

Scalable and Practical Synthesis of Halo Quinolin- 2(1*H*)-ones and Quinolines

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1. Analytical method

LC-MS method:

LC-MS method : Waters iClass, Thermo MSQ Plus and DAD

Injection volume:	0.15 µL
Column:	Zorbax RRHD SB-AQ, 1.8 µm, 2.1 x 50 mm
Column flow:	0.8 mL/min
Eluent:	Eluent A: Water, 0.04% TFA Eluent B: Acetonitrile
Gradient:	0.00 min 5% B 1.20 min 95% B 1.90 min 95% B 2.1 min 5% B
Temperature:	40 °C

The purity is given in area percent (% a/a).

2. Analytical Data of Anilides 2b-2ae and Experimental Procedures for 2a, 2e and 2p

***N*-(2-iodophenyl)-3,3-dimethoxypropanamide (2a).** 40% NaHMDS solution in THF (1400 mL, 1.5 equiv) was added over 20 min to a solution of 2-iodoaniline **1a** (401 g, 1.0 equiv) and methyl 3,3-dimethoxypropionate (330 mL, 1.2 equiv) in Me-THF (2.4 L) at 0-5 °C. The resulting solution was stirred at 0 °C for 30 min, then warmed to 22 °C and stirred at this temperature for 16 h. The reaction mixture was added over 30 min to an aqueous citric acid solution (800 g citric acid and 2.4 L H₂O) at 0-10 °C. The mixture was warmed to 22 °C and stirred for 10 min. The organic layer was separated and washed with H₂O (2.4 L). The organic layer was concentrated under reduced pressure to afford a brown solid. Yield: 653 g (crude). Purity (LC-MS): 98% (210 nm); *t_R* 0.72 min, [M + 1]⁺ = 336.

***N*-(2-Bromophenyl)-3,3-dimethoxypropanamide (2b).** 2-bromoaniline was converted according to the general amide formation procedure. Yield: 13.2 g (crude). Purity (LC-MS): 89.8% (210 nm), *t_R* 0.79 min; [M + 1]⁺ = 288, ¹H NMR (D₆-DMSO, signals of title compound only) δ : 9.48 (s, 1 H), 7.70 (m, 1 H), 7.66 (m, 1 H), 7.35-7.39 (m, 1 H), 7.11-7.14 (m, 1 H), 4.80 (t, *J* = 5.6 Hz, 1 H), 3.32 (s, 6 H), 2.72 (d, *J* = 5.6 Hz, 2 H).

***N*-(2-Chlorophenyl)-3,3-dimethoxypropanamide (2c).** 2-chloroaniline was converted according to the general amide formation procedure. Yield: 10.9 g (crude). Purity (LC-MS): 89.6% (210 nm), *t_R* 0.78 min; [M + 1]⁺ = 244, ¹H NMR (D₆-DMSO, signals of title compound only) δ : 9.54 (s, 1 H), 7.79 (m, 1 H), 7.49 (m, 1 H), 7.32 (m, 1 H), 7.18 (m, 1 H), 4.81 (t, *J* = 5.7 Hz, 1 H), 3.31 (s, 6 H), 2.74 (d, *J* = 5.6 Hz, 2 H).

***N*-(2-Fluorophenyl)-3,3-dimethoxypropanamide (2d).** 2-fluoroaniline was converted according to the general amide formation procedure. Yield: 10.0 g (crude). Purity (LC-MS): 73.8% (210 nm), *t_R* 0.70 min; [M + 1]⁺ = 228, ¹H NMR (D₆-DMSO, signals of title compound only) δ : 9.75 (s, 1 H), 7.90-7.93 (m, 1 H), 7.22-7.27 (m, 1 H), 7.12-7.19 (m, 2 H), 4.80 (t, *J* = 5.8 Hz, 1 H), 3.29 (s, 6 H), 2.74 (d, *J* = 5.8 Hz, 2 H).

***N*-(4-Iodophenyl)-3,3-dimethoxypropanamide (2e).** 4-iodoaniline was converted according to the general amide formation procedure. Yield: 13.7 g (crude). Purity (LC-MS): 83.0% (210 nm), t_R 0.83 min; $[M + 1]^+ = 336$, 1H NMR (D_6 -DMSO, signals of title compound only) δ : 10.08 (s, 1 H), 7.63 (d, $J = 8.7$ Hz, 2 H), 7.44 (d, $J = 8.7$ Hz, 2 H), 4.79 (t, $J = 5.8$ Hz, 1 H), 3.28 (s, 6 H), 2.63 (d, $J = 5.8$ Hz, 2 H).

***N*-(4-iodophenyl)-3,3-dimethoxypropanamide (2e)** 40% NaHMDS solution in THF (314 g, 1.5 equiv) was added over 20 min to a solution of 4-iodoaniline **1e** (100 g, 1.0 equiv) and methyl 3,3-dimethoxypropionate (85 g, 1.2 equiv) in Me-THF (600 mL) at 0 °C. The resulting solution was stirred at 0 °C for 10 min, then warmed to 22 °C and stirred for 16 h at this temperature. The reaction mixture was added over 20 min to 20% aqueous citric acid solution (700 mL) at 0-10 °C. The mixture was warmed to 22 °C and stirred for 10 min. The organic layer was separated and concentrated under reduced pressure. The aqueous layer was extracted with TBME (1 L). The organic layer was combined with the residue and the resulting organic solution was washed with H₂O (800 mL). The organic layer was concentrated under reduced pressure to afford a dark red solid. Yield: 169 g (crude). Purity (LC-MS): 87% (210 nm); t_R 0.84 min, $[M + 1]^+ = 336$.

***N*-(4-Bromophenyl)-3,3-dimethoxypropanamide (2f).** 4-bromoaniline was converted according to the general amide formation procedure. Yield: 11.8 g (crude). Purity (LC-MS): 87.5% (210 nm), t_R 0.81 min; $[M + 1]^+ = 288$, 1H NMR (D_6 -DMSO, signals of title compound only) δ : 10.12 (s, 1 H), 7.57 (d, $J = 8.8$ Hz, 2 H), 7.48 (d, $J = 8.8$ Hz, 2 H), 4.79 (t, $J = 5.8$ Hz, 1 H), 3.28 (s, 6 H), 2.64 (d, $J = 5.8$ Hz, 2 H).

***N*-(4-Chlorophenyl)-3,3-dimethoxypropanamide (2g).** 4-chloroaniline was converted according to the general amide formation procedure. Yield: 9.8 g (crude). Purity (LC-MS): 72% (210 nm), t_R 0.78 min; $[M + 1]^+ = 244$, 1H NMR (D_6 -DMSO, signals of title compound only) δ : 10.12 (s, 1 H), 7.62 (d, $J = 8.9$ Hz, 2 H), 7.35 (d, $J = 8.8$ Hz, 2 H), 4.79 (t, $J = 5.8$ Hz, 1 H), 3.28 (s, 6 H), 2.64 (d, $J = 5.8$ Hz, 2 H).

***N*-(4-Fluorophenyl)-3,3-dimethoxypropanamide (2h).** 4-fluoroaniline was converted according to the general amide formation procedure. Yield: 8.9 g (crude). Purity (LC-MS): 62% (210 nm), t_R 0.70 min; $[M + 1]^+ = 228$, 1H NMR (D_6 -DMSO, signals of title compound only) δ : 10.03 (s, 1 H), 7.61 (m, 2 H), 7.14 (m, 2 H), 4.79 (t, $J = 5.8$ Hz, 1 H), 3.28 (s, 6 H), 2.62 (d, $J = 5.8$ Hz, 3 H).

3,3-Dimethoxy-*N*-(2-(trifluoromethyl)phenyl)propanamide (2i). 2-(Trifluoromethyl)aniline was converted according to the general amide formation procedure. Yield: 12.0 g (crude). Purity (LC-MS): 84.1% (210 nm), t_R 0.80 min; $[M + 1]^+ = 278$, 1H NMR (D_6 -DMSO, signals of title compound only) δ : 9.58 (s, 1 H), 7.73 (m, 1 H), 7.67 (m, 1 H), 7.55 (m, 1 H), 7.44 (m, 1 H), 4.78 (t, $J = 5.7$ Hz, 1 H), 3.30 (s, 6 H), 2.69 (d, $J = 5.6$ Hz, 2 H).

3,3-Dimethoxy-*N*-(4-(trifluoromethyl)phenyl)propanamide (2j). 4-(Trifluoromethyl)aniline was converted according to the general amide formation procedure. Yield: 12.1 g (crude). Purity (LC-MS): 87.7% (210 nm), t_R 0.87 min; $[M + 1]^+ = 278$, 1H NMR (D_6 -DMSO, signals of title compound only) δ : 10.35 (s, 1 H), 7.81 (d, $J = 8.6$ Hz, 2 H), 7.66 (d, $J = 8.7$ Hz, 2 H), 4.81 (t, $J = 5.8$ Hz, 1 H), 3.29 (s, 6 H), 2.69 (d, $J = 5.9$ Hz, 2 H).

***N*-(2-Bromo-3-fluorophenyl)-3,3-dimethoxypropanamide (2k).** 2-bromo-3-fluoroaniline **1k** was converted according to the general amide formation procedure. Yield: 13.4 g (crude). Purity (LC-MS): 96% (210 nm), t_R 0.82 min; $[M + 1]^+ = 308$, 1H NMR (D_6 -DMSO, signals of title compound only) δ : 9.62 (s, 1 H), 7.58 (m, 1 H), 7.40 (m, 1 H), 7.18 (m, 1 H), 4.81 (t, $J = 5.6$ Hz, 1 H), 3.32 (s, 6 H), 2.75 (d, $J = 5.6$ Hz, 2 H).

***N*-(2-Bromo-4-fluorophenyl)-3,3-dimethoxypropanamide (2l).** 2-bromo-4-fluoroaniline **1l** was converted according to the general amide formation procedure. Yield: 12.3 g (crude). Purity (LC-MS): 97% (210 nm), t_R 0.80 min; $[M + 1]^+ = 308$, 1H NMR (D_6 -DMSO, signals of title compound only) δ : 9.55 (s, 1 H), 7.61-7.65 (m, 2 H), 7.25-7.29 (m, 1 H), 4.80 (t, $J = 5.7$ Hz, 1 H), 3.30 (s, 6 H), 2.69 (d, $J = 5.7$ Hz, 2 H).

***N*-(2-Bromo-5-fluorophenyl)-3,3-dimethoxypropanamide (2m).** 2-bromo-5-fluoroaniline **1m** was converted according to the general amide formation procedure. Yield: 12.7 g (crude). Purity (LC-MS):

97% (210 nm), t_R 0.86 min; $[M + 1]^+ = 308$, 1H NMR (D_6 -DMSO, signals of title compound only) δ : 9.54 (s, 1 H), 7.68-7.73 (m, 2 H), 7.01 (m, 1 H), 4.80 (t, $J = 5.5$ Hz, 1 H), 3.32 (s, 6 H), 2.77 (d, $J = 5.5$ Hz, 2 H).

***N*-(4-Fluoro-2-iodo-phenyl)-3,3-dimethoxypropanamide (2n).** 4-fluoro-2-iodo-aniline **1n** was converted according to the general amide formation procedure. Yield: 15.2 g (crude). Purity (LC-MS): 93% (210 nm), t_R 0.80 min; $[M + 1]^+ = 354$, 1H NMR (500 MHz, DMSO) δ : 9.48 (s, 1 H), 7.76 (dd, $J_1 = 2.9$ Hz, $J_2 = 8.2$ Hz, 1 H), 7.43 (dd, $J_1 = 5.6$ Hz, $J_2 = 8.9$ Hz, 1 H), 7.27 (td, $J_1 = 2.9$ Hz, $J_2 = 8.5$ Hz, 1 H), 4.81 (t, $J = 5.7$ Hz, 1 H), 3.31 (s, 6 H), 2.66 (d, $J = 5.7$ Hz, 2 H).

***N*-(4-Chloro-2-iodo-phenyl)-3,3-dimethoxypropanamide (2o).** 4-chloro-2-iodo-aniline **1o** was converted according to the general amide formation procedure. Yield: 15.8 g (crude). Purity (LC-MS): 87% (210 nm), t_R 0.88 min; $[M + 1]^+ = 370$, 1H NMR (500 MHz, DMSO) δ : 9.47 (s, 1 H), 7.94 (d, $J = 2.4$ Hz, 1 H), 7.51 (m, 1 H), 7.46 (dd, $J_1 = 2.4$ Hz, $J_2 = 8.7$ Hz, 1 H), 4.81 (t, $J = 5.7$ Hz, 1 H), 3.31 (s, 6 H), 2.69 (d, $J = 5.6$ Hz, 2 H).

***N*-(4-Bromo-2-iodophenyl)-3,3-dimethoxypropanamide (2p)** 40% NaHMDS solution in THF (55 g, 1.5 equiv) was added over 20 min to a solution of 4-bromo-2-iodoaniline **1p** (24.6 g, 1.0 equiv) and methyl 3,3-dimethoxypropionate (15 g, 1.2 equiv) in THF (160 mL) at 0 °C. The resulting solution was stirred at 0 °C for 10 min and allowed to warm up to 22 °C. After stirring at 22 °C for 16 h, 20% aqueous citric acid solution (120 mL) was added at 5 °C. The THF layer was separated and the aqueous layer was extracted with DCM (100 mL). The THF layer was concentrated under reduced pressure and to the residue was added DCM (200 mL) and the first DCM layer. The resulting mixture was extracted with H_2O (100 mL) and concentrated to dryness to give the intermediate as a dark brown solid. Yield: 36 g (crude). Purity (LC-MS): 92% (210 nm); t_R 0.91 min, $[M + 1]^+ = 414$; 1H NMR (D_6 -DMSO) δ : 9.45 (s, 1 H), 8.06 (d, $J = 2.0$ Hz, 1 H), 7.58 (dd, $J_1 = 8.6$ Hz, $J_2 = 2.0$ Hz, 1 H), 7.47 (d, $J = 8.6$ Hz, 1 H), 4.81 (t, $J = 5.6$ Hz, 1 H), 3.32 (s, 6 H), 2.69 (d, $J = 5.5$ Hz, 2 H).

***N*-(2-Chloro-3-methylphenyl)-3,3-dimethoxypropanamide (2q).** 2-chloro-3-methylaniline was converted according to the general amide formation procedure. Yield: 12.2 g (crude). Purity (LC-MS):

79.5% (210 nm), t_R 0.85 min; $[M + 1]^+ = 258$, 1H NMR (D_6 -DMSO, signals of title compound only) δ : 9.48 (s, 1 H), 7.67 (m, 1 H), 7.20 (m, 1 H), 7.13 (m, 1 H), 4.82 (t, $J = 5.6$ Hz, 1 H), 3.32 (s, 6 H), 2.76 (d, $J = 5.6$ Hz, 2 H), 2.35 (s, 3 H).

***N*-(2-Chloro-4-methylphenyl)-3,3-dimethoxypropanamide (2r).** 2-chloro-4-methylaniline was converted according to the general amide formation procedure. Yield: 11.9 g (crude). Purity (LC-MS): 92.6% (210 nm), t_R 0.84 min; $[M + 1]^+ = 258$, 1H NMR (D_6 -DMSO, signals of title compound only) δ : 9.46 (s, 1 H), 7.65 (d, $J = 8.2$ Hz, 1 H), 7.30 (s, 1 H), 7.11 (d, $J = 8.1$ Hz, 1 H), 4.81 (t, $J = 5.6$ Hz, 1 H), 3.31 (s, 6 H), 2.73 (d, $J = 5.7$ Hz, 2 H), 2.27 (s, 3 H).

***N*-(2-Chloro-5-methylphenyl)-3,3-dimethoxypropanamide (2s).** 2-chloro-5-methylaniline was converted according to the general amide formation procedure. Yield: 11.5 g (crude). Purity (LC-MS): 57.9% (210 nm), t_R 0.85 min; $[M + 1]^+ = 258$, 1H NMR (D_6 -DMSO, signals of title compound only) δ : 9.47 (s, 1 H), 7.62 (s, 1 H), 7.35 (d, $J = 8.1$ Hz, 1 H), 6.99 (d, $J = 8.1$ Hz, 1 H), 4.80 (t, $J = 5.6$ Hz, 1 H), 3.31 (s, 6 H), 2.73 (d, $J = 5.6$ Hz, 2 H), 2.28 (s, 3 H).

***N*-(3-Chloro-2-methylphenyl)-3,3-dimethoxypropanamide (2t).** 3-chloro-2-methylaniline was converted according to the general amide formation procedure. Yield: 10.7 g (crude). Purity (LC-MS): 76.8% (210 nm), t_R 0.79 min; $[M + 1]^+ = 258$, 1H NMR (D_6 -DMSO, signals of title compound only) δ : 9.61 (s, 1 H), 7.28-7.30 (m, 2 H), 7.20 (m, 1 H), 4.80 (t, $J = 5.8$ Hz, 1 H), 3.30 (s, 6 H), 2.67 (d, $J = 5.8$ Hz, 2 H), 2.21 (s, 3 H).

***N*-(4-Chloro-2-methylphenyl)-3,3-dimethoxypropanamide (2u).** 4-chloro-2-methylaniline was converted according to the general amide formation procedure. Yield: 10.6 g (crude). Purity (LC-MS): 51.6% (210 nm), t_R 0.80 min; $[M + 1]^+ = 258$, 1H NMR (D_6 -DMSO, signals of title compound only) δ : 9.38 (m, 1 H), 7.43 (m, 1 H), 7.21-7.30 (m, 2 H), 4.80 (s, 1 H), 3.30 (s, 6 H), 2.51 (s, 2 H), 2.19 (s, 3 H).

***N*-(5-Chloro-2-methylphenyl)-3,3-dimethoxypropanamide (2v).** 5-chloro-2-methylaniline was converted according to the general amide formation procedure. Yield: 10.4 g (crude). Purity (LC-MS): 40.6% (210 nm), t_R 0.81 min; $[M + 1]^+ = 258$, 1H NMR (D_6 -DMSO, signals of title compound only) δ :

9.39 (s, 1 H), 7.59 (m, 1 H), 7.23 (m, 1 H), 7.12 (m, 1 H), 4.80 (t, $J = 5.8$ Hz, 1 H), 3.31 (s, 6 H), 2.71 (d, $J = 5.8$ Hz, 2 H), 2.19 (s, 3 H).

***N*-(2-Chloro-3-methoxyphenyl)-3,3-dimethoxypropanamide (2w).** 2-chloro-3-methoxyaniline was converted according to the general amide formation procedure. Yield: 11.9 g (crude). Purity (LC-MS): 81.9% (210 nm), t_R 0.79 min; $[M + 1]^+ = 274$, 1H NMR (D_6 -DMSO, signals of title compound only) δ : 9.47 (s, 1 H), 7.46 (d, $J = 8.1$ Hz, 1 H), 7.26 (t, $J = 8.2$ Hz, 1 H), 6.93 (d, $J = 8.2$ Hz, 1 H), 4.81 (t, $J = 5.6$ Hz, 1 H), 3.86 (s, 3 H), 3.31 (s, 6 H), 2.75 (d, $J = 5.6$ Hz, 2 H).

***N*-(2-Chloro-4-methoxyphenyl)-3,3-dimethoxypropanamide (2x).** 2-chloro-4-methoxyaniline was converted according to the general amide formation procedure. Yield: 11.4 g (crude). Purity (LC-MS): 79.2% (210 nm), t_R 0.78 min; $[M + 1]^+ = 274$, 1H NMR (D_6 -DMSO, signals of title compound only) δ : 9.45 (s, 1 H), 7.51 (d, $J = 8.9$ Hz, 1 H), 7.08 (d, $J = 2.9$ Hz, 1 H), 6.91 (dd, $J_1 = 2.8$ Hz, $J_2 = 8.9$ Hz, 1 H), 4.79 (t, $J = 5.8$ Hz, 1 H), 3.77 (s, 3 H), 2.67 (d, $J = 5.8$ Hz, 2 H).

***N*-(2-Chloro-5-methoxyphenyl)-3,3-dimethoxypropanamide (2y).** 2-chloro-5-methoxyaniline was converted according to the general amide formation procedure. Yield: 13.1 g (crude). Purity (LC-MS): 74.9% (210 nm), t_R 0.84 min; $[M + 1]^+ = 274$, 1H NMR (D_6 -DMSO, signals of title compound only) δ : 9.44 (s, 1 H), 7.53 (d, $J = 2.8$ Hz, 1 H), 7.37 (d, $J = 8.9$ Hz, 1 H), 6.76 (dd, $J_1 = 8.9$ Hz, $J_2 = 2.9$ Hz, 1 H), 4.80 (t, $J = 5.6$ Hz, 1 H), 3.74 (s, 3 H), 2.76 (d, $J = 5.6$ Hz, 2 H).

***N*-(3-Chloro-2-methoxyphenyl)-3,3-dimethoxypropanamide (2z).** 3-chloro-2-methoxyaniline was converted according to the general amide formation procedure. Yield: 12.1 g (crude). Purity (LC-MS): 87.5% (210 nm), t_R 0.85 min; $[M + 1]^+ = 274$, 1H NMR (D_6 -DMSO, signals of title compound only) δ : 9.52 (s, 1 H), 8.01-8.02 (m, 1 H), 7.18 (m, 1 H), 7.10 (m, 1 H), 4.80 (t, $J = 5.5$ Hz, 1 H), 3.77 (s, 3 H), 3.31 (s, 6 H), 2.80 (d, $J = 5.6$ Hz, 2 H).

***N*-(4-Chloro-2-methoxyphenyl)-3,3-dimethoxypropanamide (2aa).** 4-chloro-2-methoxyaniline was converted according to the general amide formation procedure. Yield: 11.6 g (crude). Purity (LC-MS): 87.1% (210 nm), t_R 0.86 min; $[M + 1]^+ = 274$, 1H NMR (D_6 -DMSO, signals of title compound only) δ :

9.24-9.33 (m, 1 H), 8.03 (d, $J = 8.6$ Hz, 1 H), 7.11 (d, $J = 2.2$ Hz, 1 H), 6.96 (dd, $J_1 = 8.6$ Hz, $J_2 = 2.2$ Hz, 1 H), 4.78 (t, $J = 5.6$ Hz, 1 H), 3.87 (s, 3 H), 3.29 (s, 6 H), 2.74 (d, $J = 5.6$ Hz, 2 H).

***N*-(5-Chloro-2-methoxyphenyl)-3,3-dimethoxypropanamide (2ab).** 5-chloro-2-methoxyaniline was converted according to the general amide formation procedure. Yield: 12.2 g (crude). Purity (LC-MS): 78.7% (210 nm), t_R 0.87 min; $[M + 1]^+ = 274$, 1H NMR (D_6 -DMSO, signals of title compound only) δ : 9.37 (s, 1 H), 8.17 (m, 1 H), 7.09 (m, 1 H), 7.04 (m, 1 H), 4.78 (t, $J = 5.6$ Hz, 1 H), 3.85 (s, 3 H), 3.30 (s, 6 H), 2.77 (d, $J = 5.6$ Hz, 2 H).

3,3-Dimethoxy-*N*-(2-methyl-3-(trifluoromethyl)phenyl)propanamide (2ac). 2-methyl-3-(trifluoromethyl)aniline was converted according to the general amide formation procedure. Yield: 12.1 g (crude). Purity (LC-MS): 66.2% (210 nm), t_R 0.85 min; $[M + 1]^+ = 292$, 1H NMR (D_6 -DMSO, signals of title compound only) δ : 9.65 (s, 1 H), 7.59 (m, 1 H), 7.55 (m, 1 H), 7.39 (m, 1 H), 4.80 (t, $J = 5.9$ Hz, 1 H), 3.31 (s, 6 H), 2.69 (d, $J = 5.9$ Hz, 2 H), 2.28 (s, 3 H).

3,3-Dimethoxy-*N*-(2-methyl-5-(trifluoromethyl)phenyl)propanamide (2ad). 2-methyl-5-(trifluoromethyl)aniline was converted according to the general amide formation procedure. Yield: 12.5 g (crude). Purity (LC-MS): 64.6% (210 nm), t_R 0.88 min; $[M + 1]^+ = 292$, 1H NMR (D_6 -DMSO, signals of title compound only) δ : 9.45-9.56 (m, 1 H), 7.87 (m, 1 H), 7.44 (m, 2 H), 4.81 (t, $J = 5.8$ Hz, 1 H), 3.31 (s, 6 H), 2.73 (d, $J = 5.8$ Hz, 2 H), 2.30 (s, 3 H).

3,3-Dimethoxy-*N*-(5-methyl-2-(trifluoromethyl)phenyl)propanamide (2ae). 5-methyl-2-(trifluoromethyl)aniline was converted according to the general amide formation procedure. Yield: 12.3 g (crude). Purity (LC-MS): 59.5% (210 nm), t_R 0.87 min; $[M + 1]^+ = 292$, 1H NMR (D_6 -DMSO, signals of title compound only) δ : 9.52 (s, 1 H), 7.60 (d, $J = 8.0$ Hz, 1 H), 7.36 (s, 1 H), 7.24 (d, $J = 8.0$ Hz, 1 H), 4.78 (t, $J = 5.6$ Hz, 1 H), 3.30 (s, 6 H), 2.68 (d, $J = 5.6$ Hz, 2 H), 2.37 (s, 3 H).

3. Analytical Data for Quinolin-2(1*H*)-ones 3b-3ae and Experimental Procedure for 3p

8-Bromo-2-quinolin-2(1*H*)-one (3b). Obtained from amide **2b** according to the general cyclisation procedure A as yellow solid. Yield: 8.0 g (89%). Purity (LC-MS): 99.3% (210 nm), t_R 0.69 min; $[M + 1]^+ = 226$, mp 183 °C (DSC); 1H NMR (D_6 -DMSO) δ : 10.51 (s, 1 H), 7.96 (d, $J = 9.5$ Hz, 1 H), 7.83 (m, 1 H), 7.73 (m, 1 H), 7.16 (m, 1 H), 6.61 (d, $J = 9.5$ Hz, 1 H); ^{13}C NMR (D_6 -DMSO) δ : 162.3, 141.0, 136.7, 134.4, 128.5, 123.6, 123.2, 121.5, 108.5.

8-Chloro-2-quinolin-2(1*H*)-one (3c). Obtained from amide **2c** according to the general cyclisation procedure A as yellow solid. Yield: 5.2 g (72%). Purity (LC-MS): 100% (210 nm), t_R 0.67 min; $[M + 1]^+ = 180$, mp 206 °C (DSC); 1H NMR (D_6 -DMSO) δ : 11.04 (s, 1 H), 7.97 (d, $J = 9.5$ Hz, 1 H), 7.67 (m, 2 H), 7.21 (m, 1 H), 6.61 (d, $J = 9.5$ Hz, 1 H); ^{13}C NMR (D_6 -DMSO) δ : 162.4, 140.8, 135.7, 131.0, 127.7, 123.4, 123.0, 121.4, 118.9.

8-Fluoro-2-quinolin-2(1*H*)-one (3d). Obtained from amide **2d** according to the general cyclisation procedure B as brown solid. Yield: 4.8 g (74%). Purity (LC-MS): 100% (210 nm), t_R 0.59 min; $[M + 1]^+ = 164$, mp 272 °C (DSC); 1H NMR (D_6 -DMSO) δ : 11.79 (s, 1 H), 7.95 (m, 1 H), 7.50 (m, 1 H), 7.41 (m, 1 H), 7.17 (m, 1 H), 6.58 (d, $J = 9.6$ Hz, 1 H); ^{13}C NMR (D_6 -DMSO) δ : 162.1, 149.1 (d, $J = 246$ Hz), 140.3 (d, $J = 3$ Hz), 127.9 (d, $J = 13$ Hz), 124.2 (d, $J = 3$ Hz), 123.7, 122.2 (d, $J = 7$ Hz), 121.7 (d, $J = 3$ Hz), 116.1 (d, $J = 17$ Hz).

6-Iodo-2-quinolin-2(1*H*)-one (3e). Obtained from amide **2e** according to the general cyclisation procedure A as pale yellow solid after a slurry in ACN (35 mL). Yield: 8.6 g (80%). Purity (LC-MS): 98.5% (210 nm), t_R 0.75 min; $[M + 1]^+ = 272$, mp 253 °C (DSC), 1H NMR (D_6 -DMSO) δ : 11.84 (s, 1 H), 8.07 (s, 1 H), 7.85 (d, $J = 9.6$ Hz, 1 H), 7.77 (d, $J = 8.6$ Hz, 1 H), 7.12 (d, $J = 8.6$ Hz, 1 H), 6.52 (d, $J = 9.6$ Hz, 1 H); ^{13}C NMR (D_6 -DMSO) δ : 162.1, 139.5, 138.8, 137.9, 136.4, 123.3, 121.8, 117.8, 85.3.

6-Bromo-2-quinolin-2(1*H*)-one (3f). Obtained from amide **2f** according to the general cyclisation procedure A as pale yellow solid after a slurry in ACN (35 mL). Yield: 7.2 g (80%). Purity (LC-MS):

100% (210 nm), t_R 0.72 min; $[M + 1]^+ = 226$, mp 270 °C (DSC); 1H NMR (D_6 -DMSO) δ : 11.87 (s, 1 H), 7.93 (d, $J = 2.1$ Hz, 1 H), 7.88 (d, $J = 9.6$ Hz, 1 H), 7.65 (dd, $J_1 = 8.7$ Hz, $J_2 = 2.2$ Hz, 1 H), 7.25 (d, $J = 8.8$ Hz, 1 H), 6.56 (d, $J = 9.6$ Hz, 1 H); ^{13}C NMR (D_6 -DMSO) δ : 162.1, 139.6, 138.4, 133.3, 130.4, 123.6, 121.3, 117.7, 113.8.

6-Chloro-2-quinolin-2(1H)-one (3g). Obtained from amide **2g** according to the general cyclisation procedure A as yellow solid after a slurry in ACN (35 mL). Yield: 6.1 g (85%). Purity (LC-MS): 100% (210 nm), t_R 0.69 min; $[M + 1]^+ = 180$, mp 266 °C (DSC); 1H NMR (D_6 -DMSO) δ : 11.79-11.97 (m, 1 H), 7.88 (d, $J = 9.6$ Hz, 1 H), 7.79 (d, $J = 2.3$ Hz, 1 H), 7.53 (dd, $J_1 = 8.8$ Hz, $J_2 = 2.4$ Hz, 1 H), 7.31 (d, $J = 8.8$ Hz, 1 H), 6.56 (d, $J = 9.6$ Hz, 1 H); ^{13}C NMR (D_6 -DMSO) δ : 162.2, 139.7, 138.1, 130.7, 127.4, 126.0, 123.7, 120.8, 117.5.

6-Fluoro-2-quinolin-2(1H)-one (3h). Obtained from amide **2h** according to the general cyclisation procedure A as brown solid after a slurry in ACN (35 mL). Yield: 2.5 g (39%). Purity (LC-MS): 100% (210 nm), t_R 0.69 min; $[M + 1]^+ = 164$, mp 271 °C (DSC); 1H NMR (D_6 -DMSO) δ : 11.82 (s, 1 H), 7.89 (d, $J = 9.6$ Hz, 1 H), 7.54 (dd, $J_1 = 9.1$ Hz, $J_2 = 2.7$ Hz, 1 H), 7.40 (m, 1 H), 7.33 (dd, $J_1 = 9.0$ Hz, $J_2 = 4.8$ Hz, 1 H), 6.57 (d, $J = 9.6$ Hz, 1 H); ^{13}C NMR (D_6 -DMSO) δ : 162.1, 157.4 (d, $J = 238$ Hz), 139.9 (d, $J = 3$ Hz), 136.1, 123.7, 120.2 (d, $J = 9$ Hz), 118.8 (d, $J = 25$ Hz), 117.3, 113.1 (d, $J = 23$ Hz).

8-Trifluoromethyl-2-quinolin-2(1H)-one (3i). Obtained from amide **2i** according to the general cyclisation procedure B. No precipitation was observed after pouring onto ice (100 g). The aqueous phase was extracted with DCM (2 x 100 mL, 50 mL). The combined organic layers were concentrated to dryness. The crude product was purified through a slurry in ACN (35 mL) to afford a yellow solid. Yield: 2.4 g (28%). Purity (LC-MS): 100% (210 nm), t_R 0.74min; $[M + 1]^+ = 214$, mp 113 °C (DSC); 1H NMR (D_6 -DMSO) δ : 10.64-10.90 (br, 1 H), 8.09-8.10 (m, 1 H), 8.03 (m, 1 H), 7.91 (m, 1 H), 7.39 (m, 1 H), 6.72-6.73 (m, 1 H); ^{13}C NMR (D_6 -DMSO) δ : 162.2, 141.0, 135.3-135.9 (m), 133.6, 128.4 (q, $J = 5$ Hz), 127.3, 125.2, 123.0, 122.0, 113.9-115.6 (m).

6-Trifluoromethyl-2-quinolin-2(1H)-one (3j). Obtained from amide **2k** according to the general cyclisation procedure B as brown solid after a slurry in ACN (35 mL). Yield: 5.1 g (50%). Purity (LC-

MS): 98.3% (210 nm), t_R 0.76 min; $[M + 1]^+ = 214$, mp 199 °C (DSC); 1H NMR (D_6 -DMSO) δ : 12.04-12.09 (br, 1 H), 8.13 (s, 1 H), 8.04 (d, $J = 9.6$ Hz, 1 H), 7.81 (dd, $J_1 = 8.6$ Hz, $J_2 = 1.4$ Hz, 1 H), 7.46 (d, $J = 8.6$ Hz, 1 H), 6.63 (d, $J = 9.6$ Hz, 1 H); ^{13}C NMR (D_6 -DMSO) δ : 162.5 (s), 141.8 (s), 140.4 (s), 127.0 (m), 126.0 (q, $J = 4$ Hz), 123.9 (s), 123.7 (s), 122.6 (q, $J = 32$ Hz), 119.2 (s), 116.6 (s).

8-Bromo-7-fluoroquinolin-2(1H)-one (3k). Obtained from amide **2k** according to the general cyclisation procedure A as yellow solid after a slurry in ACN (35 mL). Yield: 8.94 g (92%). Purity (LC-MS): 99% (210 nm), t_R 0.73 min; $[M + 1]^+ = 242$, mp 188 °C (DSC); 1H NMR (D_6 -DMSO) δ : 10.83 (s, 1 H), 7.97 (d, $J = 9.2$ Hz, 1 H), 7.80 (dd, $J_1 = 6.1$ Hz, $J_2 = 8.5$ Hz, 1 H), 7.26 (t, $J = 8.6$ Hz, 1 H), 6.56 (d, $J = 8.8$ Hz, 1 H); ^{13}C NMR (D_6 -DMSO) δ : 162.5, 160.2 (d, $J = 247$ Hz), 140.7, 138.6, 129.9, 122.0, 117.9, 111.0 (d, $J = 25$ Hz), 95.6.

8-Bromo-6-fluoroquinolin-2(1H)-one (3l). Obtained from amide **2l** according to the general cyclisation procedure B with a cyclisation temperature of 40–60 °C. The product was slurried in ACN (35 mL) to afford yellow solid. Yield: 2.7 g (28%). Purity (LC-MS): 98.6% (210 nm), t_R 0.73 min; $[M + 1]^+ = 244$, mp 226 °C (DSC); 1H NMR (D_6 -DMSO) δ : 10.58-10.71 (br, 1 H), 7.94 (d, $J = 9.4$ Hz, 1 H), 7.87 (dd, $J_1 = 8.3$ Hz, $J_2 = 2.7$ Hz, 1 H), 7.67 (dd, $J_1 = 2.8$ Hz, $J_2 = 8.7$ Hz, 1 H), 6.67 (d, $J = 9.3$ Hz, 1 H); ^{13}C NMR (D_6 -DMSO) δ : 162.2 156.7 (d, $J = 242$ Hz), 140.2 (d, $J = 3$ Hz), 134.0, 124.3-124.5 (m), 122.4 (d, $J = 27$ Hz), 121.6-121.7 (m), 113.6 (d, $J = 23$ Hz), 108.8-109.0 (m).

8-Bromo-5-fluoroquinolin-2(1H)-one (3m). Obtained from amide **2m** according to the general cyclisation procedure A. The product was slurried in ACN (35 mL) to afford yellow solid. Yield: 7.6 g (79%). Purity (LC-MS): 98.3% (210 nm), t_R 0.74 min; $[M + 1]^+ = 244$, mp 195 °C (DSC); 1H NMR (D_6 -DMSO) δ : 10.79 (s, 1 H), 8.02 (d, $J = 9.4$ Hz, 1 H), 7.84 (m, 1 H), 7.06 (m, 1 H), 6.67 (d, $J = 9.1$ Hz, 1 H); ^{13}C NMR (D_6 -DMSO) δ : 162.1, 158.1 (d, $J = 251$ Hz), 137.9-138.0 (m), 135.0 (d, $J = 5$ Hz), 133.0 (d, $J = 5$ Hz), 123.9 (d, $J = 2$ Hz), 110.6-110.7 (m), 109.4 (d, $J = 22$ Hz), 103.3-103.4 (m).

6-Fluoro-8-iodoquinolin-2(1H)-one (3n).

Obtained from amide **2n** according to the general cyclisation procedure B as yellow solid after a slurry in ACN (35 mL). Yield: 4.0 g (35%). Purity (LC-MS): 99.4% (210 nm), t_R 0.77 min; $[M + 1]^+ = 290$, mp

261 °C (DSC); ¹H NMR (D₆-DMSO) δ: 9.60-9.99 (m, 1 H), 8.03 (d, *J* = 5.9 Hz, 1 H), 7.89-7.90 (m, 1 H), 7.68 (dd, *J*₁ = 2.0 Hz, *J*₂ = 8.5 Hz, 1 H), 6.64-6.70 (m, 1 H), ¹³C NMR (CDCl₃) δ: 162.3 (s), 157.4 (d, *J* = 248 Hz), 140.1 (d, *J* = 3 Hz), 134.9 (s), 128.5 (d, *J* = 26 Hz), 123.7 (s), 120.6 (d, *J* = 9 Hz), 113.9 (d, *J* = 22 Hz), 83.7 (d, *J* = 9 Hz).

6-Chloro-8-iodoquinolin-2(1*H*)-one (3o).

Obtained from amide **2o** according to the general cyclisation procedure B (33 equiv H₂SO₄) as yellow solid after a slurry in ACN (35 mL). Yield: 6.0 g (49%). Purity (LC-MS): 95.3% (210 nm), *t*_R 0.84 min; [M + 1]⁺ = 290, mp 217 °C (DSC); ¹H NMR (CDCl₃) δ: 8.77-9.35 (m, 1 H), 7.95 (d, *J* = 2.2 Hz, 1 H), 7.61 (d, *J* = 9.6 Hz, 1 H), 7.57 (d, *J* = 2.2 Hz, 1 H), 6.70 (d, *J* = 9.6 Hz, 1 H); ¹³C NMR (CDCl₃) δ: 162.2 (s), 139.6 (s), 136.9 (s), 128.5 (s), 127.8 (s), 124.0 (s), 120.9 (s), 84.2 (s).

6-Bromo-8-iodoquinolin-2(1*H*)-one (3p). N-(4-bromo-2-iodophenyl)-3,3-dimethoxypropan-amide **2p** (36 g, 1.0 equiv) in DCM (25 mL) was added over 10 min to concentrated H₂SO₄ (65 mL, 15.0 equiv) at 120 °C. DCM was continuously removed by distillation. After stirring at 120 °C for 0.5 h the reaction mixture was cooled to 10 °C and poured onto ice (200 g). The resulting suspension was filtered. The filter cake was washed with H₂O (2 x 50 mL), *i*PrOH (50 mL) and TBME (50 mL). The product was dissolved in DCM (400 mL) and extracted with 1 M aqueous HCl (2 x 100 mL). The organic solution was washed with H₂O (2 x 25 mL) and concentrated to dryness on a rotavap to afford beige solid. Yield: 11.2 g (40%). Purity (LC-MS): 91.1% (210 nm); *t*_R 0.86 min, [M + 1]⁺ = 351; mp 213 °C (DSC), ¹H NMR (D₆-DMSO) δ: 6.65-6.63 (m, 1 H), 7.88 (m, 1 H), 8.02 (s, 1 H), 8.19 (m, 1 H); ¹³C NMR (D₆-DMSO) δ: 162.3, 148.5, 142.0, 140.3, 139.8, 132.0, 131.1, 116.1, 114.8.

8-Chloro-7-methylquinolin-2(1*H*)-one (3q). Obtained from amide **2q** according to the general cyclisation procedure A with a reaction temperature of 22 °C. as yellow solid. Yield: 6.0 g (77%). Purity (LC-MS): 100% (210 nm), *t*_R 0.77 min; [M + 1]⁺ = 194, mp 205 °C (DSC); ¹H NMR (D₆-DMSO) δ: 7.93 (d, *J* = 9.5 Hz, 1 H), 7.57 (m, 1 H), 7.20 (m, 1 H), 6.54 (d, *J* = 9.5 Hz, 1 H), 2.44 (s, 3 H); ¹³C NMR (D₆-DMSO) δ: 162.5, 140.8, 138.7, 135.8, 126.9, 124.7, 122.1, 119.3, 118.7, 20.8.

8-Chloro-6-methylquinolin-2(1H)-one (3r). Obtained from amide **2r** according to the general cyclisation procedure A with a reaction temperature of 22 °C. as yellow solid. Yield: 6.38 g (82%). Purity (LC-MS): 100% (210 nm), t_R 0.77 min; $[M + 1]^+ = 194$, mp 186 °C (DSC); 1H NMR (D_6 -DMSO) δ : 11.01-10.91 (br, 1 H), 7.89 (d, $J = 9.5$ Hz, 1 H), 7.51 (s, 1 H), 7.47 (s, 1 H), 6.57 (d, $J = 9.5$ Hz, 1 H), 2.34 (s, 3 H); ^{13}C NMR (D_6 -DMSO) δ : 162.3, 140.5, 133.6, 132.5, 131.8, 127.5, 123.4, 121.2, 118.5, 20.4.

8-Chloro-5-methylquinolin-2(1H)-one (3s). Obtained from amide **2s** according to the general cyclisation procedure A with a reaction temperature of 22 °C. as yellow solid. Yield: 5.2 g (68%). Purity (LC-MS): 100% (210 nm), t_R 0.76 min; $[M + 1]^+ = 194$, mp 190 °C (DSC); 1H NMR ($CDCl_3$) δ : 9.18 (d, $J = 0.5$ Hz, 1 H), 7.96 (d, $J = 9.8$ Hz, 1 H), 7.45 (d, $J = 8.0$ Hz, 1 H), 7.01 (d, $J = 8.0$ Hz, 1 H), 6.73 (d, $J = 9.8$ Hz, 1 H), 2.56 (s, 3 H); ^{13}C NMR ($CDCl_3$) δ : 161.8, 137.3, 134.8, 134.7, 130.0, 124.2, 122.3, 119.7, 117.1, 18.6.

7-Chloro-8-methylquinolin-2(1H)-one (3t). Obtained from amide **2t** according to the general cyclisation procedure A with a reaction temperature of 22 °C. The crude product was purified through a slurry in ACN (35 mL) to afford yellow solid. Yield: 5.1 g (66%). Purity (LC-MS): 99.1% (210 nm), t_R 0.77 min; $[M + 1]^+ = 194$, mp 268 °C (DSC); 1H NMR ($CDCl_3$) δ : 9.65-9.47 (br, 1 H), 7.76 (d, $J = 9.5$ Hz, 1 H), 7.38 (m, 1 H), 7.26 (m, 1 H), 6.67 (d, $J = 9.5$ Hz, 1 H), 2.56 (s, 3 H); ^{13}C NMR ($CDCl_3$) δ : 163.1, 141.0, 137.6, 136.9, 126.5, 123.8, 121.2, 121.0, 118.3, 13.3.

6-Chloro-8-methylquinolin-2(1H)-one (3u). Obtained from amide **2u** according to the general cyclisation procedure A with a reaction temperature of 22 °C. The crude product was purified through a slurry in ACN (35 mL) to afford yellow solid. Yield: 5.05 g (65%). Purity (LC-MS): 100% (210 nm), t_R 0.78 min; $[M + 1]^+ = 194$, mp 260 °C (DSC); 1H NMR ($CDCl_3$) δ : 9.74 -9.69 (m, 1 H), 7.72 (d, $J = 9.6$ Hz, 1 H), 7.44 (d, $J = 1.6$ Hz, 1 H), 6.72 (d, $J = 9.5$ Hz, 1 H), 2.51 (s, 3 H); ^{13}C NMR ($CDCl_3$) δ : 162.8, 140.3, 135.4, 131.8, 127.5, 125.2, 125.0, 122.6, 120.6, 16.6.

5-Chloro-8-methylquinolin-2(1H)-one (3v) Obtained from amide **2v** according to the general cyclisation procedure A with a reaction temperature of 22 °C. The crude product was purified through a

slurry in ACN (35 mL) to afford yellow solid. Yield: 4.9 g (64%). Purity (LC-MS): 100% (210 nm), t_R 0.78 min; $[M + 1]^+ = 194$, mp 253 °C (DSC); 1H NMR (D_6 -DMSO) δ : 11.16-11.06 (br, 1 H), 8.11 (d, $J = 9.8$ Hz, 1 H), 7.36 (d, $J = 7.9$ Hz, 1 H), 7.24 (d, $J = 7.9$ Hz, 1 H), 6.66 (d, $J = 9.8$ Hz, 1 H), 2.42 (s, 3 H); ^{13}C NMR (D_6 -DMSO) δ : 162.4, 139.2, 136.6, 132.6, 129.2, 123.7, 123.6, 122.4, 116.7, 17.5.

8-Chloro-7-methoxy quinolin-2(1H)-one (3w). Obtained from amide **2w** according to the general cyclisation procedure A with a reaction temperature of 22 °C. as a yellow solid. Yield: 6.4 g (76%). Purity (LC-MS): 99.5% (210 nm), t_R 0.72 min; $[M + 1]^+ = 210$, mp 245 °C (DSC); 1H NMR (D_6 -DMSO) δ : 10.80 (s, 1 H), 7.89 (d, $J = 9.3$ Hz, 1 H), 7.67 (d, $J = 8.3$ Hz, 1 H), 7.10 (d, $J = 8.4$ Hz, 1 H), 6.41 (d, $J = 9.2$ Hz, 1 H), 3.95 (s, 3 H); ^{13}C NMR (D_6 -DMSO) δ : 162.7, 156.7, 140.8, 137.0, 128.3, 119.9, 115.0, 107.6, 105.8, 57.1.

8-Chloro-6-methoxyquinolin-2(1H)-one (3x). Obtained from amide **2x** according to the general cyclisation procedure B. The crude product was dissolved in ethyl acetate (400 mL) and filtered over silica gel (40 g). The product fractions were combined and concentrated to dryness. The product was slurried in ACN (35 mL) to afford yellow solid. Yield: 3.1 g (37%). Purity (LC-MS): 100% (210 nm), t_R 0.73 min; $[M + 1]^+ = 210$, mp 165 °C (DSC); 1H NMR (D_6 -DMSO) δ : 7.57 (d, $J = 9.0$ Hz, 1 H), 7.13 (d, $J = 2.7$ Hz, 1 H), 6.97 (d, $J = 2.7$ Hz, 1 H), 6.38 (d, $J = 9.0$ Hz, 1 H), 3.75 (s, 3 H); ^{13}C NMR (D_6 -DMSO) δ : 169.2, 151.3, 139.9, 136.7, 125.3, 122.6, 122.0, 118.1, 108.2, 56.0.

8-Chloro-5-methoxyquinolin-2(1H)-one (3y). Obtained from amide **2y** according to the general cyclisation procedure A with a reaction temperature of 22 °C. as a yellow solid. Yield: 7.8 g (93%). Purity (LC-MS): 97.3% (210 nm), t_R 0.77 min; $[M + 1]^+ = 210$, mp 200 °C (DSC); 1H NMR (D_6 -DMSO) δ : 10.99-10.84 (br, 1 H), 8.06 (d, $J = 9.8$ Hz, 1 H), 7.59 (d, $J = 8.7$ Hz, 1 H), 6.80 (d, $J = 8.8$ Hz, 1 H), 6.53 (d, $J = 9.8$ Hz, 1 H), 3.91 (s, 3 H); ^{13}C NMR (D_6 -DMSO) δ : 162.2, 155.1, 136.5, 134.7, 131.6, 121.8, 111.2, 110.6, 104.4, 56.7.

7-Chloro-8-methoxyquinolin-2(1H)-one (3z). Obtained from amide **2z** according to the general cyclisation procedure A with a reaction temperature of 22 °C. as a yellow solid. Yield: 6.64 g (79%). Purity (LC-MS): 100% (210 nm), t_R 0.73 min; $[M + 1]^+ = 210$, mp 199 °C (DSC); 1H NMR (D_6 -DMSO)

δ : 11.46 (s, 1 H), 7.92 (d, $J = 9.5$ Hz, 1 H), 7.47 (m, 1 H), 7.26 (m, 1 H), 6.54 (d, $J = 9.5$ Hz, 1 H), 3.84 (s, 3 H); ^{13}C NMR (D_6 -DMSO) δ : 162.3, 142.6, 140.4, 134.1, 128.1, 124.8, 123.2, 123.1, 120.0, 61.7.

6-Chloro-8-methoxyquinolin-2(1H)-one (3aa) Obtained from amide **2aa** according to the general cyclisation procedure B with a reaction temperature of 120 °C. No precipitation was observed after pouring onto ice (100 g). The aqueous phase was extracted with DCM (2 x 100 mL, 50 mL). The combined organic layers were concentrated to dryness. The crude product was dissolved in ethyl acetate (800 mL) and filtered over silica gel (40 g). The product fractions were combined and concentrated to dryness. The product was slurried in ACN (35 mL) to afford the product as a yellow solid. Yield: 3.4 g (41%). Purity (LC-MS): 100% (210 nm), t_{R} 0.76 min; $[\text{M} + 1]^+ = 210$, mp 186 °C (DSC); ^1H NMR (D_6 -DMSO) δ : 10.91-10.87 (br, 1 H), 7.86 (d, $J = 9.6$ Hz, 1 H), 7.37 (d, $J = 2.0$ Hz, 1 H), 7.19 (d, $J = 2.0$ Hz, 1 H), 6.58 (d, $J = 9.5$ Hz, 1 H), 3.92 (s, 3 H); ^{13}C NMR (D_6 -DMSO) δ : 161.8, 147.1, 139.8, 128.3, 126.2, 124.2, 120.5, 118.9, 111.9, 57.0.

5-Chloro-8-methoxyquinolin-2(1H)-one (3ab) Obtained from amide **2ab** according to the general cyclisation procedure A with a reaction temperature of 22 °C. The crude product was purified through a slurry in ACN (35 mL) to afford a yellow solid. Yield: 5.2 g (62%). Purity (LC-MS): 100% (210 nm), t_{R} 0.77 min; $[\text{M} + 1]^+ = 210$, mp 245 °C (DSC); ^1H NMR (D_6 -DMSO) 11.13 (s, 1 H), 8.03 (d, $J = 9.8$ Hz, 1 H), 7.25 (m, 1 H), 7.14 (m, 1 H), 6.66 (d, $J = 9.8$ Hz, 1 H), 3.90 (s, 3 H); ^{13}C NMR (D_6 -DMSO) δ : 161.5, 145.4, 136.3, 130.8, 124.5, 122.3, 122.2, 117.0, 112.1, 56.8.

8-Methyl-7-trifluoromethylquinolin-2(1H)-one (3ac). Obtained from amide **2ac** according to the general cyclisation procedure B as a beige solid after a slurry in ACN (35 mL). Yield: 4.7 g (52%). Purity (LC-MS): 95.6% (210 nm), t_{R} 0.83 min; $[\text{M} + 1]^+ = 228$, mp 216 °C (DSC); ^1H NMR (CDCl_3) δ : 10.04-9.91 (br, 1 H), 7.82 (d, $J = 9.5$ Hz, 1 H), 7.52 (m, 2 H), 6.79 (d, $J = 9.5$ Hz, 1 H), 2.63 (s, 3 H); ^{13}C NMR (CDCl_3) δ : 163.1, 140.6, 137.5, 130.7(m), 124.8 (d, $J = 284$ Hz), 120.8-127.4 (m), 123.0-125.2 (m), 122.4 (d, $J = 1$ Hz), 121.8, 119.3 (q, $J = 6$ Hz), 12.7 (d, $J = 2$ Hz).

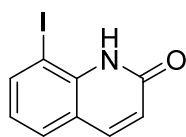
8-Methyl-5-trifluoromethylquinolin-2(1H)-one (3ad). Obtained from amide **2ad** according to the general cyclisation procedure B as a beige solid after a slurry in ACN (35 mL). Yield: 5.2 g (57%).

Purity (LC-MS): 97.8% (210 nm), t_R 0.83 min; $[M + 1]^+ = 228$, mp 208 °C (DSC); 1H NMR ($CDCl_3$) δ : 10.45-10.32 (br, 1 H), 8.12-8.14 (m, 1 H), 7.49 (m, 1 H), 7.44 (m, 1 H), 6.82 (m, 1 H), 2.63 (s, 3 H); ^{13}C NMR ($CDCl_3$) δ : 162.5, 136.9 (d, $J = 2$ Hz), 128.3-138.2 (m), 130.7, 124.9-125.6 (m), 120.7-127.3 (m), 122.9-125.1 (m), 123.3, 120.1 (q, $J = 6$ Hz), 116.0, 17.5.

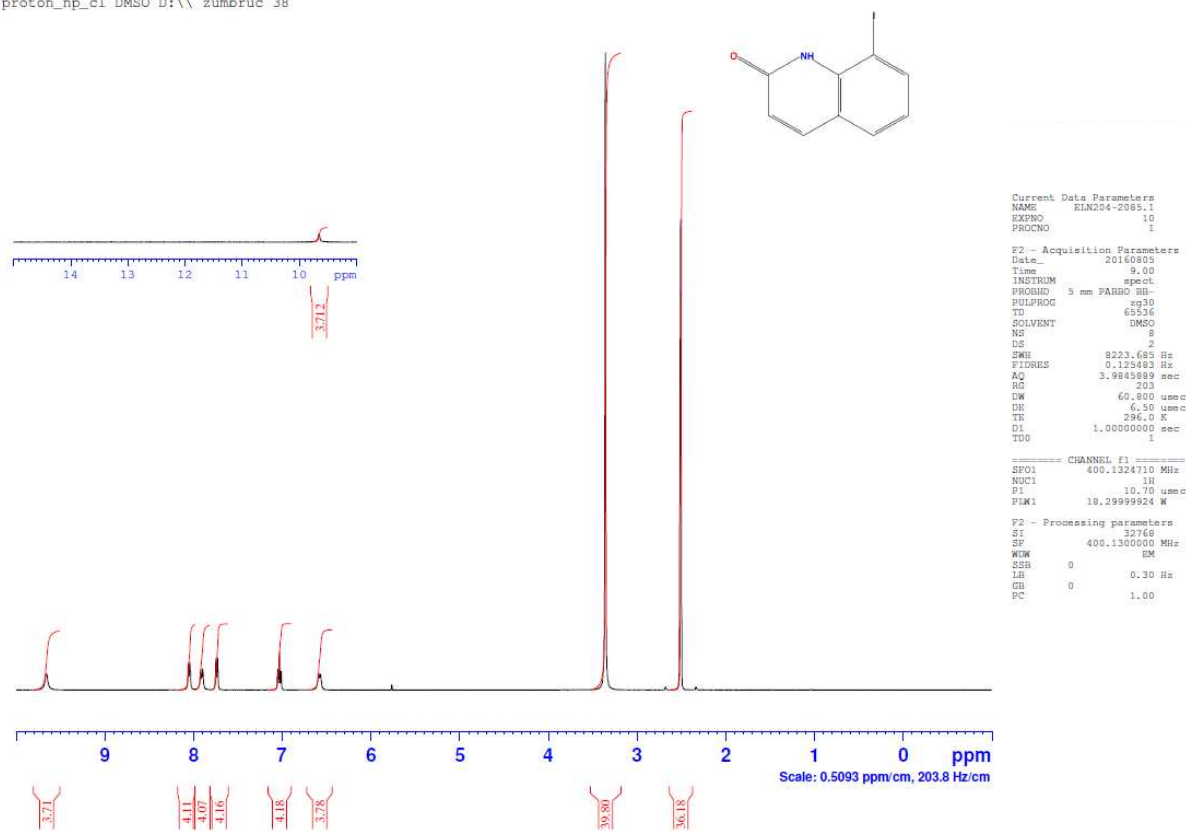
5-Methyl-8-trifluoromethylquinolin-2(1*H*)-one (3ae). Obtained from amide **2ae** according to the general cyclisation procedure B as a beige solid after a slurry in ACN (35 mL). Yield: 5.1 g (56%). Purity (LC-MS): 99.4% (210 nm), t_R 0.81 min; $[M + 1]^+ = 228$, mp 150 °C (DSC); 1H NMR ($CDCl_3$) δ : 9.04-8.90 (br, 1 H), 8.02 (d, $J = 9.9$ Hz, 1 H), 7.68 (d, $J = 7.9$ Hz, 1 H), 7.14 (d, $J = 7.8$ Hz, 1 H), 6.76 (d, $J = 9.9$ Hz, 1 H), 2.64 (s), 2.64 (s, 3 H); ^{13}C NMR ($CDCl_3$) δ : 161.5, 141.0, 137.1, 135.5, 128.0 (q, $J = 5$ Hz), 122.8-125.0 (m), 120.6-127.1 (m), 122.8 (d, $J = 122$ Hz), 119.4, 113.3 (q, $J = 31$ Hz), 19.3.

5. Proton and carbon NMR Spectra of quinolin-2(1*H*)-ones 3a-3ae

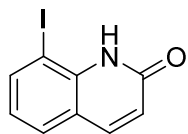
¹H NMR spectrum of 8-iodoquinolin-2(1*H*)-one **3a** (in D₆-DMSO).



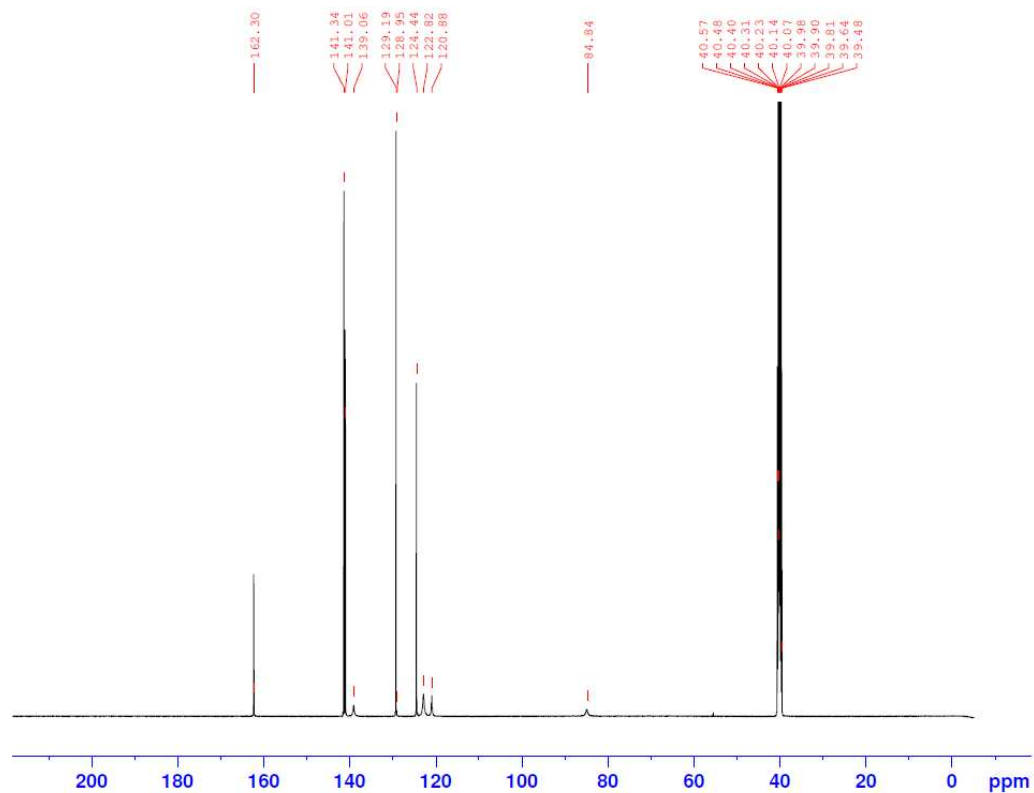
proton_np_c1 DMSO D:\zumbruc 38



^{13}C NMR spectrum of 8-iodoquinolin-2(1H)-one **3a** (in D_6 -DMSO).



C13_2048scans DMSO D:\schmidg 54



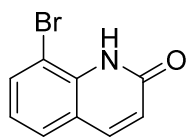
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Current Data Parameters
NAME      ELN302-0033.1_02
EXPNO     10
PROCNO    1

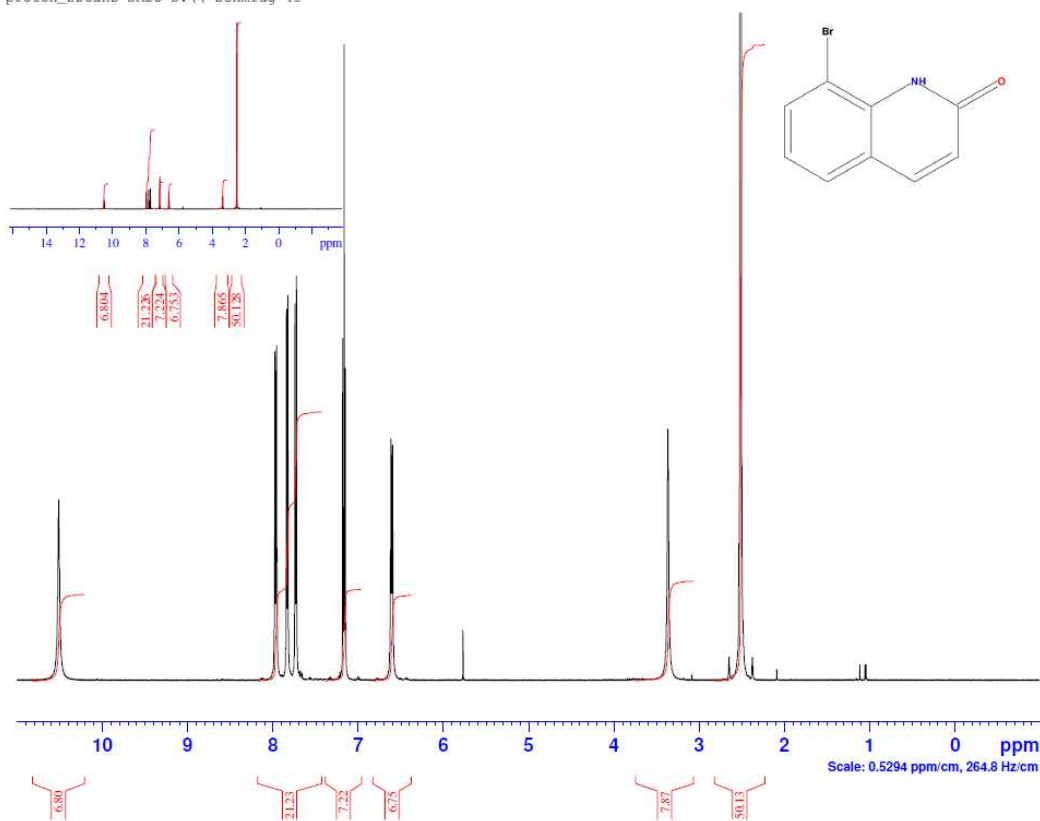
F2 - Acquisition Parameters
Date_     20170517
Time      1.05 h
INSTRUM   spect
PROBHD    Z128431_0003 (
PULPROG   zgpg30
TD         65536
SOLVENT   DMSO
NS         2048
DS         4
SWH        31512.605 Hz
FIDRES     0.961688 Hz
AQ         1.0398378 sec
RG         260.03
DW         15.867 usec
DE         19.02 usec
TE         300.2 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1
SFO1       125.7728799 MHz
NUC1       13C
P1         10.00 usec
PLM1       21.50799942 W
SFO2       500.1320005 MHz
NUC2       1H
PCPD02     waltz16
PCPD2      80.00 usec
PLM2       12.56699958 W
PLM12      0.18687931 W
PLM13      0.09316271 W

F2 - Processing parameters
SI         32768
SF         125.7577890 MHz
WDW        RM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
    
```

^1H NMR spectrum of 8-bromoquinolin-2(1H)-one **3b** (in D_6 -DMSO).



proton_2scans DMSO D:\ schmidg 43



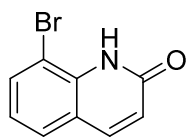
Current Data Parameters
 Name: E1N302-0034.1
 EXPNO: 10
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20160822
 Time: 12.08
 INSTRUM: spect
 PROBRD: 5 mm CPOCT 13C
 PULPROG: zg30
 TD: 65536
 SOLVENT: DMSO
 NS: 2
 DS: 5
 SWH: 10000.000 Hz
 FIDRES: 0.152588 Hz
 AQ: 3.2767999 sec
 RG: 14.06
 DW: 50.000 usec
 DE: 10.00 usec
 TE: 298.0 K
 D1: 1.00000000 sec
 TDO: 1

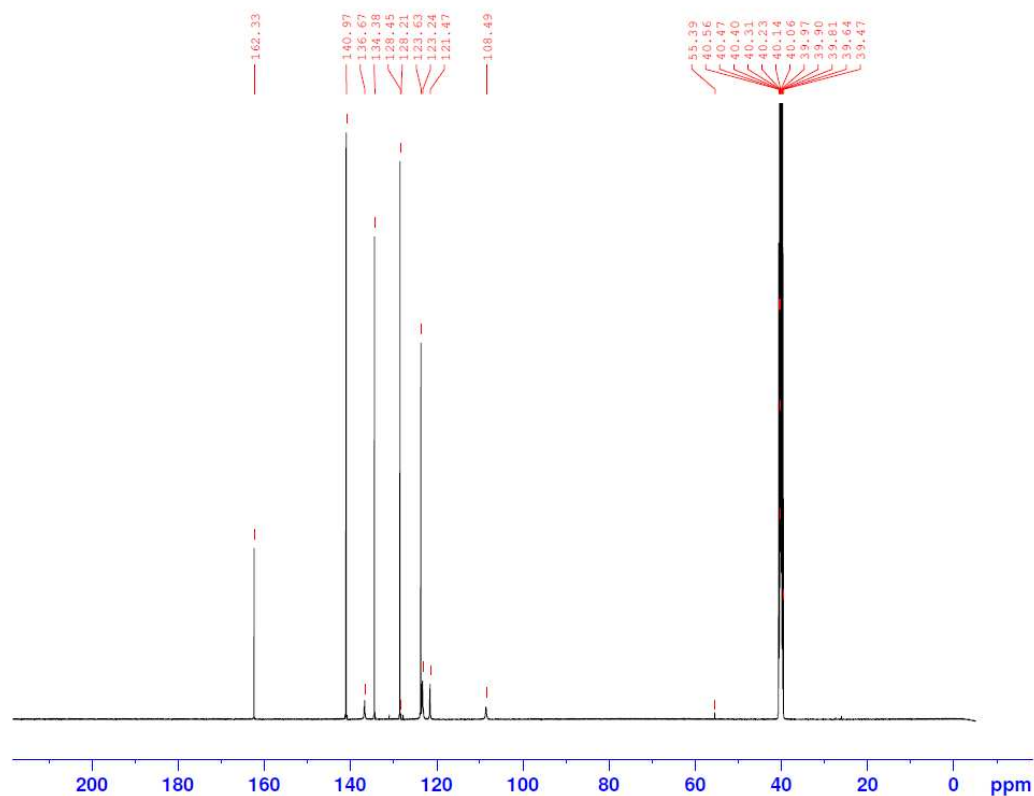
===== CHANNEL f1 =====
 SFO1: 500.1330895 MHz
 NUC1: ^1H
 P1: 10.10 usec
 PLW1: 13.00000000 W

F2 - Processing parameters
 SI: 65536
 SF: 500.1300000 MHz
 WCW: EM
 SSB: 0
 LB: 0.30 Hz
 GB: 0
 PC: 1.00

^{13}C NMR spectrum of 8-bromoquinolin-2(1H)-one **3b** (in $\text{D}_6\text{-DMSO}$).



C13_2048scans DMSO D:\ schmidg 55



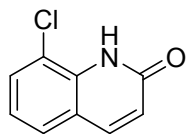
```

Current Data Parameters
NAME: E18302-0034.1.02
EXPNO: 10
PROCNO: 1

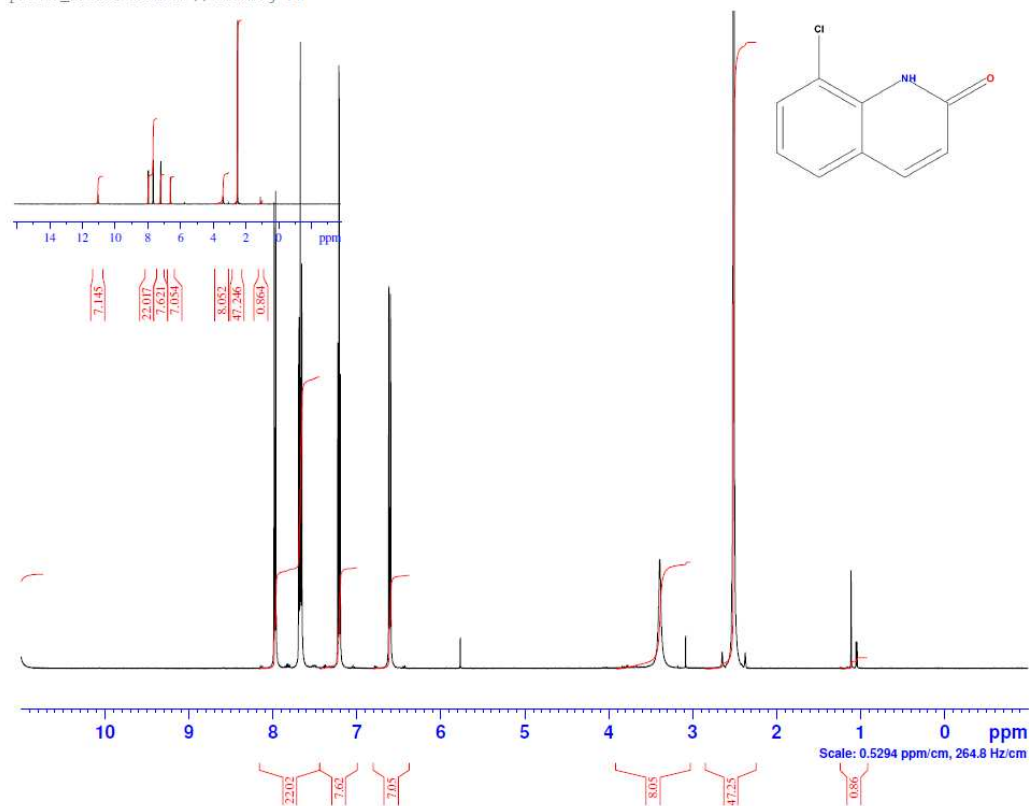
F2 - Acquisition Parameters
Date_: 20170517
Time: 2.54 h
INSTRUM: spect
PROBHD: Z128431_0003 (
PULPROG: zgpg30
TD: 65536
SOLVENT: DMSO
NS: 2048
DS: 4
SWH: 31512.605 Hz
FIDRES: 0.961688 Hz
AQ: 1.0398376 sec
RG: 200.03
RW: 15.867 usec
DE: 19.02 usec
TE: 300.0 K
D1: 2.00000000 sec
D11: 0.03000000 sec
TD0: 1
SFO1: 125.7728799 MHz
NUC1: 13C
P1: 10.00 usec
PIW1: 21.50789942 W
SFO2: 500.1320005 MHz
NUC2: 1H
CPDPRG2: waltz16
PCPD2: 80.00 usec
PIW2: 12.56499958 W
PIW12: 0.18587931 W
PIW13: 0.09316271 W

F2 - Processing parameters
SI: 32768
SF: 125.7577890 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.40
    
```

^1H NMR spectrum of 8-chloroquinolin-2(1H)-one **3c** (in D_6 -DMSO).



proton_2scans DMSO D:\ schmidg 44

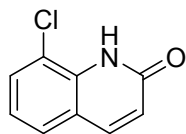


Current Data Parameters
 Date_ 20160822
 Time 12.15
 INSTRUM spect
 PROBRD 5 mm CPORC 13C
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 2
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152988 Hz
 AQ 3.2767999 sec
 RG 16.37
 DW 50.000 usec
 DE 10.00 usec
 TE 298.0 K
 D1 1.00000000 sec
 TDG 1

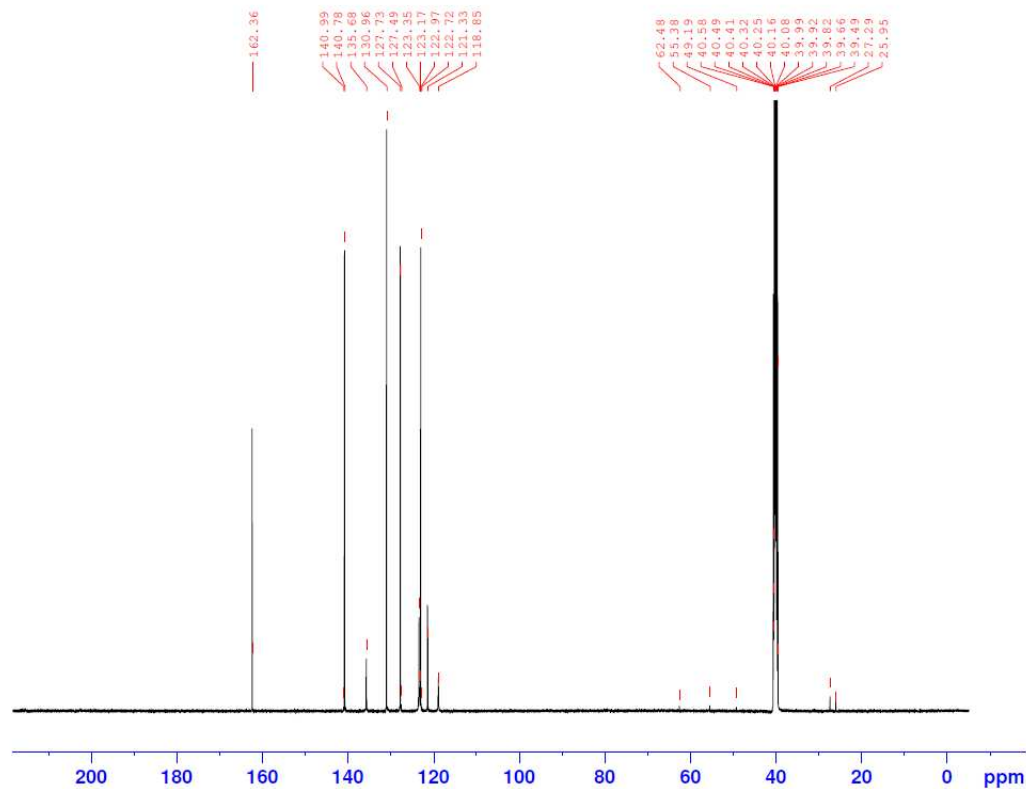
===== CHANNEL f1 =====
 SFO1 500.130885 MHz
 NUC1 1H
 P1 10.10 usec
 PLW1 13.00000000 W

F2 - Processing parameters
 SI 65536
 SF 500.1300000 MHz
 WDW RM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

^{13}C NMR spectrum of 8-chloroquinolin-2(1H)-one **3c** (in D_6 -DMSO).



C13_256scans DMSO D:\ schmidg 94



```

Current Data Parameters
NAME      ELN302-0035.1
EXPNO     20
PROCNO     1

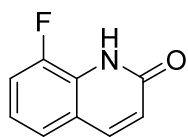
F2 - Acquisition Parameters
Date_     20160822
Time      16.48
INSTRUM    spect
PROBHD     5 mm CPDCH 13C
PULPROG    zgpg30
TD         65536
SOLVENT    DMSO
NS         256
DS         4
SWH         31512.605 Hz
FIDRES     0.480844 Hz
AQ         1.0398378 sec
RG         300.00
DW         15.867 usec
DE         60.67 usec
TE         300.2 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0         1

===== CHANNEL f1 =====
SP01      125.7728799 MHz
NUC1       13C
P1         10.00 usec
PLW1       21.00000000 W

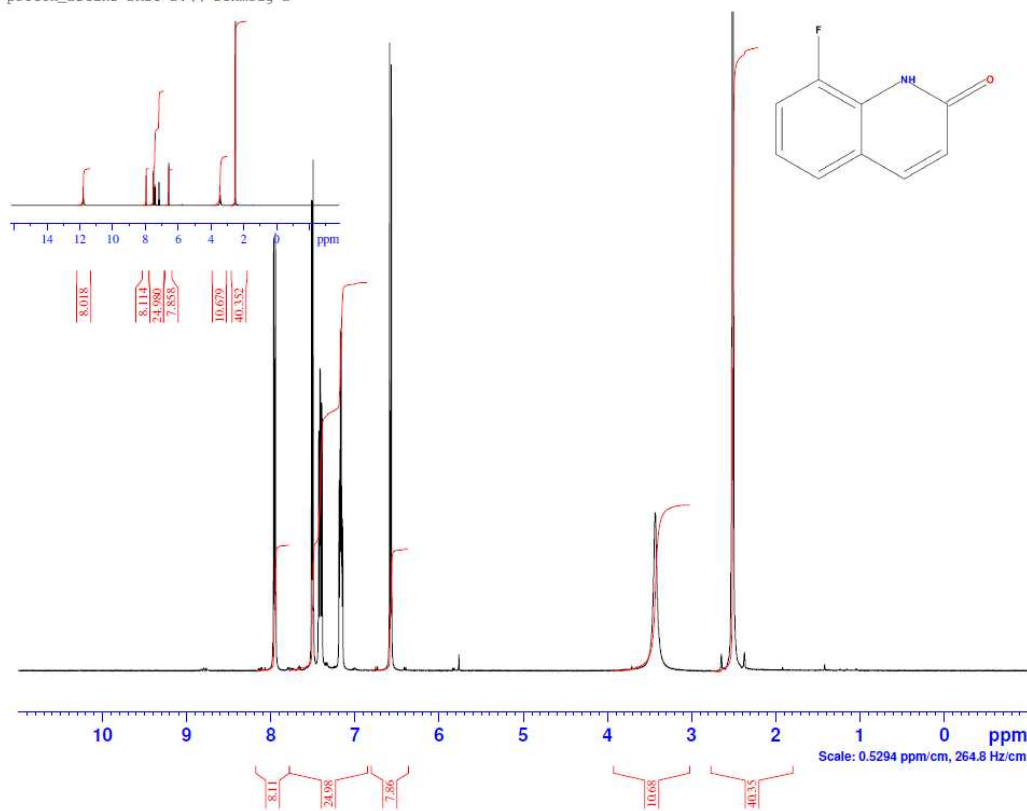
===== CHANNEL f2 =====
SP02      500.1320000 MHz
NUC2       1H
CPDPRG2    waltz16
PCPD2      80.00 usec
PLW2       13.00000000 W
PLW12      0.22395000 W
PLW13      0.11240000 W

F2 - Processing parameters
SI         32768
SF         125.7577890 MHz
WDW         0
SSB         0
LB         1.00 Hz
GB         0
PC         1.40
    
```

^1H NMR spectrum of 8-fluoroquinolin-2(1H)-one **3d** (in D_6 -DMSO).



proton_2scans DMSO D:\schmidg 2



```

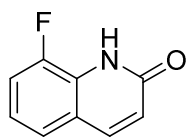
Current Data Parameters
NAME      ELM302-0049.1
EXPNO     10
PROCNO    1

F2 - Acquisition Parameters
Date_     20160826
Time      11.03
INSTRUM   spect
PROBHD    5 mm CPOCR 13C
PULPROG   zg30
TD         65536
SOLVENT   DMSO
NS         2
DS         2
SWH        10000.000 Hz
FIDRES     0.152588 Hz
AQ         3.2767999 sec
RG         11.16
DM         50.000 usec
DE         10.00 usec
TE         298.0 K
D1         1.00000000 sec
TD0        1

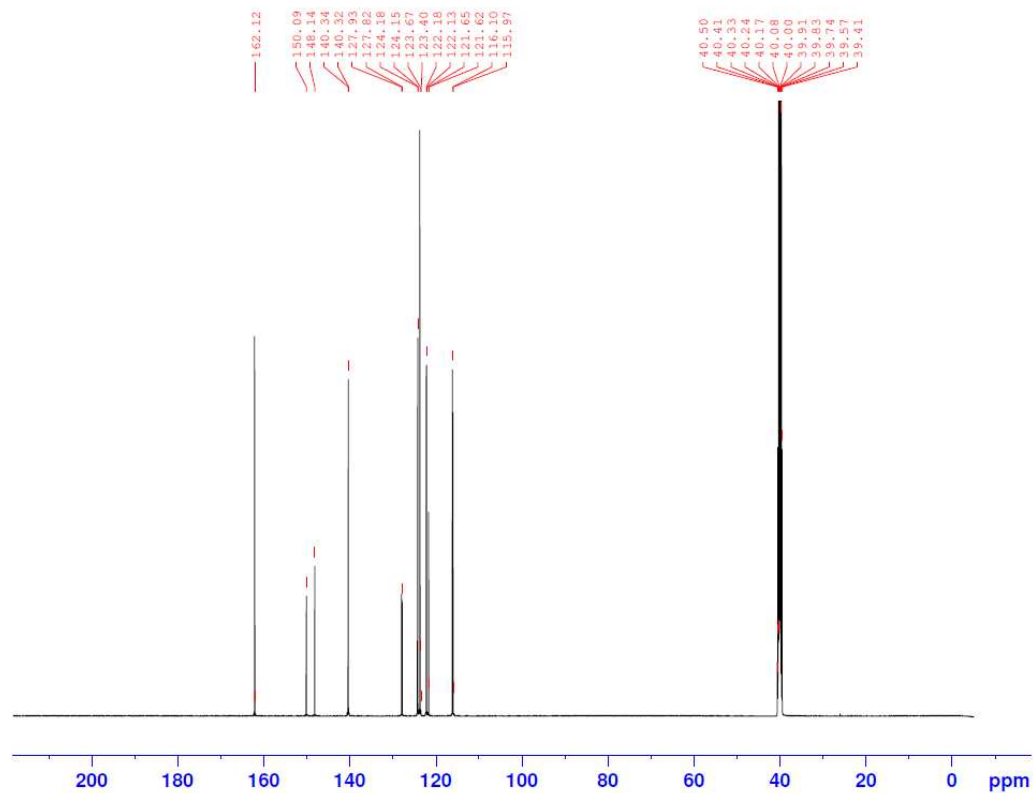
===== CHANNEL f1 =====
SFO1      500.1330885 MHz
NUC1       1H
P1         10.10 usec
PLW1      13.00000000 W

F2 - Processing parameters
SI         65536
SF         500.1330885 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
    
```

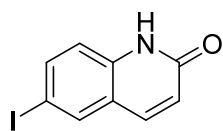

^{13}C NMR spectrum of 8-fluoroquinolin-2(1H)-one **3d** (in $\text{D}_6\text{-DMSO}$).



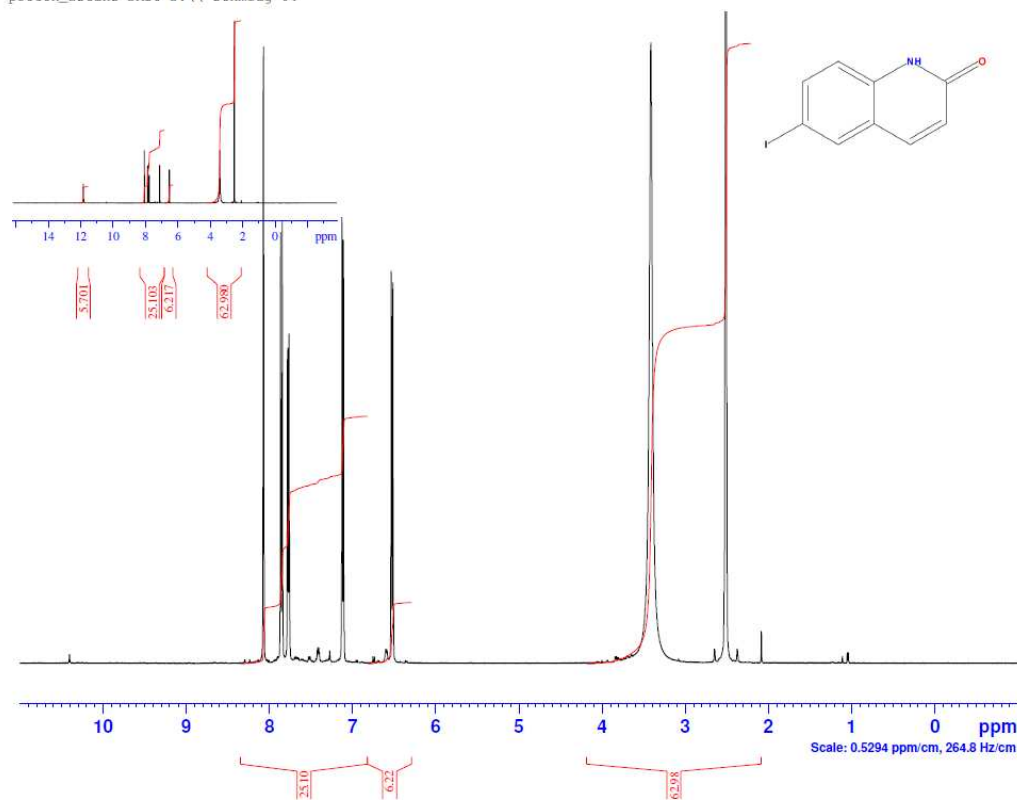
C13_2048scans DMSO D:\schmidg 33



^1H NMR spectrum of 6-iodoquinolin-2(1H)-one **3e** (in D_6 -DMSO).



after purification
proton_2scans DMSO D:\schmidg 64



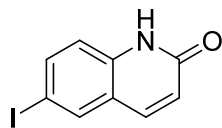
Current Data Parameters
NAME: ELM302-0131.1
EXPNO: 10
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20161014
Time: 23.43
INSTRUM: spect
PROBHD: 5 mm CPDCH 13C
PULPROG: zg30
TD: 65536
SOLVENT: DMSO
NS: 2
DS: 2
SWH: 10000.000 Hz
FIDRES: 0.152588 Hz
AQ: 3.2767999 sec
RG: 14.06
RW: 50.000 usec
DE: 10.00 usec
TE: 298.0 K
D1: 1.00000000 sec
TDO: 1

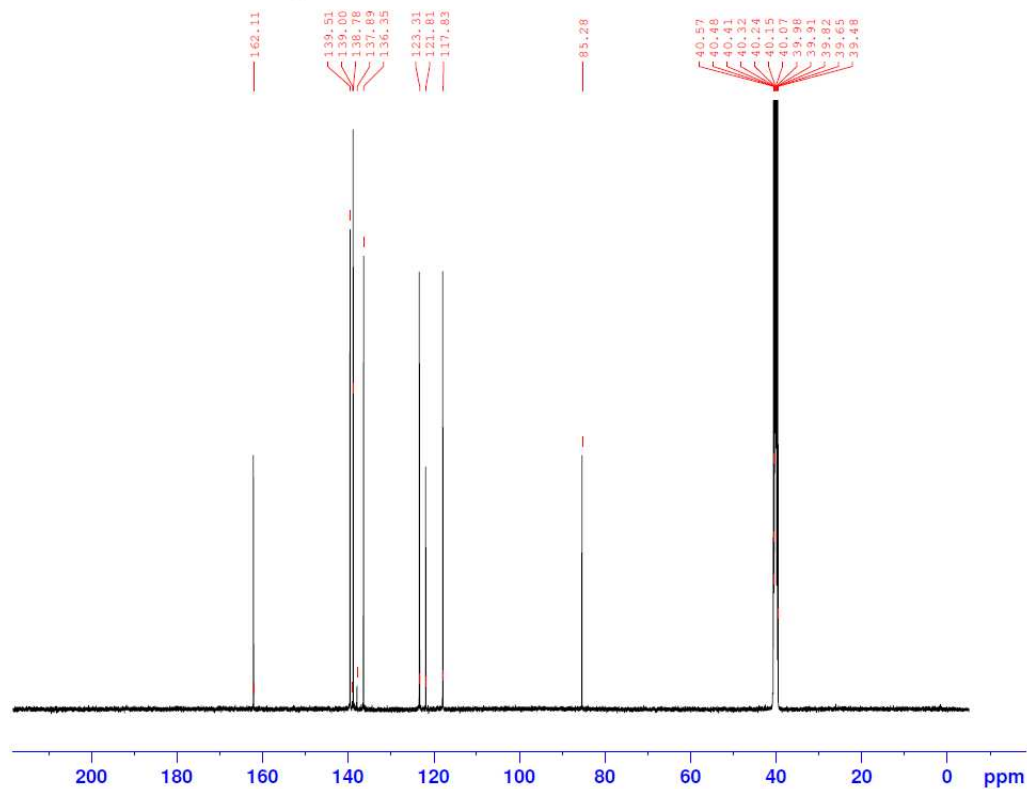
==== CHANNEL f1 =====
SFO1: 500.1330885 MHz
NUC1: 1H
P1: 10.10 usec
PLW1: 13.00000000 W

F2 - Processing parameters
S1: 65536
SF: 500.1300000 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00

^{13}C NMR spectrum of 6-iodoquinolin-2(1H)-one **3e** (in D_6 -DMSO).



after purification
C13_256scans DMSO D:\schmidg 64



```
Current Data Parameters
NAME      ELM302-0131.1
EXPNO     11
PROCNO    1

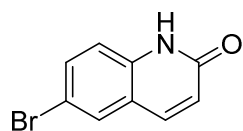
F2 - Acquisition Parameters
Date_     20161014
Time      23.58
INSTRUM   spect
PROBHD    5 mm CPOCH 13C
PULPROG   zgpg30
TD         65536
SOLVENT   DMSO
NS         256
DS         4
SWH        31512.605 Hz
FIDRES     0.488844 Hz
AQ          1.0398378 sec
RG          200.03
OW         15.867 usec
DE          60.67 usec
TE         300.0 K
D1          2.0000000 sec
D11         0.0300000 sec
TD0         1

===== CHANNEL F1 =====
SFO1       125.7708799 Mhz
NUC1        13C
P1          10.00 usec
PLW1        21.0000000 W

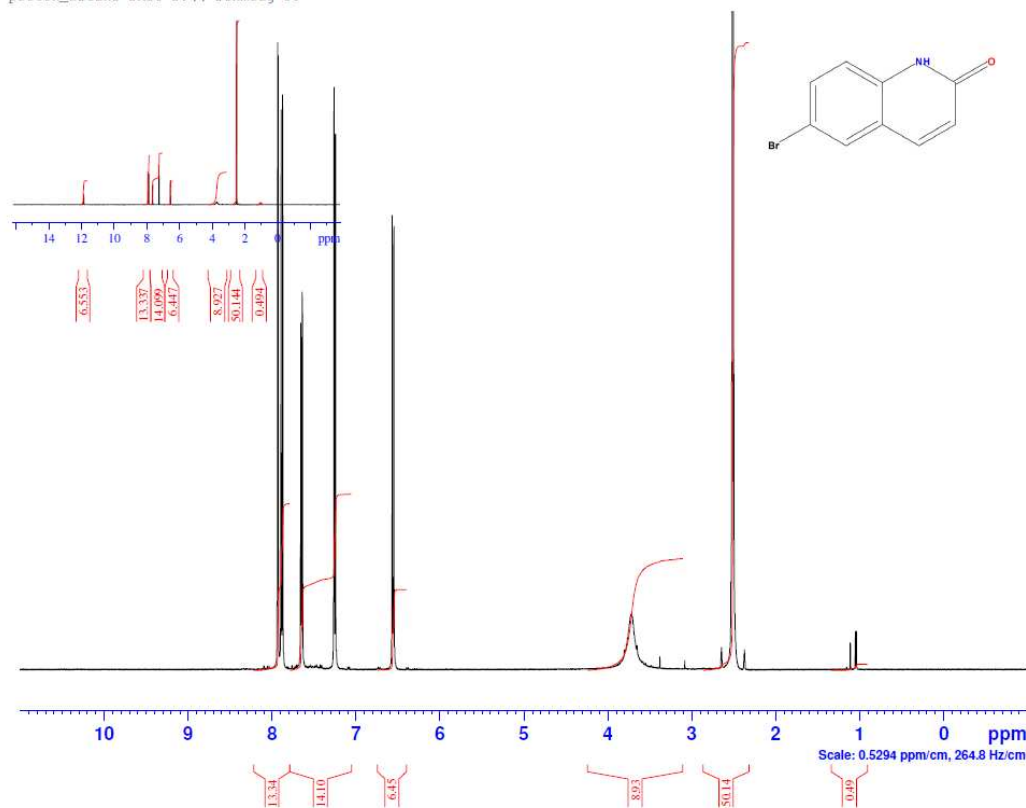
===== CHANNEL F2 =====
SFO2       500.1320005 Mhz
NUC2         1H
CPOPRG2    waltz16
PCPD2       80.00 usec
PLW2        13.0000000 W
PLW12       0.22395000 W
PLW13       0.11264000 W

F2 - Processing parameters
SI          32768
SF          125.7577890 Mhz
WDW         EM
SSB         0
LB          1.00 Hz
GB          0
PC          1.40
```

^1H NMR spectrum of 6-bromoquinolin-2(1H)-one **3f** (in $\text{D}_6\text{-DMSO}$).



proton_2scans DMSO D:\ schmidg 38



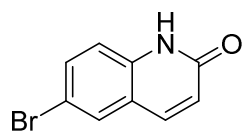
Current Data Parameters
NAME: EIN302-0026.1
EXPNO: 10
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20160816
Time: 17.15
INSTRUM: spect
PROBHD: 5 mm CPDCH 13C
PULPROG: zg30
TD: 65536
SOLVENT: DMSO
NS: 2
DS: 2
SWH: 10000.000 Hz
FIDRES: 0.152388 Hz
AQ: 3.2767999 sec
RG: 11.16
DW: 30.000 usec
DE: 10.00 usec
TE: 298.0 K
D1: 1.00000000 sec
TDO: 5

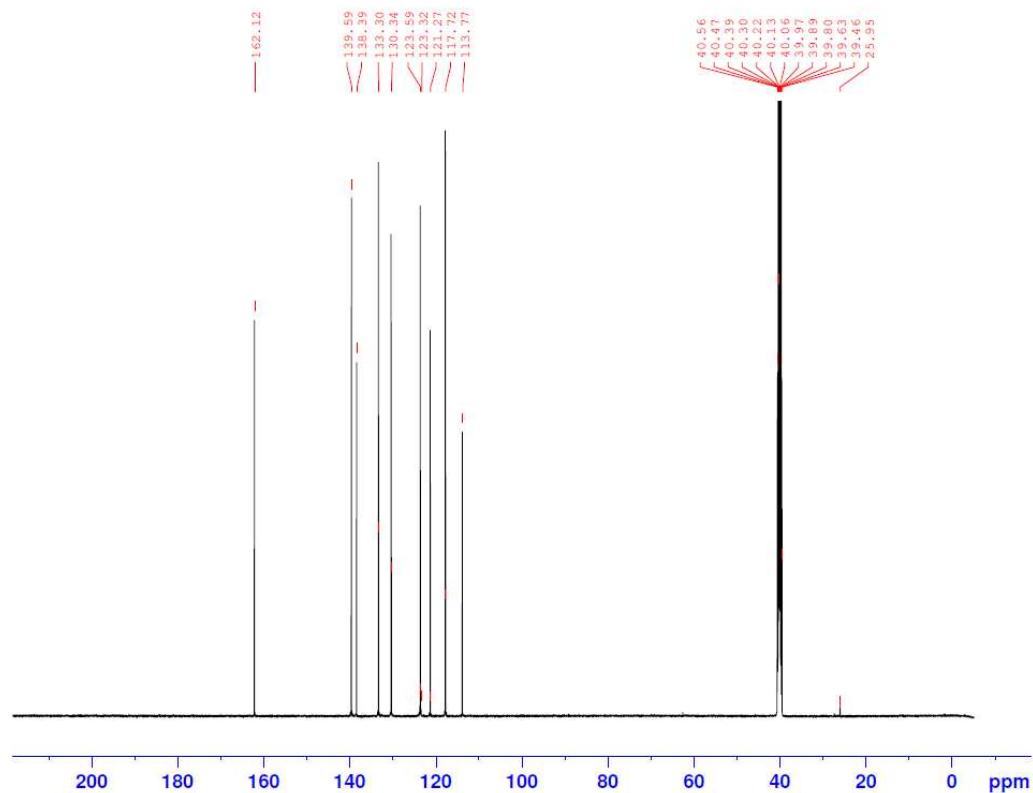
CHANNEL f1
SFO1: 500.1330885 MHz
NUC1: 1H
P1: 10.10 usec
PLW1: 13.00000000 W

F2 - Processing parameters
SI: 65536
SF: 500.1330000 MHz
WOW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00

^{13}C NMR spectrum of 6-bromoquinolin-2(1H)-one **3f** (in $\text{D}_6\text{-DMSO}$).



C13_256scans DMSO D:\schmidg 30



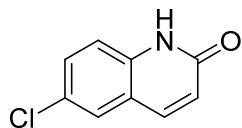
```

Current Data Parameters
NAME      EUN302-00266.1_02
EXPNO     10
PROCNO    1

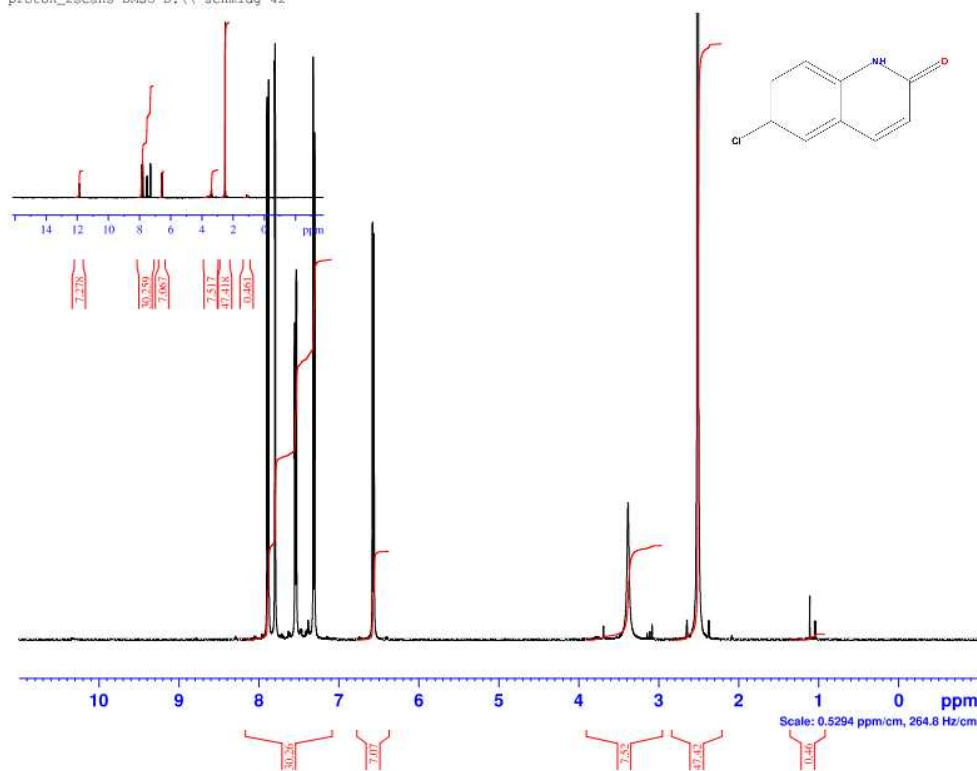
F2 - Acquisition Parameters
Date_     20170515
Time      18.00 h
INSTRUM   spect
PROBHD    Z128431.0003 (
PULPROG   zgpg30
TD         65536
SOLVENT   DMSO
NS         256
DS         4
SWH        31512.605 Hz
FIDRES     0.961688 Hz
AQ         1.0398378 sec
RG          200.03
LW         15.867 used
DE         19.02 used
TK          300.0 K
D1         2.00000000 sec
D11        0.03000000 sec
TDS        1
SFO1       125.7728799 MHz
NUC1       13C
P1         10.00 used
PLW1       21.50799942 W
SFO2       500.1320005 MHz
NUC2
CPDPRG2   waltz16
PCPD2     80.00 used
PLW2       12.56459959 W
PLW12     0.18587931 W
PLW13     0.09316271 W

F2 - Processing parameters
SI         32768
SF         125.7577890 MHz
WDW        RM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
    
```

^1H NMR spectrum of 6-chloroquinolin-2(1H)-one **3g** (in D_6 -DMSO).



after purification
proton_2scans DMSO D:\schmidg 42



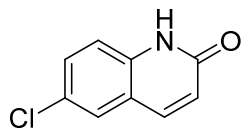
Current Data Parameters
NAME KUK302-0620.1
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160318
Time 15.37
INSTRUM spect
PROBHD 5 mm CPDPC 13C
PULPROG zg30
TE 300.2
SOLVENT DMSO
NS 2
DS 2
SWH 13008.000 Hz
FIDRES 0.155056 Hz
AQ 5.2767999 sec
RG 121.05
RW 56.000 usec
DE 10.00 usec
TE 298.2 K
D1 1.90000000 sec
TD0 1

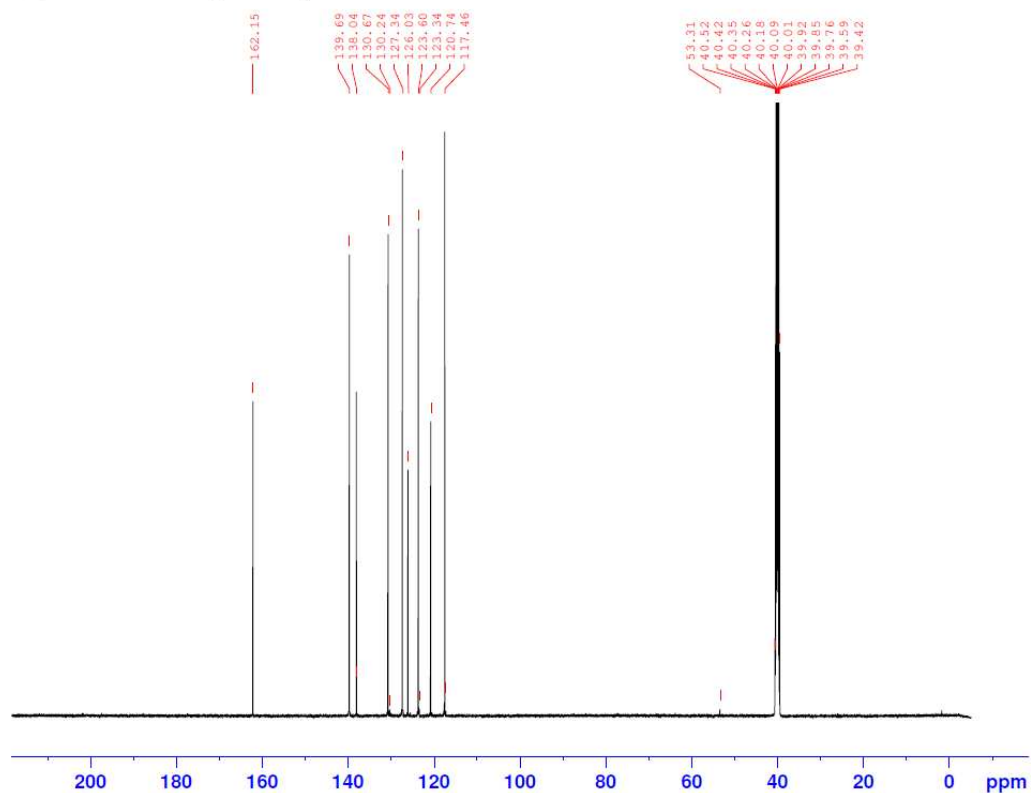
----- CHANNEL f1 -----
SFO1 500.1350883 MHz
NUC1 1H
P1 10.10 usec
PLM1 19.80000000 Hz

F2 - Processing parameters
SI 32768
SF 500.1350000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{13}C NMR spectrum of 6-chloroquinolin-2(1H)-one **3g** (in $\text{D}_6\text{-DMSO}$).



C13_256scans DMSO D:\ schmidg 31



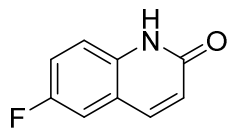
```

Current Data Parameters
NAME      ELN302-20271.02
EXPNO     10
PROCNO    1

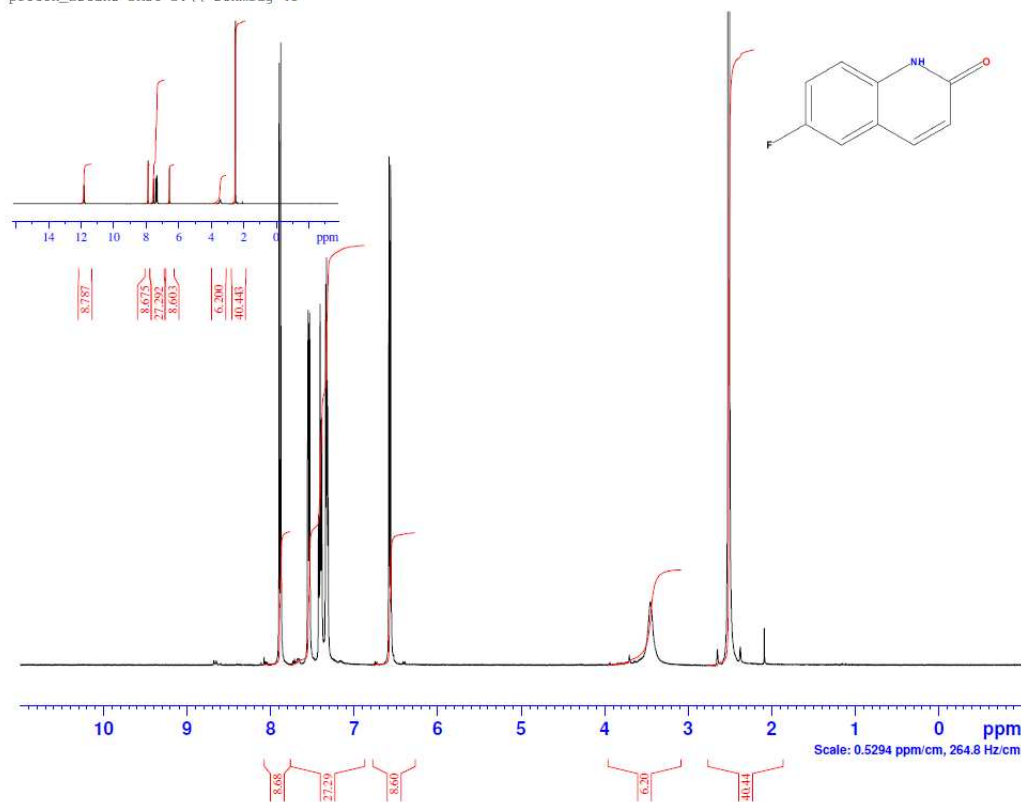
F2 - Acquisition Parameters
Data      20170515
Time      18.36 h
INSTRUM   spect
PROBHD    Z128431_003 (
PULPROG   zgpg30
TD         65536
SOLVENT   DMSO
NS         256
DS         4
SWH        31512.605 Hz
FIDRES     0.961688 Hz
AQ         1.0398378 sec
RG         200.03
DW         15.867 usec
DE         19.02 usec
TE         300.0 K
D1         2.00000000 sec
d11        0.03000000 sec
TD0        1
SFO1       125.7728799 MHz
NUC1       13C
P1         10.00 usec
PLM1       21.50799942 W
SFO2       500.1320005 MHz
NUC2       1H
CPDPRG2    waltz16
PCPD2      80.00 usec
PLM2       12.56499950 W
PLM12      0.18587931 W
PLM13      0.09316271 W

F2 - Processing parameters
SI         32768
SF         125.7577890 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
    
```

^1H NMR spectrum of 6-fluoroquinolin-2(1H)-one **3h** (in D_6 -DMSO).



after purification
proton_2scans DMSO D:\schmidg 43



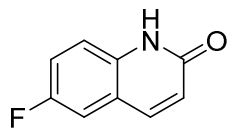
Current Data Parameters
NAME ELM302-0028.1
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160818
Time 15.11
INSTRUM spect
PROBHD 5 mm CPDCH 13C
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 2
DS 2
SWH 10000.000 Hz
FIDRES 0.132588 Hz
AQ 3.2767999 sec
RG 13.05
RW 50.000 usec
DE 10.00 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

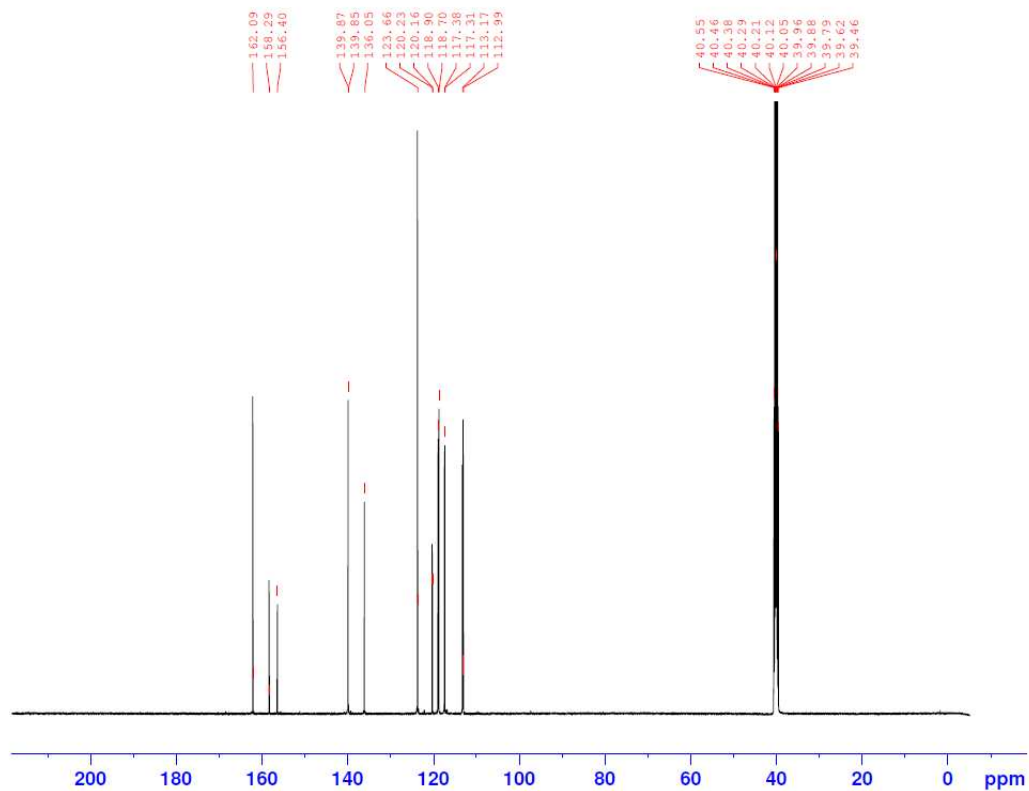
===== CHANNEL f1 =====
SFO1 500.1330885 MHz
NUC1 1H
P1 10.10 usec
PLW1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 500.1330885 MHz
WCH EM
SGB 0
LB 0.30 Hz
GB 0
PC 1.00

^{13}C NMR spectrum of 6-fluoroquinolin-2(1H)-one **3h** (in $\text{D}_6\text{-DMSO}$).



C13_256scans DMSO D:\schmidg 32



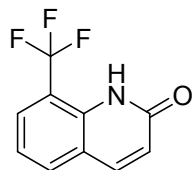
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Current Data Parameters
NAME      E13152-0029.1.02
EXPNO     10
PROCNO    1

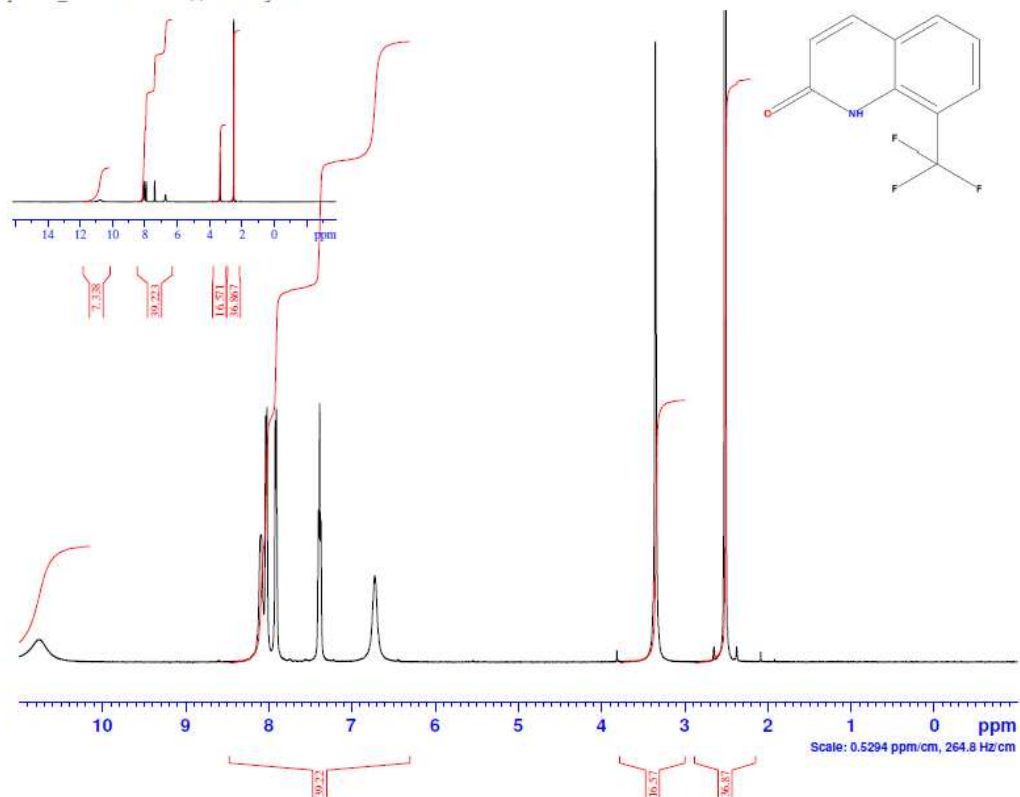
F2 - Acquisition Parameters
Date_     20170515
Time      18.53 h
INSTRUM   spect
PROBHD    Z128431_0013 (
PULPROG   zgpg30
TD         65536
SOLVENT   DMSO
NS         256
DS         4
SWH        31512.605 Hz
FIDRES     0.961698 Hz
AQ          1.5398378 sec
RG          200.03
SW          15.867 umsec
DE          19.02 umsec
TE          300.0 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0         1
SFO1       125.7728799 MHz
NUC1        13C
P1          10.00 umsec
PLM1        21.50799942 W
SFO2       500.1320005 MHz
NUC2         1H
CPDPRG2    waltz16
PCPD2       80.00 umsec
PLM2        12.56499958 W
PLM12       0.18587931 W
PLM13       0.09316271 W

F2 - Processing parameters
SI          32768
SF          125.7577890 MHz
WDM         RM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40
    
```

^1H NMR spectrum of 8-trifluoromethylquinolin-2(1H)-one **3i** (in D_6 -DMSO).



proton_2scans DMSO D:\schmidg 90



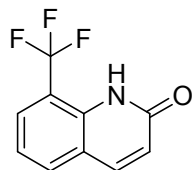
Current Data Parameters
NAME ELN302-0058.1
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160831
Time 17.05
INSTRUM spect
PROBHD 5 mm CPDCH 13C
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 2
DS 2
SWH 10000.000 Hz
FIDRES 0.182588 Hz
AQ 3.2767999 sec
RG 11.16
IN 50.000 usec
DE 10.00 usec
TE 298.0 K
D3 1.0000000 sec
TD0 1

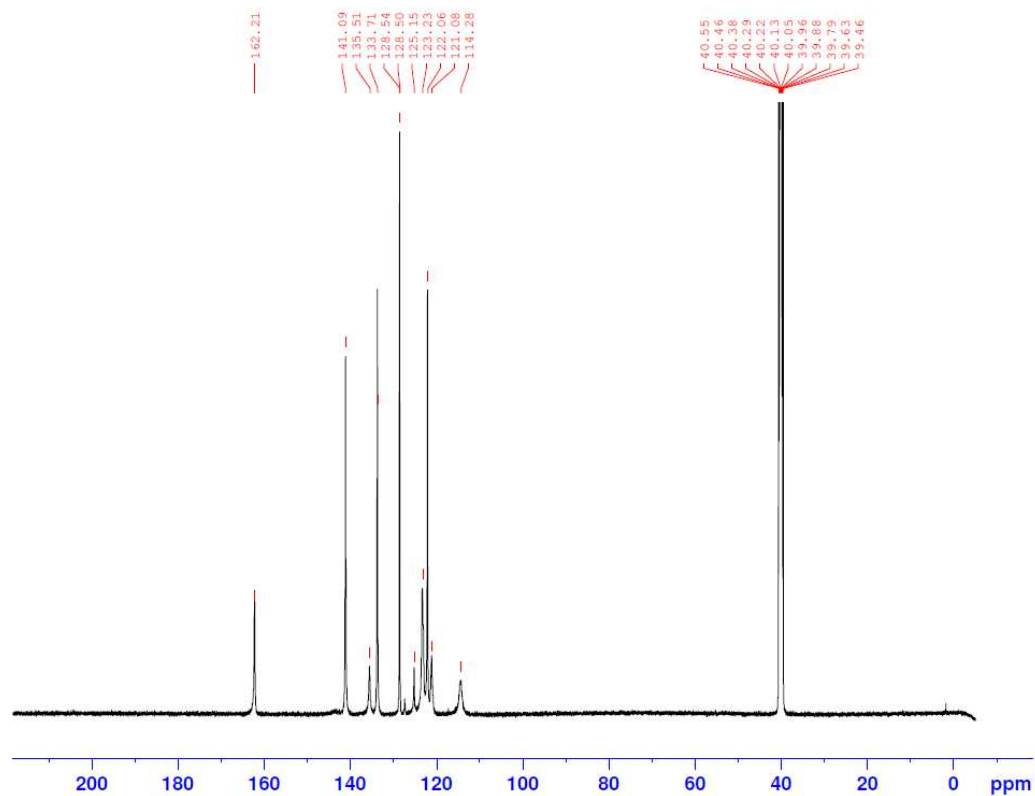
CHANNEL f1
SFO1 500.1330885 MHz
NUC1 1H
P1 10.10 usec
PLW1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 500.1330885 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{13}C NMR spectrum of 8-trifluoromethylquinolin-2(1H)-one **3i** (in D_6 -DMSO).



C13_2048scans DMSO D:\schmidg 58



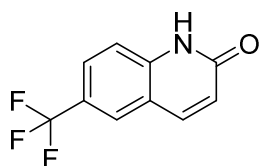
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Current Data Parameters
NAME      ELN302-0058.1.02
EXPNO     10
PROCNO    1

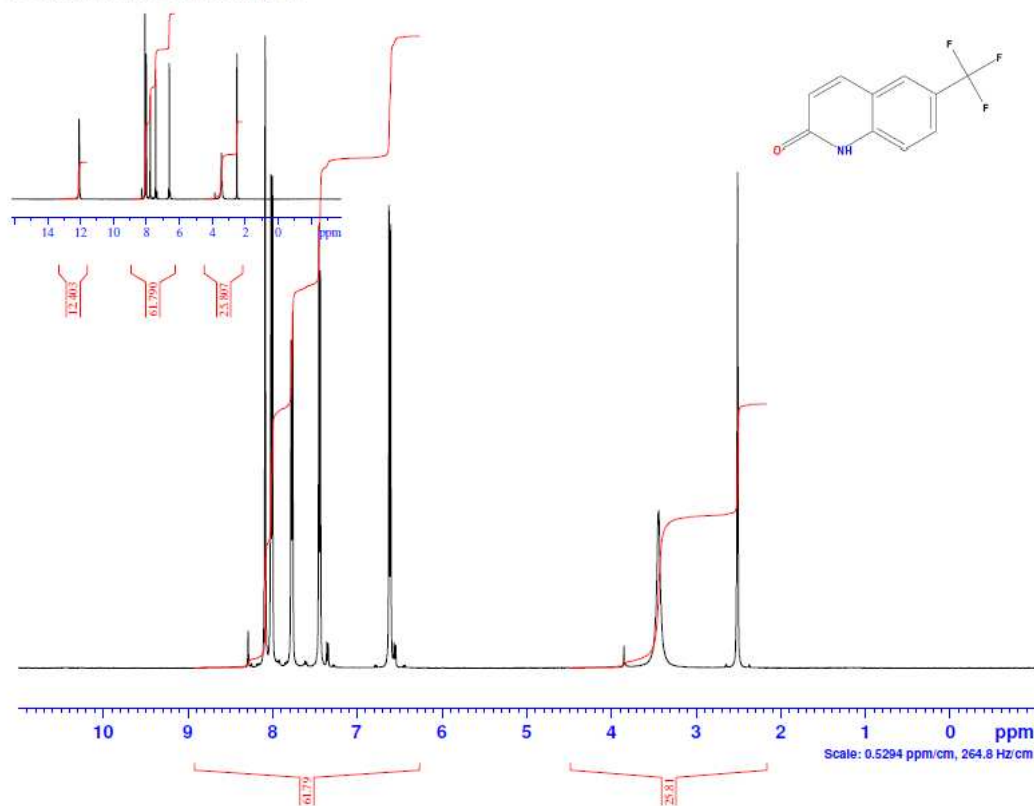
F2 - Acquisition Parameters
Date_     20170517
Time      4.44 h
INSTRUM    spect
PROBHD    Z128431.0003 (
PULPROG    zgpg30
TD         65536
SOLVENT    DMSO
NS         2048
DS         4
SWH         31512.605 Hz
FIDRES     0.961688 Hz
AQ         1.0398378 sec
RG         250.03
DM         15.867 usec
DE         19.02 usec
TE         300.0 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1
SF01       125.7728799 MHz
NUC1       13C
P1         10.00 usec
P1M1       21.50799942 W
SF02       500.1320005 MHz
NUC2       1H
CPDPRG2    waltz16
PCPD2      60.00 usec
P1W2       12.56499958 W
P1M12      0.18587931 W
P1M13      0.09316271 W

F2 - Processing parameters
SI         32768
SF         125.7577890 MHz
WDW        0
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
    
```

^1H NMR spectrum of 6-trifluoromethylquinolin-2(1H)-one **3j** (in $\text{D}_6\text{-DMSO}$).



proton_2scans DMSO D:\schmidg 25



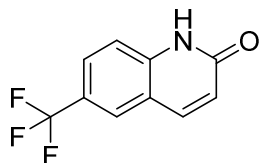
Current Data Parameters
NAME KIM302-0059.1_02
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170120
Time 14.23
INSTRUM spect
PROBHD 5 mm CPOCH 13C
PULPROG zgpg
TD 65536
SOLVENT DMSO
NS 2
DS 2
SWH 10000.000 Hz
FIDRES 0.155389 Hz
AQ 3.2767999 sec
RG 10.23
IN 50.000 uSoc
DE 10.00 uSoc
TE 298.0 K
D1 1.00000000 sec
TD0 1

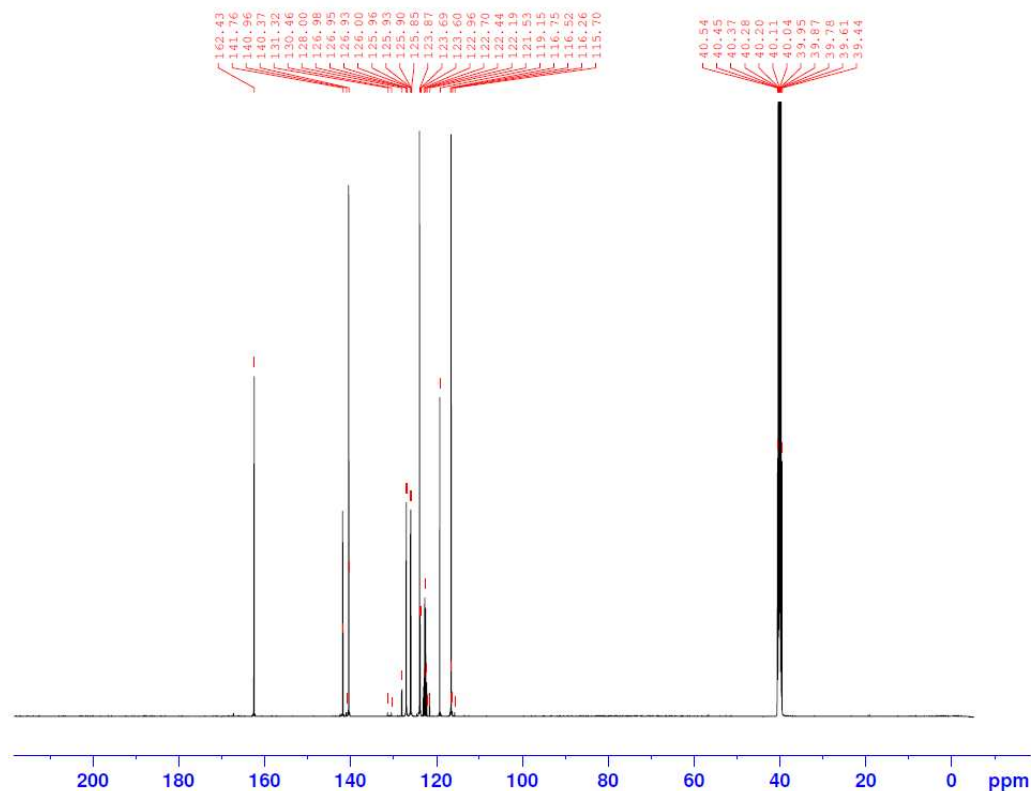
Channel f1
SFO1 500.1330885 MHz
NUC1 1H
P1 10.10 uSoc
PLW1 13.00000000 W

F2 - Processing parameters
S1 65536
SF 500.1330000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{13}C NMR spectrum of 6-trifluoromethylquinolin-2(1H)-one **3j** (in D_6 -DMSO).



C13_2048scans DMSO D:\schmidg 59



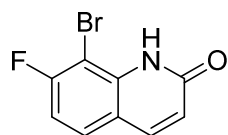
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Current Data Parameters
NAME      ELN302-0059.1_02
EXPNO     10
PROCNO     1

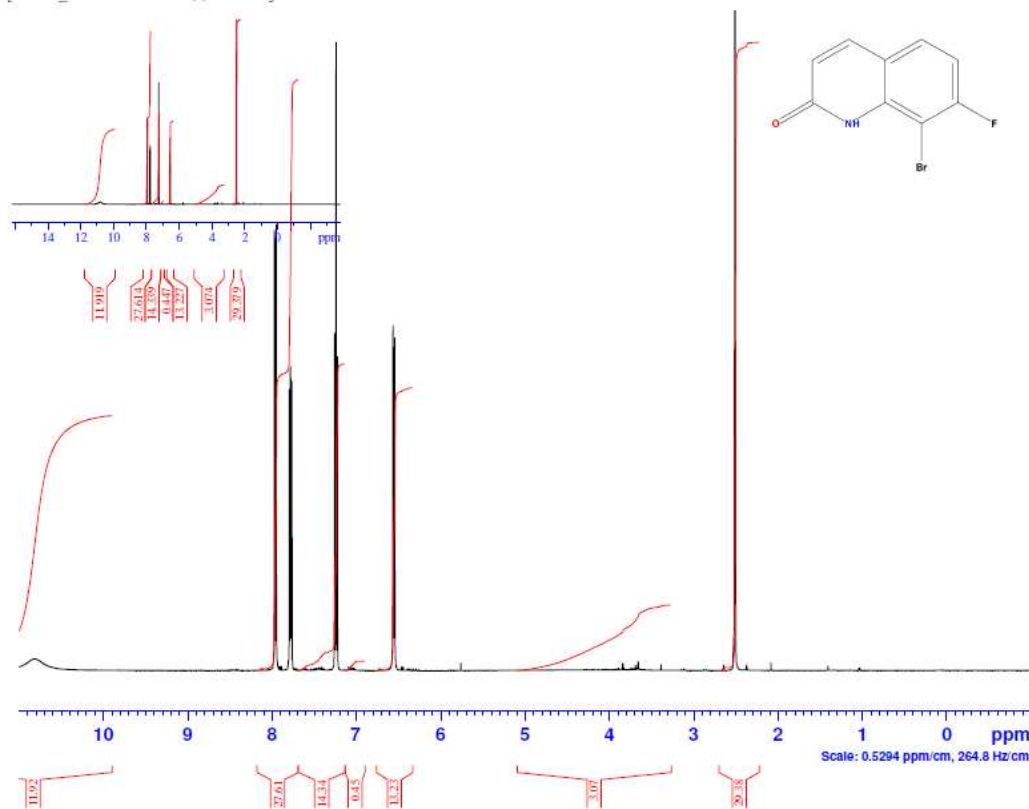
F2 - Acquisition Parameters
Date_      20170517
Time       6.33 h
INSTRUM    spect
PROBHD     Z128431.0003
PULPROG    zgpg30
TD         65536
SOLVENT    DMSO
NS         2048
DS         4
SWH         31512.605 Hz
FIDRES      0.961688 Hz
AQ          1.0398378 sec
RG          250.03
DW          15.867 usec
DE          19.02 usec
TE          300.0 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0         1
SFO1        125.7728799 MHz
NUC1        13C
P1          10.00 usec
P1M1        21.50799942 W
SFO2        500.1320005 MHz
NUC2        1H
CPDPRG2    waltz16
PCPD2       80.00 usec
P1M2        12.56489958 W
P1M12       0.18587931 W
P1M13       0.09316271 W

F2 - Processing parameters
SI          32768
SF          125.7577890 MHz
WDW         0
GB          0
LB          1.00 Hz
GB          0
PC          1.40
    
```

^1H NMR spectrum of 8-bromo-7-fluoroquinolin-2(1H)-one **3k** (in D_6 -DMSO).



proton_2scans DMSO D:\schmidg 22

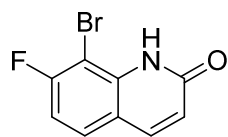


Current Data Parameters
NAME K128302-0218.1.92
EXPNO 10
PROCNO 1

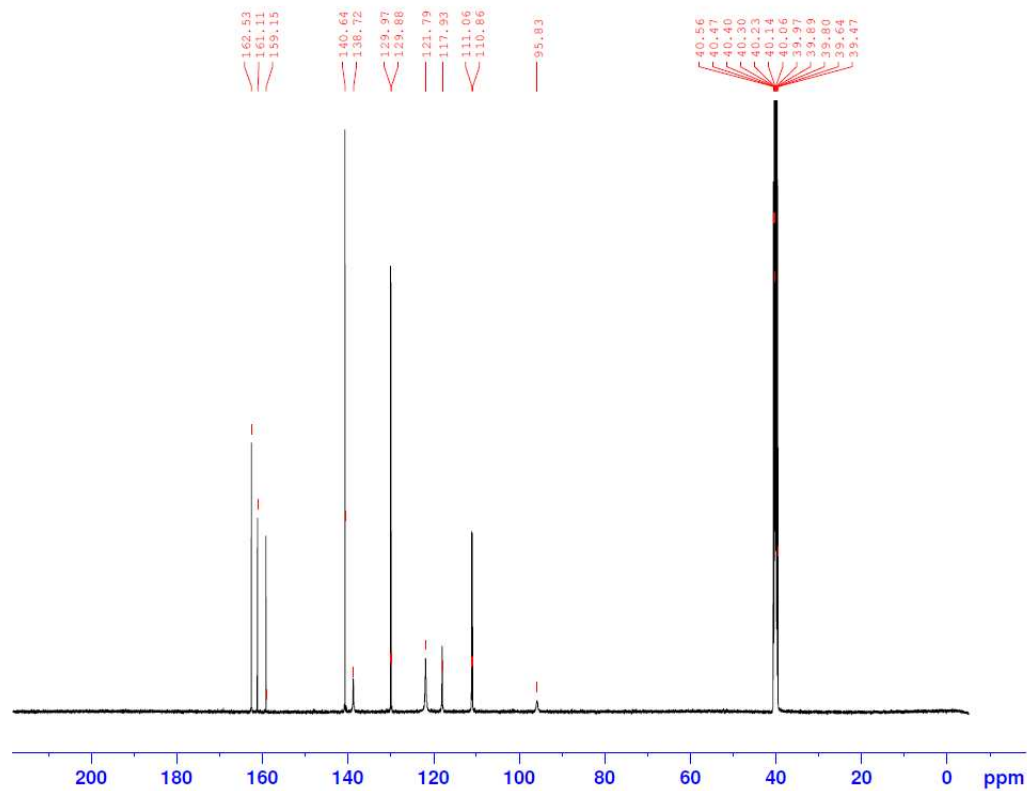
F2 - Acquisition Parameters
Date_ 20170302
Time 15.38 h
INSTRUM spect
PROBHD X128431-0003 (4
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 2
DS 2
SWH 10000.000 Hz
FIDRES 0.308176 Hz
AQ 3.2761999 sec
RG 10.23
IM 50.000 usec
DE 10.00 usec
TE 300.2 K
D1 1.00000000 sec
DS 1
SFO1 500.1330885 MHz
NUC1 1H
P1 10.00 usec
PLW1 12.56499958 W

F2 - Processing parameters
SI 65536
SF 500.1330885 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{13}C NMR spectrum of 8-bromo-7-fluoroquinolin-2(1H)-one **3k** (in D_6 -DMSO).



C13_256scans DMSO D:\ schmidg 22



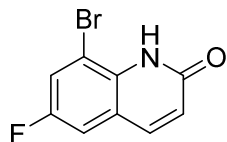
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Current Data Parameters
NAME      ELN302-0218.1.02
EXPNO     1
PROCNO    1

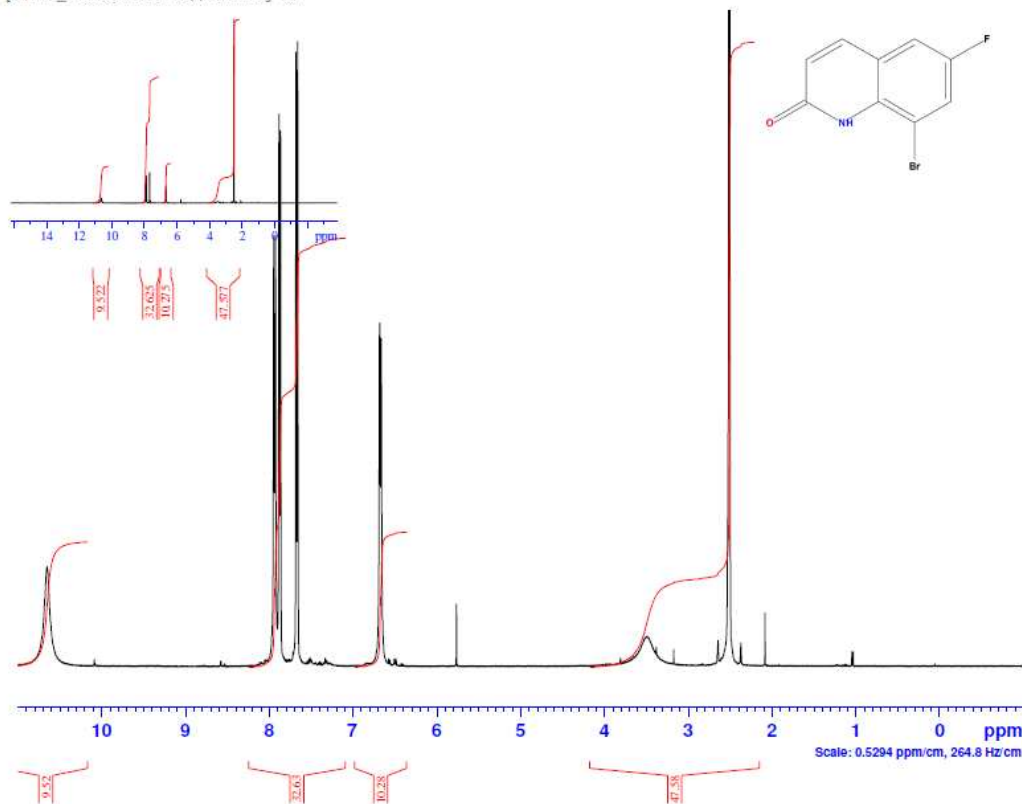
F2 - Acquisition Parameters
Date_     20170302
Time      15.52 h
INSTRUM   spect
PROBHD    Z128431-0003 (
PULPROG   zgpg30
TD         65536
SOLVENT    DMSO
NS         256
DS         4
SWH        31512.605 Hz
FIDRES     0.961688 Hz
AQ         1.0398378 sec
RG         320.03
DW         15.867 usec
DE         19.02 usec
TE         300.0 K
D1         2.00000000 sec
D11        0.03000000 sec
TDO        125.7728799 MHz
SFO1       130
NUC1       13C
P1         10.00 usec
PL1        21.50799942 W
SFO2       500.1320005 MHz
NUC2       1H
CPDPRG2    waltz16
PCPD2      80.00 usec
PLW2       12.56499958 W
PLW12      0.18587931 W
PLW13      0.09316271 W

F2 - Processing parameters
SI         32768
SF         125.7577880 MHz
WDW        0
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
    
```

^1H NMR spectrum of 8-bromo-6-fluoroquinolin-2(1H)-one **31** (in D_6 -DMSO).



proton_2scans DMSO D:\schmidg 95

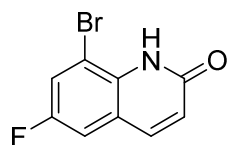


Current Data Parameters
NAME EIAN302-0214.1_02
EXPNO 20
PROCNO 1

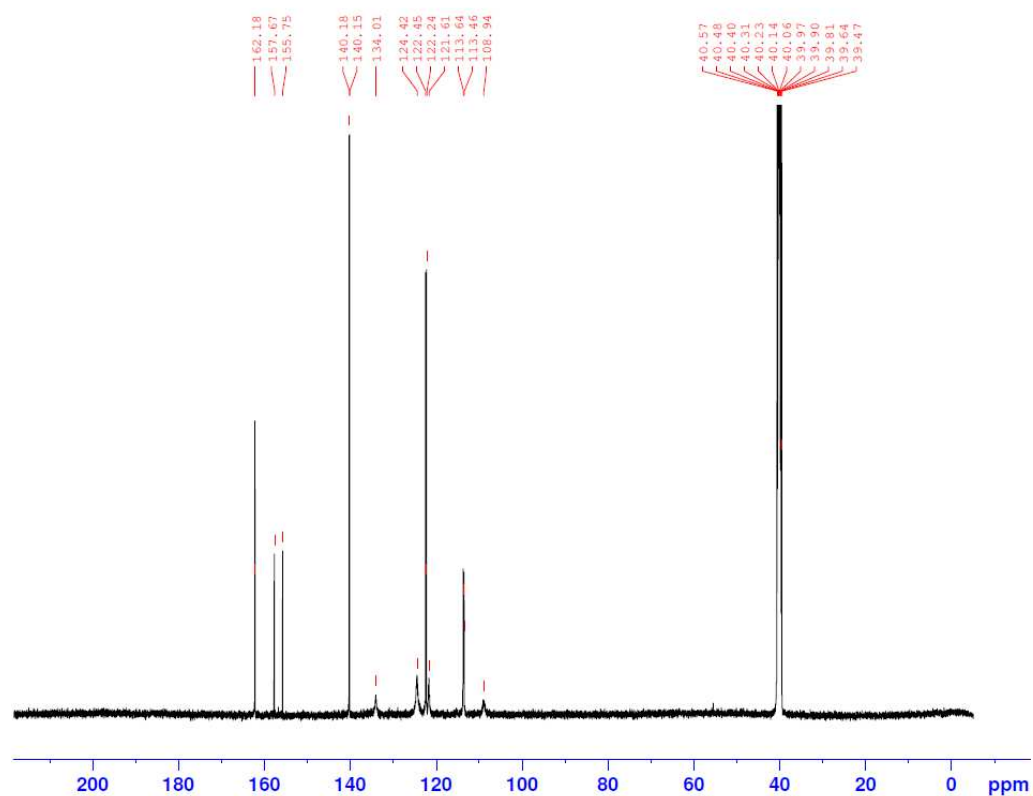
F2 - Acquisition Parameters
Date_ 20170301
Time 15.55 h
INSTRUM spect
PROBHD Z128431_0003 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 2
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.3767999 sec
RG 10.23
DM 50.000 uMHC
DE 10.00 uMHC
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 500.1330885 MHz
NUC1 1H
P1 10.00 uMHC
PLW1 12.56499958 W

F2 - Processing parameters
SI 65536
SF 500.1330885 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{13}C NMR spectrum of 8-bromo-6-fluoroquinolin-2(1H)-one **3I** (in D_6 -DMSO).



C13_256scans DMSO D:\ schmidg 95



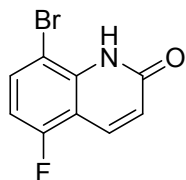
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Current Data Parameters
NAME      EIA302-C214.1_02
EXPNO     21
PROCNO    1

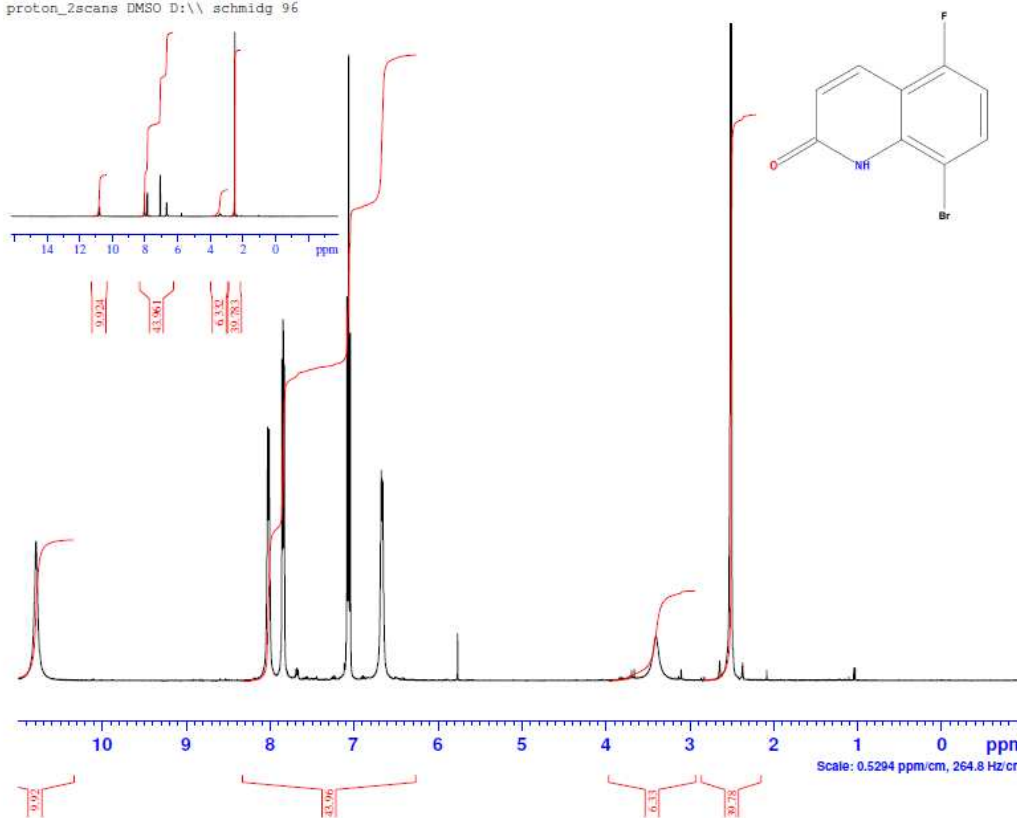
F2 - Acquisition Parameters
Date_     20170301
Time      16.10 h
INSTRUM   spect
PROBHD    Z128431_0003 (
PULPROG   zgpg30
TD         65536
SOLVENT    DMSO
NS         256
DS         4
SWH        31512.605 Hz
FIDRES     0.961688 Hz
AQ          1.0398378 sec
RG          200.03
DW          15.867 usec
DE          19.02 usec
TE          300.0 K
D1          2.00000000 sec
D11         0.03000000 sec
TDO         1
SFO1        125.7728789 MHz
NUC1        13C
P1          10.00 usec
PLM1        21.50799942 W
SFO2        500.1320005 MHz
NUC2
CPDPRG2    waltz16
PCPD2      80.00 usec
PLM2       12.56469958 W
PLM12      0.18587931 W
PLM13      0.09316271 W

F2 - Processing parameters
SI          32768
SF          125.7577890 MHz
WDW          RM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40
    
```

^1H NMR spectrum of 8-bromo-5-fluoroquinolin-2(1H)-one **3m** (in D_6 -DMSO).



proton_2scans DMSO D:\schmidg 96

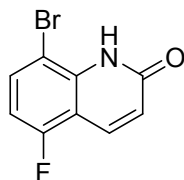


Current Data Parameters
NAME E1N302-0215.1.92
EXPNO 30
PROCNO 1

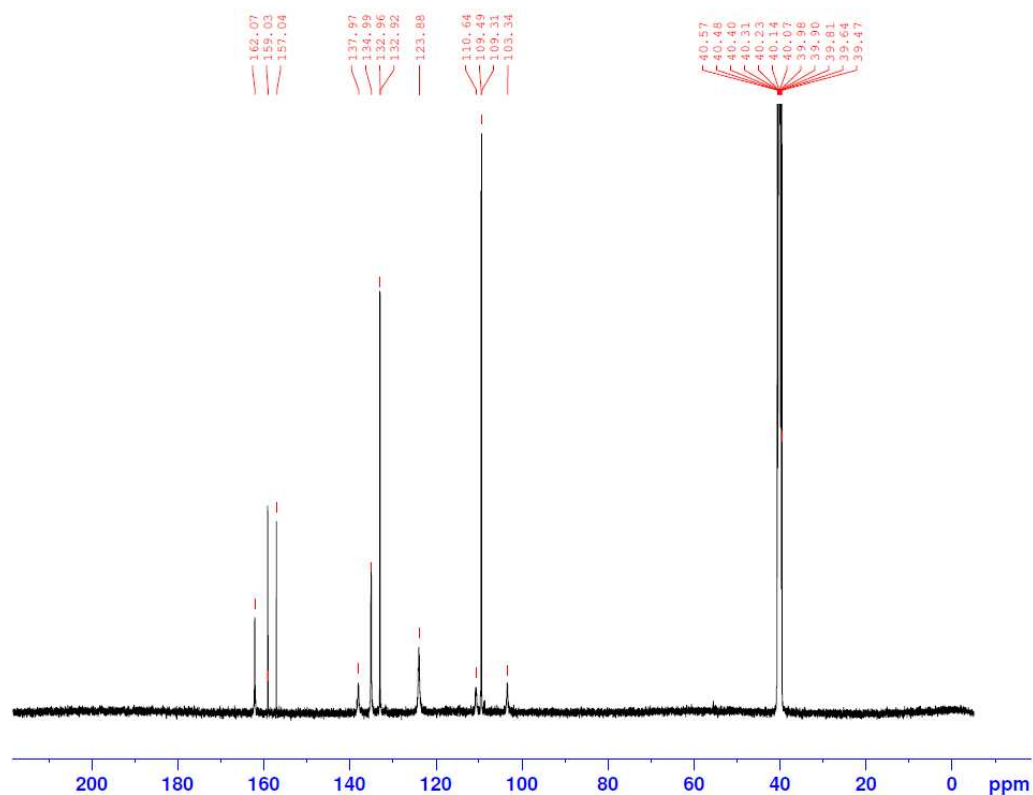
F2 - Acquisition Parameters
Date_ 20170301
Time 14.14 h
INSTRUM spect
PROBHD Z128431_0003 (4
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 2
DS 2
SWH 10056.000 Hz
FIDRES 0.393176 Hz
AQ 3.2767999 sec
RG 327.67999
IN 16.37
DE 59.800 us/c
EX 10.00 us/c
TE 296.0 K
D1 1.00000000 sec
TDO 1
SFO1 500.1300885 MHz
NUC1 1H
P1 10.00 us/c
PLW1 12.56499993 W

F2 - Processing parameters
SI 65536
SF 500.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{13}C NMR spectrum of 8-bromo-5-fluoroquinolin-2(1H)-one **3m** (in D_6 -DMSO).



C13_256scans DMSO D:\\ schmidg 96



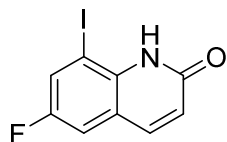
```

Current Data Parameters
NAME      ELN302-0215.1.02
EXPNO     31
PROCNO    1

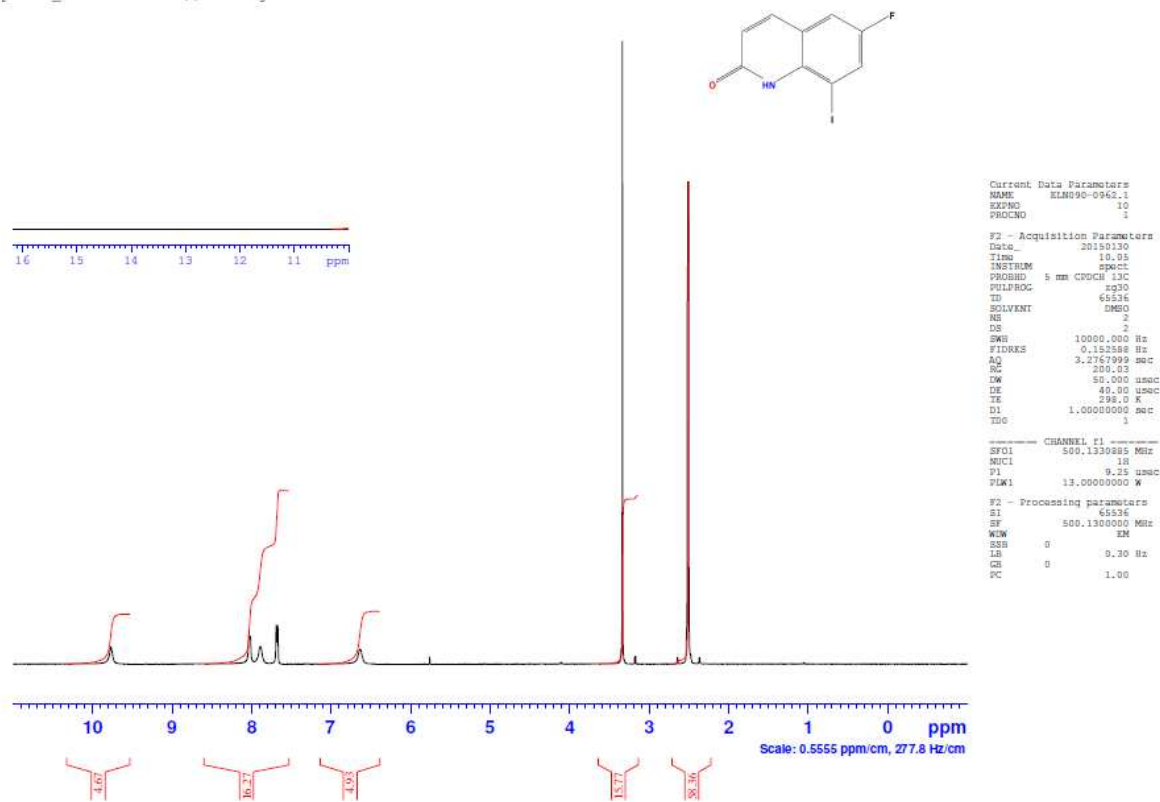
F2 - Acquisition Parameters
Date_     20170301
Time      16.29 h
INSTRUM   spect
PROBHD    Z128431_0003 (
PULPROG   zgpg30
TD         65536
SOLVENT   DMSO
NS         256
DS         4
SWH        31512.605 Hz
FIDRES     0.961688 Hz
AQ         1.0398378 sec
RG         200.03
DW         15.867 usec
DE         19.02 usec
TE         300.0 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1
SFO1       125.7728799 MHz
NUC1       13C
P1         10.00 usec
P1M1       21.50799942 W
SFO2       500.1320005 MHz
NUC2       1H
PCPD2      waltz16
PCPD2      80.00 usec
P1M2       12.56499958 W
P1M12      0.18587931 W
P1M13      0.09316271 W

F2 - Processing parameters
SI         32768
SF         125.7577850 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
    
```

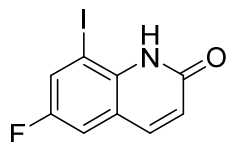
^1H NMR spectrum of 8-iodo-6-fluoroquinolin-2(1H)-one **3n** (in D_6 -DMSO).



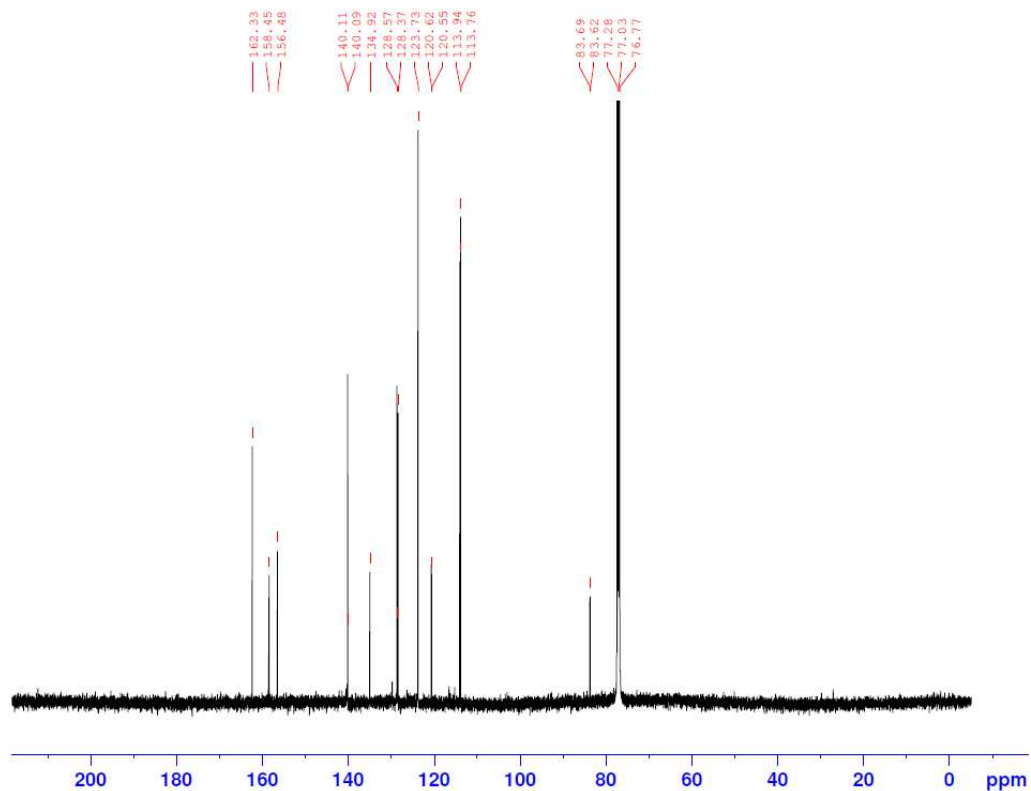
cryst1
proton_2scans DMSO D7\\ schmidg 60



^{13}C NMR spectrum of 8-iodo-6-fluoroquinolin-2(1H)-one **3n** (in CDCl_3).



cryst1
C13_256scans CDC13 D:\ schmidg 50



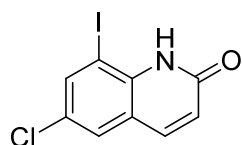
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Current Data Parameters
NAME      E18090-1320.1.02
EXPNO     11
PROCNO    1

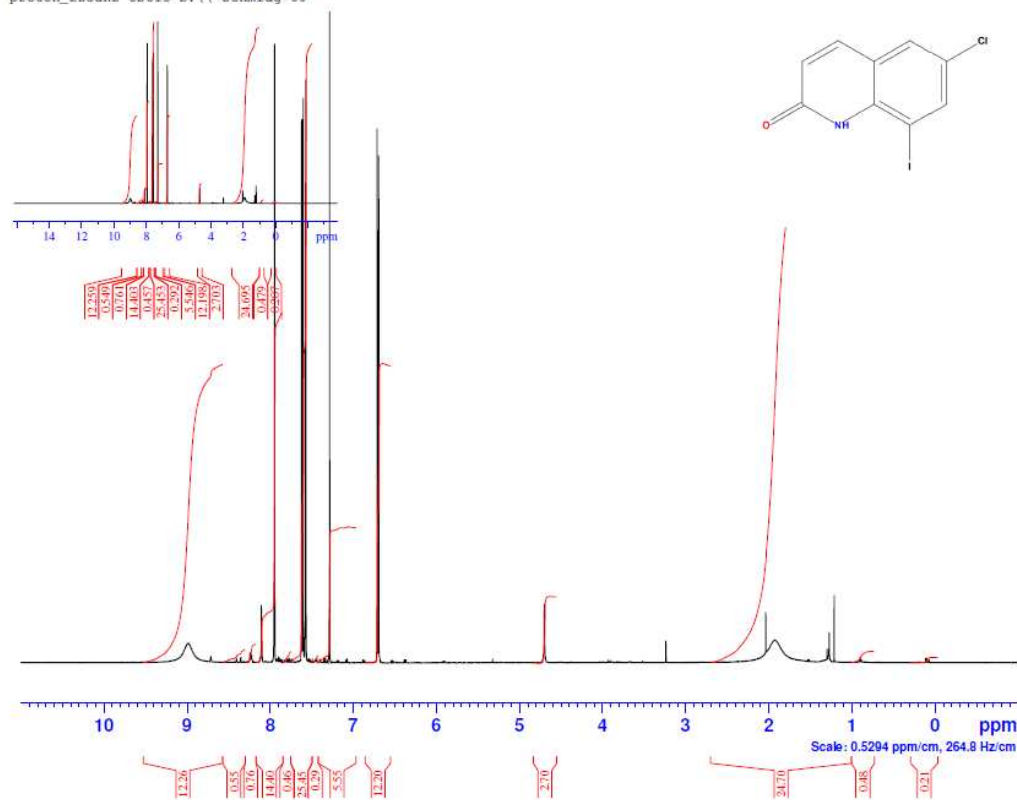
F2 - Acquisition Parameters
Date_     20170216
Time      17.13 h
INSTRUM   spect
PROBHD    Z128431_0003 (
PULPROG   zgpg30
TD         65536
SOLVENT   CDC13
NS         256
DS         4
SWH        31512.605 Hz
FIDRES     0.961688 Hz
AQ          1.03980378 sec
RG          200.03
LW         15.867 usec
DE         19.02 usec
TE          300.0 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0         1
SFO1       125.7728799 MHz
NUC1        13C
P1          10.00 usec
PLW1       21.50799942 W
SFO2       500.1320005 MHz
NUC2        1H
CPDPRG2    waltz16
PCPD2       80.00 usec
PLW2       12.56499958 W
PLW12      0.18587931 W
PLW13      0.09316271 W

F2 - Processing parameters
SI          32768
SF          125.7577890 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40
    
```

^1H NMR spectrum of 8-iodo-6-chloroquinolin-2(1H)-one **3o** (in CDCl_3).



cryst1
proton_2scans CDCl_3 D:\schmidg 60

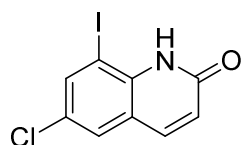


Current Data Parameters
NAME ELN090-1326_1_02
EXPNO 10
PROCNO 1

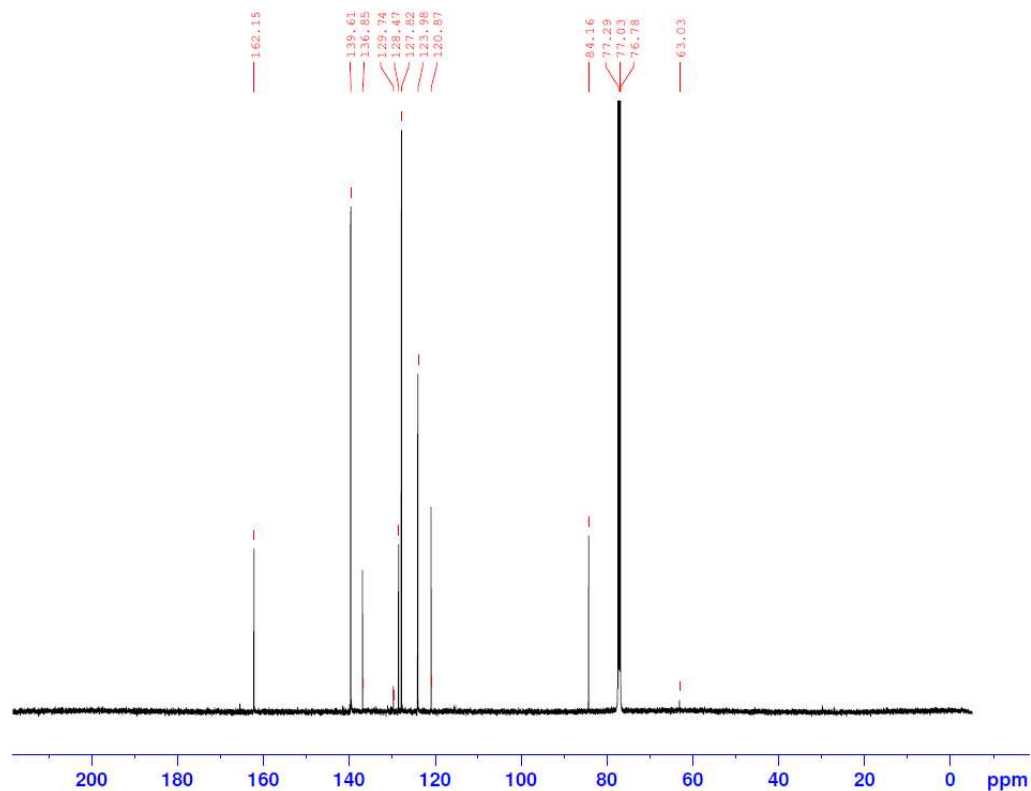
F2 - Acquisition Parameters
Date_ 20170222
Time 9.31 h
INSTRUM spect
PROBHD Z128431_0003 (4
PULPROG zg30
TD 52536
SOLVENT CDCl_3
NS 2
DS 2
SWH 10000.000 Hz
FIDRES 0.2005176 Hz
AQ 3.2767999 sec
RG 16.37
RW 50.000 usec
DE 10.00 usec
TE 298.0 K
D1 1.00000000 sec
TDO 1
SFO1 500.1330850 MHz
NUC1 1H
P1 10.00 usec
PLW1 12.56499958 W

F2 - Processing parameters
SI 52536
SF 500.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{13}C NMR spectrum of 8-iodo-6-chloroquinolin-2(1H)-one **3o** (in CDCl_3).



cryst1
C13_256scans CDC13 D:\ schmidg 60



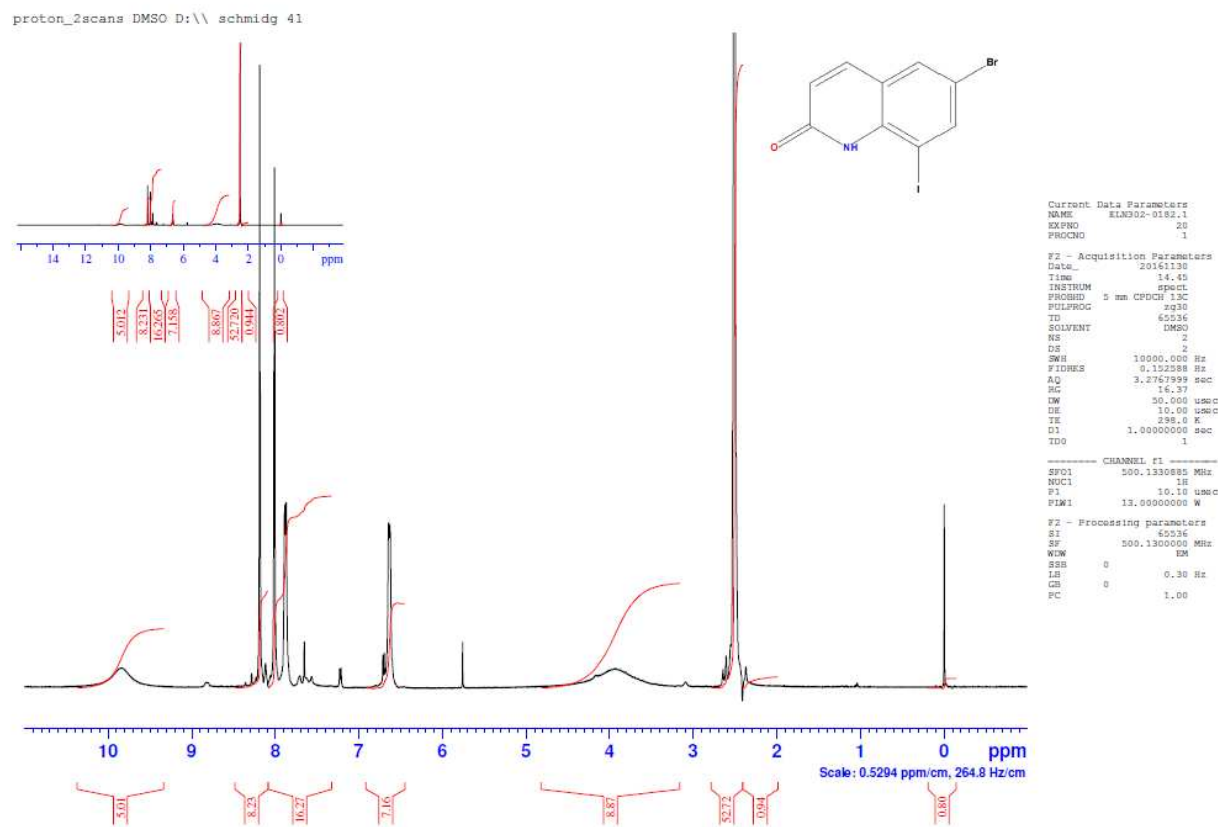
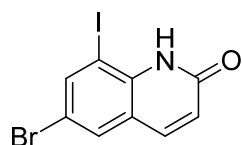
```

Current Data Parameters
NAME      E2N090-1326-1-02
EXPNO     11
PROCNO    1

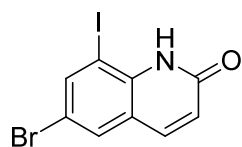
F2 - Acquisition Parameters
Date_     20170222
Time      9.46 h
INSTRUM   spect
PROBHD    Z120431_0003 (
PULPROG   zgpg30
TD         65536
SOLVENT   CDC13
NS         256
DS         4
SWH        31512.605 Hz
FIDRES     0.961668 Hz
AQ          1.0398378 sec
RG          200.03
SW          15.867 umcd
DE          19.02 umcd
TE          300.0 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0         1
SFO1       125.7728799 MHz
NUC1        13C
P1          10.00 umcd
PLW1        21.50799942 W
SFO2        500.1320005 MHz
NUC2         1H
CPDPRG2    waltz16
PCPD2       80.00 umcd
PLW2        12.56499958 W
PLW12       0.18587931 W
PLW13       0.09316271 W

F2 - Processing parameters
SI          32768
SF          125.7577890 MHz
WDM         RM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40
    
```

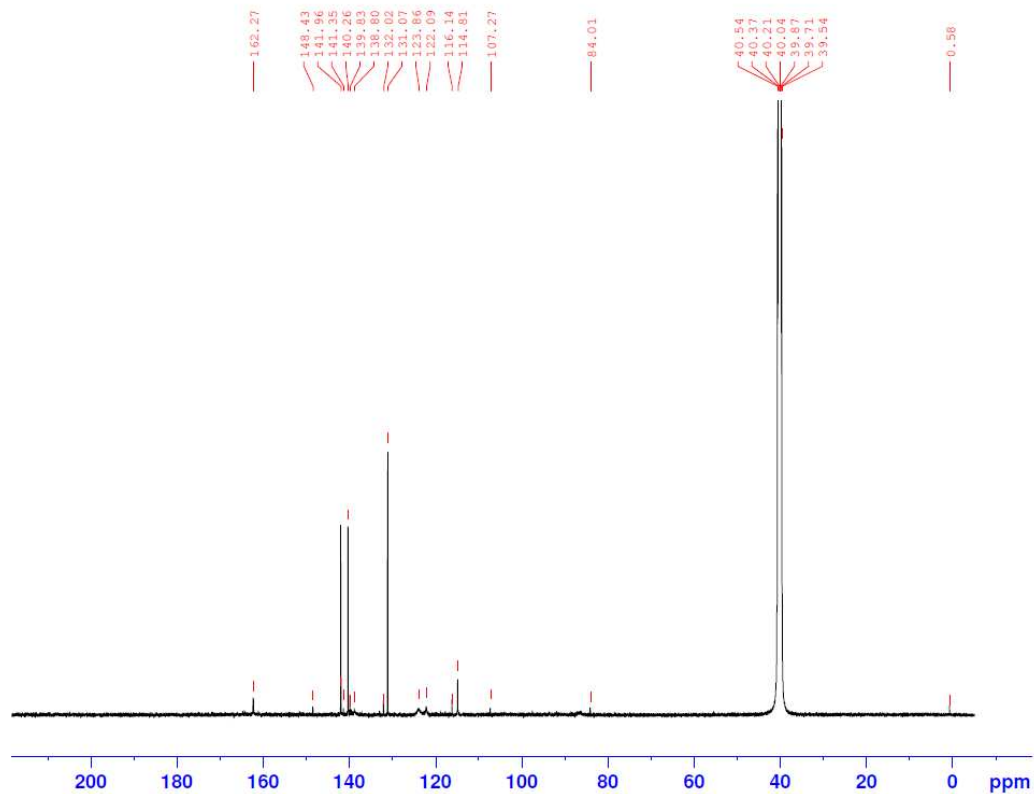
^1H NMR spectrum of 8-iodo-6-bromoquinolin-2(1H)-one **3p** (in D_6 -DMSO).



^{13}C NMR spectrum of 8-iodo-6-bromoquinolin-2(1H)-one **3p** (in $\text{D}_6\text{-DMSO}$).



C13_256scans DMSO D:\ schmidg 41



```

Current Data Parameters
NAME      EIA302-0182.1
EXPNO     21
PROCNO    1

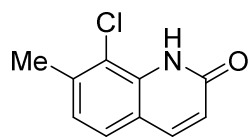
F2 - Acquisition Parameters
Date_     20161130
Time      15.00
INSTRUM   spect
PROBHD    5 mm CPOCR 13C
PULPROG   zgpg30
TD        65536
SOLVENT   DMSO
NS         256
DS         4
SWH        31512.605 Hz
FIDRES     0.480844 Hz
AQ         1.0398376 sec
RG         200.03
DW         15.867 usec
DE         60.67 usec
TE         300.0 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1

===== CHANNEL f1 =====
SFO1      125.7728799 MHz
NUC1       13C
P1         10.00 usec
PLW1       21.00000000 W

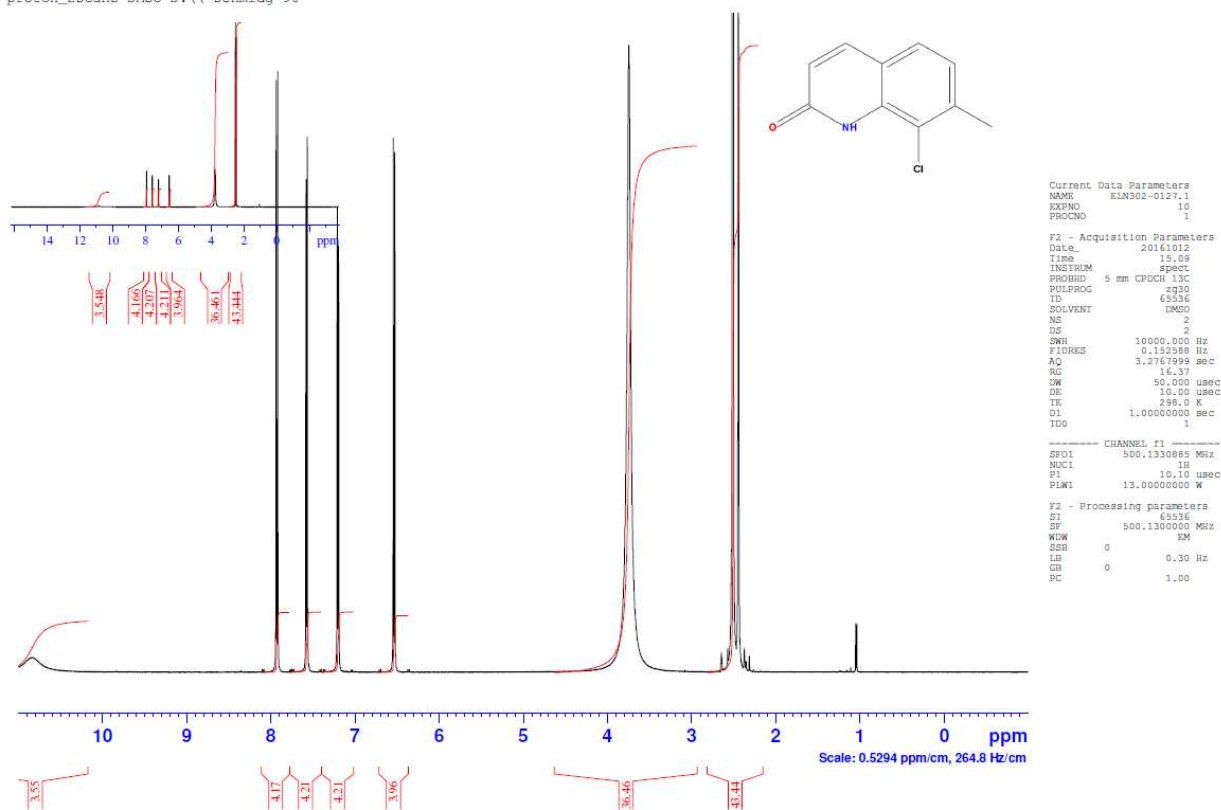
===== CHANNEL f2 =====
SFO2      500.1320005 MHz
NUC2       1H
CPOPRG2    waltz16
PCPD2      80.00 usec
PLW2       13.00000000 W
PLW12      0.22395000 W
PLW13      0.11264000 W

F2 - Processing parameters
SI         32768
SF         125.7577890 MHz
WDW        DM
SSB         0
LB          1.00 Hz
GB          0
PC          1.40
    
```

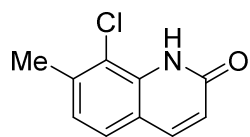
^1H NMR spectrum of 8-chloro-7-methylquinolin-2(1H)-one **3q** (in D_6 -DMSO).



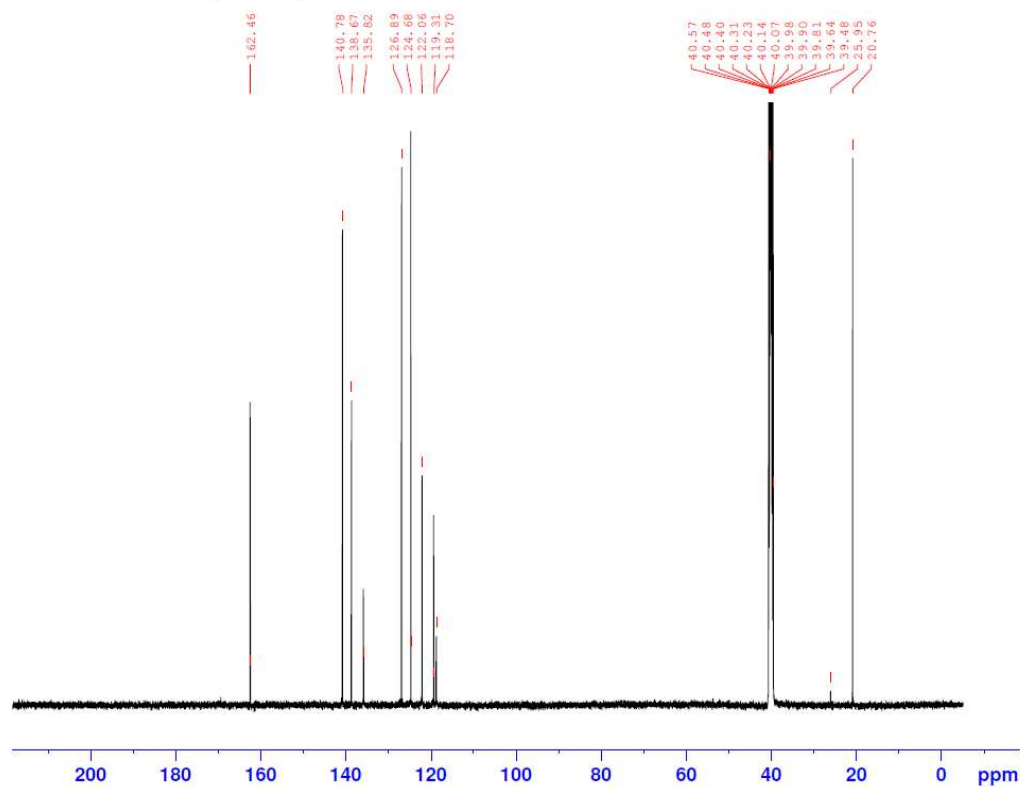
proton_2scans DMSO D:\ schmidg 96



^{13}C NMR spectrum of 8-chloro-7-methylquinolin-2(1H)-one **3q** (in $\text{D}_6\text{-DMSO}$).



C13_256scans DMSO D:\ schmidg 96



```

Current Data Parameters
NAME      ELN302-0127.1
EXPNO     11
PROCNO    1

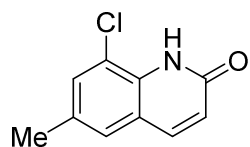
F2 - Acquisition Parameters
Date_     20161012
Time      15.24
INSTRUM   spect
PROBHD    5 mm CPDQX 13C
PULPROG   zgpg30
TD         65536
SOLVENT   DMSO
NS         256
DS         4
SWH        31512.605 Hz
FIDRES     0.480844 Hz
AQ         1.0398378 sec
RG         200.03
DW         15.867 usec
DE         60.67 usec
TE         300.0 K
D1         2.0000000 sec
D11        0.0300000 sec
TD0        1

===== CHANNEL f1 =====
SFO1      125.7728799 MHz
NUC1       13C
P1         10.00 usec
PLW1       21.00000000 W

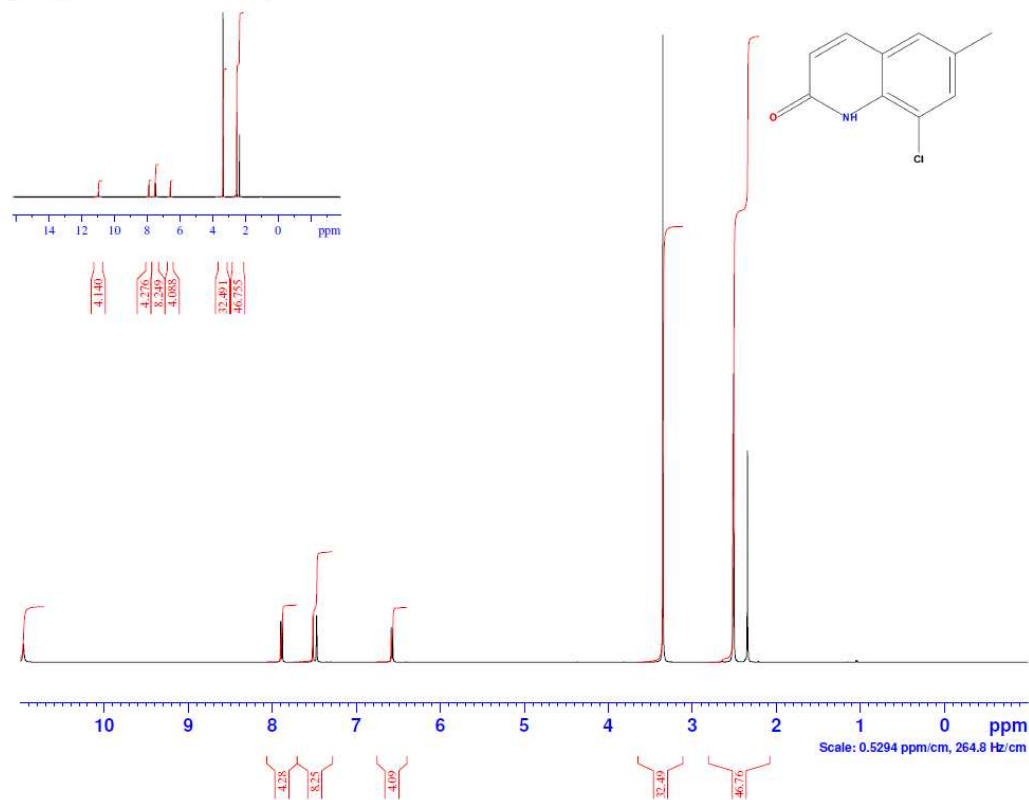
===== CHANNEL f2 =====
SFO2      500.1320095 MHz
NUC2       1H
CPDPRG2   waltz16
PCPD2     80.00 usec
PLW2       13.00000000 W
PLW12     0.22390000 W
PLW13     0.11264000 W

F2 - Processing parameters
SI         32768
SF         125.7577890 MHz
WDW        0
SSB        0
GB         0
PC         1.40
    
```

^1H NMR spectrum of 8-chloro-6-methylquinolin-2(1H)-one **3r** (in D_6 -DMSO).



proton_2scans DMSO D:\ schmidg 95



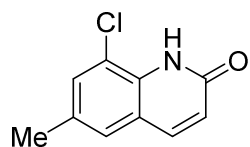
Current Data Parameters
NAME ELN302-0124.1
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161012
Time 14.51
INSTRUM spect
PROBHD 5 mm CPDCH 13C
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 2
DS 2
SWH 10000.000 Hz
FIDRES 0.192588 Hz
AQ 3.2767999 sec
RG 11.16
RW 50.000 usec
DE 10.00 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

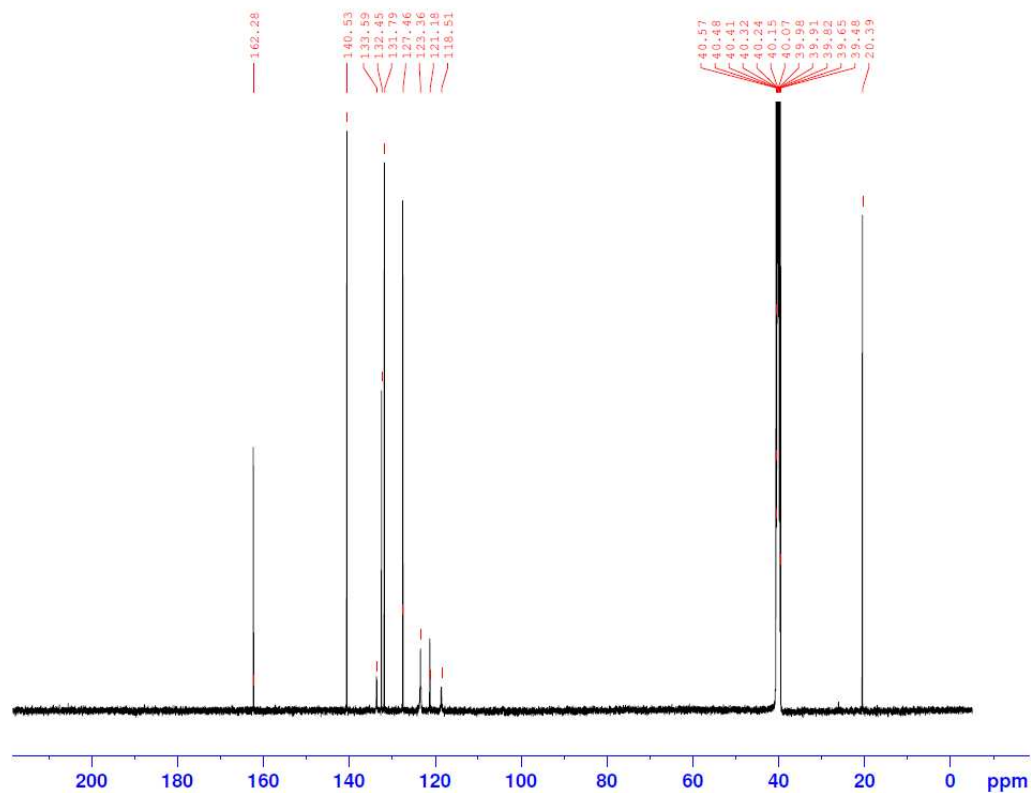
CHANNEL f1
SFO1 500.1330885 MHz
NUC1 1H
P1 10.10 usec
PLW1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 500.1330885 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{13}C NMR spectrum of 8-chloro-6-methylquinolin-2(1H)-one **3r** (in $\text{D}_6\text{-DMSO}$).



C13_256scans DMSO D:\schmidg 95



```

Current Data Parameters
NAME      E13305-0124.1
EXPNO     11
PROCNO    1

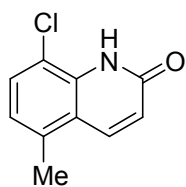
F2 - Acquisition Parameters
Date_     20161012
Time      15.06
INSTRUM   spect
PROBHD    5 mm CPOCH 13C
PULPROG   zgpg30
TD         65536
SOLVENT   DMSO
NS         256
DS         4
SWH        31512.605 Hz
FIDRES     0.480844 Hz
AQ          1.0398378 sec
RG          200.03
DW          15.867 usec
DE          60.67 usec
TE          300.0 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0         1

===== CHANNEL f1 =====
SFO1      125.7728789 MHz
NUC1       13C
P1         10.00 usec
PLM1       21.00000000 W

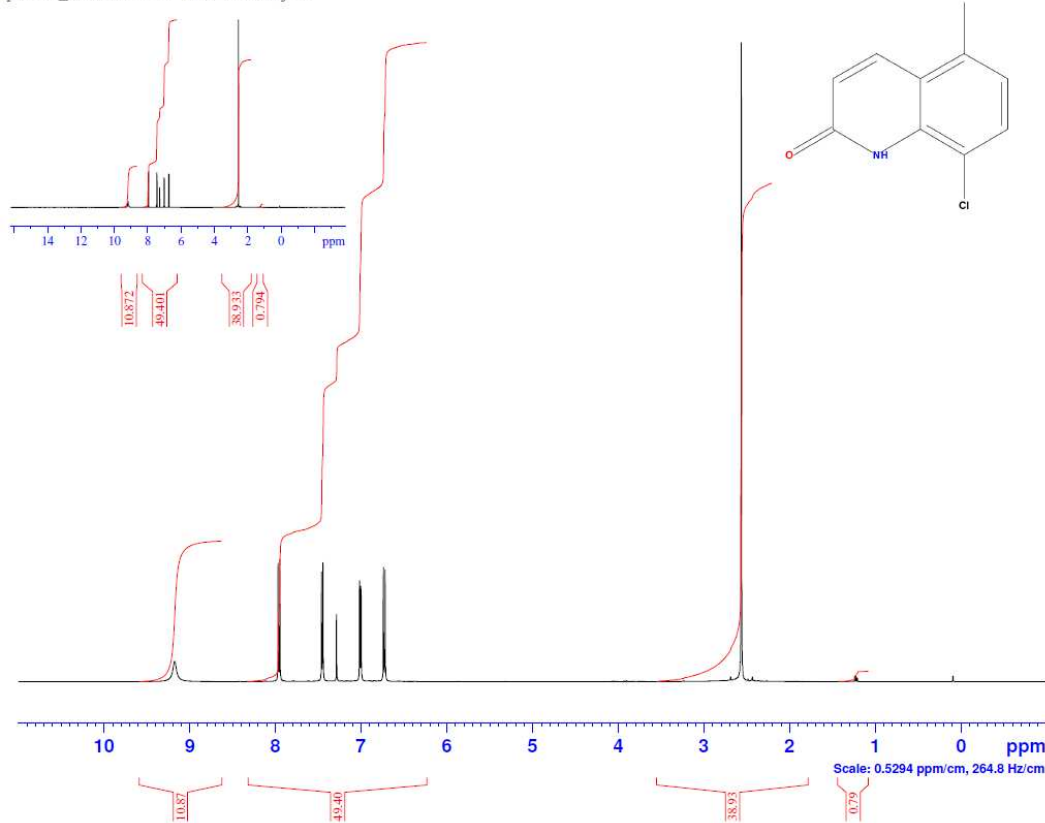
===== CHANNEL f2 =====
SFO2      500.1320005 MHz
NUC2       1H
CPOPRG12  waltz16
PCPD2      80.00 usec
PLM2       13.00000000 W
PLM12      0.22395000 W
PLM13      0.11264000 W

F2 - Processing parameters
SI          32768
SF          125.7577890 MHz
WDW         RM
SSB         0
LB          1.00 Hz
GB          0
CB          0
PC          1.40
    
```

^1H NMR spectrum of 8-chloro-5-methylquinolin-2(1H)-one **3s** (in CDCl_3).



proton_2scans CDCl_3 D:\schmidg 42



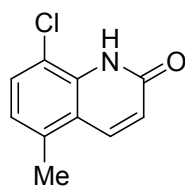
Current Data Parameters
NAME ELN302-0104.1_02
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170109
Time 12.36
INSTRUM spect
PROBHD 5 mm CPDCH 13C
PULPROG zg30
TD 65536
SOLVENT CDCl_3
NS 2
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 16.37
DW 50.000 μs
DE 15.00 μs
TE 298.0 K
D1 1.00000000 sec
D11 1
D10 1

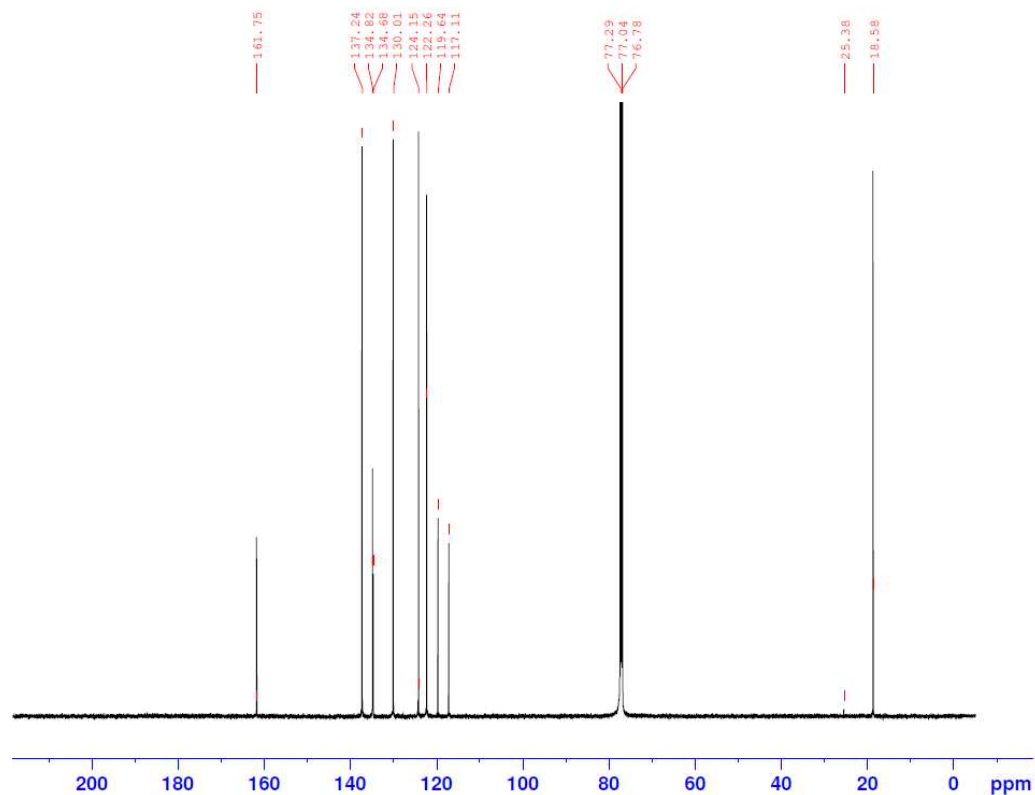
CHANNEL f1
SFO1 500.1330885 MHz
NUC1 ^1H
P1 10.10 μs
PLW1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 500.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{13}C NMR spectrum of 8-chloro-5-methylquinolin-2(1H)-one **3s** (in CDCl_3).



C13_256scans CDCl_3 D:\schmidg 42



```

Current Data Parameters
NAME      ELN302-0104.1.02
EXPNO     11
PROCNO    1

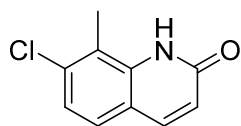
F2 - Acquisition Parameters
Date_     20170109
Time      12.51
INSTRUM   spect
PROBHD    5 mm CPDCH 13C
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         256
DS         4
SWH        31512.605 Hz
FIDRES     0.480844 Hz
AQ          1.0398378 sec
RG          200.03
RW          15.867 usec
DE          60.67 usec
TE          300.0 K
D1          2.00000000 sec
D11         0.03000000 sec
TDS         1

===== CHANNEL f1 =====
SF01       125.7728799 MHz
NUC1        13C
P1          10.00 usec
PLM1        21.00000000 W

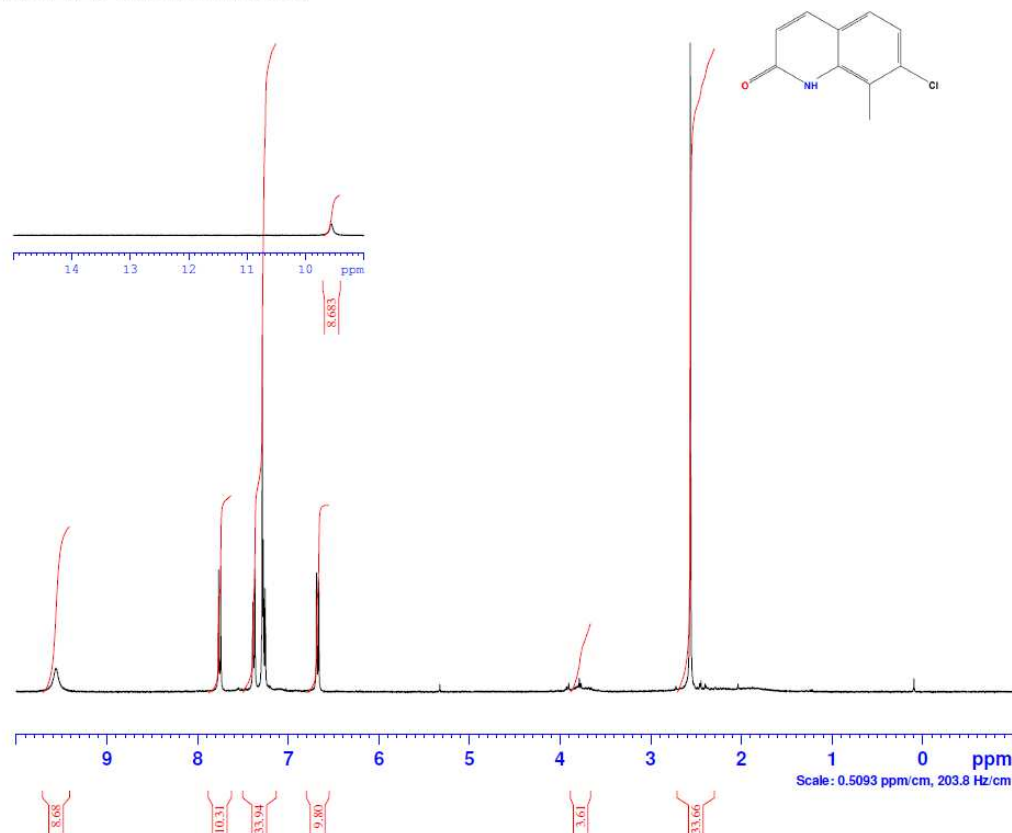
===== CHANNEL f2 =====
SF02       500.1320005 MHz
NUC2         1H
CPDPRG2    waltz16
PCPD2       40.00 usec
PLM2        13.00000000 W
PLM12       0.22395000 W
PLM13       0.11264000 W

F2 - Processing parameters
SI          32768
SF          125.7577890 MHz
WDW         0
SSB         0
LB          1.00 Hz
GB          0
PC          1.40
    
```

^1H NMR spectrum of 7-chloro-8-methylquinolin-2(1H)-one **3t** (in CDCl_3).



after purification
proton_np_cl CDCl_3 D:\schmidg 90



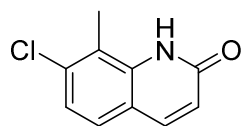
Current Data Parameters
NAME: ELN302-0092.1
EXPNO: 10
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20160927
Time: 16.18
INSTRUM: spect
PROBHD: 5 mm PABBO BB-
PULPROG: zg30
TD: 65536
SOLVENT: CDCl_3
NS: 8
DS: 2
SWH: 8223.685 Hz
FIDRES: 0.125483 Hz
AQ: 3.9845889 sec
RG: 203
DW: 60.800 usec
DE: 6.50 usec
TE: 296.0 K
D1: 1.00000000 sec
TDO: 1

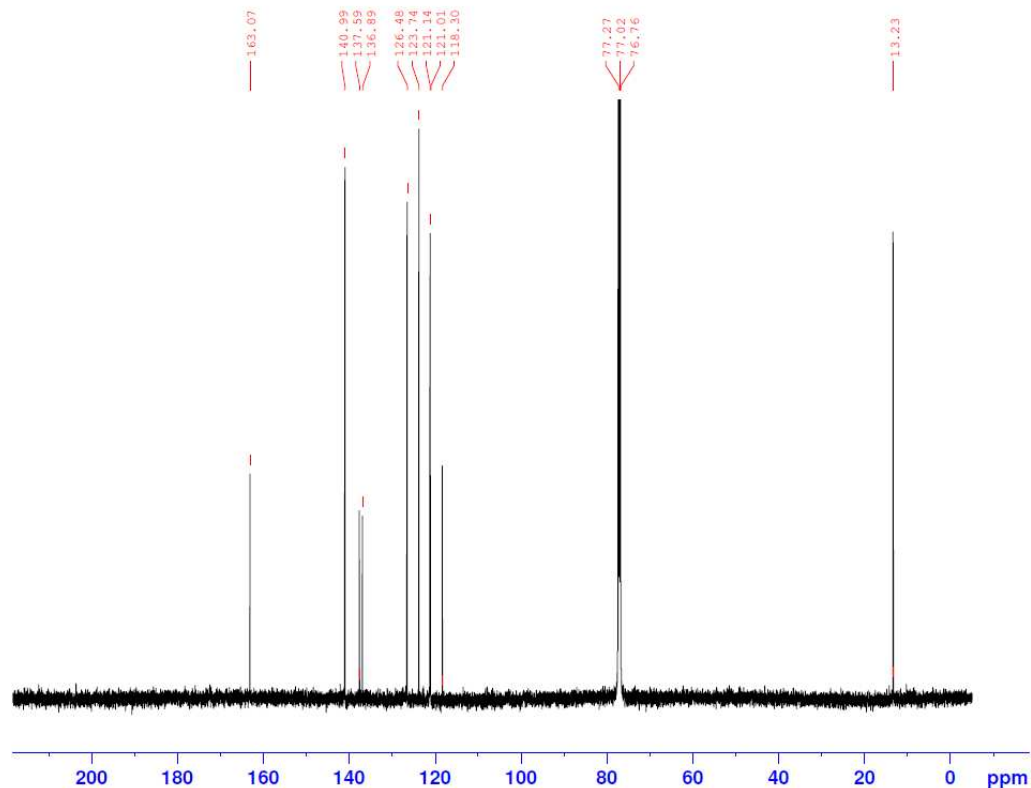
CHANNEL f1
SFO1: 400.1324710 MHz
NUC1: ^1H
P1: 10.70 usec
PLW1: 18.29999924 W

F2 - Processing parameters
SI: 32768
SF: 400.1300000 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00

^{13}C NMR spectrum of 7-chloro-8-methylquinolin-2(1H)-one **3t** (in CDCl_3).



C13_256scans CDC13 D:\ schmidg 30



```

Current Data Parameters
NAME: ELM302-0092.1
EXPNO: 11
PROCNO: 1

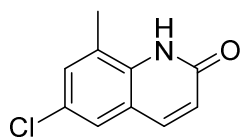
F2 - Acquisition Parameters
Date_: 20160927
Time: 10.13
INSTRUM: spect
PROBHD: 5 mm CPOCH 13C
PULPROG: zgpg30
TD: 65536
SOLVENT: CDC13
NS: 256
DS: 4
SWH: 21512.605 Hz
FIDRES: 0.480844 Hz
AQ: 1.0398378 sec
RG: 200.03
DW: 15.867 usec
DE: 60.67 usec
TE: 300.0 K
D1: 2.00000000 sec
D11: 0.03000000 sec
TD0: 1

===== CHANNEL f1 =====
SFO1: 125.7728799 MHz
NUC1: 13C
P1: 10.00 usec
PLW1: 21.00000000 W

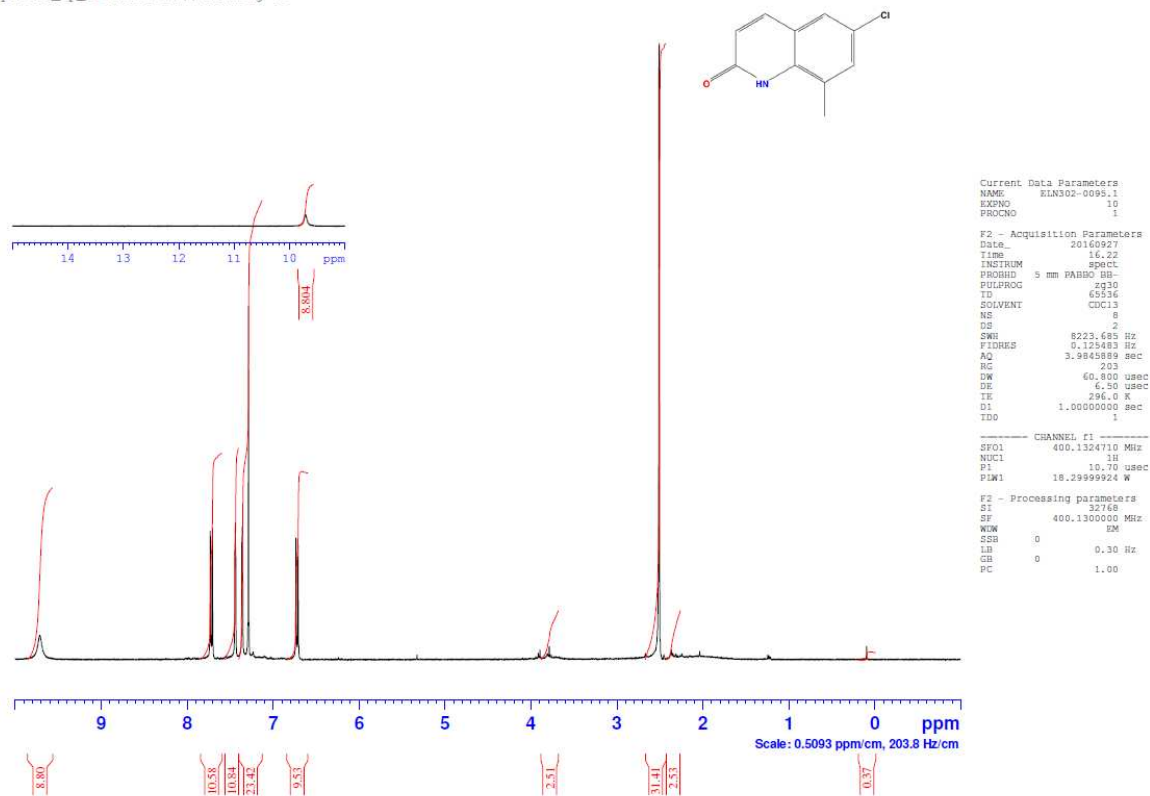
===== CHANNEL f2 =====
SFO2: 500.1320005 MHz
NUC2: 1H
CPDPRG2: waltz16
PCPD2: 80.00 usec
PLW2: 13.00000000 W
PLW12: 0.22395000 W
PLW13: 0.11264000 W

F2 - Processing parameters
SI: 32768
SF: 125.7577890 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.40
    
```

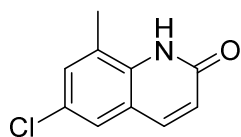
^1H NMR spectrum of 6-chloro-8-methylquinolin-2(1H)-one **3u** (in CDCl_3).



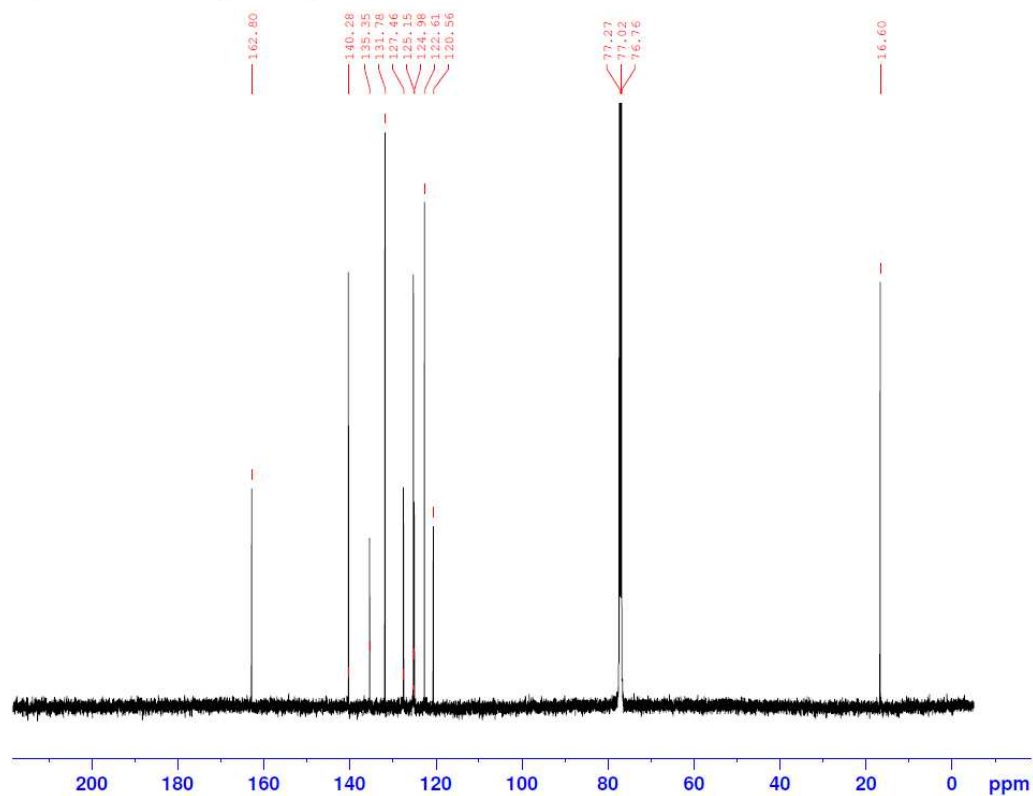
after purification
proton_np_cl CDCl_3 D:\schmidg 91



^{13}C NMR spectrum of 6-chloro-8-methylquinolin-2(1H)-one **3u** (in CDCl_3).



C13_256scans CDC13 D:\ schmidg 31



```

=====
Current Data Parameters
NAME      EIN302-0095.1
EXPNO     11
PROCNO    1

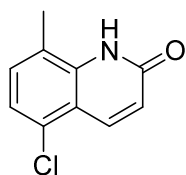
F2 - Acquisition Parameters
Date_     20160927
Time      10.31
INSTRUM   spect
PROBHD    5 mm CPOCH 13C
PULPROG   zgpg30
TD        65536
SOLVENT   CDCl3
NS         256
DS         4
SWH        31512.605 Hz
FIDRES     0.480844 Hz
AQ         1.0398378 sec
RG         200.03
DW         15.867 usec
DE         60.67 usec
TE         300.0 K
D1         2.0000000 sec
D11        0.0300000 sec
TD0        1

===== CHANNEL f1 =====
SFO1      125.7728799 MHz
NUC1       13C
P1         10.00 usec
PLW1      21.00000000 W

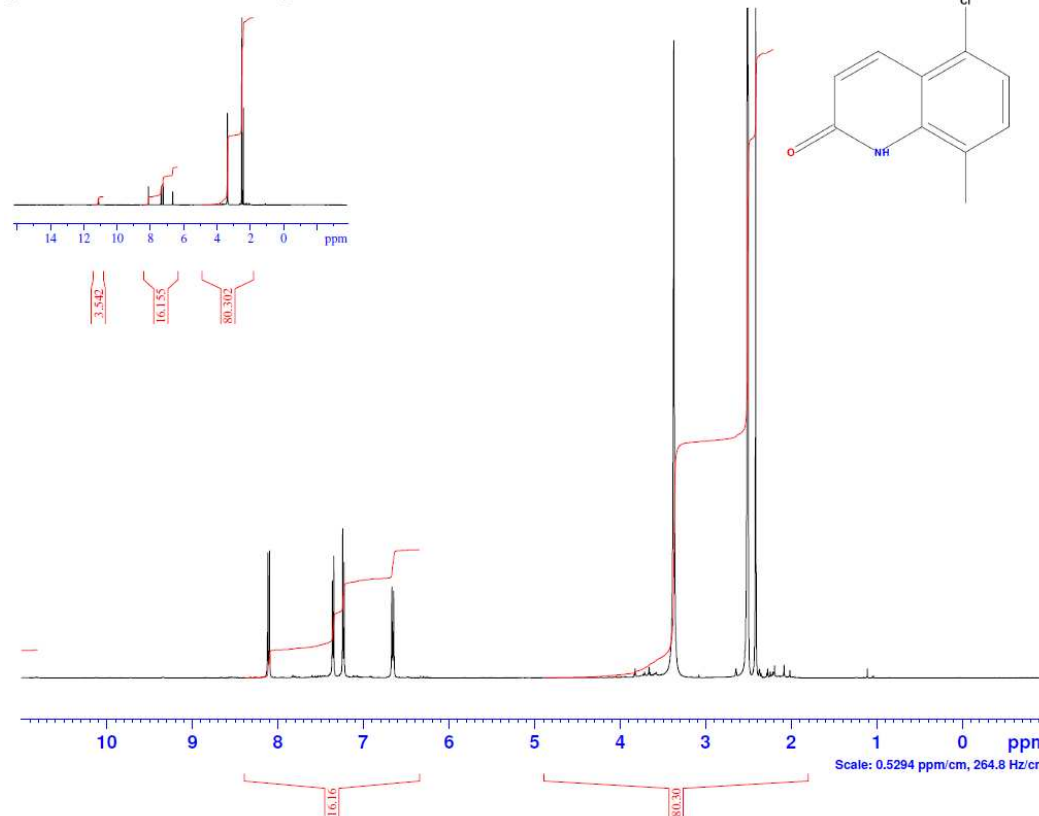
===== CHANNEL f2 =====
SFO2      500.1320005 MHz
NUC2       1H
CPDPRG2   waltz16
PCPD2     80.00 usec
PLW2      13.00000000 W
PLW12     0.22391000 W
PLW13     0.11264000 W

F2 - Processing parameters
SI         32768
SF         125.7577890 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
    
```

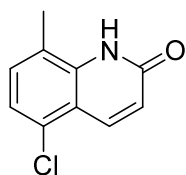
^1H NMR spectrum of 5-chloro-8-methylquinolin-2(1H)-one **3v** (in D_6 -DMSO).



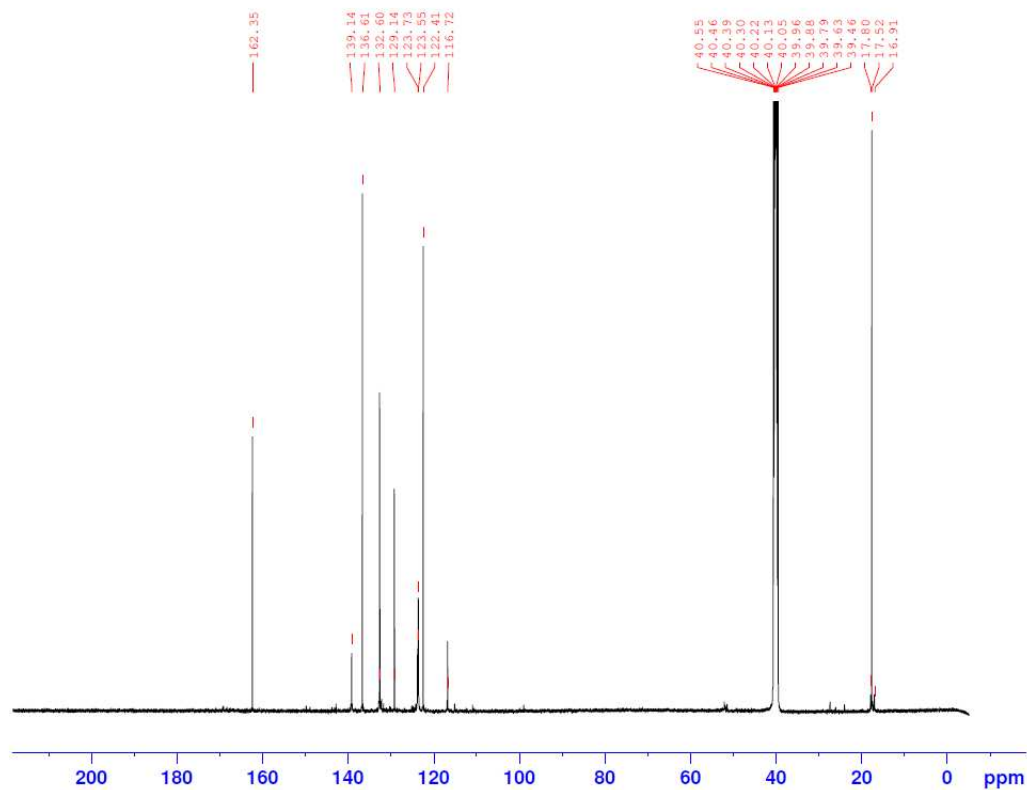
proton_32scans DMSO D:\schmidg 61



^{13}C NMR spectrum of 5-chloro-8-methylquinolin-2(1H)-one **3v** (in $\text{D}_6\text{-DMSO}$).



C13_2048scans DMSO D:\schmidg 75



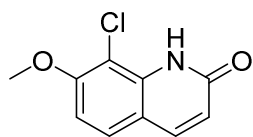
```

Current Data Parameters
NAME      ELN302-0100.1.02
EXPNO     30
PROCNO    1

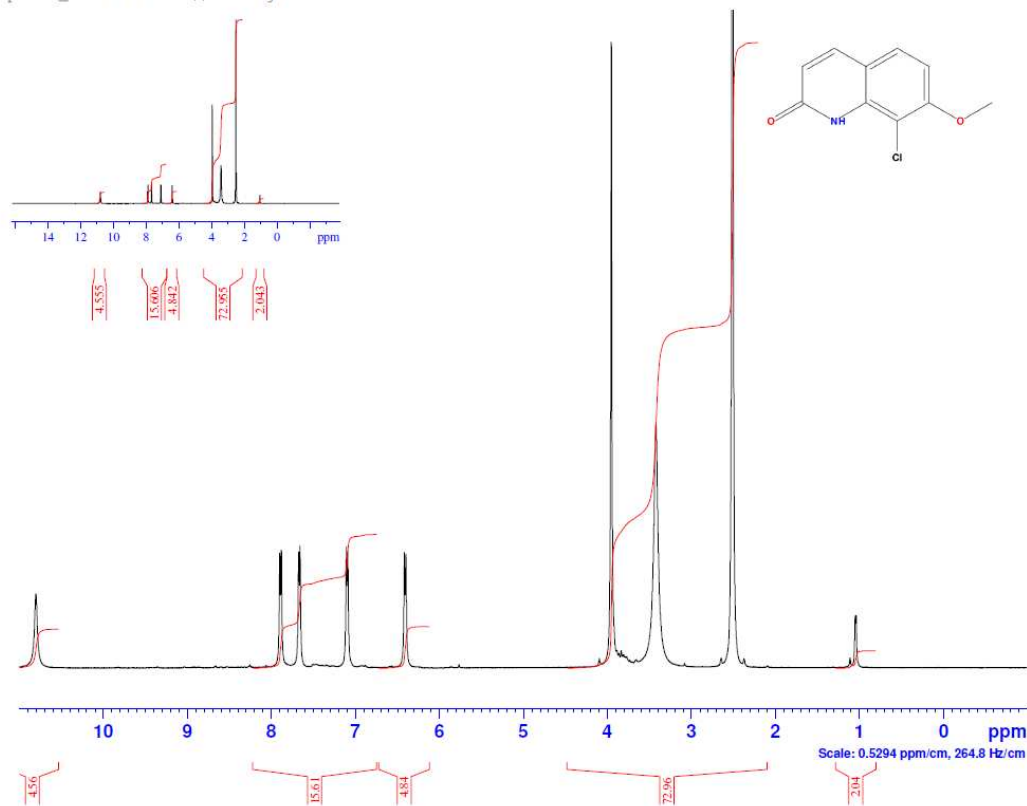
F2 - Acquisition Parameters
Date_     20170518
Time      5.40 h
INSTRUM   spect
PROBHD    Z128431_0003 (
PULPROG   zgpg30
TD         65536
SOLVENT   DMSO
NS         6048
DS         4
SWH        31512.605 Hz
FIDRES     0.961688 Hz
AQ         1.0398378 sec
RG         200.00
DW         15.867 usec
DE         19.02 usec
TE         300.0 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1
SFO1       125.7728799 MHz
NUC1       13C
P1         10.00 usec
PLM1       21.50798942 W
SFO2       500.1326005 MHz
NUC2       1H
CPDPRG2   waltz16
PCPD2      80.00 usec
PLM2       12.56499958 W
PLM12      0.18687931 W
PLM13      0.09316271 W

F2 - Processing parameters
SI         32768
SF         125.7577890 MHz
WDW        EM
SSB         0
LB         1.00 Hz
GB         0
PC         1.40
    
```

^1H NMR spectrum of 8-chloro-7-methoxyquinolin-2(1H)-one **3w** (in $\text{D}_6\text{-DMSO}$).



crude
proton_2scans DMSO D:\ schmidg 53



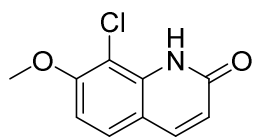
Current Data Parameters
NAME ELN302-0114.1
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161005
Time 17.09
INSTRUM spect
PROBHD 5 mm CPDCH 13C
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 2
DS 2
SWH 10000.000 Hz
FIDRES 0.132388 Hz
AQ 3.2767999 sec
RG 11.16
RW 50.000 usec
DE 10.00 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

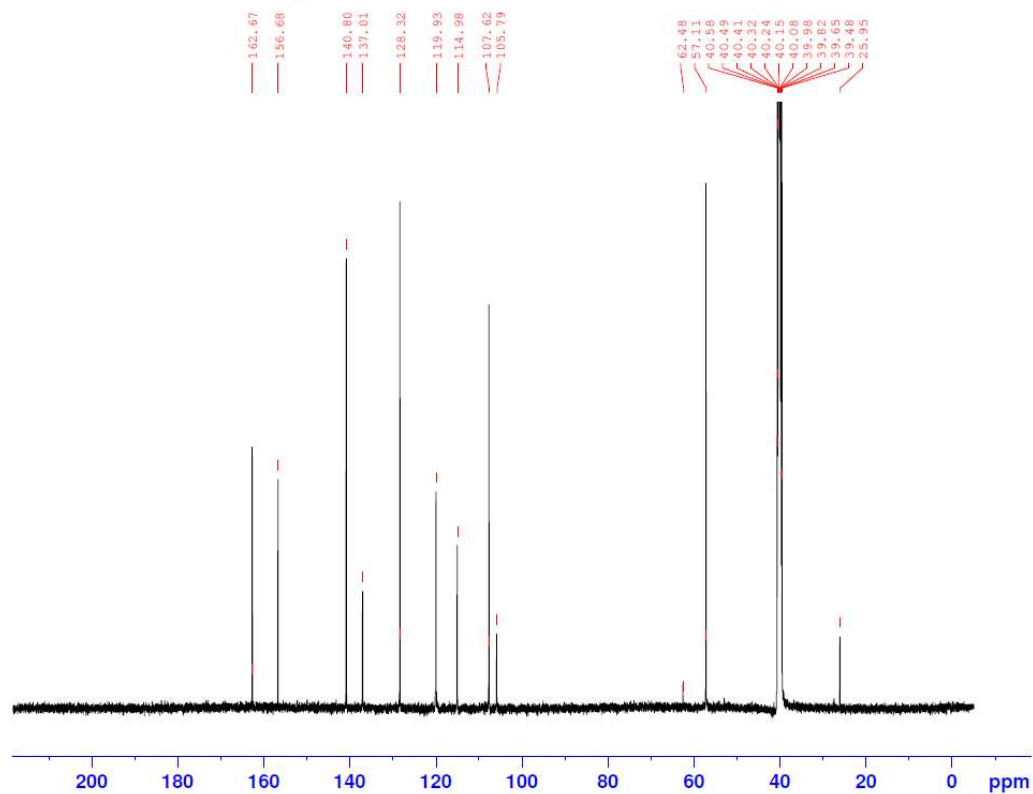
CHANNEL f1
SFO1 500.1330885 MHz
NUC1 1H
P1 10.10 usec
PLW1 13.00000000 W

F2 - Processing parameters
S1 65536
SF 500.1300000 MHz
WDW RM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{13}C NMR spectrum of 8-chloro-7-methoxyquinolin-2(1H)-one **3w** (in D_6 -DMSO).



crude
C13_256scans DMSO D:\\ schmidg 53



```

Current Data Parameters
NAME      ELN302-0114.1
EXPNO     11
PROCNO    1

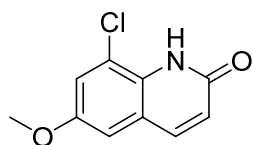
F2 - Acquisition Parameters
Date_     20161005
Time      17.24
INSTRUM   spect
PROBHD    5 mm CPDPR 13C
PULPROG   zgpg30
TD        65536
SOLVENT   DMSO
NS         256
DS         4
SWH        31512.600 Hz
FIDRES     0.480844 Hz
AQ         1.0398378 sec
RG         200.03
DW         15.867 usec
DE         60.67 usec
TE         300.0 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1

===== CHANNEL f1 =====
SP01      125.7728799 MHz
NUC1       13C
P1         10.00 usec
PLW1       21.00000000 W

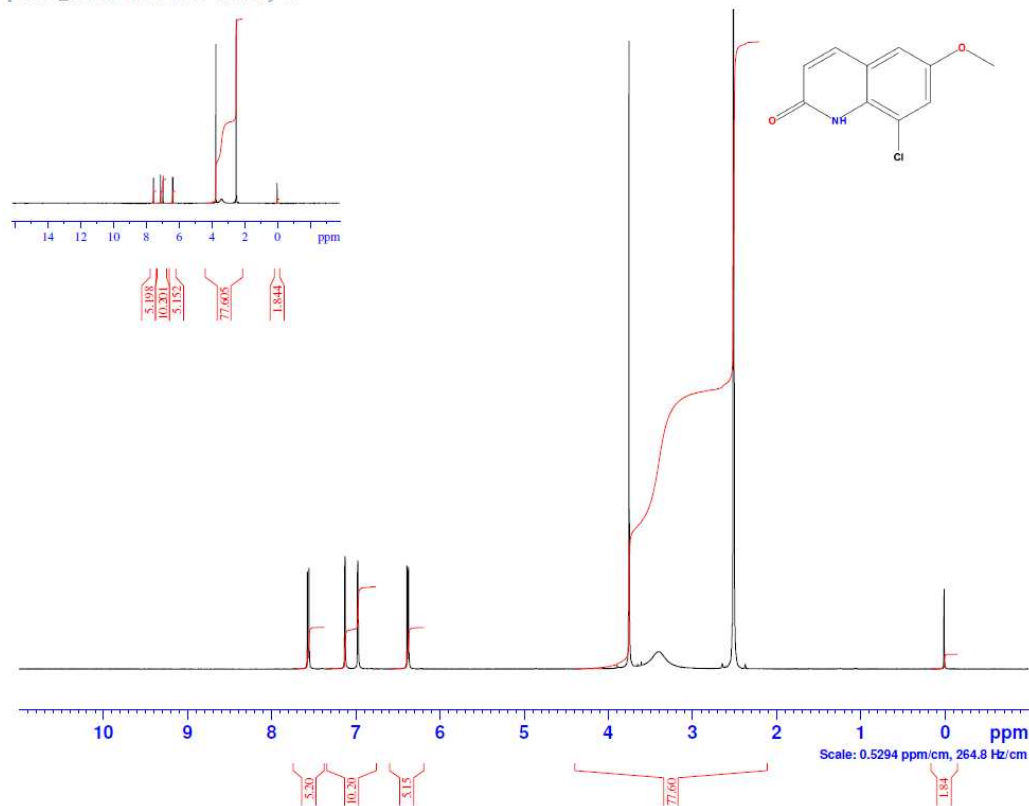
===== CHANNEL f2 =====
SP02      500.1320000 MHz
NUC2       1H
CPDPRG2    waltz16
PCPD2      80.00 usec
PLW2       13.00000000 W
PLW12      0.22395000 W
PLW13      0.11264000 W

F2 - Processing parameters
SI         32768
SF         125.7577890 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
    
```

^1H NMR spectrum of 8-chloro-6-methoxyquinolin-2(1H)-one **3x** (in D_6 -DMSO).



after purification
proton_2scans DMSO D:\ schmidg 94



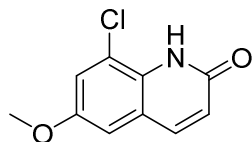
Current Data Parameters
NAME ELN302-0146.1
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161102
Time 17.02
INSTRUM spect
PROBHD 5 mm CPDCH 13C
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 2
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 34.06
RW 50.000 usec
DE 10.00 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

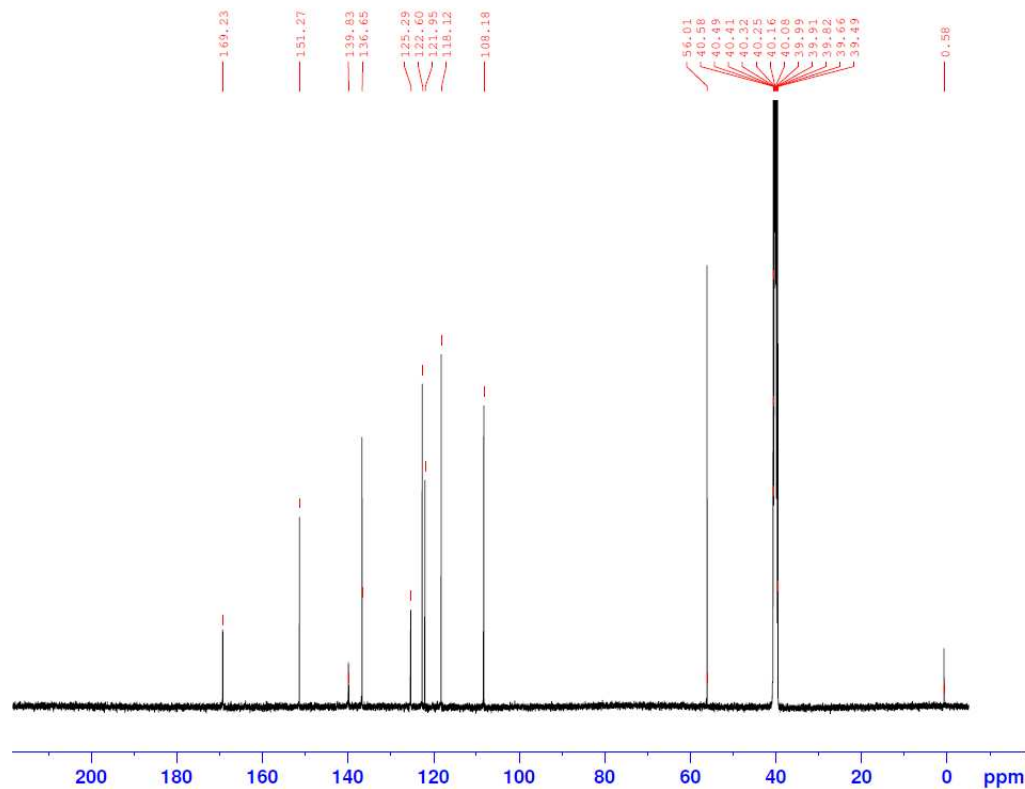
CHANNEL f1
SFO1 500.1330885 MHz
NUC1 1H
P1 10.10 usec
PLW1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 500.1330885 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{13}C NMR spectrum of 8-chloro-6-methoxyquinolin-2(1H)-one **3x** (in $\text{D}_6\text{-DMSO}$).



after purification
C13_256scans DMSO D:\ schmidg 94



```

Current Data Parameters
NAME: ELN302-0146.1
EXPNO: 21
PROCNO: 1

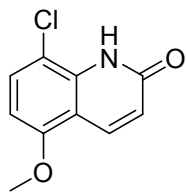
F2 - Acquisition Parameters
Date_: 20161102
Time: 17.17
INSTRUM: spect
PROBHD: 5 mm CPDCH 13C
PULPROG: zgpg30
TD: 65536
SOLVENT: DMSO
NS: 256
DS: 4
SWH: 31512.605 Hz
FIDRES: 0.480844 Hz
AQ: 1.0398378 sec
RG: 200.03
DM: 15.867 usec
DE: 60.67 usec
TK: 300.0 K
D1: 2.00000000 sec
D11: 0.03000000 sec
TD0: 1

===== CHANNEL F1 =====
SFO1: 125.7728799 MHz
NUC1: 13C
P1: 10.00 usec
PIW1: 21.00000000 W

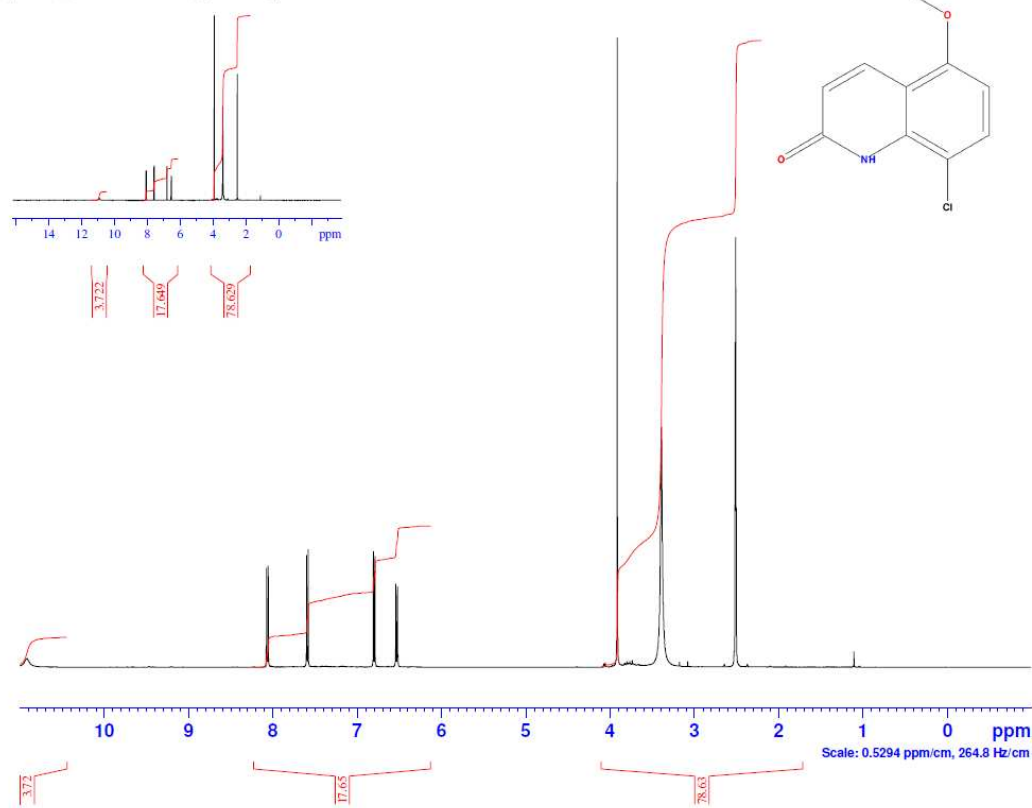
===== CHANNEL F2 =====
SFO2: 500.1320005 MHz
NUC2: 1H
PCPD2: waltz16
PCPD2: 80.00 usec
P2W2: 13.00000000 W
PIW2: 0.22395000 W
PIW13: 0.11264000 W

F2 - Processing parameters
SI: 32768
SF: 125.7677880 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.40
    
```

^1H NMR spectrum of 8-chloro-5-methoxyquinolin-2(1H)-one **3y** (in D_6 -DMSO).



proton_2scans DMSO D:\schmidg 40



Current Data Parameters

NAME	ELN302-0088.1.02
EXPNO	10
PROCNO	1

F2 - Acquisition Parameters

DATE_	20170109
TIME	12.16
INSTRUM	spect
PROBHD	5 mm CPDCH 13C
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	2
DS	2
SWH	10000.000 Hz
FIDRES	0.152588 Hz
AQ	3.2767999 sec
RG	11.16
DW	50.000 usec
DE	10.00 usec
TE	300.0 K
D1	1.00000000 sec
TD0	1

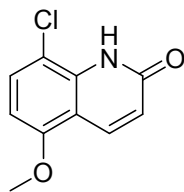
----- CHANNEL f1 -----

SFO1	500.1330885 MHz
NUC1	^1H
P1	10.10 usec
PLW1	13.00000000 W

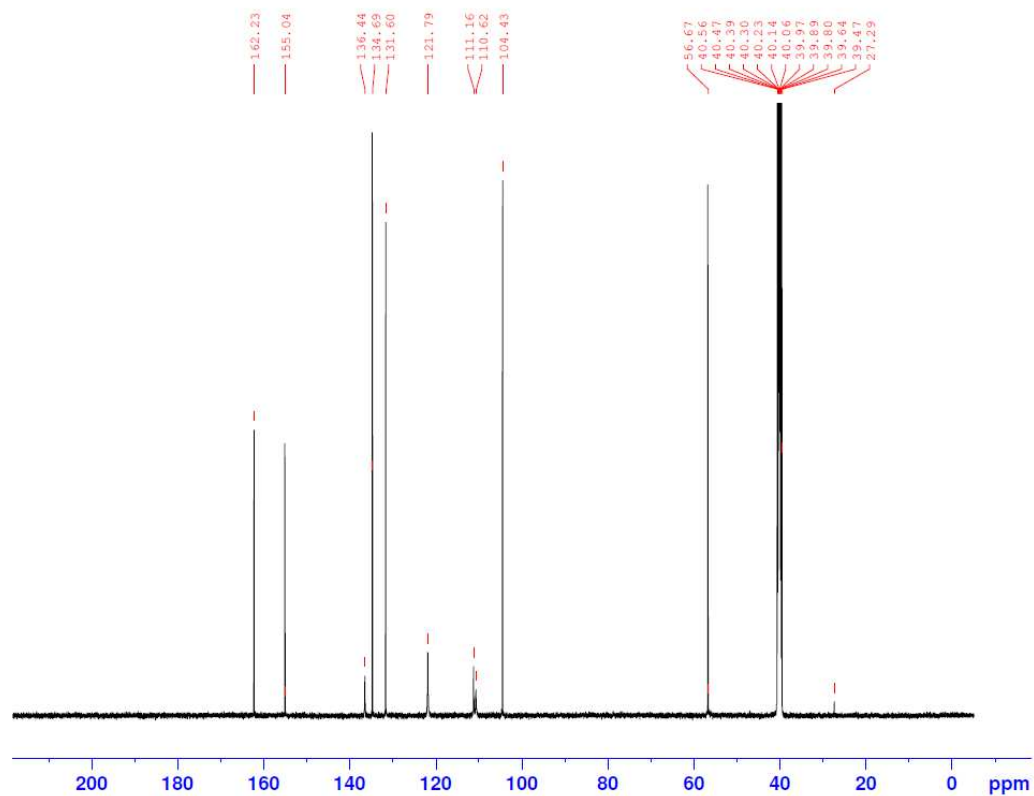
F2 - Processing parameters

SI	65536
SF	500.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

^{13}C NMR spectrum of 8-chloro-5-methoxyquinolin-2(1H)-one **3y** (in D_6 -DMSO).



C13_256scans DMSO D:\ schmidg 40



```

Current Data Parameters
NAME      ERM302-0098.1.02
EXPNO     11
PROCNO    1

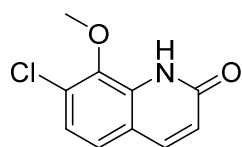
F2 - Acquisition Parameters
Date_     20170109
Time      12.31
INSTRUM   spect
PROBHD    5 mm CPOCR 13C
PULPROG   zgpg30
TD        65536
SOLVENT   DMSO
NS         256
DS         4
SWH        31512.605 Hz
FIDRES     0.480844 Hz
AQ         1.0398376 sec
RG         200.03
RW         15.967 usec
DE         60.67 usec
TE         300.0 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1

===== CHANNEL f1 =====
SFO1      125.7728799 MHz
NUC1       13C
P1         10.00 usec
PLM1       21.00000000 W

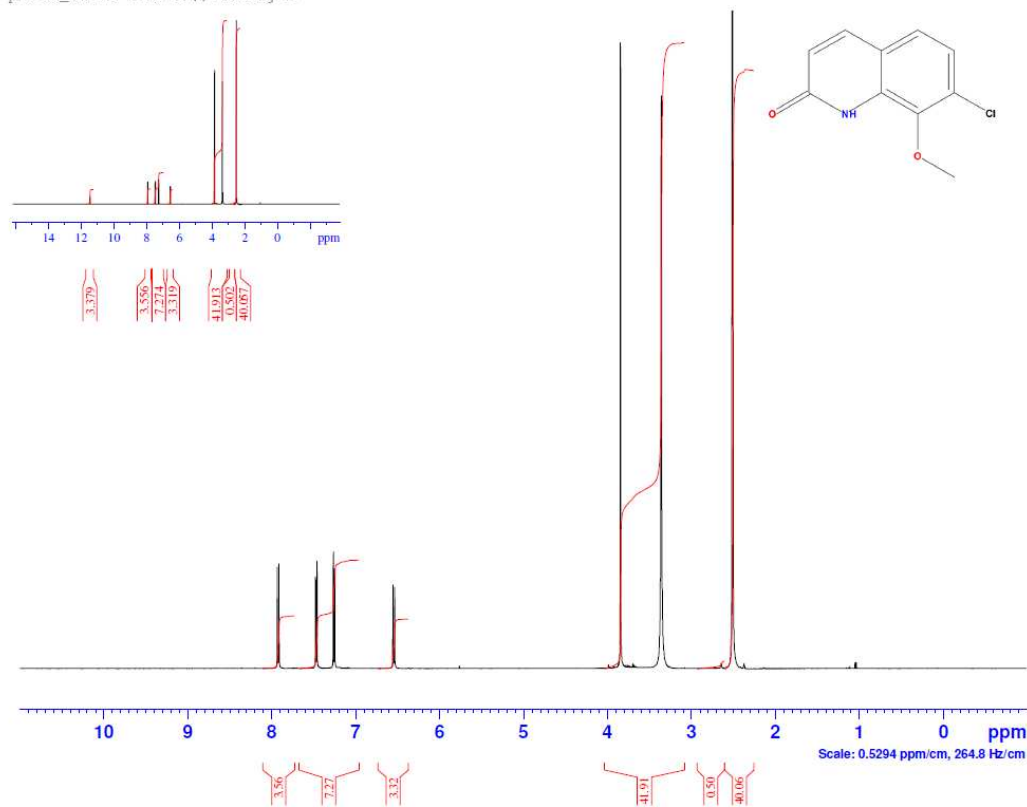
===== CHANNEL f2 =====
SFO2      500.1320005 MHz
NUC2       1H
CPOCRPG2  waltz16
PCPD2      80.00 usec
PLM2       13.00000000 W
PLM12      0.22395000 W
PLM13      0.11264000 W

F2 - Processing parameters
SI         32768
SF         125.7577890 MHz
WDW        EM
SSB         0
LB         1.00 Hz
GB         0
PC         1.40
    
```

^1H NMR spectrum of 7-chloro-8-methoxyquinolin-2(1H)-one **3z** (in D_6 -DMSO).



crude
proton_2scans DMSO D:\schmidg 47



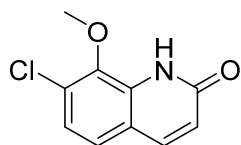
Current Data Parameters
NAME KIN302-0122.1
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Data_ 20161010
Time 17.56
INSTRUM spect
PROBHD 5 mm CPDCH 13C
PULPROG zg30
ID 65536
SOLVENT DMSO
NS 2
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 16.37
DW 50.000 usec
DE 10.00 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

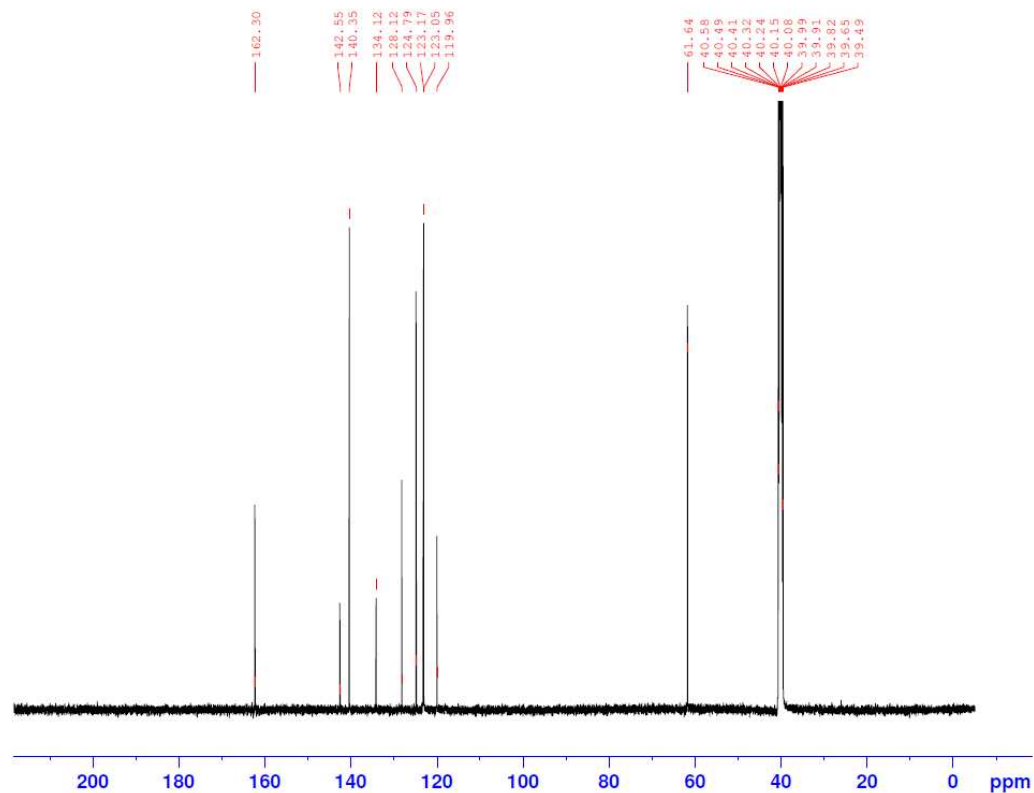
CHANNEL f1
SFO1 500.1330885 MHz
NUC1 1H
P1 10.10 usec
PLM1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 500.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{13}C NMR spectrum of 7-chloro-8-methoxyquinolin-2(1H)-one **3z** (in $\text{D}_6\text{-DMSO}$).



crude
C13_256scans DMSO D:\ schmidg 47



```

Current Data Parameters
NAME: ELM302-0122.1
EXPNO: 11
PROCNO: 1

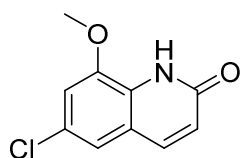
F2 - Acquisition Parameters
Date_: 20161010
Time: 17.20
INSTRUM: spect
PROBHD: 5 mm CPDCH 13C
PULPROG: zgpg30
TO: 85536
SOLVENT: DMSO
NS: 256
DS: 4
SWH: 31512.605 Hz
FIDRES: 0.480844 Hz
AQ: 1.0398378 sec
RG: 200.03
DW: 15.867 usec
DE: 60.67 usec
TE: 300.0 K
D1: 2.00000000 sec
D11: 0.03000000 sec
TD0: 1

===== CHANNEL f1 =====
SFO1: 125.772799 MHz
NUC1: 13C
P1: 10.00 usec
PLM1: 21.00000000 W

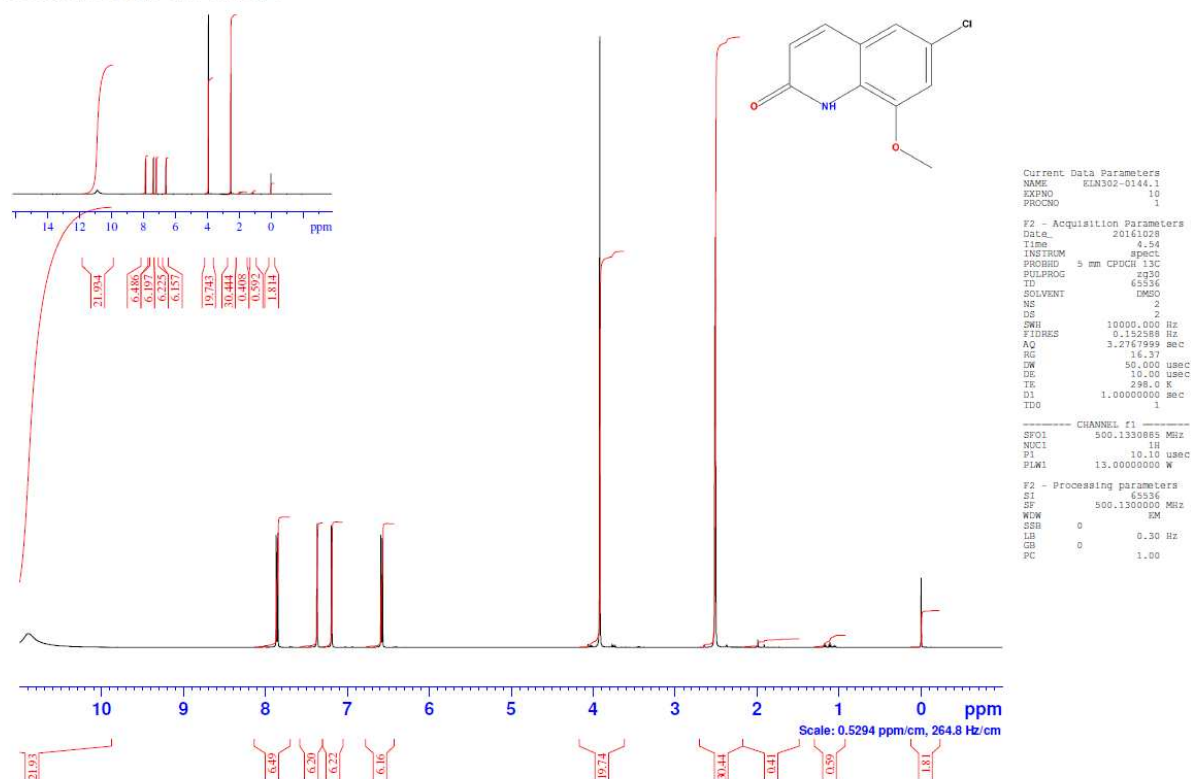
===== CHANNEL f2 =====
SFO2: 500.1320005 MHz
NUC2: 1H
CPSRG2: waltz16
PCPD2: 80.00 usec
PLM2: 13.00000000 W
PLM12: 0.22395000 W
PLM13: 0.11264000 W

F2 - Processing parameters
SI: 32768
SF: 125.7577890 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.40
    
```

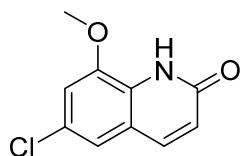
^1H NMR spectrum of 6-chloro-8-methoxyquinolin-2(1H)-one **3aa** (in D_6 -DMSO).



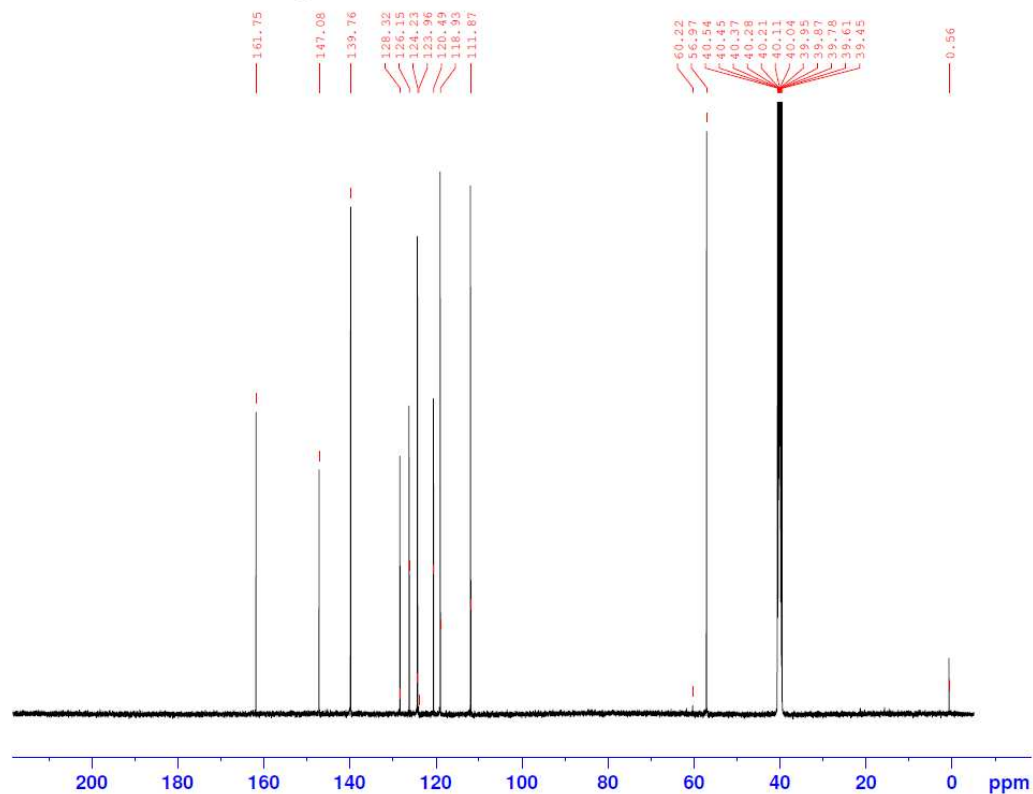
after purification
proton_2scans DMSO D:\schmidg 9



^{13}C NMR spectrum of 6-chloro-8-methoxyquinolin-2(1H)-one **3aa** (in D_6 -DMSO).



after purification
C13_256scans DMSO D:\\ schmidg 9



```
Current Data Parameters
NAME      EIA302-0144.1
EXPNO     11
PROCNO    1

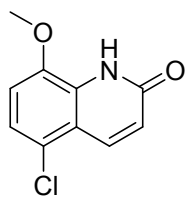
F2 - Acquisition Parameters
Date_     20161028
Time      5.59
INSTRUM    spect
PROBHD     5 mm CPDCH 13C
PULPROG    zgpg30
TD         65536
SOLVENT    DMSO
NS         256
DS         4
SWH         31512.605 Hz
FIDRES     0.480844 Hz
AQ         1.0398378 sec
RG         250.03
DW         15.867 usec
DE         60.67 usec
TE         300.0 K
D1         2.00000000 sec
D11        0.03000000 sec
TDO        1

===== CHANNEL f1 =====
SFO1      125.7728799 MHz
NUC1       13C
P1         10.00 usec
PLW1      21.00000000 W

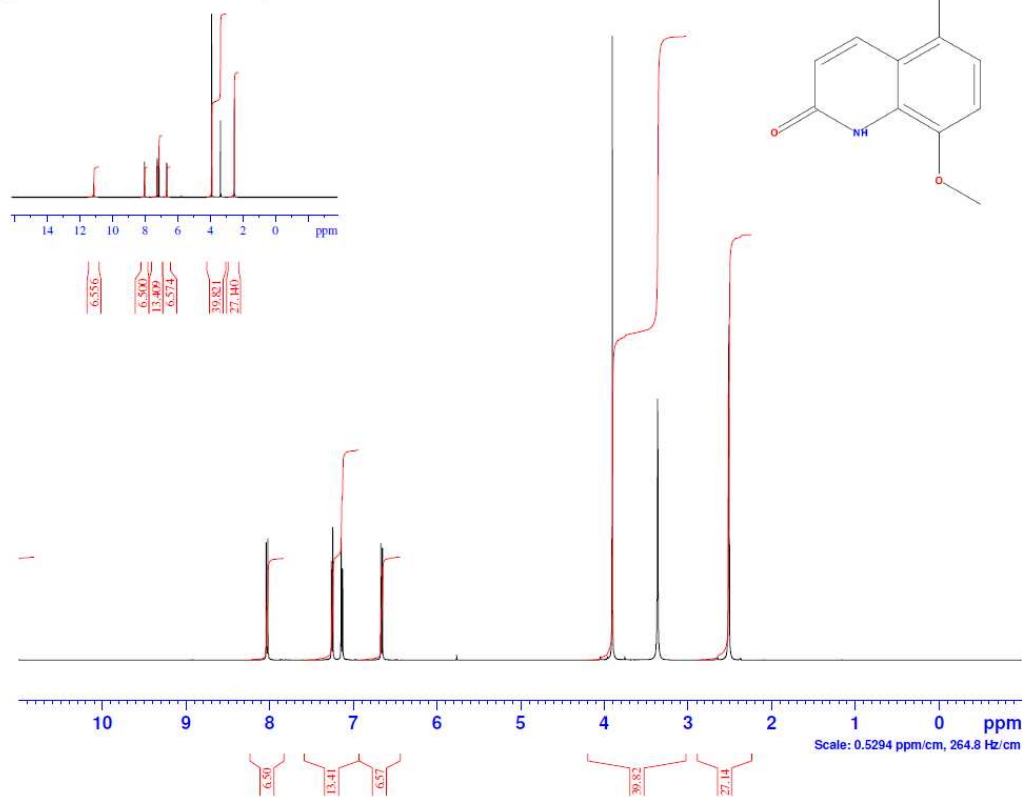
===== CHANNEL f2 =====
SFO2      500.1320000 MHz
NUC2       1H
CPDPRG2    waltz16
PCPD2      80.00 usec
PLW2      13.00000000 W
PLW12     0.22395000 W
PLW13     0.11264000 W

F2 - Processing parameters
SI         32768
SF         125.7577890 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
```

^1H NMR spectrum of 5-chloro-8-methoxyquinolin-2(1H)-one **3ab** (in D_6 -DMSO).



after purification
proton_2scans DMSO D:\schmidg 10



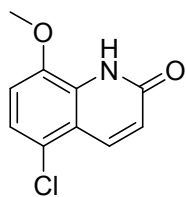
Current Data Parameters
NAME EIA302-0117.1
EXPNO 10
PROCNO 3

F2 - Acquisition Parameters
Date_ 20161007
Time 15.46
INSTRUM spect
PROBHD 5 mm CPDCH 13C
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 2
DS 3
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2167899 sec
RG 14.06
DM 50.000 usec
DE 10.00 usec
TE 298.0 K
D1 1.00000000 sec
TDO

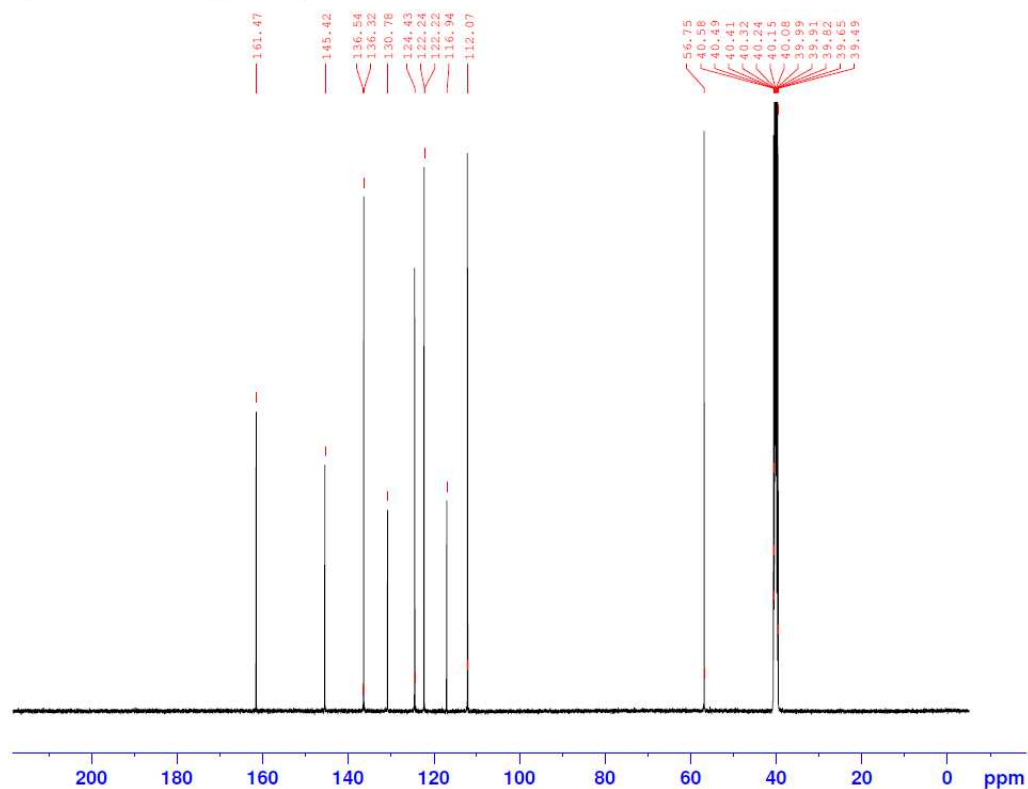
CHANNEL f1
SFO1 500.1330885 MHz
NUC1 1H
P1 10.10 usec
PLW1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 500.1330000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{13}C NMR spectrum of 5-chloro-8-methoxyquinolin-2(1H)-one **3ab** (in D_6 -DMSO).



after purification
C13_256scans DMSO D:\schmidg 10



```

Current Data Parameters
NAME      ELM302-0117.1
EXPNO     11
PROCNO    1

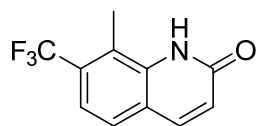
F2 - Acquisition Parameters
Date_     20161007
Time      16.01
INSTRUM   spect
PROBHD    5 mm CPDCH 13C
PULPROG   zgpg30
TD         65536
SOLVENT   DMSO
NS         256
DS         4
SWH        31512.605 Hz
FIDRES     0.480844 Hz
AQ         1.0398378 sec
RG         200.03
OW         15.867 usec
DE         60.67 usec
TE         300.0 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1

===== CHANNEL f1 =====
SFO1      125.7728799 Mhz
NUC1       13C
P1         10.00 usec
PLM1       21.00000000 W

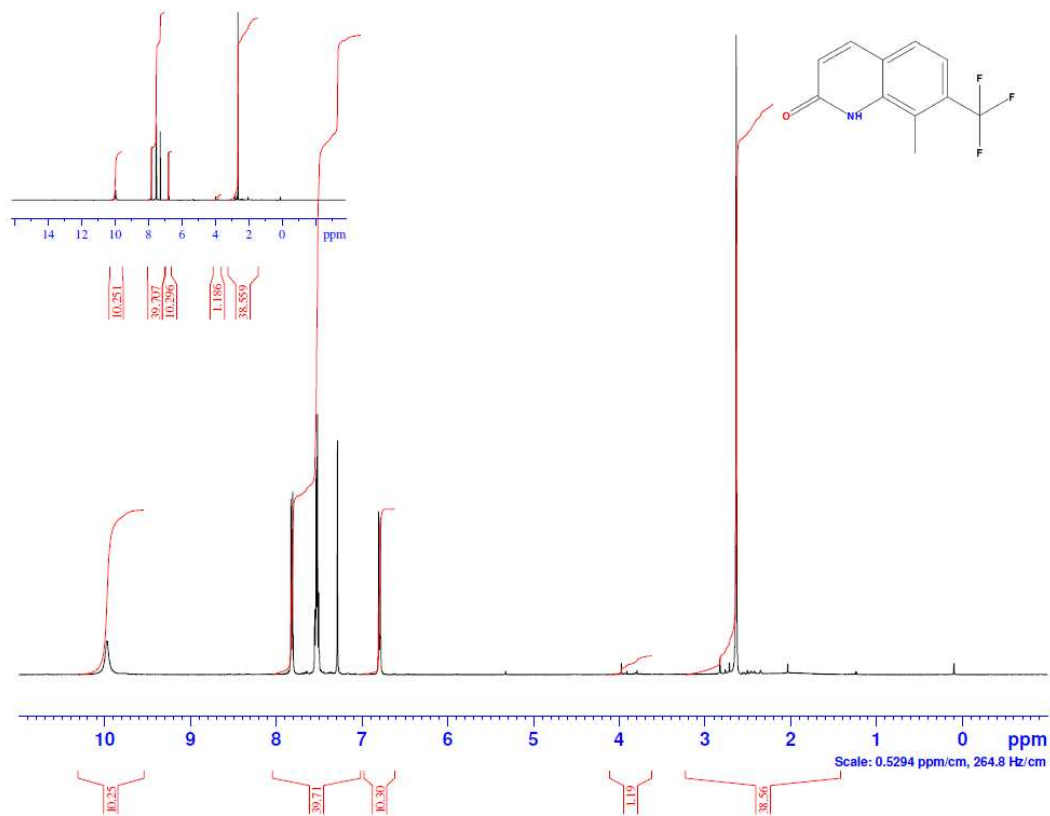
===== CHANNEL f2 =====
SFO2      500.1320005 Mhz
NUC2       1H
CPDPRG2    waltz16
PCPD2      80.00 usec
PLM2       13.00000000 W
PLM12      0.22395000 W
PLM13      0.11264000 W

F2 - Processing parameters
SI         32768
SF         125.7577890 Mhz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
    
```

^1H NMR spectrum of 8-methyl-7-(trifluoromethyl)quinolin-2(1H)-one **3ac** (in CDCl_3).



proton_2scans CDCl_3 D:\schmidg 50



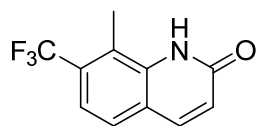
Current Data Parameters
NAME: E1N302-0167.1
EXPNO: 30
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20161114
Time: 14.43
INSTRUM: spect
PROBHD: 5 mm CPDCH 13C
PULPROG: zg30
TD: 65536
SOLVENT: CDCl_3
NS: 2
DS: 2
SWH: 10000.000 Hz
FIDRES: 0.152588 Hz
AQ: 3.2767999 sec
RG: 13.05
DW: 50.000 usec
DE: 10.00 usec
TE: 298.0 K
D1: 1.00000000 sec
TD0: 1

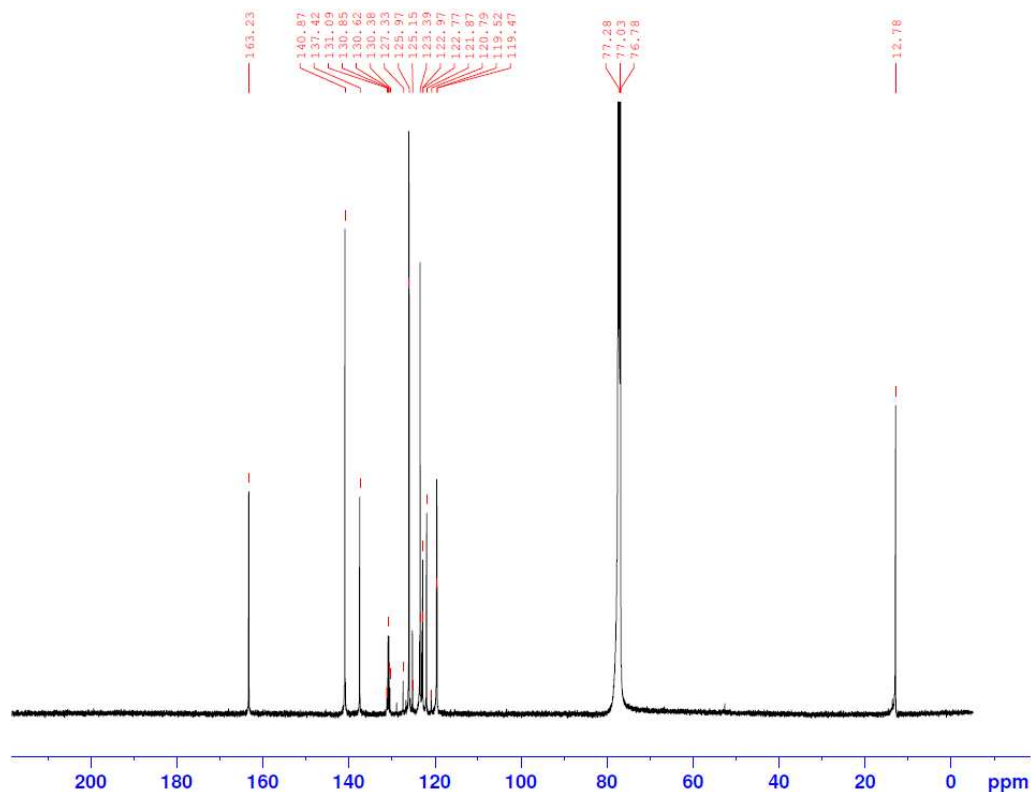
CHANNEL f1
SFO1: 500.1330885 MHz
NUC1: 1H
P1: 10.10 usec
PLW1: 13.00000000 W

F2 - Processing parameters
SI: 65536
SF: 500.1330885 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00

^{13}C NMR spectrum of 8-methyl-7-(trifluoromethyl)quinolin-2(1H)-one **3ac** (in CDCl_3).



C13_2048scans CDCl_3 D:\schmidg 1



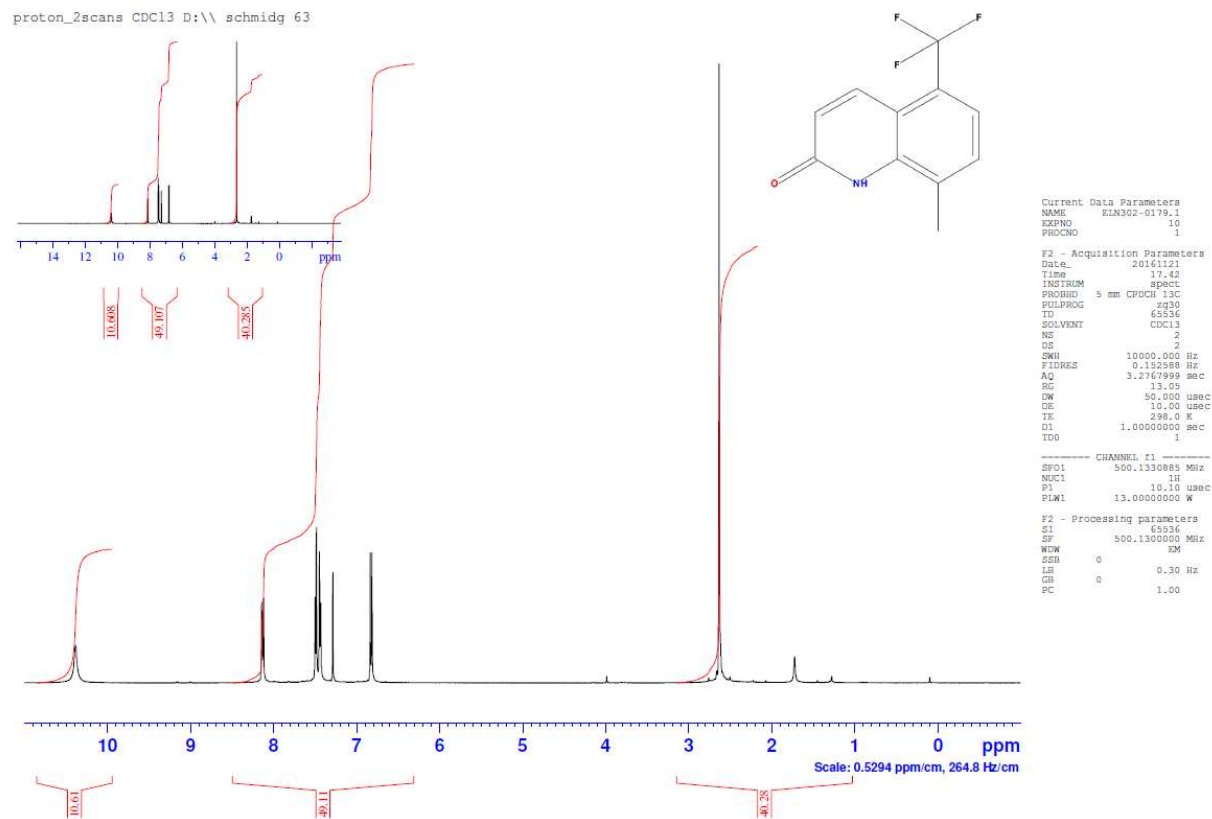
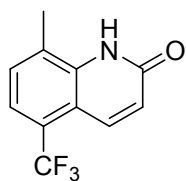
```

Current Data Parameters
NAME      ELM302-0167.1.02
EXPNO     10
PROCNO    1

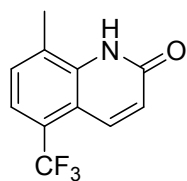
F2 - Acquisition Parameters
Date_     20170519
Time      2.25 h
INSTRUM   spect
PROBHD    Z128431_0003 (
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         2048
DS         4
SWH        31212.605 Hz
FIDRES     0.561688 Hz
AQ         1.0398378 sec
RG          200.03
DW         15.867 usec
DE         19.02 usec
TE         300.0 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1
SFO1       125.7728799 MHz
NUC1        13C
P1         10.00 usec
PLW1       21.50799942 W
SFO2       500.1350005 MHz
NUC2        1H
CPDPRG2   waltz16
PCPD2      80.00 usec
PLW2       12.56499958 W
PLW12      0.18587931 W
PLW13      0.09316271 W

F2 - Processing parameters
SI         32768
SF         125.7577890 MHz
WDW        RM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
    
```

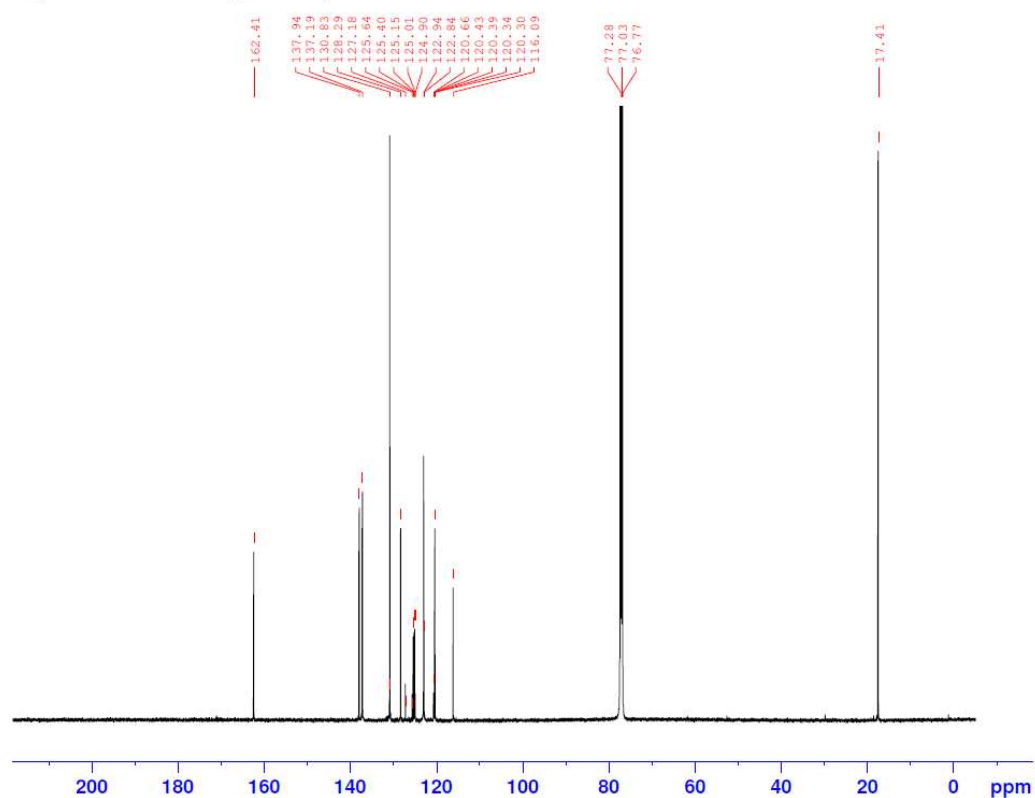
^1H NMR spectrum of 8-methyl-5-(trifluoromethyl)quinolin-2(1H)-one **3ad** (in CDCl_3).



^{13}C NMR spectrum of 8-methyl-5-(trifluoromethyl)quinolin-2(1H)-one **3ad** (in CDCl_3).



C13_2048scans CDC13 D:\\ schmidg 2



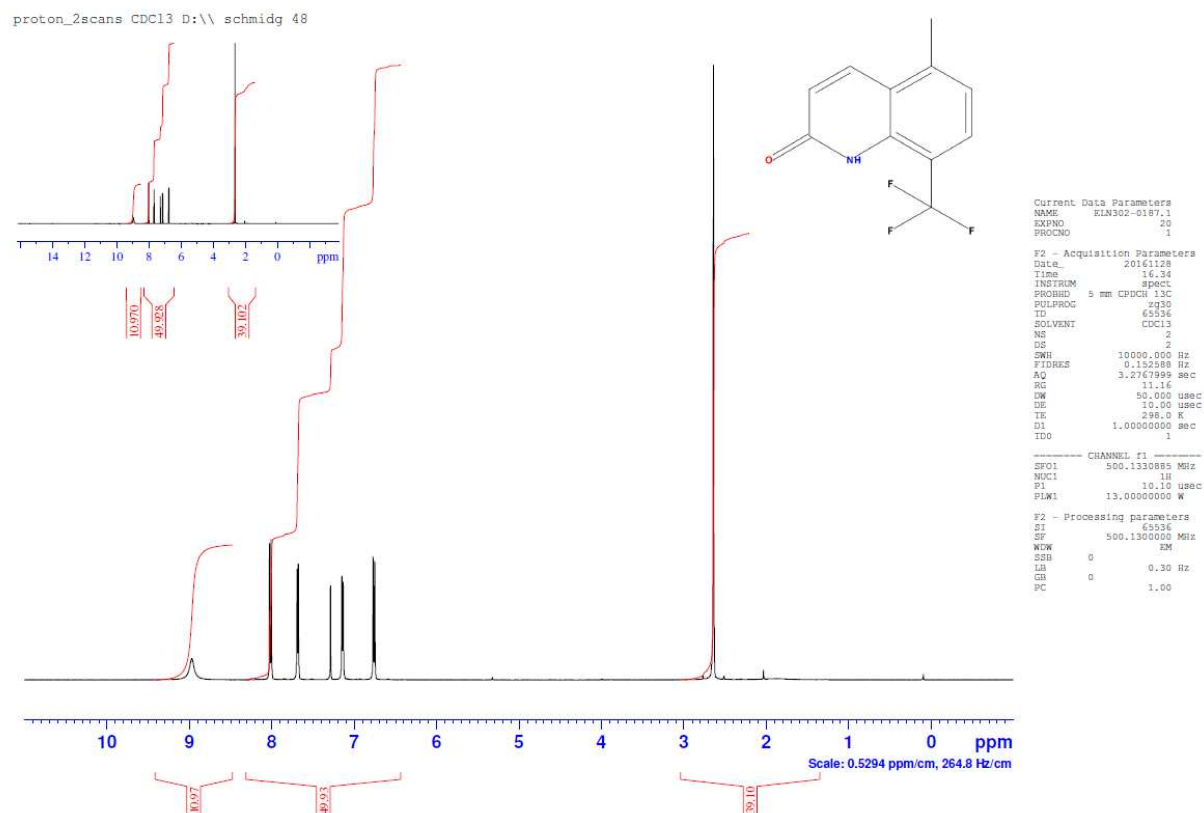
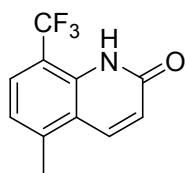
```

Current Data Parameters
NAME      ZLN302-0179.1.02
EXPNO     10
PROCNO    1

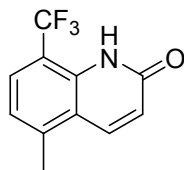
F2 - Acquisition Parameters
Date_     20170519
Time      4.14 h
INSTRUM   spect
PROBHD    Z128431.0003 (
PULPROG   zgpg30
TD         65536
SOLVENT   CDC13
NS         2048
DS         4
SWH        31512.605 Hz
FIDRES     0.961688 Hz
AQ         1.0398378 sec
RG         200.03
DW         15.867 usec
DE         19.02 usec
TE         300.0 K
D1         2.00000000 sec
D11        0.03000000 sec
TDO        1
SFO1       125.7728798 MHz
NUC1       13C
F1         10.00 usec
P1M1       21.50799942 W
SFO2       500.1320005 MHz
NUC2
CPDPRG2   waltz16
PCPD2     80.00 usec
P1M2      12.56489968 W
P1M12     0.18587931 W
P1M13     0.09316271 W

F2 - Processing parameters
SI         32768
SF         125.7577890 MHz
WDW        DM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
    
```

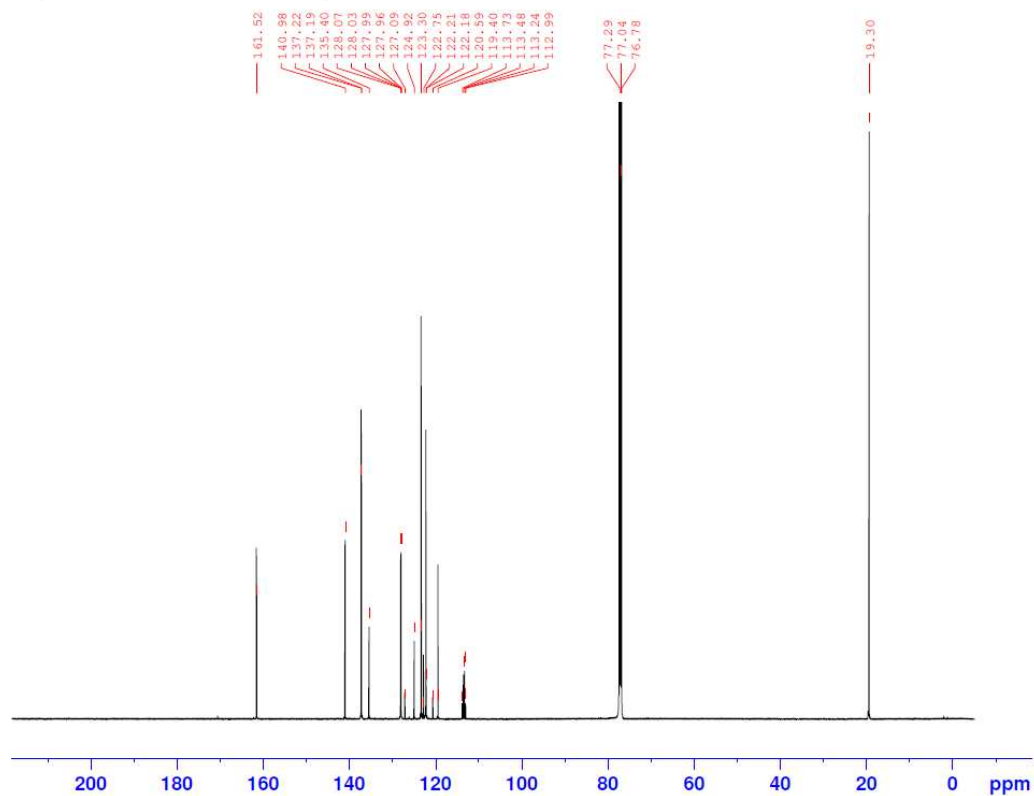
^1H NMR spectrum of 5-methyl-8-(trifluoromethyl)quinolin-2(1H)-one **3ae** (in CDCl_3).



^{13}C NMR spectrum of 5-methyl-8-(trifluoromethyl)quinolin-2(1H)-one **3ae** (in CDCl_3).



C13_2048scans CDC13 D:\\ schmidg 3



```

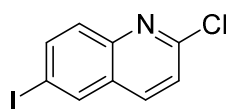
Current Data Parameters
NAME      KLN302-0187.1_02
EXPNO     10
PROCNO     1

F2 - Acquisition Parameters
Date_      20170519
Time       6.04 h
INSTRUM    spect
PROBHD     Z128431_0003 f
PULPROG    zgpg30
TD          65536
SOLVENT     CDCl3
NS          2048
DS          4
SWH         31512.605 Hz
FIDRES      0.461688 Hz
AQ          1.0398378 sec
RG          250.03
DW          15.867 usec
DE          19.02 usec
TK          300.0 K
D1          2.00000000 sec
D11         0.03000000 sec
TDS         1
SFO1        125.7728799 MHz
NUC1         13C
P1          10.00 usec
P1M1        21.50799942 W
SFO2        550.1320005 MHz
NUC2         1H
CPDPRG2     waltz16
PCPD2       10.00 usec
P1M2        12.56499958 W
P1M12       0.18587931 W
P1M13       0.09316271 W

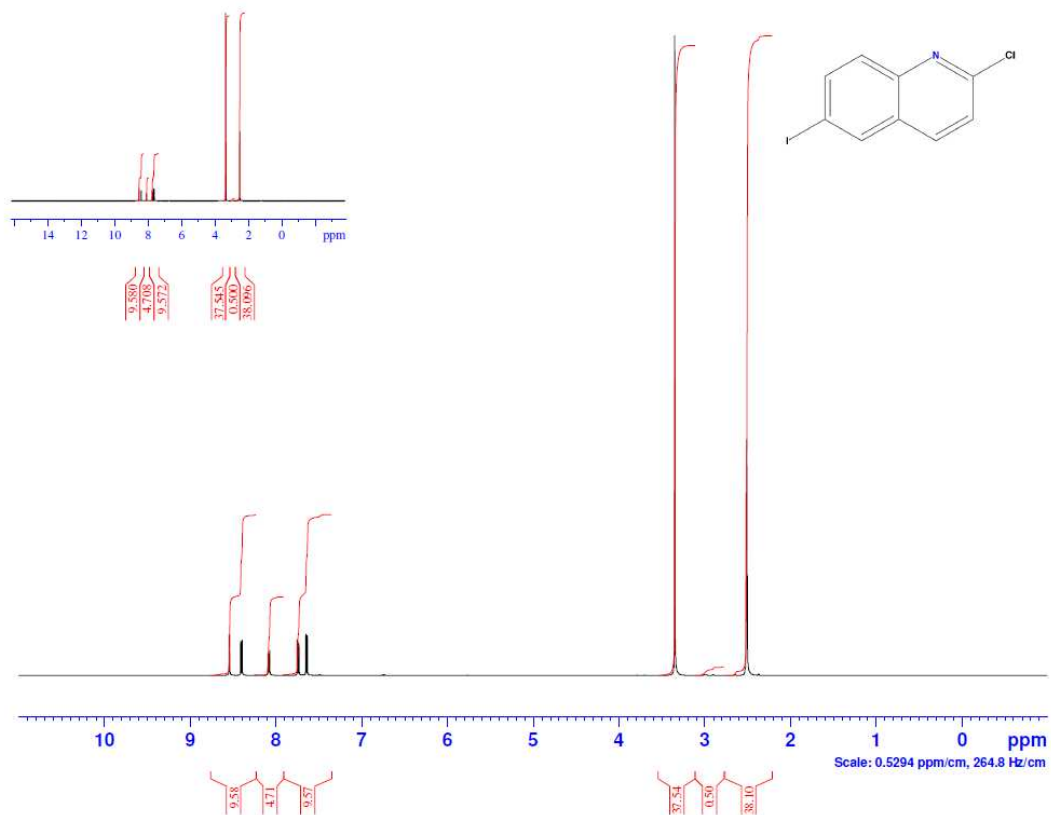
F2 - Processing parameters
SI          32768
SF          125.7577890 MHz
WDW         EM
SSB         0
LB          1.00 Hz
GB          0
PC          1.40
    
```

6. Proton and carbon NMR Spectra of quinolines 5-17

^1H NMR spectrum of 2-chloro-6-iodoquinoline **5** (in $\text{D}_6\text{-DMSO}$).



proton_2scans DMSO D:\schmidg 49



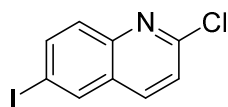
Current Data Parameters
NAME ELN302-0134.1
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161019
Time 17.48
INSTRUM spect
PROBHD 5 mm CPDCH 13C
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 2
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 11.16
DW 50.000 usec
DE 10.00 usec
TE 298.0 K
D1 1.00000000 sec
YD0 1

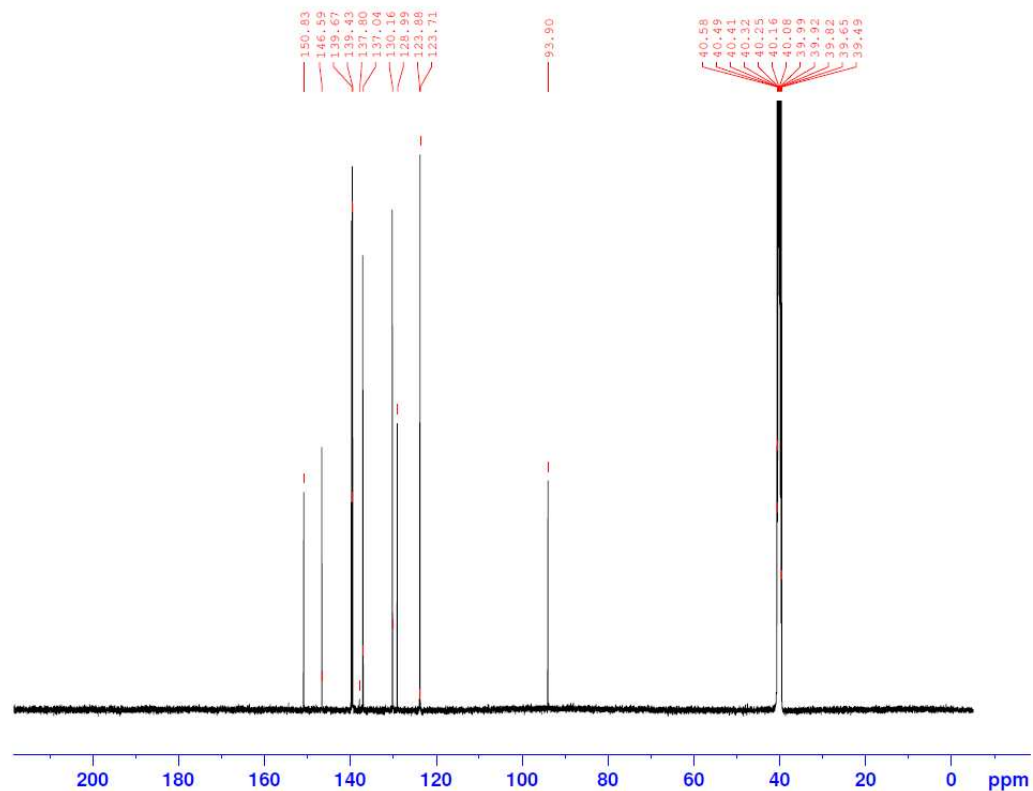
CHANNEL f1
SFO1 500.1330885 MHz
NUC1 1H
P1 10.10 usec
PLW1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 500.1330000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{13}C NMR spectrum of 2-chloro-6-iodoquinoline **5** (in $\text{D}_6\text{-DMSO}$).



C13_256scans DMSO D:\ schmidg 49



```

Current Data Parameters
NAME: ELN302-0134.1
EXPNO: 11
PROCNO: 1

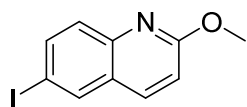
F2 - Acquisition Parameters
Date_: 20161019
Time: 18.03
INSTRUM: spect
PROBHD: 5 mm CPOCH 13C
PULPROG: zgpg30
TD: 65536
SOLVENT: DMSO
NS: 256
DS: 4
SWH: 31512.605 Hz
FIDRES: 0.480844 Hz
AQ: 1.0388378 sec
RG: 200.03
EW: 15.867 usec
DE: 60.67 usec
TE: 300.0 K
D1: 2.00000000 sec
D11: 0.03000000 sec
TD0: 1

===== CHANNEL f1 =====
SFO1: 125.7728799 MHz
NUC1: 13C
P1: 10.00 usec
PLW1: 21.00000000 W

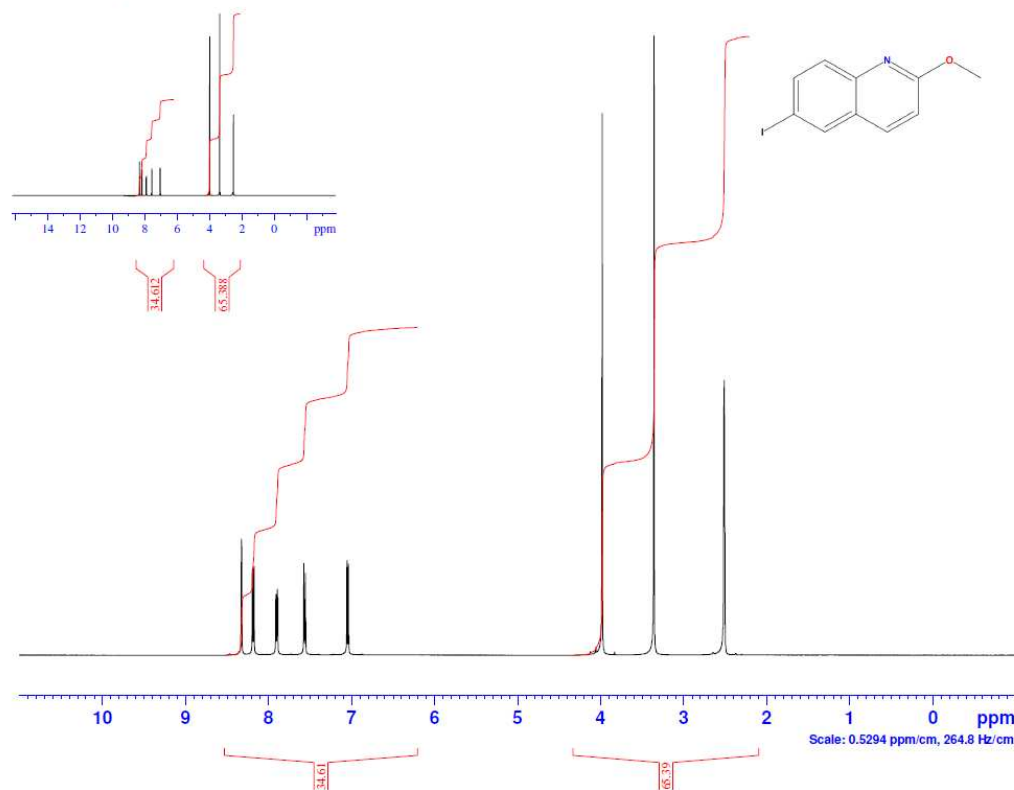
===== CHANNEL f2 =====
SFO2: 500.1320005 MHz
NUC2: 1H
PCPD2: waitz16
PCPD2: 80.00 usec
PLW2: 13.00000000 W
PLW12: 0.22395000 W
PLW13: 0.11264000 W

F2 - Processing parameters
SI: 32768
SF: 125.7577890 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.40
    
```

^1H NMR spectrum of 2-methoxy-6-iodoquinoline **12** (in $\text{D}_6\text{-DMSO}$).



proton_2scans DMSO D:\ schmidg 68



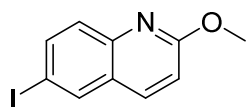
Current Data Parameters
NAME ELN302-0134.2
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161020
Time 17.47
INSTRUM spect
PROBHD 5 mm CPDCH 13C
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2
DS 2
SWH 10000.000 Hz
FIDRES 0.192388 Hz
AQ 3.2767999 sec
RG 11.16
DW 50.000 usec
DE 10.00 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

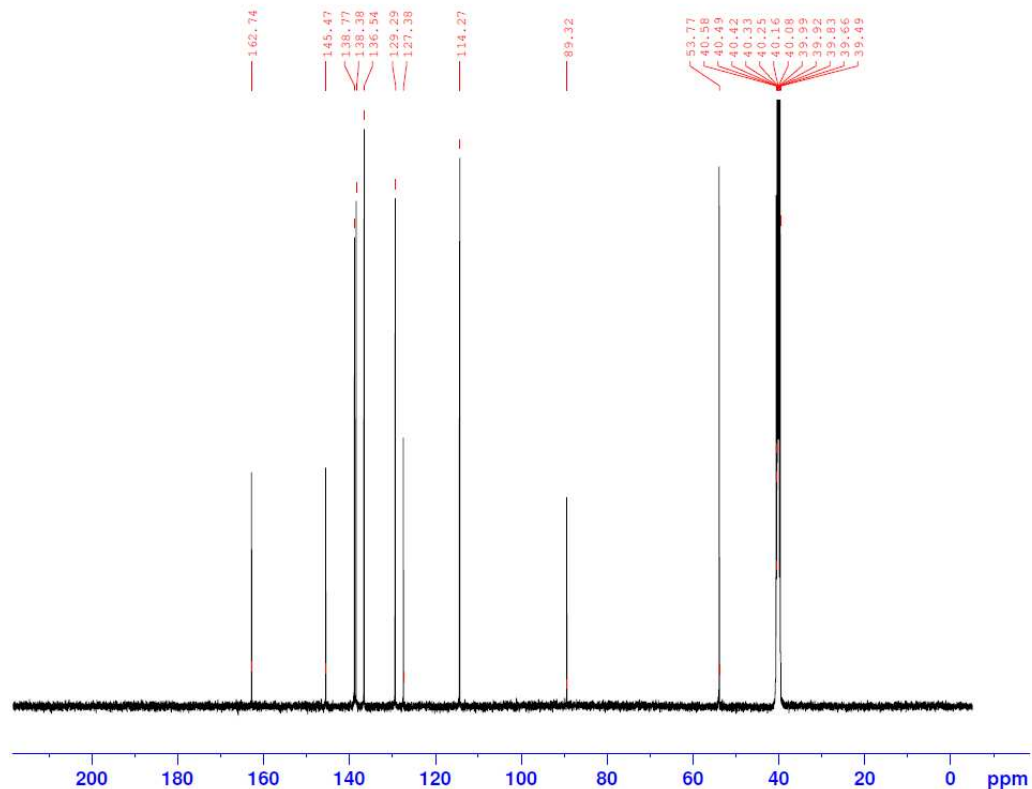
CHANNEL f1
SFO1 500.1330885 MHz
NUC1 1H
P1 10.10 usec
PLW1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 500.1330885 MHz
WDW EM
GB 0.30 Hz
GB 0
PC 1.00

^{13}C NMR spectrum of 2-methoxy-6-iodoquinoline **12** (in D_6 -DMSO).



C13_32scans DMSO D:\ schmidg 68



```

Current Data Parameters
NAME      E1N302-0134.2
EXPNO     11
PROCNO    1

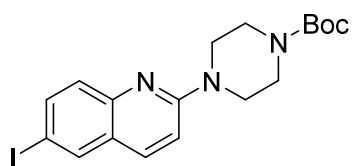
F2 - Acquisition Parameters
Date_     20161020
Time      17.50
INSTRUM   spect
PROBHD    5 mm CPDCH 13C
PULPROG   zgpg30
TD         65536
SOLVENT   DMSO
NS         32
DS         4
SWH        31512.005 Hz
FIDRES     0.450844 Hz
AQ         1.0398378 sec
RG         200.03
RW         15.867 usec
DE         60.67 usec
TE         300.0 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1

===== CHANNEL f1 =====
SFO1      125.7728799 MHz
NUC1       13C
P1         10.00 usec
PLW1       21.00000000 W

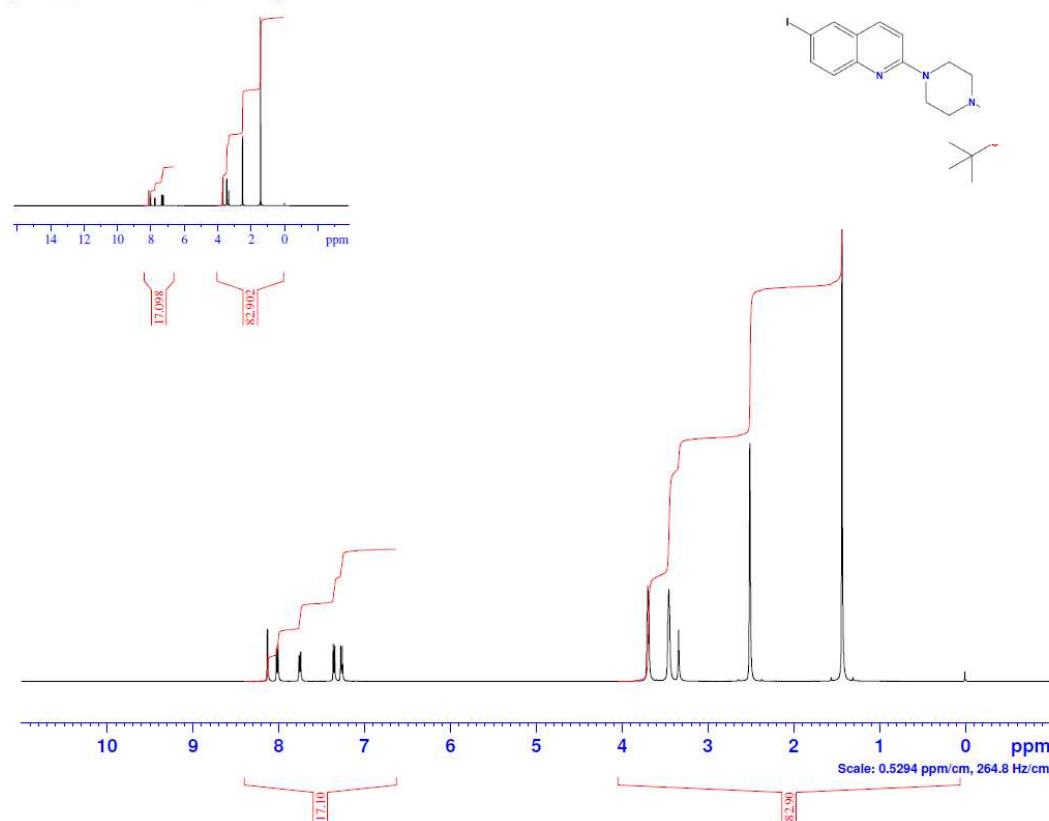
===== CHANNEL f2 =====
SFO2      500.1320005 MHz
NUC2       1H
CPDPRG2    waltz16
PCPD2      80.00 usec
PLW2       13.00000000 W
PLW12      0.22395000 W
PLW13      0.11244000 W

F2 - Processing parameters
SI         32768
SF         125.7577890 MHz
WDW        EM
SSB         0
LB          1.00 Hz
GB          0
PC          1.40
    
```

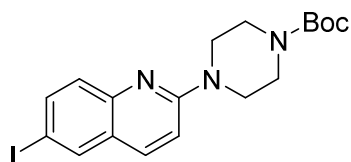
^1H NMR spectrum of tert-butyl 4-(6-iodoquinolin-2-yl)piperazine-1-carboxylate **6** (in D_6 -DMSO).



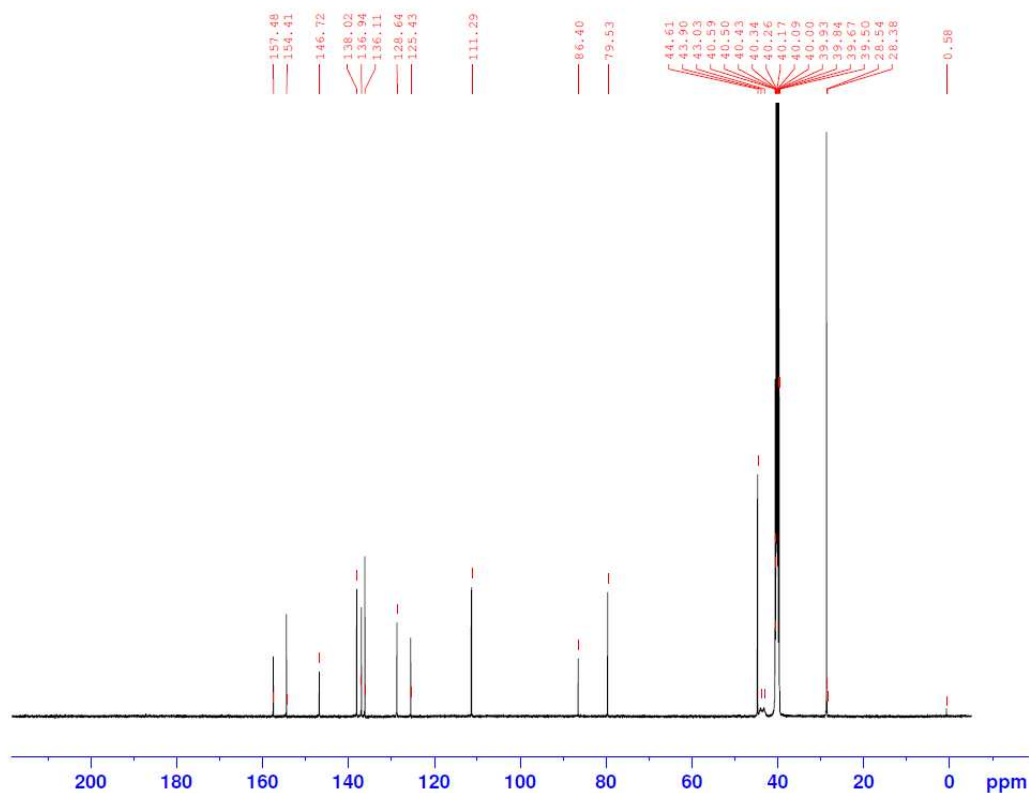
after purification
proton_2scans DMSO D:\ schmidg 30



^{13}C NMR spectrum of tert-butyl 4-(6-iodoquinolin-2-yl)piperazine-1-carboxylate **6** (in $\text{D}_6\text{-DMSO}$).



after purification
C13_256scans DMSO D:\ schmidg 30



```

Current Data Parameters
NAME      ELN302-0137.1
EXPNO     11
PROCNO    1

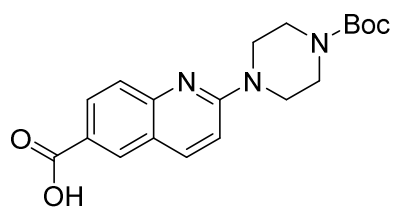
F2 - Acquisition Parameters
Date_     20161122
Time      14.10
INSTRUM   spect
PROBHD    5 mm CPDCH 13C
PULPROG   zgpg30
TD         65536
SOLVENT   DMSO
NS         256
DS         4
SWH        31512.605 Hz
FIDRES     0.480844 Hz
AQ          1.0399378 sec
RG          300.03
DW          15.867 usec
DE          60.67 usec
TR          300.0 K
D1          2.0000000 sec
D11         0.03000000 sec
TD0         1

===== CHANNEL f1 =====
SF01      125.7728799 MHz
NUC1       13C
P1         10.00 usec
PLW1       21.00000000 W

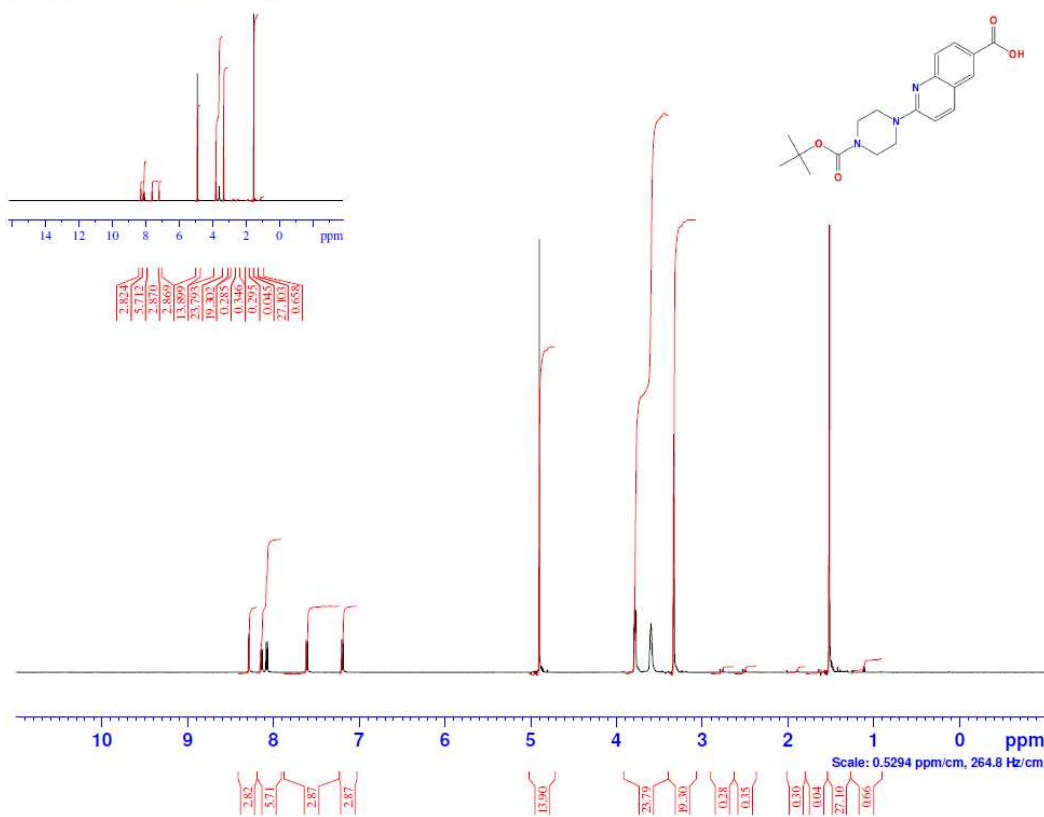
===== CHANNEL f2 =====
SF02      500.1320000 MHz
NUC2       1H
CPDPRG2    waltz16
PCPD2      80.00 usec
PLW2       13.00000000 W
PLW12      0.22395000 W
PLW13      0.11264000 W

F2 - Processing parameters
SI          32768
SF          125.7577890 MHz
WDW         EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40
    
```

^1H NMR spectrum of 2-(4-(tert-butoxycarbonyl)piperazin-1-yl)quinoline-6-carboxylic acid **7** (in CD_3OD).



proton_2scans MeOD D:\schmidg 10



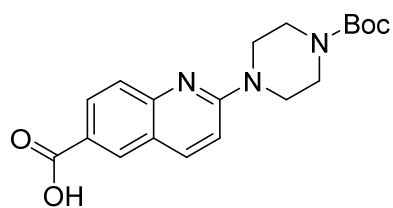
Current Data Parameters
NAME ELN302-0190.1
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161201
Time 11.27
INSTRUM spect
PROBHD 5 mm CPDCH 13C
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 2
DS 2
SWH 10000.000 Hz
FIDRES 0.132588 Hz
AQ 3.2767999 sec
RG 14.06
DW 50.000 usec
DE 10.00 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

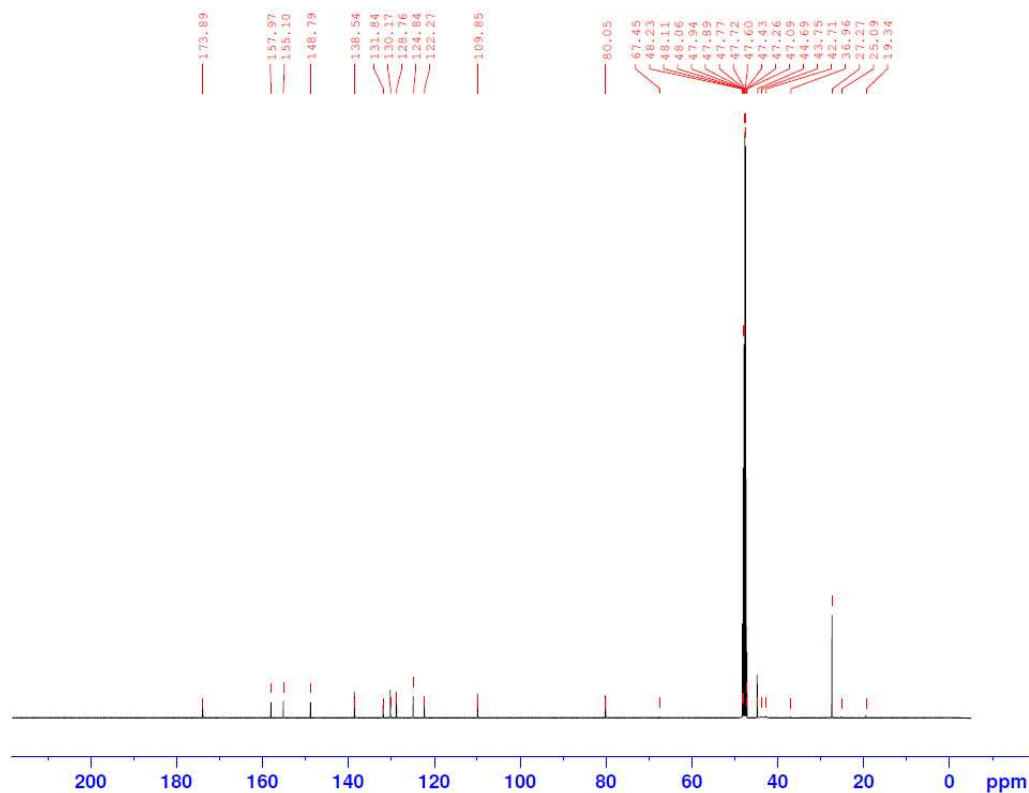
CHANNEL f1
SFO1 500.1330885 MHz
NUC1 1H
P1 10.10 usec
PLW1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 500.1330885 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{13}C NMR spectrum of 2-(4-(tert-butoxycarbonyl)piperazin-1-yl)quinoline-6-carboxylic acid **7** (in CD_3OD).



C13_2048scans MeOD D:\schmidg 35



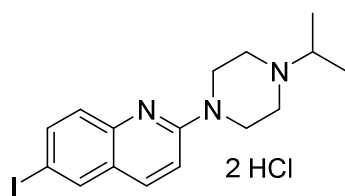
```

Current Data Parameters
NAME      ELN302-0190.1_02
EXPNO     10
PROCNO    1

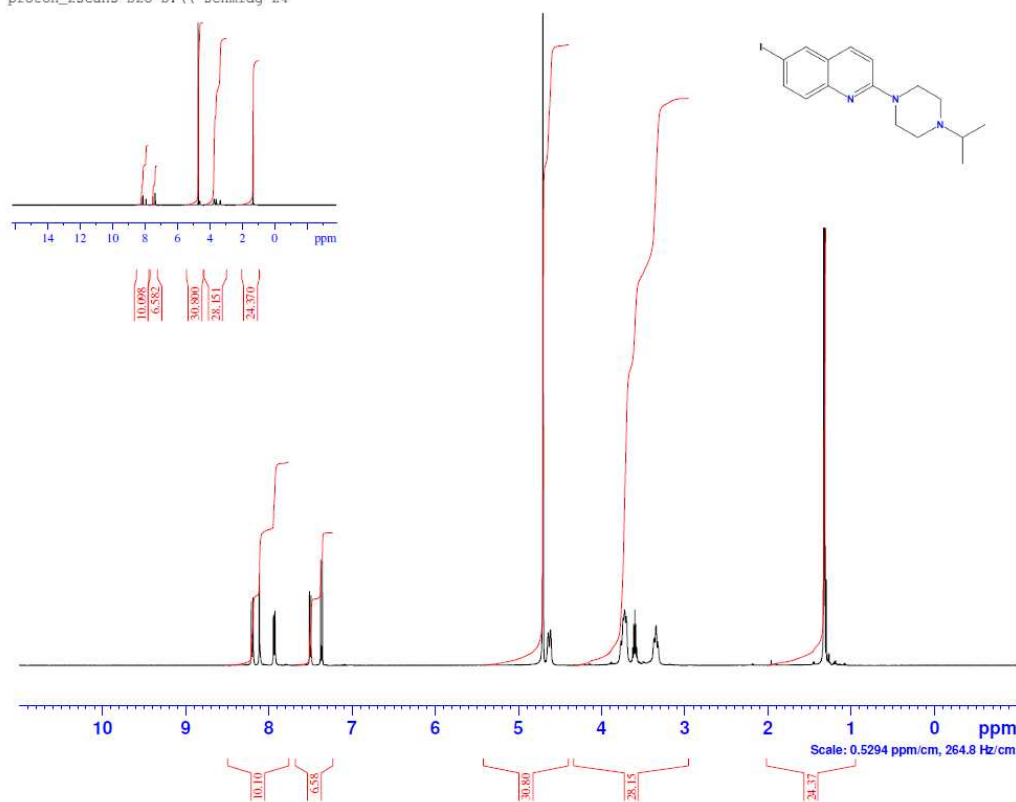
F2 - Acquisition Parameters
Date_     20170516
Time      3.53 h
INSTRUM   spect
PROBHD    Z128431_0003 (
PULPROG   zgpg30
TD         65536
SOLVENT   MeOD
NS         2048
DS         4
SWH        31512.605 Hz
FIDRES     0.961688 Hz
AQ         1.0398376 sec
RG         200.03
DW         15.867 usec
DE         19.02 usec
TE         300.0 K
D1         2.00000000 sec
D11        0.03000000 sec
TDO        1
SFO1       125.7728799 MHz
NUC1       13C
P1         10.00 usec
P1M1       21.50799942 W
SFO2       500.1320005 MHz
NUC2       1H
PCPDPRG12 waitz16
PCPD2      80.00 usec
P1M2       12.56489956 W
P1M12      0.18587931 W
P1M13      0.09316271 W

F2 - Processing parameters
SI         32768
SF         125.7577890 MHz
WDW        0
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
    
```

^1H NMR spectrum of 6-iodo-2-(4-isopropylpiperazin-1-yl)quinoline dihydrochloride **8** (in D_2O).



proton_2scans D2O D:\schmidg 24



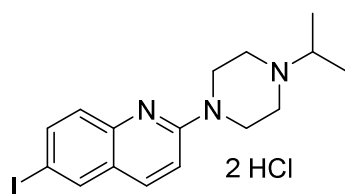
Current Data Parameters
NAME ELN302-0138.1
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161214
Time 4:55
INSTRUM spect
PROBHD 5 mm CPDCH 13C
PULPROG zg30
TD 65536
SOLVENT D2O
NS 2
DS 2
SWH 10000.000 Hz
FIDRES 0.152388 Hz
AQ 3.2767999 sec
RG 16.37
DW 50.000 usec
DE 10.00 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

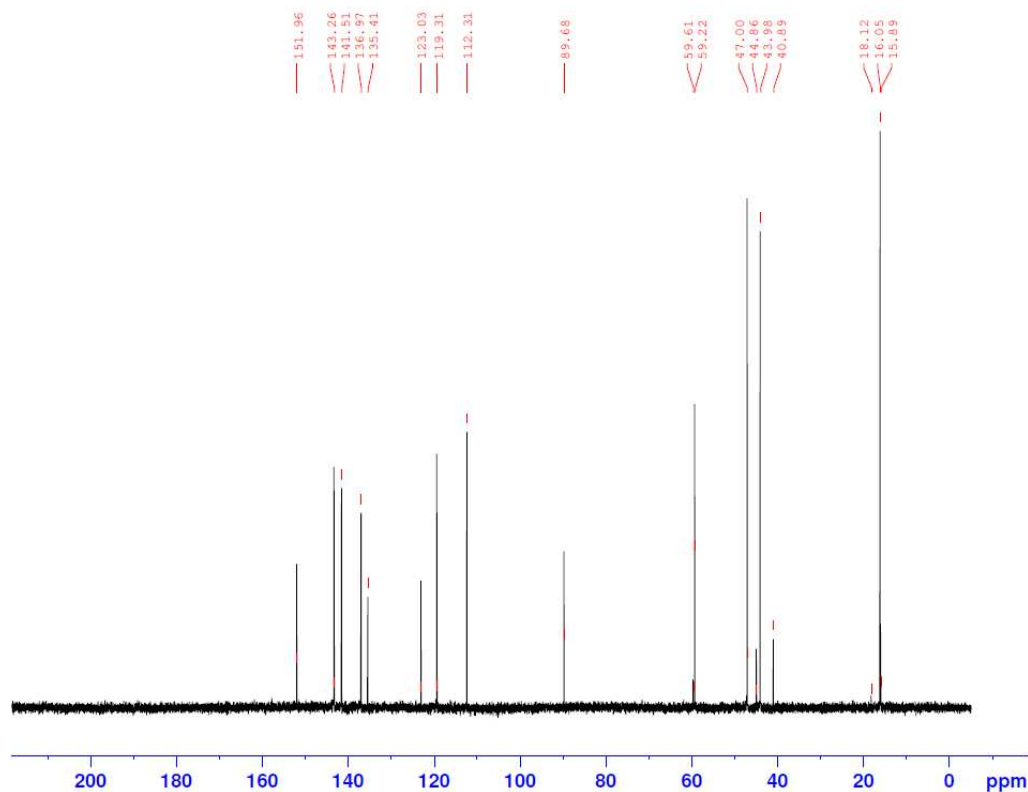
CHANNEL f1
SFO1 500.1330885 MHz
NUC1 1H
P1 10.10 usec
PLW1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 500.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{13}C NMR spectrum of 6-iodo-2-(4-isopropylpiperazin-1-yl)quinoline dihydrochloride **8** (in D_2O).



C13_256scans D2O D:\ schmidg 24



```

Current Data Parameters
NAME: E1A302-0138.1
EXPNO: 21
PROCNO: 1

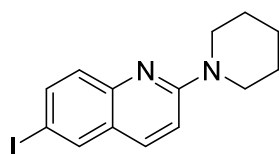
F2 - Acquisition Parameters
Date_: 20161214
Time: 5.10
INSTRUM: spect
PROBHD: 5 mm CPDQZ 13C
PULPROG: zgpg30
TD: 65536
SOLVENT: D2O
NS: 256
DS: 4
SWH: 31512.605 Hz
FIDRES: 0.480844 Hz
AQ: 1.0399378 sec
RG: 200.03
CW: 15.867 usec
DE: 60.67 usec
TE: 300.0 K
D1: 2.00000000 sec
D11: 0.03000000 sec
TDO: 1

===== CHANNEL f1 =====
SFO1: 125.772799 MHz
NUC1: 13C
P1: 10.00 usec
PLW1: 21.00000000 W

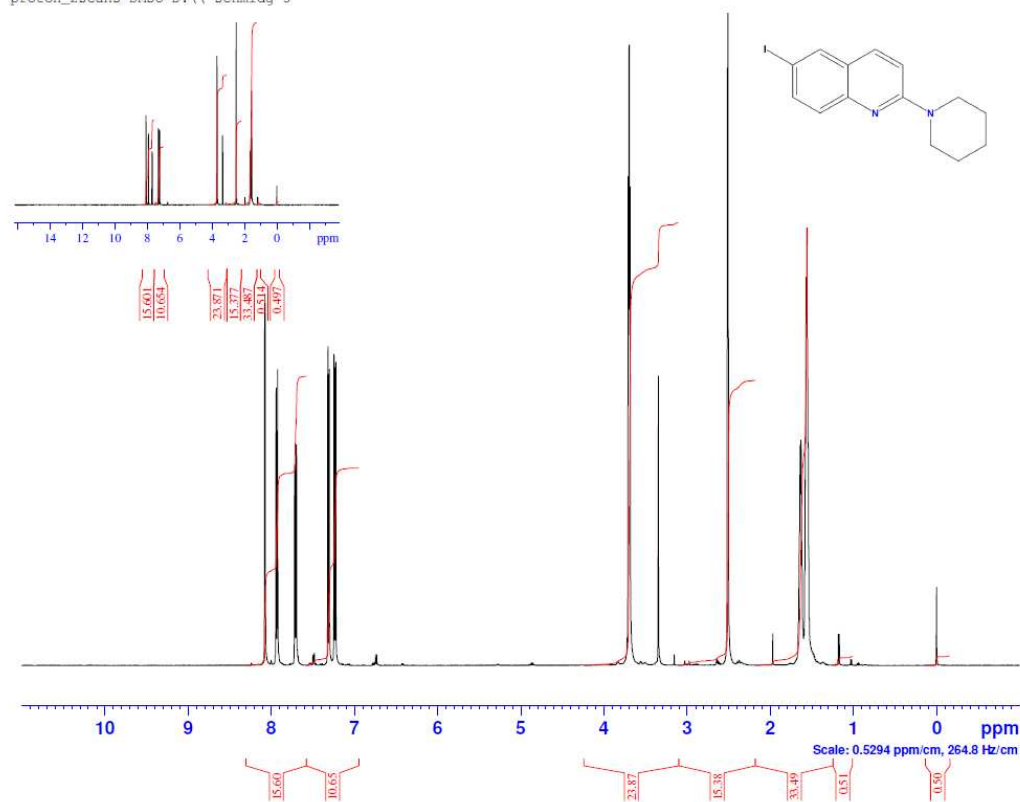
===== CHANNEL f2 =====
SFO2: 500.1320005 MHz
NUC2: 1H
CPCPD2: waltz16
PCPD2: 80.00 usec
PLW2: 13.00000000 W
PLW12: 0.12396000 W
PLW13: 0.11264000 W

F2 - Processing parameters
SI: 32768
SF: 125.7577850 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.40
    
```

^1H NMR spectrum of 6-iodo-2-(piperidin-1-yl)quinoline **9** (in D_6 -DMSO).



proton_2scans DMSO D:\schmidg 5



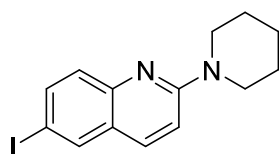
Current Data Parameters
NAME KLN302-0159.1
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161108
Time 12:11
INSTRUM spect
PROBHD 5 mm CPDCH 13C
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 2
DS 2
SWH 10000.000 Hz
FIDRES 0.132588 Hz
AQ 3.2767999 sec
RG 11.16
DW 50.000 usec
DE 10.00 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

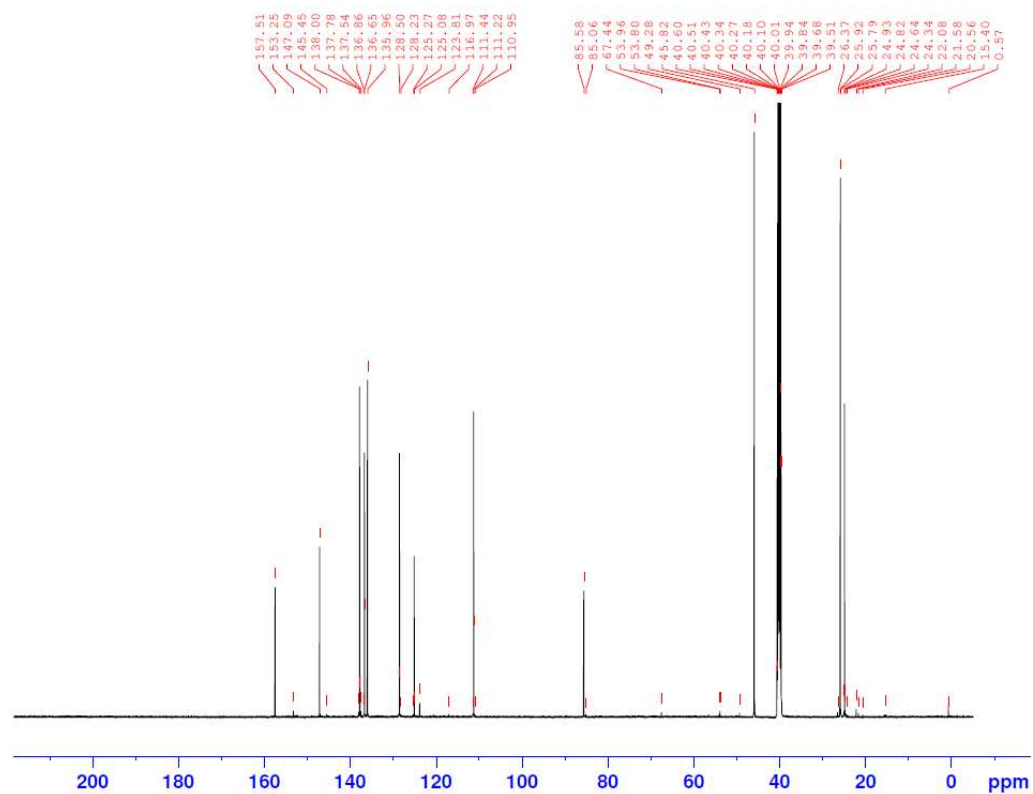
CHANNEL f1
SFO1 500.1330885 MHz
NUC1 1H
P1 10.10 usec
PLW1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 500.1330885 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{13}C NMR spectrum of 6-iodo-2-(piperidin-1-yl)quinoline **9** (in D_6 -DMSO).



C13_256scans DMSO D:\schmidg 5



```

Current Data Parameters
NAME: ELN302-0159.1
EXPNO: 11
PROCNO: 1

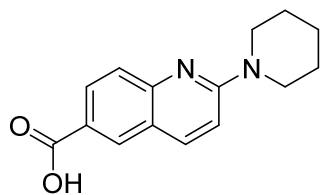
F2 - Acquisition Parameters
Date_: 20161108
Time: 12.26
INSTRUM: spect
PROBHD: 5 mm CPOCH 13C
PULPROG: zgpg30
TD: 65536
SOLVENT: DMSO
NS: 256
DS: 4
SWH: 31512.605 Hz
FIDRES: 0.480844 Hz
AQ: 1.0398378 sec
RG: 200.03
DW: 15.867 usec
DE: 60.67 usec
TE: 300.0 K
D1: 2.00000000 sec
D11: 0.03000000 sec
TD0: 1

===== CHANNEL f1 =====
SFO1: 125.7728799 MHz
NUC1: 13C
P1: 10.00 usec
PLW1: 21.00000000 W

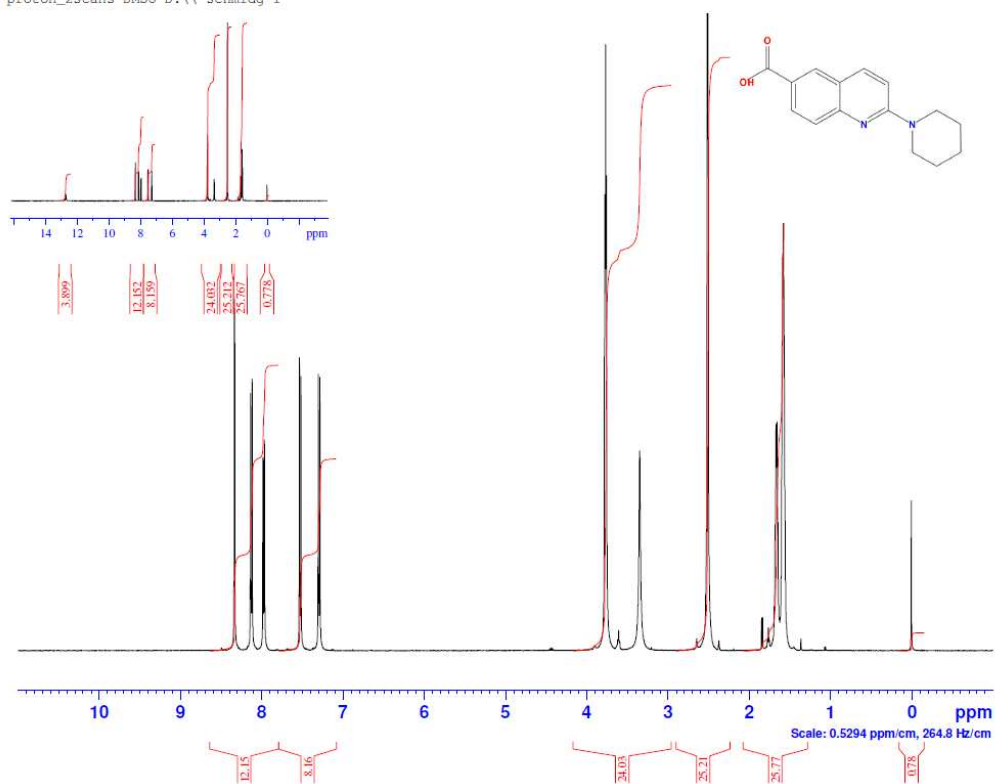
===== CHANNEL f2 =====
SFO2: 500.1320005 MHz
NUC2: 1H
CPCPRG2: waltz16
PCPD2: 80.00 usec
PLW2: 13.00000000 W
PLW12: 0.22395000 W
PLW13: 0.11264000 W

F2 - Processing parameters
SI: 32768
SF: 125.7577890 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.40
  
```

^1H NMR spectrum of 2-(piperidin-1-yl)quinoline-6-carboxylic acid **10** (in D_6 -DMSO).



crude
proton_2scans DMSO D:\schmidg 1



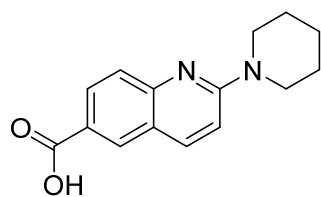
Current Data Parameters
NAME: KIN302-0161.1
EXPRO: 10
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20161109
Time: 14.52
INSTRUM: spect
PROBHD: 5 mm CPDCH 13C
PULPROG: zg30
TD: 65536
SOLVENT: DMSO
NS: 2
DS: 2
SWH: 10000.000 Hz
FIDRES: 0.132088 Hz
AQ: 3.2767999 sec
RG: 11.16
DW: 50.000 usec
DE: 10.00 usec
TE: 298.0 K
D1: 1.00000000 sec
TD0: 1

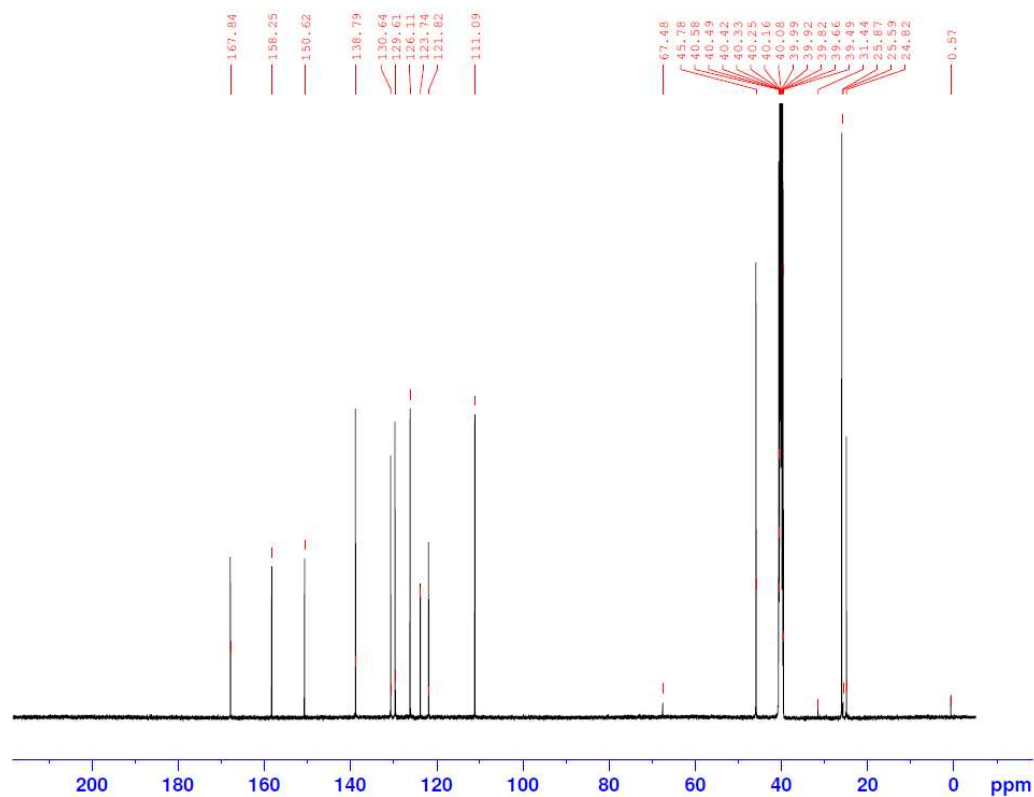
----- CHANNEL f1 -----
STO1: 500.1330889 MHz
NUC1: 1H
P1: 10.10 usec
PLW1: 13.00000000 W

F2 - Processing parameters:
SI: 65536
SF: 500.1300000 MHz
WDW: RM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00

^{13}C NMR spectrum of 2-(piperidin-1-yl)quinoline-6-carboxylic acid **10** (in D_6 -DMSO).



crude
C13_256scans DMSO D:\\ schmidg 1



Current Data Parameters
NAME ELM302-0161.1
EXPNO 11
PROCNO 1

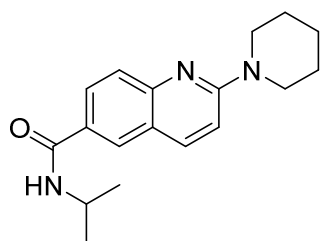
F2 - Acquisition Parameters
Date_ 20161109
Time 15.07
INSTRUM spect
PROBHD 5 mm CPDCH 13C
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 256
DS 4
SWH 31512.605 Hz
FIDRES 0.4680844 Hz
AQ 1.0398378 sec
RG 250.03
RW 15.867 usec
DE 60.67 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL F1 =====
SFO1 125.7728799 MHz
NUC1 13C
P1 10.00 usec
PLM1 21.00000000 W

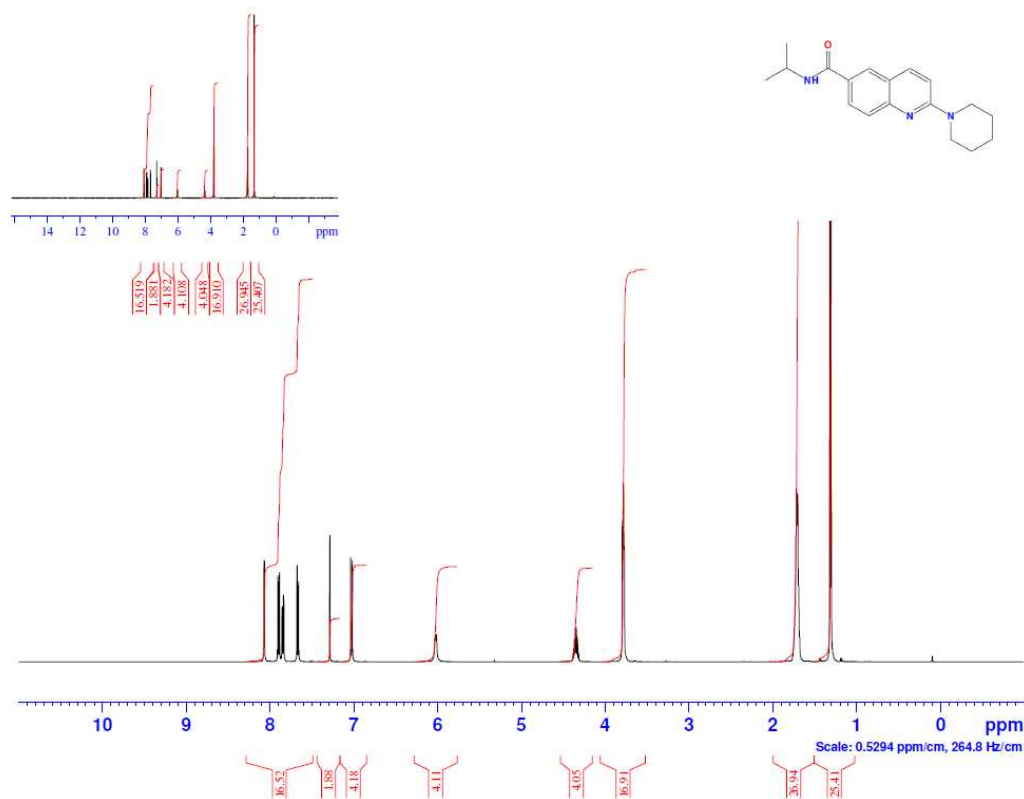
===== CHANNEL F2 =====
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 80.00 usec
PLM2 13.00000000 W
PLM12 0.22395000 W
PLM13 0.11264000 W

F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

^1H NMR spectrum of N-isopropyl-2-(piperidin-1-yl)quinoline-6-carboxamide **11** (in CDCl_3).



crude
proton_2scans CDCl_3 D:\schmidg 95



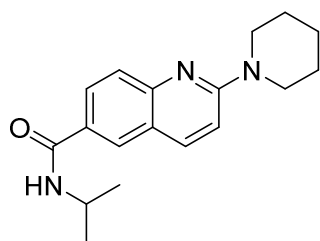
Current Data Parameters
NAME ELR302-0166.1
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
DATE_ 20161115
TIME 12:21
INSTRUM spect
PROBHD 5 mm CPDCH 13C
PULPROG zg30
TD 65536
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 11.16
DW 50.000 usec
DE 10.00 usec
TE 298.0 K
D1 1.00000000 sec
TDO 1

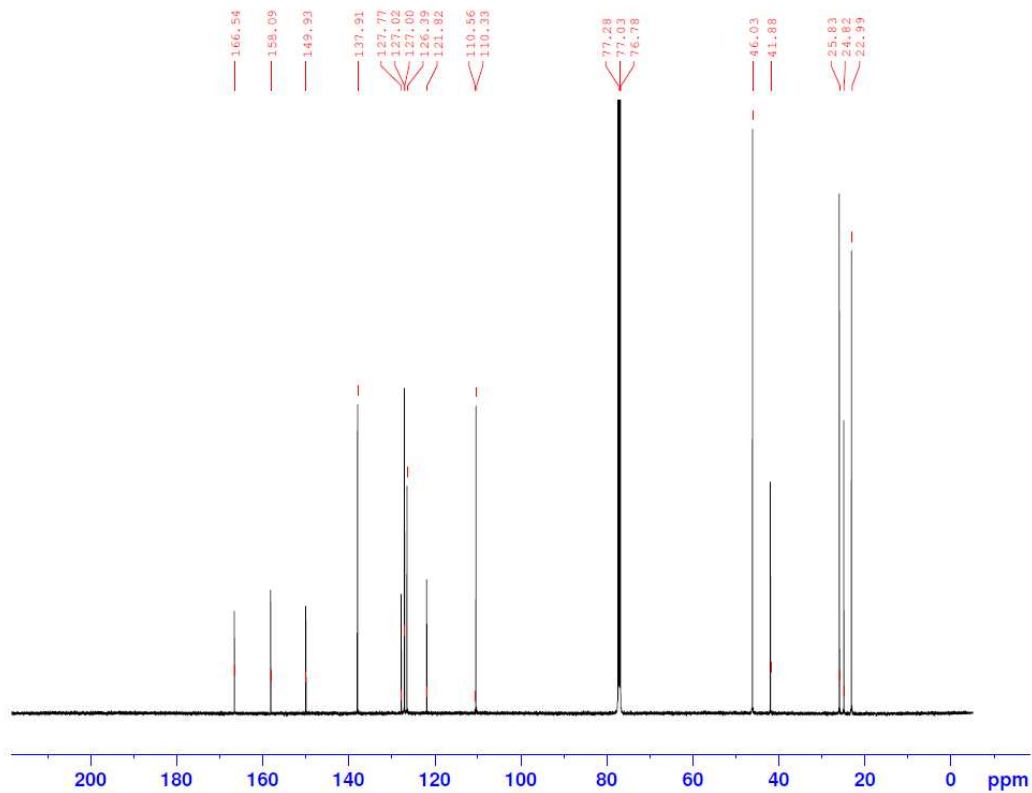
CHANNEL f1
SF01 500.1330885 MHz
NUC1 1H
P1 10.10 usec
PLW1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 500.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{13}C NMR spectrum of N-isopropyl-2-(piperidin-1-yl)quinoline-6-carboxamide **11** (in CDCl_3).



crude
C13_256scans CDC13 D:\ schmidg 95



```
Current Data Parameters
NAME      E1N302-0168.1
EXPNO     11
PROCNO    1

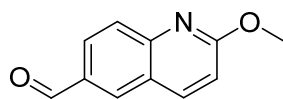
F2 - Acquisition Parameters
Date_     20161115
Time      12.36
INSTRUM   spect
PROBHD    5 mm CPOCH 13C
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         256
DS         4
SWH        31512.605 Hz
FIDRES     0.480844 Hz
AQ          1.0398378 sec
RG          200.03
EW          15.867 usec
DE          60.67 usec
TE          300.0 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0         1

===== CHANNEL f1 =====
SFO1       125.7728799 MHz
NUC1        13C
P1          10.00 usec
PLW1        21.00000000 W

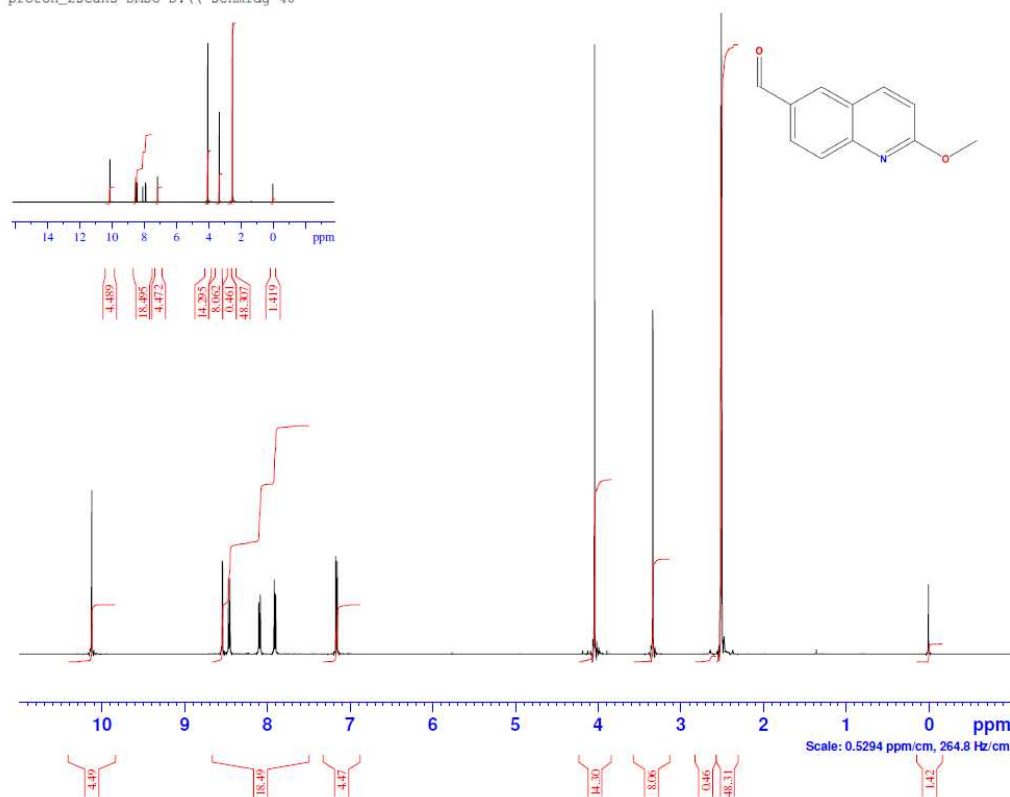
===== CHANNEL f2 =====
SFO2       500.1320005 MHz
NUC2         1H
CPOPRG12   waltz16
PCPD2       80.00 usec
PLW2        13.00000000 W
PLW12       0.22395000 W
PLW13       0.11264000 W

F2 - Processing parameters
SI          32768
SF          125.7577890 MHz
WDW         0
SSB         0
LB          1.00 Hz
GB          0
PC          1.40
```

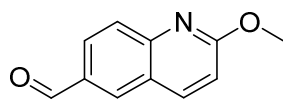
^1H NMR spectrum of 2-methoxyquinoline-6-carbaldehyde **13** (in D_6 -DMSO).



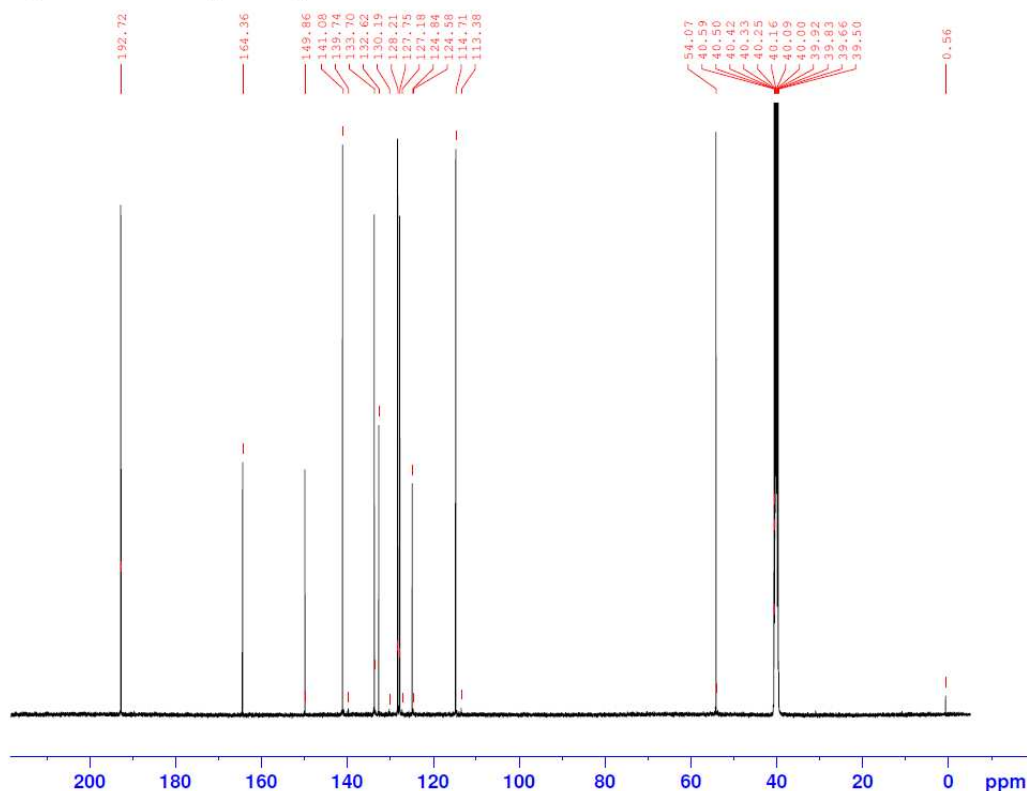
proton_2scans DMSO D:\ schmidg 40



^{13}C NMR spectrum of 2-methoxyquinoline-6-carbaldehyde **13** (in $\text{D}_6\text{-DMSO}$).



after sec. extr.
C13_256scans DMSO D:\ schmidg 8



```
Current Data Parameters
NAME      E1A302-D162.1
EXPNO     21
PROCNO    1

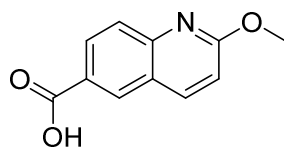
F2 - Acquisition Parameters
Date_     20161111
Time      11.13
INSTRUM    spect
PROBHD     5 mm CPDQ 13C
PULPROG    zgpg30
TD         65536
SOLVENT    DMSO
NS         256
DS         4
SWH         31512.605 Hz
FIDRES      0.480844 Hz
AQ          1.0388378 sec
RG          200.03
SW          15.867 usec
DE          60.67 usec
TE          300.0 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0         1

===== CHANNEL f1 =====
SFO1       125.7728799 MHz
NUC1       13C
PL1        10.00 usec
PLW1       21.00000000 W

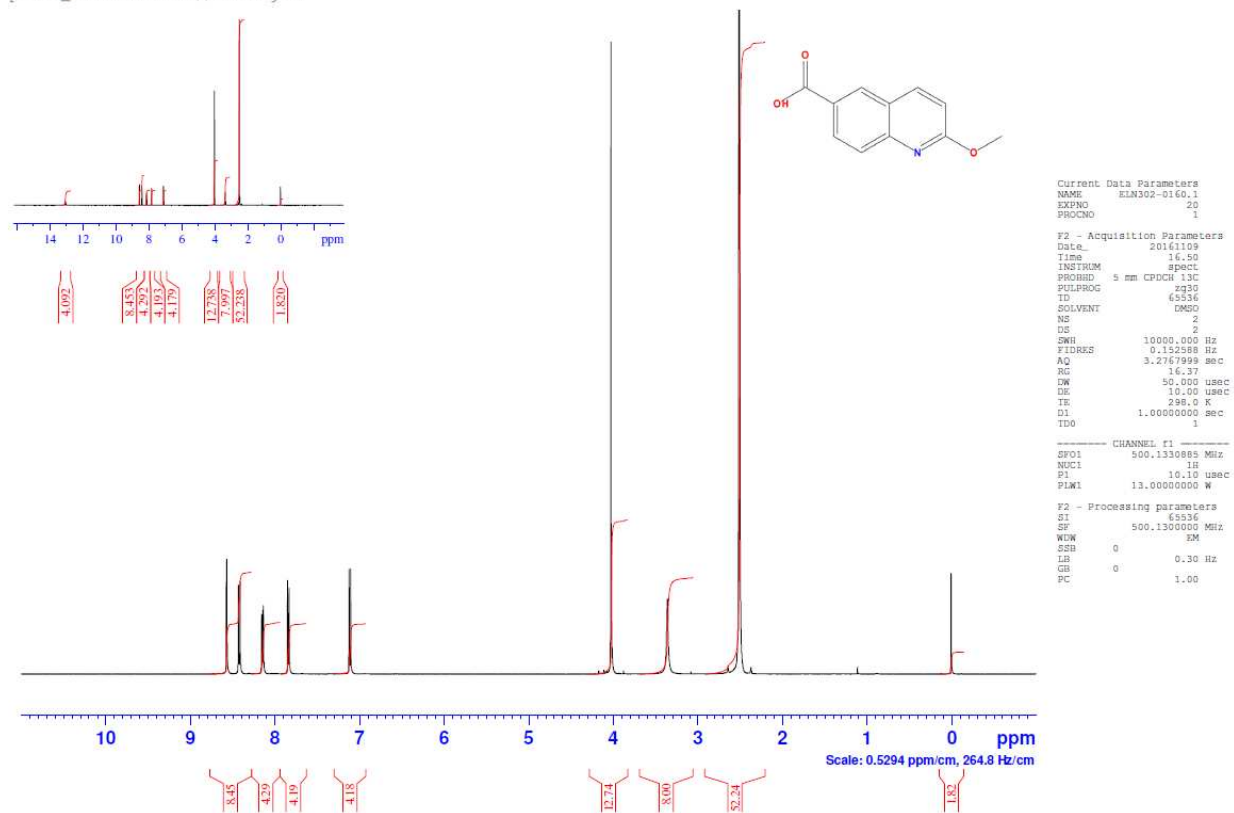
===== CHANNEL f2 =====
SFO2       500.1320005 MHz
NUC2       1H
CPDPRG2    waltz16
PCPD2      80.00 usec
PLW2       13.00000000 W
PLW12      0.22380000 W
PLW13      0.11264000 W

F2 - Processing parameters
SI         32768
SF         125.7577890 MHz
WDW         RM
SSB         0
GB          0
PC          1.40
```

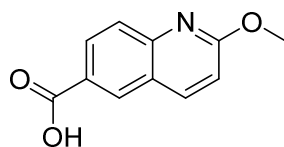
^1H NMR spectrum of 2-methoxyquinoline-6-carboxylic acid **14** (in D_6 -DMSO).



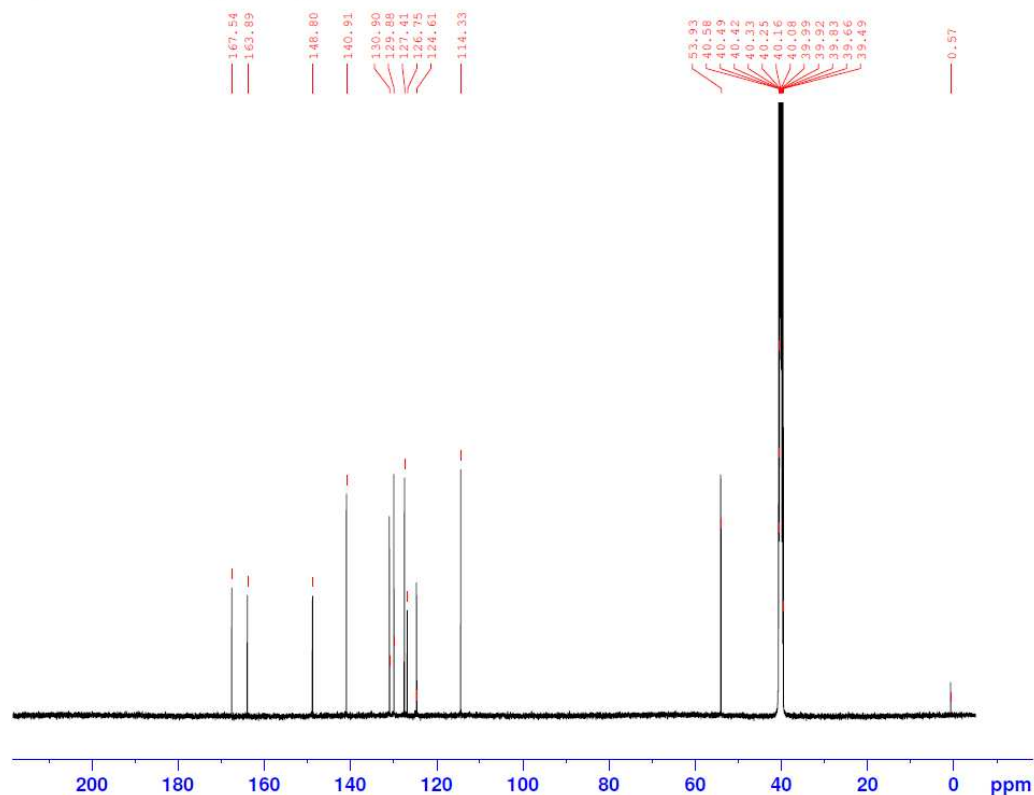
after purification
proton_2scans DMSO D:\schmidg 41



^{13}C NMR spectrum of 2-methoxyquinoline-6-carboxylic acid **14** (in D_6 -DMSO).



after purification
C13_256scans DMSO D:\\ schmidg 41



```

Current Data Parameters
NAME: E1A302-0160.1
EXPNO: 21
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20161109
Time: 17.05
INSTRUM: spect
PROBHD: 5 mm CPDCH 13C
PULPROG: zgpg30
TD: 65536
SOLVENT: DMSO
NS: 256
DS: 4
SWH: 31512.605 Hz
FIDRES: 0.480844 Hz
AQ: 1.0398376 sec
RG: 200.03
DW: 15.847 usec
DE: 60.67 usec
TE: 300.0 K
D1: 2.00000000 sec
D11: 0.03000000 sec
TD0: 1

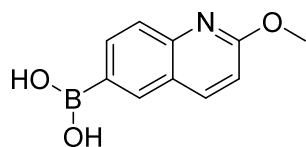
===== CHANNEL f1 =====
SFO1: 125.7728799 MHz
NUC1: 13C
P1: 10.00 usec
PLW1: 21.00000000 W

===== CHANNEL f2 =====
SFO2: 500.1300005 MHz
NUC2: 1H
CPDPRG2: waltz16
PCPD2: 80.00 usec
PLW2: 13.00000000 W
PLW12: 0.22390000 W
PLW13: 0.11264000 W

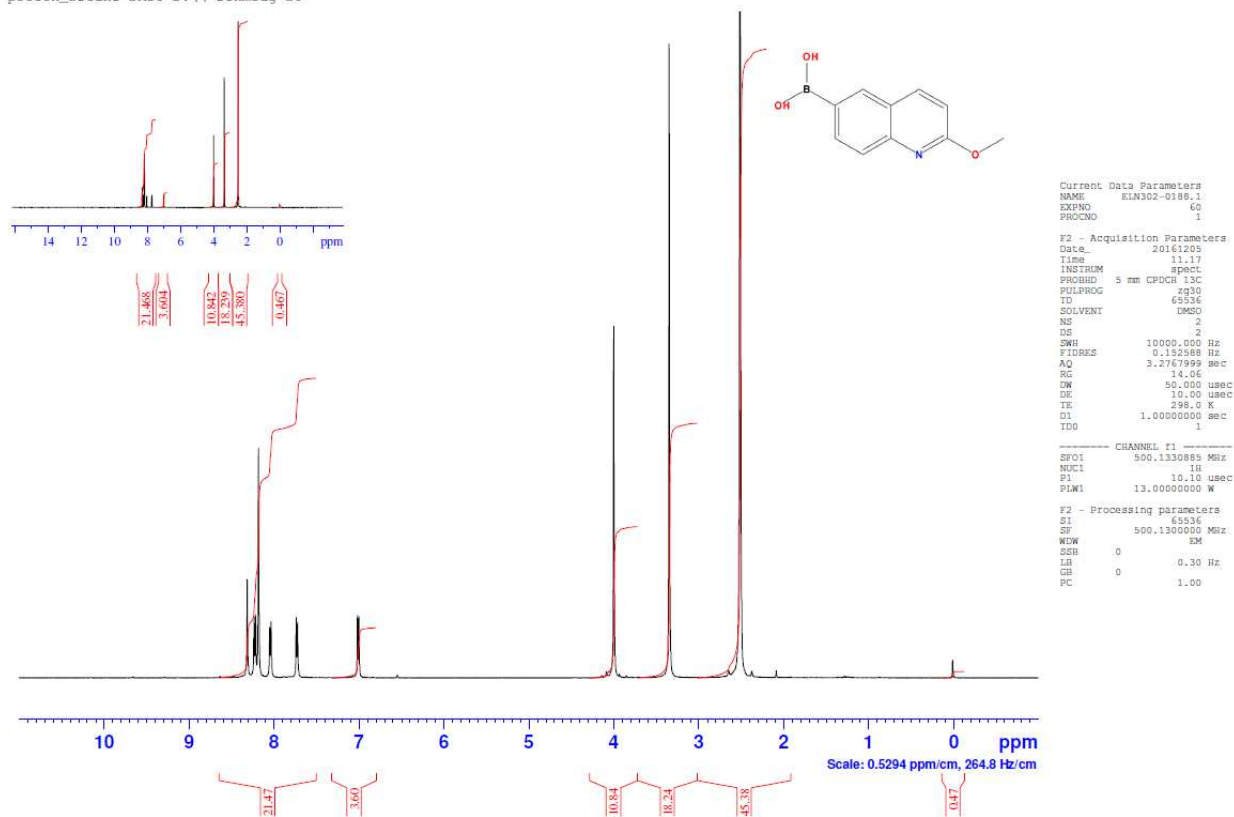
F2 - Processing parameters
SI: 32768
SF: 125.7577890 MHz
WDW: EM
SSB: 0
GB: 0
PC: 1.40

```

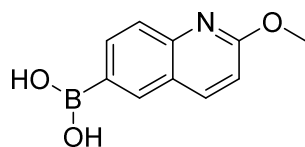
^1H NMR spectrum of (2-methoxyquinolin-6-yl)boronic acid **15** (in D_6 -DMSO).



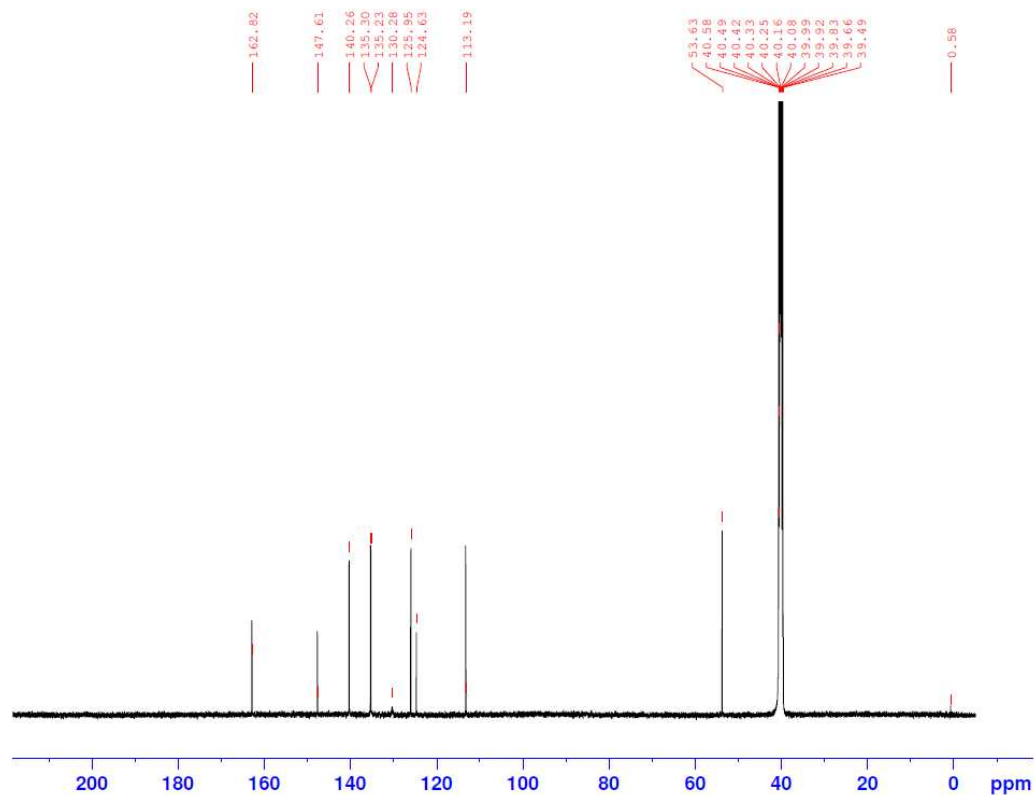
after sec. purification
proton_2scans DMSO D:\schmidg 28



^{13}C NMR spectrum of (2-methoxyquinolin-6-yl)boronic acid **15** (in D_6 -DMSO).



after sec. purification
C13_256scans DMSO D:\schmidg 28



```
Current Data Parameters
NAME      E13302-0188.1
EXPNO     61
PROCNO    1

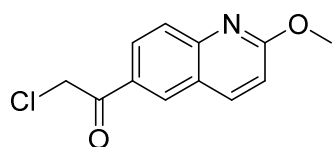
F2 - Acquisition Parameters
Date_     20161205
Time      11.31
INSTRUM    spect
PROBHD     5 mm CPQCH 13C
PULPROG    zgpg30
TD         65536
SOLVENT    DMSO
NS         256
DS         4
SWH         31512.605 Hz
FIDRES     0.480844 Hz
AQ         1.0398378 sec
RG         200.03
DW         15.867 used
DE         60.67 used
TE         300.0 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1

===== CHANNEL f1 =====
SFO1      125.7728799 MHz
NUC1       13C
P1         10.00 usec
PL1        21.00000000 W

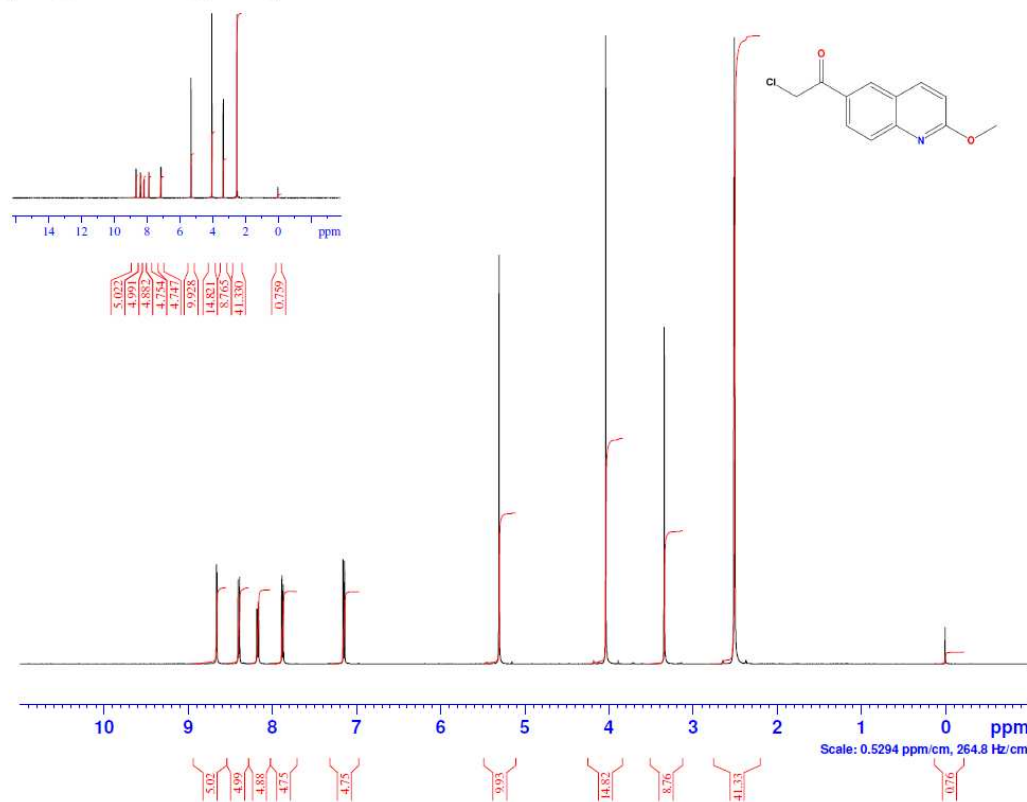
===== CHANNEL f2 =====
SFO2      500.1320005 MHz
NUC2       1H
CPDPRG2    waltz16
PCPD2       80.00 used
PL12       13.00000000 W
PL122      0.22350000 W
PL123      0.11264000 W

F2 - Processing parameters
SI         32768
SF         125.7577890 MHz
WDW        0
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
```

^1H NMR spectrum of 2-chloro-1-(2-methoxyquinolin-6-yl)ethan-1-one **16** (in D_6 -DMSO).



proton_2scans DMSO D:\schmidg 34



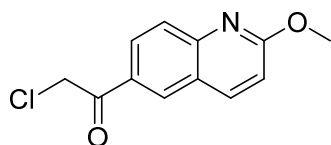
Current Data Parameters
NAME E1N302-D184.1
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161129
Time 12.14
INSTRUM spect
PROBHD 5 mm CPOCH 13C
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 2
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2747999 sec
RG 13.03
DW 50.000 usec
DE 10.00 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

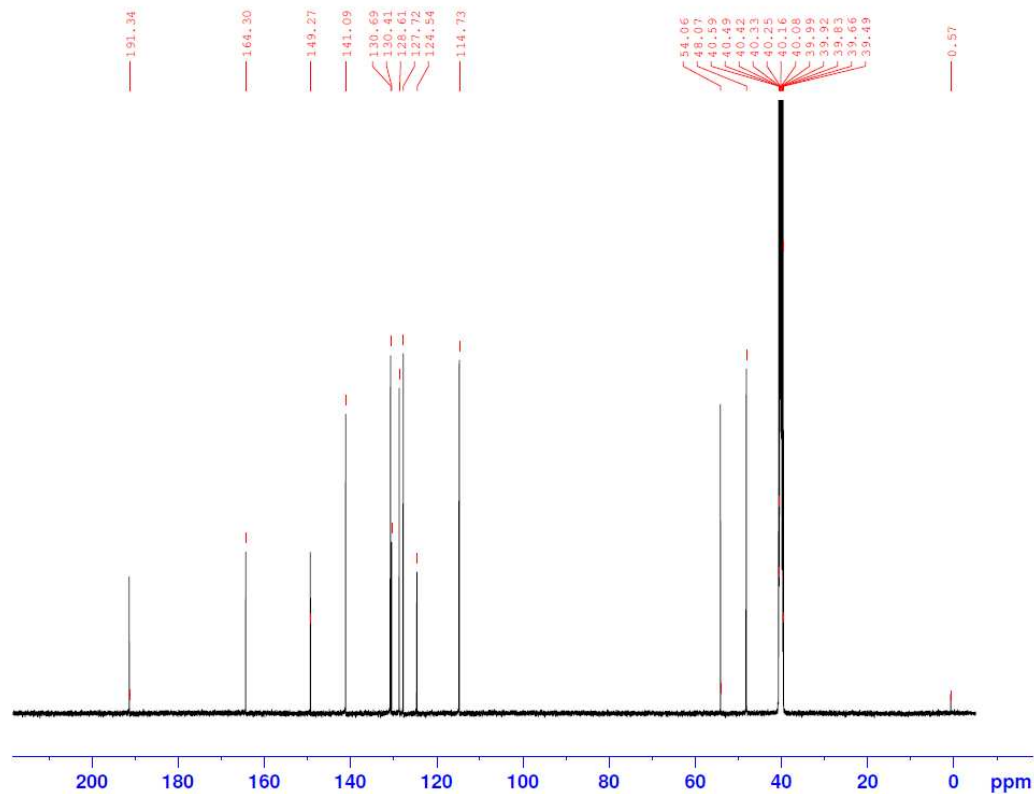
----- CHANNEL f1 -----
SFO1 500.1330885 MHz
NUC1 1H
P1 10.10 usec
PLM1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 500.1300000 MHz
WIN EM
SFR 0
LB 0.30 Hz
GB 0
PC 1.00

^{13}C NMR spectrum of 2-chloro-1-(2-methoxyquinolin-6-yl)ethan-1-one **16** (in $\text{D}_6\text{-DMSO}$).



C13_256scans DMSO D:\schmidg 34



```

Current Data Parameters
NAME: E1A302-0184.1
EXPNO: 11
PROCNO: 1

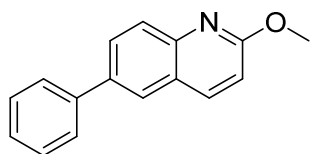
F2 - Acquisition Parameters
Date_: 20161125
Time: 12.29
INSTRUM: spect
PROBHD: 5 mm CPDQX 13C
PULPROG: zgpg30
TD: 65536
SOLVENT: DMSO
NS: 256
DS: 4
SWH: 31512.605 Hz
FIDRES: 0.480844 Hz
AQ: 1.0398378 sec
RG: 200.03
RW: 15.867 used
DE: 60.67 used
TE: 300.0 K
D1: 2.00000000 sec
D11: 0.03000000 sec
TD0: 1

===== CHANNEL f1 =====
SFO1: 125.7728799 MHz
NUC1: 13C
P1: 10.00 usec
PLW1: 21.00000000 W

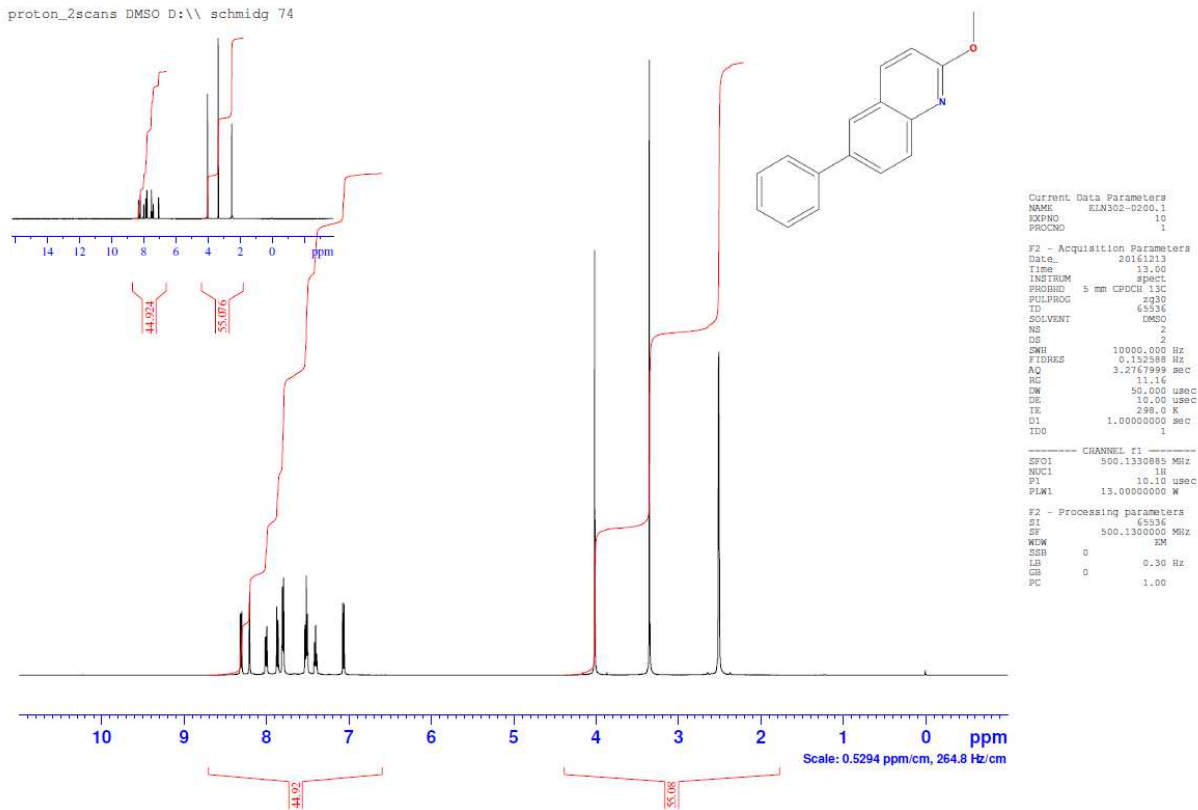
===== CHANNEL f2 =====
SFO2: 500.1320005 MHz
NUC2: 1H
PCPDG12: waltz16
PLW2: 13.00000000 W
PLW12: 0.22390000 W
PLW13: 0.11264000 W

F2 - Processing parameters
SI: 32768
SF: 125.7577890 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.40
    
```

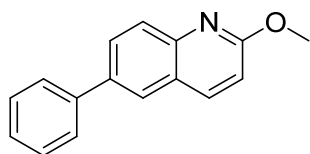
^1H NMR spectrum of 2-methoxy-6-phenylquinoline **17** (in $\text{D}_6\text{-DMSO}$).



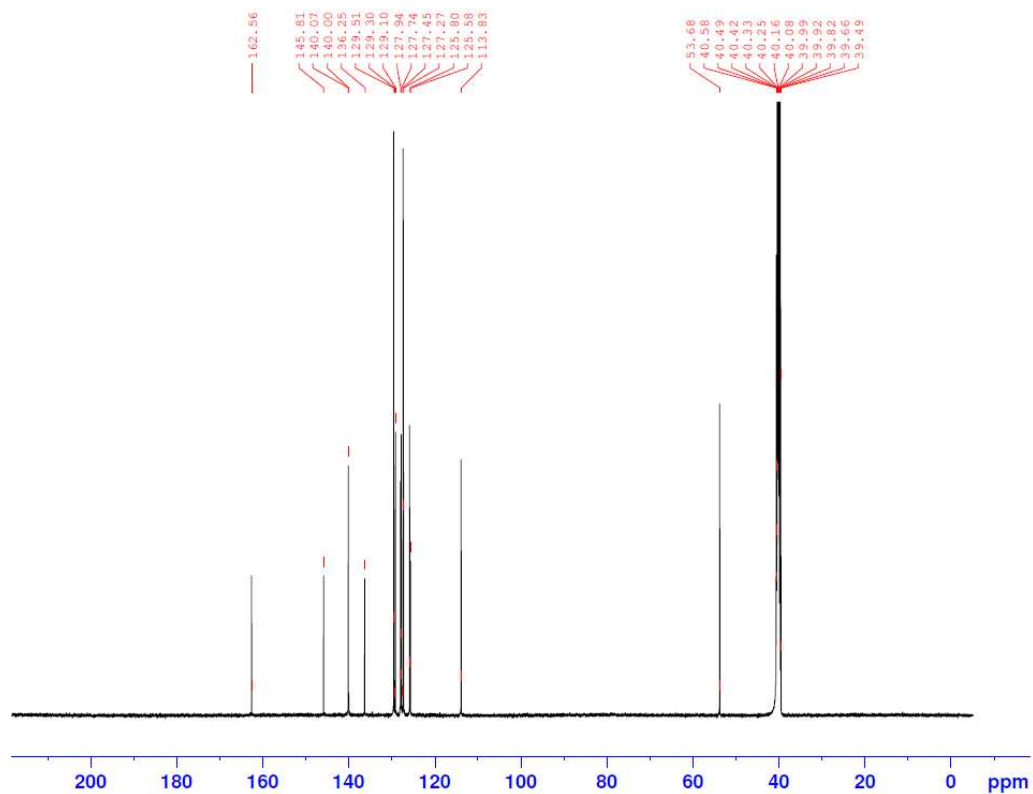
proton_2scans DMSO D:\schmidg 74



^{13}C NMR spectrum of 2-methoxy-6-phenylquinoline **17** (in D_6 -DMSO).



C13_256scans DMSO D:\ schmidg 74



```

Current Data Parameters
NAME: ELN302-0200.1
EXPNO: 11
PROCNO: 1

F2 - Acquisition Parameters
Data_: 20161213
Time: 13.15
INSTRUM: spect
PROBHD: 5 mm CPDCH 13C
PULPROG: zgpg30
TD: 65536
SOLVENT: DMSO
NS: 256
DS: 4
SWH: 31512.605 Hz
FIDRES: 0.480844 Hz
AQ: 1.0398378 sec
RG: 200.03
DW: 15.867 usec
DE: 60.67 usec
TE: 300.0 K
D1: 2.00000000 sec
D11: 0.03000000 sec
TD0: 1

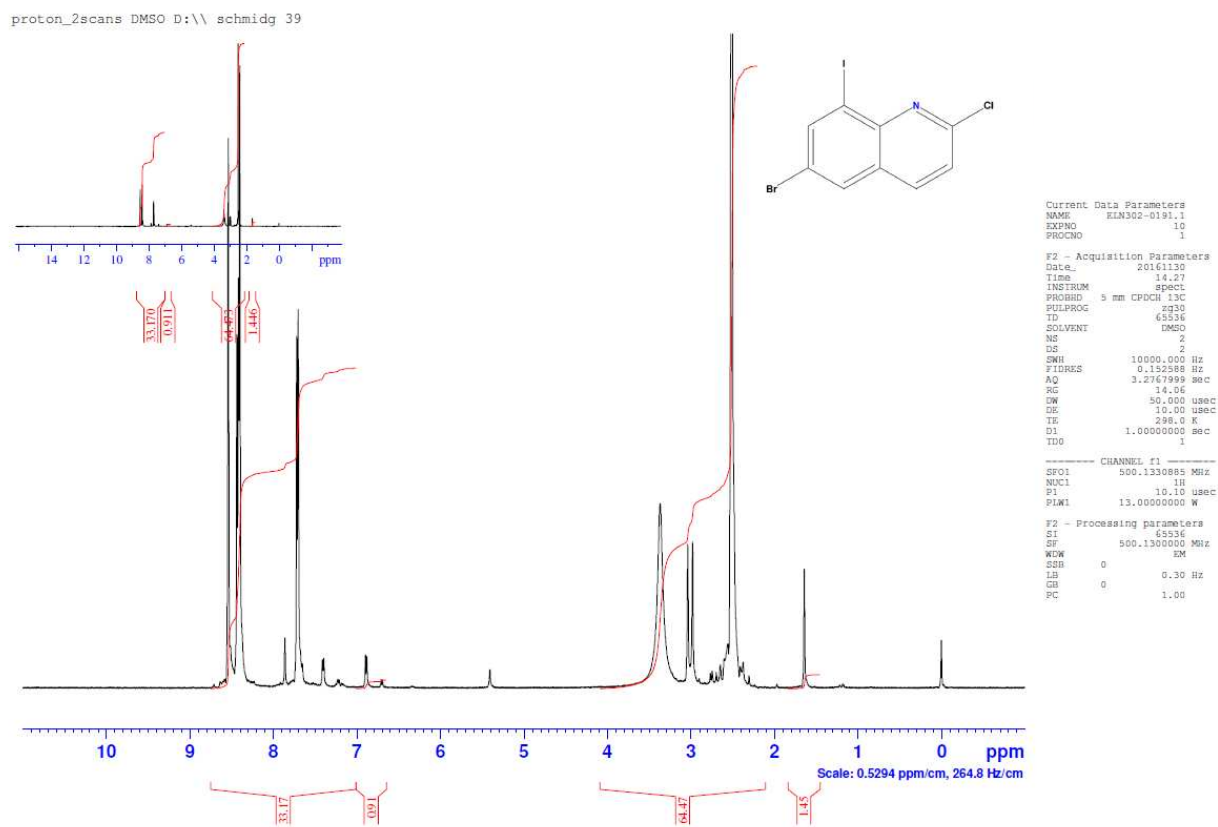
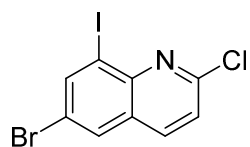
===== CHANNEL f1 =====
SFO1: 125.7728799 MHz
NUC1: 13C
P1: 10.00 usec
PLM1: 21.00000000 W

===== CHANNEL f2 =====
SFO2: 500.1320005 MHz
NUC2: 1H
CPDPRG2: waltz16
PCPD2: 80.00 usec
PLM2: 13.00000000 W
PLM12: 0.22395000 W
PLM13: 0.11264000 W

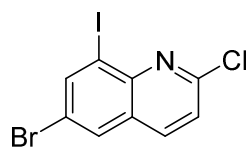
F2 - Processing parameters
SI: 32768
SF: 125.7577890 MHz
WDW: RM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.40
  
```

7. Proton and carbon NMR Spectra of quinolines 18-23

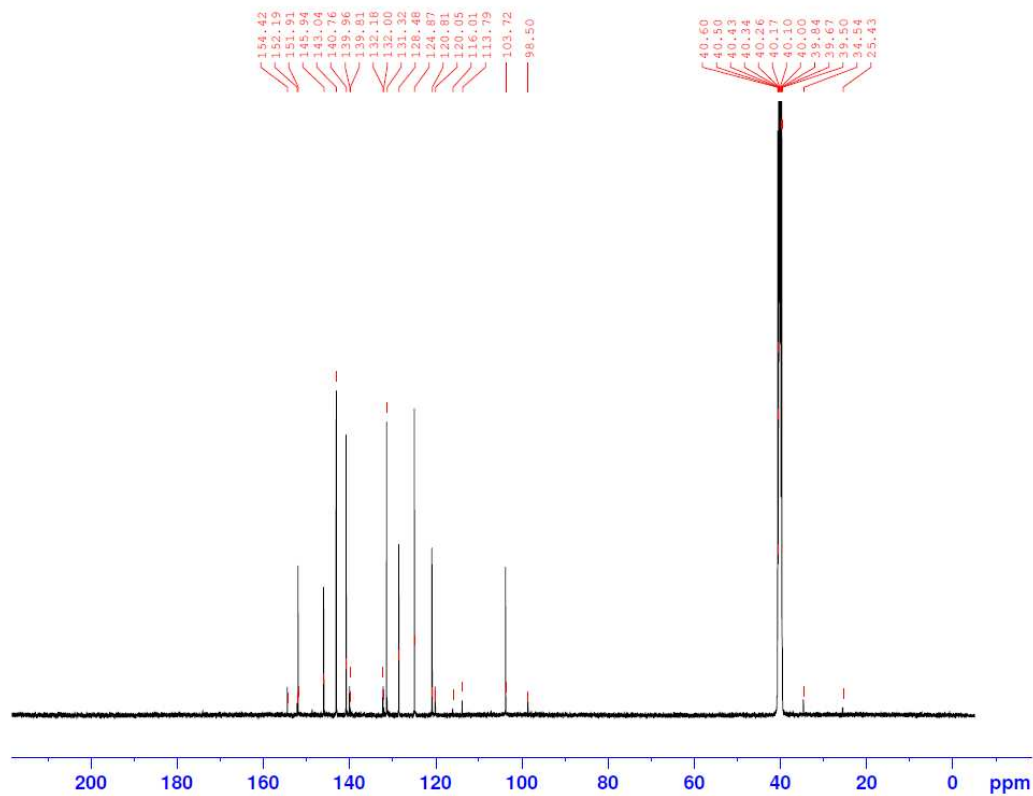
^1H NMR spectrum of 6-bromo-2-chloro-8-iodoquinoline **18** (in $\text{D}_6\text{-DMSO}$).



^{13}C NMR spectrum of 6-bromo-2-chloro-8-iodoquinoline **18** (in $\text{D}_6\text{-DMSO}$).



C13_256scans DMSO D:\ schmidg 39



```

Current Data Parameters
NAME      K1A302-D191.1
EXPNO     11
PROCNO    1

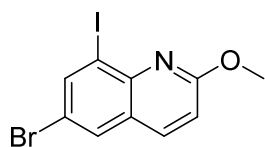
F2 - Acquisition Parameters
Date_     20161130
Time      14.42
INSTRUM   spect
PROBHD    5 mm CPDQZ 13C
PULPROG   zgpg30
TD        65536
SOLVENT   DMSO
NS         256
DS         4
SWH        31512.605 Hz
FIDRES     0.480844 Hz
AQ         1.0398378 sec
RG         200.03
DE         15.867 usec
TE         300.0 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       13C
P1         10.00 usec
PLW1       21.00000000 W

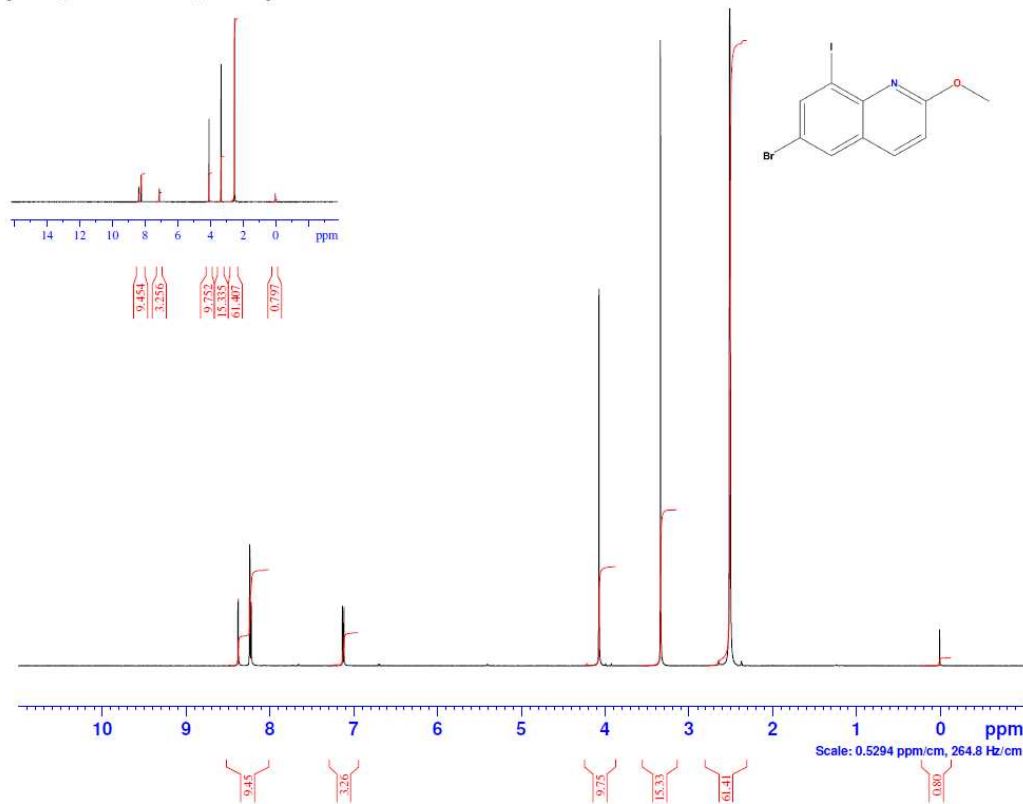
===== CHANNEL f2 =====
NUC2       1H
P2         1.00 usec
PLW2       0.11264000 W

F2 - Processing parameters
SI         32768
SF         125.7577890 MHz
WDW        EM
SSB        0
GB         0
PC         1.40
    
```

^1H NMR spectrum of 6-bromo-8-iodo-2-methoxyquinoline **19** (in $\text{D}_6\text{-DMSO}$).



proton_2scans DMSO D:\schmidg 9



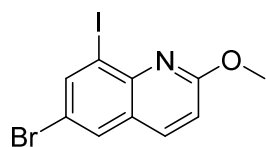
Current Data Parameters
NAME ELN302-0191.2
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161201
Time 11.45
INSTRUM spect
PROBHD 5 mm CPDOR 13C
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 2
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 16.37
LW 50.000 usec
EQ 10.00 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

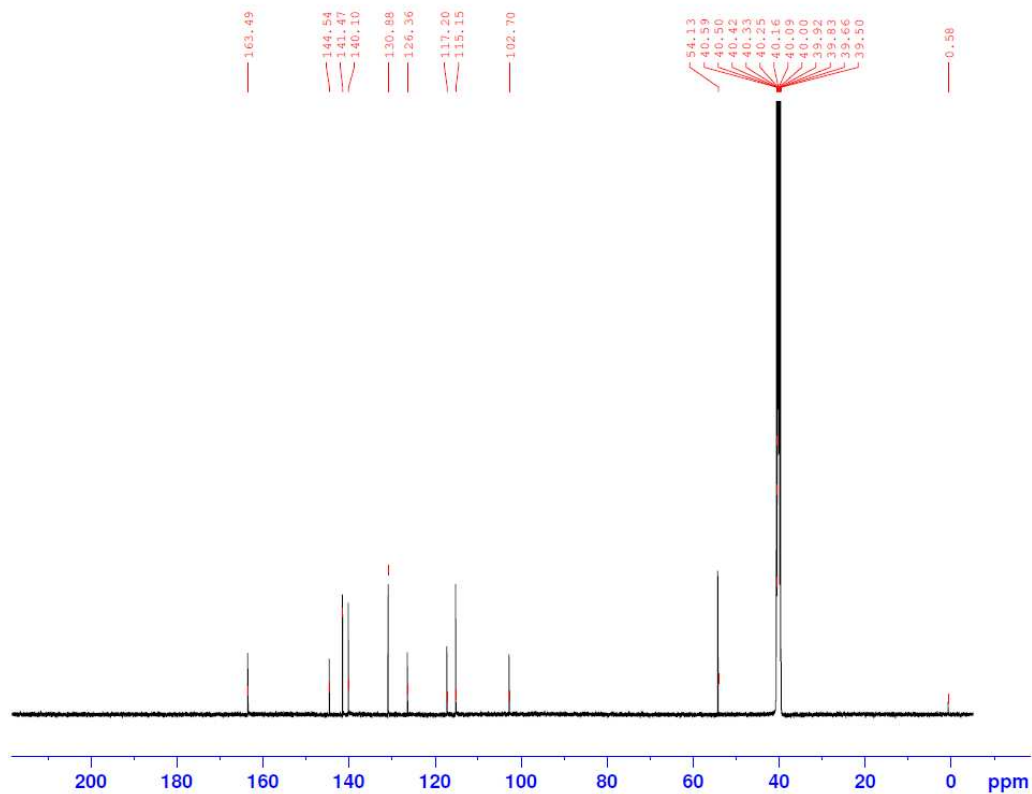
CHANNEL f1
SFO1 500.1330885 MHz
NUC1 1H
P1 10.10 usec
PLW1 13.00000000 W

F2 - Processing parameters
S1 65536
SF 500.1330000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{13}C NMR spectrum of 6-bromo-8-iodo-2-methoxyquinoline **19** (in D_6 -DMSO).



C13_256scans DMSO D:\ schmidg 9



```

Current Data Parameters
NAME: K1A302-0191.2
EXPNO: 11
PROCNO: 1

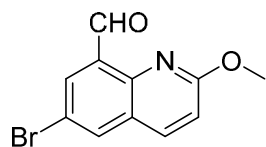
F2 - Acquisition Parameters
Date_: 20161201
Time: 12.00
INSTRUM: spect
PROBHD: 5 mm CPDCH 13C
PULPROG: zgpg30
TD: 65536
SOLVENT: DMSO
NS: 256
DS: 4
SWH: 31512.605 Hz
FIDRES: 0.480844 Hz
AQ: 1.0398378 sec
RG: 200.03
DW: 15.867 usec
DE: 60.67 usec
TR: 300.0 K
D1: 2.0000000 sec
D11: 0.0300000 sec
TDC: 1

===== CHANNEL F1 =====
SFO1: 125.7728799 MHz
NUC1: 13C
P1: 10.00 usec
PLW1: 21.00000000 W

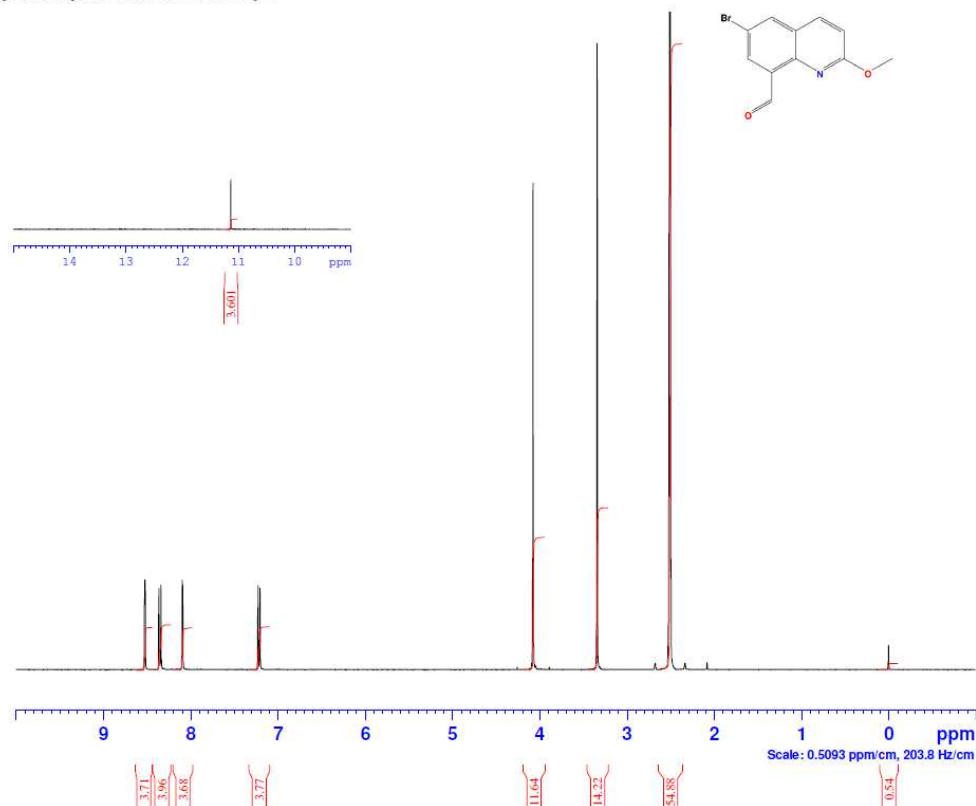
===== CHANNEL F2 =====
SFO2: 500.1320005 MHz
NUC2: 1H
CPDPRG2: waltz16
PCPD2: 80.00 usec
PLW2: 13.00000000 W
PLW12: 0.22395000 W
PLW13: 0.11264000 W

F2 - Processing parameters
SI: 32768
SF: 125.7577890 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.40
    
```

^1H NMR spectrum of 6-bromo-2-methoxyquinoline-8-carbaldehyde **20** (in D_6 -DMSO).



proton_np_c1 DMSO D:\schmidg 3



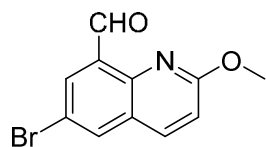
Current Data Parameters
NAME: E1N302-0201.1
EXPNO: 10
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20161208
Time: 11.01
INSTRUM: spect
PROBHD: 5 mm PABBO BB-
PULPROG: zg30
TD: 65536
SOLVENT: DMSO
NS: 8
DS: 2
SWH: 8223.685 Hz
FIDRES: 0.125483 Hz
AQ: 3.9845889 sec
RG: 203
DM: 60.800 usec
DE: 6.50 usec
TE: 296.0 K
D1: 1.00000000 sec
TDO: 1

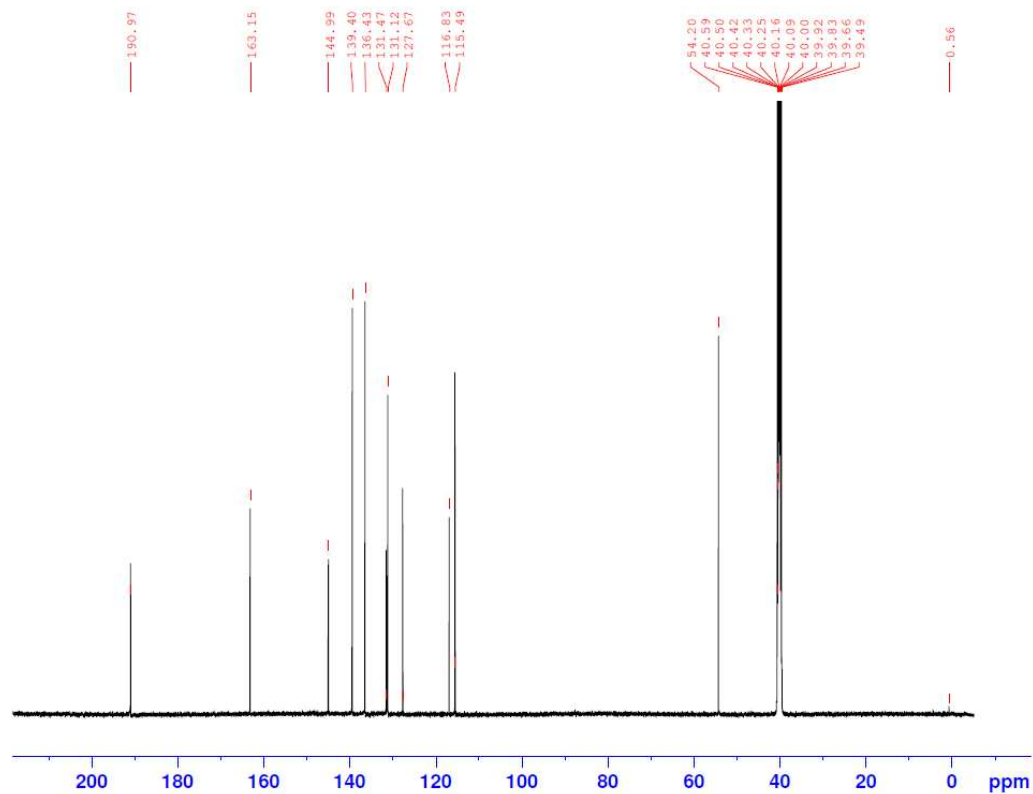
CHANNEL f1
SFO1: 400.1324710 MHz
NUC1: 1H
P1: 10.70 usec
PLW1: 18.29999924 W

F2 - Processing parameters
SI: 32768
SF: 400.1300000 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00

^{13}C NMR spectrum of 6-bromo-2-methoxyquinoline-8-carbaldehyde **20** (in D_6 -DMSO).



C13_256scans DMSO D:\schmidg 75



```

Current Data Parameters
NAME      E14302-0201-1
EXPNO     10
PROCNO    1

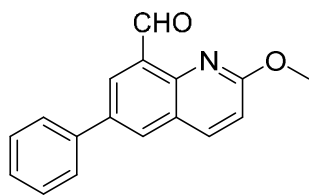
F2 - Acquisition Parameters
Date_     20161213
Time      13.32
INSTRUM   spect
PROBHD    5 mm CPDCH 13C
PULPROG   zgpg30
TD         65536
SOLVENT   DMSO
NS         256
DS         4
SWH        31512.605 Hz
FIDRES     0.480844 Hz
AQ         1.8398378 sec
RG          200.03
DW         15.867 usec
DE         60.67 usec
TE         300.0 K
D1         2.0000000 sec
D11        0.6300000 sec
TDO        1

===== CHANNEL f1 =====
SFO1      125.7727399 MHz
NUC1       13C
P1         10.00 usec
PLW1       21.0000000 W

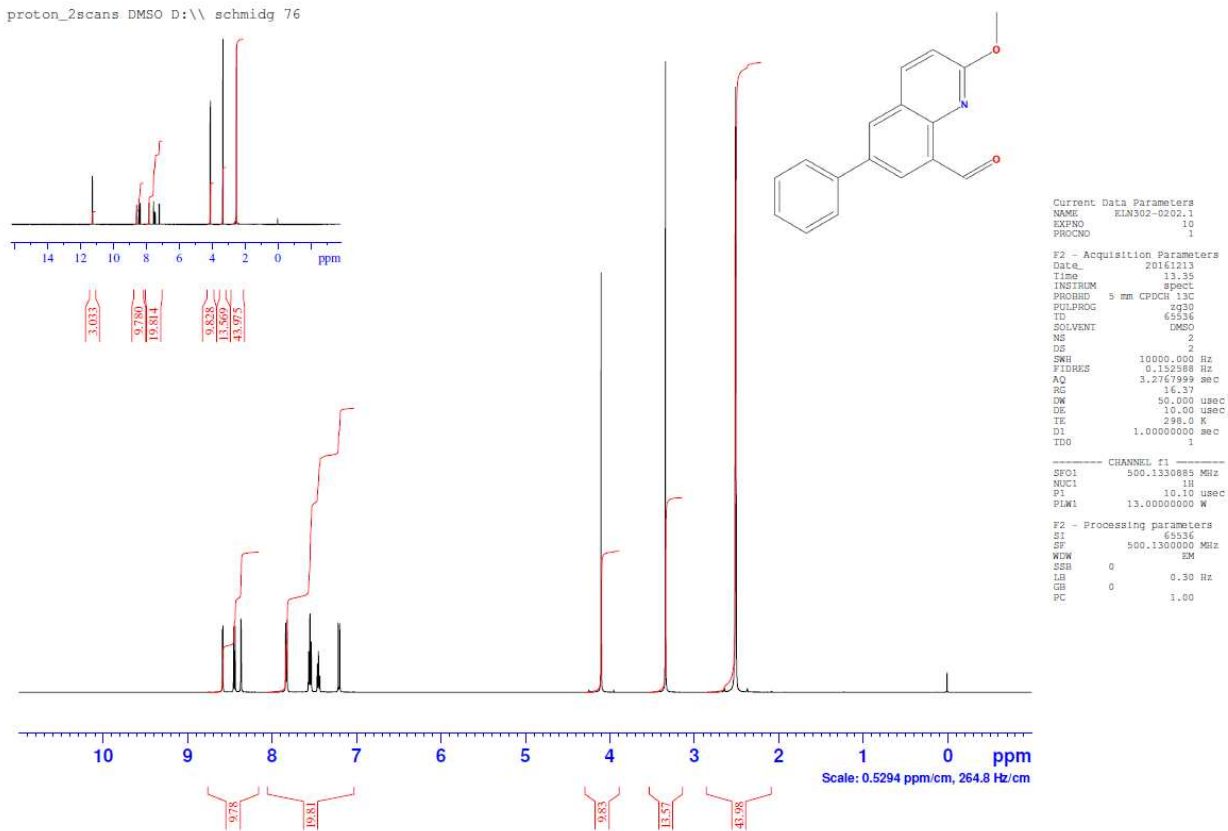
===== CHANNEL f2 =====
SFO2      500.1320005 MHz
NUC2       1H
CPCPD2    wait16
PCPD2     80.00 usec
P1W2      13.0000000 W
P1W12     0.2335000 W
P1W13     0.1126400 W

F2 - Processing parameters
SI         32768
SF         125.7577890 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
    
```

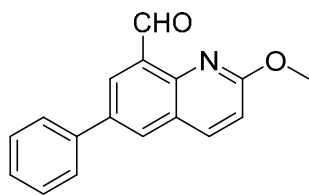
^1H NMR spectrum of 2-methoxy-6-phenylquinoline-8-carbaldehyde **21** (in D_6 -DMSO).



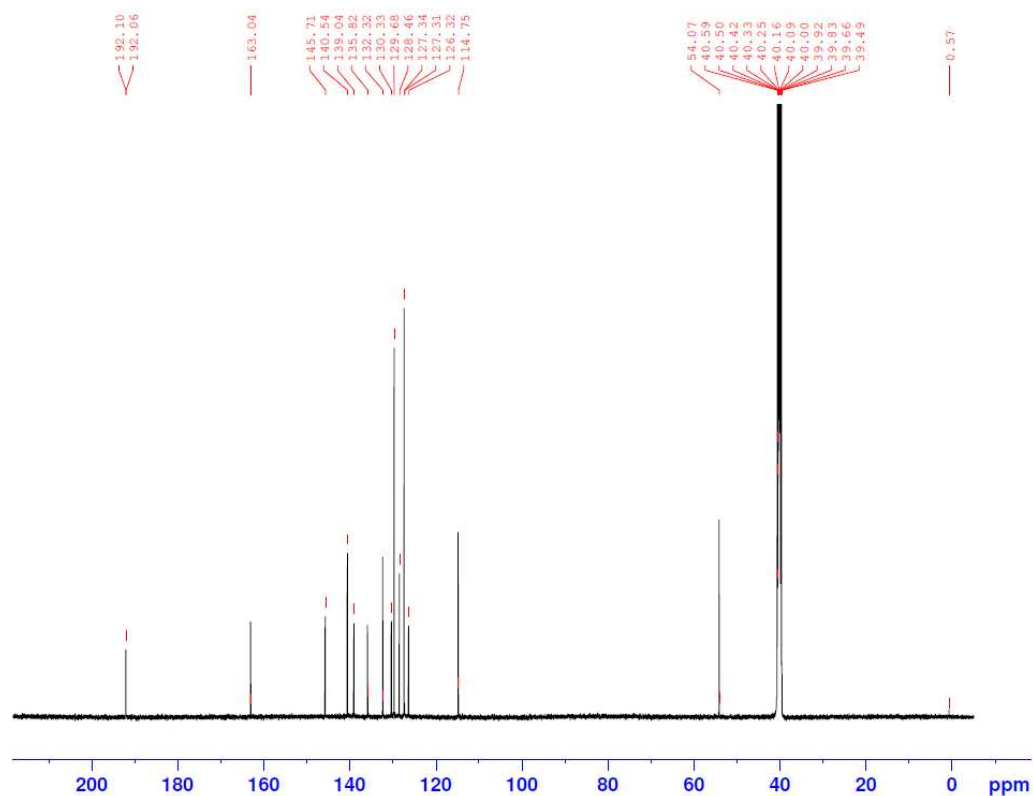
proton_2scans DMSO D:\ schmidg 76



^{13}C NMR spectrum of 2-methoxy-6-phenylquinoline-8-carbaldehyde **21** (in D_6 -DMSO).



C13_256scans DMSO D:\ schmidg 76



```

Current Data Parameters
NAME      EIA302-0202.1
EXPNO     11
PROCNO    1

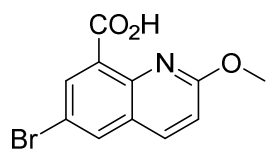
F2 - Acquisition Parameters
Date_     20161213
Time      13.50
INSTRUM   spect
PROBHD    5 mm CPOCP 13C
PULPROG   zgpg30
TD         65536
SOLVENT   DMSO
NS         256
DS         4
SWH        31512.605 Hz
FIDRES     0.480844 Hz
AQ         1.0398378 sec
RG         200.03
DW         15.867 usec
DE         60.67 usec
TE         300.0 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1

===== CHANNEL f1 =====
SFO1      125.7728799 MHz
NUC1       13C
P1        10.00 usec
P1M1      21.00000000 W

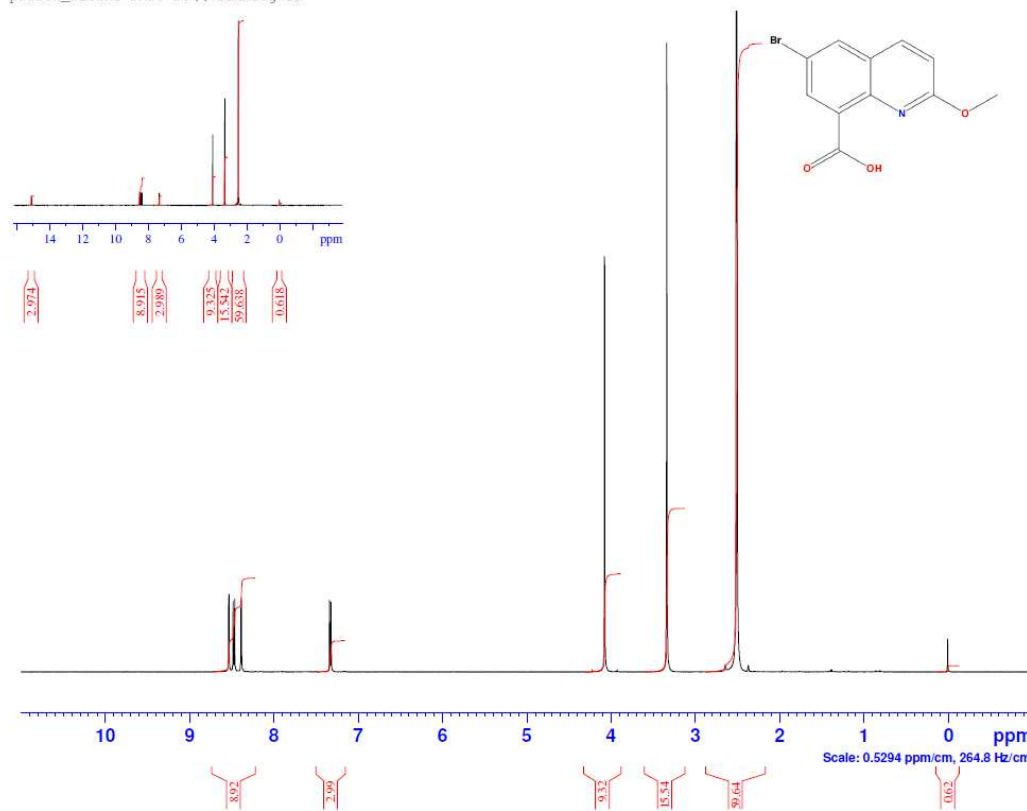
===== CHANNEL f2 =====
SFO2      500.1320005 MHz
NUC2       1H
CPCPRG2   waltz16
PCPD2     80.00 usec
P1M2      13.00000000 W
P1M12     0.22392000 W
P1M13     0.11264000 W

F2 - Processing parameters
SI         32768
SF         125.7577890 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
    
```

^1H NMR spectrum of 6-bromo-2-methoxyquinoline-8-carboxylic acid **22** (in D_6 -DMSO).



crude
proton_2scans DMSO D:\\ schmidg 30



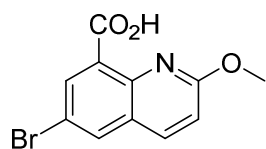
Current Data Parameters
NAME E1N302-0195.1
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161205
Time 11:54
INSTRUM spect
PROBHD 5 mm CPOCH 13C
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 2
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 16.37
DW 50.000 usec
DE 10.00 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

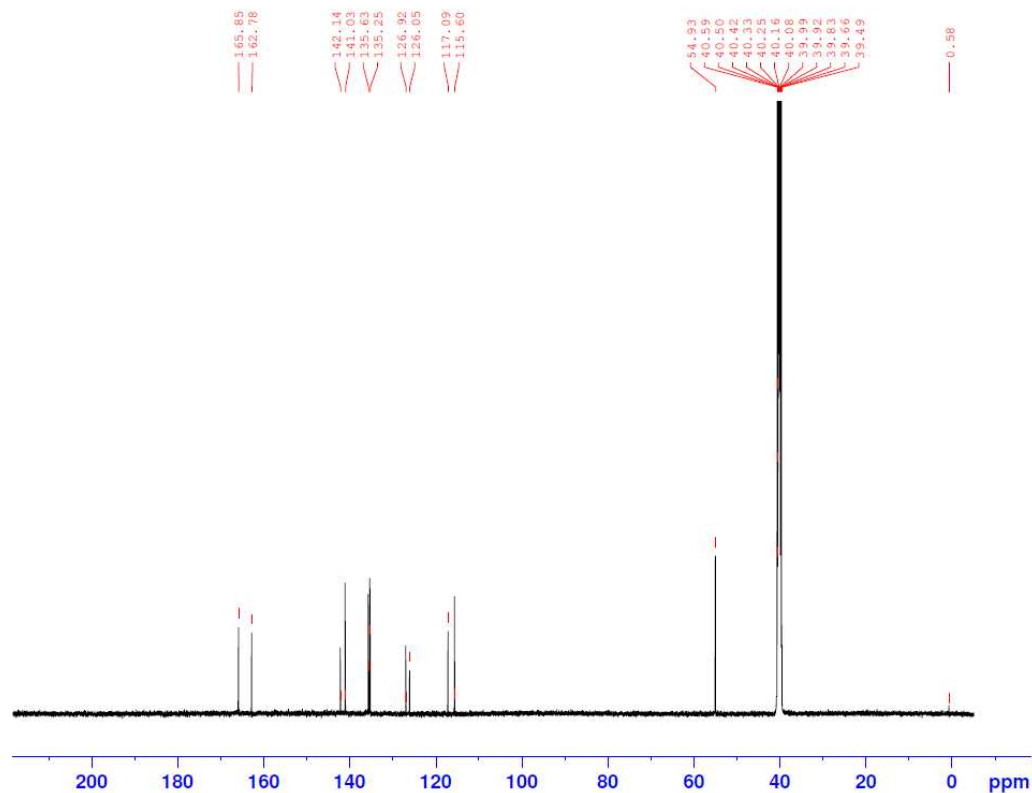
CHANNEL f1
SFO1 500.1330885 MHz
NUC1 1H
P1 10.10 usec
PLW1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 500.1330885 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{13}C NMR spectrum of 6-bromo-2-methoxyquinoline-8-carboxylic acid **22** (in D_6 -DMSO).



crude
C13_256scans DMSO D:\\ schmidg 30



```

Current Data Parameters
NAME      E14302-0195-1
EXPNO     11
PROCNO    1

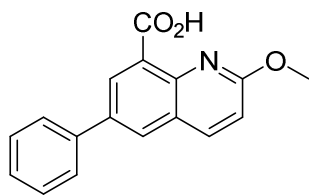
F2 - Acquisition Parameters
Date_     20161205
Time      12.09
INSTRUM   spect
PROBHD    5 mm CPOCR 13C
PULPROG   zgpg30
TD         65536
SOLVENT   DMSO
NS         256
DS         4
SWH        31512.605 Hz
FIDRES     0.480844 Hz
AQ         1.0398378 sec
RG          200.03
DE         15.867 umcd
TE         300.2 K
D1         2.0000000 sec
D11        0.0300000 sec
TD0        1

===== CHANNEL f1 =====
SFO1      125.7728799 MHz
NUC1       13C
P1         10.00 umcd
PLM1       21.0000000 W

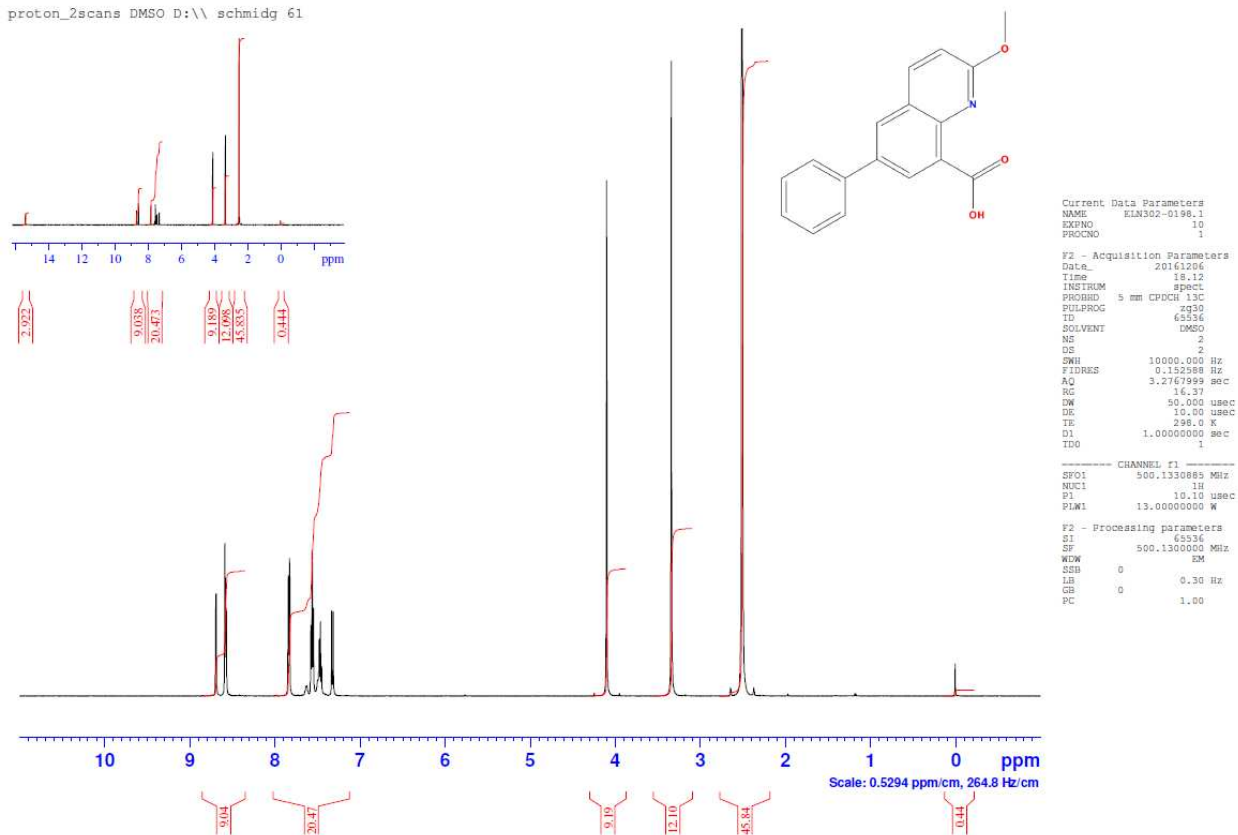
===== CHANNEL f2 =====
SFO2      500.1320005 MHz
NUC2       1H
CPCPD2    waltz16
PCPD2      80.00 umcd
PLM2       13.0000000 W
PLM12      0.2239500 W
PLM13      0.1126400 W

F2 - Processing parameters
SI         32768
SF         125.7577890 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
    
```

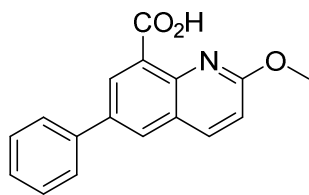
^1H NMR spectrum of 2-methoxy-6-phenylquinoline-8-carboxylic acid **23** (in D_6 -DMSO).



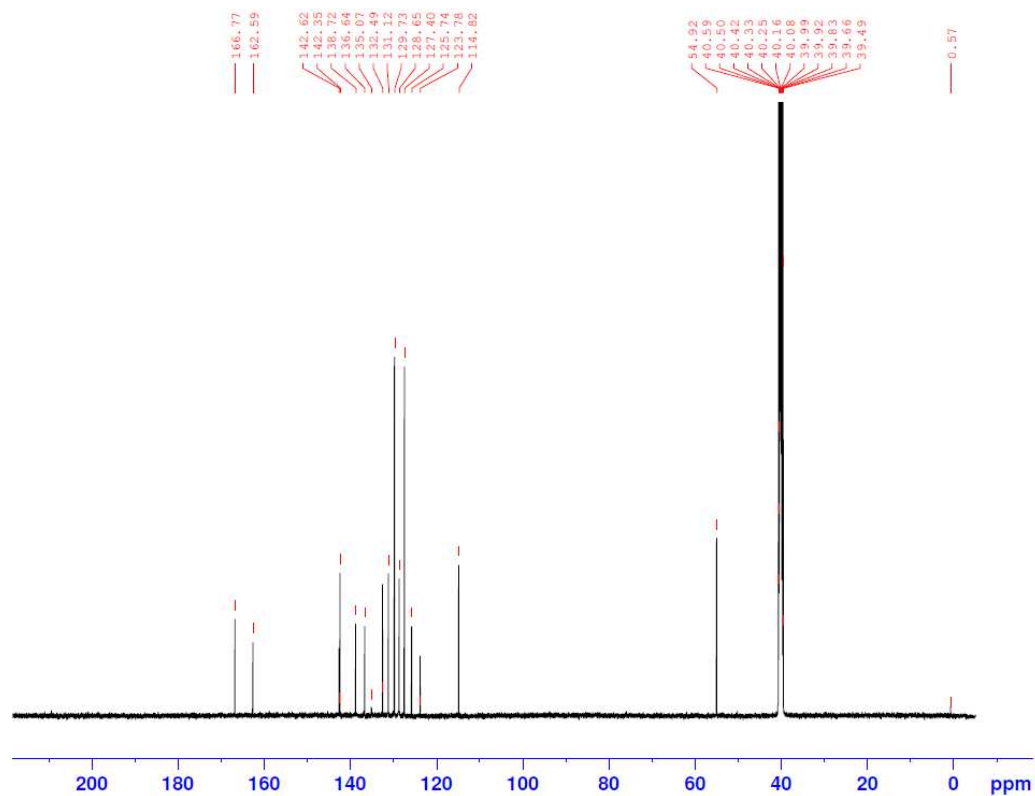
proton_2scans DMSO D:\schmidg 61



^{13}C NMR spectrum of 2-methoxy-6-phenylquinoline-8-carboxylic acid **23** (in D_6 -DMSO).



C13_256scans DMSO D:\schmidg 61



```

Current Data Parameters
NAME: EIA305-0186-1
EXPNO: 11
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20161206
Time: 18.26
INSTRUM: spect
PROBHD: 5 mm CPDQX 13C
PULPROG: zgpg30
TD: 65536
SOLVENT: DMSO
NS: 256
DS: 4
SWH: 31512.605 Hz
FIDRES: 0.480844 Hz
AQ: 1.8398378 sec
RG: 200.03
DW: 15.867 usec
DE: 60.67 usec
TE: 300.0 K
D1: 2.00000000 sec
D11: 0.03000000 sec
TD0: 1

===== CHANNEL f1 =====
SFO1: 125.772799 MHz
NUC1: 13C
P1: 10.00 usec
PLA1: 21.00000000 W

===== CHANNEL f2 =====
SFO2: 500.1320005 MHz
NUC2: 1H
CPDPRG2: waltz16
PCPD2: 80.00 usec
PLW2: 13.00000000 W
PLW12: 0.22395000 W
PLW13: 0.11264000 W

F2 - Processing parameters
SI: 32768
SF: 125.7577850 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.40
    
```