.00, H, 2.52, N, 5.73.

6-nitro-2-(trifluoromethyl)benzo[*d*]thiazole (**3l**)



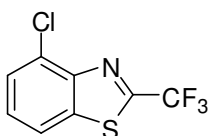
White solid, mp 93 °C; ^1H NMR (300 MHz, CDCl_3): δ 8.99 (d, $J = 2.1$ Hz, 1H), 8.51 (dd, $J_1 = 9.1$ Hz, $J_2 = 2.1$ Hz, 1H), 8.36 (d, $J = 9.1$ Hz, 1H); ^{19}F NMR (282 MHz, CDCl_3): δ -62.50 (s, 3F); ^{13}C NMR (100 MHz, CDCl_3): δ 161.2 (q, $J = 41.1$ Hz), 155.4, 146.6, 135.4, 125.7, 122.6, 119.1 (q, $J = 274.4$ Hz), 118.8; IR (film): ν 3086, 1572, 1520, 1347, 1297, 1190, 1014, 747 cm^{-1} ; MS (EI): m/z (%): 248 (100.00) [M^+]; Anal. Calcd. For $\text{C}_8\text{H}_3\text{F}_3\text{N}_2\text{O}_2\text{S}$: C, 38.72, H, 1.22, N, 11.29; Found: C, 38.68, H, 1.34, N, 11.13.

4-fluoro-2-(trifluoromethyl)benzo[*d*]thiazole (**3m**)



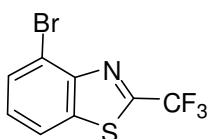
White solid, mp 54 °C; ^1H NMR (300 MHz, CDCl_3): δ 7.78 (d, $J = 8.2$ Hz, 1H), 7.60-7.50 (m, 1H), 7.36-7.29 (m, 1H); ^{19}F NMR (282 MHz, CDCl_3): δ -61.98 (s, 3F), -119.80 (m, 1F); ^{13}C NMR (100 MHz, CDCl_3): δ 158.6 (d, $J = 260.5$ Hz), 156.4 (q, $J = 41.1$ Hz), 141.4 (d, $J = 14.7$ Hz), 137.5, 128.6 (d, $J = 7.3$ Hz), 119.5 (q, $J = 273.6$ Hz), 117.7 (d, $J = 4.4$ Hz), 112.9 (d, $J = 17.6$ Hz); IR (film): ν 3080, 1575, 1517, 1477, 1337, 1305, 1252, 1196, 1140, 1025, 915, 783 cm^{-1} ; MS (EI): m/z (%): 221 (100.00) [M^+]; Anal. Calcd. For $\text{C}_8\text{H}_3\text{F}_4\text{NS}$: C, 43.44, H, 1.37, N, 6.33; Found: C, 43.52, H, 1.36, N, 6.40.

4-chloro-2-(trifluoromethyl)benzo[*d*]thiazole (**3n**)



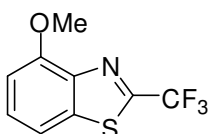
White solid, mp 49 °C; ¹H NMR (300 MHz, CDCl₃): δ 7.89 (d, *J* = 8.2 Hz, 1H), 7.64 (d, *J* = 7.7 Hz, 1H), 7.52-7.47 (m, 1H); ¹⁹F NMR (282 MHz, CDCl₃): δ -61.91 (s, 3F); ¹³C NMR (100 MHz, CDCl₃): δ 156.6 (q, *J* = 41.1 Hz), 149.4, 136.4, 130.1, 128.1, 127.6, 119.5 (q, *J* = 273.6 Hz), 120.6; IR (film): ν 3074, 1550, 1517, 1461, 1335, 1294, 1189, 1133, 1017, 778, 739 cm⁻¹; MS (EI): *m/z* (%): 237 (100.00) [M⁺]; Anal. Calcd. For C₈H₃ClF₃NS: C, 40.44, H, 1.27, N, 5.89; Found: C, 40.34, H, 1.31, N, 5.78.

4-bromo-2-(trifluoromethyl)benzo[*d*]thiazole (**3o**)



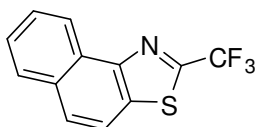
White solid, mp 65 °C; ¹H NMR (300 MHz, CDCl₃): δ 7.93 (d, *J* = 8.3 Hz, 1H), 7.80 (d, *J* = 7.6 Hz, 1H), 7.46-7.37 (m, 1H); ¹⁹F NMR (282 MHz, CDCl₃): δ -61.89 (s, 3F); ¹³C NMR (100 MHz, CDCl₃): δ 156.4 (q, *J* = 41.0 Hz), 150.6, 135.8, 130.9, 128.3, 120.9, 119.6 (q, *J* = 273.6 Hz), 118.7; IR (film): ν 3074, 1518, 1451, 1396, 1330, 1298, 1147, 1016, 775 cm⁻¹; MS (EI): *m/z* (%): 281 (100.00) [M⁺]; Anal. Calcd. For C₈H₃BrF₃NS: C, 34.06, H, 1.07, N, 4.97; Found: C, 34.14, H, 1.20, N, 4.98.

4-methoxy-2-(trifluoromethyl)benzo[*d*]thiazole (**3q**)



White solid, mp 80 °C; ¹H NMR (300 MHz, CDCl₃): δ 7.53-7.46 (m, 2H), 6.99 (dd, *J*₁ = 1.7 Hz, *J*₂ = 7.4 Hz, 1H), 4.07 (s, 3H); ¹⁹F NMR (282 MHz, CDCl₃): δ -61.58 (s, 3F); ¹³C NMR (100 MHz, CDCl₃): δ 154.7, 154.2 (q, *J* = 41.1 Hz), 142.6, 136.8, 128.8, 120.1 (q, *J* = 272.9 Hz), 113.5, 107.4, 56.1; IR (film): ν 3068, 2965, 1575, 1512, 1332, 1306, 1271, 1147, 1018, 779 cm⁻¹; MS (EI): *m/z* (%): 233 (71.13) [M⁺], 204 (100.00); Anal. Calcd. For C₉H₆F₃NOS: C, 46.35, H, 2.59, N, 6.01; Found: C, 46.29, H, 2.71, N, 5.96.

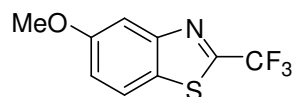
2-(trifluoromethyl)naphtho[1,2-*d*]thiazole (**3r**)



White solid, mp 87 °C; ¹H NMR (300 MHz, CDCl₃): δ 8.76 (d, *J* = 8.2 Hz, 1H), 7.89 (d, *J* = 7.9 Hz, 1H), 7.86-7.74 (m, 2H), 7.70-7.54 (m, 2H); ¹⁹F NMR (282 MHz,

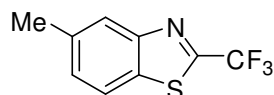
CDCl₃): δ -61.23 (s, 3F); ¹³C NMR (100 MHz, CDCl₃): δ 154.2 (q, J = 41.1 Hz), 149.1, 132.4, 132.1, 128.9, 128.5, 128.1, 127.7, 127.0, 123.8, 120.1 (q, J = 272.9 Hz), 118.3; IR (film): ν 3080, 1514, 1494, 1346, 1316, 1211, 1182, 1129, 1020, 804 cm⁻¹; MS (EI): m/z (%): 253 (100.00) [M⁺]; Anal. Calcd. For C₁₂H₆F₃NS: C, 56.91, H, 2.39, N, 5.53; Found: C, 56.70, H, 2.40, N, 5.52.

5-methoxy-2-(trifluoromethyl)benzo[*d*]thiazole (**3s**)



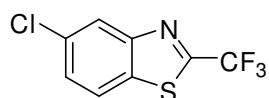
White solid, mp 60 °C; ¹H NMR (300 MHz, CDCl₃): δ 7.80 (d, J = 8.7 Hz, 1H), 7.62 (d, J = 2.2 Hz, 1H), 7.19 (dd, J_1 = 2.2 Hz, J_2 = 8.7 Hz, 1H), 3.89 (s, 3H); ¹⁹F NMR (282 MHz, CDCl₃): δ -61.74 (s, 3F); ¹³C NMR (100 MHz, CDCl₃): δ 159.8, 156.8 (q, J = 40.3 Hz), 153.6, 126.9, 122.2, 119.8 (q, q, J = 272.9 Hz), 118.5, 106.3, 55.6; IR (film): ν 3074, 3026, 1603, 1509, 1470, 1341, 1321, 1203, 1141, 1005, 829 cm⁻¹; MS (EI): m/z (%): 233 (100.00) [M⁺]; Anal. Calcd. For C₉H₆F₃NOS: C, 46.35, H, 2.59, N, 6.01; Found: C, 46.39, H, 2.68, N, 5.96.

5-methyl-2-(trifluoromethyl)benzo[*d*]thiazole (**3t**)



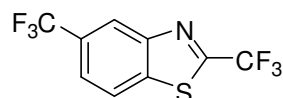
White solid, mp 45 °C; ¹H NMR (300 MHz, CDCl₃): δ 7.97 (s, 1H), 7.84 (d, J = 8.2 Hz, 1H), 7.37 (d, J = 8.2 Hz, 1H); ¹⁹F NMR (282 MHz, CDCl₃): δ -62.08 (s, 3F); ¹³C NMR (100 MHz, CDCl₃): δ 155.9 (q, J = 40.3 Hz), 152.6, 137.7, 132.0, 129.2, 124.7, 121.4, 119.8 (q, J = 272.9 Hz), 21.4; IR (film): ν 3057, 2925, 1511, 1329, 1187, 1147, 1087, 1009, 811 cm⁻¹; MS (EI): m/z (%): 217 (100.00) [M⁺]; Anal. Calcd. For C₉H₆F₃NS: C, 49.77, H, 2.78, N, 6.45; Found: C, 49.57, H, 2.84, N, 6.20.

5-chloro-2-(trifluoromethyl)benzo[*d*]thiazole (**3u**)



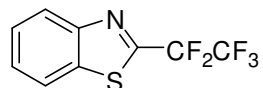
White solid, mp 64 °C; ¹H NMR (300 MHz, CDCl₃): δ 8.18 (d, J = 1.8 Hz, 1H), 7.92 (d, J = 8.8 Hz, 1H), 7.54 (dd, J_1 = 1.8 Hz, J_2 = 8.8 Hz, 1H); ¹⁹F NMR (282 MHz, CDCl₃): δ -62.29 (s, 3F); ¹³C NMR (100 MHz, CDCl₃): δ 157.7 (q, J = 41.1 Hz), 152.9, 133.7, 133.2, 128.2, 124.7, 122.8, 119.5 (q, J = 273.7 Hz); IR (film): ν 3080, 1590, 1514, 1437, 1332, 1301, 1187, 1160, 1012, 814 cm⁻¹; MS (EI): m/z (%): 237 (100.00) [M⁺]; Anal. Calcd. For C₈H₃ClF₃NS: C, 40.44, H, 1.27, N, 5.89; Found: C, 40.61, H, 1.50, N, 5.64.

2,5-bis(trifluoromethyl)benzo[*d*]thiazole (**3v**)



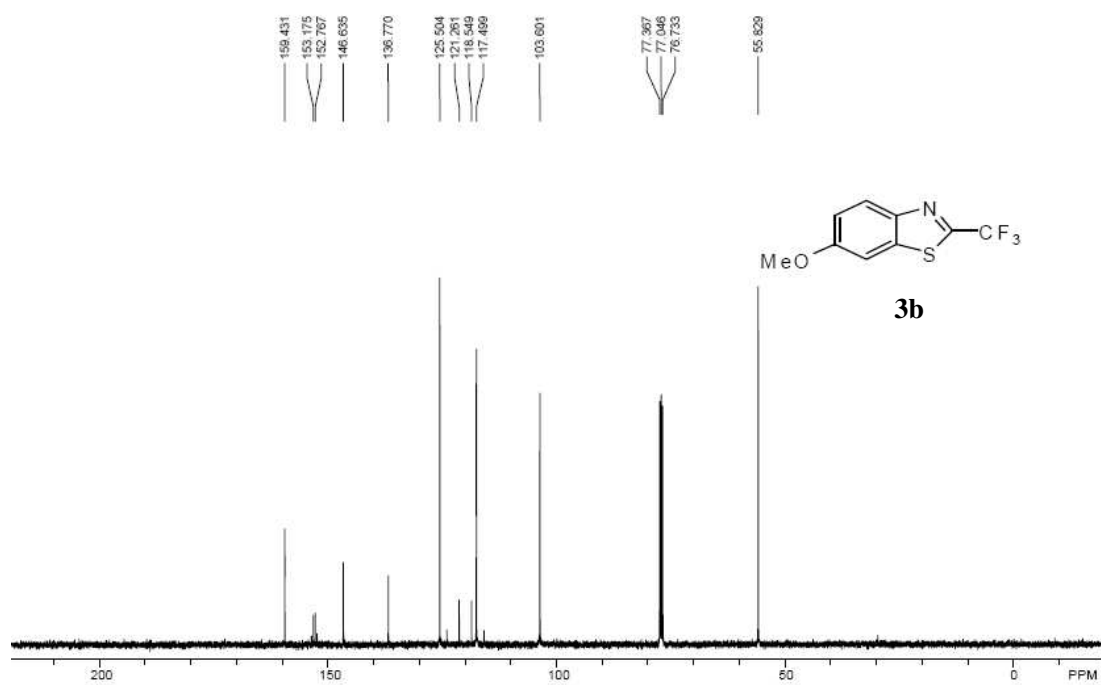
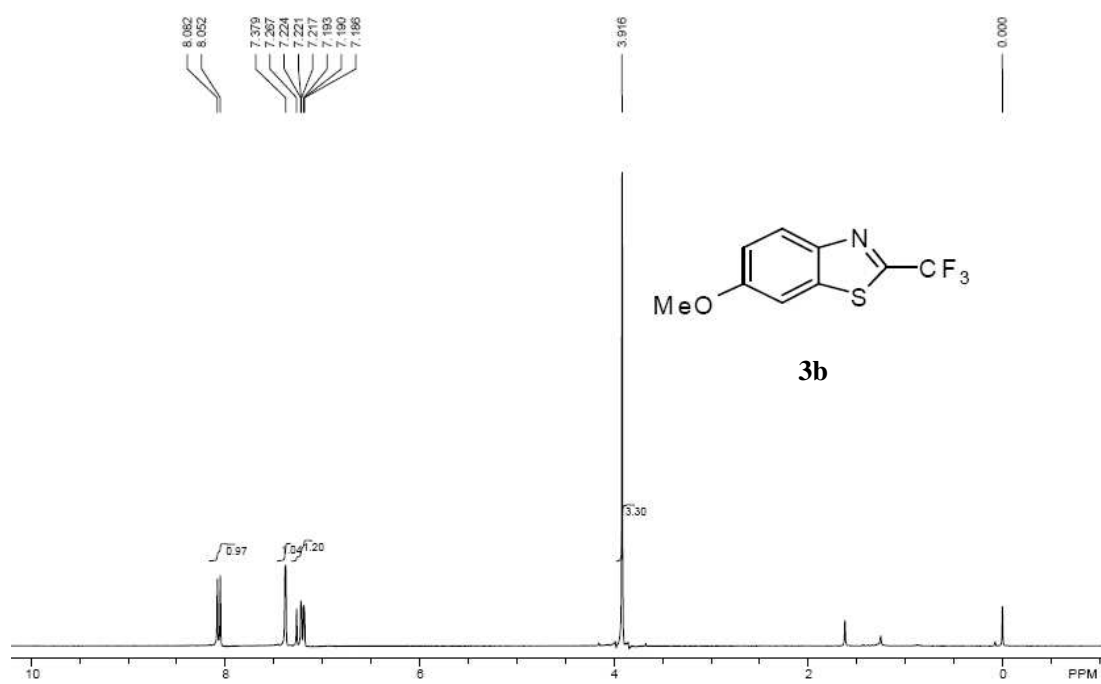
^1H NMR (300 MHz, CDCl_3): δ 8.48 (s, 1H), 8.14 (d, $J = 8.5$ Hz, 1H), 7.81 (d, $J = 8.5$ Hz, 1H); ^{19}F NMR (282 MHz, CDCl_3): δ -62.39 (s, 3F), -62.54 (s, 3F); ^{13}C NMR (100 MHz, CDCl_3): δ 158.1 (q, $J = 41.0$ Hz), 151.7, 138.2, 130.3 (q, $J = 33.7$ Hz), 123.7 (q, $J = 272.9$ Hz), 123.8 (q, $J = 2.9$ Hz), 122.9, 122.4 (q, $J = 3.7$ Hz), 119.4 (q, $J = 273.6$ Hz); IR (film): ν 3091, 1524, 1331, 1306, 1227, 1151, 1010, 820 cm^{-1} ; MS (EI): m/z (%): 271 (100.00) [M^+]; Anal. Calcd. For $\text{C}_9\text{H}_3\text{F}_6\text{NS}$: C, 39.86, H, 1.12, N, 5.17; Found: C, 39.10, H, 1.18, N, 5.06.

2-(perfluoroethyl)benzo[*d*]thiazole (**3w**)

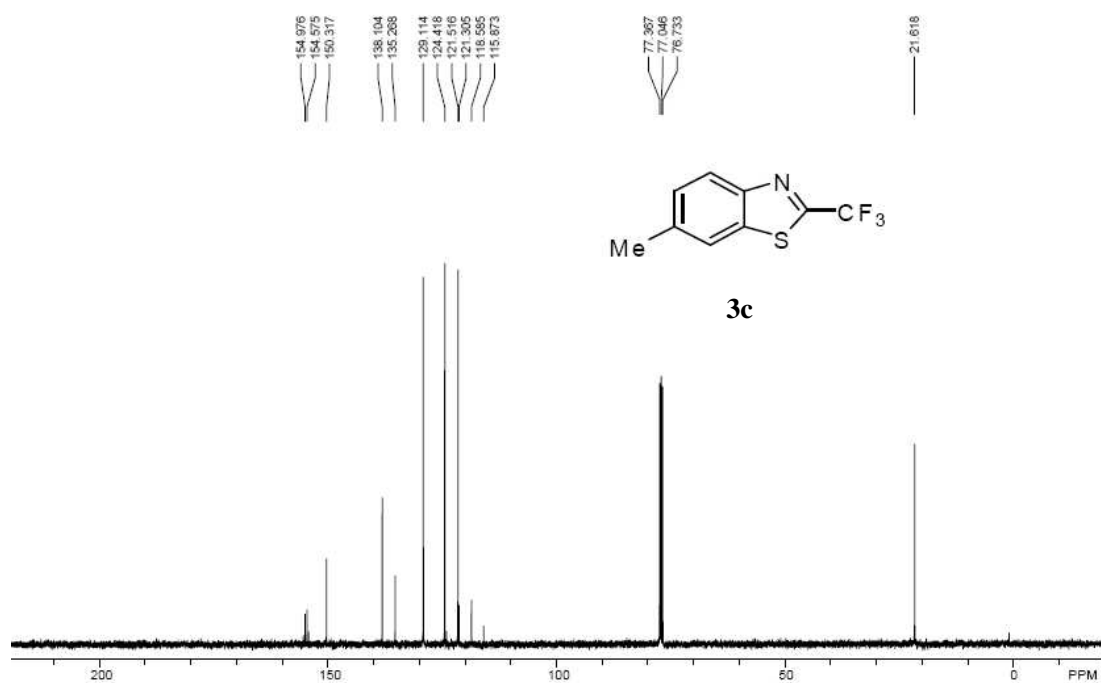
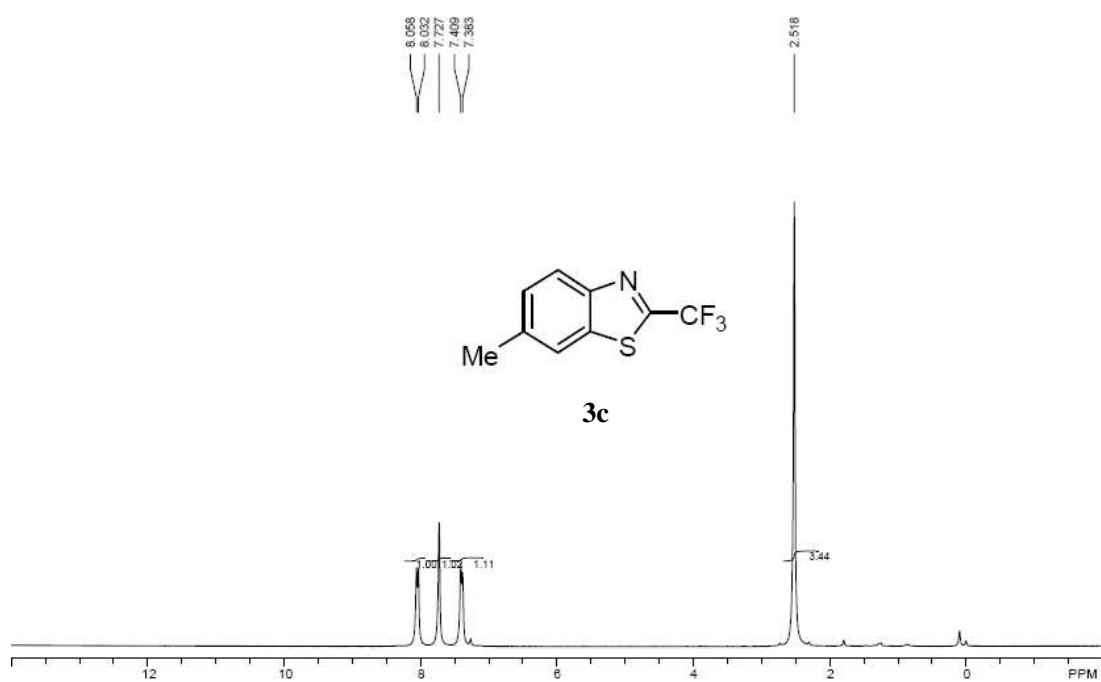


^1H NMR (300 MHz, CDCl_3): δ 8.23 (d, $J = 8.0$ Hz, 1H), 8.00 (dd, $J_1 = 7.9$ Hz, $J_2 = 1.2$ Hz, 1H), 7.65-7.52 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 155.7 (t, $J = 40.0$ Hz), 135.2, 127.4, 127.3, 125.1, 121.9, 118.3 (qt, $J_1 = 286.8$ Hz, $J_2 = 36.7$ Hz), 110.3 (tq, $J_1 = 255.3$ Hz, $J_2 = 39.6$ Hz); ^{19}F NMR (282 MHz, CDCl_3): δ -83.34 (s, 3F), -109.80 (s, 2F); IR (film): ν 3067, 1513, 1338, 1214, 1156, 1099, 927 cm^{-1} ; MS (EI): m/z (%): 253 (61.15) [M^+], 184 (100.00); HRMS Calcd for $\text{C}_9\text{H}_4\text{F}_5\text{NS}$: 252.9985, Found: 252.9989.

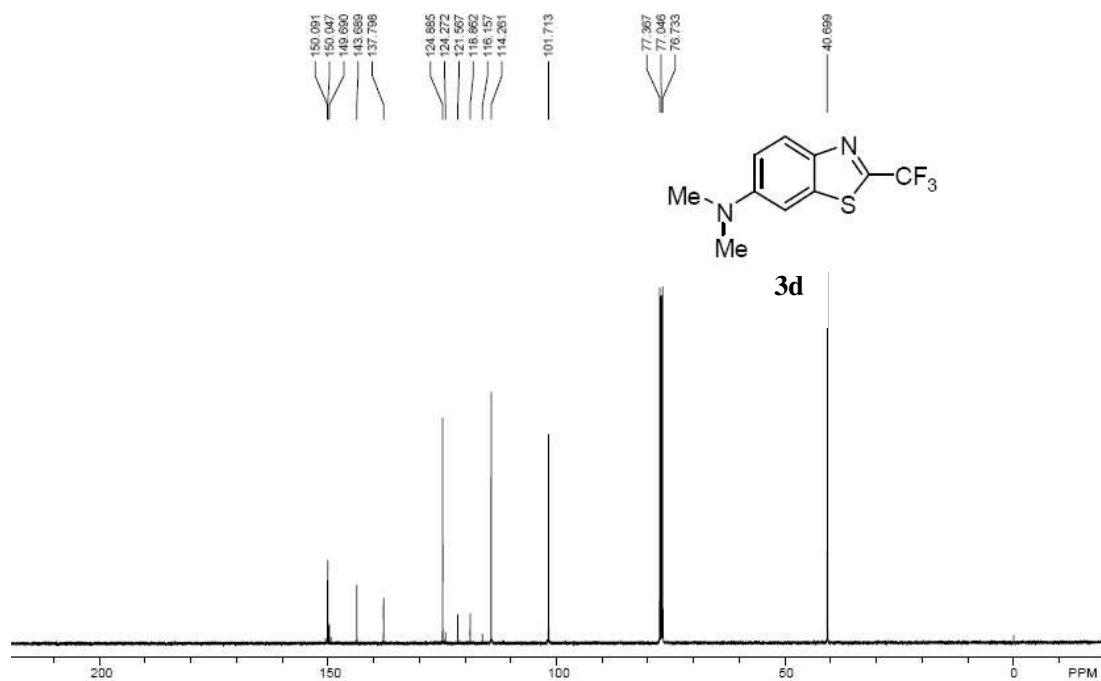
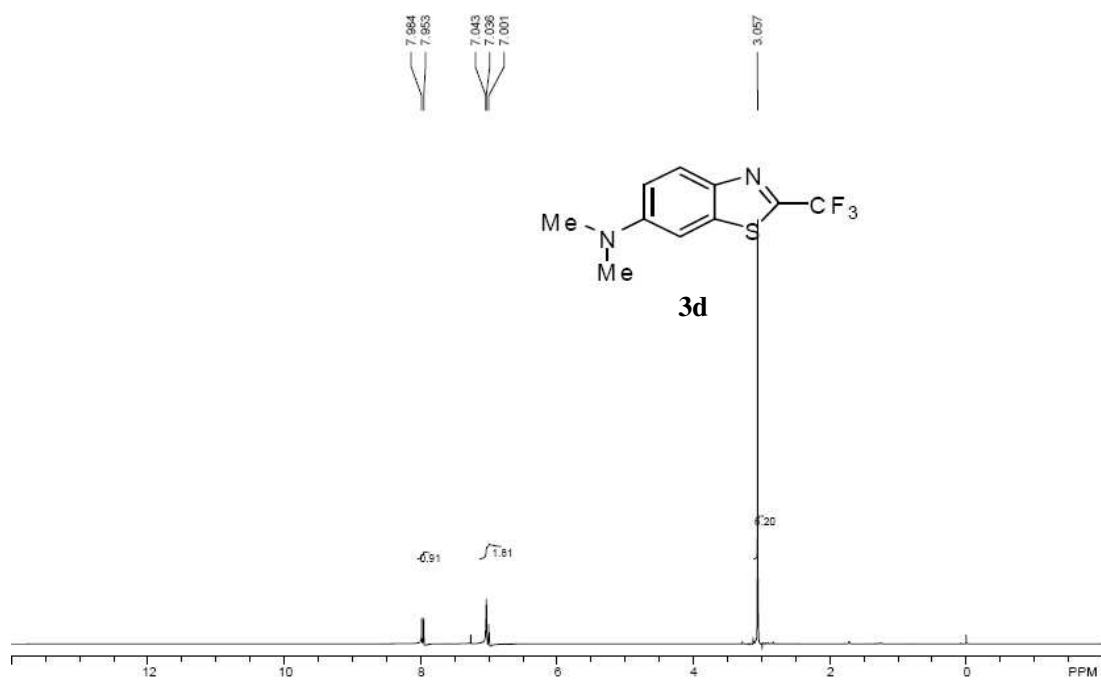
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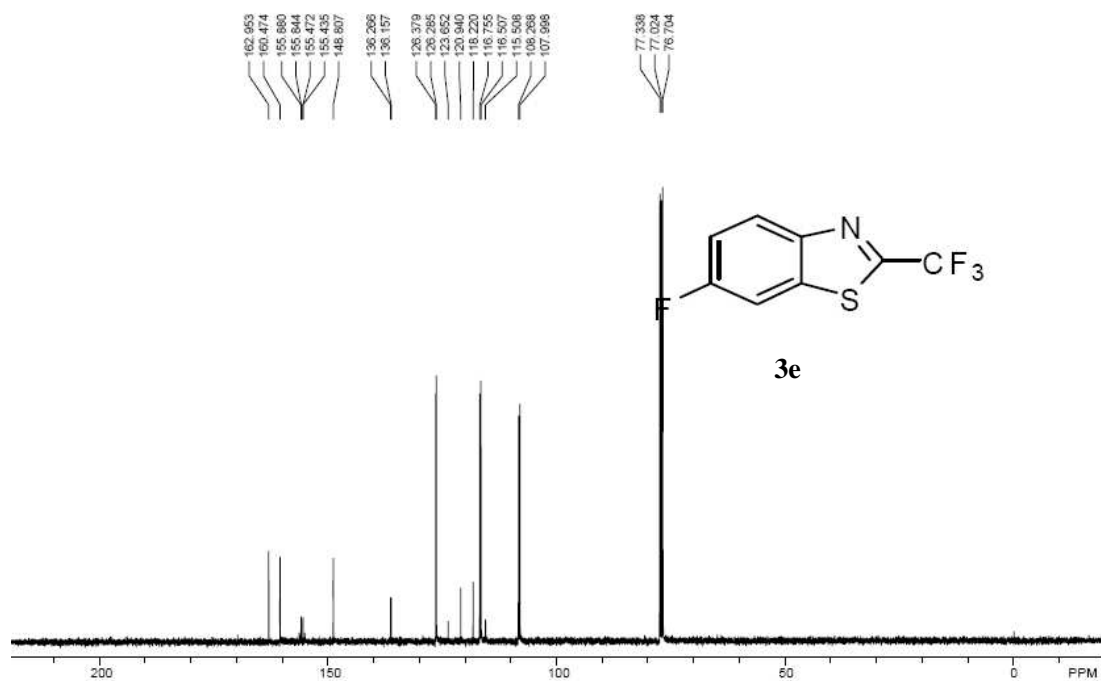
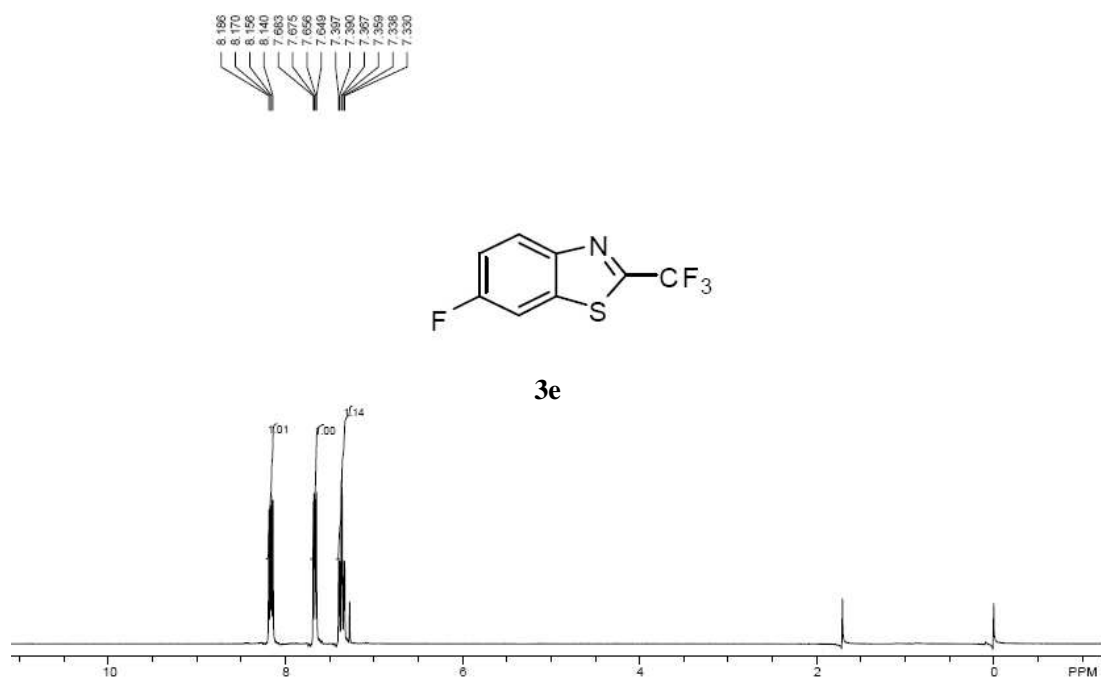
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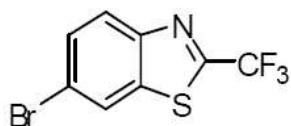
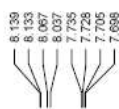
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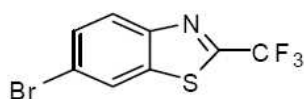
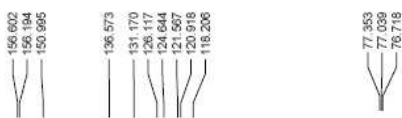
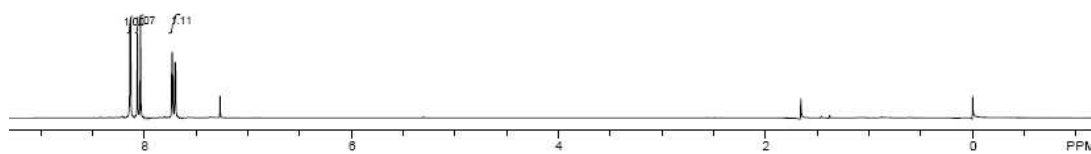
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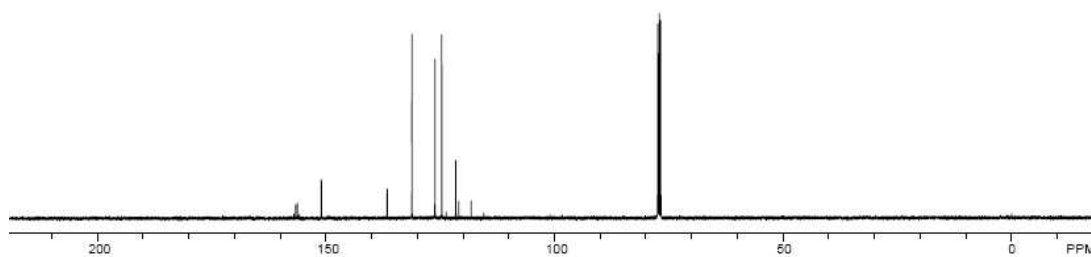
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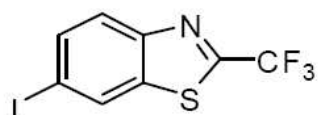
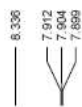
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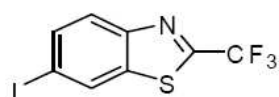
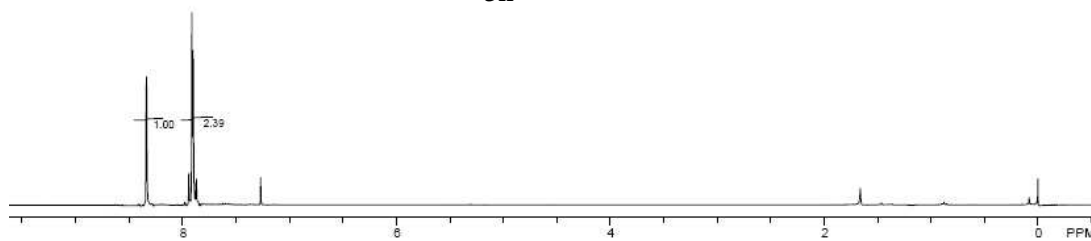
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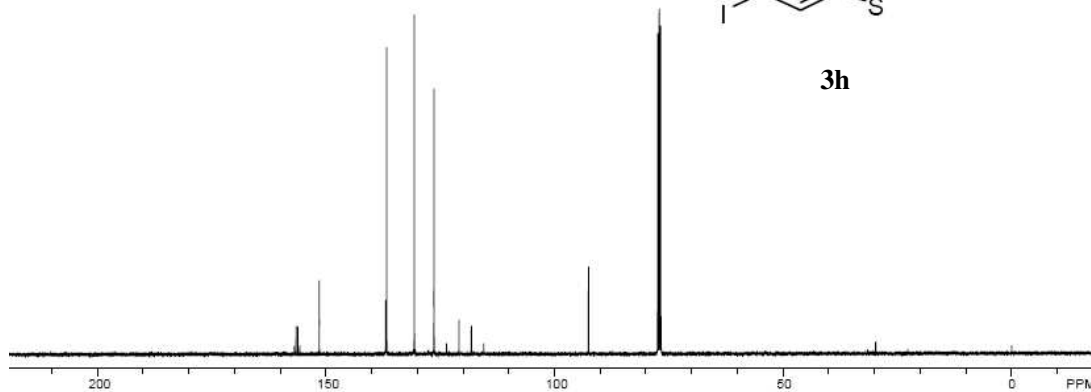
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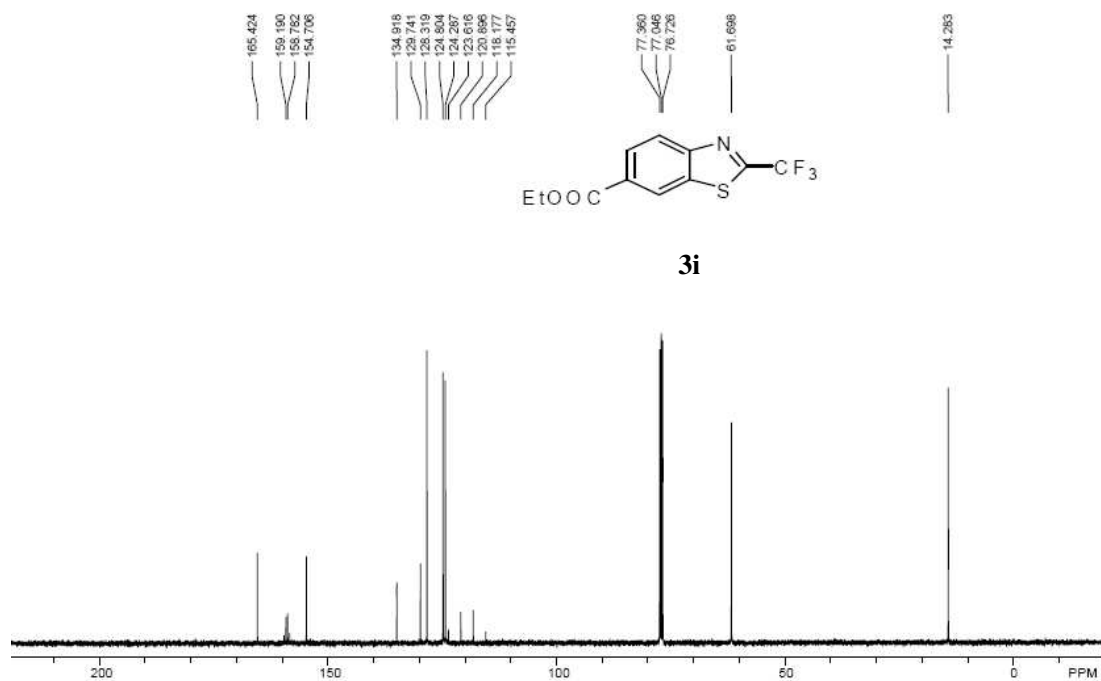
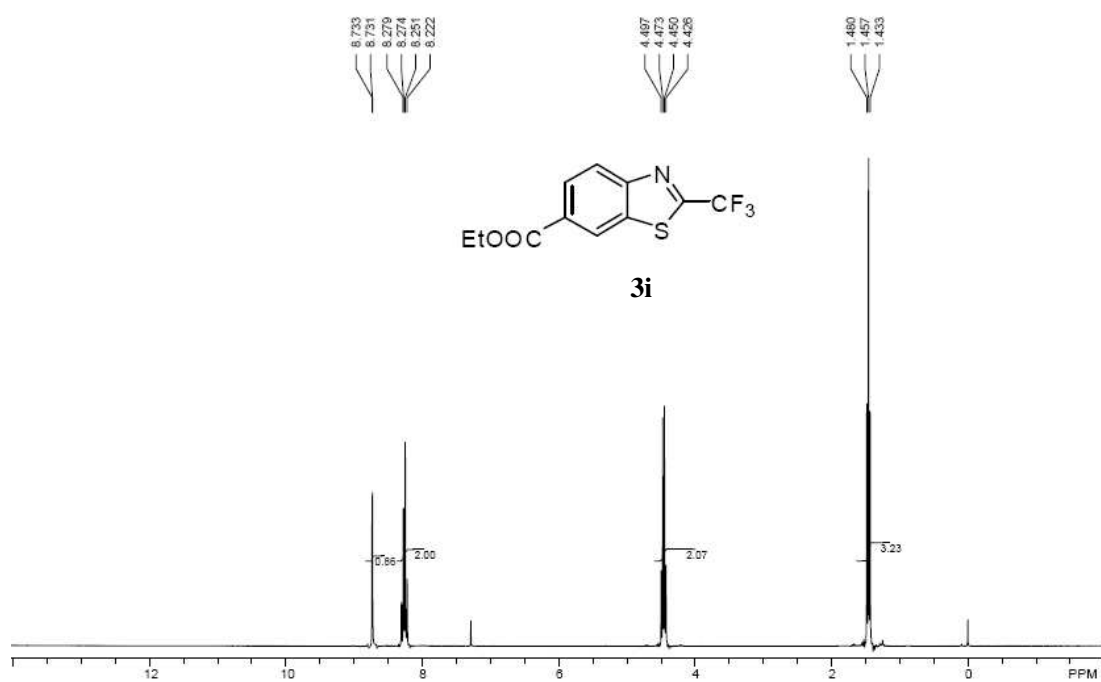
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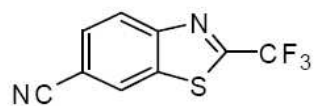
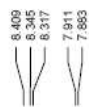
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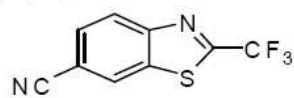
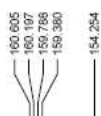
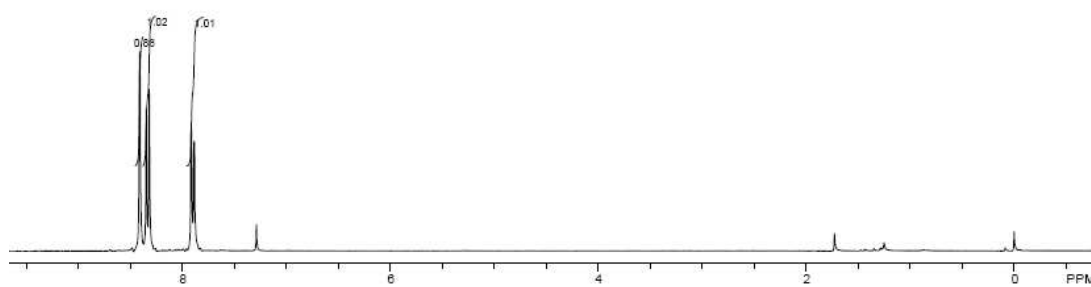
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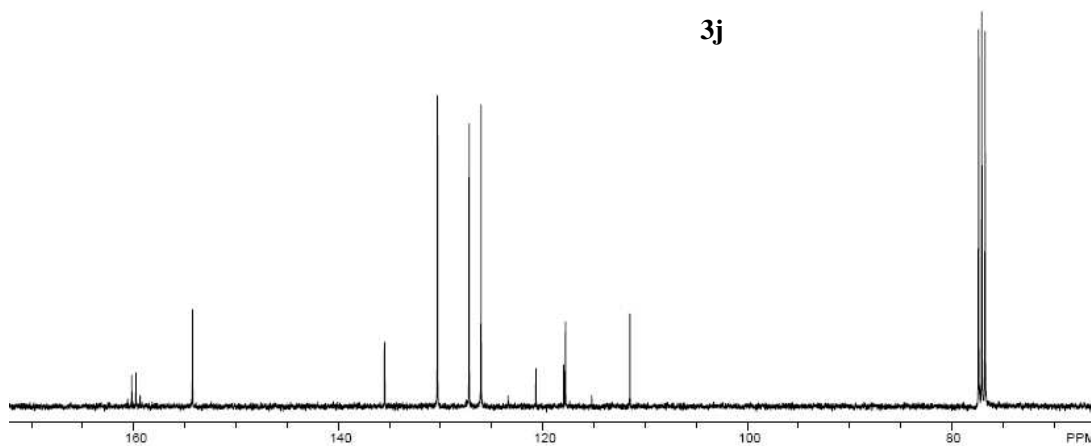
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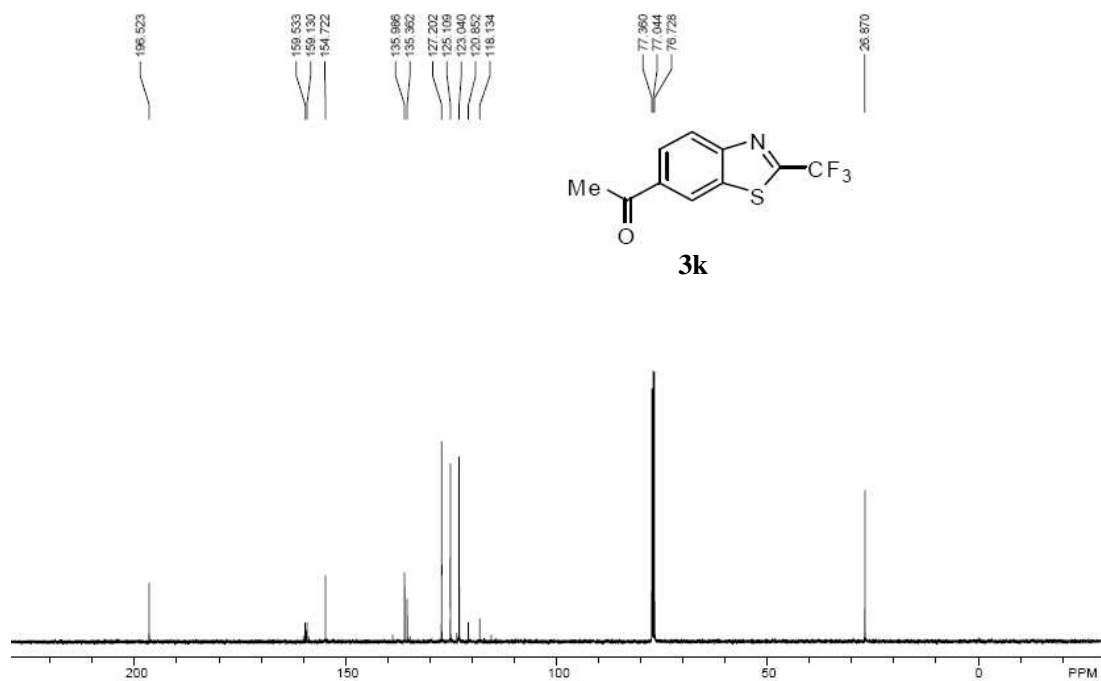
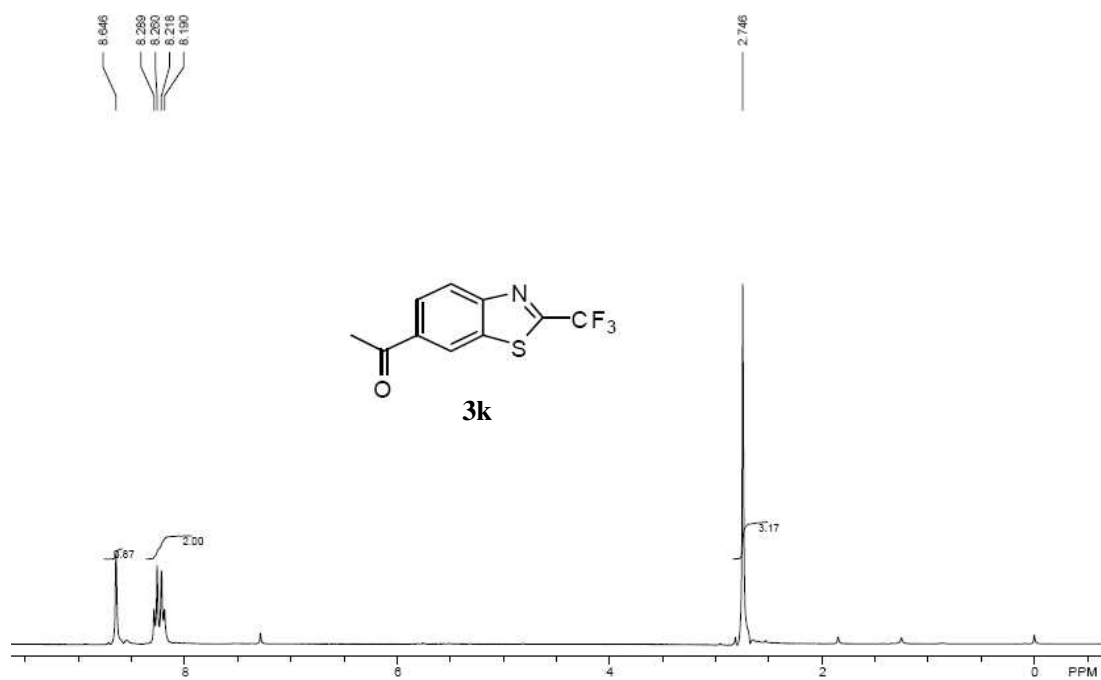
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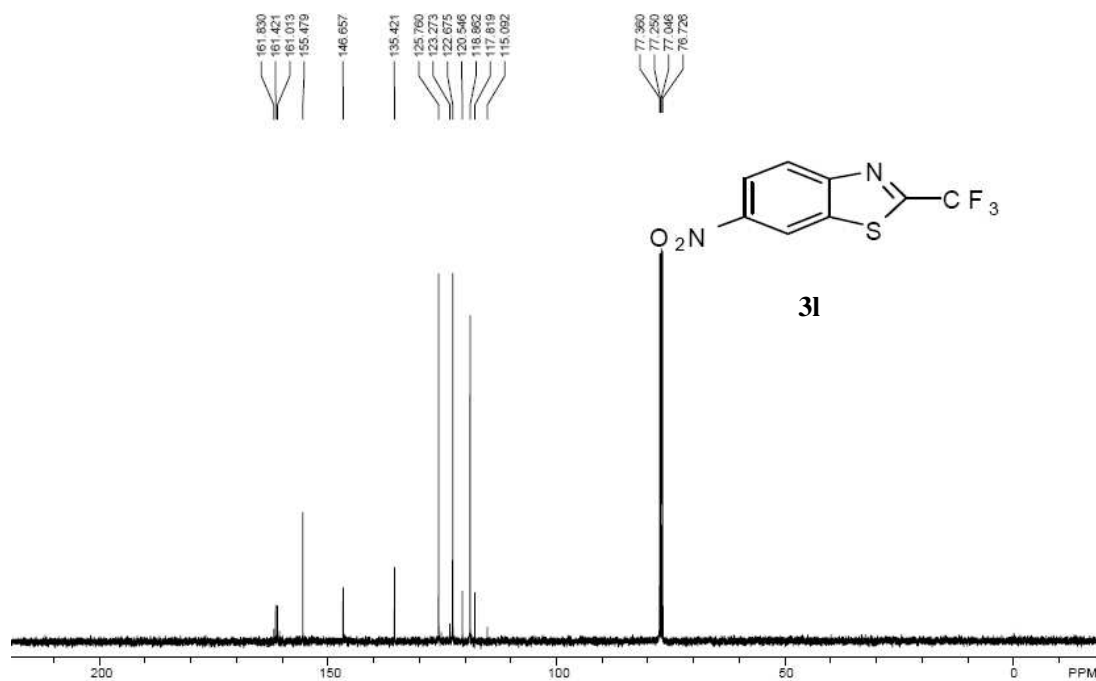
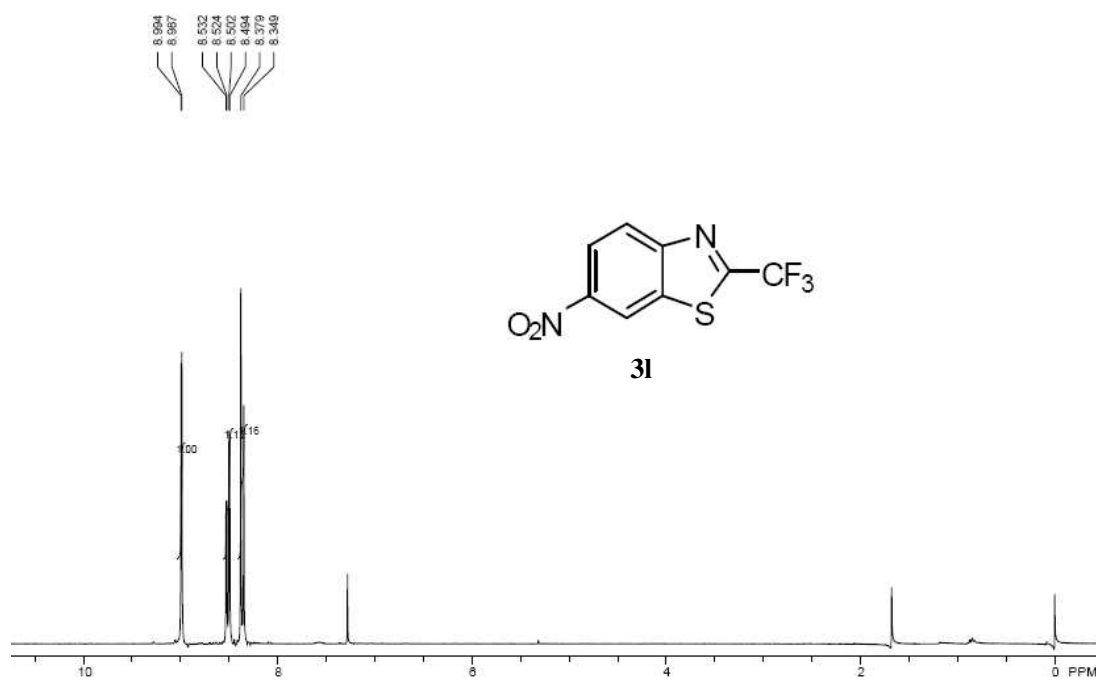
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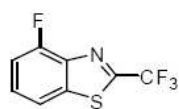
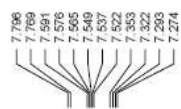
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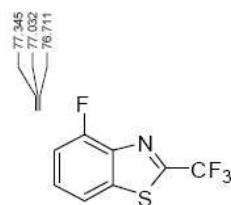
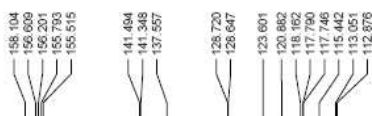
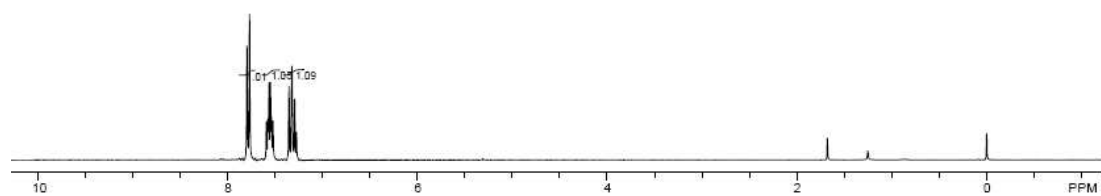
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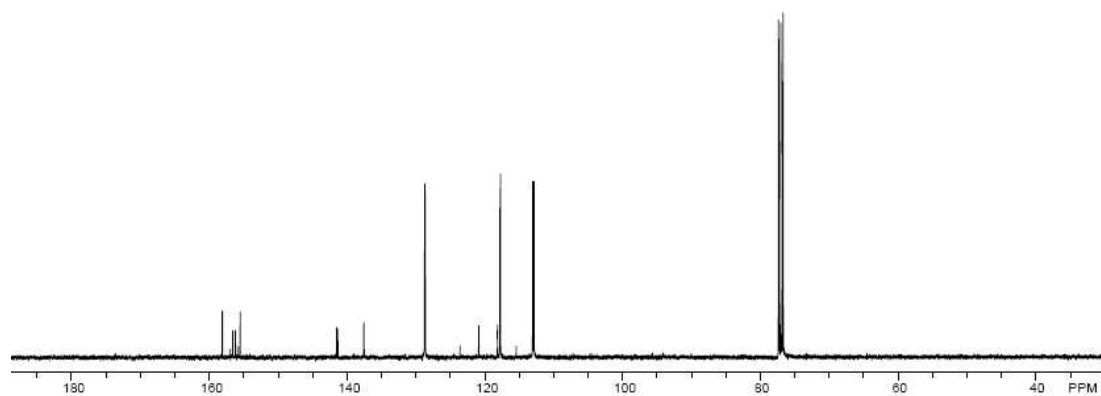
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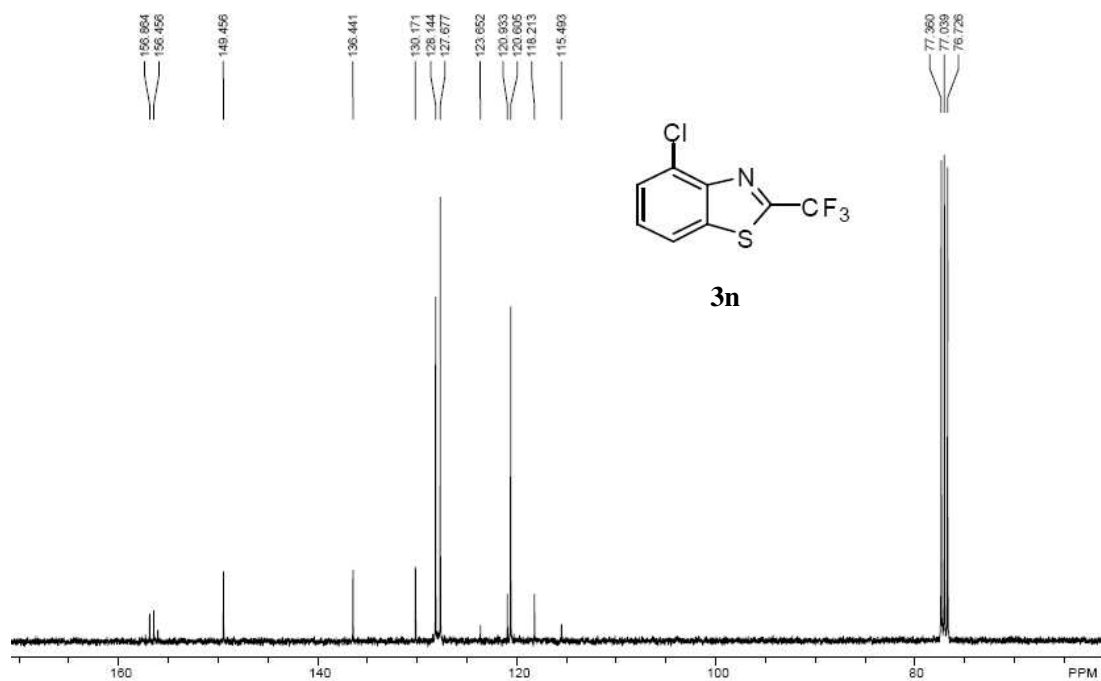
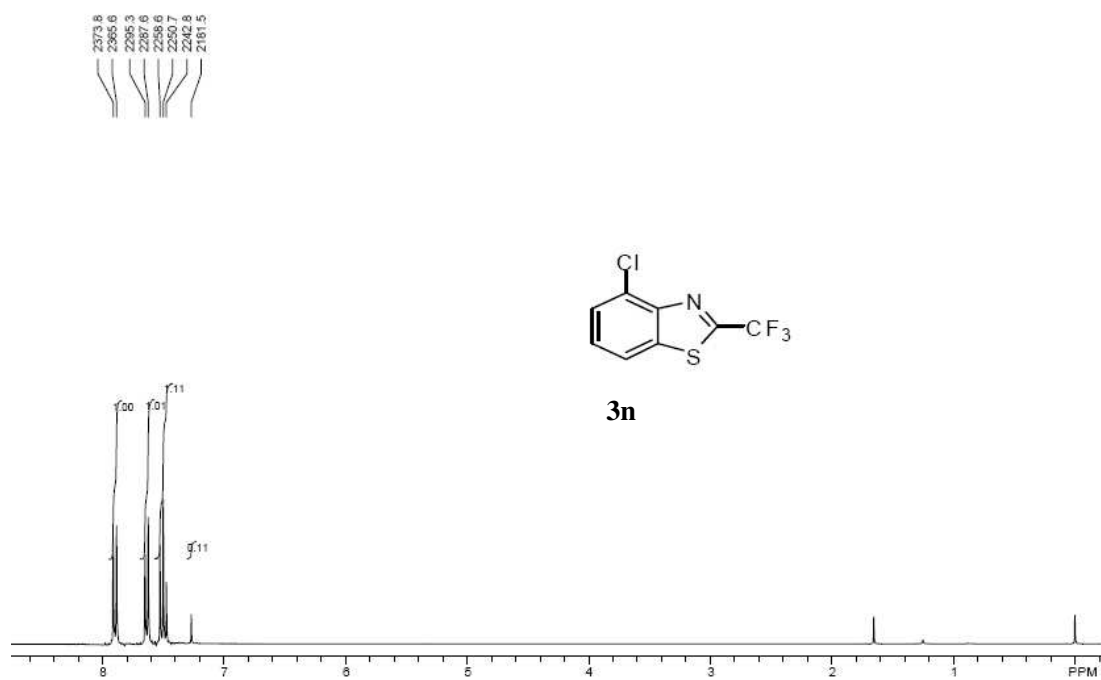
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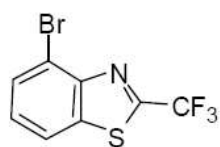
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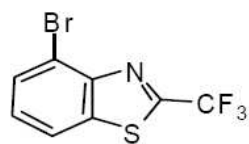
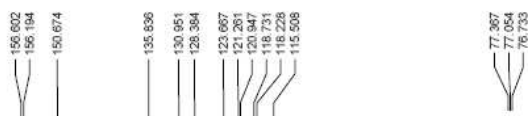
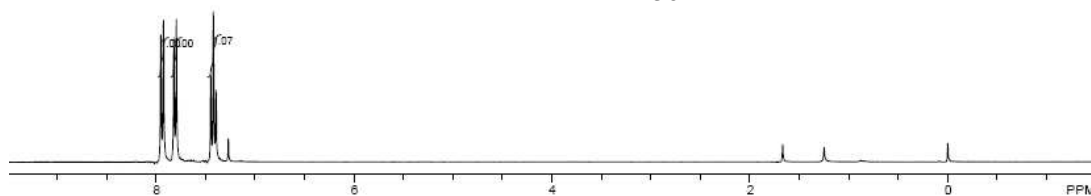
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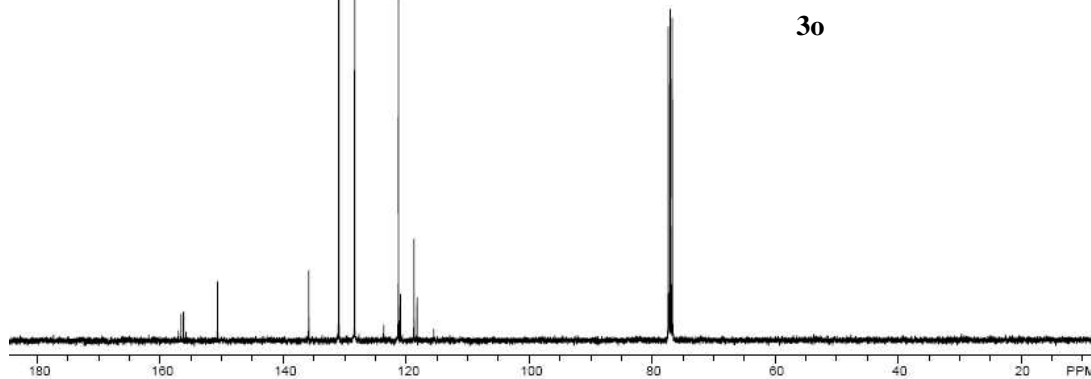
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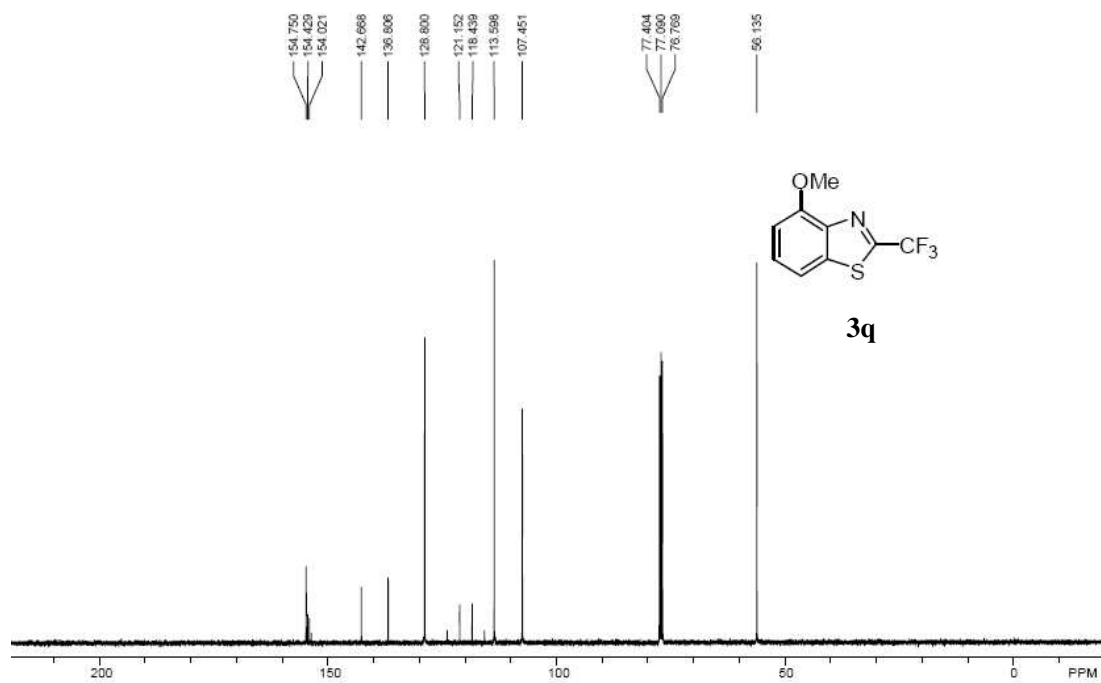
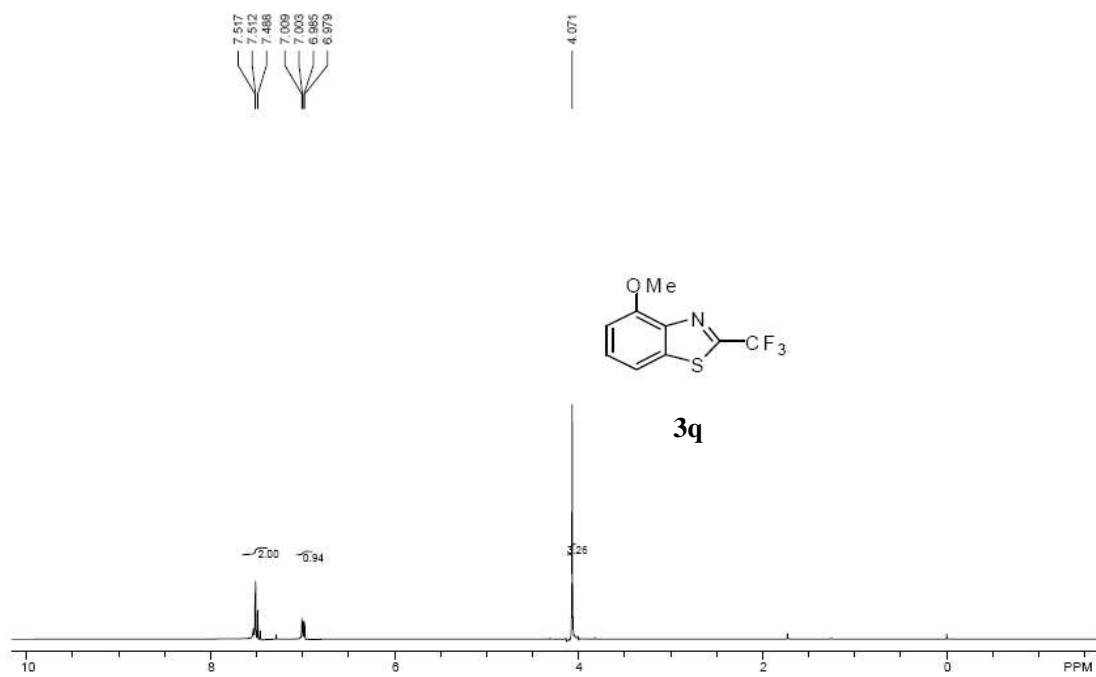
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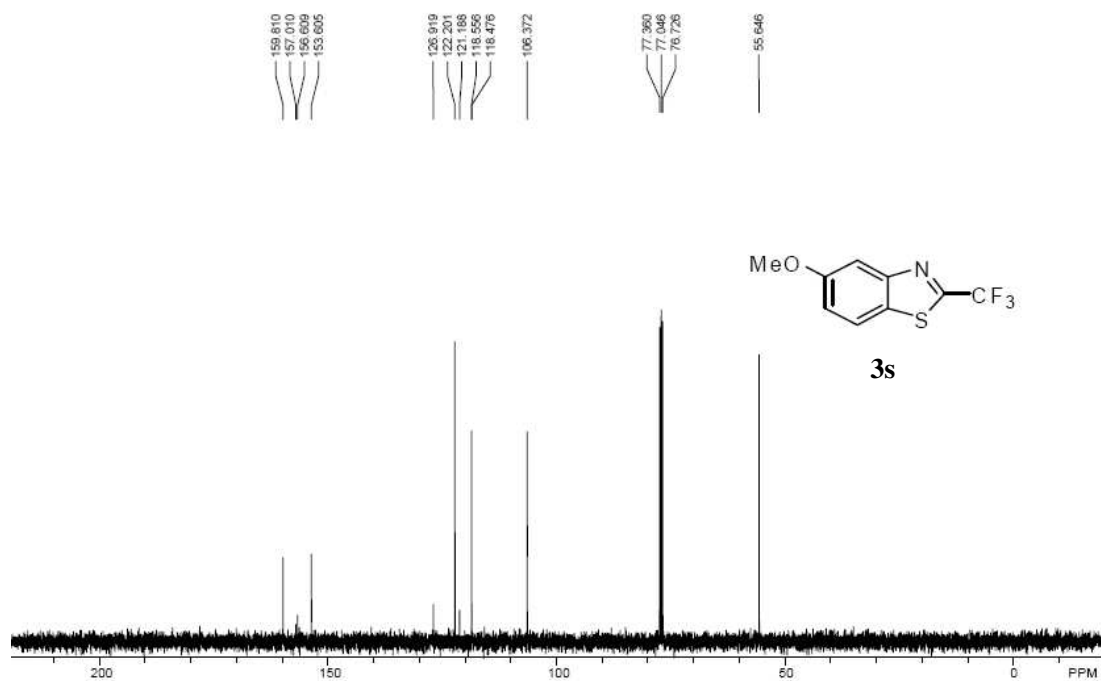
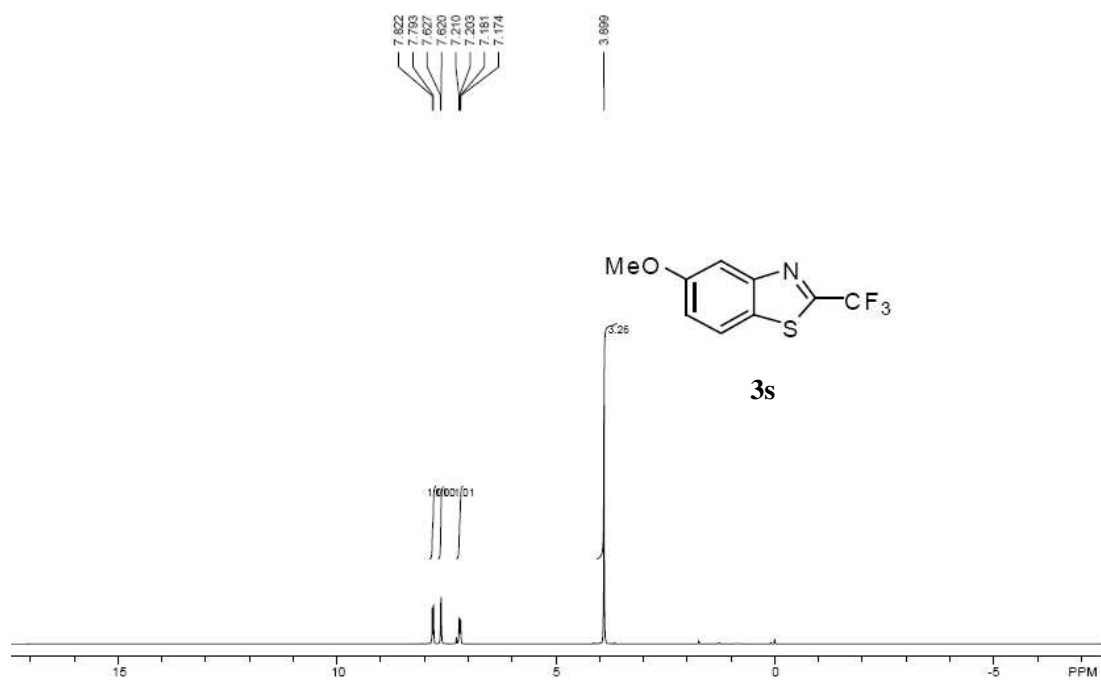
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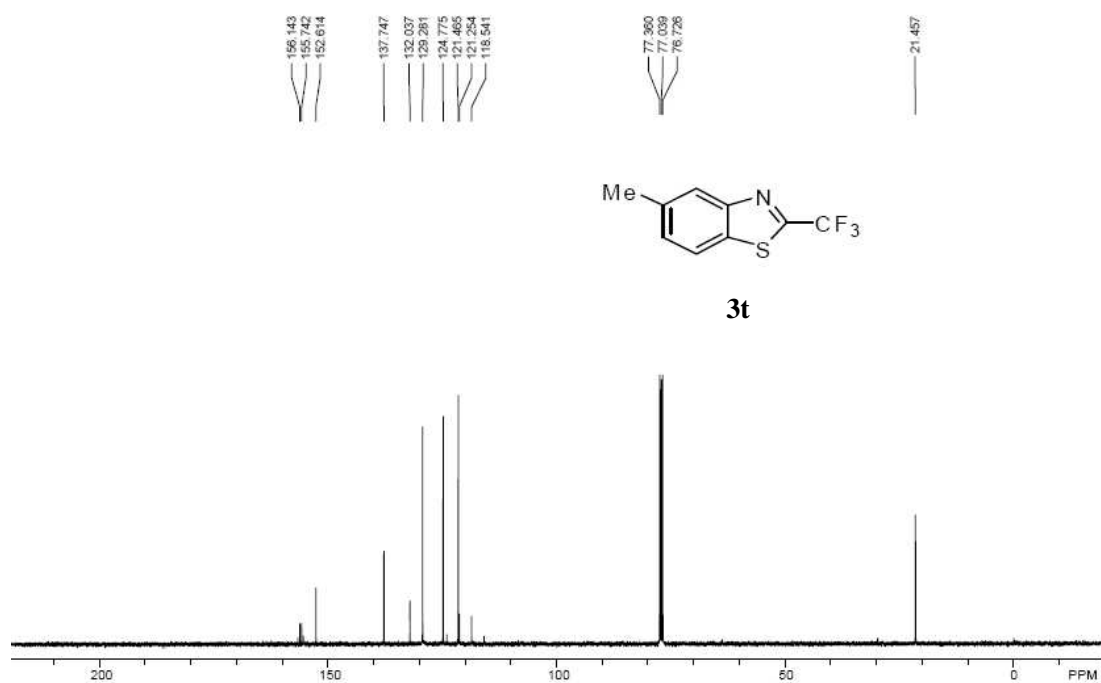
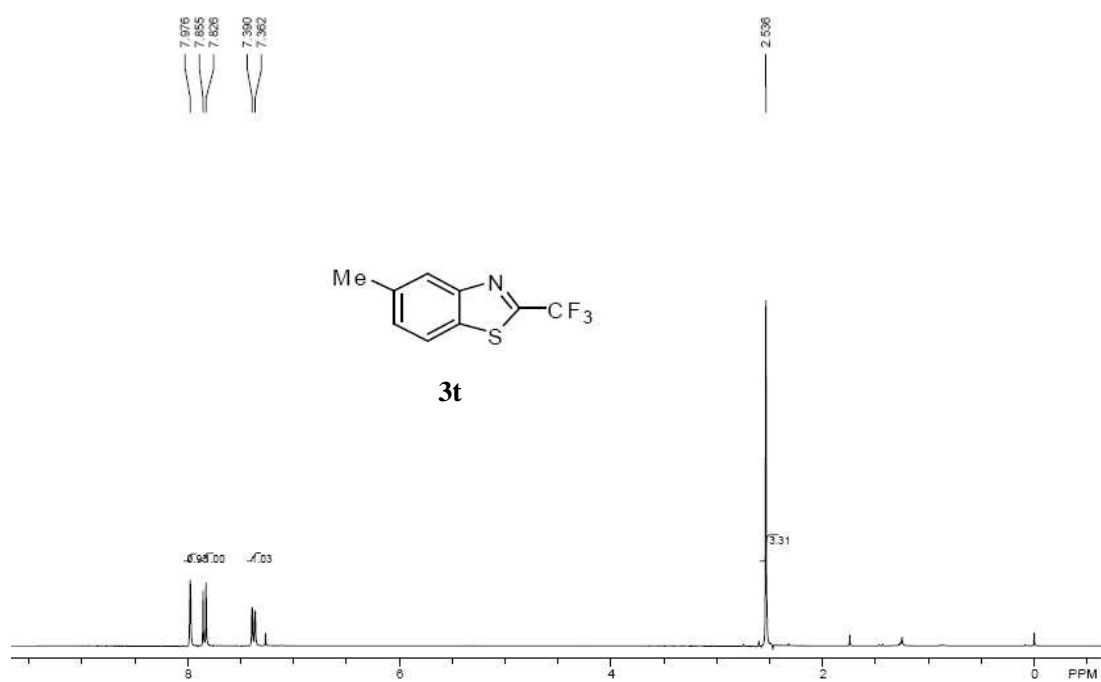
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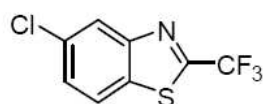
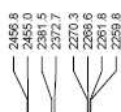
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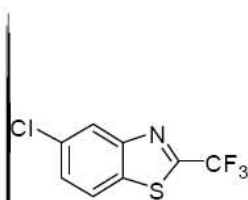
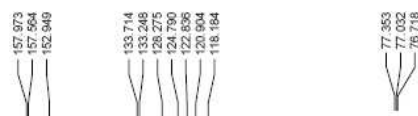
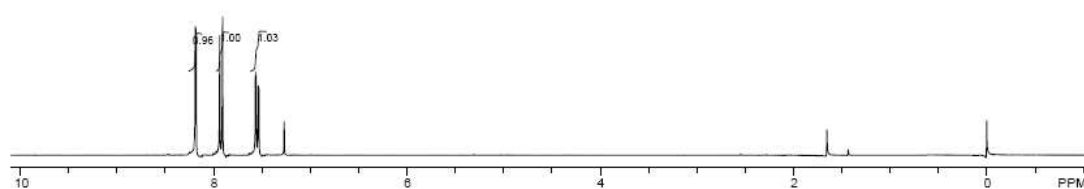
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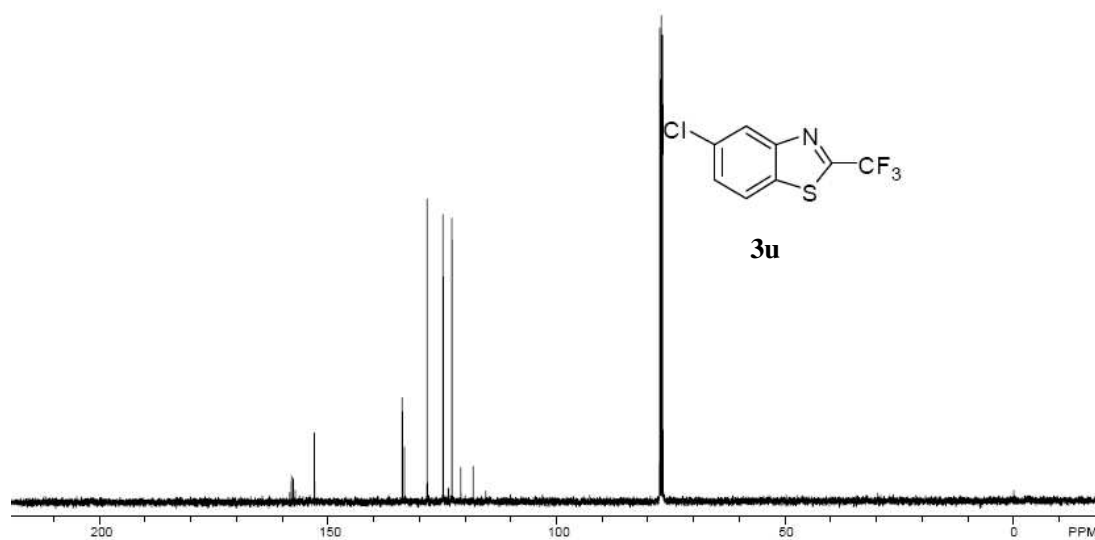
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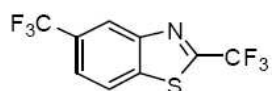
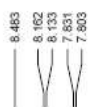
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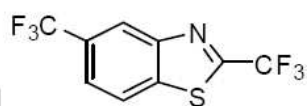
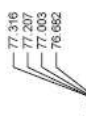
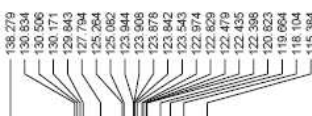
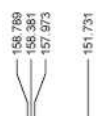
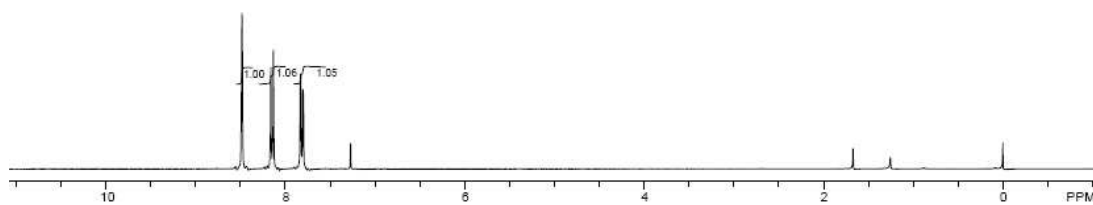
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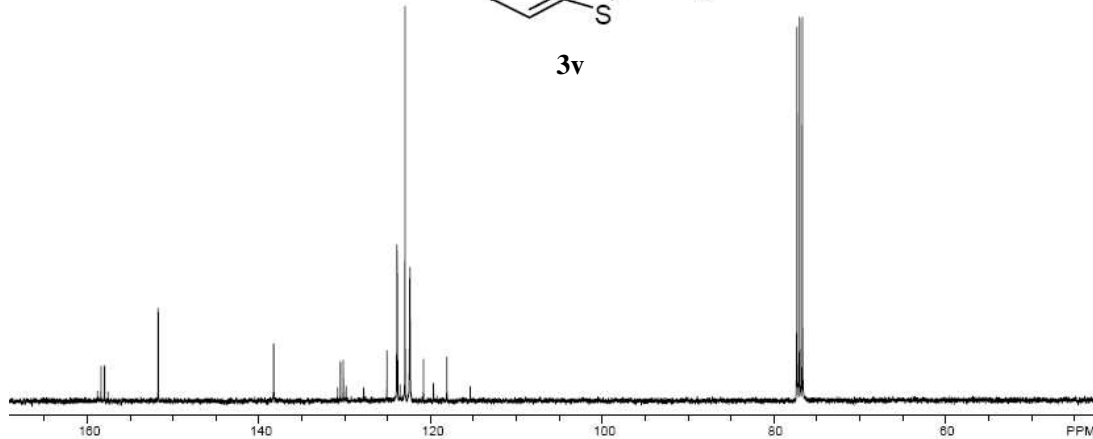
3v



3v



3v



3w

