SUPPLEMENTAL INFORMATION

Hybridation of Thiazolidinone with Hydroxamate Scaffold for Developing Novel HDAC Inhibitors with Antitumor Activities

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Part A: Biology Experimental Procedures

A.1. HDAC1 activity assay.

HDAC1 activity assay was performed as described in the study report of Shanghai Chemparter CO., LTD. The inhibitory effect of compounds on HDAC1 function was determined *in vitro* using an optimized homogenous assay performed in 384-well plate (Perkin Elmer, Cat. No. 6007279) format. In this assay, enzyme solution and substrate solution (trypsin and Ac-peptide substrate) were prepared in 1x assay buffer and solid compounds for test were dissolved to 10 mM in 100% DMSO. Firstly, Compounds were transferred to 384-well plate by Echo® Liquid Handler (Labcyte, USA) with three times dilution in 100% DMSO. 15 μL of enzyme solution or 1x assay buffer for low control was transferred to assay plate subsequently and incubated at room temperature for 15 min. And then 10 μL of substrate solution was added to each well to start reaction and incubated at room temperature for 60 min. Fluorescence measurements were obtained using a multilabel plate reader Synergy MX with excitation at 355 nm and emission at 460nm. Fit the data in XL-fit to obtain IC50 values using equation Y = Bottom + (Top-Bottom)/(1+10^((LogIC_{50}-X)*Hill Slope)) [Y is %inhibition and X is compound concentration].

A.2. Cell lines and culture conditions

Tumor cell lines used in this study were obtained from the American Type Culture Collection (ATCC). LNCaP, MCF-7 and Hela cell lines were cultured in RPMI 1640 medium, and A549 cell line was cultured in DMEM medium. Medium was supplemented with 10% FBS. All tumor cells were incubated at 37 ^{o}C and 5% CO_2

incubator.

A.3. Cell Viability assay

The cell viability of tumor cell lines in the presence of this series of compounds was determined by SRB (Sigma Aldrich) assay which was described previously.[1] In brief, cells were seeded into 96-well plates at the appropriate cell densities during the experiment. After incubation for 24 h, the cells were treated with various concentrations of the compound for 48 h. Control group were exposed to DMSO at a concentration equivalent to that of the compound-treated cells. After treatment for 48 h, 25 μL of 50% TCA was added for cell fixation at 4 ^{o}C. At least 1 h later or more, the plates were washed by water for five times. The plates were allowed to dry using hair dryer followed by being dyed with 100 μL 0.4% SRB for 10 min. After dying, the plates were washed by 1% acetic acid to remove the dye and allowed to dry using hair dryer. 100 μL of 10 mM Tris-based solution was added to each well, and absorbance was measured using a 96-well plate reader at 515 nm. The IC_{50} was calculated using GraphPad Software.

A.4. In vitro transwell migration assay

Transwell migration assay was performed as previously reported.[2] The inhibition of tumor cell migration was assessed by the Boyden chamber (Corning Falcon) migration assay in 24-well cell culture plate with 8.0-μm pore. Briefly, A549 cells were collected, centrifuged, and re-suspended with serum-free medium. The top chambers were seeded with $5*10^4$ cells in 200 μL of serum-free DMEM medium containing different concentrations of compound. The bottom chambers were filled

with 700 μL of complete medium supplemented with different concentrations of compound. After 18 h incubation, non-migrated cells were removed with cotton swabs, and migrated cells were fixed with cold 4% paraformaldehyde and stained with 0.2% crystal violet for 1 min. Then the chambers were washed using water, and the membrane was left to dry. Images were taken with an inverted microscope (Olympus) and cells from three random areas per filter were counted.

A.5. Western blotting

Western blotting was performed as described previously.[3] Cells were exposed to various concentrations of compounds for indicated time and lysed in RIPA buffer [(50 mM Tris–HCl (pH 7.4), 150 mM NaCl, 5 mM EDTA, 1 % Triton X-100, 1 % sodium deoxycholic acid, 0.1% SDS, 2 mM phenylmethanesulfonyl fluoride (PMSF), 30 mM Na_2HPO_4, 50 mM NaF, 1 mM Na_3VO_4] containing protease/phosphatase inhibitors (Roche). Lysates were combined with sample loading buffer and heated at 100 ℃. Use a Bicinchoninic acid assay (Thermo Scientific) to quantify Protein concentration. Lysates were mixed with sample loading buffer and heated at 100 ºC for 15 min. After separated by 8–15% SDS-PAGE, extracted protein were transferred to nitrocellulose membranes. Membranes were incubated in 5 % (w/v) bovine serum albumin (TBST/BSA) and stored overnight at 4 ℃ on a shaker with specific primary antibodies (1/1,000 in TBST/BSA). Then membranes were washed with TBST and incubated for 45 min with secondary antibody (1/10,000 in TBST/BSA) at room temperature. . Immunoreactive proteins were visualized using the Odyssey Fluorescence Scanner (LI-COR Bioscience, Inc., Lincoln, NE, USA).

A.6 Cell cycle analysis

Cell cycle analysis was conducted by PI staining as described previously.[4] LNCaP and A549 cells were plated in 6 cm dishes and were treated with compounds and the same amount of DMSO as control for 24 h. After ethanol fixation, cells were washed in PBS once and suspended in PBS with 200 μg/ml RNAase and 50 μg/ml propidium iodide (PI) in dark for 30 minutes. Then cells were analyzed by flow cytometry (FACS Calibur, BD Biosciences).

A.7 Apotosis assay

Apoptotic cells were monitored with Annexin V-FITC Apoptosis Detection Kit I (BD Biosciences) as described previously[4]. LNCaP and A549 cells were plated in 6 cm dishes and were treated with compounds and the same amount of DMSO as control for 48 h. Cells were washed with cold PBS, harvested and re-suspended in 100 μL 1×binding buffer, and incubated with 5 μl Annexin V fluorescein isothiocyanate and 5 μl propidium iodide for 15 min in dark at room temperature. Then 400 μl of 1×binding buffer was added and analyzed immediately with flow cytometry (FACS Calibur, BD Biosciences).

Part B: Chemistry Experimental Procedures

B.1. Chemistry: general methods

Reagents were purchased from Adamas-beta Ltd, Sigma-Aldrich Inc., J&K Inc., or Aladdin-reagents Inc., and used without further purification unless otherwise specified. All reactions were carried out with the use of standard techniques under an inert atmosphere (Ar or N_2). ^{1}H and ^{13}C NMR spectra were generated on a Varian 300 MHz or Bruker 500 Hz instruments and obtained as $CDCl_3$ or DMSO-d_6 solutions (reported in ppm), using $CDCl_3$ as the reference standard (7.26 and 77.00 ppm) or

DMSO-d_6 (2.50 and 39.51 ppm). Coupling constants (*J*) are reported in Hertz (Hz). Standard abbreviations indicating spin multiplicities are given as follow: s (singlet), d (doublet), t (triplet), q (quartet), br (broad) or m (multiplet). High resolution mass spectra were gathered on Bruker MicroTOF-Q II LCMS instrument operating in electrospray ionization (ESI). HPLC (Agilent Technologies 1200 Series) was employed for purity determination, using the following method: Eclipse XDB C18 column, 5 μm, 4.6 mm×150 mm, column temperature 40 °C; solvent A: water; solvent B: methanol; gradient of 40−70% B (0−10 min), 70−90% B (10−15 min), 90−40% B (15−20 min); flow rate of 1.5 mL/min. Compound purity was determined by high pressure liquid chromatography (HPLC) with a confirming purity of ≥95% for all of the final biologically tested compounds.

B.2. General procedure for the preparation of target compounds

N^1-hydroxy-N^4-(3-(3-(2-methoxyphenyl)-4-oxo-2-thiazolidinyl)phenyl)succinamide (**10a**) To a solution of hydroxyl amine hydrochloride (4.17 g, 60.0 mmol) in 10 mL MeOH and KOH (3.37 g, 60.0 mmol) was added to the mixture and stirred for 10 min at 40 °C, then the reaction mixture was cooled to 0 ℃ and filtered. Compound *N*-(3-(3-(2-methoxyphenyl)-4-oxo-2-thiazolidinyl)phenyl)succinamic acid methyl ester（**16a**） (500 mg, 1.2 mmol) was added to the filtrate followed by KOH (337 mg, 6.0 mmol) at room temperature for 30 min. The solvent was removed and extracted with EtOAc. The organic layer was washed with saturated NH_4Cl aqueous solution and brine, dried over Na_2SO_4, the residue was purified by column chromatography [eluting with EA followed by 10:1 CH_2Cl_2/MeOH] to give compound **10a** as a

colorless oil (134 mg, 27.8% yield). ^{1}H NMR (DMSO-d_6, 300 MHz): δ 10.43 (br s, 1H), 9.97 (br s, 1H), 8.71 (br s, 1H), 7.68 (s, 1H), 7.43 (d, *J* = 8.1 Hz, 1H), 7.23–7.13 (m, 2H), 7.02 (d, *J* = 8.4 Hz, 2H), 6.99-6.97 (m, 1H), 6.81 (dd, *J* = 7.8, 7.8 Hz, 1H), 6.08 (s, 1H), 3.93 (d, *J* = 15.9 Hz, 1H), 3.83 (d, *J* = 15.9 Hz, 1H), 3.71 (s, 3H), 2.55–2.50 (m, 2H), 2.28–2.23 (m, 2H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 170.67, 170.28, 168.30, 154.84, 140.28, 139.42, 130.01, 129.24, 128.71, 125.46, 121.89, 120.26, 118.99, 117.53, 112.34, 63.27, 55.72, 32.07, 31.44, 27.33. HPLC purity: 96.2%, t_R = 3.291 min. HRMS (ESI): calcd for $[C_{20}H_{21}N_3O_5S + Na]^+$ 438.1094, found 438.1093.

N^1-hydroxy-N^7-(3-(3-(2-methoxyphenyl)-4-oxo-2-thiazolidinyl)phenyl)heptanediamide (**10b**) Compound **10b** (18.5% yield) was prepared according to the procedure described for the preparation of compound **10a.** ^{1}H NMR (DMSO-d_6, 300 MHz): δ 10.35 (br s, 1H), 9.88 (br s, 1H), 8.67 (br s, 1H), 7.66 (s, 1H), 7.45 (d, *J* = 8.1 Hz, 1H), 7.21–7.13 (m, 2H), 7.03 (d, *J* = 8.4 Hz, 2H), 7.00-6.98 (m, 1H), 6.81 (dd, *J* = 7.8, 7.8 Hz, 1H), 6.09 (s, 1H), 3.94 (d, *J* = 15.6 Hz, 1H), 3.83 (d, *J* = 15.6 Hz, 1H), 3.78 (s, 3H), 2.26 (t, *J* = 7.5 Hz, 2H), 1.95 (t, *J* = 7.5 Hz, 2H), 1.58–1.47 (m, 4H), 1.27–1.22 (m, 2H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 171.21, 170.67, 169.02, 154.85, 140.28, 139.42, 129.99, 129.25, 128.73, 125.48, 121.91, 120.26, 119.09, 117.62, 112.34, 63.27, 55.71, 36.22, 32.12, 32.08, 28.21, 24.90, 24.74. HPLC purity: 95.5%, t_R = 4.208 min. HRMS (ESI): calcd for $[C_{23}H_{27}N_3O_5S + Na]^+$ 480.1564, found 480.1570.

N-(3-(hydroxycarbamoyl)propyl)-3-(3-(2-methoxyphenyl)-4-oxo-2-thiazolidinyl)benz-amide (**11a**)

The synthesis of intermediate **19a**

To a solution of **18** (300 mg, 0.90 mmol) in 8 mL DMF was added EDC·HCl (224 mg, 1.17 mmol) and HoBt (134 mg, 0.99 mmol), stirred for 10 min at 0 °C, then $NH_2(CH_2)_3COOCH_3$ (158 mg, 1.5 mmol) was added to the mixture. The solvent was removed and extracted with EtOAc and H_2O. The organic layer was washed with brine, dried over Na_2SO_4, the residue was purified by column chromatography [eluting with 4:1 PE/EA] to give compound **19a** as a colorless oil (290 mg, 75.4% yield).

Compound **11a** (34.1% yield) was prepared according to the last step described for the preparation of compound **10a.** ^{1}H NMR (DMSO-d_6, 300 MHz): δ 10.39 (br s, 1H), 8.72 (br s, 1H), 8.54–8.51 (m, 1H), 7.87 (s, 1H), 7.70 (d, *J* = 7.5 Hz, 1H), 7.52 (d, *J* = 7.5 Hz, 1H), 7.34 (dd, *J* = 7.5 Hz, 7.5Hz, 1H), 7.23–7.177 (m, 1H), 7.04–6.99 (m, 2H), 6.80 (dd, *J* = 7.5, 7.5 Hz, 1H), 6.21 (s, 1H), 4.03 (d, *J* = 15.6 Hz, 1H), 3.86 (d, *J* = 15.6 Hz, 1H), 3.77 (s, 3H), 3.27–3.19 (m, 2H), 2,01–1.97 (m, 2H), 1.74–1.69 (m, 2H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 170.63, 168.85, 165.52, 154.85, 140.07, 134.65, 130.15, 129.83, 129.32, 128.38, 127.41, 126.19, 125.43, 120.31, 112.37, 79.18, 63.09, 55.72, 32.20, 29.98, 25.29. HPLC purity: 95.4%, t_R = 7.355 min. HRMS (ESI): calcd for $[C_{21}H_{23}N_3O_5S + Na]^+$ 452.1251, found 452.1255.

N-(5-(hydroxycarbamoyl)pentyl)-3-(3-(2-methoxyphenyl)-4-oxo-2-thiazolidinyl)benz-amide (**11b**) Compound **11b** (31.1% yield) was prepared according to the procedure described for the preparation of compound **11a.** ^{1}H NMR (DMSO-d_6, 300 MHz): δ 10.37 (br s, 1H), 8.71 (br s, 1H), 8.49 (dd, *J* = 5.4, 5.4 Hz, 1H), 7.86 (s, 1H), 7.69 (d, *J*

= 7.8 Hz, 1H), 7.52 (d, *J* = 8.1 Hz, 1H), 7.34 (dd, *J* = 7.8, 8.1 Hz, 1H), 7.20 (dd, *J* = 7.2, 7.2 Hz, 1H), 7.04–7.00 (m, 2H), 6.83–6.78 (m, 1H), 6.21 (s, 1H), 4.03 (d, *J* = 15.6 Hz, 1H), 3.85 (d, *J* = 15.6 Hz, 1H), 3.77 (s, 3H), 3.22–3.17 (m, 2H), 1.96–1.91 (m, 2H), 1.50–1.43 (m, 4H), 1.26–1.22 (m, 2H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 170.60, 169.04, 165.37, 154.84, 140.03, 134.73, 130.08, 129.81, 129.31, 128.34, 127.38, 126.16, 125.42, 120.29, 112.36, 63.07, 55.70, 48.59, 32.21, 32.19, 28.89, 26.10, 24.90. HPLC purity: 98.2%, t_R = 3.495 min. HRMS (ESI): calcd for $[C_{23}H_{27}N_3O_5S + Na]^+$ 480.1564, found 480.1561.

4-{2-[2-(3-bromophenyl)-4-oxo-3-thiazolidinyl]phenoxy}-N-hydroxybutyramide (**12a**)

The synthesis of intermediate **22a**

To a solution of **21** (310 mg, 0.88 mmol) in 8 mL of DMF was added K_2CO_3 (243 mg, 1.76 mmol), then $Br(CH_2)_3COOCH_3$ (318 mg, 1.76 mmol) was added to the mixture. The solvent was removed and extracted with EtOAc and H_2O. The organic layer was washed with brine, dried over Na_2SO_4, the residue was purified by column chromatography [eluting with 4:1 PE/EA] to give compound **22a** as a colorless oil (340 mg, 86.1% yield).

Compound **12a** (65.2% yield) was prepared according to the last step described for the preparation of compound **10a.** ^{1}H NMR (DMSO-d_6, 300 MHz): δ 10.44 (br s, 1H), 8.75 (br s, 1H), 7.63 (s, 1H), 7.44–7.40 (m, 2H), 7.25 (d, *J* = 7.8 Hz, 1H), 7.20 (d, *J* = 7.8 Hz, 1H), 7.02– 7.00 (m, 2H), 6.87–6.81(m, 1H), 6.18 (s, 1H), 4.06 (d, *J* = 15.6 Hz, 1H), 3.98–3.94 (m, 2H), 3.84 (d, *J* = 15.6 Hz, 1H), 2.21–2.16 (m, 2H), 2.04–1.98 (m, 2H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 170.54, 168.68, 154.00, 142.72, 131.45,

130.59, 130.05, 129.35, 126.50, 125.53, 121.53, 120.34, 113.06, 67.30, 62.60, 32.02, 28.82, 24.92. HPLC purity: 97.3%, t_R = 6.745 min. HRMS (ESI): calcd for $[C_{19}H_{19}BrN_2O_4S + Na]^+$ 474.0141, found 474.0135.

5-{2-[2-(3-bromophenyl)-4-oxo-3-thiazolidinyl]phenoxy}-N-hydroxypentaneamide (**12b**) Compound **12b** (29.5% yield) was prepared according to the procedure described for the preparation of compound **12a.** ^{1}H NMR (DMSO-d_6, 300 MHz): δ 10.41 (br s, 1H), 8.73 (br s, 1H), 7.63 (s, 1H), 7.42 (dd, *J* = 7.5, 7.5 Hz, 2H), 7.25–7.17 (m, 2H), 7.01 (d, *J* = 7.8 Hz, 2H), 6.82 (dd, *J* = 7.5, 7.5 Hz, 1H), 6.16 (s, 1H), 4.02 (d, *J* = 15.6 Hz, 1H), 3.97–3.94 (m, 2H), 3.84 (d, *J* = 15.6 Hz, 1H), 2.06 (t, *J* = 6.9 Hz, 2H), 1.76-1.73 (m, 4H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 170.44, 168.95, 154.12, 142.68, 131.46, 130.59, 130.03, 129.32, 126.52, 125.59, 121.54, 120.25, 113.12, 67.42, 62.59, 32.00, 31.81, 28.17, 21.65. HPLC purity: 97.0%, t_R = 7.070 min. HRMS (ESI): calcd for $[C_{20}H_{21}BrN_2O_4S + Na]^+$ 487.0298, found 487.0293.

6-{2-[2-(3-bromophenyl)-4-oxo-3-thiazolidinyl]phenoxy}-N-hydroxylhexanamide (**12c**) Compound **12c** (70.4% yield) was prepared according to the procedure described for the preparation of compound **12a.** ^{1}H NMR (DMSO-d_6, 300 MHz): δ 10.39 (br s, 1H), 8.69 (br s, 1H), 7.63 (s, 1H), 7.41 (dd, *J* = 9.0, 9.0 Hz, 2H), 7.24 (d, *J* = 7.8 Hz, 1H), 7.19 (d, *J* = 7.8 Hz, 1H), 7.02 (d, *J* = 7.8 Hz, 2H), 6.82 (dd, *J* = 7.5, 7.5 Hz, 1H), 6.16 (s, 1H), 4.03 (d, *J* = 15.6 Hz, 1H), 3.96–3.91(m, 2H), 3.81 (d, *J* = 15.6 Hz, 1H), 2.03–1.98 (m, 2H), 1.79–1.75 (m, 2H), 1.64–1.57 (m, 2H), 1.50–1.42 (m, 2H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 170.40, 169.03, 154.17, 142.68, 131.46, 130.59, 130.01, 129.33, 126.51, 125.57, 121.54, 120.23, 113.15, 67.77, 62.57, 32.27,

32.03, 28.40, 25.13, 24.88. HPLC purity: 98.5%, t_R = 7.562 min. HRMS (ESI): calcd for $[C_{21}H_{23}BrN_2O_4S + Na]^+$ 501.0454, found 501.0439.

7-{2-[2-(3-bromophenyl)-4-oxo-3-thiazolidinyl]phenoxy}-N-hydroxyheptanamide (**12d**) Compound **12d** (24.1% yield) was prepared according to the procedure described for the preparation of compound **12a.** ^{1}H NMR (DMSO-d_6, 300 MHz): δ 10.36 (br s, 1H), 8.67 (br s, 1H), 7.63 (s, 1H), 7.45–7.38 (m, 2H), 7.25–7.17 (m, 2H), 7.02 (d, *J* = 7.8 Hz, 2H), 6.83 (dd, *J* = 7.2, 7.2 Hz, 1H), 6.17 (s, 1H), 4.05 (d, *J* = 15.6 Hz, 1H), 4.02–3.97 (m, 2H), 3.80 (d, *J* = 15.6 Hz, 1H), 2.01–1.96 (m, 2H), 1.78 (t, *J* = 7.2 Hz, 2H), 1.55 (t, *J* = 7.2 Hz, 2H), 1.50–1.47 (m, 2H), 1.42–1.38 (m, 2H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 170.34, 169.11, 154.17, 142.65, 131.48, 130.58, 129.99, 129.36, 129.32, 126.49, 125.56, 121.56, 120.22, 113.12, 67.81, 62.57, 32.26, 32.06, 28.54, 28.34, 25.20, 25.15. HPLC purity: 95.0%, t_R = 9.573 min. HRMS (ESI): calcd for $[C_{22}H_{25}BrN_2O_4S + Na]^+$ 515.0611, found 515.0597.

8-{2-[2-(3-bromophenyl)-4-oxo-3-thiazolidinyl]phenoxy}-N-hydroxyoctanamide (**12e**) Compound **12e** (65.2% yield) was prepared according to the procedure described for the preparation of compound **12a.** ^{1}H NMR ($CDCl_3$, 300 MHz): δ 7.52 (s, 1H), 7.37 (d, *J* = 7.5 Hz, 1H), 7.24–7.18 (m, 2H), 7.13 (dd, *J* = 7.5, 7.5 Hz, 1H), 6.87 (d, *J* = 7.8 Hz, 2H), 6.81 (dd, *J* = 7.5, 7.5 Hz, 1H), 5.97 (s, 1H), 4.04–3.92 (m, 4H), 2.15-2.11 (m, 2H), 1.85–1.81 (m, 2H), 1.66– 1.63 (m, 4H), 1.51–1.48 (m, 2H), 1.38–1.34 (m, 2H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 170.32, 169.09, 154.18, 142.64, 131.48, 130.58, 129.98, 129.37, 129.31, 126.48, 125.54, 121.55, 120.19, 113.10, 67.85, 62.55, 32.25, 32.07, 28.63, 28.59, 28.47, 25.37, 25.05. HPLC purity: 95.0%, t_R = 8.642 min. HRMS

(ESI): calcd for $[C_{23}H_{27}BrN_2O_4S + Na]^+$ 529.0767, found 529.0743.

4-{2-[2-(3-(4-chlorophenylethyl amino carbonyl)phenyl)-4-oxo-3-thiazolidinyl] phenoxy}-N-hydroxybutyramide (**12f**) Compound **12f** (16.1% yield) was prepared according to the procedure described for the preparation of compound **12a.** ^{1}H NMR (DMSO-d_6, 300 MHz): δ 10.45 (br s, 1H), 8.75 (br s, 1H), 8.57 (t, *J* = 5.4 Hz, 1H), 7.85 (s, 1H), 7.67 (d, *J* = 7.8 Hz, 1H), 7.53 (d, *J* = 7.8 Hz, 1H), 7.38-7.35 (m, 1H), 7.33 (d, *J* = 8.1 Hz, 2H), 7.26–7.23 (m, 2H), 7.18 (dd, *J* = 7.8, 7.5 Hz, 1H), 6.96 (dd, *J* = 7.5, 7.5 Hz, 2H), 6.78 (dd, *J* = 7.5, 7.5 Hz, 1H), 6.19 (s, 1H), 4.05 (d, *J* = 15.6 Hz, 1H), 3.99–3.92 (m, 2H), 3.87 (d, *J* = 15.6 Hz, 1H), 3.46–3.42 (m, 2H), 2.82 (t, *J* = 7.5 Hz, 2H), 2.21 (t, *J* = 7.5 Hz, 2H), 1.29–1.24 (m, 2H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 170.83, 168.73, 165.57, 154.06, 140.22, 138.54, 134.66, 130.73, 130.56, 130.23, 129.30, 128.43, 128.20, 127.39, 126.09, 125.62, 120.28, 113.05, 67.33, 63.14, 40.60, 34.27, 32.12, 30.67, 28.78, 24.87. HPLC purity: 95.9%, t_R = 9.445 min. HRMS (ESI): calcd for $[C_{28}H_{28}ClN_3O_5S + Na]^+$ 576.1330, found 576.1346.

4-{2-[2-(5-bromo-2-thiopheneyl)-4-oxo-3-thiazolidinyl]phenoxy}-N-hydroxybutyr-amide (**12g**) Compound **12g** (22.5% yield) was prepared according to the procedure described for the preparation of compound **12a.** ^{1}H NMR (DMSO-d_6, 300 MHz): δ 10.42 (br s, 1H), 8.73 (br s, 1H), 7.26 (dd, *J* = 7.5, 7.5 Hz, 1H), 7.05 (d, *J* = 7.8 Hz, 1H), 6.99–6.96 (m, 2H), 6.89 (dd, *J* = 7.5, 7.5 Hz, 1H), 6.81–6.79 (m, 1H), 6.41 (s, 1H), 4.01 (d, *J* = 15.3 Hz, 1H), 3.96–3.93 (m, 2H), 3.88 (d, *J* = 15.3 Hz, 1H), 2.15 (t, *J* = 7.5 Hz, 2H), 1.94–1.90 (m, 2H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 169.96, 168.66, 154.08, 145.74, 130.06, 129.77, 129.59, 128.65, 125.09, 120.39, 113.14, 112.99,

67.34, 58.83, 32.02, 28.78, 24.82. HPLC purity: 96.2%, t_R = 6.843 min. HRMS (ESI): calcd for $[C_{17}H_{17}BrN_2O_4S_2 + Na]^+$ 478.9705, found 478.9744.

4-{2-[2-(5-(5-pyrimidinyl)-2-thiopheneyl)-4-oxo-3-thiazolidinyl]phenoxy}-N-hydroxy -butyramide (**12h**) Compound **12h** (19.9% yield) was prepared according to the procedure described for the preparation of compound **12a.** ^{1}H NMR (DMSO-d_6, 300 MHz): δ 10.47 (br s, 1H), 9.10 (s, 1H), 9.06 (s, 2H), 8.73 (br s, 1H), 7.48 (d, *J* = 3.6 Hz, 1H), 7.25 (dd, *J* = 7.2, 7.2 Hz, 1H), 7.07 (d, *J* = 3.6 Hz, 1H), 7.03 (d, *J* = 7.8 Hz, 1H), 6.85 (dd, *J* = 7.5, 7.5 Hz, 1H), 6.65–6.62 (m, 1H), 6.48 (s, 1H), 4.02 (d, *J* = 15.3 Hz, 1H), 3.97–3.93 (m, 2H), 3.90 (d, *J* = 15.3 Hz, 1H), 2.20–2.13 (m, 2H), 1.98–1.93 (m, 2H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 170.16, 168.70, 157.20, 154.10, 153.01, 146.04, 136.83, 130.16, 129.59, 129.11, 127.65, 125.62, 125.22, 120.40, 113.02, 67.35, 58.86, 32.04, 28.78, 24.85. HPLC purity: 96.2%, t_R = 4.020 min. HRMS (ESI): calcd for $[C_{21}H_{20}N_4O_4S_2 + Na]^+$ 479.0818, found 479.0831.

4-{4-[2-(5-bromo-2-thiopheneyl)-4-oxo-3-thiazolidinyl]phenoxy}-N-hydroxybutyr- amide (**12i**) Compound **12i** (27.2 yield) was prepared according to the procedure described for the preparation of compound **12a.** ^{1}H NMR (DMSO-d_6, 300 MHz): δ 10.39 (br s, 1H), 8.68 (br s, 1H), 7.15 (d, *J* = 9.0 Hz, 2H), 6.95 (d, *J* = 3.6 Hz, 1H), 6.90-6.88 (m, 2H), 6.87 (d, *J* = 3.6 Hz, 1H), 6.65 (s, 1H), 3.97–3.92 (m, 3H), 3.85 (d, *J* = 15.9 Hz, 1H), 2.10 (t, *J* = 7.5 Hz, 2H), 1.92–1.87 (m, 2H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 153.37, 152.49, 142.54, 132.86, 118.59, 118.41, 117.54, 116.65, 105.17, 103.86, 63.49, 57.10, 33.35, 30.03, 26.58. HPLC purity: 96.4%, t_R = 7.964 min. HRMS (ESI): calcd for $[C_{17}H_{17}BrN_2O_4S_2 + Na]^+$ 478.9705, found 478.9708.

4-{4-[2-(5-(5-pyrimidinyl)-2-thiopheneyl)-4-oxo-3-thiazolidinyl]phenoxy}-N-hydroxy-butyramide (**12j**) Compound **12j** (35.1% yield) was prepared according to the procedure described for the preparation of compound **12a.** 1H NMR (DMSO-d_6, 300 MHz): 10.39 (br s, 1H), 9.10 (s, 1H), 9.06 (s, 2H), 8.68 (br s, 1H), 7.48 (d, J = 3.6 Hz, 1H), 7.25 (d, J = 7.2 Hz, 2H), 7.07 (d, J = 3.6 Hz, 1H), 7.03 (d, J = 7.8 Hz, 2H), 6.75 (s, 1H), 4.01 (d, J = 15.3 Hz, 1H), 3.96–3.93 (m, 2H), 3.90 (d, J = 15.3 Hz, 1H), 2.21–2.08 (m, 2H), 1.90–1.88 (m, 2H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 169.70, 168.56, 157.19, 153.02, 146.42, 136.72, 129.78, 129.07, 127.59, 125.70, 114.53, 66.90, 59.66, 32.53, 28.65, 24.73. HPLC purity: 98.7%, t_R = 3.788 min. HRMS (ESI): calcd for $[C_{21}H_{20}N_4O_4S_2 + Na]^+$ 479.0818, found 479.0828.

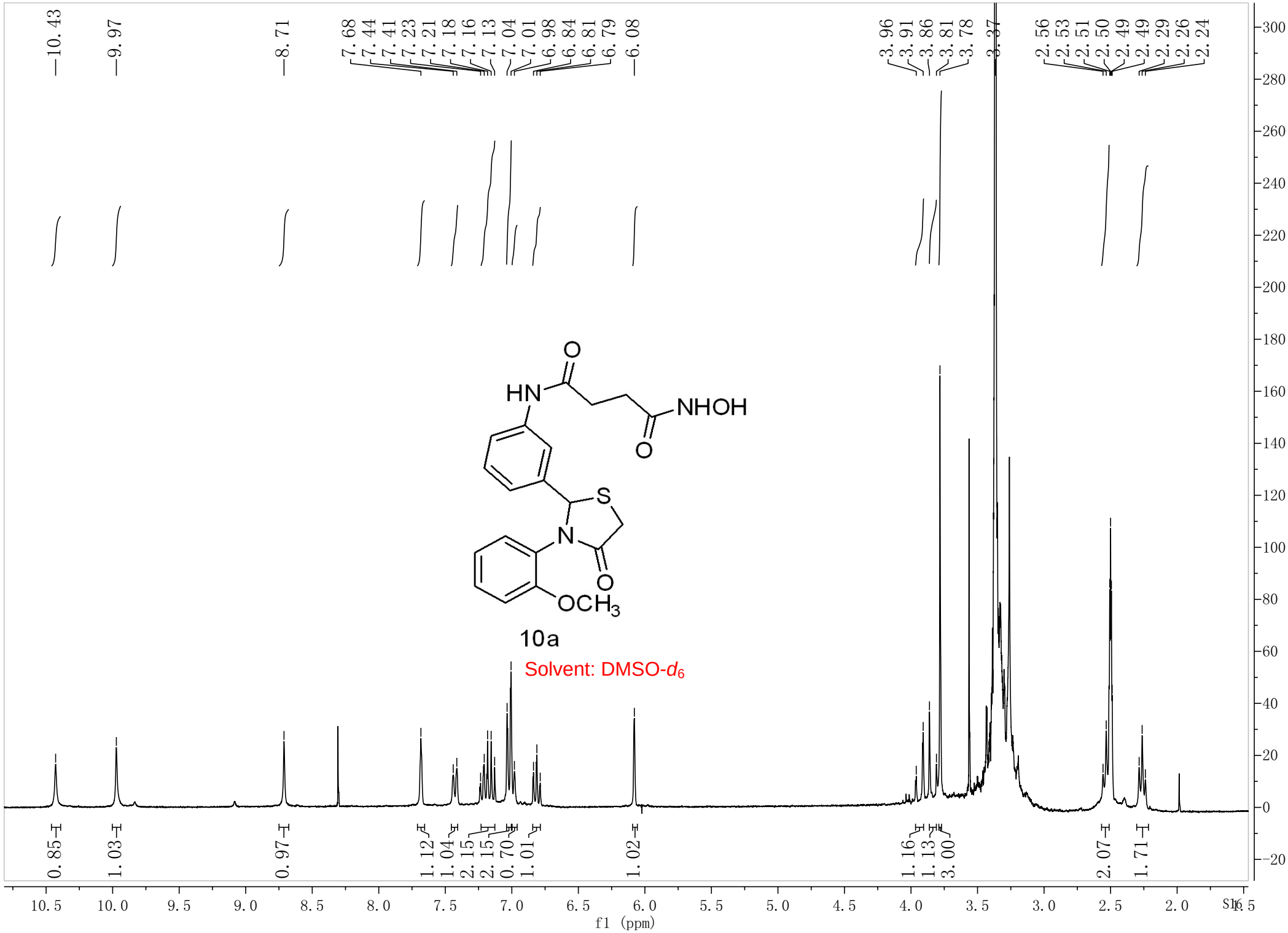
N^1-(2-(2-(3-bromophenyl)-4-oxo-3-thiazolidinyl)phenyl)-N^7-hydroxyheptanediamide (**13a**) Compound **13a** (25.1% yield) was prepared according to the procedure described for the preparation of compound **10a.** ^{1}H NMR ($CDCl_3$, 300 MHz): δ 7.74 (br s, 1H) 7.49 (s, 1H), 7,36–7.35 (m, 1H), 7.23–7.22 (m, 2H), 7.16–7.01 (m, 3H), 6.00 (s, 1H), 4.06 (d, J = 15.0 Hz, 1H), 3.93 (d, J = 15.0 Hz, 1H), 2.46–2.33 (m, 2H), 2.19–2.06 (m, 2H), 1.69–1.68 (m, 4H), 1.48–1.37 (m, 2H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 171.35, 171.26, 169.02, 141.94, 135.09, 131.69, 130.45, 126.89, 124.50, 121.56, 35.84, 32.79, 32.17, 28.32, 25.01, 24.83. HPLC purity: 96.6%, t_R = 5.787 min. HRMS (ESI): calcd for $[C_{22}H_{24}BrN_3O_4S + Na]^+$ 528.0563, found 528.0575.

N^1-(2-(2-(3-bromophenyl)-4-oxo-3-thiazolidinyl)phenyl)-N^8-hydroxyoctanediamide (**13b**) Compound **13b** (35.1% yield) was prepared according to the procedure described for the preparation of compound **10a.** ^{1}H NMR ($CDCl_3$, 300 MHz): δ 9.33 (br s, 1H), 7.76–7.70 (m, 2H), 7.47 (s, 1H), 7.41–7.7.34 (m, 1H), 7.30–7.23 (m, 2H),

7.16–7.05 (m, 3H), 6.04 (s, 1H), 4.06 (d, *J* = 15.0 Hz, 1H), 3.92 (d, *J* = 15.0 Hz, 1H), 2.32 (t, *J* = 7.2 Hz, 2H), 2.17 (t, *J* = 7.2 Hz, 2H), 1.80–1.60 (m, 4H), 1.48–1.30 (m, 4H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 171.39, 171.27, 169.08, 141.94, 135.08, 131.70, 130.52, 130.44, 128.03, 126.88, 124.54, 121.57, 79.16, 62.48, 35.94, 32.81, 32.26, 28.49, 25.07, 25.01. HPLC purity: 97.2%, t_R = 6.285 min. HR MS (ESI): calcd for $[C_{23}H_{26}BrN_3O_4S + Na]^+$ 542.0720, found 542.0732.

References:

1. C. Gao, F. J. Dai, H. W. Cui, S. H. Peng, Y. He, X. Wang, Z. F. Yi and W. W. Qiu, *Chem. Biol. Drug Design*, 2014, 84, 223-233.
2. C. Zheng, Y. Fang, W. Tong, G. Li, H. Wu, W. Zhou, Q. Lin, F. Yang, Z. Yang, P. Wang, Y. Peng, X. Pang, Z. Yi, J. Luo, M. Liu and Y. Chen, *J. Med. Chem.*, 2014, 57, 600-612.
3. F. Yang, T. Zhang, H. Wu, Y. Yang, N. Liu, A. Chen, Q. Li, J. Li, L. Qin, B. Jiang, X. Wang, X. Pang, Z. Yi, M. Liu and Y. Chen, *J. Med. Chem.*, 2014, 57, 9357-9369.
4. W. Zhou, A. Huang, Y. Zhang, Q. Lin, W. Guo, Z. You, Z. Yi, M. Liu and Y. Chen, *Eur. J. Med. Chem.*, 2015, 96, 269-280.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S
N
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Solvent: DMSO-d6
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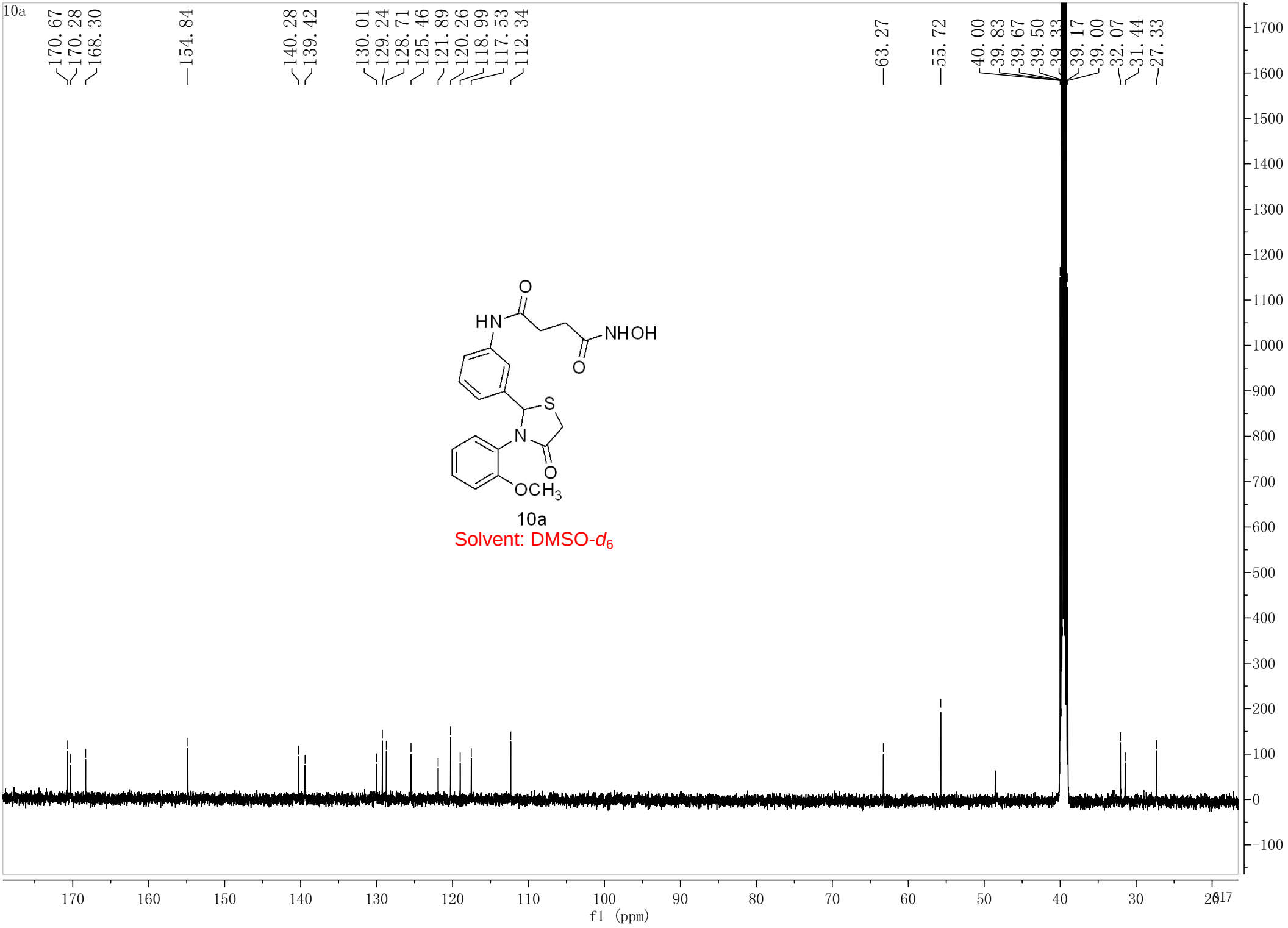
f1 (ppm)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63.27
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40.00
39.83
39.67
39.50
39.33
39.17
39.00
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10a
Solvent: DMSO-d6
f1 (ppm)

Mass Spectrum List Report

Analysis Info

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Comment			

Acquisition Parameter

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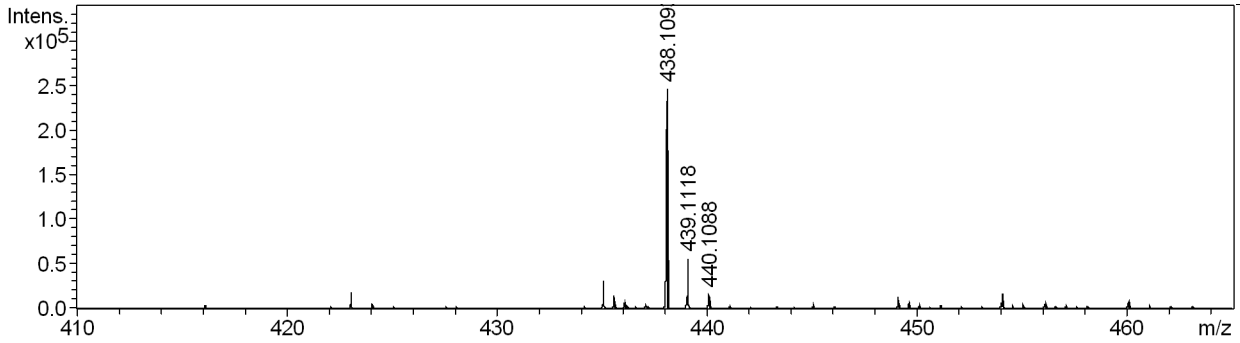

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Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e^- Conf	N-Rule
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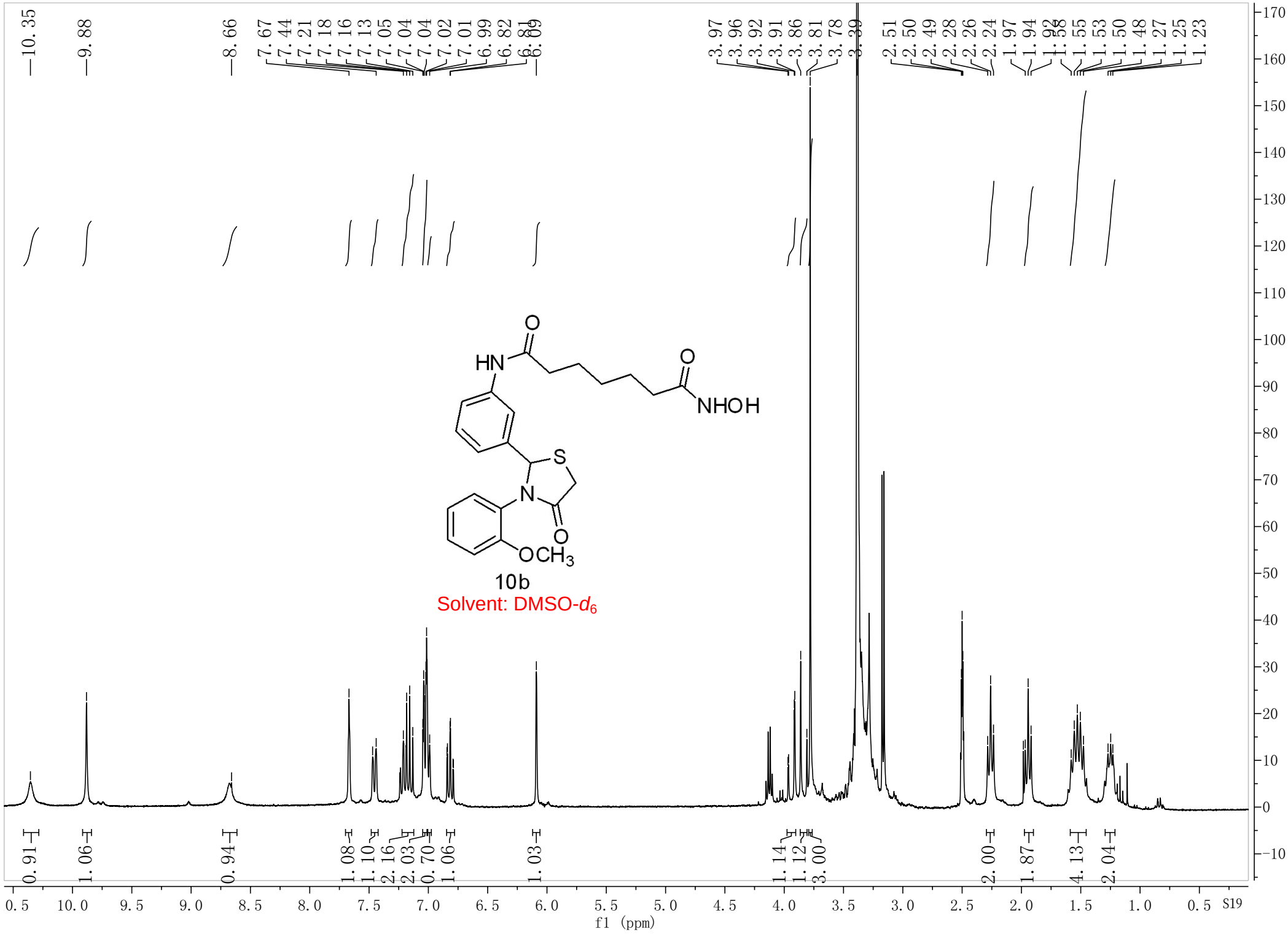
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f1 (ppm)
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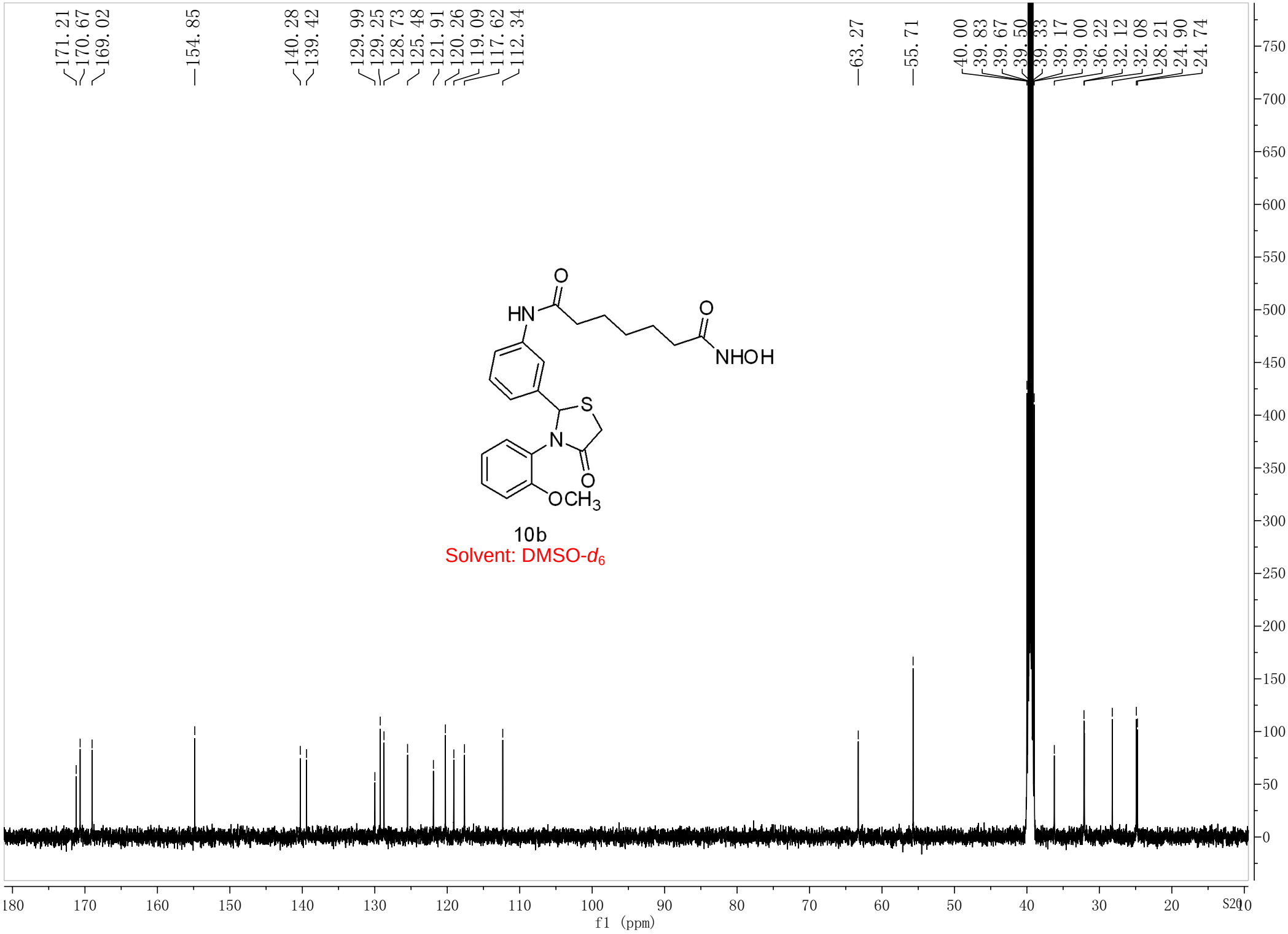
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f1 (ppm)

Mass Spectrum List Report

Analysis Info

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Sample Name	YF-457	Instrument	maXis impact 282001.00122
Comment			

Acquisition Parameter

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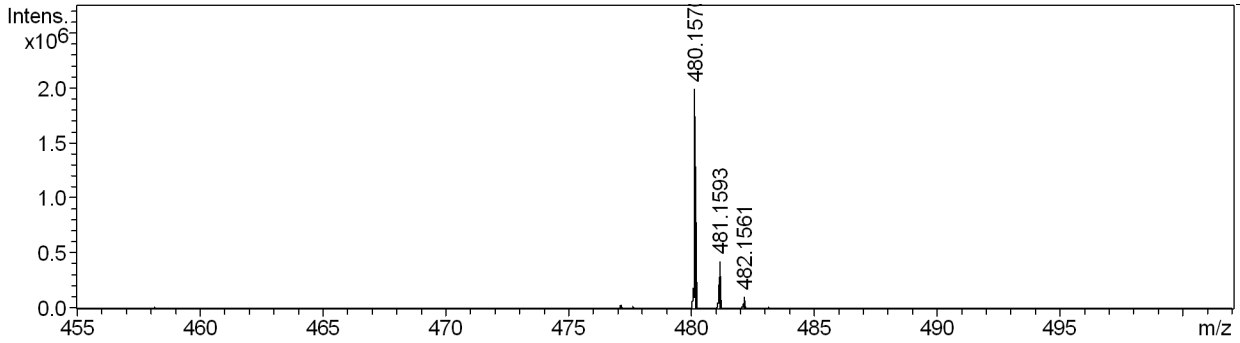

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Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e¯ Conf	N-Rule
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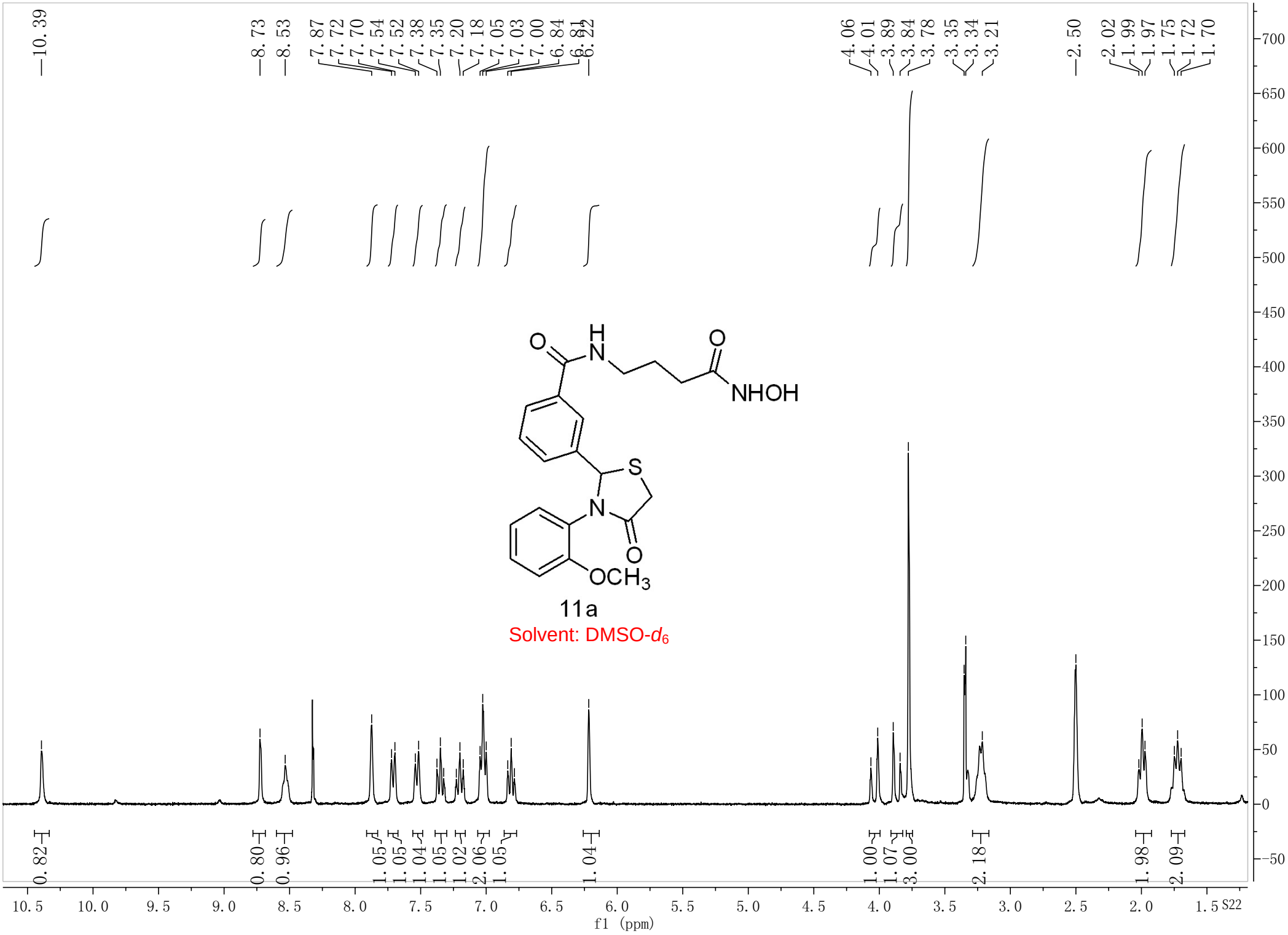
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7.00
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6.81
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O
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S
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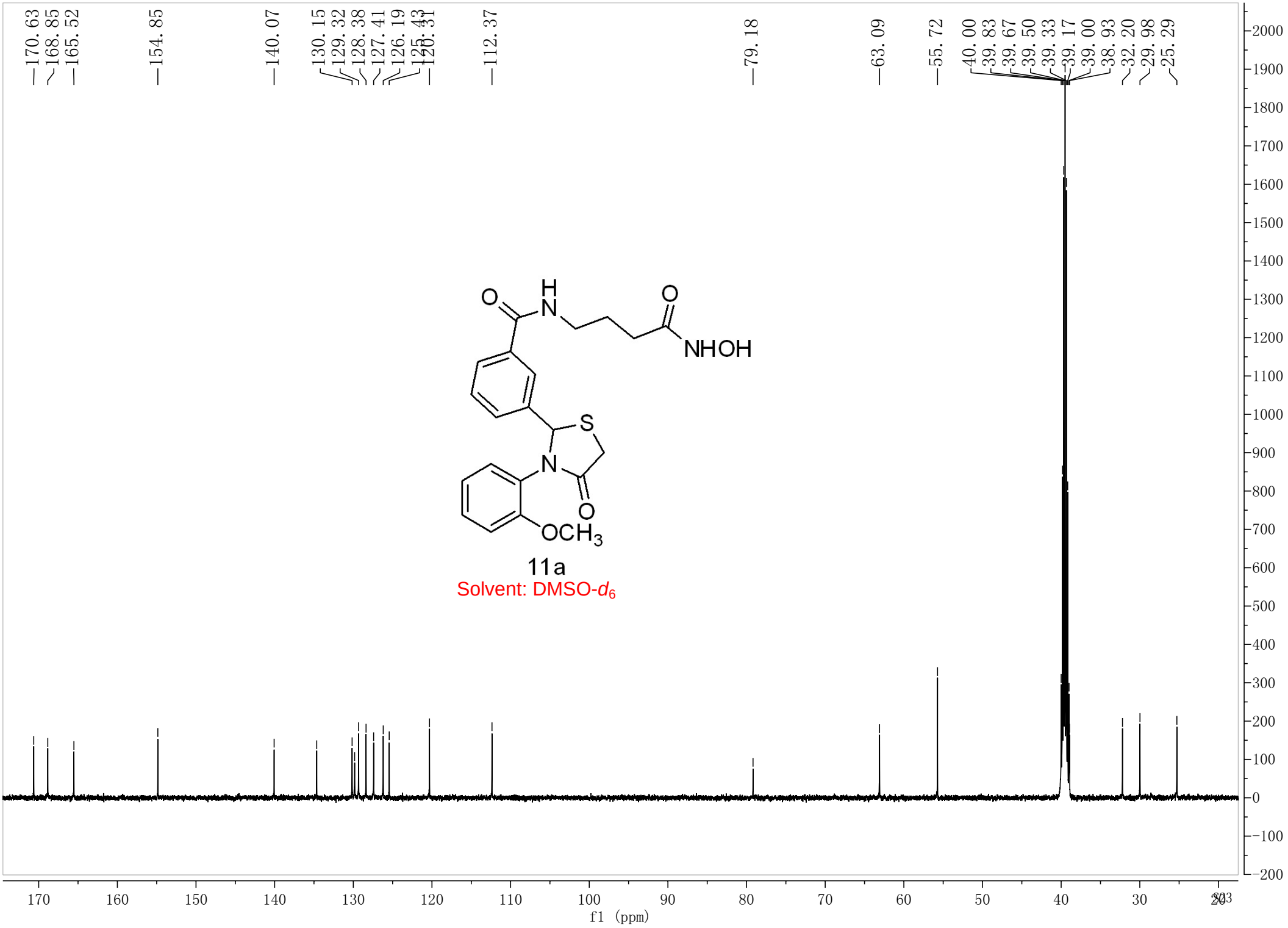
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Mass Spectrum List Report

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Sample Name	WJ-429	Instrument	maXis impact 282001.00122
Comment			

Acquisition Parameter

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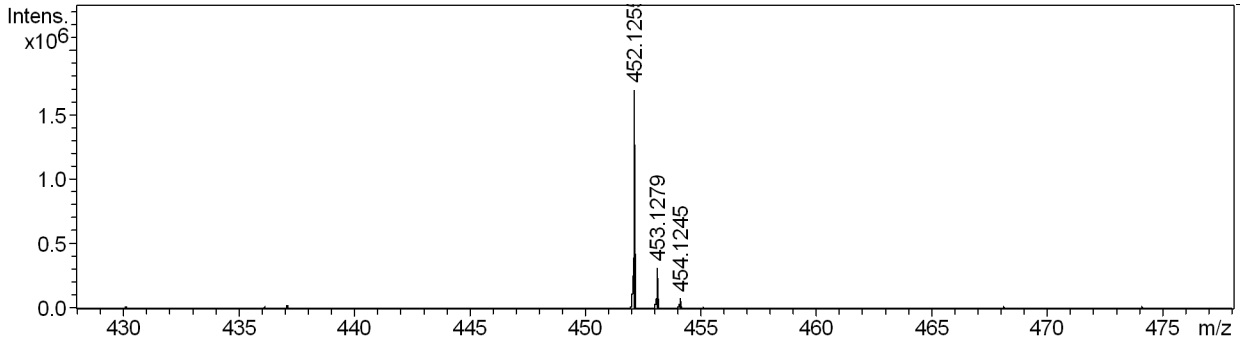

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Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e¯ Conf	N-Rule
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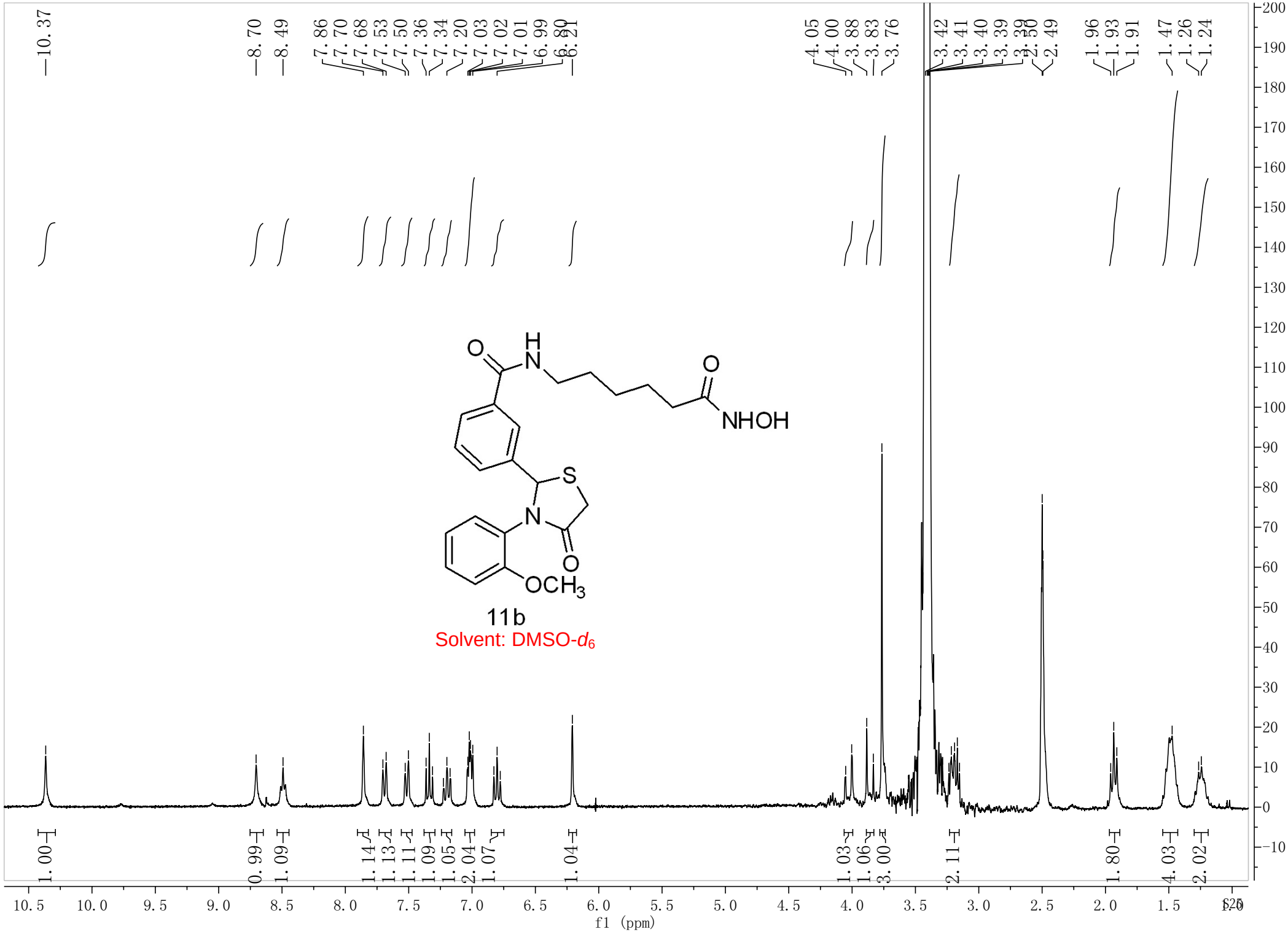
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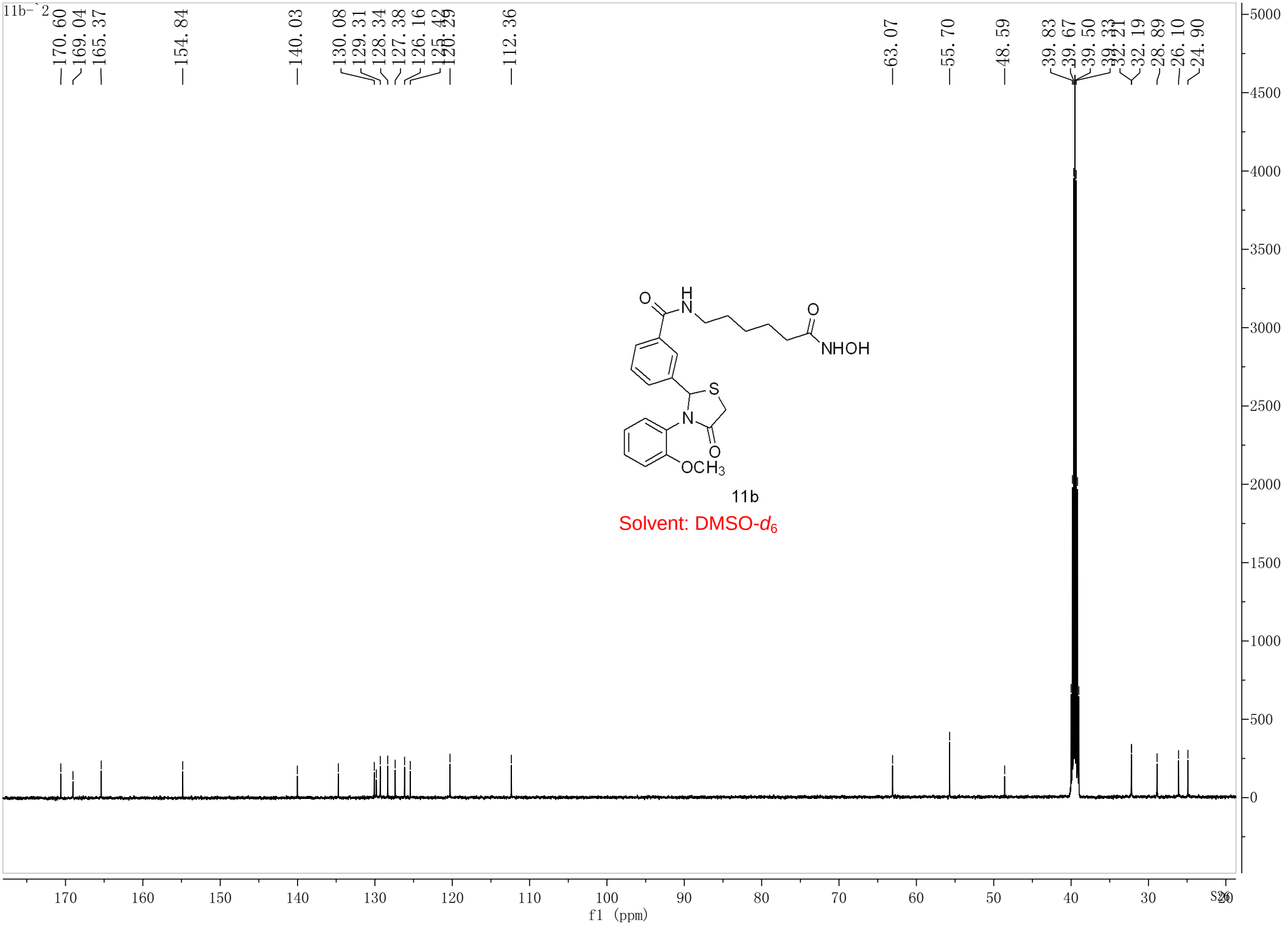
f1 (ppm)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2500
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Mass Spectrum List Report

Analysis Info

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Sample Name	YF-457A	Instrument	maXis impact 282001.00122
Comment			

Acquisition Parameter

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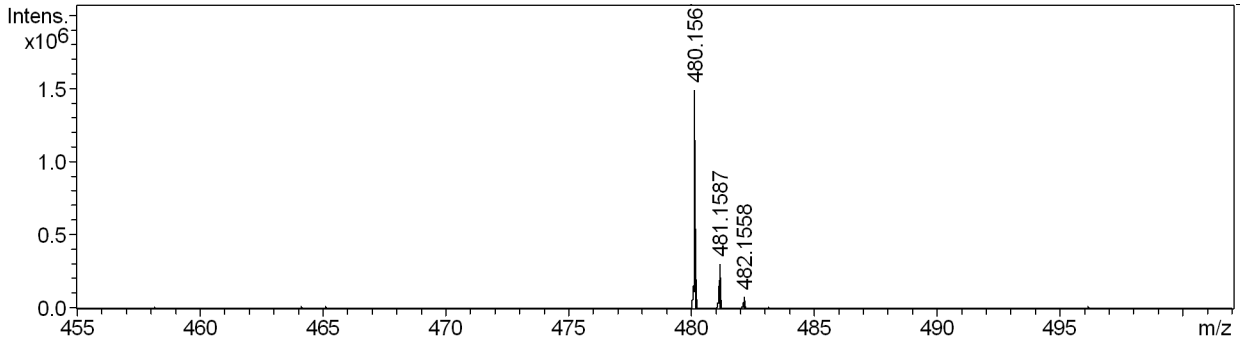
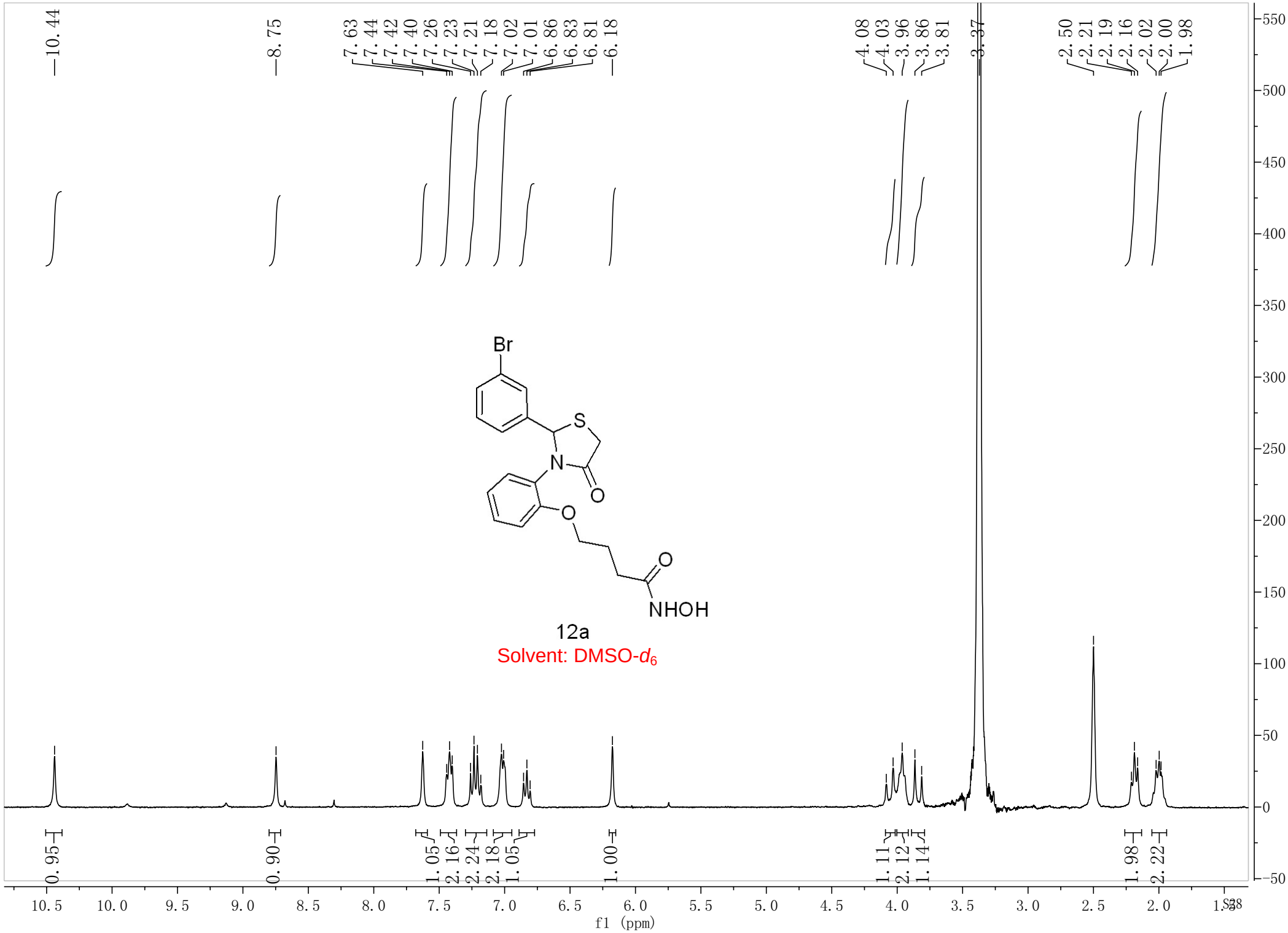
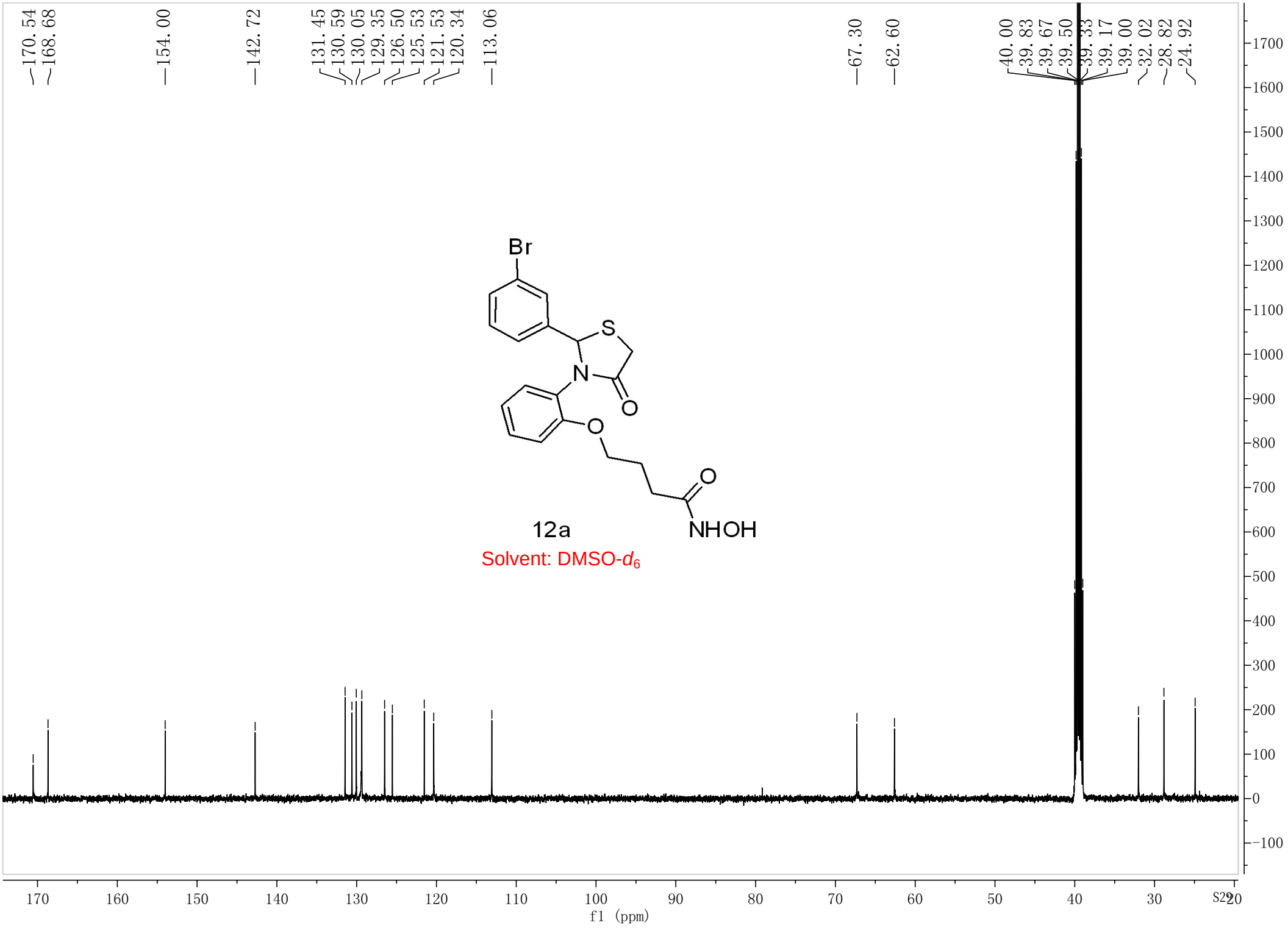


#	m/z	Res.	S/N	I	I %	FWHM
1	480.1561	37384	23799.5	1490073	100.0	0.0128
2	481.1587	25378	4907.6	307017	20.6	0.0190
3	482.1558	16908	1314.2	82201	5.5	0.0285

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e¯ Conf	N-Rule
480.1561	1	C23H27N3NaO5S	480.1564	0.6	37.9	1	100.00	11.5	even	ok


10.44
8.75
7.63
7.44
7.42
7.40
7.26
7.23
7.21
7.18
7.02
7.01
6.86
6.83
6.81
6.18
4.08
4.03
3.96
3.86
3.81
3.37
2.50
2.21
2.19
2.16
2.02
2.00
1.98
Br
S
N
O
O
O
NHOH
12a
Solvent: DMSO-d_6
0.95
0.90
1.05
2.16
2.24
2.18
1.05
1.00
1.11
2.12
1.14
1.98
2.22
f1 (ppm)


170.54
168.68
154.00
142.72
131.45
130.59
130.05
129.35
126.50
125.53
121.53
120.34
113.06
67.30
62.60
40.00
39.83
39.67
39.50
39.33
39.17
39.00
32.02
28.82
24.92
Br
S
N
O
O
O
NHOH
12a
Solvent: DMSO-d_6
f1 (ppm)

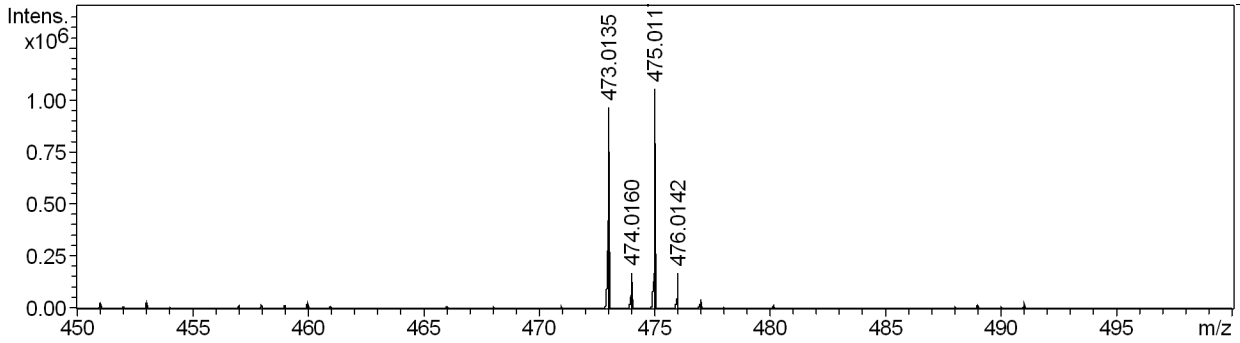
Mass Spectrum List Report

Analysis Info

Acquisition Date	4/29/2015 10:45:04 AM		
Analysis Name	D:\Data\waixi\chenyihua\20150429LIYUNQI\LW-451_P1-D-5_01_1517.d		
Method	Tune_pos_low_LC with calibration_2min.m	Operator	ECNU-Chem
Sample Name	LW-451	Instrument	maXis impact 282001.00122
Comment			

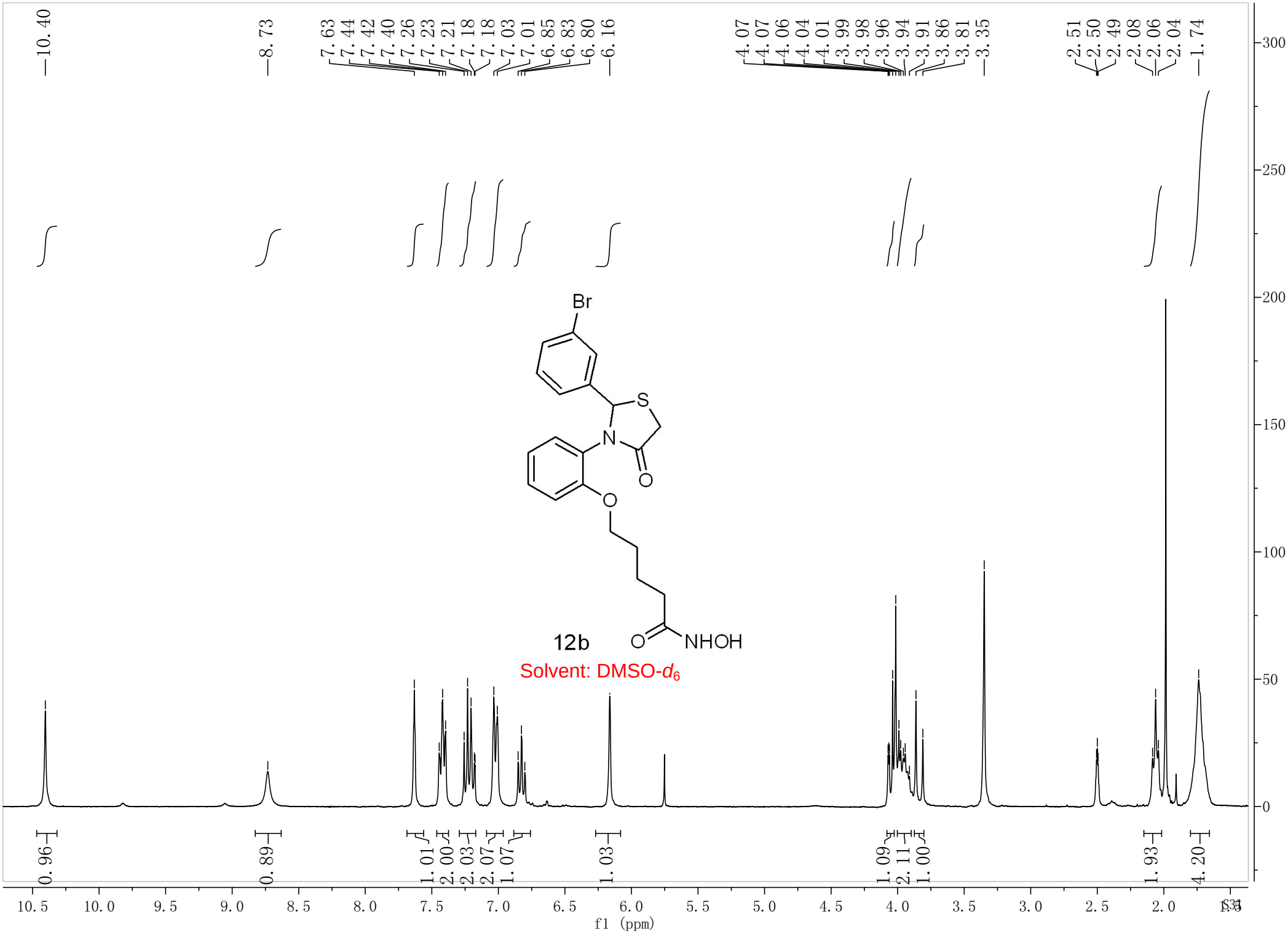
Acquisition Parameter

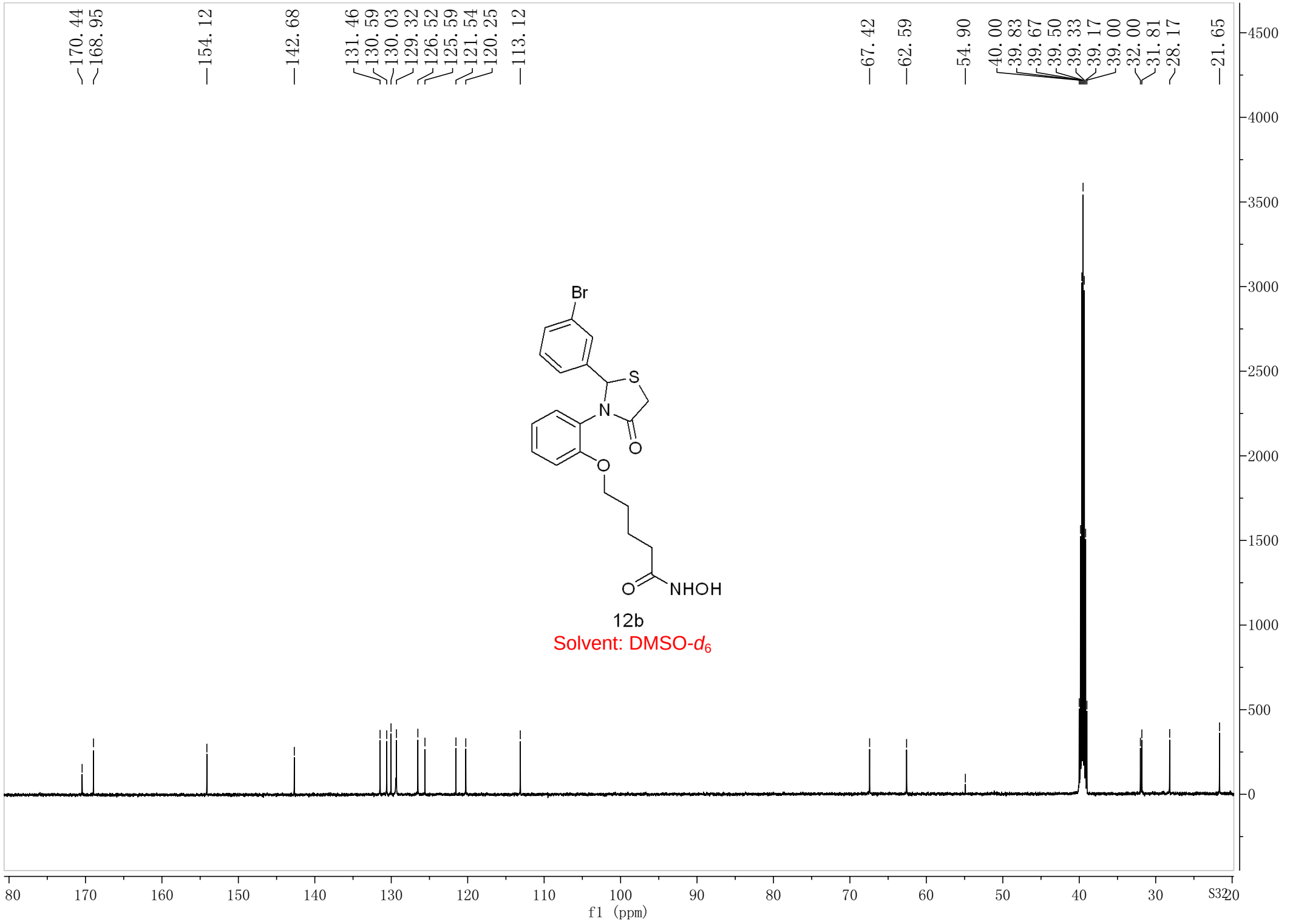
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1200 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	473.0135	34060	13690.2	964067	91.7	0.0139
2	474.0160	22824	2467.0	173659	16.5	0.0208
3	475.0117	35438	14950.5	1051065	100.0	0.0134
4	476.0142	22977	2441.9	171528	16.3	0.0207

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e^- Conf	N-Rule
473.0135	1	C19H19BrN2NaO4S	473.0141	1.3	36.1	2	59.29	10.5	even	ok


10.40
8.73
7.63
7.44
7.42
7.40
7.26
7.23
7.21
7.18
7.18
7.03
7.01
6.85
6.83
6.80
6.16
4.07
4.07
4.06
4.04
4.01
3.99
3.98
3.96
3.94
3.91
3.86
3.81
3.35
2.51
2.50
2.49
2.08
2.06
2.04
1.74
Br
S
N
O
O
O
NHOH
12b
Solvent: DMSO-d_6
0.96
0.89
1.01
2.00
2.03
2.07
1.07
1.03
1.09
2.11
1.00
1.93
4.20
f1 (ppm)


170.44
168.95
154.12
142.68
131.46
130.59
130.03
129.32
126.52
125.59
121.54
120.25
113.12
67.42
62.59
54.90
40.00
39.83
39.67
39.50
39.33
39.17
39.00
32.00
31.81
28.17
21.65
Br
S
N
O
O
O
NHOH
12b
Solvent: DMSO-d_6
f1 (ppm)

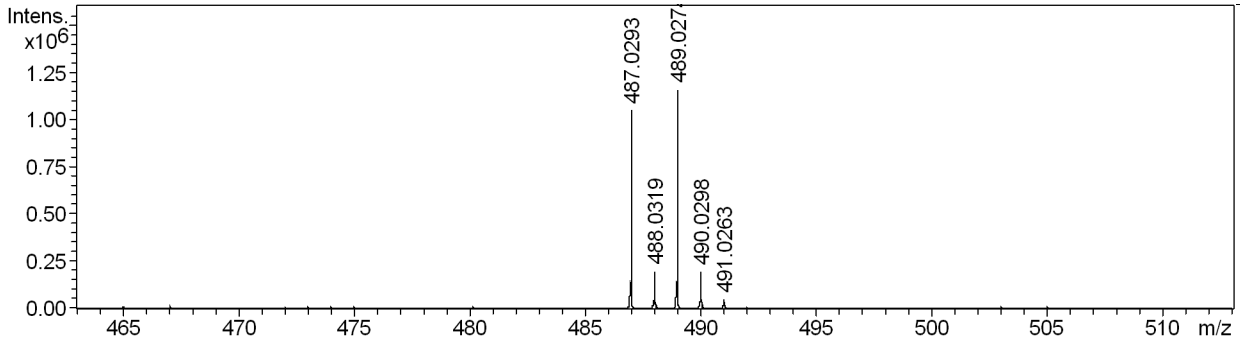
Mass Spectrum List Report

Analysis Info

Acquisition Date	4/29/2015 10:48:13 AM		
Analysis Name	D:\Data\waixi\chenyihua\20150429LIYUNQI\YF-465A_P1-D-6_01_1518.d		
Method	Tune_pos_low_LC with calibration_2min.m	Operator	ECNU-Chem
Sample Name	YF-465A	Instrument	maXis impact 282001.00122
Comment			

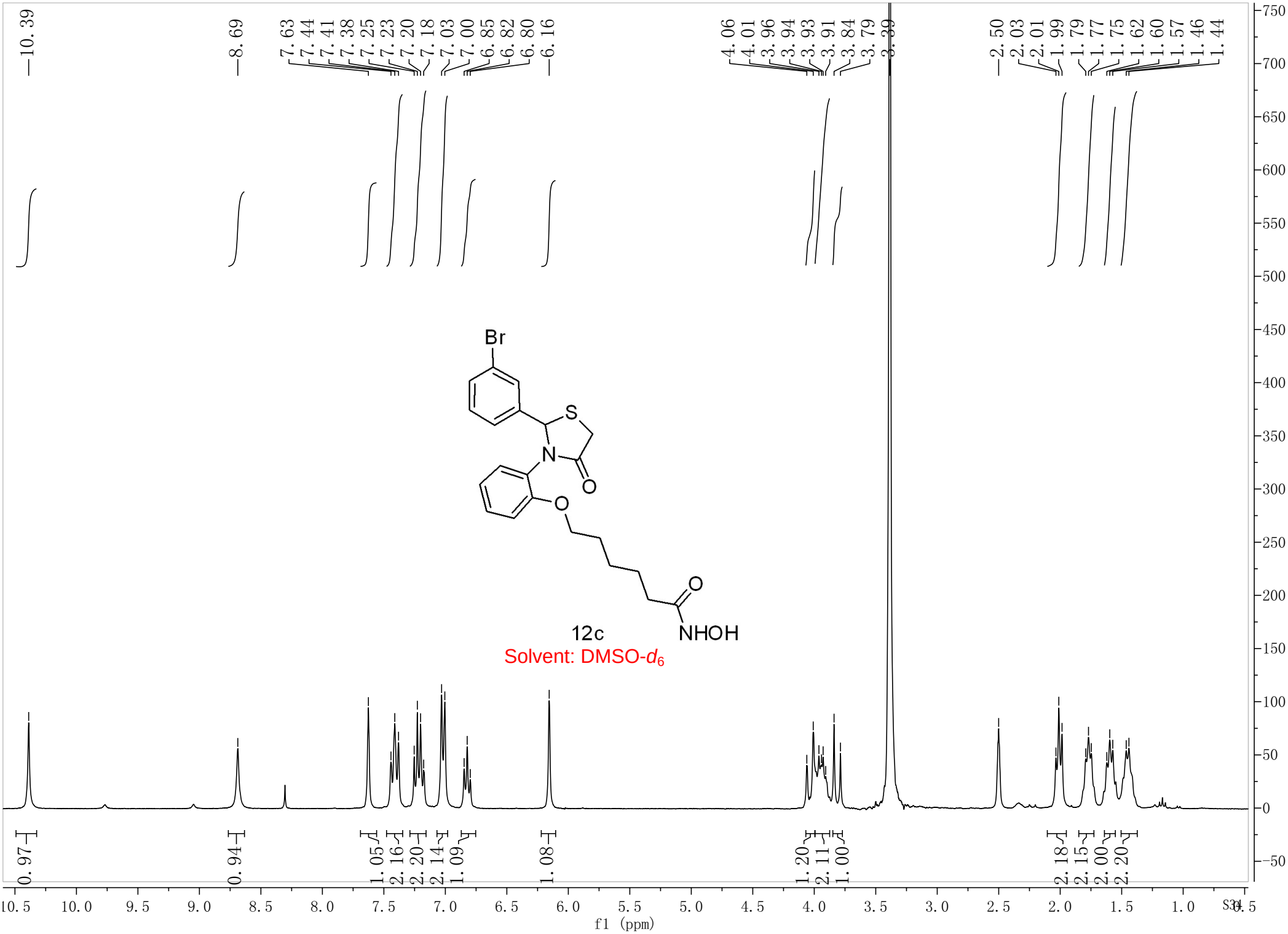
Acquisition Parameter

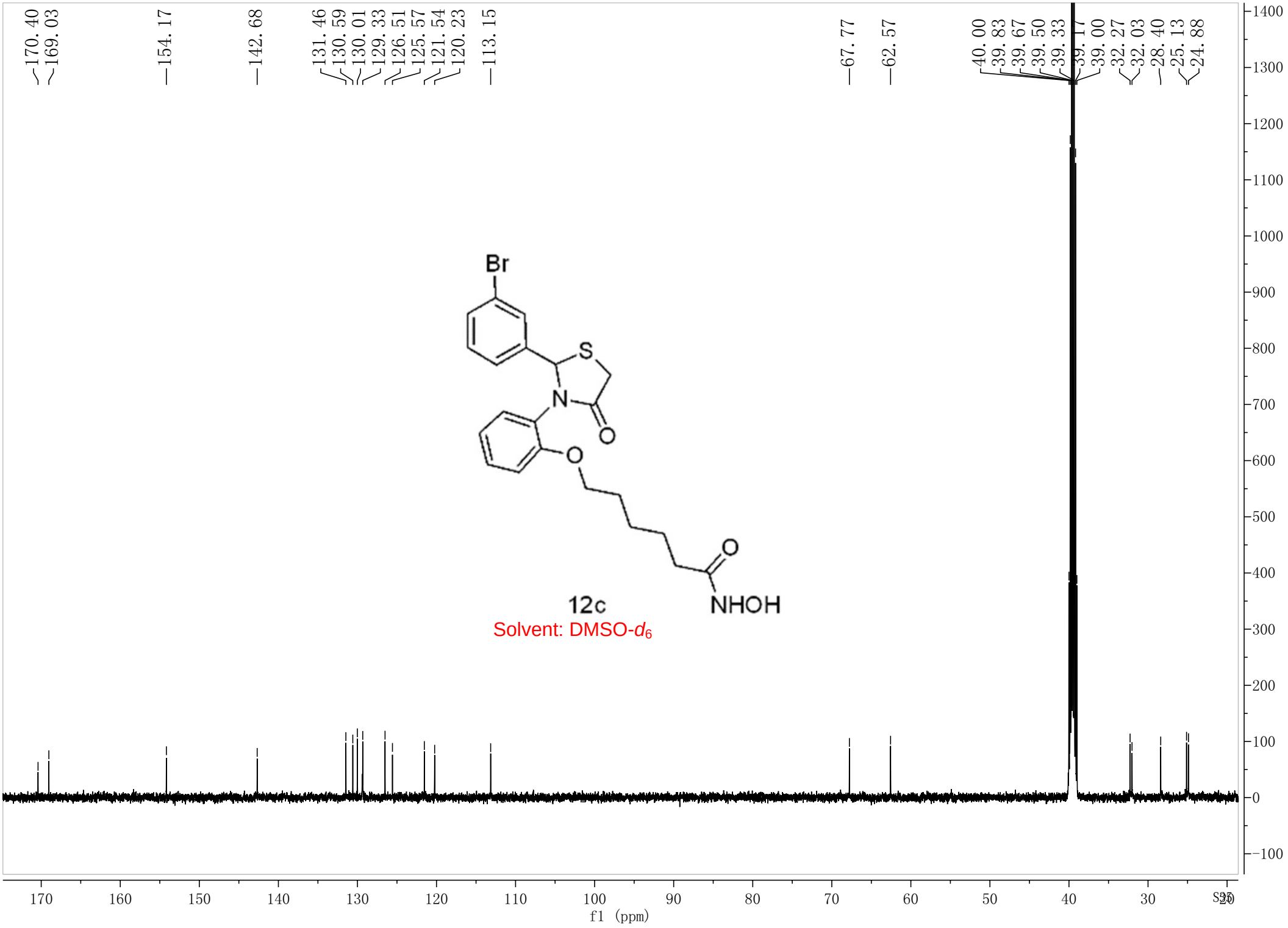
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1200 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	487.0293	34765	16144.2	1046488	90.3	0.0140
2	488.0319	23964	3073.2	198943	17.2	0.0204
3	489.0274	35934	17915.0	1158641	100.0	0.0136
4	490.0298	23353	3031.7	195895	16.9	0.0210
5	491.0263	16142	788.6	50895	4.4	0.0304

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e¯ Conf	N-Rule
487.0293	1	C20H21BrN2NaO4S	487.0298	0.9	40.4	2	63.24	10.5	even	ok


10.39
8.69
7.63
7.44
7.41
7.38
7.25
7.23
7.20
7.18
7.03
7.00
6.85
6.82
6.80
6.16
4.06
4.01
3.96
3.94
3.93
3.91
3.84
3.79
3.39
2.50
2.03
2.01
1.99
1.79
1.77
1.75
1.62
1.60
1.57
1.46
1.44
Br
S
N
O
O
O
NHOH
12c
Solvent: DMSO-d_6
0.97
0.94
1.05
2.16
2.20
2.14
1.09
1.08
1.20
2.11
1.00
2.18
2.15
2.00
2.20
f1 (ppm)


170.40
169.03
154.17
142.68
131.46
130.59
130.01
129.33
126.51
125.57
121.54
120.23
113.15
67.77
62.57
40.00
39.83
39.67
39.50
39.33
39.17
39.00
32.27
32.03
28.40
25.13
24.88
Br
S
N
O
O
O
NHOH
12c
Solvent: DMSO-d_6
f1 (ppm)

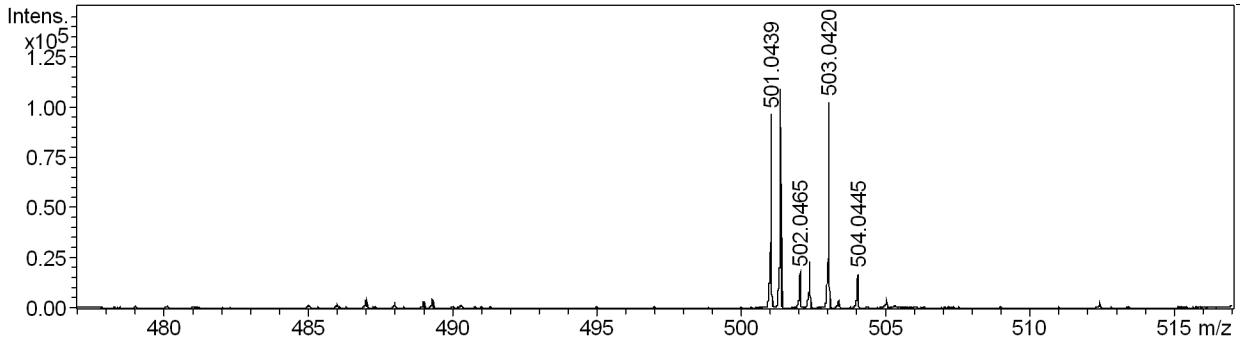
Mass Spectrum List Report

Analysis Info

		Acquisition Date	4/29/2015 10:51:22 AM
Analysis Name	D:\Data\waixi\chenyihua\20150429LIYUNQI\LW-479_P1-D-7_01_1519.d		
Method	Tune_pos_low_LC with calibration_2min.m	Operator	ECNU-Chem
Sample Name	LW-479	Instrument	maXis impact 282001.00122
Comment			

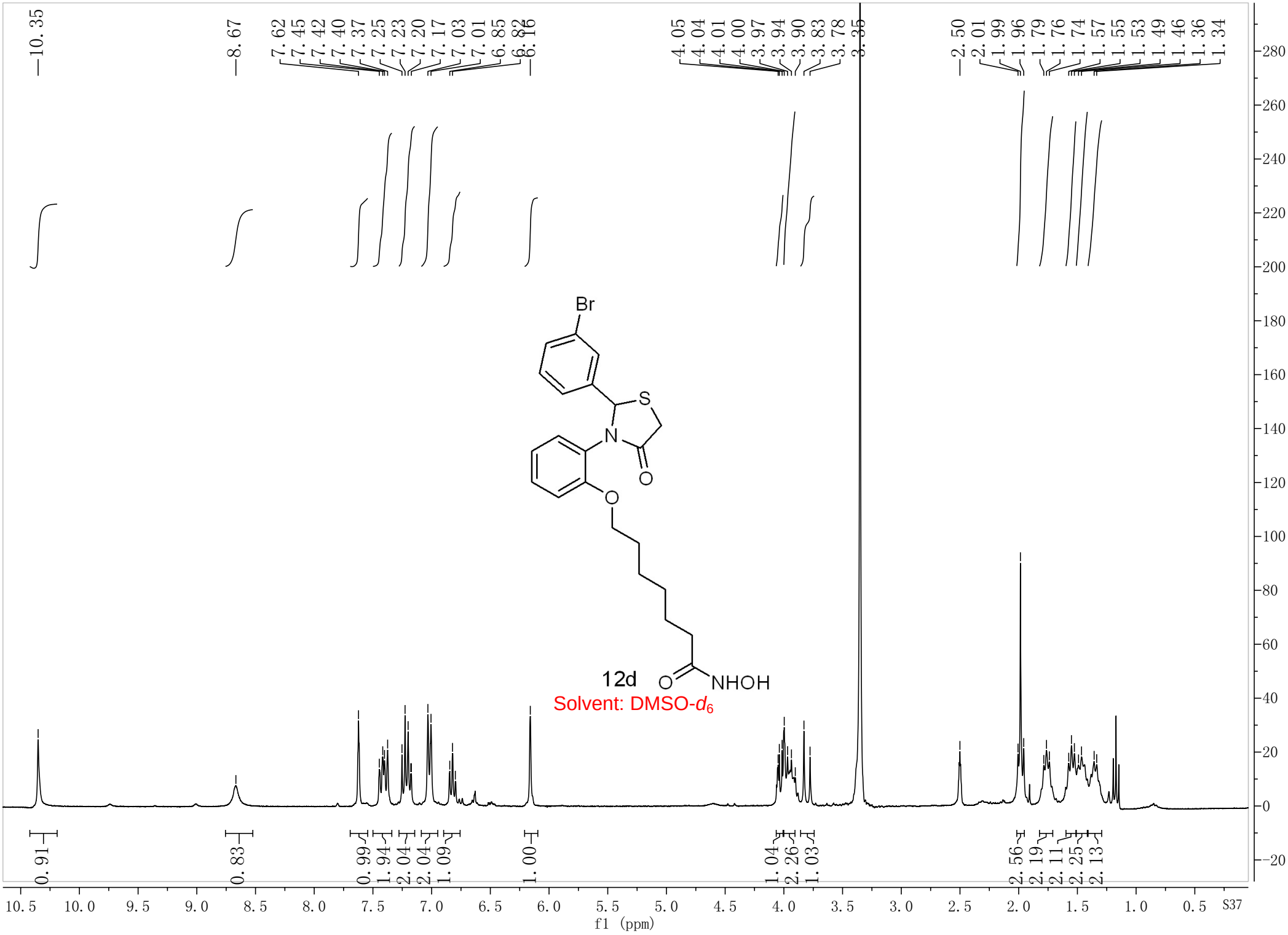
Acquisition Parameter

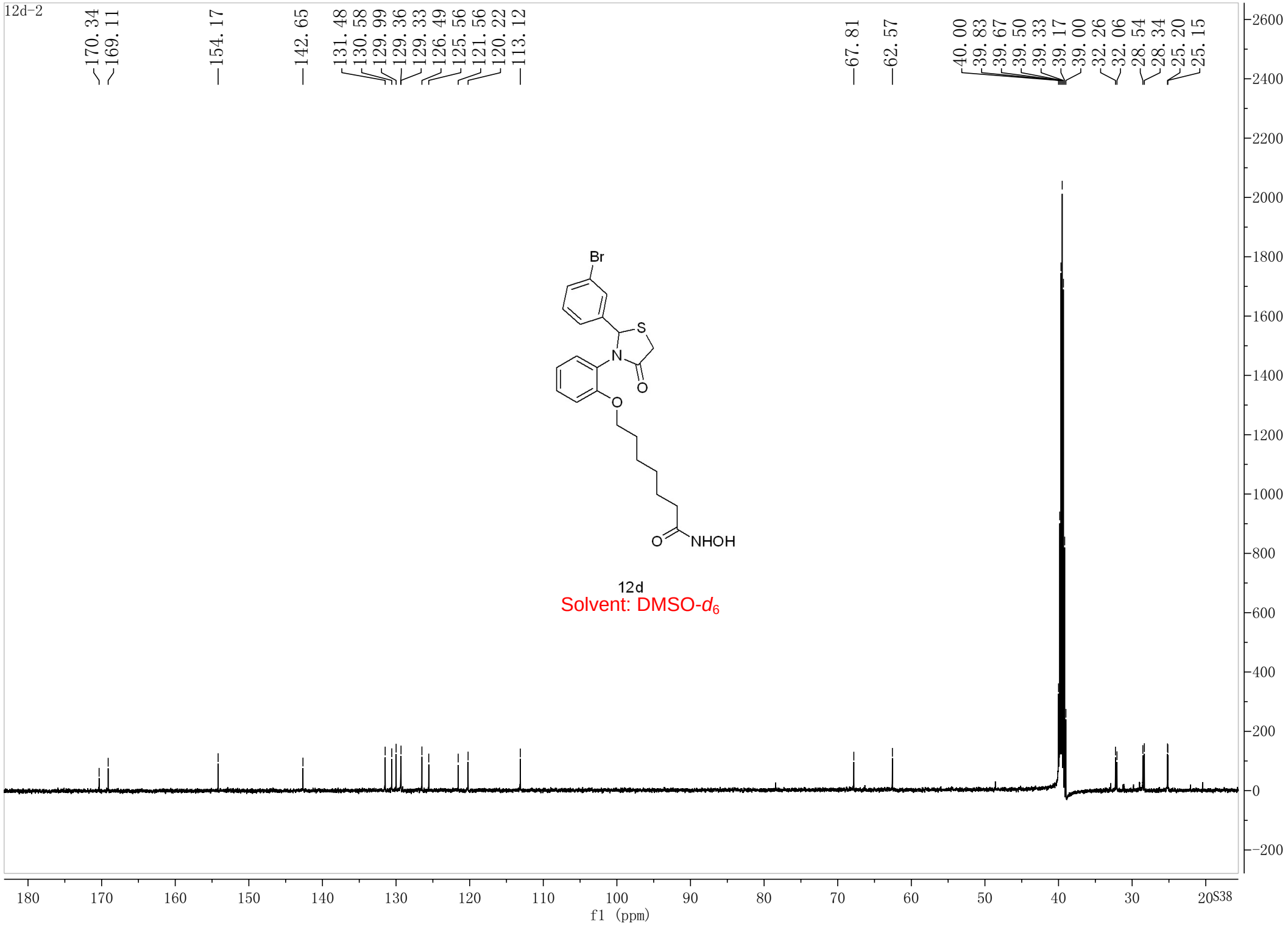
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1200 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	501.0439	24334	977.5	96047	94.1	0.0206
2	502.0465	17668	179.7	17713	17.4	0.0284
3	503.0420	24536	1033.1	102064	100.0	0.0205
4	504.0445	17506	176.6	17515	17.2	0.0288

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e¯ Conf	N-Rule
501.0439	1	C21H23BrN2NaO4S	501.0454	3.0	40.3	3	38.62	10.5	even	ok


10.35
8.67
7.62
7.45
7.42
7.40
7.37
7.25
7.23
7.20
7.17
7.03
7.01
6.85
6.82
6.16
4.05
4.04
4.01
4.00
3.97
3.94
3.90
3.83
3.78
3.35
2.50
2.01
1.99
1.96
1.79
1.76
1.74
1.57
1.55
1.53
1.49
1.46
1.36
1.34
Br
S
N
O
O
12d
O
NHOH
Solvent: DMSO-d_6
0.91
0.83
0.99
1.94
2.04
2.04
1.09
1.00
1.04
2.26
1.03
2.56
2.19
2.11
2.25
2.13
f1 (ppm)
S37


12d-2
170.34
169.11
154.17
142.65
131.48
130.58
129.99
129.36
129.33
126.49
125.56
121.56
120.22
113.12
67.81
62.57
40.00
39.83
39.67
39.50
39.33
39.17
39.00
32.26
32.06
28.54
28.34
25.20
25.15
Br
S
N
O
O
O
NHOH
12d
Solvent: DMSO-d_6
f1 (ppm)

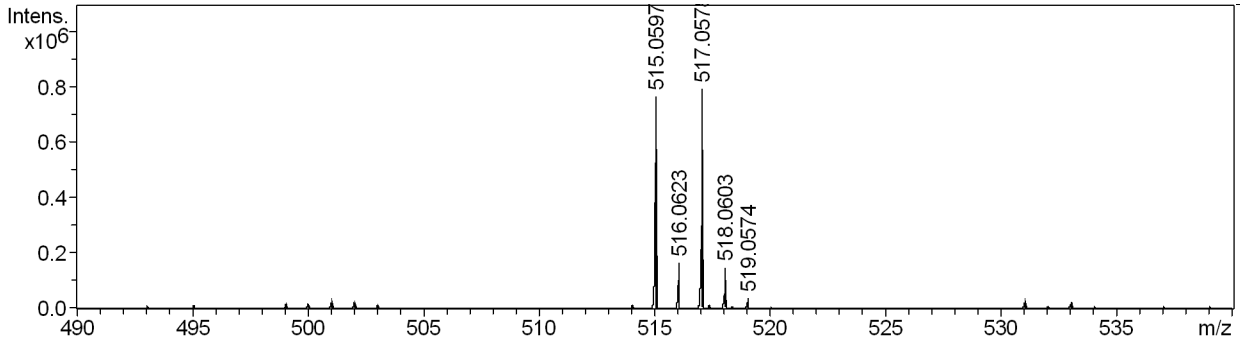
Mass Spectrum List Report

Analysis Info

Acquisition Date	4/29/2015 10:54:30 AM		
Analysis Name	D:\Data\waixi\chenyihua\20150429LIYUNQI\YF-493_P1-D-8_01_1520.d		
Method	Tune_pos_low_LC with calibration_2min.m	Operator	ECNU-Chem
Sample Name	YF-493	Instrument	maXis impact 282001.00122
Comment			

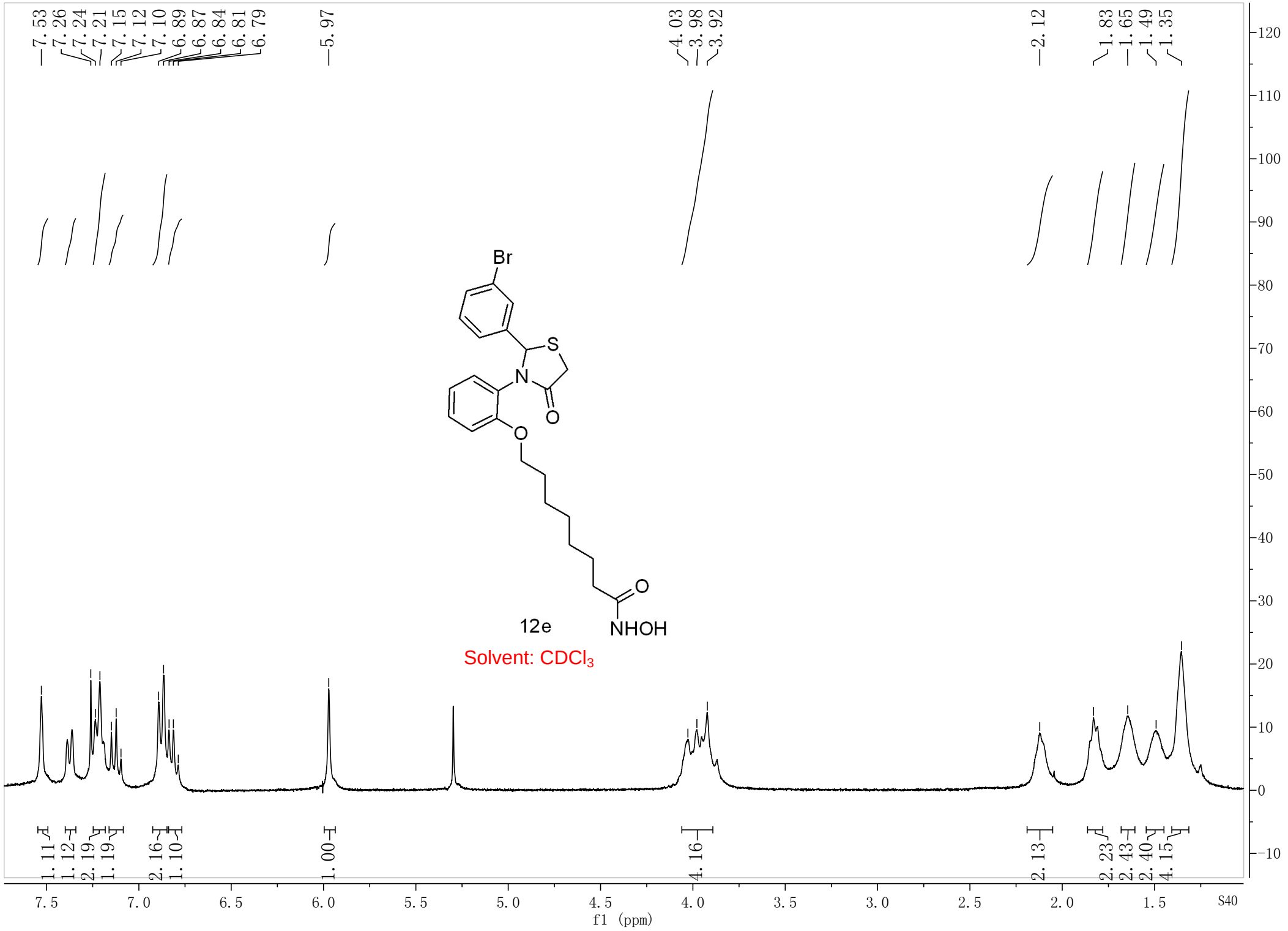
Acquisition Parameter

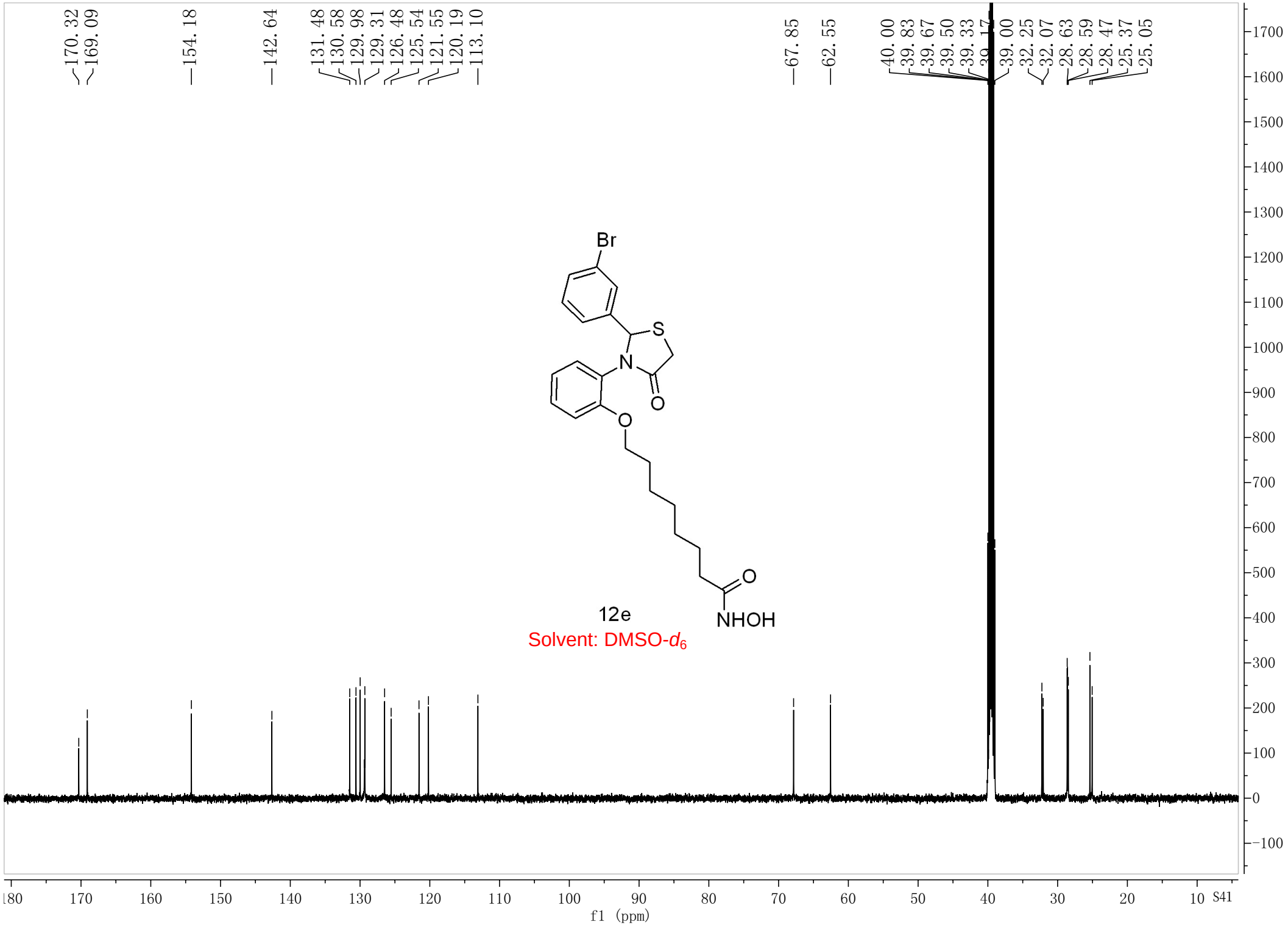
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1200 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	515.0597	34654	8666.0	763020	96.4	0.0149
2	516.0623	23747	1881.7	165565	20.9	0.0217
3	517.0578	34510	9007.7	791772	100.0	0.0150
4	518.0603	22676	1710.8	150258	19.0	0.0228
5	519.0574	15492	438.8	38520	4.9	0.0335

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e¯ Conf	N-Rule
515.0597	1	C22H25BrN2NaO4S	515.0611	2.6	32.6	1	58.76	10.5	even	ok


7.53
7.26
7.24
7.21
7.15
7.12
7.10
6.89
6.87
6.84
6.81
6.79
5.97
4.03
3.98
3.92
2.12
1.83
1.65
1.49
1.35
Br
S
N
O
O
O
NHOH
12e
Solvent: CDCl3
1.11
1.12
2.19
1.19
2.16
1.10
1.00
4.16
2.13
2.23
2.43
2.40
4.15
f1 (ppm)
S40


170.32
169.09
154.18
142.64
131.48
130.58
129.98
129.31
126.48
125.54
121.55
120.19
113.10
67.85
62.55
40.00
39.83
39.67
39.50
39.33
39.17
39.00
32.25
32.07
28.63
28.59
28.47
25.37
25.05
Br
S
N
O
O
O
NHOH
12e
Solvent: DMSO-d_6
f1 (ppm)
S41

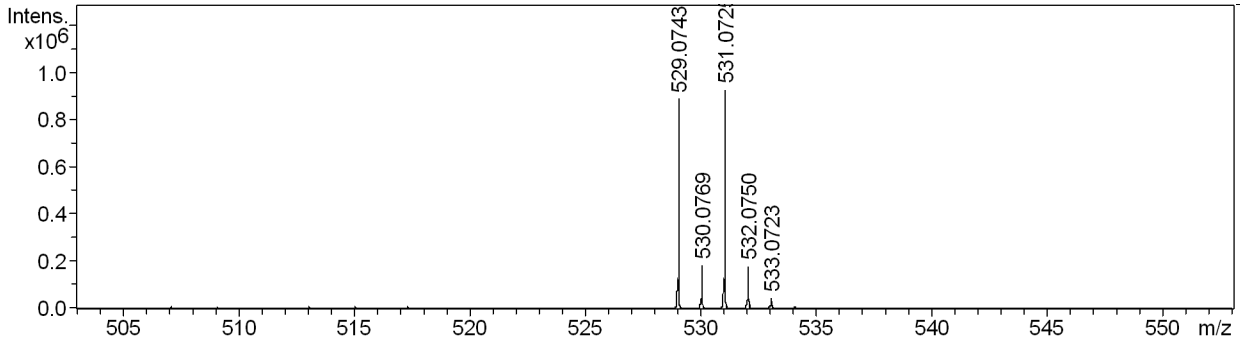
Mass Spectrum List Report

Analysis Info

Acquisition Date	4/29/2015 10:57:38 AM		
Analysis Name	D:\Data\waixi\chenyihua\20150429LIYUNQI\LW-507_P1-D-9_01_1521.d		
Method	Tune_pos_low_LC with calibration_2min.m	Operator	ECNU-Chem
Sample Name	LW-507	Instrument	maXis impact 282001.00122
Comment			

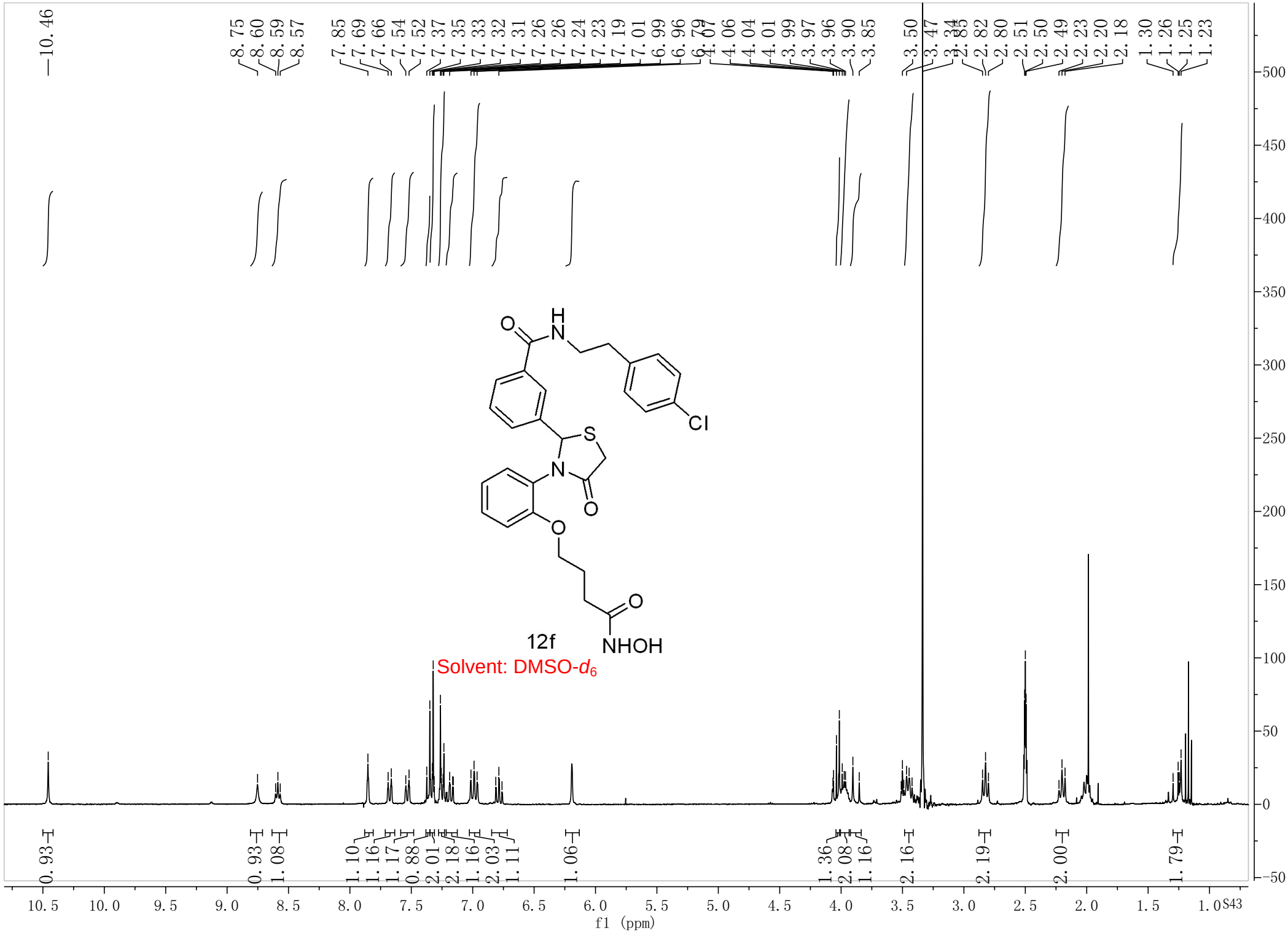
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1200 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	529.0743	34567	11298.0	884953	95.5	0.0153
2	530.0769	23614	2358.8	184629	19.9	0.0224
3	531.0725	34565	11836.9	926460	100.0	0.0154
4	532.0750	23353	2317.4	181253	19.6	0.0228
5	533.0723	15903	580.7	45419	4.9	0.0335

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e¯ Conf	N-Rule
529.0743	1	C23H27BrN2NaO4S	529.0767	4.6	38.0	1	100.00	10.5	even	ok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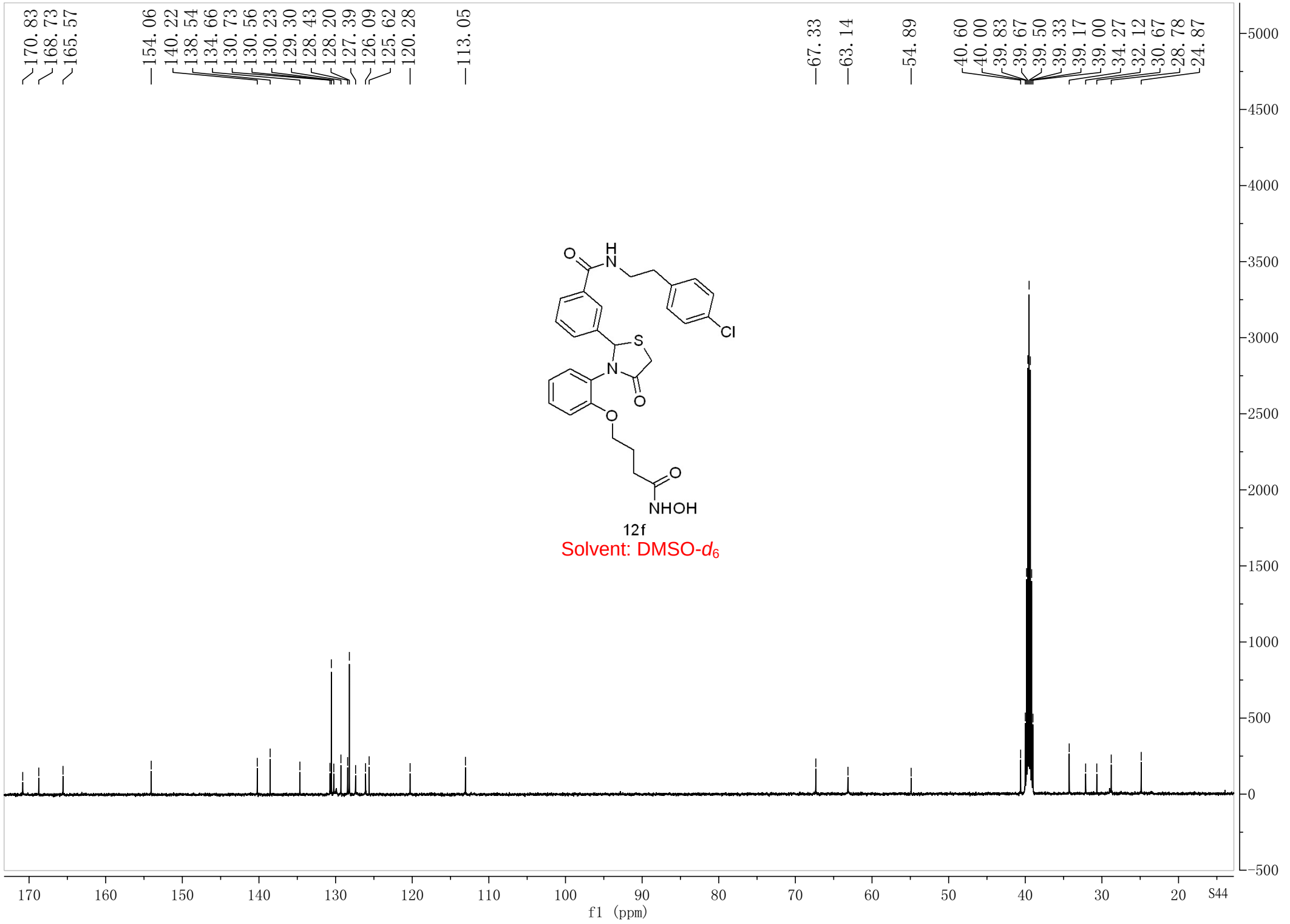
8.60
8.59
8.57
7.85
7.69
7.66
7.54
7.52
7.37
7.35
7.33
7.32
7.31
7.26
7.26
7.24
7.23
7.19
7.01
6.99
6.96
6.79
6.77
4.06
4.04
4.01
3.99
3.97
3.96
3.90
3.85
3.50
3.47
3.34
3.32
2.82
2.80
2.51
2.50
2.49
2.23
2.20
2.18
1.30
1.26
1.25
1.23
H
N
O
S
N
O
O
O
O
NHOH
Cl
12f
Solvent: DMSO-d_6
0.93
0.93
1.08
1.10
1.16
1.17
0.88
2.01
2.18
1.16
2.03
1.11
1.06
1.36
2.08
1.16
2.16
2.19
2.00
1.79
f1 (ppm)
S43


170.83
168.73
165.57
154.06
140.22
138.54
134.66
130.73
130.56
130.23
129.30
128.43
128.20
127.39
126.09
125.62
120.28
113.05
67.33
63.14
54.89
40.60
40.00
39.83
39.67
39.50
39.33
39.17
39.00
34.27
32.12
30.67
28.78
24.87
Cl
S
N
O
H
NHOH
12f
Solvent: DMSO-d_6
f1 (ppm)
S44

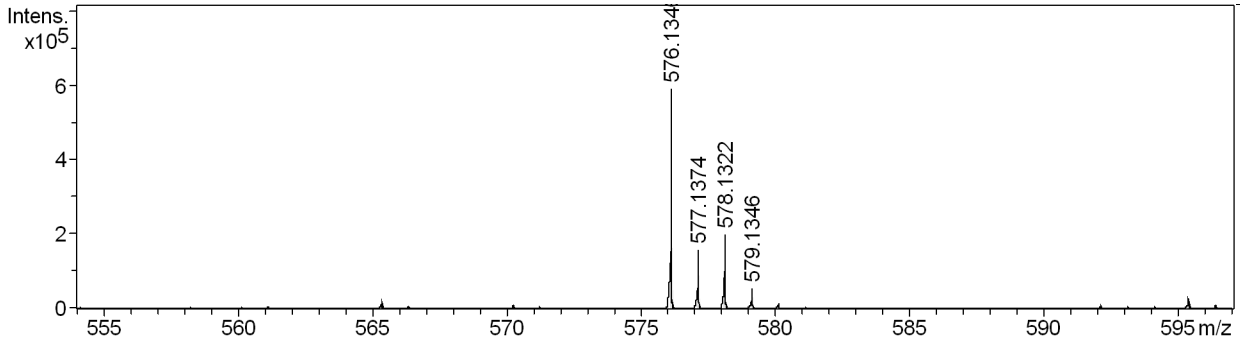
Mass Spectrum List Report

Analysis Info

		Acquisition Date	4/29/2015 1:57:28 PM
Analysis Name	D:\Data\waixi\chenyihua\20150429LIYUNQI\YF-554_P1-E-2_01_1525.d		
Method	Tune_pos_low_LC with calibration_2min.m	Operator	ECNU-Chem
Sample Name	YF-554	Instrument	maXis impact 282001.00122
Comment			

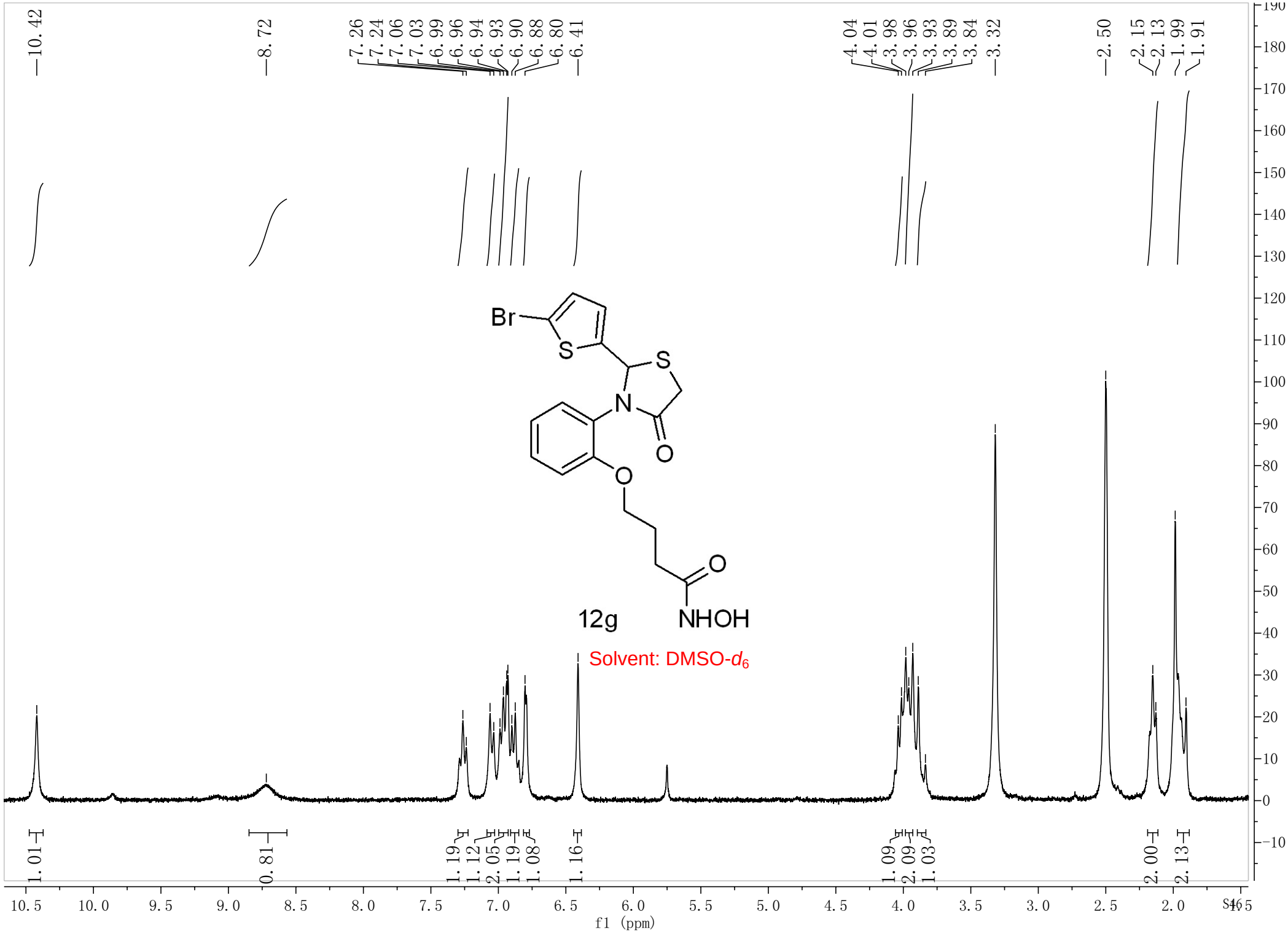
Acquisition Parameter

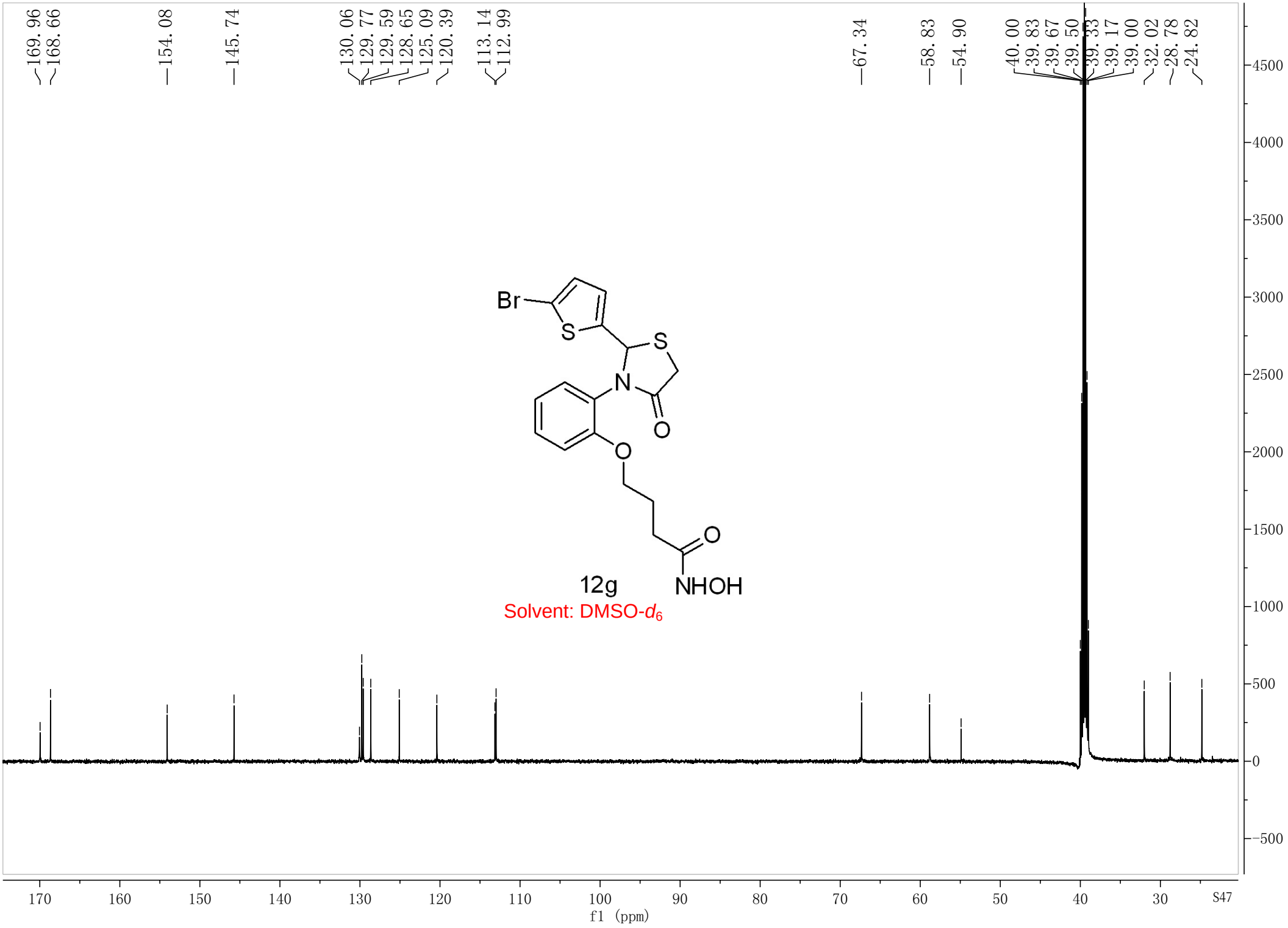
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1200 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	576.1346	31979	4958.2	589805	100.0	0.0180
2	577.1374	23218	1326.4	157626	26.7	0.0249
3	578.1322	23202	1666.6	197938	33.6	0.0249
4	579.1346	18792	458.2	54376	9.2	0.0308

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e¯ Conf	N-Rule
576.1346	1	C28H28ClN3NaO5S	576.1330	-2.6	47.1	1	100.00	15.5	even	ok


10.42
8.72
7.26
7.24
7.06
7.03
6.99
6.96
6.94
6.93
6.90
6.88
6.80
6.41
4.04
4.01
3.98
3.96
3.93
3.89
3.84
3.32
2.50
2.15
2.13
1.99
1.91
Br
S
S
N
O
O
O
NHOH
12g
Solvent: DMSO-d_6
1.01
0.81
1.19
1.12
2.05
1.19
1.08
1.16
1.09
2.09
1.03
2.00
2.13
f1 (ppm)


169.96
168.66
154.08
145.74
130.06
129.77
129.59
128.65
125.09
120.39
113.14
112.99
67.34
58.83
54.90
40.00
39.83
39.67
39.50
39.33
39.17
39.00
32.02
28.78
24.82
Br
S
S
N
O
O
O
NHOH
12g
Solvent: DMSO-d_6
4500
4000
3500
3000
2500
2000
1500
1000
500
0
−500
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
f1 (ppm)

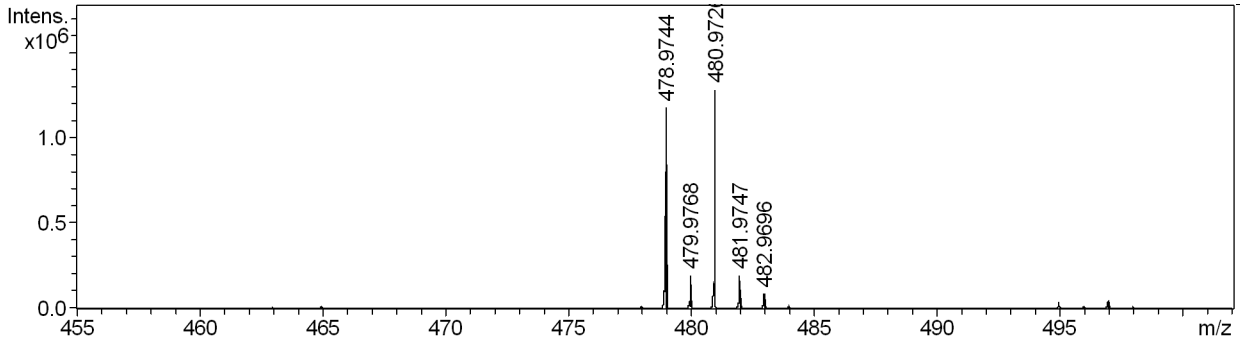
Mass Spectrum List Report

Analysis Info

		Acquisition Date	4/29/2015 2:09:58 PM
Analysis Name	D:\Data\waixi\chenyihua\20150429LIYUNQI\YF-457B_P1-E-6_01_1529.d		
Method	Tune_pos_low_LC with calibration_2min.m	Operator	ECNU-Chem
Sample Name	YF-457B	Instrument	maXis impact 282001.00122
Comment			

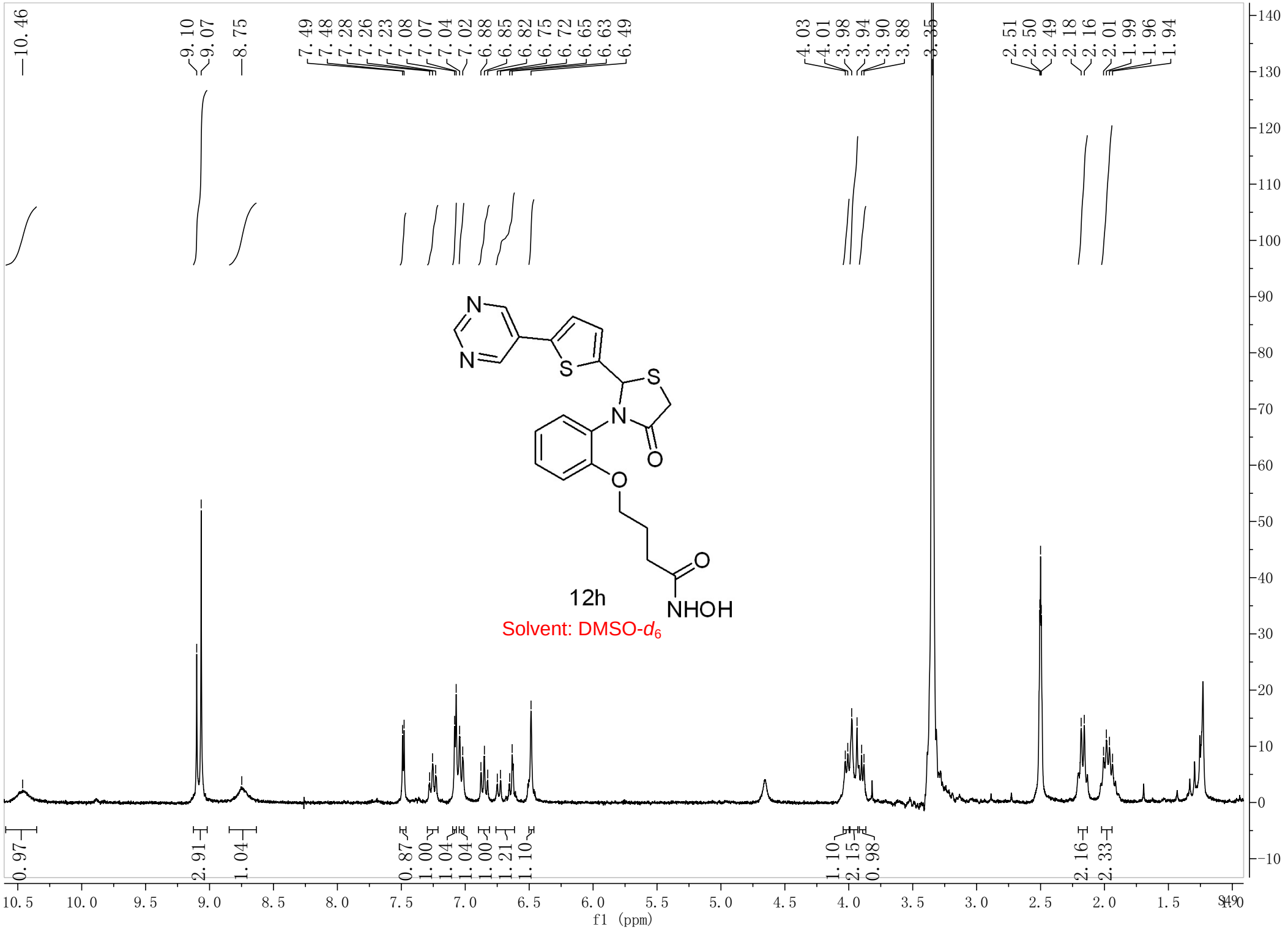
Acquisition Parameter

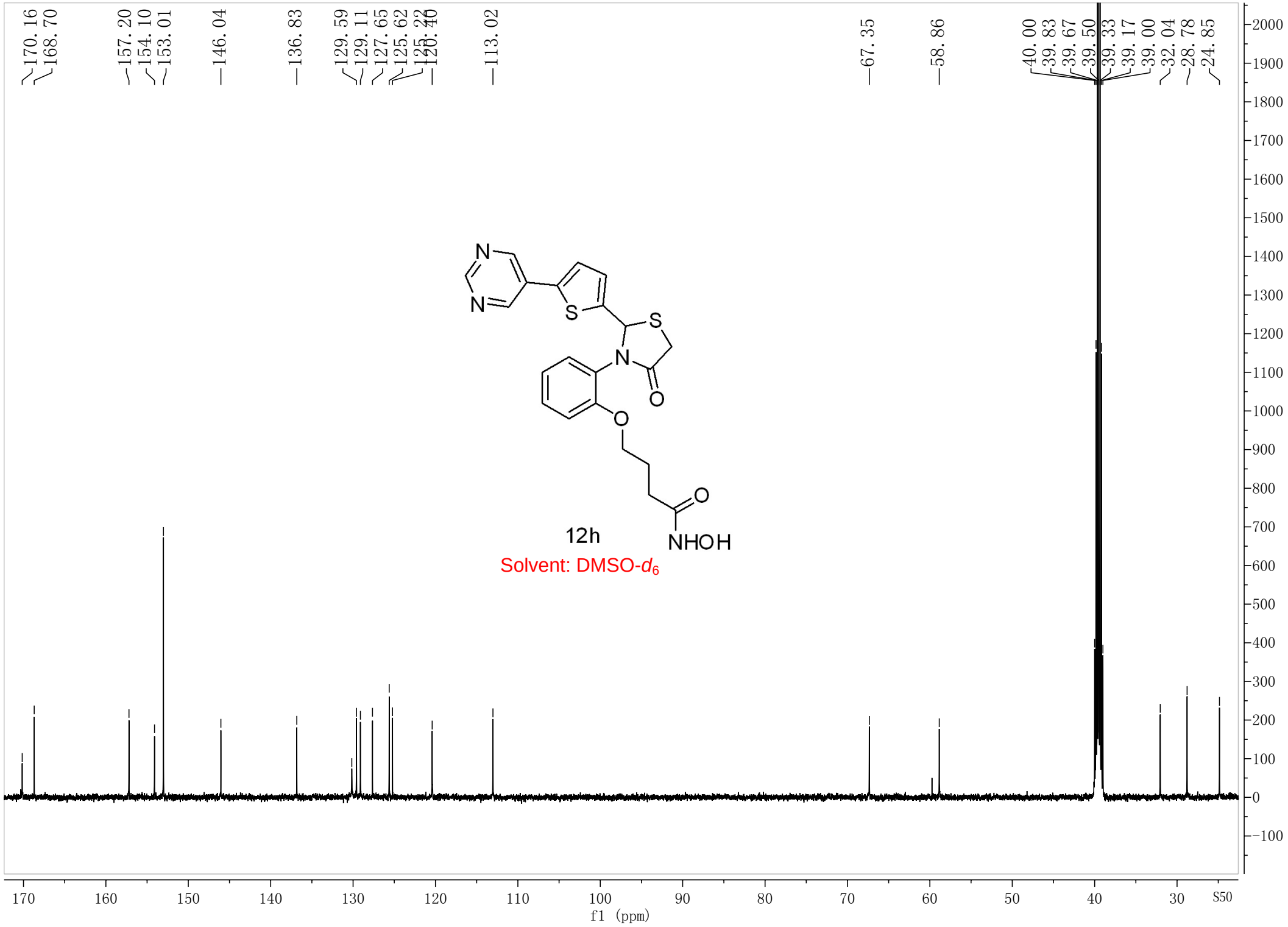
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1200 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	478.9744	36842	16035.3	1174149	91.6	0.0130
2	479.9768	23549	2631.0	192573	15.0	0.0204
3	480.9726	37530	17528.5	1282363	100.0	0.0128
4	481.9747	24074	2660.1	194719	15.2	0.0200
5	482.9696	18614	1187.3	86931	6.8	0.0259

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e⁻ Conf	N-Rule
478.9744	1	C17H17BrN2NaO4S2	478.9705	-8.1	31.1	1	100.00	9.5	even	ok


10.46
9.10
9.07
8.75
7.49
7.48
7.28
7.26
7.23
7.08
7.07
7.04
7.02
6.88
6.85
6.82
6.75
6.72
6.65
6.63
6.49
4.03
4.01
3.98
3.94
3.90
3.88
3.35
2.51
2.50
2.49
2.18
2.16
2.01
1.99
1.96
1.94
N
N
S
S
N
O
O
O
NHOH
12h
Solvent: DMSO-d_6
0.97
2.91
1.04
0.87
1.00
1.04
1.04
1.00
1.21
1.10
1.10
2.15
0.98
2.16
2.33
f1 (ppm)


170.16
168.70
157.20
154.10
153.01
146.04
136.83
129.59
129.11
127.65
125.62
113.02
67.35
58.86
40.00
39.83
39.67
39.50
39.33
39.17
39.00
32.04
28.78
24.85
12h
NHOH
Solvent: DMSO-d_6
f1 (ppm)
S50

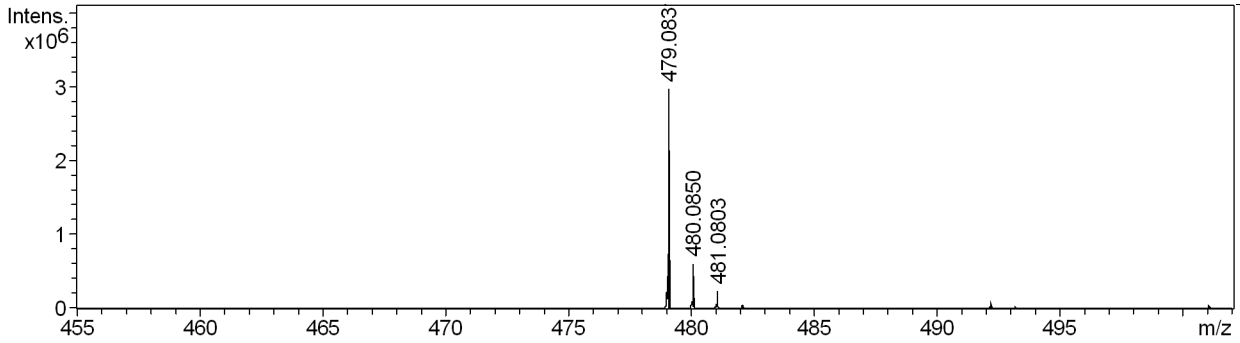
Mass Spectrum List Report

Analysis Info

		Acquisition Date	4/29/2015 2:58:15 PM
Analysis Name	D:\Data\waixi\chenyihua\20150429LIYUNQI\YF-456A-2_P1-E-7_01_1535.d		
Method	Tune_pos_low_LC with calibration_2min.m	Operator	ECNU-Chem
Sample Name	YF-456A-2	Instrument	maXis impact 282001.00122
Comment			

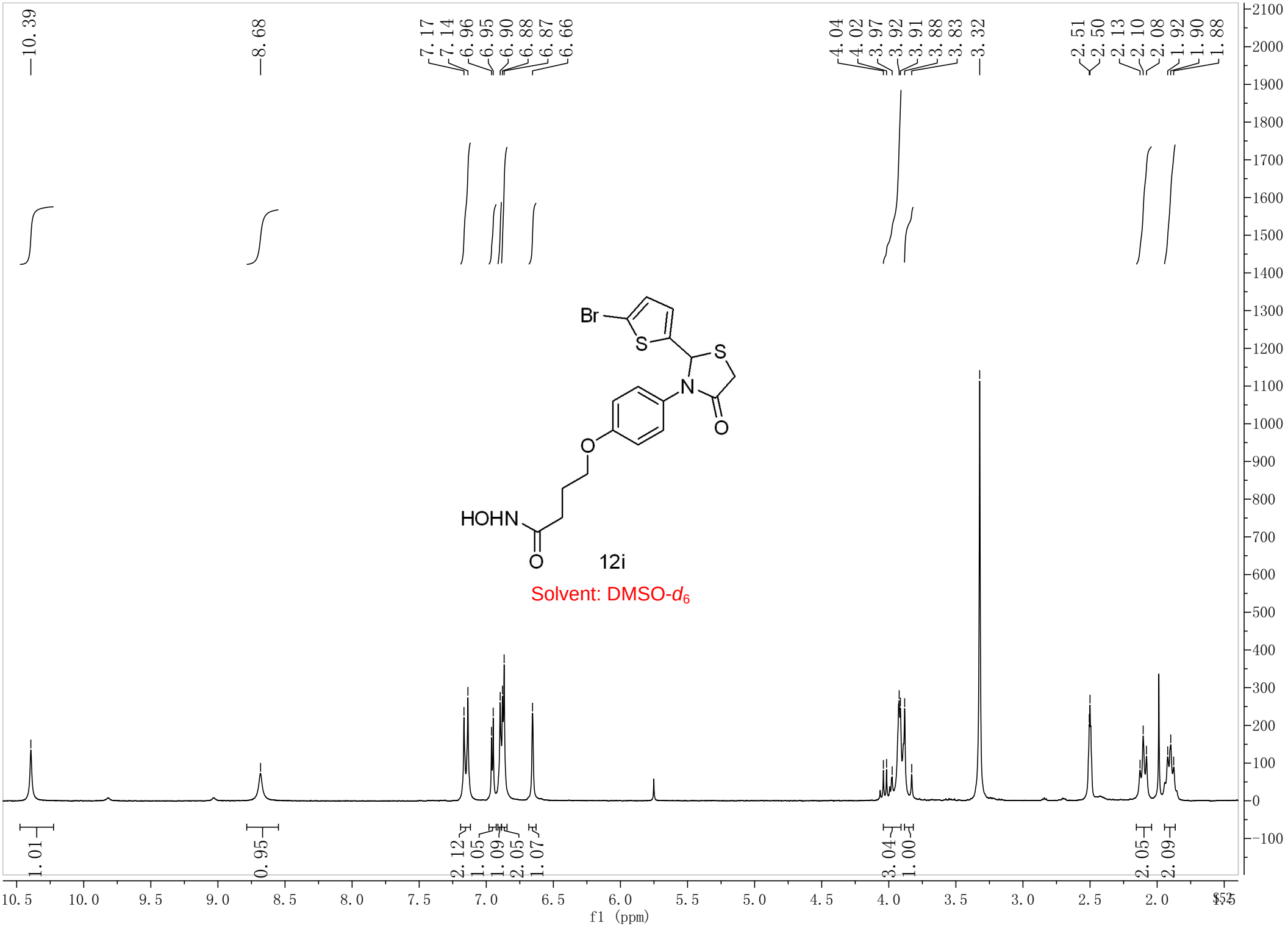
Acquisition Parameter

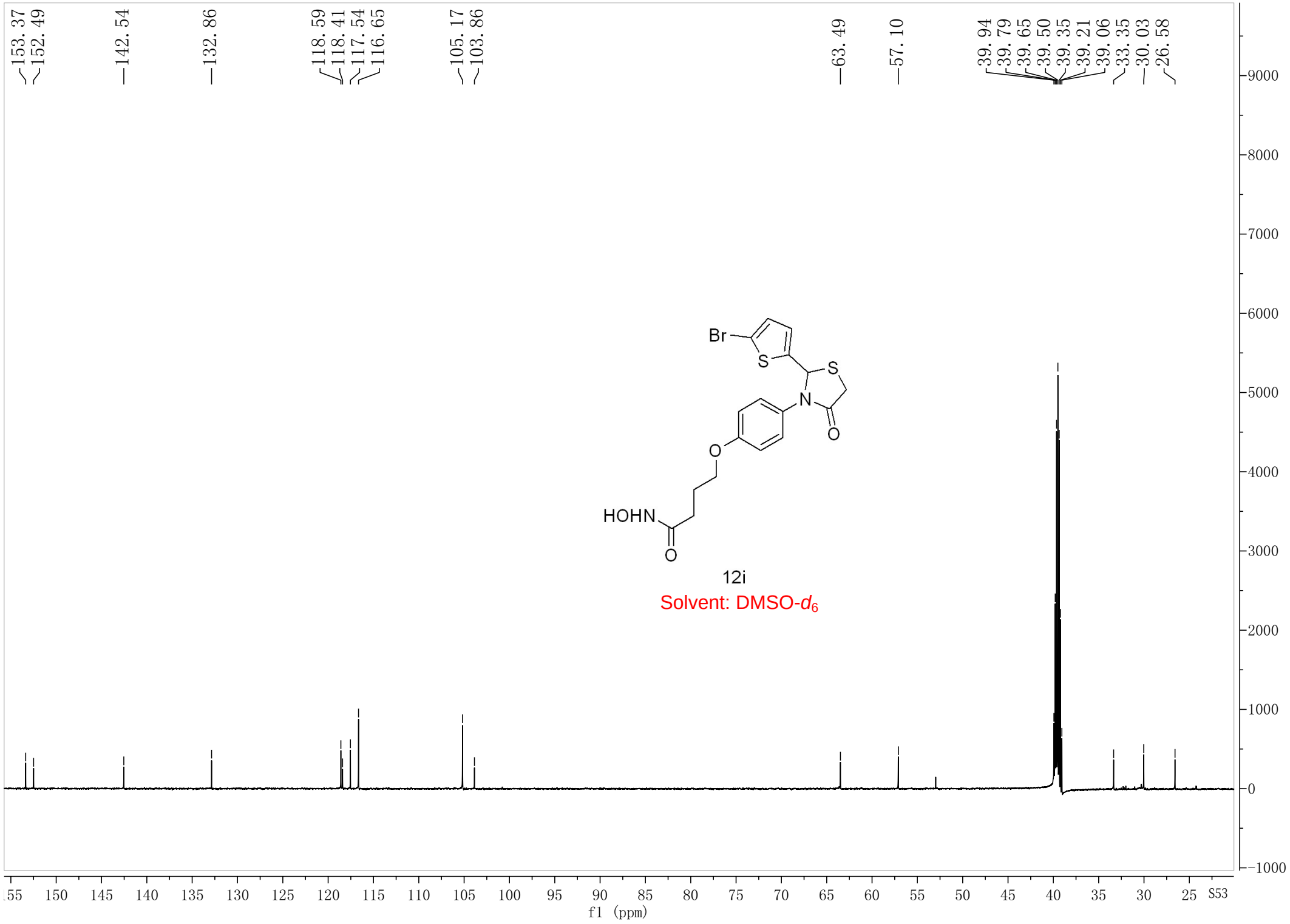
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1200 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Source



#	m/z	Res.	S/N	I	I %	FWHM
1	479.0831	25919	40727.4	2965297	100.0	0.0185
2	480.0850	30121	8391.6	610873	20.6	0.0159
3	481.0803	21775	3317.3	241286	8.1	0.0221

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e⁻ Conf	N-Rule
479.0831	1	C21H20N4NaO4S2	479.0818	-2.6	33.6	1	100.00	13.5	even	ok


10.39
8.68
7.17
7.14
6.96
6.95
6.90
6.88
6.87
6.66
4.04
4.02
3.97
3.92
3.91
3.88
3.83
3.32
2.51
2.50
2.13
2.10
2.08
1.92
1.90
1.88
Br
S
S
N
O
O
HOHN
O
12i
Solvent: DMSO-d_6
1.01
0.95
2.12
1.05
1.09
2.05
1.07
3.04
1.00
2.05
2.09
f1 (ppm)


153.37
152.49
142.54
132.86
118.59
118.41
117.54
116.65
105.17
103.86
63.49
57.10
39.94
39.79
39.65
39.50
39.35
39.21
39.06
33.35
30.03
26.58
Br
S
S
N
O
O
HOHN
O
12i
Solvent: DMSO-d_6
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
−1000
155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25
f1 (ppm)

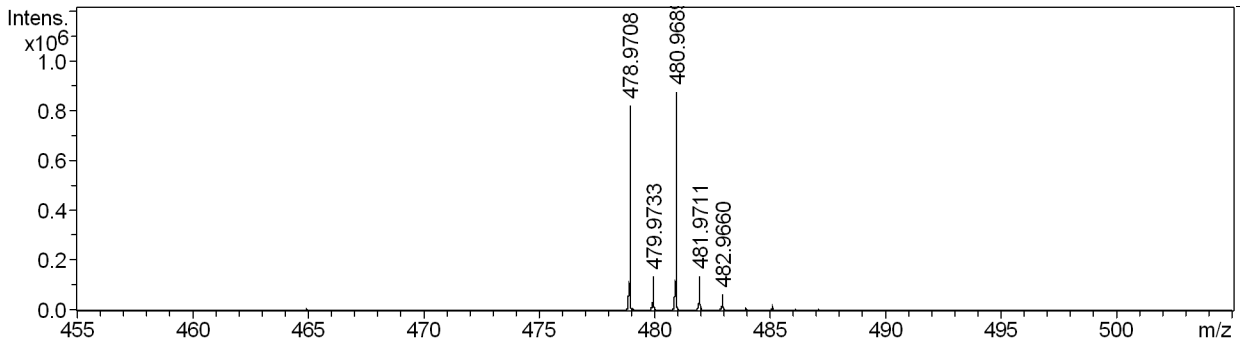
Mass Spectrum List Report

Analysis Info

Acquisition Date	4/29/2015 3:01:23 PM		
Analysis Name	D:\Data\waixi\chenyihua\20150429LIYUNQI\YF-457C-2_P1-E-8_01_1536.d		
Method	Tune_pos_low_LC with calibration_2min.m	Operator	ECNU-Chem
Sample Name	YF-457C-2	Instrument	maXis impact 282001.00122
Comment			

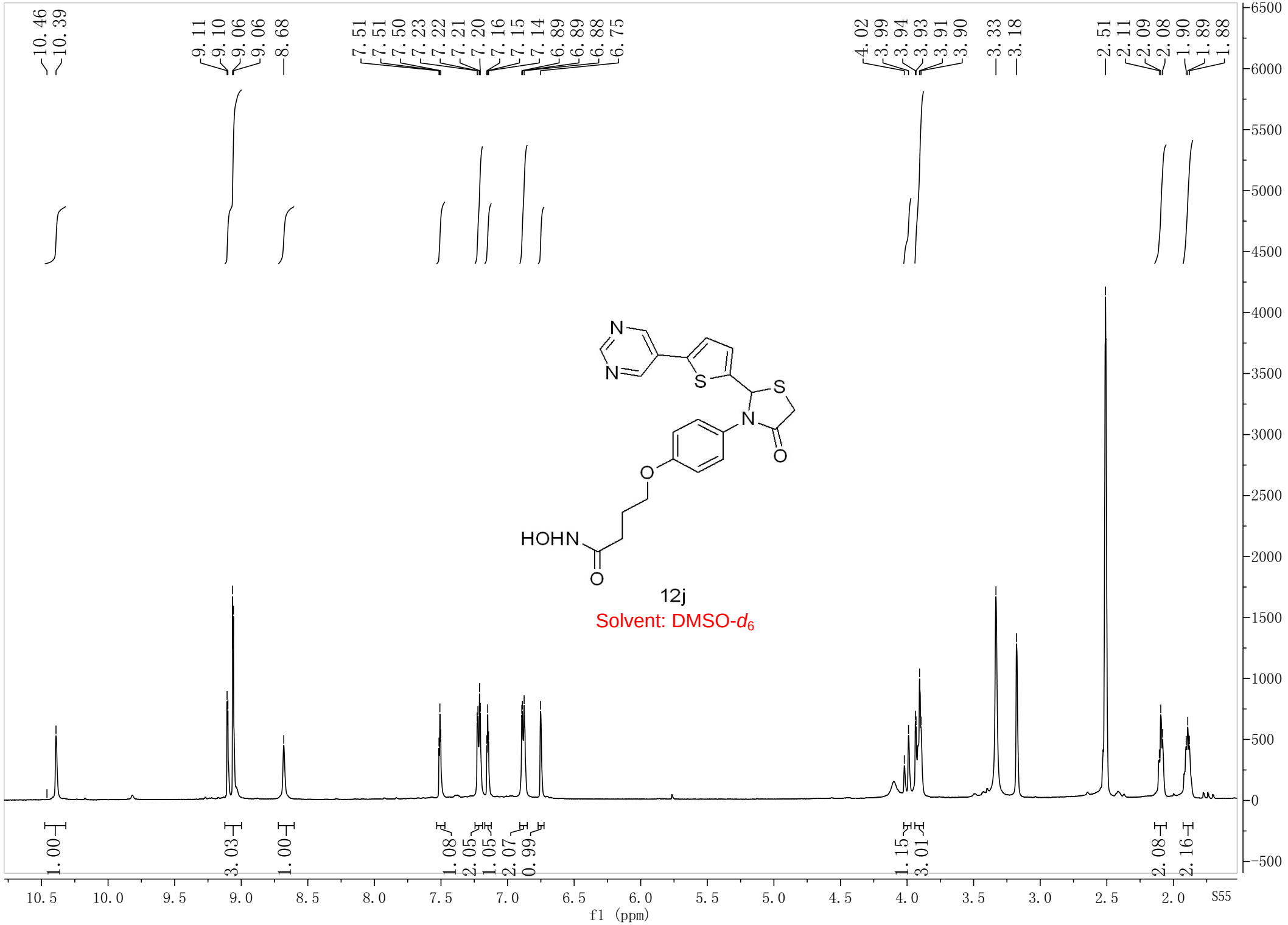
Acquisition Parameter

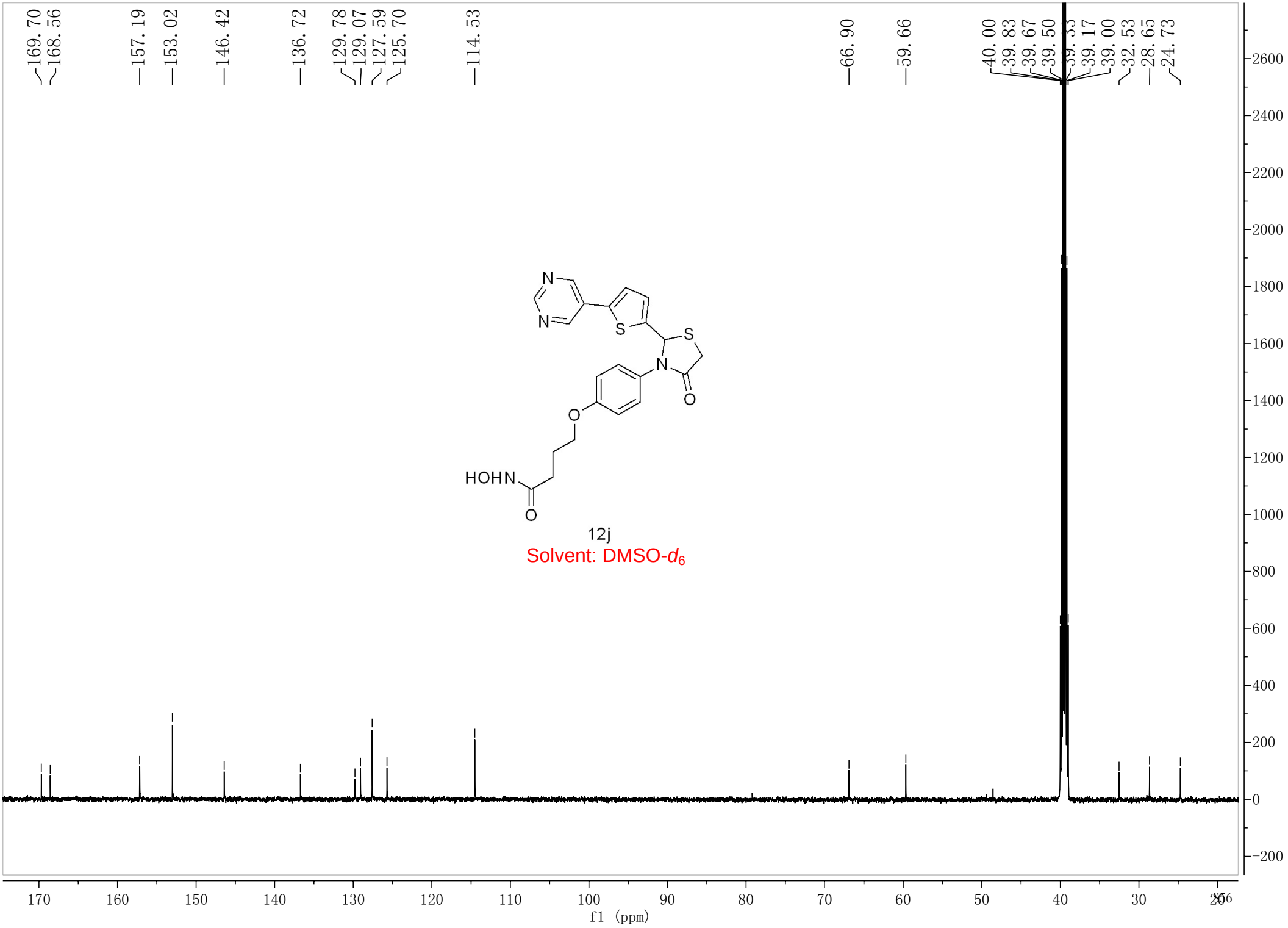
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1200 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	478.9708	33341	10510.6	819209	93.5	0.0144
2	479.9733	21658	1772.8	138119	15.8	0.0222
3	480.9689	33272	11245.8	875832	100.0	0.0145
4	481.9711	21516	1786.4	139166	15.9	0.0224
5	482.9660	17242	837.6	65202	7.4	0.0280

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e^- Conf	N-Rule
478.9708	1	C17H17BrN2NaO4S2	478.9705	-0.6	27.4	1	100.00	9.5	even	ok


10.46
10.39
9.11
9.10
9.06
9.06
8.68
7.51
7.51
7.50
7.23
7.22
7.21
7.20
7.16
7.15
7.14
6.89
6.89
6.88
6.75
4.02
3.99
3.94
3.93
3.91
3.90
3.33
3.18
2.51
2.11
2.09
2.08
1.90
1.89
1.88
N
N
S
S
N
O
O
HOHN
O
12j
Solvent: DMSO-d_6
1.00
3.03
1.00
1.08
2.05
1.05
2.07
0.99
1.15
3.01
2.08
2.16
f1 (ppm)
S55


169.70
168.56
157.19
153.02
146.42
136.72
129.78
129.07
127.59
125.70
114.53
66.90
59.66
40.00
39.83
39.67
39.50
39.33
39.17
39.00
32.53
28.65
24.73
N
N
S
S
N
O
O
HOHN
O
12j
Solvent: DMSO-d_6
f1 (ppm)

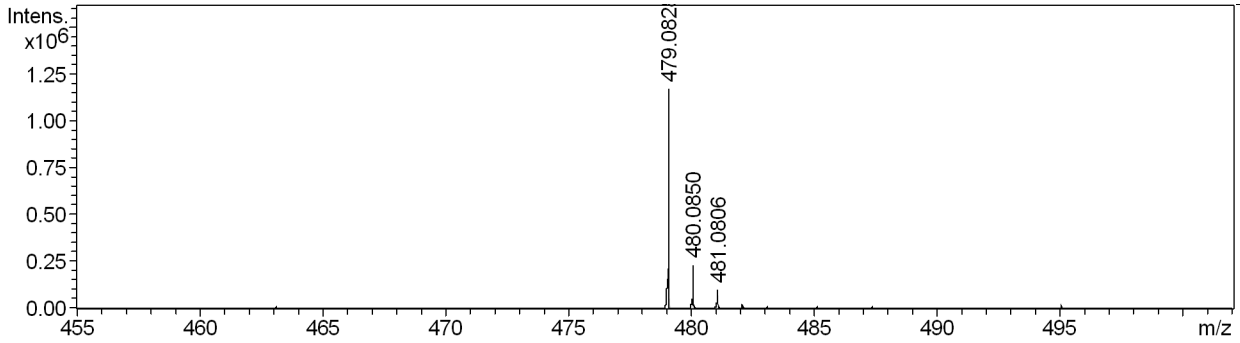
Mass Spectrum List Report

Analysis Info

		Acquisition Date	4/29/2015 3:04:30 PM
Analysis Name	D:\Data\waixi\chenyihua\20150429LIYUNQI\YF-456B-2_P1-E-9_01_1537.d		
Method	Tune_pos_low_LC with calibration_2min.m	Operator	ECNU-Chem
Sample Name	YF-456B-2	Instrument	maXis impact 282001.00122
Comment			

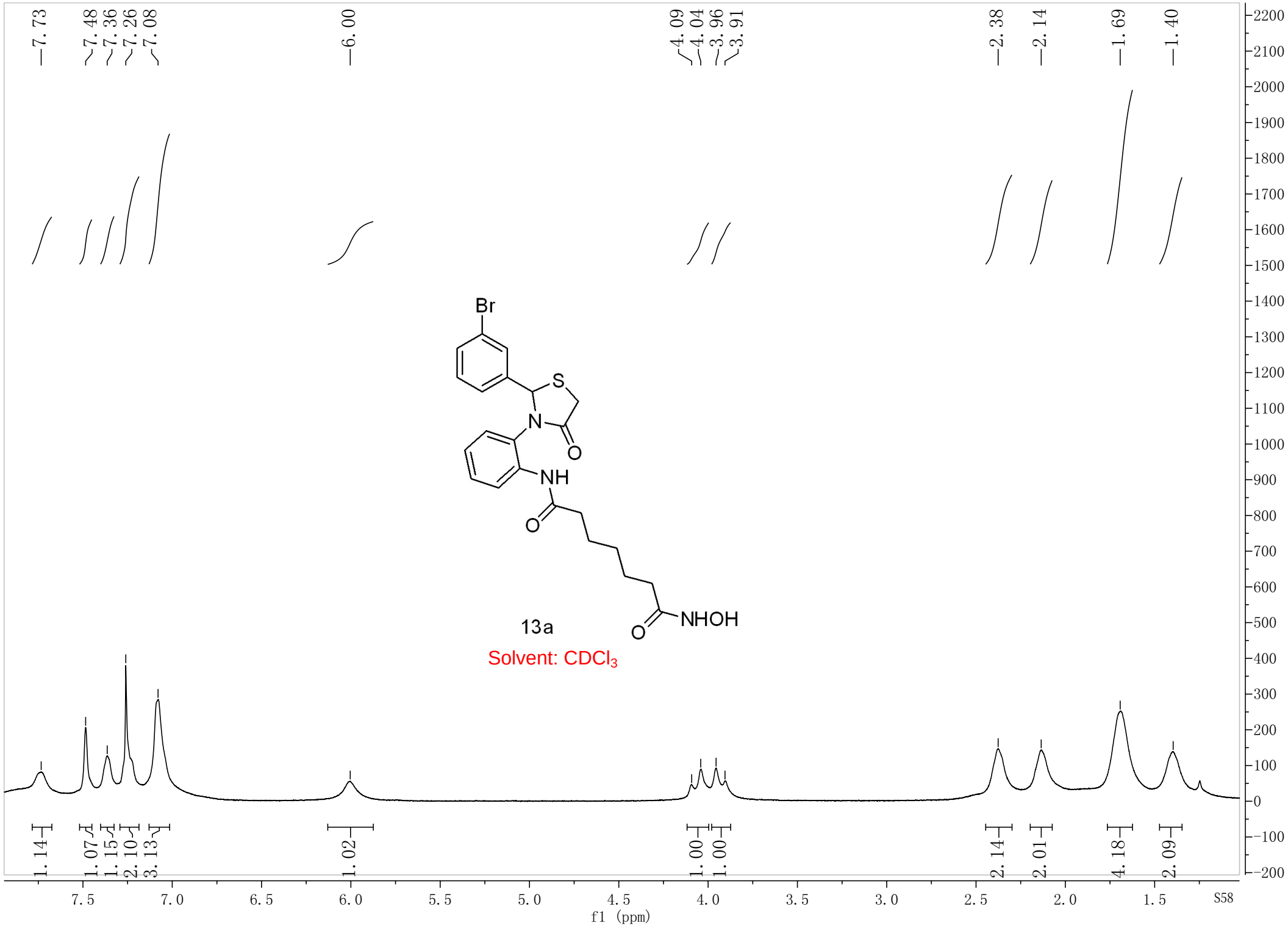
Acquisition Parameter

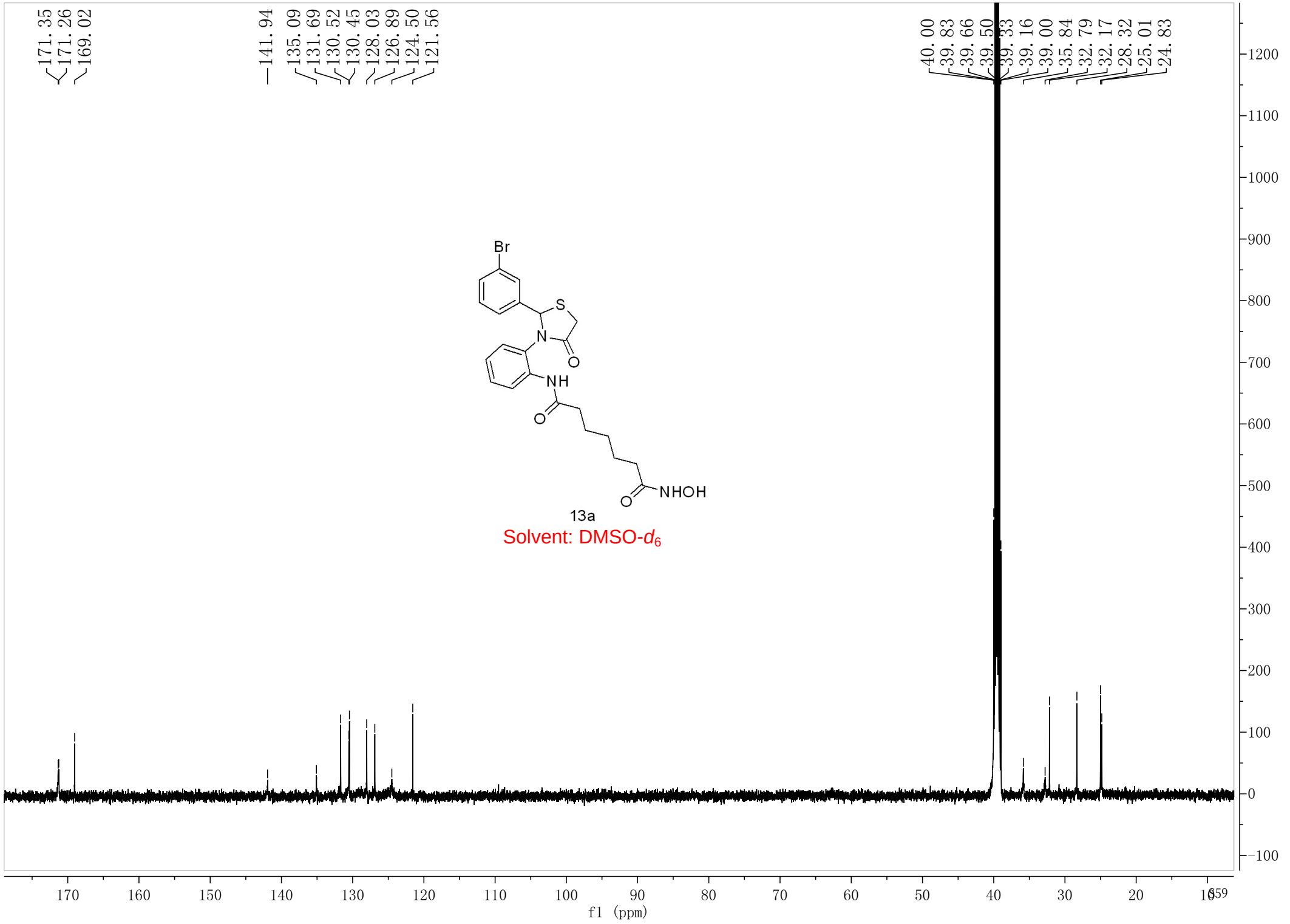
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1200 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	479.0828	34779	10985.6	1167102	100.0	0.0138
2	480.0850	23255	2208.7	234785	20.1	0.0206
3	481.0806	17680	967.2	102877	8.8	0.0272

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e¯ Conf	N-Rule
479.0828	1	C21H20N4NaO4S2	479.0818	-2.0	33.2	1	100.00	13.5	even	ok


7.73
7.48
7.36
7.26
7.08
6.00
4.09
4.04
3.96
3.91
2.38
2.14
1.69
1.40
Br
S
N
O
NH
O
O
NHOH
13a
Solvent: CDCl3
1.14
1.07
1.15
2.10
3.13
1.02
1.00
1.00
2.14
2.01
4.18
2.09
f1 (ppm)
S58


171.35
171.26
169.02
141.94
135.09
131.69
130.52
130.45
128.03
126.89
124.50
121.56
40.00
39.83
39.66
39.50
39.33
39.16
39.00
35.84
32.79
32.17
28.32
25.01
24.83
Br
S
N
O
NH
O
O
NHOH
13a
Solvent: DMSO-d_6
f1 (ppm)

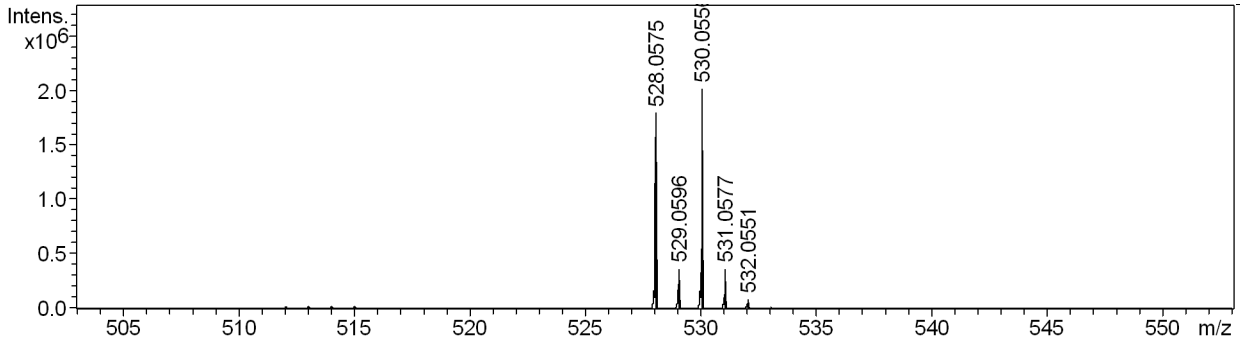
Mass Spectrum List Report

Analysis Info

		Acquisition Date	4/29/2015 3:07:37 PM
Analysis Name	D:\Data\waixi\chenyihua\20150429LIYUNQI\WJ-506-2_P1-F-1_01_1538.d		
Method	Tune_pos_low_LC with calibration_2min.m	Operator	ECNU-Chem
Sample Name	WJ-506-2	Instrument	maXis impact 282001.00122
Comment			

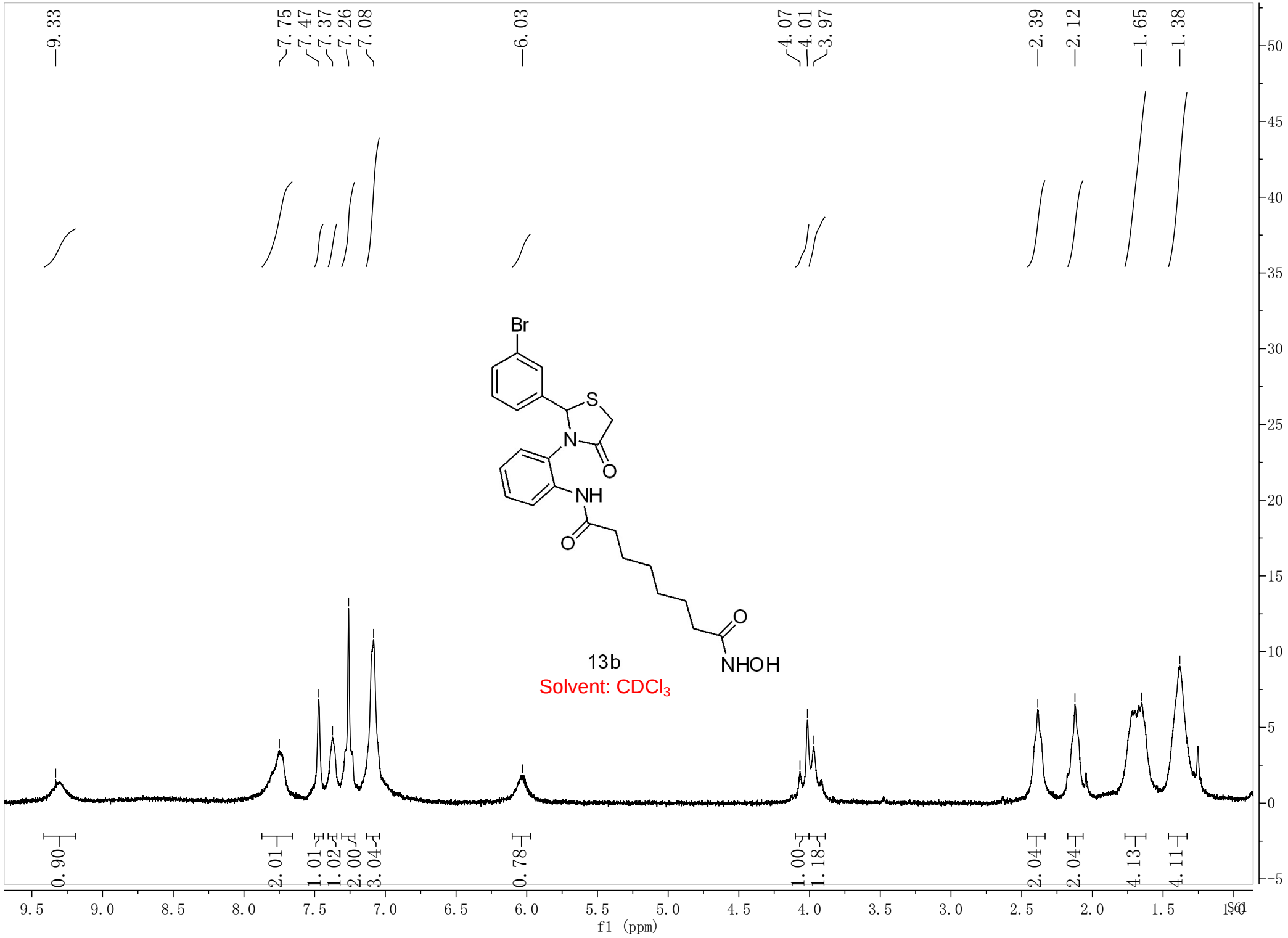
Acquisition Parameter

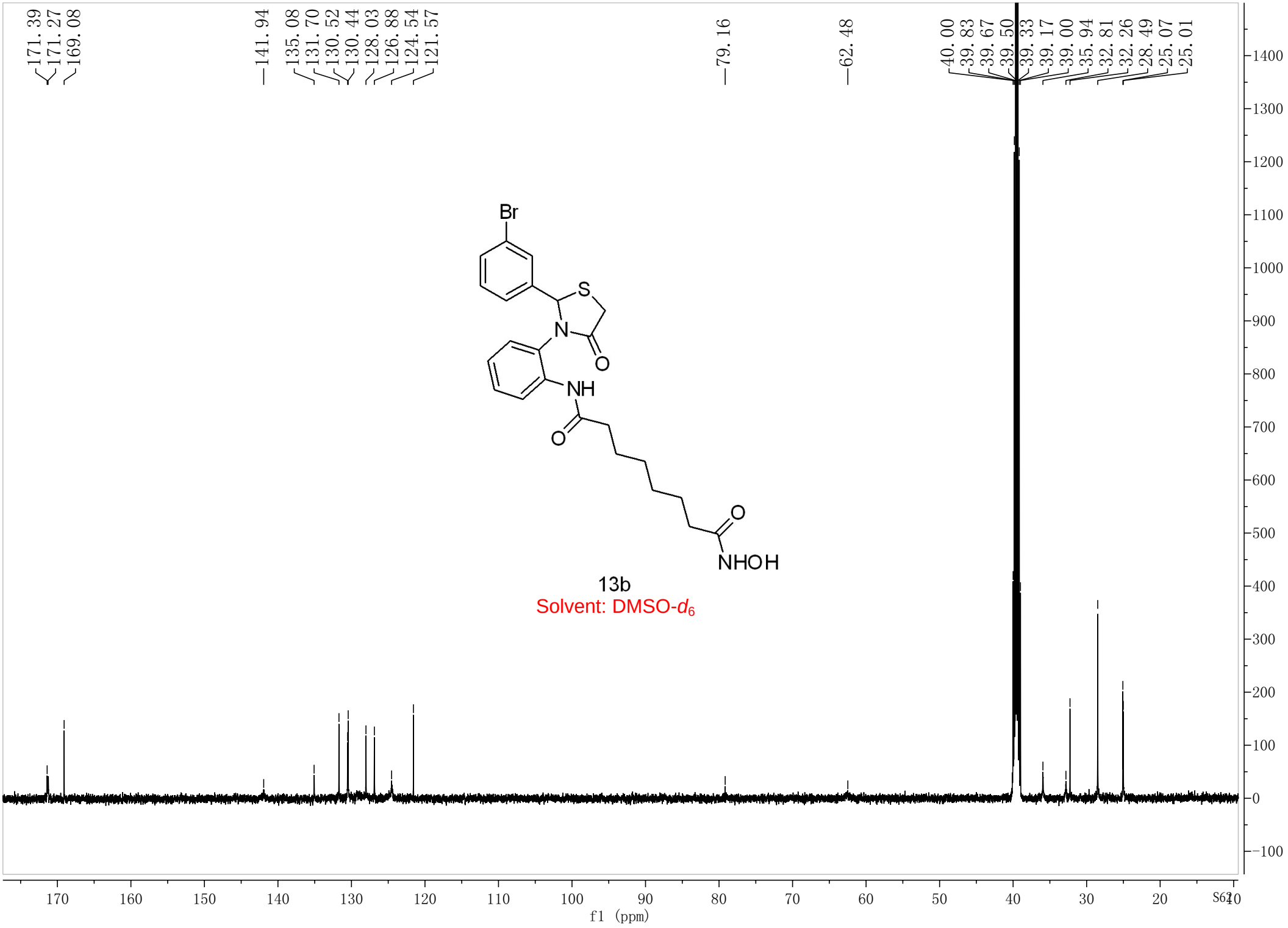
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1200 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	528.0575	37426	19624.4	1788542	88.9	0.0141
2	529.0596	27273	4026.7	366187	18.2	0.0194
3	530.0556	37825	22142.9	2010728	100.0	0.0140
4	531.0577	27587	4030.6	365390	18.2	0.0193
5	532.0551	18688	987.7	89473	4.4	0.0285

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e^- Conf	N-Rule
528.0575	1	C22H24BrN3NaO4S	528.0563	-2.2	48.3	1	100.00	11.5	even	ok


9.33
7.75
7.47
7.37
7.26
7.08
6.03
4.07
4.01
3.97
2.39
2.12
1.65
1.38
Br
S
N
O
NH
O
O
NHOH
13b
Solvent: CDCl3
0.90
2.01
1.01
1.02
2.00
3.04
0.78
1.00
1.18
2.04
2.04
4.13
4.11
f1 (ppm)


171.39
171.27
169.08
141.94
135.08
131.70
130.52
130.44
128.03
126.88
124.54
121.57
79.16
62.48
40.00
39.83
39.67
39.50
39.33
39.17
39.00
35.94
32.81
32.26
28.49
25.07
25.01
Br
S
N
O
NH
O
O
NHOH
13b
Solvent: DMSO-d_6
f1 (ppm)

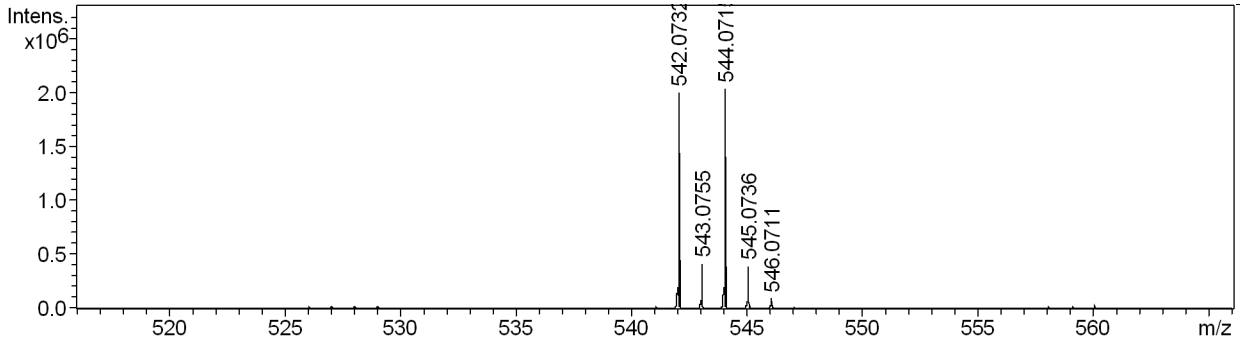
Mass Spectrum List Report

Analysis Info

		Acquisition Date	4/29/2015 3:10:45 PM
Analysis Name	D:\Data\waixi\chenyihua\20150429LIYUNQI\WJ-520-2_P1-F-2_01_1539.d		
Method	Tune_pos_low_LC with calibration_2min.m	Operator	ECNU-Chem
Sample Name	WJ-520-2	Instrument	maXis impact 282001.00122
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1200 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	542.0732	38580	19697.1	1996708	98.3	0.0141
2	543.0755	28686	4126.3	417403	20.6	0.0189
3	544.0715	37734	20123.7	2030477	100.0	0.0144
4	545.0736	27734	3956.0	398235	19.6	0.0197
5	546.0711	18836	943.3	94787	4.7	0.0290

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e¯ Conf	N-Rule
542.0732	1	C23H26BrN3NaO4S	542.0720	-2.4	41.9	2	100.00	11.5	even	ok