Electronic Supplementary Material (ESI) for RSC Advances.

Supporting information

MIC determination. MICs against replicating M. tuberculosis were determined by the microplate Alamar blue assay (MABA). PBTZ169 (synthesized by our lab), RIF and INH were included as positive controls. M. tuberculosis H37Rv（ATCC27294） and clinical isolate strains were grown to late log phase (70 to 100 Klett units) in Difco Middlebrook 7H9 Broth (catalog no. 271310) supplemented with 0.2% (vol/vol) glycerol, 0.05% Tween 80, and 10% (vol/vol) albumin-dextrosecatalase (BBL Middlebrook ADC Enrichment, catalog no. 212352) (7H9-ADCTG). Cultures were centrifuged, washed twice, and then suspended in phosphate phosphate-buffered saline. Suspensions were then passed through an 8 μm-pore-size filter to remove clumps, and aliquots were frozen at -80 °C. Two fold dilutions of test compounds and positive controls were prepared in 7H9-ADC-TG in a volume of 100 μl in 96-well, black, clear-bottom microplates (BD Biosciences, Franklin Lakes, NJ). *M. tuberculosis* (100 μl containing 2×10^5 CFU) was added, yielding a final testing volume of 200 μl. The plates were incubated at 37°C; on day 7 of incubation, 12.5 μl of 20% Tween 80 and 20 μl of Alamar blue were added to all wells. After incubation at 37 °C for 16 to 24 h, the fluorescence was read at an excitation of 530 nm and an emission of 590 nm. The MIC was defined as the lowest concentration effecting a reduction in fluorescence of ≥90% relative to the mean of replicate bacterium-only controls.

Aqueous solubility determination. Solubility was measured at pH 2.0 by using an HPLC-UV method. Test compounds were initially dissolved in 0.01 M HCl (approximately pH 2.0, 1 mL). The mixture was stirred for 12 h at room temperature and then filtered. The saturated solutions were transferred to other vials for analysis by HPLC-UV. Each sample was performed in triplicate. Aqueous concentration was determined by comparison of the peak area of the saturated solution with a standard curve plotted peak area versus known concentrations, which were prepared by solutions of test compound in ACN at 1.0, 0.1, 0.01, 0.001 mg/mL.

All samples were performed on an Agilent 1260 HPLC-UV system. Conditions (solvent A = methanol, solvent B = 0.1% TFA + H_2O): Zorbax SB-C18 column (250 mm × 4.6 mm, 5 μm, PN: 883975-902). Injection volumn: 10 μL. Flow: 0.5 mL/min. Gradient elution: 0.00 min, 40% A; 3 min, 50% A; 15 min, 100% A; 16 min, 40% A; 25 min 40%A. UV at 254 nm.

Cytotoxicity determination. Compounds were examined for toxicity (CC_{50}) in a mammalian Vero cell line at concentrations from 1000 to 4 μg/ml. The Vero cells were maintained in culture medium (Minimum Essential Medium with Earle's salt, supplemented with 10% fetal bovine serum) at 37 °C under 5% CO_2. Cells were seeded in 96-well plates at the plating density of 1×10^4 cells per well and allowed to recover for 24 h. Culture medium was replaced by assay medium containing the compound to be tested or drug-free. After 72 h of exposure, cells were harvested and cell viability was assessed by MTT assay. The CC_{50} values were calculated by Bliss analyses.

General Chemical Methods. All commercially available solvents and reagents were used without further purification. All moisture sensitive reactions were carried out under Argon atmosphere in commercially available anhydrous solvents. ^{1}H NMR spectra were determined on a Varian Mercury-400 or Bruker 500 M spectrometer in MeOD, $CDCl_3$, or DMSO-d_6 using tetramethylsilane as an internal standard. Electrospray ionization (ESI) mass spectra was obtained on an Agilent 1260-6420 Mass spectrum instruments. The reagents were all of analytical grade or chemically pure. TLC was performed on silica gel plates (Merck, ART5554 60F254).

Purity was determined by HPLC, and all target compounds were confirmed to have >95% purity.

Standard Drug. Rifampicin (RFP) and isoniazid (INH) were purchased from Sigma. PBTZ169 was synthesized according to the published procedure (EMBO Mol. Med.2014, 6 (3), 372−83.).

Purity determination. All samples were performed on an Agilent 1260 HPLC-UV system. Conditions (solvent A = methanol, solvent B = 0.1% TFA + H_2O): Zorbax SB-C18 column (250 mm × 4.6 mm, 5 μm, PN: 883975-902). Injection volumn: 10 μL. Flow: 0.5 mL/min. Gradient elution: 0.00 min, 40% A; 3 min, 50% A; 15 min, 100% A; 16 min, 40% A; 25 min 40%A. UV at 254 nm.

General synthesis procedure for synthesis of compounds 1-34. To a stirring solution of **A** (0.3 mmol) in MeOH (5 mL) was added the corresponding aldehyde (0.4 mmol) and $NaCNBH_3$ (0.5 mmol) at room temperature. The mixture was adjusted to pH 6-7, stirred

overnight at room temperature, and quenched by 1 M NaOH solution (5 mL). The mixture was diluted by H_2O (15 mL), and extracted by DCM (10 mL × 3). The combined organic layer was washed by brine, dried over anhydrous $MgSO_4$, filtered, and concentrated. The residue was purified over silica gel column (DCM : MeOH = 20 : 1) to yield oils **B1-B34**.

To a stirred solution of **B1-B34** (0.2 mmol) in DCM (5 mL) was added TFA (1 mL) at room temperature. The mixture was stirred for 2 hours and concentrated to afford the crude product **B1-34** which was used directly in the next step without further purification.

To a stirred solution of above crude **B1-34** in anhydrous MeOH (10 mL) was added BTZ core compound **D** (0.2 mmol) and Et_3N (0.6 mmol) at room temperature. The mixture was stirred overnight at 40 ^oC, and concentrated. The residue was purified by silica gel column (DCM : MeOH = 20 : 1) to yield the yellow solids **1-34. (**The data and NMR copies of compounds **1-34** were listed in the supporting information.)

2-(5-(cyclohexylmethyl)hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)-8-nitro-6-(trifluoromethyl)-4H-benzo[e][1,3]thiazin-4-one (1). According to above general procedure, employing cyclohexanecarbaldehyde afforded compound **1** as a yellow solid. ^1H NMR (500 MHz, $CDCl_3$) δ 9.21 (s, 1H), 8.81 (s, 1H), 4.23 (s, 1H), 4.02-3.96 (m, 2H), 3.66 (s, 1H), 3.14-3.02 (brs, 2H), 2.72-2.54 (brs, 4H), 2.29 (s, 2H), 1.79-1.71 (m, 6H), 1.26-1.17(m, 3H), 0.91(s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.97, 159.88, 143.59, 134.62, 133.76 (q, J = 3.46 Hz), 129.59(q, J = 34.41 Hz), 126.87, 126.51, 125.90(q, J = 3.34 Hz), 122.54 (q, J = 274.1 Hz), 62.13, 60.23, 56.37, 53.44, 41.80, 39.94, 36.81, 31.78, 26.72, 26.05; ESI-MS: 483 $(M + H)^+$. HRMS-ESI (m/z): Calcd. For $C_{22}H_{26}F_3N_4O_3S$ $(M+H)^+$: 483.1672; Found: 483.1675.

2-(5-(4-fluorobenzyl)hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)-8-nitro-6-(trifluoromethyl)-4H-benzo[e][1,3]thiazin-4-one (2). According to above general procedure, employing 4-fluorobenzaldehyde afforded compound **2** as a yellow solid. mp: 178-180 ^oC; ^1H NMR (500 MHz, $CDCl_3$) δ 9.21 (s, 1H), 8.82(s, 1H), 7.31 (s, 2H), 7.05-7.04 (s, 2H), 4.23 (s, 1H), 4.04-3.96 (m, 2H), 3.78-3.75 (m, 1H), 3.65(brs, 2H), 3.18-3.04(brs, 2H), 2.73-2.61 (brs, 3H), 1.64 (s, 1H), 1.30-1.27 (m, 3H); ^{13}C NMR(125 MHz, CDCl3) δ165.97, 143.61, 134.53, 133.79 (q, J=3.42 Hz), 130.02 (q, J = 35.30 Hz), 126.87, 125.93(q, J = 3.56 Hz), 123.78(q, J=272.01Hz), 115.42, 115.22, 59.60, 58.51, 58.35, 56.17,

53.22, 41.81, 39.99; ESI-MS: 495 $(M + H)^+$; HRMS-ESI (m/z): Calcd. For $C_{22}H_{19}F_4N_4O_3S$ $(M+H)^+$: 495.1109; Found: 495.1106.

2-(5-(4-chlorobenzyl)hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)-8-nitro-6-(trifluoromethyl)-4H-benzo[e][1,3]thiazin-4-one (3). According to above general procedure, employing 4-chlorobenzaldehyde afforded compound **3** as a yellow solid. mp: 228-230 ^oC; ^1H NMR (500 MHz, $CDCl_3$) δ 9.21(s, 1H), 8.81(s, 1H), 7.30 (s, 1H), 7.21-7.15 (m, 3H), 4.25-4.20 (brs, 1H), 4.03-3.95 (brs, 2H), 3.66 (brs, 3H), 3.17-3.04(brs, 2H), 2.74-2.64 (brs, 3H), 2.37 (s, 3H); ^{13}C NMR (125 MHz , CDCl3) δ 165.97, 159.92, 143.60, 134.60, 133.78(q, J = 3.42 Hz), 129.33 (q, J = 34.20 Hz), 128.64, 126.86, 125.90 (q, J = 3.41Hz), 122.40 (q , J = 270.12 Hz), 121.08, 59.57, 58.80, 56.20, 53.46, 53.21, 41.84, 40.01, 21.13; ESI-MS: 511 $(M + H)^+$; HRMS-ESI (m/z): Calcd. For $C_{22}H_{19}ClF_3N_4O_3S$ $(M+H)^+$: 511.0813; Found: 511.0817.

2-(5-(4-bromobenzyl)hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)-8-nitro-6-(trifluoromethyl)-4H-benzo[e][1,3]thiazin-4-one (4). According to above general procedure, employing 4-bromobenzaldehyde afforded compound **4** as a yellow solid. mp: 237-239 ^oC; ^1H NMR (500 MHz, $CDCl_3$) δ 9.20 (s, 1H), 8.81(s, 1H), 7.48 (s, 2H), 7.30-7.23 (brs, 2H), 4.22 (s, 1H), 4.01 (brs, 2H), 3.76-3.65 (brs, 3H), 3.18-3.05 (brs, 2H), 2.75-2.61 (brs, 2H), 1.64 (brs, 1H); ^{13}C NMR (125 MHz, CDCl3) δ 165.15, 159.52, 144.61, 138.93, 132.14, 131.55, 130.95, 130.12, 128.11 (q, J = 33.92 Hz), 126.71, 126.57, 123.45 (q, J = 253.41 Hz),120.25, 59.98, 59.86, 58.09, 56.35, 53.52, 41.74; ESI-MS: 555 $(M + H)^+$; HRMS-ESI (m/z): Calcd. For $C_{22}H_{19}BrF_3N_4O_3S$ $(M+H)^+$: 555.0308; Found: 555.0310.

2-(5-(4-cyanobenzyl)hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)-8-nitro-6-(trifluoromethyl)-4H-benzo[e][1,3]thiazin-4-one (5). According to above general procedure, employing 4-formylbenzonitrile afforded compound **5** as a yellow solid. mp: 232-234 ^oC; ^1H NMR (500 MHz, $CDCl_3$) δ 9.20 (s, 1H), 8.81 (s, 1H), 7.65 (s, 2H), 7.45 (s, 1H), 7.30 (s, 1H), 4.24 (s, 1H), 4.05-3.96 (m, 2H), 3.71- 3.67 (m, 3H), 3.19-3.05 (m, 2H), 2.75-2.63 (m, 2H); ^{13}C NMR(125 MHz, CDCl3) δ 165.96, 159.99, 144.18, 143.60, 134.47, 133.78, 133.75 (q, J = 3.60 Hz), 132.93, 129.70 (q, J = 35.43 Hz), 129.04, 125.97 (q, J = 3.60 Hz), 122.35 (q, J = 273.50 Hz), 120.25, 118.76, 118.33, 111.17, 59.89, 58.71, 58.47,

53.47, 53.33, 41.84, 40.04; ESI-MS: 502 $(M + H)^+$; HRMS-ESI (m/z): Calcd. For $C_{23}H_{19}F_3N_5O_3S$ $(M+H)^+$: 502.1115; Found: 502.1114.

8-nitro-2-(5-(4-nitrobenzyl)hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)-6-(trifluoromethyl)-4H-benzo[e][1,3]thiazin-4-one (6). According to above general procedure, employing 4-nitrobenzaldehyde afforded compound **6** as a yellow solid. mp: 230-232 ^oC; ^1H NMR (500 MHz, $CDCl_3$) δ 9.21 (s, 1H), 8.82 (s, 1H), 8.22-8.20 (m, 2H), 7.52-7.51 (m, 2H), 4.28-4.23 (m, 1H), 4.06-4.03 (m, 2H), 3.97-3.96 (m, 3H), 3.20-3.07 (m, 2H), 2.77-2.65 (m, 4H); ^{13}C NMR(125 MHz, CDCl3) δ 165.95, 160.01, 147.29, 146.29, 143.60, 134.46, 133.77 (q, J = 3.34 Hz), 129.25 (q, J = 35.40 Hz), 126.77, 126.47, 126.00, 125.96, 122.35 (q, J = 270.12 Hz), 59.94, 58.44, 53.35, 41.86, 40.05; ESI-MS: 522 $(M + H)^+$; HRMS-ESI (m/z): Calcd. For $C_{22}H_{19}F_3N_5O_5S$ $(M+H)^+$: 522.1054; Found: 522.1057.

8-nitro-6-(trifluoromethyl)-2-(5-(4-(trifluoromethyl)benzyl) hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)-4H-benzo[e][1,3]thiazin-4-one (7). According to above general procedure, employing 4-trifluorobenzaldehyde afforded compound **7** as a yellow solid. mp: 215-217 ^oC; ^1H NMR (500 MHz, $CDCl_3$) δ 8.88-8.87 (m, 2H), 7.68-7.66 (m, 2H), 7.55-7.54 (m, 2H), 4.05-3.97 (m, 2H), 3.75-3.61 (m, 4H), 3.34-3.31 (m, 1H), 3.10 (s, 1H), 2.97 (s, 1H), 2.72-2.65 (m, 2H); ^{13}C NMR (125 MHz, CDCl3) δ 165.14, 159.52, 144.59, 144.47, 135.18, 132.13, 132.11 (q, J = 3.70 Hz), 129.38, 127.87 (q, J = 31.82 Hz), 126.70, 126.55, 126.52，126.16，125.54 (q, J = 3.36 Hz), 123.96 (q, J = 275.64 Hz), 60.04, 59.91, 58.29, 56.48, 53.51, 49.06, 41.77; ESI-MS: 545 $(M + H)^+$; HRMS-ESI (m/z): Calcd. For $C_{23}H_{19}F_6N_4O_3S$ $(M+H)^+$: 545.1077; Found: 545.1081.

2-(5-(4-methoxybenzyl)hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)-8-nitro-6-(trifluoromethyl)-4H-benzo[e][1,3]thiazin-4-one (8). According to above general procedure, employing 4-methoxybenzaldehyde afforded compound **8** as a yellow solid. mp: 192-194 ^oC; ^1H NMR (500 MHz, $CDCl_3$) δ 9.21 (s, 1H), 8.81 (s, 1H), 7.24-7.23 (m, 2H), 6.89-6.87 (m, 2H), 4.22-4.20 (m, 1H), 4.02-3.94 (m, 2H), 3.84 (s, 3H), 3.77-3.75 (m, 2H), 3.66-3.61 (m, 2H), 3.15-3.02 (m, 2H), 2.72-2.61 (m, 4H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.97, 159.87, 158.82, 143.59, 134.62, 133.76 (q, J = 3.40 Hz), 129.07 (q, J = 35.13 Hz), 126.87, 125.91 (q, J = 3.58 Hz), 122.47 (q, J = 270.82 Hz), 114.14, 113.76 ,

59.68, 59.57, 58.47, 56.30, 55.28, 53.36, 41.84, 40.01; ESI-MS: 507 $(M + H)^+$; HRMS-ESI (m/z): Calcd. For $C_{23}H_{22}F_3N_4O_4S$ $(M+H)^+$: 507.1308; Found: 507.1305.

2-(5-(4-(tert-butyl)benzyl)hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)-8-nitro-6-(trifluoromethyl)-4H-benzo[e][1,3]thiazin-4-one (9). According to above general procedure, employing 4-tert-butylbenzaldehyde afforded compound **9** as a yellow solid. mp: 81-83 ^oC; ^1H NMR (500 MHz, DMSO) δ 8.88-8.87 (m, 2H), 7.32-7.31 (m, 2H), 7.22-7.21 (m, 2H), 4.01-3.95 (m, 2H), 3.76-3.73 (m, 1H), 3.63-3.56 (m, 3H), 3.34 (s, 2H), 3.08-2.96 (brs, 2H), 2.69-2.62 (m, 2H), 1.27 (s, 9H); ^{13}C NMR (125 MHz, DMSO) δ 165.11, 159.49, 149.56, 144.58, 136.34, 135.18, 132.10 (q, J = 3.47 Hz), 128.45, 127.77 (q, J = 34.40 Hz), 126.53 (q, J = 3.40 Hz), 125.36, 123.15 (q, J = 272.95 Hz), 60.15, 59.99, 58.61, 56.40, 53.56, 41.75, 34.59, 31.63; ESI-MS: 533 $(M + H)^+$; HRMS-ESI (m/z): Calcd. For $C_{26}H_{28}F_3N_4O_3S$ $(M+H)^+$: 533.1829; Found: 533.1833.

2-(5-(4-methylbenzyl)hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)-8-nitro-6-(trifluoromethyl)-4H-benzo[e][1,3]thiazin-4-one (10). According to above general procedure, employing 4-methylbenzaldehyde afforded compound **10** as a yellow solid. mp: 223-225 ^oC; ^1H NMR (500 MHz, $CDCl_3$) δ 9.21 (s, 1H), 8.81 (s, 1H), 7.22-7.17 (m, 4H), 4.61 (s, 1H), 4.00-3.98 (m, 2H), 3.67 (brs, 3H), 3.18-3.05 (m, 2H), 2.75 (brs, 4H), 2.37 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.97, 159.98, 143.60, 134.57, 133.78 (q, J = 3.41 Hz), 129.46 (q, J = 35.52 Hz), 129.18, 128.70, 128.59, 126.85, 126.50, 126.15, 125.91 (q, J = 3.61 Hz), 122.54 (q, J = 273.08 Hz), 59.44, 58.77, 56.10, 46.31, 41.81, 39.98, 21.13; ESI-MS: 491 $(M + H)^+$; HRMS-ESI (m/z): Calcd. For $C_{23}H_{22}F_3N_4O_3S$ $(M+H)^+$: 491.1359; Found: 491.1360.

8-nitro-2-(5-(4-(trifluoromethoxy)benzyl)hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)-6-(trifluoromethyl)-4H-benzo[e][1,3]thiazin-4-one (11). According to above general procedure, employing 4-(trifluoromethoxy)benzaldehyde afforded compound **11** as a yellow solid. mp: 188-189 ^oC; ^1H NMR (500 MHz, $CDCl_3$) δ 9.21 (s, 1H), 8.81 (s, 1H), 7.35-7.20 (m, 4H), 4.24 (s, 1H), 4.02-3.96 (m, 2H), 3.66 (brs, 3H), 3.17-3.04 (m, 1H), 2.75-2.61 (m, 4H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.95, 160.33, 143.60, 134.42, 133.78 (q, J = 3.74 Hz), 127.80(q, J = 35.40 Hz), 126.77, 125.98, 124.28, 122.40 (q, J = 273.50 Hz),

58.50, 58.28, 53.46, 41.78, 39.96; ESI-MS: 561 $(M + H)^+$; HRMS-ESI (m/z): Calcd. For $C_{23}H_{19}F_6N_4O_4S$ $(M+H)^+$: 561.1026; Found: 561.1028.

2-(5-benzylhexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)-8-nitro-6-(trifluoromethyl)-4H-benzo[e][1,3]thiazin-4-one (12). According to above general procedure, employing benzaldehyde afforded compound **12** as a yellow solid. ^{1}H NMR (500 MHz, DMSO) δ 8.88-8.87 (m, 2H), 7.30-7.24 (m, 5H), 4.03-3.96 (m, 2H), 3.74-3.72 (m, 1H), 3.60 (brs, 3H), 3.34 (brs, 1H), 3.09 (brs, 1H), 2.96 (brs, 1H), 2.69-2.62 (m, 2H); ^{13}C NMR (125 MHz, DMSO) δ 165.11, 159.48, 144.56, 139.39, 135.18, 132.11 (q, J = 3.60 Hz), 128.74, 128.65, 127.47 (q, J = 33.34 Hz), 127.27, 126.68, 126.52 (q, J = 3.46 Hz), 123.20 (q, J = 271.54 Hz), 60.07, 59.95, 58.94, 56.48, 56.38, 53.54, 41.75; ESI-MS: 477 $(M + H)^+$; HRMS-ESI (m/z): Calcd. For $C_{22}H_{20}F_3N_4O_3S$ $(M+H)^+$: 477.1203; Found: 477.1200.

2-(5-(3-fluorobenzyl)hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)-8-nitro-6-(trifluoromethyl)-4H-benzo[e][1,3]thiazin-4-one (13). According to above general procedure, employing 3-fluorobenzaldehyde afforded compound **13** as a yellow solid. mp: 176-178 ^{o}C; ^{1}H NMR (500 MHz, DMSO) δ 8.88-8.86 (m, 2H), 7.36-7.34 (m, 1H), 7.16-7.04 (m, 3H), 4.03-3.96 (m, 2H), 3.76-3.74 (m, 2H), 3.62 (s, 3H), 3.34 (s, 1H), 3.09 (brs, 1H), 2.97 (brs, 1H), 2.71-2.63 (m, 2H); ^{13}C NMR (125 MHz, DMSO) δ 165.11, 163.90, 161.48, 159.49, 144.56, 142.61, 142.54, 135.17, 132.11 (q, J = 3.53 Hz), 130.58, 130.50, 130.10, 127.79 (q, J = 34.29 Hz), 126.69, 126.53 (q, J = 3.36 Hz), , 124.66, 124.64, 123.24 (q, J = 272.89 Hz), 115.30, 115.08, 114.14, 113.93, 60.03, 59.89, 58.20, 56.32, 53.51, 41.75; ESI-MS: 495 $(M + H)^+$; HRMS-ESI (m/z): Calcd. For $C_{22}H_{19}F_4N_4O_3S$ $(M+H)^+$: 495.1109; Found: 495.1111.

2-(5-(3-chlorobenzyl)hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)-8-nitro-6-(trifluoromethyl)-4H-benzo[e][1,3]thiazin-4-one (14). According to above general procedure, employing 3-chlorobenzaldehyde afforded compound **14** as a yellow solid. mp: 177-180 ^{o}C; ^{1}H NMR (500 MHz, DMSO) δ 8.87 (s, 2H), 7.34-7.21 (m, 4H), 3.99-3.97 (m,2H), 3.77-3.75 (m,1H), 3.61 (brs, 3H), 3.34 (brs, 2H), 3.08 (brs, 1H), 2.96 (brs, 1H), 2.68-2.62 (m, 2H); ^{13}C NMR (125 MHz, DMSO) δ 165.11, 159.47, 144.56, 142.14, 135.16, 133.37, 132.12, 132.09, 130.54, 128.41, 127.76 (q, J = 34.66 Hz), 126.70, 126.52(q, J =

3.54 Hz), 123.23 (q, J = 273.27 Hz), 60.04, 59.90, 58.07, 56.29, 53.51; ESI-MS: 511 (M + H)$^+$; HRMS-ESI (m/z): Calcd. For $C_{22}H_{19}ClF_3N_4O_3S$ (M+H)$^+$: 511.0813; Found: 511.0815.

2-(5-(3-bromobenzyl)hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)-8-nitro-6-(trifluoromethyl)-4H-benzo[e][1,3]thiazin-4-one (15). According to above general procedure, employing 3-bromobenzaldehyde afforded compound **15** as a yellow solid. mp: 172-174 ^{o}C; ^{1}H NMR (500 MHz, DMSO) δ 8.88-8.87 (m, 2H), 7.48-7.42 (m, 2H), 7.32-7.28 (m, 2H), 4..01-3.95 (m, 2H), 3.78-3.75 (m, 1H), 3.63-3.60 (m, 3H), 3.34 (s, 1H), 3.09 (brs, 1H), 2.96 (brs, 1H), 2.69-2.62 (m, 2H); ESI-MS: 555 (M + H)$^+$; HRMS-ESI (m/z): Calcd. For $C_{22}H_{19}BrF_3N_4O_3S$ (M+H)$^+$: 555.0308; Found: 555.0306.

3-((5-(8-nitro-4-oxo-6-(trifluoromethyl)-4H-benzo[e][1,3]thiazin-2-yl)hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)methyl)benzonitrile (16). According to above general procedure, employing 3-formylbenzonitrile afforded compound **16** as a yellow solid. ^{1}H NMR (500 MHz, DMSO) δ 8.88-8.87 (m, 2H), 7.74-7.66 (m, 3H), 7.55-7.52 (m, 1H), 4.00-3.96 (m, 2H), 3.77-3.75 (m, 1H), 3.66-3.62 (m, 3H), 3.34 (s, 1H), 3.09 (brs, 1H), 2.97 (brs, 1H), 2.71-2.64 (m, 2H); ^{13}C NMR (125 MHz, DMSO) δ 165.11, 159.47, 144.56, 141.26, 135.17, 133.67, 132.13, 131.19, 129.95, 127.79 (q, J = 35.18 Hz), 126.68, 126.53 (q, J = 3.61 Hz), 124.48 (q, J = 270.99 Hz), 119.32, 111.68, 60.01, 59.82, 57.81, 56.28, 53.47, 41.76; ESI-MS: 502 (M + H)$^+$ HRMS-ESI (m/z): Calcd. For $C_{23}H_{19}F_4N_5O_3S$ (M+H)$^+$: 502.1155; Found: 502.1151.

8-nitro-2-(5-(3-nitrobenzyl)hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)-6-(trifluoromethyl)-4H-benzo[e][1,3]thiazin-4-one (17). According to above general procedure, employing 3-nitrobenzaldehyde afforded compound **17** as a yellow solid. mp: 199-200 ^{o}C; ^{1}H NMR (500 MHz, DMSO) δ 8.87-8.86(m, 2H), 8.13-8.09(m, 2H), 7.77-7.76(m, 1H), 7.63-7.59(m, 1H), 4.01-3.95(m, 2H), 3.79-3.74(m, 3H), 3.64-3.62(m, 1H),3.09(brs, 1H),2.97(brs, 1H),2.72-2.65(m, 2H); ^{13}C NMR(125 MHz, DMSO) δ 165.13, 159.49, 148.30, 144.57, 142.00, 135.42, 135.17, 132.12(q, J=3.52Hz), 130.22, 130.11, 127.95, 127.24 (q, J = 35.21 Hz), 126.54 (q, J = 3.47 Hz), 124.49, 122.02 (q, J = 270.12 Hz), 60.02, 59.87, 57.69, 56.29, 53.50, 41.77; ESI-MS: 522 (M + H)$^+$; HRMS-ESI (m/z): Calcd. For $C_{22}H_{19}F_3N_5O_5S$ (M+H)$^+$: 522.1054; Found: 522.1051.

8-nitro-6-(trifluoromethyl)-2-(5-(3-(trifluoromethyl)benzyl)hexahydropyrrolo [3,4-c] pyrrol-2(1H)-yl)-4H-benzo[e][1,3]thiazin-4-one (18). According to above general procedure, employing 3-(trifluoromethyl)benzaldehyde afforded compound **18** as a yellow solid. mp: 135-136 ^{o}C; ^{1}H NMR (500 MHz, DMSO) δ 8.88-8.87 (m, 2H), 7.62-7.56 (m, 4H), 4.01-3.97 (m, 3H), 3.79-3.62 (m, 5H), 3.34 (s, 1H), 3.10 (brs, 1H), 2.97 (brs, 1H), 2.70-2.63 (m, 2H); ESI-MS: 545 $(M + H)^{+}$; HRMS-ESI (m/z): Calcd. For $C_{23}H_{19}F_6N_4O_3S$ $(M+H)^{+}$: 545.1077; Found: 545.1080.

2-(5-(3-methoxybenzyl)hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)-8-nitro-6-(trifluoromethyl)-4H-benzo[e][1,3]thiazin-4-one (19). According to above general procedure, employing 3-methoxybenzaldehyde afforded compound **19** as a yellow solid. mp: 101-102 ^{o}C; ^{1}H NMR(500 MHz, $CDCl_3$) δ 9.18 (s, 2H), 8.80 (s, 1H), 6.97-6.86 (m, 4H), 4.19-3.88 (m, 9H), 3.28-2.84 (m, 6H); ESI-MS: 507 $(M + H)^{+}$; HRMS-ESI (m/z): Calcd. For $C_{23}H_{21}F_3N_4O_4S$ $(M+H)^{+}$: 507.1308; Found: 507.1305.

2-(5-(2-fluorobenzyl)hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)-8-nitro-6-(trifluoromethyl)-4H-benzo[e][1,3]thiazin-4-one (20). According to above general procedure, employing 2-fluorobenzaldehyde afforded compound **20** as a yellow solid. mp: 154-156 ^{o}C; ^{1}H NMR (500 MHz, DMSO) δ8.88-8.86 (m, 2H),7.43-7.40 (m, 1H), 7.32-7.31 (m, 1H), 7.18-7.14 (m, 2H), 4.02 (m, 2H), 3.73-3.59 (m, 5H), 3.34 (s, 3H), 3.08 (brs, 1H), 2.96 (brs, 1H), 2.71-2.64 (m, 4H); ^{13}C NMR (125 MHz, DMSO) δ 165.10, 162.09, 159.67, 159.50, 144.56, 135.17, 132.10 (q, J = 3.53 Hz), 131.58, 131.53, 130.10, 129.42, 129.34, 127.93 (q, J = 34.53 Hz), 127.25, 126.53 (q, J = 3.53 Hz), 125.65, 125.50, 124.70 (q, J = 3.25 Hz), 123.24 (q, J = 272.51 Hz), 115.66, 115.44, 59.86, 59.72, 56.33, 53.48, 51.31, 41.74; ESI-MS: 495 $(M + H)^{+}$; HRMS-ESI (m/z): Calcd. For $C_{22}H_{19}F_4N_4O_3S$ $(M+H)^{+}$: 495.1109; Found: 495.1110.

2-(5-(3,4-difluorobenzyl)hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)-8-nitro-6-(trifluoromethyl)-4H-benzo[e][1,3]thiazin-4-one (21). According to above general procedure, employing 3,4-difluorobenzaldehyde afforded compound **21** as a yellow solid. mp: 151-153 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.20 (s, 1H), 8.81 (s, 1H), 7.31 (brs, 1H), 6.88-6.84 (m, 2H), 4.23 (brs, 1H), 4.03-3.94 (m, 2H), 3.69 (brs, 3H),3.15 (brs, 1H), 3.03 (brs,1H), 2.74 (brs, 2H), 2.67 (brs,2H); ^{13}C NMR (125 MHz, DMSO) δ 165.11, 161.80 (q,

J = 247.5 Hz), 160.85 (q, *J* = 250.6 Hz), 159.51, 144.58, 135.17, 132.80 (d, *J* = 3.3 Hz), 132.11 (q, *J* = 3.7 Hz), 127.77 (q, *J* = 36.0 Hz), 126.68, 126.53 (q, *J* = 3.7 Hz), 123.13 (q, *J* = 272.7 Hz), 122.05 (d, J = 3.5 Hz), 121.90 (d, *J* =3.5 Hz), 111.82 (d, *J* = 3.8 Hz), 111.61 (d, *J* = 3.9 Hz), 104.05(t, *J* = 26.3 Hz), 59.66 (d, *J* = 14.7 Hz), 56.32, 53.46, 50.86, 41.72; ESI-MS: 513 $(M + H)^+$; HRMS-ESI (m/z): Calcd. For $C_{22}H_{18}F_5N_4O_3S$ $(M+H)^+$: 513.1014; Found: 513.1017.

2-(5-(3,4-dichlorobenzyl)hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)-8-nitro-6-(trifluoromethyl)-4H-benzo[e][1,3]thiazin-4-one (22). According to above general procedure, employing 3,4-dichlorobenzaldehyde afforded compound **22** as a yellow solid. mp: 113-115 ^oC; ^1H NMR (500 MHz, DMSO) δ 8.89 (s, 1H), 8.87 (s, 1H), 7.58 (s, 1H), 7.50 (d, *J* = 8.2Hz, 1H), 7.40 (d, J=8.2HZ, 1H), 4.03-4.00 (m, 2H), 3.75-3.72 (m, 1H), 3.69 (s, 2H), 3.63-3.60 (m, 1H), 3.10 (brs, 1H), 2.97 (brs, 1H), 2.72 (d, *J* = 8.4 Hz, 1H), 2.69 (d, J = 8.4 Hz, 1H), 2.60-2.56 (m, 2H); ^{13}C NMR (125 MHz, DMSO) δ 165.13, 159.51, 144.58, 135.90, 135.18, 134.16, 132.52, 132.13(q, J = 3.7 Hz), 129.05, 127.95, 127.74, 127.61, 127.26, 126.69, 126.54 (q, J = 3.7 Hz), 124.49, 121.78, 59.90, 56.28, 55.10, 53.49, 41.77; ESI-MS: 545 $(M + H)^+$; HRMS-ESI (m/z): Calcd. For $C_{22}H_{18}Cl_2F_3N_4O_3S$ $(M+H)^+$: 545.0423; Found: 545.0425.

2-(5-(3-chloro-4-fluorobenzyl)hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)-8-nitro-6-(trifluoromethyl)-4H-benzo[e][1,3]thiazin-4-one (23). According to above general procedure, employing 3-chloro-4-fluorobenzaldehyde afforded compound **23** as a yellow solid. mp: 73-75 ^oC; ^1H NMR (500 MHz, DMSO) δ 8.85 (d, *J* = 7.11 Hz, 2H), 7.4 (d, J = 6.77 Hz, 1H), 7.35-7.31 (m, 2H), 3.99-3.93 (m, 2H), 3.74 (d, J = 12.78 Hz, 1H), 3.61-3.58 (m, 4H), 3.06 (brs, 1H), 2.94 (brs, 1H), 2.68-2.66 (m, 1H), 2.62-2.61 (m, 1H), 2.53 (brs, 1H); ^{13}C NMR (125 MHz, DMSO) δ 165.12, 159.49, 156.622 (d, J = 246.52Hz), 144.57, 137.38, 135.16, 132.23 (q, J = 3.79 Hz), 130.58, 129.31 (d, J = 7.05Hz), 127.79 (q, J = 34.30 Hz), 126.70, 126.55 (q, J = 3.55 Hz), 123.13 (q, J = 272.73 Hz), 119.56 (d, J = 17.68 Hz), 117.08 (d, J = 20.80 Hz), 59.83, (d, J = 14.98 Hz), 57.34, 56.25, 53.45, 41.72; ESI-MS: 529 $(M + H)^+$; HRMS-ESI (m/z): Calcd. For $C_{22}H_{18}ClF_4N_4O_3S$ $(M+H)^+$: 529.0719; Found: 529.0716.

2-(5-(4-chloro-3-fluorobenzyl)hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)-8-nitro-6-(trifluoromethyl)-4H-benzo[e][1,3]thiazin-4-one (24). According to above general procedure, employing 4-chloro-3-fluorobenzaldehyde afforded compound **24** as a yellow solid. mp: 204-206 ^{o}C; ^{1}H NMR (500 MHz, DMSO) δ 9.16 (s, 1H), 8.77 (s, 1H), 7.30 (t, *J* = 7.81 Hz, 1H), 7.08 (d, J = 9.73 Hz, 1H), 7.00 (d, J = 7.85 Hz, 1H), 4.22-4.17 (m, 1H), 3.98 (t, *J* = 9.90 Hz, 1H), 3.91-3.89 (m, 1H), 3.60-3.54 (m, 3H), 3.12 (brs, 1H), 2.99 (brs, 1H), 2.69 (brs, 2H), 2.58-2.56 (m, 2H); ^{13}C NMR (125 MHz, DMSO) δ 166.09, 160.10, 159.45, 156.97, 143.72, 134.62, 133.90 (q, J = 3.35 Hz), 130.63, 129.78 (q, J = 35.51 Hz), 126.95, 126.05 (q, 3.65 Hz), 124.81, 122.54 (q, J = 273.48 Hz), 116.64 (d, J = 21.46 Hz), 59.87 (d, J = 14.46 Hz), 58.24, 56.29, 53.39, 41.96, 40.14; ESI-MS: 529 $(M + H)^{+}$; HRMS-ESI (m/z): Calcd. For $C_{22}H_{18}ClF_4N_4O_3S$ $(M+H)^{+}$: 529.0719; Found: 529.0721.

2-(5-(2-chloro-4-fluorobenzyl)hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)-8-nitro-6-(trifluoromethyl)-4H-benzo[e][1,3]thiazin-4-one (25). According to above general procedure, employing 2-chloro-4-fluorobenzaldehyde afforded compound **25** as a yellow solid. mp: 149-151 ^{o}C; ^{1}H NMR (500 MHz, DMSO) δ 8.85 (s,1H), 8.83 (s, 1H), 7.49 (t, *J* = 7.10 Hz, 1H), 7.36 (d, *J* = 8.57 Hz, 1H), 7.17 (t, *J* = 8.05 Hz, 1H), 4.14-3.94 (m, 2H), 3.71 (d, J = 12.75 Hz, 1H), 3.66 (s, 1H), 3.58 (d, J = 10.19 Hz, 1H), 3.07 (brs, 1H), 3.07 (brs, 1H), 2.95 (brs, 1H), 2.71 (d, J = 8.69 Hz, 1H), 2.65 (d, J = 8.69 Hz, 1H), 2.57 (brs, 2H); ^{13}C NMR (125 MHz, DMSO) δ 164.64, 160.80 (d, J = 246.23 Hz), 159.03, 144.10, 134.70, 133.44 (d, J = 10.57 Hz), 132.57 (d, J = 3.33 Hz), 131.80, 131.72, 131.64 (q, J = 3.71 Hz), 127.31 (q, J = 34.65 Hz), 126.21, 126.07 (q, J = 3.50 Hz), 122.66 (q, J = 272.59 Hz), 116.36 (d, J = 24.63 Hz), 114.20 (d, J = 20.61 Hz), 59.39 (d, J = 11.95 Hz), 55.83, 54.55, 53.01, 41.30; ESI-MS: 529 $(M + H)^{+}$; HRMS-ESI (m/z): Calcd. For $C_{22}H_{18}ClF_4N_4O_3S$ $(M+H)^{+}$: 529.0719; Found: 529.0717.

2-(5-(2,4-difluorobenzyl)hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)-8-nitro-6-(trifluoromethyl)-4H-benzo[e][1,3]thiazin-4-one (26). According to above general procedure, employing 2,4-difluorobenzaldehyde afforded compound **26** as a yellow solid. mp: 144-146 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.20 (s, 1H), 8.81 (s, 1H), 7.31 (brs, 1H), 6.88-6.84 (m, 2H), 4.23 (brs, 1H), 4.03-3.94 (m, 2H), 3.69 (brs, 3H),3.15 (brs, 1H), 3.03 (brs,1H), 2.74 (brs, 2H), 2.67 (brs,2H); ^{13}C NMR (125 MHz, DMSO) δ 165.11, 161.80 (q, *J* = 247.5 Hz), 160.85 (q, *J* = 250.6 Hz), 159.51, 144.58, 135.17, 132.80 (d, *J* = 3.3 Hz),

132.11 (q, *J* = 3.7 Hz), 127.77 (q, *J* = 36.0 Hz), 126.68, 126.53 (q, *J* = 3.7 Hz), 123.13 (q, *J* = 272.7 Hz), 122.05 (d, J = 3.5 Hz), 121.90 (d, *J* =3.5 Hz), 111.82 (d, *J* = 3.8 Hz), 111.61 (d, *J* = 3.9 Hz), 104.05(t, *J* = 26.3 Hz), 59.66 (d, *J* = 14.7 Hz), 56.32, 53.46, 50.86, 41.72; ESI-MS: 513 $(M + H)^+$; HRMS-ESI (m/z): Calcd. For $C_{22}H_{19}F_5N_4O_3S$ $(M+H)^+$: 513.1014; Found: 513.1016.

2-(5-(2,4-dichlorobenzyl)hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)-8-nitro-6-(trifluoromethyl)-4H-benzo[e][1,3]thiazin-4-one (27). According to above general procedure, employing 2,4-dichlorobenzaldehyde afforded compound **27** as a yellow solid. mp: 106-108 ^oC; ^1H NMR (500 MHz, DMSO) δ 8.89 (s, 1H), 8.87 (s, 1H), 7.58 (s, 1H), 7.50 (d, *J* = 8.2Hz, 1H), 7.40 (d, J=8.2HZ, 1H), 4.03-4.00 (m, 2H), 3.75-3.72 (m, 1H), 3.69 (s, 2H), 3.63-3.60 (m, 1H), 3.10 (brs, 1H), 2.97 (brs, 1H), 2.72 (d, *J* = 8.4 Hz, 1H), 2.69 (d, J = 8.4 Hz, 1H), 2.60-2.56 (m, 2H); ^{13}C NMR (125 MHz, DMSO) δ 165.13, 159.51, 144.58, 135.90, 135.18, 134.16, 132.52, 132.13(q, J = 3.7 Hz), 129.05, 127.95, 127.74, 127.61, 127.26, 126.69, 126.54 (q, J = 3.7 Hz), 124.49, 121.78, 59.90, 56.28, 55.10, 53.49, 41.77; ESI-MS: 545 $(M + H)^+$; HRMS-ESI (m/z): Calcd. For $C_{22}H_{19}F_4N_4O_3S$ $(M+H)^+$: 545.0423; Found: 545.0422.

2-(5-(2-bromo-4-fluorobenzyl)hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)-8-nitro-6-(trifluoromethyl)-4H-benzo[e][1,3]thiazin-4-one (28). According to above general procedure, employing 2-bromo-4-fluorobenzaldehyde afforded compound **28** as a yellow solid. mp: 150-151 ^oC; ^1H NMR (500 MHz, DMSO) δ 8.88 (s, 1H), 8.87 (s, 1H), 7.55-7-49 (m, 2H), 7.25-7.24 (m, 1H), 4.02-3.98 (m, 2H), 3.75-3.61 (m, 4H), 3.10 (brs, 1H), 2.98 (brs, 1H), 2.76-2.68 (m, 2H), 2.60-2.59 (m, 2H); ^{13}C NMR (125 MHz, DMSO) δ 165.12, 161.17 (d, *J* = 247.45 Hz), 159.49, 144.57, 135.18, 134.68 (d, *J* = 3.26 Hz), 132.12 (d, *J* = 8.29 Hz), 127.78 (q, *J* = 34.50 Hz), 127.26, 127.20, 126.68, 126.56, 123.90 (d, *J* = 9.64 Hz), 123.13 (q, *J* = 272.48 Hz), 119.91 (d, J = 24.48 Hz), 115.10, 59.84, 57.47, 56.48, 56.32, 53.51, 41.78; ESI-MS: 573 $(M + H)^+$; HRMS-ESI (m/z): Calcd. For $C_{22}H_{19}F_4N_4O_3S$ $(M+H)^+$: 573.0214; Found: 573.0216.

8-nitro-2-(5-(pyridin-2-ylmethyl)hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)-6-(trifluoromethyl)-4H-benzo[e][1,3]thiazin-4-one (29). According to above general procedure, employing picolinaldehyde afforded compound **29** as a yellow solid. mp: 18-

174 °C; ^{1}H NMR (500 MHz, DMSO) δ 8.88 (s, 1H), 8.87 (s, 1H), 8.50 (s, 1H), 7.76 (brs, 1H), 7.44-7.42(m, 1H), 7.28 (s, 1H), 4.05-3.98 (m, 2H), 3.79-3.63 (m, 4H), 3.13 (brs, 1H), 3.00 (brs, 1H), 2.80-2.57 (m, 4H); ^{13}C NMR (125 MHz, DMSO) δ 165.97, 160.18, 149.30, 143.59, 137.00, 134.50, 133.78, 133.75, 133.72, 129.68 (q, *J* = 35.54 Hz), 126.78, 125.95 (q, J = 3.72 Hz), 125.89, 123.41, 122.76, 122.41 (q, *J* = 272.14 Hz), 60.27, 59.48, 55.72, 52.79, 41.85, 40.05; ESI-MS: 478 $(M + H)^+$; HRMS-ESI (m/z): Calcd. For $C_{21}H_{19}F_4N_5O_3S$ $(M+H)^+$: 478.1155; Found: 478.1157.

8-nitro-2-(5-(pyridin-3-ylmethyl)hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)-6-(trifluoromethyl)-4H-benzo[e][1,3]thiazin-4-one (30). According to above general procedure, employing nicotinaldehyde afforded compound **30** as a yellow solid. mp: 124-130 °C; ^{1}H NMR (500 MHz, DMSO) δ 9.14 (s, 1H), 8.76 (s, 1H), 8.62-8.53 (m, 3H), 7.70 (brs, 1H), 4.17 (brs, 1.5H), 3.97-3.93 (m, 2.5H), 3.75-3.65 (m, 4H), 3.17 (brs, 1H), 3.04 (brs, 1H), 2.76 (brs, 3H); ESI-MS: 478 $(M + H)^+$; HRMS-ESI (m/z): Calcd. For $C_{21}H_{19}F_4N_5O_3S$ $(M+H)^+$: 478.1155; Found: 478.1153.

8-nitro-2-(5-(pyridin-4-ylmethyl)hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)-6-(trifluoromethyl)-4H-benzo[e][1,3]thiazin-4-one (31). According to above general procedure, employing isonicotinaldehyde afforded compound **31** as a yellow solid. mp: 83-90 °C; ^{1}H NMR (500 MHz, DMSO) δ 8.88 (d, J=6.0Hz, 2H), 8.51 (d,J=3.6Hz, 2H), 7.34 (d, J=3.8Hz, 2H), 4.06-3.98 (m, 2H), 3.76-3.65 (m, 4H), 3.12 (brs, 1H), 3.02 (brs, 1H), 2.75-2.53 (m, 2H); ^{13}C NMR (125 MHz, DMSO) δ 165.10, 159.50, 150.40, 149.97, 148.54, 144.55, 135.17, 132.12 (q, J = 3.61 Hz), 127.79 (q, *J* = 34.71 Hz), 126.66, 126.54 (q, J = 3.56 Hz), 123.80, 123.13 (q, *J* = 272.56 Hz), 121.69, 60.06, 59.91, 57.62, 56.32, 53.47, 41.80; ESI-MS: 478 $(M + H)^+$; HRMS-ESI (m/z): Calcd. For $C_{21}H_{19}F_4N_5O_3S$ $(M+H)^+$: 478.1155; Found: 478.1158.

2-(5-(naphthalen-2-ylmethyl)hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)-8-nitro-6-(trifluoromethyl)-4H-benzo[e][1,3]thiazin-4-one (32). According to above general procedure, employing 2-naphthaldehyde afforded compound **32** as a yellow solid. mp: 126-128 °C; ^{1}H NMR (500 MHz, DMSO) δ 8.87 (s, 2H), 7.86-7.83 (m, 3H), 7.28 (s, 1H), 7.48-7.47 (s, 3H) , 4.02-3.95 (m, 2H), 3.77-3.75 (m, 3H), 3.63-3.61 (m, 1H), 3.09 (brs, 1H), 2.97 (brs, 1H), 2.72-2.65 (m, 2H), 2.59-2.56 (m, 2H); ^{13}C NMR (125 MHz, DMSO)

δ 165.12, 159.49, 144.56, 137.17, 135.18, 133.36, 132.67, 132.10 (q, *J* = 3.5 Hz), 130.11, 128.15, 127.94 (q, *J* = 5.3 Hz), 127.59, 127.38, 127.20, 126.96, 126.70, 126.52 (q, *J* = 3.6 Hz), 126.44, 123.14 (q, J = 273.2 Hz), 121.78, 119.07, 60.13, 59.07, 56.35, 53.55, 41.78; ESI-MS: 527 $(M + H)^+$; HRMS-ESI (m/z): Calcd. For $C_{26}H_{22}F_3N_4O_3S$ $(M+H)^+$: 527.1359; Found: 527.1361.

2-(5-(naphthalen-1-ylmethyl)hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)-8-nitro-6-(trifluoromethyl)-4H-benzo[e][1,3]thiazin-4-one (33). According to above general procedure, employing 1-naphthaldehyde afforded compound **33** as a yellow solid. mp: 111-113 ^oC; ^1H NMR (500 MHz, DMSO) δ 8.87 (s, 1H), 8.85 (s, 1H), 8.265 (d, *J* = 8.1 Hz, 1H), 7.86 (d, *J* = 7.9 Hz, 1H), 7.81 (d, *J* = 7.4 Hz, 1H), 7.45-7.42 (m, 2H), 7.38-7.31 (m, 2H), 4.05-386 (m, 4H), 3.77 (d, *J* = 13.0Hz. 1H), 3.54 (d, *J* = 11.1 Hz, 1H), 3.05 (brs, 1H), 3.94 (brs, 1H), 2.68 (d, *J* = 8.9 Hz, 2H), 2.60-2.55 (m, 2H); ^{13}C NMR (125 MHz, DMSO) δ 165.06, 159.32, 144.51, 135.29, 135.13, 133.80, 132.18, 132.08 (q, *J* = 3.7 Hz), 128.59, 128.09, 127.76 (q, *J* = 34.5 Hz), 126.87, 126.69, 126.52 (q, *J* = 3.6 Hz), 125.94 (q, *J* = 5.8 Hz), 125.75, 124.94, 123.14 (q, J = 272.6 Hz), 60.25 (d, *J* = 22.4 Hz), 57.29, 56.34, 53.60, 41.72; ESI-MS: 527 $(M + H)^+$; HRMS-ESI (m/z): Calcd. For $C_{26}H_{22}F_3N_4O_3S$ $(M+H)^+$: 527.1359; Found: 527.1362.

2-(5-((5-methoxy-1H-indol-3-yl)methyl)hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)-8-nitro-6-(trifluoromethyl)-4H-benzo[e][1,3]thiazin-4-one (34). According to above general procedure, employing 5-methoxy-1H-indole-3-carbaldehyde afforded compound **34** as a yellow solid. mp: 225-228 ^oC; ^1H NMR (500 MHz, DMSO) δ 10.69 (s, 1H), 8.86 (s, 2H), 7.19 (d, J = 8.74 Hz, 1H), 7.15 (s, 1H), 7.06 (s, 1H), 6.66 (d, J = 8.57 Hz, 1H), 3.94 (q, J = 9.54 Hz, 2H), 3.74-3.70 (m, 3H), 3.57 (s, 4H), 3.04 (brs, 1H), 2.91 (brs, 1H), 2.72 (d, J = 8.84 Hz, 1H), 2.67 (d, J = 8.84 Hz, 1H), 2.45 (brs, 2H); ESI-MS: 546 $(M + H)^+$; HRMS-ESI (m/z): Calcd. For $C_{25}H_{23}F_3N_5O_4S$ $(M+H)^+$: 546.1417; Found: 546.1420.

Synthesis of compound 35. To a stirred solution of A (42 mg, 0.2 mmol) in anhydrous MeOH (10 mL) was added BTZ core compound **D** (64 mg, 0.2 mmol) and Et_3N (0.6 mmol) at room temperature. The mixture was stirred overnight at 40 ^oC, and concentrated. The residue was purified by silica gel column (DCM : MeOH = 20 : 1) to yield the yellow solids **35** (53 mg, 54% yield), mp: 204-205 ^oC; ^1H NMR (125 MHz, DMSO) δ 8.88 (s, 1H), 8.87

(s, 1H), 3.98 (brs, 2H), 3.97-3.57 (m, 4H), 3.34-3.29 (m, 1H), 3.25-3.22 (m, 1H), 3.14 (brs, 1H), 3.03 (brs, 1H); 1.43 (s, 9H); ESI-MS: 487 $(M + H)^+$; HRMS-ESI (m/z): Calcd. For $C_{20}H_{21}F_3N_4O_5S$ $(M+H)^+$: 487.1258; Found: 487.1261.

Synthesis of compound 36. To a stirred solution of **35** (97 mg, 0.2 mmol) in DCM (5 mL) was added TFA (1 mL) at room temperature. The mixture was stirred for 2 hours and concentrated. The residue was diluted by DCM, and washed by $NaHCO_3$ solution (1 M), and saturated saline, dried over anhydrous $MgSO_4$, filtered and concentrated. The residue was purified over silica gel column (DCM : MeOH = 20 : 1) to compound **36** as a yellow solid (43 mg, 56% yield), mp: 219-221 ^oC; ^1H NMR (500 MHz, DMSO) δ 8.90 (s, 1H), 8.89 (s, 1H), 4.00-3.96 (m, 2H), 3.86 (d, J = 10.7 Hz, 1H), 3.77 (d, J = 8.50 Hz, 1H), 3.50-3.46 (m, 2H), 3.33 (d, J = 9.00 Hz, 3H), 3.25-3.20 (m, 2H); ESI-MS: 387 $(M + H)^+$; HRMS-ESI (m/z): Calcd. For $C_{15}H_{13}F_3N_4O_3S$ $(M+H)^+$: 387.0733; Found: 387.0735.

General synthesis procedure of compounds 37-43. A mixture of compound **A** (0.3 mmol) and corresponding ketones (0.4 mmol) in $Ti(OPr)_4$ was stirred at 70 ^oC for 8 hours and cooled to room temperature. MeOH (5 mL) and $NaCNBH_3$ (1.6 mmol) was added to the mixture, and stirred for 5 hours at 40 ^oC. The mixture was quenched by 1 N NaOH (10 mL), filtered by celite, and washed by MeOH. The MeOH was evaporated under vacuo. The residue was diluted by H_2O, and extracted by Et_2O. The combined organic layer was washed by brine, dried over anhydrous $MgSO_4$, filtered, and concentrated. The residue was purified over silica gel column (DCM : MeOH = 30 : 1) to yield oils **B37-B43** (yield, 30-55%).

To a stirred solution of **B37-B43** in DCM (5 mL) was added TFA (1 mL) at room temperature. The mixture was stirred for 2 hours and concentrated to afford the crude product **C37-C43** which was used directly in the next step without further purification. To a stirred solution of above crude **C37-C43** in anhydrous MeOH (10 mL) was added BTZ core compound **D** (0.3 mmol) and Et_3N (0.6 mmol) at room temperature. The mixture was stirred overnight at 40 ^oC, and concentrated. The residue was purified by column chromatography over silica gel (DCM : MeOH = 20 : 1) to yield the yellow solids, which were further treated by n-hexane to give **37-43. (**The data and NMR copies of compounds **37-43** were listed in the supporting information.)

8-nitro-6-(trifluoromethyl)-2-(5-(4-(trifluoromethyl)phenyl) hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)-4H-benzo[e][1,3]thiazin-4-one (37). According to above general procedure, employing 1-(4-(trifluoromethyl)phenyl)ethan-1-one afforded compound **37** as a yellow solid, mp: 169-170 ^{o}C; 1H NMR (500 Mz, CDCl3) δ 9.16 (s,1H), 8.77 (s, 1H), 7.55-7.54 (m, 2H), 7.41-7.39 (m, 2H), 4.24-4.14 (m, 1H), 4.02-3.92 (m, 1.5H), 3.82-3.78 (m, 0.5 H), 3.73-3.66 (m, 0.5 H), 3.53-3.49 (m, 0.5 H), 3.31 (t, J = 6.5 Hz, 1H), 3.12 (brs, 0.5 H), 3.06 (brs, 0.5H), 2.99 (brs, 0.5 H), 2.92 (brs, 0.5 H), 2.87 (d, J = 9.5 Hz, 1H), 2.60-2.53 (m, 1H), 2.49-2.42 (m, 2H), 1.35 (d, J = 6.0 Hz, 3H); 13C NMR (100 MHz, CDCl3) δ 166.08, 159.98, 149.28 (d, J = 16.83 Hz), 143.71, 134.66, 133.88, 129.69 (q, J = 35.2 Hz), 129.56(q, J = 32.1 Hz), 127.29, 126.94, 126.02 (q, J = 3.0 Hz), 125.64 (q, J = 3.0 Hz), 123.91, 122.44 (q, J = 271.0 Hz), 64.24, 58.84, 58.35 (d , J = 8.10 Hz), 56.53 (d, J = 33.49 Hz), 53.59 (d, J = 22.59 Hz), 41.76, 39.90, 23.23; ESI-MS: 559 $(M + H)^{+}$; HRMS-ESI (m/z): Calcd. For $C_{24}H_{21}F_6N_4O_3S$ $(M+H)^{+}$: 559.1233; Found: 559.1236.

8-nitro-2-(5-(4-(trifluoromethoxy)phenyl)hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)-6-(trifluoromethyl)-4H-benzo[e][1,3]thiazin-4-one (38). According to above general procedure, employing 1-(4-(trifluoromethoxy)phenyl)ethan-1-one afforded compound **38** as a yellow solid. mp: 150-151 ^{o}C; ^{1}H NMR (500 Mz, $CDCl_3$) δ 9.18 (s,1H), 8.78 (s, 1H), 7.30 (brs, 2H), 7.15 (brs, 2H), 4.24-4.15 (m, 1H), 4.02-3.94 (m, 1.5H), 3.82-3.79 (m, 0.5 H), 3.68-3.66 (m, 0.5 H), 3.52 (brs, 0.5 H), 3.26 (brs, 1H), 3.12 (brs, 0.5 H), 3.06 (brs, 0.5H), 2.99 (brs, 0.5 H), 2.93 (brs, 0.5 H), 2.85 (d, *J* = 9.5 Hz, 1H), 2.58-2.54 (m, 1H), 2.48-2.45 (m, 2H), 1.33 (d, *J* = 4.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.09, 159.99, 148.29, 143.97, 143.84, 143.73, 134.69, 133.93, 129.78 (q, *J* = 35.0 Hz), 128.25, 126.99, 126.04 (q, *J* = 3.0 Hz), 122.50 (q, *J* = 255.3 Hz), 121.17, 120.60 (q, *J* = 255.3 Hz), 63.89, 58.63, 56.60, 53.64, 41.78, 39.95, 23.34; ESI-MS: 575 $(M + H)^{+}$; HRMS-ESI (m/z): Calcd. For $C_{24}H_{21}F_6N_4O_4S$ $(M+H)^{+}$: 575.1182; Found: 575.1185.

2-(5-(3,4-difluorophenyl)hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)-8-nitro-6-(trifluoromethyl)-4H-benzo[e][1,3]thiazin-4-one (39). According to above general procedure, employing 1-(3,4-difluorophenyl)ethan-1-one afforded compound **39** as a yellow solid. mp: 75-80 ^{o}C; ^{1}H NMR (500 Mz, $CDCl_3$) δ 9.17 (s, 1H), 8.78 (s, 1H), 8.77-7.06 (m, 2H), 6.99 (brs, 1H), 4.22-4.16 (m, 1H), 4.02-3.92 (m, 1.5H), 3.82-3.80 (d,

J=11.78Hz, 0.5H), 3.74 (s, 0.5H), 3.73 (s, 0.5H), 3.71 (s, 0.5H), 3.70 (s, 0.5H), 3.66-3.65 (d, J=7.64Hz, 0.5H), 3.53-3.52 (d, J=7.48Hz, 0.5H), 3.22 (brs, 1H), 3.11 (brs, 0.5H), 3.06 (brs, 1H), 2.98 (brs, 1H), 2.93 (brs, 1H), 2.83-2.82 (d, J=8.67Hz, 1H), 2.58-2.54 (m, 1H), 2.46 (brs, 1H), 1.32 (brs, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.77, 133.93, 126.05, 122.71, 117.37, 63.61, 58.82, 58.63, 58.17, 56.64, 53.64, 53.52, 41.74, 39.94, 23.20, 18.59; ESI-MS: 527 $(M + H)^+$; HRMS-ESI (m/z): Calcd. For $C_{23}H_{20}F_5N_4O_3S$ $(M+H)^+$: 527.1171; Found: 527.1173.

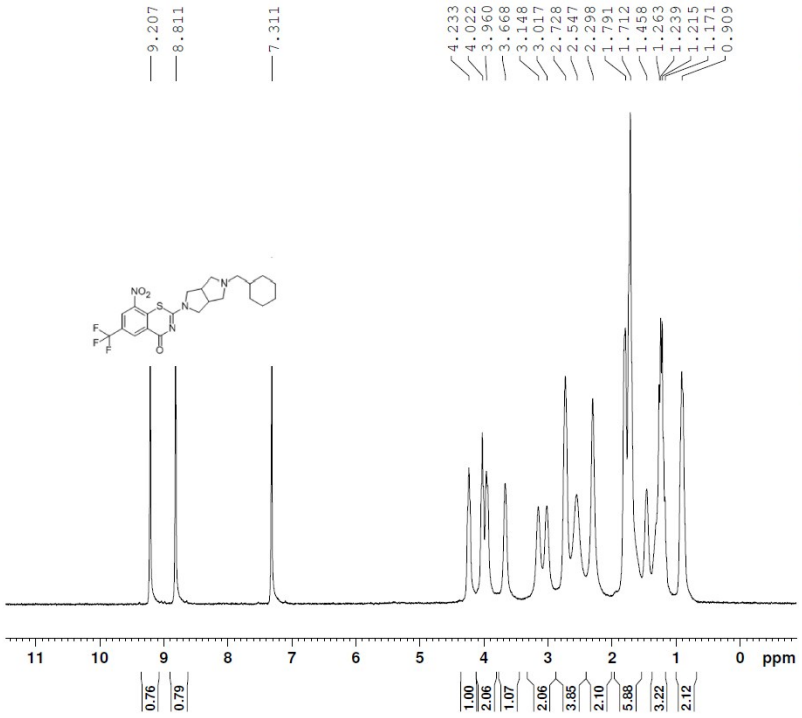
2-(5-(4-chloro-3-fluorophenyl)hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)-8-nitro-6-(trifluoromethyl)-4H-benzo[e][1,3]thiazin-4-one (40). According to above general procedure, employing 1-(4-chloro-3-fluorophenyl)ethan-1-one afforded compound **40** as a yellow solid. mp:138-139 ^oC; ^{1}H NMR (500 Mz, $CDCl_3$): δ 9.18 (s,1H), 8.78 (s, 1H), 7.31 (t, *J* = 8.0 Hz, 1H), 7.09 (t, *J* = 7.5 Hz,1H), 7.02 (d, *J* = 8.0 Hz, 1H), 4.23-4.16 (m, 1H), 4.02-3.92 (m, 1.5H), 3.82-3.80 (m, 0.5 H), 3.66-3.65 (m, 0.5 H), 3.53-3.52 (m, 0.5 H), 3.24 (brs, 1H), 3.12 (brs, 0.5 H), 3.06 (brs, 0.5H), 2.98 (brs, 0.5 H), 2.95 (brs, 0.5 H), 2.83 (brs, 1H), 2.60-2.45 (m, 3H), 1.32 (d, *J* = 5.5 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.13, 160.04, 159.56, 157.09, 146.47, 146.41, 146.26, 146.21, 143.73, 134.66, 133.92, 130.74, 129.97 (q, *J* = 70.75Hz), 129.61 (q, *J* =70.75Hz), 126.97, 126.62, 126.03 (q, *J* = 3.50Hz), 123.90 (q, *J* =275.61Hz), 123.29 (q, *J* =273.07Hz), 119.36, 118.48, 115.17, 114.93, 63.65, 58.85, 58.75, 58.28, 58.16, 56.65, 56.33, 53.63, 53.51, 51.04, 41.73, 39.92, 29.84, 23.16; ESI-MS: 543 $(M + H)^+$; HRMS-ESI (m/z): Calcd. For $C_{23}H_{19}ClF_4N_4O_3S$ $(M+H)^+$: 543.0875; Found: 543.0877.

2-(5-(3-chloro-4-fluorophenyl)hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)-8-nitro-6-(trifluoromethyl)-4H-benzo[e][1,3]thiazin-4-one (41). According to above general procedure, employing 1-(3-chloro-4-fluorophenyl)ethan-1-one afforded compound **41** as a yellow solid. mp: 168-169 ^oC; ^{1}H NMR (500 Mz, $CDCl_3$): δ 9.17 (s,1H), 8.78 (s, 1H), 7.31 (t, J = 5.9 Hz, 1H), 7.14 (brs, 1H), 7.08-7.05 (m, 1H), 4.21-4.15 (m, 1H), 4.01-3.91 (m, 1.5H), 3.82-3.80 (m, 0.5 H), 3.66-3.64 (m, 0.5 H), 3.53 (brs, 0.5 H), 3.22 (brs, 1H), 3.11 (brs, 0.5 H), 3.06 (brs, 0.5H), 2.98 (brs, 0.5 H), 2.93 (brs, 0.5 H), 2.81 (d, *J* = 6.5 Hz, 1H), 2.59-2.51 (m, 1H), 2.48-2.46 (m, 2H), 1.32 (brs, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.87, 134.04, 129.15, 126.16, 63.59, 58.74, 53.63, 40.06, 18.69; ESI-MS: 543 $(M + H)^+$; HRMS-ESI (m/z): Calcd. For $C_{23}H_{19}ClF_4N_4O_3S$ $(M+H)^+$: 543.0875; Found: 543.0877.

2-(5-(3,5-difluorophenyl)hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)-8-nitro-6-(trifluoromethyl)-4H-benzo[e][1,3]thiazin-4-one (42). According to above general procedure, employing 1-(3,5-difluorophenyl)ethan-1-one afforded compound **42** as a yellow solid. mp: 168-169 ^{o}C; ^{1}H NMR (500 Mz, $CDCl_3$): δ 9.16 (s,1H), 8.79 (s, 1H), 7.38 (brs, 1H), 6.84 (t, = 8.6 Hz,1H), 6.75 (t, = 10.0 Hz,1H), 4.22-4.14 (m, 1H), 4.02-3.95 (m, 1.5H), 3.82-3.79 (m, 0.5 H), 3.71-3.64 (m, 1.5 H), 3.53-3.49 (m, 0.5 H), 3.11 (brs, 0.5 H), 3.05 (brs, 0.5H), 2.98 (brs, 0.5 H), 2.92 (brs, 0.5 H), 2.87-2.82 (m, 1H), 2.60-2.44 (m, 3H), 1.32 (brs, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 166.0, 160.0, 143.7, 129.7 (q, J = 36.0 Hz), 129.33 (t, J = 7.5 Hz), 127.00, 126.0 (q, J = 3.0 Hz), 122.5 (q, J = 271.5 Hz), 111.7 (d, J = 22.5 Hz), 103.7 (t, J = 27.0 Hz), 60.51, 58.33, 58.22, 56.68, 56.46, 55.31, 53.80, 53.52, 41.70, 39.91, 22.06, 21.17, 14.32; ESI-MS: 527 $(M + H)^+$; HRMS-ESI (m/z): Calcd. For $C_{23}H_{20}F_5N_4O_3S$ $(M+H)^+$: 527.1171; Found: 527.1173.

8-nitro-6-(trifluoromethyl)-2-(5-(3,4,5-trifluorophenyl)hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)-4H-benzo[e][1,3]thiazin-4-one (43). According to above general procedure, employing 1-(3,4,5-trifluorophenyl)ethan-1-one afforded compound **43** as a yellow solid. mp: 158-161 ^{o}C; ^{1}H NMR (500 Mz, $CDCl_3$): δ 9.16 (s,1H), 8.77 (s, 1H), 6.92 (brs, 2H), 4.22-4.15 (m, 1H), 4.02-3.92 (m, 1.5H), 3.84-3.80 (m, 0.5 H), 3.67-3.63 (m, 0.5 H), 3.55-3.53 (m, 0.5 H), 3.20 (brs, 1H), 3.13 (brs, 0.5H), 3.08 (brs, 0.5 H), 2.99 (brs, 1H), 2.82 (brs, 1H), 2.59-2.48 (m, 3H), 1.31 (brs, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 166.07, 160.11, 151.40 (ddd, J_1 = 3.6 Hz, J_1 = 9.9 Hz, J_1 = 248.8 Hz), 143.75, 134.60, 133.89, 129.81 (q, J = 34.5 Hz), 126.97, 126.03 (q, J = 3.0 Hz), 122.50 (q, J = 276.0 Hz), 110.73 (d, J = 16.5 Hz), 63.59, 60.52, 58.39 (d, J = 106.19 Hz), 56.35, 53.51, 41.72, 39.90, 23.12, 22.98, 21.17, 14.33; ESI-MS: 545 $(M + H)^+$; HRMS-ESI (m/z): Calcd. For $C_{23}H_{19}F_6N_4O_3S$ $(M+H)^+$: 545.1077; Found: 545.1080.

NMR copies of target compounds.

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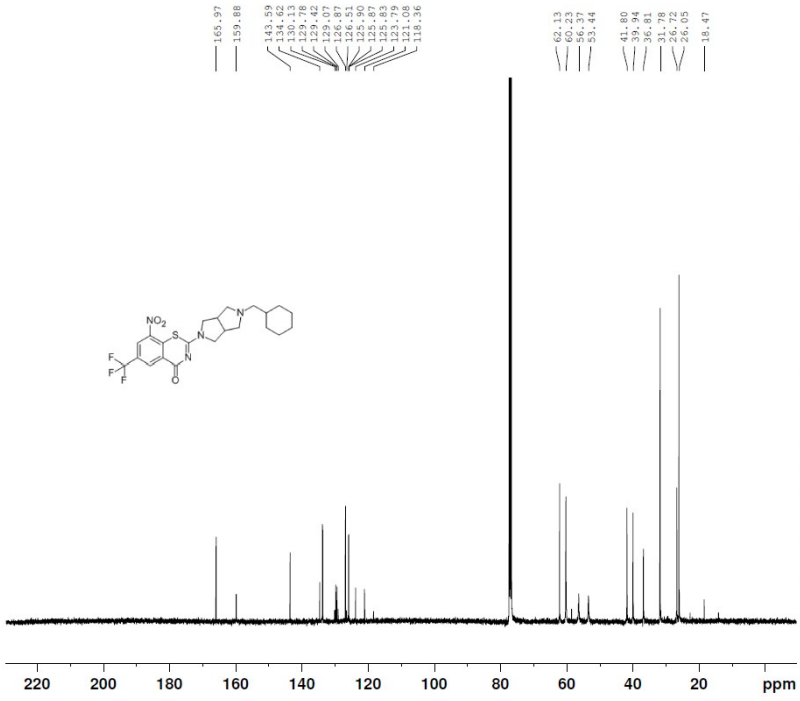


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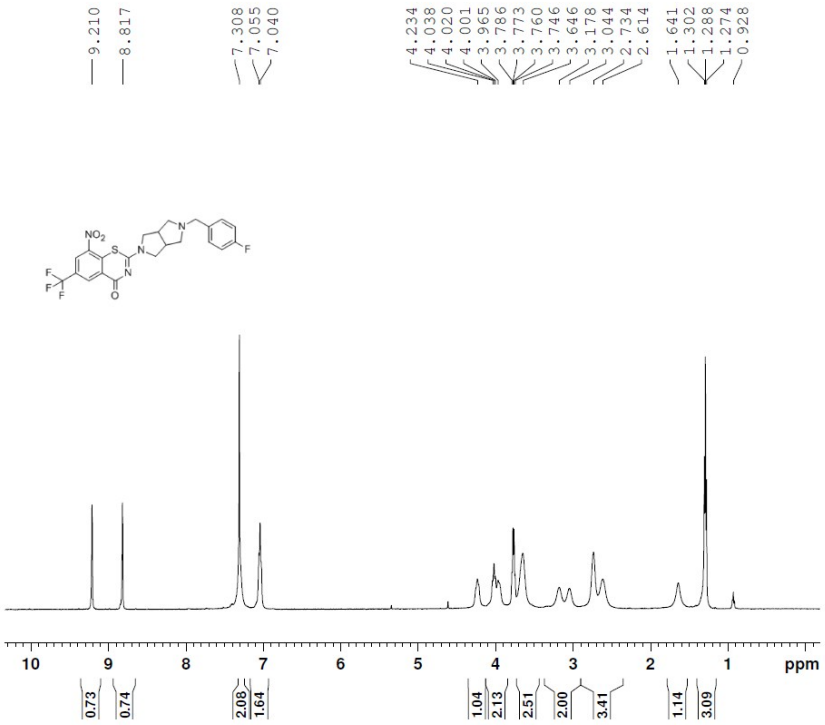


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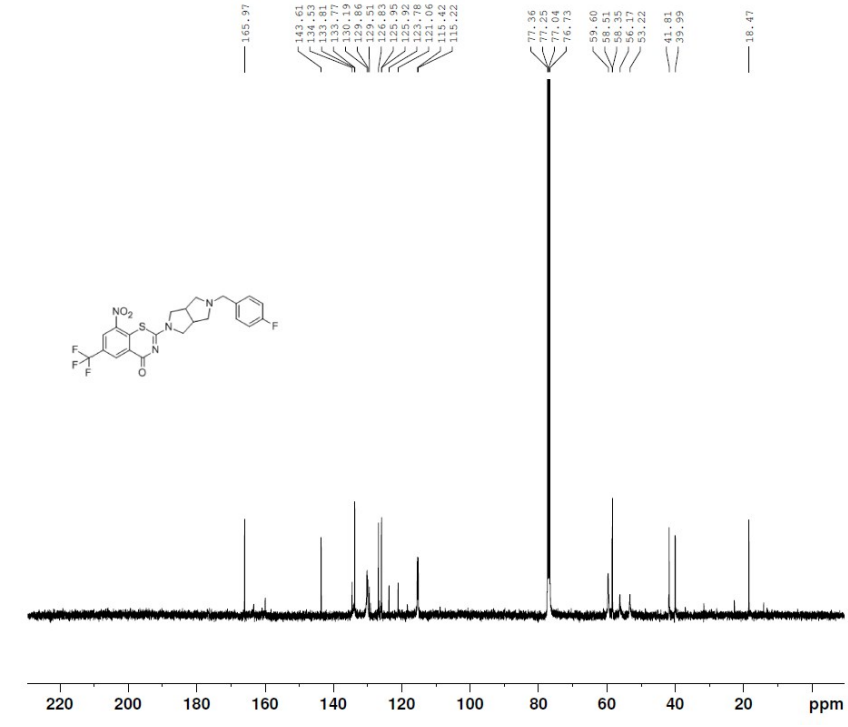


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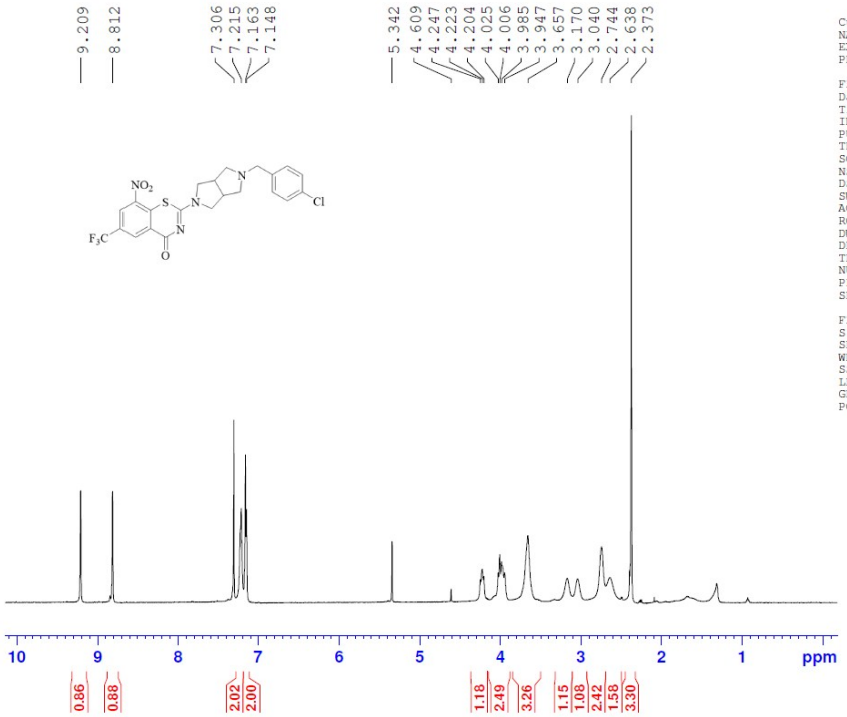
NUC2                       1H
CPDPRG[2                waltz16
PCPD2                   80.00 usec
PLW2             8.14700031 W
PLW12            0.15600000 W
PLW13            0.09983800 W

F2 - Processing parameters
SI                      32768
SF                 100.6127690 MHz
WDW                        EM
SSB       0
LB                      1.00 Hz
GB        0
PC                      1.40
```




```
Current Data Parameters
NAME        lq-2-53 0509
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_           20170508
Time               15.15
INSTRUM    WNMR-I-500MHz
PULPROG            s1pu1
TD                 48000
SOLVENT            CDCl3
NS                    10
DS                     0
SWH           12000.000 Hz
AQ             2.0000000 sec
RG                  65.6
DW                41.667 usec
DE                30.00 usec
TE                298.4 K
NUC1                  1H
PL1              120.00 dB
SFO1         499.7053818 MHz

F2 - Processing parameters
SI                 32768
SF           499.7017639 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB                  0.1
PC                 1.00
```

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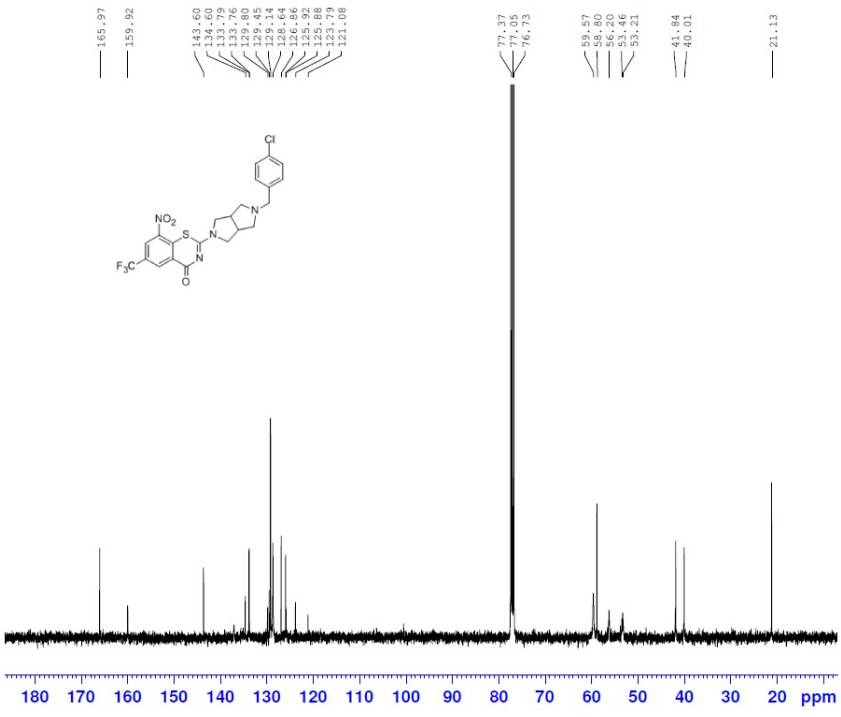


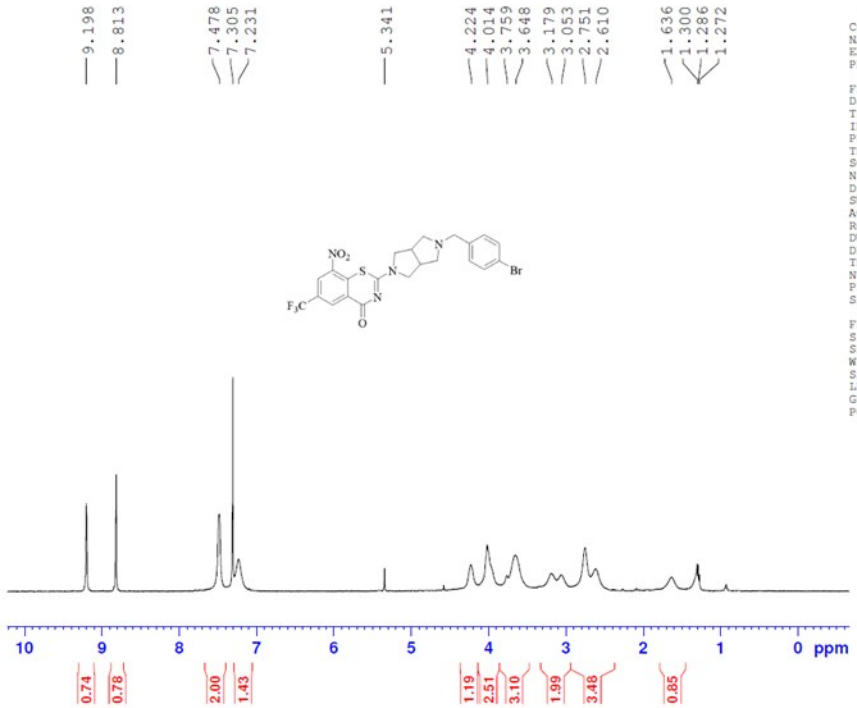

```
Current Data Parameters
NAME       20170515  lq-2-53
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_           20170515
Time               15.51
INSTRUM            spect
PROBHD   5 mm CPPBBO BB
PULPROG          zgpg30
TD                 32768
SOLVENT            CDCl3
NS                  4000
DS                     4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             0.6815744 sec
RG                  77.6
DW                20.800 usec
DE                18.00 usec
TE                298.0 K
D1             1.00000000 sec
D11            0.03000000 sec
TD0                  500

======== CHANNEL f1 ========
SFO1         100.6238345 MHz
NUC1                 13C
P1                  9.84 usec
PLW1         38.00000000 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2               80.00 usec
PLW2          8.14700031 W
PLW12         0.15600000 W
PLW13         0.09983800 W

F2 - Processing parameters
SI                 32768
SF           100.6127690 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB         0
PC                 1.40
```




```
Current Data Parameters
NAME         1q-2-61 0511
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170511
Time               14.02
INSTRUM   WNMR-I-500MHz
PULPROG            slpul
TD                 48000
SOLVENT            CDCl3
NS                     9
DS                     0
SWH          12000.000 Hz
AQ           2.0000000 sec
RG                  62.7
DW             41.667 usec
DE             30.00 usec
TE               298.1 K
NUC1                1H
PL1             120.00 dB
SFO1       499.7053818 MHz

F2 - Processing parameters
SI                 32768
SF         499.7017639 MHz
WDW                   EM
SSB       0
LB                1.00 Hz
GB                 0.1
PC                1.00
```

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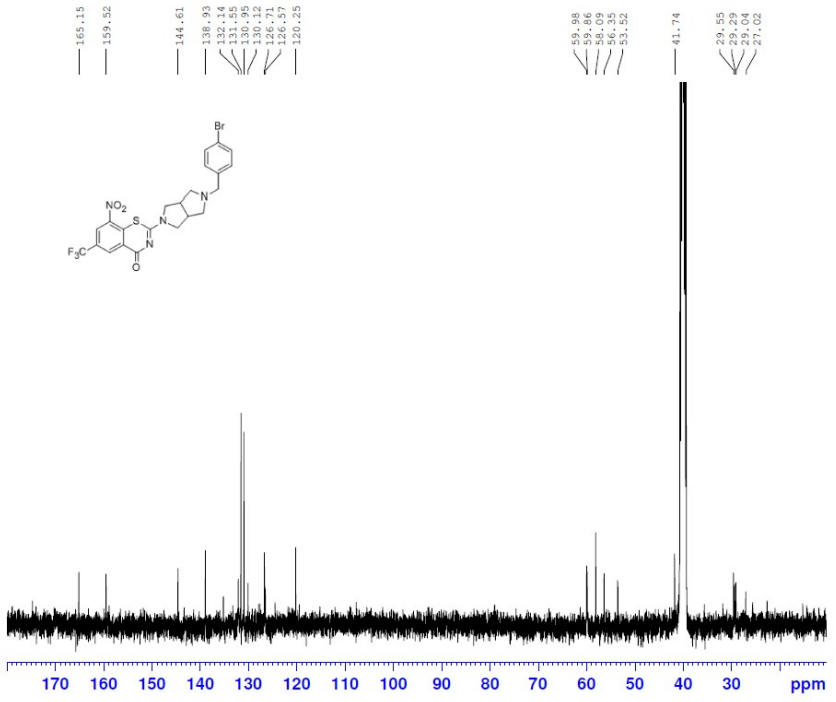


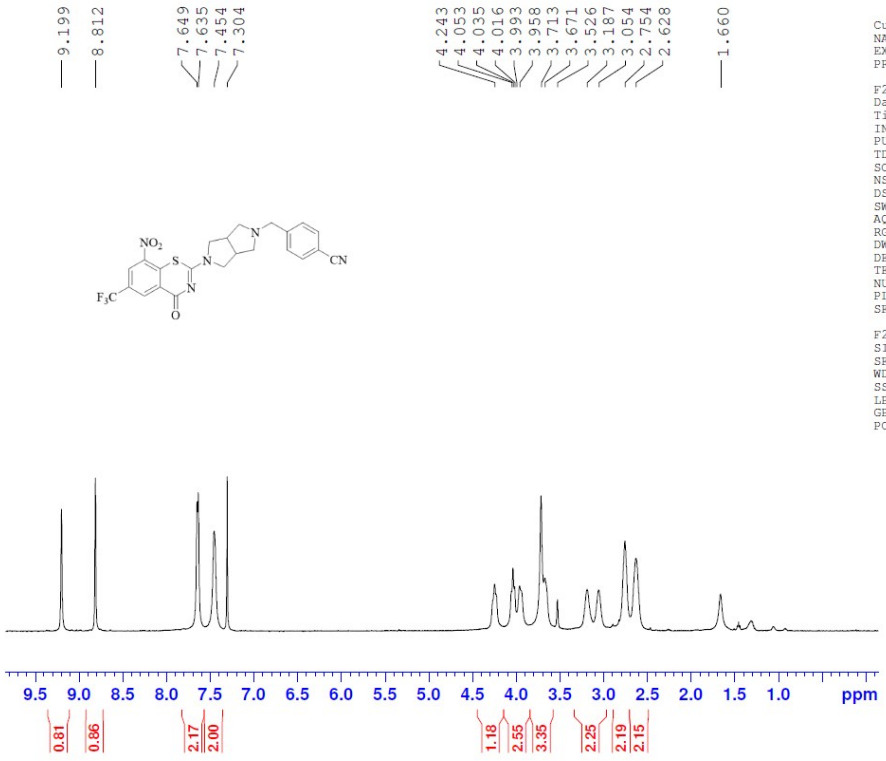

```
Current Data Parameters
NAME      20170524  1q-2-61
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170524
Time               15.31
INSTRUM             spect
PROBHD   5 mm CPPBBO BB
PULPROG          zgpg30
TD                 32768
SOLVENT             DMSO
NS                  3200
DS                     4
SWH          24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG                  77.6
DW             20.800 usec
DE             18.00 usec
TE               298.0 K
D1          1.00000000 sec
D11         0.03000000 sec
TD0                  400

======== CHANNEL f1 ========
SFO1       100.6238345 MHz
NUC1                  13C
P1                 9.84 usec
PLW1       38.00000000 W

======== CHANNEL f2 ========
SFO2       400.1316005 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2         8.14700031 W
PLW12        0.15600000 W
PLW13        0.09983800 W

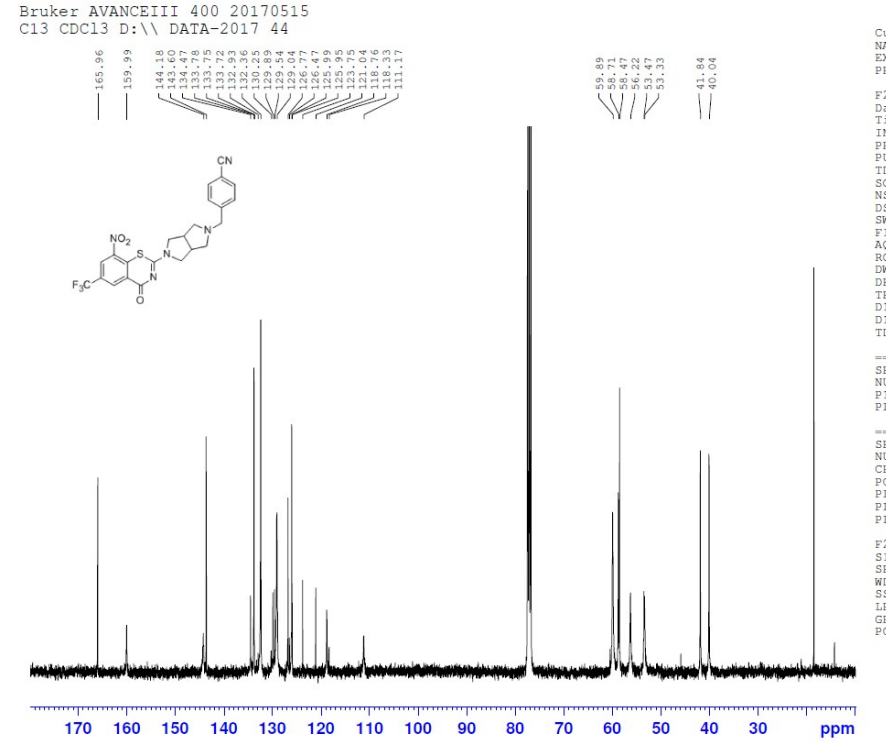
F2 - Processing parameters
SI                 32768
SF         100.6127690 MHz
WDW                   EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```




```
Current Data Parameters
NAME        1q-2-55 0509
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_           20170509
Time                9.08
INSTRUM    WNMR-I-500MHz
PULPROG             slpul
TD                  48000
SOLVENT             CDCl3
NS                      9
DS                      0
SWH            12000.000 Hz
AQ             2.0000000 sec
RG                   61.9
DW                41.667 usec
DE                 30.00 usec
TE                 298.4 K
NUC1                  1H
PL1                120.00 dB
SFO1         499.7053818 MHz

F2 - Processing parameters
SI                  32768
SF           499.7017639 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB                   0.1
PC                  1.00
```



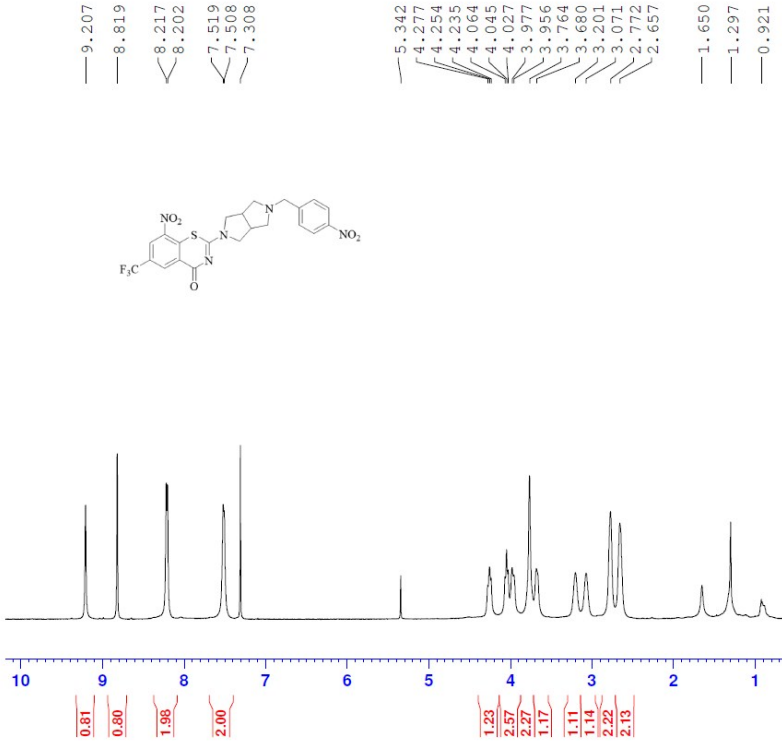

```
Current Data Parameters
NAME      20170515  1q-2-55
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20170515
Time               22.13
INSTRUM            spect
PROBHD   5 mm CPPBBO BB
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                 4000
DS                    4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             0.6815744 sec
RG                 77.6
DW                20.800 usec
DE                 18.00 usec
TE                 297.9 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                 500

======== CHANNEL f1 ========
SFO1        100.6238345 MHz
NUC1                  13C
P1                   9.84 usec
PLW1         38.00000000 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2               80.00 usec
PLW2          8.14700031 W
PLW12         0.15600000 W
PLW13         0.09983800 W

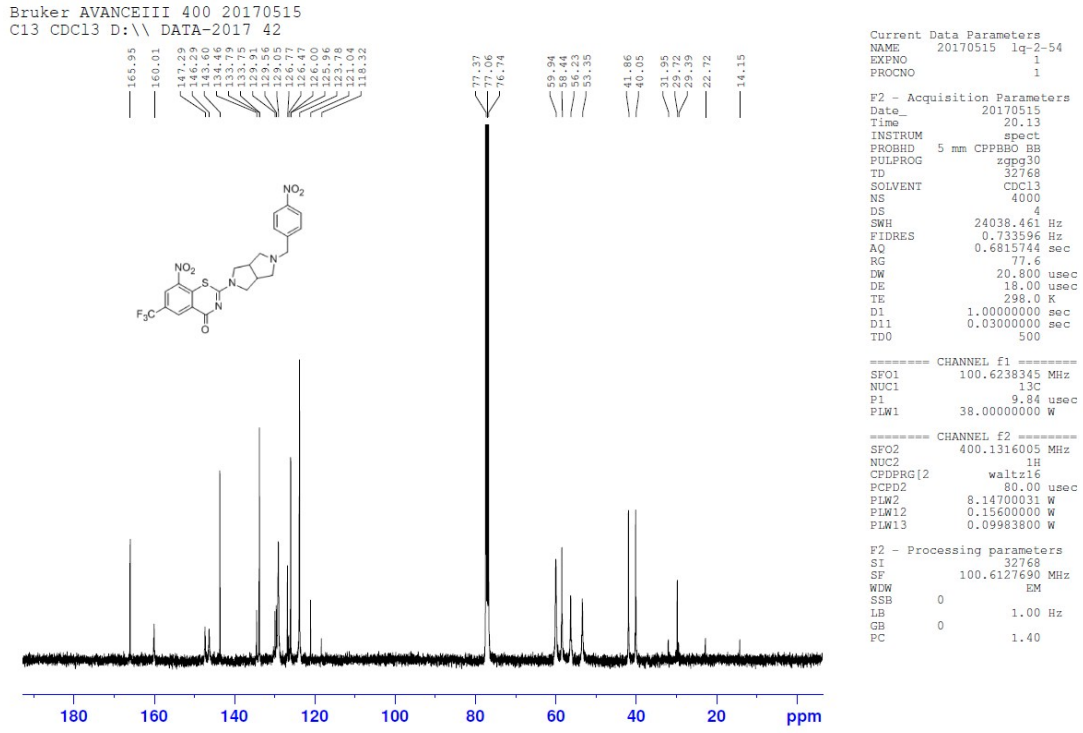
F2 - Processing parameters
SI                  32768
SF           100.6127690 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```




```
Current Data Parameters
NAME        lq-2-54 0509
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_           20170508
Time               15.12
INSTRUM   WNMR-I-500MHz
PULPROG            s1pul
TD                 48000
SOLVENT            CDCl3
NS                    18
DS                     0
SWH          12000.000 Hz
AQ           2.0000000 sec
RG                  64.8
DW             41.667 usec
DE                30.00 usec
TE                298.4 K
NUC1                  1H
PL1              120.00 dB
SFO1         499.7053818 MHz

F2 - Processing parameters
SI                 32768
SF           499.7017639 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB                  0.1
PC                 1.00
```



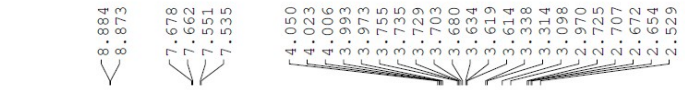

```
Current Data Parameters
NAME      20170515  lq-2-54
EXPNO                    1
PROCNO                   1

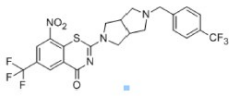
F2 - Acquisition Parameters
Date_           20170515
Time               20.13
INSTRUM            spect
PROBHD   5 mm CPPBBO BB
PULPROG         zgpg30
TD                 32768
SOLVENT            CDCl3
NS                  4000
DS                     4
SWH          24038.461 Hz
FIDRES        0.733596 Hz
AQ           0.6815744 sec
RG                  77.6
DW               20.800 usec
DE                18.00 usec
TE                298.0 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                  500

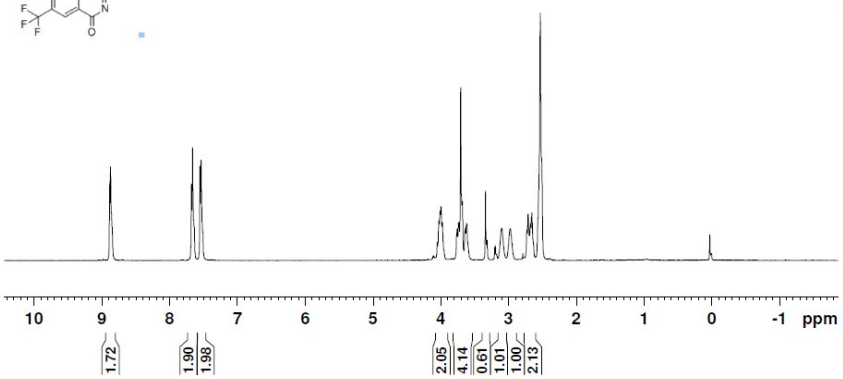
======== CHANNEL f1 ========
SFO1        100.6238345 MHz
NUC1                  13C
P1                   9.84 usec
PLW1        38.00000000 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              80.00 usec
PLW2          8.14700031 W
PLW12         0.15600000 W
PLW13         0.09983800 W

F2 - Processing parameters
SI                 32768
SF          100.6127690 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



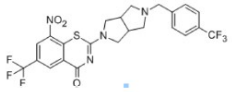


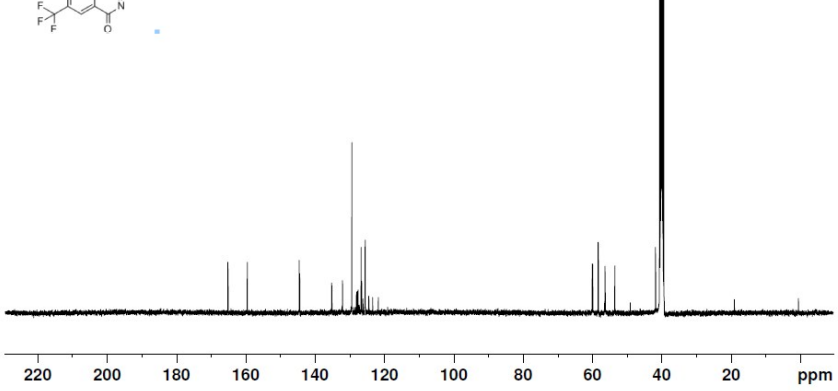



```
Current Data Parameters
NAME           tzy-2-16
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20170407
Time              15.24
INSTRUM   WNMR-I-500MHz
PULPROG           slpul
TD                48000
SOLVENT            DMSO
NS                   16
DS                    0
SWH          12000.000 Hz
AQ           2.0000000 sec
RG                 60.6
DW              41.667 usec
DE              30.00 usec
TE              298.1 K
NUC1                1H
PL1             120.00 dB
SFO1       499.7053818 MHz

F2 - Processing parameters
SI                32768
SF         499.7041375 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB                 0.1
PC                1.00
```





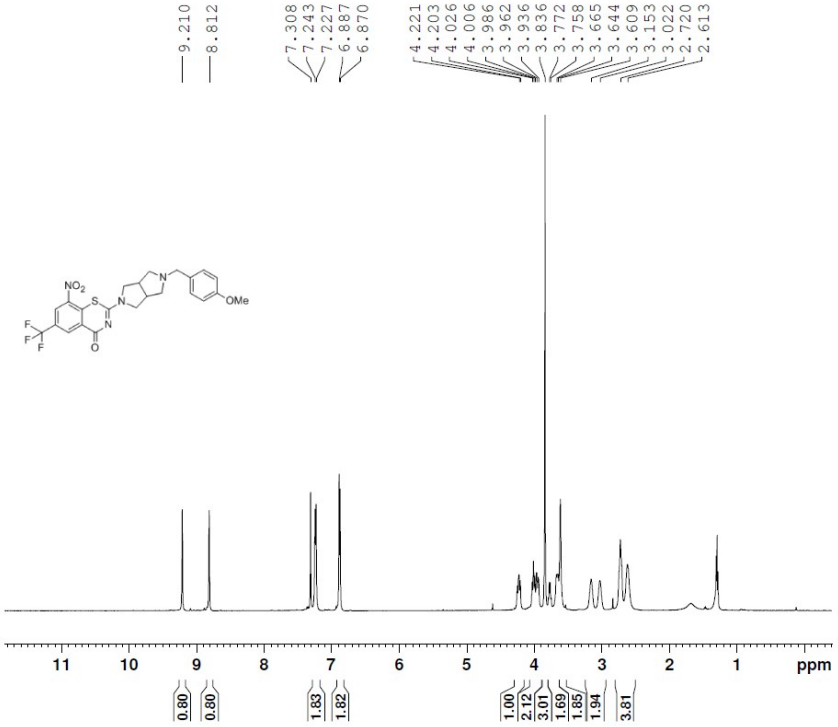

```
Current Data Parameters
NAME      20170411  tzy-2-16
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20170412
Time              18.43
INSTRUM            spect
PROBHD   5 mm CPPBBO BB
PULPROG          zgpg30
TD                32768
SOLVENT            DMSO
NS                 4800
DS                    4
SWH          24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG                 77.6
DW              20.800 usec
DE              18.00 usec
TE              298.0 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                 600

======== CHANNEL f1 ========
SFO1        100.6238345 MHz
NUC1               13C
P1                9.84 usec
PLW1        38.00000000 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2         8.14700031 W
PLW12        0.15600000 W
PLW13        0.09983800 W

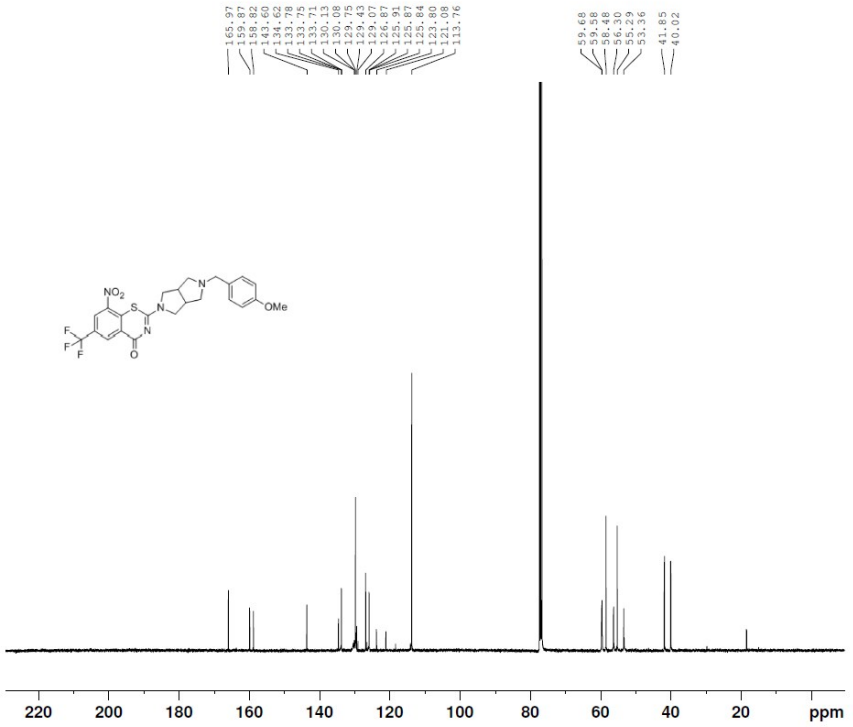
F2 - Processing parameters
SI                32768
SF         100.6127690 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```




```
Current Data Parameters
NAME              tzy-2-14-a
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_            20170405
Time                 9.46
INSTRUM   WNMR-I-500MHz
PULPROG              zlpul
TD                   48000
SOLVENT              CDCl3
NS                      16
DS                       0
SWH            12000.000 Hz
AQ             2.0000000 sec
RG                    62.2
DW                41.667 usec
DE                30.00 usec
TE                298.0 K
NUC1                   1H
PL1                120.00 dB
SFO1         499.7053818 MHz

F2 - Processing parameters
SI                   32768
SF           499.7017639 MHz
WDW                     EM
SSB       0
LB                  1.00 Hz
GB                   0.1
PC                  1.00
```



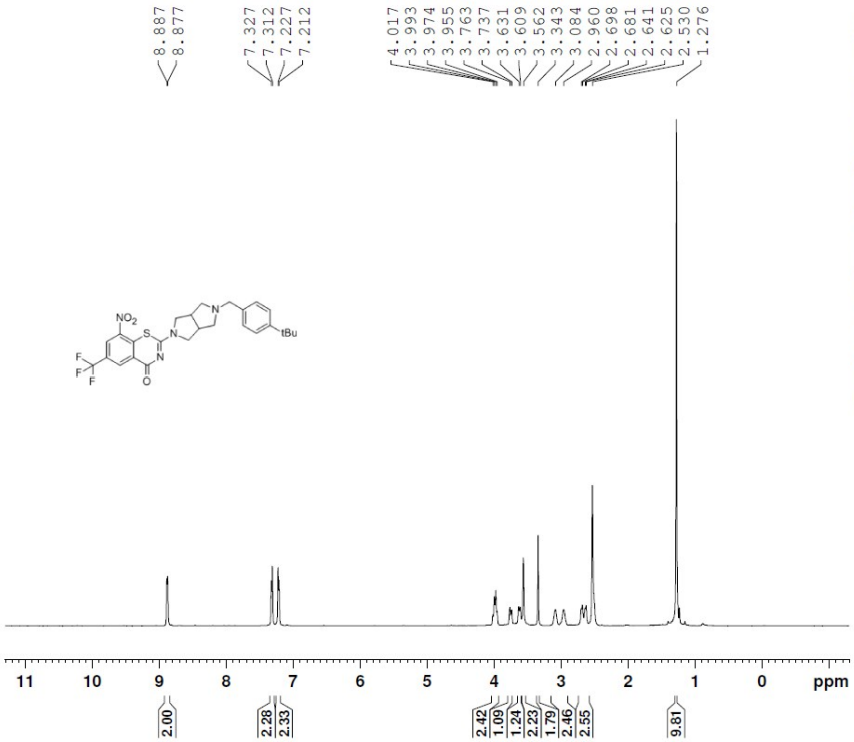

```
Current Data Parameters
NAME      20170407  tzy-2-14-a
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_            20170410
Time                 4.48
INSTRUM              spect
PROBHD   5 mm CPPBBO BB
PULPROG           zgpg30
TD                   32768
SOLVENT              CDCl3
NS                    4000
DS                       4
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ             0.6815744 sec
RG                    77.6
DW                20.800 usec
DE                18.00 usec
TE                298.0 K
D1             1.00000000 sec
D11            0.03000000 sec
TD0                    500

======== CHANNEL f1 ========
SFO1         100.6238345 MHz
NUC1                   13C
P1                    9.84 usec
PLW1         38.00000000 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2                80.00 usec
PLW2          8.14700031 W
PLW12         0.15600000 W
PLW13         0.09983800 W

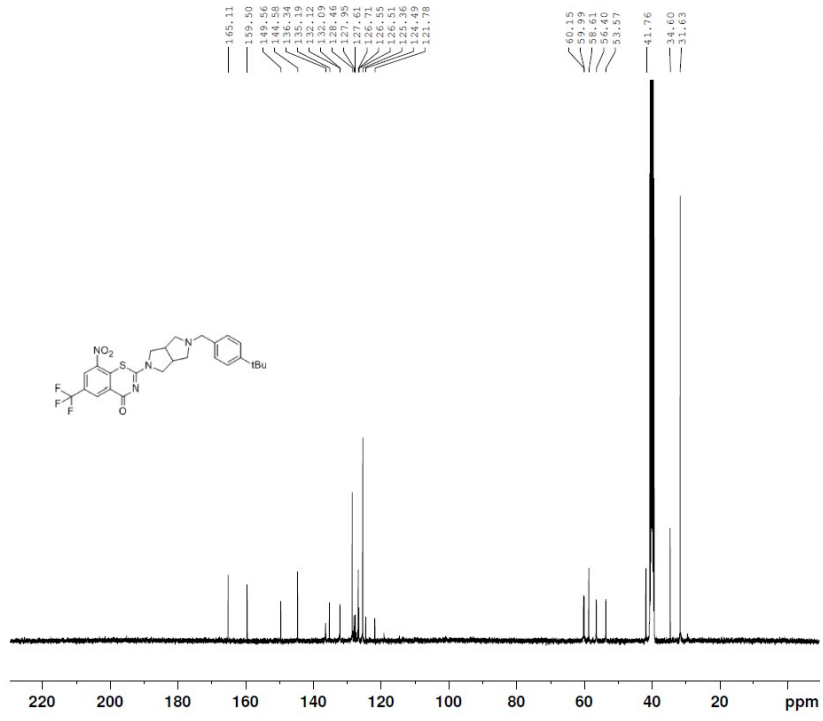
F2 - Processing parameters
SI                   32768
SF           100.6127690 MHz
WDW                     EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```




```
Current Data Parameters
NAME                  test1
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20170531
Time                  14.40
INSTRUM    WNMR-I-500MHz
PULPROG               slpul
TD                    48000
SOLVENT                DMSO
NS                       16
DS                        0
SWH             12000.000 Hz
AQ               2.0000000 sec
RG                       62
DW                 41.667 usec
DE                 30.00 usec
TE                 298.1 K
NUC1                    1H
PL1                120.00 dB
SFO1         499.7053818 MHz

F2 - Processing parameters
SI                    32768
SF           499.7041375 MHz
WDW                      EM
SSB       0
LB                  1.00 Hz
GB                   0.1
PC                  1.00
```



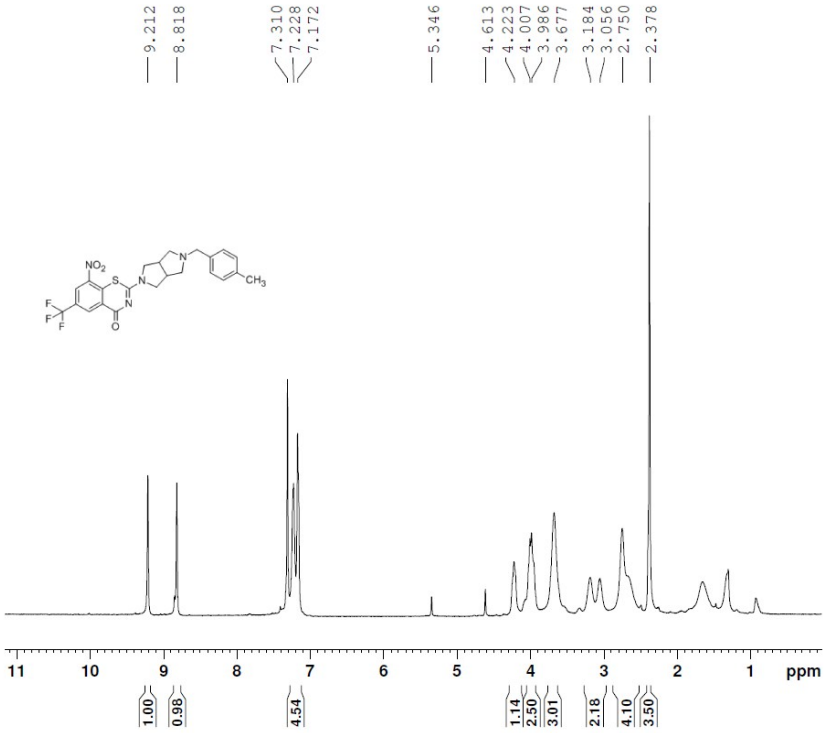

```
Current Data Parameters
NAME      20170607  test1
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20170608
Time                  15.03
INSTRUM               spect
PROBHD   5 mm CPPBBO BB
PULPROG           zgpg30
TD                    32768
SOLVENT                DMSO
NS                     4000
DS                        4
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              0.6815744 sec
RG                     77.6
DW                 20.800 usec
DE                 18.00 usec
TE                 298.0 K
D1             1.00000000 sec
D11            0.03000000 sec
TD0                    500

======== CHANNEL f1 ========
SFO1         100.6238345 MHz
NUC1                    13C
P1                    9.84 usec
PLW1         38.00000000 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                    1H
CPDPRG[2            waltz16
PCPD2                80.00 usec
PLW2          8.14700031 W
PLW12         0.15600000 W
PLW13         0.09983800 W

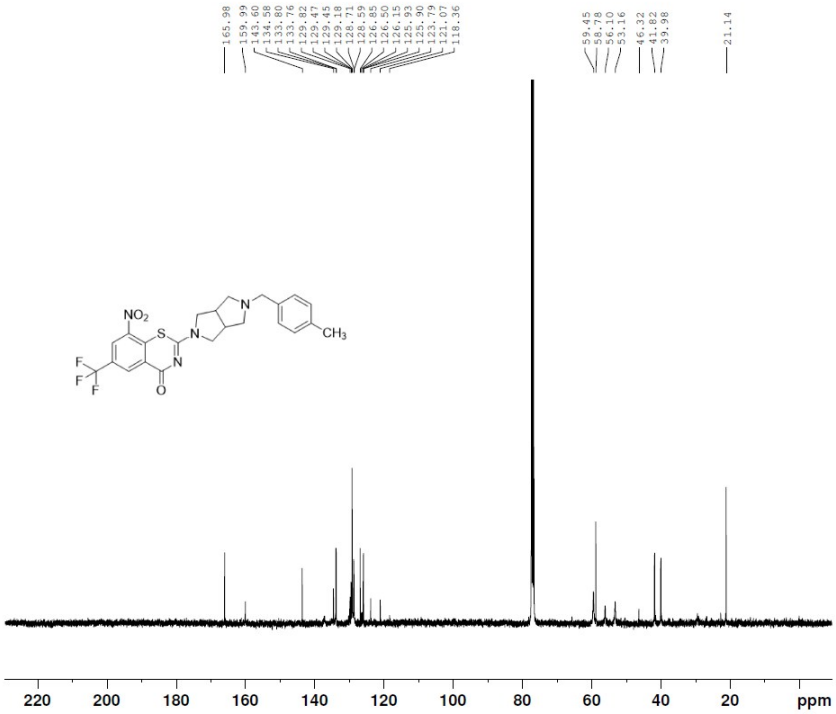
F2 - Processing parameters
SI                    32768
SF           100.6127690 MHz
WDW                      EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```




```
Current Data Parameters
NAME                  test8
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20170612
Time                   9.16
INSTRUM    WNMR-I-500MHz
PULPROG               s1pul
TD                    48000
SOLVENT               CDCl3
NS                       25
DS                        0
SWH             12000.000 Hz
AQ              2.0000000 sec
RG                     69.5
DW                 41.667 usec
DE                 30.00 usec
TE                 298.1 K
NUC1                      1H
PL1               120.00 dB
SFO1         499.7053818 MHz

F2 - Processing parameters
SI                    32768
SF           499.7017639 MHz
WDW                      EM
SSB       0
LB                  1.00 Hz
GB                   0.1
PC                  1.00
```



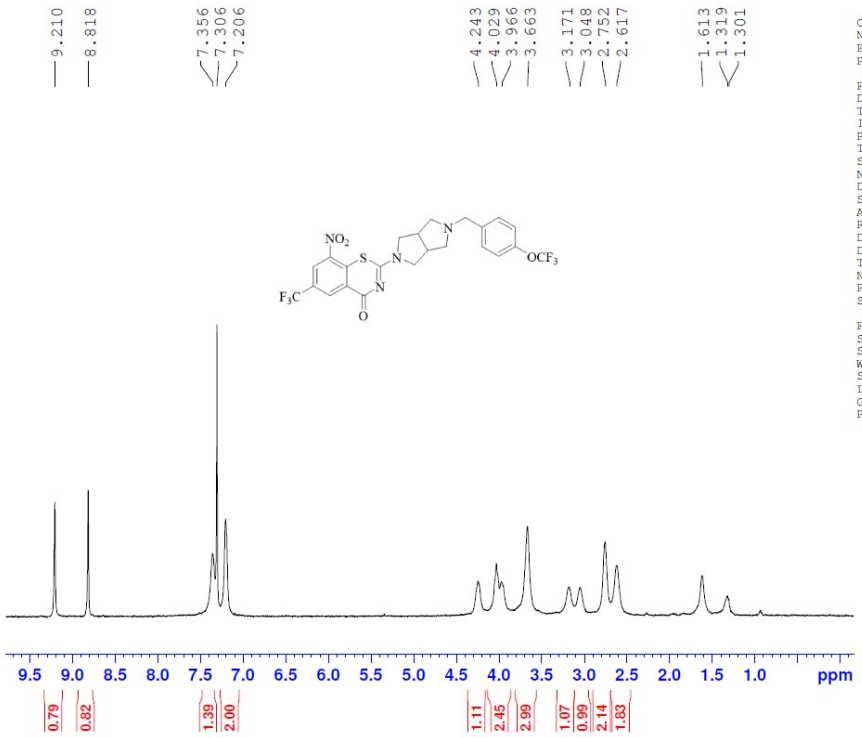

```
Current Data Parameters
NAME      20170616  test8
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20170617
Time                9.10
INSTRUM            spect
PROBHD   5 mm CPPBBO BB
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                 4800
DS                    4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            0.6815744 sec
RG                 77.6
DW               20.800 usec
DE               18.00 usec
TE               298.0 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                600

======== CHANNEL f1 ========
SFO1        100.6238345 MHz
NUC1                  13C
P1                 9.84 usec
PLW1        38.00000000 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2              80.00 usec
PLW2         8.14700031 W
PLW12        0.15600000 W
PLW13        0.09983800 W

F2 - Processing parameters
SI                 32768
SF          100.6127690 MHz
WDW                   EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

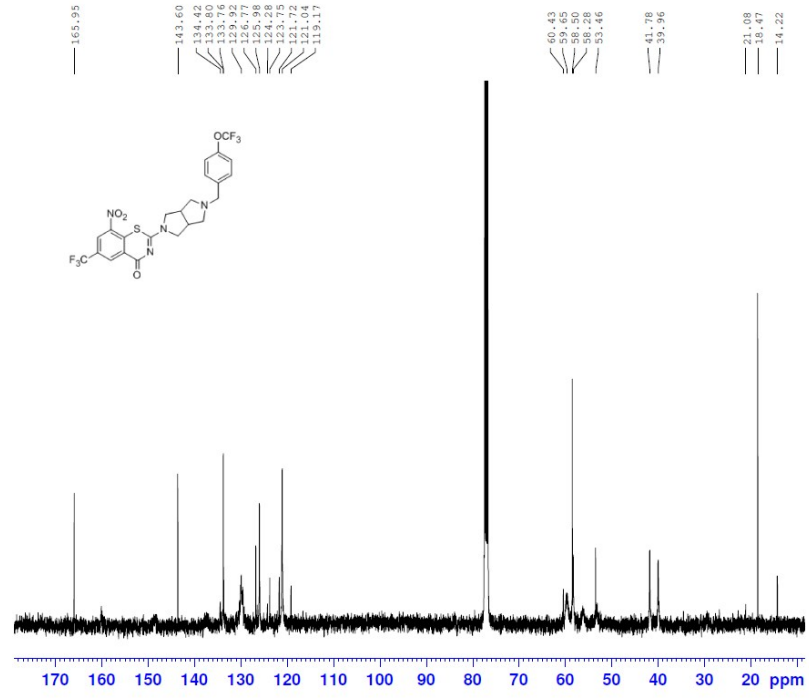



```
Current Data Parameters
NAME       lq-2-60 0509
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_           20170509
Time               9.05
INSTRUM   WNMR-I-500MHz
PULPROG            slpul
TD                 48000
SOLVENT            CDCl3
NS                     9
DS                     0
SWH            12000.000 Hz
AQ             2.0000000 sec
RG                  64.4
DW                41.667 usec
DE                30.00 usec
TE                298.4 K
NUC1                 1H
PL1               120.00 dB
SFO1         499.7053818 MHz

F2 - Processing parameters
SI                 32768
SF           499.7017639 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB                  0.1
PC                 1.00
```

Bruker AVANCEIII 400 20170515
C13 CDCl3 D:\\ DATA-2017 45



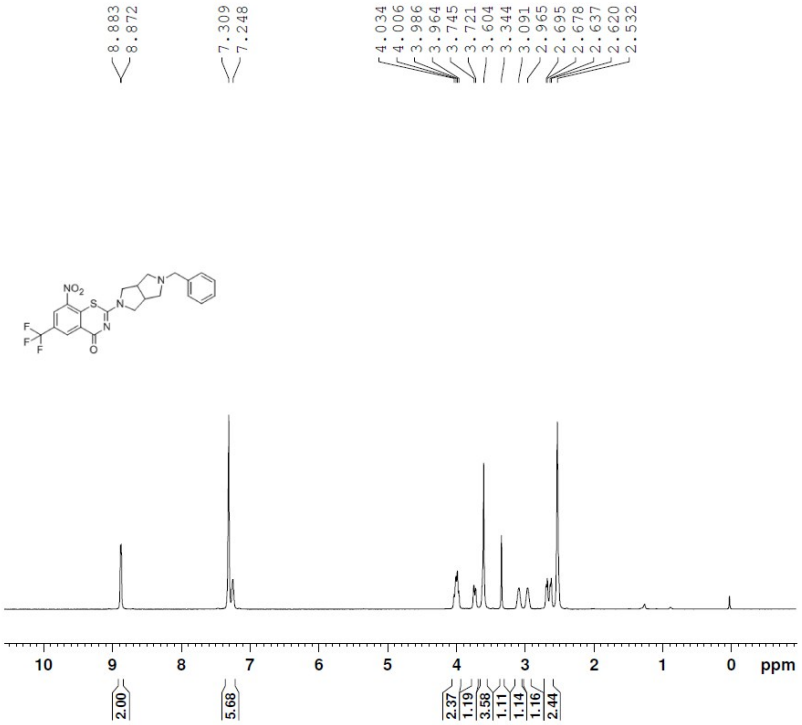

```
Current Data Parameters
NAME      20170515  lq-2-60
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_            20170516
Time                 0.12
INSTRUM             spect
PROBHD   5 mm CPPBBO BB
PULPROG           zgpg30
TD                 32768
SOLVENT            CDCl3
NS                  4000
DS                     4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             0.6815744 sec
RG                  77.6
DW                20.800 usec
DE                18.00 usec
TE                298.1 K
D1             1.00000000 sec
D11            0.03000000 sec
TD0                  500

======== CHANNEL f1 ========
SFO1         100.6238345 MHz
NUC1                   13C
P1                    9.84 usec
PLW1         38.00000000 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2               80.00 usec
PLW2          8.14700031 W
PLW12         0.15600000 W
PLW13         0.09983800 W

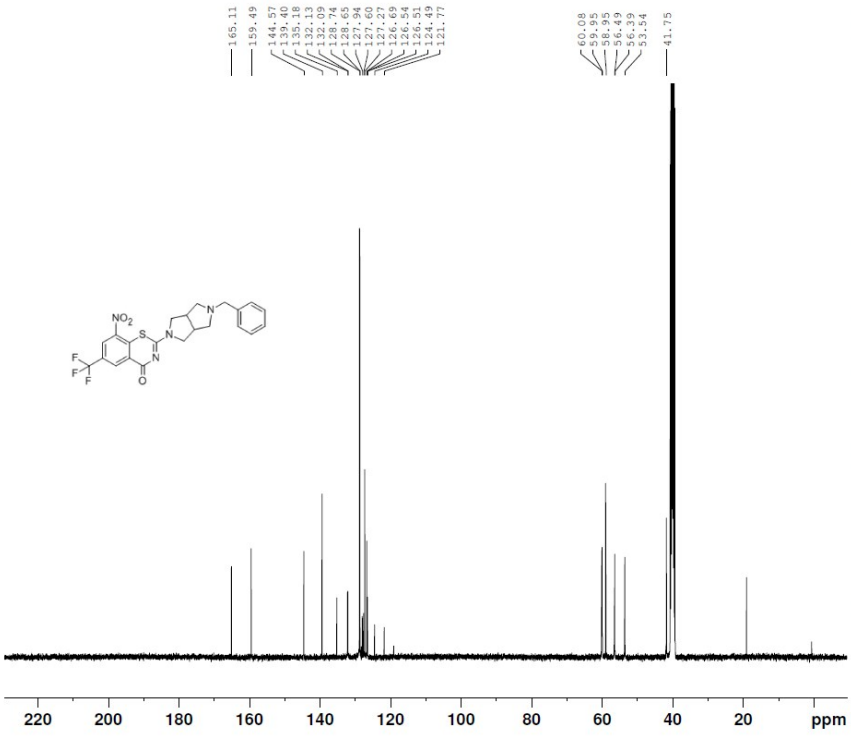
F2 - Processing parameters
SI                 32768
SF           100.6127690 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```




```
Current Data Parameters
NAME            tzy-3-32
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170526
Time               16.28
INSTRUM   WNMR-I-500MHz
PULPROG            zlpul
TD                 48000
SOLVENT              DMSO
NS                     10
DS                      0
SWH          12000.000 Hz
AQ           2.0000000 sec
RG                  63.3
DW             41.667 usec
DE              30.00 usec
TE              298.1 K
NUC1               1H
PL1             120.00 dB
SFO1        499.7053818 MHz

F2 - Processing parameters
SI                 32768
SF          499.7041375 MHz
WDW                   EM
SSB       0
LB               1.00 Hz
GB                0.1
PC               1.00
```



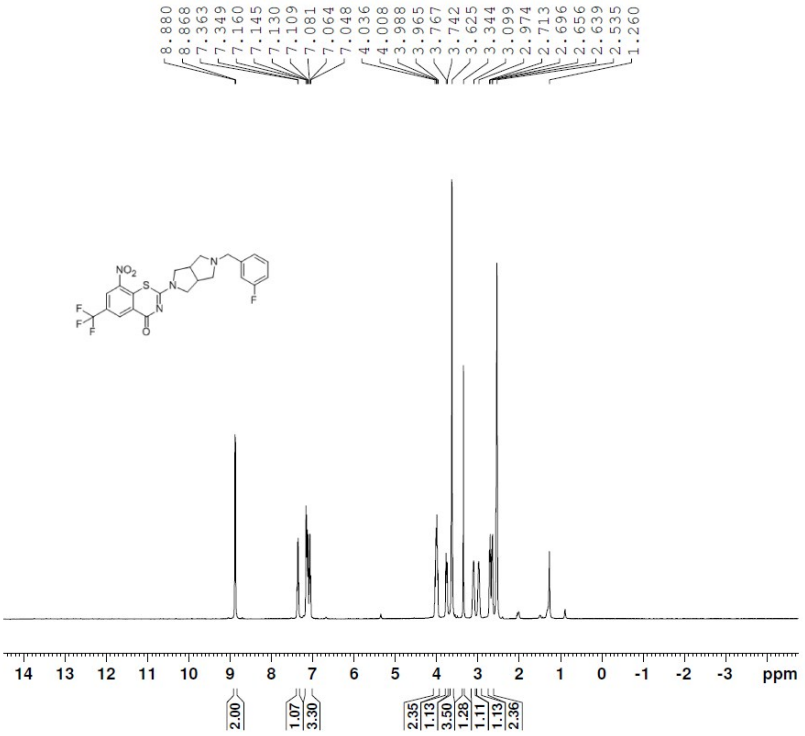

```
Current Data Parameters
NAME      20170607  TZY-3-32
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170609
Time               0.57
INSTRUM           spect
PROBHD   5 mm CPPBBO BB
PULPROG          zgpg30
TD                 32768
SOLVENT              DMSO
NS                  4000
DS                     4
SWH          24038.461 Hz
FIDRES         0.733596 Hz
AQ           0.6815744 sec
RG                  77.6
DW              20.800 usec
DE              18.00 usec
TE              298.0 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                  500

======== CHANNEL f1 ========
SFO1        100.6238345 MHz
NUC1               13C
P1                9.84 usec
PLW1       38.00000000 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2               1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2         8.14700031 W
PLW12        0.15600000 W
PLW13        0.09983800 W

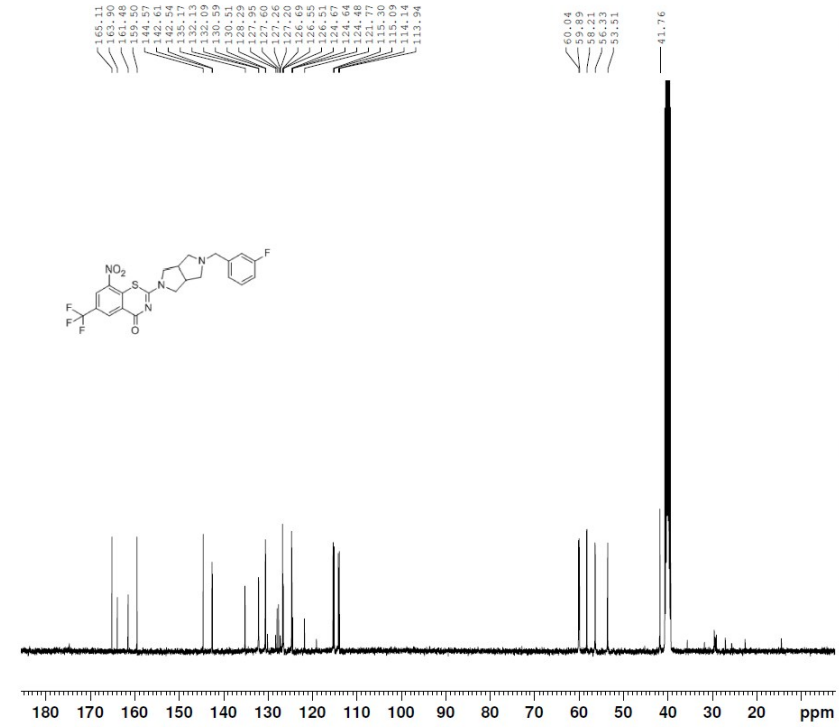
F2 - Processing parameters
SI                 32768
SF          100.6127690 MHz
WDW                   EM
SSB       0
LB               1.00 Hz
GB        0
PC               1.40
```




```
Current Data Parameters
NAME      tzy-3-28 20170522
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_           20170522
Time              10.24
INSTRUM   WNMR-I-500MHz
PULPROG           zlpul
TD                48000
SOLVENT            DMSO
NS                   14
DS                    0
SWH           12000.000 Hz
AQ            2.0000000 sec
RG                 62.1
DW               41.667 usec
DE                30.00 usec
TE               298.3 K
NUC1                 1H
PL1               120.00 dB
SFO1         499.7053818 MHz

F2 - Processing parameters
SI                32768
SF           499.7041375 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB                 0.1
PC                1.00
```



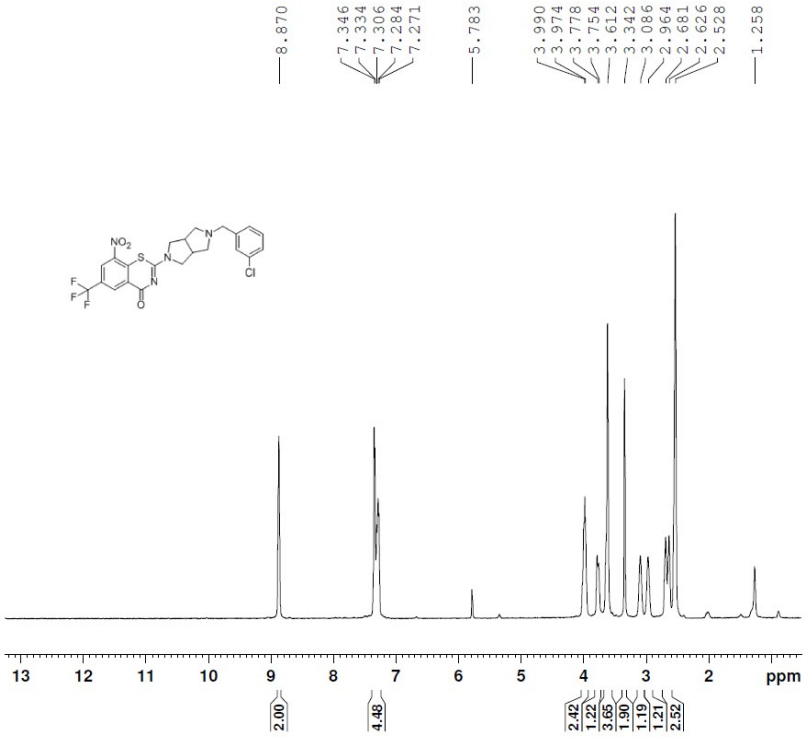

```
Current Data Parameters
NAME      20170523  TZY-3-28
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_           20170525
Time              3.31
INSTRUM          spect
PROBHD   5 mm CPPBBO BB
PULPROG          zgpg30
TD                32768
SOLVENT            DMSO
NS                 4000
DS                    4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            0.6815744 sec
RG                 77.6
DW               20.800 usec
DE                18.00 usec
TE               298.0 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                500

======== CHANNEL f1 ========
SFO1         100.6238345 MHz
NUC1                 13C
P1                  9.84 usec
PLW1         38.00000000 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2              80.00 usec
PLW2          8.14700031 W
PLW12         0.15600000 W
PLW13         0.09983800 W

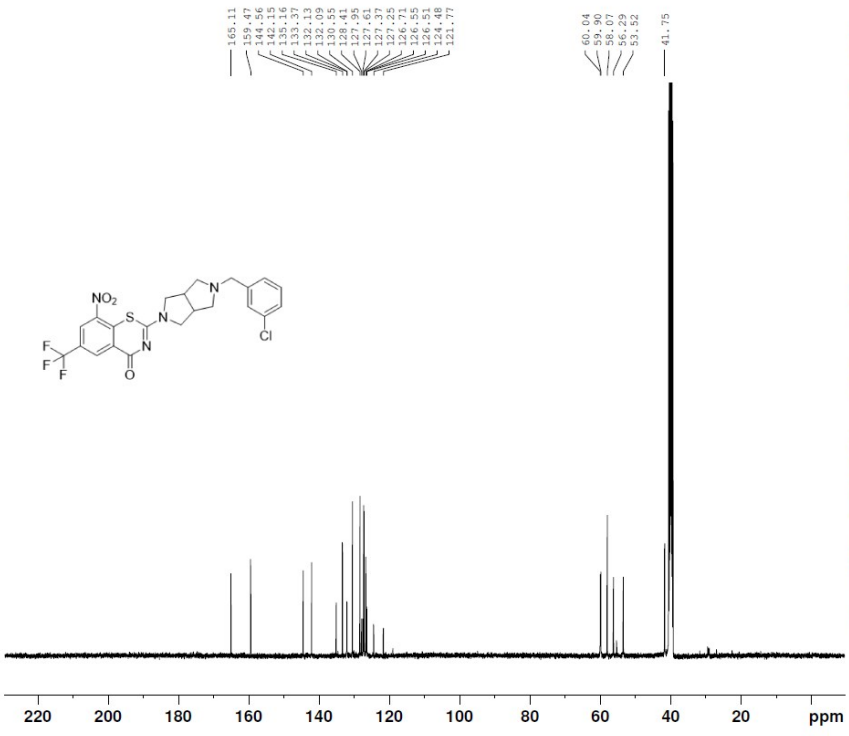
F2 - Processing parameters
SI                32768
SF           100.6127690 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB                   0
PC                1.40
```




```
Current Data Parameters
NAME                 tzy-4-9
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_               20170612
Time                    9.25
INSTRUM    WNMR-I-500MHz
PULPROG                s1pul
TD                     48000
SOLVENT                DMSO
NS                        14
DS                         0
SWH                12000.000 Hz
AQ                 2.0000000 sec
RG                      64.1
DW                    41.667 usec
DE                     30.00 usec
TE                     298.1 K
NUC1                       1H
PL1                    120.00 dB
SFO1            499.7053818 MHz

F2 - Processing parameters
SI                      32768
SF                499.7041375 MHz
WDW                        EM
SSB          0
LB                      1.00 Hz
GB                       0.1
PC                      1.00
```



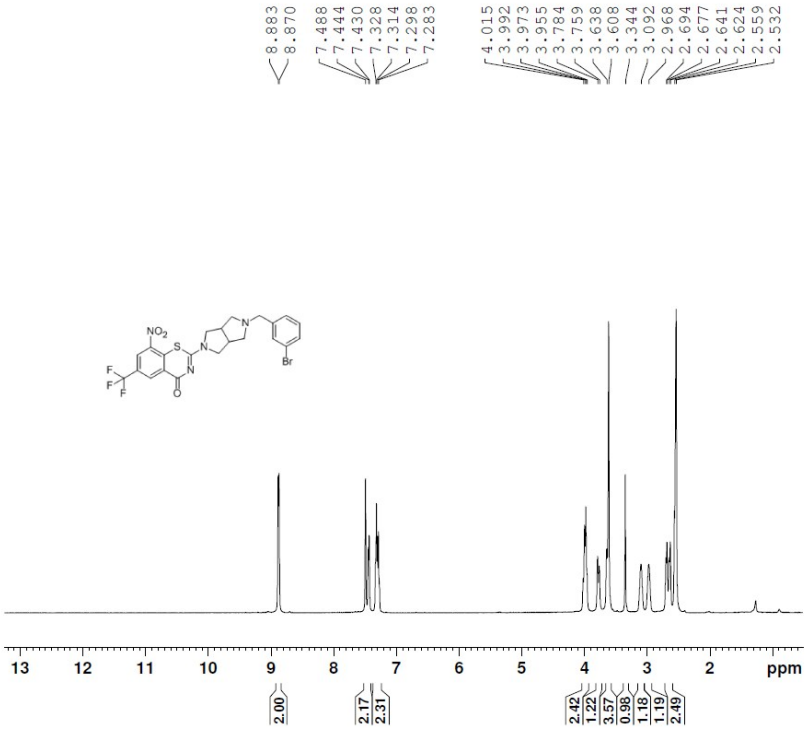

```
Current Data Parameters
NAME      20170616  tzy-4-9
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_               20170616
Time                   18.28
INSTRUM                spect
PROBHD    5 mm CPPBBO BB
PULPROG             zgpg30
TD                     32768
SOLVENT                DMSO
NS                      4800
DS                         4
SWH               24038.461 Hz
FIDRES             0.733596 Hz
AQ                 0.6815744 sec
RG                      77.6
DW                    20.800 usec
DE                     18.00 usec
TE                     298.0 K
D1                 1.00000000 sec
D11                0.03000000 sec
TD0                       600

======== CHANNEL f1 ========
SFO1            100.6238345 MHz
NUC1                     13C
P1                      9.84 usec
PLW1           38.00000000 W

======== CHANNEL f2 ========
SFO2            400.1316005 MHz
NUC2                       1H
CPDPRG[2            waltz16
PCPD2                  80.00 usec
PLW2            8.14700031 W
PLW12           0.15600000 W
PLW13           0.09983800 W

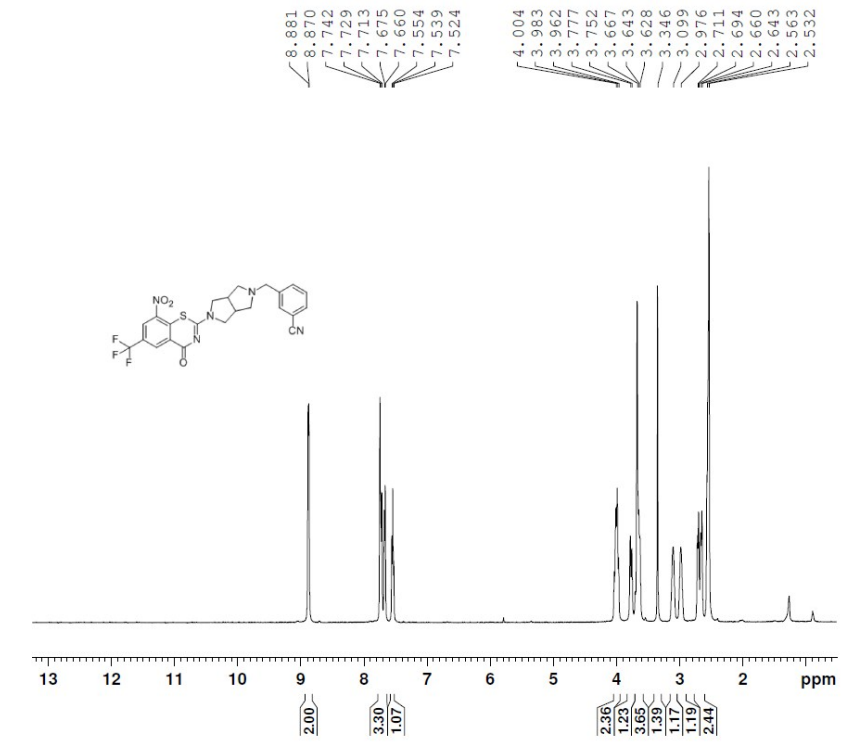
F2 - Processing parameters
SI                      32768
SF                100.6127690 MHz
WDW                        EM
SSB          0
LB                      1.00 Hz
GB           0
PC                      1.40
```




```
Current Data Parameters
NAME                  tzy-4-8
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_               20170609
Time                    8.52
INSTRUM       WNMR-I-500MHz
PULPROG                slpul
TD                     48000
SOLVENT                 DMSO
NS                        17
DS                         0
SWH                12000.000 Hz
AQ                 2.0000000 sec
RG                      62.9
DW                    41.667 usec
DE                    30.00 usec
TE                    298.1 K
NUC1                      1H
PL1                  120.00 dB
SFO1          499.7053818 MHz

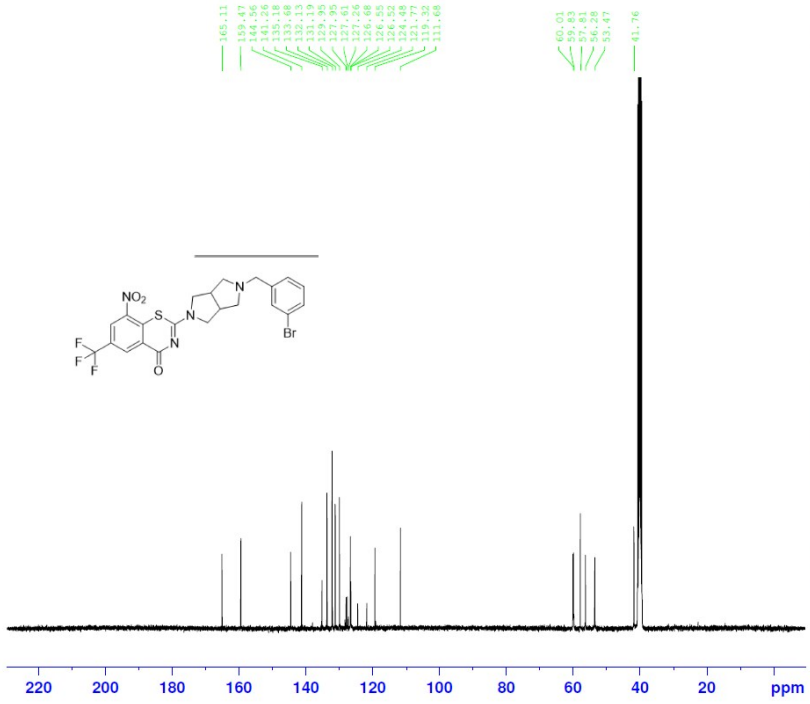
F2 - Processing parameters
SI                     32768
SF                499.7041375 MHz
WDW                       EM
SSB          0
LB                     1.00 Hz
GB                      0.1
PC                     1.00
```




```
Current Data Parameters
NAME                 tzy-4-10
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_               20170609
Time                    8.58
INSTRUM       WNMR-I-500MHz
PULPROG                slpul
TD                     48000
SOLVENT                 DMSO
NS                        10
DS                         0
SWH                12000.000 Hz
AQ                 2.0000000 sec
RG                         62
DW                    41.667 usec
DE                    30.00 usec
TE                    298.1 K
NUC1                      1H
PL1                  120.00 dB
SFO1          499.7053818 MHz

F2 - Processing parameters
SI                     32768
SF                499.7041375 MHz
WDW                       EM
SSB          0
LB                     1.00 Hz
GB                      0.1
PC                     1.00
```



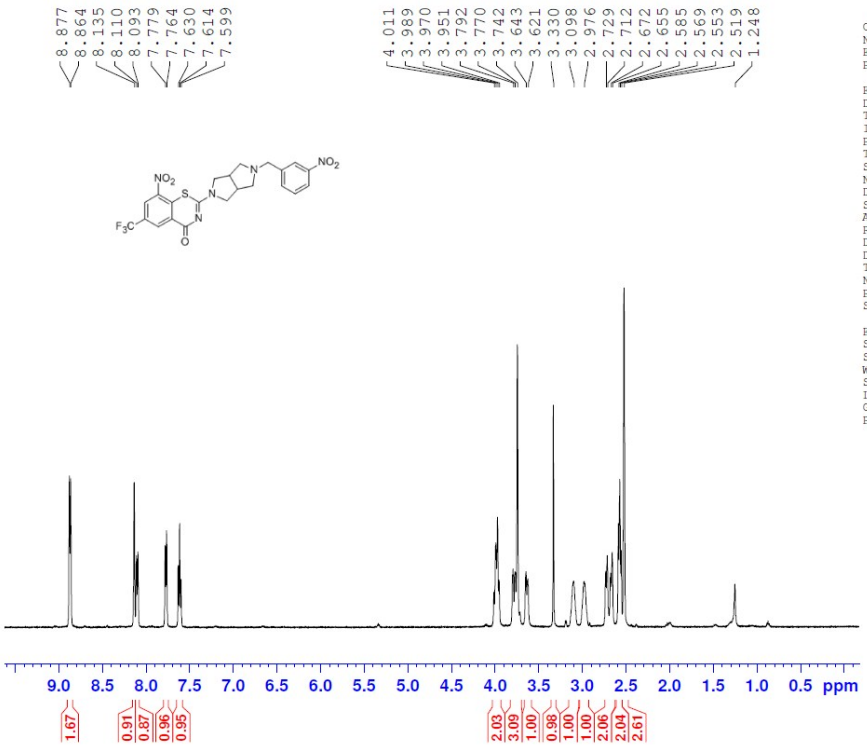

```
Current Data Parameters
NAME      20170616  tzy-4-10
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_             20170616
Time                20.50
INSTRUM             spect
PROBHD   5 mm CPPBBO BB
PULPROG           zgpg30
TD                 32768
SOLVENT              DMSO
NS                   4800
DS                      4
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ             0.6815744 sec
RG                  77.6
DW                20.800 usec
DE                18.00 usec
TE                298.0 K
D1             1.00000000 sec
D11            0.03000000 sec
TD0                  600

======== CHANNEL f1 ========
SFO1          100.6238345 MHz
NUC1                 13C
P1                  9.84 usec
PLW1          38.00000000 W

======== CHANNEL f2 ========
SFO2          400.1316005 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2              80.00 usec
PLW2           8.14700031 W
PLW12          0.15600000 W
PLW13          0.09983800 W

F2 - Processing parameters
SI                  32768
SF            100.6127690 MHz
WDW                 EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

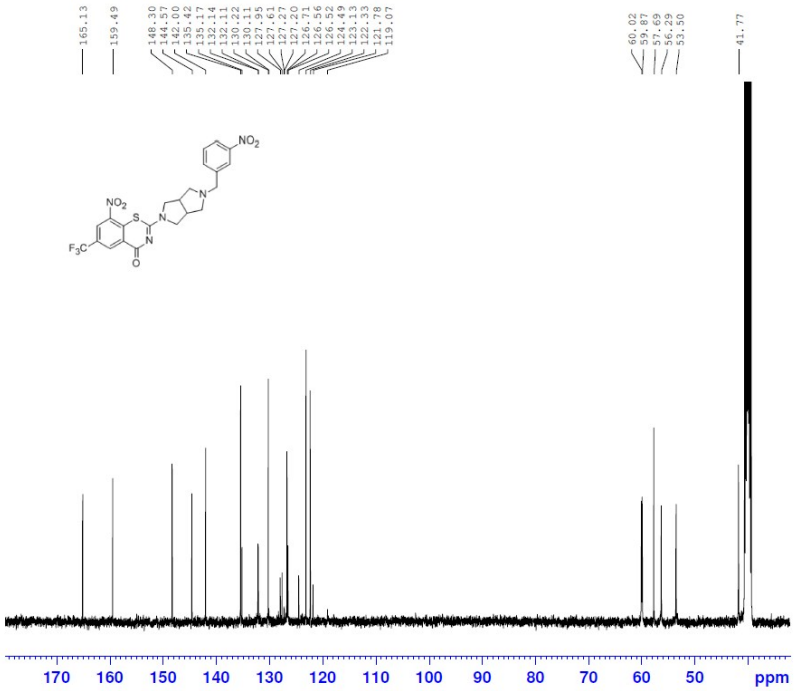



```
Current Data Parameters
NAME      lq-2-82 20170525
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_             20170525
Time                14.12
INSTRUM   WNMR-I-500MHz
PULPROG              s1pul
TD                  48000
SOLVENT              DMSO
NS                     16
DS                      0
SWH            12000.000 Hz
AQ             2.0000000 sec
RG                   63.2
DW                41.667 usec
DE                30.00 usec
TE                298.4 K
NUC1                 1H
PL1               120.00 dB
SFO1          499.7053818 MHz

F2 - Processing parameters
SI                  32768
SF            499.6981443 MHz
WDW                 no
SSB       0
LB                 1.00 Hz
GB                  0.1
PC                 1.00
```

Bruker AVANCEIII 400 20170526
C13 DMSO D:\\ DATA-2017 20



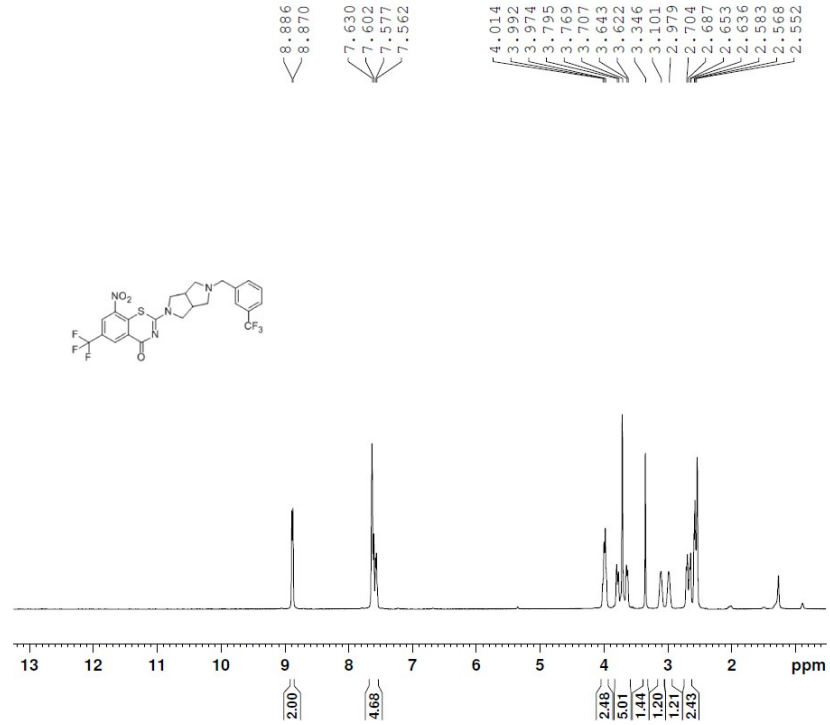

```
Current Data Parameters
NAME      20170526  LQ-2-82
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20170528
Time                 15.59
INSTRUM              spect
PROBHD   5 mm CPPBBO BB
PULPROG            zgpg30
TD                  32768
SOLVENT               DMSO
NS                    3200
DS                       4
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              0.6815744 sec
RG                    77.6
DW                20.800 usec
DE                18.00 usec
TE                298.0 K
D1             1.00000000 sec
D11            0.03000000 sec
TD0                    400

======== CHANNEL f1 ========
SFO1          100.6238345 MHz
NUC1                   13C
P1                    9.84 usec
PLW1          38.00000000 W

======== CHANNEL f2 ========
SFO2          400.1316005 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2                80.00 usec
PLW2           8.14700031 W
PLW12          0.15600000 W
PLW13          0.09983800 W

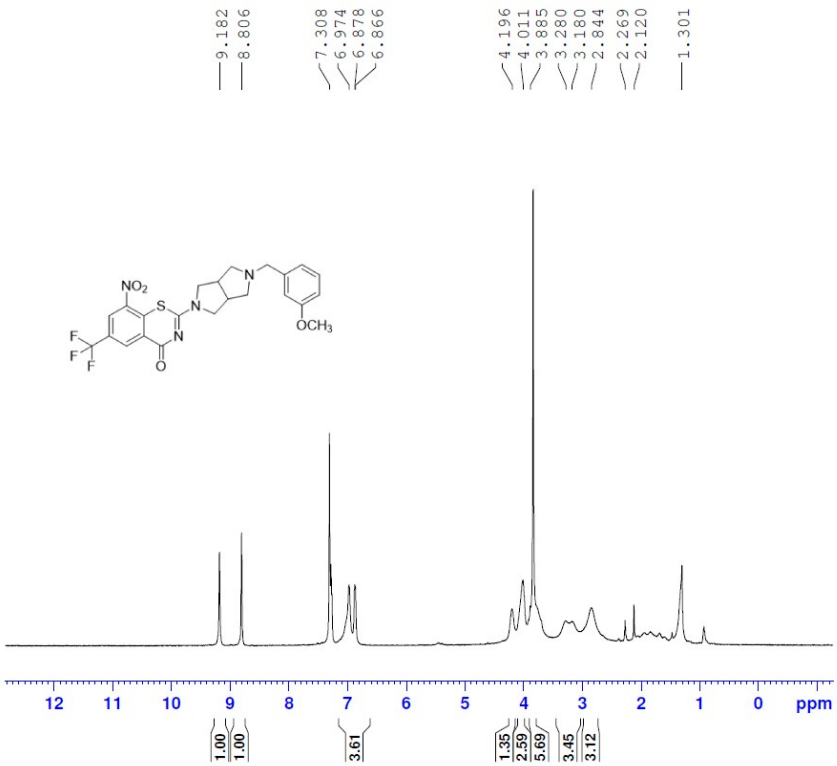
F2 - Processing parameters
SI                    32768
SF            100.6127690 MHz
WDW                      EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```




```
Current Data Parameters
NAME      tzy-3-27 20170523
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20170523
Time                 15.56
INSTRUM   WNMR-I-500MHz
PULPROG              s1pul
TD                   48000
SOLVENT               DMSO
NS                      24
DS                       0
SWH           12000.000 Hz
AQ             2.0000000 sec
RG                    62.5
DW                41.667 usec
DE                30.00 usec
TE                298.3 K
NUC1                   1H
PL1               120.00 dB
SFO1          499.7053818 MHz

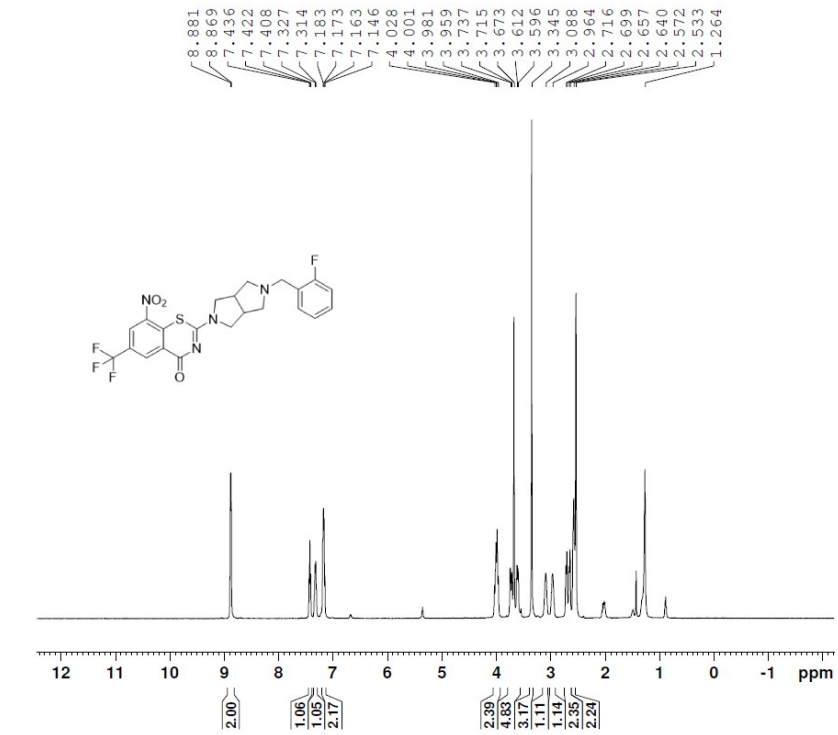
F2 - Processing parameters
SI                    32768
SF            499.7041375 MHz
WDW                      EM
SSB       0
LB                    1.00 Hz
GB                     0.1
PC                    1.00
```




```
Current Data Parameters
NAME                  test9
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20170612
Time                   9.04
INSTRUM    WNMR-I-500MHz
PULPROG               slpul
TD                    48000
SOLVENT               CDCl3
NS                       19
DS                        0
SWH             12000.000 Hz
AQ              2.0000000 sec
RG                     66.4
DW                 41.667 usec
DE                 30.00 usec
TE                 298.1 K
NUC1                     1H
PL1               120.00 dB
SFO1          499.7053818 MHz

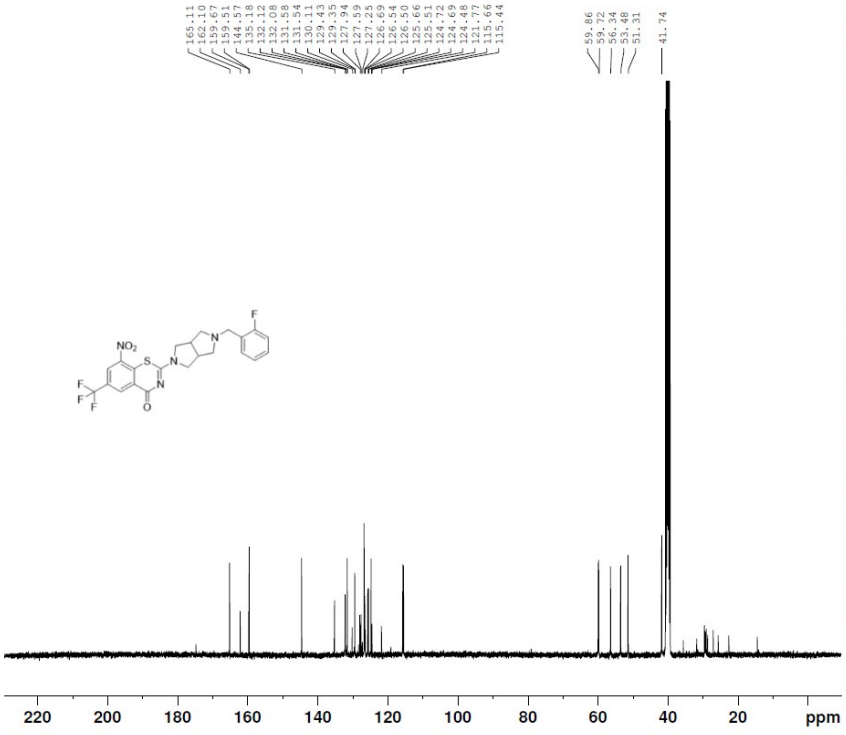
F2 - Processing parameters
SI                    32768
SF            499.7017639 MHz
WDW                      EM
SSB       0
LB                  1.00 Hz
GB                   0.1
PC                  1.00
```




```
Current Data Parameters
NAME      tzy-3-26 20170522
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20170522
Time                  10.21
INSTRUM    WNMR-I-500MHz
PULPROG               slpul
TD                    48000
SOLVENT                DMSO
NS                       20
DS                        0
SWH             12000.000 Hz
AQ              2.0000000 sec
RG                     63.8
DW                 41.667 usec
DE                 30.00 usec
TE                 298.3 K
NUC1                     1H
PL1               120.00 dB
SFO1          499.7053818 MHz

F2 - Processing parameters
SI                    32768
SF            499.7041375 MHz
WDW                      EM
SSB       0
LB                  1.00 Hz
GB                   0.1
PC                  1.00
```



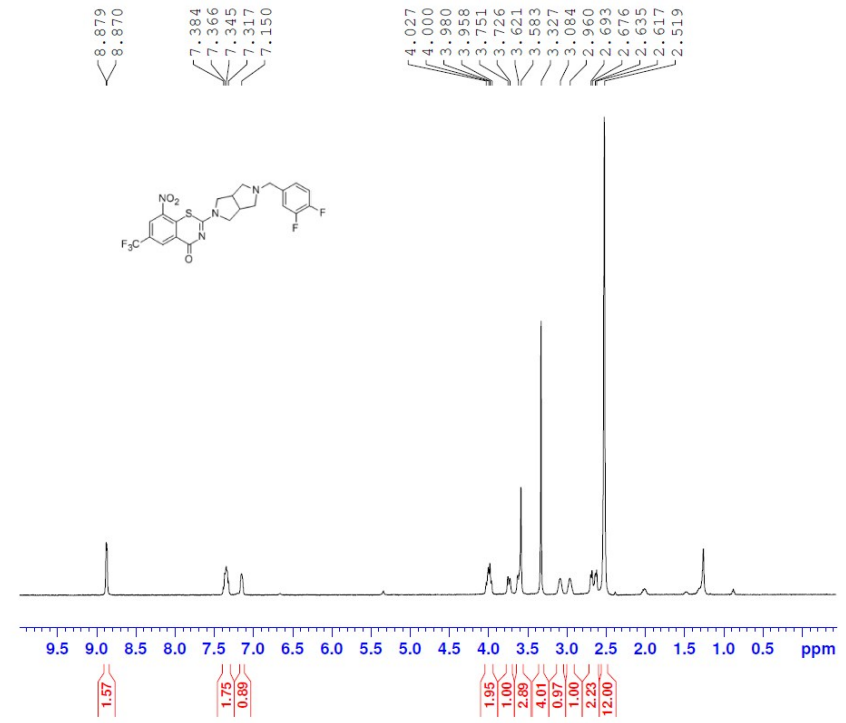

```
Current Data Parameters
NAME      20170523  TZY-3-26
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_           20170525
Time              1.32
INSTRUM           spect
PROBHD   5 mm CPPBBO BB
PULPROG          zgpg30
TD               32768
SOLVENT           DMSO
NS                4000
DS                   4
SWH          24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG                77.6
DW               20.800 usec
DE               18.00 usec
TE               298.0 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                500

======== CHANNEL f1 ========
SFO1        100.6238345 MHz
NUC1               13C
P1                9.84 usec
PLW1        38.00000000 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2               1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2         8.14700031 W
PLW12        0.15600000 W
PLW13        0.09983800 W

F2 - Processing parameters
SI                32768
SF          100.6127690 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

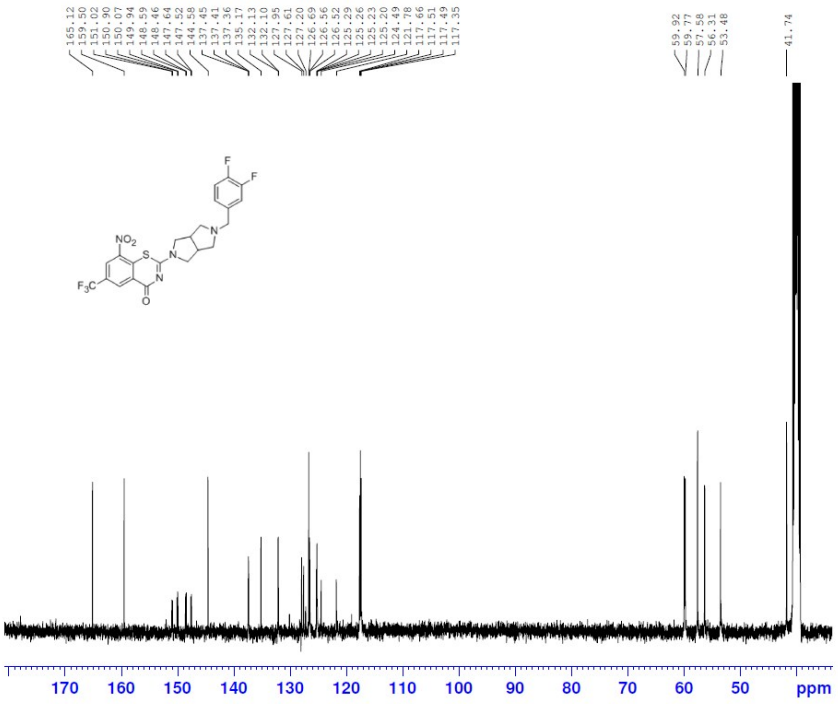



```
Current Data Parameters
NAME      lq-2-66 20170522
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_           20170522
Time              10.18
INSTRUM   WNMR-I-500MHz
PULPROG           s1pu1
TD               48000
SOLVENT           DMSO
NS                  19
DS                   0
SWH          12000.000 Hz
AQ            2.0000000 sec
RG                73.9
DW              41.667 usec
DE               30.00 usec
TE               298.4 K
NUC1               1H
PL1              120.00 dB
SFO1        499.7053818 MHz

F2 - Processing parameters
SI                32768
SF          499.6981438 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB                 0.1
PC                1.00
```

Bruker AVANCEIII 400 20170524
C13 DMSO D:\\ DATA-2017 32



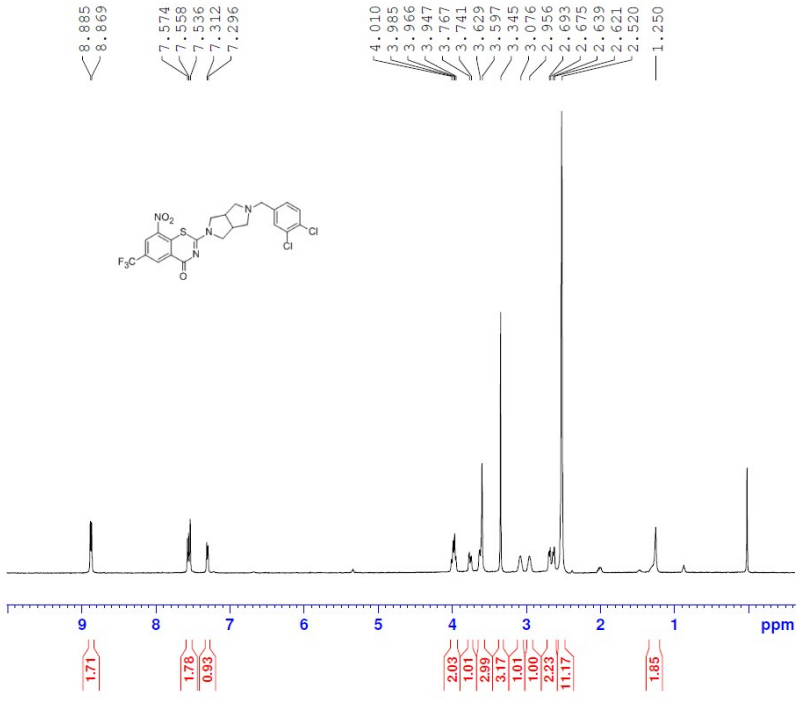
Current Data Parameters
NAME 20170524 lq-2-66
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170524
Time 17.59
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 3200
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 77.6
DW 20.800 usec
DE 18.00 usec
TE 298.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 400

======== CHANNEL f1 ========
SFO1 100.6238345 MHz
NUC1 13C
P1 9.84 usec
PLW1 38.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 8.14700031 W
PLW12 0.15600000 W
PLW13 0.09983800 W

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

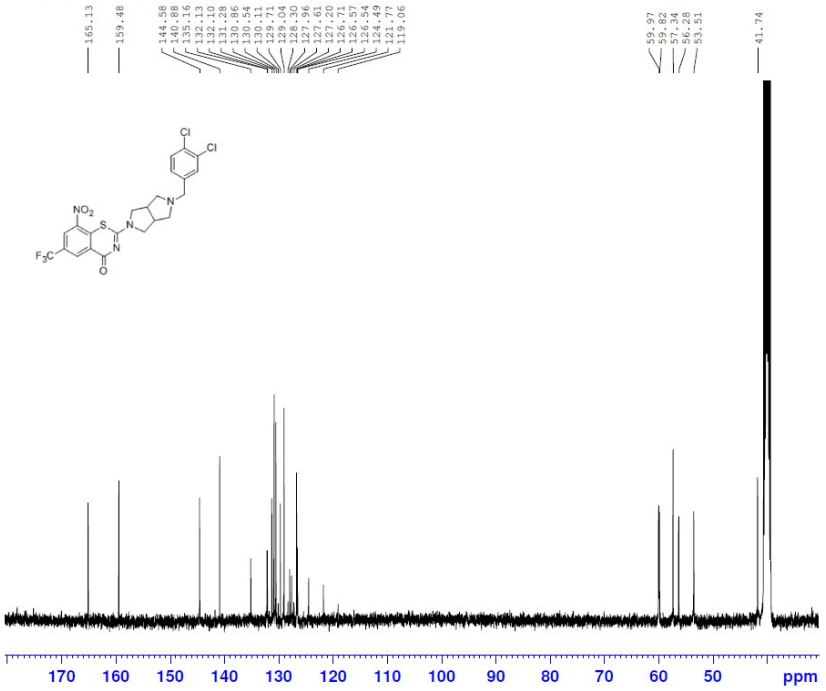


Current Data Parameters
NAME lq-2-73 5 19 2017
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170519
Time 10.30
INSTRUM WNMR-I-500MHz
PULPROG slpul
TD 48000
SOLVENT DMSO
NS 12
DS 0
SWH 12000.000 Hz
AQ 2.0000000 sec
RG 67.3
DW 41.667 usec
DE 30.00 usec
TE 293.6 K
NUC1 1H
PL1 120.00 dB
SFO1 499.7053818 MHz

F2 - Processing parameters
SI 32768
SF 499.6981427 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0.1
PC 1.00

Bruker AVANCEIII 400 20170524
C13 DMSO D:\\ DATA-2017 35



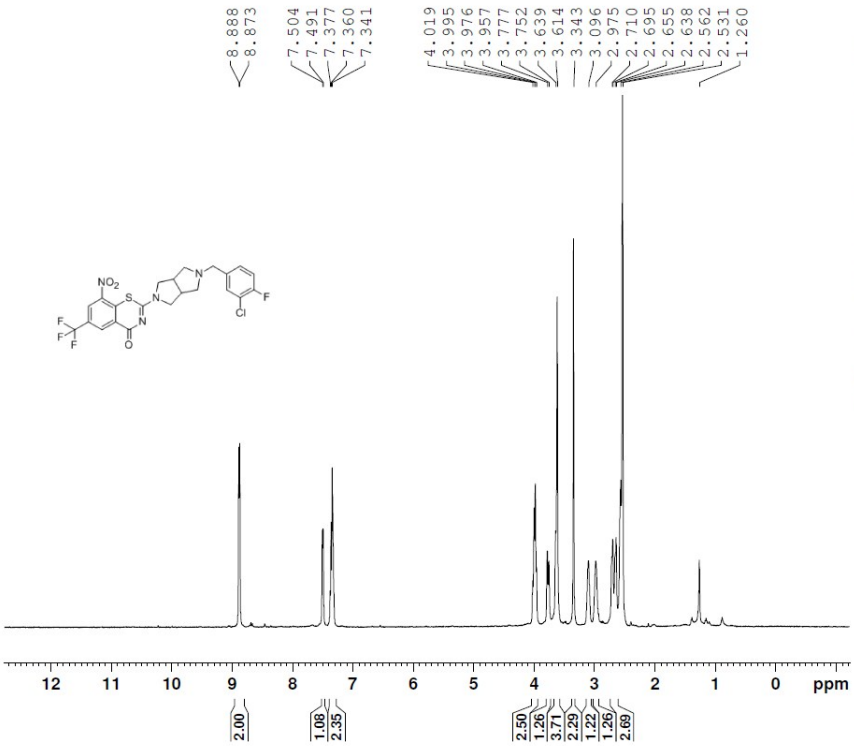

```
Current Data Parameters
NAME      20170524  lq-2-73
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20170524
Time              22.45
INSTRUM           spect
PROBHD   5 mm CPPBBO BB
PULPROG          zgpg30
TD                32768
SOLVENT            DMSO
NS                 3200
DS                    4
SWH           24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG                 77.6
DW               20.800 usec
DE               18.00 usec
TE               298.0 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                 400

======== CHANNEL f1 ========
SFO1        100.6238345 MHz
NUC1               13C
P1                9.84 usec
PLW1        38.00000000 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2         8.14700031 W
PLW12        0.15600000 W
PLW13        0.09983800 W

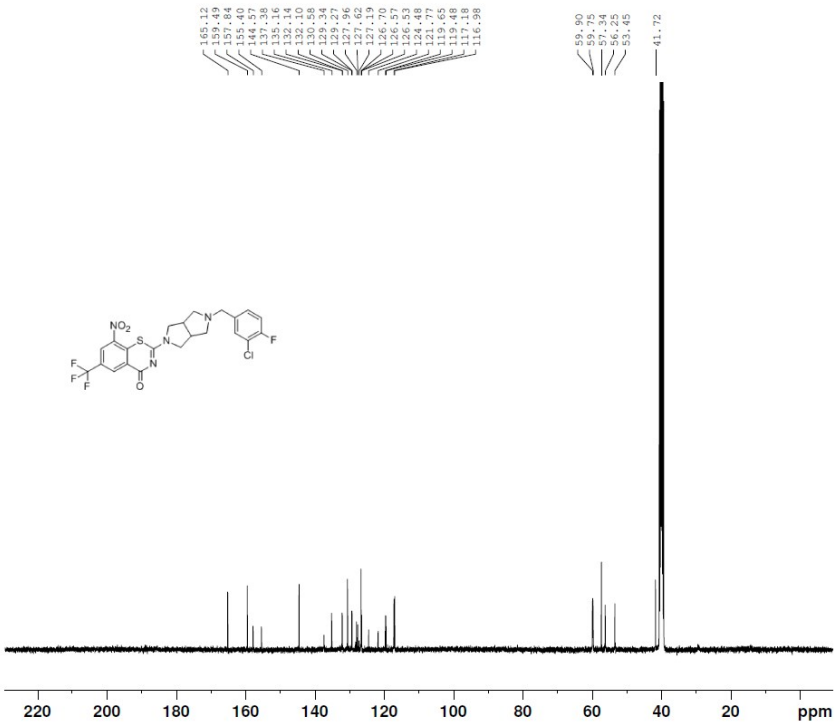
F2 - Processing parameters
SI                32768
SF          100.6127690 MHz
WDW                EM
SSB       0
LB               1.00 Hz
GB        0
PC               1.40
```




```
Current Data Parameters
NAME                 test7
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20170531
Time              14.46
INSTRUM   WNMR-I-500MHz
PULPROG             slpul
TD                48000
SOLVENT            DMSO
NS                   16
DS                    0
SWH           12000.000 Hz
AQ            2.0000000 sec
RG                 65.9
DW               41.667 usec
DE               30.00 usec
TE               298.1 K
NUC1               1H
PL1              120.00 dB
SFO1        499.7053818 MHz

F2 - Processing parameters
SI                32768
SF          499.7041375 MHz
WDW                EM
SSB       0
LB               1.00 Hz
GB                0.1
PC               1.00
```



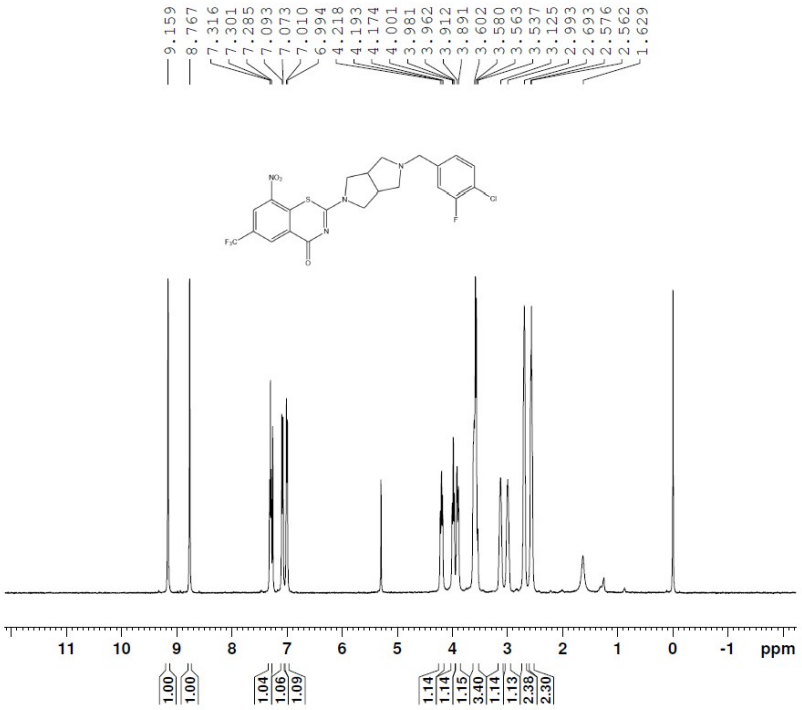

```
Current Data Parameters
NAME      20170607  test7
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_           20170608
Time               22.57
INSTRUM            spect
PROBHD   5 mm CPPBBO BB
PULPROG          zgpg30
TD                32768
SOLVENT            DMSO
NS                 4000
DS                    4
SWH           24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG                 77.6
DW               20.800 usec
DE               18.00 usec
TE               298.0 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                 500

======== CHANNEL f1 ========
SFO1        100.6238345 MHz
NUC1                13C
P1                 9.84 usec
PLW1        38.00000000 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2         8.14700031 W
PLW12        0.15600000 W
PLW13        0.09983800 W

F2 - Processing parameters
SI                 32768
SF          100.6127690 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

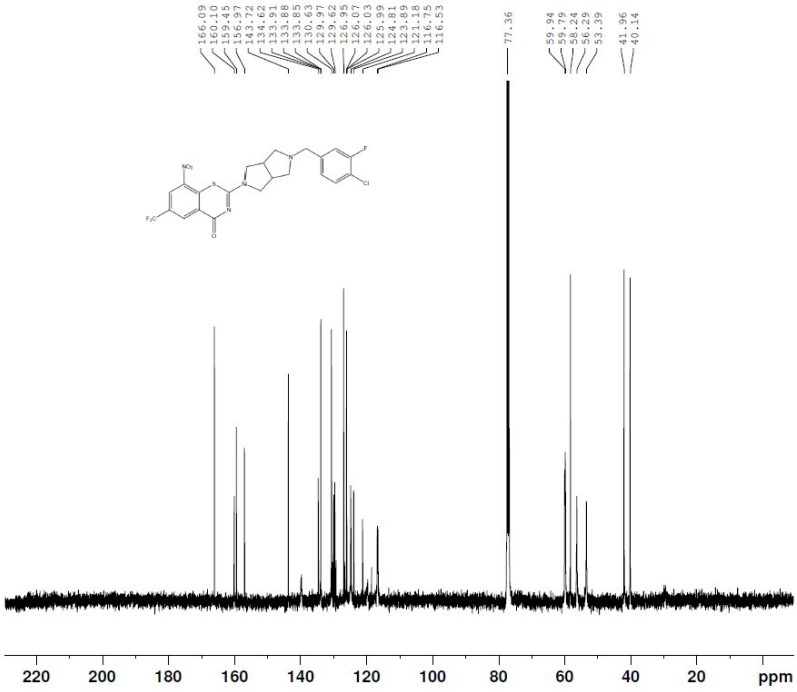



```
Current Data Parameters
NAME      tzy-2-25-20200115
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20200115
Time               16.14
INSTRUM   WNMR-I-500MHz
PULPROG             s1pul
TD                 48000
SOLVENT            CDCl3
NS                     3
DS                     0
SWH           12000.000 Hz
AQ            1.9999999 sec
RG                    35
DW               41.667 usec
DE               30.00 usec
TE               298.1 K
NUC1                1H
PL1              120.00 dB
SFO1        499.6739824 MHz

F2 - Processing parameters
SI                 32768
SF          499.6703905 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB                  0.1
PC                 1.00
```

Bruker AVANCEIII 400 20170418
C13 CDCl3 D:\\ DATA-2017 31



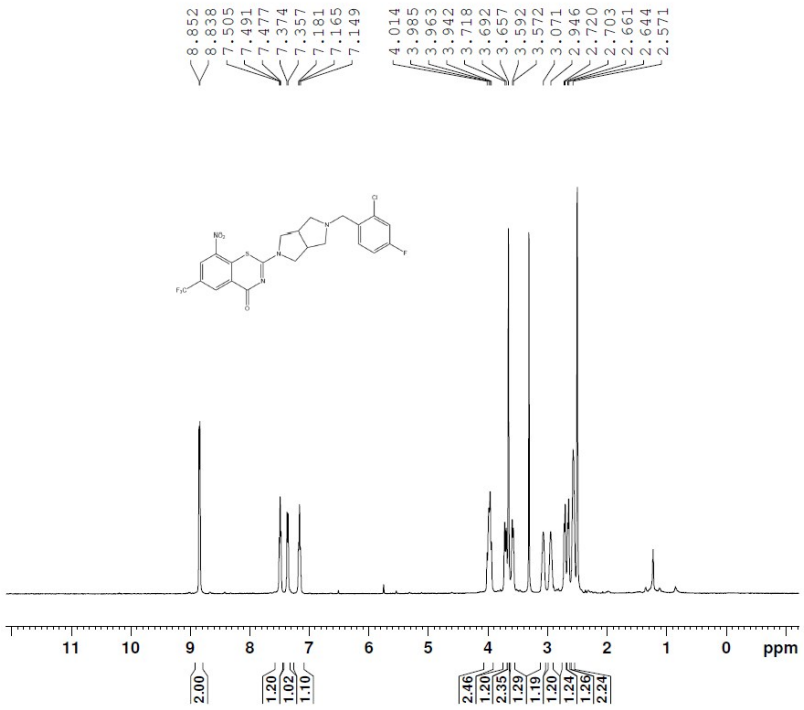

```
Current Data Parameters
NAME      20170418  tzy-2-25
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_           20170419
Time               2.54
INSTRUM           spect
PROBHD   5 mm CPPBBO BB
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                 4000
DS                    4
SWH           24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG                 77.6
DW              20.800 usec
DE              18.00 usec
TE              298.1 K
D1          1.00000000 sec
D11         0.03000000 sec
TD0                 500

======== CHANNEL f1 ========
SFO1        100.6238345 MHz
NUC1               13C
P1                9.84 usec
PLW1       38.00000000 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2        8.14700031 W
PLW12       0.15600000 W
PLW13       0.09983800 W

F2 - Processing parameters
SI                32768
SF          100.6127577 MHz
WDW                 EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

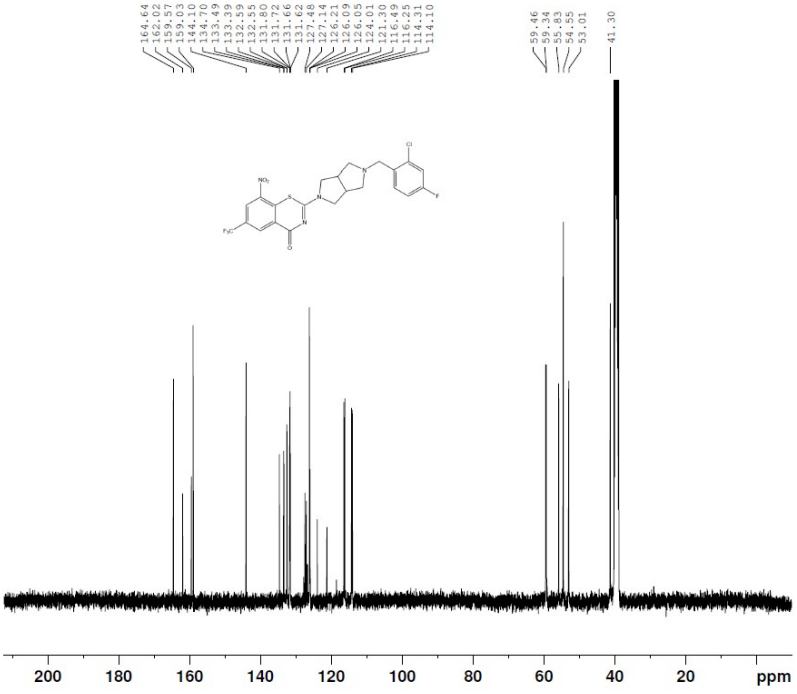



```
Current Data Parameters
NAME              test5
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_           20170531
Time              14.49
INSTRUM   WNMR-I-500MHz
PULPROG             s1pul
TD                 48000
SOLVENT             DMSO
NS                    16
DS                     0
SWH           12000.000 Hz
AQ            2.0000000 sec
RG                 64.5
DW              41.667 usec
DE              30.00 usec
TE              298.3 K
NUC1               1H
PL1             120.00 dB
SFO1        499.7053818 MHz

F2 - Processing parameters
SI                32768
SF          499.6981530 MHz
WDW                 EM
SSB       0
LB                1.00 Hz
GB                 0.1
PC                1.00
```

Bruker AVANCEIII 400 20170607
C13 DMSO D:\\ DATA-2017 36



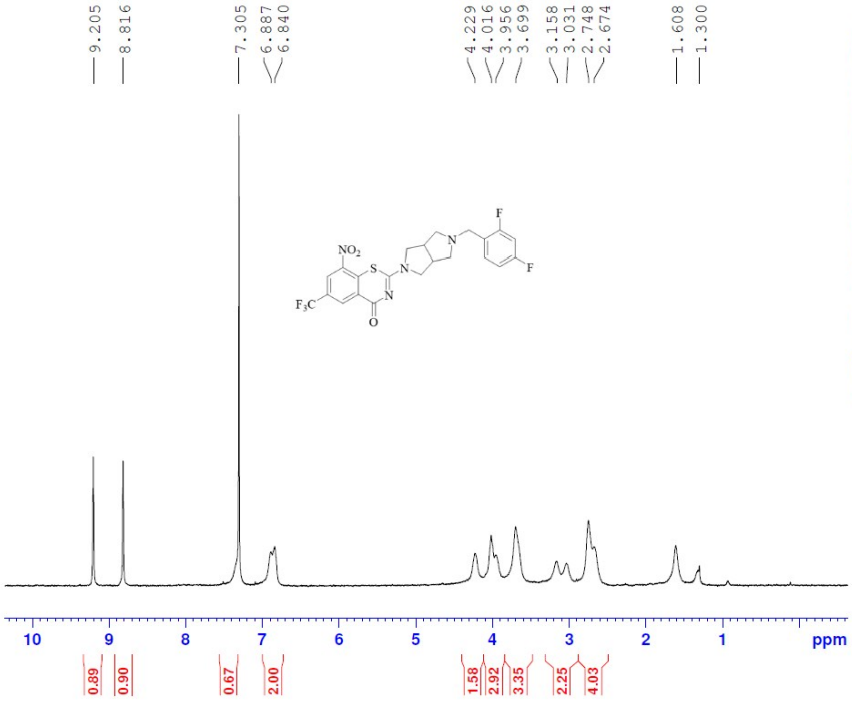
Current Data Parameters
NAME 20170607 test5
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170608
Time 19.00
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 4000
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 77.6
DW 20.800 usec
DE 18.00 usec
TE 298.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 500

======== CHANNEL f1 ========
SFO1 100.6238345 MHz
NUC1 13C
P1 9.84 usec
PLW1 38.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 8.14700031 W
PLW12 0.15600000 W
PLW13 0.09983800 W

F2 - Processing parameters
SI 32768
SF 100.6128160 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

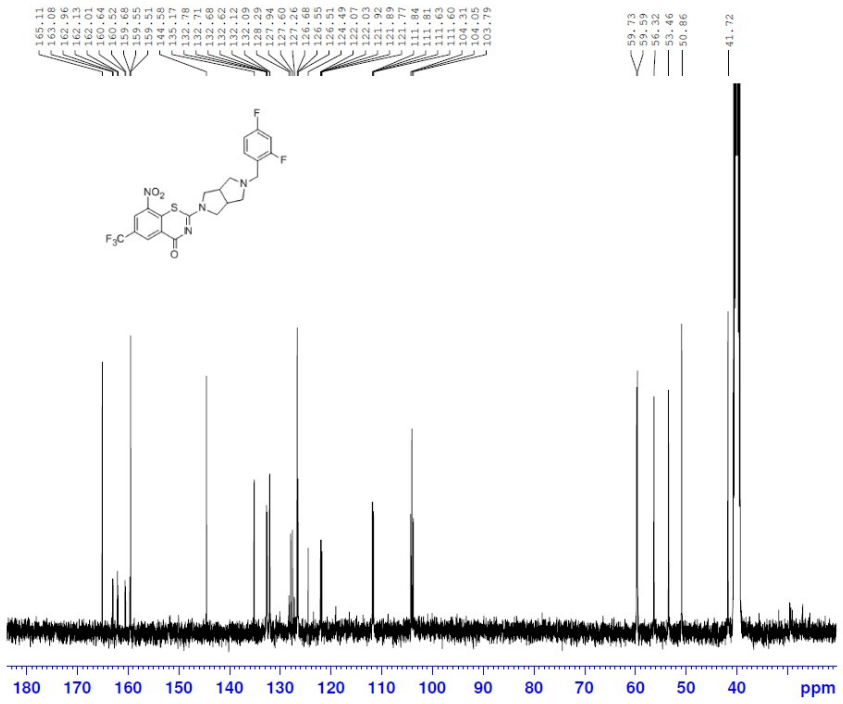


Current Data Parameters
NAME lq-2-67 0511
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170511
Time 14.25
INSTRUM WNMR-I-500MHz
PULPROG s1pul
TD 48000
SOLVENT CDCl3
NS 9
DS 0
SWH 12000.000 Hz
AQ 2.0000000 sec
RG 72.7
DW 41.667 usec
DE 30.00 usec
TE 298.3 K
NUC1 1H
PL1 120.00 dB
SFO1 499.7053818 MHz

F2 - Processing parameters
SI 32768
SF 499.7017639 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0.1
PC 1.00

Bruker AVANCEIII 400 20170524
C13 DMSO D:\\ DATA-2017 33



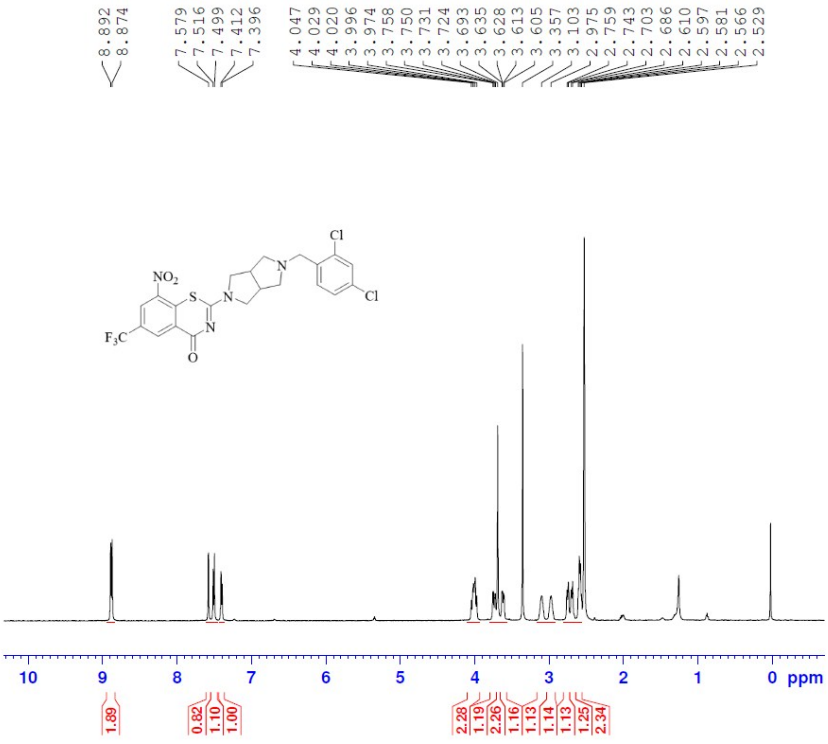

```
Current Data Parameters
NAME      20170524  1q-2-67
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_              20170524
Time                  19.34
INSTRUM               spect
PROBHD   5 mm CPPBBO BB
PULPROG             zgpg30
TD                   32768
SOLVENT               DMSO
NS                    3200
DS                       4
SWH             24038.461 Hz
FIDRES           0.733596 Hz
AQ               0.6815744 sec
RG                    77.6
DW                  20.800 usec
DE                  18.00 usec
TE                  298.0 K
D1             1.00000000 sec
D11            0.03000000 sec
TD0                    400

======== CHANNEL f1 ========
SFO1          100.6238345 MHz
NUC1                   13C
P1                    9.84 usec
PLW1          38.00000000 W

======== CHANNEL f2 ========
SFO2          400.1316005 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2                80.00 usec
PLW2           8.14700031 W
PLW12          0.15600000 W
PLW13          0.09983800 W

F2 - Processing parameters
SI                   32768
SF            100.6127690 MHz
WDW                     EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```

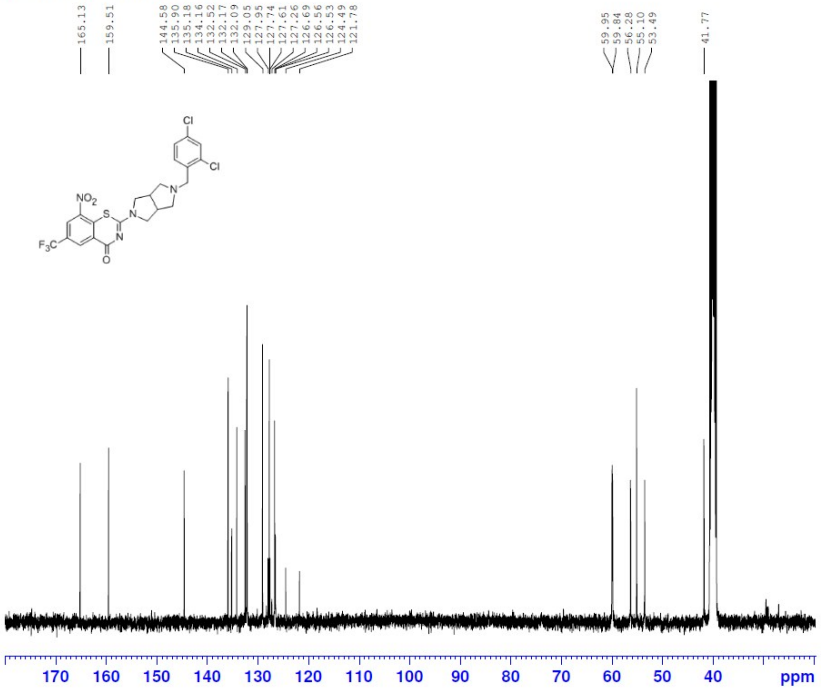



```
Current Data Parameters
NAME      1q-2-72 05192017
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_              20170519
Time                  10.28
INSTRUM   WNMR-I-500MHz
PULPROG              s1pul
TD                   48000
SOLVENT               DMSO
NS                      13
DS                       0
SWH            12000.000 Hz
AQ             2.0000000 sec
RG                    70.7
DW                 41.667 usec
DE                  30.00 usec
TE                  293.5 K
NUC1                   1H
PL1                120.00 dB
SFO1          499.7053818 MHz

F2 - Processing parameters
SI                   32768
SF            499.7041375 MHz
WDW                     EM
SSB       0
LB                    1.00 Hz
GB                     0.1
PC                    1.00
```

Bruker AVANCEIII 400 20170524
C13 DMSO D:\\ DATA-2017 34



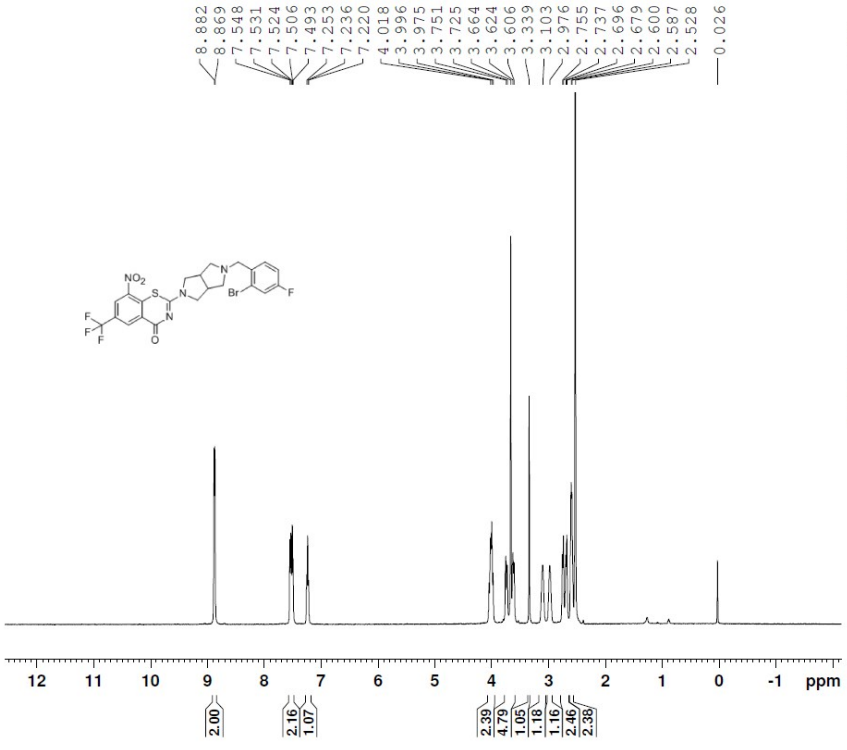

```
Current Data Parameters
NAME       20170524  lq-2-72
EXPNO             1
PROCNO            1

F2 - Acquisition Parameters
Date_          20170524
Time             21.09
INSTRUM          spect
PROBHD   5 mm CPPBBO BB
PULPROG        zgpg30
TD              32768
SOLVENT          DMSO
NS                3200
DS                   4
SWH          24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG                77.6
DW              20.800 usec
DE              18.00 usec
TE              298.0 K
D1          1.00000000 sec
D11         0.03000000 sec
TD0                400

======== CHANNEL f1 ========
SFO1       100.6238345 MHz
NUC1              13C
P1               9.84 usec
PLW1       38.00000000 W

======== CHANNEL f2 ========
SFO2       400.1316005 MHz
NUC2              1H
CPDPRG[2       waltz16
PCPD2           80.00 usec
PLW2        8.14700031 W
PLW12       0.15600000 W
PLW13       0.09983800 W

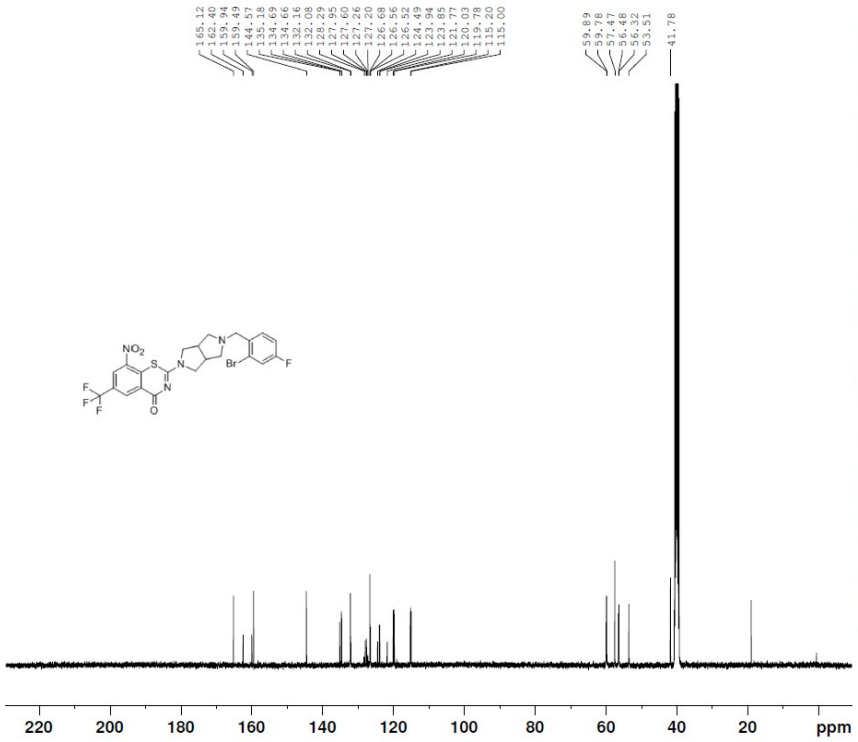
F2 - Processing parameters
SI               32768
SF         100.6127690 MHz
WDW                EM
SSB       0
LB              1.00 Hz
GB        0
PC              1.40
```




```
Current Data Parameters
NAME          tzy-3-33
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_          20170526
Time             16.30
INSTRUM   WNMR-I-500MHz
PULPROG          s1pul
TD               48000
SOLVENT           DMSO
NS                  17
DS                   0
SWH          12000.000 Hz
AQ           2.0000000 sec
RG                66.3
DW              41.667 usec
DE              30.00 usec
TE              298.1 K
NUC1               1H
PL1             120.00 dB
SFO1       499.7053818 MHz

F2 - Processing parameters
SI               32768
SF         499.7041375 MHz
WDW                EM
SSB       0
LB              1.00 Hz
GB               0.1
PC              1.00
```



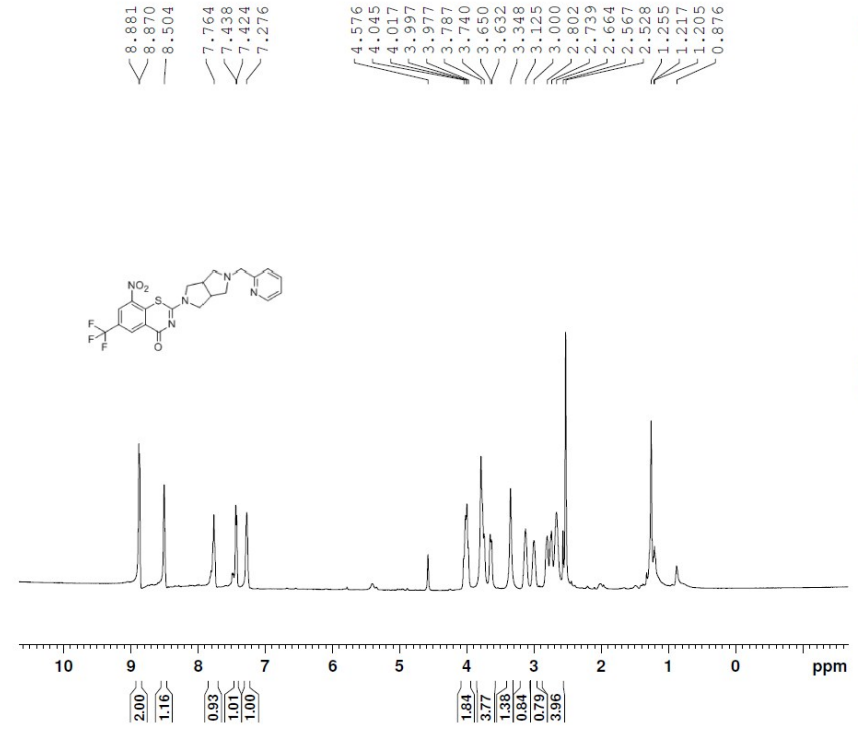

```
Current Data Parameters
NAME      20170607  TZY-3-33
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_             20170609
Time                 2.56
INSTRUM             spect
PROBHD    5 mm CPPBBO BB
PULPROG           zgpg30
TD                 32768
SOLVENT             DMSO
NS                  4000
DS                     4
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              0.6815744 sec
RG                  77.6
DW                20.800 usec
DE                18.00 usec
TE                298.0 K
D1             1.00000000 sec
D11            0.03000000 sec
TD0                  500

======== CHANNEL f1 ========
SFO1          100.6238345 MHz
NUC1                 13C
P1                  9.84 usec
PLW1          38.00000000 W

======== CHANNEL f2 ========
SFO2          400.1316005 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2              80.00 usec
PLW2           8.14700031 W
PLW12          0.15600000 W
PLW13          0.09983800 W

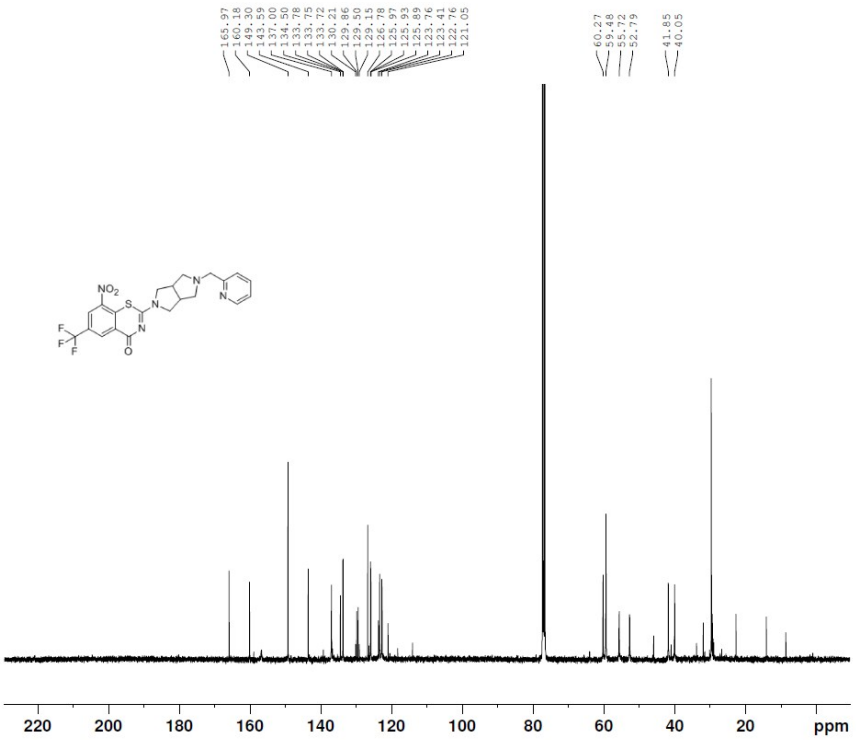
F2 - Processing parameters
SI                  32768
SF            100.6127690 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```




```
Current Data Parameters
NAME                 test2
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20170531
Time                14.29
INSTRUM   WNMR-I-500MHz
PULPROG              s1pul
TD                   48000
SOLVENT              DMSO
NS                     16
DS                      0
SWH           12000.000 Hz
AQ             2.0000000 sec
RG                   60.8
DW                41.667 usec
DE                30.00 usec
TE                298.3 K
NUC1                 1H
PL1               120.00 dB
SFO1          499.7053818 MHz

F2 - Processing parameters
SI                   32768
SF            499.7041375 MHz
WDW                     EM
SSB       0
LB                   1.00 Hz
GB                    0.1
PC                   1.00
```



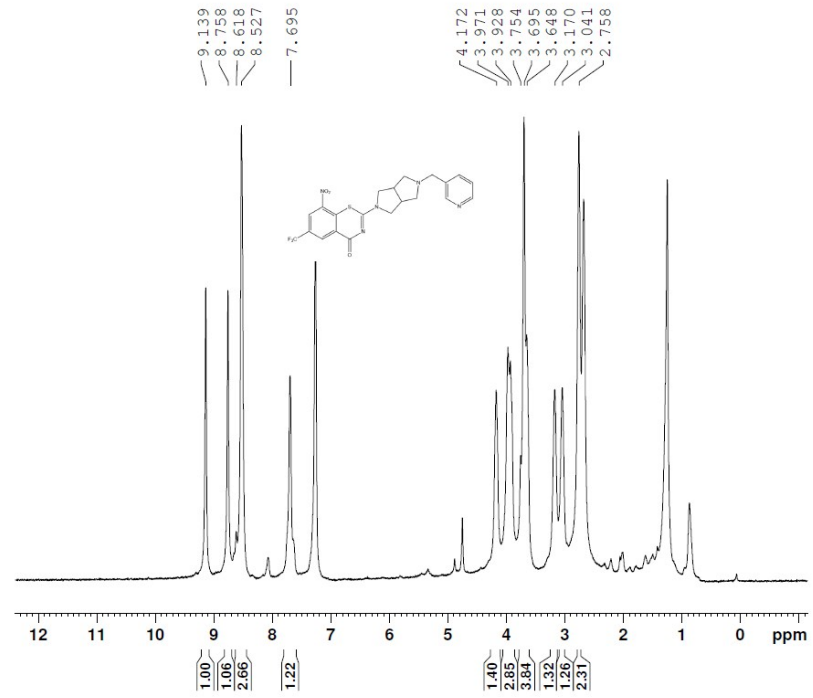

```
Current Data Parameters
NAME      20170607  test2
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_              20170609
Time                  6.54
INSTRUM              spect
PROBHD   5 mm CPPBBO BB
PULPROG           zgpg30
TD                 32768
SOLVENT            CDCl3
NS                  3521
DS                     4
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              0.6815744 sec
RG                  77.6
DW                20.800 usec
DE                18.00 usec
TE                298.0 K
D1             1.00000000 sec
D11            0.03000000 sec
TD0                  500

======== CHANNEL f1 ========
SFO1         100.6238345 MHz
NUC1                  13C
P1                   9.84 usec
PLW1         38.00000000 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2               80.00 usec
PLW2          8.14700031 W
PLW12         0.15600000 W
PLW13         0.09983800 W

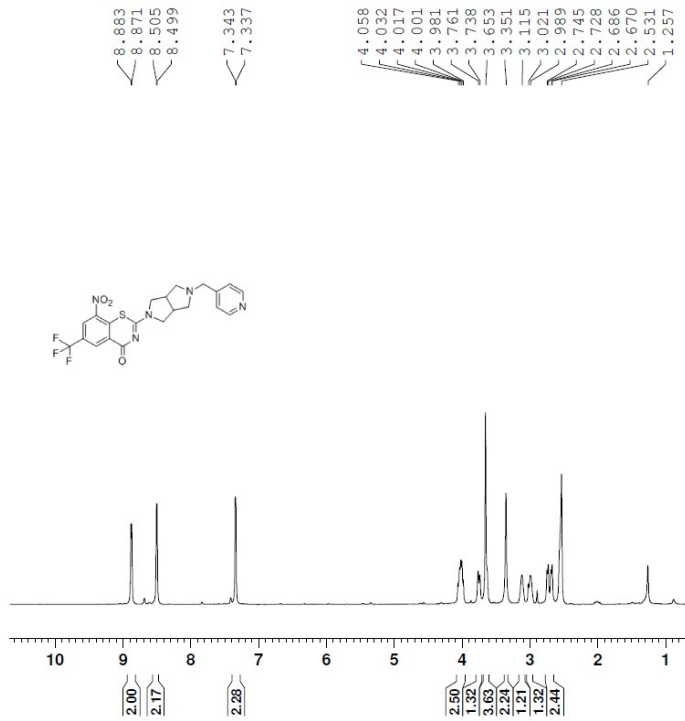
F2 - Processing parameters
SI                 32768
SF           100.6127690 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```




```
Current Data Parameters
NAME                  test3
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20170612
Time                  9.21
INSTRUM   WNMR-I-500MHz
PULPROG             s1pul
TD                  48000
SOLVENT             CDCl3
NS                     18
DS                      0
SWH            12000.000 Hz
AQ              2.0000000 sec
RG                   64.3
DW                41.667 usec
DE                30.00 usec
TE                298.1 K
NUC1                  1H
PL1                120.00 dB
SFO1         499.7053818 MHz

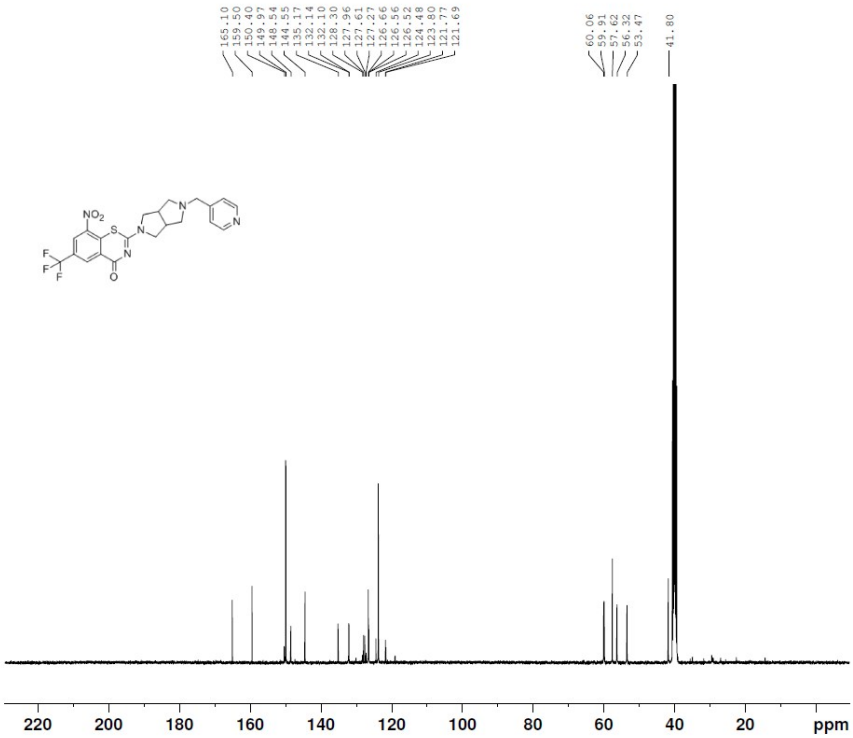
F2 - Processing parameters
SI                 32768
SF           499.6957858 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB                  0.1
PC                 1.00
```




```
Current Data Parameters
NAME                 test4
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20170531
Time                 14.36
INSTRUM   WNMR-I-500MHz
PULPROG              slpul
TD                   48000
SOLVENT               DMSO
NS                      16
DS                       0
SWH            12000.000 Hz
AQ             2.0000000 sec
RG                    60.5
DW               41.667 usec
DE                30.00 usec
TE                298.0 K
NUC1                   1H
PL1               120.00 dB
SFO1         499.7053818 MHz

F2 - Processing parameters
SI                   32768
SF            499.7041375 MHz
WDW                     EM
SSB       0
LB                 1.00 Hz
GB                  0.1
PC                 1.00
```



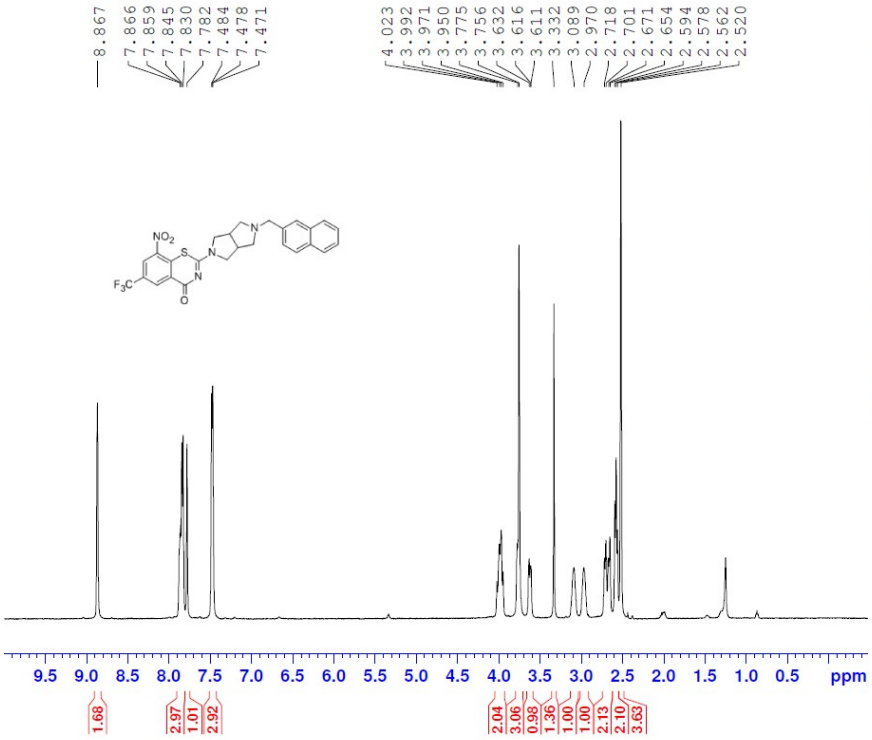

```
Current Data Parameters
NAME      20170607  test4
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20170608
Time                 17.01
INSTRUM              spect
PROBHD   5 mm CPPBBO BB
PULPROG             zgpg30
TD                   32768
SOLVENT               DMSO
NS                    4000
DS                       4
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ             0.6815744 sec
RG                    77.6
DW               20.800 usec
DE                18.00 usec
TE                298.0 K
D1             1.00000000 sec
D11            0.03000000 sec
TD0                   500

======== CHANNEL f1 ========
SFO1         100.6238345 MHz
NUC1                   13C
P1                 9.84 usec
PLW1         38.00000000 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2             80.00 usec
PLW2          8.14700031 W
PLW12         0.15600000 W
PLW13         0.09983800 W

F2 - Processing parameters
SI                   32768
SF           100.6127690 MHz
WDW                     EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

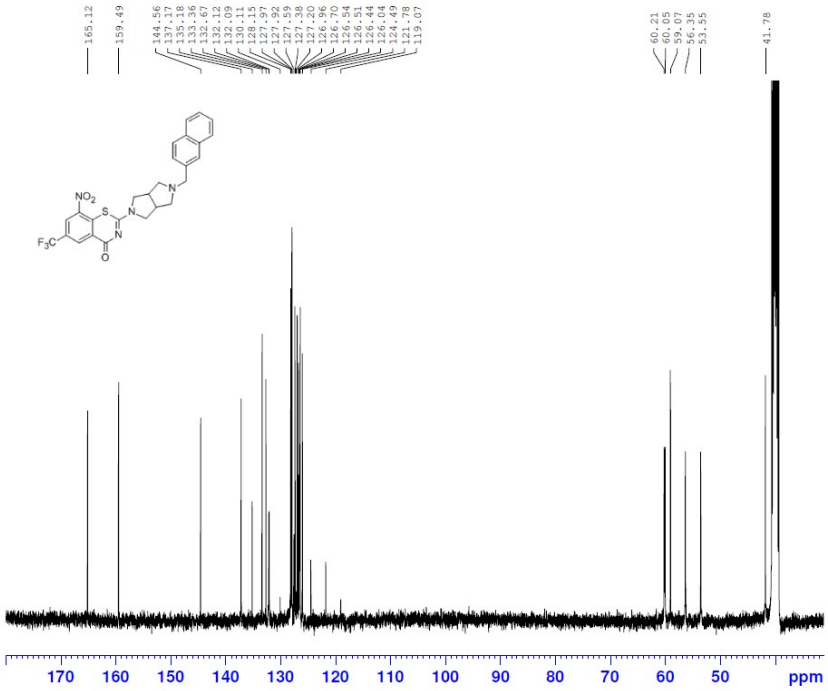



```
Current Data Parameters
NAME      1q-2-79 20170525
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_           20170525
Time              14.09
INSTRUM   WNMR-I-500MHz
PULPROG            s1pul
TD                 48000
SOLVENT             DMSO
NS                    13
DS                     0
SWH           12000.000 Hz
AQ            2.0000000 sec
RG                  61.4
DW               41.667 usec
DE                30.00 usec
TE                298.3 K
NUC1                1H
PL1              120.00 dB
SFO1         499.7053818 MHz

F2 - Processing parameters
SI                 32768
SF           499.6981441 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB                  0.1
PC                 1.00
```

Bruker AVANCEIII 400 20170526
C13 DMSO D:\\ DATA-2017 19



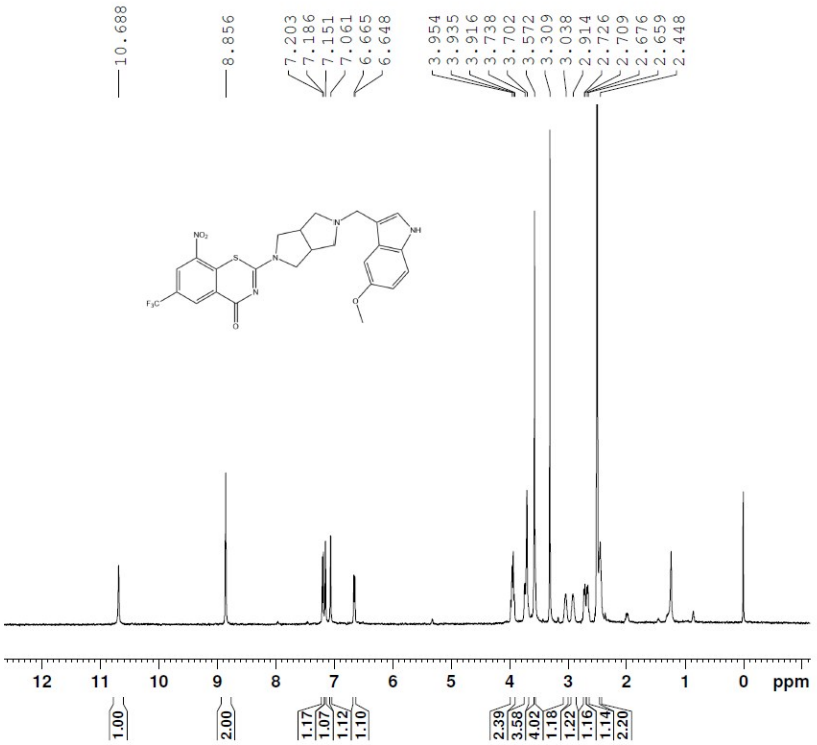

```
Current Data Parameters
NAME      20170526  LQ-2-79
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_           20170528
Time              14.24
INSTRUM            spect
PROBHD   5 mm CPPBBO BB
PULPROG          zgpg30
TD                 32768
SOLVENT             DMSO
NS                  3200
DS                     4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            0.6815744 sec
RG                  77.6
DW               20.800 usec
DE                18.00 usec
TE                298.0 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                  400

======== CHANNEL f1 ========
SFO1         100.6238345 MHz
NUC1               13C
P1                9.84 usec
PLW1         38.00000000 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2               1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2          8.14700031 W
PLW12         0.15600000 W
PLW13         0.09983800 W

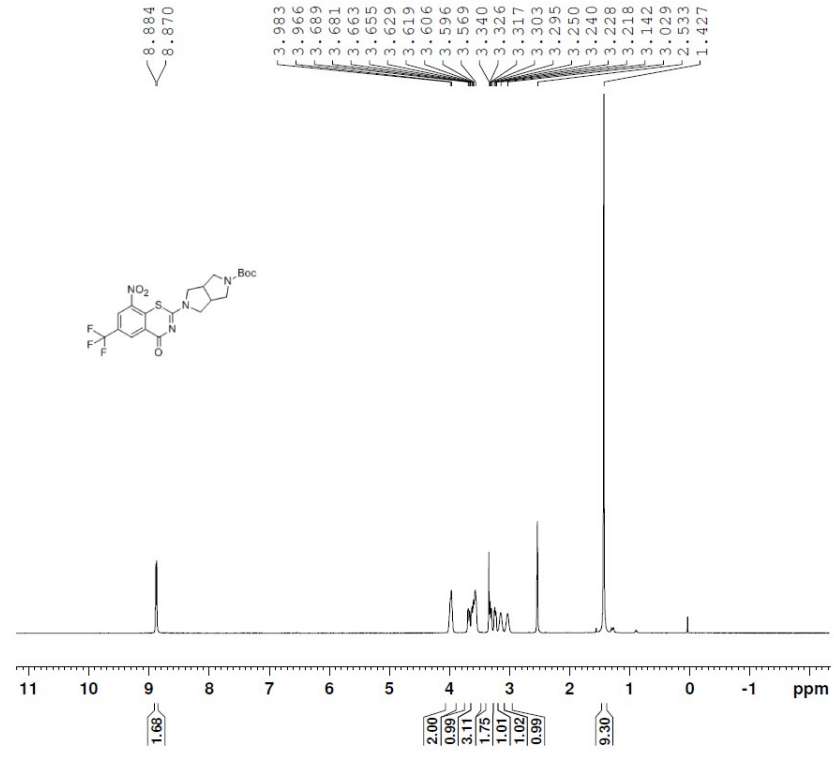
F2 - Processing parameters
SI                 32768
SF           100.6127690 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```




```
Current Data Parameters
NAME          sn-2-6-0414
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20170414
Time               16.04
INSTRUM    WNMR-I-500MHz
PULPROG            slpul
TD                 48000
SOLVENT             DMSO
NS                     8
DS                     0
SWH          12000.000 Hz
AQ           2.0000000 sec
RG                  71.6
DW             41.667 usec
DE              30.00 usec
TE              298.4 K
NUC1                1H
PL1            120.00 dB
SFO1        499.7053818 MHz

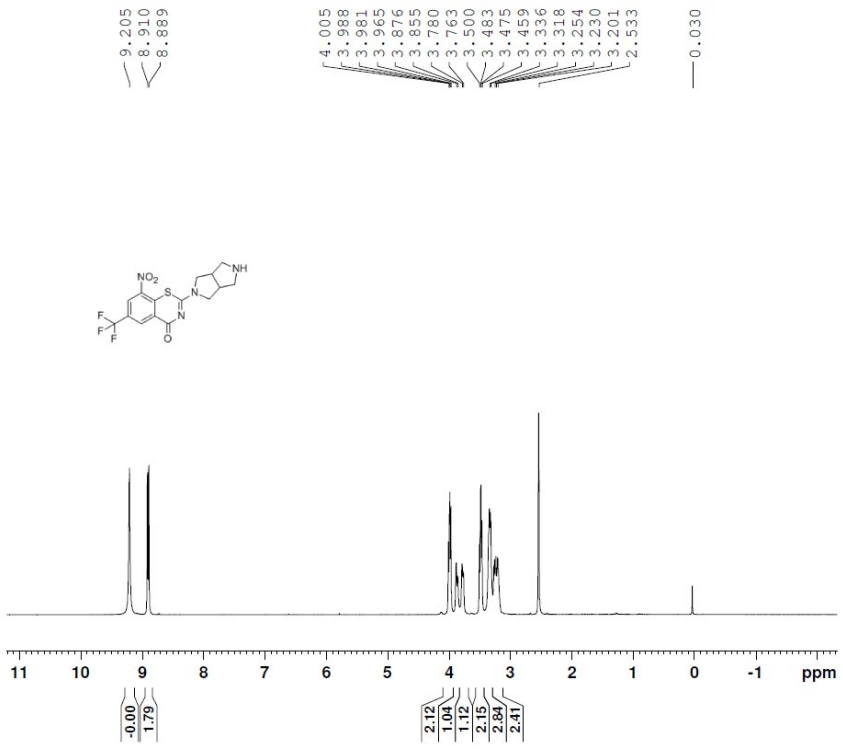
F2 - Processing parameters
SI                 32768
SF          499.6981519 MHz
WDW                   EM
SSB       0
LB              1.00 Hz
GB                 0.1
PC                1.00
```




```
Current Data Parameters
NAME            tzy-3-17
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20170502
Time               15.08
INSTRUM    WNMR-I-500MHz
PULPROG            slpul
TD                 48000
SOLVENT             DMSO
NS                    16
DS                     0
SWH          12000.000 Hz
AQ           2.0000000 sec
RG                  63.8
DW             41.667 usec
DE              30.00 usec
TE              298.4 K
NUC1                1H
PL1            120.00 dB
SFO1        499.7053818 MHz

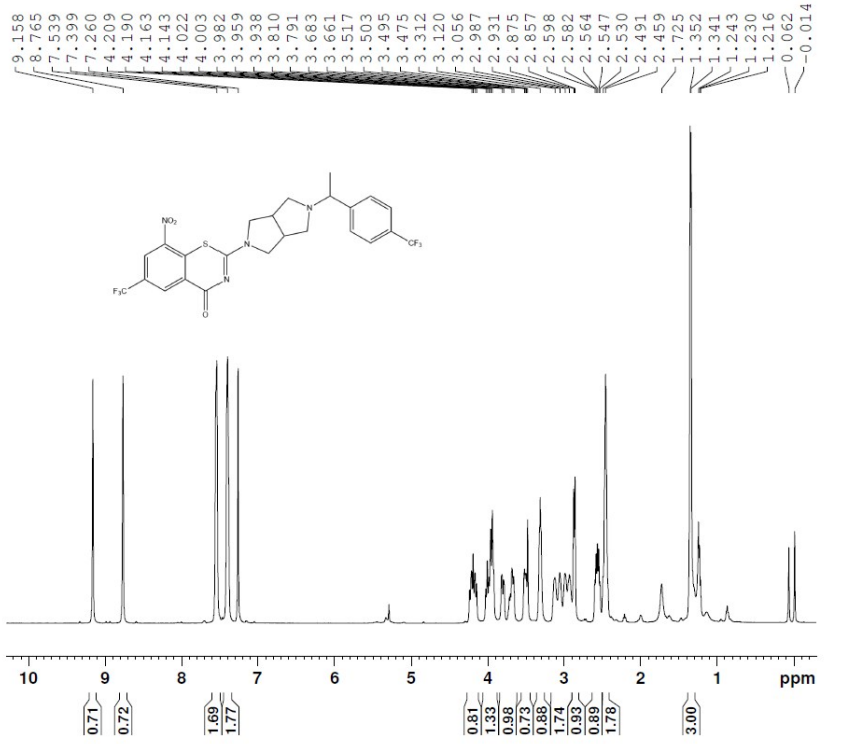
F2 - Processing parameters
SI                 32768
SF          499.7041375 MHz
WDW                   EM
SSB       0
LB              1.00 Hz
GB                 0.1
PC                1.00
```




```
Current Data Parameters
NAME                  tzy-3-18
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20170502
Time                     15.05
INSTRUM          WNMR-I-500MHz
PULPROG                  slpul
TD                       48000
SOLVENT                   DMSO
NS                           16
DS                            0
SWH                 12000.000 Hz
AQ                  2.0000000 sec
RG                        60.7
DW                      41.667 usec
DE                      30.00 usec
TE                      298.3 K
NUC1                         1H
PL1                     120.00 dB
SFO1               499.7053818 MHz

F2 - Processing parameters
SI                       32768
SF                 499.7041375 MHz
WDW                         EM
SSB                  0
LB                       1.00 Hz
GB                        0.1
PC                       1.00
```

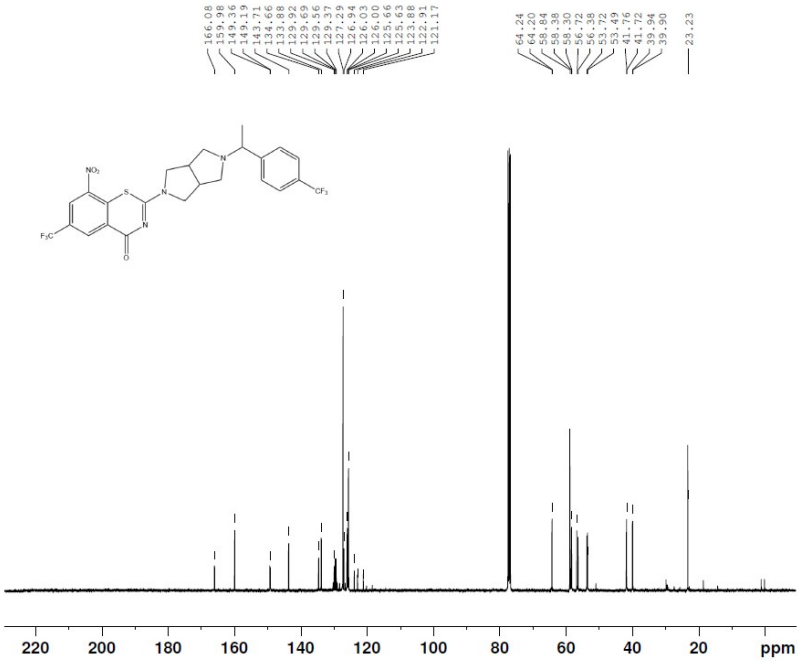



```
Current Data Parameters
NAME                  HB-1-48
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20181228
Time                     9.56
INSTRUM          WNMR-I-500MHz
PULPROG                  slpul
TD                       48000
SOLVENT                  CDCl3
NS                           31
DS                            0
SWH                 12000.000 Hz
AQ                  2.0000000 sec
RG                        42.1
DW                      41.667 usec
DE                      30.00 usec
TE                      298.1 K
NUC1                         1H
PL1                     120.00 dB
SFO1               499.6837539 MHz

F2 - Processing parameters
SI                       32768
SF                 499.6801597 MHz
WDW                         EM
SSB                  0
LB                       1.00 Hz
GB                        0.1
PC                       1.00
```

Bruker AVANCEIII 400 20181228
C13 CDCl3 D:\\ DATA-2018 32




```
Current Data Parameters
NAME      20181228  hb-1-48
EXPNO                1
PROCNO               1

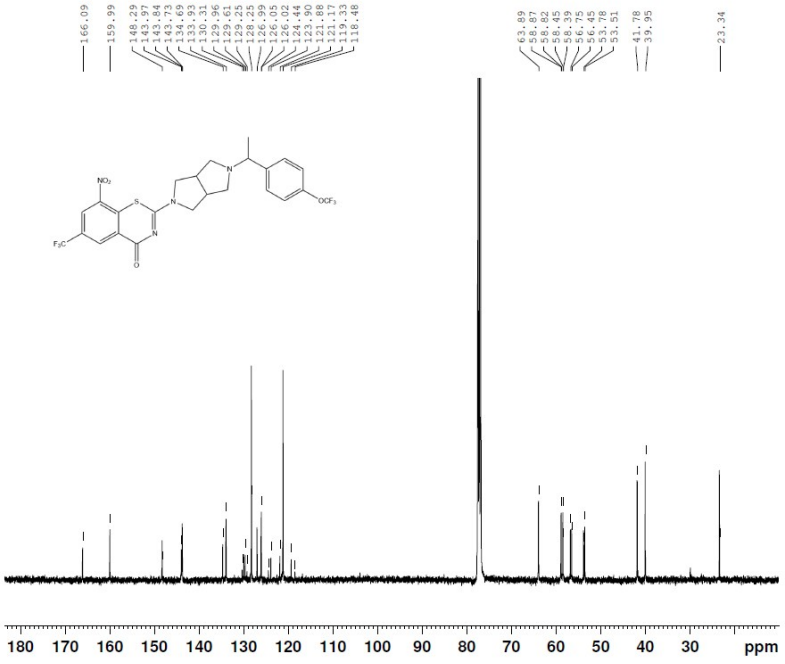
F2 - Acquisition Parameters
Date_           20181228
Time              14.39
INSTRUM           spect
PROBHD   5 mm CPPBBO BB
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                 1332
DS                    4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            0.6815744 sec
RG                 77.6
DW               20.800 usec
DE               18.00 usec
TE               298.0 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                 400

======== CHANNEL f1 ========
SFO1         100.6238345 MHz
NUC1               13C
P1                9.84 usec
PLW1        38.00000000 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2               1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2         8.14700031 W
PLW12        0.22080000 W
PLW13        0.14131001 W

F2 - Processing parameters
SI                32768
SF           100.6127596 MHz
WDW                EM
SSB       0
LB               1.00 Hz
GB        0
PC               1.40
```

Bruker AVANCEIII 400 20190102
C13 CDCl3 D:\\ DATA-2018 4



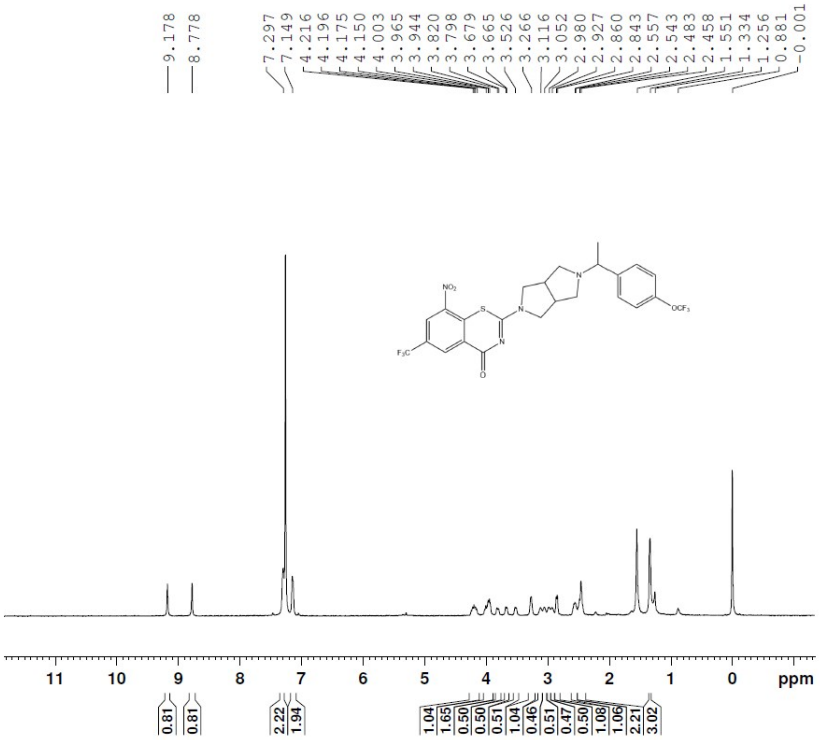

```
Current Data Parameters
NAME      20190102  hb-1-50
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_           20190102
Time              21.34
INSTRUM           spect
PROBHD   5 mm CPPBBO BB
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                 4000
DS                    4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            0.6815744 sec
RG                 77.6
DW               20.800 usec
DE               18.00 usec
TE               298.1 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                 500

======== CHANNEL f1 ========
SFO1         100.6238345 MHz
NUC1               13C
P1                9.84 usec
PLW1        38.00000000 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2               1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2         8.14700031 W
PLW12        0.22080000 W
PLW13        0.14131001 W

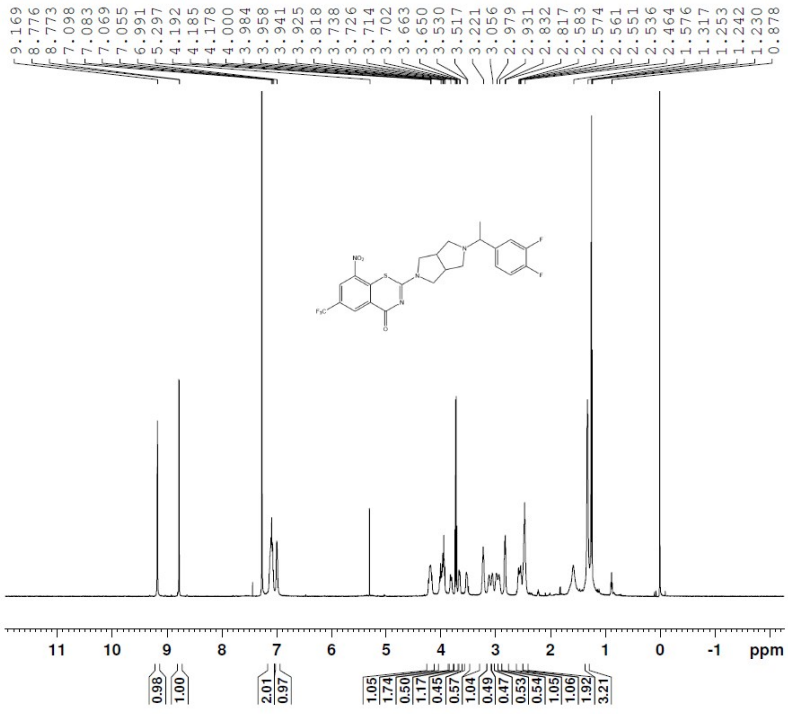
F2 - Processing parameters
SI                32768
SF           100.6127574 MHz
WDW                EM
SSB       0
LB               1.00 Hz
GB        0
PC               1.40
```




```
Current Data Parameters
NAME                  hb-1-50
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_               20190114
Time                   12.03
INSTRUM    WNMR-I-500MHz
PULPROG                s1pul
TD                     48000
SOLVENT                CDCl3
NS                        12
DS                         0
SWH                12000.000 Hz
AQ                 2.0000000 sec
RG                      58.2
DW                    41.667 usec
DE                    30.00 usec
TE                    298.1 K
NUC1                      1H
PL1                   120.00 dB
SFO1              499.6837539 MHz

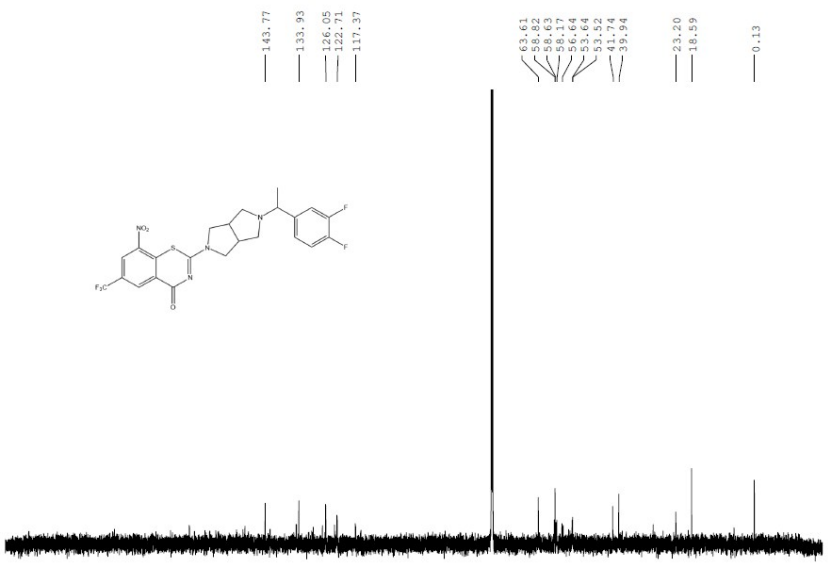
F2 - Processing parameters
SI                     32768
SF                499.6801585 MHz
WDW                       EM
SSB          0
LB                     1.00 Hz
GB                      0.1
PC                     1.00
```

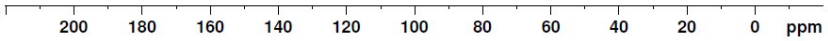



```
Current Data Parameters
NAME                  HB-1-56
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_               20190124
Time                   16.48 h
INSTRUM                spect
PROBHD    Z114607_0230 (
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                12019.230 Hz
FIDRES             0.366798 Hz
AQ                 2.7262976 sec
RG                     106.35
DW                    41.600 usec
DE                     6.50 usec
TE                    300.0 K
D1                 1.00000000 sec
TD0                        1
SFO1              600.1337058 MHz
NUC1                      1H
P0                     3.32 usec
P1                     9.97 usec
PLW1              25.38800049 W

F2 - Processing parameters
SI                     65536
SF                600.1300158 MHz
WDW                       EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```

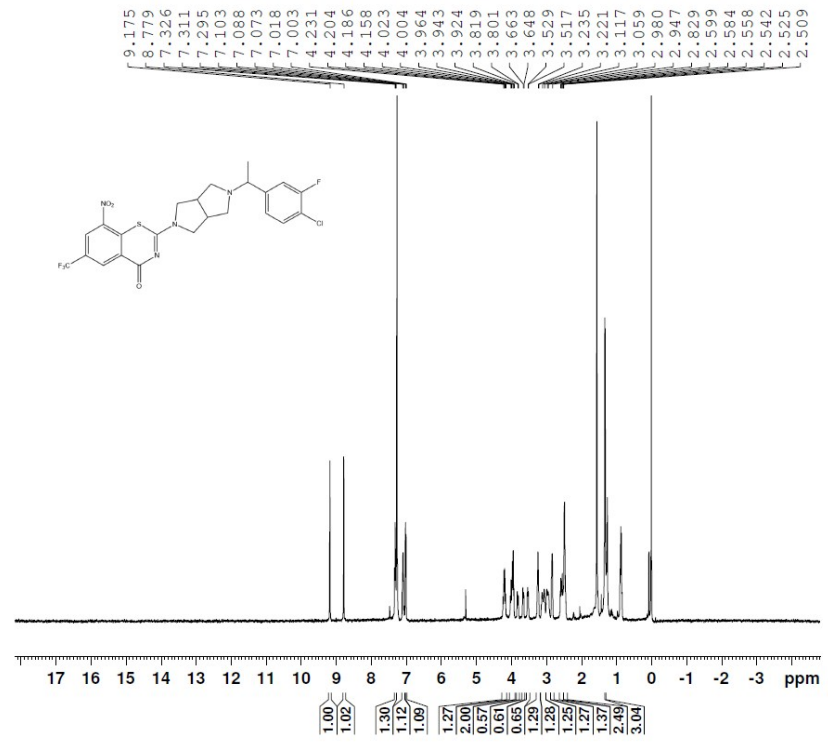





```
Current Data Parameters
NAME                  HB-1-56
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_               20190124
Time                   17.40 h
INSTRUM                spect
PROBHD    Z114607_0230 (
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH               36231.883 Hz
FIDRES             1.105709 Hz
AQ                 0.9043968 sec
RG                     189.7
DW                    13.800 usec
DE                     6.50 usec
TE                    300.0 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                        1
SFO1            150.9178988 MHz
NUC1                     13C
P0                     3.87 usec
P1                    11.60 usec
PLW1             89.20700073 W
SFO2            600.1324005 MHz
NUC2                     1H
CPDPRG[2             waltz65
PCPD2                 70.00 usec
PLW2             25.38800049 W
PLW12             0.51502001 W
PLW13             0.25905001 W

F2 - Processing parameters
SI                        32768
SF              150.9027872 MHz
WDW                          EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```




```
Current Data Parameters
NAME                  hb-1-58
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_               20190114
Time                   12.07
INSTRUM    WNMR-I-500MHz
PULPROG                 s1pul
TD                      48000
SOLVENT               CDCl3
NS                          6
DS                          0
SWH              12000.000 Hz
AQ                2.0000000 sec
RG                         35
DW                   41.667 usec
DE                    30.00 usec
TE                    298.1 K
NUC1                       1H
PL1                   120.00 dB
SFO1           499.6837539 MHz

F2 - Processing parameters
SI                        32768
SF              499.6801589 MHz
WDW                          EM
SSB          0
LB                     1.00 Hz
GB                      0.1
PC                     1.00
```

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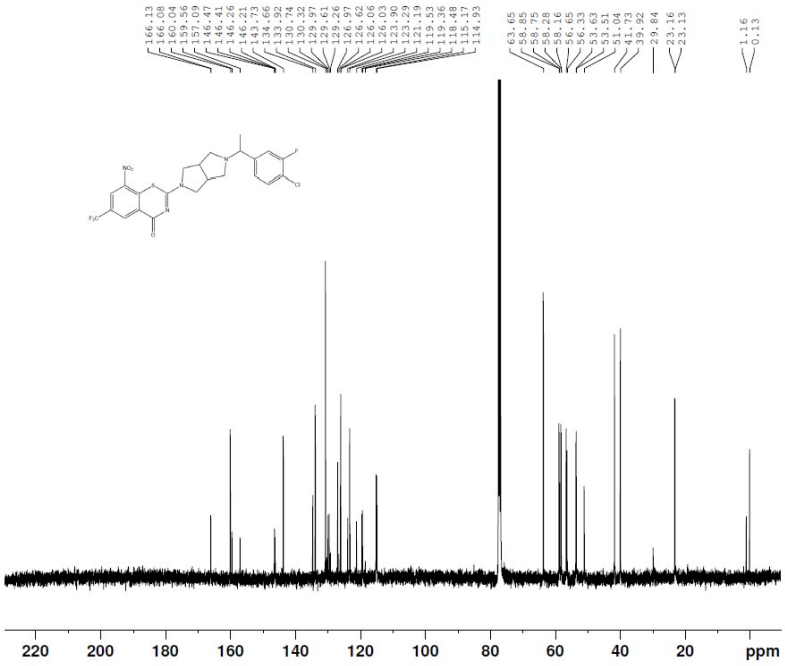
C13 CDCl3 D:\\ DATA-2018 38



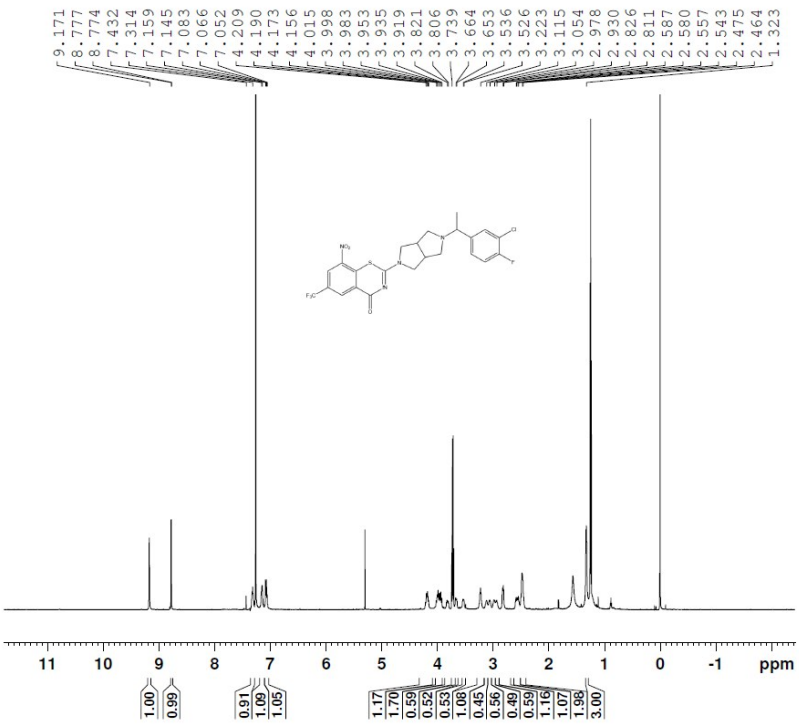

```
Current Data Parameters
NAME      20190111  hb-1-58
EXPNO             1
PROCNO            1

F2 - Acquisition Parameters
Date_          20190112
Time              0.14
INSTRUM          spect
PROBHD   5 mm CPPBBO BB
PULPROG        zgpg30
TD              32768
SOLVENT         CDCl3
NS               4000
DS                  4
SWH         24038.461 Hz
FIDRES          0.733596 Hz
AQ              0.6815744 sec
RG                77.6
DW              20.800 usec
DE              18.00 usec
TE              298.0 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                500

======== CHANNEL f1 ========
SFO1        100.6238345 MHz
NUC1               13C
P1                9.84 usec
PLW1        38.00000000 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2             80.00 usec
PLW2         8.14700031 W
PLW12        0.22080000 W
PLW13        0.14131001 W

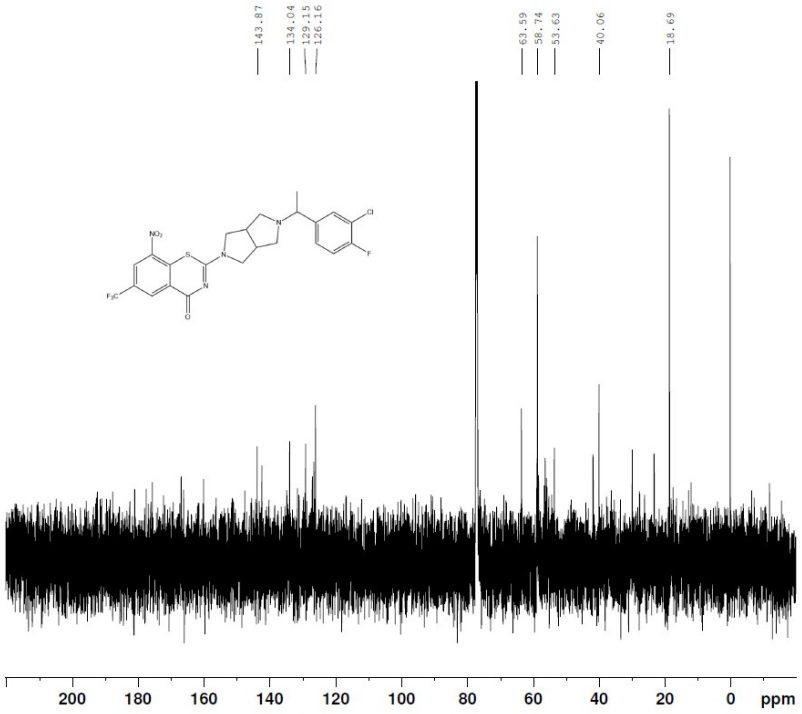
F2 - Processing parameters
SI              32768
SF          100.6127574 MHz
WDW                EM
SSB       0
LB               1.00 Hz
GB        0
PC               1.40
```




```
Current Data Parameters
NAME      HB-1-68-ZC-3-cl-4-F
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_            20190124
Time                17.45 h
INSTRUM            spect
PROBHD   Z114607_0230 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH            12019.230 Hz
FIDRES          0.366798 Hz
AQ              2.7262976 sec
RG                121.15
DW                41.600 usec
DE                 6.50 usec
TE                299.9 K
D1             1.00000000 sec
TD0                    1
SFO1          600.1337058 MHz
NUC1                   1H
P0                  3.32 usec
P1                  9.97 usec
PLW1          25.38800049 W

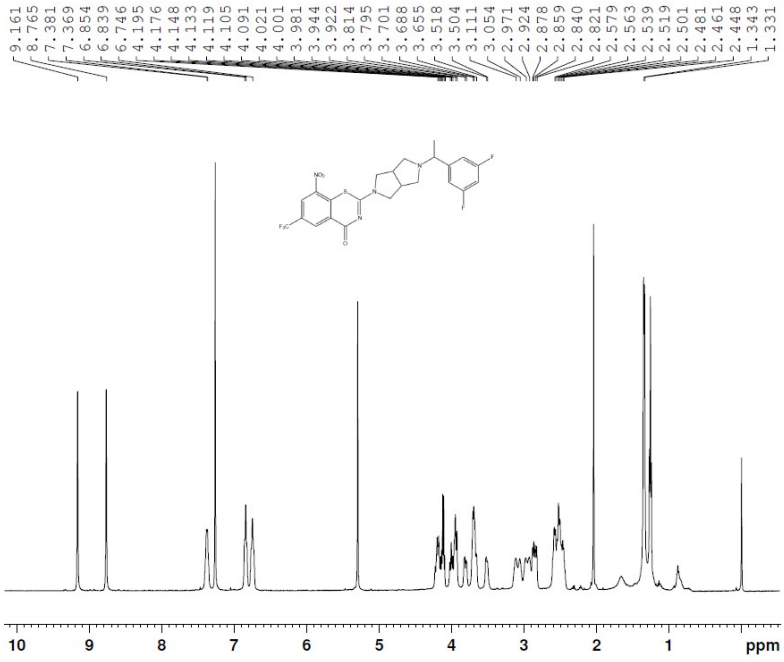
F2 - Processing parameters
SI                 65536
SF            600.1300159 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```




```
Current Data Parameters
NAME      HB-1-68-ZC-3-cl-4-F
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20190124
Time                 18.37 h
INSTRUM                spect
PROBHD    Z114607_0230 (
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    1024
DS                       4
SWH              36231.883 Hz
FIDRES           1.105709 Hz
AQ               0.9043968 sec
RG                   189.7
DW                  13.800 usec
DE                   6.50 usec
TE                  300.0 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                      1
SFO1           150.9178988 MHz
NUC1                   13C
P0                    3.87 usec
P1                   11.60 usec
PLW1          89.20700073 W
SFO2          600.1324005 MHz
NUC2                   1H
CPDPRG[2          waltz65
PCPD2                70.00 usec
PLW2          25.38800049 W
PLW12          0.51502001 W
PLW13          0.25905001 W

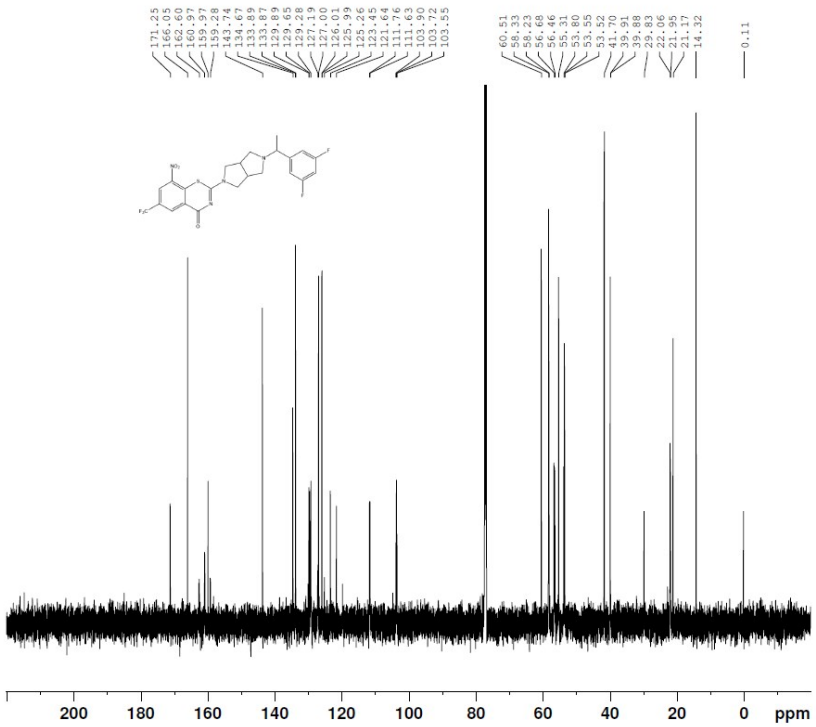
F2 - Processing parameters
SI                   32768
SF             150.9027717 MHz
WDW                     EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```




```
Current Data Parameters
NAME              hb-1-65
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_              20190122
Time                 12.17
INSTRUM   WNMR-I-500MHz
PULPROG              s1pu1
TD                   48000
SOLVENT              CDCl3
NS                       4
DS                       0
SWH              12000.000 Hz
AQ               2.0000000 sec
RG                      35
DW                 41.667 usec
DE                 30.00 usec
TE                 298.1 K
NUC1                   1H
PL1                120.00 dB
SFO1          499.6837539 MHz

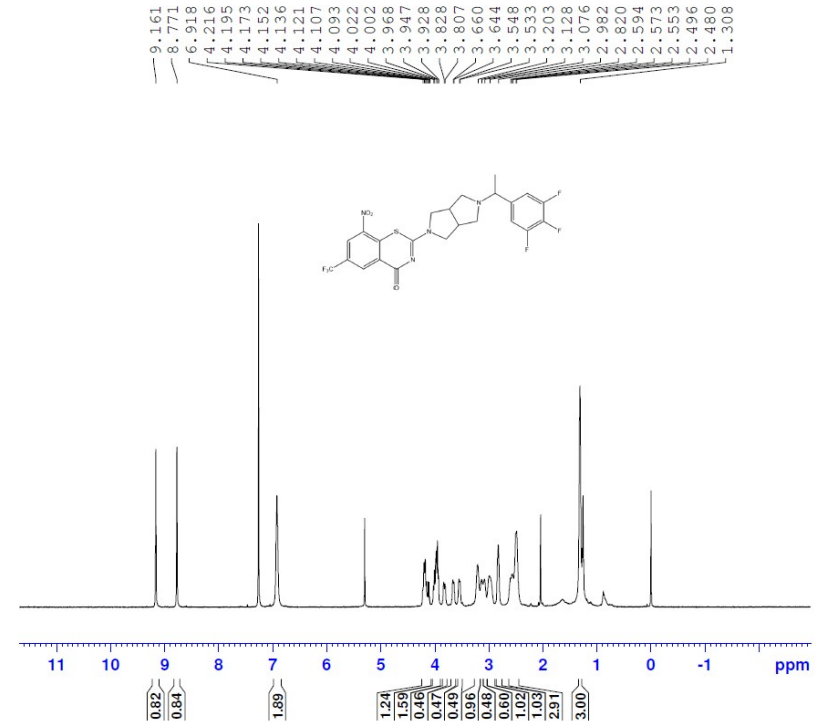
F2 - Processing parameters
SI                   32768
SF             499.6801596 MHz
WDW                     EM
SSB       0
LB                    1.00 Hz
GB                     0.1
PC                    1.00
```




```
Current Data Parameters
NAME                  HB-1-65-C
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_               20190124
Time                    11.08 h
INSTRUM                  spect
PROBHD     Z114607_0230 (
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                        1024
DS                           4
SWH                 36231.883 Hz
FIDRES              1.105709 Hz
AQ                  0.9043968 sec
RG                       189.7
DW                      13.800 usec
DE                       6.50 usec
TE                      300.0 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                          1
SFO1               150.9178988 MHz
NUC1                        13C
P0                       3.87 usec
P1                      11.60 usec
PLW1               89.20700073 W
SFO2               600.1324005 MHz
NUC2                        1H
CPDPRG[2                waltz65
PCPD2                   70.00 usec
PLW2               25.38800049 W
PLW12               0.51502001 W
PLW13               0.25905001 W

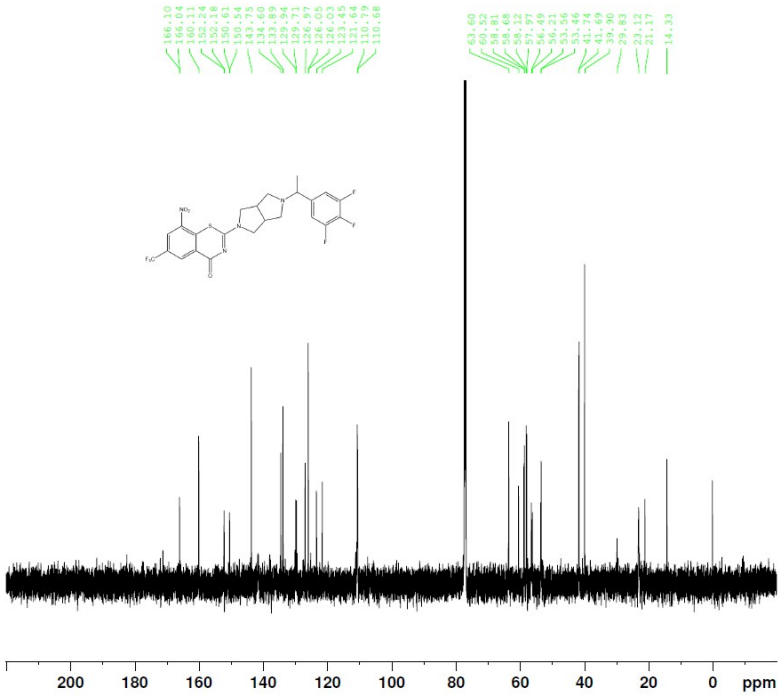
F2 - Processing parameters
SI                       32768
SF                 150.9027891 MHz
WDW                         EM
SSB          0
LB                       1.00 Hz
GB           0
PC                       1.40
```




```
Current Data Parameters
NAME                  hb-1-67
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_               20190122
Time                    12.33
INSTRUM    WNMR-I-500MHz
PULPROG                 s1pul
TD                       48000
SOLVENT                  CDCl3
NS                           3
DS                           0
SWH                 12000.000 Hz
AQ                  2.0000000 sec
RG                          50
DW                      41.667 usec
DE                      30.00 usec
TE                      298.1 K
NUC1                        1H
PL1                     120.00 dB
SFO1               499.6837539 MHz

F2 - Processing parameters
SI                       32768
SF                 499.6801593 MHz
WDW                         EM
SSB          0
LB                       1.00 Hz
GB                        0.1
PC                       1.00
```




```
Current Data Parameters
NAME      HB-1-67-ZC-3,4,5-triF
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_              20190124
Time                 12.04 h
INSTRUM                spect
PROBHD    Z114607_0230 (
PULPROG             zgpg30
TD                   65536
SOLVENT              CDC13
NS                    1024
DS                       4
SWH              36231.883 Hz
FIDRES           1.105709 Hz
AQ               0.9043968 sec
RG                   189.7
DW                  13.800 usec
DE                   6.50 usec
TE                  300.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                      1
SFO1         150.9178988 MHz
NUC1                   13C
P0                    3.87 usec
P1                   11.60 usec
PLW1         89.20700073 W
SFO2         600.1324005 MHz
NUC2                   1H
CPDPRG[2           waltz65
PCPD2                70.00 usec
PLW2         25.38800049 W
PLW12         0.51502001 W
PLW13         0.25905001 W

F2 - Processing parameters
SI                   32768
SF           150.9027883 MHz
WDW                     EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
```