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Supporting Information

Preparation of 2-Phenyl-3-Hydroxyquinoline-4(1*H*)-one-5-carboxamides as Novel Anticancer and Fluorescence Agents

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Material and Methods

Solvents and chemicals were purchased from Aldrich (Milwaukee, IL, www.sigmaaldrich.com), Acros (Geel, Belgium, www.acros.cz) and Fisher (Pittsburgh, PA, www.fishersci.com).

LC/MS analyses were carried out on UHPLC-MS system consisting of UHPLC chromatograph Accela with photodiode array detector and triple quadrupole mass spectrometer TSQ Quantum Access (both Thermo Scientific, CA, USA), using Nucleodur Gravity C18 column at 30°C and flow rate of 800 µL/min (Macherey-Nagel, 1.8 µm, 2.1 x 50 mm, Germany). Mobile phase was (A) 0.01 M amonium acetate in water, and (B) acetonitrile, linearly programmed from 10 % to 80 % B over 2.5 min, kept for 1.5 min. The column was re-equilibrated with 10 % of solution B for 1 min. The APCI source operated at discharge current of 5 µA, vaporizer temperature of 400°C and capillary temperature of 200 °C.

NMR $^{1}H/^{13}C$ spectra were obtained on a Varian (400 MHz) instrument. NMR spectra were recorded at ambient temperature (21 °C) in DMSO-d_6 or TFA-d_1 solutions and referenced to the resonance signal of DMSO of TFA. Chemical shifts δ are reported in ppm and coupling constants *J* in Hz.

HRMS analysis was performed using an Orbitrap Elite high-resolution mass spectrometer (Thermo Fischer Scientific, MA, USA) operating at positive full scan mode (120 000 FWMH) in the range of 200–900 m/z. The settings for electrospray ionization were as follows: oven temperature of 300 °C, sheath gas of 8 arb. units and source voltage of 1.5 kV. The acquired data were internally calibrated with diisooctyl phthalate as a contaminant in methanol (m/z 391.2843). Samples were diluted to a final concentration of 20 µmol/l with 0.1% formic acid in water and methanol (50:50, v/v). The samples were injected by direct infusion into the mass spectrometer.

Crystallography. The single-crystal X-ray experiment was performed at room temperature. For this measurement, colorless single crystal of good quality was preselected under a polarization microscope. The crystal was mounted on a quartz capillary. The data were collected using SuperNova kappa diffractometer with Atlas CCD detector (Agilent Technologies, Yarnton, UK). Accurate cell parameters were determined and refined using CrysAlis CCD program (version 1.171.37.35, Agilent Technologies, Yarnton, UK). For the integration of the collected data, the CrysAlis RED program (version 1.171.37.35, Agilent Technologies) was used.

The structure was solved using direct method with SHELXS-2014 [Sheldrick, 2008] = [Sheldrick, G. M. (2008). Acta Cryst. A64, 112-122] program and then the solution was refined using SHELXL-2014 [Sheldrick, 2008] program. The aromatic hydrogen atoms were treated as “riding” on their parent carbon atoms with d(C H) = 0.93 Å and assigned isotropic atomic displacement parameters equal to 1.2 times the value of the equivalent atomic displacement parameters of the parent carbon atom [Uiso(H) = 1.2Ueq(C)]. The methylene H atoms were constrained to an ideal geometry with d(C H) = 0.97 Å and Uiso(H) = 1.2Ueq(C). Methyl H atoms were constrained as riding atoms, fixed to the parent atoms with distance of 0.96 Å and Uiso(H) = 1.5Ueq(C). Hydrogen atoms involved in H-bonding were introduced into the calculated positions and then refined freely with isotropic atomic displacement parameters.

The crystal structure has been deposited at the Cambridge Crystallographic Data Centre and allocated the deposition number CCDC 1057862.

Cytotoxic MTT assay. Cell suspensions were prepared and diluted according to the particular cell type and the expected target cell density (2 500–30 000 cells/well based on cell growth characteristics). Cells were added by pipette (80 μL) into 96-well microtiter plates. Inoculates were allowed a pre-incubation period of 24 h at 37 °C and 5 % CO_2 for stabilisation. Four-fold dilutions, in 20-μL aliquots, of the intended test concentration were added to the microtiter plate wells at time zero. All test compound concentrations were examined in duplicate. Incubation of the cells with the test compounds lasted for 72 h at 37 °C, in a 5 % CO_2 atmosphere at 100 % humidity. At the end of the incubation period, the cells were assayed using MTT. Aliquots (10 μL) of the MTT stock solution were pipetted into each well and incubated for a further 1–4 h. After this incubation period the formazan produced was dissolved by the addition of 100 μL/well of 10 % aq SDS (pH = 5.5), followed by a further incubation at 37 °C overnight. The optical density (OD) was measured at 540 nm with a Labsystem iEMS Reader MF. Tumour cell survival (TCS) was calculated using the following equation: TCS = ($OD_{drug\text{-}exposed\ well}$ / mean $OD_{control\ wells}$) x 100 %. The IC_{50} value, the drug concentration lethal to 50 % of the tumour cells, was calculated from appropriate dose-response curves.

Fluorescent microscop assay. U2OS osteosacroma cancer cells were plated into 384 wells PerkinElmer CellCarrier plate in densities 2000 cells per well and left overnight in incubator. Next day live cells were exposed to 10 M compound concentration for 30 min. Live cell images were captured with the aid of Yokogawa CellVoyager7000 automated microscope with 60x water immersion objective. Cells were illuminated with 488 nm and 561 nm lasers and images were acquired respectively with 525/50 nm and 620/70 nm band pass filters

Experimental procedures:

Preparation of 2-(methoxycarbonyl)-3-nitrobenzoic acid (2):

3-Nitrophtalic anhydride (10 g) was dissolved in methanol (30 mL) under boiling and subsequently refluxed for 16 hours. Methanol was removed *in vacuo* and the residue (white solid compound) was recrystallized from water. If the compound purity was insufficient the recrystallization was repeated.

Preparation of 3-amino-2-(methoxycarbonyl)benzoic acid (3):

The compound **2** (0.57 g) and 10% Pd/C (0.057 g) were mixed with methanol (15 mL) and the reaction mixture was kept under the hydrogen atmosphere for 2 hours. The reaction mixture was filtered and evaporated *in vacuo*. The resulting compound was purified by silica gel column chromatography (Hex:EtOAc 7:3).

Preparation of *N*-propyl-3-nitrophtalic anhydride (5):

The compound **2** (2 g, 8.9 mmol) was mixed with thionylchloride (10 mL) and the reaction mixture was stirred at 35-40°C to obtain the yellow limpid solution. The mixture is concentrated and the residue dissolved in dry toluene (2 mL) and again concentrated. This process is repeated. The residue (white solid compound) was dissolved in dry THF (15 mL) and added in several portions to the solution of propylamine (0.73 mL, 8.9 mmol) and TEA (1.6 mL, 11.5 mmol) in dry THF (20 mL). After 2 hours of stirring the mixture was diluted with water (50 mL) and extracted with EtAc (3x 25 mL). The combined organic layers were washed with saturated $NaHCO_3$ (aq.), water and brine and finally concentrated *in vacuo*.

Preparation of 2-nitro-6-(propylcarbamoyl)benzoic acid (6):

The compound **5** (1.5 g) was added to the 10% NaOH solution in methanol (20 mL). The reaction mixture was refluxed for 2 hours and then concentrated *in vacuo*. The residue was dissolved in water and adjusted to pH 3 with hydrochloric acid. The resulting suspension was filtered and washed with water.

Preparation of dimethyl 3-nitrophthalate (8):

The compound **2** (2 g) was mixed with thionylchloride (8 mL) and the reaction mixture was stirred at 35-40°C until the yellow limpid solution is formed. The evaporation of thionylchloride yielded the white solid compound which was dissolved in methanol (15 mL) and refluxed for 4 hours. The reaction mixture was cooled down to room temperature, diluted with water (30 mL) and extracted with EtAc (3x 15 mL). The combined organic layers were washed with saturated $NaHCO_3$ (aq.), water and brine and concentrated *in vacuo* to give the white solid compound.

Preparation of dimethyl 3-aminophthalate (9):

The compound **8** (3.5 g) and 10% Pd/C (0.3 g) were mixed with methanol and the reaction mixture was kept under the hydrogen atmosphere for 2 hours. The reaction mixture was filtered and concentrated *in vacuo* to obtain yellowish viscous liquid.

Preparation of 3-aminophthalic acid (10):

The compound **9** (2 g) was mixed with 10% solution of NaOH in methanol (20 mL). The reaction mixture was refluxed for 2 hours and then concentrated *in vacuo*. The residue was dissolved in water, adjusted to pH 6 with hydrochloric acid. The resulting suspension was filtered and washed with water.

Preparation of 3-nitrophthalic acid (11):

The compound **8** (2 g) was added to the 10% NaOH solution in methanol (20 mL). The reaction mixture was heated under reflux for 2 hours and concentrated *in vacuo*. The residue was dissolved in water, adjusted to pH 3 with hydrochloric acid. The yielded suspension was filtered and washed with water.

Preparation of bis(2-oxo-2-phenylethyl) 3-nitrophthalate (12a):

The compound **11** (0.4 g, 1.9 mmol) was added to the solution of TEA (0.58 mL, 4.2 mmol) in DMF (5 mL). After 10 minutes of stirring bromoacetophenone (0.72 g, 3.6 mmol) was added and the reaction mixture was stirred for 2 hours at room temperature. Water was added and the formed precipitation was filtered off and washed with water. The dry crude product was suspended in methanol and filtered.

General synthesis methods of compounds 13a-g

3-Aminophtalic acid (**10**) (0.4 g, 2.2 mmol) was dissolved in the mixture of TEA (0.675 mL, 4.9 mmol) and DMF (10 mL) and stirred for 10 minutes. The bromoacetophenone (4.2 mmol) was added and the reaction mixture was stirred for 2 hours at room temperature (the precipitation was formed gradually). The reaction mixture was poured into the water (50 mL) and the precipitated compound was filtered off and washed with water thoroughly.
Purification of **13a**, **13c-e**: The dry crude product was suspended in methanol and filtered.
Purification of **13b**, **13f-g**: The dry crude product was suspended in ethanol and filtered.

Preparation of bis(2-(3-nitro-4-(piperidin-1-yl)phenyl)-2-oxoethyl) 3-aminophthalate (13h):

The compound **13g** (0.2 g, 0.35 mmol) was dissolved in solution of piperidine (0.42 mL, 4.05 mmol) and DMF (6 mL). The reaction mixture was stirred for 2 hours at room temperature and then poured into the water. The pH was adjusted to 5 with hydrochloric acid and the precipitated compound was filtered off and washed with water.

General synthesis methods of compounds 14a-f

The compound **13a-f** (200 mg) was dissolved in trifluoroacetic acid (3 mL) and the reaction mixture was refluxed for 2 hours (6 hours for compound **13b**). Trifluoracetic acid was evaporated and the residue was mixed with Et_2O, filtered and washed with Et_2O. The dry crude product was suspended in solution water:ethanol (1:1), warmed to boiling point, filtered hot and washed with water:ethanol (1:1) and Et_2O.

General synthesis methods of compounds 14g-h

The compound **13g-h** (0.2 g) was suspended in polyphosphoric acid (3 mL) and the reaction mixture was heated to 100°C. After 6 hours of heating the reaction mixture was poured into the ice-water and the formed crystals were filtered off and washed with water and Et_2O. The dry crude product was mixed with water:ethanol (1:1). The suspension was heated to boiling point, filtered hot, washed with water:ethanol (1:1) and Et_2O.

General synthesis methods of compounds 15a-f and 15h-i

The compound **14a-f** (0.2 g) was dissolved in 10% amine in DMF (2 mL). The reaction mixture was stirred for 2 hours at 50°C. After addition of water the yielded suspension was filtered off and washed with water.
Purification of **15a**, **15d**, **15e**, **15h**: The dry crude product was dissolved in ethanol, then water was added and the resulting precipitation was filtered off and washed with water.
Purification **15b**: The dry crude product was shortly boiled in EtAc, filtered and washed with Et_2O.

Purification of **15c**: The dry crude product was dissolved in EtOH and precipitated with Et_2O. The formed suspension was filtered and washed with Et_2O.
Purification of **15f**: The dry crude product was shortly boiled in Et_2O and filtered.
Purification of **15i**: The dry crude product was purified by silica gel column chromatography (EtAc:Tol /1:1).

Preparation of compound 15g

The compound **14b** (0.2 g) was mixed with 2-aminoethanol (2 mL) and the reaction mixture was stirred for 2 hours at 50°C. The reaction mixture was poured into water and the resulting precipitation was filtered off and washed with water. The dry crude product was suspended in Et_2O, filtered and washed with Et_2O.

Preparation of compound 15l

The compound **14b** (0.2 g) was mixed with saturated solution of ammonia in methanol (2 mL) and with DMF (2 mL). The reaction mixture was stirred for 2 hours at 50°C, water was added and pH was adjusted to 7 with hydrochloric acid. The formed suspension was filtered off and washed with water. The dry crude product was suspended in methanol, filtered and washed with Et_2O.

General synthesis methods of compounds 16a-b

The compound **14** (0.2 g) was mixed with 0.25M NaOH in metanol (6 mL). The reaction mixture was refluxed for 1 hour and cooled down to room temperature. The precipitated crystals were filtered off and washed with small amount of cold methanol.

Analytical data:

2-(Methoxycarbonyl)-3-nitrobenzoic acid (2):

Yield 8.32 g (71 %). ^{1}H NMR (400 MHz, DMSO-d_6) δ ppm 8.41 (dd, *J*=1.3, 8.3 Hz, 1 H), 8.32 (dd, *J*=1.1, 7.7 Hz, 1 H), 7.87 (t, *J*=7.9 Hz, 1 H), 3.85 (s, 3 H). ^{13}C NMR (101MHz, DMSO-d_6) δ ppm 165.4, 165.2, 146.1, 135.7, 131.4, 131.1, 129.4, 128.3, 53.2.

3-Amino-2-(methoxycarbonyl)benzoic acid (3):

Yield 0.24 g (48 %). ^{1}H NMR (400MHz, DMSO-d_6) δ ppm 7.26 - 7.15 (m, 1 H), 6.87 (dd, *J*=1.2, 8.2 Hz, 1 H), 6.82 (dd, *J*=1.2, 7.4 Hz, 1 H), 5.78 (br. s., 2 H), 3.71 (s, 3 H). ^{13}C NMR (101MHz, DMSO-d_6) δ ppm 169.3, 168.2, 147.8, 134.5, 131.2, 118.6, 116.1, 113.0, 51.9.

***N*-Propyl-3-nitrophtalic anhydride (5):**

Yield 1.41 g (68 %). ^{1}H NMR (400MHz ,DMSO-d_6) δ ppm 7.45 - 7.38 (m, 1 H), 7.00 - 6.92 (m, 2 H), 6.44 (br. s., 2 H), 3.45 (t, *J*=7.2 Hz, 2 H), 1.56 (sxt, *J*=7.3 Hz, 2 H), 0.84 (t, *J*=7.5 Hz, 3 H). ^{13}C NMR (101MHz, DMSO-d_6) δ ppm 169.5, 168.1, 146.4, 135.0, 132.3, 121.3, 110.6, 108.9, 38.5, 21.4, 11.2.

2-Nitro-6-(propylcarbamoyl)benzoic acid (6):

Yield 1.53 g (95 %). ^{1}H NMR (400MHz, DMSO-d_6) δ ppm 13.64 (br. s., 1 H), 8.81 - 8.60 (m, 1 H), 8.12 (d, *J*=7.5 Hz, 1 H), 7.86 (d, *J*=7.0 Hz, 1 H), 7.73 (t, *J*=7.9 Hz, 1 H), 3.24 - 3.13 (m, 2 H), 1.51 (sxt, *J*=7.3 Hz, 2 H), 0.90 (t, *J*=7.5 Hz, 3 H). ^{13}C NMR (101MHz, DMSO-d_6) δ ppm 165.8, 165.6, 147.0, 137.1, 132.5, 130.3, 128.2, 125.1, 41.0, 22.2, 11.4.

Dimethyl 3-nitrophthalate (8):

Yield 1.82 g (86 %). ^{1}H NMR (400MHz, DMSO-d_6) δ ppm 8.45 (dd, *J*=1.1, 8.1 Hz, 1 H), 8.34 (dd, *J*=1.3, 7.9 Hz, 1 H), 7.90 (t, *J*=8.1 Hz, 1 H), 3.88 (s, 3 H), 3.88 (s, 3 H). ^{13}C NMR (101MHz, DMSO-d_6) δ ppm 165.1, 164.1, 146.1, 135.7, 131.6, 129.5, 129.3, 128.8, 53.3.

Dimethyl 3-aminophthalate (9):

Yield 3.01 g (98 %). ^{1}H NMR (400MHz, DMSO-d_6) δ ppm 7.27 - 7.22 (m, 1 H), 6.92 (dd, *J*=0.9, 8.3 Hz, 1 H), 6.75 (dd, *J*=1.1, 7.2 Hz, 1 H), 6.09 (s, 2 H), 3.75 (s, 3 H), 3.74 (s, 3 H). ^{13}C NMR (101MHz, DMSO-d_6) δ ppm 168.6, 167.6, 148.7, 133.6, 131.8, 119.0, 115.6, 111.0, 52.3, 52.0.

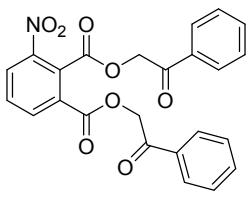
3-Aminophthalic acid (10):

Yield 1.44 g (81 %). ^{1}H NMR (400MHz, DMSO-d_6) δ ppm 7.18 (dd, *J*=7.5, 8.3 Hz, 1 H), 6.84 (dd, *J*=0.9, 8.3 Hz, 1 H), 6.67 (dd, *J*=1.1, 7.2 Hz, 1 H). ^{13}C NMR (101MHz, DMSO-d_6) δ ppm 170.0, 169.1, 148.7, 135.8, 131.3, 118.1, 115.2, 111.9.

3-Nitrophthalic acid (11):

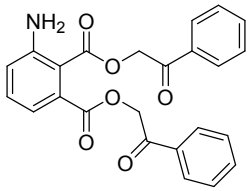
Yield 1.64 g (93 %). ^{1}H NMR (400MHz, DMSO-d_6) δ ppm 8.17 (dd, *J*=1.3, 7.9 Hz, 1 H), 7.86 (dd, *J*=1.3, 8.3 Hz, 1 H), 7.59 (t, *J*=7.9 Hz, 1 H). ^{13}C NMR (101MHz, DMSO-d_6) δ ppm 166.8, 166.1, 151.0, 134.5, 134.0, 132.9, 129.1, 125.8.

Bis(2-oxo-2-phenylethyl) 3-nitrophthalate (12a):



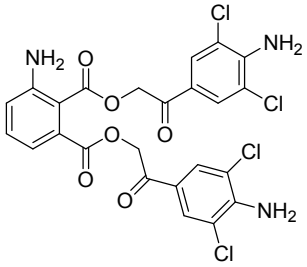
Yield 0,58 g (72 %). ^{1}H NMR (400MHz, DMSO-d_6) δ ppm 8.54 (dd, *J*=1.3, 8.3 Hz, 1 H), 8.49 (dd, *J*=1.3, 7.9 Hz, 1 H), 8.05 - 7.96 (m, 5 H), 7.75 - 7.65 (m, 2 H), 7.61 - 7.50 (m, 4 H), 5.85 (s, 2 H), 5.68 (s, 2 H). ^{13}C NMR (101MHz, DMSO-d_6) δ ppm 191.8, 191.8, 163.9, 163.3, 146.5, 135.7, 134.2, 134.1, 133.9, 133.6, 132.2, 129.3, 129.2, 129.0, 128.9, 128.6, 128.0, 127.9, 68.4, 68.2.

Bis(2-oxo-2-phenylethyl) 3-aminophthalate (13a):



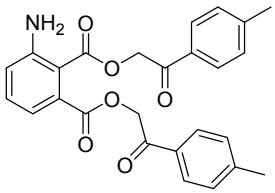
Yield 0.61 g (70 %). ^{1}H NMR (400MHz, DMSO-d_6) δ ppm 8.06 - 7.98 (m, 4 H), 7.76 - 7.67 (m, 2 H), 7.63 - 7.54 (m, 4 H), 7.39 - 7.32 (m, 1 H), 7.05 - 6.99 (m, 2 H), 6.29 (br. s., 2 H), 5.71 (s, 2 H), 5.65 (s, 2 H). ^{13}C NMR (101MHz, DMSO-d_6) δ ppm 193.5, 192.6, 166.7, 166.5, 148.2, 134.2, 133.9, 133.8, 133.6, 131.6, 131.6, 128.9, 128.9, 127.9, 127.7, 119.5, 116.2, 112.1, 67.2, 67.0. HRMS: Calcd for $C_{24}H_{19}NO_6$ = 417.1212, Found m/z 417.1208.

Bis(2-(4-amino-3,5-dichlorophenyl)-2-oxoethyl) 3-aminophthalate (13b):



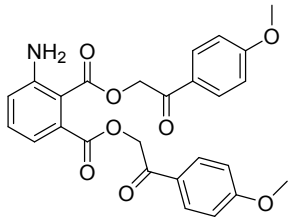
Yield 0.83 g (68 %). ^{1}H NMR (400MHz, DMSO-d_6) δ ppm 7.90 (s, 2 H), 7.86 (s, 2 H), 7.33 (t, *J*=8.0 Hz, 1 H), 7.02 - 6.97 (m, 2 H), 6.63 (s, 2 H), 6.58 (s, 2 H), 6.25 (br. s, 2 H), 5.57 (s, 2 H), 5.51 (s, 2 H). ^{13}C NMR (101MHz, DMSO-d_6) δ ppm 189.8, 188.9, 166.6, 148.2, 146.3, 146.1, 131.5, 131.5, 128.4, 128.2, 122.3, 121.9, 119.5, 117.4, 117.4, 116.3, 112.6, 66.6, 66.5. HRMS: Calcd for $C_{24}H_{17}N_3O_6$ = 582.9871, Found m/z 582.9874.

Bis(2-oxo-2-(p-tolyl)ethyl) 3-aminophthalate (13c):



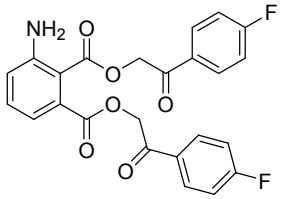
Yield 0.78 g (84 %). ^{1}H NMR (400MHz, DMSO-d_6) δ ppm7.95 - 7.86 (m, 4 H), 7.42 - 7.30 (m, 5 H), 7.04 - 7.00 (m, 2 H), 6.28 (br. s, 2 H), 5.66 (s, 2 H), 5.61 (s, 2 H), 2.40 (s, 3 H), 2.40 (s, 3 H). ^{13}C NMR (101MHz, DMSO-d_6) δ ppm 193.0, 192.0, 166.6, 166.5, 148.1, 144.7, 144.4, 131.5, 131.5, 131.4, 131.1, 129.4, 129.4, 128.0, 127.8, 119.4, 116.2, 112.3, 67.0, 66.9, 21.2, 21.2. HRMS: Calcd for $C_{26}H_{23}NO_6$ = 445.1525, Found m/z 445,1527.

Bis(2-(4-methoxyphenyl)-2-oxoethyl) 3-aminophthalate (13d):



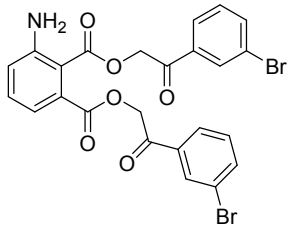
Yield 0.65 g (65 %). ^{1}H NMR (400MHz, DMSO-d_6) δ ppm 8.03 - 7.95 (m, 4 H), 7.34 (t, *J*=8.0 Hz, 1 H), 7.13 - 7.07 (m, 4 H), 7.05 - 6.99 (m, 2 H), 6.27 (br. s, 2 H), 5.64 (s, 2 H), 5.58 (s, 2 H), 3.87 (s, 3 H), 3.86 (s, 3 H). ^{13}C NMR (101MHz, DMSO-d_6) δ ppm 191.8, 190.8, 166.6, 166.5, 163.8, 163.6, 148.0, 131.4, 131.3, 130.3, 130.1, 126.7, 126.4, 119.4, 116.2, 114.1, 114.1, 112.7, 66.8, 66.7, 55.6, 55.6. HRMS: Calcd for $C_{26}H_{23}NO_8$ = 477.1424, Found m/z 477.1425.

Bis(2-(4-fluorophenyl)-2-oxoethyl) 3-aminophthalate (13e):



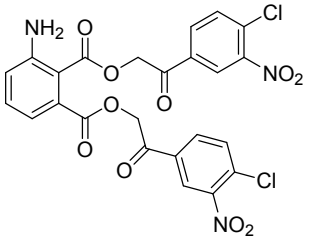
Yield 0.78 g (82 %). ^{1}H NMR (400MHz, DMSO-d_6) δ ppm 8.16 - 8.05 (m, 4 H), 7.46 - 7.38 (m, 4 H), 7.38 - 7.31 (m, 1 H), 7.05 - 6.98 (m, 2 H), 6.28 (br. s., 2 H), 5.69 (s, 2 H), 5.63 (s, 2 H). ^{13}C NMR (101MHz, DMSO-d_6) δ ppm 192.2, 191.3, 166.8, 166.6, 165.5 (d, *J*=247 Hz, 1 C), 165,3 (d, *J*=240 Hz, 1 C), 148.3, 131.7, 131.2, 131.1, 131.0, 130.9, 130.7, 130.5, 130.4, 119.6, 116.3, 116.2, 116.2, 116.0, 115.9, 112.1, 67.1, 67.0. HRMS: Calcd for $C_{24}H_{17}F_2NO_6$ = 453.1024, Found m/z 453.1026.

Bis(2-(3-bromophenyl)-2-oxoethyl) 3-aminophthalate (13f):



Yield 0.92 g (77 %). ^{1}H NMR (400MHz, DMSO-d_6) δ ppm 8.17 (t, *J*=1.8 Hz, 1 H), 8.13 (t, *J*=1.8 Hz, 1 H), 8.02 (td, *J*=1.3, 7.9 Hz, 1 H), 7.99 (td, *J*=1.4, 7.7 Hz, 1 H), 7.95 - 7.89 (m, 2 H), 7.59 - 7.51 (m, 2 H), 7.39 - 7.33 (m, 1 H), 7.03 (dd, *J*=0.9, 8.3 Hz, 1 H), 6.99 (dd, *J*=1.1, 7.2 Hz, 1 H), 6.29 (br. s., 2 H), 5.70 (s, 2 H), 5.65 (s, 2 H). ^{13}C NMR (101MHz, DMSO-d_6) δ ppm 192.6, 191.8, 166.8, 166.4, 148.5, 136.8, 136.6, 135.9, 135.7, 131.9, 131.8, 131.2, 131.2, 130.5, 130.4, 127.0, 126.9, 122.3, 122.3, 119.6, 116.2, 111.6, 67.2, 67.1. HRMS: Calcd for $C_{24}H_{17}Br_2NO_6$ = 572.9423, Found m/z 572.9417.

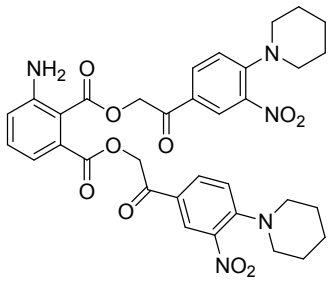
Bis(2-(4-chloro-3-nitrophenyl)-2-oxoethyl) 3-aminophthalate (13g):



Yield 0.82 g (68 %). ^{1}H NMR (400MHz, DMSO-d_6) δ ppm8.63 (d, *J*=2.2 Hz, 1 H), 8.60 (d, *J*=2.2 Hz, 1 H), 8.31 - 8.22 (m, 2 H), 8.02 (s, 1 H), 8.00 (s, 1 H), 7.40 - 7.32 (m, 1 H), 7.05 - 7.00 (m, 1 H), 6.98 (dd,

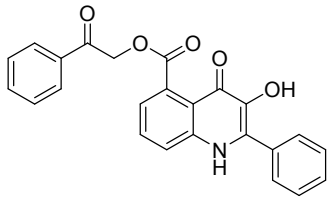
J=0.9, 7.5 Hz, 1 H), 6.29 (br. s, 2 H), 5.72 (s, 2 H), 5.68 (s, 2 H). ^{13}C NMR (101MHz, DMSO-d_6) δ ppm 192.0, 191.3, 167.3, 166.8, 149.1, 148.4, 148.4, 134.0, 133.9, 133.1, 133.0, 132.9, 132.9, 132.4, 132.4, 130.7, 130.6, 125.3, 125.2, 120.1, 116.7, 111.6, 67.7, 67.6. HRMS: Calcd for $C_{24}H_{15}Cl_2N_3O_{10}$ = 575.0134, Found m/z 575.0134.

Bis(2-(3-nitro-4-(piperidin-1-yl)phenyl)-2-oxoethyl) 3-aminophthalate (13h):



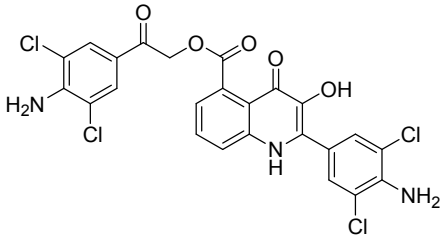
Yield 0.21 mg (87 %). ^{1}H NMR (400MHz, DMSO-d_6) δ ppm 8.36 (d, *J*=2.3 Hz, 1 H), 8.33 (d, *J*=2.3 Hz, 1 H), 8.07 - 8.00 (m, 2 H), 7.37 - 7.30 (m, 3 H), 7.04 - 6.97 (m, 2 H), 6.27 (br. s, 2 H), 5.63 (s, 2 H), 5.57 (s, 2 H), 3.17 (br. s., 8 H), 1.61 (br. s., 12 H). ^{13}C NMR (101MHz, DMSO-d_6) δ ppm 190.6, 189.7, 166.7, 166.5, 148.8, 148.7, 148.3, 138.4, 138.4, 132.7, 132.6, 131.6, 127.2, 127.0, 123.5, 123.1, 119.8, 119.8, 119.5, 116.3, 112.3, 66.8, 66.7, 51.1, 51.1, 25.2, 23.2. HRMS: Calcd for $C_{34}H_{35}N_5O_{10}$ = 673.2384, Found m/z 673.2376.

2-Oxo-2-phenylethyl 2-phenyl-3-hydroxyquinoline-4(1*H*)-one-5-carboxylate (14a):



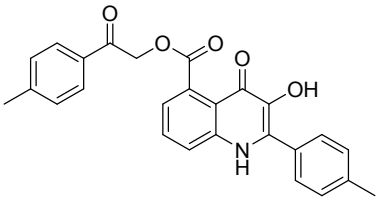
Yield 168 mg (88 %). ^{1}H NMR (400MHz, DMSO-d_6) δ ppm 11.84 (s, 1 H), 8.70 (br. s, 1 H), 8.09 - 8.02 (m, 2 H), 7.89 - 7.78 (m, 3 H), 7.76 - 7.65 (m, 2 H), 7.65 - 7.49 (m, 5 H), 7.31 (dd, *J*=0.9, 7.0 Hz, 1 H), 5.66 (s, 2 H). ^{13}C NMR (101MHz, DMSO-d_6) δ ppm 193.1, 169.2, 168.8, 138.4, 138.0, 134.1, 134.0, 132.0, 131.9, 131.6, 130.0, 129.4, 129.3, 129.0, 128.4, 127.9, 120.8, 120.1, 118.1, 67.1. HRMS: Calcd for $C_{24}H_{17}NO_5$ = 399.1107, Found m/z 399.1101.

2-(4-Amino-3,5-dichlorophenyl)-2-oxoethyl 2-(4-amino-3,5-dichlorophenyl)-3-hydroxyquinoline-4(1*H*)-one-5-carboxylate (14b):



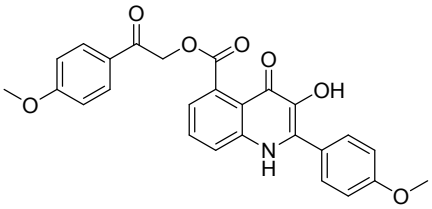
Yield 169 mg (87 %). ^{1}H NMR (400MHz, DMSO-d_6) δ ppm 11.62 (s, 1 H), 7.90 (s, 2 H), 7.83 (dd, *J*=0.8, 8.6 Hz, 1 H), 7.79 (s, 2 H), 7.70 - 7.62 (m, 1 H), 7.28 (dd, *J*=0.8, 7.0 Hz, 1 H), 6.59 (br. s, 2 H), 6.05 (br. s., 2 H), 5.51 (s, 2 H). ^{13}C NMR (101MHz, DMSO-d_6) δ ppm 189.3, 169.0, 168.4, 146.0, 142.1, 138.0, 137.8, 131.5, 129.9, 129.6, 128.6, 128.3, 122.4, 120.6, 119.8, 119.7, 117.8, 117.3, 117.3, 66.6. HRMS: Calcd for $C_{24}H_{15}Cl_4N_3O_5$ = 564.9766 Found m/z 564.9758.

2-Oxo-2-(*p*-tolyl)ethyl 2-(*p*-tolyl)-3-hydroxyquinoline-4(1*H*)-one-5-carboxylate (14c):



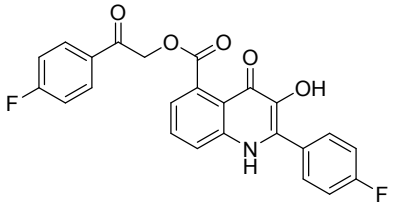
Yield 178 mg (93 %). ^{1}H NMR (400MHz, TFA-d_1) δ ppm 8.94 (d, *J*=7.4 Hz, 1 H), 8.42 (d, *J*=8.6 Hz, 1 H), 7.98 (t, *J*=8.0 Hz, 1 H), 7.93 (d, *J*=8.6 Hz, 2 H), 7.82 (d, *J*=8.2 Hz, 2 H), 7.44 (d, *J*=7.8 Hz, 2 H), 7.38 (d, *J*=8.2 Hz, 2 H), 5.98 (s, 2 H), 2.45 (s, 3 H), 2.44 (s, 3 H). ^{13}C NMR (101MHz, TFA-d_1) δ ppm 197.7, 172.9, 158.1, 151.0, 147.3, 145.8, 140.6, 139.1, 138.2, 133.3, 132.0, 131.9, 131.7, 130.9, 130.4, 129.7, 126.4, 126.0, 118.8, 70.7, 22.2, 21.9. HRMS: Calcd for $C_{26}H_{21}NO_5$ = 427.1420 Found m/z 427.1418.

2-(4-Methoxyphenyl)-2-oxoethyl 2-(4-methoxyphenyl)-3-hydroxyquinoline-4(1*H*)-one-5-carboxylate (14d):



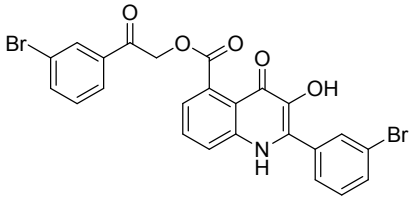
Yield 162 mg (84 %). ^{1}H NMR (400MHz, DMSO-d_6) δ ppm 11.71 (s, 1 H), 8.51 (br. s., 1 H), 8.06 - 7.99 (m, 2 H), 7.84 (dd, *J*=1.0, 8.6 Hz, 1 H), 7.82 - 7.76 (m, 2 H), 7.70 - 7.63 (m, 1 H), 7.30 (dd, *J*=1.0, 7.0 Hz, 1 H), 7.16 - 7.12 (m, 2 H), 7.12 - 7.08 (m, 2 H), 5.59 (s, 2 H), 3.87 (s, 3 H), 3.85 (s, 3 H). ^{13}C NMR (101MHz, DMSO-d_6) δ ppm 191.3, 169.2, 168.5, 163.6, 160.1, 138.0, 137.9, 131.7, 131.7, 130.7, 130.3, 129.8, 127.0, 124.1, 120.7, 119.9, 117.9, 114.2, 113.8, 66.8, 55.6, 55.4. HRMS: Calcd for $C_{26}H_{21}NO_7$ = 459.1318 Found m/z 459.1315.

2-(4-Fluorophenyl)-2-oxoethyl 2-(4-fluorophenyl)-3-hydroxyquinoline-4(1*H*)-one-5-carboxylate (14e):



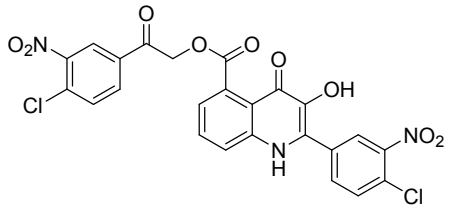
Yield 173 mg (90 %). ^{1}H NMR (400MHz, DMSO-d_6) δ ppm 11.83 (s, 1 H), 8.67 (br. s., 1 H), 8.18 - 8.10 (m, 2 H), 7.91 - 7.85 (m, 2 H), 7.83 (dd, *J*=0.9, 7.5 Hz, 1 H), 7.73 - 7.65 (m, 1 H), 7.47 - 7.38 (m, 4 H), 7.30 (dd, *J*=0.9, 7.0 Hz, 1 H), 5.64 (s, 2 H). ^{13}C NMR (101MHz, DMSO-d_6) δ ppm 191.8, 169.1, 168.7, 165.2 (d, *J*=291 Hz, 1 C), 164.1, 161.3, 162.7 (d, *J*=287 Hz, 1 C), 138.3, 137.9, 131.7, 131.6, 131.6, 131.1, 131.0, 130.9, 130.9, 130.9, 130.0, 128.3, 128.3, 120.8, 120.0, 118.1, 116.1 (d, *J*=22 Hz, 1 C), 115.3 (d, *J*=22 Hz, 1 C), 67.0. HRMS: Calcd for $C_{24}H_{15}F_2NO_5$ = 435.0918 Found m/z 435.0919.

2-(3-Bromophenyl)-2-oxoethyl 2-(3-bromophenyl)-3-hydroxyquinoline-4(1*H*)-one-5-carboxylate (14f):



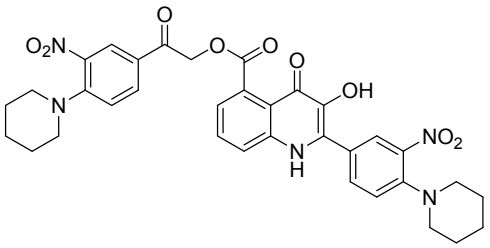
Yield 184 mg (95 %). ^{1}H NMR (400MHz, DMSO-d_6) δ ppm 11.86 (s, 1 H), 8.82 (br. s., 1 H), 8.17 (t, *J*=1.8 Hz, 1 H), 8.05 (d, *J*=7.9 Hz, 1 H), 8.00 (t, *J*=1.8 Hz, 1 H), 7.95 - 7.90 (m, 1 H), 7.84 (s, 1 H), 7.82 (s, 1 H), 7.77 - 7.72 (m, 1 H), 7.72 - 7.65 (m, 1 H), 7.60 - 7.50 (m, 2 H), 7.29 (d, *J* = 6.1 Hz, 1 H), 5.65 (s, 2 H). ^{13}C NMR (101MHz, DMSO-d_6) δ ppm 192.3, 169.1, 168.8, 138.5, 138.0, 136.5, 136.1, 134.1, 132.1, 131.7, 131.5, 131.2, 130.5, 130.4, 130.2, 130.1, 128.5, 127.0, 122.3, 121.5, 120.8, 120.1, 118.1, 67.2. HRMS: Calcd for $C_{24}H_{15}Br_2NO_5$ = 554.9317 Found m/z 554.9315.

2-(4-Chloro-3-nitrophenyl)-2-oxoethyl 2-(4-chloro-3-nitrophenyl)-3-hydroxyquinoline-4(1*H*)-one-5-carboxylate (14g):



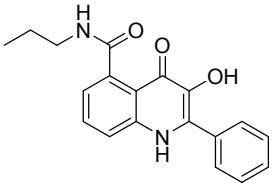
Yield 157 mg (81 %). ^{1}H NMR (400MHz, DMSO-d_6) δ ppm 11.97 (s, 1 H), 9.11 (br. s., 1 H), 8.65 (d, *J*=2.2 Hz, 1 H), 8.53 (d, *J*=2.2 Hz, 1 H), 8.31 (dd, *J*=2.0, 8.6 Hz, 1 H), 8.15 (dd, *J*=2.0, 8.6 Hz, 1 H), 8.03 (s, 1 H), 8.00 (s, 1 H), 7.82 (d, *J*=8.3 Hz, 1 H), 7.76 - 7.67 (m, 1 H), 7.31 (d, *J* = 6.6 Hz, 1 H), 5.70 (s, 2 H). ^{13}C NMR (101MHz, DMSO-d_6) δ ppm 191.3, 169.0, 147.9, 147.4, 138.9, 138.1, 134.6, 133.7, 132.8, 132.4, 132.1, 131.6, 131.4, 130.5, 130.1, 128.4, 126.2, 125.6, 124.9, 121.0, 120.2, 118.2, 112.1, 67.3. HRMS: Calcd for $C_{24}H_{13}Cl_2N_3O_9$ = 557.0029 Found m/z 557.0020.

2-(3-Nitro-4-(piperidin-1-yl)phenyl)-2-oxoethyl 2-(3-nitro-4-(piperidin-1-yl)phenyl)- 3-hydroxy-quinoline-4(1*H*)-one-5-carboxylate (14h):



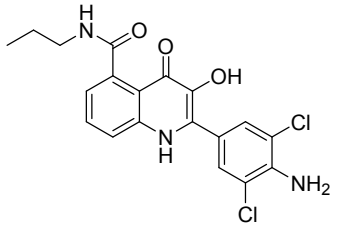
Yield 154 mg (79 %). ^{1}H NMR (400MHz, DMSO-d_6) δ ppm 11.78 (s, 1 H), 8.80 (br. s., 1 H), 8.37 (d, *J*=2.2 Hz, 1 H), 8.28 (d, *J*=1.3 Hz, 1 H), 8.09 (dd, *J*=1.8, 8.8 Hz, 1 H), 8.00 (d, *J*=8.3 Hz, 1 H), 7.82 (d, *J*=8.3 Hz, 1 H), 7.68 (t, *J*=7.7 Hz, 1 H), 7.44 (d, *J*=8.8 Hz, 1 H), 7.35 (d, *J*=8.8 Hz, 1 H), 7.30 (d, *J*=7.0 Hz, 1 H), 5.58 (s, 2 H), 3.18 (br. s., 4 H), 3.08 (br. s., 4 H), 1.61 (br. s., 12 H). ^{13}C NMR (101MHz, DMSO-d_6) δ ppm 190.2, 169.1, 168.6, 148.7, 146.2, 140.3, 138.5, 138.4, 137.9, 134.3, 132.8, 131.6, 130.1, 129.7, 127.1, 126.7, 123.7, 122.9, 120.8, 120.4, 120.0, 119.9, 118.0, 66.8, 51.8, 51.1, 25.4, 25.2, 23.4, 23.2. HRMS: Calcd for $C_{34}H_{33}N_5O_9$ = 655.2278 Found m/z 655.2270

***N*-Propyl-2-phenyl-3-hydroxyquinoline-4(1*H*)-one-5-carboxamide (15a):**



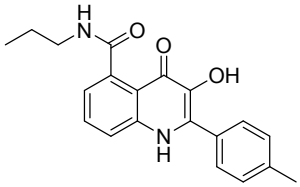
Yield 57 mg (35 %). ^{1}H NMR (400MHz, DMSO-d_6) δ ppm 11.54 (s, 1 H), 8.44 (br. s., 1 H), 7.91 (t, *J*=5.5 Hz, 1 H), 7.82 - 7.78 (m, 2 H), 7.72 (dd, *J*=0.9, 8.3 Hz, 1 H), 7.61 - 7.50 (m, 4 H), 7.02 (dd, *J*=1.3, 7.0 Hz, 1 H), 3.24 - 3.14 (m, 2 H), 1.57 (sxt, *J*=7.3 Hz, 2 H), 0.93 (t, *J*=7.5 Hz, 3 H). ^{13}C NMR (101MHz, DMSO-d_6) δ ppm 169.7, 166.4, 138.1, 138.0, 135.9, 134.0, 131.4, 130.0, 129.8, 129.5, 128.4, 123.0, 120.0, 117.6, 41.3, 22.1, 11.7. HRMS: Calcd for $C_{19}H_{18}N_2O_3$ = 322.1317 Found m/z 322.1317.

***N*-Propyl-2-(4-amino-3,5-dichlorophenyl)-3-hydroxyquinoline-4(1*H*)-one-5-carboxamide (15b)**



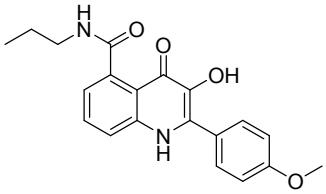
Yield 64 mg (45 %). ^{1}H NMR (400MHz, DMSO-d_6) δ ppm 11.35 (s, 1 H), 7.91 (t, *J*=5.5 Hz, 1 H), 7.78 (s, 2 H), 7.71 (d, *J*=8.8 Hz, 1 H), 7.53 (dd, *J*=7.0, 8.8 Hz, 1 H), 7.00 (d, *J*=7.0 Hz, 1 H), 6.02 (br. s., 2 H), 3.23 - 3.13 (m, 2 H), 1.56 (sxt, *J*=7.3 Hz, 2 H), 0.92 (t, *J*=7.2 Hz, 3 H). ^{13}C NMR (101MHz, DMSO-d_6) δ ppm 169.6, 168.9, 141.9, 138.3, 138.0, 137.4, 129.7, 128.4, 128.0, 120.8, 119.9, 118.5, 117.8, 117.4, 41.0, 22.1, 11.6. Calcd for $C_{19}H_{17}Cl_2N_3O_3$ = 405.0647 Found m/z 405.0644.

***N*-Propyl-2-(*p*-tolyl)-3-hydroxyquinoline-4(1*H*)-one-5-carboxamide (15c):**



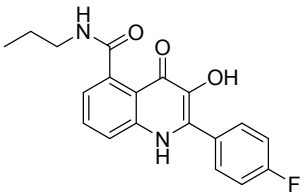
Yield 101 g (64 %). ^{1}H NMR (400MHz, DMSO-d_6) δ ppm 12.80 (br. s., 1 H), 8.51 (br. s., 1 H), 8.03 (d, *J*=8.8 Hz, 1 H), 7.76 (d, *J*=8.3 Hz, 2 H), 7.68 (t, *J*=7.0 Hz, 1 H), 7.41 (d, *J*=7.9 Hz, 1 H), 7.34 (d, *J*=7.0 Hz, 1 H), 3.32 - 3.19 (m, 2 H), 2.42 (s, 3 H), 1.59 (sxt, *J*=7.3 Hz, 2 H), 0.94 (t, *J*=7.5 Hz, 3 H). ^{13}C NMR (101MHz, DMSO-d_6) δ ppm 169.7, 165.1, 139.8, 137.9, 137.7, 135.5, 135.3, 130.0, 129.5, 128.9, 128.2, 123.7, 120.4, 117.4, 41.4, 22.1, 21.1, 11.7. Calcd for $C_{20}H_{20}N_2O_3$ = 336.1474 Found m/z 336.1464.

***N*-Propyl-2-(4-Methoxyphenyl)-3-hydroxyquinoline-4(1*H*)-one-5-carboxamide (15d):**



Yield 62 mg (40 %). ^{1}H NMR (400MHz, DMSO-d_6) δ ppm 12.21 (br. s., 1 H), 8.27 (br. s., 1 H), 7.90 (dd, *J*=0.9, 8.8 Hz, 1 H), 7.84 - 7.78 (m, 2 H), 7.66 - 7.57 (m, 1 H), 7.21 (dd, *J*=0.9, 7.0 Hz, 1 H), 7.17 - 7.11 (m, 2 H), 3.85 (s, 3 H), 3.28 - 3.17 (m, 2 H), 1.65 - 1.51 (m, 1 H), 0.93 (t, *J*=7.2 Hz, 3 H). ^{13}C NMR (101MHz, DMSO-d_6) δ ppm 169.7, 166.6, 160.3, 138.0, 137.8, 136.1, 133.3, 130.9, 129.8, 123.6, 122.5, 119.7, 117.6, 113.8, 55.4, 41.3, 22.1, 11.7. Calcd for $C_{20}H_{20}N_2O_4$ = 352.1423 Found m/z 352.1412.

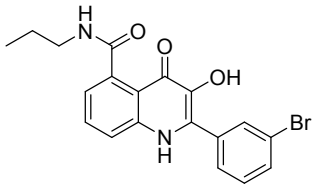
***N*-Propyl-2-(4-fluorophenyl)-3-hydroxyquinoline-4(1*H*)-one-5-carboxamide (15e):**



Yield 48 g (31 %). ^{1}H NMR (400MHz, DMSO-d_6) δ ppm 11.55 (br. s., 1 H), 7.92 (t, *J*=4.8 Hz, 1 H), 7.86 (dd, *J*=5.7, 8.8 Hz, 2 H), 7.71 (d, *J*=8.3 Hz, 1 H), 7.55 (t, *J*=7.5 Hz, 1 H), 7.48 - 7.35 (m, 2 H), 7.02 (d, *J*=6.6 Hz, 1 H), 3.20 (q, *J*=6.1 Hz, 2 H), 1.57 (sxt, *J*=7.3 Hz, 2 H), 0.93 (t, *J*=7.2 Hz, 3 H). ^{13}C NMR (101MHz, DMSO-d_6) δ ppm 169.7, 169.3, 162.4 (d, *J*=247, 1 C), 138.4, 138.3, 137.5, 131.6, 131.5,

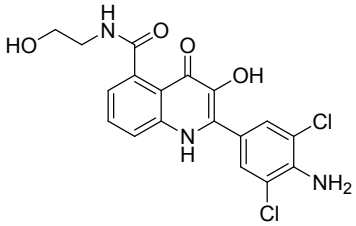
129.9, 129.3, 128.5, 121.0, 118.7, 118.1, 115.4, 115.2, 41.1, 22.2, 11.7. Calcd for $C_{19}H_{17}FN_2O_3$ = 340.1223 Found m/z 340.1221.

***N*-Propyl-2-(3-bromophenyl)-3-hydroxyquinoline-4(1*H*)-one-5-carboxamide (15f):**



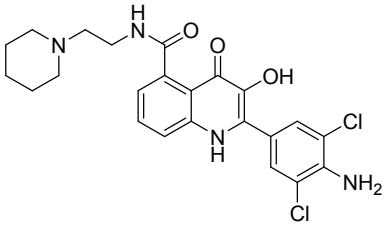
Yield 125 mg (81 %). ^{1}H NMR (400MHz, DMSO-d_6) δ ppm 11.56 (s, 1 H), 8.63 (br. s., 1 H), 7.99 (s, 1 H), 7.92 (t, *J*=5.5 Hz, 1 H), 7.82 (d, *J*=7.5 Hz, 1 H), 7.77 - 7.65 (m, 2 H), 7.61 - 7.48 (m, 2 H), 7.02 (d, *J*=6.6 Hz, 1 H), 3.20 (q, *J*=6.6 Hz, 1 H), 1.57 (sxt, *J*=7.3 Hz, 2 H), 0.93 (t, *J*=7.5 Hz, 3 H). ^{13}C NMR (101MHz, DMSO-d_6) δ = 169.6, 169.4, 138.5, 138.5, 137.6, 134.3, 131.9, 131.5, 130.5, 130.0, 128.4, 128.3, 121.5, 121.0, 118.7, 118.1, 41.1, 22.2, 11.7. Calcd for $C_{19}H_{17}BrN_2O_3$ = 400.0423 Found m/z 400.0413.

***N*-(2-Hydroxyethyl)-2-(4-amino-3,5-dichlorophenyl)-3-hydroxyquinoline-4(1*H*)-one-5-carboxamide (15g):**



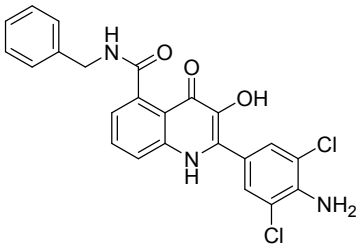
Yield 20 mg (35 %). ^{1}H NMR (400MHz, DMSO-d_6) δ ppm 11.47 (s, 1 H), 8.50 (br. s., 1 H), 7.92 (t, *J*=5.7 Hz, 1 H), 7.79 (s, 2 H), 7.73 (dd, *J*=0.9, 8.8 Hz, 1 H), 7.59 - 7.50 (m, 1 H), 7.04 (dd, *J*=0.9, 7.0 Hz, 1 H), 6.04 (s, 2 H), 4.71 (br. s., 1 H), 3.60 (t, *J*=6.1 Hz, 2 H), 3.32 (t, *J*=6.1 Hz, 2 H). ^{13}C NMR (101MHz, DMSO) δ ppm 169.9, 168.9, 142.0, 138.1, 138.0, 137.0, 129.7, 128.6, 128.5, 120.9, 119.7, 118.7, 117.7, 117.4, 59.8, 42.0. Calcd for $C_{18}H_{15}Cl_2N_3O_4$ = 407.0440 Found m/z 407.0431.

***N*-(2-(Piperidin-1-yl)ethyl)-2-(4-amino-3,5-dichlorophenyl)-3-hydroxyquinoline-4(1*H*)-one-5-carboxamide (15h):**



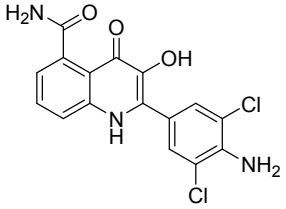
Yield 41 mg (24 %). ^{1}H NMR (400MHz, DMSO-d_6) δ ppm 11.35 (s, 1 H), 8.08 - 7.76 (m, 2 H), 7.69 (d, *J*=7.9 Hz, 1 H), 7.47 (t, *J*=7.7 Hz, 1 H), 6.99 (d, *J*=6.6 Hz, 1 H), 5.95 (br. s., 2 H), 3.67 - 3.20 (m, 6 H), 2.65 - 2.52 (m, 2 H), 1.63 - 1.44 (m, 4 H), 1.44 - 1.28 (m, 2 H). ^{13}C NMR (101MHz, DMSO-d_6) δ ppm 170.4, 142.3, 142.2, 142.2, 142.1, 138.7, 138.6, 137.2, 129.5, 128.9, 121.3, 118.4, 117.9, 117.9, 57.7, 54.3, 40.6, 31.1, 26.8. Calcd for $C_{23}H_{24}Cl_2N_4O_3$ = 474.1225 Found m/z 474.1223.

***N*-Benzyl-2-(4-amino-3,5-dichlorophenyl)-3-hydroxyquinoline-4(1*H*)-one-5-carboxamide (15i):**



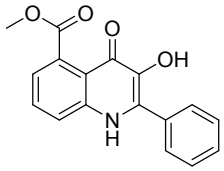
Yield 55 mg (34 %). ^{1}H NMR (400MHz, DMSO-d_6) δ ppm 11.39 (s, 1 H), 8.49 (t, *J* = 5.9 Hz, 1 H), 7.80 (s, 2 H), 7.74 (d, *J*=7.9 Hz, 1 H), 7.60 - 7.51 (m, 1 H), 7.46 (d, *J*=7.0 Hz, 2 H), 7.34 (t, *J*=7.7 Hz, 2 H), 7.29 - 7.21 (m, 1 H), 7.07 (d, *J* = 6.6 Hz, 1 H), 6.03 (br. s, 2 H), 4.49 (d, *J*=6.1 Hz, 2 H). ^{13}C NMR (101MHz, DMSO-d_6) δ ppm 169.7, 168.9, 142.0, 139.8, 138.3, 138.0, 136.9, 128.8, 128.4, 128.1, 128.1, 127.2, 126.4, 120.9, 119.8, 118.7, 117.8, 117.4, 42.5. Calcd for $C_{23}H_{17}Cl_2N_3O_3$ = 453.0647 Found m/z 4530637.

2-(4-Amino-3,5-dichlorophenyl)-3-hydroxyquinoline-4(1*H*)-one-5-carboxamide (15l):



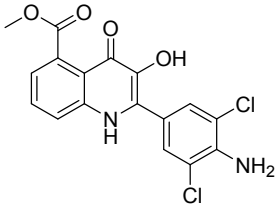
Yield 39 mg (30 %). ^{1}H NMR (400MHz, DMSO-d_6) δ ppm 11.34 (s, 1 H), 7.79 (s, 2 H), 7.70 (d, *J*=8.8 Hz, 1 H), 7.58 - 7.49 (m, 1 H), 7.44 (br. s., 1 H), 7.18 (br. s., 1 H), 7.03 (d, *J* = 6.1 Hz, 1 H), 6.03 (s, 2 H). ^{13}C NMR (101MHz, DMSO-d_6) δ ppm 171.6, 169.0, 142.0, 138.4, 138.0, 137.5, 129.8, 128.5, 128.0, 120.7, 119.9, 118.5, 117.5, 117.5. Calcd for $C_{16}H_{11}Cl_2N_3O_3$ = 363.0177 Found m/z 363,0175.

Methyl 2-phenyl-3-hydroxyquinoline-4(1*H*)-one-5-carboxylate (16a)



Yield 50 mg (34 %). ^{1}H NMR (400MHz, DMSO-d_6) δ ppm 11.76 (br. s., 1 H), 8.59 (br. s., 1 H), 7.82 - 7.78 (m, 3 H), 7.64 - 7.48 (m, 4 H), 7.18 (dd, *J*=0.9, 7.0 Hz, 1 H), 3.84 (s, 3 H). ^{13}C NMR (101MHz, DMSO-d_6) δ ppm 170.3, 168.8, 138.3, 138.0, 132.2, 132.0, 131.6, 129.8, 129.3, 129.2, 128.3, 120.2, 119.8, 118.1, 52.0. Calcd for $C_{17}H_{13}NO_4$ = 295.0845 Found m/z 295.0843.

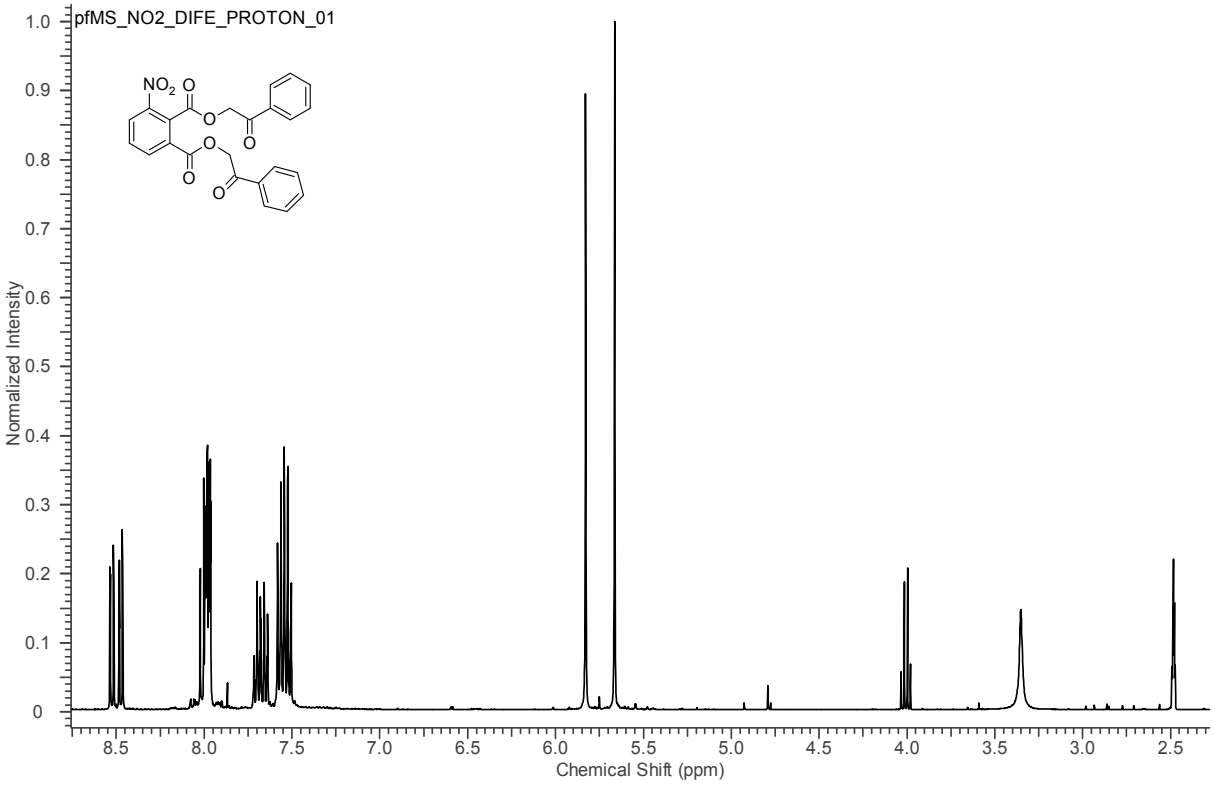
Methyl 2-(4-amino-3,5-dichlorophenyl)-3-hydroxyquinoline-4(1*H*)-one-5-carboxylate (16b)

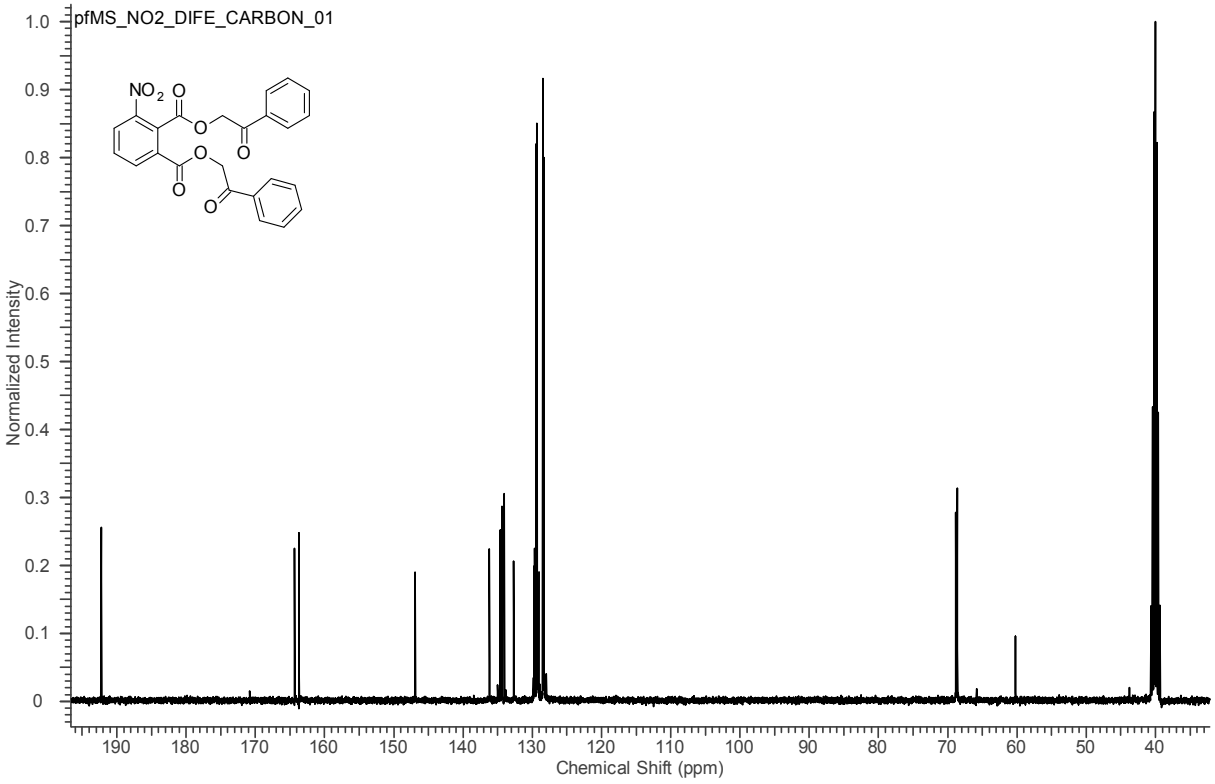


Yield 43 mg (32 %). ^{1}H NMR (400MHz, DMSO-d_6) δ ppm 11.56 (br. s., 1 H), 7.82 - 7.75 (m, 3 H), 7.63 - 7.55 (m, 1 H), 7.15 (d, *J*=6.6 Hz, 1 H), 6.02 (s, 2 H), 3.83 (s, 3 H). ^{13}C NMR (101MHz, DMSO-d_6) δ ppm 170.3, 168.5, 142.1, 138.1, 137.9, 132.2, 129.8, 129.5, 128.6, 120.1, 119.9, 119.8, 118.0, 117.4, 52.0. Calcd for $C_{17}H_{12}Cl_2N_2O_4$ = 378.0174 Found m/z 378.0131.

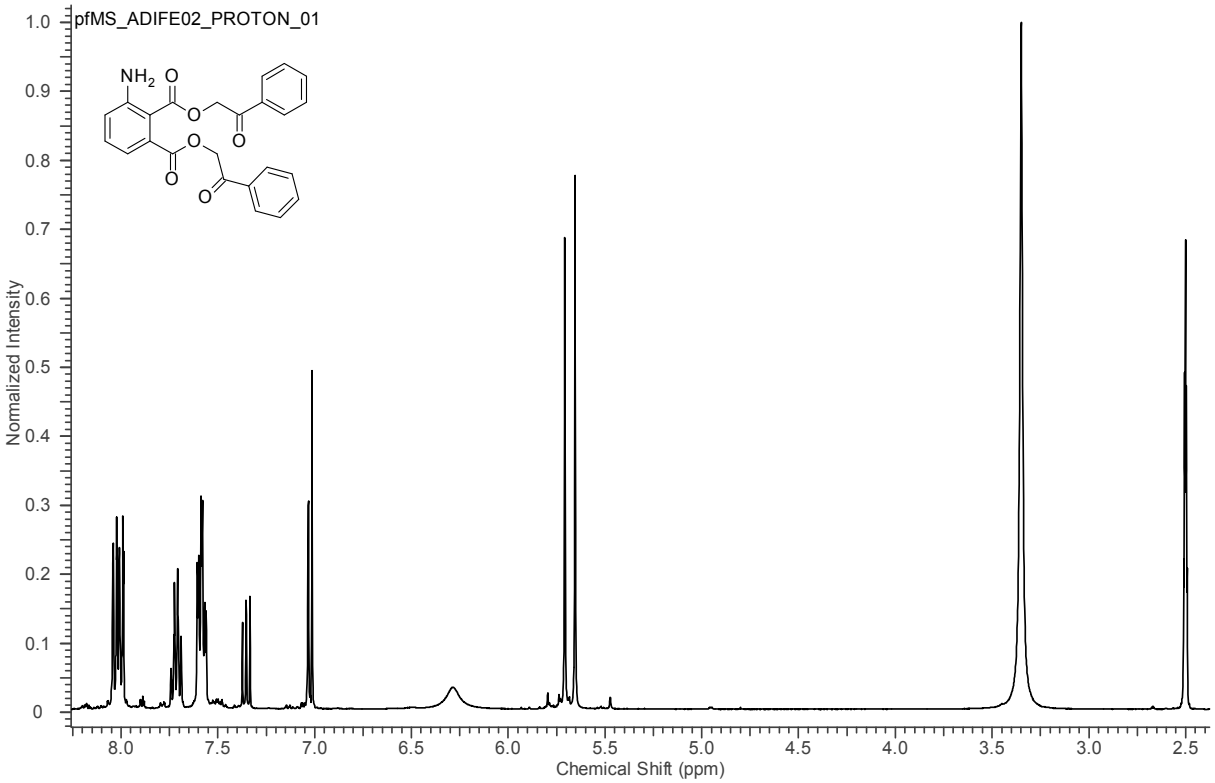
Original ^{1}H and ^{13}C NMR spectra

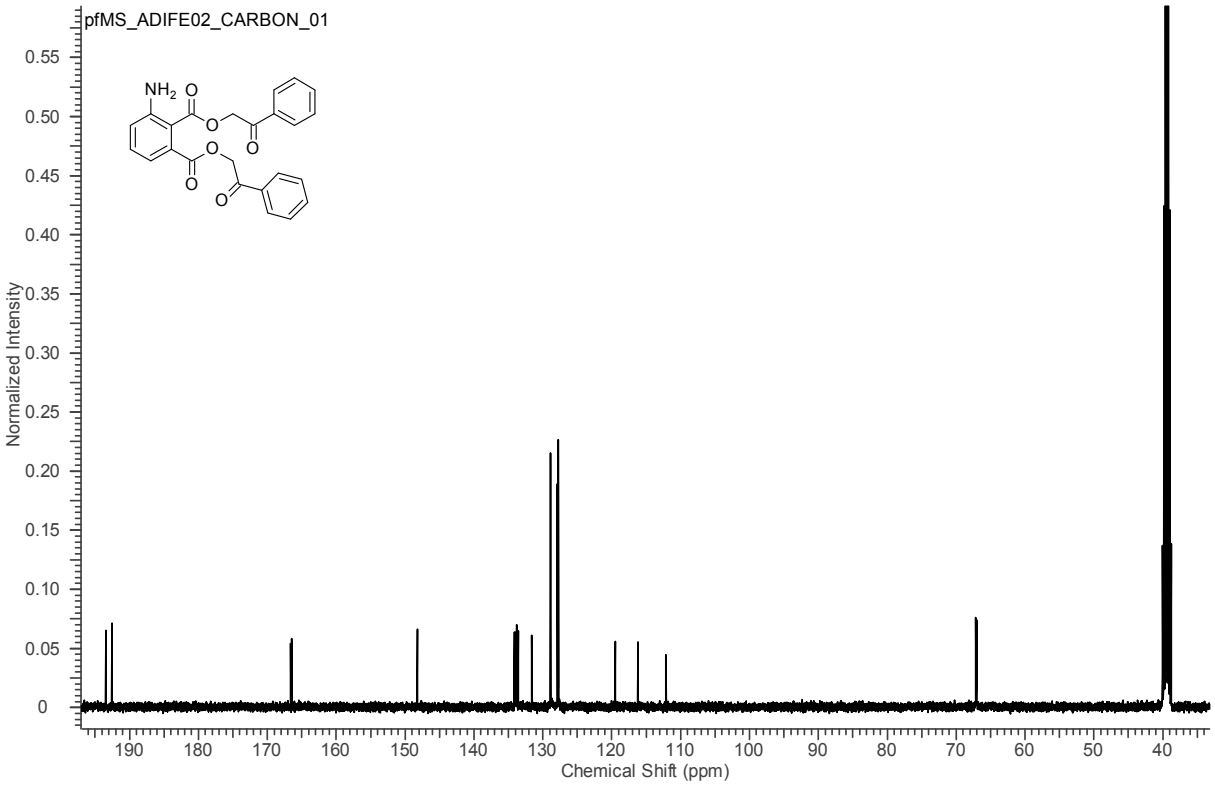
Bis(2-oxo-2-phenylethyl) 3-nitrophthalate (12a):



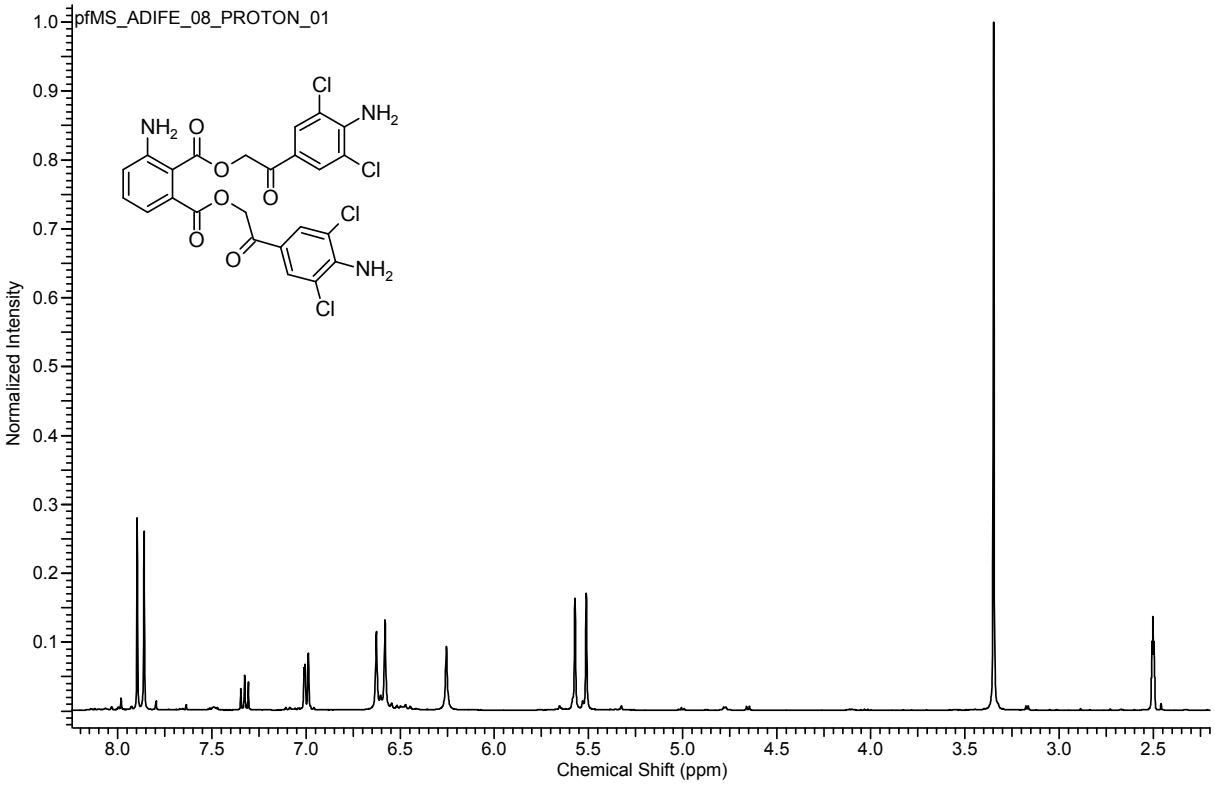


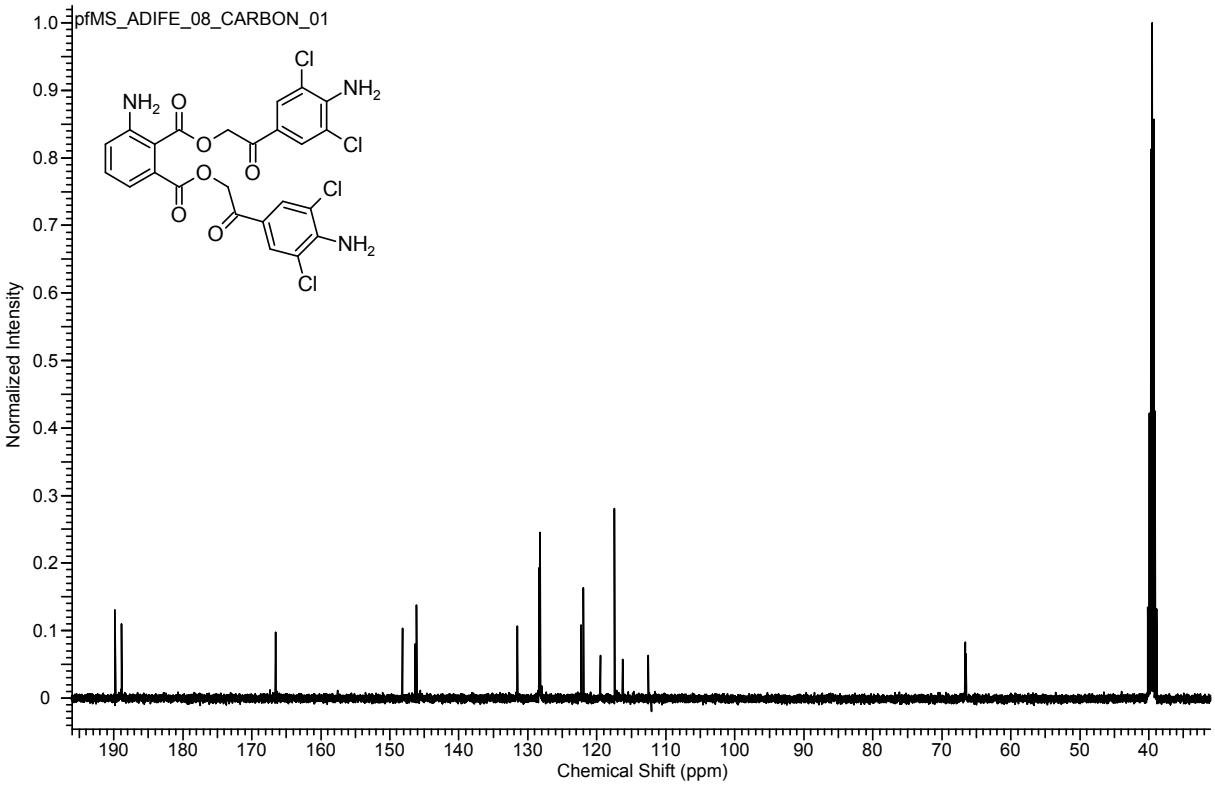
Bis(2-oxo-2-phenylethyl) 3-aminophthalate (13a):



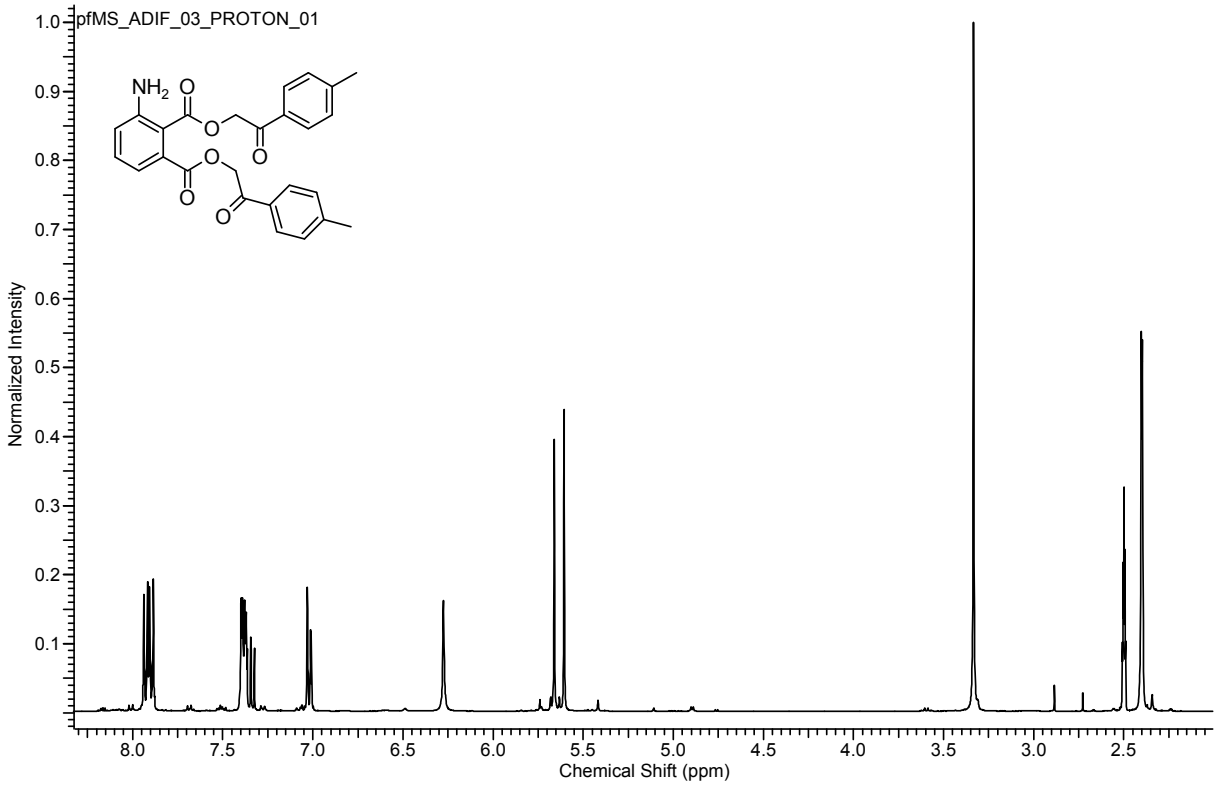


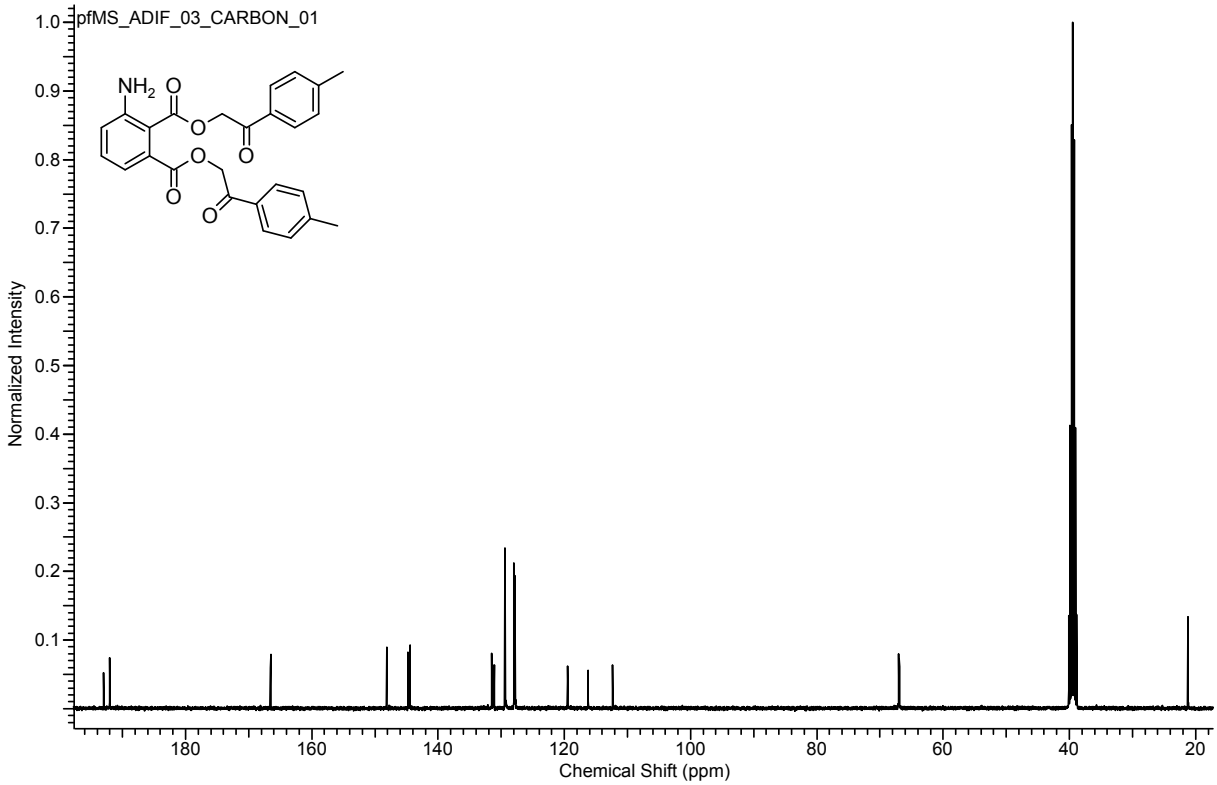
Bis(2-(4-amino-3,5-dichlorophenyl)-2-oxoethyl) 3-aminophthalate (13b):



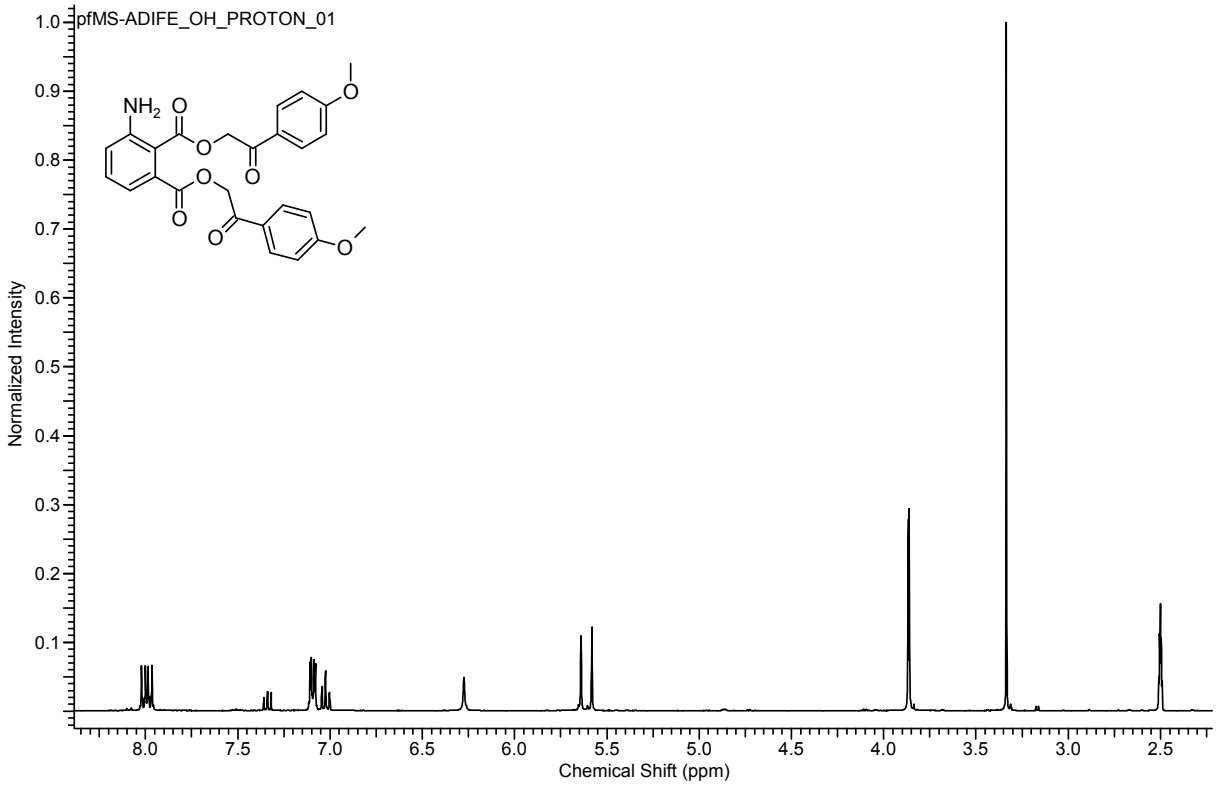


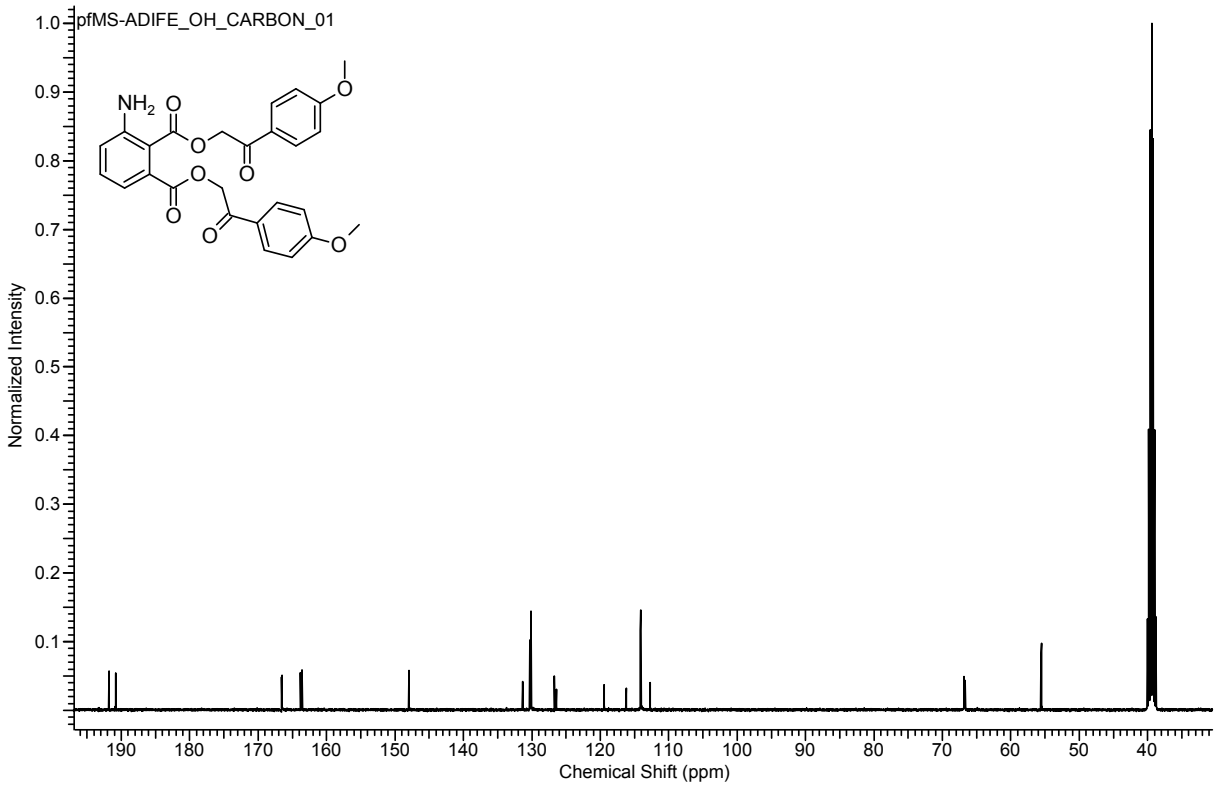
Bis(2-oxo-2-(*p*-tolyl)ethyl) 3-aminophthalate (13c):



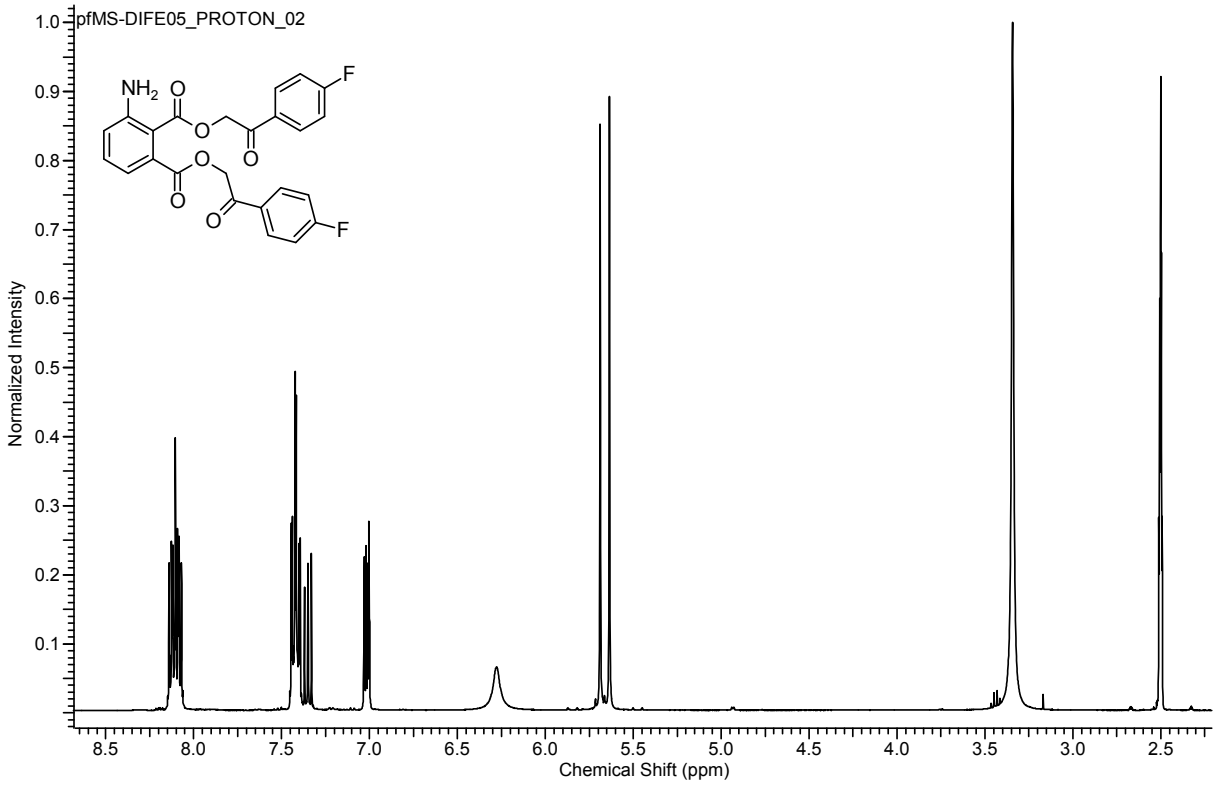


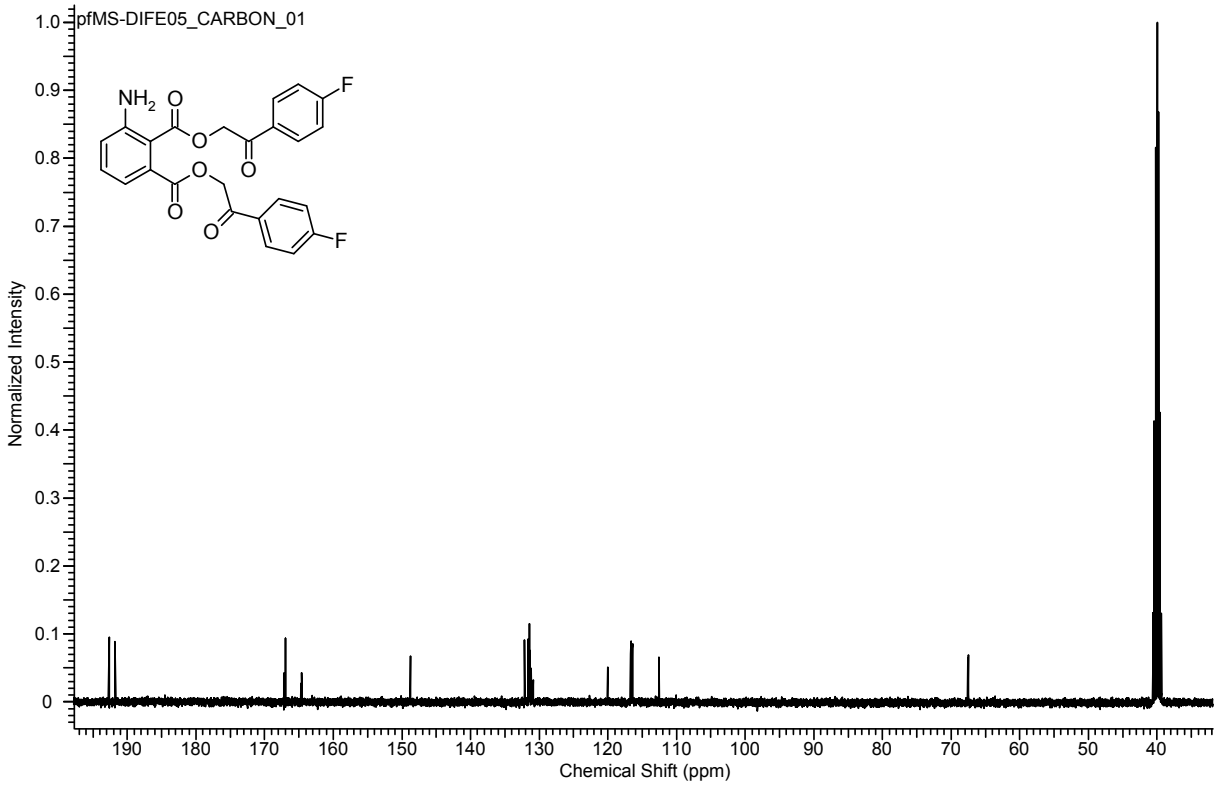
Bis(2-(4-methoxyphenyl)-2-oxoethyl) 3-aminophthalate (13d):



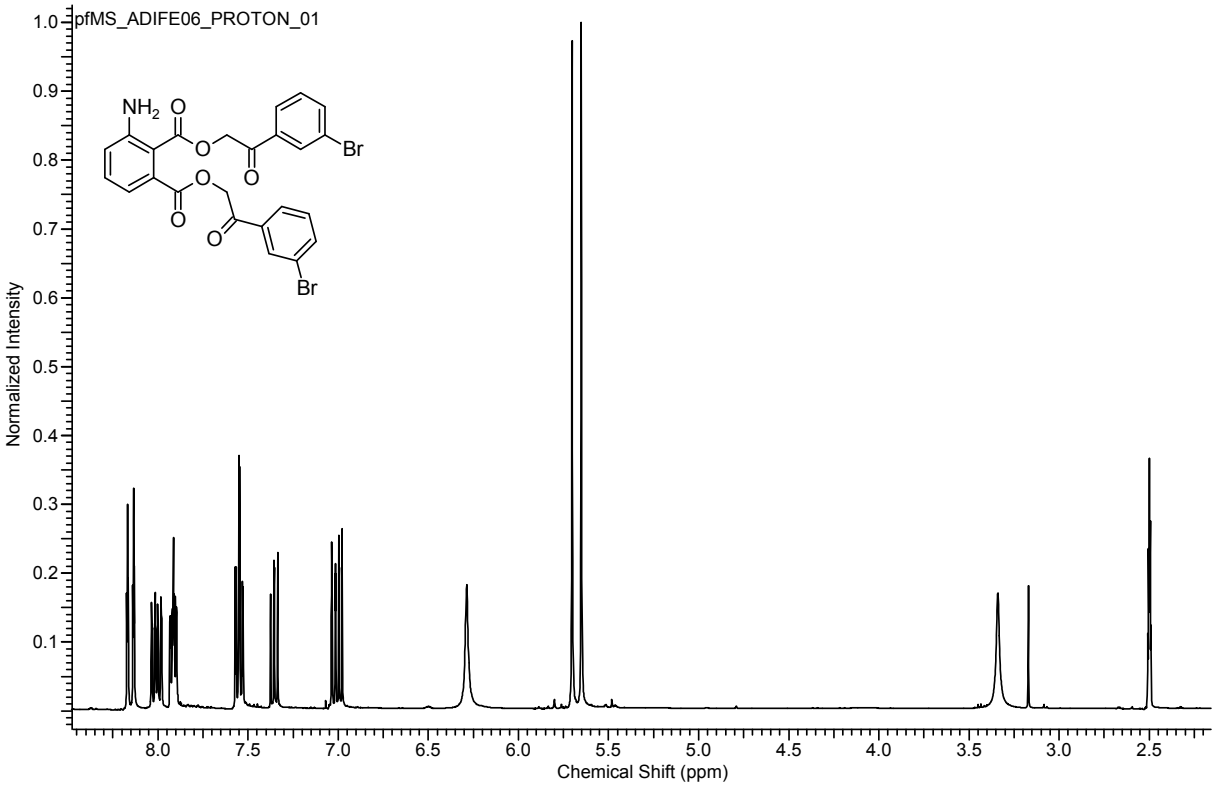


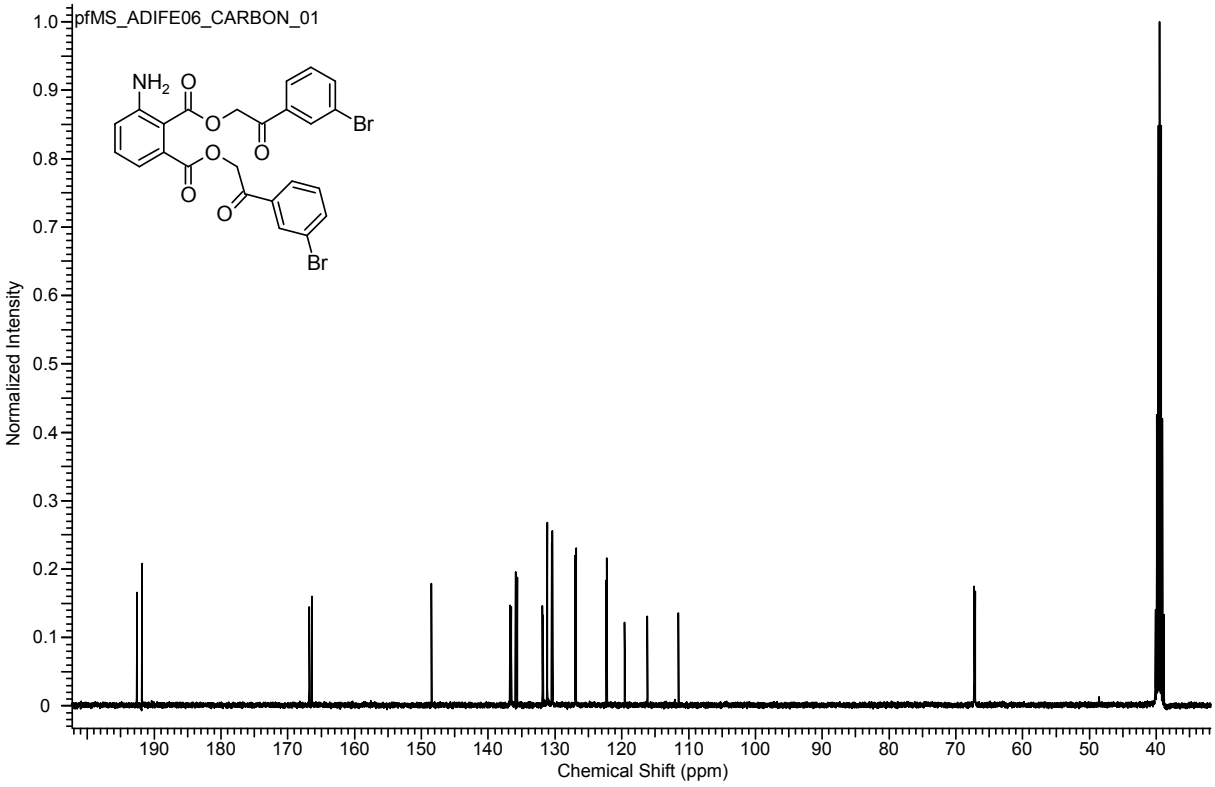
Bis(2-(4-fluorophenyl)-2-oxoethyl) 3-aminophthalate (13e):



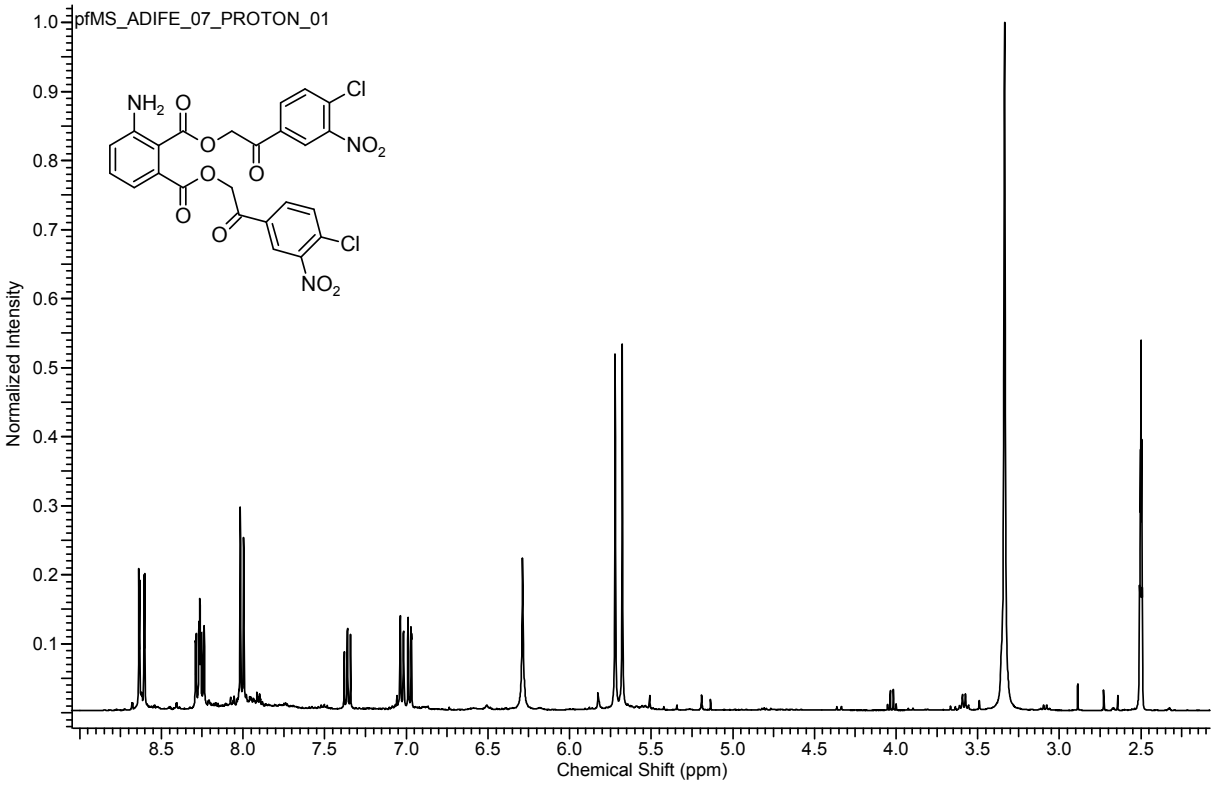


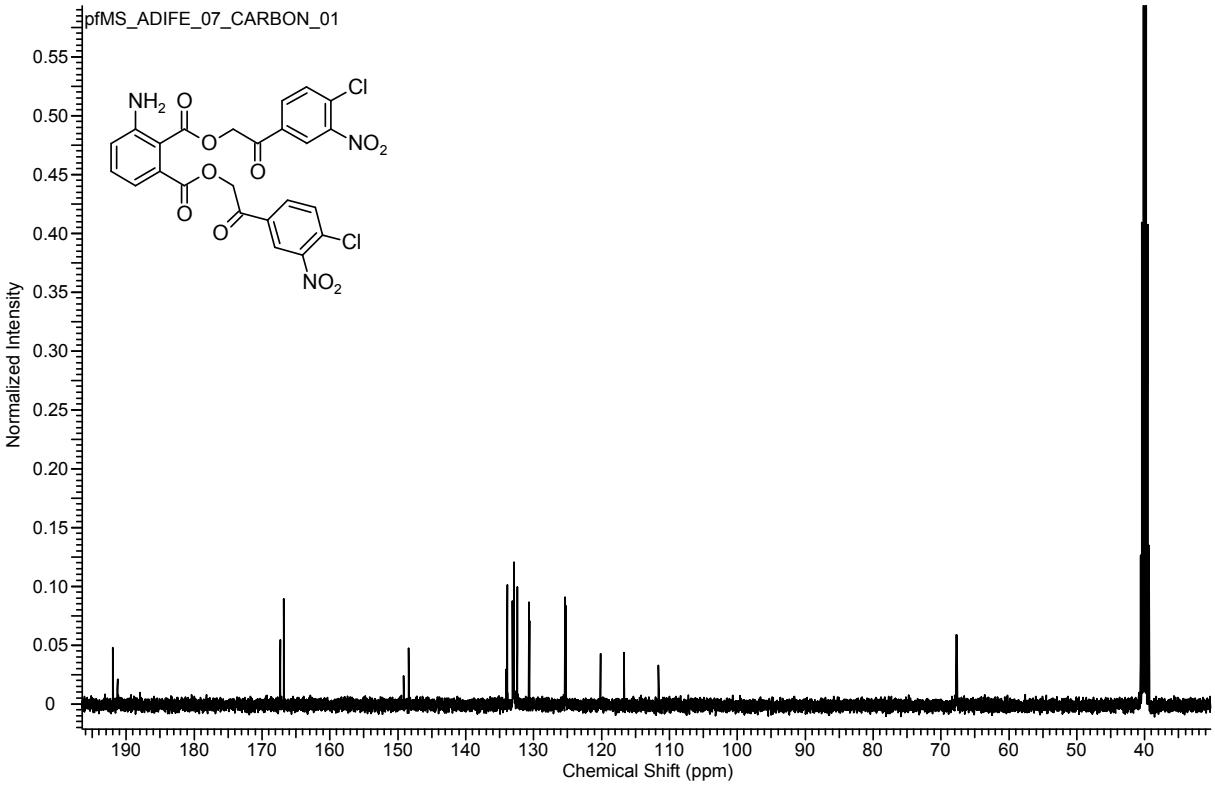
Bis(2-(3-bromophenyl)-2-oxoethyl) 3-aminophthalate (13f):



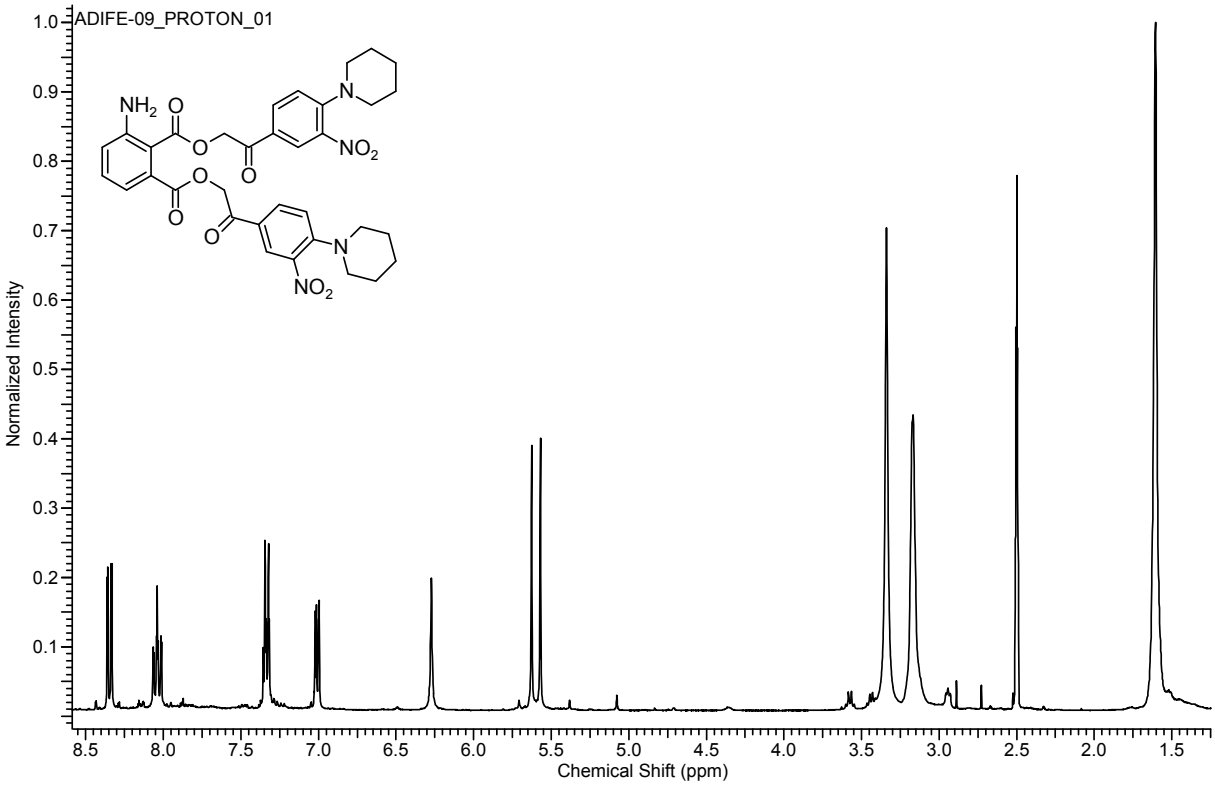


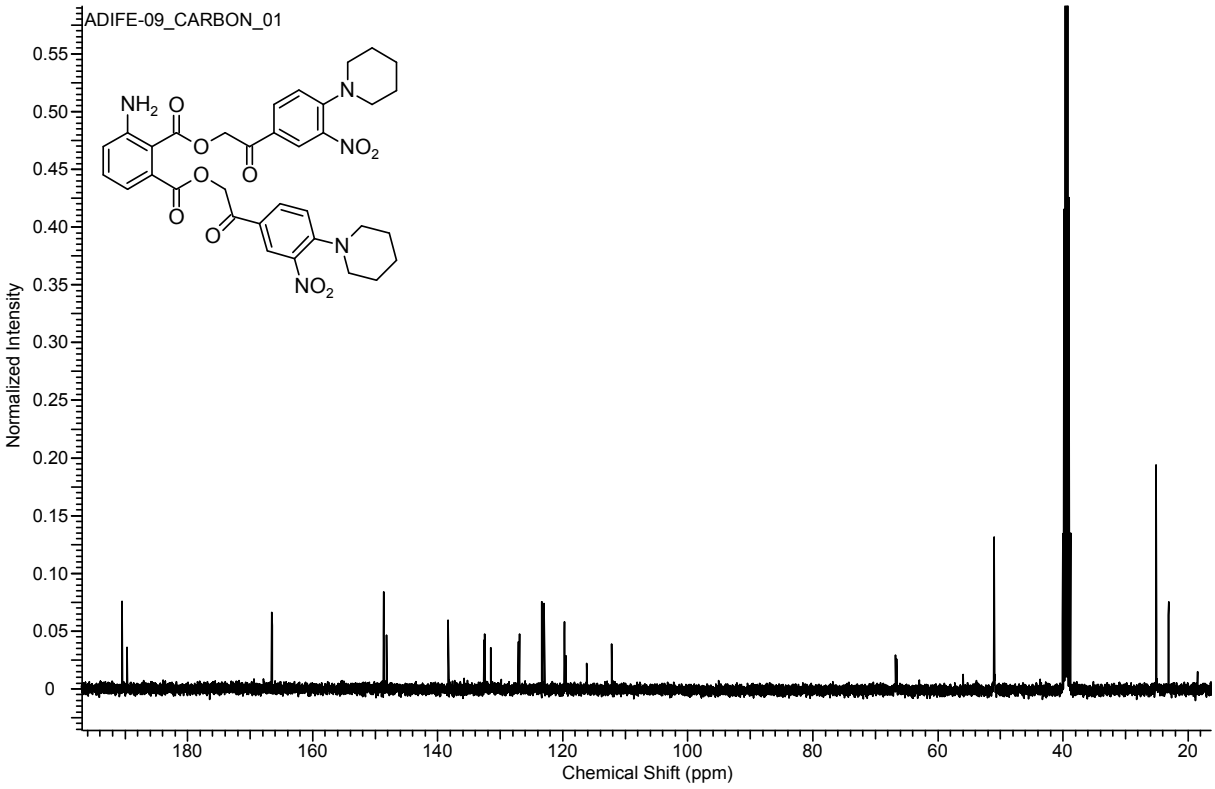
Bis(2-(4-chloro-3-nitrophenyl)-2-oxoethyl) 3-aminophthalate (13g):



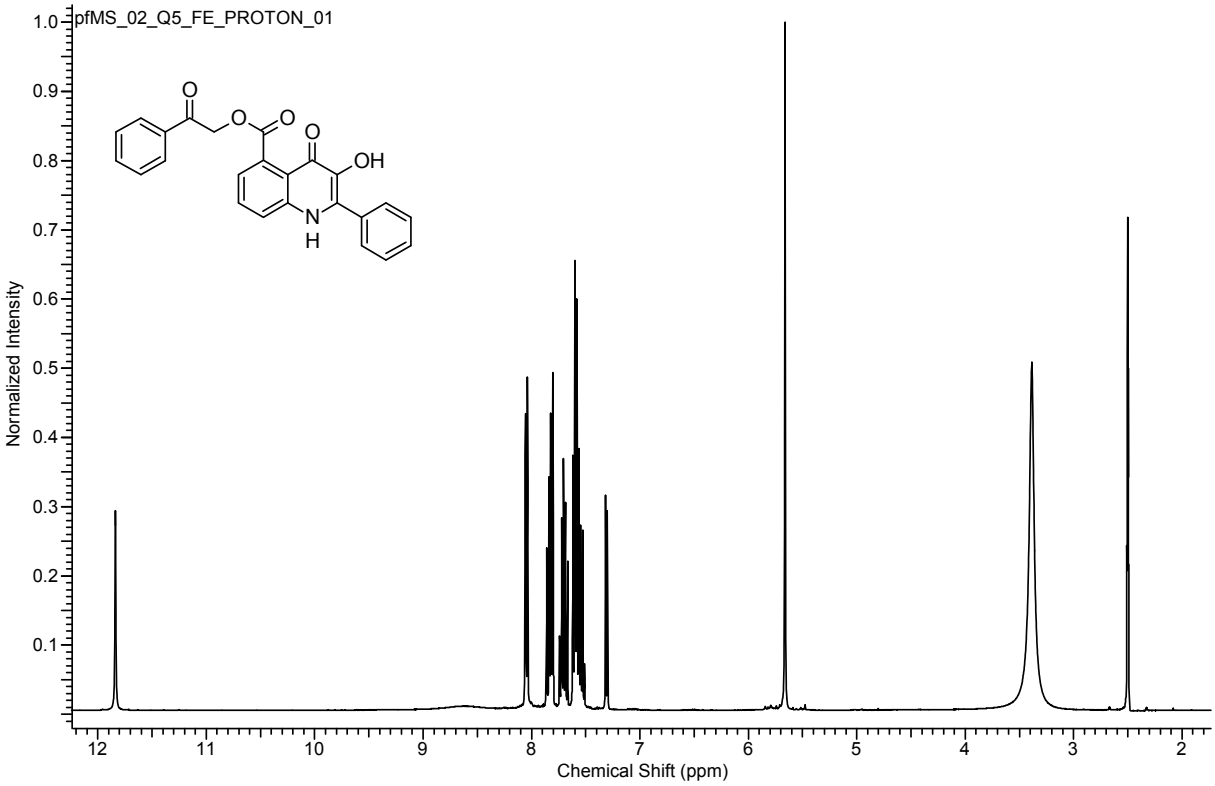


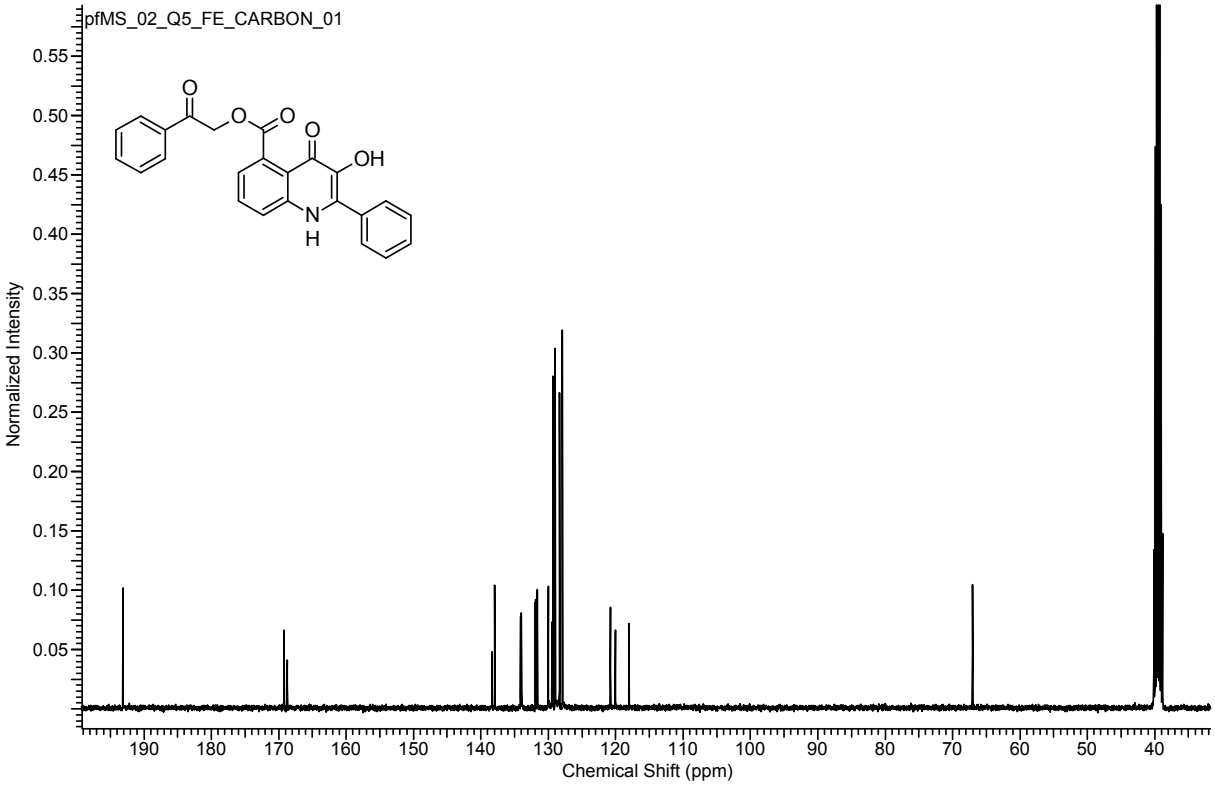
Bis(2-(3-nitro-4-(piperidin-1-yl)phenyl)-2-oxoethyl) 3-aminophthalate (13h):



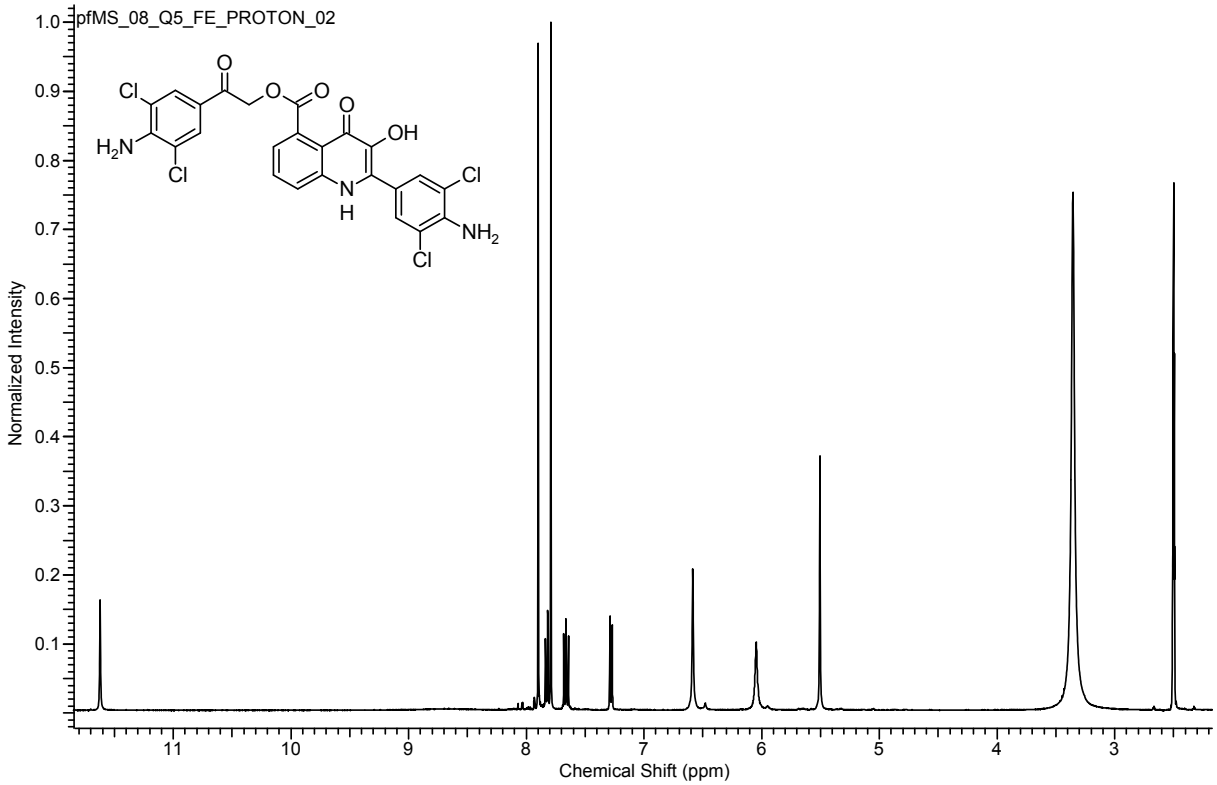


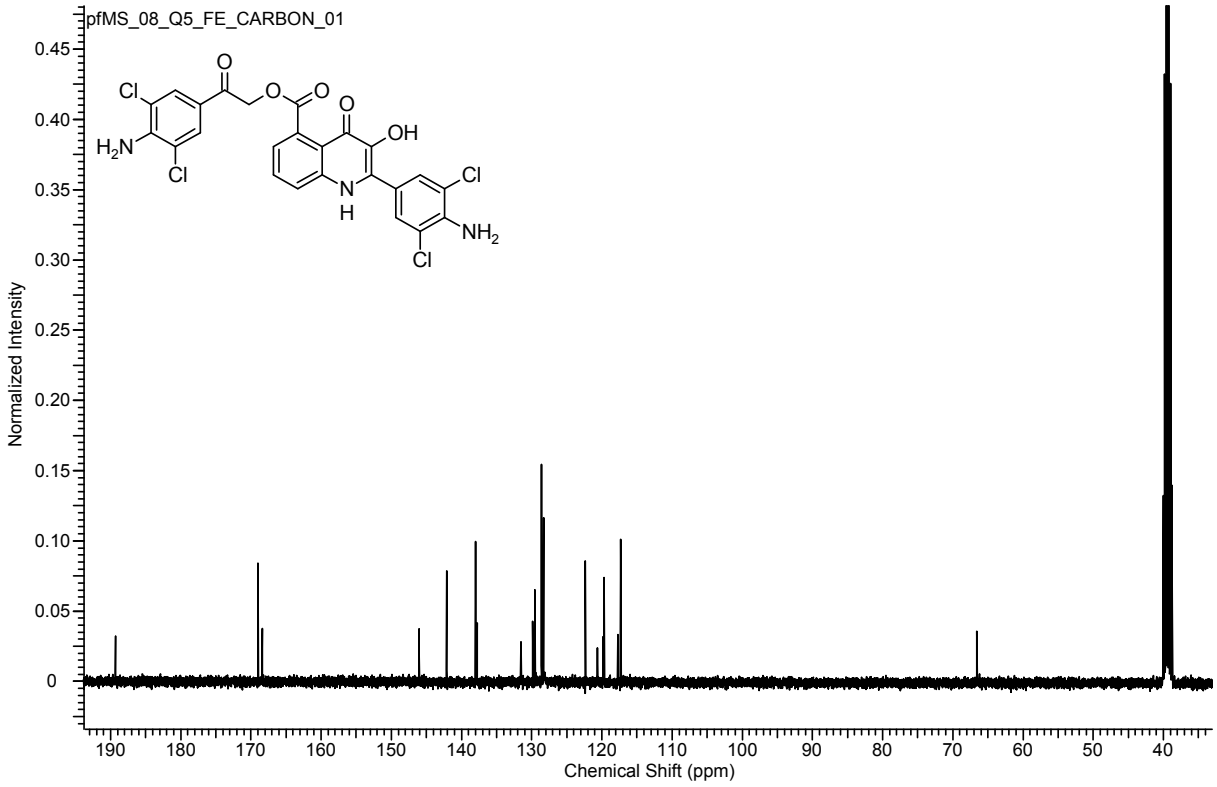
2-Oxo-2-phenylethyl 2-phenyl-3-hydroxyquinoline-4(1*H*)-one-5-carboxylate (14a):



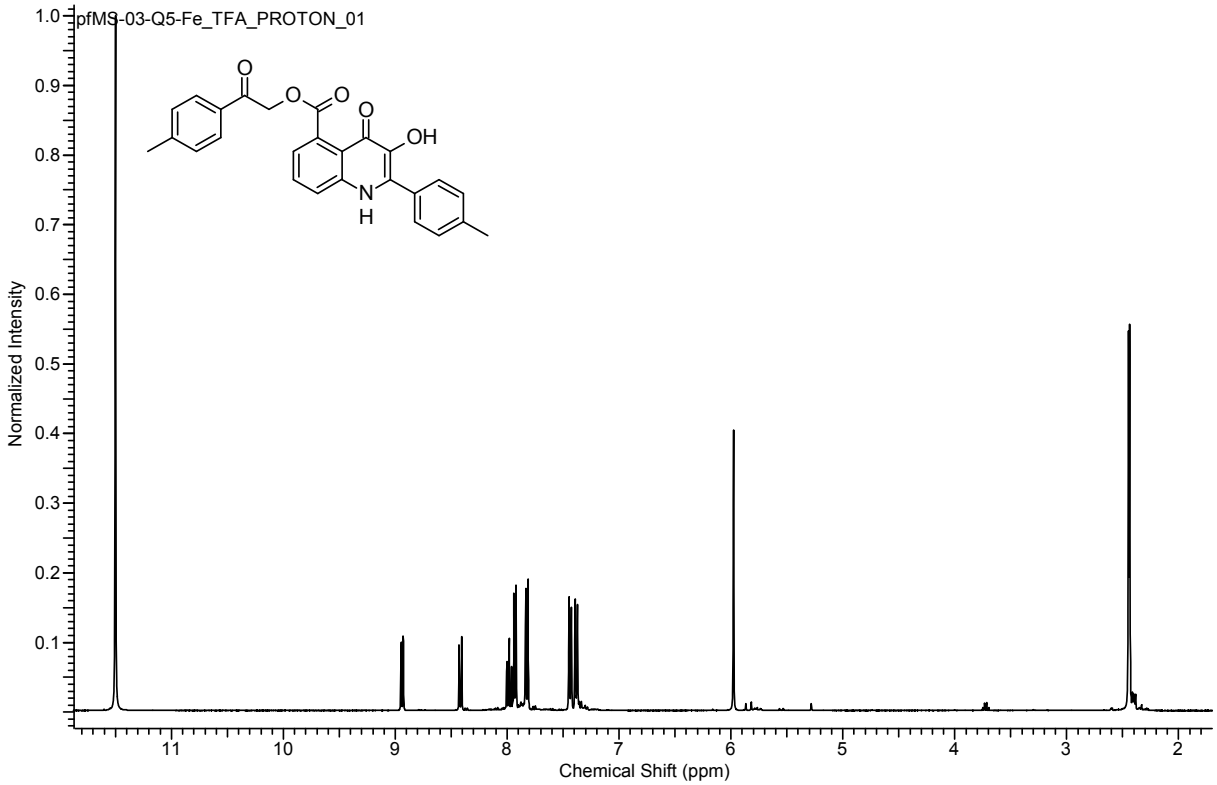


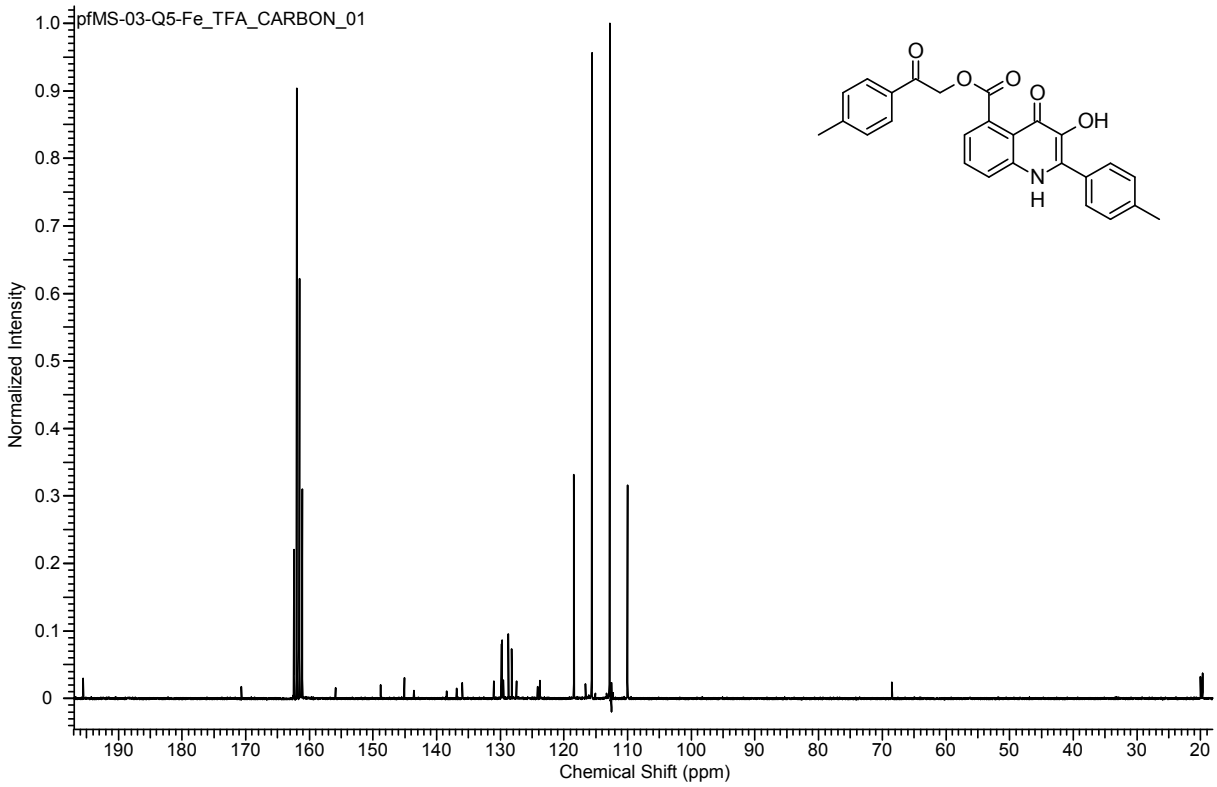
2-(4-Amino-3,5-dichlorophenyl)-2-oxoethyl 2-(4-amino-3,5-dichlorophenyl)- hydroxyquinoline-4(1*H*)-one-5-carboxylate (14b):



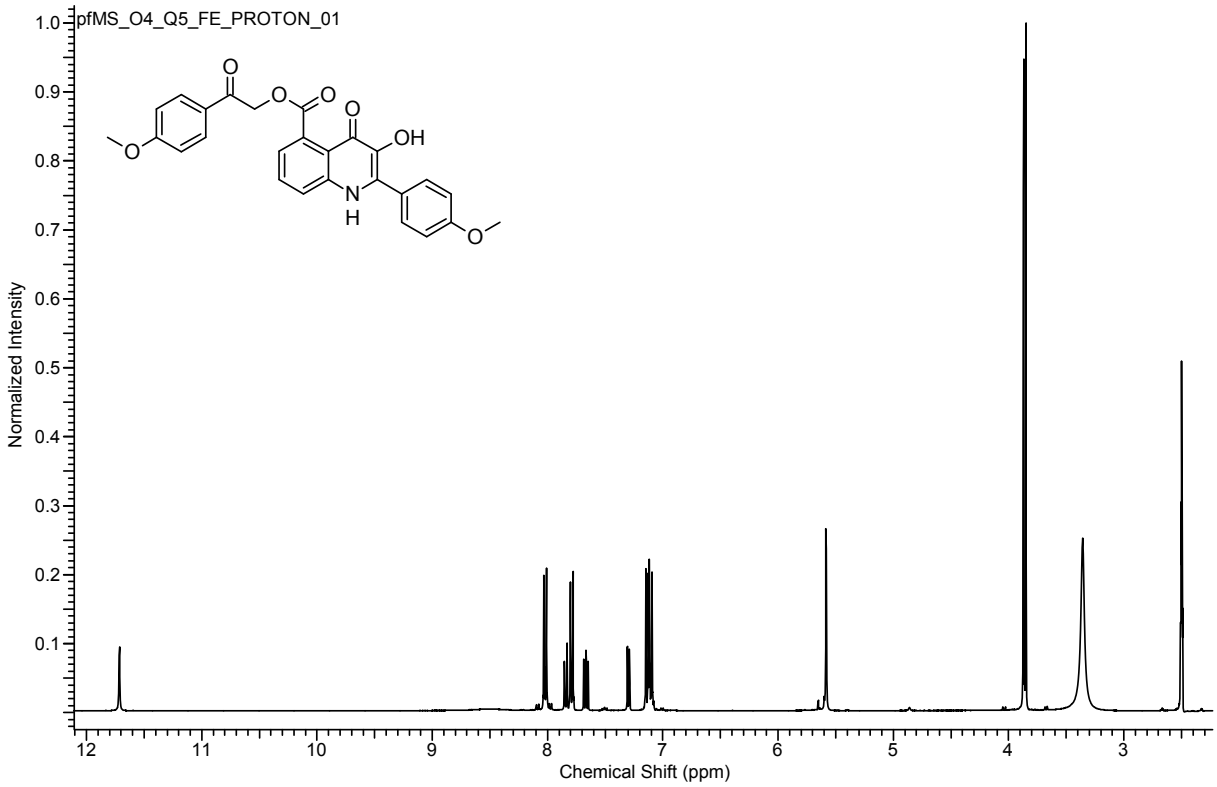


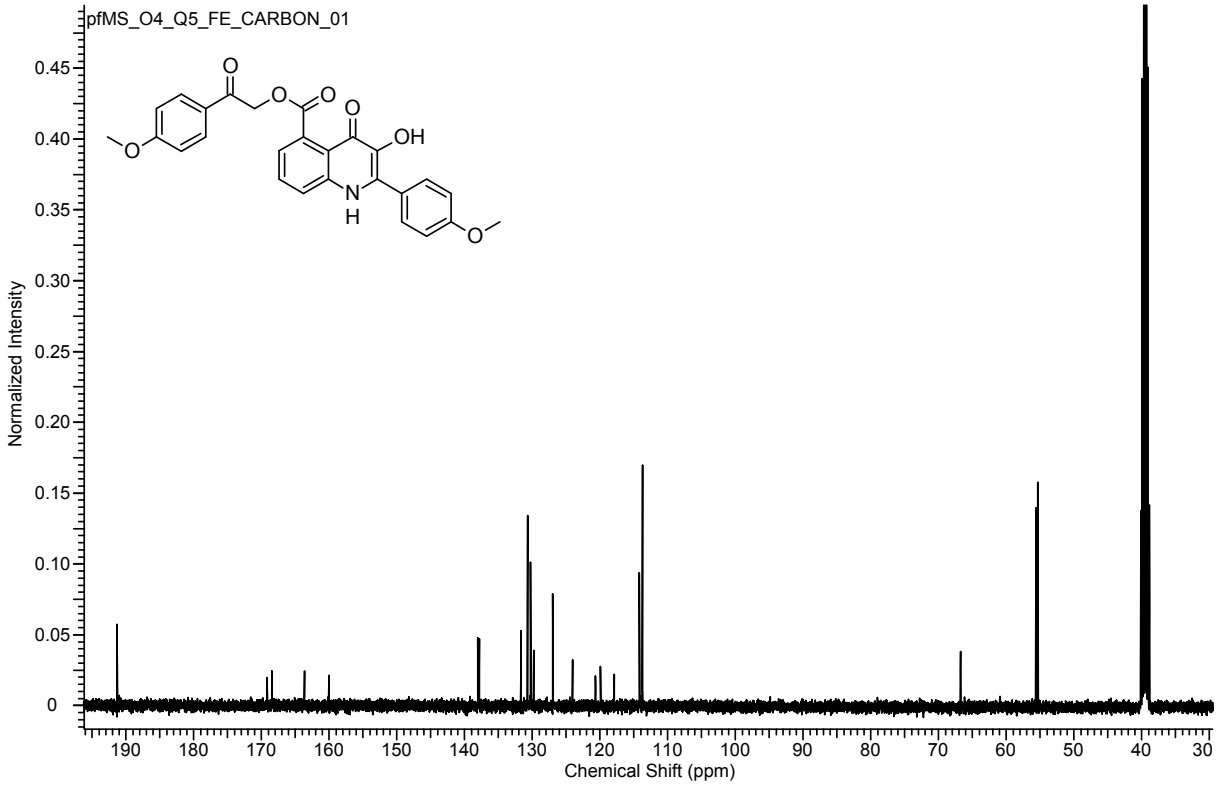
2-Oxo-2-(*p*-tolyl)ethyl 2-(*p*-tolyl)-3-hydroxyquinoline-4(1*H*)-one-5-carboxylate (14c):



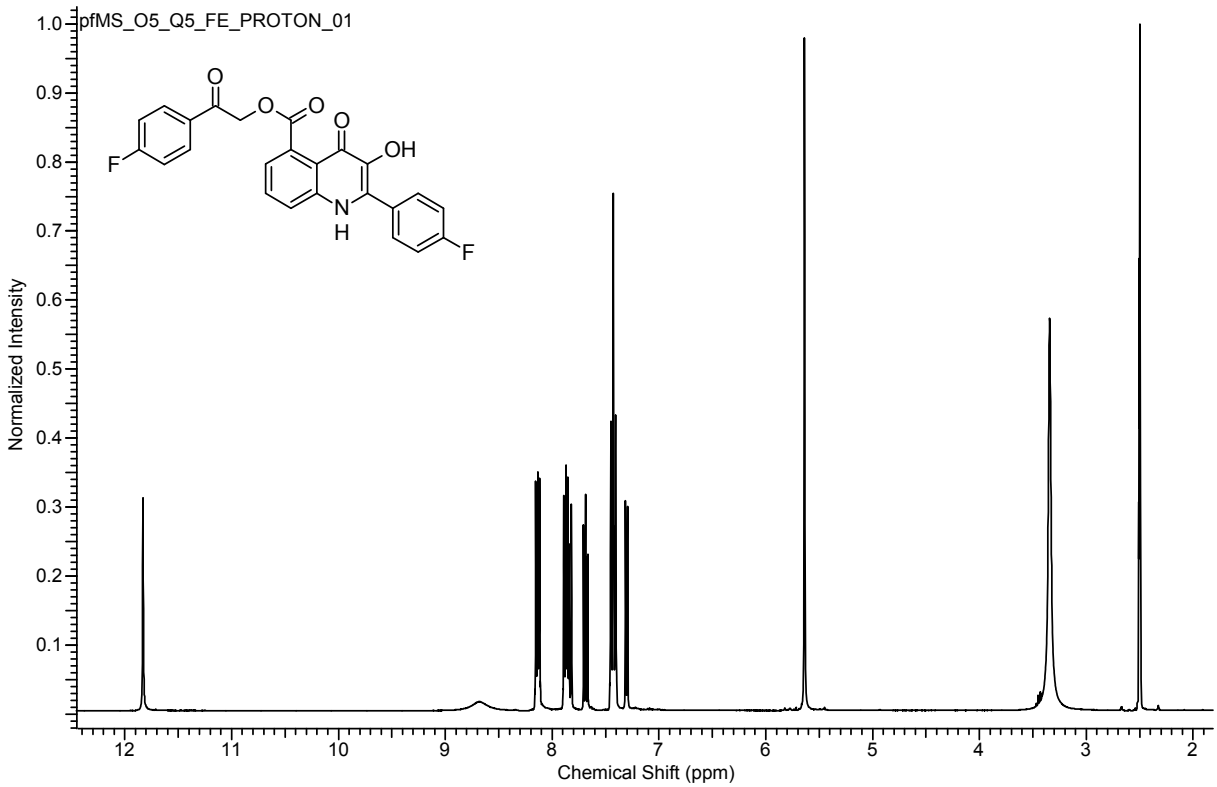


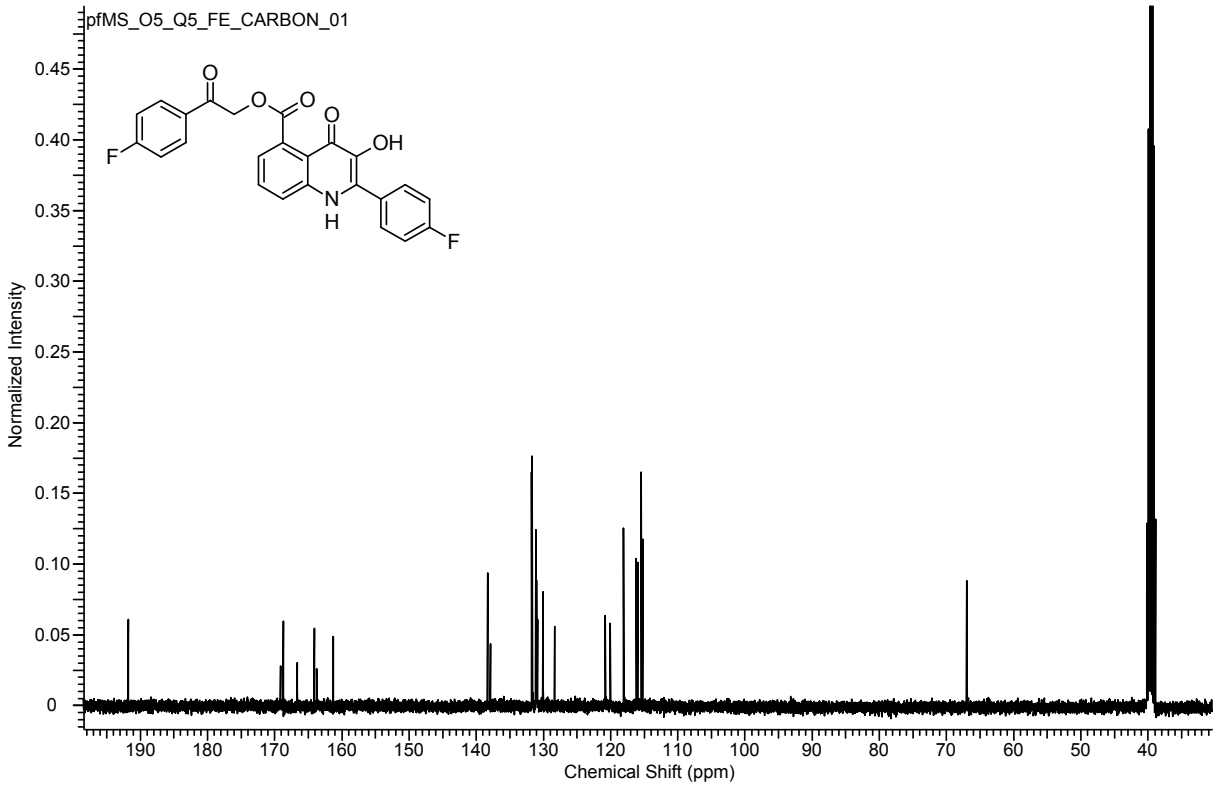
2-(4-Methoxyphenyl)-2-oxoethyl 2-(4-methoxyphenyl)-3-hydroxyquinoline-4(1*H*)-one-5-carboxylate (14d):



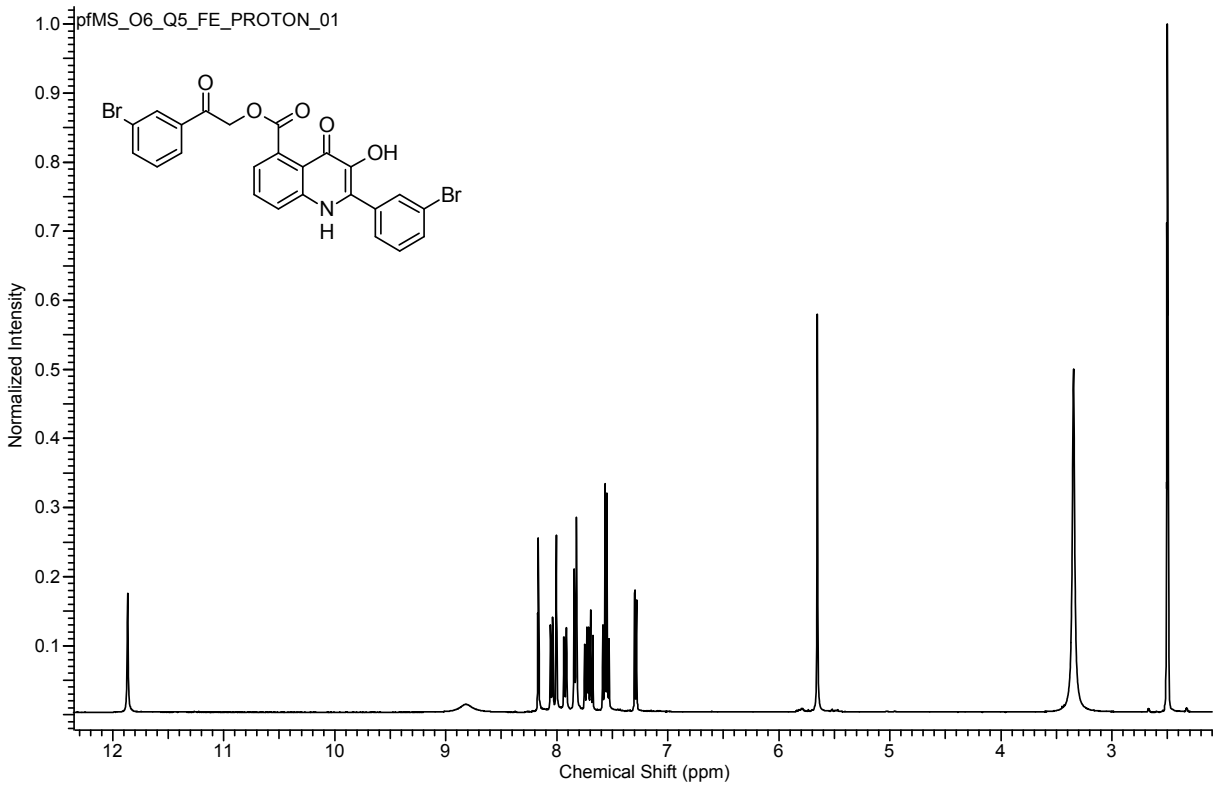


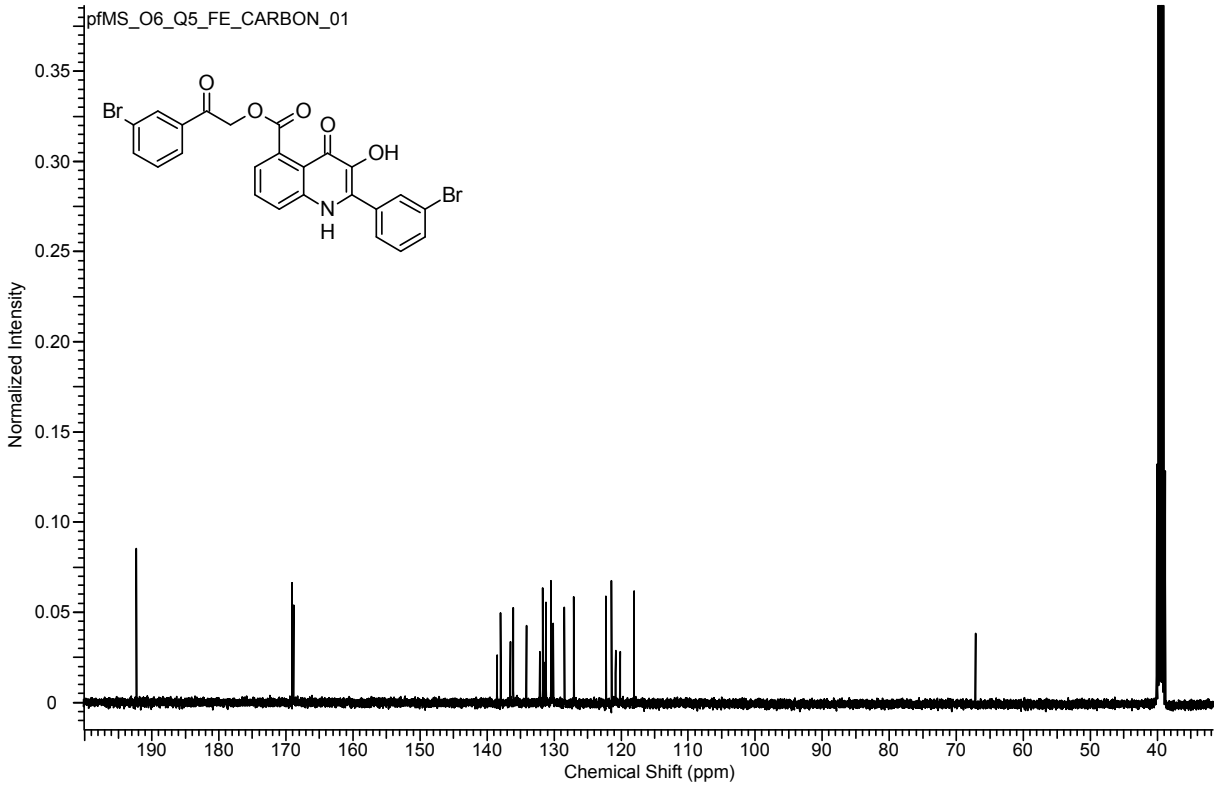
2-(4-Fluorophenyl)-2-oxoethyl 2-(4-fluorophenyl)-3-hydroxyquinoline-4(1*H*)-one-5-carboxylate (14e):



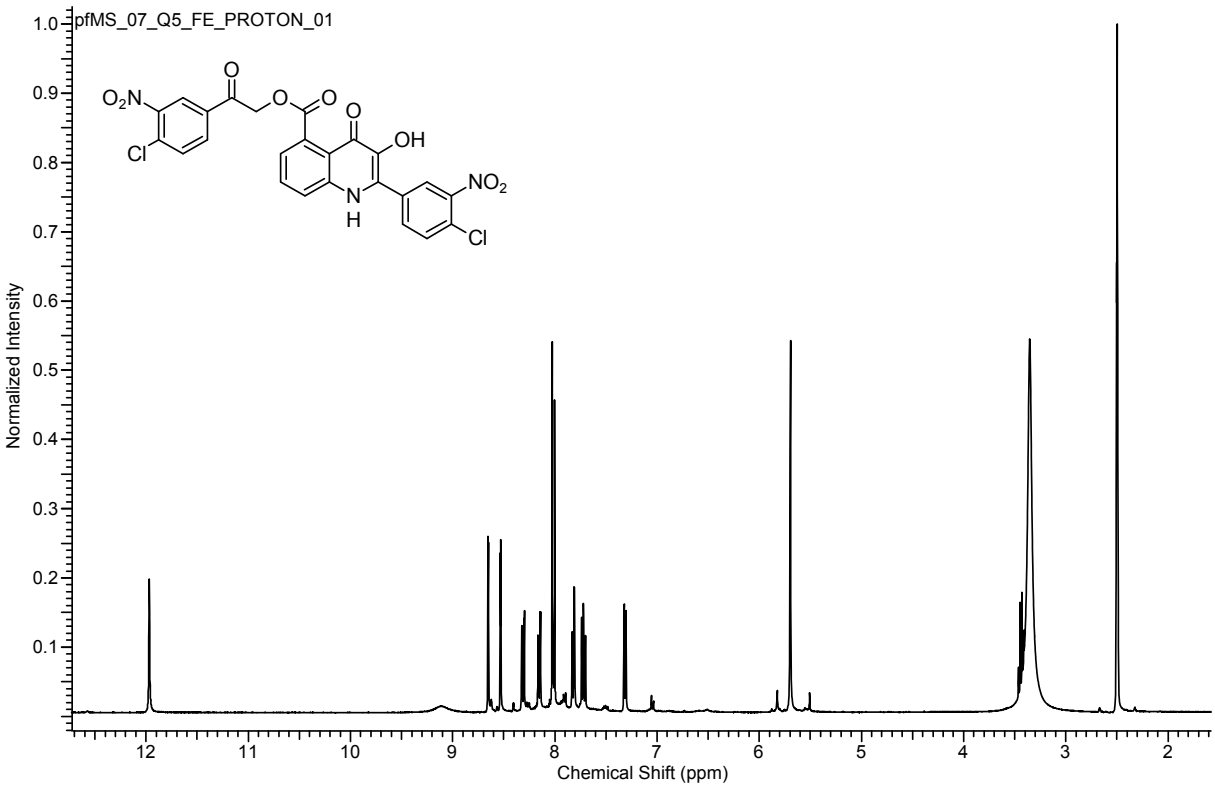


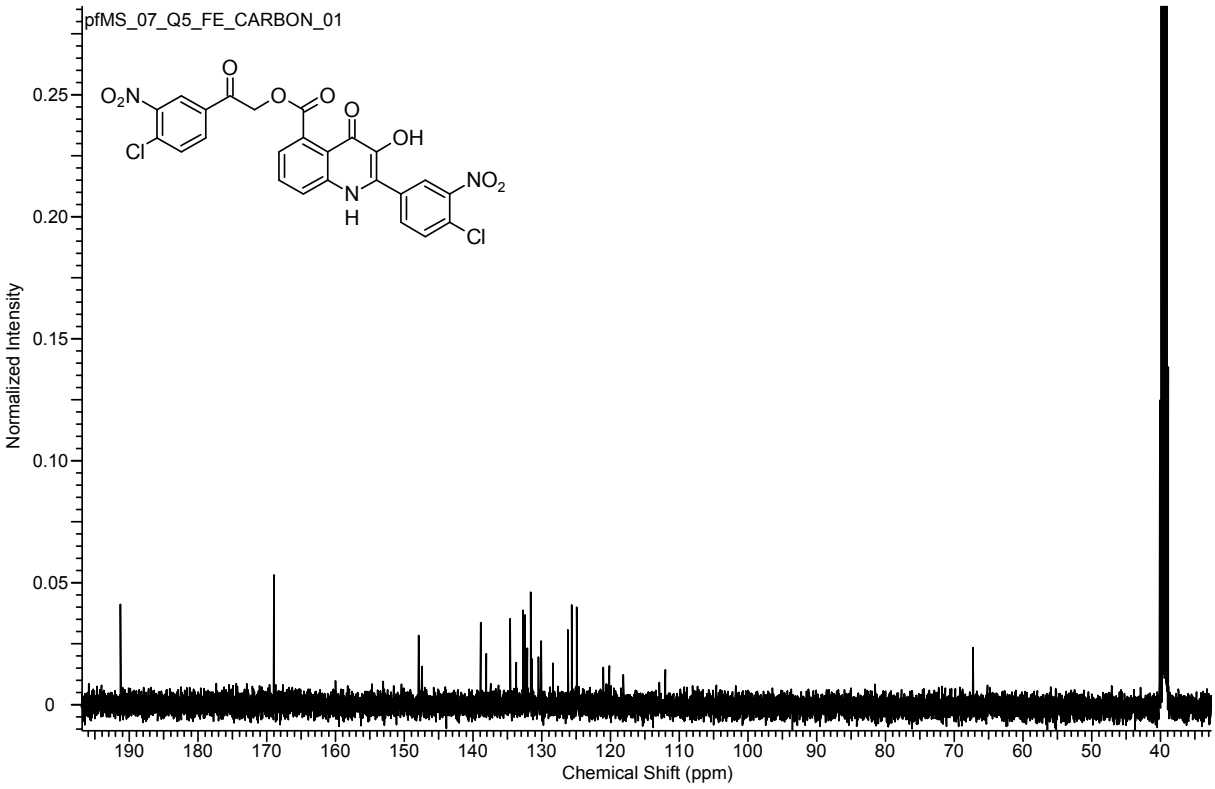
2-(3-Bromophenyl)-2-oxoethyl 2-(3-bromophenyl)-3-hydroxyquinoline-4(1*H*)-one-5-carboxylate (14f):



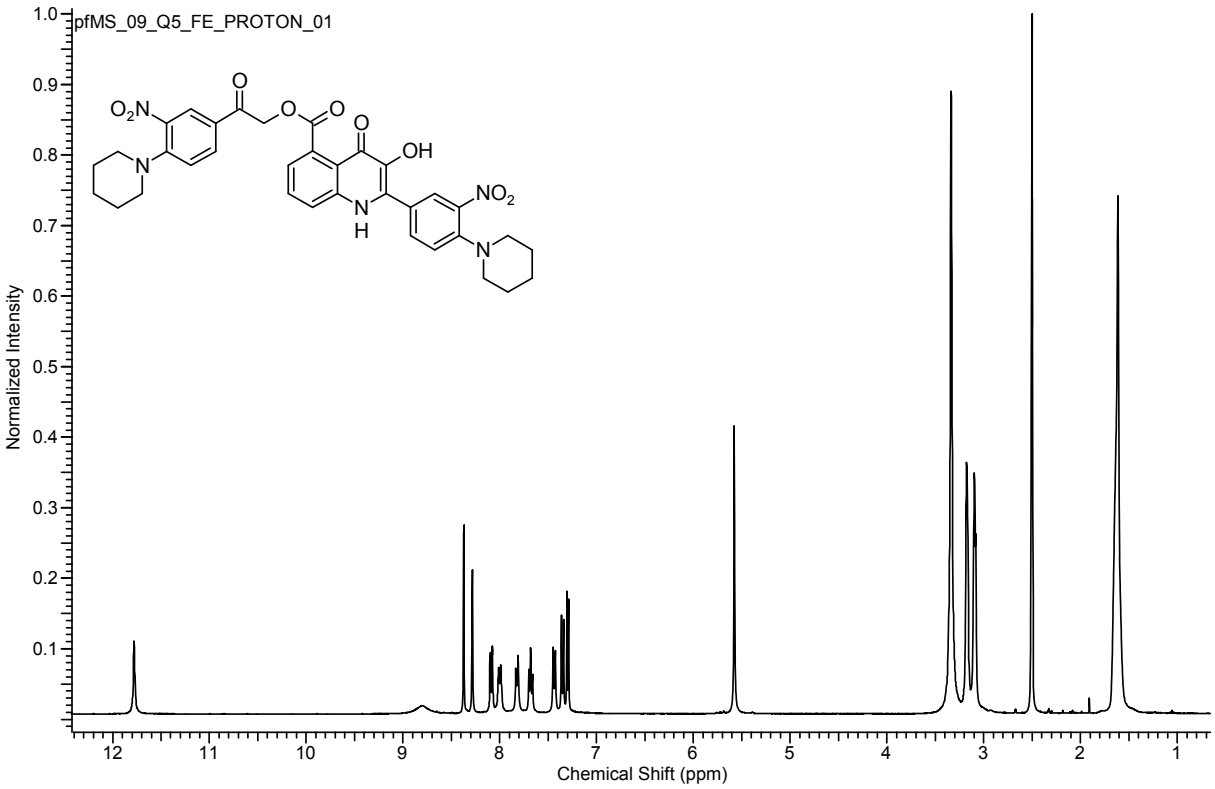


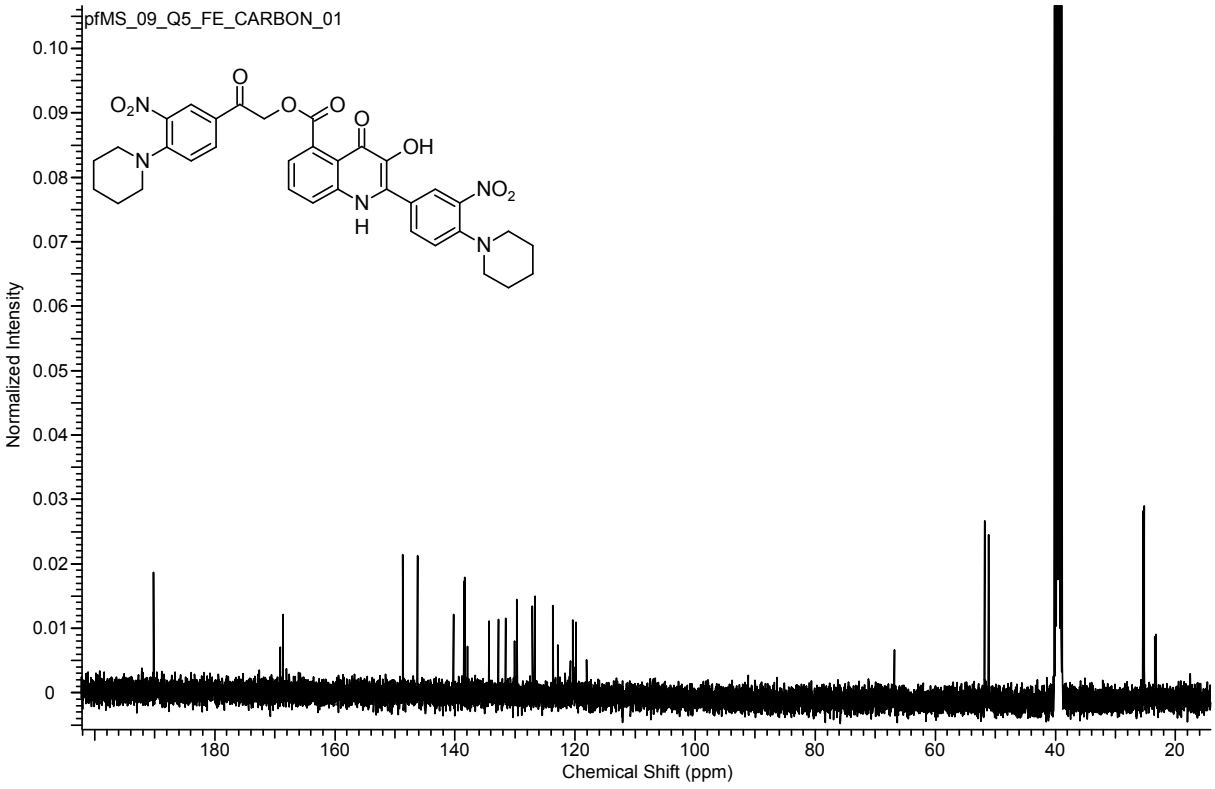
2-(4-Chloro-3-nitrophenyl)-2-oxoethyl 2-(4-chloro-3-nitrophenyl)-3-hydroxyquinoline-4(1*H*)-one-5-carboxylate (14g):



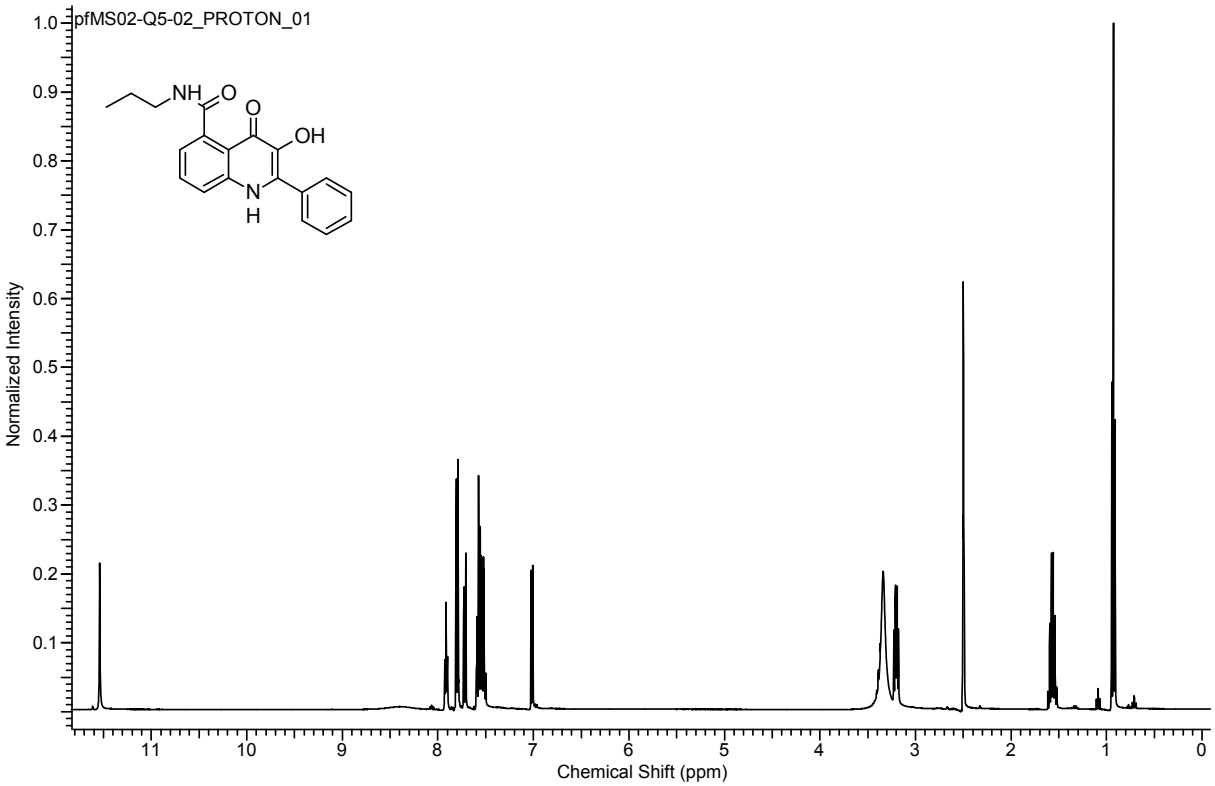


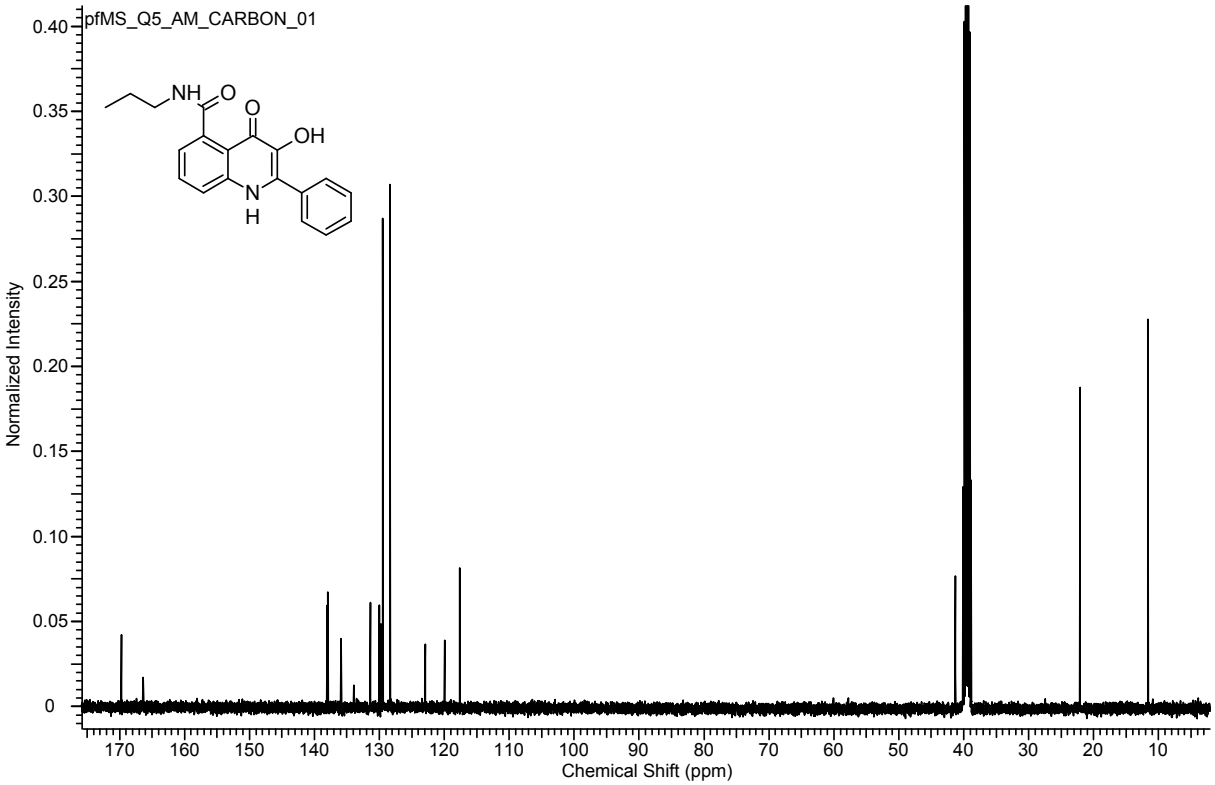
2-(3-Nitro-4-(piperidin-1-yl)phenyl)-2-oxoethyl 2-(3-nitro-4-(piperidin-1-yl)phenyl)- 3-hydroxy-quinoline-4(1*H*)-one-5-carboxylate (14h):



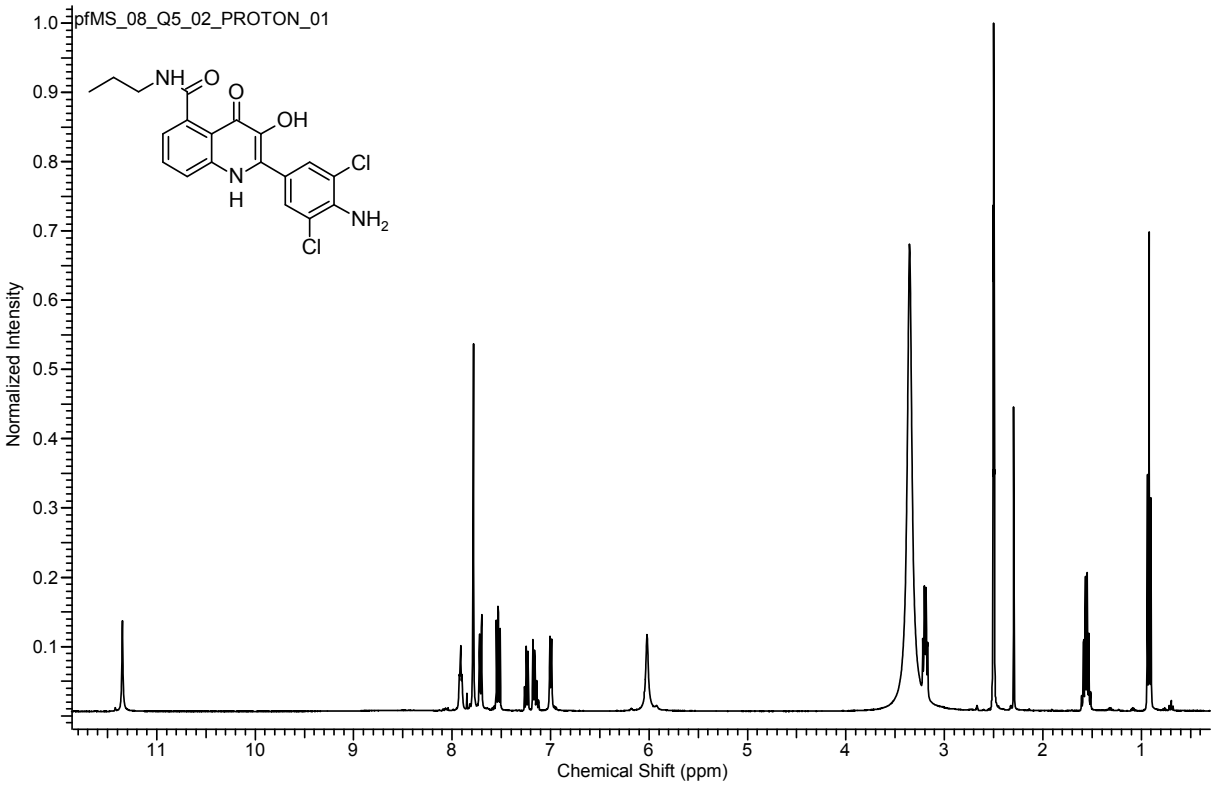


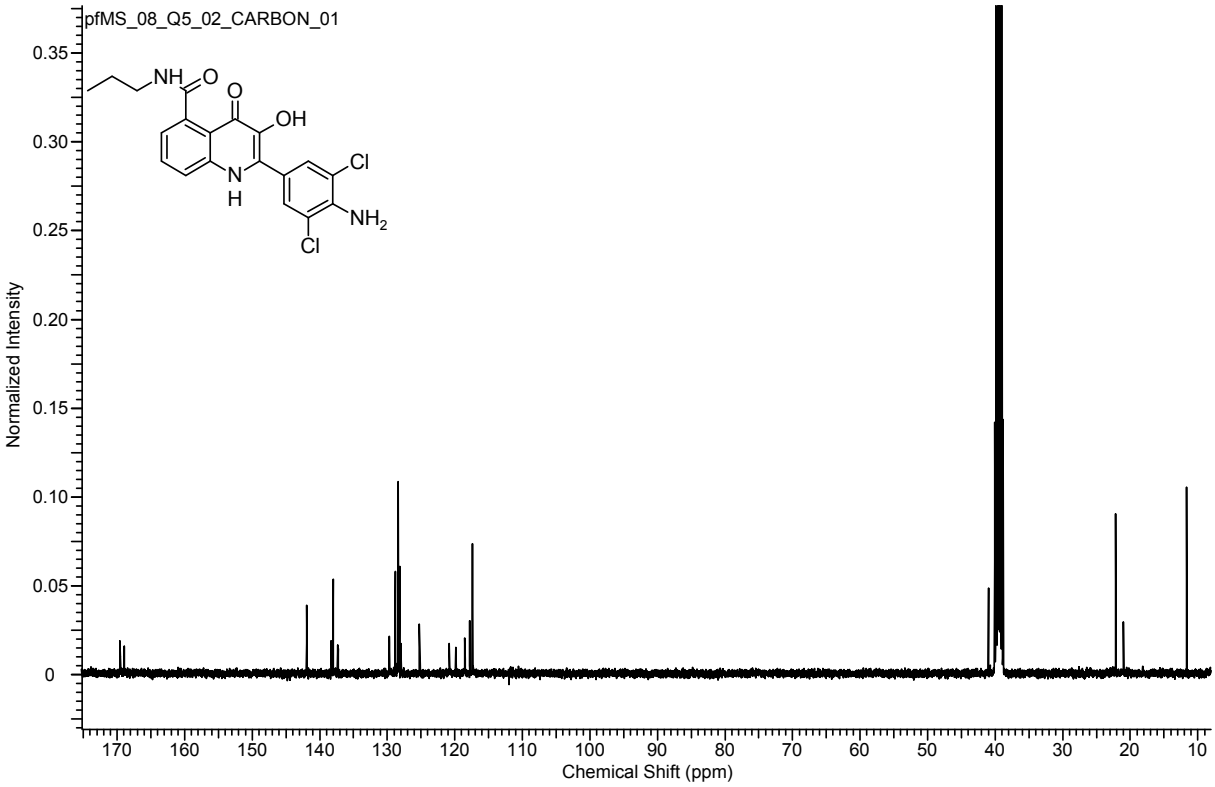
_N_-Propyl-2-phenyl-3-hydroxyquinoline-4(1_H_)-one-5-carboxamide (15a):



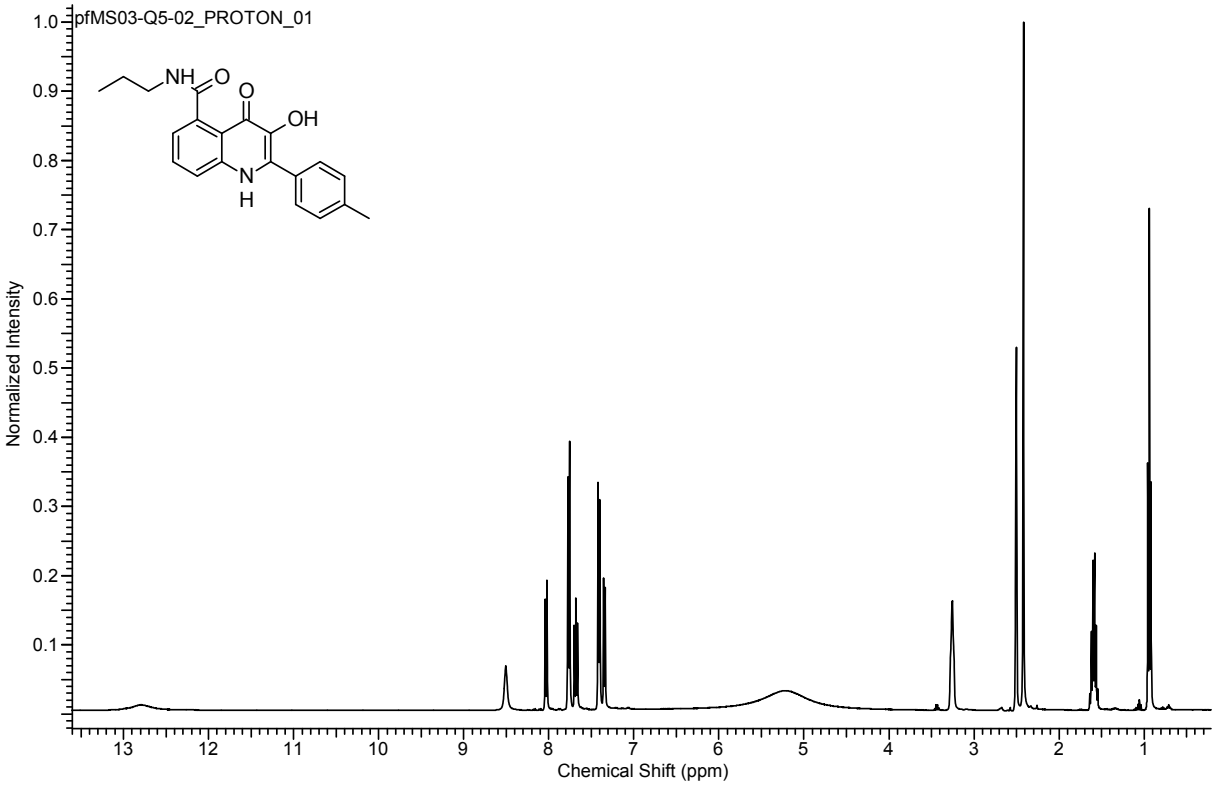


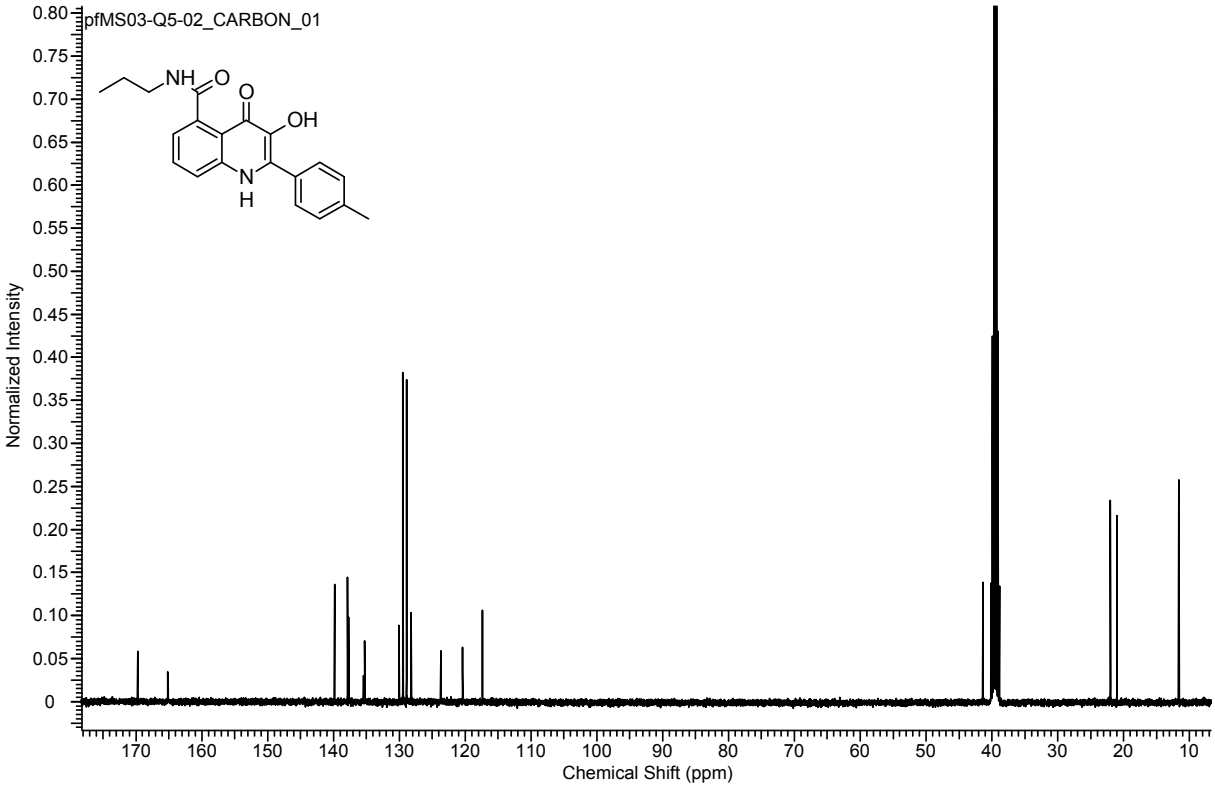
_N_-Propyl-2-(4-amino-3,5-dichlorophenyl)-3-hydroxyquinoline-4(1_H_)-one-5-carboxamide (15b)



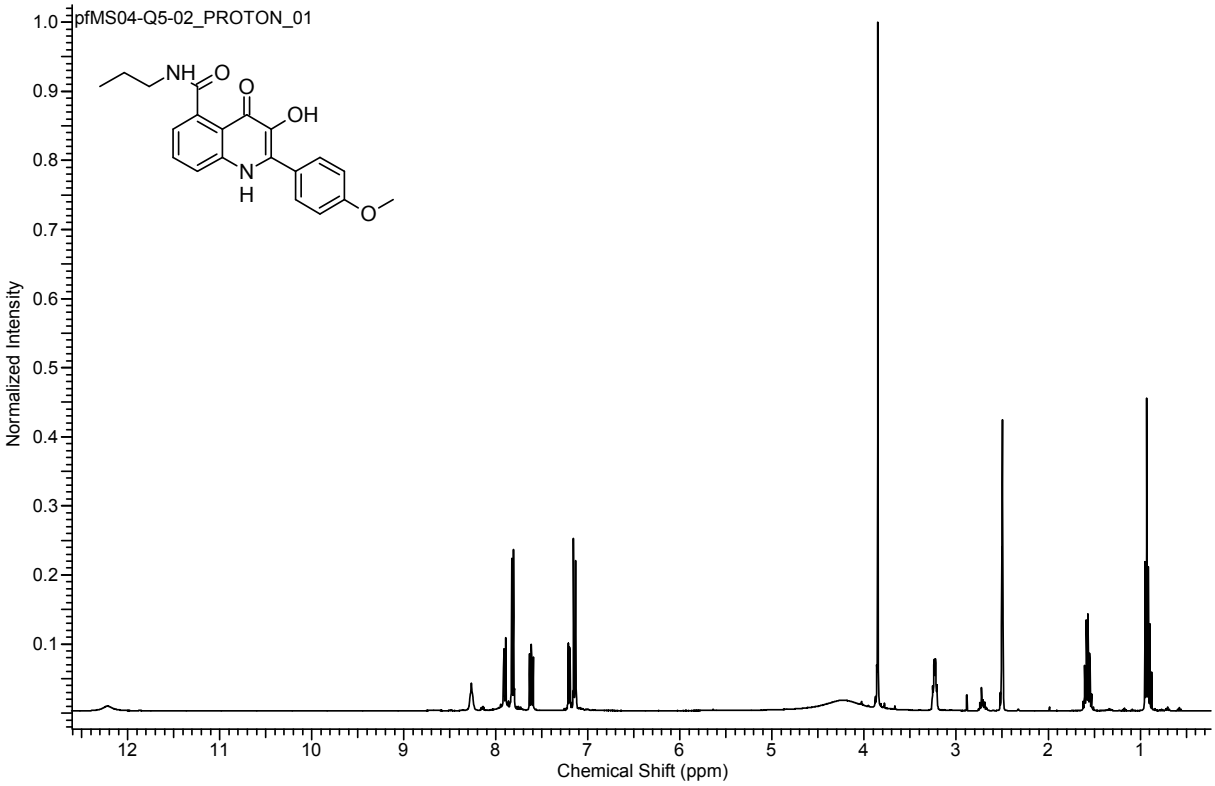


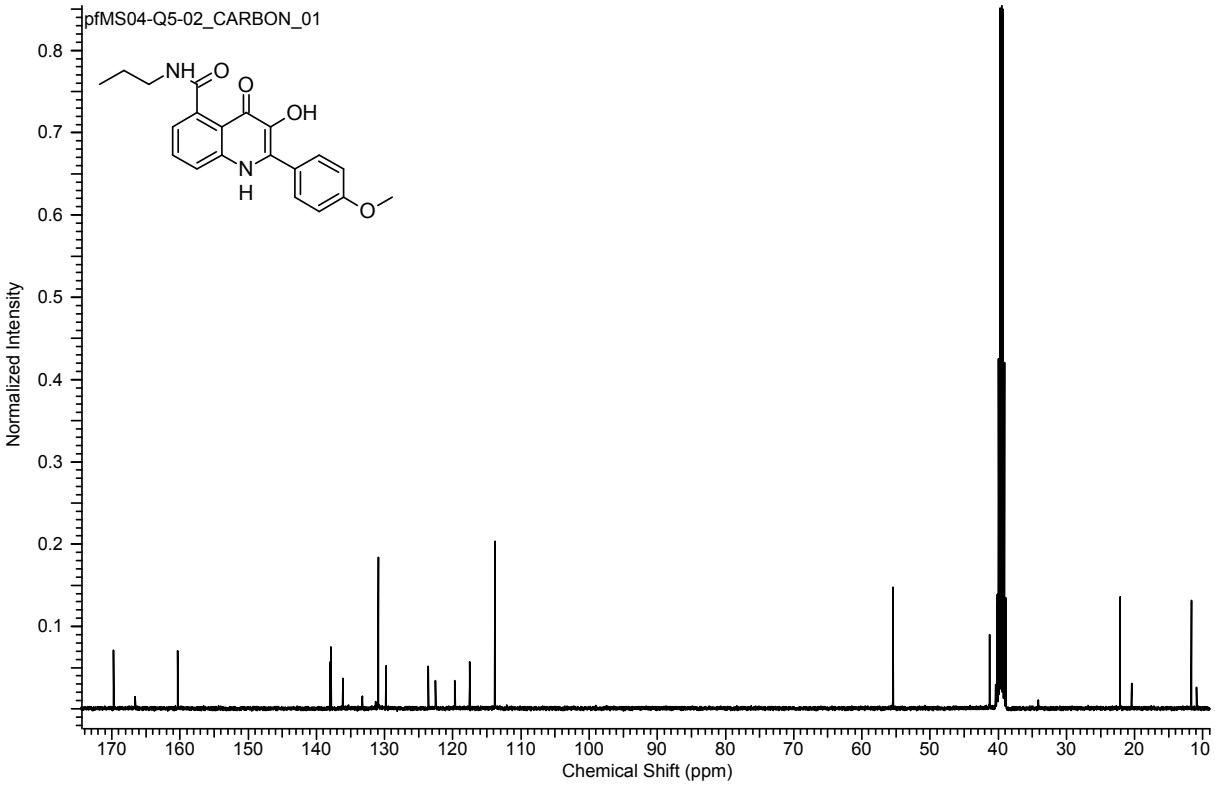
***N*-Propyl-2-(*p*-tolyl)-3-hydroxyquinoline-4(1*H*)-one-5-carboxamide (15c):**



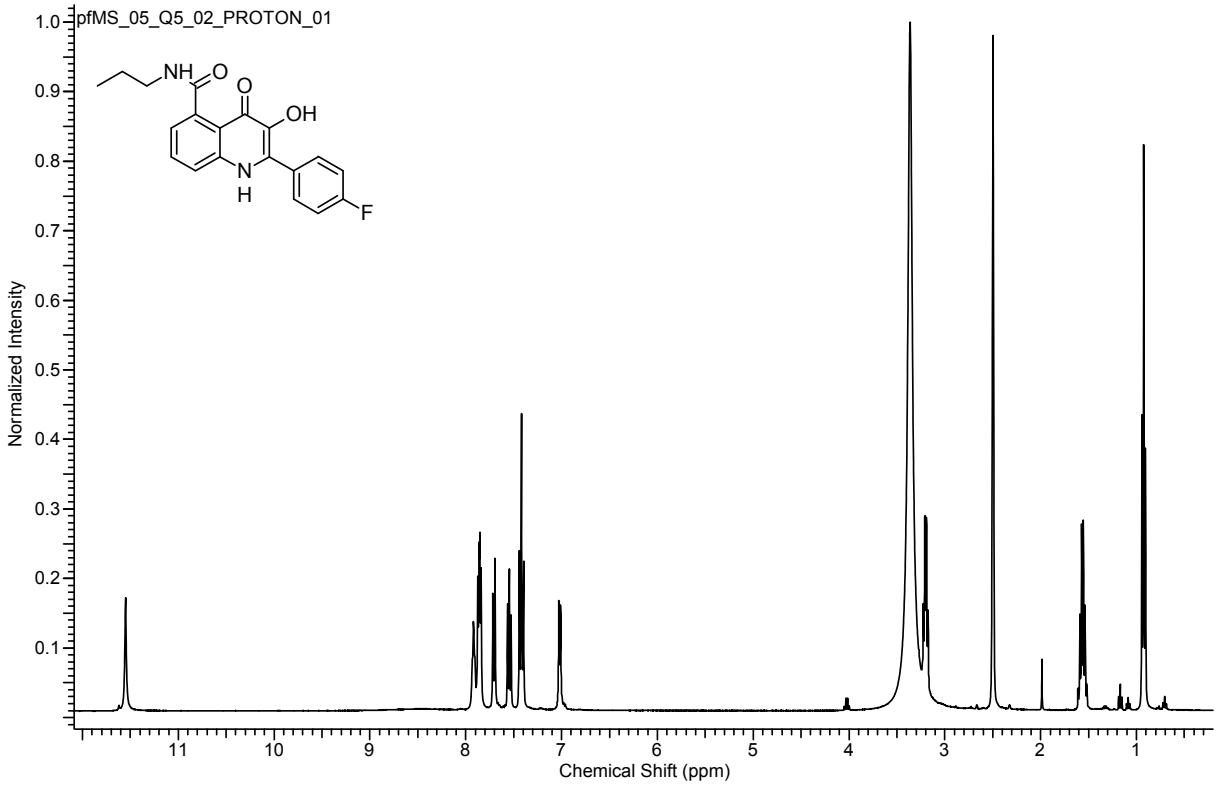


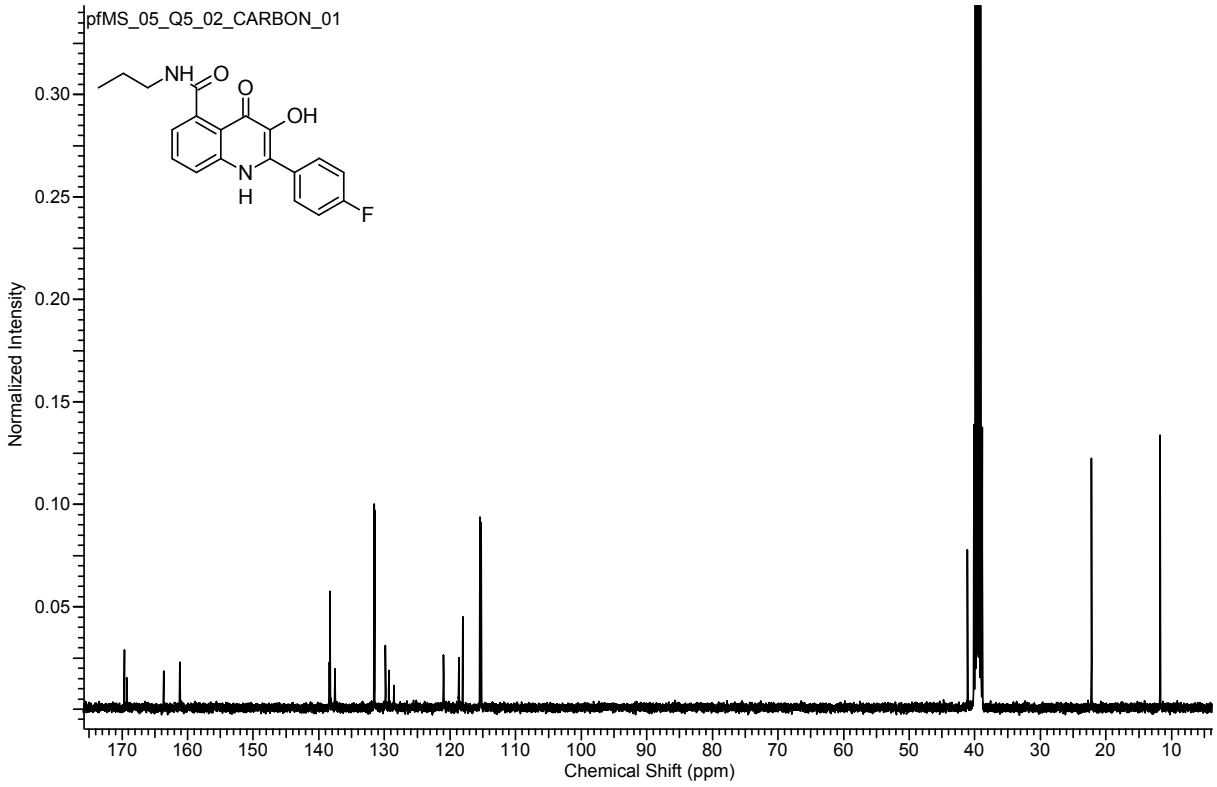
***N*-Propyl-2-(4-Methoxyphenyl)-3-hydroxyquinoline-4(1*H*)-one-5-carboxamide (15d):**



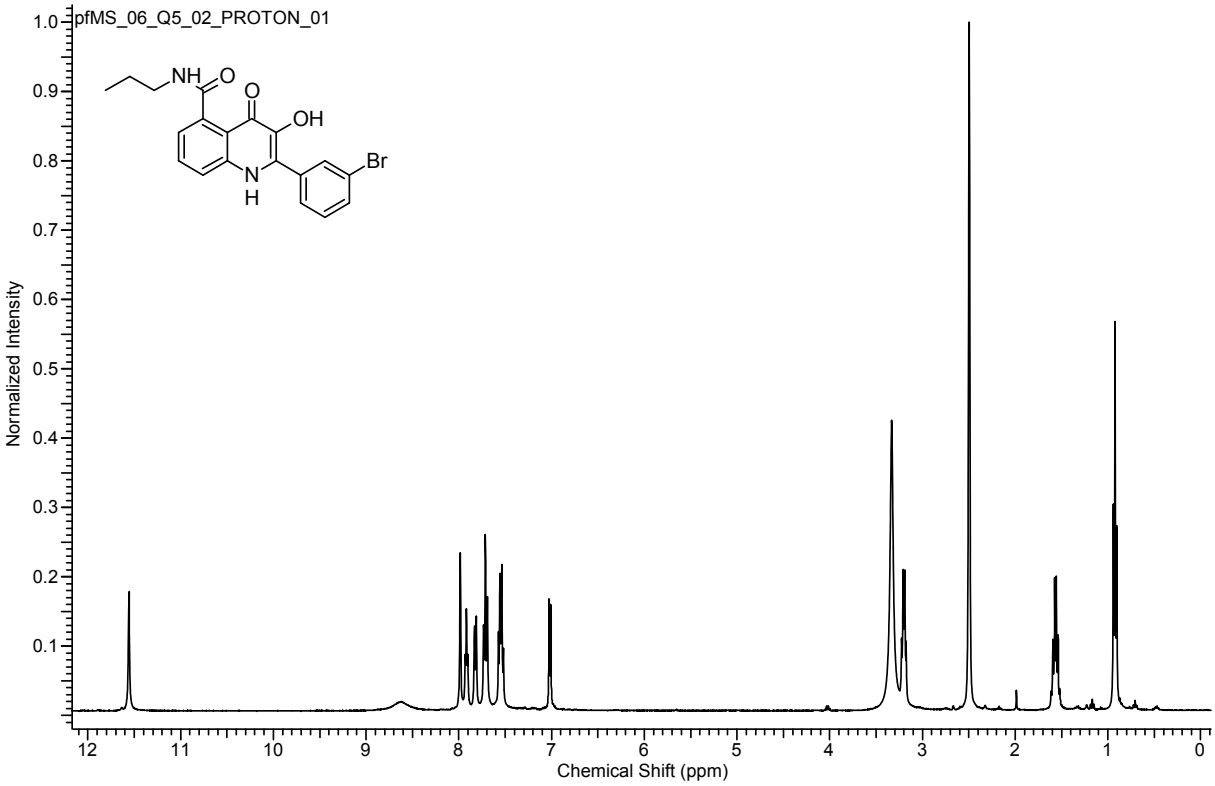


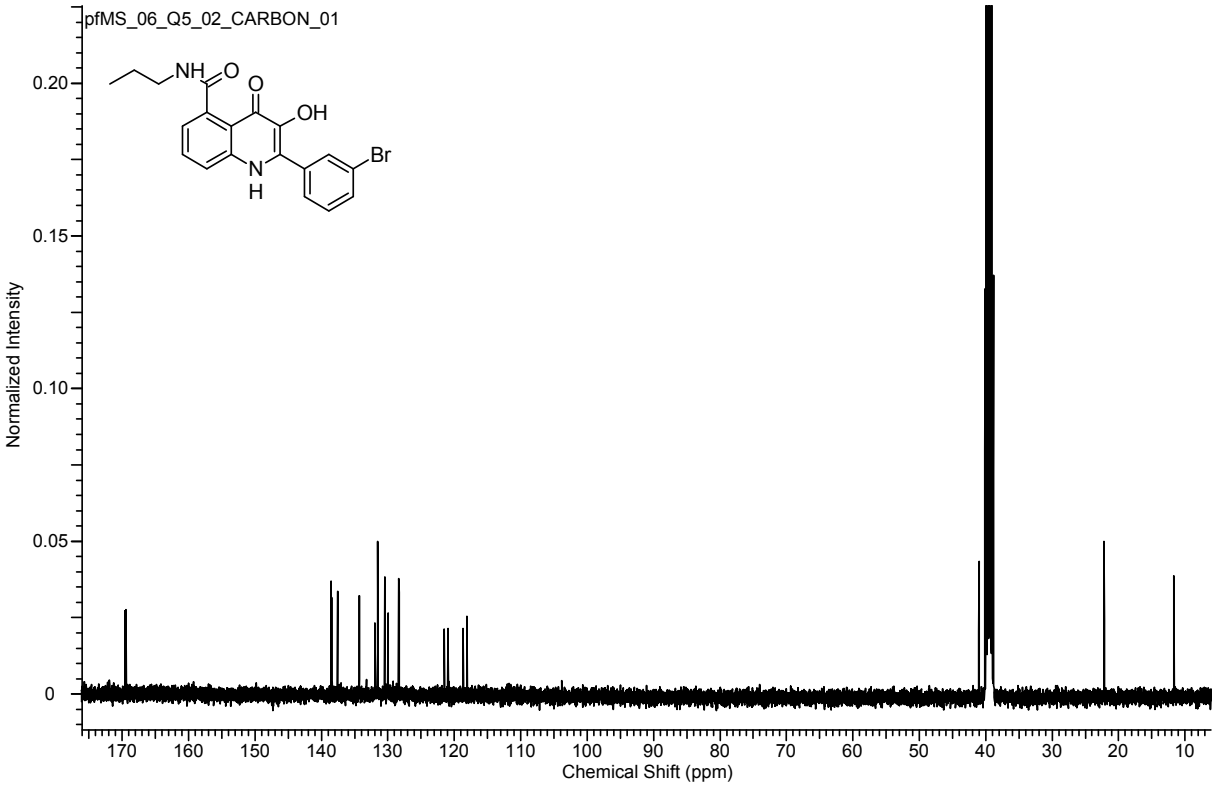
***N*-Propyl-2-(4-fluorophenyl)- 3-hydroxyquinoline-4(1*H*)-one-5-carboxamide (15e):**



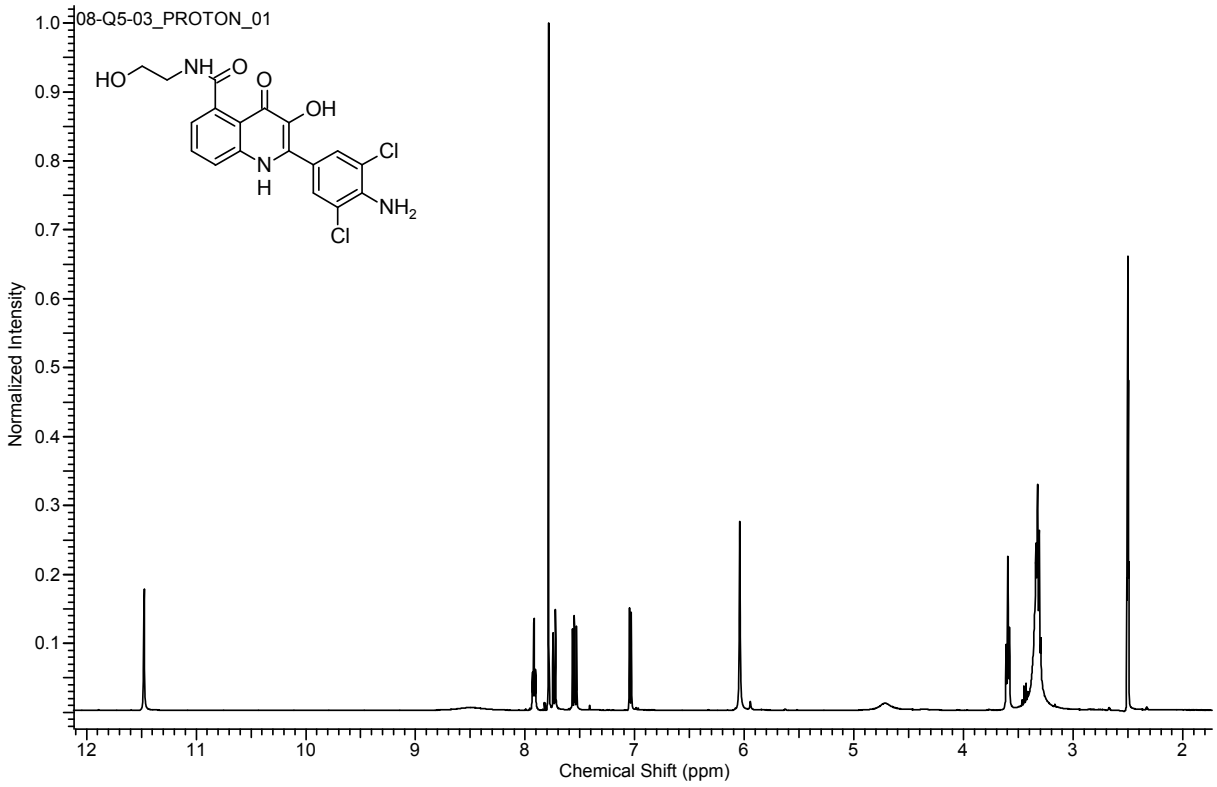


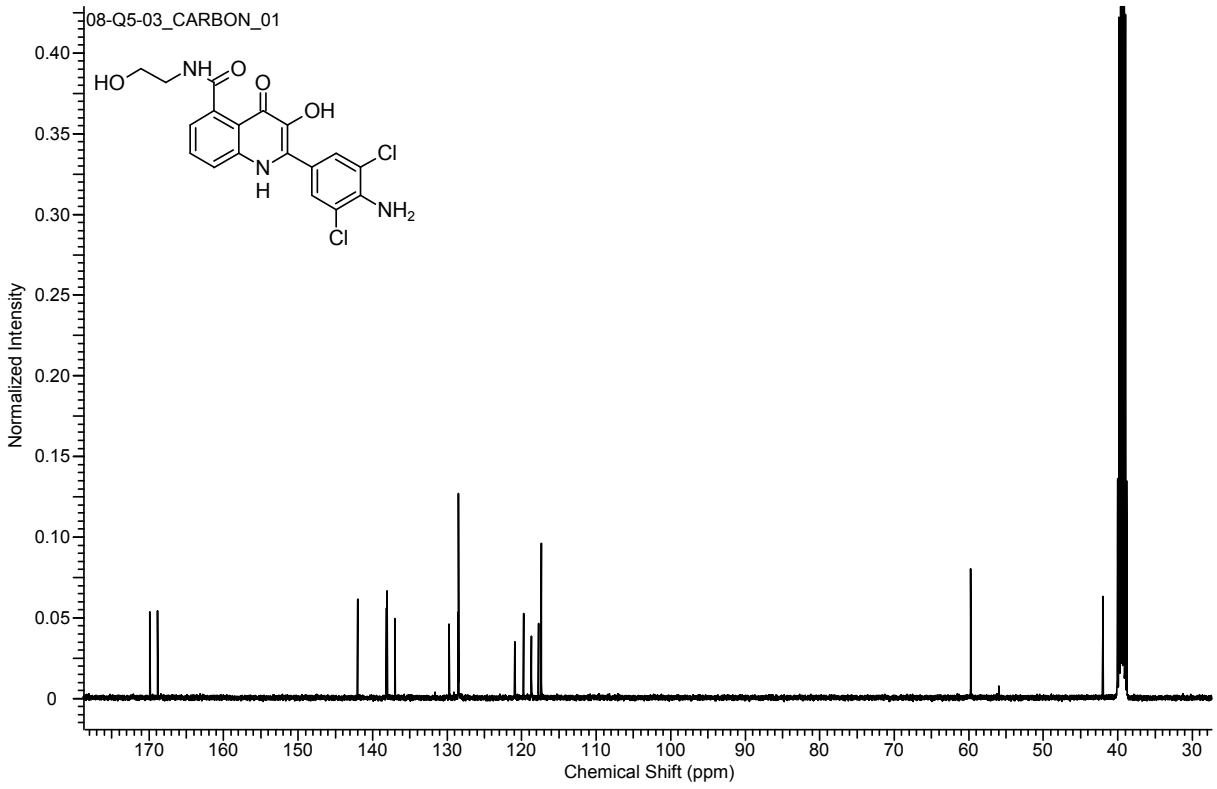
***N*-Propyl-2-(3-bromophenyl)-3-hydroxyquinoline-4(1*H*)-one-5-carboxamide (15f):**



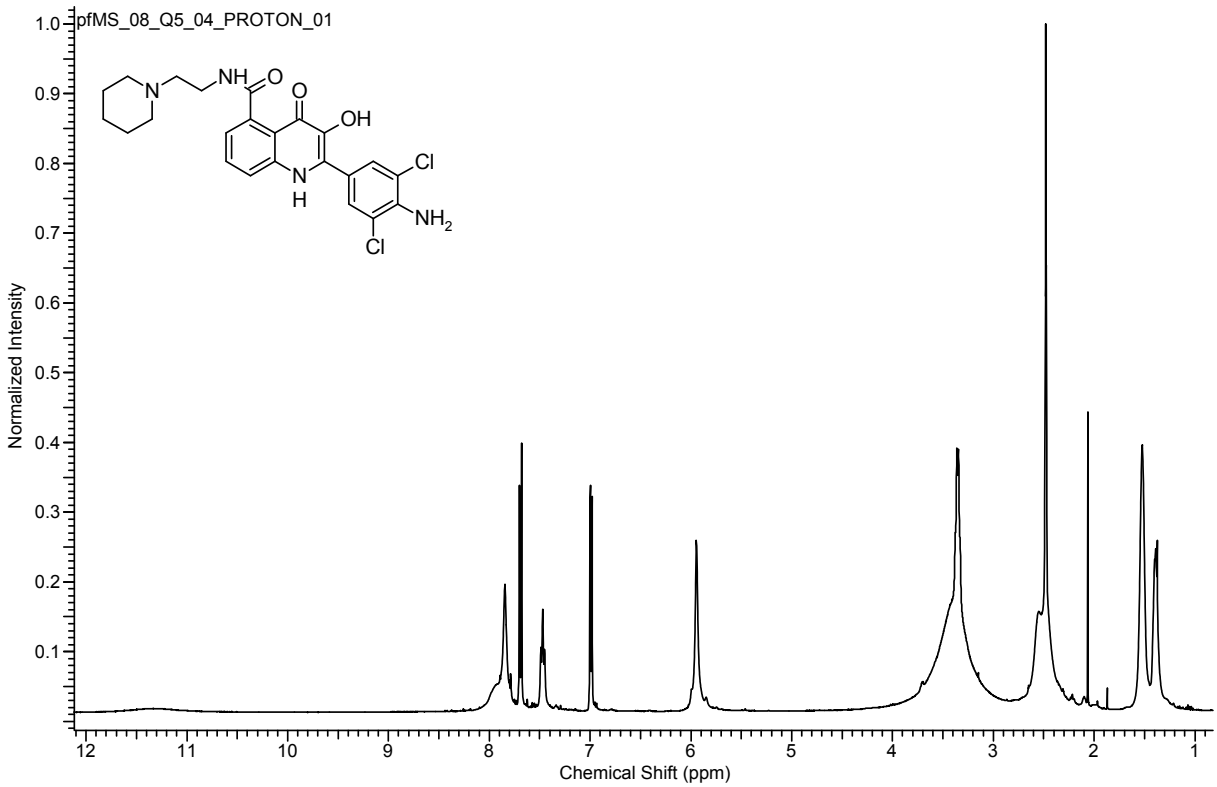


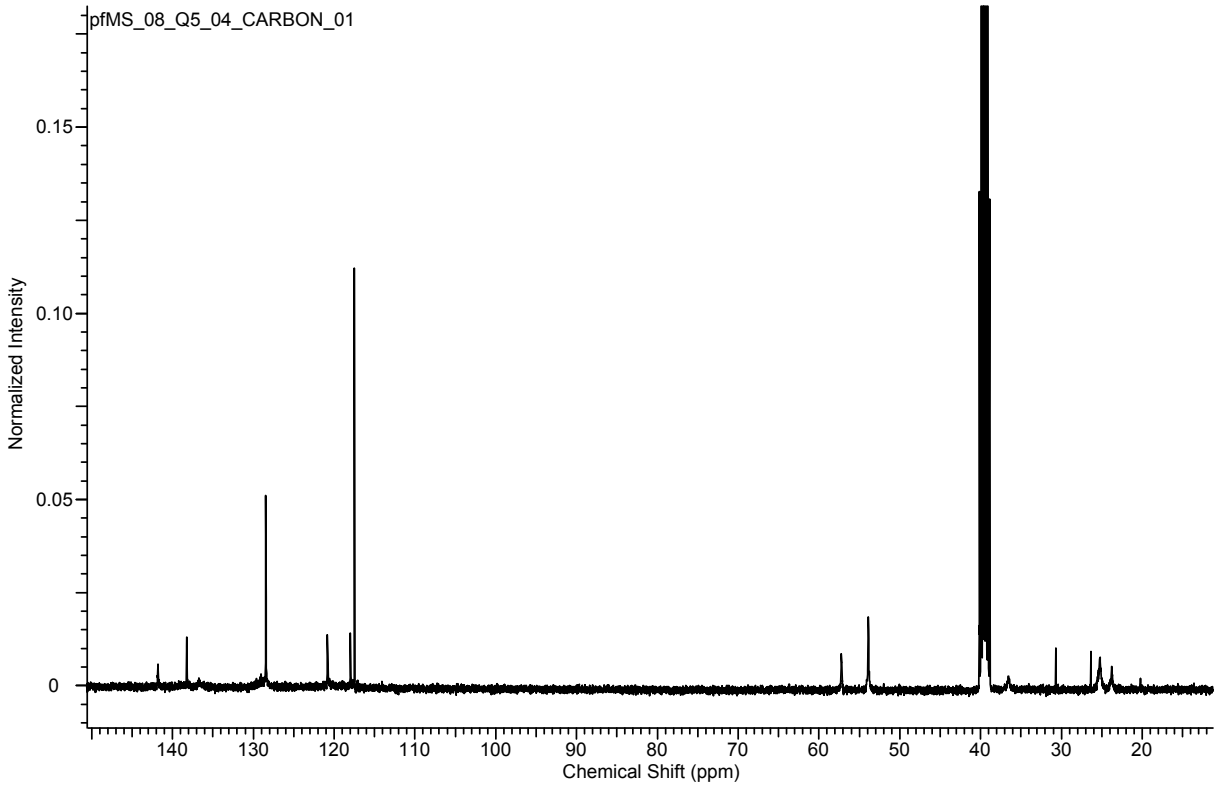
***N*-(2-Hydroxyethyl)-2-(4-amino-3,5-dichlorophenyl)-3-hydroxyquinoline-4(1*H*)-one-5-carboxamide (15g):**



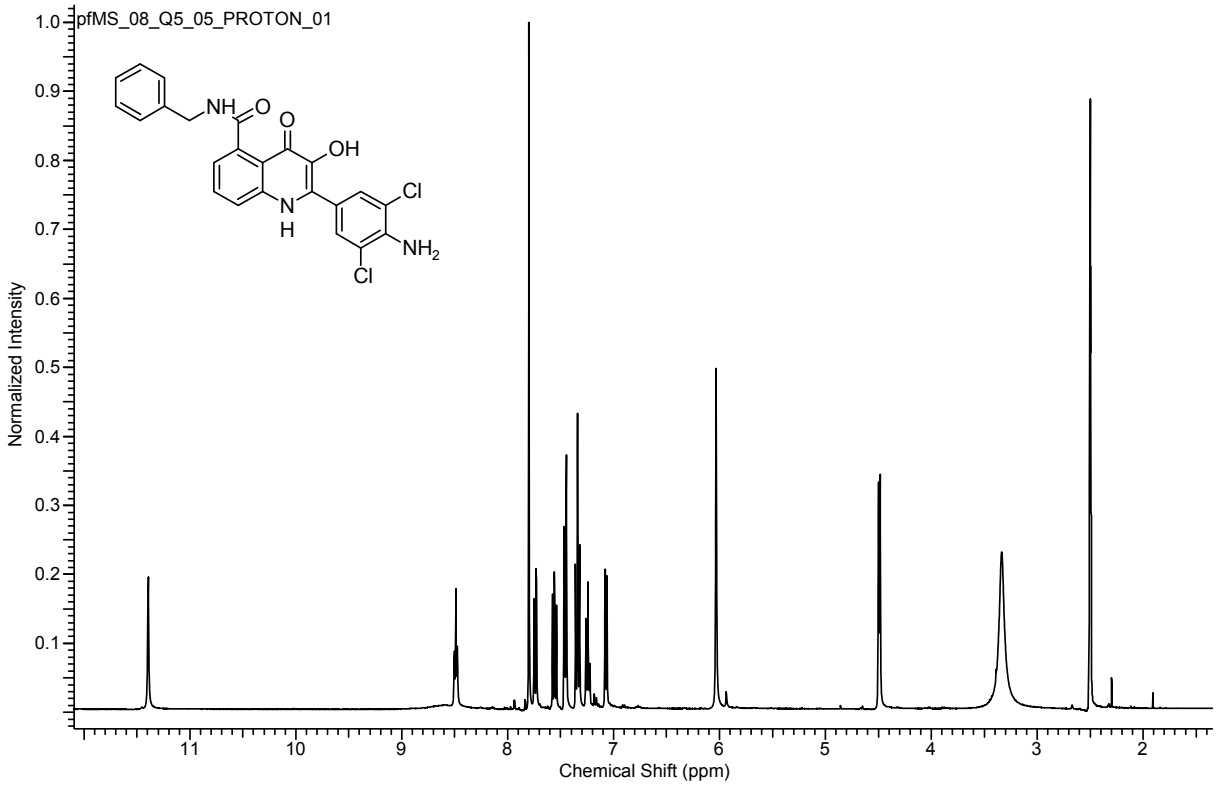


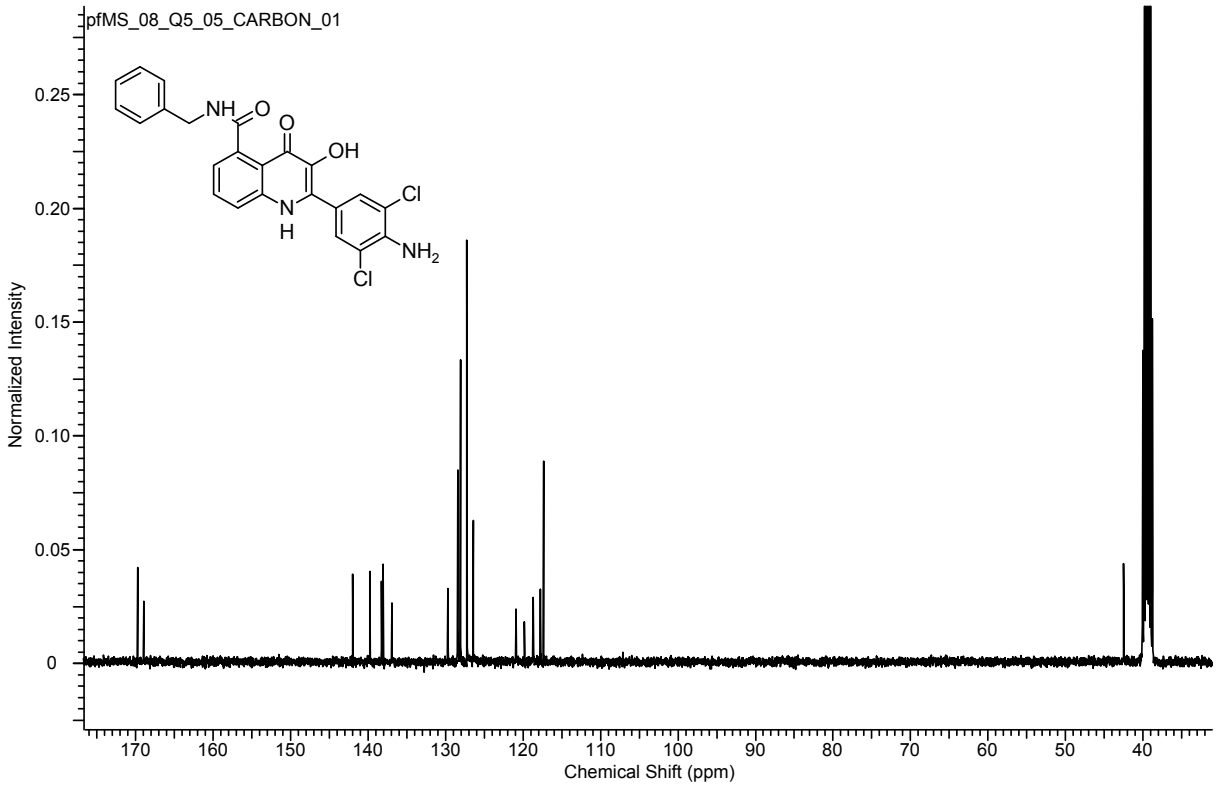
***N*-(2-(Piperidin-1-yl)ethyl)-2-(4-amino-3,5-dichlorophenyl)-3-hydroxyquinoline-4(1*H*)-one-5-carboxamide (15h):**



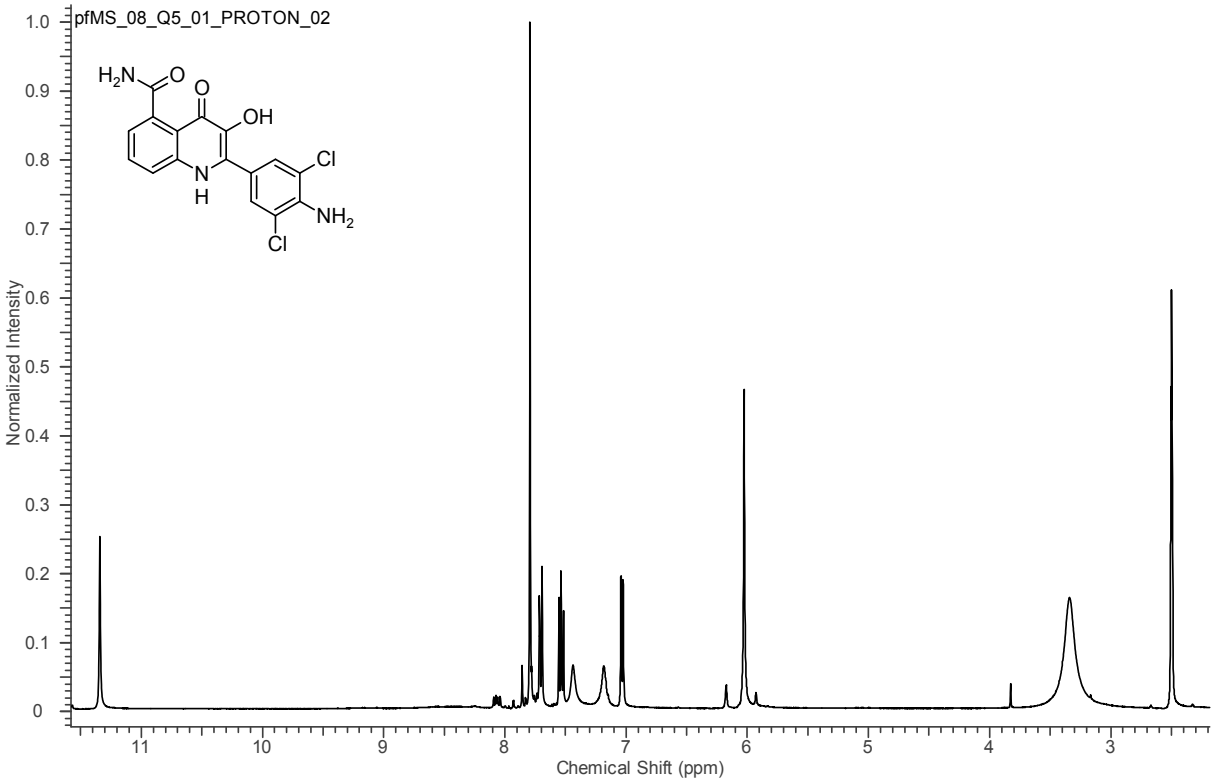


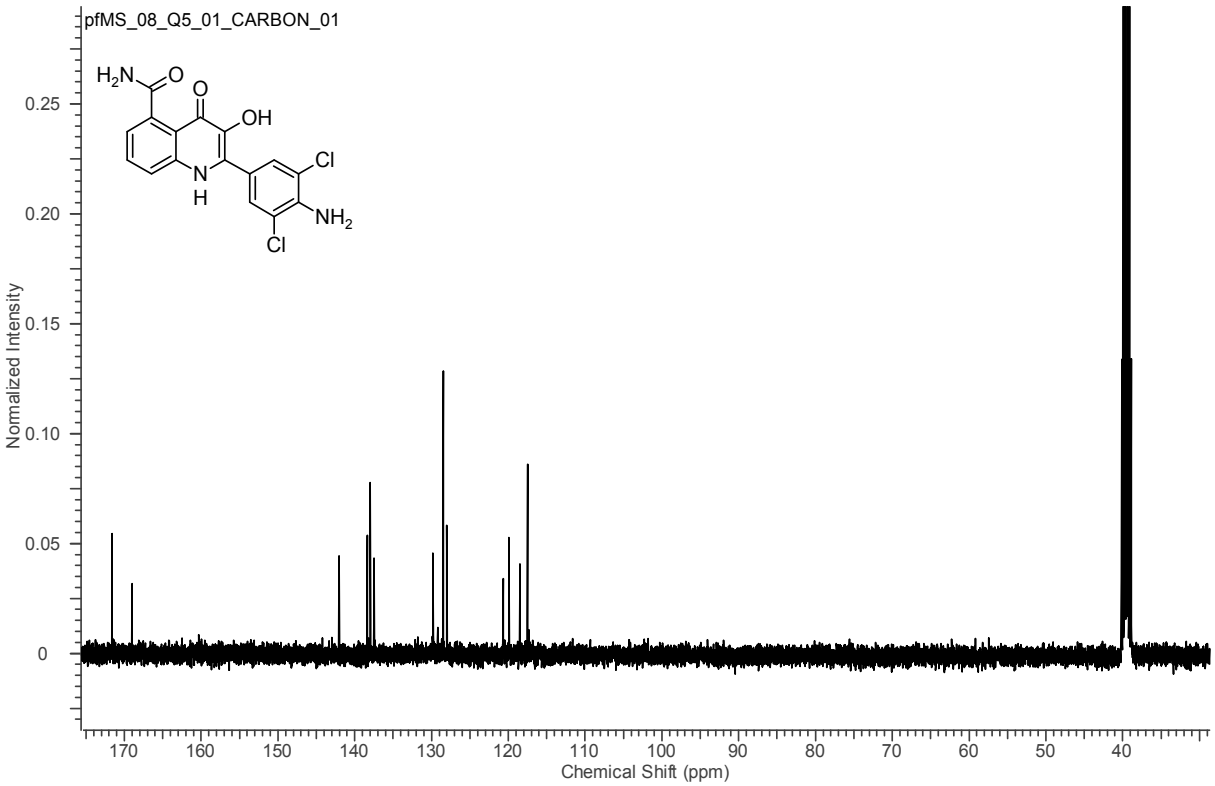
***N*-Benzyl-2-(4-amino-3,5-dichlorophenyl)-3-hydroxyquinoline-4(1*H*)-one-5-carboxamide (15i):**



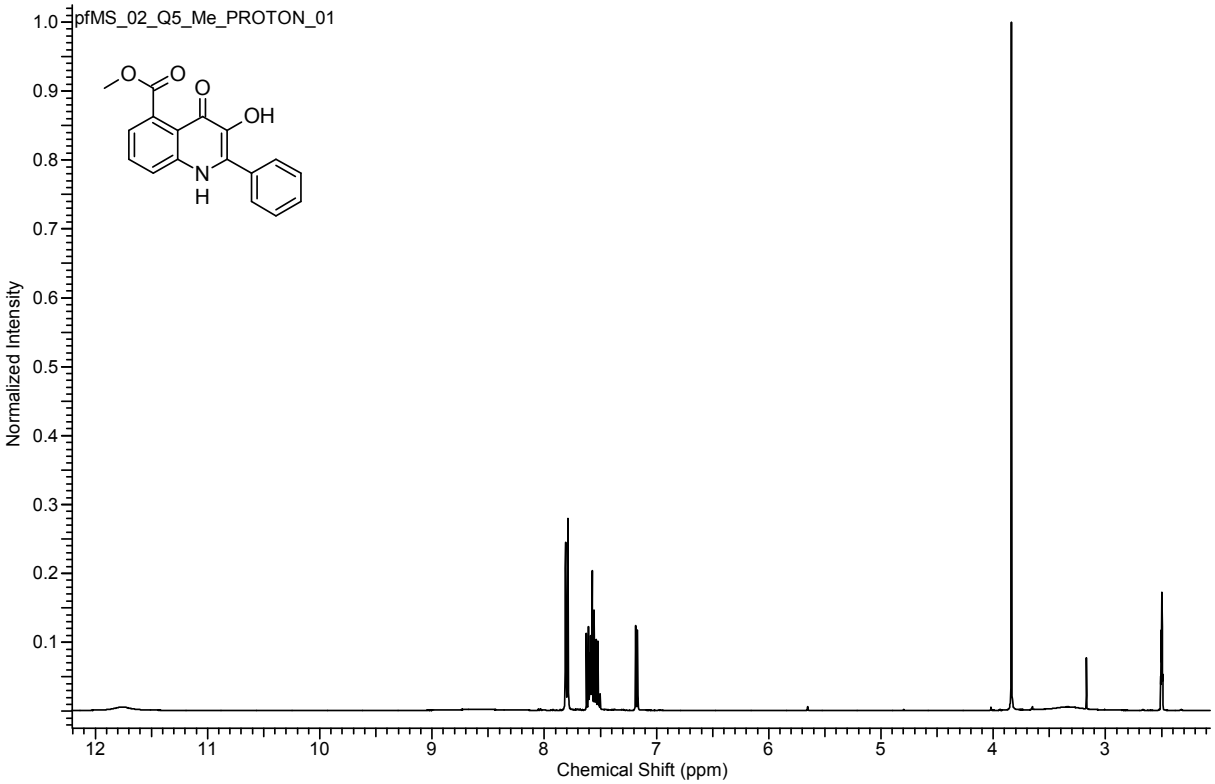


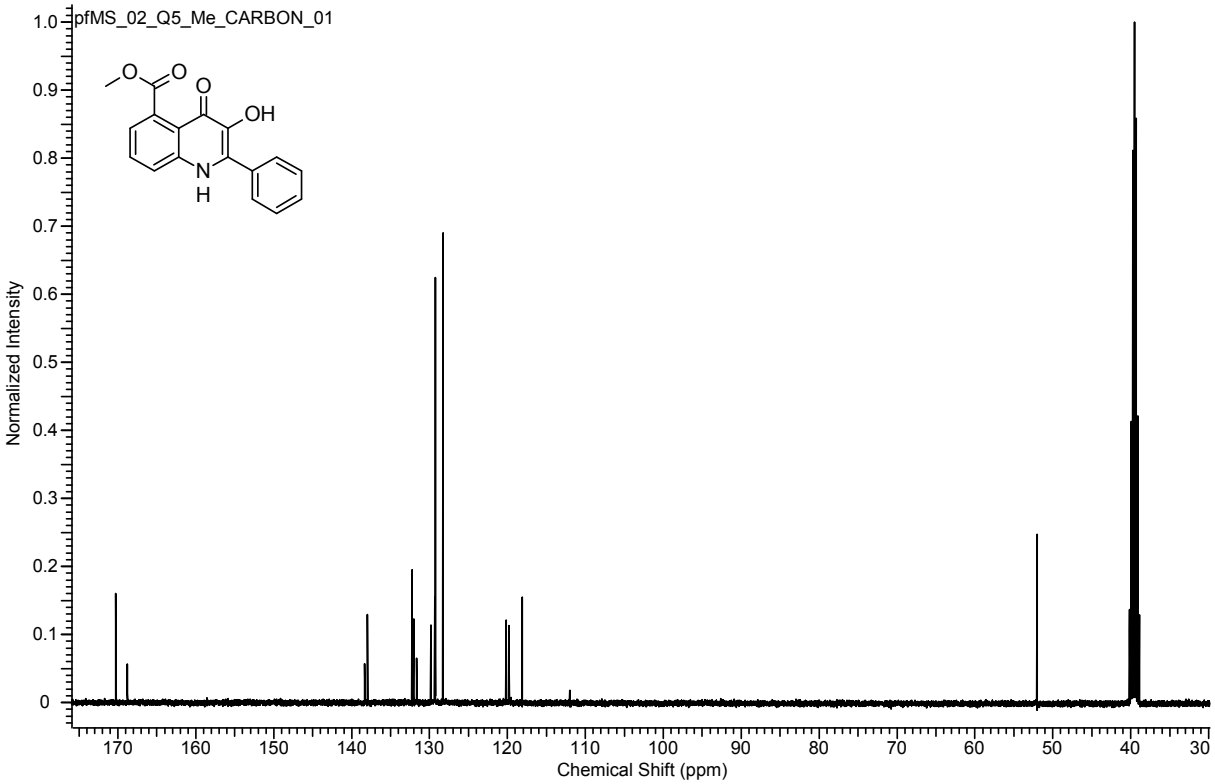
2-(4-Amino-3,5-dichlorophenyl)-3-hydroxyquinoline-4(1*H*)-one-5-carboxamide (15l):



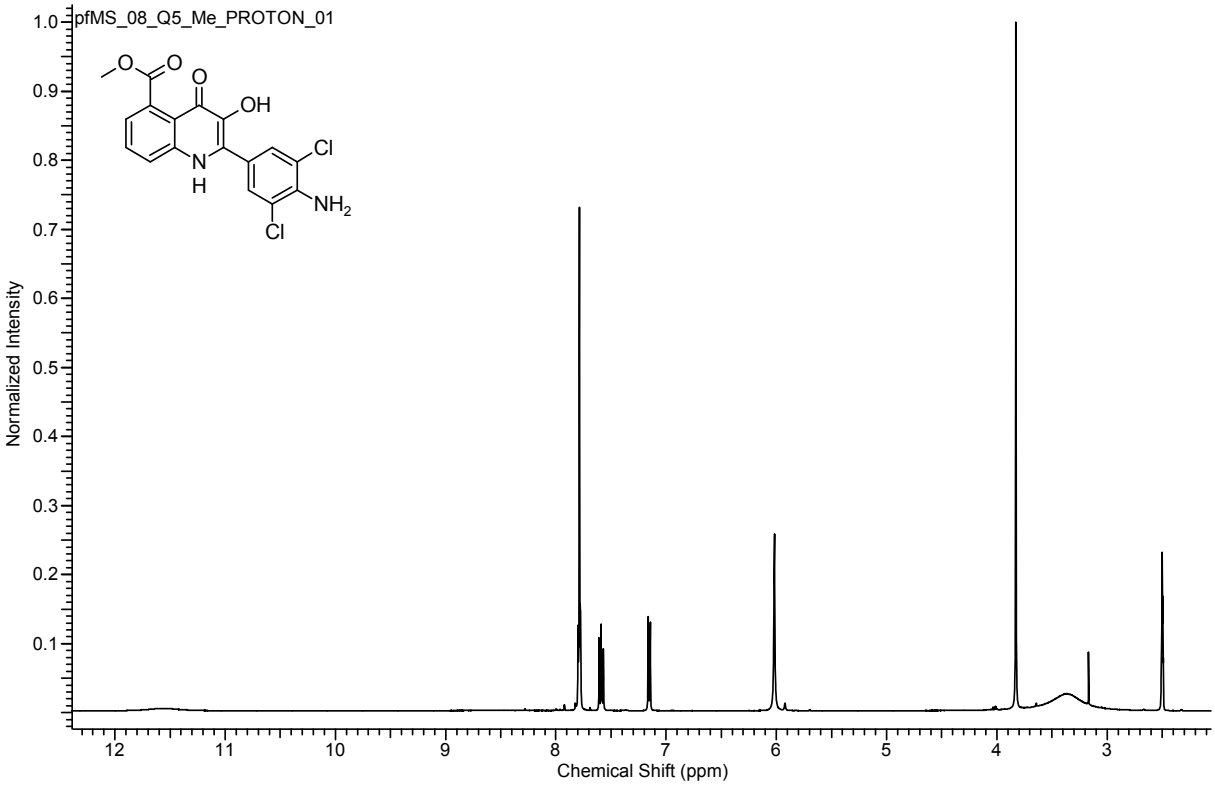


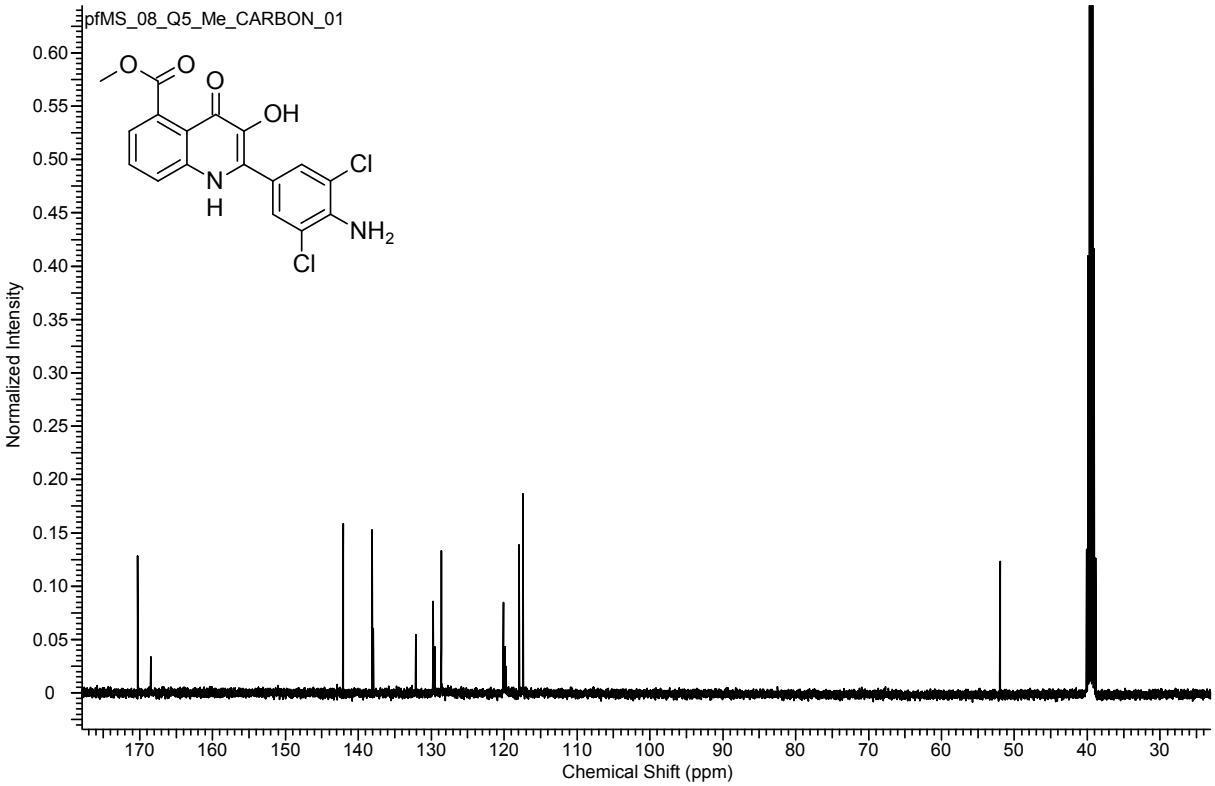
Methyl 2-phenyl-3-hydroxyquinoline-4(1*H*)-one-5-carboxylate (16a)





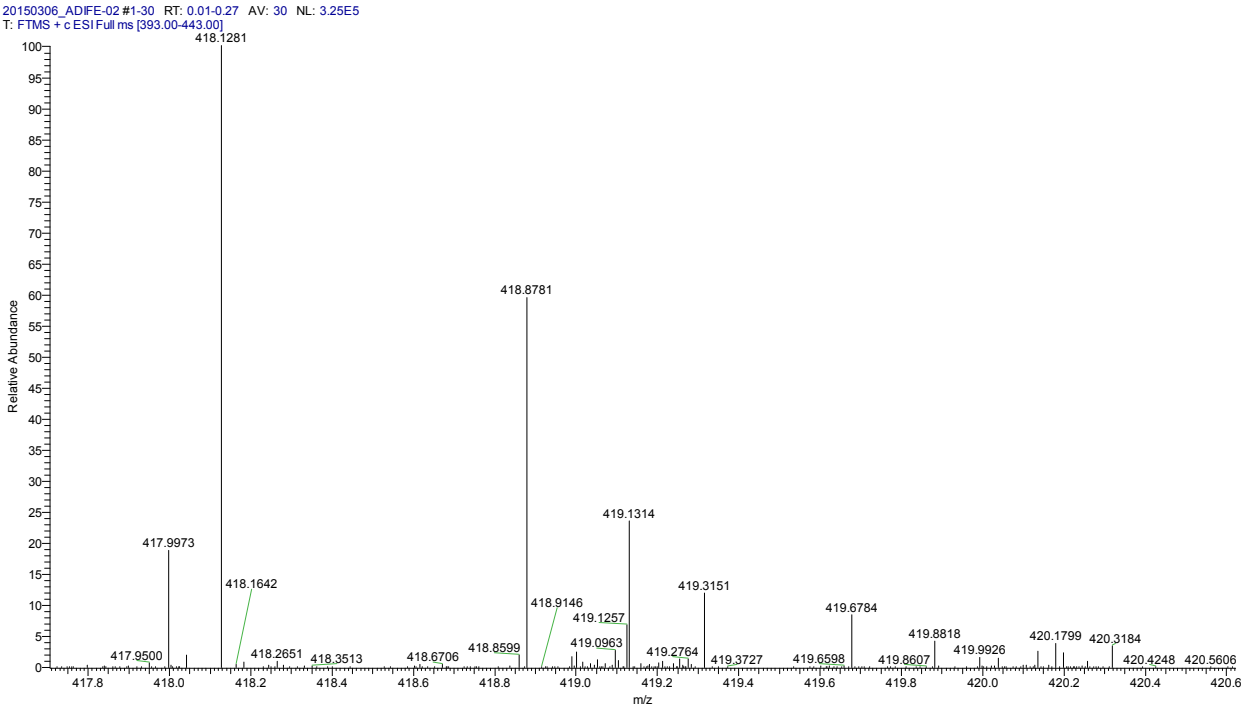
Methyl 2-(4-amino-3,5-dichlorophenyl)-3-hydroxyquinoline-4(1*H*)-one-5-carboxylate (16b)



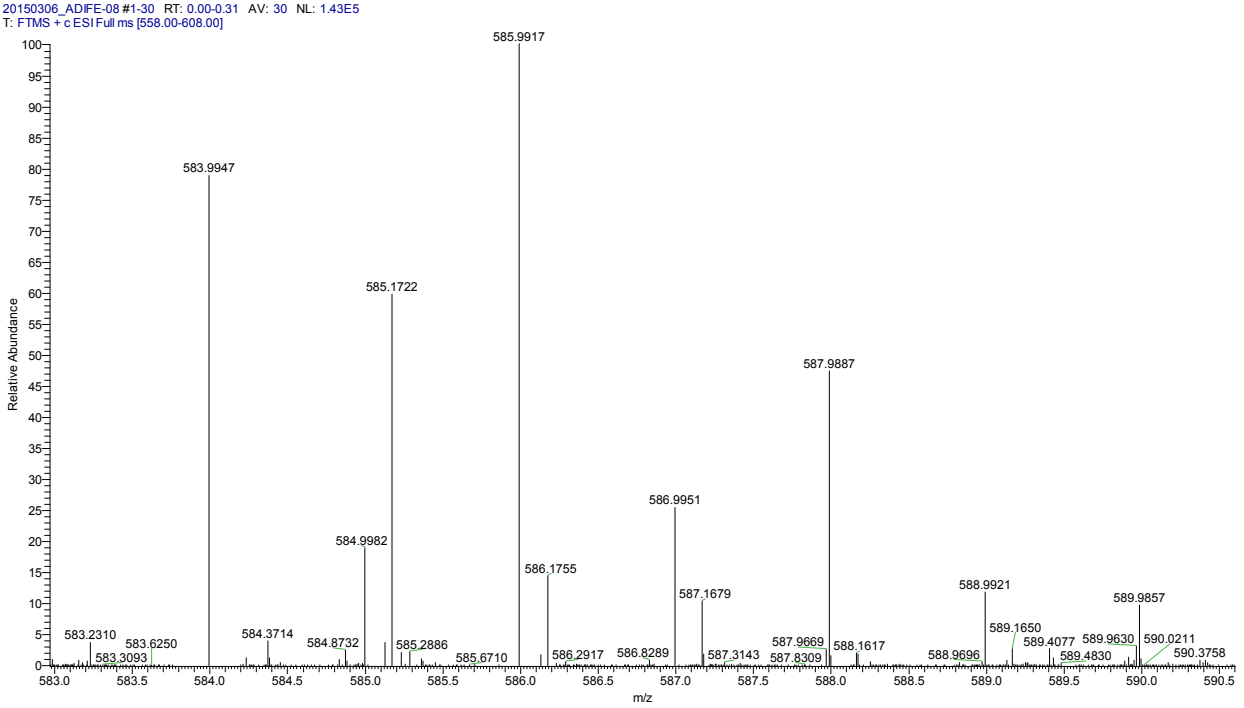


Original HRMS spectra

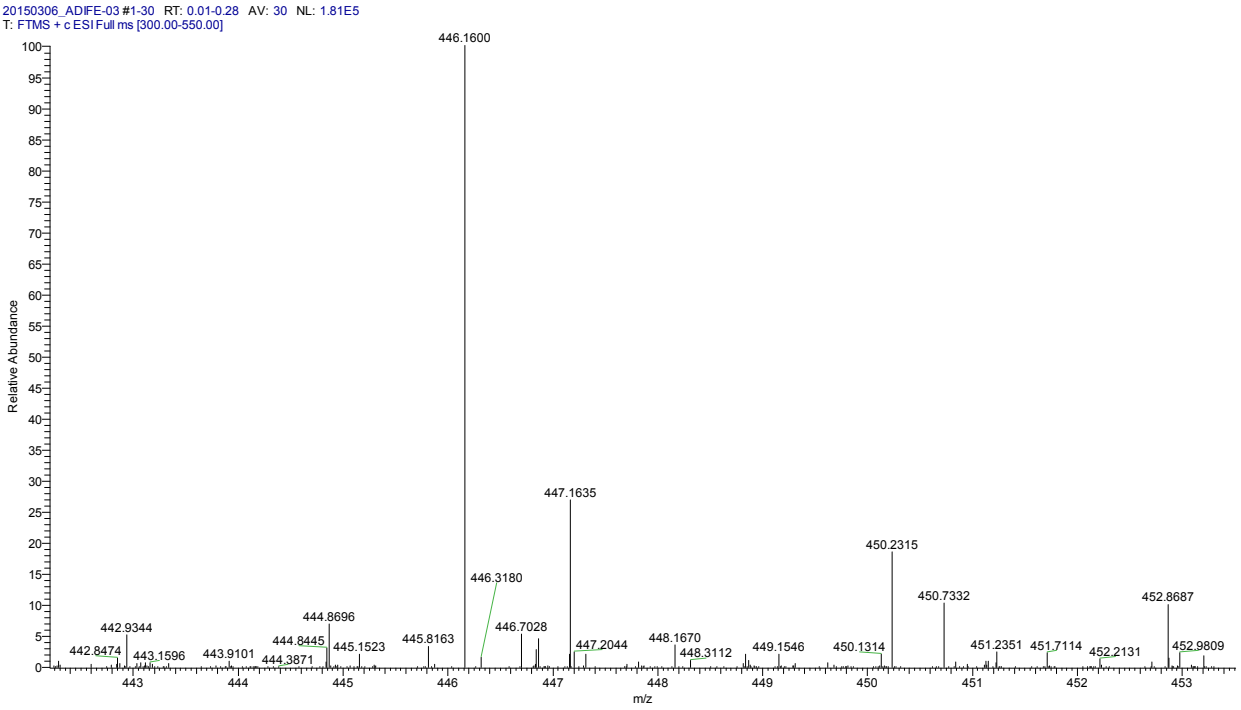
Bis(2-oxo-2-phenylethyl) 3-aminophthalate (13a):



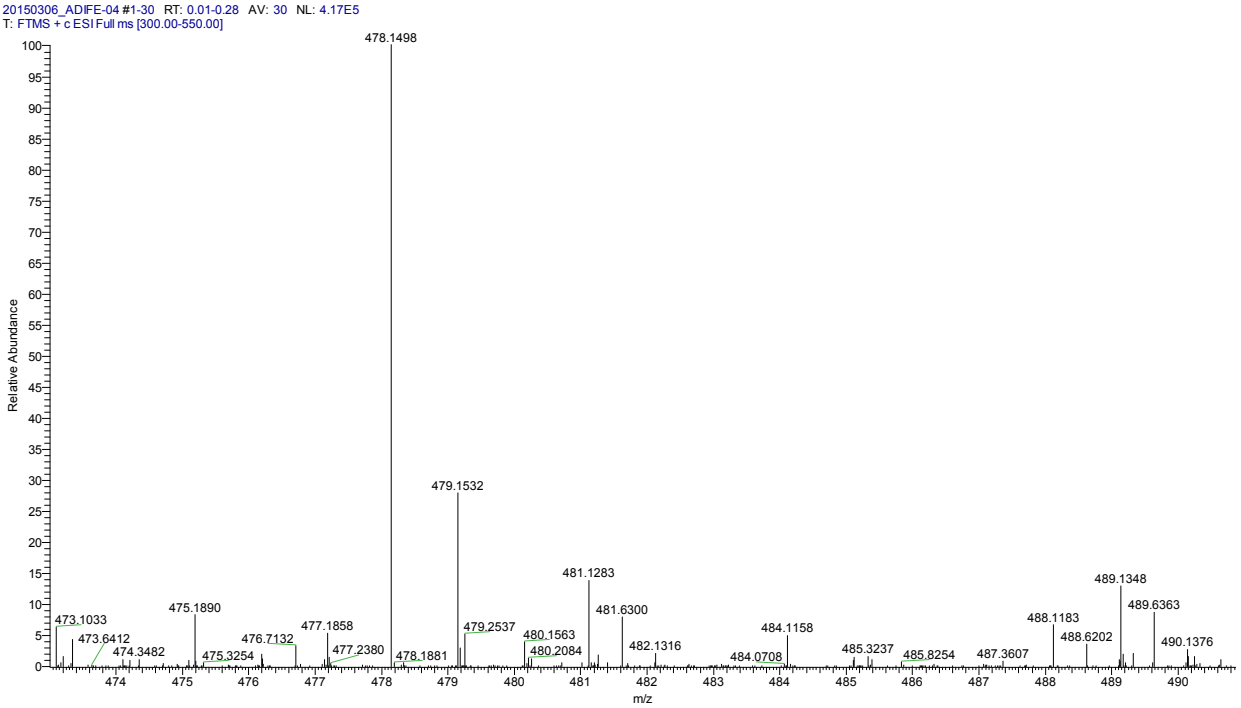
Bis(2-(4-amino-3,5-dichlorophenyl)-2-oxoethyl) 3-aminophthalate (13b):



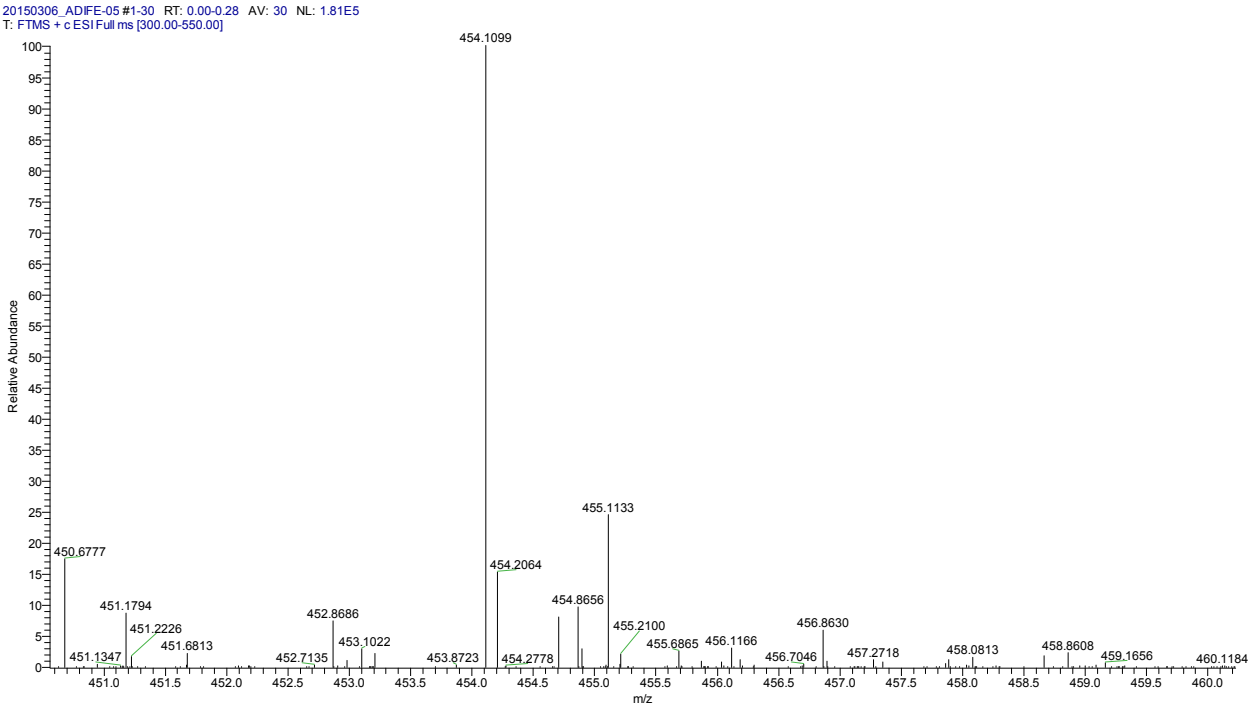
Bis(2-oxo-2-(*p*-tolyl)ethyl) 3-aminophthalate (13c):



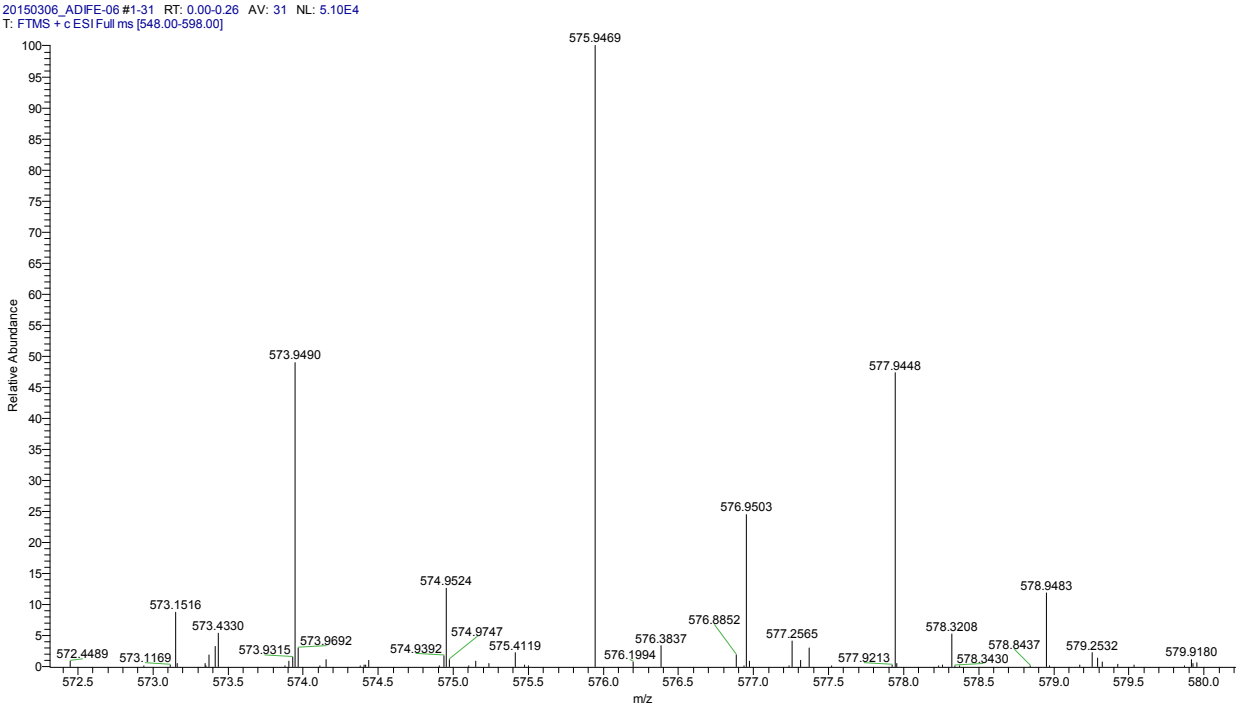
Bis(2-(4-methoxyphenyl)-2-oxoethyl) 3-aminophthalate (13d):



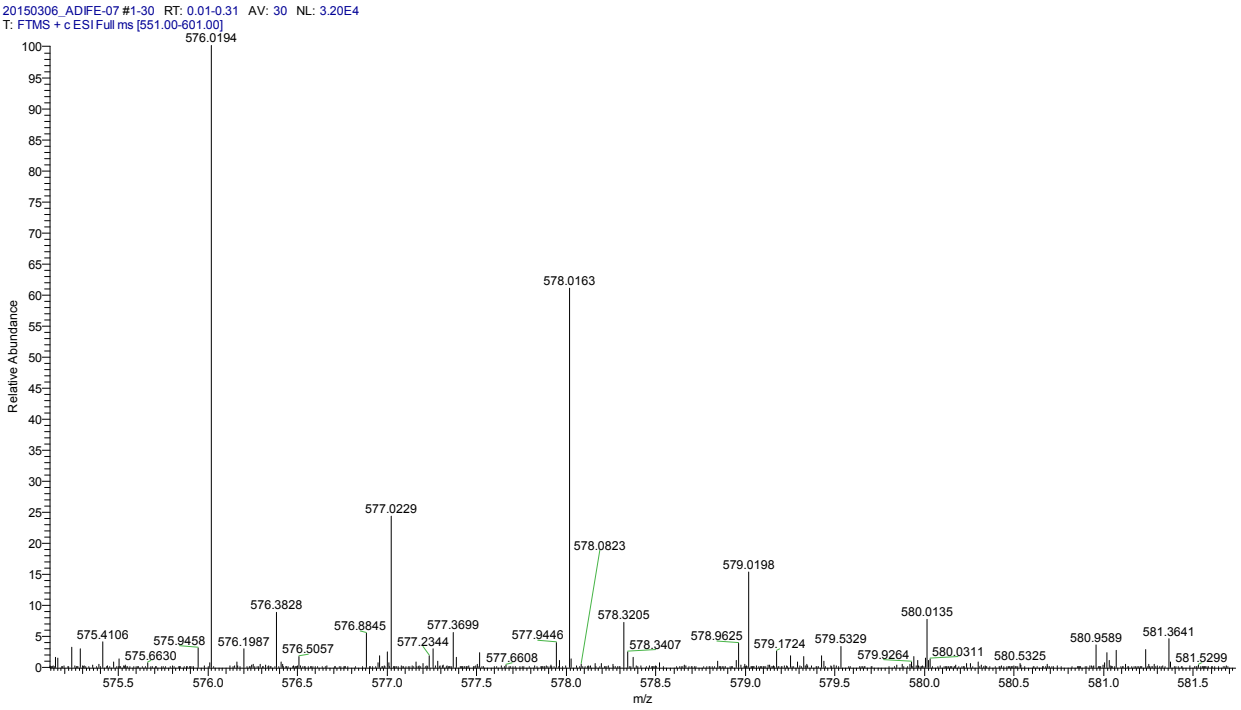
Bis(2-(4-fluorophenyl)-2-oxoethyl) 3-aminophthalate (13e):



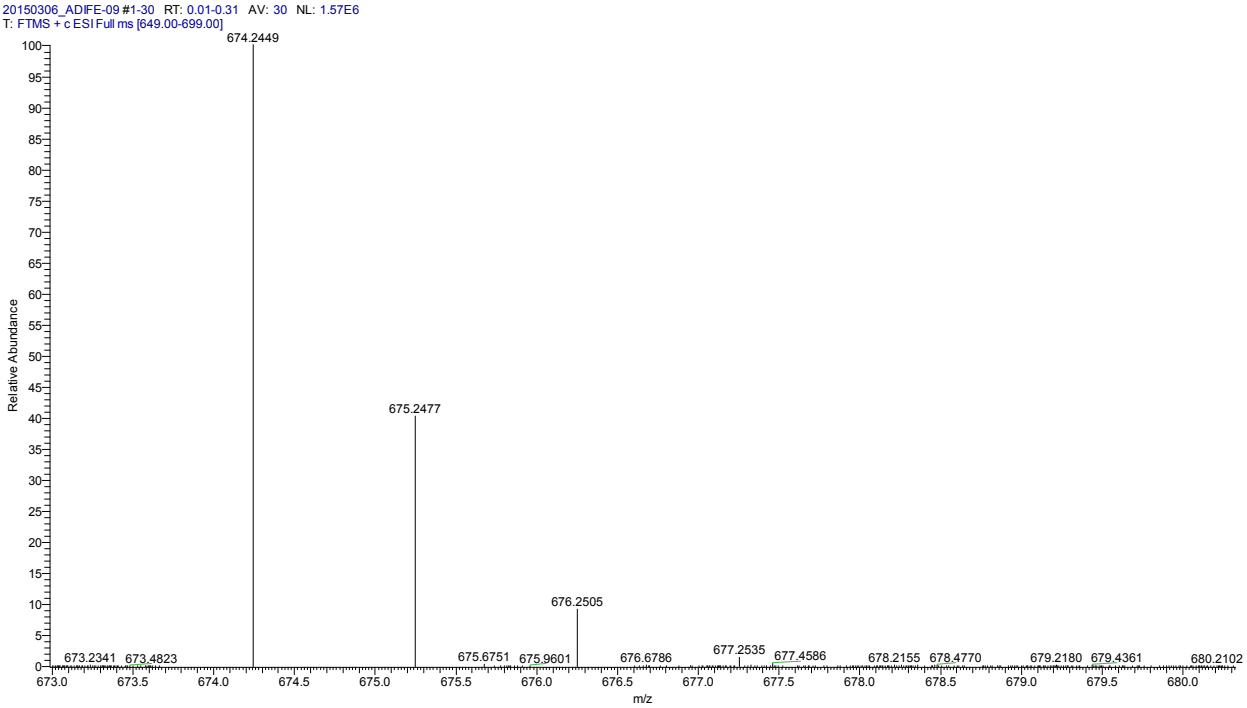
Bis(2-(3-bromophenyl)-2-oxoethyl) 3-aminophthalate (13f):



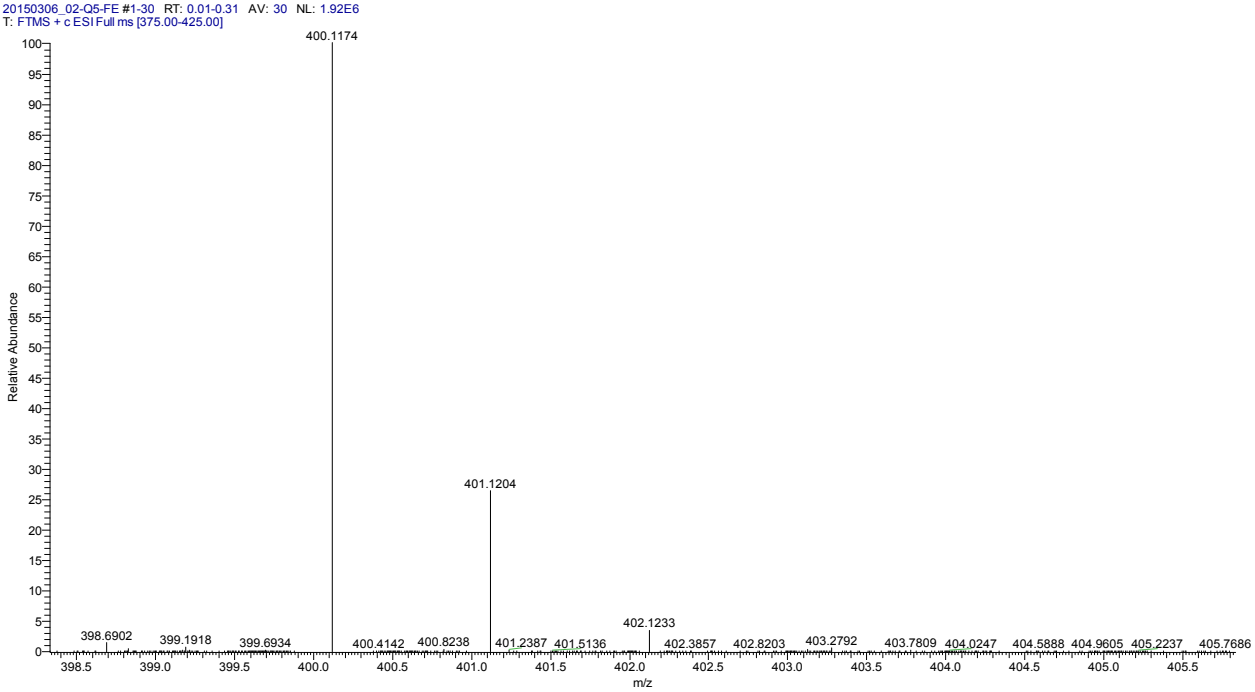
Bis(2-(4-chloro-3-nitrophenyl)-2-oxoethyl) 3-aminophthalate (13g):



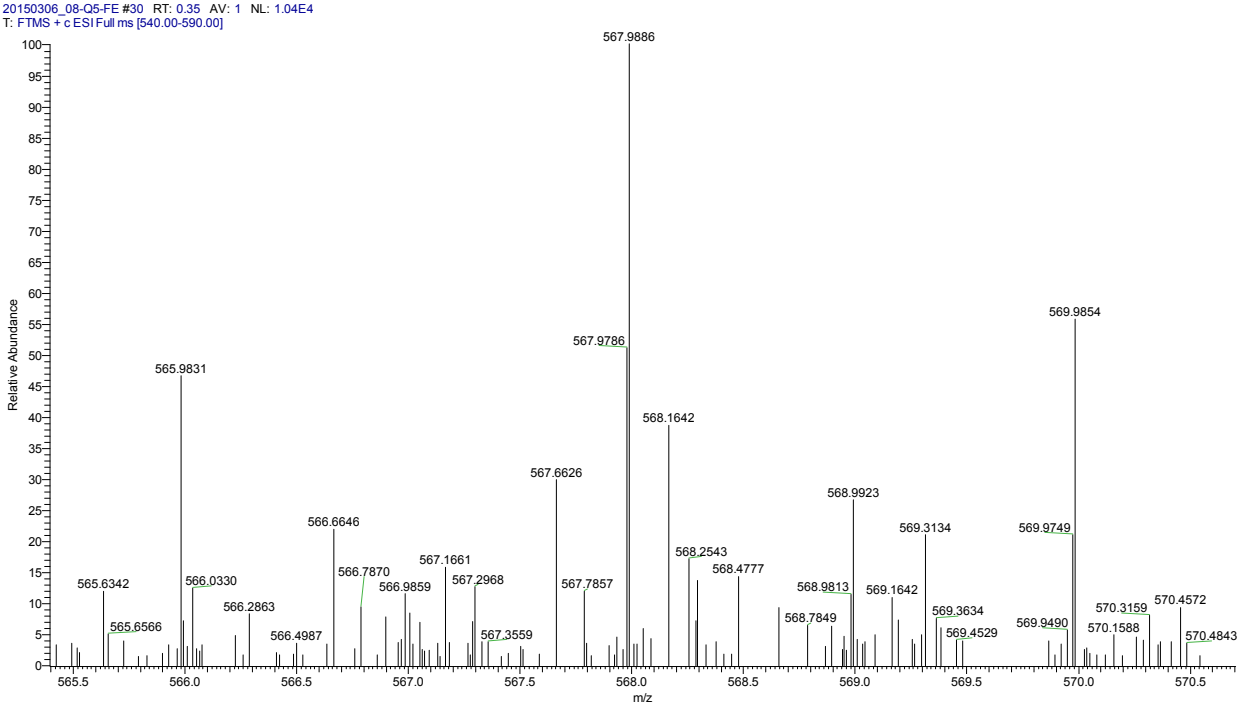
Bis(2-(3-nitro-4-(piperidin-1-yl)phenyl)-2-oxoethyl) 3-aminophthalate (13h):



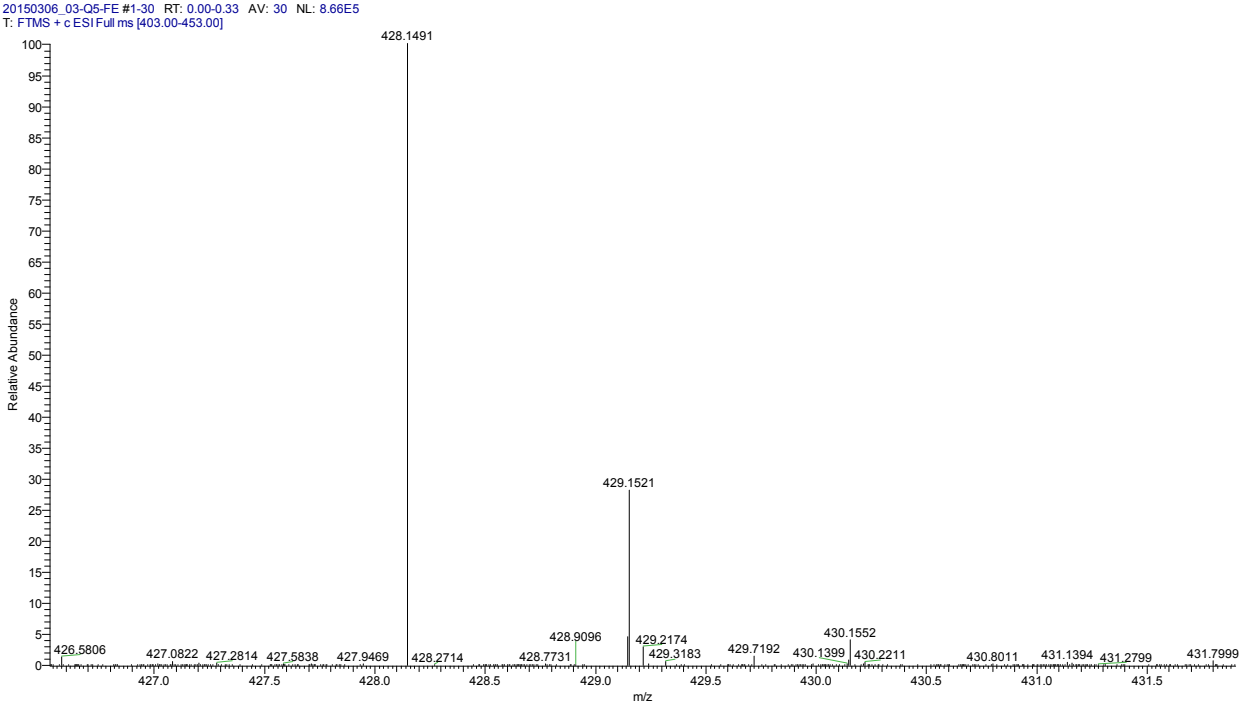
2-Oxo-2-phenylethyl 2-phenyl-3-hydroxyquinoline-4(1*H*)-one-5-carboxylate (14a):



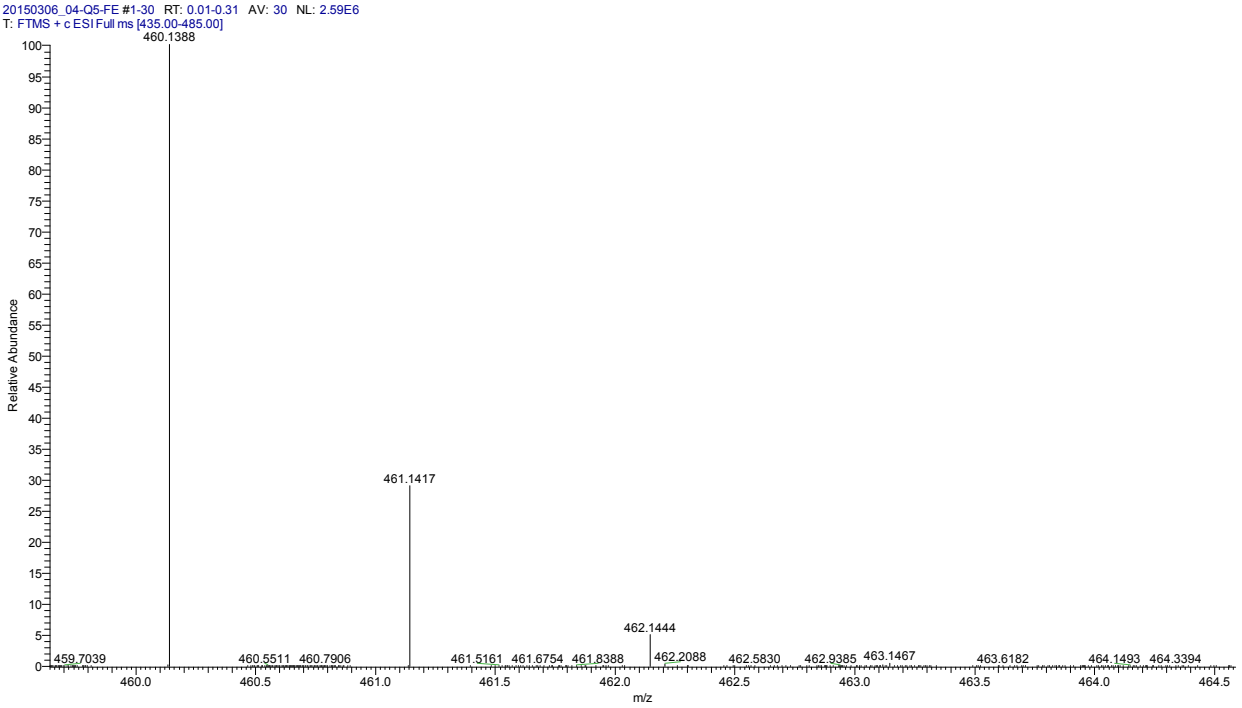
2-(4-Amino-3,5-dichlorophenyl)-2-oxoethyl 2-(4-amino-3,5-dichlorophenyl)- hydroxyquinoline-4(1*H*)-one-5-carboxylate (14b):



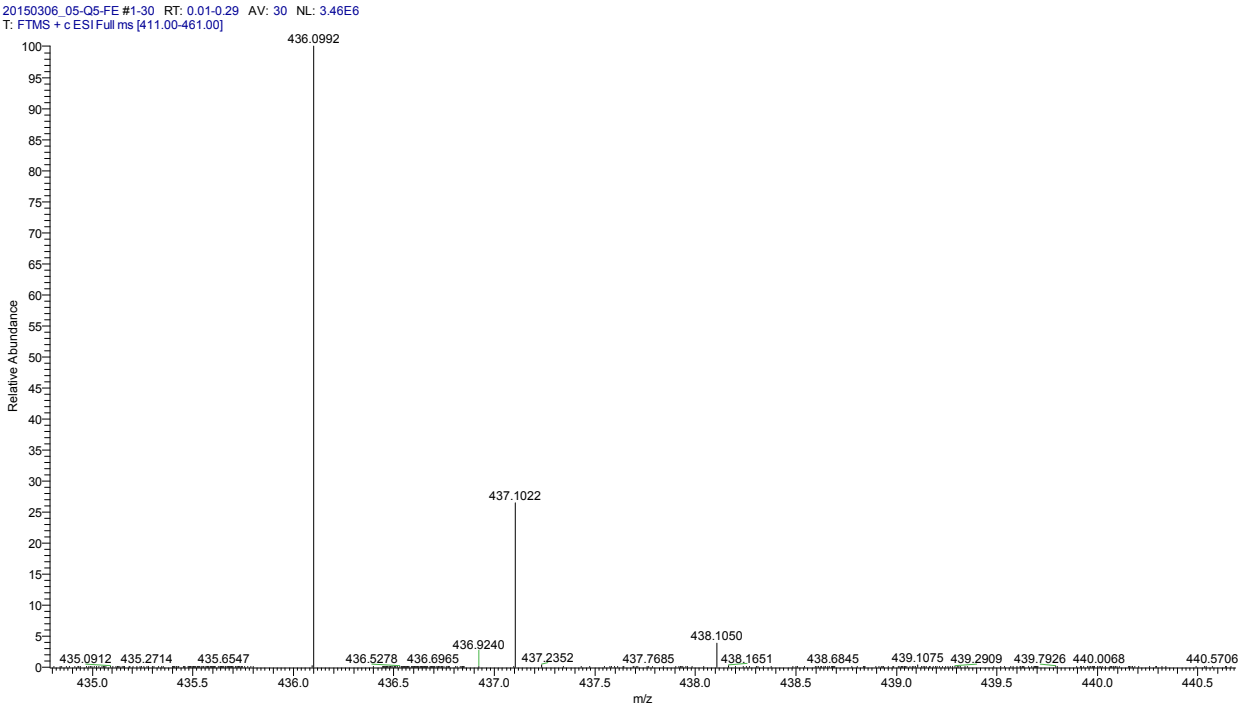
2-Oxo-2-(*p*-tolyl)ethyl 2-(*p*-tolyl)-3-hydroxyquinoline-4(1*H*)-one-5-carboxylate (14c):



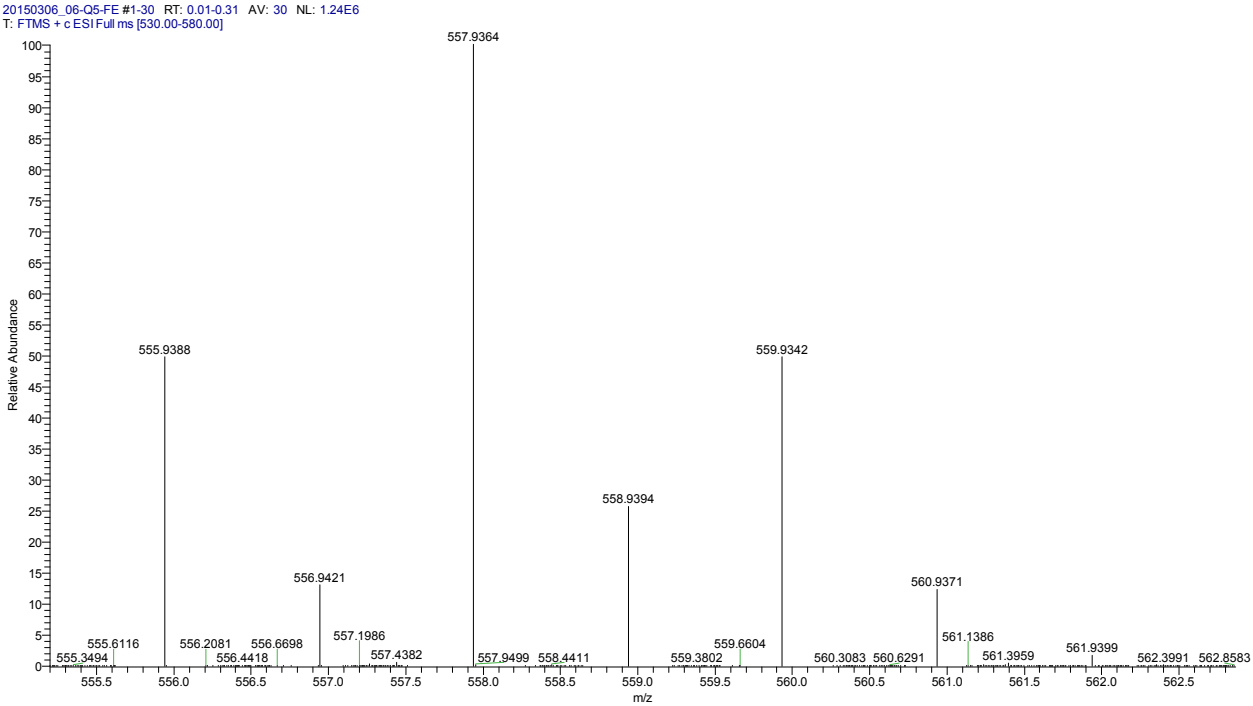
2-(4-Methoxyphenyl)-2-oxoethyl 2-(4-methoxyphenyl)-3-hydroxyquinoline-4(1*H*)-one-5-carboxylate (14d):



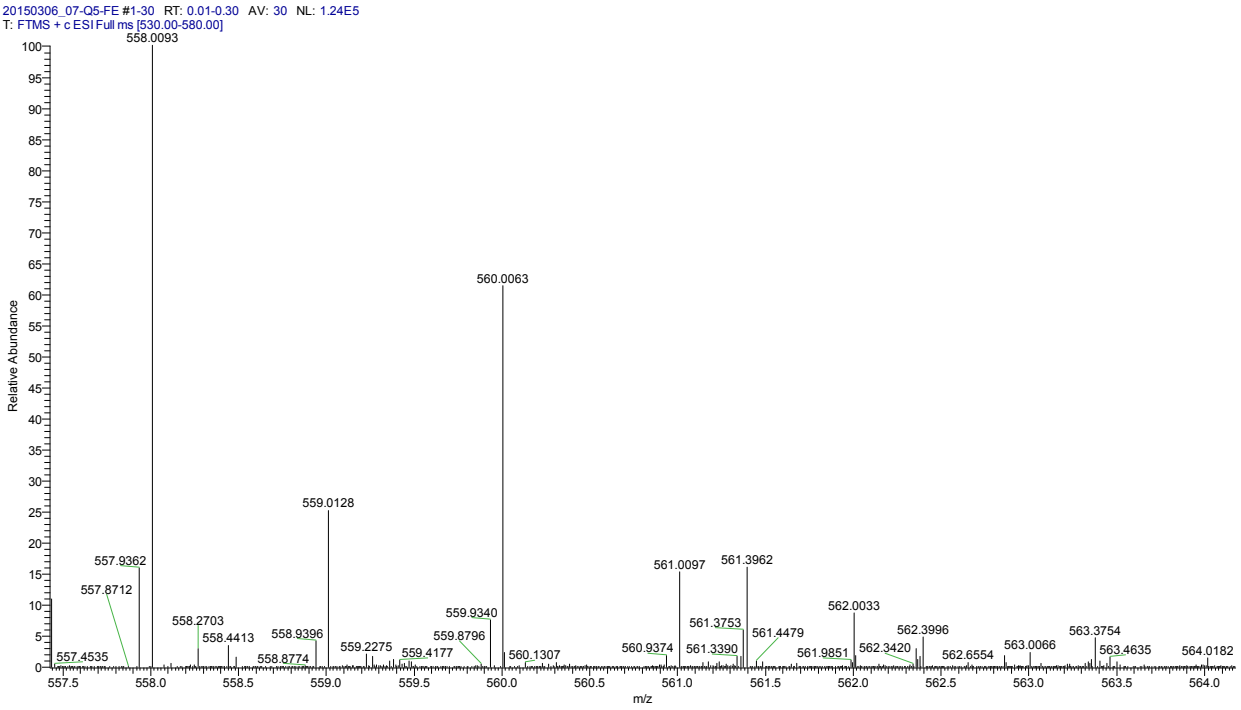
2-(4-Fluorophenyl)-2-oxoethyl 2-(4-fluorophenyl)-3-hydroxyquinoline-4(1*H*)-one-5-carboxylate (14e):



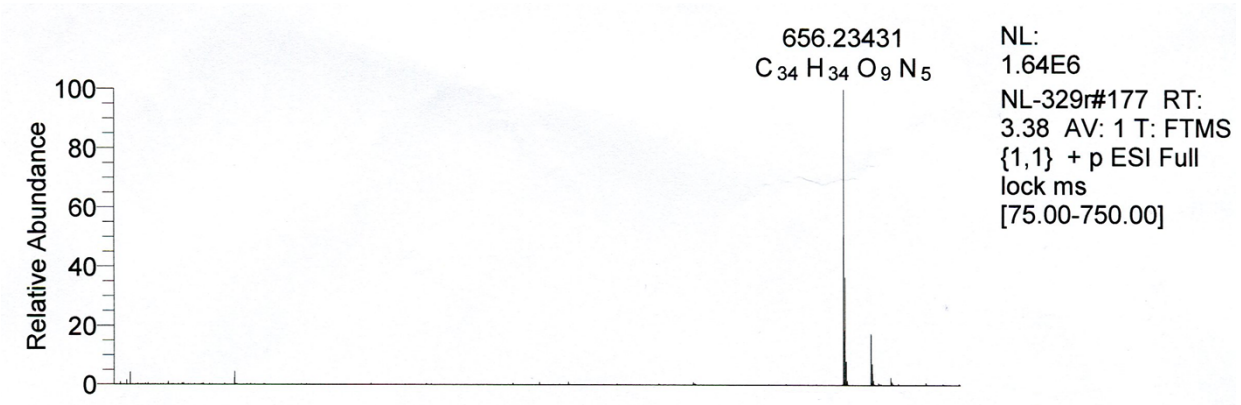
2-(3-Bromophenyl)-2-oxoethyl 2-(3-bromophenyl)-3-hydroxyquinoline-4(1*H*)-one-5-carboxylate (14f):



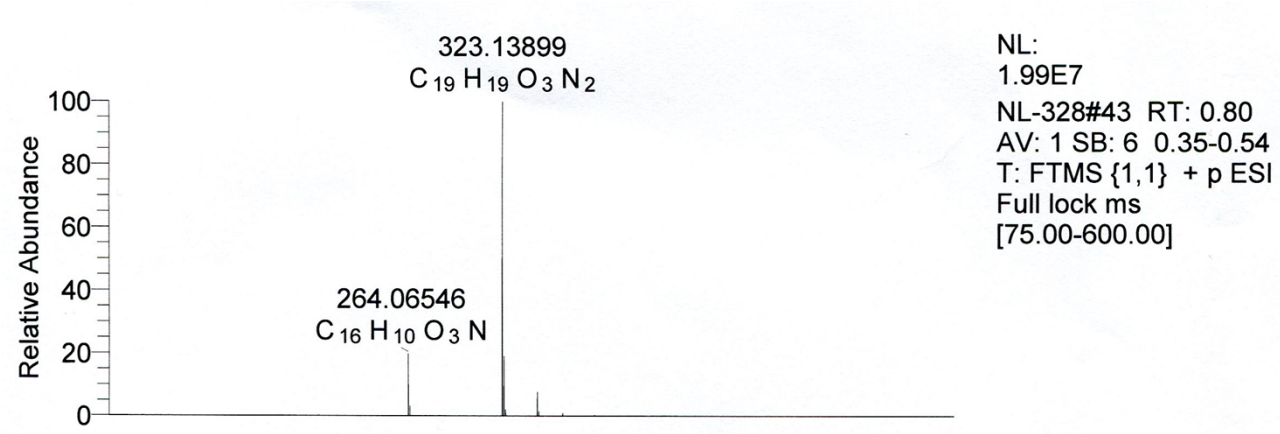
2-(4-Chloro-3-nitrophenyl)-2-oxoethyl 2-(4-chloro-3-nitrophenyl)-3-hydroxyquinoline-4(1*H*)-one-5-carboxylate (14g):



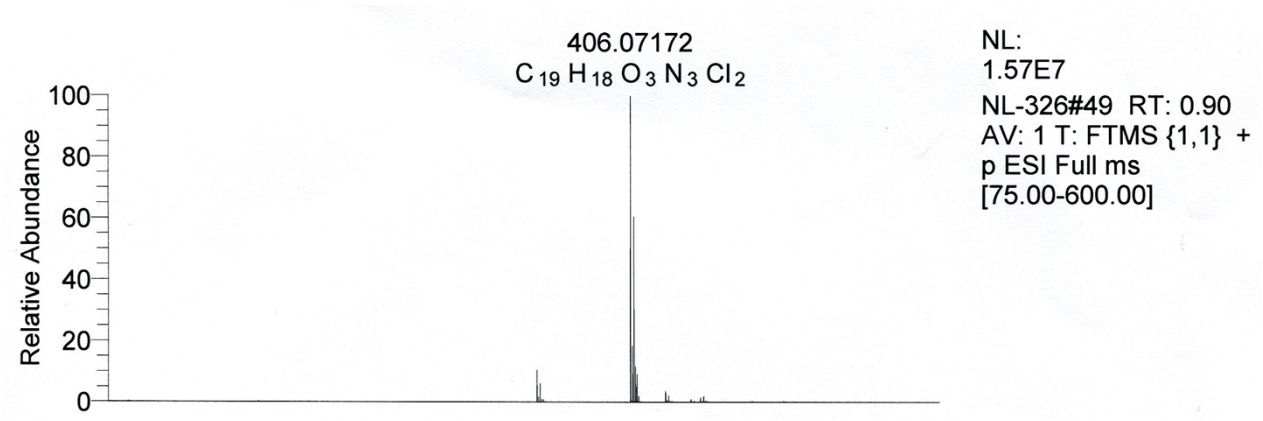
2-(3-Nitro-4-(piperidin-1-yl)phenyl)-2-oxoethyl 2-(3-nitro-4-(piperidin-1-yl)phenyl)- 3-hydroxy-quinoline-4(1*H*)-one-5-carboxylate (14h):



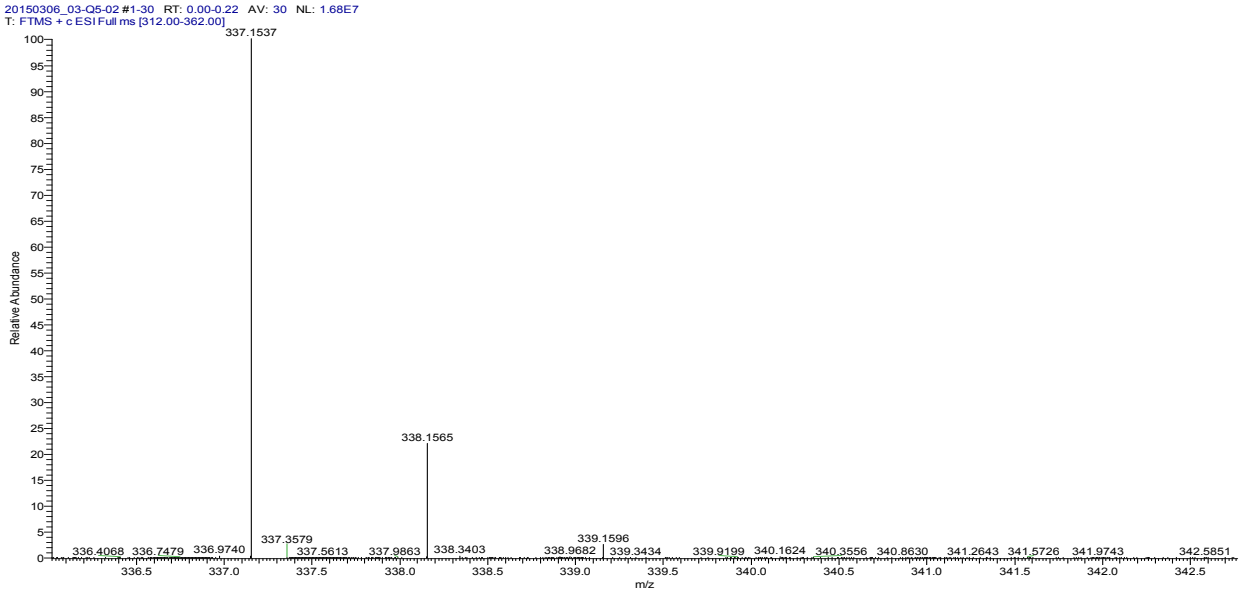
***N*-Propyl-2-phenyl-3-hydroxyquinoline-4(1*H*)-one-5-carboxamide (15a):**



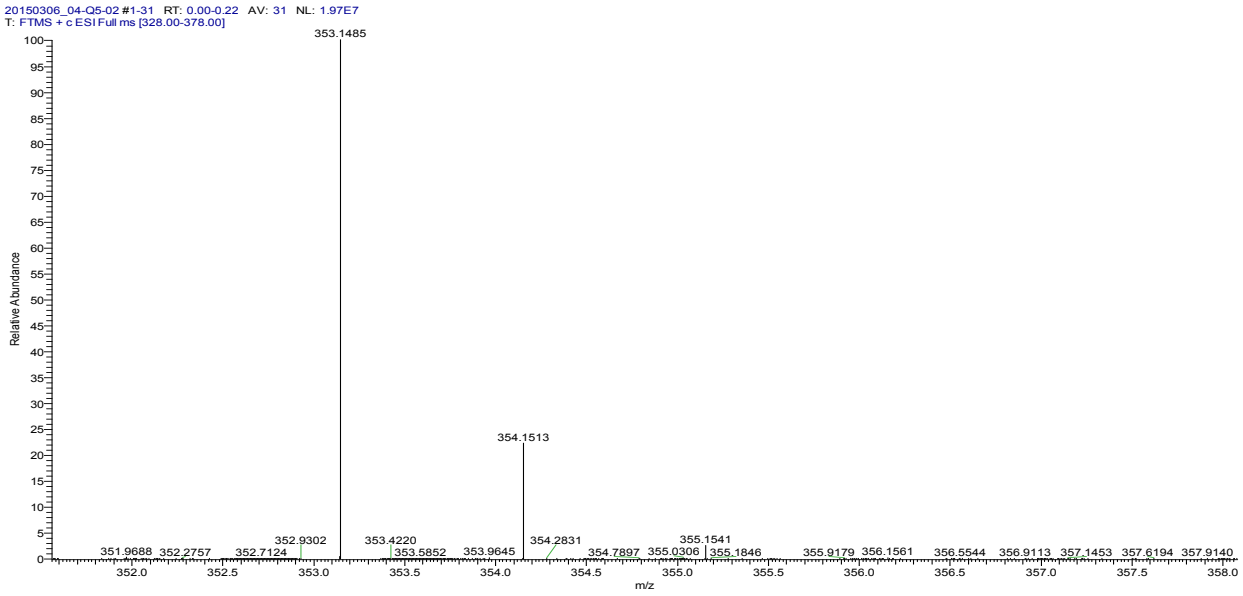
***N*-Propyl-2-(4-amino-3,5-dichlorophenyl)-3-hydroxyquinoline-4(1*H*)-one-5-carboxamide (15b):**



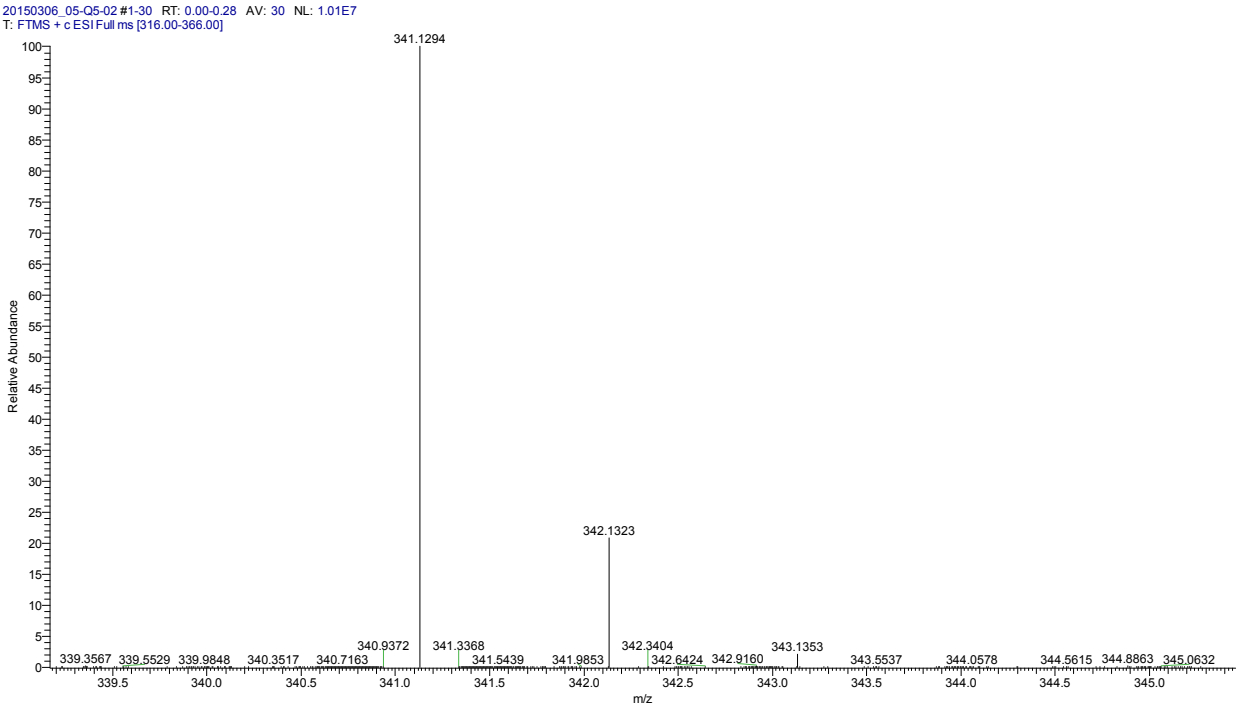
***N*-Propyl-2-(*p*-tolyl)-3-hydroxyquinoline-4(1*H*)-one-5-carboxamide (15c):**



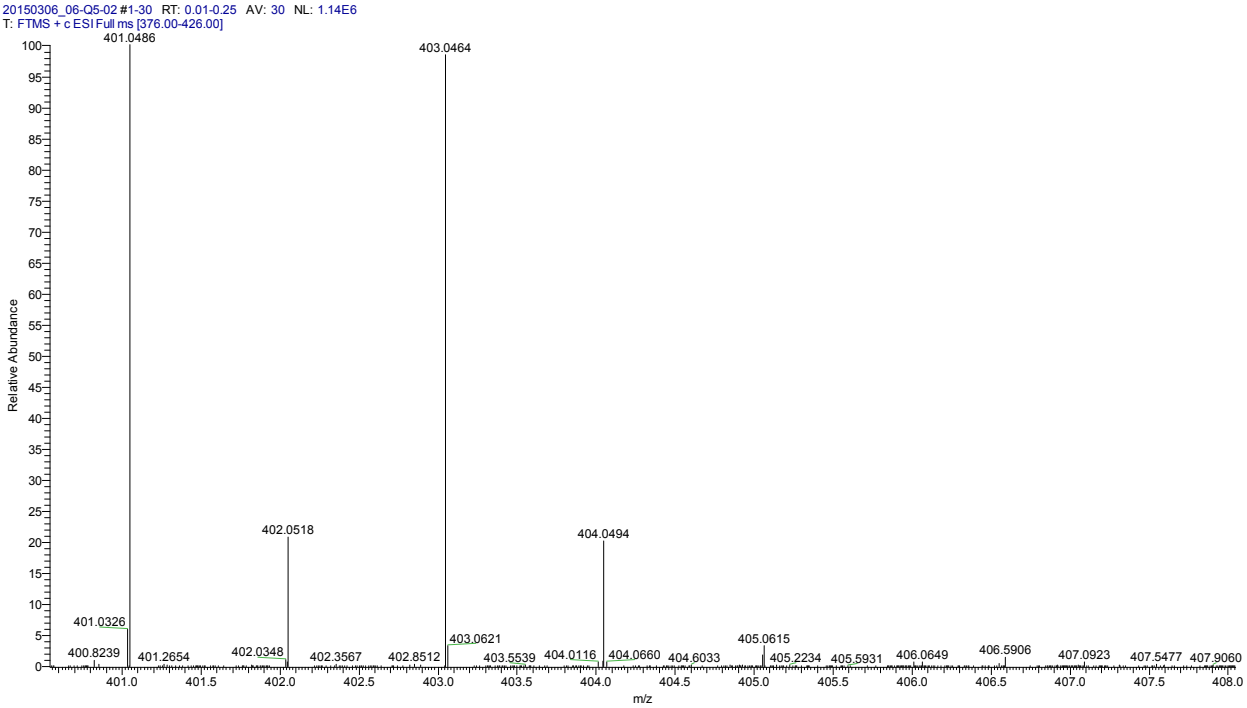
***N*-Propyl-2-(4-Methoxyphenyl)-3-hydroxyquinoline-4(1*H*)-one-5-carboxamide (15d):**



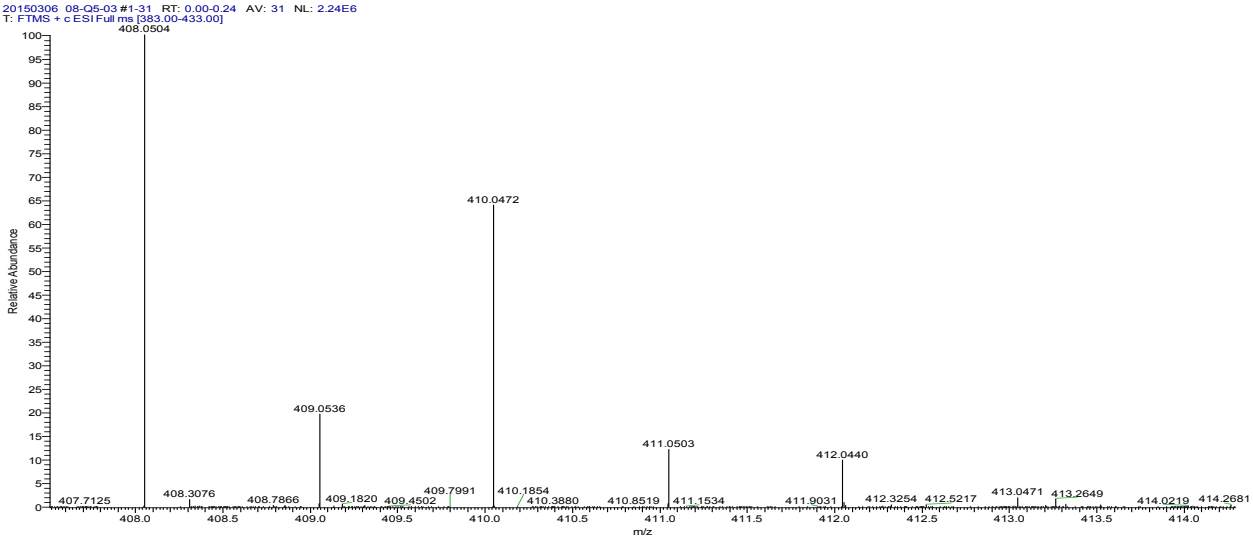
N-Propyl-2-(4-fluorophenyl)- 3-hydroxyquinoline-4(1*H*)-one-5-carboxamide (15e):



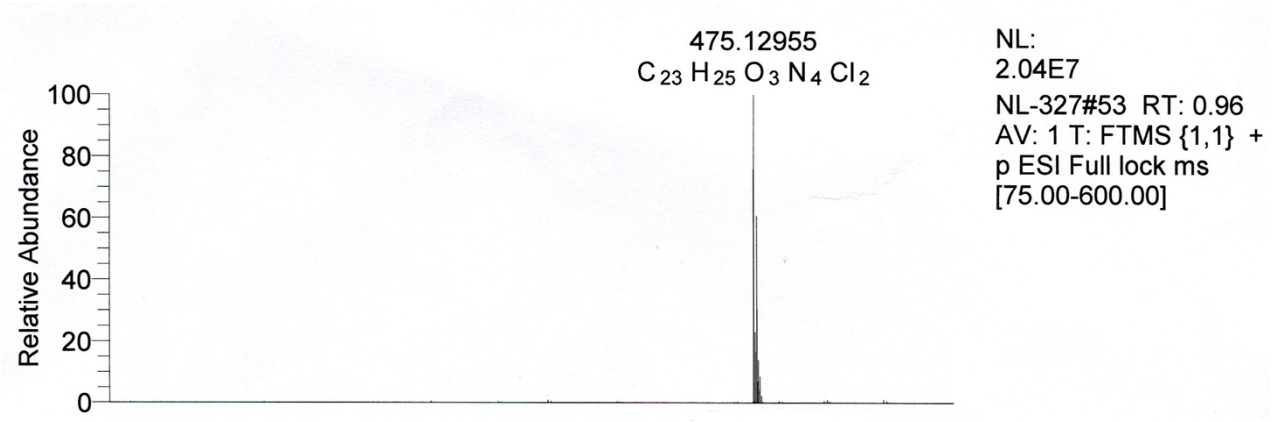
N-Propyl-2-(3-bromophenyl)-3-hydroxyquinoline-4(1*H*)-one-5-carboxamide (15f):



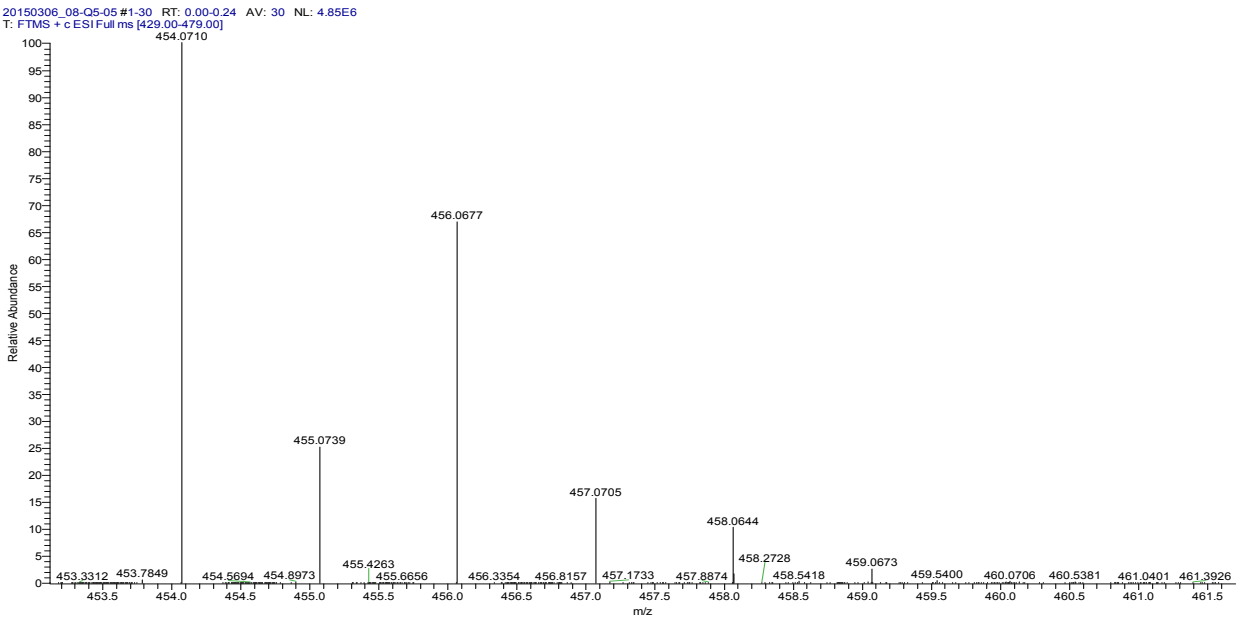
***N*-(2-Hydroxyethyl)-2-(4-amino-3,5-dichlorophenyl)-3-hydroxyquinoline-4(1*H*)-one-5-carboxamide (15g):**



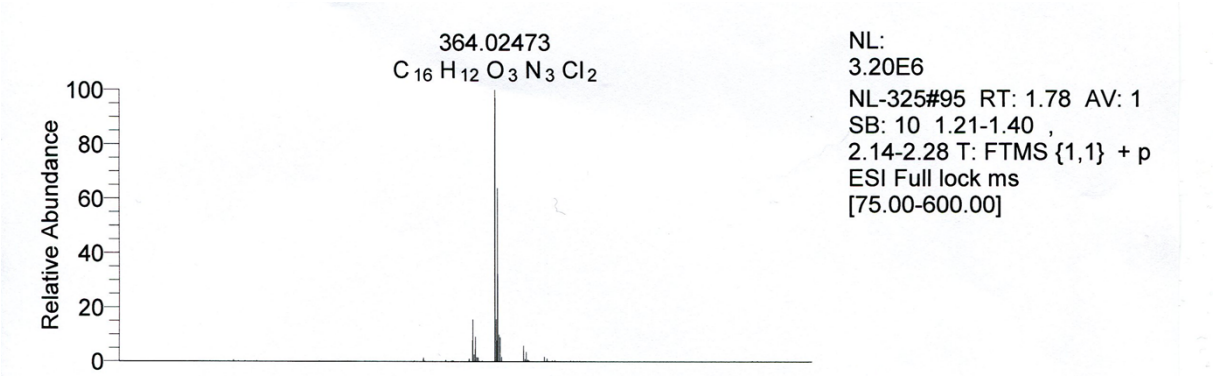
***N*-(2-(Piperidin-1-yl)ethyl)-2-(4-amino-3,5-dichlorophenyl)-3-hydroxyquinoline-4(1*H*)-one-5-carboxamide (15h):**



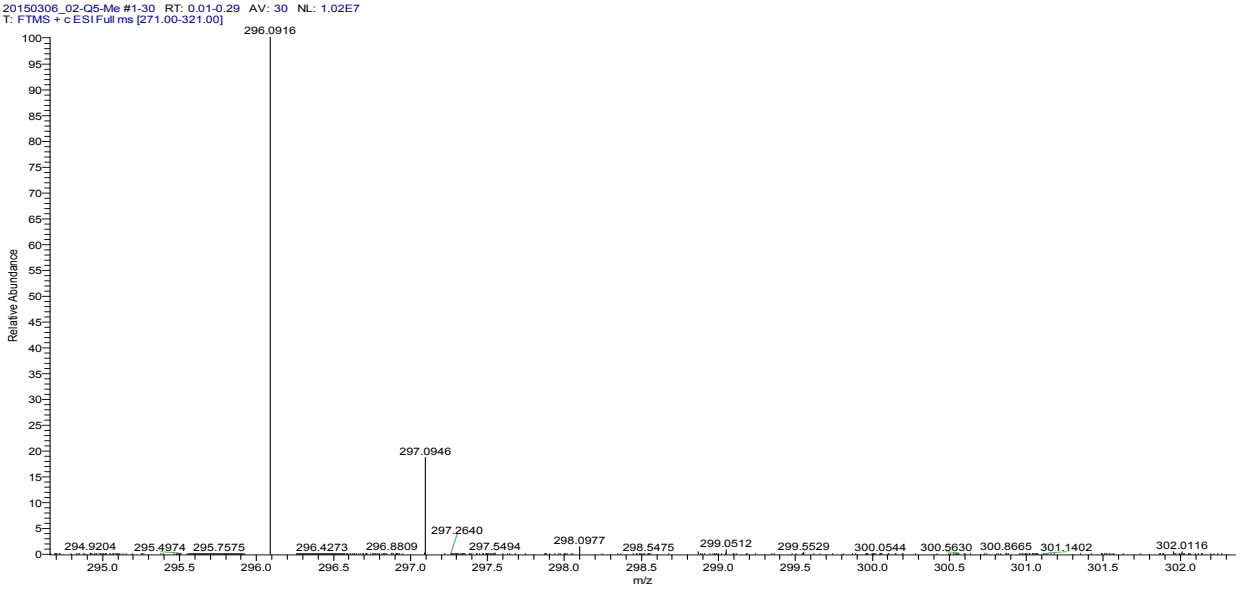
***N*-Benzyl-2-(4-amino-3,5-dichlorophenyl)-3-hydroxyquinoline-4(1*H*)-one-5-carboxamide (15i):**



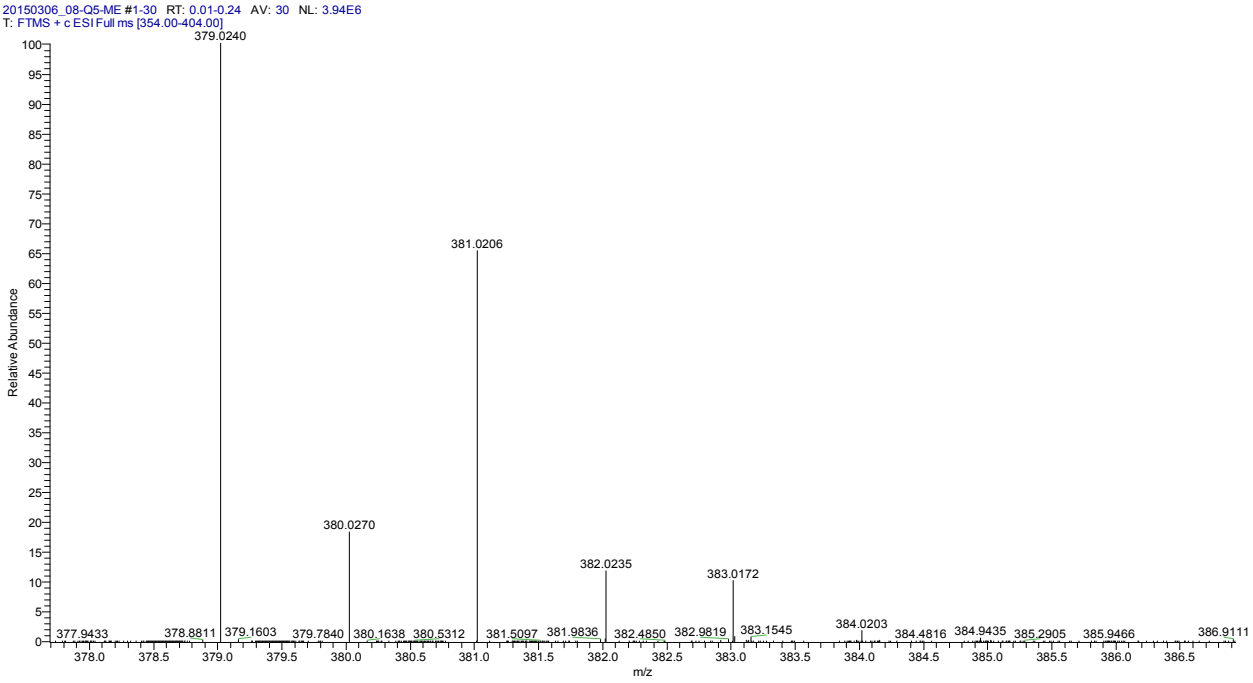
2-(4-Amino-3,5-dichlorophenyl)-3-hydroxyquinoline-4(1*H*)-one-5-carboxamide (15l):



Methyl 2-phenyl-3-hydroxyquinoline-4(1*H*)-one-5-carboxylate (16a)



Methyl 2-(4-amino-3,5-dichlorophenyl)-3-hydroxyquinoline-4(1*H*)-one-5-carboxylate (16b)



Crystallography data

Table 1: Experimental data

Crystal data	
Chemical formula	$C_{19}H_{18}N_2O_3 \cdot C_3H_6O$
M_r	380.43
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	298 (1)
a, b, c (Å)	12.5280 (3), 10.6895 (2), 15.9537 (4)
β (°)	104.877 (3)
V (Å^3)	2064.87 (9)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	0.22 × 0.13 × 0.05
Data collection	
Diffractometer	SuperNova diffractometer (Agilent Technologies) with Atlas detector
Absorption correction	Multi-scan *CrysAlis PRO*, Agilent Technologies, Version 1.171.37.35 Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.
T_{min}, T_{max}	0.583, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	31019, 3914, 3154
R_{int}	0.028
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.610
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.067, 0.204, 1.06
No. of reflections	3914
No. of parameters	275
No. of restraints	6
H-atom treatment	H-atom parameters constrained
$\Delta\rangle_{max}$, $\Delta\rangle_{min}$ (e Å^{-3})	0.53, -0.35

Computer programs: *CrysAlis PRO*, Agilent Technologies, Version 1.171.37.35, *SHELXS2013* (Sheldrick, 2014), *SHELXL2014*/6 (Sheldrick, 2014).

Table 2. Geometric parameters (Å, °).

O1—C3	1.354 (3)	C13—C14	1.394 (5)

O1—H1	0.8200	C13—H13	0.9300
O2—C4	1.249 (3)	C14—H14	0.9300
O3—C15	1.227 (3)	C16A—C17A	1.486 (9)
N2—C16B	1.26 (2)	C16A—H16A	0.9700
N2—C15	1.322 (3)	C16A—H16B	0.9700
N2—C16A	1.512 (6)	C17A—C18A	1.444 (11)
N2—H2	0.8600	C17A—H17A	0.9700
N1—C8A	1.361 (3)	C17A—H17B	0.9700
N1—C2	1.364 (3)	C18A—H18A	0.9600
N1—H1A	0.8600	C18A—H18B	0.9600
C2—C3	1.369 (3)	C18A—H18C	0.9600
C2—C9	1.482 (3)	C16B—C17B	1.46 (4)
C3—C4	1.424 (3)	C16B—H16C	0.9700
C4—C4A	1.445 (3)	C16B—H16D	0.9700
C4A—C8A	1.410 (3)	C17B—C18B	1.24 (4)
C4A—C5	1.418 (3)	C17B—H17C	0.9700
C5—C6	1.369 (4)	C17B—H17D	0.9700
C5—C15	1.497 (3)	C18B—H18D	0.9600
C6—C7	1.395 (4)	C18B—H18E	0.9600
C6—H6	0.9300	C18B—H18F	0.9600
C7—C8	1.359 (4)	C31—C88B	1.513 (15)
C7—H7	0.9300	C31—C88A	1.5198 (5)
C8—C8A	1.399 (3)	C31—H31A	0.9600
C8—H8	0.9300	C31—H31B	0.9600
C9—C14	1.379 (4)	C31—H31C	0.9600
C9—C10	1.380 (4)	C30—C88A	1.5199 (5)
C10—C11	1.380 (4)	C30—C88B	1.5200 (4)
C10—H10	0.9300	C30—H30A	0.9600
C11—C12	1.350 (6)	C30—H30B	0.9600
C11—H11	0.9300	C30—H30C	0.9600
C12—C13	1.370 (6)	C88A—O77A	1.2131 (5)
C12—H12	0.9300	C88B—O77B	1.2132 (5)

C2—N1—C8A	122.8 (2)	N1—C8A—C4A	119.9 (2)
C3—O1—H1	109.00	N1—C8A—C8	119.5 (2)
C15—N2—C16B	126.7 (10)	C2—C9—C14	121.1 (3)
C15—N2—C16A	119.4 (3)	C10—C9—C14	118.7 (3)
C8A—N1—H1A	119.00	C2—C9—C10	120.2 (3)
C2—N1—H1A	119.00	C9—C10—C11	121.0 (3)
N1—C2—C9	117.0 (2)	C10—C11—C12	120.3 (4)
N1—C2—C3	119.1 (2)	C11—C12—C13	119.9 (4)
C3—C2—C9	124.0 (2)	C12—C13—C14	120.6 (4)
C16B—N2—H2	110.00	C9—C14—C13	119.5 (3)
C15—N2—H2	120.00	N2—C15—C5	115.6 (2)
C16A—N2—H2	120.00	O3—C15—N2	122.1 (2)
O1—C3—C4	118.5 (2)	O3—C15—C5	122.3 (2)
O1—C3—C2	119.0 (2)	N2—C16A—C17A	113.2 (5)
C2—C3—C4	122.5 (2)	N2—C16B—C17B	113.7 (18)
O2—C4—C3	120.3 (2)	C16A—C17A—C18A	117.8 (6)
O2—C4—C4A	123.4 (2)	C16B—C17B—C18B	117 (3)
C3—C4—C4A	116.3 (2)	C5—C6—H6	120.00
C4—C4A—C8A	119.3 (2)	C7—C6—H6	120.00
C5—C4A—C8A	118.0 (2)	C6—C7—H7	120.00
C4—C4A—C5	122.6 (2)	C8—C7—H7	120.00
C4A—C5—C15	121.7 (2)	C7—C8—H8	120.00
C4A—C5—C6	120.1 (2)	C8A—C8—H8	120.00

C6—C5—C15	118.3 (2)	C9—C10—H10	119.00
C5—C6—C7	120.7 (3)	C11—C10—H10	120.00
C6—C7—C8	120.7 (3)	C10—C11—H11	120.00
C7—C8—C8A	119.8 (3)	C12—C11—H11	120.00
C4A—C8A—C8	120.7 (2)	C11—C12—H12	120.00
C13—C12—H12	120.00	H18A—C18A—H18B	109.00
C12—C13—H13	120.00	H18A—C18A—H18C	110.00
C14—C13—H13	120.00	C17A—C18A—H18A	109.00
C9—C14—H14	120.00	C17B—C18B—H18D	110.00
C13—C14—H14	120.00	C17B—C18B—H18E	109.00
N2—C16A—H16A	109.00	C17B—C18B—H18F	110.00
N2—C16A—H16B	109.00	H18D—C18B—H18E	109.00
C17A—C16A—H16A	109.00	H18D—C18B—H18F	110.00
C17A—C16A—H16B	109.00	H18E—C18B—H18F	109.00
H16A—C16A—H16B	108.00	O77A—C88A—C30	141.3 (8)
H16C—C16B—H16D	108.00	O77A—C88A—C31	108.7 (7)
N2—C16B—H16C	109.00	C30—C88A—C31	108.3 (6)
N2—C16B—H16D	109.00	O77B—C88B—C30	93.3 (10)
C17B—C16B—H16C	109.00	O77B—C88B—C31	156.1 (12)
C17B—C16B—H16D	109.00	C30—C88B—C31	108.6 (10)
C18A—C17A—H17A	108.00	C88A—C30—H30A	110.00
C18A—C17A—H17B	108.00	C88A—C30—H30B	109.00
C16A—C17A—H17B	108.00	C88A—C30—H30C	110.00
C16A—C17A—H17A	108.00	C88B—C30—H30A	106.00
H17A—C17A—H17B	107.00	C88B—C30—H30B	100.00
C16B—C17B—H17C	108.00	C88B—C30—H30C	122.00
C16B—C17B—H17D	108.00	H30A—C30—H30B	109.00
H17C—C17B—H17D	107.00	H30A—C30—H30C	109.00
C18B—C17B—H17D	109.00	H30B—C30—H30C	109.00
C18B—C17B—H17C	108.00	C88A—C31—H31A	109.00
C17A—C18A—H18C	109.00	C88A—C31—H31B	109.00
C17A—C18A—H18B	109.00	C88A—C31—H31C	109.00
C88B—C31—H31B	102.00	H31A—C31—H31C	110.00
C88B—C31—H31C	104.00	H31B—C31—H31C	109.00
H31A—C31—H31B	109.00		

C8A—N1—C2—C3	3.2 (3)	C8A—C4A—C5—C15	178.0 (2)
C8A—N1—C2—C9	-177.0 (2)	C4—C4A—C8A—N1	1.0 (3)
C2—N1—C8A—C4A	-3.9 (3)	C4—C4A—C8A—C8	-178.1 (2)
C2—N1—C8A—C8	175.2 (2)	C5—C4A—C8A—N1	180.0 (2)
C16A—N2—C15—O3	-16.4 (5)	C5—C4A—C8A—C8	0.9 (3)
C16A—N2—C15—C5	167.2 (4)	C4A—C5—C6—C7	1.2 (4)
C15—N2—C16A—C17A	-173.0 (5)	C15—C5—C6—C7	-178.5 (3)
N1—C2—C3—O1	178.8 (2)	C4A—C5—C15—O3	101.1 (3)
N1—C2—C3—C4	0.5 (3)	C4A—C5—C15—N2	-82.5 (3)
C9—C2—C3—O1	-0.9 (4)	C6—C5—C15—O3	-79.3 (3)
C9—C2—C3—C4	-179.2 (2)	C6—C5—C15—N2	97.2 (3)
N1—C2—C9—C10	131.9 (3)	C5—C6—C7—C8	0.2 (5)
N1—C2—C9—C14	-47.3 (4)	C6—C7—C8—C8A	-1.0 (5)
C3—C2—C9—C10	-48.3 (4)	C7—C8—C8A—N1	-178.6 (3)
C3—C2—C9—C14	132.5 (3)	C7—C8—C8A—C4A	0.5 (4)
O1—C3—C4—O2	0.0 (3)	C2—C9—C10—C11	179.7 (3)
O1—C3—C4—C4A	178.5 (2)	C14—C9—C10—C11	-1.0 (5)
C2—C3—C4—O2	178.3 (2)	C2—C9—C14—C13	-179.2 (3)
C2—C3—C4—C4A	-3.2 (3)	C10—C9—C14—C13	1.5 (5)

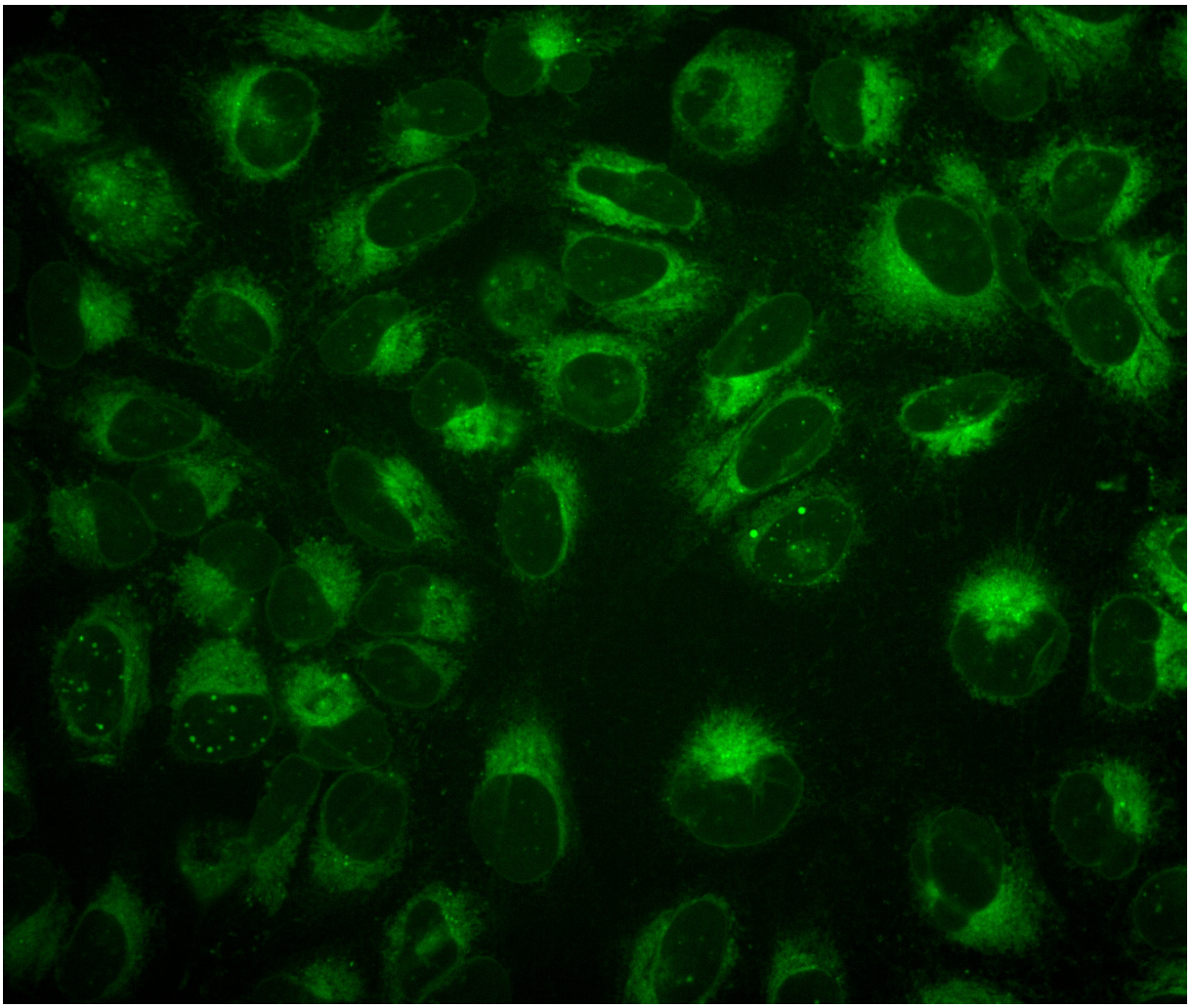
O2—C4—C4A—C5	1.9 (3)	C9—C10—C11—C12	-0.1 (6)
O2—C4—C4A—C8A	-179.2 (2)	C10—C11—C12—C13	0.7 (7)
C3—C4—C4A—C5	-176.5 (2)	C11—C12—C13—C14	-0.2 (7)
C3—C4—C4A—C8A	2.4 (3)	C12—C13—C14—C9	-1.0 (6)
C4—C4A—C5—C6	177.3 (2)	N2—C16A—C17A—C18A	-70.4 (8)
C4—C4A—C5—C15	-3.0 (3)	C8A—C4A—C5—C15	178.0 (2)
C8A—C4A—C5—C6	-1.7 (3)	C4—C4A—C8A—N1	1.0 (3)

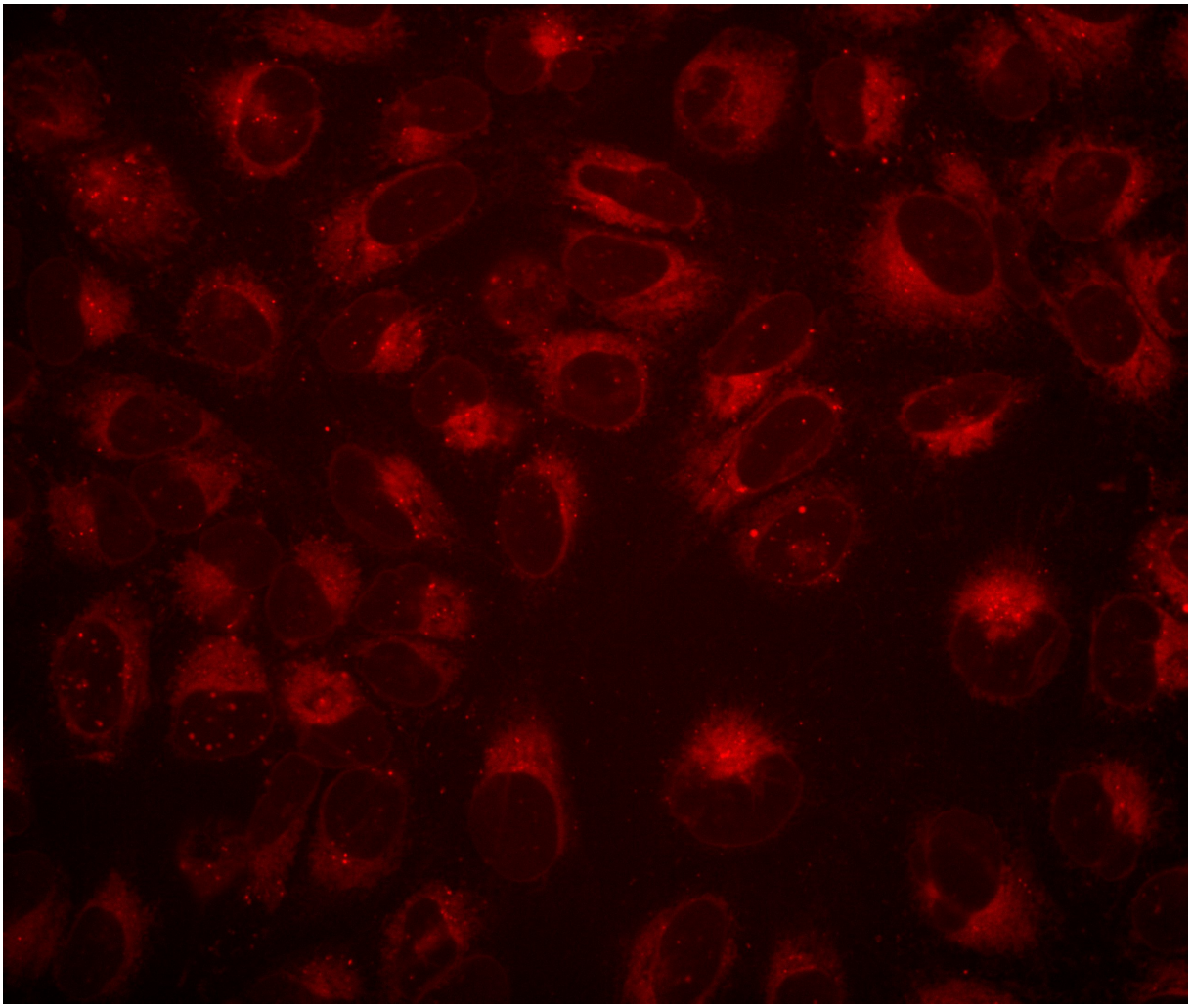
Table 3. Hydrogen bond geometric parameters (Å, °).

D-H···A	d(D-H)	d(H..A)	d(D..A)	<DHA
O1-H1···O2	0.8200	2.2700	2.701 (3)	113.00
O1-H1···O2^{i}	0.8200	1.9900	2.729 (3)	151.00
N1-H1A···O3^{ii}	0.8600	1.9500	2.798 (3)	170.00
N2-H2···O77A^{iii}	0.8600	2.0400	2.894 (7)	172.00
C8-H8···O2^{ii}	0.9300	2.4200	3.244 (3)	148.00

i: -x, -y, -z+1
ii: -x, y+1/2, -z+3/2
iii: -x, -y+1, -z+1

Fluorescent microscope images of compound 14b





Fluorescent microscope images of compound 15i