Supporting Information

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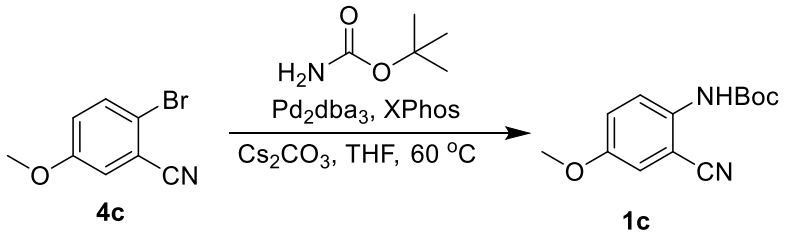
General Information:

The reagents and solvents were obtained from commercial suppliers and used without further purification. ^{1}H and ^{13}C NMR spectra were recorded on an instrument at 400 MHz for ^{1}H and 101 MHz for ^{13}C using dimethyl sulfoxide (DMSO-d6) as a solvent. Chemical shifts are in parts per million (ppm) and were referenced to the residual proton peaks in deuterated solvents. Mass spectra were recorded with an LCMS (Agilent). LCMS analysis was performed using a Kinetex XB- C18 column (75x3mm) 2.6 μm. High-resolution mass spectrometry (HRMS) data were measured on Thermo Orbitrap Exploris spectrometer. Standard column chromatography was performed using 100-200 mesh silica gel. Reverse-phase HPLC purification was performed using a Kinetex XB - C18 column (250 mm × 30 mm, 10 μm) eluting with a gradient of MeCN/water containing 10 mM Ammonium formate.

Experimental Section

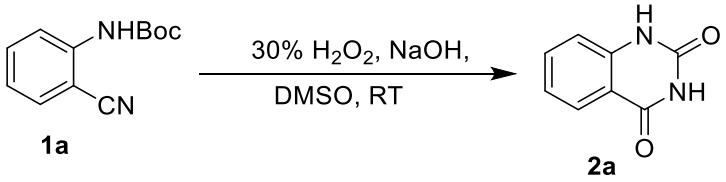
General procedure: Synthesis of 1b-1p:



4c **1c**

A mixture of 2-bromo-5-methoxybenzonitrile **4c** (1 mmol, 1 eq), *tert*-butyl carbamate (2 mmol, 2 eq), and Cs_2CO_3 (2 mmol, 2 eq) in THF (6 mL) was purged with N_2 gas for 5 min and then added Pd_2dba_3 (0.05 eq) and XPhos (0.1 eq) under N_2 atmosphere at room temperature. The reaction mixture was stirred at 60 ^oC for 4 h. After completion of starting material, the reaction mixture was filtered through a pad of Celite, and filtrate was concentrated under reduced pressure afforded crude residue. The residue was purified by silica gel column chromatography (30% EtOAc/hexanes) to afford *tert*-butyl (2-cyano-4-methoxyphenyl)carbamate **1c** (670 mg, 58% yield) as an off-white solid.

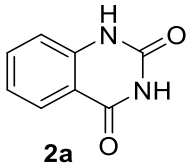
General procedure for synthesis of quinazoline-2,4(1*H*,3*H*)-dione:



1a **2a**

To a stirred solution of *tert*-butyl (2-cyanophenyl)carbamate **1a** (1 mmol, 1 eq) in DMSO (2 mL) were added NaOH (6 eq) followed by 35% H_2O_2 (1 eq) at 0 ^oC under N_2 atmosphere. The reaction mixture was stirred at room temperature for 16 h. The reaction was monitored by TLC and UPLC. After completion of starting material, the reaction mixture was quenched with 10% sodium metabisulfite solution and stirred for 5 min and extracted with EtOAc (3x50 mL). The combined organic layers were dried over Na_2SO_4, filtered, and concentrated in *vacuo* afforded crude residue. The crude residue was purified by Reverse-phase column chromatography to afford quinazoline-2,4(1*H*,3*H*)-dione **2a** as a white solid.

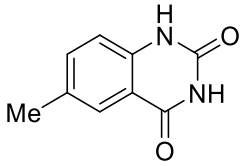
Quinazoline-2,4(1*H*,3*H*)-dione (**2a**):



2a

Quinazoline-2,4(1*H*,3*H*)-dione **2a** (160 mg, 0.987 mmol) was synthesised from *tert*-butyl (2-cyanophenyl)carbamate **1a** (218 mg, 1 mmol) by following the general procedure. Yield: 98%; White solid. Melting point: melting not observed, decomposed at ~380 ^{o}C. ^{1}H NMR (400 MHz, DMSO-d_6): δ 11.18 (brs, 2H), 7.88 (dd, *J* = 8.51, 1.50 Hz, 1H), 7.63 (td, *J* = 7.76, 1.50 Hz, 1H), 7.19 - 7.15 (m, 2 H). ^{13}C NMR (101 MHz, DMSO-d_6): δ = 162.79, 150.27, 140.87, 134.90, 126.91, 122.26, 115.29, 114.30. HRMS (ESI-TOF) *m/z*: calcd for $C_8H_7N_2O_2$ $(M+H)^+$ 163.0508, found 163.0494.

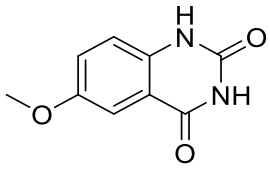
6-Methylquinazoline-2,4(1*H*,3*H*)-dione (2b):



2b

6-Methylquinazoline-2,4(1*H*,3*H*)-dione **2b** (170 mg, 0.965 mmol) was synthesised from *tert*-butyl (2-cyano-4-methylphenyl)carbamate **1b** (232 mg, 1 mmol) by following the general procedure. Yield: 96%; White solid. Melting point = 313 – 316 °C. ^{1}H NMR (400 MHz, DMSO-d6): δ 11.10 (br*s*, 1H), 7.68 (m, 1H), 7.45 (dd, *J* = 2.0, 8.4 Hz, 1H), 7.06 (d, *J* = 8.3 Hz, 1H), 2.32 (s, 2H). ^{13}C NMR (101 MHz, DMSO-d_6): δ 162.80, 150.25, 138.69, 135.93, 131.50, 126.44, 115.25, 114.13, 20.19. HRMS (ESI-TOF) *m/z*: calcd for $C_9H_9N_2O_2$ $(M+H)^+$ 177.0664, found 177.0653.

6-Methoxyquinazoline-2,4(1*H*,3*H*)-dione (2c):

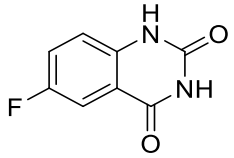


2c

6-Methoxyquinazoline-2,4(1*H*,3*H*)-dione **2c** (190 mg, 0.984 mmol) was synthesised from *tert*-butyl (2-cyano-4-methoxyphenyl) carbamate **1c** (248 mg, 1 mmol) by following the general procedure. Yield: 98%; Off-white solid. Melting point = 313 – 315 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ 10.94 (br*s*, 2H), 7.33 (d, *J* = 3.0 Hz, 1H), 7.30 - 7.25 (m, 1H), 7.12 (d, *J* = 8.5 Hz, 1H), 3.78 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6): δ 162.79, 154.45, 150.22, 135.28,

123.68, 117.01, 114.82, 107.96, 55.49. HRMS (ESI-TOF) *m/z*: calcd for $C_9H_9N_2O3$ $(M+H)^+$ 193.0613, found 193.0603.

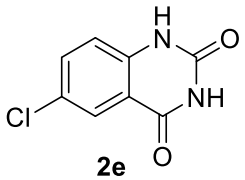
6-Fluoroquinazoline-2,4(1*H*,3*H*)-dione (2d):



2d

6-Fluoroquinazoline-2,4(1*H*,3*H*)-dione **2d** (173 mg, 0.961 mmol) was synthesised from *tert*-butyl (2-cyano-4-fluorophenyl)carbamate **1d** (236 mg, 1 mmol) by following the general procedure. Yield: 96%; White solid. Melting point = 295 – 297 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ 11.52 - 11.05 (m, 2H), 7.65 - 7.43 (m, 2H), 7.20 (dd, *J* = 4.4, 9.0 Hz, 1H). ^{13}C NMR (101 MHz, DMSO-d_6): δ 161.95, 150.09, 143.76, 131.25 (m, 1C), 124.20 (q, $J_{C,F}$ = 5.05 Hz, 1C), 123.90 (q, $J_{C,F}$ = 272.7 Hz, 1C), 122.60 (q, $J_{C,F}$ = 32.32 Hz, 1C), 116.61, 114.48. ^{19}F NMR (376 MHz, DMSO-d_6): δ –120.3. HRMS (ESI-TOF) *m/z*: calcd for $C_8H_4FN_2O_2$ $(M-H)^+$ 179.0257, found 179.0260.

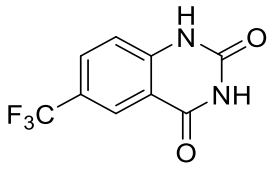
6-Chloroquinazoline-2,4(1*H*,3*H*)-dione (2e):



2e

6-Chloroquinazoline-2,4(1*H*,3*H*)-dione **2e** (183 mg, 0.933 mmol) was synthesised from *tert*-butyl (4-chloro-2-cyanophenyl)carbamate **1e** (252 mg, 1 mmol) by following the general procedure. Yield: 93%; White solid. Melting point = 285 – 287 °C. ^{1}H NMR (400 MHz, DMSO-d6): δ 10.88 (brs, 2H), 7.81 (d, *J* = 2.0 Hz, 1H), 7.68 (dd, *J* = 2.8, 8.8 Hz, 1H), 7.19 (d, *J* = 9.0 Hz, 1H). ^{13}C NMR (101 MHz, DMSO-d_6): δ 161.79, 150.01, 139.74, 134.77, 126.23, 125.88, 117.52, 115.76. HRMS (ESI-TOF) *m/z*: calcd for $C_8H_4ClN_2O_2$ $(M-H)^+$ 194.9961, found 194.9965.

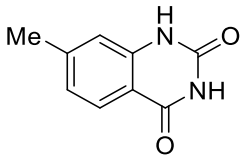
6-(Trifluoromethyl)quinazoline-2,4(1*H*,3*H*)-dione (2f):



2f

6-(Trifluoromethyl)quinazoline-2,4(1*H*,3*H*)-dione **2f** (147 mg, 0.639 mmol) was synthesised from *tert*-butyl (2-cyano-4-(trifluoromethyl)phenyl)carbamate **1f** (286 mg, 1 mmol) by following the general procedure. Yield: 64%; White solid. Melting point = 293 – 295 °C. ^{1}H NMR (400 MHz, DMSO-d$_6$): δ 11.53 (brs, 2H), 8.10 (d, *J* = 1.5 Hz, 1H), 7.97 (dd, *J* = 2.0, 8.5 Hz, 1H), 7.34 (d, *J* = 8.5 Hz, 1H). ^{13}C NMR (101 MHz, DMSO-d$_6$): δ 161.94, 150.09, 143.76, 131.27 (d, $J_{C,F}$ = 3.03 Hz, 1C), 124.17 (q, $J_{C,F}$ = 4.04 Hz, 1C), 123.89 (q, $J_{C,F}$ = 272 Hz, 1C), 122.57 (q, $J_{C,F}$ = 33.33 Hz, 1C), 116.60, 114.48. ^{19}F NMR (376 MHz, DMSO-d$_6$): δ –60.6. HRMS (ESI-TOF) *m/z*: calcd for $C_9H_4F_3N_2O_2$ $(M-H)^+$ 229.0225, found 229.0228.

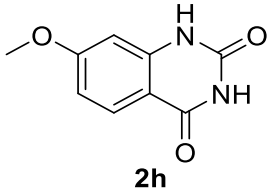
7-Methylquinazoline-2,4(1*H*,3*H*)-dione (2g):



2g

7-Methylquinazoline-2,4(1*H*,3*H*)-dione **2g** (120 mg, 0.681 mmol) was synthesised from *tert*-butyl (2-cyano-5-methylphenyl)carbamate **1g** (232 mg, 1 mmol) by following the general procedure. Yield: 68%; White solid. Melting point = 285 – 288 °C. ^{1}H NMR (400 MHz, DMSO-d6): δ 11.20 (brs, 2H), 8.51 (s, 1H), 7.77 (d, *J* = 7.9 Hz, 1H), 7.02 - 6.97 (m, 2H), 2.36 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d6): δ 162.71, 150.49, 145.50, 141.03, 126.86, 123.56, 115.09, 112.03, 21.41. HRMS (ESI-TOF) *m/z*: calcd for $C_9H_9N_2O_2$ $(M+H)^+$ 177.0664, found 177.0648.

7-Methoxyquinazoline-2,4(1*H*,3*H*)-dione (2h):

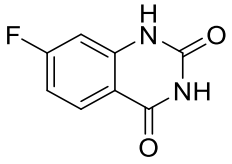


2h

7-Methoxyquinazoline-2,4(1*H*,3*H*)-dione **2h** (143 mg, 0.739 mmol) was synthesised from *tert*-butyl (2-cyano-5-methoxyphenyl)carbamate **1h** (248 mg, 1 mmol) by following the general procedure. Yield: 74%; White solid. Melting point: melting not observed, decomposed

between 314 – 327 °C. ^{1}H NMR (400 MHz, DMSO-d6): δ 11.03 (brs, 2H), 7.79 (d, *J* = 8.9 Hz, 1H), 6.76 (dd, *J* = 2.4, 8.8 Hz, 1H), 6.62 (d, *J* = 2.4 Hz, 1H), 3.82 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d6): δ 164.34, 162.32, 150.53, 142.80, 128.81, 110.48, 107.66, 98.32, 55.59. HRMS (ESI-TOF) *m/z*: calcd for $C_9H_7N_2O_3$ $(M-H)^+$ 191.0457, found 191.0460.

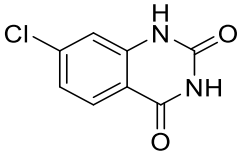
7-Fluoroquinazoline-2,4(1*H*,3*H*)-dione (2i):



2i

7-Fluoroquinazoline-2,4(1*H*,3*H*)-dione **2i** (130 mg, 0.722 mmol) was synthesised from *tert*-butyl (2-cyano-5-fluorophenyl)carbamate **1i** (236 mg, 1 mmol) by following the general procedure. Yield: 72%; Off-white solid. Melting point: melting not observed, decomposed at between 354 – 364 ºC. ^{1}H NMR (400 MHz, DMSO-d6): δ 11.25 (brs, 2H), 7.94 (dd, *J* = 6.2, 8.8 Hz, 1H), 7.02 (dt, *J* = 2.4, 8.7 Hz, 1H), 6.89 (dd, *J* = 2.4, 9.9 Hz, 1H). ^{13}C NMR (101 MHz, DMSO-d6): δ 165.78 (d, $J_{C,F}$ = 252 Hz, 1C), 161.94, 150.28, 142.90 (d, $J_{C,F}$ = 13.13 Hz, 1C), 130.17 (d, $J_{C,F}$ = 11.11 Hz, 1C), 111.33, 110.27 (d, $J_{C,F}$ = 23.23 Hz, 1C), 101.49 (d, $J_{C,F}$ = 26.26 Hz, 1C). ^{19}F NMR (376 MHz, DMSO-d_6): δ –103.5. HRMS (ESI-TOF) *m/z*: calcd for $C_8H_6FN_2O_2$ $(M+H)^+$ 181.0413, found 181.0397.

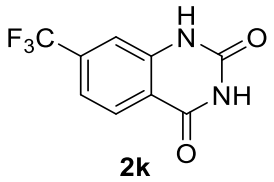
7-Chloroquinazoline-2,4(1*H*,3*H*)-dione (2j):



2j

7-Chloroquinazoline-2,4(1*H*,3*H*)-dione **2j** (159 mg, 0.811 mmol) was synthesised from *tert*-butyl (5-chloro-2-cyanophenyl)carbamate **1j** (252 mg, 1 mmol) by following the general procedure. Yield: 81%; Brown solid. Melting point = 298 – 300 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ 11.46 - 11.02 (m, 2H), 7.64 - 7.51 (m, 2H), 7.20 (dd, *J* = 4.5, 9.0 Hz, 1H). ^{13}C NMR (101 MHz, DMSO-d_6): δ 165.99, 162.17, 150.31, 142.26, 139.24, 128.94, 122.35, 114.89, 113.31. HRMS (ESI-TOF) *m/z*: calcd for $C_8H_4ClN_2O_2$ $(M-H)^+$ 194.9961, found 194.9965.

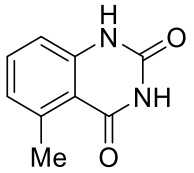
7-(Trifluoromethyl)quinazoline-2,4(1*H*,3*H*)-dione (2k):



2k

7-(Trifluoromethyl)quinazoline-2,4(1*H*,3*H*)-dione **2k** (156 mg, 0.677 mmol) was synthesised from *tert*-butyl (2-cyano-5-(trifluoromethyl)phenyl)carbamate **1k** (286 mg, 1 mmol) by following the general procedure. Yield: 67%; Off-white solid. Melting point: melting not observed, decomposed between 221 - 230 ºC. ^{1}H NMR (400 MHz, DMSO-d6): δ 11.56 (brs, 2H), 8.07 (d, *J* = 8.3 Hz, 1H), 7.51 - 7.43 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d6): δ 162.06, 150.26, 141.60, 134.08 (d, $J_{C,F}$ = 31.31 Hz, 1C), 128.58, 124.74 (m, 1C), 118.03 (d, $J_{C,F}$ = 3.03 Hz, 1C), 117.43, 112.44 (m, 1C). ^{19}F NMR (376 MHz, DMSO-d_6): δ –62.1. HRMS (ESI-TOF) *m/z*: calcd for $C9H_4F_3N_2O_2$ $(M-H)^+$ 229.0225, found 229.0223.

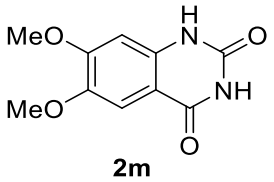
5-Methylquinazoline-2,4(1*H*,3*H*)-dione (2l):



2l

5-Methylquinazoline-2,4(1*H*,3*H*)-dione **2l** (154 mg, 0.875 mmol) was synthesised from *tert*-butyl (2-cyano-3-methylphenyl)carbamate **1l** (278 mg, 1 mmol) by following the general procedure. Yield: 87%; Brown solid. Melting point = 271 – 273 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ 10.92 (brs, 2H), 7.44 (t, *J* = 7.8 Hz, 1H), 7.02 (d, *J* = 8.0 Hz, 1H), 6.93 (d, *J* = 7.4 Hz, 1H), 2.64 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d6): δ 163.63, 150.04, 142.20, 140.92, 133.73, 125.12, 113.47, 112.46, 22.05. HRMS (ESI-TOF) *m/z*: calcd for $C_9H_9N_2O_2$ $(M+H)^+$ 177.0664, found 177.0651.

6,7-Dimethoxyquinazoline-2,4(1*H*,3*H*)-dione (2m):

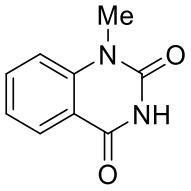


2m

6,7-Dimethoxyquinazoline-2,4(1*H*,3*H*)-dione **2m** (201 mg, 0.905 mmol) was synthesised from *tert*-butyl (2-cyano-4,5-dimethoxyphenyl)carbamate **1m** (278 mg, 1 mmol)

by following the general procedure. Yield: 90%; Brown solid. Melting point = 319 – 321 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ 8.42 (s, 2H), 7.25 (s, 1H), 6.73 (s, 1H), 3.82 (s, 3H), 3.78 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d6): δ 162.41, 154.88, 150.38, 144.99, 136.61, 107.14, 106.18, 97.85, 55.80, 55.69. HRMS (ESI-TOF) *m/z*: calcd for $C_{10}H_{11}N_2O_4$ $(M+H)^+$ 223.0719, found 223.0699.

1-Methylquinazoline-2,4(1*H*,3*H*)-dione (2n):



2n

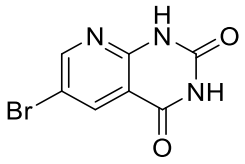
1-Methylquinazoline-2,4(1*H*,3*H*)-dione **2n** (136 mg, 0.772 mmol) was synthesised from *tert*-butyl (2-cyanophenyl)(methyl)carbamate **1n** (232 mg, 1 mmol) by following the general procedure. Yield: 77%; White solid. Melting point: melting not observed, decomposed above ~253 °C. ^{1}H NMR (400 MHz, DMSO-d6): δ 11.51 (brs, 1H), 7.98 (dd, *J* = 1.5, 7.5 Hz, 1H), 7.74 (ddd, *J* = 1.8, 7.1, 8.6 Hz, 1H), 7.40 (d, *J* = 8.5 Hz, 1H), 7.26 (t, *J* = 7.5 Hz, 1H), 3.43 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d6): δ 161.78, 150.22, 141.66, 135.21, 127.28, 122.43, 115.54, 114.68, 29.44. HRMS (ESI-TOF) *m/z*: calcd for $C_9H_9N_2O_2$ $(M+H)^+$ 177.0664, found 177.0649.

Pyrido[2,3-d]pyrimidine-2,4(1*H*,3*H*)-dione (2o):

2o

Pyrido[2,3-d]pyrimidine-2,4(1*H*,3*H*)-dione **2o** (117 mg, 0.717 mmol) was synthesised from *tert*-butyl (3-cyanopyridin-2-yl)carbamate **1o** (220 mg, 1 mmol) by following the general procedure. Yield: 71%; Off-white solid. Melting point = 315 – 317 °C. ^{1}H NMR (400 MHz, DMSO-d6): δ 11.65 (s, 1H), 11.45 (s, 1H), 8.59 (dd, *J* = 1.9, 4.8 Hz, 1H), 8.25 (dd, *J* = 1.6, 7.8 Hz, 1H), 7.24 (dd, *J* = 4.9, 7.8 Hz, 1H). ^{13}C NMR (101 MHz, DMSO-d6): δ 162.35, 154.52, 152.37, 150.37, 136.35, 118.83, 109.88. HRMS (ESI-TOF) *m/z*: calcd for $C_7H_4N_3O_2$ $(M-H)^+$ 162.0304, found 162.0307.

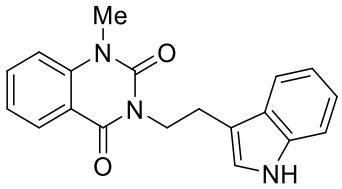
6-Bromopyrido[2,3-d]pyrimidine-2,4(1*H*,3*H*)-dione (2p):



2p

6-Bromopyrido[2,3-d]pyrimidine-2,4(1*H*,3*H*)-dione **2p** (220 mg, 0.912 mmol) was synthesised from *tert*-butyl (5-bromo-3-cyanopyridin-2-yl)carbamate **1p** (298 mg, 1 mmol) by following the general procedure. Yield: 91%; White solid. Melting point = 292 – 294 °C. ^{1}H NMR (400 MHz, DMSO-d6): δ 11.53 (brs, 2H), 8.71 (d, *J* = 2.5 Hz, 1H), 8.34 (d, *J* = 2.5 Hz, 1H). ^{13}C NMR (101 MHz, DMSO-d_6): δ 161.39, 154.85, 151.29, 150.23, 137.83, 112.54, 111.61. HRMS (ESI-TOF) *m/z*: calcd for $C_7H_3BrN_3O_2$ $(M-H)^+$ 239.9409, found 239.9413.

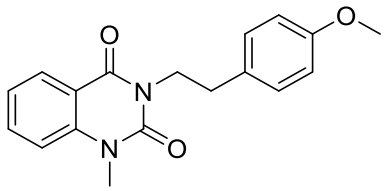
Goshuyuamide II:



Goshuyuamide II

To a stirred solution of 1-methylquinazoline-2,4(1*H*,3*H*)-dione **2n** (30 mg, 0.170 mmol) in DMF (1 mL) was added Cs_2CO_3 (111 mg, 0.341 mmol) at room temperature and stirred for 15 min. To this reaction mixture, 3-(2-bromoethyl)-1*H*-indole **6** (38.2 mg, 0.170 mmol) was added and stirred at 80 ^{o}C for 16 h. The reaction was monitored by UPLC-MS. After completion starting material, the reaction mixture was quenched with ice cold water and extracted with EtOAc (3x20 mL). The combined organic layers were dried over Na_2SO_4, filtered, and concentrated in *vacuo* afforded crude residue which was purified by Prep-HPLC (ACN/H_2O (5mM Ammonium formate)) followed by lyophilization afforded **Goshuyuamide II** (39 mg, 0.117 mmol, 69% yield) as a white solid. Melting point = 220 – 222 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ 10.84 (brs, 1H), 8.09 (dd, *J* = 1.5, 7.9 Hz, 1H), 7.79 (ddd, *J* = 1.6, 7.1, 8.5 Hz, 1H), 7.72 (d, *J* = 7.8 Hz, 1H), 7.47 (d, *J* = 8.4 Hz, 1H), 7.37 - 7.29 (m, 2H), 7.22 (d, *J* = 2.3 Hz, 1H), 7.08 (dt, *J* = 1.2, 7.5 Hz, 1H), 7.03 - 6.98 (m, 1H), 4.24 - 4.18 (m, 2H), 3.56 (s, 3H), 3.02 - 2.94 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 161.01, 150.27, 140.40, 136.28, 135.24, 127.74, 127.18, 122.81, 122.69, 121.00, 118.31, 114.85, 114.57, 111.41, 110.95, 41.80, 30.57, 23.44. HRMS (ESI-TOF) *m/z*: calcd for $C_{19}H_{18}N_3O_2$ $(M+H)^+$ 320.1399, found 320.1381.

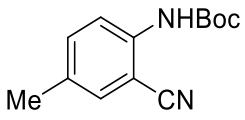
3-(4-Methoxyphenethyl)-1-methylquinazoline-2,4(1*H*,3*H*)-dione (Alkaloid):



Alkaloid

To a solution of 1-methylquinazoline-2,4(1*H*,3*H*)-dione **2n** (30 mg, 0.170 mmol) in DMF (1 mL) was added Cs_2CO_3 (111 mg, 0.341 mmol) at room temperature and stirred for 15 min. To this reaction mixture, 1-(2-bromoethyl)-4-methoxybenzene **7** (36.6 mg, 0.170 mmol) was added and stirred at 80 ^oC for 16 h. The reaction was monitored by UPLC. After completion starting material, the reaction mixture was quenched with ice cold water and extracted with EtOAc (3x20 mL). The combined organic layers were dried over Na_2SO_4, filtered, and concentrated in reduced pressure afforded crude residue which was purified by Prep-HPLC (ACN/H_2O (5mM Ammonium formate)) followed by lyophilization afforded 3-(4-methoxyphenethyl)-1-methylquinazoline-2,4(1*H*,3*H*)-dione (38 mg, 0.122 mmol, 72% yield) as a white solid. Melting point = 136 – 138 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ 8.05 (dd, *J* = 1.5, 7.9 Hz, 1H), 7.78 (ddd, *J* = 1.7, 7.1, 8.6 Hz, 1H), 7.45 (d, *J* = 8.4 Hz, 1H), 7.34 - 7.28 (m, 1H), 7.19 - 7.13 (m, 2H), 6.89 - 6.84 (m, 2H), 4.13 - 4.07 (m, 2H), 3.72 (s, 3H), 3.53 (s, 3H), 2.83 - 2.77 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d6): δ 160.88, 157.81, 150.14, 140.35, 135.26, 130.43, 129.53, 127.72, 122.70, 114.76, 114.58, 113.88, 54.96, 42.59, 32.39, 30.55. HRMS (ESI-TOF) *m/z*: calcd for $C_{18}H_{19}N_2O_3$ $(M+H)^+$ 311.1396, found 311.1376.

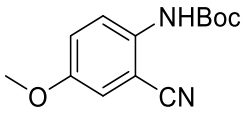
***tert*-Butyl (2-cyano-4-methylphenyl)carbamate (1b):**



1b

tert-Butyl (2-cyano-4-methylphenyl)carbamate **1b** (738 mg, 3.181 mmol, 62%) was synthesised from 2-bromo-5-methylbenzonitrile (1 g, 5.102 mmol) by following the general procedure. Yellow solid; Melting point = 102 – 104 °C. ^{1}H NMR (400 MHz, DMSO-d6): δ 9.27 (s, 1H), 7.57 (d, *J* = 2.0 Hz, 1H), 7.45 (dd, *J* = 1.5, 8.3 Hz, 1H), 7.33 (d, *J* = 8.4 Hz, 1H), 2.30 (s, 3H), 1.46 (s, 9H). ^{13}C NMR (101 MHz, DMSO-d6): δ 153.03, 138.32, 134.78, 134.28, 132.90, 125.13, 117.07, 107.55, 79.71, 27.96, 19.87. LCMS: m/z: 233 $[M+H]^+$. HRMS (ESI-TOF) *m/z*: calcd for $C_{13}H_{17}N_2O_2$ $(M+H)^+$ 233.1290, found 233.1284.

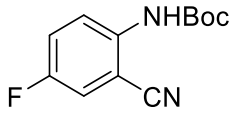
***tert*-Butyl (2-cyano-4-methoxyphenyl)carbamate (1c):**



1c

tert-Butyl (2-cyano-4-methoxyphenyl)carbamate **1c** (670 mg, 2.701 mmol, 58%) was synthesised from 2-bromo-5-methoxybenzonitrile (1 g, 4.716 mmol) by following the general procedure. Yellow solid; Melting point = 98 – 99 °C. ^{1}H NMR (400 MHz, DMSO-d6): δ 9.16 (brs, 1H), 7.36 - 7.29 (m, 2H), 7.24 - 7.19 (m, 1H), 3.78 (s, 3H), 1.45 (s, 9H). ^{13}C NMR (101 MHz, DMSO-d6): δ 156.20, 153.35, 133.83, 127.44, 120.27, 116.70, 109.29, 79.52, 55.81, 27.98. LCMS: m/z: 249 $[M+H]^+$. HRMS (ESI-TOF) *m/z*: calcd for $C_{13}H_{17}N_2O_3$ $(M+H)^+$ 249.1239, found 249.1233.

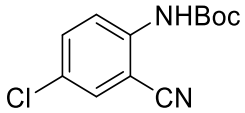
***tert*-Butyl (2-cyano-4-fluorophenyl)carbamate (1d):**



1d

tert-Butyl (2-cyano-4-methoxyphenyl)carbamate **1d** (1.05 g, 4.449 mmol, 88%) was synthesised from 2-bromo-5-fluorobenzonitrile (1 g, 5.000 mmol) by following the general procedure. Yellow solid; Melting point = 92 – 94 °C. ^{1}H NMR (400 MHz, DMSO-d6): δ 9.81 (s, 1H), 8.24 (d, *J* = 1.6 Hz, 1H), 7.99 (dd, *J* = 1.9, 8.8 Hz, 1H), 7.77 (d, *J* = 8.6 Hz, 1H), 1.49 (s, 9H). ^{13}C NMR (101 MHz, DMSO-d6): δ 152.37, 144.54, 130.56 (qd, $J_{C,F}$ = 3.6, 24.0 Hz, 1C), 130.44 (q, $J_{C,F}$ = 3.4 Hz, 1C), 124.70 (q, $J_{C,F}$ = 33.33 Hz, 1C), 127.28-119.17 (m, 1C), 124.35, 115.68, 106.52, 80.75, 27.84. ^{19}F NMR (376 MHz, DMSO-d_6): δ –102.8. LCMS: m/z: 235 $[M-H]^+$. HRMS (ESI-TOF) *m/z*: calcd for $C_{12}H_{12}FN_2O_2$ $(M-H)^+$ 235.0883, found 235.0890.

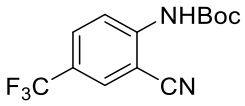
***tert*-Butyl (4-chloro-2-cyanophenyl)carbamate (1e):**



1e

tert-Butyl (4-chloro-2-cyanophenyl)carbamate **1e** (284 mg, 1.127 mmol, 49%) was synthesised from 2-bromo-5-chlorobenzonitrile (500 mg, 2.314 mmol) by following the general procedure. White solid; Melting point = 119 –121 °C. ^{1}H NMR (400 MHz, DMSO-d6): δ 9.53 (s, 1H), 7.95 (d, *J* = 2.5 Hz, 1H), 7.71 (dd, *J* = 2.6, 8.8 Hz, 1H), 7.49 (d, *J* = 8.9 Hz, 1H), 1.47 (s, 9H). ^{13}C NMR (101 MHz, DMSO-d6): δ 152.71, 139.99, 133.73, 132.34, 128.63, 126.36, 115.69, 108.64, 80.26, 27.90. LCMS: m/z: 251 $[M-H]^+$. HRMS (ESI-TOF) *m/z*: calcd for $C_{12}H_{12}ClN_2O_2$ $(M-H)^+$ 251.0587, found 251.0592.

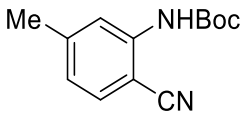
***tert*-Butyl (2-cyano-4-(trifluoromethyl)phenyl)carbamate (1f):**



1f

tert-Butyl (2-cyano-4-(trifluoromethyl)phenyl)carbamate **1f** (835 mg, 2.919 mmol, 73%) was synthesised from 2-bromo-5-(trifluoromethyl)benzonitrile (1 g, 4.000 mmol) by following the general procedure. Yellow solid; Melting point = 110 – 112 °C. ^{1}H NMR (400 MHz, DMSO-d6): δ 9.82 (s, 1H), 8.25 (d, *J* = 1.6 Hz, 1H), 8.00 (dd, *J* = 1.8, 8.8 Hz, 1H), 7.76 (d, *J* = 8.6 Hz, 1H), 1.49 (s, 9H). ^{13}C NMR (101 MHz, DMSO-d6): δ 152.38, 144.54, 130.72 (q, $J_{C,F}$ = 5.05 Hz, 1C), 130.47 (q, $J_{C,F}$ = 4.04 Hz, 1C), 124.80 (q, $J_{C,F}$ = 33.33 Hz, 1C), 124.40, 121.89, 115.69, 106.56, 80.77, 27.85. ^{19}F NMR (376 MHz, DMSO-d_6): δ –60.9. LCMS: m/z: 287 $[M+H]^+$. HRMS (ESI-TOF) *m/z*: calcd for $C_{13}H_{12}F_3N_2O_2$ $(M-H)^+$ 285.0851, found 285.0857.

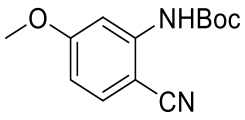
***tert*-Butyl (2-cyano-5-methylphenyl)carbamate (1g):**



1g

tert-Butyl (2-cyano-5-methylphenyl)carbamate **1g** (900 mg, 3.879 mmol, 76%) was synthesised from 2-bromo-4-methylbenzonitrile (1 g, 5.102 mmol) by following the general procedure. Off-white solid; Melting point = 113 – 115 °C. ^{1}H NMR (400 MHz, DMSO-d6): δ 9.32 (s, 1H), 7.63 (d, *J* = 8.0 Hz, 1H), 7.29 (s, 1H), 7.14 - 7.07 (m, 1H), 2.35 (s, 3H), 1.47 (s, 9H). ^{13}C NMR (101 MHz, DMSO-d6): δ 152.90, 144.29, 140.71, 132.85, 125.81, 125.28, 117.18, 104.51, 79.84, 27.94, 21.25. LCMS: m/z: 233 $[M+H]^+$. HRMS (ESI-TOF) *m/z*: calcd for $C_{13}H_{17}N_2O_2$ $(M+H)^+$ 233.1290, found 233.1284.

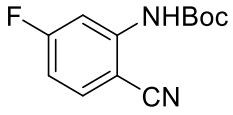
***tert*-Butyl (2-cyano-5-methoxyphenyl)carbamate (1h):**



1h

tert-Butyl (2-cyano-5-methoxyphenyl)carbamate **1h** (920 mg, 3.709 mmol, 78%) was synthesised from 2-bromo-4-methoxybenzonitrile (1 g, 4.717 mmol) by following the general procedure. Off-white solid; Melting point = 117 – 119 °C. ^{1}H NMR (400 MHz, DMSO-d6): δ 9.20 (brs, 1H), 7.67 (d, *J* = 8.6 Hz, 1H), 7.06 (d, *J* = 2.4 Hz, 1H), 6.85 (dd, *J* = 2.5, 8.8 Hz, 1H), 3.81 (s, 3H), 1.47 (s, 9H). ^{13}C NMR (101 MHz, DMSO-d6): δ 162.91, 152.71, 142.70, 134.53, 117.26, 111.04, 109.76, 98.74, 79.98, 55.70, 27.93. LCMS: m/z: 247 $[M-H]^+$. HRMS (ESI-TOF) *m/z*: calcd for $C_{13}H_{17}N_2O_3$ $(M+H)^+$ 249.1239, found 249.1232.

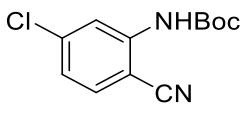
***tert*-Butyl (2-cyano-5-fluorophenyl)carbamate (1i):**



1i

tert-Butyl (2-cyano-5-fluorophenyl)carbamate **1i** (405 mg, 1.176 mmol, 68%) was synthesised from 2-bromo-4-fluorobenzonitrile (500 mg, 2.500 mmol) by following the general procedure. Off-white solid; Melting point = 92 – 94 °C. ^{1}H NMR (400 MHz, DMSO-d6): δ 9.59 (s, 1H), 7.86 (dd, *J* = 6.2, 8.7 Hz, 1H), 7.41 (dd, *J* = 2.6, 10.8 Hz, 1H), 7.15 (dt, *J* = 2.6, 8.4 Hz, 1H), 1.48 (s, 9H). ^{13}C NMR (101 MHz, DMSO-d6): δ 164.45 (d, $J_{C,F}$ = 251 Hz, 1C), 152.53, 143.50 (d, $J_{C,F}$ = 12.36 Hz, 1C), 135.67 (d, $J_{C,F}$ = 10.90 Hz, 1C), 116.26, 112.25 (d, $J_{C,F}$ = 22.53 Hz, 1C), 111.19 (d, $J_{C,F}$ = 26.16 Hz, 1C), 102.73 (d, $J_{C,F}$ = 2.90 Hz, 1C), 80.47, 27.87. ^{19}F NMR (376 MHz, DMSO-d_6): δ –102.8. LCMS: m/z: 235 $[M-H]^+$. HRMS (ESI-TOF) *m/z*: calcd for $C_{12}H_{12}FN_2O_2$ $(M-H)^+$ 235.0883, found 235.0888.

***tert*-Butyl (5-chloro-2-cyanophenyl)carbamate (1j):**

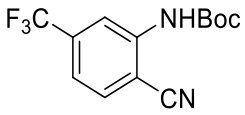


1j

tert-butyl (5-chloro-2-cyanophenyl)carbamate **1j** (521 mg, 2.067 mmol, 89%) was synthesised from 2-bromo-4-chlorobenzonitrile (500 mg, 2.315 mmol) by following the

general procedure. White solid; Melting point = 97 – 99 °C. ^{1}H NMR (400 MHz, DMSO-d6): δ 9.61 (s, 1H), 7.81 (d, *J* = 8.5 Hz, 1H), 7.61 (d, *J* = 2.0 Hz, 1H), 7.37 (dd, *J* = 2.1, 8.4 Hz, 1H), 1.48 (s, 9H). ^{13}C NMR (101 MHz, DMSO-d6): δ 152.57, 142.27, 138.17, 134.72, 124.89, 124.03, 116.20, 105.45, 80.51, 27.88. LCMS: m/z: 251 $[M-H]^+$. HRMS (ESI-TOF) *m/z*: calcd for $C_{12}H_{12}ClN_2O_2$ $(M-H)^+$ 251.0587, found 251.0593.

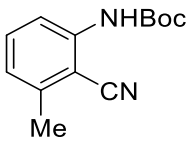
***tert*-Butyl (2-cyano-5-(trifluoromethyl)phenyl)carbamate (1k):**



1k

tert-butyl (2-cyano-5-(trifluoromethyl)phenyl)carbamate **1k** (521 mg, 1.821 mmol, 91%) was synthesised from 2-bromo-4-(trifluoromethyl)benzonitrile (500 mg, 2.000 mmol) by following the general procedure. Pale brown solid; Melting point = 91 – 93 °C. ^{1}H NMR (400 MHz, DMSO-d6): δ 9.77 (s, 1H), 8.03 (d, *J* = 8.1 Hz, 1H), 7.88 (s, 1H), 7.64 (dd, *J* = 1.1, 8.1 Hz, 1H), 1.49 (s, 9H). ^{13}C NMR (DMSO-d_6, 101 MHz) δ 152.6, 141.8, 134.72, 133.21 (q, $J_{C,F}$ = 32.32 Hz, 1C), 123.07 (q, $J_{C,F}$ = 272.7 Hz, 1C), 121.08 (q, $J_{C,F}$ = 5.05 Hz, 1C), 120.59 (q, $J_{C,F}$ = 3.03, 4.04 Hz, 1C), 115.81, 110.22, 80.71, 27.88. ^{19}F NMR (376 MHz, DMSO-d_6): δ –62.2. LCMS: m/z: 285 $[M-H]^+$. HRMS (ESI-TOF) *m/z*: calcd for $C_{13}H_{12}F_3N_2O_2$ $(M-H)^+$ 285.0851, found 285.0857.

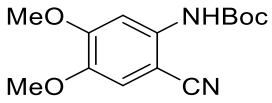
***tert*-Butyl (2-cyano-3-methylphenyl)carbamate (1l):**



1l

tert-butyl (2-cyano-3-methylphenyl)carbamate **1l** (495 mg, 2.133 mmol, 83%) was synthesised from 2-bromo-6-methylbenzonitrile (500 mg, 2.551 mmol) by following the general procedure. Yellow solid; Melting point = 83 – 85 °C. ^{1}H NMR (400 MHz, DMSO-d6): δ 9.31 (s, 1H), 7.54 - 7.47 (m, 1H), 7.28 (d, *J* = 8.1 Hz, 1H), 7.20 (d, *J* = 7.6 Hz, 1H), 2.45 (s, 3H), 1.47 (s, 9H). ^{13}C NMR (101 MHz, DMSO-d6): δ 152.97, 142.18, 141.13, 132.90, 125.98, 122.28, 115.91, 108.23, 79.79, 27.96, 20.21. LCMS: m/z: 233 $[M+H]^+$. HRMS (ESI-TOF) *m/z*: calcd for $C_{13}H_{17}N_2O_2$ $(M+H)^+$ 233.1290, found 233.1284.

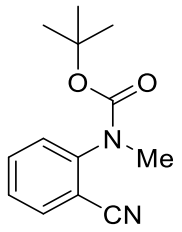
***tert*-Butyl (2-cyano-4,5-dimethoxyphenyl)carbamate (1m):**



1m

tert-butyl (2-cyano-4,5-dimethoxyphenyl)carbamate **1m** (405 mg, 1.457 mmol, 70%) was synthesised from 2-bromo-4,5-dimethoxybenzonitrile (500 mg, 2.066 mmol) by following the general procedure. Yellow solid; Melting point = 131 – 133 °C. ^{1}H NMR (400 MHz, DMSO-d6): δ 9.14 (s, 1H), 7.27 (s, 1H), 7.01 (s, 1H), 3.80 (s, 3H), 3.78 (s, 3H), 1.46 (s, 9H). ^{13}C NMR (101 MHz, DMSO-d6): δ 153.10, 152.58, 145.97, 135.80, 117.33, 114.19, 108.98, 98.79, 79.59, 56.04, 55.80, 28.01. LCMS: m/z: 277 $[M-H]^+$. HRMS (ESI-TOF) *m/z*: calcd for $C_{14}H_{19}N_2O_4$ $(M+H)^+$ 279.1345, found 279.1339.

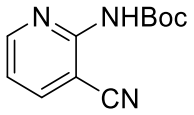
***tert*-Butyl (2-cyanophenyl)(methyl)carbamate (1n):**



1n

To a stirred solution of *tert*-butyl (2-cyanophenyl)carbamate (500 mg, 2.291 mmol) in THF (10 mL) was added sodium hydride (92 mg, 2.291 mmol) at 0 ^{o}C under N_2 atmosphere. Iodomethane (0.143 mL, 2.291 mmol) was added at 0 ^{o}C and the reaction mixture was stirred for 16 h. The reaction was monitored by TLC and UPLC. After completion of starting material, the reaction mixture was quenched with ice water and extracted with EtOAc (2 x 50 mL). Combined organic layers were dried over Na_2SO_4, filtered, and concentrated in *vacuo* yield crude residue which was purified by silica gel column chromatography (20% EtOAc/hexanes) obtained *tert*-butyl (2-cyanophenyl)(methyl)carbamate **1n** (450 mg, 1.926 mmol, 84% yield) as a colourless oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.66 (dd, *J* = 1.4, 8.0 Hz, 1H), 7.60 (dt, *J* = 1.6, 7.8 Hz, 1H), 7.37 - 7.29 (m, 2H), 3.29 (s, 3H), 1.44 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 153.78, 146.59, 133.48, 133.19, 127.75, 126.88, 116.74, 112.35, 81.42, 37.33, 28.07. LCMS: m/z: 177 $[M-56+H]^+$. HRMS (ESI-TOF) *m/z*: calcd for $C_{13}H_{17}N_2O_2$ $(M+H)^+$ 233.1290, found 233.1284.

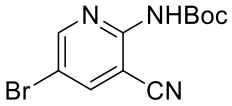
***tert*-Butyl (3-cyanopyridin-2-yl)carbamate (1o):**



1o

tert-butyl (3-cyanopyridin-2-yl)carbamate **1o** (775 mg, 3.539 mmol, 65%) was synthesised from 2-bromonicotinonitrile (1 g, 5.464 mmol) by following the general procedure. Pale green solid; Melting point = 159 – 161 °C. ^{1}H NMR (400 MHz, DMSO-d6): δ 10.09 (s, 1H), 8.62 (dd, *J* = 1.9, 4.9 Hz, 1H), 8.29 (dd, *J* = 1.9, 7.8 Hz, 1H), 7.37 (dd, *J* = 4.9, 7.8 Hz, 1H), 1.47 (s, 9H). ^{13}C NMR (101 MHz, DMSO-d6): δ 152.66, 152.52, 152.24, 142.68, 120.41, 115.87, 104.23, 80.45, 27.86. LCMS: m/z: 218 $[M-H]^+$. HRMS (ESI-TOF) *m/z*: calcd for $C_{13}H_{17}N_2O_2$ $(M-56+H)^+$ 164.0460, found 164.0454.

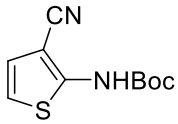
***tert*-Butyl (5-bromo-3-cyanopyridin-2-yl)carbamate (1p):**



1p

tert-butyl (3-cyanopyridin-2-yl)carbamate **1p** (308 mg, 1.033 mmol, 41%) was synthesised from 2-amino-5-bromonicotinonitrile (500 mg, 2.525 mmol) by following the procedure for **1q**. White solid; Melting point = 104 – 106 °C. ^{1}H NMR (400 MHz, DMSO-d6): δ 10.25 (s, 1H), 8.76 (d, *J* = 2.5 Hz, 1H), 8.65 (d, *J* = 2.4 Hz, 1H), 1.47 (s, 9H). ^{13}C NMR (101 MHz, DMSO-d6): δ 153.08, 152.23, 151.67, 144.44, 114.60, 114.57, 105.39, 80.79, 27.81. LCMS: m/z: 296 $[M-H]^+$. HRMS (ESI-TOF) *m/z*: calcd for $C_{11}H_{11}BrN_3O_2$ $(M-H)^+$ 296.0035, found 296.0040.

***tert*-Butyl (3-cyanothiophen-2-yl)carbamate (1q):**

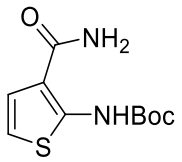


1q

To a stirred solution of 2-aminothiophene-3-carbonitrile (500 mg, 4.03 mmol) in THF (8 mL) were added Et_3N (1.4 mL, 10.07 mmol), DMAP (98 mg, 0.80 mmol) and Boc_2O (1.32 g, 6.04 mmol) under N2 atmosphere. The reaction mixture was stirred at room temperature for 16 h. After completion of starting material, the reaction mixture was quenched with water and extracted with EtOAc (2x50 mL). The combined organic layers were dried over Na_2SO_4,

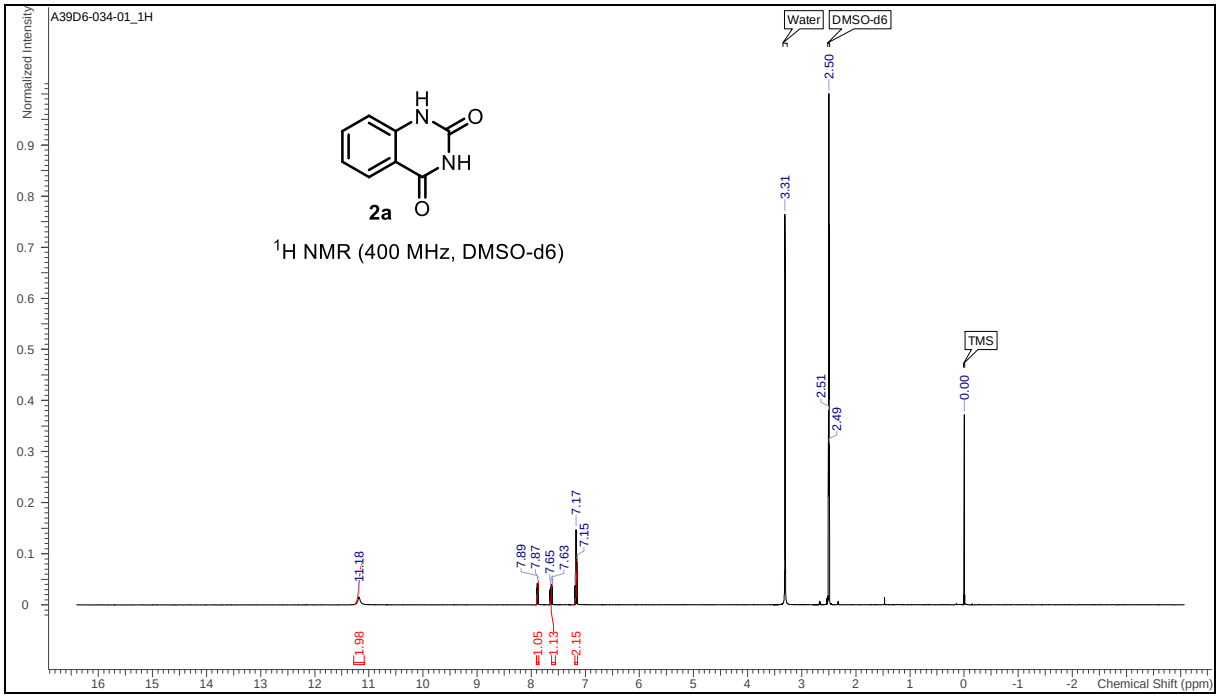
filtered, and concentrated in *vacuo* afforded crude residue. The crude residue was purified by Silica gel column chromatography to afford *tert*-Butyl (3-cyanothiophen-2-yl)carbamate **1q** (550 mg, 2.45 mmol, 61%) as an off-white solid. Melting point = 92 – 94 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ 10.97 (brs, 1H), 7.15 - 7.06 (m, 2H), 1.48 (s, 9H). ^{13}C NMR (126 MHz, DMSO-d6): δ 152.56, 151.25, 125.27, 118.45, 114.56, 92.87, 81.26, 27.79. LCMS: m/z: 223 $[M-H]^+$. HRMS (ESI-TOF) *m/z*: calcd for $C_{10}H_{11}N_2O_2S$ $(M-H)^+$ 223.0541, found 223.0545.

***tert*-Butyl (3-carbamoylthiophen-2-yl)carbamate (3q):**



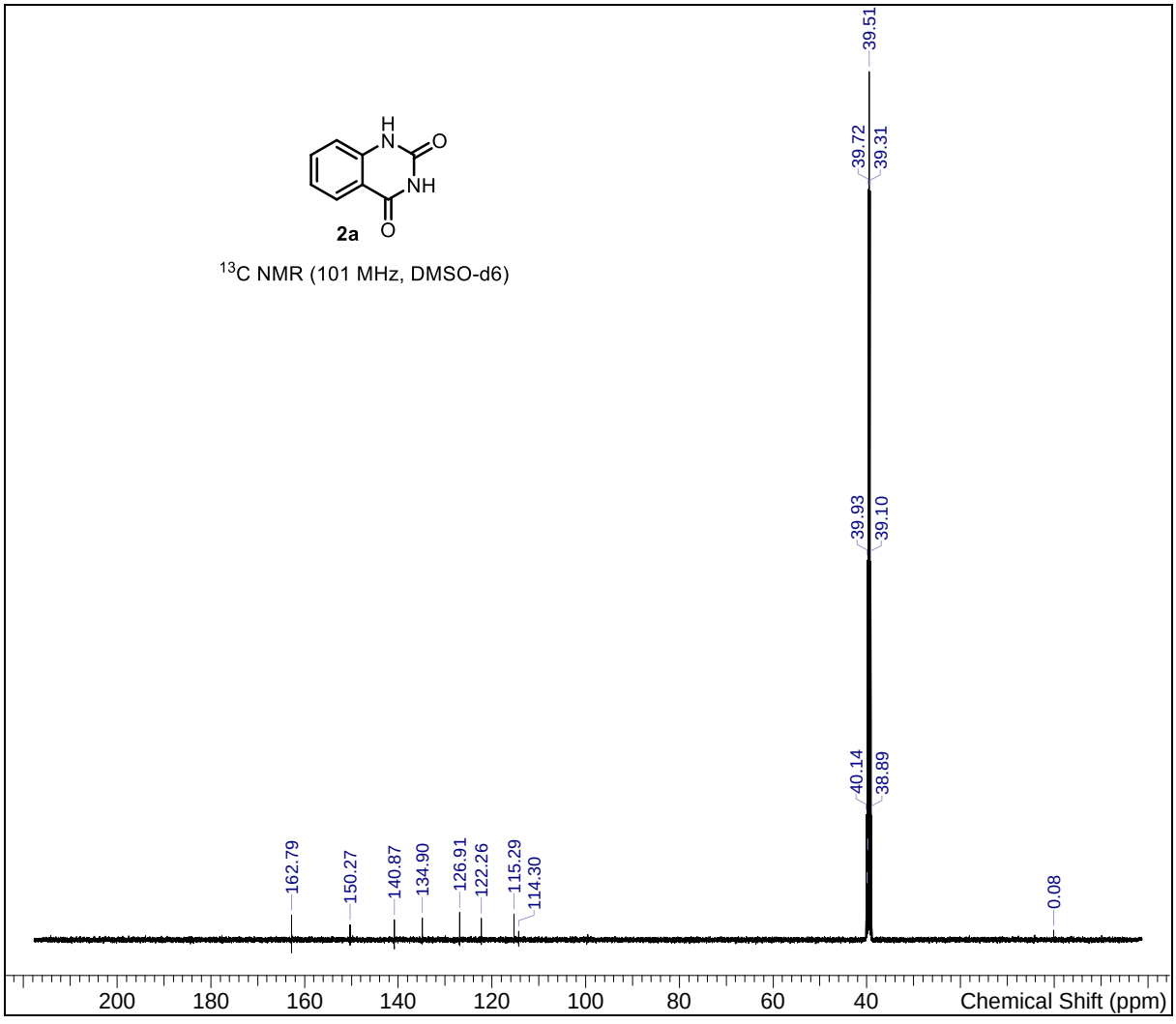
3q

tert-Butyl (3-carbamoylthiophen-2-yl)carbamate **3q** (180 mg, 0.74 mmol) was obtained from *tert*-butyl (3-cyanothiophen-2-yl)carbamate **1q** (224 mg, 1 mmol) by following the general procedure. Yield: 74%; Off-white solid. Melting point = 137 – 139 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ 11.30 (brs, 1H), 7.85 (brs, 1H), 7.50 (brs, 1H), 7.36 (d, *J* = 5.9 Hz, 1H), 6.91 (d, *J* = 5.8 Hz, 1H), 1.49 (s, 10H). ^{13}C NMR (101 MHz, DMSO-d_6): δ 166.97, 151.47, 147.67, 123.44, 114.88, 113.67, 81.31, 27.81. LCMS: m/z: 241 $[M-H]^+$. HRMS (ESI-TOF) *m/z*: calcd for $C_{10}H_{13}N_2O_3S$ $(M-H)^+$ 241.0647, found 241.0652.



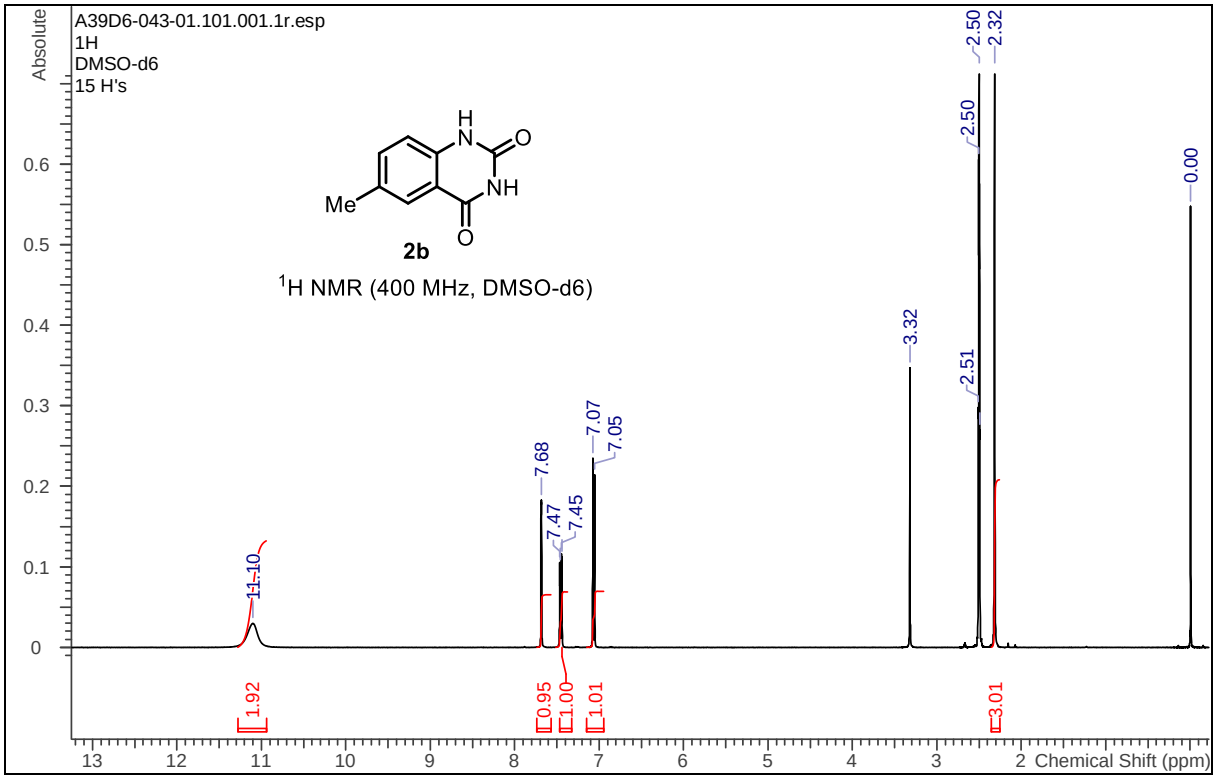
2a

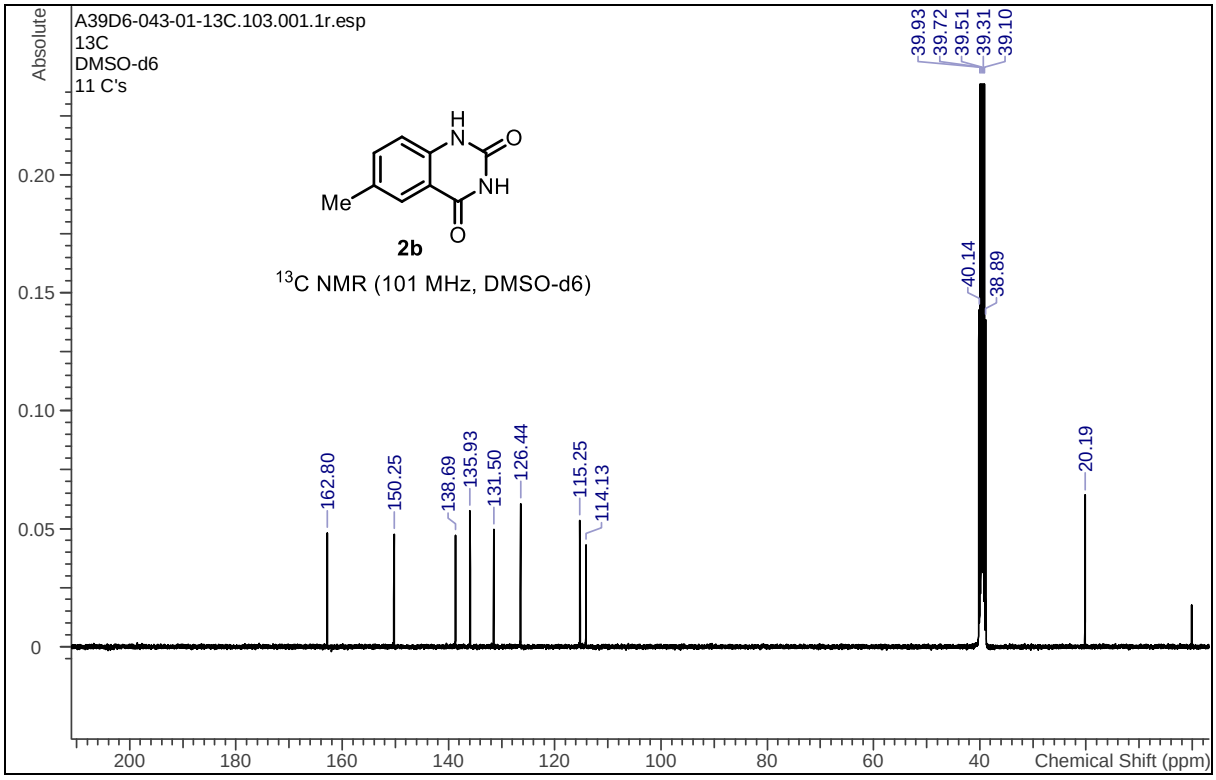
^{1}H NMR (400 MHz, DMSO-d6)

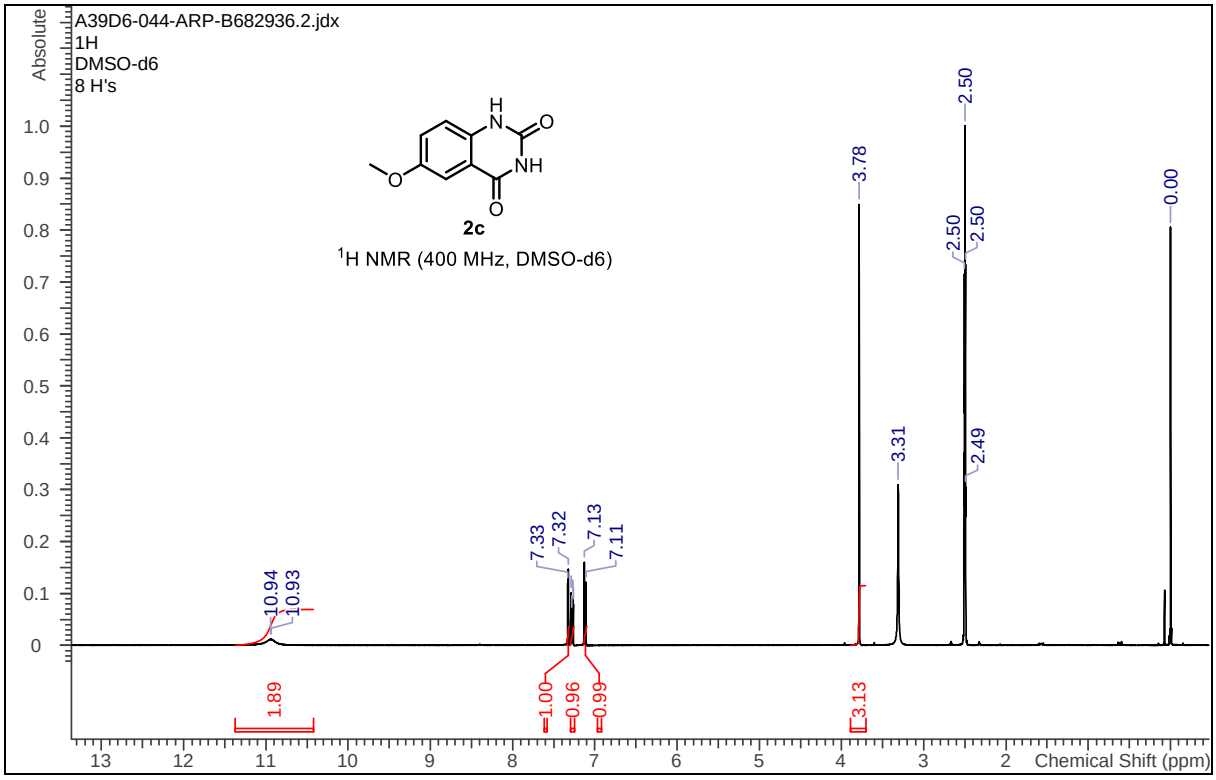


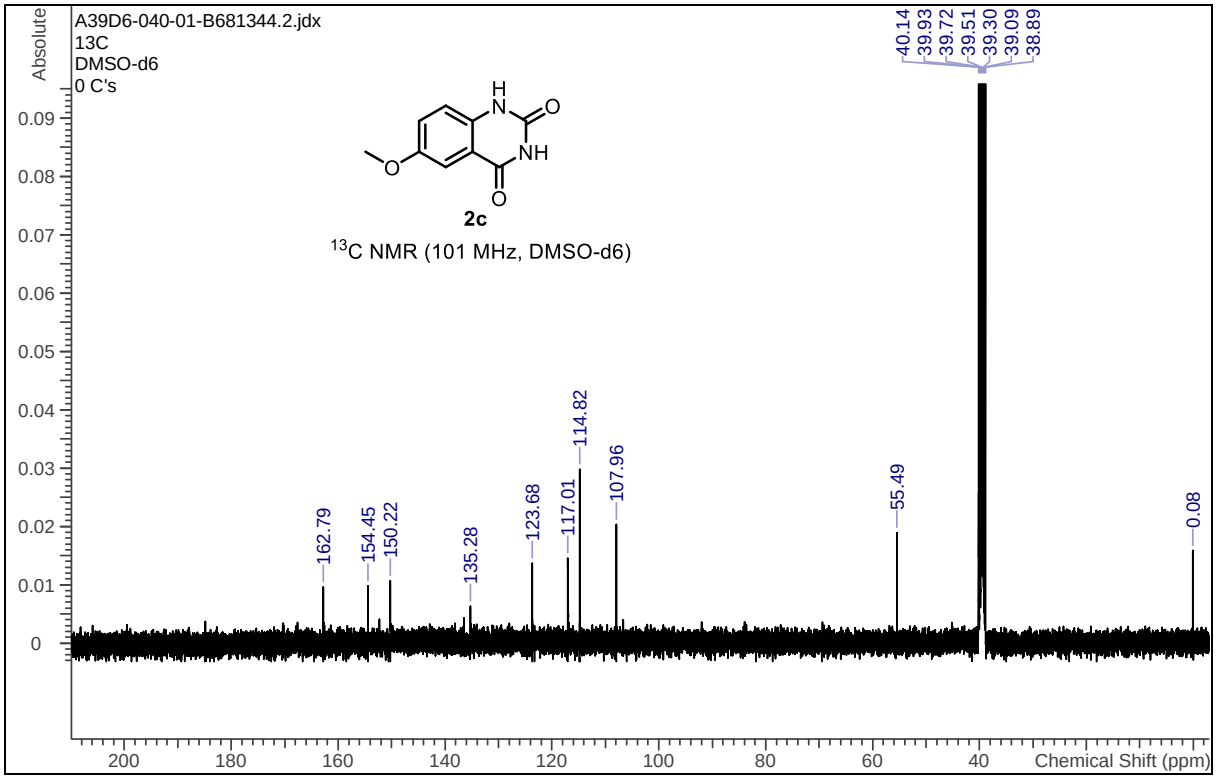
2a

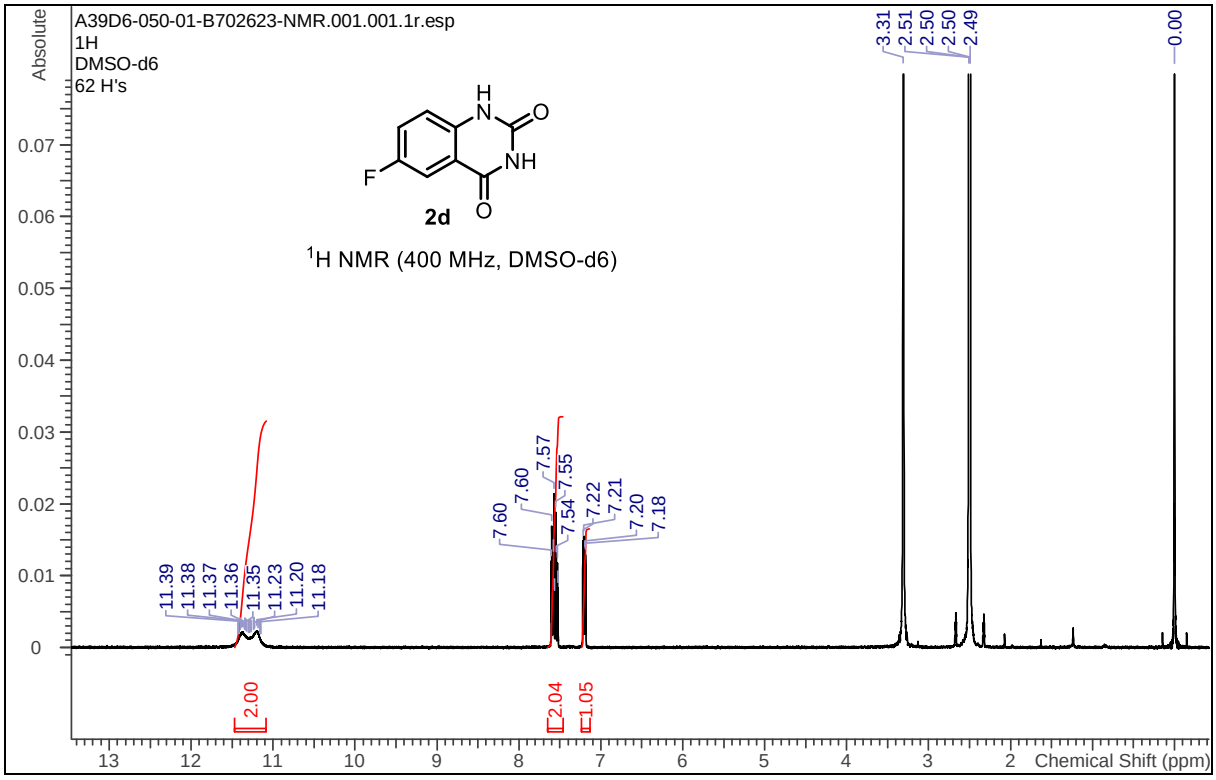
^{13}C NMR (101 MHz, DMSO-d6)

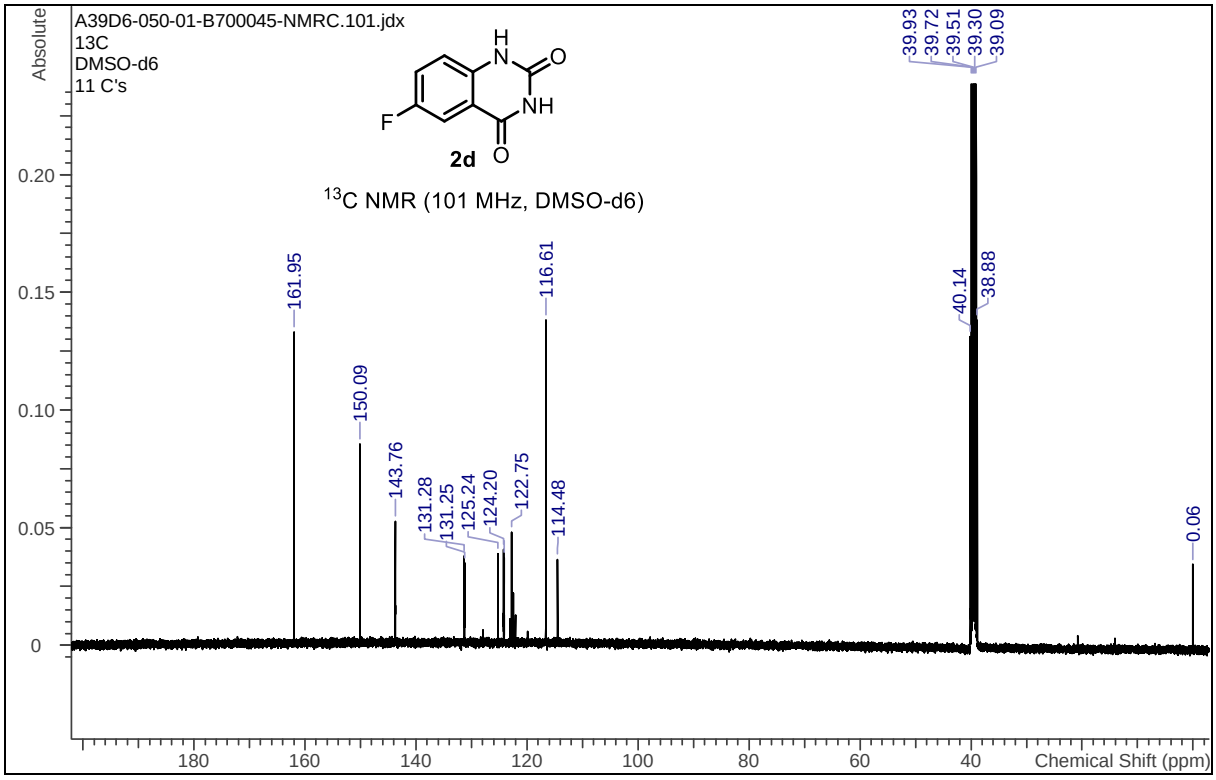

A39D6-043-01.101.001.1r.esp
1H
DMSO-d6
15 H's
Absolute
2b
1H NMR (400 MHz, DMSO-d6)
Chemical Shift (ppm)

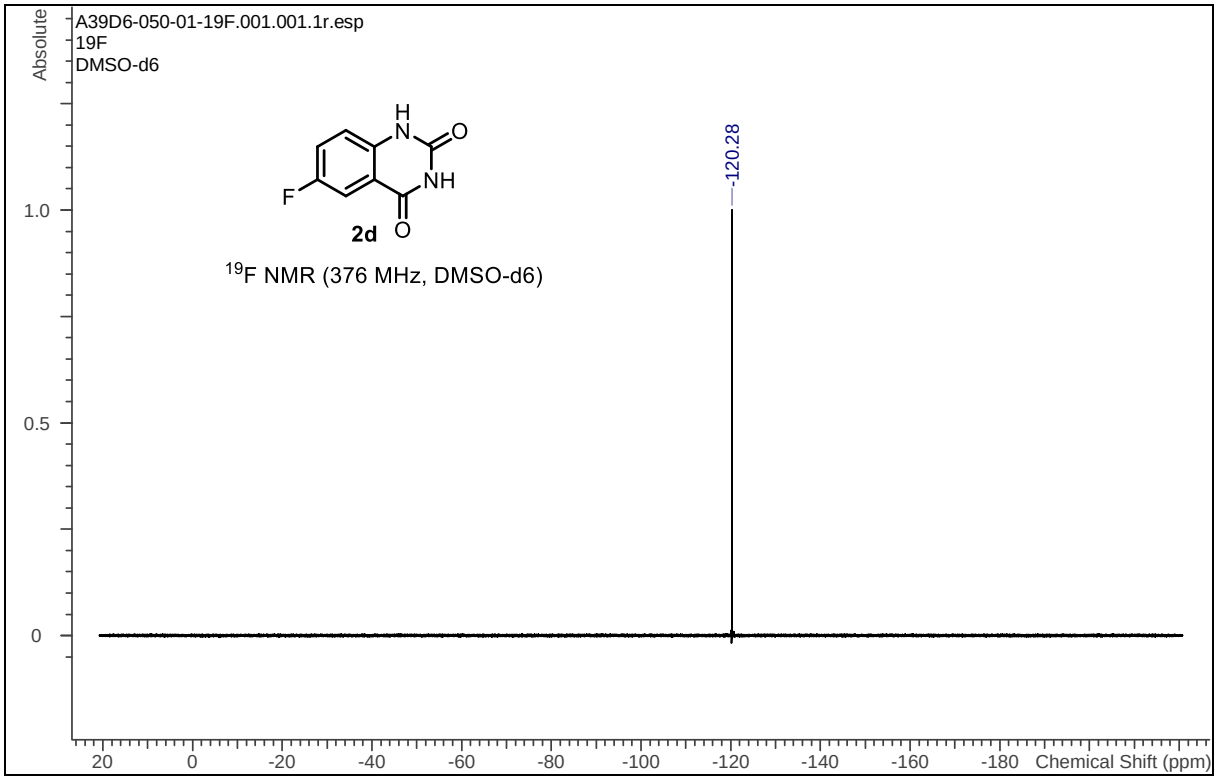

A39D6-043-01-13C.103.001.1r.esp
13C
DMSO-d6
11 C's
Absolute
2b
13C NMR (101 MHz, DMSO-d6)
Chemical Shift (ppm)

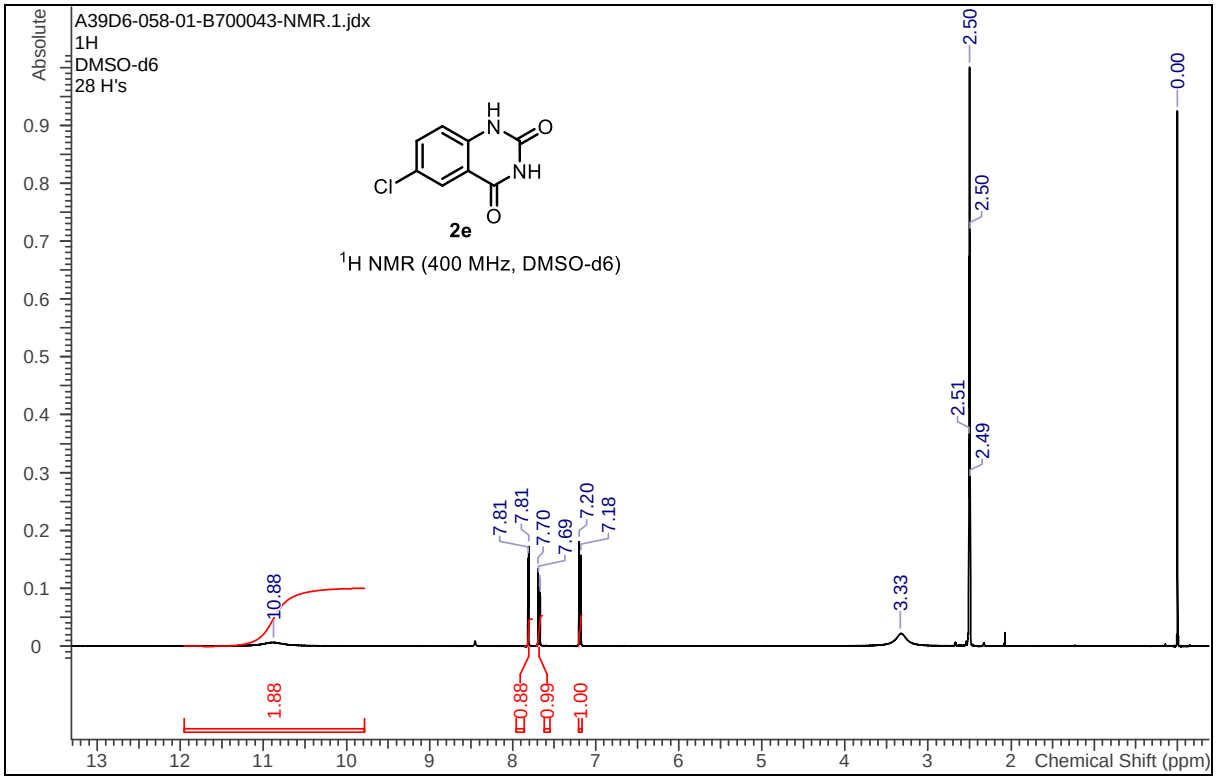

A39D6-044-ARP-B682936.2.jdx
1H
DMSO-d6
8 H's
Absolute
2c
1H NMR (400 MHz, DMSO-d6)
10.94
10.93
7.33
7.32
7.13
7.11
3.78
3.31
2.50
2.50
2.50
2.49
0.00
1.89
1.00
0.96
0.99
3.13
Chemical Shift (ppm)

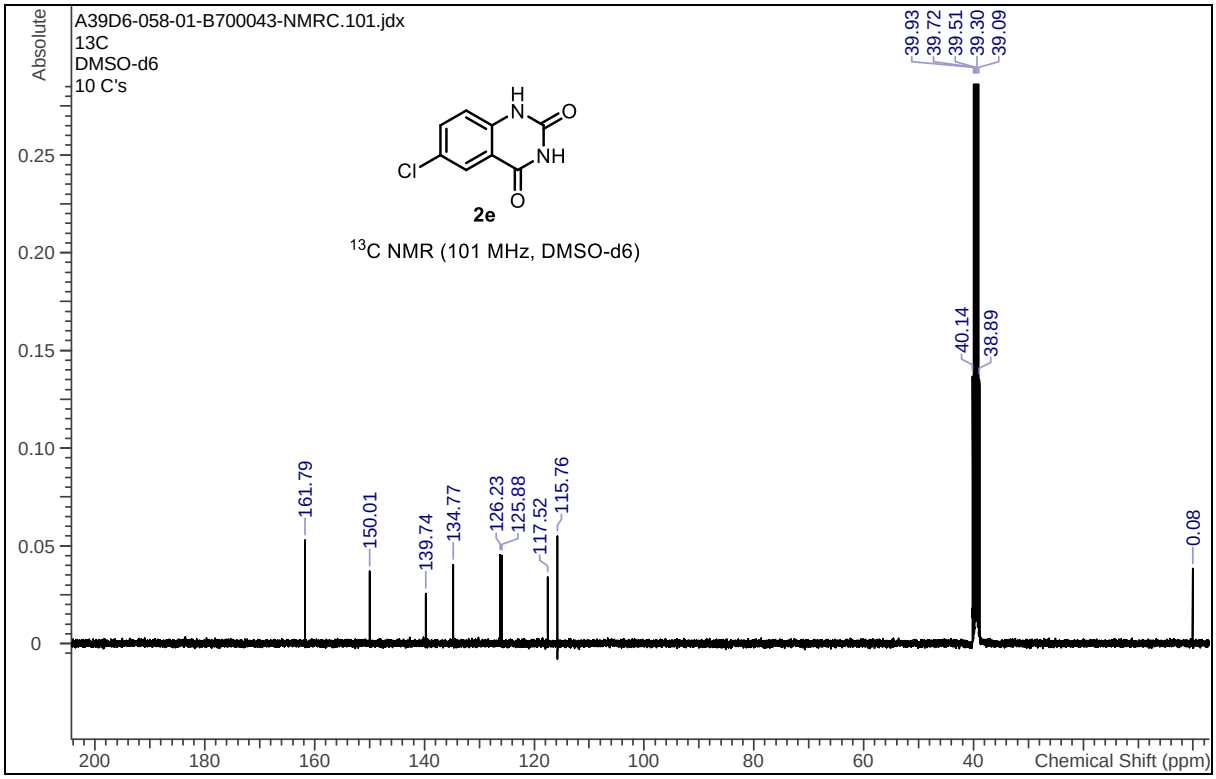

A39D6-040-01-B681344.2.jdx
13C
DMSO-d6
0 C's
Absolute
2c
13C NMR (101 MHz, DMSO-d6)
40.14
39.93
39.72
39.51
39.30
39.09
38.89
162.79
154.45
150.22
135.28
123.68
117.01
114.82
107.96
55.49
0.08
Chemical Shift (ppm)

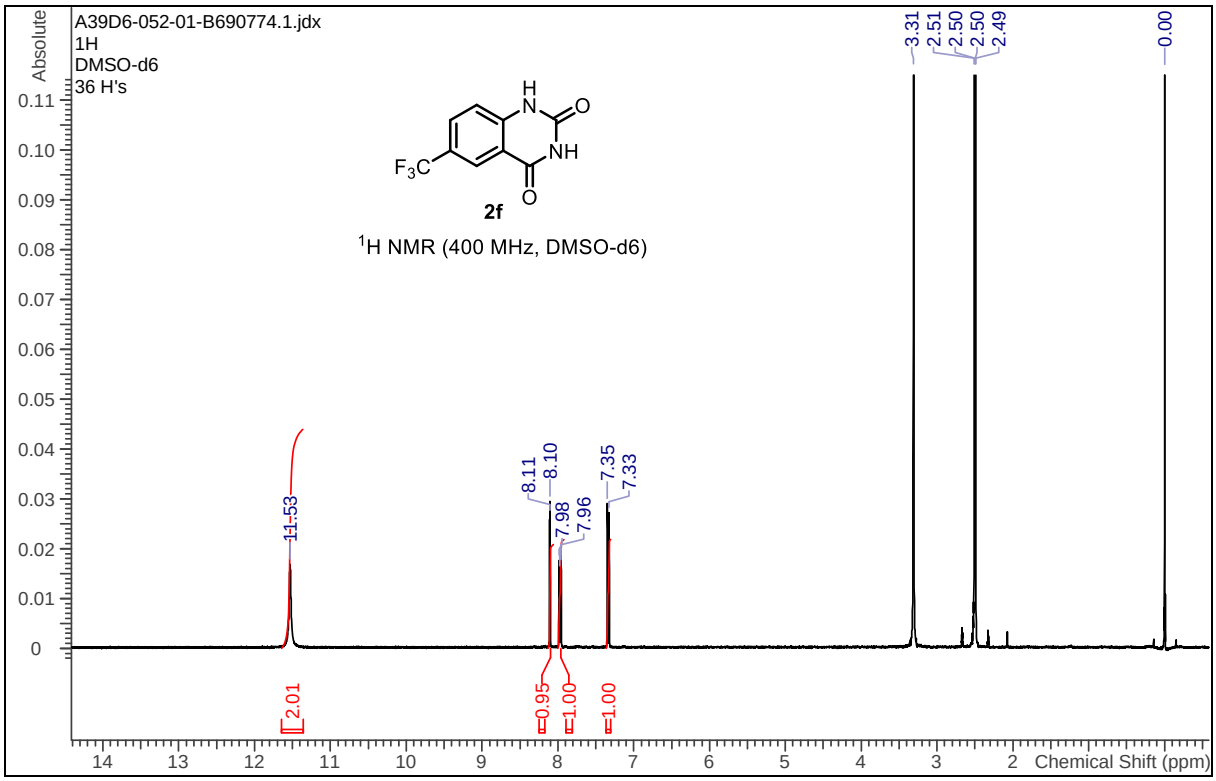

A39D6-050-01-B702623-NMR.001.001.1r.esp
1H
DMSO-d6
62 H's
2d
1H NMR (400 MHz, DMSO-d6)
Absolute
Chemical Shift (ppm)
3.31
2.51
2.50
2.50
2.49
0.00
11.39
11.38
11.37
11.36
11.35
11.23
11.20
11.18
7.60
7.60
7.57
7.55
7.54
7.22
7.21
7.20
7.18
2.00
2.04
1.05

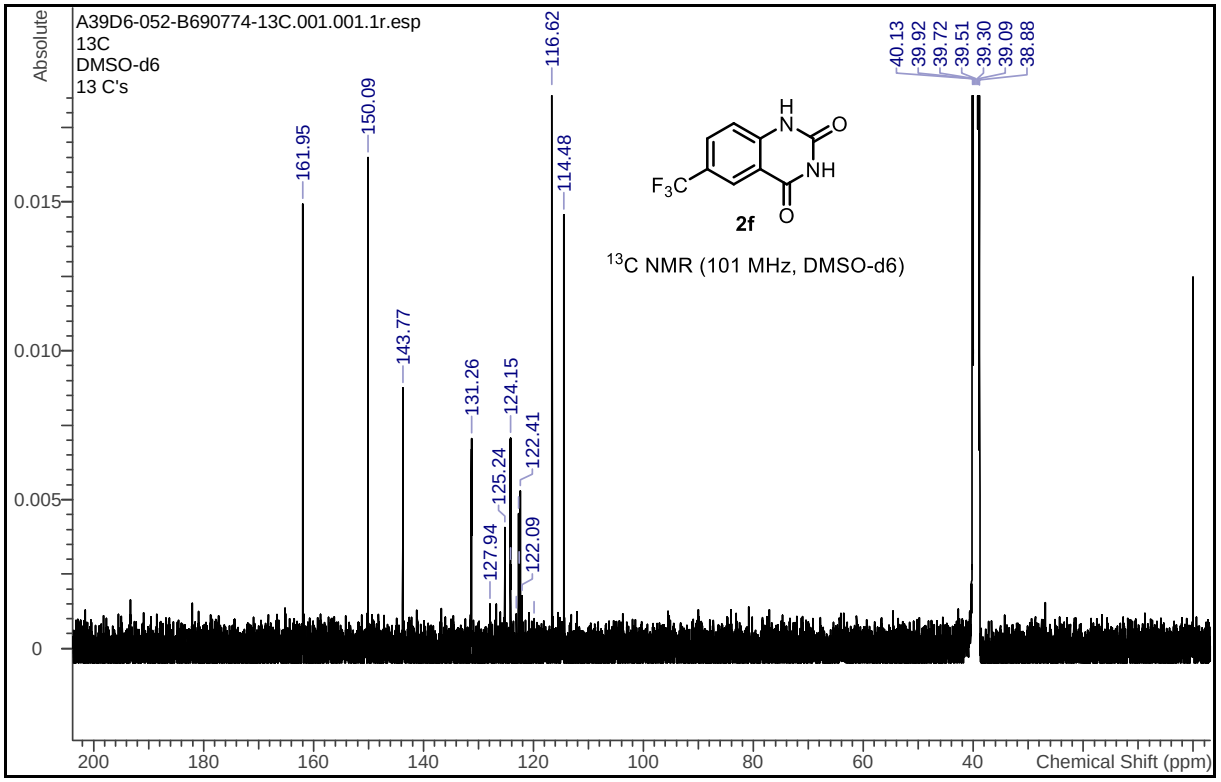

A39D6-050-01-B700045-NMRC.101.jdx
13C
DMSO-d6
11 C's
2d
13C NMR (101 MHz, DMSO-d6)
Absolute
Chemical Shift (ppm)
39.93
39.72
39.51
39.30
39.09
161.95
150.09
143.76
131.28
131.25
125.24
124.20
122.75
116.61
114.48
40.14
38.88
0.06

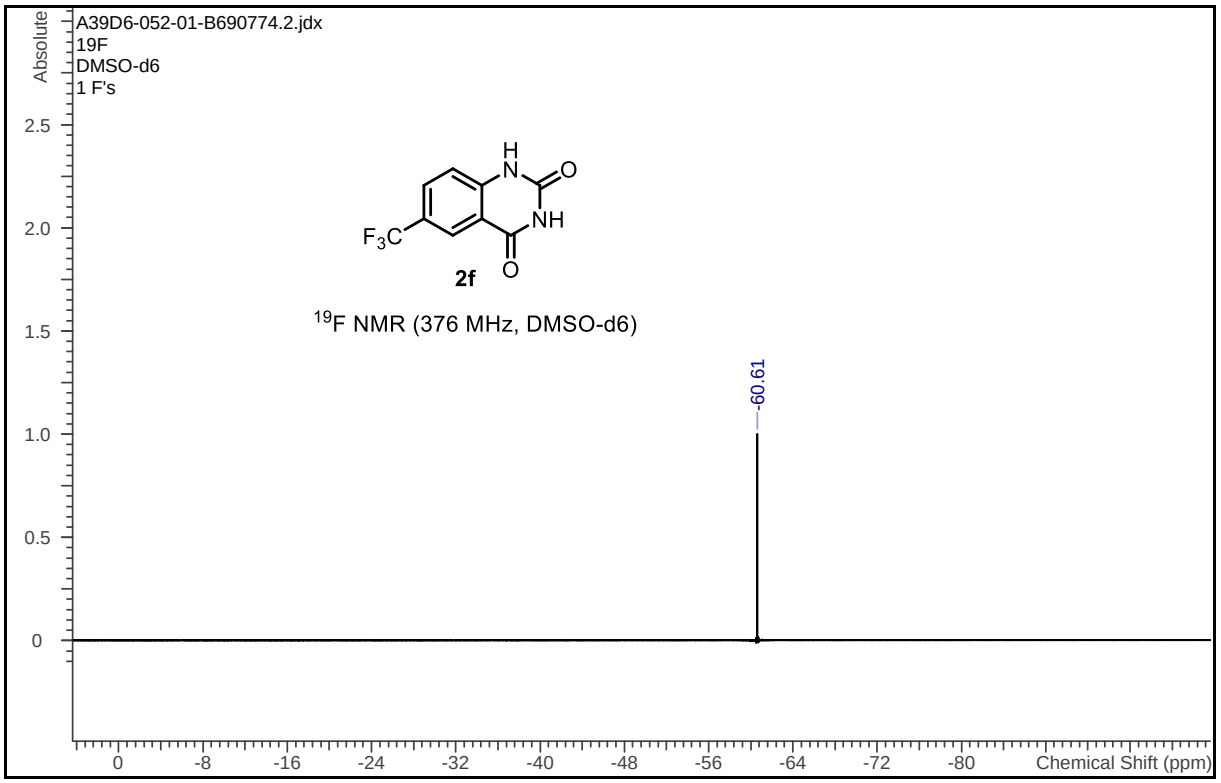

A39D6-050-01-19F.001.001.1r.esp
19F
DMSO-d6
Absolute
2d
19F NMR (376 MHz, DMSO-d6)
-120.28
Chemical Shift (ppm)

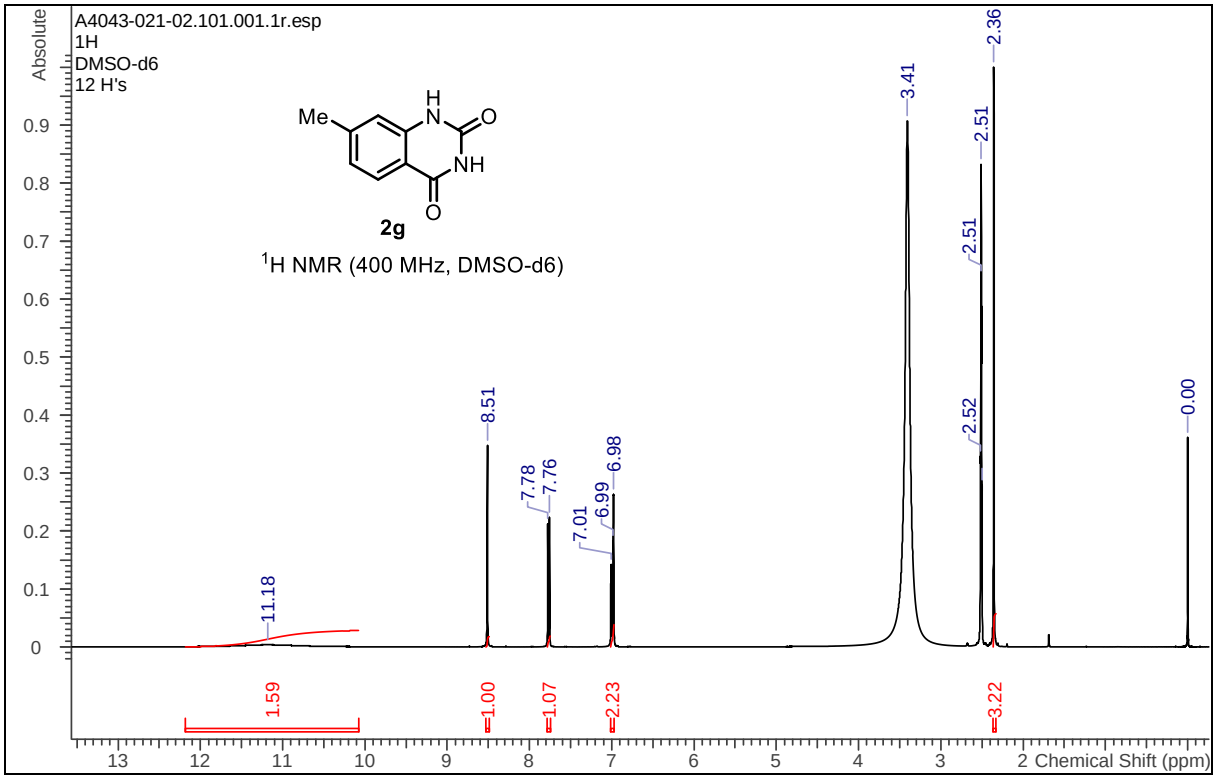

A39D6-058-01-B700043-NMR.1.jdx
1H
DMSO-d6
28 H's
Absolute
2e
1H NMR (400 MHz, DMSO-d6)
2.50
0.00
2.51
2.49
7.81
7.81
7.70
7.69
7.20
7.18
3.33
10.88
1.88
0.88
0.99
1.00
Chemical Shift (ppm)

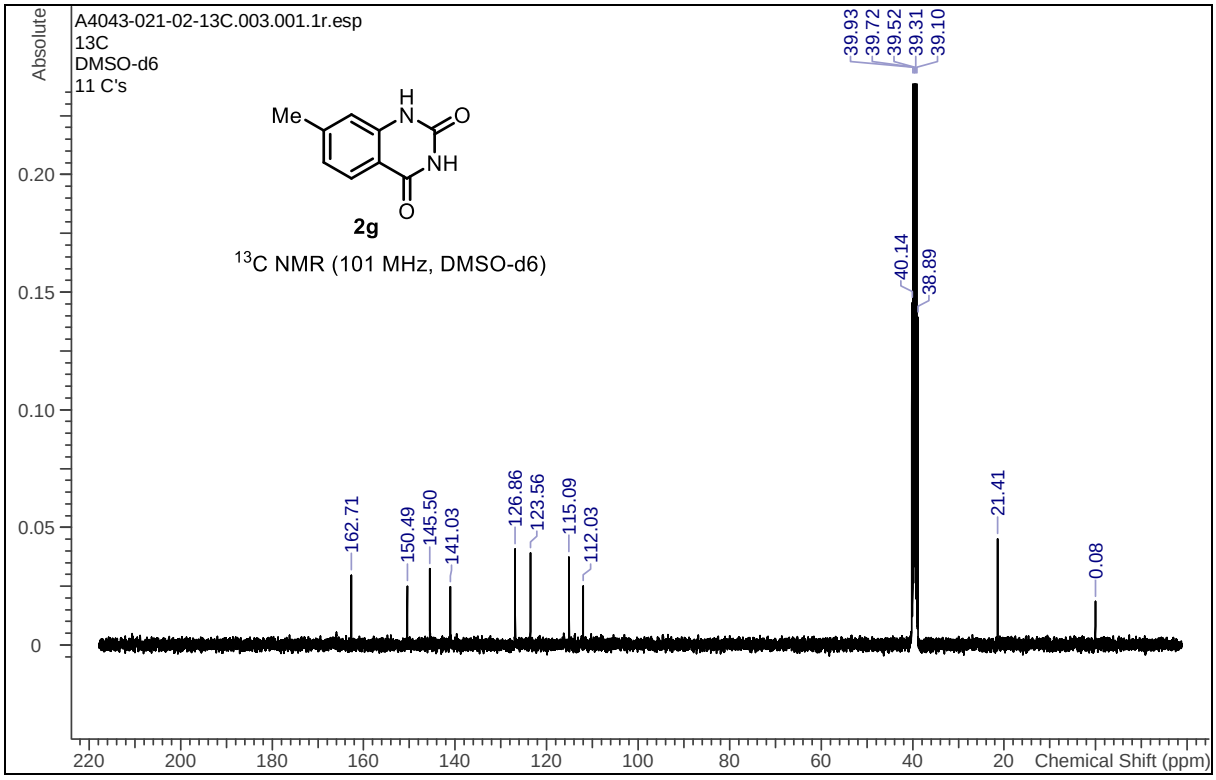

A39D6-058-01-B700043-NMRC.101.jdx
13C
DMSO-d6
10 C's
Absolute
2e
13C NMR (101 MHz, DMSO-d6)
39.93
39.72
39.51
39.30
39.09
40.14
38.89
161.79
150.01
139.74
134.77
126.23
125.88
117.52
115.76
0.08
Chemical Shift (ppm)

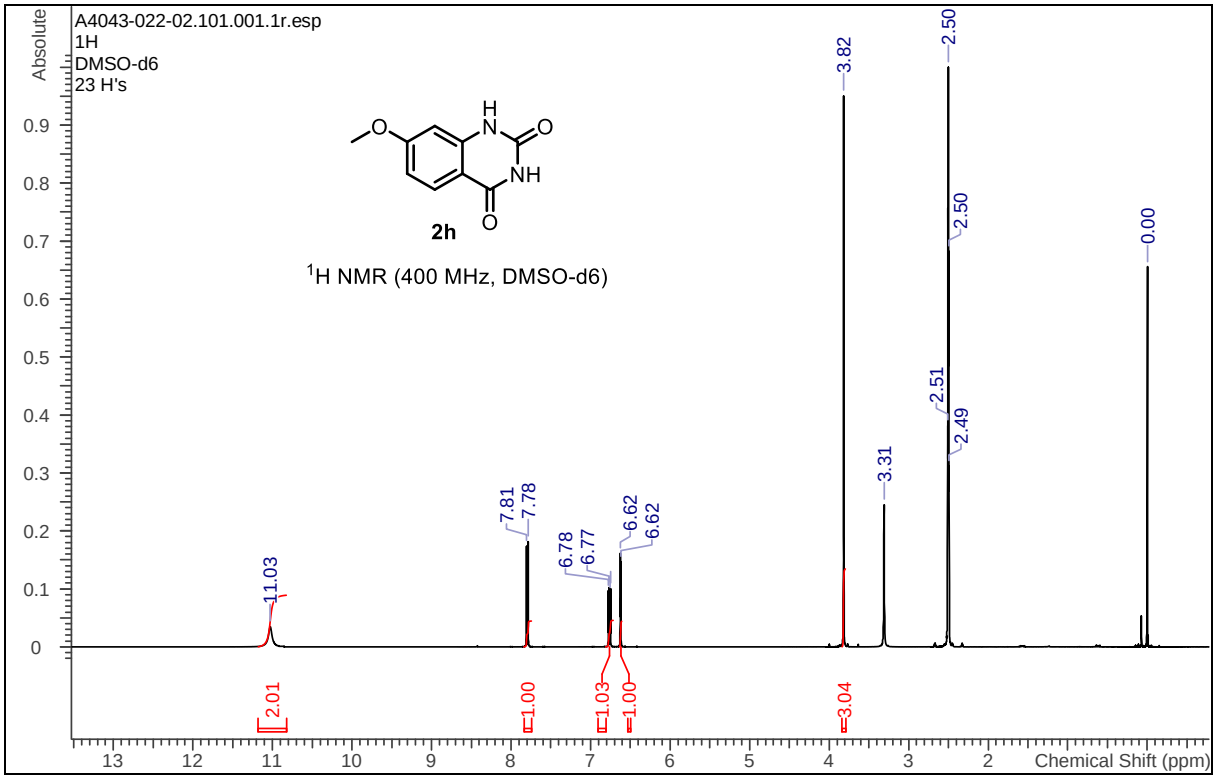

A39D6-052-01-B690774.1.jdx
1H
DMSO-d6
36 H's
Absolute
2f
1H NMR (400 MHz, DMSO-d6)
3.31
2.51
2.50
2.50
2.49
0.00
11.53
8.11
8.10
7.98
7.96
7.35
7.33
2.01
0.95
1.00
1.00
Chemical Shift (ppm)

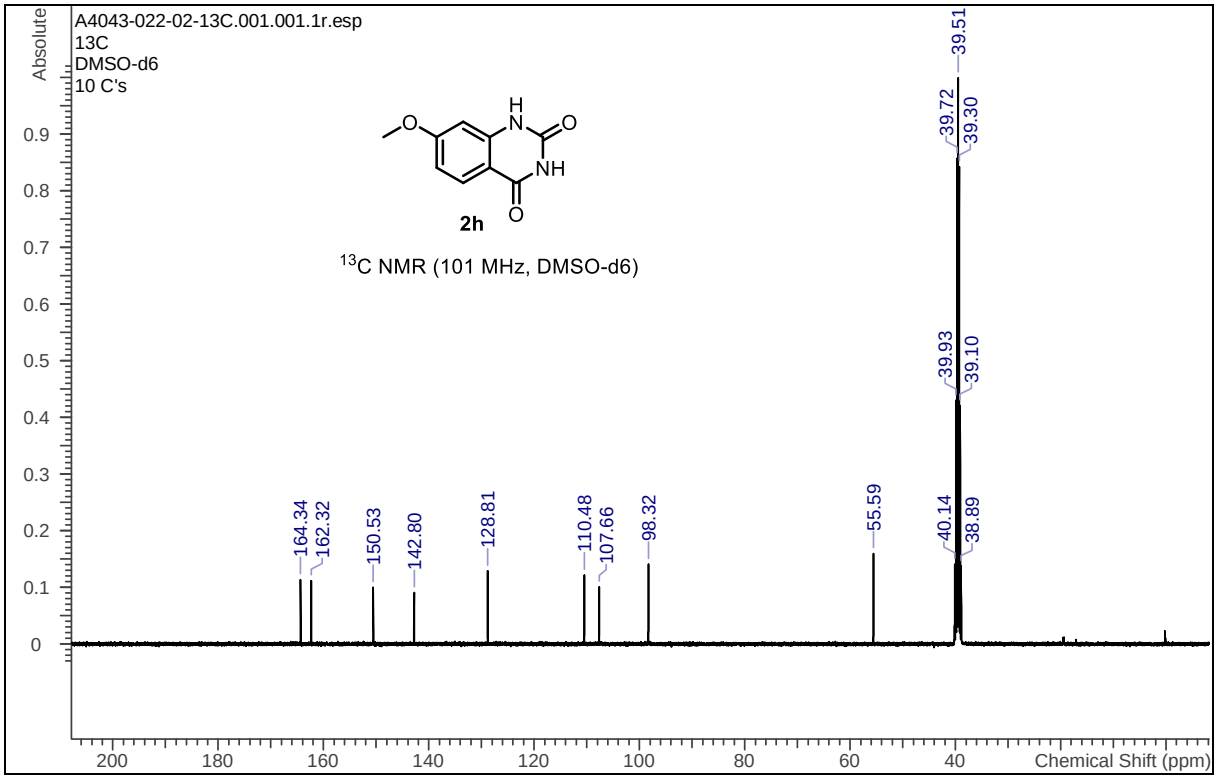

A39D6-052-B690774-13C.001.001.1r.esp
13C
DMSO-d6
13 C's
Absolute
161.95
150.09
143.77
131.26
127.94
125.24
124.15
122.41
122.09
116.62
114.48
40.13
39.92
39.72
39.51
39.30
39.09
38.88
2f
13C NMR (101 MHz, DMSO-d6)
Chemical Shift (ppm)

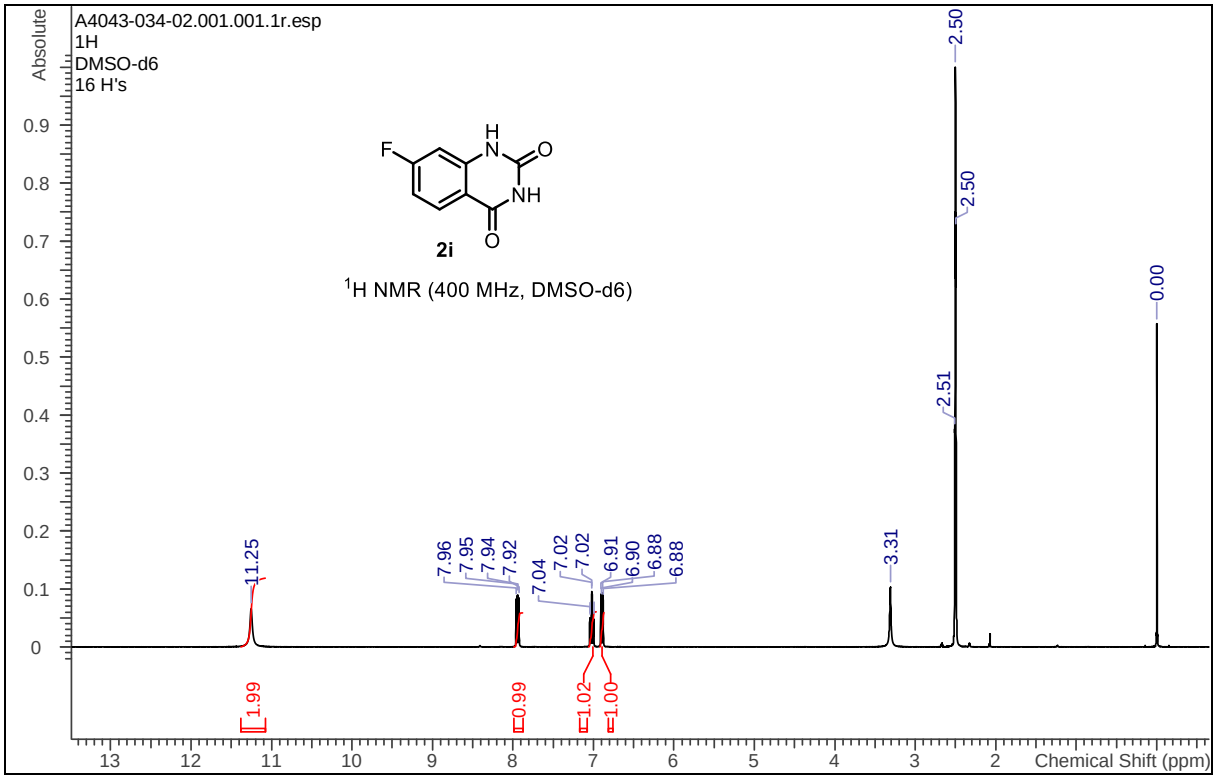

A39D6-052-01-B690774.2.jdx
19F
DMSO-d6
1 F's
Absolute
-60.61
2f
19F NMR (376 MHz, DMSO-d6)
Chemical Shift (ppm)

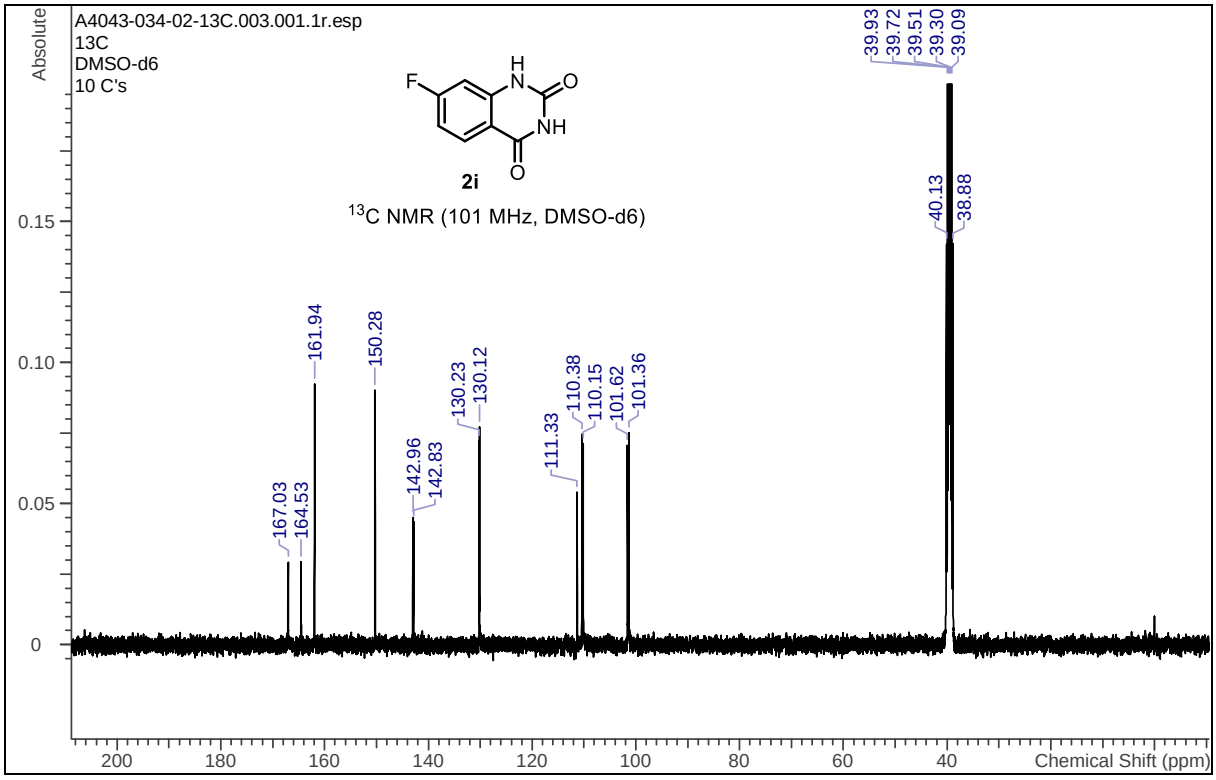

A4043-021-02.101.001.1r.esp
1H
DMSO-d6
12 H's
Me
H
N
O
NH
O
2g
1H NMR (400 MHz, DMSO-d6)
Absolute
11.18
8.51
7.78
7.76
7.01
6.99
6.98
3.41
2.51
2.51
2.36
2.52
0.00
1.59
1.00
1.07
2.23
3.22
Chemical Shift (ppm)


A4043-021-02-13C.003.001.1r.esp
13C
DMSO-d6
11 C's
Me
H
N
O
NH
O
2g
13C NMR (101 MHz, DMSO-d6)
Absolute
39.93
39.72
39.52
39.31
39.10
40.14
38.89
162.71
150.49
145.50
141.03
126.86
123.56
115.09
112.03
21.41
0.08
Chemical Shift (ppm)


A4043-022-02.101.001.1r.esp
1H
DMSO-d6
23 H's
2h
^{1}H NMR (400 MHz, DMSO-d6)
Absolute
Chemical Shift (ppm)
11.03
7.81
7.78
6.78
6.77
6.62
6.62
3.82
3.31
2.51
2.50
2.49
2.50
0.00
2.01
1.00
1.03
1.00
3.04


A4043-022-02-13C.001.001.1r.esp
13C
DMSO-d6
10 C's
2h
^{13}C NMR (101 MHz, DMSO-d6)
Absolute
Chemical Shift (ppm)
164.34
162.32
150.53
142.80
128.81
110.48
107.66
98.32
55.59
39.93
39.72
39.51
39.30
39.10
40.14
38.89


A4043-034-02.001.001.1r.esp
1H
DMSO-d6
16 H's
2i
1H NMR (400 MHz, DMSO-d6)
Absolute
Chemical Shift (ppm)
11.25
7.96
7.95
7.94
7.92
7.04
7.02
7.02
6.91
6.90
6.88
6.88
3.31
2.50
2.50
2.51
0.00
1.99
0.99
1.02
1.00


A4043-034-02-13C.003.001.1r.esp
13C
DMSO-d6
10 C's
2i
13C NMR (101 MHz, DMSO-d6)
Absolute
Chemical Shift (ppm)
39.93
39.72
39.51
39.30
39.09
40.13
38.88
167.03
164.53
161.94
150.28
142.96
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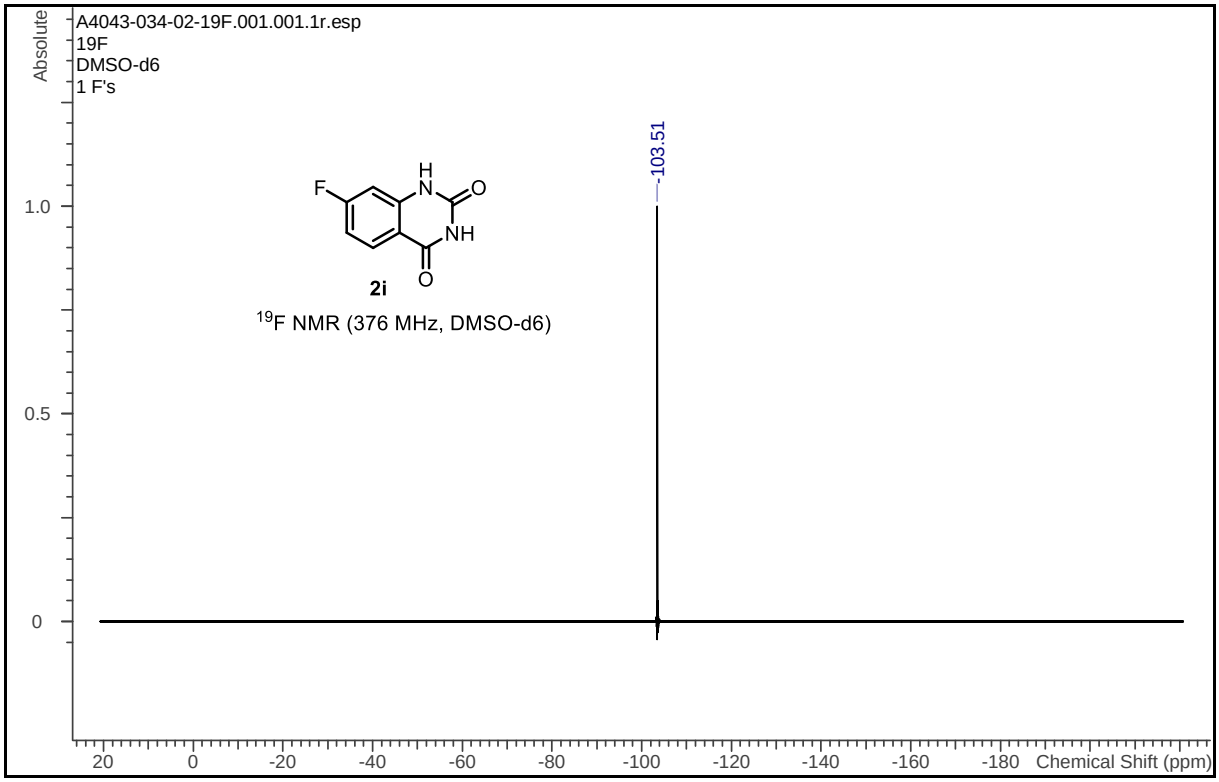
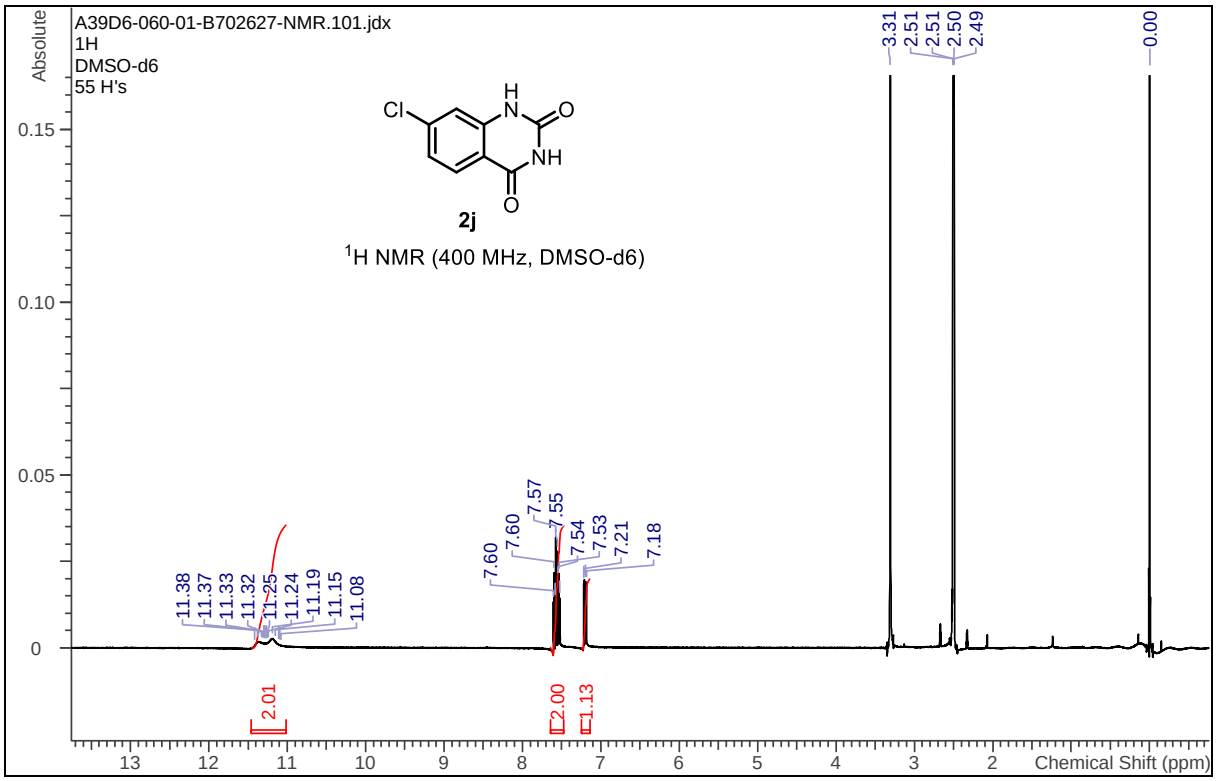
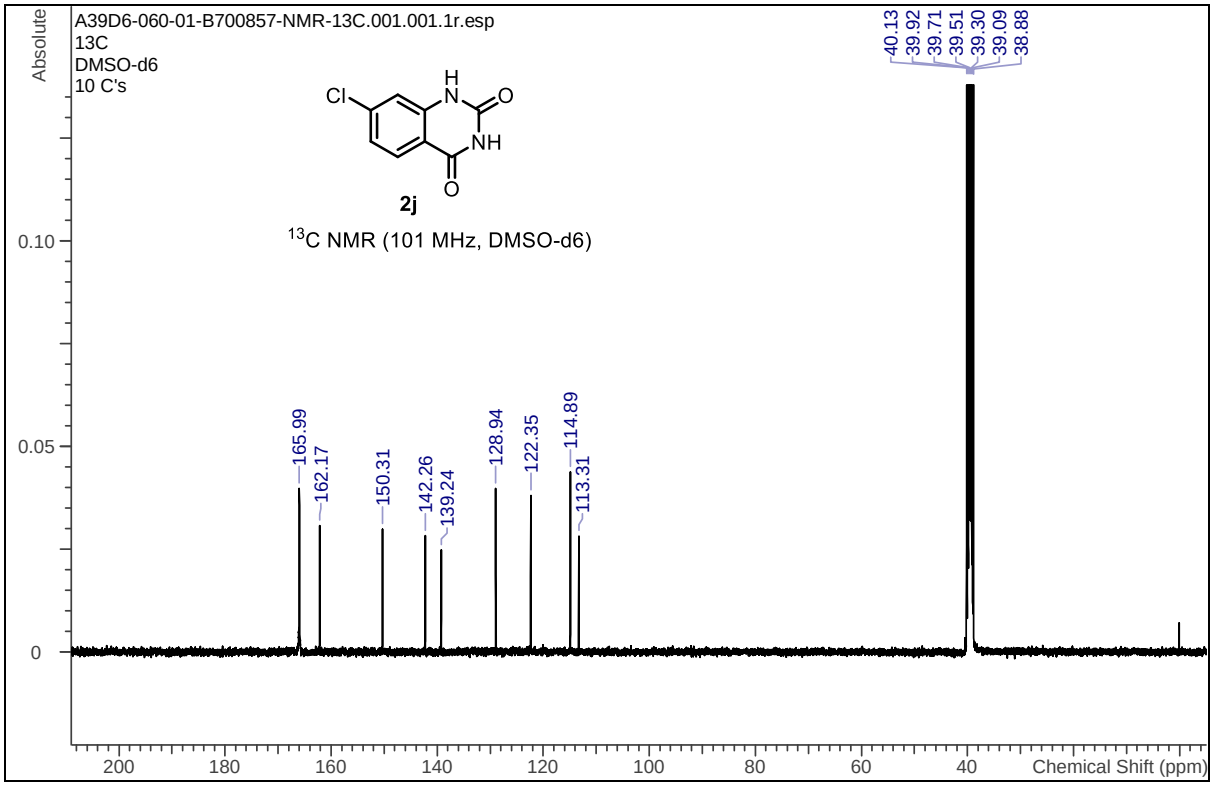
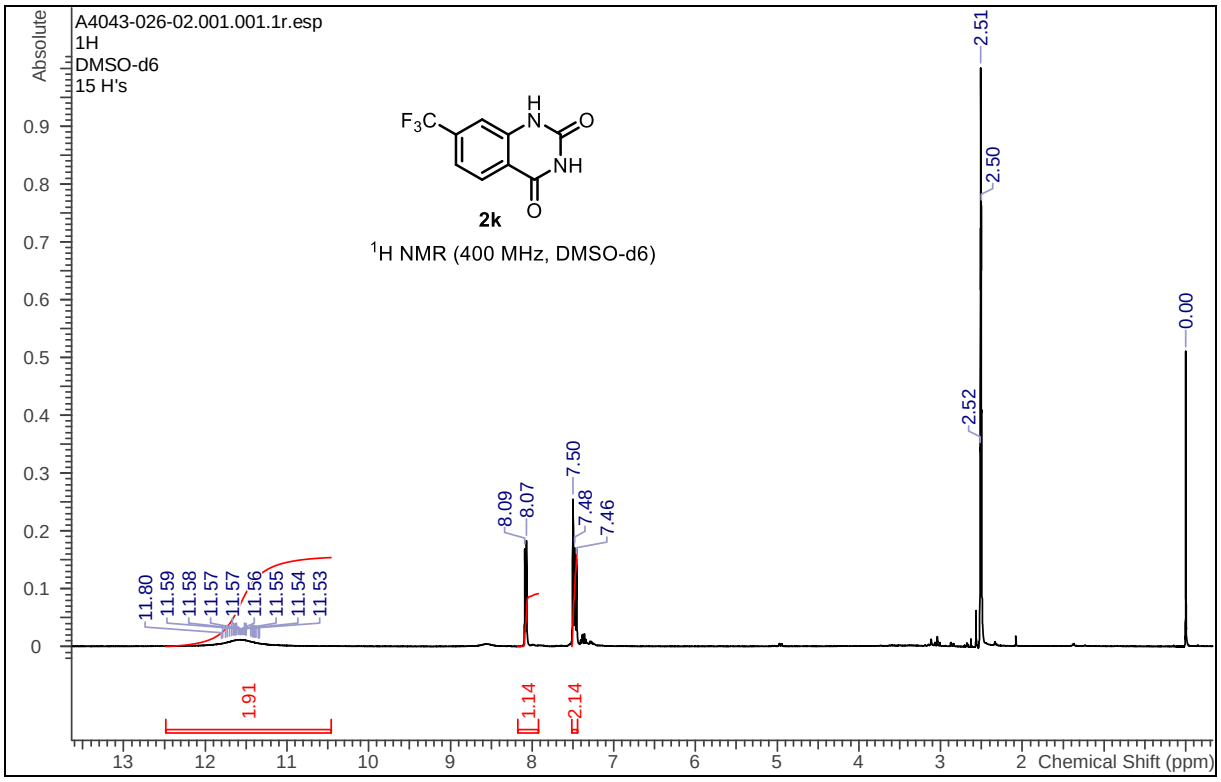
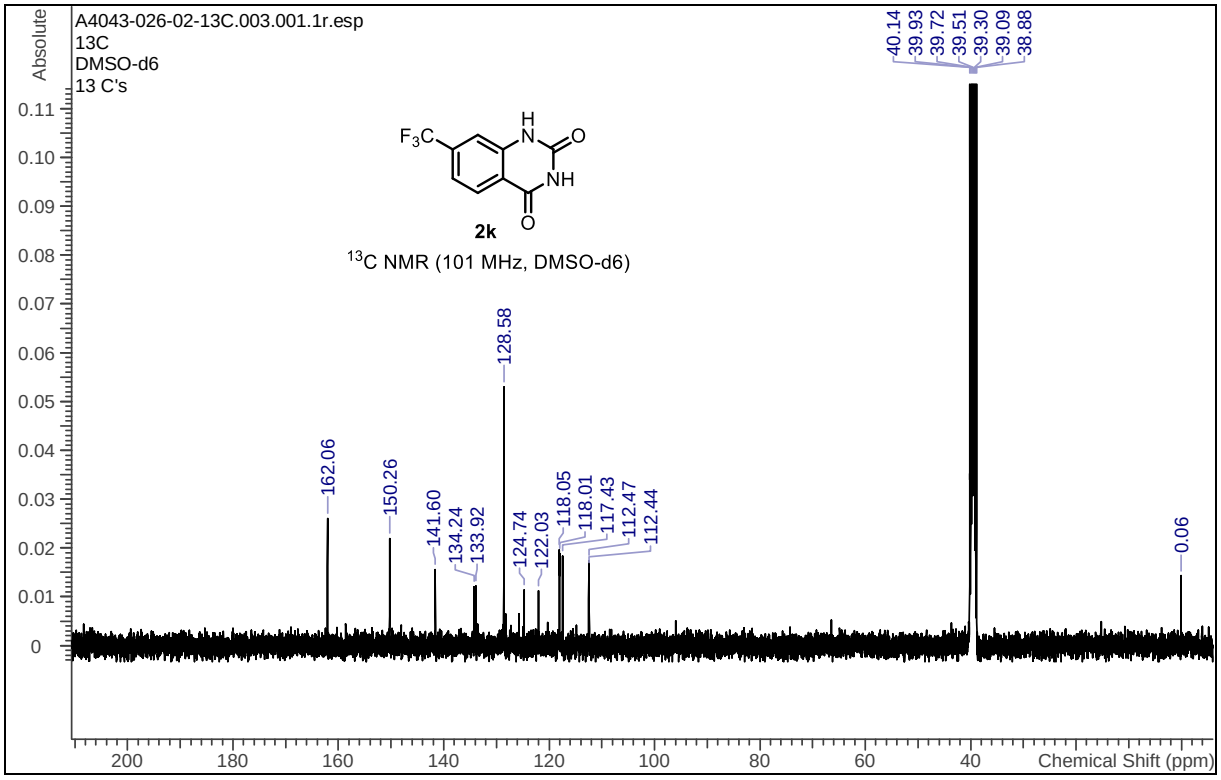
130.12
111.33
110.38
110.15
101.62
101.36

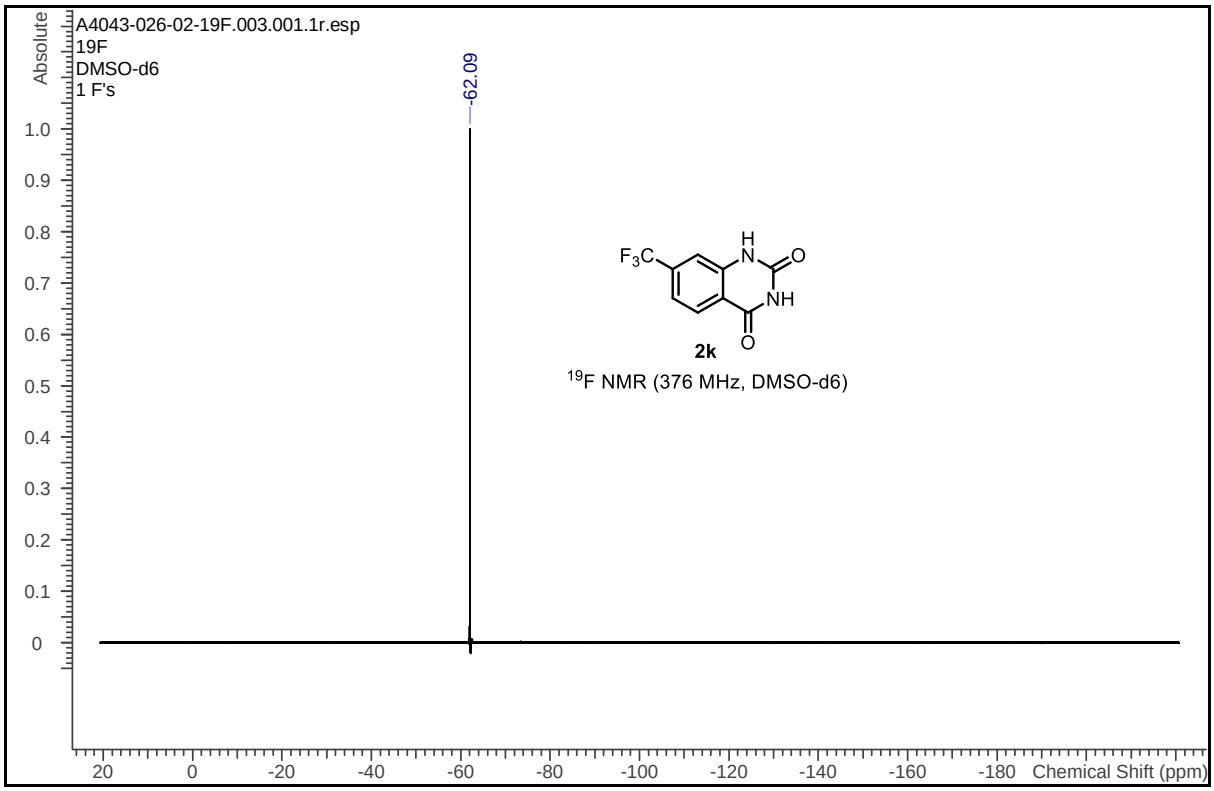

A4043-034-02-19F.001.001.1r.esp
19F
DMSO-d6
1 F's
Absolute
-103.51
2i
19F NMR (376 MHz, DMSO-d6)
Chemical Shift (ppm)

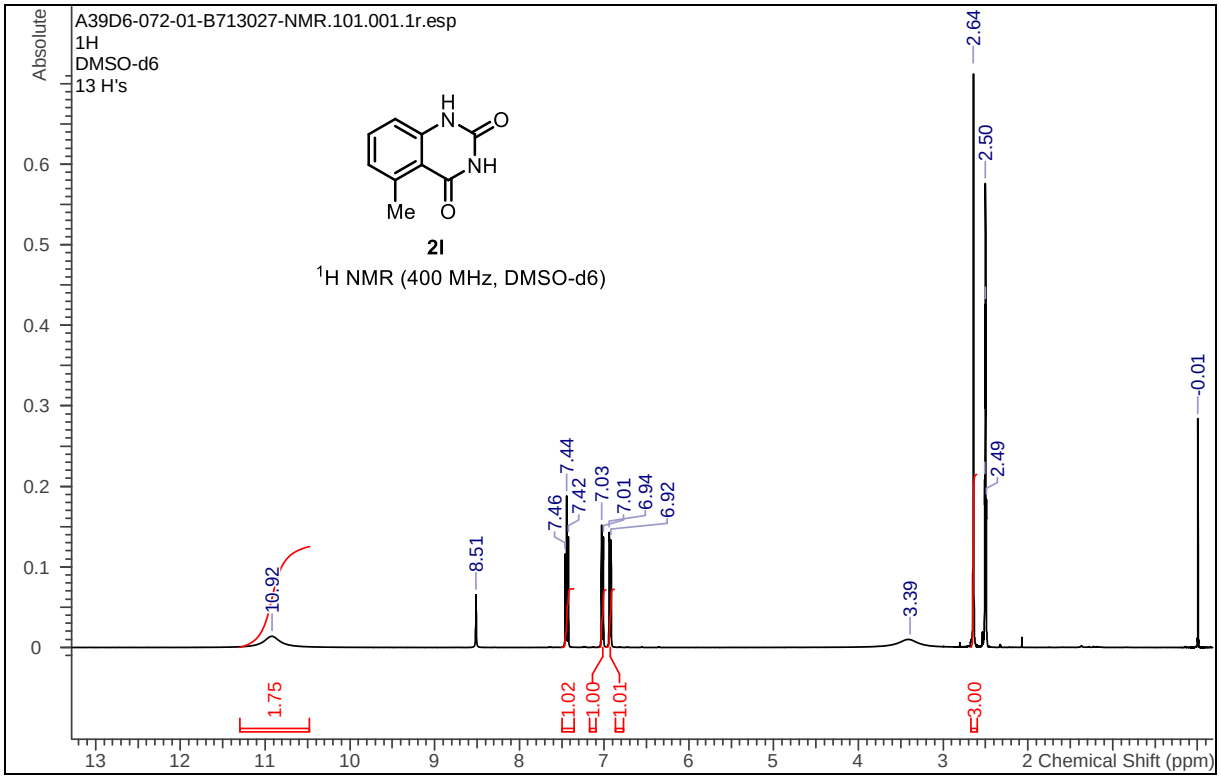

A39D6-060-01-B702627-NMR.101.jdx
1H
DMSO-d6
55 H's
Absolute
3.31
2.51
2.51
2.50
2.49
0.00
11.38
11.37
11.33
11.32
11.25
11.24
11.19
11.15
11.08
7.60
7.60
7.57
7.55
7.54
7.53
7.21
7.18
2.01
2.00
1.13
2j
1H NMR (400 MHz, DMSO-d6)
Chemical Shift (ppm)

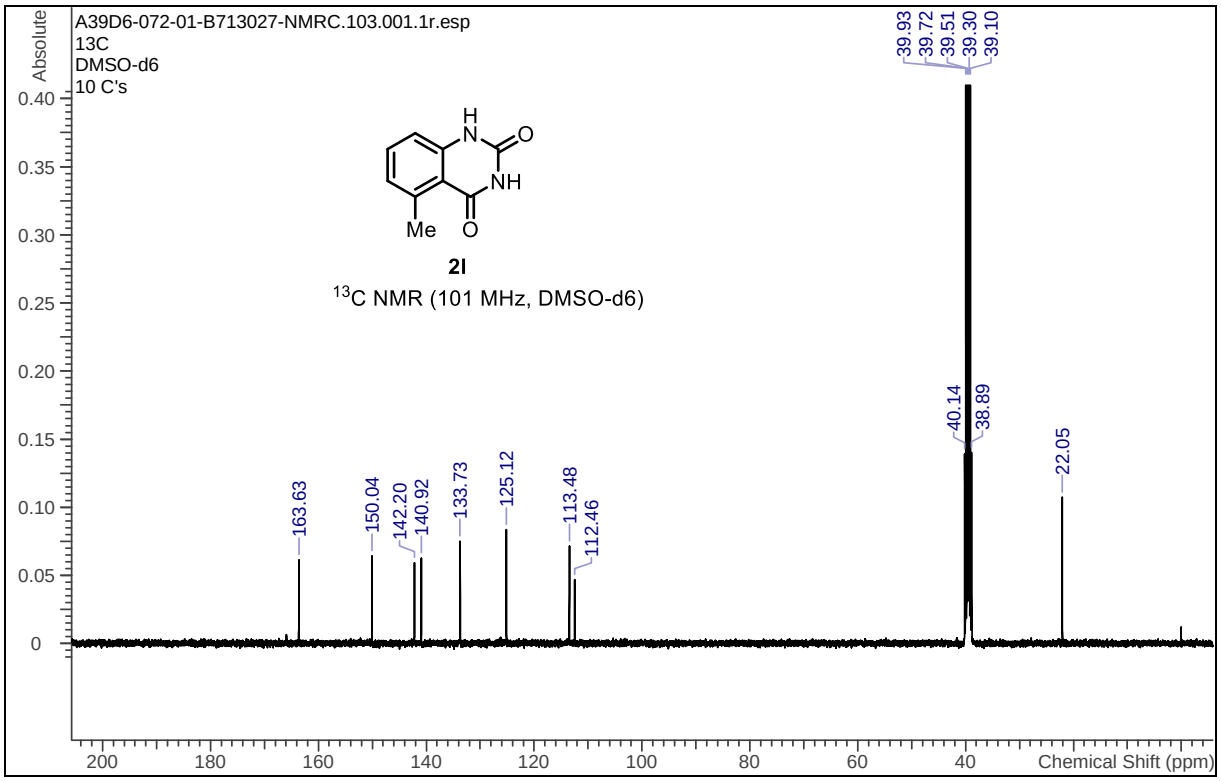

A39D6-060-01-B700857-NMR-13C.001.001.1r.esp
13C
DMSO-d6
10 C's
Absolute
Cl
H
N
O
NH
O
2j
^{13}C NMR (101 MHz, DMSO-d6)
40.13
39.92
39.71
39.51
39.30
39.09
38.88
165.99
162.17
150.31
142.26
139.24
128.94
122.35
114.89
113.31
0.10
0.05
0
200
180
160
140
120
100
80
60
40
Chemical Shift (ppm)

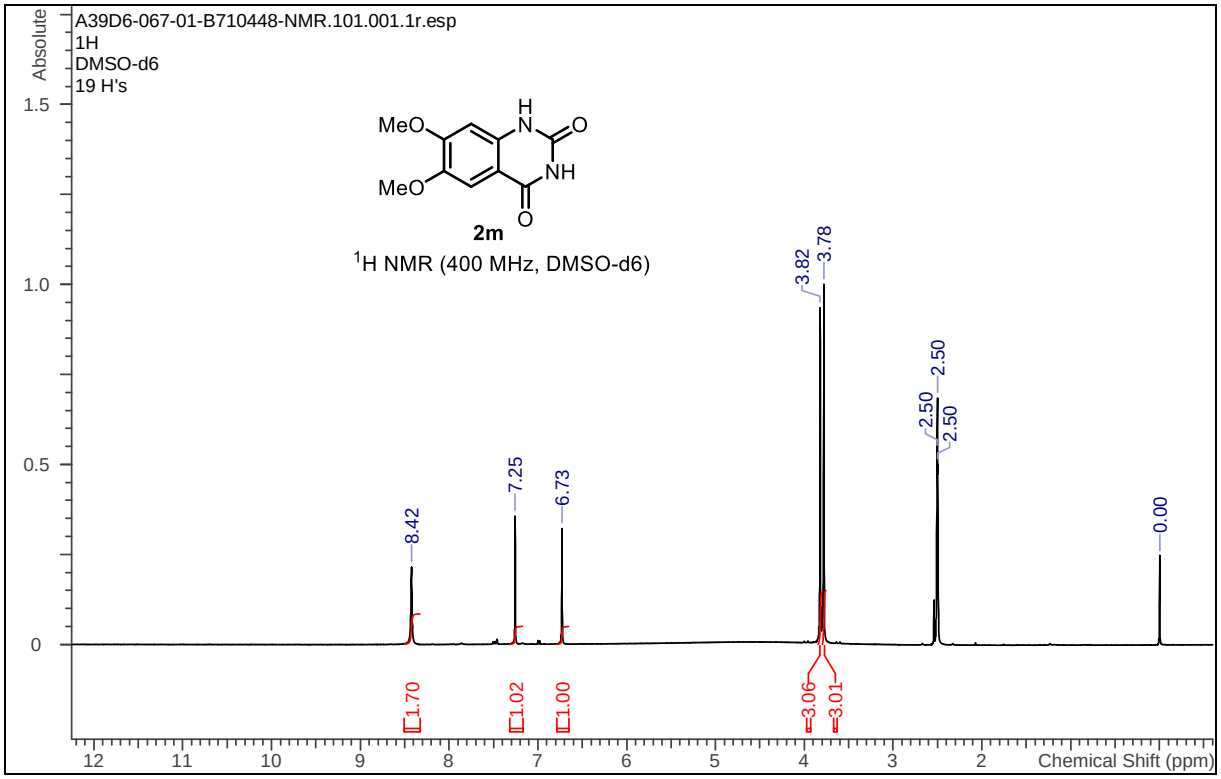

A4043-026-02.001.001.1r.esp
1H
DMSO-d6
15 H's
Absolute
F_3C
H
N
O
NH
O
2k
^{1}H NMR (400 MHz, DMSO-d6)
2.51
2.50
2.52
0.00
8.09
8.07
7.50
7.48
7.46
11.80
11.59
11.58
11.57
11.57
11.56
11.55
11.54
11.53
1.91
1.14
2.14
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
13
12
11
10
9
8
7
6
5
4
3
2
Chemical Shift (ppm)

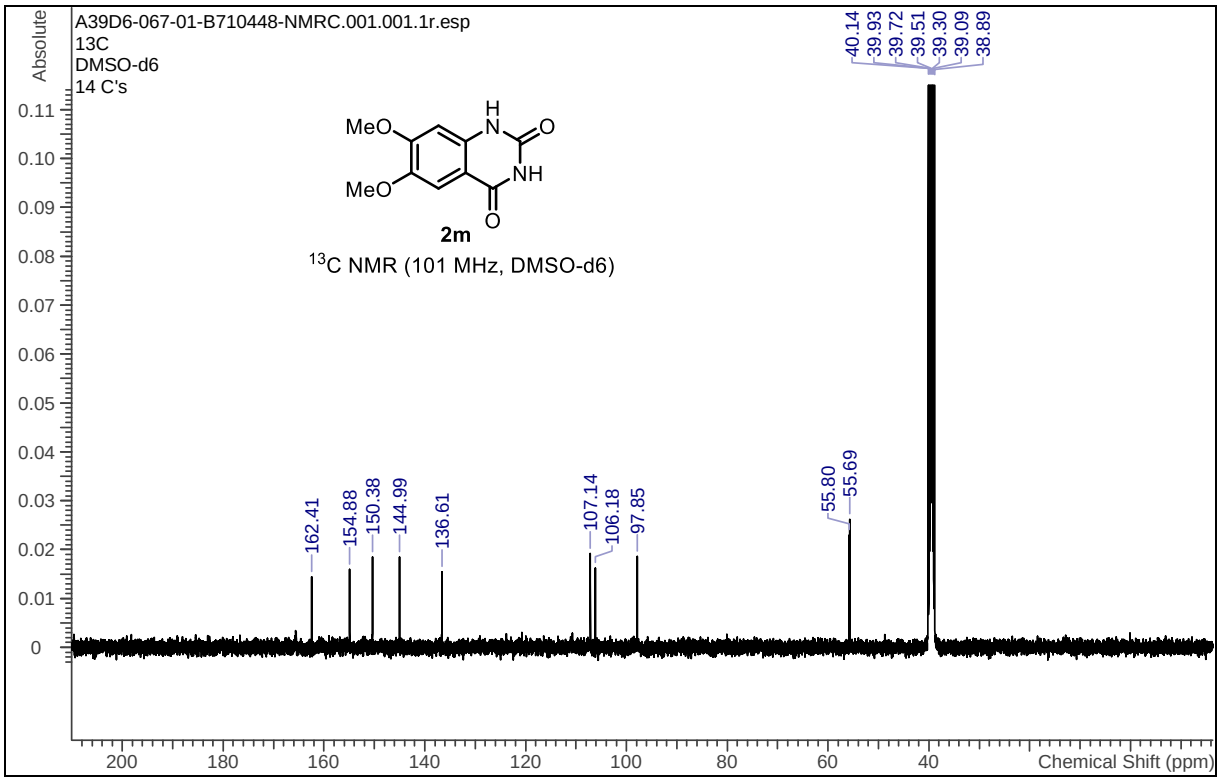

A4043-026-02-13C.003.001.1r.esp
13C
DMSO-d6
13 C's
Absolute
40.14
39.93
39.72
39.51
39.30
39.09
38.88
128.58
162.06
150.26
141.60
134.24
133.92
124.74
122.03
118.05
118.01
117.43
112.47
112.44
0.06
2k
13C NMR (101 MHz, DMSO-d6)
Chemical Shift (ppm)

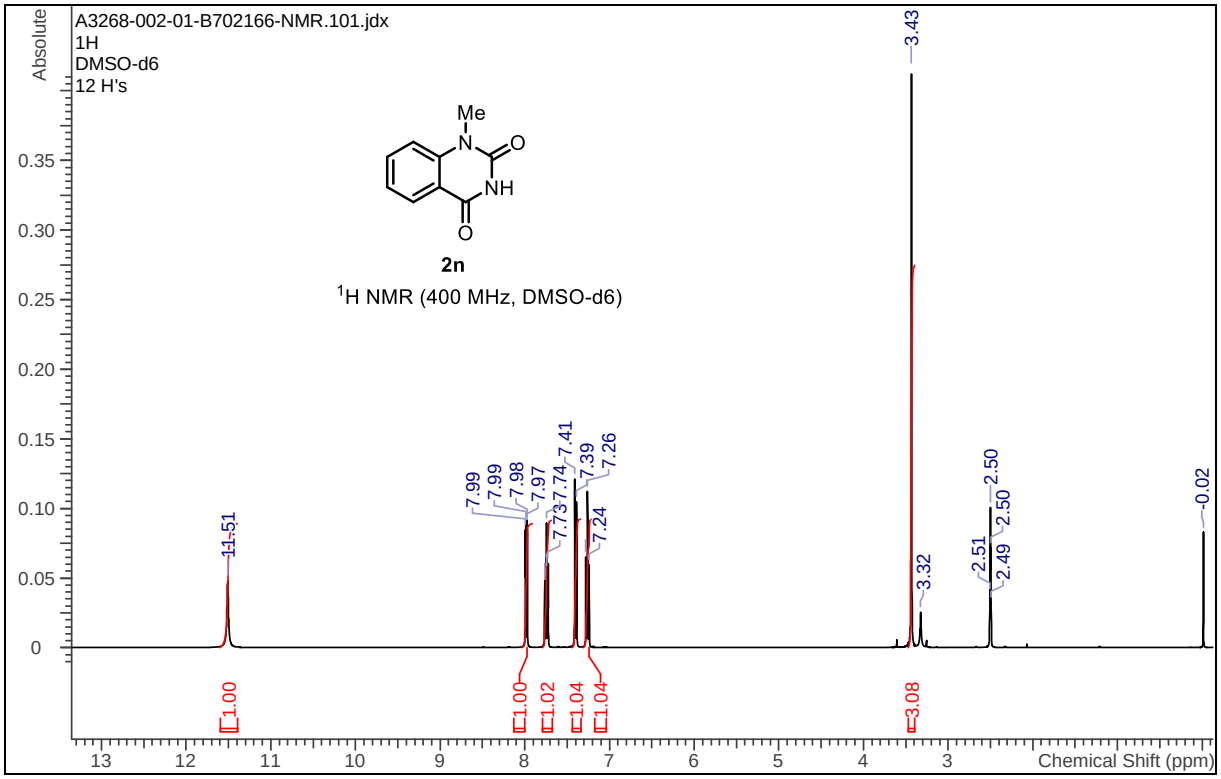

A4043-026-02-19F.003.001.1r.esp
19F
DMSO-d6
1 F's
Absolute
-62.09
2k
19F NMR (376 MHz, DMSO-d6)
Chemical Shift (ppm)

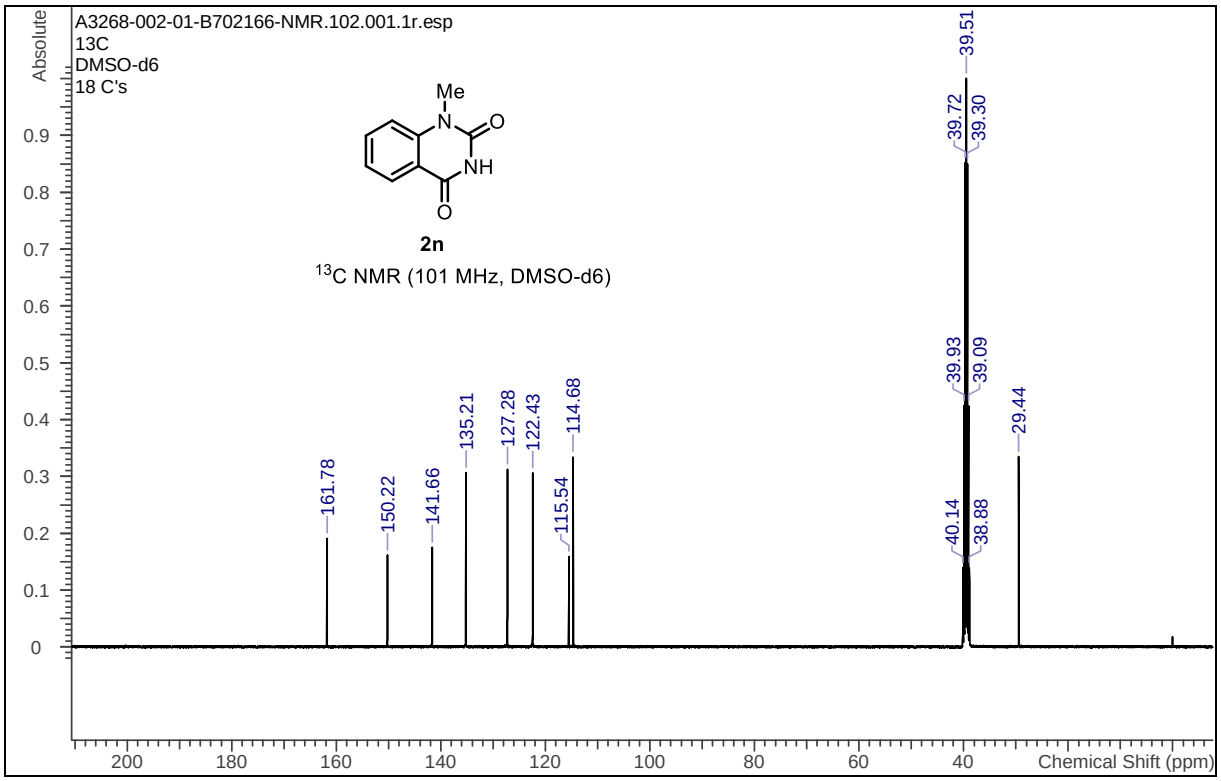

A39D6-072-01-B713027-NMR.101.001.1r.esp
1H
DMSO-d6
13 H's
2l
1H NMR (400 MHz, DMSO-d6)
Absolute
2.64
2.50
2.49
0.01
10.92
8.51
7.46
7.44
7.42
7.03
7.01
6.94
6.92
3.39
1.75
1.02
1.00
1.01
3.00
2 Chemical Shift (ppm)

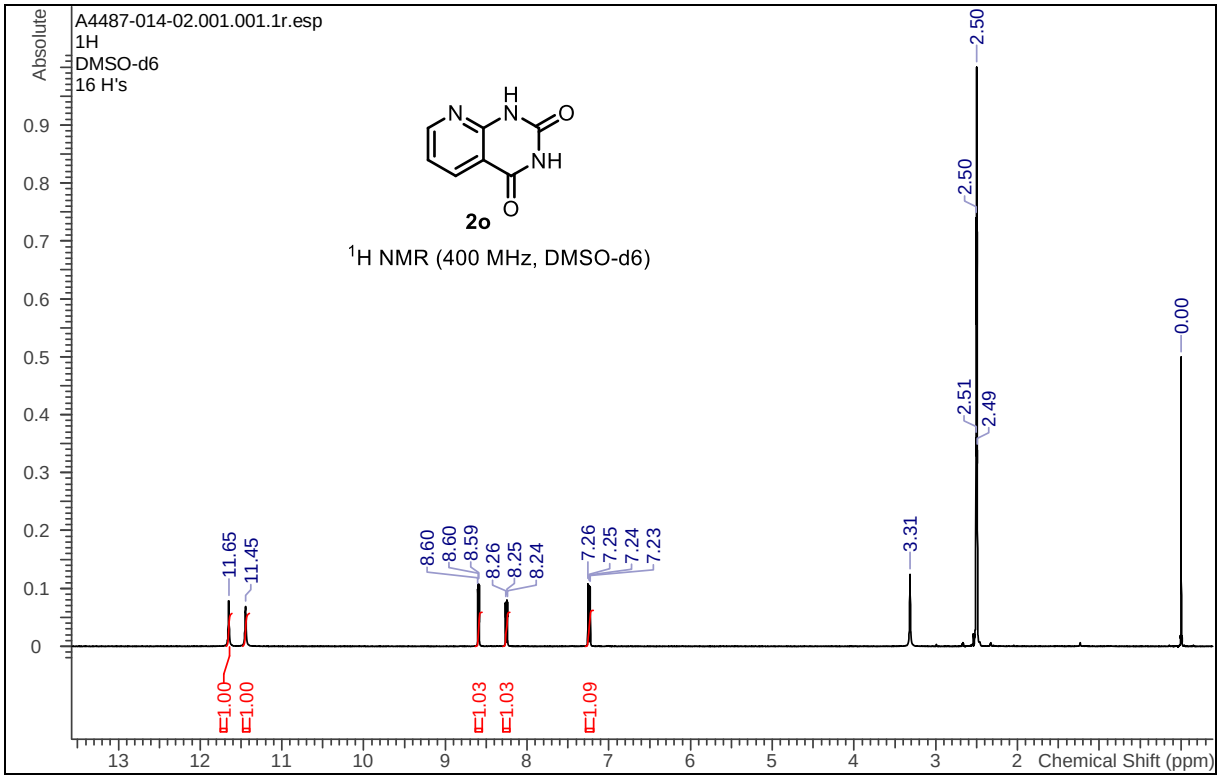

A39D6-072-01-B713027-NMRC.103.001.1r.esp
13C
DMSO-d6
10 C's
2l
13C NMR (101 MHz, DMSO-d6)
Absolute
39.93
39.72
39.51
39.30
39.10
40.14
38.89
22.05
163.63
150.04
142.20
140.92
133.73
125.12
113.48
112.46
Chemical Shift (ppm)

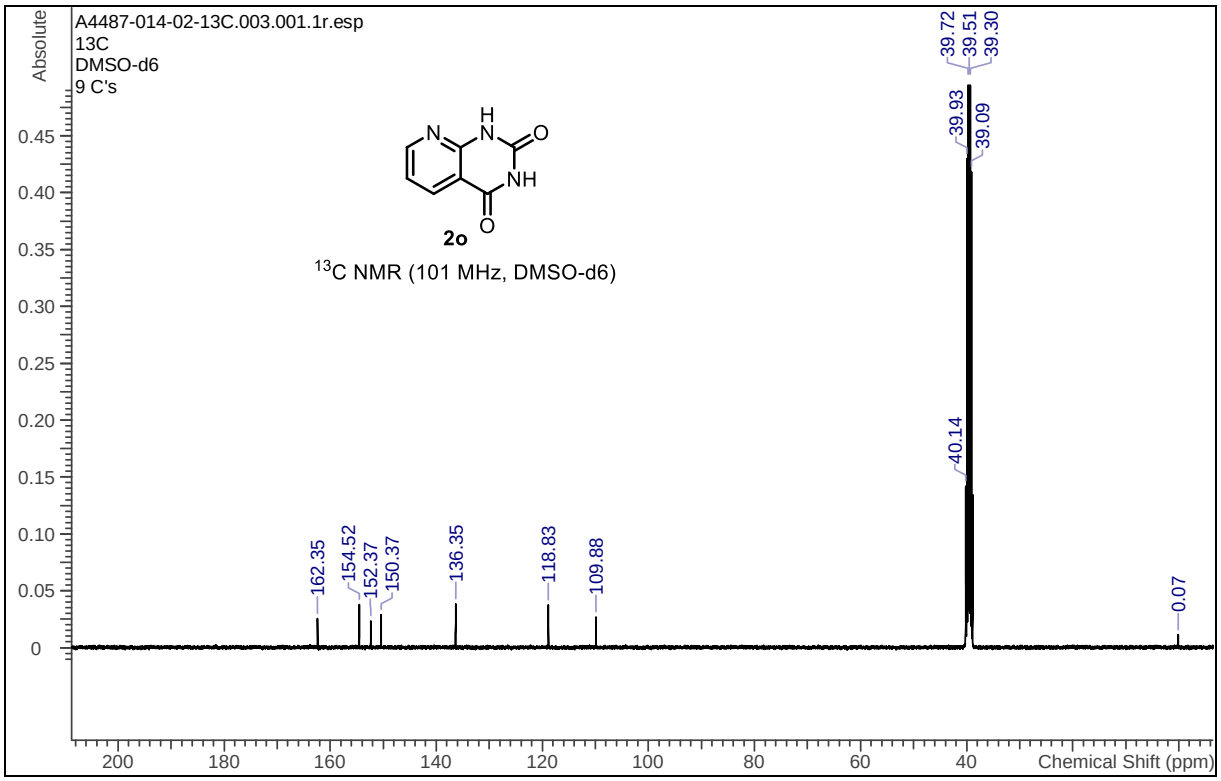

A39D6-067-01-B710448-NMR.101.001.1r.esp
1H
DMSO-d6
19 H's
Absolute
MeO
MeO
H
N
O
NH
O
2m
1H NMR (400 MHz, DMSO-d6)
8.42
7.25
6.73
3.82
3.78
2.50
2.50
2.50
0.00
1.70
1.02
1.00
3.06
3.01
Chemical Shift (ppm)

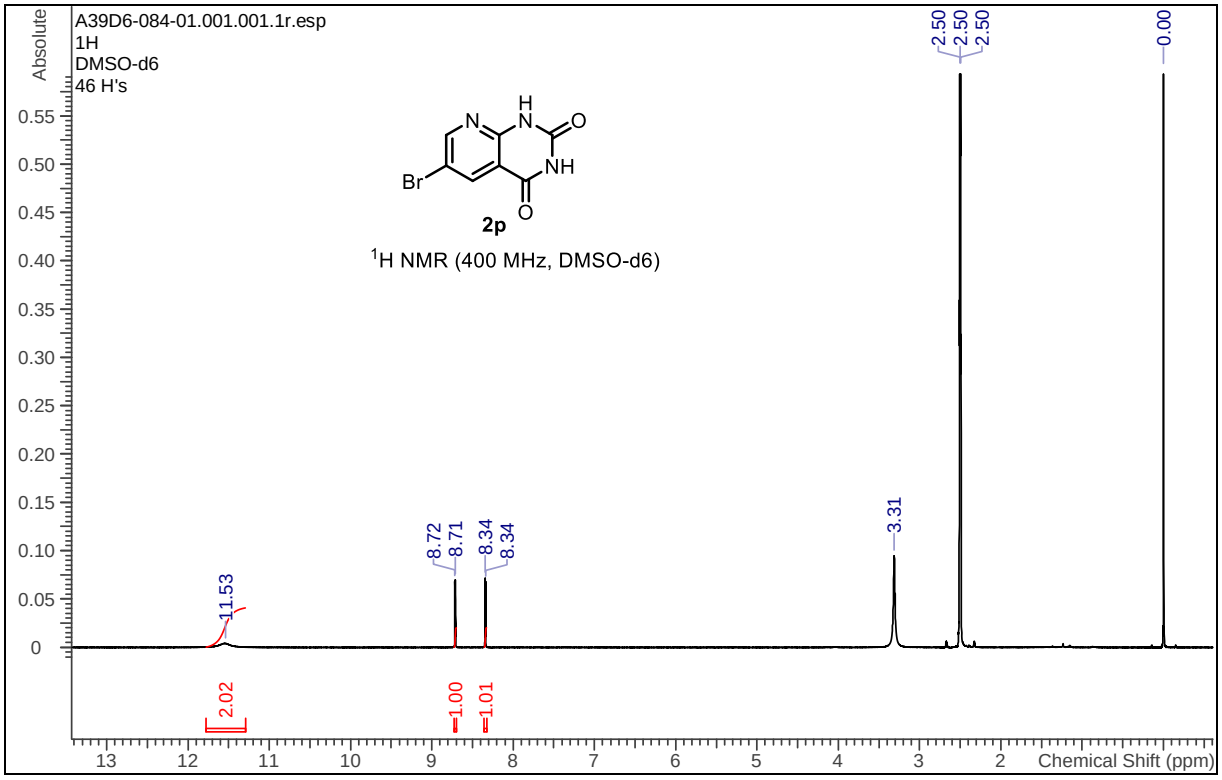

A39D6-067-01-B710448-NMRC.001.001.1r.esp
13C
DMSO-d6
14 C's
Absolute
MeO
MeO
H
N
O
NH
O
2m
13C NMR (101 MHz, DMSO-d6)
40.14
39.93
39.72
39.51
39.30
39.09
38.89
162.41
154.88
150.38
144.99
136.61
107.14
106.18
97.85
55.80
55.69
Chemical Shift (ppm)

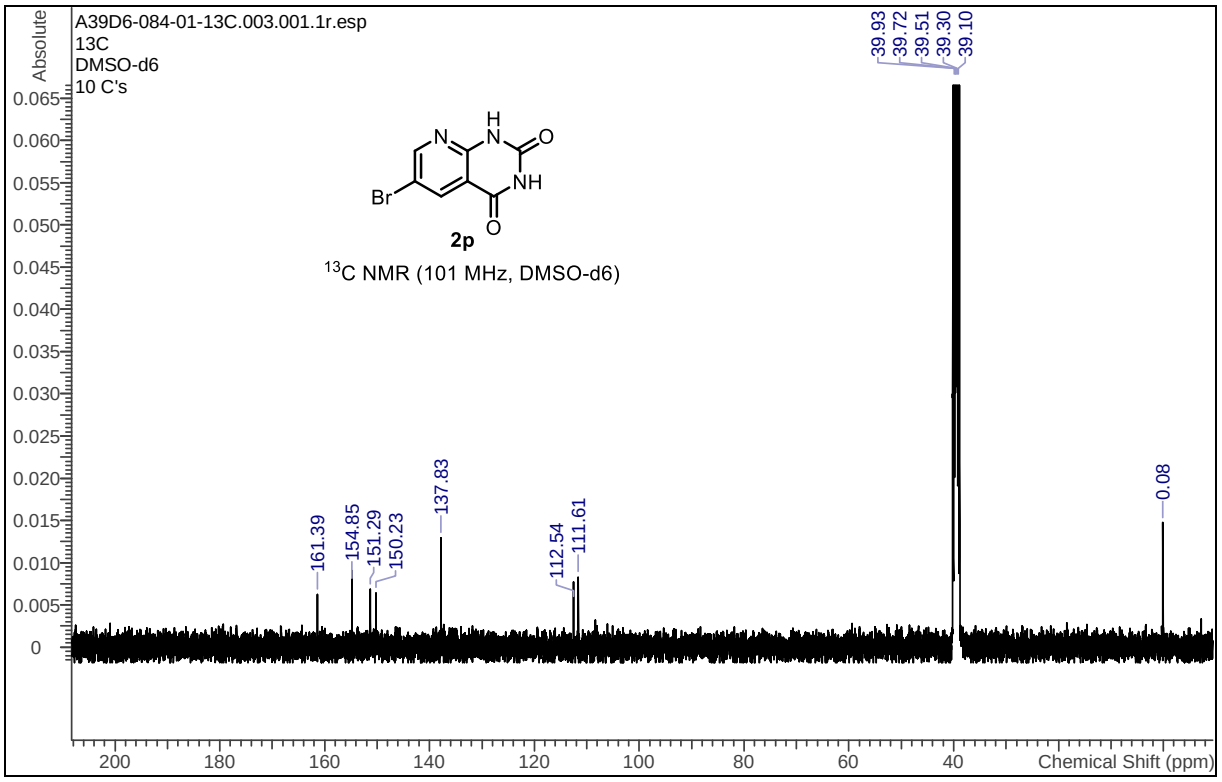

A3268-002-01-B702166-NMR.101.jdx
1H
DMSO-d6
12 H's
Absolute
Me
N
O
NH
O
2n
1H NMR (400 MHz, DMSO-d6)
3.43
11.51
7.99
7.99
7.98
7.97
7.74
7.73
7.41
7.39
7.26
7.24
2.50
2.50
2.51
2.49
3.32
-0.02
1.00
1.00
1.02
1.04
1.04
3.08
Chemical Shift (ppm)

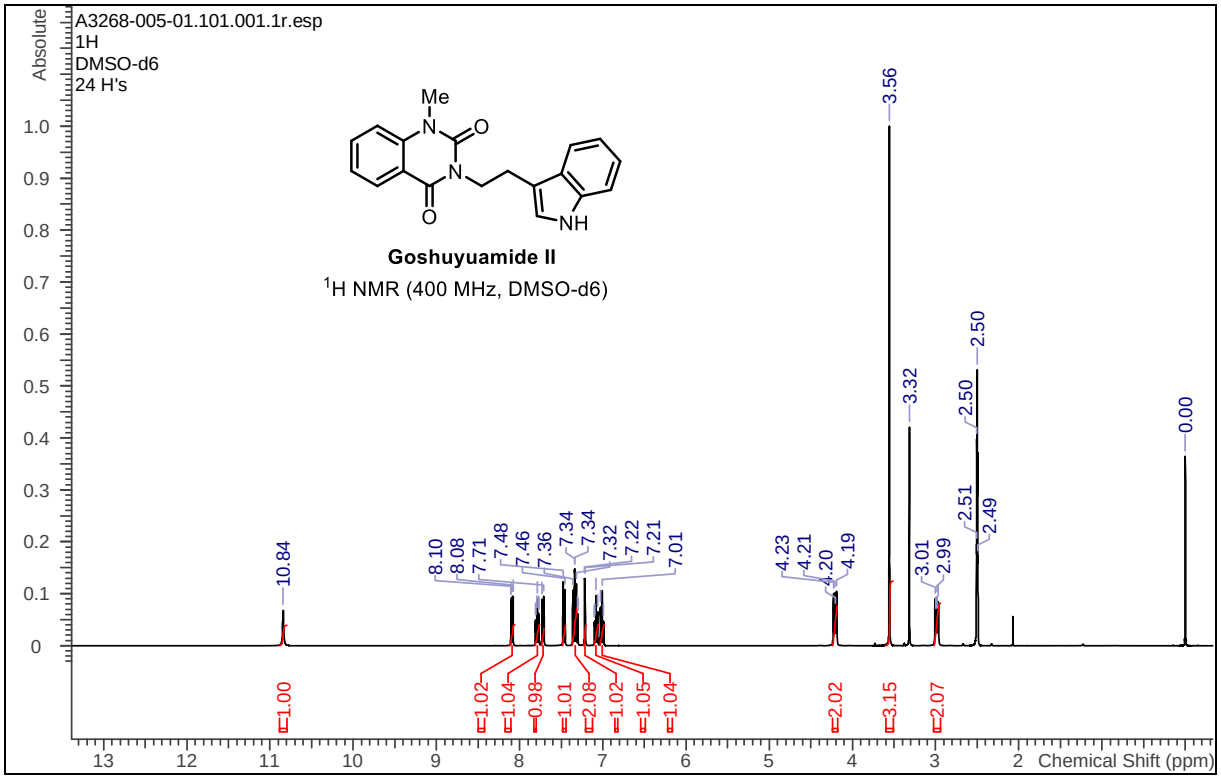

A3268-002-01-B702166-NMR.102.001.1r.esp
13C
DMSO-d6
18 C's
Absolute
Me
N
O
NH
O
2n
13C NMR (101 MHz, DMSO-d6)
39.51
39.72
39.30
39.93
39.09
29.44
40.14
38.88
161.78
150.22
141.66
135.21
127.28
122.43
115.54
114.68
Chemical Shift (ppm)

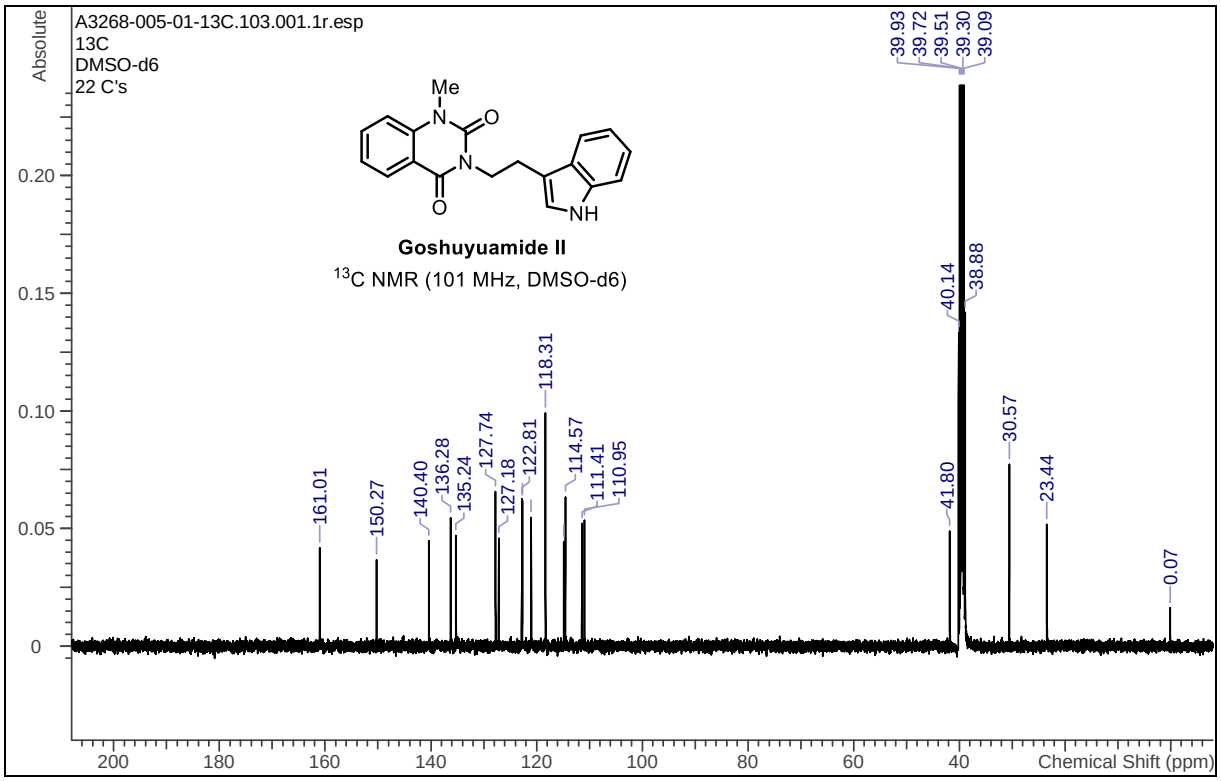

A4487-014-02.001.001.1r.esp
1H
DMSO-d6
16 H's
Absolute
2o
^{1}H NMR (400 MHz, DMSO-d6)
11.65
11.45
8.60
8.60
8.59
8.26
8.25
8.24
7.26
7.25
7.24
7.23
3.31
2.50
2.50
2.51
2.49
0.00
1.00
1.00
1.03
1.03
1.09
Chemical Shift (ppm)

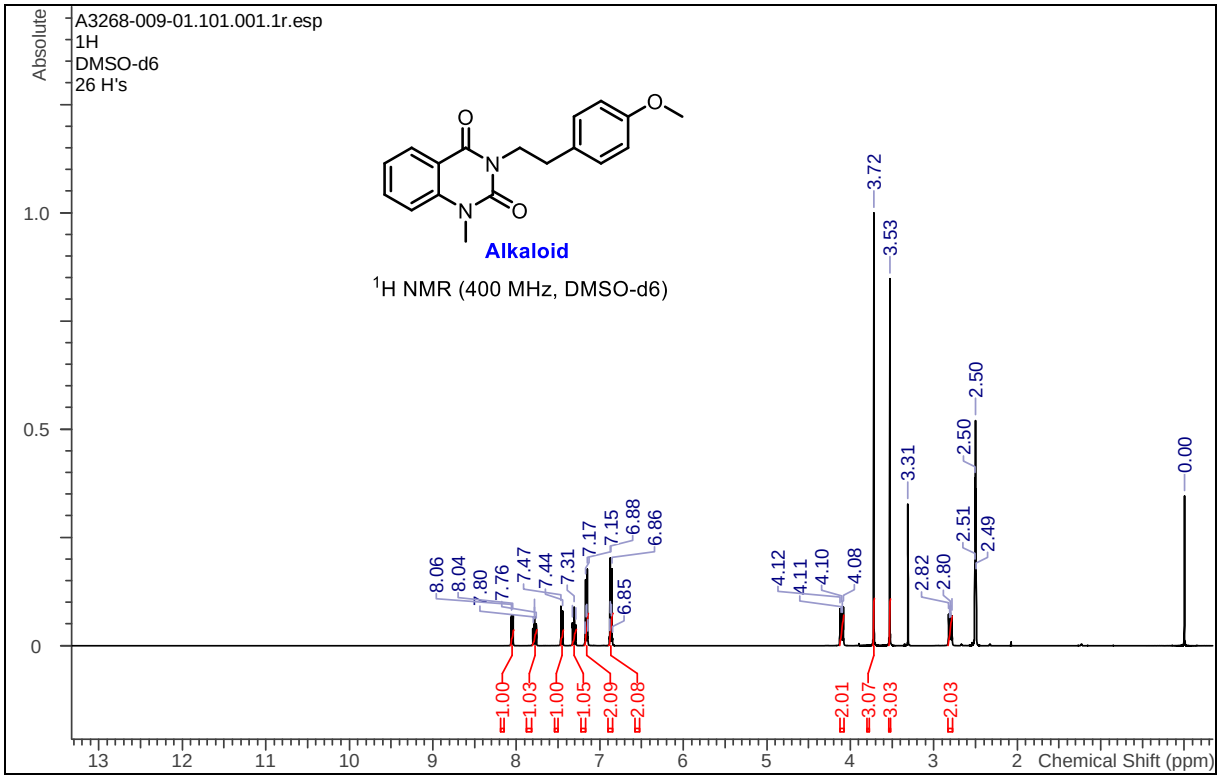

A4487-014-02-13C.003.001.1r.esp
13C
DMSO-d6
9 C's
Absolute
2o
^{13}C NMR (101 MHz, DMSO-d6)
39.72
39.51
39.30
39.93
39.09
40.14
162.35
154.52
152.37
150.37
136.35
118.83
109.88
0.07
Chemical Shift (ppm)

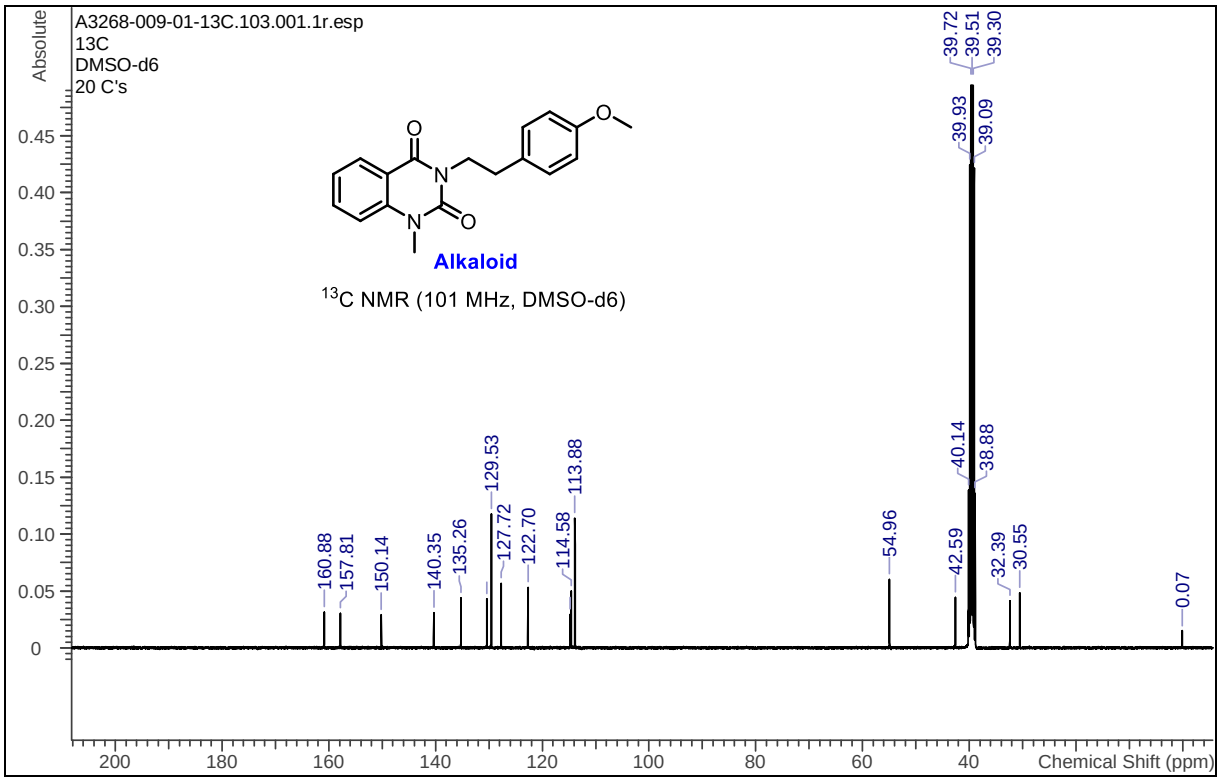

A39D6-084-01.001.001.1r.esp
1H
DMSO-d6
46 H's
Absolute
2.50
2.50
2.50
0.00
11.53
8.72
8.71
8.34
8.34
3.31
2.02
1.00
1.01
Chemical Shift (ppm)

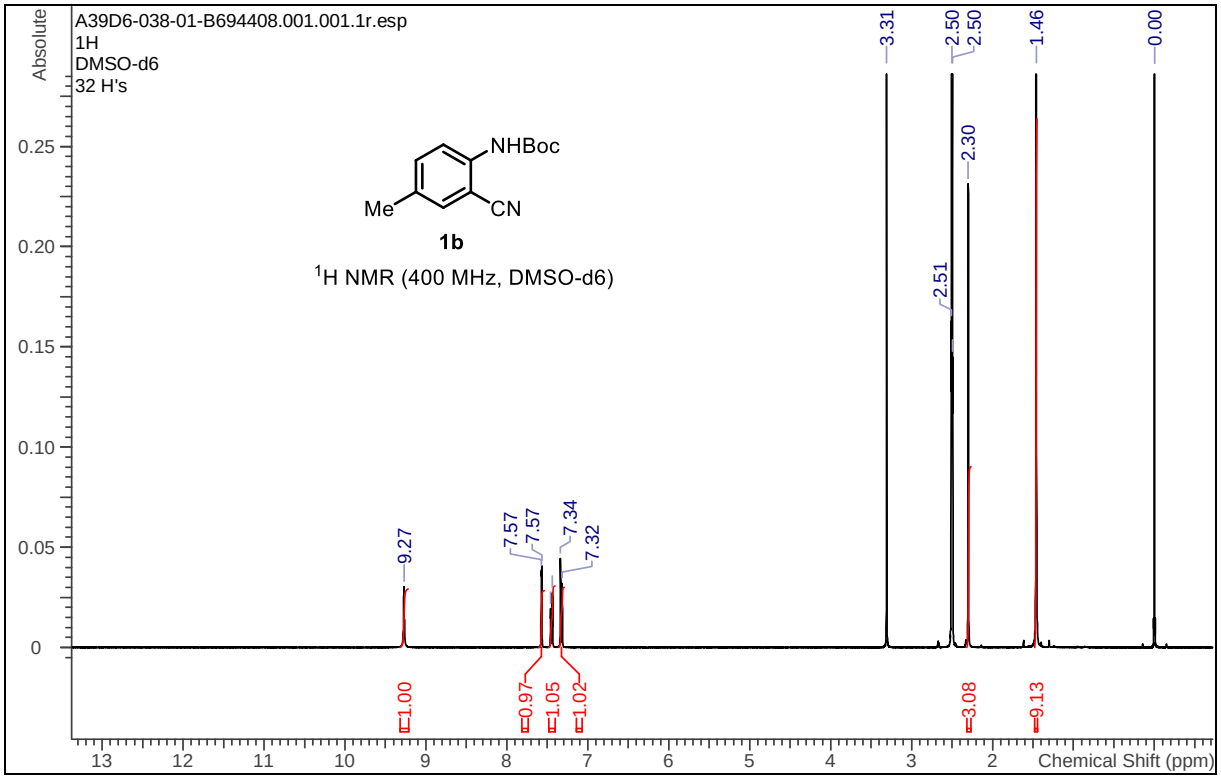

A39D6-084-01-13C.003.001.1r.esp
13C
DMSO-d6
10 C's
Absolute
39.93
39.72
39.51
39.30
39.10
161.39
154.85
151.29
150.23
137.83
112.54
111.61
0.08
Chemical Shift (ppm)

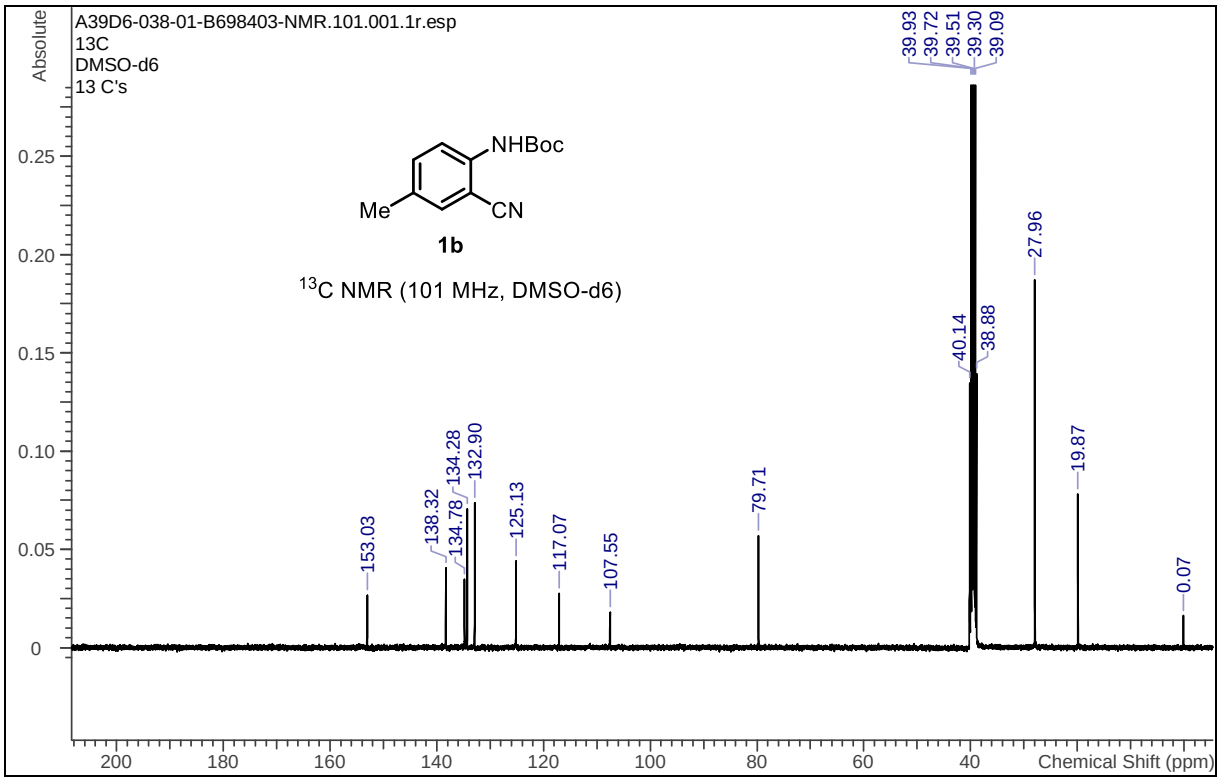

A3268-005-01.101.001.1r.esp
1H
DMSO-d6
24 H's
Absolute
Me
N
O
N
O
NH
Goshuyuamide II
1H NMR (400 MHz, DMSO-d6)
10.84
8.10
8.08
7.71
7.48
7.46
7.36
7.34
7.34
7.32
7.22
7.21
7.01
4.23
4.21
4.20
4.19
3.56
3.32
3.01
2.99
2.50
2.50
2.51
2.49
0.00
1.00
1.02
1.04
0.98
1.01
2.08
1.02
1.05
1.04
2.02
3.15
2.07
Chemical Shift (ppm)

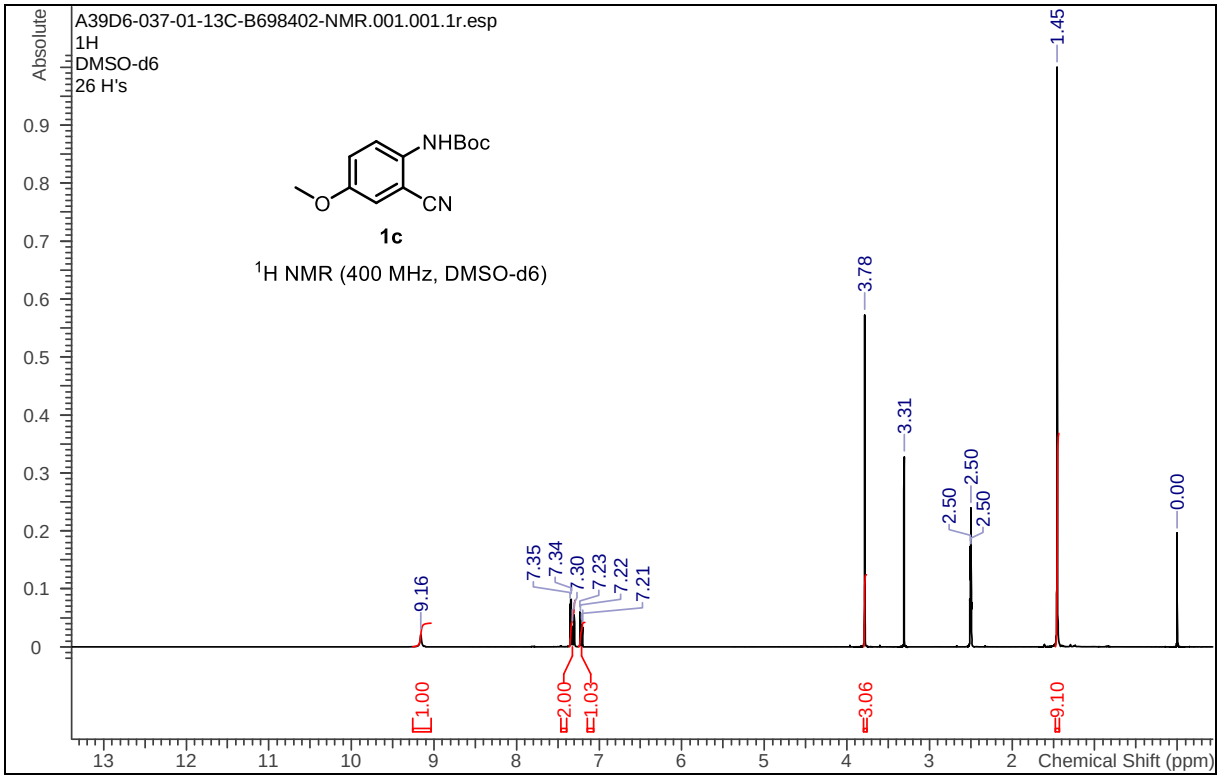

A3268-005-01-13C.103.001.1r.esp
13C
DMSO-d6
22 C's
Absolute
Me
N
O
N
O
NH
Goshuyuamide II
13C NMR (101 MHz, DMSO-d6)
39.93
39.72
39.51
39.30
39.09
40.14
38.88
30.57
23.44
41.80
0.07
161.01
150.27
140.40
136.28
135.24
127.74
127.18
122.81
118.31
114.57
111.41
110.95
Chemical Shift (ppm)

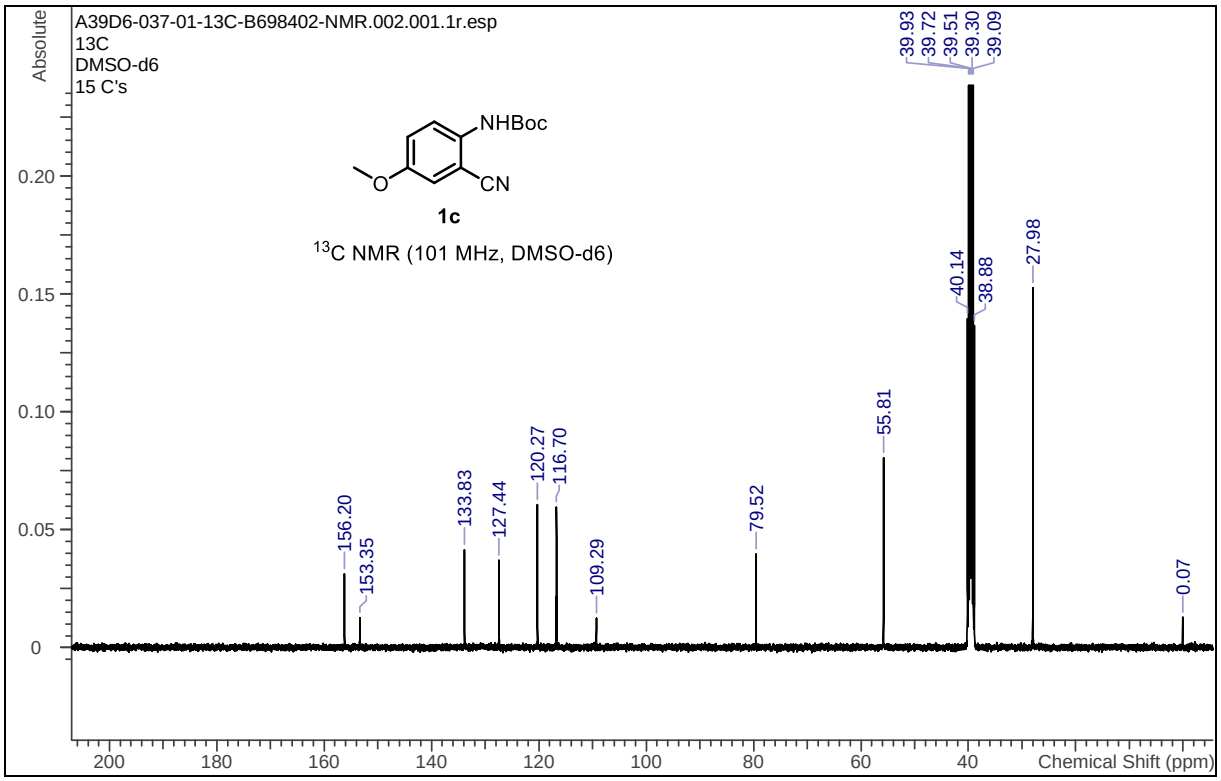

A3268-009-01.101.001.1r.esp
1H
DMSO-d6
26 H's
Absolute
Alkaloid
^{1}H NMR (400 MHz, DMSO-d6)
Chemical Shift (ppm)

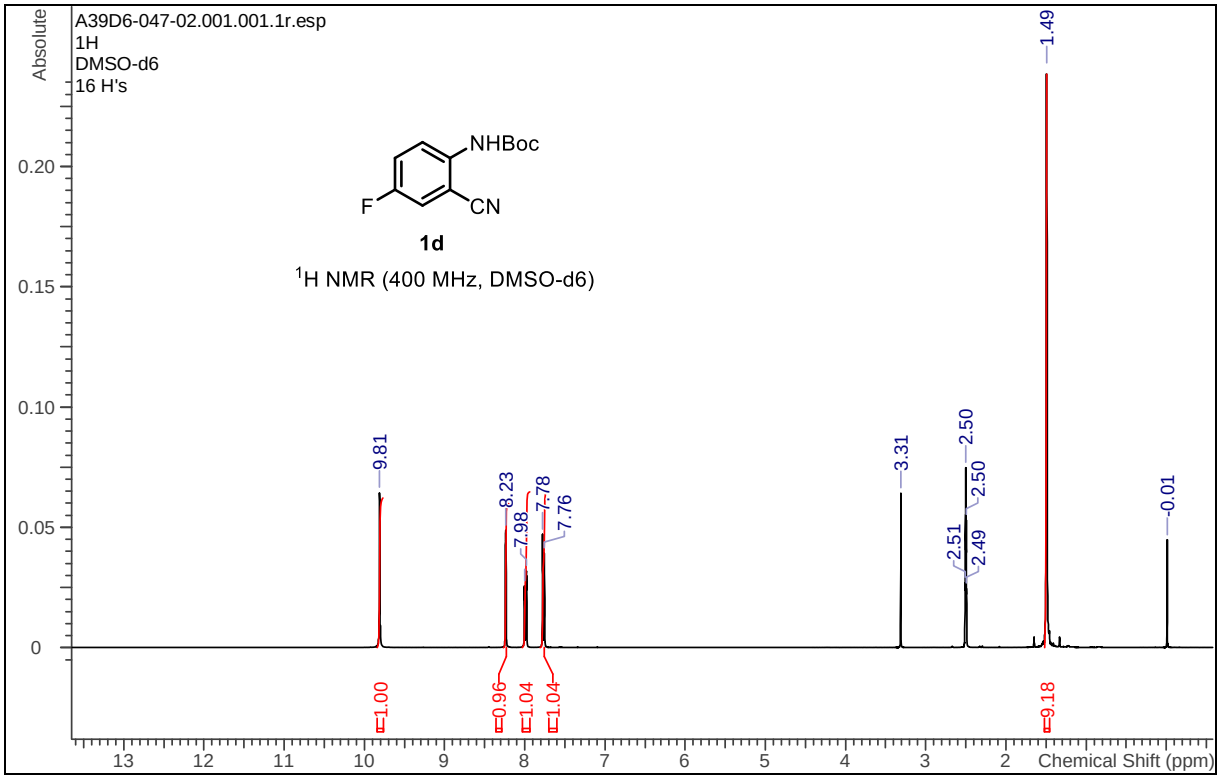

A3268-009-01-13C.103.001.1r.esp
13C
DMSO-d6
20 C's
Absolute
Alkaloid
^{13}C NMR (101 MHz, DMSO-d6)
Chemical Shift (ppm)

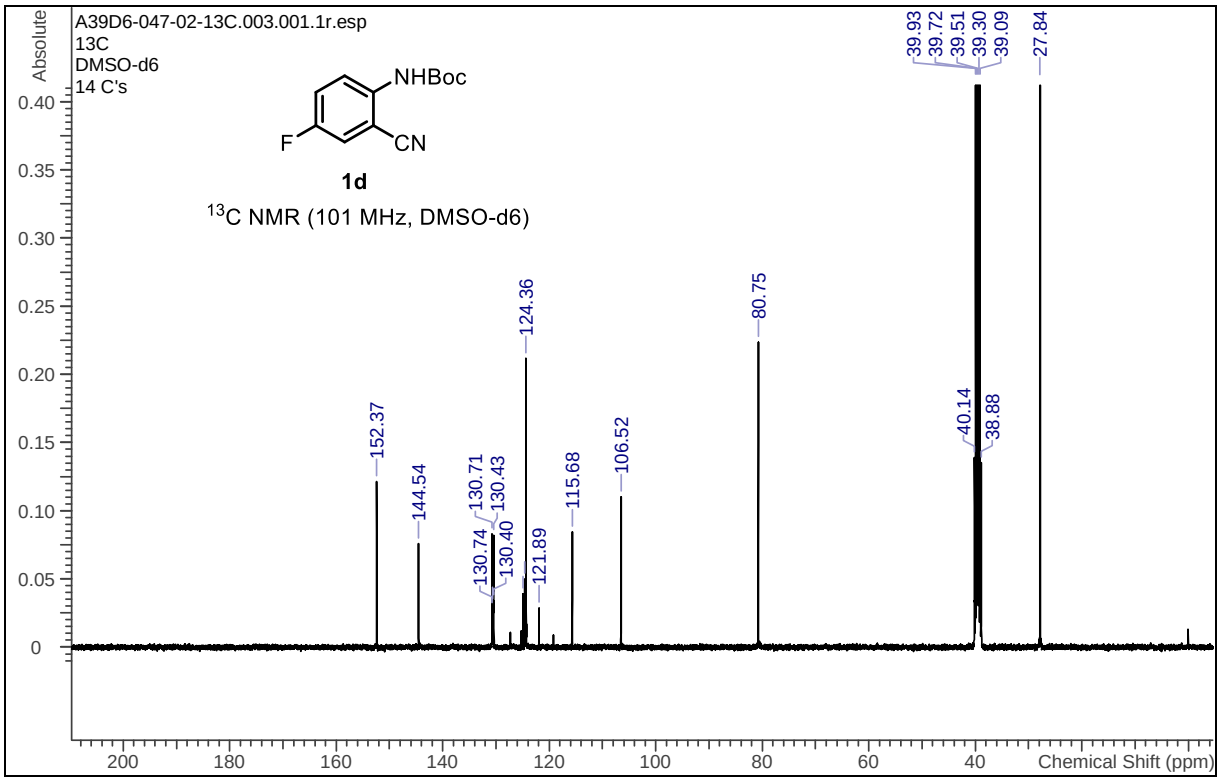

A39D6-038-01-B694408.001.001.1r.esp
1H
DMSO-d6
32 H's
NHBoc
Me
CN
1b
1H NMR (400 MHz, DMSO-d6)
Absolute
Chemical Shift (ppm)
3.31
2.50
2.50
1.46
0.00
2.30
2.51
9.27
7.57
7.57
7.34
7.32
1.00
0.97
1.05
1.02
3.08
9.13

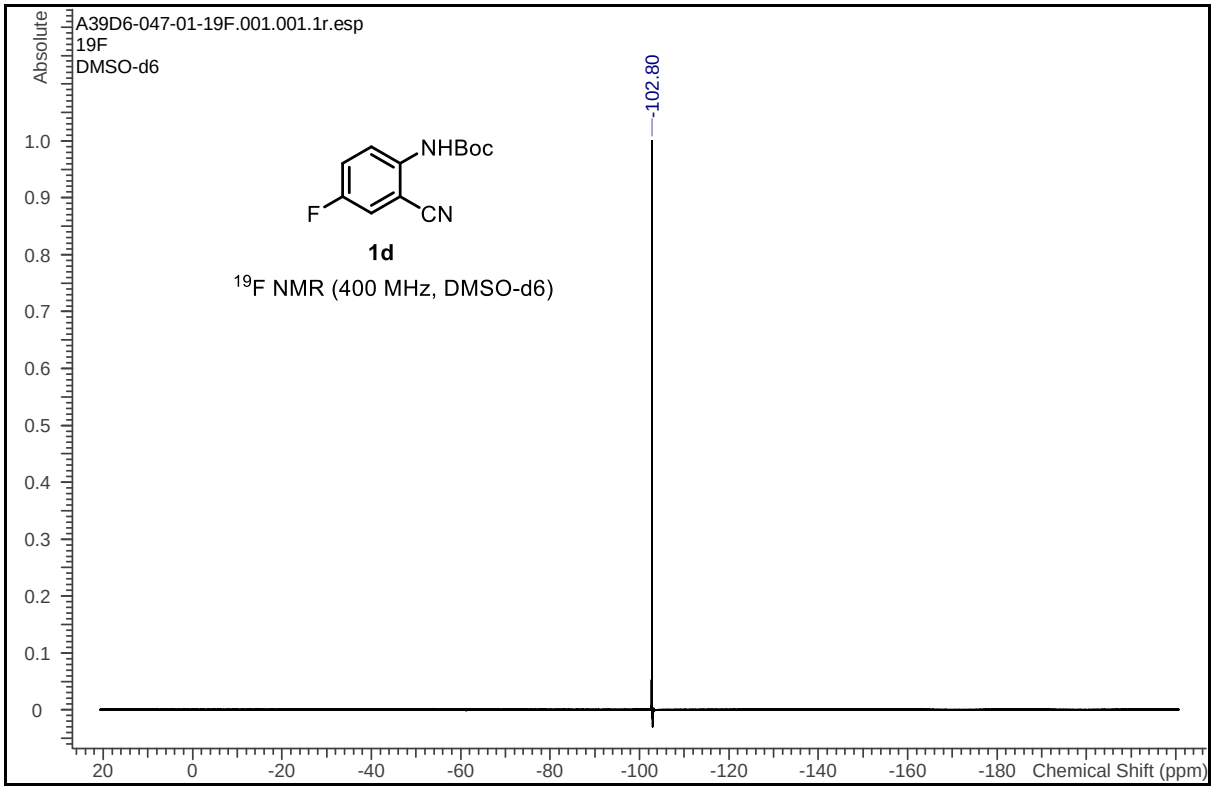

A39D6-038-01-B698403-NMR.101.001.1r.esp
13C
DMSO-d6
13 C's
NHBoc
Me
CN
1b
13C NMR (101 MHz, DMSO-d6)
Absolute
Chemical Shift (ppm)
39.93
39.72
39.51
39.30
39.09
27.96
40.14
38.88
19.87
153.03
138.32
134.78
134.28
132.90
125.13
117.07
107.55
79.71
0.07

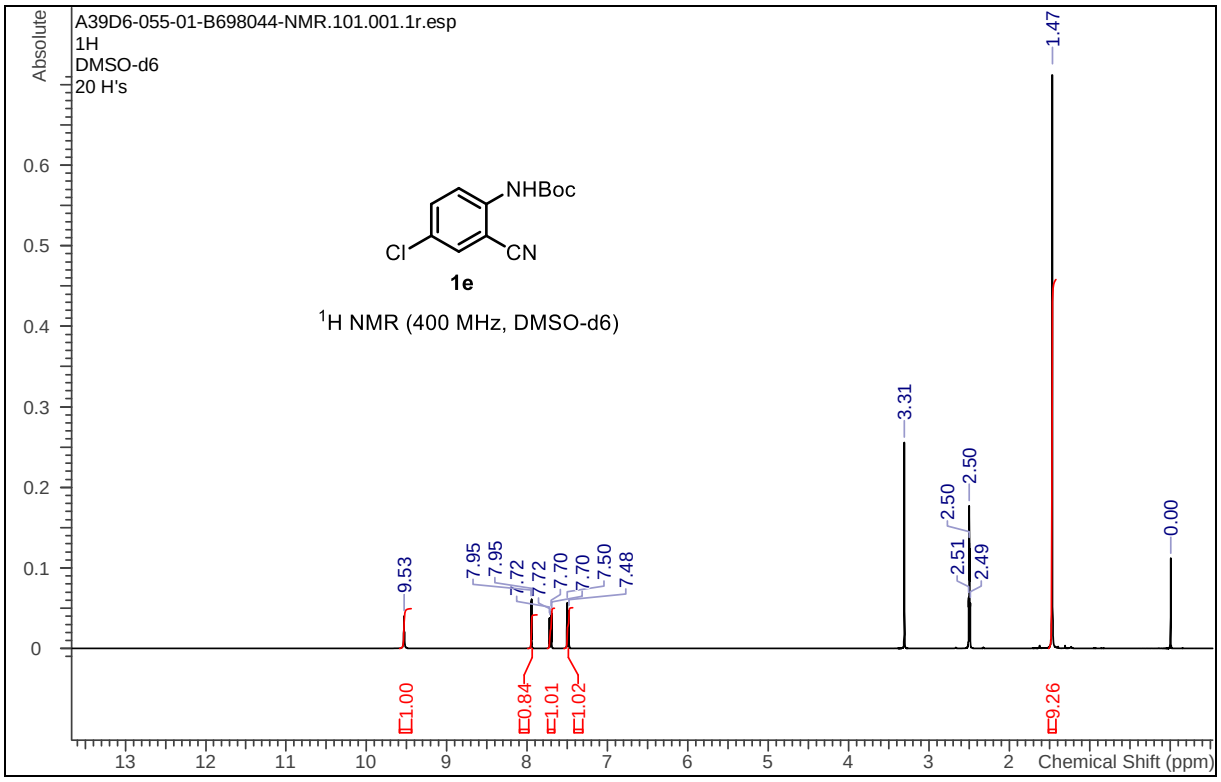

A39D6-037-01-13C-B698402-NMR.001.001.1r.esp
1H
DMSO-d6
26 H's
NHBoc
O
CN
1c
1H NMR (400 MHz, DMSO-d6)
Absolute
Chemical Shift (ppm)
9.16
7.35
7.34
7.30
7.23
7.22
7.21
3.78
3.31
2.50
2.50
2.50
1.45
0.00
1.00
2.00
1.03
3.06
9.10

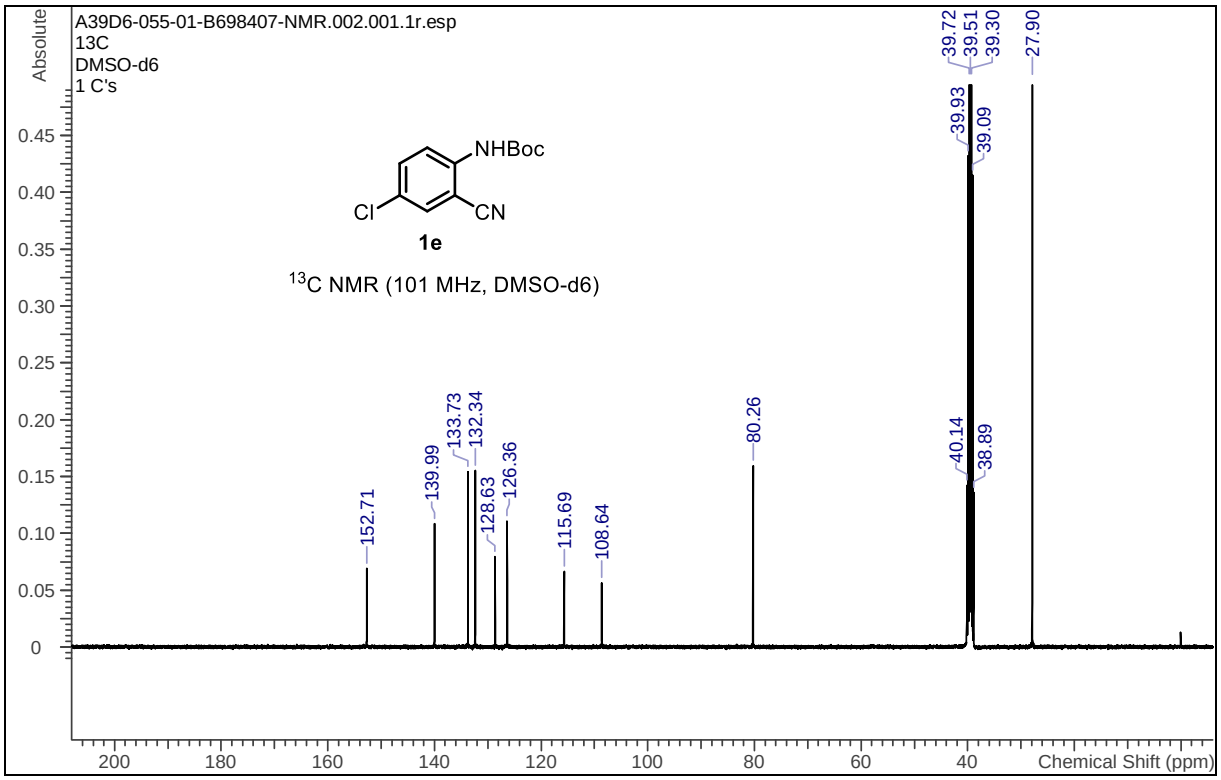

A39D6-037-01-13C-B698402-NMR.002.001.1r.esp
13C
DMSO-d6
15 C's
NHBoc
O
CN
1c
13C NMR (101 MHz, DMSO-d6)
Absolute
Chemical Shift (ppm)
39.93
39.72
39.51
39.30
39.09
40.14
38.88
27.98
55.81
156.20
153.35
133.83
127.44
120.27
116.70
109.29
79.52
0.07

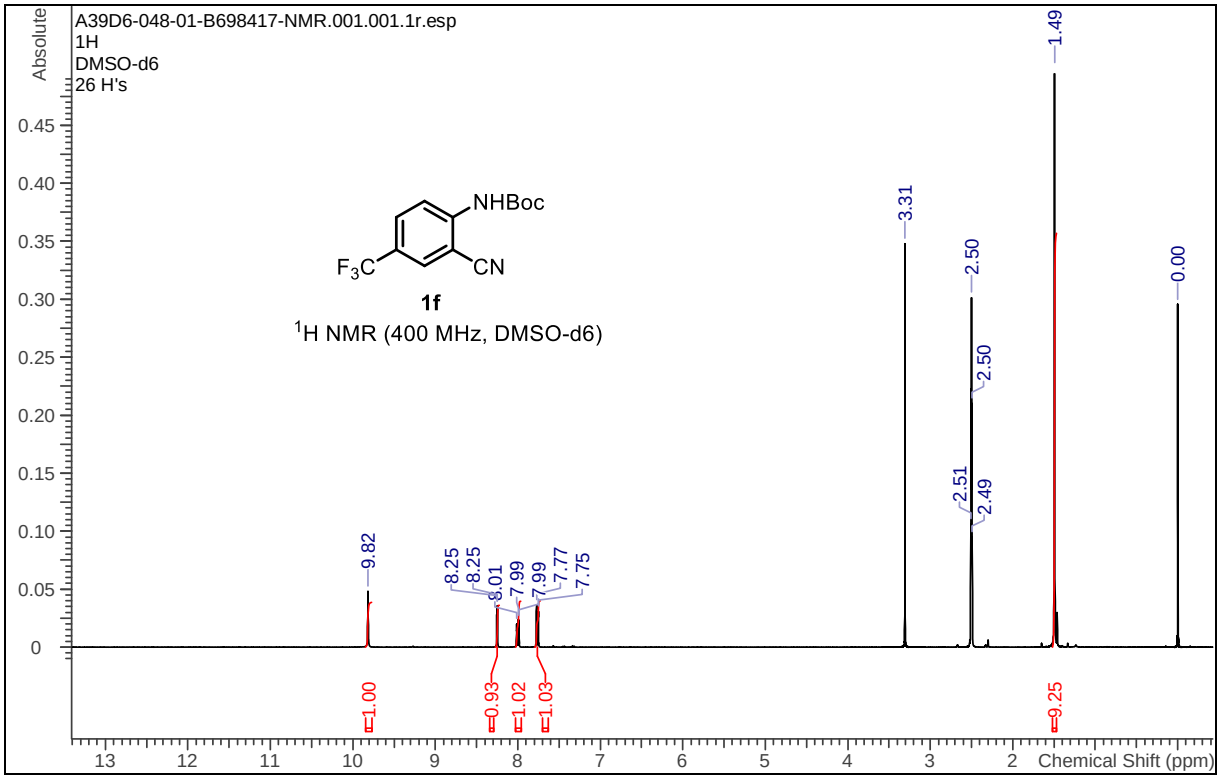

A39D6-047-02.001.001.1r.esp
1H
DMSO-d6
16 H's
NHBoc
F
CN
1d
1H NMR (400 MHz, DMSO-d6)
Absolute
Chemical Shift (ppm)
1.49
9.81
8.23
7.98
7.78
7.76
3.31
2.50
2.50
2.51
2.49
0.01
1.00
0.96
1.04
1.04
9.18

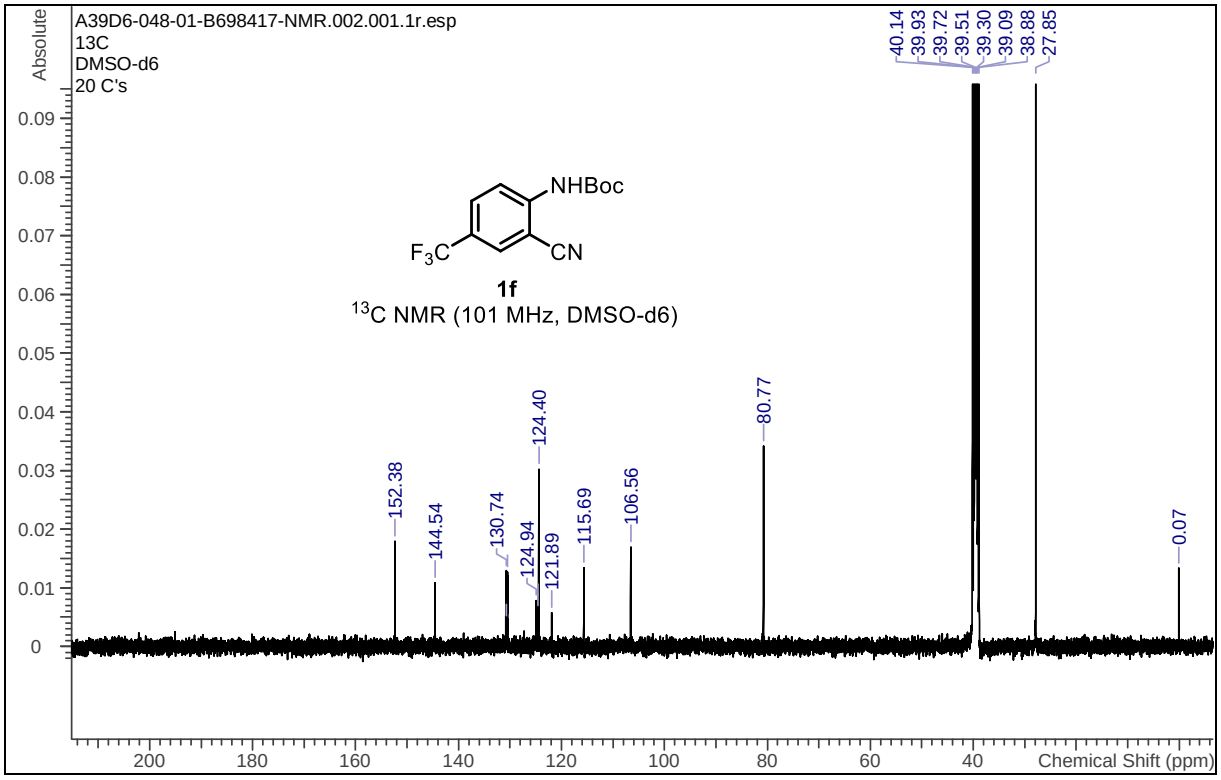

A39D6-047-02-13C.003.001.1r.esp
13C
DMSO-d6
14 C's
NHBoc
F
CN
1d
13C NMR (101 MHz, DMSO-d6)
Absolute
Chemical Shift (ppm)
39.93
39.72
39.51
39.30
39.09
27.84
80.75
124.36
152.37
144.54
130.71
130.43
130.74
130.40
121.89
115.68
106.52
40.14
38.88

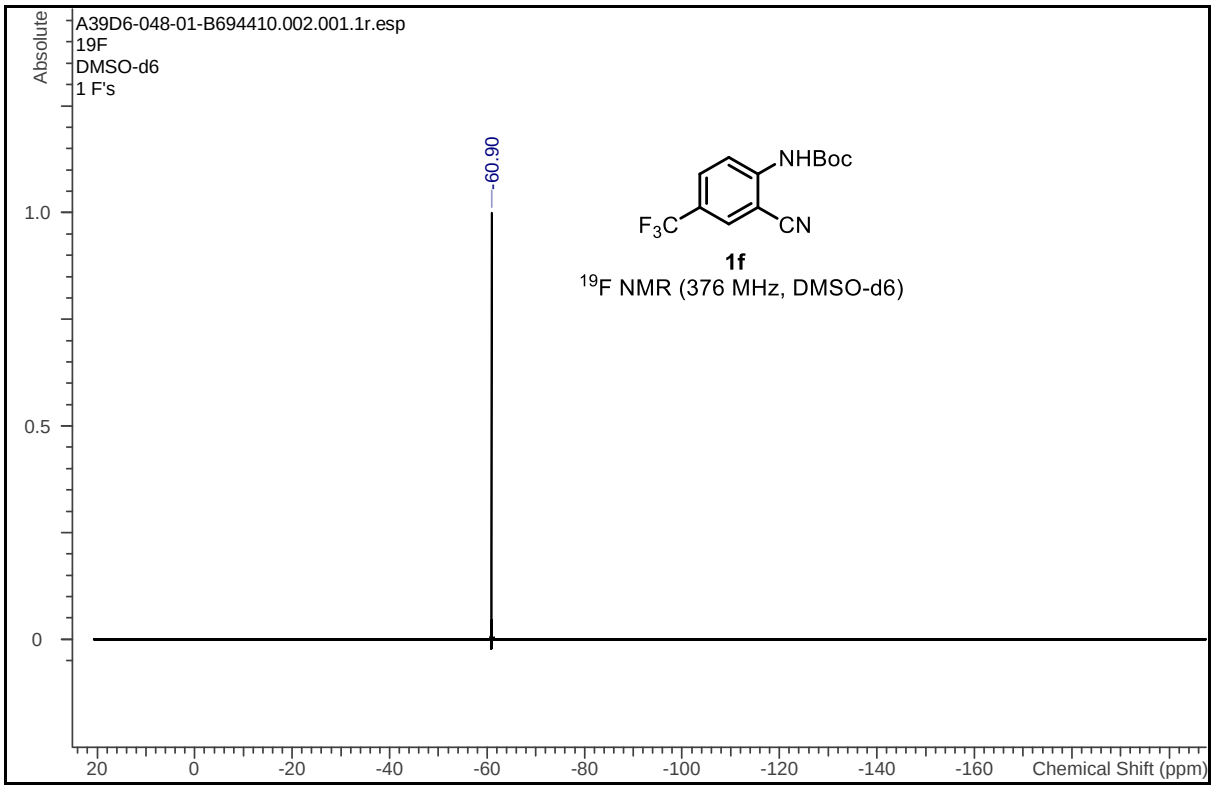

A39D6-047-01-19F.001.001.1r.esp
19F
DMSO-d6
Absolute
-102.80
NHBoc
F
CN
1d
19F NMR (400 MHz, DMSO-d6)
Chemical Shift (ppm)

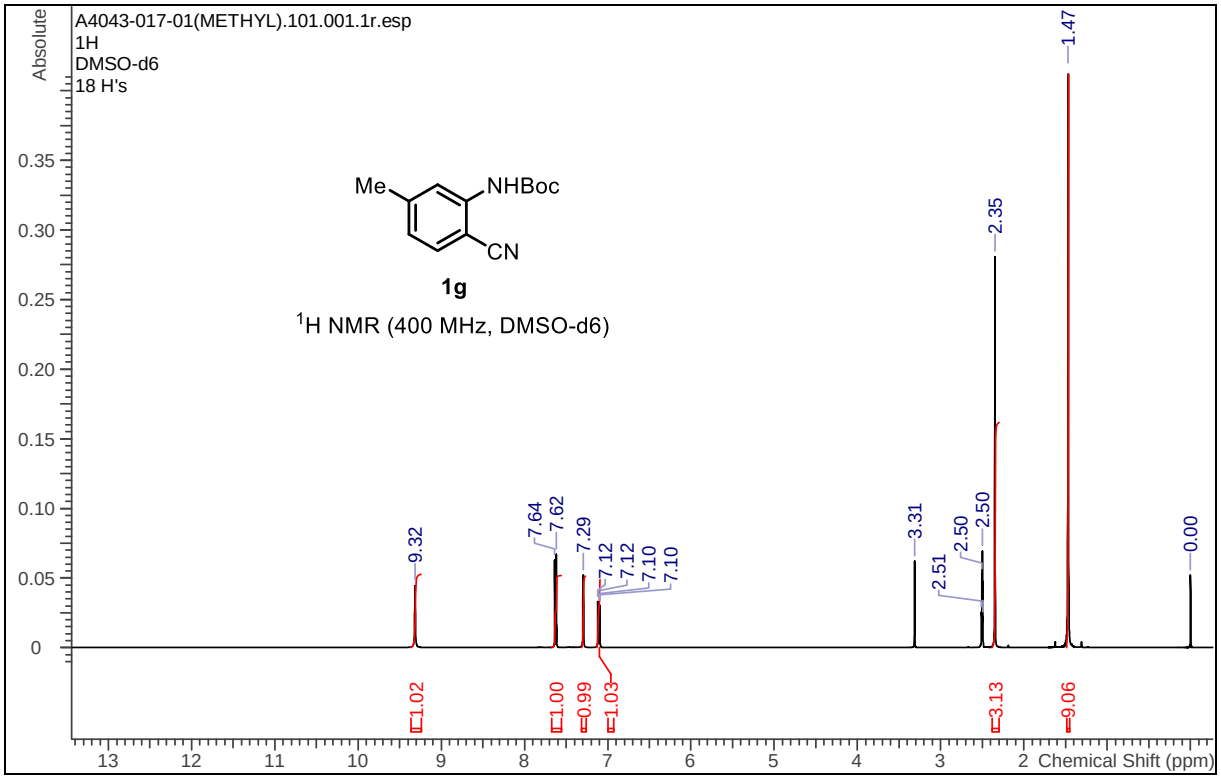

A39D6-055-01-B698044-NMR.101.001.1r.esp
1H
DMSO-d6
20 H's
Absolute
NHBoc
Cl
CN
1e
1H NMR (400 MHz, DMSO-d6)
9.53
7.95
7.95
7.72
7.72
7.70
7.70
7.50
7.48
3.31
2.50
2.50
2.51
2.49
1.47
0.00
1.00
0.84
1.01
1.02
9.26
Chemical Shift (ppm)

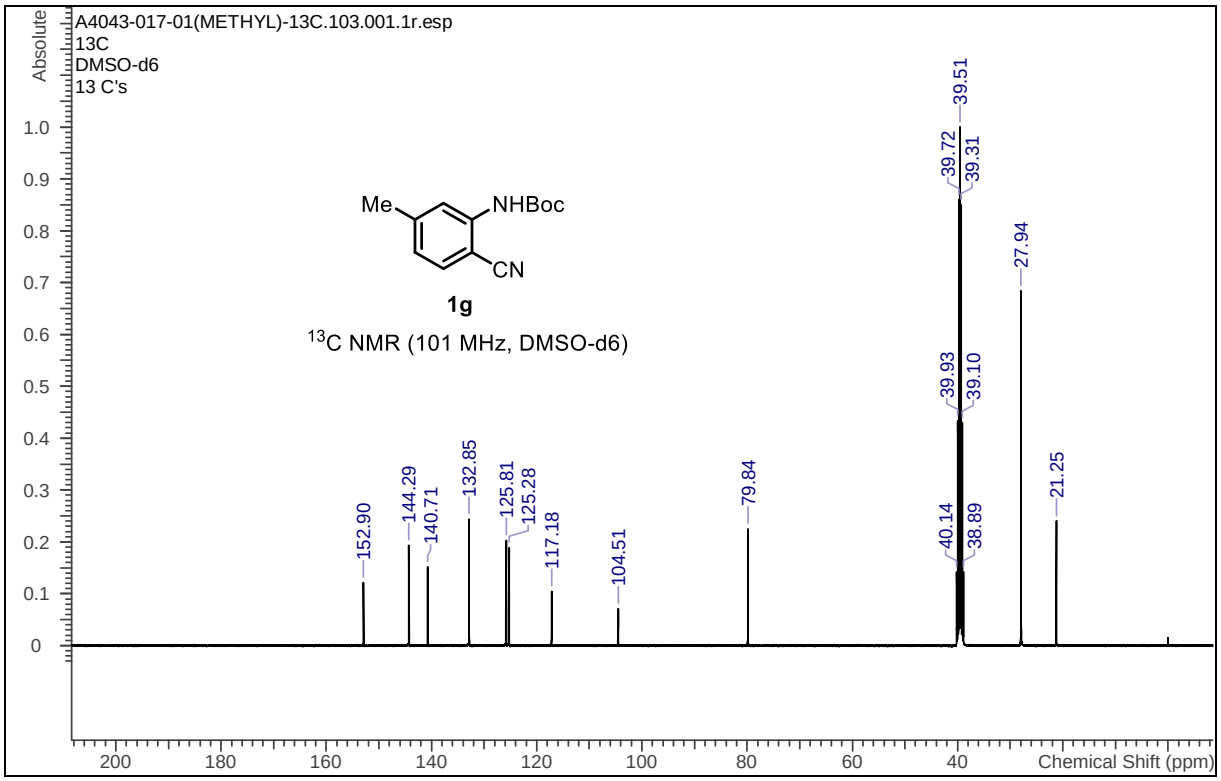

A39D6-055-01-B698407-NMR.002.001.1r.esp
13C
DMSO-d6
1 C's
NHBoc
Cl
CN
1e
13C NMR (101 MHz, DMSO-d6)
Absolute
Chemical Shift (ppm)

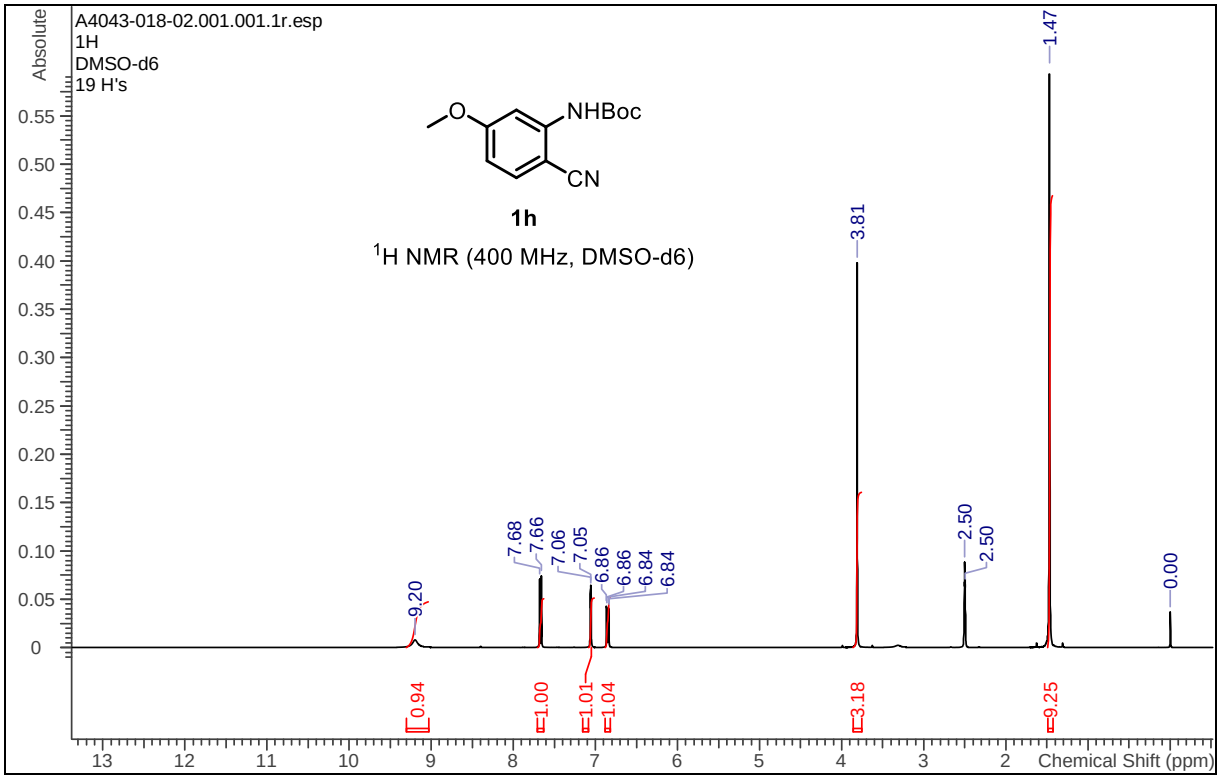

A39D6-048-01-B698417-NMR.001.001.1r.esp
1H
DMSO-d6
26 H's
NHBoc
F3C
CN
1f
1H NMR (400 MHz, DMSO-d6)
Absolute
Chemical Shift (ppm)

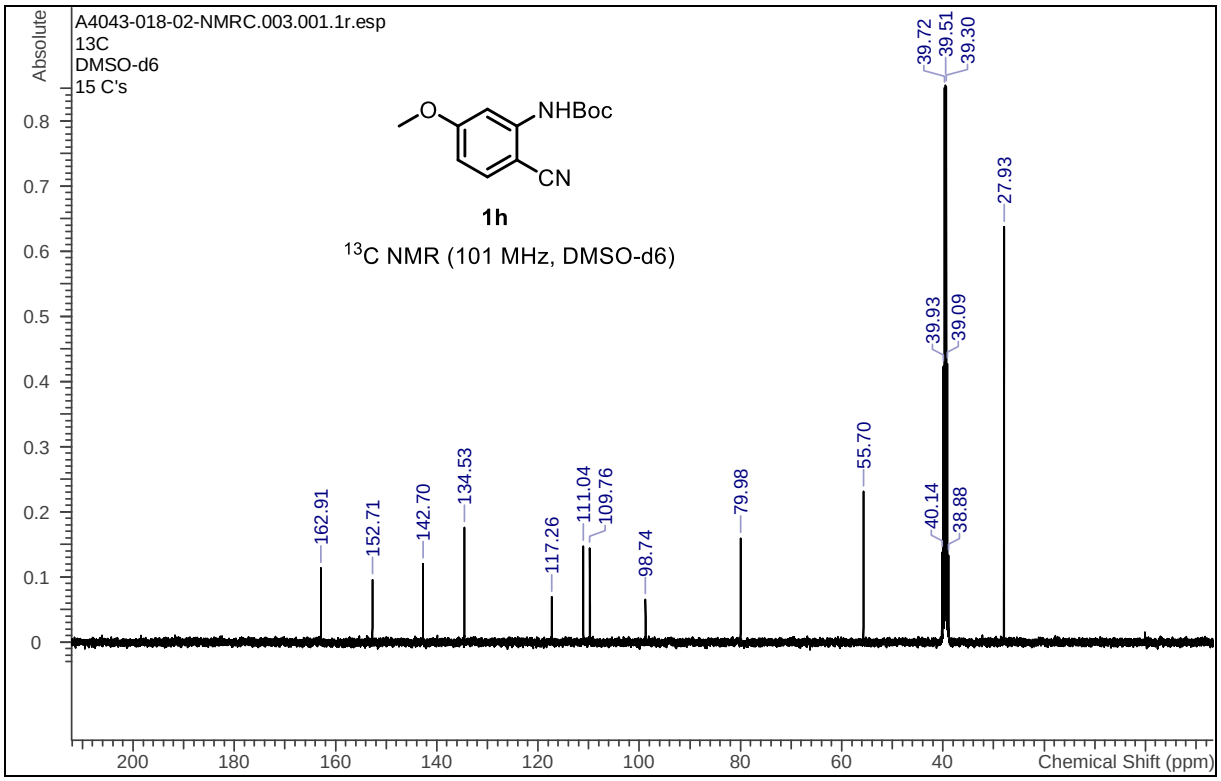

A39D6-048-01-B698417-NMR.002.001.1r.esp
13C
DMSO-d6
20 C's
Absolute
40.14
39.93
39.72
39.51
39.30
39.09
38.88
27.85
NHBoc
F3C
CN
1f
13C NMR (101 MHz, DMSO-d6)
80.77
124.40
152.38
144.54
130.74
124.94
121.89
115.69
106.56
0.07
Chemical Shift (ppm)

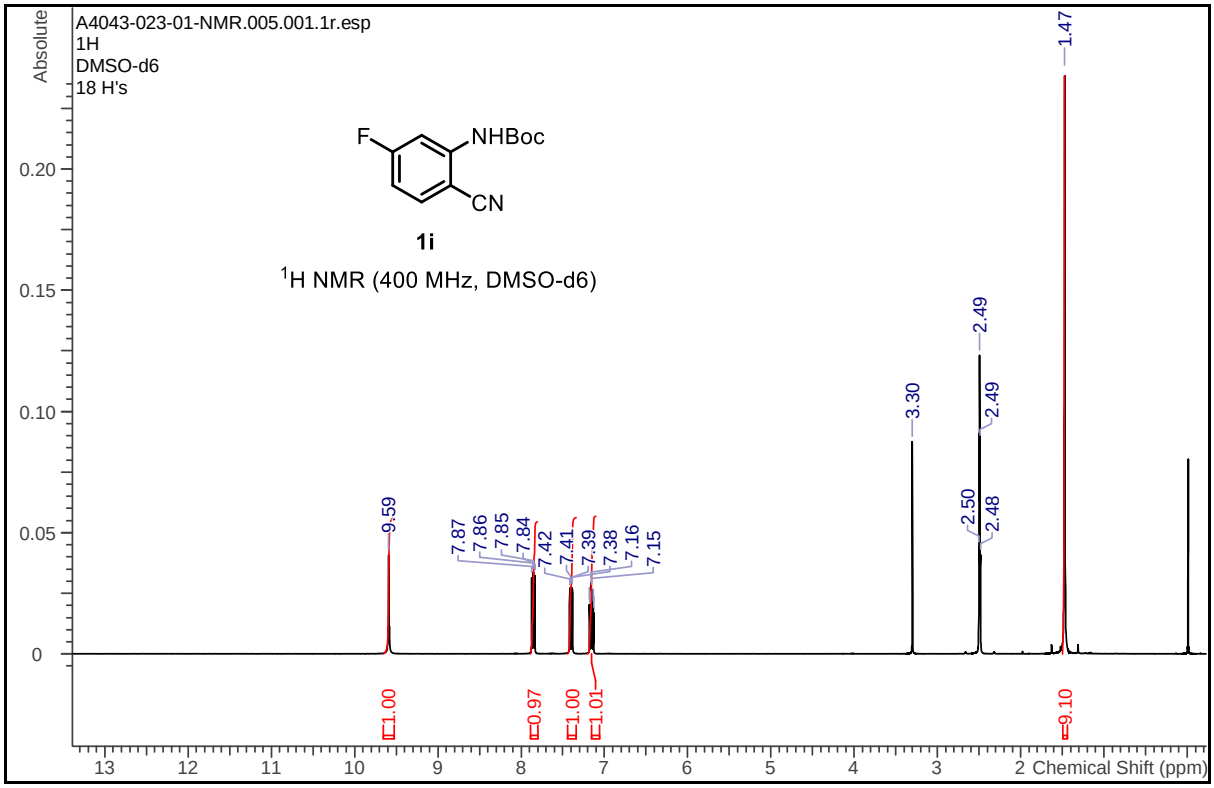

A39D6-048-01-B694410.002.001.1r.esp
19F
DMSO-d6
1 F's
Absolute
60.90
NHBoc
F3C
CN
1f
19F NMR (376 MHz, DMSO-d6)
Chemical Shift (ppm)

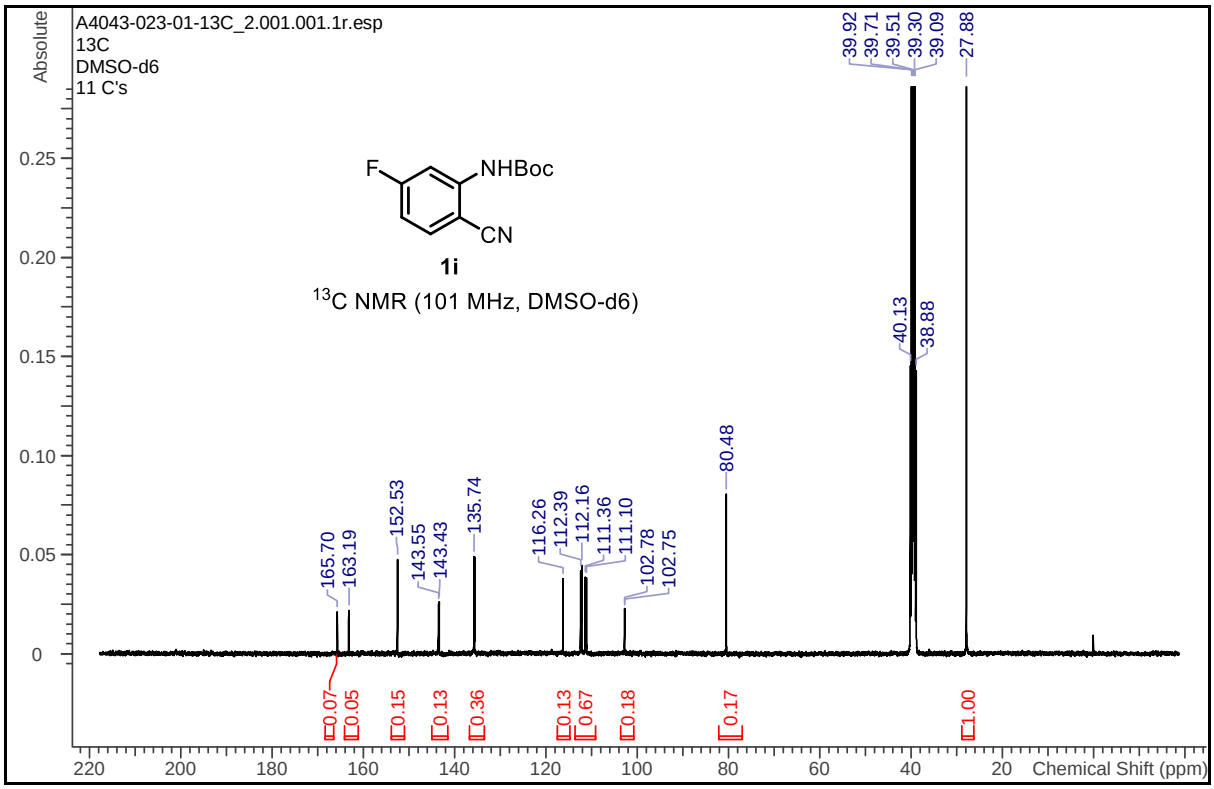

A4043-017-01(METHYL).101.001.1r.esp
1H
DMSO-d6
18 H's
Absolute
Me
NHBoc
CN
1g
1H NMR (400 MHz, DMSO-d6)
9.32
7.64
7.62
7.29
7.12
7.12
7.10
7.10
3.31
2.51
2.50
2.50
2.35
1.47
0.00
1.02
1.00
0.99
1.03
3.13
9.06
Chemical Shift (ppm)

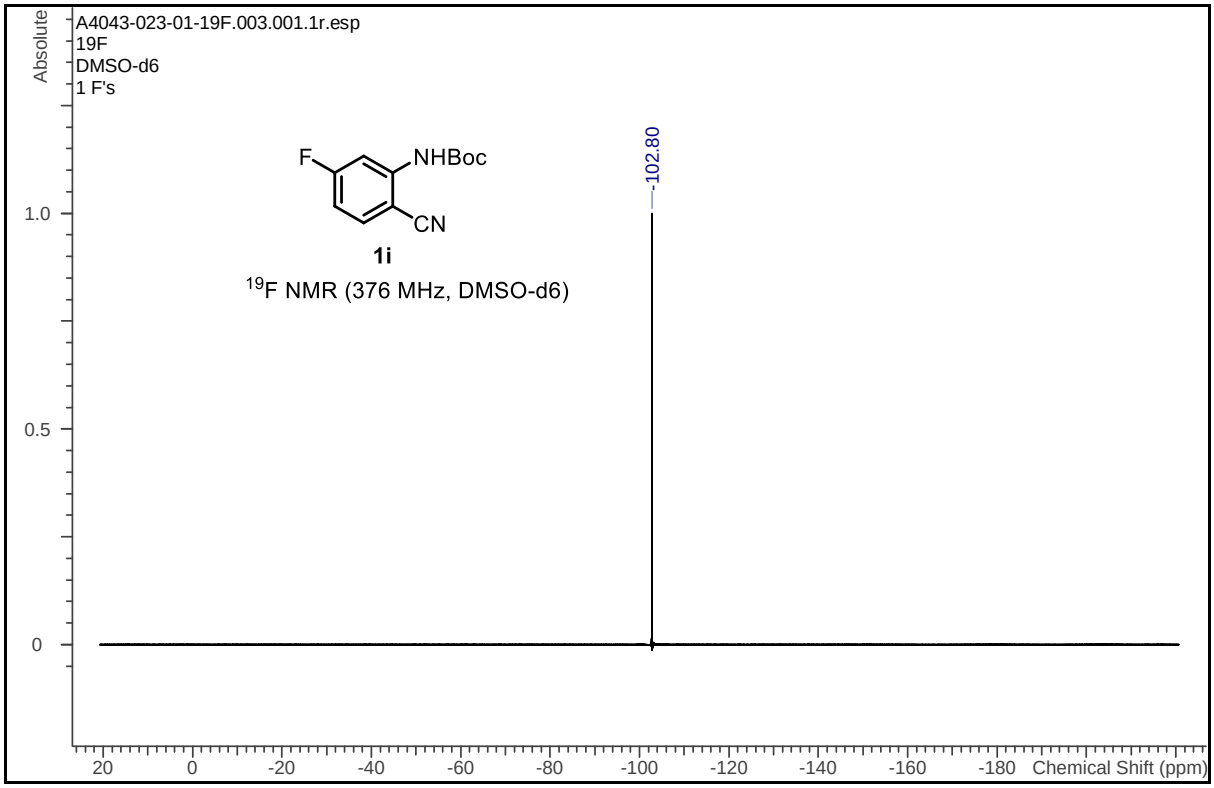

A4043-017-01(METHYL)-13C.103.001.1r.esp
13C
DMSO-d6
13 C's
Absolute
Me
NHBoc
CN
1g
13C NMR (101 MHz, DMSO-d6)
152.90
144.29
140.71
132.85
125.81
125.28
117.18
104.51
79.84
39.93
39.72
39.51
39.31
39.10
40.14
38.89
27.94
21.25
Chemical Shift (ppm)

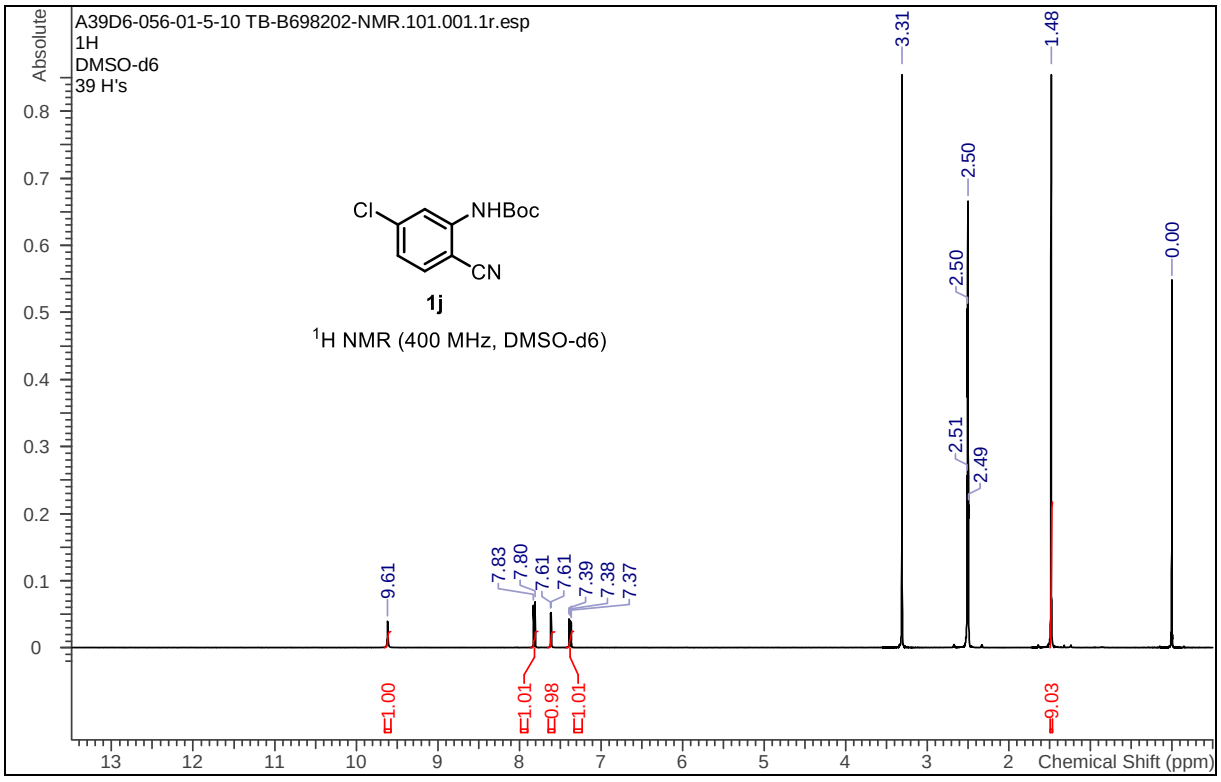

A4043-018-02.001.001.1r.esp
1H
DMSO-d6
19 H's
NHBoc
CN
1h
1H NMR (400 MHz, DMSO-d6)
Absolute
Chemical Shift (ppm)
1.47
3.81
2.50
2.50
0.00
9.20
7.68
7.66
7.06
7.05
6.86
6.86
6.84
6.84
0.94
1.00
1.01
1.04
3.18
9.25

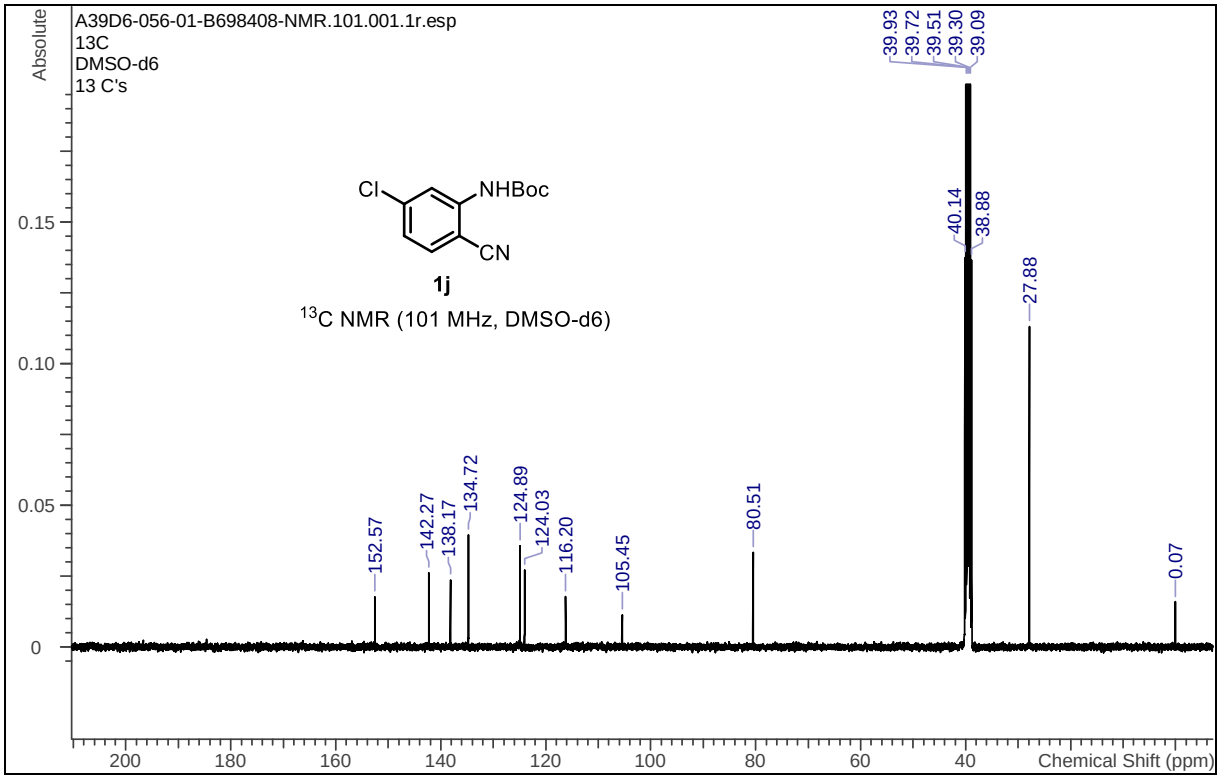

A4043-018-02-NMRC.003.001.1r.esp
13C
DMSO-d6
15 C's
NHBoc
CN
1h
13C NMR (101 MHz, DMSO-d6)
Absolute
Chemical Shift (ppm)
39.72
39.51
39.30
27.93
39.93
39.09
55.70
40.14
38.88
162.91
152.71
142.70
134.53
117.26
111.04
109.76
98.74
79.98

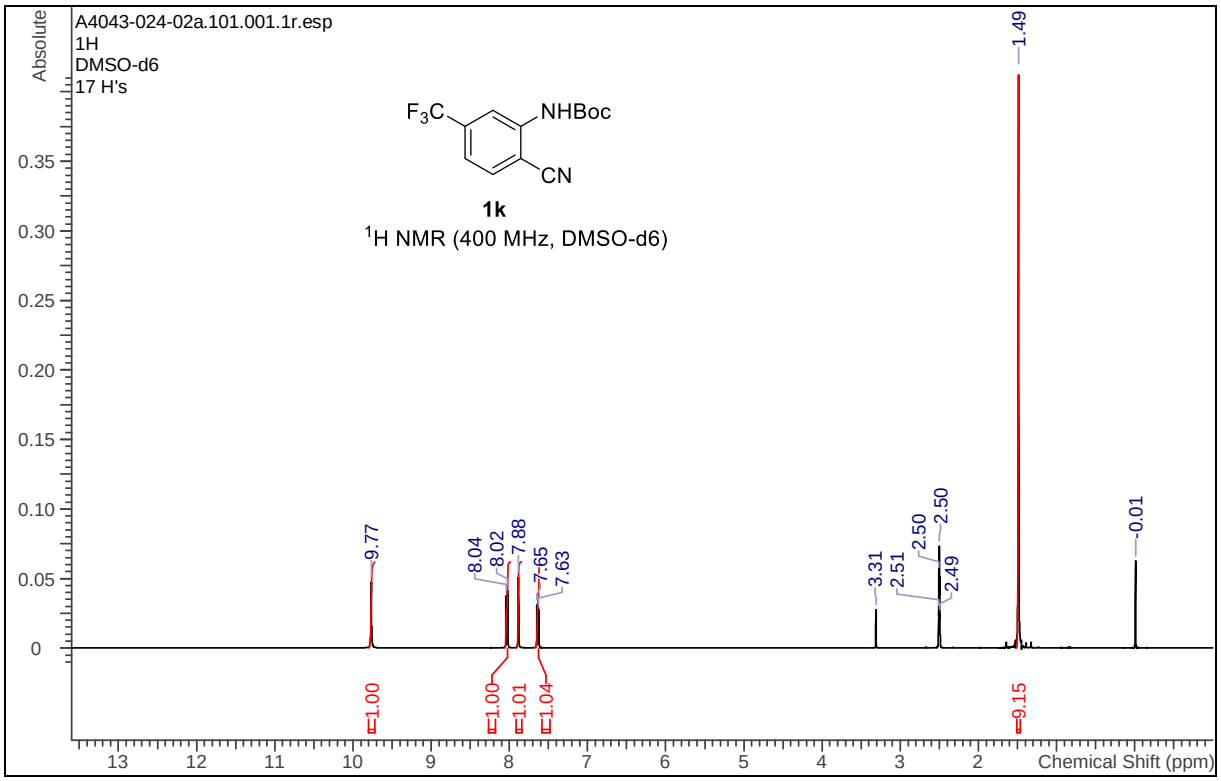

A4043-023-01-NMR.005.001.1r.esp
1H
DMSO-d6
18 H's
F
NHBoc
CN
1i
1H NMR (400 MHz, DMSO-d6)
Absolute
1.47
3.30
2.49
2.49
2.50
2.48
9.59
7.87
7.86
7.85
7.84
7.42
7.41
7.39
7.38
7.16
7.15
1.00
0.97
1.00
1.01
9.10
Chemical Shift (ppm)

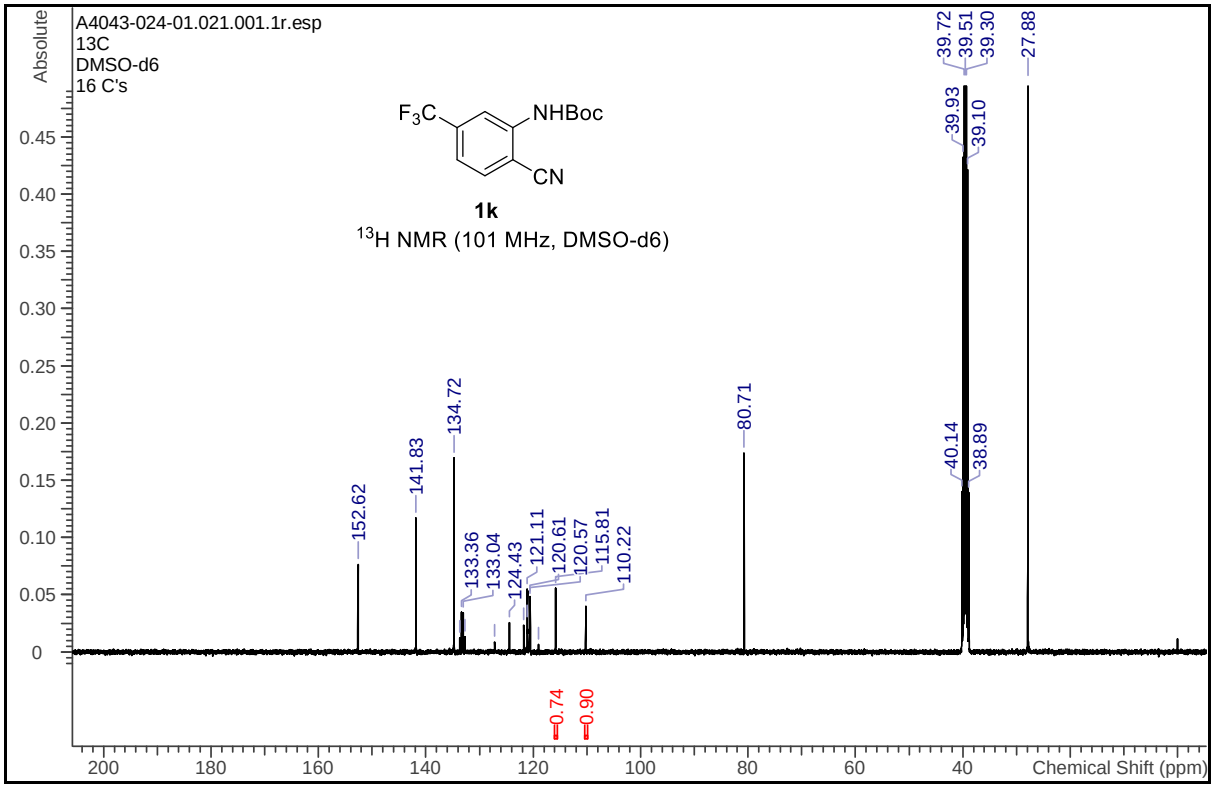

A4043-023-01-13C_2.001.001.1r.esp
13C
DMSO-d6
11 C's
F
NHBoc
CN
1i
13C NMR (101 MHz, DMSO-d6)
Absolute
39.92
39.71
39.51
39.30
39.09
27.88
40.13
38.88
80.48
165.70
163.19
152.53
143.55
143.43
135.74
116.26
112.39
112.16
111.36
111.10
102.78
102.75
0.07
0.05
0.15
0.13
0.36
0.13
0.67
0.18
0.17
1.00
Chemical Shift (ppm)

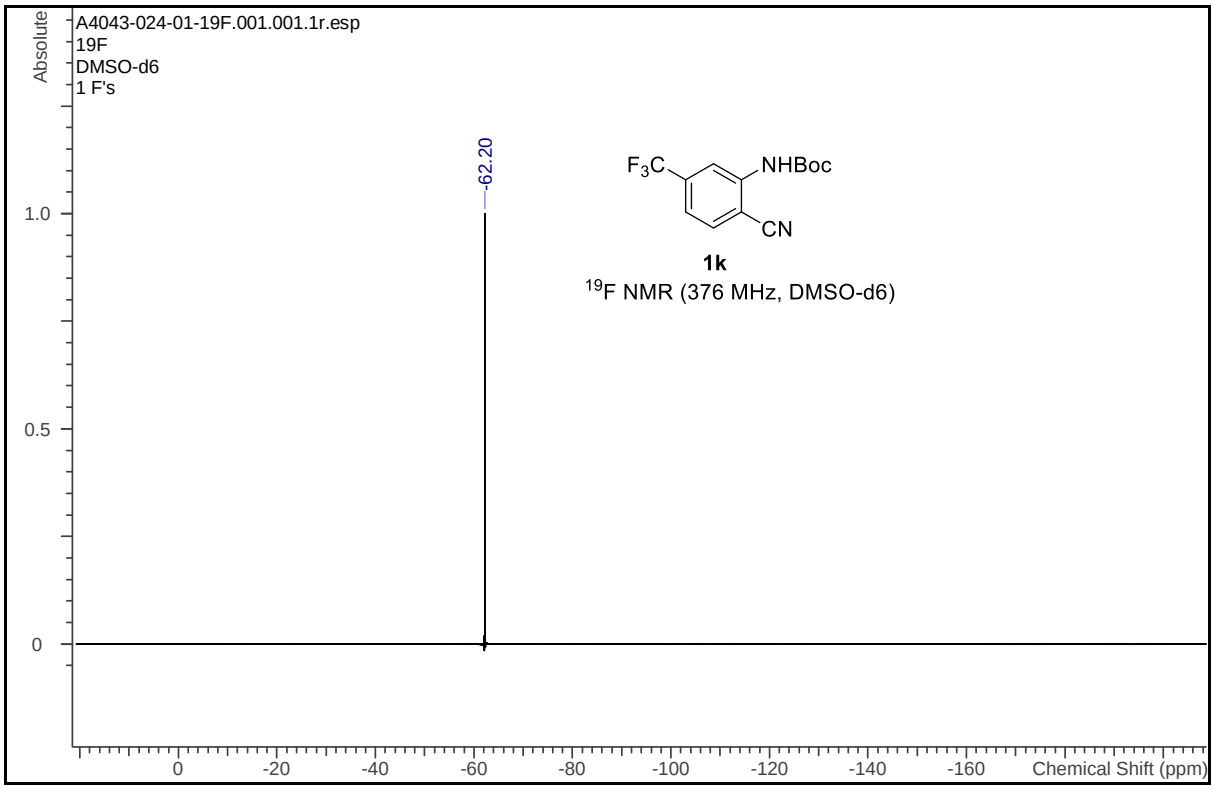

A4043-023-01-19F.003.001.1r.esp
19F
DMSO-d6
1 F's
Absolute
F
NHBoc
CN
1i
19F NMR (376 MHz, DMSO-d6)
-102.80
1.0
0.5
0
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
Chemical Shift (ppm)

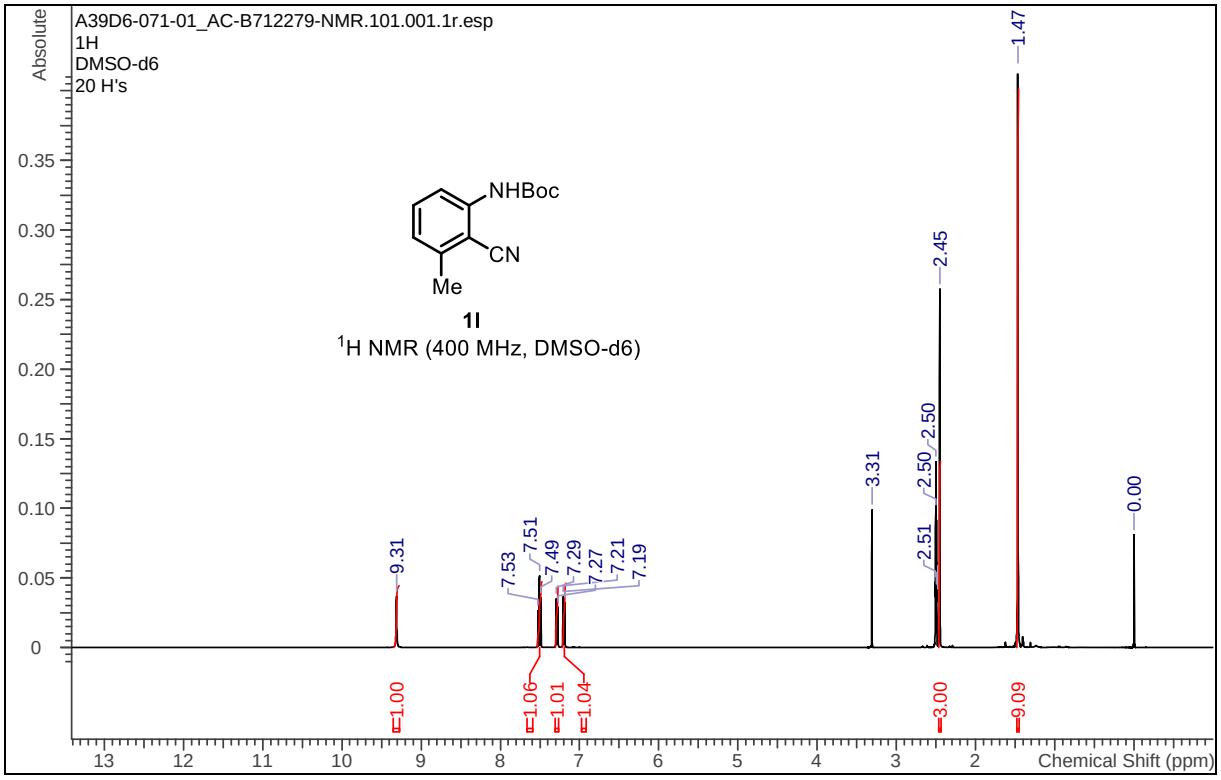

A39D6-056-01-5-10 TB-B698202-NMR.101.001.1r.esp
1H
DMSO-d6
39 H's
Absolute
Cl
NHBoc
CN
1j
1H NMR (400 MHz, DMSO-d6)
3.31
1.48
2.50
2.50
0.00
2.51
2.49
9.61
7.83
7.80
7.61
7.61
7.39
7.38
7.37
1.00
1.01
0.98
1.01
9.03
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
13
12
11
10
9
8
7
6
5
4
3
2
Chemical Shift (ppm)

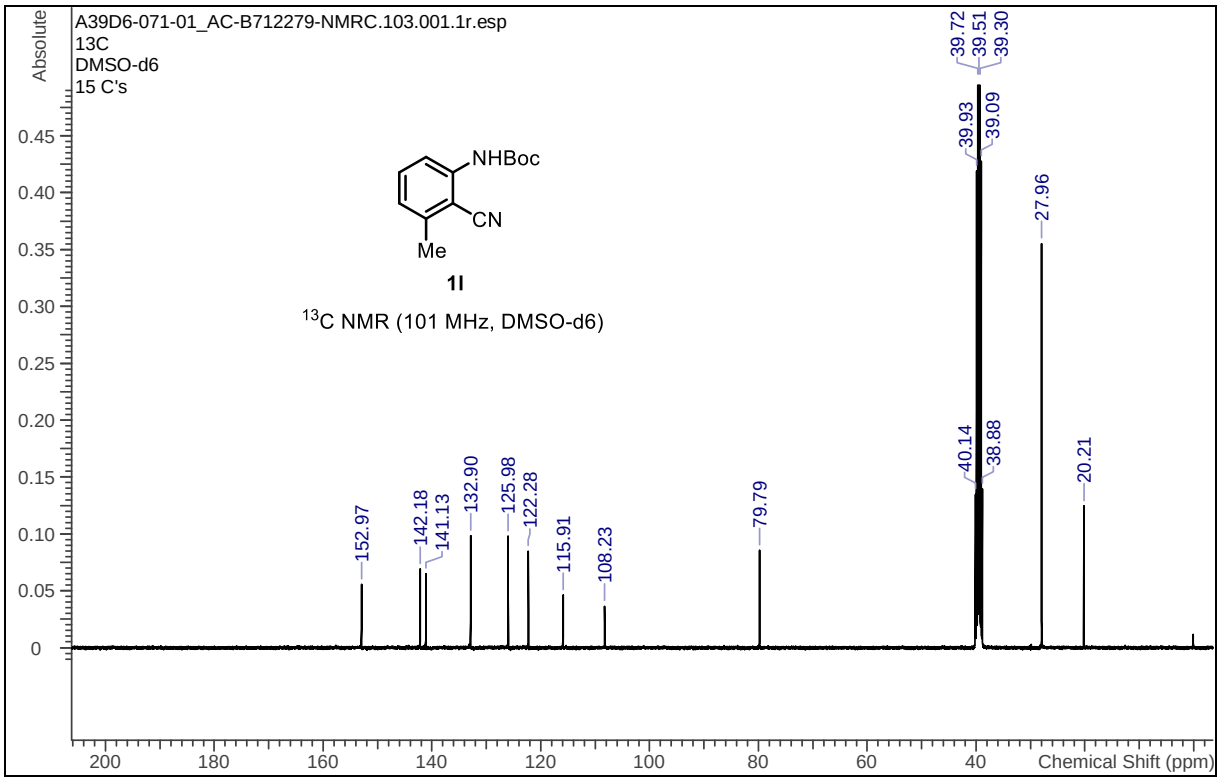

A39D6-056-01-B698408-NMR.101.001.1r.esp
13C
DMSO-d6
13 C's
Cl
NHBoc
CN
1j
^{13}C NMR (101 MHz, DMSO-d6)
Absolute
Chemical Shift (ppm)
39.93
39.72
39.51
39.30
39.09
40.14
38.88
27.88
152.57
142.27
138.17
134.72
124.89
124.03
116.20
105.45
80.51
0.07

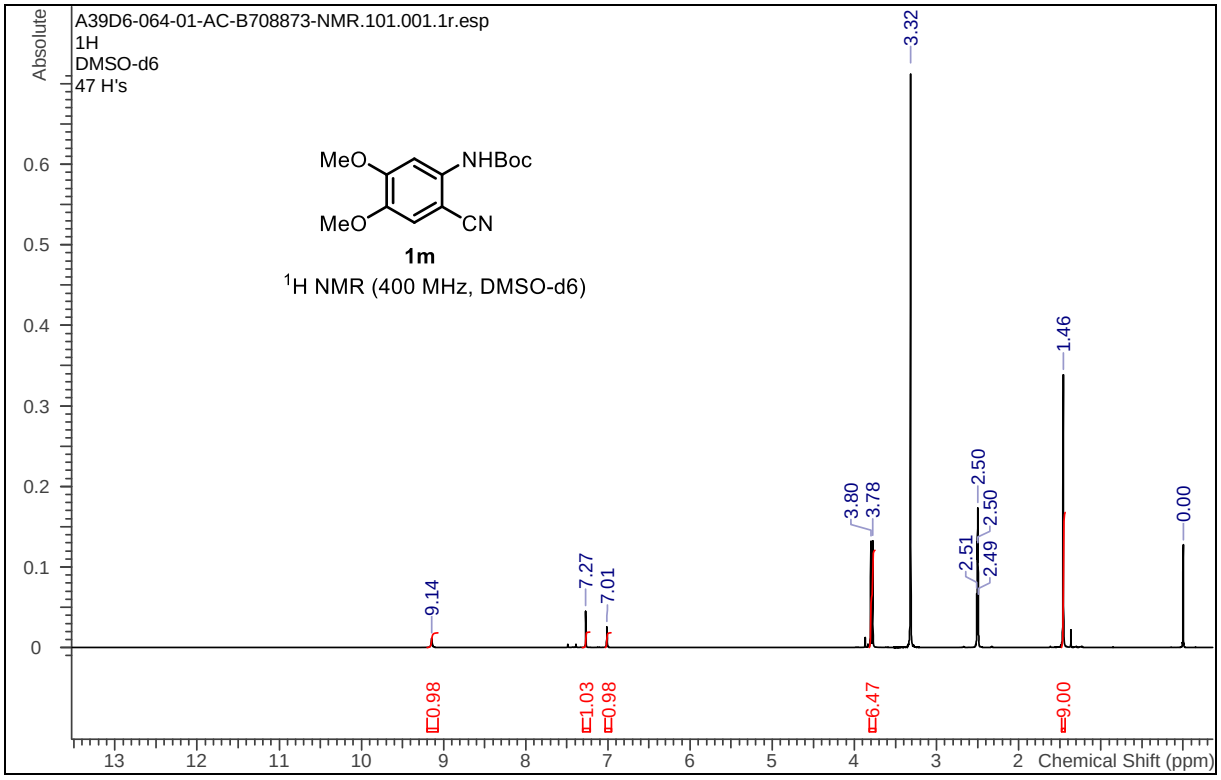

A4043-024-02a.101.001.1r.esp
1H
DMSO-d6
17 H's
F_3C
NHBoc
CN
1k
^{1}H NMR (400 MHz, DMSO-d6)
Absolute
Chemical Shift (ppm)
1.49
9.77
8.04
8.02
7.88
7.65
7.63
3.31
2.51
2.50
2.50
2.49
0.01
1.00
1.00
1.01
1.04
9.15

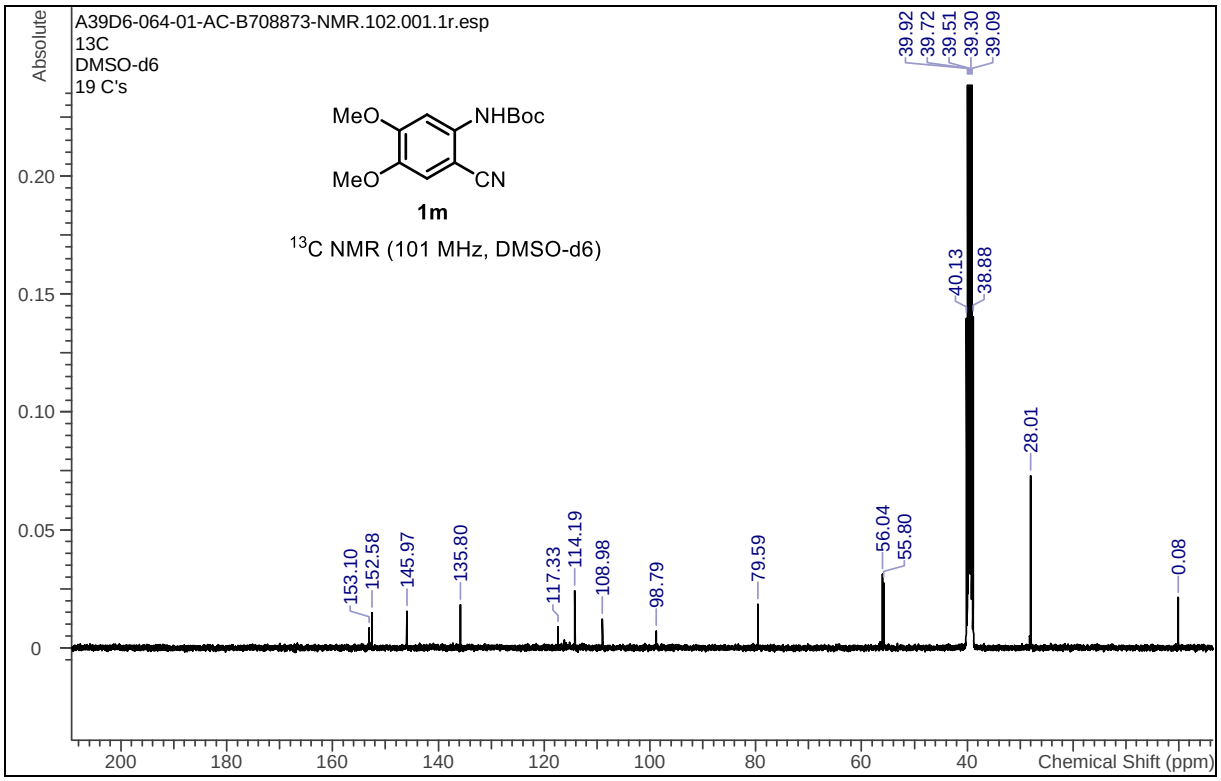

A4043-024-01.021.001.1r.esp
13C
DMSO-d6
16 C's
Absolute
F3C
NHBoc
CN
1k
13H NMR (101 MHz, DMSO-d6)
39.72
39.51
39.30
27.88
39.93
39.10
134.72
80.71
141.83
40.14
38.89
152.62
133.36
133.04
124.43
121.11
120.61
120.57
115.81
110.22
0.74
0.90
Chemical Shift (ppm)

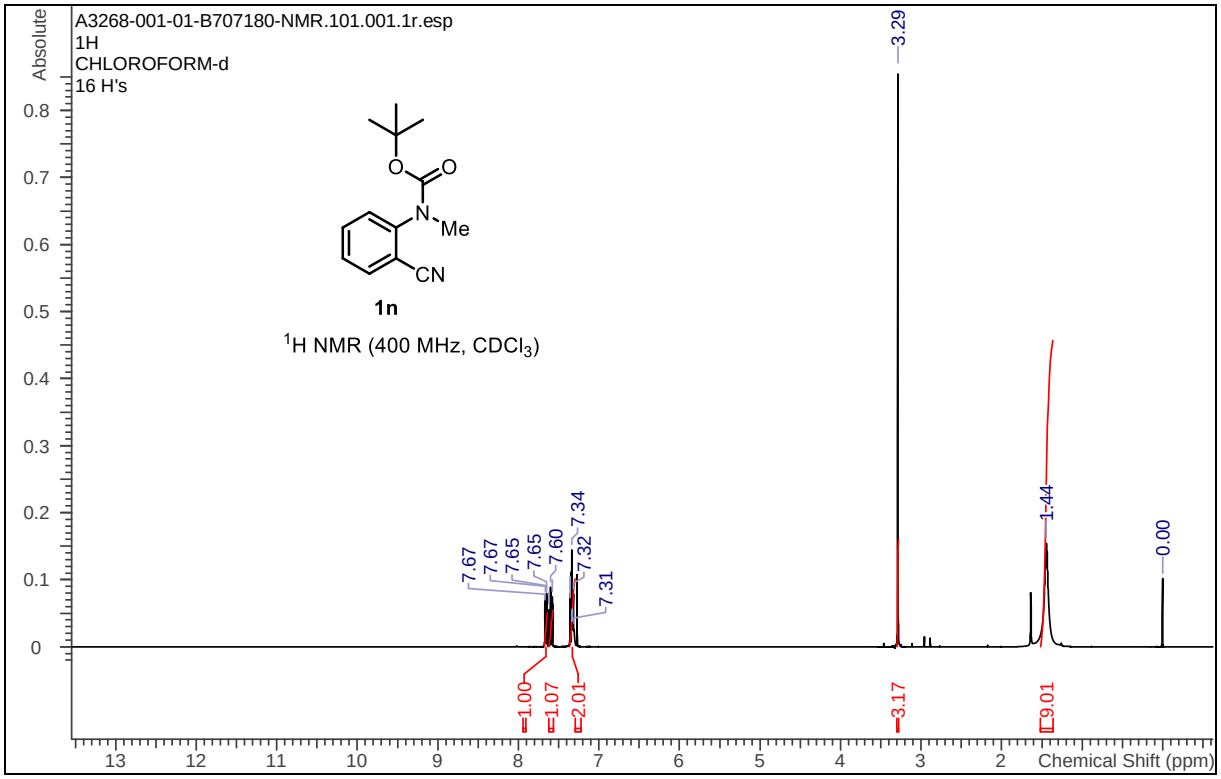

A4043-024-01-19F.001.001.1r.esp
19F
DMSO-d6
1 F's
Absolute
-62.20
F3C
NHBoc
CN
1k
19F NMR (376 MHz, DMSO-d6)
Chemical Shift (ppm)

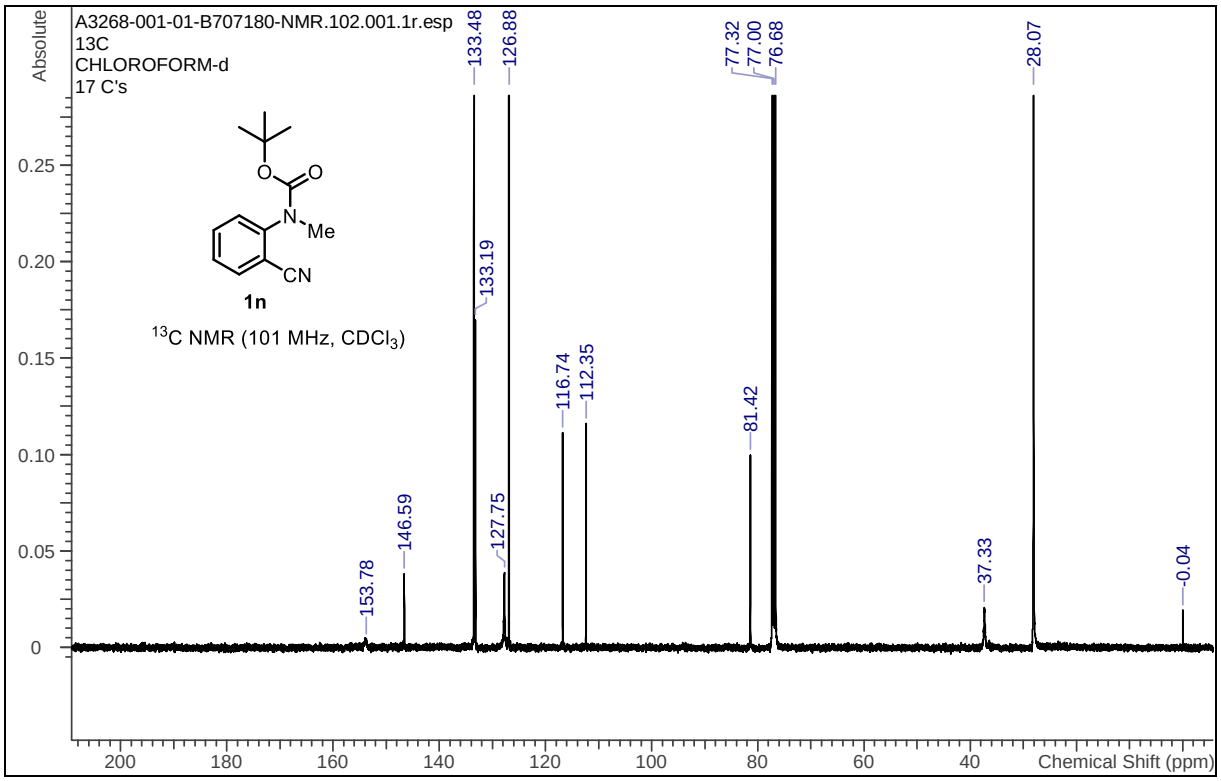

A39D6-071-01_AC-B712279-NMR.101.001.1r.esp
1H
DMSO-d6
20 H's
NHBoc
CN
Me
1l
1H NMR (400 MHz, DMSO-d6)
Absolute
Chemical Shift (ppm)
9.31
7.53
7.51
7.49
7.29
7.27
7.21
7.19
3.31
2.51
2.50
2.50
2.45
1.47
0.00
1.00
1.06
1.01
1.04
3.00
9.09

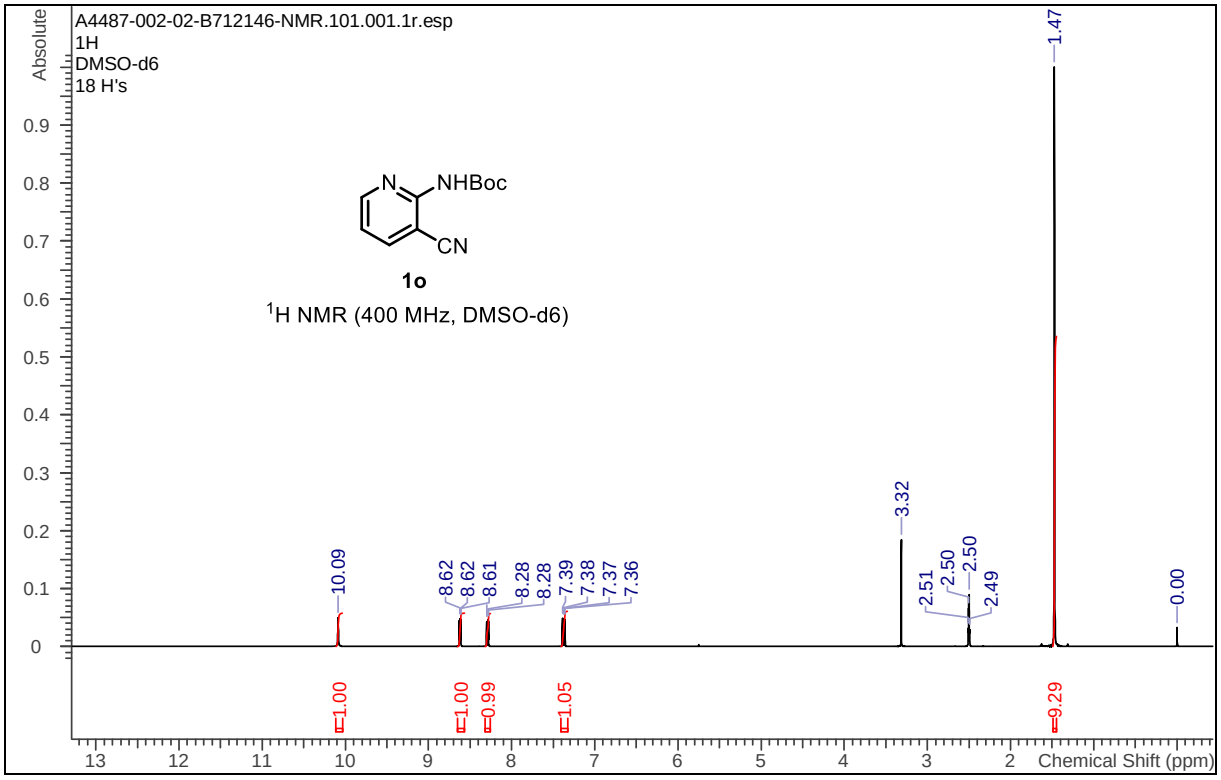

A39D6-071-01_AC-B712279-NMRC.103.001.1r.esp
13C
DMSO-d6
15 C's
NHBoc
CN
Me
1l
13C NMR (101 MHz, DMSO-d6)
Absolute
Chemical Shift (ppm)
152.97
142.18
141.13
132.90
125.98
122.28
115.91
108.23
79.79
40.14
39.93
39.72
39.51
39.30
39.09
38.88
27.96
20.21

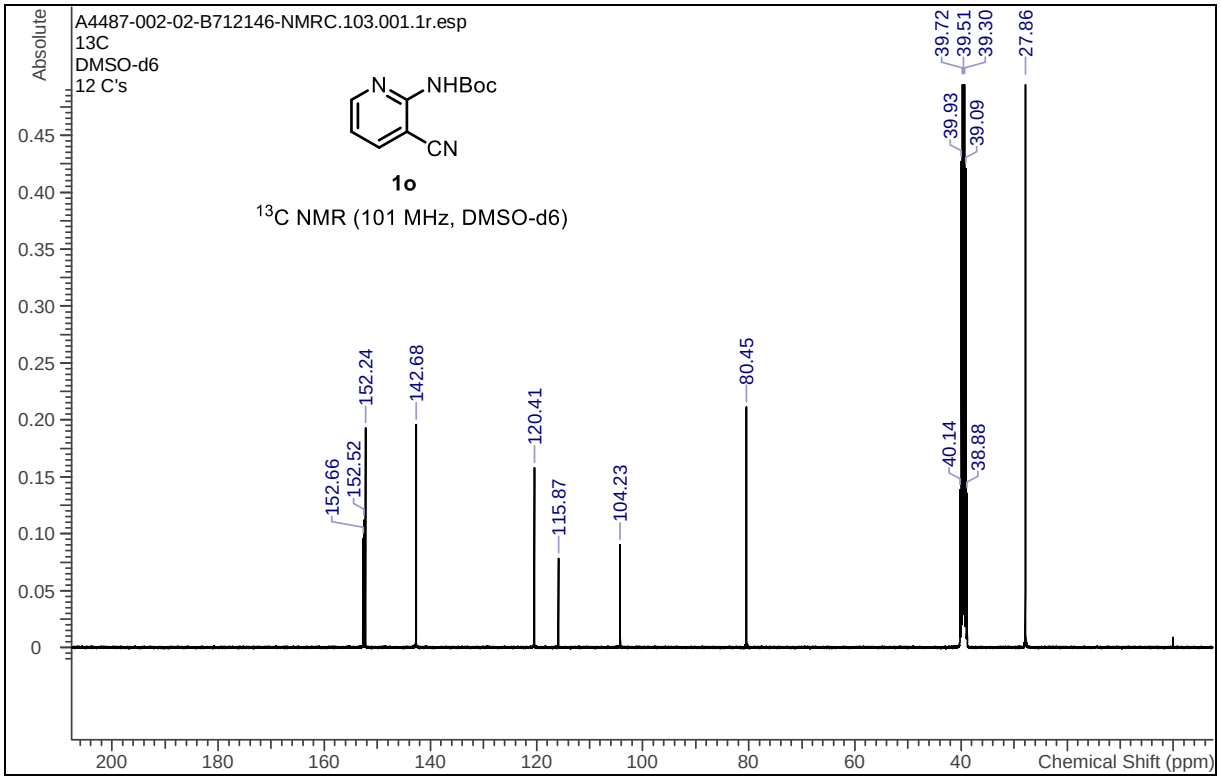

A39D6-064-01-AC-B708873-NMR.101.001.1r.esp
1H
DMSO-d6
47 H's
MeO
NHBoc
MeO
CN
1m
1H NMR (400 MHz, DMSO-d6)
Absolute
Chemical Shift (ppm)
3.32
1.46
3.80
3.78
2.50
2.50
2.51
2.49
0.00
9.14
7.27
7.01
0.98
1.03
0.98
6.47
9.00

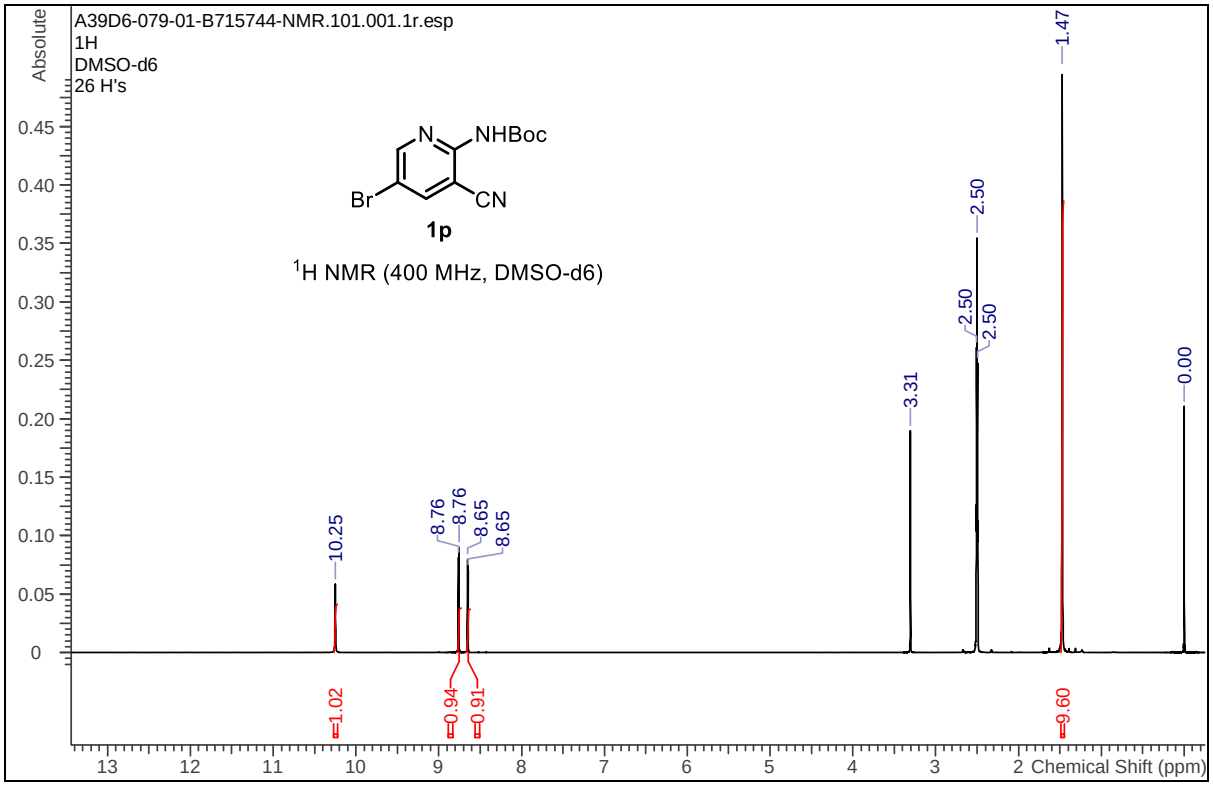

A39D6-064-01-AC-B708873-NMR.102.001.1r.esp
13C
DMSO-d6
19 C's
MeO
NHBoc
MeO
CN
1m
13C NMR (101 MHz, DMSO-d6)
Absolute
Chemical Shift (ppm)
39.92
39.72
39.51
39.30
39.09
40.13
38.88
28.01
153.10
152.58
145.97
135.80
117.33
114.19
108.98
98.79
79.59
56.04
55.80
0.08

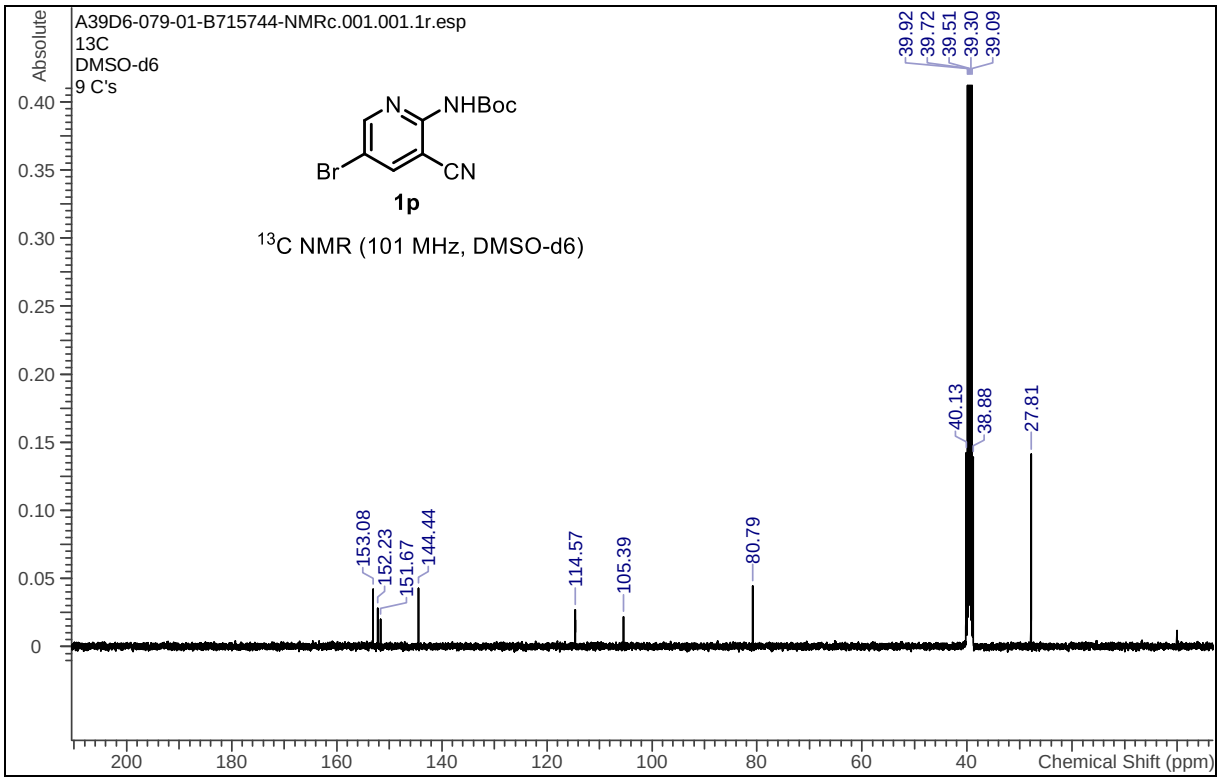

A3268-001-01-B707180-NMR.101.001.1r.esp
1H
CHLOROFORM-d
16 H's
Absolute
1n
^{1}H NMR (400 MHz, $CDCl_3$)
3.29
1.44
0.00
7.67
7.67
7.65
7.65
7.60
7.34
7.32
7.31
1.00
1.07
2.01
3.17
9.01
Chemical Shift (ppm)

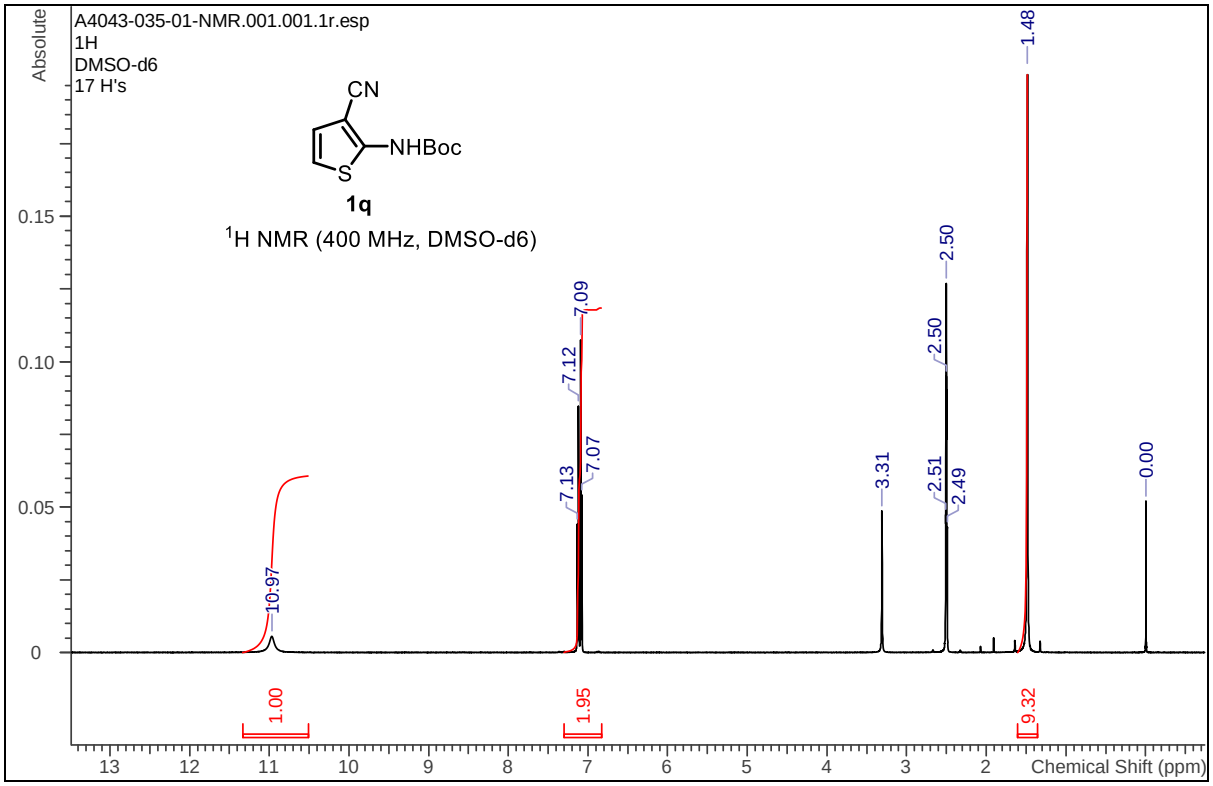

A3268-001-01-B707180-NMR.102.001.1r.esp
13C
CHLOROFORM-d
17 C's
Absolute
1n
^{13}C NMR (101 MHz, $CDCl_3$)
133.48
126.88
77.32
77.00
76.68
28.07
133.19
116.74
112.35
81.42
153.78
146.59
127.75
37.33
-0.04
Chemical Shift (ppm)

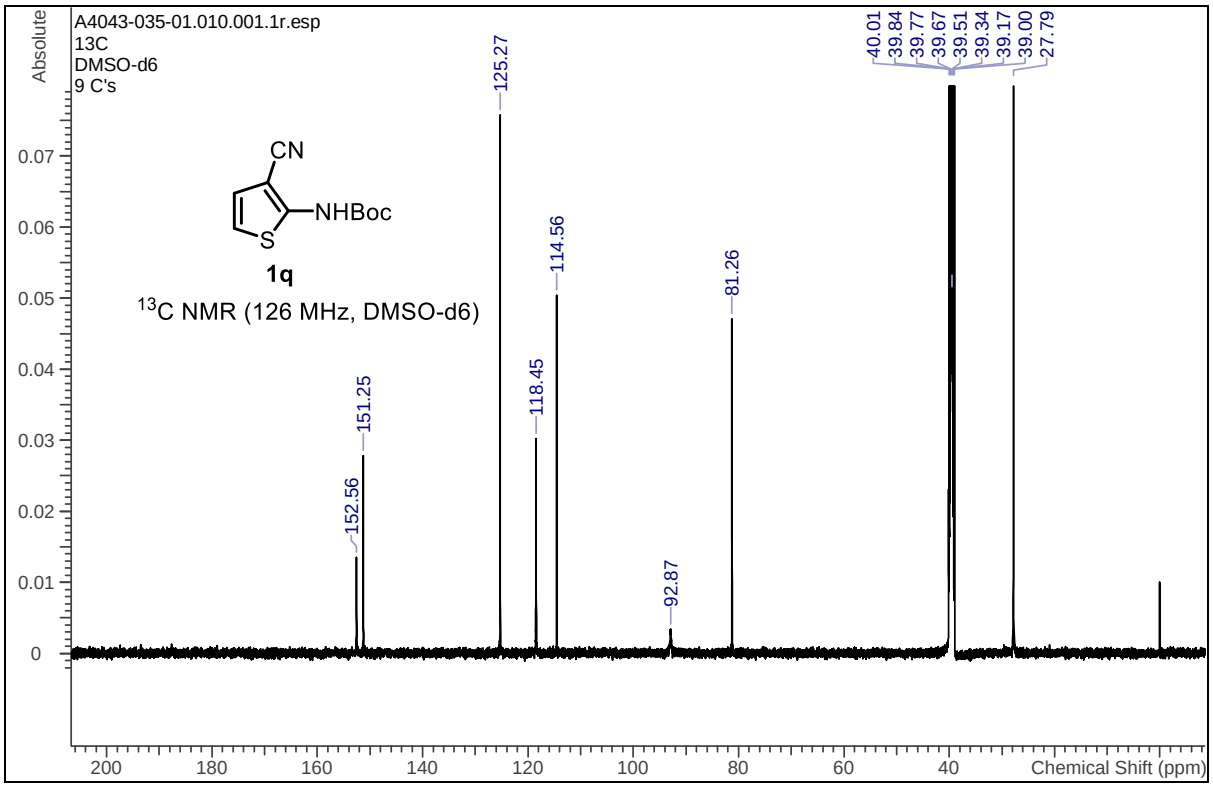

A4487-002-02-B712146-NMR.101.001.1r.esp
1H
DMSO-d6
18 H's
NHBoc
CN
1o
1H NMR (400 MHz, DMSO-d6)
Absolute
Chemical Shift (ppm)
1.47
3.32
2.51
2.50
2.50
2.49
0.00
10.09
8.62
8.62
8.61
8.28
8.28
7.39
7.38
7.37
7.36
1.00
1.00
0.99
1.05
9.29

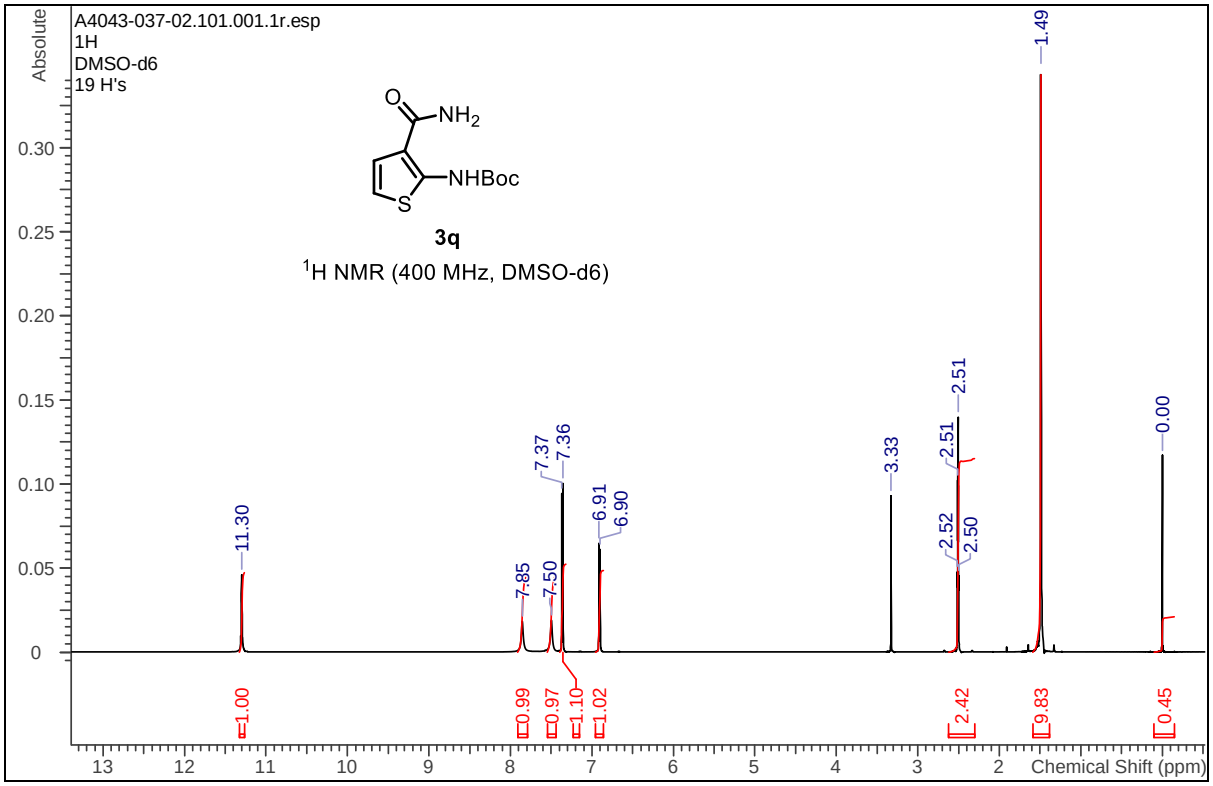

A4487-002-02-B712146-NMRC.103.001.1r.esp
13C
DMSO-d6
12 C's
NHBoc
CN
1o
13C NMR (101 MHz, DMSO-d6)
Absolute
Chemical Shift (ppm)
39.72
39.51
39.30
27.86
39.93
39.09
80.45
152.24
142.68
120.41
152.66
152.52
115.87
104.23
40.14
38.88

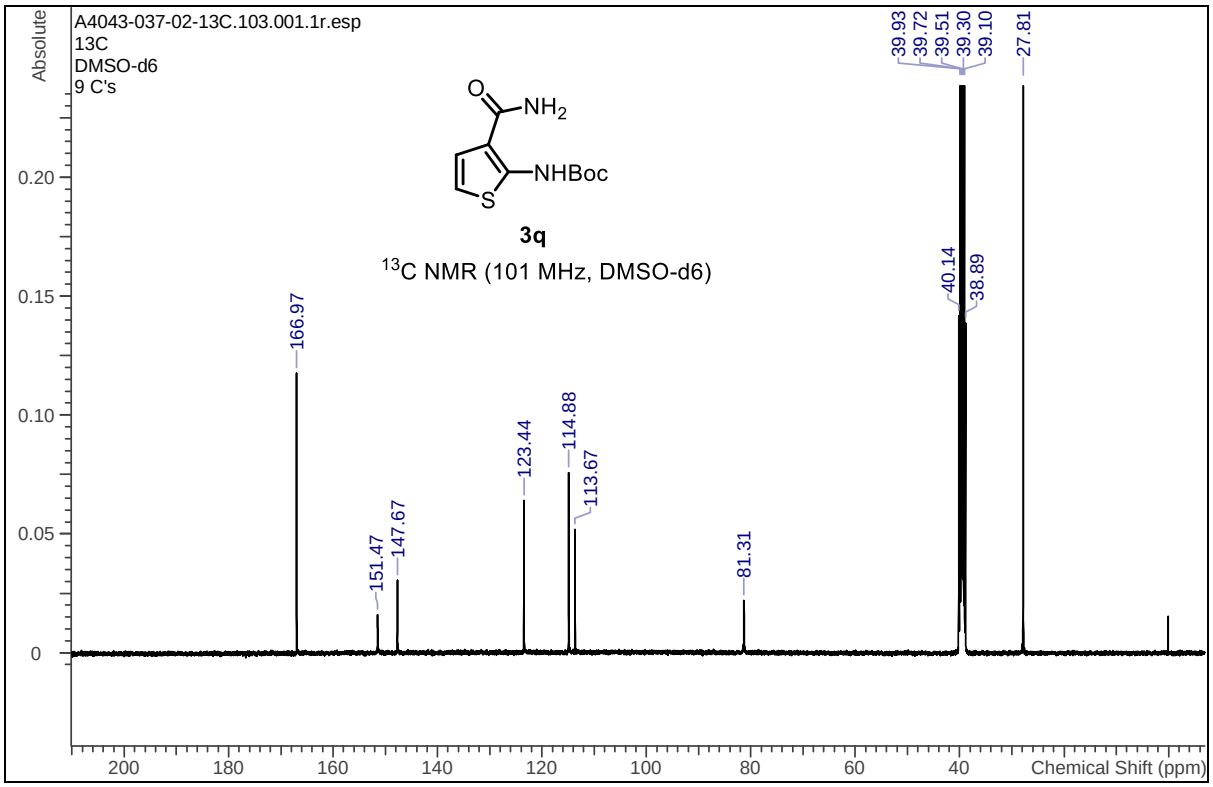

A39D6-079-01-B715744-NMR.101.001.1r.esp
1H
DMSO-d6
26 H's
Absolute
NHBoc
Br
CN
1p
1H NMR (400 MHz, DMSO-d6)
10.25
8.76
8.76
8.65
8.65
3.31
2.50
2.50
2.50
1.47
0.00
=1.02
=0.94
=0.91
=9.60
Chemical Shift (ppm)


A39D6-079-01-B715744-NMRc.001.001.1r.esp
13C
DMSO-d6
9 C's
Absolute
NHBoc
Br
CN
1p
13C NMR (101 MHz, DMSO-d6)
39.92
39.72
39.51
39.30
39.09
40.13
38.88
27.81
153.08
152.23
151.67
144.44
114.57
105.39
80.79
Chemical Shift (ppm)


A4043-035-01-NMR.001.001.1r.esp
1H
DMSO-d6
17 H's
CN
NHBoc
S
1q
1H NMR (400 MHz, DMSO-d6)
Absolute
1.48
2.50
2.50
7.09
7.12
7.07
7.13
3.31
2.51
2.49
0.00
10.97
1.00
1.95
9.32
Chemical Shift (ppm)


A4043-035-01.010.001.1r.esp
13C
DMSO-d6
9 C's
CN
NHBoc
S
1q
13C NMR (126 MHz, DMSO-d6)
Absolute
40.01
39.84
39.77
39.67
39.51
39.34
39.17
39.00
27.79
125.27
114.56
81.26
118.45
151.25
152.56
92.87
Chemical Shift (ppm)


A4043-037-02.101.001.1r.esp
1H
DMSO-d6
19 H's
Absolute
O
NH2
NHBoc
S
3q
1H NMR (400 MHz, DMSO-d6)
11.30
7.85
7.50
7.37
7.36
6.91
6.90
3.33
2.52
2.51
2.50
1.49
0.00
1.00
0.99
0.97
1.10
1.02
2.42
9.83
0.45
Chemical Shift (ppm)


A4043-037-02-13C.103.001.1r.esp
13C
DMSO-d6
9 C's
Absolute
O
NH2
NHBoc
S
3q
13C NMR (101 MHz, DMSO-d6)
166.97
151.47
147.67
123.44
114.88
113.67
81.31
40.14
38.89
39.93
39.72
39.51
39.30
39.10
27.81
Chemical Shift (ppm)