Supporting Information

Rh(I)-Catalyzed Alkylation of *ortho* C-H Bonds in Aromatic Amides with Maleimides

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I. General Information.

^{1}H NMR and ^{13}C NMR spectra were recorded on a JEOL ECS-400 spectrometer in $CDCl_3$ with tetramethylsilane as the internal standard. Data are reported as follows: chemical shift in ppm (δ), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, brs = broad singlet, and m = multiplet), coupling constant (Hz), and integration. In some cases, some peaks in the ^{13}C NMR spectra cannot be analyzed because of overlapping peaks. Infrared spectra (IR) were obtained using a JASCO FT/IR-4200 spectrometer; absorptions are reported in reciprocal centimeters with the following relative intensities: s (strong), m (medium), or w (weak). Mass spectra and high resolution mass spectra (HRMS) were obtained using a JEOL JMS-700 spectrometer. Melting points were determined using a Yamato melting point apparatus. Column chromatography was performed with SiO_2 (Silicycle SiliaFlash F60 (230-400 mesh)). Some compounds were purified by LC-908 HPLC (GPC).

II. Materials.

Toluene (Kanto Chemical) was purified by passage through activated alumina using a GlassContour Solvent Dispensing System. 8-Aminoquinoline (CAS 578-66-5), maleimide (CAS 541-59-3), *N*-methylmaleimide (CAS 930-88-1), *N*-ethylmaleimide (CAS 128-53-0), *N*-cyclohexylmaleimide (CAS: 1631-25-0), *N*-phenylmaleimide (CAS: 941-69-5), *N*-benzylmaleimide (CAS: 1631-26-1), 2-methylbenzoic acid (CAS: 118-90-1) were purchased from Tokyo Chemical Industry Co., Ltd. $[Ru(p\text{-cymene})Cl]_2$ (CAS: 52462-29-0) was purchased from Sigma-Aldrich Co. $[Rh(OAc)(cod)]_2$ was prepared according to literature procedures.[1]

III. Synthesis of Starting Materials.

All amides bearing an 8-aminoquinoline moiety were prepared by reacting the corresponding acid or the corresponding acid chlorides with 8-aminoquinoline.[2]

General Procedure for the Preparation of Starting Amides.

(1) Synthesis of amides from acid chlorides.

The acid chloride (15 mmol) was dissolved in CH_2Cl_2 (20 mL). After cooling the reaction mixture to 0 °C, a solution of 8-aminoquinoline (15 mmol) and triethylamine (36 mmol) in 10 mL of CH_2Cl_2 was added dropwise. The resulting mixture was allowed to warm to rt and was then stirred overnight. The crude mixture was then washed with saturated aqueous $NaHCO_3$ (20 mL), and CH_2Cl_2 (3x20 mL). The combined organic layers were washed with 1 M HCl aq. (20 mL). The organic phase was dried over anhydrous Na_2SO_4 and the solution taken to dryness. The resulting crude amide was purified by flash chromatography on silica gel (eluent: hexanes/EtOAc = 5/1).

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[1] Chatt, J.; Venanzi, L. M. *J. Chem. Soc.* **1957**, 4735.
[2] Shibata, K.; Chatani, N. *Org. Lett.* **2014**, *16*, 5148.

(2) Synthesis of amides from carboxylic acid.

To a stirred solution of carboxylic acid (15 mmol) and DMF (5 drops) in CH_2Cl_2 (10 mL), $(COCl)_2$ (1.5 mL, 18 mmol) was added dropwise. The solution was magnetically stirred at room temperature for 2 h. The solvent was then eliminated under reduced pressure, and the resulting residue was dissolved in CH_2Cl_2 (15 mL). After cooling the reaction mixture to 0 °C, a solution of 8-aminoquinoline (15 mmol) and triethylamine (36 mmol) in 10 mL of the same solvent were added dropwise. The resulting mixture was allowed to warm to rt and stirred overnight. The crude product was washed with saturated aqueous $NaHCO_3$ (20 mL), and CH_2Cl_2 (3x20 mL). The organic phase was washed with 1 M HCl aq. (20 mL). The organic phase was dried over anhydrous Na_2SO_4 and the solvent removed by evaporation of the solvent. The resulting crude amide was purified by flash chromatography on silica gel (eluent: hexanes/EtOAc = 5/1).

IV. Synthesis of Alkylation Products.

(1) General procedure for the Rh(I)-catalyzed alkylation of aromatic amides with *N*-methylmaleimide.

To an oven-dried 5 mL screw-capped vial, 2-methyl-*N*-(quinolin-8-yl)benzamide (**1a**) (78.7 mg, 0.3 mmol), *N*-methylmaleimide (39.6 mg, 0.36 mmol), $[Rh(OAc)(cod)]_2$ (4.1 mg, 0.0075 mmol) and toluene (1 mL) were added. The mixture was stirred for 12 hours at 160 °C and then cooled to room temperature. The resulting mixture was filtered through a celite pad and then concentrated *in vacuo*. The residue was purified by column chromatography on silica gel (eluent: hexane/EtOAc = 1.5:1) and further purified through GPC to afford the alkylation product **2a** (93.0 mg, 83%) as a white powder.

(2) General procedure for the Ru(II)-catalyzed alkylation of aromatic amides with *N*-methylmaleimide.

To an oven-dried 5 mL screw-capped vial, 2-methyl-*N*-(quinolin-8-yl)benzamide (**1a**) (78.7 mg, 0.3 mmol), *N*-methylmaleimide (39.6 mg, 0.36 mmol), 2-methylbenzoic acid (40.9 mg, 0.3 mmol), $[RuCl_2(p\text{-cymene})]_2$ (4.6 mg, 0.0075 mmol) and toluene (1 mL) were added. The mixture was stirred for 12 hours at 160 °C and then cooled to room temperature. The resulting mixture was filtered through a celite pad and washed with saturated aqueous $NaHCO_3$ (20 mL), and EtOAc (3x20 mL); then concentrated *in vacuo*. The residue was purified by column chromatography on silica gel (eluent: hexane/EtOAc = 1.5:1) and further purified through GPC to afford the alkylation product **2a** (75.1 mg, 67%) as a white powder.

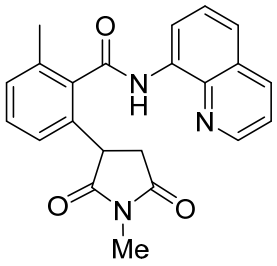
(3) A gram scale reaction

To an oven-dried 40 mL screw-capped vial , 2-methyl-N-(quinolin-8-yl)benzamide (**1a)** (1049.2

mg, 4.0 mmol), *N*-methylmaleimide (132.1 mg, 1.2 mmol), $[Rh(OAc)(cod)]_2$ (54.0 mg, 0.1 mmol) and toluene (14 mL) were added. The mixture was stirred for 12 hours at 160 °C and then cooled to room temperature. The resulting mixture was filtered through a celite pad and then concentrated in vacuo. The residue was purified by column chromatography on silica gel (eluent: hexane/EtOAc= 1.5:1) to afford the alkylation product **2a** (1401.1 mg, 94%) as a white powder.

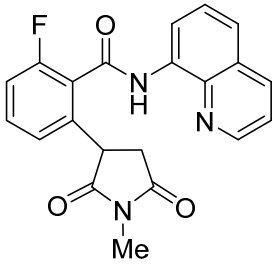
V. Spectroscopic Data.

2-methyl-6-(1-methyl-2,5-dioxopyrrolidin-3-yl)-*N*-(quinolin-8-yl)benzamide (2a)



93.0 mg, 83% yield (Rh(I)-catalyzed); 75.1 mg, 67% yield (Ru(II)-catalyzed). R_f 0.23 (hexane/EtOAc = 1.5:1). White powder. M.p. 103.4-103.9 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.48 (s, 3H), 2.88-2.94 (m, 1H), 2.93 (s, 3H), 3.24 (dd, *J* = 18.3, 9.6 Hz, 1H), 4.28 (dd, *J* = 9.6, 5.5 Hz, 1H), 7.02 (d, *J* = 7.8 Hz, 1H), 7.25 (d, *J* = 6.4 Hz, 1H), 7.36 (t, *J* = 7.8 Hz, 1H), 7.44-7.48 (m, 1H), 7.57-7.59 (m, 2H), 8.18 (dd, *J* = 8.2, 1.4 Hz, 1H), 8.80 (dd, *J* = 4.1, 1.4 Hz, 1H), 8.91 (dd, *J* = 5.5, 3.7 Hz, 1H), 10.19 (s, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 19.97, 25.24, 38.28, 44.41, 116.93, 121.94, 122.55, 125.00, 127.33, 128.11, 130.14, 130.29, 134.13, 134.87, 135.66, 136.41, 138.10, 138.62, 148.71, 167.82, 176.32, 177.97; IR (ATR) 3337 w 2951 w 1776 w 1699 s 1669 m, 1596 w, 1520 s, 1483 m, 1425 m, 1383 m, 1325 w, 1281 m, 1120 w, 758 m; MS *m*/*z* (relative intensity, %) 373 (M^+, 23), 231 (12), 230 (82), 229 (100), 160 (20), 145 (52), 144 (81), 117 (12), 115 (11); HRMS Calcd for $C_{22}H_{19}N_3O_3$: 373.1426; Found: 373.1423.

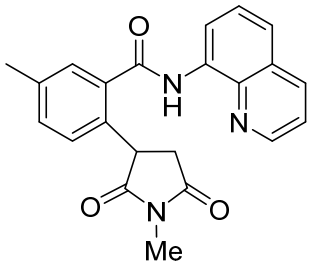
2-fluoro-6-(1-methyl-2,5-dioxopyrrolidin-3-yl)-*N*-(quinolin-8-yl)benzamide (2b)



67.2 mg, 60% yield. R_f 0.34 (hexane/EtOAc = 1:1). White powder. M.p. 75.8-76.1 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.94-3.01 (m, 1H), 3.00 (s, 3H), 3.29 (dd, *J* = 18.3, 9.6 Hz, 1H), 4.43 (dd, *J* = 9.6, 5.5 Hz, 1H), 7.07 (d, *J* = 7.8 Hz, 1H), 7.22 (dd, *J* = 9.6, 8.7 Hz, 1H), 7.47-7.49 (m, 2H), 7.57-7.59 (m, 2H), 8.18 (dd, *J* = 8.5, 1.6 Hz, 1H), 8.81-8.83 (m, 2H), 10.51 (s, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 25.29, 38.22, 44.91, 116.15 (d, *J* = 22.9 Hz), 116.85, 121.96, 122.62, 124.71 (d, *J* = 17.2 Hz), 125.41, 127.35, 128.10, 132.23 (d, *J* = 9.5 Hz), 134.26, 136.42, 138.60, 138.86, 148.67, 159.89 (d, *J* = 247.9 Hz), 162.60, 176.19, 177.69; IR (ATR) 3340 w, 3016 w, 2945 w,

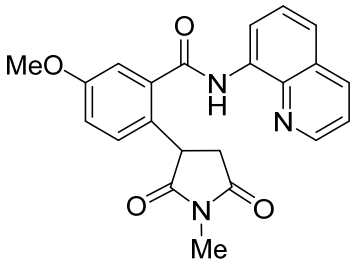
1176 w, 1698 s, 1667 m, 1612 w, 1576 w, 1524 s, 1485 m, 1427 m, 1384 m, 1327 m, 1281 m, 1120 m, 827 w, 791 m, 752 s, 692 m; MS *m*/*z* (relative intensity, %) 377 (M^+, 20), 234 (24), 233 (14), 149 (21), 145 (17), 144 (100); HRMS Calcd for $C_{21}H_{16}FN_3O_3$: 377.1176; Found: 377.1174.

5-methyl-2-(1-methyl-2, 5-dioxopyrrolidin-3-yl)-*N*-(quinolin-8-yl)benzamide (2c)



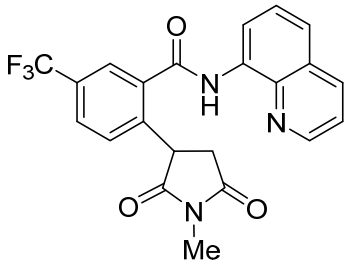
92.8 mg, 83% yield. R_f 0.25 (hexane/EtOAc = 1.5:1). Yellow powder. M.p. 116.6-116.8 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.46 (s, 3H), 2.94 (dd, *J* = 18.1, 5.9 Hz, 1H), 3.04 (s, 3H), 3.29 (dd, *J* = 18.1, 9.5 Hz, 1H), 4.48 (dd, *J* = 9.5, 5.9 Hz, 1H), 7.16 (d, *J* = 8.2 Hz, 1H), 7.33 (d, *J* = 7.8 Hz, 1H), 7.47 (dd, *J* = 8.2, 4.1 Hz, 1H), 7.56-7.57 (m, 2H), 7.62 (s, 1H), 8.18 (dd, *J* = 8.2, 1.4 Hz, 1H), 8.78-8.83 (m, 2H), 10.43 (s, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.27, 25.19, 38.49, 44.78, 116.58, 121.88, 122.21, 127.42, 128.10, 128.51, 130.23, 132.20, 133.78, 134.62, 135.83, 136.48, 138.45, 138.73, 148.52, 167.55, 176.75, 178.62. IR (ATR) 3343 w, 3015 w, 2950 w, 1176 w, 1698 s, 1667 m, 1597 w, 1573 w, 1522 s, 1482 m, 1425 m, 1383 m, 1326 m, 1281 m, 1119 m, 1041 w, 953 m, 827 m, 792 m, 751 s, 693 m; MS *m*/*z* (relative intensity, %) 373 (M^+, 14), 230 (50), 229 (100), 188 (20), 160 (25), 145 (29), 144 (65), 130 (10), 117 (10), 115 (10); HRMS Calcd for $C_{22}H_{19}N_3O_3$: 373.1426; Found: 373.1427.

5-methoxy-2-(1-methyl-2,5-dioxopyrrolidin-3-yl)-*N*-(quinolin-8-yl)benzamide (2d)



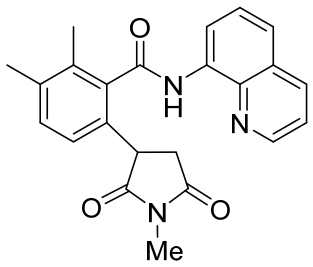
63.0 mg, 54% yield. R_f 0.18 (hexane/EtOAc = 2:1). Pale yellow powder. M.p. 81.2-81.6 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.93 (dd, *J* = 18.3, 5.9 Hz, 1H), 3.04 (s, 3H), 3.28 (dd, *J* = 18.3, 9.5 Hz, 1H), 3.89 (s, 3H), 4.44 (dd, *J* = 9.5, 5.9 Hz, 1H), 7.05 (dd, *J* = 8.5, 2.5 Hz, 1H), 7.20 (d, *J* = 8.2 Hz, 1H), 7.34 (d, *J* = 2.7 Hz, 1H), 7.47 (dd, *J* = 8.2, 4.1 Hz, 1H), 7.57 (d, *J* = 4.6 Hz, 2H), 8.19 (dd, *J* = 8.2, 1.4 Hz, 1H), 8.79 (m, 2H), 10.44 (s, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 25.20, 38.53, 44.47, 55.78, 114.05, 116.33, 116.61, 121.93, 122.32, 127.40, 128.09, 128.52, 131.56, 134.52, 136.48, 137.02, 138.72, 148.56, 159.25, 167.14, 176.76, 178.75; IR (ATR) 3341 w, 3012 w, 2947 w, 2360 m, 2340 w, 1776 w, 1697 s, 1670 m, 1606 w, 1576 w, 1525 s, 1482 m, 1425 m, 1383 m, 1326 m, 1281 m, 1223 m, 1119 m, 1041 w, 955 w, 826 m, 792 m, 751 s, 694 m; MS *m*/*z* (relative intensity, %) 389 (M^+, 13), 246 (22), 245 (100), 204 (29), 176 (10), 144 (17); HRMS Calcd for $C_{22}H_{19}N_3O_4$: 389.1376; Found: 389.1378.

2-(1-methyl-2,5-dioxopyrrolidin-3-yl)-*N*-(quinolin-8-yl)-5-(trifluoromethyl)benzamide (2e)



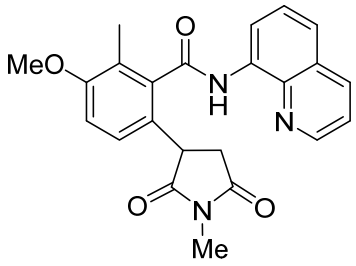
84.5 mg, 66% yield. R_f 0.20 (hexane/EtOAc = 1.5:1). White powder. M.p. 84.9-85.4 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.97 (dd, *J* = 18.1, 6.0 Hz, 1H), 3.03 (s, 3H), 3.33 (dd, *J* = 18.1, 9.6 Hz, 1H), 4.56 (dd, *J* = 9.6, 6.0 Hz, 1H), 7.44 (d, *J* = 7.8 Hz, 1H), 7.49 (q, *J* = 4.3 Hz, 1H), 7.57-7.62 (m, 2H), 7.79 (dd, *J* = 8.2, 1.4 Hz, 1H), 8.05 (d, *J* = 0.9 Hz, 1H), 8.20 (dd, *J* = 8.2, 1.8 Hz, 1H), 8.76 (dd, *J* = 6.4, 2.3 Hz, 1H), 8.83 (m, 1H), 10.49 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 25.30, 38.11, 45.02, 116.81, 120.77 (q, *J* = 270.2 Hz), 122.06, 122.76, 124.86 (d, *J* = 3.1 Hz), 127.32, 128.11, 130.48 (q, *J* = 33.0 Hz), 130.98, 131.03, 134.19, 136.53, 136.95, 138.67, 140.60, 148.77, 166.01, 175.96, 177.55; IR (ATR) 3333 w, 3016 w, 2945 m, 1778 m, 1700 s, 1672 m, 1525 s, 1484 m, 1429 m, 1384 m, 1333 m, 1282 m, 1172 m, 1124 s, 1085 w, 955 w, 916 w, 756 m; MS *m*/*z* (relative intensity, %) 427 (M^+, 11), 199 (11), 171 (10), 145 (15), 144 (100); HRMS Calcd for $C_{22}H_{16}FN_3O_3$: 427.1144; Found: 427.1142.

2,3-dimethyl-6-(1-methyl-2,5-dioxopyrrolidin-3-yl)-*N*-(quinolin-8-yl)benzamide (2f)



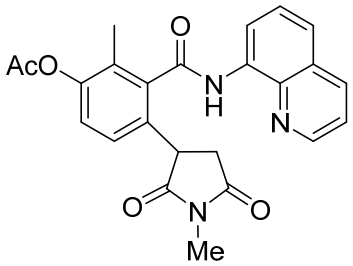
116.1 mg, 100% yield. R_f 0.24 (hexane/EtOAc = 1.5:1). White powder. M.p. 104.2-104.7 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.32 (s, 3H), 2.35 (s, 3H), 2.86-2.92 (m, 1H), 2.91 (s, 3H), 3.21 (dd, *J* = 18.8, 9.6 Hz, 1H), 4.22 (dd, *J* = 9.6, 5.5 Hz, 1H), 6.93 (d, *J* = 7.8 Hz, 1H), 7.24 (d, *J* = 7.8 Hz, 1H), 7.46 (dd, *J* = 8.2, 4.1 Hz, 1H), 7.58-7.59 (m, 2H), 8.18 (d, *J* = 8.2 Hz, 1H), 8.79 (dd, *J* = 4.1, 1.4 Hz, 1H), 8.91-8.94 (m, 1H), 10.16 (s, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 17.03, 20.20, 25.20, 38.28, 44.25, 116.91, 121.93, 122.52, 124.67, 127.32, 128.10, 131.45, 132.19, 133.94, 134.17, 136.38, 137.52, 138.38, 138.60, 148.68, 168.44, 176.42, 178.10; IR (ATR) 3338 w, 3014 w, 2948 w, 1777w, 1697 s, 1669 m, 1597 w, 1577 w, 1520 s, 1483 m, 1425 m, 1384 m , 1326 m, 1281 m, 1119 m, 827 w, 793 w, 753 m, 692 w; MS *m*/*z* (relative intensity, %) 387 (M^+, 17), 245 (11), 244 (71), 243 (100), 174 (21), 159 (21), 144 (16); HRMS Calcd for $C_{23}H_{21}N_3O_3$: 387.1583; Found: 387.1588.

3-methoxy-2-methyl-6-(1-methyl-2,5-dioxopyrrolidin-3-yl)-*N*-(quinolin-8-yl)benzamide (2g)



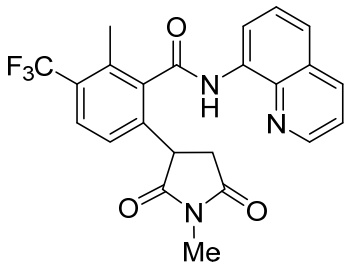
120.6 mg, 99% yield. R_f 0.33 (hexane/EtOAc = 1:1). Pale yellow powder. M.p. 97.9-98.3 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.31 (s, 3H), 2.86-2.92 (m, 1H), 2.91 (s, 3H), 3.21 (dd, *J* = 18.5, 9.5 Hz, 1H), 3.86 (s, 3H), 4.20 (dd, *J* = 9.5, 5.5 Hz, 1H), 6.91 (d, *J* = 8.7 Hz, 1H), 7.01 (d, *J* = 8.2 Hz, 1H), 7.45 (dd, *J* = 8.2, 4.1 Hz, 1H), 7.57-7.59 (m, 2H), 8.17 (d, *J* = 8.2 Hz, 1H), 8.78 (dd, *J* = 4.1, 1.4 Hz, 1H), 8.87-8.91 (m, 1H), 10.16 (s, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 13.39, 25.15, 38.35, 44.00, 55.78, 111.41, 116.84, 121.92, 122.50, 124.41, 126.15, 126.28, 127.30, 128.08, 134.10, 136.36, 138.57, 139.14, 148.65, 157.49, 167.64, 176.46, 178.30. IR (ATR) 3337 w, 3014 w, 2946 w, 1776 w, 1697 s, 1671 m, 1583 w, 1521 s, 1482 m, 1429 m, 1384 m, 1326 m, 1273 m, 1118 w, 1096 m, 826 w, 793 w, 752 m, 692 m; MS *m*/*z* (relative intensity, %) 403 (M^+, 16), 260 (41), 259 (100), 218 (31), 190 (17); HRMS Calcd for $C_{23}H_{21}N_3O_4$: 403.1532; Found: 403.1527.

2-methyl-4-(1-methyl-2,5-dioxopyrrolidin-3-yl)-3-(quinolin-8-ylcarbamoyl)phenyl acetate (2h)



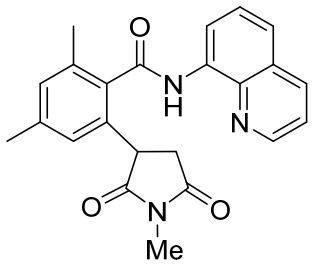
122.9 mg, 95% yield. R_f 0.24 (hexane/EtOAc = 1:1). Pale pink powder. M.p. 105.2-105.4 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.28 (s, 3H), 2.35 (s, 3H), 2.88-2.92 (m, 1H), 2.92 (s, 3H), 3.21 (dd, *J* = 18.3, 9.6 Hz, 1H), 4.26 (dd, *J* = 9.6, 5.5 Hz, 1H), 7.06 (d, *J* = 8.7 Hz, 1H), 7.15 (d, *J* = 8.2 Hz, 1H), 7.46 (qd, *J* = 4.1, 1.8 Hz, 1H), 7.58-7.59 (m, 2H), 8.18 (dt, *J* = 8.2, 1.6 Hz, 1H), 8.80-8.81 (m, 1H), 8.89 (t, *J* = 4.4 Hz, 1H), 10.20 (s, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 13.70, 20.91, 25.22, 38.11, 44.10, 116.97, 121.99, 122.71, 123.91, 126.20, 127.23, 128.06, 128.24, 132.49, 133.95, 136.35, 138.56, 139.72, 148.78, 149.11, 166.69, 169.08, 176.04, 177.55. IR (ATR) 3332 w, 3018 w, 2939 w, 1761 w, 1698 s, 1670 m, 1595 w, 1521 s, 1483 m, 1427 m, 1383 m, 1326 m, 1281 m, 1200 m, 1119 m, 898 w, 827 w, 793 w, 749 s; MS *m*/*z* (relative intensity, %) 431 (M^+, 16), 289 (12), 288 (70), 287 (78), 246 (23), 245 (100), 244 (10), 204 (63), 176 (24), 171 (10), 161 (21), 145 (18), 144 (55); HRMS Calcd for $C_{24}H_{21}N_3O_5$: 431.1481; Found: 431.1481.

2-methyl-6-(1-methyl-2,5-dioxopyrrolidin-3-yl)-*N*-(quinolin-8-yl)-3-(trifluoromethyl) benzamide (2i)



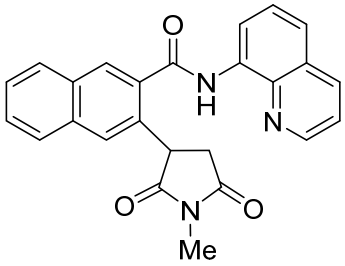
119.5 mg, 90% yield. R_f 0.26 (hexane/EtOAc = 1.5:1). White powder. M.p. 93.7-94.2 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.58 (s, 3H), 2.85-2.94 (m, 1H), 2.92 (s, 3H), 3.25 (dd, *J* = 18.8, 9.6 Hz, 1H), 4.29 (dd, *J* = 9.6, 5.5 Hz, 1H), 7.15 (d, *J* = 8.2 Hz, 1H), 7.49 (dd, *J* = 8.5, 4.4 Hz, 1H), 7.61-7.63 (m, 2H), 7.73 (d, 8.2 Hz, 1H), 8.20 (dd, *J* = 8.5, 1.6 Hz, 1H), 8.82 (dd, *J* = 4.4, 1.6 Hz, 1H), 8.90 (dd, *J* = 6.0, 2.7 Hz, 1H), 10.23 (s, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 16.57, 25.38, 37.92, 44.38, 117.19, 122.12, 123.03, 124.03(d, *J* = 272.6 Hz), 125.12, 125.40, 127.31, 127.58 (d, *J* = 5.7 Hz), 128.15, 129.63 (q, *J* = 29.5 Hz), 133.79, 134.89, 136.52, 138.55, 140.54, 148.89, 166.65, 175.72, 177.16; IR (ATR) 3329 w, 3020 w, 2943 w, 1778 w, 1699 s, 1670 m, 1598 w, 1522 s, 1484 m, 1427 m, 1384 m, 1319 m, 1281 m, 1184 w, 1121 m, 1110 m, 898 m, 793 m, 753, m, 695 m; MS *m*/*z* (relative intensity, %) 441 (M^+, 16), 298 (27), 213 (27), 145 (16), 144 (100); HRMS Calcd for $C_{23}H_{18}F_3N_3O_3$: 441.1300; Found: 441.1299.

2,4-dimethyl-6-(1-methyl-2,5-dioxopyrrolidin-3-yl)-*N*-(quinolin-8-yl)benzamide (2j)



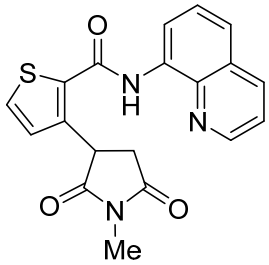
109.1 mg, 94% yield. R_f 0.20 (hexane/EtOAc = 1.5:1). Yellow powder. M.p. 86.4-86.7 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.34 (s, 3H), 2.44 (s, 3H), 2.87-2.94 (m, 1H), 2.94 (s, 3H), 3.23 (dd, *J* = 18.3, 9.6 Hz, 1H), 4.25 (dd, *J* = 9.6, 5.5 Hz, 1H), 6.81 (s, 1H), 7.06 (s, 1H), 7.44 (qd, *J* = 4.1, 1.5 Hz, 1H), 7.55-7.60 (m, 2H), 8.16 (dd, *J* = 8.2, 1.8 Hz, 1H), 8.78 (t, *J* = 2.1 Hz, 1H), 8.89 (q, *J* = 3.1 Hz, 1H), 10.16 (s, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 19.90, 21.35, 25.20, 38.31, 44.33, 116.77, 121.88, 122.38, 125.60, 127.29, 128.06, 131.02, 134.18, 134.87, 135.37, 135.49, 136.34, 138.56, 140.13, 148.62, 168.01, 176.40, 178.10; IR (ATR); 3339 w, 3014 w, 1776 w, 1697 s, 1668 m, 1610 w, 1520 s, 1483 m, 1425 m, 1383 m, 1325 m, 1281 m, 1117 m, 827 w, 763 w, 751 s, 680 m; MS *m*/*z* (relative intensity, %) 387 (M^+, 10), 245 (12), 244 (82), 243 (100), 174 (23), 159 (43), 144 (26); HRMS Calcd for $C_{23}H_{21}N_3O_3$: 387.1583; Found: 387.1577.

3-(1-methyl-2,5-dioxopyrrolidin-3-yl)-*N*-(quinolin-8-yl)-2-naphthamide (2k)



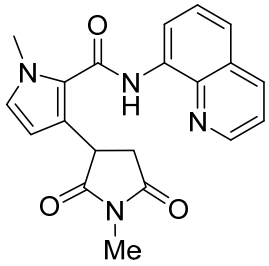
62.0 mg, 51% yield. R_f 0.24 (hexane/EtOAc = 1.5:1). Pale yellow powder. M.p. 216.0-216.5 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 3.04-3.10 (m, 1H), 3.09 (s, 3H), 3.34 (dd, *J* = 18.1, 9.4 Hz, 1H), 4.67 (dd, *J* = 9.4, 5.7 Hz, 1H), 7.48 (dd, *J* = 8.2, 4.1 Hz, 1H), 7.58-7.63 (m, 4H), 7.76 (s, 1H), 7.85 (d, *J* = 6.9 Hz, 1H), 7.98 (d, *J* = 7.3 Hz, 1H), 8.19 (d, *J* = 8.2 Hz, 1H), 8.34 (s, 1H), 8.82-8.84 (m, 2H), 10.61 (s, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 25.25, 38.49, 45.47, 116.61, 121.92, 122.29, 127.40, 127.47, 127.74, 128.16, 128.36, 128.47, 128.53, 130.70, 132.17, 133.22, 133.56, 134.29, 134.73, 136.53, 138.79, 148.56, 167.62, 176.72, 179.60. IR (ATR) 3342 w, 3015 w, 2948 w, 1776 w, 1697 s, 1668 m, 1597 w, 1522 s, 1484 m, 1427 m, 1384 m, 1326 w, 1281 m, 1120 w, 827 w, 793 w, 752 m, 695 w; MS *m*/*z* (relative intensity, %) 409 (M^+, 15), 266 (40), 265 (100), 224 (15), 196 (20), 181 (11), 153 (10), 152(11), 144 (17); HRMS Calcd for $C_{25}H_{19}N_3O_3$: 409.1426; Found: 409.1428.

3-(1-methyl-2,5-dioxopyrrolidin-3-yl)-*N*-(quinolin-8-yl)thiophene-2-carboxamide (2l)



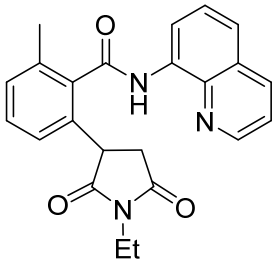
78.8 mg, 72% yield. R_f 0.23 (hexane/EtOAc = 1:1). Brown powder. M.p. 187.4-187.8 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.86 (dd, *J* = 18.3, 6.0 Hz, 1H), 3.12 (s, 3H), 3.31 (dd, *J* = 18.3, 9.6 Hz, 1H), 4.85 (dd, *J* = 9.2, 6.0 Hz, 1H), 7.02 (d, *J* = 5.0 Hz, 1H), 7.46-7.49 (m, 2H), 7.54-7.55 (m, 2H), 8.17 (dd, *J* = 8.2, 1.8 Hz, 1H), 8.72 (dd, *J* = 5.5, 3.7 Hz, 1H), 8.84 (dd, *J* = 4.4, 1.6 Hz, 1H), 10.49 (s, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 25.27, 37.41, 41.30, 116.75, 121.89, 122.12, 127.39, 127.93, 128.03, 130.12, 132.61, 134.32,136.48, 138.57, 141.94, 148.53, 160.27, 176.52, 177.75; IR (ATR) 3310 w, 3015 w, 2945 w, 1777 w, 1697 s, 1658 m, 1596 w, 1523 s, 1484 m, 1424 m, 1383 m, 1327 m, 1281 m, 1215w, 1118 m, 956 w, 792 m, 752 m, 752 s, 691 m, 665 m; MS *m*/*z* (relative intensity, %) 365 (M^+, 31), 222 (21), 221 (24), 180 (15), 145 (17), 144 (100), 137 (21); HRMS Calcd for $C_{19}H_{15}N_3O_3S$: 365.0834; Found: 365.0836.

1-methyl-3-(1-methyl-2,5-dioxopyrrolidin-3-yl)-*N*-(quinolin-8-yl)-1*H*-pyrrole-2-carboxamide (2m)



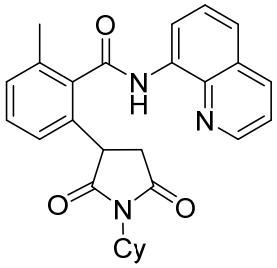
88.4 mg, 82% yield. R_f 0.28 (hexane/EtOAc = 1:1). Brown powder. M.p. 67.0-67.2 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.90 (dd, *J* = 18.3, 5.0 Hz, 1H), 3.06 (s, 3H), 3.37 (dd, *J* = 18.3, 9.6 Hz, 1H), 3.94 (s, 3H), 4.63 (dd, *J* = 9.4, 5.3 Hz, 1H), 5.99 (d, *J* = 2.7 Hz, 1H), 6.75 (d, *J* = 2.7 Hz, 1H), 7.46 (dd, *J* = 8.2, 4.1 Hz, 1H), 7.56-7.58 (m, 2H), 8.18 (dd, *J* = 8.2, 1.4 Hz, 1H), 8.75-8.80 (m, 2H), 10.35 (s, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 25.30, 36.84, 37.70, 39.16, 106.23, 117.57, 121.81, 122.15, 123.14, 126.43, 127.36, 127.46, 128.21, 134.74, 136.54, 139.09, 148.54, 160.04, 176.63, 178.62; IR (ATR) 3347 w, 3014 w, 2950 w, 1776 w, 1697 s, 1658 m, 1521 s, 1482 m, 1425 m, 1383 m, 1326 m, 1281 m, 1119 m, 956 w, 887 w, 827 w, 792 w, 753 m, 689 w; MS *m*/*z* (relative intensity, %) 362 (M^+, 20), 219 (27), 218 (100), 177 (54), 134 (17); HRMS Calcd for $C_{20}H_{18}N_4O_3$: 362.1379; Found: 362.1384.

2-(1-ethyl-2,5-dioxopyrrolidin-3-yl)-6-methyl-*N*-(quinolin-8-yl)benzamide (3a)



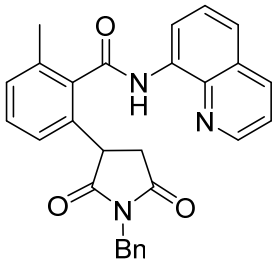
99.9 mg, 86% yield. R_f 0.17 (hexane/EtOAc = 2:1). White powder. M.p. 82.1-82.5 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.14 (t, *J* = 7.2 Hz, 3H), 2.48 (s, 3H), 2.87 (dd, *J* = 18.4, 5.4 Hz, 1H), 3.22 (dd, *J* = 18.4, 9.6 Hz, 1H), 3.54 (q, *J* = 7.2 Hz, 2H), 4.26 (dd, *J* = 9.6, 5.4 Hz, 1H), 7.00 (d, *J* = 7.8 Hz, 1H), 7.25 (d, *J* = 8.7 Hz, 1H), 7.36 (t, *J* = 7.8 Hz, 1H), 7.46 (qd, *J* = 4.1, 1.4 Hz, 1H), 7.58-7.61 (m, 2H), 8.18 (dt. *J* = 8.2, 1.6 Hz, 1H), 8.79-8.80 (m, 1H), 8.93 (m, 1H), 10.18 (s, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 13.12, 19.97, 34.12, 38.38, 44.20, 116.98, 121.92, 122.53, 124.68, 127.32, 128.12, 130.17, 130.22, 134.15, 135.16, 135.65, 136.39, 138.17, 138.66, 148.69, 167.82, 176.09, 177.65; IR (ATR) 3334 w, 2951 w, 2876 w, 2360 w, 1772 w, 1701 s, 1673 m, 1522 s, 1483 m, 1400 m, 1326 m, 1224 m, 1126 m, 789 m, 773 m; MS *m*/*z* (relative intensity, %) 387 (M^+, 11), 245 (11), 244 (77), 243 (100) 174 (11), 146 (12), 145 (49), 144 (53), 130 (10), 117 (11), 115 (11); HRMS Calcd for $C_{23}H_{21}N_3O_3$: 387.1583; Found: 387.1578.

2-(1-cyclohexyl-2,5-dioxopyrrolidin-3-yl)-6-methyl-*N*-(quinolin-8-yl)benzamide (4a)



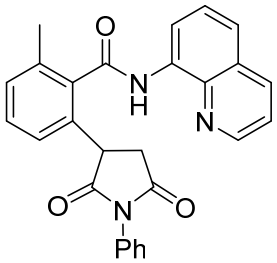
95.1 mg, 72% yield. R_f 0.29 (hexane/EtOAc = 2:1). White powder. M.p. 102.8-103.3 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.15-1.29 (m, 3H), 1.15-1.63 (m, 3H), 1.71-1.86 (m, 2H), 2.10-2.16 (m, 2H), 2.47 (s, 3H), 2.80 (dd, *J* = 18.7, 5.2 Hz, 1H), 3.17 (dd, *J* = 18.7, 9.6 Hz, 1H), 3.97-4.01 (m, 1H), 4.21 (dd, *J* = 9.6, 5.2 Hz, 1H), 6.97 (d, *J* = 7.8 Hz, 1H), 7.24 (d, *J* = 7.8 Hz, 1H), 7.35 (t, *J* = 7.8 Hz, 1H), 7.46 (dd, *J* = 8.2, 4.6 Hz, 1H), 7.58-7.60 (m, 2H), 8.18 (dd, *J* = 8.2, 1.8 Hz, 1H), 8.80 (dd, *J* = 4.1, 1.8 Hz, 1H), 8.93 (dd, *J* = 6.0, 3.2 Hz, 1H), 10.19 (s, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 19.97, 25.03, 25.85, 28.83, 38.26, 43.73, 52.05, 117.02, 121.90, 122.50, 124.35, 127.29, 128.10, 130.11, 130.16, 134.16, 135.54, 135.58, 136.39, 138.17, 138.63, 148.65, 167.85, 176.38, 177.88; IR (ATR) 3338 w, 3016 w, 2932 w, 2856 w, 1773 w, 1696 s, 1671 m, 1596 w, 1521 s, 1483 m, 1424 m, 1373 m, 1325 m, 1261 w, 1188 m, 1143 w, 897 w, 826 w, 752 s, 666 w; MS *m*/*z* (relative intensity, %) 441 (M^+, 14), 298 (44), 297 (100), 217 (10), 216 (78), 215 (47), 146 (20), 145 (49), 144 (36), 117 (12), 115 (10); HRMS Calcd for $C_{27}H_{27}N_3O_3$: 441.2052; Found: 441.2057.

2-(1-benzyl-2,5-dioxopyrrolidin-3-yl)-6-methyl-*N*-(quinolin-8-yl)benzamide (5a)



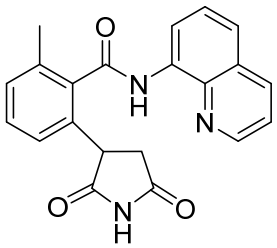
98.5 mg, 73% yield. R_f 0.33 (hexane/EtOAc = 2:1). White powder. m.p. 86.4-86.9 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.47 (s, 3H), 2.86 (dd, *J* = 18.7, 5.2 Hz, 1H), 3.23 (dd, *J* = 18.7, 9.6 Hz, 1H), 4.28 (dd, *J* = 9.6, 5.0 Hz, 1H), 4.58 (d, *J* = 14.0 Hz, 1H), 4.66 (d, *J* = 14.0 Hz, 1H), 6.90 (d, *J* = 7.8 Hz, 1H), 7.22-7.36 (m, 6H), 7.45 (dd, *J* = 8.2, 4.1 Hz, 1H), 7.56-7.61 (m, 2H), 8.17 (dd, *J* = 8.2, 1.4 Hz, 1H), 8.78 (dd, *J* = 4.4, 1.6 Hz, 1H), 8.90 (dd, *J* = 5.5, 3.7 Hz, 1 H), 10.18 (s, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 19.97, 38.35, 42.72, 44.12, 116.99, 121.95, 122.55, 124.57, 127.32, 128.01, 128.08, 128.69, 128.86, 130.17, 130.21, 134.10, 135.05, 135.60, 135.81, 136.40, 138.14, 148.66, 167.77, 175.81, 177.51; IR (ATR) 3339 w, 3018 w, 2939 w, 1776 w, 1701 s, 1669 m, 1596 w, 1521 s, 1483 m, 1425 m, 1392 m, 1325 m, 1167 m, 827 s, 754 m, 701 m; MS *m*/*z* (relative intensity, %) 449 (M^+, 17), 307 (10), 306 (55), 305 (95), 145 (20), 144 (34), 91 (100); HRMS Calcd for $C_{28}H_{23}N_3O_3$: 449.1739; Found: 449.1735.

2-(2,5-dioxo-1-phenylpyrrolidin-3-yl)-6-methyl-*N*-(quinolin-8-yl)benzamide (6a)



118.1 mg, 90% yield. R_f 0.21 (hexane/EtOAc = 2:1). Pale yellow powder. M.p. 91.0-91.4 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.51 (s, 3H), 3.10 (dd, *J* = 18.5, 5.6 Hz, 1H), 3.40 (dd, *J* = 18.5, 9.7 Hz, 1H), 4.45 (dd, *J* = 9.7, 5.6 Hz, 1H), 7.16 (d, *J* = 7.8 Hz, 1H), 7.25-7.44 (m, 8H), 7.58-7.59 (m, 2H), 8.16 (dd, *J* = 8.2, 1.4 Hz, 1H), 8.75 (t, *J* = 2.1 Hz, 1H), 8.93 (dd, *J* = 6.0, 3.2 Hz, 1H), 10.21 (s, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 20.16, 38.40, 44.72, 117.04, 121.94, 122.58, 125.46, 126.61, 127.33, 128.13, 128.67, 129.17, 130.29, 130.54, 132.05, 134.12, 135.06, 135.84, 136.41, 137.91, 138.66, 148.70, 167.87, 175.25, 176.79; IR (ATR) 3338 w, 3015 w, 2941 w, 1779 w, 1711 s, 1666 m, 1596 w, 1521 s, 1483 m, 1424 m, 1382 s, 1326 m, 1269 w, 1179 m, 838 w, 751 s, 695 m, 664 m; MS *m*/*z* (relative intensity, %) 435 (M^+, 25), 293 (12), 292 (71), 291 (100), 222 (10), 171 (10), 145 (81), 144 (54), 116 (10), 115 (15); HRMS Calcd for $C_{27}H_{21}N_3O_3$: 435.1583; Found: 435.1588.

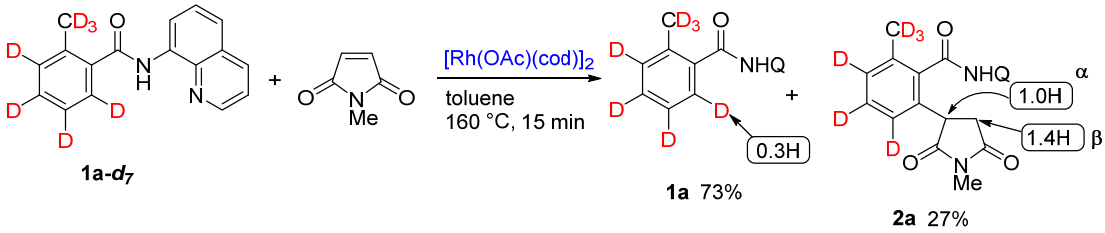
2-(2,5-dioxopyrrolidin-3-yl)-6-methyl-*N*-(quinolin-8-yl)benzamide (7a)



100.6 mg, 93% yield. R_f 0.43 (hexane/EtOAc = 1:2). White powder. M.p.163.7-164.2 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.48 (s, 3H), 2.94 (dd, *J* = 18.8, 5.5 Hz, 1H), 3.25 (dd, *J* = 18.8, 9.6 Hz, 1H), 4.33 (dd, *J* = 9.6, 5.5 Hz, 1H), 7.09 (d, *J* = 7.8 Hz, 1H), 7.27 (d, *J* = 6.9 Hz, 1H), 7.38 (t, *J* = 7.8 Hz, 1H), 7.45 (dd, *J* = 8.2, 4.6 Hz, 1H), 7.58-7.60 (m, 2H), 8.17-8.19 (m, 2H), 8.79 (dd, *J* = 4.1, 1.8 Hz, 1H), 8.92 (dd, *J* = 5.5, 3.2 Hz, 1H), 10.18 (s, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 20.02, 39.39, 45.67, 117.12, 122.01, 122.65, 124.82, 127.43, 128.20, 130.27, 130.48, 134.19, 134.45, 135.81, 136.47, 138.23, 138.70, 148.76, 167.84, 175.82, 177.81; IR (ATR) 3333 w, 3074 w, 2987 w, 1775 w, 1705 s, 1669 m, 1596 w, 1521 s, 1483 m, 1425 m, 1384 m, 1326 m, 1244 m, 1177 w, 1126 w, 1045 w, 828 w, 792 w, 696 w; MS *m*/*z* (relative intensity, %) 359 (M^+, 13), 216 (7),145 (37), 144 (100); HRMS Calcd for $C_{21}H_{17}N_3O_3$: 359.1270; Found: 359.1271.

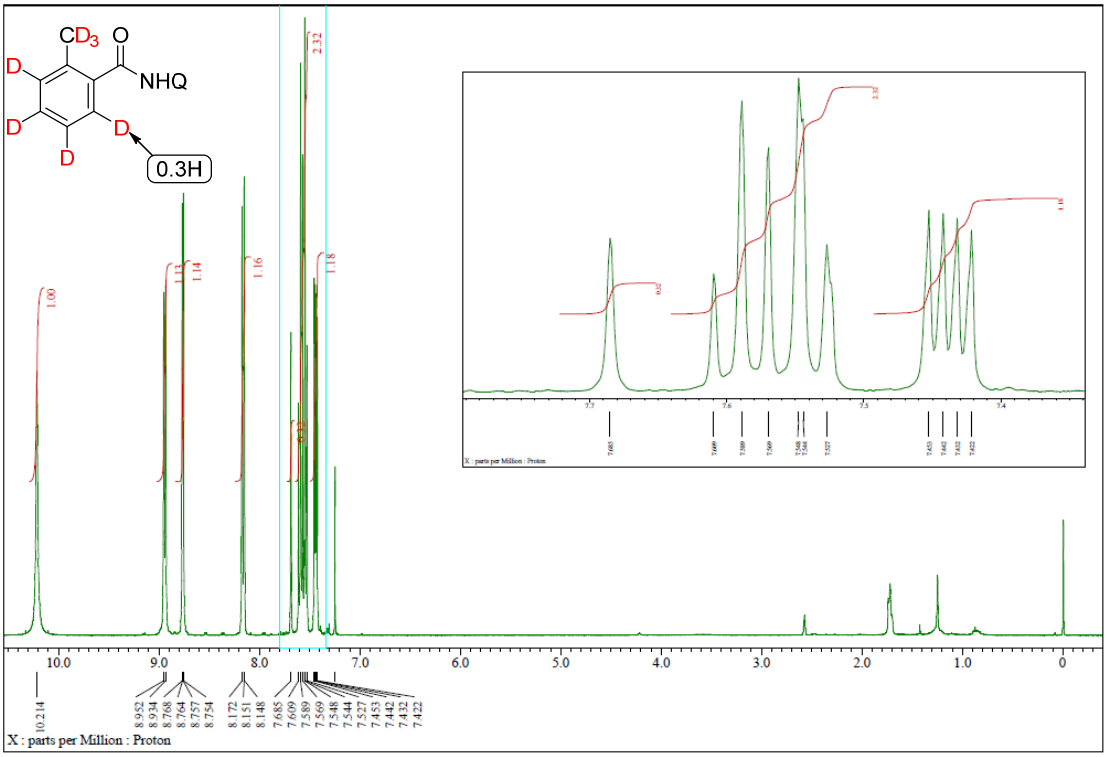
VI. Deuterium Labeling Experiments

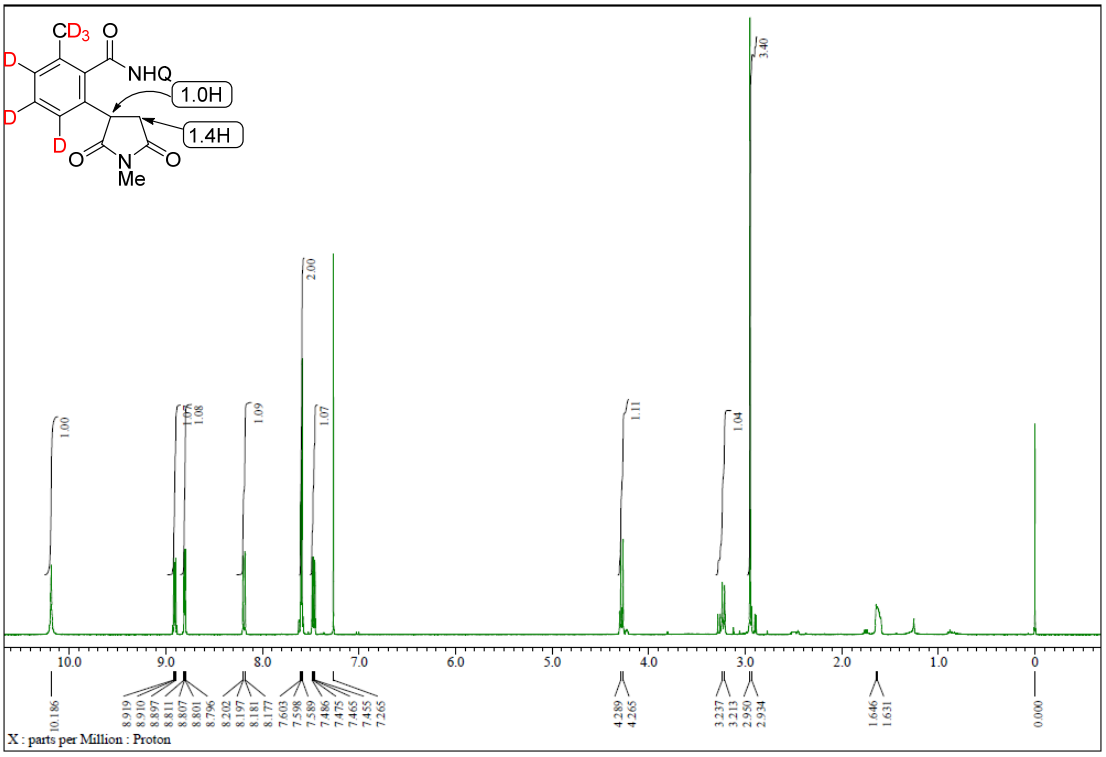
(a) Rh (I) system



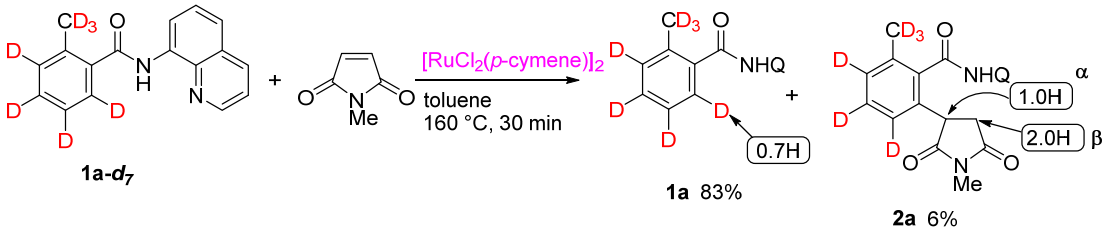
Representative procedure.

To an oven-dried 5 mL screw-capped vial, 2-methyl-*N*-(quinolin-8-yl)benzamide **1a-*d*$_7$** (80.8 mg, 0.3 mmol), *N*-methylmaleimide (39.6 mg, 0.36 mmol), $[Rh(OAc)(cod)]_2$ (4.1 mg, 0.0075 mmol) and toluene (1 mL) were added. The mixture was stirred for 15 minutes at 160 °C and then cooled to room temperature. The resulting mixture was filtered through a celite pad and then concentrated *in vacuo*. The residue was purified by column chromatography on silica gel (eluent: hexane/EtOAc = 1.5:1) to afford the desired product and starting material.



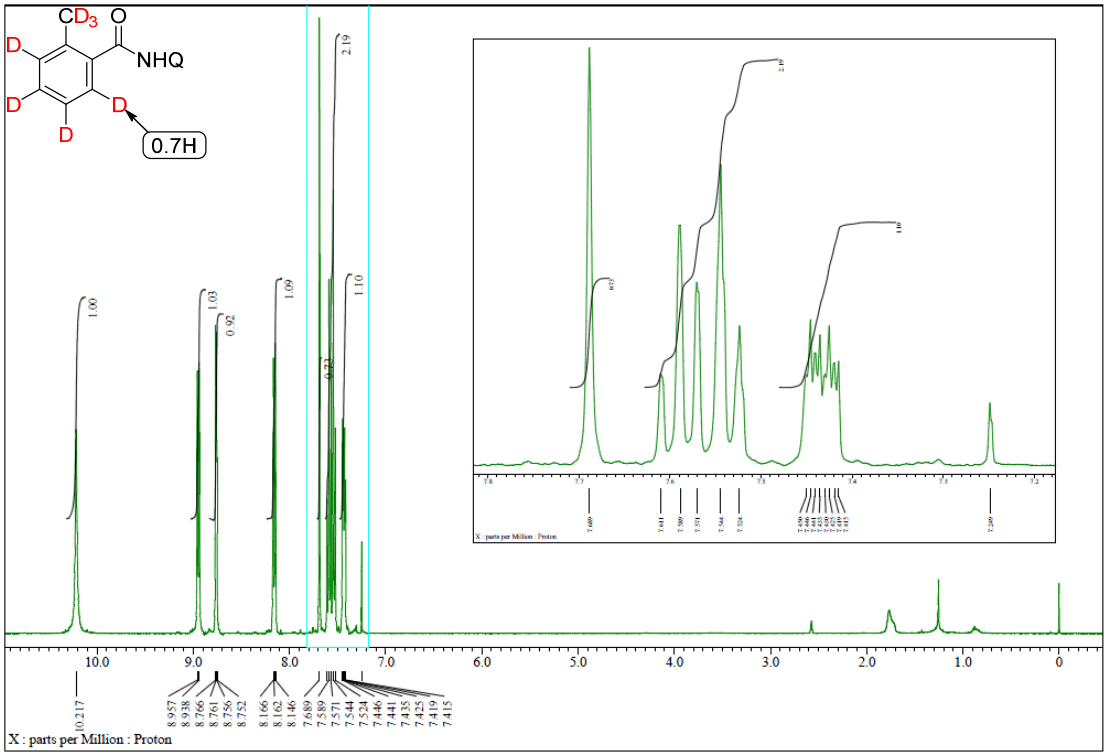


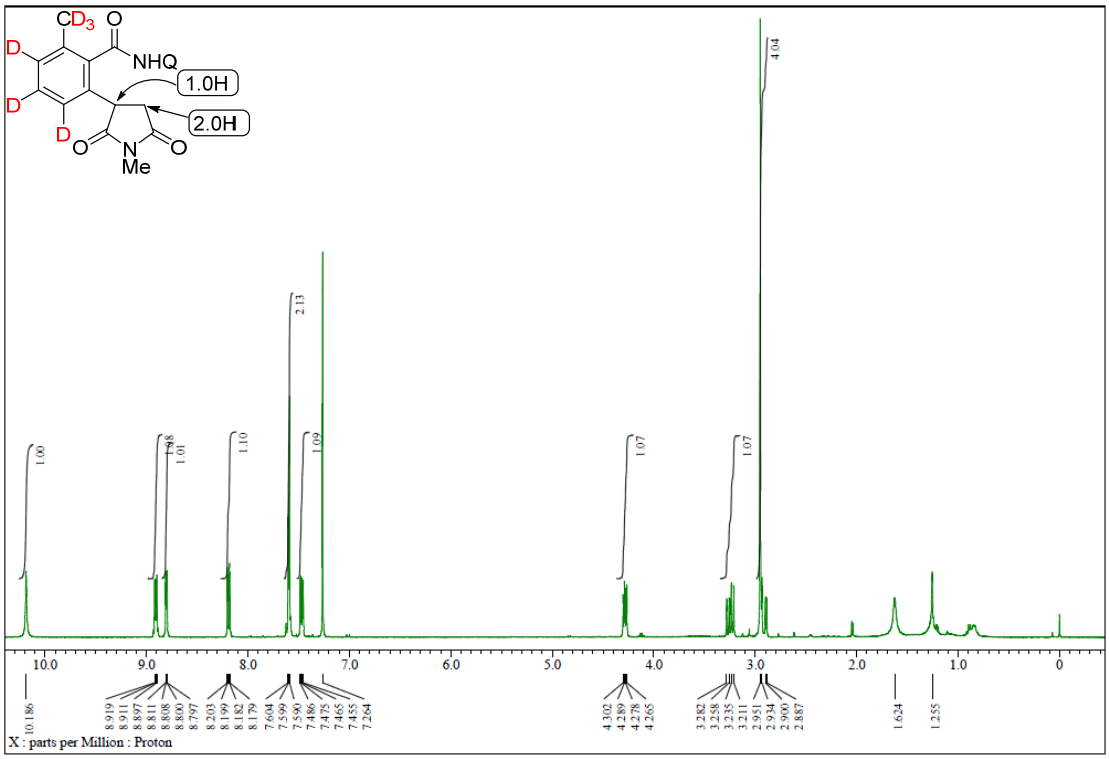
(a) Ru (II) system



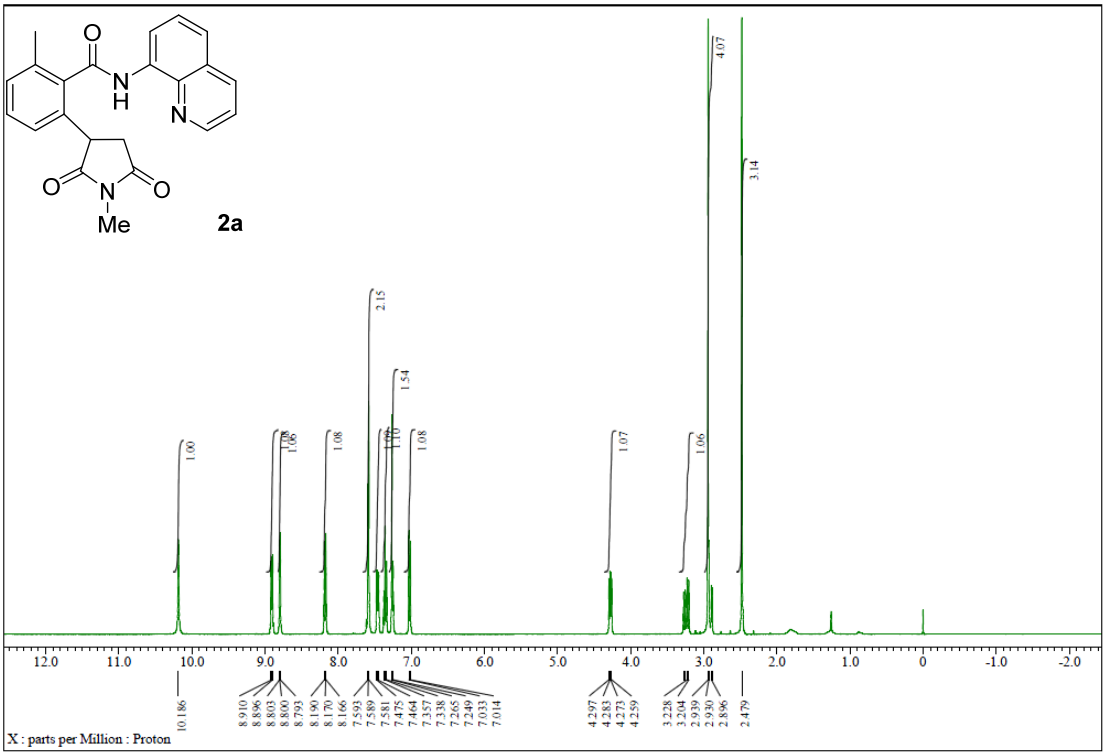
Representative procedure.

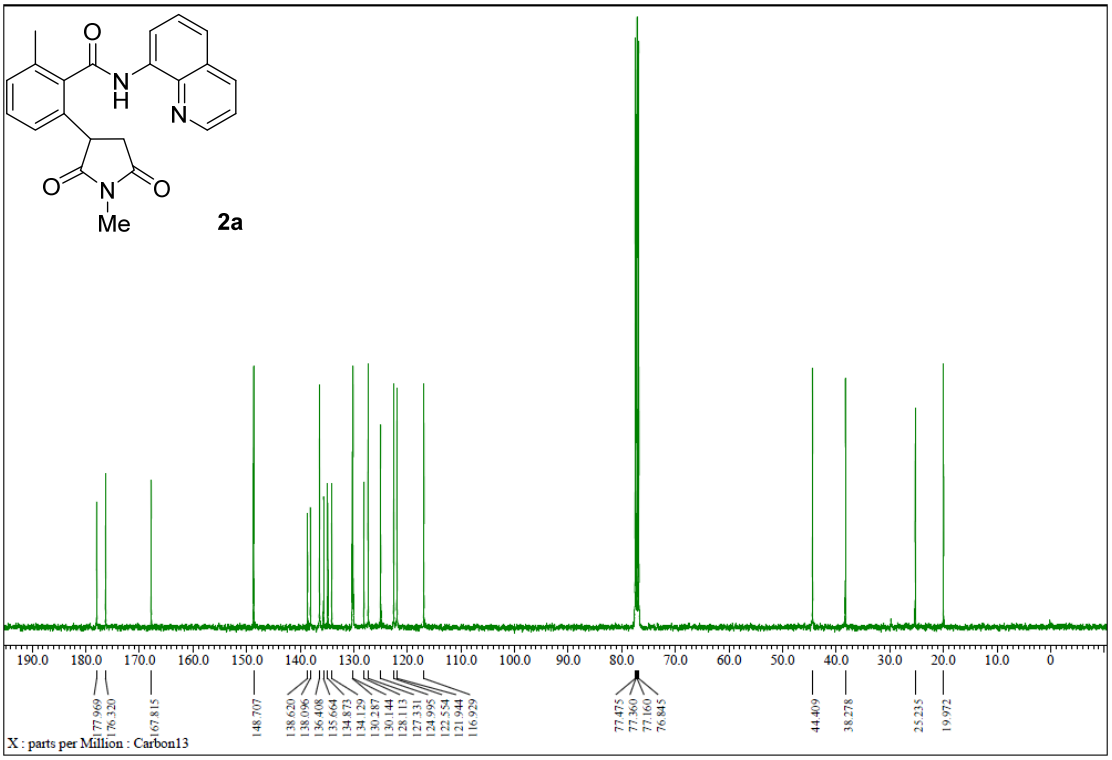
To an oven-dried 5 mL screw-capped vial, 2-methyl-*N*-(quinolin-8-yl)benzamide (80.8 mg, 0.3 mmol), *N*-methylmaleimide (39.6 mg, 0.36 mmol), 2-methylbenzoic acid (40.9 mg, 0.3 mmol), $[RuCl_2(p\text{-cymene})]_2$ (4.6 mg, 0.0075 mmol) and toluene (1 mL) were added. The mixture was stirred for 30 minutes at 160 °C and then cooled to room temperature. The resulting mixture was filtered through a celite pad and washed with saturated aqueous $NaHCO_3$ (20 mL), and EtOAc (3x20 mL); then concentrated *in vacuo*. The residue was purified by column chromatography on silica gel (eluent: hexane/EtOAc = 1.5:1) to afford the desired product and starting material.

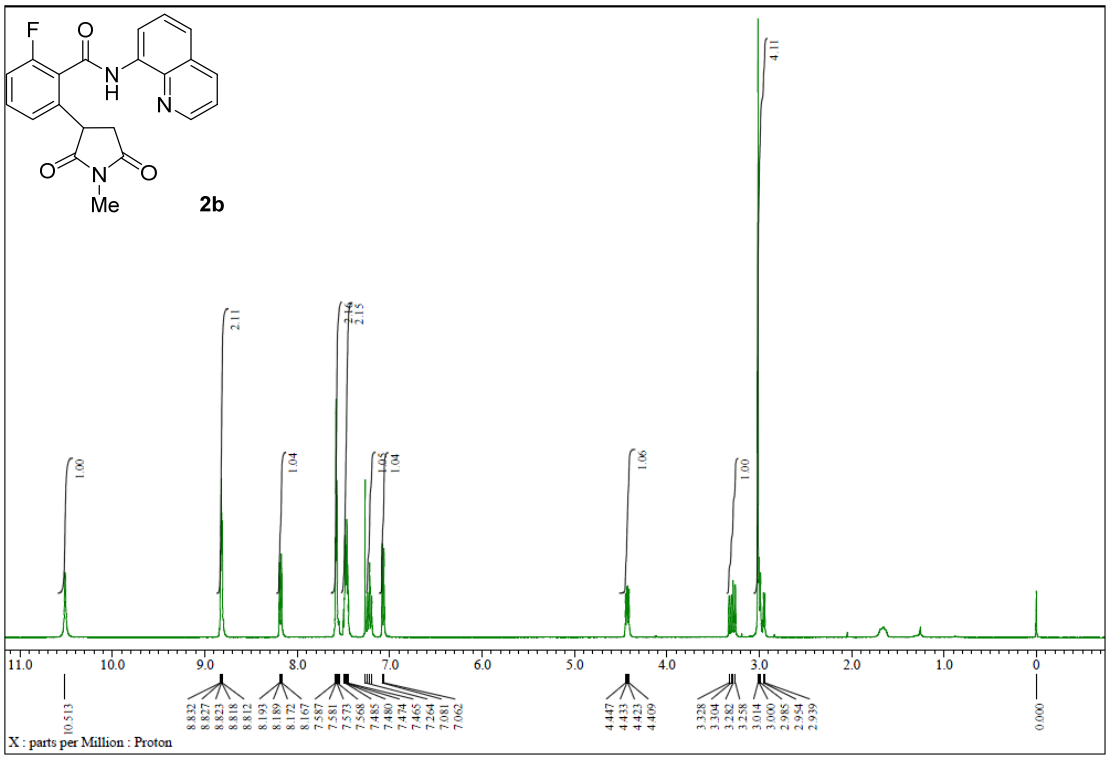

CD3
O
NHQ
D
D
D
D
0.7H
X : parts per Million : Proton

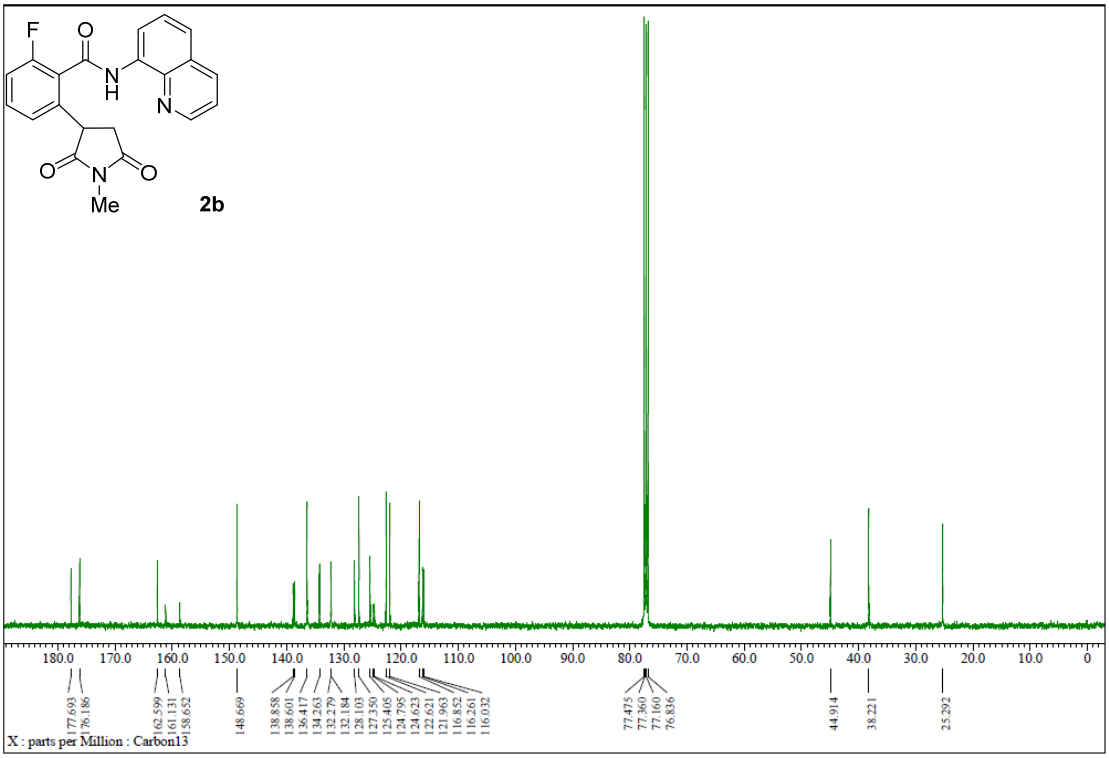

CD3
O
NHQ
D
D
D
1.0H
2.0H
O
N
Me
O
X : parts per Million : Proton

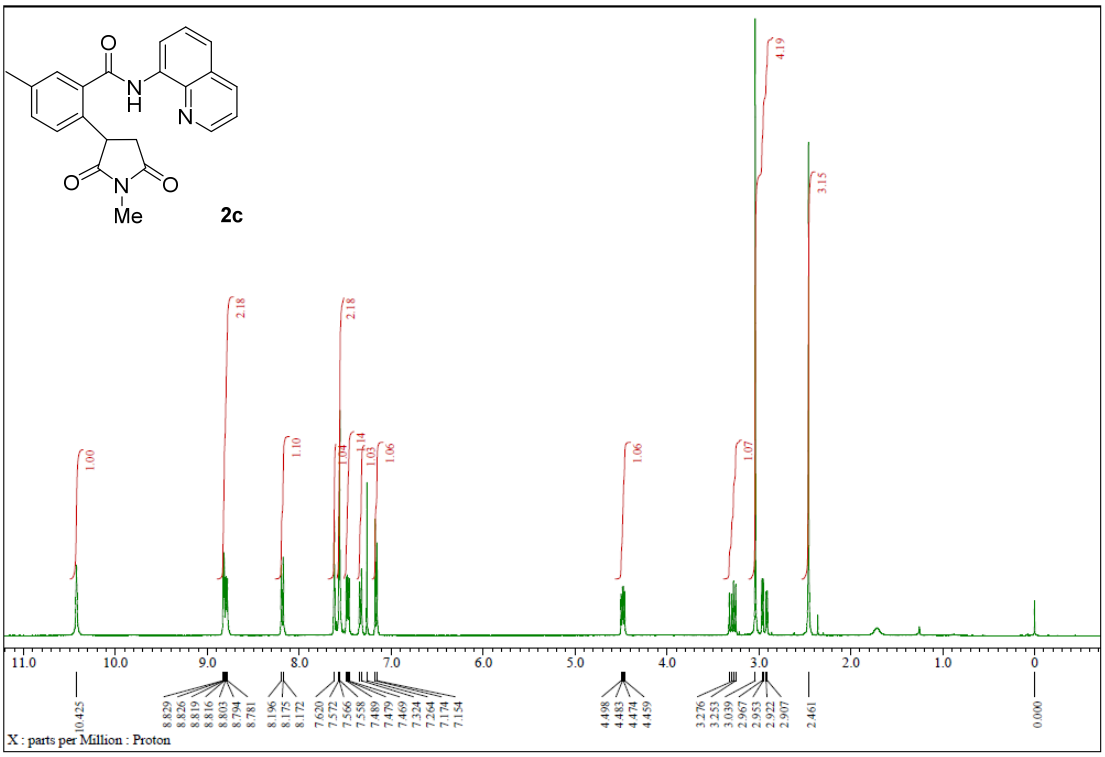
VII. Copies of ^{1}H and ^{13}C NMR Spectra

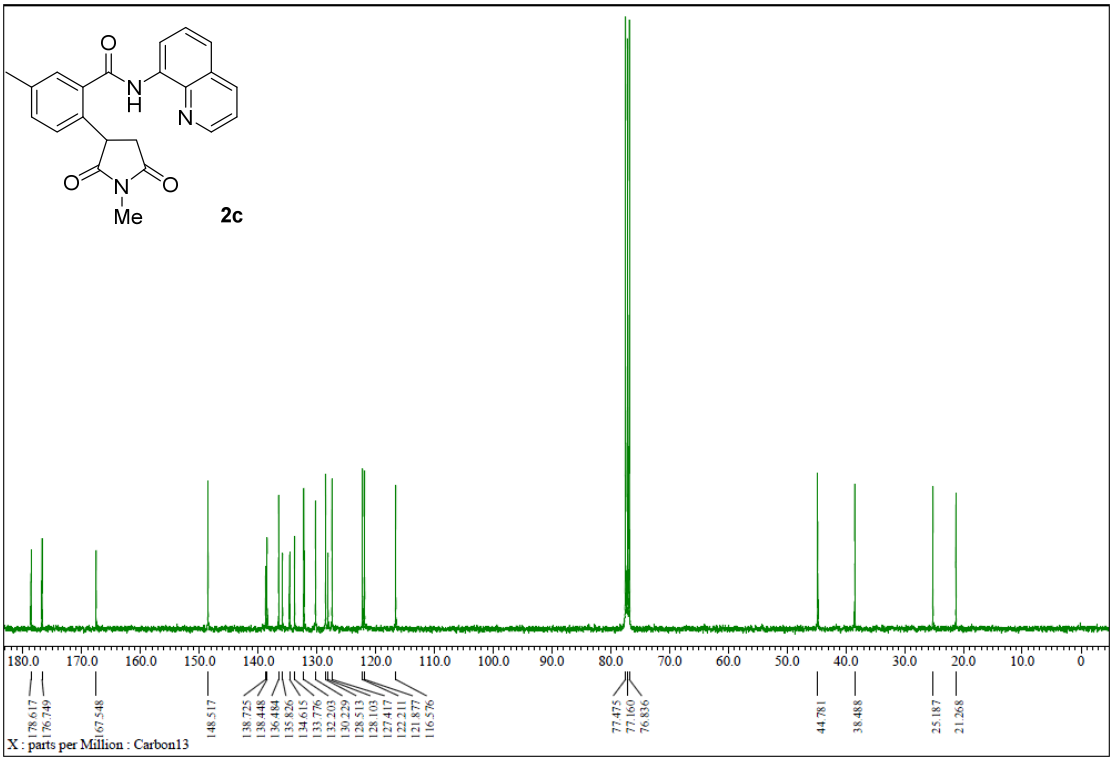


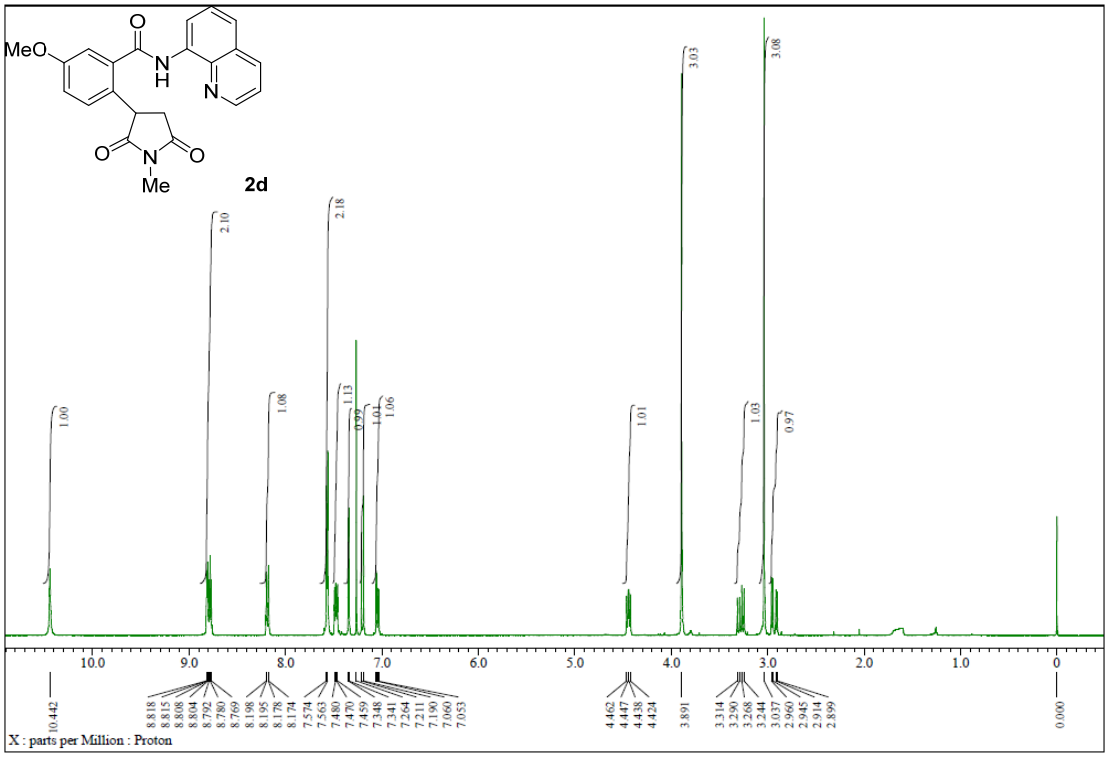


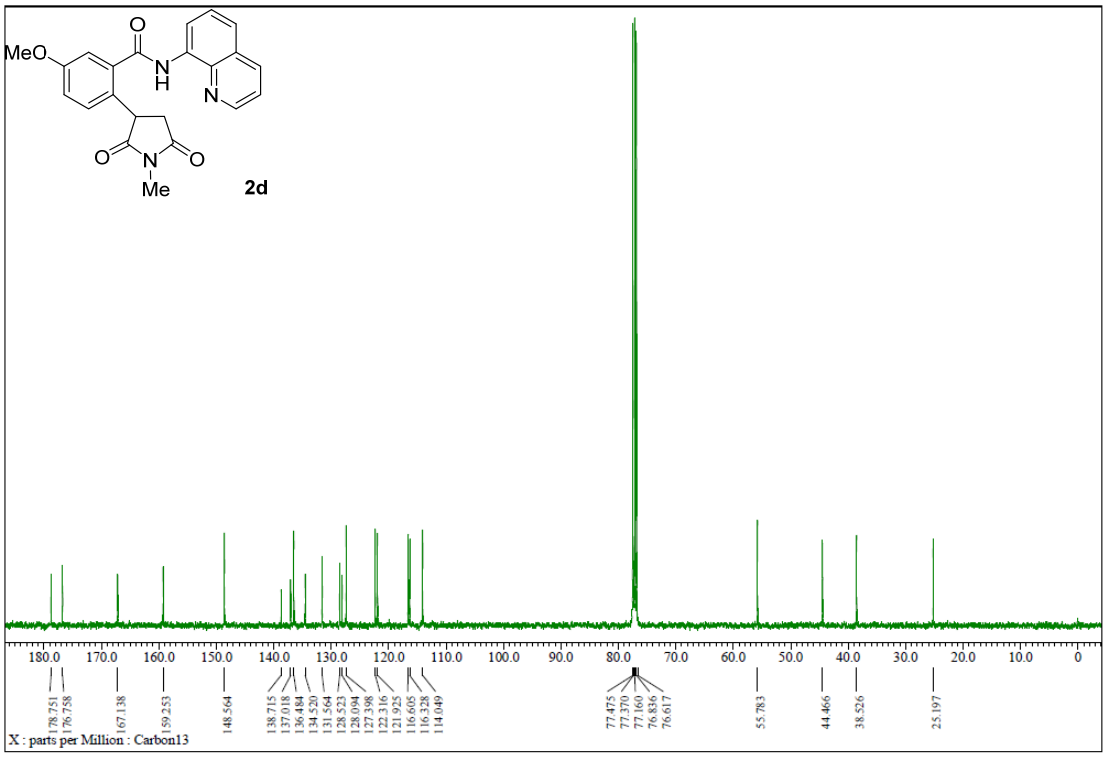

F
O
N
H
N
O
N
O
Me
2b
X : parts per Million : Proton

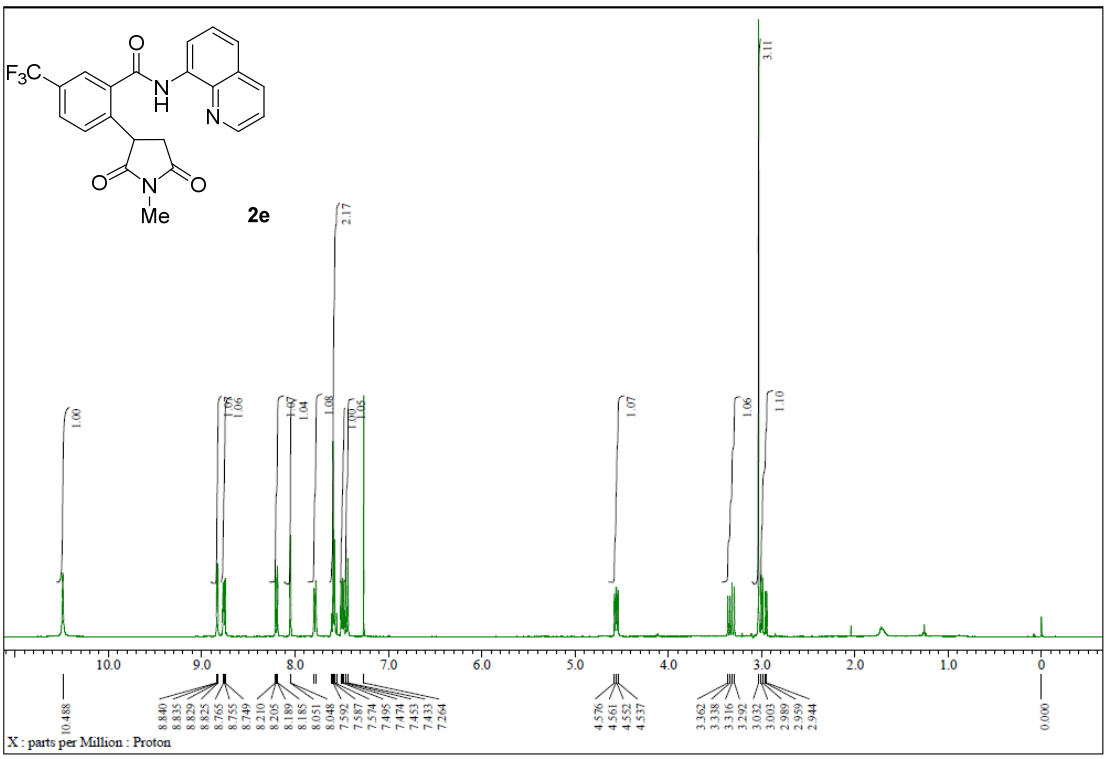

F
O
N
H
N
O
N
O
Me
2b
X : parts per Million : Carbon13

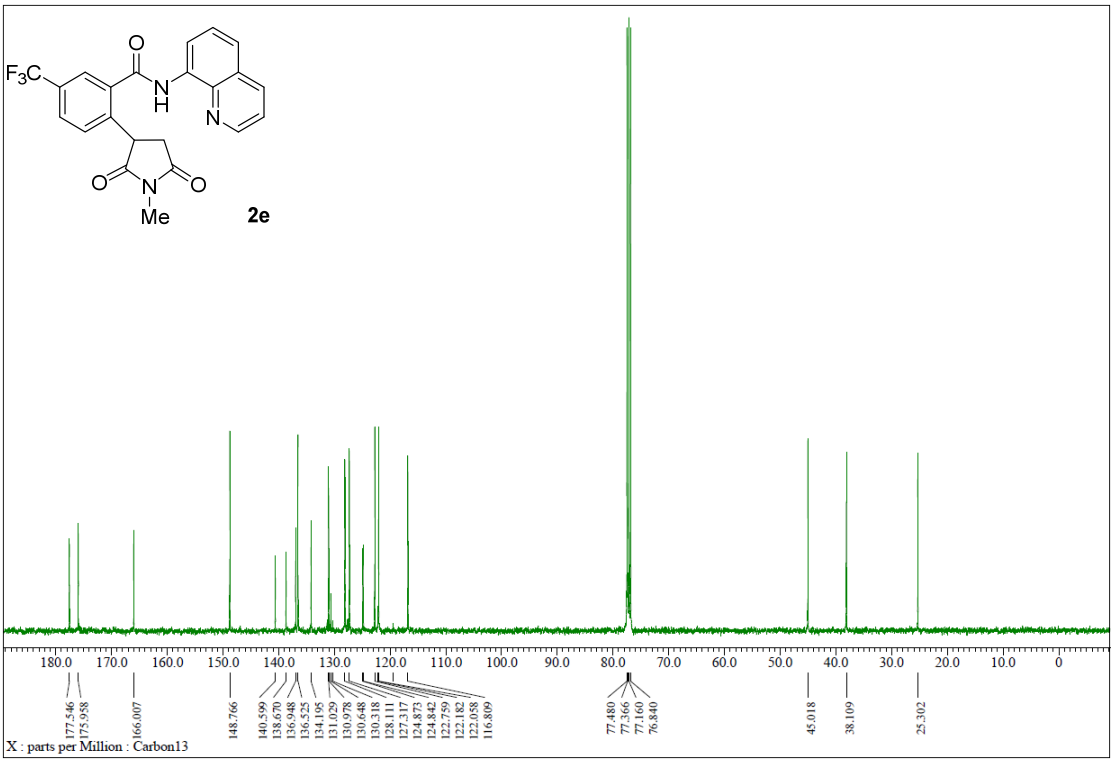

2c
X : parts per Million : Proton

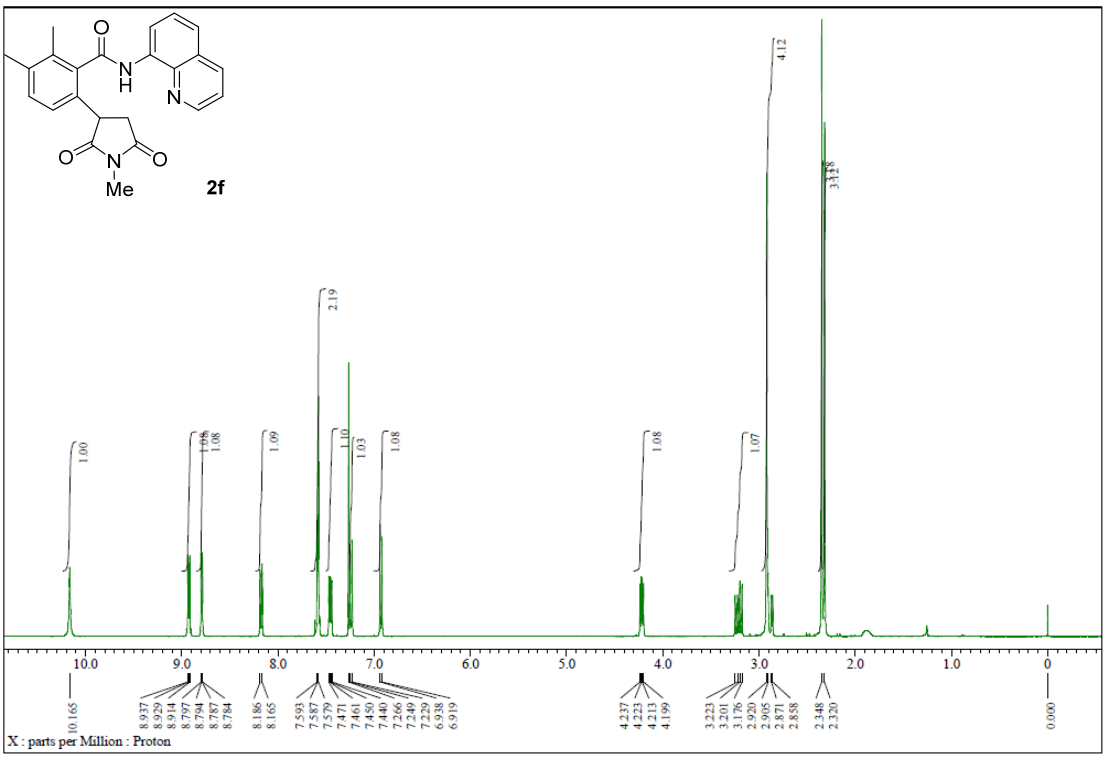

2c
X : parts per Million : Carbon13

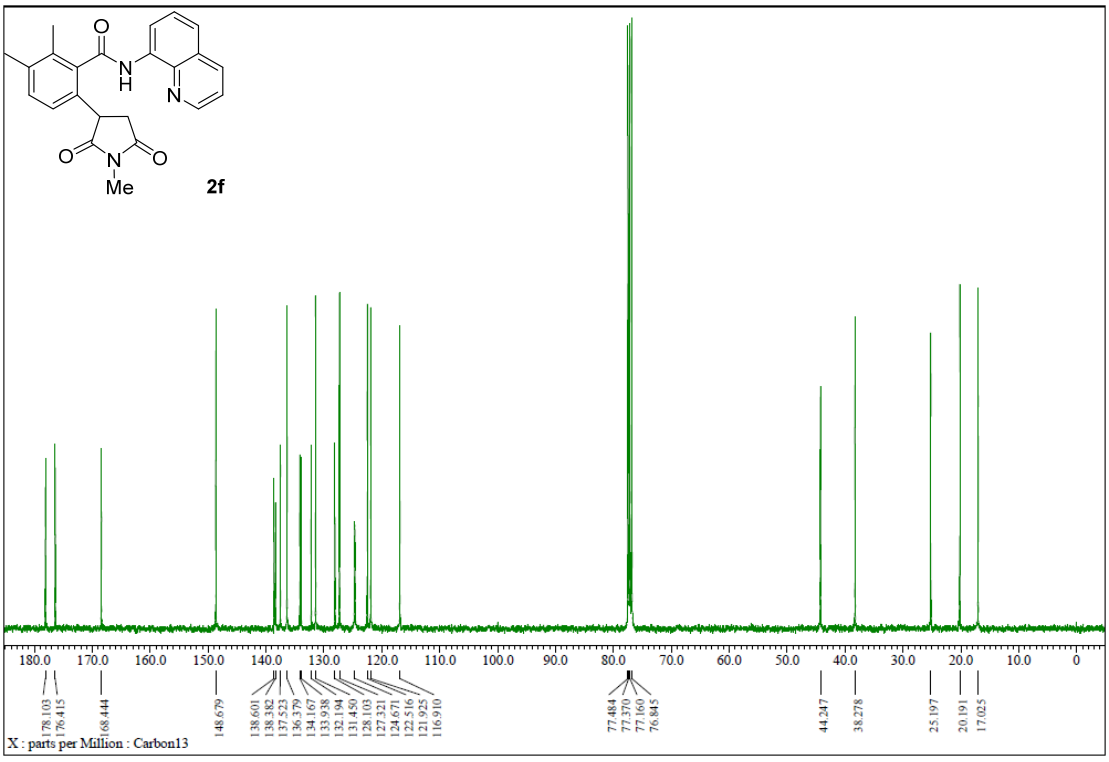

MeO
O
N
H
N
O
N
O
Me
2d
10.442
8.818
8.815
8.808
8.804
8.792
8.780
8.769
8.198
8.195
8.178
8.174
7.574
7.563
7.480
7.470
7.459
7.448
7.341
7.264
7.211
7.190
7.060
7.053
4.462
4.447
4.438
4.424
3.891
3.314
3.290
3.268
3.244
3.037
2.960
2.945
2.914
2.899
0.000
X : parts per Million : Proton

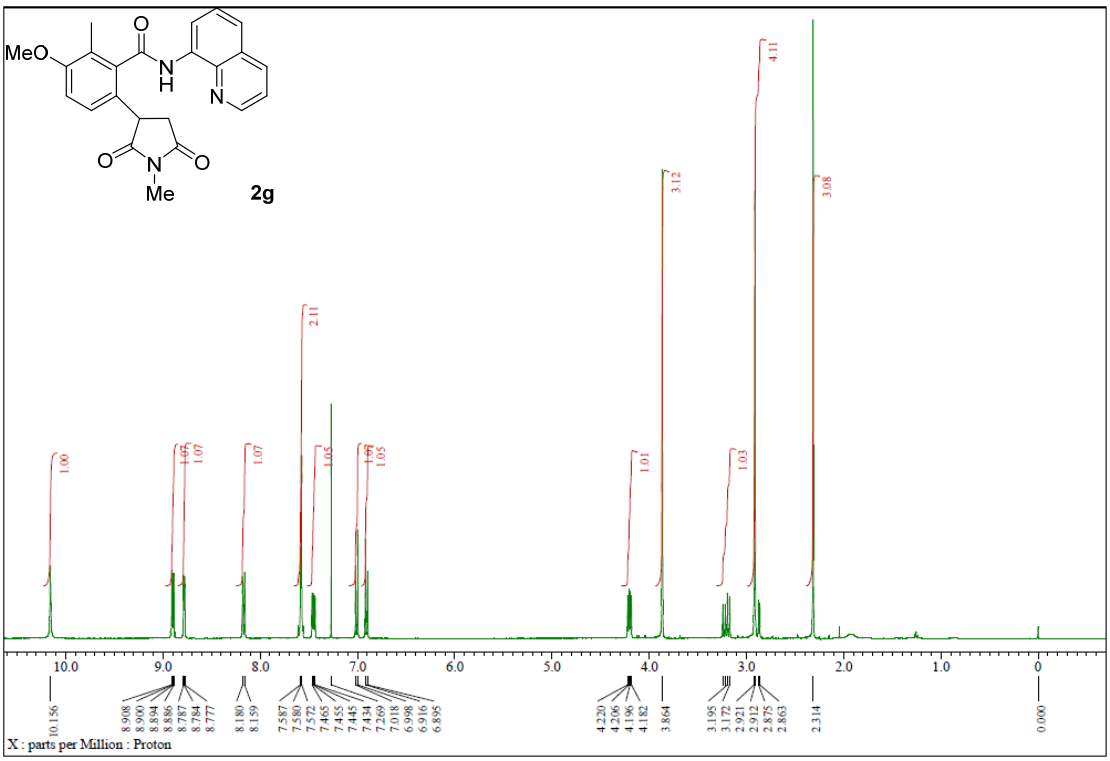

MeO
O
N
H
N
O
N
O
Me
2d
178.751
176.758
167.138
159.253
148.564
138.715
137.018
136.484
134.520
131.564
128.523
128.094
127.398
122.316
121.925
116.605
116.328
114.049
77.475
77.370
77.160
76.836
76.617
55.783
44.466
38.526
25.197
X : parts per Million : Carbon13

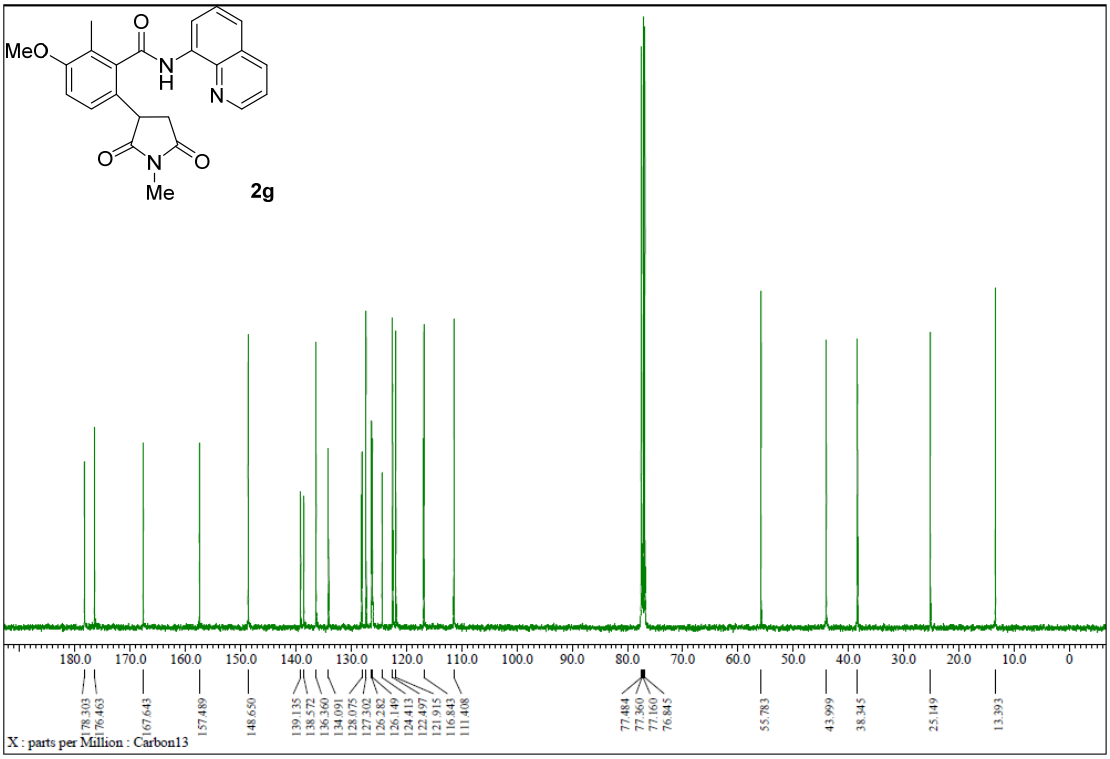

2e
X : parts per Million : Proton

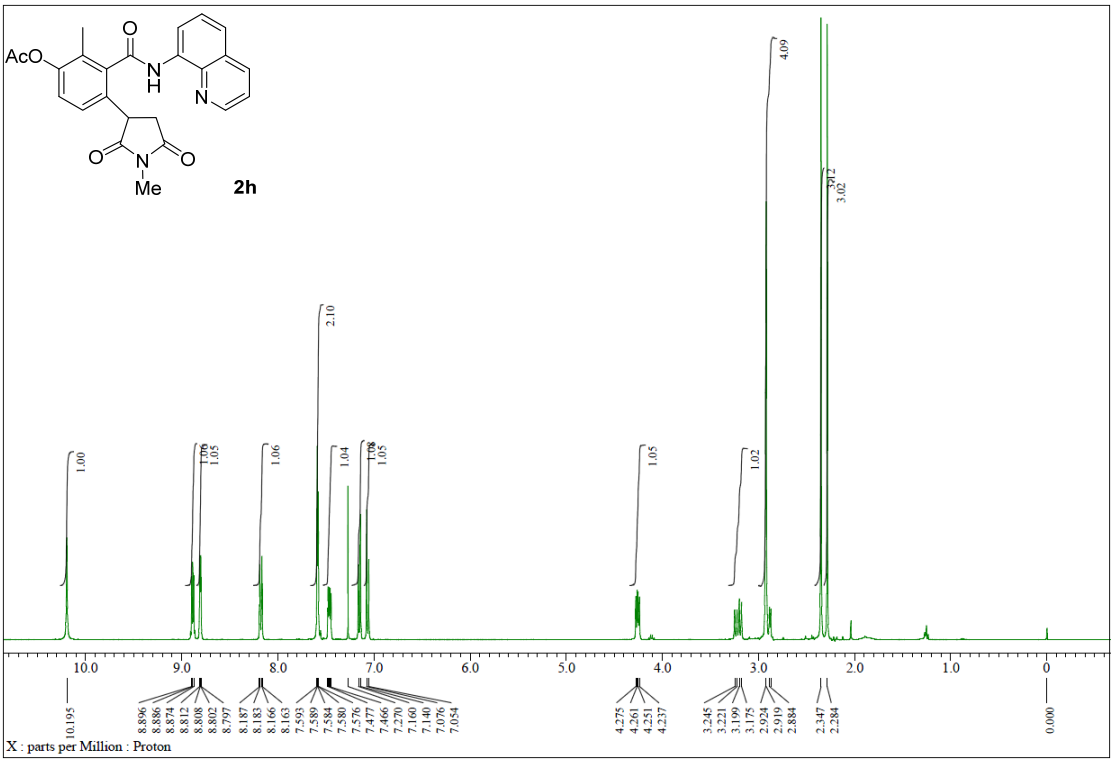

2e
X : parts per Million : Carbon13

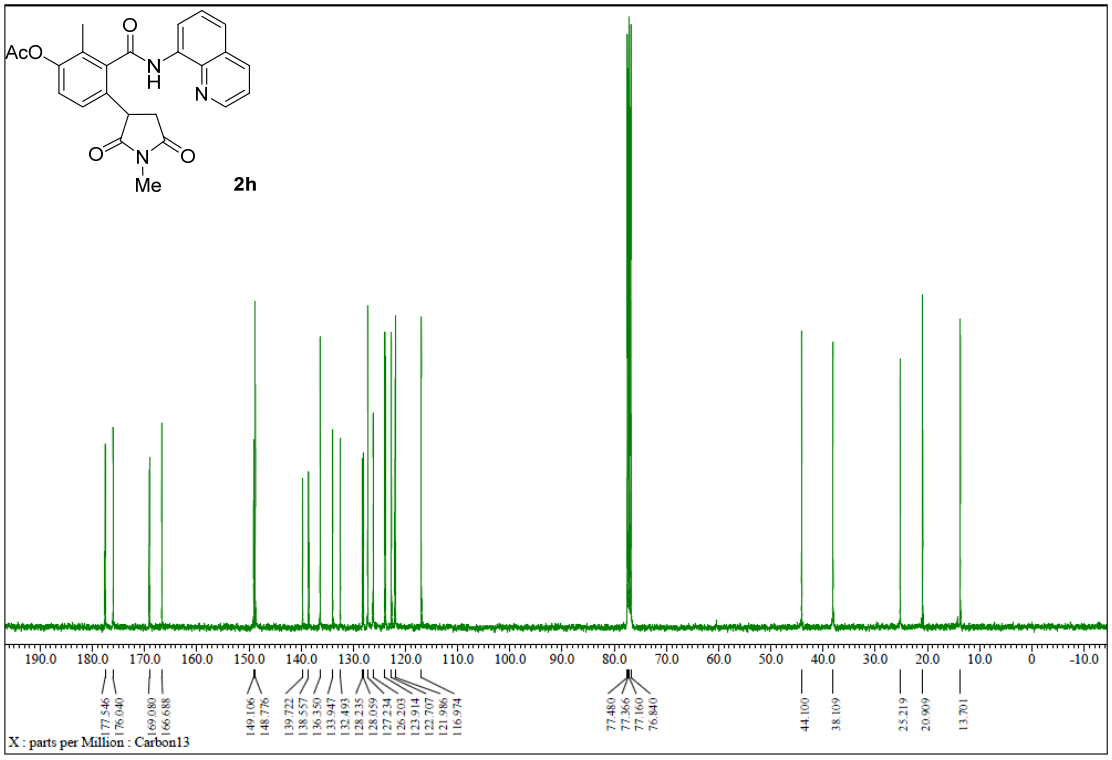

2f
X : parts per Million : Proton

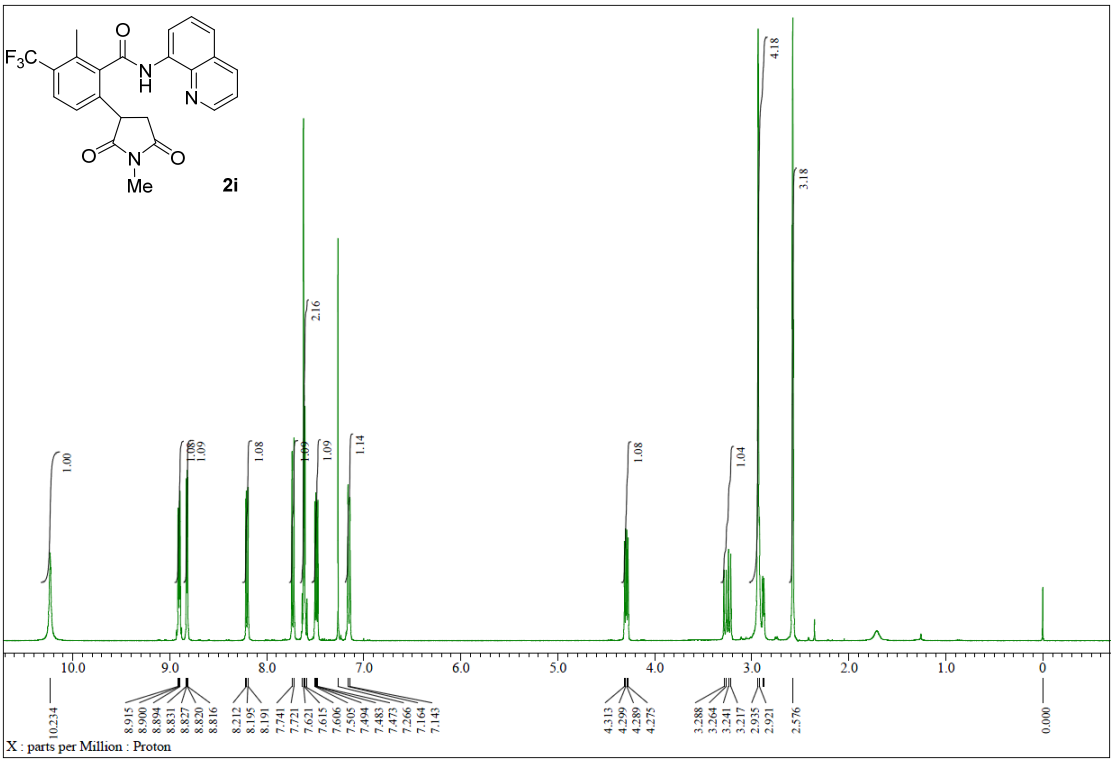

2f
X : parts per Million : Carbon13


MeO
O
N
H
N
O
N
O
Me
2g
4.11
3.12
3.08
2.11
1.00
1.07
1.07
1.05
1.01
1.03
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
X : parts per Million : Proton


MeO
O
N
H
N
O
N
O
Me
2g
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
X : parts per Million : Carbon13


AcO
O
N
H
N
O
N
O
Me
2h
4.09
3.12
3.02
2.10
1.00
1.06
1.04
1.05
1.02
10.195
8.896
8.886
8.874
8.812
8.808
8.802
8.797
8.187
8.183
8.166
8.163
7.593
7.589
7.584
7.580
7.576
7.477
7.466
7.270
7.160
7.140
7.076
7.054
4.275
4.261
4.251
4.237
3.245
3.221
3.199
3.175
2.924
2.919
2.884
2.347
2.284
0.000
X : parts per Million : Proton


AcO
O
N
H
N
O
N
O
Me
2h
77.546
77.040
169.080
166.688
149.106
148.776
139.722
138.557
136.350
133.947
132.493
128.235
128.059
127.234
126.203
123.914
122.707
121.986
116.974
77.480
77.366
77.160
76.840
44.100
38.109
25.219
20.909
13.701
X : parts per Million : Carbon13


F3C
O
N
H
N
O
N
O
Me
2i
4.18
3.18
2.16
1.00
1.08
1.09
1.08
1.09
1.09
1.14
1.08
1.04
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
10.234
8.915
8.900
8.894
8.831
8.827
8.820
8.816
8.212
8.195
8.191
7.741
7.721
7.621
7.615
7.606
7.505
7.494
7.483
7.473
7.266
7.164
7.143
4.313
4.299
4.289
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3.264
3.241
3.217
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2.921
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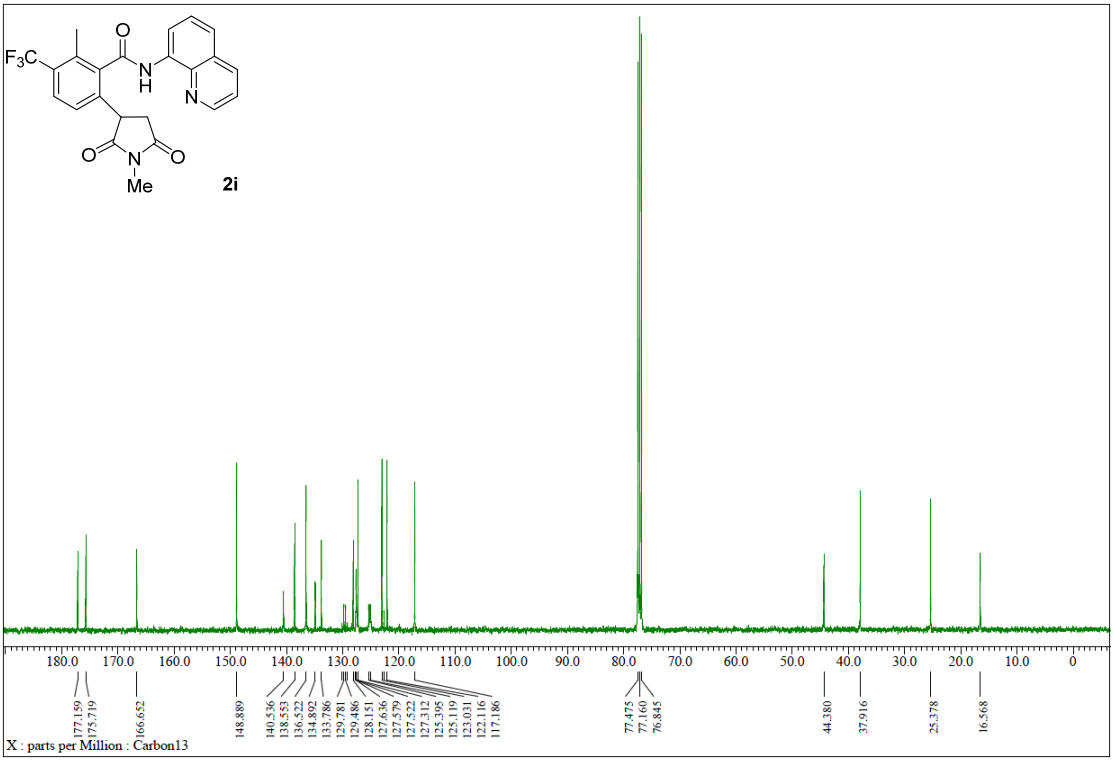
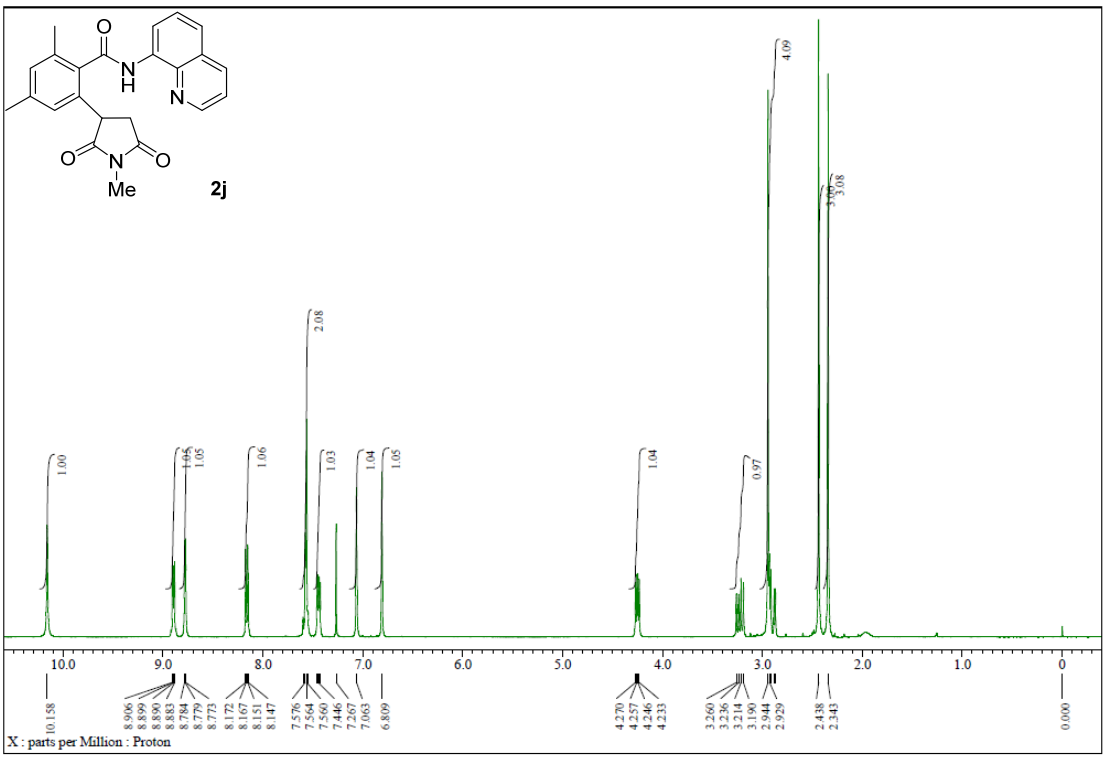
0.000
X : parts per Million : Proton


F3C
O
N
H
N
O
N
O
Me
2i
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
177.159
175.719
166.652
148.889
140.536
138.553
136.522
134.892
133.786
129.781
129.486
128.151
127.636
127.579
127.522
127.312
125.395
125.119
123.031
122.116
117.186
77.475
77.160
76.845
44.380
37.916
25.378
16.568
X : parts per Million : Carbon13


2j
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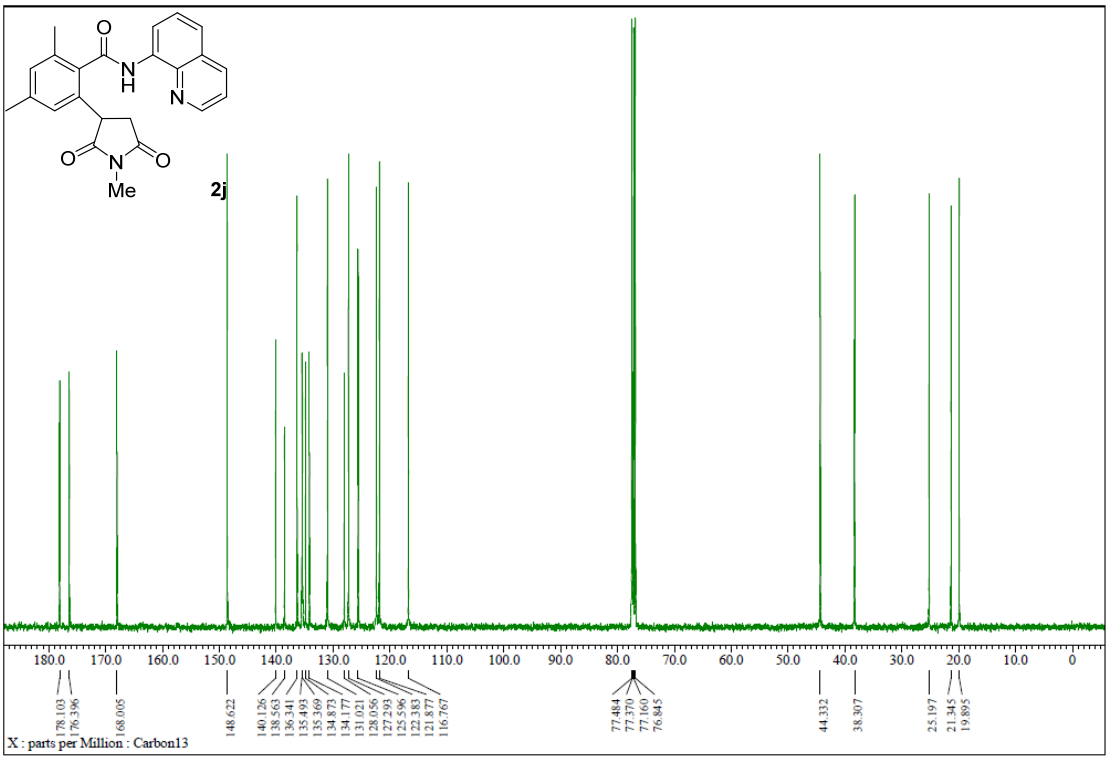
2j
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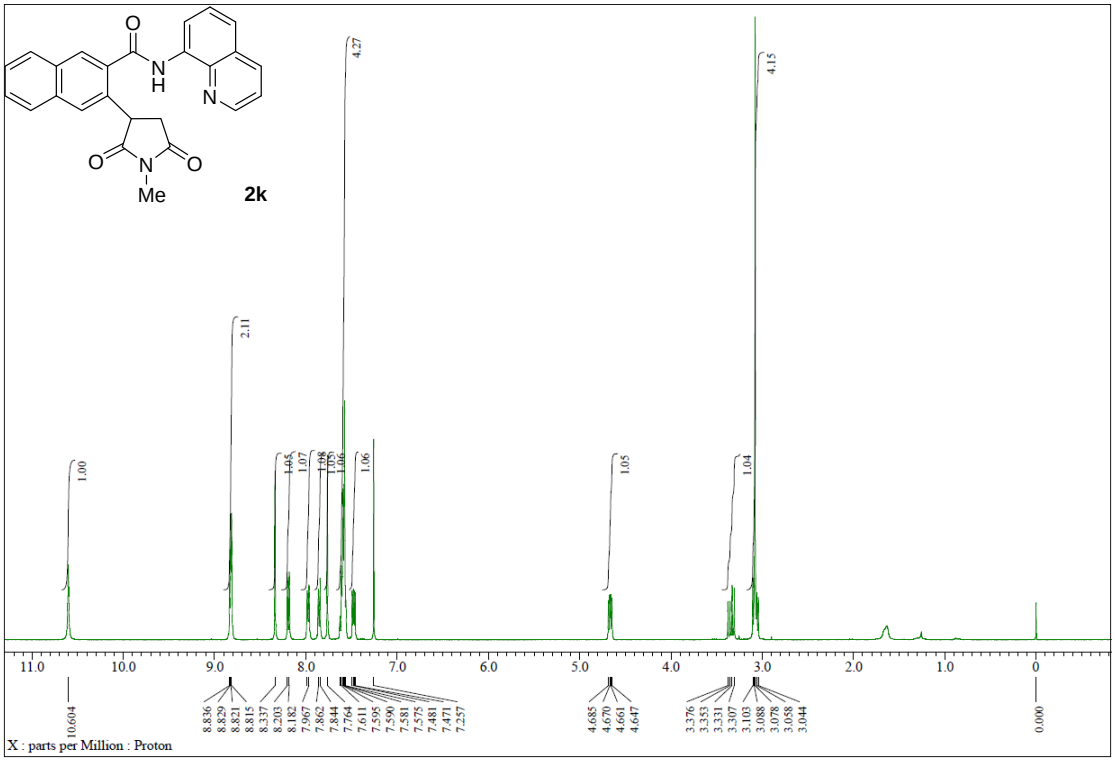
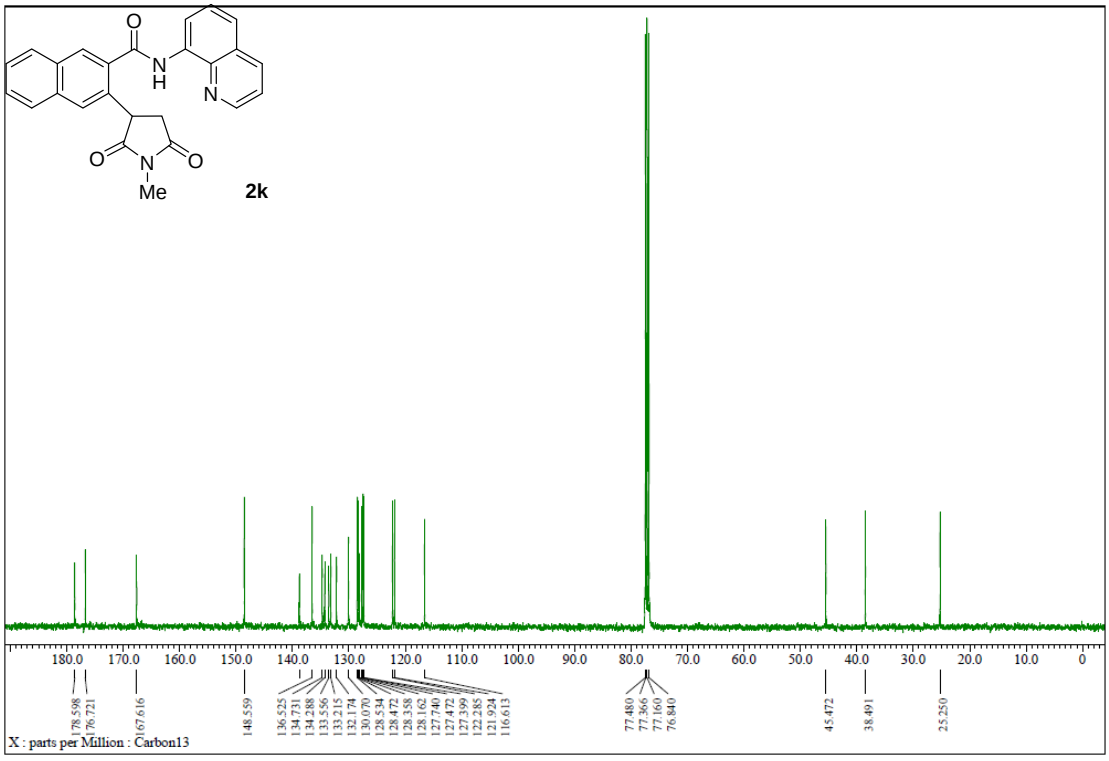
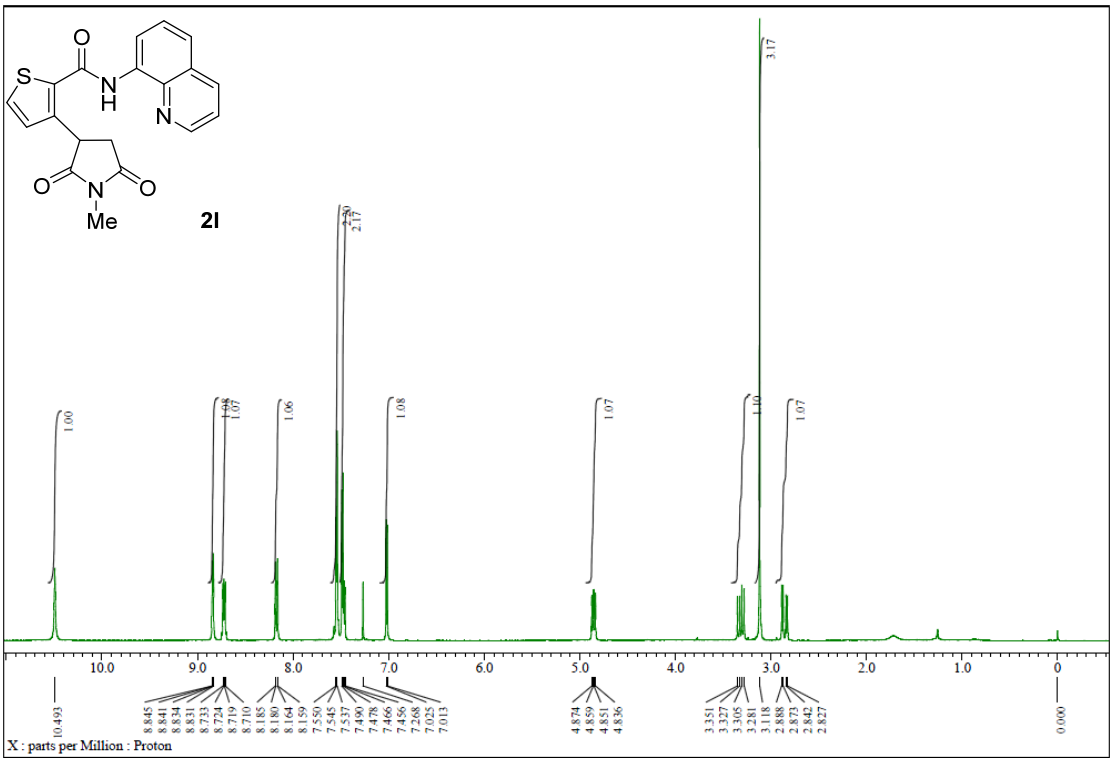
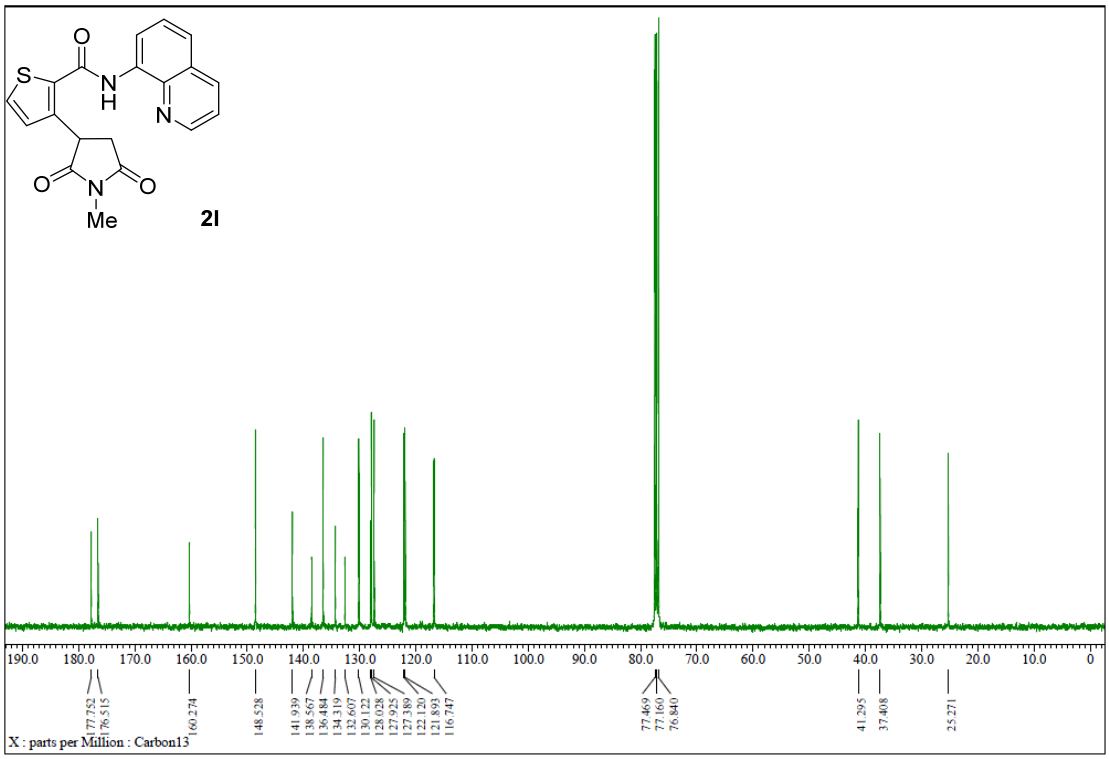
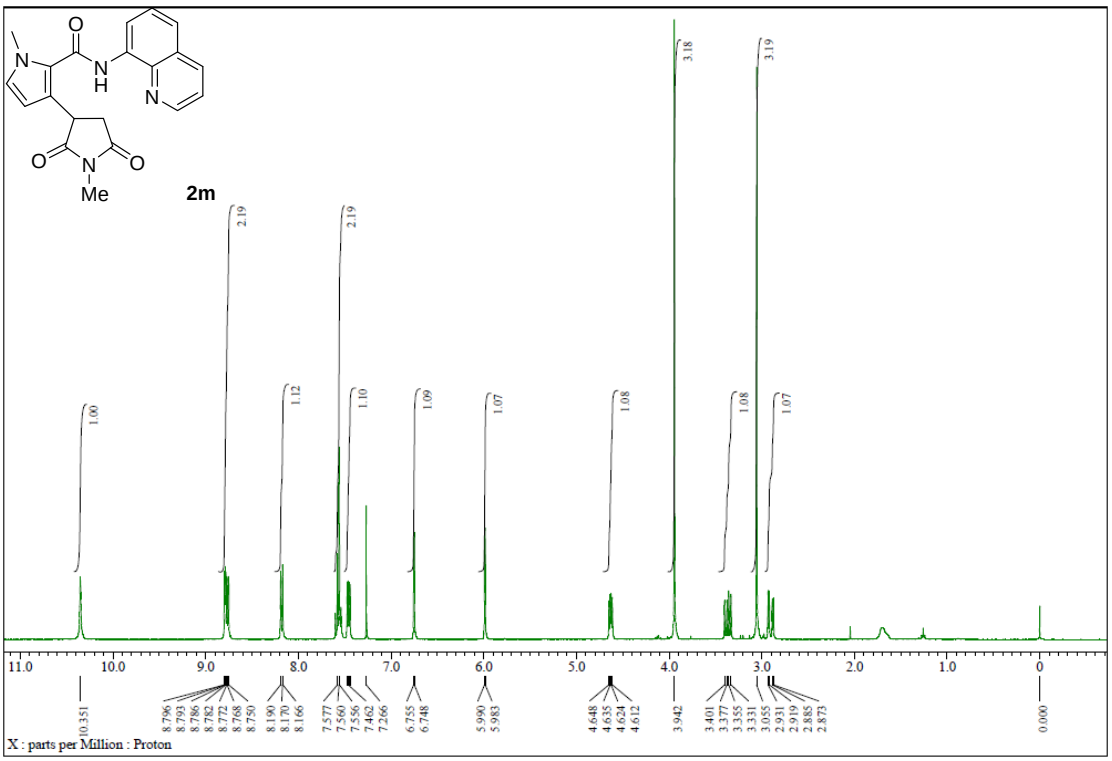

2k
X : parts per Million : Proton


2k
X : parts per Million : Carbon13


2l
X : parts per Million : Proton


2l
X : parts per Million : Carbon13


2m
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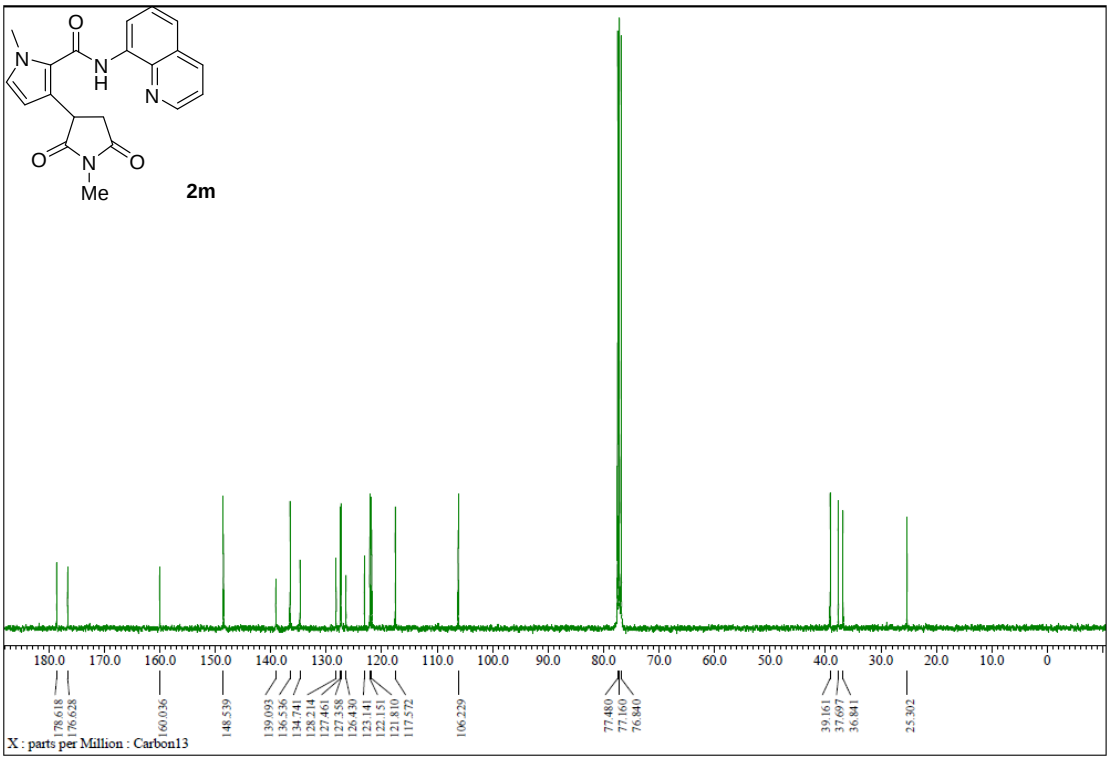
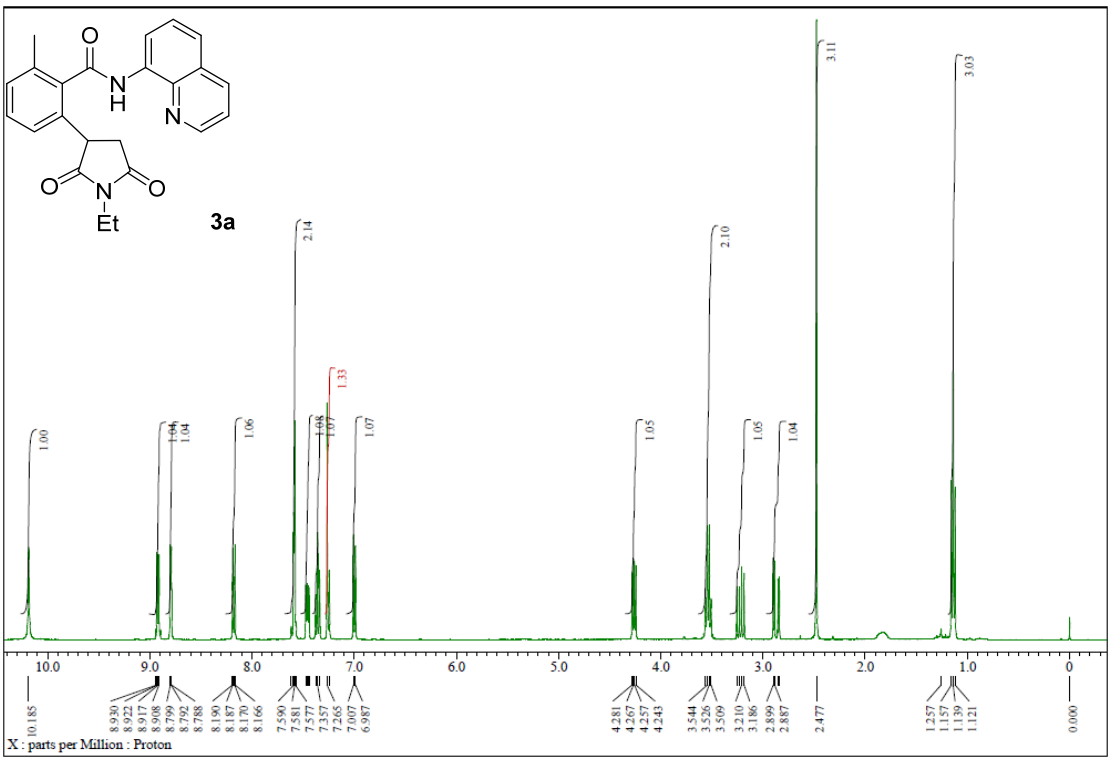
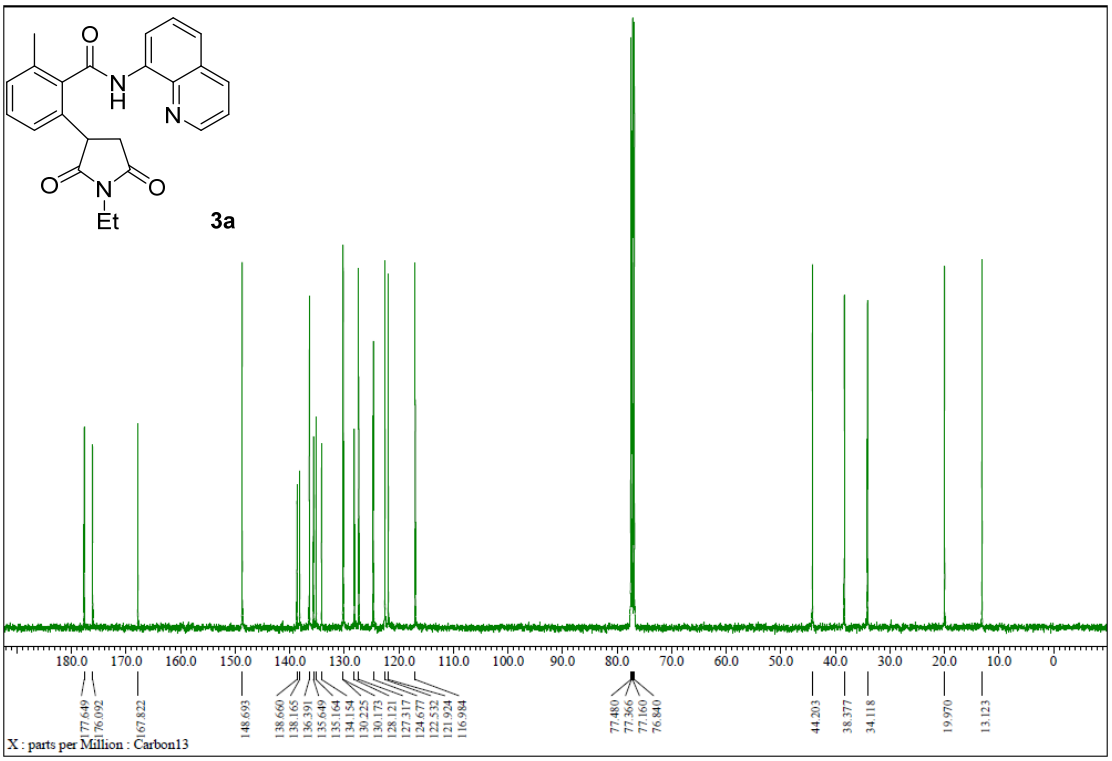
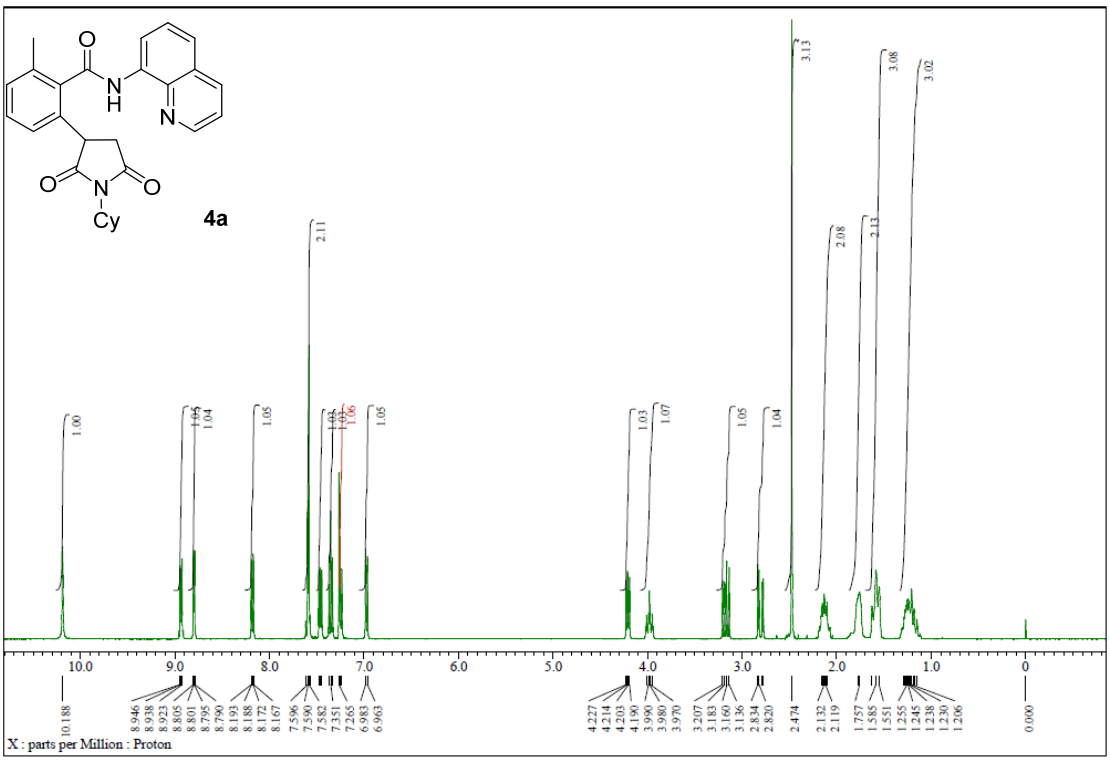
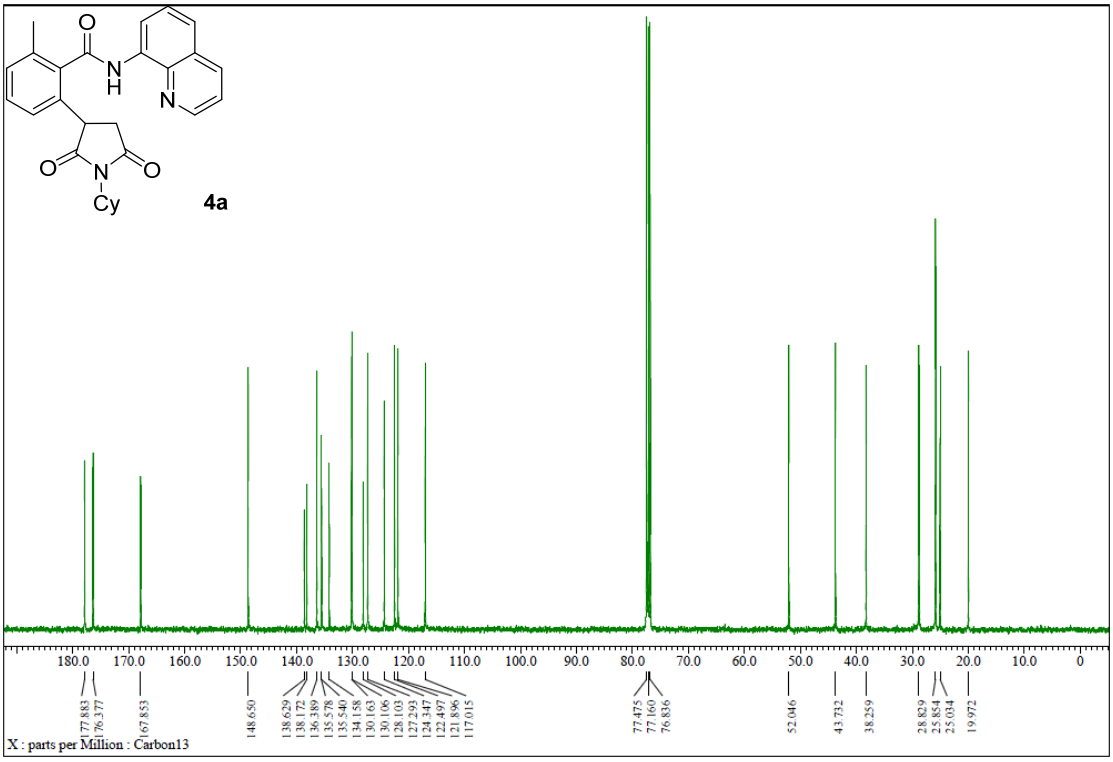
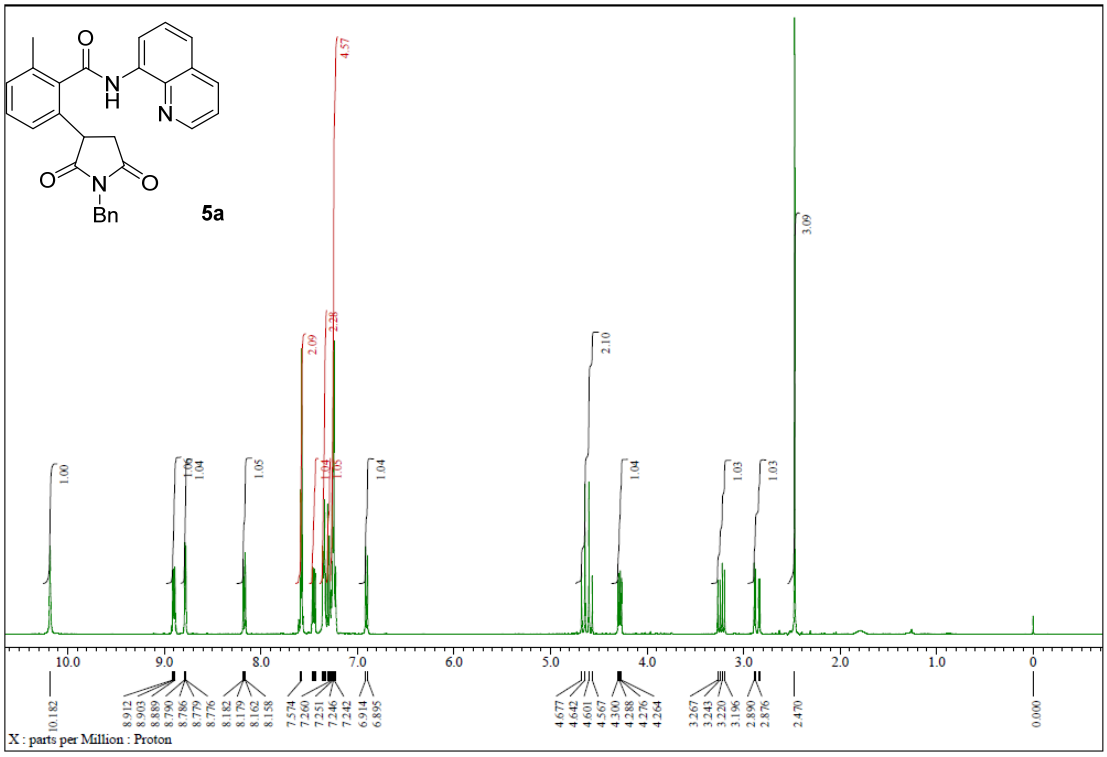

2m
X : parts per Million : Carbon13

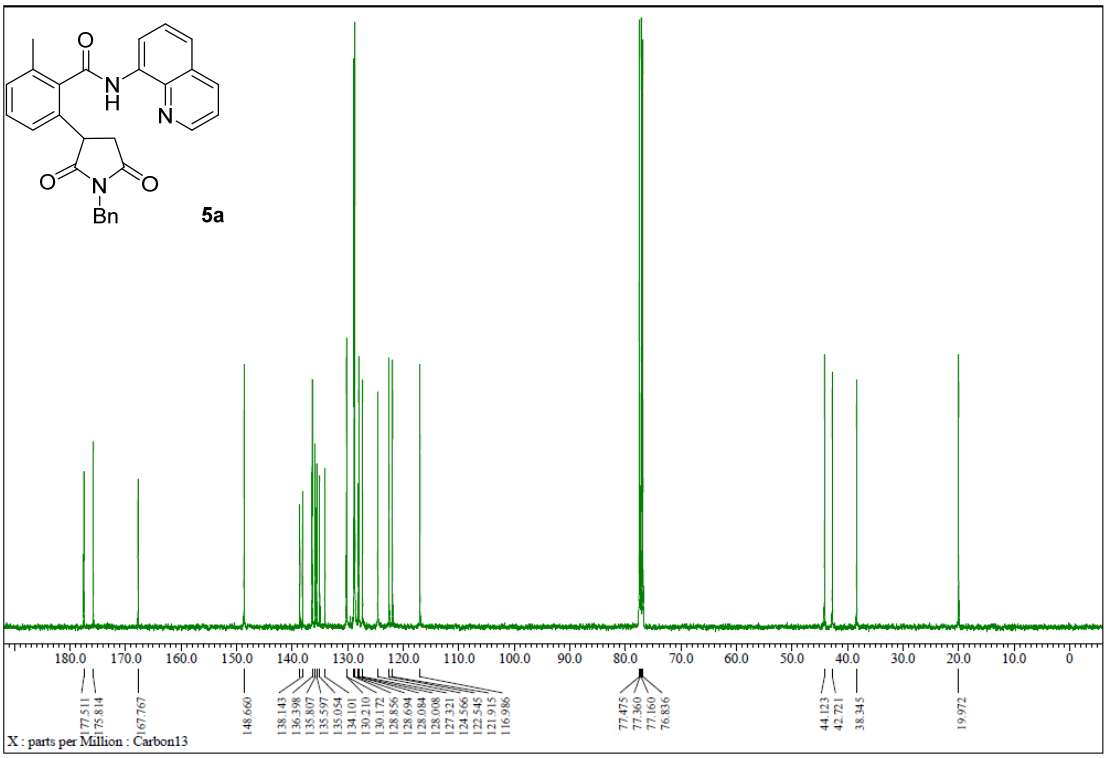

3a
X : parts per Million : Proton

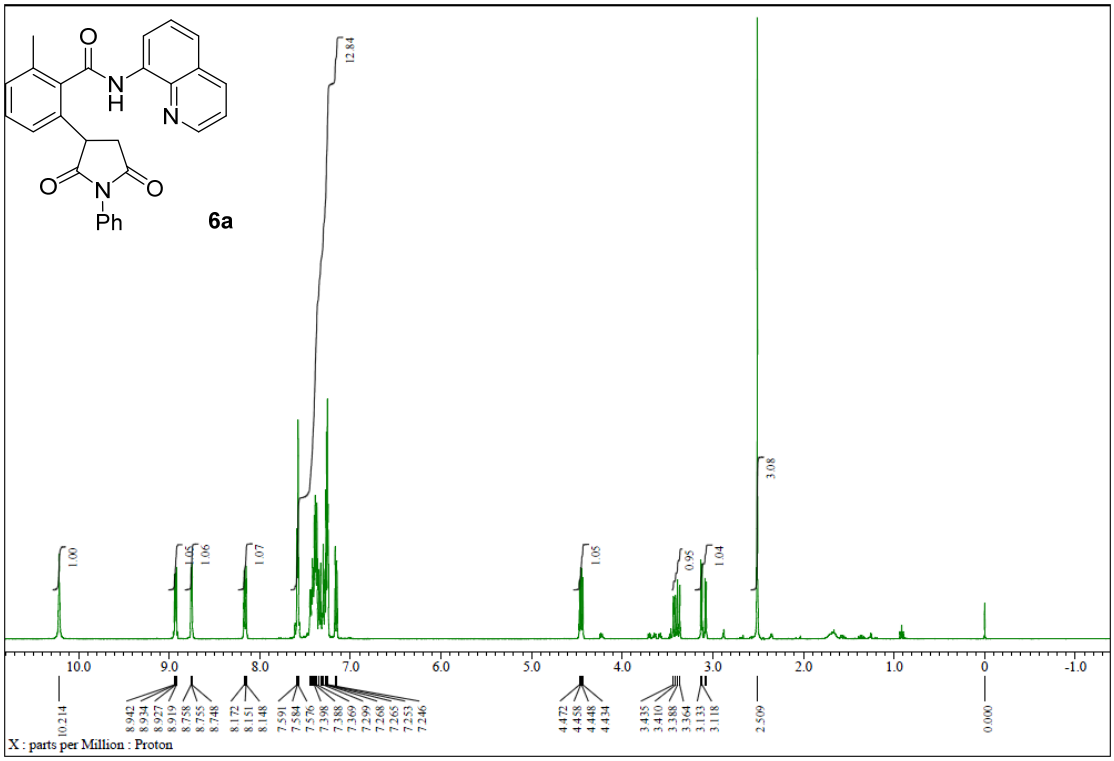

3a
X : parts per Million : Carbon13

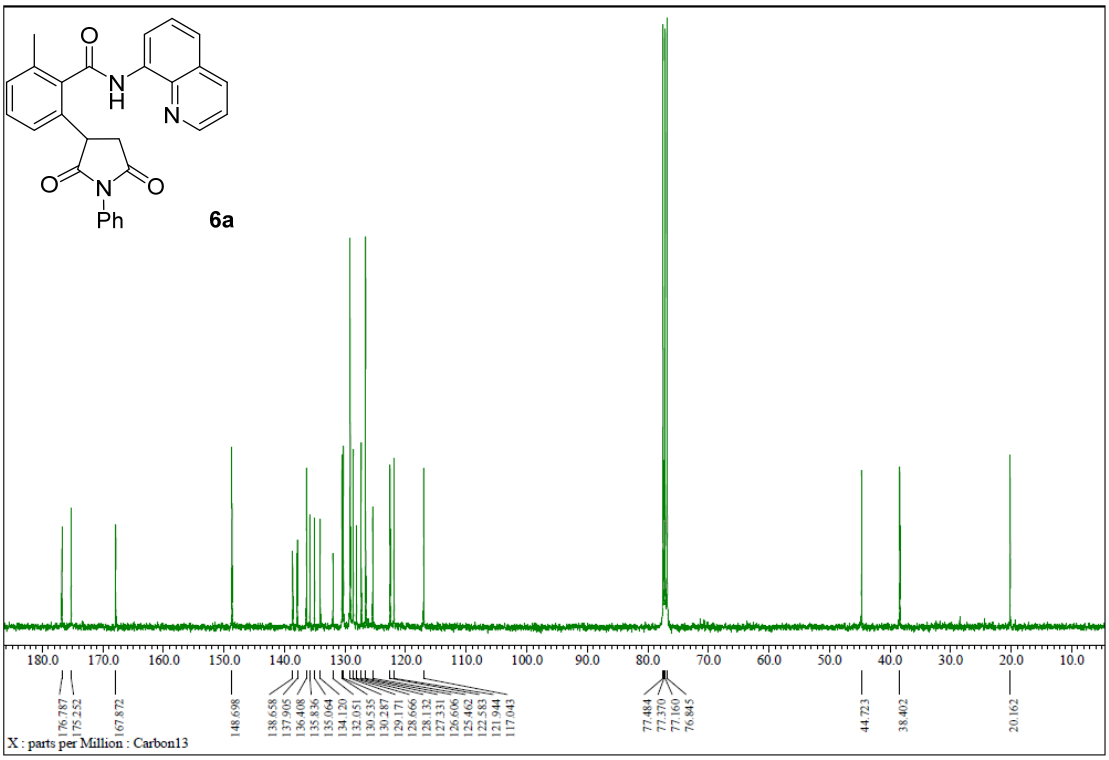

4a
X : parts per Million : Proton

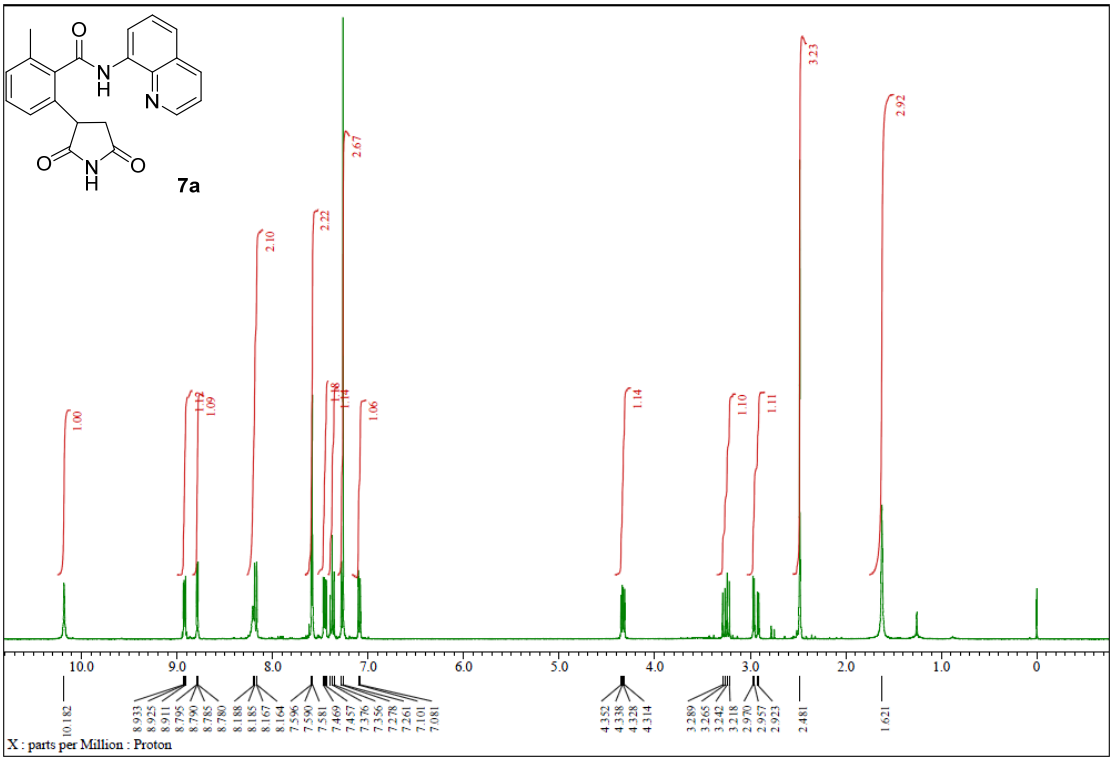

4a
X : parts per Million : Carbon13

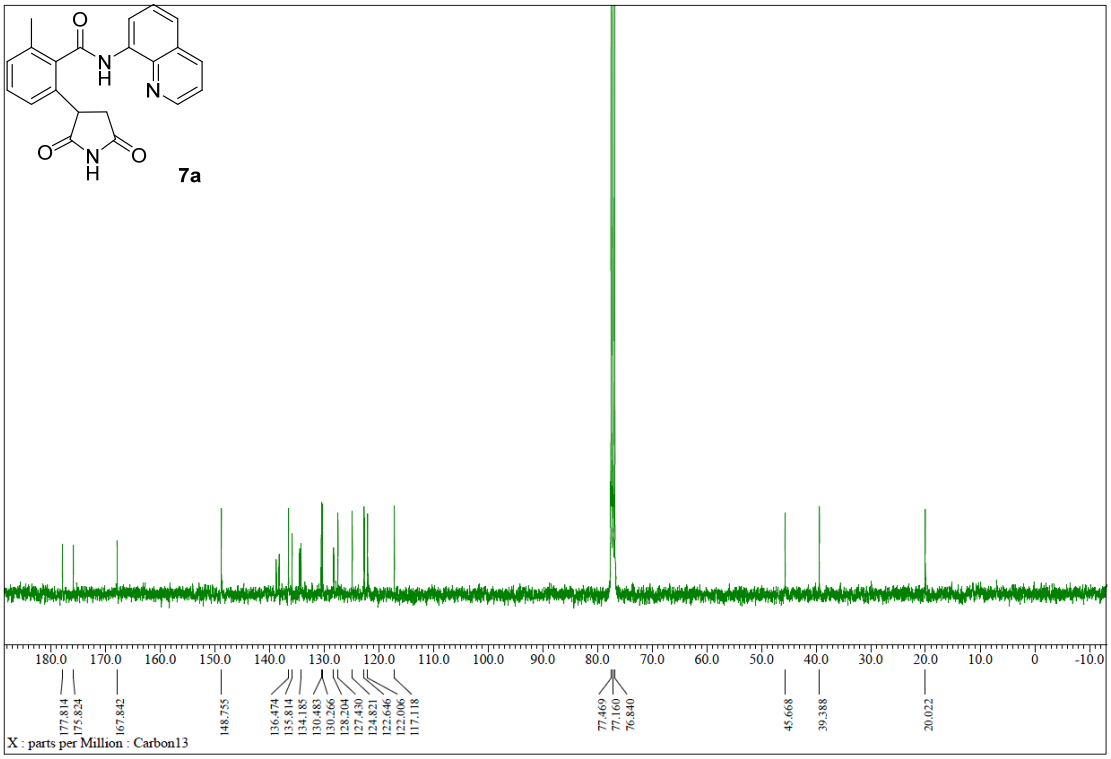

5a
X : parts per Million : Proton


5a
X : parts per Million : Carbon13


6a
X : parts per Million : Proton


6a
X : parts per Million : Carbon13


7a
X : parts per Million : Proton


7a
X : parts per Million : Carbon13