

Supporting Information
for
Reagent-controlled regiodivergent intermolecular
cyclization of 2-aminobenzothiazoles with β -ketoesters and
 β -ketoamides

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General information

The following chemicals were obtained from Alfa-Aesar, Sigma-Aldrich, and TCI and used as received: CBrCl_3 , KO^tBu , MeCN, $\text{In}(\text{OTf})_3$, toluene, methyl acetoacetate and their derivatives, 2-aminobenzothiazole and their derivatives. Thin-layer chromatography (TLC) was performed using TLC silica gel 60 F_{254} glass plates. Silica gel 60 (230–400 mesh) was used for column chromatography. The ^1H NMR and ^{13}C NMR of samples in CDCl_3 were measured using a Bruker Avance 300 (AV300) spectrometer with tetramethylsilane as an internal standard. For ^1H NMR spectra, chemical shifts were reported in ppm (δ), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, b = broad) and coupling constant (Hz). Detection of compounds by gas chromatography was performed using an Agilent 6890N gas chromatograph equipped with a HP-5 column and an FID detector. Analysis of samples by gas chromatography mass spectrometry was carried out using a Hewlett-Packard HP6890 gas chromatograph with 5973 mass selective detector. Mass spectra measurements were recorded on Bruker microTOFQII under electrospray ionization (ESI) mode. Melting points were recorded with samples in capillary tubes using an automated melting point system.

General procedure for the synthesis of benzo[d]imidazo[2,1-b]thiazole

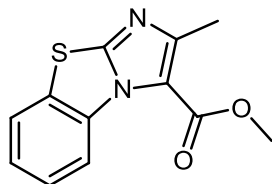
A 25 mL two-neck round-bottomed flask was charged with 2-aminobenzothiazole (**1a**, 180 mg, 1.2 mmol), methyl acetoacetate (**2a**, 108 μL , 1.0 mmol), in 3 mL of $\text{CBrCl}_3/\text{MeCN}$ 1:9 (v/v) solvent mixture. KO^tBu (224 mg, 2.0 mmol) was added slowly at room temperature and the reaction mixture was stirred under reflux for 16 h. Upon completion, the reaction mixture was diluted with 30 mL of ethyl acetate, filtered through a short pad of silica gel and washed down with an additional 60 mL ethyl acetate. The filtrate was washed with distilled water ($3 \times 30 \text{ mL}$) and the organic phase was dried with anhydrous Na_2SO_4 . After filtration, the solvent was removed by rotary evaporation and the residue was purified by column chromatography using hexane and ethyl acetate (v/v = 8:1) as eluent to afford **3a** with 84% yield.

General procedure for the synthesis of benzo[4,5]thiazolo[3,2-a]pyrimidin-4-ones

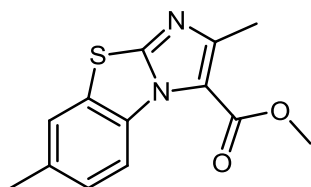
A 10 mL round-bottomed flask was charged with 2-aminobenzothiazole (**1a**, 150 mg, 1.0 mmol), methyl acetoacetate (**2a**, 162 μL , 1.5 mmol) and indium(III) trifluoromethanesulfonate (56 mg,

0.1 mmol) in 1.5 mL of toluene. After stirring at 100 °C for 16 h, the reaction was diluted with water and extracted with EtOAc (15 mL × 5). The combined organic layers were washed with brine and dried with anhydrous Na₂SO₄. After filtration, the solvent was removed by rotary evaporation, and the residue was cleaned up by column chromatography using hexane and ethyl acetate (v/v = 4:1) as eluent to afford **5a** with 95% yield.

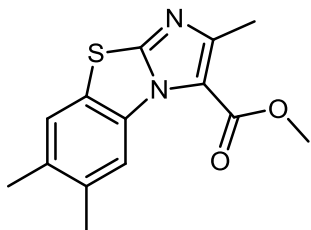
Analytical Data for Products



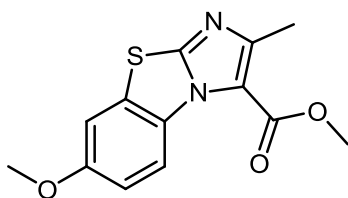
Methyl 2-methylbenzo[d]imidazo[2,1-b]thiazole-3-carboxylate (3a). Obtained as a yellow semi-solid (206 mg, 84%); ¹H NMR (300 MHz, CDCl₃) δ 8.95 (d, *J* = 8.1 Hz, 1H), 7.66 (d, *J* = 7.8 Hz, 1H), 7.45 (t, *J* = 8.0 Hz, 1H), 7.34 (t, *J* = 7.5 Hz, 1H), 3.97 (s, 3H), 2.63 (s, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 161.1, 154.4, 151.7, 134.0, 129.7, 126.3, 125.0, 123.6, 118.3, 117.6, 51.6, 16.9. HRMS (ESI) calcd for C₁₂H₁₁N₂O₂S [M+H]⁺: 247.0536; found 247.0533.



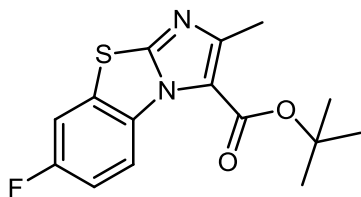
Methyl 2,7-dimethylbenzo[d]imidazo[2,1-b]thiazole-3-carboxylate (3b). Obtained as a yellow solid (240 mg, 92%); mp 145-147 °C; ¹H NMR (300 MHz, CDCl₃) δ 8.79 (d, *J* = 8.7 Hz, 1H), 7.44 (s, 1H), 7.23 (d, *J* = 8.7 Hz, 1H), 3.96 (s, 3H), 2.62 (s, 3H), 2.44 (s, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 161.1, 153.9, 151.5, 135.1, 132.0, 129.8, 127.3, 123.5, 118.2, 117.2, 51.5, 21.1, 16.8. HRMS (ESI) calcd for C₁₃H₁₃N₂O₂S [M+H]⁺: 261.0692; found 261.0695.



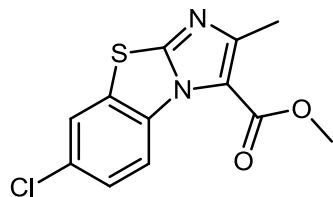
Methyl 2,6,7-trimethylbenzo[d]imidazo[2,1-*b*]thiazole-3-carboxylate (3c). Obtained as a yellow semi-solid (246 mg, 90%); ^1H NMR (75 MHz, CDCl_3) δ 8.70 (s, 1H), 7.38 (s, 1H), 3.97 (s, 3H), 2.62 (s, 3H), 2.39 (s, 3H), 2.33 (s, 3H); ^{13}C NMR (300 MHz, CDCl_3) δ 161.2, 154.0, 151.8, 135.4, 134.1, 132.4, 126.7, 123.7, 118.1, 118.0, 51.5, 20.4, 19.7, 16.9. HRMS (ESI) calcd for $\text{C}_{14}\text{H}_{15}\text{N}_2\text{O}_2\text{S}$ $[\text{M}+\text{H}]^+$: 275.0849; found 275.0850.



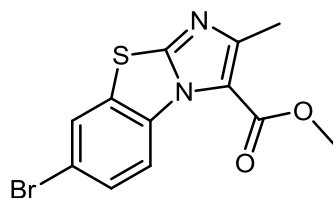
Methyl 2-methyl-7-methoxybenzo[d]imidazo[2,1-*b*]thiazole-3-carboxylate (3d). Obtained as a yellow-orange semi-solid (234 mg, 85%); ^1H NMR (300 MHz, CDCl_3) δ 8.80 (d, $J = 9.3$ Hz, 1H), 7.10 (s, 1H), 6.95 (d, $J = 9.1$ Hz, 1H), 3.94 (s, 3H), 3.83 (s, 3H), 2.59 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 161.1, 152.0, 153.6, 150.9, 131.4, 128.3, 118.3, 118.1, 113.4, 107.6, 55.7, 51.4, 16.8. HRMS (ESI) calcd for $\text{C}_{13}\text{H}_{13}\text{N}_2\text{O}_3\text{S}$ $[\text{M}+\text{H}]^+$: 277.0641; found 277.0638.



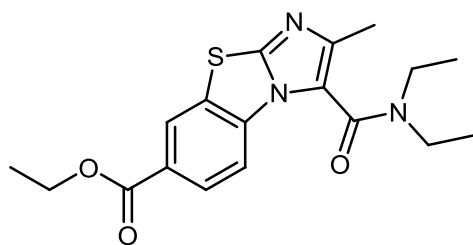
***tert*-Butyl 7-fluoro-2-methylbenzo[d]imidazo[2,1-*b*]thiazole-3-carboxylate (3e).** Obtained as a yellow solid (223 mg, 73%); mp 102-104 $^\circ\text{C}$; ^1H NMR (300 MHz, CDCl_3) δ 9.01 (d, $J = 9.1$ Hz, 1H), 7.36 (d, $J = 7.8$ Hz, 1H), 7.16 (d, $J = 8.4$ Hz, 1H), 2.60 (s, 3H), 1.65 (s, 9H); ^{13}C NMR (75 MHz, CDCl_3) δ 161.2, 160.1, 157.9, 152.9, 150.5, 131.1, 131.0, 130.6, 119.9, 119.1, 119.0, 113.9, 113.5, 110.4, 110.0, 82.1, 28.4, 17.1. HRMS (ESI) calcd for $\text{C}_{15}\text{H}_{16}\text{FN}_2\text{O}_2\text{S}$ $[\text{M}+\text{H}]^+$: 307.0911; found 307.0914.



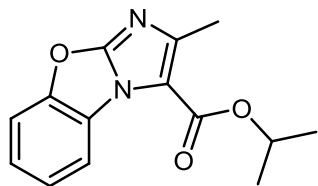
Methyl 7-chloro-2-methylbenzo[d]imidazo[2,1-b]thiazole-3-carboxylate (3f). Obtained as a yellow solid (220 mg, 78%); mp 139-141 °C; ^1H NMR (300 MHz, CDCl_3) δ 8.91 (d, J = 9.0 Hz, 1H), 7.62 (s, 1H), 7.39 (d, J = 9.0 Hz, 1H), 3.96 (s, 3H), 2.62 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 161.0, 154.4, 151.4, 132.6, 131.2, 130.3, 126.6, 123.1, 120.7, 118.6, 51.7, 16.9. HRMS (ESI) calcd for $\text{C}_{12}\text{H}_{10}\text{ClN}_2\text{O}_2\text{S}$ $[\text{M}+\text{H}]^+$: 281.0146; found 281.0149.



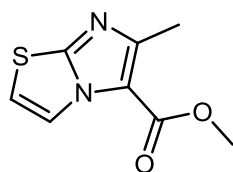
Methyl 7-bromo-2-methylbenzo[d]imidazo[2,1-b]thiazole-3-carboxylate (3g). Obtained as a yellow solid (270 mg, 83%); mp 170-172 °C; ^1H NMR (300 MHz, CDCl_3) δ 8.86 (d, J = 9.0 Hz, 1H), 7.78 (s, 1H), 7.53 (d, J = 9.0 Hz, 1H), 3.97 (s, 3H), 2.62 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 161.1, 154.5, 151.3, 133.0, 131.5, 129.5, 126.0, 123.8, 118.9, 118.0, 51.7, 16.9. HRMS (ESI) calcd for $\text{C}_{12}\text{H}_{10}\text{BrN}_2\text{O}_2\text{S}$ $[\text{M}+\text{H}]^+$: 324.9641; found 324.9643.



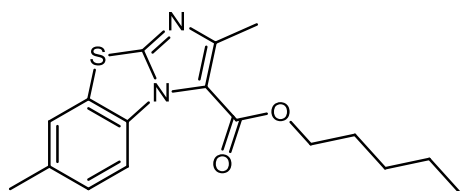
Ethyl 3-(diethylcarbamoyl)-2-methyl-benzo[d]imidazo[2,1-b] thiazole-7-carboxylate (3h). Obtained as a yellow semi-solid (281 mg, 78 %); ^1H NMR (300 MHz, CDCl_3) δ 8.36 (s, 1H), 8.06 (d, J = 8.7 Hz, 1H), 7.71 (d, J = 7.8 Hz, 1H), 4.38 (q, J = 7.2 Hz, 2H), 3.55 (broad, 4H), 1.38 (q, J = 7.2 Hz, 3H), 1.22 (broad, 6H); ^{13}C NMR (75 MHz, CDCl_3) δ 165.3, 161.8, 149.0, 144.1, 135.0, 130.0, 127.9, 127.0, 125.7, 113.6, 61.3, 42.9, 40.1, 14.5, 14.2, 14.0. HRMS (ESI) calcd for $\text{C}_{18}\text{H}_{22}\text{N}_3\text{O}_3\text{S}$ $[\text{M}+\text{H}]^+$: 360.1377; found 360.1375.



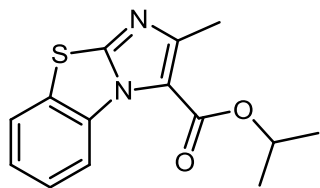
Isopropyl 2-methylbenzo[d]imidazo[2,1-b]oxazole-3-carboxylate (3j). Obtained as a pale yellow semi-solid (218 mg, 84%); ^1H NMR (300 MHz, CDCl_3) δ 8.28 (d, J = 9.3 Hz, 1H), 7.48 (d, J = 9.3 Hz, 1H), 7.35-7.25 (m, 2H), 5.37-5.22 (m, 1H), 2.60 (s, 3H), 1.42 (d, J = 6.3 Hz, 6H); ^{13}C NMR (75 MHz, CDCl_3) δ 160.0, 155.5, 150.6, 150.5, 127.3, 124.5, 124.3, 115.1, 113.8, 112.0, 68.4, 22.1, 16.2. HRMS (ESI) calcd for $\text{C}_{14}\text{H}_{15}\text{N}_2\text{O}_3$ $[\text{M}+\text{H}]^+$: 259.1077; found 259.1079.



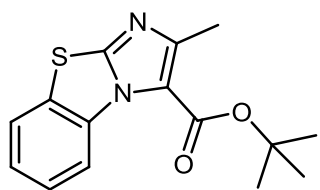
Methyl 6-methylimidazo[2,1-b]thiazole-5-carboxylate (3k). Obtained as a white solid (181 mg, 92%); mp 97-99 °C; ^1H NMR (300 MHz, CDCl_3) δ 8.02 (d, J = 4.5 Hz, 1H), 6.88 (d, J = 4.5 Hz, 1H), 3.90 (s, 3H), 2.59 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 160.8, 153.2, 152.3, 121.1, 115.2, 112.6, 51.3, 15.9. HRMS (ESI) calcd for $\text{C}_8\text{H}_9\text{N}_2\text{O}_2\text{S}$ $[\text{M}+\text{H}]^+$: 197.0379; found 197.0379.



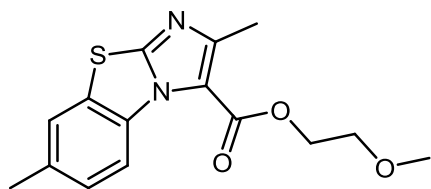
Pentyl 2,7-dimethyl-benzo[d]imidazo[2,1-b]thiazole-3-carboxylate (3l). Obtained as a yellow solid (262 mg, 83%); mp 59-62 °C; ^1H NMR (300 MHz, CDCl_3) δ 8.80 (d, J = 8.7 Hz, 1H), 7.41 (s, 1H), 7.20 (d, J = 9.0 Hz, 1H), 4.35 (t, J = 6.8 Hz, 2H), 2.62 (s, 3H), 2.42 (s, 3H), 1.83-1.75 (m, 2H), 1.47-1.33 (m, 4H), 0.93 (t, J = 6.9 Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 160.8, 153.7, 151.3, 135.0, 132.0, 129.7, 127.2, 123.5, 118.4, 117.3, 64.8, 28.4, 22.8, 28.2, 22.3, 21.1, 17.0, 13.9. HRMS (ESI) calcd for $\text{C}_{17}\text{H}_{21}\text{N}_2\text{O}_2\text{S}$ $[\text{M}+\text{H}]^+$: 317.1319; found 317.1322.



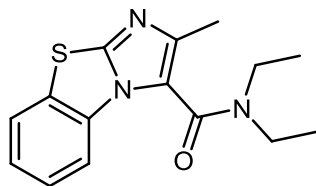
Isopropyl 2-methyl-benzo[d]imidazo[2,1-b]thiazole-3-carboxylate (3m). Obtained as a yellow oil (256 mg, 93%); ^1H NMR (300 MHz, CDCl_3) δ 8.95 (d, J = 8.4 Hz, 1H), 7.62 (d, J = 8.1 Hz, 1H), 7.41 (t, J = 8.0 Hz, 1H), 7.30 (t, J = 7.7 Hz, 1H), 5.36-5.22 (m, 1H), 2.62 (s, 3H), 1.42 (d, J = 6.3 Hz, 6H); ^{13}C NMR (75 MHz, CDCl_3) δ 160.2, 153.9, 151.3, 134.0, 129.6, 126.1, 124.8, 123.4, 118.8, 117.7, 68.5, 22.1, 17.0. HRMS (ESI) calcd for $\text{C}_{14}\text{H}_{15}\text{N}_2\text{O}_2\text{S}$ $[\text{M}+\text{H}]^+$: 275.0849; found 275.0849.



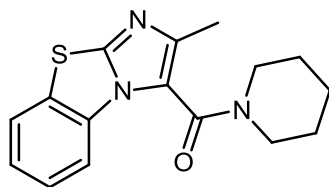
tert-Butyl 2-methylbenzo[d]imidazo[2,1-b]thiazole-3-carboxylate (3n). Obtained as a yellow oil (259 mg, 90%); ^1H NMR (300 MHz, CDCl_3) δ 8.96 (d, J = 8.4 Hz, 1H), 7.64 (d, J = 8.1 Hz, 1H), 7.43 (t, J = 8.0 Hz, 1H), 7.32 (t, J = 7.7 Hz, 1H), 2.61 (s, 3H), 1.65 (s, 9H); ^{13}C NMR (75 MHz, CDCl_3) δ 160.1, 153.2, 150.9, 134.1, 129.7, 126.1, 124.8, 123.5, 119.8, 117.8, 81.9, 28.5, 17.1. HRMS (ESI) calcd for $\text{C}_{15}\text{H}_{17}\text{N}_2\text{O}_2\text{S}$ $[\text{M}+\text{H}]^+$: 289.1005; found 289.1007.



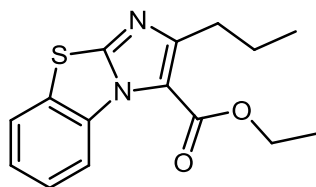
2-Methoxyethyl 2,7-dimethylbenzo[d]imidazo[2,1-b]thiazole-3-carboxylate (3o). Obtained as a yellow-orange solid (268 mg, 88%); mp 110-112 $^{\circ}\text{C}$; ^1H NMR (300 MHz, CDCl_3) δ 8.76 (d, J = 8.7 Hz, 1H), 7.41 (s, 1H), 7.19 (d, J = 8.4 Hz, 1H), 4.50 (t, J = 4.7 Hz, 2H), 3.74 (t, J = 4.7 Hz, 2H), 3.43 (s, 3H), 2.64 (s, 3H), 2.42 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 160.5, 154.4, 151.5, 135.0, 131.9, 129.7, 127.3, 123.5, 118.0, 117.2, 70.5, 63.5, 58.9, 21.1, 16.9. HRMS (ESI) calcd for $\text{C}_{15}\text{H}_{17}\text{N}_2\text{O}_3\text{S}$ $[\text{M}+\text{H}]^+$: 305.0954; found 305.0955.



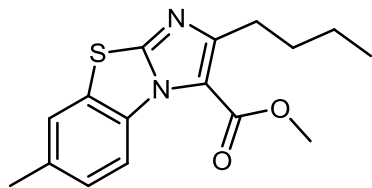
N,N-Diethyl 2-methylbenzo[d]imidazo[2,1-b]thiazole-3-carboxamide (3p). Obtained as a yellow oil (256 mg, 89%); ^1H NMR (300 MHz, CDCl_3) δ 7.62 (t, J = 8.0 Hz, 2H), 7.33 (t, J = 7.8 Hz, 1H), 7.24 (t, J = 7.7 Hz, 1H), 3.52 (broad, 4H), 2.33 (s, 3H), 1.20 (broad, 6H); ^{13}C NMR (75 MHz, CDCl_3) δ 162.1, 148.1, 143.2, 132.2, 129.8, 126.1, 124.5, 123.9, 118.9, 113.9, 42.9, 39.7, 14.4, 13.8. HRMS (ESI) calcd for $\text{C}_{15}\text{H}_{18}\text{N}_3\text{OS}$ $[\text{M}+\text{H}]^+$: 288.1165; found 288.1168.



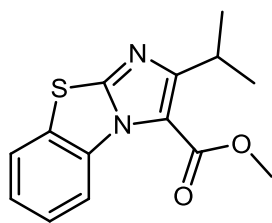
(2-Methylbenzo[d]imidazo[2,1-b]thiazol-3-yl)(piperidin-1-yl)methanone (3q). Obtained as a yellow-orange oil (263 mg, 88%); ^1H NMR (300 MHz, CDCl_3) δ 7.78 (d, J = 8.1 Hz, 1H), 7.64 (d, J = 8.1 Hz, 1H), 7.37 (t, J = 7.7 Hz, 1H), 7.28 (t, J = 7.7 Hz, 1H), 3.47 (broad, 4H), 2.36 (s, 3H), 1.67 (broad, 6H); ^{13}C NMR (75 MHz, CDCl_3) δ 161.3, 148.8, 144.2, 132.5, 129.9, 126.2, 124.6, 123.9, 118.7, 114.5, 47.4, 44.3, 26.4, 24.5, 14.7. HRMS (ESI) calcd for $\text{C}_{16}\text{H}_{18}\text{N}_3\text{OS}$ $[\text{M}+\text{H}]^+$: 300.1165; found 300.1167.



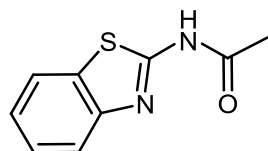
Ethyl 2-propylbenzo[d]imidazo[2,1-b]thiazole-3-carboxylate (3r). Obtained as a yellow solid (238 mg, 83%); mp 58-61 $^{\circ}\text{C}$; ^1H NMR (300 MHz, CDCl_3) δ 8.90 (d, J = 8.4 Hz, 1H), 7.62 (d, J = 7.8 Hz, 1H), 7.40 (t, J = 7.8 Hz, 1H), 7.29 (t, J = 7.7 Hz, 1H), 4.42 (q, J = 7.2 Hz, 2H), 2.97 (t, J = 7.5 Hz, 2H), 1.83-1.69 (m, 2H), 1.43 (t, J = 7.2 Hz, 3H), 1.00 (t, J = 7.5 Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 160.6, 158.3, 151.6, 134.0, 129.7, 126.1, 124.8, 123.5, 118.2, 117.6, 60.6, 32.3, 22.8, 14.3, 13.9. HRMS (ESI) calcd for $\text{C}_{15}\text{H}_{17}\text{N}_2\text{O}_2\text{S}$ $[\text{M}+\text{H}]^+$: 289.1005; found 289.1008.



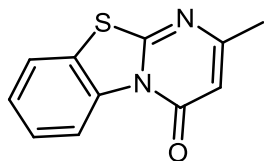
Methyl 2-butyl-7-methylbenzo[d]imidazo[2,1-b]thiazole-3-carboxylate (3s). Obtained as a yellow semi-solid (251 mg, 83%); ^1H NMR (300 MHz, CDCl_3) δ 8.67 (d, J = 8.7 Hz, 1H), 7.34 (s, 1H), 7.13 (d, J = 8.7 Hz, 1H), 3.91 (s, 3H), 2.94 (t, J = 7.7 Hz, 2H), 2.36 (s, 3H), 1.74-1.64 (m, 2H), 1.45-1.33 (m, 2H), 0.92 (t, J = 7.4 Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 161.0, 158.3, 151.5, 134.8, 131.9, 129.7, 127.1, 123.3, 117.6, 117.0, 51.3, 31.5, 29.8, 22.5, 20.9, 13.8. HRMS (ESI) calcd for $\text{C}_{16}\text{H}_{19}\text{N}_2\text{O}_2\text{S}$ $[\text{M}+\text{H}]^+$: 303.1161; found 303.1164.



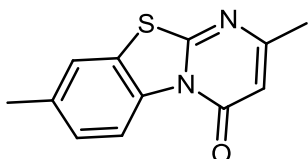
Methyl 2-isopropylbenzo[d]imidazo[2,1-b]thiazole-3-carboxylate (3t). Obtained as a yellow semi-solid (190 mg, 69%); ^1H NMR (300 MHz, CDCl_3) δ 8.80 (d, J = 8.4 Hz, 1H), 7.59 (d, J = 7.5 Hz, 1H), 7.37 (t, J = 8.0 Hz, 1H), 7.26 (t, J = 7.7 Hz, 1H), 3.95 (s, 3H), 3.77-3.61 (m, 1H), 1.32 (d, J = 6.9 Hz, 6H); ^{13}C NMR (75 MHz, CDCl_3) δ 163.4, 161.1, 151.9, 133.9, 129.8, 126.0, 124.8, 123.4, 117.4, 116.7, 51.5, 28.0, 22.2. HRMS (ESI) calcd for $\text{C}_{14}\text{H}_{15}\text{N}_2\text{O}_2\text{S}$ $[\text{M}+\text{H}]^+$: 275.0849; found 275.0852.



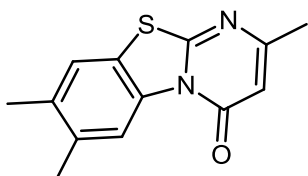
N-(benzo[d]thiazol-2-yl)acetamide (4)^[a] ^1H NMR (300 MHz, CDCl_3) δ 12.21 (broad, 1H), 7.84 (d, J = 7.8 Hz, 1H), 7.76 (d, J = 8.1 Hz, 1H), 7.45 (t, J = 7.2 Hz, 1H), 7.33 (t, J = 7.2 Hz, 1H), 2.28 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 169.0, 160.2, 147.5, 131.8, 126.3, 124.0, 121.6, 120.2, 23.4. HRMS (ESI) calcd for $\text{C}_9\text{H}_9\text{N}_2\text{OS}$ $[\text{M}+\text{H}]^+$: 193.0430; found 193.0432.



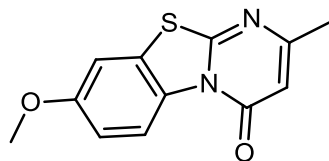
2-Methyl-4H-benzo[4,5]thiazolo[3,2-a]pyrimidin-4-one (5a)^{lb} Obtained as a light yellow solid (206 mg, 95%); mp 202-204 °C; ¹H NMR (300 MHz, CDCl₃) δ 8.94 (d, *J* = 7.5 Hz, 1H), 7.57 (d, *J* = 7.2 Hz, 1H), 7.44-7.33 (m, 2H), 6.16 (s, 1H), 2.30 (s, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 162.6, 161.1, 160.8, 135.8, 126.7, 126.6, 123.8, 121.5, 119.7, 106.9, 23.5. HRMS (ESI) calcd for C₁₁H₉N₂OS [M+H]⁺: 217.0430; found 217.0432.



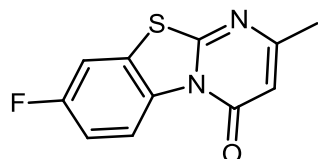
2,8-Dimethyl-4H-benzo[4,5]thiazolo[3,2-a]pyrimidin-4-one (5b). Obtained as a white solid (228 mg, 99%); mp 193-195 °C; ¹H NMR (300 MHz, CDCl₃) δ 8.79 (d, *J* = 8.7 Hz, 1H), 7.35 (s, 1H), 7.19 (d, *J* = 8.7 Hz, 1H), 6.15 (s, 1H), 2.39 (s, 3H), 2.31 (s, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 162.5, 161.2, 160.8, 137.1, 133.7, 127.7, 126.6, 123.8, 121.5, 119.4, 106.8, 23.5, 21.2. HRMS (ESI) calcd for C₁₂H₁₁N₂OS [M+H]⁺: 231.0586; found 231.0587.



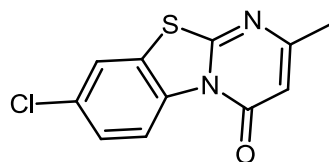
2,7,8-Trimethyl-4H-benzo[4,5]thiazolo[3,2-a]pyrimidin-4-one (5c). Obtained as a light yellow solid (237 mg, 97%); mp 178-180 °C; ¹H NMR (300 MHz, CDCl₃) δ 8.55 (s, 1H), 7.15 (s, 1H), 6.05 (s, 1H), 2.24 (s, 3H), 2.20 (s, 3H), 2.17 (s, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 162.1, 161.3, 160.5, 135.8, 135.6, 133.8, 121.4, 120.5, 119.9, 106.5, 23.4, 19.9, 19.7. HRMS (ESI) calcd for C₁₃H₁₃N₂OS [M+H]⁺: 245.0743; found 245.0744.



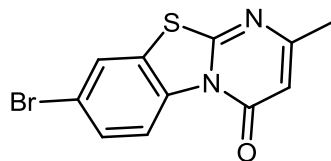
8-Methoxy-2-methyl-4H-benzo[4,5]thiazolo[3,2-a]pyrimidin-4-one (5d). Obtained as a yellow solid (222 mg, 90%); mp 175-177 °C; ^1H NMR (300 MHz, CDCl_3) δ 8.90 (d, J = 9.3 Hz, 1H), 7.09 (s, 1H), 6.99 (d, J = 9.3 Hz, 1H), 6.20 (s, 1H), 3.84 (s, 3H), 2.34 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 162.4, 161.0, 160.7, 158.4, 129.8, 125.4, 120.8, 113.5, 106.9, 106.0, 55.7, 23.6. HRMS (ESI) calcd for $\text{C}_{12}\text{H}_{11}\text{N}_2\text{O}_2\text{S}$ $[\text{M}+\text{H}]^+$: 247.0535; found 247.0538.



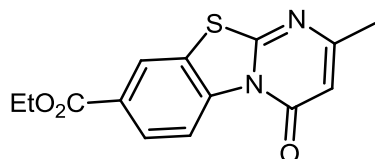
8-Fluoro-2-methyl-4H-benzo[4,5]thiazolo[3,2-a]pyrimidin-4-one (5e). Obtained as a white solid (222 mg, 95%); mp 200-202 °C; ^1H NMR (300 MHz, CDCl_3) δ 9.02-8.95 (m, 1H), 7.33 (d, J = 7.8 Hz, 1H), 7.16 (t, J = 8.9 Hz, 1H), 6.20 (s, 1H), 2.34 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 162.8, 162.3, 160.9, 160.6, 159.0, 132.3, 125.7, 125.5, 121.3, 121.2, 114.5, 114.2, 108.9, 108.6, 107.2, 23.6. HRMS (ESI) calcd for $\text{C}_{11}\text{H}_8\text{FN}_2\text{OS}$ $[\text{M}+\text{H}]^+$: 235.0336; found 235.0336.



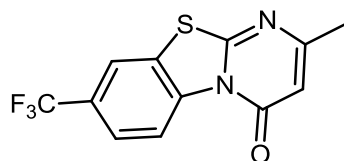
8-Chloro-2-methyl-4H-benzo[4,5]thiazolo[3,2-a]pyrimidin-4-one (5f). Obtained as a white solid (231 mg, 92%); mp 212-214 °C; ^1H NMR (300 MHz, CDCl_3) δ 8.96 (d, J = 9.0 Hz, 1H), 7.62 (s, 1H), 7.45 (d, J = 9.0 Hz, 1H), 6.24 (s, 1H), 2.37 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 163.1, 160.8, 160.7, 134.5, 132.7, 127.3, 125.6, 121.5, 120.8, 107.3, 23.7. HRMS (ESI) calcd for $\text{C}_{11}\text{H}_8\text{ClN}_2\text{OS}$ $[\text{M}+\text{H}]^+$: 251.0040; found 251.0042.



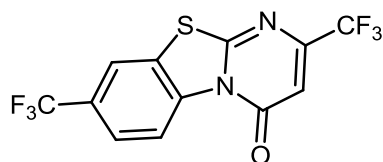
8-Bromo-2-methyl-4H-benzo[4,5]thiazolo[3,2-a]pyrimidin-4-one (5g). Obtained as a yellow solid (272 mg, 92%); mp 227-229 °C; ^1H NMR (300 MHz, CDCl_3) δ 8.89 (d, J = 9.0 Hz, 1H), 7.77 (s, 1H), 7.58 (d, J = 9.0 Hz, 1H), 6.23 (s, 1H), 2.36 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 163.1, 160.7, 160.7, 134.9, 130.1, 125.9, 124.3, 121.0, 120.2, 107.3, 23.7. HRMS (ESI) calcd for $\text{C}_{11}\text{H}_8\text{BrN}_2\text{OS}$ $[\text{M}+\text{H}]^+$: 294.9535; found 294.9532.



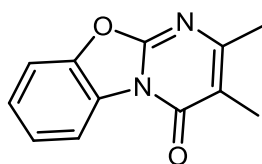
Ethyl 2-methyl-4-oxo-4H-benzo[4,5]thiazolo[3,2-a]pyrimidine-8-carboxylate (5h). Obtained as a white solid (246 mg, 85%); mp 196-198 °C; ^1H NMR (300 MHz, CDCl_3) δ 9.09 (d, J = 9.0 Hz, 1H), 8.35 (s, 1H), 8.16 (d, J = 9.0 Hz, 1H), 6.26 (s, 1H), 4.42 (q, J = 7.1 Hz, 2H), 2.38 (s, 3H), 1.42 (t, J = 7.1 Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 165.0, 163.2, 161.5, 160.9, 129.2, 128.9, 128.3, 124.3, 123.2, 119.5, 107.3, 61.6, 23.7, 14.3. HRMS (ESI) calcd for $\text{C}_{14}\text{H}_{13}\text{N}_2\text{O}_3\text{S}$ $[\text{M}+\text{H}]^+$: 289.0642; found 289.0645.



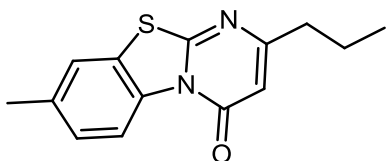
2-Methyl-8-(trifluoromethyl)-4H-benzo[4,5]thiazolo[3,2-a]pyrimidin-4-one (5i). Obtained as a white solid (258 mg, 91%); mp 179-181 °C; ^1H NMR (300 MHz, CDCl_3) δ 9.08 (d, J = 8.7 Hz, 1H), 7.90 (s, 1H), 7.69 (d, J = 8.7 Hz, 1H), 6.20 (s, 1H), 2.34 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 163.2, 161.0, 160.6, 138.1, 129.8, 129.4, 128.9, 128.7, 128.5, 125.1, 124.9, 124.0, 123.9, 123.9, 123.8, 121.5, 119.9, 119.1, 119.0, 119.0, 118.9, 117.9, 107.3, 23.6. HRMS (ESI) calcd for $\text{C}_{12}\text{H}_8\text{F}_3\text{N}_2\text{OS}$ $[\text{M}+\text{H}]^+$: 285.0304; found 285.0306.



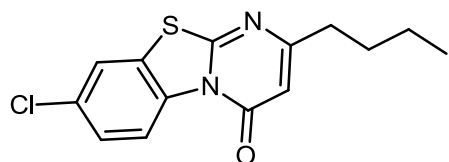
2,8-Bis(trifluoromethyl)-4H-benzo[4,5]thiazolo[3,2-a]pyrimidin-4-one (5j). Obtained as a yellow solid (321 mg, 95%); mp 178-180 °C; ^1H NMR (300 MHz, CDCl_3) δ 9.18 (d, J = 8.7 Hz, 1H), 8.04 (s, 1H), 7.83 (d, J = 8.7 Hz, 1H), 6.79 (s, 1H); ^{13}C NMR (75 MHz, CDCl_3) δ 163.6, 159.9, 151.7, 151.2, 150.7, 150.2, 137.5, 131.0, 130.5, 130.1, 129.6, 128.6, 125.7, 125.3, 125.0, 124.7, 124.6, 124.6, 122.1, 121.4, 120.4, 119.5, 119.5, 119.4, 119.4, 118.4, 117.8, 114.8, 107.2, 107.2, 107.1, 107.1. HRMS (ESI) calcd for $\text{C}_{12}\text{H}_5\text{F}_6\text{N}_2\text{OS}$ $[\text{M}+\text{H}]^+$: 339.0021; found 339.0023.



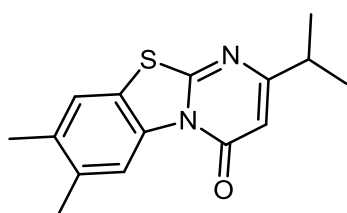
2,3-Dimethyl-4H-benzo[4,5]oxazolo[3,2-a]pyrimidin-4-one (5k). Obtained as a white solid (170 mg, 79%); mp 155-157 °C; ^1H NMR (300 MHz, CDCl_3) δ 8.37 (d, J = 6.9 Hz, 1H), 7.50-7.36 (m, 3H), 2.40 (s, 3H), 2.14 (s, 3H); ^{13}C NMR 75 MHz, CDCl_3) δ 159.8, 159.4, 152.5, 144.6, 126.9, 126.3, 125.0, 116.3, 113.6, 110.7, 22.4, 11.0. HRMS (ESI) calcd for $\text{C}_{12}\text{H}_{11}\text{N}_2\text{O}_2$ $[\text{M}+\text{H}]^+$: 215.0815; found 215.0818.



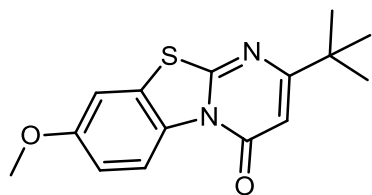
8-Methyl-2-propyl-4H-benzo[4,5]thiazolo[3,2-a]pyrimidin-4-one (5l). Obtained as a light yellow solid (226 mg, 88%); mp 95-97 °C; ^1H NMR (300 MHz, CDCl_3) δ 8.71 (d, J = 8.4 Hz, 1H), 7.27 (s, 1H), 7.11 (d, J = 8.4 Hz, 1H), 6.09 (s, 1H), 2.46 (t, J = 7.7 Hz, 2H), 2.31 (s, 3H), 1.72-1.58 (m, 2H), 0.92 (t, J = 7.4 Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 165.9, 161.0, 160.8, 136.9, 133.5, 122.4, 123.8, 121.3, 119.1, 106.1, 39.0, 21.1, 21.1, 13.5. HRMS (ESI) calcd for $\text{C}_{14}\text{H}_{15}\text{N}_2\text{OS}$ $[\text{M}+\text{H}]^+$: 259.0900; found 259.0903.



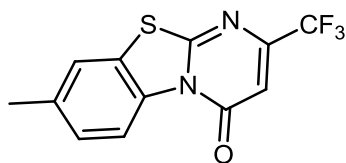
2-Butyl-8-chloro-4H-benzo[4,5]thiazolo[3,2-a]pyrimidin-4-one (5m). Obtained as a light yellow solid (252 mg, 86%); mp 113-115 °C; ^1H NMR (300 MHz, CDCl_3) δ 8.62 (d, J = 9.0 Hz, 1H), 7.36 (s, 1H), 7.14 (d, J = 8.7 Hz, 1H), 5.99 (s, 1H), 2.40 (t, J = 7.7 Hz, 2H), 1.58-1.46 (m, 2H), 1.32-1.18 (m, 2H), 0.80 (t, J = 7.2 Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 166.3, 160.2, 160.2, 133.9, 132.0, 126.5, 125.2, 120.9, 120.0, 106.1, 36.6, 29.7, 21.9, 13.5. HRMS (ESI) calcd for $\text{C}_{14}\text{H}_{14}\text{ClN}_2\text{OS}$ $[\text{M}+\text{H}]^+$: 293.0510; found 293.0513.



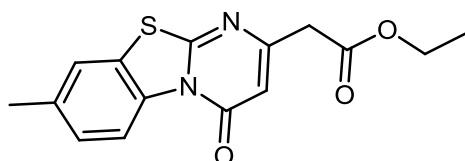
2-Isopropyl-7,8-dimethyl-4H-benzo[4,5]thiazolo[3,2-a]pyrimidin-4-one (5n). Obtained as a yellow solid (210 mg, 77%); mp 145-147 °C; ^1H NMR (300 MHz, CDCl_3) δ 8.72 (s, 1H), 7.28 (s, 1H), 6.20 (s, 1H), 2.86-2.72 (m, 1H), 2.31 (s, 3H), 2.27 (s, 3H), 1.25 (d, J = 6.6 Hz, 6H); ^{13}C NMR (75 MHz, CDCl_3) δ 171.2, 161.5, 161.4, 136.0, 135.7, 134.0, 121.6, 120.9, 120.2, 104.1, 36.3, 21.1, 20.0, 19.8. HRMS (ESI) calcd for $\text{C}_{15}\text{H}_{17}\text{N}_2\text{OS}$ $[\text{M}+\text{H}]^+$: 273.1056; found 273.1018.



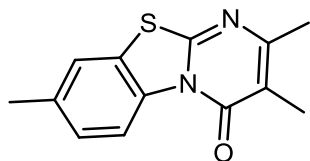
2-(tert-Butyl)-8-methoxy-4H-benzo[4,5]thiazolo[3,2-a]pyrimidin-4-one (5o). Obtained as a yellow solid (202 mg, 70%); mp 196-198 °C; ^1H NMR (300 MHz, CDCl_3) δ 8.93 (d, J = 9.3 Hz, 1H), 7.12 (s, 1H), 7.00 (d, J = 9.3 Hz, 1H), 6.35 (s, 1H), 3.86 (s, 3H), 1.30 (s, 9H); ^{13}C NMR (75 MHz, CDCl_3) δ 173.4, 161.7, 160.3, 158.3, 129.8, 125.7, 120.7, 113.3, 106.1, 103.4, 55.7, 37.2, 28.8. HRMS (ESI) calcd for $\text{C}_{15}\text{H}_{17}\text{N}_2\text{O}_2\text{S}$ $[\text{M}+\text{H}]^+$: 289.1005; found 289.1008.



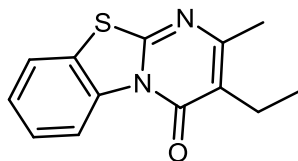
8-Methyl-2-(trifluoromethyl)-4H-benzo[4,5]thiazolo[3,2-a]pyrimidin-4-one (5p). Obtained as a yellow solid (281 mg, 99%); mp 192-194 °C; ^1H NMR (300 MHz, CDCl_3) δ 8.80 (d, J = 8.4 Hz, 1H), 7.46 (s, 1H), 7.28 (d, J = 8.7 Hz, 1H), 6.66 (s, 1H), 2.46 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 163.5, 159.8, 151.0, 150.6, 150.1, 149.6, 138.4, 133.0, 128.3, 125.9, 124.3, 122.1, 121.8, 119.6, 118.6, 114.9, 106.4, 106.3, 106.3, 106.2, 21.3. HRMS (ESI) calcd for $\text{C}_{12}\text{H}_8\text{F}_3\text{N}_2\text{OS}$ $[\text{M}+\text{H}]^+$: 285.0305; found 285.0305.



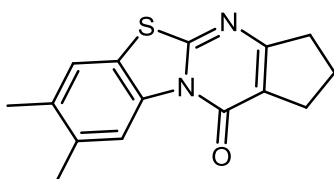
Ethyl 2-(8-methyl-4-oxo-4H-benzo[4,5]thiazolo[3,2-a]pyrimidin-2-yl)acetate (5q). Obtained as a light yellow solid (278 mg, 92%); mp 119-121 °C; ^1H NMR (300 MHz, CDCl_3) δ 8.67 (d, J = 8.7 Hz, 1H), 7.28 (s, 1H), 7.11 (d, J = 8.7 Hz, 1H), 6.23 (s, 1H), 4.12 (q, J = 7.2 Hz, 2H), 3.53 (s, 2H), 2.31 (s, 3H), 1.20 (t, J = 7.2 Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 168.8, 161.4, 160.3, 157.8, 137.2, 133.2, 127.5, 123.8, 121.4, 119.1, 108.0, 61.0, 42.5, 21.0, 13.9. HRMS (ESI) calcd for $\text{C}_{15}\text{H}_{15}\text{N}_2\text{O}_3\text{S}$ $[\text{M}+\text{H}]^+$: 303.0798; found 303.0799.



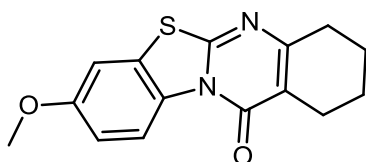
2,3,8-Trimethyl-4H-benzo[4,5]thiazolo[3,2-a]pyrimidin-4-one (5r). Obtained as a light yellow solid (230 mg, 94%); mp 156-158 °C; ^1H NMR (300 MHz, CDCl_3) δ 8.79 (d, J = 8.4 Hz, 1H), 7.30 (s, 1H), 7.16 (d, J = 8.7 Hz, 1H), 2.36 (s, 3H), 2.30 (s, 3H), 2.09 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 161.3, 157.8, 157.2, 136.8, 133.7, 127.4, 124.1, 121.5, 119.1, 114.3, 21.8, 21.2, 11.1. HRMS (ESI) calcd for $\text{C}_{13}\text{H}_{13}\text{N}_2\text{OS}$ $[\text{M}+\text{H}]^+$: 245.0743; found 245.0745.



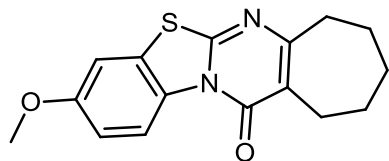
3-Ethyl-2-methyl-4H-benzo[4,5]thiazolo[3,2-a]pyrimidin-4-one (5s). Obtained as a light yellow solid (220 mg, 90%); mp 130-132 °C; ^1H NMR (300 MHz, CDCl_3) δ 8.21 (d, J = 7.8 Hz, 1H), 7.30 (d, J = 7.8 Hz, 1H), 7.18-7.06 (m, 2H), 2.40 (q, J = 7.4 Hz, 2H), 2.14 (s, 3H), 0.96 (t, J = 7.4 Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 160.5, 157.1, 156.8, 135.5, 126.0, 125.9, 123.7, 121.0, 119.8, 119.0, 20.8, 18.7, 12.3. HRMS (ESI) calcd for $\text{C}_{13}\text{H}_{13}\text{N}_2\text{OS}$ $[\text{M}+\text{H}]^+$: 245.0743; found 245.0746.



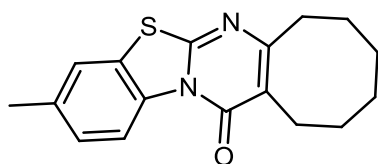
7,8-Dimethyl-2,3-dihydrobenzo[4,5]thiazolo[3,2-a]cyclopenta [d]pyrimidin-11(1H)-one (5t). Obtained as a yellow solid (238 mg, 88%); mp 167-169 °C; ^1H NMR (300 MHz, CDCl_3) δ 8.68 (s, 1H), 7.20 (s, 1H), 2.87-2.79 (m, 4H), 2.25 (s, 3H), 2.21 (s, 3H), 2.15-2.01 (m, 2H); ^{13}C NMR (75 MHz, CDCl_3) δ 167.4, 161.4, 159.1, 135.7, 135.5, 134.0, 121.5, 121.0, 120.1, 118.6, 34.5, 27.0, 21.4, 20.0, 19.7. HRMS (ESI) calcd for $\text{C}_{15}\text{H}_{15}\text{N}_2\text{OS}$ $[\text{M}+\text{H}]^+$: 271.0900; found 271.0898.



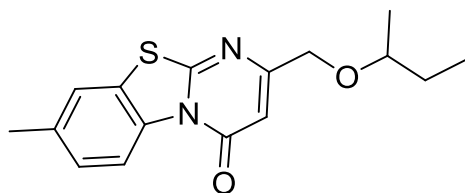
8-Methoxy-3,4-dihydro-1H-benzo[4,5]thiazolo[2,3-b]quinazolin-12(2H)-one (5u). Obtained as a yellow solid (249 mg, 87%); mp 181-183 °C; ^1H NMR (300 MHz, CDCl_3) δ 8.81 (d, J = 9.0 Hz, 1H), 7.00 (s, 1H), 6.89 (d, J = 9.3 Hz, 1H), 3.78 (s, 3H), 2.65-2.52 (m, 4H), 1.81-1.70 (m, 4H); ^{13}C NMR (75 MHz, CDCl_3) δ 160.9, 158.8, 158.0, 157.2, 129.7, 125.4, 120.0, 115.9, 113.0, 106.0, 55.6, 31.6, 22.1, 22.1, 21.8. HRMS (ESI) calcd for $\text{C}_{15}\text{H}_{15}\text{N}_2\text{O}_2\text{S}$ $[\text{M}+\text{H}]^+$: 287.0849; found 287.0851.



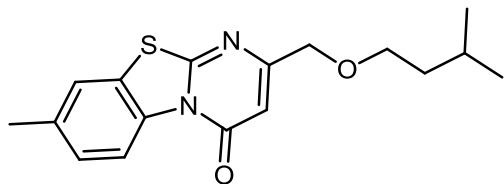
3-Methoxy-8,9,10,11-tetrahydrobenzo[4,5]thiazolo[3,2-*a*]cyclohepta[*d*]pyrimidin-12(7*H*)-one (5v). Obtained as a light yellow solid (265 mg, 88%); mp 174-176 °C; ^1H NMR (300 MHz, CDCl_3) δ 8.93 (d, J = 9.3 Hz, 1H), 7.06 (s, 1H), 6.96 (d, J = 9.0 Hz, 1H), 3.83 (s, 3H), 2.87-2.80 (m, 4H), 1.89-1.79 (m, 2H), 1.71-1.55 (m, 4H); ^{13}C NMR (75 MHz, CDCl_3) δ 164.9, 161.1, 158.2, 157.2, 130.1, 125.8, 120.7, 120.5, 113.2, 106.0, 55.6, 38.2, 32.3, 26.5, 25.4, 24.0. HRMS (ESI) calcd for $\text{C}_{16}\text{H}_{17}\text{N}_2\text{O}_2\text{S}$ $[\text{M}+\text{H}]^+$: 301.1005; found 301.1008.



3-Methyl-9,10,11,12-tetrahydro-7*H*-benzo[4,5]thiazolo[3,2-*a*]cycloocta[*d*]pyrimidin-13(8*H*)-one (5w). Obtained as a light yellow solid (251 mg, 84%); mp 172-174 °C; ^1H NMR (300 MHz, CDCl_3) δ 8.90 (d, J = 8.7 Hz, 1H), 7.40 (s, 1H), 7.25 (d, J = 8.7 Hz, 1H), 2.83-2.74 (m, 4H), 2.43 (s, 3H), 1.83-1.69 (m, 4H), 1.50-1.39 (m, 4H); ^{13}C NMR (75MHz, CDCl_3) δ 162.4, 161.0, 158.1, 137.0, 134.1, 127.6, 124.3, 121.7, 119.4, 118.5, 34.4, 29.6, 29.2, 26.4, 26.1, 23.9, 21.3. HRMS (ESI) calcd for $\text{C}_{17}\text{H}_{19}\text{N}_2\text{OS}$ $[\text{M}+\text{H}]^+$: 299.1213; found 299.1216.



2-(*sec*-Butoxymethyl)-8-methyl-4*H*-benzo[4,5]thiazolo[3,2-*a*]pyrimidin-4-one (5x). Obtained as a yellow semisolid (197 mg, 65%); ^1H NMR (300 MHz, CDCl_3) δ 7.66 (s, 1H), 7.47-7.38 (m, 2H), 7.20 (d, J = 8.4 Hz, 1H), 5.00-4.85 (m, 1H), 3.77 (s, 2H), 2.44 (s, 3H), 1.68-1.51 (m, 2H), 1.24 (d, J = 6.3 Hz, 3H), 0.90 (t, J = 7.5 Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 170.5, 146.0, 140.6, 134.8, 130.2, 130.1, 127.0, 124.3, 112.2, 109.7, 73.0, 35.4, 28.7, 21.3, 19.4, 9.6. HRMS (ESI) calcd for $\text{C}_{16}\text{H}_{19}\text{N}_2\text{O}_2\text{S}$ $[\text{M}+\text{H}]^+$: 303.1162; found 303.1165.



2-((Isopentyloxy)methyl)-8-methyl-4H-benzo[4,5]thiazolo[3,2-a]pyrimidin-4-one (5y).

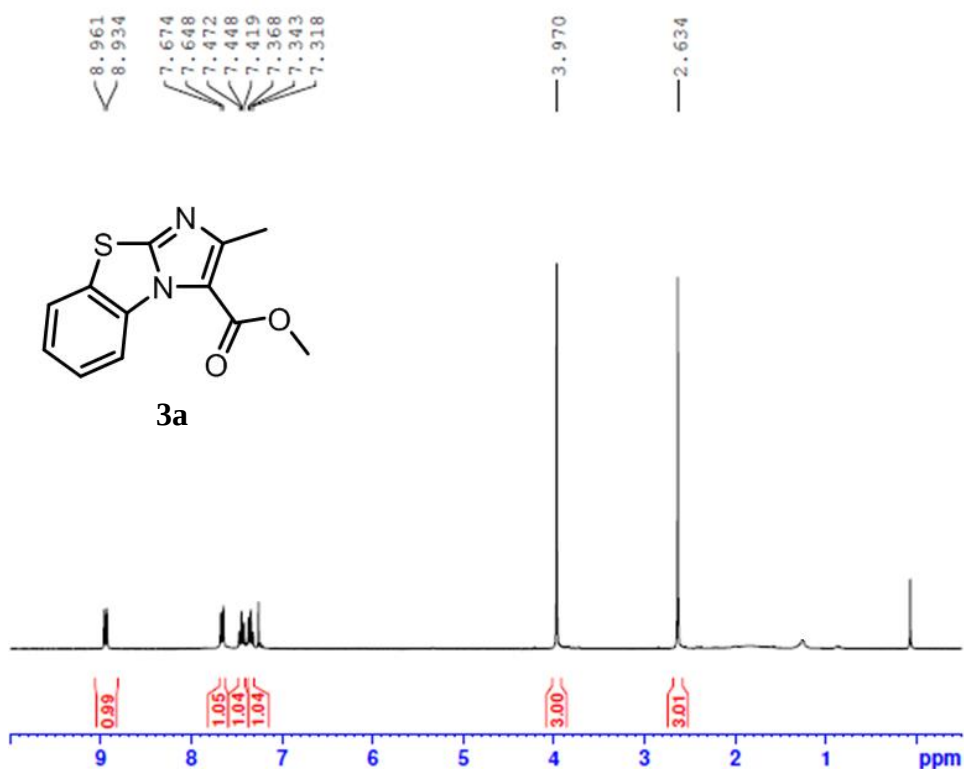
Obtained as a yellow semisolid (220 mg, 69%); ^1H NMR (300 MHz, CDCl_3) δ 7.63 (s, 1H), 7.43 (s, 1H), 7.38 (d, $J = 8.1$ Hz, 1H), 7.18 (d, $J = 8.1$ Hz, 1H), 4.17 (t, $J = 6.9$ Hz, 2H), 3.77 (s, 2H), 2.42 (s, 3H), 1.76-1.60 (m, 1H), 1.54 (q, $J = 6.8$ Hz, 2H), 0.90 (d, $J = 6.6$ Hz, 6H); ^{13}C NMR (75 MHz, CDCl_3) δ 170.9, 146.9, 140.4, 134.7, 130.1, 130.1, 127.0, 124.2, 112.1, 109.7, 63.7, 37.2, 35.1, 25.0, 22.4, 21.2. HRMS (ESI) calcd for $\text{C}_{17}\text{H}_{21}\text{N}_2\text{O}_2\text{S}$ $[\text{M}+\text{H}]^+$: 317.1318; found 317.1319.

References

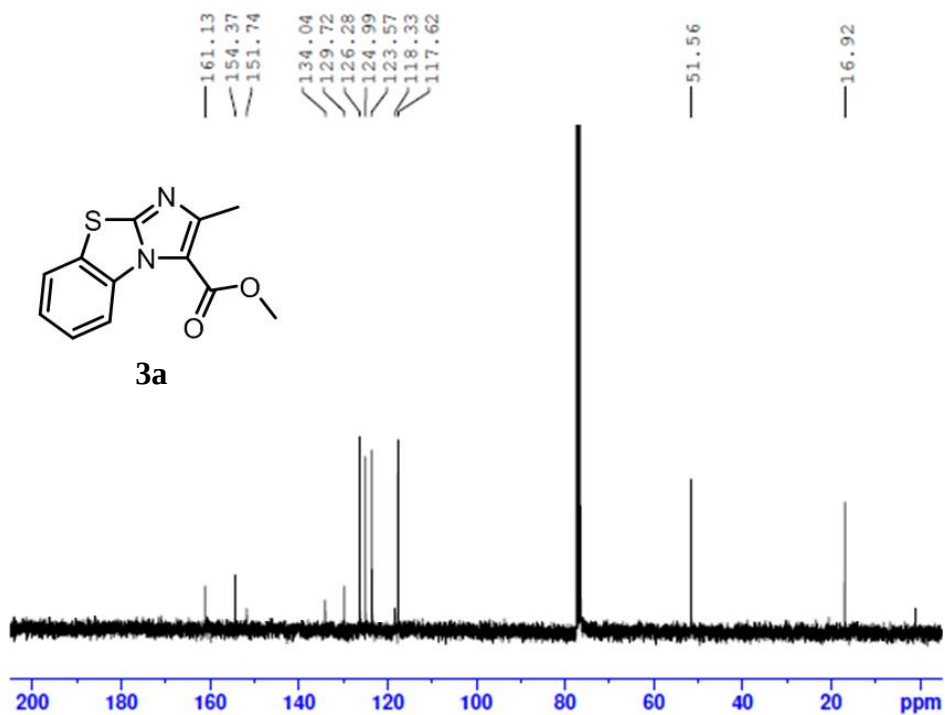
- [a] Rothweiler, U.; Stensen, W.; Brandsdal, B. O.; Isaksson, J.; Leeson, F. A.; Engh, R. A.; Svendsen, J. S. M. *J. Med. Chem.* **2016**, 59, 9814–9824.
- [b] Landreau, C.; Deniaud, D.; Evian, M.; Reliquet, A.; Meslin, J. C. *J. Chem.Soc., Perkin Trans. I* **2002**, 741–745.

NMR Spectra

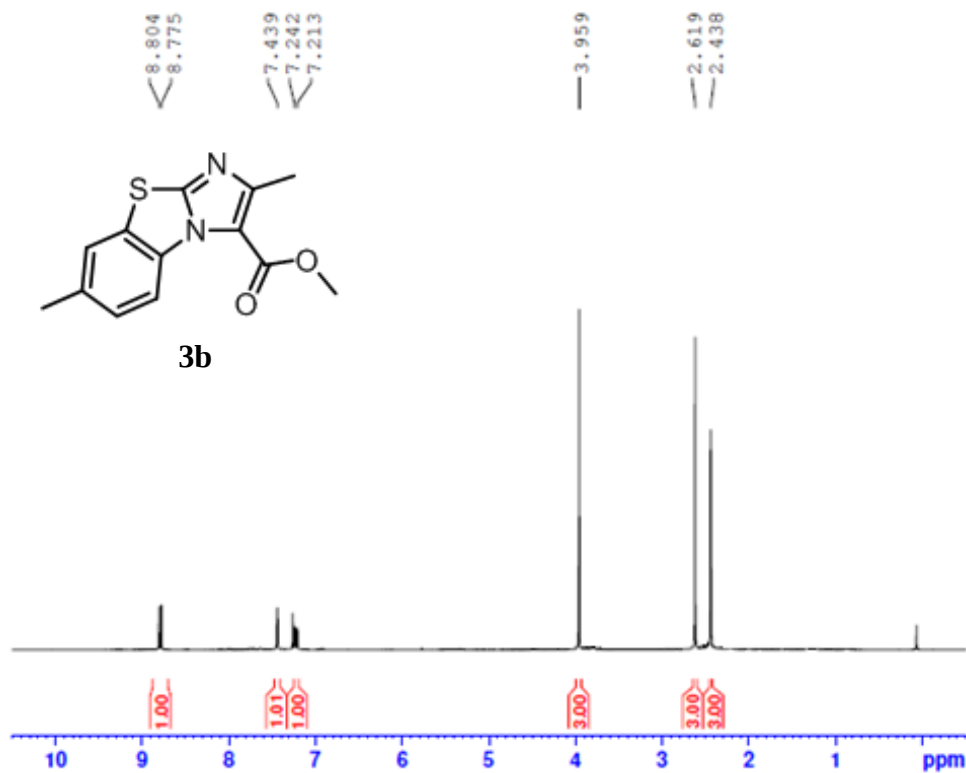
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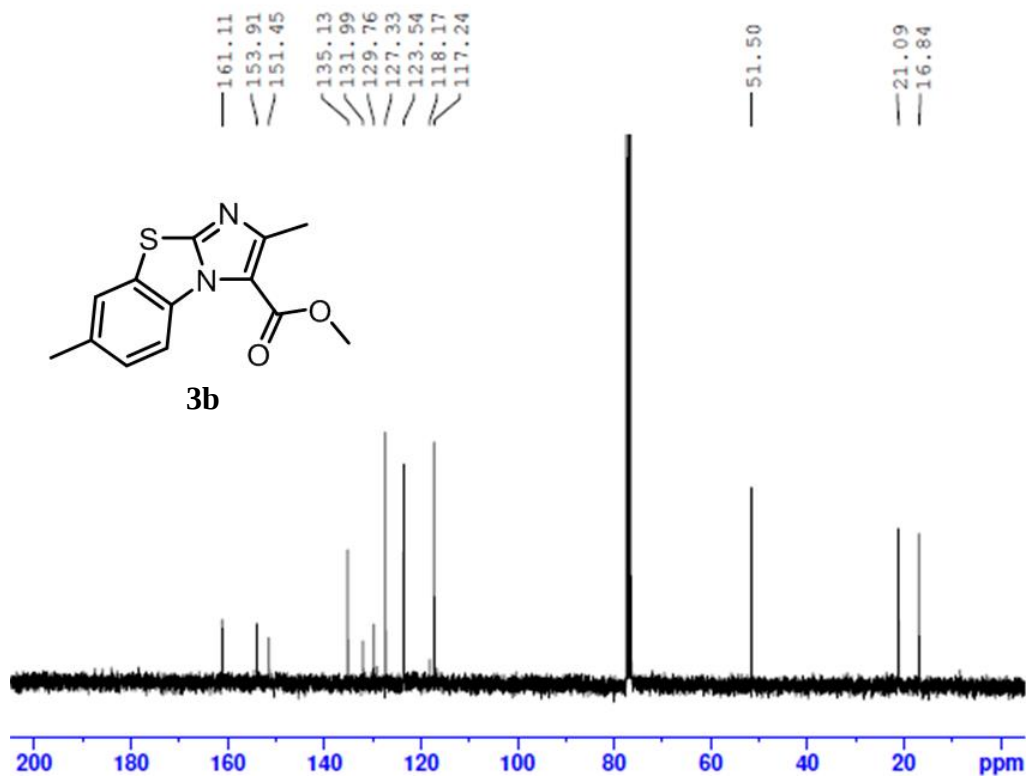
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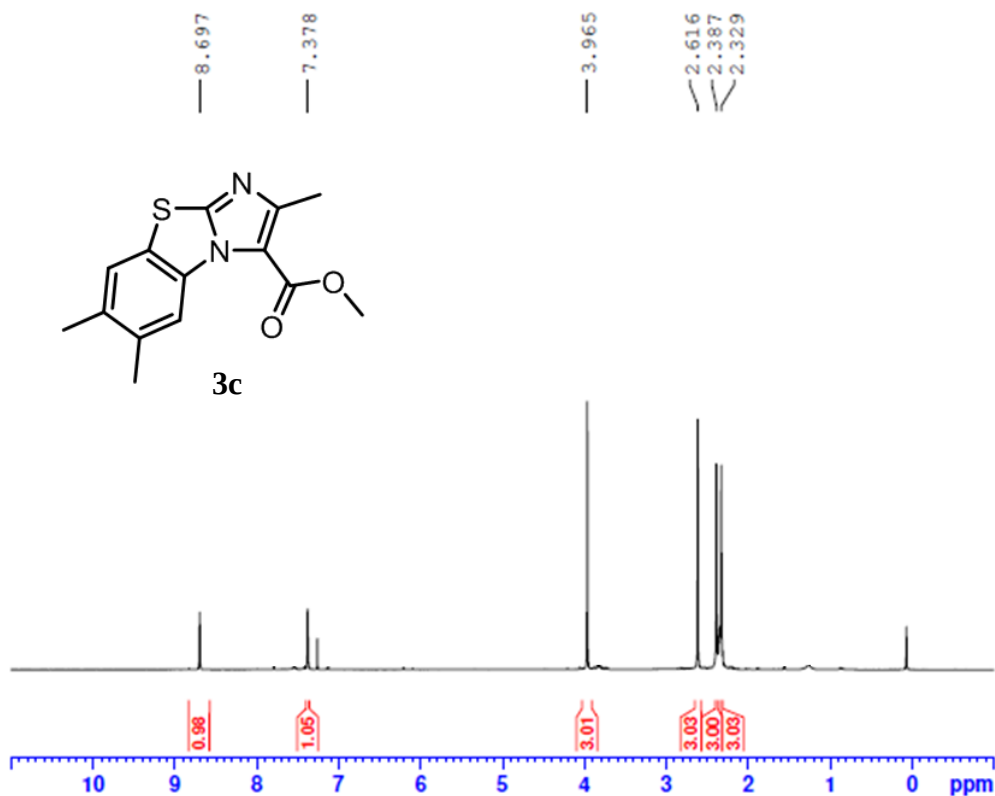
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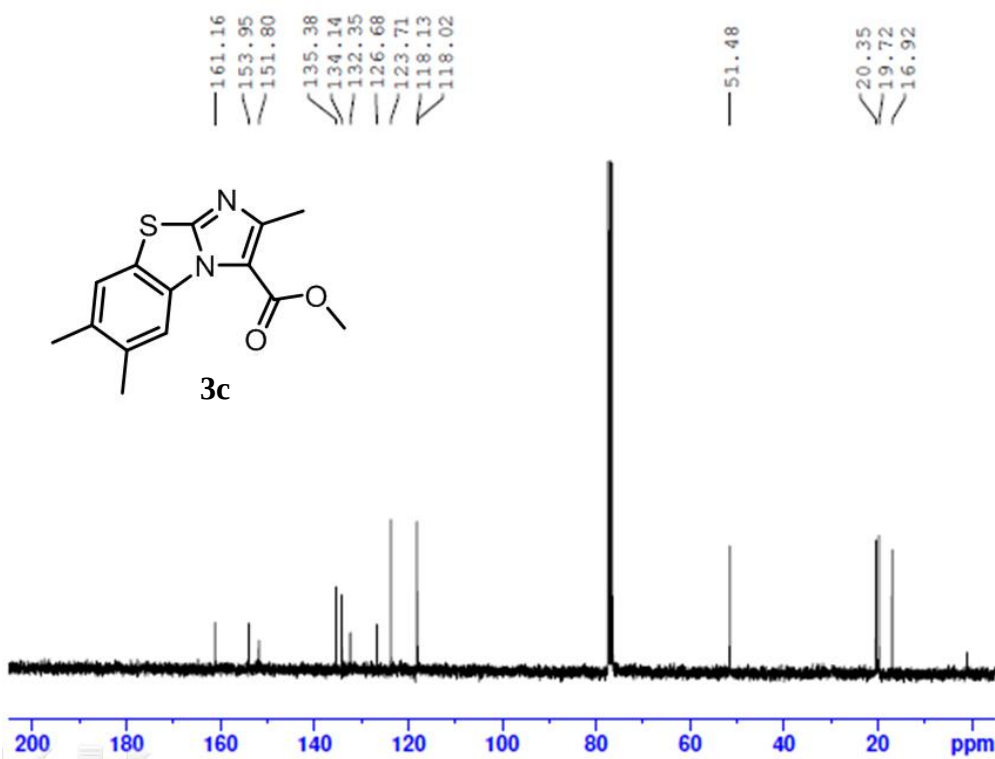
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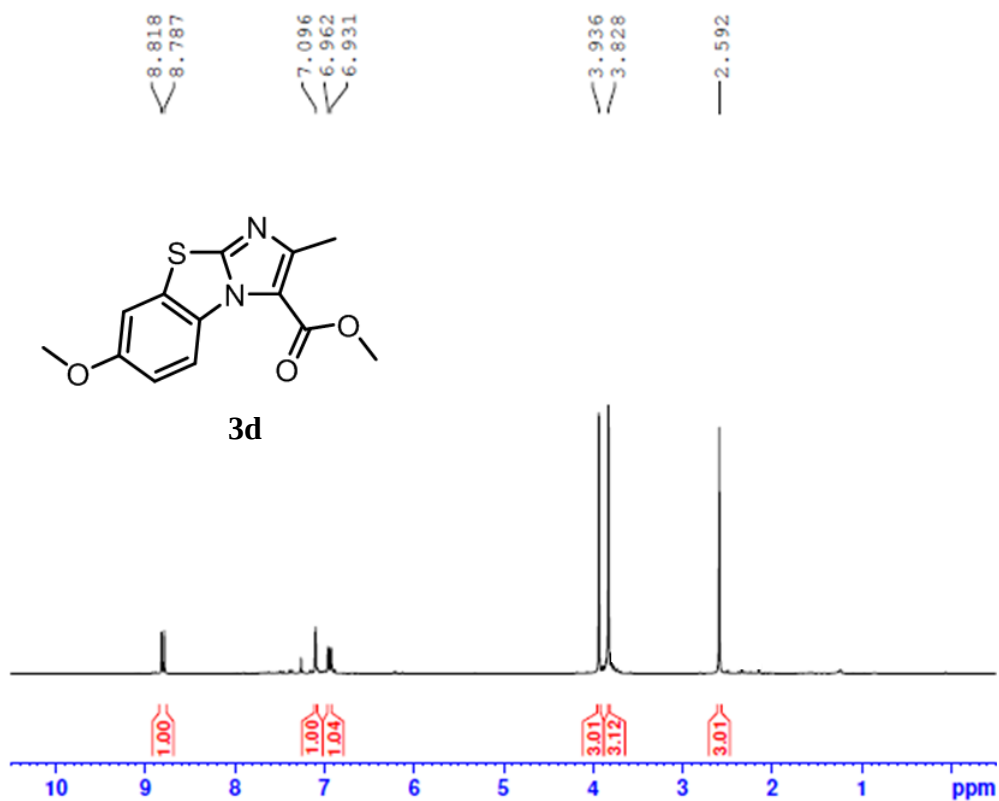
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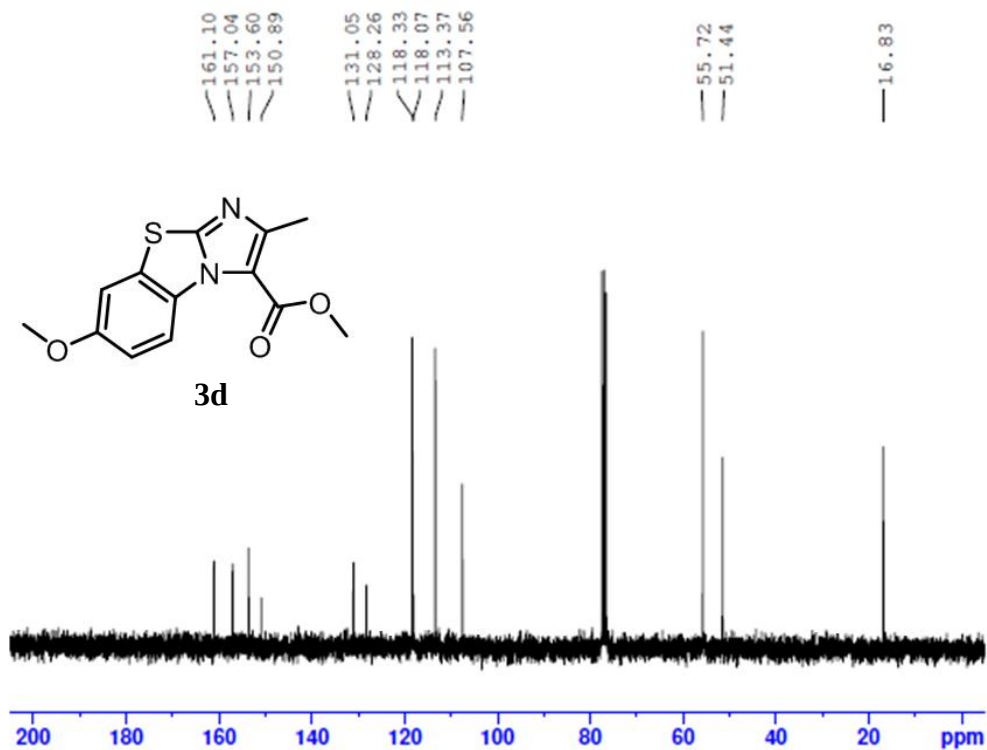
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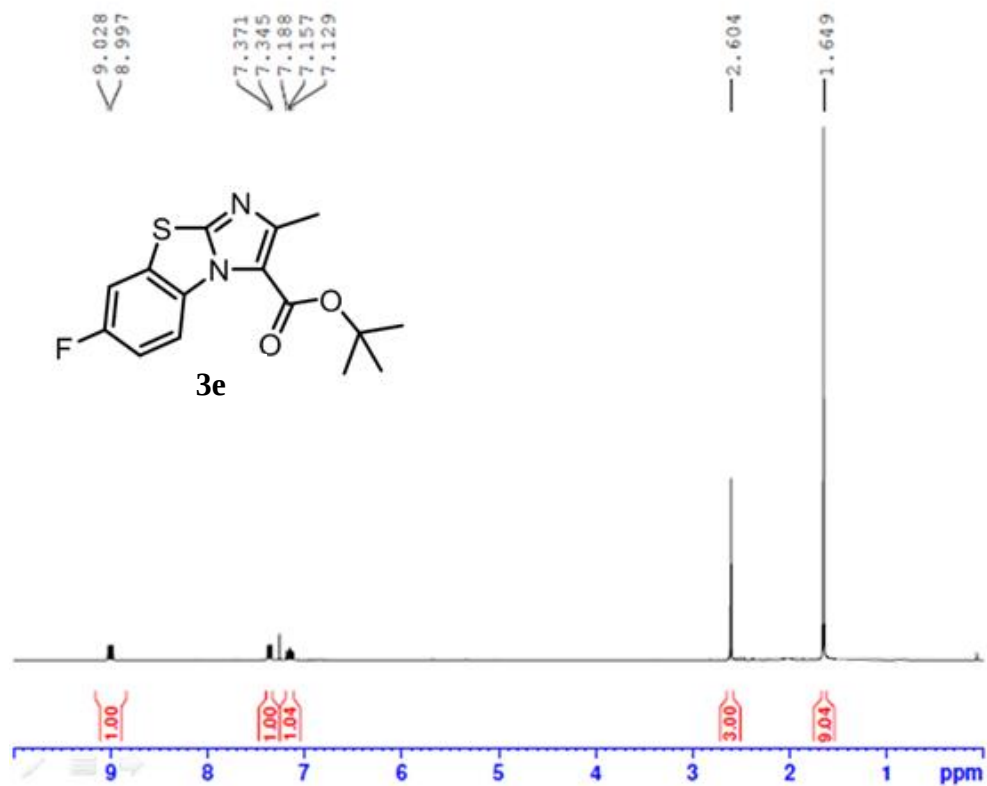
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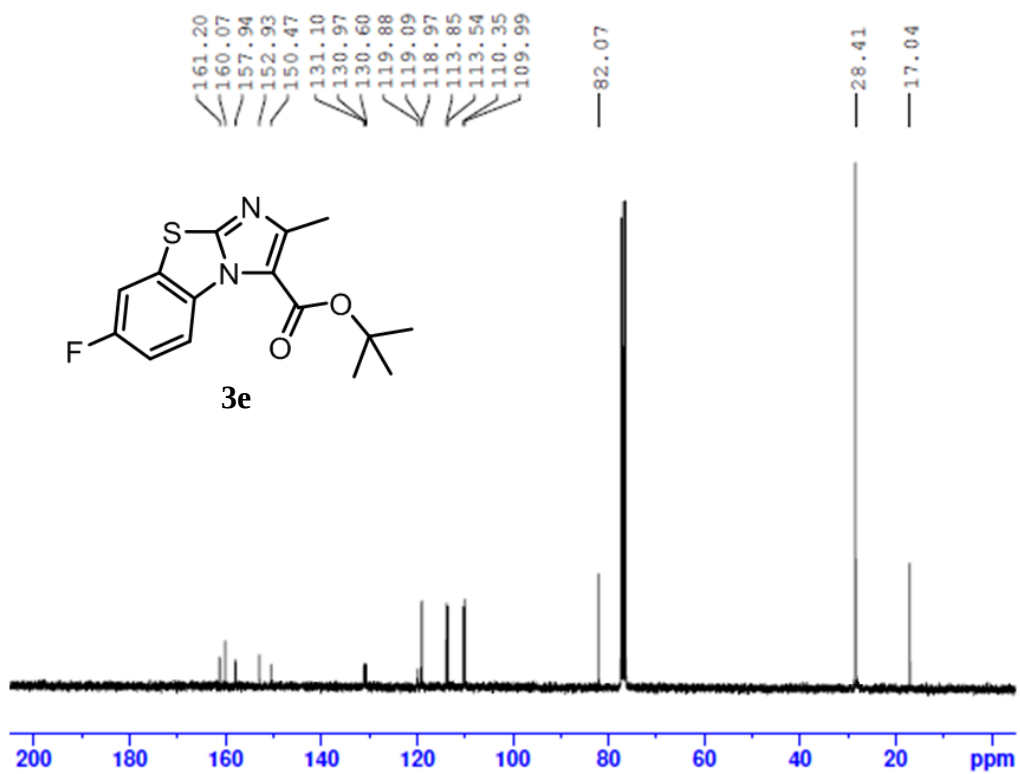
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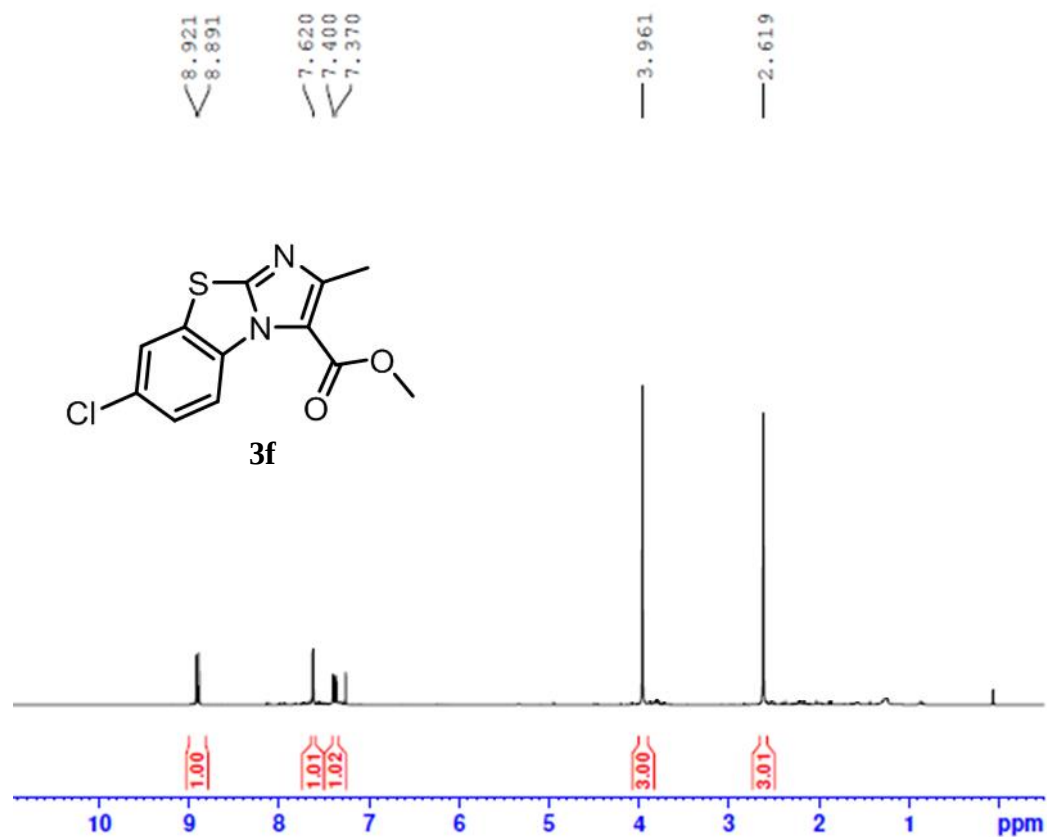
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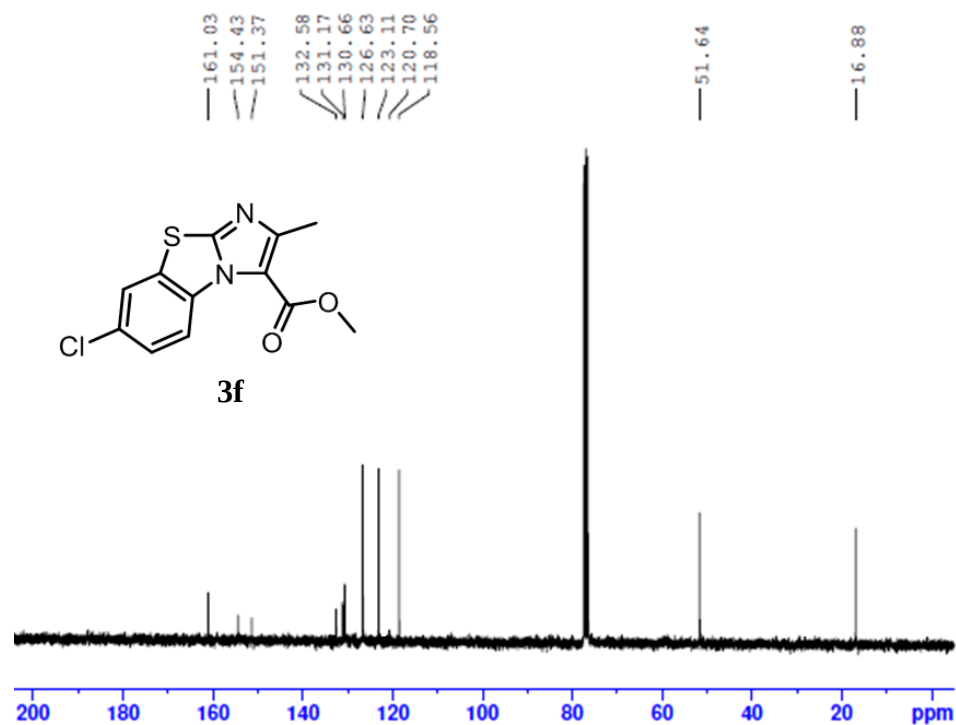
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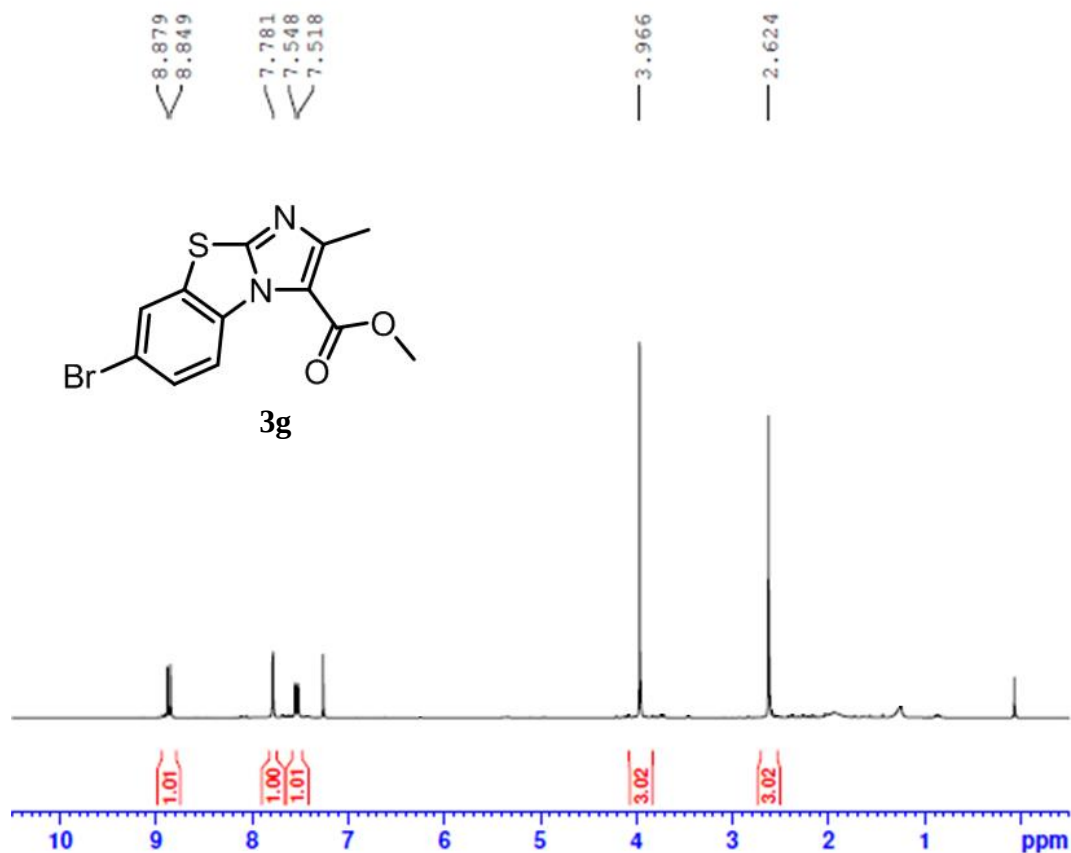
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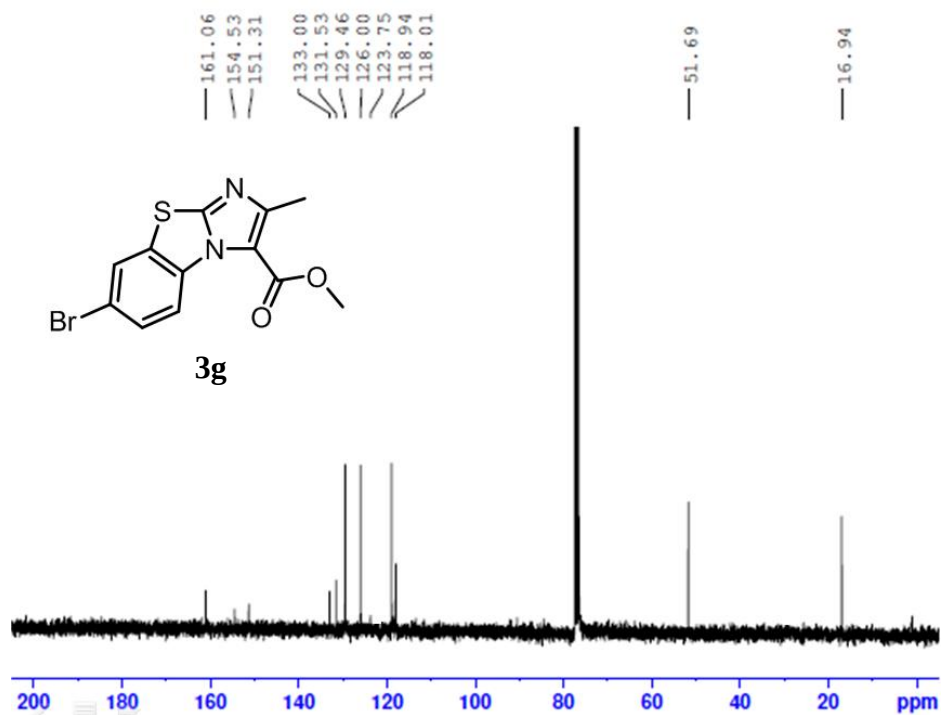
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¹H normal range AC300



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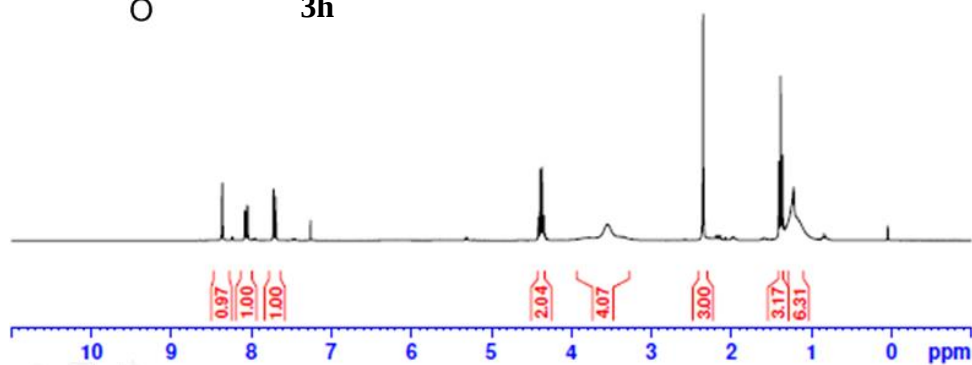
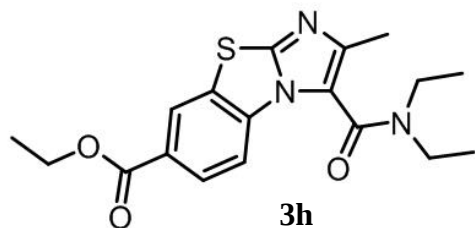


¹H normal range AC300

8.362
8.075
8.046
7.723
7.694

4.413
4.389
4.365
4.342
3.545

2.353
1.407
1.383
1.359
1.221



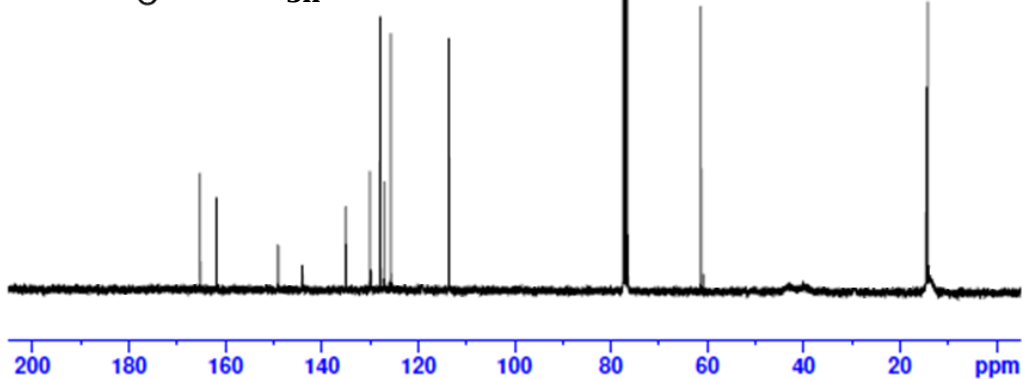
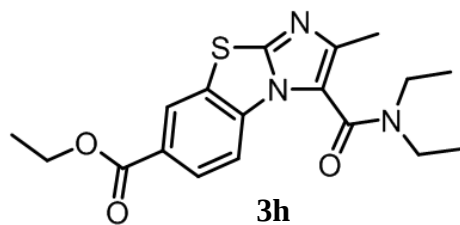
¹³C Standard AC300

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144.05
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130.04
127.88
126.98
125.67
113.58

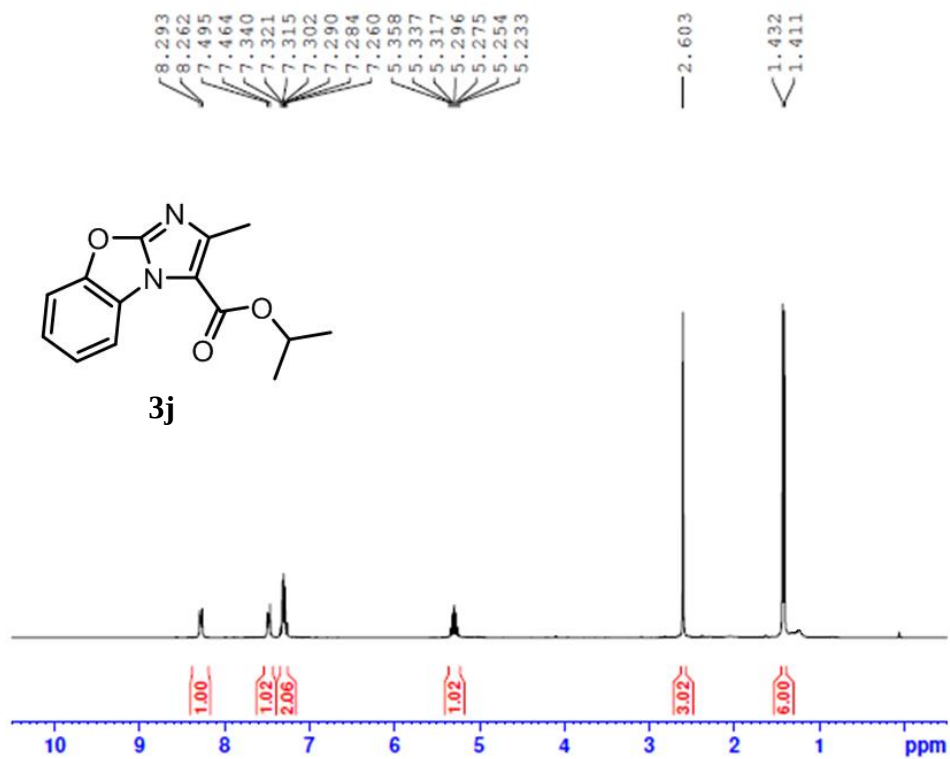
61.31

42.91
40.11

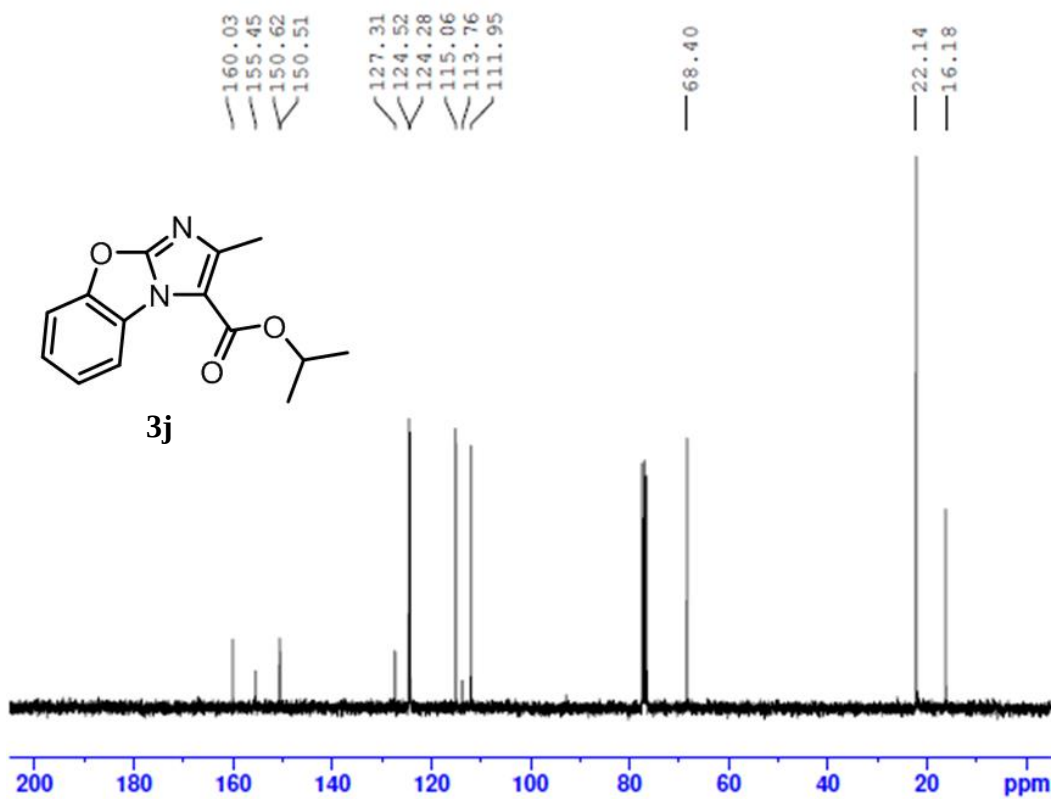
14.53
14.21
13.98



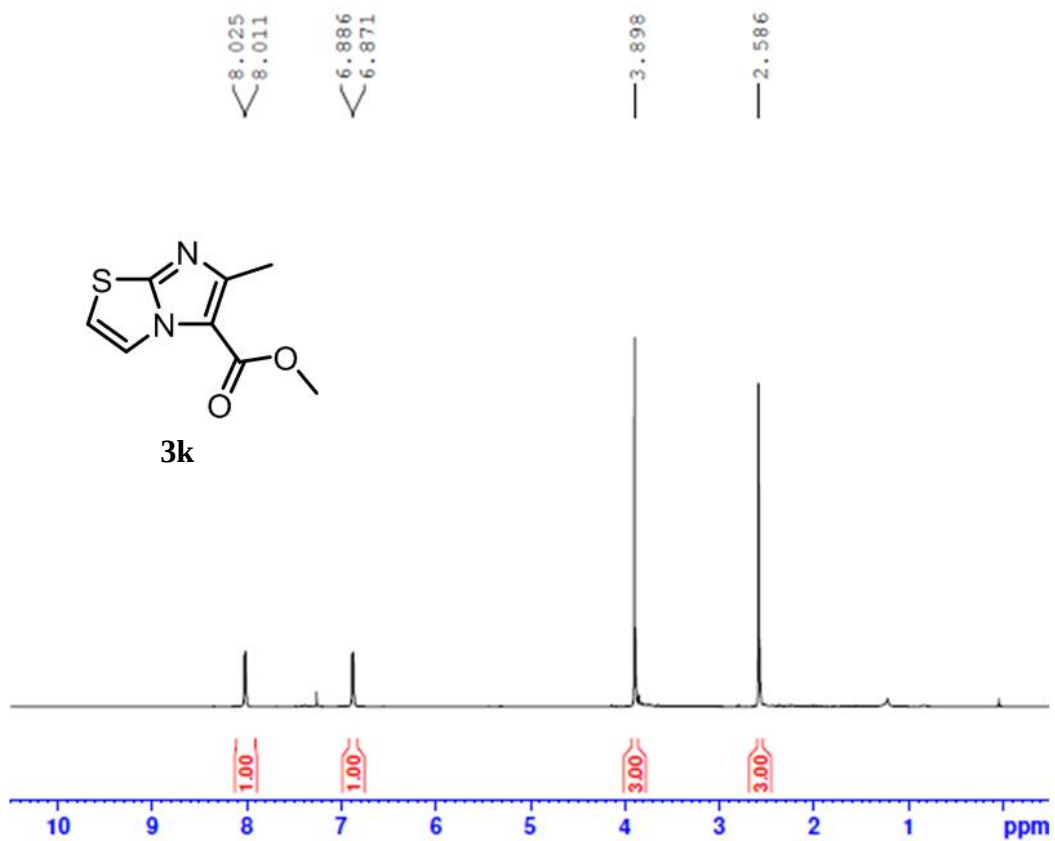
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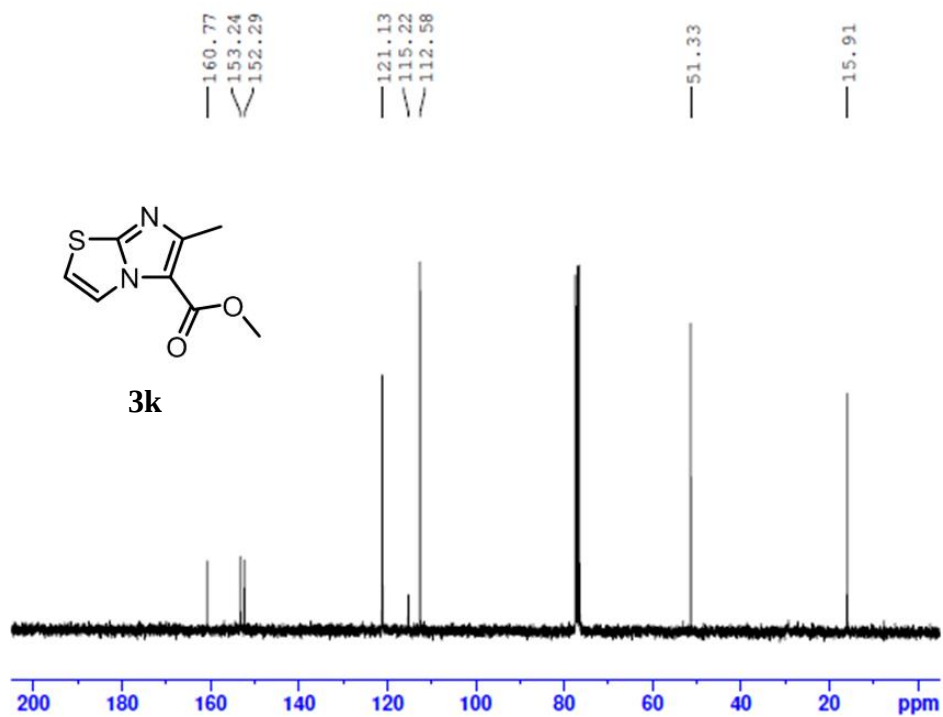
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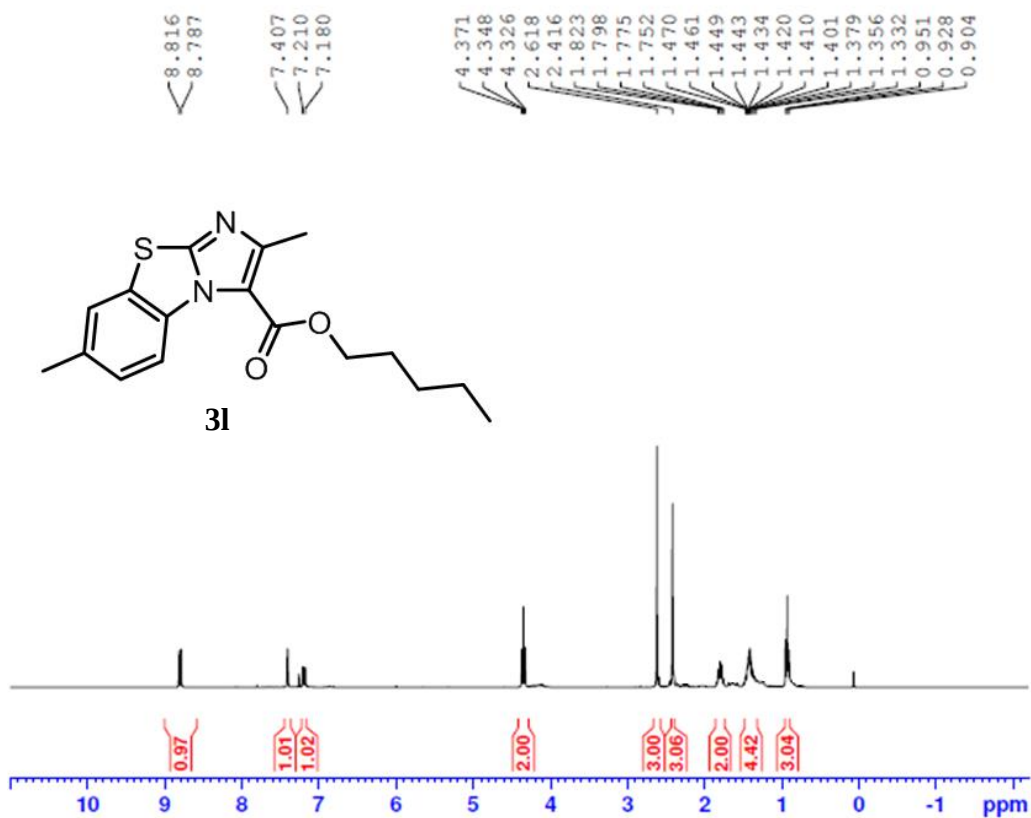
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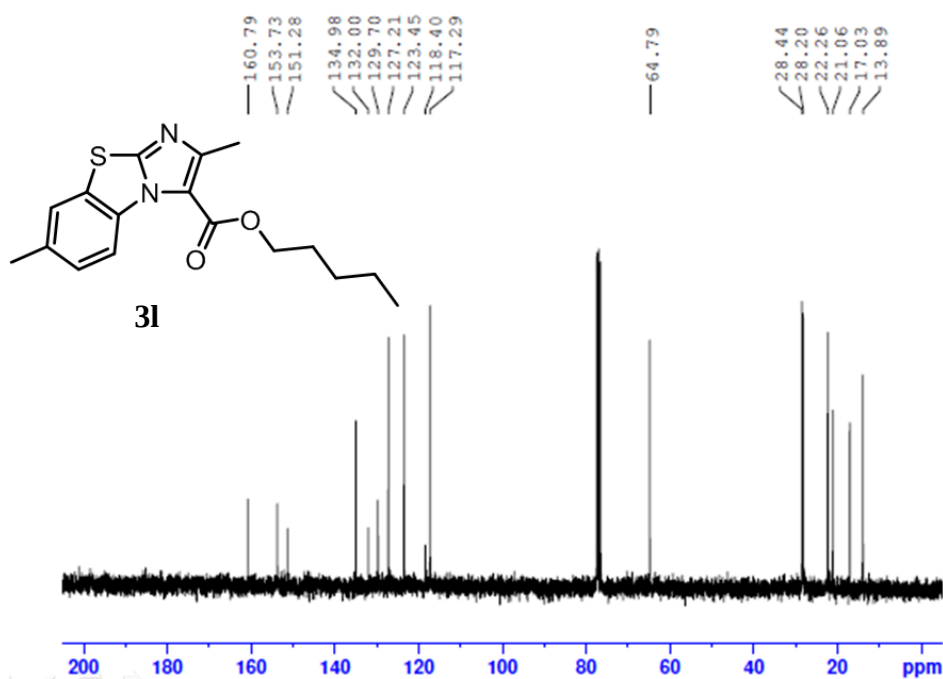
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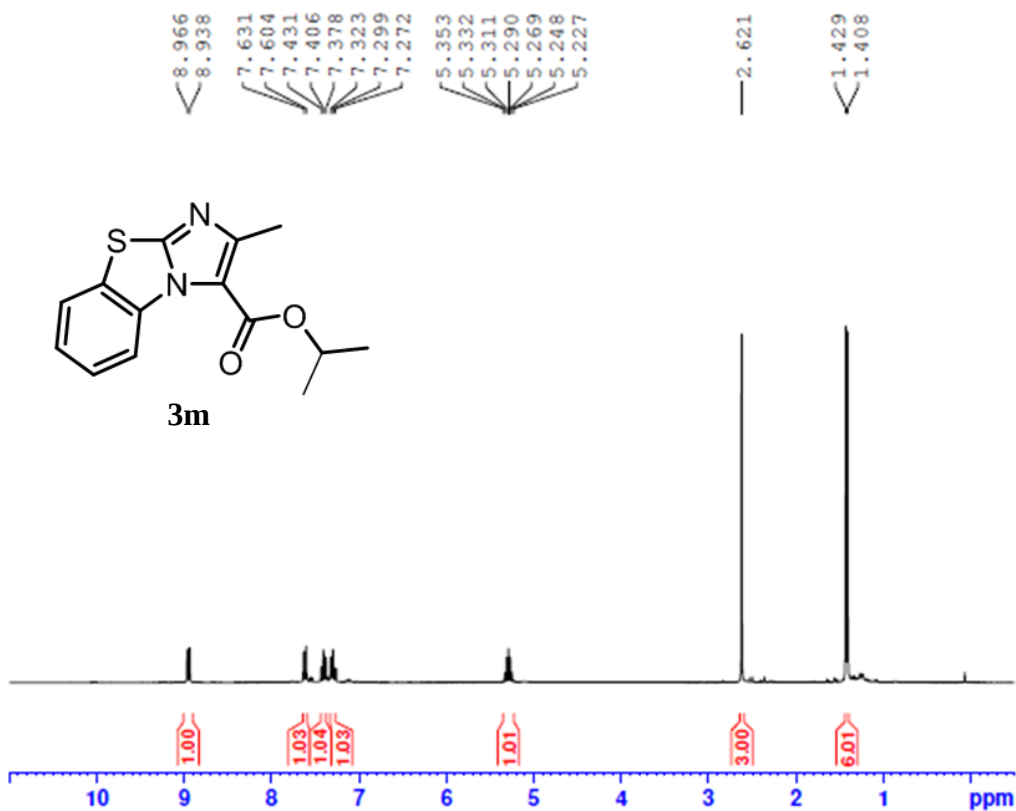
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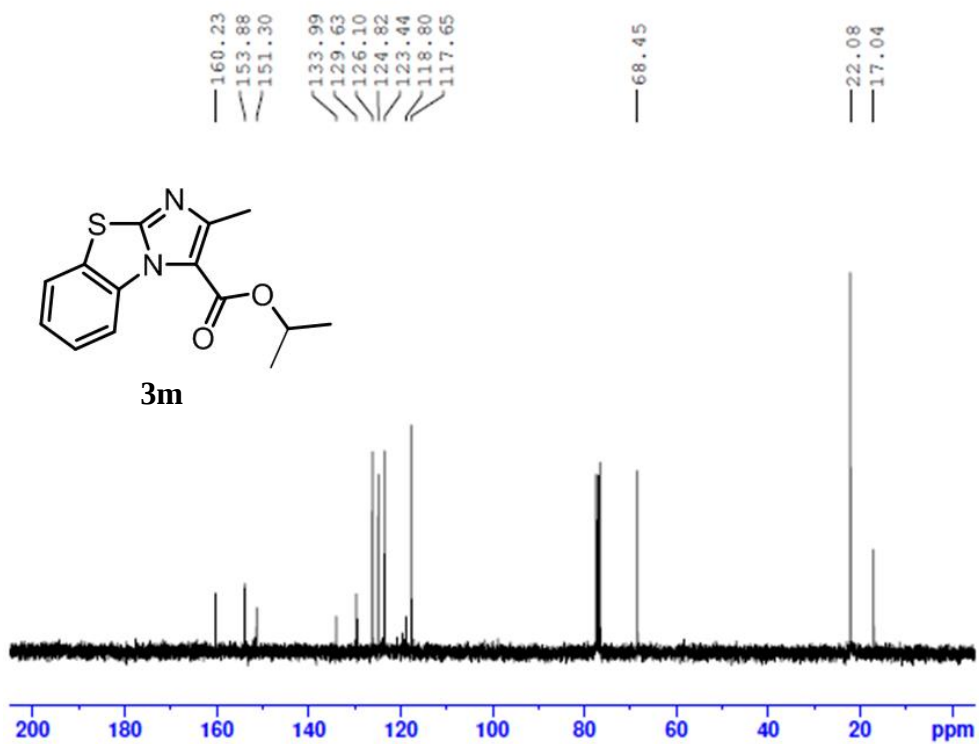
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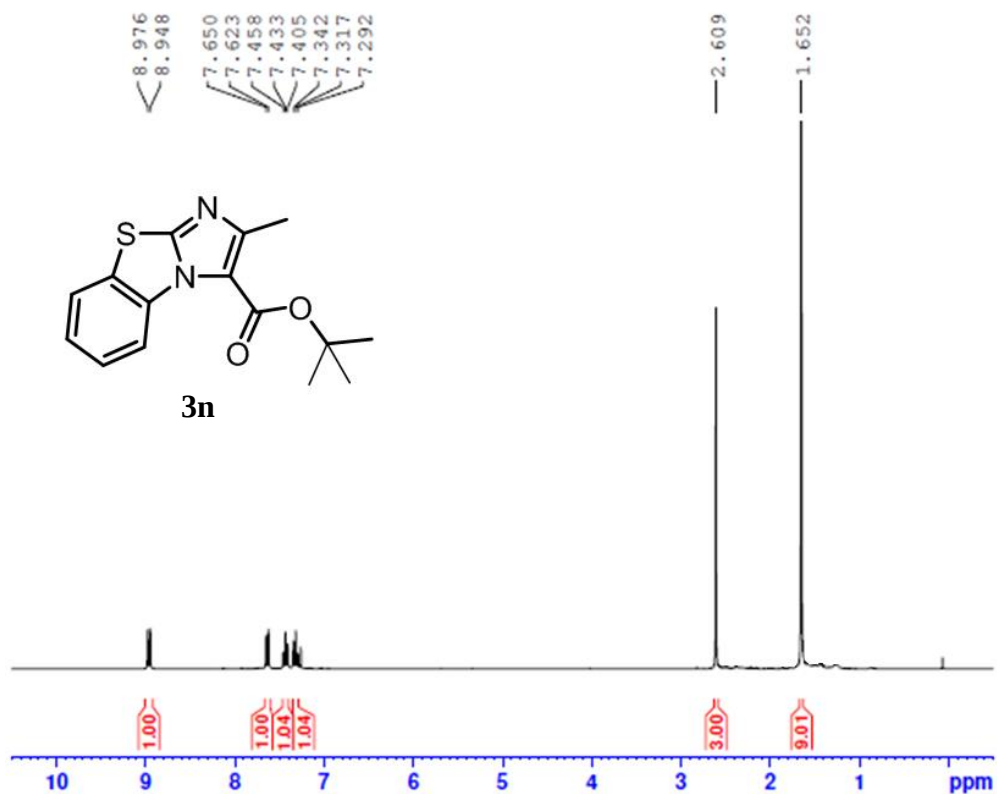
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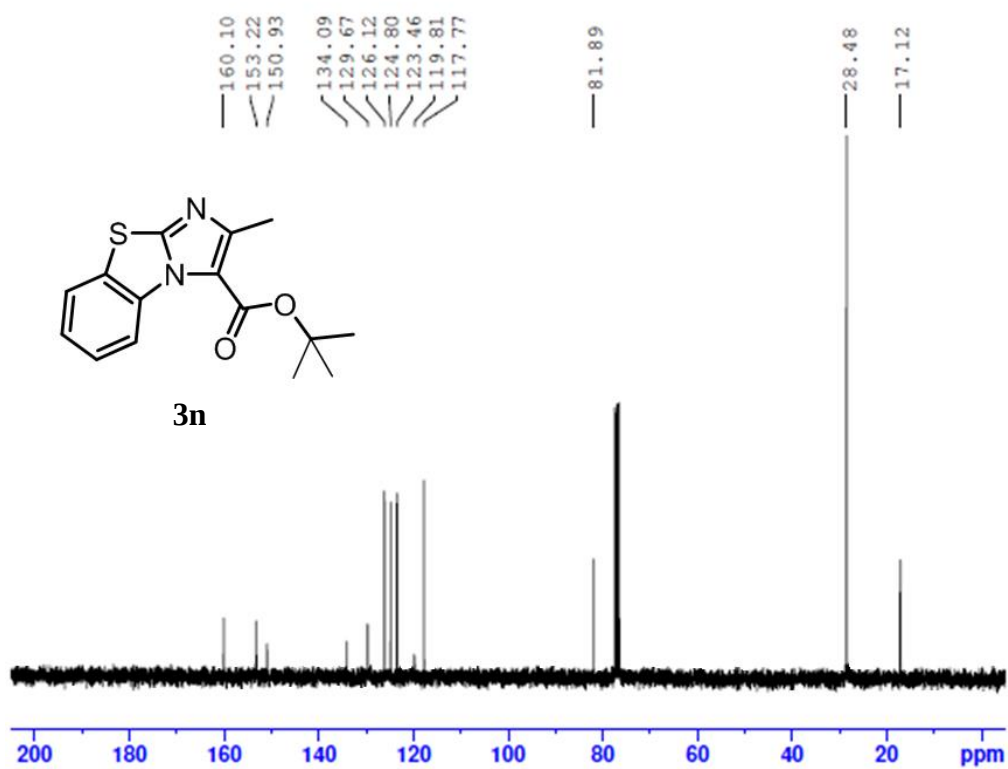
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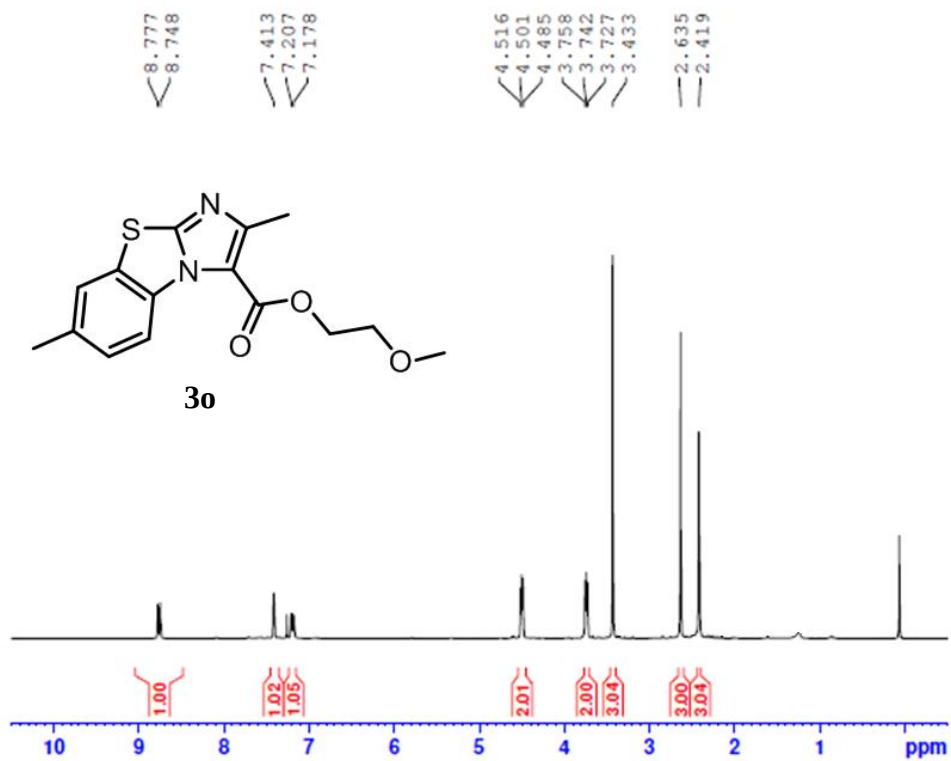
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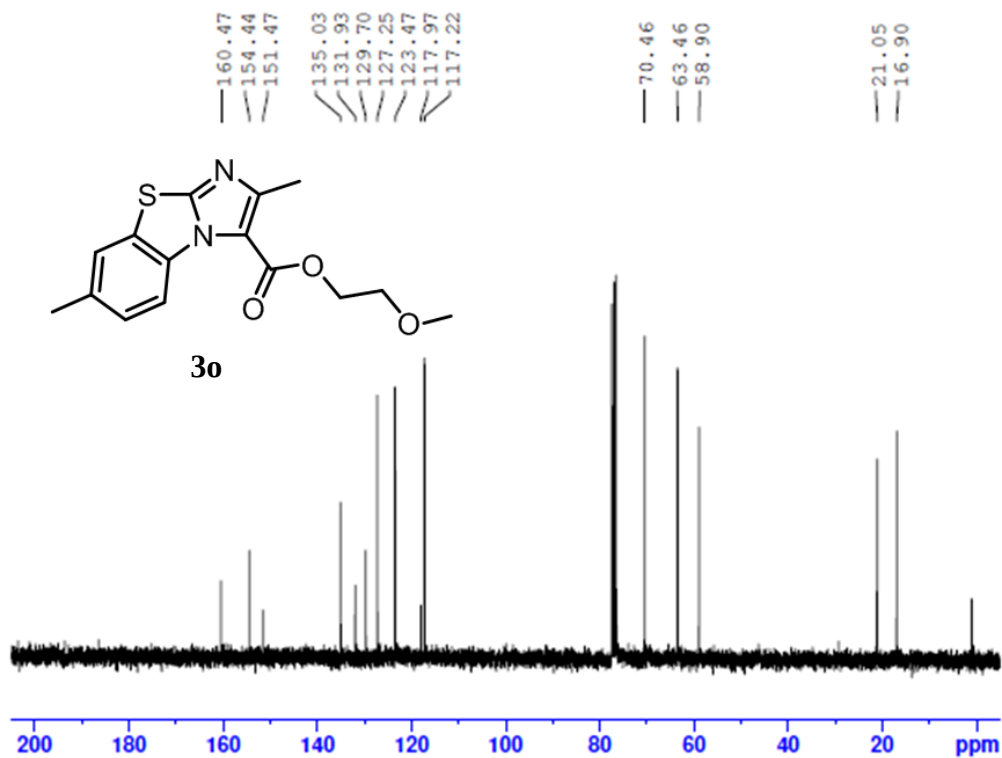
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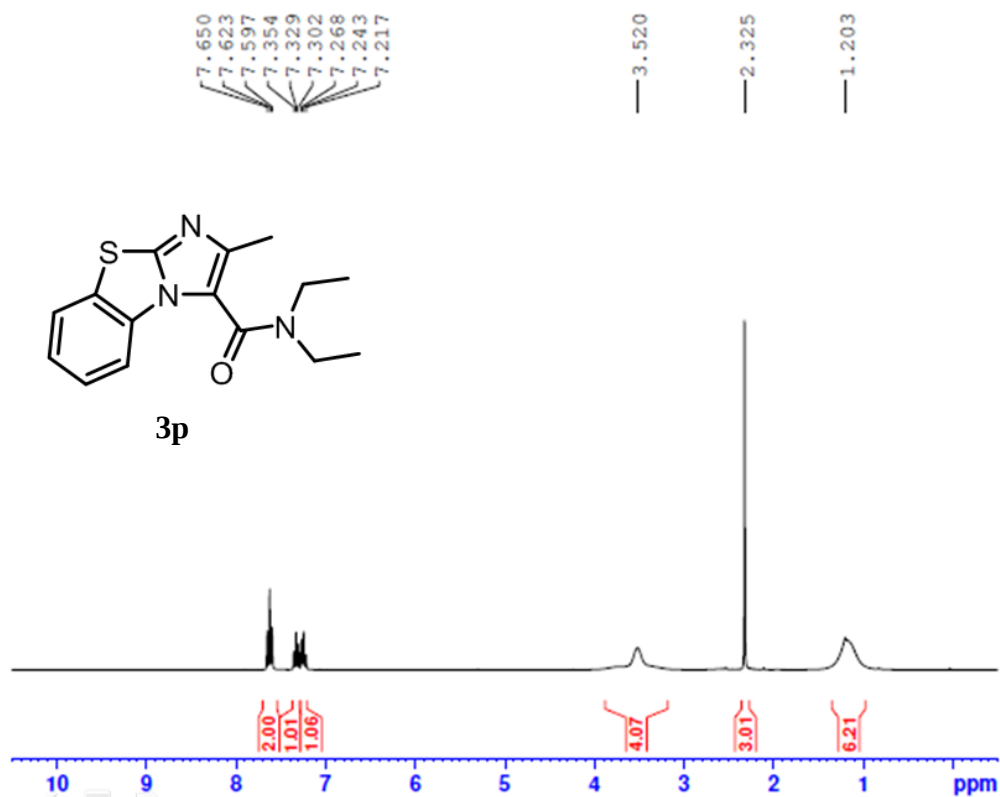
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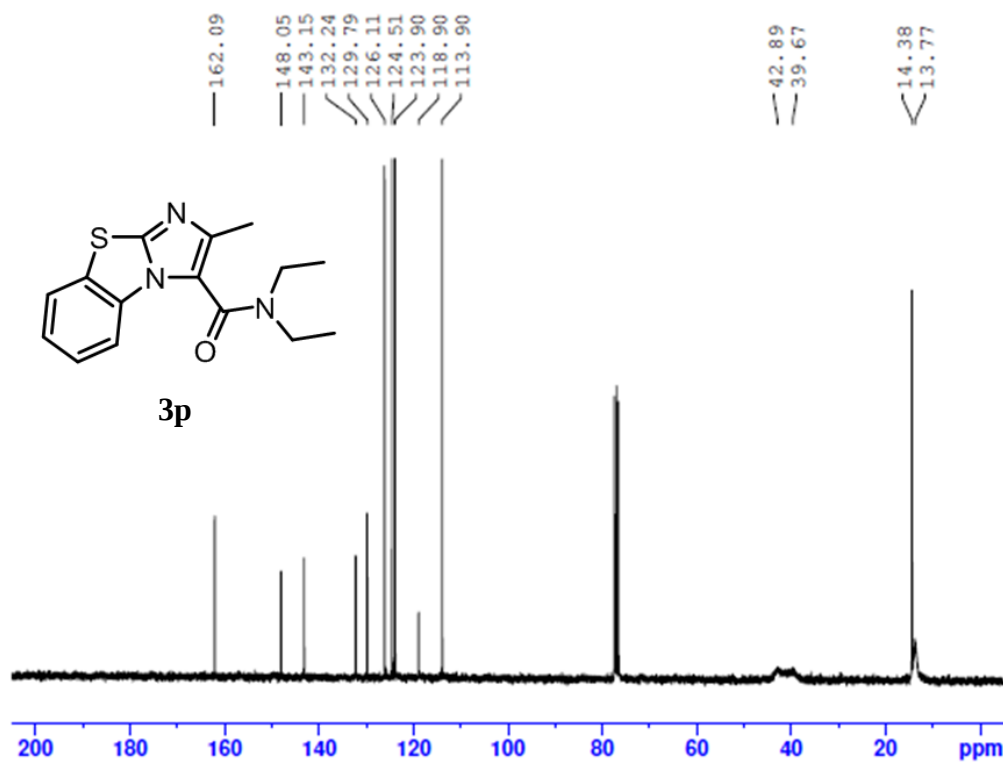
13C Standard AC300



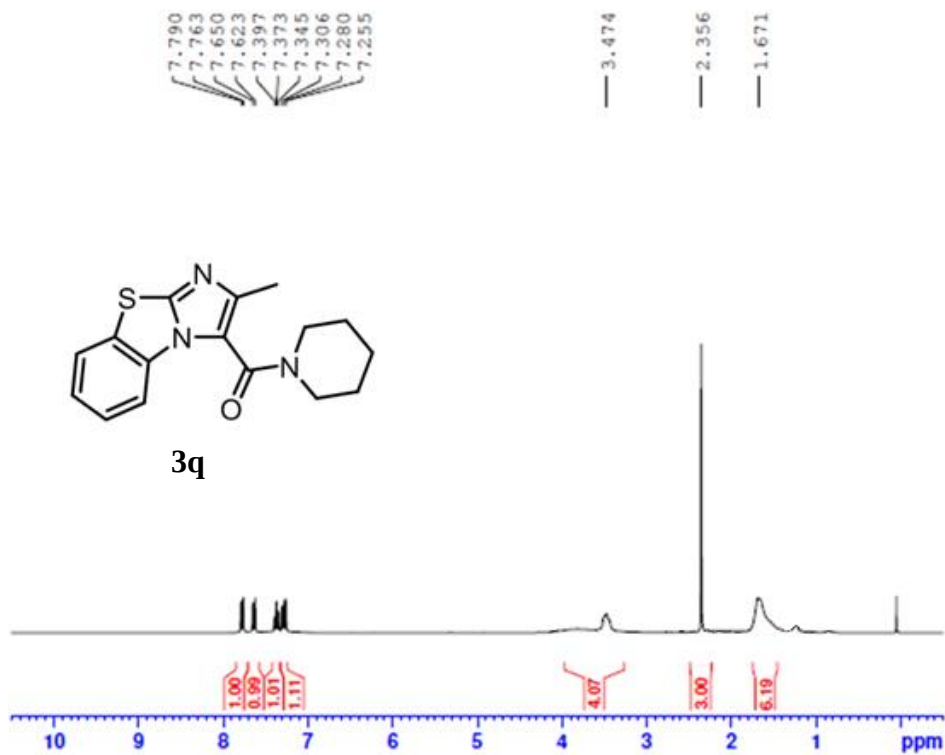
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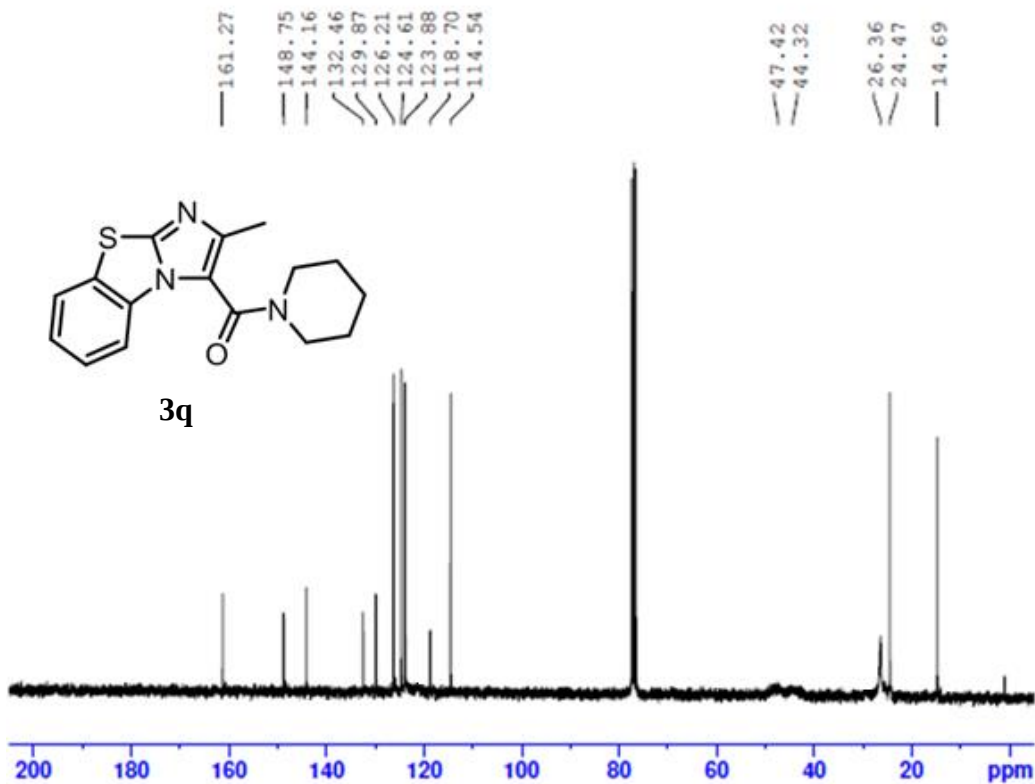
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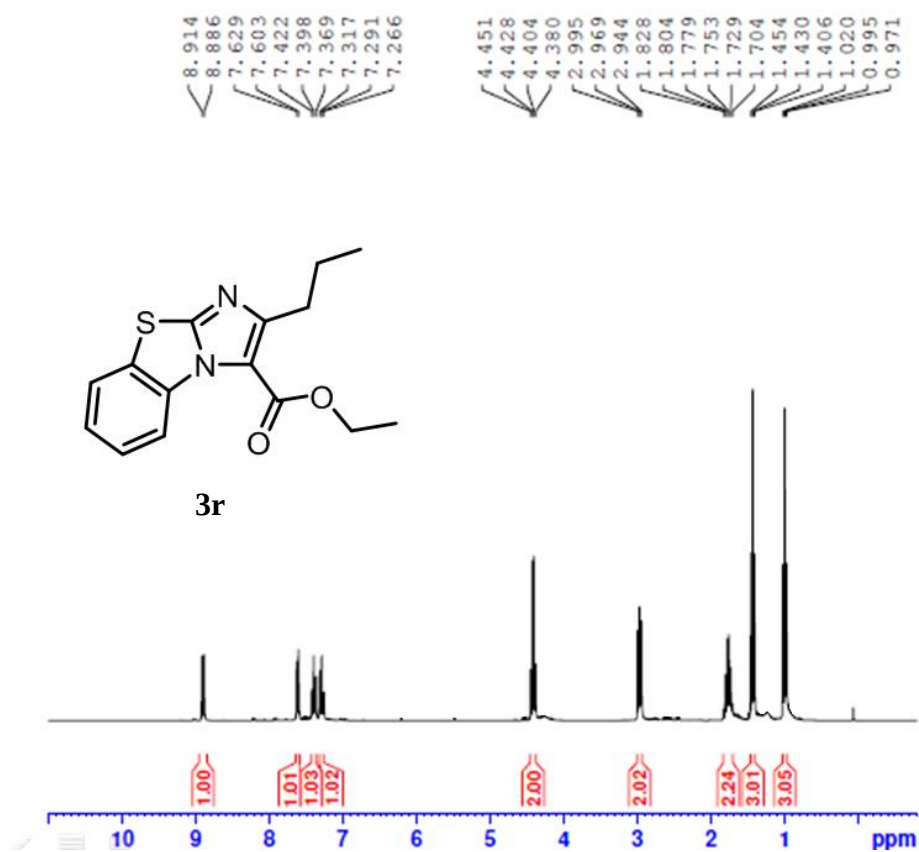
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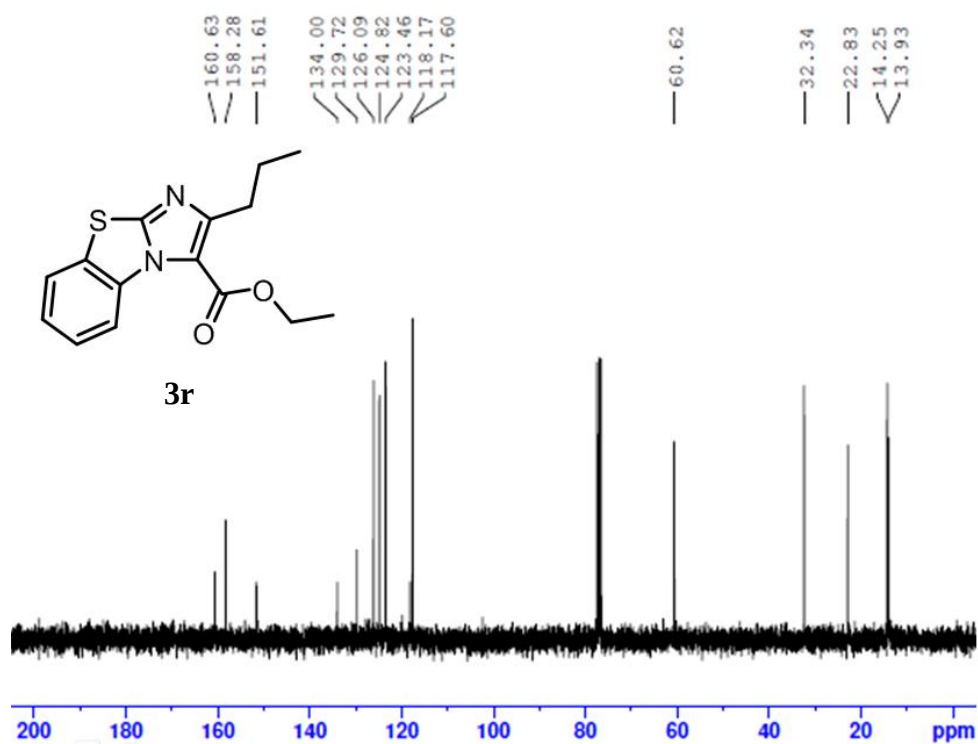
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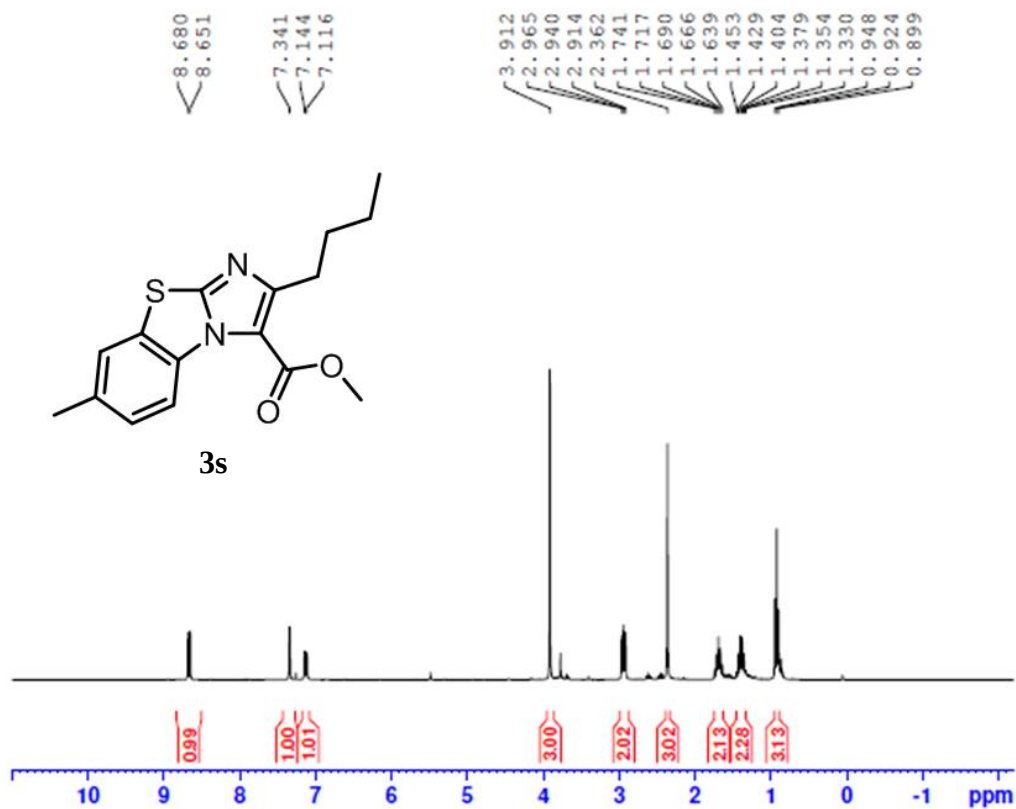
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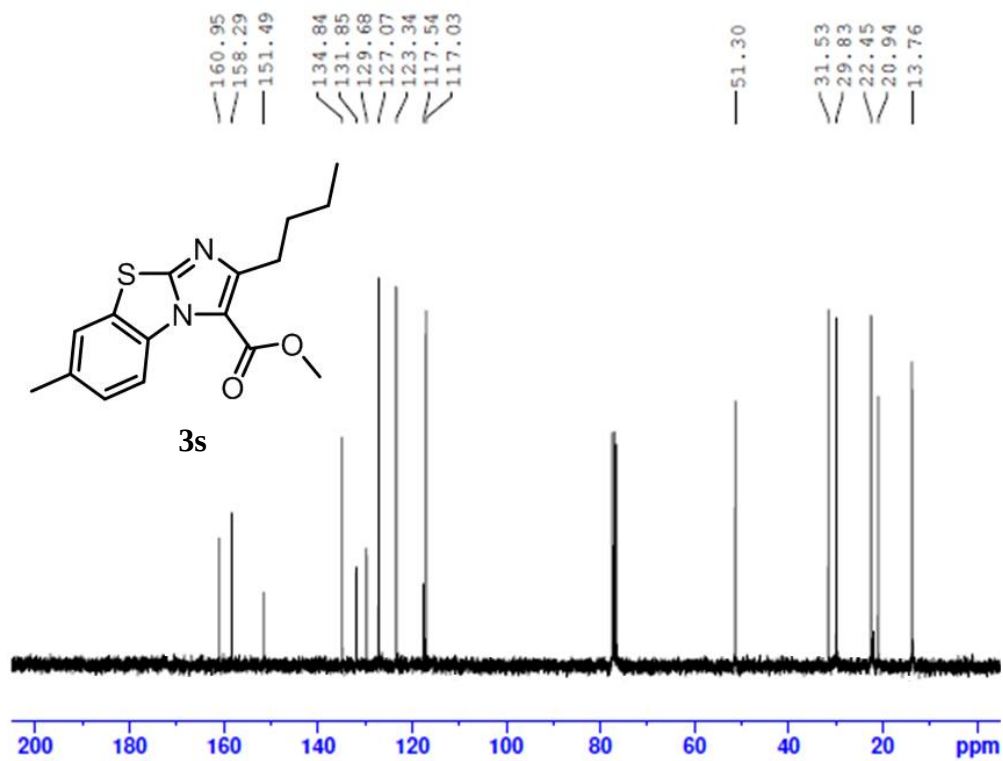
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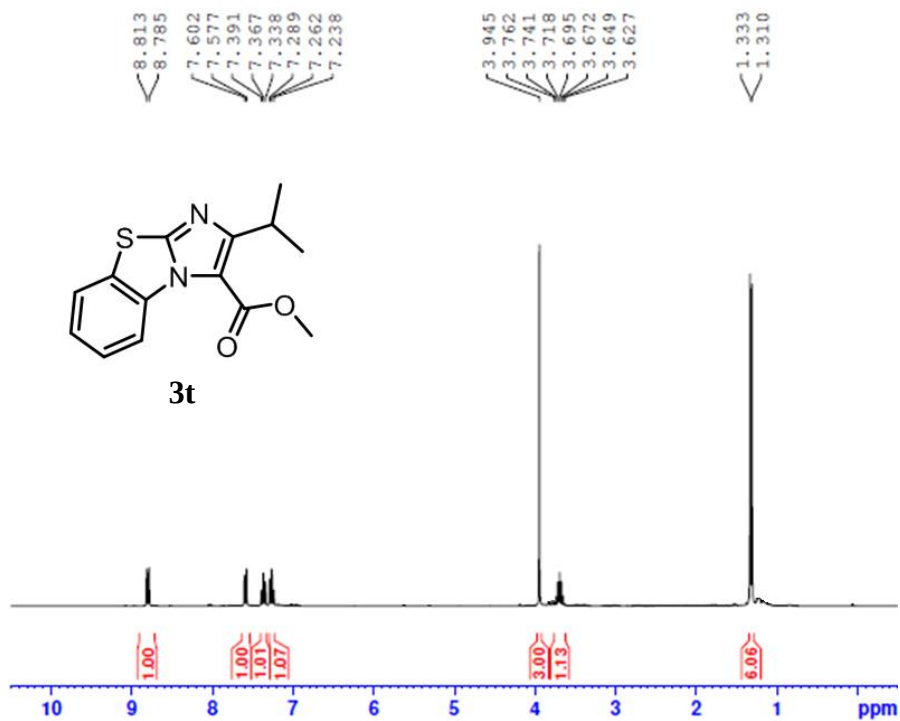
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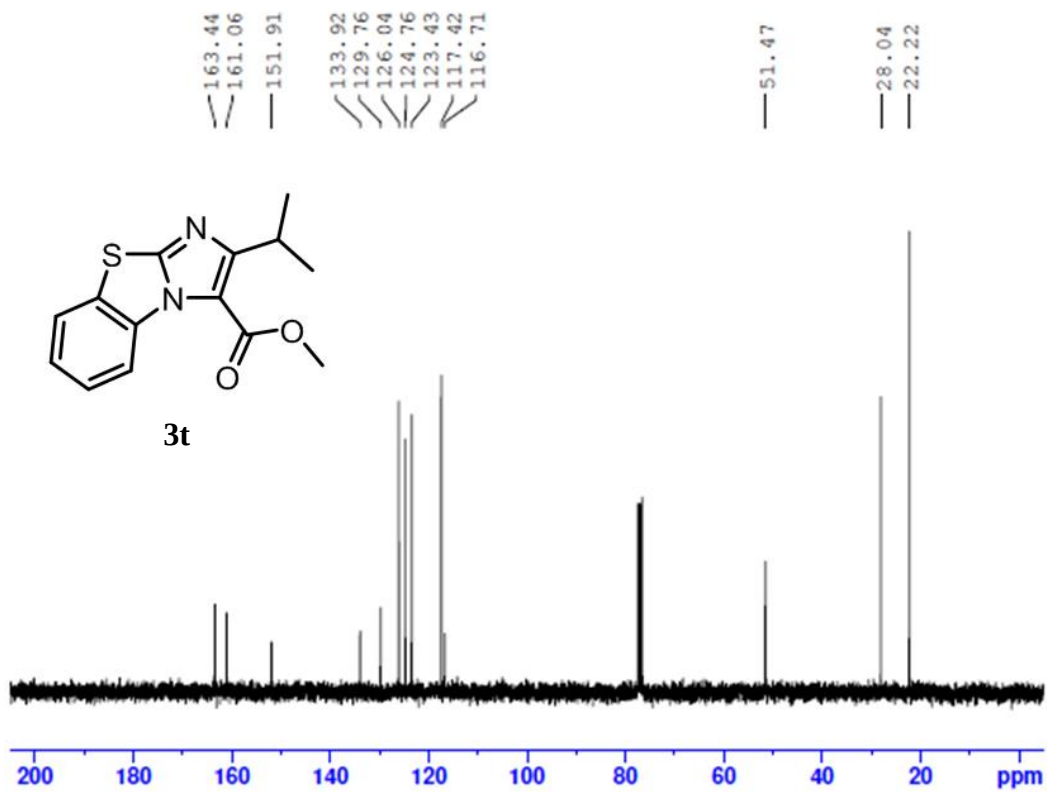
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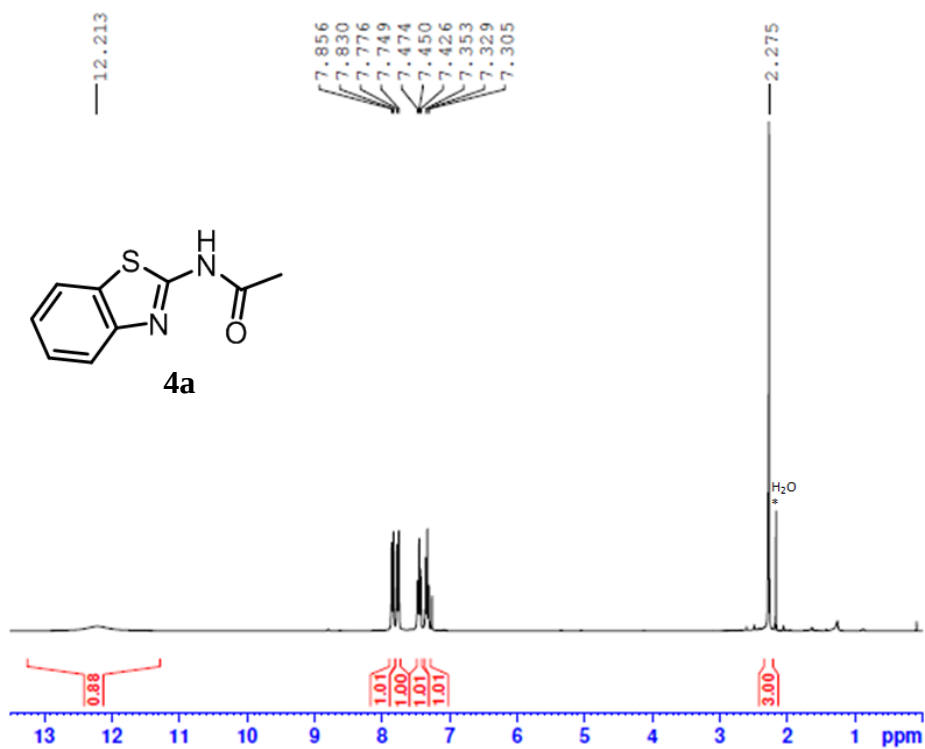
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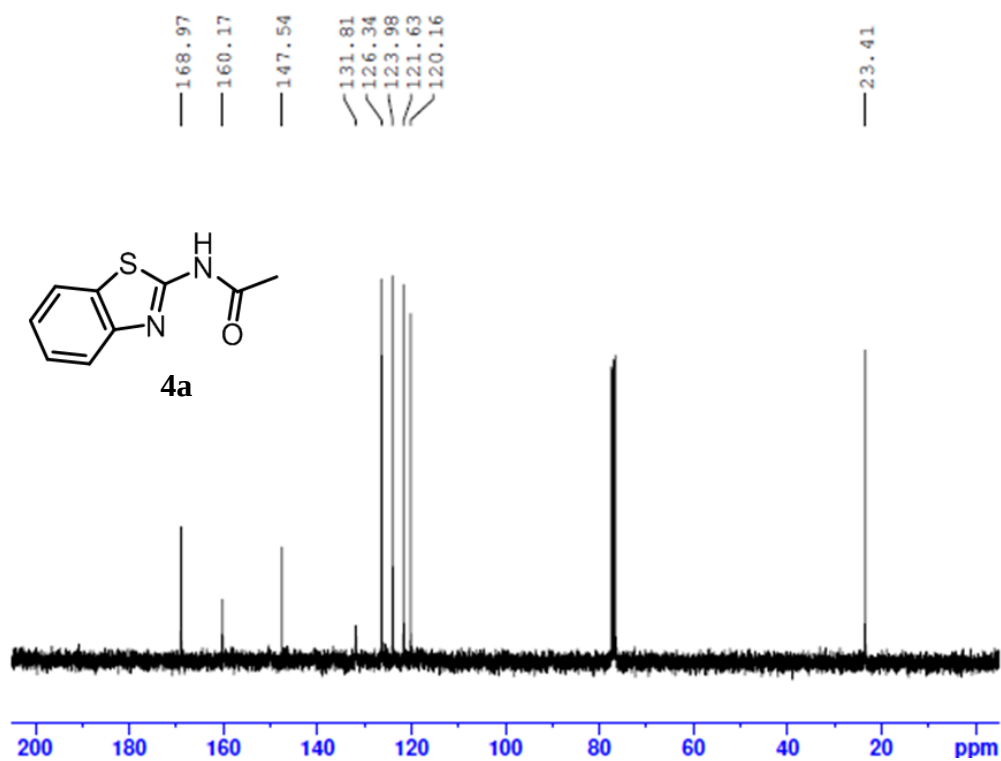
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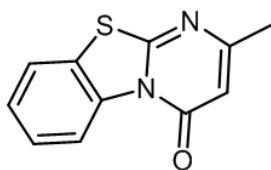
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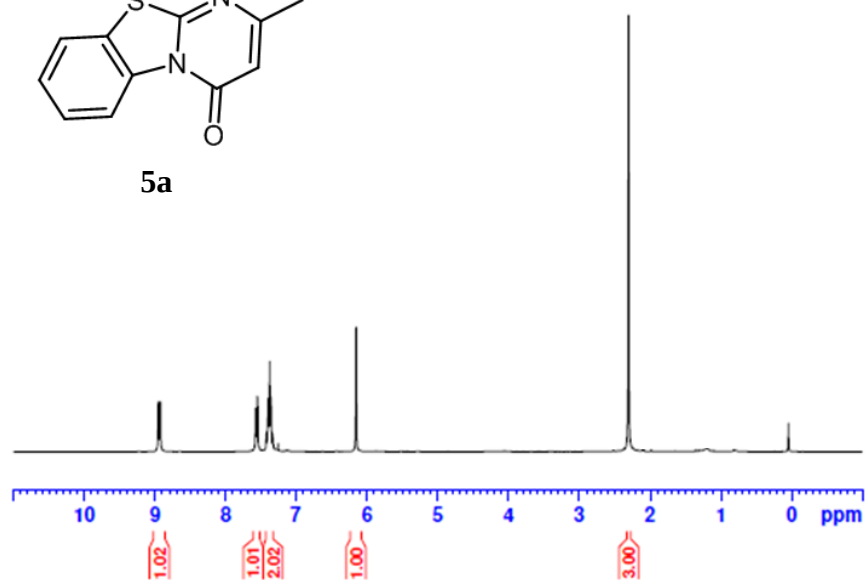
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8.950
8.925
7.579
7.555
7.424
7.405
7.380
7.361
7.336
6.158

2.304



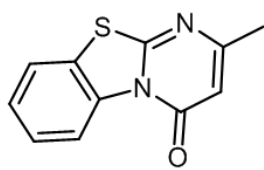
5a



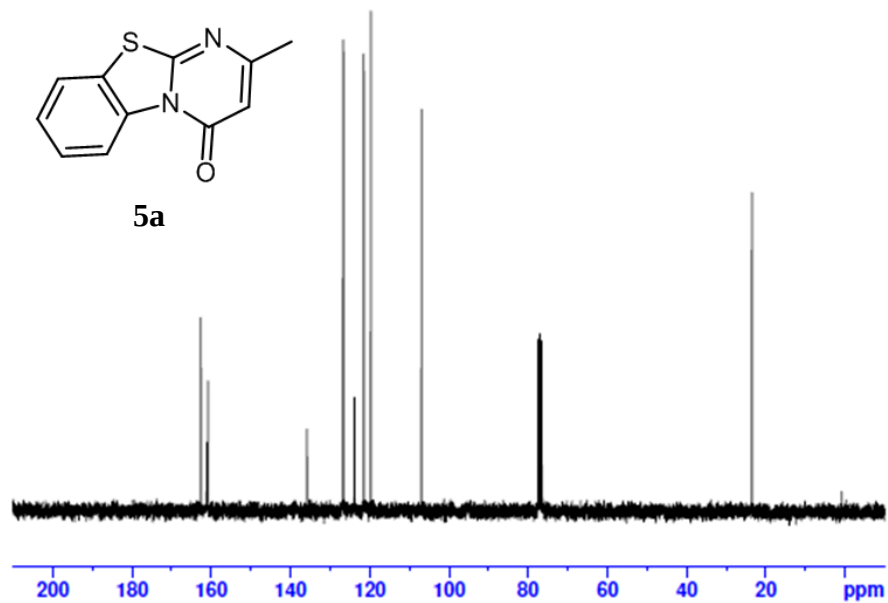
¹³C Standard AC300

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161.14
160.82
135.82
126.72
126.62
123.84
121.48
119.72
106.92

23.50

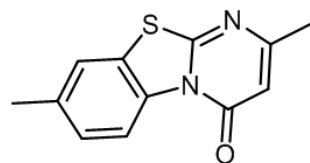


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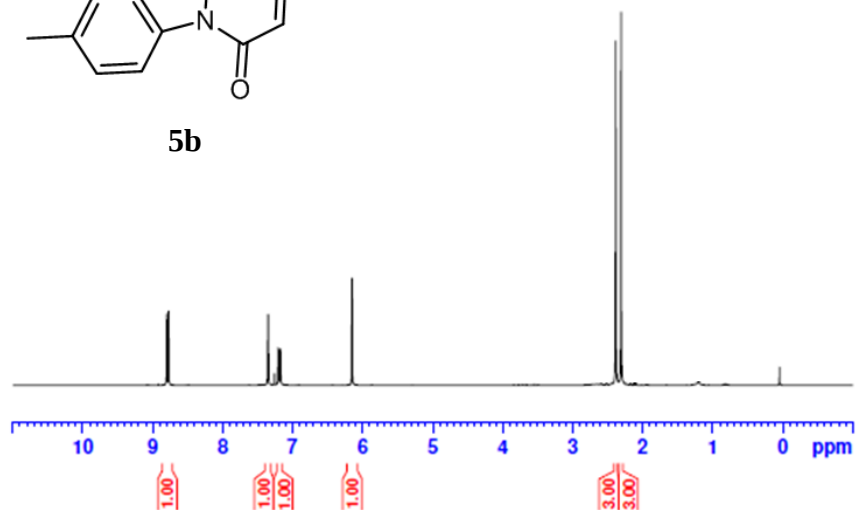


¹H normal range AC300

8.802
8.773
7.352
7.208
7.179
6.153
2.385
2.309

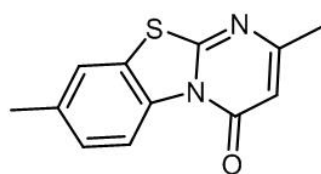


5b

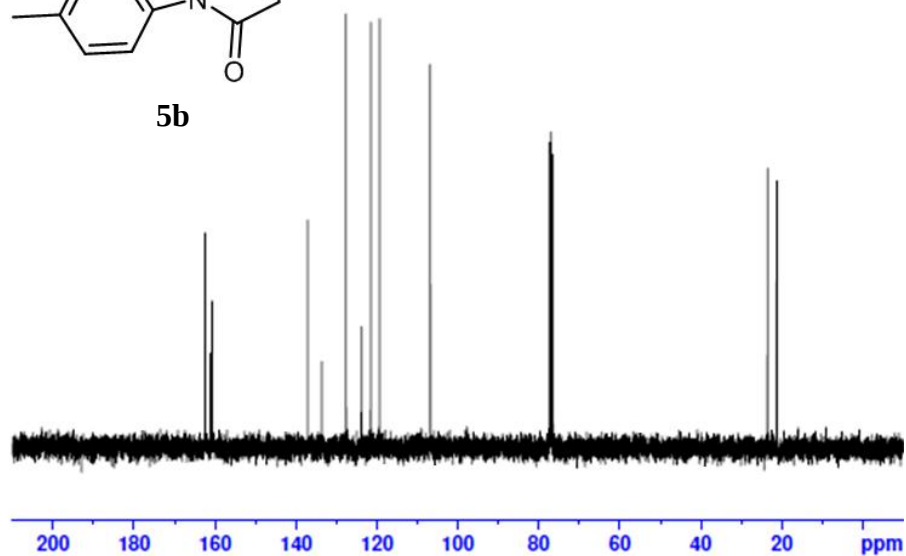


¹³C Standard AC300

162.47
161.16
160.75
137.12
133.65
127.65
123.82
121.51
119.35
106.83
23.50
21.23

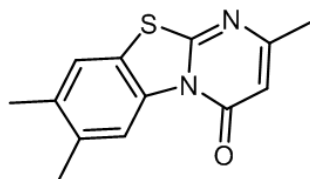


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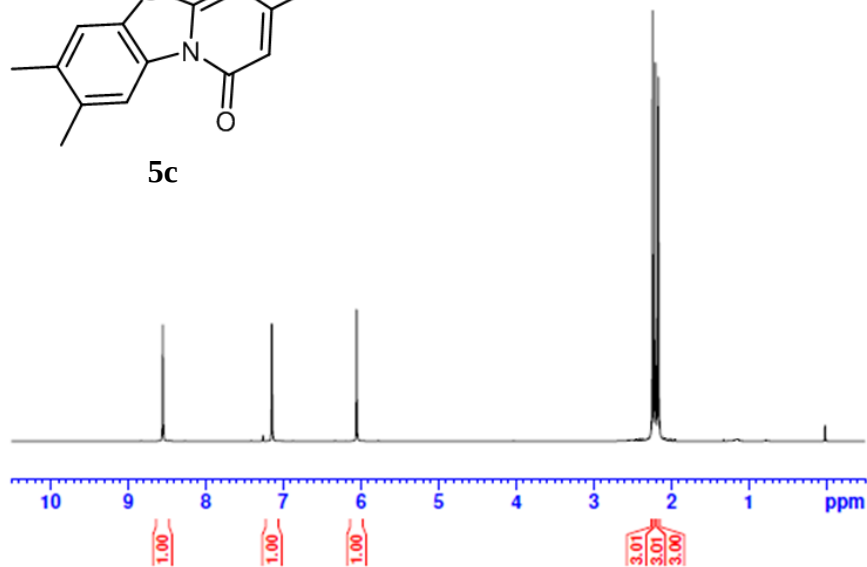


1H normal range AC300

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7.146
6.053
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2.204
2.165

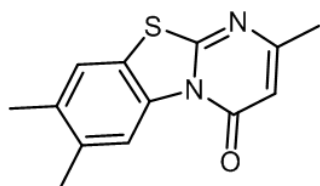


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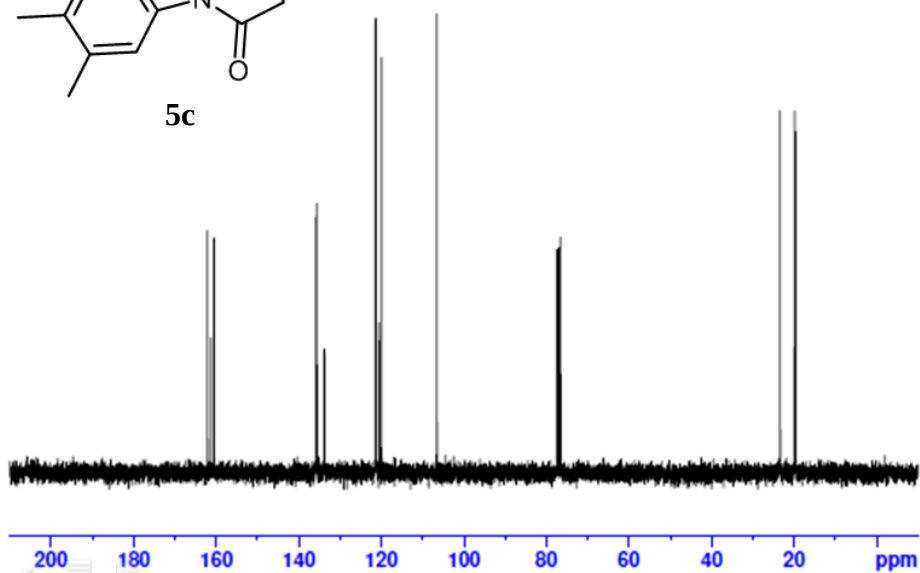


13C Standard AC300

162.103
161.26
160.50
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135.60
133.75
121.37
120.51
119.91
106.54
23.37
19.87
19.66

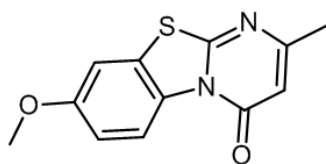


5c

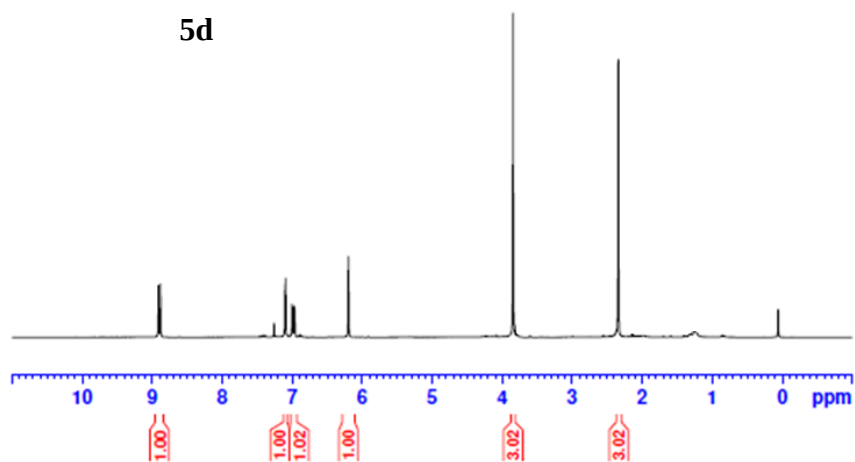


1H normal range AC300

8.912
8.881
7.093
7.002
6.971
6.195
3.844
2.341

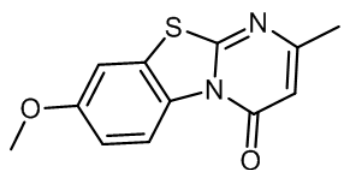


5d

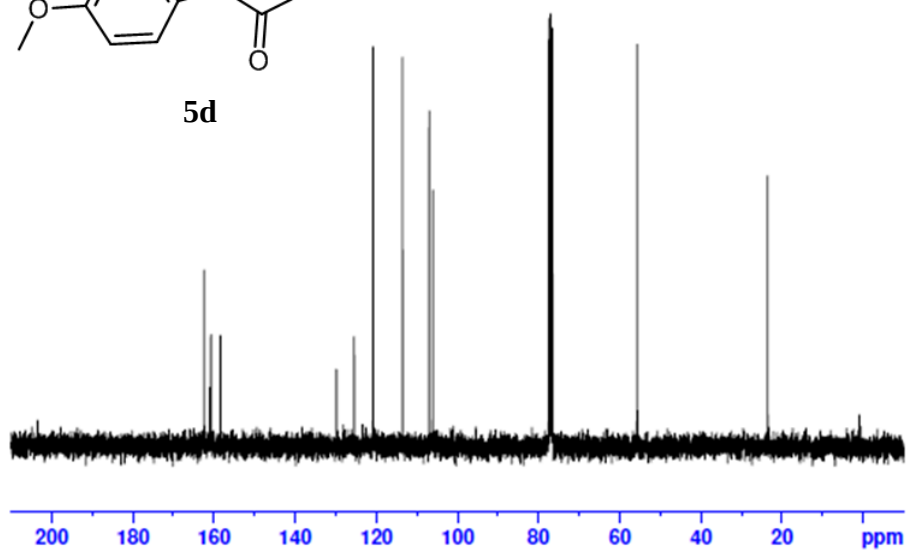


13C Standard AC300

162.41
160.96
160.74
158.37
129.78
125.43
120.78
113.51
106.94
106.02
55.70
23.55

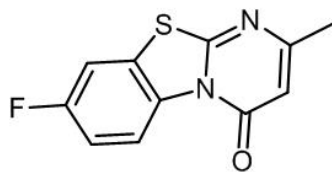


5d

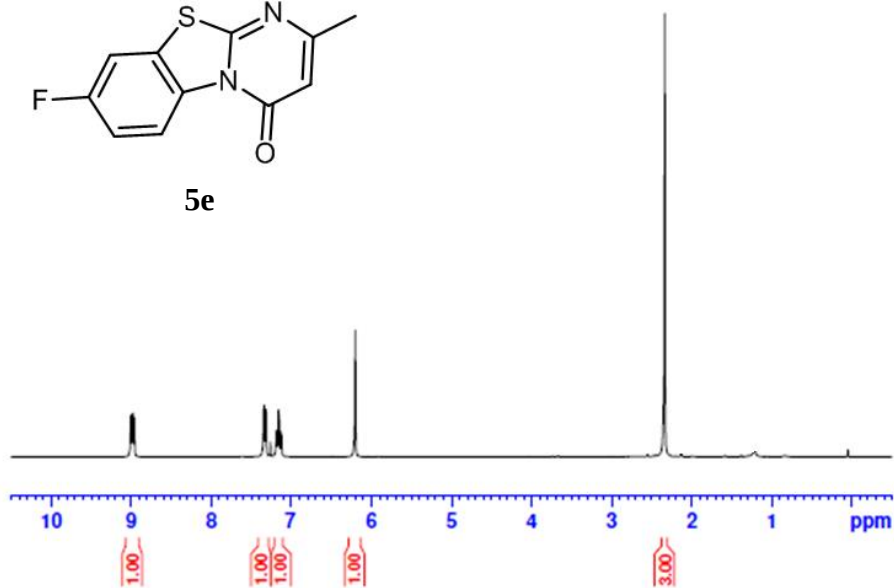


¹H normal range AC300

9.005
8.989
8.974
8.958
7.340
7.314
7.188
7.159
7.129
6.202
2.338

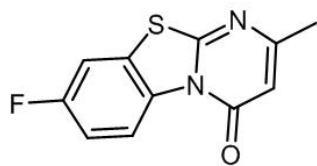


5e

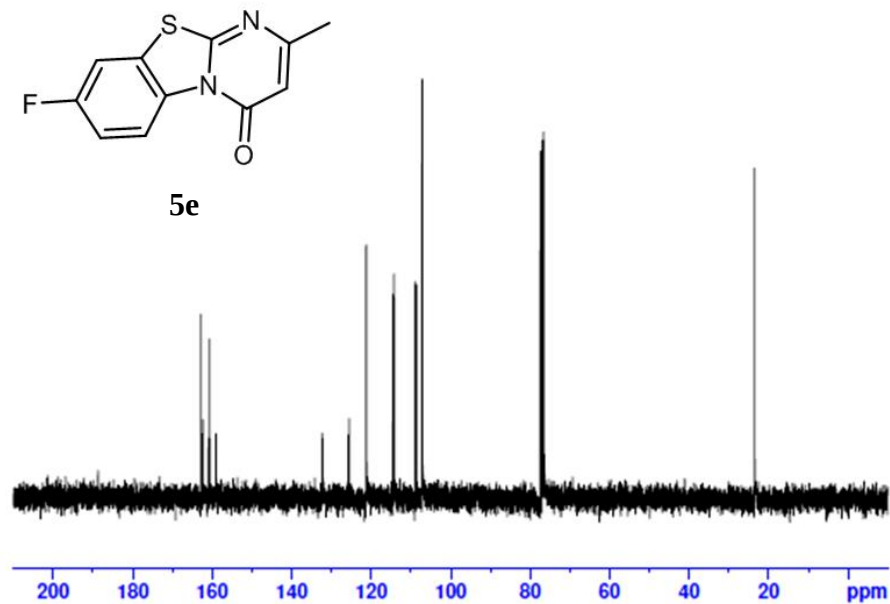


¹³C Standard AC300

162.78
162.31
160.89
160.60
159.01
132.26
125.67
125.53
121.28
121.16
114.51
114.20
108.91
108.55
107.15
23.55



5e



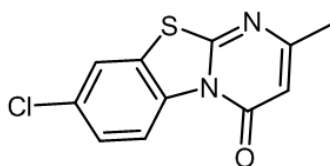
1H normal range AC300

8.978
8.948

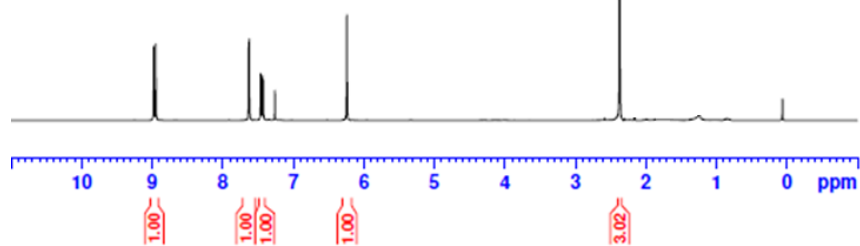
7.624
7.462
7.432

6.240

2.370



5f

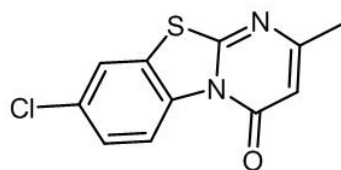


13C Standard AC300

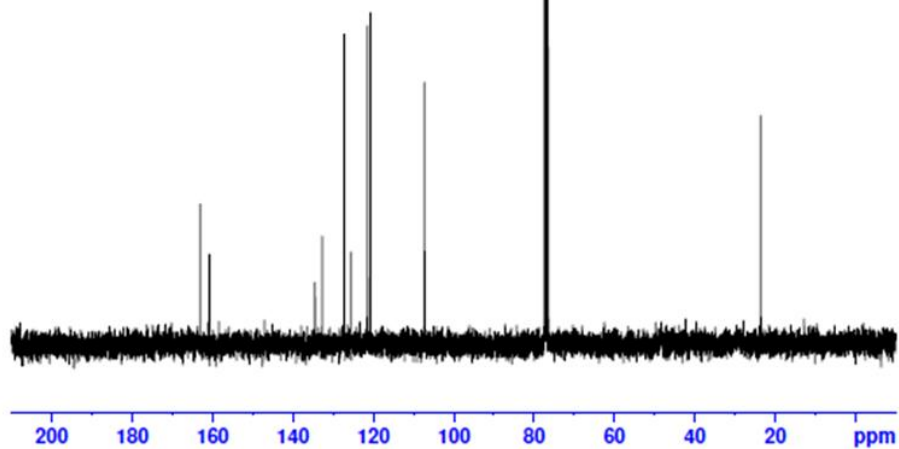
163.07
160.81
160.73

134.51
132.73
127.26
125.60
121.48
120.75

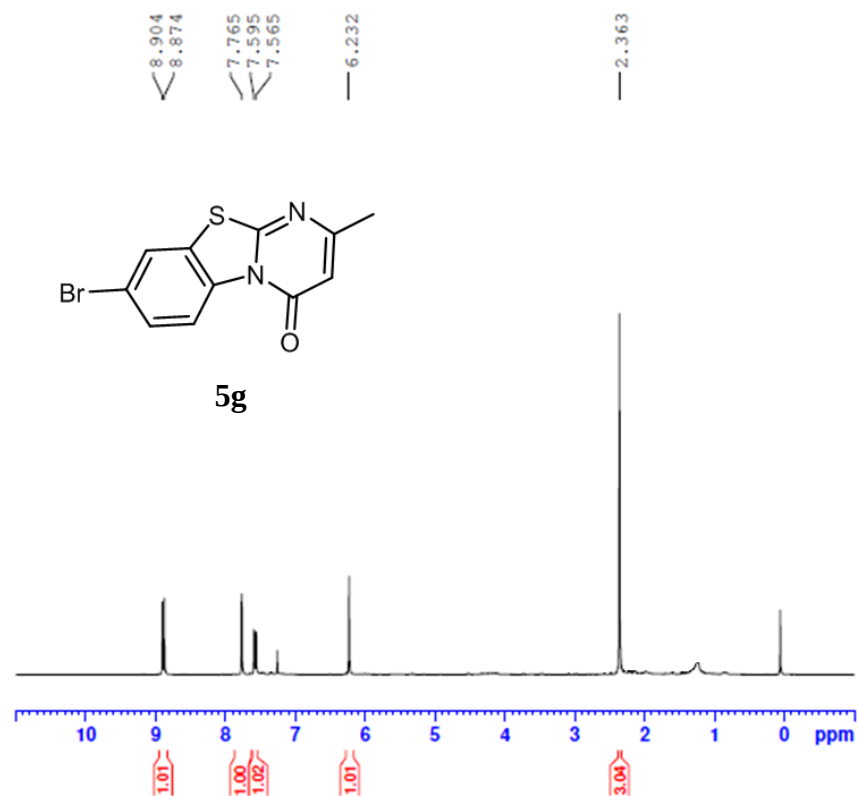
23.66



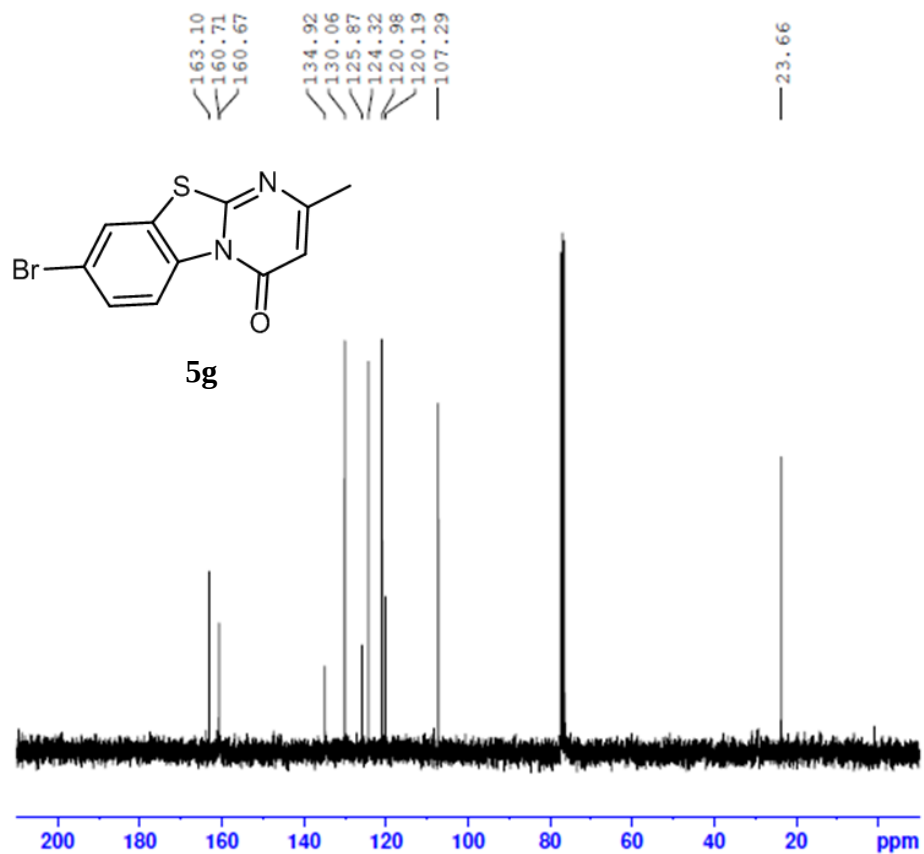
5f



¹H normal range AC300



¹³C Standard AC300



1H normal range AC300

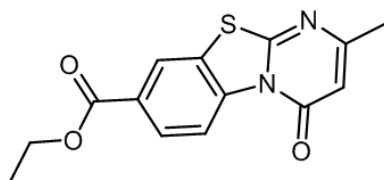
9.100
9.070
8.345
8.177
8.147

6.255

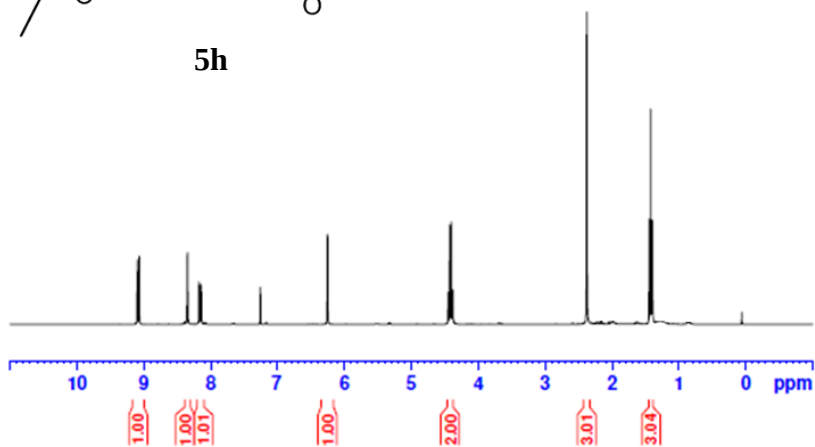
4.451
4.427
4.403
4.380

2.377

1.443
1.419
1.396



5h



13C Standard AC300

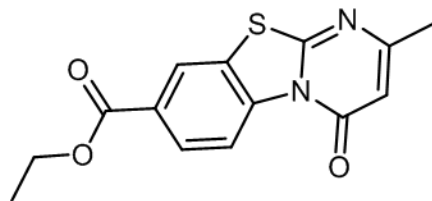
165.01
163.16
161.49
160.86

138.88
129.15
128.29
124.30
123.21
119.47
107.28

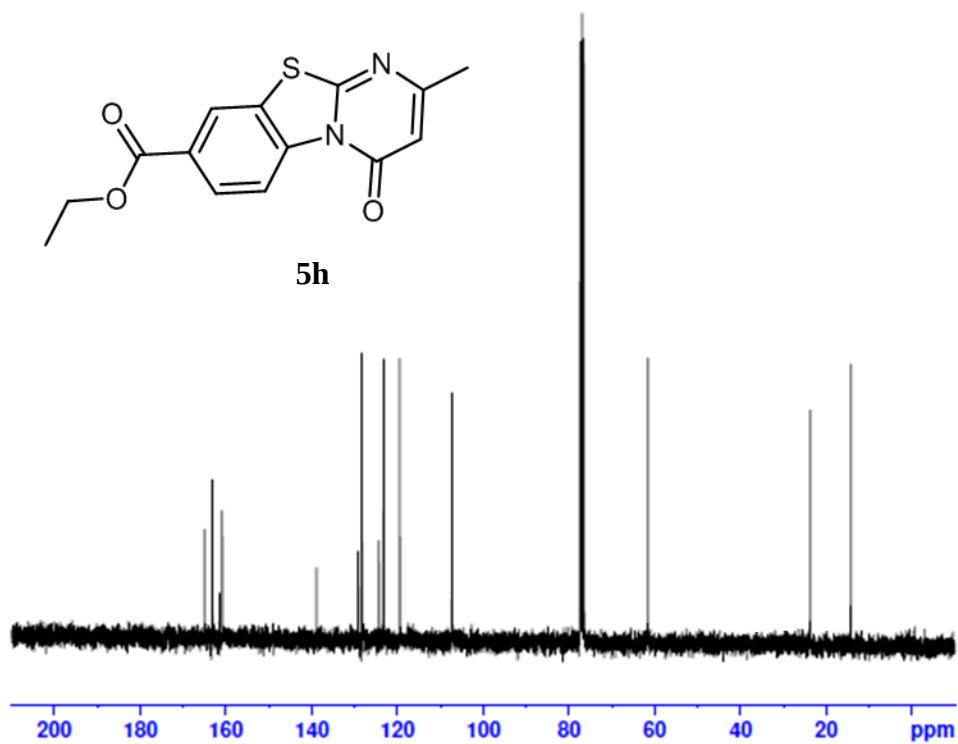
61.57

23.69

14.25

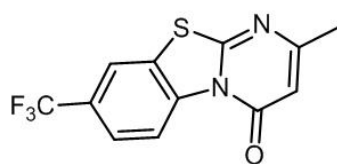


5h

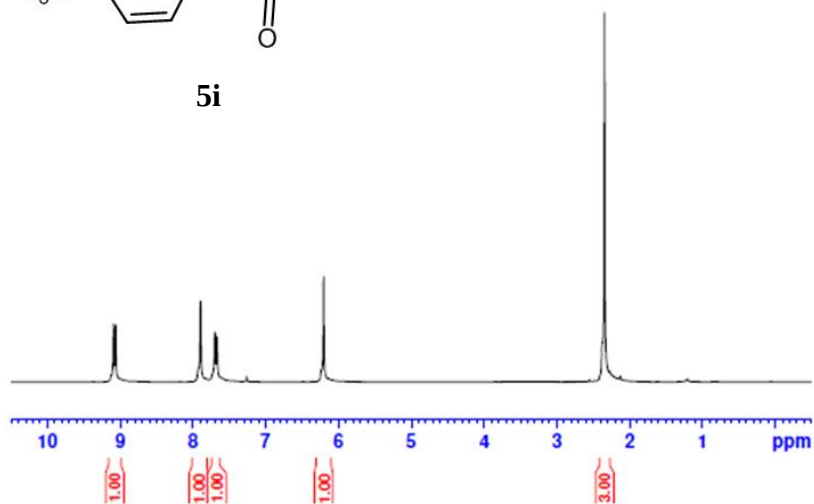


¹H normal range AC300

$\swarrow$ 9.092
 $\swarrow$ 9.063
 $\swarrow$ 7.896
 $\swarrow$ 7.700
 $\swarrow$ 7.671
 — 6.204
 — 2.342

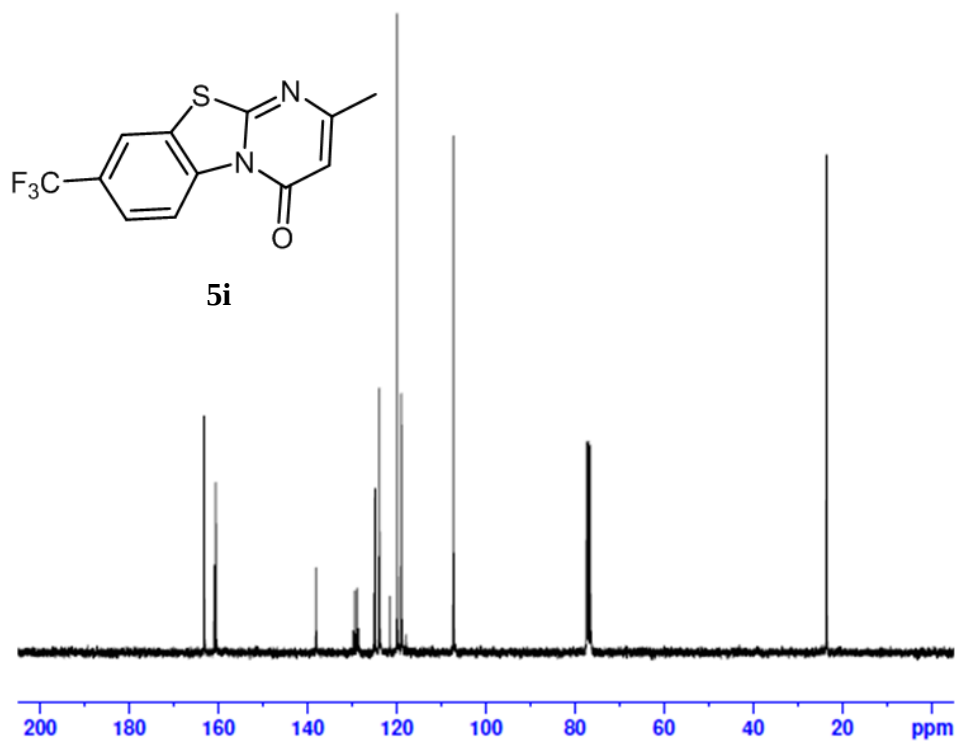


5i



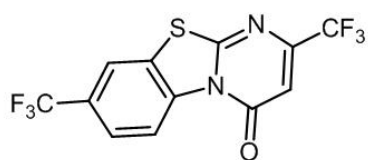
¹³C Standard AC300

$\swarrow$ 163.21
 $\swarrow$ 160.96
 $\swarrow$ 160.36
 $\swarrow$ 138.12
 $\swarrow$ 129.82
 $\swarrow$ 129.38
 $\swarrow$ 128.30
 $\swarrow$ 128.73
 $\swarrow$ 128.49
 $\swarrow$ 125.12
 $\swarrow$ 124.86
 $\swarrow$ 123.96
 $\swarrow$ 123.93
 $\swarrow$ 123.88
 $\swarrow$ 123.86
 $\swarrow$ 123.80
 $\swarrow$ 119.90
 $\swarrow$ 119.06
 $\swarrow$ 119.01
 $\swarrow$ 118.96
 $\swarrow$ 118.91
 $\swarrow$ 117.89
 $\swarrow$ 101.29
 — 23.58

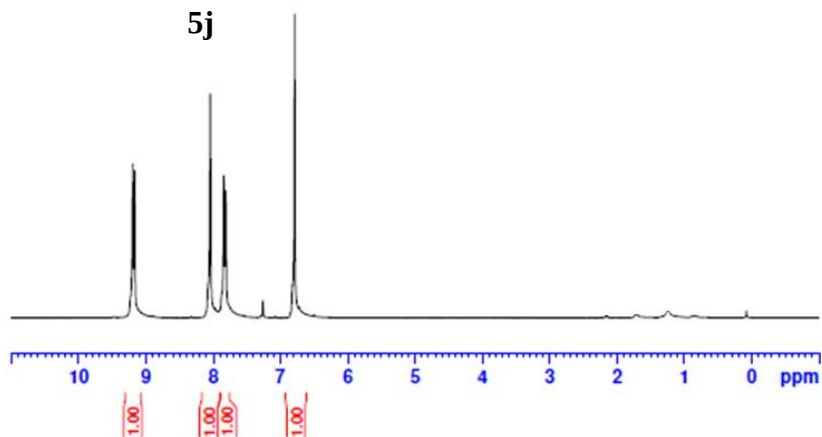


¹H normal range AC300

9.197
9.167
8.044
7.842
7.813
6.790

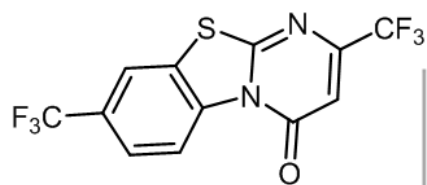


5j

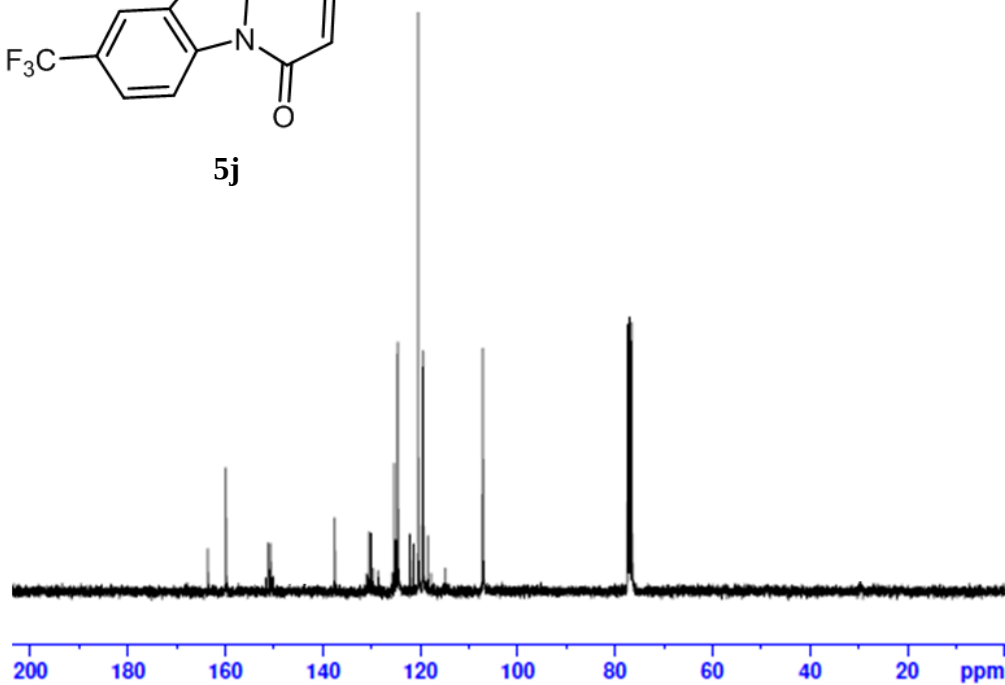


¹³C Standard AC300

163.59
159.89
151.86
151.38
150.70
150.22
137.55
136.99
136.54
136.09
129.65
128.62
128.74
125.32
125.01
124.65
124.65
124.56
122.09
121.39
120.41
119.52
119.46
119.41
119.36
116.45
117.78
114.80
107.22
107.14
107.10



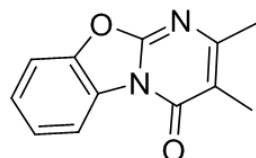
5j



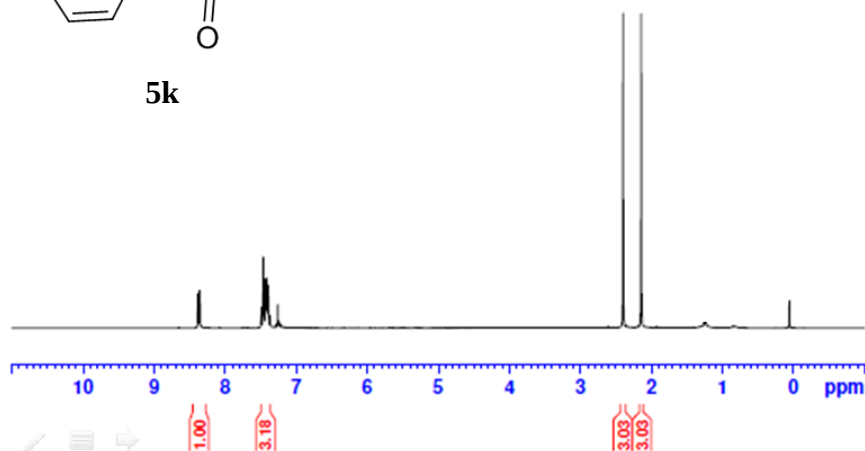
¹H normal range AC300

8.384
8.361
7.487
7.461
7.436
7.421
7.412
7.396
7.371

2.399
2.143



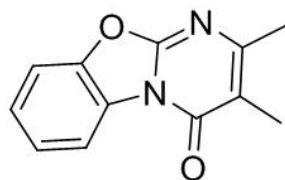
5k



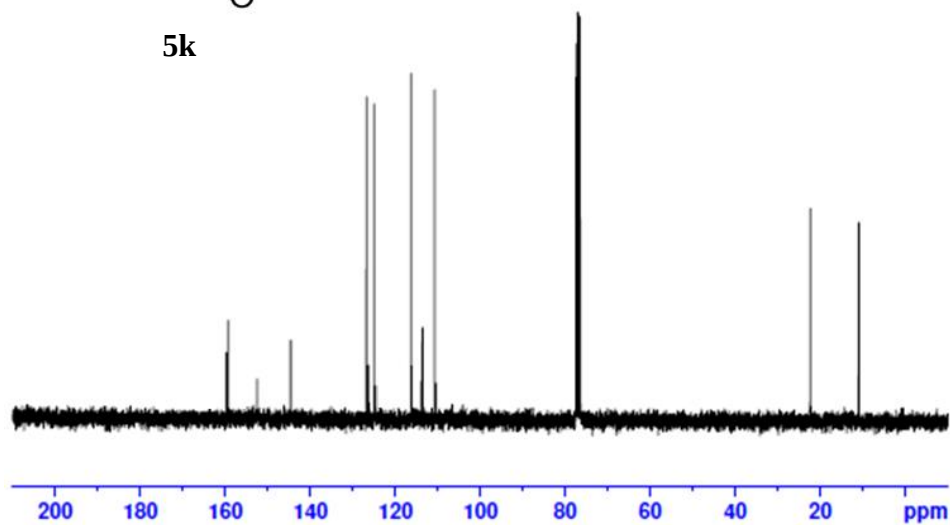
¹³C Standard AC300

159.77
159.35
152.48
144.61
126.77
126.27
124.98
116.26
113.62
110.74

22.36
10.96



5k



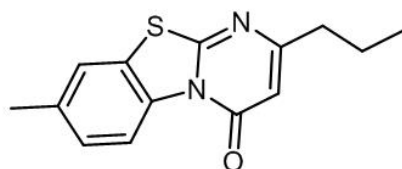
1H normal range AC300

8.726
8.698

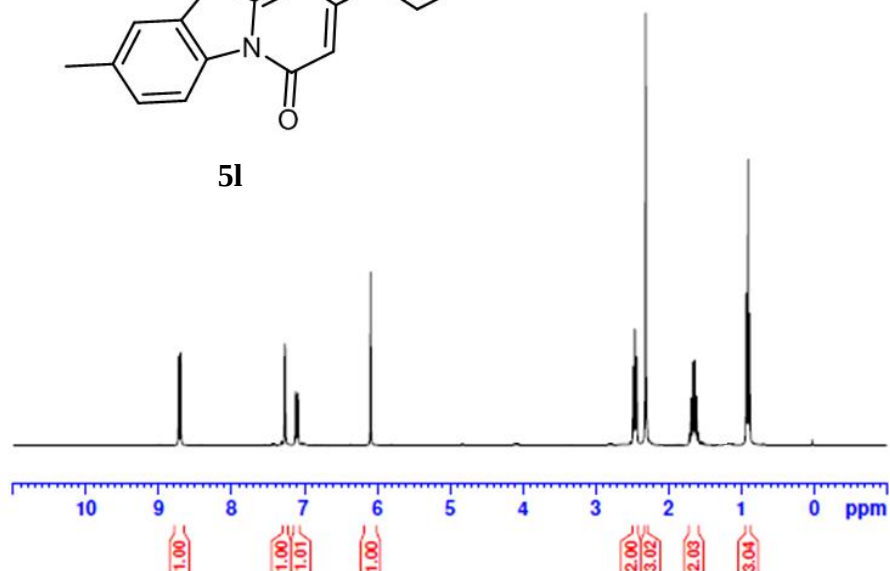
7.265
7.119
7.091

6.089

2.484
2.459
2.433
2.312
1.712
1.688
1.663
1.637
1.613
1.588
0.930
0.906
0.881



5l



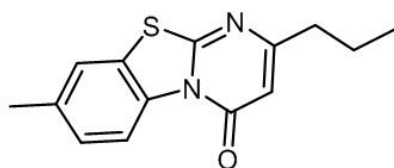
13C Standard AC300

165.93
161.04
160.76

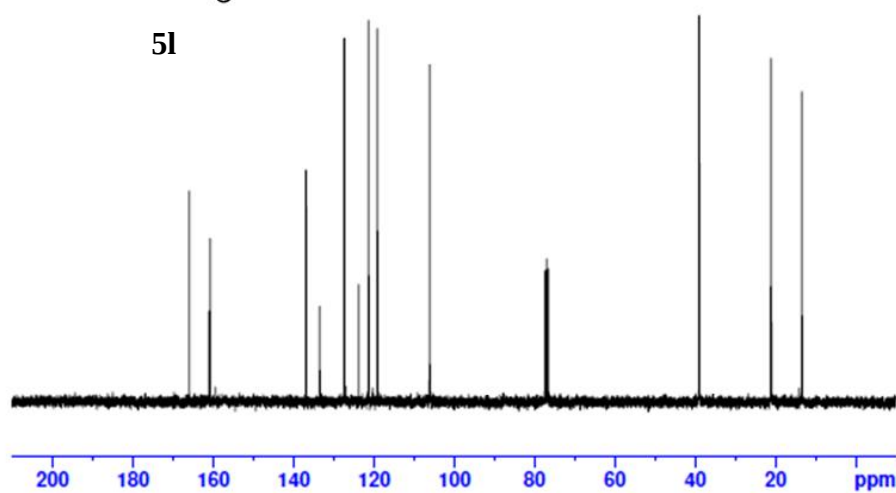
136.86
133.51
127.40
123.75
121.32
119.14
106.13

39.01

21.14
21.08
13.47



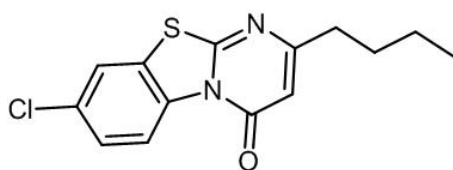
5l



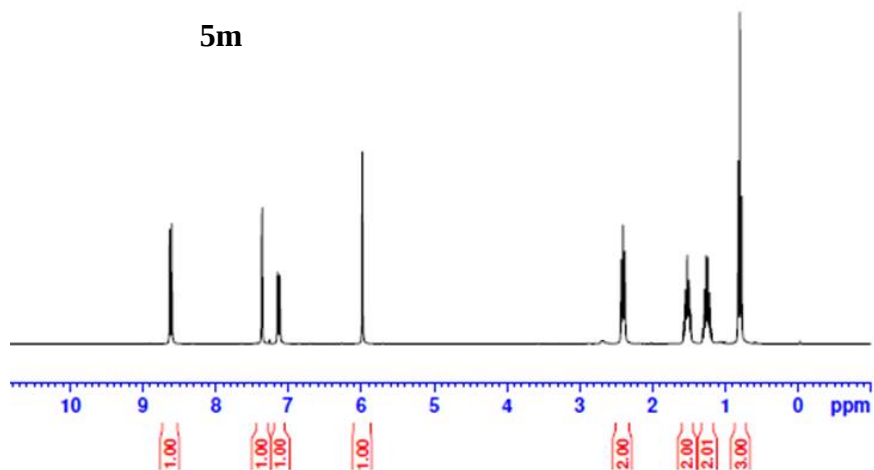
¹H normal range AC300

8.633
8.603
7.362
7.154
7.125
5.986

2.429
2.404
2.378
1.571
1.547
1.521
1.496
1.470
1.311
1.287
1.262
1.237
1.212
1.188
0.822
0.798
0.774



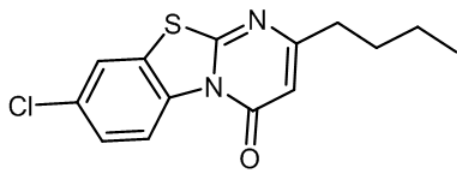
5m



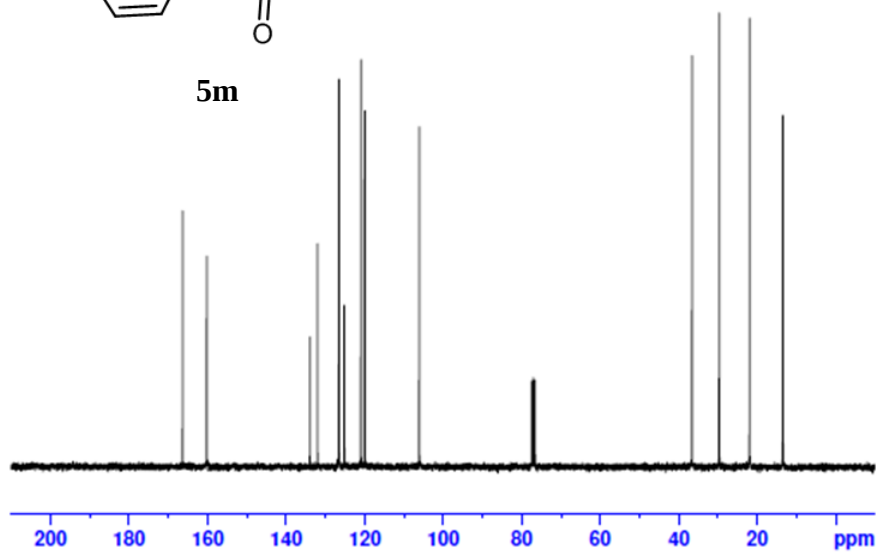
¹³C Standard AC300

166.33
160.24
160.15
133.88
131.98
126.53
125.16
120.93
119.95
106.07

36.59
29.65
21.94
13.46



5m



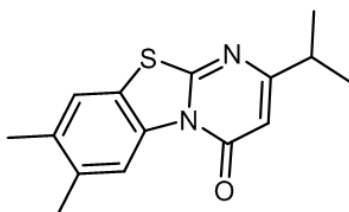
¹H normal range AC300

8.723

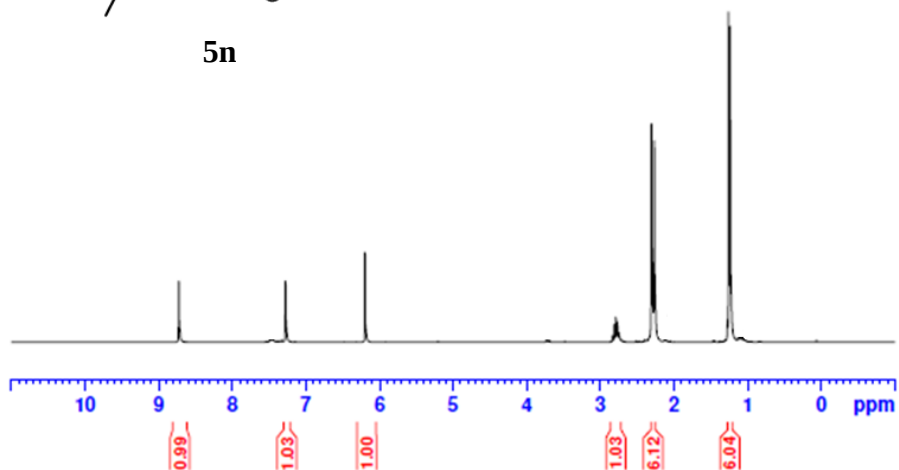
7.276

6.196

2.857
2.834
2.811
2.789
2.766
2.744
2.721
2.306
2.267
1.257
1.235



5n



¹³C Standard AC300

171.22

161.53
161.43

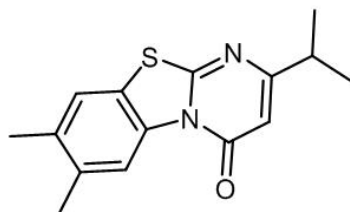
135.97
135.72
134.01

121.63
120.86
120.19

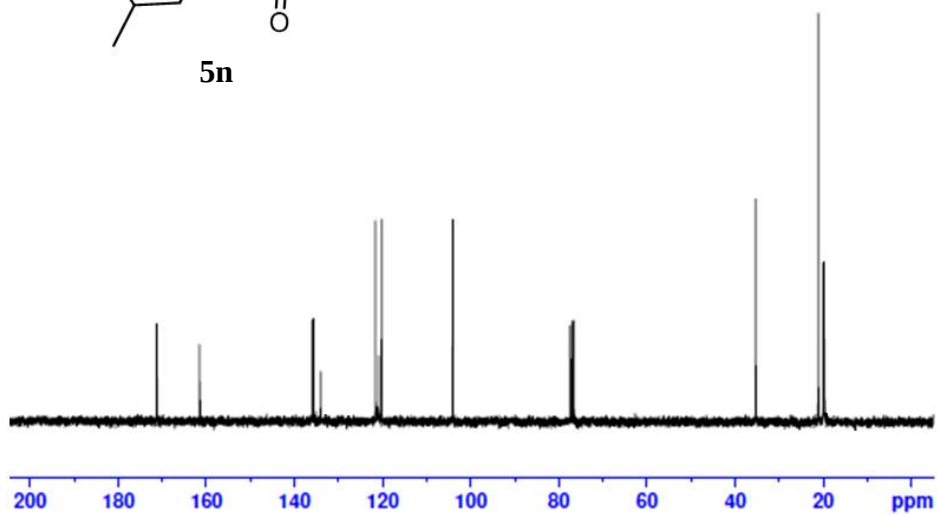
104.09

35.34

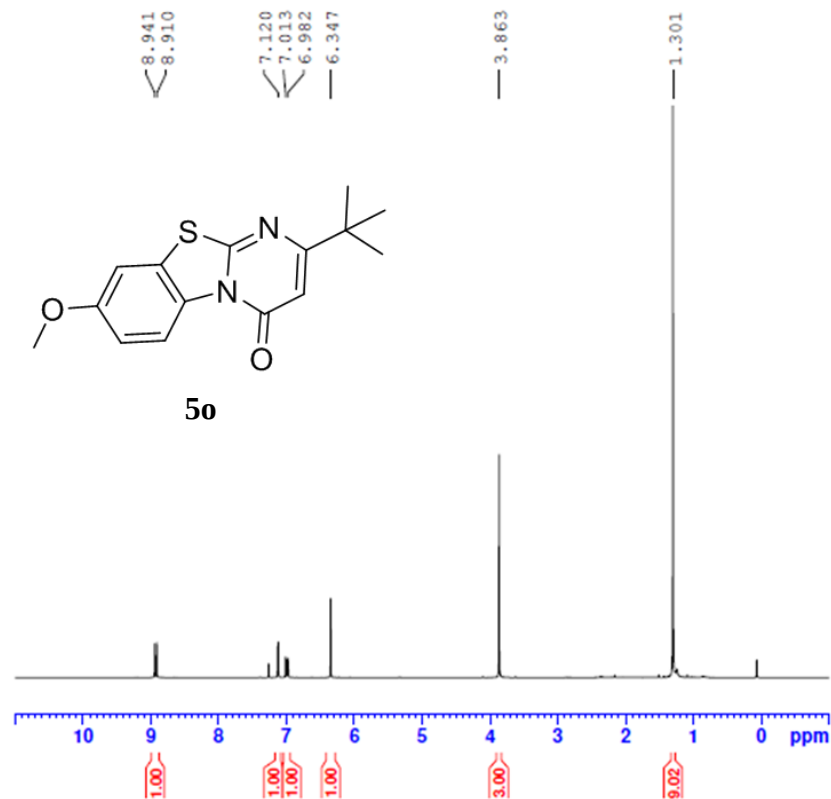
21.13
20.02
19.82



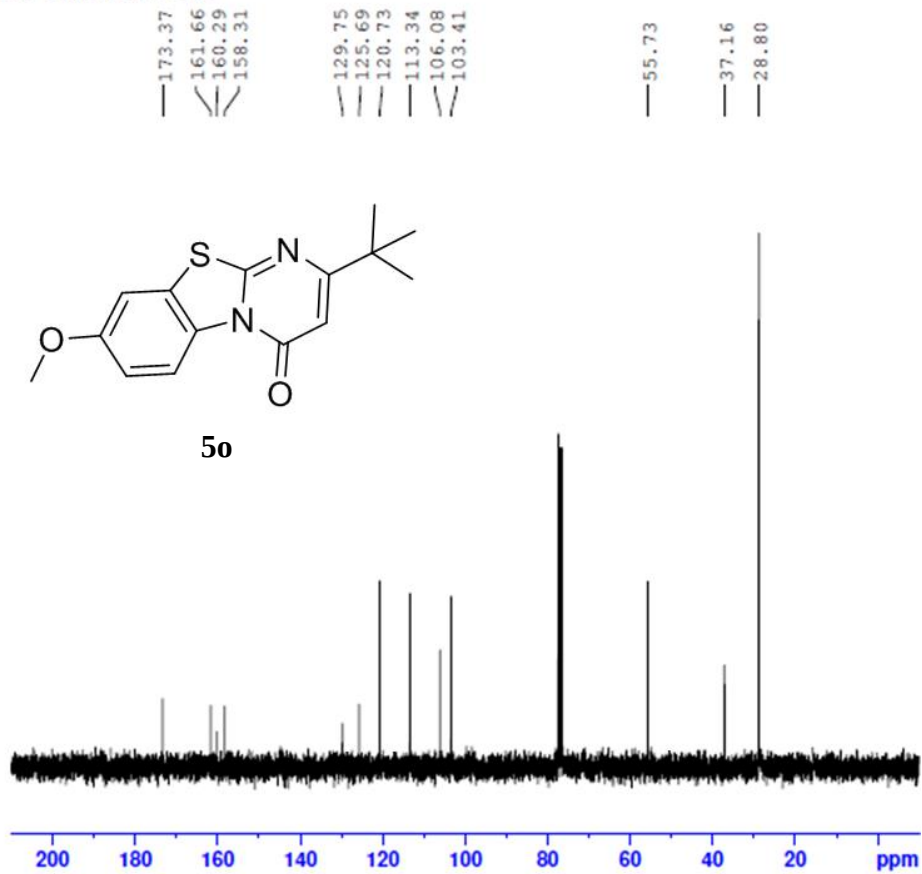
5n



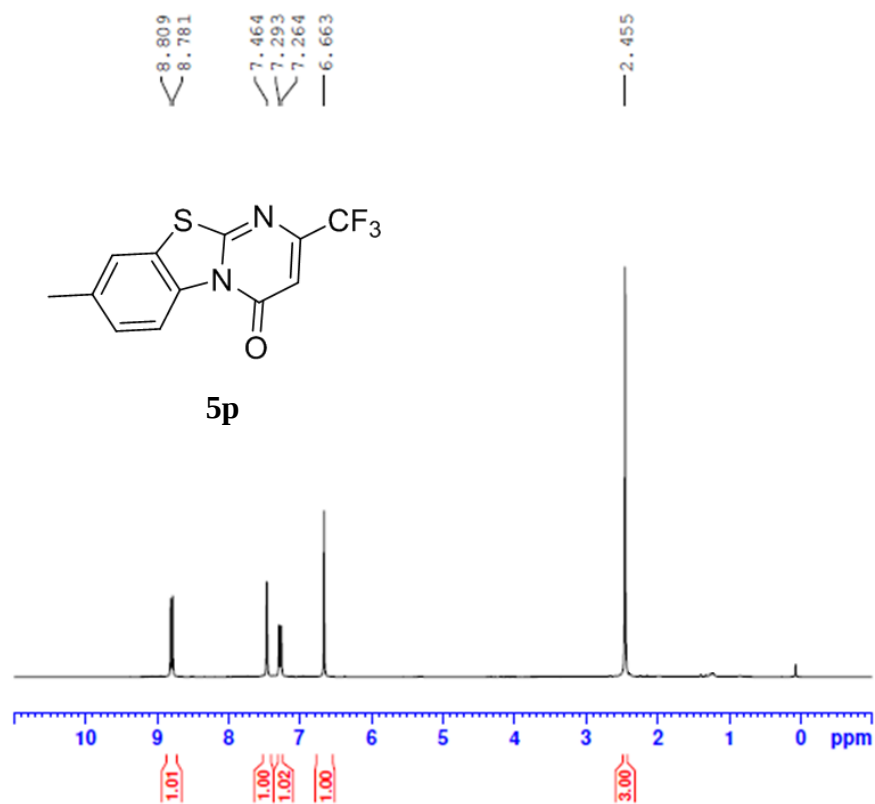
1H normal range AC300



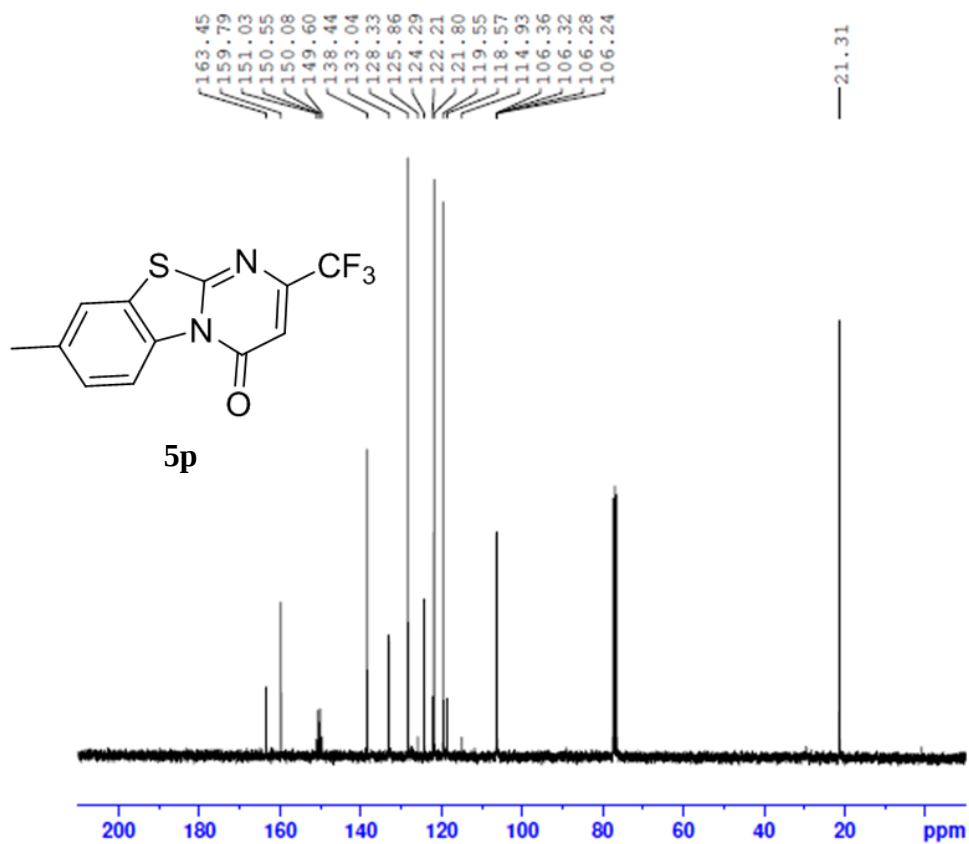
13C Standard AC300



¹H normal range AC300

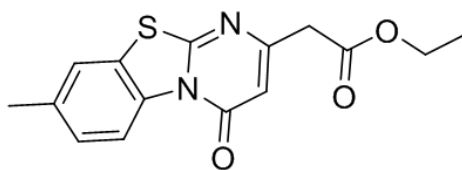


¹³C Standard AC300

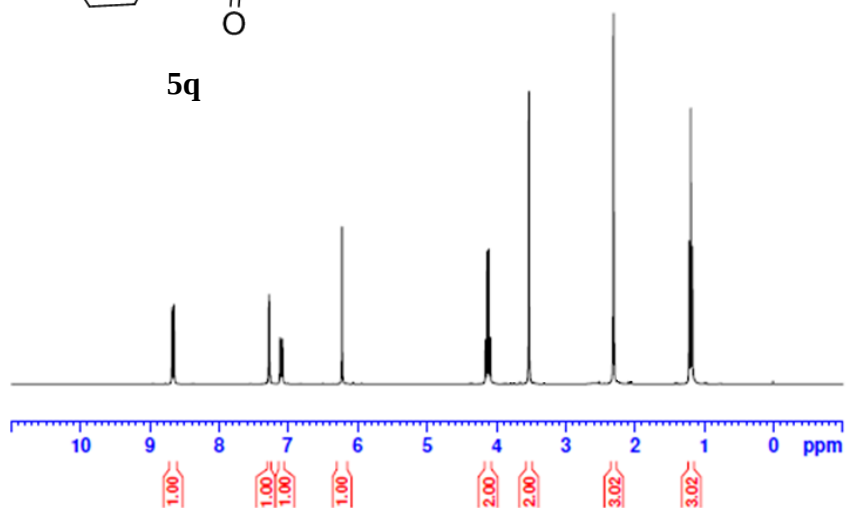


¹H normal range AC300

8.682
8.653
7.282
7.121
7.092
6.227
4.159
4.135
4.111
4.088
3.531
2.310
1.219
1.195
1.171

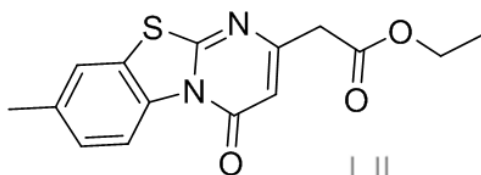


5q

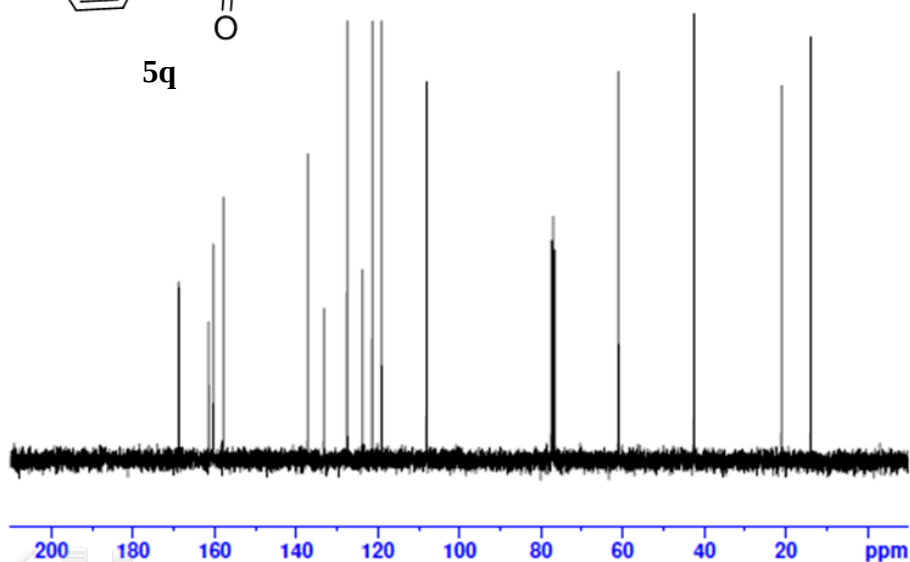


¹³C Standard AC300

168.77
161.40
160.29
157.82
137.16
133.20
127.51
123.75
121.35
119.08
108.02
61.03
42.48
21.04
13.87



5q

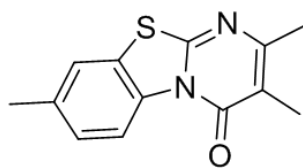


¹H normal range AC300

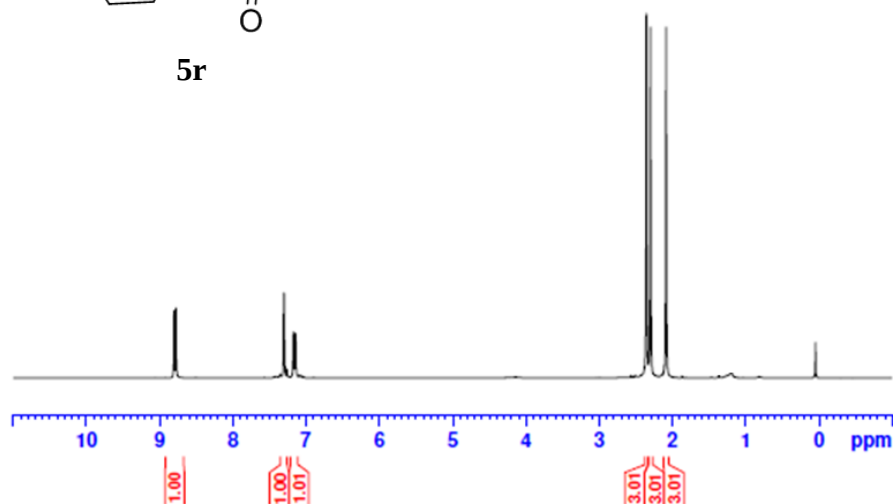
8.804
8.776

7.302
7.176
7.147

2.355
2.299
2.086



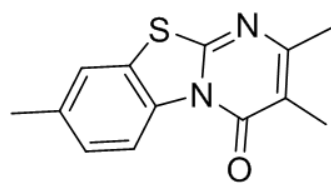
5r



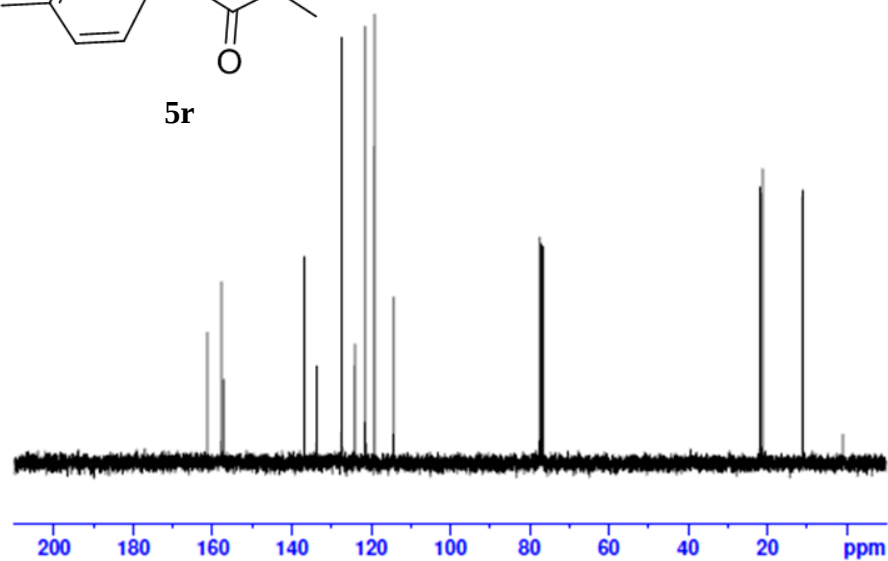
¹³C Standard AC300

161.30
157.77
157.21
136.84
133.73
127.41
124.08
121.46
119.14
114.29

21.79
21.17
11.05



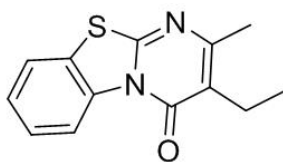
5r



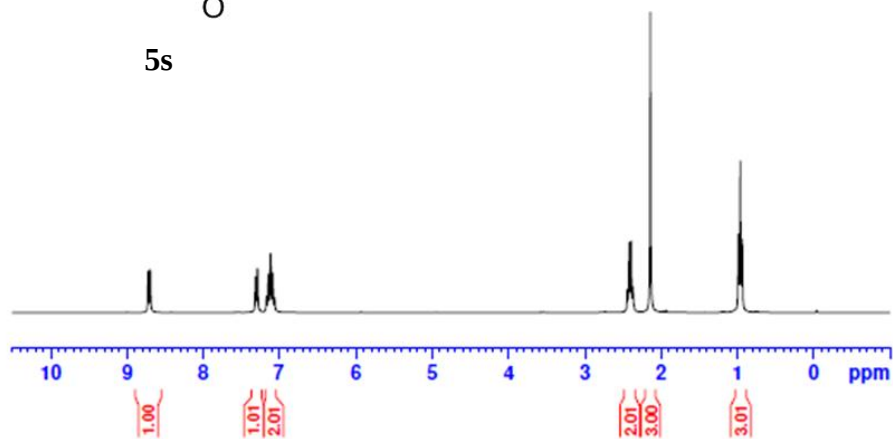
¹H normal range AC300

8.721
8.695
7.315
7.289
7.171
7.149
7.118
7.091
7.067

2.442
2.417
2.392
2.368
2.141
0.986
0.962
0.937



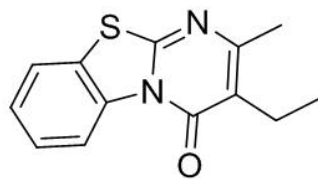
5s



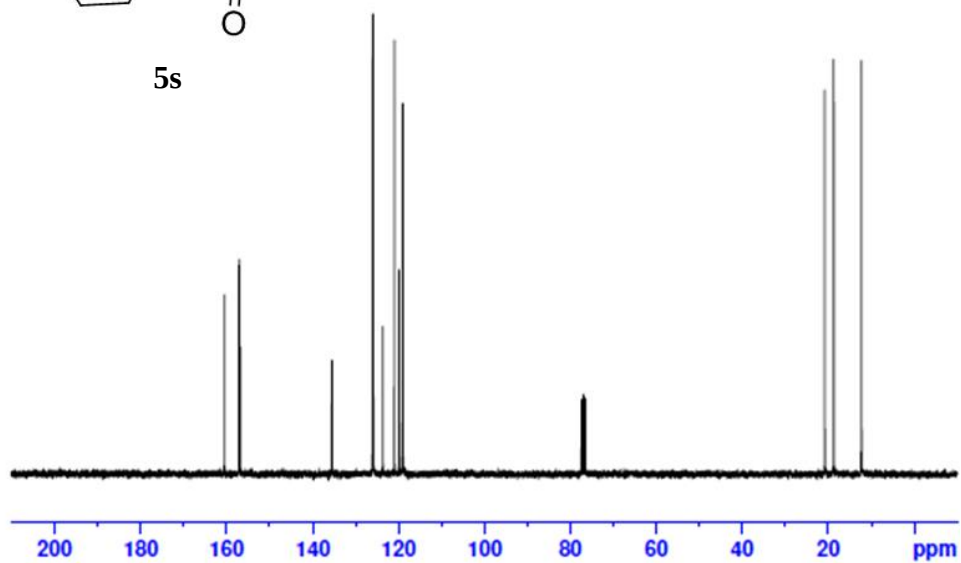
¹³C Standard AC300

160.48
157.06
156.82
135.49
125.99
125.90
123.65
120.97
119.84
119.00

20.82
18.74
12.28



5s

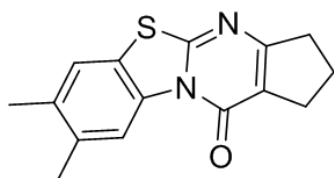


¹H normal range AC300

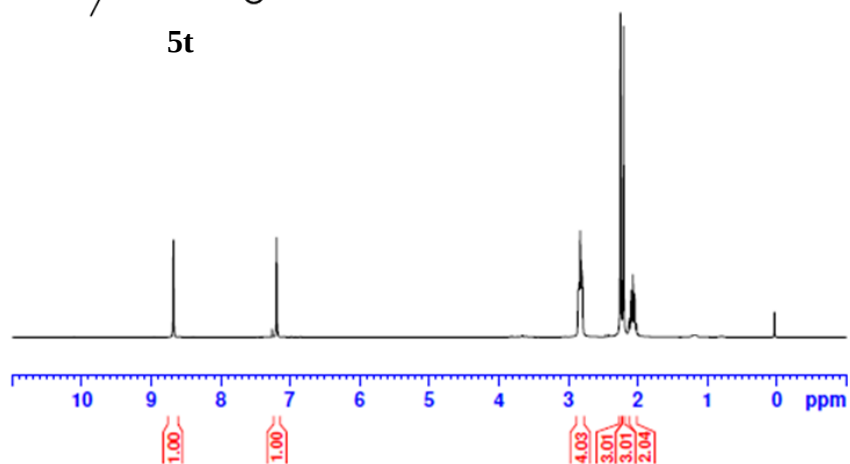
8.680

7.195

2.853
2.828
2.803
2.249
2.206
2.120
2.094
2.069
2.043
2.018



5t

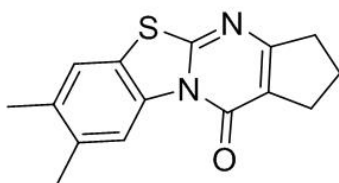


¹³C Standard AC300

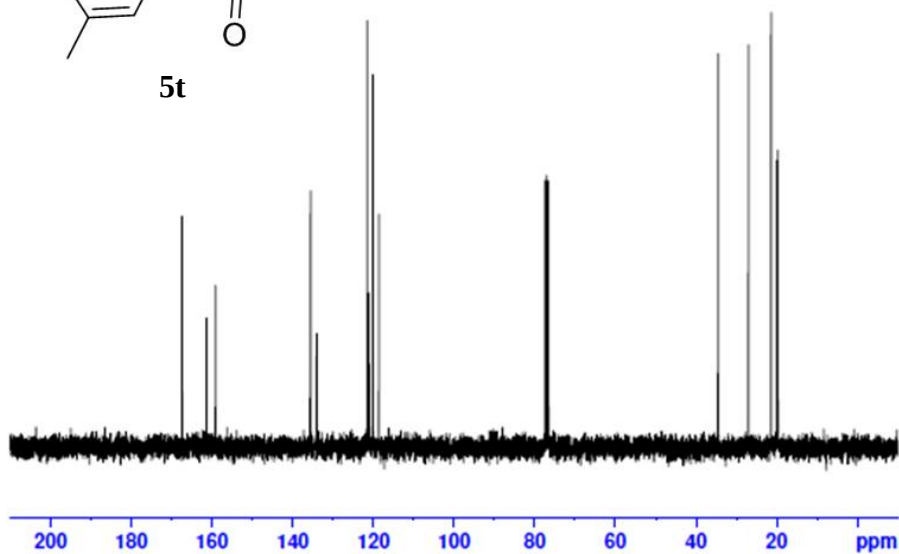
167.38
161.35
159.10

135.65
135.49
134.04
121.50
121.04
120.10
118.61

34.49
27.02
21.39
20.01
19.69



5t

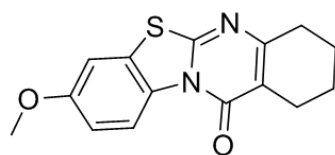


¹H normal range AC300

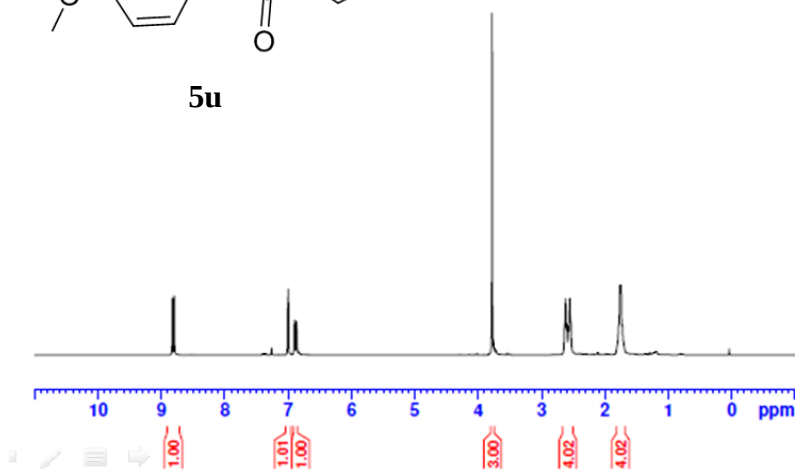
8.827
8.797

6.997
6.903
6.872

3.781
2.635
2.618
2.600
2.574
2.555
2.539
1.786
1.764
1.754
1.745
1.725



5u



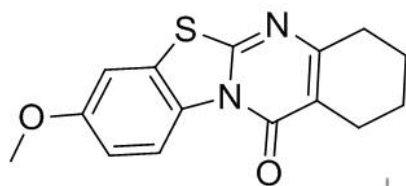
¹³C Standard AC300

160.87
158.77
158.02
157.20

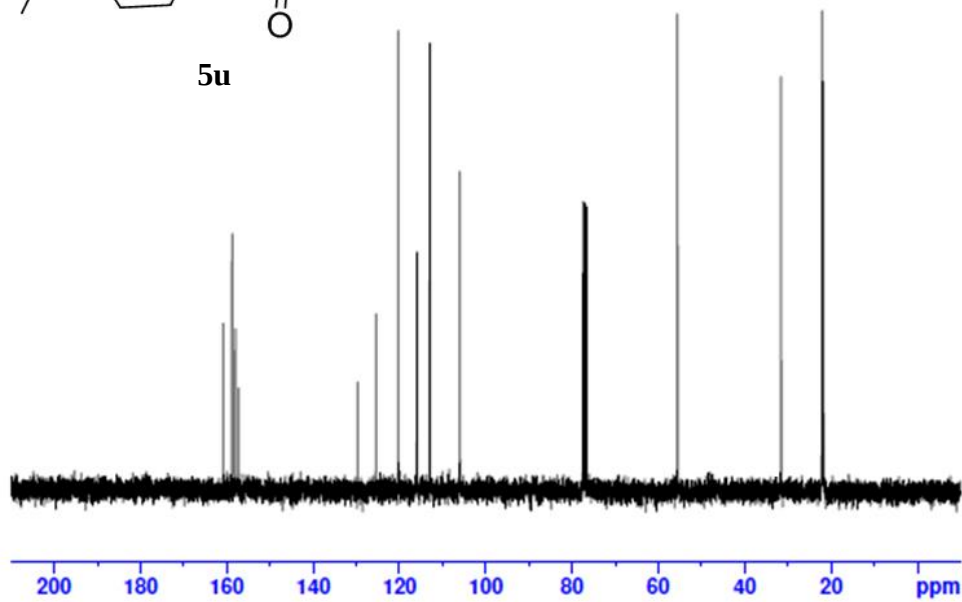
129.69
125.42
120.28
115.94
112.96
105.99

55.56

31.55
22.09
22.05
21.75



5u

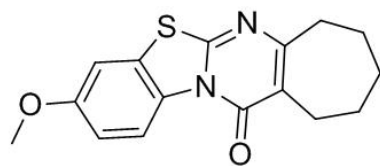


¹H normal range AC300

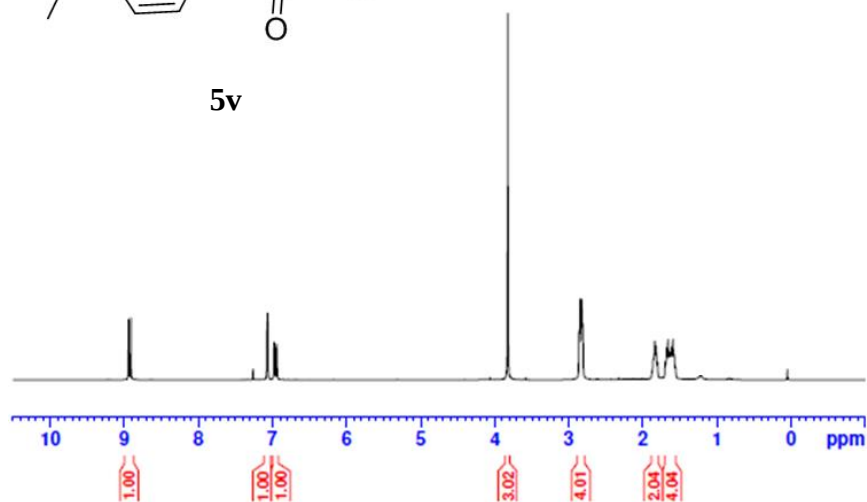
8.942
8.911

7.064
6.978
6.948

3.825
2.862
2.846
2.826
2.810
2.801
1.861
1.841
1.823
1.803
1.700
1.681
1.664
1.646
1.634
1.626
1.614
1.597
1.580
1.560



5v



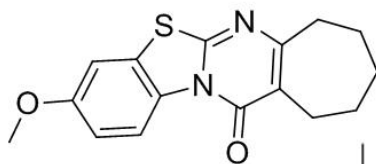
¹³C Standard AC300

164.86
161.14
158.19
157.18

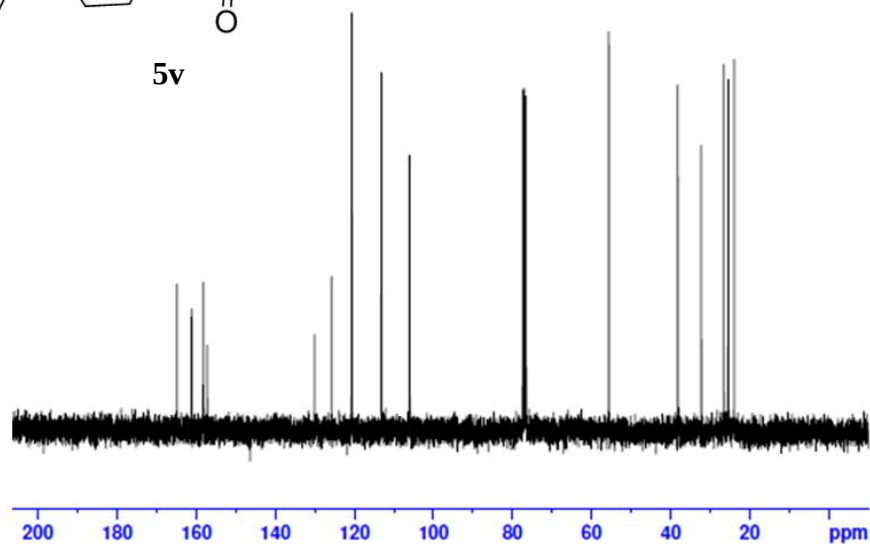
130.06
125.78
120.67
120.54
113.17
106.03

55.64

38.21
32.26
26.53
25.43
23.95



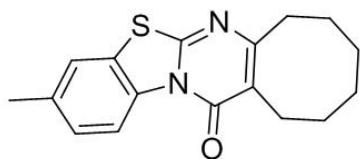
5v



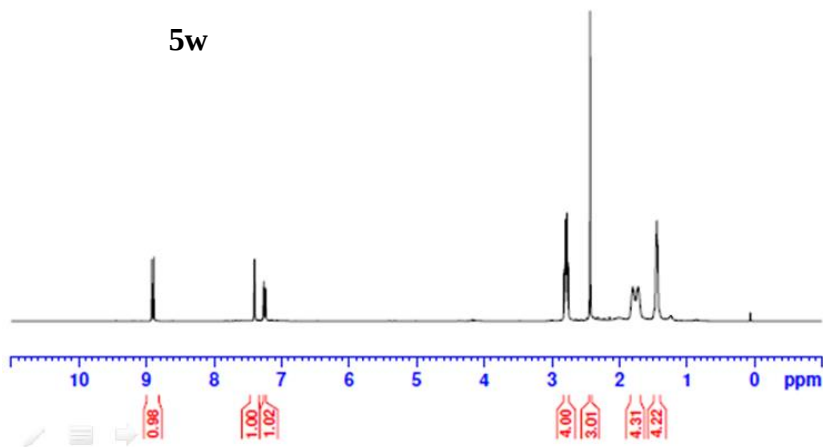
1H normal range AC300

8.919
8.890
7.399
7.268
7.239

2.817
2.797
2.788
2.776
2.755
2.431
1.797
1.757
1.723
1.489
1.453
1.434
1.404



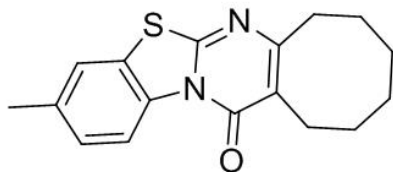
5w



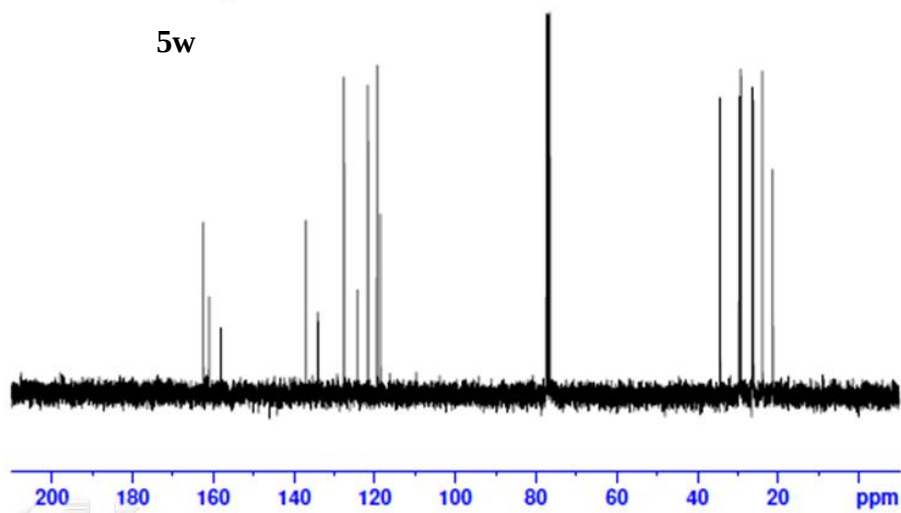
13C Standard AC300

162.42
161.04
158.12
137.00
134.05
127.58
124.26
121.65
119.39
118.54

34.39
29.64
29.20
26.37
26.13
23.91
21.30



5w



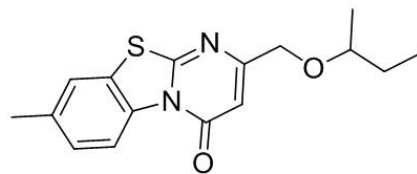
1H normal range AC300

7.658
7.454
7.426
7.399
7.214
7.186

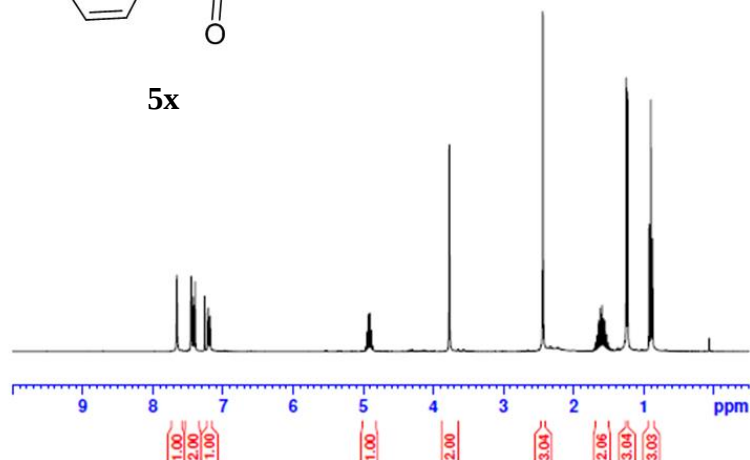
4.966
4.945
4.924
4.903
4.882
4.861

3.772

2.438
1.666
1.643
1.619
1.595
1.577
1.572
1.552
1.527
1.250
1.229
0.823
0.898
0.874



5x



13C Standard AC300

170.51

146.88

140.55

134.78

130.18

130.13

127.02

124.30

112.18

109.73

77.42

76.99

76.57

72.96

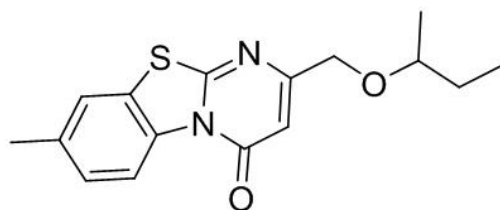
35.39

28.75

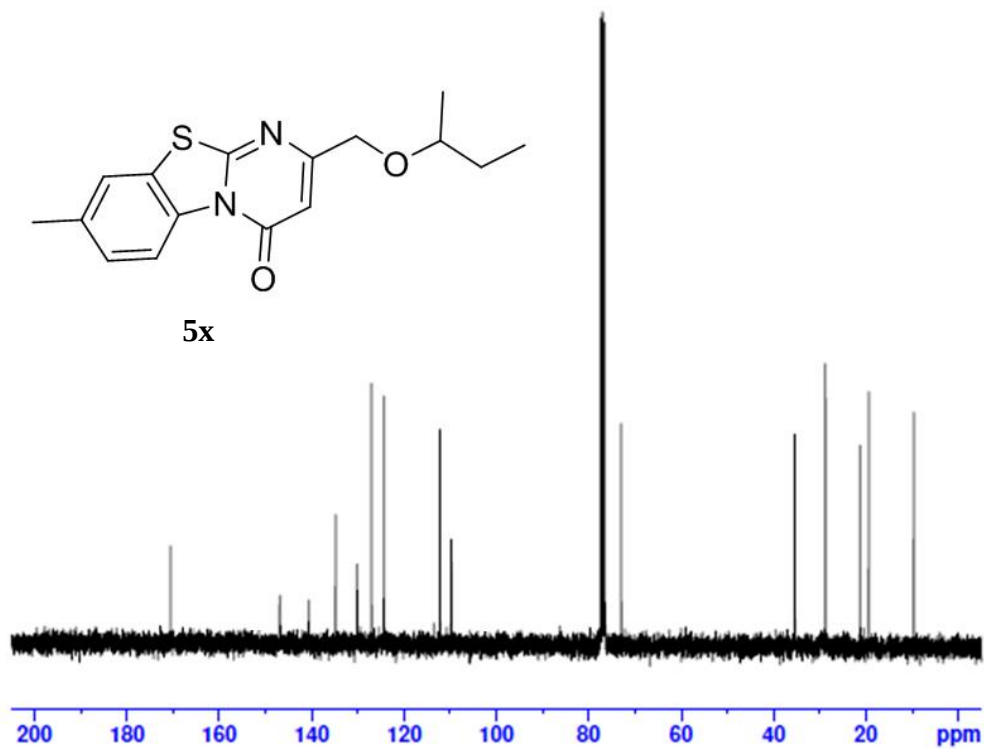
21.27

19.39

9.63

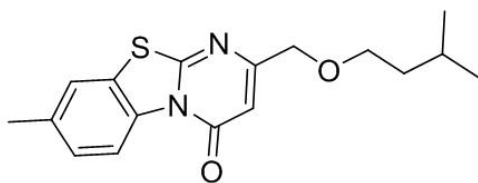


5x

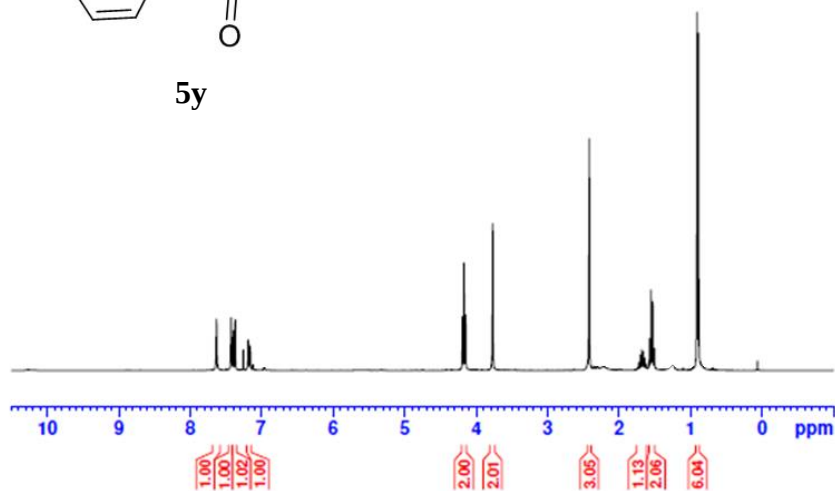


1H normal range AC300

7.632
7.428
7.398
7.371
7.190
7.163
4.192
4.169
4.146
3.769
2.419
1.752
1.726
1.704
1.681
1.659
1.637
1.615
1.573
1.550
1.527
1.505
0.910
0.888

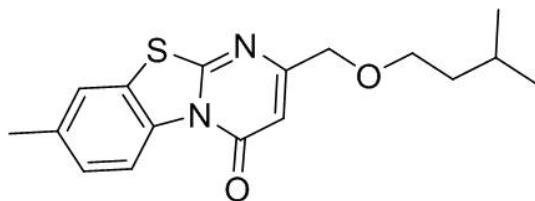


5y



13C Standard AC300

170.91
146.93
140.43
134.71
130.10
130.06
126.95
124.23
112.10
109.71
63.68
37.20
35.14
24.98
22.35
21.20



5y

