SUPPORTING INFORMATION

On Water: Catalyst−free chemoselective synthesis of highly functionalized tetrahydroquinazolines from 2-aminophenylacrylate

Rakesh K. Saunthwal,[a] Monika Patel,[a] Rakesh K. Tiwari,[b] Keykavous Parang [b] and Akhilesh K. Verma, * [a]

[a]*Synthetic Organic Chemistry Research Laboratory, Department of Chemistry, University of Delhi, Delhi – 110007, India*

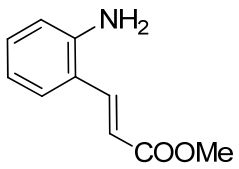
[b]*College of Pharmacy, Chapman University, Orange, California 92866, USA*

Email: averma@acbr.du.ac.in

Experimental section

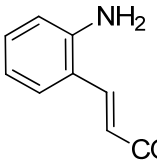
General Information and Method. All the reactions were performed in an oven-dried Schlenk flask under an argon atmosphere. Column chromatography was cperformed using silica gel (mesh 100-200). TLC analysis was performed on commercially prepared 60 F_{254} silica gel plates. Visualization of spots on TLC plate was accomplished with UV light (254 nm) and staining over I_2 chamber. ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra were recorded in $CDCl_3$ and $(CD_3)_2SO$. Chemical shifts for carbons are reported in ppm from tetramethylsilane and are referenced to the carbon resonance of the solvent. Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = doublet of doublet, br s = broad singlet), coupling constants in Hertz, and integration. High-resolution mass spectra were recorded with q-TOF electrospray mass spectrometer and Infrared spectra were recorded on a FT-IR spectrophotometer. All purchased chemicals were used as received. All melting points are uncorrected.
Few data's were recorded in $CDCl_3$ which does not show the –NH proton, to confirm –NH proton we have reported the IR data's.

General procedure for the synthesis of 2-aminophenyl acrylate 1a–l. To probe the viability of the designed strategy, the substrates **1a-l** required for the reaction were readily prepared by the Heck cross−coupling[10] of the commercially available and readily accessible substituted and unsubstituted bromo/iodoanilines with acrylates by using 5 mol % of $PdCl_2(PPh_3)_2$ and triethylamine as base The structure and purity of known starting materials were confirmed by comparison of their physical and spectral data (^{1}H NMR, ^{13}C NMR, and HRMS) with those reported in literature.

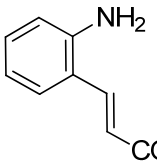


(*E*)-Methyl 3-(2-aminophenyl)acrylate (1a). The product was obtained as yellow needles (DCM/Ether), (90%): mp 60–62 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, J = 14.6 Hz, 1H), 7.35 (d, J = 8.0 Hz, 1H), 7.17–7.12 (m, 1H), 6.74 (t, J = 7.3 Hz, 1H), 6.67 (d, J = 8.0 Hz, 1H), 6.33 (d, J = 15.4 Hz, 1H), 3.96 (br s, 2H), 3.77 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.7, 145.5, 140.3, 131.3, 128.0, 119.8, 118.9, 117.6, 116.7, 51.6; IR spectrum in film (ν_{max}, cm^{-1}) 3481, 3361, 1654, 1629,

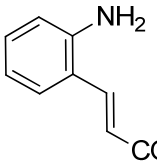
1597, 1468, 1448, 1324, 1299, 1182, 1113, 999, 839,753; HRMS (ESI) $(M)^+$ Calcd for $C_{10}H_{11}NO_2$ 177.0790, found 177.0790.



(*E*)-Ethyl 3-(2-aminophenyl)acrylate (1b). The product was obtained as yellow needles (DCM/Ether) (90%): mp 64–67 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, J =16.1 Hz, 1H), 7.31–7.29 (m, 1H), 7.11–7.07 (m, 1H), 6.71–6.67 (m, 1H), 6.63–6.61 (m, 1H), 6.27 (d, J = 15.4 Hz, 1H), 4.18 (q, J = 6.6 Hz, 2H), 3.44 (br s, 2H), 1.26 (t, J = 6.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.3, 145.5, 140.0, 131.2, 128.1, 119.9, 118.9, 118.1, 116.7, 60.4, 14.3; IR spectrum in film (ν_{max}, cm^{-1}) 3371, 3245, 1699, 1654, 1620, 1490, 1460, 1367, 1321, 1263, 1197, 1035, 980, 863, 755. HRMS (ESI) $(M)^+$ Calcd for $C_{11}H_{13}NO_2$ 191.0946, found 191.0946.

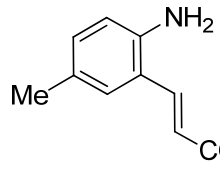


(*E*)-Butyl 3-(2-aminophenyl)acrylate (1c). The product was obtained as yellow oil, (91%): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, J = 15.4 Hz, 1H), 7.45–7.43 (m, 1H), 7.24–7.19 (m, 1H), 6.81 (t, J = 7.3 Hz, 1H), 6.75 (d, J = 8.0 Hz, 1H), 6.42 (d, J =16.1 Hz, 1H), 4.27 (t, J = 6.5 Hz, 2H), 4.11 (br s, 2H), 1.78–1.71 (m, 2H), 1.54–1.45 (m, 2H), 1.03 (t, J = 7.5 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.3, 145.6, 139.9, 131.1, 127.8, 119.6, 118.6, 117.7, 116.6, 64.2, 30.6, 19.0, 13.6; IR spectrum in film (ν_{max}, cm^{-1}) 3456, 3373, 2959, 1701, 1654, 1623, 1490, 1459, 1323, 1303, 1177, 1063, 982, 863, 755 . HRMS (ESI) $(M)^+$ Calcd for $C_{13}H_{17}NO_2$ 219.1259, found 219.1258.

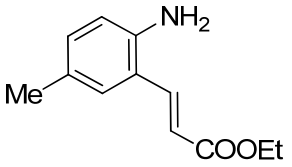


(*E*)-*tert*-Butyl 3-(2-aminophenyl)acrylate (1d). The product was obtained as a yellow needles (DCM/Ether), (89%): mp 69–71 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, J = 16.5 Hz, 1H), 7.36–7.34 (m, 1H), 7.16–7.12 (m, 1H), 6.74 (t, J = 8.0 Hz, 1H), 6.69–6.66 (m, 1H), 6.27 (d, J = 15.9 Hz, 1H), 3.93 (br s, 2H), 1.52 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.6, 145.3, 139.0, 130.9, 128.1, 120.2, 120.1,

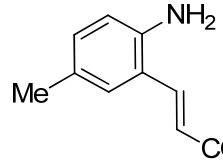
118.9, 116.6, 80.4, 28.2; IR spectrum in film (ν_{max}, cm^{-1}) 3404, 3343, 1705, 1626, 1493, 1341, 1287, 1262, 1178, 1156, 1008, 980, 857; HRMS (ESI) $(M)^+$ Calcd for $C_{13}H_{17}NO_2$ 219.1259, found 219.1258.



(*E*)-Methyl 3-(2-amino-5-methylphenyl)acrylate (1e). The product was obtained as yellow needles (DCM/Ether), (85%): mp 54–56 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, J = 16.0 Hz,1H), 7.24 (s, 1H), 7.04–7.02 (m, 1H), 6.66 (d, J = 8.2 Hz, 1H), 6.39 (d, J =16.0 Hz, 1H), 3.95 (br s, 2H), 3.84 (s, 3H), 2.28 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.7, 143.3, 140.3, 132.1, 128.0, 127.9, 119.6, 117.0, 116.9, 51.5, 20.2; IR spectrum in film (ν_{max}, cm^{-1}) 3457, 3375, 1701, 1618, 1500, 1435, 1307, 1259, 1193, 1161, 1038, 981, 858, 817; HRMS (ESI) $(M)^+$ Calcd for $C_{11}H_{13}NO_2$ 191.0946, found 191.0946.

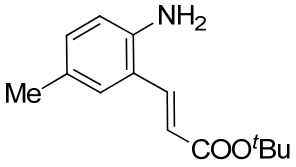


(*E*)-Ethyl 3-(2-amino-5-methylphenyl)acrylate (1f). The product was obtained as a yellow needles (DCM/Ether), (83%): mp 61–63 °C: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, J =15.8 Hz, 1H), 7.17 (d, J = 1.8 Hz, 1H), 6.98–6.95 (m, 1H), 6.59 (d, J =7.9 Hz, 1H), 6.32 (d, J =15.8 Hz, 1H), 4.24 (q, J = 6.7 Hz, 2H), 3.84 (br s, 2H), 2.21 (s, 3H), 1.31 (t, J = 1.32 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.3, 143.2, 140.1, 132.1, 128.0, 119.7, 117.6, 116.9, 60.3, 20.3, 14.3; IR spectrum in film (ν_{max}, cm^{-1}) 3407, 3350, 2920, 1704, 1621, 1502, 1449, 1431, 1337, 1326, 1194, 1177, 1161,1015, 981, 851, 812, 755; HRMS (ESI) $(M)^+$ Calcd for $C_{12}H_{15}NO_2$ 205.1103, found 205.1103.

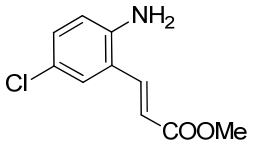


(*E*)-Butyl 3-(2-amino-5-methylphenyl)acrylate (1g). The product was obtained as yellow oil, (82%): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (d, J = 16.0 Hz, 1H), 7.24 (s, 1H), 7.02 (d, J = 8.2 Hz, 1H), 6.65 (d, J = 8.2 Hz, 1H), 6.39 (d, J = 16.0 Hz, 1H), 4.24 (t, J = 6.9 Hz, 2H), 3.86 (br s, 2H), 2.27 (s, 3H), 1.76–1.68 (m,

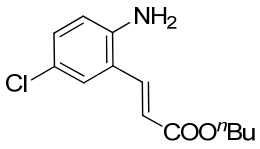
2H), 1.51–1.44 (m, 2H), 1.00 (t, J = 7.3 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.4, 143.2, 140.1, 132.1, 128.0, 127.9, 119.7, 117.6, 116.9, 64.3, 30.7, 20.3, 19.1, 13.7; IR spectrum in film (ν_{max}, cm^{-1}) 3390, 3372, 2958, 1703, 1620, 1501, 1329, 1300, 1259, 1176, 1160, 1063, 981, 859, 815; HRMS (ESI) $(M)^+$ Calcd for $C_{14}H_{19}NO_2$ 233.1416, found 233.1415.



(*E*)-*tert*-Butyl 3-(2-amino-5-methylphenyl)acrylate (1h). The product was obtained as yellow needles (DCM/Ether) (90%): mp 64–67 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, J =16.0 Hz, 1H), 7.10 (s, 1H), 6.90–6.88 (m, 1H), 6.53 (d, J = 8.2 Hz, 1H), 6.10 (d, J =16.0 Hz, 1H), 3.74 (br s, 2H), 2.15 (s, 3H), 1.45 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.7, 143.0, 139.1, 131.8, 128.2, 128.0, 120.1, 119.8, 116.8, 80.3, 28.2, 20.3; HRMS (ESI) $(M)^+$ Calcd for $C_{14}H_{19}NO_2$ 233.1416, found 233.1415.

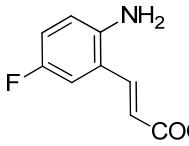


(*E*)-Methyl 3-(2-amino-5-chlorophenyl)acrylate (1i). The product was obtained as a yellow needles (DCM/Ether) (80%): mp 70–72 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, J = 15.6 Hz, 1H), 7.24 (d, J = 2.3 Hz, 1H), 7.00 (dd, J = 8.7 and 2.3 Hz, 1H), 6.57 (d, J = 8.7 Hz, 1H), 6.24 (d, J =15.6 Hz, 1H), 3.94 (br s, 2H), 3.71 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.3, 144.0, 138.8, 130.9, 127.2, 123.5, 120.9, 118.7, 51.7; IR spectrum in film (ν_{max}, cm^{-1}) 3459, 3353, 2961, 1724, 1541, 1507, 1490, 1301, 1285, 1252, 1148, 1105, 1027, 856, 818, 763; HRMS (ESI) $(M)^+$ Calcd for $C_{10}H_{10}ClNO_2$ 211.0400, found 211.0403.

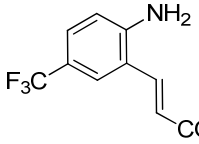


(*E*)-Butyl 3-(2-amino-5-chlorophenyl)acrylate (1j). The product was obtained as yellow oil, (91%): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, J = 15.9 Hz, 1H), 7.31 (d, J = 2.4 Hz, 1H), 7.08 (dd, J = 8.5 and 2.4 Hz, 1H), 6.60 (d, J = 8.5 Hz, 1H), 6.31 (d, J = 15.9 Hz, 1H), 4.17 (t, J = 6.4 Hz, 2H), 3.96 (br s, 2H), 1.69–1.62 (m, 2H), 1.45–1.35 (m, 2H), 0.93 (t, J = 7.4 Hz, 3H); ^{13}C NMR (100 MHz,

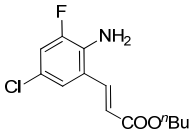
$CDCl_3$) δ 167.0, 143.9, 138.5, 130.8, 127.2, 123.5, 121.1, 119.3, 117.8, 64.5, 30.7, 19.1, 13.7; HRMS (ESI) $(M)^+$ Calcd for $C_{13}H_{16}ClNO_2$ 253.0870, found 253.0870.



(*E*)-Methyl 3-(2-amino-5-fluorophenyl)acrylate (1k). The product was obtained as a yellow needles (DCM/Ether), (89%): mp 69–71 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, J = 16.0 Hz, 1H), 7.06 (dd, J = 10.0 and 4.6 Hz, 1H), 6.91–6.86 (m, 1H), 6.64–6.61 (m, 1H), 6.31 (d, J = 15.6 Hz, 1H), 3.78 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.3, 156.3 (d, J = 236.7 Hz, 1C), 147.7, 139.1, 120.8 (d, J = 7.7 Hz, 1C), 118.9, 118.4, 117.7 (d, J = 7.6 Hz, 1C), 113.4 (d, J = 23.0 Hz, 1C), 51.8; HRMS (ESI) $(M)^+$ Calcd for $C_{10}H_{10}FNO_2$ 195.0696, found 195.0696.

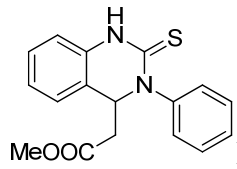


(*E*)-Methyl 3-(2-amino-5-(trifluoromethyl)phenyl) acrylate (1l). The product was obtained as a pale yellow needles (DCM/Ether) (70%): mp 80–82 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, J = 15.8 Hz, 1H), 7.58 (s, 1H), 7.36–7.34 (m, 1H), 6.71 (d, J = 8.5 Hz, 1H),), 6.38 (d, J = 15.8 Hz, 1H), 4.33 (br s, 2H), 3.79 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.3, 148.0, 138.9, 127.8, 127.79, 125.3 (q, J = 15.2 Hz, 1C), 119.3, 118.9, 116.2, 51.8; IR spectrum in film (ν_{max}, cm^{-1}) 3380, 3246, 2954, 1702, 1629, 1509, 1438, 1347, 1324, 1166, 1110, 1076, 980, 864, 772; HRMS (ESI) $(M)^+$ Calcd for $C_{11}H_{10}F_3NO_2$ 245.0664, found 245.0664.

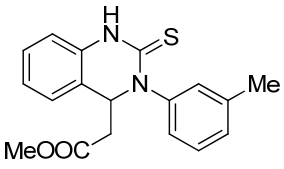


(*E*)-Butyl 3-(2-amino-5-chloro-3-fluorophenyl)acrylate (1m). The product was obtained as a pale yellow needles (DCM/Ether) (70%): mp 85–87 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (d, J = 16.0 Hz, 1H), 7.13–7.12 (m, 1H), 6.98 (dd, J = 10.5 and 2.3 Hz, 1H), 6.32 (d, J = 16.0 Hz, 1H), 4.17 (t, J = 6.4 Hz, 2H), 4.05 (br s, 2H), 1.68–1.61 (m, 2H), 1.42–1.36 (m, 2H), 0.93 (t, J = 7.3 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.7, 151.5 (d, J = 242.5 Hz, 1C), 137.4 (d, J = 3.8 Hz, 1C), 132.9 (d, J = 13.4 Hz, 1C), 122.6 (d, J = 2.9 Hz, 1C), 122.4 (d, J = 3.8 Hz, 1C), 122.3 (d, J = 10.5 Hz, 1C), 120.3, 116.6 (d, J = 22.0 Hz, 1C), 64.7, 30.7, 19.1, 13.7; HRMS (ESI) $(M)^+$ Calcd for $C_{13}H_{15}ClFNO_2$ 271.0775, found 271.0774.

General procedure for the synthesis of 2-thioxo-1,2,3,4-tetrahydroquinazoline (3a-l and 4a-o). An oven-dried Schlenk tube with a Teflon screw valve was charged with 0.5 mmol of 2-aminophenylacrylate **1a-1l**, and 0.5 mmol of isothiocyanates **2a–j** .The Schlenk tube was capped with a rubber septum and then evacuated and backfilled with nitrogen. The septum was then replaced with a Teflon screw valve, and the Schlenk tube was sealed. The reaction mixture was heated to 80 °C for 16-20 h until 2-aminophenylacrylate **1a-1l**, had been completely consumed (as determined by TLC). The reaction was allowed to cool at room temperature. The reaction mixture was diluted with ethyl acetate (10 mL) and water (15 mL). Organic layer was concentrated under reduced pressure. The crude material so obtained was purified by column chromatography on silica gel using hexane-ethyl acetate mixture (80: 20).

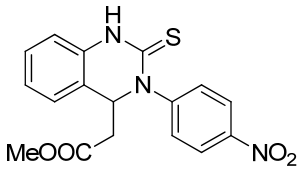


Methyl 2-(3-phenyl-2-thioxo-1,2,3,4-etrahydroquinazolin -4-yl) acetate (3a). The product was obtained as a white needles (DCM/Ether), (90%) : mp 144–142 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.76 (br s, 1H), 7.47–7.43 (m, 2H), 7.39–7.37 (m, 3H), 7.28–7.26 (m, 1H), 7.13 (d, J = 7.3 Hz, 1H), 7.06–7.02 (m, 1H), 6.86 (d, J = 7.9 Hz, 1H), 5.24 (dd, J = 8.6 and 4.3 Hz, 1H), 3.53 (s, 3H), 2.95–2.81 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 177.3, 169.9, 143.8, 134.4, 129.4, 129.3, 129.1, 129.0, 128.5, 128.3, 125.8, 123.9, 120.7, 113.9, 60.8, 51.9, 39.5; HRMS (ESI) $(M)^+$ Calcd for $C_{17}H_{16}N_2O_2S$ 312.0932, found 312.0930.

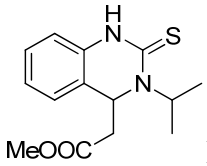


Methyl 2-(2-thioxo-3-(*m*-tolyl)-1,2,3,4-tetrahydro quinazolin -4-yl)acetate (3b). The product was obtained as a yellow needles (DCM/Ether), (83%) : mp 115–117 °C: ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.29 (br s, 1H), 7.33 (t, J = 7.9 Hz, 1H), 7.29–7.24 (m, 1H), 7.22–7.16 (m, 3H), 7.12 (d, J = 6.7 Hz, 1H), 7.03 (t, J = 7.9 Hz, 1H), 6.92 (d, J = 7.9 Hz, 1H), 5.22 (dd, J = 9.1 and 4.8 Hz, 1H), 3.53 (s, 3H), 2.92–2.90 (m, 1H), 2.86–2.80 (m, 1H), 2.38 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ

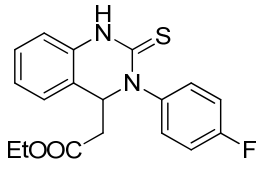
177.0, 169.9, 143.6, 139.5, 134.4, 129.2, 129.1, 128.8, 125.7, 123.7, 120.6, 114.1, 60.8, 51.8, 39.4, 21.3; HRMS (ESI) $(M)^+$ Calcd for $C_{18}H_{18}N_2O_2S$ 326.1089, found 326.
1089.



Methyl 2-(3-(4-nitrophenyl)-2-thioxo-1,2,3,4-tetrahydro quinazolin-4-yl)acetate (3c). The product was obtained as a yellow needles (DCM/Ether), (95%) : mp 144–142 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.56 (br s, 1H), 8.29 (d, J = 8.5 Hz, 2H), 7.62 (d, J = 7.9 Hz, 2H), 7.27–7.24 (m, 1H), 7.15–7.05 (m, 2H), 6.93 (d, J = 7.9 Hz, 1H), 5.29 (dd, J = 6.4 and 4.9 Hz, 1H), 3.54 (s, 3H), 2.92–2.78 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.9, 169.6, 149.1, 146.8, 134.0, 129.7, 129.5, 125.8, 125.0, 124.7, 124.4, 120.5, 114.2, 60.5, 52.1, 39.7; HRMS (ESI) $(M)^+$ Calcd for $C_{17}H_{15}N_3O_4S$ 357.0783 found 357.0784.

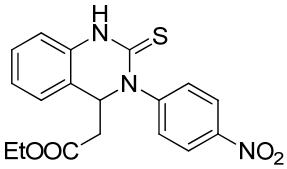


Methyl 2-(3-isopropyl-2-thioxo-1,2,3,4-tetrahydro quinazolin-4-yl)acetate (3d). The product was obtained as a yellow oil, (75%): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.71(br s, 1H), 7.24–7.20 (m, 1H), 7.14 (d, J = 7.8 Hz, 1H), 7.00 (t, J = 7.5 Hz, 1H), 6.86 (d, J = 8.2 Hz, 1H), 5.61–5.55 (m, 1H), 5.05 (dd, J = 9.6 and 2.3 Hz, 1H), 3.56 (s, 3H), 2.81–2.74 (m, 1H), 2.58–2.53 (m, 1H), 1.40 (d, J = 6.9 Hz, 3H), 1.21 (d, J = 6.9 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 177.1, 170.3, 134.4, 128.9, 125.2, 123.6, 121.8, 113.6, 52.6, 51.8, 50.2, 40.0, 20.6, 20.4; HRMS (ESI) $(M)^+$ Calcd for $C_{14}H_{18}N_2O_2S$ 278.1089, found 326.1088.

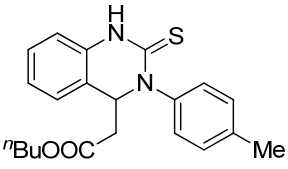


Ethyl 2-(3-(4-fluorophenyl)-2-thioxo-1,2,3,4-tetrahydro quinazolin-4-yl)acetate (3e). The product was obtained as a white needles (DCM/Ether), (92%) : mp 135–137 °C: ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.25 (br s, 1H), 7.34–7.30 (m, 2H), 7.21–7.17 (m, 1H), 7.08 (t, J = 8.2 Hz, 3H), 6.99 (t, J = 4.12 Hz,

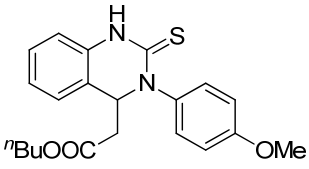
1H), 6.85 (d, J = 4.1 Hz, 1H), 5.16 (dd, J = 8.2 and 5.0 Hz, 1H), 3.97–3.89 (m, 2H), 2.84–2.75 (m, 2H), 1.06 (t, J = 7.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 177.4, 169.5, 162.0 (d, J = 248.2 Hz, 1C), 139.7 (d, J = 2.9 Hz, 1C), 134.5, 130.6 (d, J = 8.6 Hz, 1C), 129.4, 125.9, 124.1, 120.7, 116.5 (d, J = 22.0 Hz, 1C), 114.1, 61.2, 61.0, 39.9, 14.1; HRMS (ESI) $(M)^+$ Calcd for $C_{18}H_{17}FN_2O_2S$ 344.0995, found 344.0997.



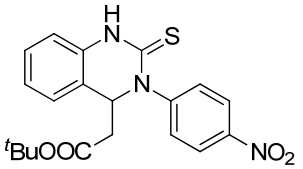
Ethyl 2-(3-(4-nitrophenyl)-2-thioxo-1,2,3,4-tetrahydro quinazolin-4-yl)acetate (3f). The product was obtained as a yellow needles (DCM/Ether), (94%) : mp 137–139 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.19 (br s, 1H), 8.30 (d, J = 9.2 Hz, 2H), 7.64–7.61 (m, 2H), 7.28 (t, J = 7.6 Hz, 1H), 7.15 (d, J = 6.9 Hz, 1H), 7.08 (t, J = 7.6 Hz, 1H), 6.90 (d, J = 8.4 Hz, 1H), 5.29 (dd, J = 7.6 and 4.5 Hz, 1H), 4.03–3.95 (m, 2H), 2.90–2.78 (m, 2H), 1.12 (t, J = 6.9 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.8, 169.2, 149.1, 146.7, 134.0, 129.8, 129.5, 125.8, 124.7, 124.3, 120.5, 114.1, 61.2, 60.5, 39.9, 13.9; HRMS (ESI) $(M)^+$ Calcd for $C_{18}H_{17}N_3O_4S$ 371.0940, found 371.0941.



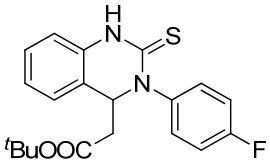
Butyl 2-(2-thioxo-3-(*p*-tolyl)-1,2,3,4-tetrahydro quinazolin-4-yl)acetate (3g). The product was obtained as a yellow oil (84%): ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.51 (br s, 1H), 7.18–7.14 (m, 5H), 7.05–7.04 (d, J = 6.1 Hz, 1H), 6.98–6.94 (m, 1H), 6.91 (d, J = 7.9 Hz, 1H), 5.14 (dd, J = 8.5 and 4.9 Hz, 1H), 3.85 (t, J = 6.7 Hz, 2H), 2.85–2.72 (m, 2H), 2.31 (s, 3H), 1.41–1.35 (m, 2H), 1.18–1.11 (m, 2H), 0.81–0.76 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 177.9, 170.3, 133.5, 130.1, 129.5, 128.6, 126.4, 125.5, 124.1, 122.3, 122.1, 121.1, 68.5, 64.7, 41.5, 30.5, 19.0, 13.6; HRMS (ESI) $(M)^+$ Calcd for $C_{21}H_{24}N_2O_2S$ 384.1558, found 384.1560.



Butyl 2-(3-(4-methoxyphenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin -4-yl) acetate (3h). The product was obtained as a dark brown needles (DCM/Ether), (80%) : mp 144–146 °C: ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.05 (br s, 1H), 7.30–7.28 (m, 2H), 7.26–7.22 (m, 2H), 7.12 (d, J = 6.7 Hz, 1H), 7.05–7.00 (m, 1H), 6.95 (d, J = 9.1 Hz, 2H), 6.89 (d, J = 7.9 Hz, 1H), 5.20 (dd, J = 8.5 and 4.8 Hz, 1H), 3.92 (t, J = 6.1 Hz, 2H), 3.82 (s, 3H), 2.92–2.78 (m, 2H), 1.47–1.42 (m, 2H), 1.27–1.17 (m, 2H), 0.84 (t, J =7.3 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 177.4, 169.6, 159.1, 136.5, 135.2, 134.3, 129.6, 129.1, 125.8, 125.0, 123.7, 120.7, 114.6, 113.9, 64.9, 61.0, 55.4, 39.7, 23.4, 18.9, 13.6; HRMS (ESI) $(M)^+$ Calcd for $C_{21}H_{24}N_2O_3S$ 384.1508, found 384.1510.

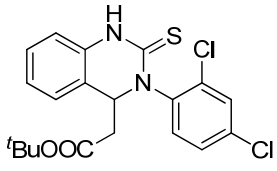


***tert*-Butyl2-(3-(4-nitrophenyl)-2-thioxo-1,2,3,4-tetra hydroquinazolin-4-yl)acetate (3i).** The product was obtained as a yellow oil, (90%) : ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.29 (br s, 1H), 8.26–8.24 (m, 2H), 7.59–7.57 (m, 2H), 7.24–7.19 (m, 1H), 7.10 (d, J = 7.3 Hz, 1H), 7.04–7.00 (m, 1H), 6.85 (d, J = 6.4 Hz, 1H**),** 5.19 (dd, J = 6.8 and 4.1 Hz, 1H), 2.75–2.64 (m, 2H), 1.26 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.8, 168.4, 149.2, 146.8, 134.0, 129.8, 129.4, 126.0, 124.7, 124.2, 120.6, 114.1, 82.0, 60.7, 41.1, 27.8; HRMS (ESI) $(M)^+$ Calcd for $C_{20}H_{21}N_3O_4S$ 399.1253, found 399.1255.

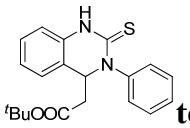


***tert*-Butyl 2-(3-(4-fluorophenyl)-2-thioxo-1,2,3,4-tetra hydroquinazolin-4-yl)acetate (3j).** The product was obtained as a white needles, (92%) : mp 137–140 °C: ^{1}H NMR (400 MHz, DMSO–d_6) δ 9.56 (br s, 1H), 7.39–7.36 (m, 2H), 7.24–7.20 (m, 1H), 7.13 (t, J = 8.2 Hz, 3H), 7.04–7.00 (m, 1H), 6.91(d, J = 7.8, 1H), 5.15 (dd, J = 7.3 and 5.9 Hz, 1H), 2.75–2.73 (m, 2H), 1.30 (s, 9H); ^{13}C NMR (100 MHz, DMSO–d_6) δ 177.0, 168.6, 161.9 (d, J = 248.2 Hz, 1C), 139.6 (d, J = 2.9 Hz, 1C), 134.2, 130.5 (d, J = 8.6 Hz, 1C), 129.1, 125.9, 123.8, 120.5, 116.4 (d, J =

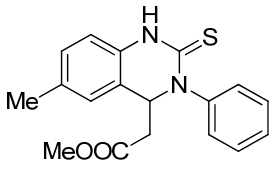
23.0 Hz, 1C), 114.1, 81.7, 61.0, 40.9, 27.8; HRMS (ESI) $(M)^+$ Calcd for $C_{20}H_{21}FN_2O_2S$ 372.1308, found 372.1241.



***tert*-Butyl 2-(3-(2,4-dichlorophenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (3k).** The product was obtained as a dark brown oil, (93%) : ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.0 (br s, 1H), 7.54 (d, J = 8.7 Hz, 1H), 7.46 (d, J = 2.3 Hz, 1H), 7.29 (dd, J = 8.2 and 2.3 Hz, 1H), 7.15–7.11 (m, 1H), 7.05 (d, J = 7.3 Hz, 1H**),** 6.98–6.94 (m, 1H), 6.91 (d, J = 7.8 Hz, 1H), 5.00 (dd, J = 6.9 and 5.5 Hz, 1H), 2.69–2.61 (m, 2H), 1.24 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.4, 168.5, 138.8, 134.8, 134.1, 133.9, 132.3, 130.4, 128.9, 127.5, 125.7, 123.9, 120.2, 114.2, 81.7, 65.7, 41.2, 27.7; HRMS (ESI) $(M)^+$ Calcd for $C_{20}H_{20}Cl_2N_2O_2S$ 422.0623, found 422.0624.

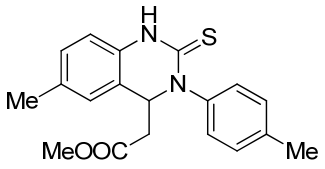


tert-Butyl 2-(3-phenyl-2-thioxo-1,2,3,4-tetrahydro quinazolin-4-yl)acetate (3l). The product was obtained as a white needles, (84%) : mp 139–141 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.9 (br s, 1H), 7.46–7.40 (m, 4H), 7.36–7.32 (m, 1H), 7.26–7.22 (m, 1H), 7.15 (d, J = 7.8 Hz, 1H), 7.06 (d, J = 8.2 Hz, 1H), 7.03–6.99 (m, 1H), 5.19 (dd, J = 6.4 and 4.1 Hz, 1H), 2.67–2.52 (m, 2H), 1.27 (s, 9H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 175.9, 168.4, 143.9, 134.7, 129.1, 129.0, 128.6, 127.5, 126.0, 122.8, 120.3, 113.8, 80.5, 60.1, 41.0, 27.4; HRMS (ESI) $(M)^+$ Calcd for $C_{20}H_{22}N_2O_2S$ 354.1402, found 354.1403

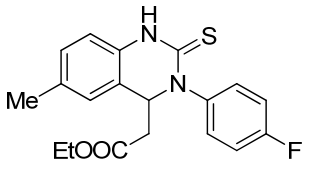


Methyl 2-(6-methyl-3-phenyl-2-thioxo-1,2,3,4-tetra hydroquinazolin-4-yl)acetate (4a). The product was obtained as a yellow needles (DCM/Ether), (92%) : mp 129–131 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.41 (br s, 1H), 7.46–7.40 (m, 2H), 7.37–7.35 (m, 3H), 7.04 (d, J = 7.8 Hz, 1H), 6.91 (s, 1H), 6.84 (d, J = 8.2 Hz, 1H) 5.20 (dd, J = 8.2 and 4.6 Hz, 1H), 3.56 (s, 3H), 2.93–2.79 (m, 2H),

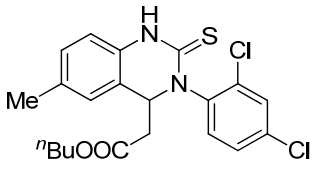
2.27 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.7, 169.9, 137.0, 133.5, 132.0, 129.7, 129.5, 129.4, 128.6, 128.2, 126.9, 125.2, 120.6, 113.9, 60.8. 51.8, 39.6, 20.8; HRMS (ESI) $(M)^+$ Calcd for $C_{18}H_{18}N_2O_2S$ 326.1089, found 326.1089.



Methyl 2-(6-methyl-2-thioxo-3-(*p*-tolyl)-1,2,3,4-tetra hydroquinazolin-4-yl)acetate (4b). The product was obtained as a yellow needles (DCM/Ether), (87%) : mp 131–133 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.17 (br s, 1H), 7.24–7.21 (m, 4H), 7.02 (d, J = 8.2 Hz, 1H), 6.90 (s, 1H), 6.79 (d, J = 8.2 Hz, 1H), 5.15 (dd, J = 8.2 and 4.1 Hz, 1H), 3.53 (s, 3H), 2.88–2.78 (m, 2H), 2.37 (s, 3H), 2.26 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.9, 170.0, 141.2, 138.2, 134.2, 133.5, 132.0, 130.0, 129.7, 128.6, 128.2, 126.0, 120.6,113.9, 60.8, 51.8, 39.6, 21.2, 20.8; HRMS (ESI) $(M)^+$ Calcd for $C_{19}H_{20}N_2O_2S$ 340.1245, found 340.1246

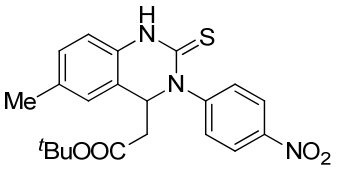


Ethyl 2-(3-(4-fluorophenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4c). The product was obtained as a yellow needles (DCM/Ether), (93%): mp: 140–143 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.02 (br s, 1H), 7.37–7.34 (m, 2H), 7.11 (t, J = 8.2 Hz, 2H), 7.05–7.03 (m, 1H), 6.92 (s, 1H), 6.77 (d, J = 7.8 Hz, 1H) 5.15 (dd, J = 8.2 and 5.0 Hz, 1H), 4.02–3.96 (m, 2H), 2.87–2.82 (m, 1H), 2.80–2.75 (m, 1H), 2.27 (s, 3H), 1.12 (t, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 177.4, 169.5, 161.9 (d, J = 249.2 Hz, 1C), 139.7 (d, J = 2.9 Hz, 1C), 133.7, 131.9, 130.5 (d, J = 8.6 Hz, 1C), 129.8, 126.1, 120.5, 116.3 (d, J = 23.0 Hz, 1C), 113.9, 61.0, 60.9, 39.8, 20.8, 13.9; HRMS (ESI) $(M)^+$ Calcd for $C_{19}H_{19}FN_2O_2S$ 358.1151, found 358.1150

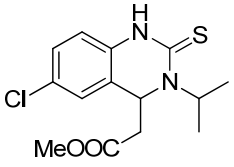


Butyl 2-(3-(2,4-dichlorophenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate: (4d) The product was obtained as a dark

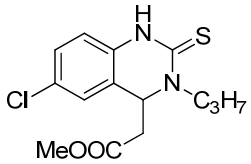
brown needles (DCM/Ether), (94%): mp: 110–113 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 9.78 (br s, 1H), 7.45–7.42 (m, 2H), 7.26 –7.23 (m, 1H), 6.99–6.97 (m, 1H), 6.85 (s, 1H), 6.81 (d, *J* = 8.2 Hz, 1H), 5.00 (dd, *J* = 5.0 and 2.3 Hz, 1H), 3.89–3.85 (m, 2H), 2.78–2.67 (m, 2H), 2.22 (s, 3H), 1.41–1.35 (m, 2H), 1.18–1.13 (m, 2H), 0.78 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 175.6, 169.4, 138.4, 135.1, 134.3, 133.9, 132.3, 131.3, 130.5, 129.8, 127.4, 126.0, 120.2, 114.5, 65.0, 59.3, 40.2, 30.3, 20.9, 18.9, 13.6; HRMS (ESI) $(M+H)^+$ Calcd for $C_{21}H_{22}Cl_2N_2O_2S$: 437.0857, found 437.0868.



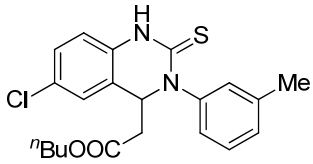
***tert*-Butyl 2-(6-methyl-3-(4-nitrophenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4e).** The product was obtained as a yellow needles (DCM/Ether), (92%): mp: 205–207 °C; ^{1}H NMR (400 MHz, $CDCl_3$) *δ* 9.09 (br s, 1H), 8.24 (d, *J* = 9.2 Hz, 2H), 7.57 (d, *J* = 9.2 Hz, 2H), 7.03–7.00 (m, 1H), 6.89 (s, 1H), 6.73 (d, *J* = 7.9 Hz, 1H), 5.14 (dd, *J* = 7.9 and 4.9 Hz, 1H), 2.74–2.62 (m, 2H), 2.22 (s, 3H), 1.27 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) *δ* 176.5, 168.4, 149.3, 146.7, 134.0, 131.6, 129.9, 129.8, 126.3, 124.7, 120.5, 113.9, 81.9, 60.8, 41.1, 27.8, 20.9.; HRMS (ESI) $(M)^+$ Calcd for $C_{21}H_{23}N_3O_4S$ 413.1409, found 413.1410.



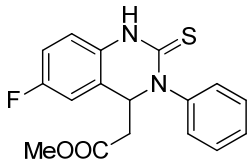
Methyl 2-(6-chloro-3-isopropyl-2-thioxo-1,2,3,4-tetra hydroquinazolin-4-yl)acetate: (4f) The product was obtained as a yellow oil (68%): ^{1}H NMR (400 MHz, $CDCl_3$) *δ*: 9.29 (br s, 1H), 7.14–7.10 (m, 2H), 6.84 (d, *J* = 8.2 Hz, 1H), 5.54–5.57 (m, 1H), 4.97 (dd, *J* = 11 and 3.2 Hz, 1H), 3.56 (s, 3H), 2.76–2.69 (m, 1H), 2.57–2.49 (m, 1H), 1.34 (d, *J* = 6.8 Hz, 3H), 1.14 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) *δ*: 176.9, 170.0, 133.1, 128.9, 128.4, 125.2, 123.3, 115.0, 52.6, 51.9, 49.7, 39.8, 20.6, 20.3; HRMS (ESI) $(M+H)^+$ Calcd for $C_{14}H_{17}ClN_2O_2S$: 312.0699, found 312.0699.



Methyl 2-(6-chloro-3-propyl-2-thioxo-1,2,3,4-tetra hydroquinazolin-4-yl)acetate (4g). The product was obtained as a yellow oil, (62%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.84 (br s, 1H), 7.13 (dd, J = 8.2 and 2.3 Hz, 1H), 7.06 (d, J = 2.3 Hz, 1H) 6.75 (d, J = 8.3 Hz, 1H), 4.87 (dd, J = 8.7 and 5.0 Hz, 1H), 3.63–3.56 (m, 5H), 2.70–2.61 (m, 2H), 1.70–1.64 (m, 2H), 0.86 (t, J = 7.3 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.5, 170.2, 132.9, 129.1, 128.5, 125.6, 122.2, 114.9, 56.4, 53.9, 52.1, 38.7, 20.9, 11.0; HRMS (ESI) $(M)^+$ Calcd for $C_{14}H_{17}ClN_2O_2S$ 312.0699, found 312.0699.

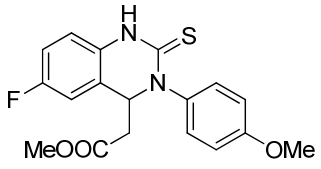


Butyl 2-(6-chloro-2-thioxo-3-(*m*-tolyl)-1,2,3,4-tetra hydroquinazolin-4-yl)acetate (4h). The product was obtained as a pale yellow oil; (77%): ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.68 (br s, 1H), 7.30–7.26 (m, 1H), 7.22–7.18 (m, 1H), 7.14–7.03 (m, 4H), 6.99 (d, J = 7.4 Hz 1H), 5.09 (dd, J = 9.2 and 5.0 Hz, 1H), 3.92–3.87 (m, 2H), 2.84–2.74 (m, 2H), 2.27 (s, 3H), 1.41–1.38 (m, 2H), 1.20–1.10 (m, 2H), 0.80–0.77 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.8, 169.4, 143.3, 139.6, 139.58, 137.0, 136.6, 133.1, 129.2, 129.18, 129.1, 125.8, 122.3, 115.3, 65.0, 60.4, 39.4, 30.3, 21.3, 18.9, 13.6; HRMS (ESI) $(M)^+$ Calcd for $C_{21}H_{23}ClN_2O_2S$ 402.1169, found 402.1170.

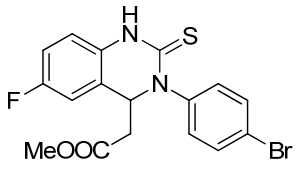


Methyl 2-(6-fluoro-3-phenyl-2-thioxo-1,2,3,4-tetra hydroquinazolin-4-yl)acetate (4i). The product was obtained as a as a pale white needles (DCM/Ether), (75%): mp: 137–139 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.10 (br s, 1H), 7.47–7.43 (m, 2H), 7.40–7.35 (m, 3H), 6.98–6.93 (m, 1H), 6.89–6.84 (m, 2H), 5.19 (dd, J = 8.7 and 4.5 Hz, 1H), 3.55 (s, 3H), 2.96–2.81 (m, 2H), ^{13}C NMR (100 MHz, $CDCl_3$) δ 177.0, 169.7, 158.9 (d, J = 249.2 Hz, 1C), 143.5, 130.8 (d, J = 2.9 Hz, 1C), 129.5, 128.5, 128.4, 122.2 (d, J = 7.6 Hz, 1C), 116.2 (d, J = 23.0 Hz, 1C),

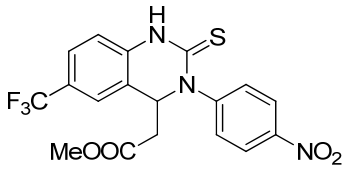
115.3 (d, J = 7.6 Hz, 1C), 113.0, 112.8, 61.4, 52.0, 39.1; HRMS (ESI) $(M)^+$ Calcd for $C_{17}H_{15}FN_2O_2S$ 330.0838, found 330.0840.



Methyl 2-(6-fluoro-3-(4-methoxyphenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4j). The product was obtained as a pale white needles (DCM/Ether), (68%): mp: 160–168 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.64 (br s, 1H), 7.28 (d, J = 8.7 Hz, 2H), 6.96 (d, J = 9.2 Hz, 1H), 6.93–6.90 (m, 2H), 6.87–6.84 (m, 1H), 5.15 (dd, J = 8.7 and 4.2 Hz, 1H), 3.81 (s, 3H), 3.56 (s, 3H), 2.94–2.81 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 177.1, 169.8, 159.1 (d, J = 243.4 Hz, 1C), 136.2, 130.7 (d, J = 2.9 Hz, 1C), 129.5, 122.2 (d, J = 7.7 Hz, 1C), 116.0 (d, J = 23.0 Hz, 1C), 115.4 (d, J = 7.7 Hz, 1C), 114.6, 112.7 (d, J = 24.9 Hz, 1C), 60.6, 55.4, 52.0, 39.1; HRMS (ESI) $(M)^+$ Calcd for $C_{18}H_{17}FN_2O_3S$ 360.0944, found 360.0942.

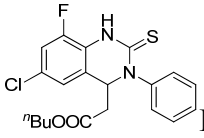


Methyl 2-(3-(4-bromophenyl)-6-fluoro-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4k). The product was obtained as a white needles; (78%): mp: 160–168 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 9.81 (br s, 1H), 7.53–7.50 (m, 2H), 7.34–7.32 (m, 2H), 6.95–6.92 (m, 2H), 6.89–6.86 (m, 1H), 5.18(dd, J = 8.2 and 4.6 Hz, 1H), 3.57 (s, 3H), 2.91–2.82 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.6, 169.6, 158.9 (d, J = 243.4 Hz, 1C), 144.4, 131.8, 131.6, 130.6 (d, J = 2.9 Hz, 1C), 129.5, 127.6, 122.6, 122.1 (d, J = 7.7 Hz, 1C), 116.2 (d, J = 23.0 Hz, 1C), 115.6 (d, J = 7.7 Hz, 1C), 112.7 (d, J = 23.9 Hz, 1C), 61.3, 51.1, 39.2; HRMS (ESI) $(M)^+$ Calcd for $C_{17}H_{14}BrFN_2O_2S$ 407.9943, found 407.9943.

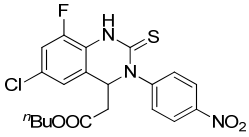


Methyl 2-(3-(4-nitrophenyl)-2-thioxo-6-(trifluoromethyl) -1,2,3,4-tetrahydroquinazolin-4-yl) acetate (4l). The product was obtained as a yellow semi–solid; (65%): ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.19 (br s,

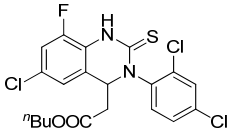
1H), 8.32 (d, J = 9.2 Hz, 2H), 7.61–7.55 (m, 3H), 7.44 (s, 1H), 7.01 (d, J = 8.3 Hz, 1H) 5.31 (dd, J = 8.2 and 5.2 Hz, 1H), 3.56 (s, 3H), 2.95–2.81 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 177.2, 169.2, 148.6, 147.1, 136.6, 129.7, 127.0, 126.9, 126.6, 126.2, 124.9, 123.5 (q, J = 34.7 Hz, 1C) 122.2, 120.8, 114.3, 60.3, 52.3, 39.4; HRMS (ESI) $(M)^+$ Calcd for $C_{18}H_{14}F_3N_3O_4S$ 425.0657, found 425.0658.



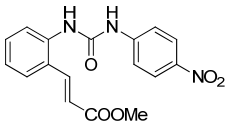
Butyl 2-(6-chloro-8-fluoro-3-phenyl-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4m). The product was obtained as a yellow needles, (136.0 mg, 67%): mp 150–152 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (br s, 1H), 7.48–7.44 (m, 2H), 7.41–7.39 (m, 1H), 7.38–7.34 (m, 2H), 7.12–7.09 (m, 1H), 6.98 (s, 1H), 5.20 (dd, J = 8.7 and 4.6 Hz, 1H), 4.00–3.93 (m, 2H), 2.95–2.80 (m, 2H), 1.52–1.44 (m, 2H), 1.26–1.20 (m, 2H), 0.88–0.84 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.9, 169.1, 147.9 (d, J = 250.1 Hz, 1C), 143.3, 129.6, 128.6, 128.4, 123.7, 122.0 (d, J = 14.3 Hz, 1C), 121.7 (d, J = 3.8 Hz, 1C),116.2, 116.0, 65.2, 60.2, 39.3, 30.3, 18.9, 13.6; HRMS (ESI) $(M)^+$ Calcd for $C_{20}H_{20}ClFN_2O_2S$ 406.0918, found 406.0919.



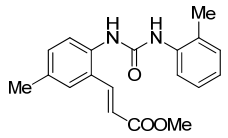
Butyl 2-(6-chloro-8-fluoro-3-(4-nitrophenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4n). The product was obtained as a yellow needles, (169.1 mg, 75%): mp 152–154 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (br s, 1H), 8.30 (d, J = 8.7 Hz, 2H), 7.58 (d, J = 8.7 Hz, 2H), 7.14 (dd, J = 9.6 and 1.3 Hz, 1H), 7.00 (s, 1H), 5.24 (dd, J = 8.2 and 4.6 Hz, 1H), 3.98 (t, J = 6.4 Hz, 2H), 2.92–2.80 (m, 2H), 1.52–1.45 (m, 2H), 1.28–1.18 (m, 2H), 0.86 (t, J = 7.3 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.7, 168.8, 148.6, 148.0 (d, J = 250.1 Hz, 1C), 146.9, 129.7, 128.9 (d, J = 8.6 Hz, 1C), 124.8, 123.5, 121.6 (d, J = 2.3 Hz, 1C), 116.5, 116.3, 65.4, 60.0, 39.5, 30.3, 18.9, 13.5; HRMS (ESI) $(M)^+$ Calcd for $C_{20}H_{19}ClFN_3O_4S$ 451.0769, found 451.0770.



Butyl 2-(6-chloro-3-(2,4-dichlorophenyl)-8-fluoro-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4o). The product was obtained as a white needles , (166.2 mg, 70%), mp 164–166 °C : ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40 (br s, 1H), 7.52–7.49 (m, 2H), 7.36–7.33 (m, 1H), 7.11 (dd, J = 9.6 and 1.8 Hz, 1H), 6.99 (s, 1H), 5.05 (dd, J = 7.8 and 5.0 Hz, 1H), 4.00–3.95 (m, 2H), 2.86–2.80 (m, 2H), 1.52–1.45 (m, 2H), 1.28–1.18 (m, 2H), 0.86 (t, J = 8.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.8, 168.9, 148.0 (d, J = 250.2 Hz, 1C), 138.5, 135.4, 133.7, 132.1, 130.7, 128.6 (d, J = 8.6 Hz, 1C), 127.7, 123.6, 121.5 (d, J = 2.9 Hz, 1C), 116.3, 116.1, 65.3, 58.7, 39.5, 30.3, 18.9, 13.6; HRMS (ESI) $(M+H)^+$ Calcd for $C_{20}H_{18}Cl_3FN_3O_2S$ 475.0127, found 475.0230.

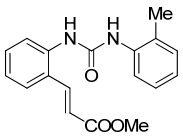


(*E*)-Methyl 3-(2-(3-(4-nitrophenyl)ureido)phenyl) acrylate (6a). The product was obtained as a yellow needles (DCM/Ether), (92%): mp 175–178 °C; ^{1}H NMR (400 MHz, DMSO–d_6) δ 9.67 (s, 1H), 8.73 (s, 1H), 8.20–8.17 (m, 2H), 7.85 (d, J = 15.6 Hz, 1H), 7.79 (d, J = 6.8 Hz, 1H) 7.71–7.68 (m, 3H), 7.43–7.39 (m, 1H), 7.18 (t, J = 8.2 Hz, 1H), 6.60 (d, J = 16.0 Hz, 1H), 3.72 (s, 3H); ^{13}C NMR (100 MHz, DMSO–d_6) δ 166.7, 152.4, 146.3, 141.1, 139.6, 137.1, 130.8, 126.8, 125.2, 124.7, 124.4, 119.1, 117.6, 51.6; IR spectrum in film (ν_{max}, cm^{-1}) 3361, 3270, 2954, 1724, 1673, 1504, 1274, 1217, 1187, 1166, 1111, 1015, 981, 937, 856, 838; HRMS (ESI) $(M)^+$ Calcd for $C_{17}H_{15}N_3O_5$ 341.1012, found 341.1015.

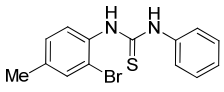


(*E*)-Methyl 3-(2-(3-(2-fluorophenyl)ureido)-5-methylphenyl)acrylate (6b). The product was obtained as a white needles (DCM/Ether), (90%): mp 178–180 °C; ^{1}H NMR (400 MHz, DMSO–d_6) δ 8.82 (s, 1H), 8.77 (s, 1H), 8.15–8.10 (m, 1H), 7.85 (d, J = 16.0 Hz, 1H),7.60 (t, J = 8.7 Hz, 2H), 7.25–7.17 (m, 2H), 7.13–7.08 (m, 1H), 7.00–6.95 (m, 1H), 6.56 (d, J = 16.0 Hz, 1H), 3.72 (s, 3H), 2.27 (s, 3H); ^{13}C NMR (100 MHz, DMSO–d_6) δ 166.7, 152.5, 139.7, 135.0, 133.2, 131.5, 127.1, 125.9, 124.5, 123.9, 122.4, 122.3, 120.5, 118.6, 115.0,

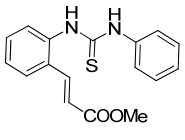
114.8, 51.6, 20.0; IR spectrum in film (ν_{max}, cm^{-1}) 3286, 3233, 2927, 1734, 1645, 1560, 1500, 1491, 1300, 1284, 1254, 1198, 1106, 1031, 936, 849, 810 ; HRMS (ESI) $(M)^+$ Calcd for $C_{18}H_{17}FN_2O_3$ 328.1223, found 328.1223.



(*E*)-Methyl 3-(2-(3-(*o*-tolyl)ureido)phenyl)acrylate (6c). The product was obtained as a pale yellow needles (DCM/Ether), (85%): mp 158–160 °C; ^{1}H NMR (400 MHz, DMSO–d_6) δ 8.91 (s, 1H), 8.89 (s, 1H), 8.17 (t, J = 8.0 Hz, 1H), 7.91 (d, J = 15.6 Hz, 1H), 7.80–7.74 (m, 2H), 7.39 (t, J = 7.3 Hz, 1H), 7.26–7.21 (m, 1H), 7.12 (t, J = 7.8 Hz, 2H), 7.02–6.97 (m, 1H), 6.59 (d, J = 15.6 Hz, 1H), 3.73 (s, 3H), 3.35 (s, 3H); ^{13}C NMR (100 MHz, DMSO–d_6) δ 166.7, 152.4, 139.6, 137.5, 130.7, 127.1, 125.8, 124.5, 123.9, 123.5, 122.5, 122.4, 120.5, 119.0, 115.0, 114.8, 51.5, 20.7; HRMS (ESI) $(M)^+$ Calcd for $C_{18}H_{18}N_2O_3$ 310.1317, found 310.1317



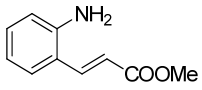
1-(2-Bromo-4-methylphenyl)-3-phenylthiourea (10). The product was obtained as a white needles (DCM/Ether), (90%): mp 166–168 °C; ^{1}H NMR (400 MHz, DMSO–d_6) δ 9.90 (s, 1H), 9.30 (s, 1H), 7.53 (d, J = 8.2 Hz, 2H), 7.48 (s, 1H), 7.40 (d, J = 8.2 Hz, 1H), 7.34 (t, J = 7.8 Hz, 2H), 7.18–7.11 (m, 2H), 2.29 (s, 3H); ^{13}C NMR (100 MHz, DMSO–d_6) δ 180.3, 139.2, 137.8, 135.2, 132.6, 129.9, 128.5, 128.4, 124.6, 123.7, 121.1, 20.2; HRMS (ESI) $(M)^+$ Calcd for $C_{14}H_{13}BrN_2S$ 319.9983, found 319.9980.



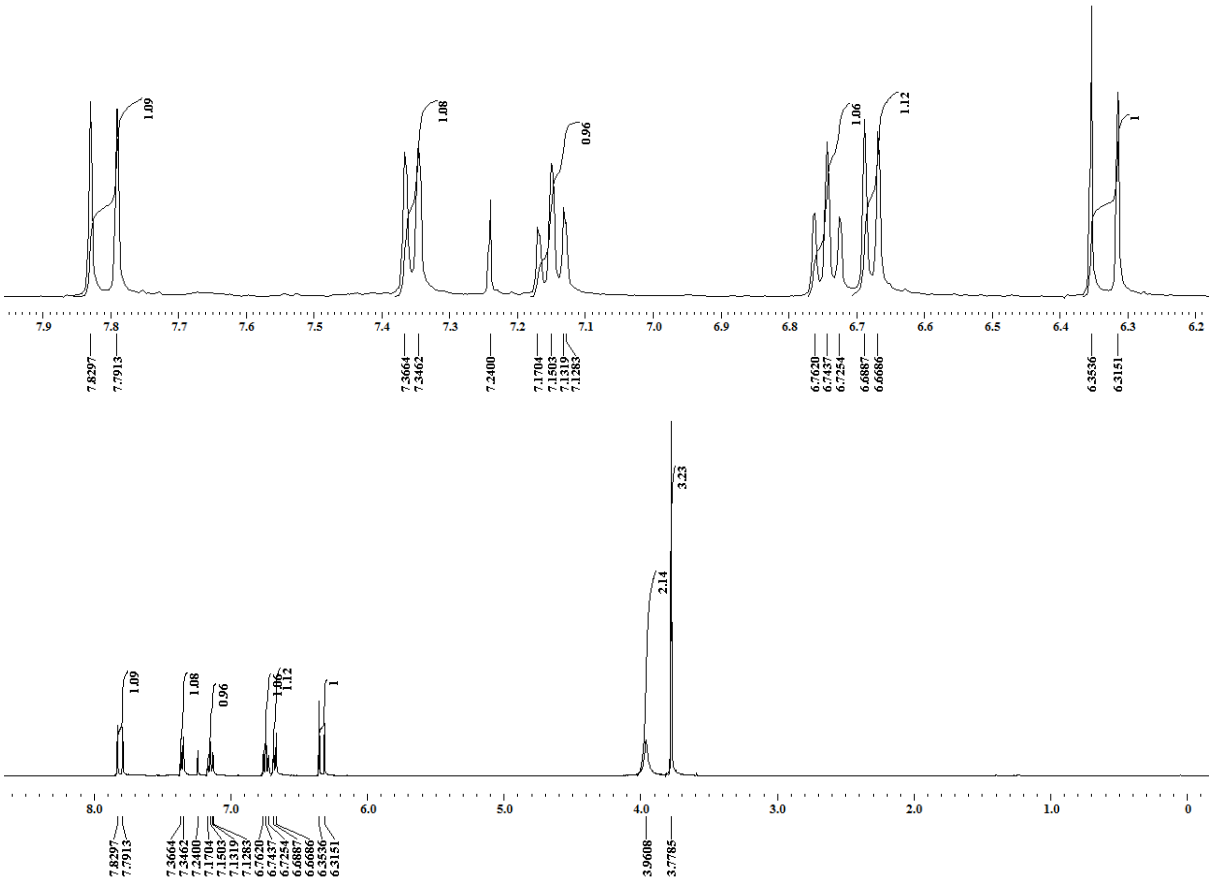
(*E*)-methyl 3-(2-(3-phenylthioureido)phenyl)acrylate (P). The product was obtained as a brown needles (DCM/Ether), mp 165–167 °C; ^{1}H NMR (400 MHz, DMSO–d_6) δ 9.85 (br s, 1H), 9.68 (br s, 1H), 7.86 (d, J = 7.8 Hz, 1H). 7.77 (d, J = 16.0 Hz, 1H), 7.48–7.41 (m, 3H), 7.35–7.28 (m, 4H), 7.13 (t, J = 7.3 Hz, 1H), 6.61 (d, J = 16.0 Hz, 1H), 3.72 (m, 3H); ^{13}C NMR (100 MHz, DMSO–d_6) δ 181.2, 166.8, 140.5, 139.4, 138.8, 131.1, 130.7, 129.1, 129.0, 128.5, 126.8, 124.7, 123.9, 118.4, 51.6 ; HRMS (ESI) $(M)^+$ Calcd for $C_{17}H_{16}N_2O_2S$ 312.0932, found 312.0930.

SPECTRA

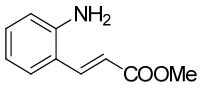
^{1}H NMR



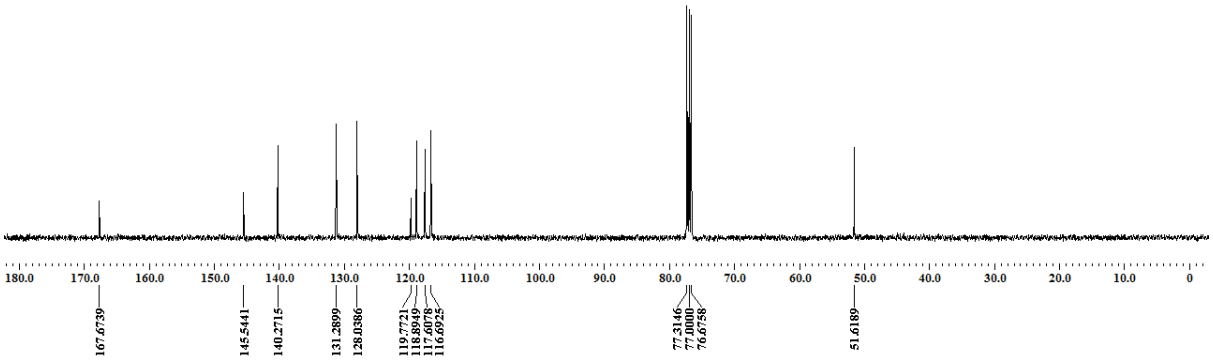
(*E*)-Methyl 3-(2-aminophenyl)acrylate (1a)



^{13}C NMR



(*E*)-Methyl 3-(2-aminophenyl)acrylate (1a)



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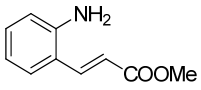
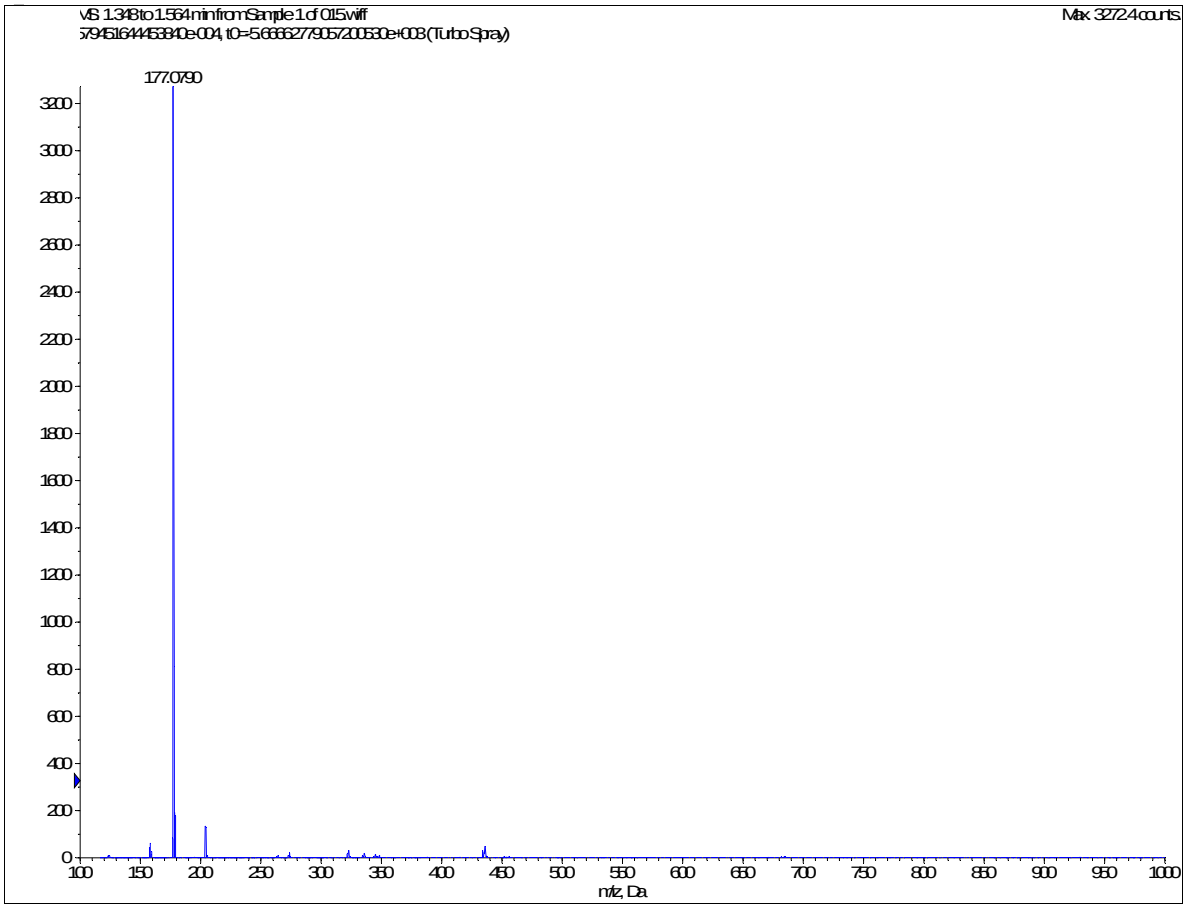
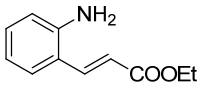
HRMS



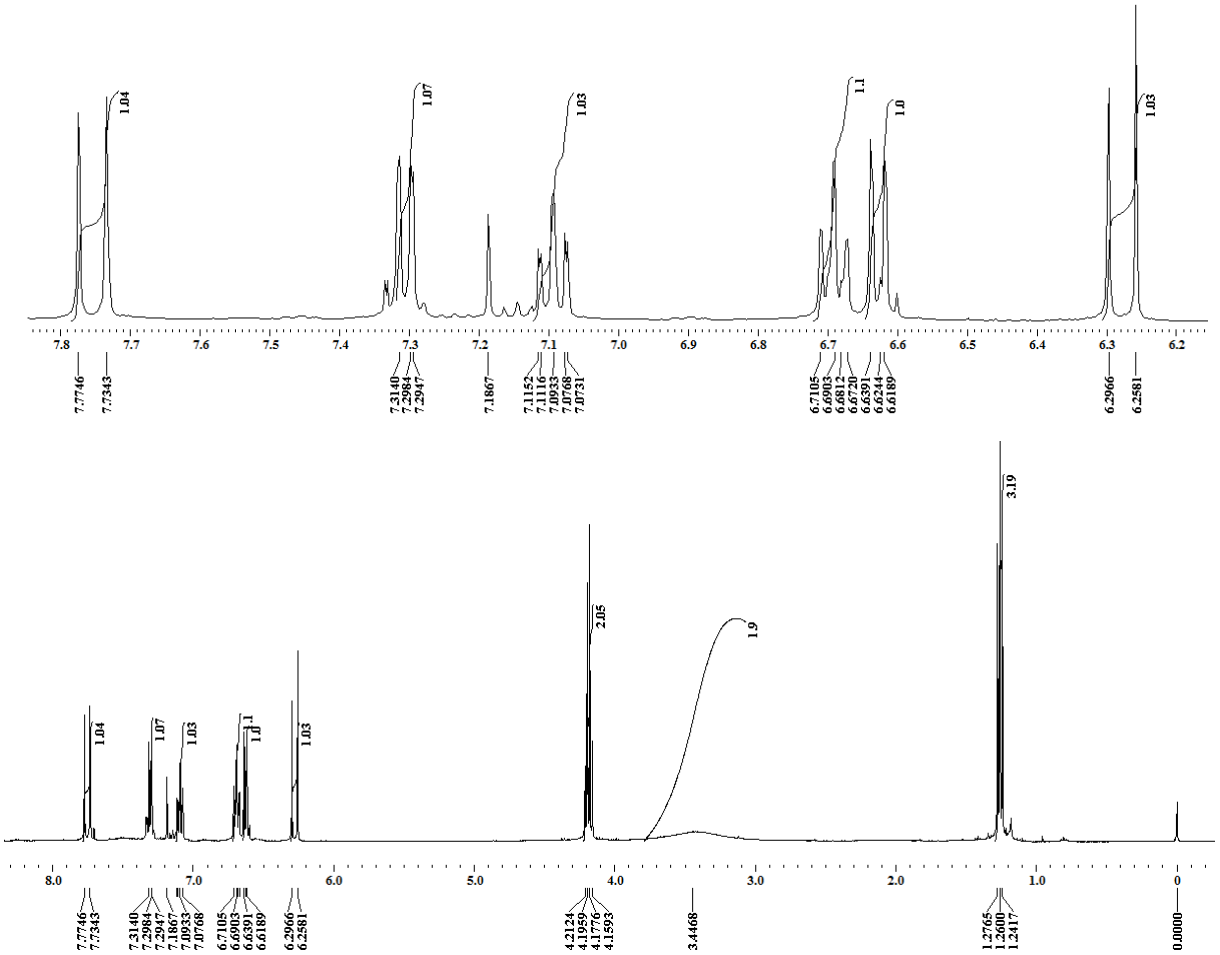
(*E*)-Methyl 3-(2-aminophenyl)acrylate (1a)



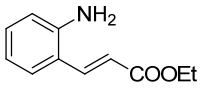
^{1}H NMR



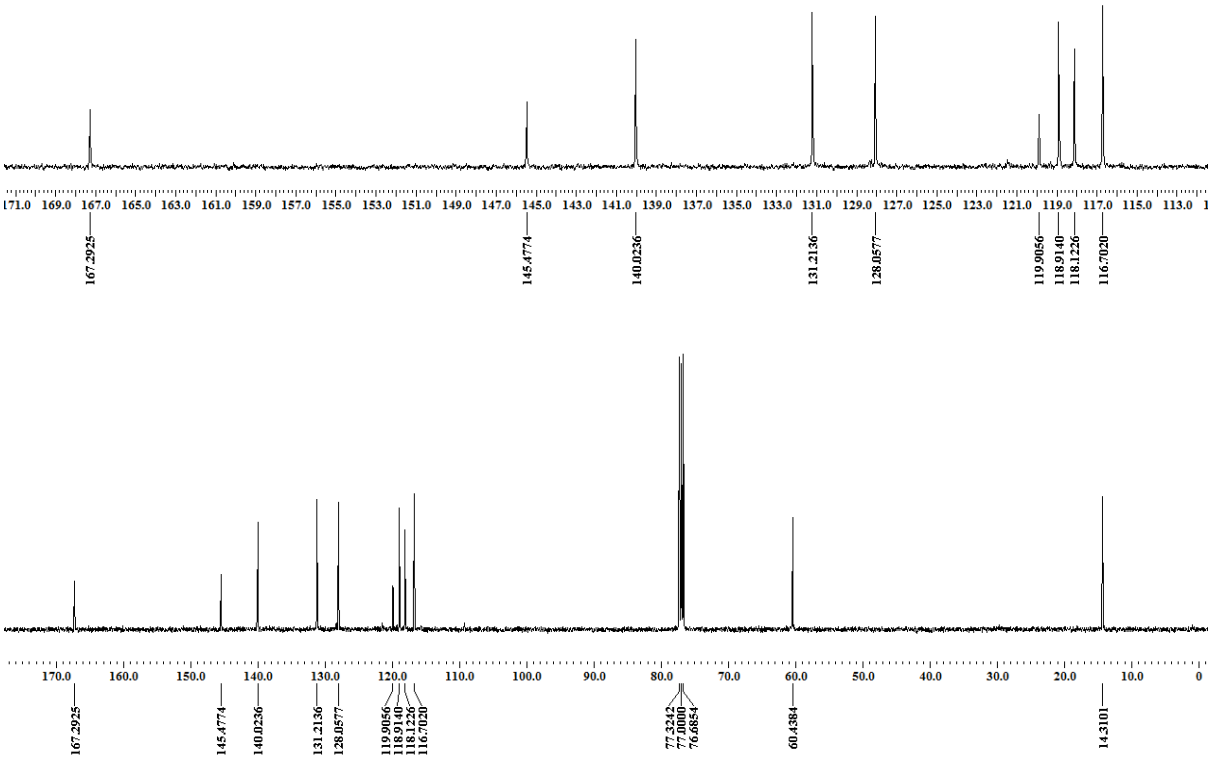
(*E*)-Ethyl 3-(2-aminophenyl)acrylate (1b)



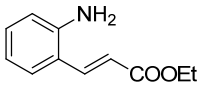
^{13}C NMR



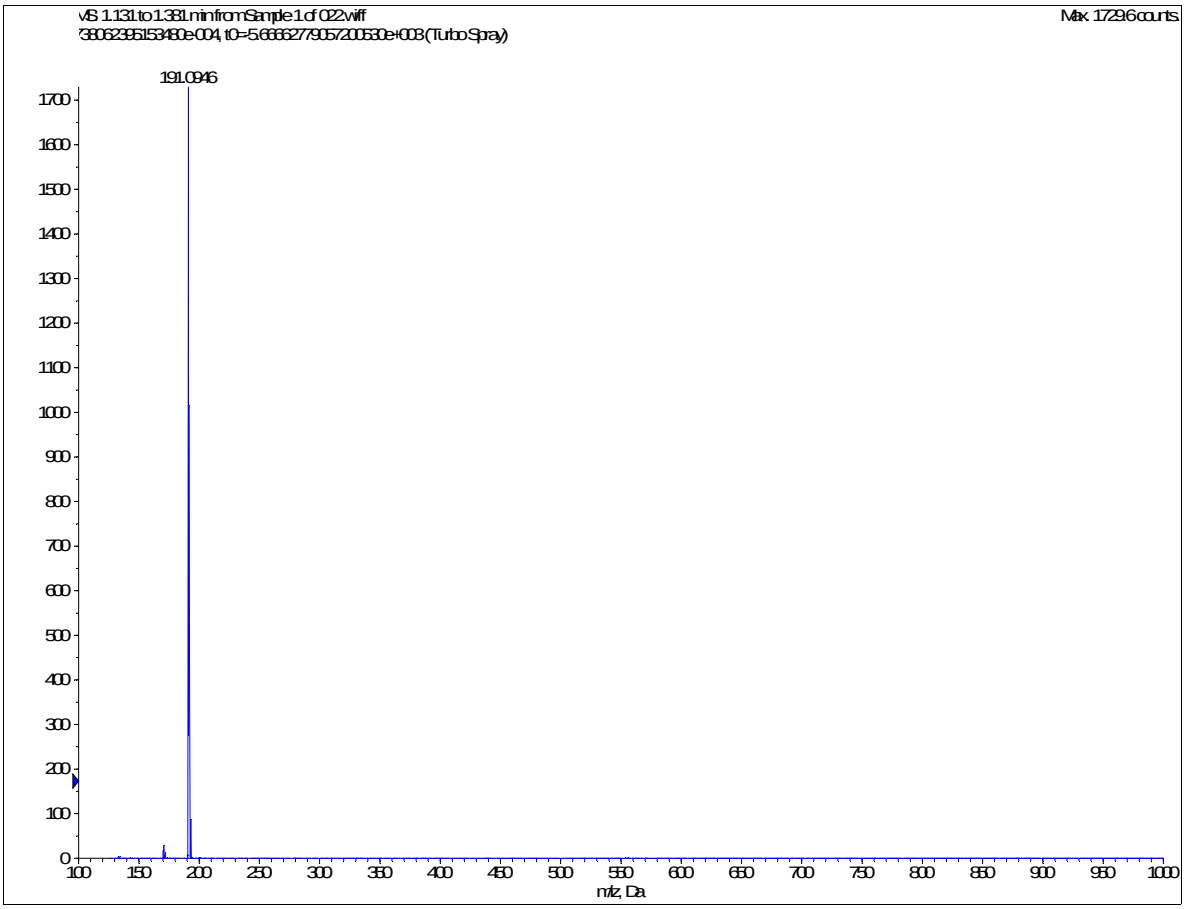
(*E*)-Ethyl 3-(2-aminophenyl)acrylate (1b)



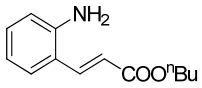
HRMS



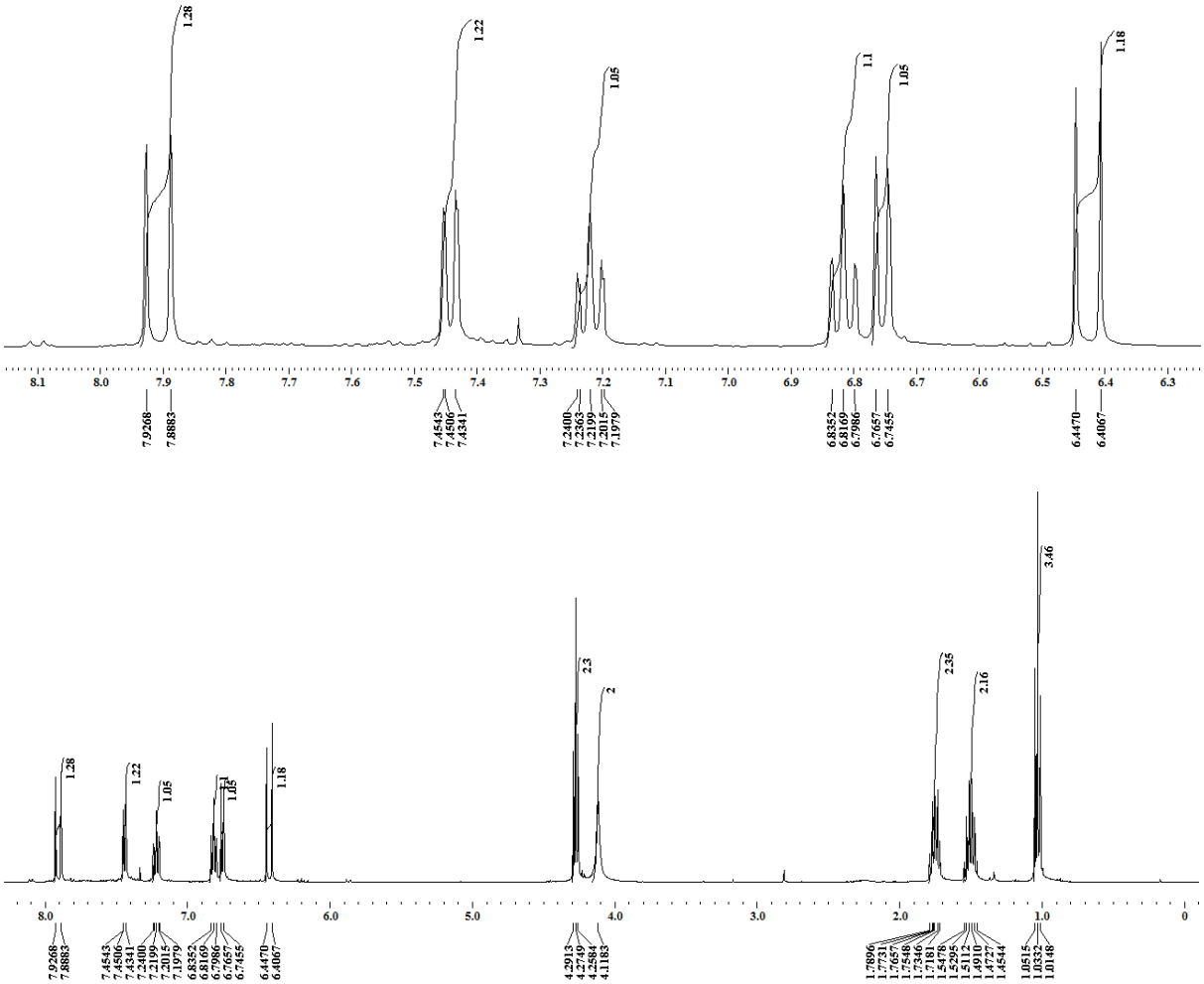
(*E*)-Ethyl 3-(2-aminophenyl)acrylate (1b)



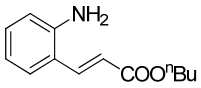
^{1}H NMR



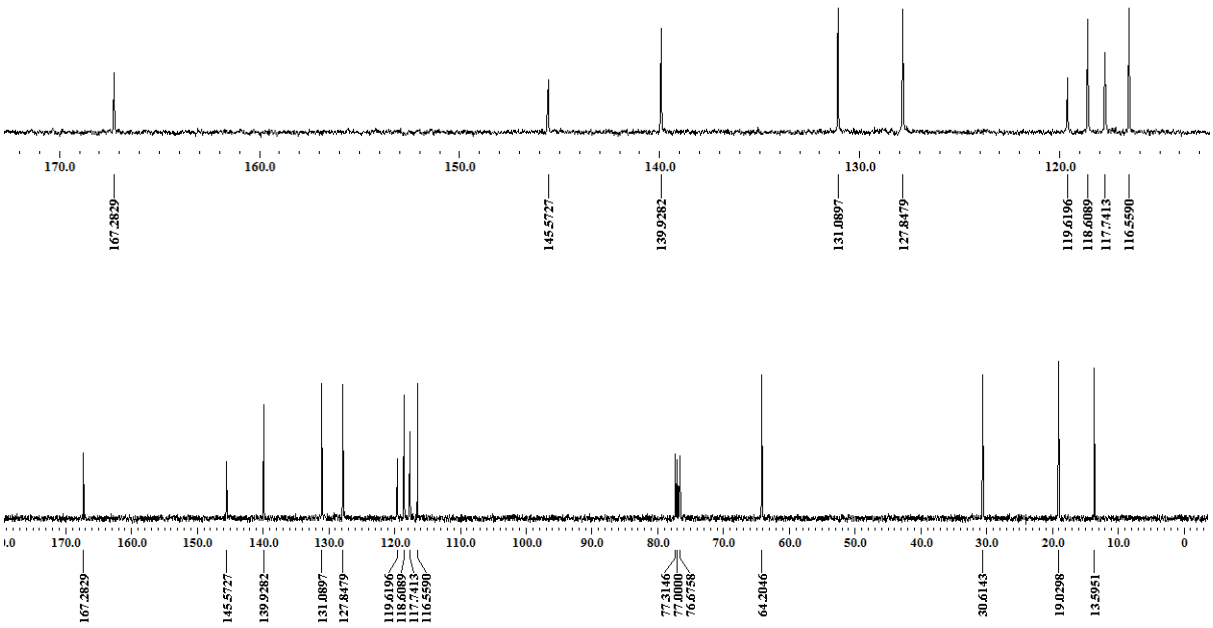
(*E*)-Butyl 3-(2-aminophenyl)acrylate (1c)



^{13}C NMR



(*E*)-Butyl 3-(2-aminophenyl)acrylate (1c)



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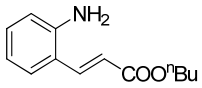
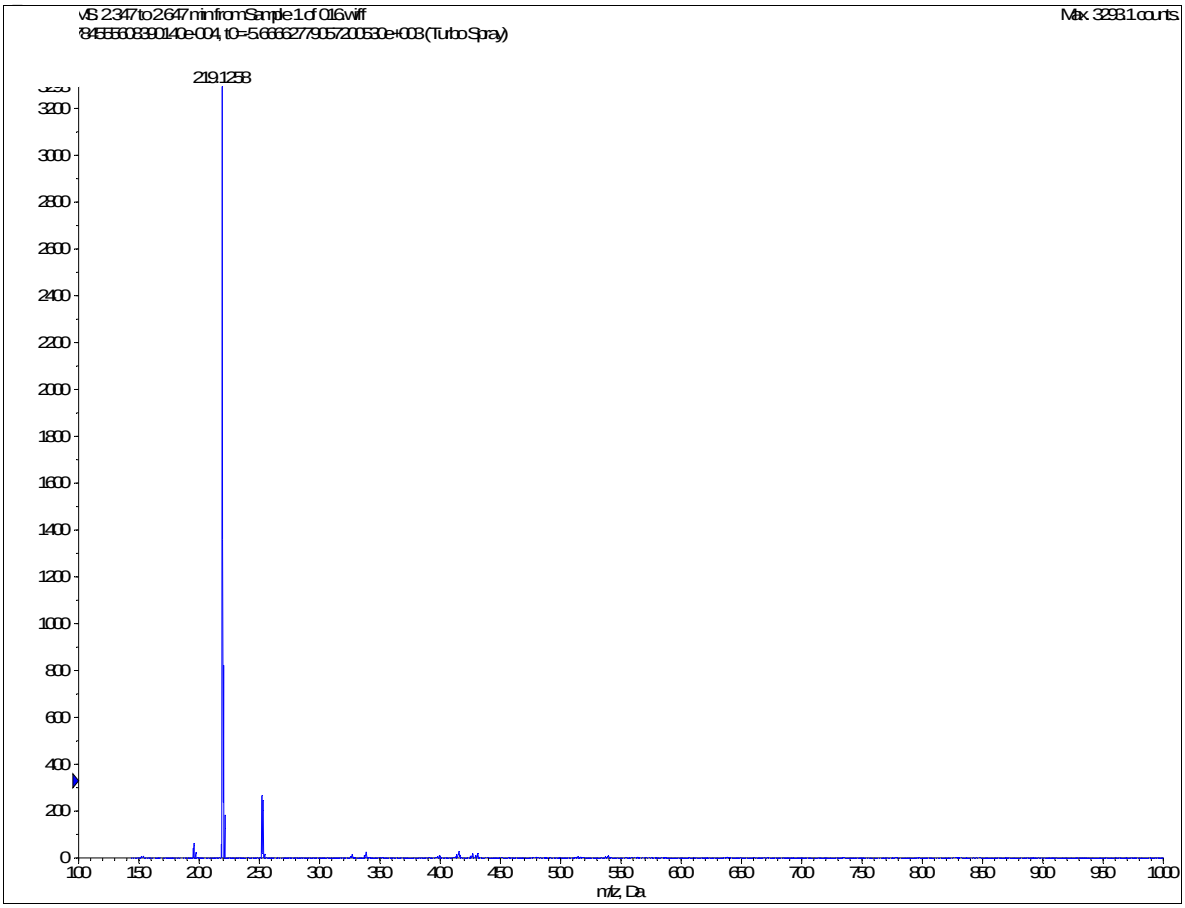


(*E*)-Butyl 3-(2-aminophenyl)acrylate (1c)



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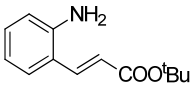
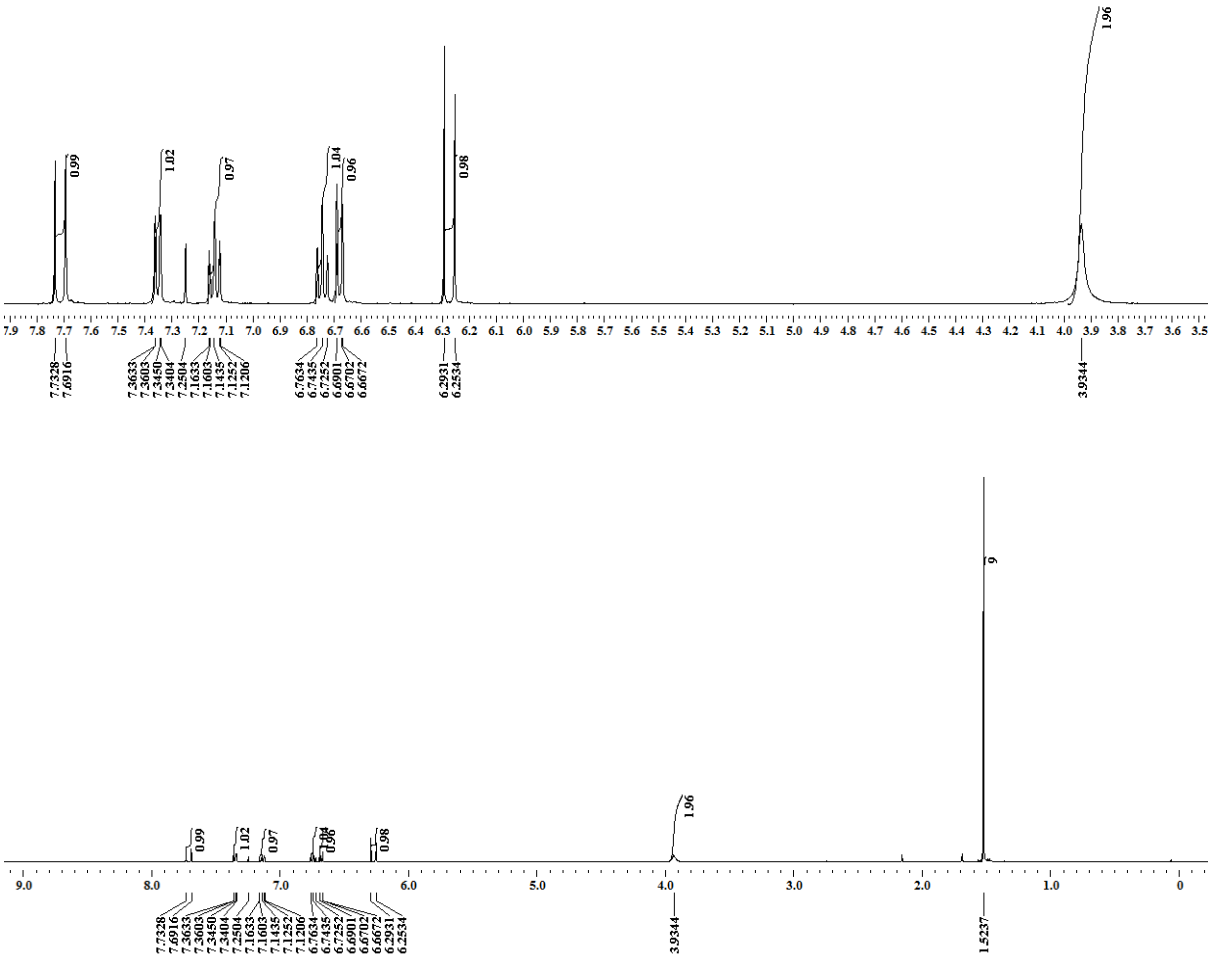


(*E*)-*tert*-Butyl 3-(2-aminophenyl)acrylate (1d)



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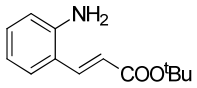
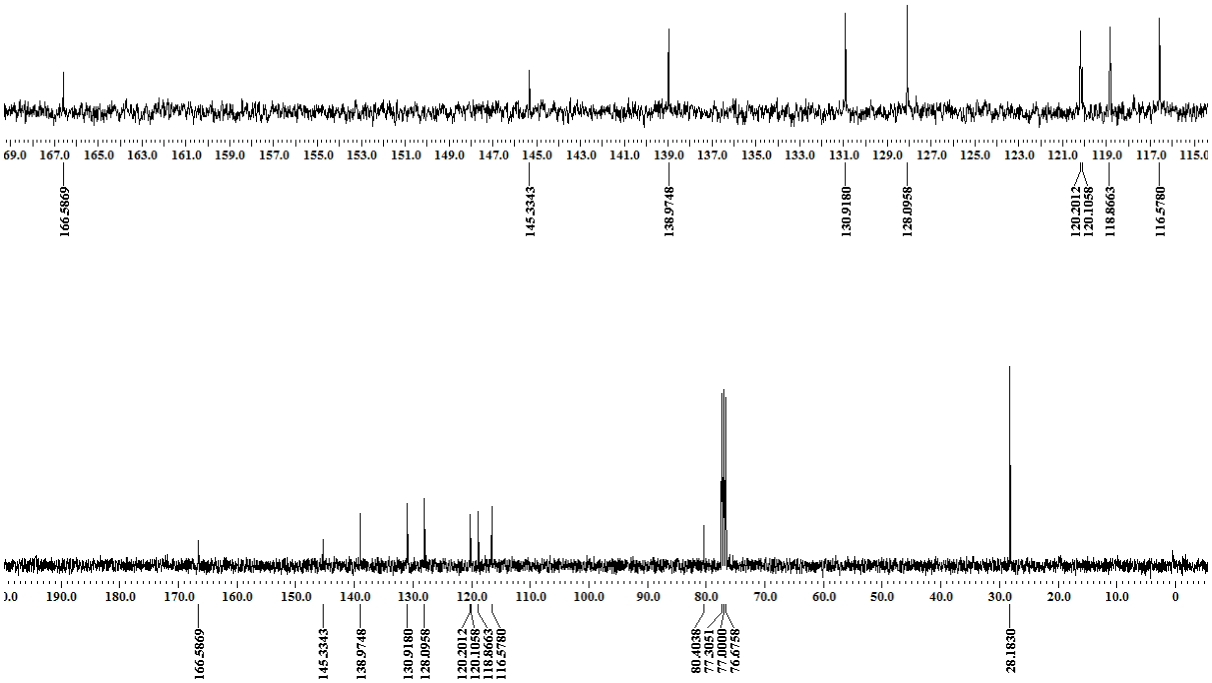


(*E*)-*tert*-Butyl 3-(2-aminophenyl)acrylate (1d)



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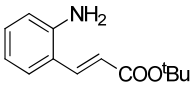
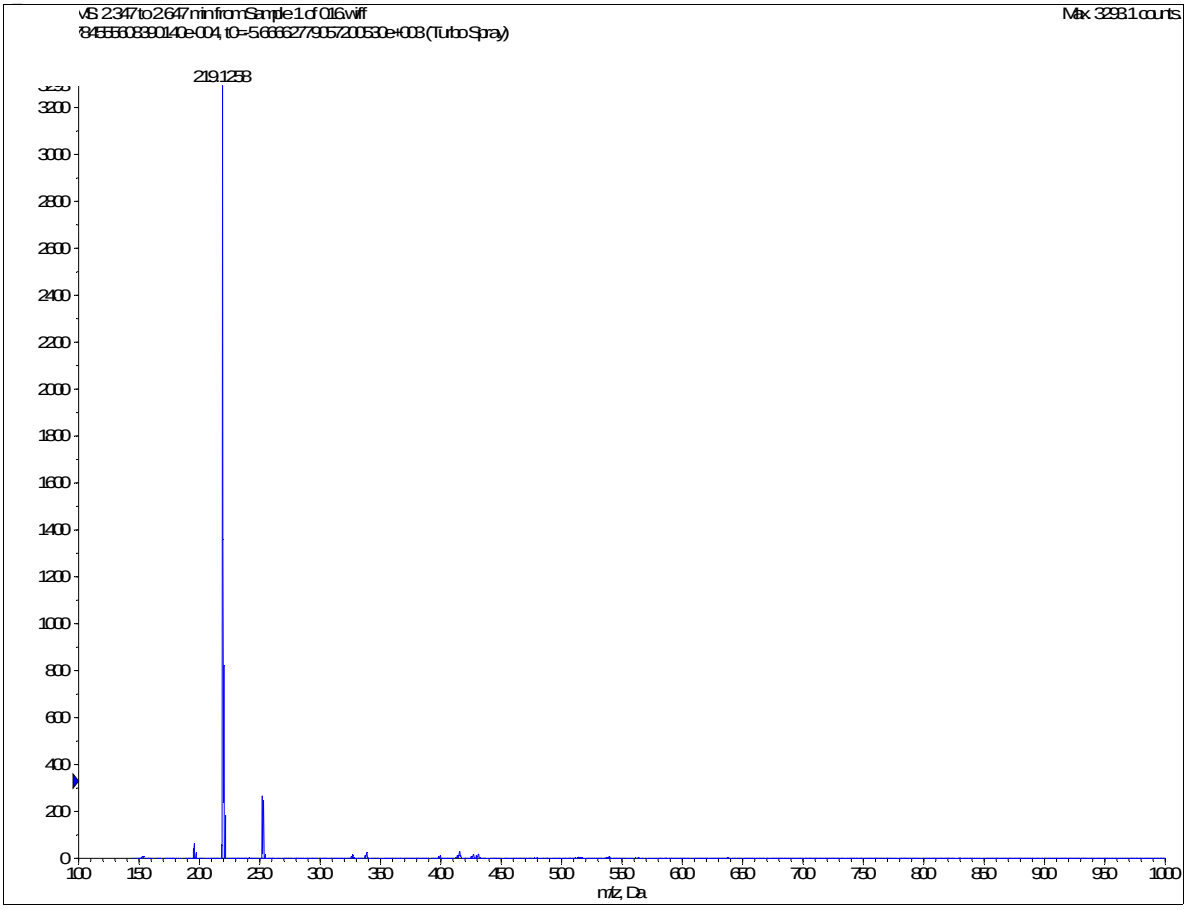


(*E*)-*tert*-Butyl 3-(2-aminophenyl)acrylate (1d)



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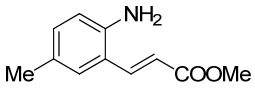
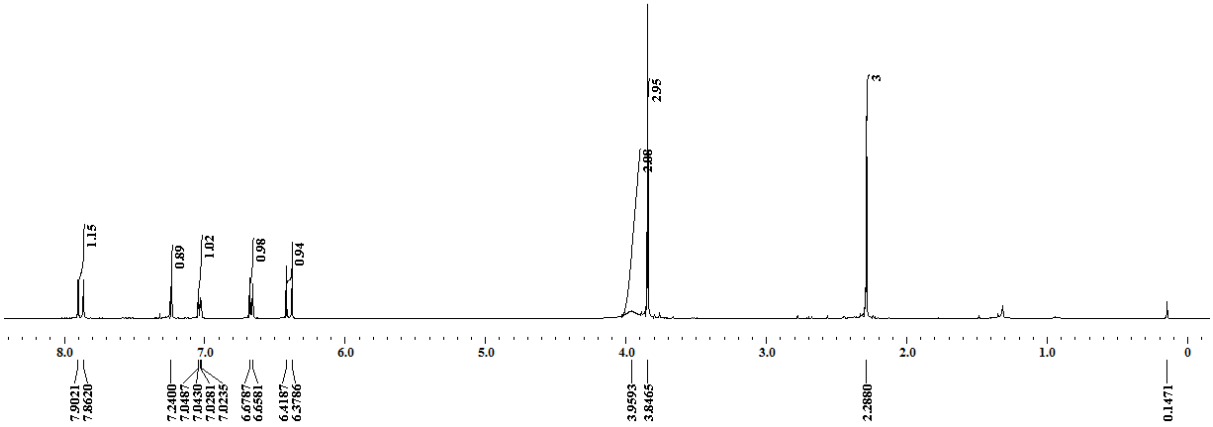
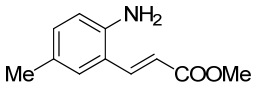


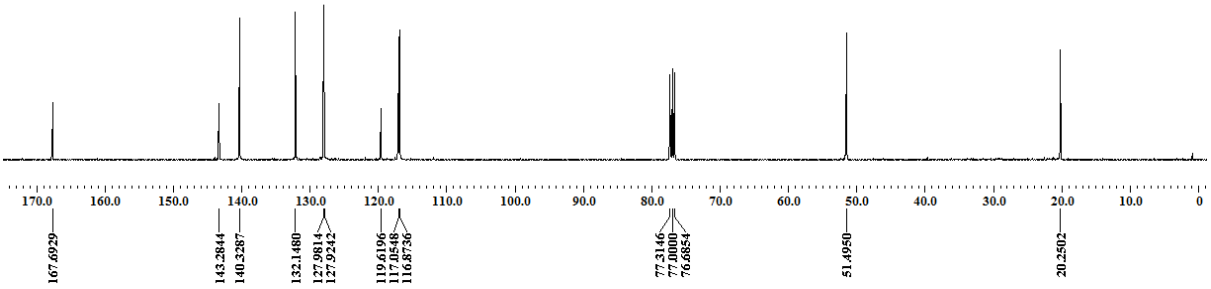
(*E*)-Methyl 3-(2-amino-5-methylphenyl)acrylate (1e)



^{13}C NMR



(*E*)-Methyl 3-(2-amino-5-methylphenyl)acrylate (1e)



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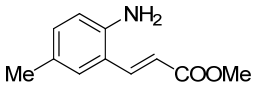
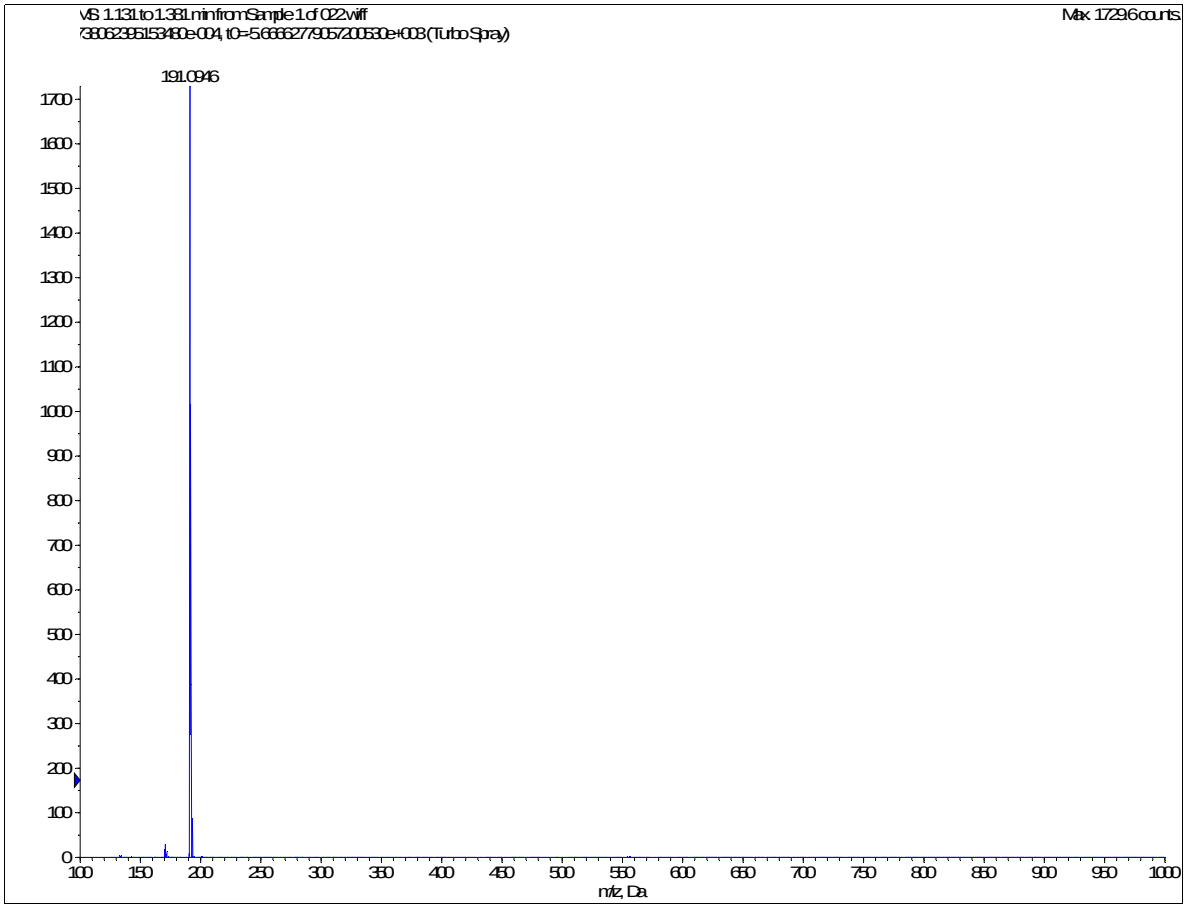
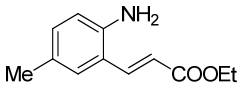


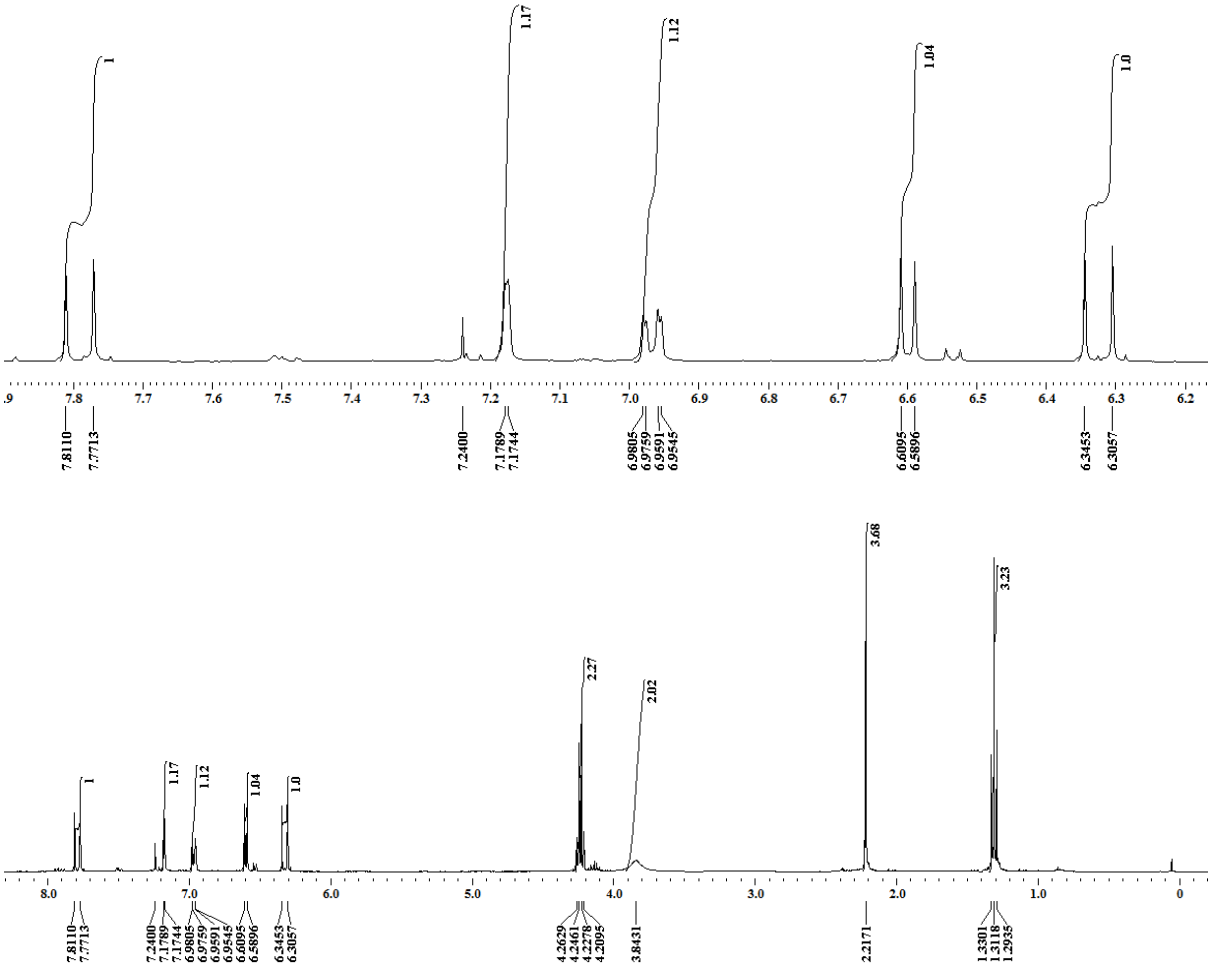
(*E*)-Methyl 3-(2-amino-5-methylphenyl)acrylate (1e)



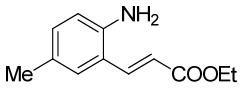
^{1}H NMR



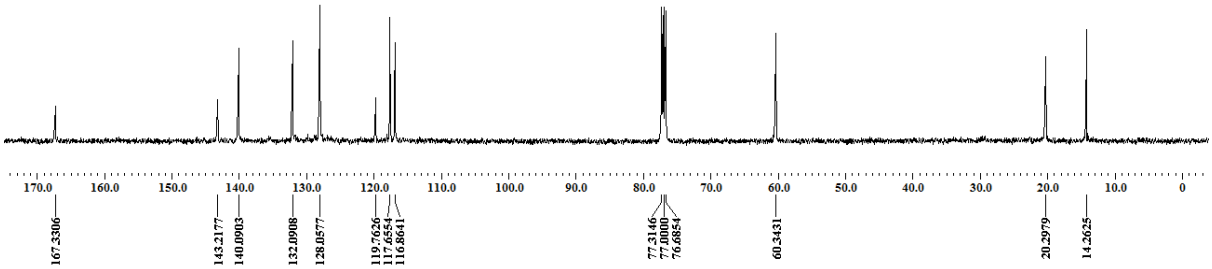
(*E*)-Ethyl 3-(2-amino-5-methylphenyl)acrylate (1f)



^{13}C NMR



(*E*)-Ethyl 3-(2-amino-5-methylphenyl)acrylate (1f)



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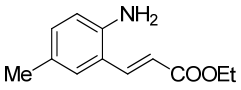
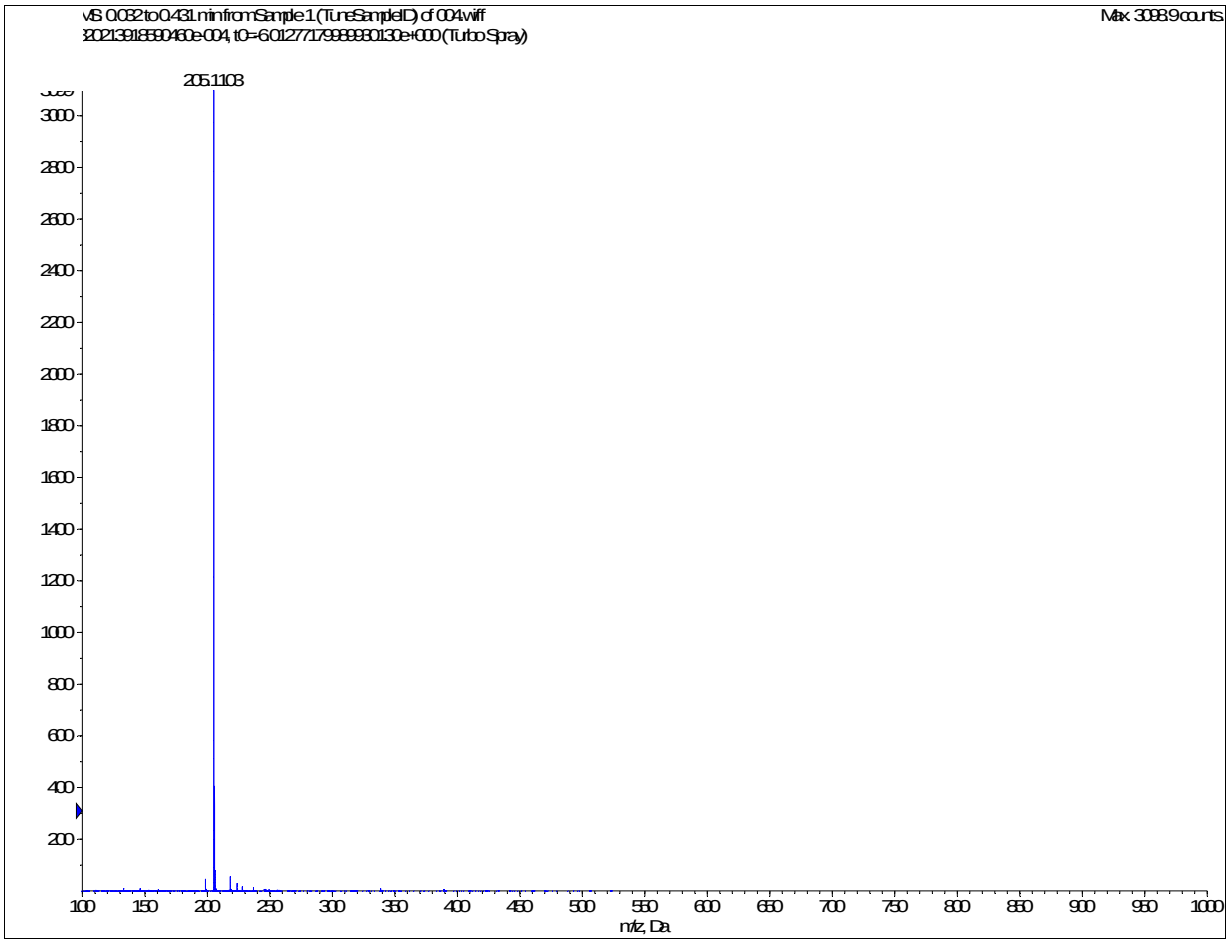
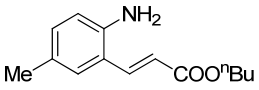


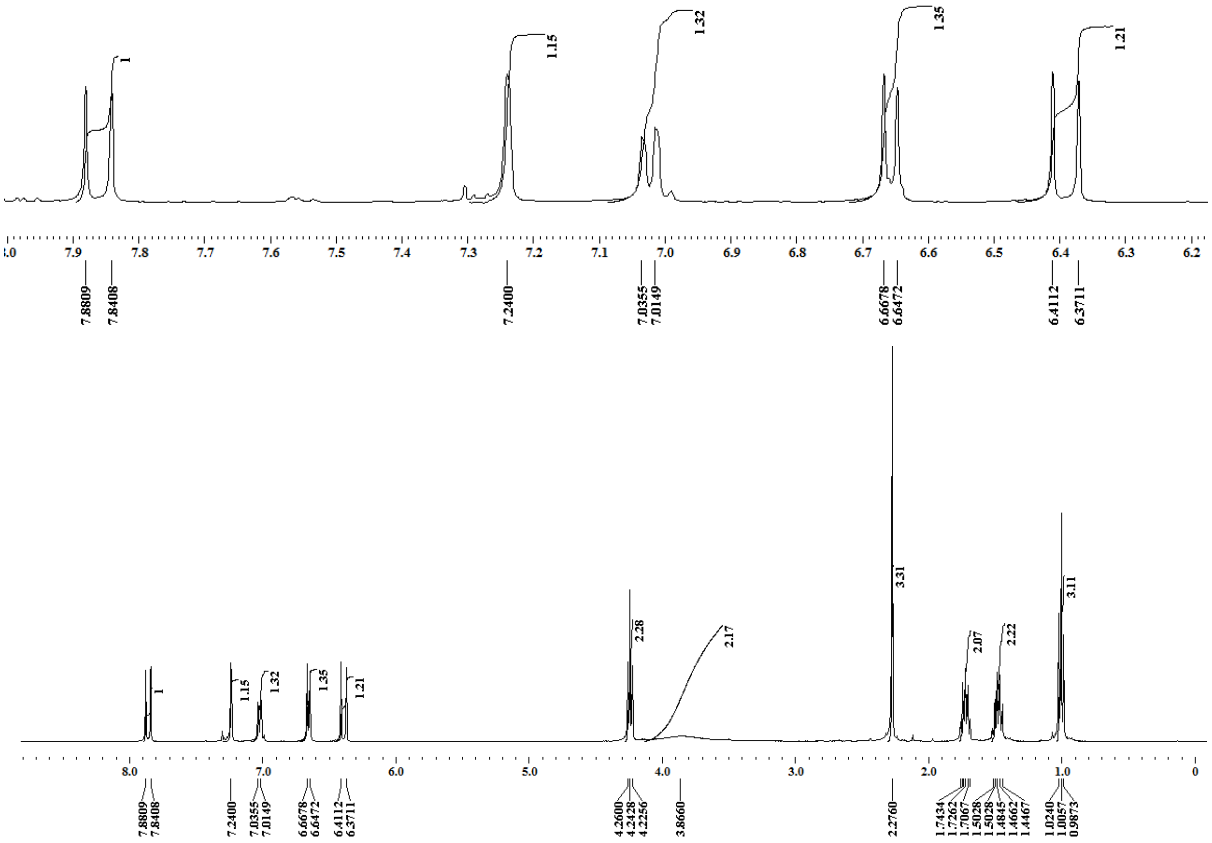
(*E*)-Ethyl 3-(2-amino-5-methylphenyl)acrylate (1f)



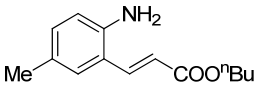
^{1}H NMR



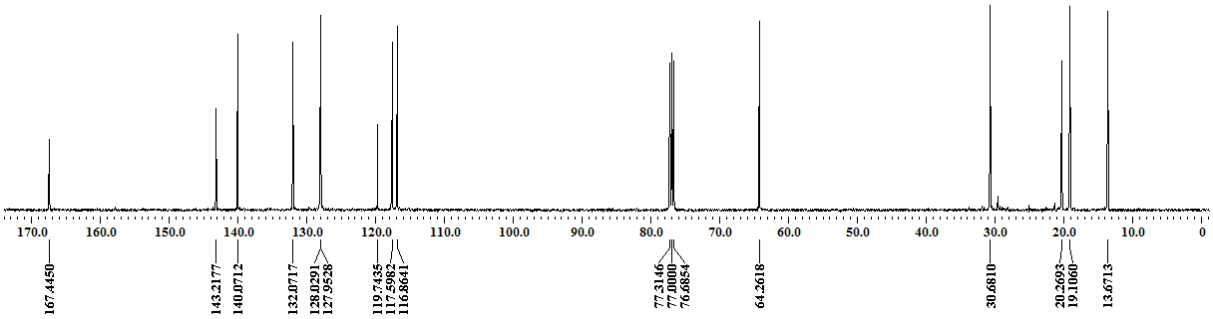
(*E*)-Butyl 3-(2-amino-5-methylphenyl)acrylate (1g)



^{13}C NMR



(*E*)-Butyl 3-(2-amino-5-methylphenyl)acrylate (1g)



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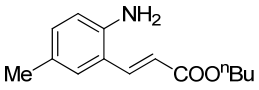
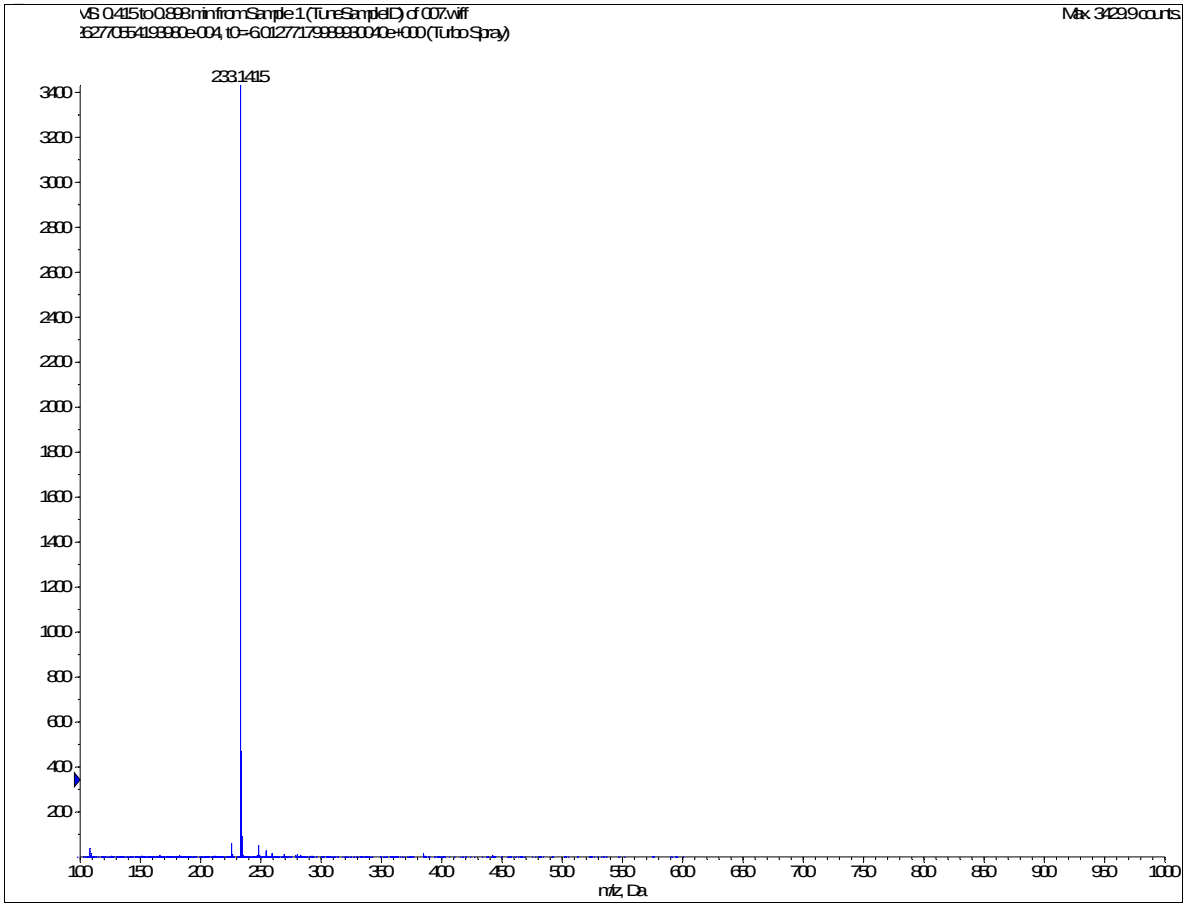
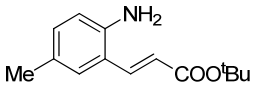


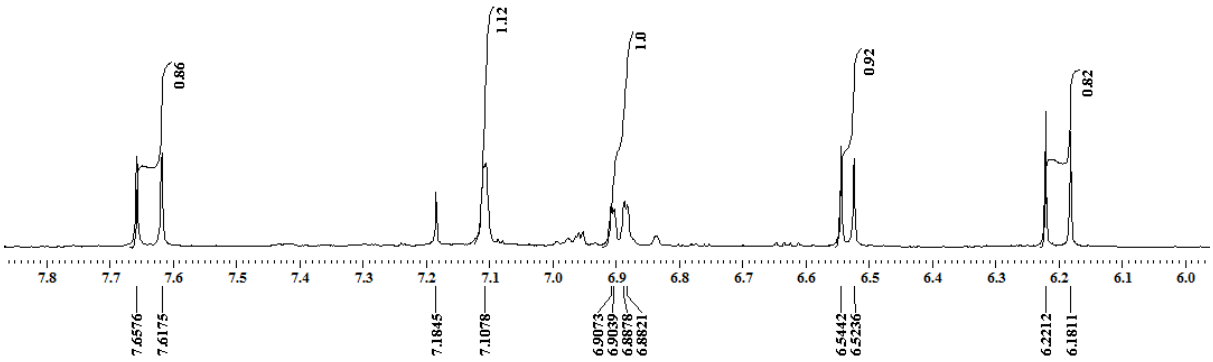
(*E*)-Butyl 3-(2-amino-5-methylphenyl)acrylate (1g)

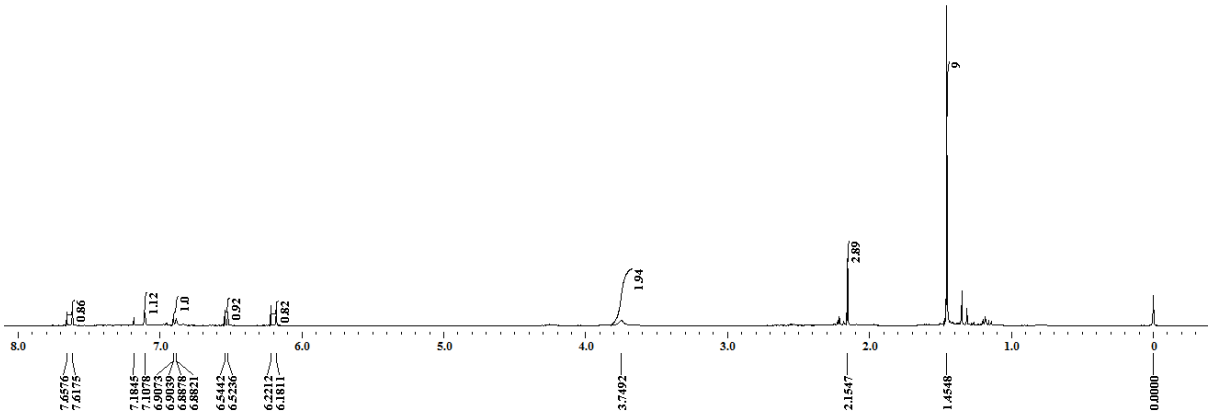


^{1}H NMR

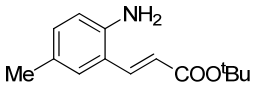


(*E*)-*tert*-Butyl 3-(2-amino-5-methylphenyl)acrylate (1h)

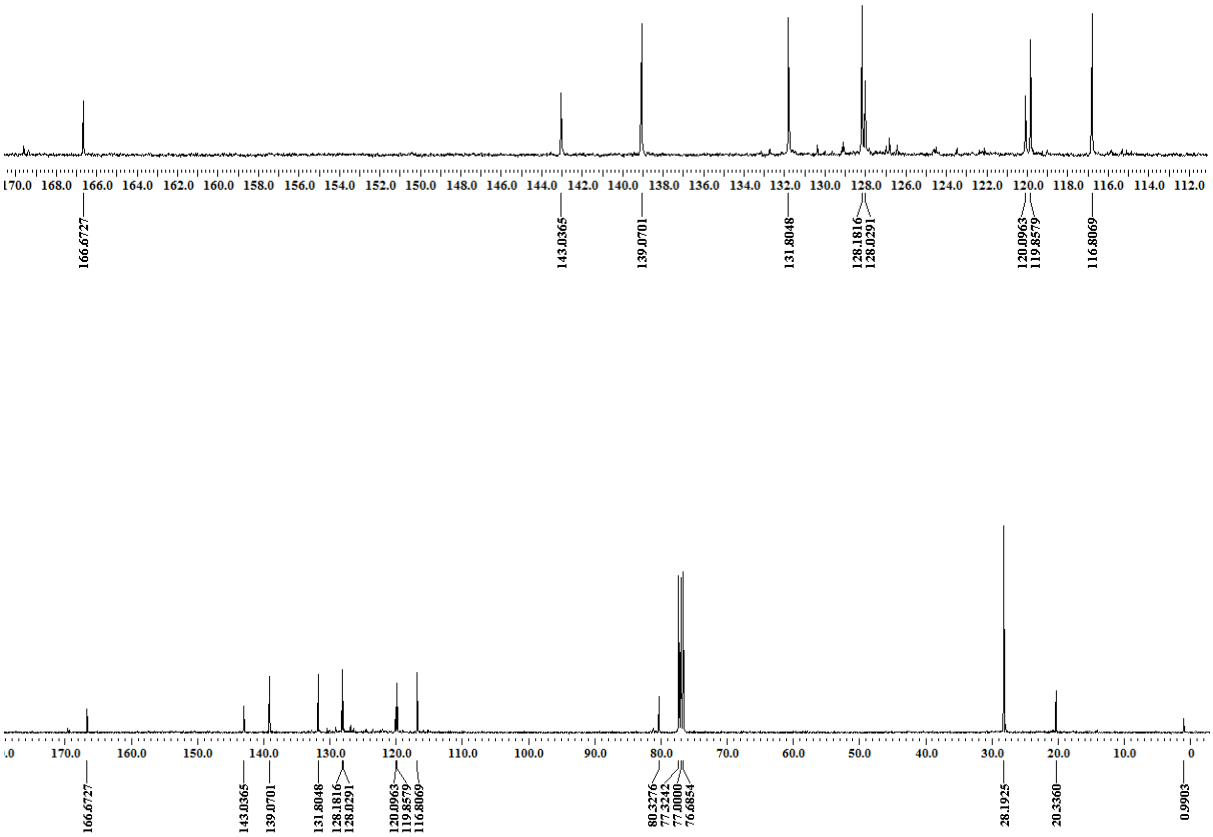




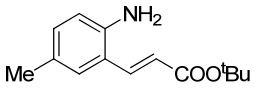
^{13}C NMR



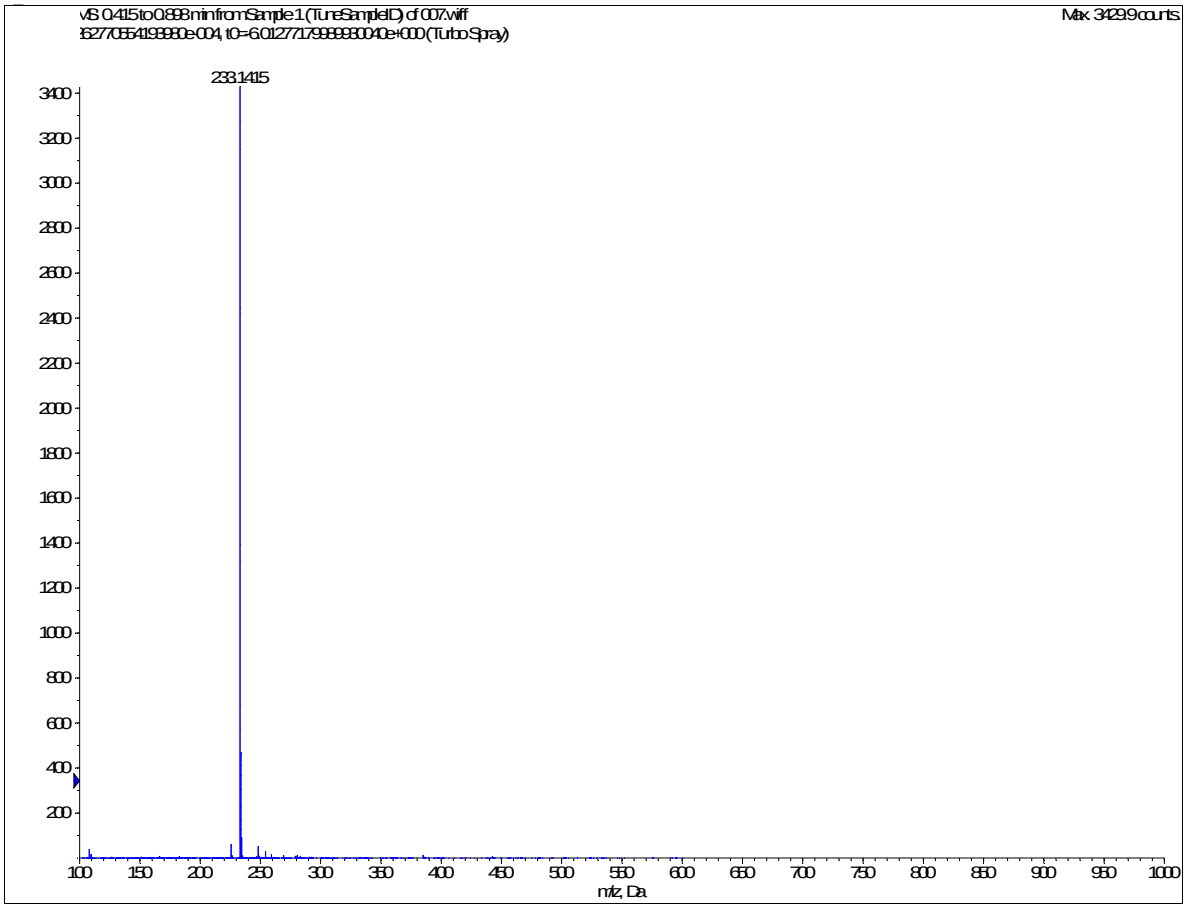
(*E*)-*tert*-Butyl 3-(2-amino-5-methylphenyl)acrylate (1h)



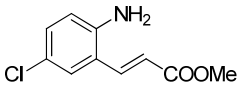
HRMS



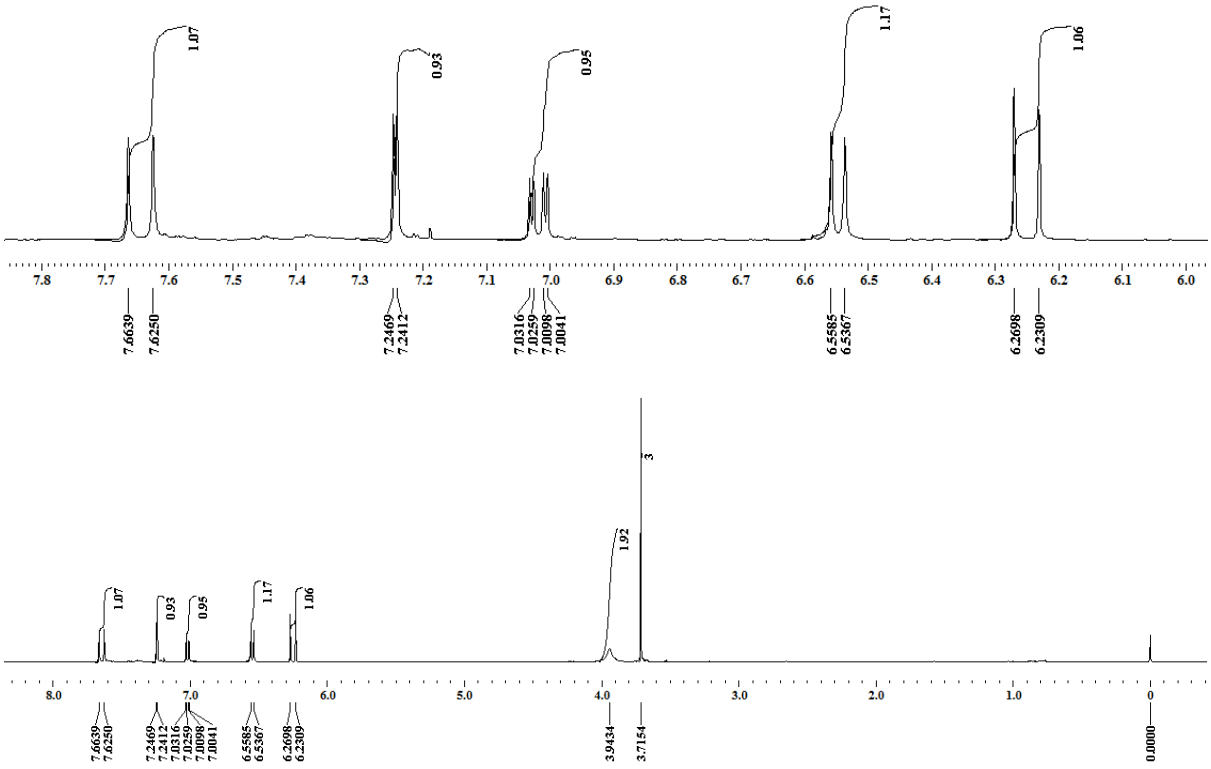
(*E*)-*tert*-Butyl 3-(2-amino-5-methylphenyl)acrylate (1h)



^{1}H NMR



(*E*)-Methyl 3-(2-amino-5-chlorophenyl)acrylate (1i)



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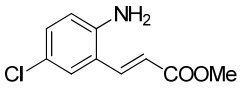
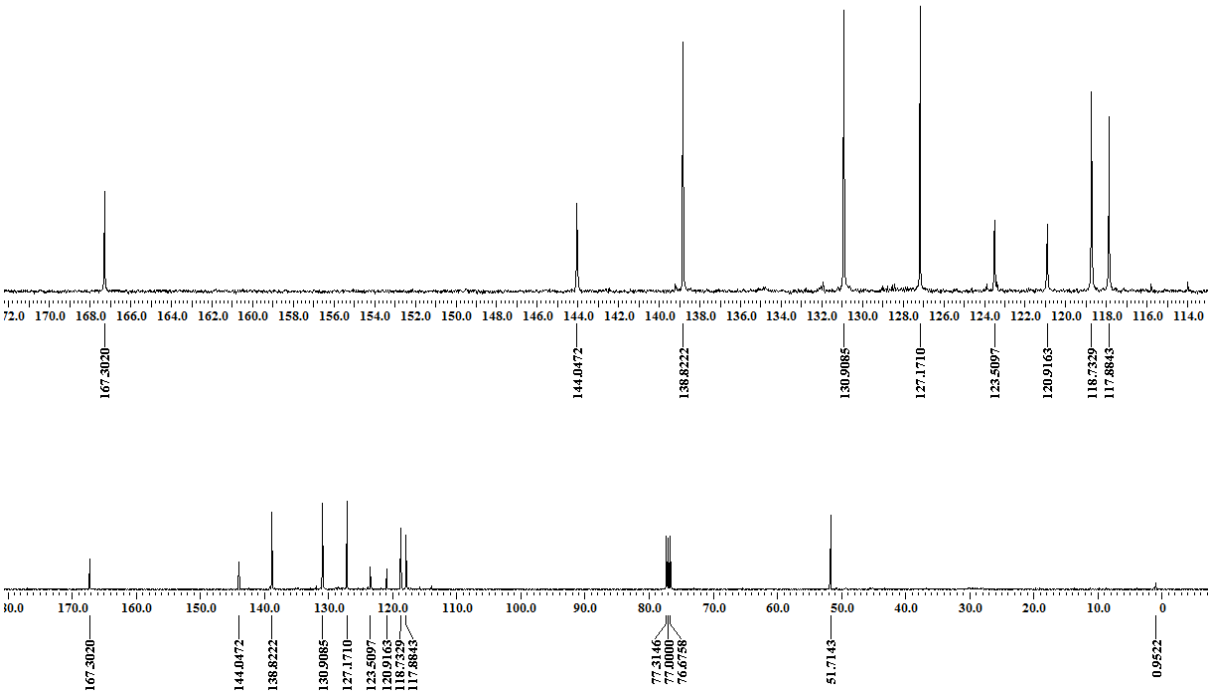
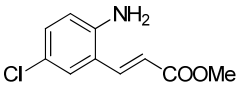


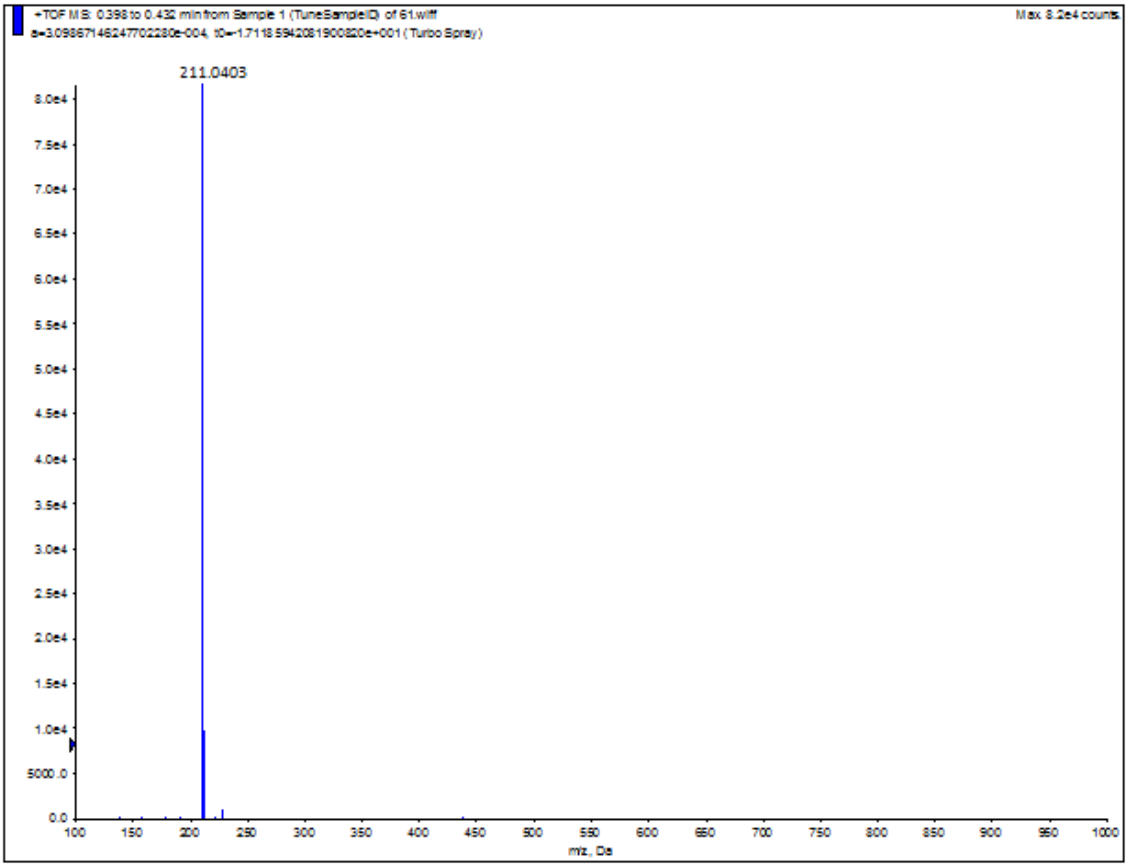
(*E*)-Methyl 3-(2-amino-5-chlorophenyl)acrylate (1i)



HRMS



(*E*)-Methyl 3-(2-amino-5-chlorophenyl)acrylate (1i)



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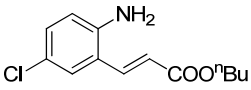
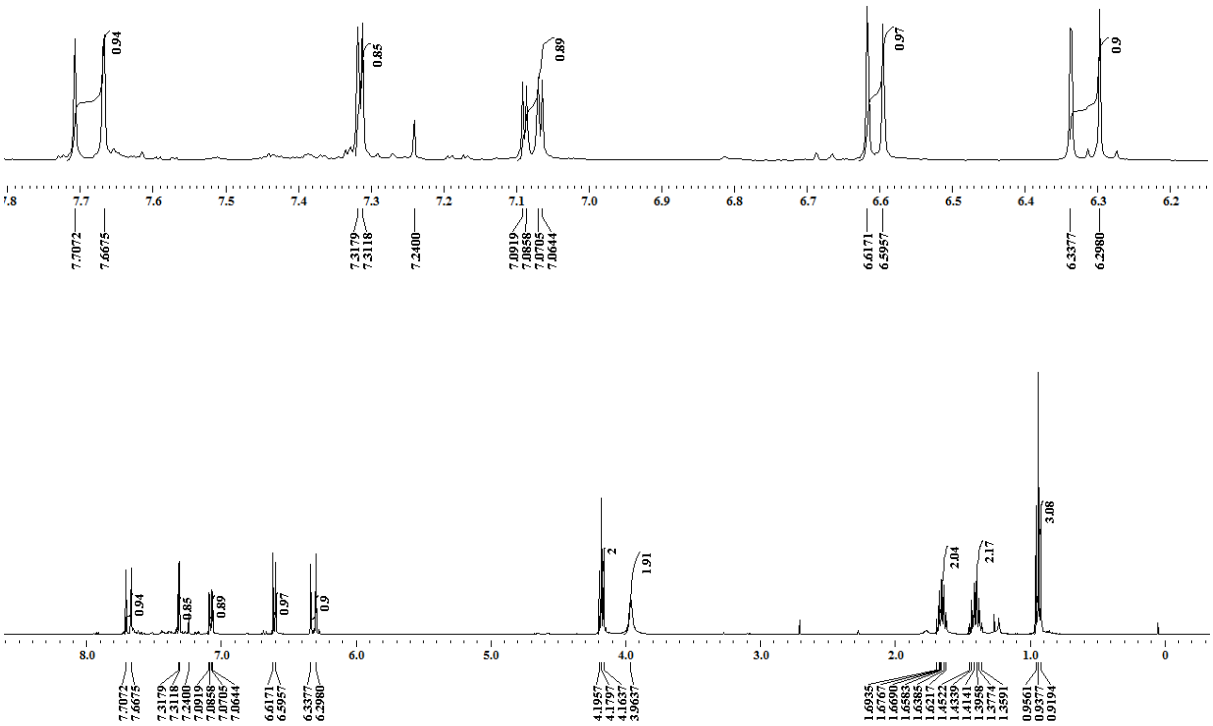


(*E*)-Butyl 3-(2-amino-5-chlorophenyl)acrylate (1j)



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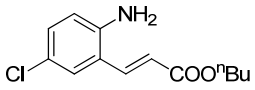

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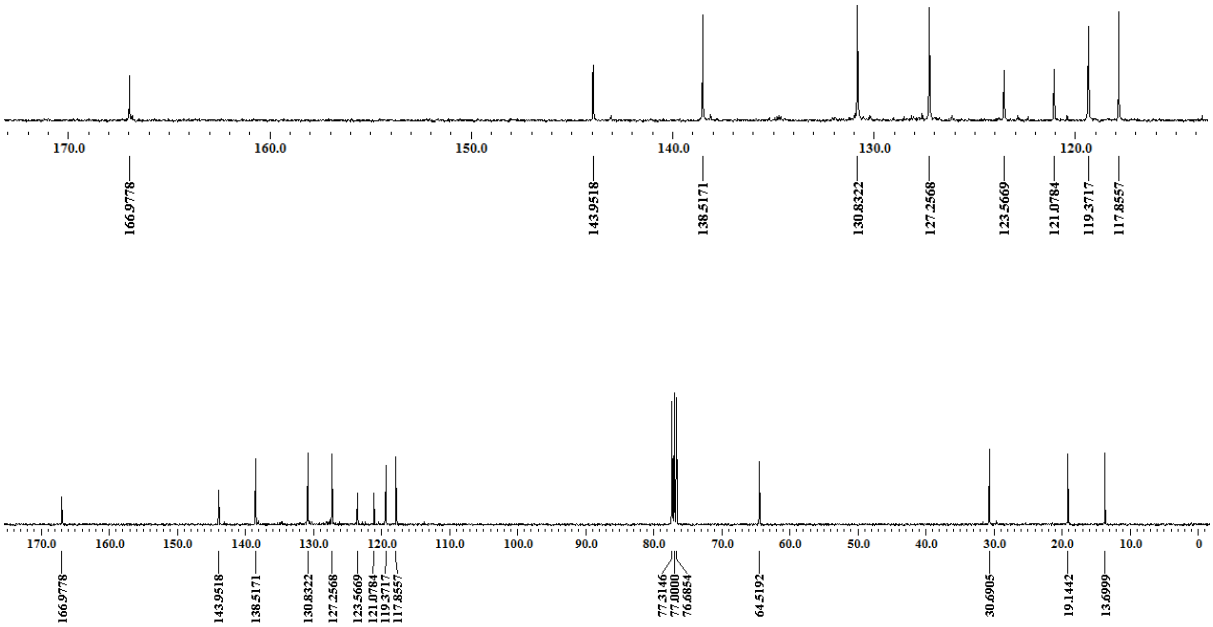
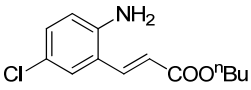
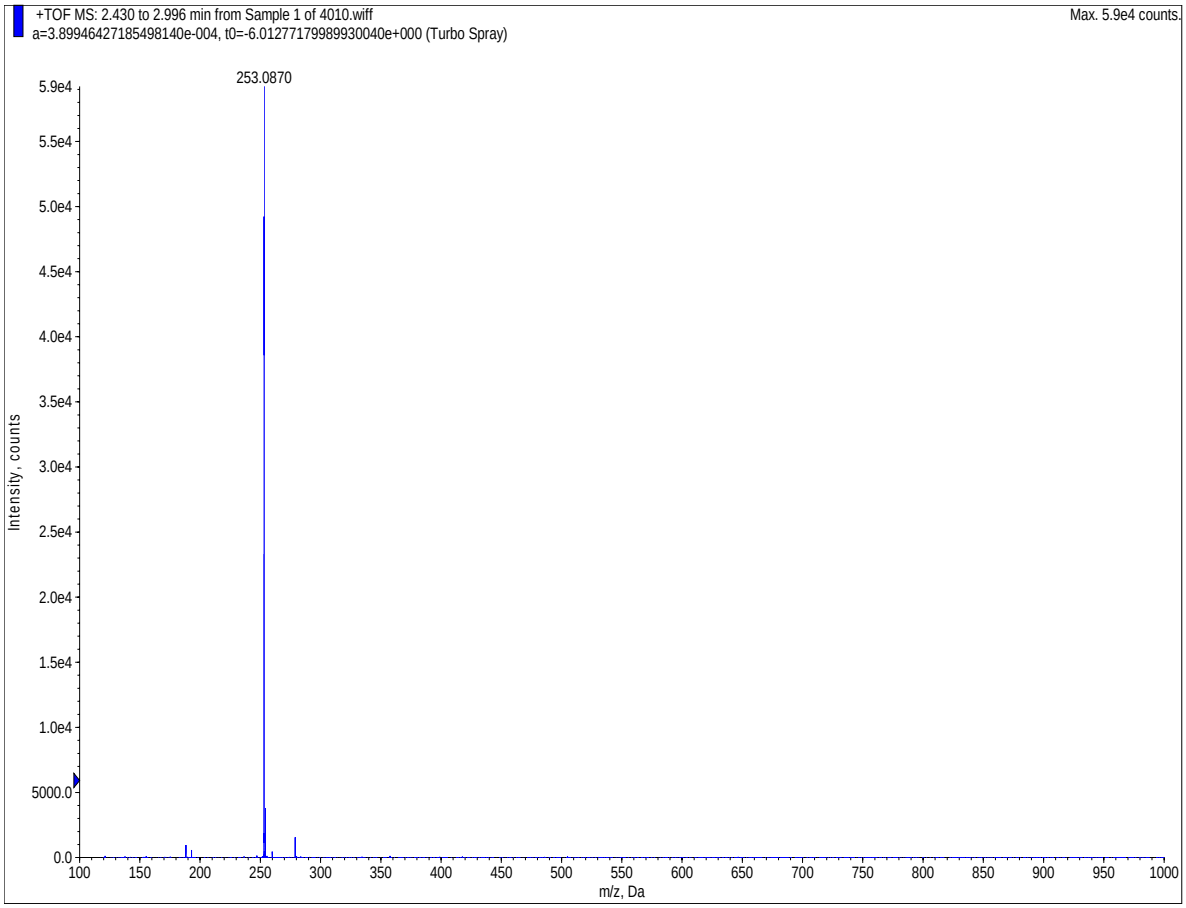


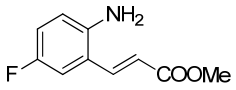
HRMS



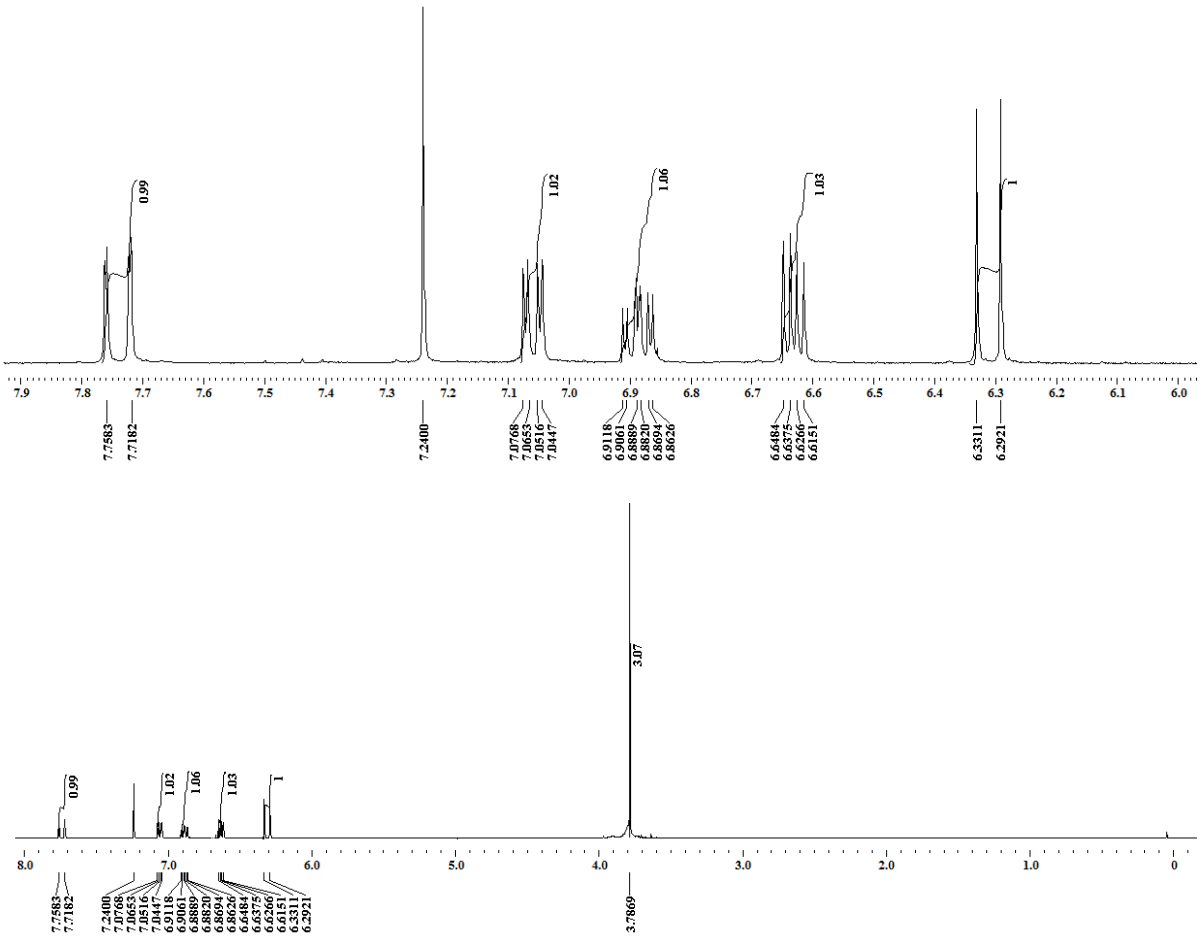
(*E*)-Butyl 3-(2-amino-5-chlorophenyl)acrylate (1j)



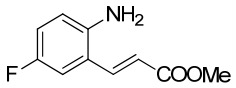
^{1}H NMR



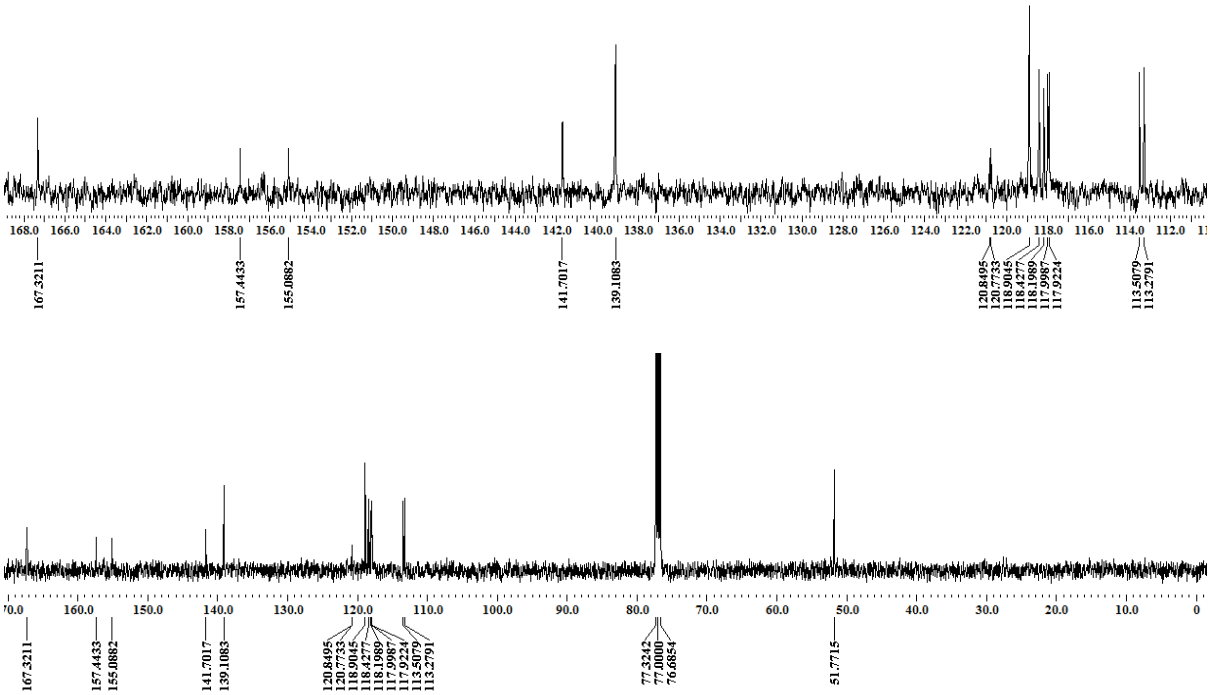
(*E*)-methyl 3-(2-amino-5-fluorophenyl)acrylate (1k)



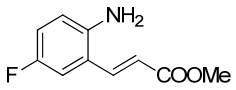
^{13}C NMR



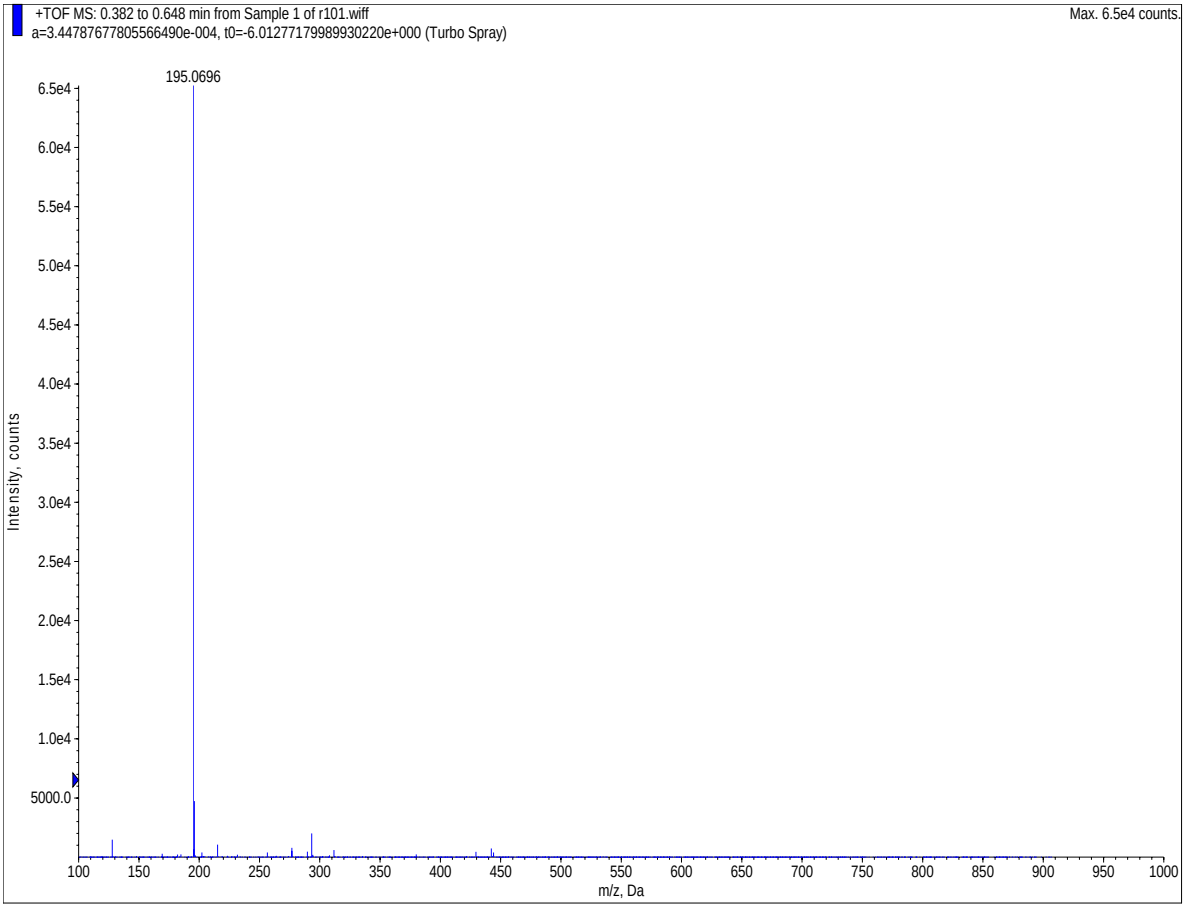
(*E*)-methyl 3-(2-amino-5-fluorophenyl)acrylate (1k)



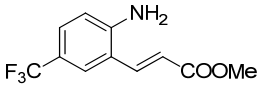
HRMS



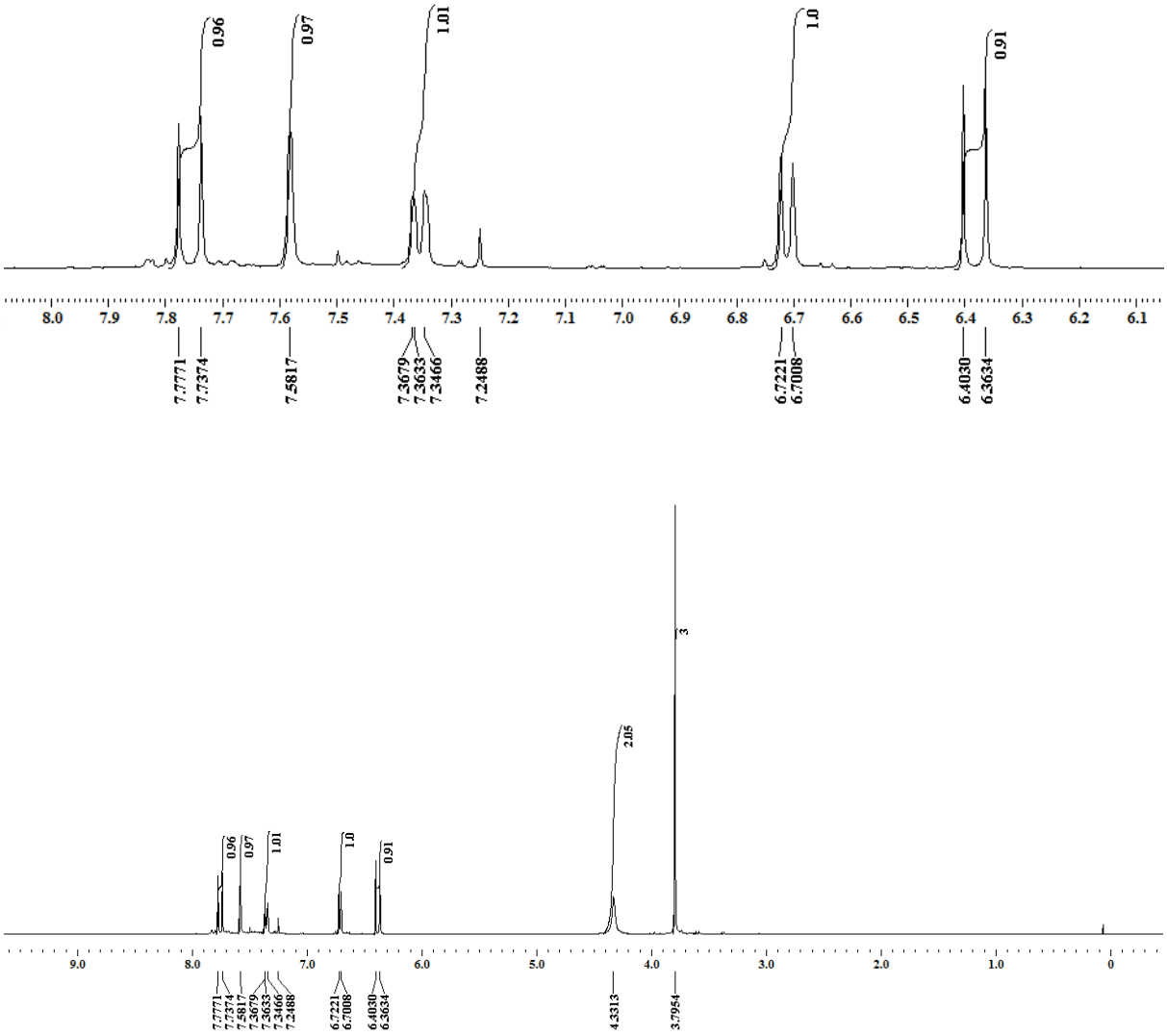
(*E*)-methyl 3-(2-amino-5-fluorophenyl)acrylate (1k)



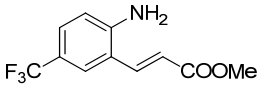
^{1}H NMR



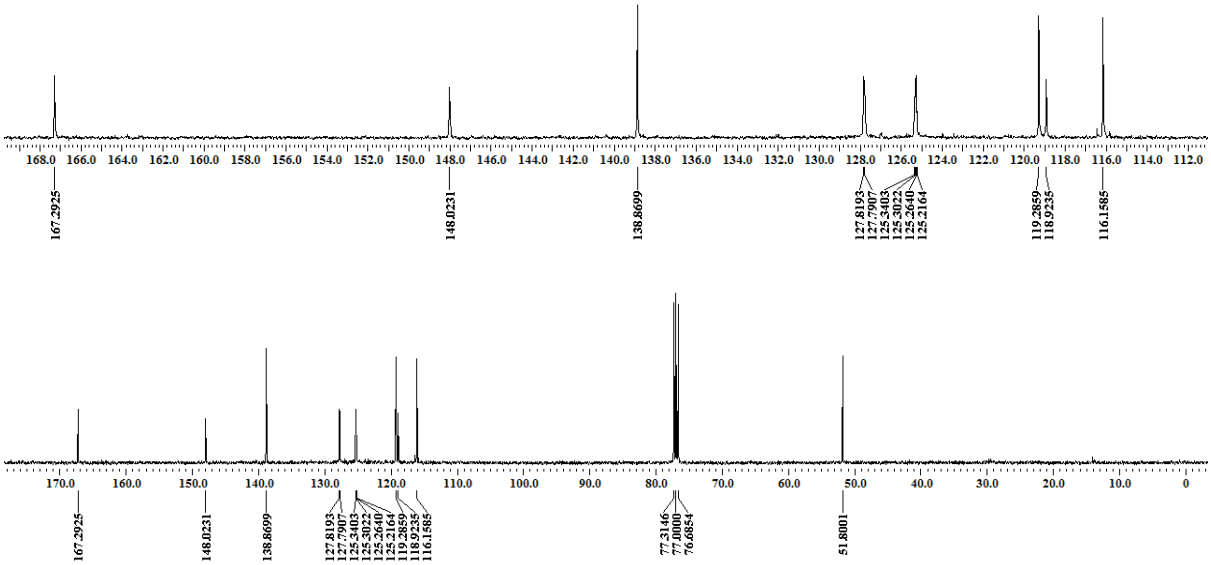
(*E*)-Methyl 3-(2-amino-5-(trifluoromethyl)phenyl)acrylate (1l)



^{13}C NMR



(*E*)-Methyl 3-(2-amino-5-(trifluoromethyl)phenyl)acrylate (1l)



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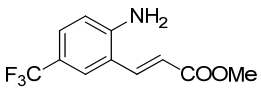
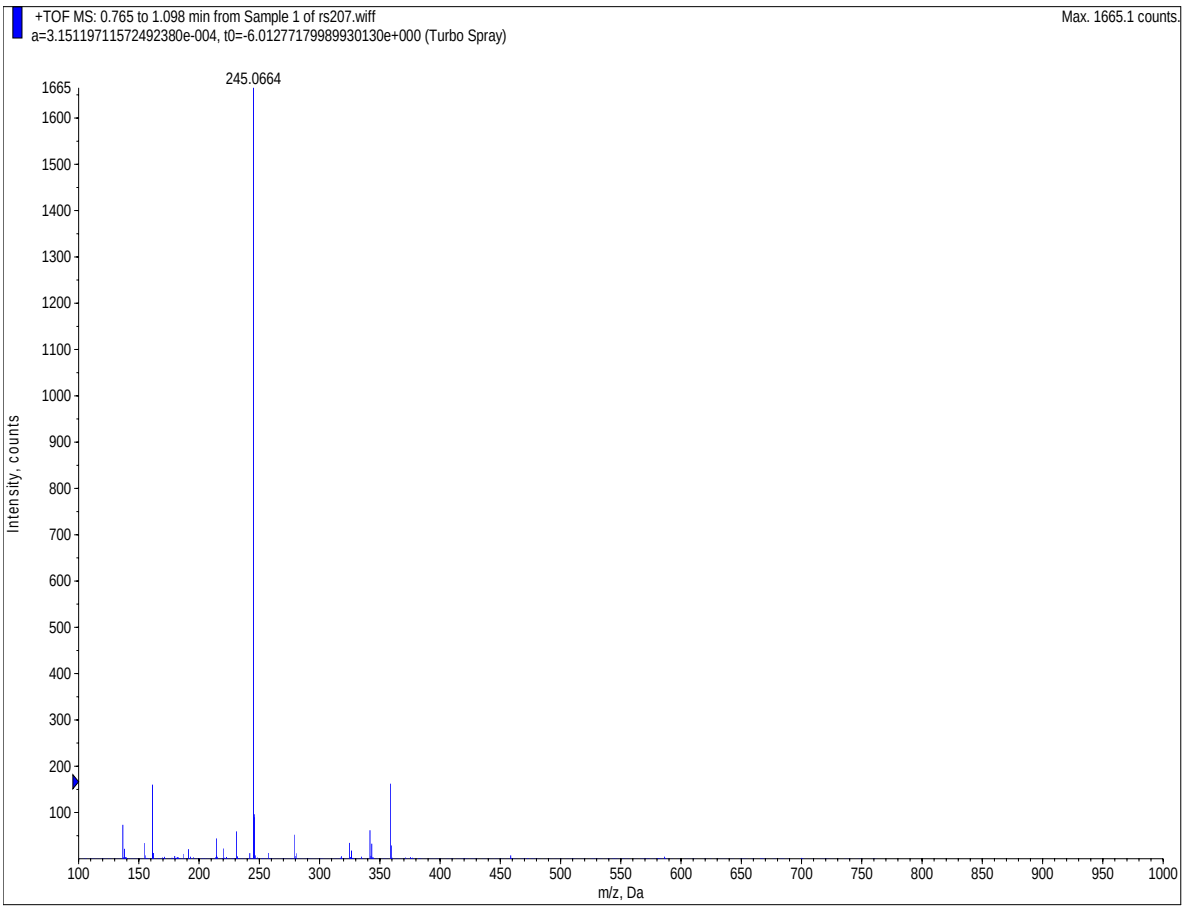
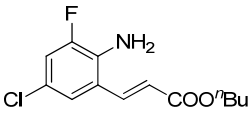


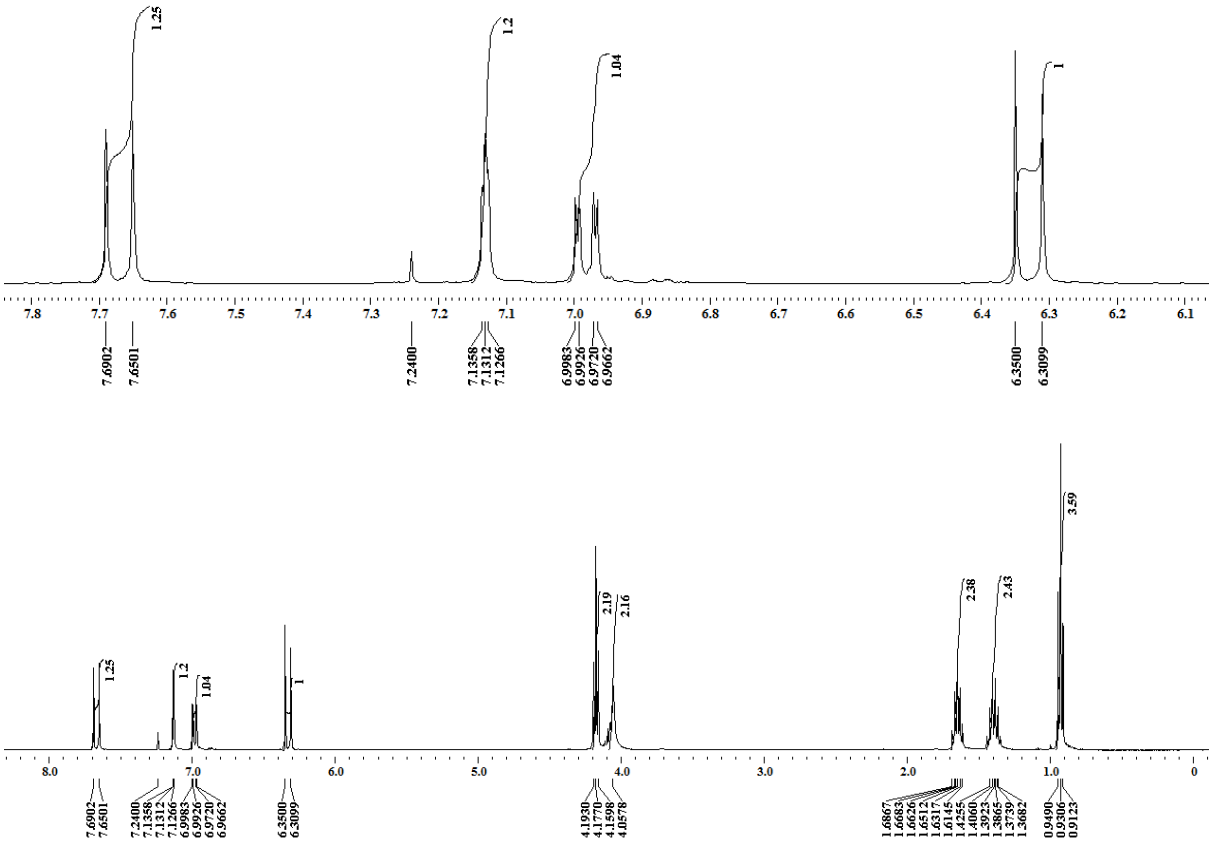
(*E*)-Methyl 3-(2-amino-5-(trifluoromethyl)phenyl)acrylate (1l)



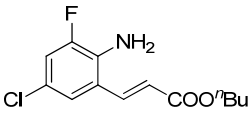
^{1}H NMR



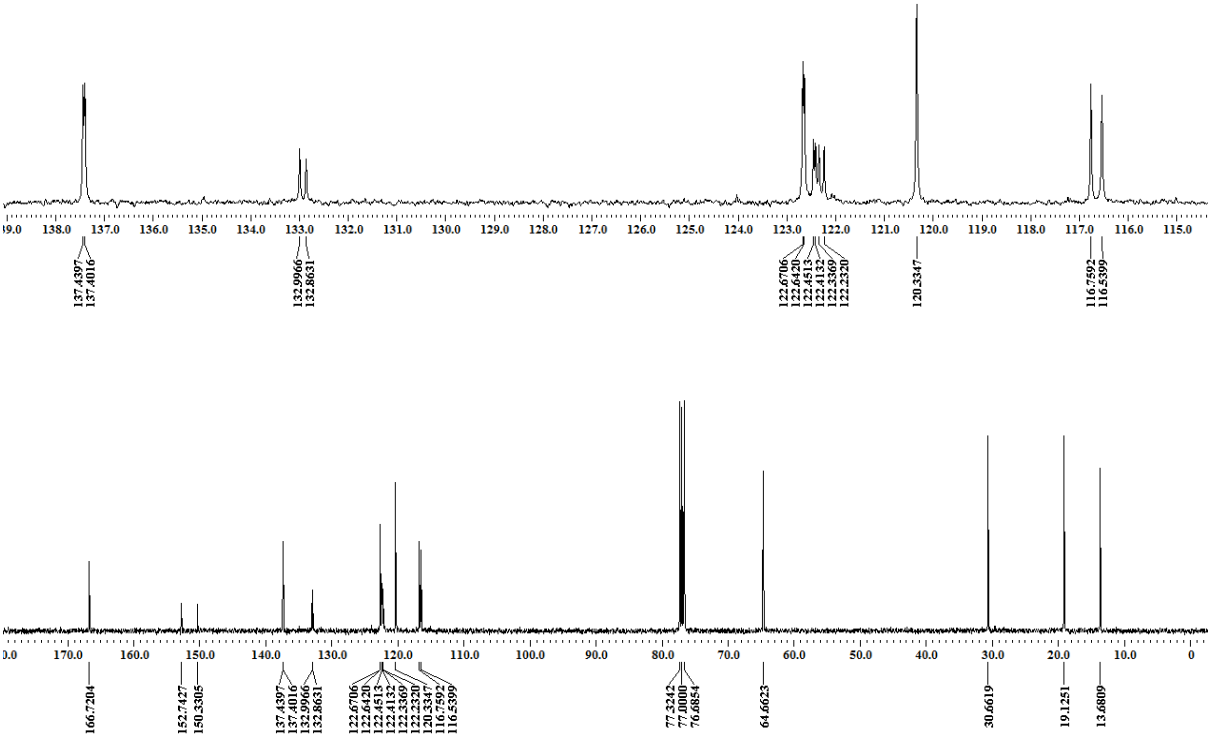
(*E*)-butyl 3-(2-amino-5-chloro-3-fluorophenyl)acrylate (1m)



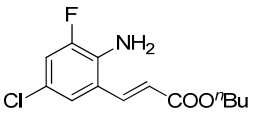
^{13}C NMR



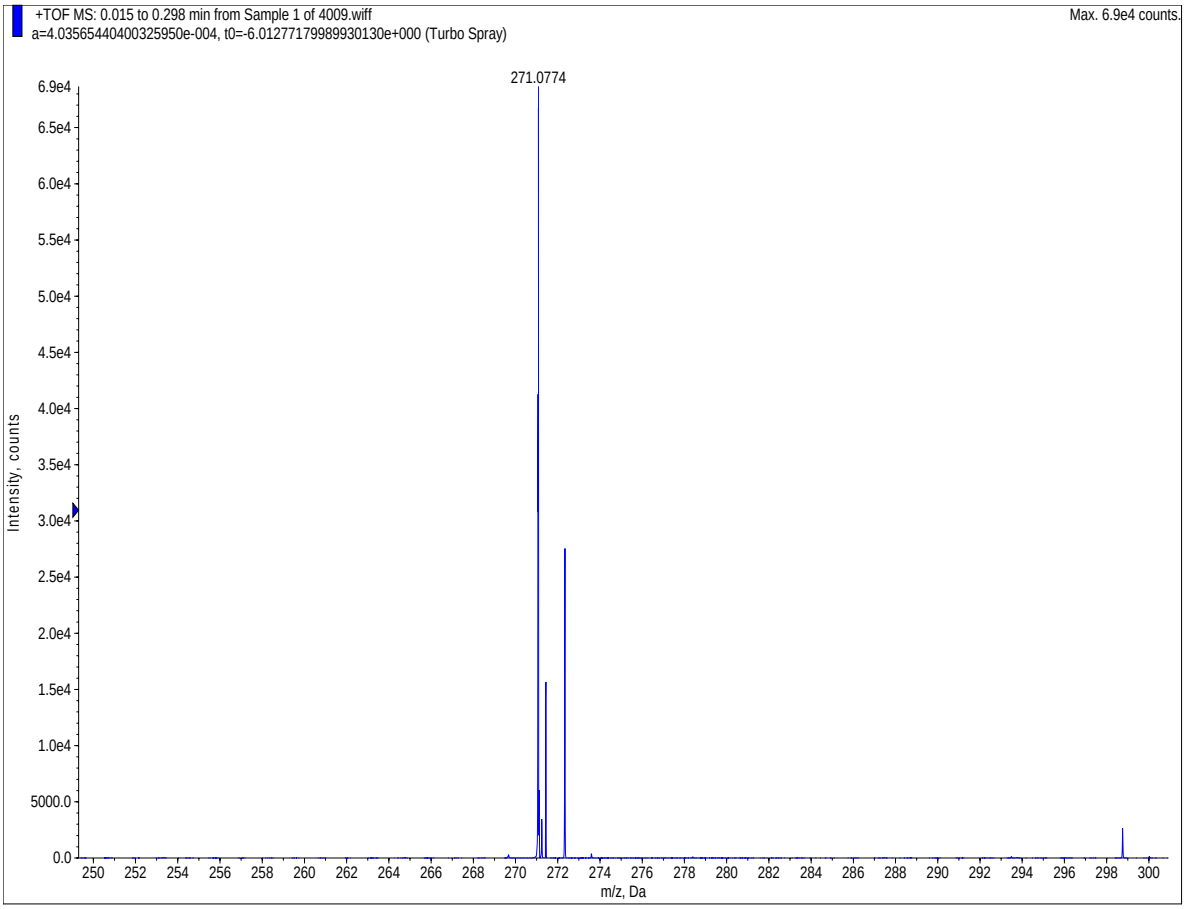
(*E*)-butyl 3-(2-amino-5-chloro-3-fluorophenyl)acrylate (1m)



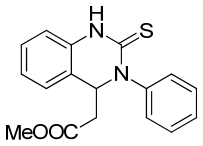
HRMS



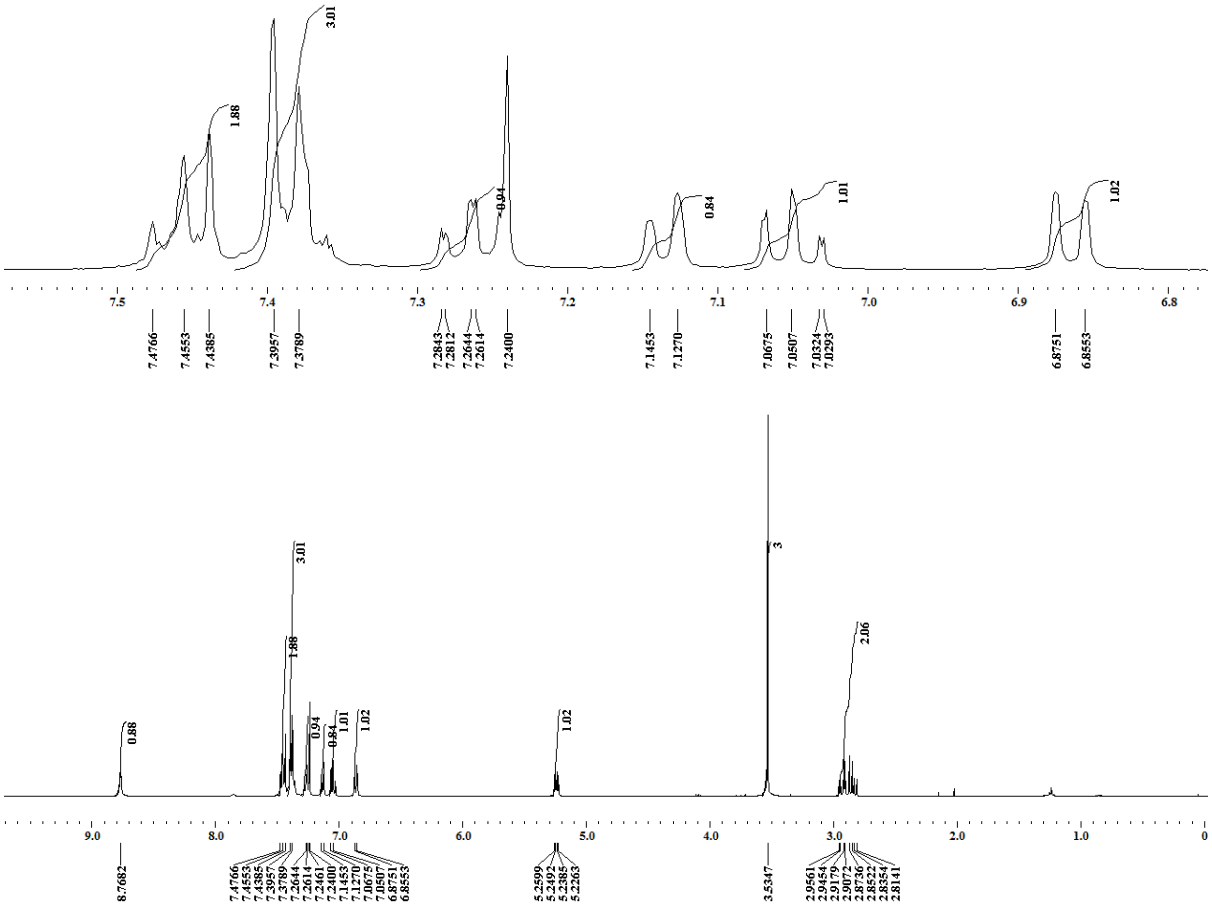
(E)-butyl 3-(2-amino-5-chloro-3-fluorophenyl)acrylate (1m)



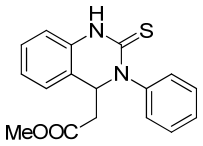
^{1}H NMR



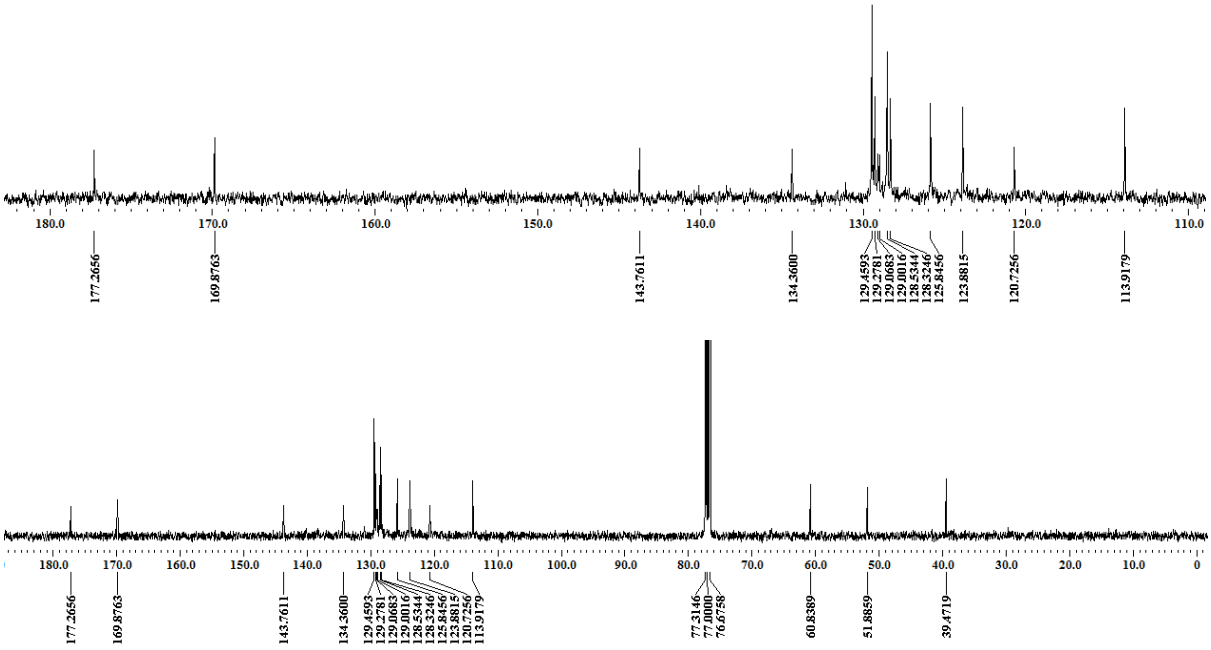
Methyl 2-(3-phenyl-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (3a)



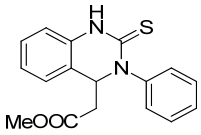
^{13}C NMR



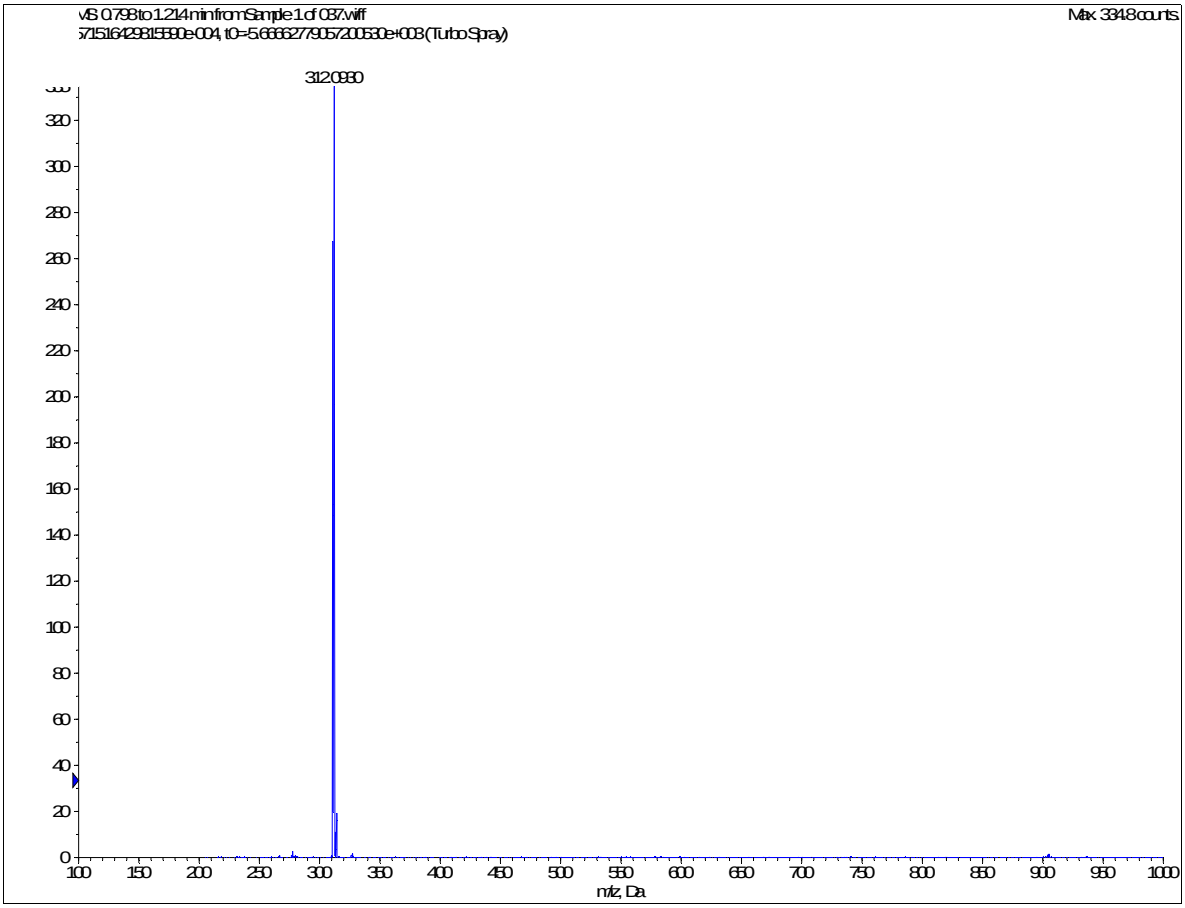
Methyl 2-(3-phenyl-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (3a)



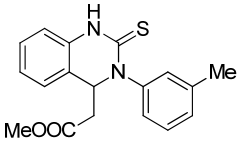
HRMS



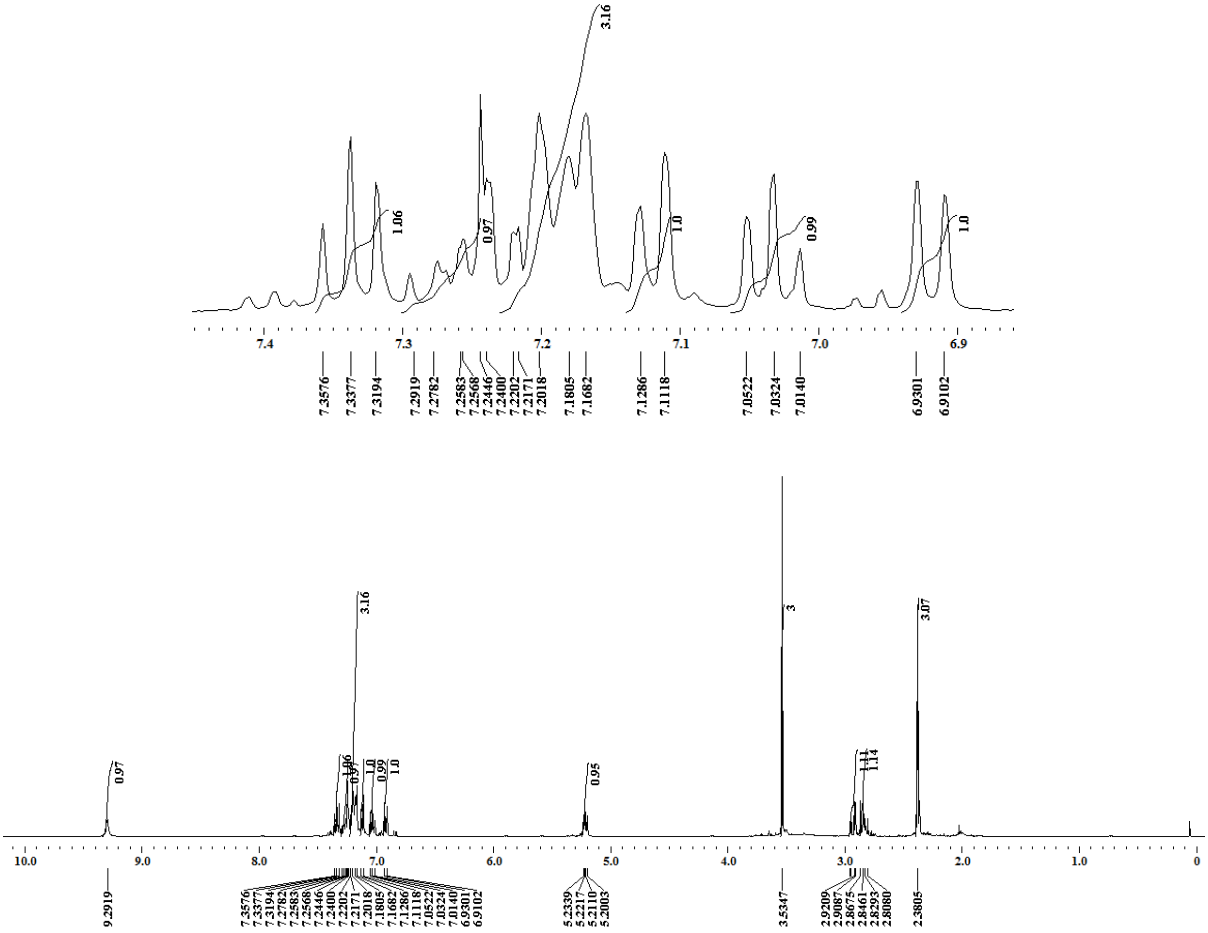
Methyl 2-(3-phenyl-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (3a)



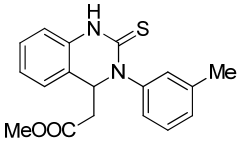
^{1}H NMR



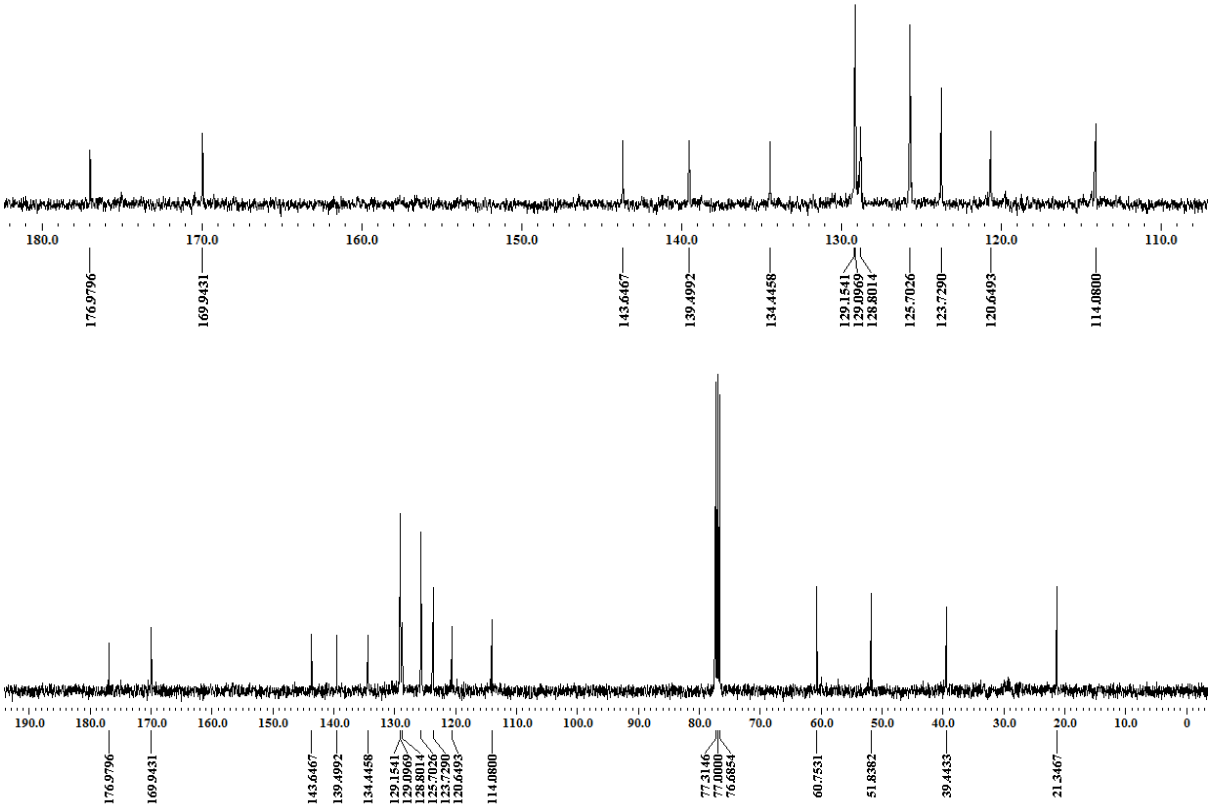
Methyl 2-(2-thioxo-3-(*m*-tolyl)-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (3b)



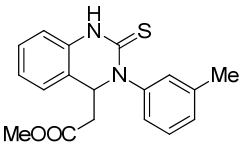
^{13}C NMR



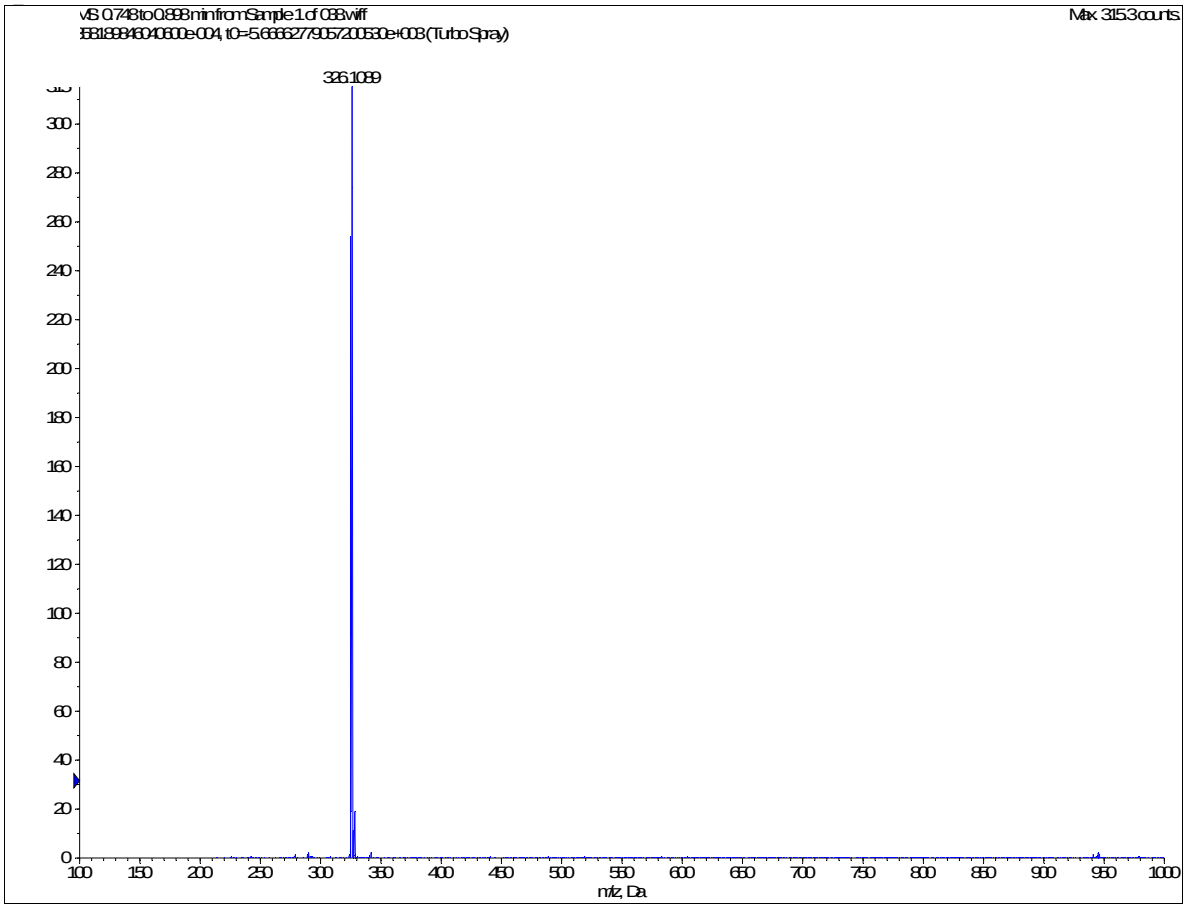
Methyl 2-(2-thioxo-3-(*m*-tolyl)-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (3b)



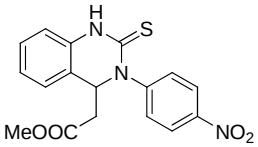
HRMS



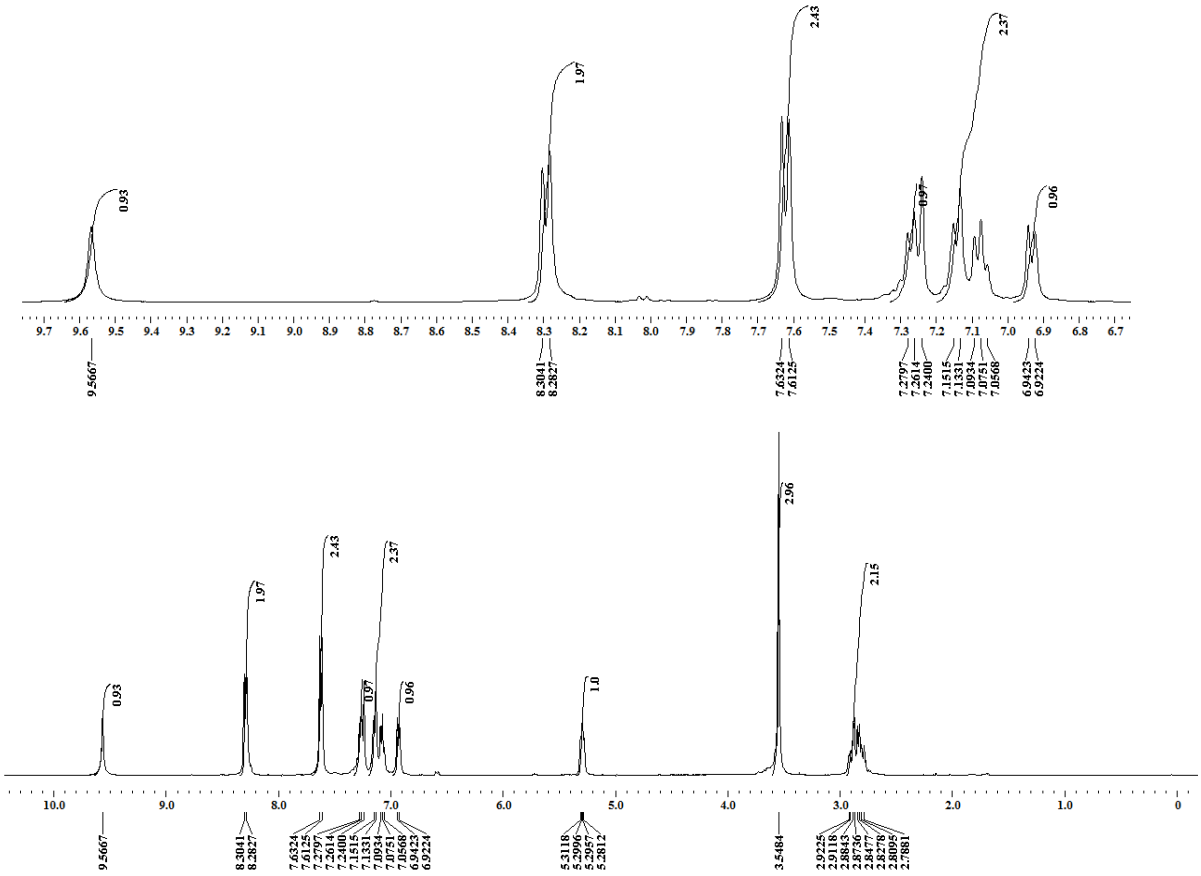
Methyl 2-(2-thioxo-3-(*m*-tolyl)-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (3b)



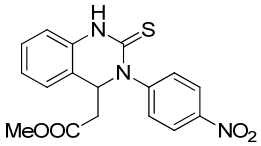
^{1}H NMR



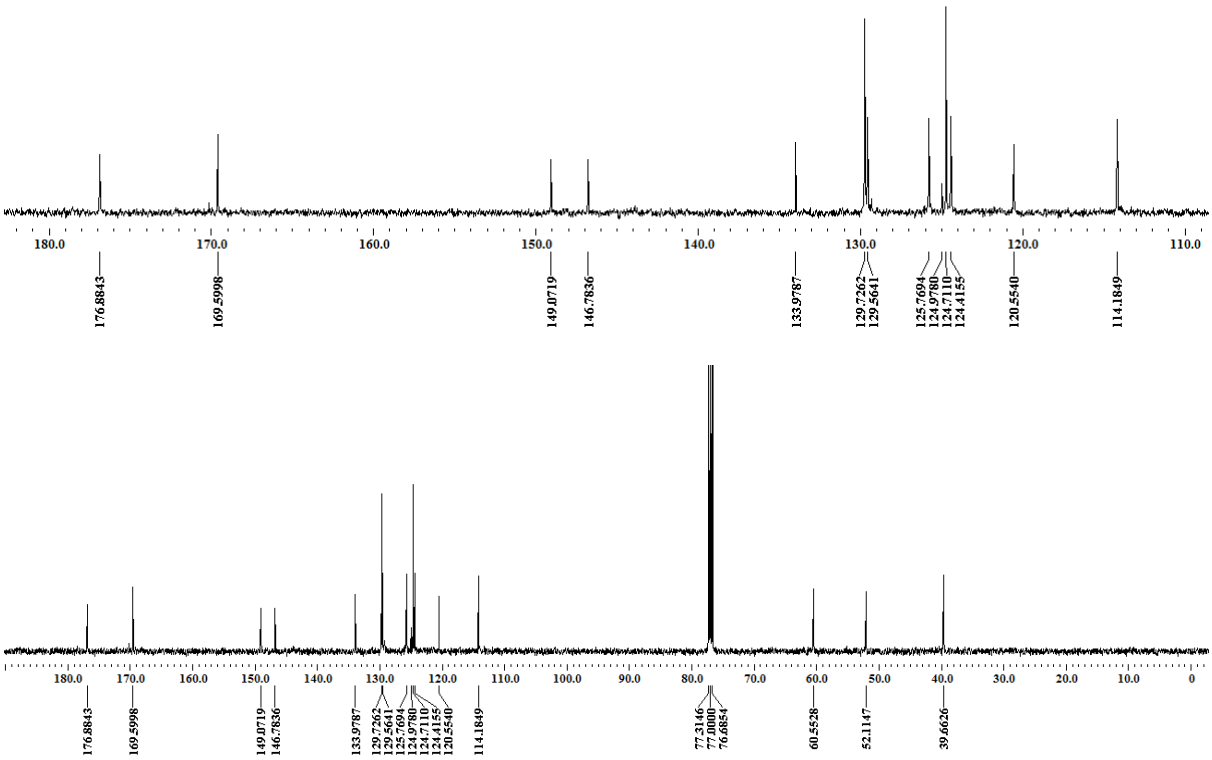
Methyl 2-(3-(4-nitrophenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (3c)



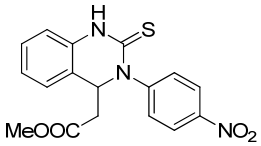
^{13}C NMR



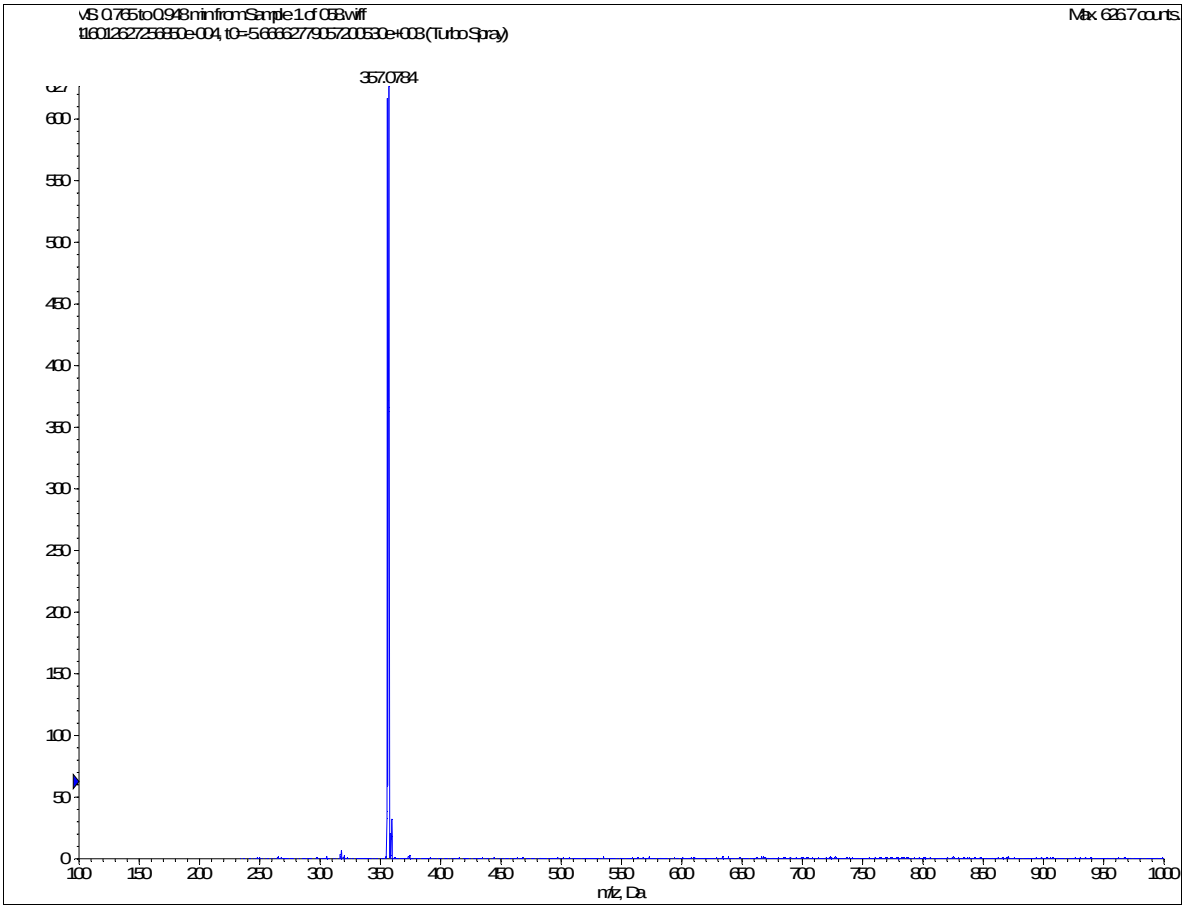
Methyl 2-(3-(4-nitrophenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (3c)



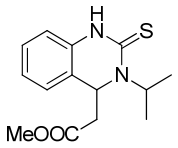
HRMS



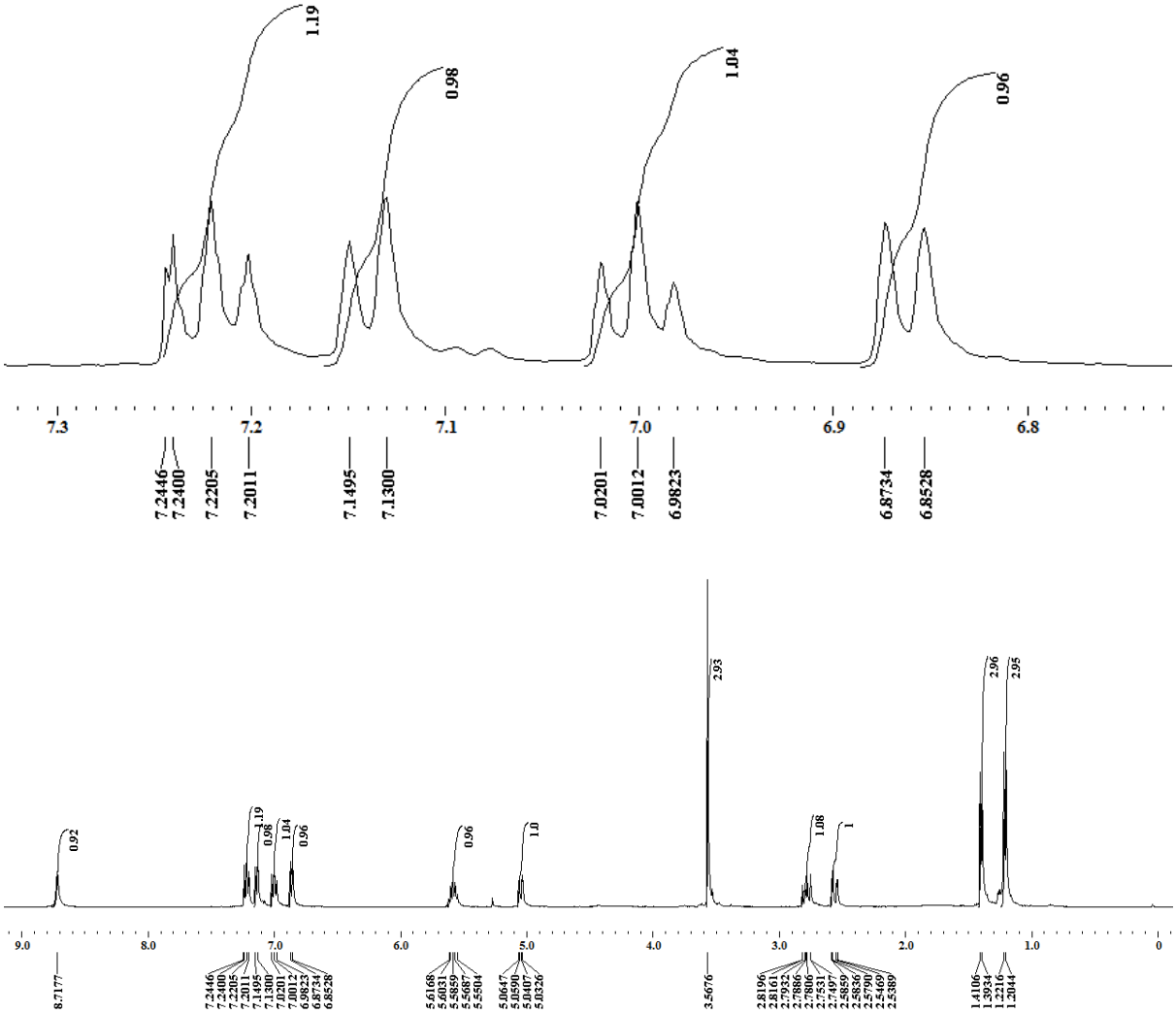
Methyl 2-(3-(4-nitrophenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (3c)



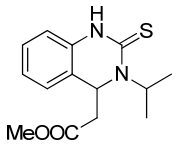
^{1}H NMR



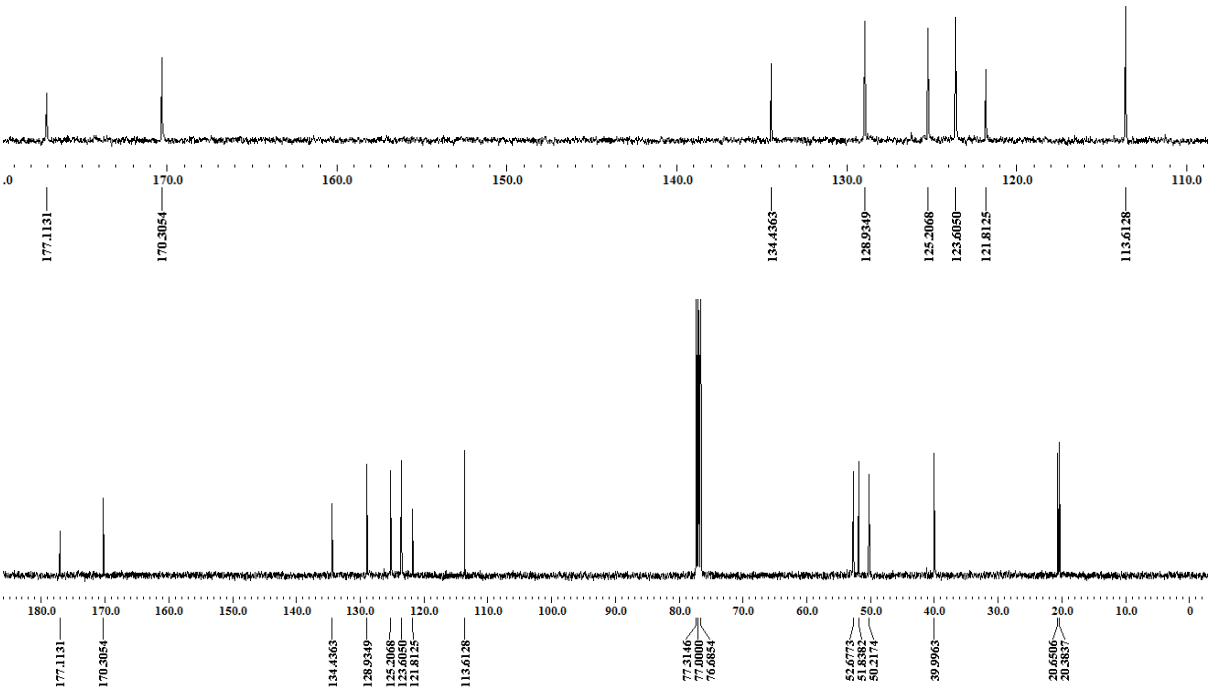
Methyl 2-(3-isopropyl-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (3d)



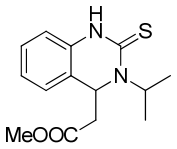
^{13}C NMR



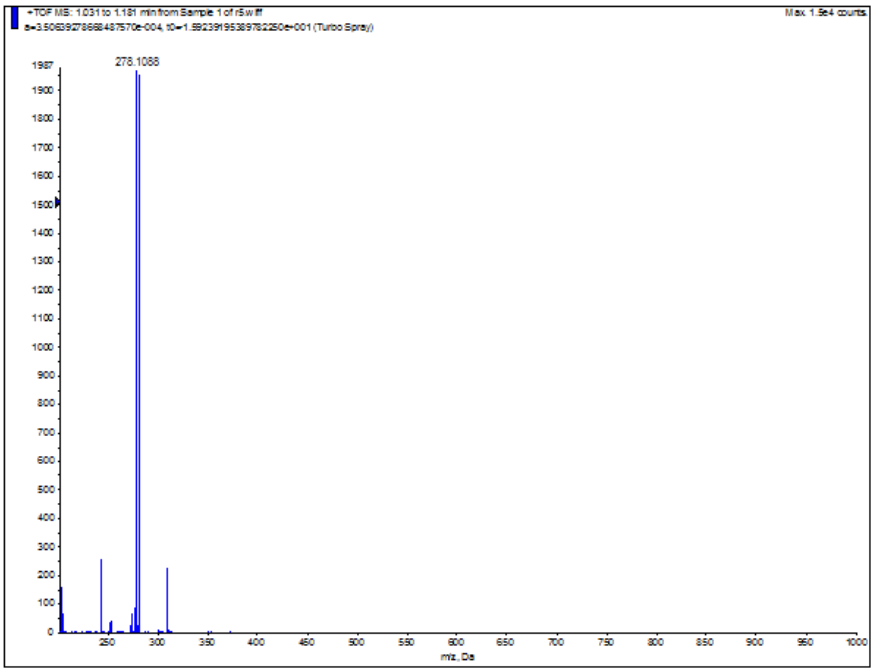
Methyl 2-(3-isopropyl-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (3d)



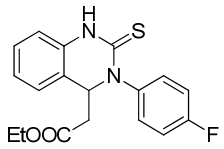
HRMS



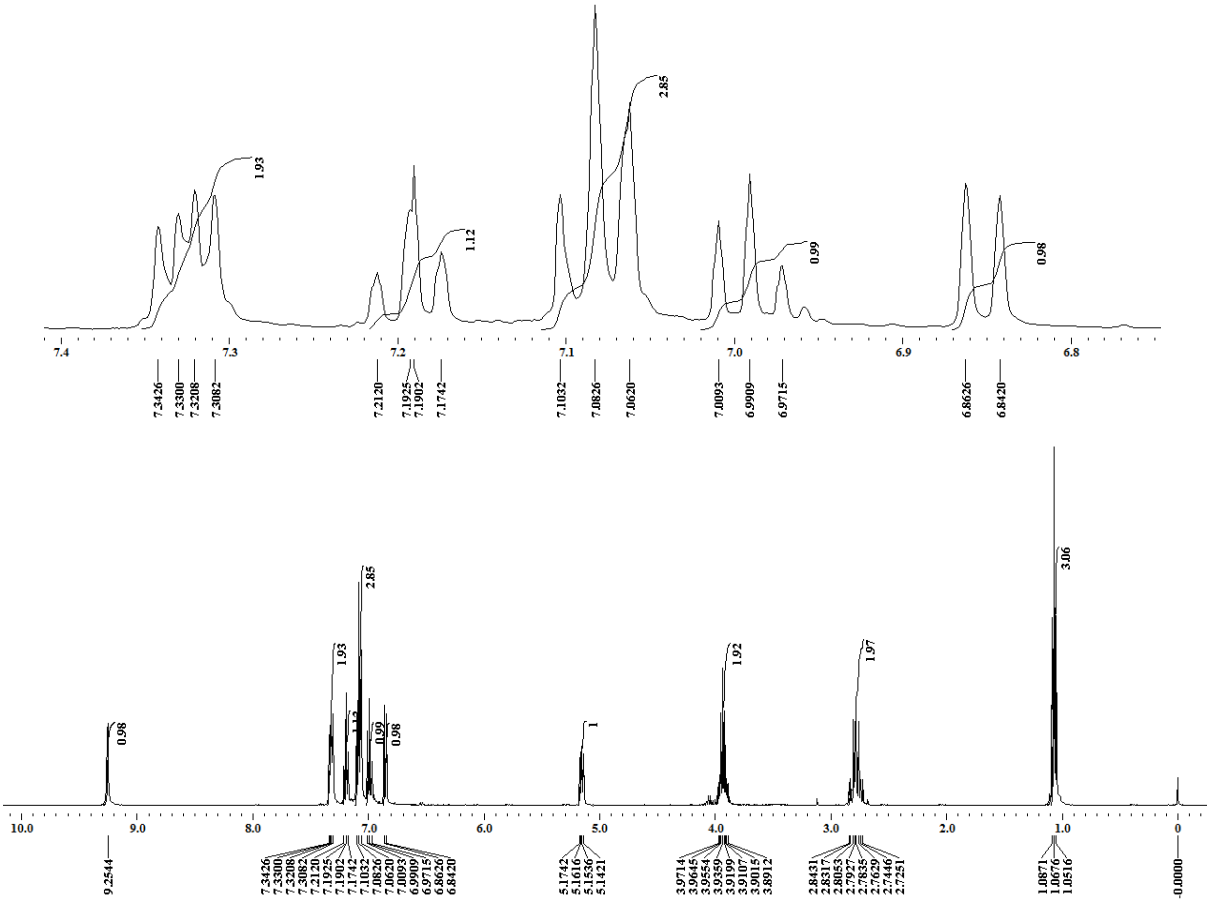
Methyl 2-(3-isopropyl-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (3d)



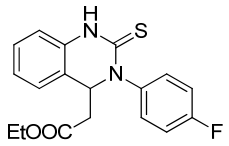
H NMR



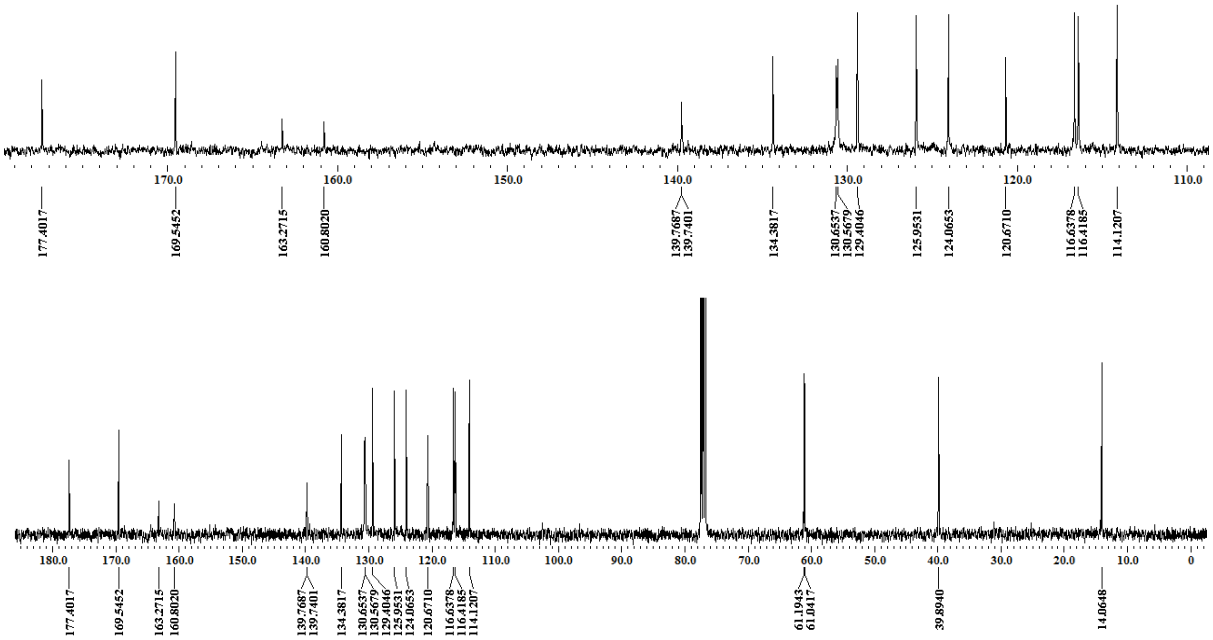
Ethyl 2-(3-(4-fluorophenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (3e)



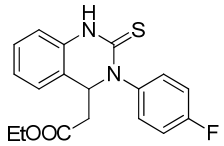
^{13}C NMR



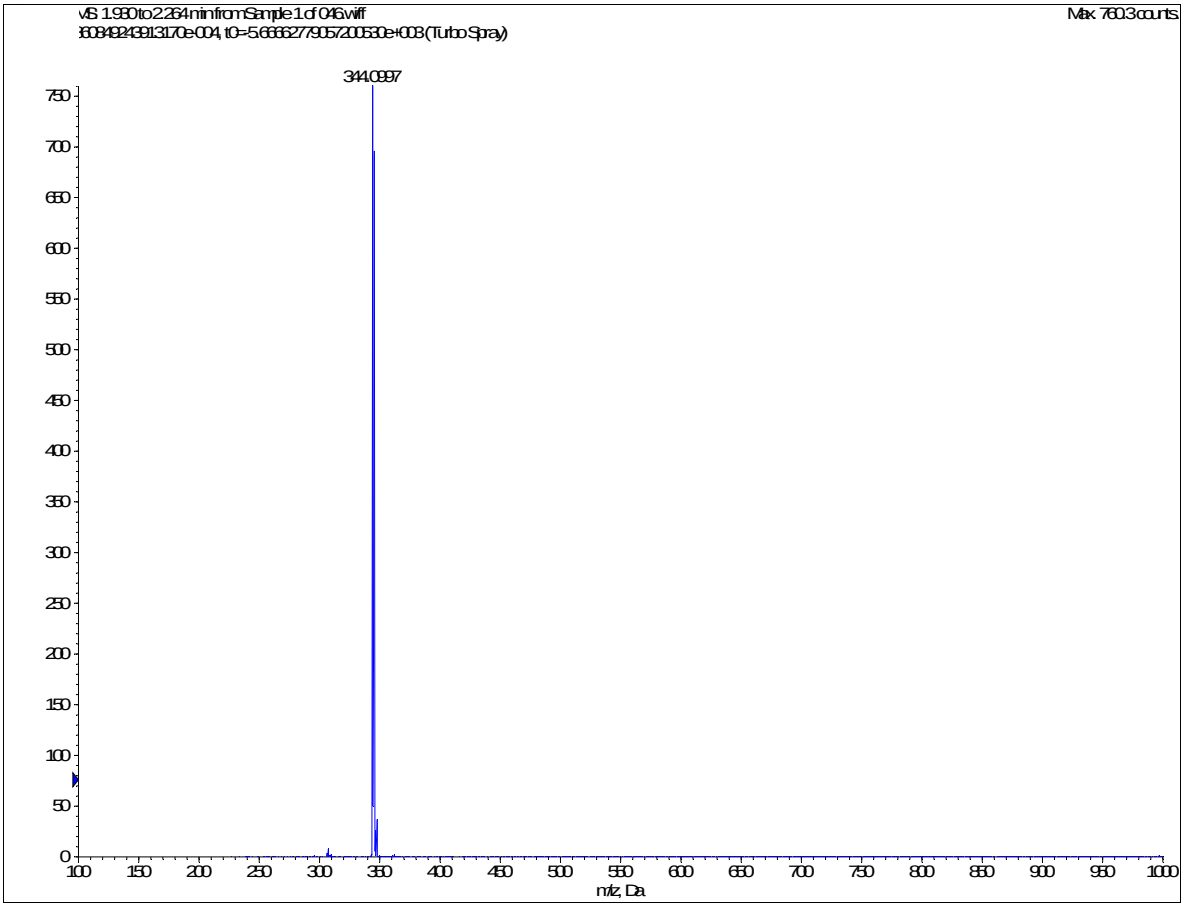
Ethyl 2-(3-(4-fluorophenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (3e)



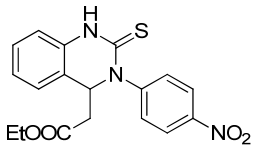
HRMS



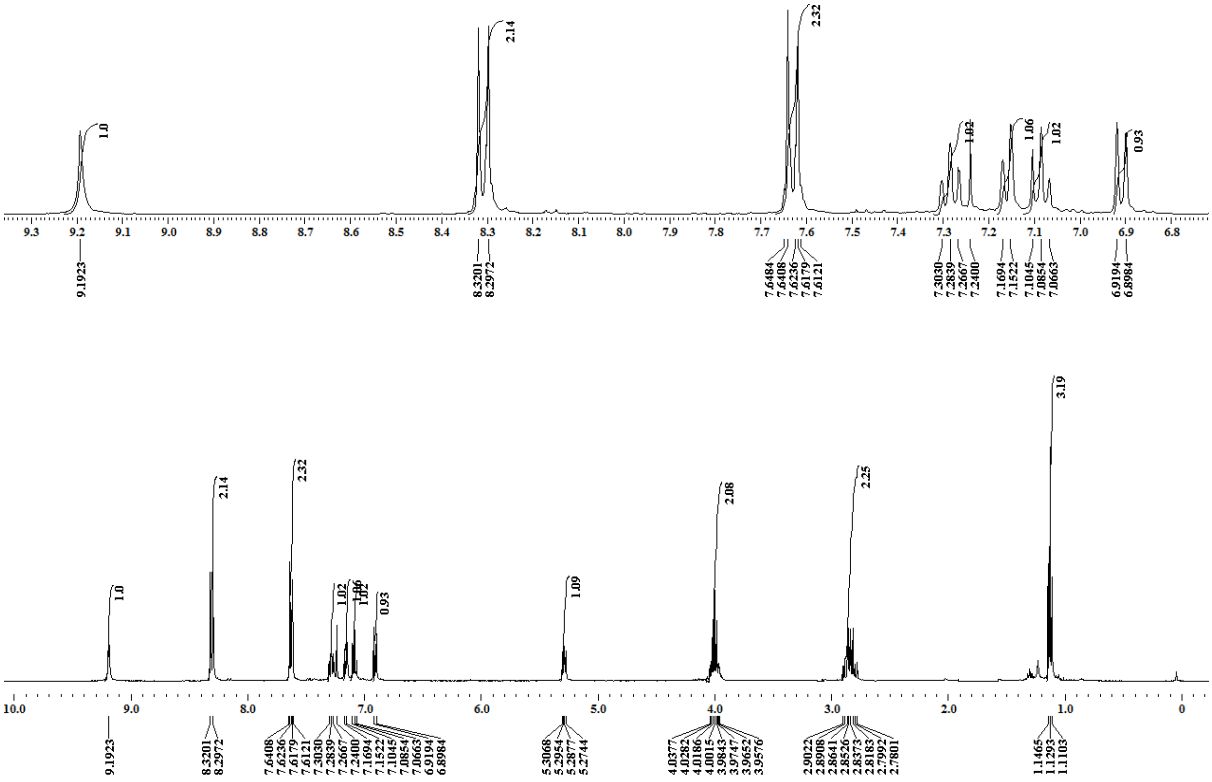
Ethyl 2-(3-(4-fluorophenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (3e)



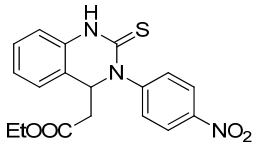
^{1}H NMR



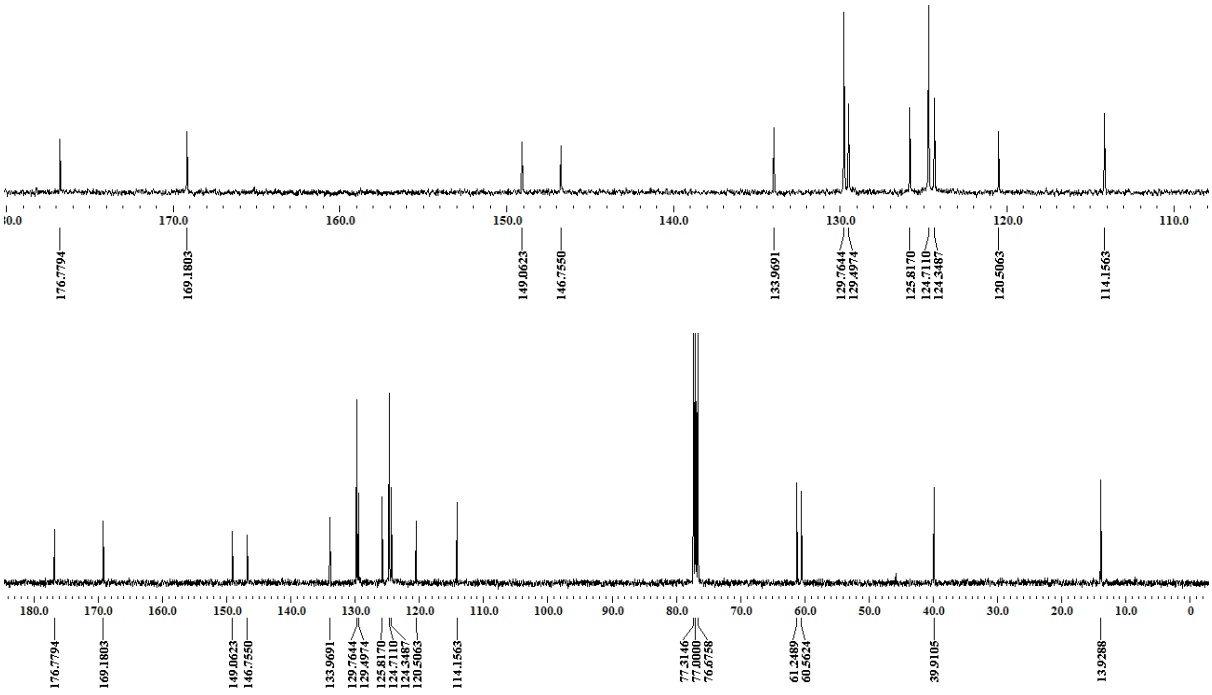
Ethyl 2-(3-(4-nitrophenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (3f)



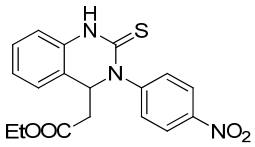
^{13}C NMR



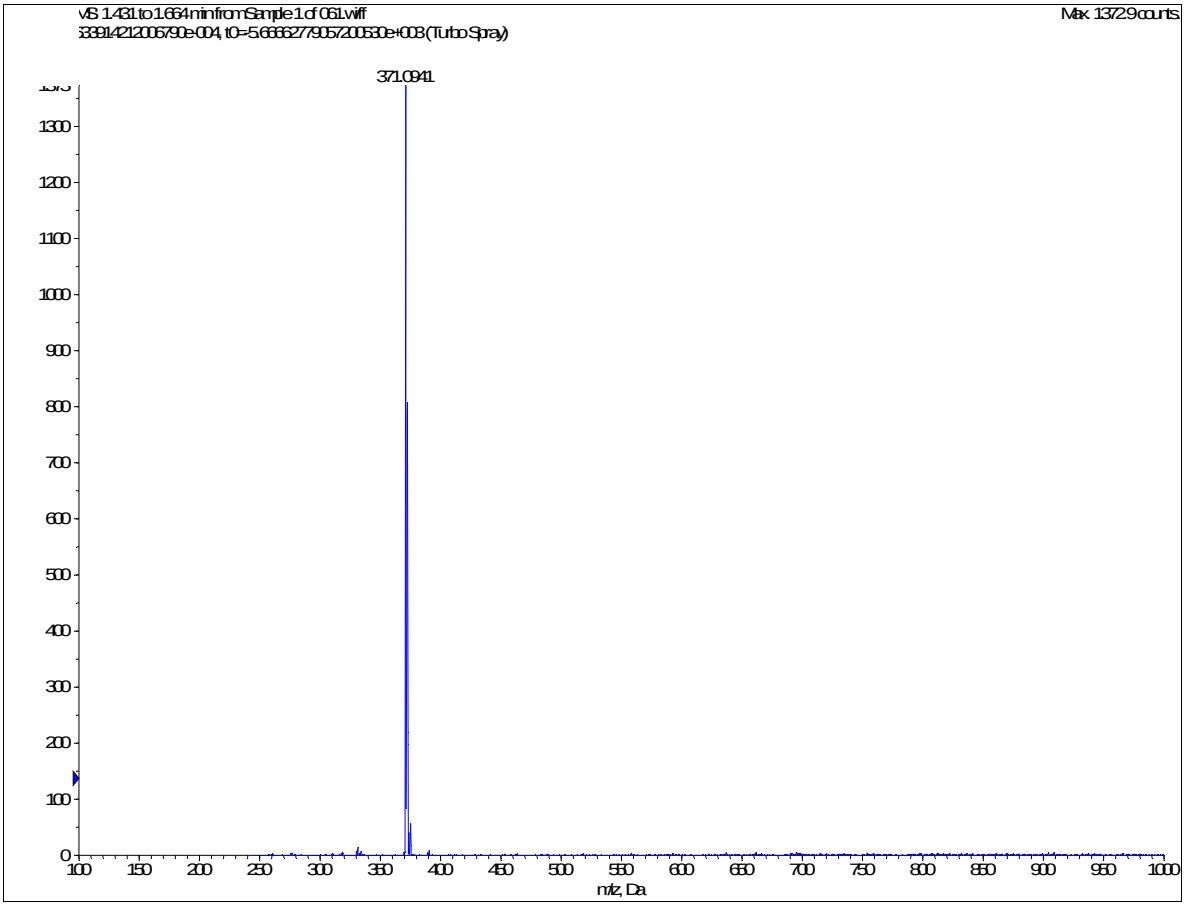
Ethyl 2-(3-(4-nitrophenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (3f)



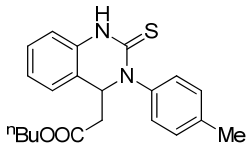
HRMS



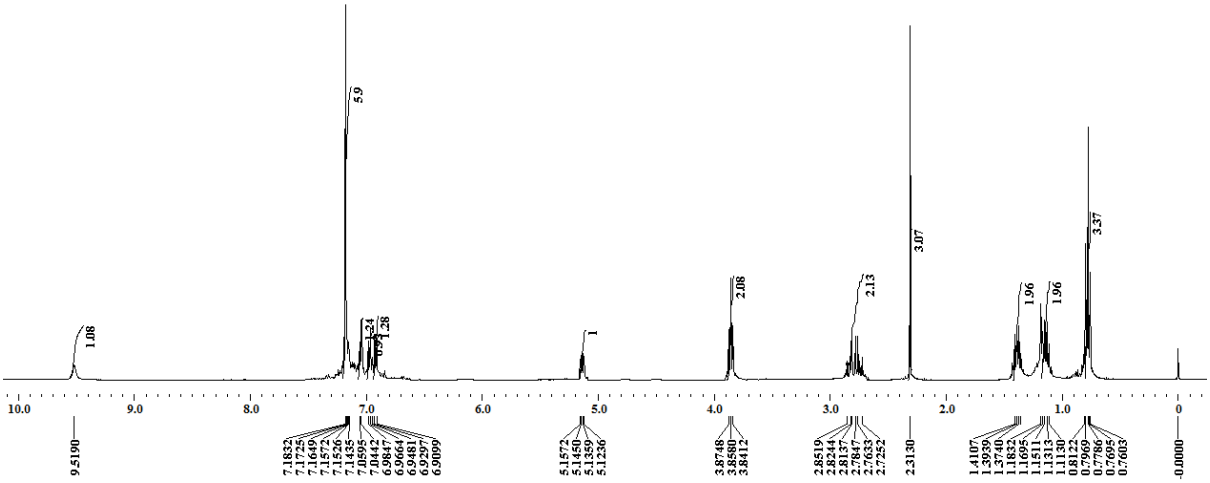
Ethyl 2-(3-(4-nitrophenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (3f)



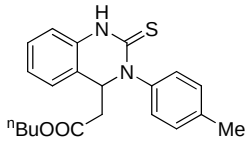
^{1}H NMR



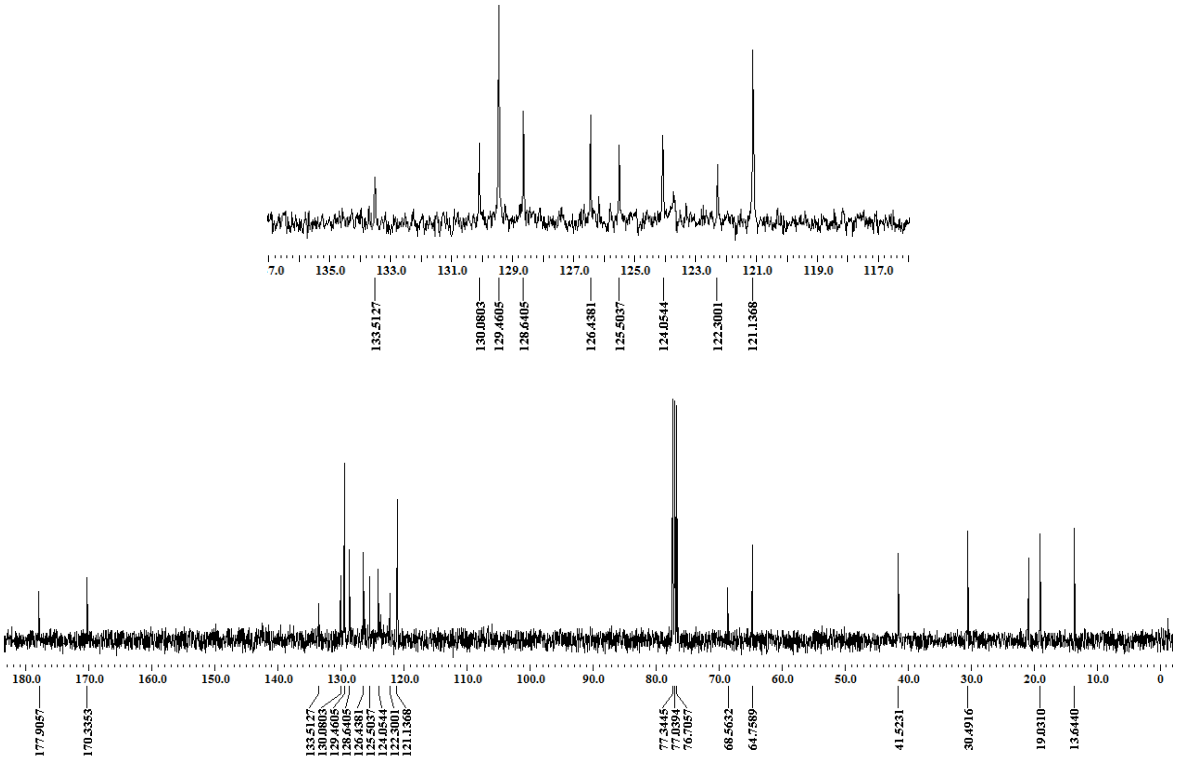
Butyl 2-(2-thioxo-3-(*p*-tolyl)-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (3g)



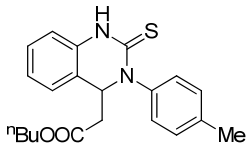
^{13}C NMR



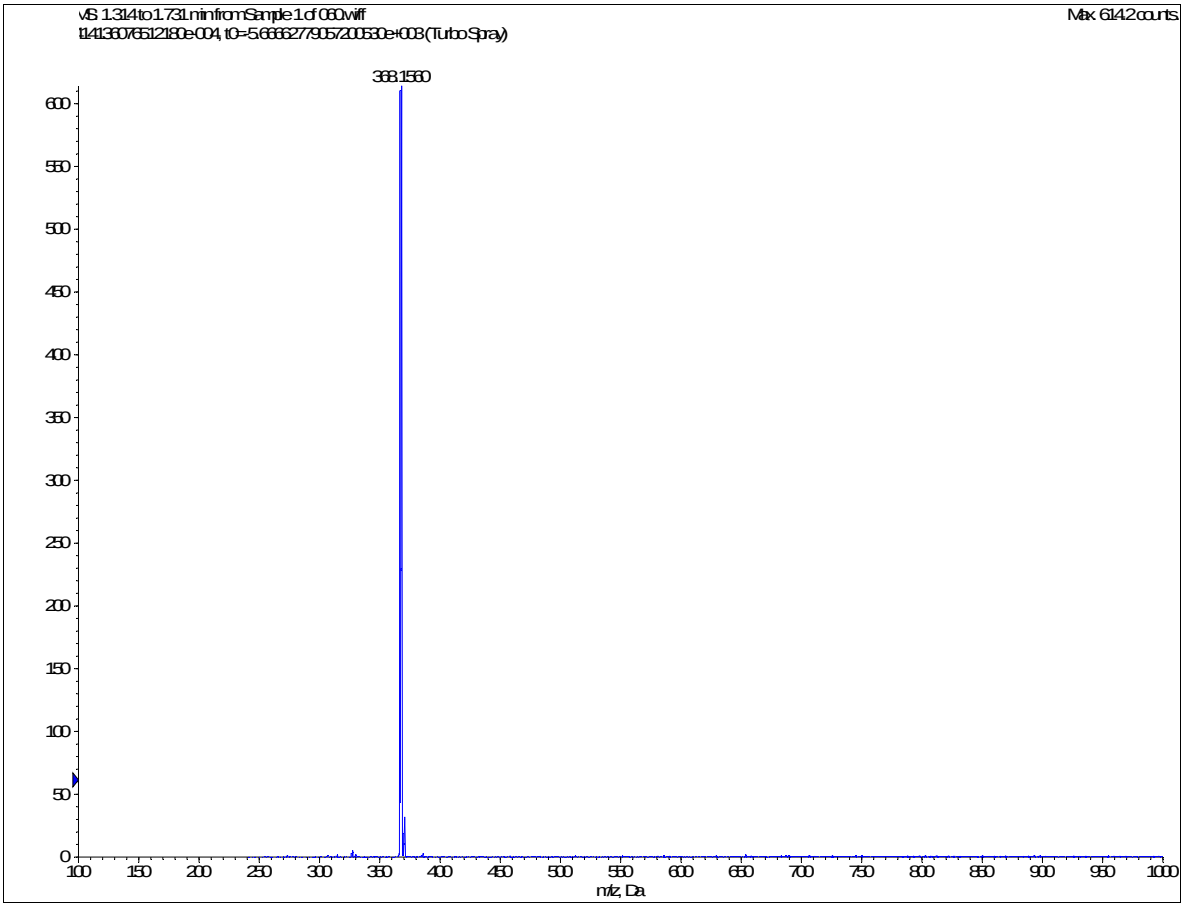
Butyl 2-(2-thioxo-3-(*p*-tolyl)-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (3g)



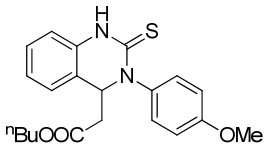
HRMS



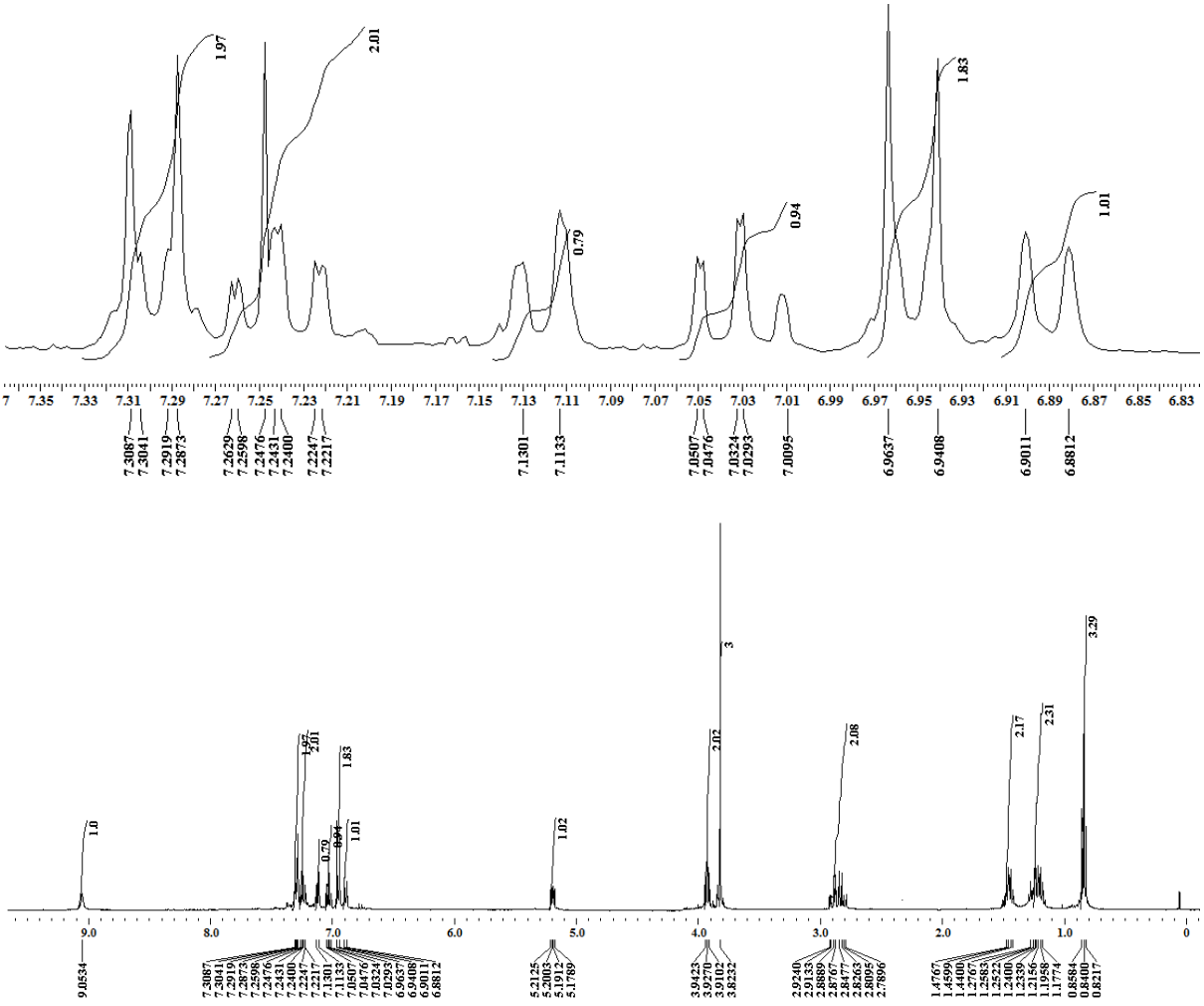
Butyl 2-(2-thioxo-3-(*p*-tolyl)-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (3g)



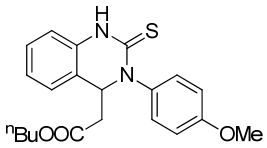
^{1}H NMR



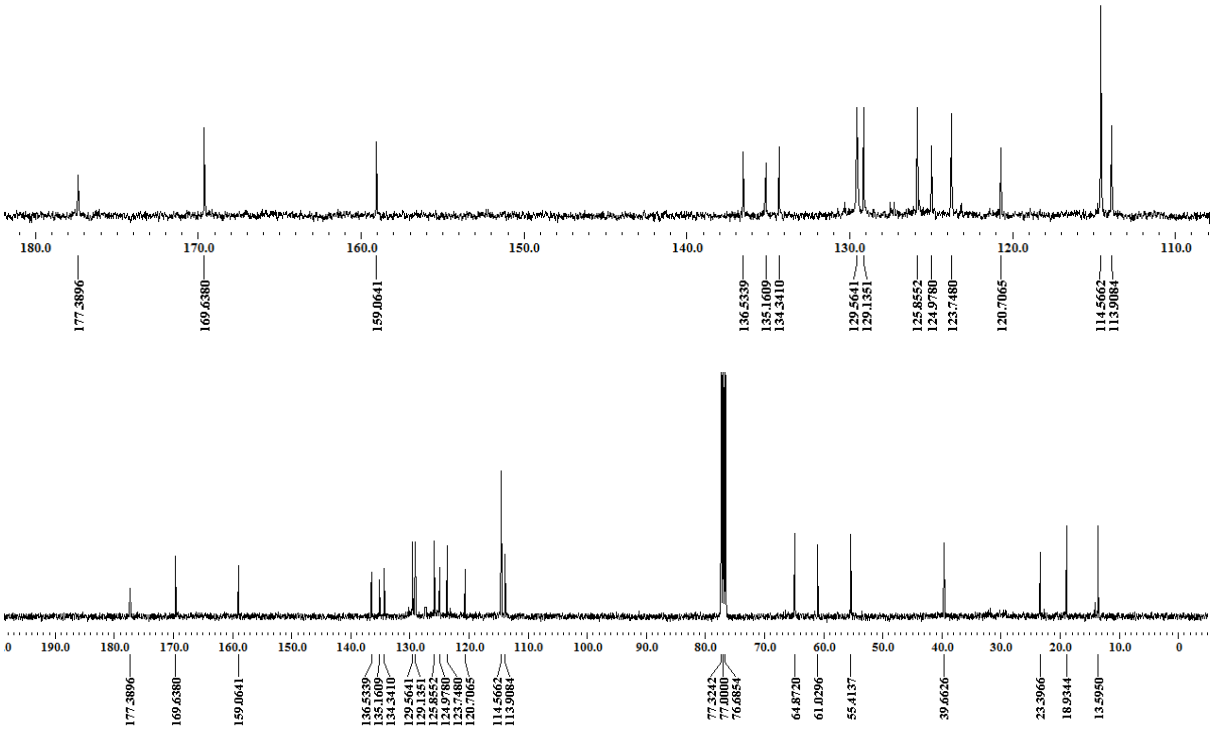
Butyl 2-(3-(4-methoxyphenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (3h)



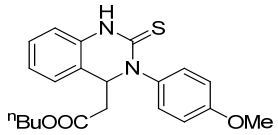
^{13}C NMR



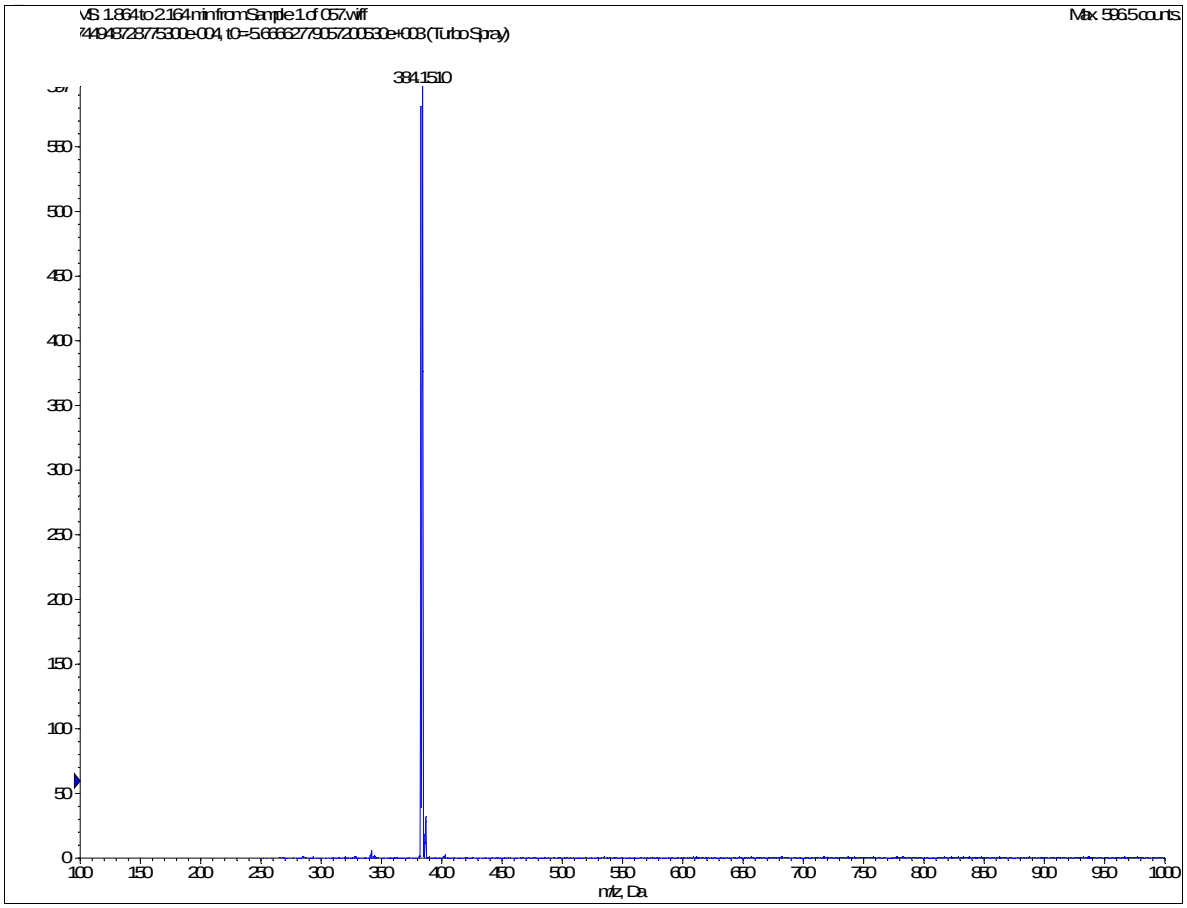
Butyl 2-(3-(4-methoxyphenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (3h)



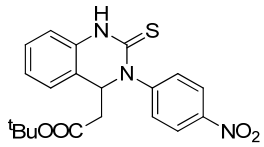
HRMS



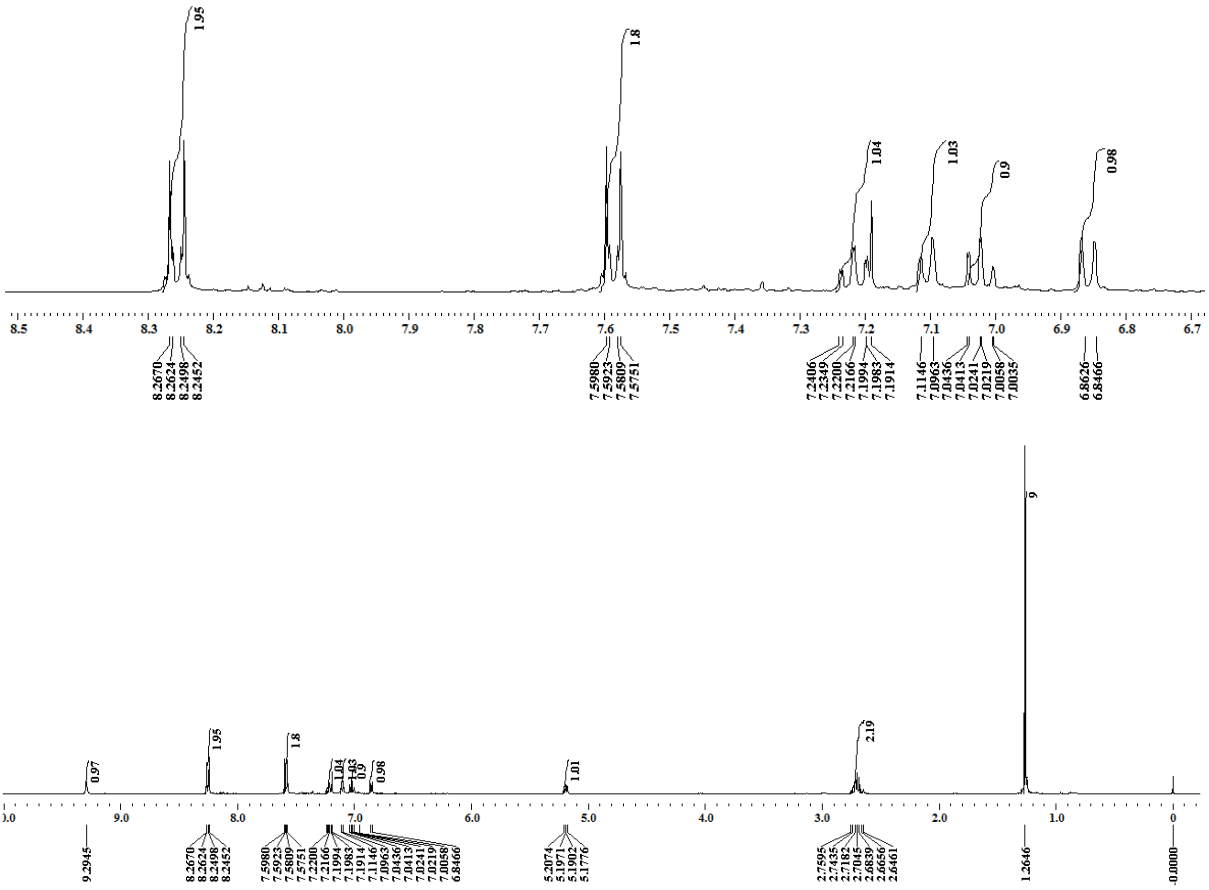
Butyl 2-(3-(4-methoxyphenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (3h)



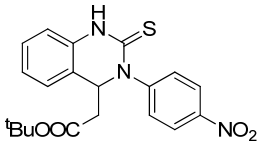
^{1}H NMR



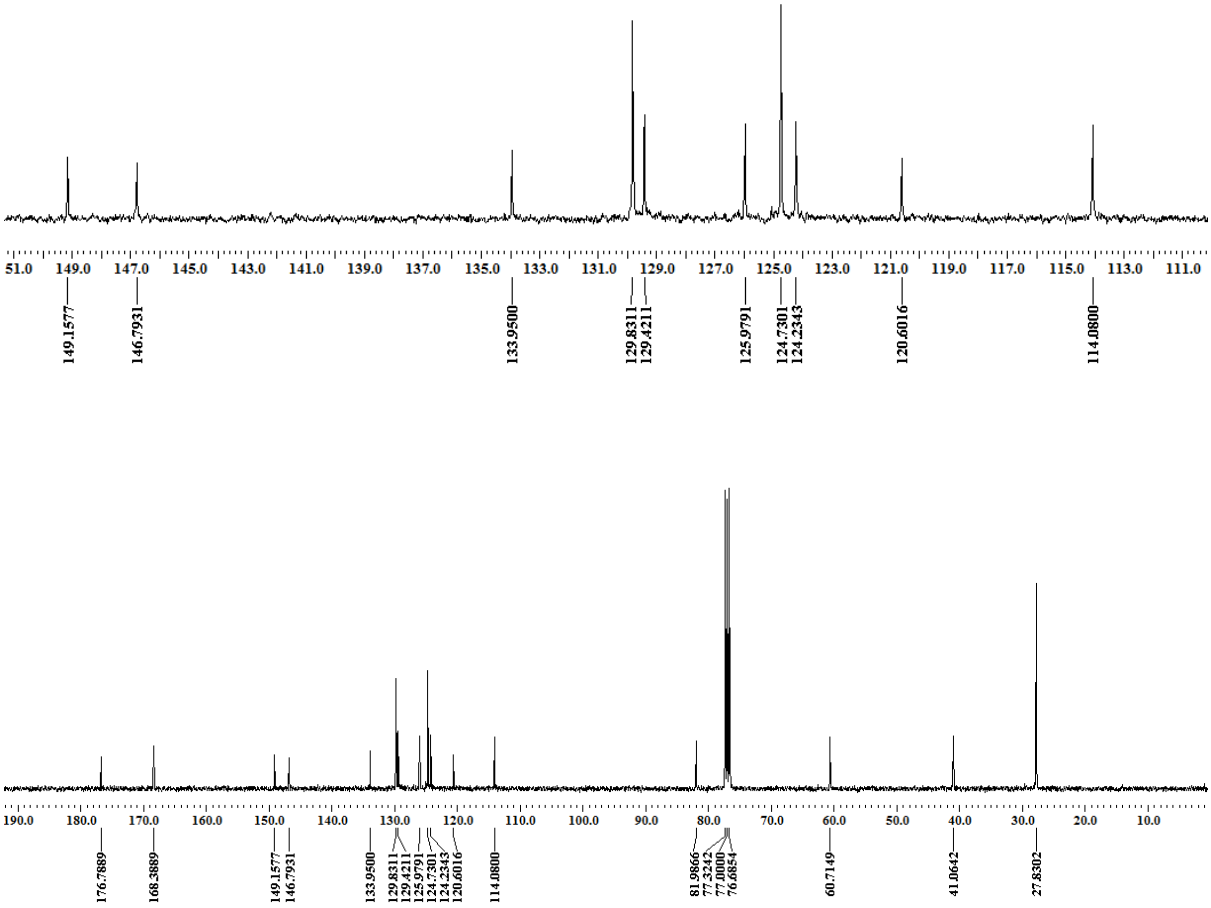
***tert*-Butyl 2-(3-(4-nitrophenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (3i)**



^{13}C NMR

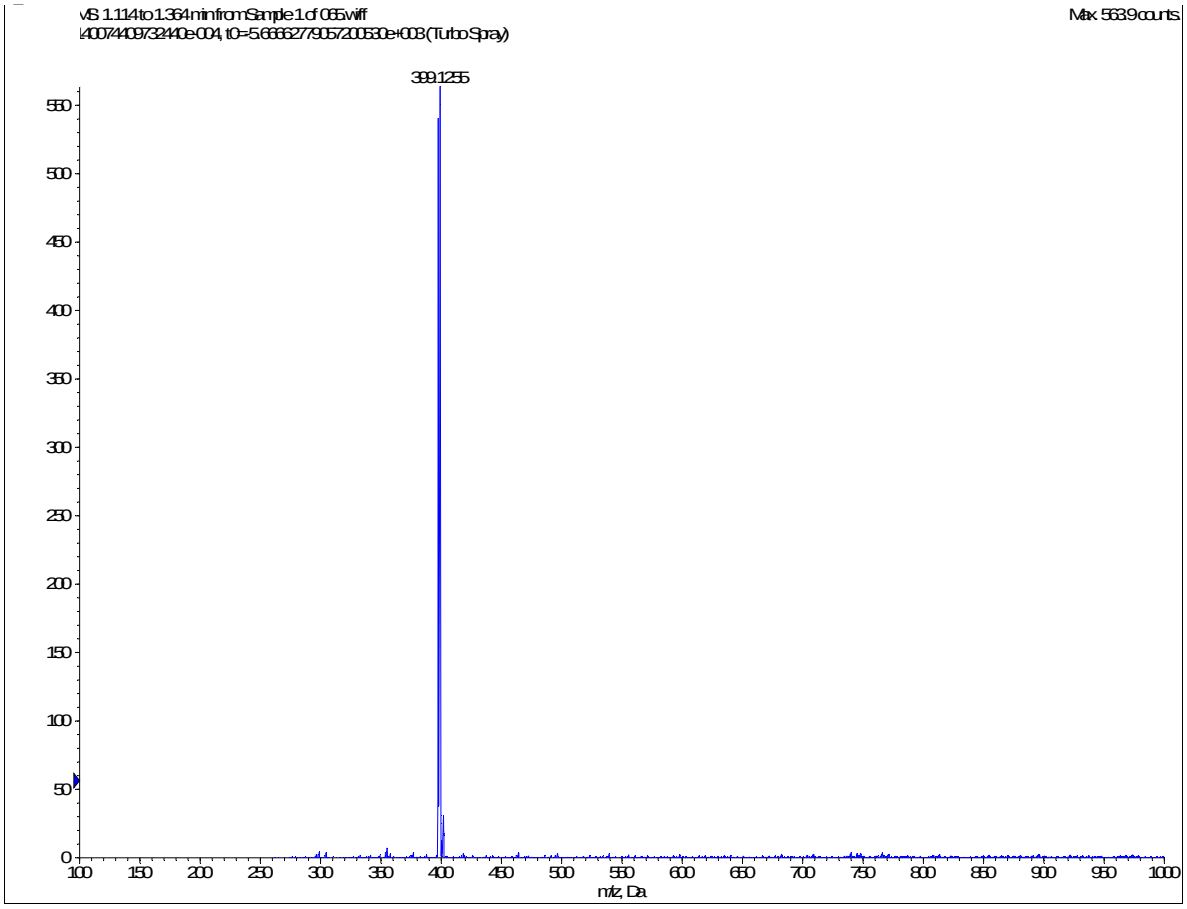


tert-Butyl 2-(3-(4-nitrophenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (3i)

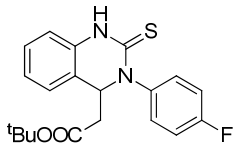


HRMS

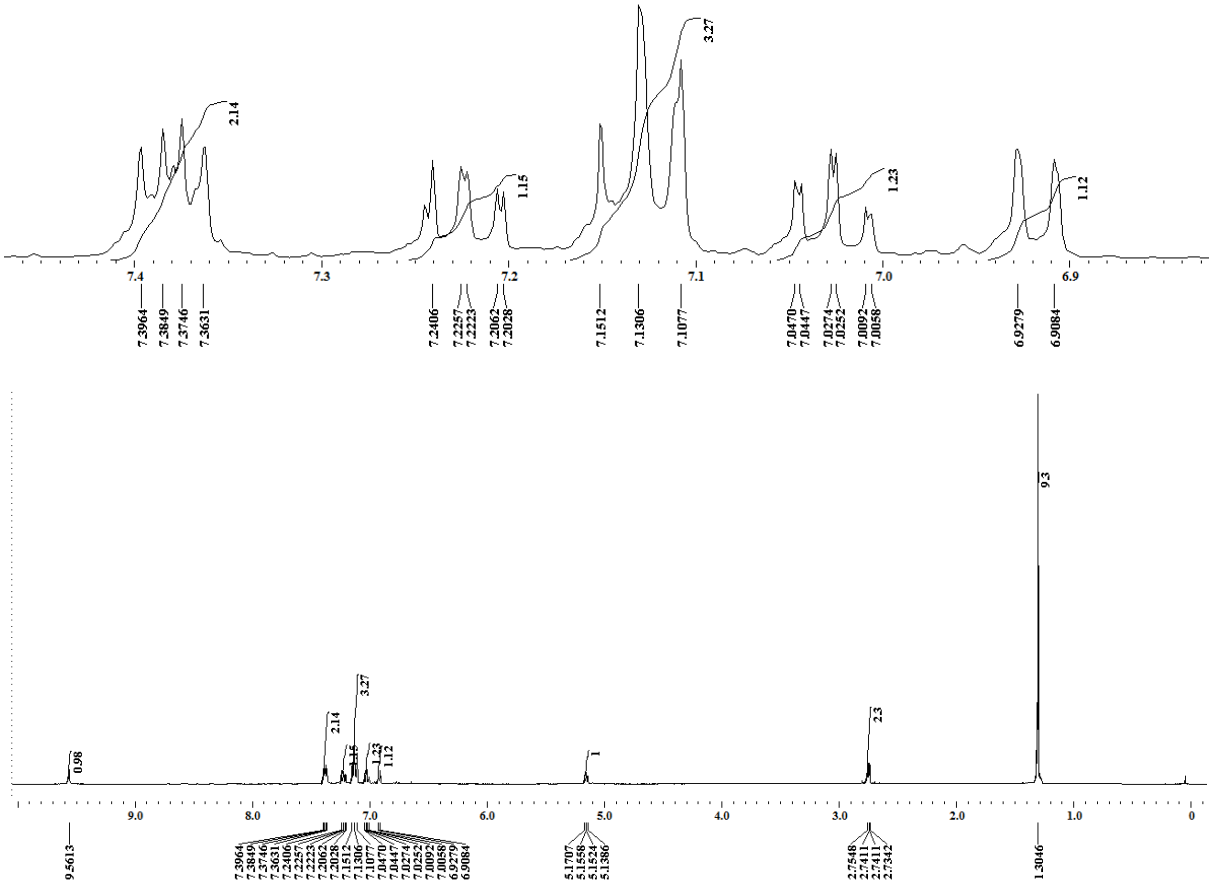
tert-butyl 2-(3-(4-nitrophenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (3i)



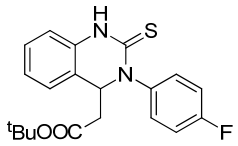
^{1}H NMR



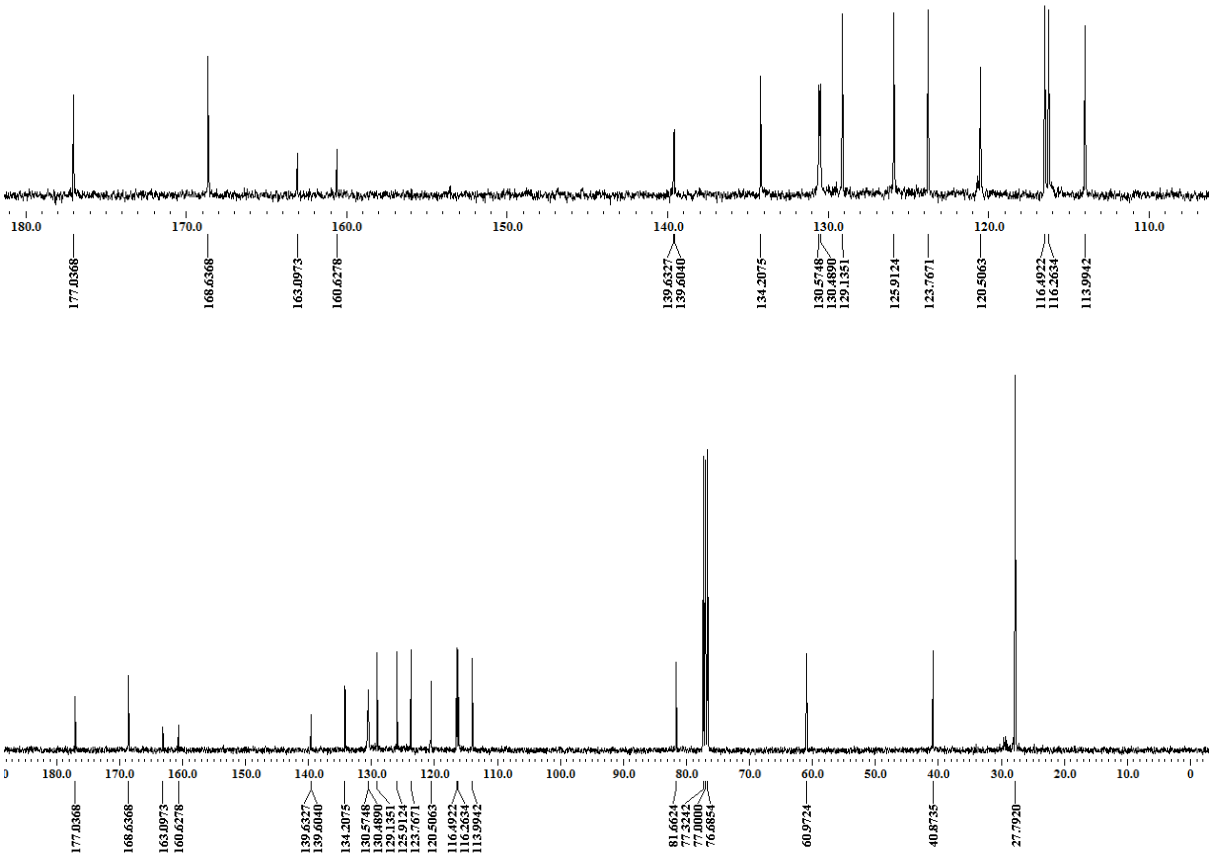
***tert*-butyl 2-(3-(4-fluorophenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (3j)**



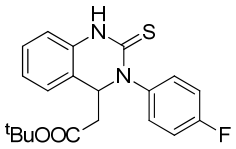
^{13}C NMR



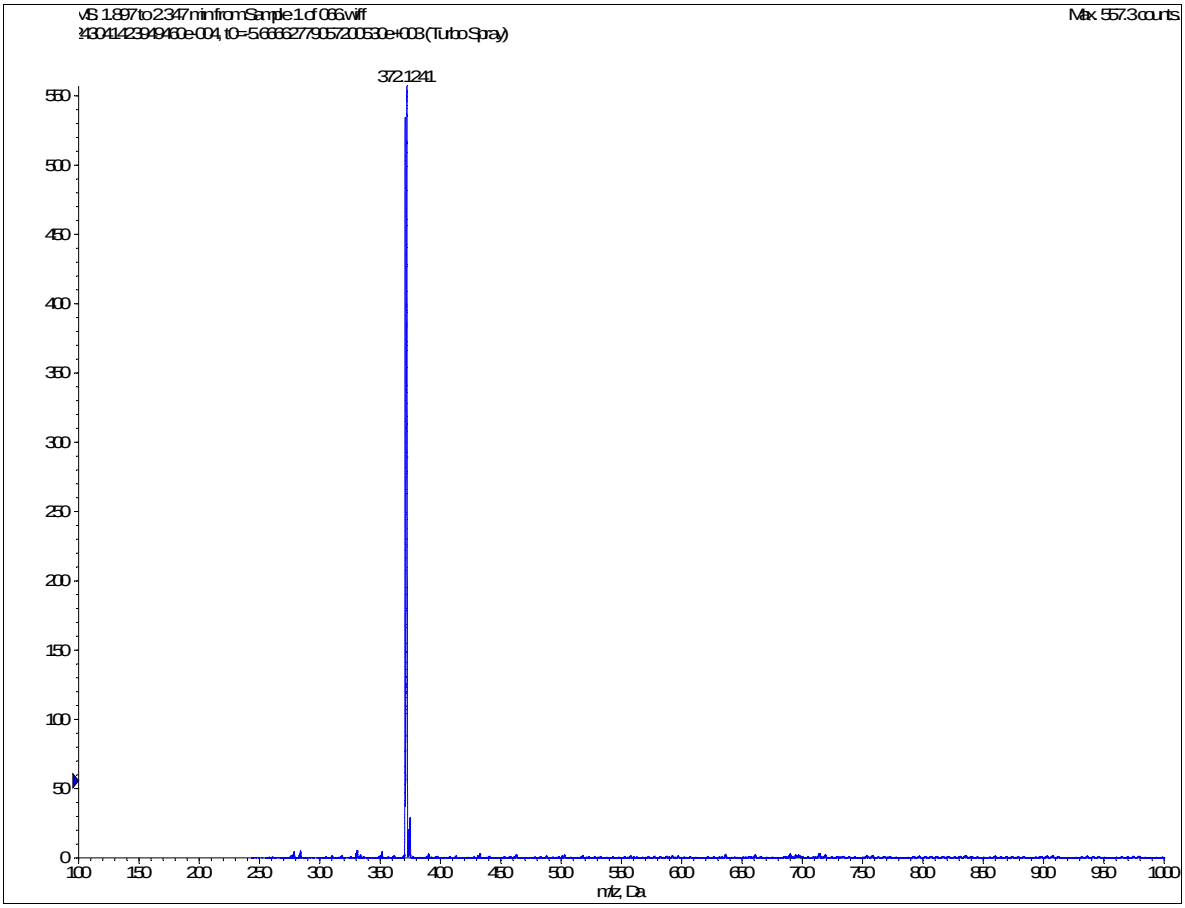
tert-butyl 2-(3-(4-fluorophenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (3j)



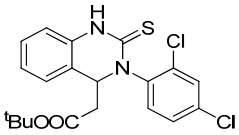
HRMS



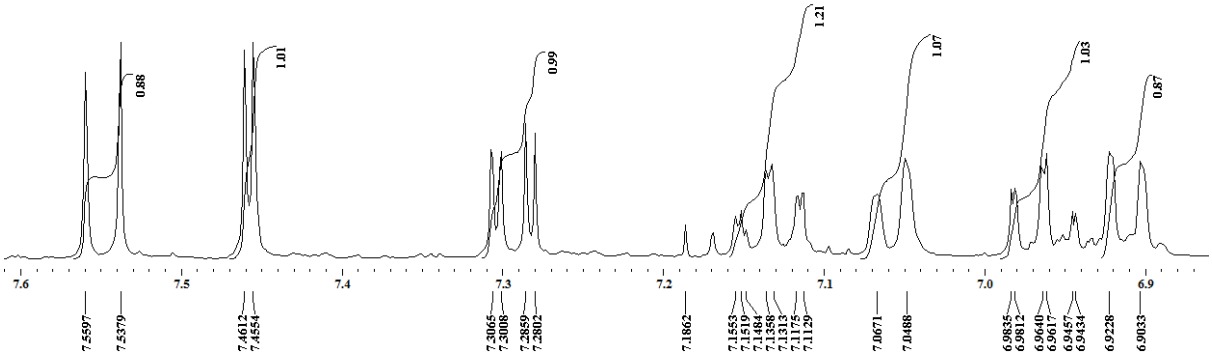
***tert*-butyl 2-(3-(4-fluorophenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (3j)**

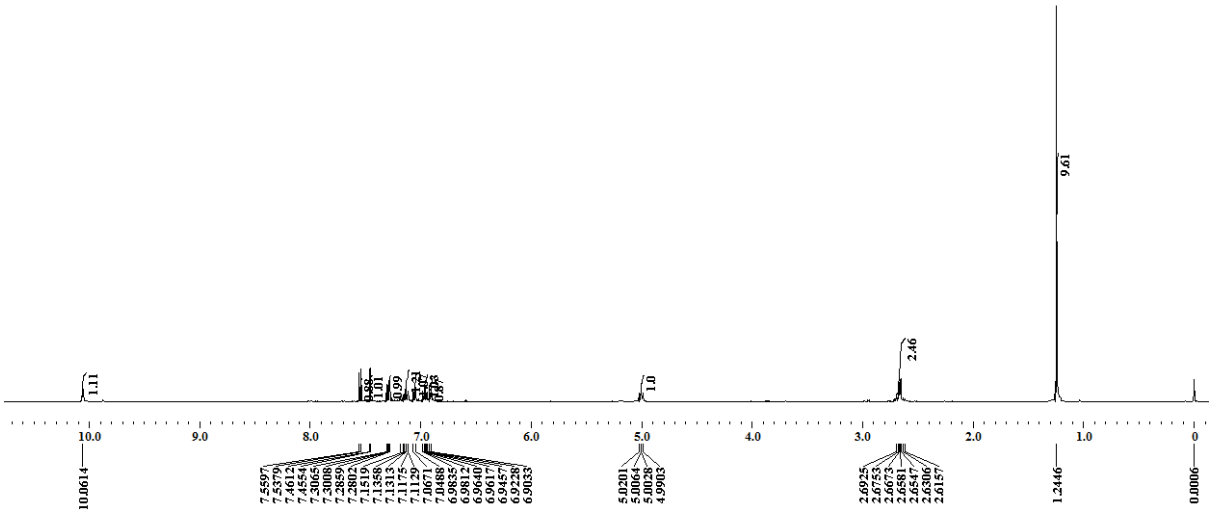


^{1}H NMR

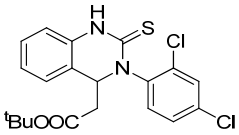


tert-butyl 2-(3-(2,4-dichlorophenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (3k)

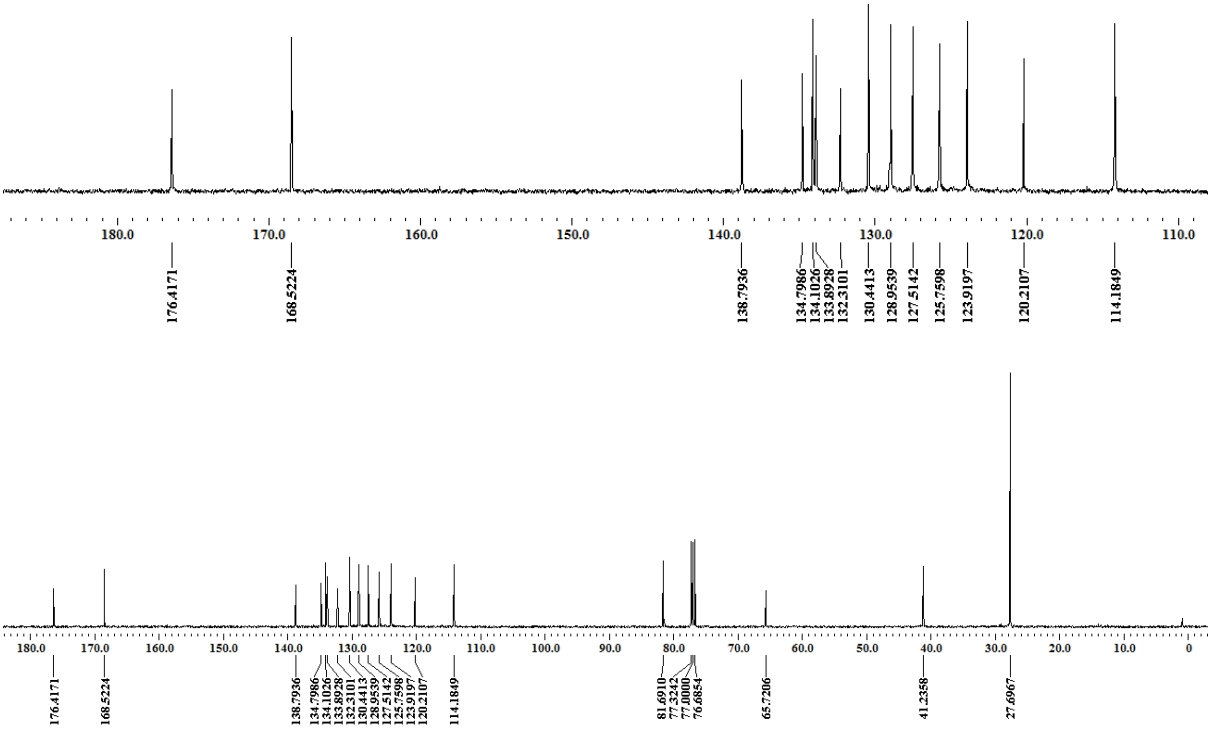




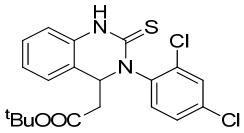
^{13}C NMR



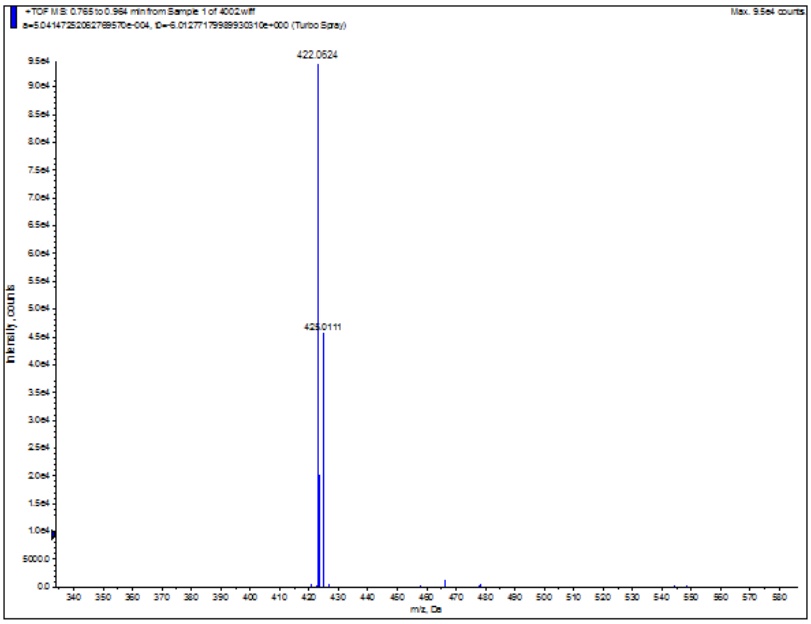
tert-butyl 2-(3-(2,4-dichlorophenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (3k)



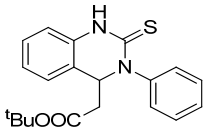
HRMS



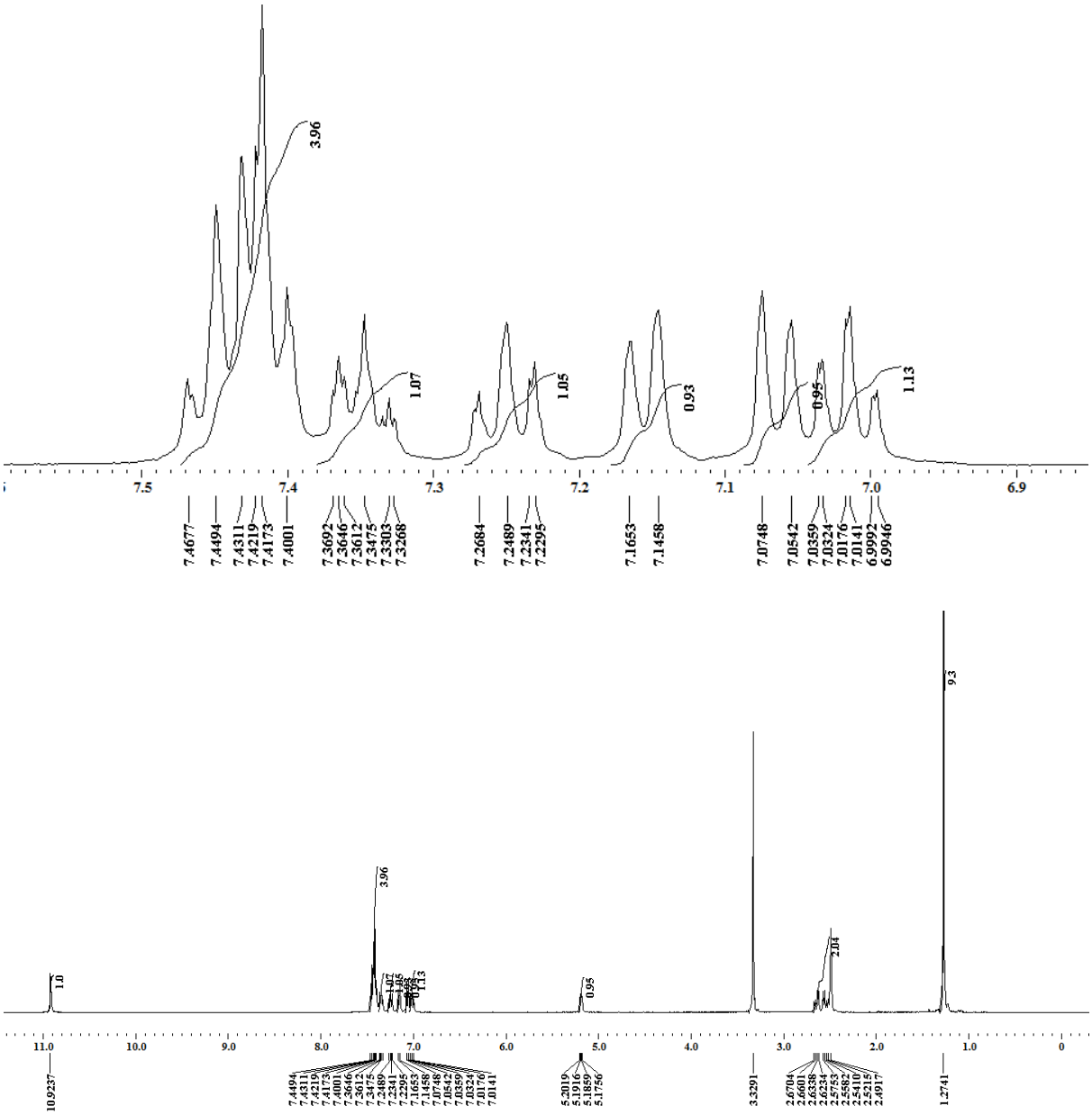
tert-butyl 2-(3-(2,4-dichlorophenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (3k)



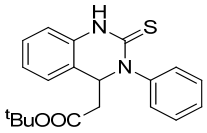
^{1}H NMR



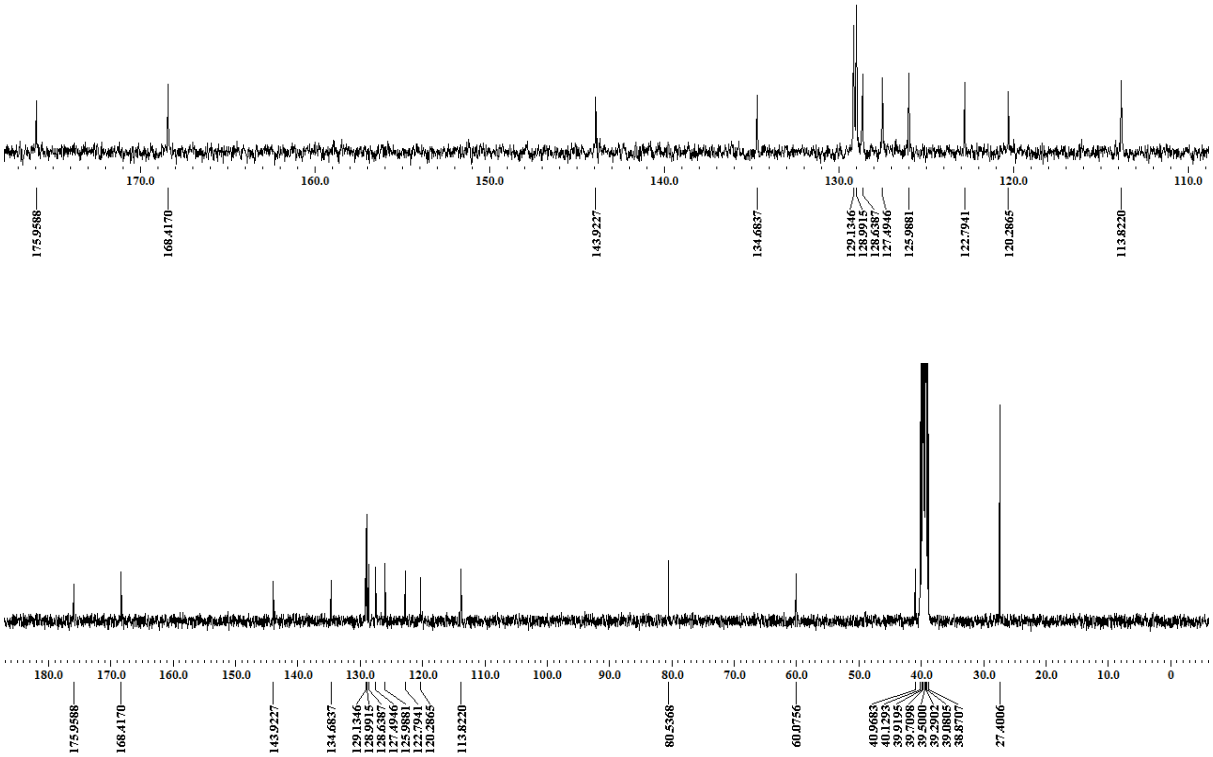
***tert*-butyl 2-(3-phenyl-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (3l)**



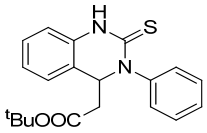
^{13}C NMR



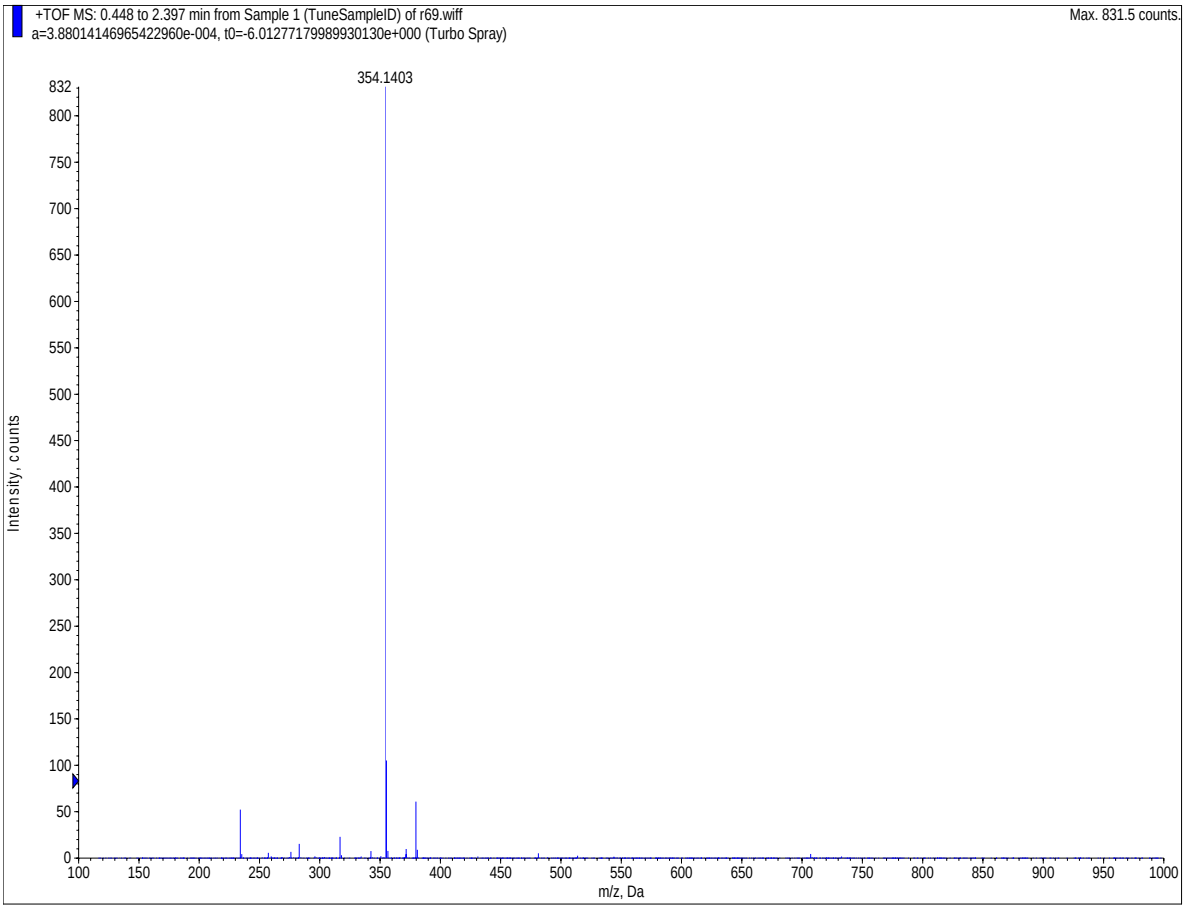
***tert*-butyl 2-(3-phenyl-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (3l)**



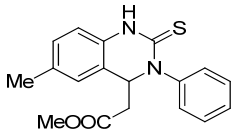
HRMS



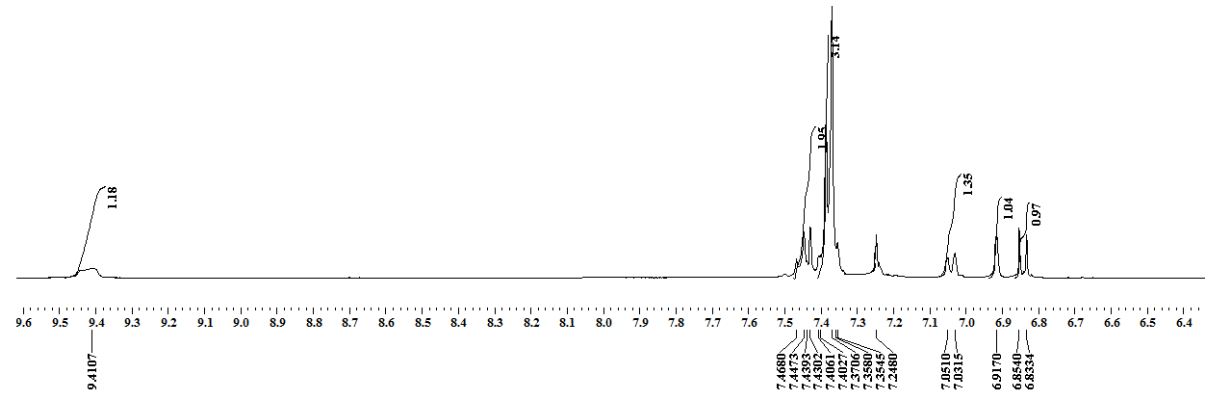
tert-butyl 2-(3-phenyl-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (3l)

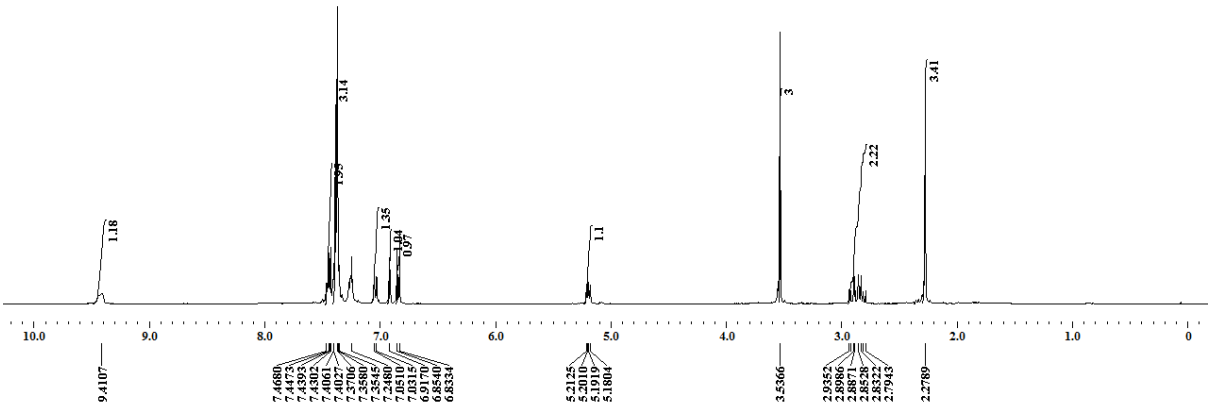


^{1}H NMR

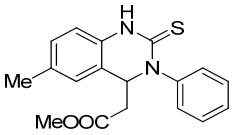


Methyl 2-(6-methyl-3-phenyl-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4a)

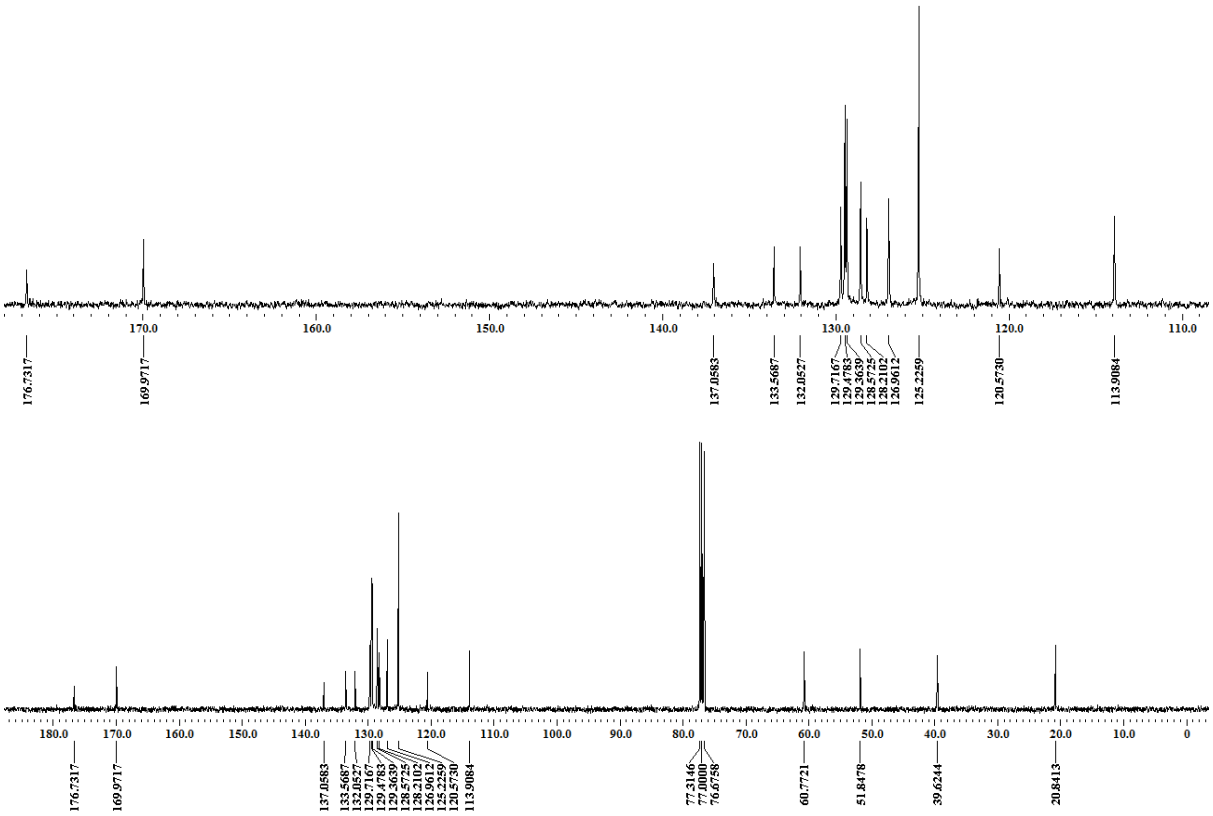




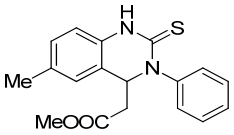
^{13}C NMR



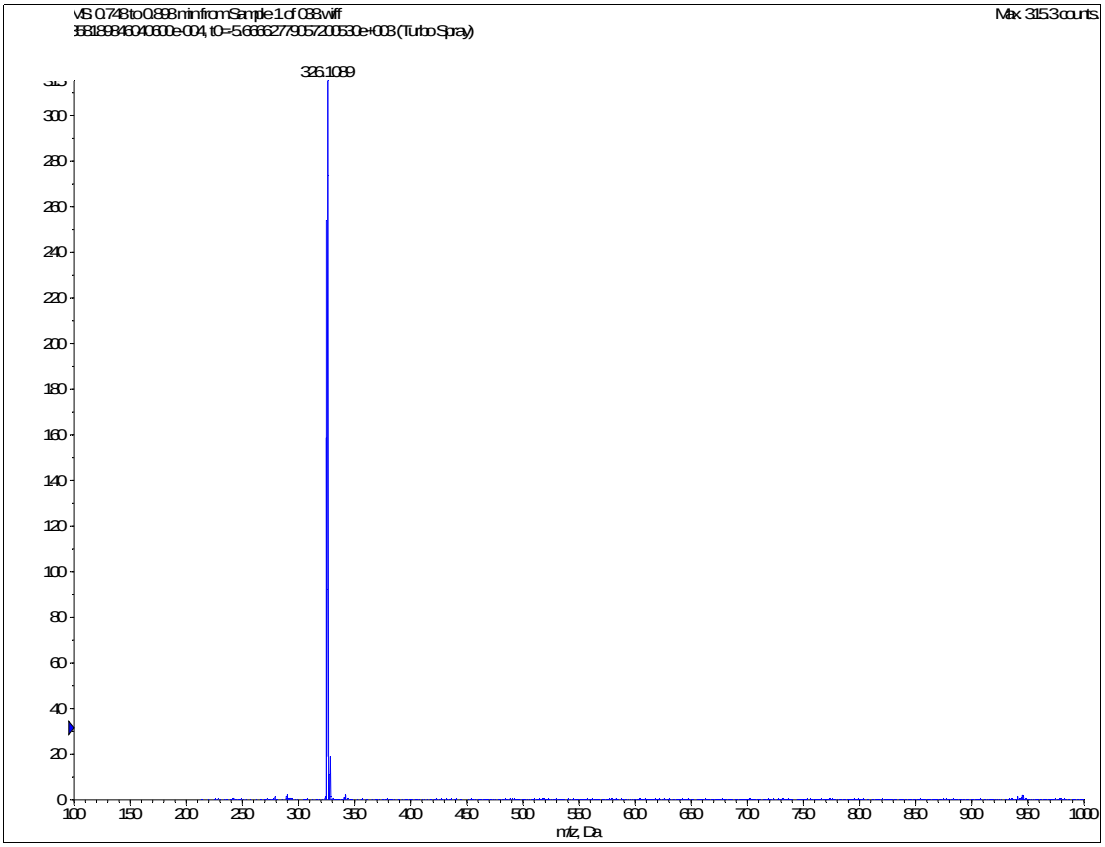
Methyl 2-(6-methyl-3-phenyl-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4a)



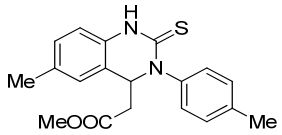
HRMS



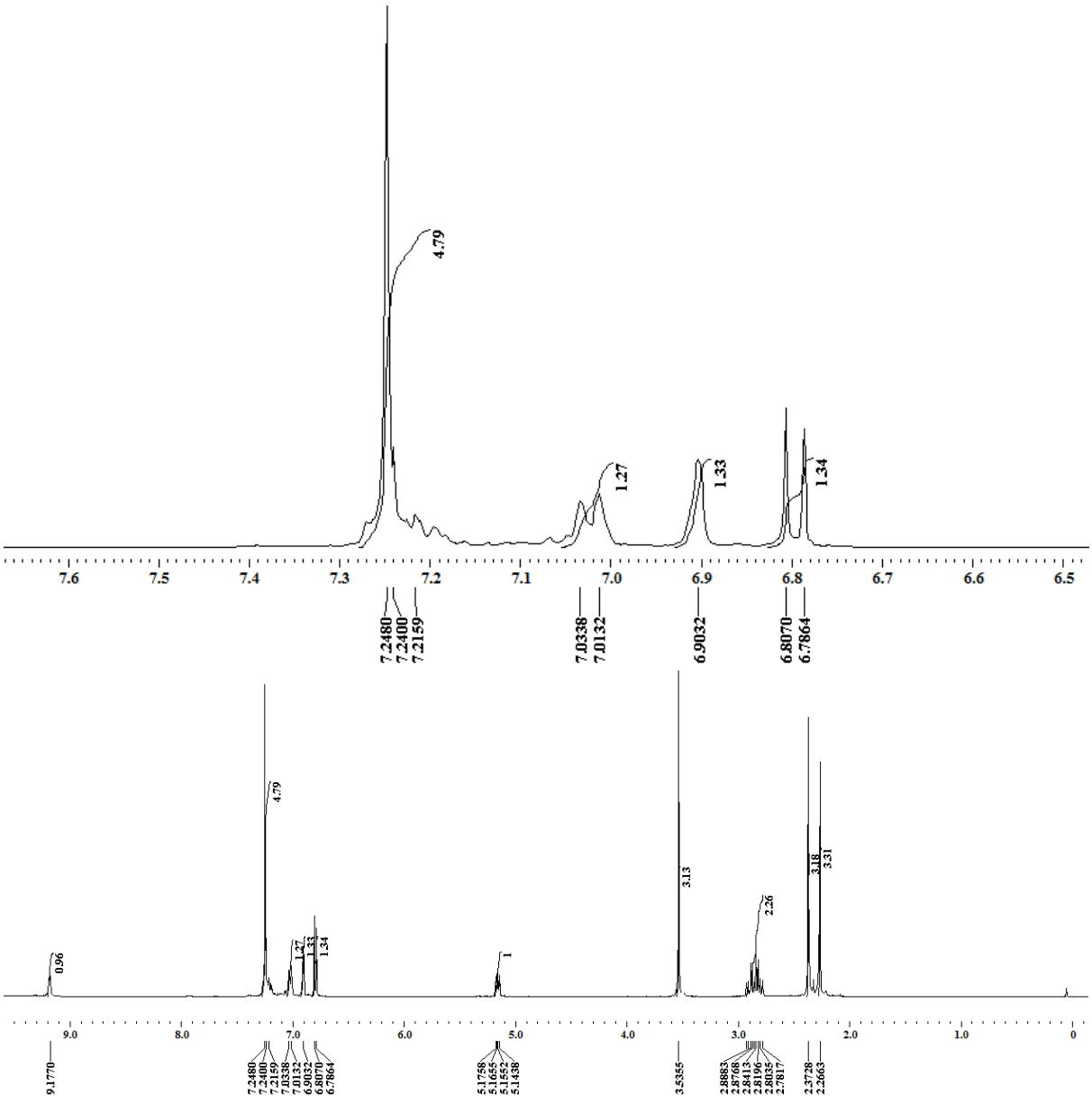
Methyl 2-(6-methyl-3-phenyl-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4a)



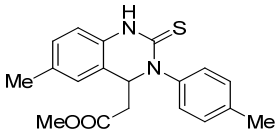
^{1}H NMR



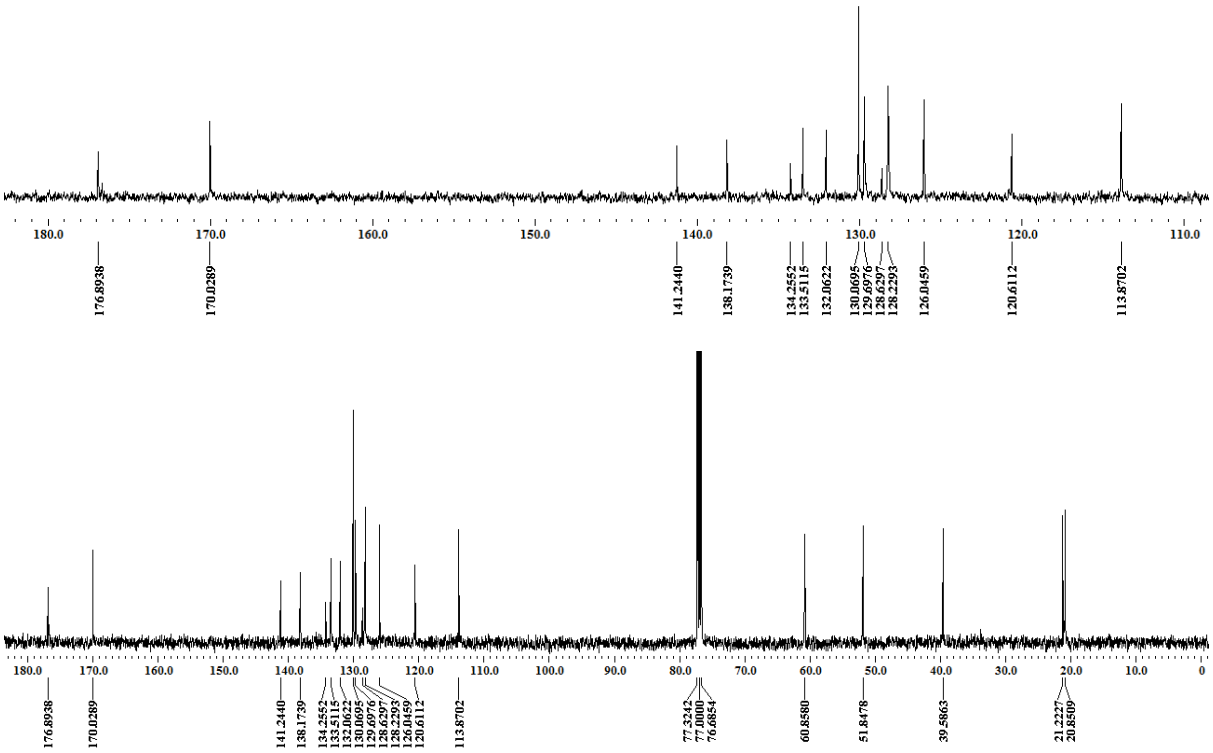
Methyl 2-(6-methyl-2-thioxo-3-(p-tolyl)-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4b)



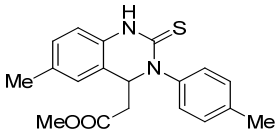
^{13}C NMR



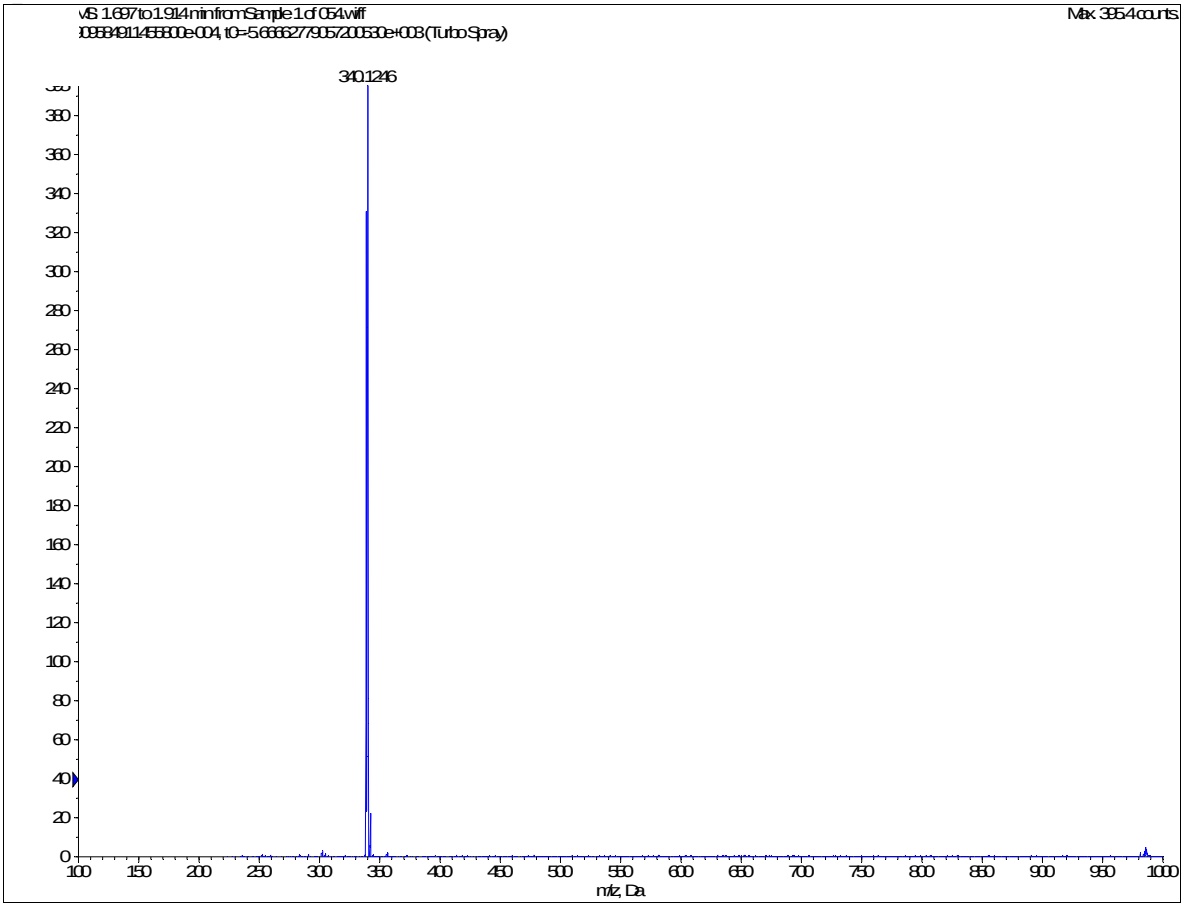
Methyl 2-(6-methyl-2-thioxo-3-(p-tolyl)-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4b)



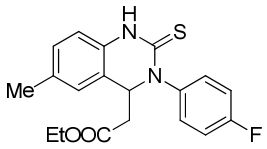
HRMS



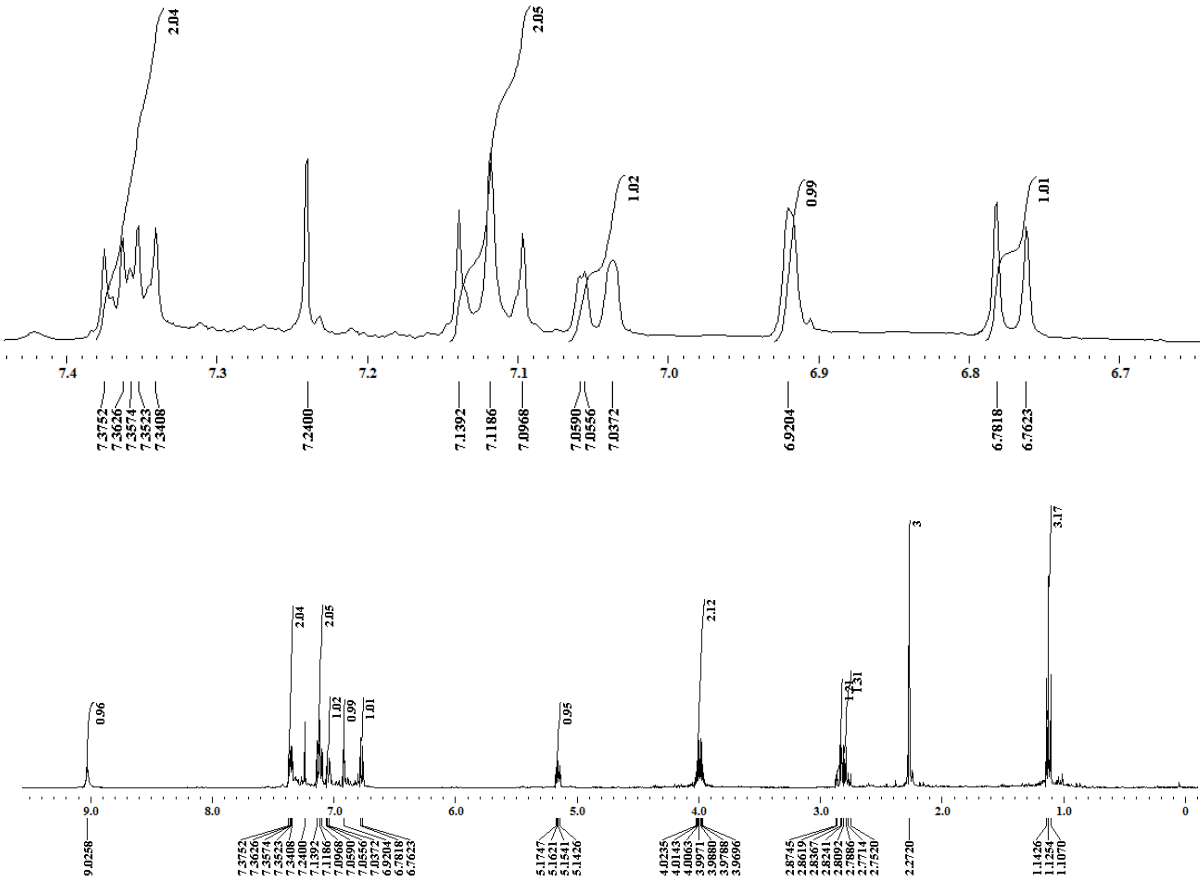
Methyl 2-(6-methyl-2-thioxo-3-(p-tolyl)-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4b)



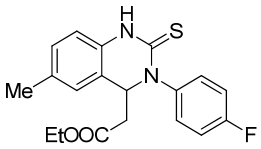
^{1}H NMR



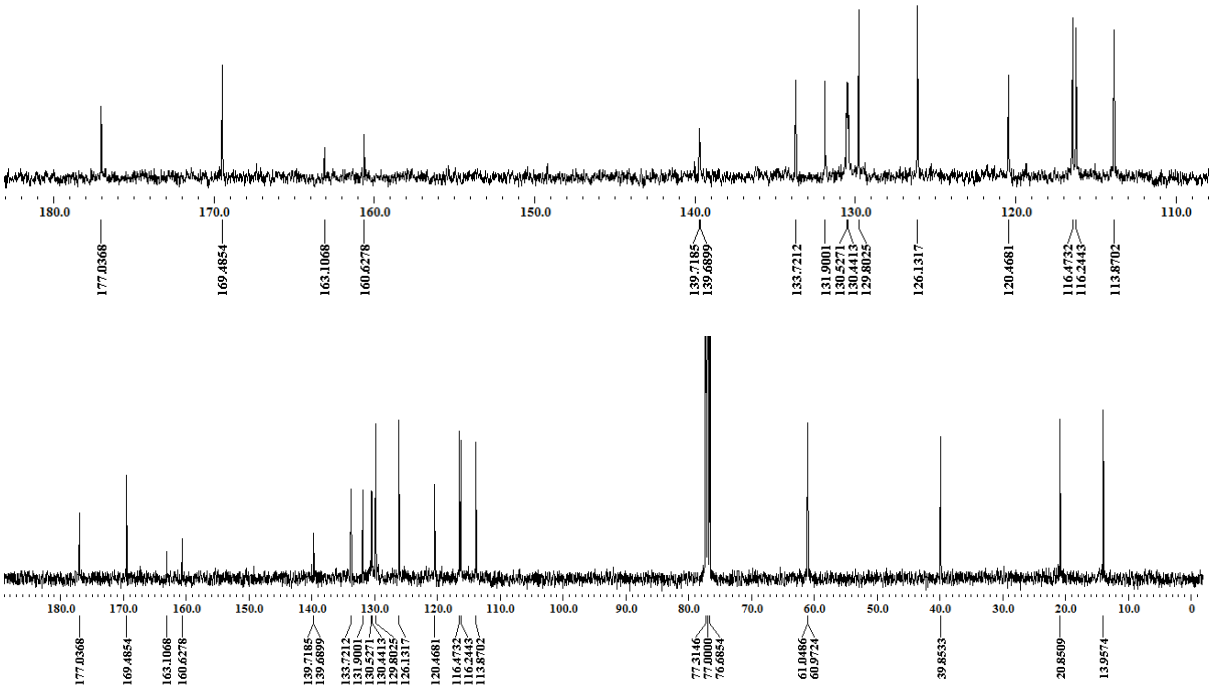
Ethyl 2-(3-(4-fluorophenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4c)



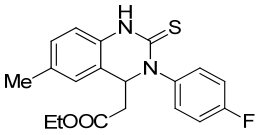
^{13}C NMR



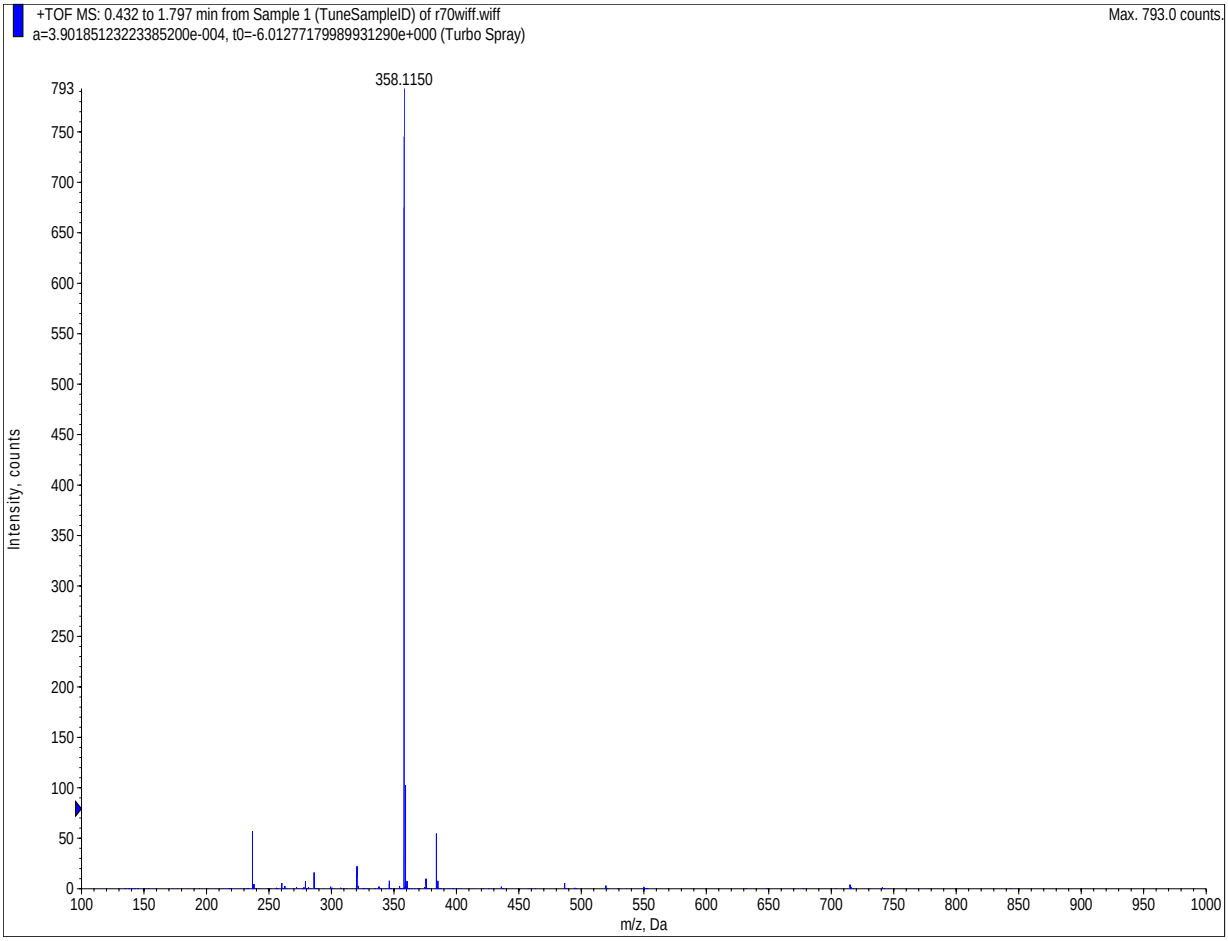
Ethyl 2-(3-(4-fluorophenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4c)



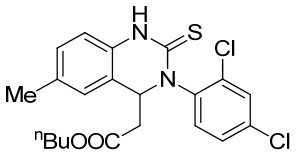
HRMS



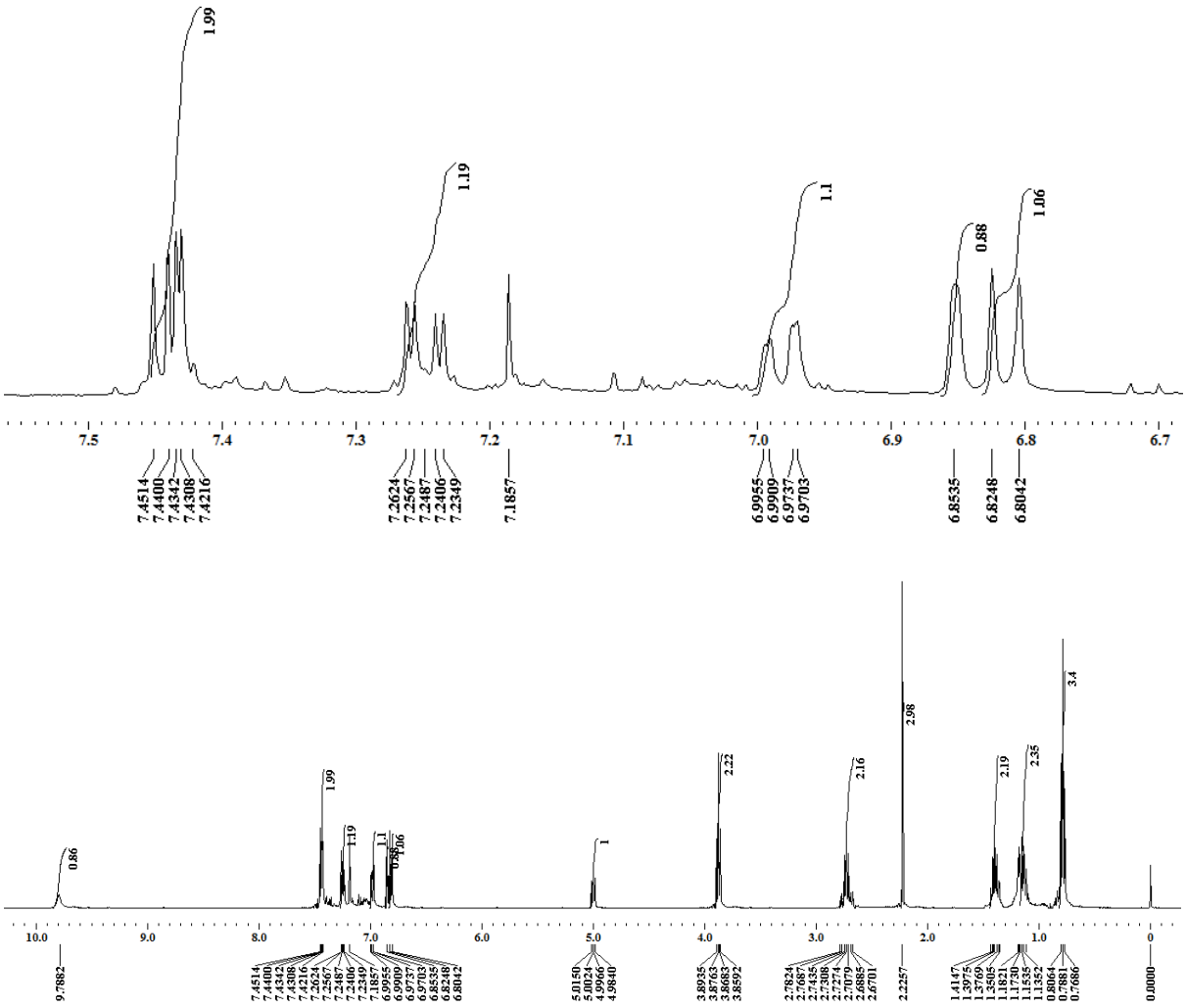
Ethyl 2-(3-(4-fluorophenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4c)



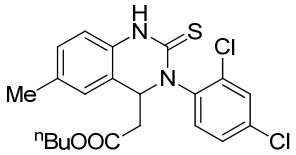
^{1}H NMR



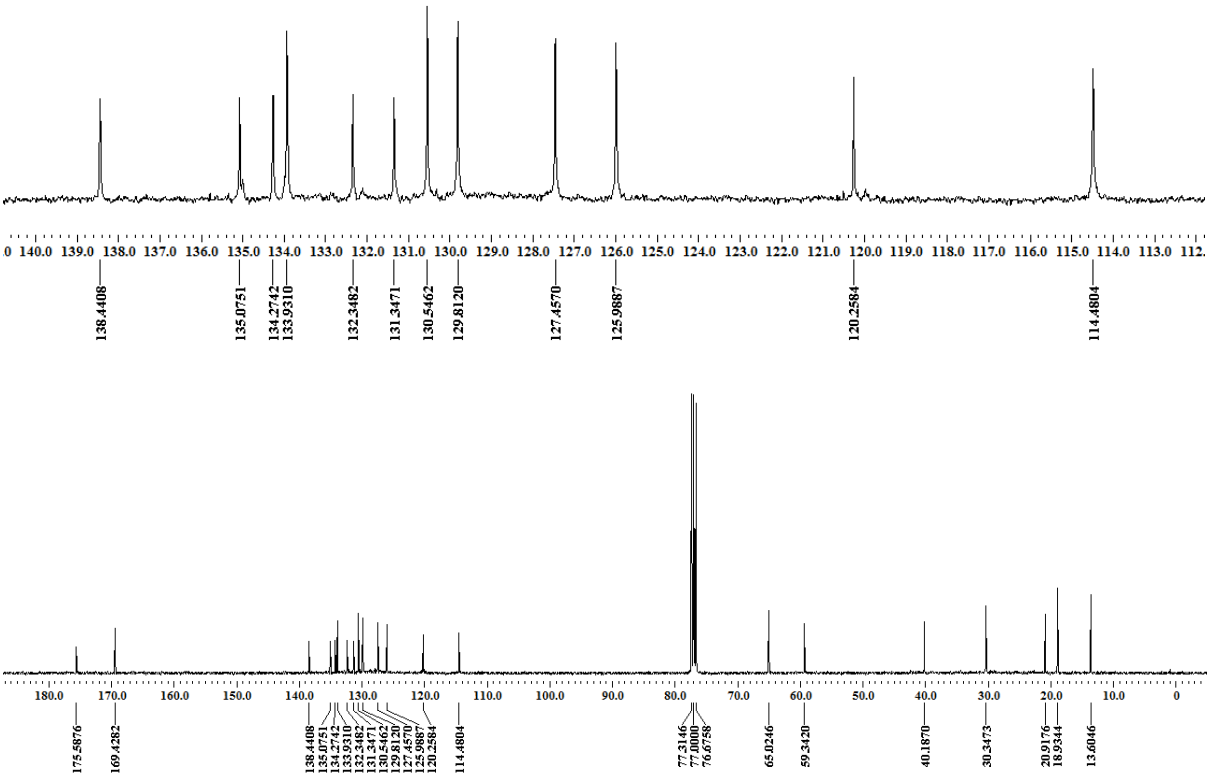
Butyl 2-(3-(2,4-dichlorophenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4d)



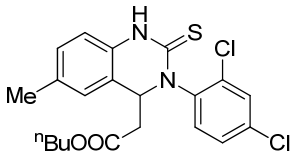
^{13}C NMR



Butyl 2-(3-(2,4-dichlorophenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4d)



HRMS



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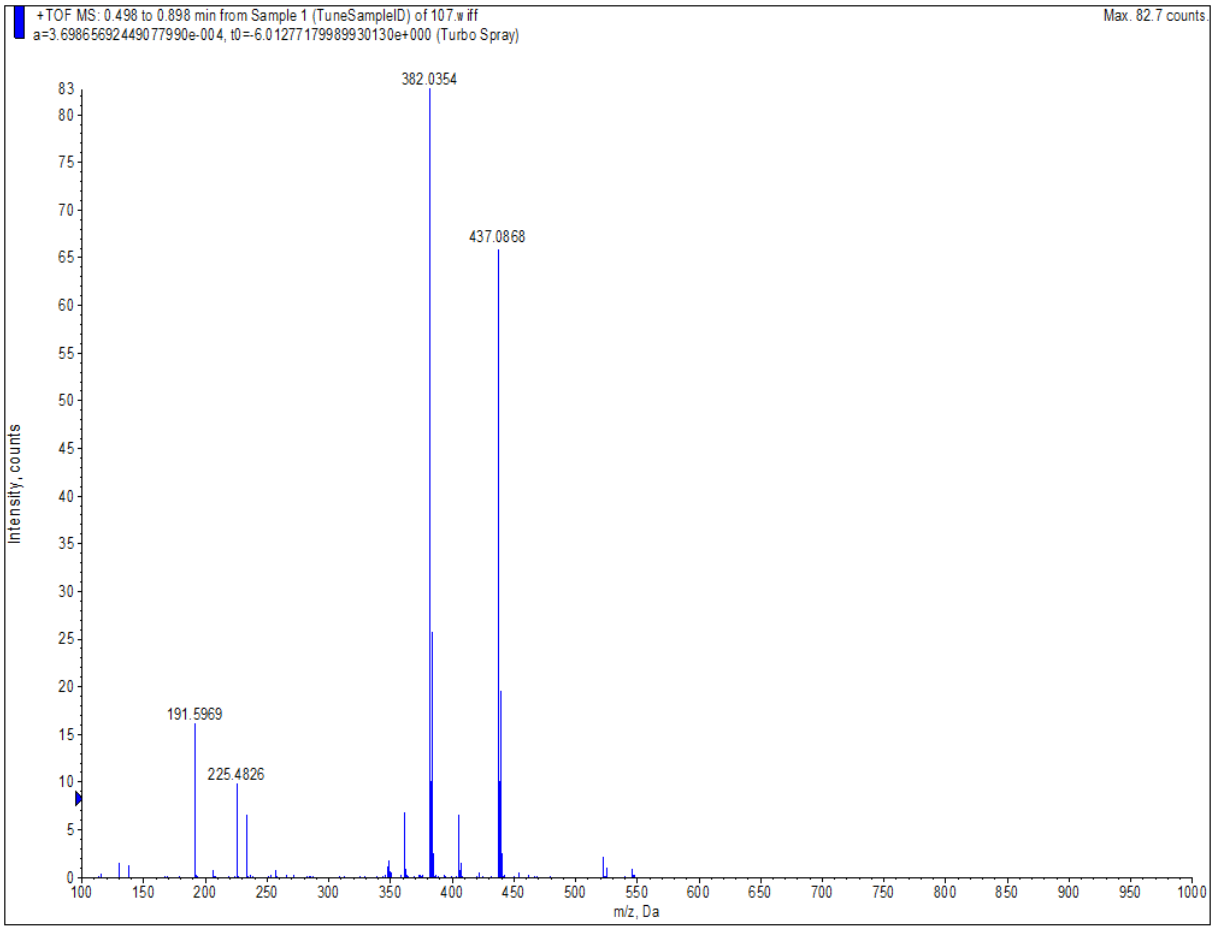
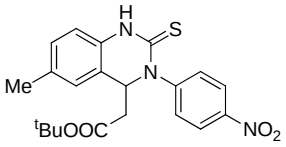
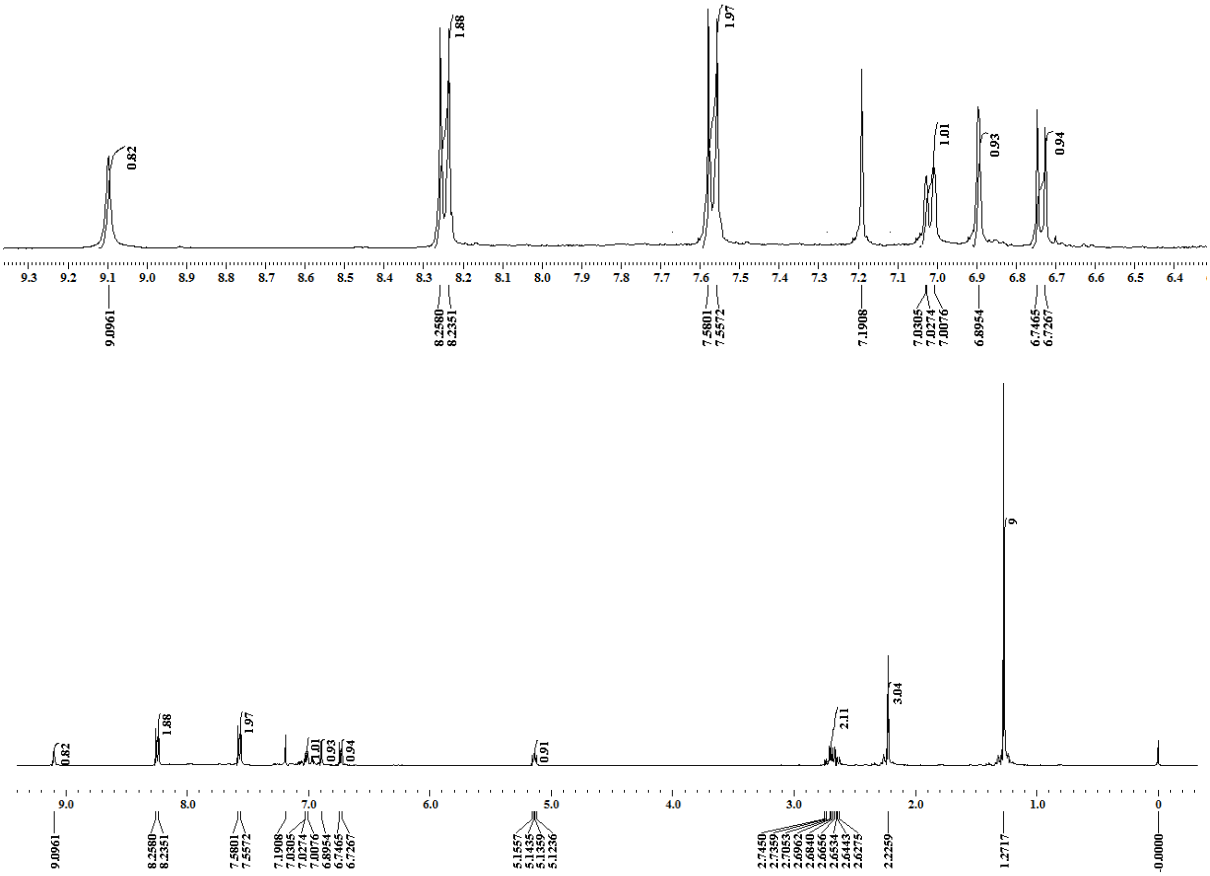


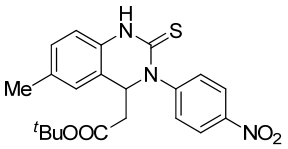
^{1}H NMR



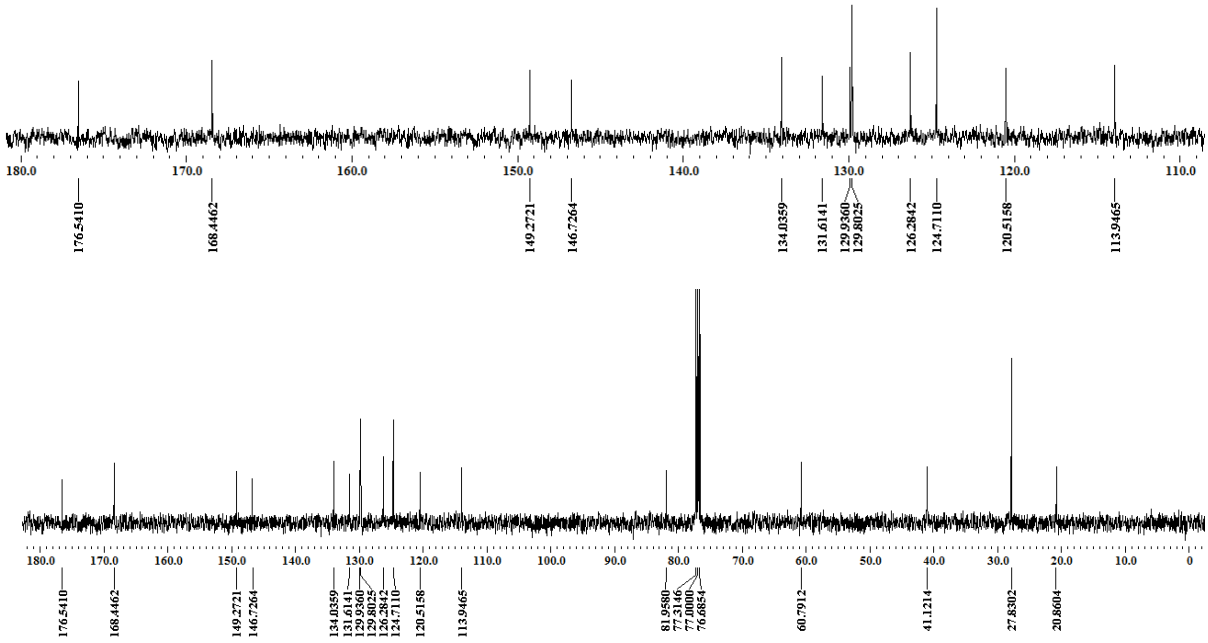
tert-Butyl 2-(6-methyl-3-(4-nitrophenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4e)



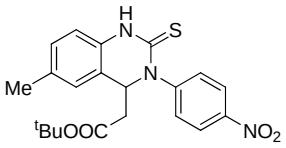
^{13}C NMR



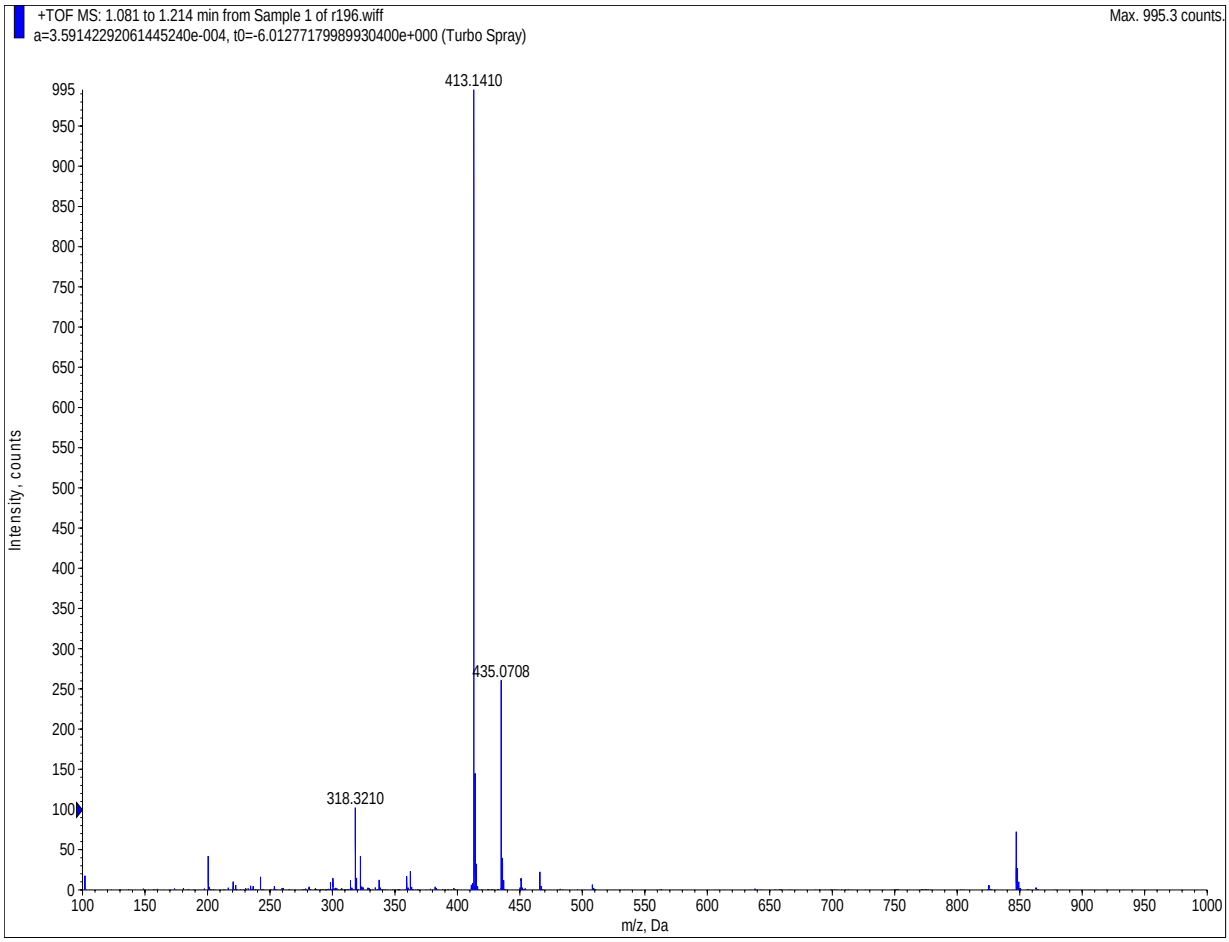
tert-Butyl 2-(6-methyl-3-(4-nitrophenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4e)



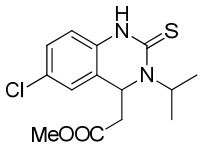
HRMS



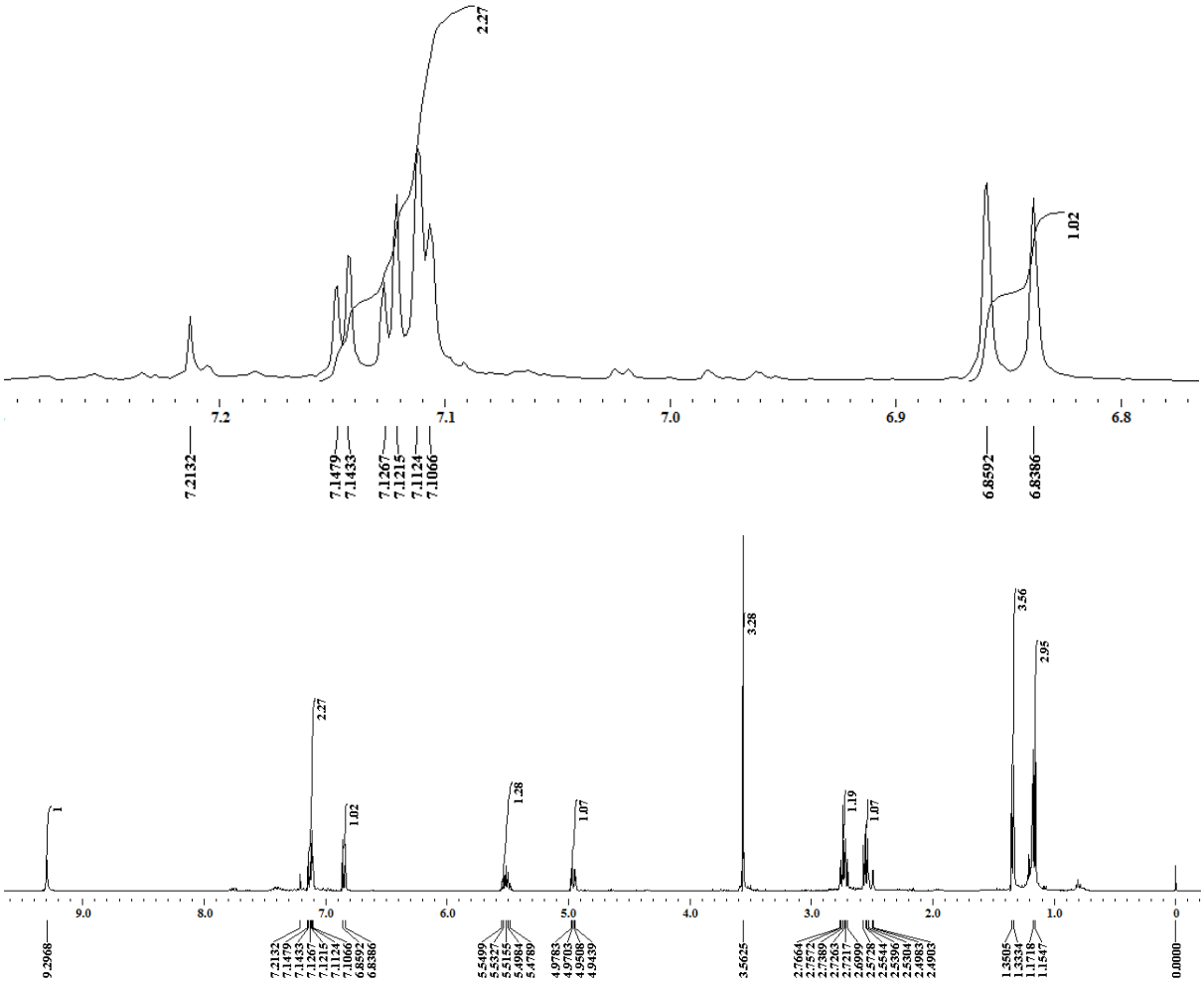
tert-Butyl 2-(6-methyl-3-(4-nitrophenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4e)



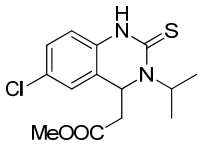
^{1}H NMR



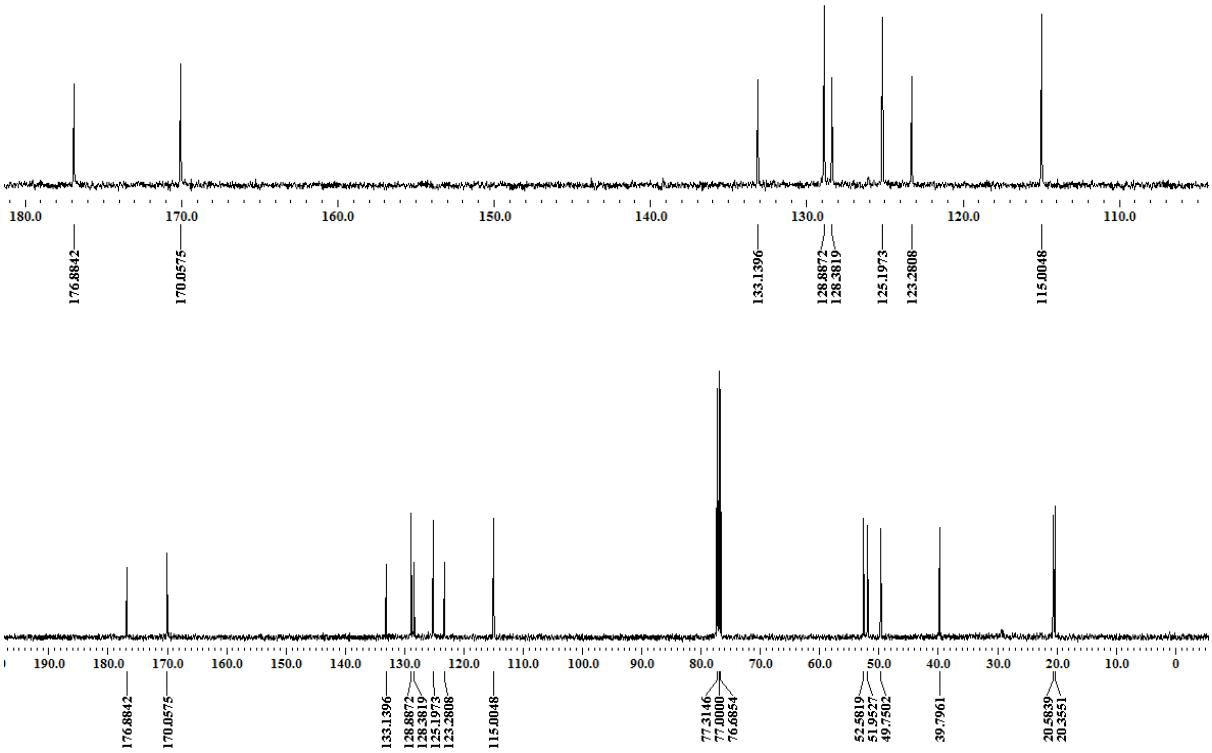
Methyl 2-(6-chloro-3-isopropyl-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4f)



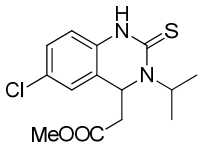
^{13}C NMR



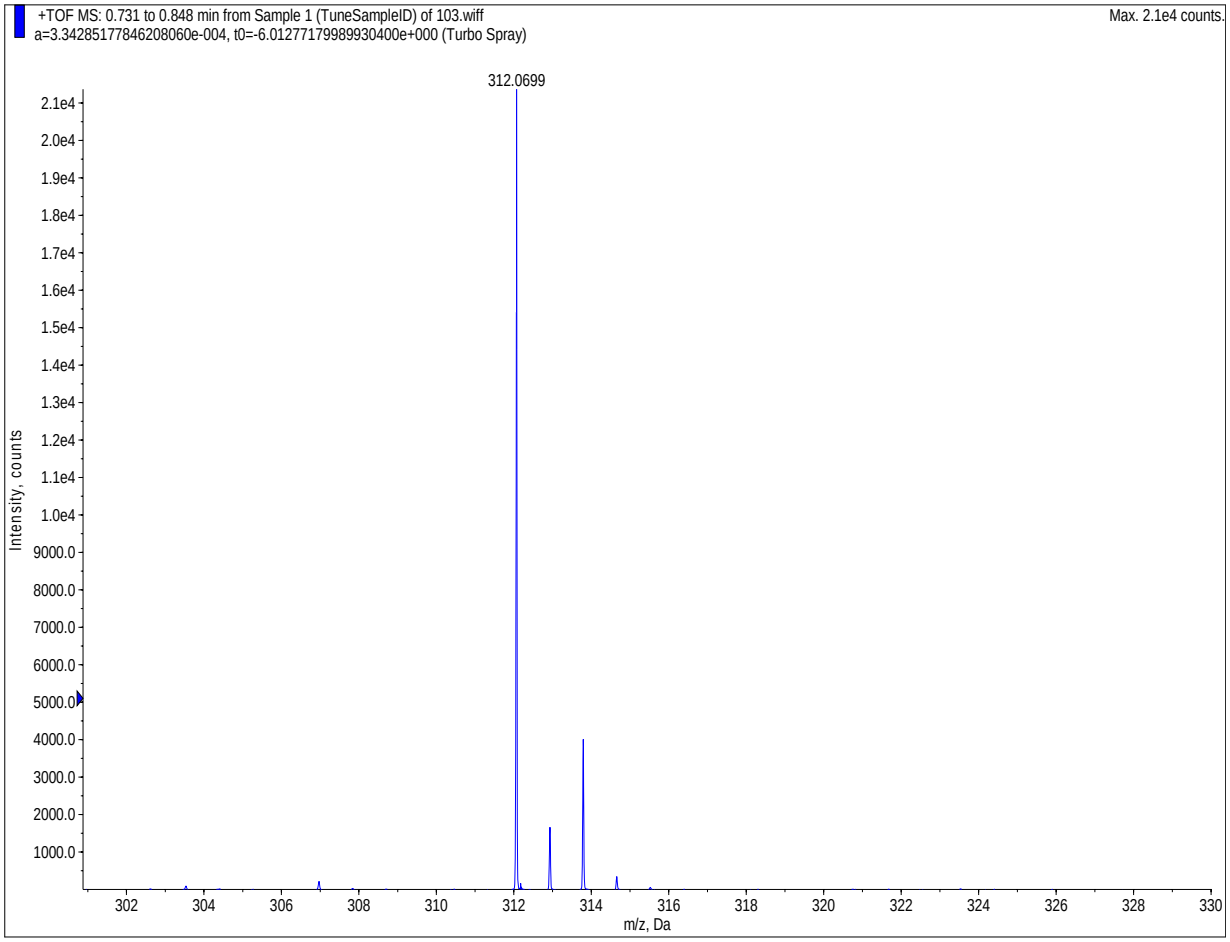
Methyl 2-(6-chloro-3-isopropyl-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4f)



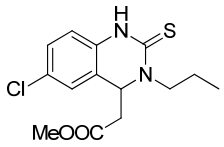
HRMS



Methyl 2-(6-chloro-3-isopropyl-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4f)



^{1}H NMR



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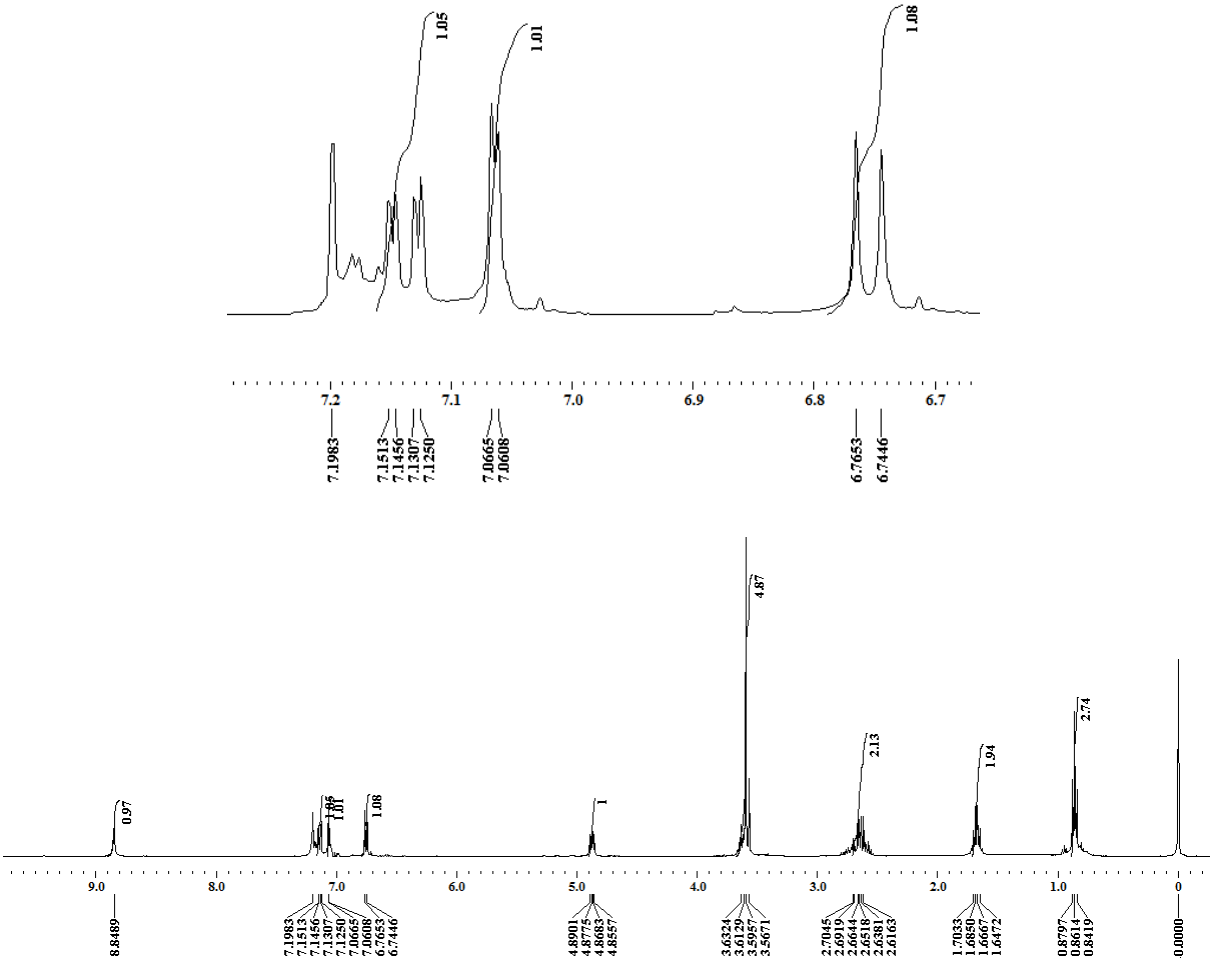
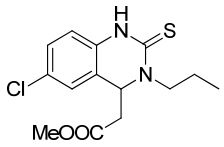
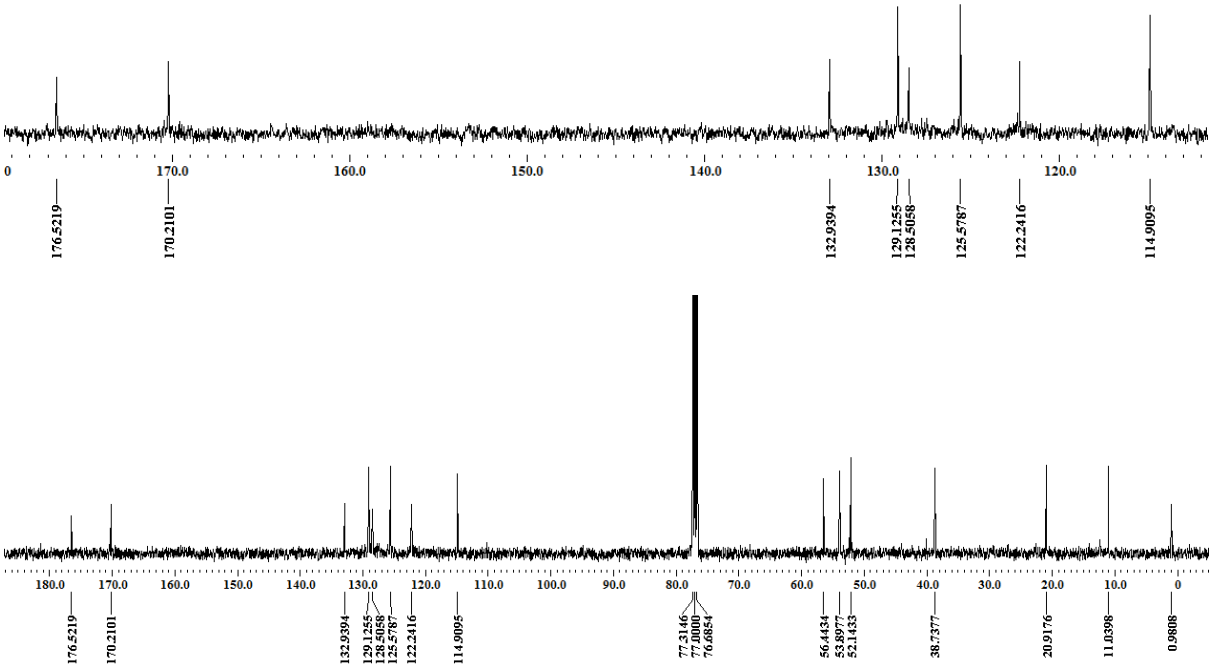


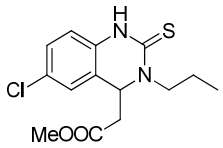
^{13}C NMR



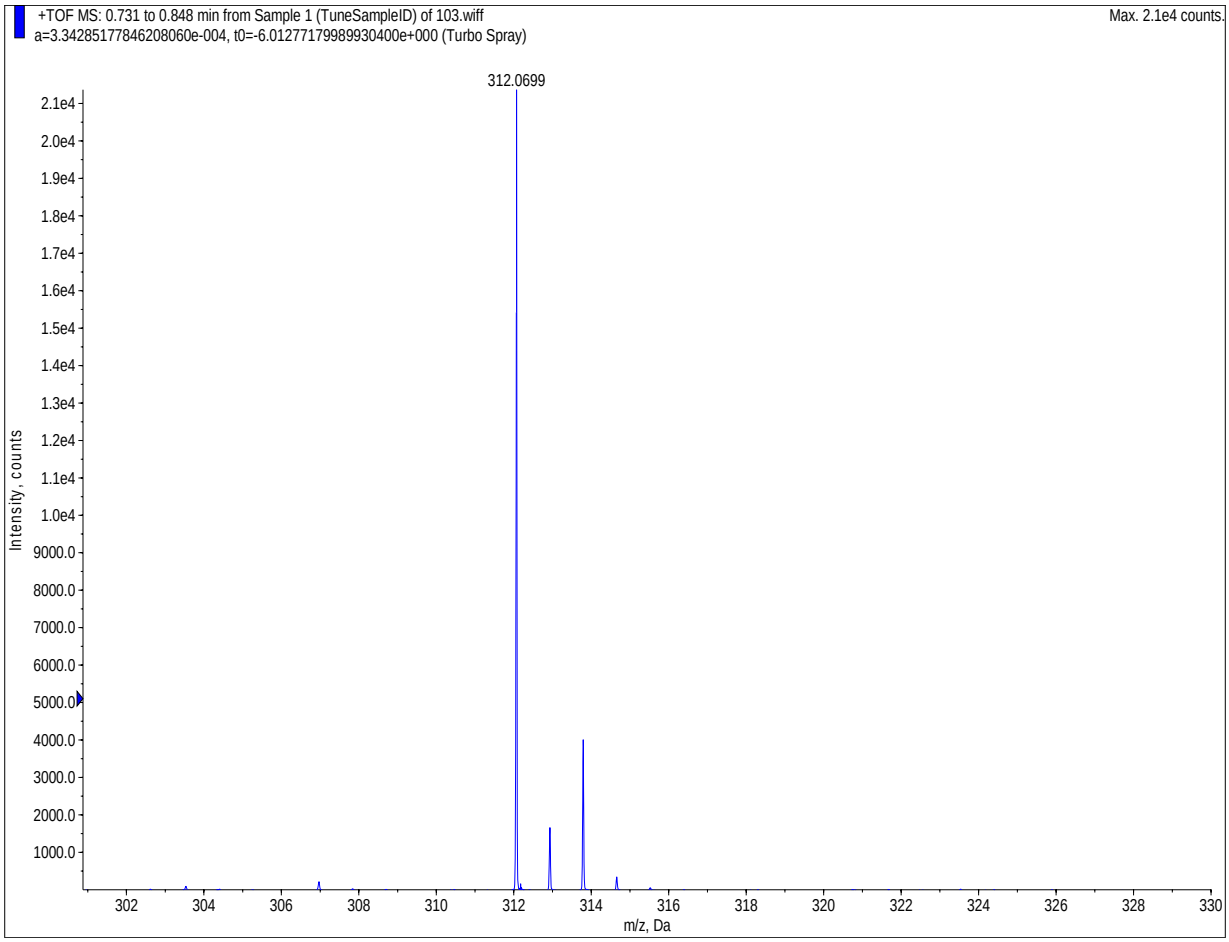
Methyl 2-(6-chloro-3-propyl-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4g)



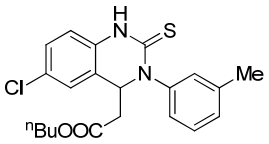
HRMS



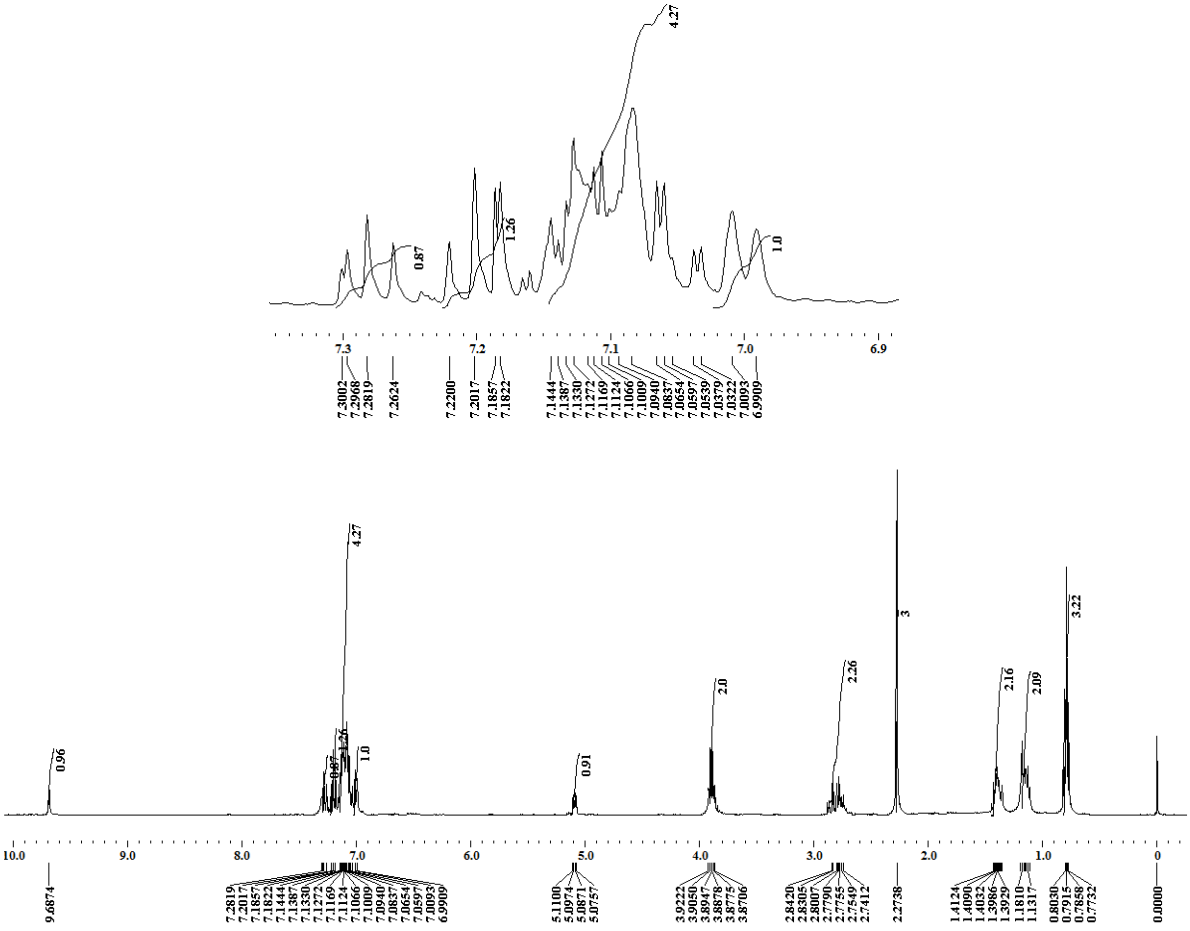
Methyl 2-(6-chloro-3-propyl-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4g)



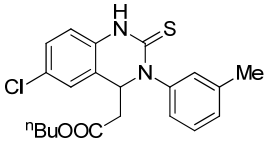
^{1}H NMR



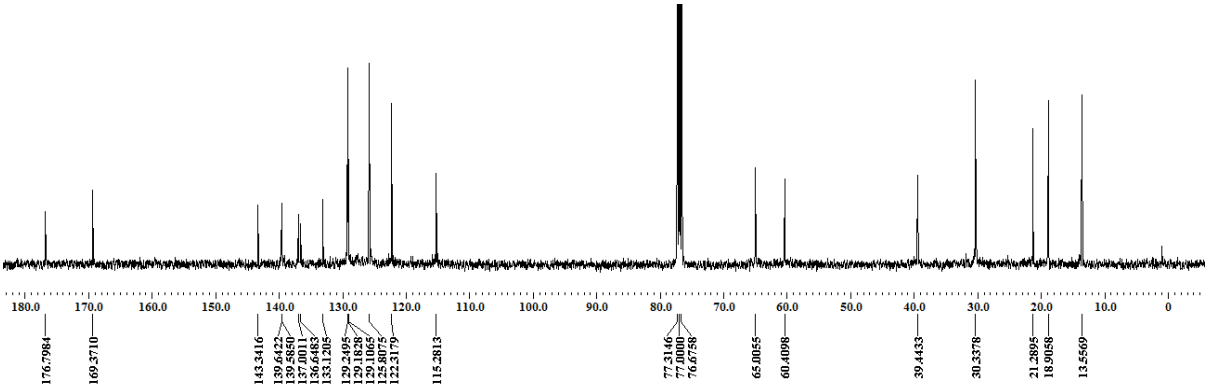
Butyl 2-(6-chloro-2-thioxo-3-(*m*-tolyl)-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4h)



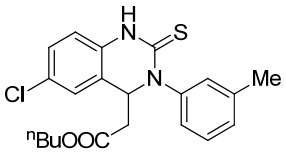
^{13}C NMR



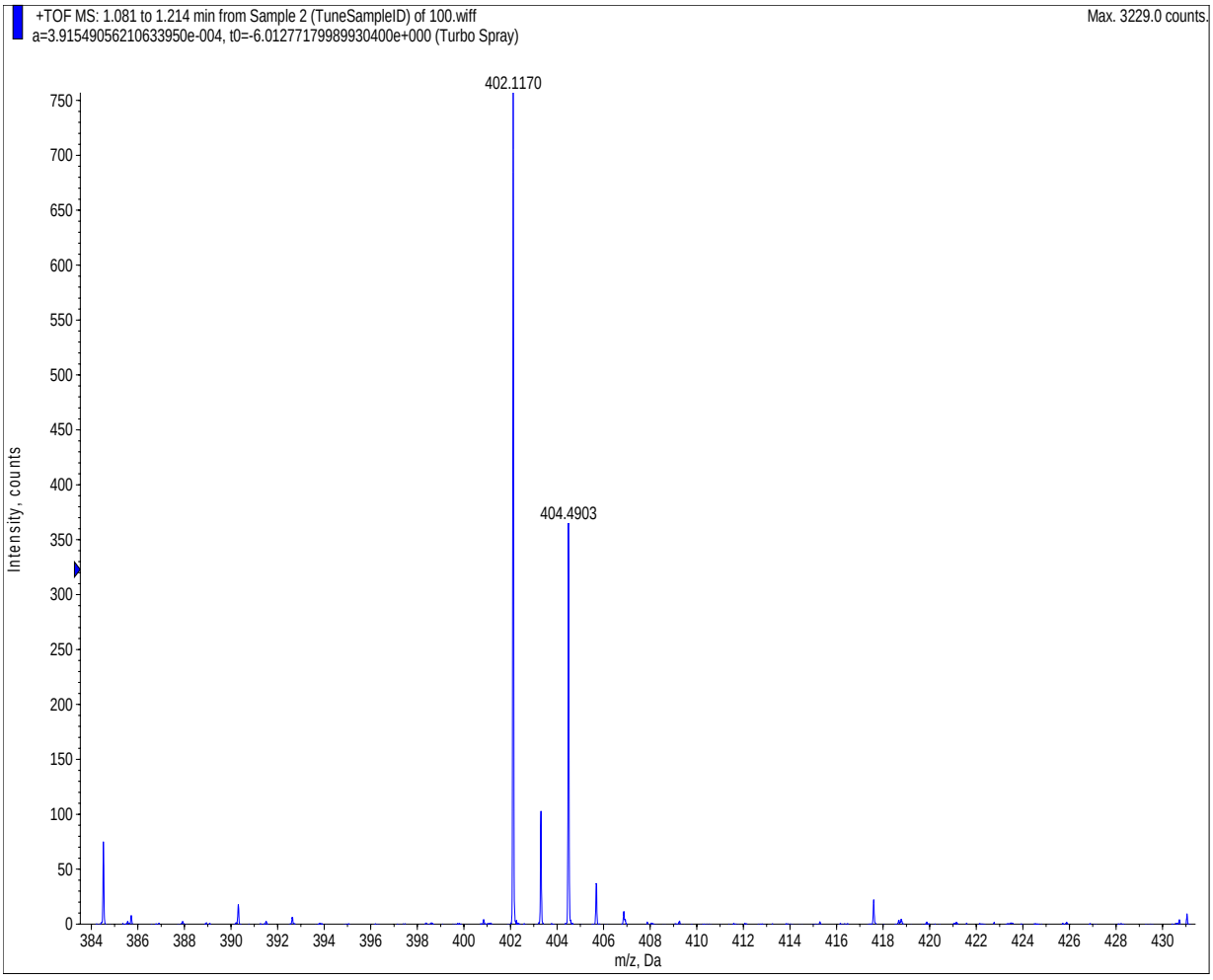
Butyl 2-(6-chloro-2-thioxo-3-(*m*-tolyl)-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4h)



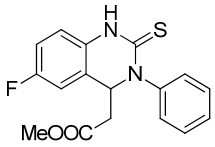
HRMS



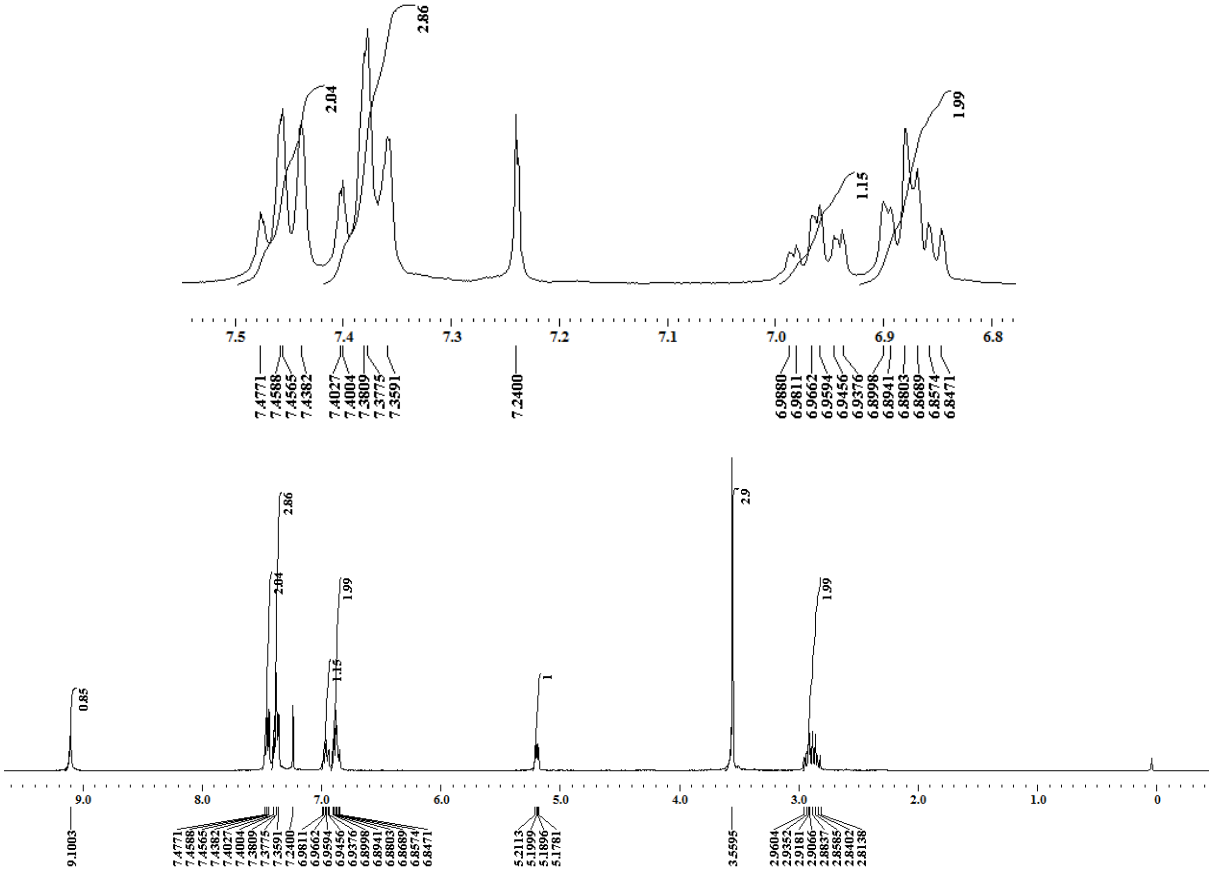
Butyl 2-(6-chloro-2-thioxo-3-(*m*-tolyl)-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4h)



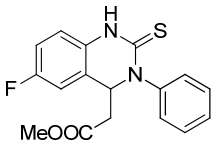
^{1}H NMR



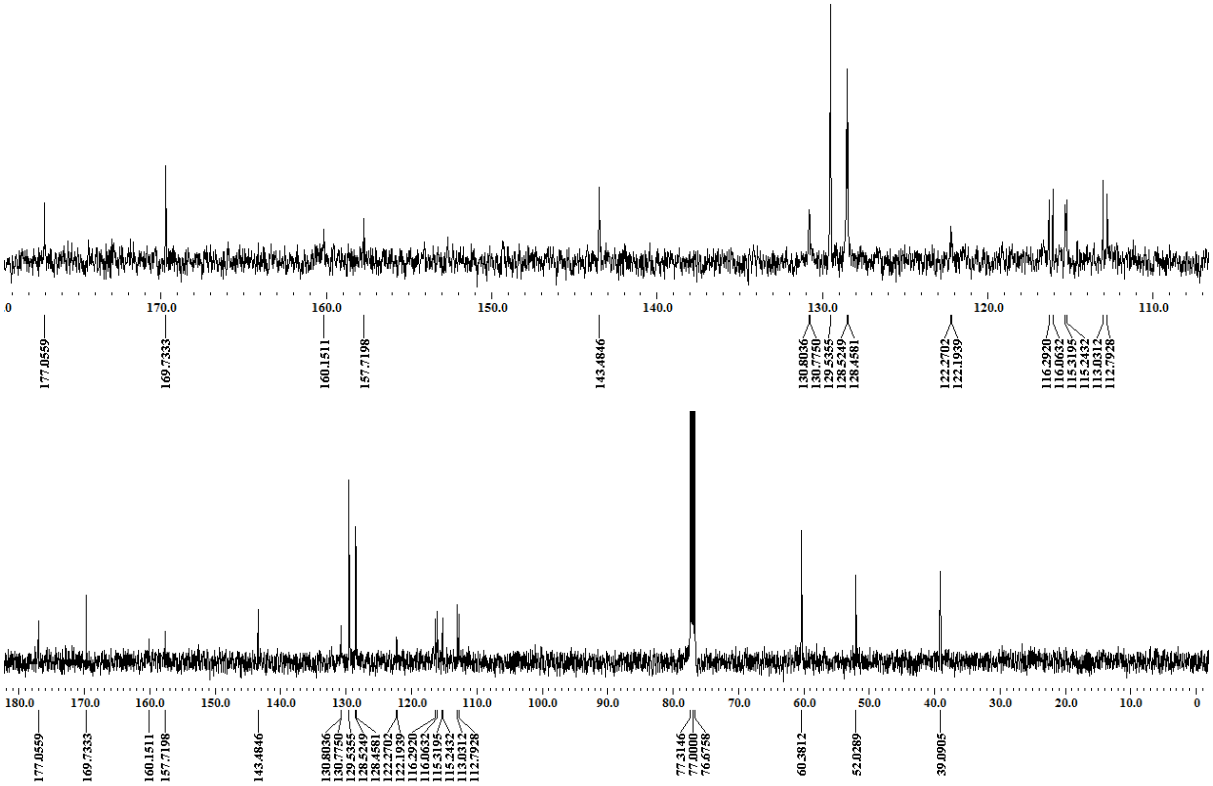
Methyl 2-(6-fluoro-3-phenyl-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4i)



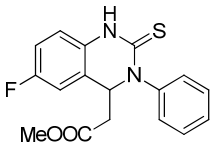
^{13}C NMR



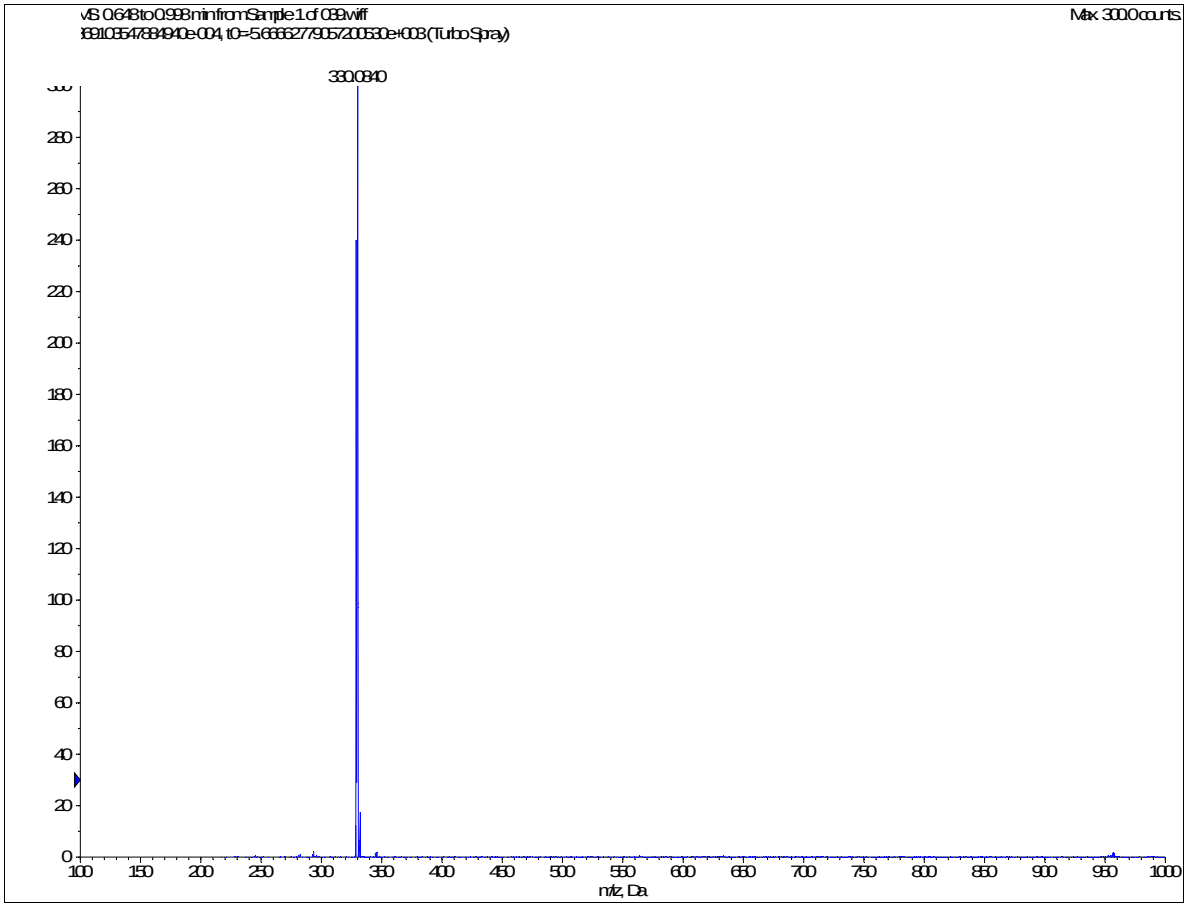
Methyl 2-(6-fluoro-3-phenyl-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4i)



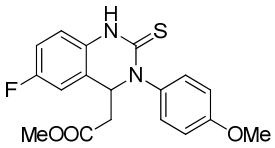
HRMS



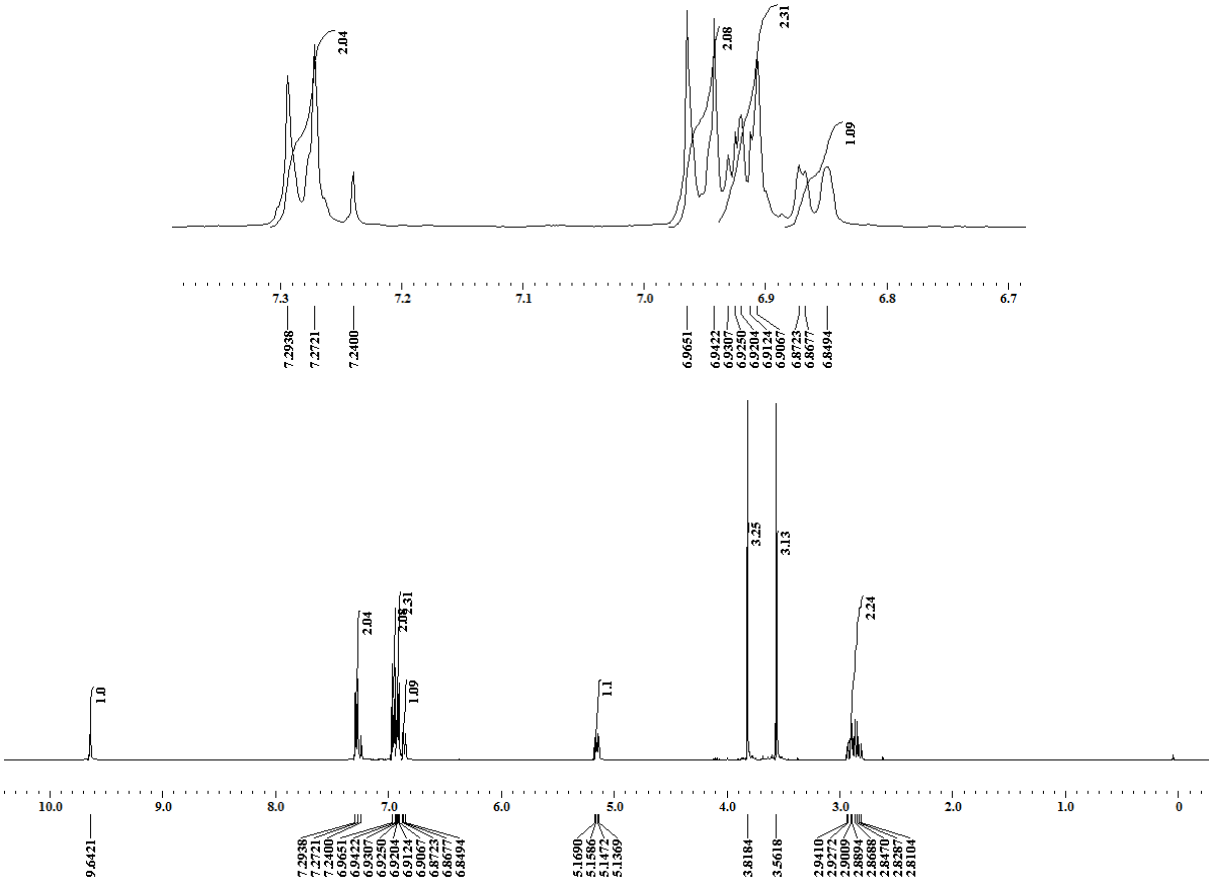
Methyl 2-(6-fluoro-3-phenyl-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4i)



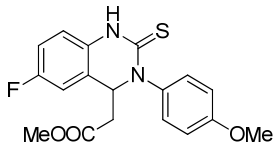
^{1}H NMR



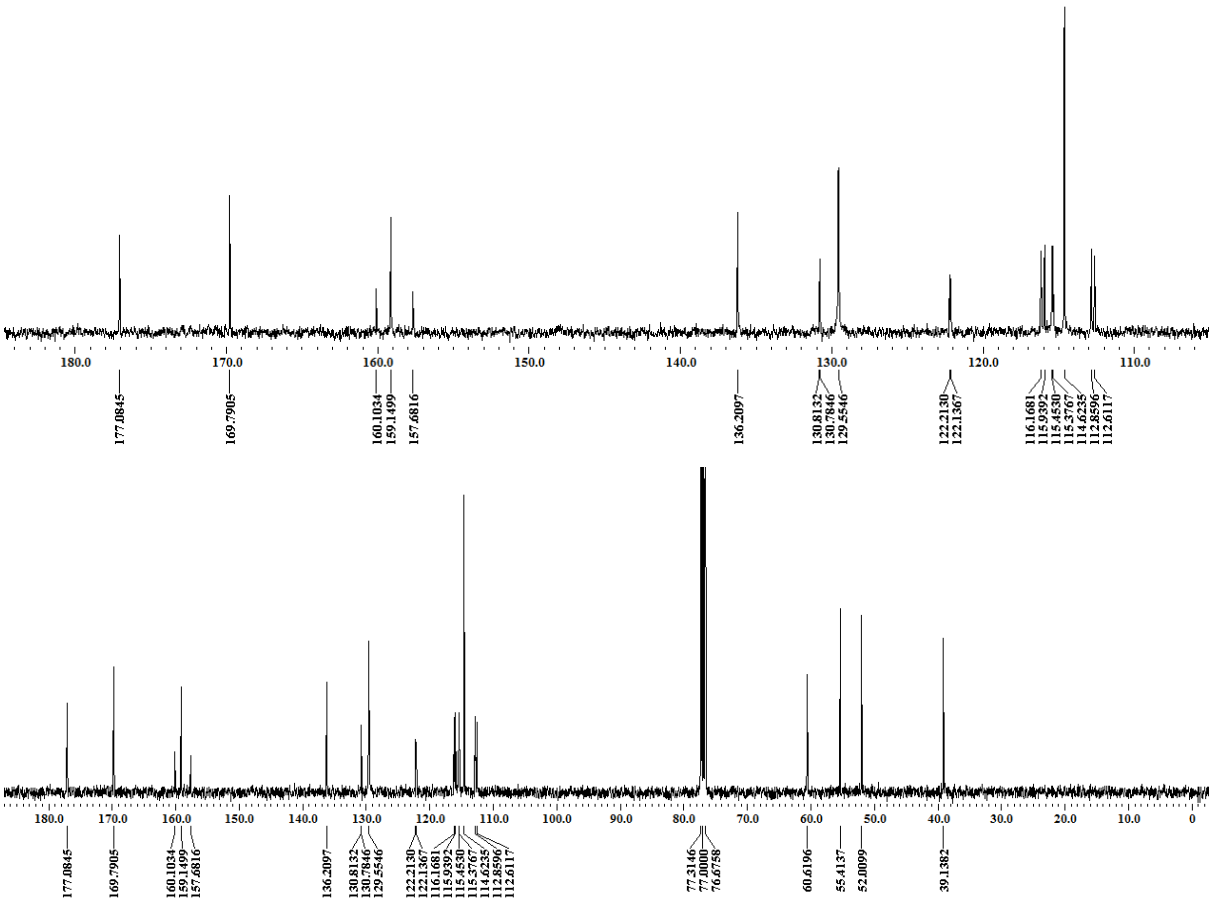
Methyl 2-(6-fluoro-3-(4-methoxyphenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4j)



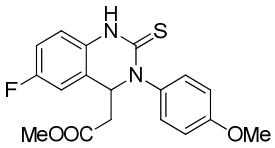
^{13}C NMR



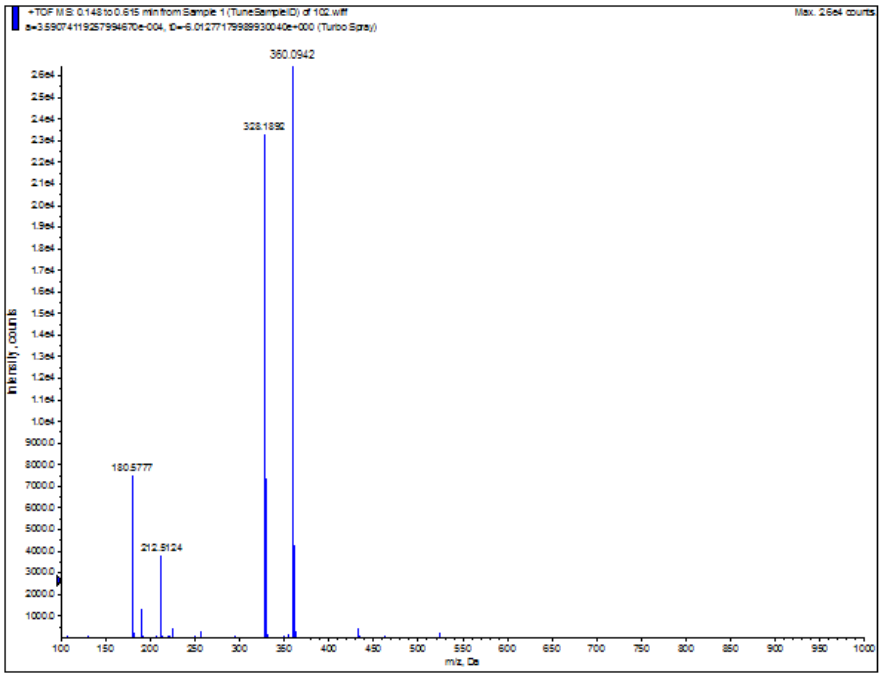
methyl 2-(6-fluoro-3-(4-methoxyphenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4j)



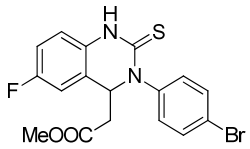
HRMS



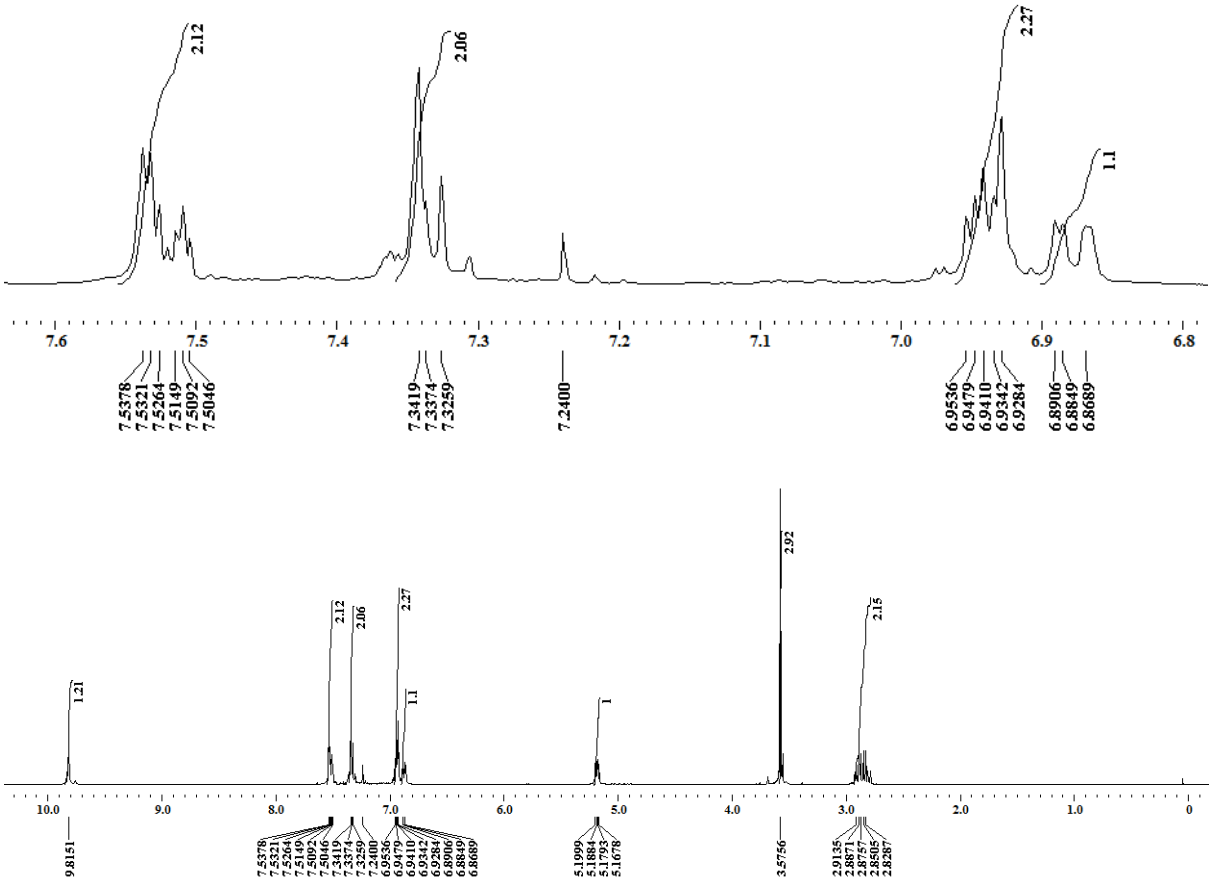
methyl 2-(6-fluoro-3-(4-methoxyphenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4j)



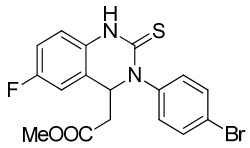
^{1}H NMR



Methyl 2-(3-(4-bromophenyl)-6-fluoro-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4k)



^{13}C NMR



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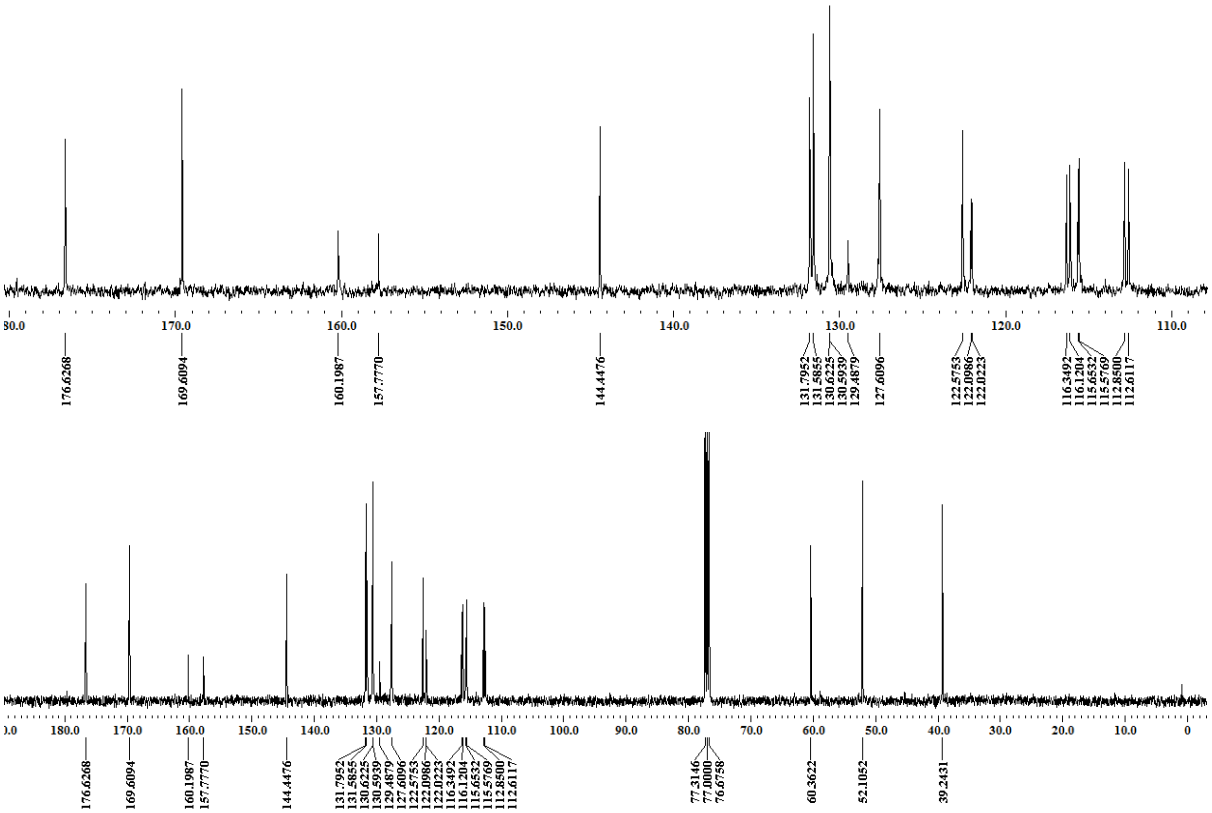
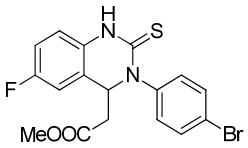


HRMS



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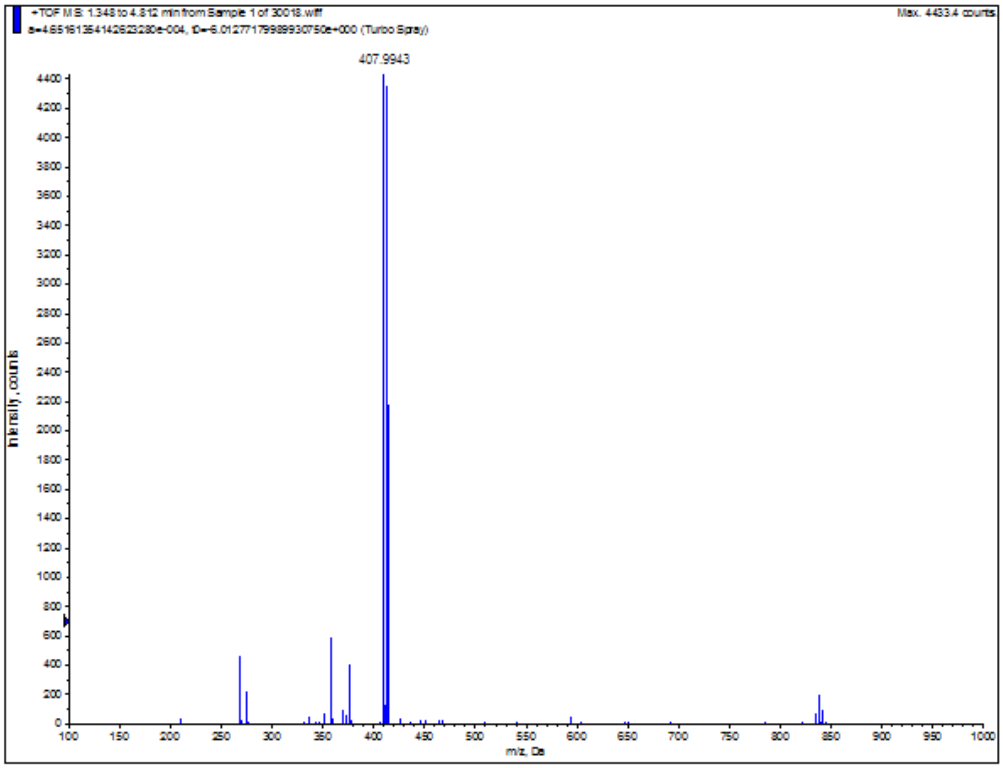
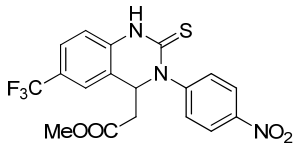
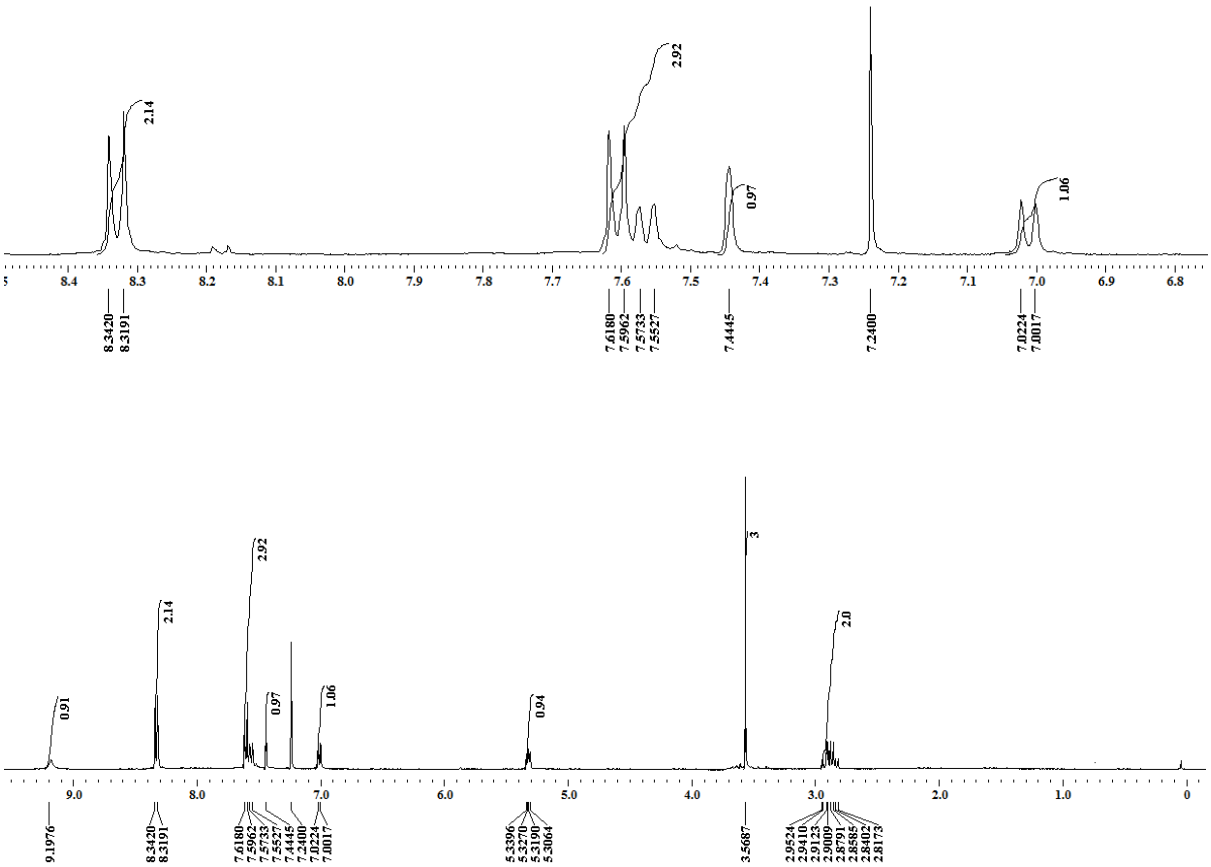


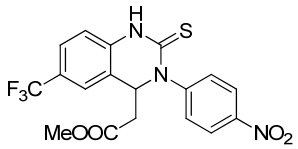
^{1}H NMR



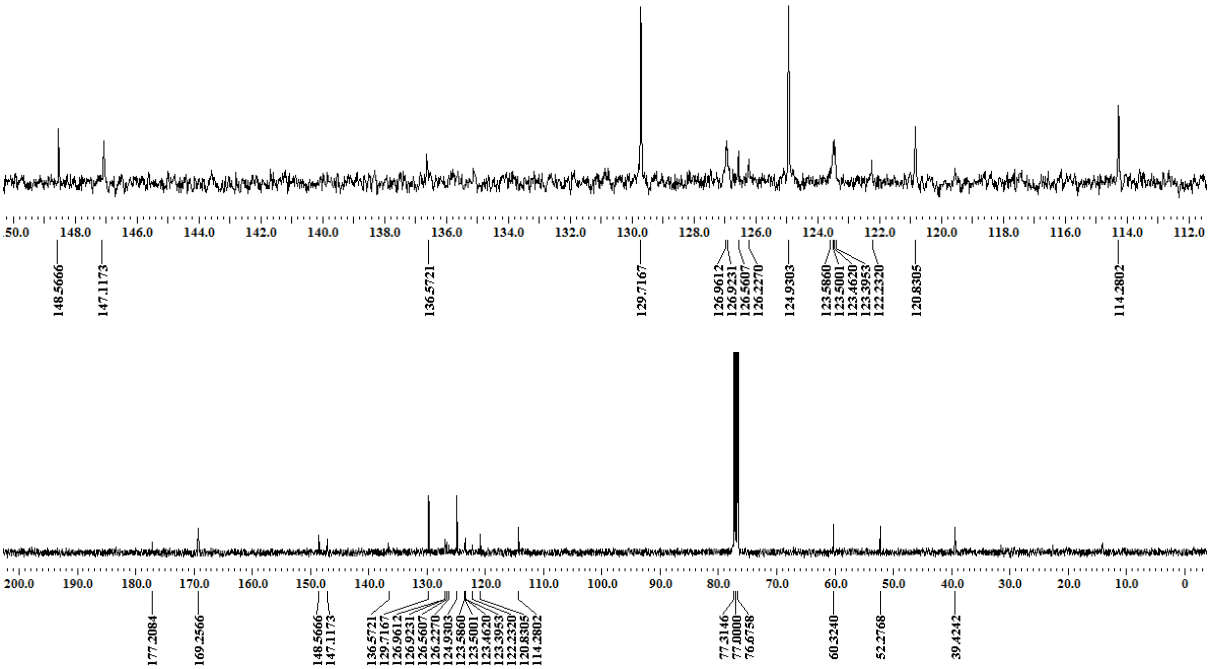
Methyl 2-(3-(4-nitrophenyl)-2-thioxo-6-(trifluoromethyl)-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4l)



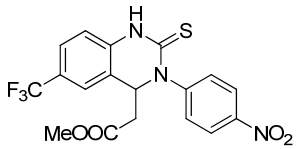
^{13}C NMR



Methyl 2-(3-(4-nitrophenyl)-2-thioxo-6-(trifluoromethyl)-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4l)



HRMS



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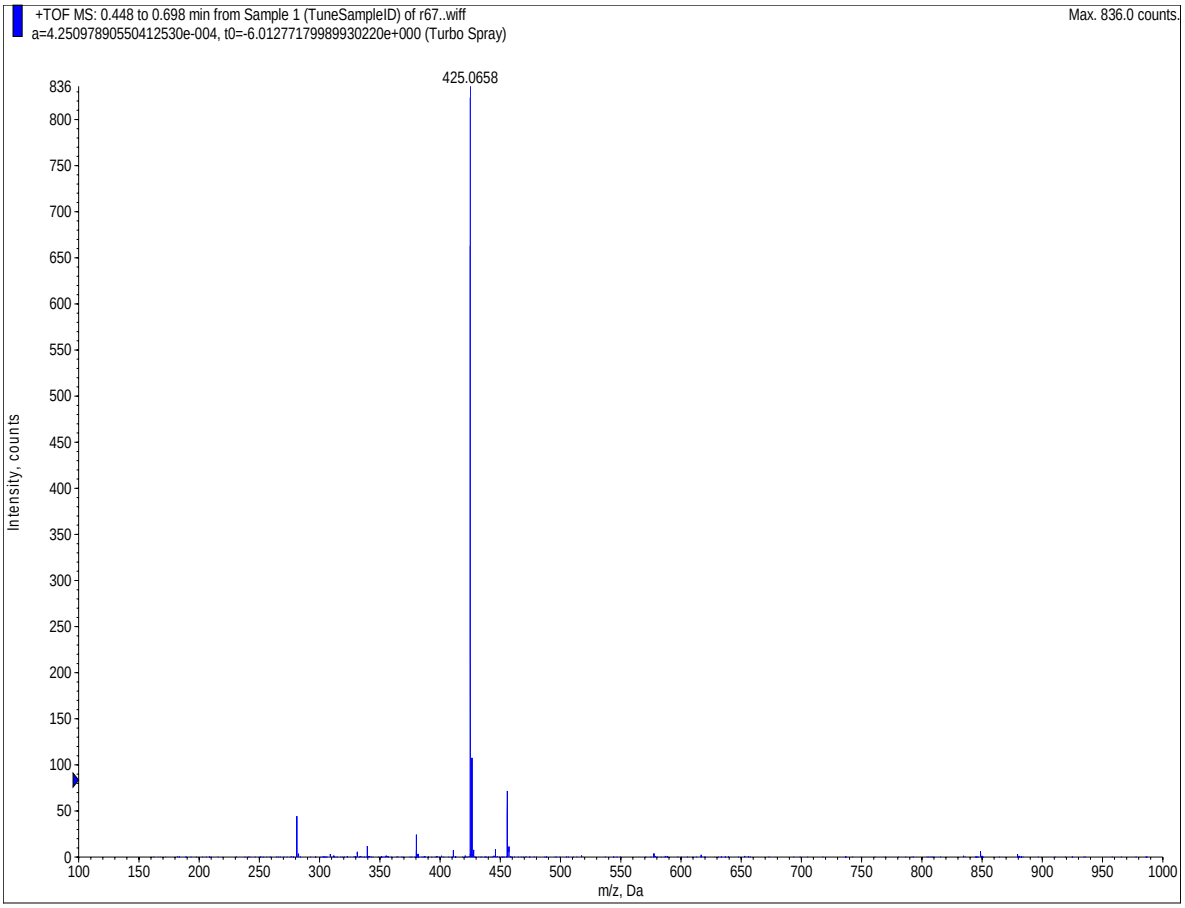
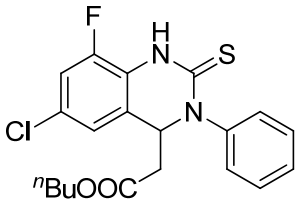
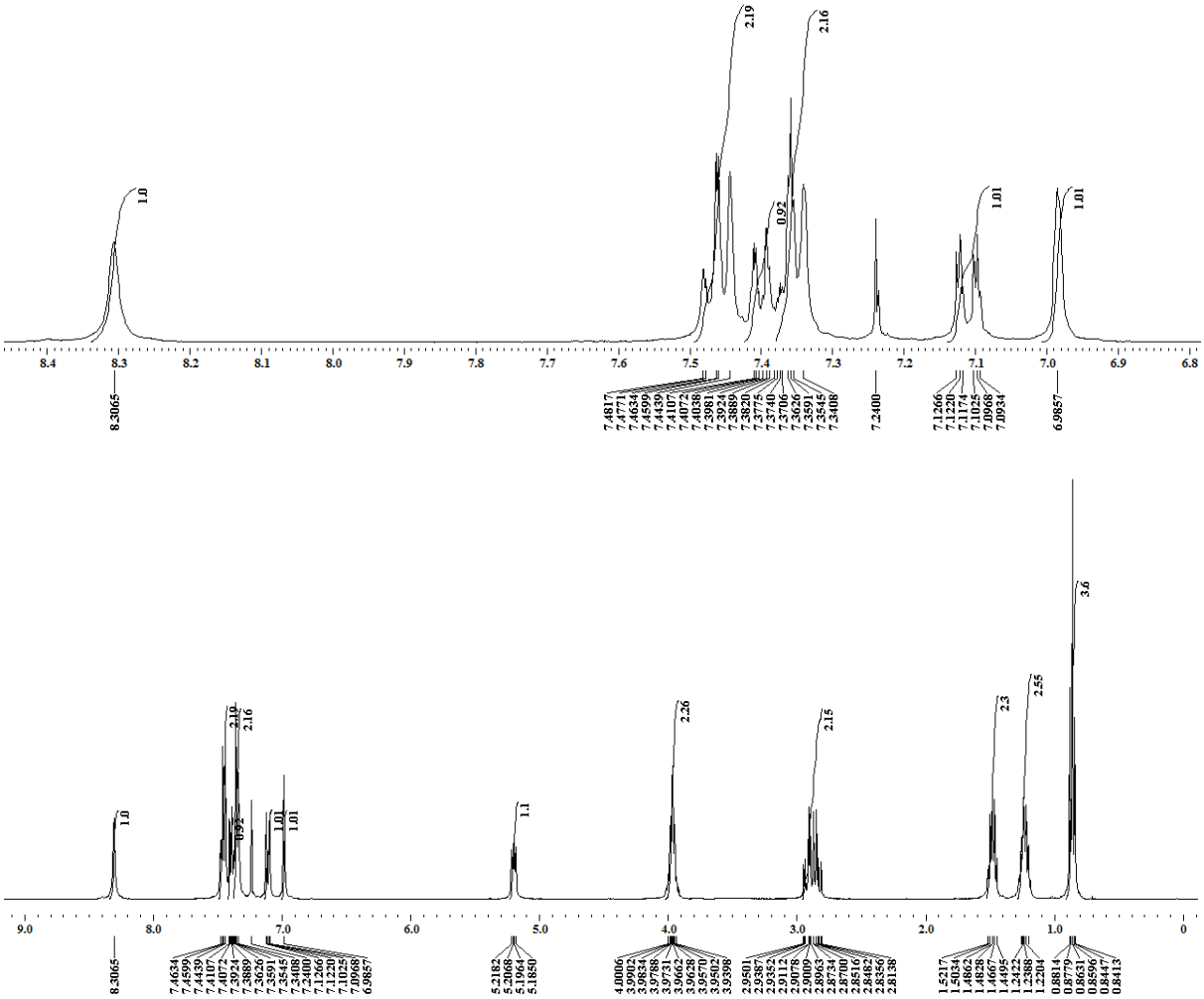


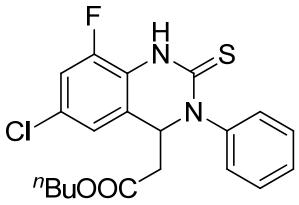
^{1}H NMR



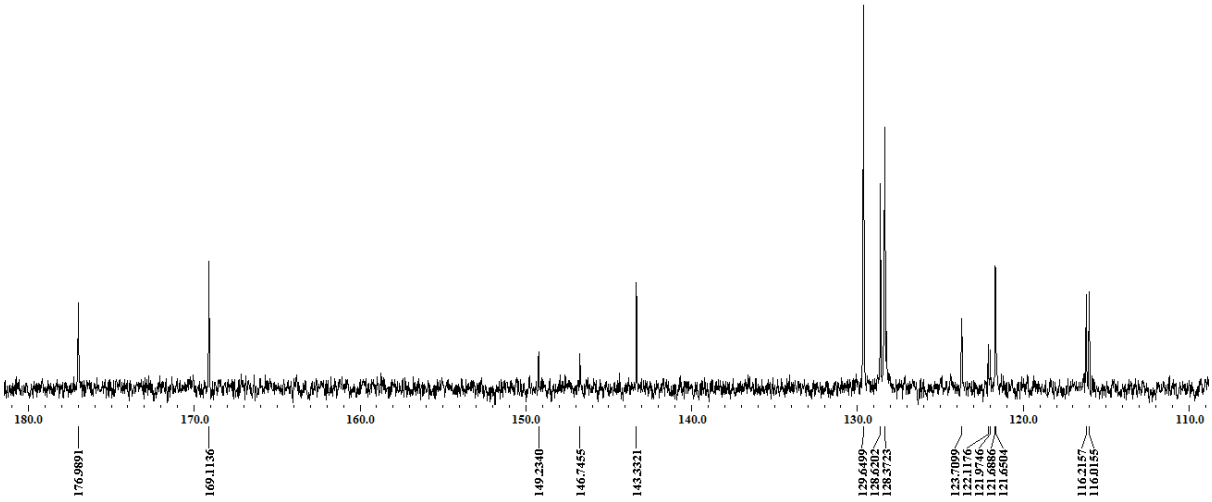
Butyl 2-(6-chloro-8-fluoro-3-phenyl-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4m)

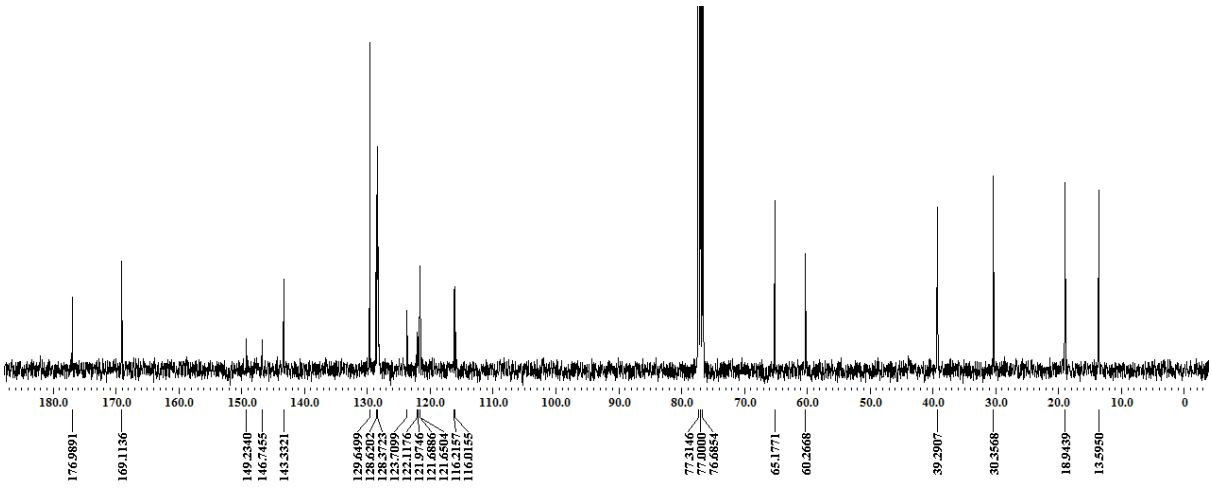


^{13}C NMR

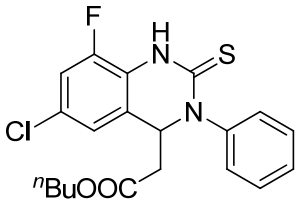


Butyl 2-(6-chloro-8-fluoro-3-phenyl-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4m)

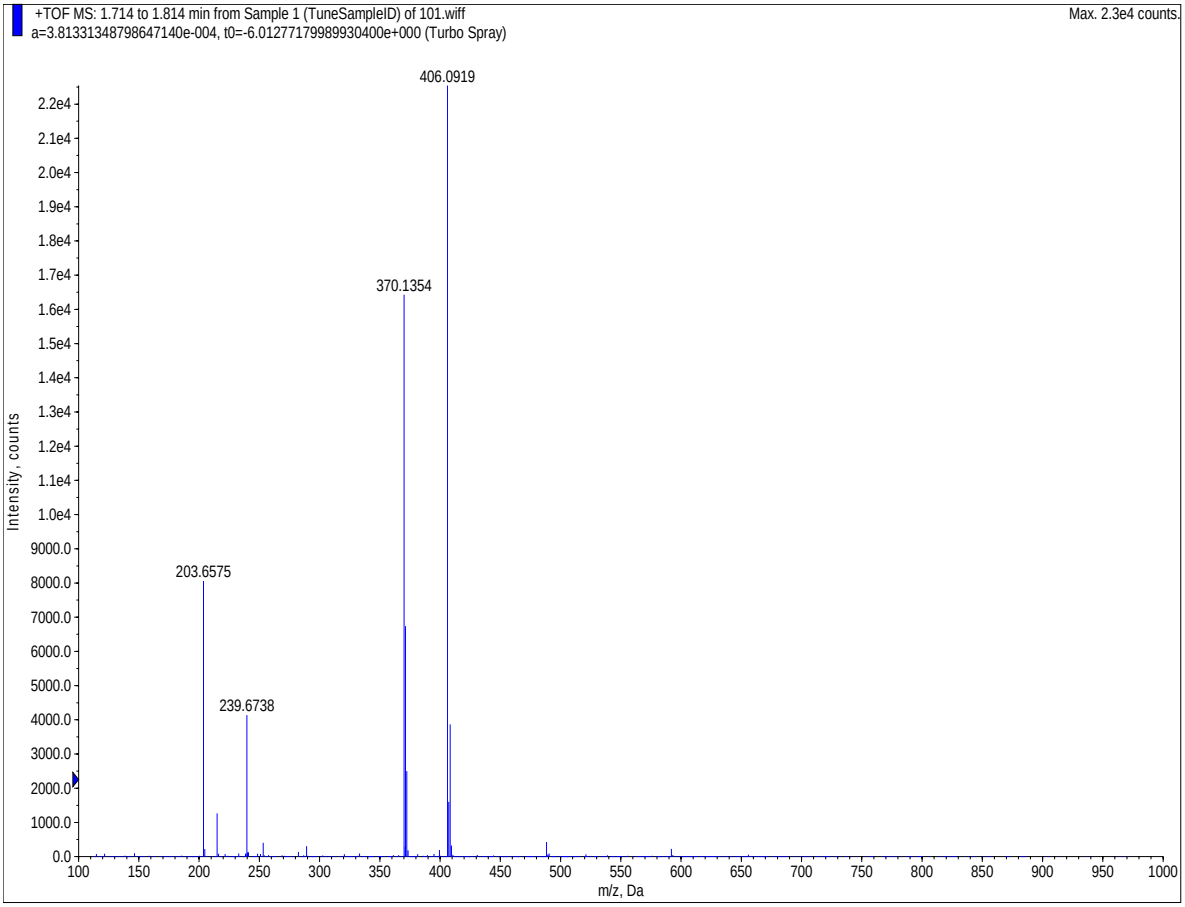




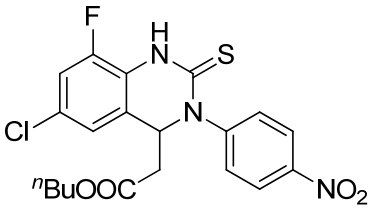
HRMS



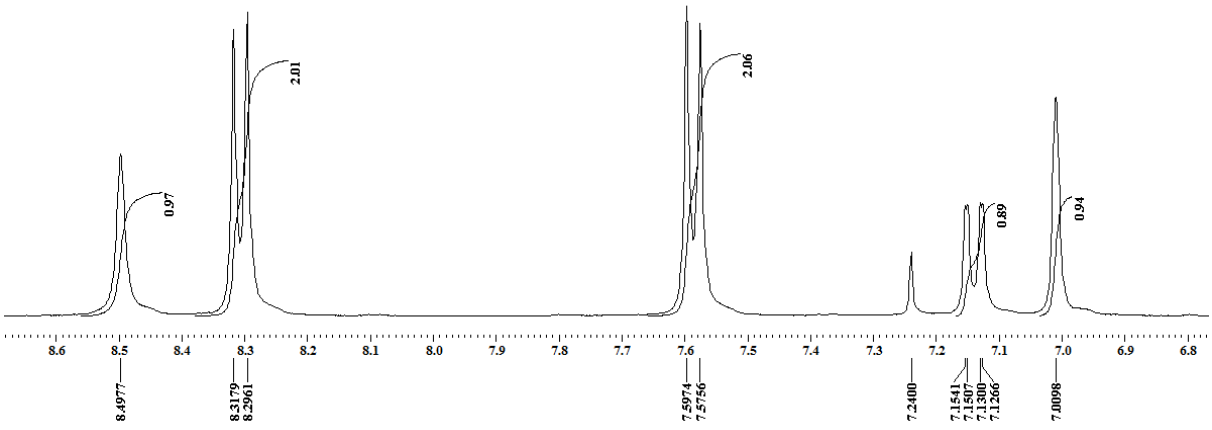
Butyl 2-(6-chloro-8-fluoro-3-phenyl-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4m)

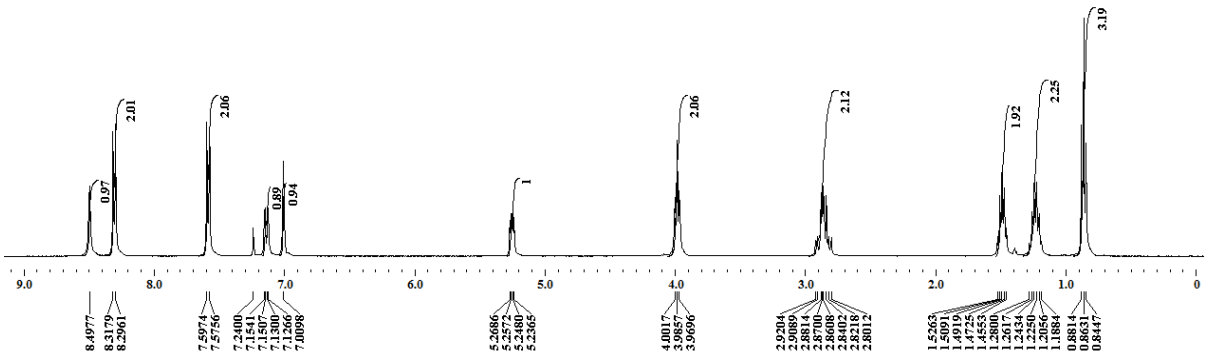


^{1}H NMR

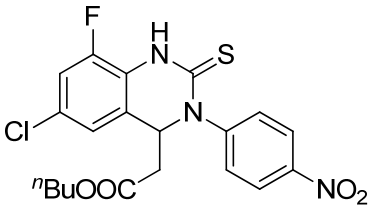


Butyl 2-(6-chloro-8-fluoro-3-(4-nitrophenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4n)

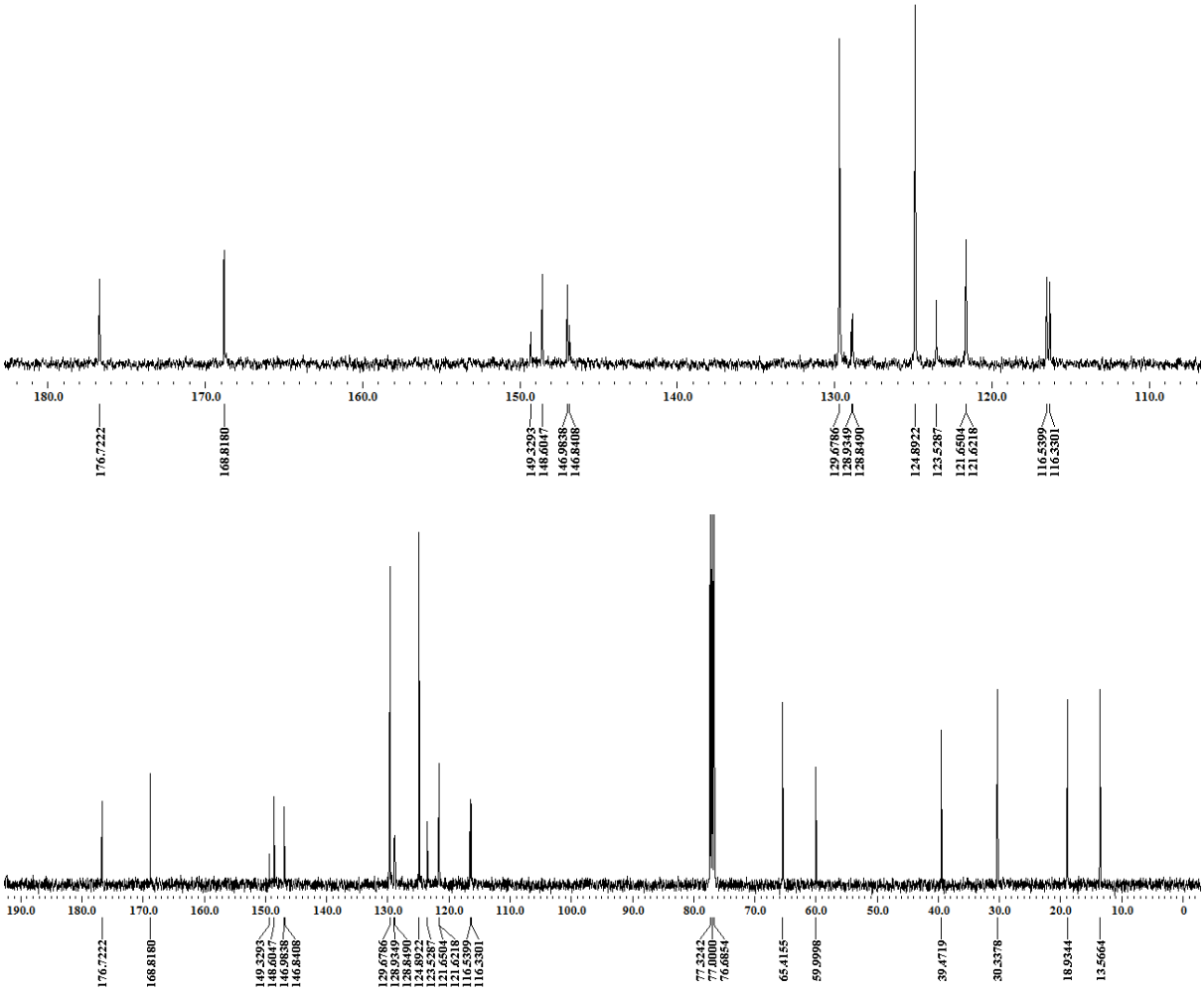




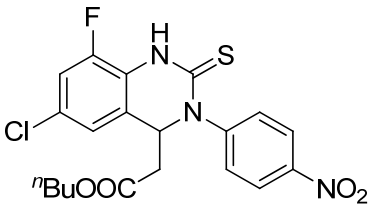
^{13}C NMR



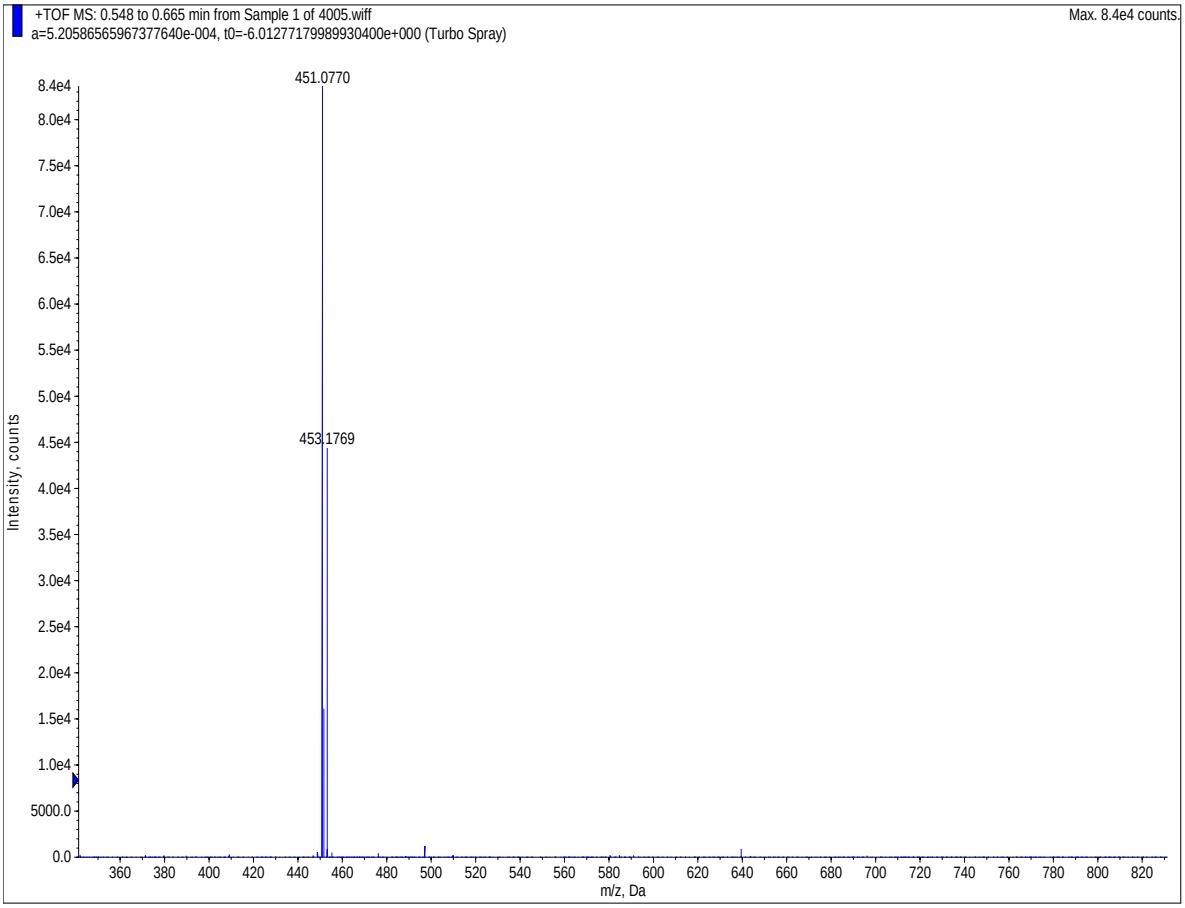
Butyl 2-(6-chloro-8-fluoro-3-(4-nitrophenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4n)



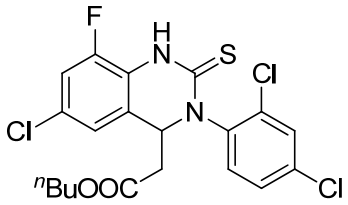
HRMS



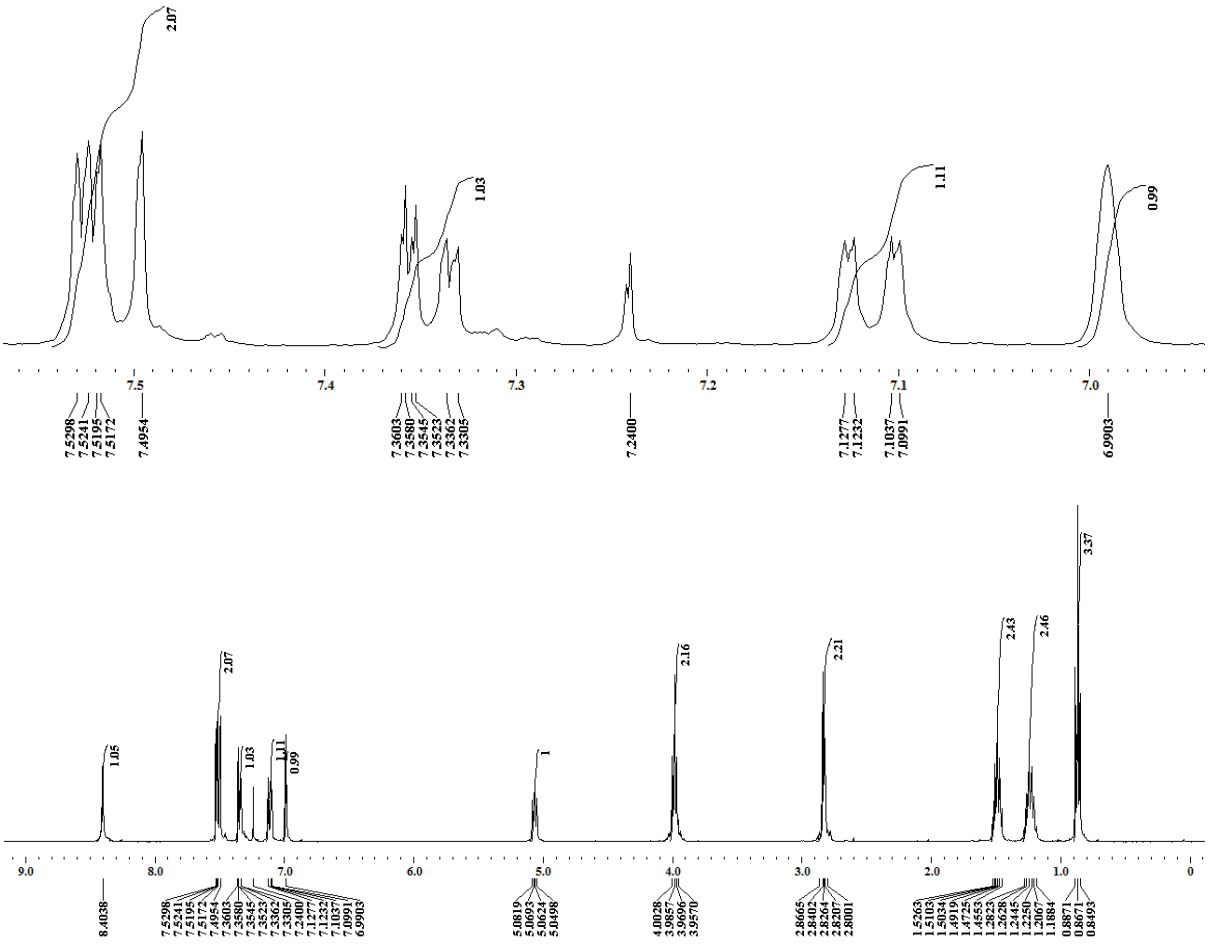
Butyl 2-(6-chloro-8-fluoro-3-(4-nitrophenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4n)



^{1}H NMR



Butyl 2-(6-chloro-3-(2,4-dichlorophenyl)-8-fluoro-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4o)



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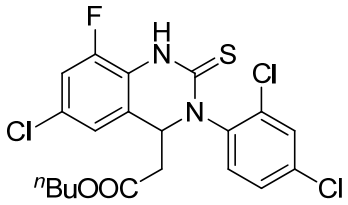
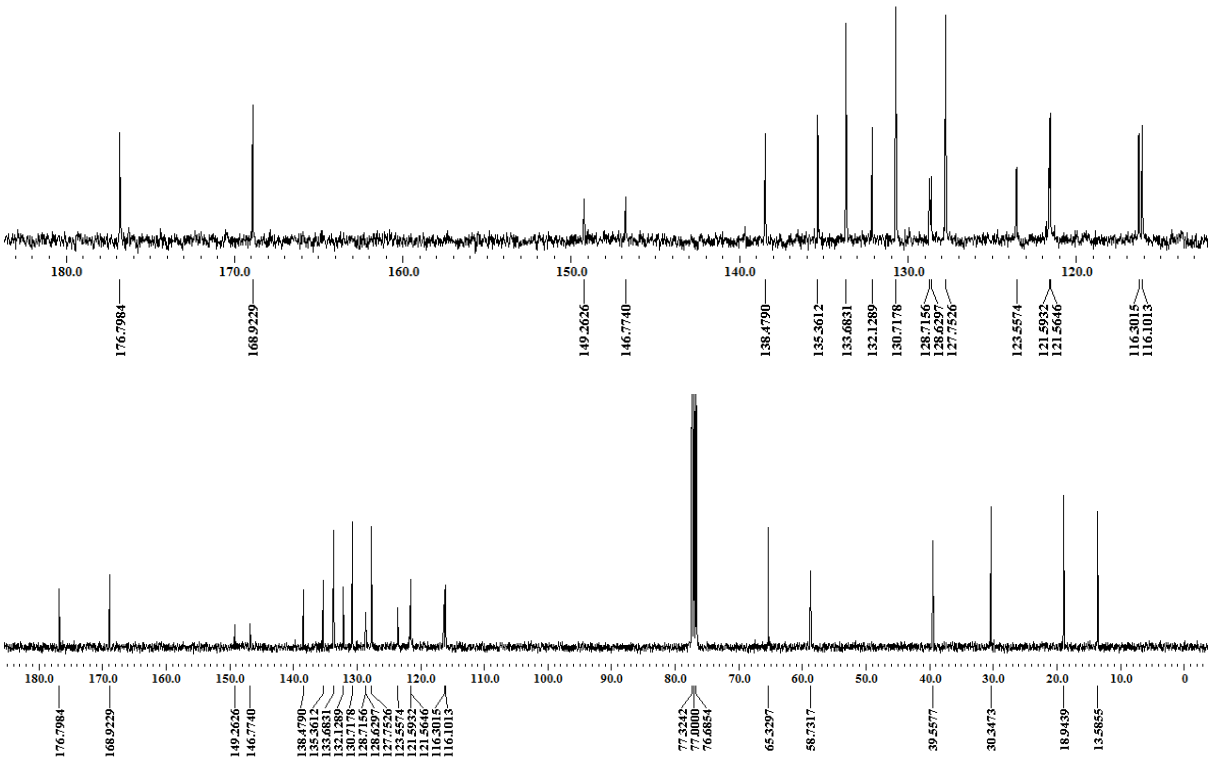
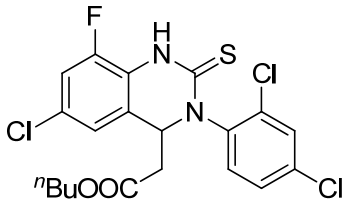


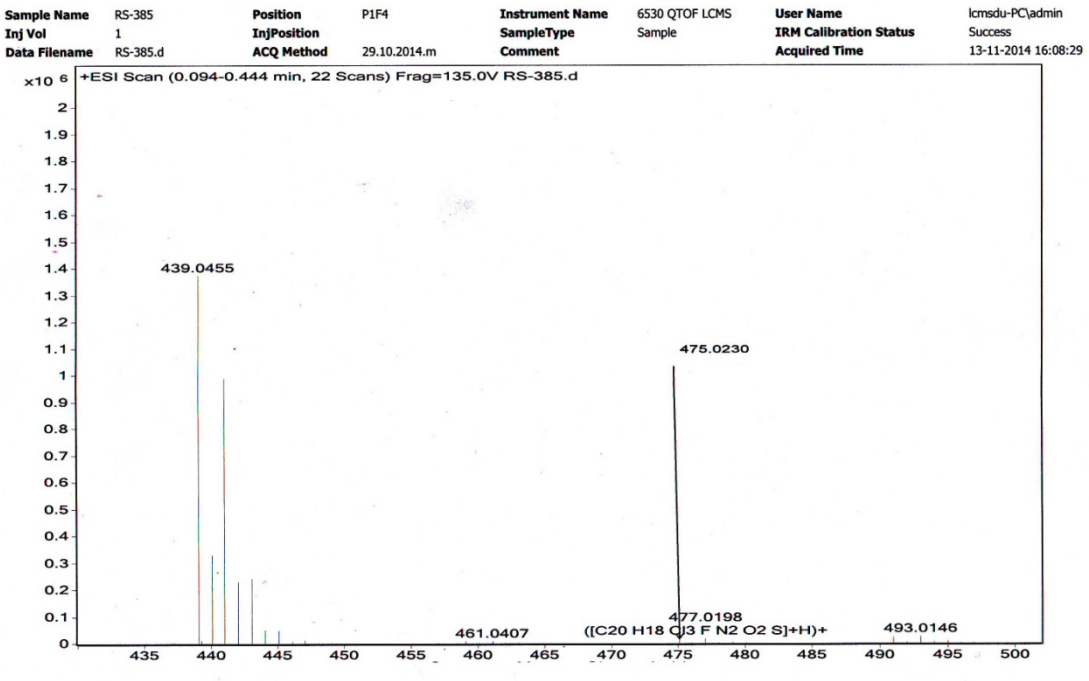
Butyl 2-(6-chloro-3-(2,4-dichlorophenyl)-8-fluoro-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4o)



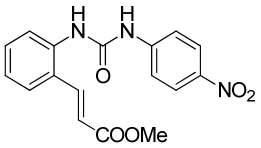
HRMS



Butyl 2-(6-chloro-3-(2,4-dichlorophenyl)-8-fluoro-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4o)

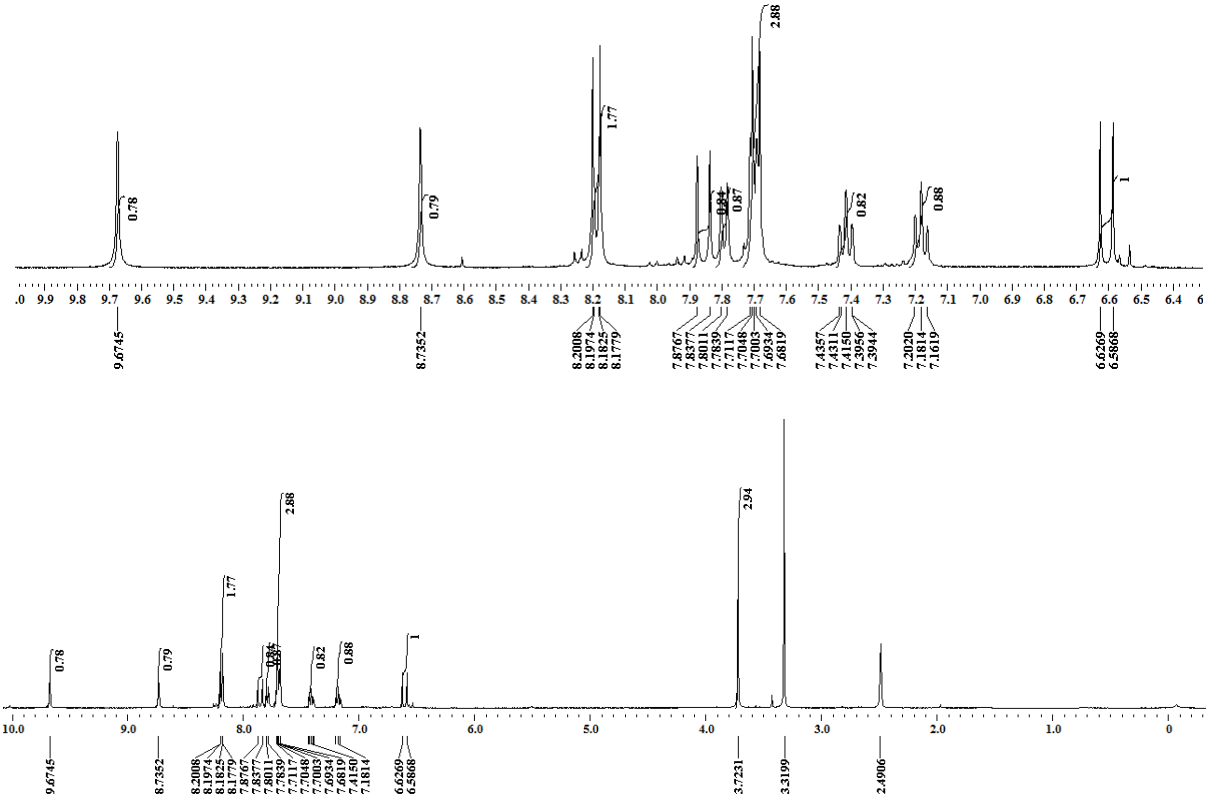


^{1}H NMR

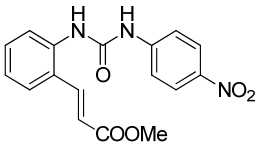


(*E*)-Methyl 3-(2-(3-(4-nitrophenyl)ureido)phenyl)acrylate

(6a)

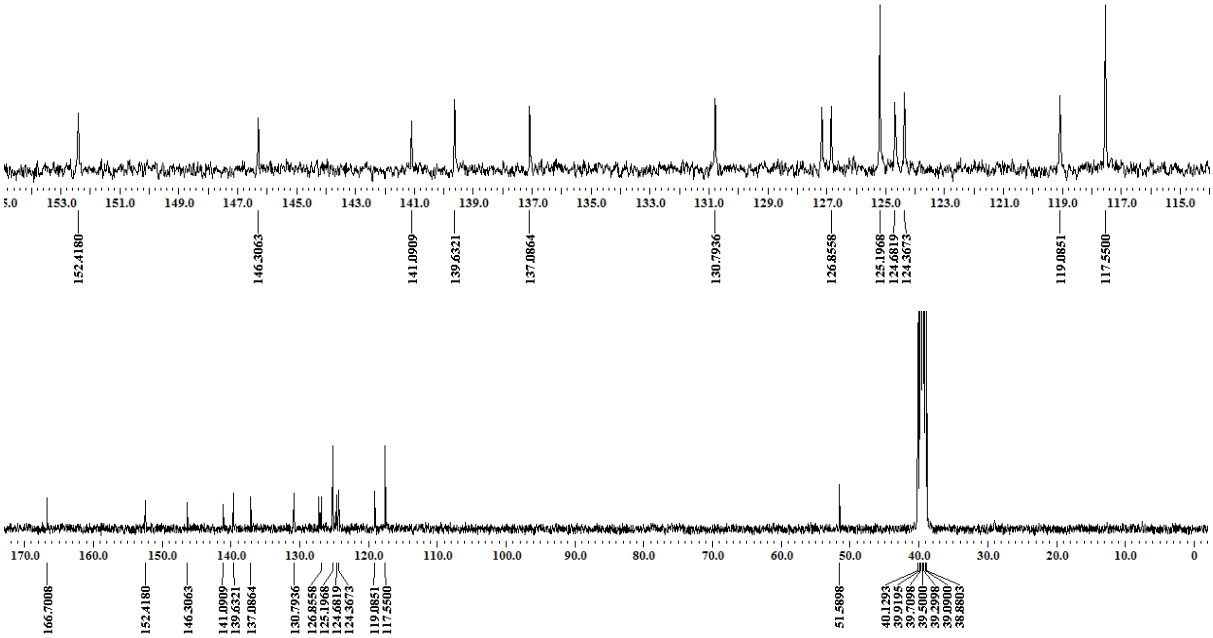


^{13}C NMR

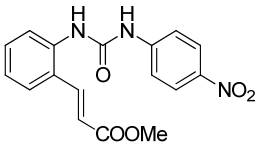


(*E*)-Methyl 3-(2-(3-(4-nitrophenyl)ureido)phenyl)acrylate

(6a)

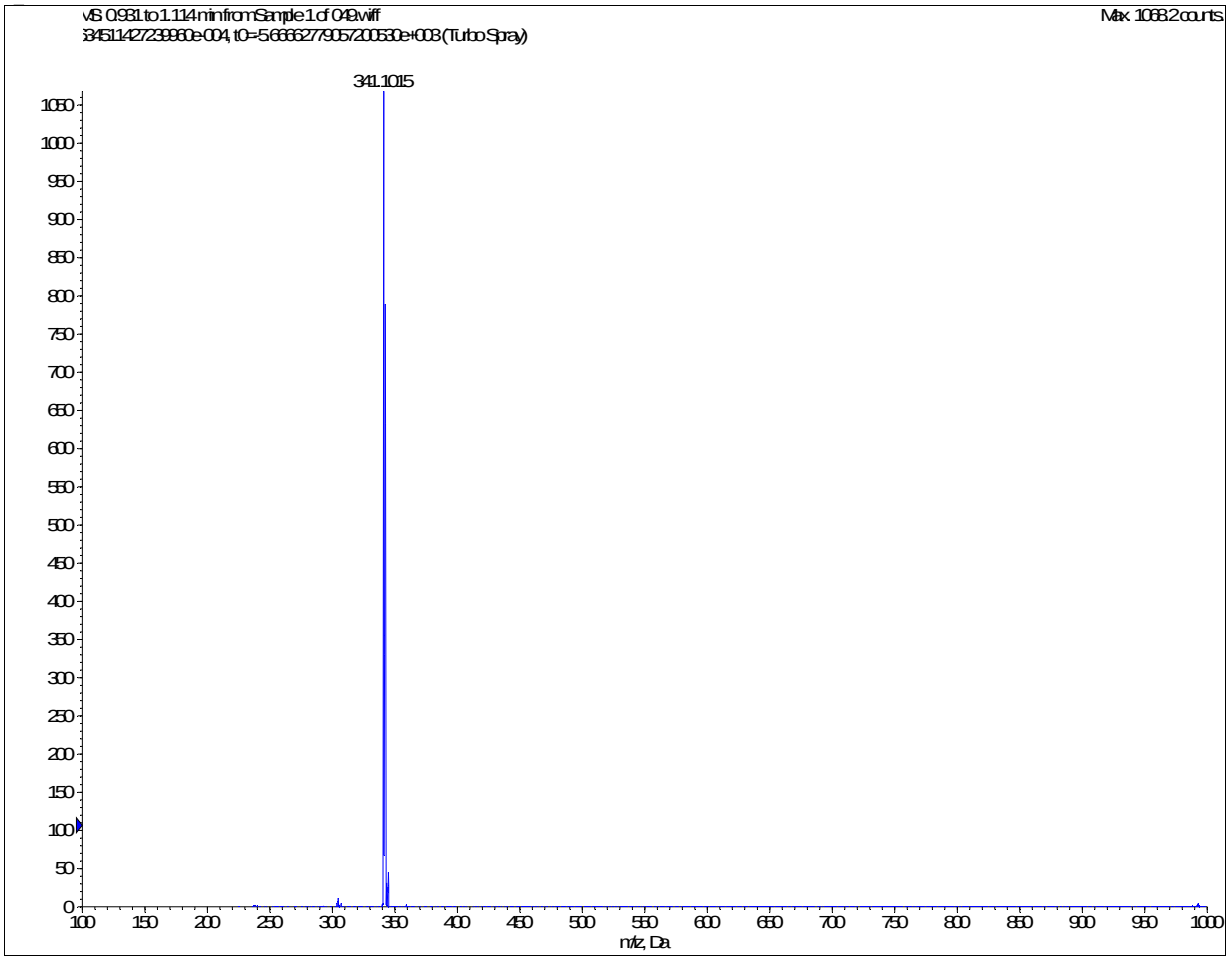


HRMS

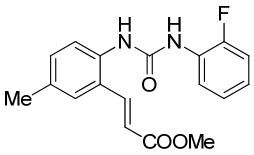


(*E*)-Methyl 3-(2-(3-(4-nitrophenyl)ureido)phenyl)acrylate

(6a)

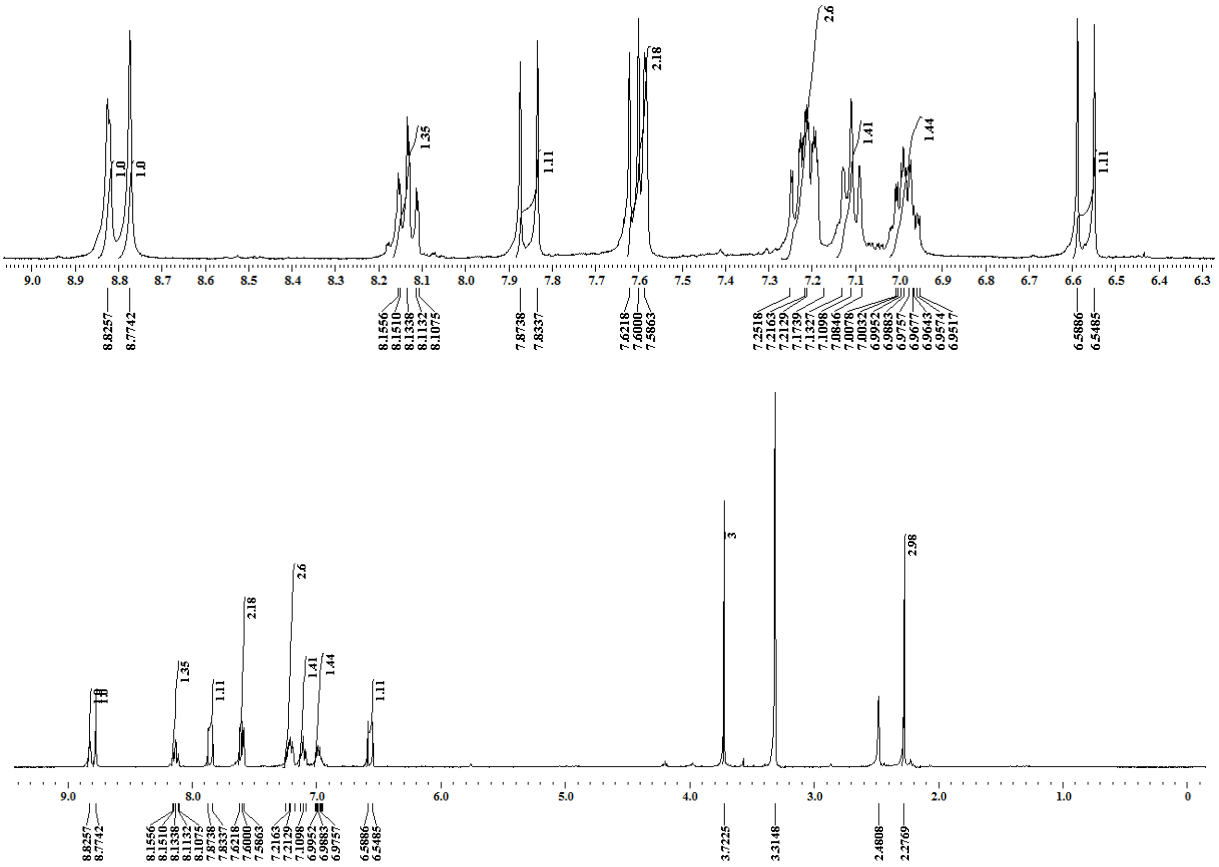


^{1}H NMR

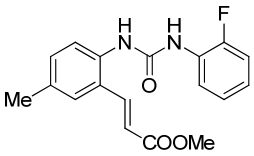


(*E*)-Methyl 3-(2-(3-(2-fluorophenyl)ureido)-5-methylphenyl)acrylate

(6b)

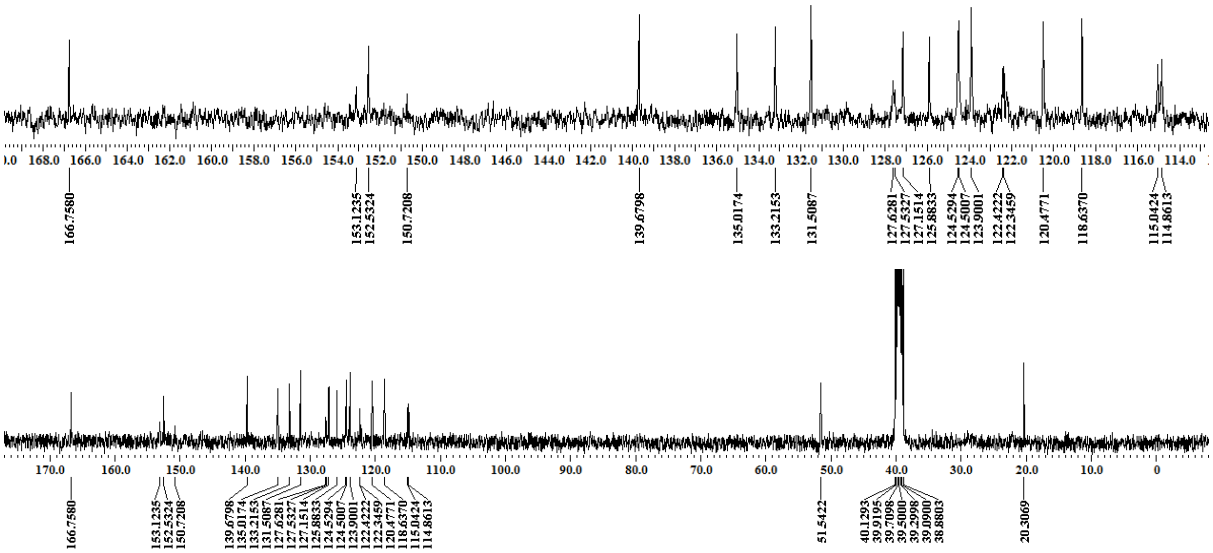


^{13}C NMR

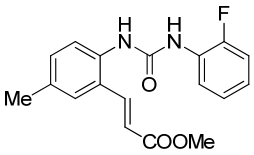


(*E*)-Methyl 3-(2-(3-(2-fluorophenyl)ureido)-5-methylphenyl)acrylate

(6b)

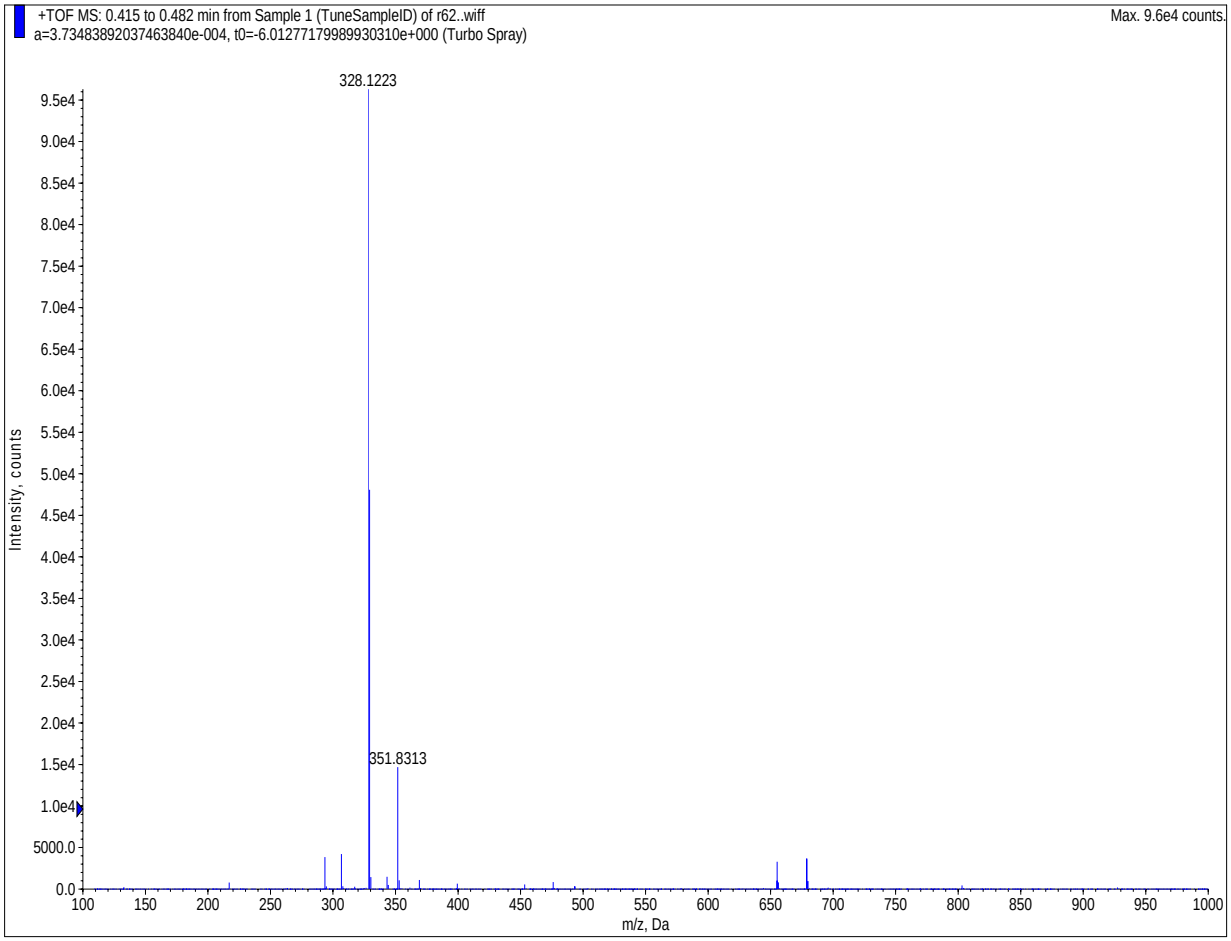


HRMS

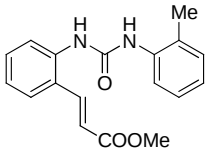


(*E*)-Methyl 3-(2-(3-(2-fluorophenyl)ureido)-5-methylphenyl)acrylate

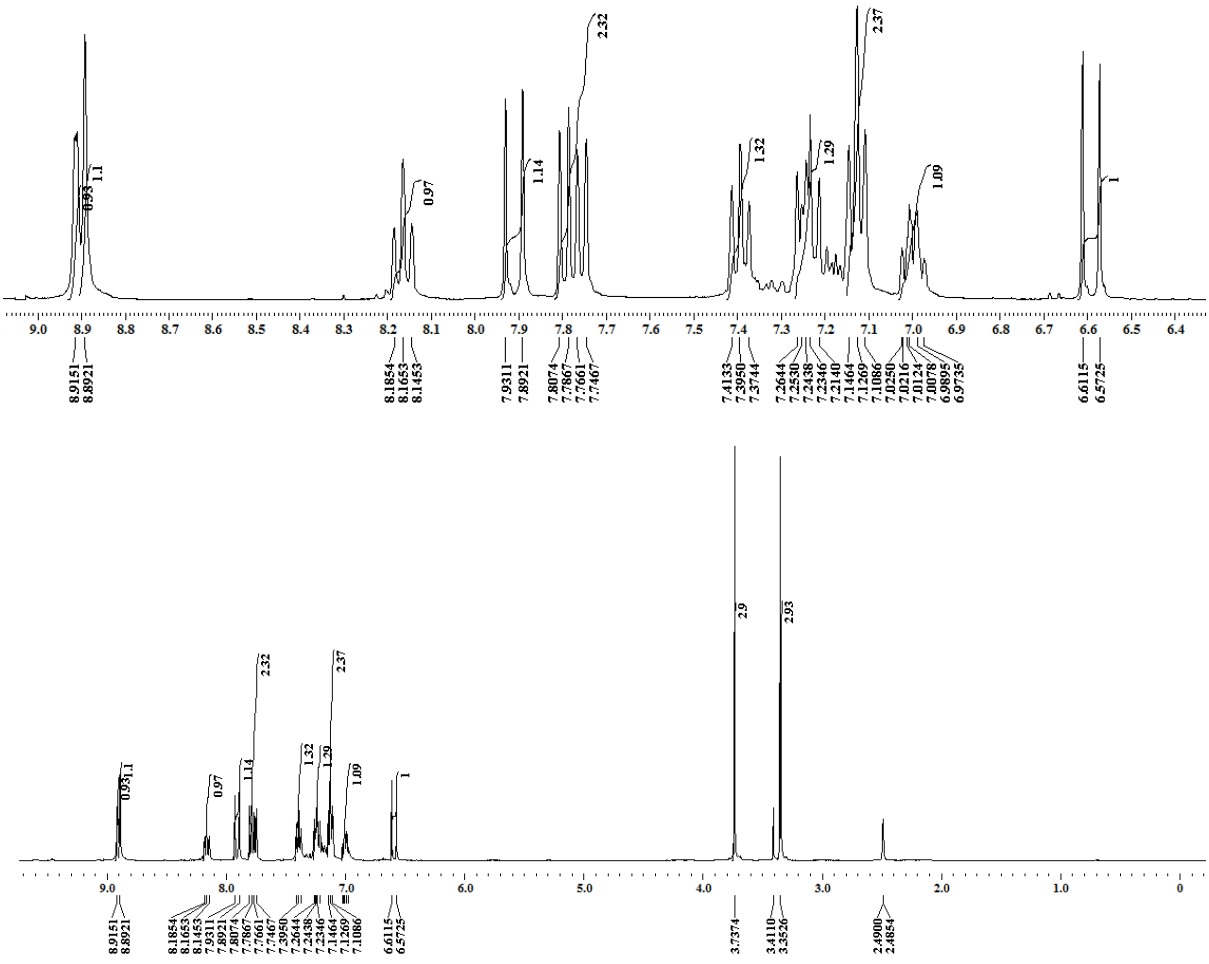
(6b)



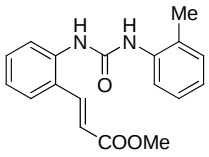
^{1}H NMR



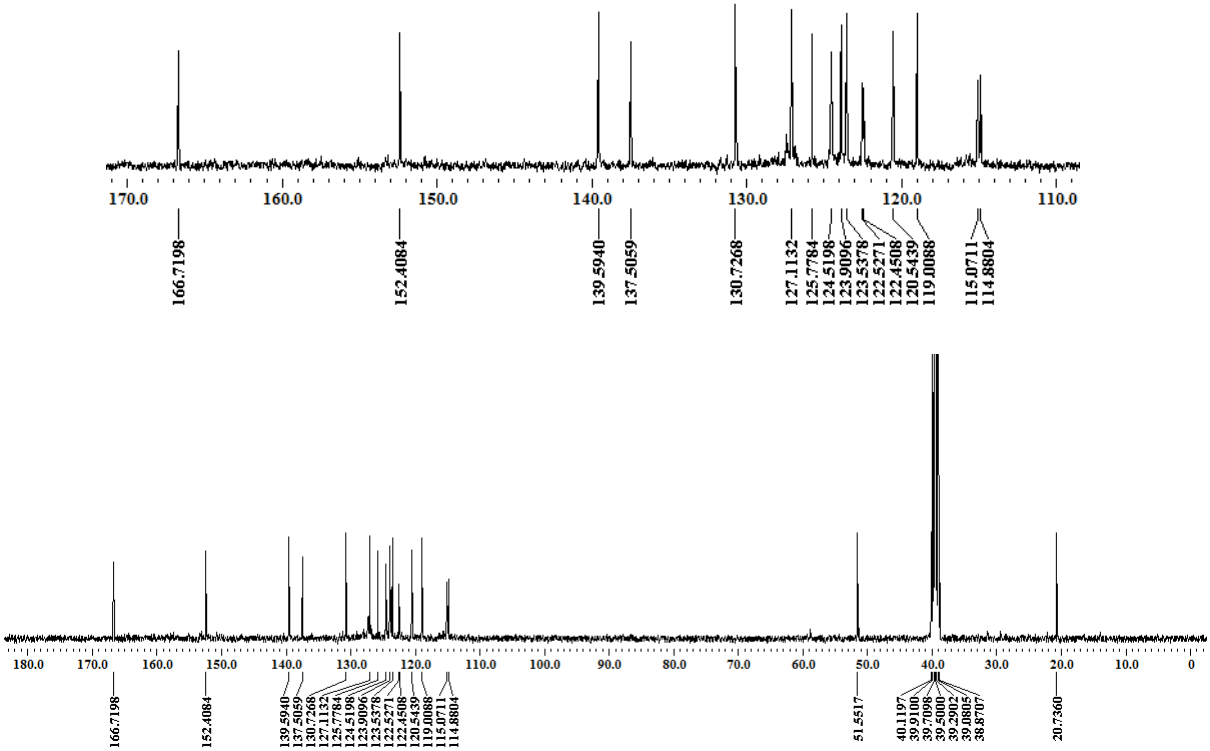
(*E*)-Methyl 3-(2-(3-(o-tolyl)ureido)phenyl)acrylate (6c)



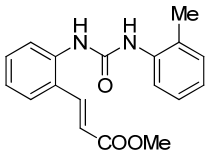
^{13}C NMR



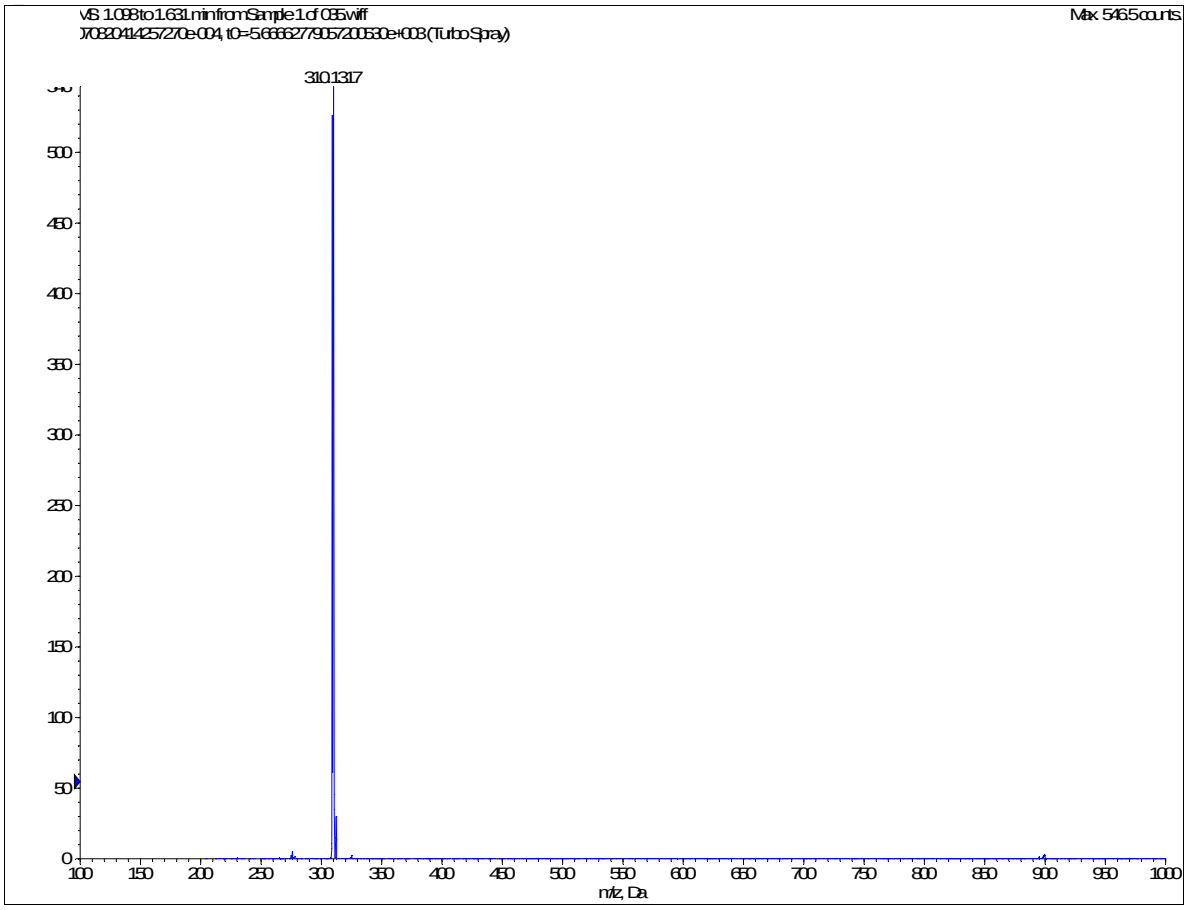
(*E*)-Methyl 3-(2-(3-(o-tolyl)ureido)phenyl)acrylate (6c)



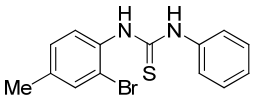
HRMS



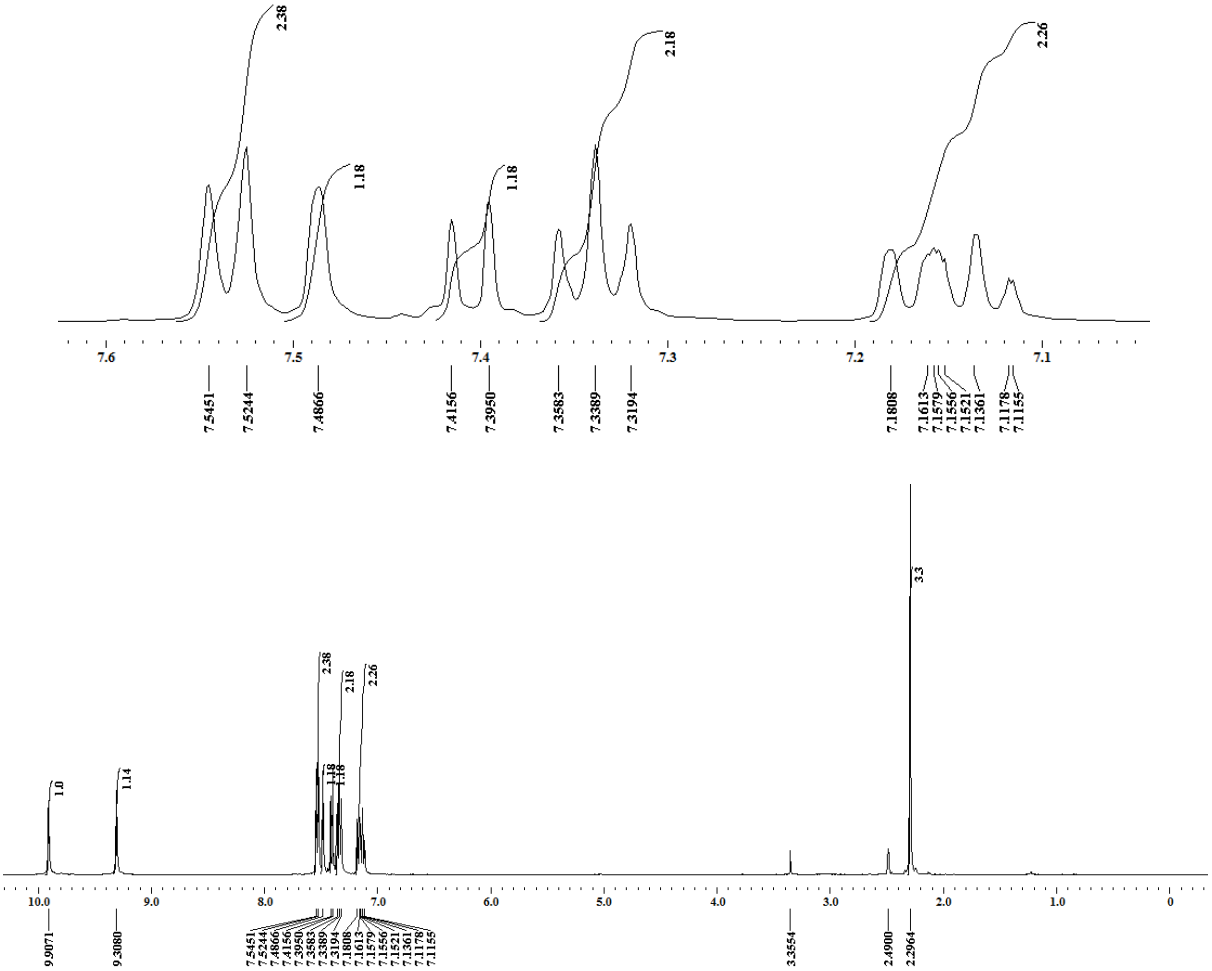
(*E*)-Methyl 3-(2-(3-(o-tolyl)ureido)phenyl)acrylate (6c)



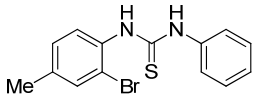
^{1}H NMR



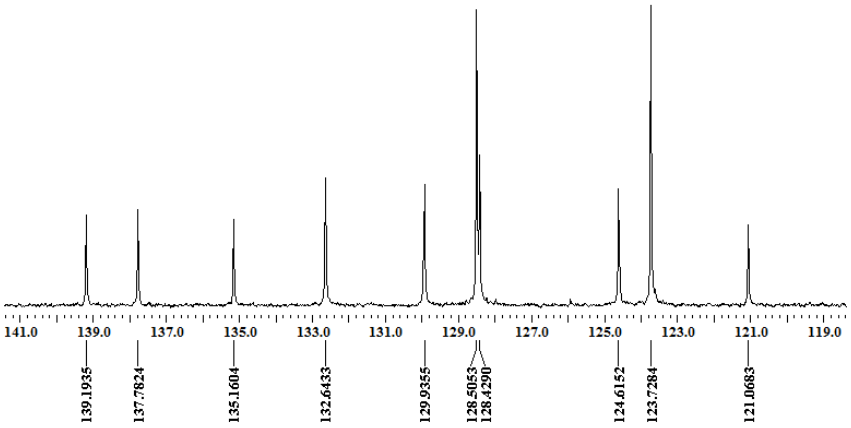
1-(2-Bromo-4-methylphenyl)-3-phenylthiourea (10)

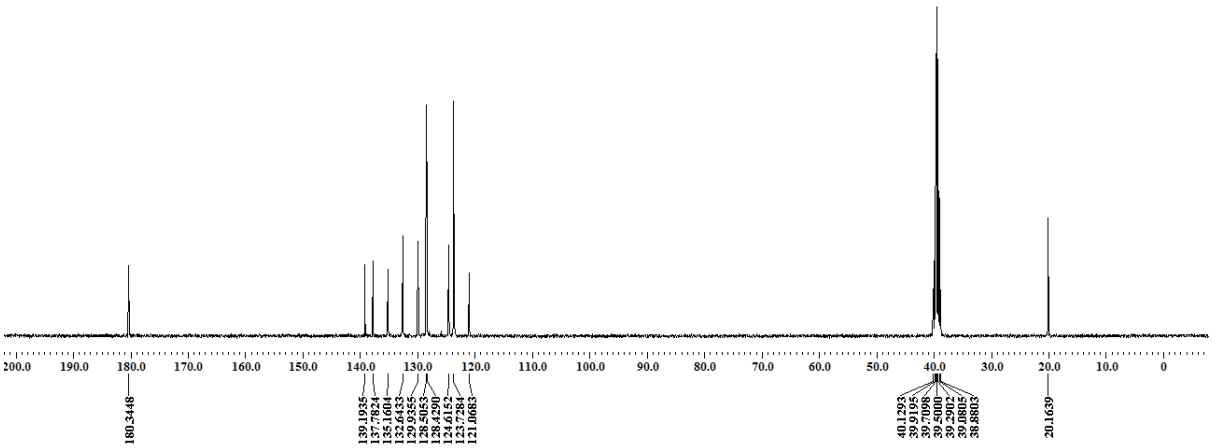


^{13}C NMR

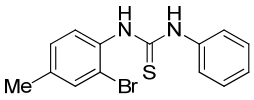


1-(2-Bromo-4-methylphenyl)-3-phenylthiourea (10)

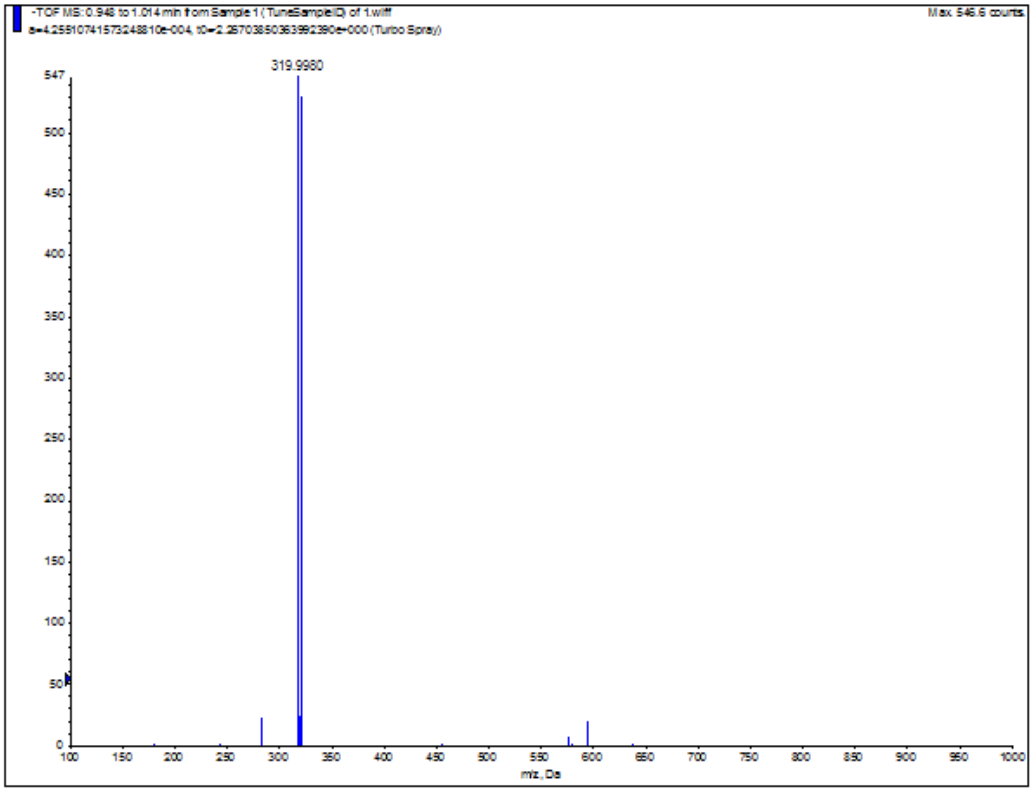




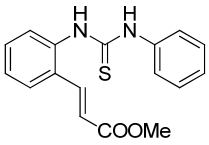
HRMS



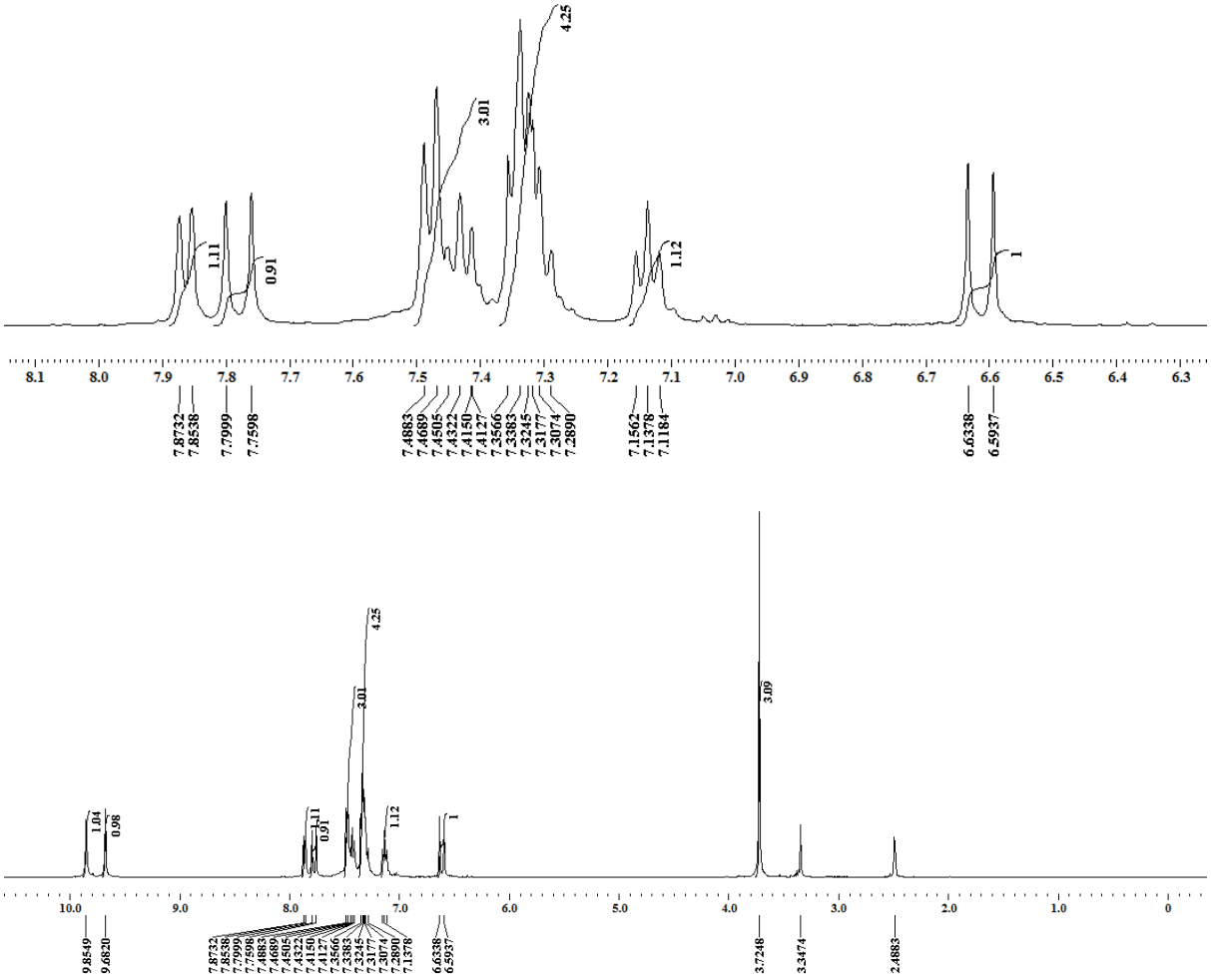
1-(2-Bromo-4-methylphenyl)-3-phenylthiourea (10)



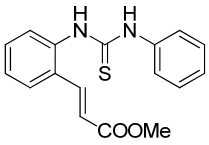
^{1}H NMR



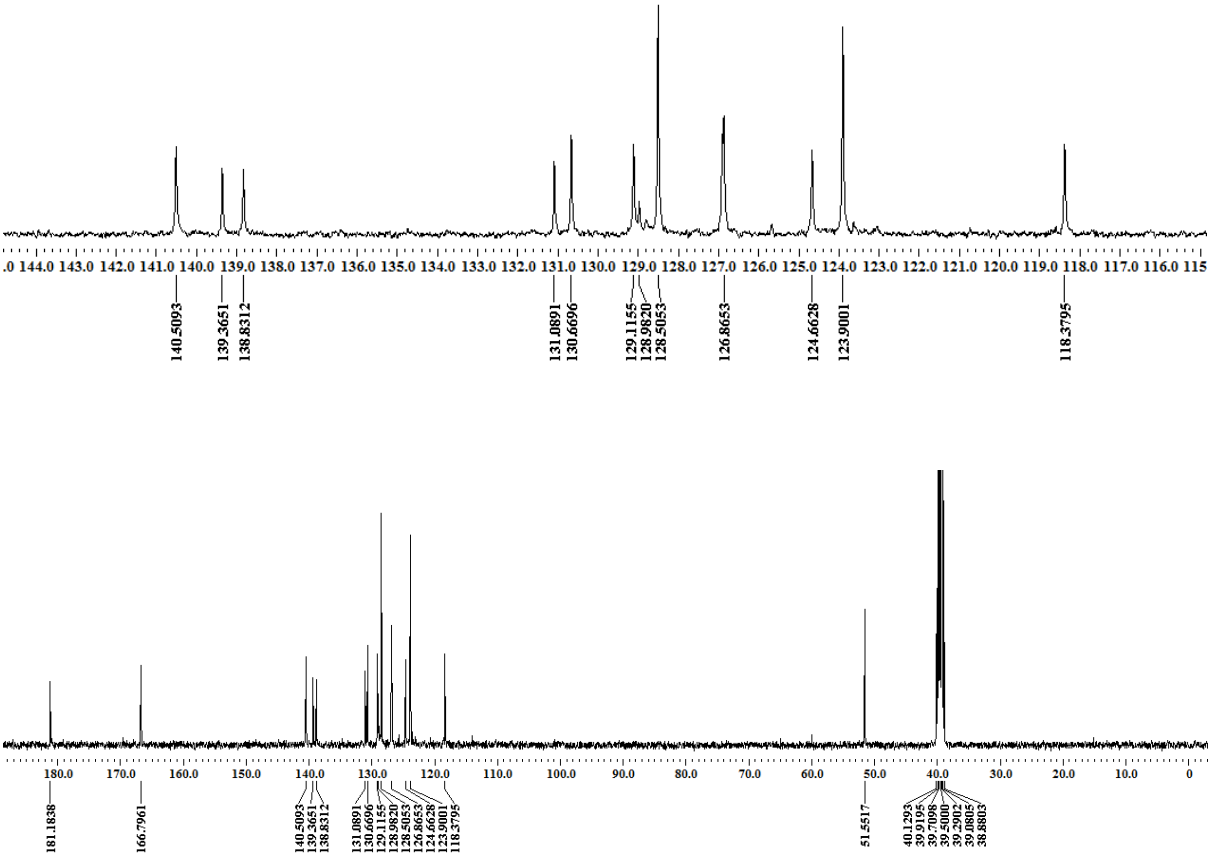
(*E*)-methyl 3-(2-(3-phenylthioureido)phenyl)acrylate (P)



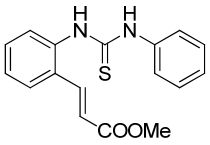
^{13}C NMR



(*E*)-methyl 3-(2-(3-phenylthioureido)phenyl)acrylate (P)



HRMS



(*E*)-methyl 3-(2-(3-phenylthioureido)phenyl)acrylate (P)