Supplementary Material (ESI) for Chemical Communications


# Chemo-/Regioselective Synthesis of 6-Unsubstituted Dihydropyrimidinones, 1,3-Thiazines and Chromones via Novel Variants of Biginelli Reaction

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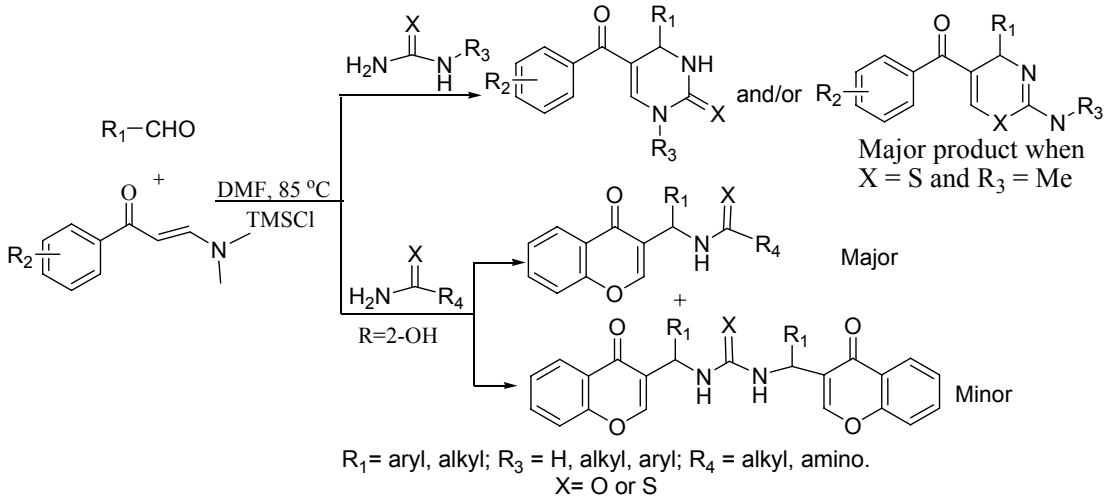
## Contents



**General.** All experiments were carried out at open atmosphere, enaminones used in the experiment were prepared following literature method,[1] all other chemicals were obtained from commercial resource and used without further purification. Organic solvents were all dried by standard procedure prior to use. $^{1}$H and $^{13}$C NMR were recorded in on Bruker AVANCE DMX-500 spectrometry in DMSO-$d_6$ at 500 MHz and 125 MHz, respectively. Chemical shift are reported in ppm ($\delta$) relative to DMSO-$d_6$ (2.50 for $^{1}$H and 40.7 for $^{13}$C spectra). Mass spectra were performed on a Bruker Esquire 3000plus mass spectrometer (Bruker-Franzen Analytik GmbH Breman, Germany) equipped with ESI interface and ion trap analyzer. HRMS were obtained on a Bruker 7-tesla FT-ICR MS equipped with an electrospray source (Billelica, MA, USA). Infrared spectra were obtained on a FTIR spectrometer. Melting point was tested in X-4 apparatus and was not corrected.

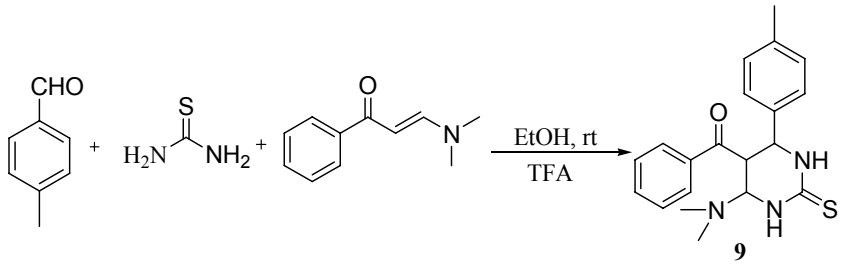
**Synthesis of 6-unsubstituted DHPMs, 1,3-thiazines and 3-substituted chromones** (Scheme 1). Aldehyde 0.3 mmol, enaminone 0.3 mmol and urea/thiourea/amide 0.35




**Scheme 1**

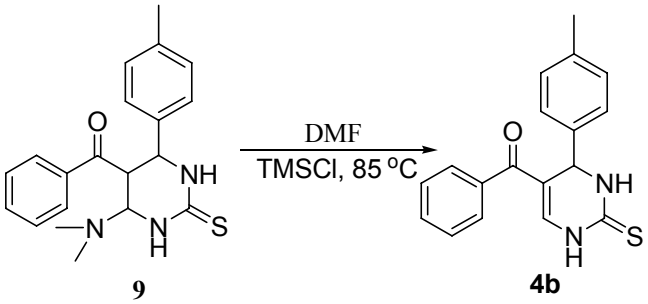
mmol were mixed in 2 mL DMF in a vessel, 0.45 mmol TMSCl was added and the mixture was stirred at 85 $^{o}$C for 10 h. After cooled down to room temperature, 5 mL $H_2O$ was added to the vessel and the mixture was extracted with ethyl acetate (3×10 mL). The combined organic layers were dried overnight with anhydrous $Na_2SO4$. Corresponding products were purified by silica gel chromatography with elution of mixed petroleum ether and ethyl acetate ($V_{PET}$ : $V_{EA}$=3:1).

**Synthesis of intermediate tetrahydropyrimidinone 9** (Scheme 2). Tolualdehyde 0.3 mmol, enaminone 0.3 mmol and thiourea 0.35 mol mixed with 2 mL EtOH in a vessel, 50 mol % TFA was then added and the mixture was stirred at room temperature for 12 h. The solid precipitated form the reaction was filtered and recrystalized in EtOH/DMF ($V_{EtOH}$ : $V_{DMF}$ = 3:1) to give pure product.



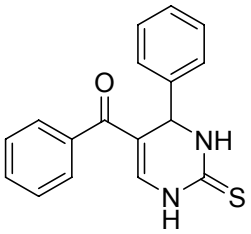

**Scheme 2**

**Synthesis of corresponding DHPM from 9 (Scheme 3).** The purified **9** was subjected to identical conditions as mentioned in standard three-component synthesis to give corresponding DHPM.

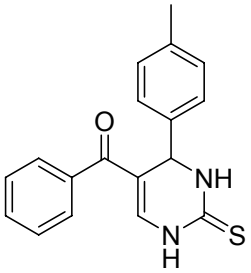



**Scheme 3**

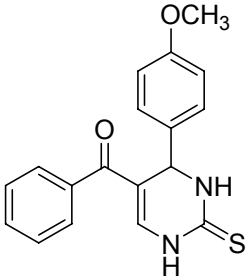
(1) El-Taweel, F. M. A. A.; Elnagdi, M. H. *J. Heterocyclic Chem.* **2001**, *38*, 981.




4-Phenyl-5-phenylmethanone-yl-3,4-dihydropyrimidine-2(1*H*)-thione (**4a**). Pale yellow crystal; m. p. 277-280 $^{o}$C; $^{1}$H NMR (DMSO-$d_6$, 500 MHz) $\delta$ = 10.46 (d, 1H, $J$ = 4.6 Hz), 9.79 (s, 1H), 7.57-7.45 (m, 5H), 7.40-7.29 (m, 5H), 6.88 (d, 1H, $J$ = 5.8 Hz), 5.44 (d, 1H, J=3.3 Hz); $^{13}$C NMR (DMSO-$d_6$, 125 MHz) $\delta$ = 193.0, 175.0, 144.0, 139.3, 138.7, 132.5, 129.9, 129.7, 129.3, 129.0, 127.8, 114.4, 54.7; IR (KBr, cm$^{-1}$): 3323, 3155, 2960, 1652, 1625, 1565, 1470, 1205, 1133, 1031, 892; ESI-MS: m/z 295 ([M+H]$^{+}$); ESI-HRMS: Calcd for $C_{17}H_{14}N_2OSNa$ ([M+Na]$^{+}$), 317.0719; Found, 317.0729.

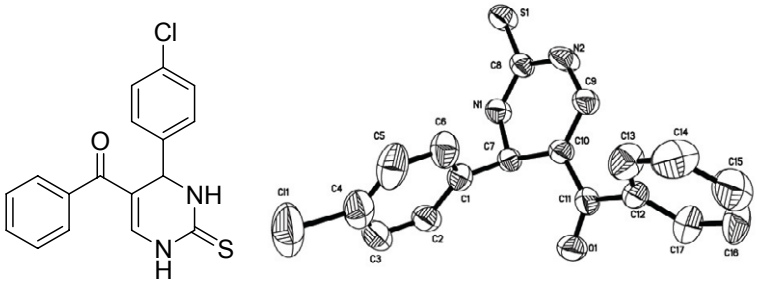



4-(4-Methylphenyl)-5-phenylmethanone-yl-3,4-dihydropyrimidine-2(1*H*)-thione (**4b**). Yellow solid; m. p. 279-281 $^{o}$C; $^{1}$H NMR (DMSO-$d_6$, 500 MHz) $\delta$ = 10.43 (d, 1H, $J$ = 4.5 Hz), 9.75 (s, 1H), 7.55-7.45 (m, 5H), 7.22-7.16 (m, 4H), 6.87 (d, 1H, $J$= 5.6 Hz), 5.40 (d, 1H, $J$ = 3.3 Hz), 2.27 (s, 3H); $^{13}$C NMR (DMSO-$d_6$, 125 MHz) $\delta$ = 193.0, 174.9, 141.2, 139.3, 138.5, 138.3, 132.5, 130.4, 129.7, 129.2, 127.7, 114.6, 54.4, 21.9; IR (KBr, cm$^{-1}$): 3310, 3148, 3060, 2975, 1671, 1620, 1559, 1461, 1204, 1128, 1029; ESI-MS: m/z 309 ([M+H]$^{+}$); ESI-HRMS: Calcd for $C_{18}H_{16}N_2OSNa$ ([M+Na]$^{+}$), 331.0876; Found, 331.0870.

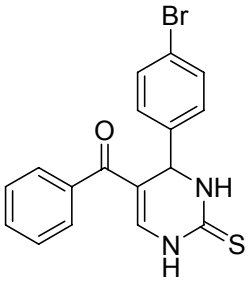



4-(4-Methoxyphenyl)-5-phenylmethanone-yl-3,4-dihydropyrimidine-2(1*H*)-thione (**4c**). Yellow solid; m. p. 267-269 $^{o}$C; $^{1}$H NMR (DMSO-$d_6$, 500 MHz) $\delta$ = 10.42 (d, 1H, $J$ = 4.5 Hz), 9.74 (s, 1H), 7.61-7.46 (m, 5H), 7.26 (d, 2H, $J$ = 8.4 Hz), 6.94-6.92 (m, 2H), 6.88 (d, 1H, $J$ = 5.6 Hz), 5.40 (d, 1H, $J$ = 2.9 Hz), 3.73 (s, 3H); $^{13}$C NMR (DMSO-$d_6$, 125 MHz) $\delta$ = 193.06, 174.81, 160.07, 139.34, 138.48, 136.27, 132.50, 129.70, 129.27, 129.11, 115.21, 114.67, 56.33, 54.11; IR (KBr, cm$^{-1}$): 3274, 3158, 3101, 2997, 1653, 1622, 1574, 1510, 1475, 1203, 1138, 1032; ESI-MS: m/z 325 ([M+H]$^{+}$); ESI-HRMS: Calcd for $C_{18}H_{16}N_2O_2SNa$ ([M+Na]$^{+}$), 347.0825; Found,

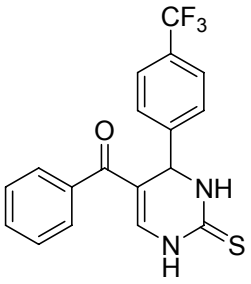
347.0820.




4-(4-Chlorophenyl)-5-phenylmethanone-yl-3,4-dihydropyrimidine-2(1*H*)-thione (**4d**). Yellow solid; m. p. 269-271 $^{o}$C; $^{1}$H NMR (DMSO-$d_6$, 500 MHz) $\delta$ = 10.51 (d, 1H, $J$ = 4.8 Hz), 9.81 (s, 1H), 7.57-7.44 (m, 7H), 7.34 (d, 2H, $J$ = 5.6 Hz), 6.89 (d, 1H, $J$= 5.6 Hz), 5.44 (d, 1H, $J$ = 3.2 Hz); ); $^{13}$C NMR (DMSO-$d_6$, 125 MHz) $\delta$ = 192.9, 175.0, 142.9, 139.2, 138.9, 133.6, 132.5, 129.9, 129.8, 129.7, 129.3, 114.0, 54.1; IR (KBr, cm$^{-1}$): 3389, 3170, 3081, 2979, 1660, 1627, 1555, 1470, 1260, 1204, 1089, 1014; ESI-MS: m/z 329 ([M+H]$^{+}$); ESI-HRMS: Calcd for $C_{17}H_{14}ClN_2OS$ ([M+H]$^{+}$), 329.0510; Found, 329.0516.

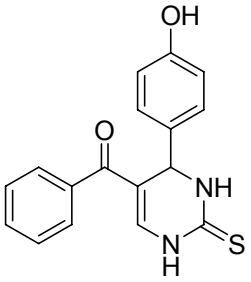



4-(4-Bromophenyl)-5-phenylmethanone-yl-3,4-dihydropyrimidine-2(1*H*)-thione (**4e**). Pale yellow solid; m. p. 282-283 $^{o}$C; $^{1}$H NMR (DMSO-$d_6$, 500 MHz) $\delta$ = 10.51 (d, 1H, $J$ = 4.6 Hz), 9.80 (s, 1H), 7.59-7.45 (m, 7H), 7.29 (d, 2H, $J$ = 8.4 Hz), 6.89 (d, 1H, $J$ = 5.4 Hz), 5.43 (d, 1H, $J$ = 3.2 Hz); $^{13}$C NMR (DMSO-$d_6$, 125 MHz) $\delta$ = 192.9, 175.0, 143.3, 139.2, 138.9, 132.8, 132.5, 130.1, 129.8, 129.3, 122.2, 113.9, 54.2; IR (KBr, cm$^{-1}$): 3367, 3150, 2969, 1661, 1630, 1558, 1472, 1360, 1201, 1131, 1045; ESI-MS: m/z 373 ([M+H]$^{+}$); ESI-HRMS: Calcd for $C_{17}H_{13}BrN_2OSNa$ ([M+Na]$^{+}$), 394.9824; Found, 394.9842.

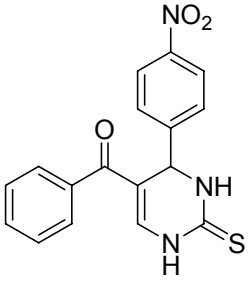



4-(4-Trifluoromethylphenyl)-5-phenylmethanone-yl-3,4-dihydropyrimidine-2(1*H*)-thi one (**4f**). Yellow solid; m. p. 267-270 $^{o}$C; $^{1}$H NMR (DMSO-$d_6$, 500 MHz) $\delta$ = 10.57 (d, 1H, $J$ = 4.6 Hz), 9.85 (s, 1H), 7.77 (d, 2H, $J$ = 8.2 Hz), 7.56-7.45 (m, 7H), 6.93 (d, 1H, $J$ = 5.8 Hz), 5.54 (d, 1H, $J$ = 3.2 Hz); $^{13}$C NMR (DMSO-$d_6$, 125 MHz) $\delta$ = 192.9,

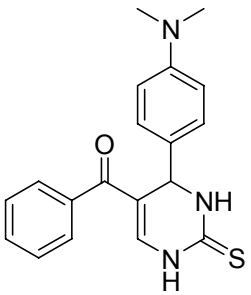
175.2, 148.3, 139.2, 139.1, 132.6, 129.7, 129.4, 128.8, 126.9, 126.8, 113.7, 54.4; IR (KBr, $cm^{-1}$): 3410, 3167, 3084, 1993, 1661, 1628, 1558, 1469, 1365, 1326, 1260, 1204, 1129, 1068, 1017; ESI-MS: m/z 363 ($[M+H]^+$); ESI-HRMS: Calcd for $C_{18}H_{14}F_3N_2OS$ ($[M+H]^+$), 363.0773; Found, 363.0776.




4-(4-Hydroxylphenyl)-5-phenylmethanone-yl-3,4-dihydropyrimidine-2(1*H*)-thione (**4g**). Yellow crystal; m. p. 269-271 $^oC$; $^1H$ NMR (DMSO-$d_6$, 500 MHz) $\delta$ = 10.36 (d, 1H, $J$ = 5.4 Hz), 9.69 (s, 1H), 9.44 (s, 1H), 7.55-7.45 (m, 5H), 7.13 (d, 2H, $J$ = 8.5 Hz), 6.84 (d, 1H, $J$ = 6.0 Hz), 6.73 (d, 2H, $J$ = 8.5 Hz), 5.33 (d, 1H, $J$ = 3.2 Hz); $^{13}C$ NMR (DMSO-$d_6$, 125 MHz) $\delta$ = 192.9, 174.6, 158.2, 139.4, 138.2, 134.6, 132.4, 129.6, 129.2, 129.1, 116.4, 114.8, 54.1; IR (KBr, $cm^{-1}$): 3374, 3183, 3007, 1660, 1629, 1563, 1446, 1206, 1134, 1023; ESI-MS: m/z 311 ($[M+H]^+$); ESI-HRMS: Calcd for $C_{17}H_{15}N_2O_2S$ ($[M+H]^+$), 311.0849; Found, 311.0848.

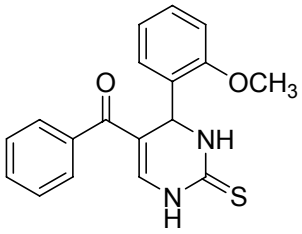



4-(4-Nitrophenyl)-5-phenylmethanone-yl-3,4-dihydropyrimidine-2(1*H*)-thione (**4h**). Colorless crystal; m. p. 288-291 $^oC$; $^1H$ NMR (DMSO-$d_6$, 500 MHz) $\delta$ = 10.62 (s, 1H), 9.88 (d, 1H, $J$ = 2.4 Hz), 8.26 (d, 2H, $J$ = 8.7 Hz), 7.61-7.45 (m, 7H), 6.95 (s, 1H), 5.58 (d, 1H, $J$ = 3.0 Hz); $^{13}C$ NMR (DMSO-$d_6$, 125 MHz) $\delta$ = 192.9, 175.2, 150.9, 148.2, 139.3, 139.0, 132.6, 129.7, 129.3, 125.2, 113.5, 54.4; IR (KBr, $cm^{-1}$): 3318, 3075, 2981, 1658, 1625, 1578, 1476, 1362, 1201, 1130, 1040; ESI-MS: m/z 340 ($[M+H]^+$); ESI-HRMS: Calcd for $C_{17}H_{14}N_3O_3S$ ($[M+H]^+$), 340.0750; Found, 340.0720.

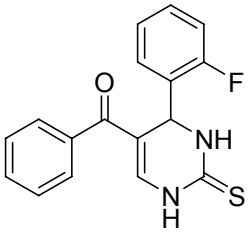



4-(4-*N,N*-Dimethylaminophenyl)-5-phenylmethanone-yl-3,4-dihydropyrimidine-2(1*H*)-thione (**4i**). Brown solid; m. p. 266-269 $^oC$; $^1H$ NMR (DMSO-$d_6$, 500 MHz) $\delta$ =

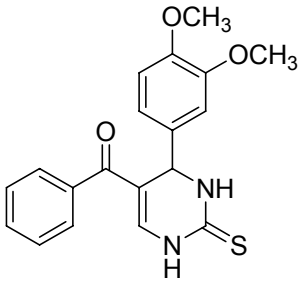
10.34 (d, 1H, $J$ = 4.7 Hz), 9.67 (s, 1H), 7.55-7.47 (m, 5H), 7.13 (d, 2H, $J$ = 8.6 Hz), 6.84 (d, 1H, $J$ = 5.5 Hz), 6.68 (d, 2H, $J$ = 8.6 Hz), 5.32 (d, 1H, $J$ = 3.0 Hz), 2.86 (s, 6H); $^{13}$C NMR (DMSO-$d_6$, 125 MHz) $\delta$= 193.1, 174.6, 151.2, 139.4, 138.1, 132.4, 131.7, 129.7, 129.2, 128.6, 114.9, 113.6, 54.1, 41.3; IR (KBr, cm$^{-1}$): 3311, 3173, 3111, 2993, 2926, 1652, 1628, 1571, 1475, 1199, 1014; ESI-MS: m/z 338 ([M+H]$^+$); ESI-HRMS: Calcd for $C_{19}H_{20}N_3OS$ ([M+H]$^+$), 338.1322; Found, 338.1321.




4-(2-Methoxyphenyl)-5-phenylmethanone-yl-3,4-dihydropyrimidine-2(1*H*)-thione (**4j**). Colorless crystal; m. p. 263-265 $^o$C; $^1$H NMR (DMSO-$d_6$, 500 MHz) $\delta$= 10.34 (d, 1H, $J$ = 5.0 Hz), 9.37 (s, 1H), 7.56-7.47 (m, 5H), 7.28-7.19 (m, 2H), 7.05-6.92 (m, 2H), 6.85 (d, 1H, $J$ = 5.6 Hz), 5.70 (d, 1H, $J$ = 3.0 Hz), 3.81 (s, 3H); $^{13}$C NMR (DMSO-$d_6$, 125 MHz) $\delta$= 192.8, 175.1, 158.2, 139.4, 138.7, 132.4, 131.0, 130.5, 129.6, 129.4, 129.2, 121.5, 113.4, 112.7, 56.8, 50.8; IR (KBr, cm$^{-1}$): 3316, 3155, 2957, 1661, 1623, 1558, 1481, 1205, 1035; ESI-MS: m/z 325 ([M+H]$^+$); ESI-HRMS: Calcd for $C_{18}H_{17}N_2O_2S$ ([M+H]$^+$), 325.1005; Found, 325.1004.

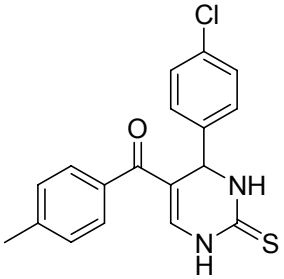



4-(2-Fluorophenyl)-5-phenylmethanone-yl-3,4-dihydropyrimidine-2(1*H*)-thione (**4k**). Yellow solid; m. p. 268-271 $^o$C; $^1$H NMR (DMSO-$d_6$, 500 MHz) $\delta$ = 10.48 (d, 1H, $J$ = 5.4 Hz), 9.73 (s, 1H), 7.55-7.35 (m, 7H), 7.22-7.18 (m, 2H), 6.89 (d, 1H, $J$ = 5.8 Hz), 5.67 (d, 1H, $J$ = 2.6 Hz); $^{13}$C NMR (DMSO-$d_6$, 125 MHz) $\delta$ = 192.8, 174.9, 139.2, 138.9, 132.6, 131.3, 131.2, 130.8, 129.7, 129.3, 125.9, 117.0, 116.8, 113.1, 49.9; IR (KBr, cm$^{-1}$): 3321, 3161, 2960, 1652, 1624, 1560, 1438, 1351, 1204, 1046; ESI-MS: m/z 313 ([M+H]$^+$); ESI-HRMS: Calcd for $C_{17}H_{14}FN_2OS$ ([M+H]$^+$), 313.0805; Found, 313.0806.

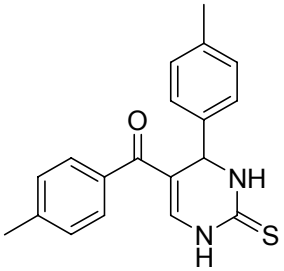



4-(3,4-Dimethoxyphenyl)-5-phenylmethanone-yl-3,4-dihydropyrimidine-2(1*H*)-thion e (**4l**). Pale yellow solid; m. p. 235-237 $^o$C; $^1$H NMR (DMSO-$d_6$, 500 MHz) $\delta$ = 10.41 (d, 1H, $J$ = 4.6 Hz), 9.72 (s, 1H), 7.59-7.46 (m, 5H), 6.95-6.88 (m, 3H), 6.82 (d, 1H, $J$

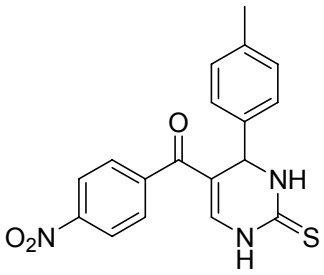
= 8.2 Hz), 5.40 (d, 1H, *J* = 2.9 Hz), 3.74 (s, 3H), 3.73 (s, 3H); $^{13}$C NMR (DMSO-$d_6$, 125 MHz) $\delta$ =193.1, 174.8, 152.5, 149.7, 139.4, 138.7, 136.4, 132.5, 129.7, 129.3, 119.7, 114.4, 113.1, 111.9, 56.8, 56.7, 54.2; IR (KBr, cm$^{-1}$): 3316, 3174, 2981, 1661, 1628, 1561, 1481, 1362, 1205, 1167, 1051; ESI-MS: m/z 355 ([M+H]$^+$); ESI-HRMS: Calcd for $C_{19}H_{19}N_2O_3S$ ([M+H]$^+$), 355.1111; Found, 355.1112.




4-(4-Chlorophenyl)-5-(4-methylphenyl)-methanone-yl-3,4-dihydropyrimidine-2(1*H*)-thione (**4m**). Yellow solid; m.p. 277-279 $^o$C; $^1$H NMR (DMSO-$d_6$, 500 MHz) $\delta$ = 10.49 (d, 1H, *J* = 4.8 Hz), 9.76 (s, 1H), 7.45-7.41 (m, 4H), 7.33 (d, 2H, *J* = 8.4 Hz), 7.27 (d, 2H, *J* = 7.8 Hz), 6.90 (d, 1H, *J* = 5.6 Hz), 5.44 (d, 1H, *J* = 3.1 Hz), 2.35 (s, 3H); $^{13}$C NMR (DMSO-$d_6$, 125 MHz) $\delta$= 192.7, 175.1, 143.0, 142.7, 138.4, 136.4, 133.6, 130.2, 129.9, 129.8, 129.4, 114.1, 54.2, 22.2; IR (KBr, cm$^{-1}$): 3312, 3161, 2985, 2912, 1662, 1620, 1554, 1468, 1204, 1046; ESI-MS: m/z 343 ([M+H]$^+$); ESI-HRMS: Calcd for $C_{18}H_{16}ClN_2OS$ ([M+H]$^+$), 343.0666; Found, 343.0665.

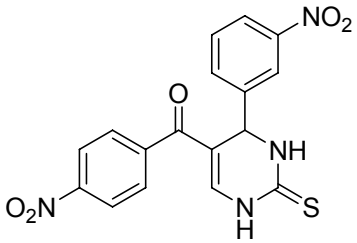



4-(4-Methylphenyl)-5-(4-methylphenyl)-methanone-yl-3,4-dihydropyrimidine-2(1*H*)-thione (**4n**). Yellow solid; m.p. 279-281 $^o$C; $^1$H NMR (DMSO-$d_6$, 500 MHz) $\delta$ = 10.39 (d, 1H, *J* = 5.2 Hz), 9.7 (s, 1H), 7.41 (d, 2H, *J* = 7.9 Hz), 7.27 (d, 2H, *J* = 7.9 Hz), 7.21-7.15 (m, 4H), 6.86 (d, 1H, *J* = 5.6 Hz ), 5.40 (d, 1H, *J* = 3.2 Hz), 2.27 (s, 3H), 2.08 (s, 3H); $^{13}$C NMR (DMSO-$d_6$, 125 MHz) $\delta$ = 192.7, 174.9, 142.6, 141.2, 138.2, 138.0, 136.5, 130.3, 130.2, 129.4, 127.7, 114.6, 54.4, 22.2, 21.8; IR (KBr, cm$^{-1}$): 3334, 3154, 2989, 1649, 1622, 1569, 1472, 1365, 1205, 1180, 1032; ESI-MS: m/z 323 ([M+H]$^+$); ESI-HRMS: Calcd for $C_{19}H_{19}N_2OS$ ([M+H]$^+$), 323.1213; Found, 323.1215.

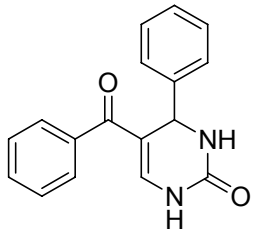



4-(4-Methylphenyl)-5-(4-nitrophenyl)-methanone-yl-3,4-dihydropyrimidine-2(1*H*)-thi

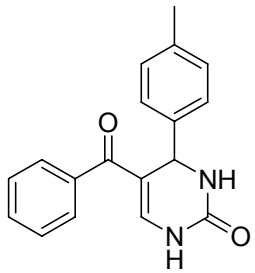
one (**4o**). Yellow solid; m.p. 237-240 °C; $^1$H NMR (DMSO-$d_6$, 500 MHz) $\delta$ = 10.63 (d, 1H, $J$ = 4.5 Hz), 9.84 (s, 1H), 8.28 (d, 2H, $J$ = 8.6 Hz), 7.74 (d, 2H, $J$ = 8.6 Hz), 7.23-7.17 (m, 4H), 6.91 (d, 1H, $J$ = 5.7 Hz), 5.40 (d, 1H, $J$ = 3.0 Hz), 2.28 (s, 3H); $^{13}$C NMR (DMSO-$d_6$, 125 MHz) $\delta$ = 191.5, 175.0, 149.9, 145.0, 141.0, 140.0, 138.4, 130.6, 130.4, 127.8, 124.9, 114.4, 54.2, 21.9; IR (KBr, cm$^{-1}$): 3321, 3159, 2971, 1663, 1625, 1557, 1468, 1360, 1204, 1128, 1016; ESI-MS: m/z 354 ([M+H]$^+$); ESI-HRMS: Calcd for $C_{18}H_{16}N_3O_3S$ ([M+H]$^+$), 354.0907; Found, 354.0904.




4-(3-Nitrophenyl)-5-(4-nitrophenyl)-methanone-yl-3,4-dihydropyrimidine-2(1*H*)-thione (**4p**). Pale orange solid; m.p. 273-275 °C; $^1$H NMR (DMSO-$d_6$, 500 MHz) $\delta$ = 10.83 (d, 1H, $J$ = 5.4 Hz), 9.98 (s, 1H), 8.31-8.27 (m, 2H), 8.18-8.17 (t, 2H, $J$ = 2.1 Hz), 7.86-7.69 (m, 4H), 7.01 (d, 1H, $J$ = 5.8 Hz), 5.61 (d, 1H, $J$ = 3.0 Hz); ); $^{13}$C NMR (DMSO-$d_6$, 125 MHz) $\delta$ = 191.4, 175.2, 150.0, 149.1, 145.8, 144.7, 140.8, 134.6, 131.7, 130.7, 129.6, 124.8, 122.7, 113.2, 54.1; IR (KBr, cm$^{-1}$): 3361, 3160, 2987, 1664, 1628, 1556, 1470, 1360, 1205, 1043; ESI-MS: m/z 385 ([M+H]$^+$); ESI-HRMS: Calcd for $C_{17}H_{13}N_4O_5S$ ([M+H]$^+$), 385.0601; Found, 385.0595.

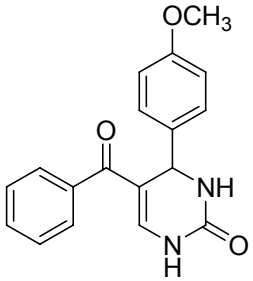



4-Phenyl-5-phenylmethanone-yl-3,4-dihydropyrimidine-2(1*H*)-one (**4q**). Yellow solid; m. p. 281-284 °C; $^1$H NMR (DMSO-$d_6$, 500 MHz) $\delta$ = 9.37 (br, 1H), 7.86 (s, 1H), 7.85-7.43 (m, 5H), 7.35-7.27 (m, 4H), 7.28-7.25 (m, 1H), 7.03 (s, 1H), 5.43 (d, 1H, $J$ = 2.9 Hz); $^{13}$C NMR (DMSO-$d_6$, 125 MHz) $\delta$ = 192.7, 152.5, 145.3, 143.1, 139.8, 132.0, 129.6, 129.5, 129.2, 128.6, 127.6, 113.6, 54.5; IR (KBr, cm$^{-1}$): 3352, 3207, 1684, 1665, 1620, 1442, 1372, 1210, 1160, 903; ESI-MS: m/z 279 ([M+H]$^+$); ESI-HRMS: Calcd for $C_{17}H_{15}N_2O_2$ ([M+H]$^+$), 279.1128; Found, 279.1130.

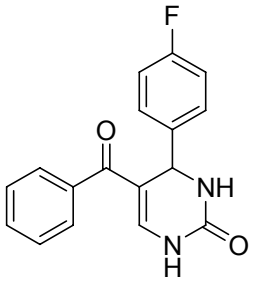



4-(4-Methylphenyl)-5-phenylmethanone-yl-3,4-dihydropyrimidine-2(1*H*)-one (**4r**). Yellow solid; m. p. 230-233 °C; $^1$H NMR (DMSO-$d_6$, 500 MHz) $\delta$ = 9.29 (d, 1H, $J$ = 5.1 Hz), 7.82 (s, 1H), 7.54-7.43 (m, 5H), 7.23 (d, 2H, $J$ = 7.9 Hz), 7.15 (d, 2H, $J$ = 7.9

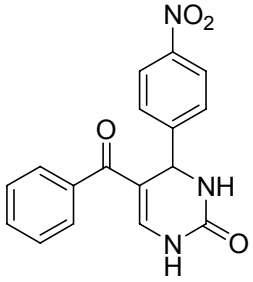
Hz), 6.99 (d, 1H, *J* = 6.0 Hz), 5.39 (d, 1H, *J* = 2.9 Hz), 2.27 (s, 3H); $^{13}$C NMR (DMSO-$d_6$, 125 MHz) $\delta$ = 192.8, 152.4, 142.7, 142.4, 139.8, 137.8, 132.1, 130.2, 129.6, 129.2, 127.5, 113.9, 54.2, 21.8; IR (KBr, cm$^{-1}$): 3332, 3210, 3090, 2924, 1692, 1655, 1621, 1440, 1369, 1216, 1179, 902; ESI-MS: m/z 293 ([M+H]$^+$); ESI-HRMS: Calcd for $C_{18}H_{17}N_2O_2$ ([M+H]$^+$), 293.1285; Found, 293.1282.




4-(4-Methoxylphenyl)-5-phenylmethanone-yl-3,4-dihydropyrimidine-2(1*H*)-one (**4s**). Yellow solid; m. p. 230-233 $^o$C; $^1$H NMR (DMSO-$d_6$, 500 MHz) $\delta$ = 9.29 (d, 1H, *J* = 4.8 Hz), 7.80 (s, 1H), 7.52-7.45 (m, 5H), 7.26 (d, 2H, *J* = 8.6 Hz), 6.99 (d, 1H, *J* = 6.0 Hz), 6.90 (d, 2H, *J* = 8.6 Hz), 5.38 (d, 1H, *J* = 2.8 Hz), 3.73 (s, 3H); $^{13}$C NMR (DMSO-$d_6$, 125 MHz) $\delta$ = 192.7, 159.7, 152.4, 142.6, 139.8, 137.4, 132.8, 129.6, 129.2, 128.8, 115.0, 113.9, 56.2, 53.9; IR (KBr, cm$^{-1}$): 3337, 3213, 3089, 2930, 1693, 1654, 1612, 1443, 1370, 1217, 1178, 1058, 905; ESI-MS: m/z 309 ([M+H]$^+$); ESI-HRMS: Calcd for $C_{18}H_{16}N_2O_3Na$ ([M+Na]$^+$), 331.1053; Found, 331.1049.

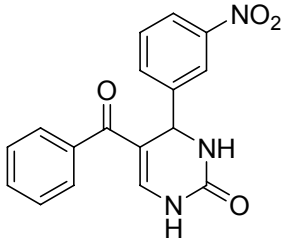



4-(4-Fluorophenyl)-5-phenylmethanone-yl-3,4-dihydropyrimidine-2(1*H*)-one (**4t**). Yellow solid; m. p. 310-312 $^o$C; $^1$H NMR (DMSO-$d_6$, 500 MHz) $\delta$ = 9.37 (d, 1H, *J* = 4.2 Hz), 7.87 (s, 1H), 7.55-7.36 (m, 7H), 7.19-7.16 (m, 2H), 7.03 (d, 1H, *J* = 6.0 Hz), 5.44 (d, 1H, *J* = 2.8 Hz); $^{13}$C NMR (DMSO-$d_6$, 125 MHz) $\delta$ = 192.7, 152.2, 143.0, 139.7, 132.1, 129.7, 129.6, 129.5, 129.2, 116.5, 116.3, 113.4, 53.9; IR (KBr, cm$^{-1}$): 3289, 3142, 1682, 1651, 1613, 1446, 1368, 1209, 1160, 906; 11ESI-MS: m/z 297 ([M+H]$^+$); ESI-HRMS: Calcd for $C_{17}H_{14}FN_2O_2$ ([M+H]$^+$), 297.1032; Found, 297.1034.

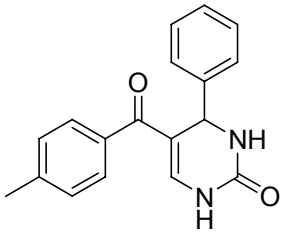



4-(4-Nitrophenyl)-5-phenylmethanone-yl-3,4-dihydropyrimidine-2(1*H*)-one (**4u**). Yellow solid; m. p. 251-253 $^o$C; $^1$H NMR (DMSO-$d_6$, 500 MHz) $\delta$ = 9.50 (d, 1H, *J* =

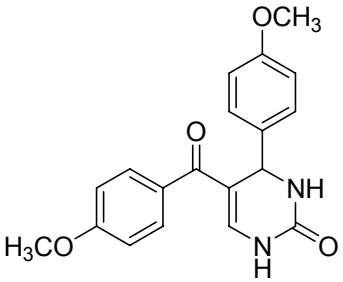
5.8 Hz), 8.24 (d, 2H, *J* = 8.6 Hz), 8.02 (s, 1H), 7.63 (d, 2H, *J* = 8.6 Hz), 7.55-7.45 (m, 5H), 7.08 (d, 1H, *J* = 6.1 Hz), 5.58 (d, 1H, *J* = 2.8 Hz); $^{13}$C NMR (DMSO-$d_6$, 125 MHz) $\delta$ = 192.6, 152.3, 152.0, 148.0, 143.6, 139.5, 132.2, 129.6, 129.2, 129.1, 125.0, 112.6, 54.3; IR (KBr, cm$^{-1}$): 3339, 3212, 3084, 2929, 1696, 1656, 1611, 1445, 1373, 1350, 1213, 1156, 1086, 902; ESI-MS: m/z 324 ([M+H]$^+$); ESI-HRMS: Calcd for $C_{17}H_{14}N_3O_4$ ([M+H]$^+$), 324.0979; Found, 324.0981.




4-(3-Nitrophenyl)-5-phenylmethanone-yl-3,4-dihydropyrimidine-2(1*H*)-one (**4v**). Yellow solid; m. p. 287-290 $^o$C; $^1$H NMR (DMSO-$d_6$, 500 MHz) $\delta$ = 9.50 (d, 1H, *J* = 5.4 Hz), 8.15-8.11 (m, 2H), 7.99 (s, 1H), 7.80 (d, 1H, *J* = 7.7 Hz), 7.65-7.32 (m, 1H), 7.48-7.42 (m, 5H), 7.08 (d, 1H, *J* = 6.0 Hz), 5.56 (d, 1H, *J* = 2.8 Hz); $^{13}$C NMR (DMSO-$d_6$, 125 MHz) $\delta$ = 192.7, 152.0, 149.0, 147.3, 143.8, 139.5, 134.4, 132.2, 131.5, 129.6, 129.2, 123.7, 122.4, 112.6, 54.2; IR (KBr, cm$^{-1}$): 3358, 3210, 3096, 2932, 1693, 1657, 1617, 1532, 1445, 1355, 1212, 1153, 1091, 905; ESI-MS: m/z 324 ([M+H]$^+$); ESI-HRMS: Calcd for $C_{17}H_{14}N_3O_4$ ([M+H]$^+$), 324.0979; Found, 324.0979.

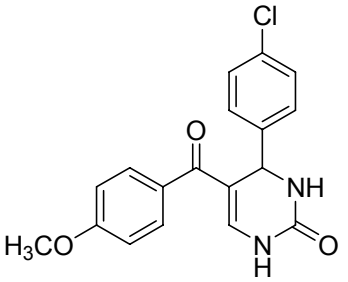



4-phenyl-5-(4-Methylphenyl)methanone-yl-3,4-dihydropyrimidine-2(1*H*)-one (**4w**). Yellow solid; m. p. 311-313 $^o$C; $^1$H NMR (DMSO-$d_6$, 500 MHz) $\delta$ = 9.31 (d, 1H, *J* = 5.2 Hz), 7.84 (s, 1H), 7-40-7.23 (m, 9H), 7.01 (d, 1H, *J* = 6.0 Hz), 5.42 (d, 1H, *J* = 3.0 Hz), 2.34 (s, 3H); $^{13}$C NMR (DMSO-$d_6$, 125 MHz) $\delta$ = 192.5, 152.4, 145.3, 142.3, 142.1, 137.0, 130.0, 129.6, 129.3, 128.6, 127.6, 113.7, 54.5, 22.1; IR (KBr, cm$^{-1}$): 3399, 3204, 3106, 2957, 1689, 1661, 1623, 1446, 1371, 1220, 1176, 1154, 902; ESI-MS: m/z 293 ([M+H]$^+$); ESI-HRMS: Calcd for $C_{18}H_{17}NO_2$ ([M+H]$^+$), 293.1285; Found, 293.1286.

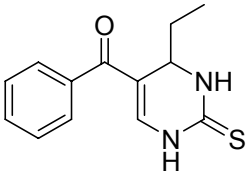



4-(4-Methoxyphenyl)-5-(4-methoxylphenyl)methanone-yl-3,4-dihydropyrimidine-2(1*H*)-one (**4x**). Orange solid; m. p. 254-256 $^o$C; $^1$H NMR (DMSO-$d_6$, 500 MHz) $\delta$ = 9.23 (d, 1H, *J* = 5.3 Hz), 7.74 (s, 1H), 7.49 (d, 2H, *J* = 8.6 Hz), 7.25 (d, 2H, *J* = 8.6

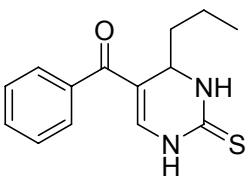
Hz), 7.01-6.98 (m, 3H), 6.89 (d, 2H, $J$ = 8.6 Hz), 5.38 (d, 1H, $J$ = 2.8 Hz), 3.80 (s, 3H), 3.72 (s, 3H); $^{13}$C NMR (DMSO-$d_6$, 125 MHz) $\delta$ = 191.6, 162.8, 159.7, 152.5, 141.3, 137.5, 132.0, 131.4, 128.8, 115.0, 114.8, 113.9, 56.5, 56.3, 54.1; IR (KBr, cm$^{-1}$): 3277, 2931, 2835, 1704, 1670, 1650, 1509, 1443, 1367, 1246, 1170, 1029, 905; ESI-MS: m/z 339 ([M+H]$^+$); ESI-HRMS: Calcd for $C_{19}H_{18}N_2O_4Na$ ([M+Na]$^+$), 361.1159; Found, 361.1154.




4-(4-Chlorophenyl)-5-(4-methoxylphenyl)methanone-yl-3,4-dihydropyrimidine-2(1*H*)-one (**4y**). Colorless crystal; m. p. 298-299 $^o$C; $^1$H NMR (DMSO-$d_6$, 500 MHz) $\delta$ = 9.32 (d, 1H, $J$ = 4.4 Hz), 7.84 (s, 1H), 7.49 (d, 2H, $J$ = 8.6 Hz), 7.40 (d, 2H, $J$ = 8.5 Hz), 7.34 (d, 2H, $J$ = 8.5 Hz), 7.04 (d, 1H, $J$ = 6.0 Hz), 6.98 (d, 2H, $J$ = 1.8 Hz), 5.42 (d, 1H, $J$ = 2.9 Hz), 3.80 (s, 3H); $^{13}$C NMR (DMSO-$d_6$, 125 MHz) $\delta$ = 191.6, 162.8, 152.4, 144.3, 141.9, 133.1, 131.9, 131.5, 129.7, 129.6, 114.9, 113.2, 16.6, 54.2; IR (KBr, cm$^{-1}$): 3263, 2925, 1696, 1673, 1654, 1603, 1458, 1365, 1256, 1169, 1086, 905; ESI-MS: m/z 343 ([M+H]$^+$); ESI-HRMS: Calcd for $C_{18}H_{15}ClN_2O_3Na$ ([M+Na]$^+$), 365.0663; Found, 365.0658.

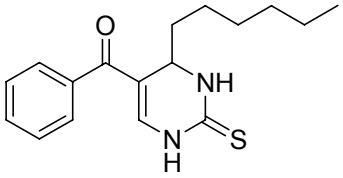



4-Ethyl-5-phenylmethanone-yl-3,4-dihydropyrimidine-2(1*H*)-thione (**6a**). Yellow solid; m. p. 225-228 $^o$C; $^1$H NMR (DMSO-$d_6$, 500 MHz) $\delta$ = 10.18 (d, 1H, $J$ = 4.7 Hz), 9.33 (s, 1H), 7.57-7.46 (m, 5H), 6.73 (d, 1H, $J$ = 5.6 Hz), 4.43 (dd, $J_1$ = 4.2 Hz, $J_2$ = 3.5 Hz), 1.59-1.53 (m, 2H), 0.85 (t, 3H, $J$ = 7.4 Hz); $^{13}$C NMR (DMSO-$d_6$, 125 MHz) $\delta$ = 193.4, 176.1, 139.5, 139.4, 132.3, 129.6, 129.2, 113.7, 52.4, 29.7, 9.1; IR (KBr, cm$^{-1}$): 3279, 3186, 2962, 1618, 1576, 1466, 1381, 1200, 1104, 986; ESI-MS: m/z 247 ([M+H]$^+$); ESI-HRMS: Calcd for $C_{13}H_{14}N_2OSNa$ ([M+Na]$^+$), 269.0719; Found, 269.0723.

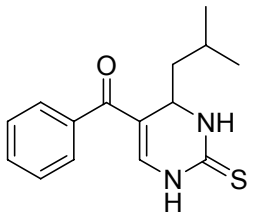



4-Propyl-5-phenylmethanone-yl-3,4-dihydropyrimidine-2(1*H*)-thione (**6b**). Colorless crystal; m. p. 197-199 $^o$C; $^1$H NMR (DMSO-$d_6$, 500 MHz) $\delta$ = 10.19 (d, 1H, $J$ = 5.2 Hz), 9.38 (s, 1H), 7.58-7.47 (m, 5H), 6.70 (d, 1H, $J$ = 5.6 Hz), 4.42 (dd, $J_1$ = 4.4 Hz, $J_2$ = 4.7 Hz), 1.54-1.47 (m, 2H), 1.36-1.26 (m, 2H), 0.88 (t, 3H, $J$ = 7.3 Hz); $^{13}$C NMR

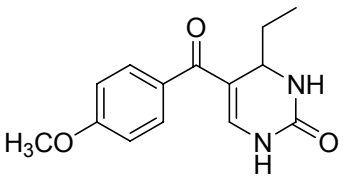
(DMSO-$d_6$, 125 MHz) $\delta$ = 193.3, 175.9, 139.5, 139.2, 132.3, 129.6, 129.2, 114.4, 51.2, 39.2, 17.8, 15.0; IR (KBr, $cm^{-1}$): 3275, 3169, 2948, 1625, 1572, 1463, 1377, 1203, 1120, 1047; ESI-MS: m/z 261 ($[M+H]^+$); ESI-HRMS: Calcd for $C_{14}H_{16}N_2OSNa$ ($[M+Na]^+$), 283.0876; Found, 283.0873.




4-Hexyl-5-phenylmethanone-yl-3,4-dihydropyrimidine-2(1*H*)-thione (**6c**). Yellow solid; m. p. 169-172$^o$C; $^1$H NMR (DMSO-$d_6$, 500 MHz) $\delta$ = 10.18 (d, 1H, $J$ = 4.6 Hz), 9.36 (s, 1H), 7.63-7.47 (m, 5H), 6.71 (d, 1H, $J$ = 5.5 Hz), 4.41 (d, 1H, $J$ = 3.2 Hz), 1.54-1.49 (m, 2H), 1.24-1.22 (m, 8H), 0.84 (t, 3H, $J$ = 6.8 Hz); $^{13}$C NMR (DMSO-$d_6$, 125 MHz) $\delta$ = 193.4, 175.9, 139.5, 139.2, 132.4, 129.6, 129.2, 114.4, 51.3, 36.8, 32.4, 29.6, 24.4, 23.2, 15.1; IR (KBr, $cm^{-1}$): 3406, 3273, 2926, 2855, 1628, 1571, 1462, 1375, 1200, 1118, 1016; ESI-MS: m/z 303 ($[M+H]^+$); ESI-HRMS: Calcd for $C_{17}H_{22}N_2OSNa$ ($[M+Na]^+$), 325.1345; Found, 325.1345.

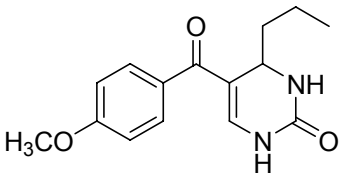



4-Isobutyl-5-phenylmethanone-yl-3,4-dihydropyrimidine-2(1*H*)-thione (**6d**). Yellow solid; m. p. 233-235 $^o$C; $^1$H NMR (DMSO-$d_6$, 500 MHz) $\delta$ = 10.25 (d, 1H, $J$ = 4.7 Hz), 9.48 (s, 1H), 7.58-7.47 (m, 5H), 6.71 (d, 1H, $J$ = 5.6 Hz), 4.43-4.40 (m, 1H), 1.74-1.71 (m, 1H), 1.50-1.44 (m, 1H), 1.31-1.25 (m, 1H), 0.93 (d, 3H, $J$ = 6.6 Hz), 0.88 (d, 3H, $J$ = 6.6 Hz); $^{13}$C NMR (DMSO-$d_6$, 125 MHz) $\delta$ = 193.1, 175.9, 139.4, 139.0, 132.4, 129.6, 129.2, 115.5, 19.4, 46.3, 24.6, 24.0, 23.1; IR (KBr, $cm^{-1}$): 3177, 2954, 2926, 1652, 1620, 1577, 1477, 1367, 1209, 1127, 987, 713; ESI-MS: m/z 275 ($[M+H]^+$); ESI-HRMS: Calcd for $C_{15}H_{19}N_2OS$ ($[M+H]^+$), 275.1213; Found, 275.1217.

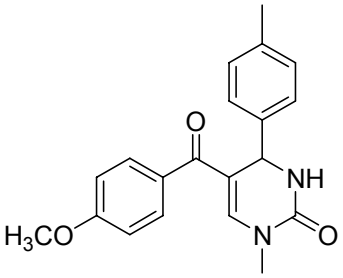



4-Ethyl-5-phenylmethanone-yl-3,4-dihydropyrimidine-2(1*H*)-one (**6e**). White solid; m. p. 190-193 $^o$C; $^1$H NMR (DMSO-$d_6$, 500 MHz) $\delta$ = 8.99 (d, 1H, $J$ = 4.8 Hz), 7.52 (d, 2H, $J$ = 8.6 Hz), 7.34 (s, 1H), 7.01 (d, 2H, $J$ = 8.6 Hz), 6.89 (d, 1H, $J$= 5.9 Hz), 4.37 (dd, 1H, $J_1$= 4.8 Hz, $J_2$ = 2.9 Hz), 3.81 (s, 3H), 1.55-1.50 (m, 2H), 0.85 (t, 3H, $J$ = 7.4 Hz); $^{13}$C NMR (DMSO-$d_6$, 125 MHz) $\delta$ = 192.2, 162.7, 153.3, 142.3, 132.3, 131.5, 114.8, 113.1, 56.6, 52.2, 30.1, 9.33; IR (KBr, $cm^{-1}$): 3279, 2957, 1932, 2839,

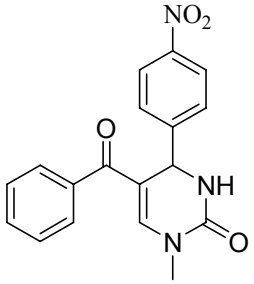
1720, 1685, 1593, 1460, 1379, 1202, 1113, 1030, 903; ESI-MS: m/z 261 ($[M+H]^+$); ESI-HRMS: Calcd for $C_{14}H_{16}N_2O_3Na([M+Na]^+)$, 283.1053; Found, 283.1052.



4-Propyl-5-phenylmethanone-yl-3,4-dihydropyrimidine-2(1*H*)-one (**6f**). Yellow solid; m. p. 173-176 $^oC$; $^1H$ NMR (DMSO-$d_6$, 500 MHz) $\delta$ = 9.00 (d, 1H, $J$ = 4.8 Hz), 7.52 (d, 2H, $J$ = 8.6 Hz), 7.39 (s, 1H), 7.01 (d, 2H, $J$ = 8.6 Hz), 6.87 (d, 1H, $J$ = 5.9 Hz), 4.37 (t, 1H, $J$ = 2.7 Hz), 3.81 (s, 3H), 1.51-1.22 (m, 4H), 0.87 (t, 3H, $J$ = 7.2 Hz); $^{13}C$ NMR (DMSO-$d_6$, 125 MHz) $\delta$ = 192.1, 162.7, 153.3, 142.0, 132.3, 131.4, 114.8, 113.8, 56.6, 50.9, 39.8, 18.1, 15.1; IR (KBr, $cm^{-1}$): 3277, 2958, 2932, 1699, 1682, 1594, 1459, 1379, 1202, 1171, 1113, 1030, 905; ESI-MS: m/z 275 ($[M+H]^+$); ESI-HRMS: Calcd for $C_{15}H_{19}N_2O_3Na([M+Na]^+)$, 297.1210; Found, 297.1207.

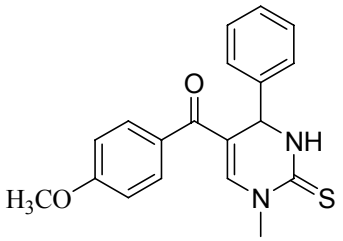


1-Methyl-4-(4-methylphenyl)-5-(4-methoxyphenyl)methanone-yl-3,4-dihydropyrimid ine-2(1*H*)-one (**7a**). Yellow oil; $^1H$ NMR (DMSO-$d_6$, 500 MHz) $\delta$ = 7.92 (brs, 1H), 7.56 (d, 2H, $J$ = 8.2 Hz), 7.27 (s, 1H) 7.3 (d, 2H, $J$ = 7.7 Hz), 7.13 (d, 2H, $J$ = 7.5 Hz), 7.00 (d, 1H), 6.98 (s, 1H), 5.44 (d, 1H, $J$ = 2.5 Hz), 3.80 (s, 3H), 3.10 (s, 3H), 2.56 (s, 3H); $^{13}C$ NMR (DMSO-$d_6$, 125 MHz) $\delta$ = 191.4, 162.9, 153.1, 145.7, 142.3, 137.8, 132.1, 131.7, 130.4, 127.5, 114.8, 114.2, 56.6, 54.6, 36.0, 21.8; IR (film, $cm^{-1}$): 3418, 2927, 1681, 1647, 1620, 1512, 1318, 1243, 1173, 1027; ESI-MS: m/z 337 ($[M+H]^+$); ESI-HRMS: Calcd for $C_{20}H_{20}N_2O_3Na([M+Na]^+)$, 359.1366; Found, 359.1361.

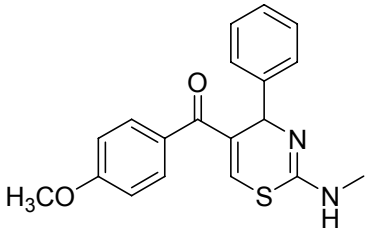


1-Methyl-4-(4-nitrophenyl)-5-phenylmethanone-yl-3,4-dihydropyrimidine-2(1*H*)-one (**7b**). White solid; m.p. 222-223 $^oC$; $^1H$ NMR (DMSO-$d_6$, 500 MHz) $\delta$ = 8.22 (d, 2H, $J$ = 8.7 Hz), 8.16 (d, 1H, $J$ = 2.9 Hz), 7.63 (d, 2 H, $J$ = 8.7 Hz), 7.56-7.53 (m, 3H), 7.47-7.44 (m, 2H), 7.37 (s, 1H), 5.58 (d, 1H, $J$ = 2.9 Hz), 3.12 (s, 3H); $^{13}C$ NMR (DMSO-$d_6$, 125 MHz) $\delta$ = 192.3, 152.6, 152.2, 148.0, 147.9, 139.4, 132.3, 129.6, 129.5, 129.1, 125.0, 112.7, 54.5, 36.2; IR (KBr film, $cm^{-1}$): ESI-MS: 3358, 3069, 2943, 1700, 1652, 1606, 1521, 1445, 1348, 1241, 1122, 1050, 947; m/z 338 ($[M+H]^+$);

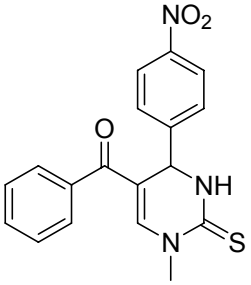
ESI-HRMS: Calcd for $C_{18}H_{15}N_3O_4Na([M+Na]^+)$, 360.0955; Found, 360.0954.



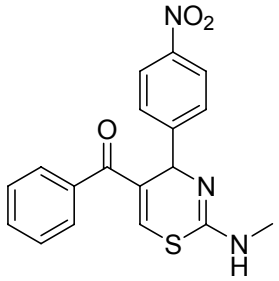

1-Methyl-4phenyl-5-(4-methoxyphenyl)methanone-yl-3,4-dihydropyrimidine-2(1*H*)-thione (**7c**). Yellow solid; m. p. 219-221 $^oC$; $^1H$ NMR (DMSO-$d_6$, 500 MHz) $\delta$ = 9.72 (d, 1H, $J$ = 8.4 Hz), 7.63-7.61 (m, 2H), 7.43-7.26 (m, 6H), 7.05-7.00 (m, 2H), 5.42 (d, 1H, $J$ = 3.2 Hz), 3.84 (s, 3H), 3.46 (s, 3H); $^{13}C$ NMR (DMSO-$d_6$, 125 MHz) $\delta$ = 191.6, 177.3, 163.3, 143.9, 142.2, 131.9, 131.5, 129.8, 128.9, 127.7, 115.6, 115.0, 56.6, 54.5, 41.9; IR (KBr, $cm^{-1}$): 3447, 2924, 2854, 1655, 1620, 1601, 1508, 1458, 1377, 1254, 1153, 1103; ESI-MS: m/z 339 ($[M+H]^+$); ESI-HRMS: Calcd for $C_{19}H_{18}N_2O_2SNa([M+Na]+)$, 361.0981; Found, 361.0971.



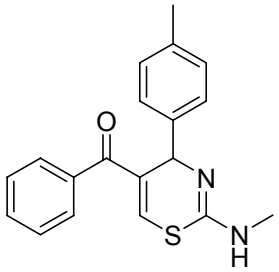

2-Methylamino-4-phenyl-5-(4-methoxyphenyl)methanone-yl-4*H*-1,3-thiazine (**8c**). Yellow oil; $^1H$ NMR (DMSO-$d_6$, 500 MHz) $\delta$ = 8.25 (d, 1H, $J$ = 4.3 Hz), 7.72 (s, 1H), 7.58 (d, 2H, $J$ = 8.6 Hz), 7.31-7.23 (m, 5H), 7.03 (s, 1H ), 7.01 (s, 1H), 5.52 (s, 1H), 3.83 (s, 3H), 2.86 (d, 3H, $J$ = 4.3 Hz); $^{13}C$ NMR (DMSO-$d_6$, 125 MHz) $\delta$ = 193.2, 162.7, 157.8, 154.3, 143.8, 132.6, 131.9, 129.8, 128.5, 127.7, 115.0, 114.7, 56.6, 56.5, 30.1; IR (film, $cm^{-1}$): 3286, 2968, 2931, 1599, 1535, 1512, 1454, 1375, 1250, 1170, 1110, 1029, 953; ESI-MS: m/z 339 ($[M+H]^+$); ESI-HRMS: Calcd for $C_{19}H_{18}N_2O_2SNa([M+Na]^+)$, 361.0981; Found, 361.0980.



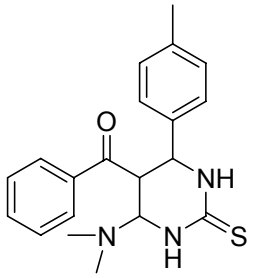

1-Methyl-4-(4-nitrophenyl)-5-phenylmethanone-yl-3,4-dihydropyrimidine-2(1*H*)-thione (**7d**). Pale orange crystal; m. p. 266-268 $^oC$; $^1H$ NMR (DMSO-$d_6$, 500 MHz) $\delta$ = 9.92 (d, 1H, $J$ = 3.4 Hz), 8.24 (t, 2H, $J$ = 1.9 Hz), 7.61-7.58 (m, 5H), 7.50-7.46 (m, 2H), 7.44 (s, 1H), 5.55 (d, 1H, $J$ = 3.4 Hz), 3.48 (s, 3H); $^{13}C$ NMR (DMSO-$d_6$, 125 MHz) $\delta$ = 192.7, 171.5, 150.7, 148.2, 144.2, 138.9, 132.8, 129.7, 129.2, 125.2, 114.4, 54.1, 42.1; IR (KBr, $cm^{-1}$): 3449, 3317, 2925, 1650, 1612, 1521, 1445, 1349, 1251, 1154, 1097, 946; ESI-MS: m/z 354 ($[M+H]^+$); ESI-HRMS: Calcd for $C_{18}H_{16}N_3O_3S([M+H]^+)$, 354.0907; Found, 354.0904.



2-Methylamino-4-(4-nitrophenyl)-5-phenylmethanone-yl-4*H*-1,3-thiazine (**8d**). Brown oil; $^{1}$H NMR (DMSO-$d_6$, 500 MHz) $\delta$ = 8.49 (d, 1H, $J$ = 4.6 Hz), 8.18 (d, 2H, $J$ = 8.7 Hz), 7.76 (s, 1H), 7.58-7.46 (m, 7H), 5.73 (s, 1H), 2.87 (d, 3H, $J$ = 4.6 Hz); $^{13}$C NMR (DMSO-$d_6$, 125 MHz) $\delta$ = 194.2, 158.1, 156.1, 151.2, 147.8, 140.1, 132.0, 129.8, 129.7, 129.2, 125.2, 113.6, 39.9, 30.2; IR (film, cm$^{-1}$): 3271, 3035, 2970, 2935, 1732, 1598, 1518, 1405, 1344, 1290, 1109, 1048, 956; ESI-MS: m/z 354 ([M+H]$^{+}$); ESI-HRMS: Calcd for $C_{18}H_{15}N_3O_3SNa$([M+Na]$^{+}$), 376.0726; Found, 376.0725.

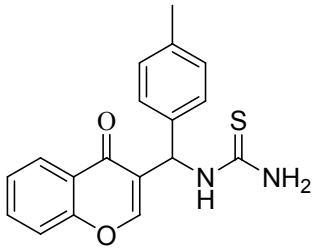


2-Methylamino-4-(4-methylphenyl)-5-phenylmethanone-yl-4*H*-1,3-thiazine (**8e**). Yellow oil; $^{1}$H NMR (DMSO-$d_6$, 500 MHz) $\delta$ = 8.32 (brs, 1H), 7.68 (s, 1H), 7.54-7.47 (m, 5H), 7.14-7.09 (m, 4H), 5.50 (s, 1H), 2.85 (brs, 3H), 2.25 (s, 3H); $^{13}$C NMR (DMSO-$d_6$, 125 MHz) $\delta$ = 194.3, 158.4, 155.4, 140.8, 140.5, 137.8, 131.8, 130.4, 129.5, 129.4, 127.6, 114.8, 40.3, 30.1, 21.8; IR (film, cm$^{-1}$): 3415, 3255, 3027, 2929, 1620, 1543, 1510, 1405, 1376, 1289, 1211, 1107, 1027; ESI-MS: m/z 323 ([M+H]$^{+}$); ESI-HRMS: Calcd for $C_{19}H_{18}N_2OSNa$([M+Na]$^{+}$), 345.1032; Found, 345.1038.

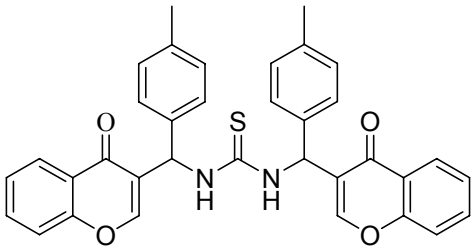


4-(4-Methylphenyl)-5-phenylmethanone-yl-6-dimethylaminotetrahydropyrimidine-2(1*H*)-thione (**9**). White solid; m. p. 202-205 $^{o}$C; $^{1}$H NMR (DMSO-$d_6$, 500 MHz) $\delta$ = 8.30 (s, 1H), 8.22 (s, 1H), 7.73-7.70 (m, 2H), 7.50-7.46 (m, 1H), 7.34-7.31 (m, 2H), 7.21 (d, 2H, $J$ = 8.0 Hz), 6.98 (d, 2H, $J$ = 7.9 Hz), 4.58 (d, 1H, $J$ = 10.3 Hz), 4.50 (d, 1H, $J$ = 9.8 Hz), 4.22 (t, 1H, $J$ = 10.0 Hz), 2.23 (s, 6H), 2.13 (s, 3H); IR (KBr cm$^{-1}$); $^{13}$C NMR (DMSO-$d_6$, 125 MHz) $\delta$= 200.6, 178.9, 138.3, 138.1, 136.0, 134.4, 129.9, 129.6, 129.2, 128.8, 77.3, 60.2, 48.5, 40.3, 21.8; IR (KBr, cm$^{-1}$): 3347, 3195, 2940, 1666, 1543, 1508, 1447, 1356, 1196, 1034, 944; ESI-MS: m/z 376 ([M+Na]$^{+}$);

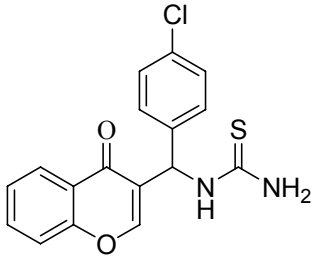
ESI-HRMS: Calcd for $C_{20}H_{23}N_3OSNa([M+Na]^+)$, 376.1454; Found, 376.1450.



1-((4-Oxo-4*H*-chromen-3-yl)(*p*-tolyl)methyl)thiourea (**11a**). White solid; m. p. 239-241 $^oC$; $^1H$ NMR (DMSO-$d_6$, 500 MHz) $\delta$ = 8.52 (s, 1H), 8.35 (d, 1H, $J$ = 8.5 Hz), 8.00 (d, 1H, $J$ = 7.8 Hz), 7.84-7.80 (m, 1H), 7.68 (d, 1H, $J$ = 8.5 Hz), 7.50-7.47 (m, 1H), 7.38 (brs, 2H), 7.21 (d, 2H, $J$ = 7.8 Hz), 7.11 (d, 2H, $J$ = 7.8 Hz), 6.50 (d, 1H, $J$ = 8.2 Hz), 2.25 (s, 3H); IR (KBr $cm^{-1}$); $^{13}C$ NMR (DMSO-$d_6$, 125 MHz) $\delta$= 184.1, 177.0, 157.0, 155.9, 138.9, 137.1, 135.6, 129.8, 127.5, 126.7, 126.0, 124.8, 124.7, 119.7, 56.3, 21.7; IR (KBr, $cm^{-1}$): 3365, 3158, 2965, 1630, 1531, 1465, 1350, 12238, 1132; ESI-MS: m/z 347 ($[M+Na]^+$); ESI-HRMS: Calcd for $C_{18}H_{16}N_2O_2SNa([M+Na]^+)$, 347.0825; Found, 347.0811.

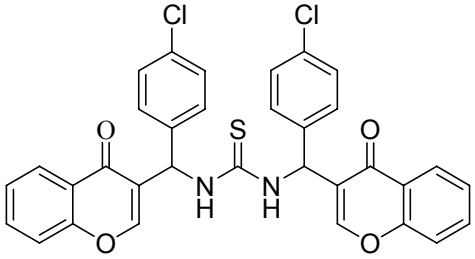


1,3-Bis((4-oxo-4*H*-chromen-3-yl)(*p*-tolyl)methyl)thiourea (**12a**). White solid; m. p. 212-214 $^oC$; $^1H$ NMR (DMSO-$d_6$, 500 MHz) $\delta$ = 8.73 (Brs, 2H), 8.48 (s, 2H), 8.00-7.96 (m, 2H), 7.99-7.76 (m, 2H), 7.68-7.62 (m, 2H), 7.49-7.44 (m, 2H), 7.26-7.21 (m, 4H), 7.13-7.07 (m, 4H), 6.59 (d, 1H, $J$ = 8.4 Hz), 2.26 (s, 6H); $^{13}C$ NMR (DMSO-$d_6$, 125 MHz) $\delta$ = 176.8, 158.2, 156.9, 155.7, 137.3, 135.5, 129.9, 127.8, 126.7, 126.0, 125.1, 124.7, 119.7, 113.5, 55.9, 21.8; IR (KBr, $cm^{-1}$): 3433, 3332, 3068, 2921, 1636, 1512, 1465, 1404, 1353, 1139, 1056, 760; ESI-MS: m/z 595 ($[M+Na]^+$); ESI-HRMS: Calcd for $C_{35}H_{28}N_2O_4SNa$, 595.1662; Found, 595.1643.

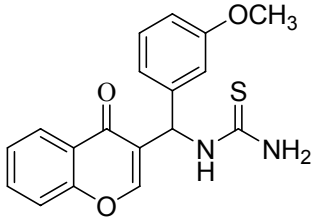


1-((4-Chlorophenyl)(4-oxo-4*H*-chromen-3-yl)methyl)thiourea (**11b**). White solid; m. p. 228-230 $^oC$; $^1H$ NMR (DMSO-$d_6$, 500 MHz) $\delta$ = 8.60 (s, 1H), 8.42 (d, 1H, $J$ = 8.4 Hz), 8.00 (d, 1H, $J$ = 7.8 Hz), 7.85-7.81 (m, 1H), 7.69 (d, 1H, $J$ = 8.5 Hz), 7.51-7.38 (m, 3H), 7.37-7.34 (m, 4H), 6.55 (d, 1H, $J$ = 8.3 Hz); $^{13}C$ NMR (DMSO-$d_6$, 125 MHz) $\delta$ = 184.2, 177.0, 157.0, 156.4, 141.0, 135.7, 132.6, 129.4, 129.2, 126.8, 126.0, 124.6,

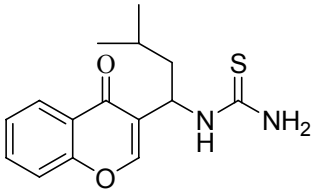
124.2, 119.7, 56.1; IR (KBr, $cm^{-1}$): 3393, 3337, 3167, 1628, 1526, 1464, 1415, 1354, 1246, 1135, 1012, 759; ESI-MS: m/z 367 ($[M+Na]^+$); ESI-HRMS: Calcd for $C_{17}H_{13}ClN_2O_2SNa([M+Na]^+)$, 367.0278; Found, 367.0269.



1,3-Bis((4-chlorophenyl)(4-oxo-4*H*-chromen-3-yl)methyl)thiourea (**12b**). White solid; m. p. 245-247 $^oC$; $^1H$ NMR (DMSO-$d_6$, 500 MHz) $\delta$ = 8.89 (brs, 1H), 8.81 (brs, 1H), 8.58 (s, 1H), 8.55 (s, 1H), 8.01-7.96 (m, 2H), 7.85-7.78 (m, 2H), 7.70-7.63 (m, 2H), 7.50-7.34 (m, 10H), 6.63 (t, 2H, $J$ = 8.6 Hz); $^{13}C$ NMR (DMSO-$d_6$, 125 MHz) $\delta$ = 176.9, 157.2, 156.2, 135.7, 132.7, 129.7, 129.3, 126.8, 126.0, 124.7, 124.4, 119.7, 56.8; IR (KBr, $cm^{-1}$): 3433, 3301, 2925, 1640, 1513, 1465, 1405, 1354, 1092, 761; ESI-MS: m/z 613 ($[M+H]^+$); ESI-HRMS: Calcd for $C_{33}H_{22}Cl_2N_2O_4SNa([M+Na]^+)$, 635.0570; Found, 635.0550.

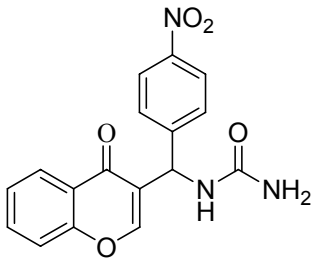


1-((3-Methoxyphenyl)(4-oxo-4*H*-chromen-3-yl)methyl)thiourea (**11c**). Pale yellow solid; m. p. 219-223 $^oC$; $^1H$ NMR (DMSO-$d_6$, 500 MHz) $\delta$ = 8.55 (s, 1H), 8.42 (d, 1H, $J$ = 8.6 Hz), 8.00 (d, 1H, $J$ = 7.7 Hz), 7.81-7.77 (m, 1H), 7.65 (d, 1H, $J$ = 8.4 Hz), 7.47-7.42 (m, 3H), 7.24-7.21 (m, 1H), 6.93-6.91 (m, 2H), 6.80 (d, 1H, $J$ = 8.5 Hz), 6.54 (d, 1H, $J$ = 8.5 Hz), 3.71 (s, 3H); $^{13}C$ NMR (DMSO-$d_6$, 125 MHz) $\delta$ = 184.1, 177.0, 160.4, 156.9, 156.0, 143.6, 135.6, 130.4, 126.7, 126.0, 124.7, 124.6, 120.2, 119.9, 119.6, 113.9, 112.9, 56.5, 56.2; IR (KBr, $cm^{-1}$): 3407, 3302, 3173, 3083, 1634, 1556, 1465, 1350, 1263, 1137, 1046, 851; ESI-MS: m/z 363 ($[M+Na]^+$); ESI-HRMS: Calcd for $C_{18}H_{16}N_2O_3SNa([M+Na]^+)$, 363.0774; Found, 363.0761.

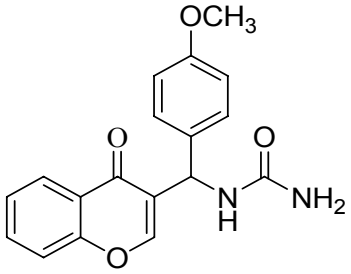


1-(3-Methyl-1-(4-oxo-4*H*-chromen-3-yl)butyl)thiourea (**11d**). White solid; m. p. 211-212 $^oC$; $^1H$ NMR (DMSO-$d_6$, 500 MHz) $\delta$ = 8.28 (s, 1H), 8.07 (d, 1H, $J$ = 7.8 Hz), 7.92-7.79 (m, 2H), 7.65 (d, 1H, $J$ = 8.5 Hz), 7.52-7.48 (m, 1H), 7.10 (brs, 2H), 5.24 (d, 1H, $J$ = 6.5 Hz), 1.77-1.53 (m, 3H), 0.90 (d, 6H, $J$ = 6.5 Hz); $^{13}C$ NMR (DMSO-$d_6$, 125 MHz) $\delta$ = 183.7, 177.5, 156.8, 155.2, 135.4, 134.9, 126.6, 126.0, 125.0, 119.1, 52.3, 43.4, 26.0, 23.7, 23.4; ; IR (KBr, $cm^{-1}$): 3319, 3174, 2956, 1630, 1537, 1465,

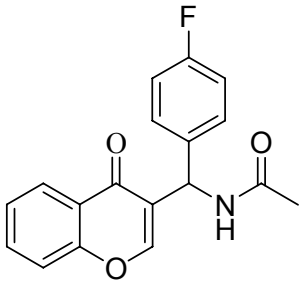
1350, 1218, 1139, 762; ESI-MS: m/z 313 ([M+Na]$^+$); ESI-HRMS: Calcd for $C_{18}H_{18}N_2O_2SNa$([M+Na]$^+$), 313.0981; Found, 313.0980.



1-((4-Nitrophenyl)(4-oxo-4*H*-chromen-3-yl)methyl)urea (**11e**). White solid; m. p. 259-261 $^o$C; $^1$H NMR (DMSO-$d_6$, 500 MHz) $\delta$ = 8.66 (s, 1H), 8.17 (d, 2H, $J$ = 8.9 Hz), 8.00-7.98 (m, 1H), 7.84-7.81 (m, 1H), 7.70 (d, 1H, $J$ = 8.2 Hz), 7.63 (d, 2H, $J$ = 8.6 Hz), 7.51-7.47 (m, 1H), 7.07 (d, 1H, $J$ = 9.1 Hz), 5.99 (d, 1H, $J$ = 9.1 Hz) 5.89 (s, 2H); $^{13}$C NMR (DMSO-$d_6$, 125 MHz) $\delta$ = 176.9, 159.0, 157.0, 156.4, 151.3, 147.5, 135.7, 128.8, 126.8, 126.0, 124.9, 124.7, 124.4, 119.7, 51.6; IR (KBr, cm$^{-1}$): 3442, 3281, 3103, 2925, 1658, 1633, 1562, 1520, 1465, 1356, 1168, 764; ESI-MS: m/z 340 ([M+H]$^+$); ESI-HRMS: Calcd for $C_{17}H_{13}N_3O_5Na$([M+Na]$^+$), 362.0747; Found, 362.0740.

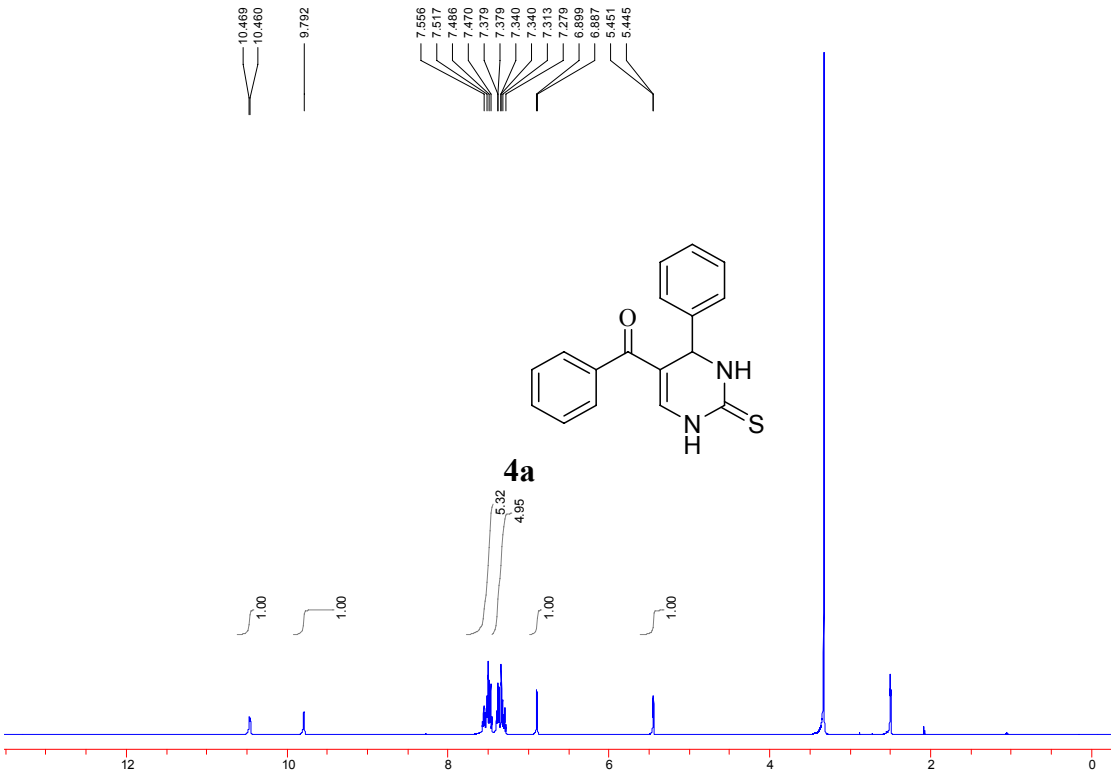


1-((4-Methoxyphenyl)(4-oxo-4*H*-chromen-3-yl)methyl)urea (**11f**). White solid; m. p. 219-222 $^o$C; $^1$H NMR (DMSO-$d_6$, 500 MHz) $\delta$ = 8.47 (s, 1H), 8.00 (d, 1H, $J$ = 7.9 Hz), 7.82-7.79 (m, 1H), 7.66 (d, 1H, $J$ = 8.5 Hz), 7.49 (t, 1H, $J$ = 7.5 Hz), 7.26 (d, 2H, $J$ = 8.5 Hz), 6.86-6.81 (m, 3H), 5.80 (d, 1H, $J$ = 8.9 Hz), 5.74 (s, 2H); $^{13}$C NMR (DMSO-$d_6$, 125 MHz) $\delta$ = 177.0, 159.2, 159.0, 157.0, 155.3, 135.4, 135.1, 128.9, 126.6, 126.3, 126.0, 124.7, 119.6, 114.6, 56.2, 51.1; IR (KBr, cm$^{-1}$): 3450, 3349, 3284, 2926, 1658, 1637, 1562, 1465, 1353, 1250, 1176, 764; ESI-MS: m/z 347 ([M+Na]$^+$); ESI-HRMS: Calcd for $C_{18}H_{16}N_2O_4Na$([M+Na]$^+$), 347.1002; Found, 347.0995.



*N*-((4-Fluorophenyl)(4-oxo-4*H*-chromen-3-yl)methyl)acetamide (**11g**). White solid; m. p. 247-249 $^o$C; $^1$H NMR (DMSO-$d_6$, 500 MHz) $\delta$ = 8.52 (d, 1H, $J$ = 8.3 Hz), 8.34 (s, 1H), 8.03-8.01 (m, 1H), 7.82-7.80 (m, 1H), 7.67 (d, 1H, $J$ = 8.4 Hz), 7.50 (d, 1H, $J$ = 7.4 Hz), 7.39-7.36 (m, 2H), 7.15 (t, 2H, $J$ = 8.3 Hz), 6.13 (d, 1H, $J$ = 8.3 Hz), 1.92 (s,

3H); $^{13}$C NMR (DMSO-$d_6$, 125 MHz) $\delta$ = 176.5, 169.9, 163.4, 161.4, 157.0, 155.7, 138.0, 135.5, 130.3, 126.7, 126.2, 125.6, 116.2, 116.0, 49.4, 23.8; IR (KBr, $cm^{-1}$): 3298, 3075, 1641, 1537, 1508, 1470, 1360, 1221, 1155, 754; ESI-MS: m/z 334 ($[M+Na]^+$); ESI-HRMS: Calcd for $C_{18}H_{14}FNO_3Na$($[M+Na]^+$), 334.0850; Found, 334.0842.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7.470
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7.279
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6.887
5.451
5.445
O
NH
N
H
S
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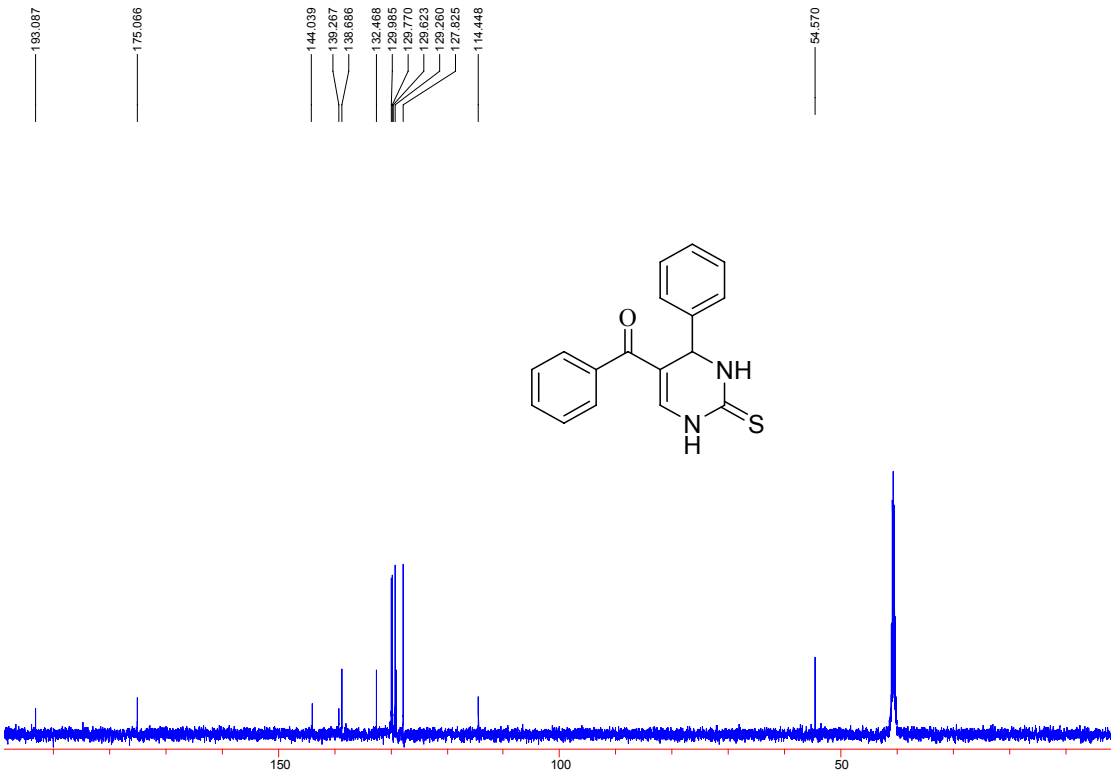
1.00
1.00
12
10
8
6
4
2
0

**4a**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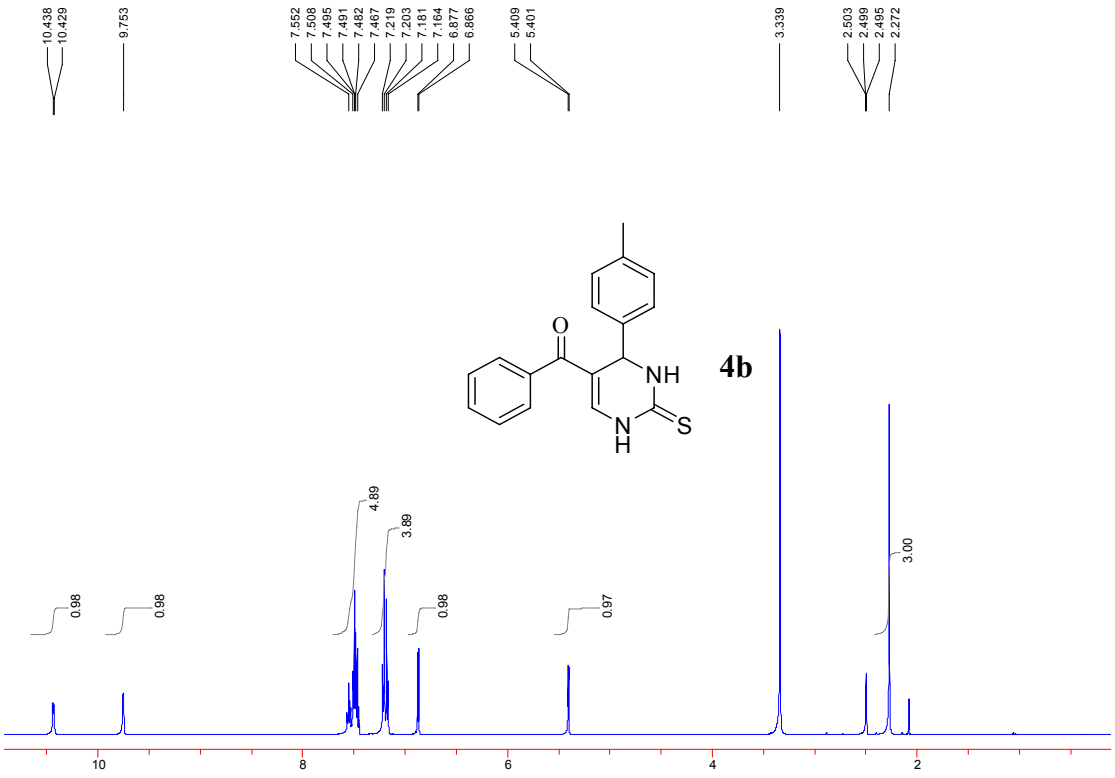
N
H
S
150
100
50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7.491
7.482
7.467
7.219
7.203
7.181
7.164
6.877
6.866
5.409
5.401
3.339
2.503
2.499
2.495
2.272
O
NH
N
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10
8
6
4
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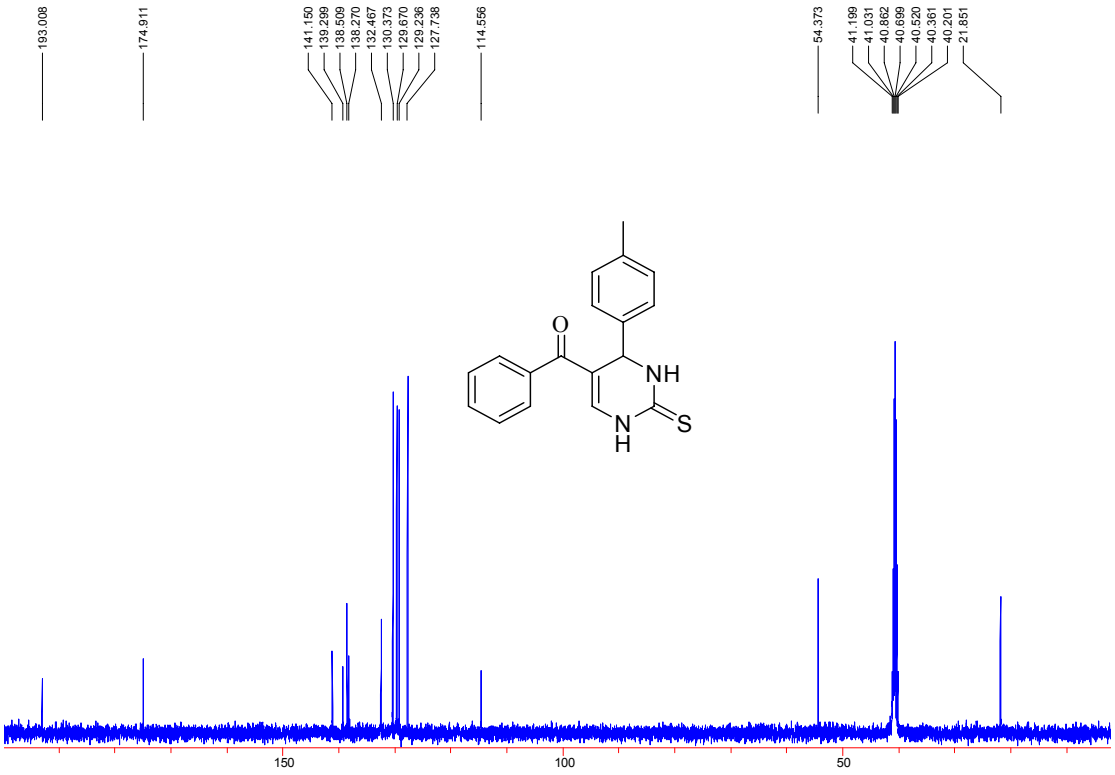
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127.738
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S
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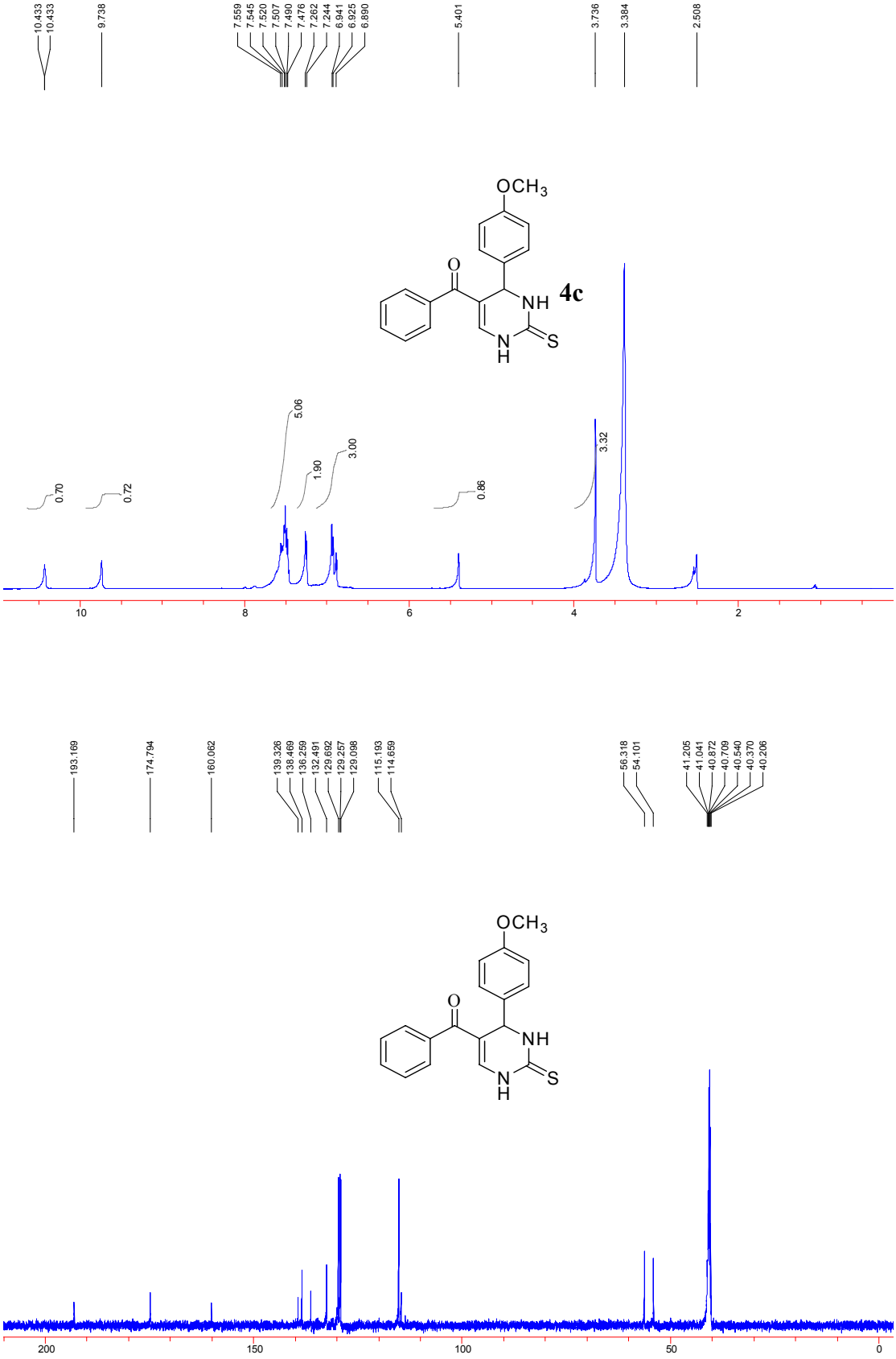
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6.890
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3.384
2.508
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N
H
S
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3.32
10
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4
2
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41.041
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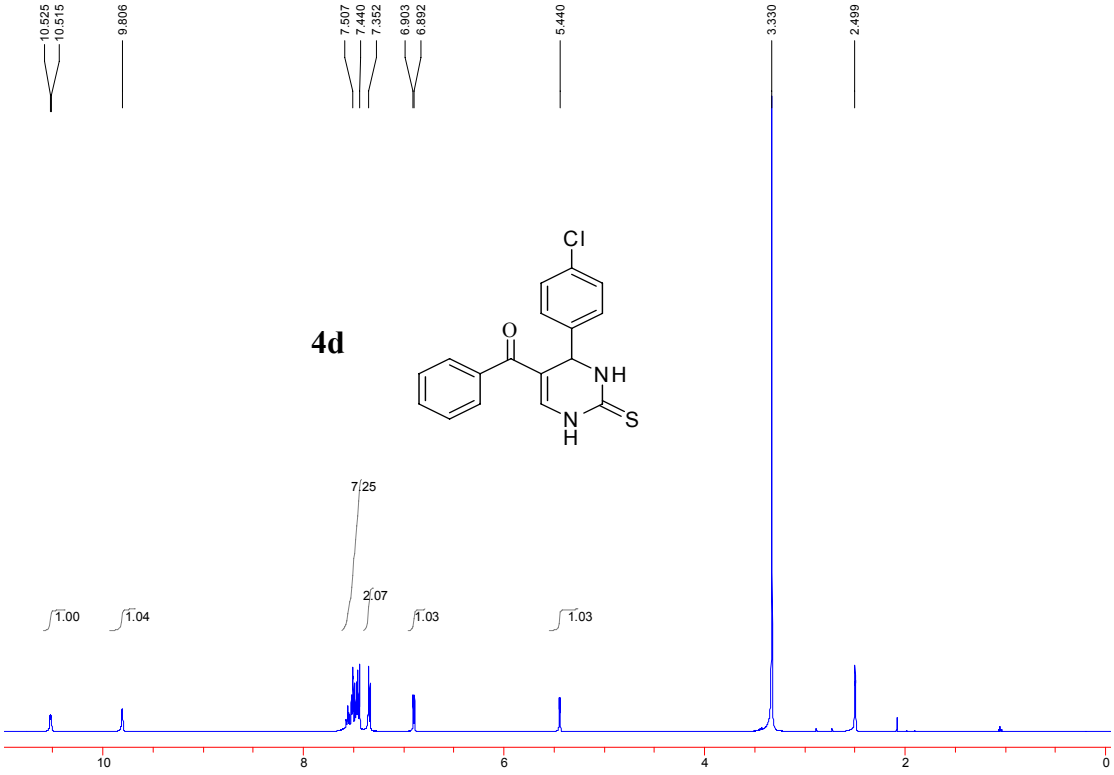
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1.03
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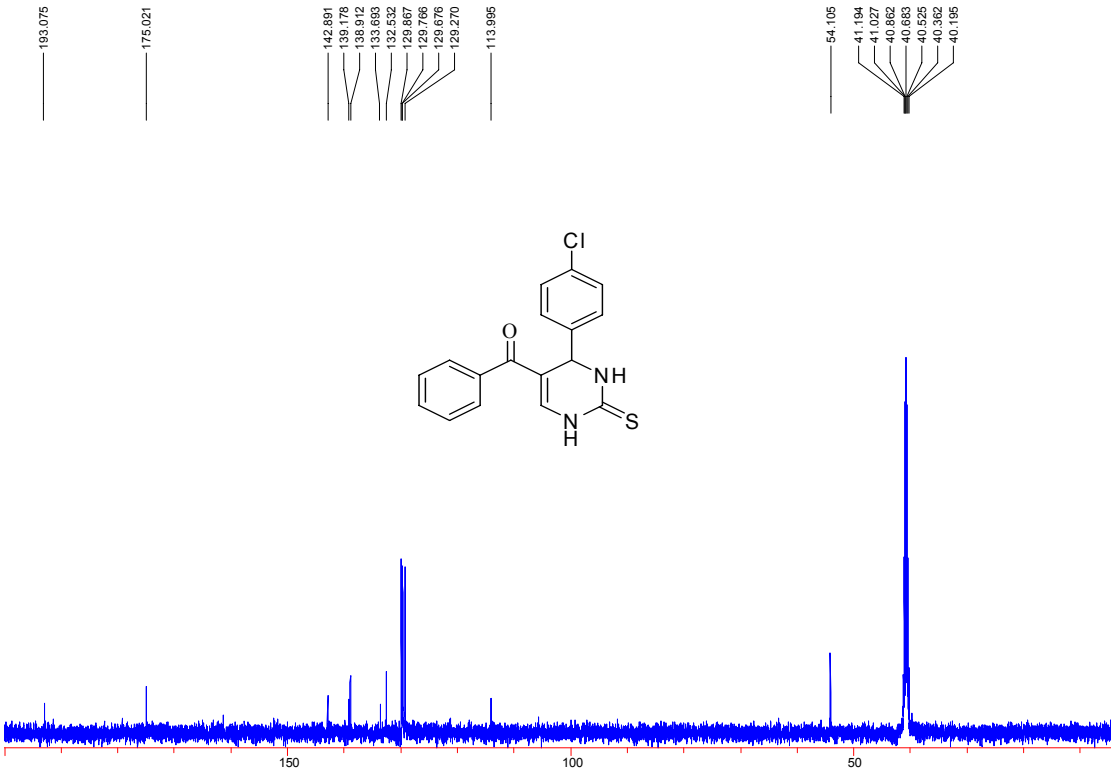
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40.362
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S
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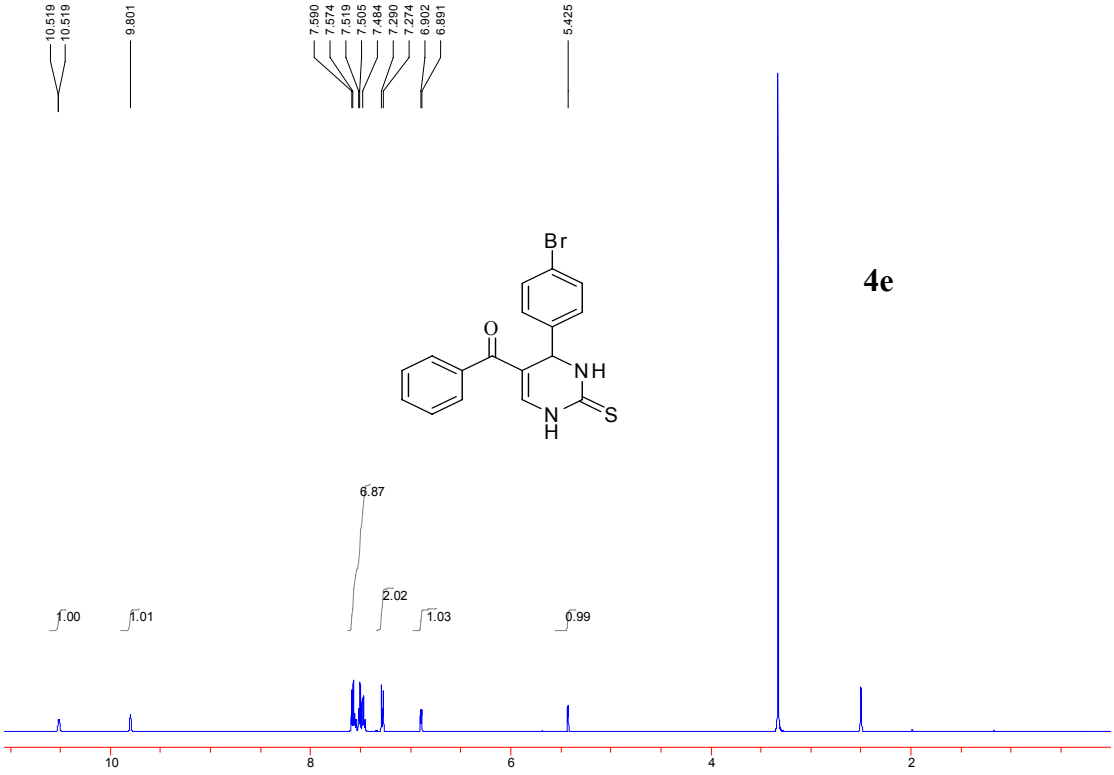
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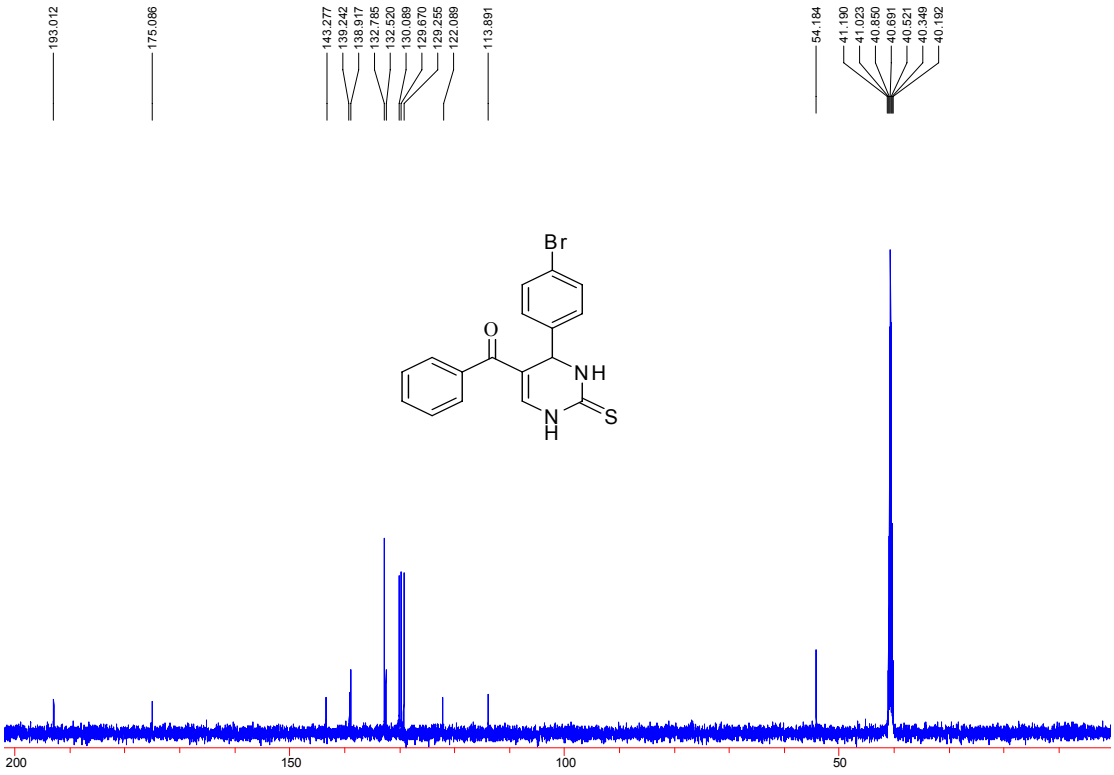
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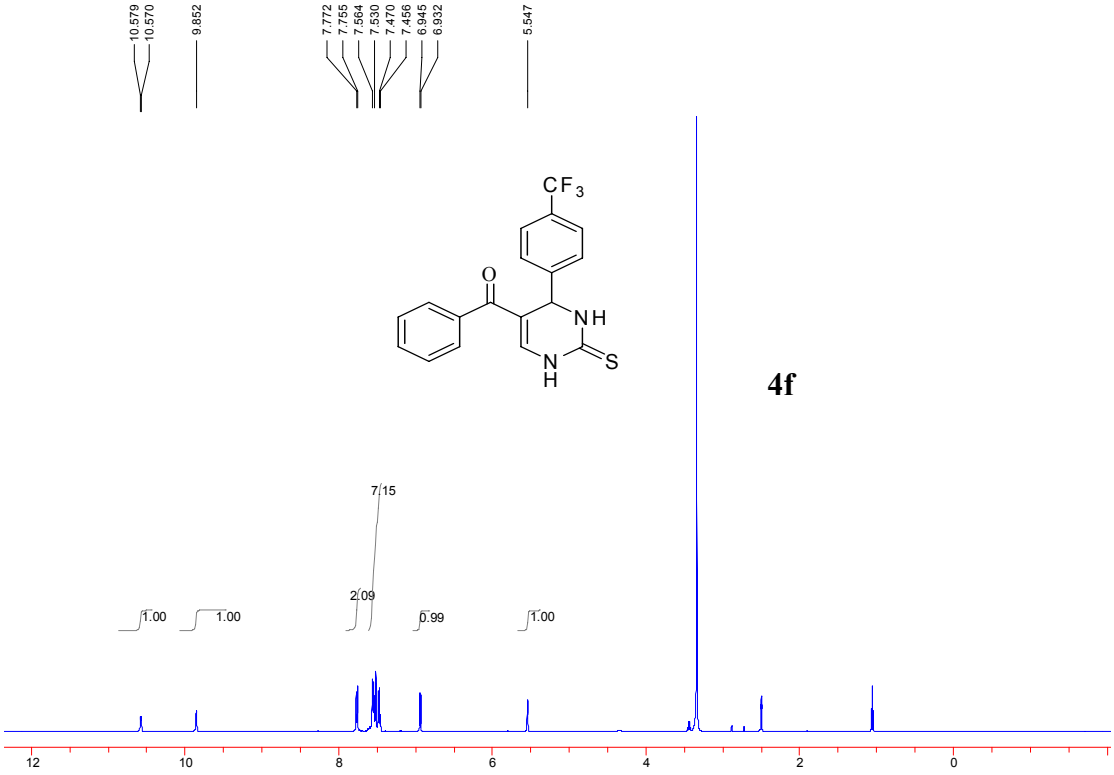
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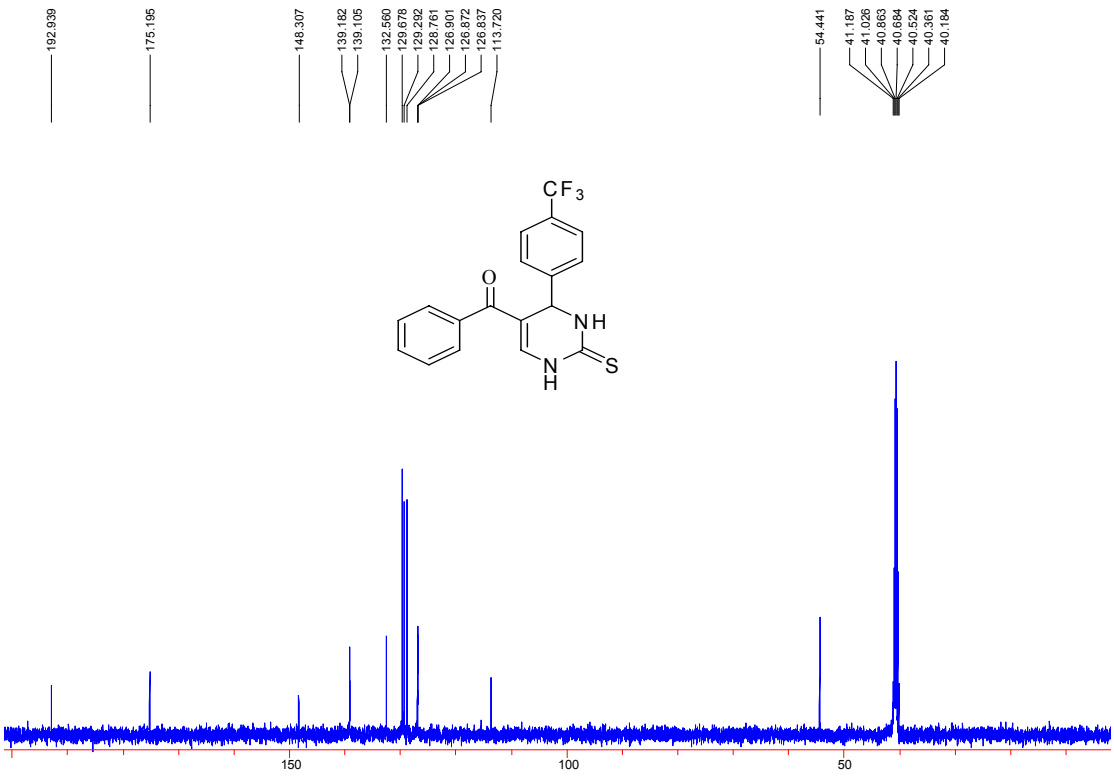
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S
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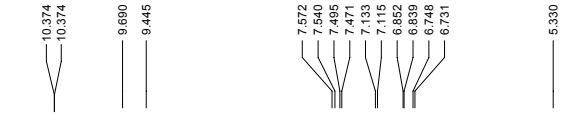
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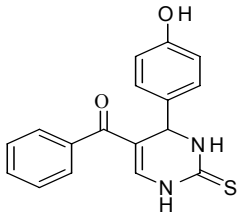
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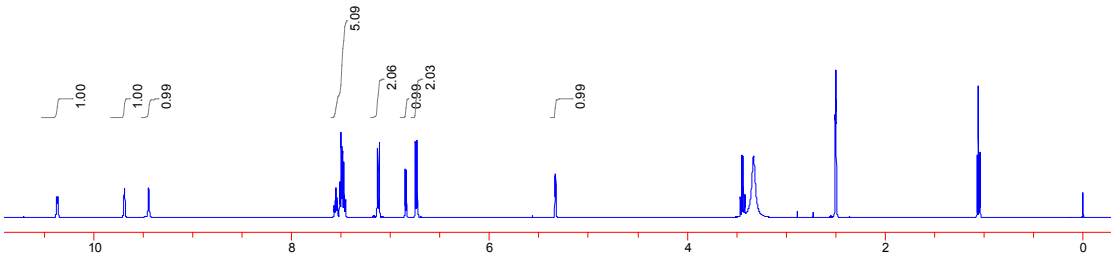
**4g**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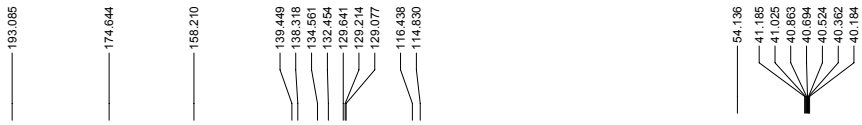
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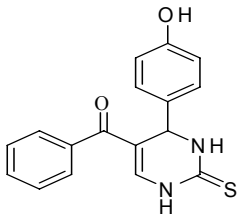
40.362
40.184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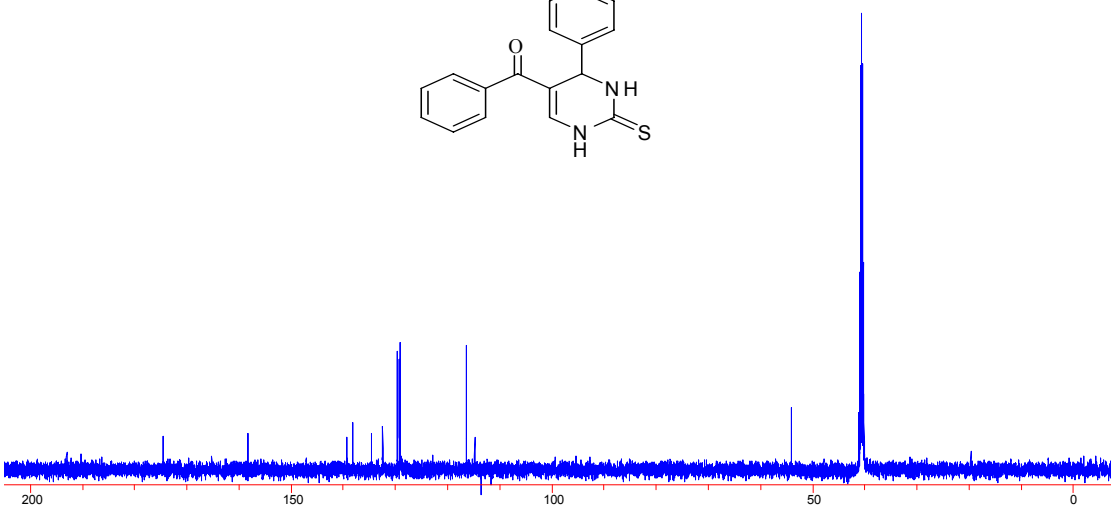
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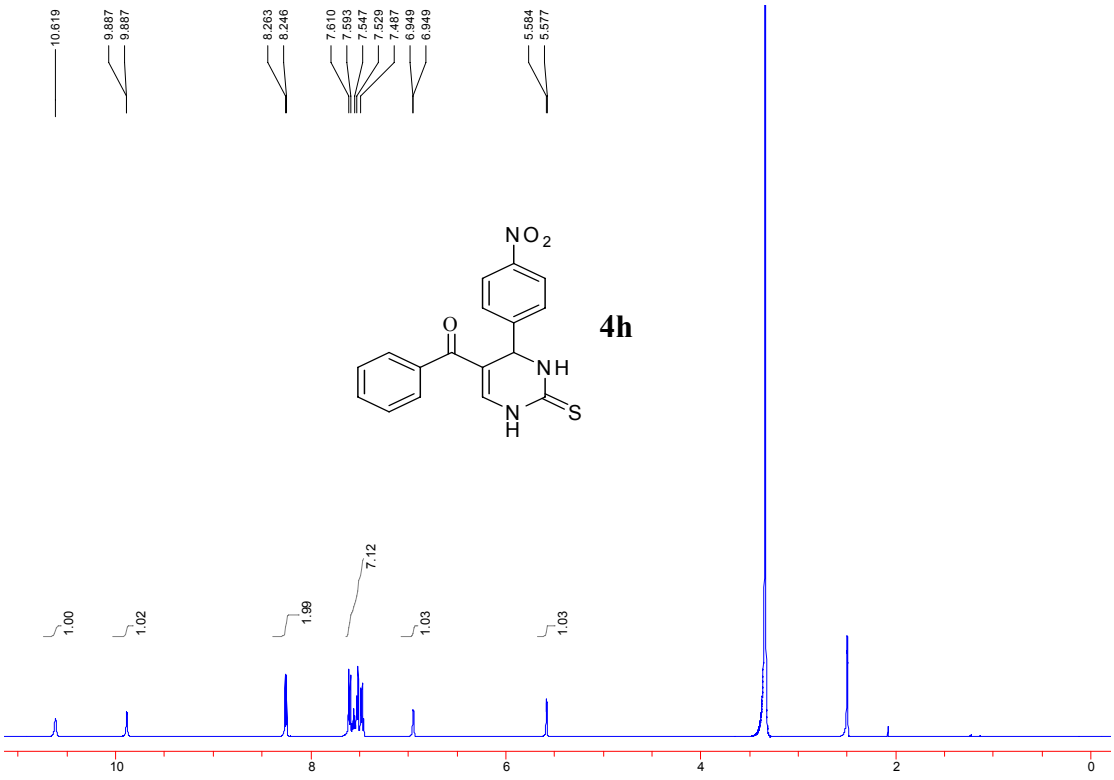
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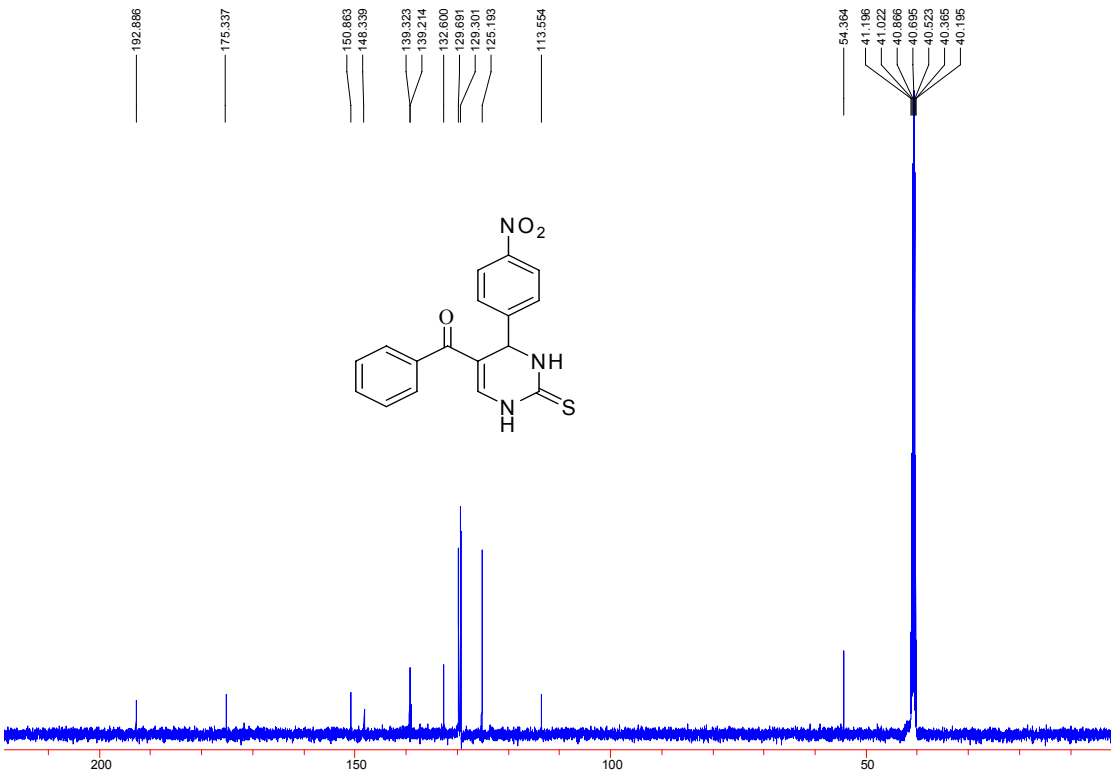
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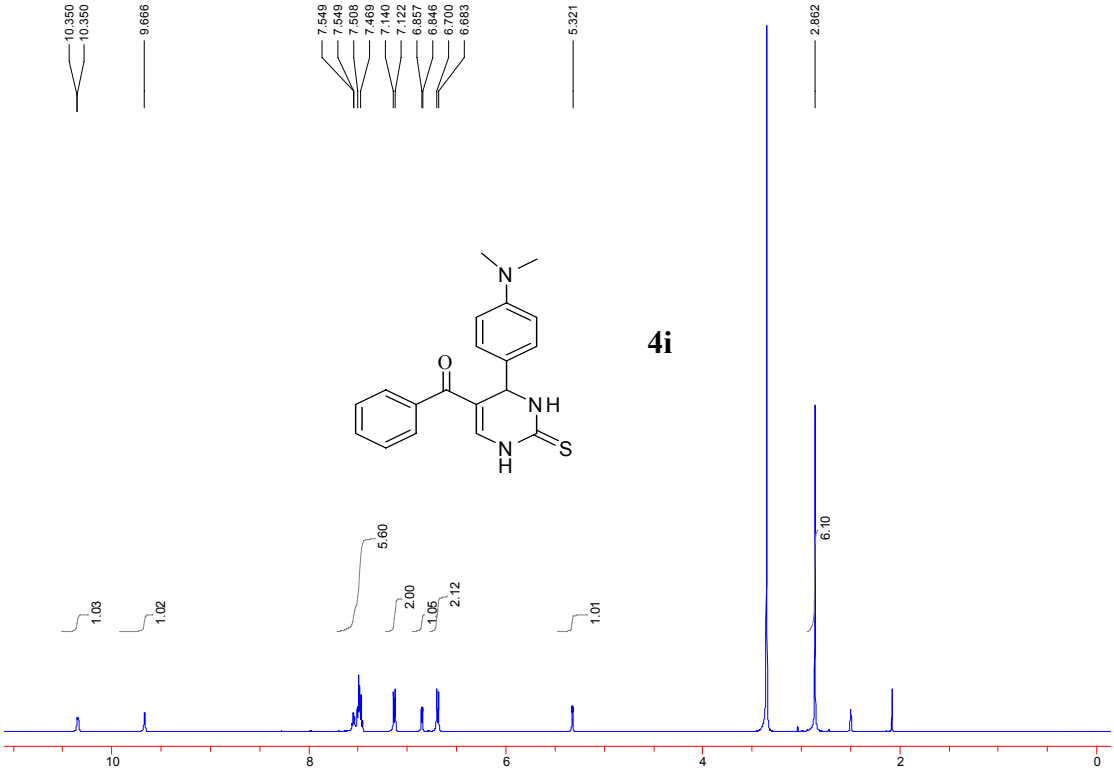
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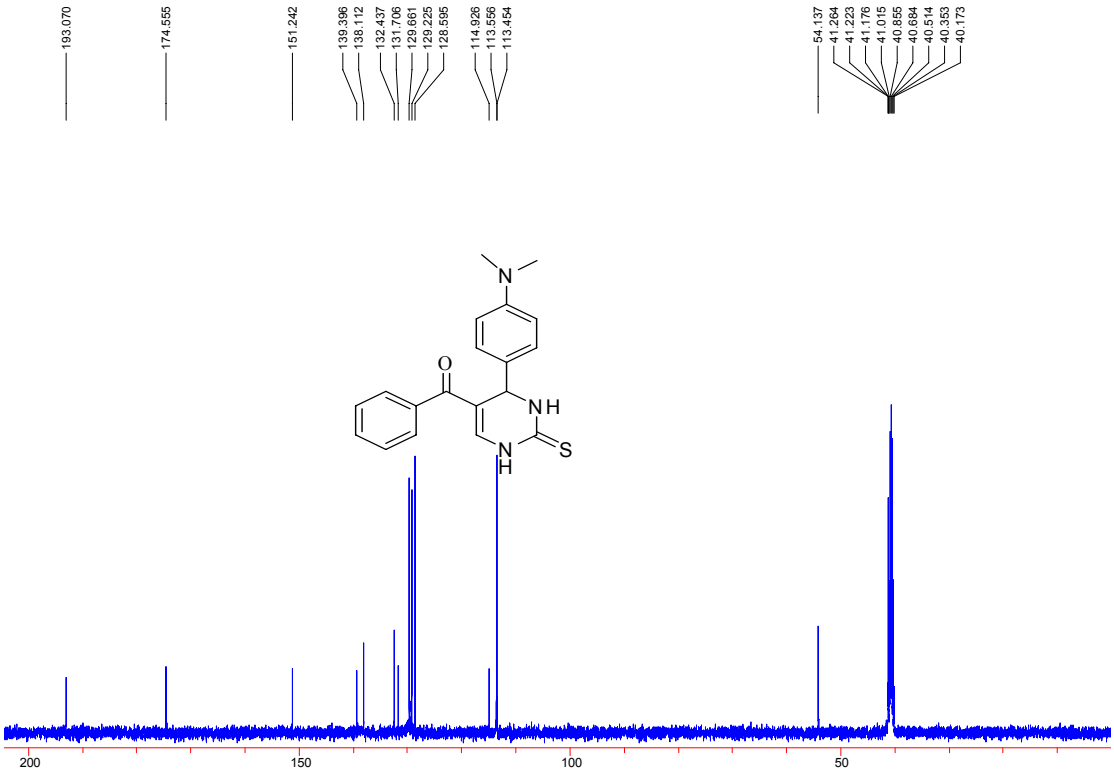
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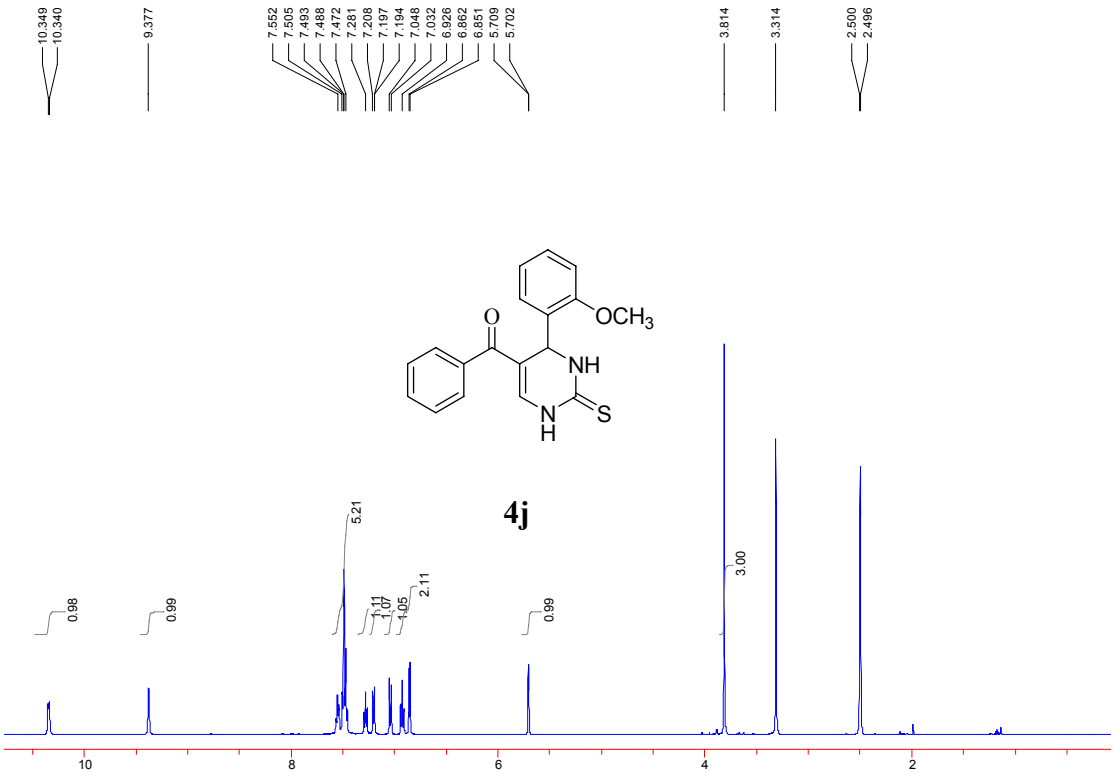
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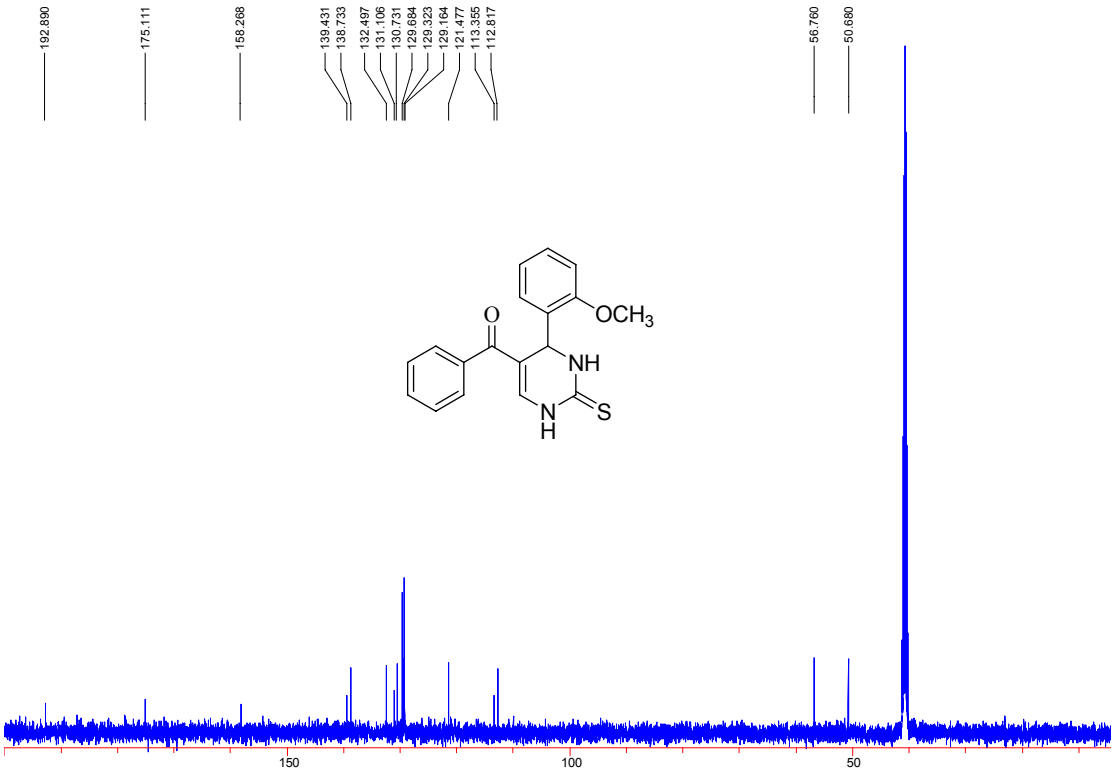
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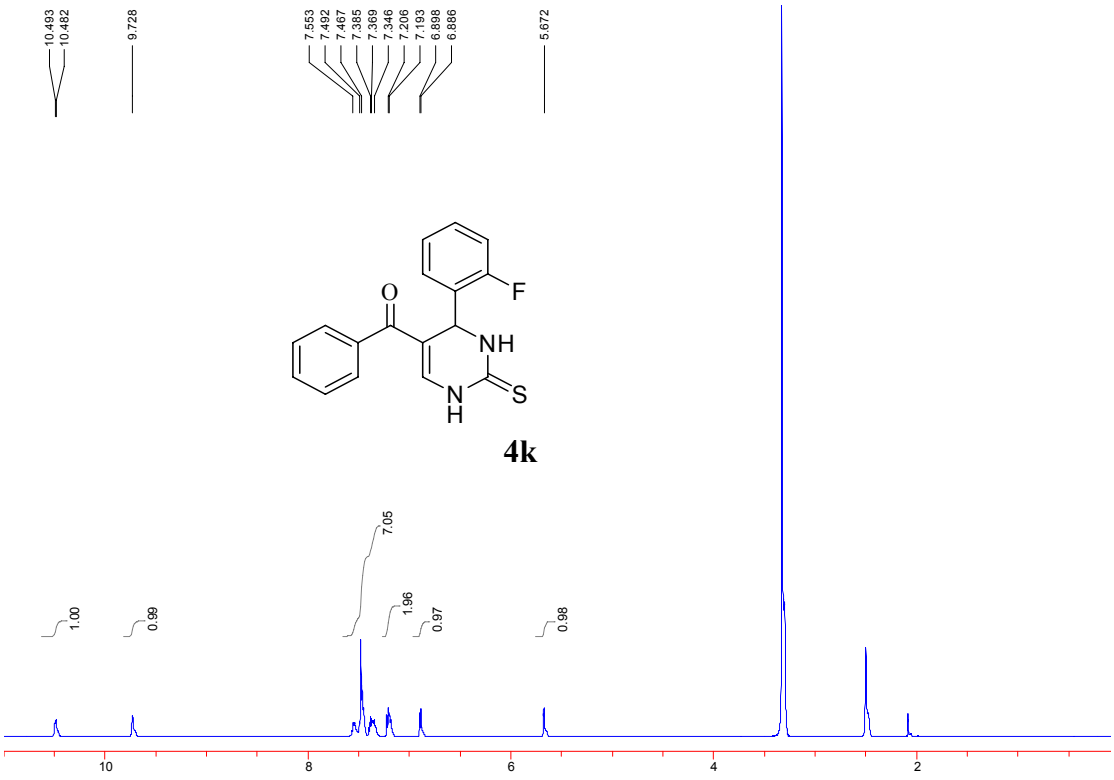
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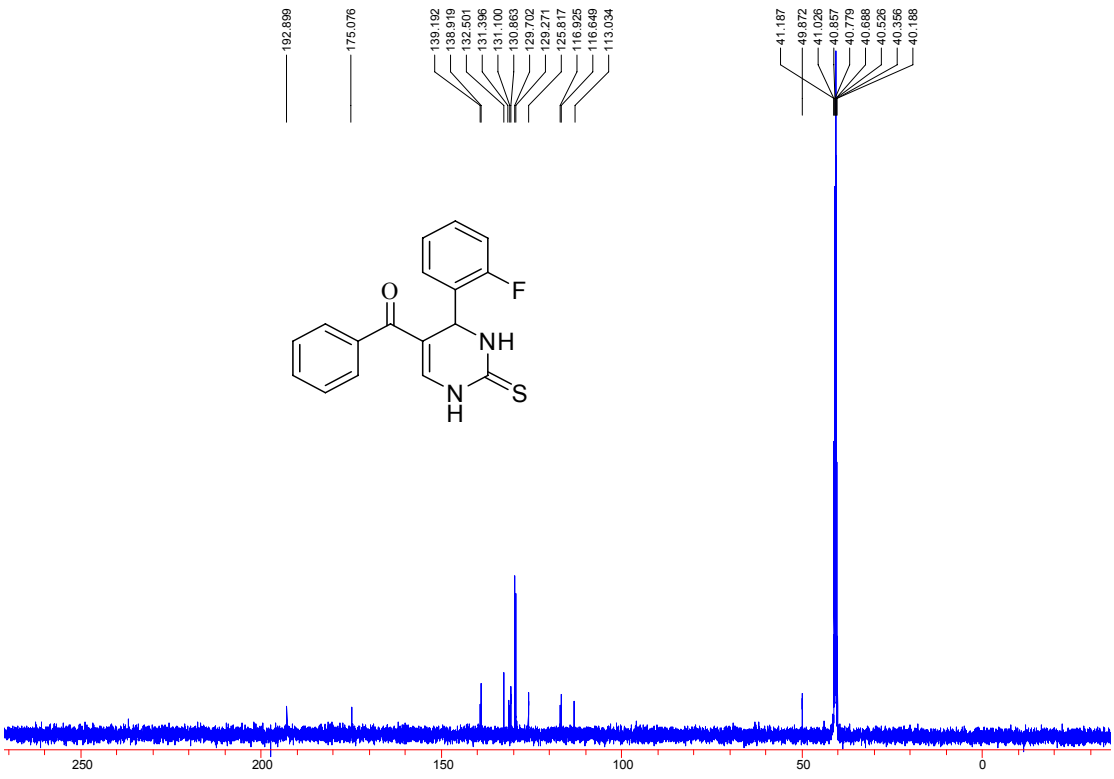
**4k**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H
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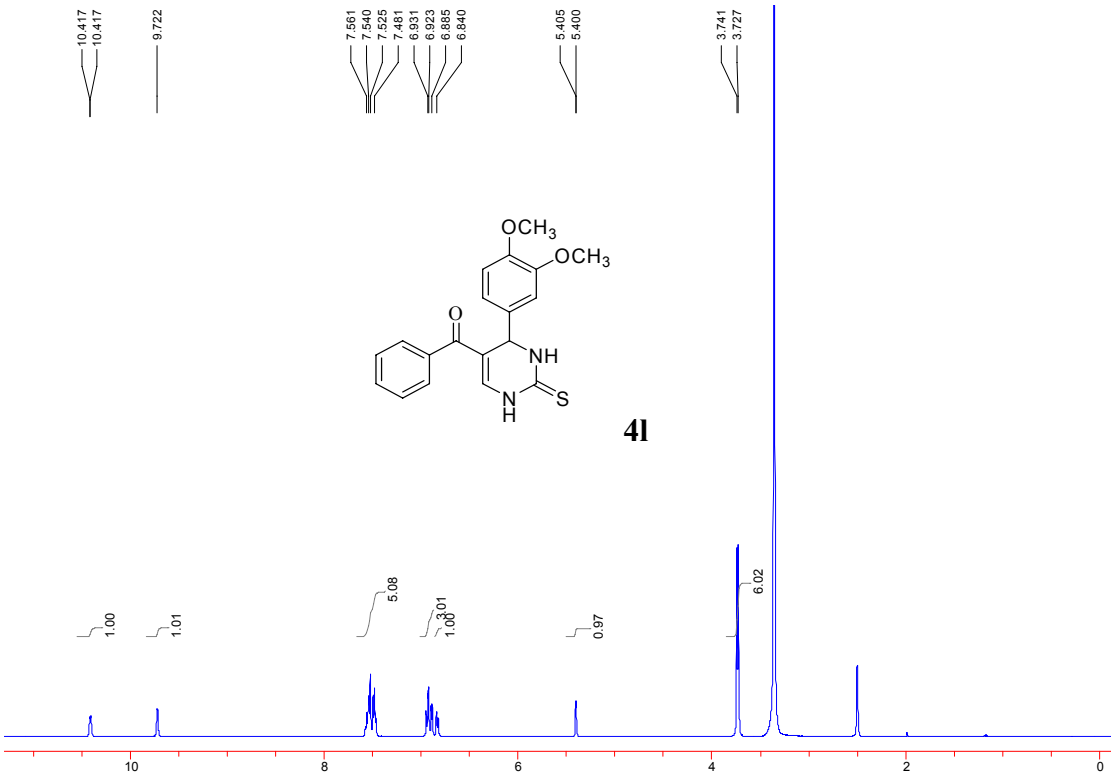
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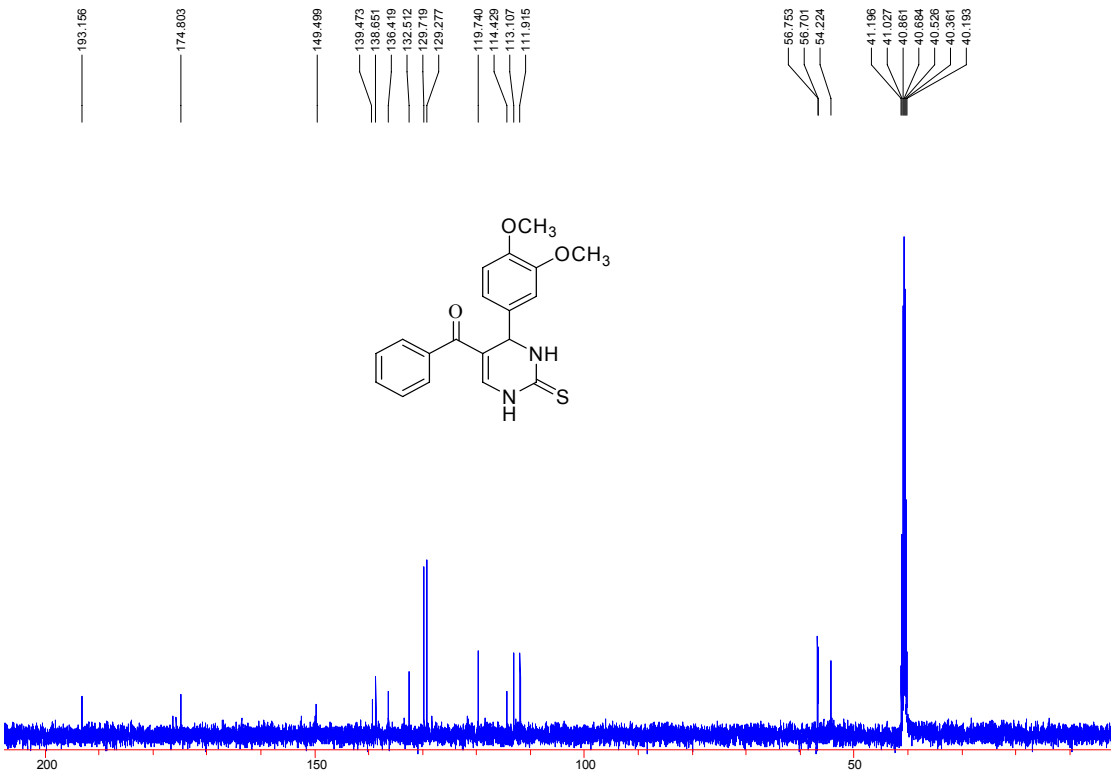
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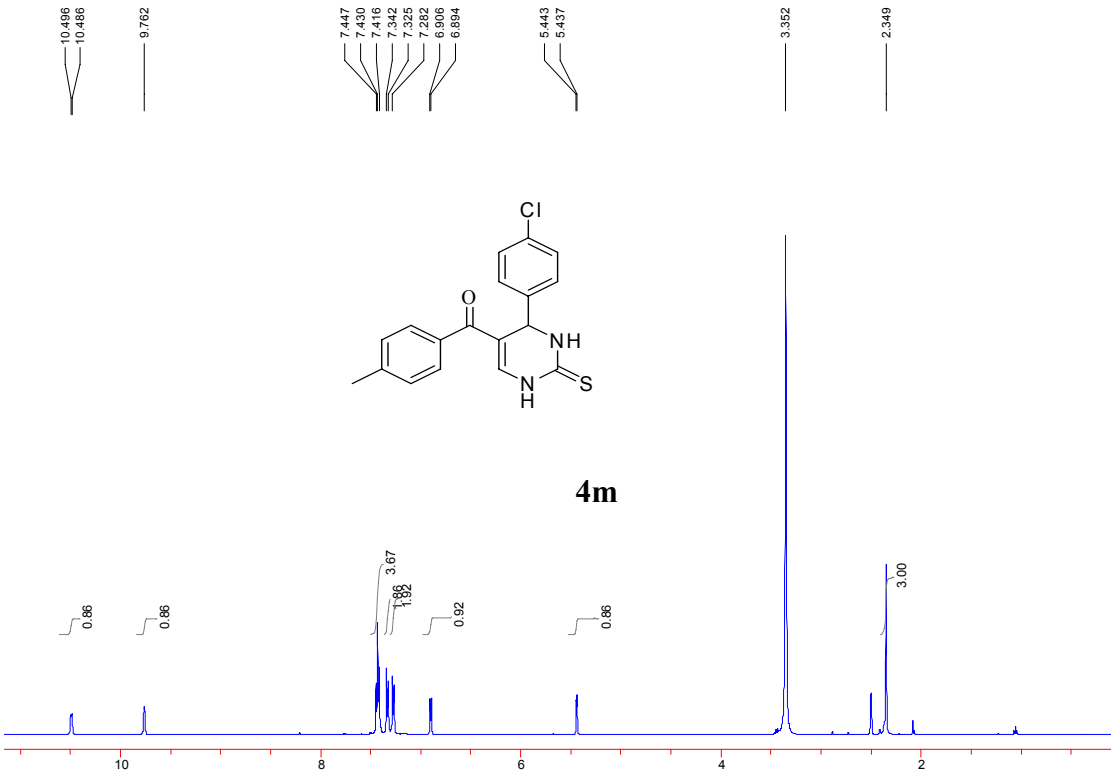
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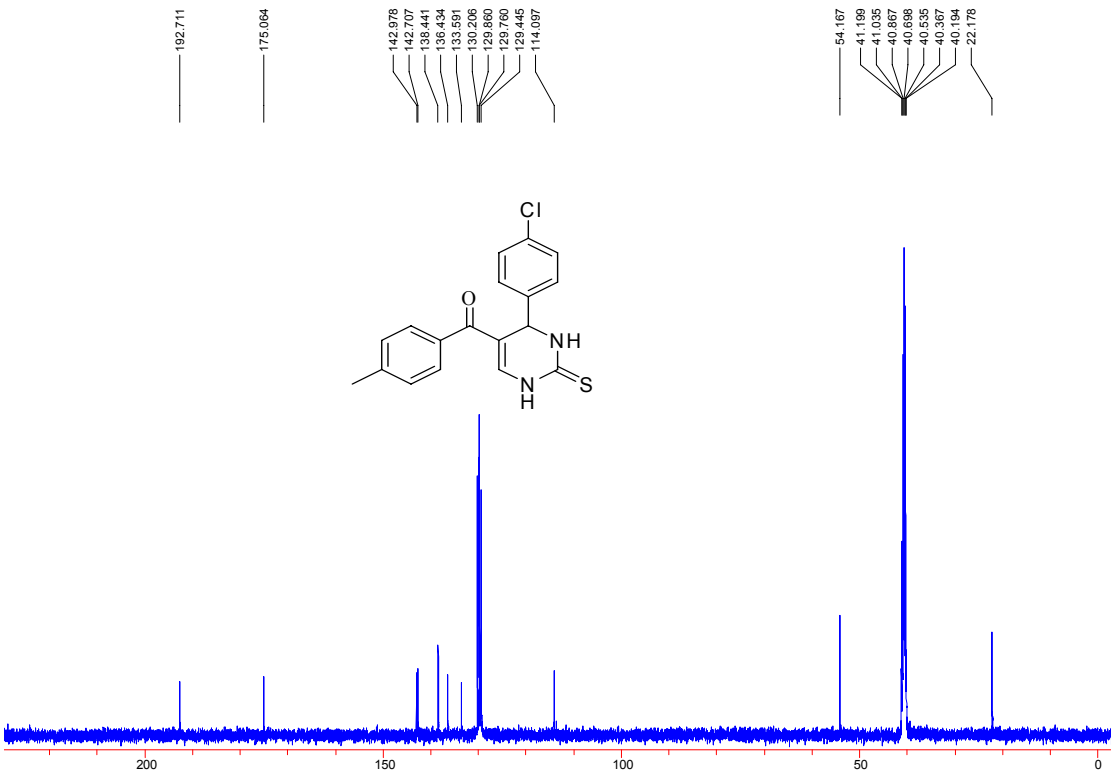
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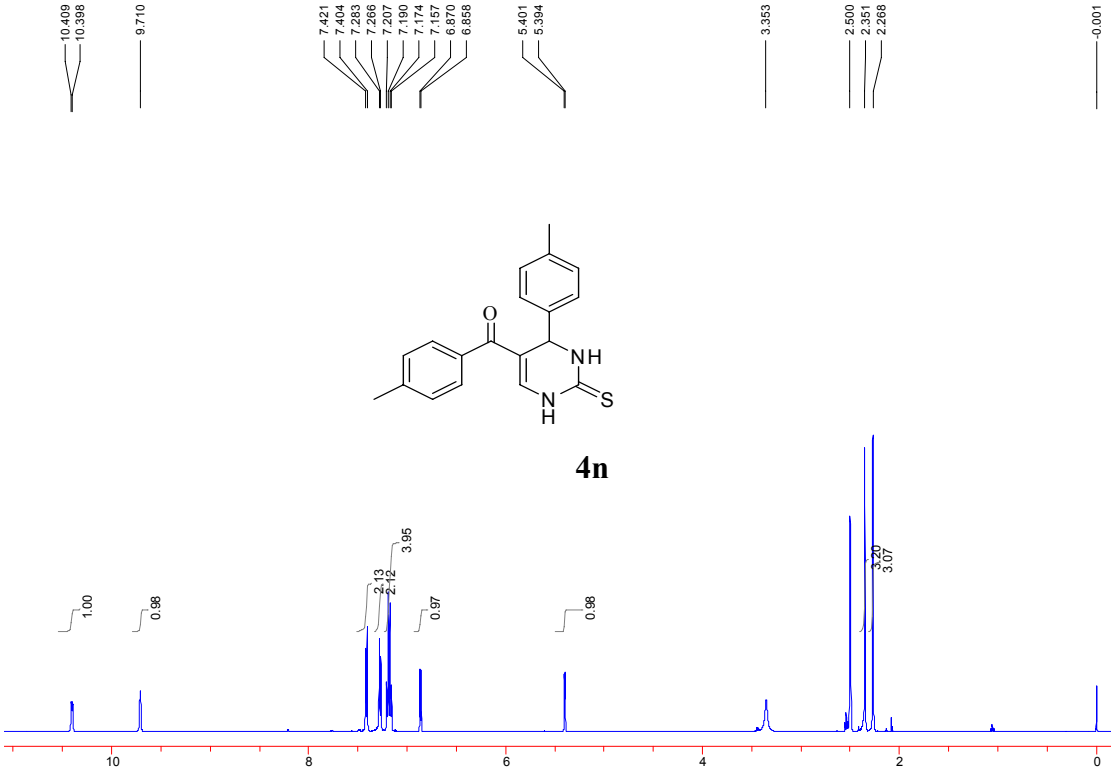
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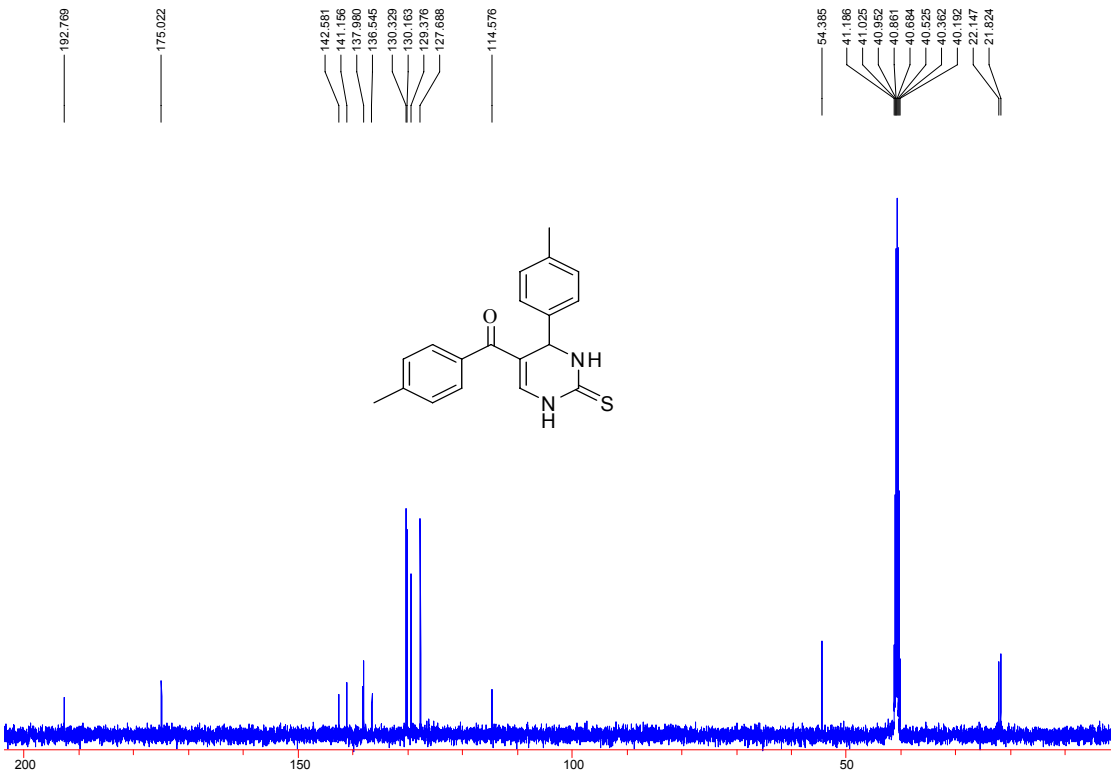
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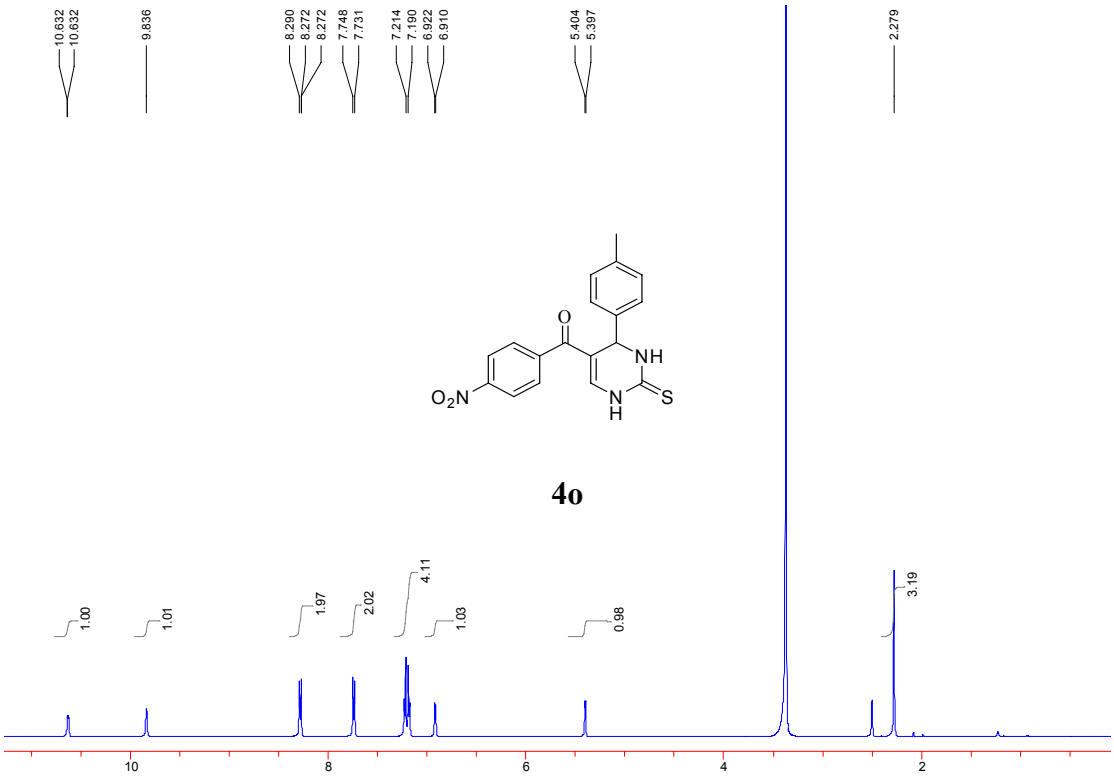
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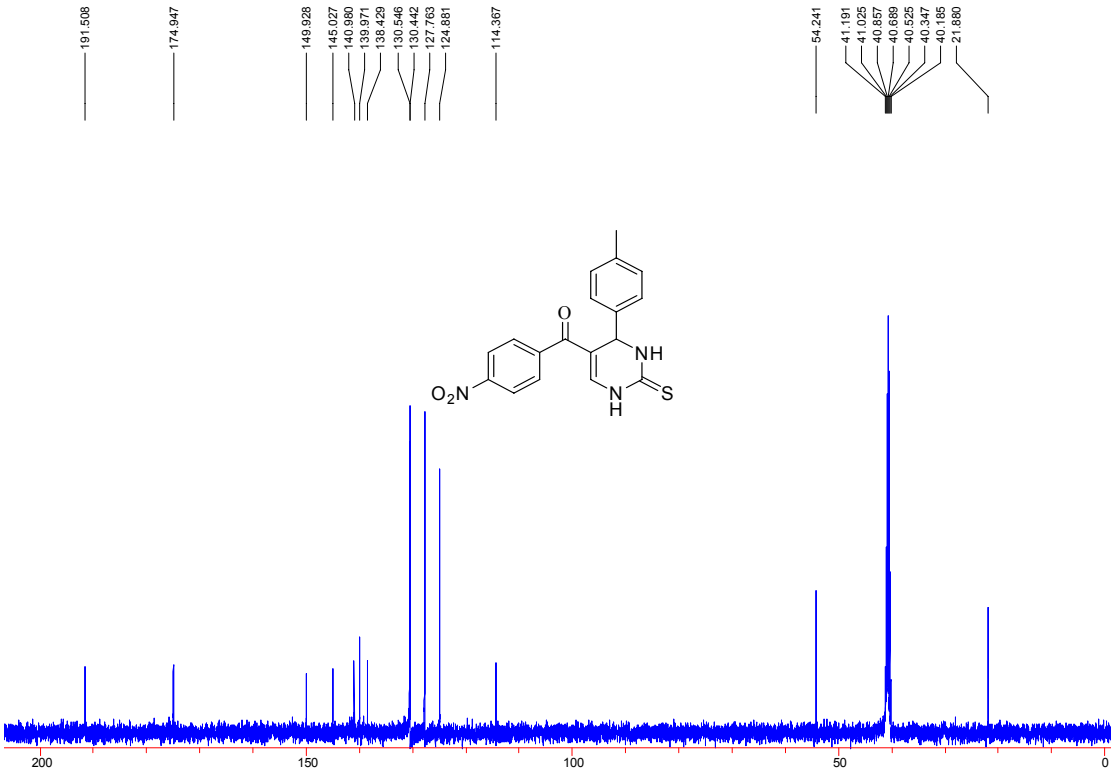
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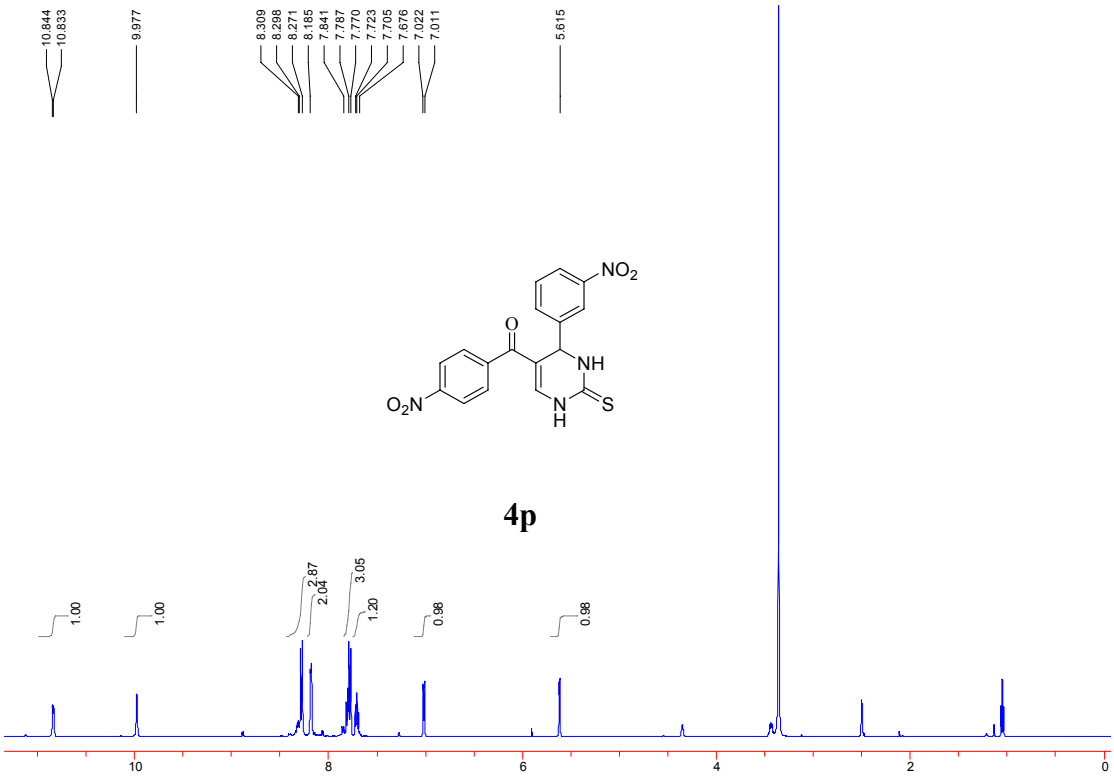
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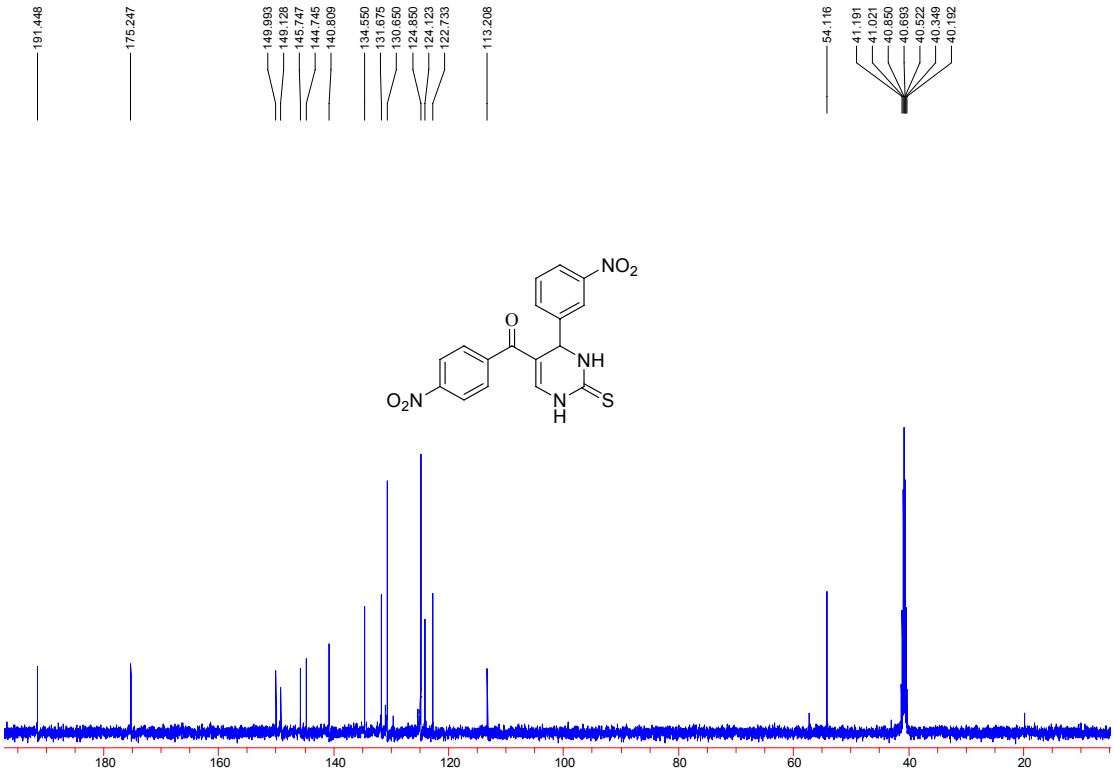
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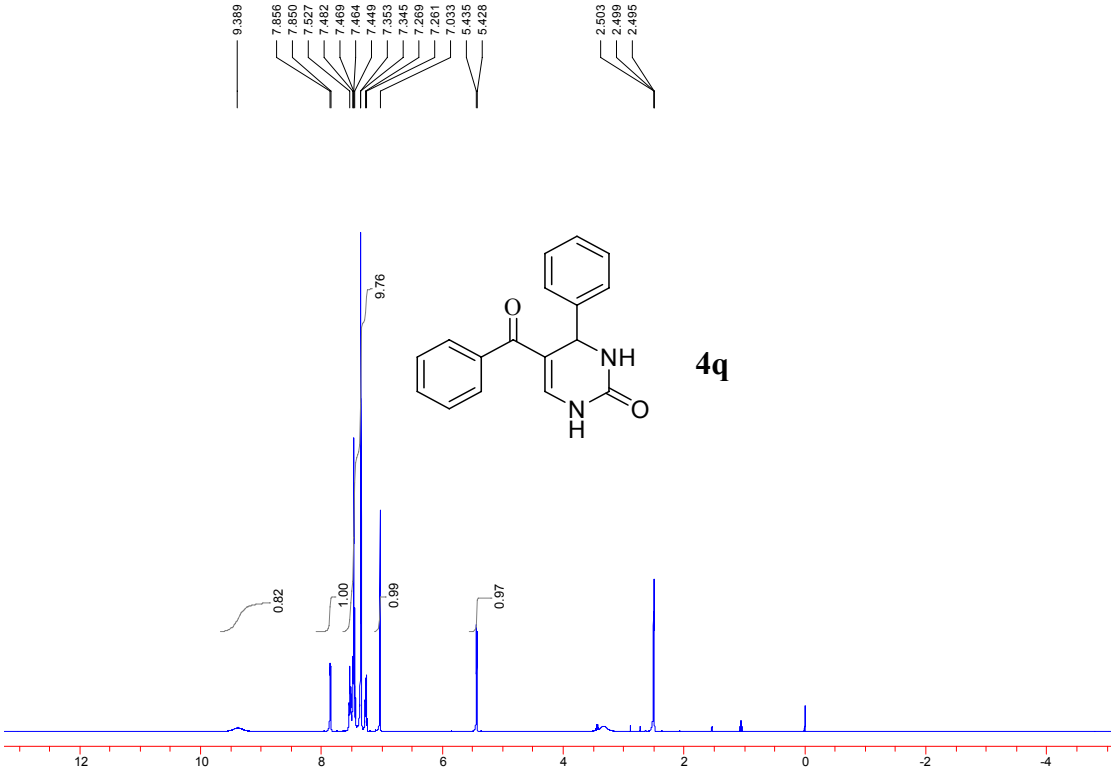
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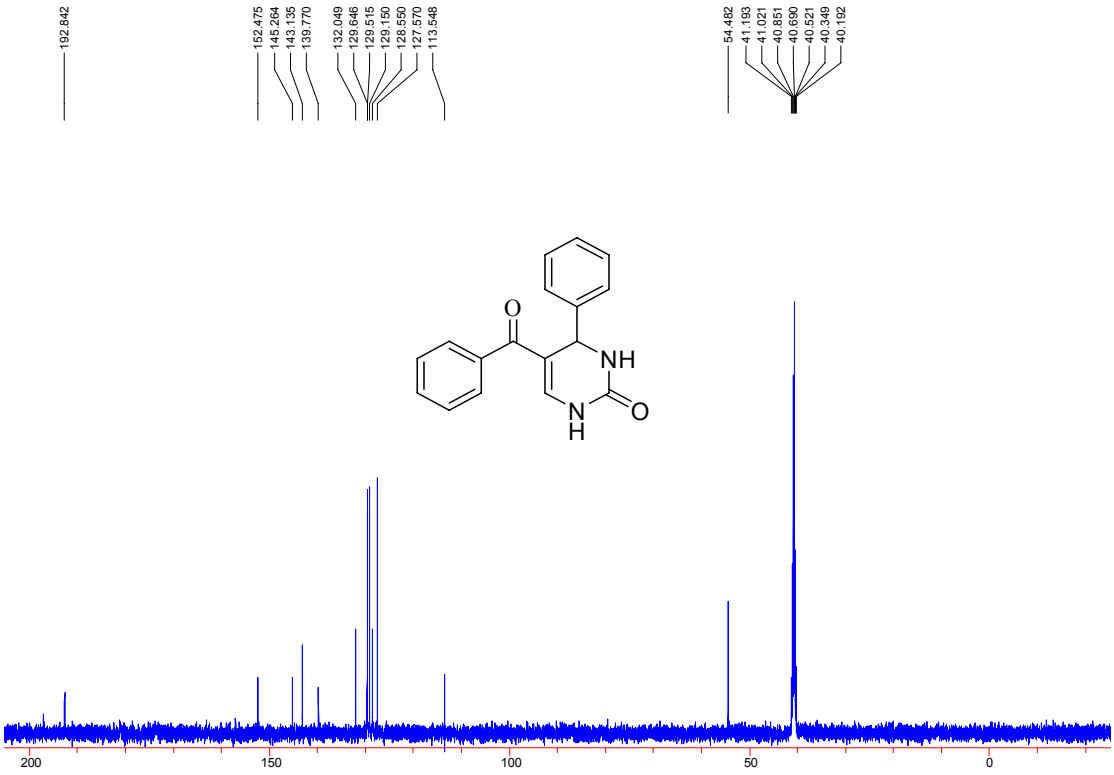
**4q**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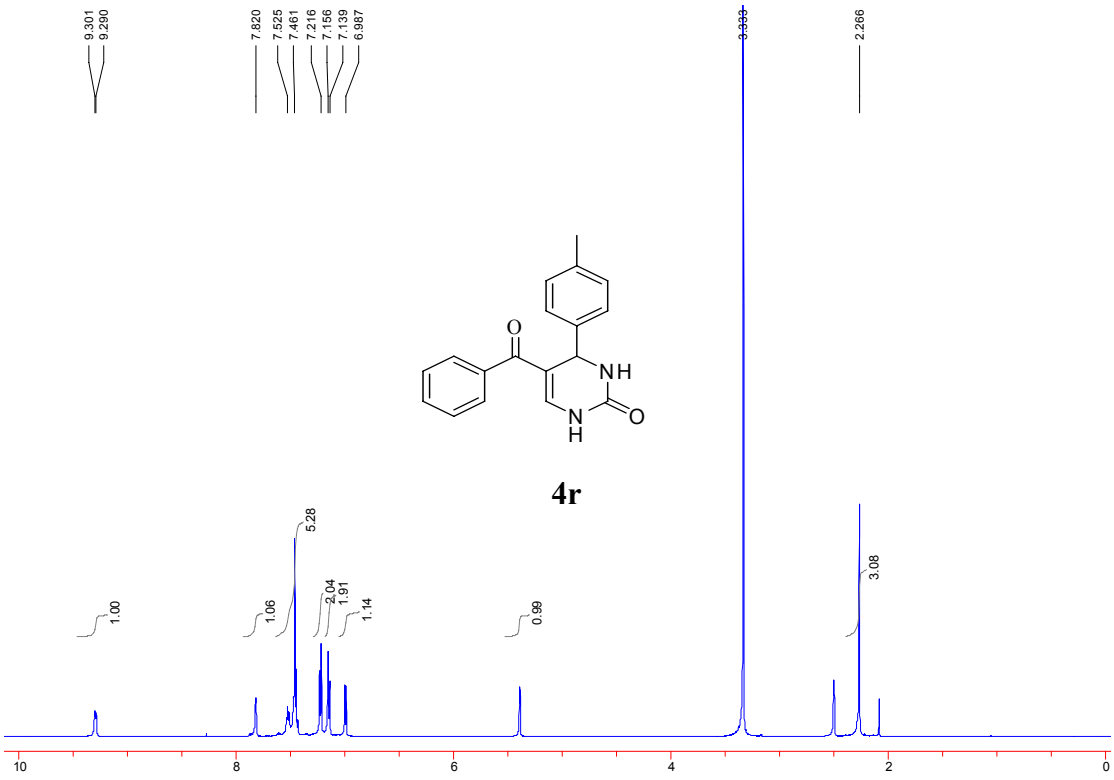
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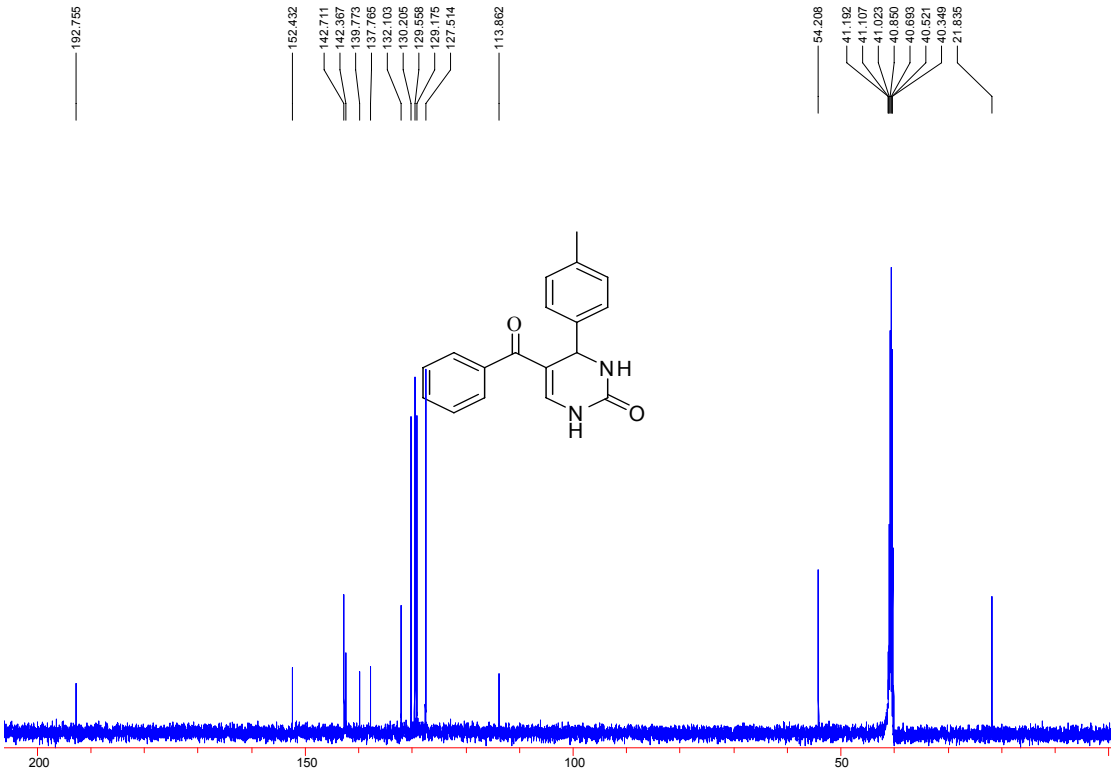
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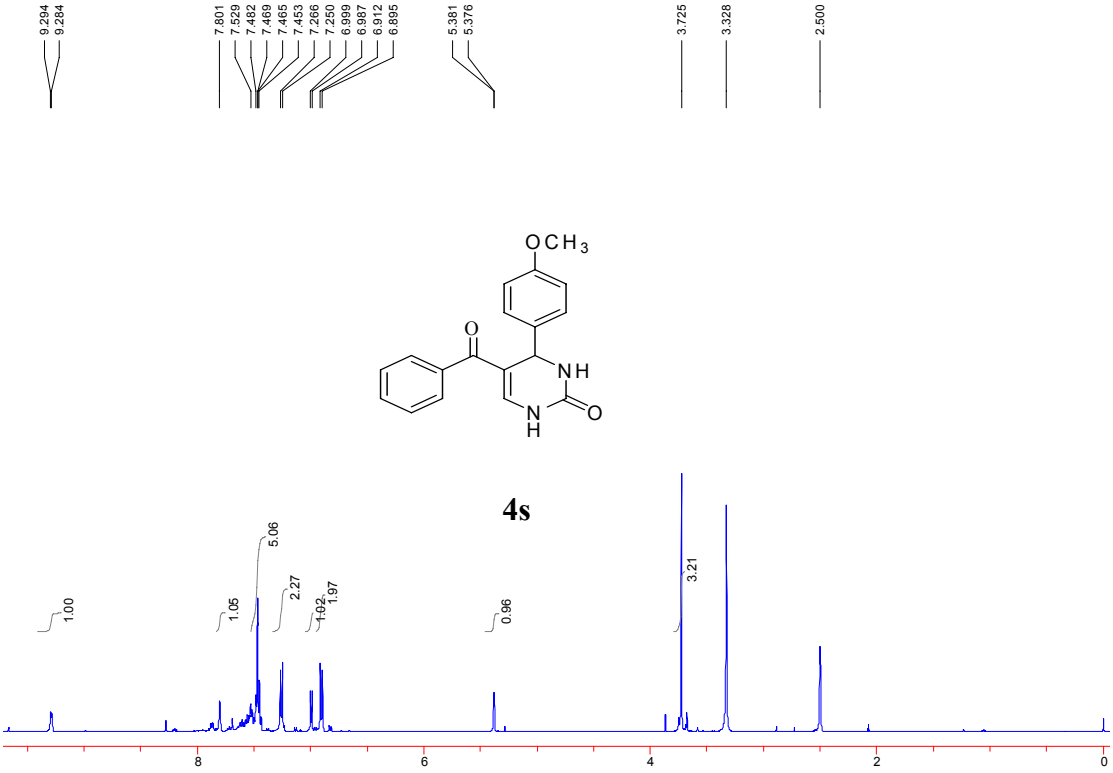
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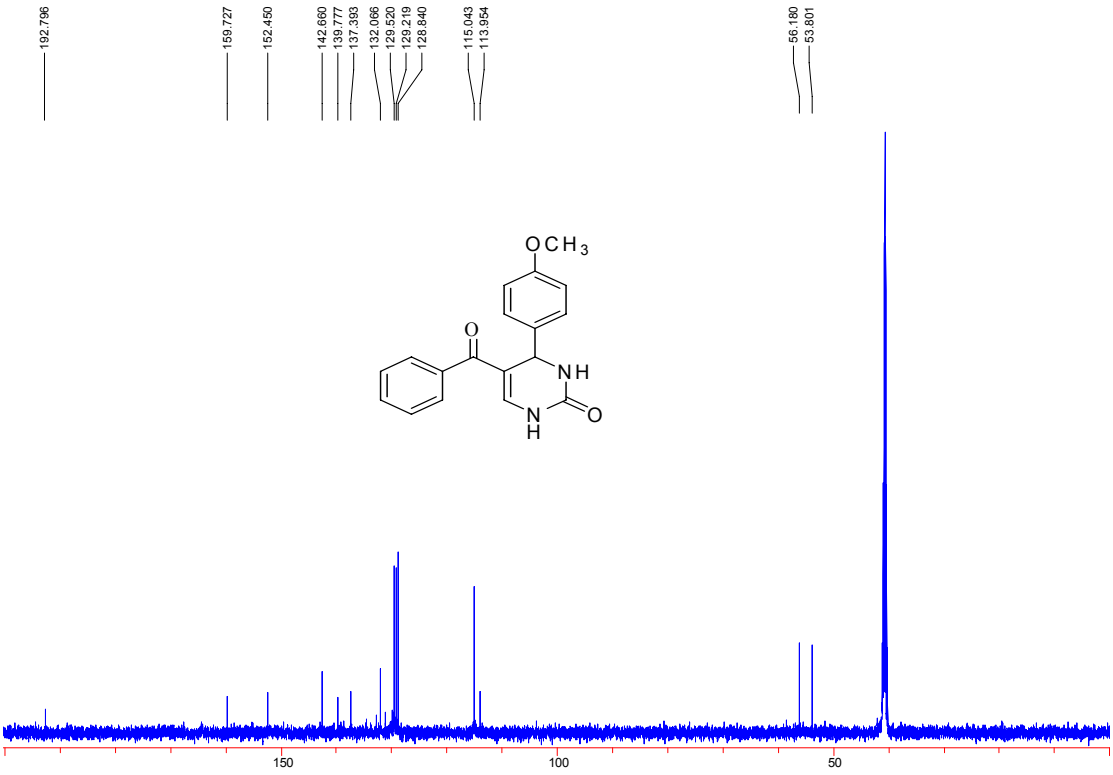
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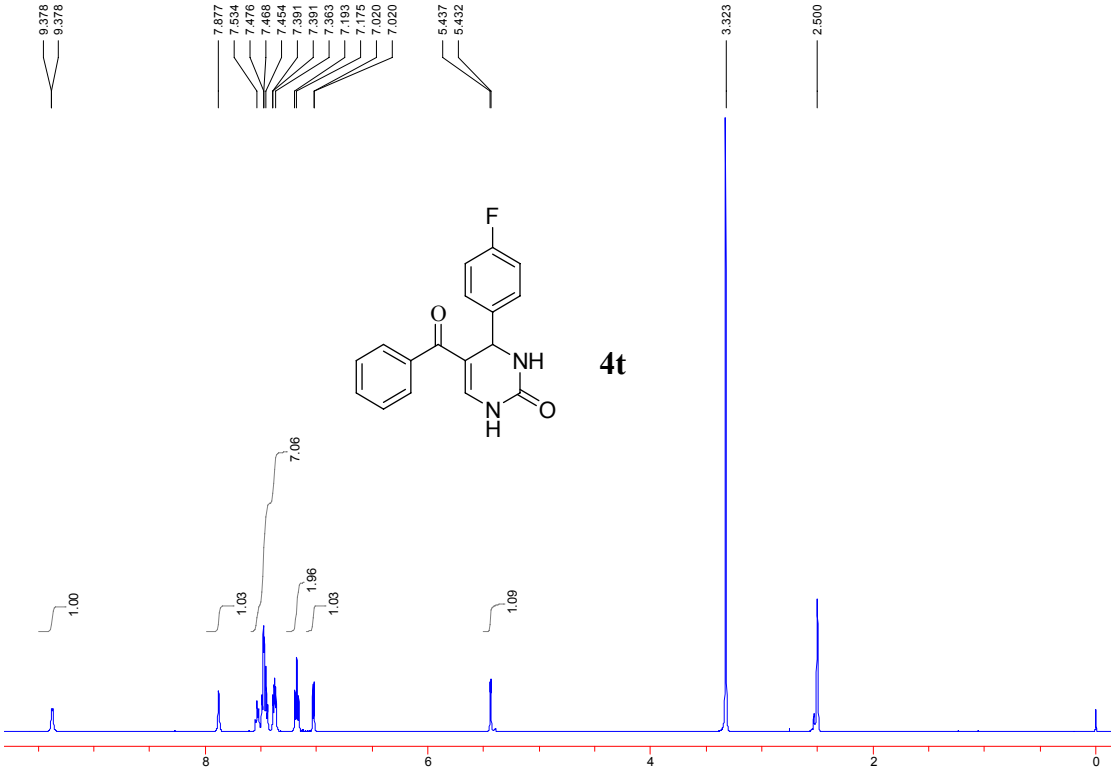
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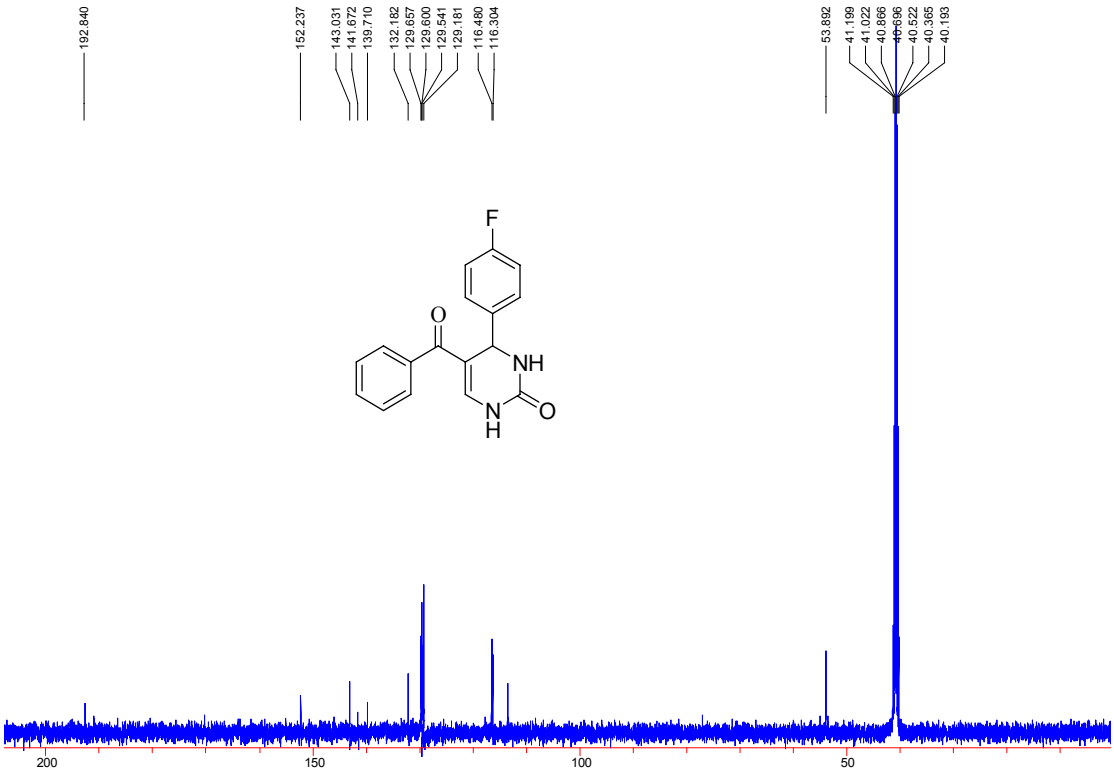
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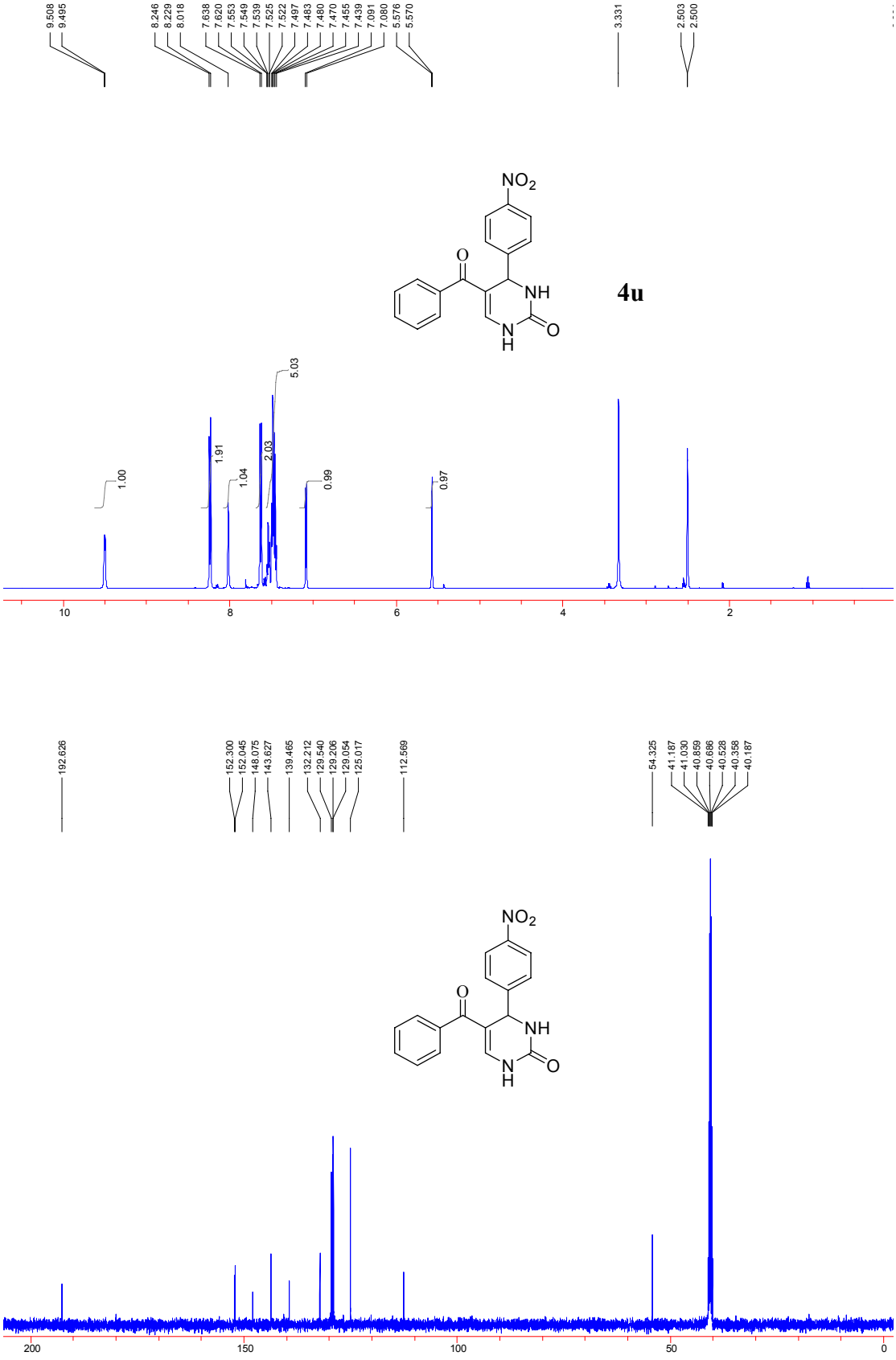
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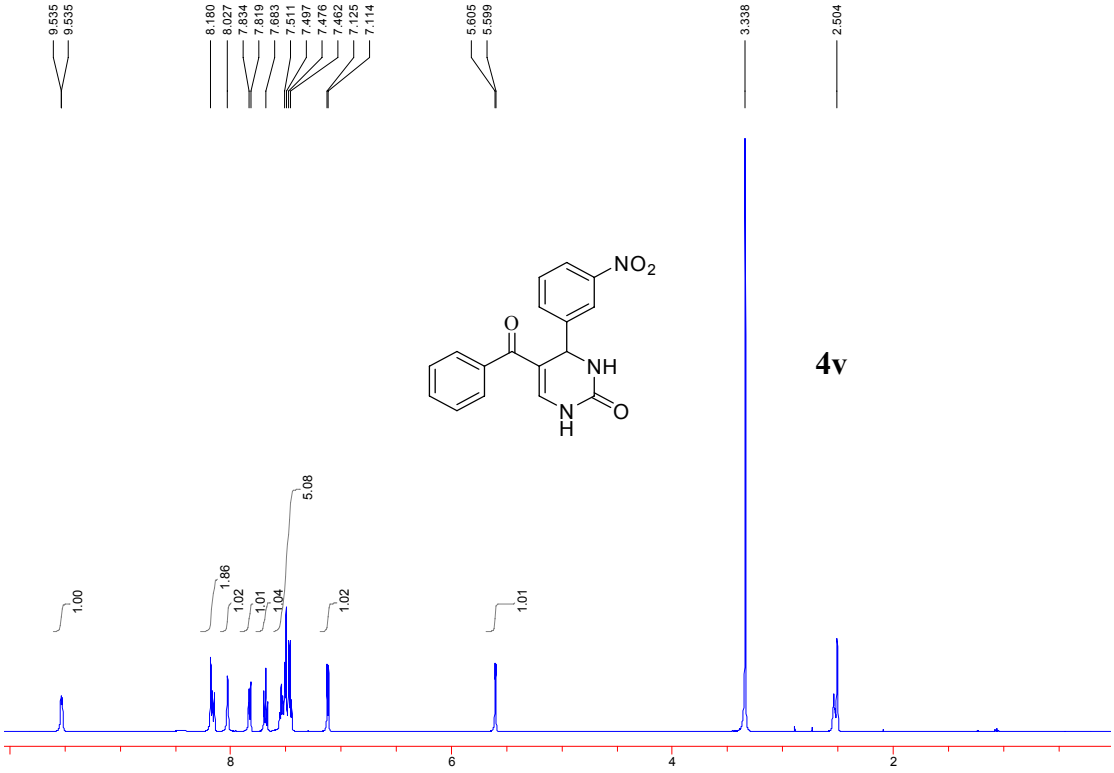
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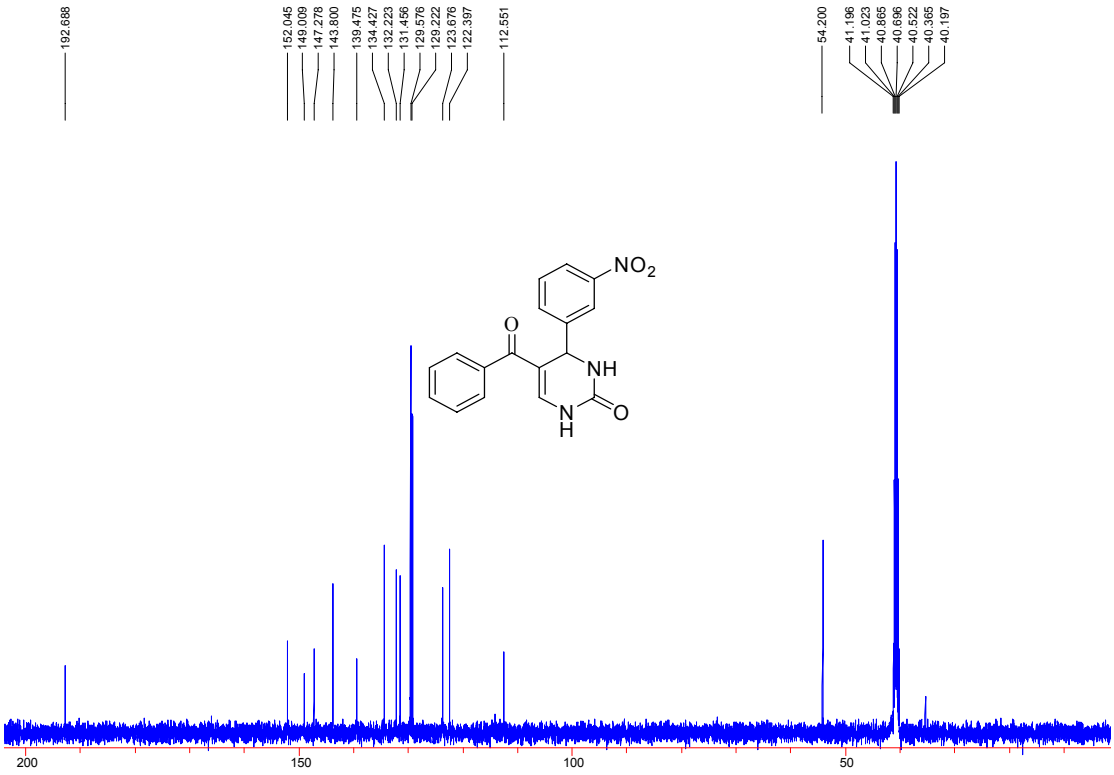
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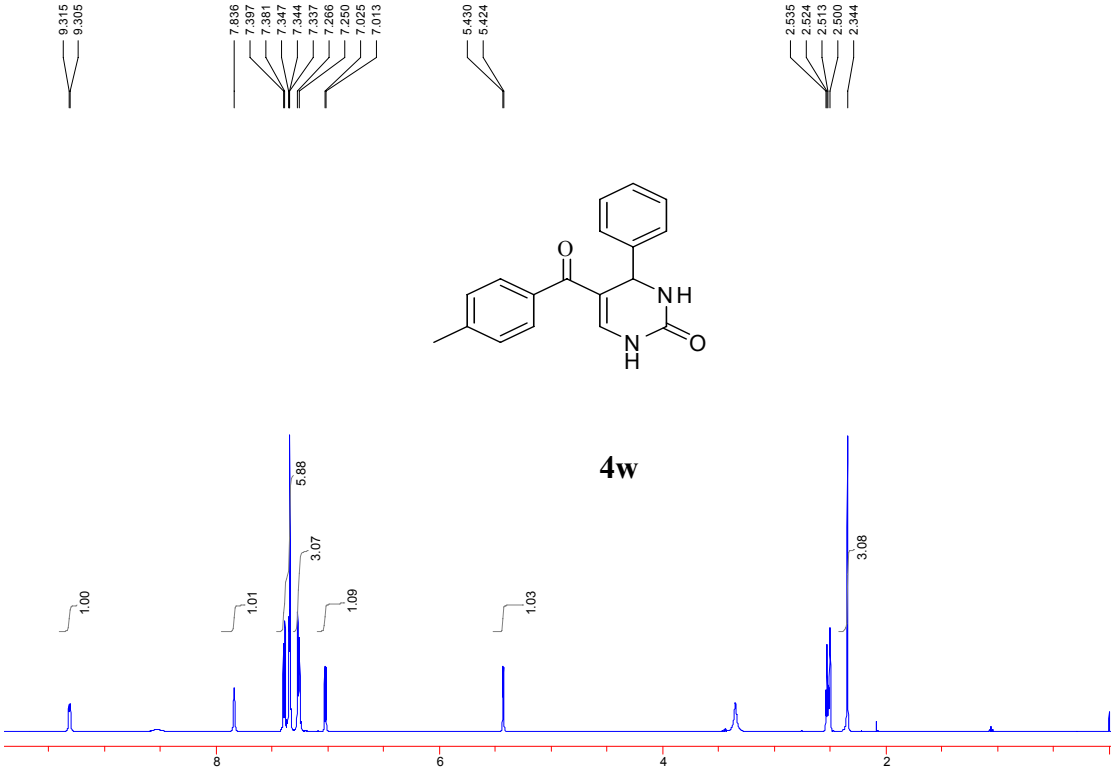
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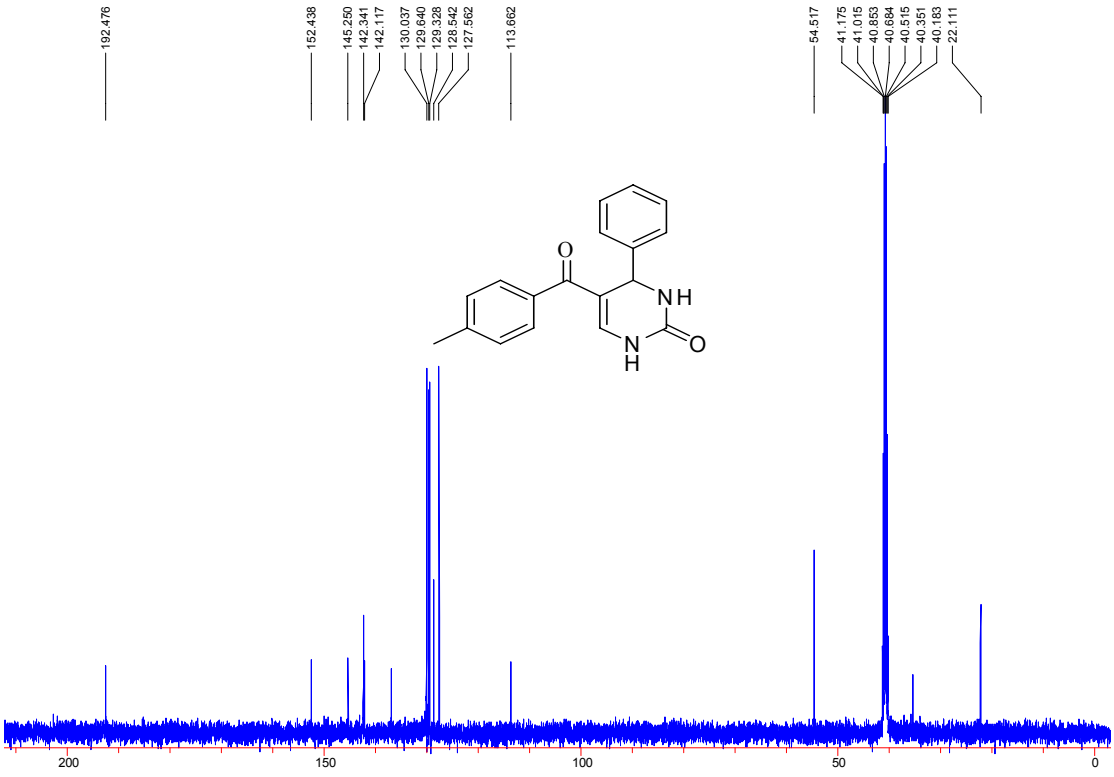
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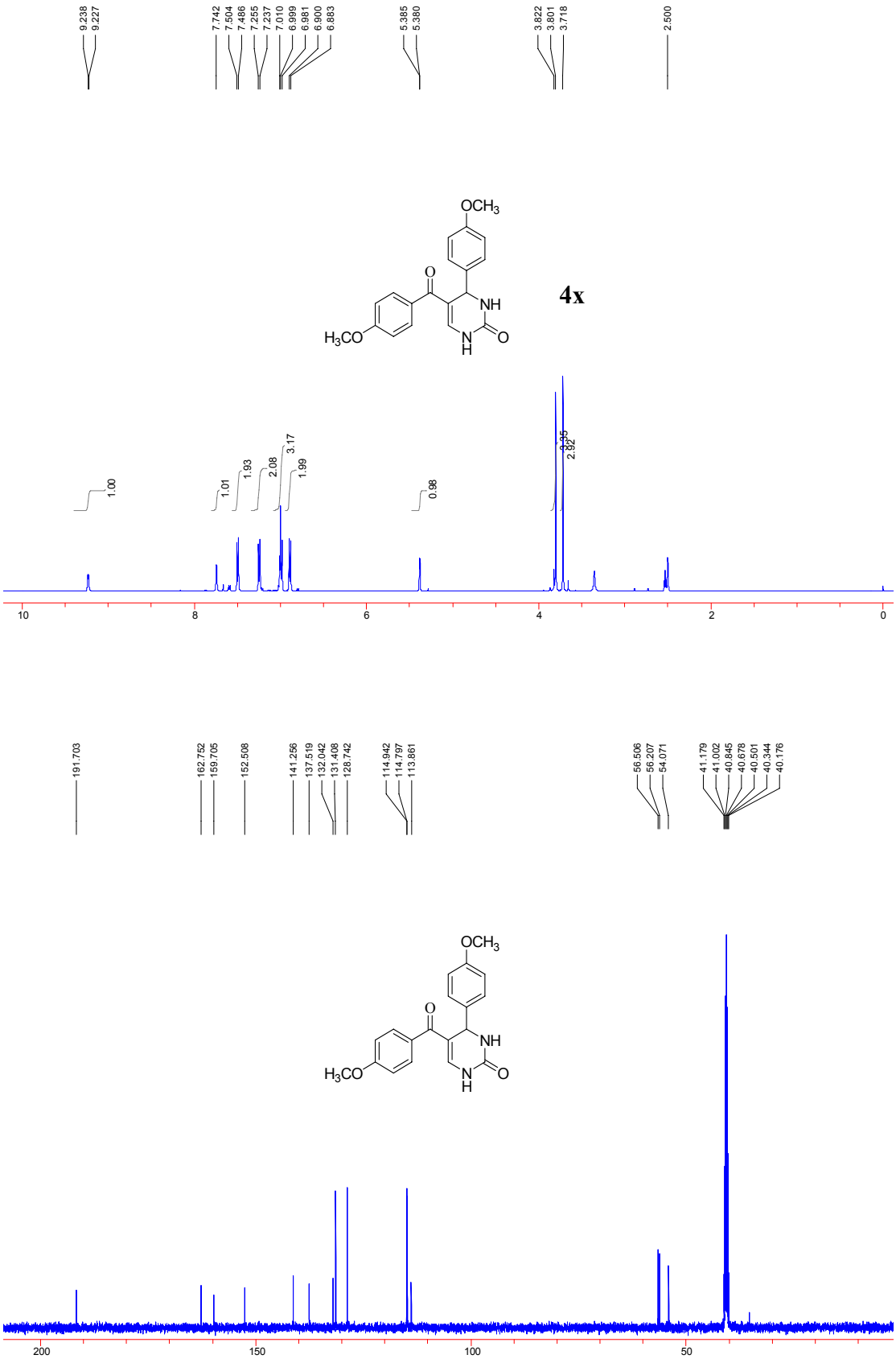
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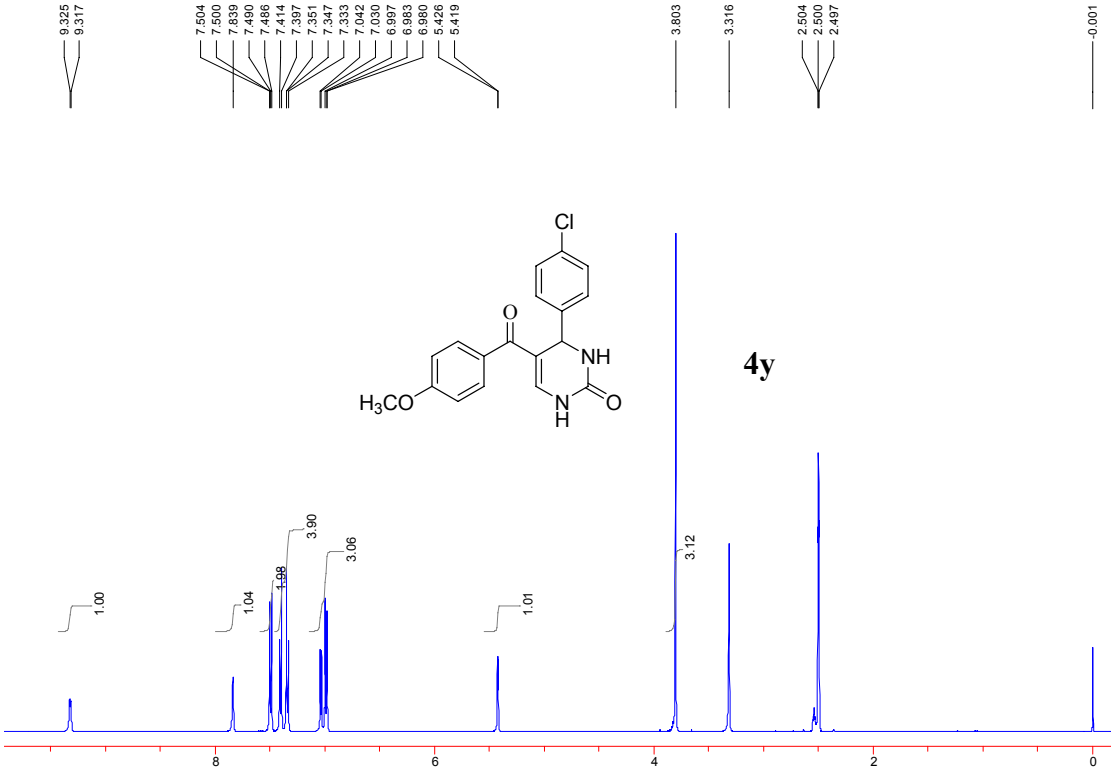
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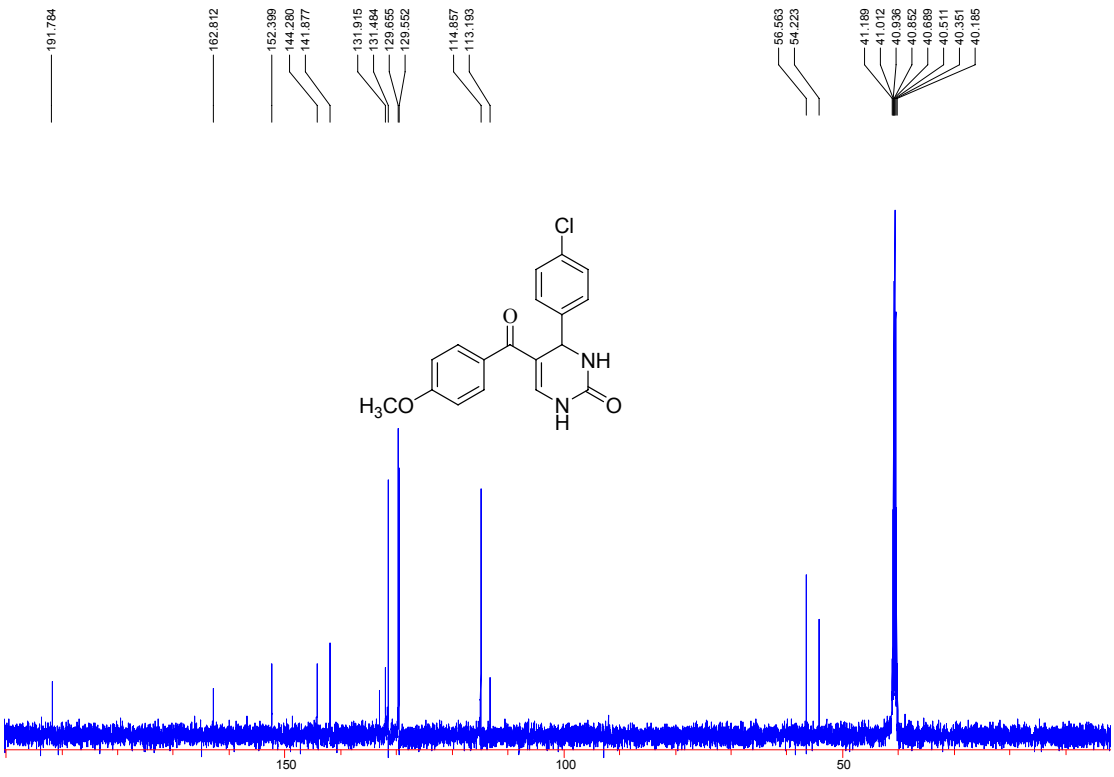
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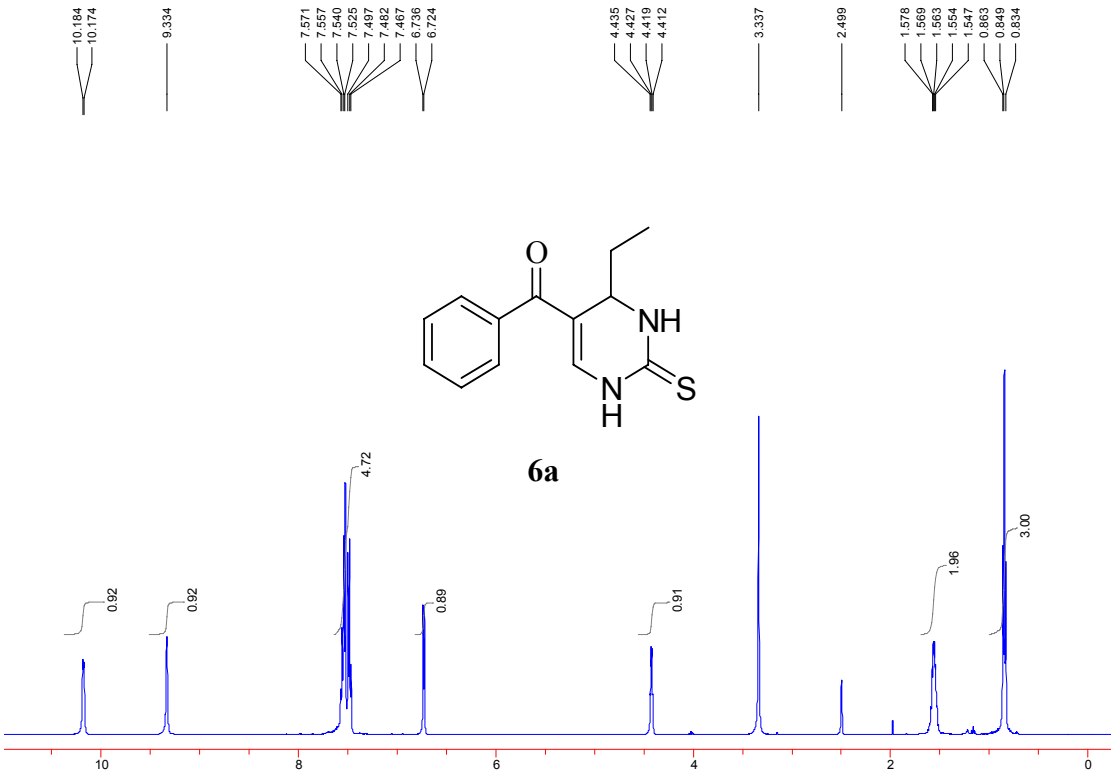
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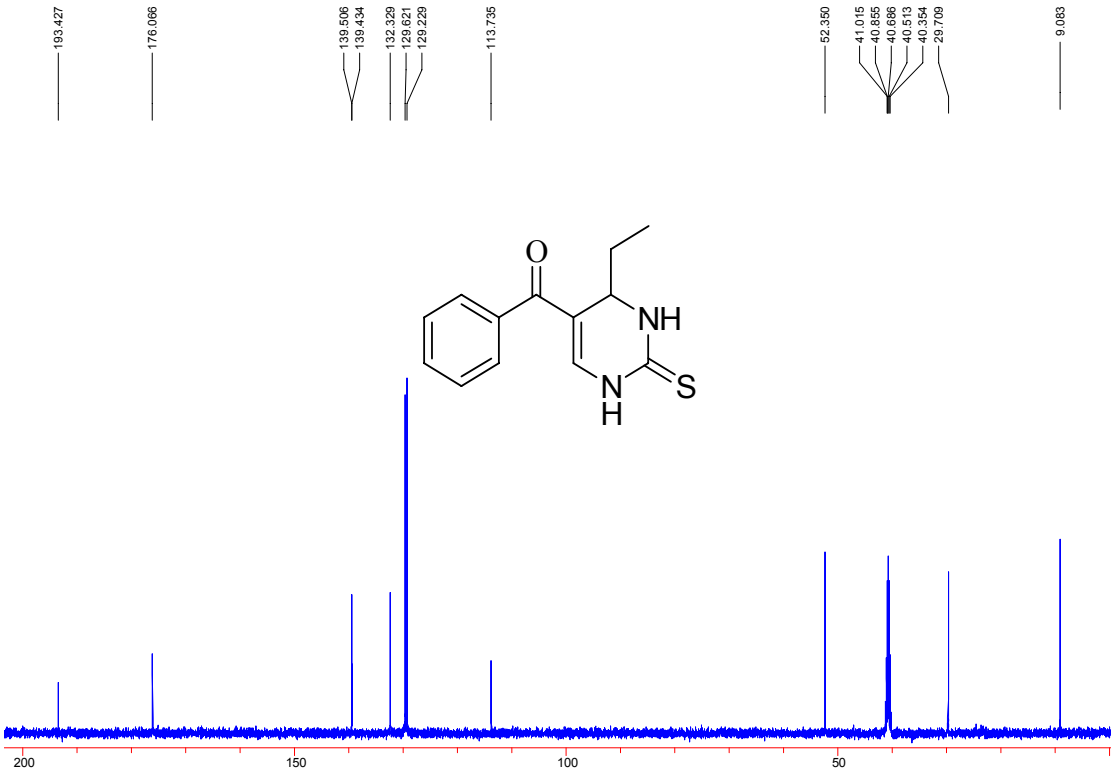
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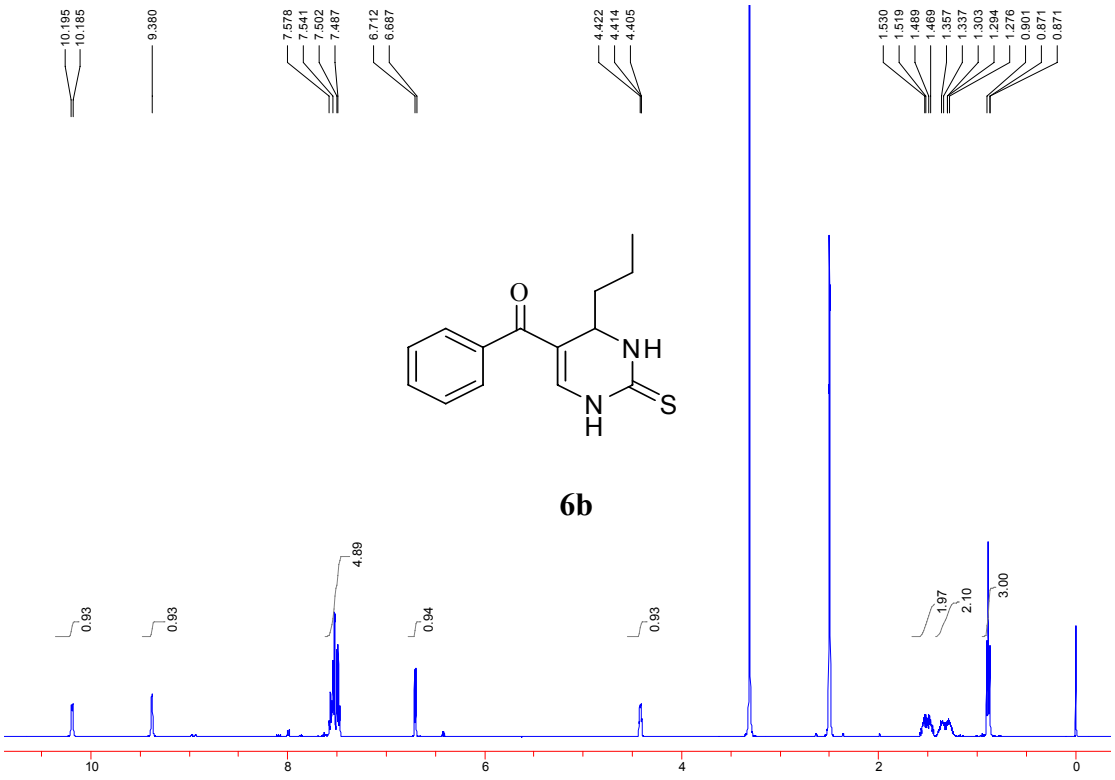
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0.901
0.871
0.871
O
NH
N
H
S
0.93
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0.93
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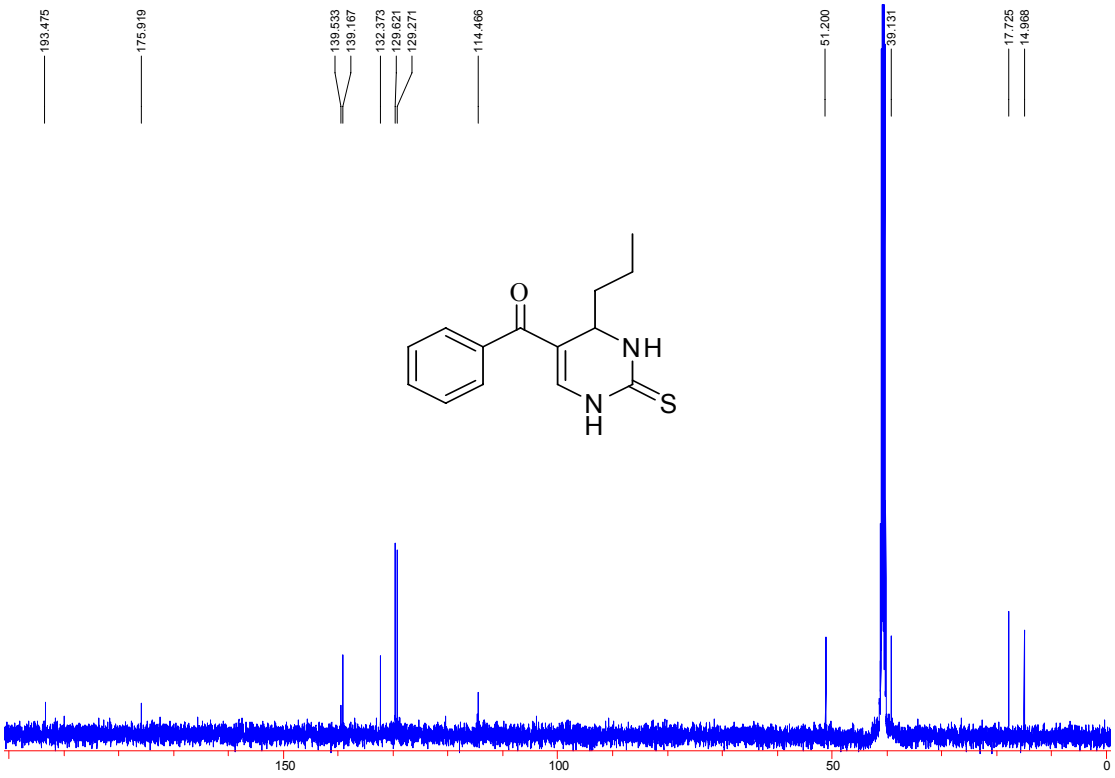
**6b**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39.131
17.725
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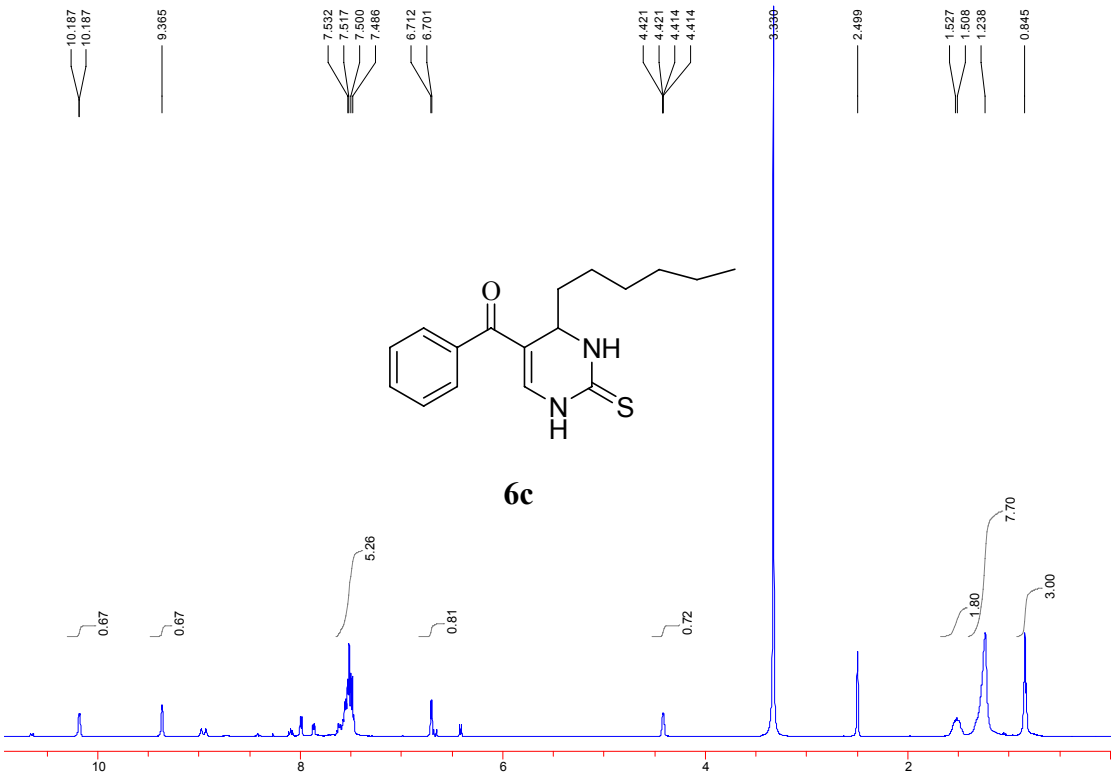
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7.517
7.500
7.486
6.712
6.701
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4.421
4.414
4.414
3.330
2.499
1.527
1.508
1.238
0.845
O
NH
N
H
S
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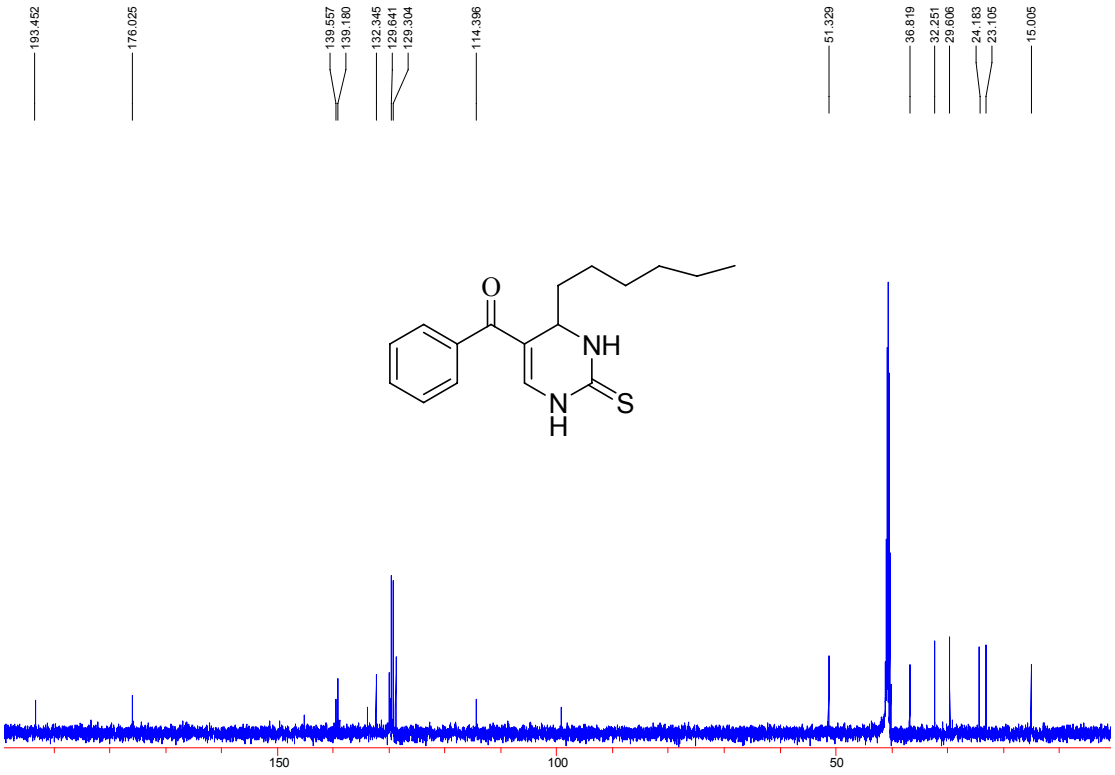
**6c**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129.641
129.304
114.396
51.329
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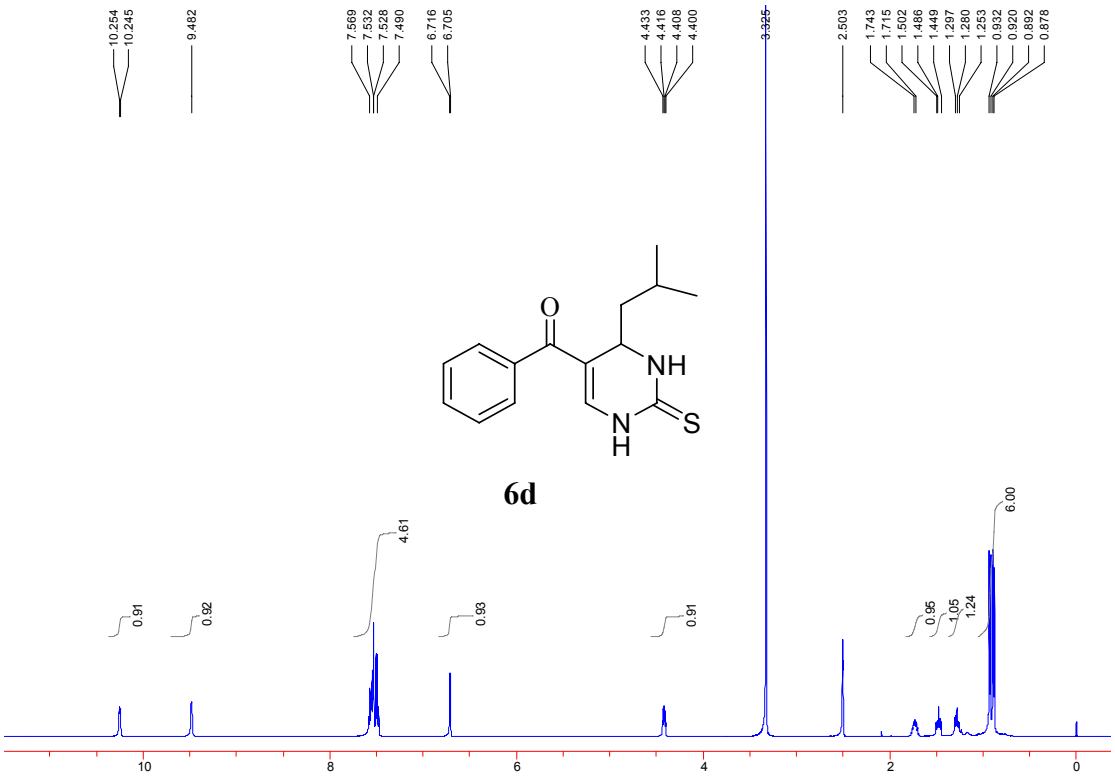
32.251
29.606
24.183
23.105
15.005
O
NH
N
H
S
150
100
50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7.532
7.528
7.490
6.716
6.705
4.433
4.416
4.408
4.400
3.325
2.503
1.743
1.715
1.502
1.486
1.449
1.297
1.280
1.253
0.932
0.920
0.892
0.878
O
NH
N
H
S
6d
0.91
0.92
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0.93
0.91
0.95
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1.24
6.00
10
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6
4
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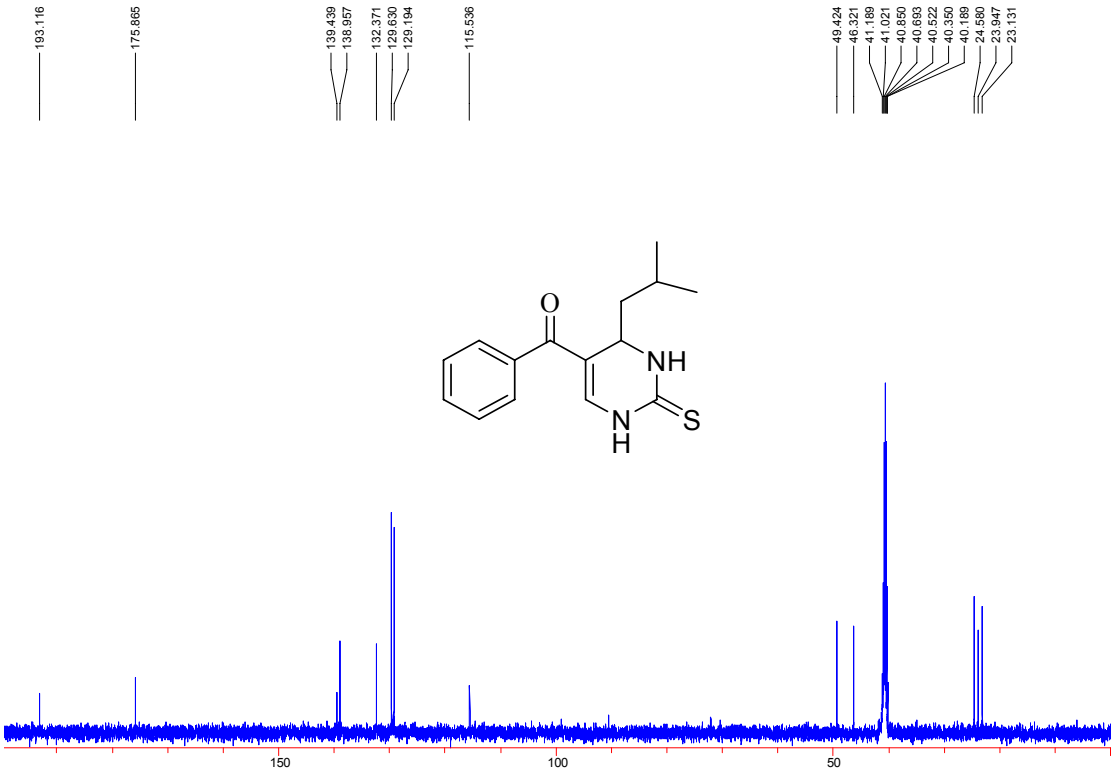
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139.439
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132.371
129.630
129.194
115.536
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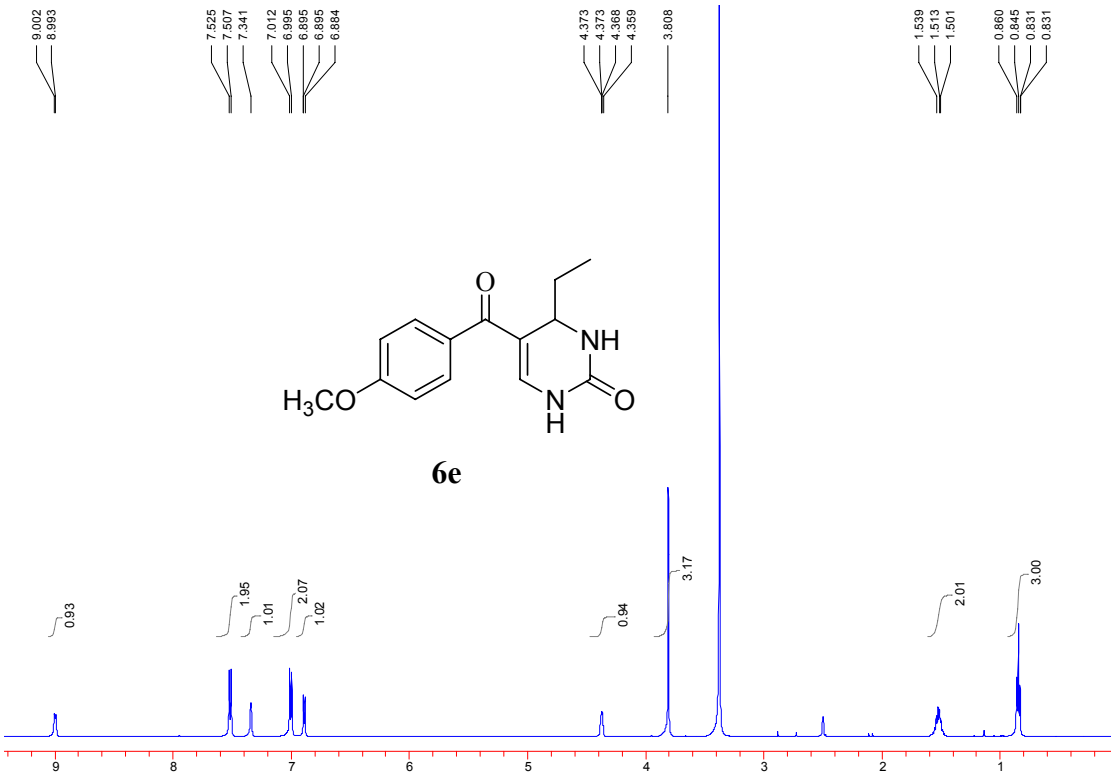
46.321
41.189
41.021
40.850
40.693
40.522
40.350
40.189
24.580
23.947
23.131
O
NH
N
H
S
150
100
50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7.507
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7.012
6.995
6.895
6.895
6.884
4.373
4.373
4.368
4.359
3.808
1.539
1.513
1.501
0.860
0.845
0.831
0.831
O
NH
H3CO
N
H
O
0.93
1.95
1.01
2.07
1.02
0.94
3.17
2.01
3.00
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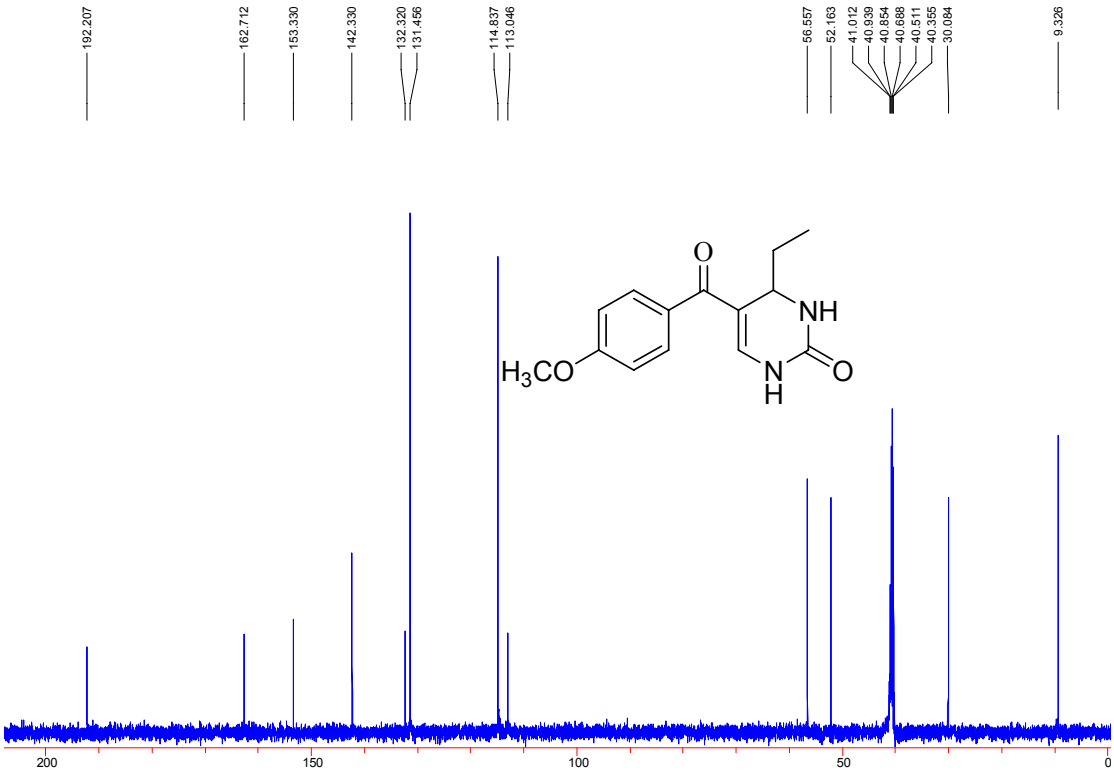
8
7
6
5
4
3
2
1

**6e**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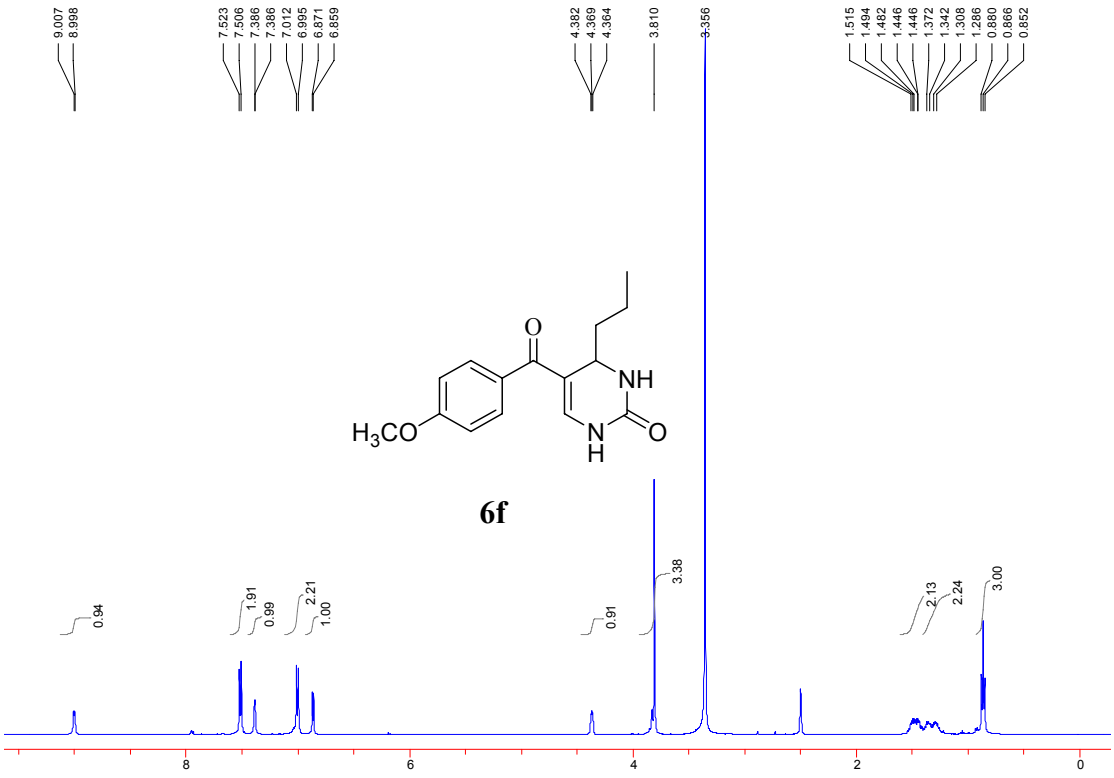
153.330
142.330
132.320
131.456
114.837
113.046
56.557
52.163
41.012
40.939
40.854
40.688
40.511
40.355
30.084
9.326
O
NH
H3CO
N
H
O
200
150
100
50
0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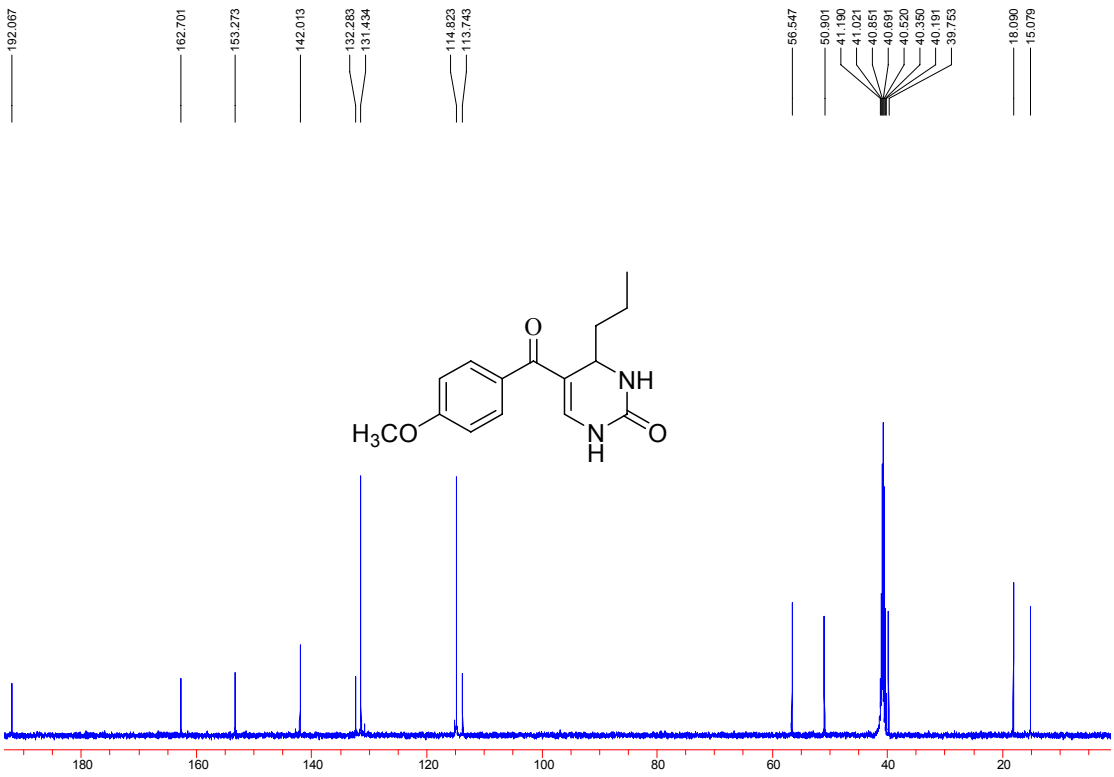
7.506
7.386
7.386
7.012
6.995
6.871
6.859
4.382
4.369
4.364
3.810
3.356
1.515
1.494
1.482
1.446
1.446
1.372
1.342
1.308
1.286
0.880
0.866
0.852
O
NH
H3CO
N
H
O
0.94
1.91
0.99
2.21
1.00
0.91
3.38
2.13
2.24
3.00
8
6
4
2
0

**6f**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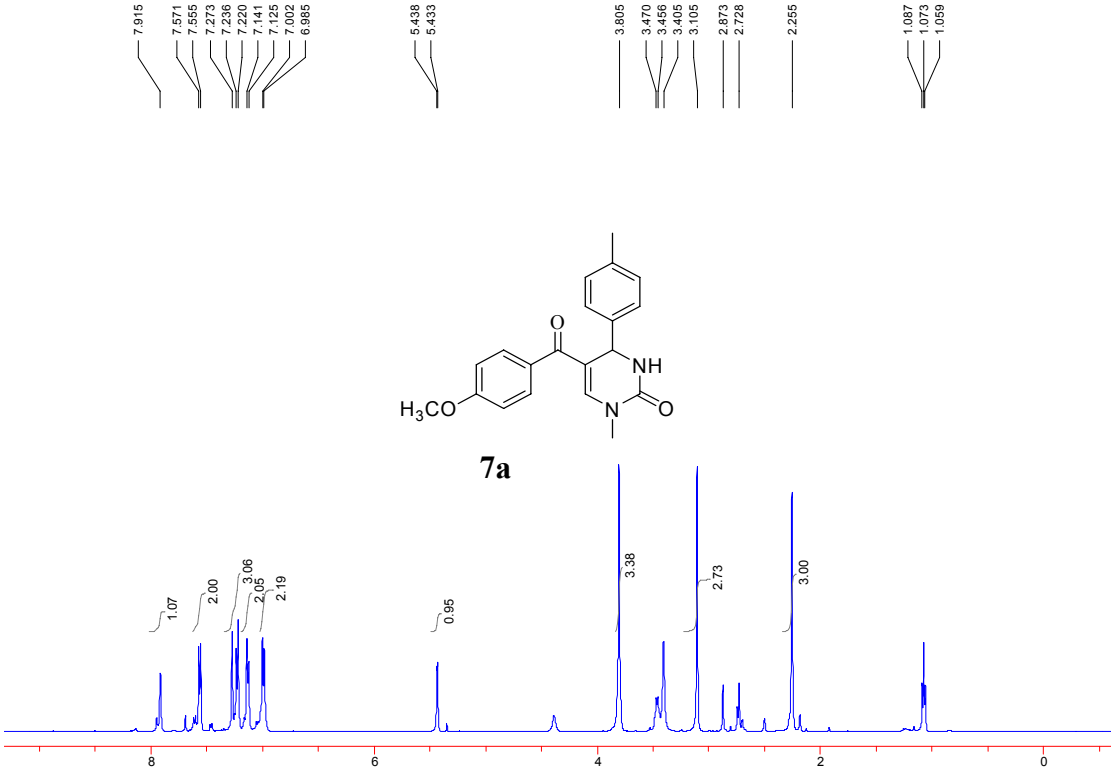
153.273
142.013
132.283
131.434
114.823
113.743
56.547
50.901
41.190
41.021
40.851
40.691
40.520
40.350
40.191
39.753
18.090
15.079
O
NH
H3CO
N
H
O
180
160
140
120
100
80
60
40
20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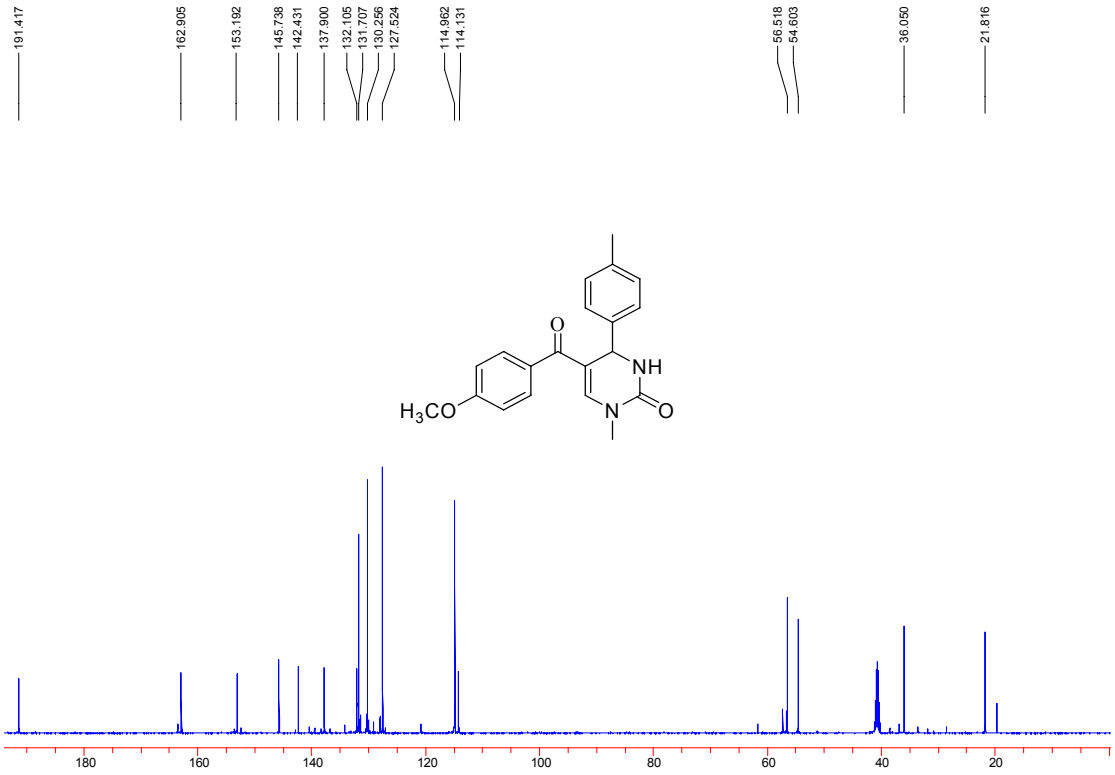
7.571
7.555
7.273
7.236
7.220
7.141
7.125
7.002
6.985
5.438
5.433
3.805
3.470
3.456
3.405
3.105
2.873
2.728
2.255
1.087
1.073
1.059
O
NH
H3CO
N
O
1.07
2.00
3.06
2.05
2.19
0.95
3.38
2.73
3.00
8
6
4
2
0

**7a**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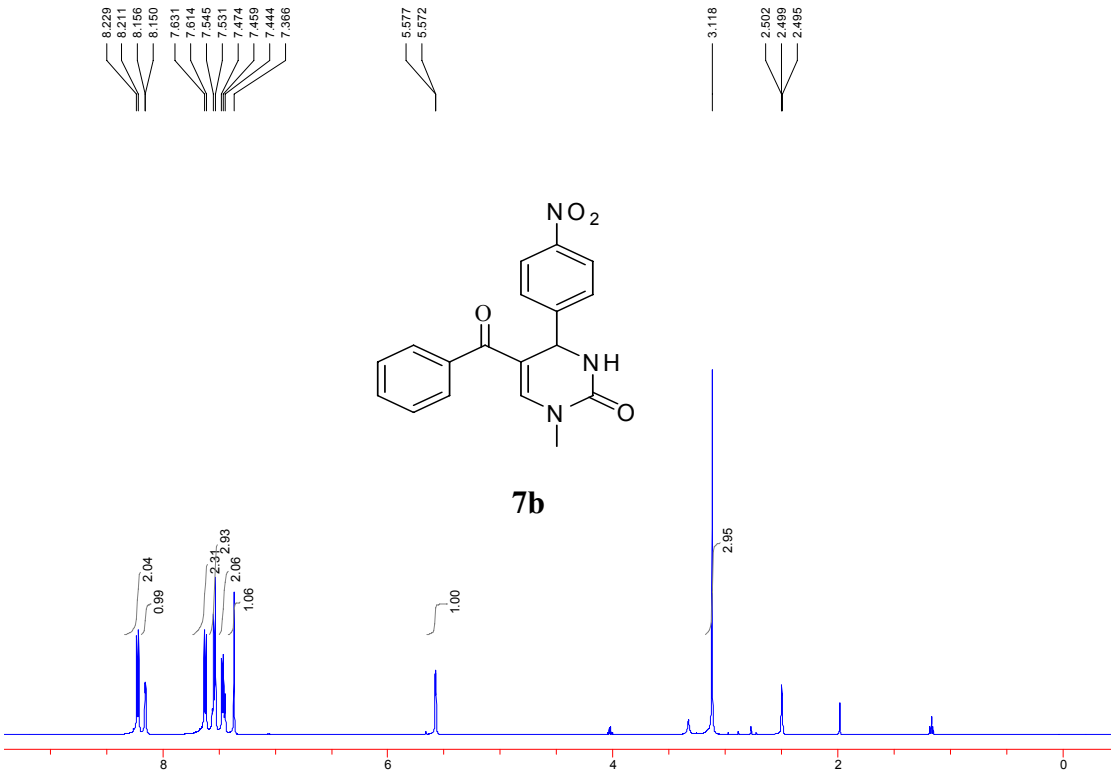
153.192
145.738
142.431
137.900
132.105
131.707
130.256
127.524
114.962
114.131
56.518
54.603
36.050
21.816
O
NH
H3CO
N
O
180
160
140
120
100
80
60
40
20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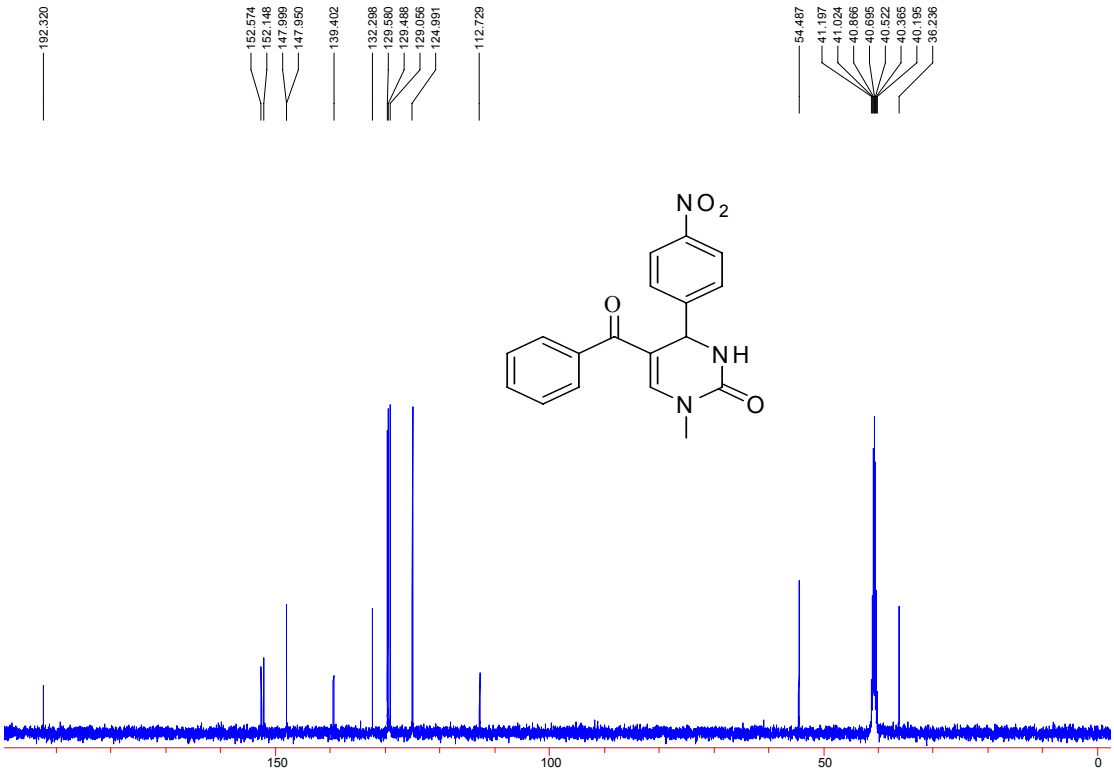
8.156
8.150
7.631
7.614
7.545
7.531
7.474
7.459
7.444
7.366
5.577
5.572
3.118
2.502
2.499
2.495
NO2
O
NH
N
O
7b
2.04
0.99
2.31
2.83
2.06
1.06
1.00
2.95
8
6
4
2
0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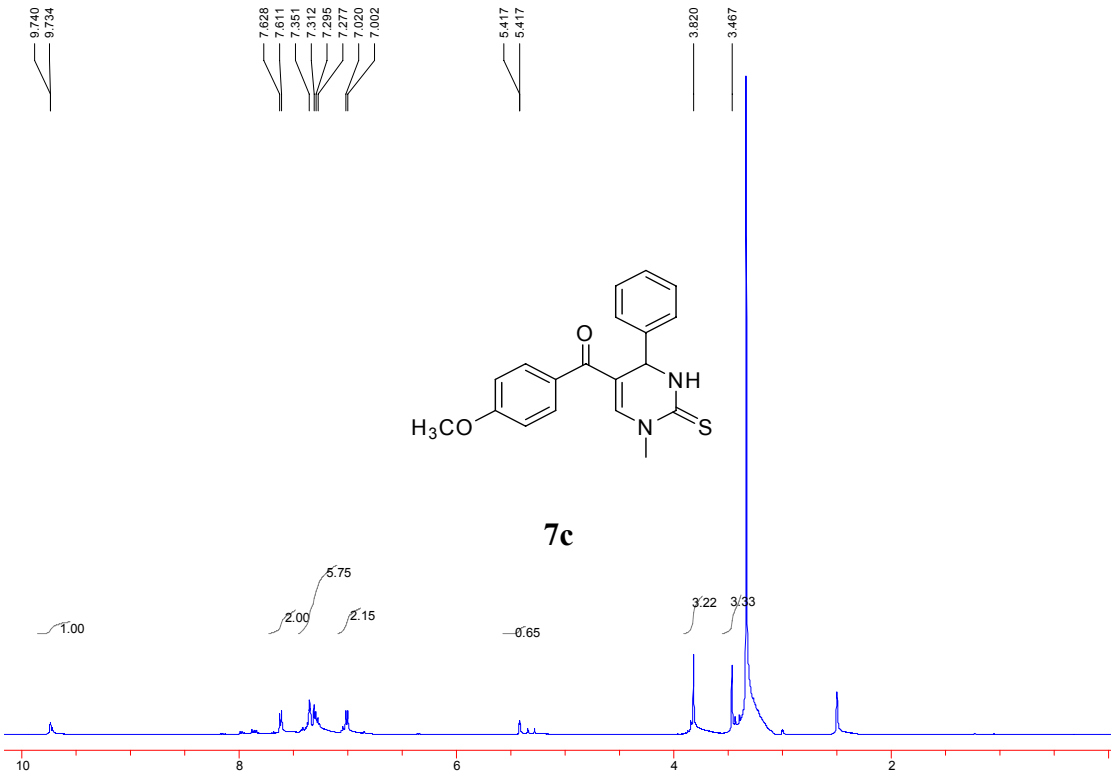
152.148
147.999
147.950
139.402
132.298
129.580
129.488
129.056
124.991
112.729
54.487
41.197
41.024
40.866
40.695
40.522
40.365
40.195
36.236
NO2
O
NH
N
O
150
100
50
0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9.734
7.628
7.611
7.351
7.312
7.295
7.277
7.020
7.002
5.417
5.417
3.820
3.467
O
NH
H3CO
N
S
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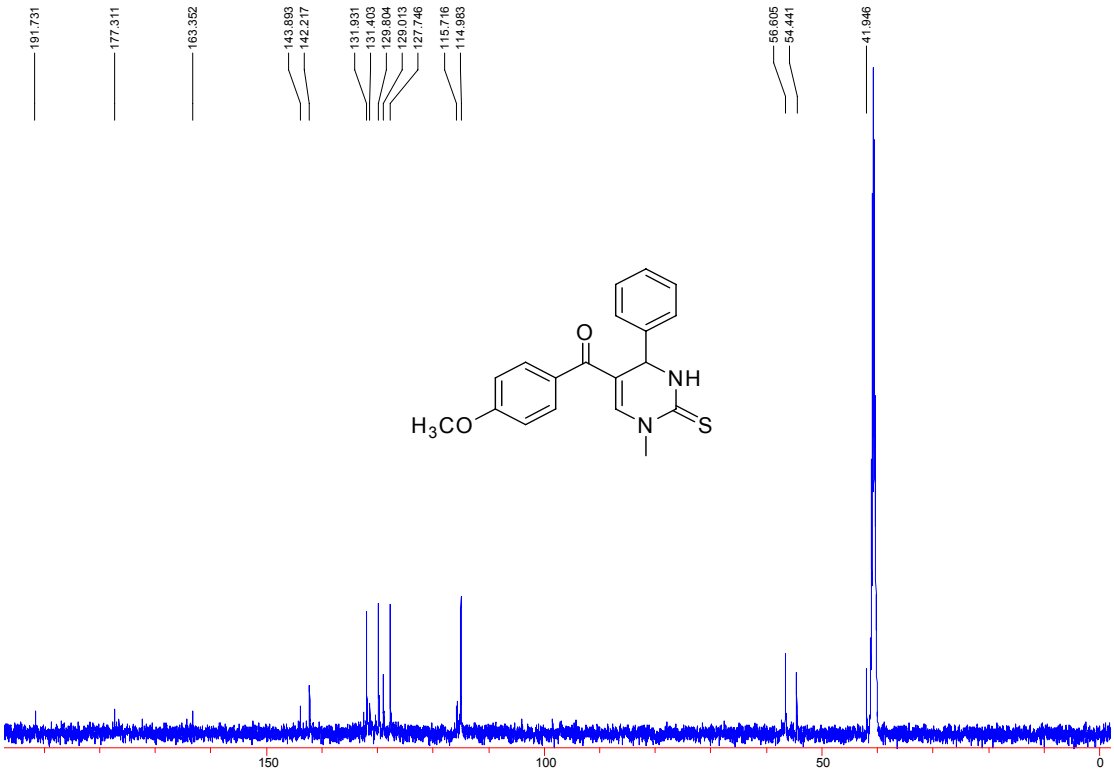
2.00
5.75
2.15
0.65
3.22
3.33
10
8
6
4
2

**7c**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163.352
143.893
142.217
131.931
131.403
129.804
129.013
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114.983
56.605
54.441
41.946
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H3CO
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S
150
100
50
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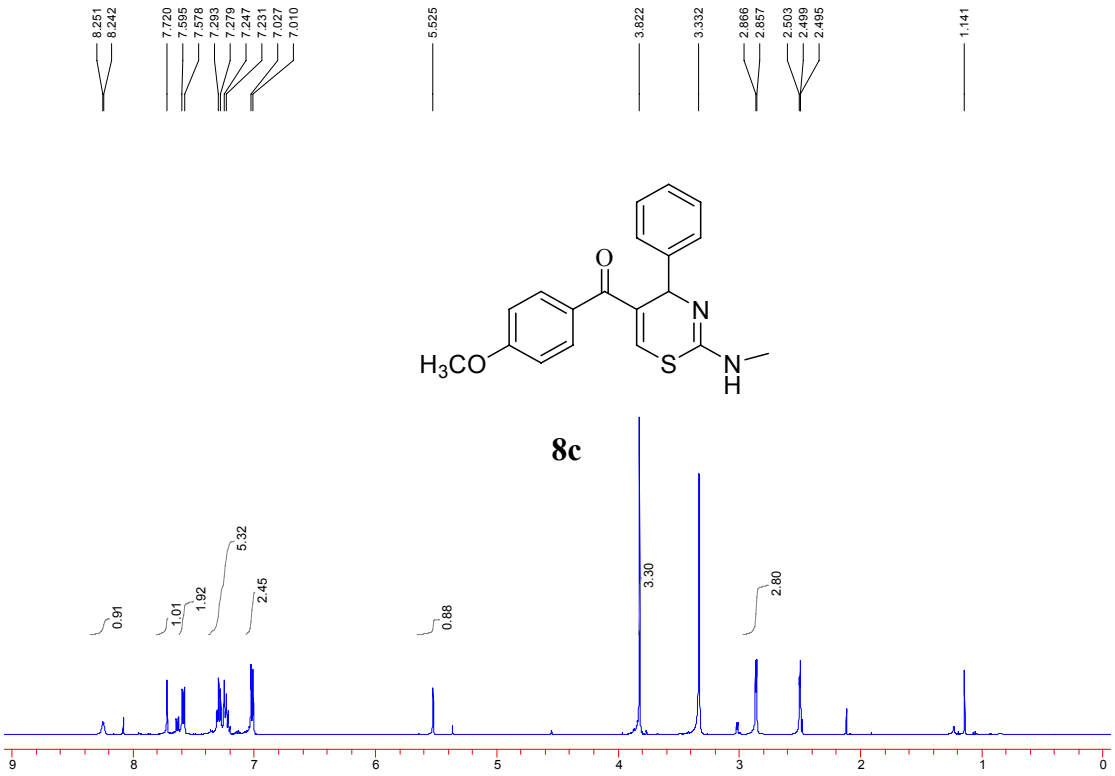
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7.720
7.595
7.578
7.293
7.279
7.247
7.231
7.027
7.010
5.525
3.822
3.332
2.866
2.857
2.503
2.499
2.495
1.141
O
N
S
N
H
H3CO
8c
0.91
1.01
1.92
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0.88
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2.80
9
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7
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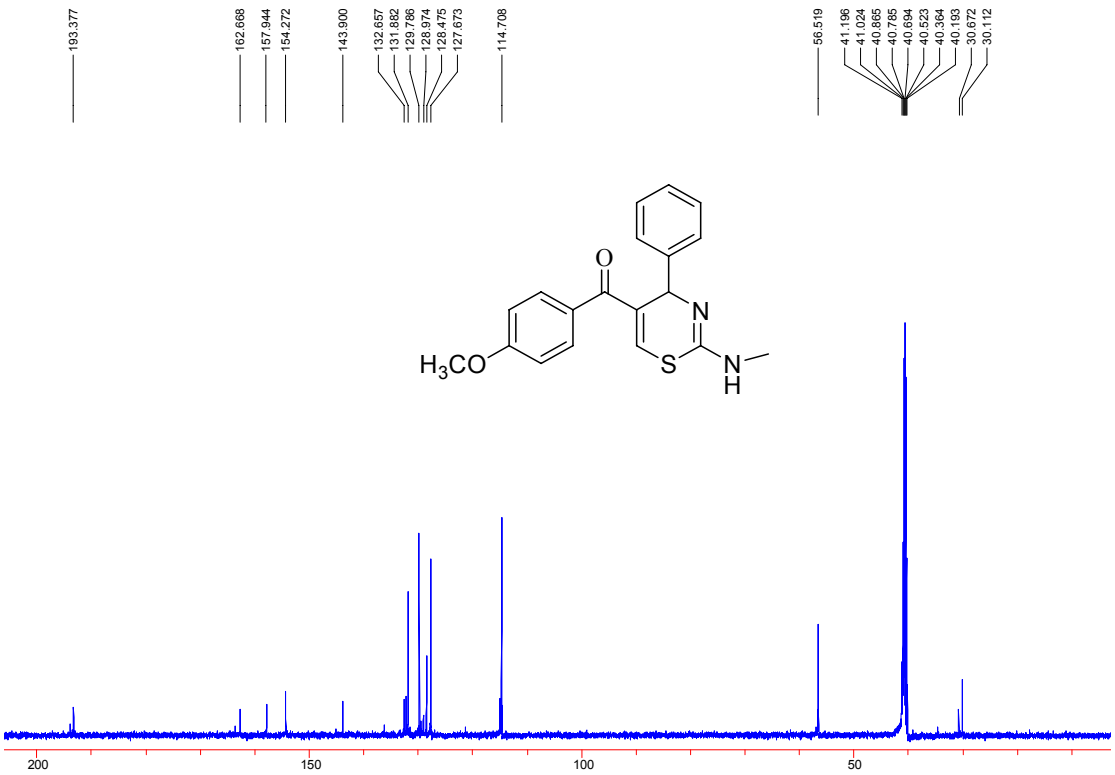
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56.519
41.196
41.024
40.865
40.785
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30.672
30.112
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N
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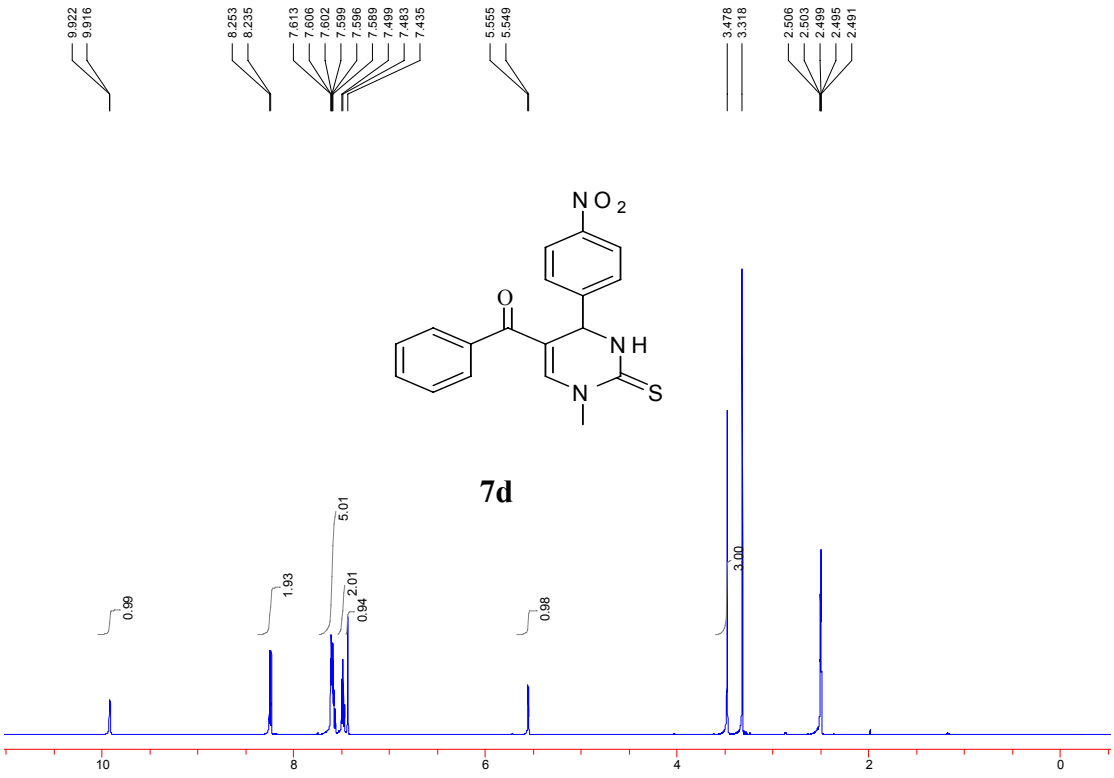
H3CO
200
150
100
50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7.606
7.602
7.599
7.596
7.589
7.499
7.483
7.435
5.555
5.549
3.478
3.318
2.506
2.503
2.499
2.495
2.491
NO2
O
NH
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5.01
2.01
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3.00
10
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2
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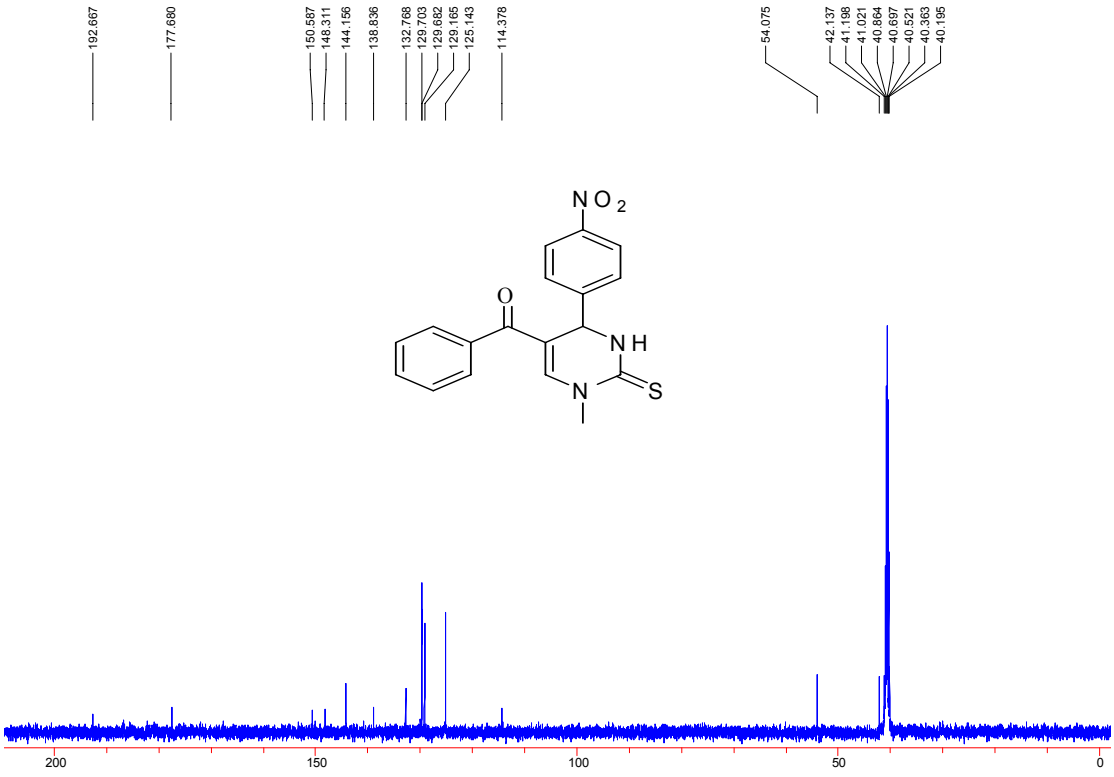
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129.165
125.143
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54.075
42.137
41.198
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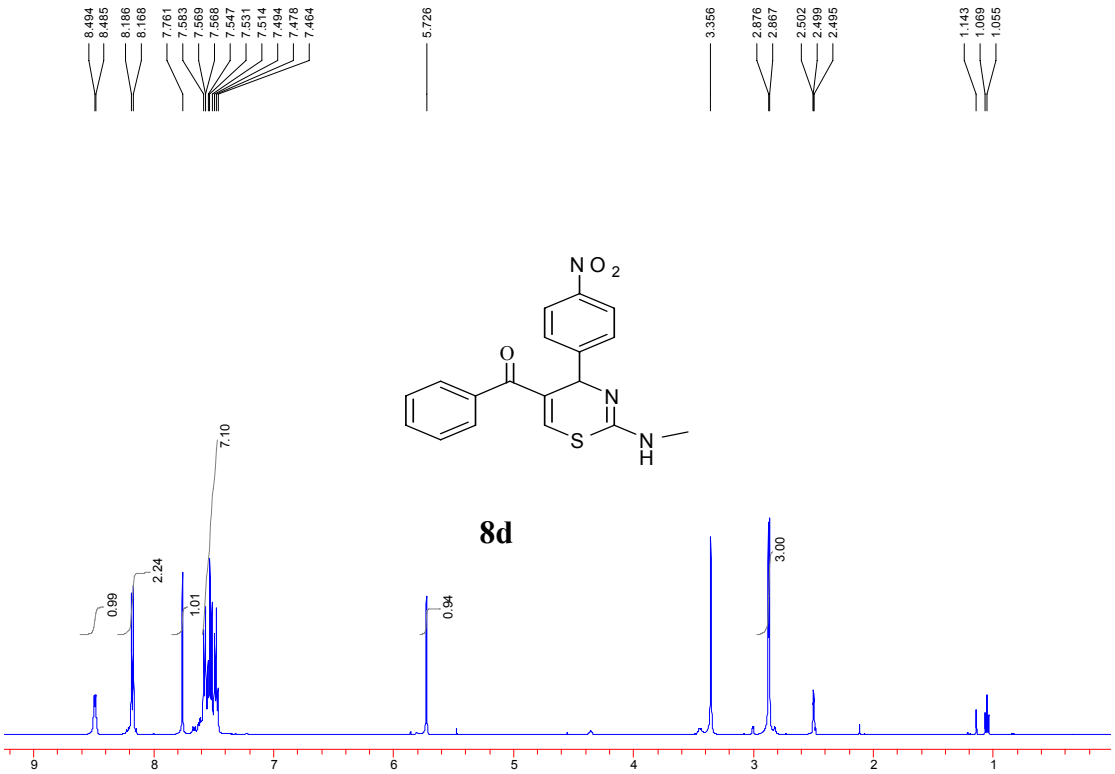
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7.568
7.547
7.531
7.514
7.494
7.478
7.464
5.726
3.356
2.876
2.867
2.502
2.499
2.495
1.143
1.069
1.055
NO2
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N
S
N
H
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0.94
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8
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4
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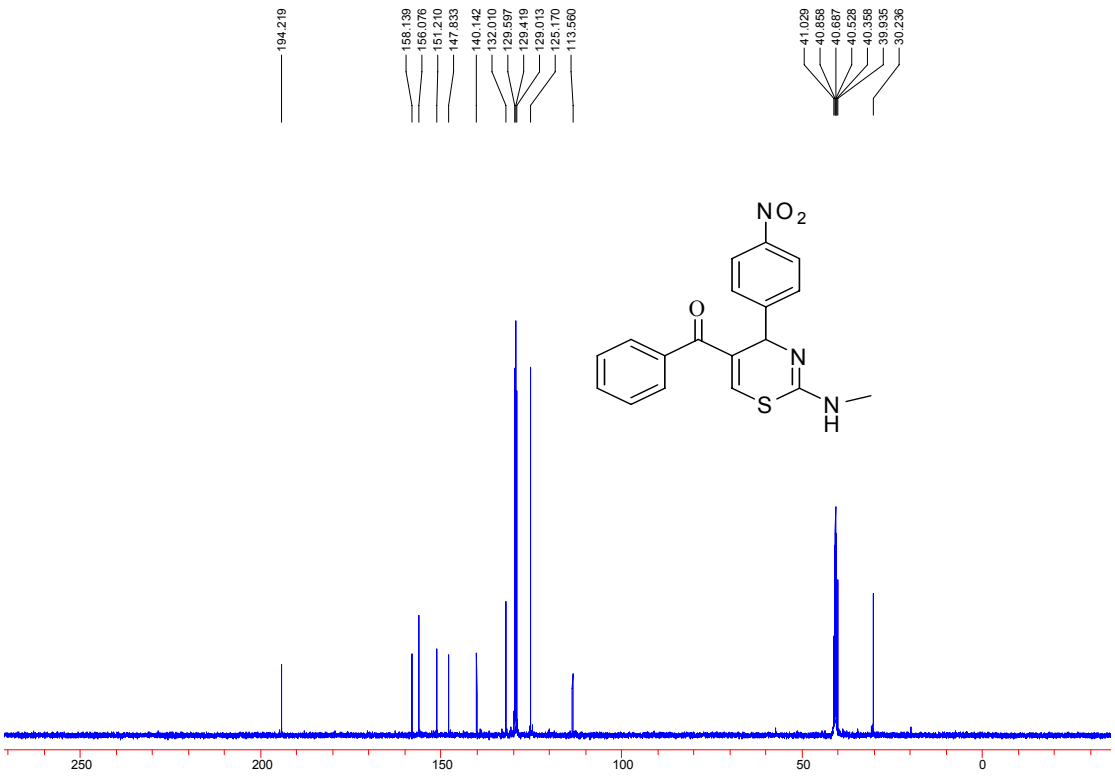
2
1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129.597
129.419
129.013
125.170
113.560
41.029
40.858
40.687
40.528
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39.935
30.236
NO2
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N
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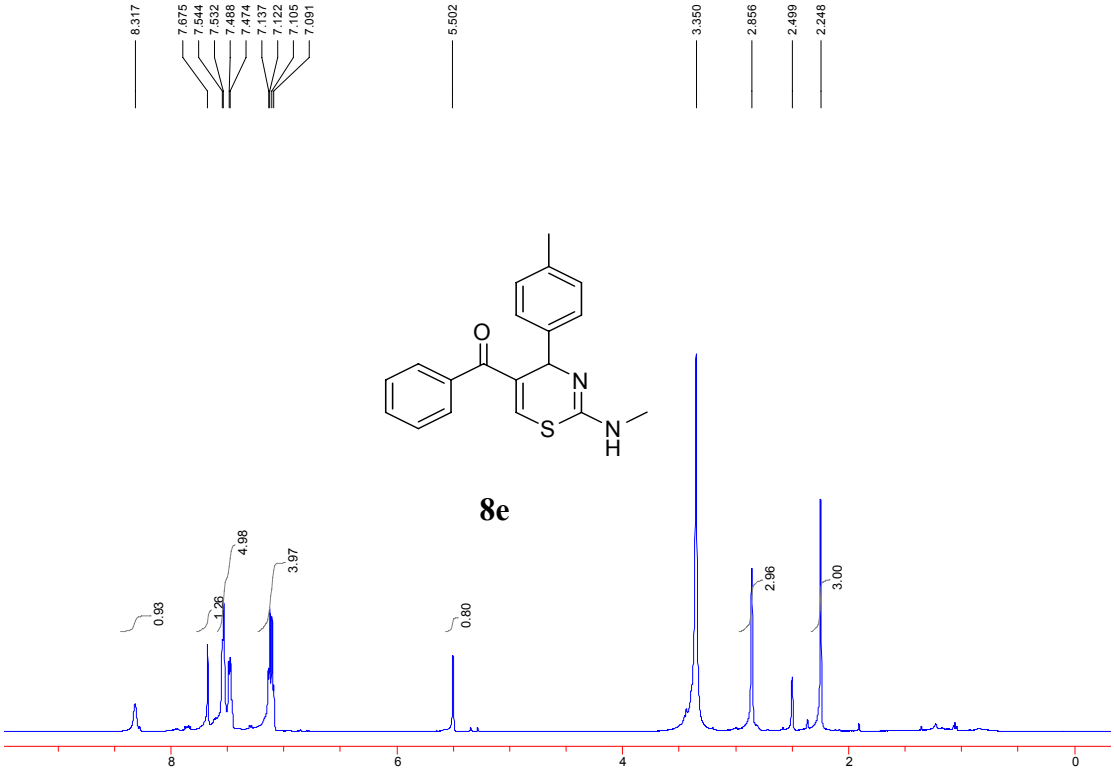
100
50
0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7.122
7.105
7.091
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3.350
2.856
2.499
2.248
O
N
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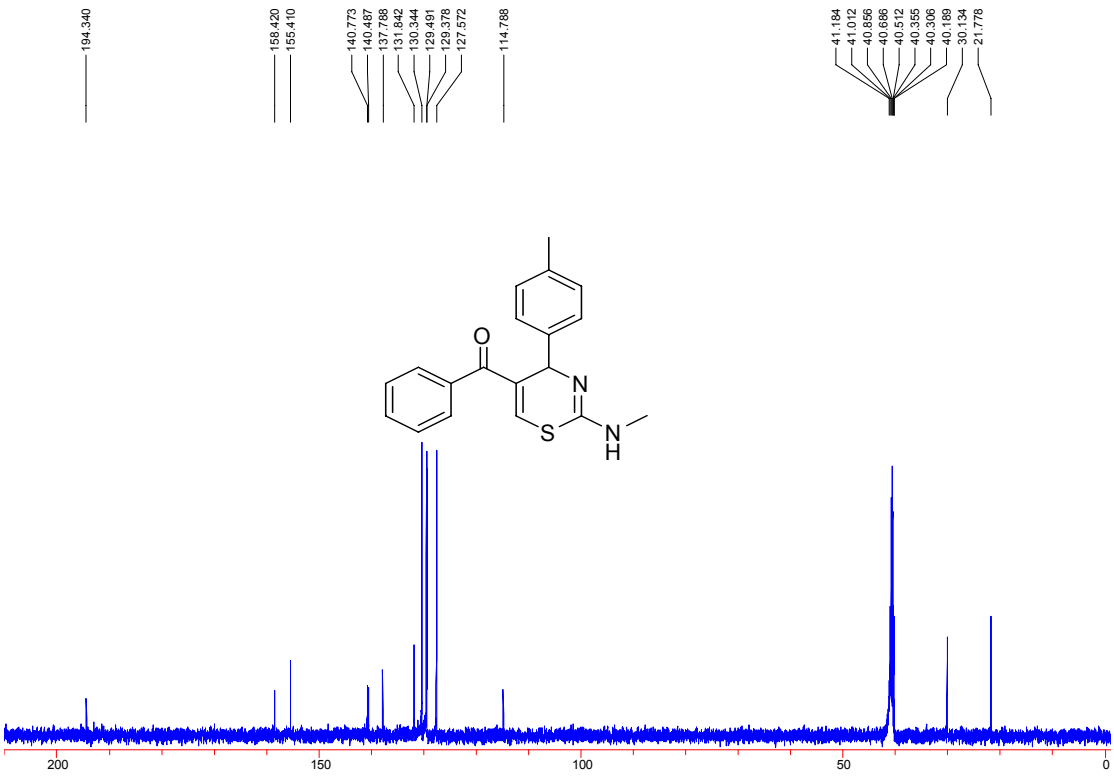
0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129.378
127.572
114.788
41.184
41.012
40.856
40.686
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40.189
30.134
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50
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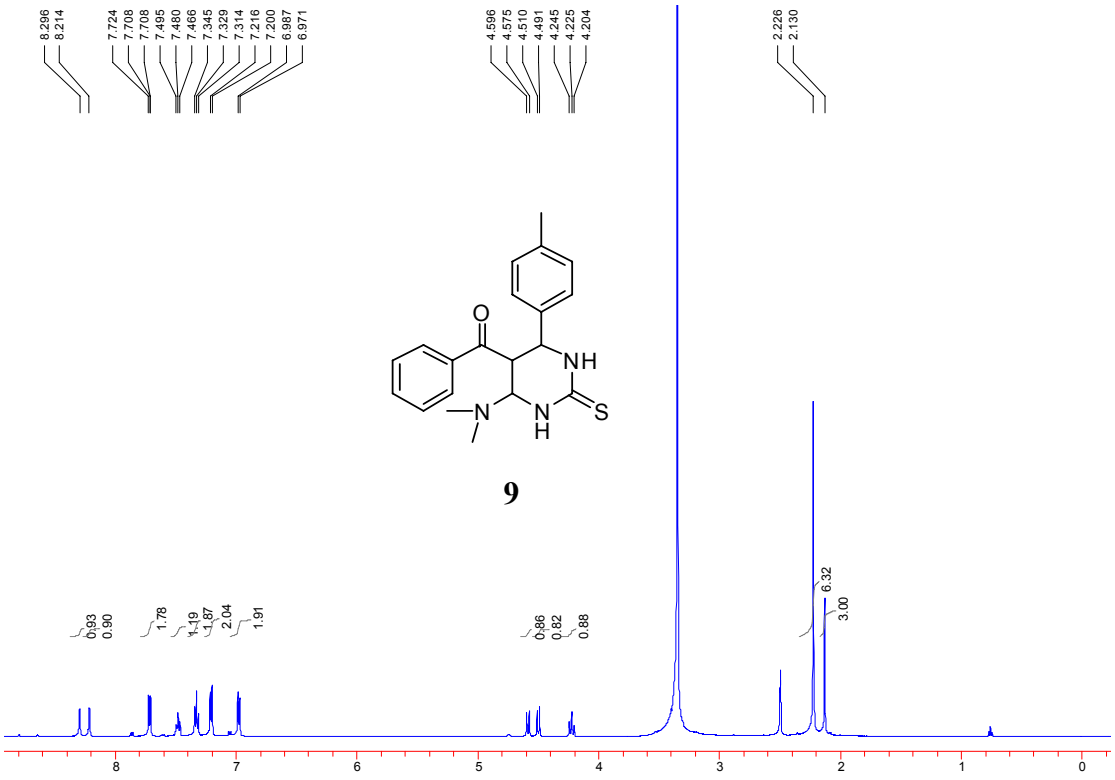
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7.466
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7.329
7.314
7.216
7.200
6.987
6.971
4.596
4.575
4.510
4.491
4.245
4.225
4.204
2.226
2.130
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NH
N
N
H
S
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0.90
1.78
1.19
1.87
2.04
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5
4
3
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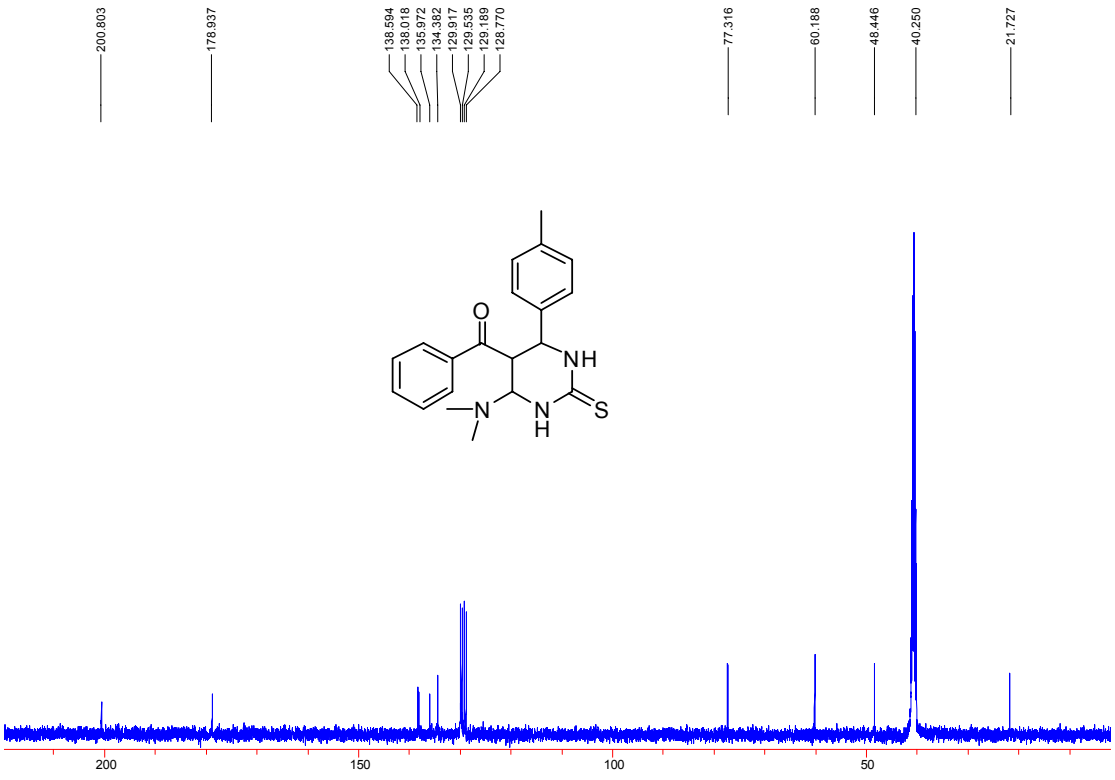
1
0

**9**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129.535
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60.188
48.446
40.250
21.727
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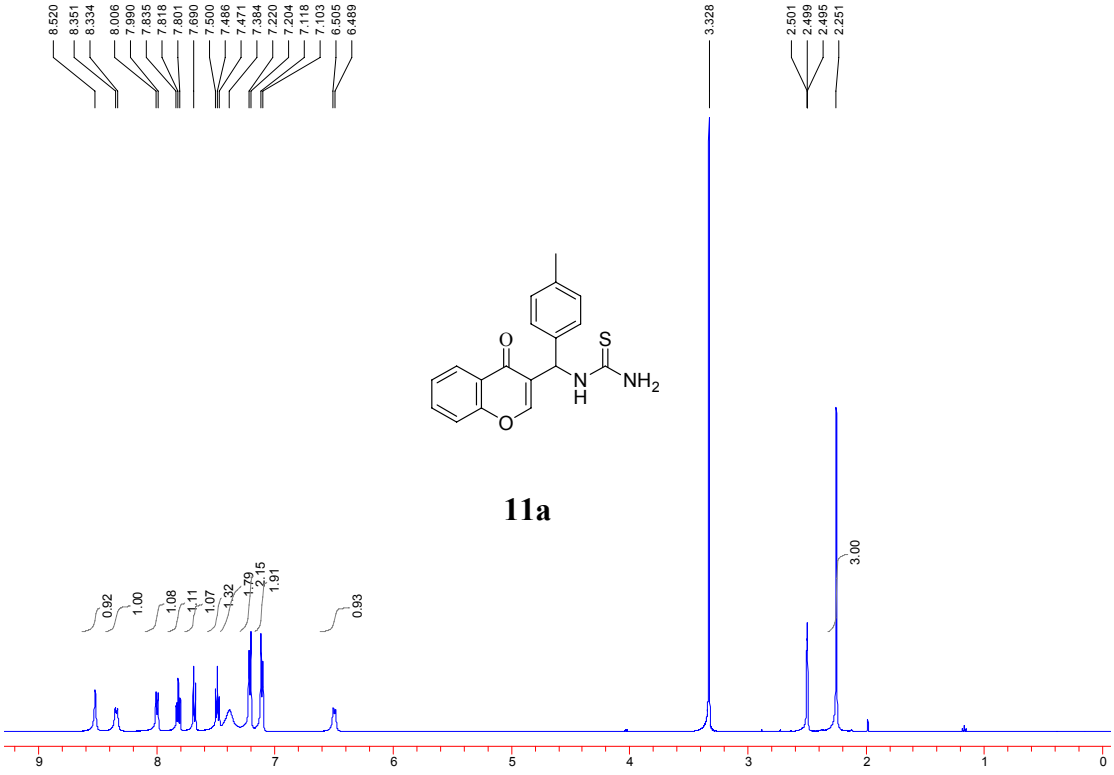
N
N
H
S
200
150
100
50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7.835
7.818
7.801
7.690
7.500
7.486
7.471
7.384
7.220
7.204
7.118
7.103
6.505
6.489
3.328
2.501
2.499
2.495
2.251
O
S
N
H
NH2
O
11a
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1.00
1.08
1.11
1.07
1.32
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2.15
1.91
0.93
3.00
9
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7
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1
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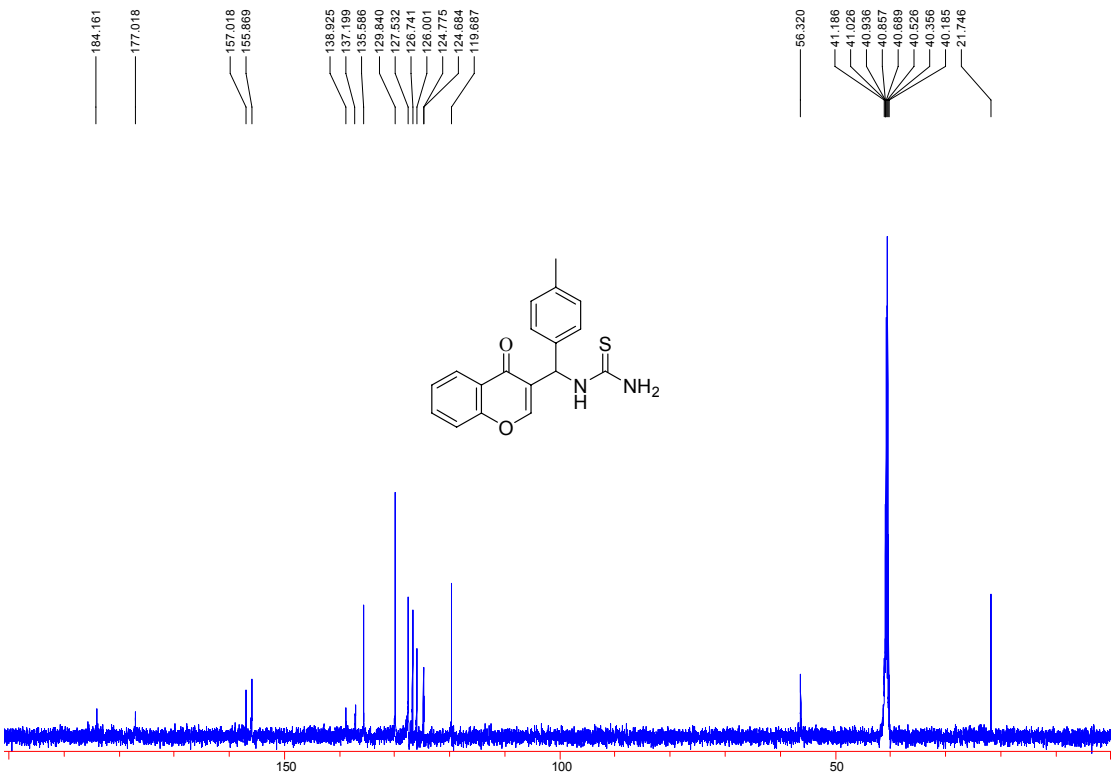
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157.018
155.869
138.925
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135.586
129.840
127.532
126.741
126.001
124.775
124.684
119.687
56.320
41.186
41.026
40.936
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40.526
40.356
40.185
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S
N
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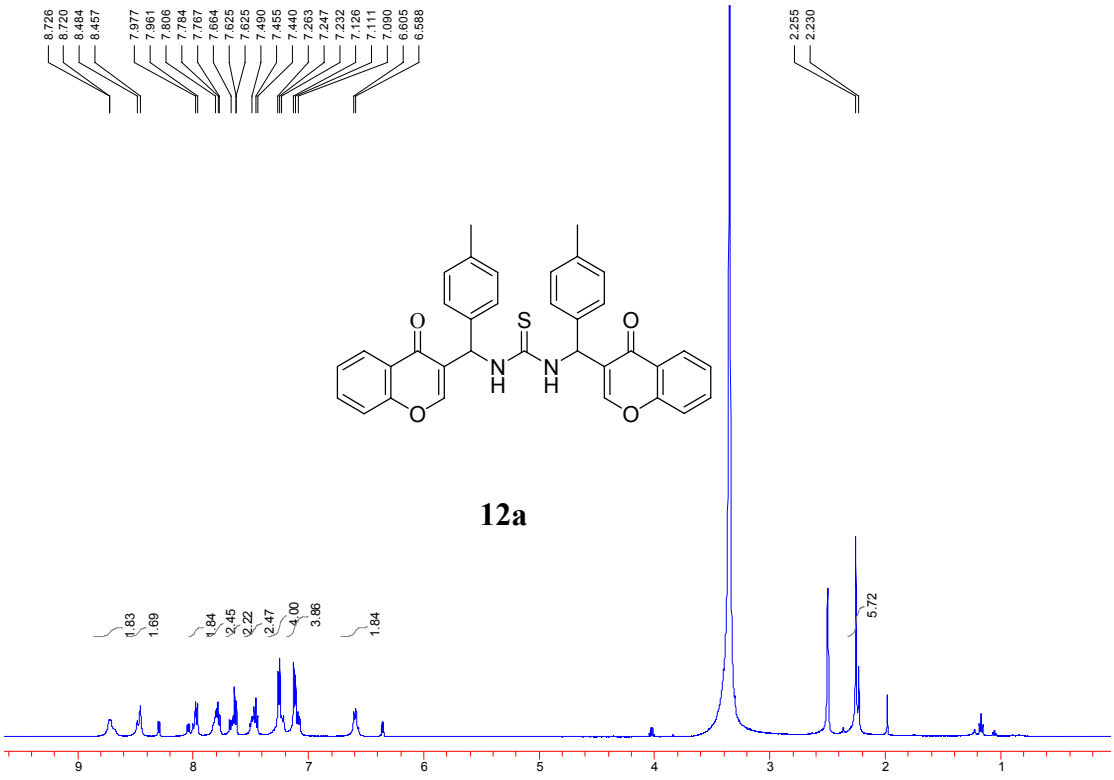
NH2
O
150
100
50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8.457
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7.961
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7.664
7.625
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7.455
7.440
7.263
7.247
7.232
7.126
7.111
7.090
6.605
6.588
2.255
2.230
O
S
N
H
N
H
O
O
O
1.83
1.69
1.84
2.45
2.22
2.47
4.00
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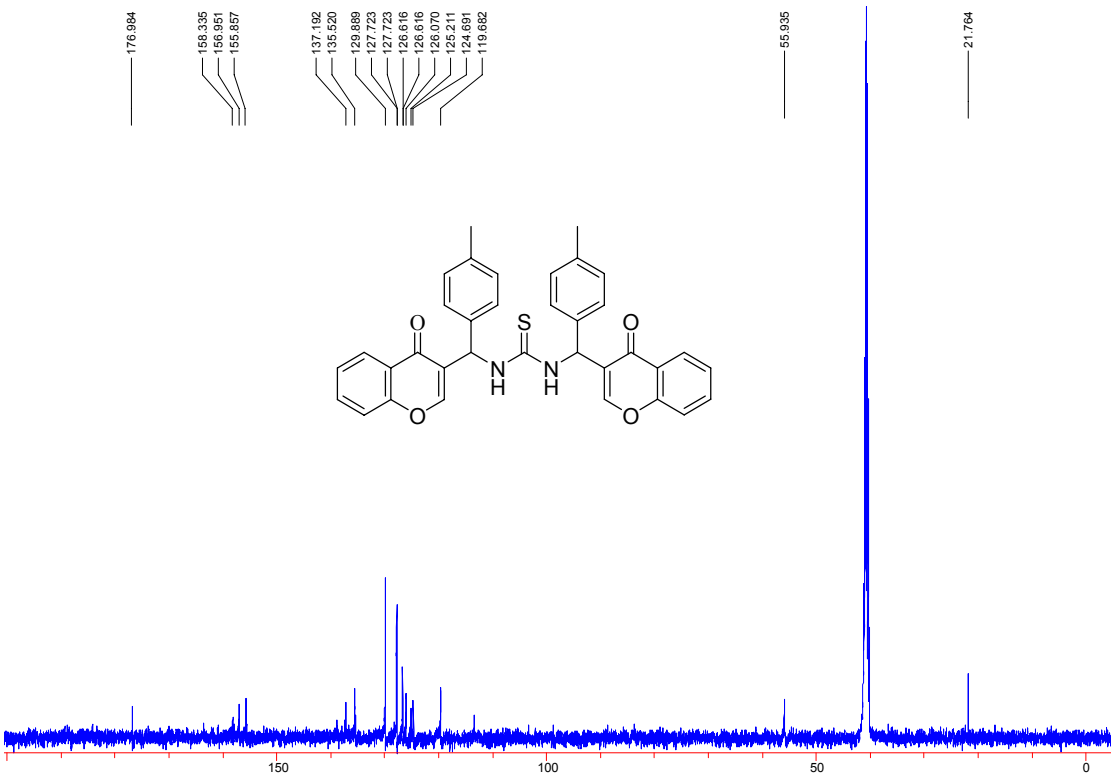
1.84
5.72
9
8
7
6
5
4
3
2
1

**12a**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135.520
129.889
127.723
127.723
126.616
126.616
126.070
125.211
124.691
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21.764
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N
H
N
H
O
O
O
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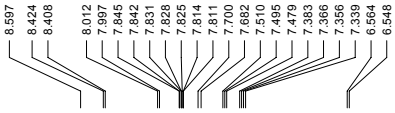
100
50
0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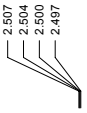
7.845
7.842
7.831
7.828
7.825
7.814
7.811
7.700
7.682
7.510
7.495
7.479
7.383
7.366
7.356
7.339
6.564
6.548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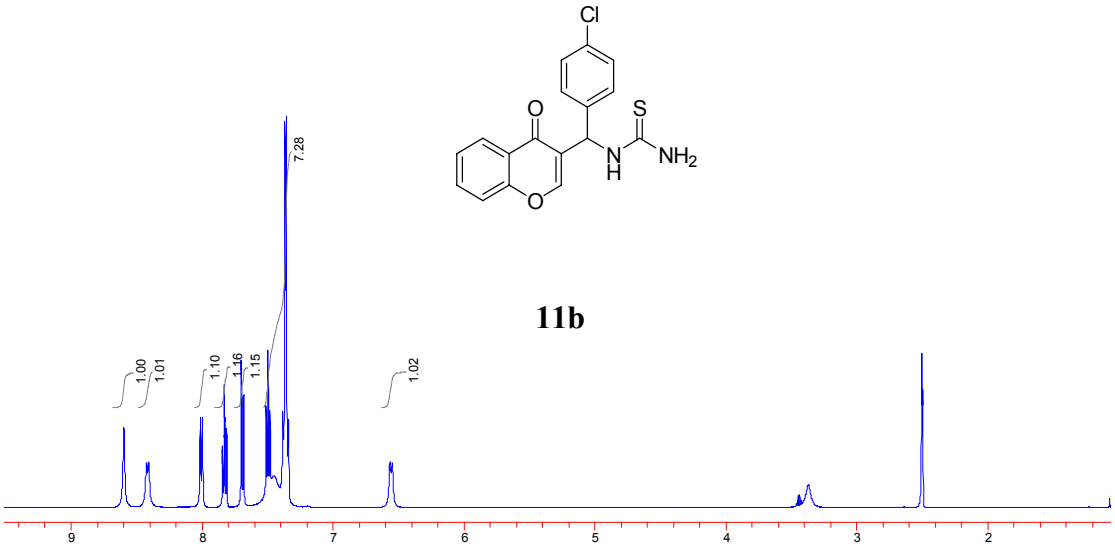
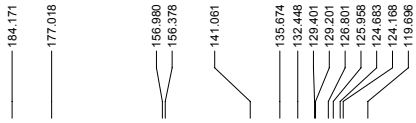
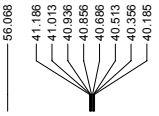
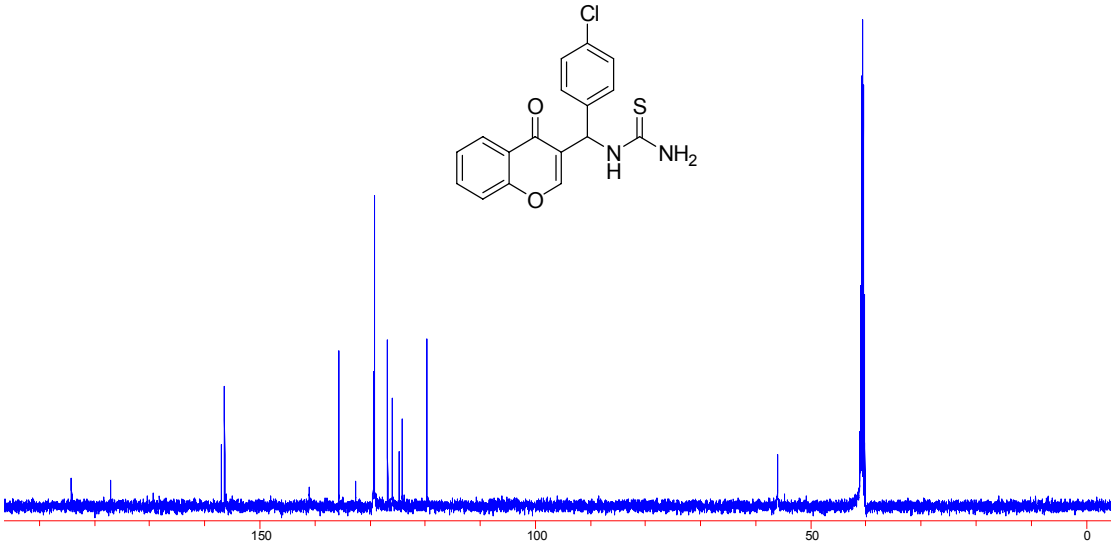
2.504
2.500
2.497

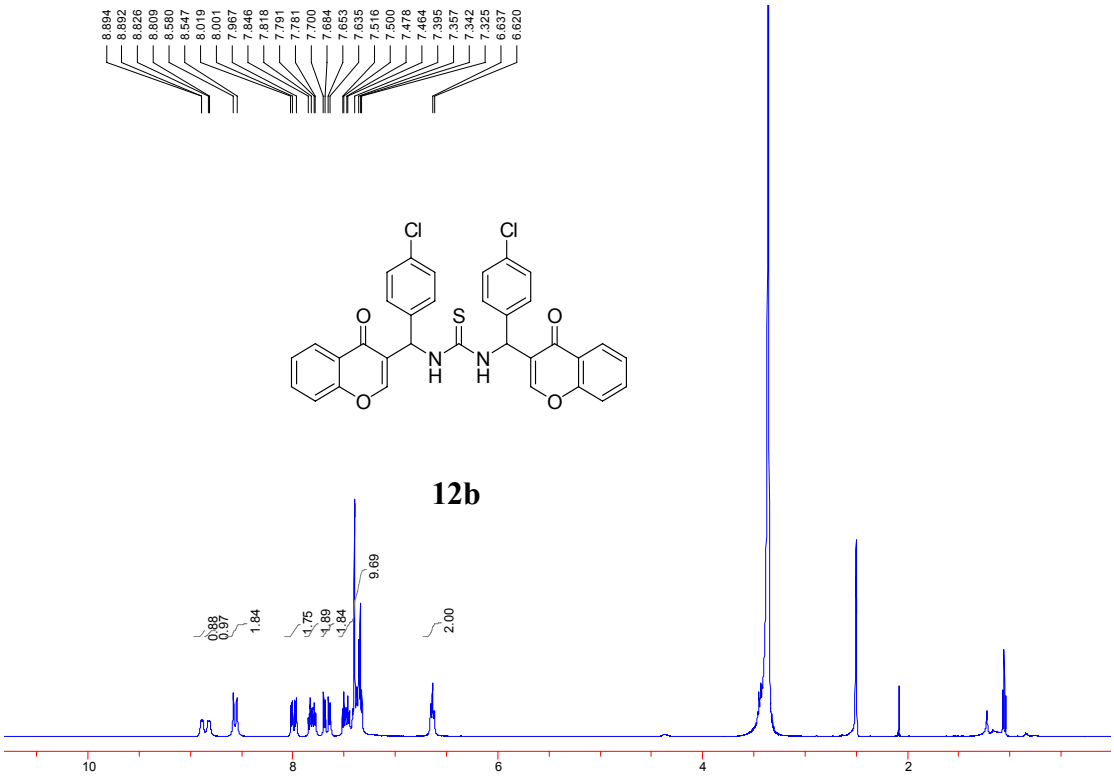

Cl
O
S
N
H
NH2
O
7.28
1.00
1.01
1.10
1.16
1.15
1.02
9
8
7
6
5
4
3
2

**11b**


184.171
177.018
156.980
156.378
141.061
135.674
132.448
129.401
129.201
126.801
125.958
124.683
124.168
119.696


56.068
41.186
41.013
40.936
40.856
40.686
40.513
40.356
40.185


Cl
O
S
N
H
NH2
O
150
100
50
0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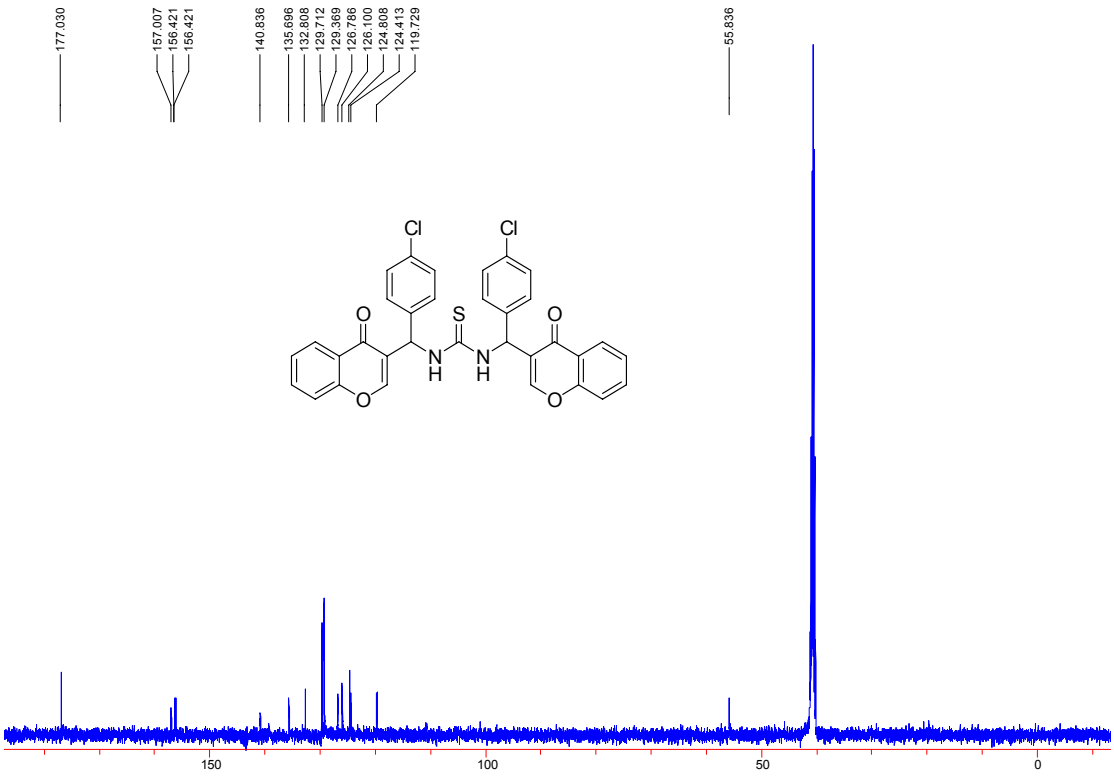
8.892
8.826
8.809
8.580
8.547
8.019
8.001
7.967
7.846
7.818
7.791
7.781
7.700
7.684
7.653
7.635
7.516
7.500
7.478
7.464
7.395
7.357
7.342
7.325
6.637
6.620
Cl
Cl
O
S
O
N
H
N
H
O
O
9.69
0.88
0.97
1.84
1.75
1.89
1.84
2.00
10
8
6
4
2

**12b**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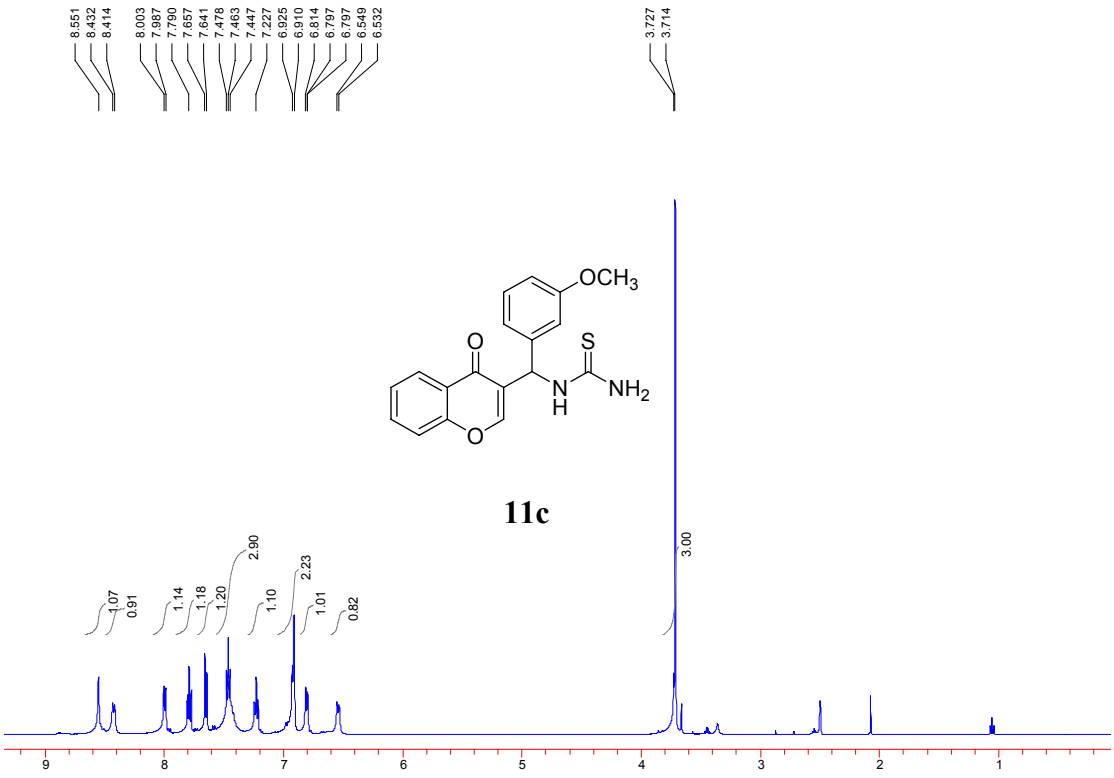
156.421
156.421
140.836
135.696
132.808
129.712
129.369
126.786
126.100
124.808
124.413
119.729
55.836
Cl
Cl
O
S
O
N
H
N
H
O
O
150
100
50
0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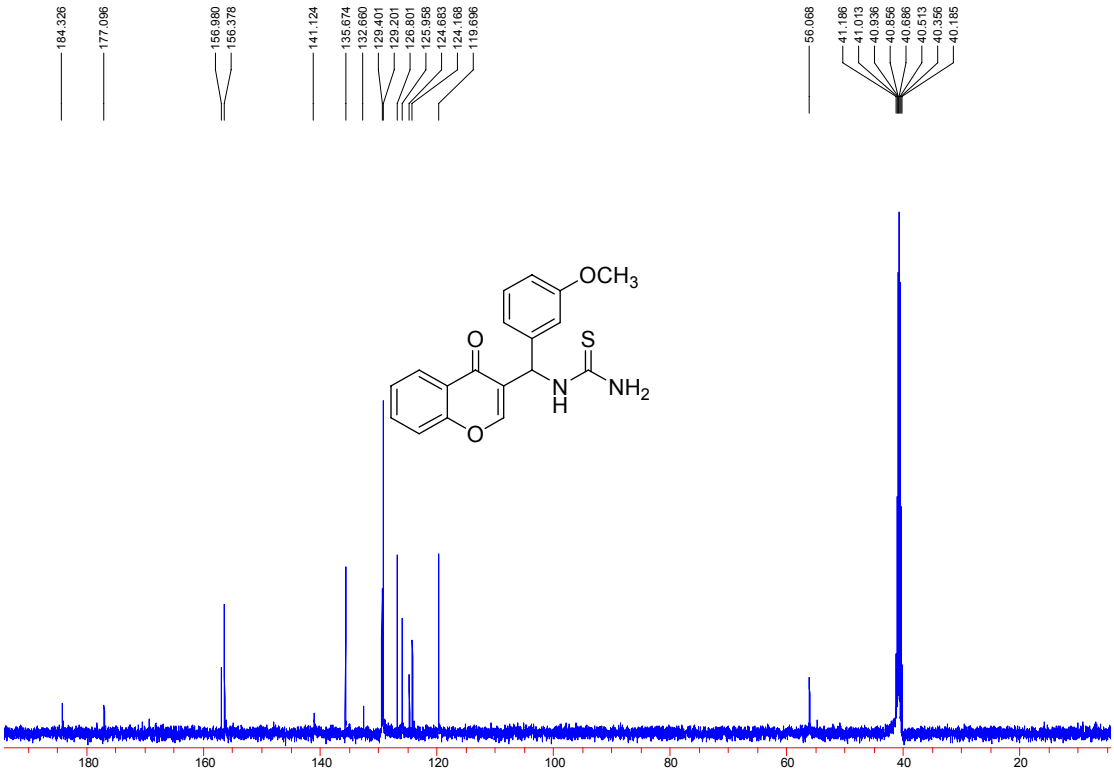
8.432
8.414
8.003
7.987
7.790
7.657
7.641
7.478
7.463
7.447
7.227
6.925
6.910
6.814
6.797
6.797
6.549
6.532
3.727
3.714
OCH3
O
S
N
H
NH2
O
11c
1.07
0.91
1.14
1.18
1.20
2.90
1.10
2.23
1.01
0.82
3.00
9
8
7
6
5
4
3
2
1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135.674
132.660
129.401
129.201
126.801
125.958
124.683
124.168
119.696
56.068
41.186
41.013
40.936
40.856
40.686
40.513
40.356
40.185
OCH3
O
S
N
H
NH2
O
180
160
140
120
100
80
60
40
20


8.275
8.081
8.065
7.917
7.893
7.883
7.827
7.812
7.797
7.657
7.640
7.517
7.502
7.488
7.101
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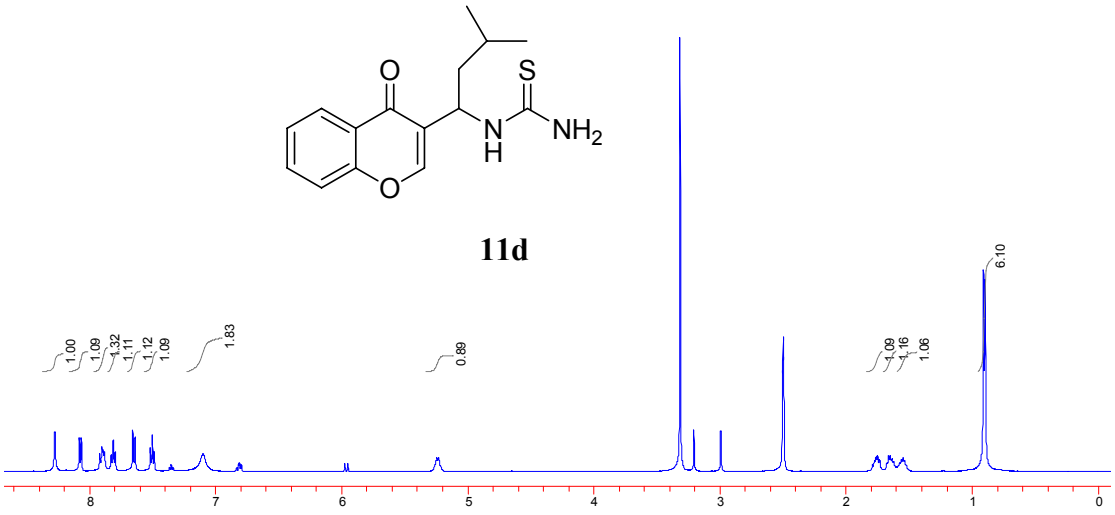
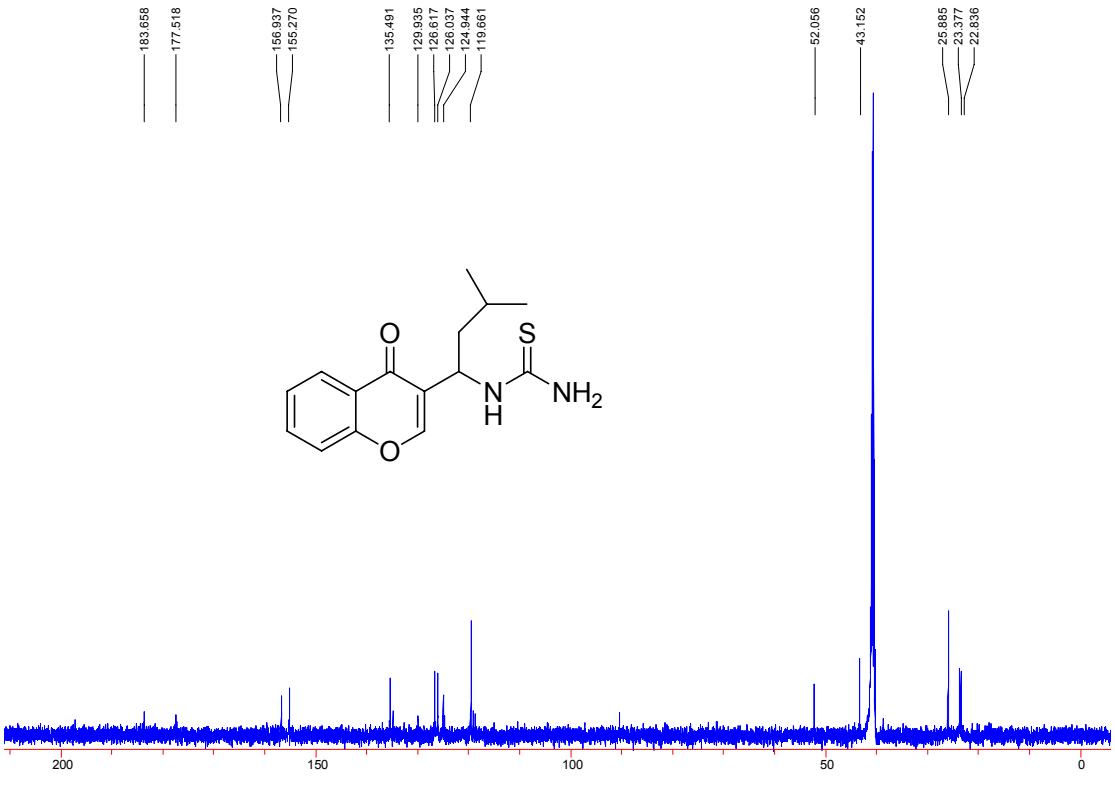
1.734
1.663
1.637
1.562
1.549
1.524
0.910
0.910
0.897


O
S
N
H
NH2
O
11d
1.00
1.09
1.32
1.11
1.12
1.09
1.83
0.89
1.09
1.16
1.06
6.10
8
7
6
5
4
3
2
1
0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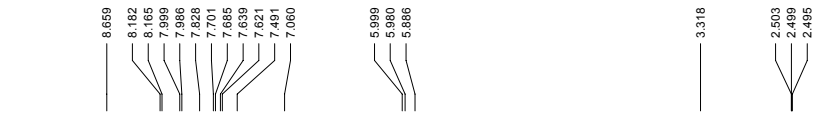
177.518
156.937
155.270
135.491
129.935
126.617
126.037
124.944
119.661
52.056
43.152
25.885
23.377
22.836
O
S
N
H
NH2
O
200
150
100
50
0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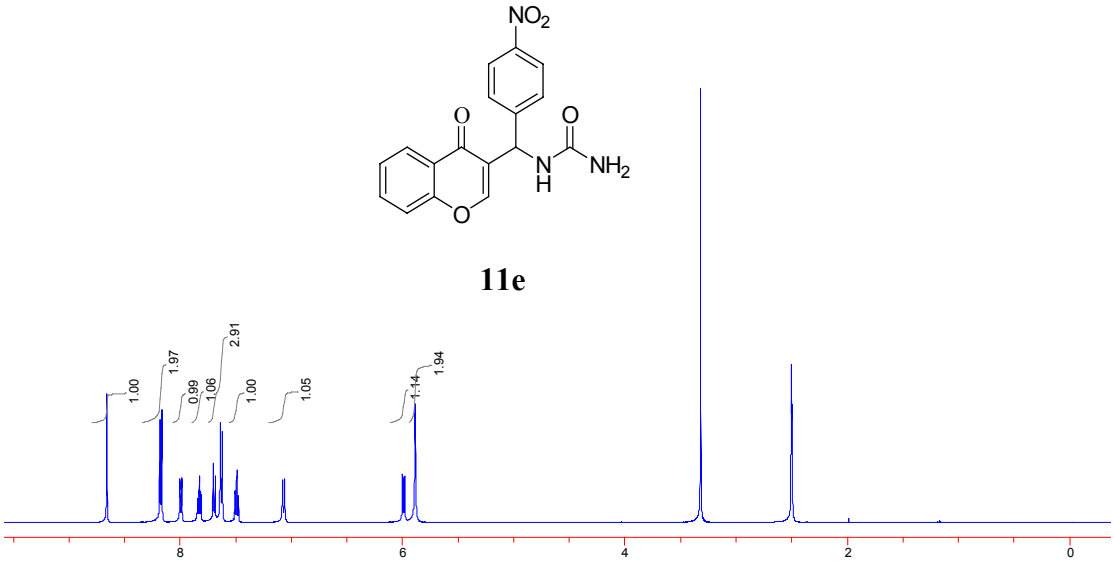
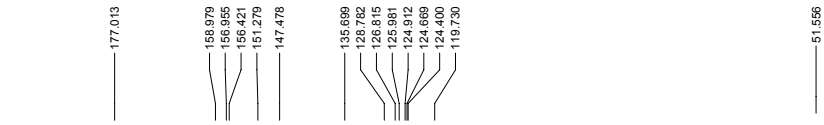
8.182
8.165
7.999
7.986
7.828
7.701
7.685
7.639
7.621
7.491
7.060
5.999
5.980
5.886
3.318
2.503
2.499
2.495


NO2
O
O
N
H
NH2
O
1.00
1.97
0.99
1.06
2.91
1.00
1.05
1.14
1.94
8
6
4
2
0

**11e**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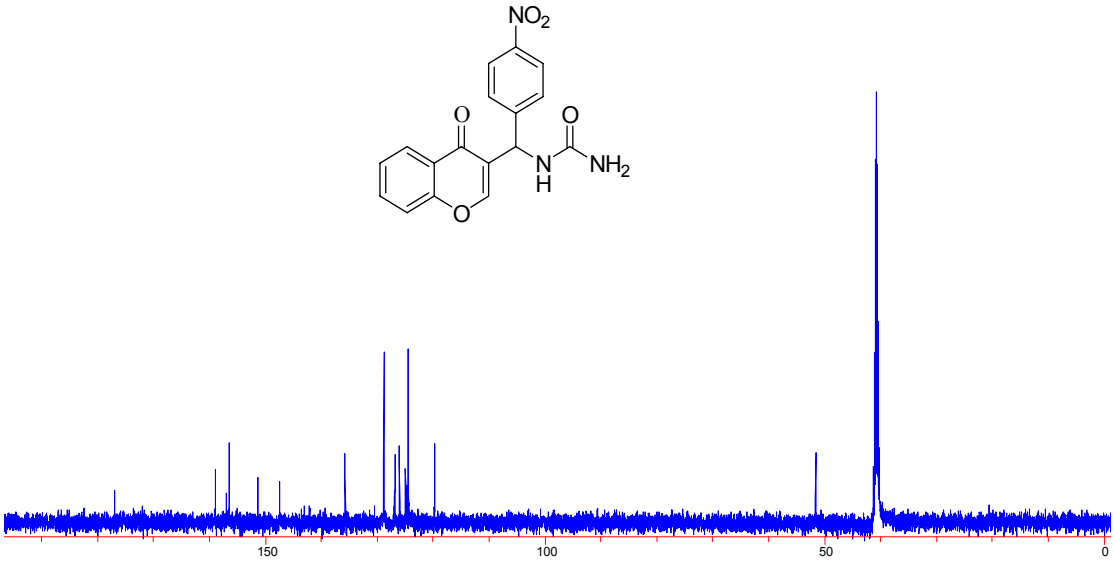
156.421
151.279
147.478
135.699
128.782
126.815
125.981
124.912
124.669
124.400
119.730
51.556
41.187
41.011
40.943
40.853
40.688
40.520
40.351
40.184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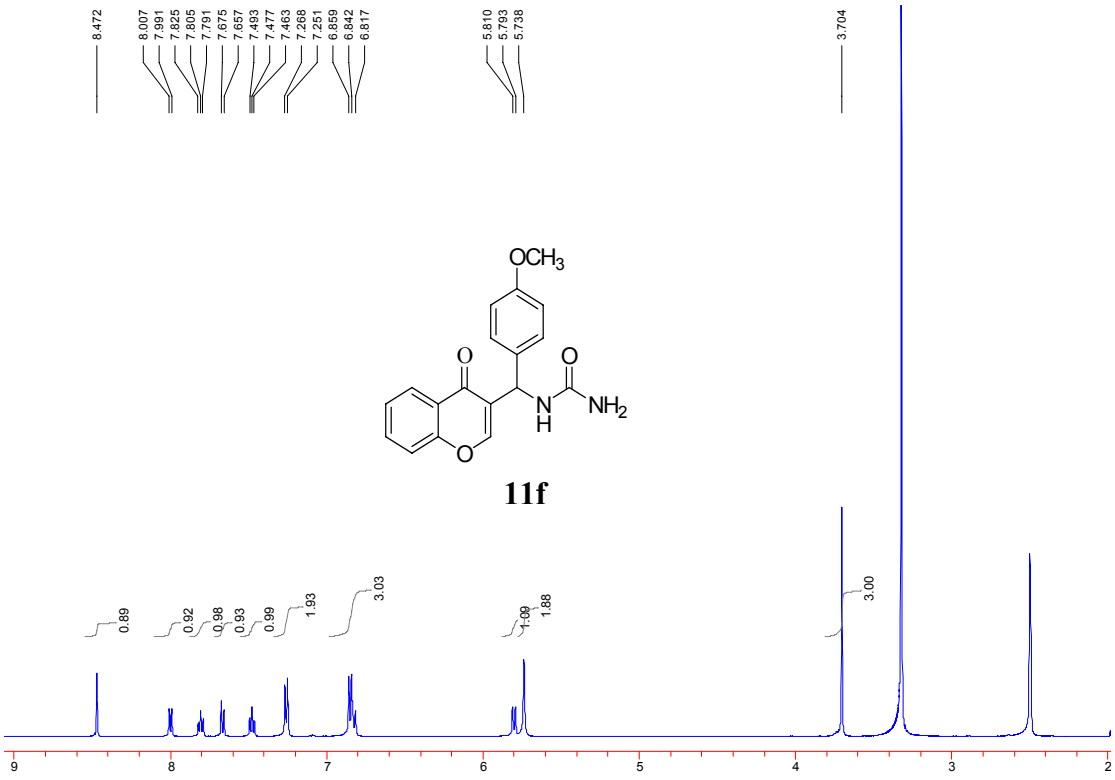
O
N
H
NH2
O
150
100
50
0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7.657
7.493
7.477
7.463
7.268
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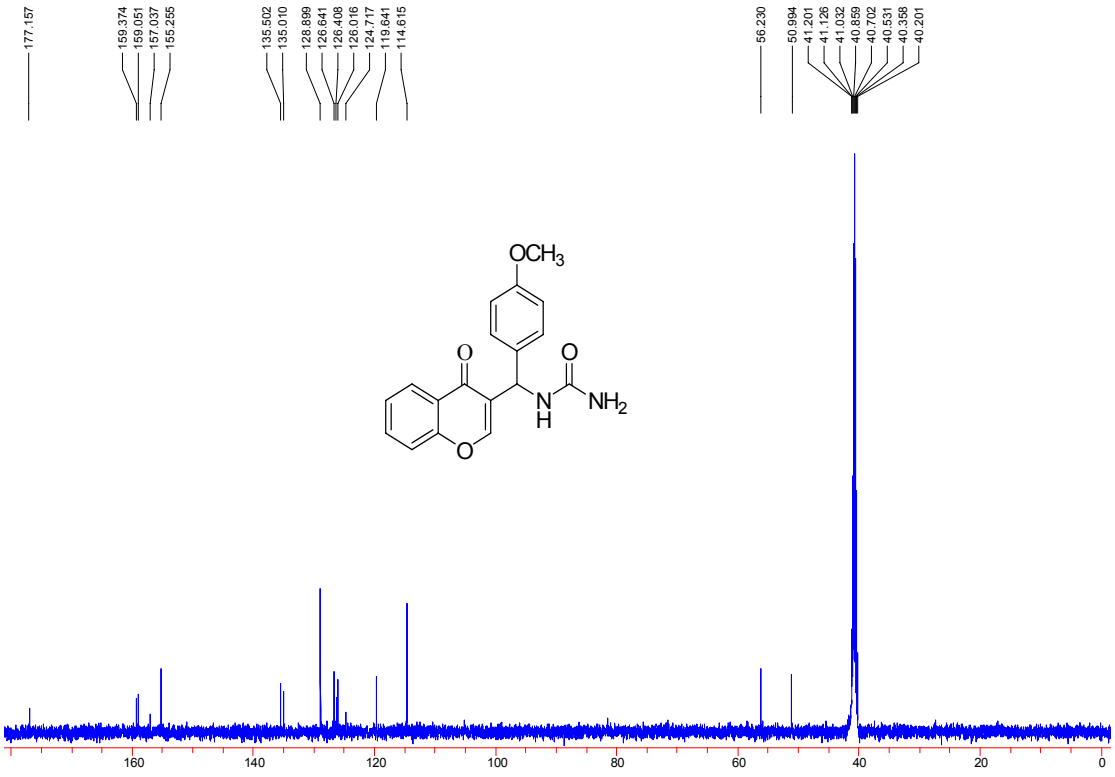
6.859
6.842
6.817
5.810
5.793
5.738
3.704
OCH3
O
O
N
H
NH2
O
0.89
0.92
0.98
0.93
0.99
1.93
3.03
1.00
1.88
3.00
9
8
7
6
5
4
3
2

**11f**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159.051
157.037
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135.502
135.010
128.899
126.641
126.408
126.016
124.717
119.641
114.615
56.230
50.994
41.201
41.126
41.032
40.859
40.702
40.531
40.358
40.201
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O
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H
NH2
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140
120
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80
60
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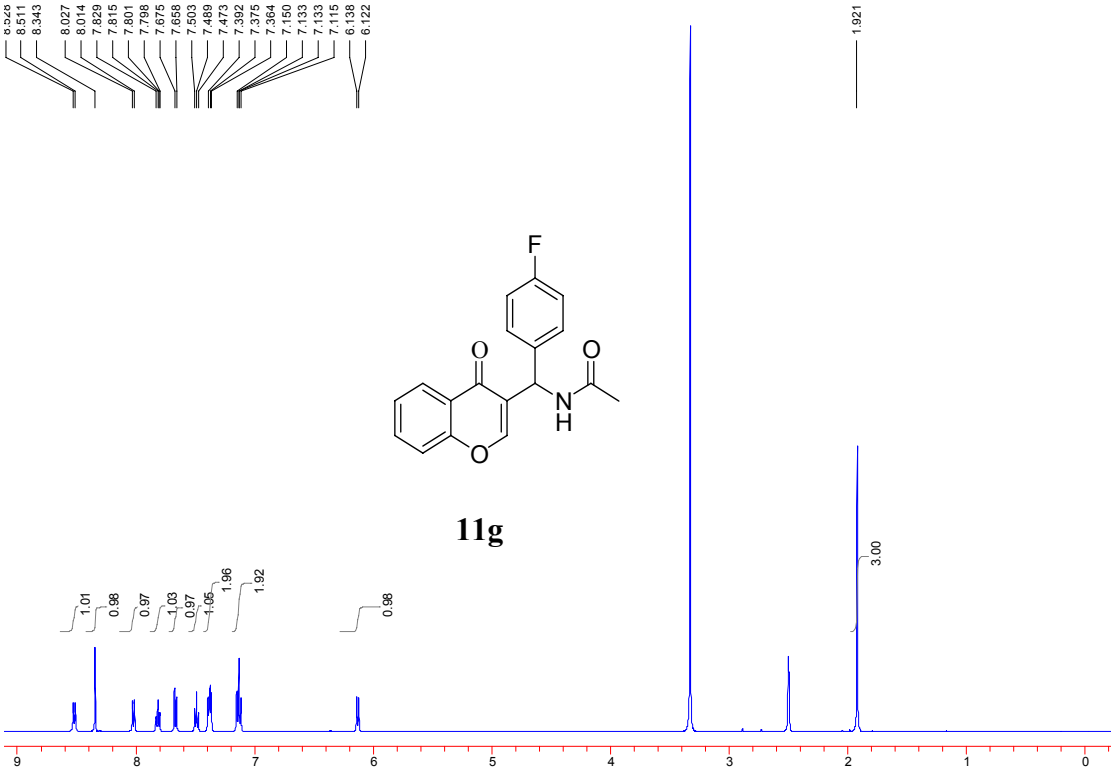
20
0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7.829
7.815
7.801
7.798
7.675
7.658
7.503
7.489
7.473
7.392
7.375
7.364
7.150
7.133
7.133
7.115
6.138
6.122
1.921
F
O
O
N
H
O
11g
1.01
0.98
0.97
1.03
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1.92
0.98
3.00
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7
6
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4
3
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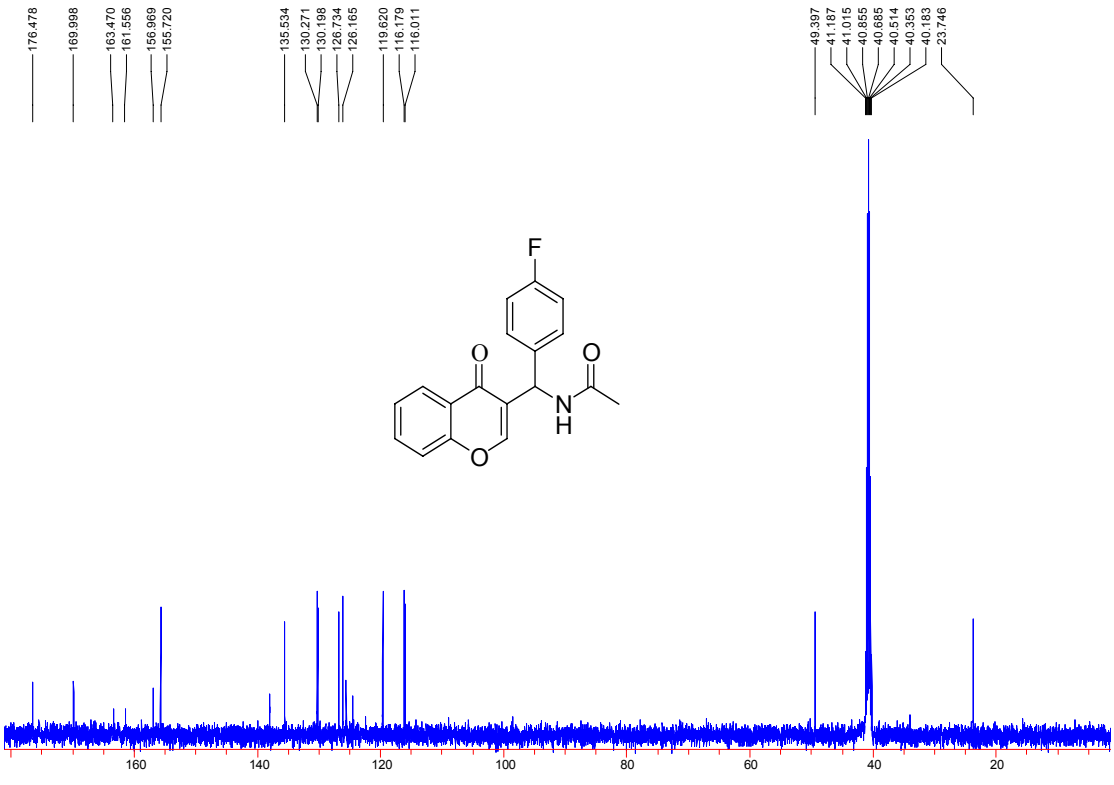
1
0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163.470
161.556
156.969
155.720
135.534
130.271
130.198
126.734
126.165
119.620
116.179
116.011
49.397
41.187
41.015
40.855
40.685
40.514
40.353
40.183
23.746
F
O
O
N
H
O
160
140
120
100
80
60
40
20