Electronic Supplementary Material (ESI) for RSC Advances.

Selective Targeting of CD38 Hydrolase and Cyclase Activity as an Approach to Immunostimulation

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Supporting Information

In Silico Analysis

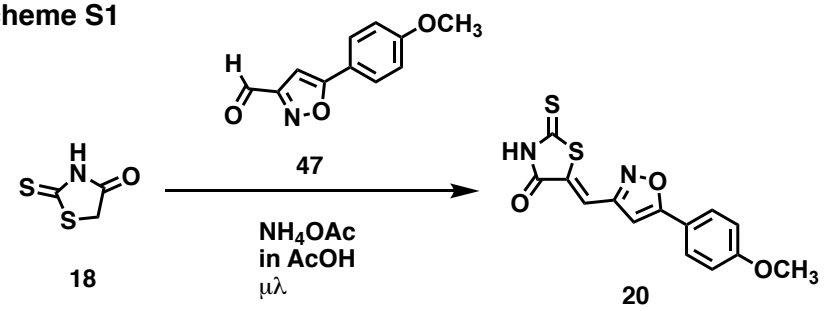
A modified PDB was prepared from PDB 4XJT (human CD38 complexed with inhibitor 2 [4-[(2,6-dimethylbenzyl)amino]-2-methylquinoline-8-carboxamide]). PDB 4XJT was imported into the AMBER10 program, and prepared by first breaking the bond between ADPr phosphate and Gln226 (mutated from Glu226) followed by substitution of a hydroxyl on the 1' position of ADPr phosphate. The Gln226 was repacked as Glu226. The 2' phosphate was removed from ADPr phosphate rendering ADPr. The complex was protonated at 310 K and pH 7.4 and was minimized. A compound (ligand) database of the 100 compounds populating the curated database outlined in the main manuscript was created, and structures were protonated at pH 7.4 and minimized. The 2-methylquinoline-8-carboxamide inhibitor in PDB 4XJT was removed from the complex and dummy atoms were used to map the active site. Compounds were docked into the active site using a triangle matcher and 50 poses were scored using London dG. Placements were further refined using an induced fit method and the top 5 poses were scored with GBVI/WSA dG. The docking campaign was designed such that ADPr and CD38 active site moieties would interact with docking compounds—simulating uncompetitive binding. Protein Ligand Interaction Fingerprints (PLIFs) were used to assess and annotate predictive binding poses along with observations from cocrystal structures described herein. The resulting preliminary binding poses were analyzed and visualized using the Molecular Operating Environment (MOE, Montreal, Quebec, Canada).

Synthesis

All reagents and dry solvents were purchased from Aldrich Chemical Co. (Milwaukee, WI), Sigma Chemical Co. (St. Louis, MO), VWR (Radnor, PA) or Fisher Scientific (Chicago, IL) and were used without further purification except as noted below. Triethylamine was distilled from potassium hydroxide and stored in a nitrogen atmosphere. Dry methanol, ethyl acetate, tetrahydrofuran, dimethyl formamide and hexane were either purchased (VWR) or prepared using a Glass Contour Solvent Purification System (Pure Process Technology, LLC, Nashua, NH). Microwave synthetic procedures were conducted on an Initiator 8 microwave synthesizer (Biotage, Charlotte, NC). Preparative scale chromatographic procedures were carried out using a Biotage Selekt chromatography system (Biotage, Charlotte, NC) fitted with silica gel 60 cartridges (230-440 mesh). Thin layer chromatography was conducted on Merck precoated silica gel 60 F-254. Apigenin, quercetin and compound **17** were purchased from Selleckchem (Houston, TX), and compounds **1**-**16** were purchased from Chembridge (San Diego, CA).

All ^{1}H- and ^{13}C-NMR spectra were recorded on a Bruker Avance 600 MHz spectrometer, and all chemical shifts are reported as δ values referenced to TMS or DSS. Splitting patterns are indicated as follows: s, singlet; d, doublet; t, triplet; m, multiplet; br, broad peak. In all cases, ^{1}H-NMR, ^{13}C-NMR and MS spectra were consistent with assigned structures, and ^{13}C peak assignments appear on the spectrum. . Mass spectra were recorded by LC/MS on a Waters UPLC/MS system with a model QDa mass spectrometer detector. Prior to biological testing procedures, all compounds were determined to be >95% pure by UPLC chromatography (9:1 H_2O: acetonitrile, +0.1% formic acid to 1:9 H_2O/ acetonitrile +0.1% formic acid over 8 minutes) using a Waters Acquity H-series ultrahigh-performance liquid chromatograph fitted with a C18 reversed-phase column (Acquity UPLC BEH C18 1.7 M, 2.1 X 100 mm). Compounds **20**-**46** were synthesized according to the general procedure described below.

Scheme S1



*Synthesis of (Z)-5-((5-(4-methoxyphenyl)isoxazol-3-yl)methylene)-2-thioxothiazolidin-4-one (**20**).*
A 0.05 g portion of 2-thioxothiazolidin-4-one **18** (0.43 mmol), 0.087 g (0.43 mmol) of 5-(4-methoxyphenyl)isoxazole-3-carbaldehyde **47** and 0.66 mg (0.86 mmol) of ammonium acetate were added to a microwave vial along with 2 mL of glacial acetic acid, a stirring bar was added and the vial was sealed. The sealed vial was microwave irradiated for 10 minutes at 180 ^{o}C, during which time the reaction mixture changed from a colorless solution to a vibrant orange-yellow suspension. The reaction mixture was allowed to cool to room temperature, the vial was opened and completion of the reaction was verified by TLC (1:1 EtOAc/hexane). The reaction product was precipitated by adding 5 mL of water, the mixture was centrifuged (10,000 X G, 10^{o}C, 5 minutes) and the liquid was decanted. The resulting solid was then washed with an additional 5 mL of water, re-centrifuged and the liquid was decanted. Residual water was removed from the solid by lyophilization to afford (Z)-5-((5-(4-methoxyphenyl)isoxazol-3-yl)methylene)-2-thioxothiazolidin-4-one **20** (104 mg, 76.1%) as a yellowish solid. ^{1}H NMR (600 MHz, D_6-DMSO/TMS): δ 7.84 (d, J = 8.7 Hz, 2H, H-7, H-11), 7.49 (s, 1H, H-21), 7.19 (s, 1H, H-4), 7.13–7.09 (m, 2H, H-10, H-8), 3.83 ppm (s, 3H, H-13). ^{13}C NMR (600 MHz, D_6-DMSO/TMS) δ 55.48 ($\underline{C}H_3$-O); 100.39 (N-C-$\underline{C}$H); 114.85 (O-C-$\underline{C}$H); 116.38 (O-C-$\underline{C}$H); 127.60 (CH-$\underline{C}$); 158.24 (N-$\underline{C}$); 161.30 (O-$\underline{C}$); 168.68 ($\underline{C}$O); 170.05 ($\underline{C}$S). UPLC retention time: 7.23 min. MS: calculated, 319.3650, found, 318.9710.

Synthesis of (Z)-5-(4-(methylsulfonyl)benzylidene)-2-thioxothiazolidin-4-one *(**21**).*
Compound **21** was synthesized from 2-thioxothiazolidin-4-one and 4-(methylsulfonyl)benzaldehyde exactly as described for compound **20** and isolated as a dark yellow solid in 71.2% yield. ^{1}H NMR (600 MHz, D_6-DMSO/TMS) δ 7.84 (d, J = 8.7 Hz, 2H, H-7, H-11), 7.49 (s, 1H, H-21), 7.19 (s, 1H, H-4), 7.13–7.09 (m, 2H, H-10, H-8), 3.83 ppm (s, 3H, H-13). ^{13}C NMR (600 MHz, D_6-DMSO/TMS) δ 43.80 (CH_3); 128.18 (C-$\underline{C}$H); 129.61 ($\underline{C}$-CH); 129.66 (C-$\underline{C}$H); 138.18 ($\underline{C}$-CH); 142.02 ($\underline{C}$-CH); 195.84 ($\underline{C}$S). UPLC retention time: 5.21 min. MS: calculated, 298.3770, found, 298.0614.

*Synthesis of (Z)-2-thioxo-5-(4-(trifluoromethoxy)benzylidene)thiazolidin-4-one (**22**).*

Compound **22** was synthesized from 2-thioxothiazolidin-4-one and 4-(trifluoromethoxy)benzaldehyde exactly as described for compound **20** and isolated as a dark orange-yellow solid in 70.4% yield. ^{1}H NMR (600 MHz, D_6-DMSO/TMS) δ 7.75–7.67 (m, 3H, H-7, H-18, H-9), 7.52 ppm (d, J = 8.0 Hz, 2H, H-10, H-17). ^{13}C NMR (600 MHz, D_6-DMSO/TMS) δ 122.07 (C-CH); 127.16 (C-CH); 130.32 (C-CH); 132.63 (C-CH); 132.90 (C-CH); 149.76 (C-CH); 169.71 (CO); 195.89 (CS). UPLC retention time 7.56 min. MS: calculated, 304.2892, found, 304.0641.

*Synthesis of (Z)-2-thioxo-5-(4-(trifluoromethyl)benzylidene)thiazolidin-4-one (**23**).*
Compound **23** was synthesized from 2-thioxothiazolidin-4-one and 4-(trifluoromethyl)benzaldehyde exactly as described for compound **20** and isolated as a yellow solid in 79.8% yield. ^{1}H NMR (600 MHz, D_6-DMSO/TMS) δ 7.90–7.79 (m, 4H, H-10, H-16, H-17, H-9), 7.71 ppm (s, 1H, H-7). UPLC retention time 7.43 min. MS calculated, 288.0568, found, 288.0568.

*Synthesis of (Z)-5-((4'-methoxy-[1,1'-biphenyl]-4-yl)methylene)-3-methyl-2-thioxothiazolidin-4-one (**24**).*
Compound **24** was synthesized from 3-methyl-2-thioxothiazolidin-4-one and 4'-methoxy-[1,1'-biphenyl]-4-carbaldehyde exactly as described for compound **20** and isolated as a yellow solid in 70.6% yield. ^{1}H NMR (600 MHz, D_6-DMSO/TMS) δ 7.85–7.82 (m, 3H), 7.74–7.69 (m, 4H), 7.05 (d, J = 8.7 Hz, 2H), 3.81 (s, 3H, H-23), 3.41 ppm (s, 3H, H-8). ^{13}C NMR (600 MHz, D_6-DMSO/TMS) δ 55.74 (CH_3); 115.08 (C-CH); 127.40 (C-CH); 128.55 (C-CH); 131.87 (C-CH); 132.97 (C-CH). UPLC retention time 8.817 min. MS calculated, 342.05442, found, 342.0713.

*Synthesis of (Z)-5-(quinolin-6-ylmethylene)-2-thioxothiazolidin-4-one (**25**).*
Compound **25** was synthesized from 2-thioxothiazolidin-4-one and quinoline-6-carbaldehyde exactly as described for compound **20** and isolated as a light yellow solid in 50.7% yield. ^{1}H NMR (600 MHz, D_6-DMSO/TMS) δ 8.97 (dd, J = 0.9, 4.1 Hz, 1H), 8.52 (d, J = 8.2 Hz, 1H), 8.22 (s, 1H), 8.11 (d, J = 8.7 Hz, 1H), 7.93 (dd, J = 1.8, 8.7 Hz, 1H), 7.80 (s, 1H), 7.61 ppm (dd, J = 4.2, 8.3 Hz, 1H, H-11). ^{13}C NMR (600 MHz, D_6-DMSO/TMS) δ 123.00 (C-CH); 128.42 (C-CH); 130.52 (C-CH); 130.71 (C-CH); 130.89 (C-CH); 131.51 (C-CH); 137.41 (C-CH); 148.21 (CO); 152.79 (C-CH); 196.41 (CS). UPLC retention time 1.55 min. MS calculated, 273.00780, found, 272.9719.

*Synthesis of (Z)-5-(dibenzo[b,d]furan-2-ylmethylene)-2-thioxothiazolidin-4-one (**26**).*
Compound **26** was synthesized from 2-thioxothiazolidin-4-one and dibenzo[*b*,*d*]furan-2-carbaldehyde exactly as described for compound **20** and isolated as an off-white solid in 71.1% yield. ^{1}H NMR (600 MHz, D_6-DMSO/TMS) δ 8.31 (s, 1H, H-8), 8.20 (d, J = 7.7 Hz, 1H), 7.83 (d, J = 8.6 Hz, 1H), 7.77 (s, 1H), 7.72 (d, J = 8.5 Hz, 2H), 7.57 (t, J = 7.7 Hz, 1H), 7.44 ppm (t, J = 7.4 Hz, 1H). ^{13}C NMR (600 MHz, D_6-DMSO/TMS) δ 112.36 (C-CH); 113.34(C-CH); 122.18 (C-CH); 123.18 (C-CH); 123.90 (C-CH); 124.20 (C-CH); 125.24 (C-CH); 128.82 (C-CH); 129.06 (C-CH); 130.66 (C-CH); 132.32 (C-CH); 156.81 (CO).UPLC retention time 7.94 min. MS calculated, 311.00747, found, 312.0881.

*Synthesis of (Z)-5-(4-phenoxybenzylidene)-2-thioxothiazolidin-4-one (**27**).*
Compound **27** was synthesized from 2-thioxothiazolidin-4-one and 4-phenoxybenzaldehyde exactly as described for compound **20** and isolated as a yellow solid in 55.9% yield. ^{1}H NMR (600 MHz,) D_6-DMSO/TMS δ 7.62–7.59 (m, 3H), 7.47–7.42 (m, 2H), 7.25–7.07 ppm (m, 5H). ^{13}C NMR (600 MHz, D_6-DMSO/TMS) δ 117.96 (C-CH); 120.19 (C-CH); 124.25 (C-CH); 125.14 (C-CH); 128.12 (C-CH); 130.17 (C-CH); 131.66 (C-CH); 133.23 (C-CH); 155.54 (C-CH); 159.66 (C-CH); 169.84 (CO); 195.96 (CS). UPLC retention time 7.73 min. MS calculated, 314.02312, found, 314.0204.

*Synthesis of (Z)-5-((2,3-dihydrobenzo[b][1,4]dioxin-6-yl)methylene)-2-thioxothiazolidin-4-one (**28**).*
Compound **28** was synthesized from 2-thioxothiazolidin-4-one and 2,3-dihydrobenzo[*b*][1,4]dioxine-6-carbaldehyde exactly as described for compound **20** and isolated as a dark orange solid in 63.8% yield. ^{1}H NMR (600 MHz, D_6-DMSO/TMS) δ 7.52 (s, 1H, H-15), 7.09–7.06 (m, 2H), 7.00 (d, J = 8.5 Hz, 1H), 4.30 ppm (dd, J = 4.5, 17.6 Hz, 4H, H-13, H-14). ^{13}C NMR (600 MHz, D_6-DMSO/TMS) δ 64.46 (CH_2); 65.01 (CH_2); 118.65 (C-CH); 118.67 (C-CH); 119.60 (C-CH); 119.62 (C-CH); 124.84 (C-CH);

124.86 (C-CH); 126.73 (C-CH); 132.22 (C-CH); 132.24 (CO); 144.29 (CS). UPLC retention time 5.83 min. MS calculated, 280.00238, found, 279.9747.

*Synthesis of (Z)-5-((4'-methyl-[1,1'-biphenyl]-3-yl)methylene)-2-thioxothiazolidin-4-one (**29**)*
Compound **29** was synthesized from 2-thioxothiazolidin-4-one and 4'-methyl-[1,1'-biphenyl]-3-carbaldehyde exactly as described for compound **20** and isolated as a dark red-orange solid in 64.3% yield. ^{1}H NMR (600 MHz, D_6-DMSO/TMS) δ 7.80 (s, 1H, H-8), 7.74–7.55 (m, 5H), 7.50 (d, J = 7.7 Hz, 1H), 7.28 (d, J = 7.7 Hz, 2H), 2.35–2.31 ppm (m, 3H, H-21). ^{13}C NMR (600 MHz, D_6-DMSO/TMS) δ 21.15 (CH_3); 126.43 (C-CH); 127.07 (C-CH); 129.09 (C-CH); 129.13 (C-CH); 130.08 (C-CH); 130.17 (C-CH); 130.52 (C-CH); 132.10 (C-CH); 134.14 (C-CH); 136.62 (C-CH); 137.93 (C-CH); 141.59 (C-CH); 169.90 (CO); 196.13 (CS). UPLC retention time 8.34 min. MS calculated, 312.04386, found, 312.0044.

*Synthesis of (Z)-5-((6-chloro-[1,3]dioxolo[4,5-g]quinolin-7-yl)methylene)-2-thioxothiazolidin-4-one (**30**).*
Compound **30** was synthesized from 2-thioxothiazolidin-4-one and 6-chloro-[1,3]dioxolo[4,5-*g*]quinoline-7-carbaldehyde exactly as described for compound **20** and isolated as a dark orange solid in 40.2% yield. ^{1}H NMR (600 MHz, D_6-DMSO/TMS) δ 8.12 (s, 1H), 7.65 (s, 1H), 7.58 (s, 1H), 7.28 (s, 1H), 6.25 ppm (s, 2H, H-18). ^{13}C NMR (600 MHz, D_6-DMSO/TMS) δ 60.73 (CH_2); 72.71 (C-CH); 103.41 (C-CH); 104.05 (C-CH); 104.68 (C-CH); 123.63 (C-CH); 124.49 (C-CH); 125.25 (C-CH); 137.04 (C-CH); 145.98 (C-CH); 148.00 (C-CH); 149.25 (C-CH); 153.55 (CO). UPLC retention time 6.48 min. MS calculated, 350.95866, found, 350.9773.

*Synthesis of (Z)-5-((9H-fluoren-3-yl)methylene)-2-thioxothiazolidin-4-one (**31**).*
Compound **31** was synthesized from 2-thioxothiazolidin-4-one and 9*H*-fluorene-3-carbaldehyde exactly as described for compound **20** and isolated as an orange solid in 72.4% yield. ^{1}H NMR (600 MHz, D_6-DMSO/TMS) δ 8.06–8.03 (m, 1H), 7.97 (s, 1H, H-8), 7.78–7.68 (m, 2H), 7.62 (s, 2H), 7.44–7.36 (m, 2H), 4.00 ppm (s, 2H, H-9). ^{13}C NMR (600 MHz, D_6-DMSO/TMS) δ 36.89 (CH_2); 121.33 (C-CH); 121.41 (C-CH); 125.82 (C-CH); 127.41 (C-CH); 127.56 (C-CH); 128.53 (C-CH); 130.57 (C-CH);131.85 (C-CH); 132.71 (C-CH); 144.21 (C-CH); 144.62 (C-CH); 170.02 (CO). UPLC retention time 8.10 min. MS calculated, 310.02821, found, 309.9631.

*Synthesis of (Z)-2-thioxo-5-((4'-(trifluoromethyl)-[1,1'-biphenyl]-4-yl)methylene)thiazolidin-4-one (**32**).*
Compound **32** was synthesized from 2-thioxothiazolidin-4-one and 4'-(trifluoromethyl)-[1,1'-biphenyl]-4-carbaldehyde exactly as described for compound **20** and isolated as an orange solid in 66.5% yield. ^{1}H NMR (600 MHz, D_6-DMSO/TMS) δ 7.99–7.69 ppm (m, 9H). ^{13}C NMR (600 MHz, D_6-DMSO/TMS) δ 125.95 (CF_3, C-CH); 127.60 (C-CH); 127.79 (C-CH); 127.99 (C-CH)); 130.90 (C-CH); 131.23 (C-CH); 132.12 (C-CH); 140.34 (C-CH); 142.81 (C-CH); 169.36 (CO). UPLC retention time 8.51 min. MS: calculated, 364.3882, found, 364.0916.

*Synthesis of (Z)-5-((4'-methyl-[1,1'-biphenyl]-4-yl)methylene)-2-thioxothiazolidin-4-one (**33**).*
Compound **33** was synthesized from 2-thioxothiazolidin-4-one and 4'-methyl-[1,1'-biphenyl]-4-carbaldehyde exactly as described for compound **20** and isolated as a yellow solid in 77.6% yield. ^{1}H NMR (600 MHz, D_6-DMSO/TMS) δ 7.85–7.81 (m, 2H), 7.68–7.62 (m, 5H), 7.30 (d, J = 7.4 Hz, 2H), 2.34 ppm (s, 3H, H-16). ^{13}C NMR (600 MHz, D_6-DMSO/TMS) δ 20.74 (CH_3); 125.04 (C-CH); 126.67 (C-CH); 127.23(C-CH)); 129.75 (C-CH, C-CH); 131.22 (C-CH); 137.94(C-CH); 142.08 (C-CH); 169.39(CO); 195.54 (CS). UPLC retention time 8.50 min. MS calculated, 310.4170, found, 310.0669.

*Synthesis of (Z)-5-(4-(pyridin-2-yl)benzylidene)-2-thioxothiazolidin-4-one (**34**).*
Compound **34** was synthesized from 2-thioxothiazolidin-4-one and 4-(pyridin-2-yl)benzaldehyde exactly as described for compound **20** and isolated as a yellow solid in 68.8% yield. ^{1}H NMR (600 MHz, D_6-DMSO/TMS) δ 8.69 (d, J = 4.6 Hz, 1H), 8.23 (d, J = 8.2 Hz, 2H), 8.02 (d, J = 8.0 Hz, 1H), 7.90 (t, J = 7.6 Hz, 1H), 7.70–7.65 (m, 3H), 7.41–7.36 ppm (m, 1H). ^{13}C NMR (600 MHz, D_6-DMSO/TMS) δ 121.30 (C-CH); 123.82 (C-CH); 127.81 (C-CH); 131.39 (C-CH); 131.43 (C-CH); 133.92 (C-CH); 137.98 (C-

CH); 140.78 (C-CH); 155.11 (CO). UPLC retention time 5.56 min. MS calculated, 299.02345, found, 298.9749.

*Synthesis of (Z)-2-thioxo-5-((5-(3-(trifluoromethyl)phenyl)furan-2-yl)methylene)thiazolidin-4-one (**35**).* Compound **35** was synthesized from 2-thioxothiazolidin-4-one and 5-(3-(trifluoromethyl)phenyl)furan-2-carbaldehyde exactly as described for compound **20** and isolated as a yellow solid in 69.0% yield. ^{1}H NMR (600 MHz, D_6-DMSO/TMS) δ 8.08 (s, 1H, H-7), 8.03 (d, J = 7.7 Hz, 1H), 7.77–7.70 (m, 2H), 7.47–7.45 (m, 2H), 7.27 ppm (d, J = 3.7 Hz, 1H). ^{13}C NMR (600 MHz, D_6-DMSO/TMS) δ 111.98 (C-CH); 117.46 (C-CH); 121.07 (C-CH); 122.56 (C-CH); 123.35 (C-CH); 125.73 (C-CH); 128.25 (C-CH); 130.03 (C-CH); 130.47 (CF_3); 130.68 (CF_3); 131.03 (C-CH); 150.12 (C-CH); 156.13 (C-CH); 169.37(CO); 196.52 (CS). UPLC retention time 7.69 min. MS calculated, 355.99485, found, 356.0168.

*Synthesis of (Z)-5-((6-methoxynaphthalen-2-yl)methylene)-2-thioxothiazolidin-4-one (**36**).* Compound **36** was synthesized from 2-thioxothiazolidin-4-one and 6-methoxy-2-naphthaldehyde exactly as described for compound **20** and isolated as an orange solid in 68.4% yield. ^{1}H NMR (600 MHz, D_6-DMSO/TMS) δ 8.04 (s, 1H), 7.91 (dd, J = 8.8, 29.0 Hz, 2H), 7.68 (s, 1H, H-8), 7.56 (dd, J = 1.3, 8.6 Hz, 1H), 7.34 (d, J = 1.8 Hz, 1H), 7.22 (dd, J = 2.3, 9.0 Hz, 1H), 3.89 ppm (s, 3H, H-20). ^{13}C NMR (600 MHz, D_6-DMSO/TMS) δ 55.93 (CH_3); 106.687 (C-CH); 120.26 (C-CH); 127.39 (C-CH)); 128.41 (C-CH); 128.70 (); 131.07 (C-CH); 132.04 (C-CH); 132.49 (C-CH); 135.69 (C-CH); 159.66 (CO). UPLC retention time 7.20 min. MS calculated, 302.02312, found, 301.9300.

*Synthesis of (Z)-5-((4'-methyl-[1,1'-biphenyl]-4-yl)methylene)2-thioxothiazolidin-4-one (**37**).* Compound **37** was synthesized from 2-thioxothiazolidin-4-one and 4'-methyl-[1,1'-biphenyl]-4-carbaldehyde exactly as described for compound **20** and isolated as an off-white solid in 50.3% yield. ^{1}H NMR (600 MHz, D_6-DMSO/TMS) δ 11.10–11.07 (m, 1H, H-5), 7.84–7.82 (m, 3H, H-12, H-8, H-6), 7.70 (d, J = 8.2 Hz, 2H, H-11, H-9), 7.66–7.62 (m, 2H, H-18, H- 14), 7.33–7.29 (m, 2H, H-17, H-15), 2.37 ppm (s, 3H, H-19). ^{13}C NMR (600 MHz, D_6-DMSO/TMS) δ 21.18 (CH_3); 123.61 (C-CH); 127.08 (C-CH); 127.54 (C-CH); 130.15 (C-CH); 131.15 (C-CH); 131.85 (C-CH); 132.24 (C-CH); 136.40 (C-CH);138.21 (C-CH); 142.19 (C-CH); 167.82 (CO); 168.26 (CO). UPLC retention time 7.61 min. MS, calculated, 294.3560, found, 294.1762.

*Synthesis of (Z)-5-(4-(benzyloxy)benzylidene)-2-thioxothiazolidin-4-one (**38**).*
Compound **38** was synthesized from 2-thioxothiazolidin-4-one and 4-(benzyloxy)benzaldehyde exactly as described for compound **20** and isolated as a yellow-orange solid in 16.8% yield. ^{1}H NMR (600 MHz, D_6-DMSO/TMS) δ 12.18 (s, 1H, H-5), 7.61–7.58 (m, 3H), 7.50 (d, J = 7.4 Hz, 2H), 7.40 (t, J = 7.6 Hz, 2H), 7.34 (t, J = 7.3 Hz, 1H), 7.23–7.20 (m, 2H), 5.20 ppm (s, 2H, H-16). ^{13}C NMR (600 MHz, D_6-DMSO/TMS) δ 70.06 (CH_2); 116.36 (C-CH); 122.89 (C-CH); 126.17 (C-CH); 128.27 (C-CH); 128.50 (C-CH); 128.96 (C-CH); 132.27 (C-CH); 133.13 (C-CH); 136.92 (C-CH); 160.91 (C-CH); 169.88 (CO); 195.95 (CS). UPLC retention time 8.49 min. MS calculated, 328.03877, found, 328.0041.

*Synthesis of (Z)-2-thioxo-5-(3,4,5-trimethoxybenzylidene)thiazolidin-4-one (**39**).*
Compound **39** was synthesized from 2-thioxothiazolidin-4-one and 3,4,5-trimethoxybenzaldehyde exactly as described for compound **20** and isolated as a dark red-orange solid in 8.3% yield. ^{1}H NMR (600 MHz, D_6-DMSO/TMS) δ 12.21 (d, J = 20.6 Hz, 1H, H-17), 7.57 (s, 1H, H-13), 6.90 (s, 2H, H-2, H-6), 3.92 (s, 6H, H-12, H-10), 3.81 ppm (s, 3H, H-11). ^{13}C NMR (600 MHz, D_6-DMSO/TMS) δ 56.56 (O-CH_3); 60.72 (O-CH_3); 108.51 (C-CH); 128.93 (C-CH); 132.51 (C-CH); 153.78 (CO). UPLC retention time 5.74 min. MS calculated, 312.02860, found, 311.9912.

*Synthesis of (Z)-5-([1,1'-biphenyl]-4-ylmethylene)-2-thioxothiazolidin-4-one (**40**).*
Compound **40** was synthesized from 2-thioxothiazolidin-4-one and [1,1'-biphenyl]-4-carbaldehyde exactly as described for compound **20** and isolated as a dark orange solid in 58.9% yield. ^{1}H NMR (600 MHz, D_6-DMSO/TMS) δ 12.31–12.20 (m, 1H, H-4), 7.88 (d, J = 8.2 Hz, 2H, H-14, H-18), 7.74 (dd, J = 7.9, 18.0 Hz, 4H, H-11, H-9, H-8, H-12), 7.68 (s, 1H, H-6), 7.50 (dd, J = 6.9, 8.2 Hz, 2H, H-17, H-15),

7.42 ppm (t, J = 7.3 Hz, 1H, H-16). ^{13}C NMR (600 MHz, D_6-DMSO/TMS) δ 125.71 (C-CH); 127.22 (C-CH); 127.93 (C-CH); 128.81 (C-CH); 129.59 (C-CH); 131.62 (C-CH); 132.34 (C-CH); 139.11 (C-CH); 142.54 (C-CH); 169.93 (CO); 196.00 (CS). UPLC retention time 7.85 min. MS calculated, 298.3900, found, 297.9619.

*Synthesis of (Z)-2-thioxo-5-(2-(trifluoromethyl)benzylidene)thiazolidin-4-one (**41**).*
Compound **41** was synthesized from 2-thioxothiazolidin-4-one and 2-(trifluoromethyl)benzaldehyde exactly as described for compound **20** and isolated as a an off-white solid in 60.7% yield. ^{1}H NMR (600 MHz, D_6-DMSO/TMS) δ 12.41 (s, 1H, H-15), 7.92–7.81 (m, 3H, H-5, H-3, H-2), 7.76–7.69 ppm (m, 2H, H-6, H-4). ^{13}C NMR (600 MHz, D_6-DMSO/TMS) δ 123.39 (C-CH); 125.21 (C-CH); 125.90 (C-CH); 127.02 (C-CH); 127.29 (C-CH); 127.33 (C-CH); 127.37(C-CH); 128.03 (CF_3); 128.23 (CF_3); 128.42 (CF_3); 128.62 (CF_3); 129.77 (C-CH); 131.04 (C-CH); 131.35 (C-CH); 131.67 (C-CH); 133.96 (C-CH), 169.27 (CO); 196.06 (CS). UPLC retention time 6.68 min. MS calculated, 287.98429, found, 288.0781.

*Synthesis of (Z)-2-thioxo-5-(2-(trifluoromethoxy)benzylidene)thiazolidin-4-one (**42**).*
Compound **42** was synthesized from 3-methyl-2-thioxothiazolidin-4-one and 4'-methoxy-[1,1'-biphenyl]-4-carbaldehyde exactly as described for compound **20** and isolated as a an off-white solid in 70.6% yield. ^{1}H NMR (600 MHz, D_6-DMSO/TMS) δ 12.40 (s, 1H, H-14), 7.76 (s, 1H, H-6), 7.70–7.59 (m, 3H, H-10, H-11, H-12), 7.53 ppm (d, J = 8.3 Hz, 1H, H-9). ^{13}C NMR (600 MHz, D_6-DMSO/TMS) δ 122.29 (C-CH); 123.06 (C-CH); 126.62 (C-CH); 128.96 (C-CH); 129.83 (C-CH); 129.88 (C-CH); 132.94 (C-CH); 147.50 (C-CH); 169.56 (CO); 195.80 (CS). UPLC retention time 6.93 min. MS calculated, 304.2892, measured 304.0848.

Synthesis of (Z)-3-methyl-5-((4'-methyl-[1,1'-biphenyl]-4-yl)methylene)-2-thioxothiazolidin-4-one *(**43**)*.
Compound **43** was synthesized from 4'-methyl-[1,1'-biphenyl]-4-carbaldehyde exactly as described for compound **24** and isolated as a yellow solid in 30.1% yield. 1H NMR (600 MHz, D_6-acetone): δ 7.88–7.85 (m, 2H, H-11, H-15), 7.80 (s, 1H, H-9), 7.72 (d, J = 8.2 Hz, 2H, H-14, H-12), 7.66–7.64 (m, 2H, H-21, H-17), 7.32 (d, J = 8.0 Hz, 2H, H-20, H-18), 3.49 (s, 3H, H-8), 2.38 ppm (s, 3H, H-22). ^{13}C NMR (600 MHz, D_6-DMSO/TMS) δ 21.20 (CH_3); 31.68 (CH_3); 127.15 (C-CH); 127.43 (C-CH); 130.21 (C-CH); 131.84 (C-CH); 132.22 (C-CH); 132.87 (C-CH); 138.42 (C-CH). UPLC retention time 9.49min. MS calculated, 326.4440, measured 326.0348.

*Synthesis of (Z)-2-(5-((4'-methyl-[1,1'-biphenyl]-4-yl)methylene)-4-oxo-2-thioxothiazolidin-3-yl)acetic acid (**44**).*
Compound **44** was synthesized from 4'-methyl-[1,1'-biphenyl]-4-carbaldehyde exactly as described from compound **24** and isolated as a yellow solid. 1H NMR (600 MHz, D_6-Acetone): δ 7.89–7.85 (m, 3H, H-11, H-15, H-9), 7.75 (d, J = 8.2 Hz, 2H, H-12, H-14), 7.67–7.65 (m, 2H, H-17, H-21), 7.32 (d, J = 7.8 Hz, 2H, H-18, H-20), 4.85 (s, 2H, H-8), 2.38 ppm (s, 3H, H-22). ^{13}C NMR (600 MHz, D_6-DMSO/TMS) δ 47.05 (CH_3); 127.14 (C-CH); 127.71 (C-CH); 130.18 (C-CH); 131.85 (C-CH); 132.16 (C-CH); 133.16 (C-CH); 136.26 (C-CH); 138.39 (C-CH);142.72 (C-CH); 167.09 (CO); 167.59 (COOH); 193.50 (CS). UPLC retention time 8.20 min. MS calculated, 368.4530, measured 368.2621.

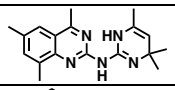
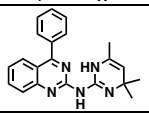
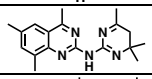
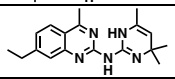
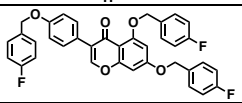
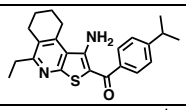
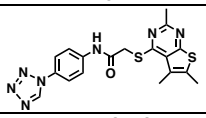
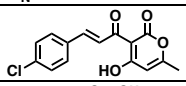
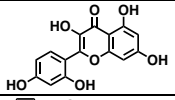
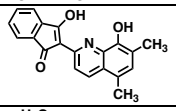
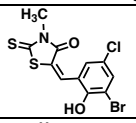
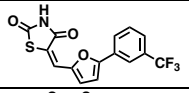
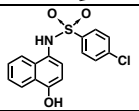
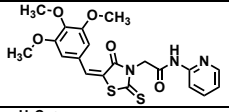
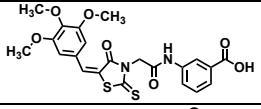
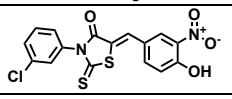
*Synthesis of (Z)-5-((4'-methoxy-[1,1'-biphenyl]-4-yl)methylene)-2-thioxothiazolidin-4-one (**45**).*
Compound **45** was synthesized from 4'-methoxy-[1,1'-biphenyl]-4-carbaldehyde exactly as described from compound **24** and isolated as an orange solid. 1H NMR (600 MHz, D_6-DMSO): δ 7.81 (d, J = 8.2 Hz, 2H), 7.73–7.63 (m, 5H), 7.05 (d, J = 8.6 Hz, 2H), 3.80 ppm (s, 3H, H-22). ^{13}C NMR (600 MHz, D_6-DMSO/TMS) δ 55.72 (O-CH_3); 115.05 (C-CH); 127.30 (C-CH); 128.49 (C-CH); 131.18 (C-CH); 131.47 (C-CH); 131.60 (C-CH); 131.88 (C-CH); 142.10 (C-CH); 160.09 (CO). UPLC retention time 7.69min. MS calculated, 328.03877, measured 328.0452.

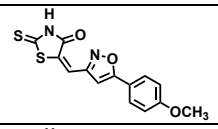
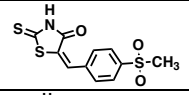
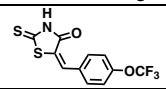
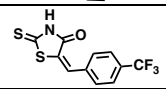
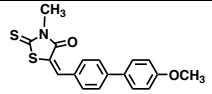
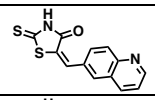
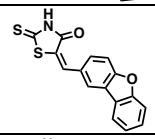
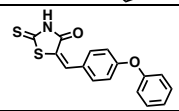
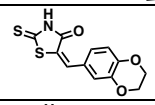
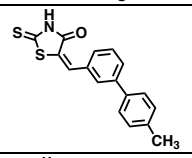
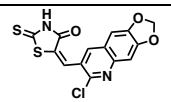
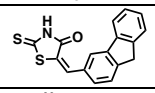
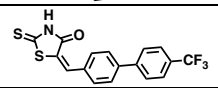
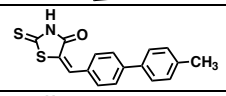
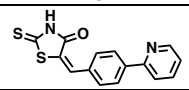
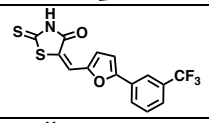
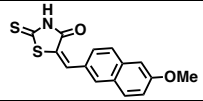
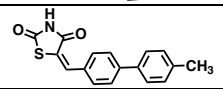
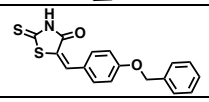
*Synthesis of (Z)-5-((4'-(trifluoromethyl)-[1,1'-biphenyl]-4-yl)methylene)-2-thioxothiazolidin-4-one (**46**).*
Compound **46** was synthesized from 4'-(trifluoromethyl)-[1,1'-biphenyl]-4-carbaldehyde exactly as described from compound **24** and isolated as an off white solid. 1H NMR (600 MHz, D_6-DMSO): δ 7.94 (dd, J = 8.3, 28.4 Hz, 4H), 7.85–7.82 (m, 3H), 7.74–7.71 ppm (m, 2H). ^{13}C NMR (600 MHz, D_6-

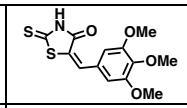
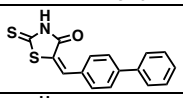
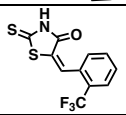
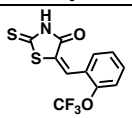
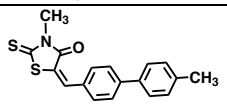
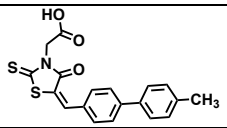
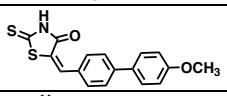
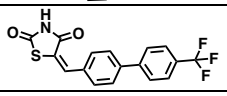
DMSO/TMS) δ 124.57 (C-CH); 126.33 (C-CH); 128.07 (C-CH); 128.26 (C-CH); 131.17 (C-CH); 131.45 (C-CH); 133.55 (C-CH); 140.46 (C-CH); 143.31 (C-CH); 167.76 (CO); 168.17 (CO). UPLC retention time 7.69 min. MS calculated, 349.03843, measured 342.0713.

Physicochemical Properties

Table S1. Structures of CD38 Inhibitors and their Activity Against CD38 Cyclase

Compound	Structure	MW	CLogP	tPSA	pKa*
1		309.42	2.871	61.14	4.7, 4.8, 7.1, 11.4, 11.9
2		343.43	3.472	61.14	4.4, 4.6, 7.1, 11.1, 11.3
3		309.42	2.105	61.47	4.8, 5.0, 7.0, 7.9, 11.0
4		309.42	2.901	61.14	4.6, 5.1, 7.2, 11.4, 11.8
5		594.59	8.470	53.99	--
6		378.53	6.173	55.45	5.3, 7.1
7		411.50	2.062	94.14	1.9, 2.2, 3.0, 12.1
8		290.70	2.515	63.60	5.1
9		302.24	0.445	127.45	6.0, 6.2, 6.3, 6.4, 6.4
10		317.34	2.851	69.89	4.0, 4.4, 6.5
11		364.66	2.767	40.54	2.0, 6.0
12		333.29	3.869	55.40	7.3
13		333.79	3.800	72.06	8.1, 8.8
14		445.51	0.388	89.46	1.9, 3.2, 12.3
15		488.53	1.628	114.40	1.8, 4.1, 13.1
16		392.83	3.836	92.35	5.4

20		318.37	1.798	59.92	6.5
21		299.38	0.161	68.9	7.5
22		309.25	2.83	38.33	7.5
23		289.29	2.685	29.10	7.5
24		341.44	3.945	29.54	2.0
25		272.34	1.689	41.46	3.8, 6.4
26		311.37	3.746	38.33	7.7
27		313.39	3.9	38.33	7.7
28		279.33	1.556	47.56	7.6
29		311.43	1.556	47.56	7.5
30		350.79	2.197	59.92	1.6, 6.2
31		309.40	3.735	29.1	7.8
32		365.39	4.573	29.1	7.7
33		311.42	4.189	29.1	7.7
34		298.38	2.403	41.46	4.3, 7.6
35		355.35	3.959	38.33	7.3
36		301.38	2.895	38.33	7.5
37		295.36	4.099	46.17	7.5
38		327.42	3.489	38.33	7.7

39		311.37	0.859	56.79	7.3
40		297.39	3.69	29.1	7.7
41		289.29	2.685	29.1	7.5
42		305.29	2.83	38.33	7.3
43		325.44	4.525	20.31	2.0
44		369.45	3.815	57.61	1.8, 3.7
45		327.42	3.609	38.33	7.7
46		349.33	4.483	46.17	7.5

cLogP and tPSA values are estimated using ChemDraw 20.0; pKa values were estimated using the MolGpKa software routine: https://xundrug.cn/molgpka (J. *Chem. Inf. Modeling* **2021**, *67 (7),* 3159-3165).

Enzyme Assay

CD38 cyclase activity. Compounds were screened for the ability to inhibit the cyclase activity of recombinant human CD38 in a fluorometric assay. In brief, recombinant CD38 was diluted to a working concentration of 40 nM (4x) in assay diluent (PBS, 0.002% Tween-20, pH7.4) and 25 µL were pipetted into a black 96 well plate. Screening compounds were diluted using assay diluent to 4x the desired screening concentration and 25 µL of this mixture was added to each wells. DMSO was screened as a vehicle control. After 15 mins incubation on an orbital shaker, 50 µL of a 50 µM solution of NGD^+ (2x) was added to each well, initiating the reaction. The final concentration of CD38 and NGD^+ in the reaction are, 10 nM and 25 µM respectively. With an excitation at 300nm and 410nm emission, the reaction was monitored for 10 mins. Initial rates (velocities) were calculated by determining the slope over the first 5 mins. Mean fluorescence for the vehicle treated control was used to normalize each treatment group, and values were expressed as percent activity of CD38. Each assay was conducted in at least technical duplicates and experimental triplicates and compared to the literature described CD38 cyclase inhibitor quercetin (Q).

CD38 hydrolase activity. The hydrolase screening assay was conducted using the same procedure as the cyclase screen, substituting 20µM ε-NAD^+ working solution for NGD^+, resulting in a final concentration of 10µM. Initial rates were calculated for the first 2.5mins.

Dose dependence and kinetic mechanism of inhibition. Selected hit compounds were assayed for dose dependent inhibition of CD38 cyclase using the general workflow described above at concentrations between 0 and 100 µM. Serial dilutions of each compound were adjusted to establish an eight-point concentration curve. Likewise, Michalis-Menton enzyme kinetics were assessed by varying substrate (8-point curve) and compound concentrations. All enzyme reactions were kept at a standard ratio of CD38/compound/substrate (4x/4x/2x). Data from each experiment was collected in technical and experimental triplicates.

Cell Culture

Primary culture. All PBMC and T cells were cultured in accordance with the Stem Cell Technology T-cell Expansion Protocol. In brief, for expansion of T cells in PBMC cultures, an initial culture was seeded at 1 X 10^6 cells/mL in ImmunoCult XF expansion media with 3-10 ng/mL of IL-2 (complete media). The culture was diluted 4- to 8-fold every 2 to 3 days with complete media.

T cell activation. PBMCs were cultured as above with the addition of 20 μL/mL of anti-CD3/CD38 tetramer on day 0. Activated T cell cultures were maintained for 14 days on average. For re-stimulation challenges, 20 μL/mL of anti-CD3/CD28 was added to activated T cells (day 9-12).

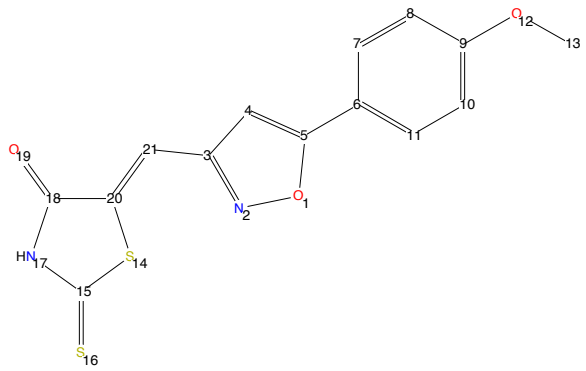
PBMC toxicity. Cytotoxicity of CD38 hit inhibitors were assessed against T cell activated PBMCs. After a 48 hr treatment, cell viability was assessed using CellTiter-Glo (Promega), with all experiments performed according to the manufacturers directions. Viability was assessed in three separate donors. Experiments were conducted in triplicates and mean values normalized to vehicle treated controls.

Cytokine Analysis (Interferon-γ). T cells were activated and cultured as described above for 12 days. Secreted cytokines were measured in the supernatants from T cells by ELISA (Biolegend). For acute T cell activity and screening of CD38 inhibitors, supernatants were analyzed 48 hrs post-activation. Supernatants were also collected on day 14, 48 hrs after restimulation of T cell cultures to assess effects of CD38 inhibitors in a re-challenge/expansion model. Initial interferon-γ screens were conducted with a single donor in triplicate and results recorded as percent difference from vehicle treated control. Screening of novel CD38 inhibitors was conducted with three donors and presented as mean percent difference from vehicle treated control.

Cellular NADH levels. Cellular NADH levels were measured using the NAD-Glo kit (Promega)— with all experiments performed according to the manufacturers directions. In short, NADH was measured in resting PBMCs, and PBMCs 30 and 60 mins after activation.

CMC-assist

CMM210212 **TZB-001**



Consistency: Unknown*, unknown purity*

Data set 1H: CMM210212 1 1 /opt/topspin4.1.3
Structure: /opt/topspin4.1.3/CMM210212/1/structure.mol
Acquisition date: February 12, 2021 9:08:39 AM EST
Solvent: DMSO
Probe: 5 mm PATXI 1H/D/19F-13C/15N Z-GRD Z855801/0017
Eretic reference:

Sum formula: $C_{14}H_{10}N_2O_3S_2$

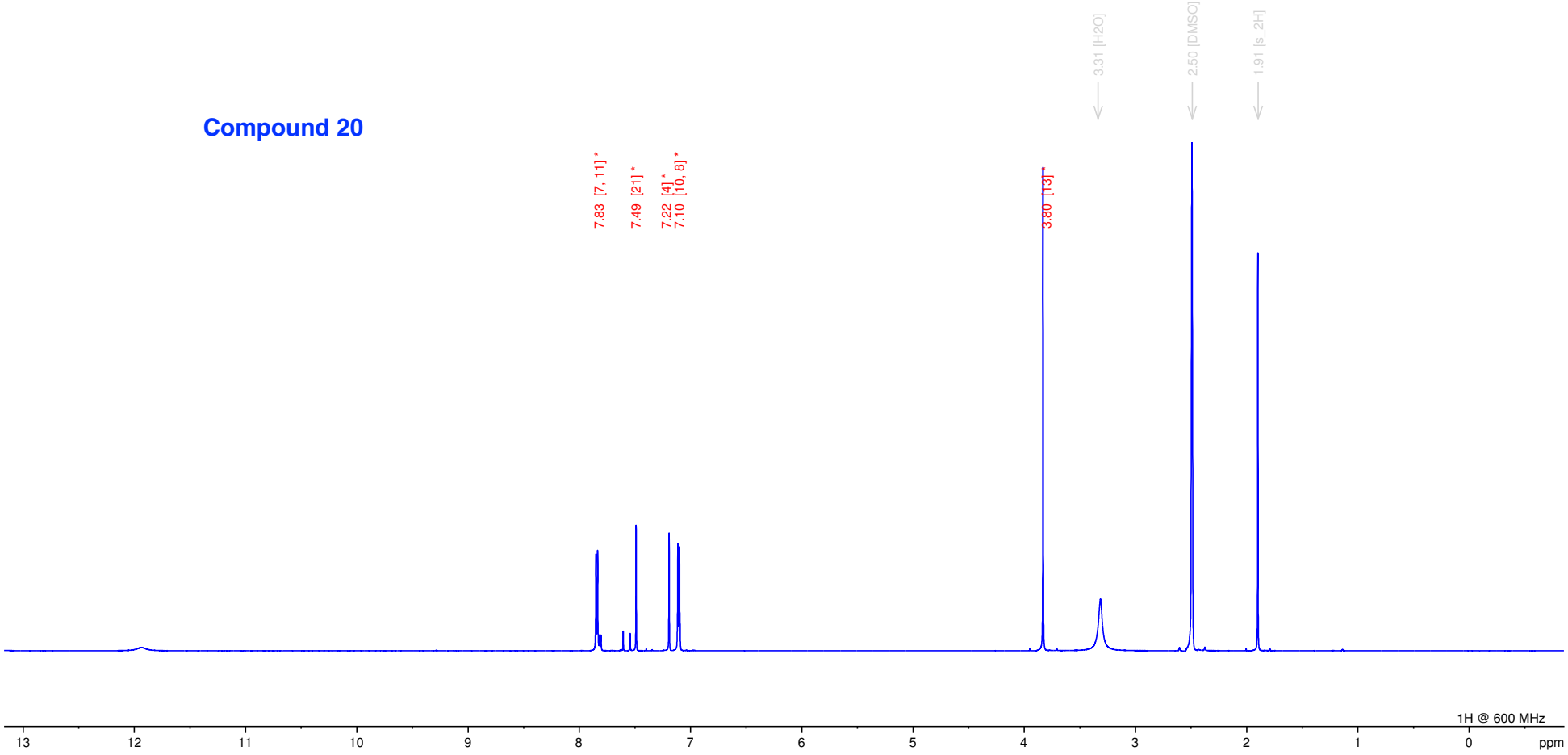
Molecular Mass: 318.01 Da

Comments:
Multiplet interpretation available for spectrum.
A multiplet interpretation for all major signals in the spectrum could be found. All given impurities could be assigned to regions in the spectrum.

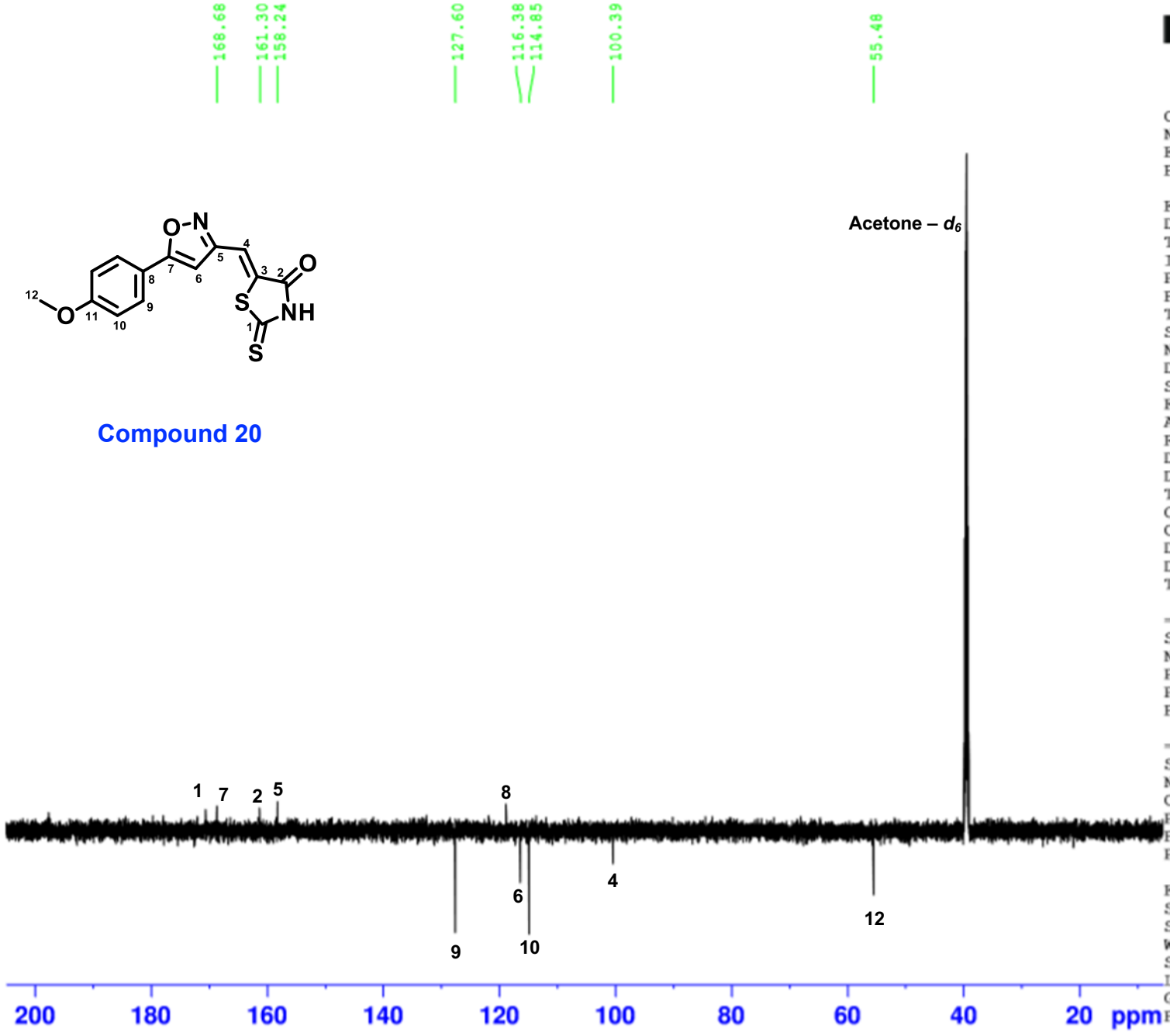
Signature:

Automatic analysis generated by Bruker CMC (b:17).
One or more results have not been created by automatic analysis, or edited manually: marked by '*'.
Report generated by Bruker CMC-assist TopSpin 4.1.3 (of 2021-06-28 13:00:50), on 'MacBook-Pro.local' as 'tzbenton'

Compound 20



103dx-001

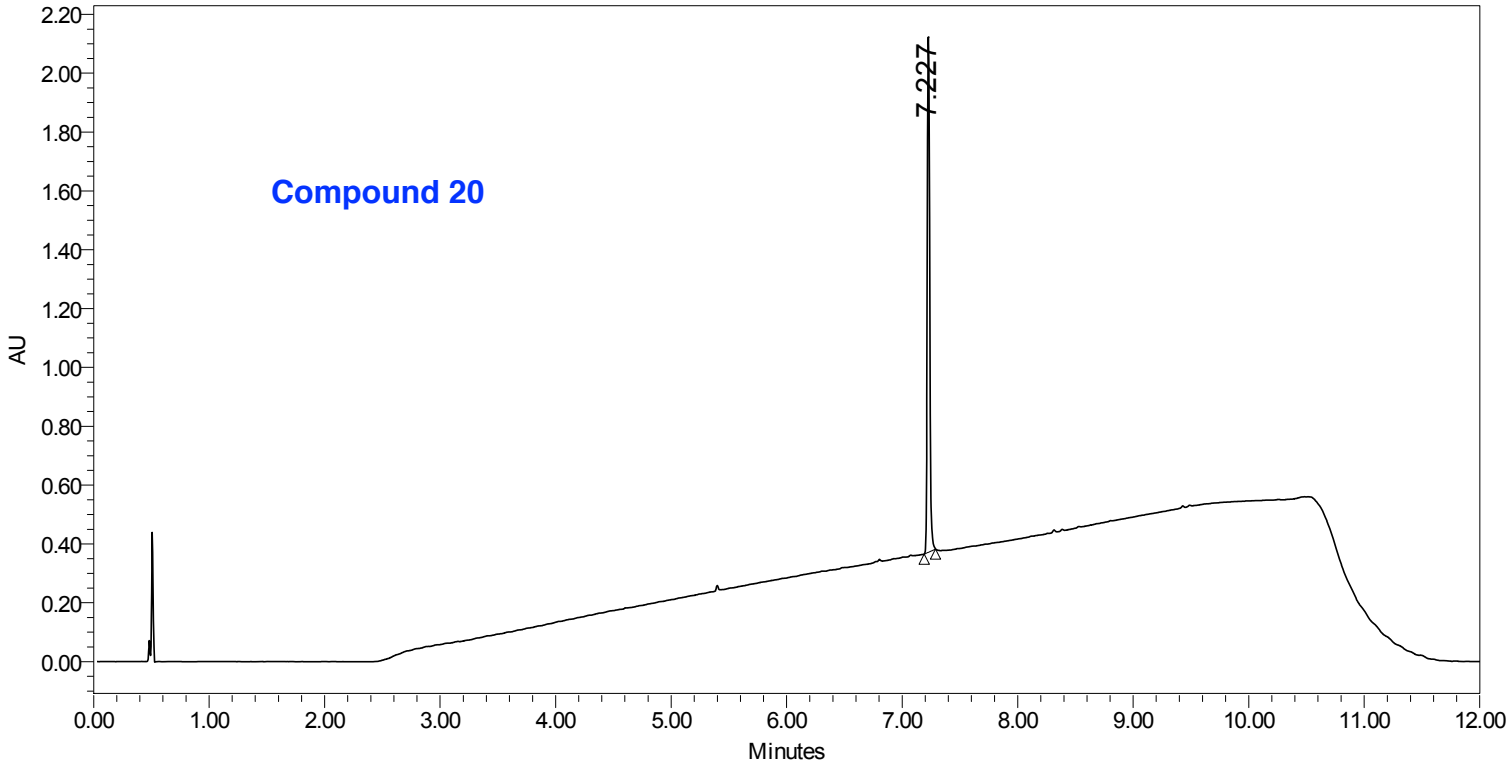


Compound 20

```
Current Data Parameters
NAME                 CMM210913
EXPNO                        3
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20210913
Time                     14.10
INSTRUM                  spect
PROBHD     5 mm PATXI 1H/
PULPROG                  jmod
TD                      65536
SOLVENT                Acetone
NS                        2000
DS                           4
SWH                  36057.691 Hz
FIDRES                0.550197 Hz
AQ                    0.9087659 sec
RG                        2050
DW                      13.867 usec
DE                        6.50 usec
TE                       301.5 K
CNST2                145.0000000
CNST11                 1.0000000
D1                     2.00000000 sec
D20                    0.00689655 sec
TD0                          1

======== CHANNEL f1 ========
SFO1                150.9178988 MHz
NUC1                        13C
P1                        11.80 usec
P2                        23.60 usec
PLW1               202.10000610 W

======== CHANNEL f2 ========
SFO2                600.1324005 MHz
NUC2                        1H
CPDPRG[2                waltz16
PCPD2                     70.00 usec
PLW2                13.69999981 W
PLW12                0.17449000 W

F2 - Processing parameters
SI                        32768
SF                  150.9028090 MHz
WDW                          EM
SSB                 0
LB                        1.00 Hz
GB                  0
PC                        1.40
```

SAMPLE INFORMATION

Sample Name:	2021Feb05_TZB103dx_001	Acquired By:	System
Sample Type:	Unknown	Sample Set Name	TZB_103dx
Vial:	1:C,1	Acq. Method Set:	ReversePhase_12min_Max Plot
Injection #:	1	Processing Methoc	ReversePhase_Purity_MAX Plot
Injection Volume:	1.00 ul	Channel Name:	PDA Max Plot 190.0 - 800.0
Run Time:	12.0 Minutes	Proc. Chnl. Descr.:	PDA MaxPlot (190.0 nm to 800.0
Date Acquired:	2/5/2021 3:00:30 PM EST		
Date Processed:	8/31/2021 3:48:20 PM EDT		

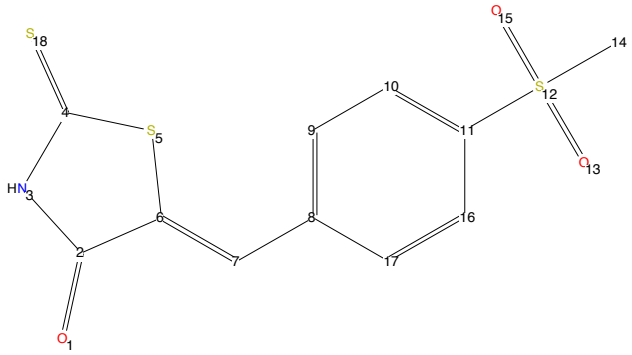


	RT	Area	% Area	Height	Peak Lambda Max.
1	7.227	2581126	100.00	1751520	358.9

CMC-assist

CMM210212 **TZB-002**

Consistency: Unknown*, unknown purity*



Data set 1H: CMM210212 5 1 /opt/topspin4.1.3
Structure: /opt/topspin4.1.3/CMM210212/5/structure.mol
Acquisition date: February 12, 2021 9:26:26 AM EST
Solvent: DMSO
Probe: 5 mm PATXI 1H/D/19F-13C/15N Z-GRD Z855801/0017
Eretic reference:

Sum formula: $C_{11}H_9NO_3S_3$

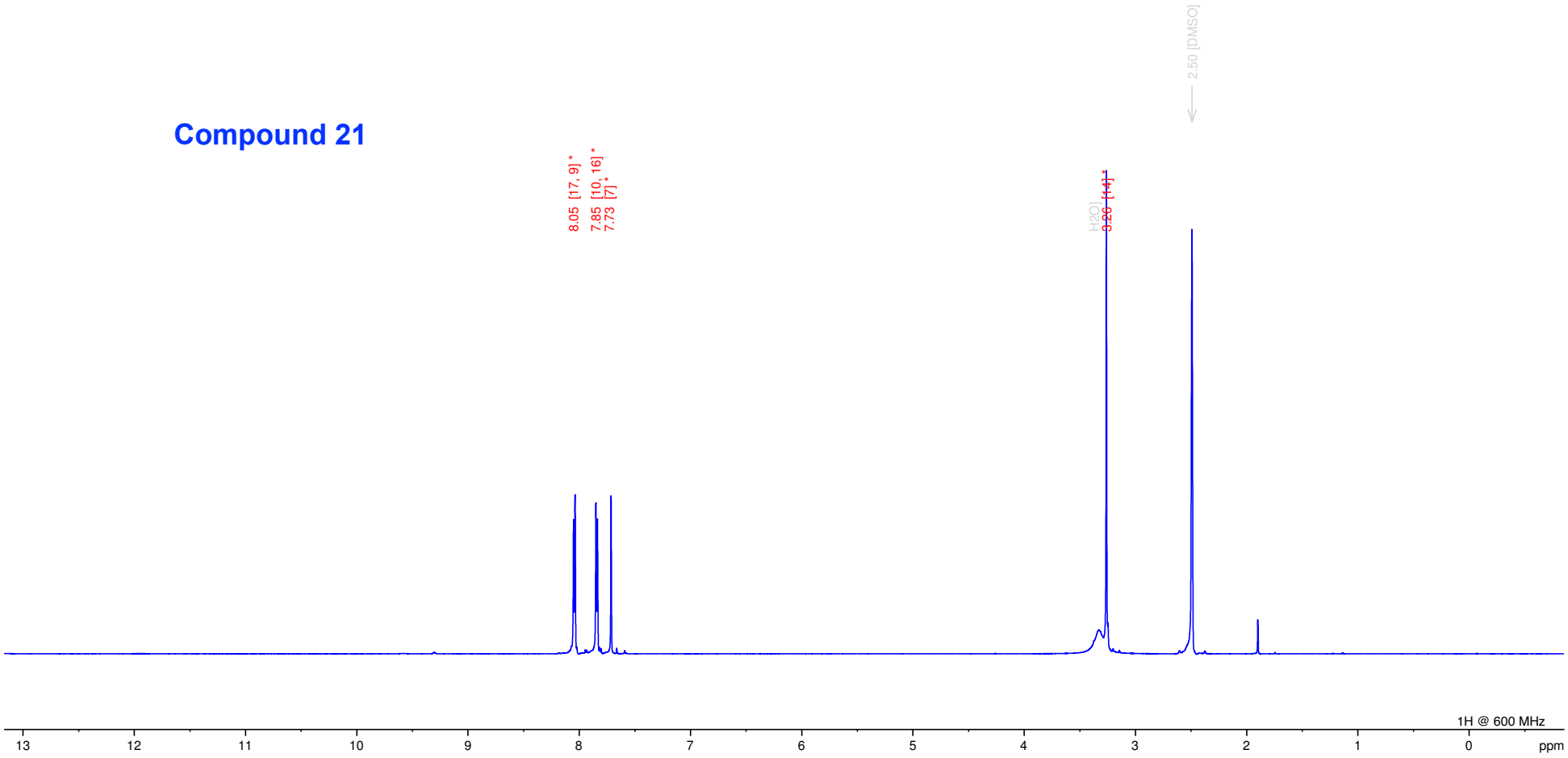
Molecular Mass: 298.97 Da

Comments:
Multiplet interpretation available for spectrum.
A multiplet interpretation for all major signals in the spectrum could be found. All given impurities could be assigned to regions in the spectrum.

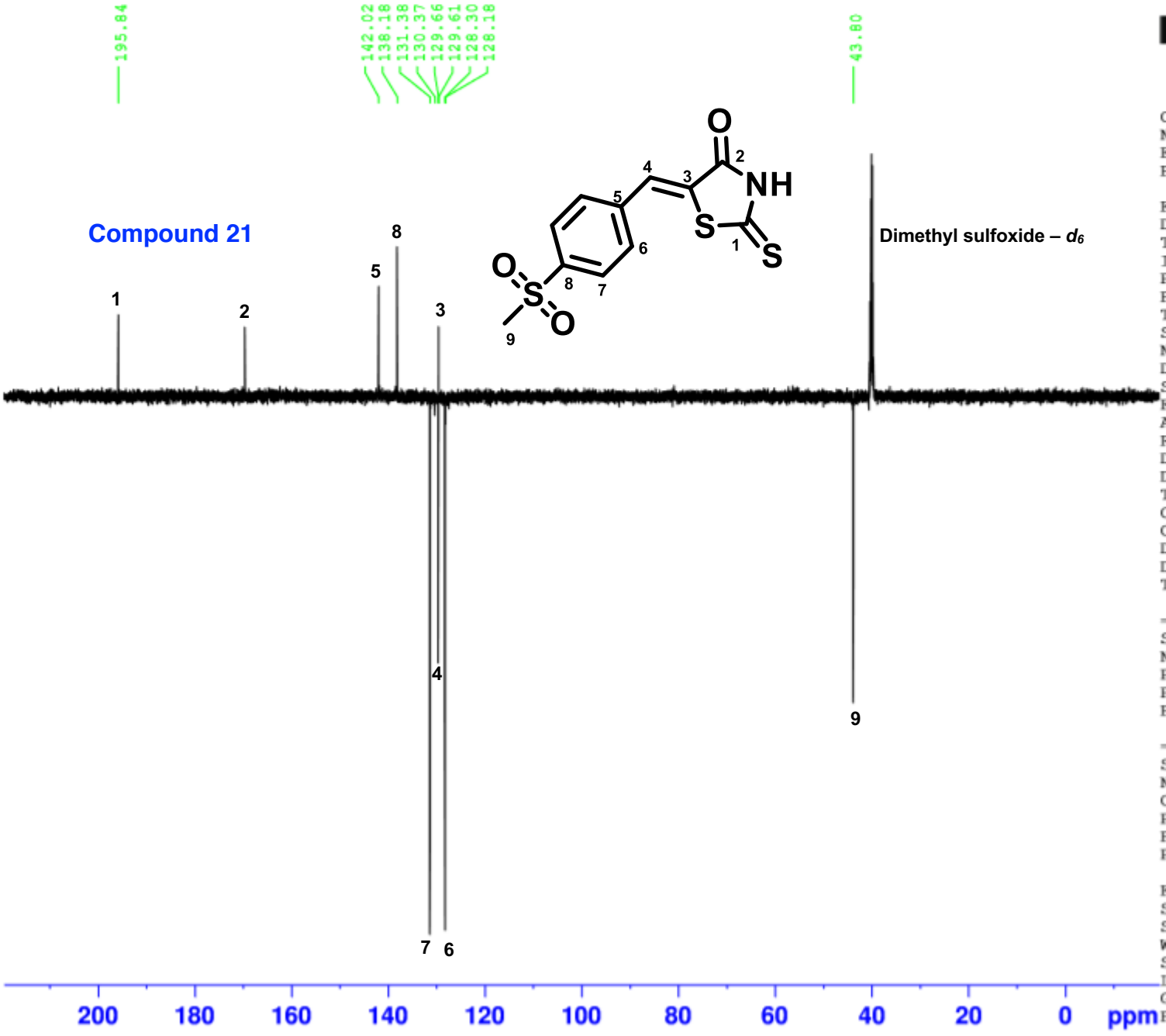
Signature:

Automatic analysis generated by Bruker CMC (b:17).
One or more results have not been created by automatic analysis, or edited manually: marked by '*'.
Report generated by Bruker CMC-assist TopSpin 4.1.3 (of 2021-06-28 13:00:50), on 'MacBook-Pro.local' as 'tzbenton'

Compound 21



21 (TZB103dx-002)

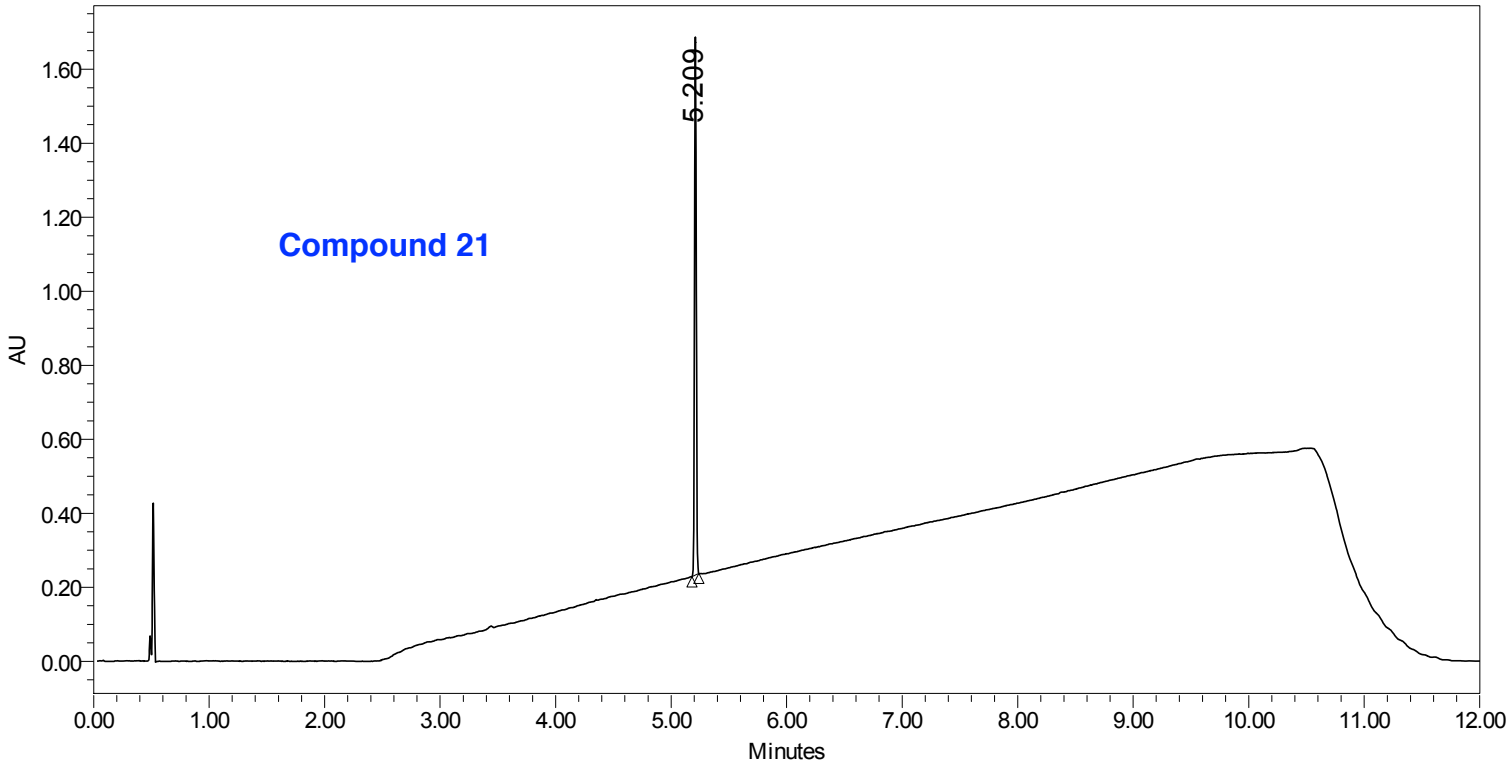


BRUKER

```
Current Data Parameters
NAME                  CMM210917
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20210917
Time                       8.38
INSTRUM                   spect
PROBHD    5 mm PATXI 1H/
PULPROG                   jmod
TD                       65536
SOLVENT                   DMSO
NS                        1000
DS                           4
SWH                  36057.691 Hz
FIDRES                0.550197 Hz
AQ                    0.9087659 sec
RG                         2050
DW                       13.867 usec
DE                         6.50 usec
TE                        301.4 K
CNST2                145.0000000
CNST11                 1.0000000
D1                     2.00000000 sec
D20                    0.00689655 sec
TD0                           1

======== CHANNEL f1 ========
SFO1                150.9178988 MHz
NUC1                        13C
P1                        11.80 usec
P2                        23.60 usec
PLW1               202.10000610 W

======== CHANNEL f2 ========
SFO2                600.1324005 MHz
NUC2                        1H
CPDPRG[2                waltz16
PCPD2                     70.00 usec
PLW2                13.69999981 W
PLW12                0.17449000 W

F2 - Processing parameters
SI                         32768
SF                  150.9028090 MHz
WDW                           EM
SSB                0
LB                         1.00 Hz
GB                 0
PC                         1.40
```

SAMPLE INFORMATION

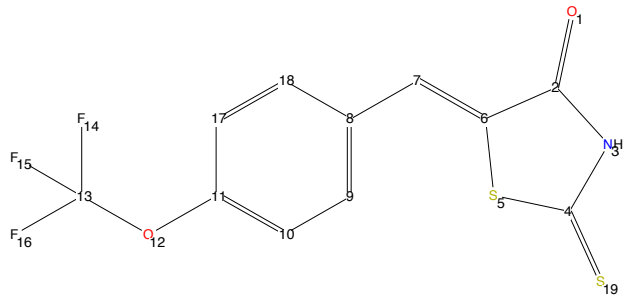
Sample Name:	2021Feb08_TZB103dx_004	Acquired By:	System
Sample Type:	Unknown	Sample Set Name	TZB_103dx
Vial:	1:F,6	Acq. Method Set:	ReversePhase_12min_Max Plot
Injection #:	1	Processing Methoc	ReversePhase_Purity_MAX Plot
Injection Volume:	1.00 ul	Channel Name:	PDA Max Plot 190.0 - 800.0
Run Time:	12.0 Minutes	Proc. Chnl. Descr.:	PDA MaxPlot (190.0 nm to 800.0
Date Acquired:	2/8/2021 3:10:01 PM EST		
Date Processed:	2/8/2021 4:03:43 PM EST		



	RT	Area	% Area	Height	Peak Lambda Max.
1	5.209	1617665	100.00	1457785	373.8

CMC-assist

CMM210212 **TZB-004**



Consistency: Unknown*, unknown purity*

Sum formula: $C_{11}H_6F_3NO_2S_2$

Molecular Mass: 304.98 Da

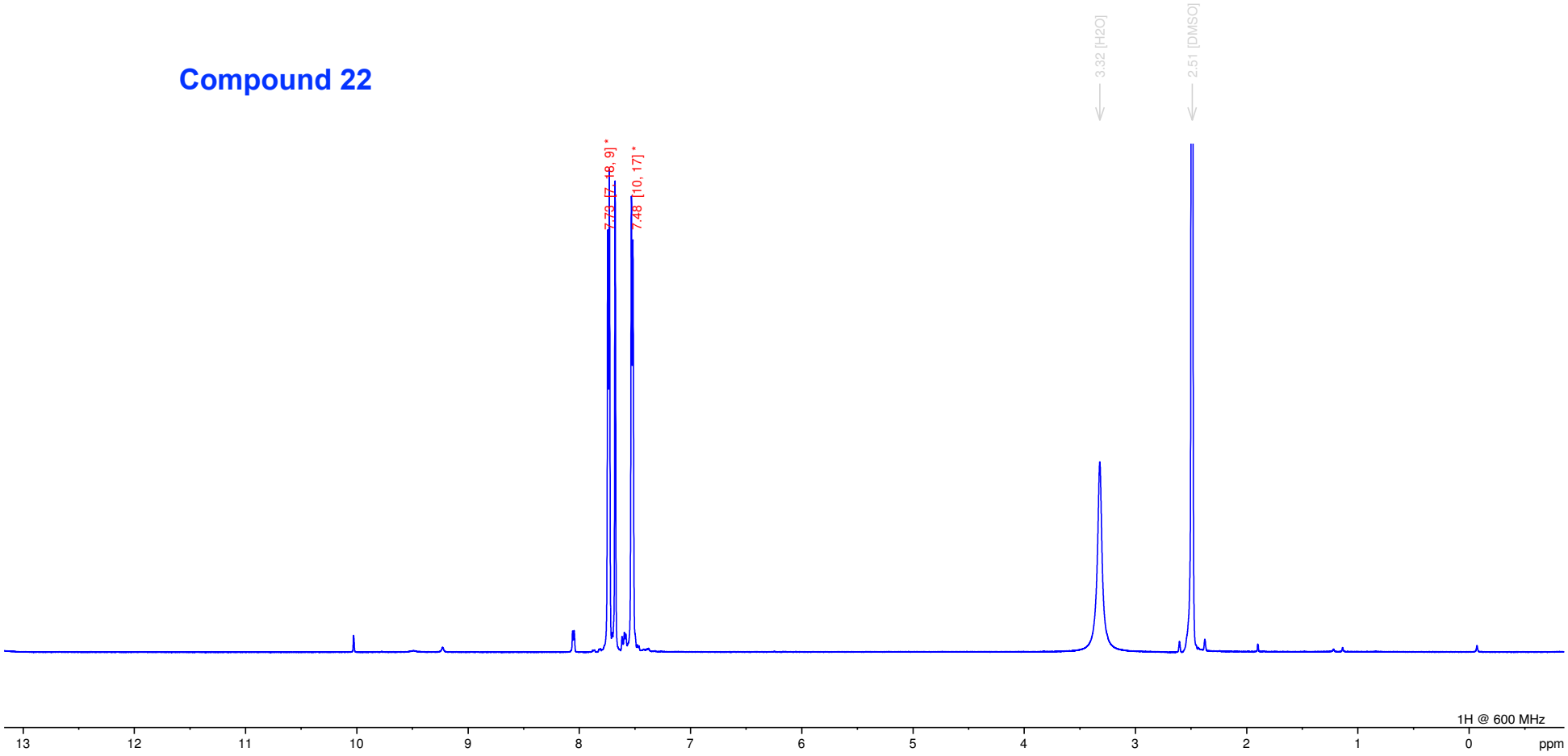
Data set 1H: CMM210212 6 1 /opt/topspin4.1.3
Structure: /opt/topspin4.1.3/CMM210212/6/structure.mol
Acquisition date: February 12, 2021 9:30:28 AM EST
Solvent: DMSO
Probe: 5 mm PATXI 1H/D/19F-13C/15N Z-GRD Z855801/0017
Eretic reference:

Comments:
Multiplet interpretation available for spectrum.
A multiplet interpretation for all major signals in the spectrum could be found. All given impurities could be assigned to regions in the spectrum.

Signature:

Automatic analysis generated by Bruker CMC (b:17).
One or more results have not been created by automatic analysis, or edited manually: marked by '*'.
Report generated by Bruker CMC-assist TopSpin 4.1.3 (of 2021-06-28 13:00:50), on 'MacBook-Pro.local' as 'tzbenton'

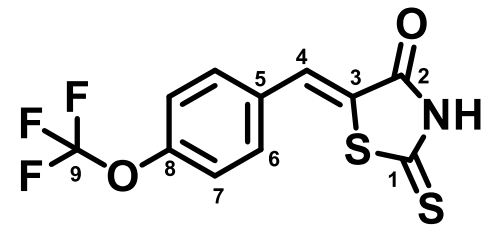
Compound 22



22 (TZB103dx-004)

195.89 169.71 149.76 132.90 132.63 131.73 130.32 127.16 122.07

Compound 22



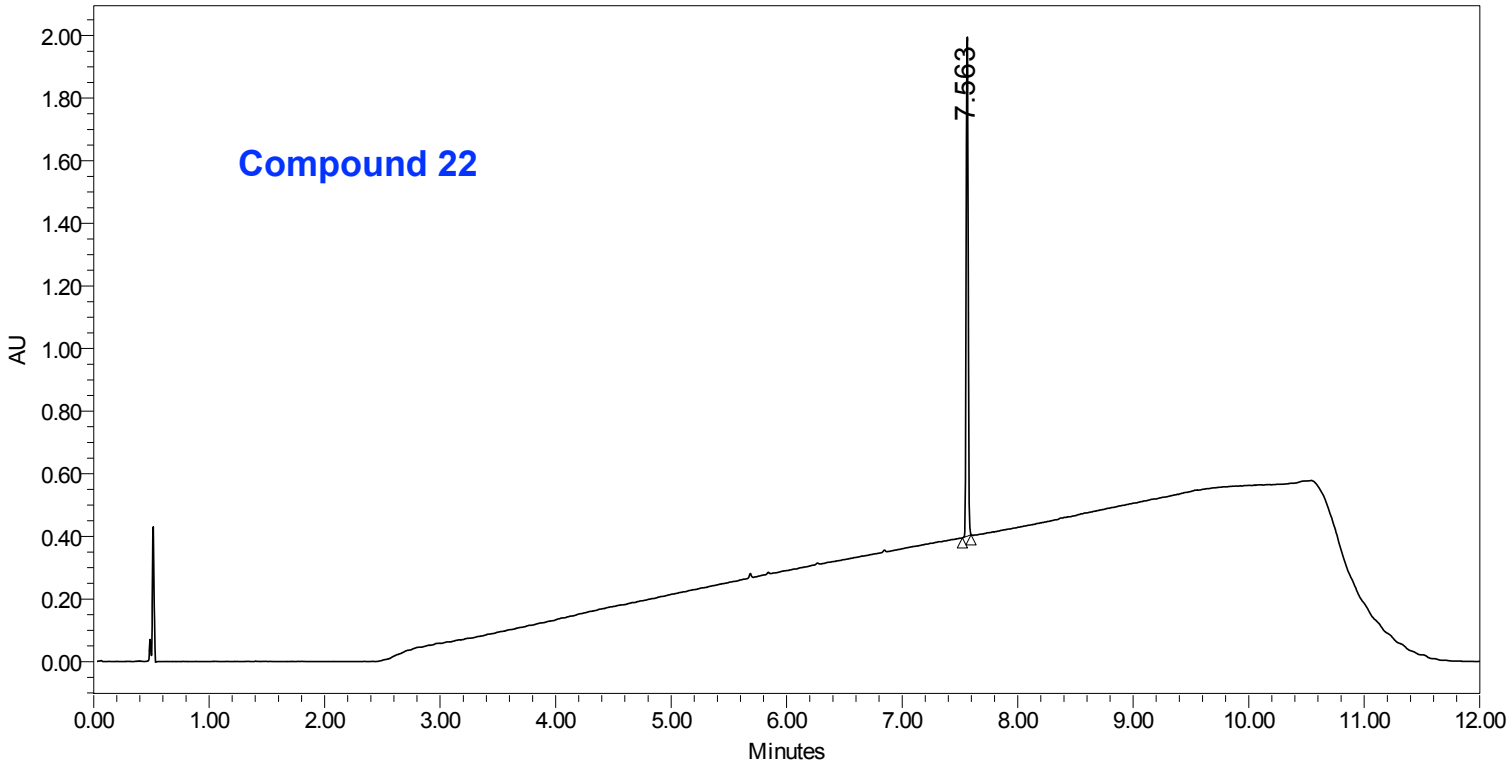
Dimethyl sulfoxide – d_6

BRUKER

```
Current Data Parameters
NAME                  CMM210917
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20210917
Time                       9.34
INSTRUM                   spect
PROBHD     5 mm PATXI 1H/
PULPROG                   jmod
TD                       65536
SOLVENT                   DMSO
NS                        1000
DS                           4
SWH                36057.691 Hz
FIDRES             0.550197 Hz
AQ                 0.9087659 sec
RG                        2050
DW                   13.867 usec
DE                    6.50 usec
TE                    301.3 K
CNST2              145.0000000
CNST11               1.0000000
D1                 2.00000000 sec
D20                0.00689655 sec
TD0                           1

======== CHANNEL f1 ========
SFO1               150.9178988 MHz
NUC1                       13C
P1                    11.80 usec
P2                    23.60 usec
PLW1            202.10000610 W

======== CHANNEL f2 ========
SFO2               600.1324005 MHz
NUC2                       1H
CPDPRG[2                waltz16
PCPD2                 70.00 usec
PLW2             13.69999981 W
PLW12             0.17449000 W

F2 - Processing parameters
SI                        32768
SF                 150.9028090 MHz
WDW                          EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

SAMPLE INFORMATION

Sample Name:	2021Feb08_TZB103dx_004	Acquired By:	System
Sample Type:	Unknown	Sample Set Name	TZB_103dx
Vial:	1:F,4	Acq. Method Set:	ReversePhase_12min_Max Plot
Injection #:	1	Processing Methoc	ReversePhase_Purity_MAX Plot
Injection Volume:	1.00 ul	Channel Name:	PDA Max Plot 190.0 - 800.0
Run Time:	12.0 Minutes	Proc. Chnl. Descr.:	PDA MaxPlot (190.0 nm to 800.0
Date Acquired:	2/8/2021 2:44:46 PM EST		
Date Processed:	8/31/2021 3:51:55 PM EDT		

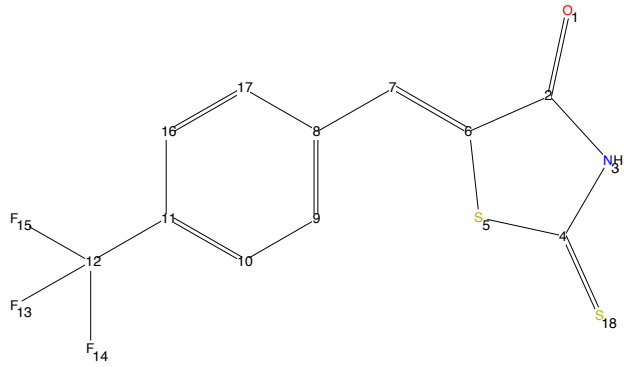


	RT	Area	% Area	Height	Peak Lambda Max.
1	7.563	1952785	100.00	1596133	370.7

CMC-assist

CMM210212 **TZB-005**

Consistency: Unknown*, unknown purity*



Sum formula:
$C_{11}H_6F_3NOS_2$

Molecular Mass:
288.98 Da

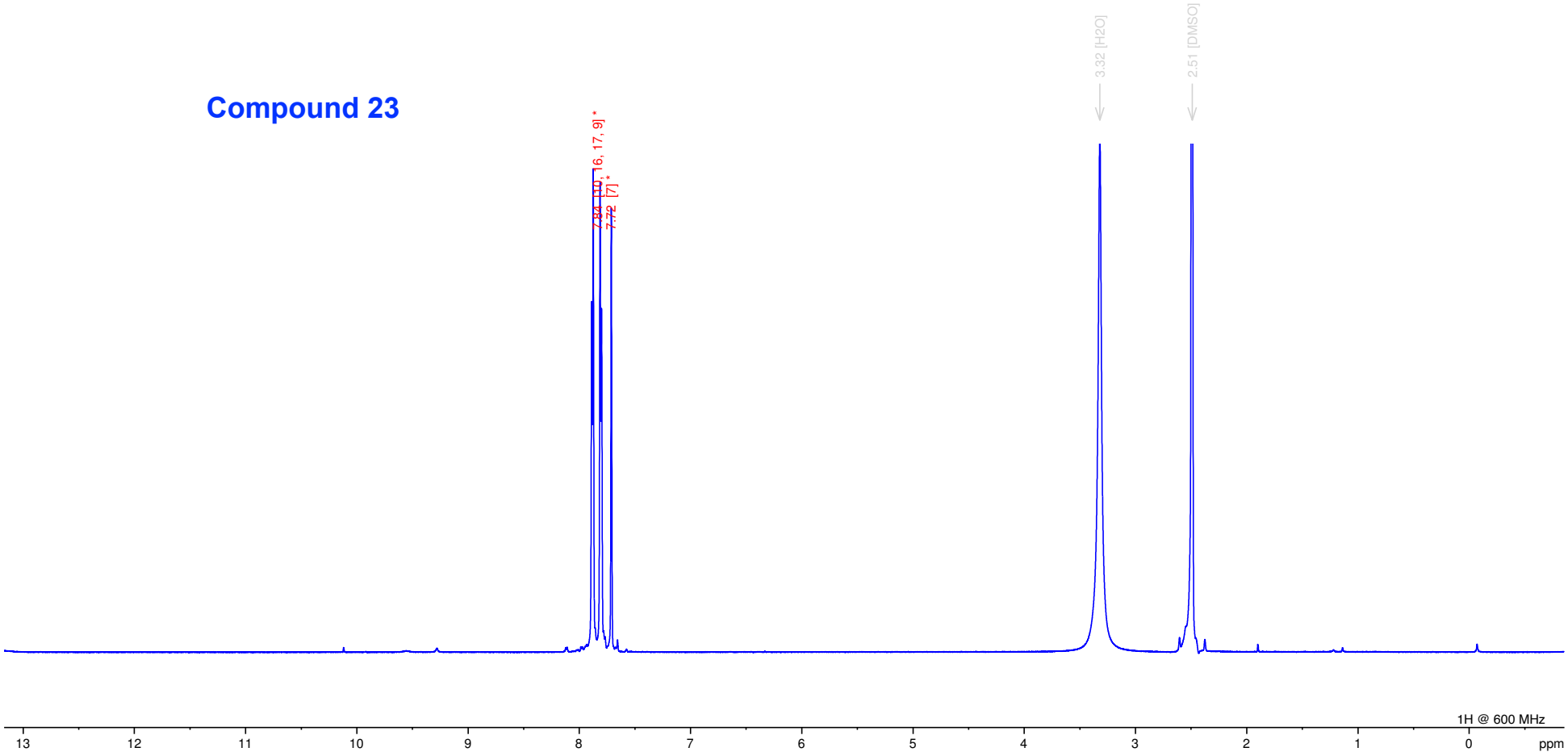
Data set 1H: CMM210212 4 1 /opt/topspin4.1.3
Structure: /opt/topspin4.1.3/CMM210212/4/structure.mol
Acquisition date: February 12, 2021 9:22:19 AM EST
Solvent: DMSO
Probe: 5 mm PATXI 1H/D/19F-13C/15N Z-GRD Z855801/0017
Eretic reference:

Comments:
Multiplet interpretation available for spectrum.
A multiplet interpretation for all major signals in the spectrum could be found. All given impurities could be assigned to regions in the spectrum.

Signature:

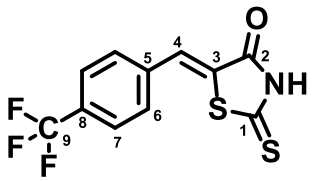
Automatic analysis generated by Bruker CMC (b:17).
One or more results have not been created by automatic analysis, or edited manually: marked by '*'.
Report generated by Bruker CMC-assist TopSpin 4.1.3 (of 2021-06-28 13:00:50), on 'MacBook-Pro.local' as 'tzbenton'

Compound 23



103dx-005

195.50
169.45
136.62
130.73
129.77
128.43
126.11



Compound 23

Acetone – d_6

1 2 5 3 4 9 6,7

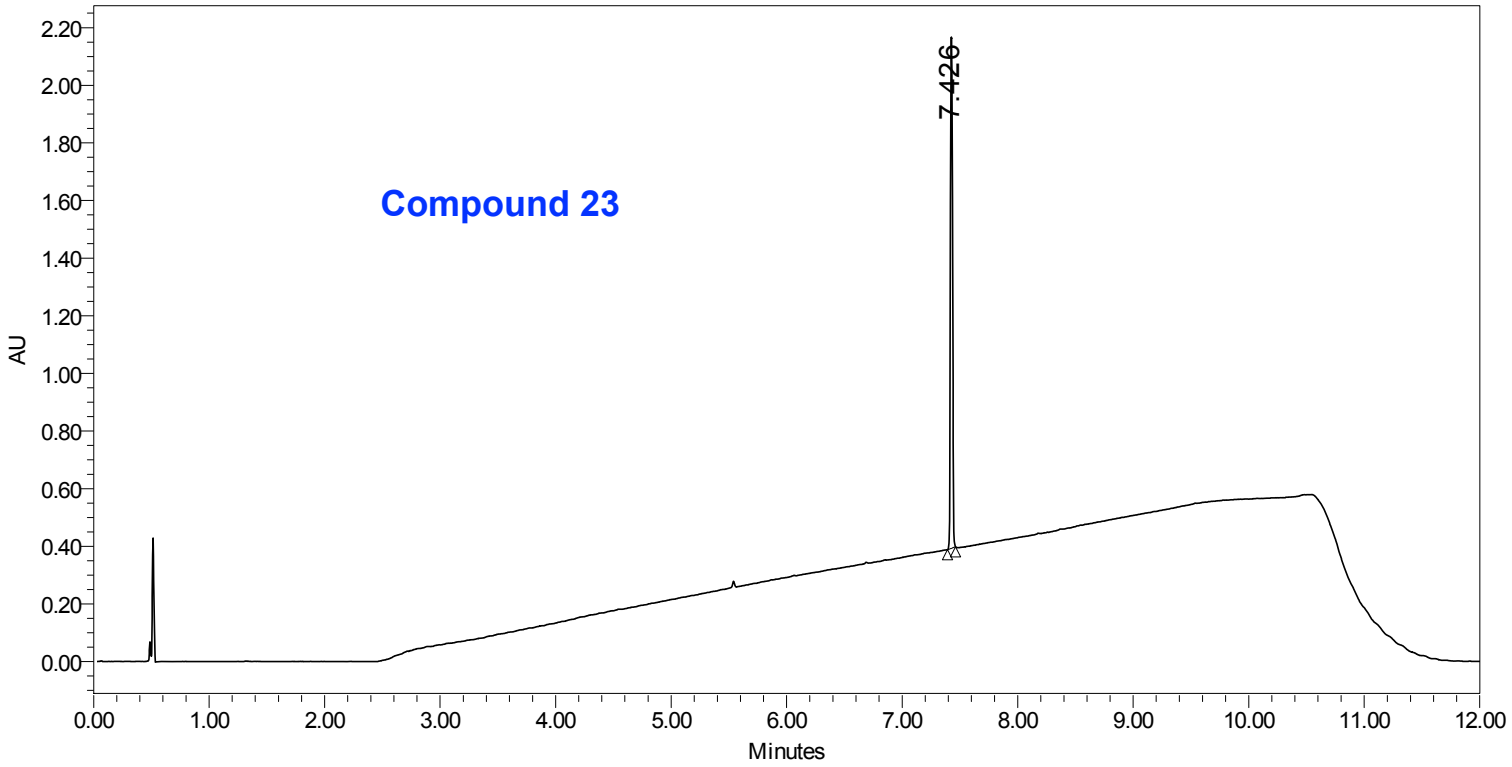
200 180 160 140 120 100 80 60 40 20 ppm

BRUKER

```
Current Data Parameters
NAME            CMM210910
EXPNO                   5
PROCNO                  1

F2 - Acquisition Parameters
Date_            20210910
Time                19.52
INSTRUM             spect
PROBHD   5 mm PATXI 1H/
PULPROG             jmod
TD                 65536
SOLVENT          Acetone
NS                    4000
DS                       4
SWH            36057.691 Hz
FIDRES          0.550197 Hz
AQ             0.9087659 sec
RG                    2050
DW               13.867 usec
DE                6.50 usec
TE                301.3 K
CNST2         145.0000000
CNST11          1.0000000
D1             2.00000000 sec
D20            0.00689655 sec
TD0                      1

======== CHANNEL f1 ========
SFO1       150.9178988 MHz
NUC1                 13C
P1                11.80 usec
P2                23.60 usec
PLW1      202.10000610 W

======== CHANNEL f2 ========
SFO2       600.1324005 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2             70.00 usec
PLW2       13.69999981 W
PLW12       0.17449000 W

F2 - Processing parameters
SI                   32768
SF         150.9028090 MHz
WDW                    EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

SAMPLE INFORMATION

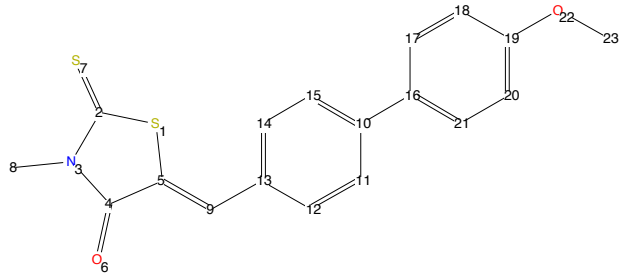
Sample Name:	2021Feb08_TZB103dx_005	Acquired By:	System
Sample Type:	Unknown	Sample Set Name	TZB_103dx
Vial:	1:F,3	Acq. Method Set:	ReversePhase_12min_Max Plot
Injection #:	1	Processing Methoc	ReversePhase_Purity_MAX Plot
Injection Volume:	1.00 ul	Channel Name:	PDA Max Plot 190.0 - 800.0
Run Time:	12.0 Minutes	Proc. Chnl. Descr.:	PDA MaxPlot (190.0 nm to 800.0
Date Acquired:	2/8/2021 2:32:10 PM EST		
Date Processed:	8/31/2021 3:50:59 PM EDT		



	RT	Area	% Area	Height	Peak Lambda Max.
1	7.426	2274749	100.00	1774733	358.9

CMC-assist

CMM210625 **MJF-28**



Consistency: Unknown*, unknown purity*

Sum formula: $C_{18}H_{15}NO_2S_2$

Molecular Mass: 341.05 Da

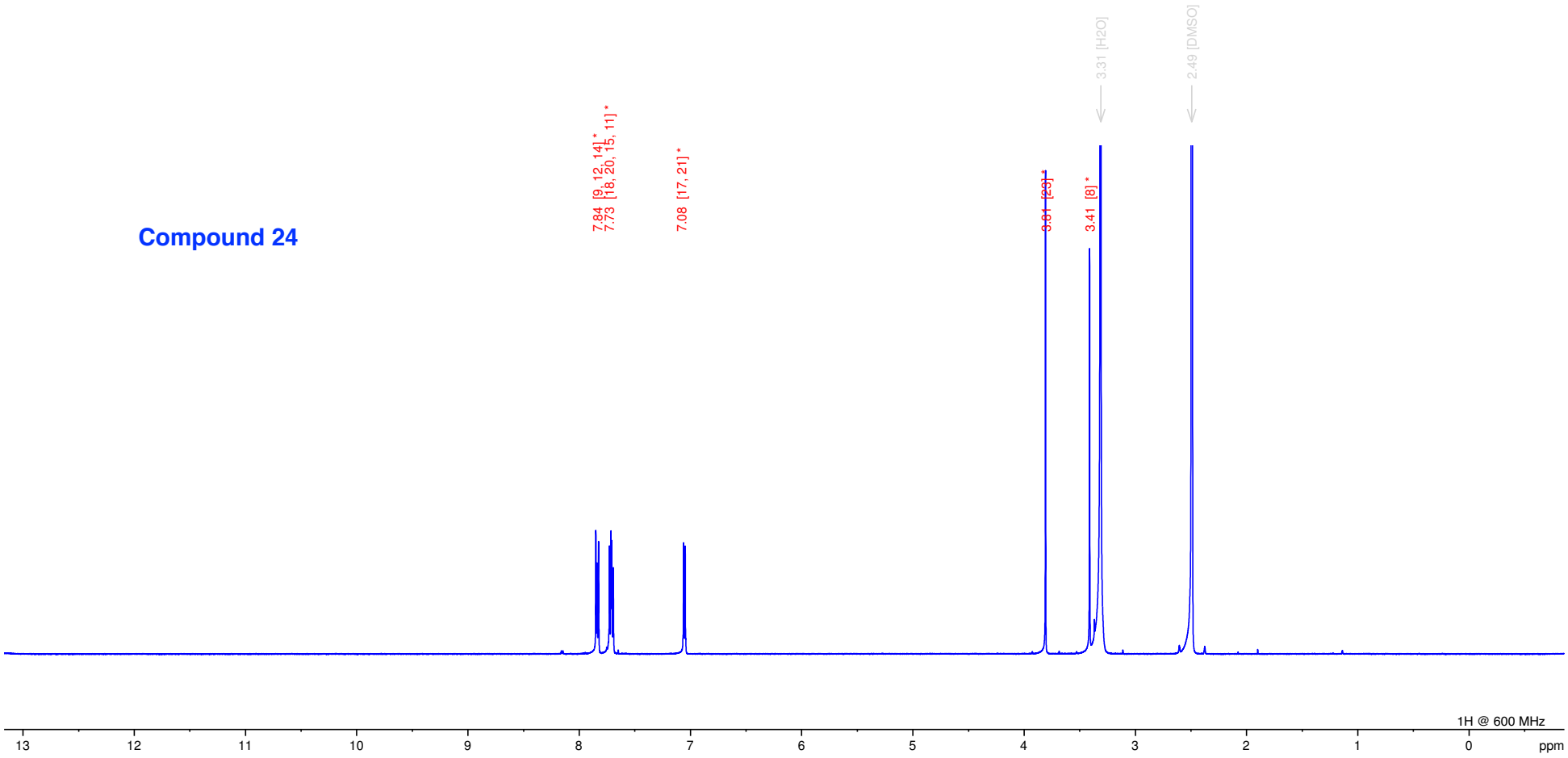
Data set 1H:	CMM210625 3 1 /opt/topspin4.1.3
Structure:	/opt/topspin4.1.3/CMM210625/3/structure.mol
Acquisition date:	June 25, 2021 2:40:32 PM EDT
Solvent:	DMSO
Probe:	5 mm PATXI 1H/D/19F-13C/15N Z-GRD Z855801/0017
Eretic reference:	

Comments:
Multiplet interpretation available for spectrum.
A multiplet interpretation for all major signals in the spectrum could be found. All given impurities could be assigned to regions in the spectrum.

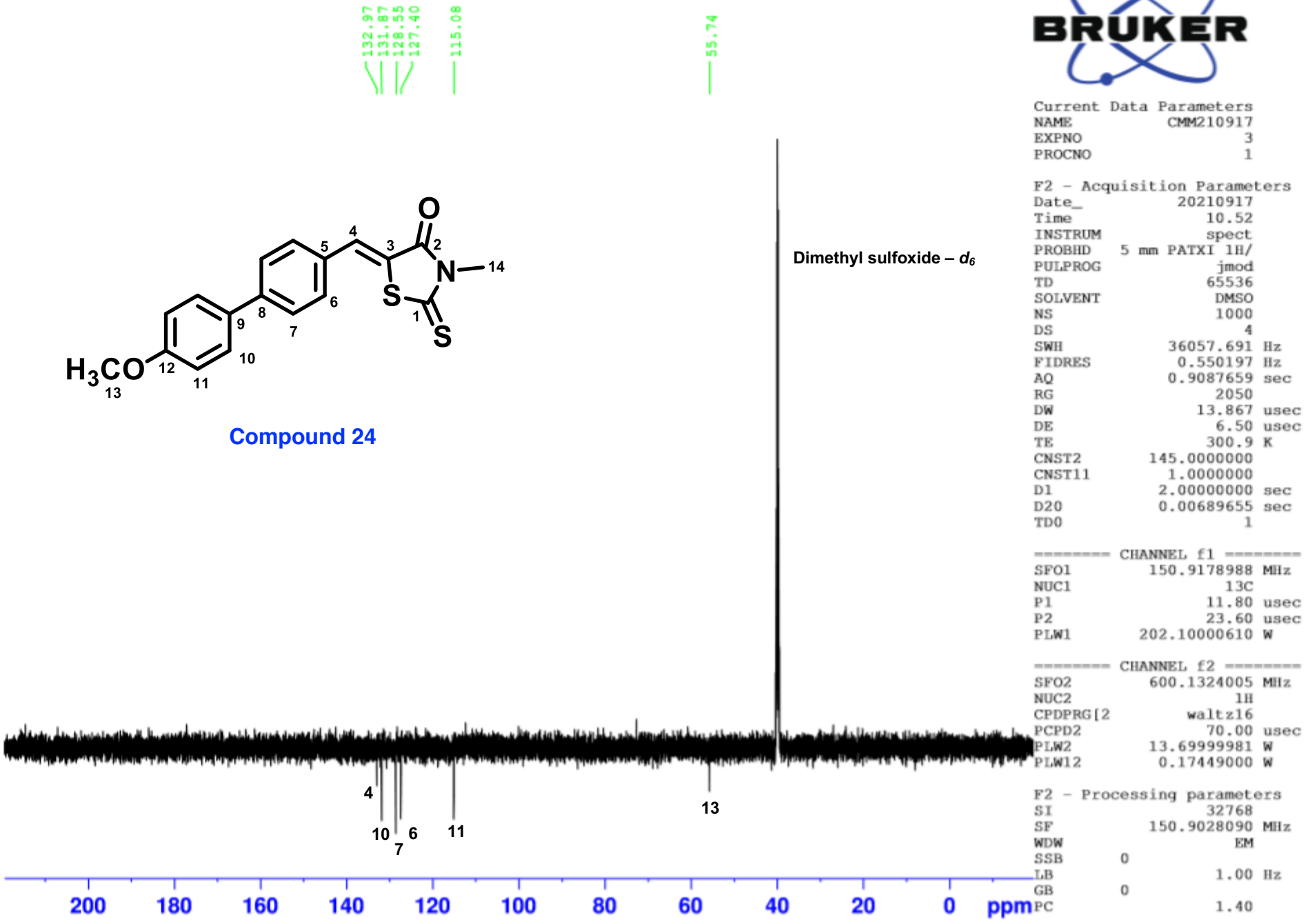
Signature:

Automatic analysis generated by Bruker CMC (b:17).
One or more results have not been created by automatic analysis, or edited manually: marked by '*'.
Report generated by Bruker CMC-assist TopSpin 4.1.3 (of 2021-06-28 13:00:50), on 'MacBook-Pro.local' as 'tzbenton'

Compound 24



24 (MJF28)

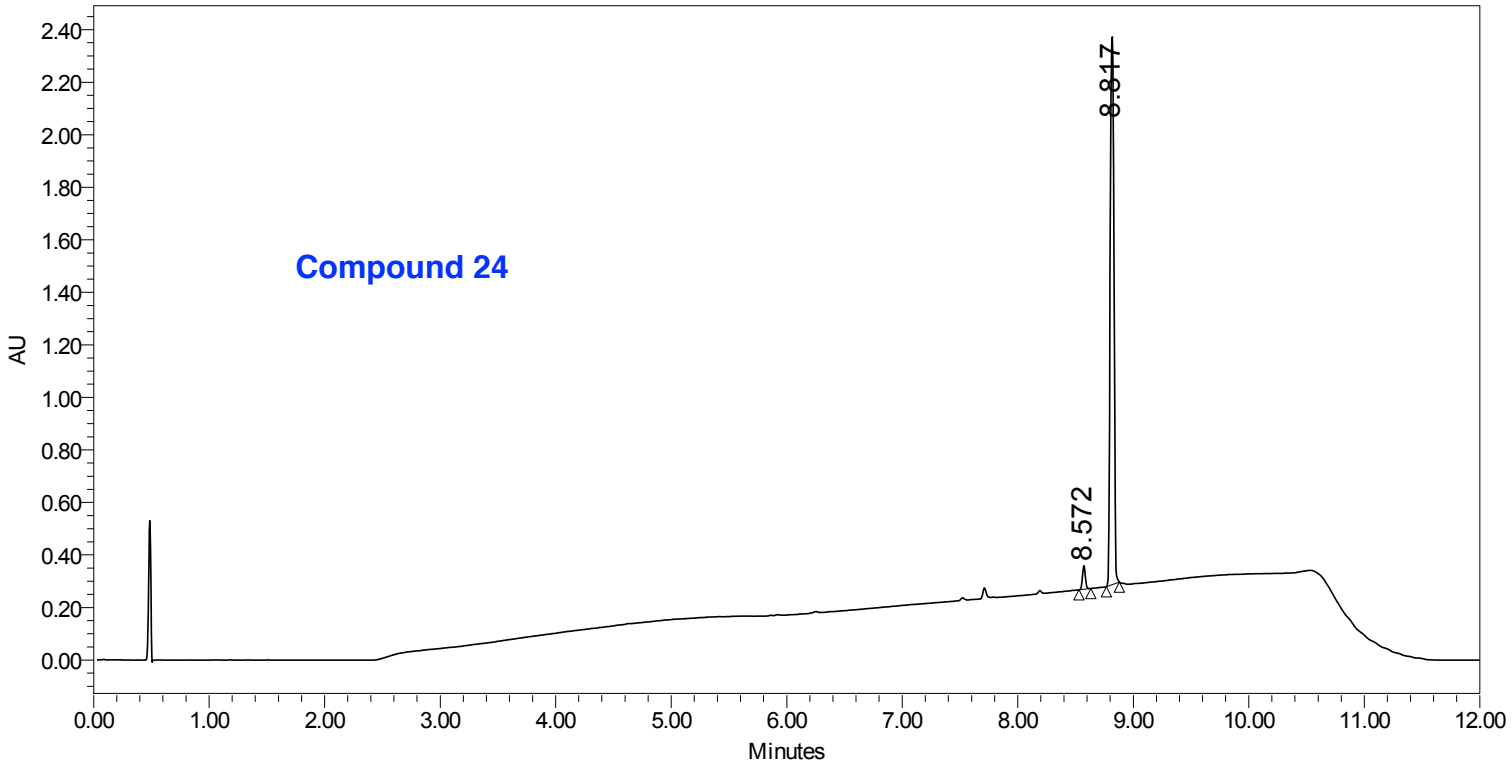


Compound 24

```
Current Data Parameters
NAME                 CMM210917
EXPNO                        3
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20210917
Time                     10.52
INSTRUM                  spect
PROBHD    5 mm PATXI 1H/
PULPROG                  jmod
TD                      65536
SOLVENT                  DMSO
NS                       1000
DS                          4
SWH                 36057.691 Hz
FIDRES              0.550197 Hz
AQ                  0.9087659 sec
RG                       2050
DW                     13.867 usec
DE                      6.50 usec
TE                     300.9 K
CNST2               145.0000000
CNST11                1.0000000
D1                    2.00000000 sec
D20                   0.00689655 sec
TD0                          1

======== CHANNEL f1 ========
SFO1               150.9178988 MHz
NUC1                        13C
P1                       11.80 usec
P2                       23.60 usec
PLW1              202.10000610 W

======== CHANNEL f2 ========
SFO2               600.1324005 MHz
NUC2                        1H
CPDPRG[2                waltz16
PCPD2                    70.00 usec
PLW2               13.69999981 W
PLW12               0.17449000 W

F2 - Processing parameters
SI                       32768
SF                 150.9028090 MHz
WDW                         EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
```

SAMPLE INFORMATION

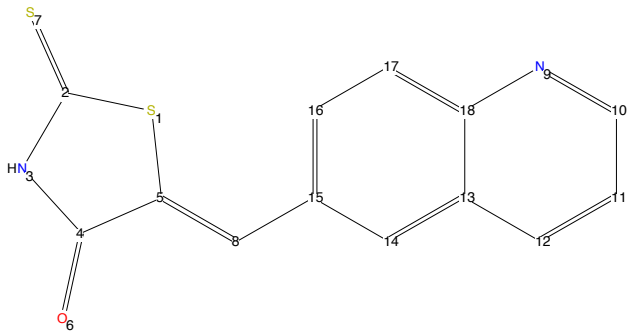
Sample Name:	2021June24_MJF_28_2	Acquired By:	System
Sample Type:	Unknown	Sample Set Name	TZB_103dx
Vial:	1:A,2	Acq. Method Set:	ReversePhase_12min_Max Plot
Injection #:	1	Processing Methoc	ReversePhase_Purity_MAX Plot
Injection Volume:	5.00 ul	Channel Name:	PDA Max Plot 190.0 - 800.0
Run Time:	12.0 Minutes	Proc. Chnl. Descr.:	PDA MaxPlot (190.0 nm to 800.0
Date Acquired:	6/24/2021 10:21:57 AM EDT		
Date Processed:	8/31/2021 4:00:53 PM EDT		



	RT	Area	% Area	Height	Peak Lambda Max.
1	8.572	152765	3.12	89487	407.4
2	8.817	4751200	96.88	2086075	392.4

CMC-assist

CMM210623



Consistency: Unknown*, unknown purity*

Sum formula: $C_{13}H_8N_2OS_2$

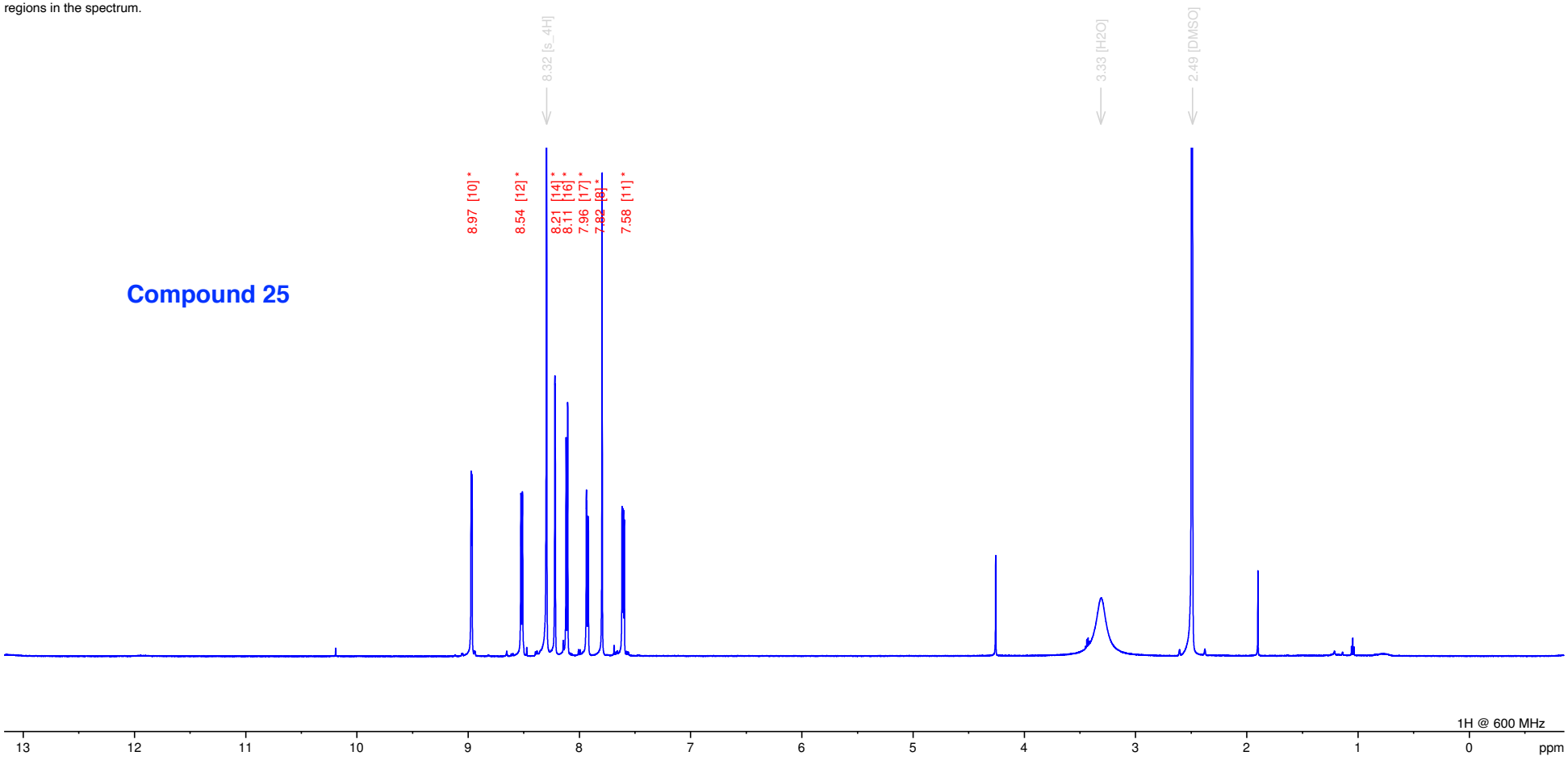
Molecular Mass: 272.01 Da

Data set 1H:	CMM210623 3 1 /opt/topspin4.1.3
Structure:	/opt/topspin4.1.3/CMM210623/3/structure.mol
Acquisition date:	June 23, 2021 1:45:00 PM EDT
Solvent:	DMSO
Probe:	5 mm PATXI 1H/D/19F-13C/15N Z-GRD Z855801/0017
Eretic reference:	

Comments:
Multiplet interpretation available for spectrum.Multiplet interpretation available for spectrum.
A multiplet interpretation for all major signals in the spectrum could be found. All given impurities could be assigned to regions in the spectrum.A multiplet interpretation for all major signals in the spectrum could be found. All given impurities could be assigned to regions in the spectrum.

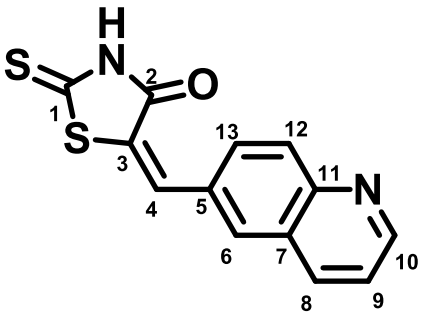
Signature:

Automatic analysis generated by Bruker CMC (b:17).
One or more results have not been created by automatic analysis, or edited manually: marked by '*'.
Report generated by Bruker CMC-assist TopSpin 4.1.3 (of 2021-06-28 13:00:50), on 'MacBook-Pro.local' as 'tzbenton'



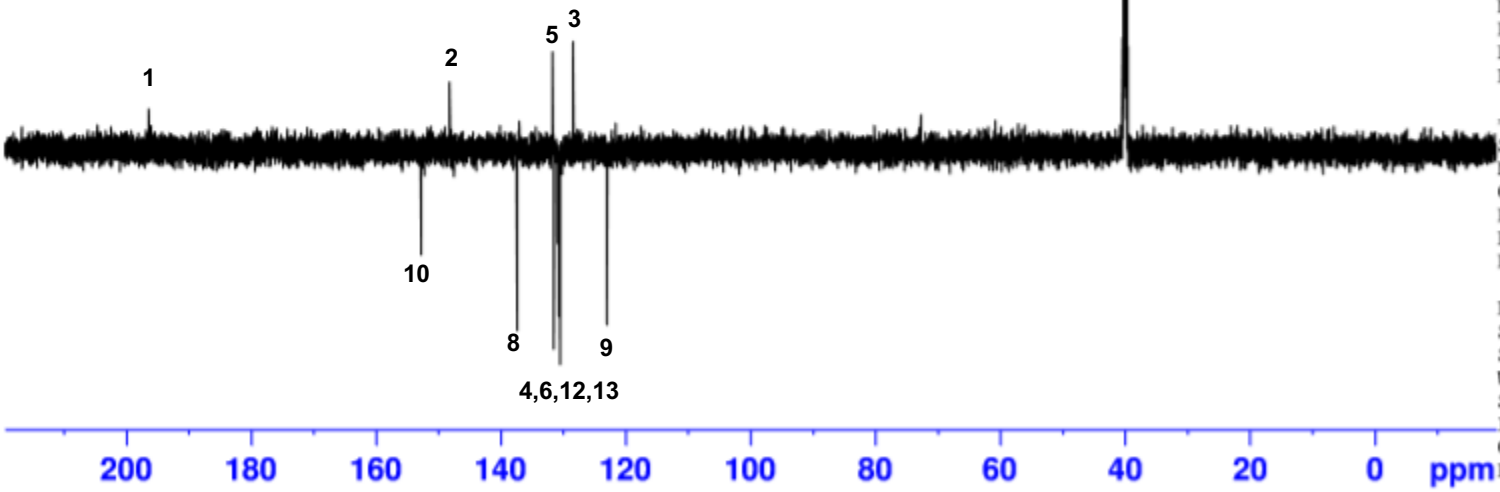
25 (JMT-175)

196.41
152.79
148.21
137.41
131.51
130.89
130.71
130.52
128.42
123.00



Compound 25

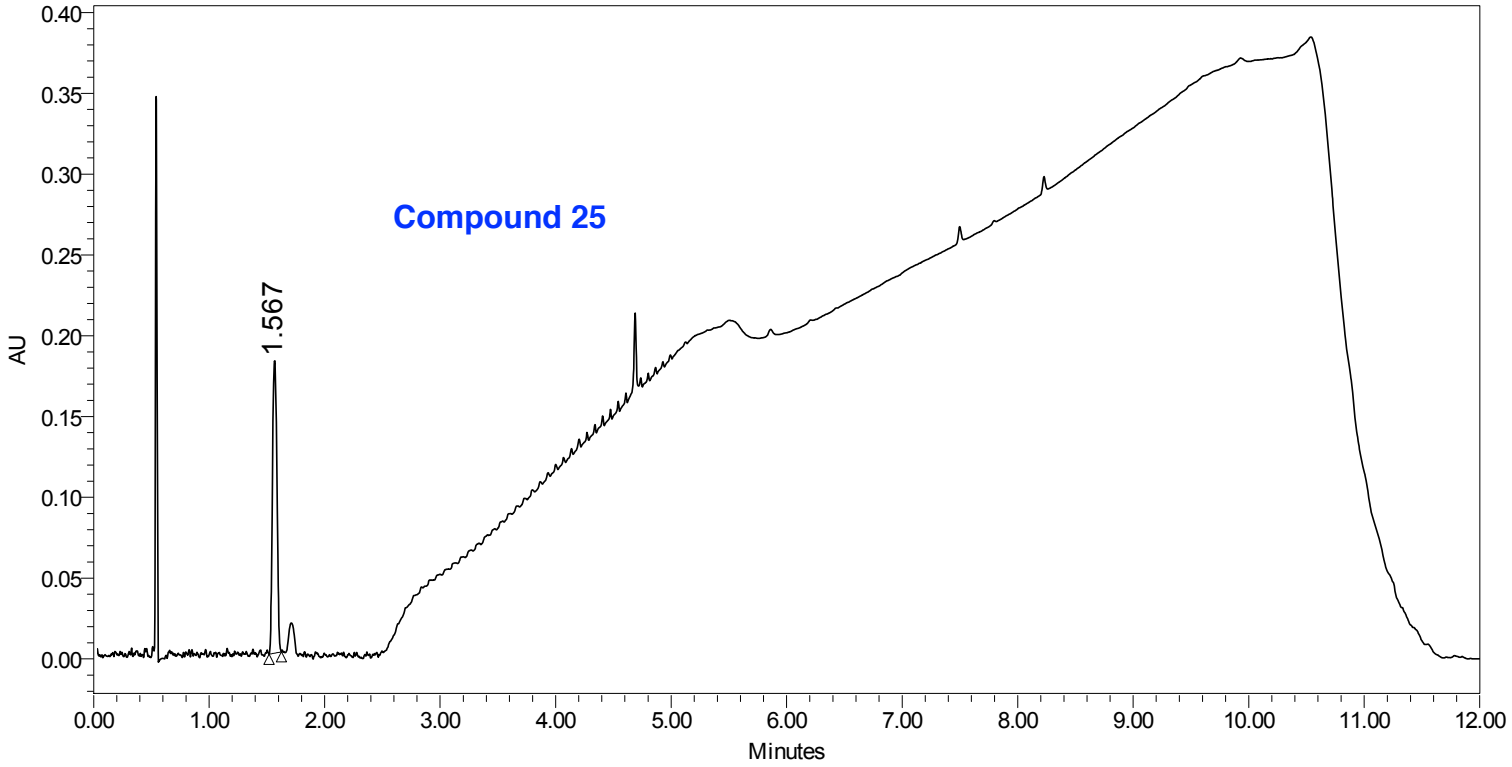
Dimethyl sulfoxide – d_6




```
Current Data Parameters
NAME                  CMM210916
EXPNO                         4
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20210916
Time                      12.57
INSTRUM                   spect
PROBHD    5 mm PATXI 1H/
PULPROG                   jmod
TD                       65536
SOLVENT                   DMSO
NS                        1000
DS                           4
SWH                  36057.691 Hz
FIDRES                0.550197 Hz
AQ                    0.9087659 sec
RG                         2050
DW                       13.867 usec
DE                         6.50 usec
TE                        301.2 K
CNST2                145.0000000
CNST11                 1.0000000
D1                     2.00000000 sec
D20                    0.00689655 sec
TD0                           1

======== CHANNEL f1 ========
SFO1                150.9178988 MHz
NUC1                        13C
P1                        11.80 usec
P2                        23.60 usec
PLW1               202.10000610 W

======== CHANNEL f2 ========
SFO2                600.1324005 MHz
NUC2                        1H
CPDPRG[2                waltz16
PCPD2                     70.00 usec
PLW2               13.69999981 W
PLW12               0.17449000 W

F2 - Processing parameters
SI                        32768
SF                  150.9028090 MHz
WDW                          EM
SSB          0
LB                         1.00 Hz
GB           0
PC                         1.40
```

SAMPLE INFORMATION

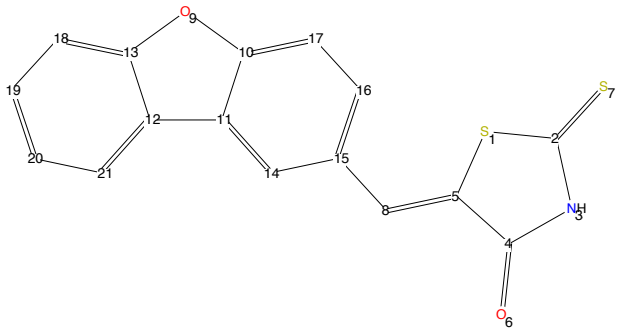
Sample Name:	175	Acquired By:	System
Sample Type:	Unknown	Sample Set Name	103dx_JMT
Vial:	1:B,7	Acq. Method Set:	ReversePhase_12min_Max Plot
Injection #:	1	Processing Methoc	ReversePhase_Purity_MAX Plot
Injection Volume:	1.00 ul	Channel Name:	PDA Max Plot 190.0 - 800.0
Run Time:	12.0 Minutes	Proc. Chnl. Descr.:	PDA MaxPlot (190.0 nm to 800.0
Date Acquired:	7/28/2021 9:30:13 AM EDT		
Date Processed:	8/31/2021 4:08:39 PM EDT		



	RT	Area	% Area	Height	Peak Lambda Max.
1	1.567	490728	100.00	180849	296.3

CMC-assist

CMM210622 JMT-166



Consistency: Unknown*, unknown purity*

Sum formula: $C_{16}H_9NO_2S_2$

Molecular Mass: 311.01 Da

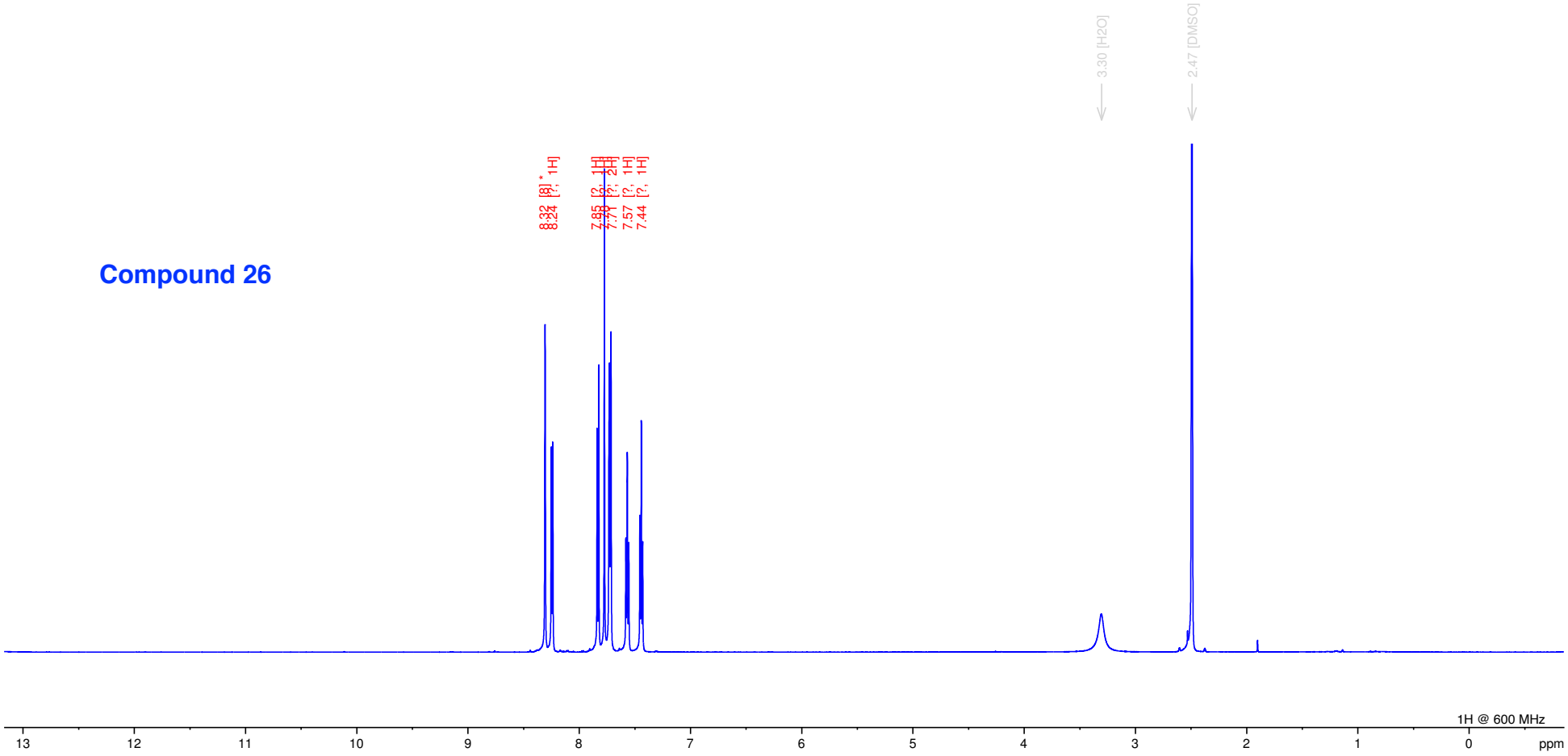
Data set 1H: CMM210622 11 1 /opt/topspin4.1.3
Structure: /opt/topspin4.1.3/CMM210622/11/structure.mol
Acquisition date: June 22, 2021 12:06:35 PM EDT
Solvent: DMSO
Probe: 5 mm PATXI 1H/D/19F-13C/15N Z-GRD Z855801/0017
Eretic reference:

Comments:
Multiplet interpretation available for spectrum.
A multiplet interpretation for all major signals in the spectrum could be found. All given impurities could be assigned to regions in the spectrum.

Signature:

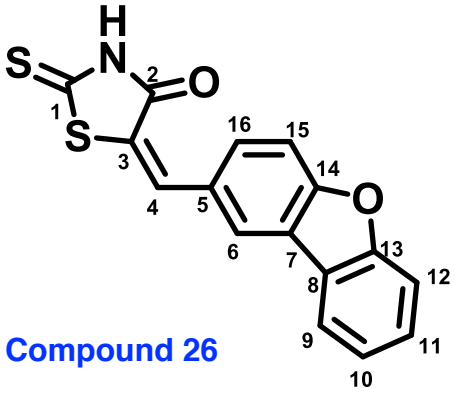
Automatic analysis generated by Bruker CMC (b:17).
One or more results have not been created by automatic analysis, or edited manually: marked by '*'.
Report generated by Bruker CMC-assist TopSpin 4.1.3 (of 2021-06-28 13:00:50), on 'MacBook-Pro.local' as 'tzbenton'

Compound 26



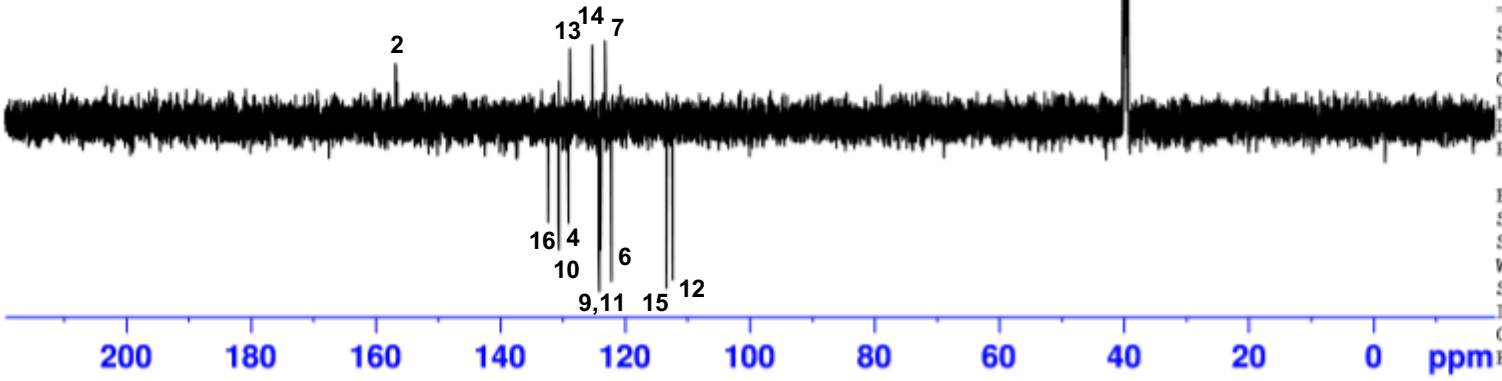
26 (JMT-166)

156.81
132.32
130.66
129.06
128.82
125.24
124.20
123.90
123.18
122.18
113.34
112.36



Compound 26

Dimethyl sulfoxide – d_6

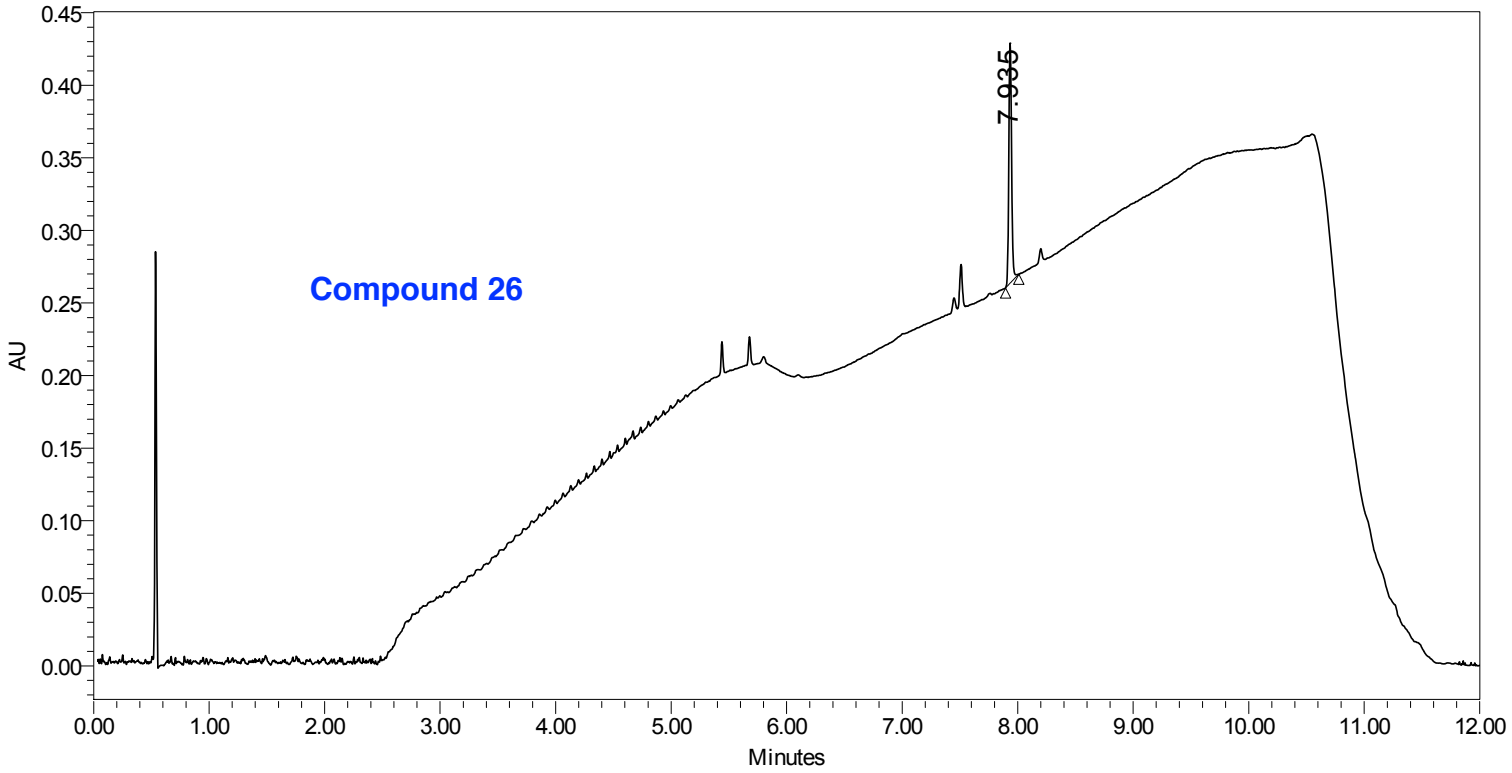


BRUKER

```
Current Data Parameters
NAME                  CMM210916
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20210916
Time                      10.51
INSTRUM                   spect
PROBHD    5 mm PATXI 1H/
PULPROG                   jmod
TD                       65536
SOLVENT                   DMSO
NS                        1000
DS                           4
SWH                  36057.691 Hz
FIDRES               0.550197 Hz
AQ                   0.9087659 sec
RG                        2050
DW                      13.867 usec
DE                        6.50 usec
TE                       301.1 K
CNST2               145.0000000
CNST11                1.0000000
D1                   2.00000000 sec
D20                  0.00689655 sec
TD0                           1

======== CHANNEL f1 ========
SFO1            150.9178988 MHz
NUC1                      13C
P1                      11.80 usec
P2                      23.60 usec
PLW1           202.10000610 W

======== CHANNEL f2 ========
SFO2            600.1324005 MHz
NUC2                      1H
CPDPRG[2              waltz16
PCPD2                   70.00 usec
PLW2            13.69999981 W
PLW12            0.17449000 W

F2 - Processing parameters
SI                        32768
SF              150.9028090 MHz
WDW                          EM
SSB          0
LB                       1.00 Hz
GB           0
PC                       1.40
```

SAMPLE INFORMATION

Sample Name:	166	Acquired By:	System
Sample Type:	Unknown	Sample Set Name	103dx_JMT
Vial:	1:B,3	Acq. Method Set:	ReversePhase_12min_Max Plot
Injection #:	1	Processing Methoc	ReversePhase_Purity_MAX Plot
Injection Volume:	1.00 ul	Channel Name:	PDA Max Plot 190.0 - 800.0
Run Time:	12.0 Minutes	Proc. Chnl. Descr.:	PDA MaxPlot (190.0 nm to 800.0
Date Acquired:	7/27/2021 8:46:42 PM EDT		
Date Processed:	8/31/2021 3:41:45 PM EDT		



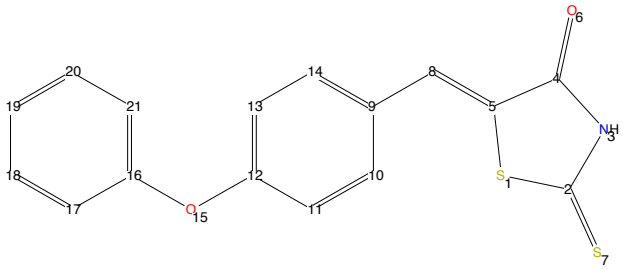
	RT	Area	% Area	Height	Peak Lambda Max.
1	7.935	274502	100.00	165424	386.8

CMC-assist

CMM210622

Consistency: Unknown*, unknown purity*

Data set 1H: CMM210622 8 1 /opt/topspin4.1.3
Structure: /opt/topspin4.1.3/CMM210622/8/structure.mol
Acquisition date: June 22, 2021 11:43:17 AM EDT
Solvent: DMSO
Probe: 5 mm PATXI 1H/D/19F-13C/15N Z-GRD Z855801/0017
Eretic reference:



Sum formula:
$C_{16}H_{11}NO_2S_2$

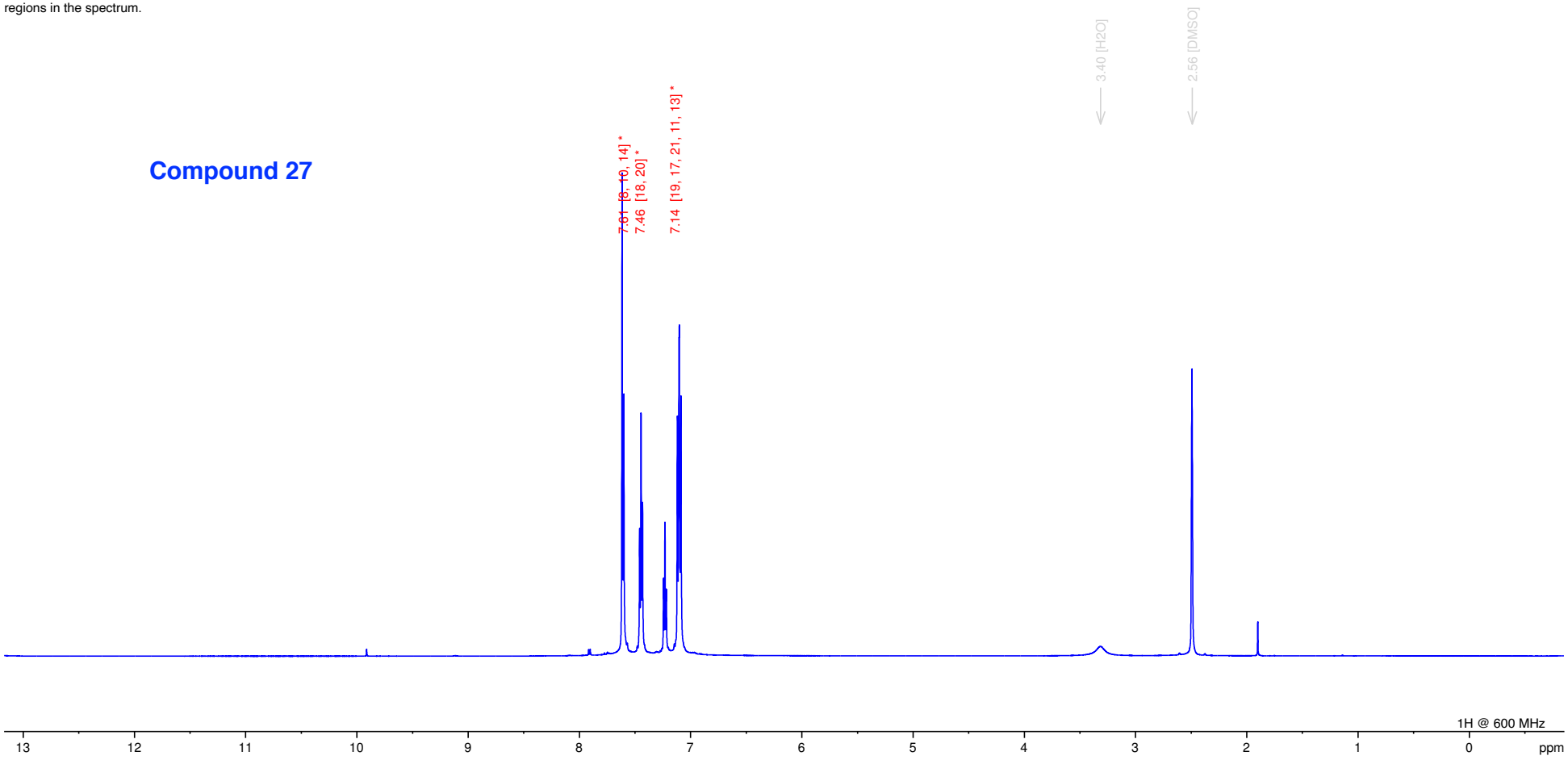
Molecular Mass:
313.02 Da

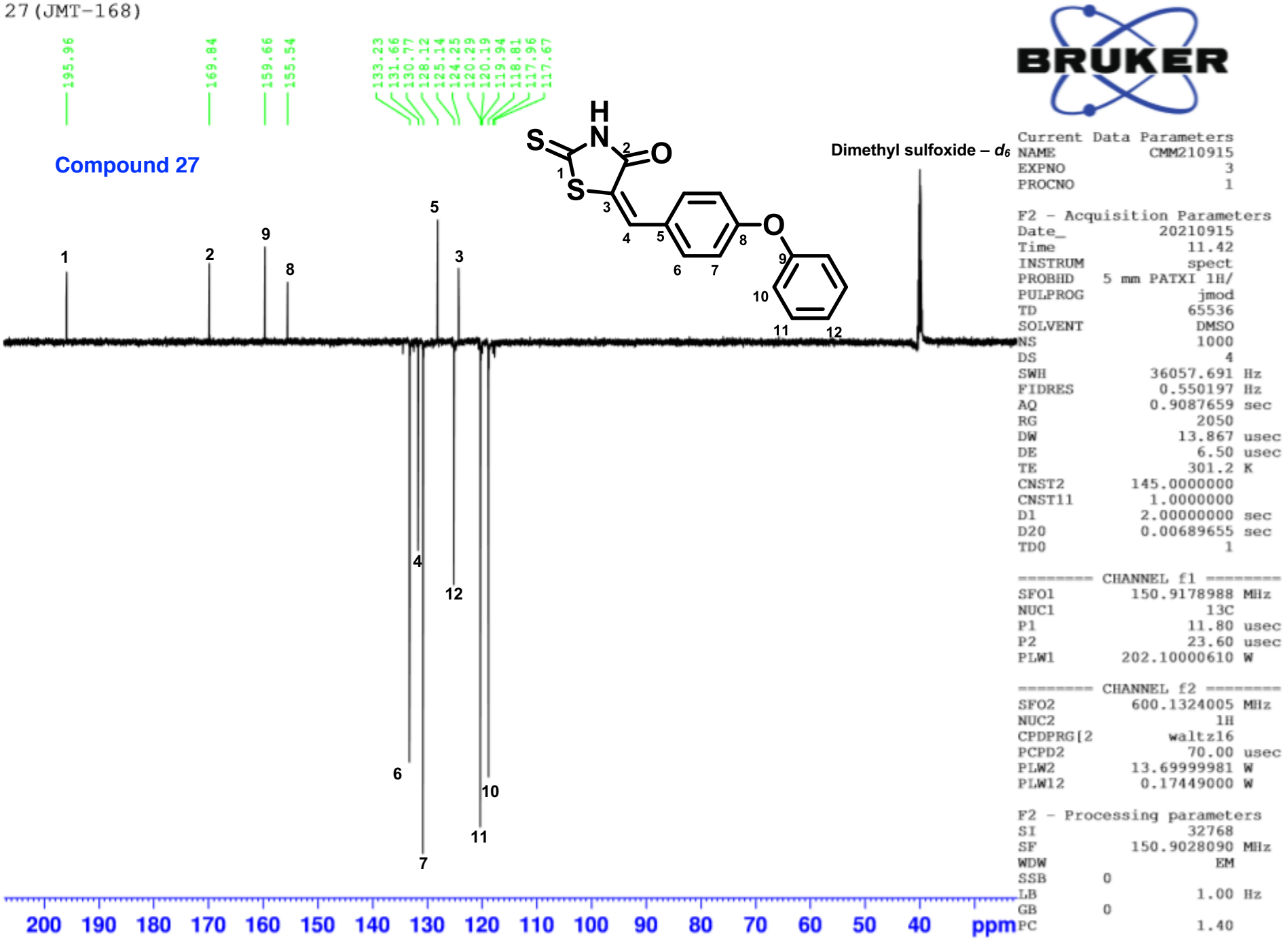
Comments:
Multiplet interpretation available for spectrum.Multiplet interpretation available for spectrum.
A multiplet interpretation for all major signals in the spectrum could be found. All given impurities could be assigned to regions in the spectrum.A multiplet interpretation for all major signals in the spectrum could be found. All given impurities could be assigned to regions in the spectrum.

Signature:

Automatic analysis generated by Bruker CMC (b:17).
One or more results have not been created by automatic analysis, or edited manually: marked by '*'.
Report generated by Bruker CMC-assist TopSpin 4.1.3 (of 2021-06-28 13:00:50), on 'MacBook-Pro.local' as 'tzbenton'

Compound 27





BRUKER

Current Data Parameters

NAME	CMM210915
EXPNO	3
PROCNO	1

F2 - Acquisition Parameters

Date_	20210915
Time	11.42
INSTRUM	spect
PROBHD	5 mm PATXI 1H/
PULPROG	jmod
TD	65536
SOLVENT	DMSO
NS	1000
DS	4
SWH	36057.691 Hz
FIDRES	0.550197 Hz
AQ	0.9087659 sec
RG	2050
DW	13.867 usec
DE	6.50 usec
TE	301.2 K
CNST2	145.0000000
CNST11	1.0000000
D1	2.00000000 sec
D20	0.00689655 sec
TD0	1

======== CHANNEL f1 ========

SFO1	150.9178988 MHz
NUC1	13C
P1	11.80 usec
P2	23.60 usec
PLW1	202.10000610 W

======== CHANNEL f2 ========

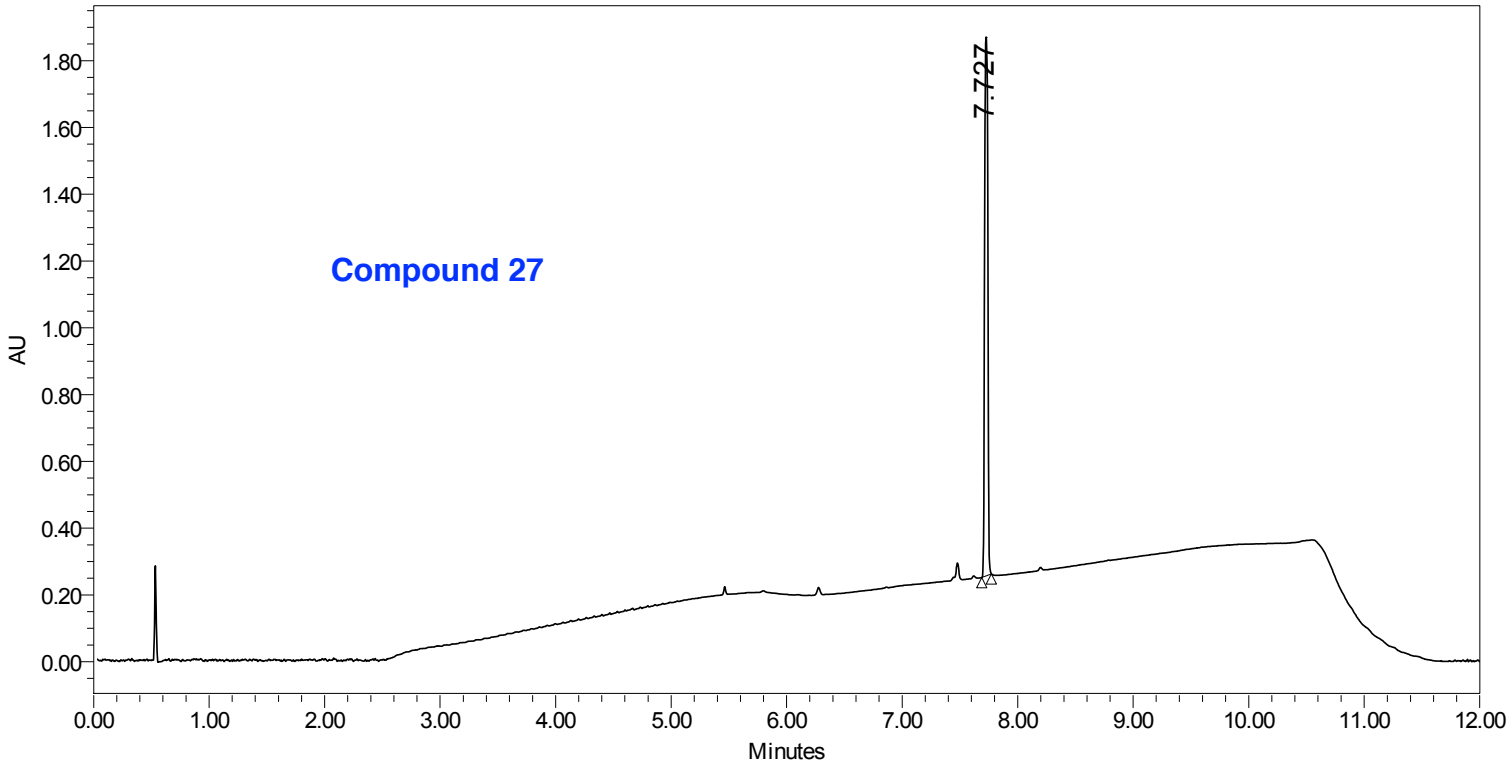
SFO2	600.1324005 MHz
NUC2	1H
CPDPRG[2	waltz16
PCPD2	70.00 usec
PLW2	13.69999981 W
PLW12	0.17449000 W

F2 - Processing parameters

SI	32768
SF	150.9028090 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

SAMPLE INFORMATION

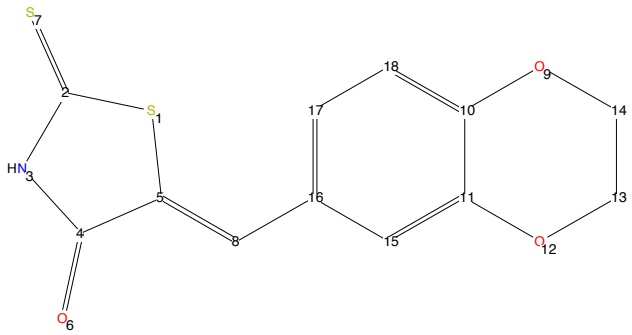
Sample Name:	168	Acquired By:	System
Sample Type:	Unknown	Sample Set Name	103dx_JMT
Vial:	1:B,5	Acq. Method Set:	ReversePhase_12min_Max Plot
Injection #:	1	Processing Method	ReversePhase_Purity_MAX Plot
Injection Volume:	1.00 ul	Channel Name:	PDA Max Plot 190.0 - 800.0
Run Time:	12.0 Minutes	Proc. Chnl. Descr.:	PDA MaxPlot (190.0 nm to 800.0
Date Acquired:	7/27/2021 9:10:46 PM EDT		
Date Processed:	8/31/2021 3:44:49 PM EDT		



	RT	Area	% Area	Height	Peak Lambda Max.
1	7.727	3128203	100.00	1614391	373.8

CMC-assist

CMM210622



Consistency: Unknown*, unknown purity*

Sum formula:
$C_{12}H_9NO_3S_2$

Molecular Mass:
279.00 Da

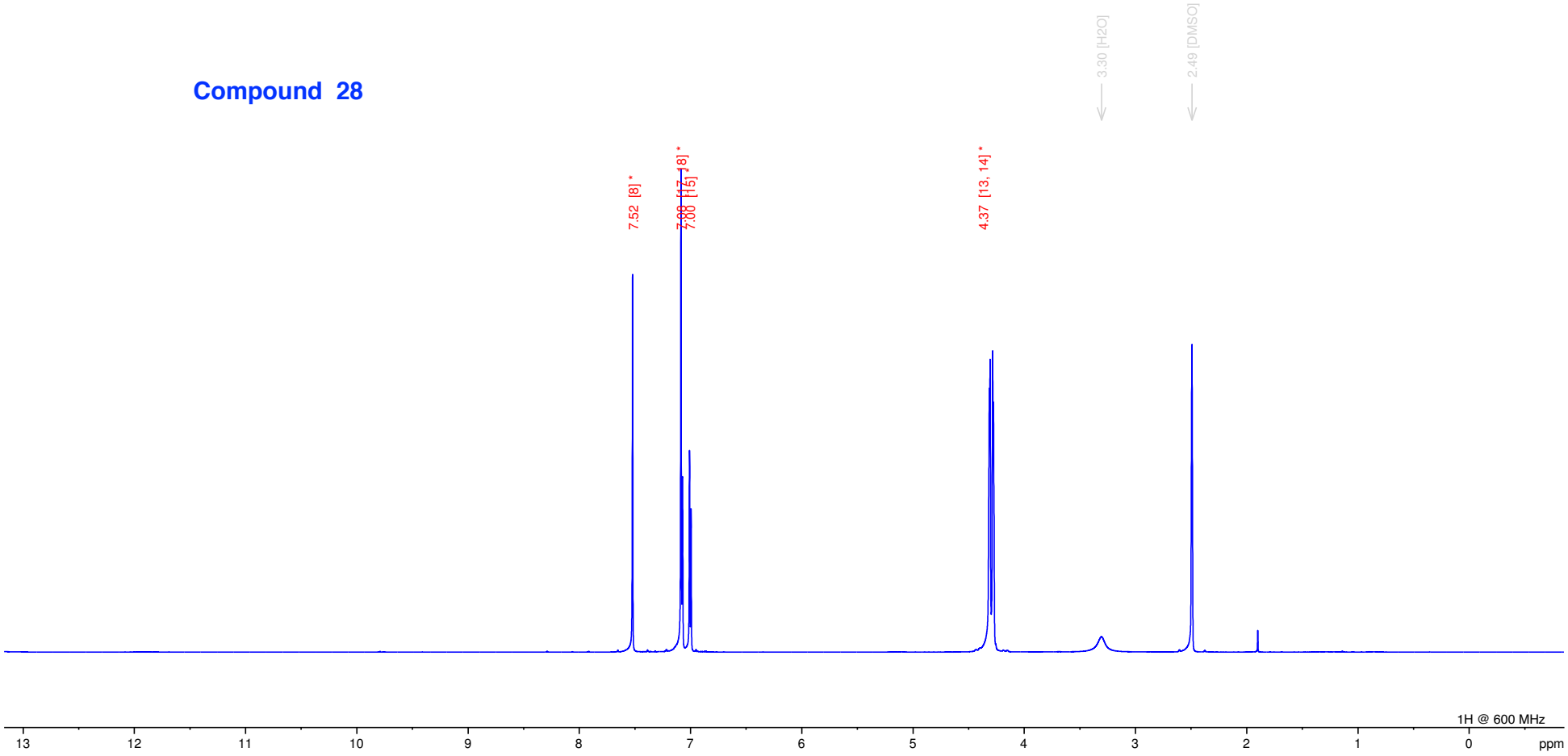
Data set 1H: CMM210622 5 1 /opt/topspin4.1.3
Structure: /opt/topspin4.1.3/CMM210622/5/structure.mol
Acquisition date: June 22, 2021 11:25:46 AM EDT
Solvent: DMSO
Probe: 5 mm PATXI 1H/D/19F-13C/15N Z-GRD Z855801/0017
Eretic reference:

Comments:
Multiplet interpretation available for spectrum.
A multiplet interpretation for all major signals in the spectrum could be found. All given impurities could be assigned to regions in the spectrum.

Signature:

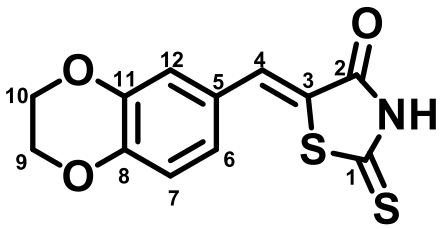
Automatic analysis generated by Bruker CMC (b:17).
One or more results have not been created by automatic analysis, or edited manually: marked by '*'.
Report generated by Bruker CMC-assist TopSpin 4.1.3 (of 2021-06-28 13:00:50), on 'MacBook-Pro.local' as 'tzbenton'

Compound 28



28 (JMT-178)

195.90
144.29
132.24
132.22
126.73
124.86
124.84
119.62
119.60
118.67
118.65
65.01
64.46



Compound 28

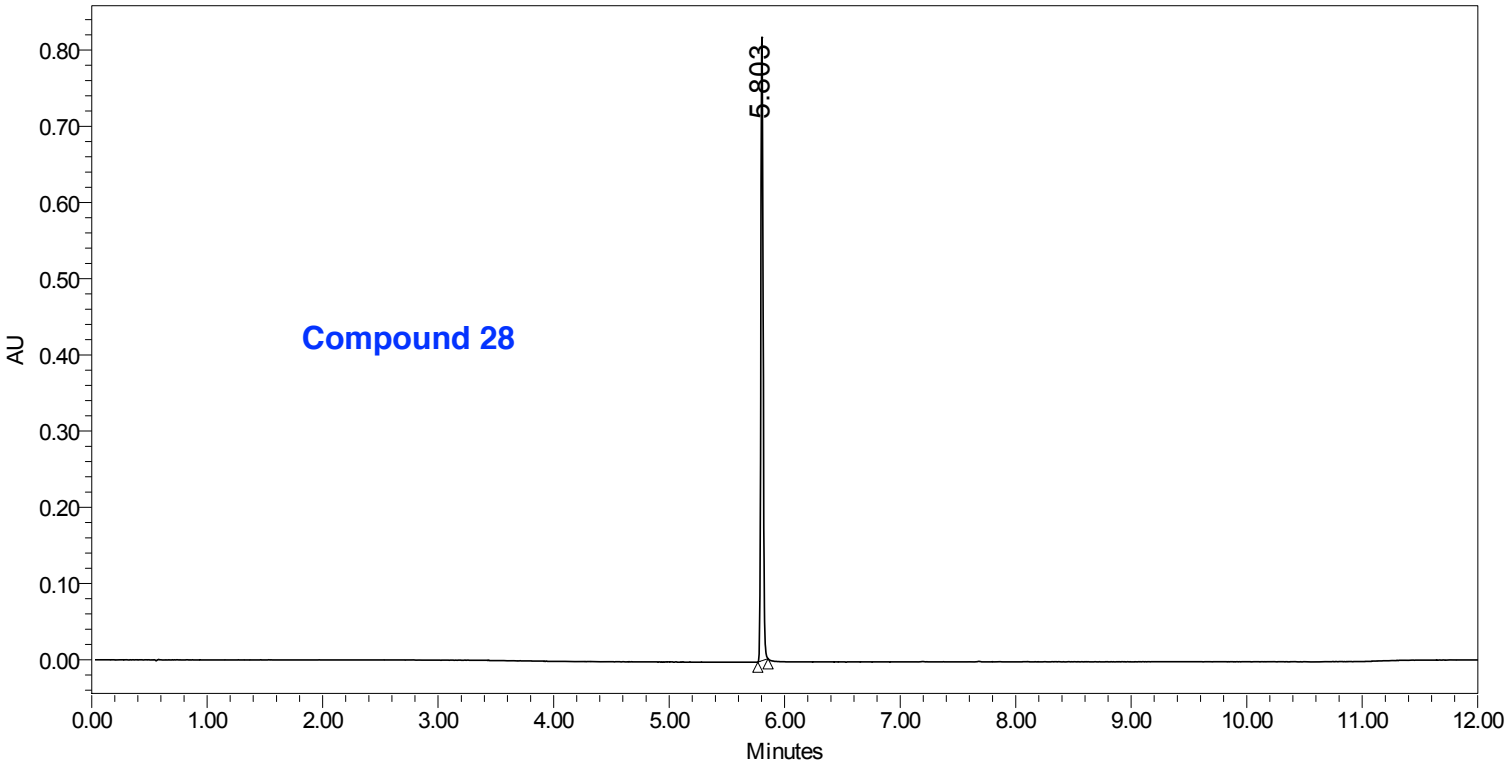
Dimethyl sulfoxide – d_6

BRUKER

```
Current Data Parameters
NAME              CMM210914
EXPNO                     3
PROCNO                    1

F2 - Acquisition Parameters
Date_              20210914
Time                 11.29
INSTRUM              spect
PROBHD    5 mm PATXI 1H/
PULPROG              jmod
TD                  65536
SOLVENT              DMSO
NS                   1000
DS                      4
SWH            36057.691 Hz
FIDRES          0.550197 Hz
AQ              0.9087659 sec
RG                   2050
DW                13.867 usec
DE                 6.50 usec
TE                301.2 K
CNST2         145.0000000
CNST11          1.0000000
D1              2.00000000 sec
D20             0.00689655 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          150.9178988 MHz
NUC1                  13C
P1                 11.80 usec
P2                 23.60 usec
PLW1         202.10000610 W

======== CHANNEL f2 ========
SFO2          600.1324005 MHz
NUC2                  1H
CPDPRG[2           waltz16
PCPD2              70.00 usec
PLW2          13.69999981 W
PLW12          0.17449000 W

F2 - Processing parameters
SI                    32768
SF            150.9028090 MHz
WDW                     EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

SAMPLE INFORMATION

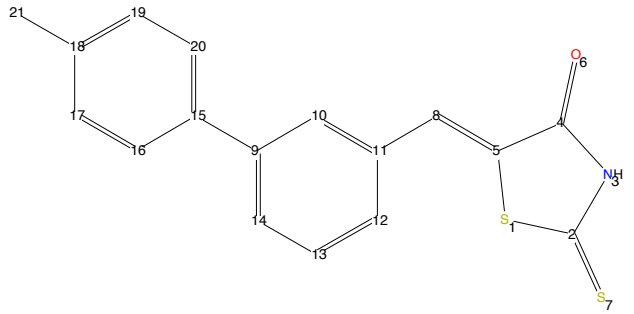
Sample Name:	178	Acquired By:	System
Sample Type:	Unknown	Sample Set Name	103dx_JMT
Vial:	1:C,2	Acq. Method Set:	ReversePhase_12min_Max Plot
Injection #:	1	Processing Methoc	ReversePhase_Purity_MAX Plot
Injection Volume:	1.00 ul	Channel Name:	400.0nm
Run Time:	12.0 Minutes	Proc. Chnl. Descr.:	PDA 400.0 nm, Smoothed by 7
Date Acquired:	7/27/2021 10:13:28 PM EDT		
Date Processed:	8/31/2021 3:33:40 PM EDT		



	RT	Area	% Area	Height	Peak Lambda Max.
1	5.803	1130101	100.00	818367	397.4

CMC-assist

CMM210622



Consistency: Unknown*, unknown purity*

Data set 1H: CMM210622 2 1 /opt/topspin4.1.3
Structure: /opt/topspin4.1.3/CMM210622/2/structure.mol
Acquisition date: June 22, 2021 11:08:05 AM EDT
Solvent: DMSO
Probe: 5 mm PATXI 1H/D/19F-13C/15N Z-GRD Z855801/0017
Eretic reference:

Sum formula: $C_{17}H_{13}NOS_2$

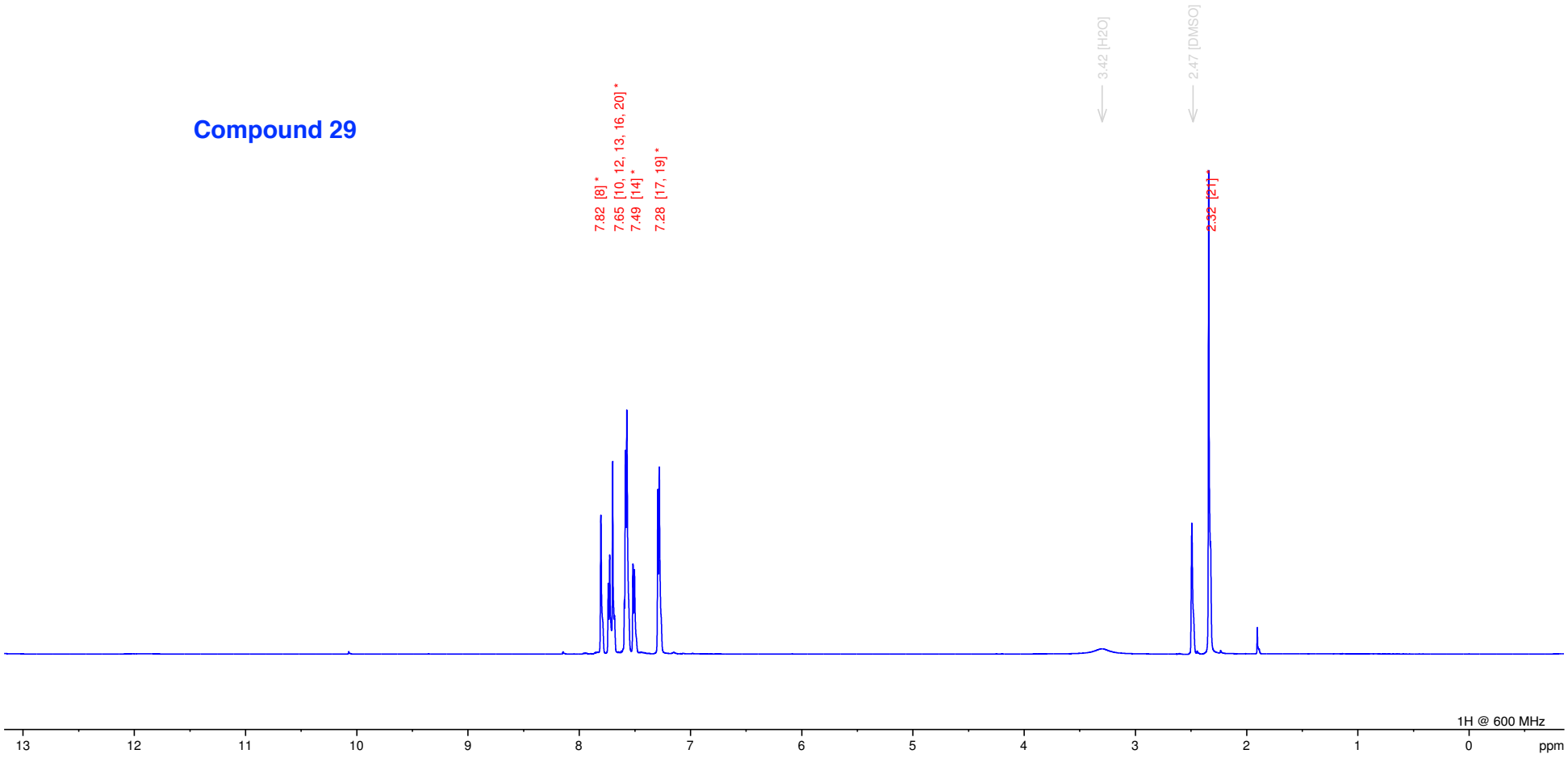
Molecular Mass: 311.04 Da

Comments:
Multiplet interpretation available for spectrum.
A multiplet interpretation for all major signals in the spectrum could be found. All given impurities could be assigned to regions in the spectrum.

Signature:

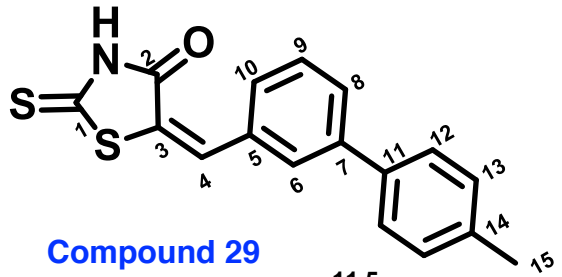
Automatic analysis generated by Bruker CMC (b:17).
One or more results have not been created by automatic analysis, or edited manually: marked by '*'.
Report generated by Bruker CMC-assist TopSpin 4.1.3 (of 2021-06-28 13:00:50), on 'MacBook-Pro.local' as 'tzbenton'

Compound 29



29 (JMT-171)

196.13 169.90 141.59 137.93 136.62 134.14 132.10 130.52 130.17 130.08 129.13 129.09 127.07 126.97 126.43 21.15



Compound 29

Dimethyl sulfoxide – d_6

11,5 7 14 1 2 3 4 15 6,8,9,10,12,13

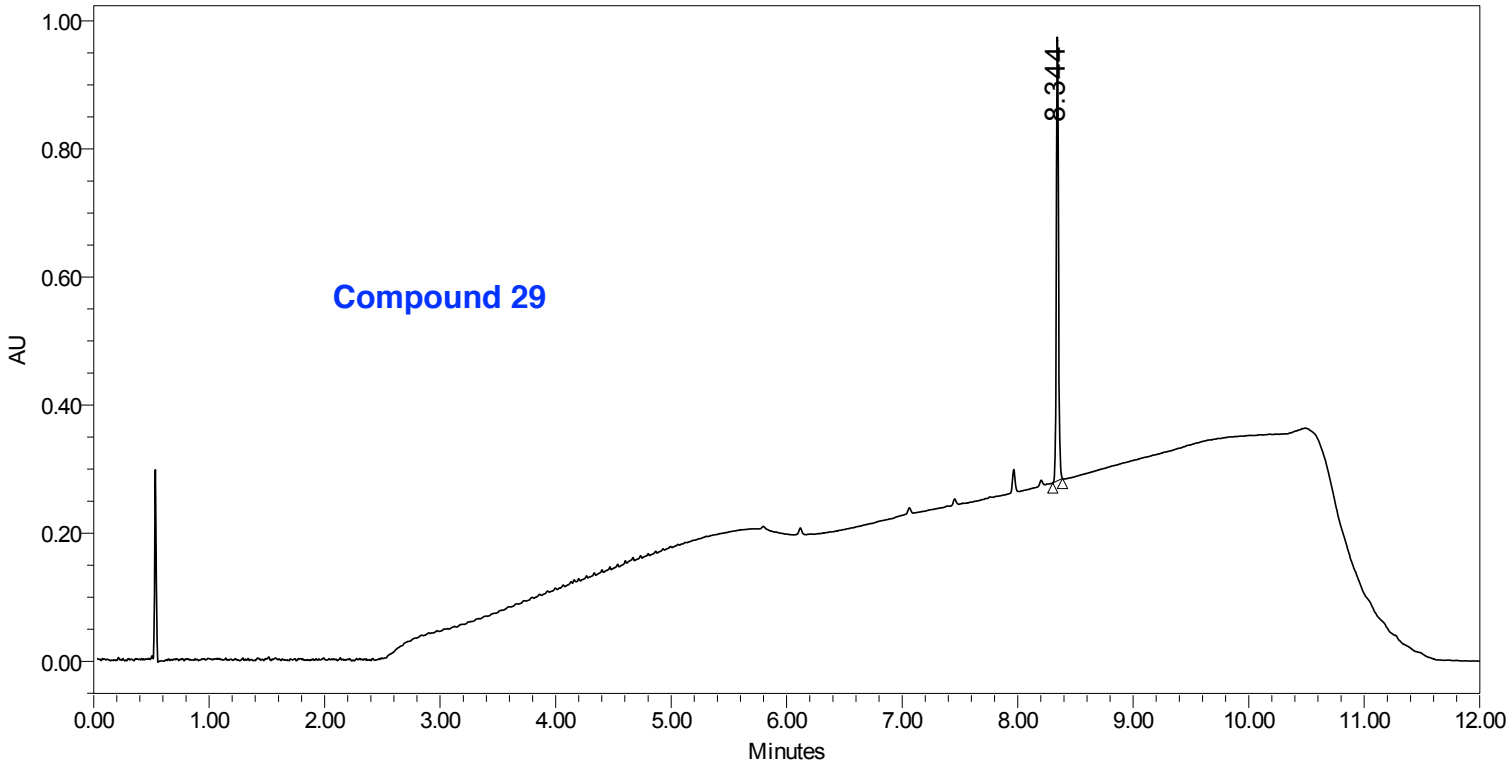
200 180 160 140 120 100 80 60 40 20 0 ppm

BRUKER

```
Current Data Parameters
NAME                CMM210914
EXPNO                       8
PROCNO                      1

F2 - Acquisition Parameters
Date_              20210914
Time                  19.24
INSTRUM               spect
PROBHD    5 mm PATXI 1H/
PULPROG               jmod
TD                   65536
SOLVENT                DMSO
NS                     2000
DS                        4
SWH               36057.691 Hz
FIDRES             0.550197 Hz
AQ                 0.9087659 sec
RG                     2050
DW                   13.867 usec
DE                     6.50 usec
TE                    301.4 K
CNST2             145.0000000
CNST11              1.0000000
D1                  2.00000000 sec
D20                 0.00689655 sec
TD0                         1

======== CHANNEL f1 ========
SFO1           150.9178988 MHz
NUC1                     13C
P1                     11.80 usec
P2                     23.60 usec
PLW1          202.10000610 W

======== CHANNEL f2 ========
SFO2           600.1324005 MHz
NUC2                     1H
CPDPRG[2             waltz16
PCPD2                  70.00 usec
PLW2           13.69999981 W
PLW12           0.17449000 W

F2 - Processing parameters
SI                       32768
SF             150.9028090 MHz
WDW                         EM
SSB          0
LB                      1.00 Hz
GB           0
PC                      1.40
```

SAMPLE INFORMATION

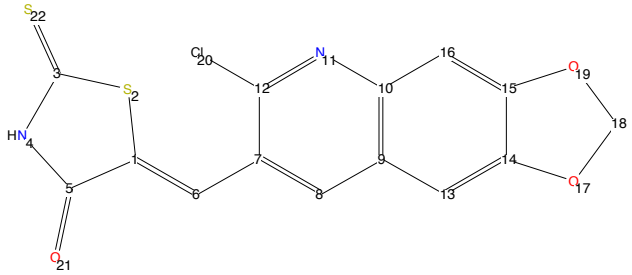
Sample Name:	171	Acquired By:	System
Sample Type:	Unknown	Sample Set Name	103dx_JMT
Vial:	1:C,4	Acq. Method Set:	ReversePhase_12min_Max Plot
Injection #:	1	Processing Methoc	ReversePhase_Purity_MAX Plot
Injection Volume:	1.00 ul	Channel Name:	PDA Max Plot 190.0 - 800.0
Run Time:	12.0 Minutes	Proc. Chnl. Descr.:	PDA MaxPlot (190.0 nm to 800.0
Date Acquired:	7/27/2021 10:38:33 PM EDT		
Date Processed:	8/31/2021 3:19:34 PM EDT		



	RT	Area	% Area	Height	Peak Lambda Max.
1	8.344	893834	100.00	694220	376.3

CMC-assist

CMM210623 JM T-13 2



Consistency: Unknown*, unknown purity*

Data set 1H: CMM210623 5 1 /opt/topspin4.1.3
Structure: /opt/topspin4.1.3/CMM210623/5/structure.mol
Acquisition date: June 23, 2021 1:55:35 PM EDT
Solvent: DMSO
Probe: 5 mm PATXI 1H/D/19F-13C/15N Z-GRD Z855801/0017
Eretic reference:

Sum formula: $C_{14}H_7ClN_2O_3S_2$

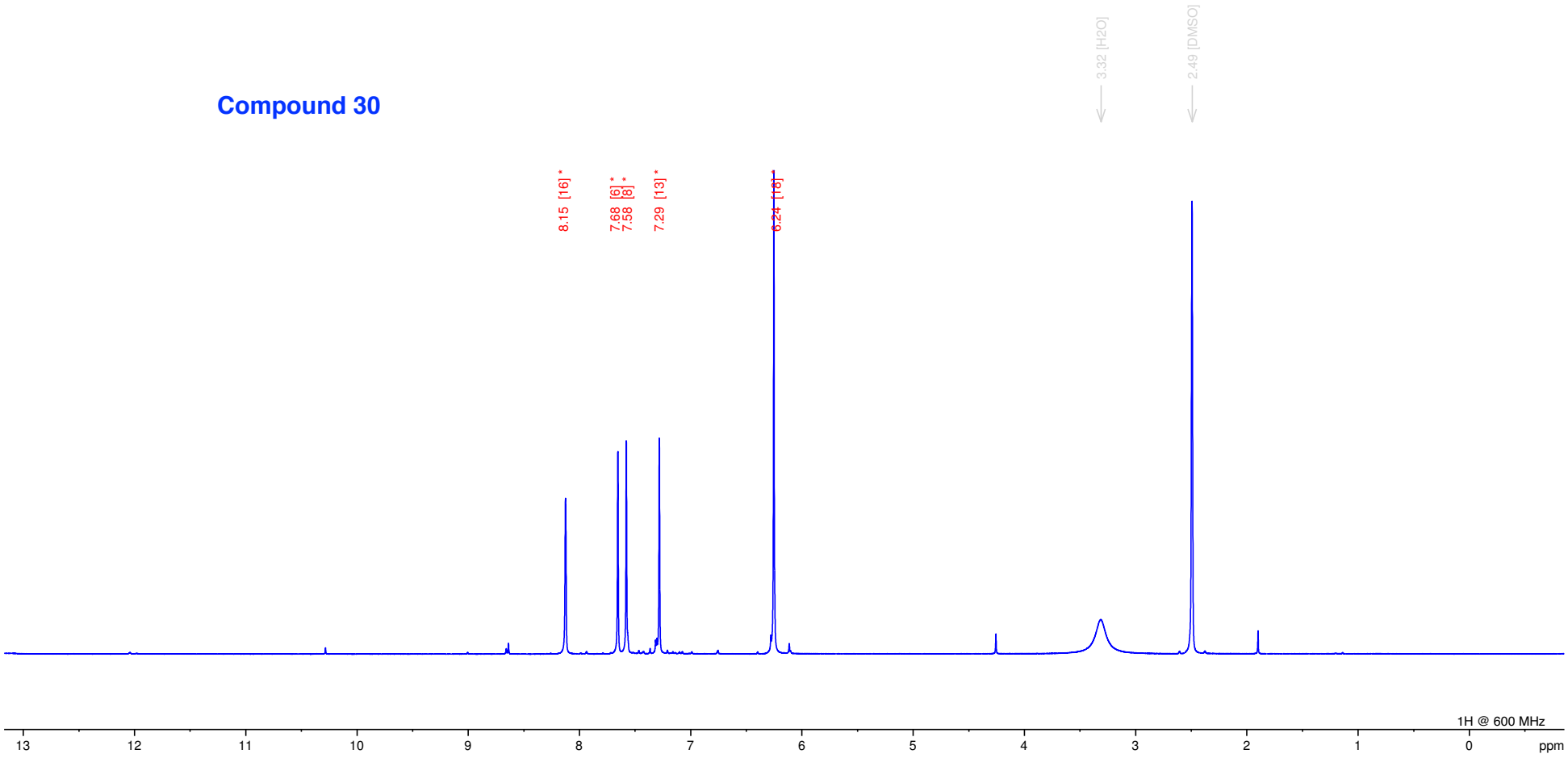
Molecular Mass: 349.96 Da

Comments:
Multiplet interpretation available for spectrum.
A multiplet interpretation for all major signals in the spectrum could be found. All given impurities could be assigned to regions in the spectrum.

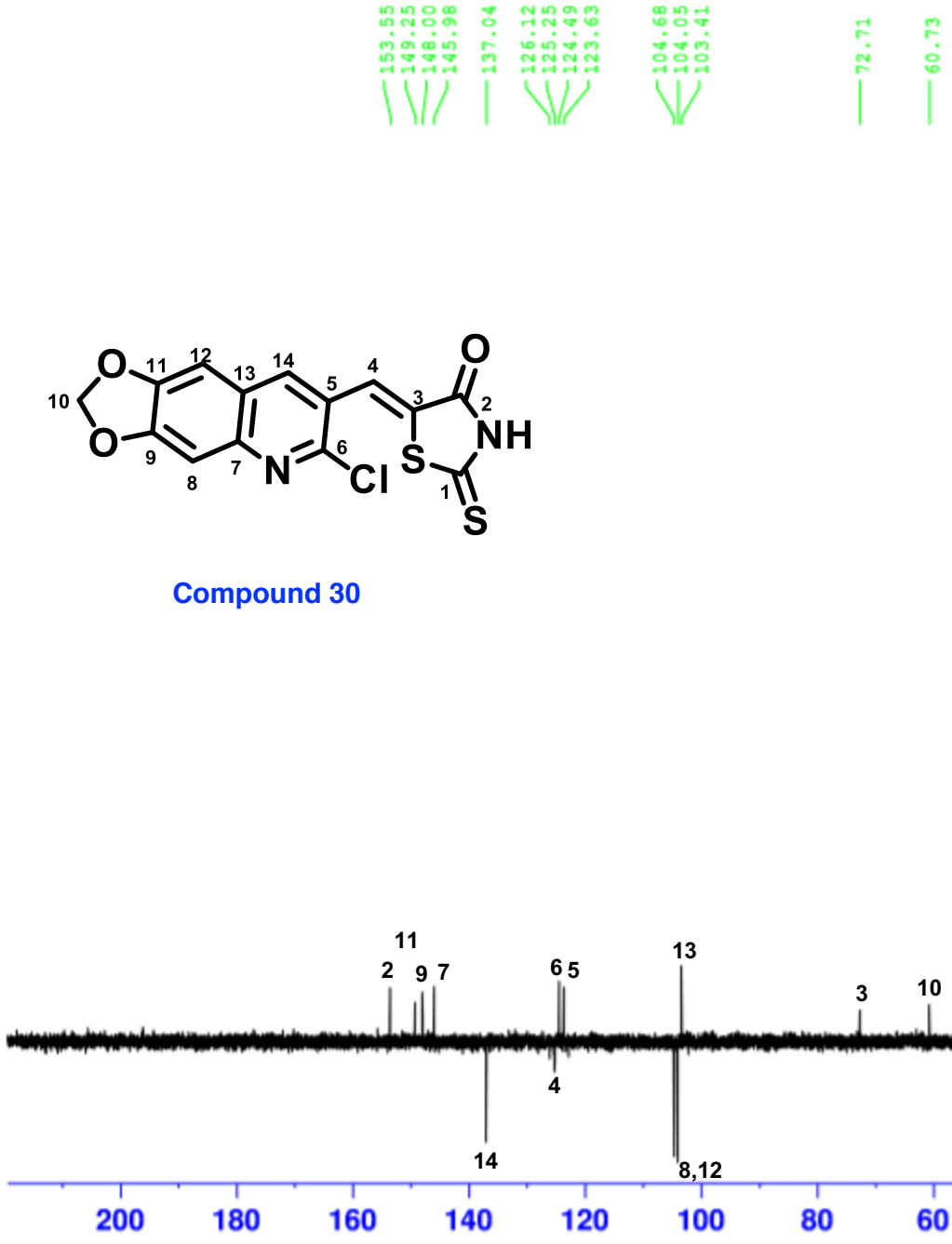
Signature:

Automatic analysis generated by Bruker CMC (b:17).
One or more results have not been created by automatic analysis, or edited manually: marked by '*'.
Report generated by Bruker CMC-assist TopSpin 4.1.3 (of 2021-06-28 13:00:50), on 'MacBook-Pro.local' as 'tzbenton'

Compound 30



30 (JMT-132)



Compound 30

Current Data Parameters
NAME CMM210916
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210916
Time 23.05
INSTRUM spect
PROBHD 5 mm PATXI 1H/
PULPROG jmod
TD 65536
SOLVENT DMSO
NS 8000
DS 4
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 2050
DW 13.867 usec
DE 6.50 usec
TE 301.4 K
CNST2 145.0000000
CNST11 1.0000000
D1 2.00000000 sec
D20 0.00689655 sec
TD0 1

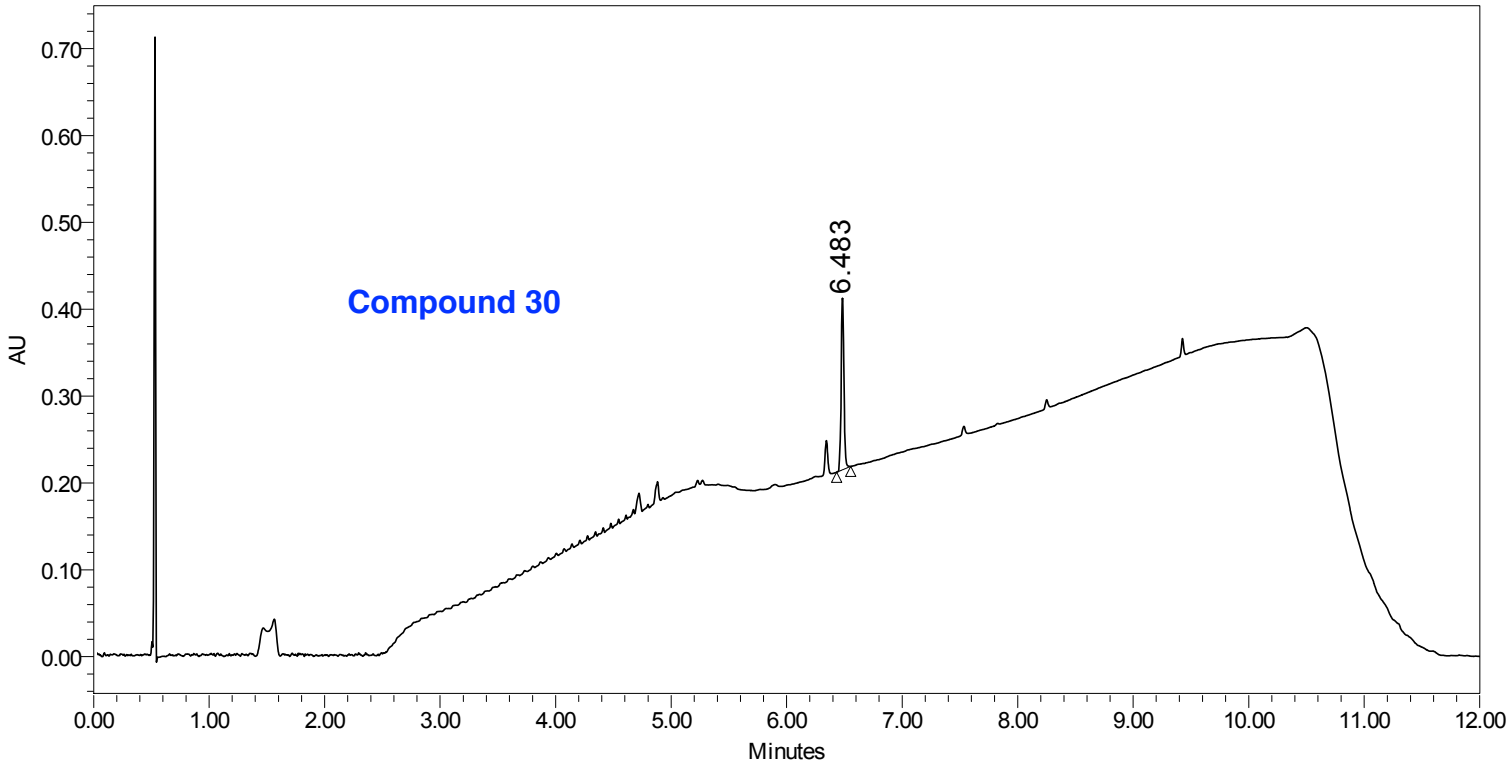
======== CHANNEL f1 ========
SFO1 150.9178988 MHz
NUC1 13C
P1 11.80 usec
P2 23.60 usec
PLW1 202.10000610 W

======== CHANNEL f2 ========
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 70.00 usec
PLW2 13.69999981 W
PLW12 0.17449000 W

F2 - Processing parameters
SI 32768
SF 150.9028090 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

SAMPLE INFORMATION

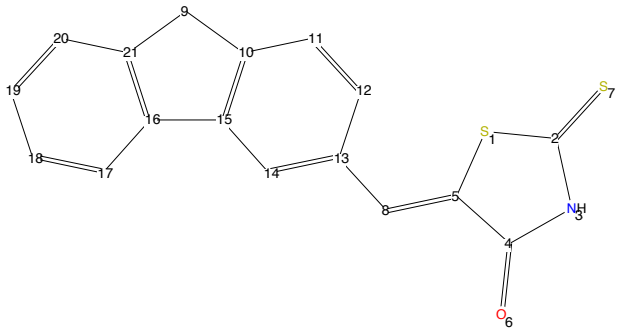
Sample Name:	132	Acquired By:	System
Sample Type:	Unknown	Sample Set Name	103dx_JMT
Vial:	1:B,4	Acq. Method Set:	ReversePhase_12min_Max Plot
Injection #:	1	Processing Method	ReversePhase_Purity_MAX Plot
Injection Volume:	3.00 ul	Channel Name:	PDA Max Plot 190.0 - 800.0
Run Time:	12.0 Minutes	Proc. Chnl. Descr.:	PDA MaxPlot (190.0 nm to 800.0
Date Acquired:	7/28/2021 12:10:19 PM EDT		
Date Processed:	8/31/2021 3:29:13 PM EDT		



	RT	Area	% Area	Height	Peak Lambda Max.
1	6.483	331432	100.00	197687	396.2

CMC-assist

CMM210618 JMT-165



Consistency: Unknown*, unknown purity*

Data set 1H: CMM210618 4 1 /opt/topspin4.1.3
Structure: /opt/topspin4.1.3/CMM210618/4/structure.mol
Acquisition date: June 18, 2021 3:25:08 PM EDT
Solvent: DMSO
Probe: 5 mm PATXI 1H/D/19F-13C/15N Z-GRD Z855801/0017
Eretic reference:

Sum formula: $C_{17}H_{11}NOS_2$

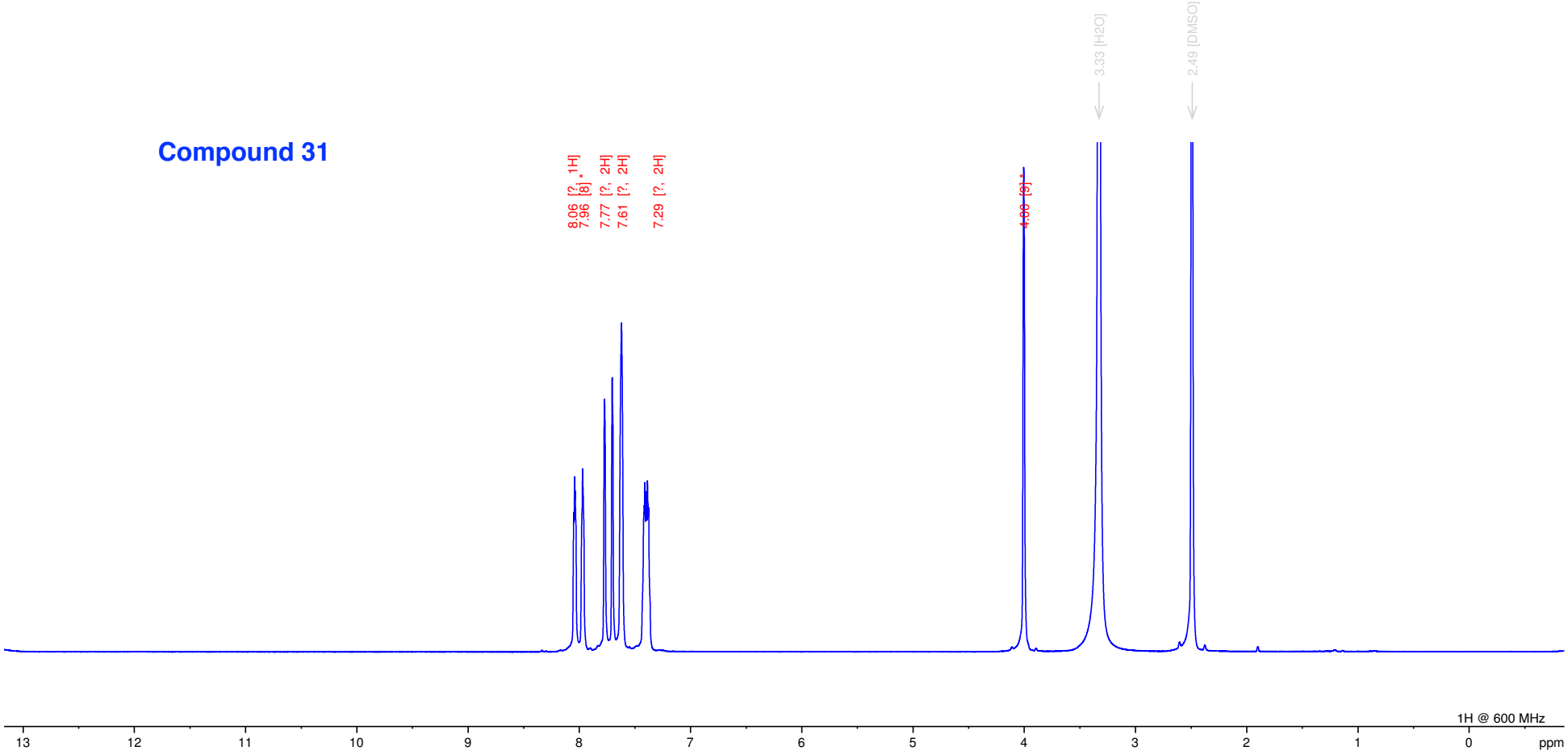
Molecular Mass: 309.03 Da

Comments:
Multiplet interpretation available for spectrum.
A multiplet interpretation for all major signals in the spectrum could be found. All given impurities could be assigned to regions in the spectrum.

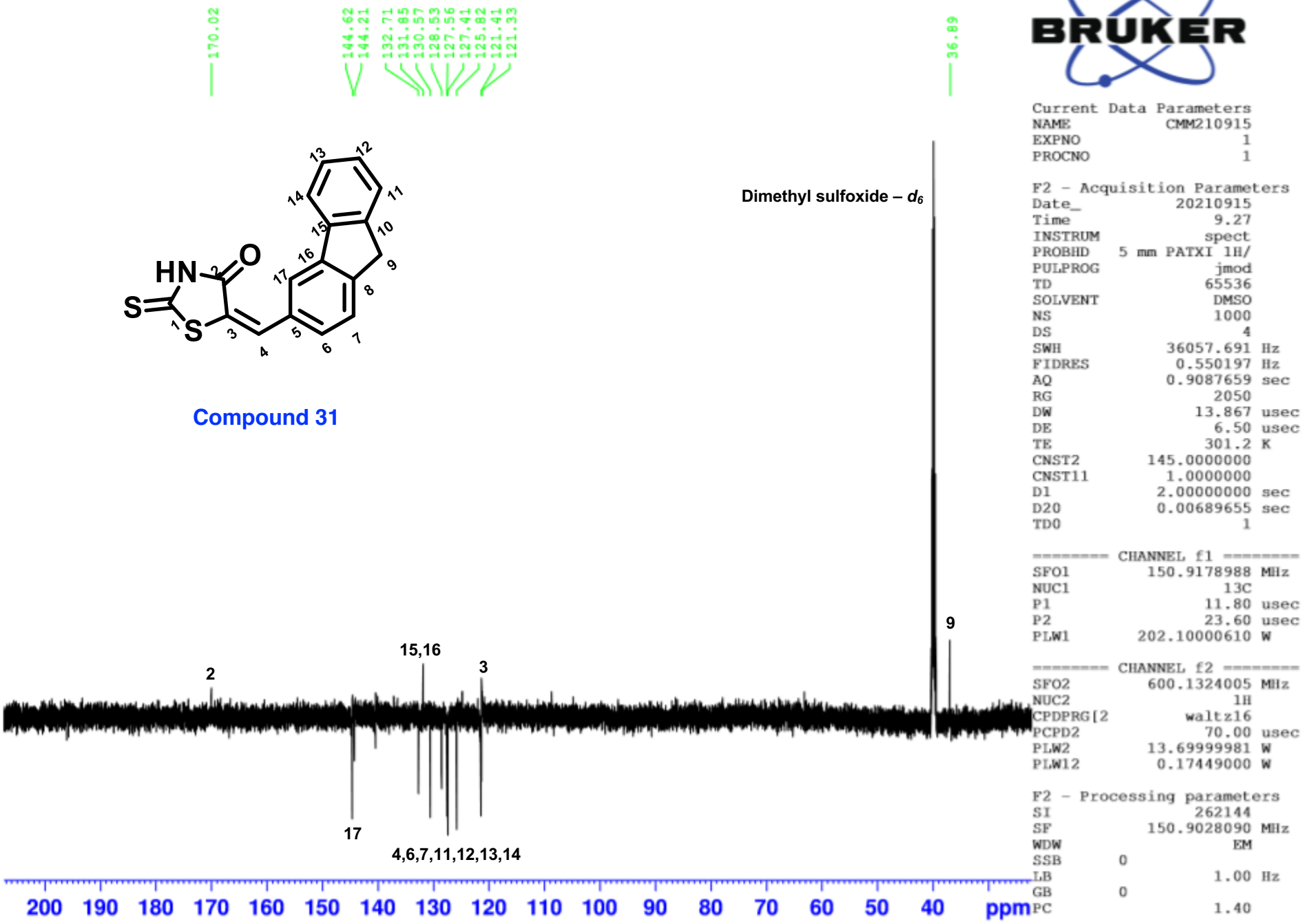
Signature:

Automatic analysis generated by Bruker CMC (b:17).
One or more results have not been created by automatic analysis, or edited manually: marked by '*'.
Report generated by Bruker CMC-assist TopSpin 4.1.3 (of 2021-06-28 13:00:50), on 'MacBook-Pro.local' as 'tzbenton'

Compound 31



31 (JMT-165)



Compound 31

BRUKER

Current Data Parameters
NAME CMM210915
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210915
Time 9.27
INSTRUM spect
PROBHD 5 mm PATXI 1H/
PULPROG jmod
TD 65536
SOLVENT DMSO
NS 1000
DS 4
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 2050
DW 13.867 usec
DE 6.50 usec
TE 301.2 K
CNST2 145.0000000
CNST11 1.0000000
D1 2.00000000 sec
D20 0.00689655 sec
TD0 1

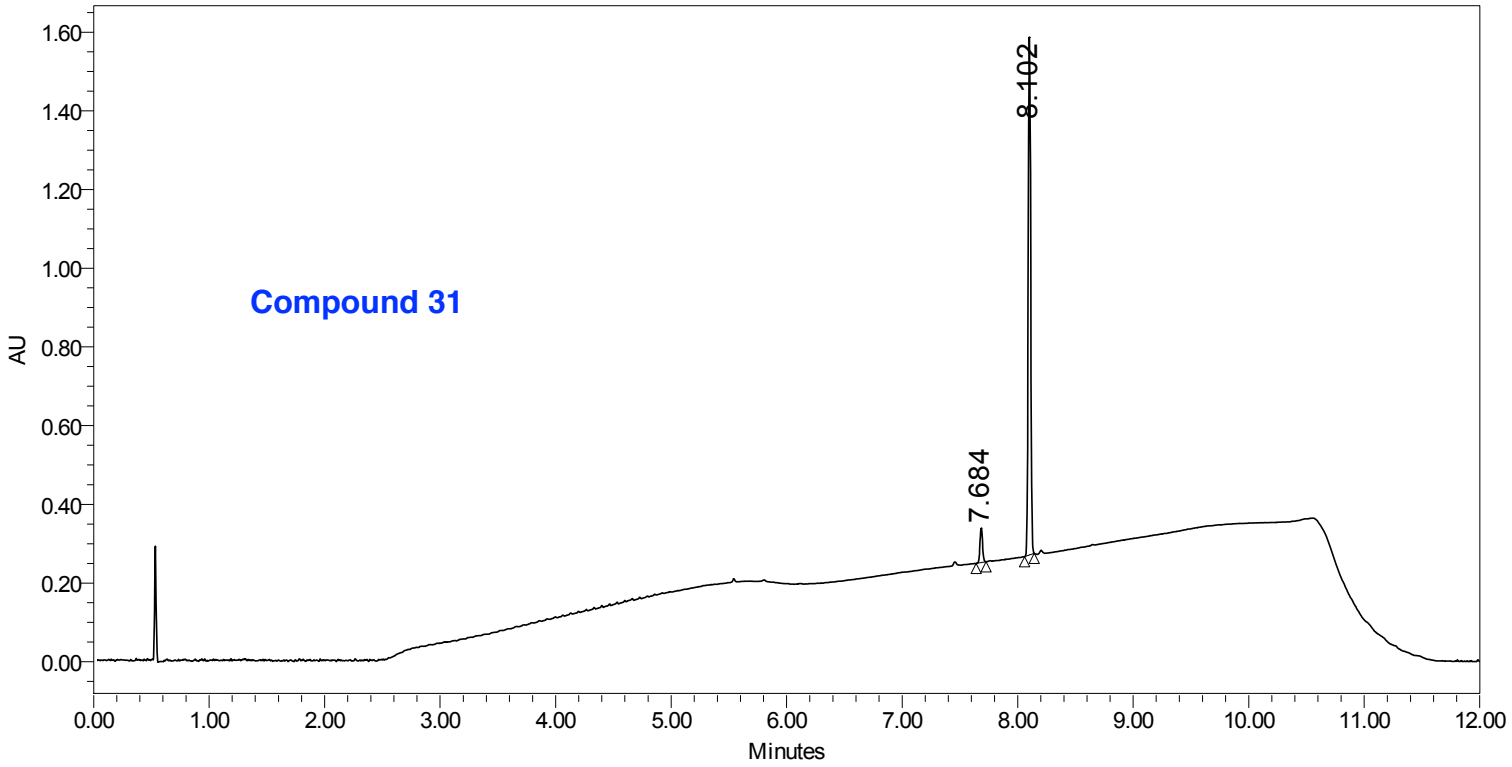
======== CHANNEL f1 ========
SFO1 150.9178988 MHz
NUC1 13C
P1 11.80 usec
P2 23.60 usec
PLW1 202.10000610 W

======== CHANNEL f2 ========
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 70.00 usec
PLW2 13.69999981 W
PLW12 0.17449000 W

F2 - Processing parameters
SI 262144
SF 150.9028090 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

SAMPLE INFORMATION

Sample Name:	165	Acquired By:	System
Sample Type:	Unknown	Sample Set Name	103dx_JMT
Vial:	1:B,8	Acq. Method Set:	ReversePhase_12min_Max Plot
Injection #:	1	Processing Methoc	ReversePhase_Purity_MAX Plot
Injection Volume:	1.00 ul	Channel Name:	PDA Max Plot 190.0 - 800.0
Run Time:	12.0 Minutes	Proc. Chnl. Descr.:	PDA MaxPlot (190.0 nm to 800.0
Date Acquired:	7/27/2021 9:48:22 PM EDT		
Date Processed:	8/31/2021 3:39:41 PM EDT		

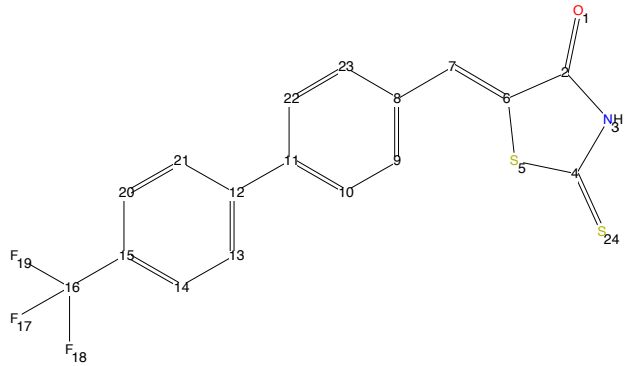


	RT	Area	% Area	Height	Peak Lambda Max.
1	7.684	133736	6.44	87393	412.4
2	8.102	1943048	93.56	1316459	406.8

CMC-assist

CMM210212 **TZB-006**

Consistency: Unknown*, unknown purity*



Sum formula: $C_{17}H_{10}F_3NOS_2$

Molecular Mass: 365.02 Da

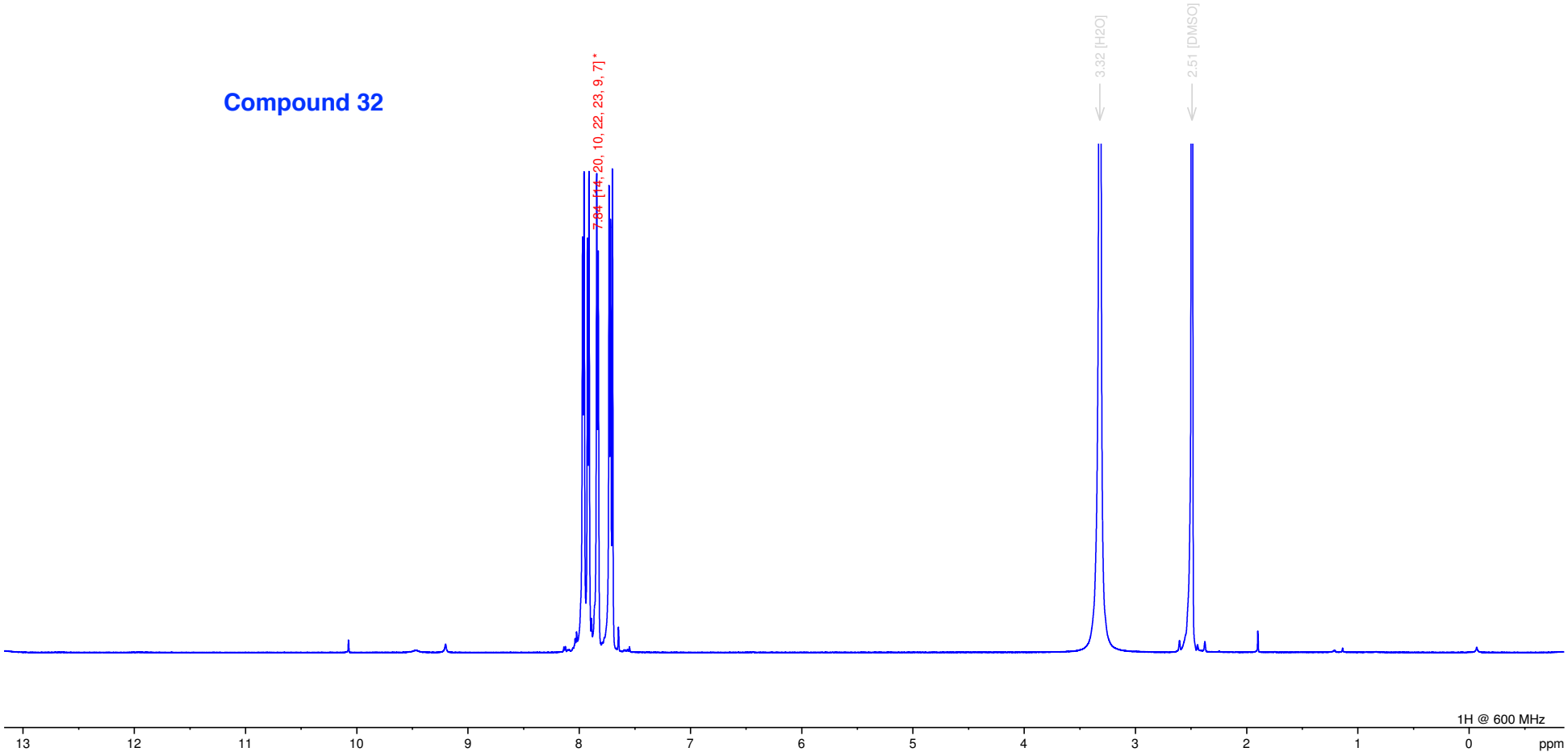
Data set 1H: CMM210212 2 1 /opt/topspin4.1.3
Structure: /opt/topspin4.1.3/CMM210212/2/structure.mol
Acquisition date: February 12, 2021 9:13:01 AM EST
Solvent: DMSO
Probe: 5 mm PATXI 1H/D/19F-13C/15N Z-GRD Z855801/0017
Eretic reference:

Comments:
Multiplet interpretation available for spectrum.
A multiplet interpretation for all major signals in the spectrum could be found. All given impurities could be assigned to regions in the spectrum.

Signature:

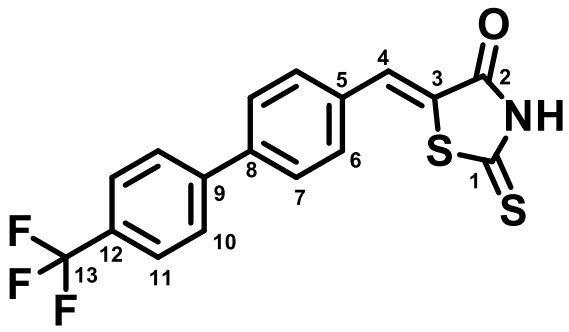
Automatic analysis generated by Bruker CMC (b:17).
One or more results have not been created by automatic analysis, or edited manually: marked by '*'.
Report generated by Bruker CMC-assist TopSpin 4.1.3 (of 2021-06-28 13:00:50), on 'MacBook-Pro.local' as 'tzbenton'

Compound 32



103dx-006

169.36
142.81
140.34
133.01
132.12
131.23
130.90
127.99
127.70
127.60
125.95



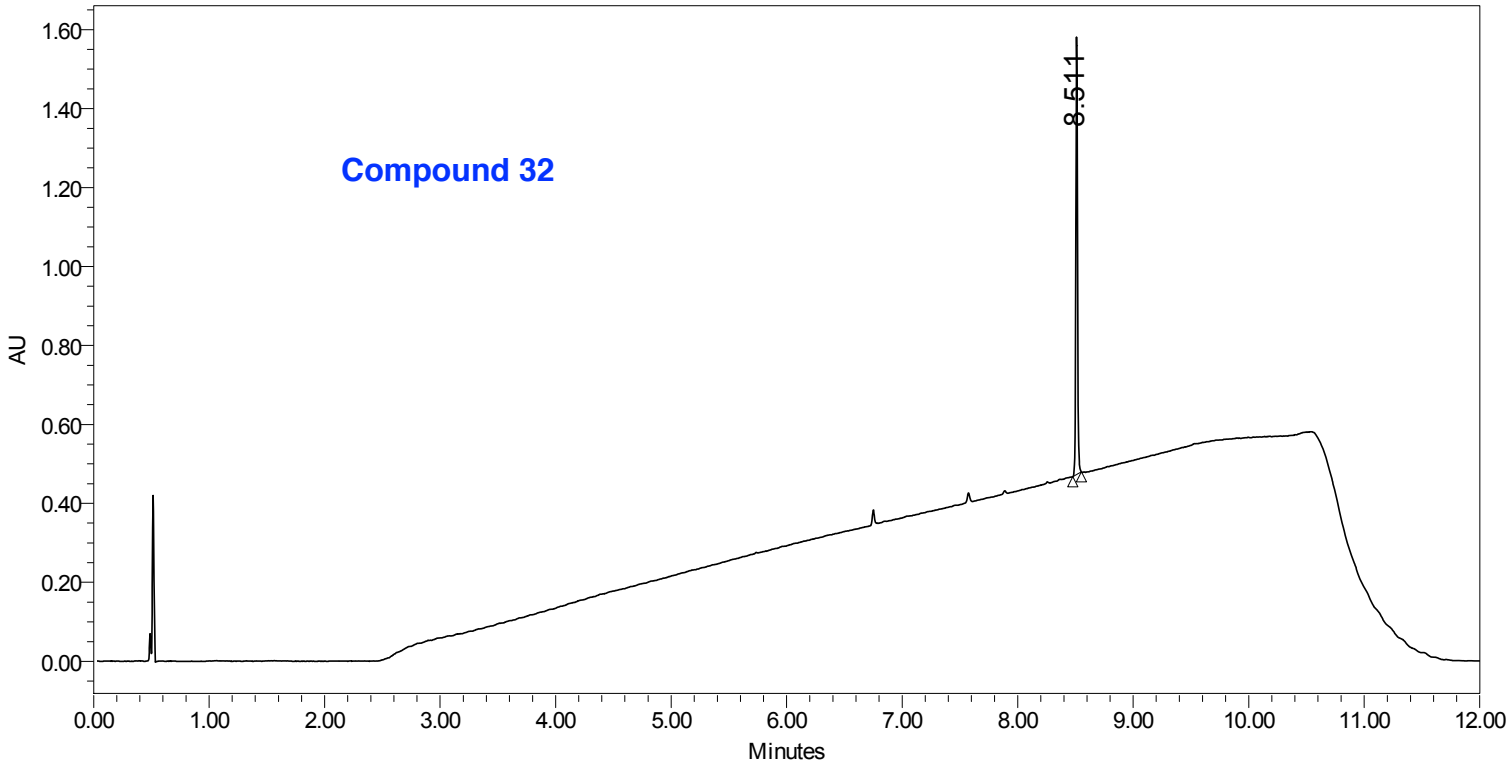
Compound 32

Dimethyl sulfoxide – d_6


```
Current Data Parameters
NAME            CMM210914
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20210914
Time                9.33
INSTRUM            spect
PROBHD   5 mm PATXI 1H/
PULPROG             jmod
TD                 65536
SOLVENT          Acetone
NS                  2000
DS                     4
SWH            36057.691 Hz
FIDRES          0.550197 Hz
AQ              0.9087659 sec
RG                  2050
DW                13.867 usec
DE                 6.50 usec
TE                301.4 K
CNST2         145.0000000
CNST11          1.0000000
D1              2.00000000 sec
D20             0.00689655 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         150.9178988 MHz
NUC1                13C
P1                11.80 usec
P2                23.60 usec
PLW1        202.10000610 W

======== CHANNEL f2 ========
SFO2         600.1324005 MHz
NUC2                1H
CPDPRG[2          waltz16
PCPD2             70.00 usec
PLW2         13.69999981 W
PLW12         0.17449000 W

F2 - Processing parameters
SI                 32768
SF           150.9028090 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

SAMPLE INFORMATION

Sample Name:	2021Feb08_TZB103dx_006	Acquired By:	System
Sample Type:	Unknown	Sample Set Name	TZB_103dx
Vial:	1:F,2	Acq. Method Set:	ReversePhase_12min_Max Plot
Injection #:	1	Processing Method	ReversePhase_Purity_MAX Plot
Injection Volume:	1.00 ul	Channel Name:	PDA Max Plot 190.0 - 800.0
Run Time:	12.0 Minutes	Proc. Chnl. Descr.:	PDA MaxPlot (190.0 nm to 800.0
Date Acquired:	2/8/2021 2:19:18 PM EST		
Date Processed:	8/31/2021 3:49:53 PM EDT		



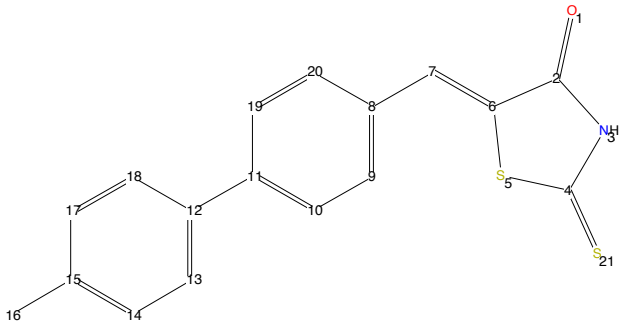
	RT	Area	% Area	Height	Peak Lambda Max.
1	8.511	1165347	100.00	1112283	383.7

CMC-assist

CMM210212

Consistency: Unknown*, unknown purity*

Data set 1H: CMM210212 3 1 /opt/topspin4.1.3
Structure: /opt/topspin4.1.3/CMM210212/3/structure.mol
Acquisition date: February 12, 2021 9:18:02 AM EST
Solvent: DMSO
Probe: 5 mm PATXI 1H/D/19F-13C/15N Z-GRD Z855801/0017
Eretic reference:



Sum formula: $C_{17}H_{13}NOS_2$

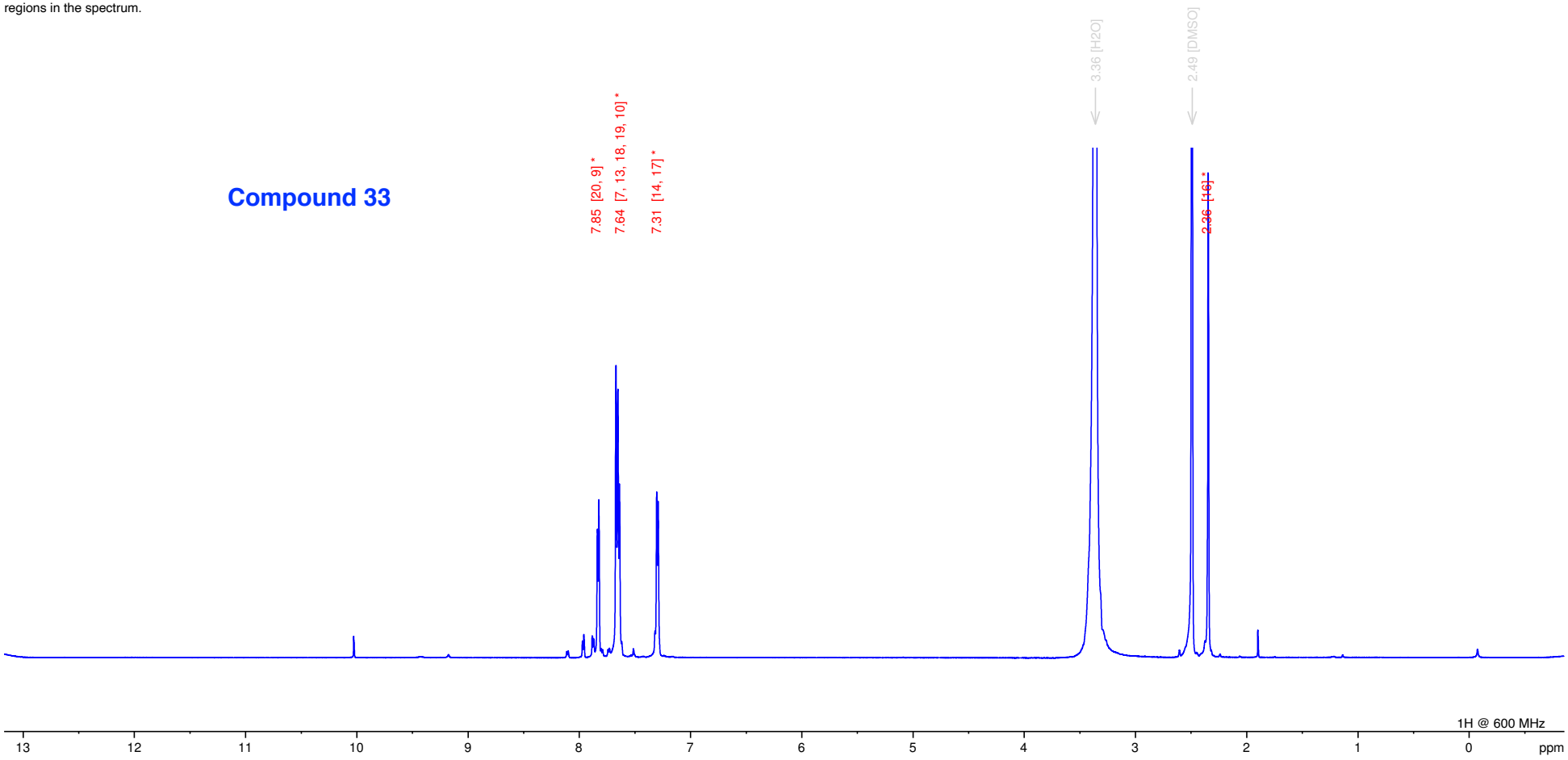
Molecular Mass: 311.04 Da

Comments:
Multiplet interpretation available for spectrum.Multiplet interpretation available for spectrum.
A multiplet interpretation for all major signals in the spectrum could be found. All given impurities could be assigned to regions in the spectrum.A multiplet interpretation for all major signals in the spectrum could be found. All given impurities could be assigned to regions in the spectrum.

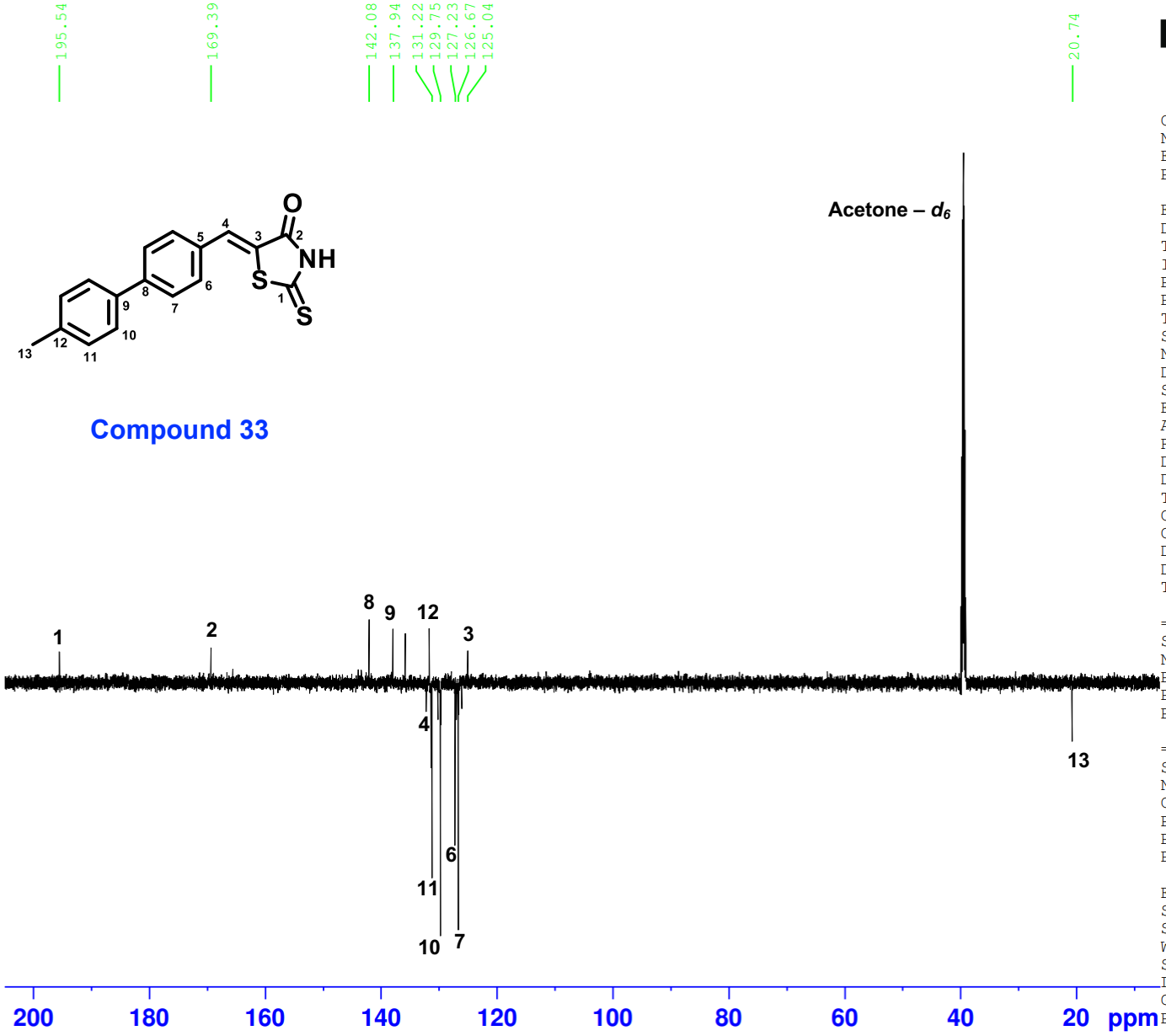
Signature:

Automatic analysis generated by Bruker CMC (b:17).
One or more results have not been created by automatic analysis, or edited manually: marked by '*'.
Report generated by Bruker CMC-assist TopSpin 4.1.3 (of 2021-06-28 13:00:50), on 'MacBook-Pro.local' as 'tzbenton'

Compound 33



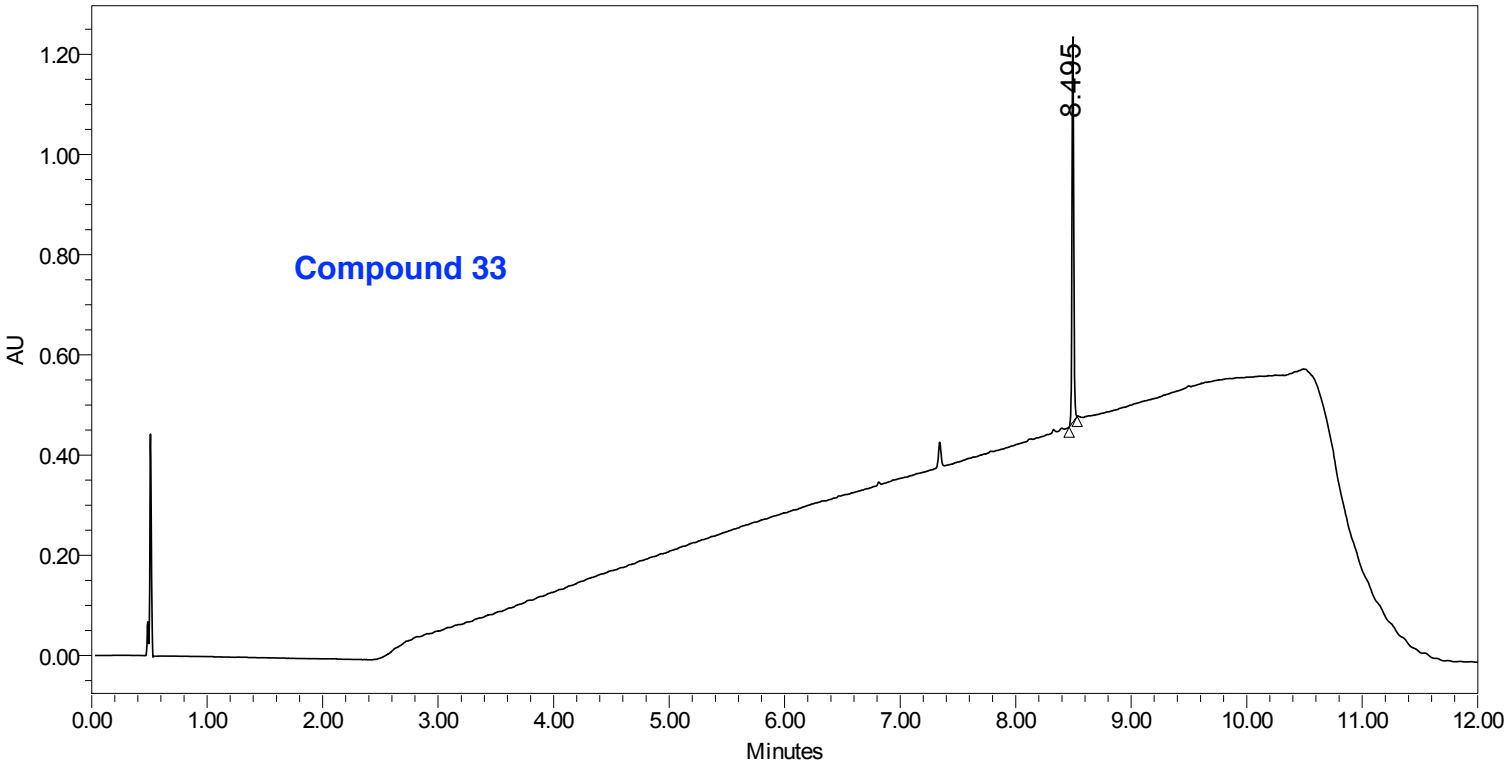
103dx-007-apt




```
Current Data Parameters
NAME         CMM210910-t
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210910
Time               12.28
INSTRUM            spect
PROBHD   5 mm PATXI 1H/
PULPROG             jmod
TD                 65536
SOLVENT          Acetone
NS                  2064
DS                     4
SWH            36057.691 Hz
FIDRES          0.550197 Hz
AQ             0.9087659 sec
RG                  2050
DW                13.867 usec
DE                 6.50 usec
TE                301.3 K
CNST2         145.0000000
CNST11          1.0000000
D1             2.00000000 sec
D20            0.00689655 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          150.9178988 MHz
NUC1                 13C
P1                11.80 usec
P2                23.60 usec
PLW1        202.10000610 W

======== CHANNEL f2 ========
SFO2          600.1324005 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2             70.00 usec
PLW2          13.69999981 W
PLW12          0.17449000 W

F2 - Processing parameters
SI                 32768
SF            150.9028090 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

SAMPLE INFORMATION

Sample Name:	2021Feb08_TZB103dx_007	Acquired By:	System
Sample Type:	Unknown	Sample Set Name	TZB_103dx
Vial:	1:F,1	Acq. Method Set:	ReversePhase_12min_Max Plot
Injection #:	1	Processing Methoc	ReversePhase_Purity_MAX Plot
Injection Volume:	1.00 ul	Channel Name:	PDA Max Plot 190.0 - 800.0
Run Time:	12.0 Minutes	Proc. Chnl. Descr.:	PDA MaxPlot (190.0 nm to 800.0
Date Acquired:	2/8/2021 2:05:57 PM EST		
Date Processed:	8/31/2021 3:47:16 PM EDT		



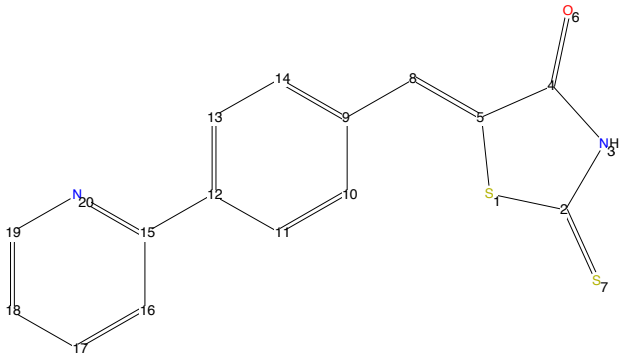
	RT	Area	% Area	Height	Peak Lambda Max.
1	8.495	790841	100.00	768406	392.4

CMC-assist

CMM210622 JM T-16 7

Consistency: Unknown*, unknown purity*

Data set 1H: CMM210622 6 1 /opt/topspin4.1.3
Structure: /opt/topspin4.1.3/CMM210622/6/structure.mol
Acquisition date: June 22, 2021 11:30:54 AM EDT
Solvent: DMSO
Probe: 5 mm PATXI 1H/D/19F-13C/15N Z-GRD Z855801/0017
Eretic reference:



Sum formula:
$C_{15}H_{10}N_2OS_2$

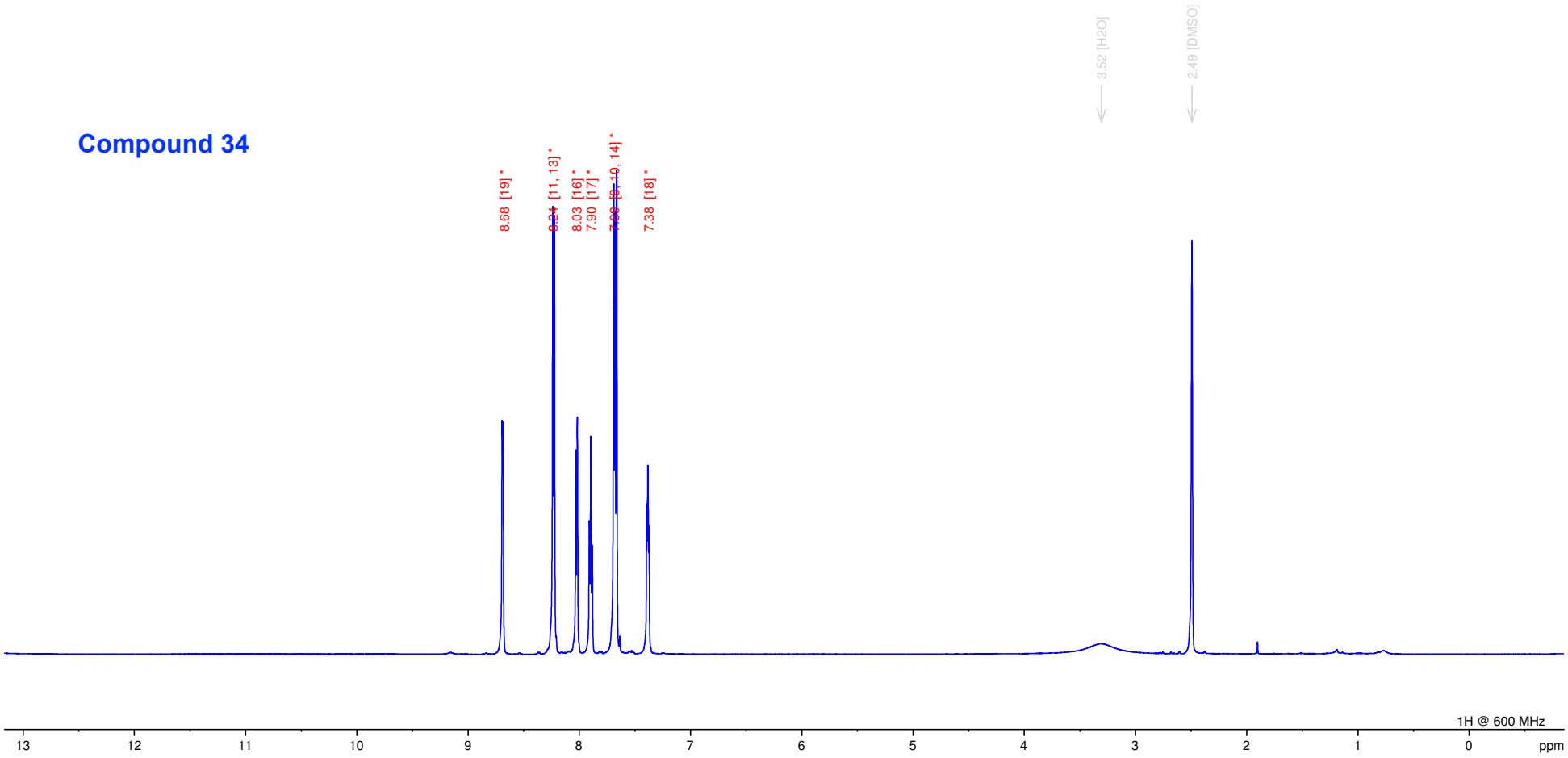
Molecular Mass:
298.02 Da

Comments:
Multiplet interpretation available for spectrum.
A multiplet interpretation for all major signals in the spectrum could be found. All given impurities could be assigned to regions in the spectrum.

Signature:

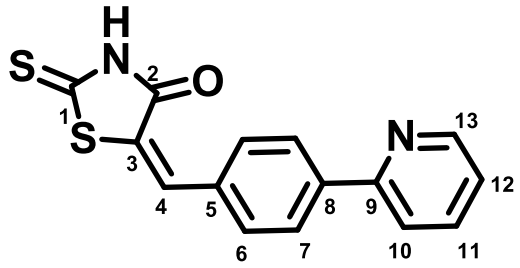
Automatic analysis generated by Bruker CMC (b:17).
One or more results have not been created by automatic analysis, or edited manually: marked by '*'.
Report generated by Bruker CMC-assist TopSpin 4.1.3 (of 2021-06-28 13:00:50), on 'MacBook-Pro.local' as 'tzbenton'

Compound 34



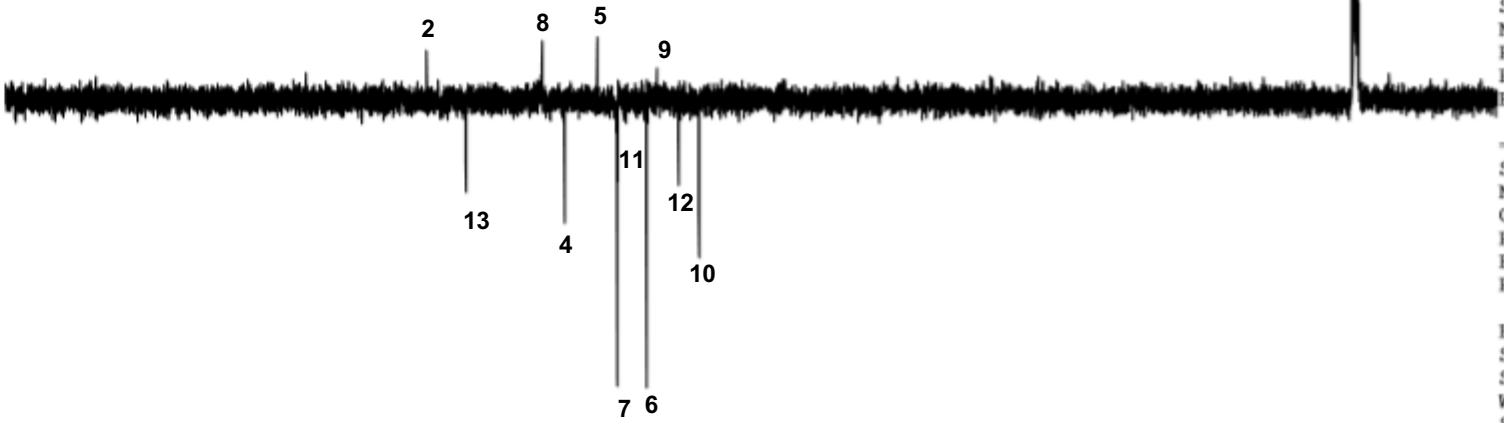
34 (JMT-167)

155.11
150.23
140.78
137.98
133.92
131.43
131.39
127.81
123.82
121.30



Compound 34

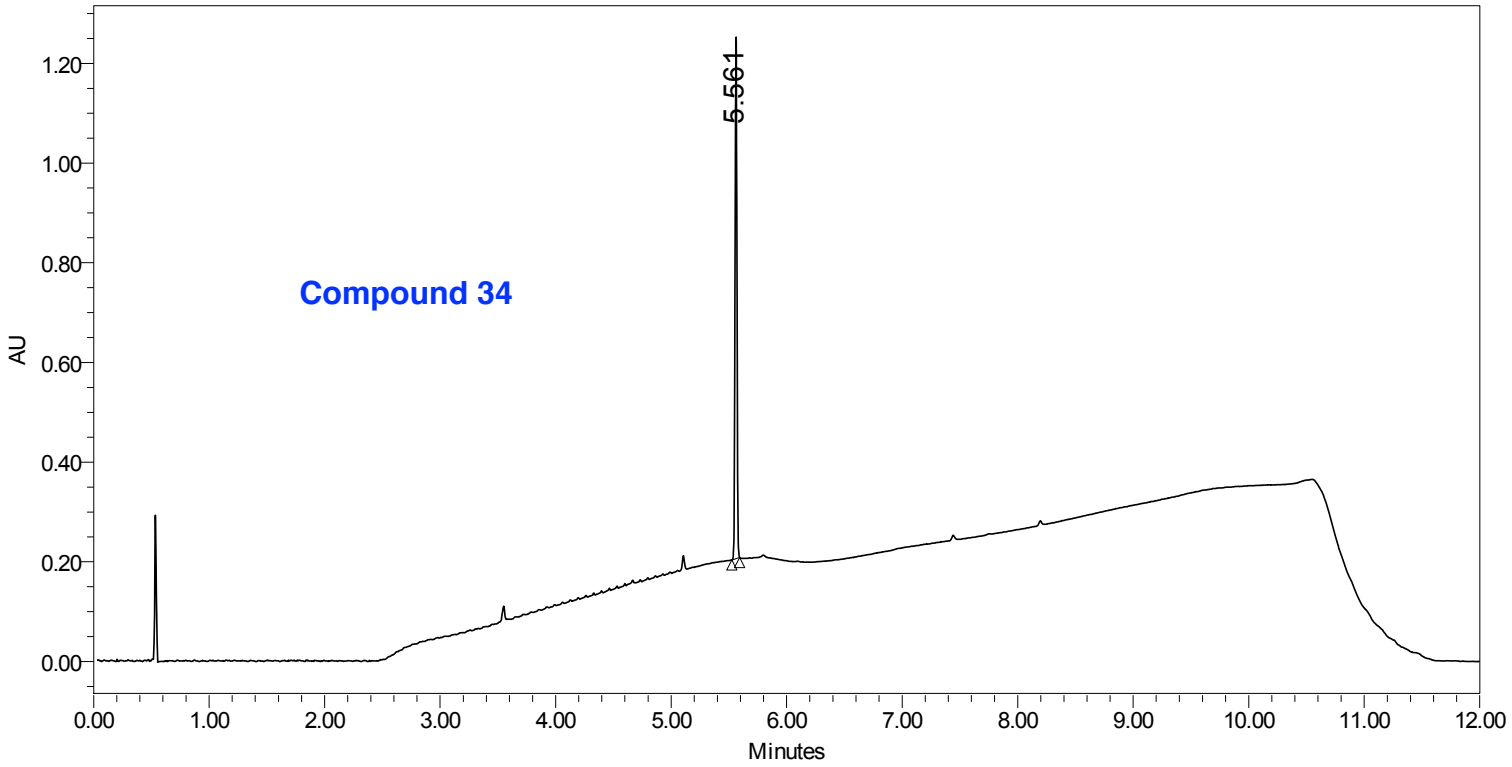
Dimethyl sulfoxide – d_6




```
Current Data Parameters
NAME                  CMM210915
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20210915
Time                      10.38
INSTRUM                   spect
PROBHD    5 mm PATXI 1H/
PULPROG                   jmod
TD                       65536
SOLVENT                   DMSO
NS                        1000
DS                           4
SWH                  36057.691 Hz
FIDRES                0.550197 Hz
AQ                    0.9087659 sec
RG                         2050
DW                       13.867 usec
DE                         6.50 usec
TE                        301.2 K
CNST2                145.0000000
CNST11                 1.0000000
D1                     2.00000000 sec
D20                    0.00689655 sec
TD0                           1

======== CHANNEL f1 ========
SFO1                 150.9178988 MHz
NUC1                         13C
P1                         11.80 usec
P2                         23.60 usec
PLW1                202.10000610 W

======== CHANNEL f2 ========
SFO2                 600.1324005 MHz
NUC2                         1H
CPDPRG[2                 waltz16
PCPD2                      70.00 usec
PLW2                 13.69999981 W
PLW12                 0.17449000 W

F2 - Processing parameters
SI                           32768
SF                  150.9028090 MHz
WDW                             EM
SSB                  0
LB                            1.00 Hz
GB                   0
PC                            1.40
```

SAMPLE INFORMATION

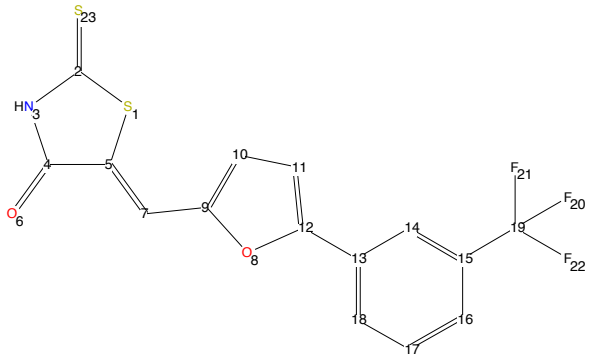
Sample Name:	167	Acquired By:	System
Sample Type:	Unknown	Sample Set Name	103dx_JMT
Vial:	1:B,2	Acq. Method Set:	ReversePhase_12min_Max Plot
Injection #:	1	Processing Methoc	ReversePhase_Purity_MAX Plot
Injection Volume:	1.00 ul	Channel Name:	PDA Max Plot 190.0 - 800.0
Run Time:	12.0 Minutes	Proc. Chnl. Descr.:	PDA MaxPlot (190.0 nm to 800.0
Date Acquired:	7/27/2021 8:34:05 PM EDT		
Date Processed:	8/31/2021 3:42:43 PM EDT		



	RT	Area	% Area	Height	Peak Lambda Max.
1	5.561	1199345	100.00	1047356	388.1

CMC-assist

CMM210622



Consistency: Unknown*, unknown purity*

Sum formula: $C_{15}H_8F_3NO_2S_2$

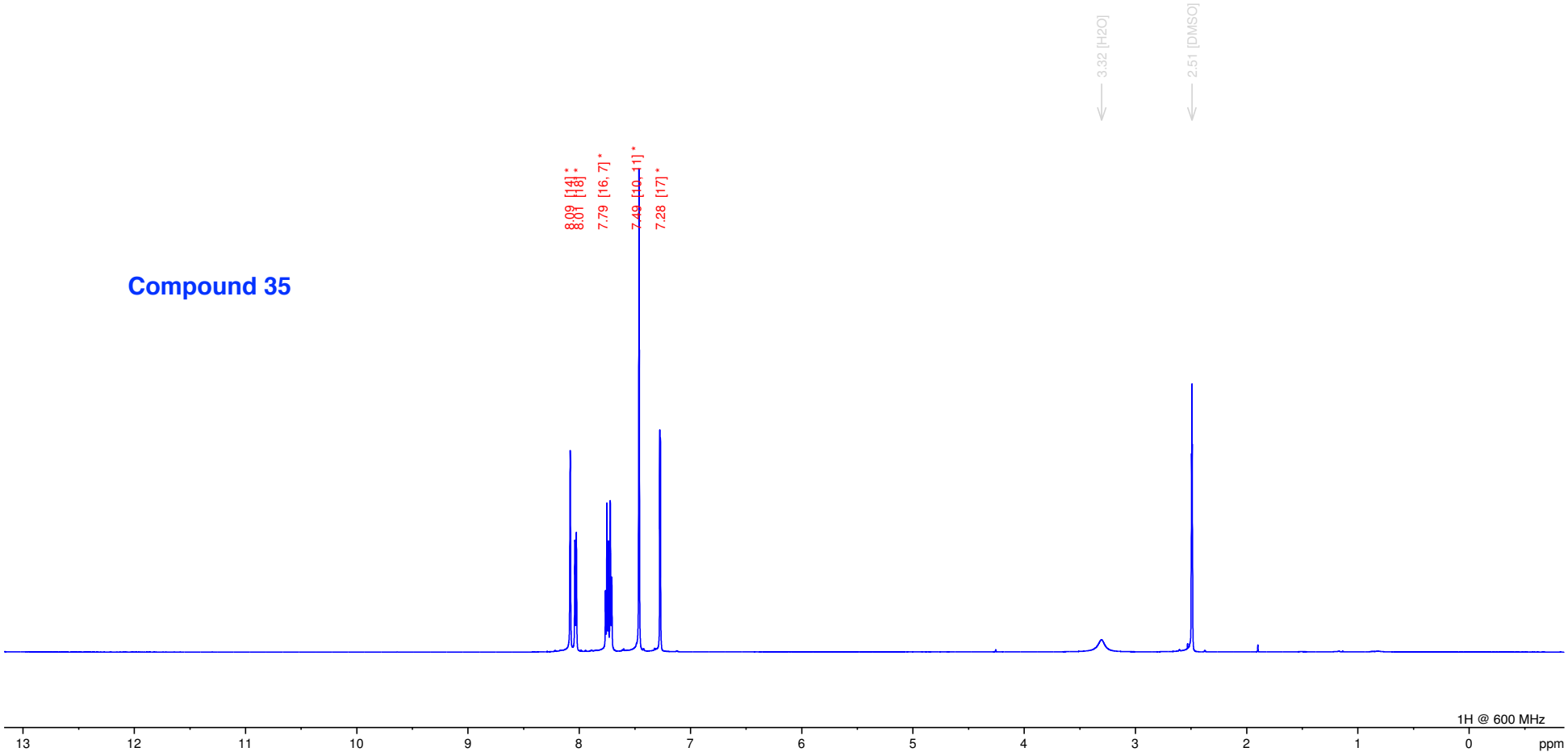
Molecular Mass: 354.99 Da

Data set 1H:	CMM210622 7 1 /opt/topspin4.1.3
Structure:	/opt/topspin4.1.3/CMM210622/7/structure.mol
Acquisition date:	June 22, 2021 11:36:16 AM EDT
Solvent:	DMSO
Probe:	5 mm PATXI 1H/D/19F-13C/15N Z-GRD Z855801/0017
Eretic reference:	

Comments:
Multiplet interpretation available for spectrum.
A multiplet interpretation for all major signals in the spectrum could be found. All given impurities could be assigned to regions in the spectrum.

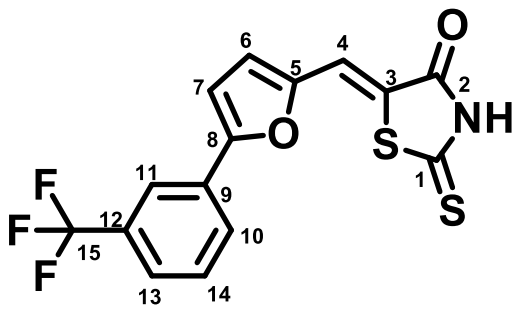
Signature:

Automatic analysis generated by Bruker CMC (b:17).
One or more results have not been created by automatic analysis, or edited manually: marked by '*'.
Report generated by Bruker CMC-assist TopSpin 4.1.3 (of 2021-06-28 13:00:50), on 'MacBook-Pro.local' as 'tzbenton'



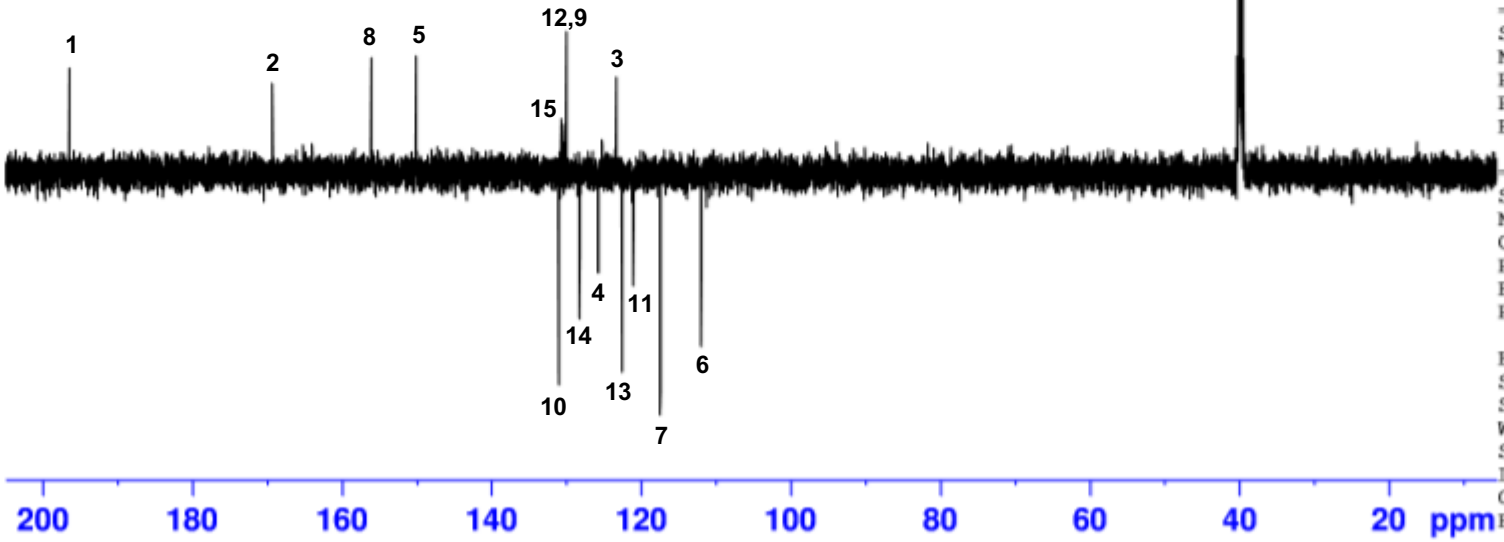
35 (JMT-169)

196.52 169.37 156.13 150.12 131.03 130.68 130.47 130.03 128.25 125.73 123.35 122.56 121.07 117.46 111.98



Compound 35

Dimethyl sulfoxide – d_6

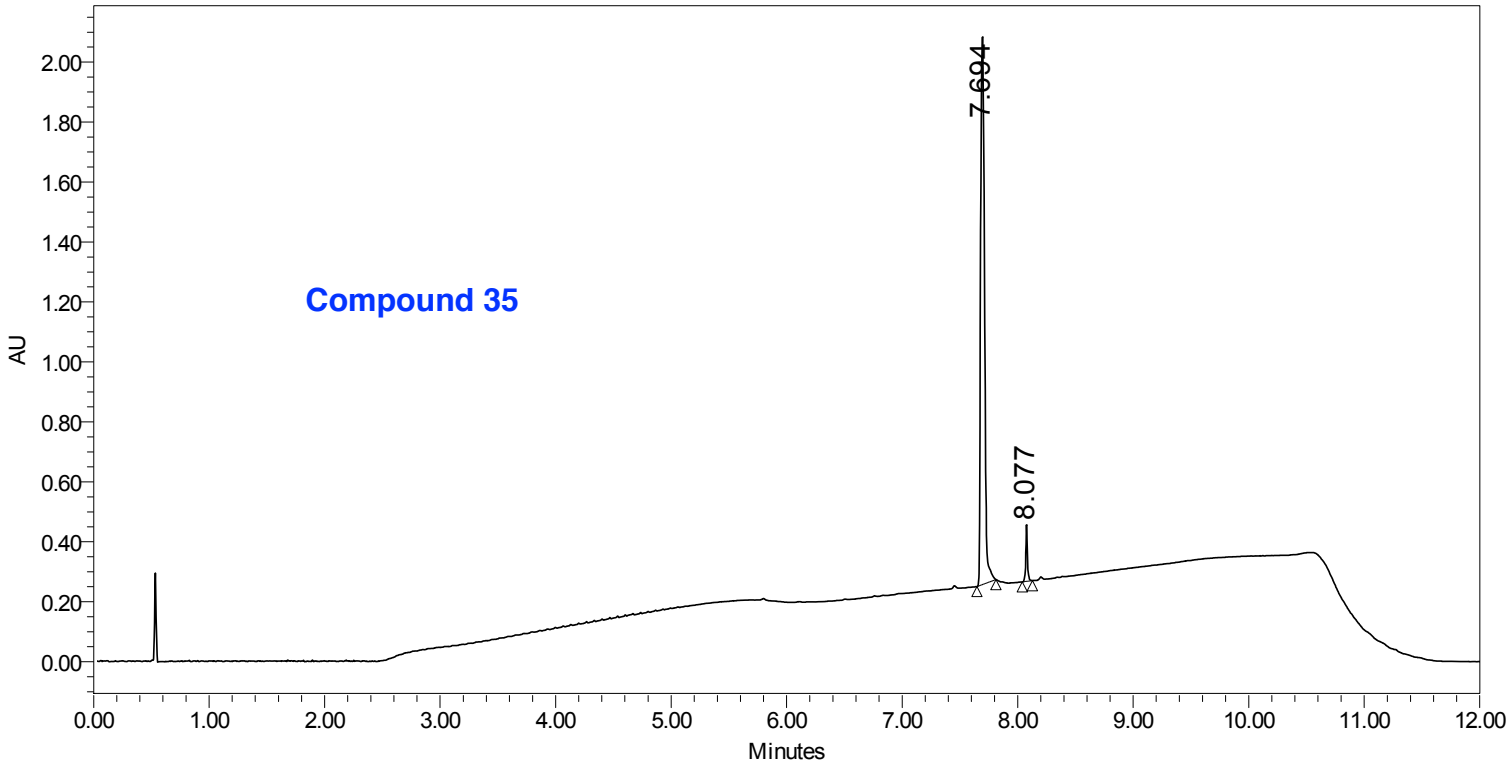


BRUKER

```
Current Data Parameters
NAME                 CMM210914
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_               20210914
Time                   10.30
INSTRUM                spect
PROBHD    5 mm PATXI 1H/
PULPROG                 jmod
TD                     65536
SOLVENT                 DMSO
NS                      1000
DS                         4
SWH                36057.691 Hz
FIDRES             0.550197 Hz
AQ                 0.9087659 sec
RG                      2050
DW                   13.867 usec
DE                     6.50 usec
TE                    301.3 K
CNST2              145.0000000
CNST11               1.0000000
D1                 2.00000000 sec
D20                0.00689655 sec
TD0                          1

======== CHANNEL f1 ========
SFO1            150.9178988 MHz
NUC1                      13C
P1                      11.80 usec
P2                      23.60 usec
PLW1           202.10000610 W

======== CHANNEL f2 ========
SFO2            600.1324005 MHz
NUC2                       1H
CPDPRG[2              waltz16
PCPD2                   70.00 usec
PLW2           13.69999981 W
PLW12           0.17449000 W

F2 - Processing parameters
SI                       32768
SF              150.9028090 MHz
WDW                         EM
SSB          0
LB                      1.00 Hz
GB           0
PC                      1.40
```

SAMPLE INFORMATION

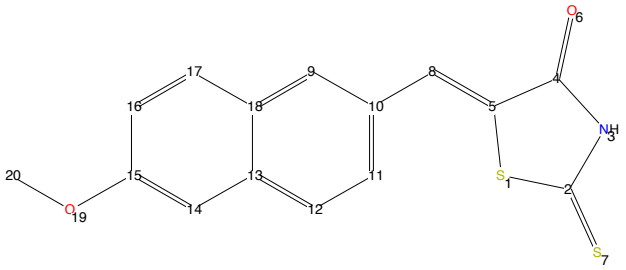
Sample Name:	169	Acquired By:	System
Sample Type:	Unknown	Sample Set Name	103dx_JMT
Vial:	1:C,3	Acq. Method Set:	ReversePhase_12min_Max Plot
Injection #:	1	Processing Method	ReversePhase_Purity_MAX Plot
Injection Volume:	1.00 ul	Channel Name:	PDA Max Plot 190.0 - 800.0
Run Time:	12.0 Minutes	Proc. Chnl. Descr.:	PDA MaxPlot (190.0 nm to 800.0
Date Acquired:	7/27/2021 10:26:00 PM EDT		
Date Processed:	8/31/2021 3:45:39 PM EDT		



	RT	Area	% Area	Height	Peak Lambda Max.
1	7.694	4321518	95.76	1827309	304.9
2	8.077	191439	4.24	189068	441.7

CMC-assist

CMM210622 **JMT-173**



Consistency: Unknown*, unknown purity*

Sum formula: $C_{15}H_{11}NO_2S_2$

Molecular Mass: 301.02 Da

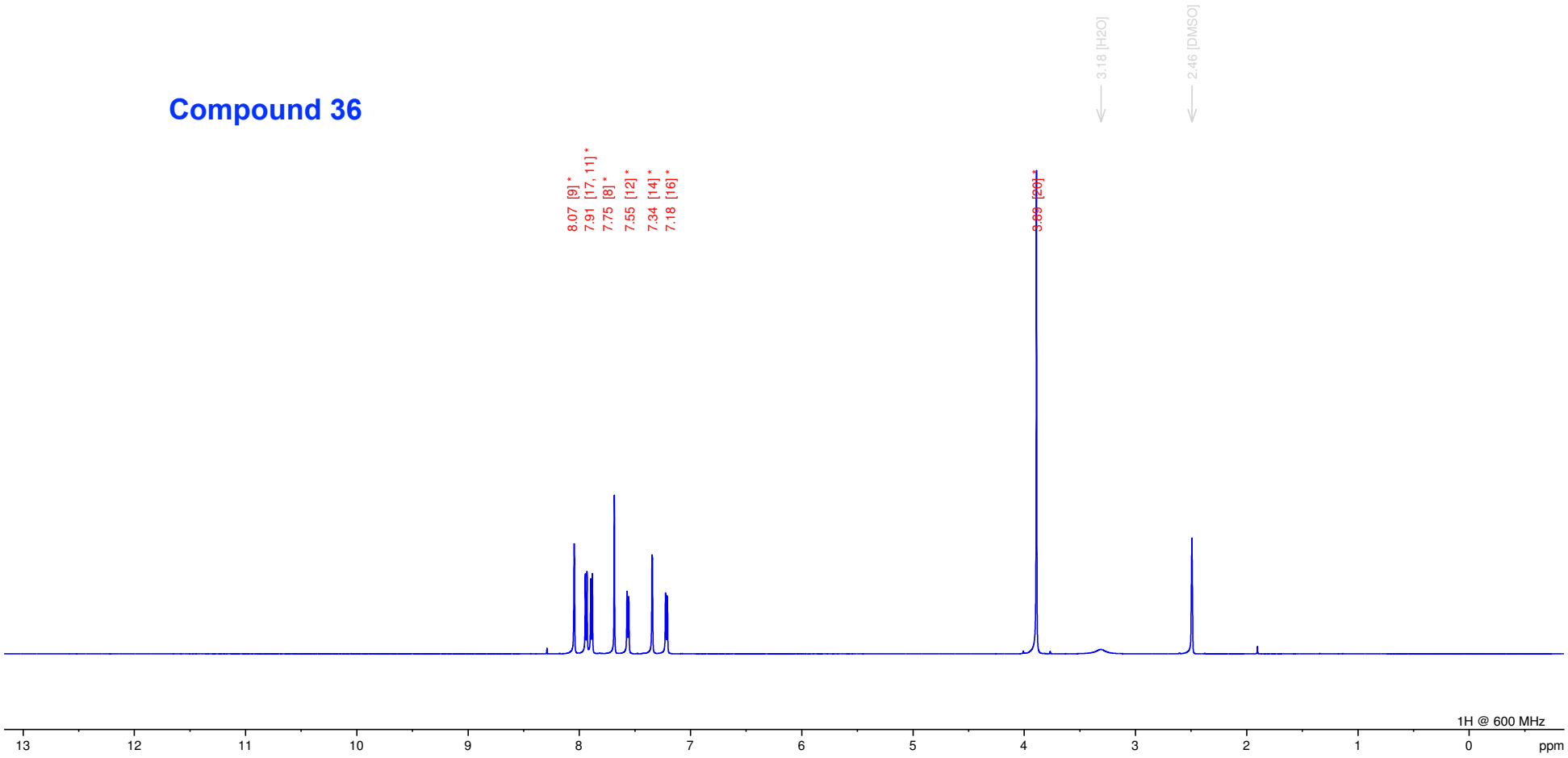
Data set 1H: CMM210622 4 1 /opt/topspin4.1.3
Structure: /opt/topspin4.1.3/CMM210622/4/structure.mol
Acquisition date: June 22, 2021 11:20:30 AM EDT
Solvent: DMSO
Probe: 5 mm PATXI 1H/D/19F-13C/15N Z-GRD Z855801/0017
Eretic reference:

Comments:
Multiplet interpretation available for spectrum.
A multiplet interpretation for all major signals in the spectrum could be found. All given impurities could be assigned to regions in the spectrum.

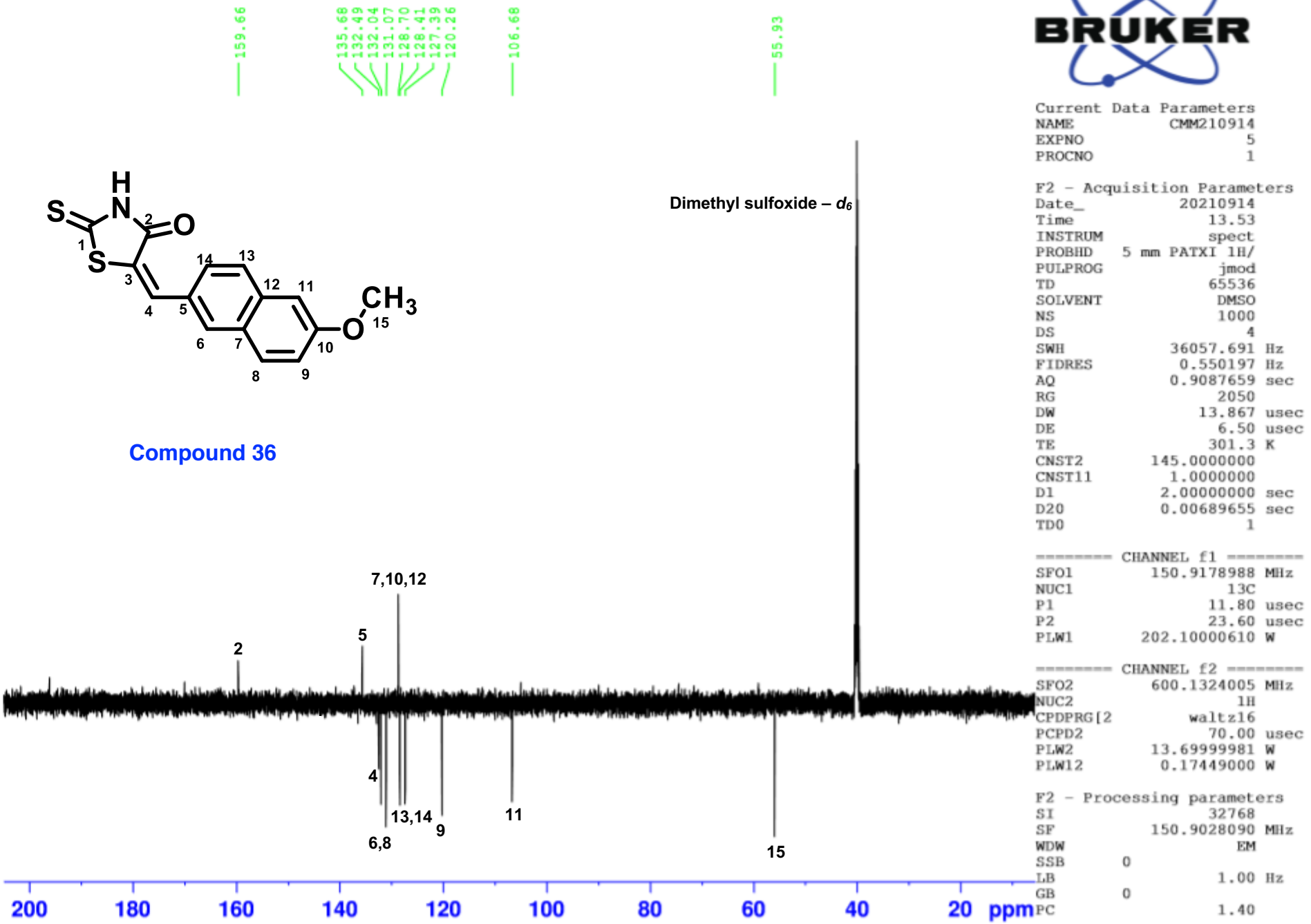
Signature:

Automatic analysis generated by Bruker CMC (b:17).
One or more results have not been created by automatic analysis, or edited manually: marked by '*'.
Report generated by Bruker CMC-assist TopSpin 4.1.3 (of 2021-06-28 13:00:50), on 'MacBook-Pro.local' as 'tzbenton'

Compound 36



36 (JMT-173)

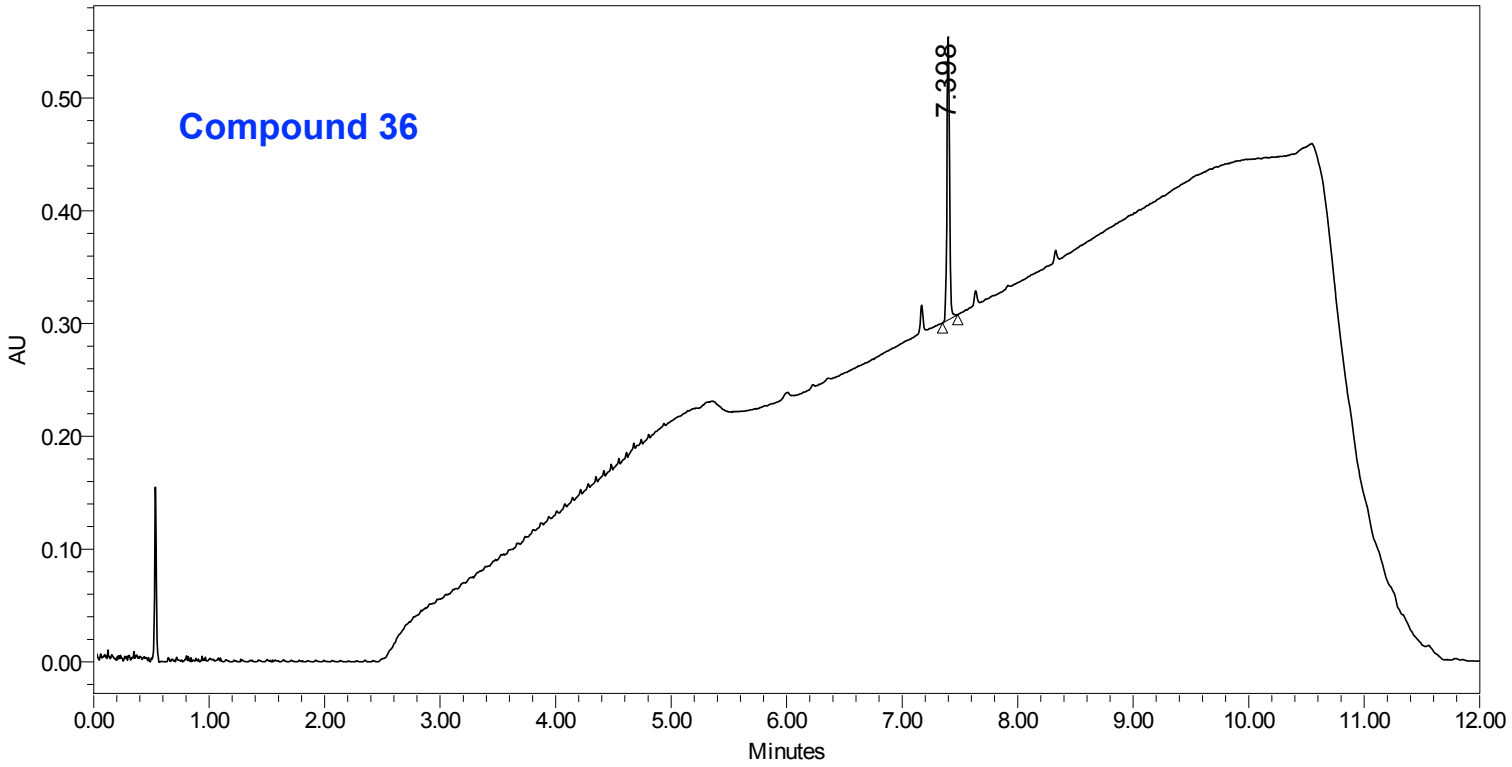


Compound 36

```
Current Data Parameters
NAME            CMM210914
EXPNO                   5
PROCNO                  1

F2 - Acquisition Parameters
Date_            20210914
Time                13.53
INSTRUM             spect
PROBHD   5 mm PATXI 1H/
PULPROG             jmod
TD                 65536
SOLVENT             DMSO
NS                  1000
DS                     4
SWH           36057.691 Hz
FIDRES         0.550197 Hz
AQ            0.9087659 sec
RG                  2050
DW               13.867 usec
DE                6.50 usec
TE               301.3 K
CNST2        145.0000000
CNST11         1.0000000
D1            2.00000000 sec
D20           0.00689655 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         150.9178988 MHz
NUC1                13C
P1               11.80 usec
P2               23.60 usec
PLW1       202.10000610 W

======== CHANNEL f2 ========
SFO2         600.1324005 MHz
NUC2                1H
CPDPRG[2          waltz16
PCPD2              70.00 usec
PLW2         13.69999981 W
PLW12         0.17449000 W

F2 - Processing parameters
SI                 32768
SF           150.9028090 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

SAMPLE INFORMATION

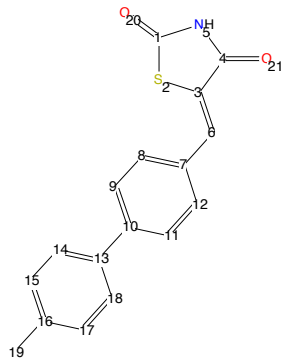
Sample Name:	173	Acquired By:	System
Sample Type:	Unknown	Sample Set Name	103dx_JMT_2
Vial:	1:D,1	Acq. Method Set:	ReversePhase_12min_Max Plot
Injection #:	1	Processing Methoc	ReversePhase_Purity_MAX Plot
Injection Volume:	2.00 ul	Channel Name:	PDA Max Plot 190.0 - 800.0
Run Time:	12.0 Minutes	Proc. Chnl. Descr.:	PDA MaxPlot (190.0 nm to 800.0
Date Acquired:	8/31/2021 4:51:35 PM EDT		
Date Processed:	9/1/2021 10:43:08 AM EDT		



	RT	Area	% Area	Height	Peak Lambda Max.
1	7.398	393044	100.00	250883	407.4

CMC-assist

TZB-009_2



Consistency: Unknown*, unknown purity*

Data set 1H: TZB-009_2 1 1 /opt/topspin4.1.3
Structure: /opt/topspin4.1.3/TZB-009_2/1/structure.mol
Acquisition date: July 21, 2021 9:01:46 AM EDT
Solvent: Acetone
Probe: 5 mm PATXI 1H/D/19F-13C/15N Z-GRD Z855801/0017
Eretic reference:

Sum formula: $C_{17}H_{13}NO_2S$

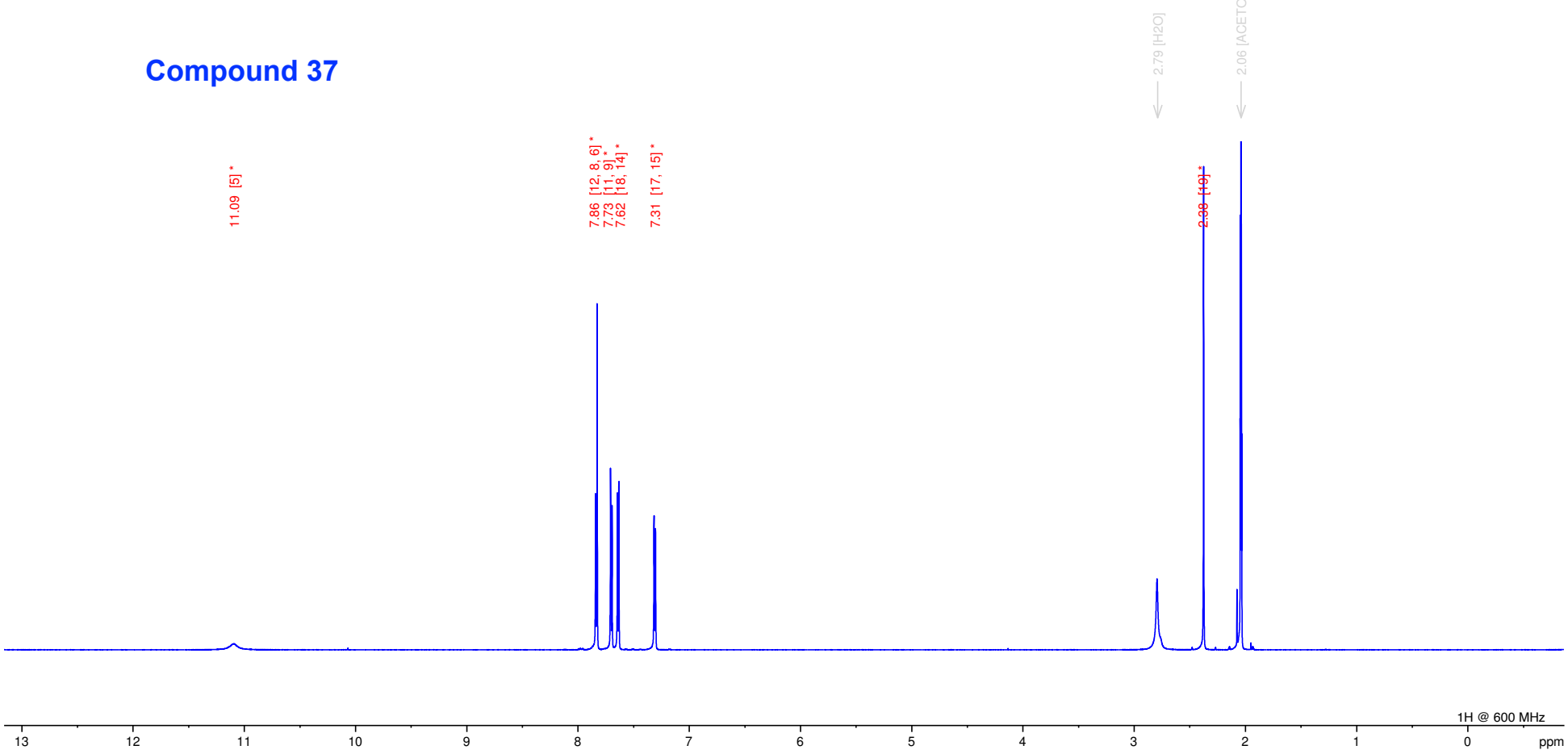
Molecular Mass: 295.07 Da

Comments:
Multiplet interpretation available for spectrum.
A multiplet interpretation for all major signals in the spectrum could be found. All given impurities could be assigned to regions in the spectrum.

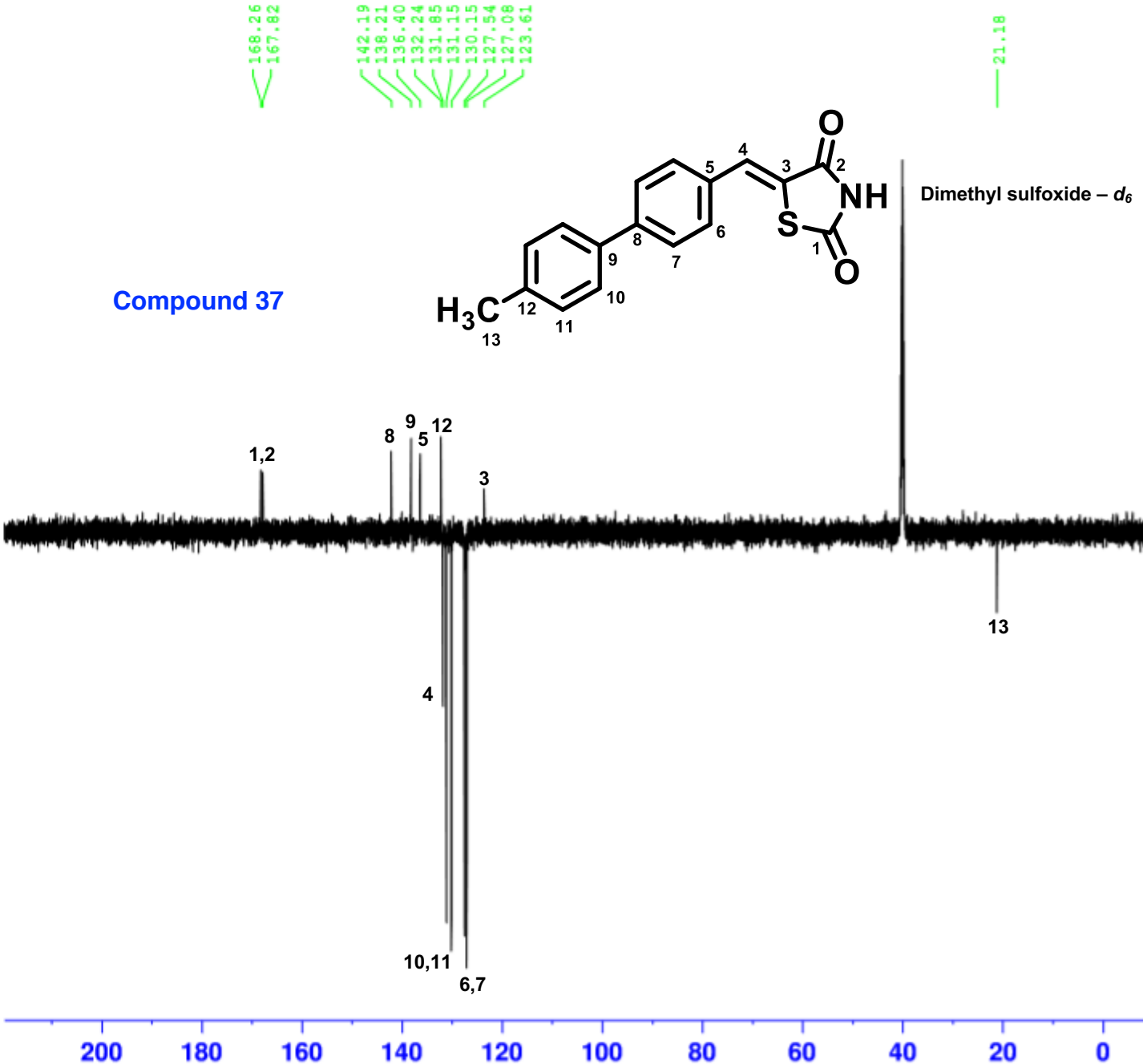
Signature:

Automatic analysis generated by Bruker CMC (b:17).
One or more results have not been created by automatic analysis, or edited manually: marked by '*'.
Report generated by Bruker CMC-assist TopSpin 4.1.3 (of 2021-06-28 13:00:50), on 'MacBook-Pro.local' as 'tzbenton'

Compound 37



37 (TZB103dx009)

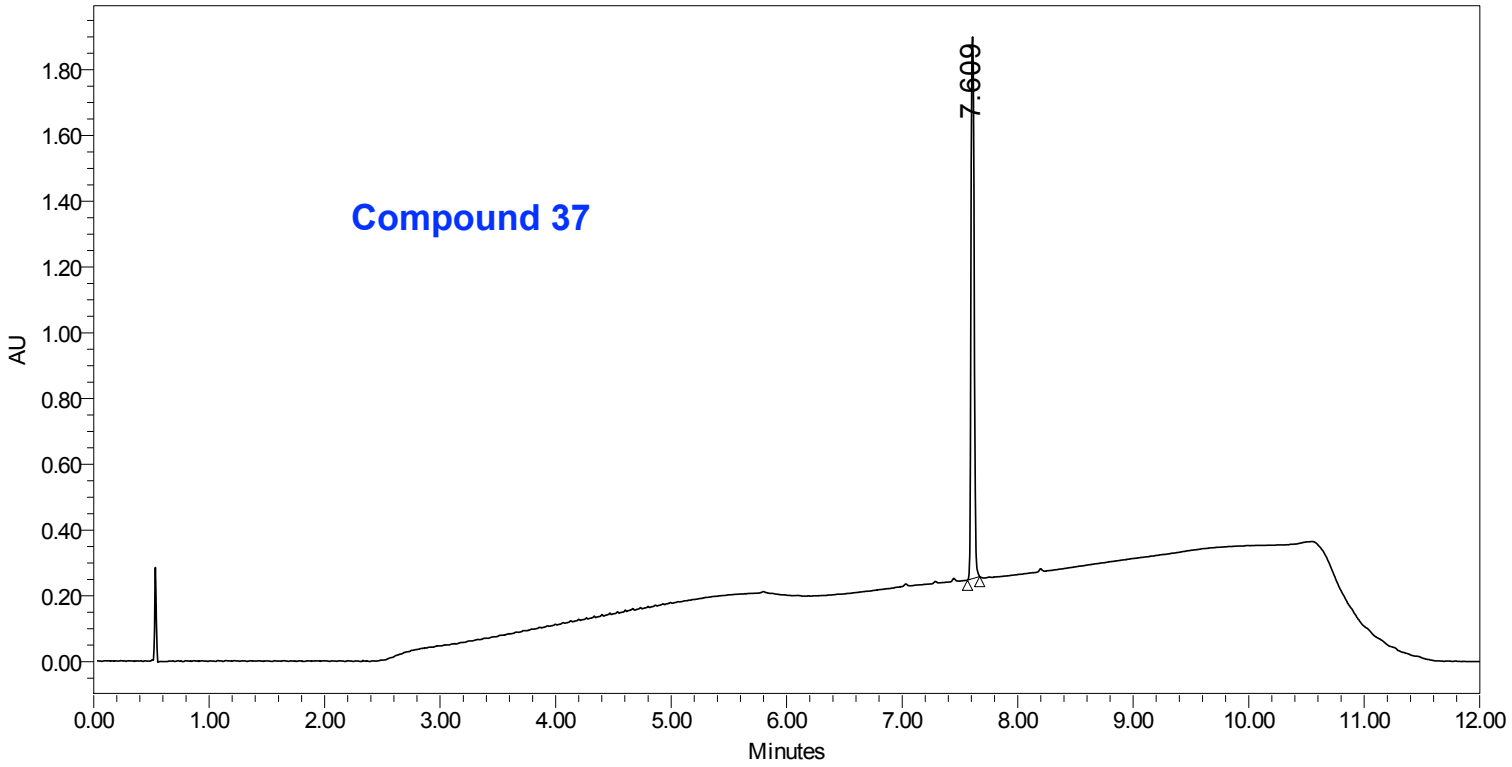


BRUKER

```
Current Data Parameters
NAME                  CMM210917
EXPNO                         6
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20210917
Time                      14.02
INSTRUM                   spect
PROBHD    5 mm PATXI 1H/
PULPROG                   jmod
TD                       65536
SOLVENT                   DMSO
NS                        1000
DS                           4
SWH                  36057.691 Hz
FIDRES                0.550197 Hz
AQ                    0.9087659 sec
RG                         2050
DW                       13.867 usec
DE                        6.50 usec
TE                       302.7 K
CNST2                145.0000000
CNST11                 1.0000000
D1                     2.00000000 sec
D20                    0.00689655 sec
TD0                           1

======== CHANNEL f1 ========
SFO1                 150.9178988 MHz
NUC1                         13C
P1                         11.80 usec
P2                         23.60 usec
PLW1               202.10000610 W

======== CHANNEL f2 ========
SFO2                 600.1324005 MHz
NUC2                         1H
CPDPRG[2                 waltz16
PCPD2                      70.00 usec
PLW2                13.69999981 W
PLW12                0.17449000 W

F2 - Processing parameters
SI                           32768
SF                  150.9028090 MHz
WDW                             EM
SSB                  0
LB                         1.00 Hz
GB                   0
PC                         1.40
```

SAMPLE INFORMATION

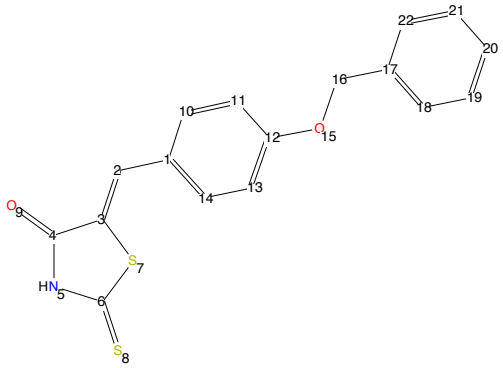
Sample Name:	009	Acquired By:	System
Sample Type:	Unknown	Sample Set Name	103dx_JMT
Vial:	1:B,6	Acq. Method Set:	ReversePhase_12min_Max Plot
Injection #:	1	Processing Methoc	ReversePhase_Purity_MAX Plot
Injection Volume:	1.00 ul	Channel Name:	PDA Max Plot 190.0 - 800.0
Run Time:	12.0 Minutes	Proc. Chnl. Descr.:	PDA MaxPlot (190.0 nm to 800.0
Date Acquired:	7/27/2021 9:23:17 PM EDT		
Date Processed:	8/31/2021 3:25:18 PM EDT		



	RT	Area	% Area	Height	Peak Lambda Max.
1	7.609	3114188	100.00	1648063	345.8

CMC-assist

JMT_129



Consistency: Unknown*, unknown purity*

Sum formula:
$C_{17}H_{13}NO_2S_2$

Molecular Mass:
327.04 Da

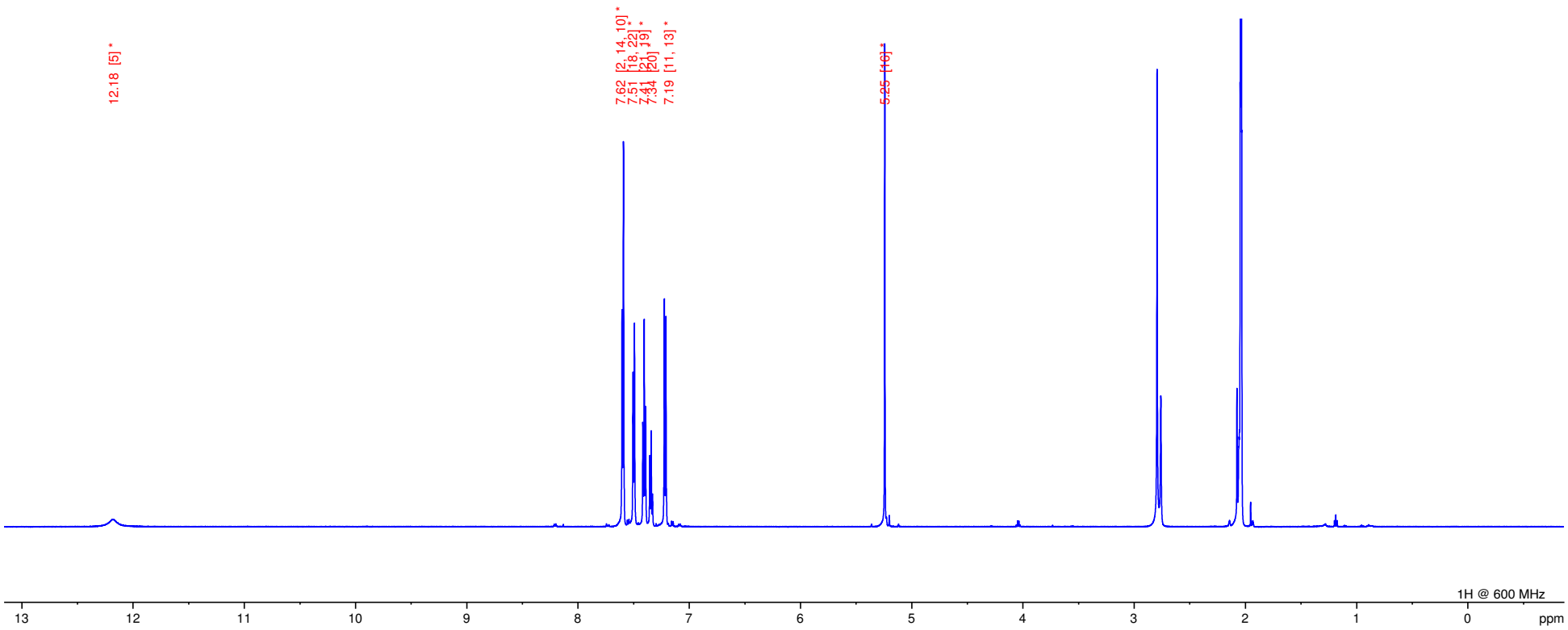
Data set 1H: JMT_129 1 1 /opt/topspin4.1.3
Structure: /opt/topspin4.1.3/JMT_129/structure.mol
Acquisition date: July 18, 2021 5:12:28 PM EDT
Solvent: Acetone
Probe: 5 mm PATXI 1H/D/19F-13C/15N Z-GRD Z855801/0017
Eretic reference:

Comments:
Multiplet interpretation available for spectrum.
A multiplet interpretation for all major signals in the spectrum could be found. All given impurities could be assigned to regions in the spectrum.

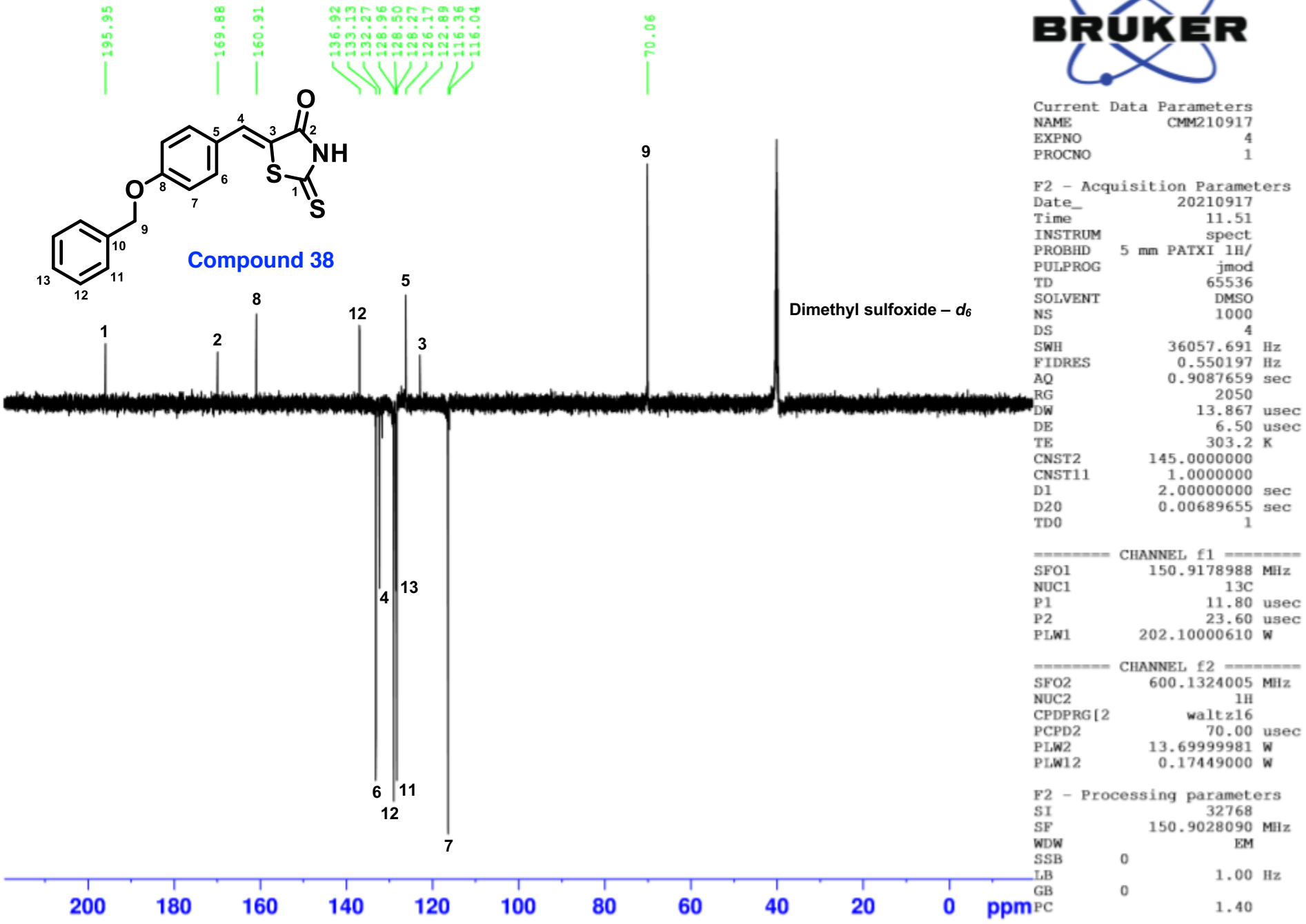
Signature:

Automatic analysis generated by Bruker CMC (b:17).
One or more results have not been created by automatic analysis, or edited manually: marked by '*'.
Report generated by Bruker CMC-assist TopSpin 4.1.3 (of 2021-06-28 13:00:50), on 'MacBook-Pro.local' as 'tzbenton'

Compound 38



38 (JMT129)

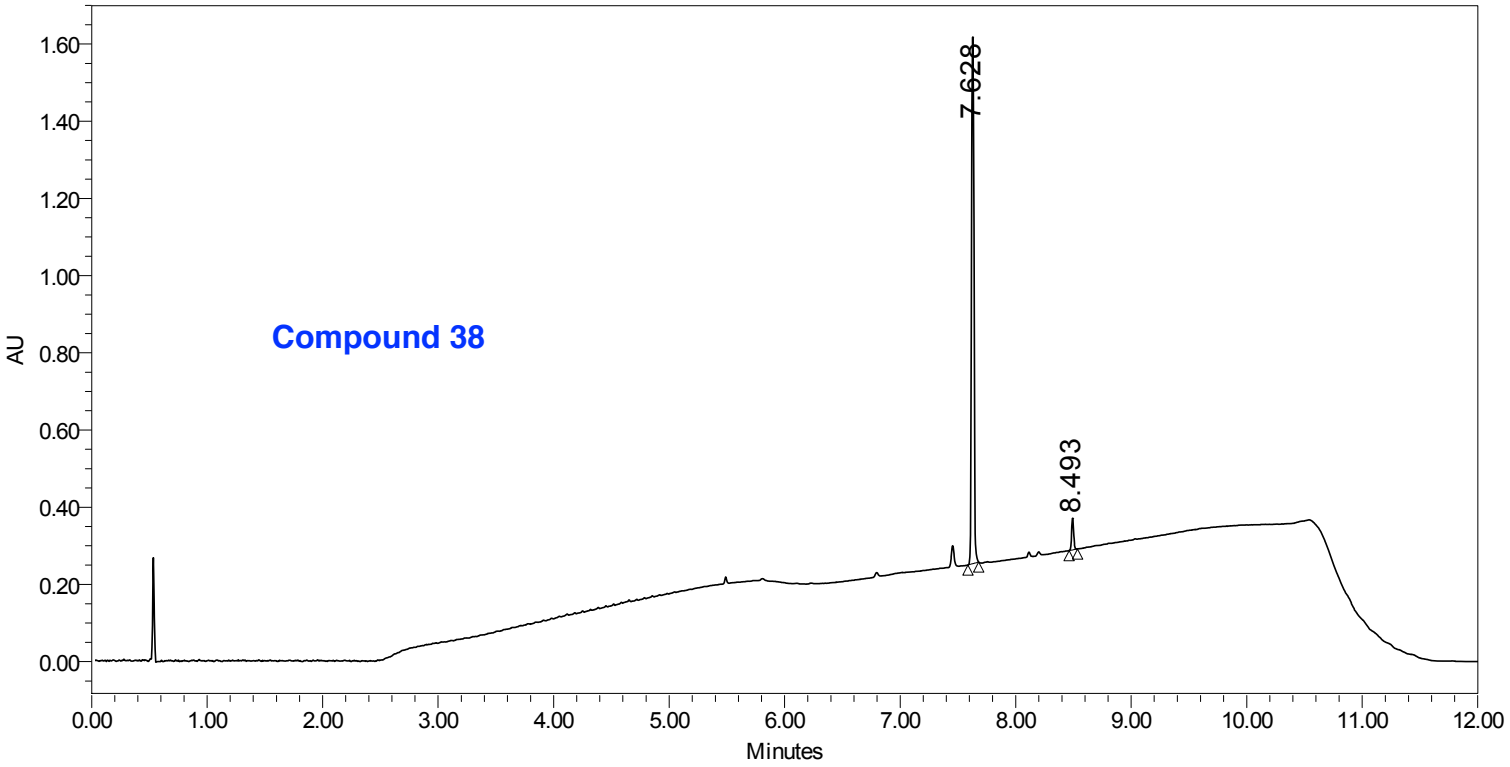


BRUKER

```
Current Data Parameters
NAME                 CMM210917
EXPNO                        4
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20210917
Time                     11.51
INSTRUM                  spect
PROBHD     5 mm PATXI 1H/
PULPROG                  jmod
TD                       65536
SOLVENT                  DMSO
NS                       1000
DS                          4
SWH                  36057.691 Hz
FIDRES                0.550197 Hz
AQ                    0.9087659 sec
RG                        2050
DW                      13.867 usec
DE                        6.50 usec
TE                       303.2 K
CNST2                145.0000000
CNST11                 1.0000000
D1                     2.00000000 sec
D20                    0.00689655 sec
TD0                          1

======== CHANNEL f1 ========
SFO1               150.9178988 MHz
NUC1                       13C
P1                       11.80 usec
P2                       23.60 usec
PLW1              202.10000610 W

======== CHANNEL f2 ========
SFO2               600.1324005 MHz
NUC2                       1H
CPDPRG[2                waltz16
PCPD2                    70.00 usec
PLW2              13.69999981 W
PLW12              0.17449000 W

F2 - Processing parameters
SI                       32768
SF                 150.9028090 MHz
WDW                         EM
SSB          0
LB                        1.00 Hz
GB           0
PC                        1.40
```

SAMPLE INFORMATION

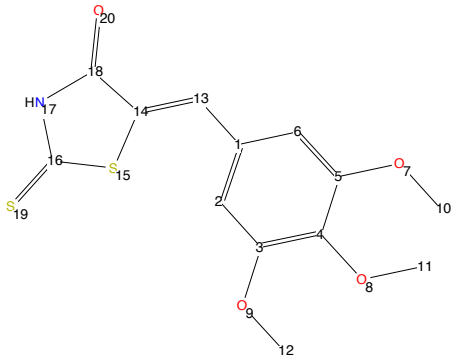
Sample Name:	129	Acquired By:	System
Sample Type:	Unknown	Sample Set Name	103dx_JMT
Vial:	1:A,6	Acq. Method Set:	ReversePhase_12min_Max Plot
Injection #:	1	Processing Method	ReversePhase_Purity_MAX Plot
Injection Volume:	1.00 ul	Channel Name:	PDA Max Plot 190.0 - 800.0
Run Time:	12.0 Minutes	Proc. Chnl. Descr.:	PDA MaxPlot (190.0 nm to 800.0
Date Acquired:	7/27/2021 7:43:54 PM EDT		
Date Processed:	8/31/2021 3:03:27 PM EDT		



	RT	Area	% Area	Height	Peak Lambda Max.
1	7.628	2077553	95.35	1366786	392.4
2	8.493	101326	4.65	82128	236.1

CMC-assist

JMT_134



Consistency: Unknown*, unknown purity*

Data set 1H: JMT_134 1 1 /opt/topspin4.1.3
Structure: /opt/topspin4.1.3/JMT_134/1/structure.mol
Acquisition date: July 18, 2021 4:56:18 PM EDT
Solvent: Acetone
Probe: 5 mm PATXI 1H/D/19F-13C/15N Z-GRD Z855801/0017
Eretic reference:

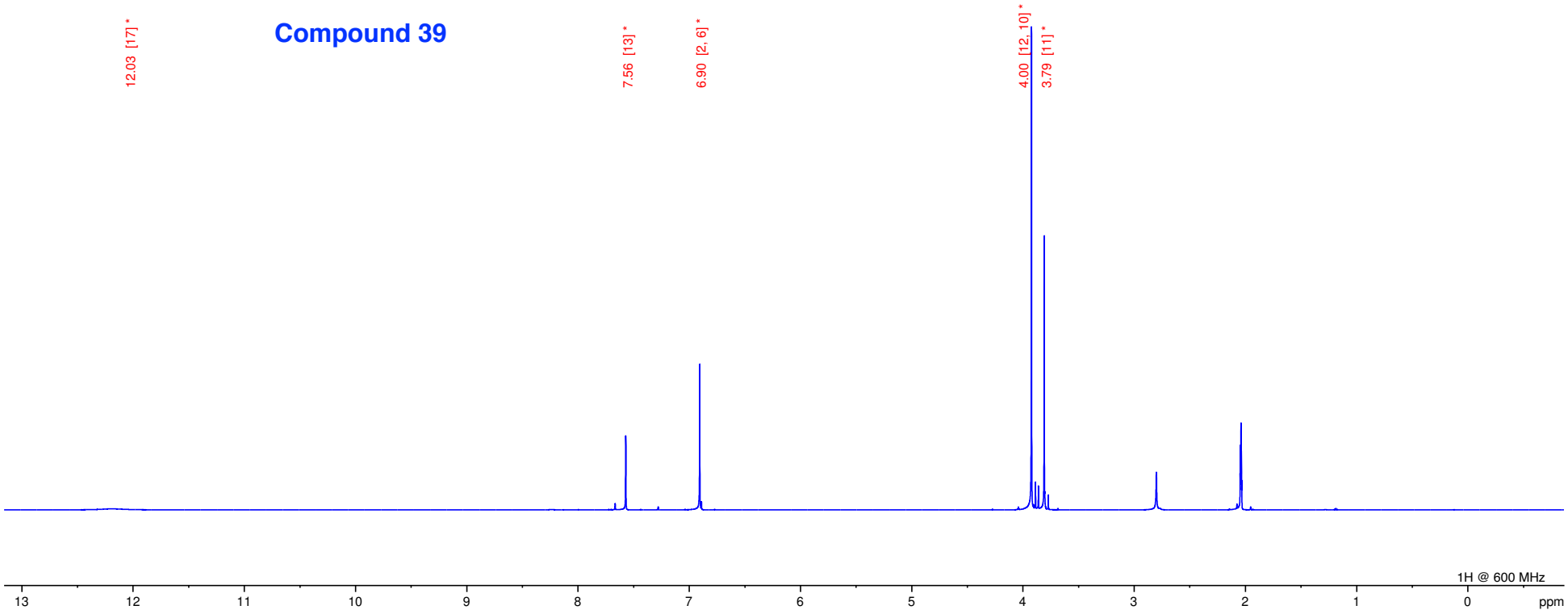
Sum formula: $C_{13}H_{13}NO_4S_2$

Molecular Mass: 311.03 Da

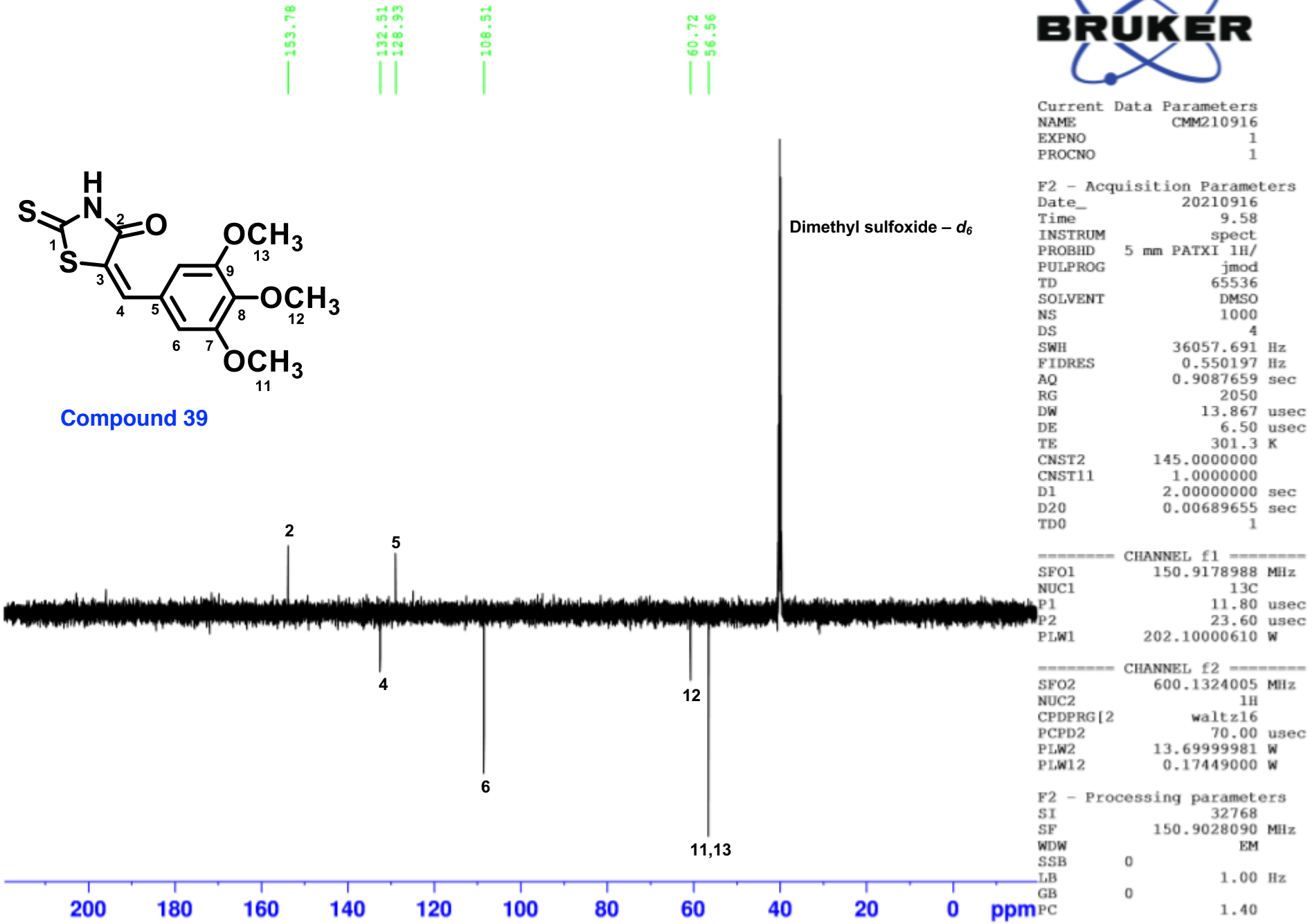
Comments:
Multiplet interpretation available for spectrum.Multiplet interpretation available for spectrum.
A multiplet interpretation for all major signals in the spectrum could be found. All given impurities could be assigned to regions in the spectrum.A multiplet interpretation for all major signals in the spectrum could be found. All given impurities could be assigned to regions in the spectrum.

Signature:

Automatic analysis generated by Bruker CMC (b:17).
One or more results have not been created by automatic analysis, or edited manually: marked by '*'.
Report generated by Bruker CMC-assist TopSpin 4.1.3 (of 2021-06-28 13:00:50), on 'MacBook-Pro.local' as 'tzbenton'



39 (JMT-134)

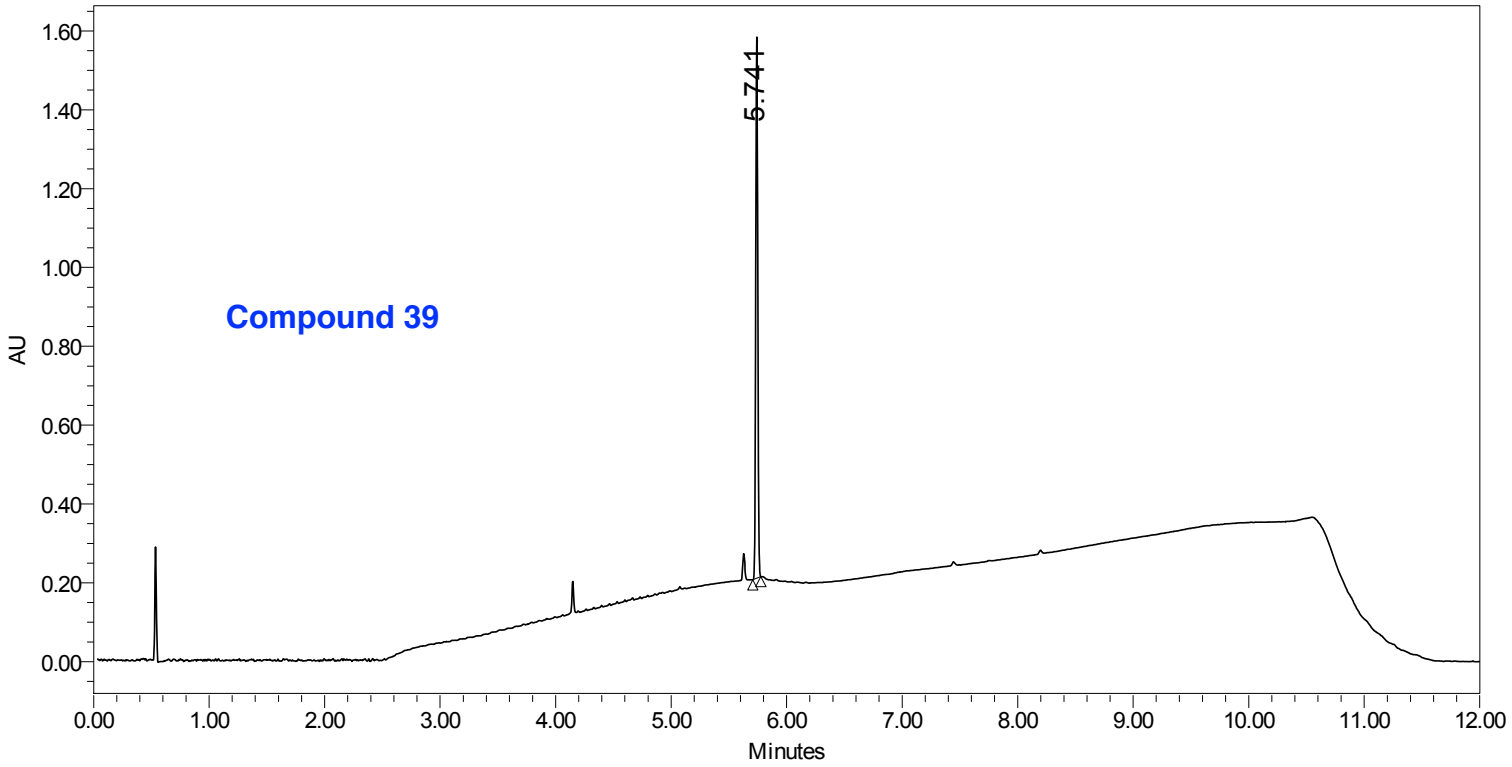


Compound 39

```
Current Data Parameters
NAME                 CMM210916
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_               20210916
Time                    9.58
INSTRUM                spect
PROBHD    5 mm PATXI 1H/
PULPROG                 jmod
TD                     65536
SOLVENT                DMSO
NS                     1000
DS                        4
SWH                36057.691 Hz
FIDRES             0.550197 Hz
AQ                 0.9087659 sec
RG                      2050
DW                    13.867 usec
DE                      6.50 usec
TE                     301.3 K
CNST2             145.0000000
CNST11              1.0000000
D1                  2.00000000 sec
D20                 0.00689655 sec
TD0                          1

======== CHANNEL f1 ========
SFO1             150.9178988 MHz
NUC1                      13C
P1                      11.80 usec
P2                      23.60 usec
PLW1            202.10000610 W

======== CHANNEL f2 ========
SFO2             600.1324005 MHz
NUC2                      1H
CPDPRG[2               waltz16
PCPD2                   70.00 usec
PLW2             13.69999981 W
PLW12             0.17449000 W

F2 - Processing parameters
SI                       32768
SF               150.9028090 MHz
WDW                         EM
SSB          0
LB                      1.00 Hz
GB           0
PC                      1.40
```

SAMPLE INFORMATION

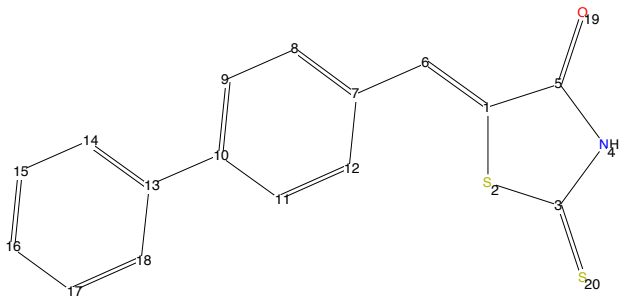
Sample Name:	134	Acquired By:	System
Sample Type:	Unknown	Sample Set Name	103dx_JMT
Vial:	1:B,1	Acq. Method Set:	ReversePhase_12min_Max Plot
Injection #:	1	Processing Methoc	ReversePhase_Purity_MAX Plot
Injection Volume:	1.00 ul	Channel Name:	PDA Max Plot 190.0 - 800.0
Run Time:	12.0 Minutes	Proc. Chnl. Descr.:	PDA MaxPlot (190.0 nm to 800.0
Date Acquired:	7/27/2021 8:21:34 PM EDT		
Date Processed:	8/31/2021 3:06:18 PM EDT		



	RT	Area	% Area	Height	Peak Lambda Max.
1	5.741	1697320	100.00	1375780	392.4

• CMC-assist

JMT_144



Consistency: Unknown*, unknown purity*

Sum formula: $C_{16}H_{11}NOS_2$

Molecular Mass: 297.03 Da

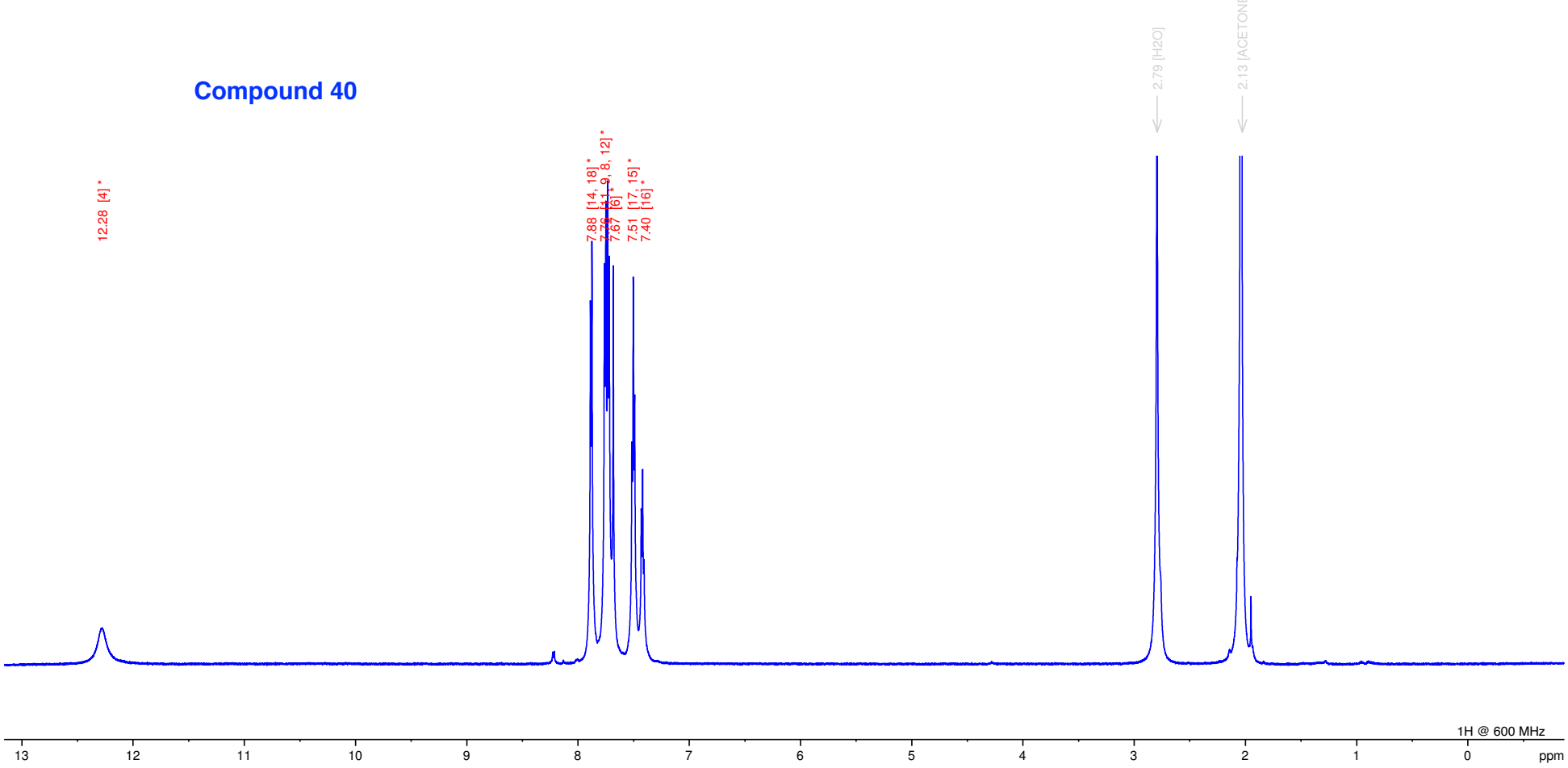
Data set 1H:	JMT_144 1 1 /opt/topspin4.1.3
Structure:	/opt/topspin4.1.3/JMT_144/1/structure.mol
Acquisition date:	July 19, 2021 2:35:45 PM EDT
Solvent:	Acetone
Probe:	5 mm PATXI 1H/D/19F-13C/15N Z-GRD Z855801/0017
Eretic reference:	

Comments:
Multiplet interpretation available for spectrum.
A multiplet interpretation for all major signals in the spectrum could be found. All given impurities could be assigned to regions in the spectrum.

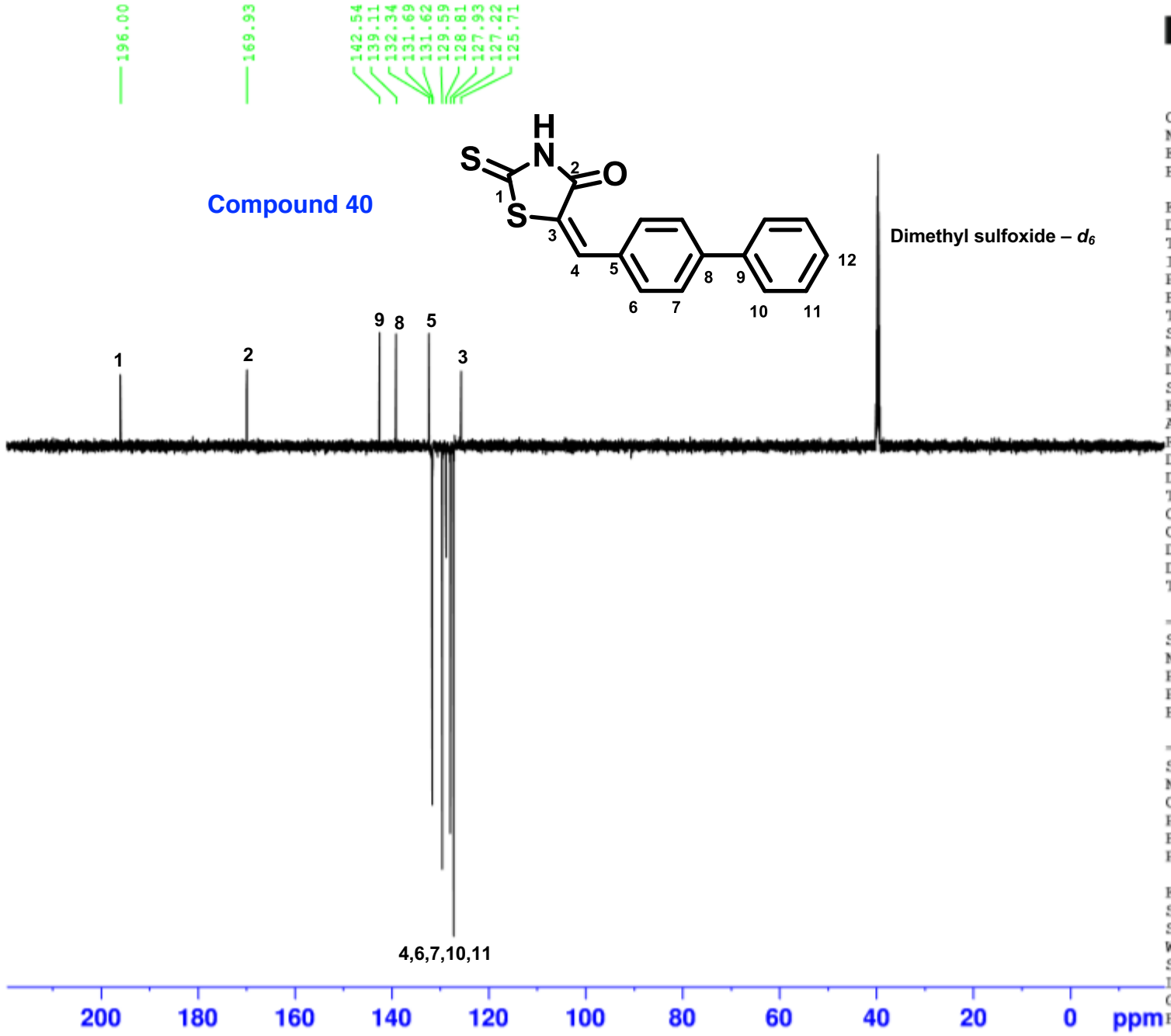
Signature:

Automatic analysis generated by Bruker CMC (b:17).
One or more results have not been created by automatic analysis, or edited manually: marked by '*'.
Report generated by Bruker CMC-assist TopSpin 4.1.3 (of 2021-06-28 13:00:50), on 'MacBook-Pro.local' as 'tzbenton'

Compound 40



40 (JMT-144)

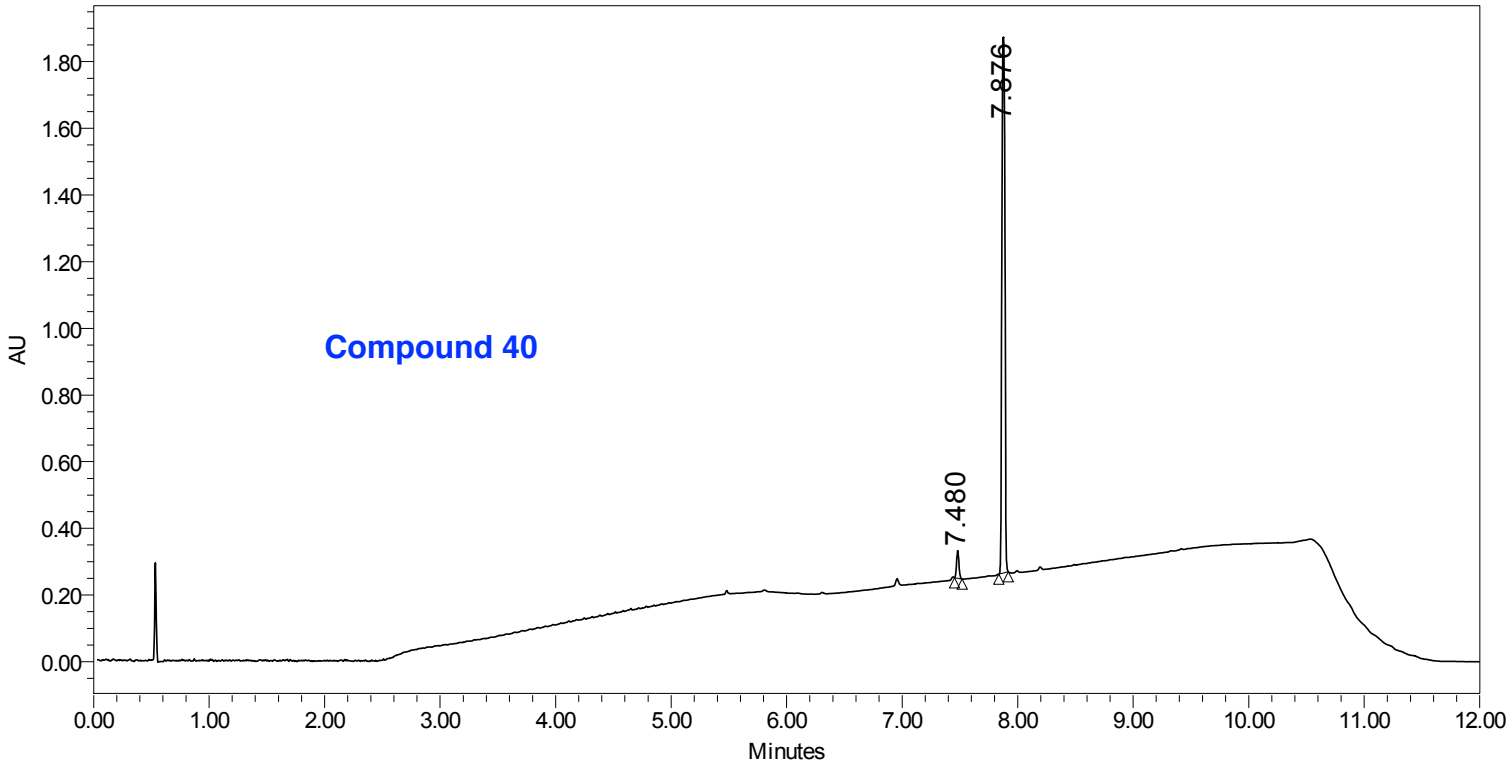


BRUKER

```
Current Data Parameters
NAME                CMM210916
EXPNO                       6
PROCNO                      1

F2 - Acquisition Parameters
Date_                20210916
Time                    15.19
INSTRUM                 spect
PROBHD    5 mm PATXI 1H/
PULPROG                 jmod
TD                      65536
SOLVENT                 DMSO
NS                      1000
DS                         4
SWH                36057.691 Hz
FIDRES              0.550197 Hz
AQ                  0.9087659 sec
RG                       2050
DW                     13.867 usec
DE                       6.50 usec
TE                      301.2 K
CNST2              145.0000000
CNST11               1.0000000
D1                   2.00000000 sec
D20                  0.00689655 sec
TD0                         1

======== CHANNEL f1 ========
SFO1               150.9178988 MHz
NUC1                       13C
P1                       11.80 usec
P2                       23.60 usec
PLW1            202.10000610 W

======== CHANNEL f2 ========
SFO2               600.1324005 MHz
NUC2                       1H
CPDPRG[2                waltz16
PCPD2                    70.00 usec
PLW2               13.69999981 W
PLW12               0.17449000 W

F2 - Processing parameters
SI                         32768
SF                 150.9028090 MHz
WDW                           EM
SSB          0
LB                        1.00 Hz
GB           0
PC                        1.40
```

SAMPLE INFORMATION

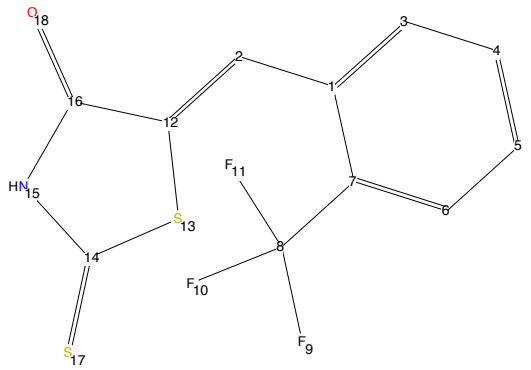
Sample Name:	144	Acquired By:	System
Sample Type:	Unknown	Sample Set Name	103dx_JMT
Vial:	1:A,5	Acq. Method Set:	ReversePhase_12min_Max Plot
Injection #:	1	Processing Method	ReversePhase_Purity_MAX Plot
Injection Volume:	1.00 ul	Channel Name:	PDA Max Plot 190.0 - 800.0
Run Time:	12.0 Minutes	Proc. Chnl. Descr.:	PDA MaxPlot (190.0 nm to 800.0
Date Acquired:	7/27/2021 7:31:19 PM EDT		
Date Processed:	8/31/2021 3:36:51 PM EDT		



	RT	Area	% Area	Height	Peak Lambda Max.
1	7.480	115051	3.72	82555	394.3
2	7.876	2978135	96.28	1608789	388.1

CMC-assist

JMT_187



Consistency: Unknown*, unknown purity*

Data set 1H:	JMT_187 1 1 /opt/topspin4.1.3
Structure:	/opt/topspin4.1.3/JMT_187/1/structure.mol
Acquisition date:	July 18, 2021 4:33:05 PM EDT
Solvent:	Acetone
Probe:	5 mm PATXI 1H/D/19F-13C/15N Z-GRD Z855801/0017
Eretic reference:	

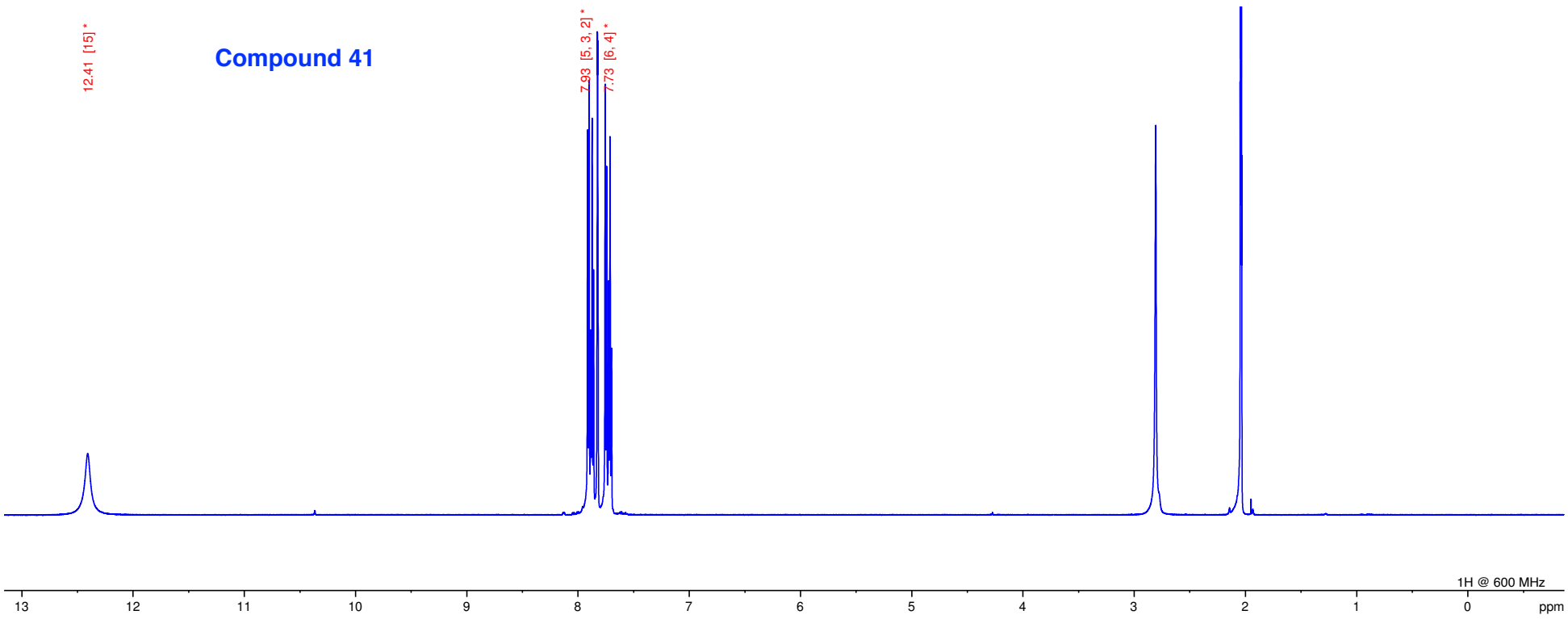
Sum formula:
$C_{11}H_6F_3NOS_2$

Molecular Mass:
288.98 Da

Comments:
Multiplet interpretation available for spectrum.
A multiplet interpretation for all major signals in the spectrum could be found. All given impurities could be assigned to regions in the spectrum.

Signature:

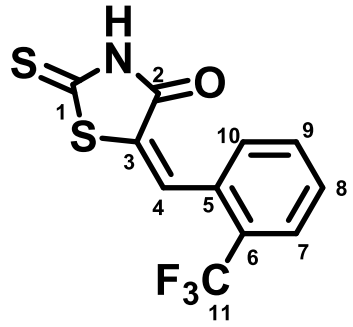
Automatic analysis generated by Bruker CMC (b:17).
One or more results have not been created by automatic analysis, or edited manually: marked by '*'.
Report generated by Bruker CMC-assist TopSpin 4.1.3 (of 2021-06-28 13:00:50), on 'MacBook-Pro.local' as 'tzbenton'



41 (JMT-187)

196.06
169.27
133.96
131.67
131.35
131.04
129.77
128.62
128.42
128.23
128.03
127.37
127.33
127.29
127.02
125.90
125.21
123.39

Compound 41



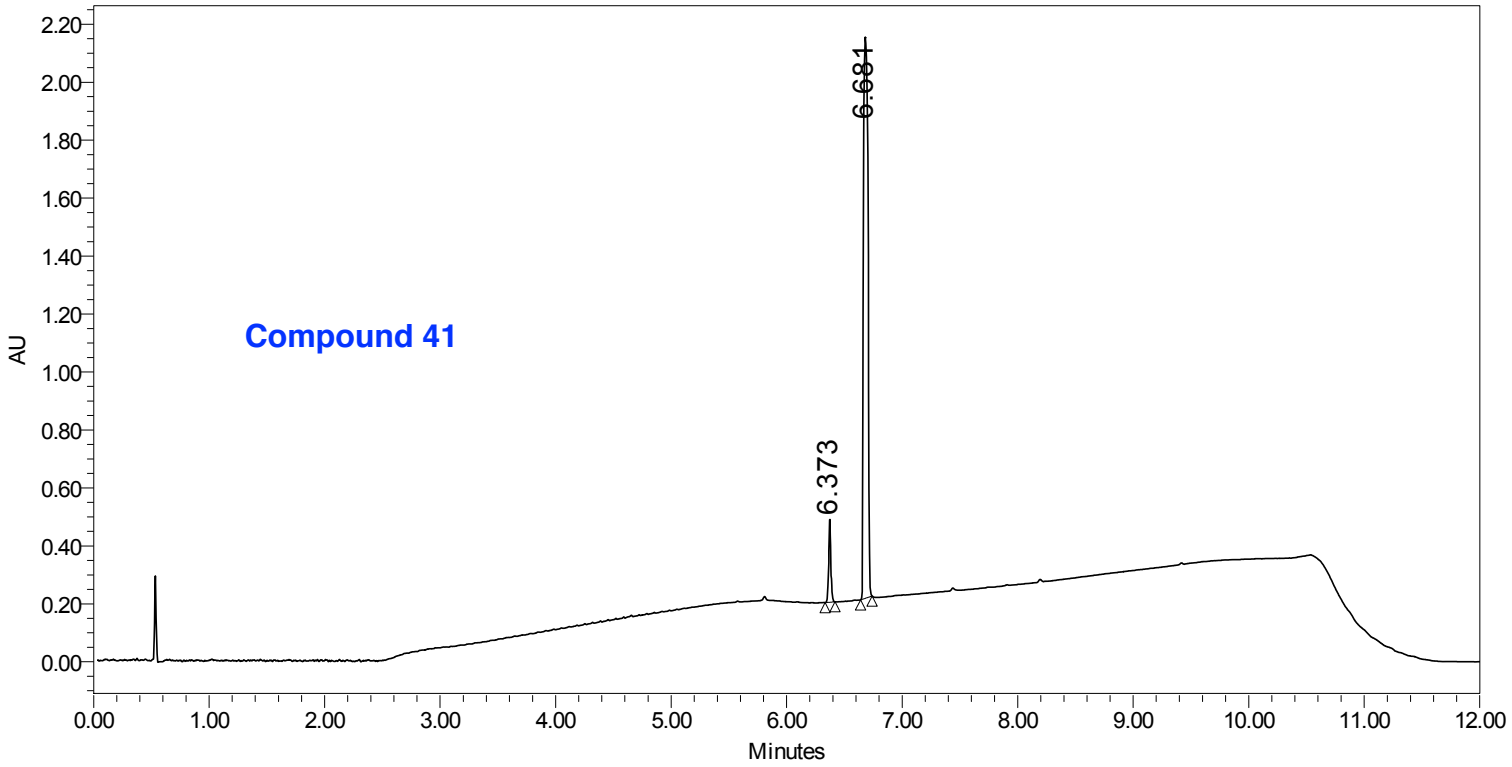
Dimethyl sulfoxide – d_6

BRUKER

```
Current Data Parameters
NAME                  CMM210915
EXPNO                         7
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20210915
Time                      16.17
INSTRUM                   spect
PROBHD    5 mm PATXI 1H/
PULPROG                   jmod
TD                       65536
SOLVENT                   DMSO
NS                        1000
DS                           4
SWH                  36057.691 Hz
FIDRES                0.550197 Hz
AQ                    0.9087659 sec
RG                         2050
DW                       13.867 usec
DE                        6.50 usec
TE                       301.3 K
CNST2                145.0000000
CNST11                 1.0000000
D1                     2.00000000 sec
D20                    0.00689655 sec
TD0                           1

======== CHANNEL f1 ========
SFO1                150.9178988 MHz
NUC1                        13C
P1                       11.80 usec
P2                       23.60 usec
PLW1               202.10000610 W

======== CHANNEL f2 ========
SFO2                600.1324005 MHz
NUC2                        1H
CPDPRG[2                waltz16
PCPD2                    70.00 usec
PLW2                13.69999981 W
PLW12                0.17449000 W

F2 - Processing parameters
SI                          32768
SF                  150.9028090 MHz
WDW                            EM
SSB                 0
LB                       1.00 Hz
GB                  0
PC                       1.40
```

SAMPLE INFORMATION

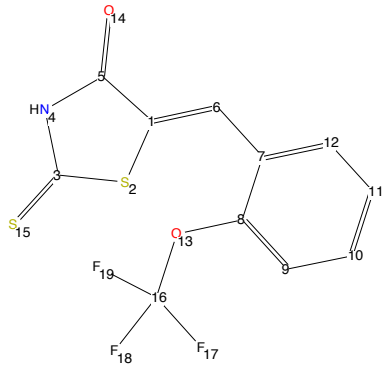
Sample Name:	187	Acquired By:	System
Sample Type:	Unknown	Sample Set Name	103dx_JMT
Vial:	1:A,4	Acq. Method Set:	ReversePhase_12min_Max Plot
Injection #:	1	Processing Methoc	ReversePhase_Purity_MAX Plot
Injection Volume:	1.00 ul	Channel Name:	PDA Max Plot 190.0 - 800.0
Run Time:	12.0 Minutes	Proc. Chnl. Descr.:	PDA MaxPlot (190.0 nm to 800.0
Date Acquired:	7/27/2021 7:18:44 PM EDT		
Date Processed:	8/31/2021 3:57:16 PM EDT		



	RT	Area	% Area	Height	Peak Lambda Max.
1	6.373	374327	6.75	286232	345.8
2	6.681	5174718	93.25	1936031	275.3

CMC-assist

JMT_188



Consistency: Unknown*, unknown purity*

Sum formula:
$C_{11}H_6F_3NO_2S_2$

Molecular Mass:
304.98 Da

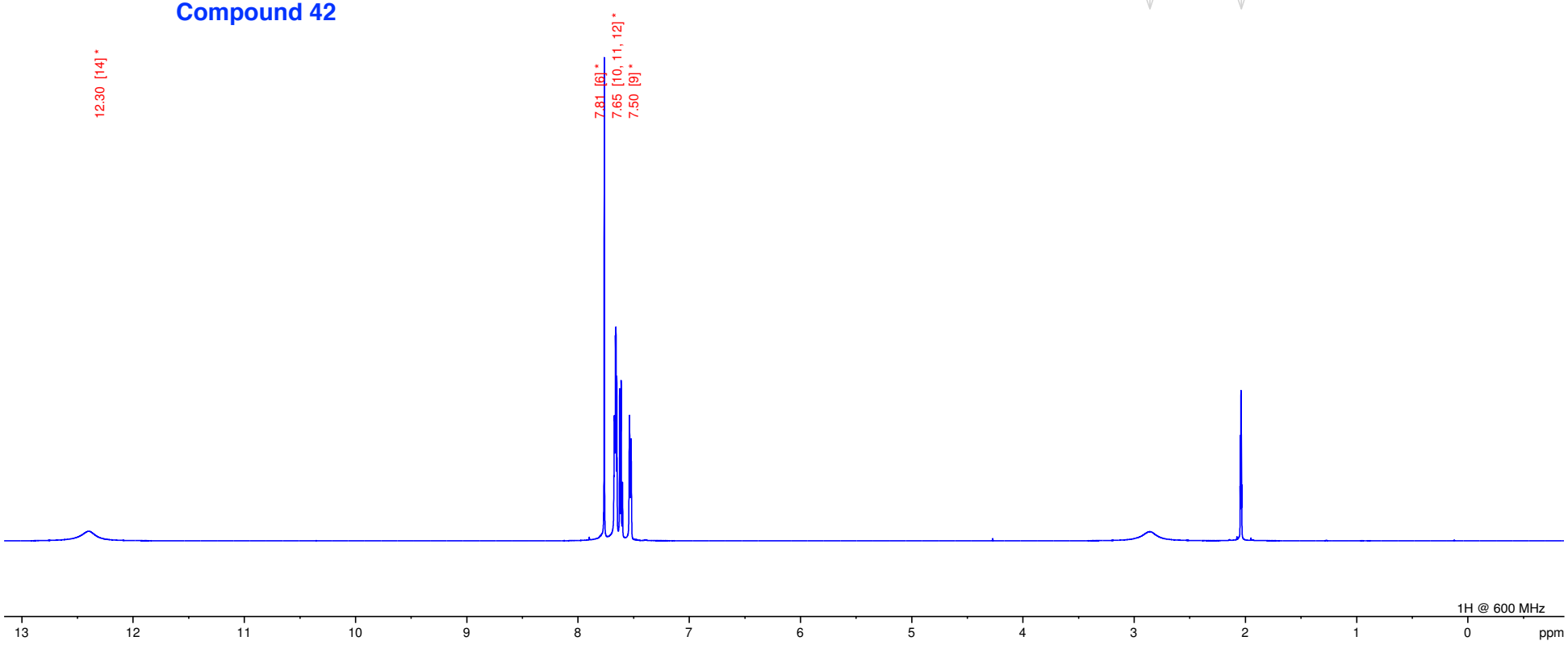
Data set 1H:	JMT_188 1 1 /opt/topspin4.1.3
Structure:	/opt/topspin4.1.3/JMT_188/1/structure.mol
Acquisition date:	July 18, 2021 5:06:13 PM EDT
Solvent:	Acetone
Probe:	5 mm PATXI 1H/D/19F-13C/15N Z-GRD Z855801/0017
Eretic reference:	

Comments:
Multiplet interpretation available for spectrum.
A multiplet interpretation for all major signals in the spectrum could be found. All given impurities could be assigned to regions in the spectrum.

Signature:

Automatic analysis generated by Bruker CMC (b:17).
One or more results have not been created by automatic analysis, or edited manually: marked by '*'.
Report generated by Bruker CMC-assist TopSpin 4.1.3 (of 2021-06-28 13:00:50), on 'MacBook-Pro.local' as 'tzbenton'

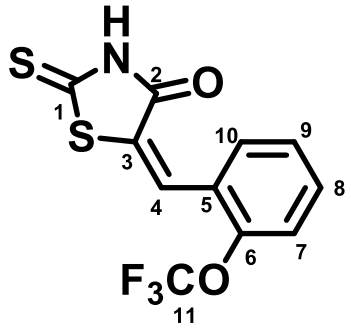
Compound 42



42 (JMT-188)

195.80 169.56 147.50 132.94 129.88 129.83 128.96 126.62 123.06 122.29 121.33 119.62

Compound 42



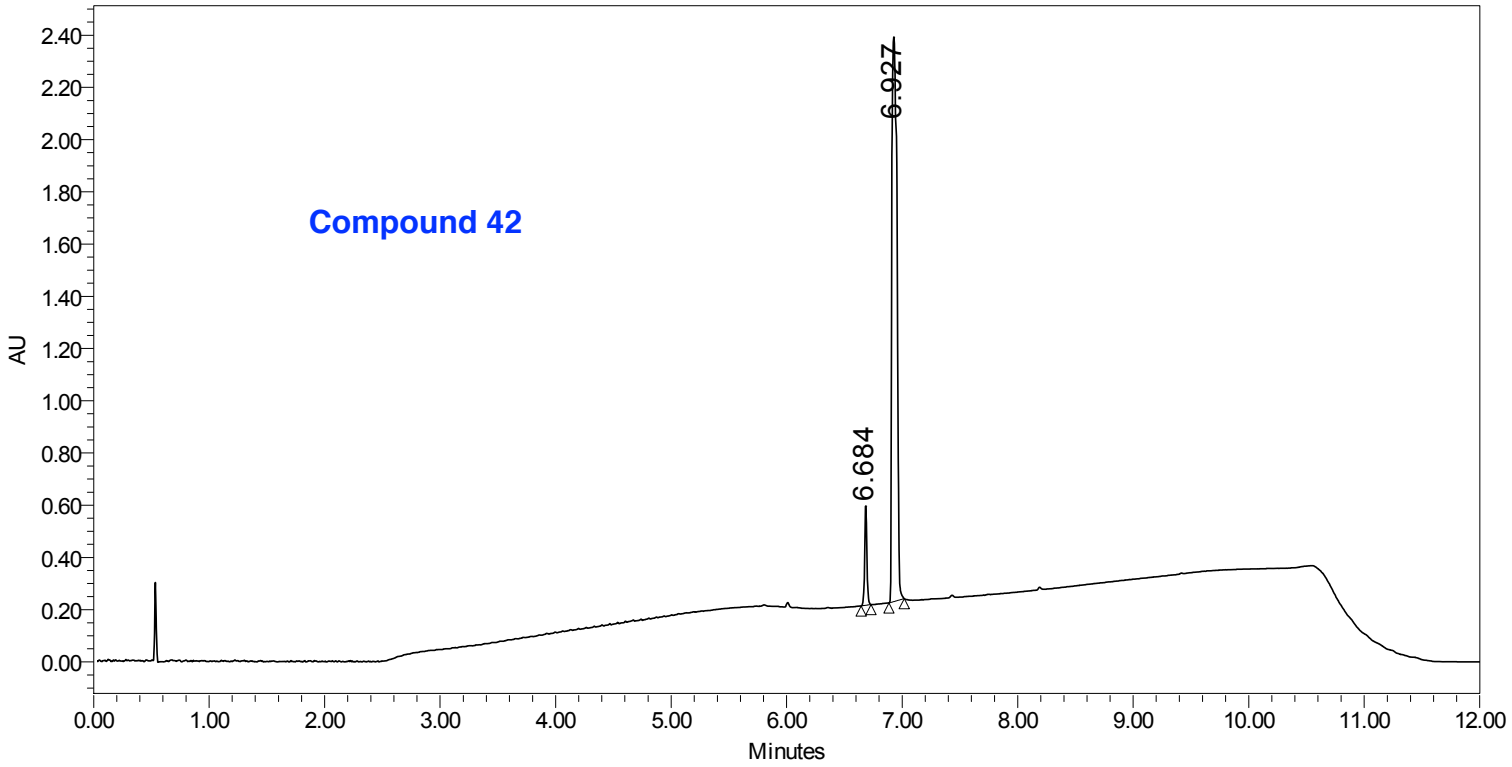
Dimethyl sulfoxide – d_6

BRUKER

```
Current Data Parameters
NAME                  CMM210915
EXPNO                         8
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20210915
Time                      17.10
INSTRUM                   spect
PROBHD    5 mm PATXI 1H/
PULPROG                   jmod
TD                       65536
SOLVENT                   DMSO
NS                        1000
DS                           4
SWH                  36057.691 Hz
FIDRES               0.550197 Hz
AQ                   0.9087659 sec
RG                        2050
DW                      13.867 usec
DE                        6.50 usec
TE                       301.4 K
CNST2                145.0000000
CNST11                 1.0000000
D1                     2.00000000 sec
D20                    0.00689655 sec
TD0                           1

======== CHANNEL f1 ========
SFO1                150.9178988 MHz
NUC1                        13C
P1                        11.80 usec
P2                        23.60 usec
PLW1               202.10000610 W

======== CHANNEL f2 ========
SFO2                600.1324005 MHz
NUC2                        1H
CPDPRG[2                waltz16
PCPD2                     70.00 usec
PLW2                13.69999981 W
PLW12                0.17449000 W

F2 - Processing parameters
SI                        32768
SF                  150.9028090 MHz
WDW                          EM
SSB                 0
LB                        1.00 Hz
GB                  0
PC                        1.40
```

SAMPLE INFORMATION

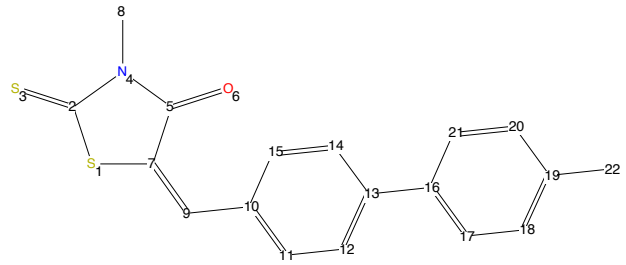
Sample Name:	188	Acquired By:	System
Sample Type:	Unknown	Sample Set Name	103dx_JMT
Vial:	1:A,2	Acq. Method Set:	ReversePhase_12min_Max Plot
Injection #:	1	Processing Methoc	ReversePhase_Purity_MAX Plot
Injection Volume:	1.00 ul	Channel Name:	PDA Max Plot 190.0 - 800.0
Run Time:	12.0 Minutes	Proc. Chnl. Descr.:	PDA MaxPlot (190.0 nm to 800.0
Date Acquired:	7/27/2021 6:53:33 PM EDT		
Date Processed:	8/31/2021 3:58:18 PM EDT		



	RT	Area	% Area	Height	Peak Lambda Max.
1	6.684	511370	7.08	380475	359.5
2	6.927	6712585	92.92	2162816	259.4

CMC-assist

JMT193



Consistency: Unknown*, unknown purity*

Sum formula: $C_{18}H_{15}NOS_2$

Molecular Mass: 325.06 Da

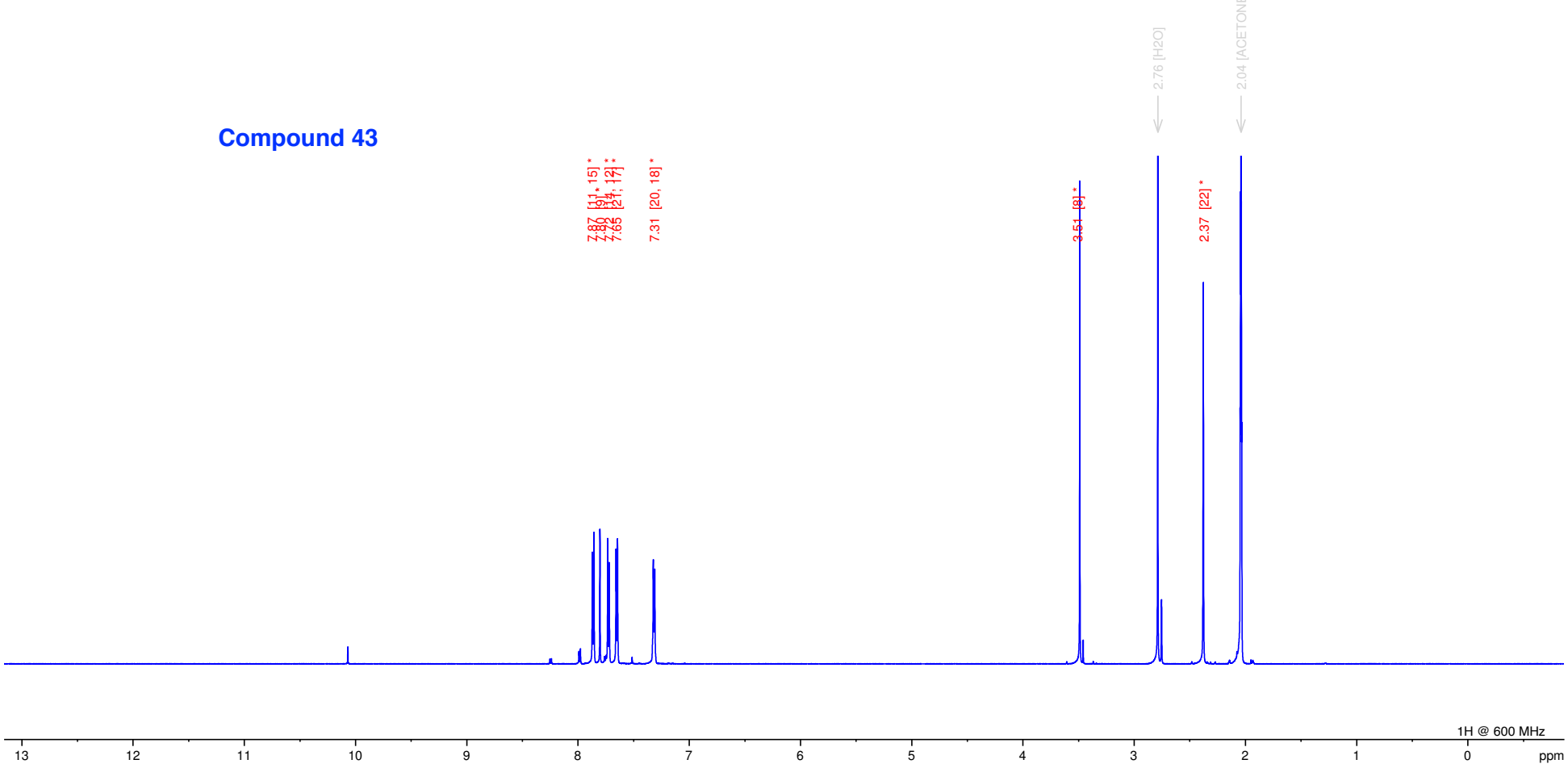
Data set 1H:	JMT193 1 1 /opt/topspin4.1.3
Structure:	/opt/topspin4.1.3/JMT193/1/structure.mol
Acquisition date:	July 19, 2021 3:05:59 PM EDT
Solvent:	Acetone
Probe:	5 mm PATXI 1H/D/19F-13C/15N Z-GRD Z855801/0017
Eretic reference:	

Comments:
Multiplet interpretation available for spectrum.
A multiplet interpretation for all major signals in the spectrum could be found. All given impurities could be assigned to regions in the spectrum.

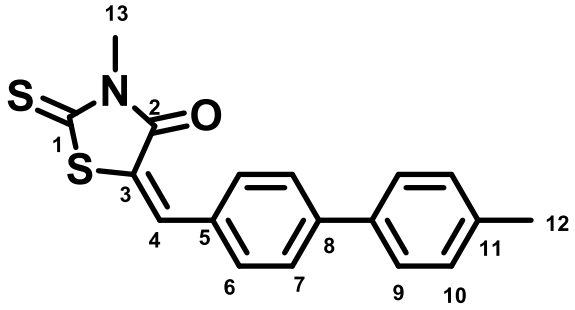
Signature:

Automatic analysis generated by Bruker CMC (b:17).
One or more results have not been created by automatic analysis, or edited manually: marked by '*'.
Report generated by Bruker CMC-assist TopSpin 4.1.3 (of 2021-06-28 13:00:50), on 'MacBook-Pro.local' as 'tzbenton'

Compound 43



43 (JMT193)



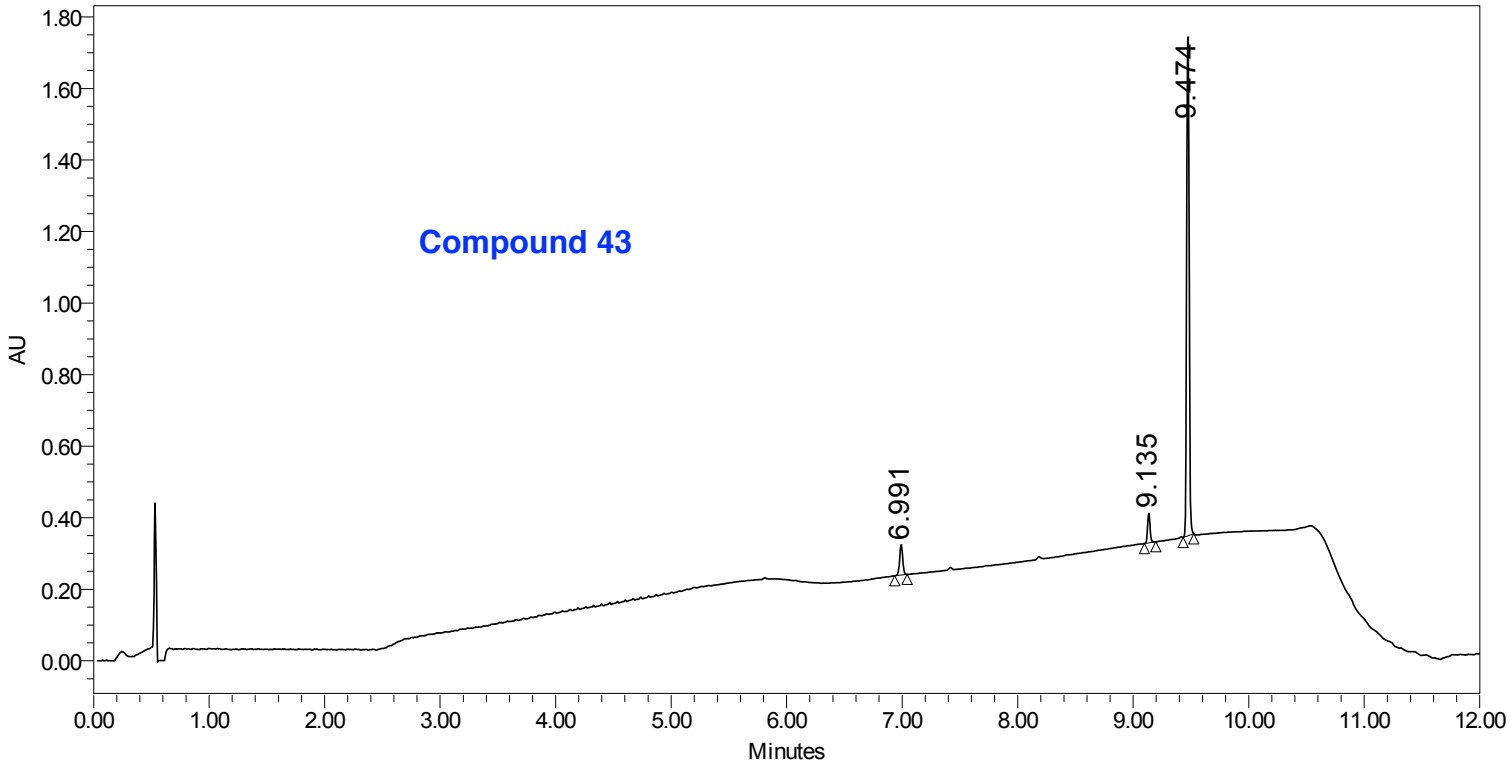
Compound 43

Dimethyl sulfoxide – d_6


```
Current Data Parameters
NAME                  CMM210917
EXPNO                         7
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20210917
Time                      14.55
INSTRUM                   spect
PROBHD    5 mm PATXI 1H/
PULPROG                    jmod
TD                        65536
SOLVENT                    DMSO
NS                         1000
DS                            4
SWH                   36057.691 Hz
FIDRES                0.550197 Hz
AQ                    0.9087659 sec
RG                         2050
DW                       13.867 usec
DE                         6.50 usec
TE                        302.0 K
CNST2                145.0000000
CNST11                 1.0000000
D1                     2.00000000 sec
D20                    0.00689655 sec
TD0                           1

======== CHANNEL f1 ========
SFO1                150.9178988 MHz
NUC1                        13C
P1                        11.80 usec
P2                        23.60 usec
PLW1                202.10000610 W

======== CHANNEL f2 ========
SFO2                600.1324005 MHz
NUC2                        1H
CPDPRG[2                waltz16
PCPD2                     70.00 usec
PLW2                13.69999981 W
PLW12                0.17449000 W

F2 - Processing parameters
SI                         32768
SF                  150.9028090 MHz
WDW                           EM
SSB                0
LB                         1.00 Hz
GB                 0
PC                         1.40
```

SAMPLE INFORMATION

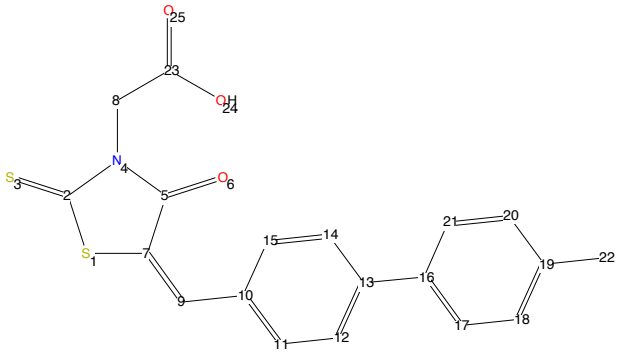
Sample Name:	193	Acquired By:	System
Sample Type:	Unknown	Sample Set Name	103dx_JMT
Vial:	1:A,1	Acq. Method Set:	ReversePhase_12min_Max Plot
Injection #:	1	Processing Methoc	ReversePhase_Purity_MAX Plot
Injection Volume:	1.00 ul	Channel Name:	PDA Max Plot 190.0 - 800.0
Run Time:	12.0 Minutes	Proc. Chnl. Descr.:	PDA MaxPlot (190.0 nm to 800.0
Date Acquired:	7/27/2021 6:40:58 PM EDT		
Date Processed:	8/31/2021 3:59:11 PM EDT		



	RT	Area	% Area	Height	Peak Lambda Max.
1	6.991	154167	6.43	84249	298.7
2	9.135	121661	5.07	82622	399.3
3	9.474	2123174	88.50	1394426	392.4

CMC-assist

JMT194



Consistency: Unknown*, unknown purity*

Sum formula: $C_{19}H_{15}NO_3S_2$

Molecular Mass: 369.05 Da

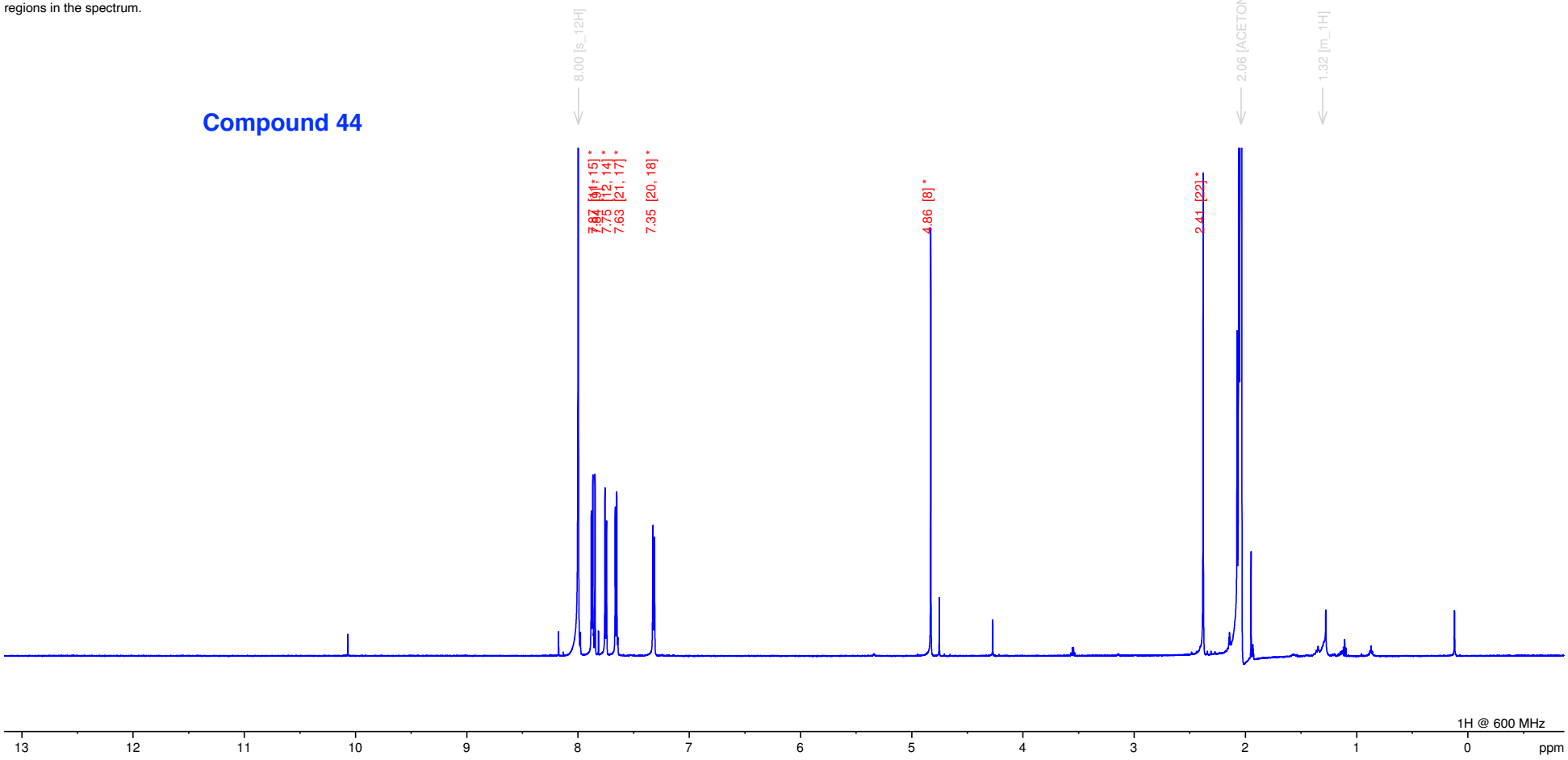
Data set 1H:	JMT194 1 1 /opt/topspin4.1.3
Structure:	/opt/topspin4.1.3/JMT194/1/structure.mol
Acquisition date:	July 19, 2021 2:59:06 PM EDT
Solvent:	Acetone
Probe:	5 mm PATXI 1H/D/19F-13C/15N Z-GRD Z855801/0017
Eretic reference:	

Comments:
Multiplet interpretation available for spectrum.Multiplet interpretation available for spectrum.
A multiplet interpretation for all major signals in the spectrum could be found. All given impurities could be assigned to regions in the spectrum.A multiplet interpretation for all major signals in the spectrum could be found. All given impurities could be assigned to regions in the spectrum.

Signature:

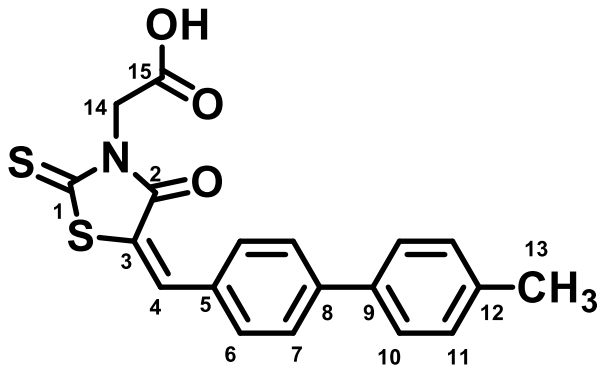
Automatic analysis generated by Bruker CMC (b:17).
One or more results have not been created by automatic analysis, or edited manually: marked by '*'.
Report generated by Bruker CMC-assist TopSpin 4.1.3 (of 2021-06-28 13:00:50), on 'MacBook-Pro.local' as 'tzbenton'

Compound 44



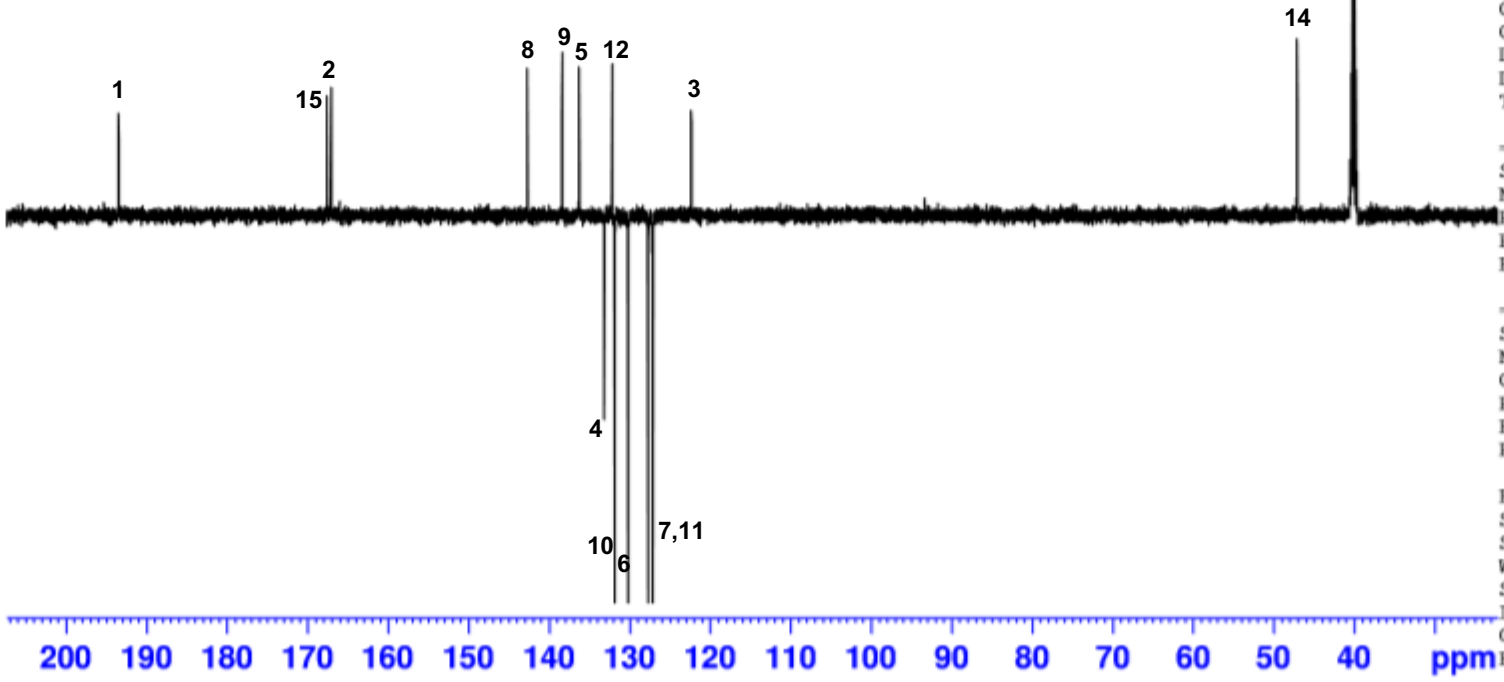
44 (JMT-194)

193.50
167.59
167.09
142.72
138.39
136.26
133.16
132.16
131.85
130.18
127.71
127.14
122.33
47.05



Compound 44

Dimethyl sulfoxide – d_6



BRUKER

Current Data Parameters
NAME CMM210915
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210915
Time 12.46
INSTRUM spect
PROBHD 5 mm PATXI 1H/
PULPROG jmod
TD 65536
SOLVENT DMSO
NS 1000
DS 4
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 2050
DW 13.867 usec
DE 6.50 usec
TE 301.2 K
CNST2 145.0000000
CNST11 1.0000000
D1 2.00000000 sec
D20 0.00689655 sec
TD0 1

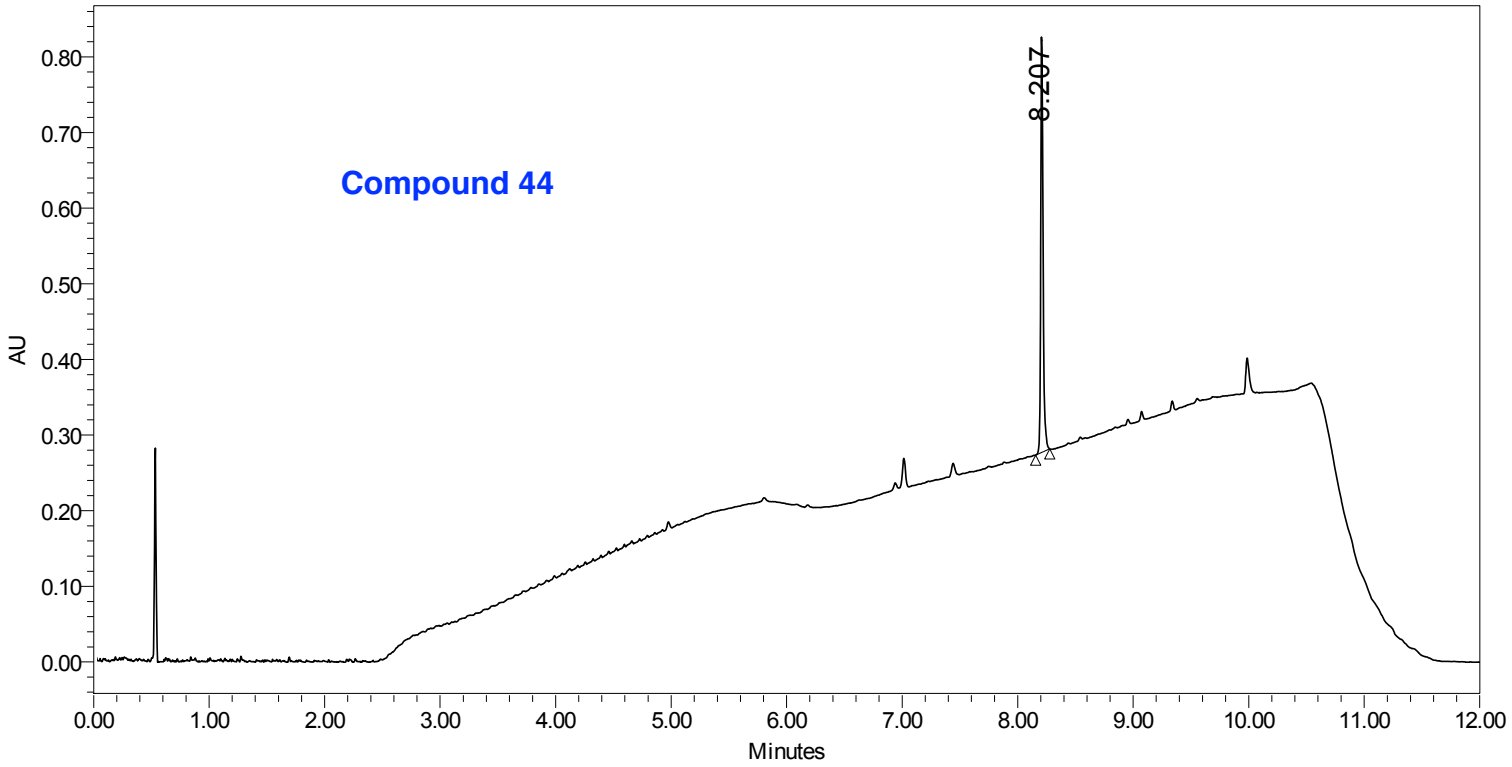
======== CHANNEL f1 ========
SFO1 150.9178988 MHz
NUC1 13C
P1 11.80 usec
P2 23.60 usec
PLW1 202.10000610 W

======== CHANNEL f2 ========
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 70.00 usec
PLW2 13.69999981 W
PLW12 0.17449000 W

F2 - Processing parameters
SI 32768
SF 150.9028090 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

SAMPLE INFORMATION

Sample Name:	194	Acquired By:	System
Sample Type:	Unknown	Sample Set Name	103dx_JMT
Vial:	1:A,3	Acq. Method Set:	ReversePhase_12min_Max Plot
Injection #:	1	Processing Methoc	ReversePhase_Purity_MAX Plot
Injection Volume:	1.00 ul	Channel Name:	PDA Max Plot 190.0 - 800.0
Run Time:	12.0 Minutes	Proc. Chnl. Descr.:	PDA MaxPlot (190.0 nm to 800.0
Date Acquired:	7/27/2021 7:06:09 PM EDT		
Date Processed:	8/31/2021 4:11:37 PM EDT		

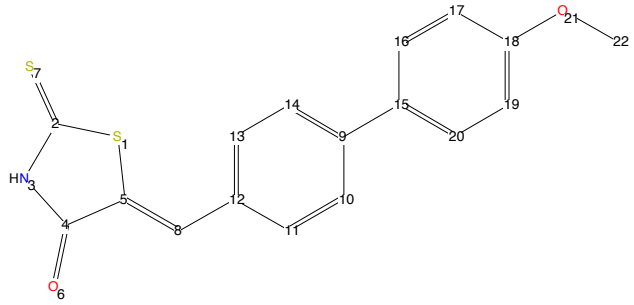


	RT	Area	% Area	Height	Peak Lambda Max.
1	8.207	782016	100.00	551272	394.3

CMC-assist

CMM210625

Consistency: Unknown*, unknown purity*



Data set 1H: CMM210625 5 1 /opt/topspin4.1.3
Structure: /opt/topspin4.1.3/CMM210625/5/structure.mol
Acquisition date: June 25, 2021 2:52:22 PM EDT
Solvent: DMSO
Probe: 5 mm PATXI 1H/D/19F-13C/15N Z-GRD Z855801/0017
Eretic reference:

Sum formula: $C_{17}H_{13}NO_2S_2$

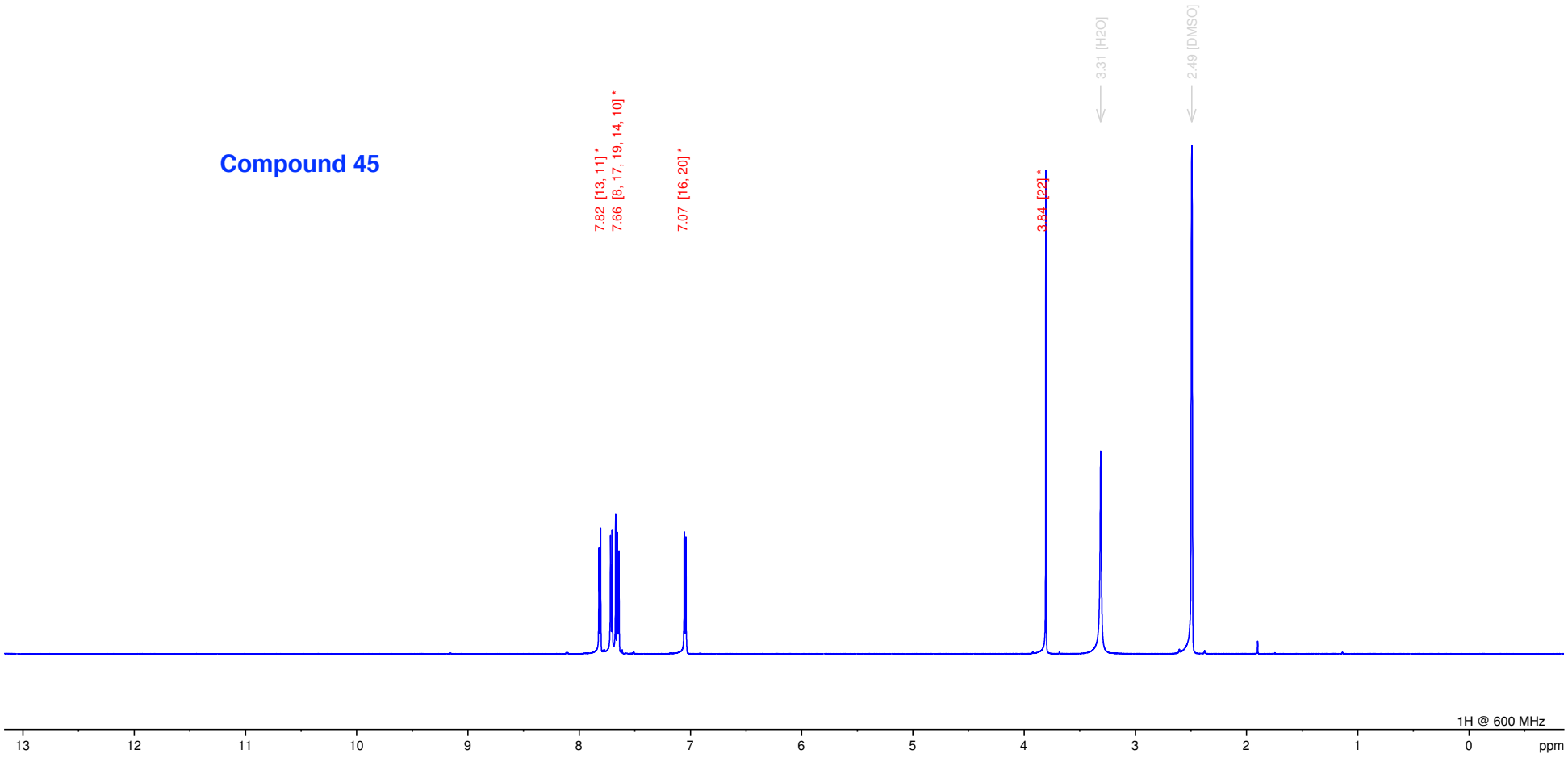
Molecular Mass: 327.04 Da

Comments:
Multiplet interpretation available for spectrum.
A multiplet interpretation for all major signals in the spectrum could be found. All given impurities could be assigned to regions in the spectrum.

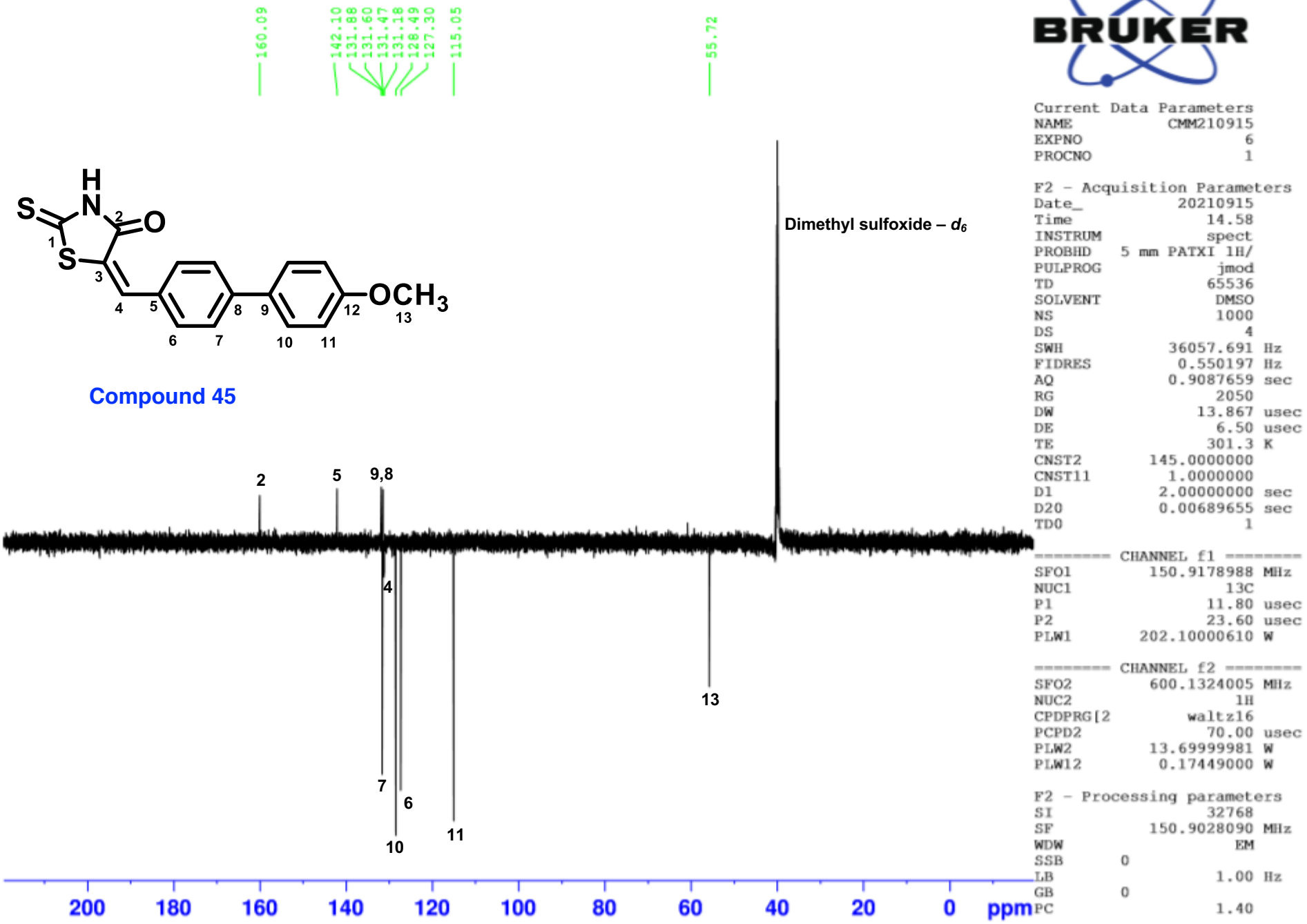
Signature:

Automatic analysis generated by Bruker CMC (b:17).
One or more results have not been created by automatic analysis, or edited manually: marked by '*'.
Report generated by Bruker CMC-assist TopSpin 4.1.3 (of 2021-06-28 13:00:50), on 'MacBook-Pro.local' as 'tzbenton'

Compound 45



45 (JMT-170)

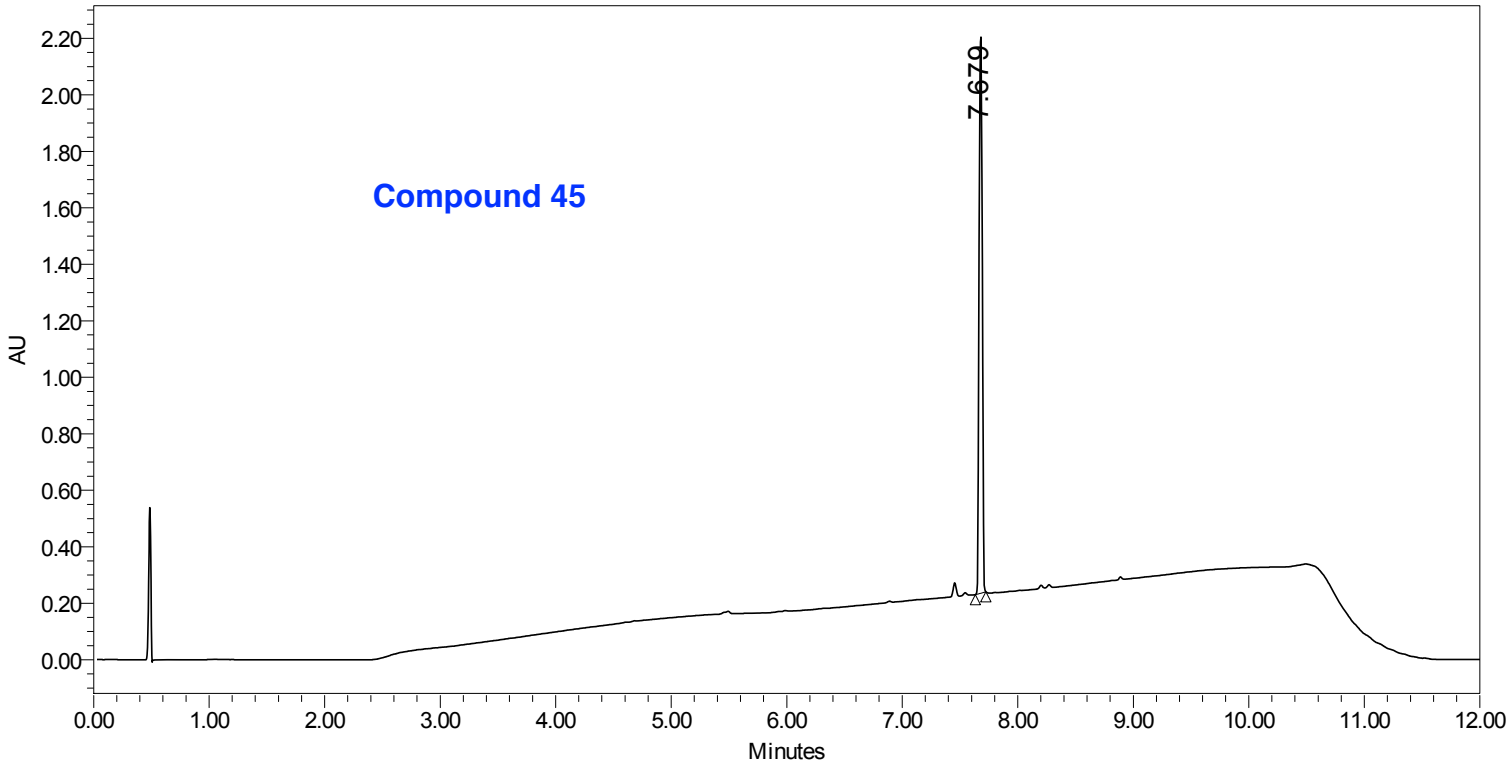


Compound 45

```
Current Data Parameters
NAME                  CMM210915
EXPNO                         6
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20210915
Time                      14.58
INSTRUM                   spect
PROBHD     5 mm PATXI 1H/
PULPROG                   jmod
TD                       65536
SOLVENT                   DMSO
NS                        1000
DS                           4
SWH                  36057.691 Hz
FIDRES               0.550197 Hz
AQ                   0.9087659 sec
RG                        2050
DW                      13.867 usec
DE                        6.50 usec
TE                       301.3 K
CNST2                145.0000000
CNST11                 1.0000000
D1                     2.00000000 sec
D20                    0.00689655 sec
TD0                           1

======== CHANNEL f1 ========
SFO1                 150.9178988 MHz
NUC1                         13C
P1                         11.80 usec
P2                         23.60 usec
PLW1                202.10000610 W

======== CHANNEL f2 ========
SFO2                 600.1324005 MHz
NUC2                         1H
CPDPRG[2                 waltz16
PCPD2                      70.00 usec
PLW2                 13.69999981 W
PLW12                 0.17449000 W

F2 - Processing parameters
SI                           32768
SF                   150.9028090 MHz
WDW                             EM
SSB                  0
LB                         1.00 Hz
GB                   0
PC                         1.40
```

SAMPLE INFORMATION

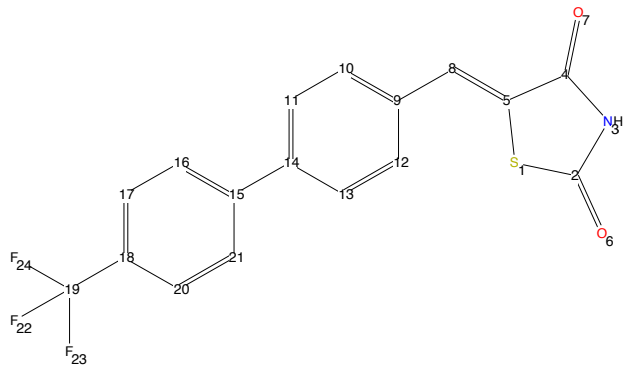
Sample Name:	2021June24_MJF_30	Acquired By:	System
Sample Type:	Unknown	Sample Set Name	TZB_103dx
Vial:	1:A,4	Acq. Method Set:	ReversePhase_12min_Max Plot
Injection #:	1	Processing Method	ReversePhase_Purity_MAX Plot
Injection Volume:	5.00 ul	Channel Name:	PDA Max Plot 190.0 - 800.0
Run Time:	12.0 Minutes	Proc. Chnl. Descr.:	PDA MaxPlot (190.0 nm to 800.0
Date Acquired:	6/24/2021 10:47:26 AM EDT		
Date Processed:	8/31/2021 4:01:45 PM EDT		



	RT	Area	% Area	Height	Peak Lambda Max.
1	7.679	3784346	100.00	1973427	393.1

CMC-assist

CMM210618



Consistency: Unknown*, unknown purity*

Sum formula:
$C_{17}H_{10}F_3NO_2S$

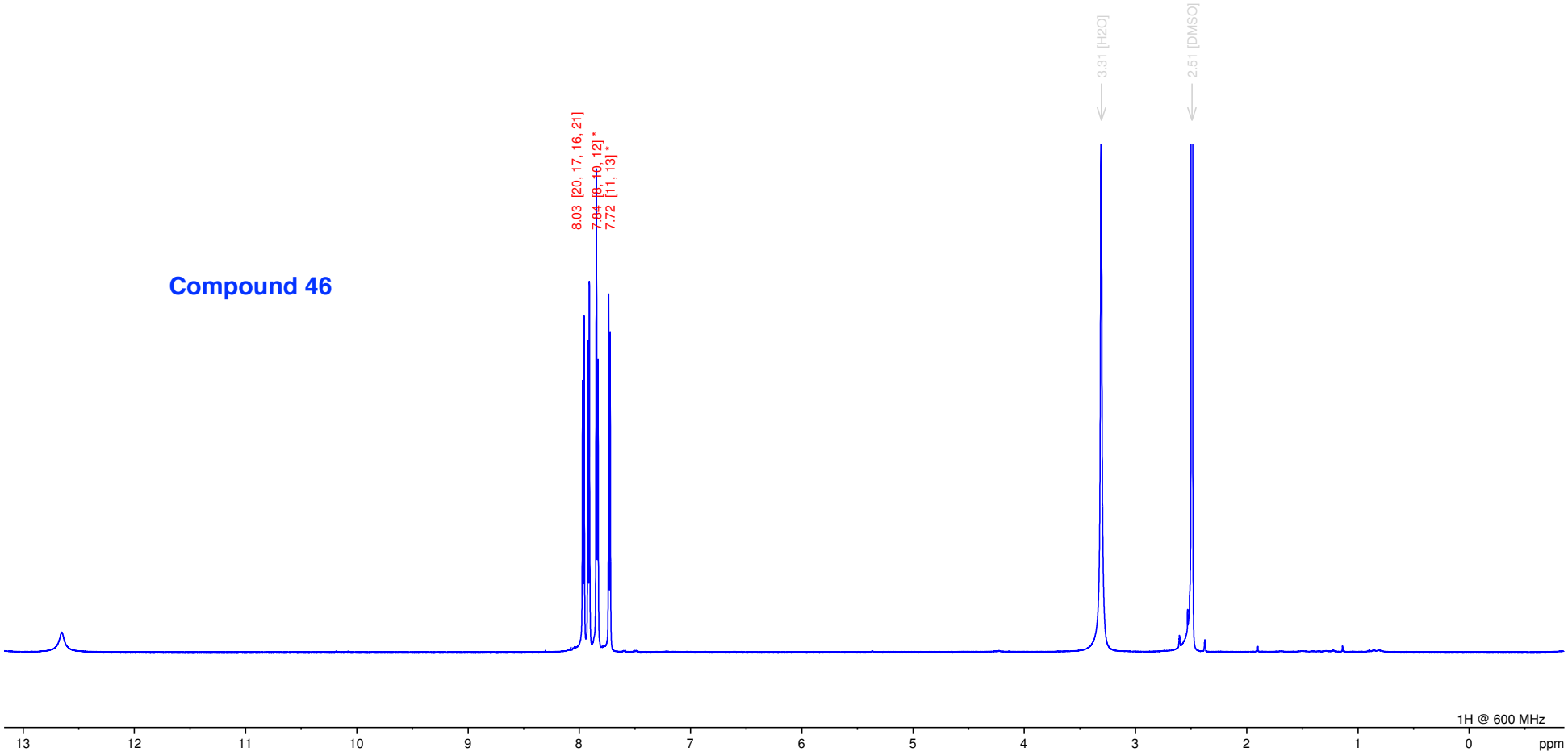
Molecular Mass:
349.04 Da

Data set 1H: CMM210618 2 1 /opt/topspin4.1.3
Structure: /opt/topspin4.1.3/CMM210618/2/structure.mol
Acquisition date: June 18, 2021 3:08:52 PM EDT
Solvent: DMSO
Probe: 5 mm PATXI 1H/D/19F-13C/15N Z-GRD Z855801/0017
Eretic reference:

Comments:
Multiplet interpretation available for spectrum.
A multiplet interpretation for all major signals in the spectrum could be found. All given impurities could be assigned to regions in the spectrum.

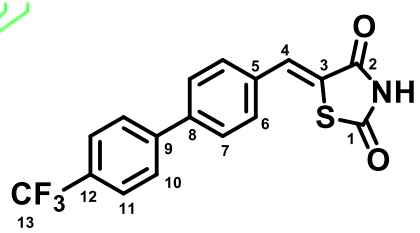
Signature:

Automatic analysis generated by Bruker CMC (b:17).
One or more results have not been created by automatic analysis, or edited manually: marked by '*'.
Report generated by Bruker CMC-assist TopSpin 4.1.3 (of 2021-06-28 13:00:50), on 'MacBook-Pro.local' as 'tzbenton'



46 (JMT200)

168.17
167.76
143.31
140.46
133.55
131.45
131.17
128.26
128.07
126.33
124.57



Compound 46

Dimethyl sulfoxide – d_6

1,2
9
8
5
3
13
4
6
11
10,7

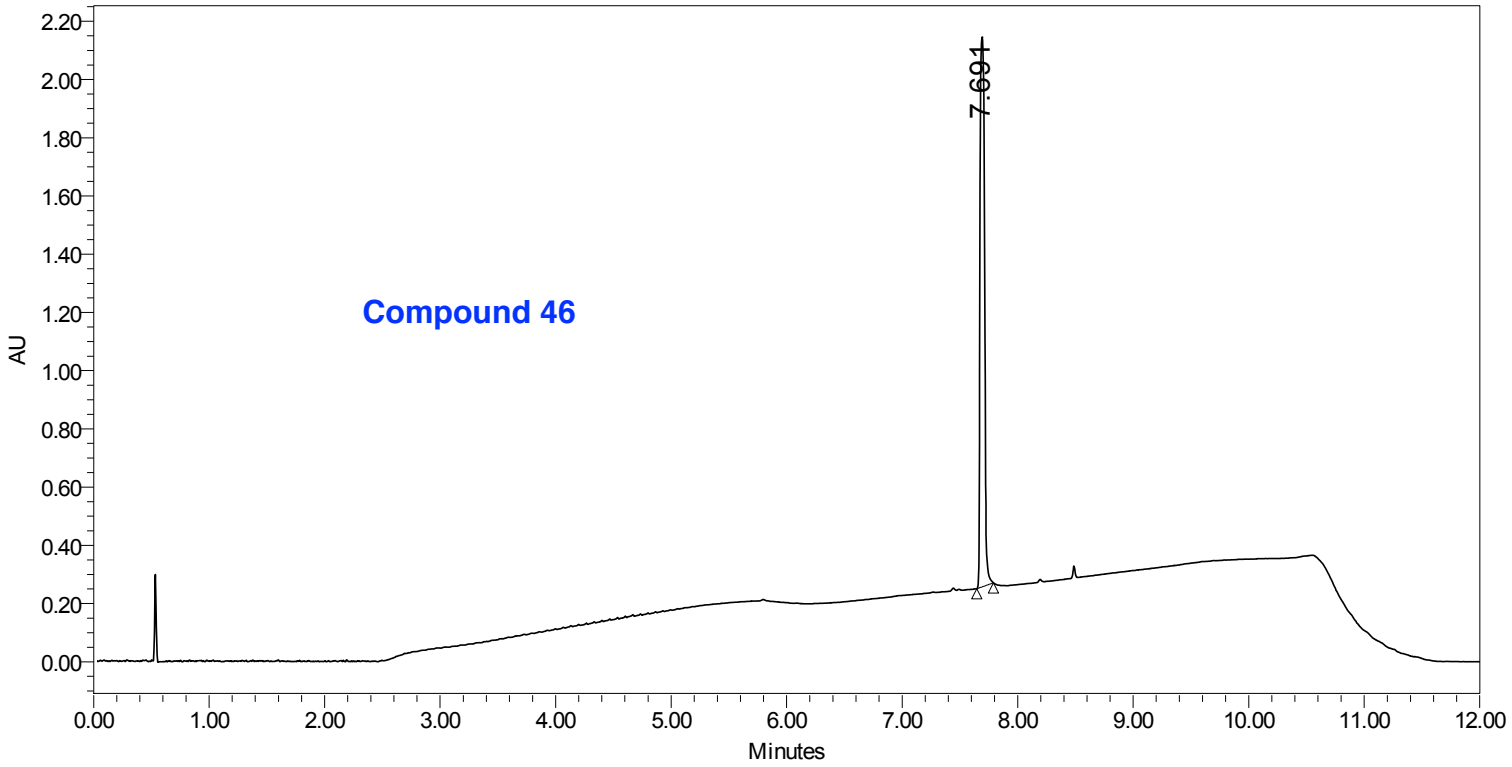
200 180 160 140 120 100 80 60 40 20 0 ppm

BRUKER

```
Current Data Parameters
NAME                  CMM210917
EXPNO                         5
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20210917
Time                      12.45
INSTRUM                   spect
PROBHD    5 mm PATXI 1H/
PULPROG                   jmod
TD                       65536
SOLVENT                   DMSO
NS                        1000
DS                           4
SWH                  36057.691 Hz
FIDRES                0.550197 Hz
AQ                    0.9087659 sec
RG                        2050
DW                      13.867 usec
DE                        6.50 usec
TE                       304.1 K
CNST2                145.0000000
CNST11                 1.0000000
D1                     2.00000000 sec
D20                    0.00689655 sec
TD0                           1

======== CHANNEL f1 ========
SFO1               150.9178988 MHz
NUC1                        13C
P1                        11.80 usec
P2                        23.60 usec
PLW1              202.10000610 W

======== CHANNEL f2 ========
SFO2               600.1324005 MHz
NUC2                        1H
CPDPRG[2                waltz16
PCPD2                     70.00 usec
PLW2               13.69999981 W
PLW12               0.17449000 W

F2 - Processing parameters
SI                        32768
SF                 150.9028090 MHz
WDW                          EM
SSB          0
LB                        1.00 Hz
GB           0
PC                        1.40
```

SAMPLE INFORMATION

Sample Name:	Ds3	Acquired By:	System
Sample Type:	Unknown	Sample Set Name	103dx_JMT
Vial:	1:A,7	Acq. Method Set:	ReversePhase_12min_Max Plot
Injection #:	1	Processing Method	ReversePhase_Purity_MAX Plot
Injection Volume:	1.00 ul	Channel Name:	PDA Max Plot 190.0 - 800.0
Run Time:	12.0 Minutes	Proc. Chnl. Descr.:	PDA MaxPlot (190.0 nm to 800.0
Date Acquired:	7/27/2021 7:56:30 PM EDT		
Date Processed:	8/31/2021 2:47:35 PM EDT		



	RT	Area	% Area	Height	Peak Lambda Max.
1	7.691	5106805	100.00	1888896	317.3