

Supporting Information for:
**Water-Driven Ligations Using Cyclic Amino
Squarates: Making SN1-Like Reactions Useful**

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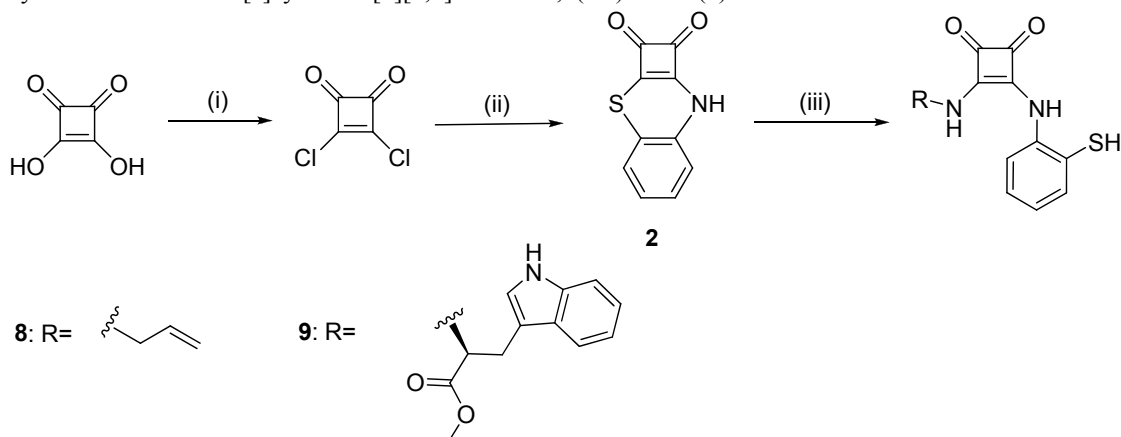
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1. General Information of the synthesis and characterization of the new compounds.

General Experimental Methods. ^1H NMR and ^{13}C NMR spectra were recorded on a 300 MHz spectrometer and the chemical shifts were measured from the solvent peak as an internal standard. Chemical shifts and coupling constants (J -value) are reported in ppm and Hertz respectively. The following abbreviations are used for spin multiplicity: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad. High Resolution Mass spectra (HRMS) samples were analyzed by positive ion electrospray. Analytical thin-layer chromatography (TLC) was performed using silica gel 60 F254 pre-coated plates (0.25-mm thickness). Preparative TLC separations were made on precoated analytical plates, 0.50 mm thick, silica gel 60 F254. Flash column chromatography was performed with Silica-P Flash Silica Gel (ultra pure 40-63 μm). Reagents and solvents purchased from Aldrich Chemical Co., Acros Organics, VWR International Inc., Pfaltz & Bauer and Pharmco and used without any further purification. All reactions were carried out in oven-dried glassware under argon or nitrogen atmosphere unless otherwise specified.

1.1 Synthesis of 1H-benzo[e]cyclobuta[b][1,4]thiazine-1,2(8H)-dione (**2**)



Reagents and conditions: (i) oxalyl chloride, DMF, CCl_4 , -78°C to reflux, 3hr; (ii) 2-aminothiophenol, TEA, benzene, 0°C to reflux, 16hr; (iii) RNH_2 , TEA, THF, r.t., 16hr.

(1) Synthesis of **2**

Finely powdered 1,2-Dihydroxycyclobutene-3,4-dione (0.57 g, 5 mmol), carbon tetrachloride (10 mL), and DMF (0.05mL), were introduced into a 25 mL round-bottomed flask previously filled with argon. The mixture was frozen by immersion in dry ice-acetone and oxalyl chloride (0.85 mL, 10 mmol) was introduced at once through the condenser's outlet. Then the flask was allowed to warm to room temperature, agitation started at 300 rpm, and the flask was then lowered into an oil bath thermostatted to $50\text{--}60^\circ\text{C}$. Regular gas evolution started immediately and was no more apparent after 50 min. After further 2hr, heating and agitation were discontinued. The solvent was removed to give 1,2-dichlorocyclobutene-3,4-dione (0.6g) as yellow crystal.

1,2-Dichlorocyclobutene-3,4-dione (0.6g) was dissolved in dry benzene (50mL) and cooled down to 0°C under argon atmosphere. 1 eq of thiophenol was added in one portion, followed by addition of excess of triethylamine (2.2eq) in anhydrous benzene (5mL). Reaction mixture was stirred at 0°C for 0.5hr, at r.t. for 0.5hr and at reflux overnight. The mixture was filtered and the solid was washed with water and methanol to give a yellow solid. Yield: 0.45g (55%). ^1H NMR (300 MHz, DMSO-d_6) : δ 7.35-6.89 (m, 3H), 6.73-6.70 (m, 1H). ^{13}C NMR (75 MHz, DMSO-d_6) : δ 183.84, 183.39, 179.66, 164.62, 134.48, 129.57, 128.39, 126.63, 119.14, 115.03. MS: cacl. for M^+ : 203, found: 203.

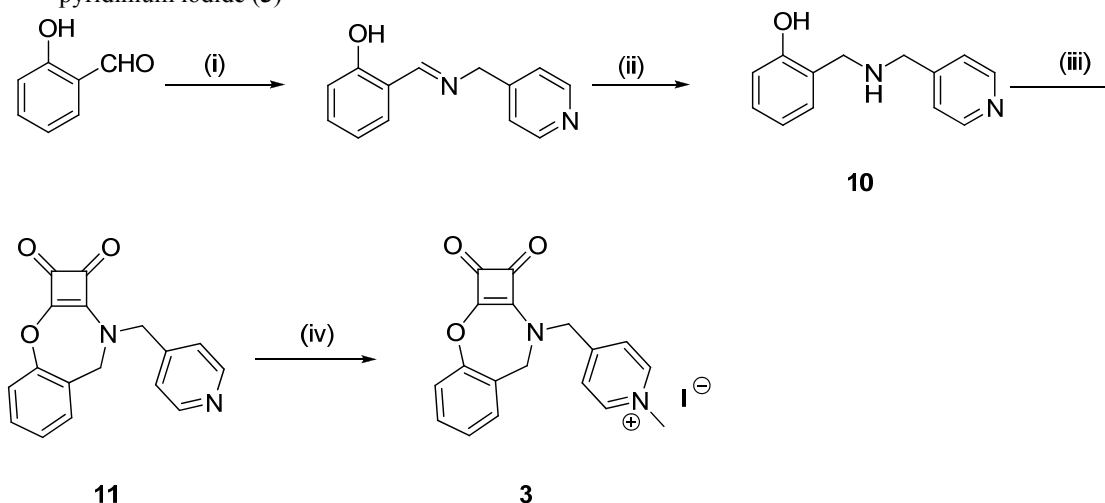
(2) General procedures for the synthesis of **8** and **9**

To a mixture of **2** (1mmol, 1eq) and TEA (2mmol, 2eq) in dry THF (20mL) at r.t. under Ar was added substituted amine (3mmol, 1.5eq). The mixture was stirred at r.t. overnight. The mixture was concentrated and the residue was partitioned between water and ethyl acetate. The organic layer was separated, washed with brine, dried and concentrated. The residue was purified by flash chromatography using PE:EA (1:1) as eluent to give a yellow solid. 3-(Allylamino)-4-(2-mercaptophenylamino)cyclobut-3-ene-1,2-dione (**8**): Yield 0.17g (65%). MS m/z (%): cacl. for $[\text{M}+\text{H}]^+$: 261.1, found: 261.1; ^1H NMR (300 MHz, DMSO-d_6) : δ 9.59 (brs, 1H), 8.70-8.66 (1H), 8.19 (s, 1H), 6.91-6.74 (m, 3H), 6.54 (dd, $J = 7.5$ Hz, 3Hz, 1H), 5.85-5.72 (m, 1H), 5.11-5.01 (m, 2H), 3.73-3.68 (m, 2H).

^{13}C NMR (75MHz, DMSO-d_6) : δ 177.52, 163.26, 147.03, 135.38, 135.27, 128.19, 127.72, 126.83, 120.97, 117.66, 116.26, 102.40, 41.64.

(S)-methyl-3-(1H-indol-3-yl)-2-(2-(2-mercaptophenylamino)-3,4-dioxocyclobut-1-enylamino)propanoate (**9**). Yield 0.23g (55%). MS m/z (%): cacl. for $[\text{M}+\text{H}]^+$: 422.1, found: 422.1; ^1H NMR (300 MHz, DMSO-d_6) : δ 10.86 (s, 1H), 9.73 (s, 1H), 8.73 (d, J = 7.8 Hz, 1H), 8.03 (s, 1H), 7.46 (d, J = 7.8 Hz, 1H), 7.33 (d, J = 7.8 Hz, 1H), 7.13 (s, 1H), 7.06-6.78 (m, 5H), 6.56 (d, J = 7.8 Hz, 1H), 4.53 (m, 1H), 3.62 (s, 3H), 3.21 (m, 2H); ^{13}C NMR (75MHz, DMSO-d_6) : δ 176.24, 171.77, 162.83, 146.36, 136.21, 134.43, 127.48, 127.09, 126.99, 126.20, 123.92, 121.14, 120.14, 118.59, 118.08, 117.02, 111.62, 109.38, 101.63, 53.04, 52.23, 26.43.

1.2 Synthesis of 4-((1,2-dioxo-1,2-dihydrobenzo[*f*]cyclobuta[*b*][1,4]oxazepin-9(8H)-yl)-methyl)-1-methylpyridinium iodide (**3**)



Reagents and conditions: (i) 4-aminomethyl pyridine, EtOH, r.t. 1hr; (ii) NaBH_4 , EtOH, 0°C to r.t., 1hr; (iii) 3,4-dichlorocyclobutene-1,2-dione, TEA, benzene, 0°C to reflux, 16hr; (iv) CH_3I , CH_2Cl_2 , r.t., 16hr

(1) Synthesis of 2-((pyridin-4-ylmethylamino)methyl)phenol (**10**)

A mixture of salicylaldehyde (10mmol) and amine (1eq) in EtOH (10mL) was stirred at r.t. for 2hr. The mixture was cooled to 0°C and NaBH_4 (1.2 eq) was added in portions. The mixture was then stirred at that temp. for 2hr. The reaction was quenched by water and concentrated. The residue was partitioned between water and DCM. The organic layers were combined, dried and concentrated. The residue was purified by flash chromatography using DCM:MeOH (20:1) as eluent to give a colorless sticky oil. Yield 1.9g (90%). ^1H NMR (300 MHz, CDCl_3) : δ 8.61-8.56 (m, 2H), 7.26-7.01 (m, 3H), 7.01-6.78 (m, 3H), 4.06 (s, 2H), 3.85 (s, 2H).

(2) Synthesis of 9-(pyridin-4-ylmethyl)-8,9-dihydrobenzo[*f*]cyclobuta[*b*][1,4]oxazepin-1,2-dione (**11**)

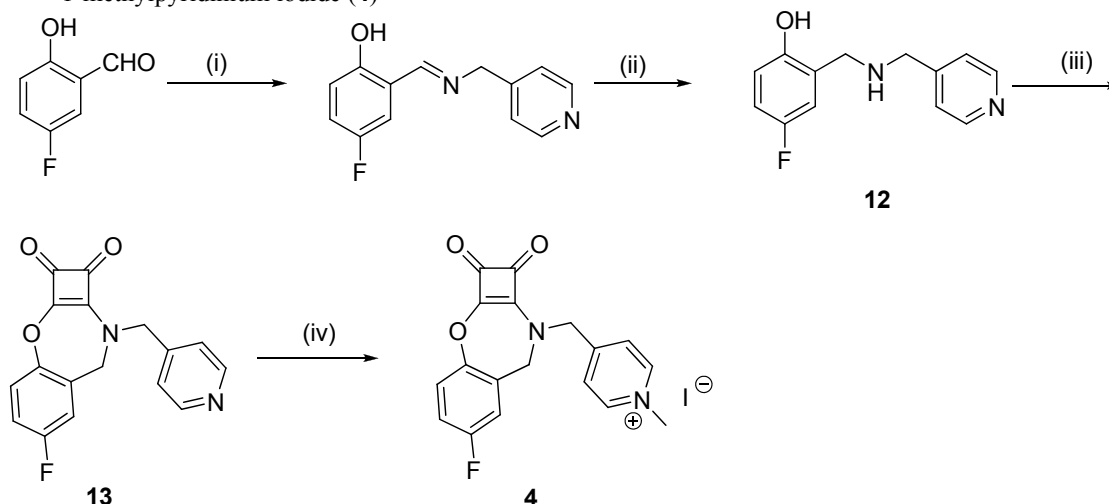
1,2-Dichlorocyclobutene-3,4-dione (0.6g) was dissolved in dry benzene (50mL) and cooled down to 0°C under argon atmosphere. 1 eq of 2-((pyridin-4-ylmethylamino)-methyl)phenol in anhydrous benzene (25mL) was added dropwise, accompanied by addition of excess of triethyl amine (2.2eq) in anhydrous benzene (25mL). Reaction mixture was stirred at 0°C for 0.5hr, at r.t. for 0.5hr and at reflux overnight. The reaction mixture was then filtered and concentrated. Flash chromatography using Hexanes (100mL), DCM (100mL), DCM:MeOH (100:1, 200mL), DCM:MeOH (80:1, 200mL), DCM:MeOH (60:1) as eluent afforded a brown sticky oil, which was dried under high vacuum to give a foamy solid. Yield: 0.19g (16.3%). MS m/z (%): cacl. for $[\text{M}+\text{H}]^+$: 293.1, found: 293.1; ^1H NMR (300 MHz, DMSO-d_6) : δ 8.57 (dd, J = 1.5, 4.5Hz, 2H), 7.48-7.31 (m, 5H), 7.22-7.16 (m, 1H), 4.89 (s, 2H), 4.67 (s, 2H).

(3) Synthesis of 4-((1,2-dioxo-1,2-dihydrobenzo[*f*]cyclobuta[*b*][1,4]oxazepin-9(8H)-yl)methyl)-1-methylpyridinium iodide (**3**)

A mixture of 9-(pyridin-4-ylmethyl)-8,9-dihydrobenzo[*f*]cyclobuta[*b*][1,4]oxazepin-1,2-dione (20mg) and iodomethane (excess) in anhydrous DCM (0.4mL) was stirred at r.t. for overnight. The mixture was filtered and the solid was dried under high vacuum to give a pale white solid with rather good water solubility. Yield : 18.9mg

(90%). HRMS m/z : cacl. for $[M+H-I]^+$: 307.1082, found: 307.1083; $^1\text{H NMR}$ (300 MHz, DMSO-d_6): δ 8.96 (d, $J=6.3\text{Hz}$, 2H), 8.11 (d, $J=6.0\text{Hz}$, 2H), 7.51-7.19 (m, 4H), 5.16 (s, 2H), 4.74 (s, 2H), 4.32 (s, 3H). $^{13}\text{C NMR}$ (75MHz, DMSO-d_6): δ 188.44, 181.18, 175.26, 173.81, 155.30, 154.41, 145.69, 132.27, 130.86, 125.91, 125.37, 123.61, 120.50, 53.86, 52.73, 47.65.

1.3 Synthesis of 4-((6-fluoro-1,2-dioxo-1,2-dihydrobenzo[f]cyclobuta[b][1,4]oxazepin-9(8H)-yl)methyl)-1-methylpyridinium iodide (**4**)



Reagents and conditions: (i) 4-aminomethyl pyridine, EtOH, r.t. 1hr; (ii) NaBH_4 , EtOH, 0°C to r.t., 1hr; (iii) 3,4-dichlorocyclobutene-1,2-dione, TEA, benzene, 0°C to reflux, 16hr; (iv) CH_3I , CH_2Cl_2 , r.t., 16hr

(1) Synthesis of 4-fluoro-2-((pyridin-4-ylmethylamino)methyl)phenol (**12**)

A mixture of aldehyde (10mmol) and amine (1eq) in EtOH (10mL) was stirred at r.t. for 2hr. The mixture was then cooled to 0°C and NaBH_4 (1.2 eq) was added in portions. The mixture was then stirred at that temp. for 2hr. The reaction solution was quenched by water at 0°C and concentrated. The residue was extracted by DCM. The organic layers were combined, dried and concentrated. The residue was purified by flash chromatography using DCM:MeOH (20:1) as eluent to give a colorless sticky oil. Yield 1.44g (65%). $^1\text{H NMR}$ (300 MHz, DMSO-d_6): δ 8.50 (d, $J=6\text{Hz}$, 2H), 7.35 (d, $J=6\text{Hz}$, 2H), 7.03 (dd, $J=9, 3\text{Hz}$, 1H), 6.89 (m, 1H), 6.74-6.69 (m, 1H), 3.73 (s, 2H), 3.70 (s, 2H).

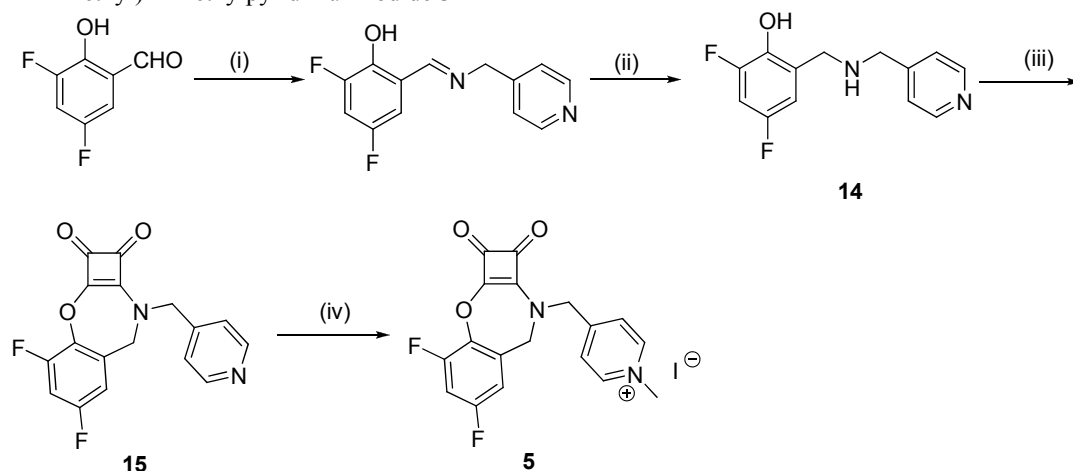
(3) Synthesis of 6-fluoro-9-((pyridin-4-ylmethyl)-8,9-dihydrobenzo[f]cyclobuta[b][1,4]-oxazepine-1,2-dione (**13**)

1,2-Dichlorocyclobutene-3,4-dione (0.6g) was dissolved in dry benzene (40mL) and cooled down to 0°C under argon atmosphere. 1 eq of phenol in anhydrous benzene (30 mL) was added dropwise, accompanied by addition of excess of triethyl amine (2.2eq) in anhydrous benzene (30 mL). Reaction mixture was stirred at 0°C for 0.5hr, at r.t. for 0.5hr and at reflux overnight. The reaction mixture was then filtered and concentrated. Flash chromatography using PE (100mL), DCM (100mL), DCM:MeOH (100:1, 200mL), DCM:MeOH (80:1, 200mL), DCM:MeOH (60:1) as eluent afforded a brown sticky oil, which was dried under high vacuum to give a foamy solid. Yield 0.31g (25%). HRMS m/z : cacl. for $[M+H]^+$: 311.0832, found: 311.0822; $^1\text{H NMR}$ (300 MHz, DMSO-d_6): δ 8.59-8.58 (m, 2H), 7.46-7.26 (m, 5H), 4.98 (s, 2H), 4.66 (s, 2H).

(3) Synthesis of 4-((6-fluoro-1,2-dioxo-1,2-dihydrobenzo[f]cyclobuta[b][1,4]oxazepin-9(8H)-yl)methyl)-1-methylpyridinium iodide (**4**)

A mixture of 6-fluoro-9-((pyridin-4-ylmethyl)-8,9-dihydrobenzo[f]cyclobuta[b][1,4]-oxazepine-1,2-dione (20mg) and iodomethane (excess) in anhydrous DCM (0.4mL) was stirred at r.t. overnight. The mixture was filtered and the solid was washed with large amount of DCM, dried under high vacuum to give a pale white solid with rather good water solubility. Yield: 18.8 mg (90%). HRMS m/z : cacl. for $[M+H-I]^+$: 325.0988, found: 325.0996; $^1\text{H NMR}$ (300 MHz, DMSO-d_6): δ 8.97 (m, 2H), 8.13-8.11 (m, 2H), 7.50-7.23 (m, 3H), 5.15 (s, 2H), 4.72 (s, 2H), 4.33 (3H). $^{13}\text{C NMR}$ (75MHz, DMSO-d_6): δ 188.33, 181.08, 175.32, 173.72, 159.47, 156.26, 155.05, 150.82, 150.78, 145.68, 126.02, 125.62, 125.51, 122.59, 122.48, 118.58, 118.26, 117.47, 117.16, 53.02, 52.71, 47.72.

1.4 Synthesis of 4-((4,6-difluoro-1,2-dioxo-1,2-dihydrobenzo[f]cyclobuta[b][1,4]-oxazepin-9(8H)-yl)-methyl)-1-methylpyridinium iodide **5**



Reagents and conditions: (i) 4-aminomethyl pyridine, EtOH, r.t. 1hr; (ii) NaBH₄, EtOH, 0°C to r.t., 1hr; (iii) 3,4-dichlorocyclobutene-1,2-dione, TEA, benzene, 0°C to reflux, 16hr; (iv) CH₃I, CH₂Cl₂, r.t., 16hr

(1) Synthesis of 4,6-difluoro-2-((pyridin-4-ylmethylamino)methyl)phenol (**14**)

A mixture of aldehyde (10mmol) and amine (1eq) in EtOH (10mL) was stirred at r.t. for 2hr. The mixture was then cooled to 0°C and NaBH₄ (1.2 eq) was added in portions. The mixture was then stirred at that temp. for 2hr. The reaction solution was quenched by water at 0°C and concentrated. The residue was extracted by DCM. The organic layers were combined, dried and concentrated. The residue was purified by flash chromatography using DCM:MeOH (20:1) as eluent to give a colorless sticky oil. Yield 1.63g (65%). ¹HNMR (300 MHz, DMSO-d₆) : δ 8.61 (d, *J* = 4 Hz, 2H), 7.27-6.84 (m, 2H), 6.84-6.76 (m, 1H), 6.56-6.53 (m, 1H), 4.04 (s, 3H), 3.85 (s, 3H).

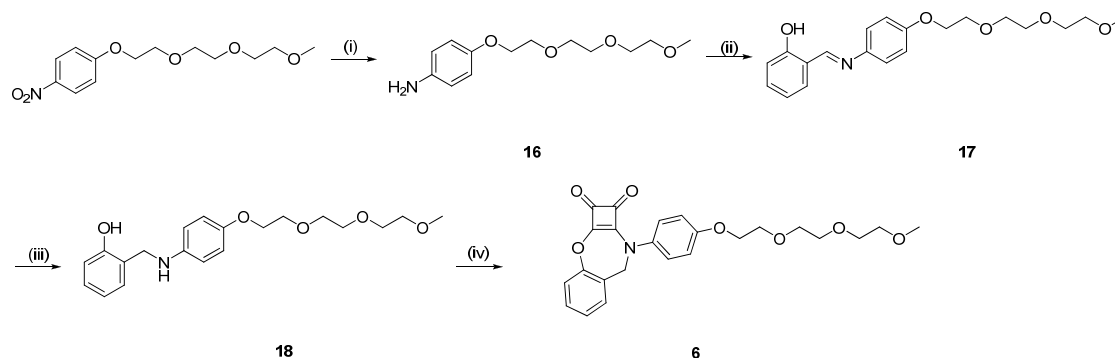
(2) Synthesis of 4,6-difluoro-9-(pyridin-4-ylmethyl)-8,9-dihydrobenzo[f]cyclobuta-[b][1,4]oxazepine-1,2-dione (**15**)

1,2-Dichlorocyclobutene-3,4-dione (0.6g) was dissolved in dry benzene (40mL) and cooled down to 0 °C under argon atmosphere. 1 eq of phenol in anhydrous benzene (30 mL) was added dropwise, accompanied by addition of excess of triethyl amine (2.2eq) in anhydrous benzene (30 mL). Reaction mixture was stirred at 0°C for 0.5hr, at r.t. for 0.5hr and at reflux overnight. The reaction mixture was then filtered and concentrated. Flash chromatography using PE (100mL), DCM (100mL), DCM:MeOH (100:1, 200mL), DCM:MeOH (80:1, 200mL), DCM:MeOH (60:1) as eluent afforded a brown sticky oil, which was dried under high vacuum to give a foamy solid. Yield 0.33g (25%). HRMS *m/z*: cacl. for [M+H]⁺: 329.0738, found: 329.0737; ¹HNMR (300 MHz, DMSO-d₆) : δ 8.70-8.69 (m, 2H), 7.27-7.23 (m, 2H), 7.08-7.01 (m, 1H), 6.64-6.60 (m, 1H), 4.94 (s, 2H), 4.74 (s, 2H).

(3) Synthesis of 4-((4,6-difluoro-1,2-dioxo-1,2-dihydrobenzo[f]cyclobuta[b][1,4]-oxazepin-9(8H)-yl)-methyl)-1-methylpyridinium iodide (**5**)

A mixture of 6-fluoro-9-(pyridin-4-ylmethyl)-8,9-dihydrobenzo[f]cyclobuta[b][1,4]-oxazepine-1,2-dione (20mg) and iodomethane (excess) in anhydrous DCM (0.4mL) was stirred at r.t. for overnight. The mixture was filtered and the solid was washed with large amount of DCM, dried under high vacuum to give a pale white solid with rather good water solubility. Yield : 19mg (90%). HRMS *m/z*: cacl. for [M+H-I]⁺: 343.0894, found: 343.0903; ¹HNMR (300 MHz, DMSO-d₆) : δ 8.98 (d, *J* = 4Hz, 2H), 8.12 (d, *J* = 4Hz, 2H), 7.67-7.60 (m, 1H), 7.15-7.11 (m, 1H), 5.16 (s, 2H), 4.78 (s, 2H), 4.33 (3H). ¹³CNMR (75MHz, DMSO-d₆) : δ 188.37, 180.68, 175.31, 172.86, 158.61, 158.45, 155.37, 155.20, 155.03, 153.80, 150.49, 150.31, 145.67, 139.74, 139.69, 139.58, 139.52, 127.13, 127.00, 125.92, 113.82, 113.77, 113.49, 113.45, 106.54, 106.23, 106.18, 105.87, 53.00, 52.83, 47.68.

1.5 Synthesis of 9-(4-(2-(2-(2-methoxyethoxy)ethoxy)ethoxy)phenyl)-8,9-dihydrobenzo[f]cyclobuta[b][1,4]oxazepine-1,2-dione (**6**)



Reagents and conditions: (i) Pd/C, H₂, MeOH; (ii) salicy aldehyde, EtOH, r.t. 1hr; (iii) NaBH₄, EtOH, 0°C to r.t., 1hr; (iv) 3,4-dichlorocyclobutene-1,2-dione, TEA, benzene, 0°C to reflux, 16hr.

(1) Synthesis of 4-(2-(2-(2-methoxyethoxy)ethoxy)ethoxy)aniline (**16**)

A mixture of **1** (10 mmol) and 10% Pd/C (10%wt) in MeOH (50 mL) was hydrogenated at room temperature under a hydrogen balloon, with vigorous stirring, overnight. The catalyst was filtered through Celite, and the filtrate was concentrated to give a brown sticky oil. The oil was used directly for the next step without further purification.

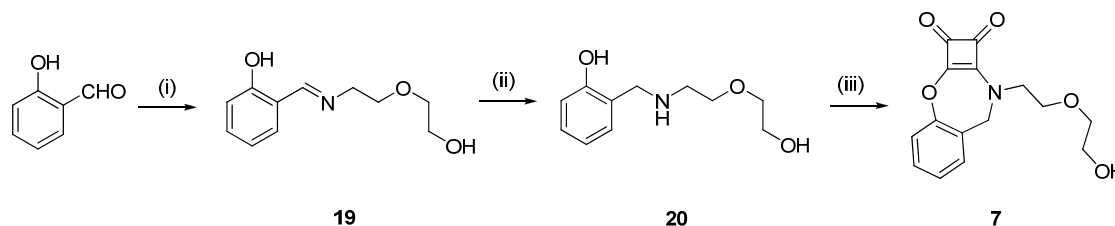
(2) Synthesis of 2-((4-(2-(2-(2-methoxyethoxy)ethoxy)ethoxy)phenylamino)methyl)phenol (**18**)

A mixture of aldehyde (10mmol) and amine (1eq) in EtOH was stirred at r.t. for 2hr. The mixture was cooled to 0°C and NaBH₄ (1.2eq) was added in portions. The mixture was then stirred at that temp. for 2hr. The reaction was solution was quenched by water and concentrated. The residue was extracted by DCM. The organic layers were combined, dried and concentrated to give a brown sticky oil. The oil was used directly for the next step without further purification.

(3) Synthesis of 9-(4-(2-(2-(2-methoxyethoxy)ethoxy)ethoxy)phenyl)-8,9-dihydrobenzo[f]cyclobuta[b][1,4]-oxazepine-1,2-dione (**6**)

1,2-Dichlorocyclobutene-3,4-dione (0.6g) was dissolved in dry benzene (50mL) and cooled down to 0 °C under argon atmosphere. 1 eq of phenol in anhydrous benzene (5mL) was added dropwise, accompanied by addition of excess of triethyl amine (2.2eq) in anhydrous benzene (5mL). Reaction mixture was stirred at 0°C for 0.5hr, at r.t. for 0.5hr and at reflux overnight. Flash chromatography using Hexanes:EtOAc (1:1) as eluent afforded a yellow sticky oil, which was dried under high vacuum to give semi solid. Total yield (three steps): 52.7%. HRMS *m/z*: cacl.: 440.1709 [M+H]⁺, found: 440.1700; ¹HNMR (300 MHz, CDCl₃) : δ 7.50-7.15 (m, 6H), 6.98 (d, *J* = 9.0 Hz, 2H), 4.99 (s, 2H), 4.16-4.14 (m, 2H), 3.89-3.86 (m, 2H), 3.76-3.57 (m, 8H), 3.39 (s, 3H).

1.6 Synthesis of 9-(2-(2-(2-hydroxyethoxy)ethyl)-8,9-dihydrobenzo[f]cyclobuta[b][1,4]-oxazepine-1,2-dione (**7**)



(1) Synthesis of 2-((2-(2-(2-hydroxyethoxy)ethyl)amino)methyl)phenol (**20**)

A mixture of aldehyde (10mmol) and amine (1eq) in EtOH was stirred at r.t. for 2hr. The mixture was cooled to 0°C and NaBH₄ (1.2eq) was added in portions. The mixture was then stirred at that temp. for 2hr. The reaction was solution was quenched by water and concentrated. The residue was extracted by DCM. The organic layers were combined, dried and concentrated to give a yellow sticky oil. The oil was used directly for the next step without further purification.

(2) Synthesis of 9-(2-(2-(2-hydroxyethoxy)ethyl)-8,9-dihydrobenzo[f]cyclobuta[b][1,4]-oxazepine-1,2-dione (**7**)

1,2-Dichlorocyclobutene-3,4-dione (0.6g) was dissolved in dry benzene (50mL) and cooled down to 0 °C under argon atmosphere. 1 eq of phenol in anhydrous benzene (5mL) was added dropwise, accompanied by addition of excess of triethyl amine (2.2eq) in anhydrous benzene (5mL). Reaction mixture was stirred at 0°C for 0.5hr, at r.t. for 0.5hr and at reflux overnight. Flash chromatography using Hexanes:EtOAc (1:1) as eluent afforded a yellow sticky oil. Total yield (two steps): 23.1%. HRMS m/z (%): cacl.: 290.1023 [M+H]⁺, found: 290.1026; ¹HNMR (300 MHz, CDCl₃): δ 7.42-6.89 (m, 4H), 4.68 (s, 2H), 3.96-3.56 (m, 8H).

2. Ligation of cyclic squarate derivative **3** with L-cysteine and L-cysteine ethyl ester

Table S1. Ligation of cyclic squarate derivative **3** with L-cysteine and L-cysteine ethyl ester (Scheme 1).^a

Entry	Reactant	Product	Time (Conv >95%)
1			5 min
2			5 min

^aReaction conditions: H₂O, r.t.

3. UV spectra of **3**, NHS-Biotin and SQ-Biotin

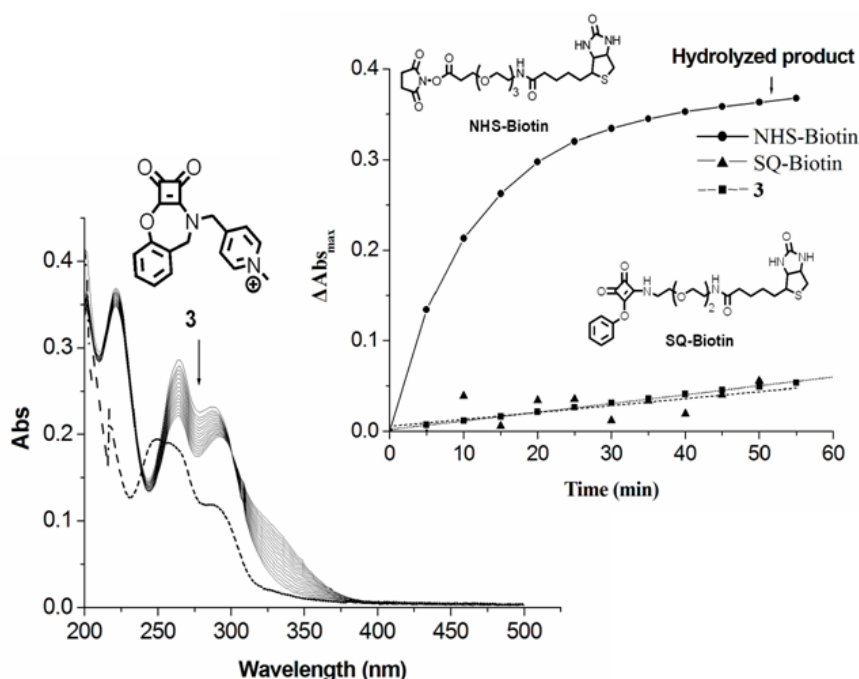


Fig1 UV spectra of 10 μM of **3** in PBS buffer (10 mM, pH 8.02) at increment of 5 min from 0 to 70 min (solid line), and in CH₃CN (dash line). The insert shows the plot of (Abs_{max(0 min)}-Abs_{max(t)}) at 264 nm of **3**, NHS-Biotin and SQ-Biotin versus time in PBS buffer (10 mM, pH 8.02).

4. The Maldi-Tof spectra for the ligation of the proteins using squarate pyridium salts.

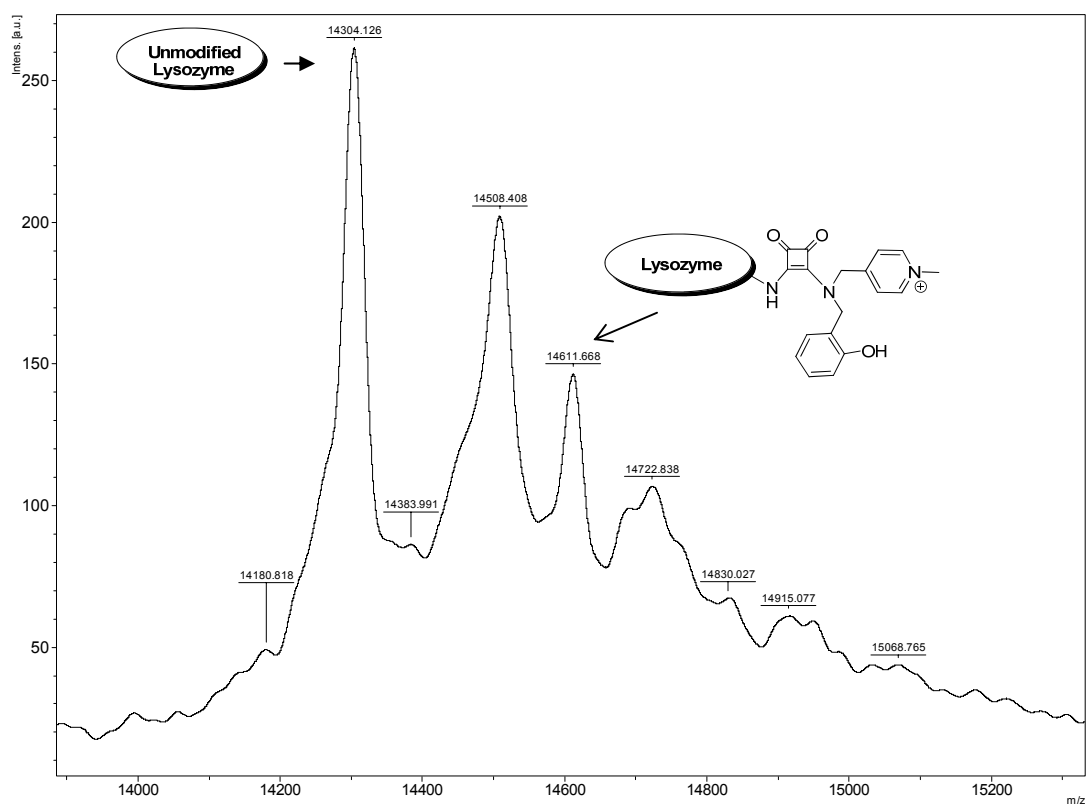


Figure 2. The spectrum of Maldi-Tof of modified Lysozyme by **3** at pH 7.75 in 10mM PBS buffer.

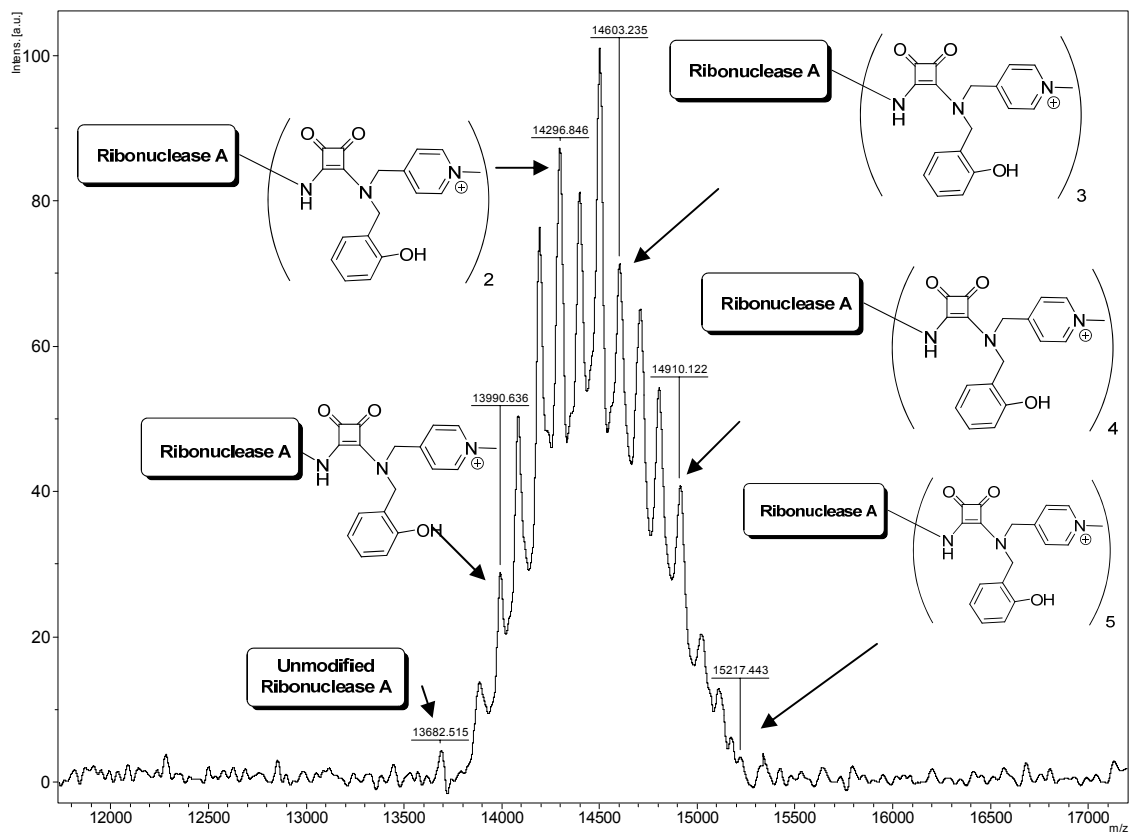


Figure 3. The spectrum of Maldi-Tof of modified Ribonuclease A by **3** at pH 7.75 in 10mM PBS buffer.

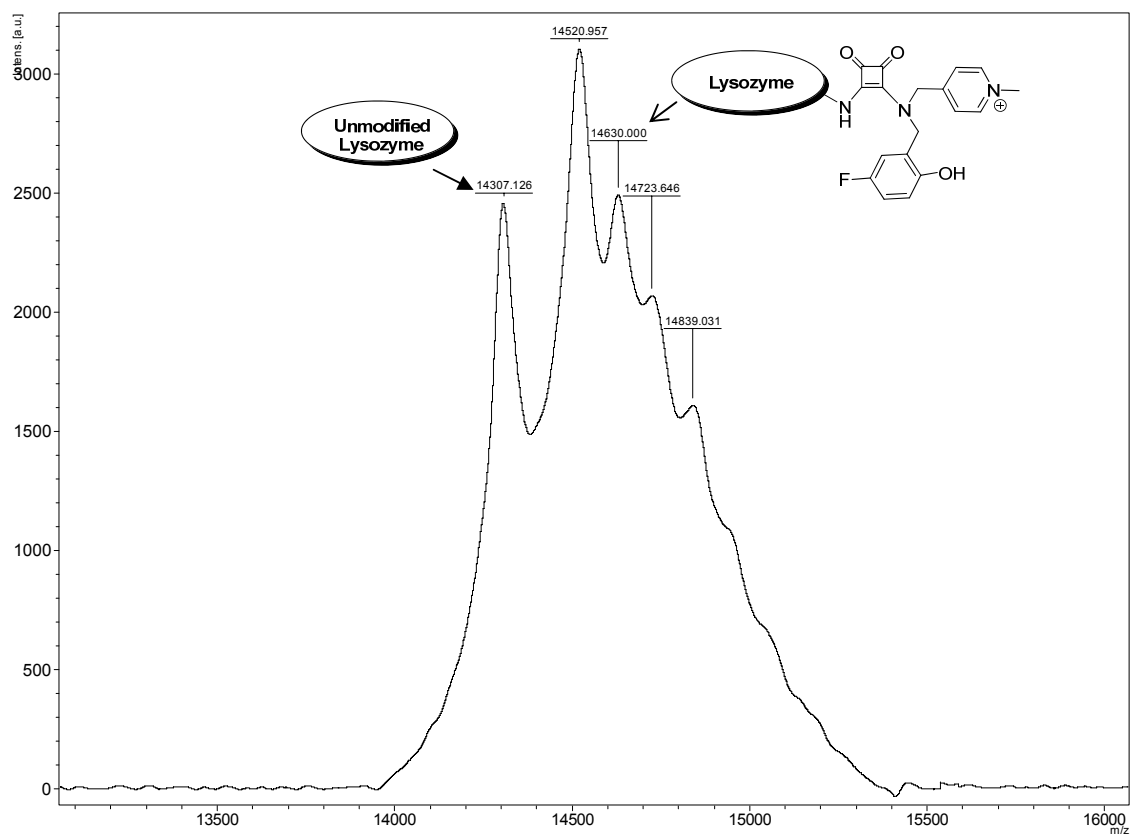


Figure 4. The spectrum of Maldi-ToF of modified Lysozyme by **4** at pH 7.75 in 10mM PBS buffer.

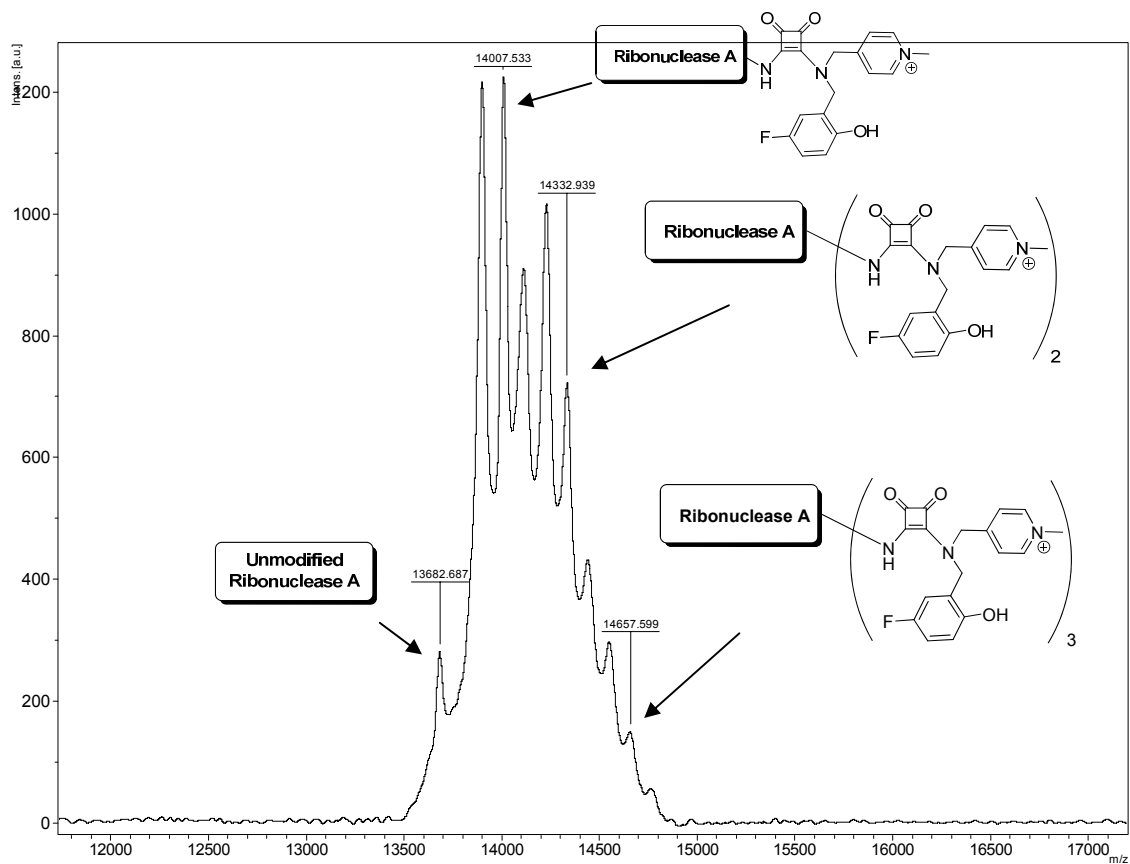


Figure 5. The spectrum of Maldi-ToF of modified Ribonuclease A by 4 at pH 7.75 in 10mM PBS buffer.

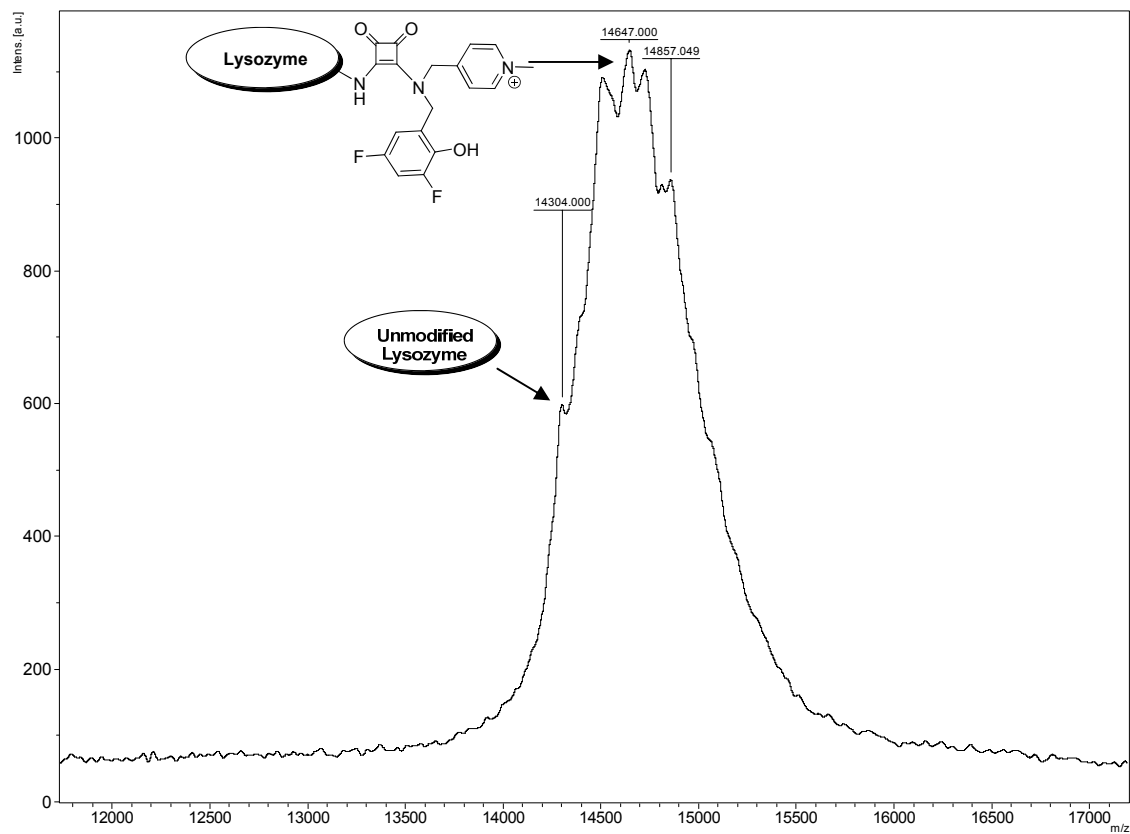


Figure 6. The spectrum of Maldi-ToF of modified Lysozyme by **5** at pH 7.75 in 10mM PBS buffer.

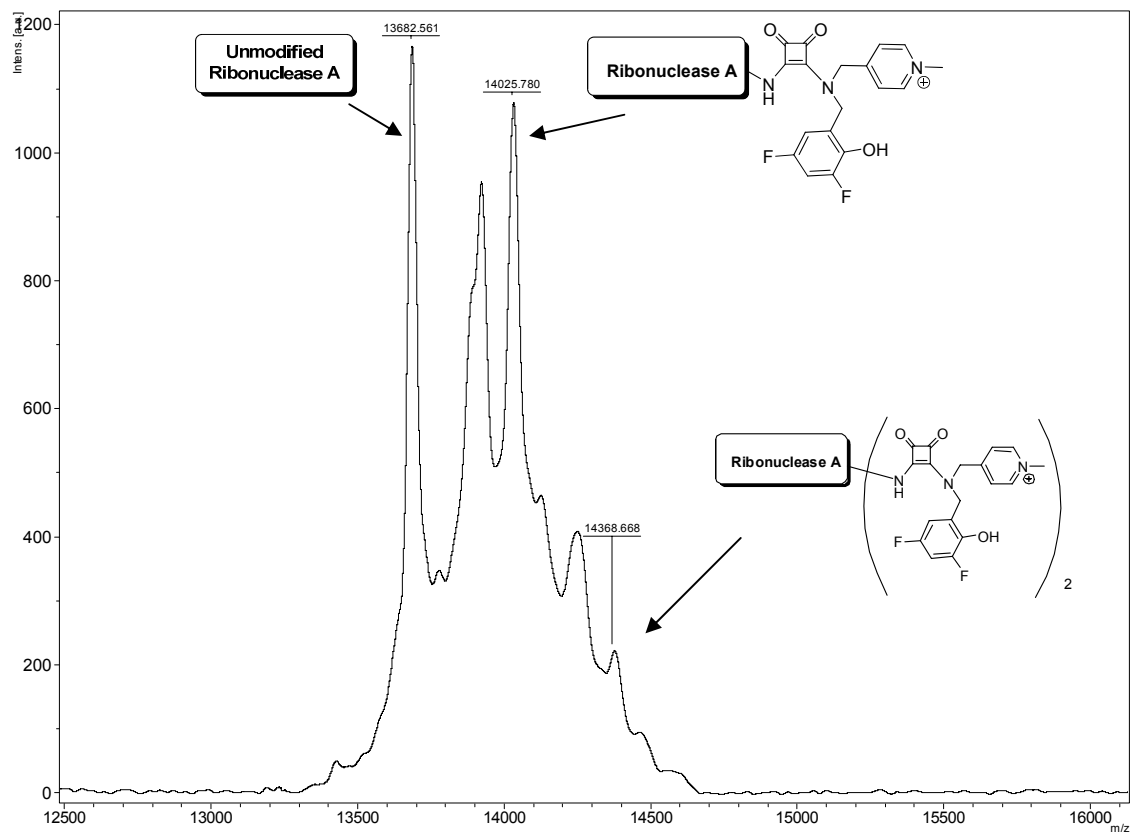
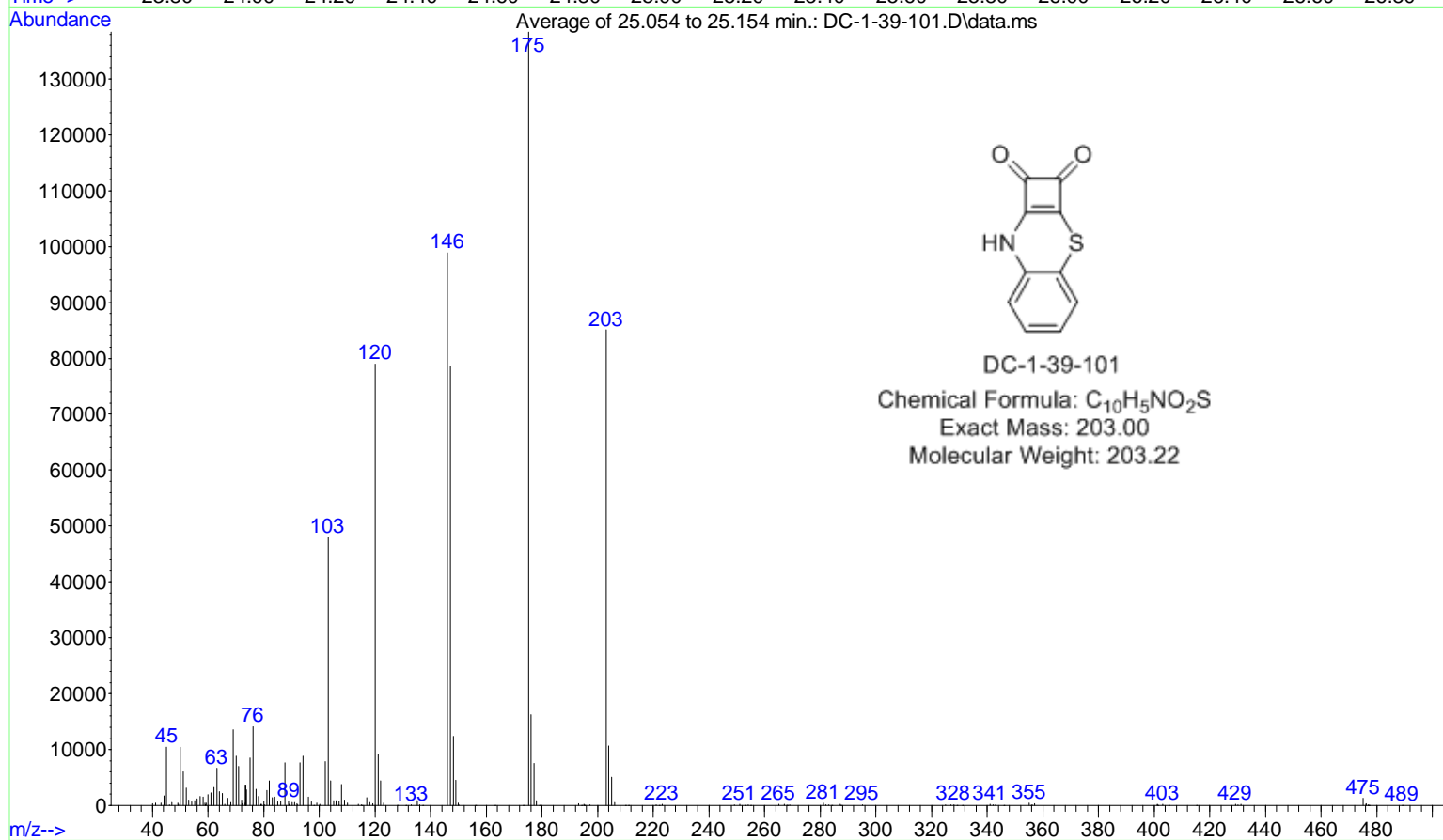
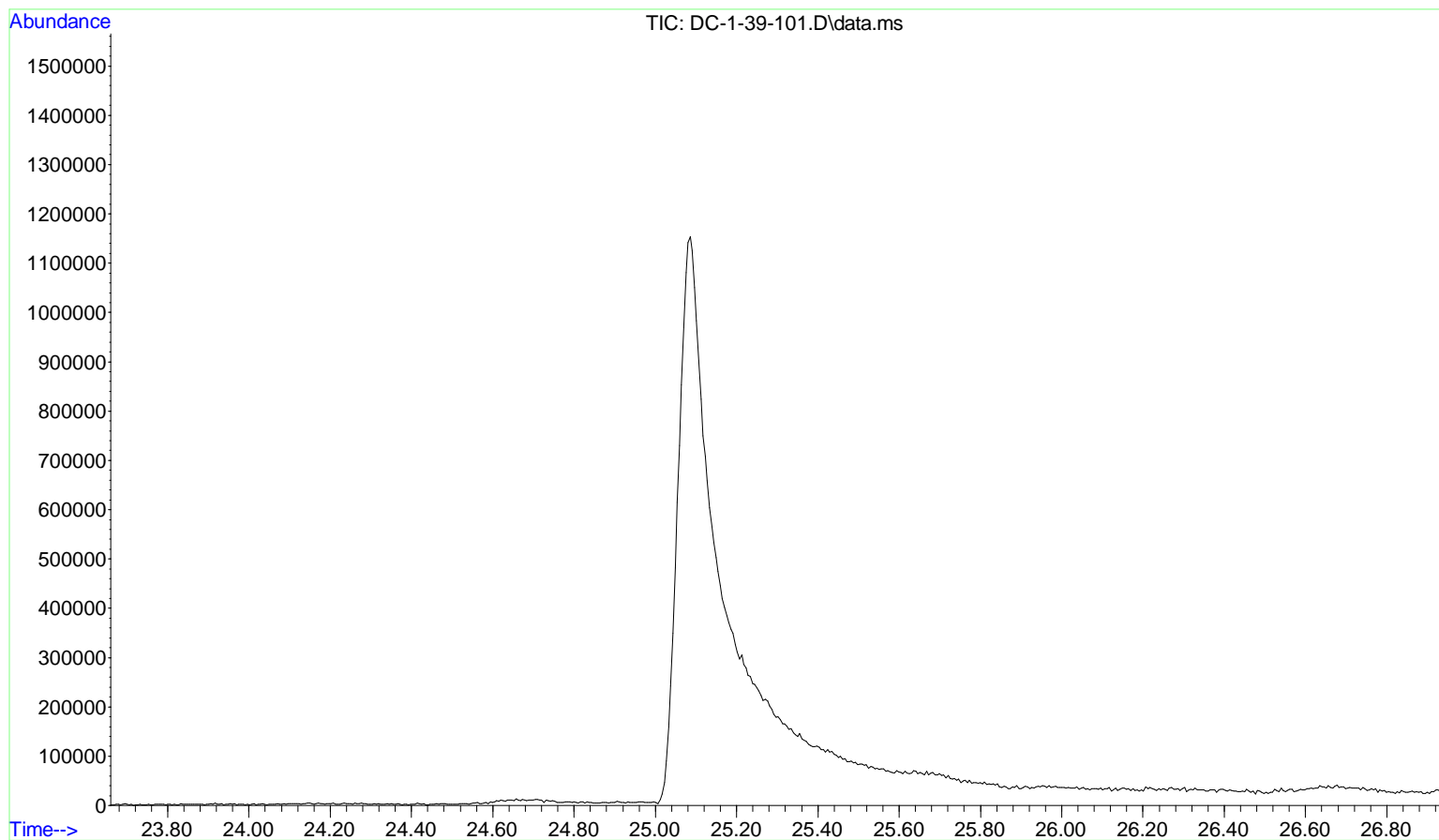


Figure 7. The spectrum of Maldi-ToF of modified Ribonuclease A by **5** at pH 7.75 in 10mM PBS buffer.

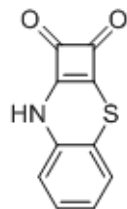
File : C:\MSDCHEM\1\Default\Data\BSB\DC-1-39-101.D This journal is (c) The Royal Society of Chemistry 2011
Operator : amh
Acquired : 11 Dec 2009 11:30 using AcqMethod 00_GEN 30_1 SPLIT ALS_INJ_EI 40C 40_500DA.M
Instrument : Instrument #1
Sample Name: dc-1-39-101
Misc Info :
Vial Number: 11



7.360
7.091
7.084
7.069
7.065
7.062
7.058
7.043
7.035
7.006
6.987
6.980
6.961
6.954
6.950
6.932
6.928
6.925
6.906
6.902
6.744
6.740
6.718
6.713

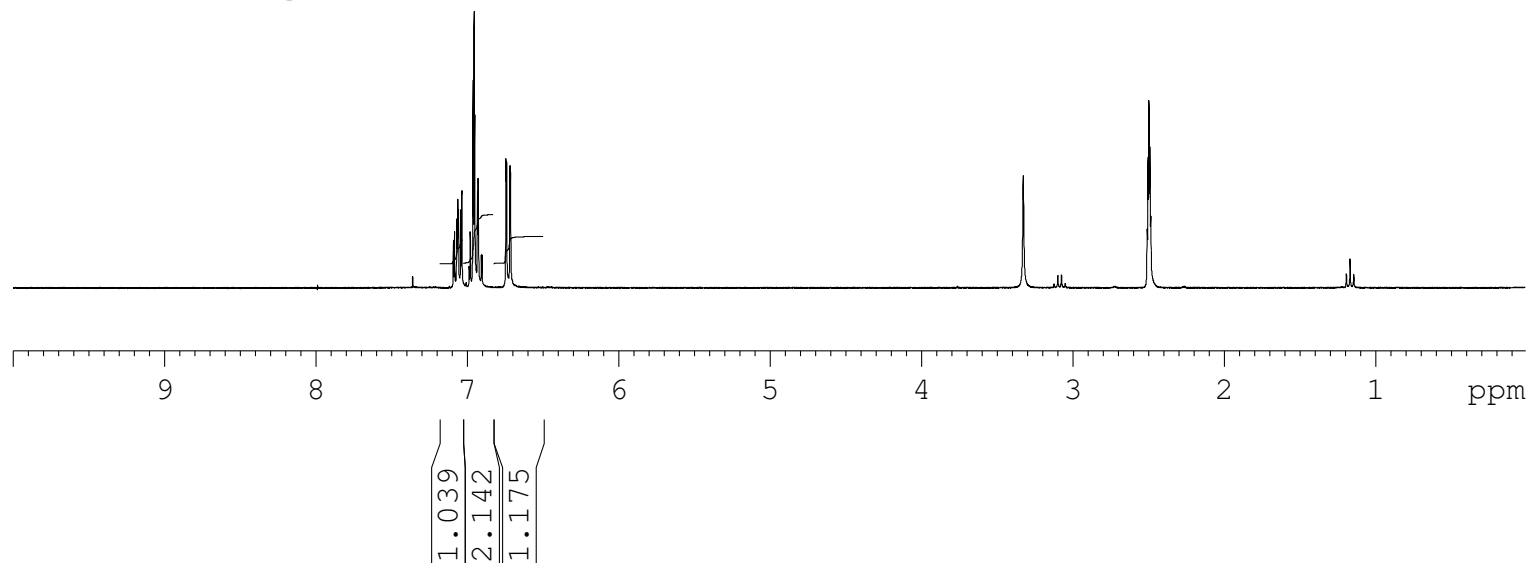
3.326
3.098
3.073
3.049
2.507
2.502
2.495
2.489
2.483
1.191
1.167
1.143

dc-1-39-101



DC-1-39-101

Chemical Formula: C₁₀H₅NO₂S
 Exact Mass: 203.00
 Molecular Weight: 203.22



Current Data Parameters

NAME dc-1-39-101
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20100622
 Time 17.43
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT DMSO
 NS 16
 DS 0
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 812.7
 DW 104.400 usec
 DE 54.00 usec
 TE 296.2 K
 D1 1.00000000 sec
 TD0 1

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

NUC1 1H
 P1 9.75 usec
 PL1 0.00 dB
 SFO1 300.1324000 MHz

F2 - Processing parameters

SI 32768
 SF 300.1300024 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

DC-1-39-101

DMSO-d₆

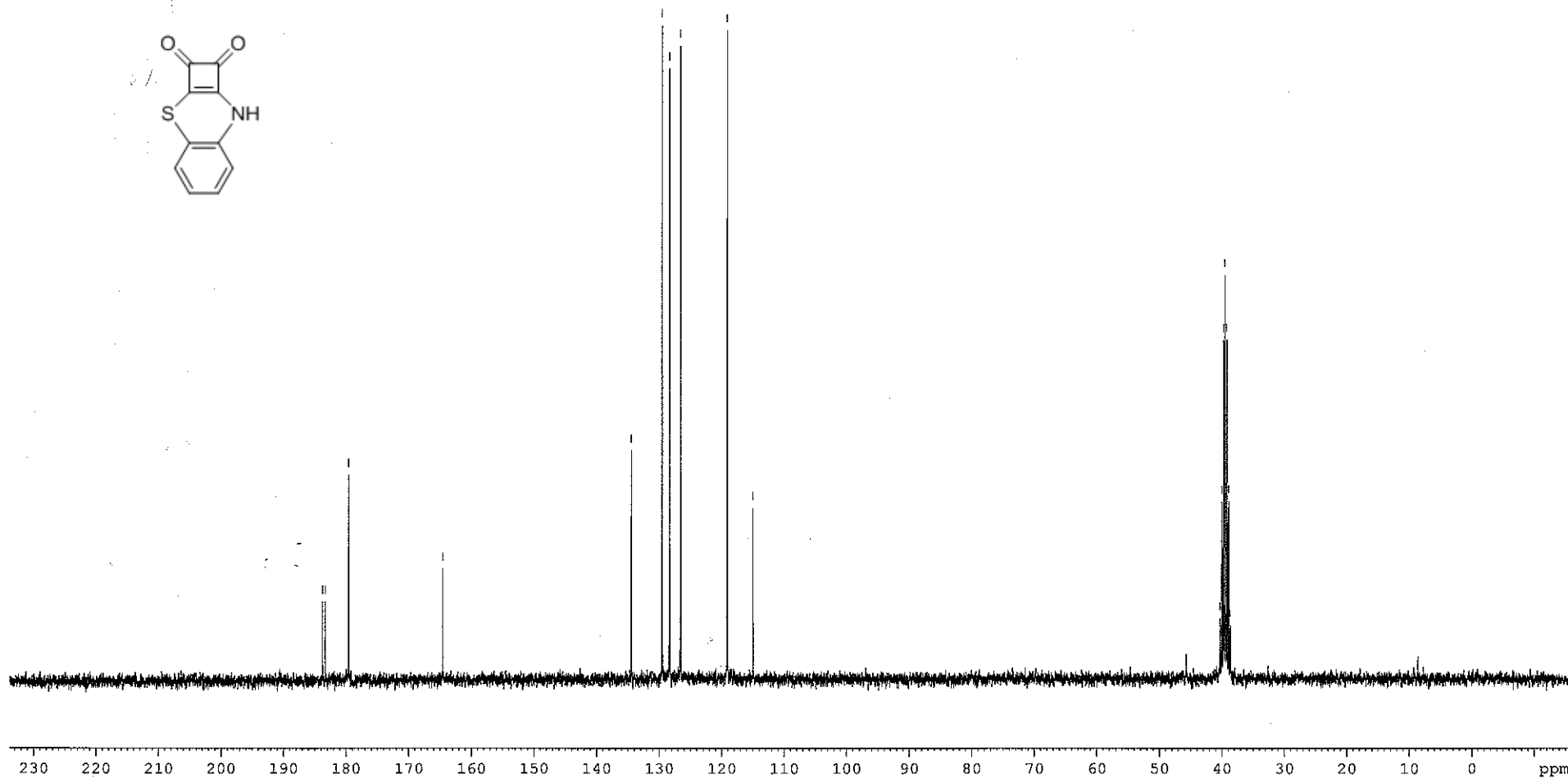
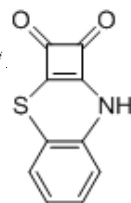
183.846
183.388
179.656

164.621

134.487
129.571
128.394
126.637

119.138
115.033

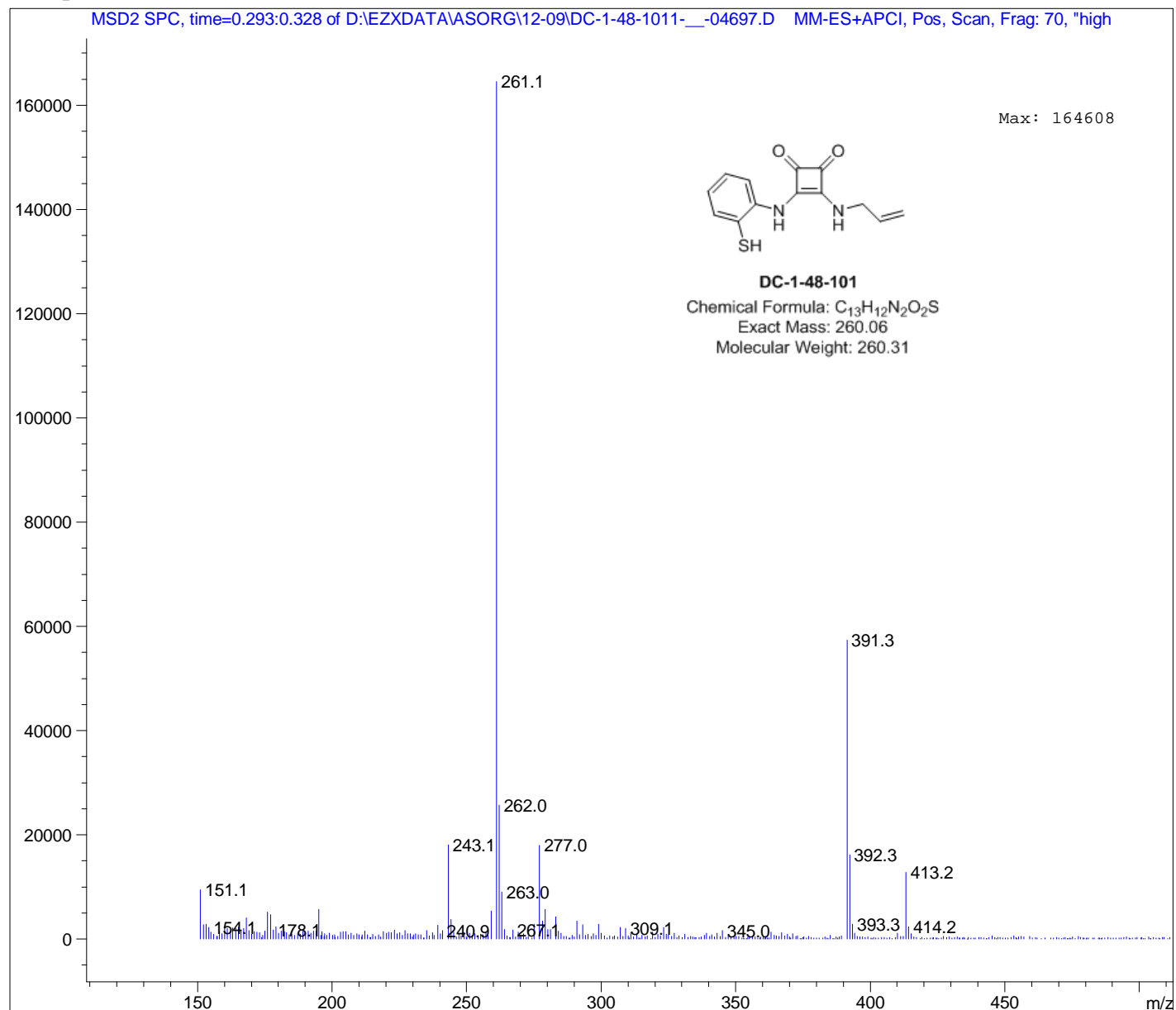
40.342
40.065
39.788
39.510
39.233
38.954
38.676



Sample Name : dc-1-48-101

=====
Acq. Operator : Angela Hansen
Acq. Instrument : INSTRUMENT 1 Location : Vial 2
Injection Date : 12/17/2009 12:23:56 PM Inj : 1
Inj Volume : 10 µl
Acq. Method : D:\METHODS\POS_MIXED_LOOP_150_
Last changed : 12/17/2009 12:23:35 PM by Angela Hansen
(modified after loading)
Analysis Method : D:\METHODS\16MIN_150_1000_LCMS_BOTH_POS.M
Last changed : 12/15/2009 2:38:59 PM by David Dye
(modified after loading)
Method Info : Method for loop analysis of small organics
Sample Info : test
Easy-Access Method: 'pos_mixed_loop_150_1000'
Database #:

MS Spectrum

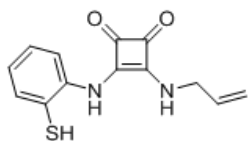


8.68
 8.69
 6.88
 6.86
 6.85
 6.83
 6.83
 6.80
 6.80
 6.78
 6.78
 6.77
 6.76
 6.74
 6.55
 6.55
 6.53
 6.52
 5.77
 5.74
 5.11
 5.10
 5.06
 5.05
 5.05
 5.04
 5.02
 5.02
 3.73
 3.73
 3.72
 3.71
 3.70
 3.69
 3.68
 3.31
 2.50
 2.49
 2.48
 2.48
 2.47

Current Data Parameters
 NAME dc-1-48-101dms0
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20091221
 Time 12.08
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT DMSO
 NS 16
 DS 0
 SWH 3591.954 Hz
 FIDRES 0.109618 Hz
 AQ 4.5613556 sec
 RG 574.7
 DW 139.200 usec
 DE 54.00 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

dc-1-48-101dms0

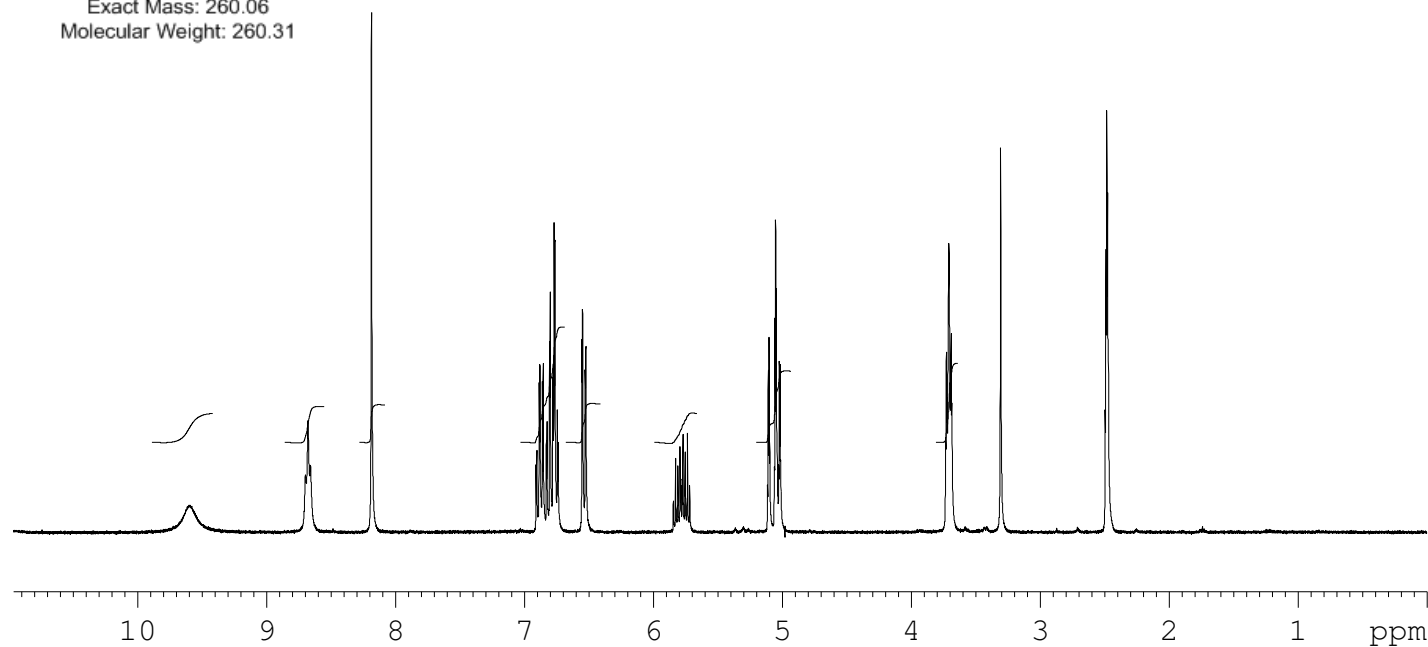


DC-1-48-101

Chemical Formula: C₁₃H₁₂N₂O₂S
 Exact Mass: 260.06
 Molecular Weight: 260.31

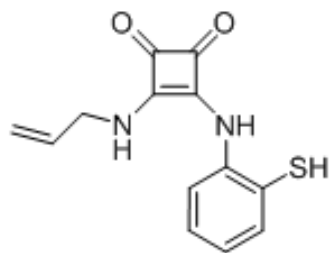
==== CHANNEL f1 =====
 NUC1 1H
 P1 9.75 usec
 PL1 0.00 dB
 SFO1 300.1315007 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300063 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00



0.75
 0.93
 0.98
 3.02
 1.00
 0.75
 1.86
 2.08

dc-1-48-101



177.521
 163.263
 147.030
 135.383
 135.270
 128.187
 127.721
 126.825
 120.967
 117.660
 116.257
 102.404

41.643
 41.198
 40.930
 40.654
 40.375
 40.098
 39.821
 39.540

Current Data Parameters
 NAME dc-1-48-101
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20100105
 Time 16.40
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zgdc
 TD 65536
 SOLVENT DMSO
 NS 300
 DS 0
 SWH 18832.393 Hz
 FIDRES 0.287360 Hz
 AQ 1.7400308 sec
 RG 1448.2
 DW 26.550 usec
 DE 6.00 usec
 TE 298.2 K
 D1 1.00000000 sec
 d11 0.03000000 sec
 TD0 1

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

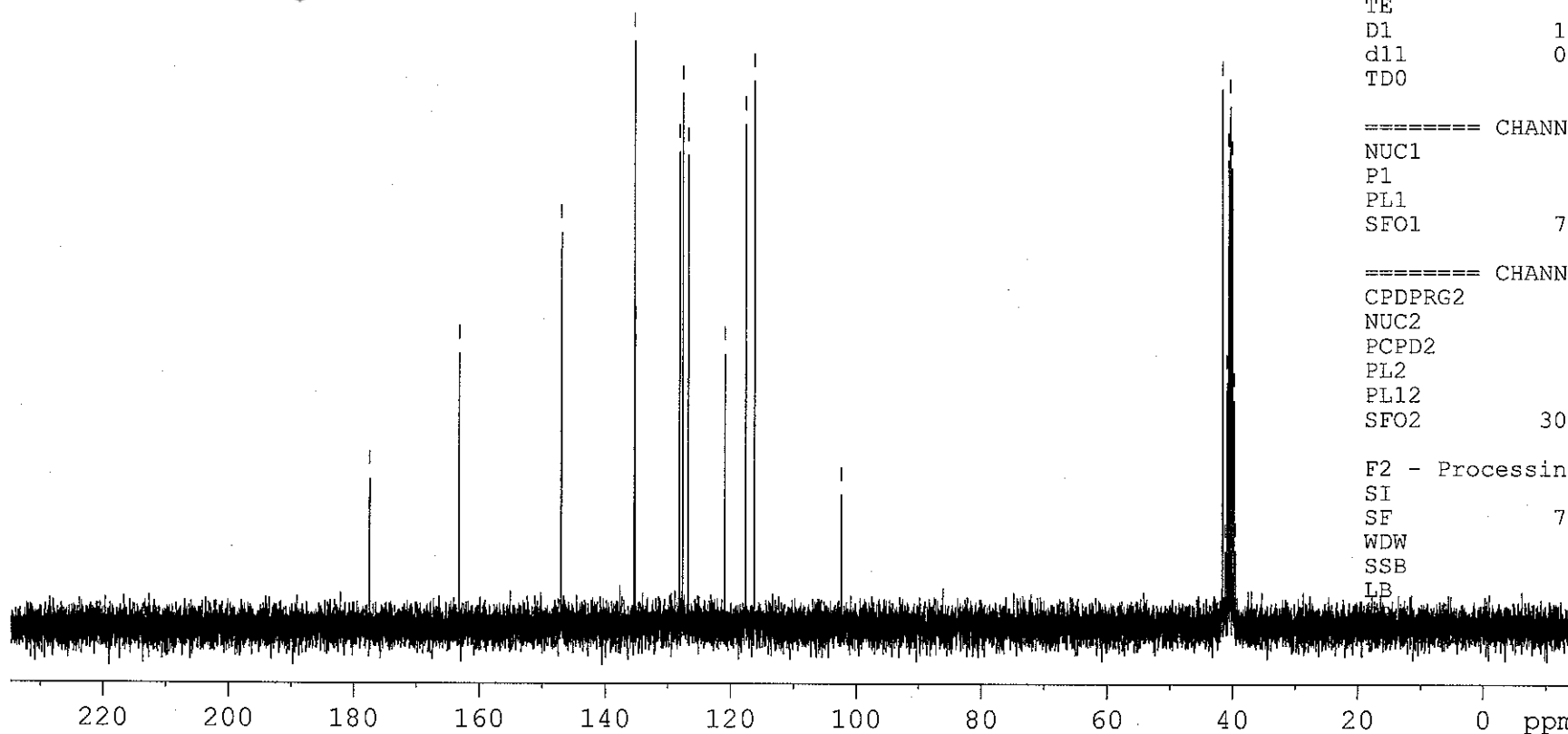
NUC1 13C
 P1 11.80 usec
 PL1 0.00 dB
 SFO1 75.4760200 MHz

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

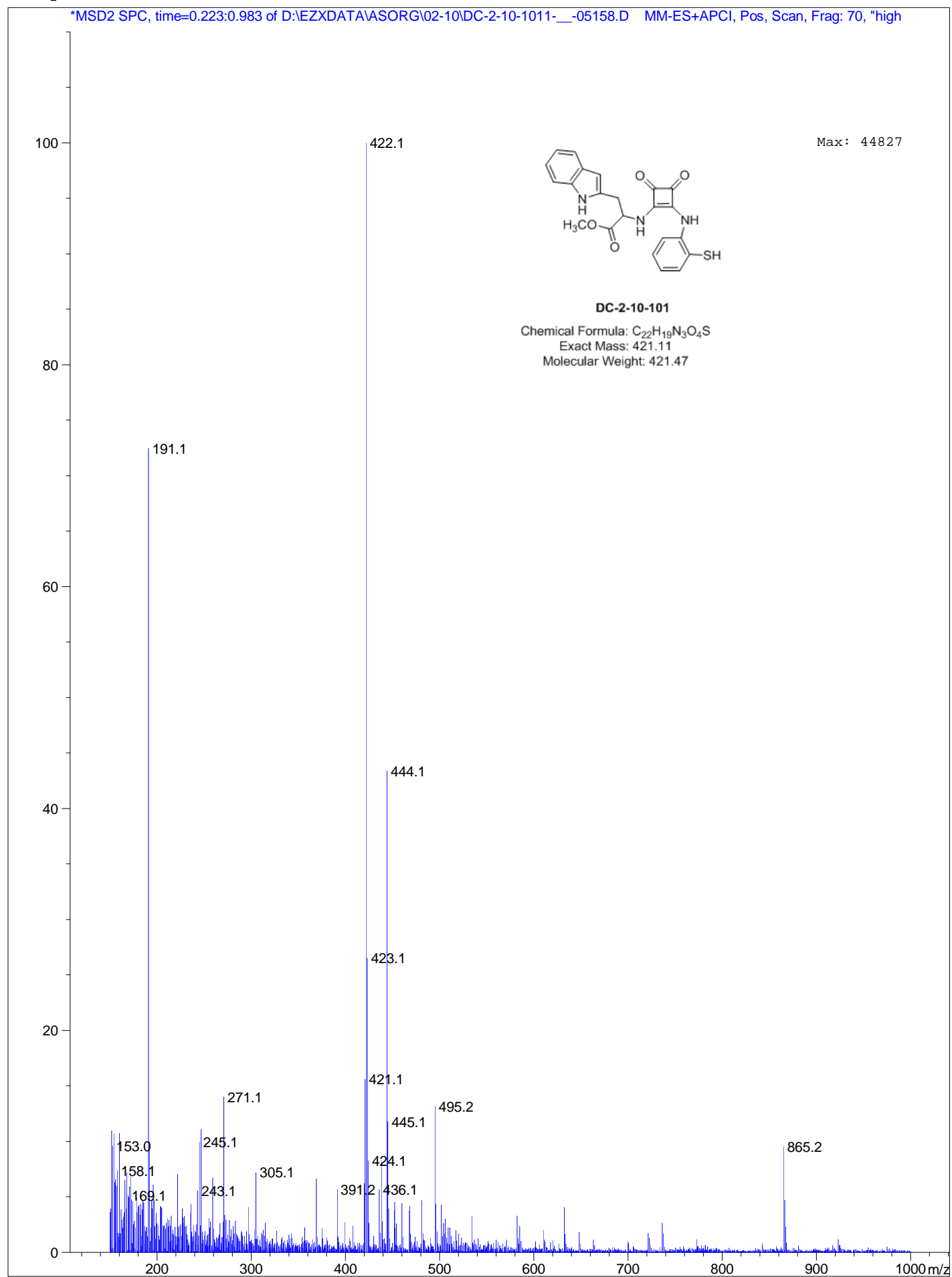
CPDPRG2 waltz16
 NUC2 1H
 PCPD2 95.00 usec
 PL2 0.00 dB
 PL12 18.00 dB
 SFO2 300.1312005 MHz

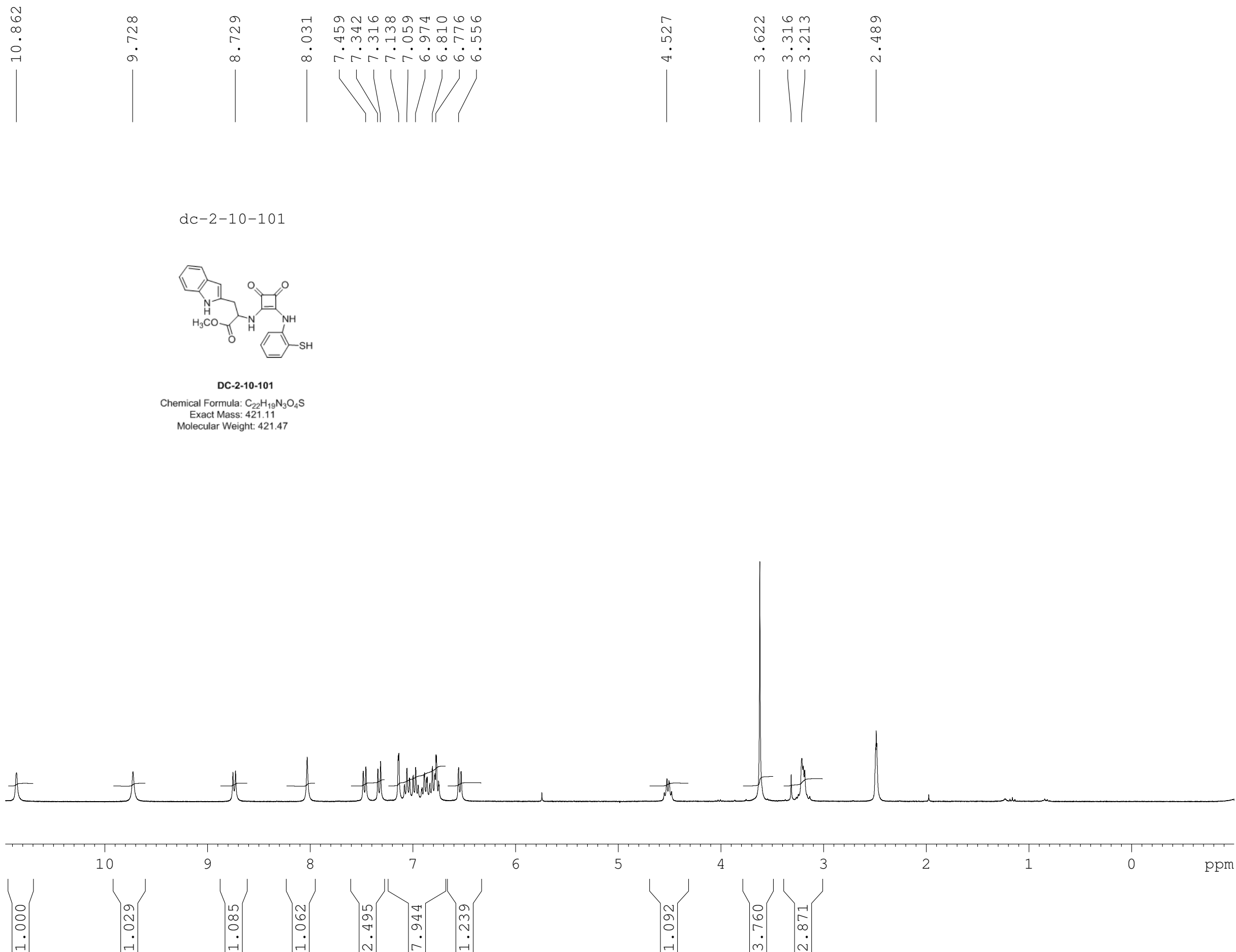
F2 - Processing parameters

SI 32768
 SF 75.4677190 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 0
 1.40



MS Spectrum





Current Data Parameters

NAME dc-2-10-101
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20100130
Time 15.02
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT DMSO
NS 16
DS 0
SWH 3591.954 Hz
FIDRES 0.109618 Hz
AQ 4.5613556 sec
RG 456.1
DW 139.200 usec
DE 54.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

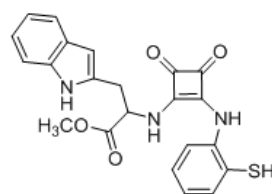
==== CHANNEL f1 =====

NUC1 1H
P1 9.75 usec
PL1 0.00 dB
SFO1 300.1315007 MHz

F2 - Processing parameters

SI 32768
SF 300.1300042 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

DC-2-10-carbon2



DC-2-10-101

Chemical Formula: C₂₂H₁₉N₃O₄S
 Exact Mass: 421.11
 Molecular Weight: 421.47

176.242
 171.773
 162.831
 146.357
 136.214
 134.433
 127.480
 127.095
 126.993
 126.201
 123.920
 121.137
 120.145
 118.587
 118.075
 117.017
 111.617
 109.382
 101.634

53.041
 52.226
 40.461
 40.274
 40.186
 39.910
 39.631
 39.354
 39.075
 38.792
 26.425

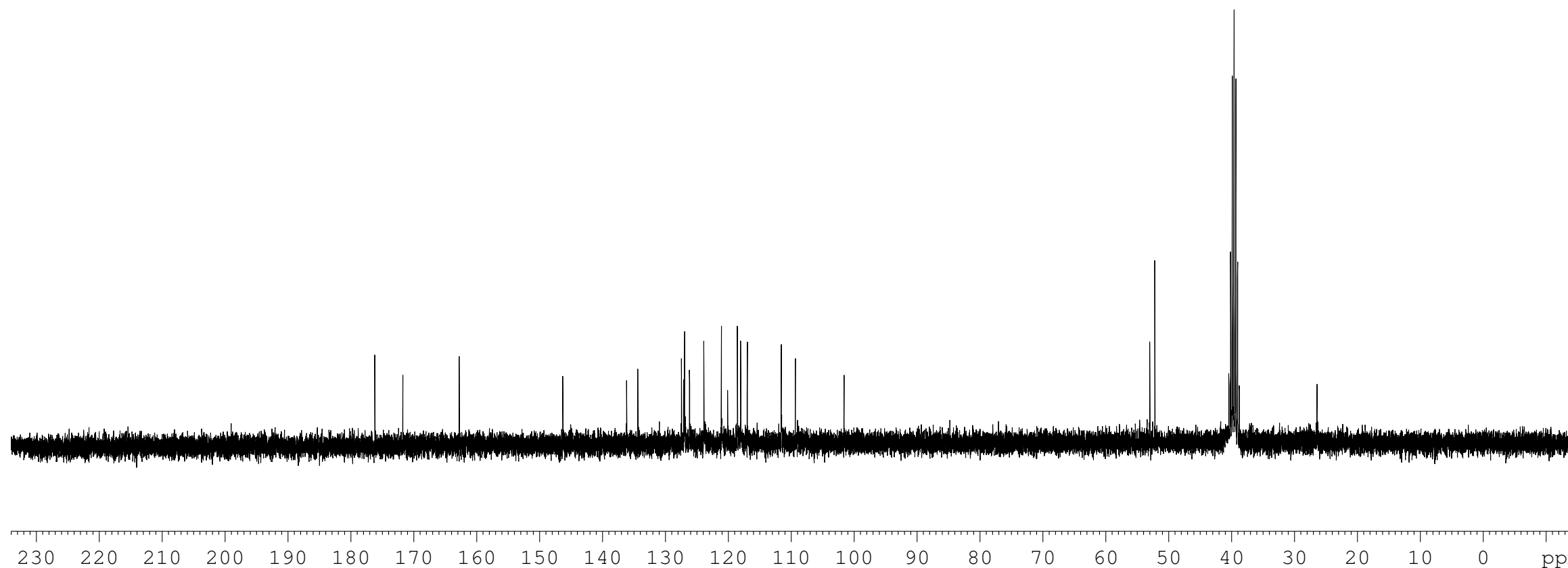
Current Data Parameters
 NAME DC-2-10-carbon2
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100130
 Time 16.42
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zgdc
 TD 65536
 SOLVENT DMSO
 NS 800
 DS 0
 SWH 18832.393 Hz
 FIDRES 0.287360 Hz
 AQ 1.7400308 sec
 RG 4597.6
 DW 26.550 usec
 DE 6.00 usec
 TE 298.2 K
 D1 1.00000000 sec
 d11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 13C
 P1 11.80 usec
 PL1 0.00 dB
 SFO1 75.4760200 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 95.00 usec
 PL2 0.00 dB
 PL12 18.00 dB
 SFO2 300.1312005 MHz

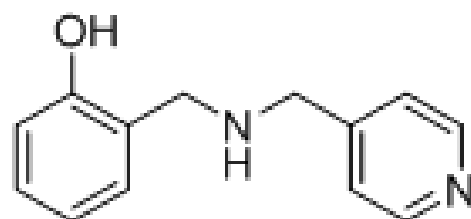
F2 - Processing parameters
 SI 32768
 SF 75.4677751 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00



8.607
 8.602
 8.593
 8.588
 8.577
 8.555
 7.266
 7.247
 7.233
 7.227
 7.206
 7.204
 7.203
 7.181
 7.176
 7.013
 7.012
 7.009
 7.008
 6.989
 6.987
 6.983
 6.891
 6.887
 6.864
 6.860
 6.835
 6.831
 6.811
 6.807
 6.786
 6.782
 5.303

4.058
 4.037
 3.953
 3.851

DC-2-32-102

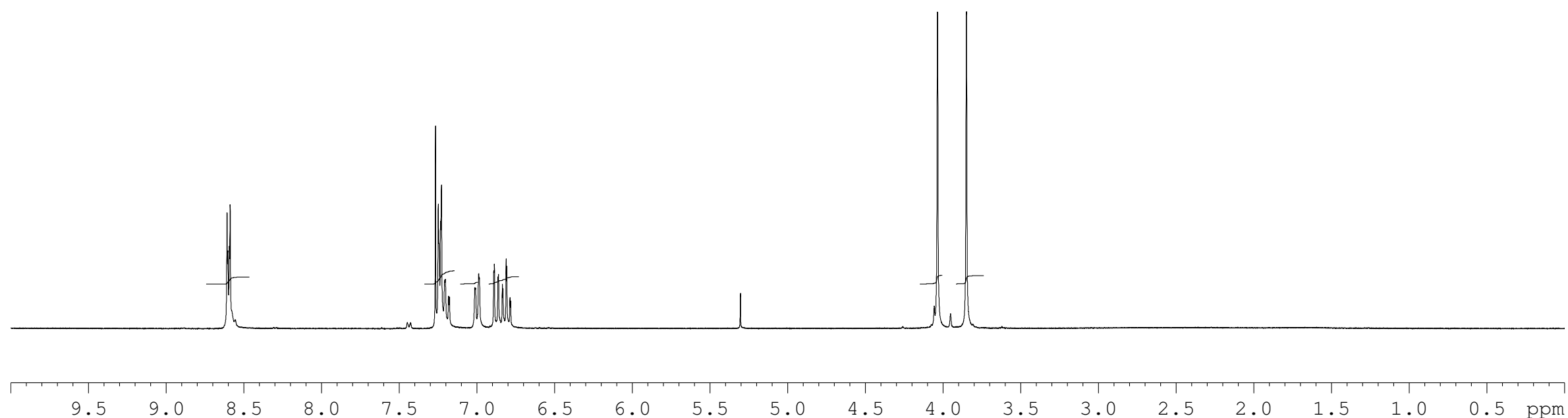


Current Data Parameters
 NAME DC-2-32-102
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100208
 Time 18.41
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT CDC13
 NS 16
 DS 0
 SWH 3591.954 Hz
 FIDRES 0.109618 Hz
 AQ 4.5613556 sec
 RG 574.7
 DW 139.200 usec
 DE 54.00 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 9.75 usec
 PL1 0.00 dB
 SFO1 300.1315007 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300042 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00



1.661
 3.158
 0.454
 1.749
 2.089
 2.000

8.585
 8.580
 8.570
 8.565
 7.486
 7.481
 7.457
 7.453
 7.435
 7.429
 7.405
 7.399
 7.390
 7.385
 7.372
 7.368
 7.344
 7.340
 7.321
 7.316
 7.222
 7.217
 7.197
 7.193
 7.173
 7.168
 5.745

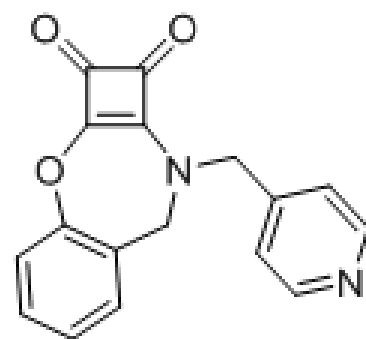
4.897
 4.670

3.306

2.502
 2.496
 2.490
 2.484
 2.478

1.225

Dc-2-119-101

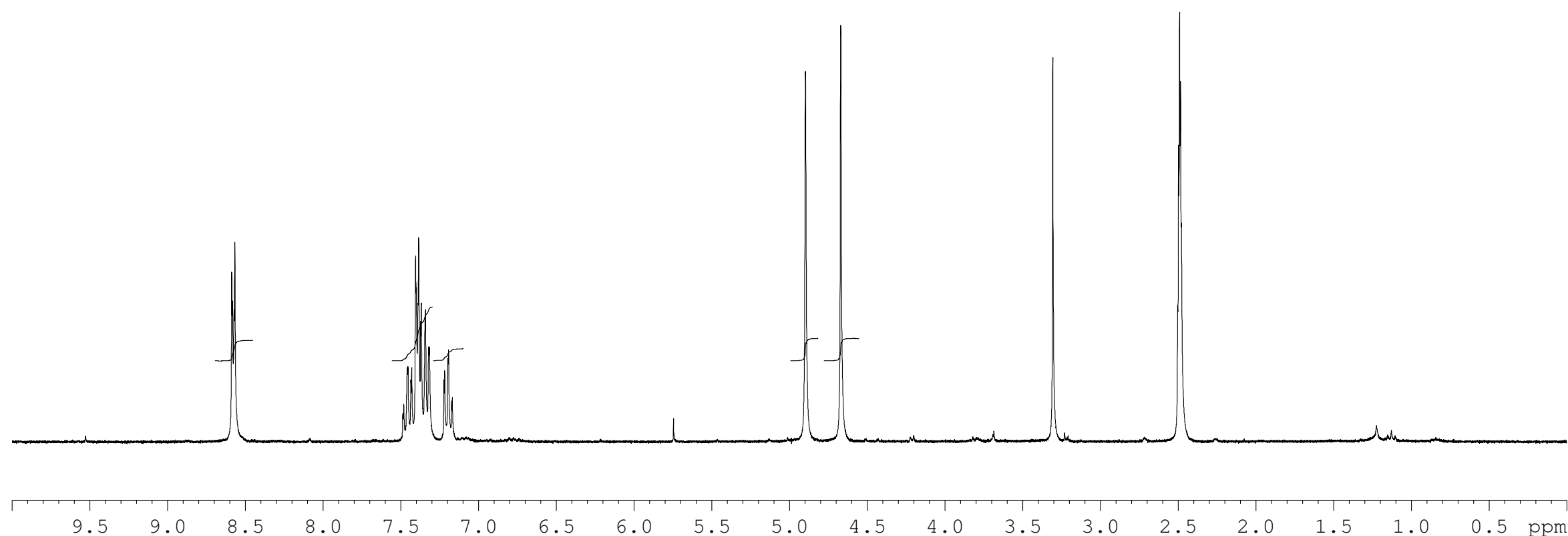


Current Data Parameters
 NAME Dc-2-119-101
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100312
 Time 16.03
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT CDC13
 NS 32
 DS 0
 SWH 3591.954 Hz
 FIDRES 0.109618 Hz
 AQ 4.5613556 sec
 RG 1024
 DW 139.200 usec
 DE 54.00 usec
 TE 299.2 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 9.75 usec
 PL1 0.00 dB
 SFO1 300.1315007 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300042 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00



1.818

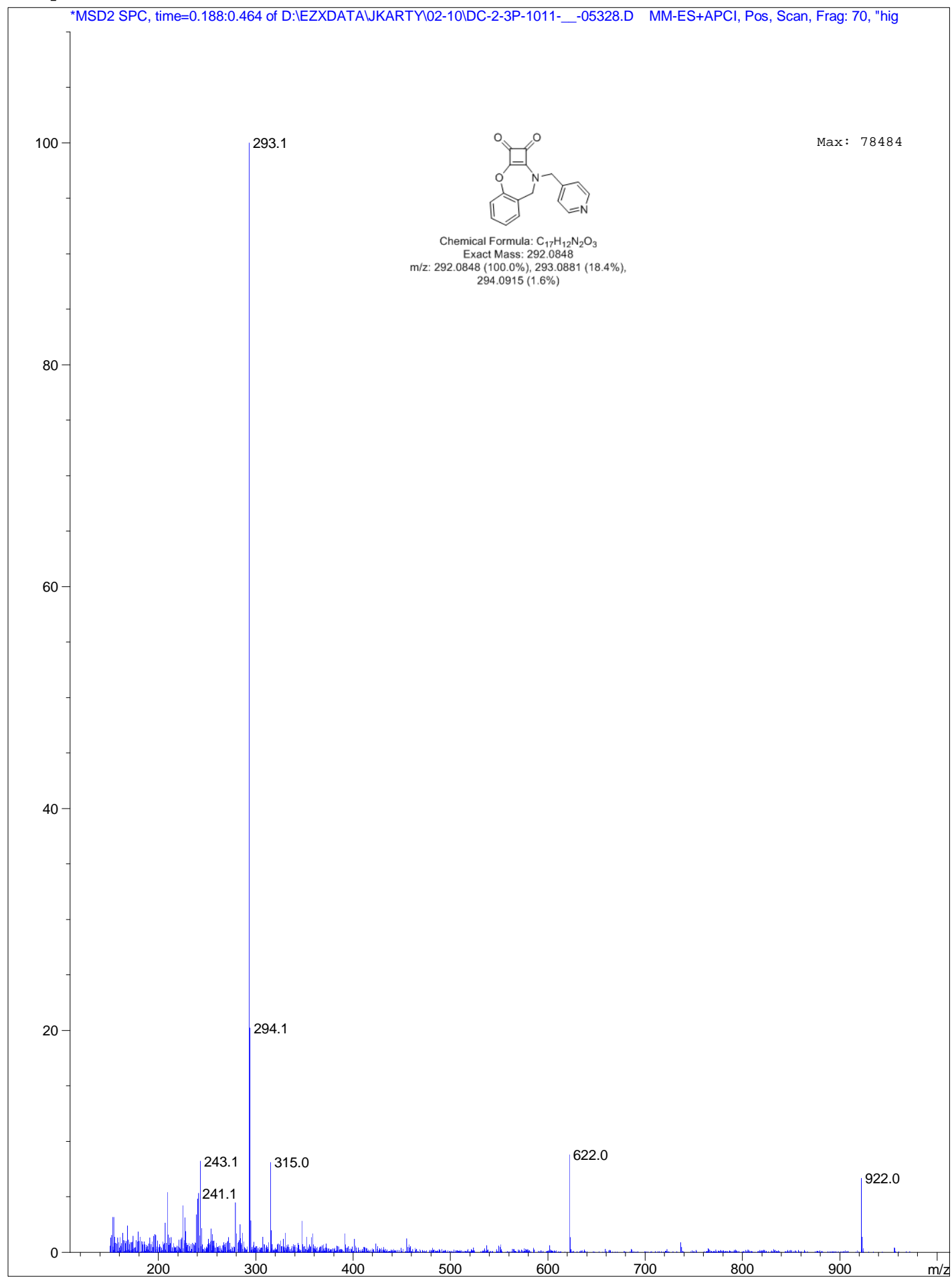
4.813

1.086

2.003

2.000

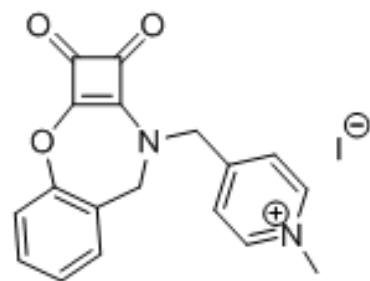
MS Spectrum



8.978
8.957
8.128
8.108
7.512
7.486
7.461
7.410
7.386
7.383
7.346
7.320
7.244
7.220
7.198
7.195

5.168
4.742
4.321
3.309
2.491
2.486

DC-2-45-103

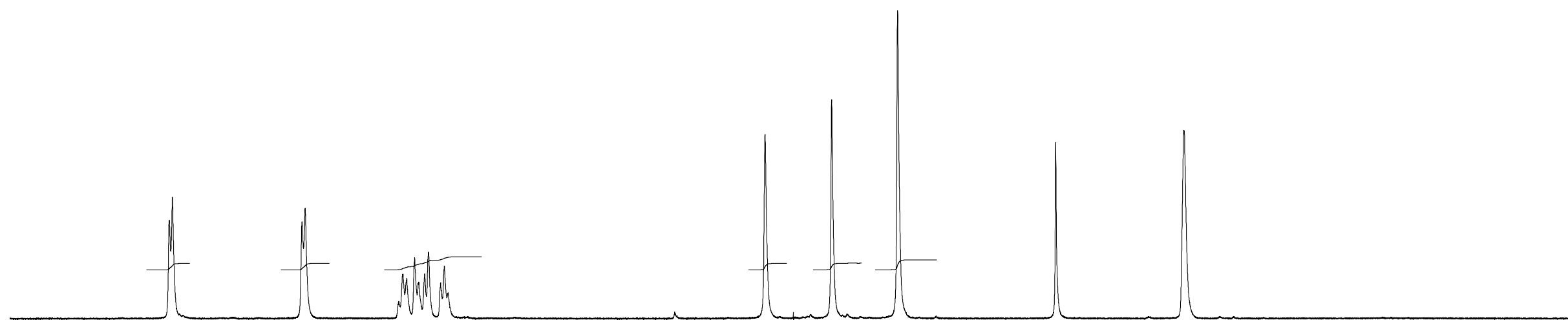


Current Data Parameters
 NAME DC-2-45-103
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100212
 Time 15.04
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT DMSO
 NS 32
 DS 0
 SWH 3591.954 Hz
 FIDRES 0.109618 Hz
 AQ 4.5613556 sec
 RG 645.1
 DW 139.200 usec
 DE 54.00 usec
 TE 299.2 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 9.75 usec
 PL1 0.00 dB
 SFO1 300.1315007 MHz

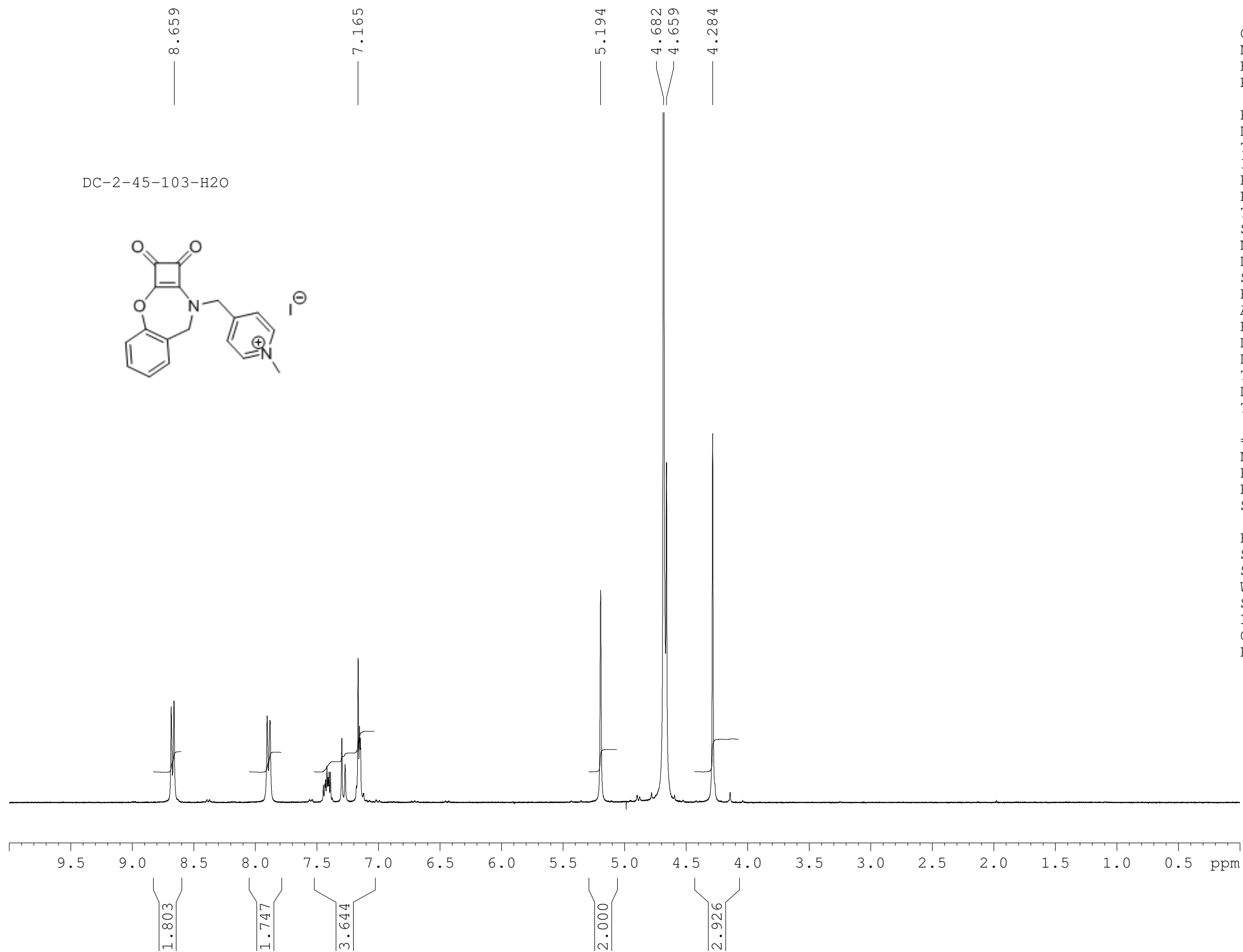
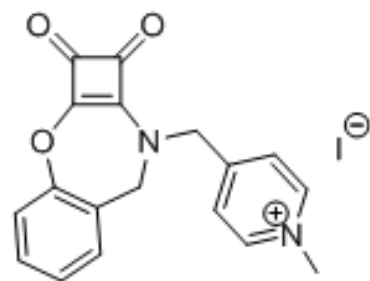
F2 - Processing parameters
 SI 32768
 SF 300.1300042 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00



9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

2.012
1.981
4.037
2.000
2.077
3.095

DC-2-45-103-H2O



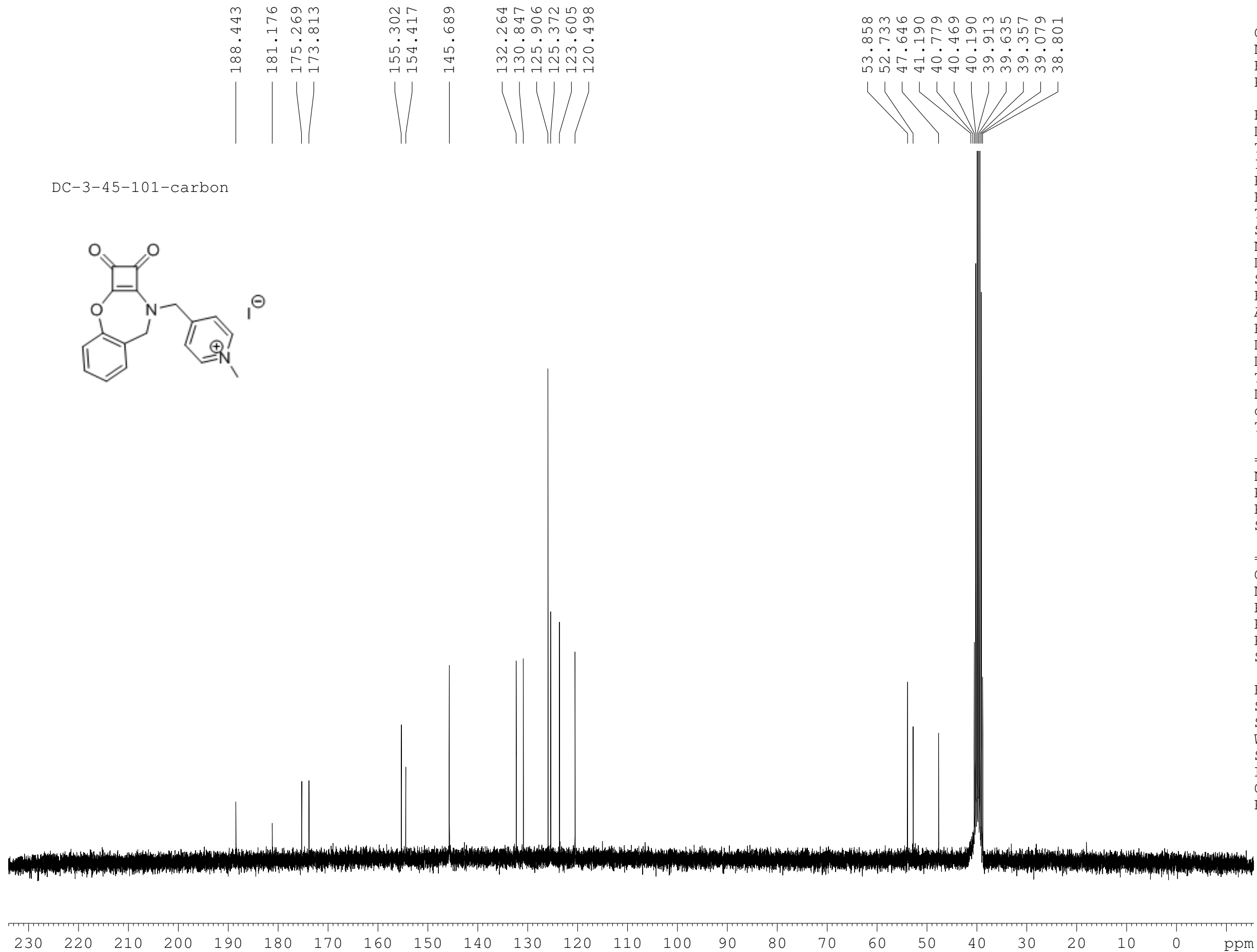
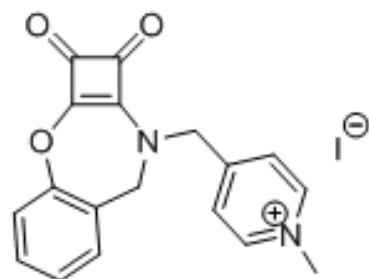
Current Data Parameters
NAME DC-2-45-103-H2O
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100218
Time 10.05
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT D2O
NS 32
DS 0
SWH 3591.954 Hz
FIDRES 0.109618 Hz
AQ 4.5613556 sec
RG 256
DW 139.200 usec
DE 54.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 9.75 usec
PL1 0.00 dB
SFO1 300.1315007 MHz

F2 - Processing parameters
SI 32768
SF 300.1300042 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

DC-3-45-101-carbon



Current Data Parameters
 NAME DC-3-45-101-carbon
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100513
 Time 7.53
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zgdc
 TD 65536
 SOLVENT DMSO
 NS 13000
 DS 0
 SWH 18832.393 Hz
 FIDRES 0.287360 Hz
 AQ 1.7400308 sec
 RG 2048
 DW 26.550 usec
 DE 6.00 usec
 TE 297.2 K
 D1 1.00000000 sec
 d11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 13C
 P1 11.80 usec
 PL1 0.00 dB
 SFO1 75.4760200 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 95.00 usec
 PL2 0.00 dB
 PL12 18.00 dB
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677751 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

Elemental Composition Report

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 80.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

13 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-18 H: 0-15 N: 0-2 O: 0-3 Na: 0-1

File name: dc-2-45-103

Instrument: LCT KC366

Method: ESI-TOF

dc-2-45-103c 28 (0.702) AM (Cen,6, 90.00, Ar,6000.0,1222.14,0.70,LS 4); Sm (SG, 2x6.00); Cm (27:28)

Notebook Ref:

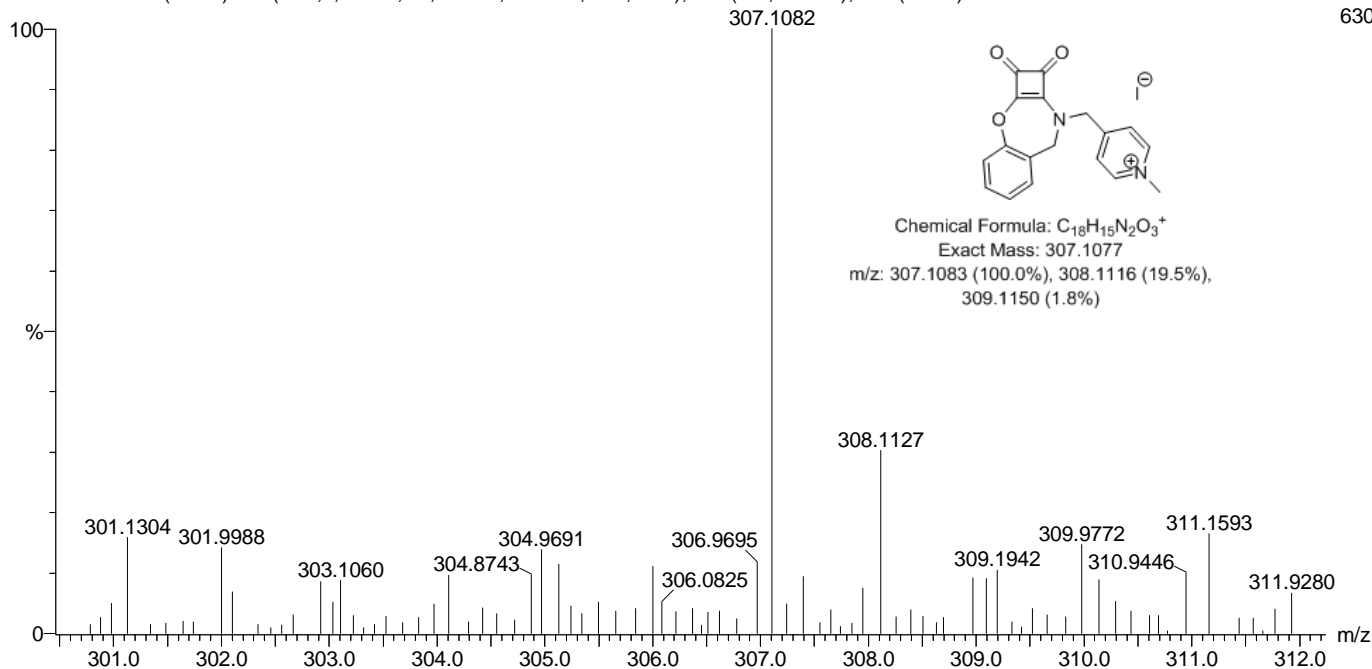
Test name: Accurate Mass

Base Peak Mass: 307.10818481

IU Database#:

26-Feb-2010 14:45:30

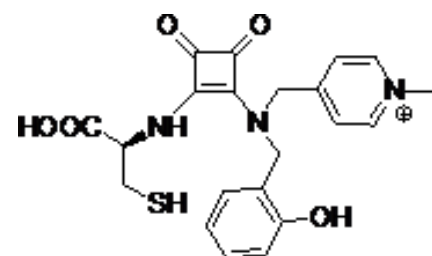
1: TOF MS ES+
630



Minimum: 80.00
 Maximum: 100.00

Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
307.1082	100.00	307.1083	-0.1	-0.3	12.5	21.1	C18 H15 N2 O3

DC-2-65-100



DC-2-65-1
Chemical Formula: C₂₁H₂₂N₃O₅S⁺
Exact Mass: 428.1275
Molecular Weight: 428.4809

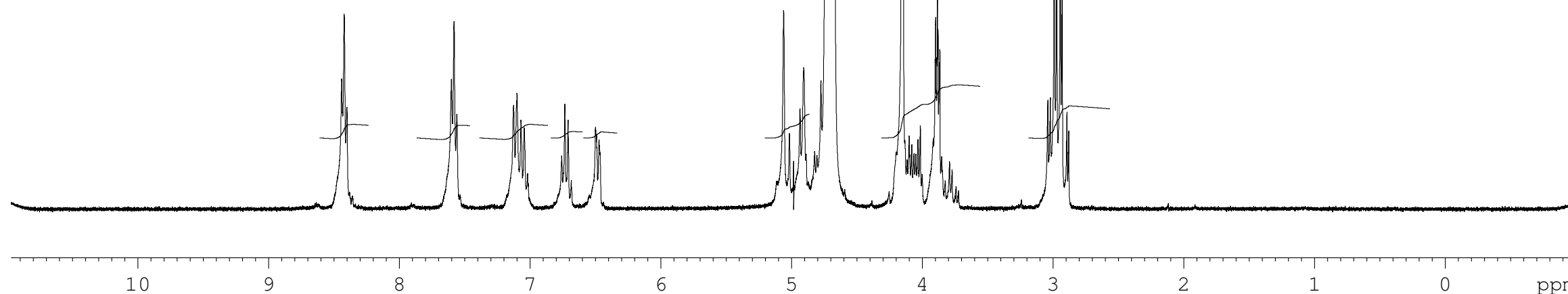
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 8.402
 7.603
 7.583
 7.562
 7.128
 7.102
 7.072
 7.046
 6.736
 6.711
 6.501
 5.062
 4.937
 4.908
 4.777
 4.733
 4.719
 4.704
 4.700
 4.681
 4.677
 4.159
 4.148
 4.017
 3.900
 3.890
 3.885
 3.881
 3.871
 3.868
 3.041
 3.022
 2.991
 2.972
 2.945
 2.931
 2.895
 2.881

Current Data Parameters
 NAME DC-2-65-100
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100218
 Time 11.07
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT D2O
 NS 32
 DS 0
 SWH 3591.954 Hz
 FIDRES 0.109618 Hz
 AQ 4.5613556 sec
 RG 362
 DW 139.200 usec
 DE 54.00 usec
 TE 298.2 K
 D1 1.0000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 9.75 usec
 PL1 0.00 dB
 SFO1 300.1315007 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300042 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00



2.120
 2.062
 2.103
 1.000
 0.818
 4.008
 8.716
 4.900

10 9 8 7 6 5 4 3 2 1 0 ppm

Elemental Composition Report

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 80.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

81 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-21 H: 0-22 N: 0-3 O: 0-5 Na: 0-1 S: 0-1

File name: dc-2-65-1

Notebook Ref:

Instrument: LCT KC366

Test name: Accurate Mass

IU Database#:

26-Feb-2010 12:25:12

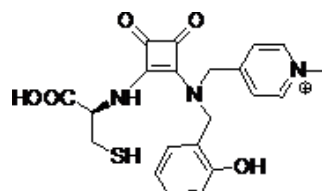
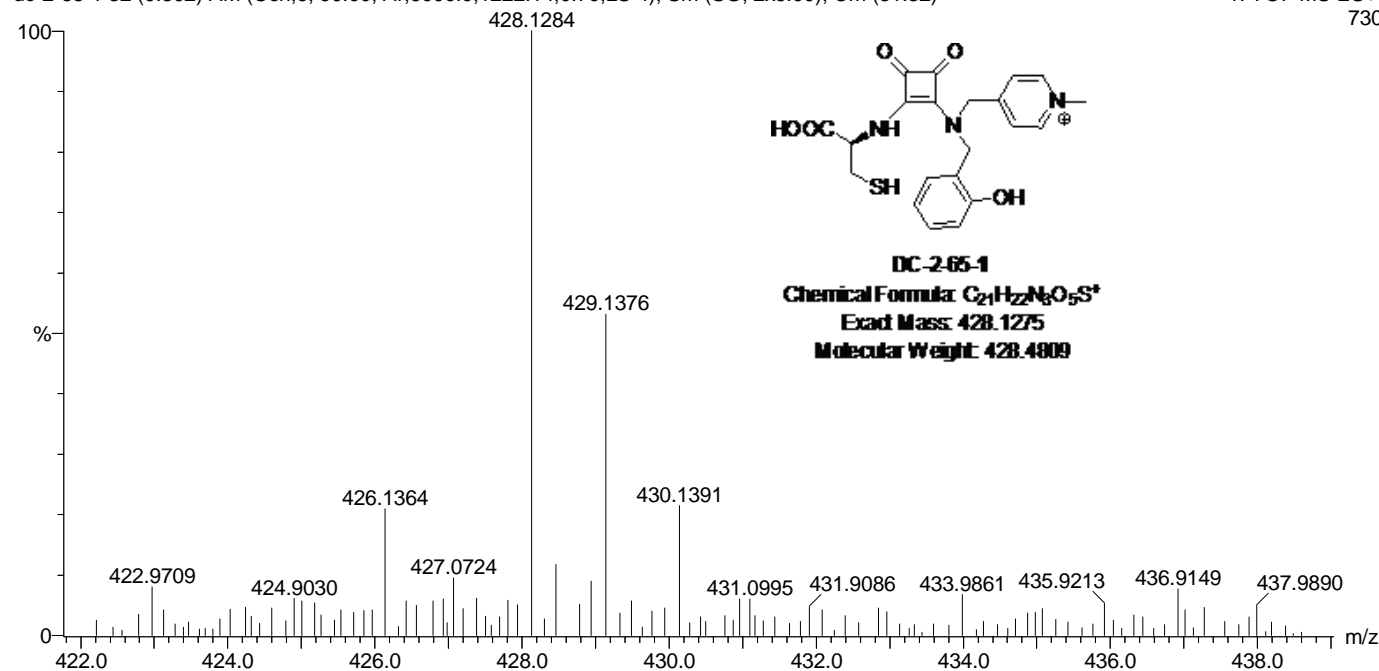
Method: ESI-TOF

Base Peak Mass: 428.1283745

dc-2-65-1 32 (0.802) AM (Cen,6, 90.00, Ar,6000.0,1222.14,0.70,LS 4); Sm (SG, 2x6.00); Cm (31:32)

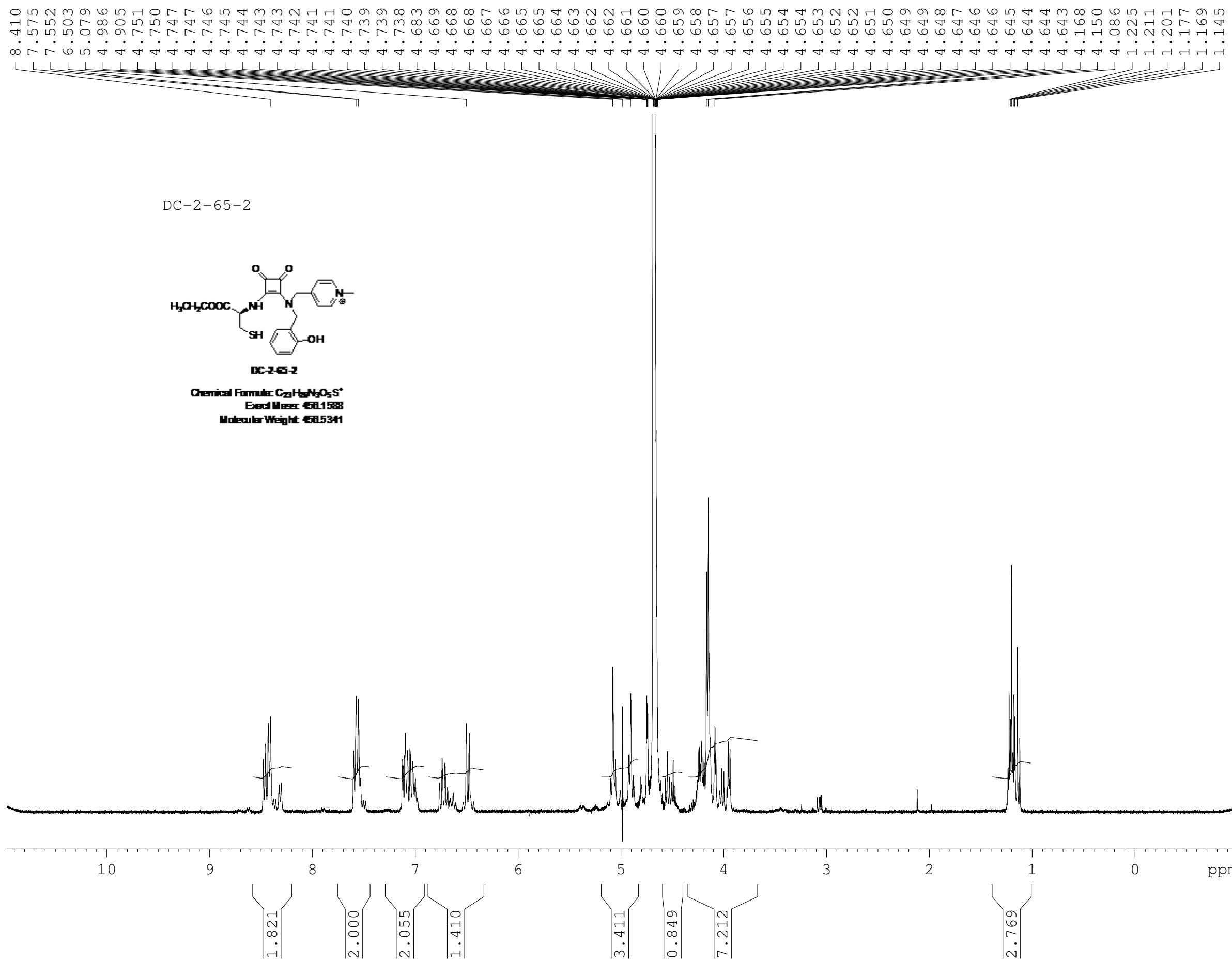
1: TOF MS ES+

730



DC-2-65-1
Chemical Formula: C₂₁H₂₂N₃O₅S⁺
Exact Mass: 428.1275
Molecular Weight: 428.4809

Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
428.1284	100.00	428.1280	0.4	0.9	12.5	68.7	C ₂₁ H ₂₂ N ₃ O ₅ S



Current Data Parameters
 NAME DC-2-65-2
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100222
 Time 9.07
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT D2O
 NS 32
 DS 0
 SWH 3591.954 Hz
 FIDRES 0.109618 Hz
 AQ 4.5613556 sec
 RG 362
 DW 139.200 usec
 DE 54.00 usec
 TE 298.2 K
 D1 1.0000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 9.75 usec
 PL1 0.00 dB
 SFO1 300.1315007 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300042 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

Elemental Composition Report

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 80.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

81 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-23 H: 0-26 N: 0-3 O: 0-5 Na: 0-1 S: 0-1

File name: dc-2-65-2

Notebook Ref:

Instrument: LCT KC366

Test name: Accurate Mass

IU Database#:

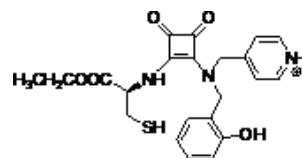
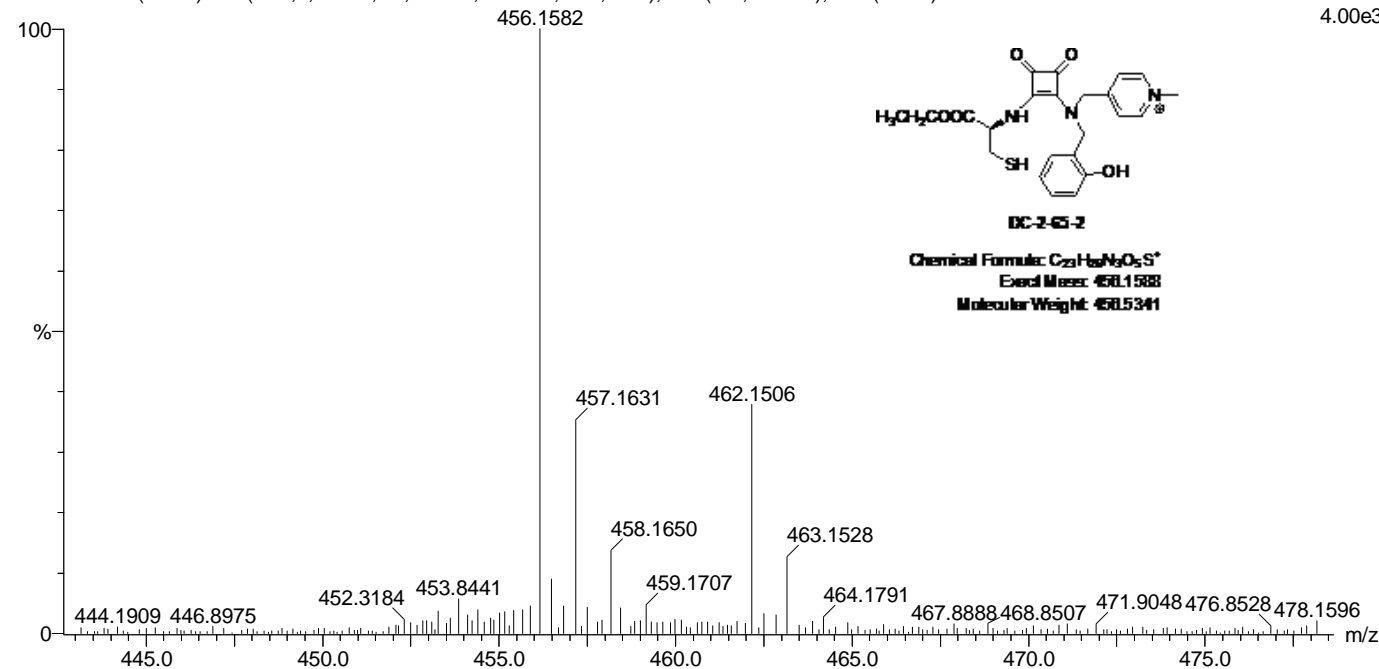
26-Feb-2010 12:21:02

Method: ESI-TOF

Base Peak Mass: 456.15817261

dc-2-65-2 30 (0.752) AM (Cen,6, 90.00, Ar,6000.0,1222.14,0.70,LS 4); Sm (SG, 2x6.00); Cm (29:30)

1: TOF MS ES+
4.00e3



DC-2-65-2

Chemical Formula: C₂₃H₂₆N₃O₅S⁺

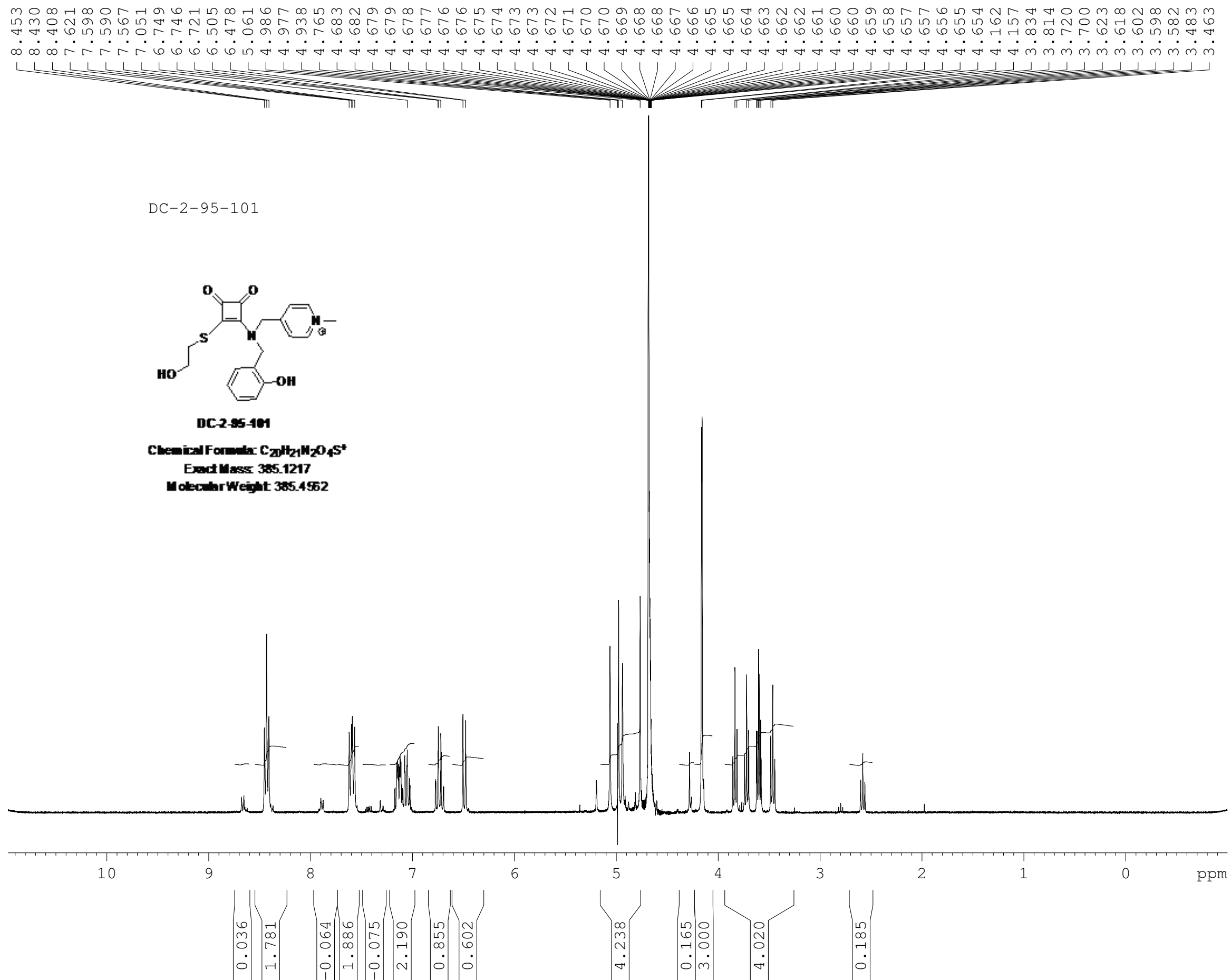
Exact Mass: 456.1588

Molecular Weight: 456.5341

Minimum: 80.00
 Maximum: 100.00

-1.5
 80.0

Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
456.1582	100.00	456.1593	-1.1	-2.4	12.5	44.9	C ₂₃ H ₂₆ N ₃ O ₅ S



Current Data Parameters
 NAME DC-2-95-101
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100226
 Time 18.36
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT D2O
 NS 32
 DS 0
 SWH 3591.954 Hz
 FIDRES 0.109618 Hz
 AQ 4.5613556 sec
 RG 645.1
 DW 139.200 usec
 DE 54.00 usec
 TE 299.2 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 9.75 usec
 PL1 0.00 dB
 SFO1 300.1315007 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300042 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

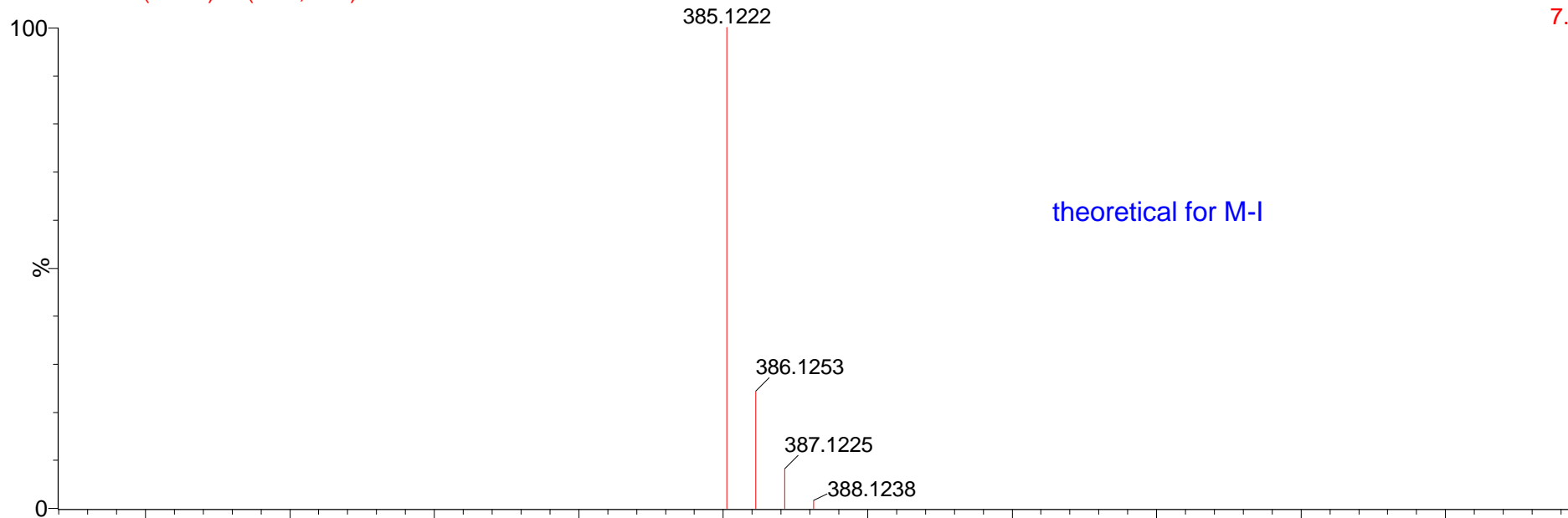
File name: dc-2-95-101
Instrument: LCT KC366
Method: ESI-TOF

Notebook Ref: 24821
Test name: Accurate Mass
Base Peak Mass: 387.13412476

IU Database#: 24821
06-May-2010 11:34:47

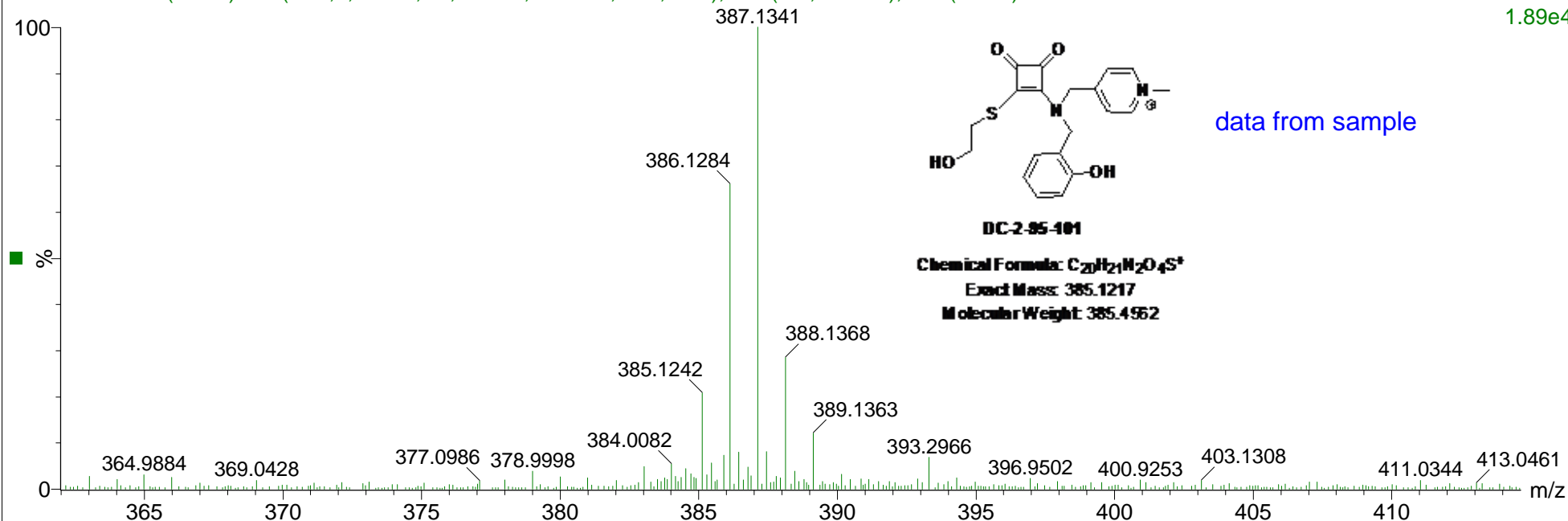
dc-2-94-201 (0.035) Is (0.50,0.50) C₂₀H₂₁N₂O₄S

1: TOF MS ES+
7.47e12



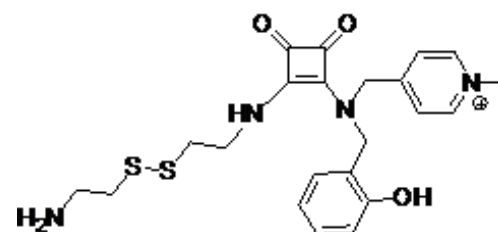
dc-2-95-101 64 (1.603) AM (Cen,8, 90.00, Ar,4000.0,1222.14,0.70,LS 6); Sm (SG, 2x4.00); Cm (63:71)

1: TOF MS ES+
1.89e4



8.477
 8.454
 8.424
 8.402
 8.377
 8.292
 8.270
 7.615
 7.596
 7.573
 7.554
 7.545
 7.538
 7.516
 7.080
 7.055
 7.032
 7.026
 7.007
 6.981
 6.935
 6.913
 6.693
 6.668
 6.643
 6.614
 6.594
 6.572
 6.548
 6.525
 6.499
 6.463
 4.954
 4.913
 4.883
 4.815
 4.753
 4.683
 4.607
 4.266
 4.175
 4.150
 4.140
 4.087
 4.067
 3.974
 3.793
 3.772
 3.751
 3.649
 3.039
 3.017
 2.995
 2.713
 2.690
 2.667
 2.645

Dc-2-117-101



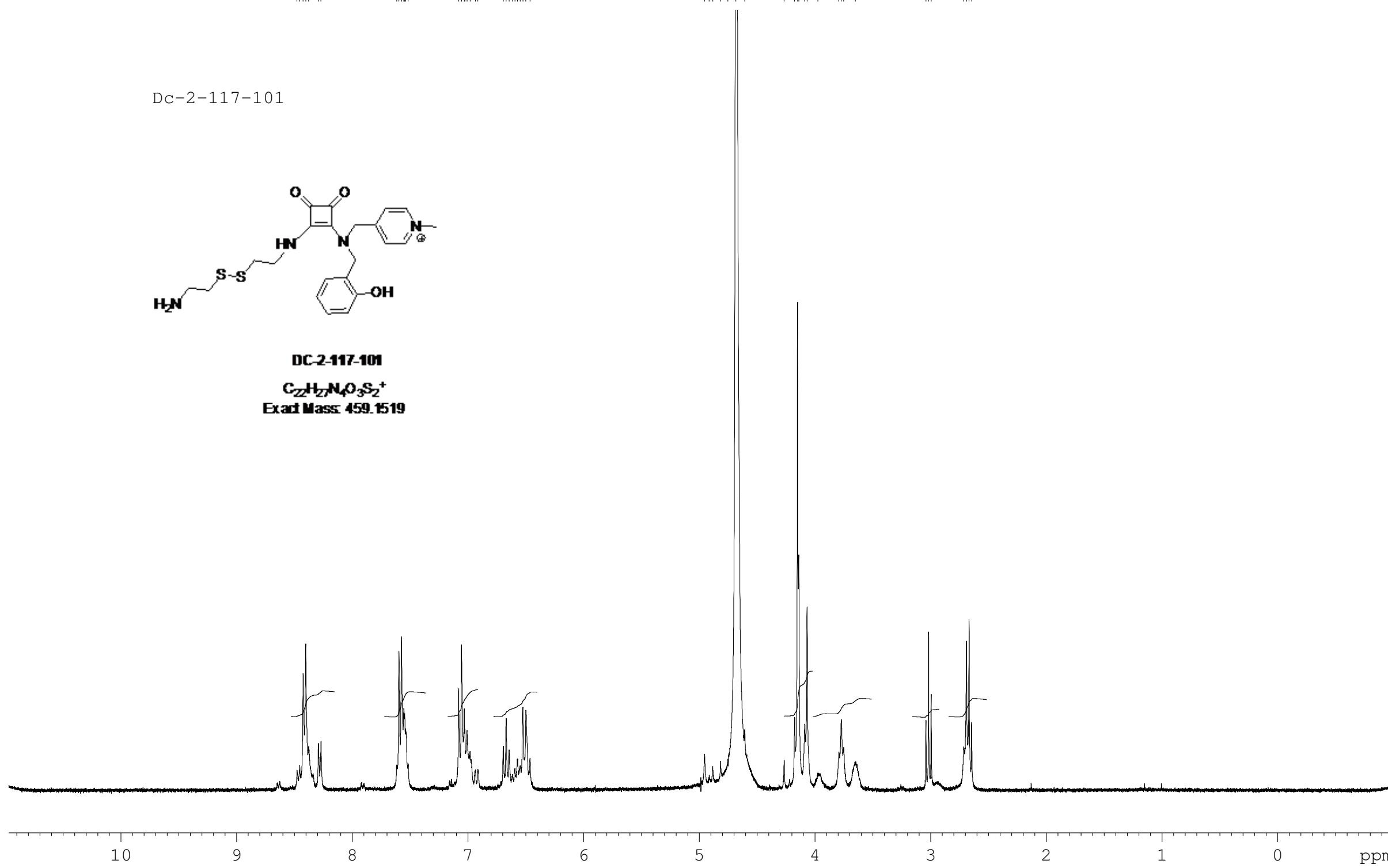
DC-2-117-101
 $C_{22}H_{27}N_4O_3S_2^+$
 Exact Mass: 459.1519

Current Data Parameters
 NAME Dc-2-117-101
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100310
 Time 15.18
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT D2O
 NS 32
 DS 0
 SWH 3591.954 Hz
 FIDRES 0.109618 Hz
 AQ 4.5613556 sec
 RG 256
 DW 139.200 usec
 DE 54.00 usec
 TE 299.2 K
 D1 1.0000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 9.75 usec
 PL1 0.00 dB
 SFO1 300.1315007 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300042 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00



2.039
 1.938
 2.256
 2.000
 3.755
 1.431
 0.607
 1.388

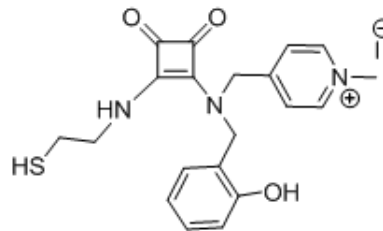
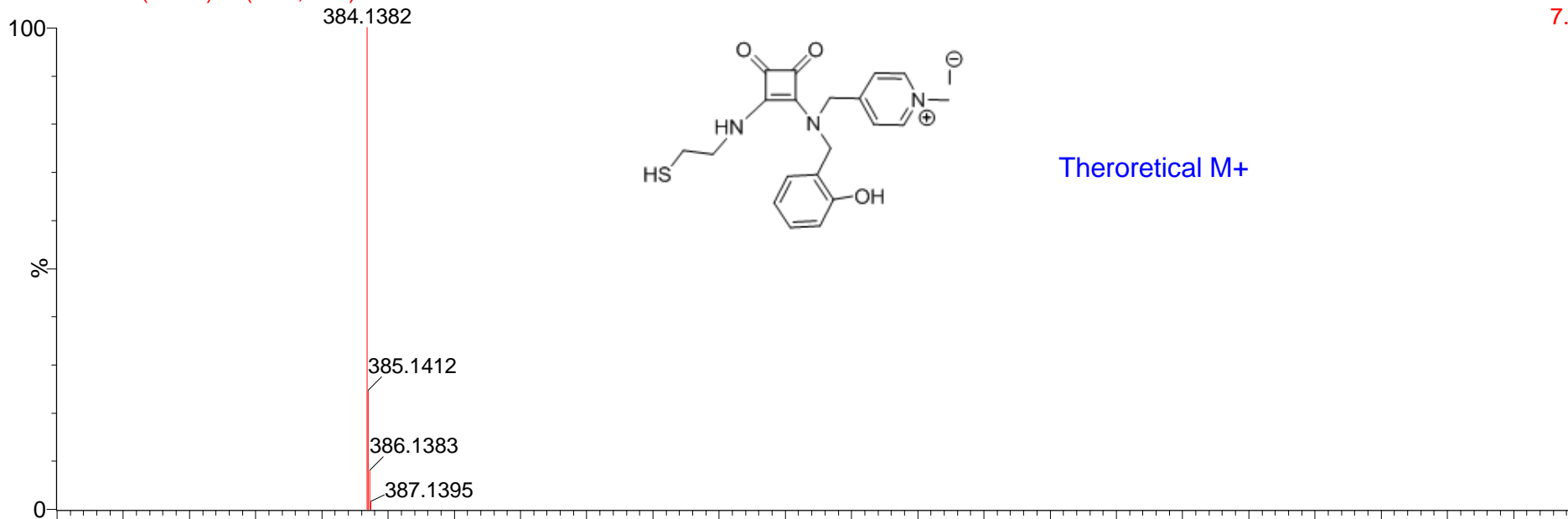
File name: dc-2-117-101B
Instrument: LCT KC366
Method: ESI-TOF

Notebook Ref: 24952
Test name: Accurate Mass
Base Peak Mass: 459.15127563

IU Database#: 24952
13-May-2010 12:39:59

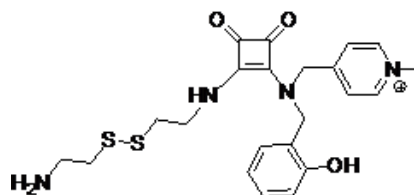
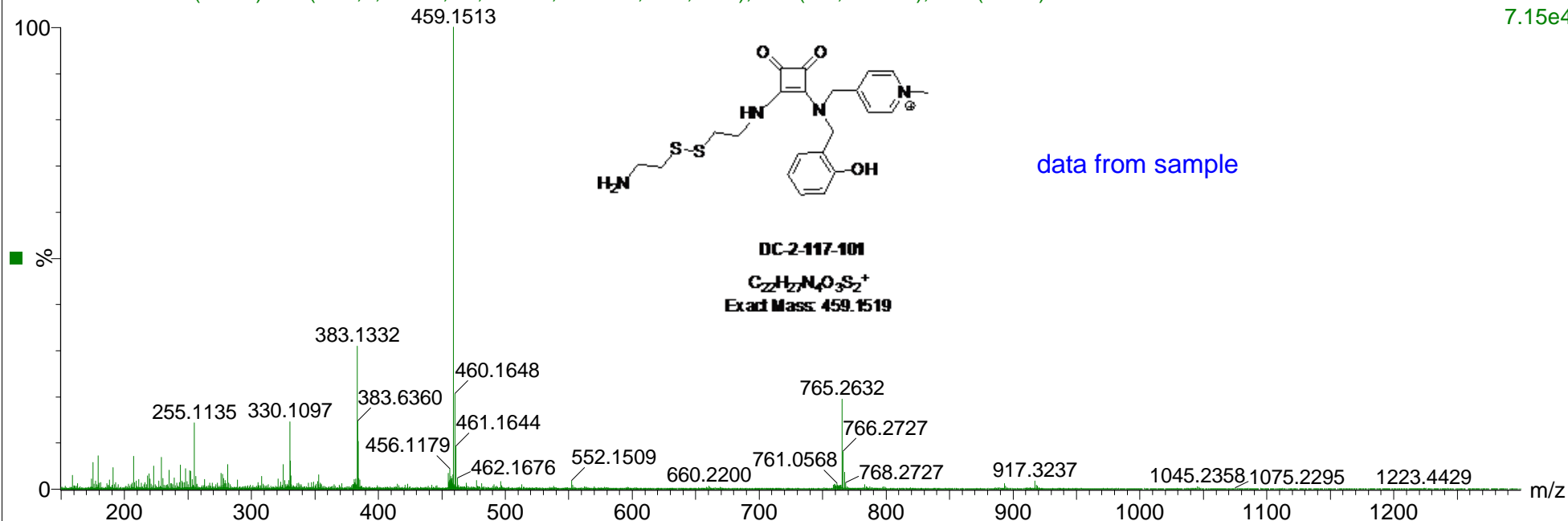
dc-3-86-101 (0.035) Is (0.50,0.50) C₂₀H₂₂N₃O₃S

1: TOF MS ES+
7.45e12

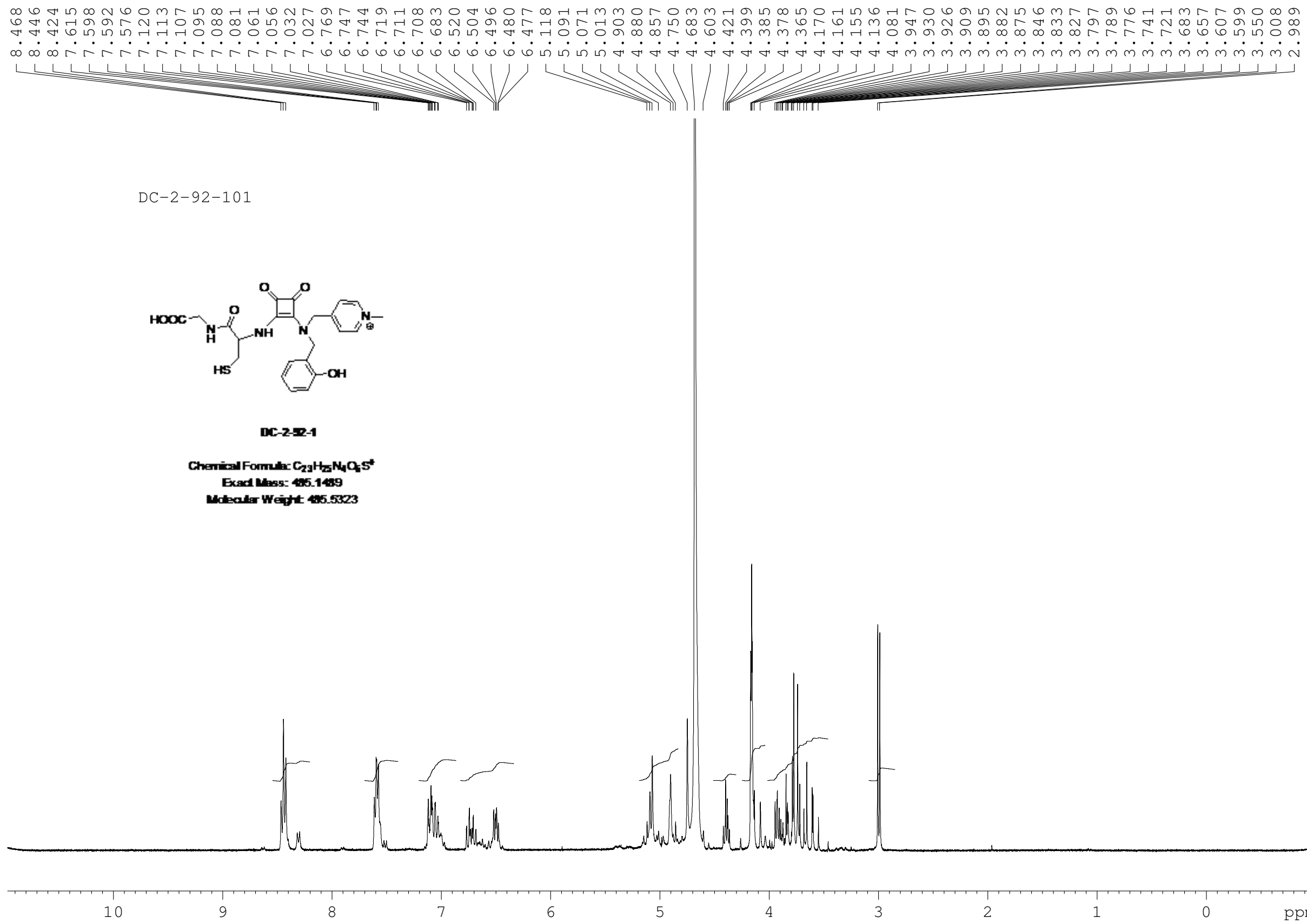


dc-2-117-101B 34 (0.852) AM (Cen,8, 90.00, Ar,5000.0,1222.14,0.70,LS 6); Sm (SG, 2x4.00); Cm (23:40)

1: TOF MS ES+
7.15e4

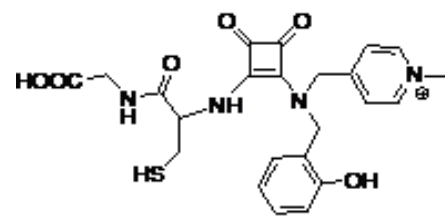


DC-2-117-101
C₂₂H₂₇N₄O₃S₂⁺
Exact Mass: 459.1519



8.468
 8.446
 8.424
 7.615
 7.598
 7.592
 7.576
 7.120
 7.113
 7.107
 7.095
 7.088
 7.081
 7.061
 7.056
 7.032
 7.027
 6.769
 6.747
 6.744
 6.719
 6.711
 6.708
 6.683
 6.520
 6.504
 6.496
 6.480
 6.477
 5.118
 5.091
 5.071
 5.013
 4.903
 4.880
 4.857
 4.750
 4.683
 4.603
 4.421
 4.399
 4.385
 4.378
 4.365
 4.170
 4.161
 4.155
 4.136
 4.081
 3.947
 3.930
 3.926
 3.909
 3.895
 3.882
 3.875
 3.846
 3.833
 3.827
 3.797
 3.789
 3.776
 3.741
 3.721
 3.683
 3.657
 3.607
 3.599
 3.550
 3.008
 2.989

DC-2-92-101



DC-2-92-1

Chemical Formula: $C_{23}H_{25}N_4O_3S^+$
 Exact Mass: 485.1489
 Molecular Weight: 485.5323

Current Data Parameters
 NAME DC-2-92-101
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100226
 Time 14.48
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT D2O
 NS 32
 DS 0
 SWH 3591.954 Hz
 FIDRES 0.109618 Hz
 AQ 4.5613556 sec
 RG 256
 DW 139.200 usec
 DE 54.00 usec
 TE 299.2 K
 D1 1.0000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 9.75 usec
 PL1 0.00 dB
 SFO1 300.1315007 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300042 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

2.211
 2.256
 2.379
 2.000
 3.787
 0.685
 4.236
 4.974
 1.297

Elemental Composition Report

Multiple Mass Analysis: 2 mass(es) processed

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 80.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

31200 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 23-23 N: 0-4 O: 0-6 Na: 0-1 S: 0-1 2H: 1-5 1H: 1-29

File name: dc-2-92-101

Instrument: LCT KC366

Method: ESI-TOF

dc-2-92-101 31 (0.785) AM (Cen,6, 90.00, Ar,4000.0,922.36,0.70,LS 4); Sm (SG, 2x4.00); Cm (29:45)

Notebook Ref: 24694

Test name: Accurate Mass

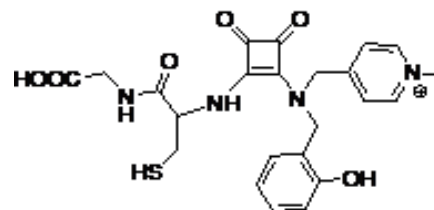
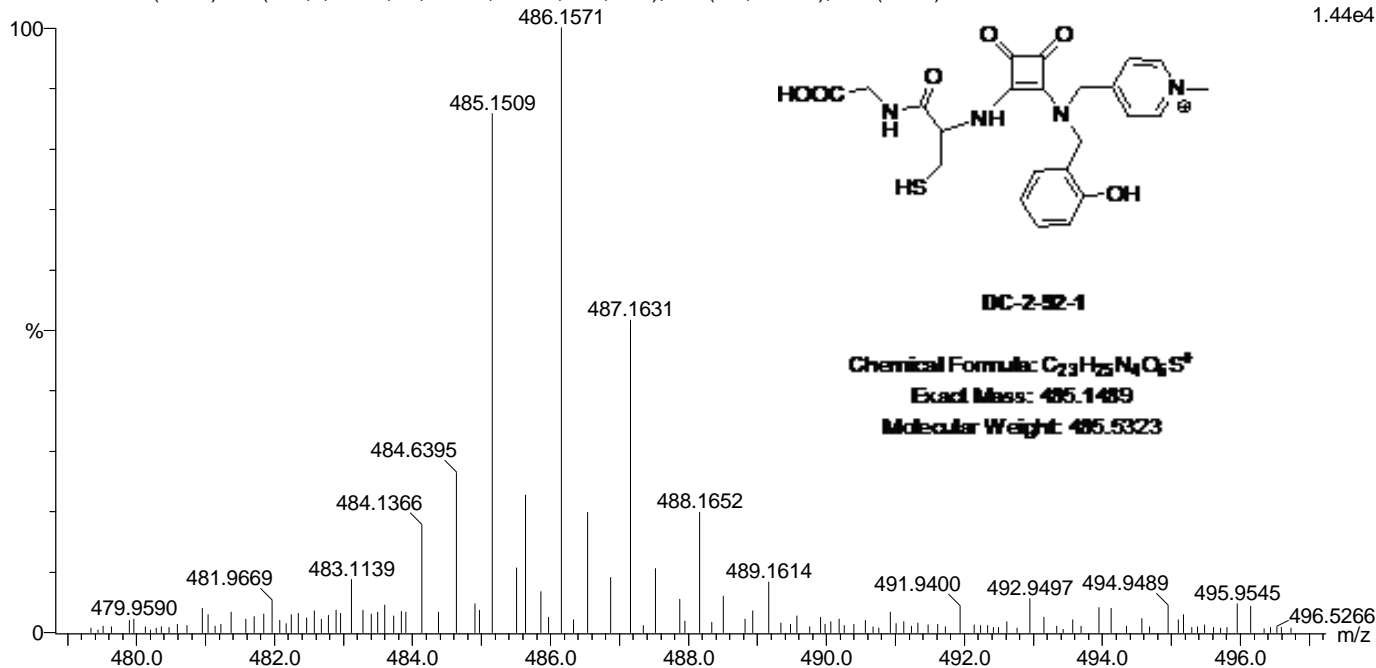
Base Peak Mass: 486.15707397

IU Database#: 24694

28-Apr-2010 12:17:42

1: TOF MS ES+

1.44e4



DC-2-92-1

Chemical Formula: C₂₃H₂₅N₄O₆S⁺

Exact Mass: 486.1489

Molecular Weight: 486.5323

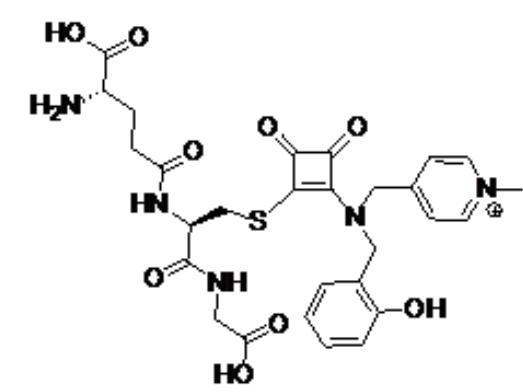
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
485.1509	85.78	485.1464	4.5	9.3	14.5	8216.9	C23 N4 O6 S 2H2 1H21
486.1571	100.00	486.1558	1.3	2.7	13.5	953.5	C23 N4 O6 S 2H 1H24
		486.1527	4.4	9.1	14.5	2915.8	C23 N4 O6 S 2H3 1H20

8.656
 8.634
 8.435
 8.419
 8.398
 7.878
 7.857
 7.569
 7.547
 7.284
 7.146
 7.133
 7.099
 7.094
 7.081
 7.075
 7.056
 7.051
 7.024
 6.740
 6.715
 6.684
 6.484
 6.473
 6.458
 6.446
 5.171
 5.045
 5.021
 4.974
 4.905
 4.865
 4.801
 4.784
 4.773
 4.755
 4.700
 4.688
 4.635
 4.259
 4.149
 4.137
 4.096
 4.080
 4.048
 4.033
 3.865
 3.808
 3.721
 3.695
 3.677
 3.553
 3.526
 3.506
 3.478
 2.838
 2.819
 2.813
 2.438
 2.414
 2.387
 2.353
 2.325
 2.084
 2.066
 2.044
 2.019
 1.994

Current Data Parameters
 NAME DC-3-82-101-5min
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100503
 Time 17.31
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT D2O
 NS 32
 DS 0
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 512
 DW 104.400 usec
 DE 54.00 usec
 TE 296.2 K
 D1 1.00000000 sec
 TD0 1

DC-3-82-101-5min

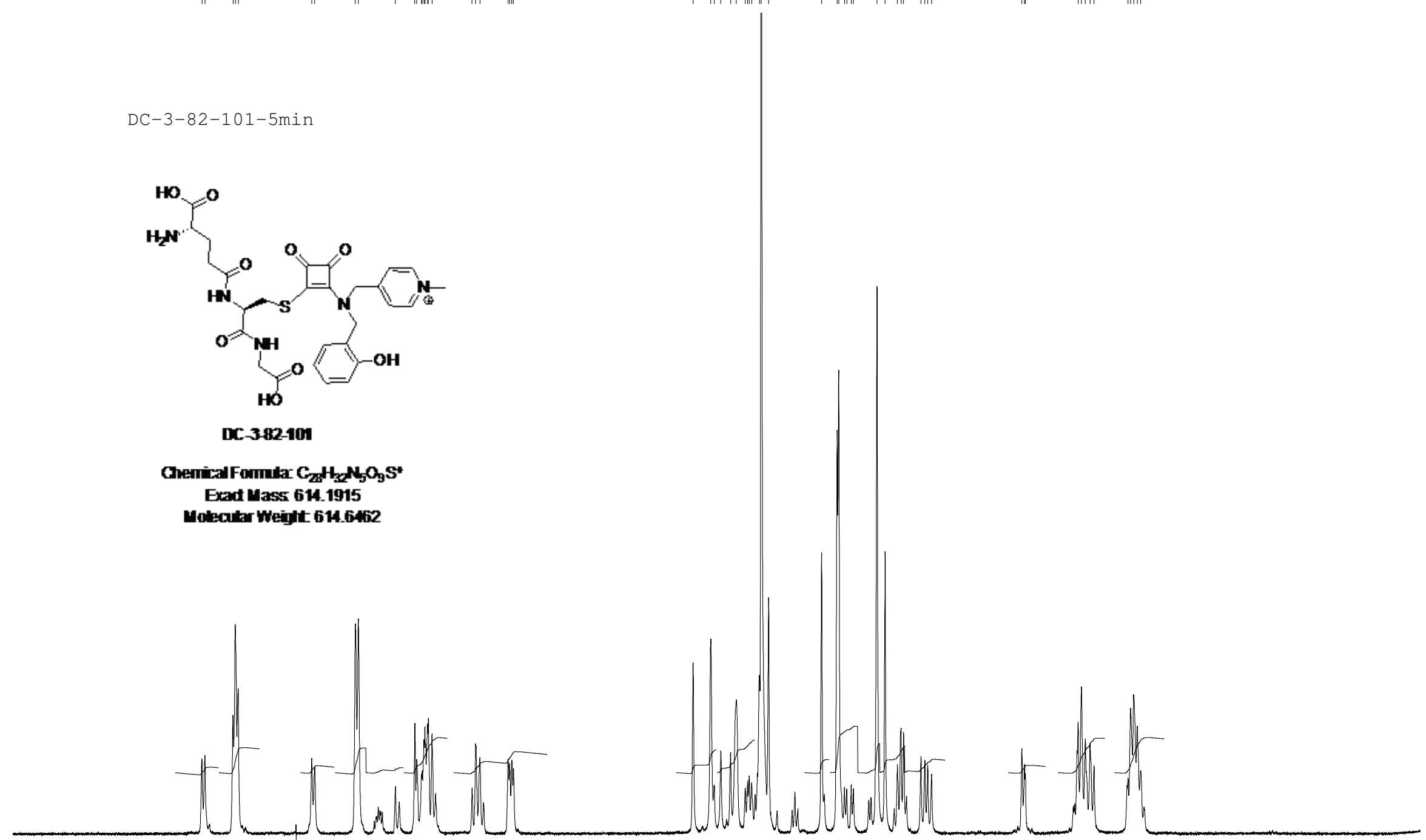


DC-3-82-101

Chemical Formula: $C_{28}H_{32}N_5O_9S^+$
 Exact Mass: 614.1915
 Molecular Weight: 614.6462

==== CHANNEL f1 =====
 NUC1 1H
 P1 9.75 usec
 PL1 0.00 dB
 SFO1 300.1324000 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300024 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

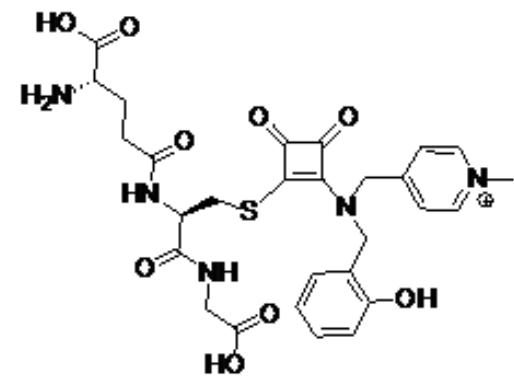


9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

0.287
 1.407
 0.322
 1.436
 0.292
 2.030
 1.076
 1.344
 1.935
 0.765
 2.738
 2.471
 1.691
 0.738
 0.362
 2.021
 2.000

8.427
 8.411
 8.405
 8.389
 7.558
 7.538
 7.090
 7.076
 7.070
 7.065
 7.051
 7.045
 7.040
 7.019
 7.013
 6.731
 6.709
 6.706
 6.700
 6.679
 6.675
 6.476
 6.468
 6.465
 6.452
 6.441
 6.438
 5.037
 5.018
 4.970
 4.902
 4.855
 4.794
 4.778
 4.766
 4.750
 4.708
 4.688
 4.140
 4.128
 4.091
 4.075
 4.043
 4.027
 3.862
 3.806
 3.692
 3.675
 3.547
 3.519
 3.499
 3.471
 2.431
 2.408
 2.402
 2.380
 2.373
 2.348
 2.340
 2.319
 2.077
 2.055
 2.050
 2.034
 2.028
 2.012
 2.006
 1.987

DC-3-82-101-1h



DC-3-82-101

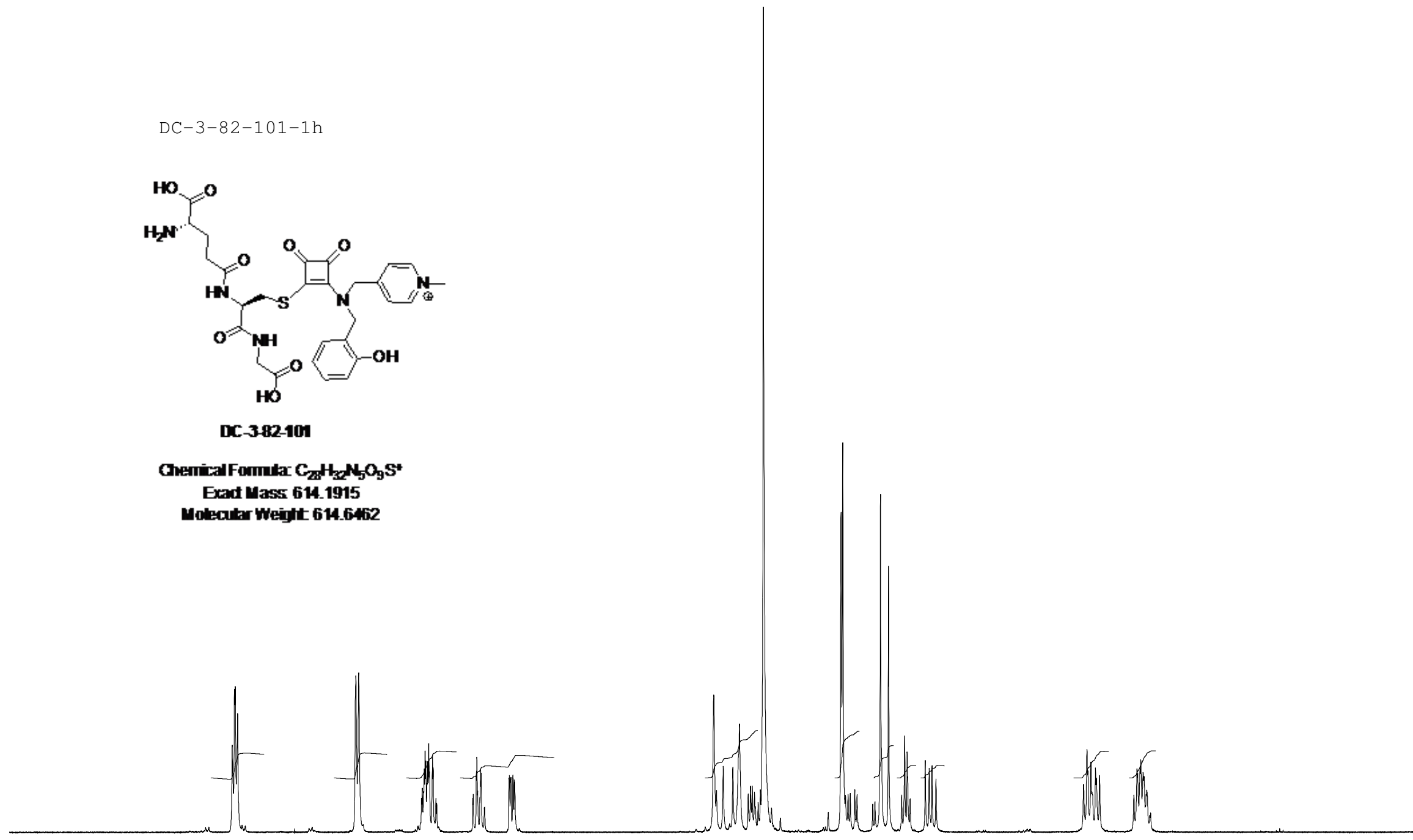
Chemical Formula: $C_{28}H_{32}N_5O_9S^+$
 Exact Mass: 614.1915
 Molecular Weight: 614.6462

Current Data Parameters
 NAME DC-3-82-101-1h
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100504
 Time 8.55
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT D2O
 NS 32
 DS 0
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 512
 DW 104.400 usec
 DE 54.00 usec
 TE 683.2 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 9.75 usec
 PL1 0.00 dB
 SFO1 300.1324000 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300024 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00



9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

1.927
 1.925
 2.115
 1.647
 3.901
 3.815
 2.640
 1.006
 0.993
 2.160
 2.206

Elemental Composition Report

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 80.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

114 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-28 H: 0-32 N: 0-5 O: 0-9 S: 0-1

File name: dc-3-82-101

Instrument: LCT KC366

Method: ESI-TOF

dc-3-82-101 57 (1.436) AM (Cen,8, 90.00, Ar,4000.0,1222.14,0.70,LS 6); Sm (SG, 2x4.00); Cm (57:60)

Notebook Ref: 24823

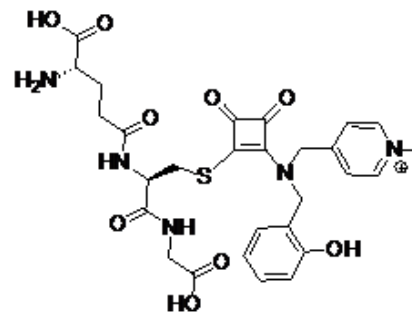
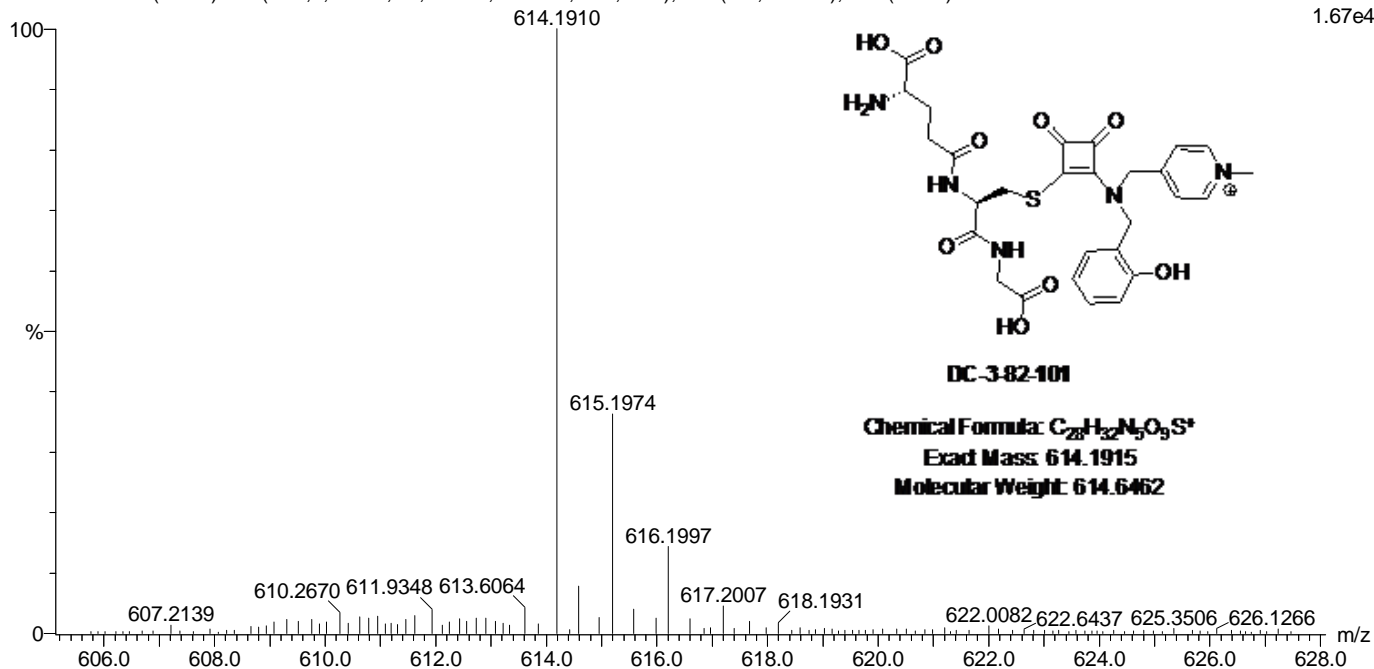
Test name: Accurate Mass

Base Peak Mass: 614.19097900

IU Database#: 24823

06-May-2010 11:43:09

1: TOF MS ES+
1.67e4



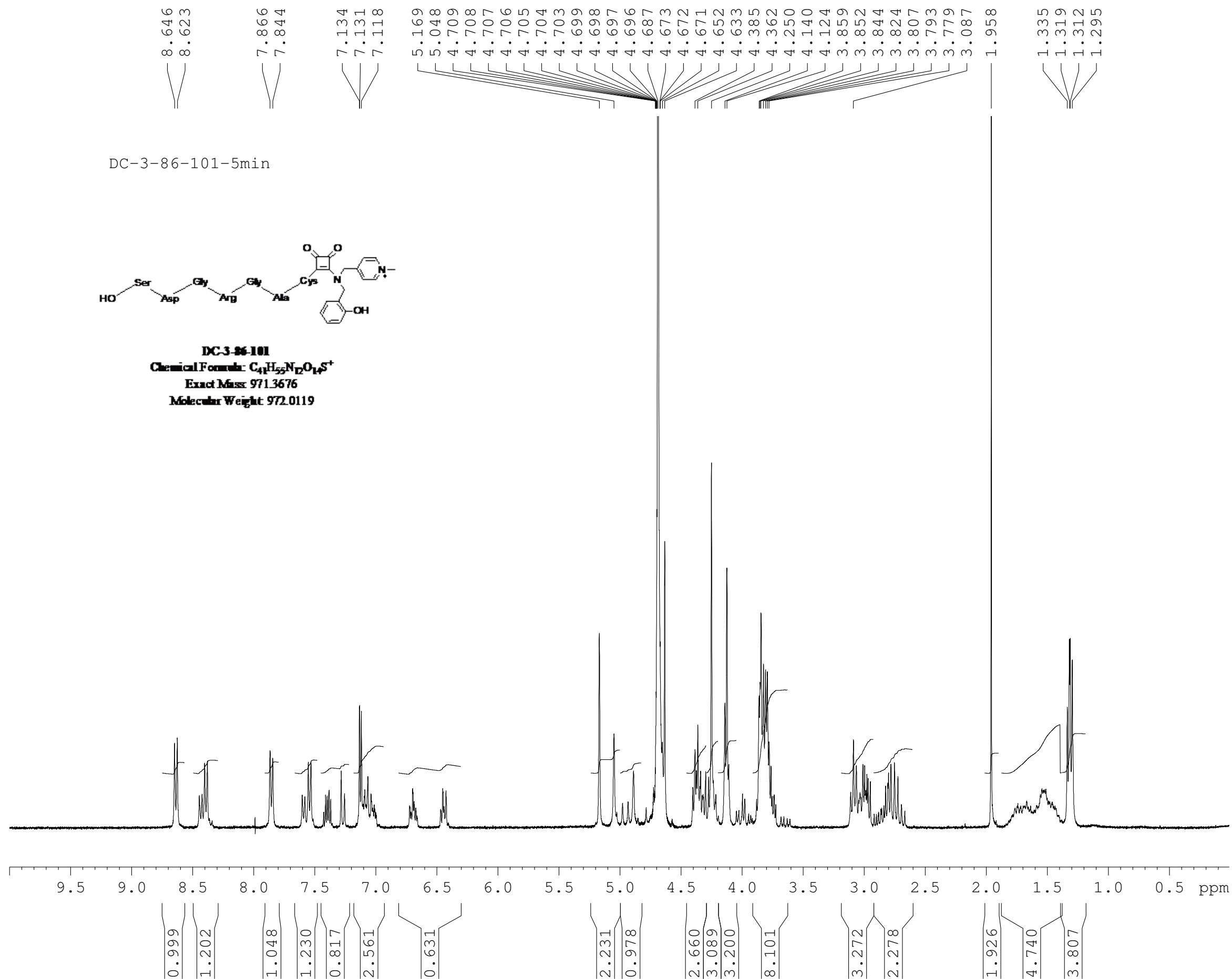
DC-3-82-101

Chemical Formula: C₂₈H₃₂N₅O₉S⁺

Exact Mass: 614.1915

Molecular Weight: 614.6462

Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
614.1910	100.00	614.1921	-1.1	-1.8	15.5	30.9	C ₂₈ H ₃₂ N ₅ O ₉ S



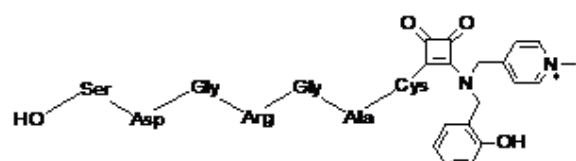
Current Data Parameters
NAME DC-3-86-101-5min
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100505
Time 15.45
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT D2O
NS 64
DS 0
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 512
DW 104.400 usec
DE 54.00 usec
TE 683.2 K
D1 1.00000000 sec
TD0 1

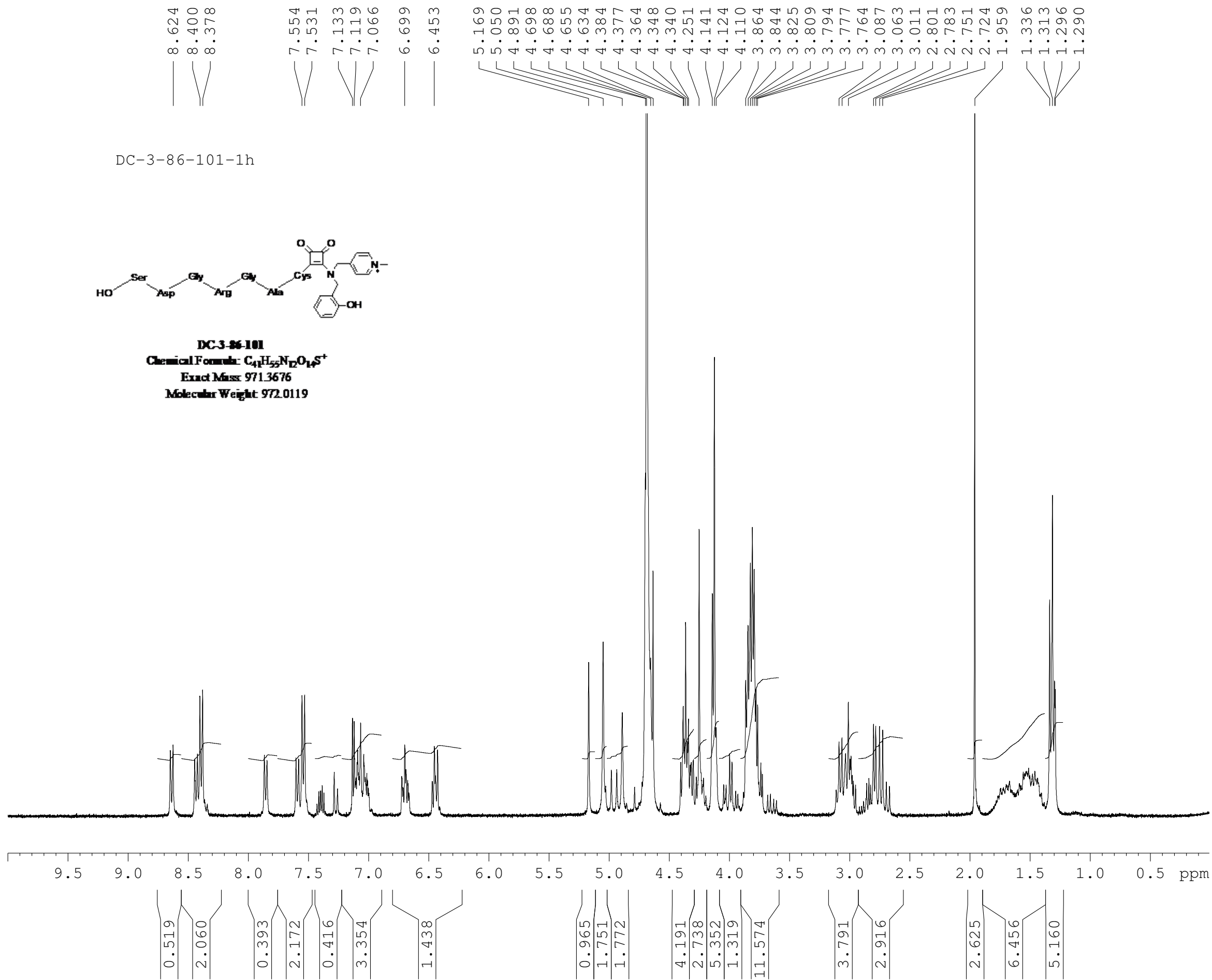
==== CHANNEL f1 =====
NUC1 1H
P1 9.75 usec
PL1 0.00 dB
SFO1 300.1324000 MHz

F2 - Processing parameters
SI 32768
SF 300.1300024 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

DC-3-86-101-1h



DC-3-86-101
Chemical Formula: C₄₁H₅₅N₁₂O₁₄S⁺
Exact Mass: 971.3676
Molecular Weight: 972.0119



Current Data Parameters

NAME DC-3-86-101-1h
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

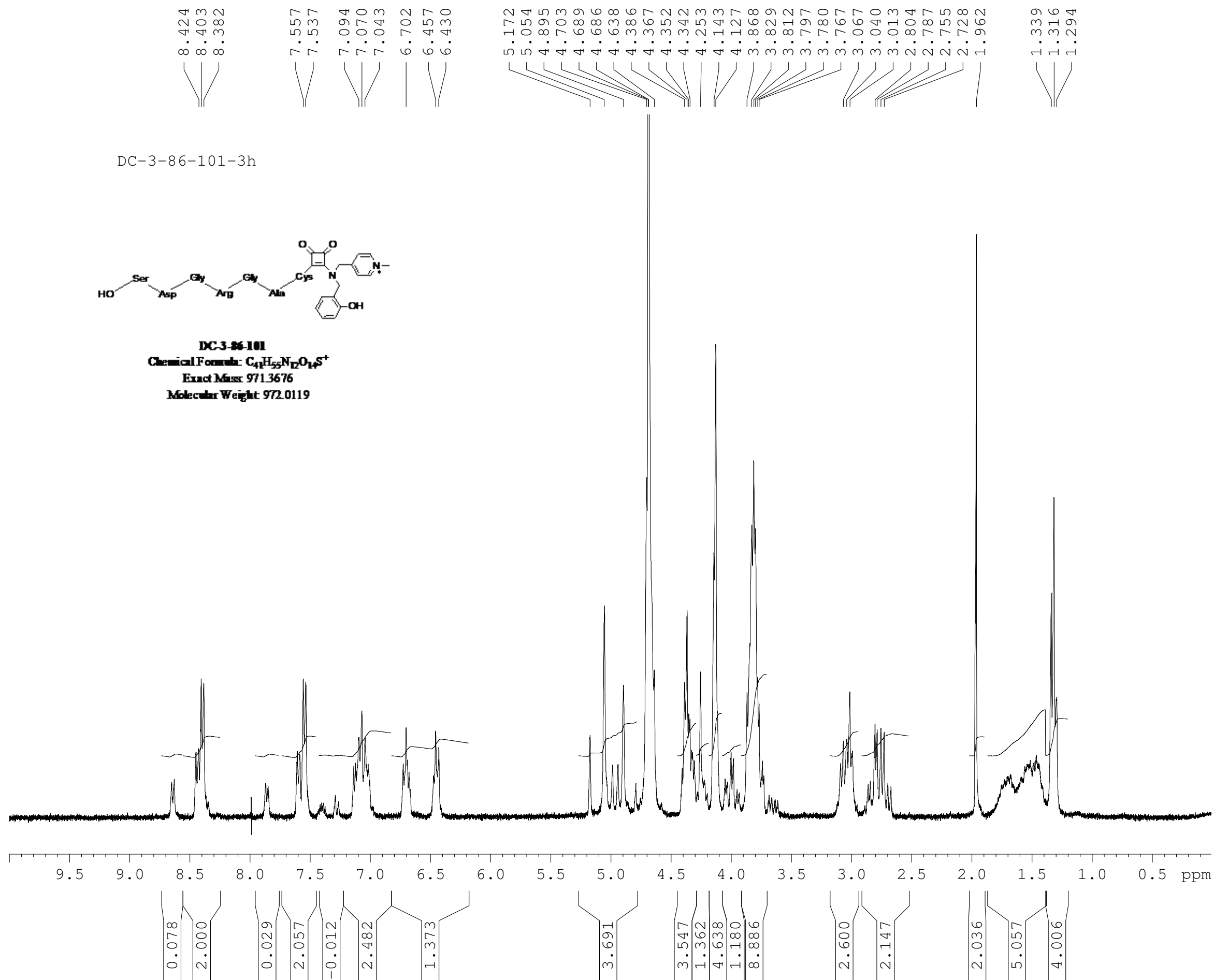
Date_ 20100505
 Time 16.33
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT D2O
 NS 64
 DS 0
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 512
 DW 104.400 usec
 DE 54.00 usec
 TE 683.2 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====

NUC1 1H
 P1 9.75 usec
 PL1 0.00 dB
 SFO1 300.1324000 MHz

F2 - Processing parameters

SI 32768
 SF 300.1300024 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00



Current Data Parameters

NAME DC-3-86-101-3h
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

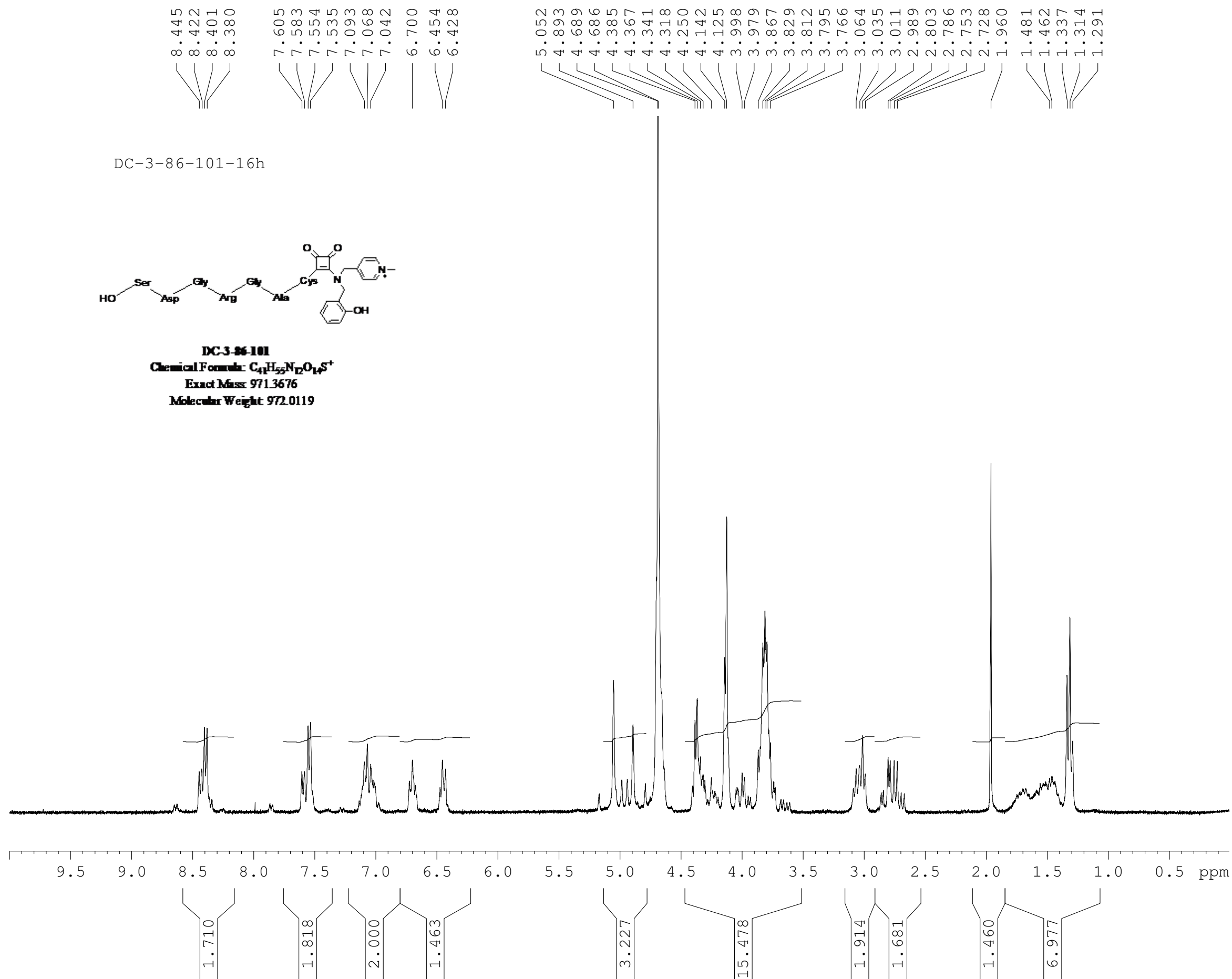
Date_ 20100505
Time 18.32
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT D2O
NS 32
DS 0
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 512
DW 104.400 usec
DE 54.00 usec
TE 683.2 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====

NUC1 1H
P1 9.75 usec
PL1 0.00 dB
SFO1 300.1324000 MHz

F2 - Processing parameters

SI 32768
SF 300.1300024 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



Current Data Parameters
 NAME DC-3-86-101-16h
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100506
 Time 9.39
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT D2O
 NS 32
 DS 0
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 512
 DW 104.400 usec
 DE 54.00 usec
 TE 683.2 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 9.75 usec
 PL1 0.00 dB
 SFO1 300.1324000 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300024 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

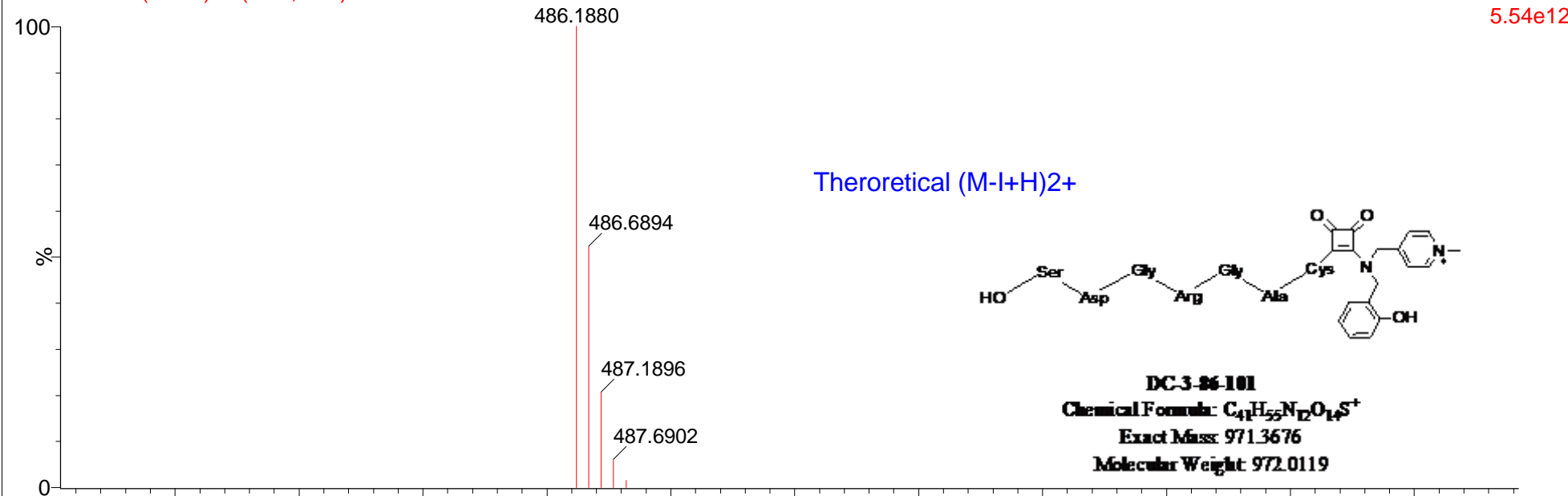
File name: dc-3-86-101
Instrument: LCT KC366
Method: ESI-TOF

Notebook Ref: 24947
Test name: Accurate Mass
Base Peak Mass: 486.18878174

IU Database#: 24947
13-May-2010 12:23:17

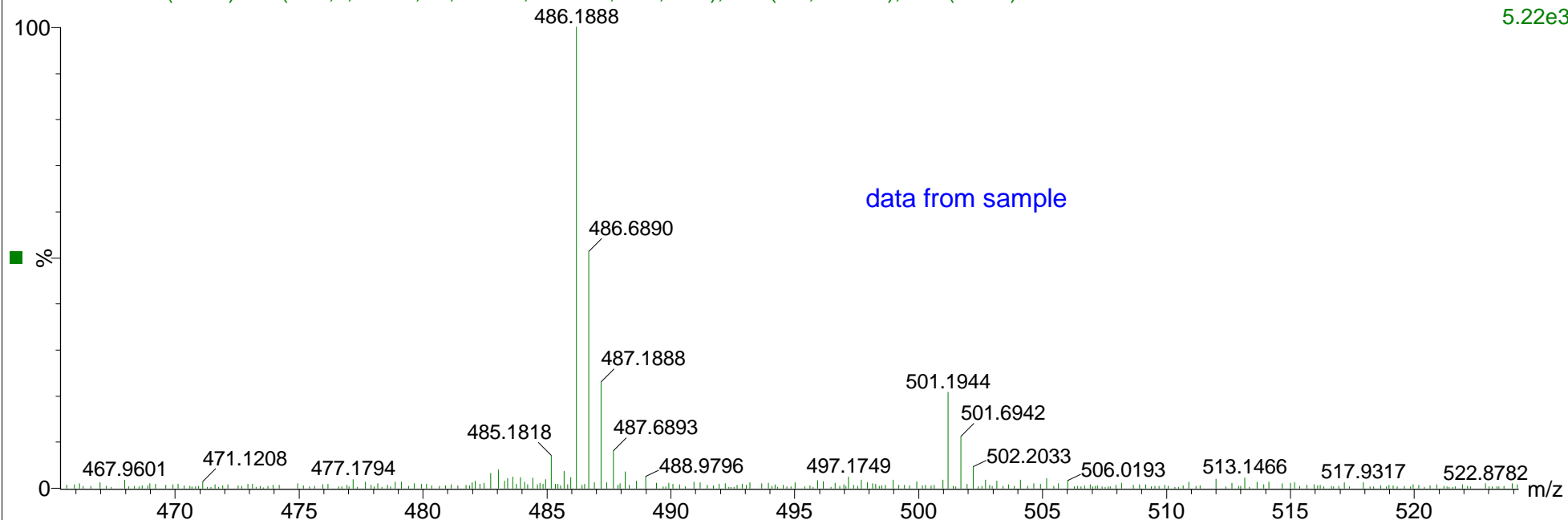
dc-3-86-101 (0.035) Is (0.50,0.50) C₄₁H₅₄N₁₂O₁₄S

1: TOF MS ES+
5.54e12

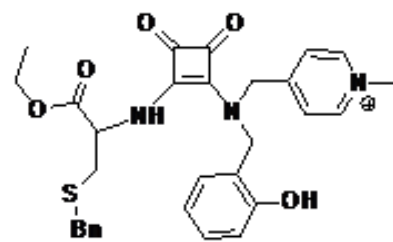


dc-3-86-101 48 (1.202) AM (Cen,8, 90.00, Ar,5000.0,1971.61,0.70,LS 6); Sm (SG, 2x4.00); Cm (48:54)

1: TOF MS ES+
5.22e3



DC-2-92-201-5min



DC-2-92-201

Chemical Formula: C₃₀H₃₂N₃O₅⁺

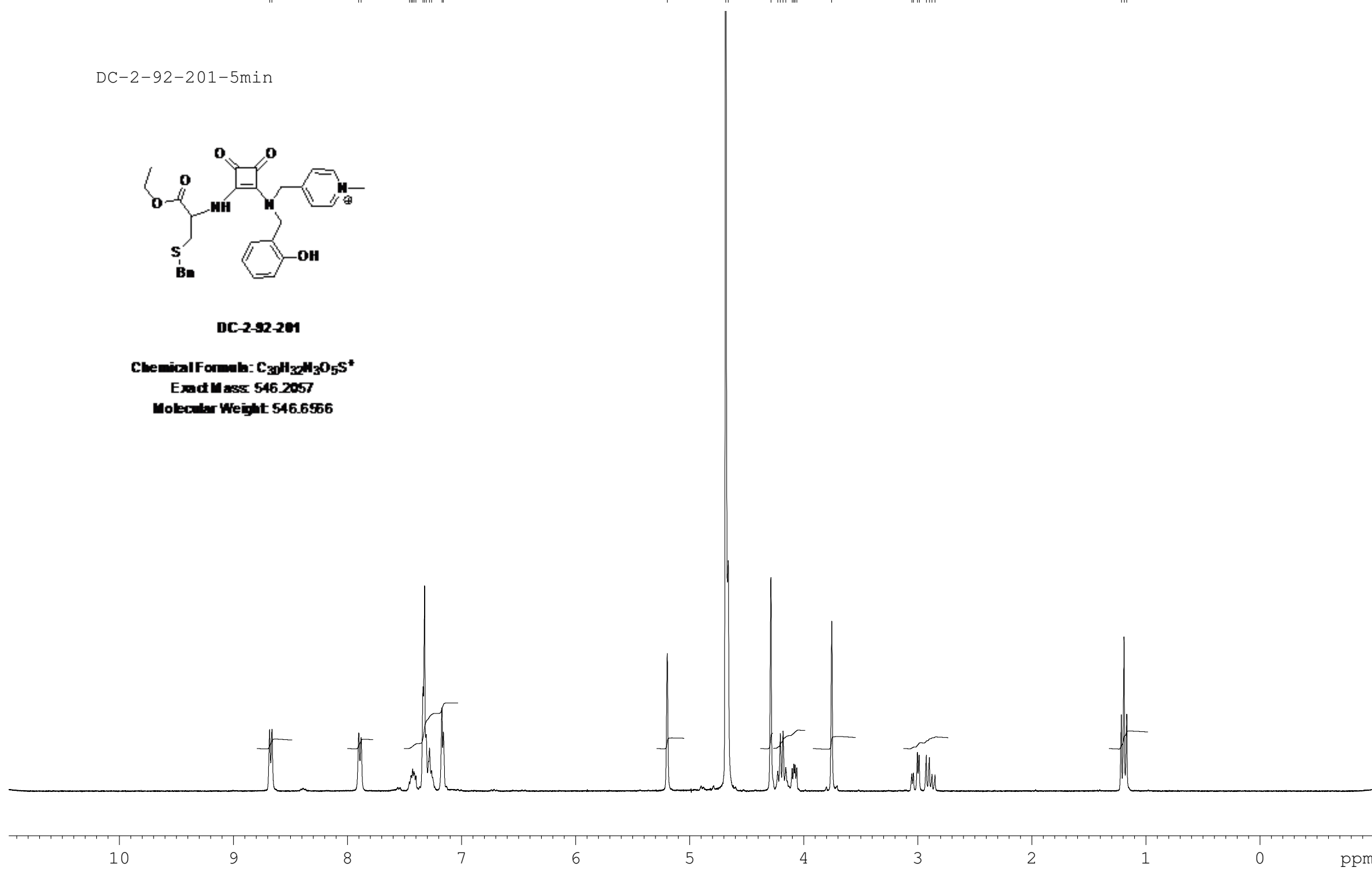
Exact Mass: 546.2057

Molecular Weight: 546.6566

8.682
8.661
7.900
7.880
7.457
7.440
7.428
7.415
7.399
7.337
7.323
7.308
7.280
7.262
7.171
7.159

5.196
4.682
4.661
4.287
4.228
4.205
4.180
4.157
4.101
4.085
4.074
4.059
3.753
3.052
3.037
3.002
2.987
2.924
2.898
2.874
2.848

1.214
1.190
1.167



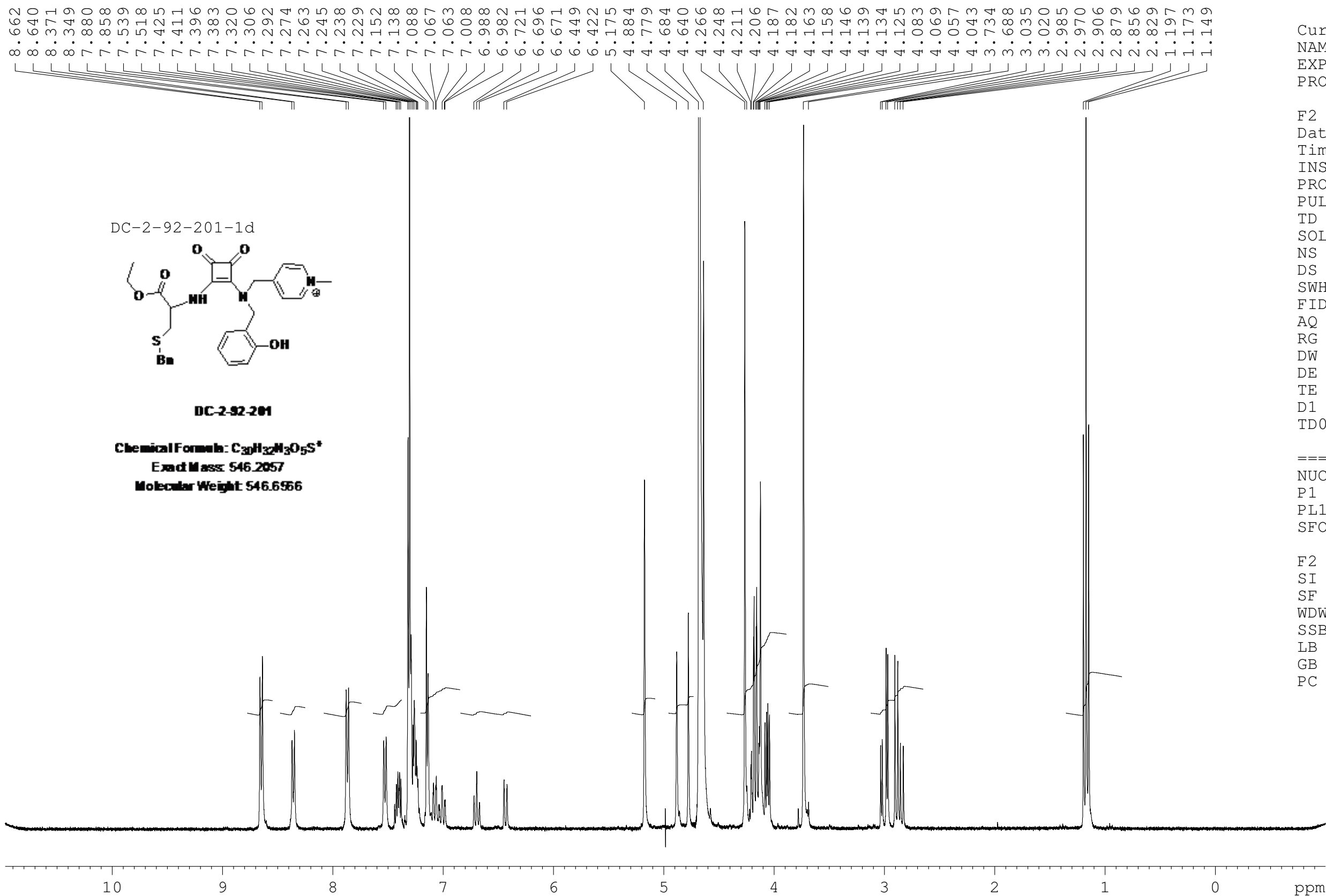
1.651
1.731
8.927
2.000
3.029
3.523
2.156
2.119
3.243

Current Data Parameters
 NAME DC-2-92-201-5min
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100226
 Time 14.42
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT D2O
 NS 32
 DS 0
 SWH 3591.954 Hz
 FIDRES 0.109618 Hz
 AQ 4.5613556 sec
 RG 256
 DW 139.200 usec
 DE 54.00 usec
 TE 299.2 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 9.75 usec
 PL1 0.00 dB
 SFO1 300.1315007 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300042 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00



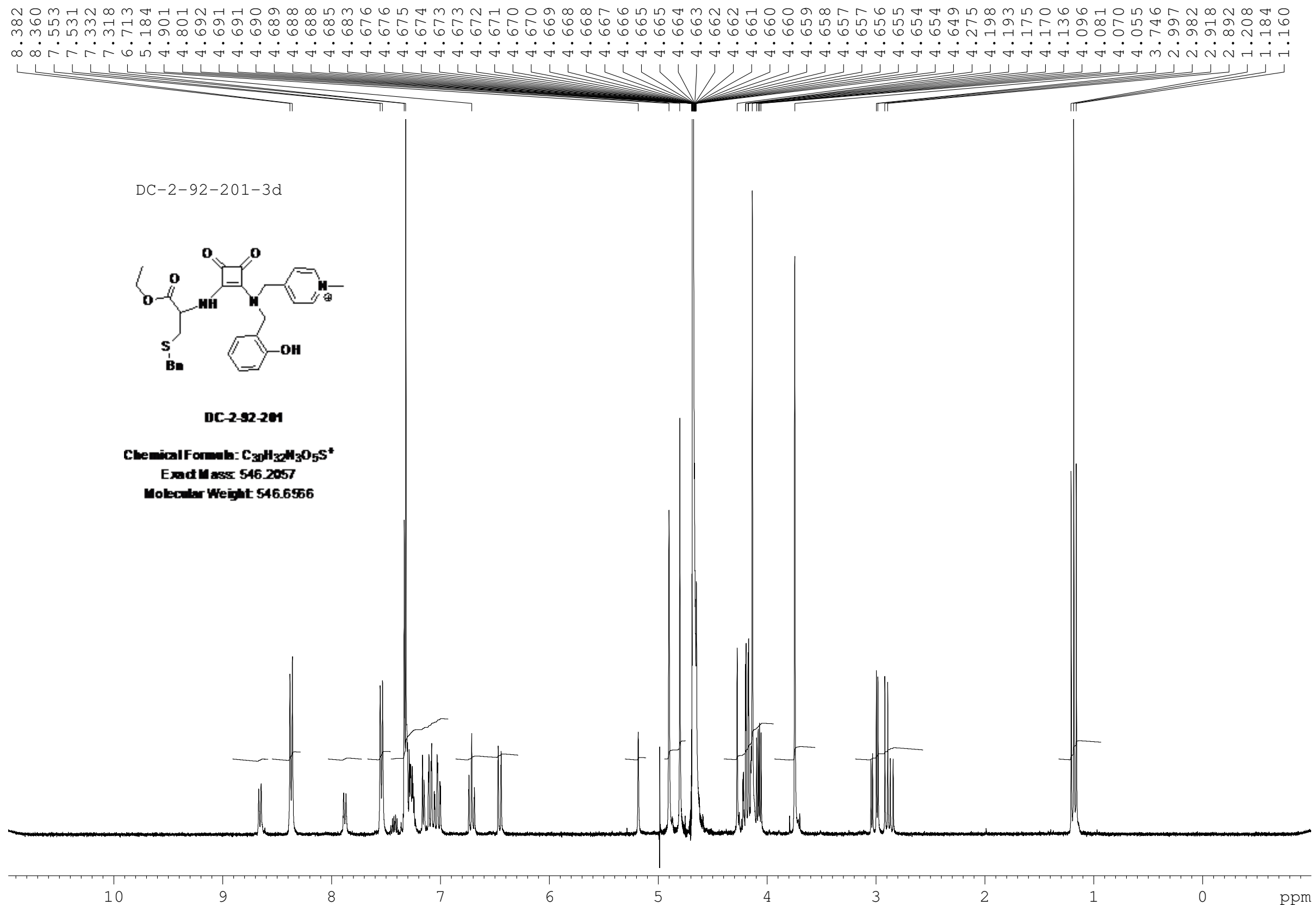
Current Data Parameters
 NAME DC-2-92-201-1d
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100227
 Time 11.31
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT D2O
 NS 32
 DS 0
 SWH 3591.954 Hz
 FIDRES 0.109618 Hz
 AQ 4.5613556 sec
 RG 512
 DW 139.200 usec
 DE 54.00 usec
 TE 298.2 K
 D1 1.0000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 9.75 usec
 PL1 0.00 dB
 SFO1 300.1315007 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300042 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

Integration values:
 1.000
 0.433
 0.783
 1.068
 1.882
 -0.230
 1.153
 1.335
 6.368
 2.140
 1.931
 2.932



Current Data Parameters
 NAME DC-2-92-201-3d
 EXPNO 1
 PROCNO 1

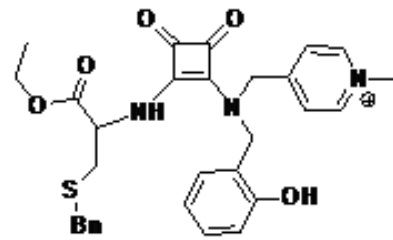
F2 - Acquisition Parameters
 Date_ 20100301
 Time 18.23
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT D2O
 NS 16
 DS 0
 SWH 3591.954 Hz
 FIDRES 0.109618 Hz
 AQ 4.5613556 sec
 RG 456.1
 DW 139.200 usec
 DE 54.00 usec
 TE 299.2 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 9.75 usec
 PL1 0.00 dB
 SFO1 300.1315007 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300042 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

8.384
8.361
7.556
7.534
7.338
7.335
7.321
6.716
4.904
4.807
4.685
4.683
4.675
4.674
4.673
4.672
4.671
4.670
4.669
4.668
4.667
4.666
4.665
4.665
4.664
4.663
4.662
4.662
4.661
4.660
4.660
4.659
4.658
4.657
4.657
4.656
4.655
4.654
4.654
4.653
4.652
4.651
4.651
4.650
4.649
4.649
4.648
4.647
4.200
4.195
4.176
4.171
4.137
4.072
4.057
3.748
2.999
2.984
2.921
2.894
1.210
1.208
1.186
1.184
1.162

Dc-2-92-201-6d



DC-2-92-201

Chemical Formula: C₃₀H₃₂N₃O₅S⁺

Exact Mass: 546.2057

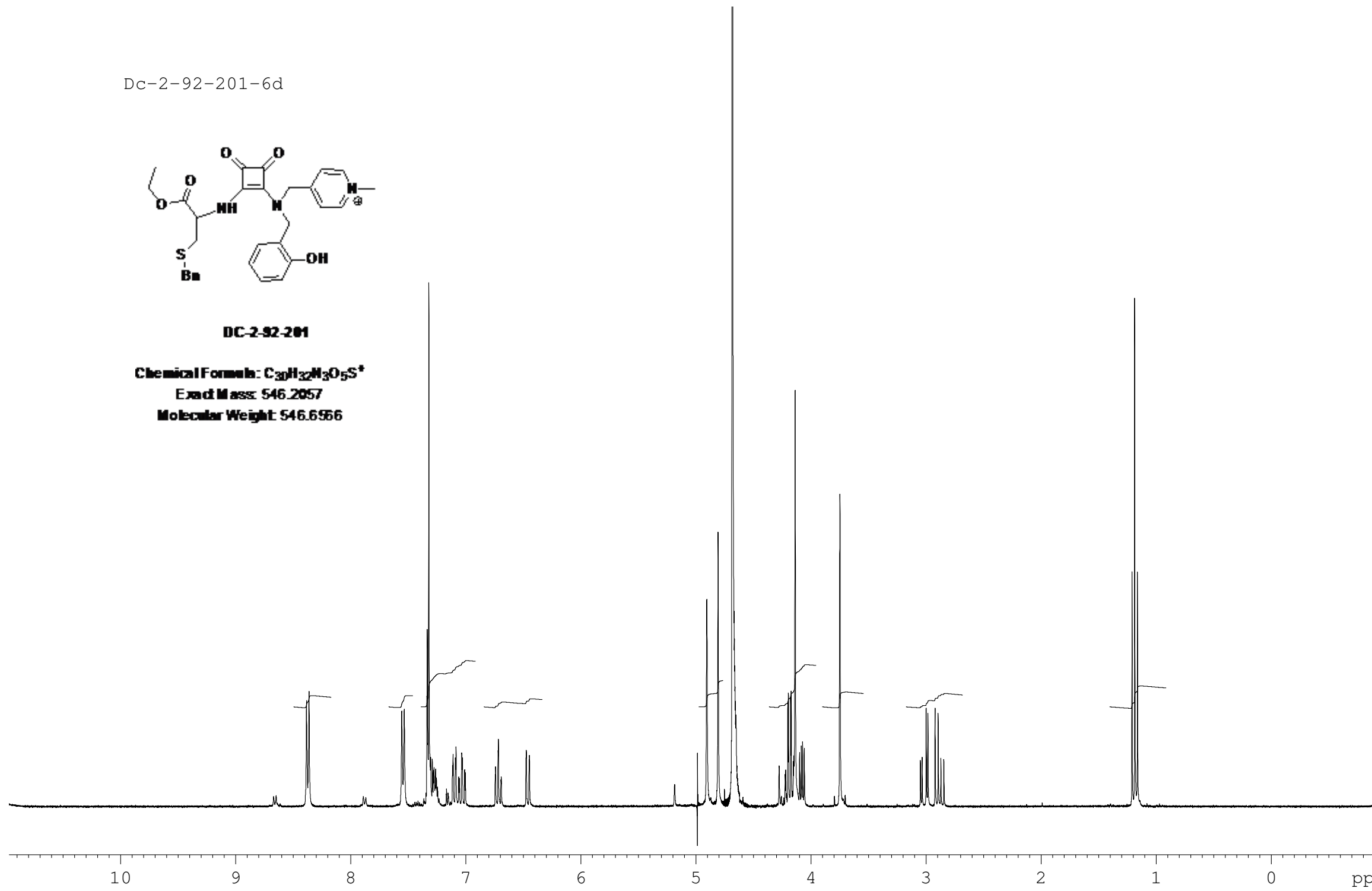
Molecular Weight: 546.6566

Current Data Parameters
NAME Dc-2-92-201-6d
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100303
Time 18.12
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT D2O
NS 16
DS 0
SWH 3591.954 Hz
FIDRES 0.109618 Hz
AQ 4.5613556 sec
RG 456.1
DW 139.200 usec
DE 54.00 usec
TE 299.2 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 9.75 usec
PL1 0.00 dB
SFO1 300.1315007 MHz

F2 - Processing parameters
SI 32768
SF 300.1300042 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



1.438
1.653
6.828
1.081
3.941
6.216
2.000
1.774
2.837

Elemental Composition Report

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 80.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

74 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-30 H: 0-32 N: 0-3 O: 0-5 Na: 0-1 S: 0-1

File name: dc-2-92-201b

Notebook Ref: 25563

IU Database#: 25563

Instrument: LCT KC366

Test name: Accurate Mass

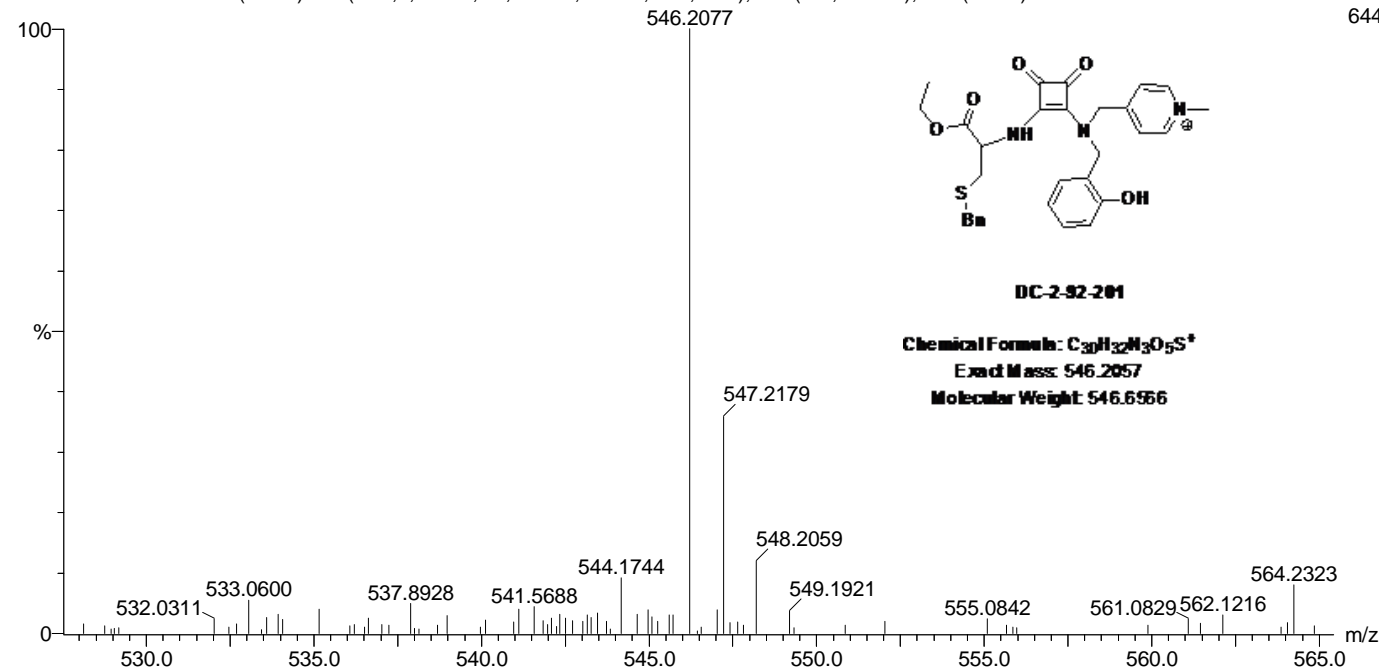
15-Jun-2010 17:23:10

Method: ESI-TOF

Base Peak Mass: 546.20770264

dc-2-92-201b-rerun5 67 (1.686) AM (Cen,8, 90.00, Ar,5000.0,922.36,0.70,LS 7); Sm (SG, 2x4.00); Cm (67:68)

1: TOF MS ES+
644



Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
546.2077	100.00	546.2063	1.4	2.6	16.5	0.2	C30 H32 N3 O5 S

8.679
 8.657
 7.900
 7.878
 7.438
 7.426
 7.409
 7.396
 7.308
 7.281
 7.167
 7.152
 5.197
 4.718
 4.716
 4.714
 4.712
 4.712
 4.711
 4.710
 4.710
 4.709
 4.708
 4.707
 4.707
 4.706
 4.705
 4.704
 4.704
 4.703
 4.702
 4.702
 4.701
 4.700
 4.699
 4.699
 4.698
 4.697
 4.696
 4.696
 4.695
 4.694
 4.693
 4.683
 4.668
 4.668
 4.664
 4.283
 3.917
 3.903
 3.876
 3.864
 3.847
 3.824
 3.806
 3.756
 3.743
 3.739
 3.725

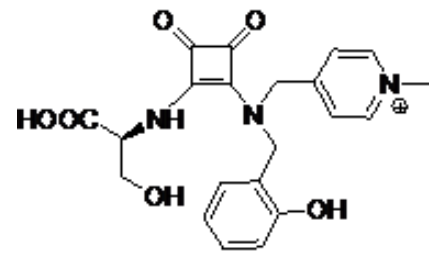
Current Data Parameters
 NAME DC-2-69-100-5min
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100219
 Time 10.08
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT D2O
 NS 32
 DS 0
 SWH 3591.954 Hz
 FIDRES 0.109618 Hz
 AQ 4.5613556 sec
 RG 256
 DW 139.200 usec
 DE 54.00 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 9.75 usec
 PL1 0.00 dB
 SFO1 300.1315007 MHz

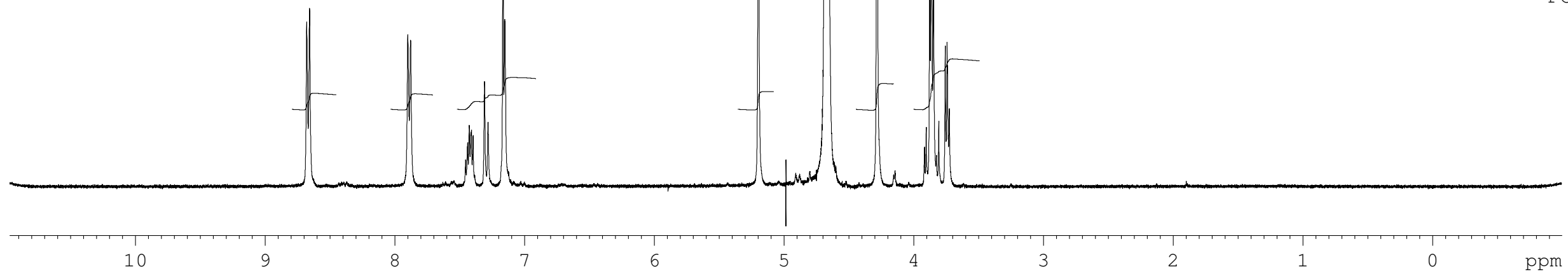
F2 - Processing parameters
 SI 32768
 SF 300.1300042 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

DC-2-69-100-5min



DC-2-69-1

Chemical Formula: C₂₁H₂₂N₃O₆⁺
Exact Mass: 412.1503
Molecular Weight: 412.4153



2.000
 1.983
 4.230
 2.420
 3.523
 6.683

8.672
8.650
8.388
8.365
7.894
7.872
7.562
7.539
7.308
7.162
7.148
7.144
5.191
4.910
4.806
4.704
4.703
4.702
4.702
4.701
4.700
4.699
4.699
4.698
4.697
4.696
4.696
4.695
4.694
4.693
4.693
4.692
4.691
4.690
4.690
4.689
4.683
4.682
4.676
4.675
4.674
4.673
4.673
4.672
4.671
4.670
4.670
4.669
4.668
4.667
4.666
4.665
4.665
4.664
4.663
4.662
4.662
4.657
4.642
4.640
4.639
4.277
4.138
3.886
3.885
3.884
3.871
3.869
3.815
3.800
3.785

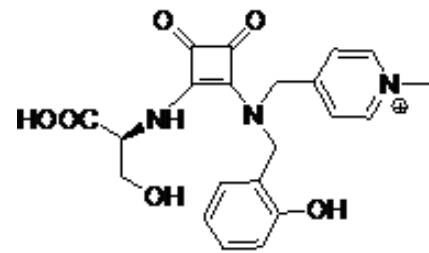
Current Data Parameters
NAME DC-2-69-100-1d
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100220
Time 10.42
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT D2O
NS 32
DS 0
SWH 3591.954 Hz
FIDRES 0.109618 Hz
AQ 4.5613556 sec
RG 574.7
DW 139.200 usec
DE 54.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 9.75 usec
PL1 0.00 dB
SFO1 300.1315007 MHz

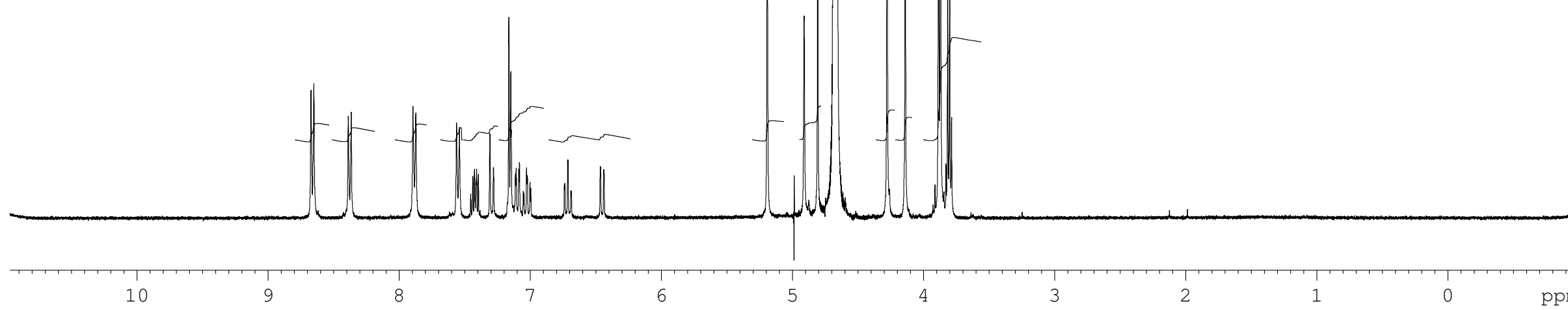
F2 - Processing parameters
SI 32768
SF 300.1300042 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

DC-2-69-100-1d

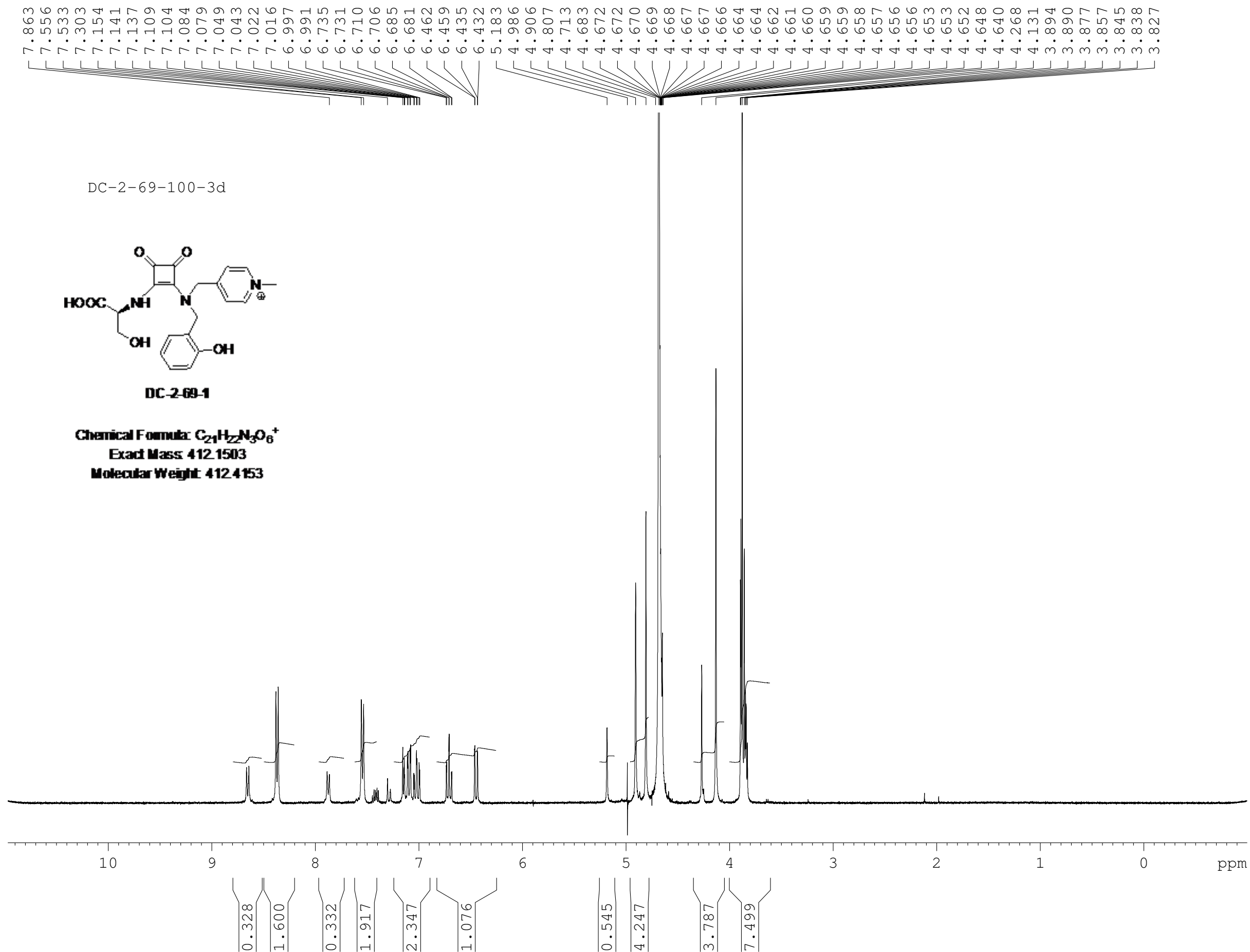


DC-2-69-1

Chemical Formula: $C_{21}H_{22}N_3O_6^+$
Exact Mass: 412.1503
Molecular Weight: 412.4153



1.000
0.572
1.012
0.826
0.921
2.172
0.059
1.248
2.337
2.035
1.530
6.744



Current Data Parameters
 NAME DC-2-69-100-3d
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100222
 Time 9.14
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT D2O
 NS 32
 DS 0
 SWH 3591.954 Hz
 FIDRES 0.109618 Hz
 AQ 4.5613556 sec
 RG 362
 DW 139.200 usec
 DE 54.00 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 9.75 usec
 PL1 0.00 dB
 SFO1 300.1315007 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300042 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

8.386
 8.363
 7.562
 7.540
 7.118
 7.112
 7.093
 7.087
 7.057
 7.051
 7.031
 7.026
 7.005
 6.999
 6.743
 6.739
 6.718
 6.714
 6.693
 6.689
 6.471
 6.468
 6.444
 6.441
 4.914
 4.817
 4.720
 4.715
 4.715
 4.714
 4.712
 4.712
 4.711
 4.710
 4.710
 4.709
 4.708
 4.707
 4.707
 4.706
 4.705
 4.704
 4.704
 4.703
 4.702
 4.701
 4.701
 4.700
 4.699
 4.698
 4.697
 4.696
 4.696
 4.683
 4.653
 4.273
 4.137
 3.911
 3.900
 3.892
 3.886
 3.878
 3.867
 3.859

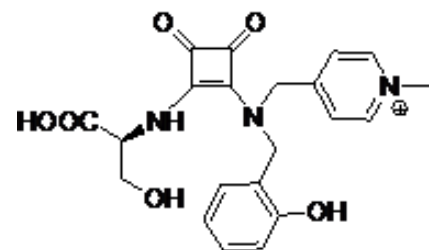
Current Data Parameters
 NAME DC-2-69-100-6d
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100225
 Time 10.34
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT D2O
 NS 32
 DS 0
 SWH 3591.954 Hz
 FIDRES 0.109618 Hz
 AQ 4.5613556 sec
 RG 574.7
 DW 139.200 usec
 DE 54.00 usec
 TE 298.2 K
 D1 1.0000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 9.75 usec
 PL1 0.00 dB
 SFO1 300.1315007 MHz

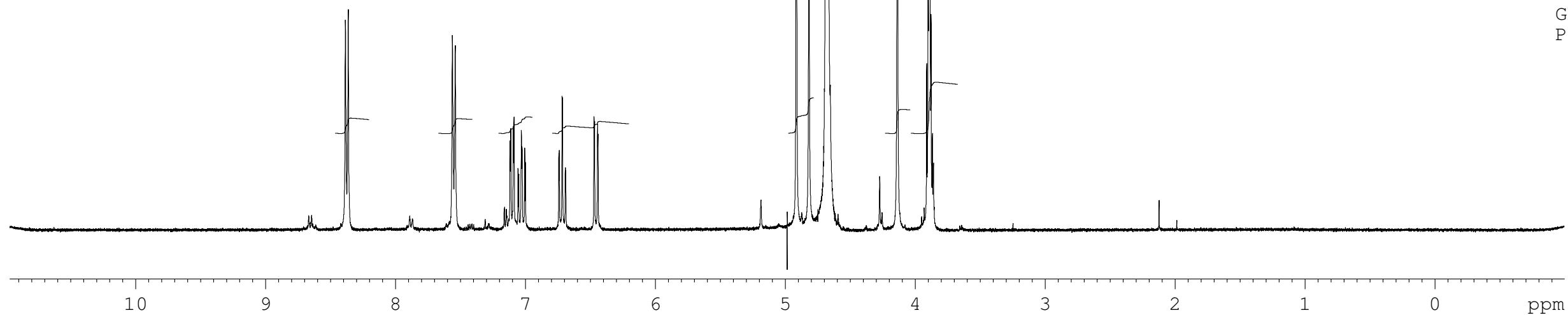
F2 - Processing parameters
 SI 32768
 SF 300.1300042 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

DC-2-69-100-6d



DC-2-69-1

Chemical Formula: $C_{21}H_{22}N_3O_6^+$
 Exact Mass: 412.1503
 Molecular Weight: 412.4153



2.000
 2.050
 2.356
 1.375
 5.246
 3.437
 7.213

Elemental Composition Report

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 80.0
 Selected filters: None

Monoisotopic Mass, Even Electron Ions

23 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-21 H: 0-22 N: 0-3 O: 0-6

File name: dc-2-69-100

Instrument: LCT KC366

Method: ESI-TOF

dc-2-69-100 48 (1.203) AM (Cen,8, 90.00, Ar,4000.0,1222.14,0.70,LS 6); Sm (SG, 2x4.00); Cm (48:74)

Notebook Ref: 24824

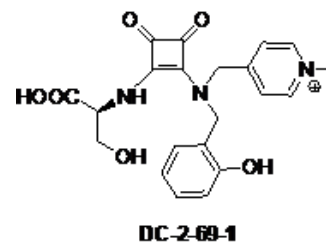
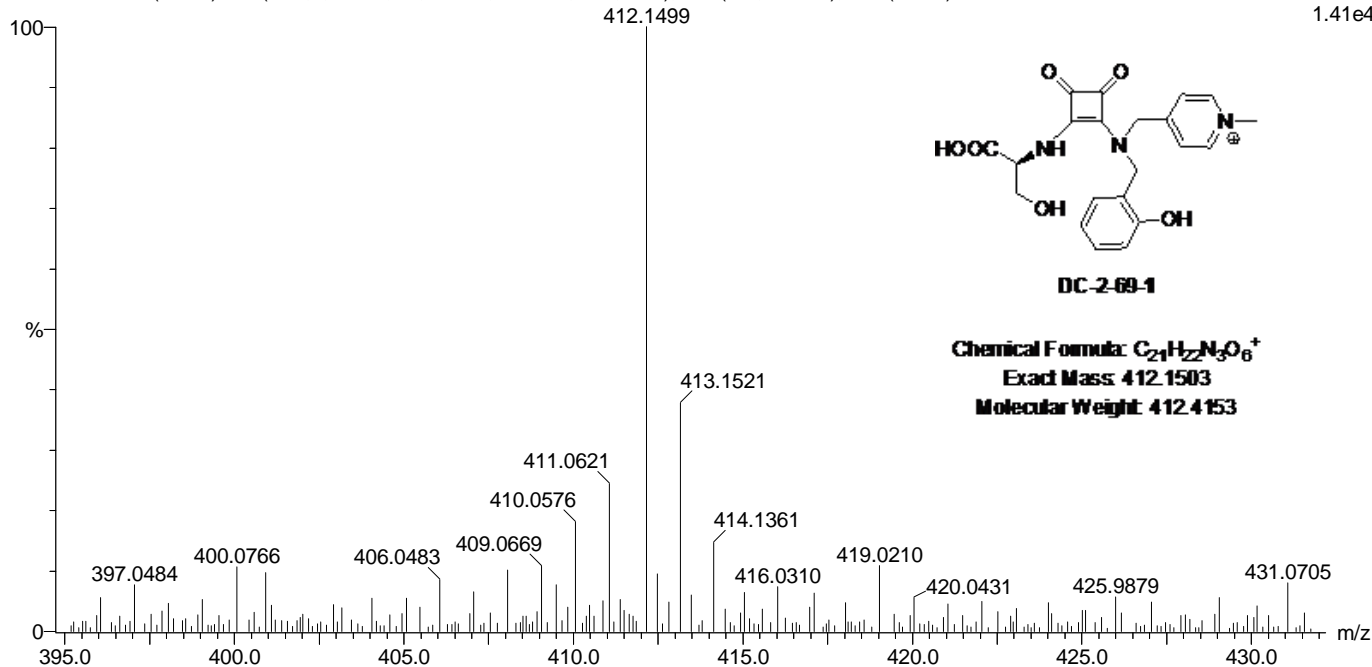
Test name: Accurate Mass

Base Peak Mass: 412.14990234

IU Database#: 24824

06-May-2010 11:47:20

1: TOF MS ES+
 1.41e4

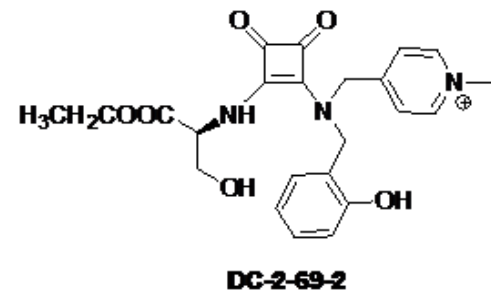


Chemical Formula: C₂₁H₂₂N₃O₆⁺
Exact Mass: 412.1503
Molecular Weight: 412.4153

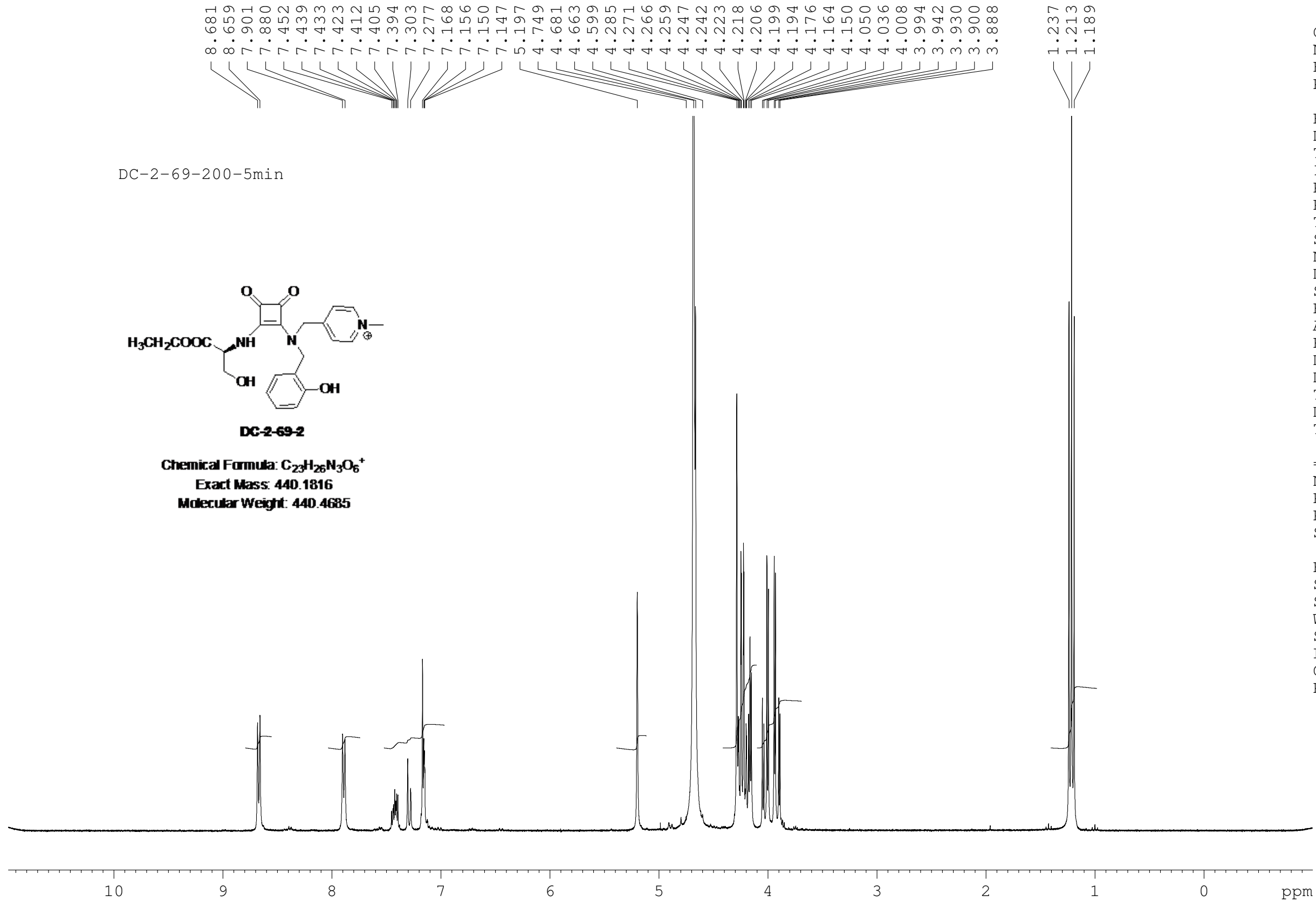
Minimum: 80.00 -1.5
 Maximum: 100.00 5.0 5.0 80.0

Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
412.1499	100.00	412.1509	-1.0	-2.4	12.5	761.1	C21 H22 N3 O6

DC-2-69-200-5min



Chemical Formula: $C_{23}H_{26}N_3O_6^+$
 Exact Mass: 440.1816
 Molecular Weight: 440.4685

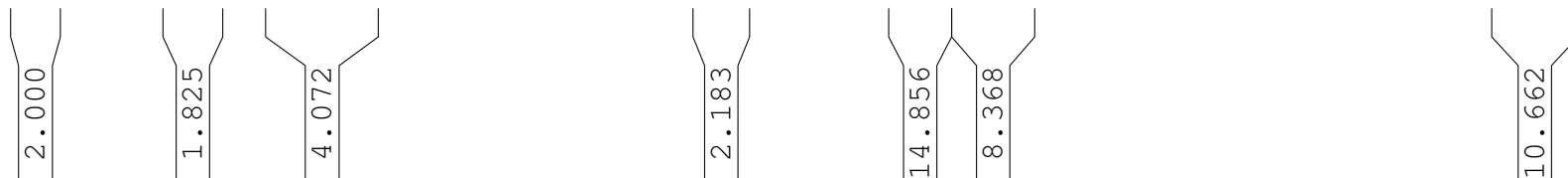


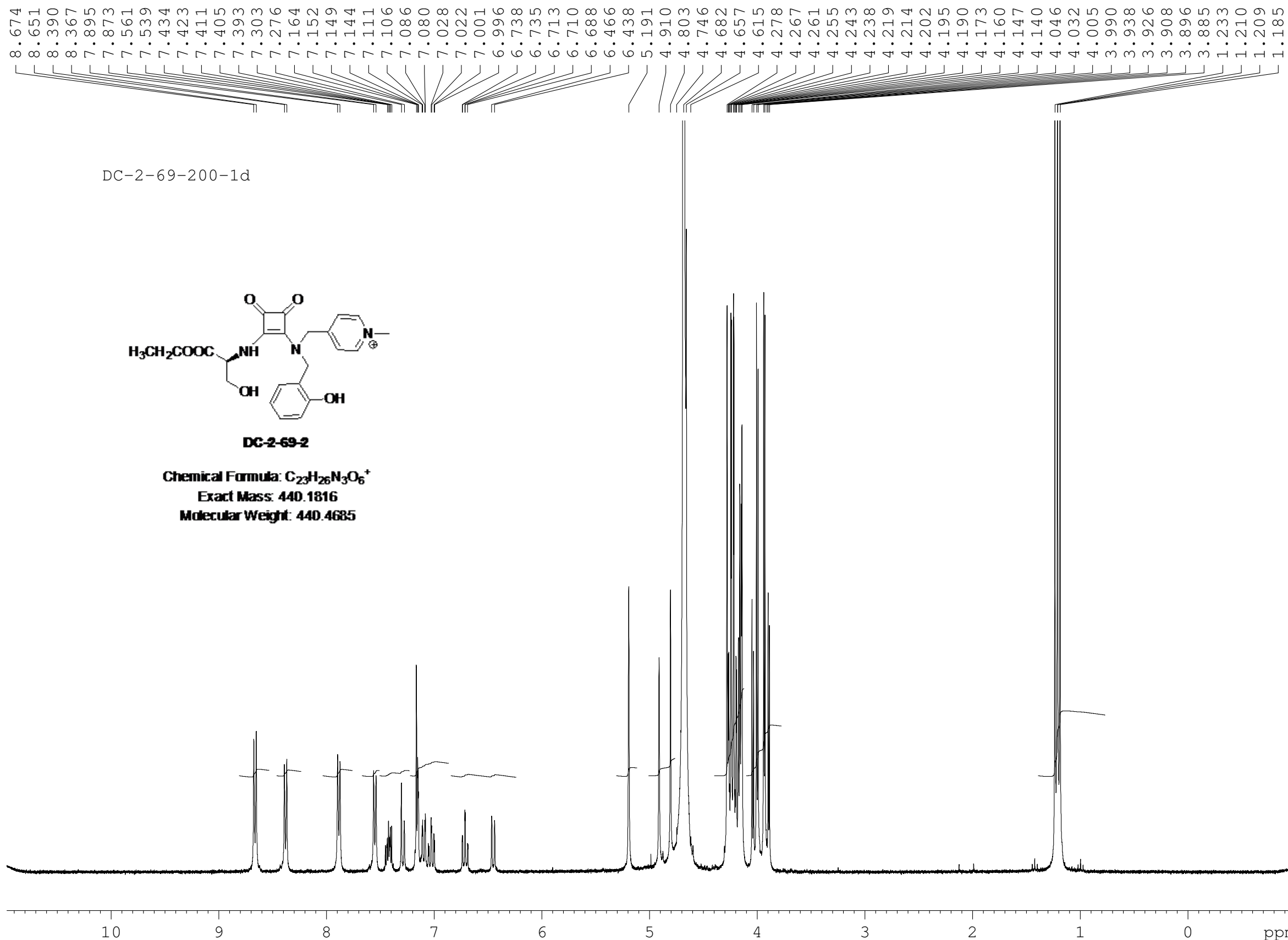
Current Data Parameters
 NAME DC-2-69-200-5min
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100219
 Time 10.15
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT D2O
 NS 32
 DS 0
 SWH 3591.954 Hz
 FIDRES 0.109618 Hz
 AQ 4.5613556 sec
 RG 256
 DW 139.200 usec
 DE 54.00 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 9.75 usec
 PL1 0.00 dB
 SFO1 300.1315007 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300042 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00





Current Data Parameters
 NAME DC-2-69-200-1d
 EXPNO 1
 PROCNO 1

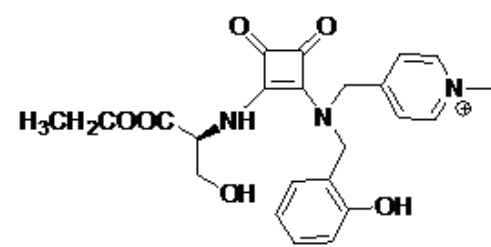
F2 - Acquisition Parameters
 Date_ 20100220
 Time 10.50
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT D2O
 NS 32
 DS 0
 SWH 3591.954 Hz
 FIDRES 0.109618 Hz
 AQ 4.5613556 sec
 RG 362
 DW 139.200 usec
 DE 54.00 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 9.75 usec
 PL1 0.00 dB
 SFO1 300.1315007 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300042 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

8.664
8.642
8.382
8.360
7.887
7.865
7.555
7.533
7.299
7.157
7.142
7.108
7.103
7.083
7.078
7.049
7.043
7.024
7.018
6.997
6.992
6.733
6.708
6.684
6.461
6.434
5.183
4.907
4.805
4.684
4.683
4.648
4.270
4.259
4.254
4.248
4.235
4.230
4.211
4.207
4.194
4.187
4.183
4.165
4.153
4.139
4.132
4.039
4.025
3.997
3.983
3.958
3.930
3.919
3.889
3.877
1.225
1.201
1.178

DC-2-69-200-3d



DC-2-69-2

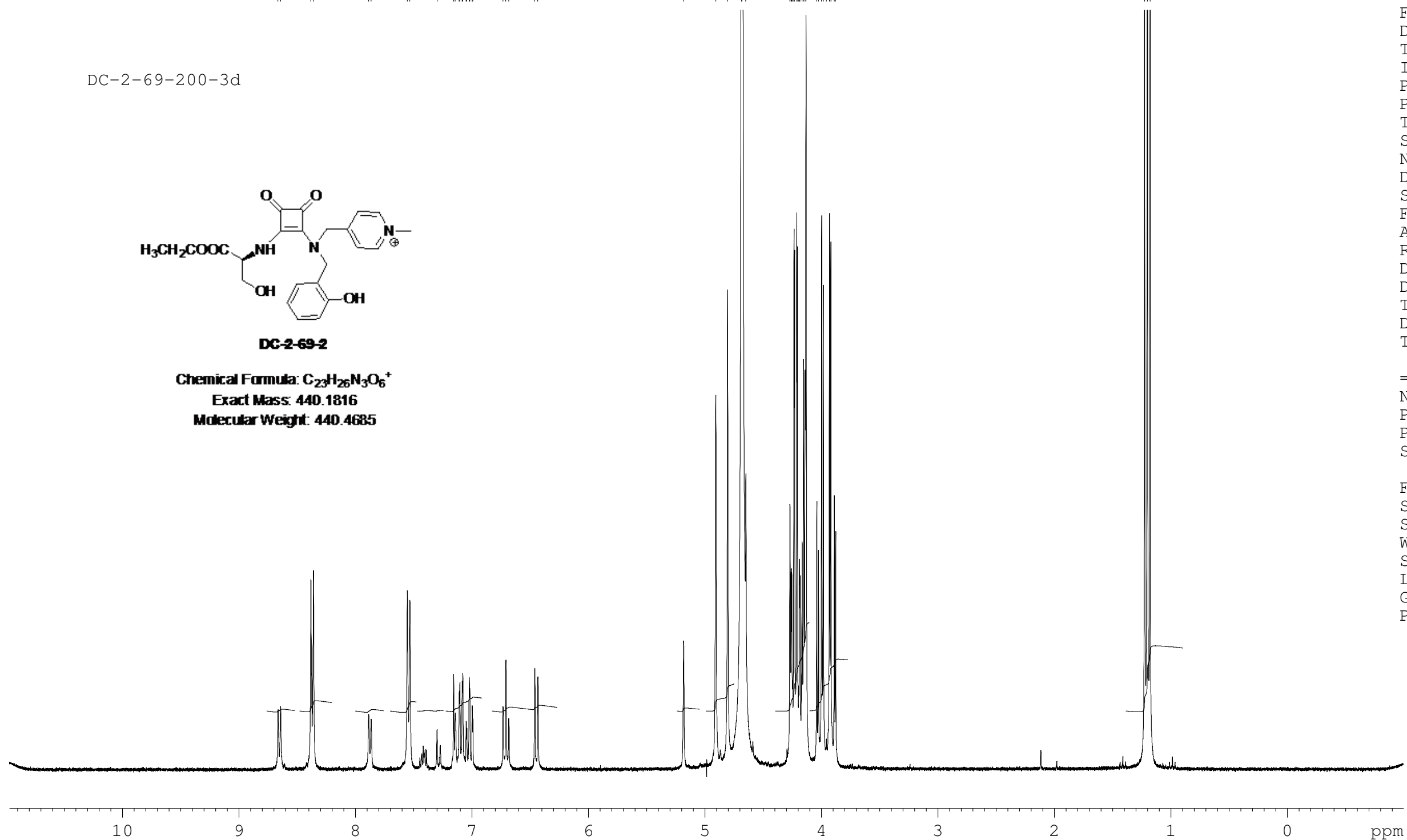
Chemical Formula: C₂₃H₂₆N₃O₆⁺
Exact Mass: 440.1816
Molecular Weight: 440.4685

Current Data Parameters
 NAME DC-2-69-200-3d
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100222
 Time 9.21
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT D2O
 NS 32
 DS 0
 SWH 3591.954 Hz
 FIDRES 0.109618 Hz
 AQ 4.5613556 sec
 RG 322.5
 DW 139.200 usec
 DE 54.00 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 9.75 usec
 PL1 0.00 dB
 SFO1 300.1315007 MHz

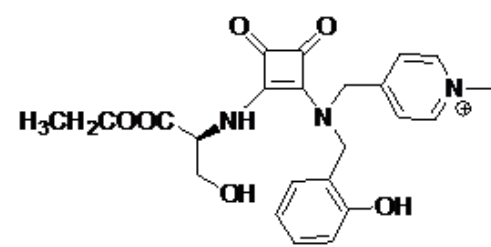
F2 - Processing parameters
 SI 32768
 SF 300.1300042 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00



0.076
1.600
0.049
1.714
0.097
2.457
0.683
0.352
5.189
16.760
9.720
11.944

8.387
 8.365
 7.561
 7.538
 7.116
 7.111
 7.091
 7.086
 7.057
 7.051
 7.032
 7.026
 7.005
 7.000
 6.741
 6.738
 6.716
 6.713
 6.691
 6.688
 6.471
 6.467
 6.444
 6.440
 5.186
 4.914
 4.815
 4.753
 4.683
 4.276
 4.264
 4.259
 4.252
 4.240
 4.236
 4.216
 4.212
 4.200
 4.192
 4.188
 4.170
 4.158
 4.144
 4.137
 4.044
 4.030
 4.003
 3.988
 3.936
 3.924
 3.894
 3.883
 2.122
 1.231
 1.207
 1.183

DC-2-69-200-6d



DC-2-69-2

Chemical Formula: C₂₃H₂₆N₃O₆⁺

Exact Mass: 440.1816

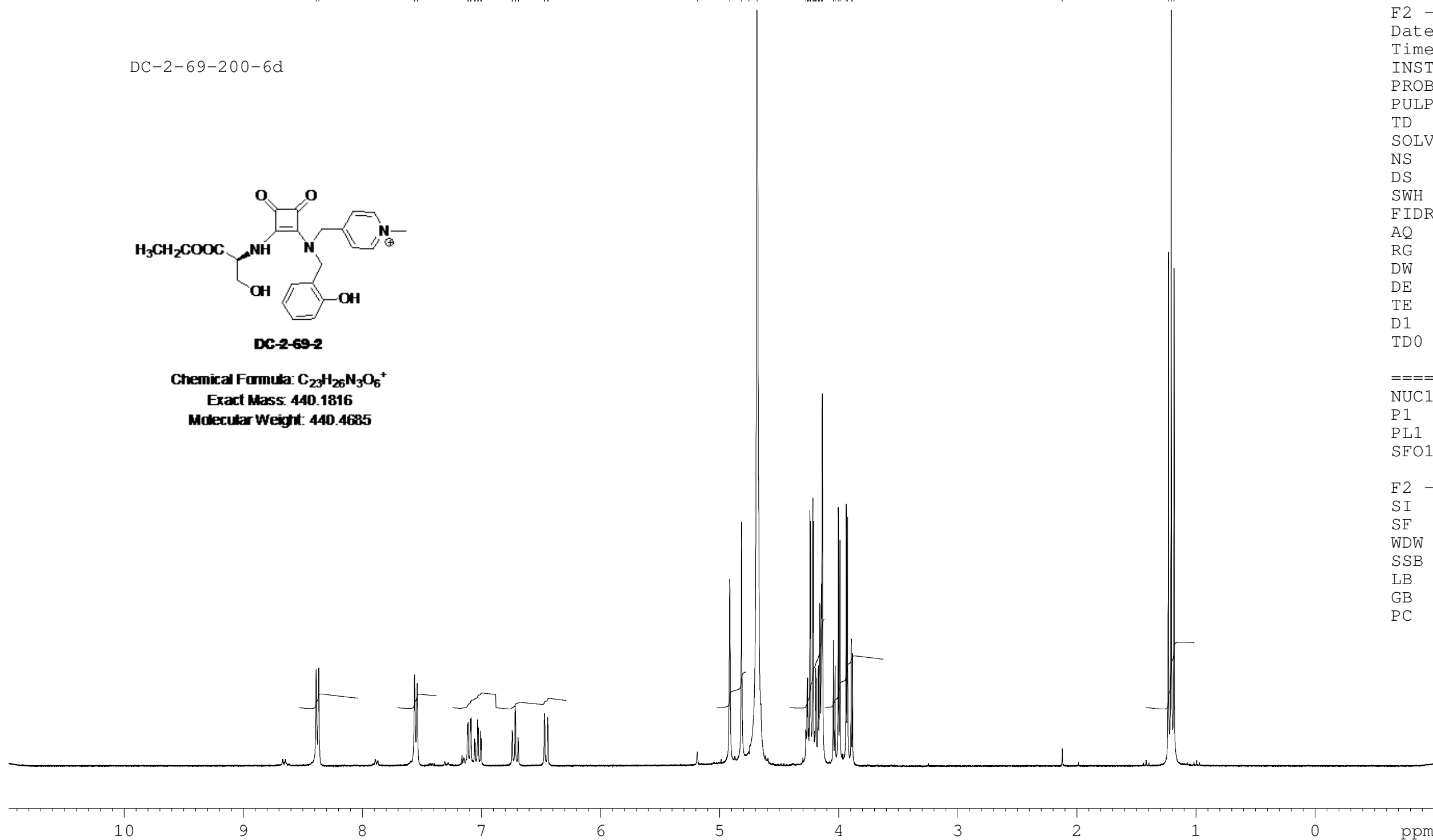
Molecular Weight: 440.4685

Current Data Parameters
 NAME DC-2-69-200-6d
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100225
 Time 10.42
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT D2O
 NS 32
 DS 0
 SWH 3591.954 Hz
 FIDRES 0.109618 Hz
 AQ 4.5613556 sec
 RG 406.4
 DW 139.200 usec
 DE 54.00 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 9.75 usec
 PL1 0.00 dB
 SFO1 300.1315007 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300042 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00



2.000
 2.539
 2.646
 1.515
 7.524
 18.566
 10.167
 13.635

Elemental Composition Report

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 80.0
 Selected filters: None

Monoisotopic Mass, Even Electron Ions

23 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-23 H: 0-26 N: 0-3 O: 0-6

File name: dc-2-69-200

Instrument: LCT KC366

Method: ESI-TOF

dc-2-69-200 44 (1.102) AM (Cen,8, 90.00, Ar,4000.0,1222.14,0.70,LS 6); Sm (SG, 2x4.00); Cm (44:49)

Notebook Ref: 24825

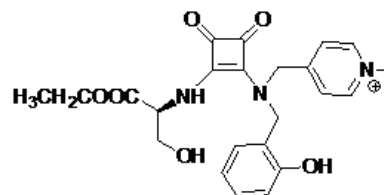
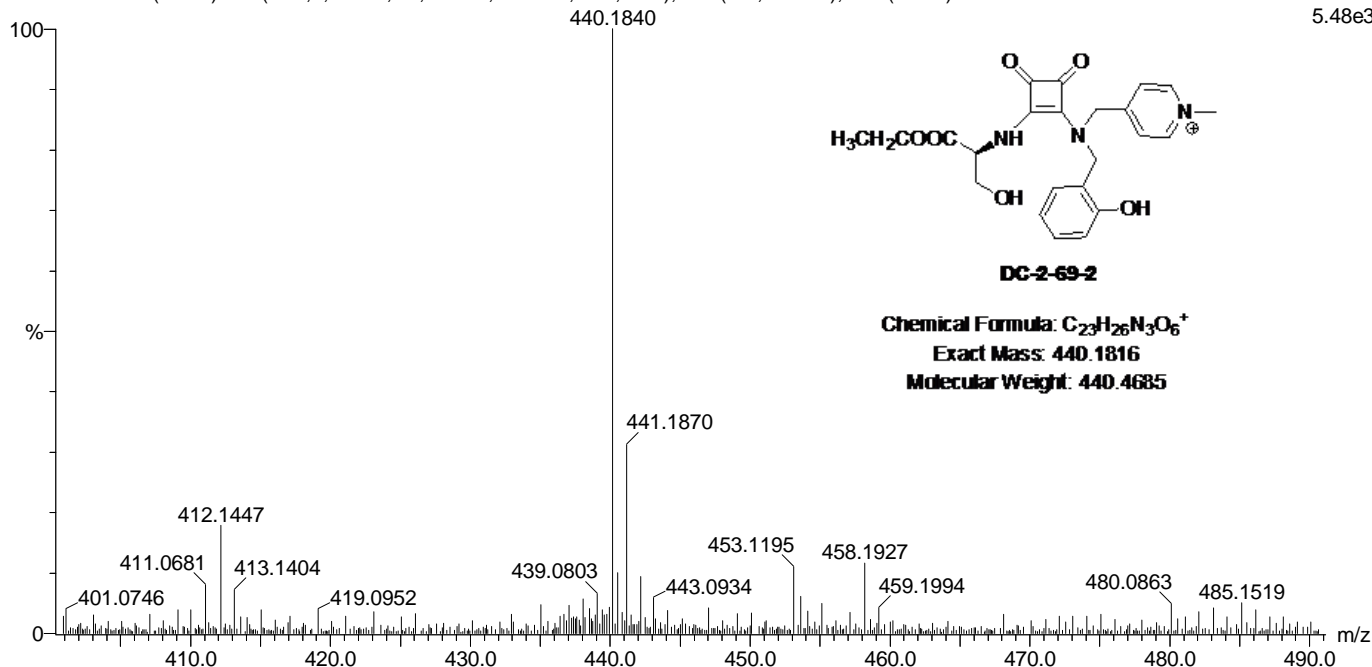
Test name: Accurate Mass

Base Peak Mass: 440.1839048

IU Database#: 24825

06-May-2010 11:51:31

1: TOF MS ES+
 5.48e3



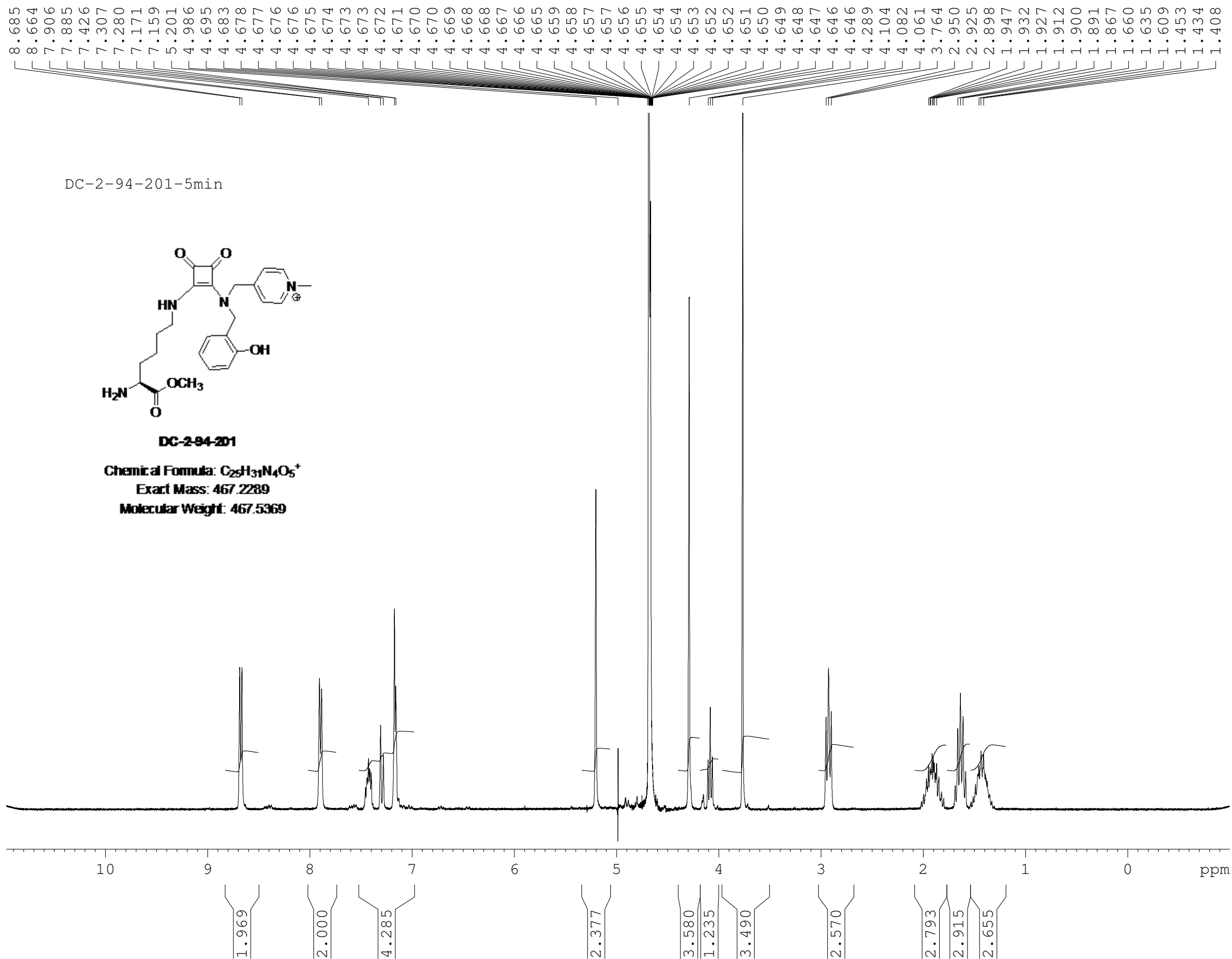
DC-2-69-2

Chemical Formula: C₂₃H₂₆N₃O₆⁺

Exact Mass: 440.1816

Molecular Weight: 440.4685

Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
440.1840	100.00	440.1822	1.8	4.1	12.5	66.5	C ₂₃ H ₂₆ N ₃ O ₆

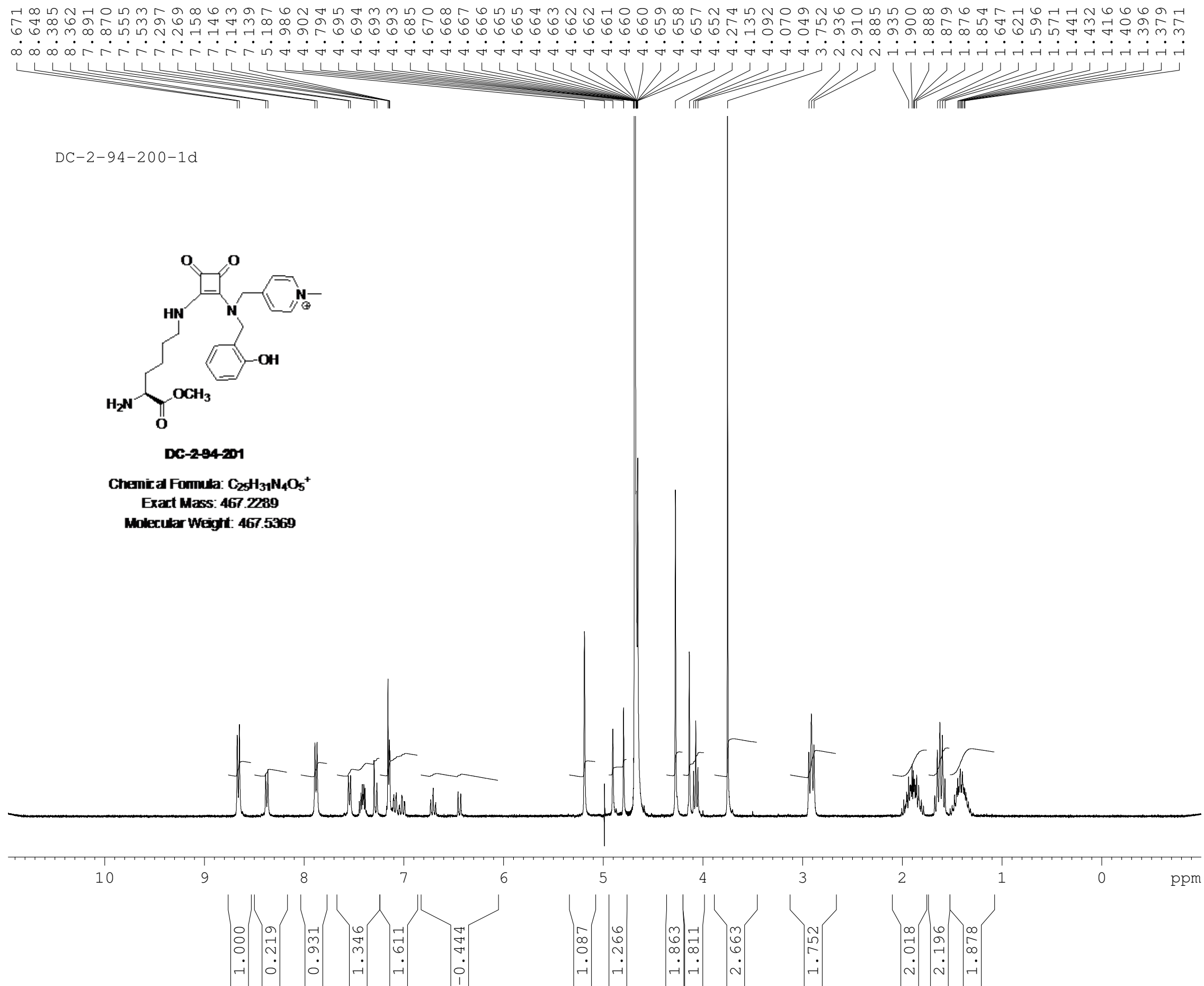


Current Data Parameters
 NAME DC-2-94-201-5min
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100226
 Time 16.13
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT D2O
 NS 32
 DS 0
 SWH 3591.954 Hz
 FIDRES 0.109618 Hz
 AQ 4.5613556 sec
 RG 256
 DW 139.200 usec
 DE 54.00 usec
 TE 299.2 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 9.75 usec
 PL1 0.00 dB
 SFO1 300.1315007 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300042 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME DC-2-94-201-1d
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100227
 Time 11.41
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT D2O
 NS 16
 DS 0
 SWH 3591.954 Hz
 FIDRES 0.109618 Hz
 AQ 4.5613556 sec
 RG 512
 DW 139.200 usec
 DE 54.00 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 9.75 usec
 PL1 0.00 dB
 SFO1 300.1315007 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300042 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

8.391
 8.368
 7.563
 7.541
 7.086
 6.719
 6.715
 6.469
 5.190
 4.986
 4.915
 4.813
 4.692
 4.691
 4.690
 4.689
 4.689
 4.685
 4.683
 4.672
 4.671
 4.670
 4.670
 4.669
 4.668
 4.668
 4.667
 4.666
 4.665
 4.665
 4.664
 4.663
 4.662
 4.662
 4.661
 4.660
 4.659
 4.659
 4.658
 4.657
 4.657
 4.656
 4.655
 4.654
 4.652
 4.652
 4.651
 4.650
 4.649
 4.649
 4.648
 4.647
 4.646
 4.646
 4.644
 4.643
 4.277
 4.141
 4.097
 4.076
 4.054
 3.758
 2.942
 2.917
 2.891
 1.906
 1.894
 1.653
 1.627
 1.602
 1.422

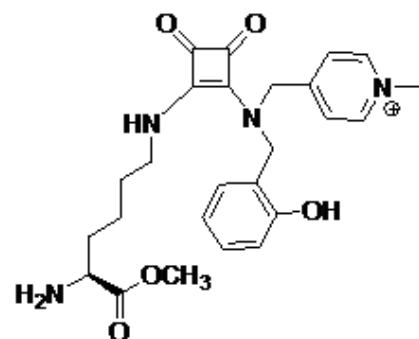
Current Data Parameters
 NAME DC-2-94-201-3d
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100301
 Time 18.32
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT D2O
 NS 16
 DS 0
 SWH 3591.954 Hz
 FIDRES 0.109618 Hz
 AQ 4.5613556 sec
 RG 456.1
 DW 139.200 usec
 DE 54.00 usec
 TE 299.2 K
 D1 1.0000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 9.75 usec
 PL1 0.00 dB
 SFO1 300.1315007 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300042 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

DC-2-94-201-3d

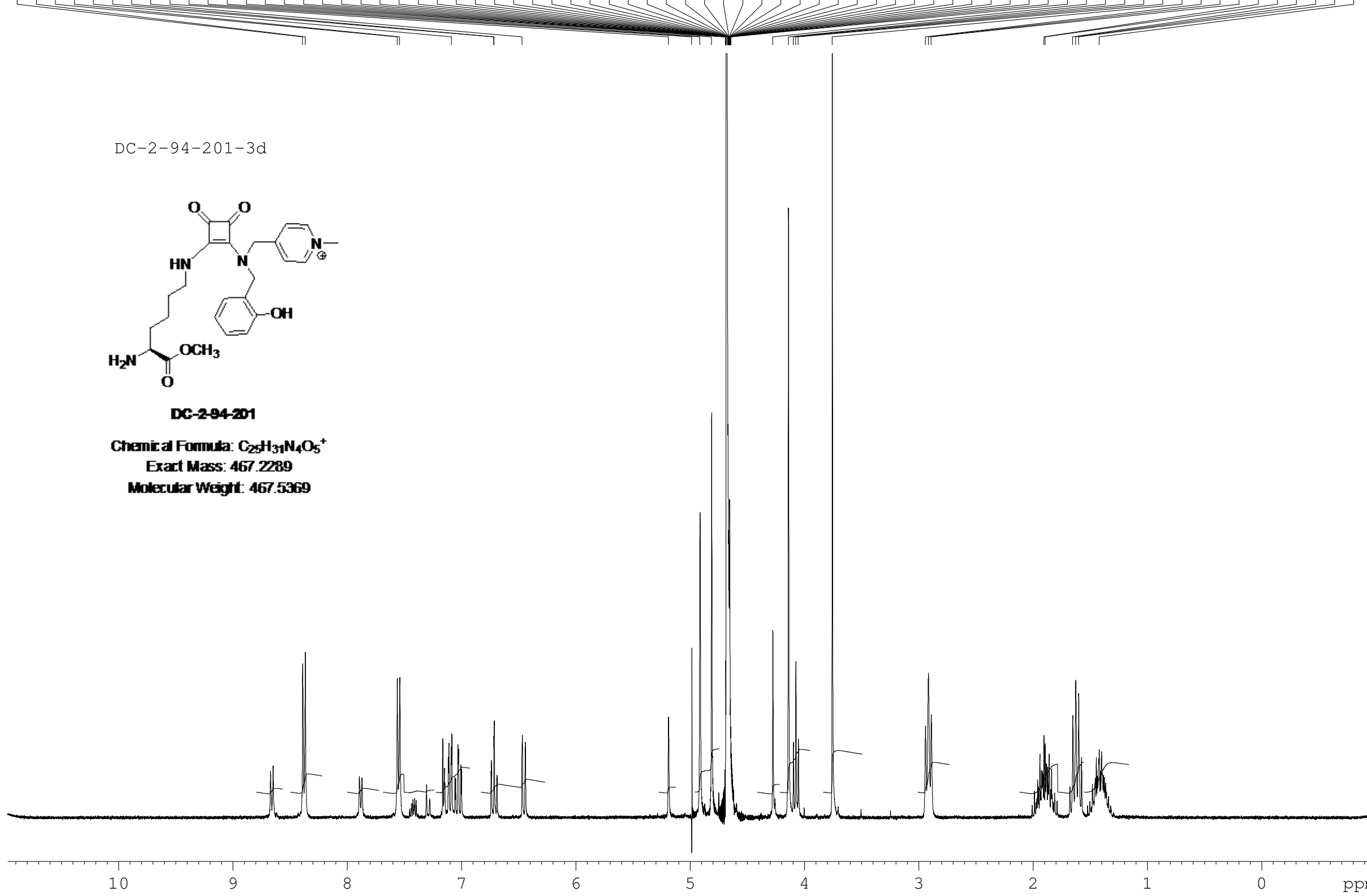


DC-2-94-201

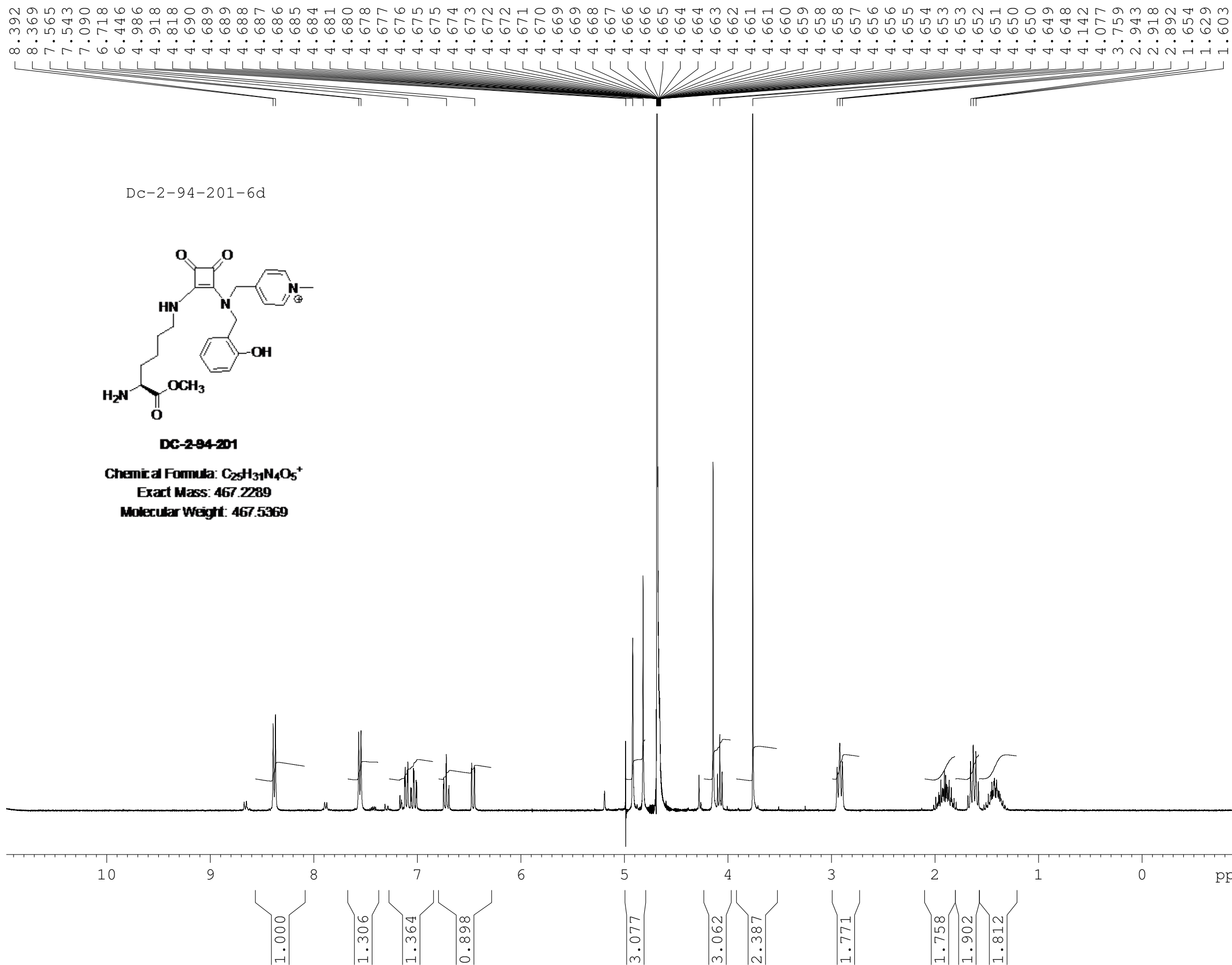
Chemical Formula: C₂₅H₃₁N₄O₅⁺

Exact Mass: 467.2289

Molecular Weight: 467.5369



0.213
 1.172
 0.121
 1.260
 0.129
 1.736
 0.717
 0.344
 3.172
 0.546
 3.025
 2.764
 1.999
 2.022
 2.172
 2.000



Current Data Parameters
 NAME Dc-2-94-201-6d
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100303
 Time 18.31
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT D2O
 NS 16
 DS 0
 SWH 3591.954 Hz
 FIDRES 0.109618 Hz
 AQ 4.5613556 sec
 RG 406.4
 DW 139.200 usec
 DE 54.00 usec
 TE 299.2 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 9.75 usec
 PL1 0.00 dB
 SFO1 300.1315007 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300042 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

Elemental Composition Report

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 80.0
 Selected filters: None

Monoisotopic Mass, Even Electron Ions

25 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-25 H: 0-31 N: 0-4 O: 0-5

File name: dc-2-94-201

Instrument: LCT KC366

Method: ESI-TOF

dc-2-94-201 30 (0.752) AM (Cen,8, 90.00, Ar,4000.0,1222.14,0.70,LS 6); Sm (SG, 2x4.00); Cm (29:36)

Notebook Ref: 24820

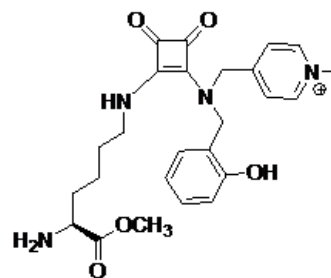
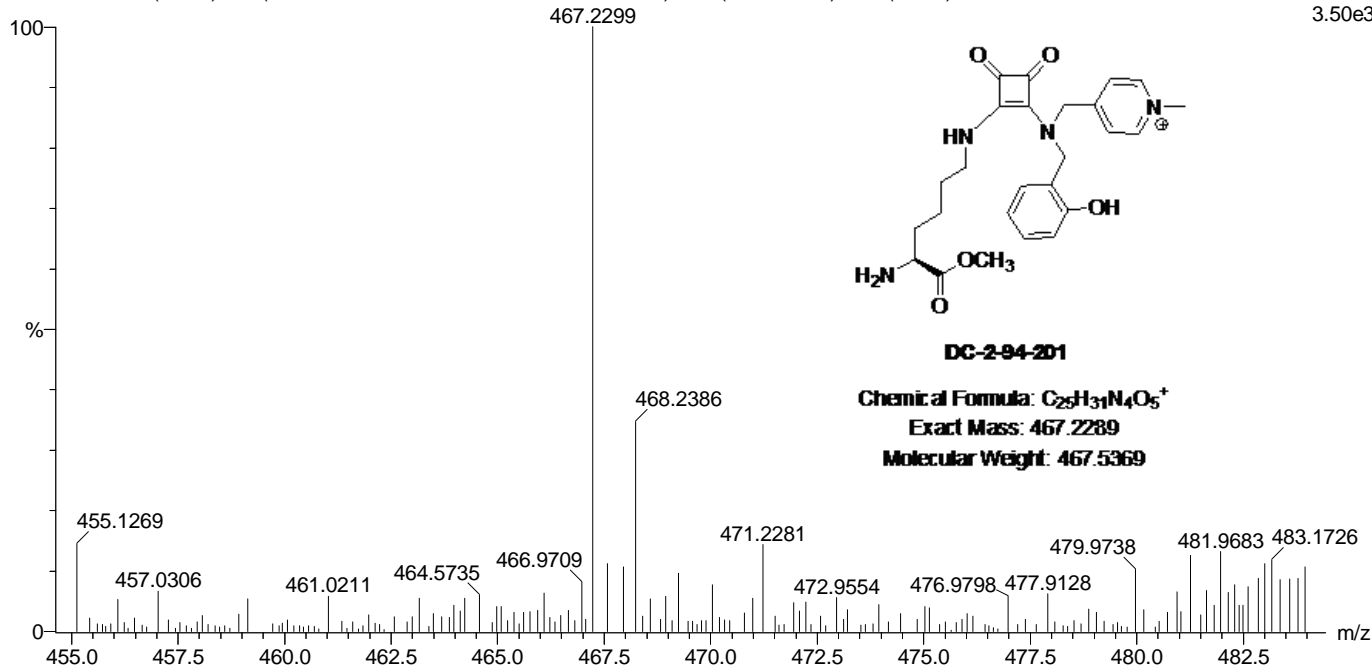
Test name: Accurate Mass

Base Peak Mass: 467.22994995

IU Database#: 24820

06-May-2010 11:30:37

1: TOF MS ES+
 3.50e3



DC-2-94-201

Chemical Formula: C₂₅H₃₁N₄O₅⁺

Exact Mass: 467.2289

Molecular Weight: 467.5369

Minimum: 80.00
 Maximum: 100.00

Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
467.2299	100.00	467.2294	0.5	1.1	12.5	38.6	C ₂₅ H ₃₁ N ₄ O ₅

8.651
 8.628
 7.854
 7.833
 7.606
 7.604
 7.580
 7.578
 7.408
 7.405
 7.381
 7.378
 7.296
 7.187
 7.165
 7.161
 7.147
 7.090
 7.066
 7.063
 5.127
 4.986
 4.690
 4.689
 4.689
 4.688
 4.687
 4.684
 4.682
 4.679
 4.678
 4.678
 4.677
 4.676
 4.675
 4.675
 4.674
 4.673
 4.672
 4.672
 4.671
 4.670
 4.669
 4.669
 4.668
 4.667
 4.666
 4.666
 4.665
 4.664
 4.664
 4.663
 4.662
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 4.661
 4.660
 4.659
 4.658
 4.658
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 4.653
 4.597
 4.266
 3.341
 3.325
 3.212
 3.185

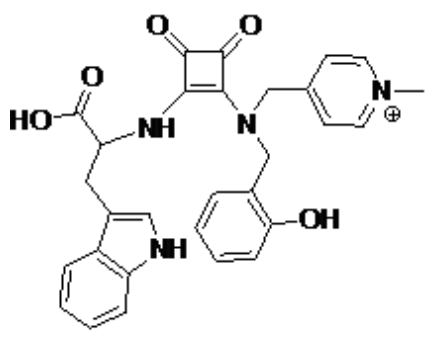
Current Data Parameters
 NAME DC-2-91-101-5min
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100226
 Time 9.14
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT D2O
 NS 32
 DS 0
 SWH 3591.954 Hz
 FIDRES 0.109618 Hz
 AQ 4.5613556 sec
 RG 406.4
 DW 139.200 usec
 DE 54.00 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 9.75 usec
 PL1 0.00 dB
 SFO1 300.1315007 MHz

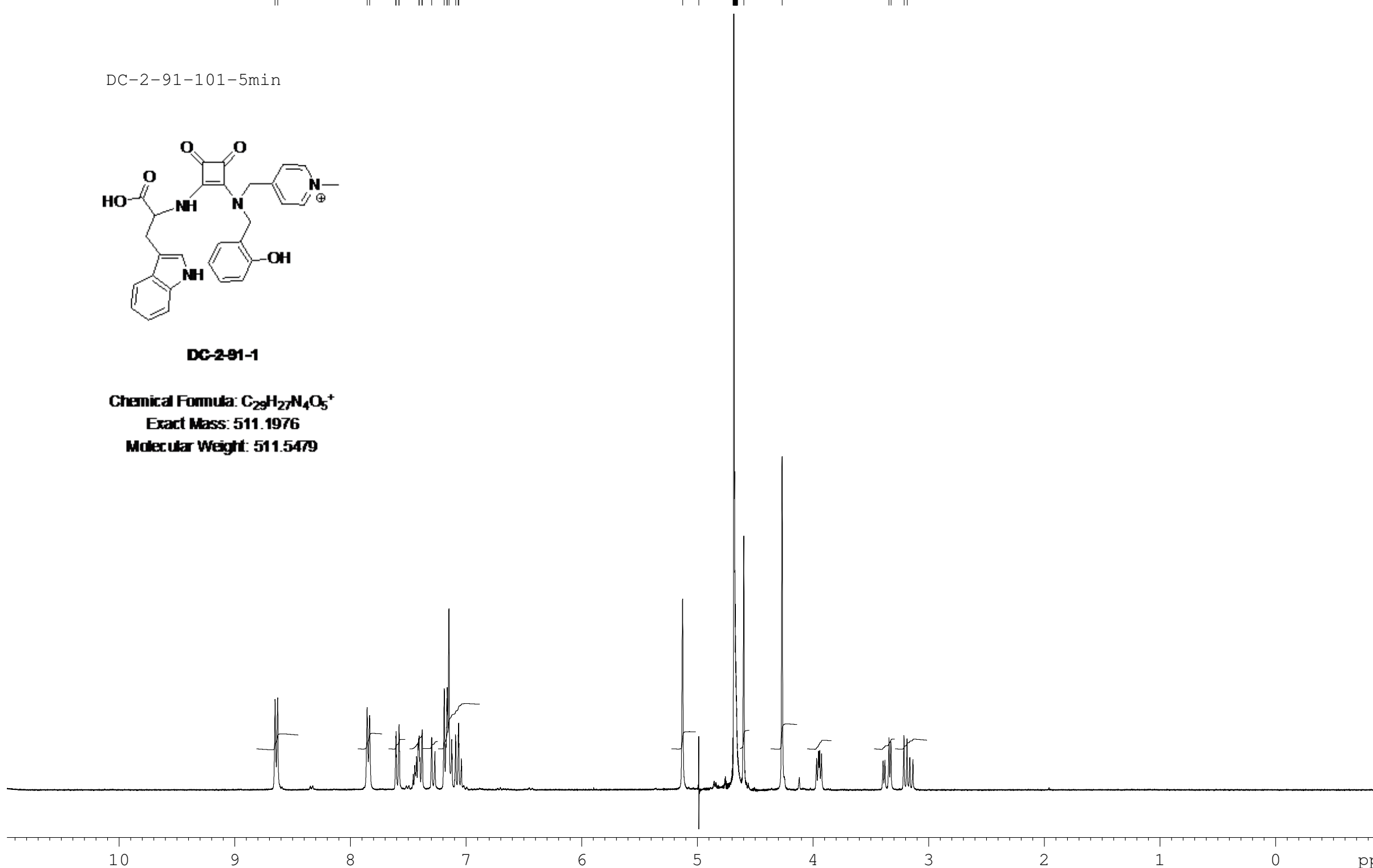
F2 - Processing parameters
 SI 32768
 SF 300.1300042 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

DC-2-91-101-5min

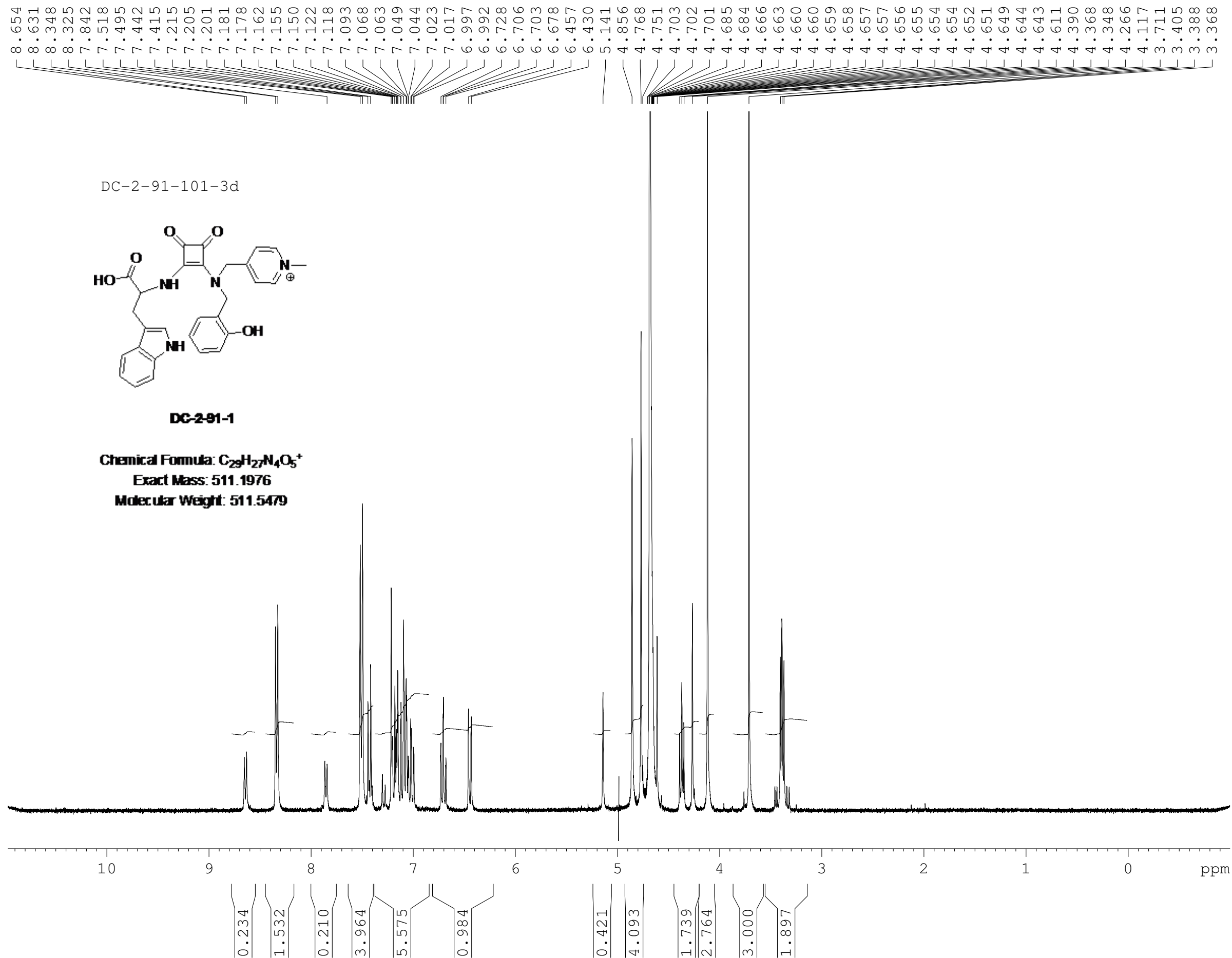


DC-2-91-1

Chemical Formula: C₂₉H₂₇N₄O₅⁺
Exact Mass: 511.1976
Molecular Weight: 511.5479



1.715
 1.860
 1.172
 1.959
 0.891
 5.552
 2.123
 2.318
 3.014
 1.000
 1.197
 1.067



Current Data Parameters
 NAME DC-2-91-101-3d
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100301
 Time 18.18
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT D2O
 NS 16
 DS 0
 SWH 3591.954 Hz
 FIDRES 0.109618 Hz
 AQ 4.5613556 sec
 RG 512
 DW 139.200 usec
 DE 54.00 usec
 TE 299.2 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 9.75 usec
 PL1 0.00 dB
 SFO1 300.1315007 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300042 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

8.338
 8.316
 7.614
 7.611
 7.589
 7.587
 7.585
 7.511
 7.489
 7.439
 7.437
 7.416
 7.412
 7.410
 7.221
 7.203
 7.199
 7.179
 7.175
 7.152
 7.151
 7.148
 7.116
 7.115
 7.112
 7.093
 7.089
 7.086
 7.069
 7.064
 7.063
 7.051
 7.045
 7.025
 7.019
 6.999
 6.994
 6.735
 6.731
 6.710
 6.706
 6.681
 6.463
 6.460
 6.436
 6.433
 4.852
 4.771
 4.694
 4.692
 4.692
 4.691
 4.690
 4.685
 4.683
 4.597
 4.262
 4.175
 4.158
 4.150
 4.133
 4.113
 3.446
 3.429
 3.395
 3.378
 3.322
 3.297
 3.271
 3.245

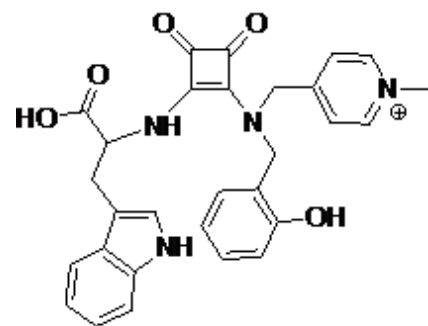
Current Data Parameters
 NAME Dc-2-91-101-6d
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100303
 Time 18.18
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT D2O
 NS 16
 DS 0
 SWH 3591.954 Hz
 FIDRES 0.109618 Hz
 AQ 4.5613556 sec
 RG 574.7
 DW 139.200 usec
 DE 54.00 usec
 TE 299.2 K
 D1 1.0000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 9.75 usec
 PL1 0.00 dB
 SFO1 300.1315007 MHz

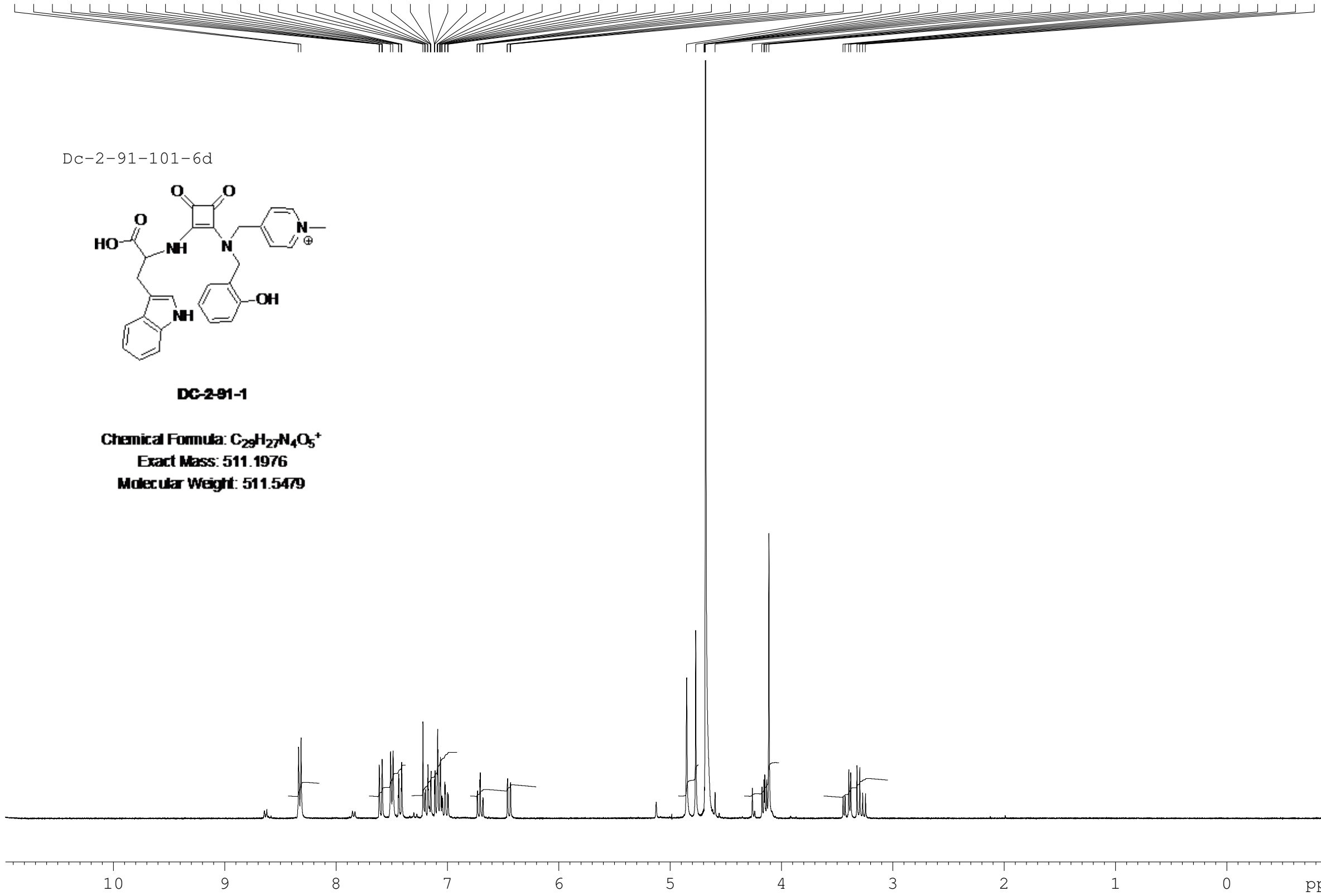
F2 - Processing parameters
 SI 32768
 SF 300.1300042 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

Dc-2-91-101-6d



DC-2-91-1

Chemical Formula: C₂₉H₂₇N₄O₅⁺
Exact Mass: 511.1976
Molecular Weight: 511.5479



1.594
 3.899
 5.504
 1.149
 3.929
 4.194
 2.000

Elemental Composition Report

Multiple Mass Analysis: 2 mass(es) processed

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 80.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

82 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-29 H: 0-27 N: 0-4 O: 0-5 Na: 0-1

File name: dc-2-91-101

Instrument: LCT KC366

Method: ESI-TOF

dc-2-91-101 31 (0.786) AM (Cen,6, 90.00, Ar,4000.0,922.36,0.70,LS 4); Sm (SG, 2x4.00); Cm (27:50)

Notebook Ref: 24689

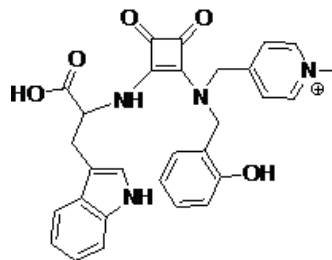
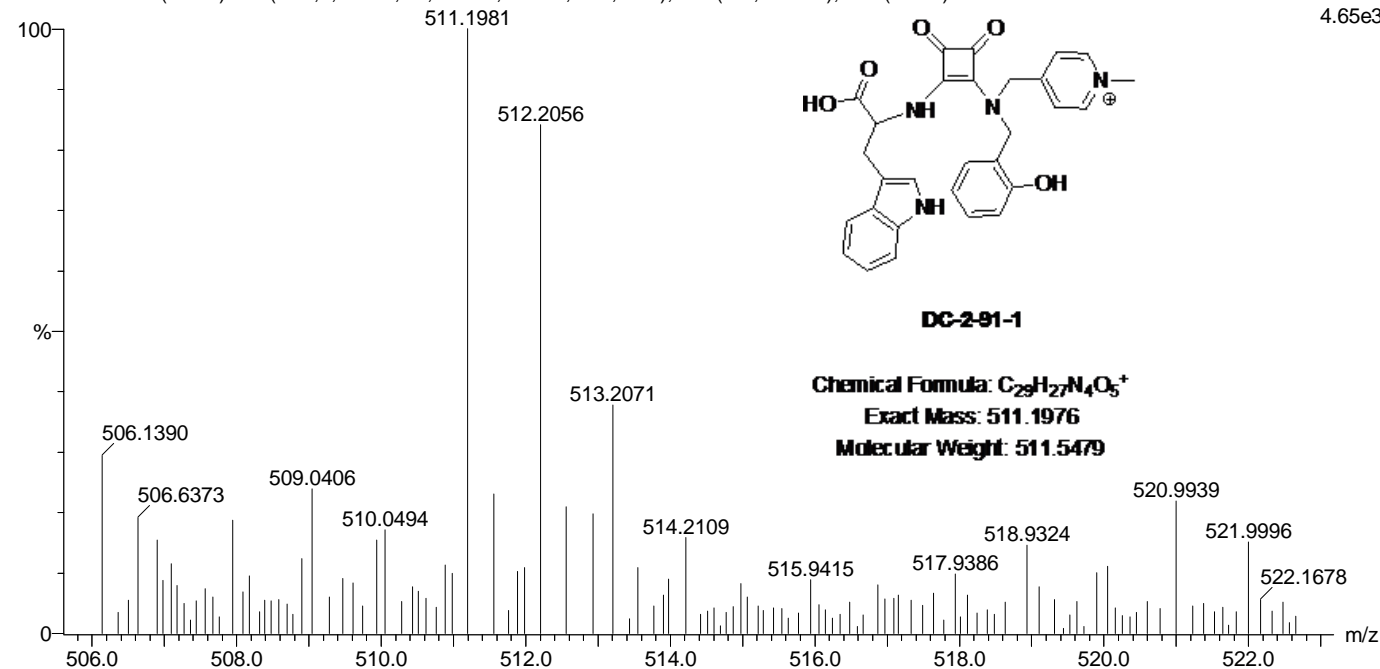
Test name: Accurate Mass

Base Peak Mass: 511.19808960

IU Database#: 24689

28-Apr-2010 11:56:47

1: TOF MS ES+
4.65e3



DC-2-91-1

Chemical Formula: C₂₉H₂₇N₄O₅⁺

Exact Mass: 511.1976

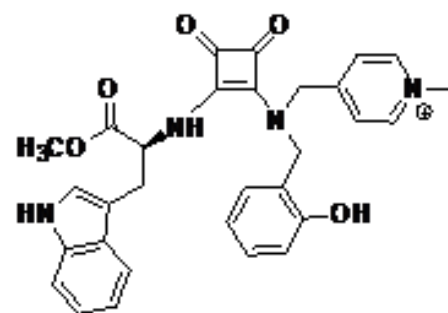
Molecular Weight: 511.5479

Minimum: 80.00 -1.5
 Maximum: 100.00 5.0 10.0 80.0

Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
511.1981	100.00	511.1981	0.0	0.0	18.5	1145.0	C29 H27 N4 O5
512.2056	84.11	---					

8.664
 8.641
 7.873
 7.851
 7.506
 7.483
 7.480
 7.427
 7.412
 7.403
 7.400
 7.397
 7.298
 7.208
 7.165
 7.151
 7.143
 7.111
 7.107
 7.084
 5.150
 4.696
 4.695
 4.694
 4.694
 4.693
 4.685
 4.682
 4.677
 4.676
 4.675
 4.675
 4.674
 4.673
 4.672
 4.672
 4.671
 4.670
 4.669
 4.669
 4.668
 4.667
 4.667
 4.666
 4.665
 4.664
 4.664
 4.663
 4.662
 4.661
 4.661
 4.660
 4.659
 4.658
 4.658
 4.657
 4.656
 4.656
 4.655
 4.654
 4.654
 4.620
 4.368
 4.365
 4.345
 4.274
 3.713
 3.397
 3.382
 3.379
 3.361

DC-2-91-201-5min



DC-2-91-201

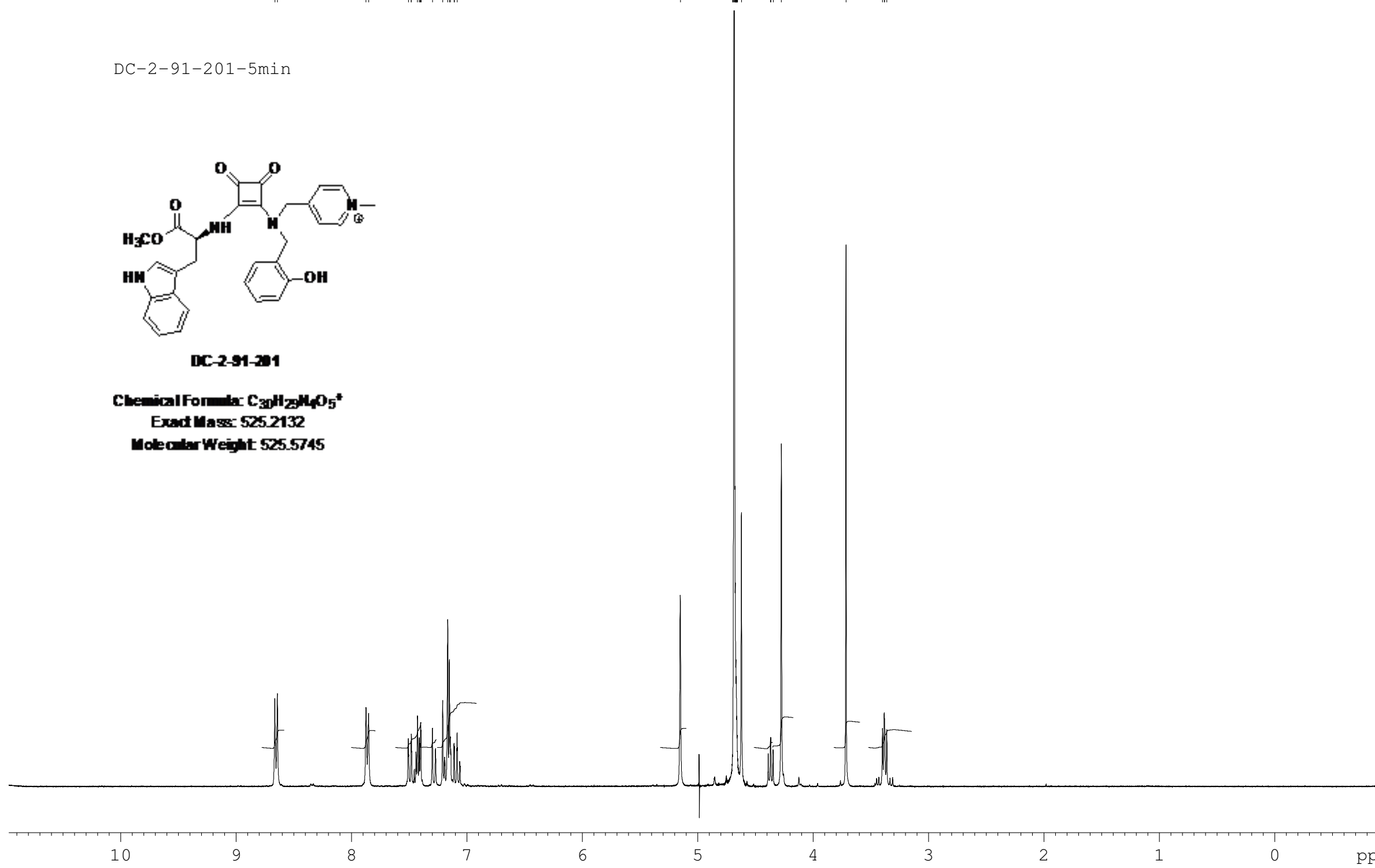
Chemical Formula: $C_{23}H_{23}N_4O_5^+$
 Exact Mass: 525.2132
 Molecular Weight: 525.5745

Current Data Parameters
 NAME DC-2-91-201-5min
 EXPNO 1
 PROCNO 1

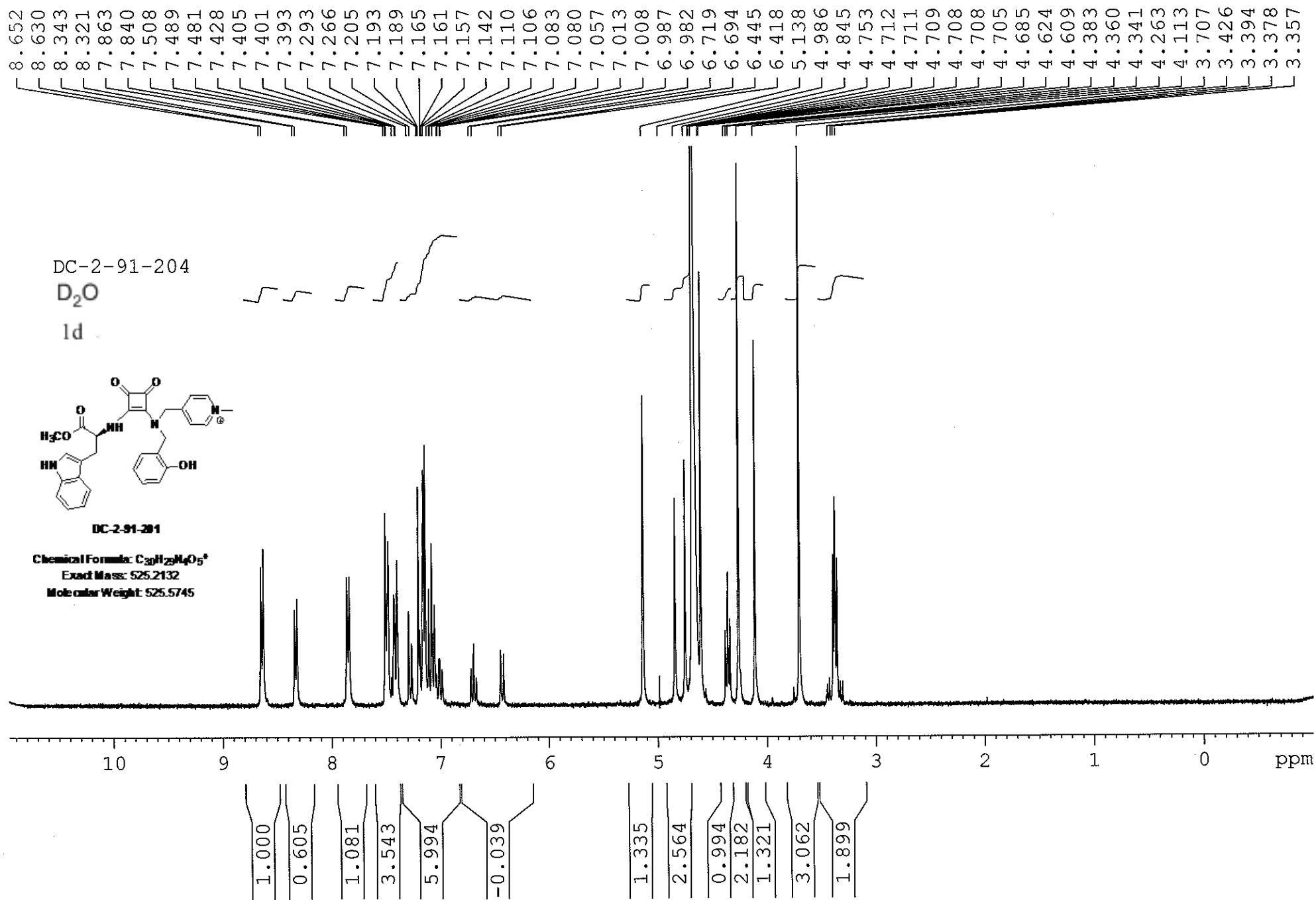
F2 - Acquisition Parameters
 Date_ 20100226
 Time 9.21
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT D2O
 NS 32
 DS 0
 SWH 3591.954 Hz
 FIDRES 0.109618 Hz
 AQ 4.5613556 sec
 RG 574.7
 DW 139.200 usec
 DE 54.00 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

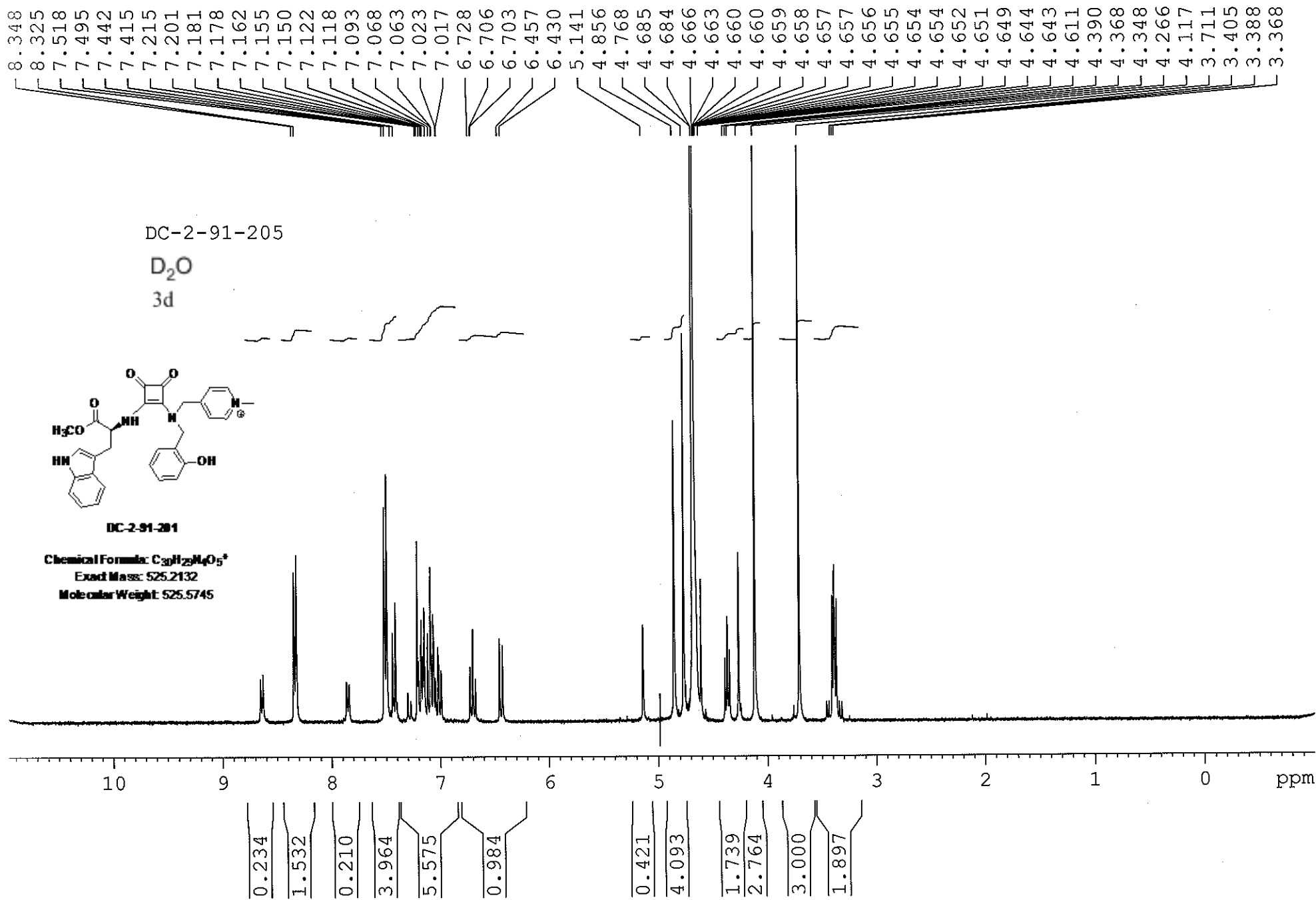
==== CHANNEL f1 =====
 NUC1 1H
 P1 9.75 usec
 PL1 0.00 dB
 SFO1 300.1315007 MHz

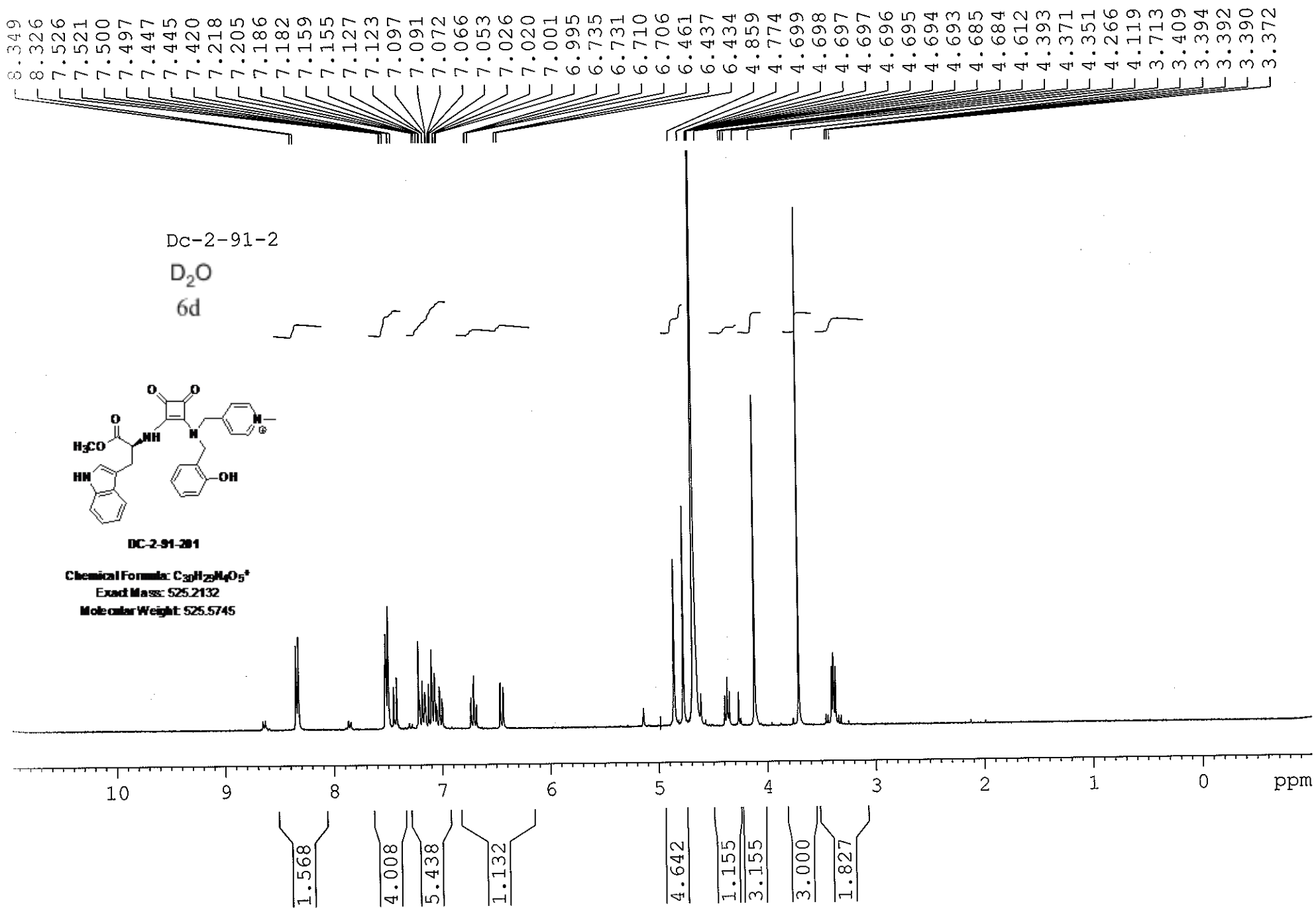
F2 - Processing parameters
 SI 32768
 SF 300.1300042 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00



2.042
 1.980
 2.961
 0.915
 5.241
 2.254
 0.653
 3.550
 3.000
 1.906







Elemental Composition Report

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 80.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

22 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-30 H: 0-29 N: 0-4 O: 0-5

File name: dc-2-91-201

Instrument: LCT KC366

Method: ESI-TOF

dc-2-91-201 34 (0.853) AM (Cen,8, 90.00, Ar,4000.0,1222.14,0.70,LS 6); Sm (SG, 2x4.00); Cm (27:42)

Notebook Ref: 24822

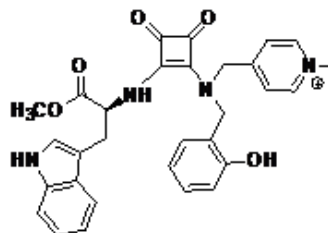
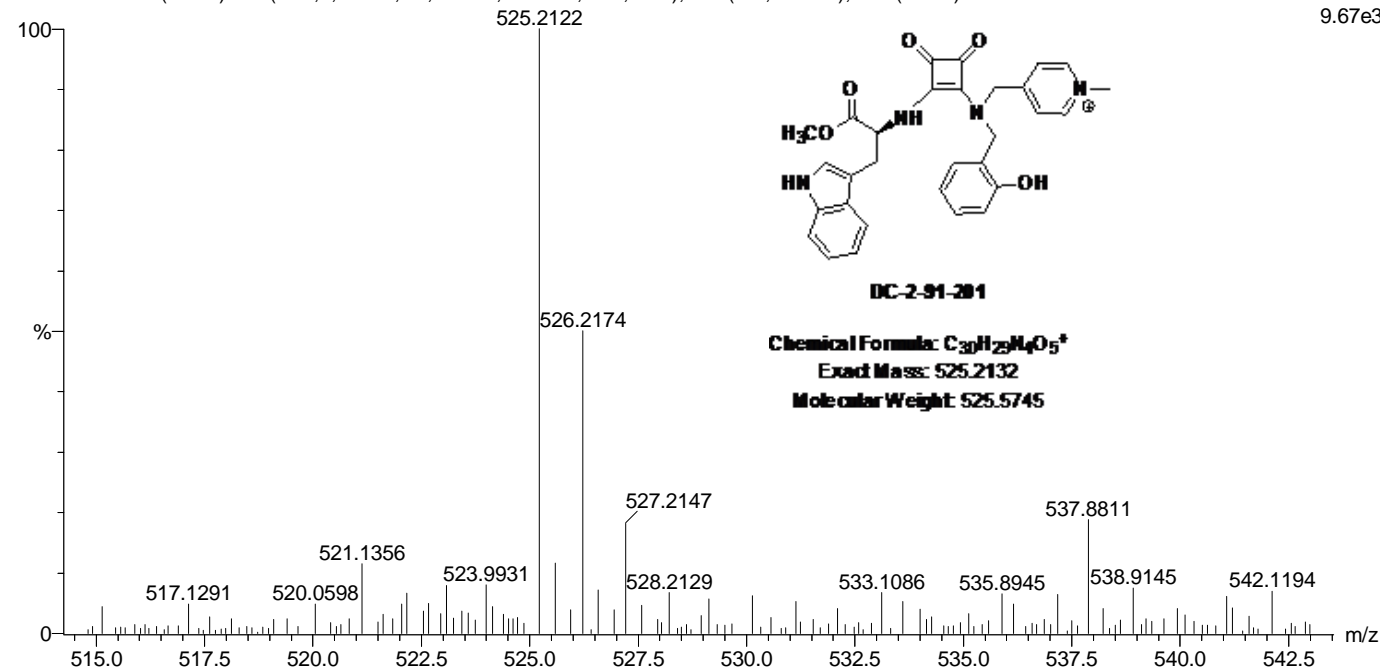
Test name: Accurate Mass

Base Peak Mass: 525.21215820

IU Database#: 24822

06-May-2010 11:38:59

1: TOF MS ES+
9.67e3



DC-2-91-201

Chemical Formula: $C_{30}H_{29}N_4O_5^+$

Exact Mass: 525.2132

Molecular Weight: 525.5745

Minimum: 80.00
 Maximum: 100.00

-1.5
 80.0

Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
525.2122	100.00	525.2138	-1.6	-3.0	18.5	447.6	C30 H29 N4 O5

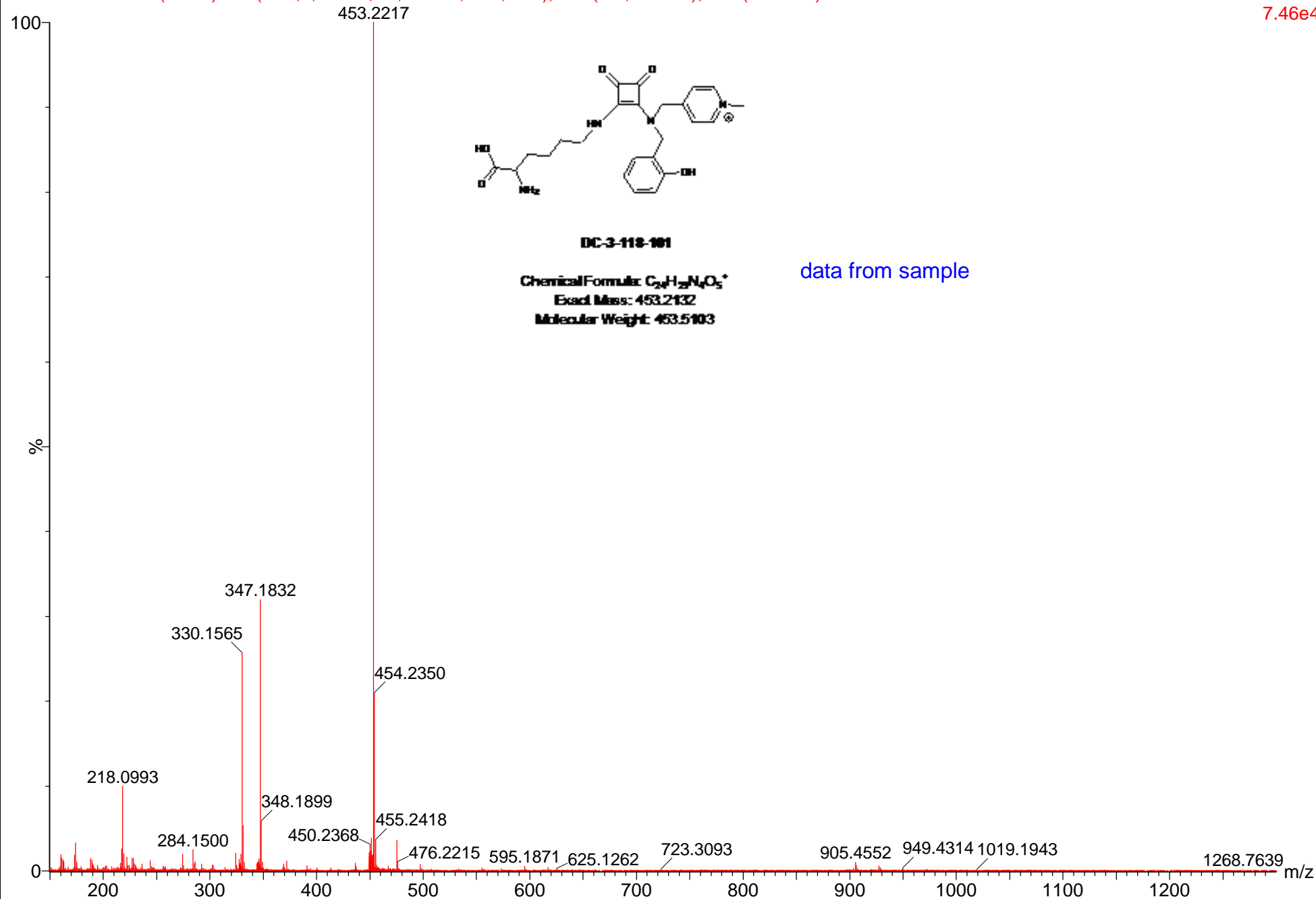
File name: dc-3-118-101
Instrument: LCT KC366
Method: ESI-TOF

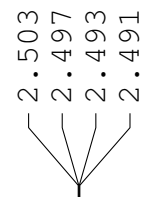
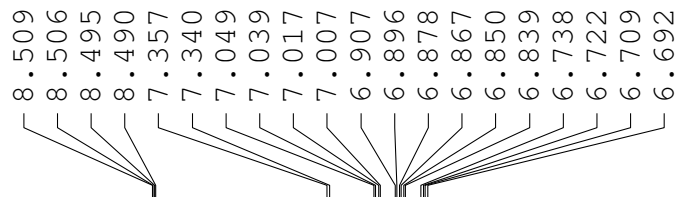
Notebook Ref: 25174
Test name: Accurate Mass
Base Peak Mass: 453.22174072

IU Database#: 25174
01-Jun-2010 15:51:53

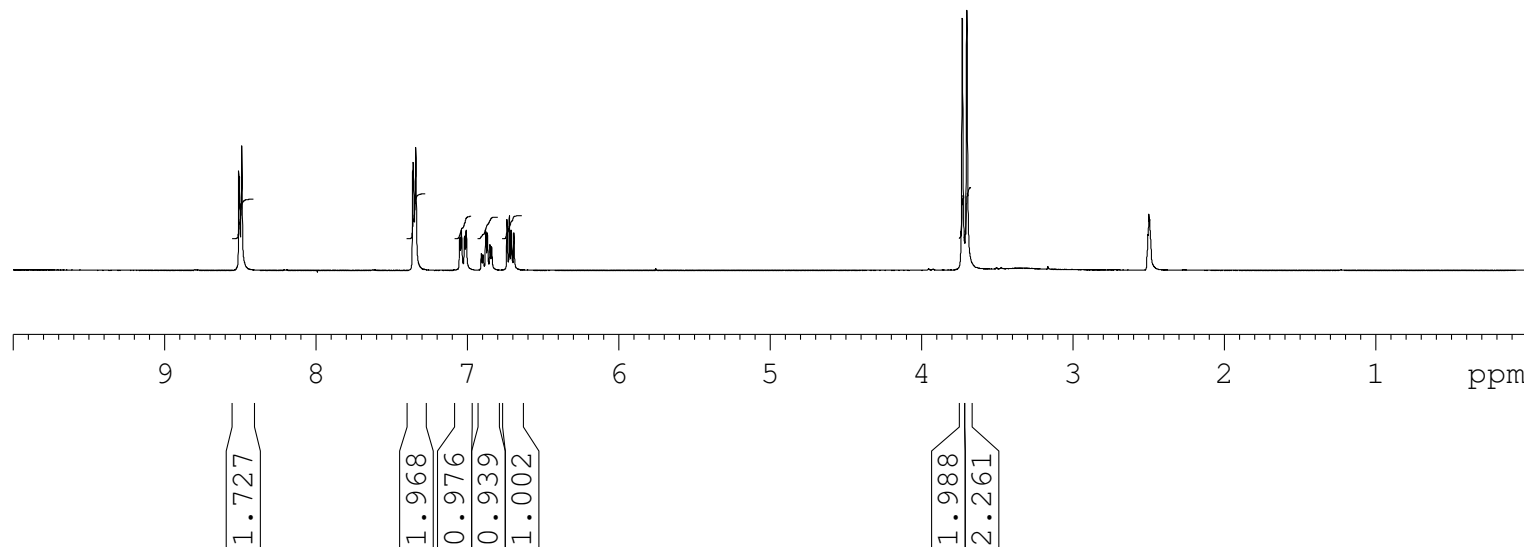
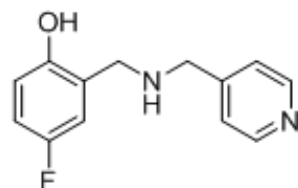
dc-3-118-101 146 (3.254) AM (Cen,8, 80.00, Ar,6000.0,0.00,0.70); Sm (SG, 2x4.00); Cm (140:159)

1: TOF MS ES+
7.46e4





dc-3-127-101



Current Data Parameters

NAME dc-3-127-101
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20100604
 Time 10.38
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT DMSO
 NS 16
 DS 0
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 406.4
 DW 104.400 usec
 DE 54.00 usec
 TE 296.2 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====

NUC1 1H
 P1 9.75 usec
 PL1 0.00 dB
 SFO1 300.1324000 MHz

F2 - Processing parameters

SI 32768
 SF 300.1300024 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

8.595
 8.579
 7.457
 7.441
 7.428
 7.409
 7.389
 7.352
 7.342
 7.326
 7.313
 7.302
 7.293
 7.287
 7.272
 7.262

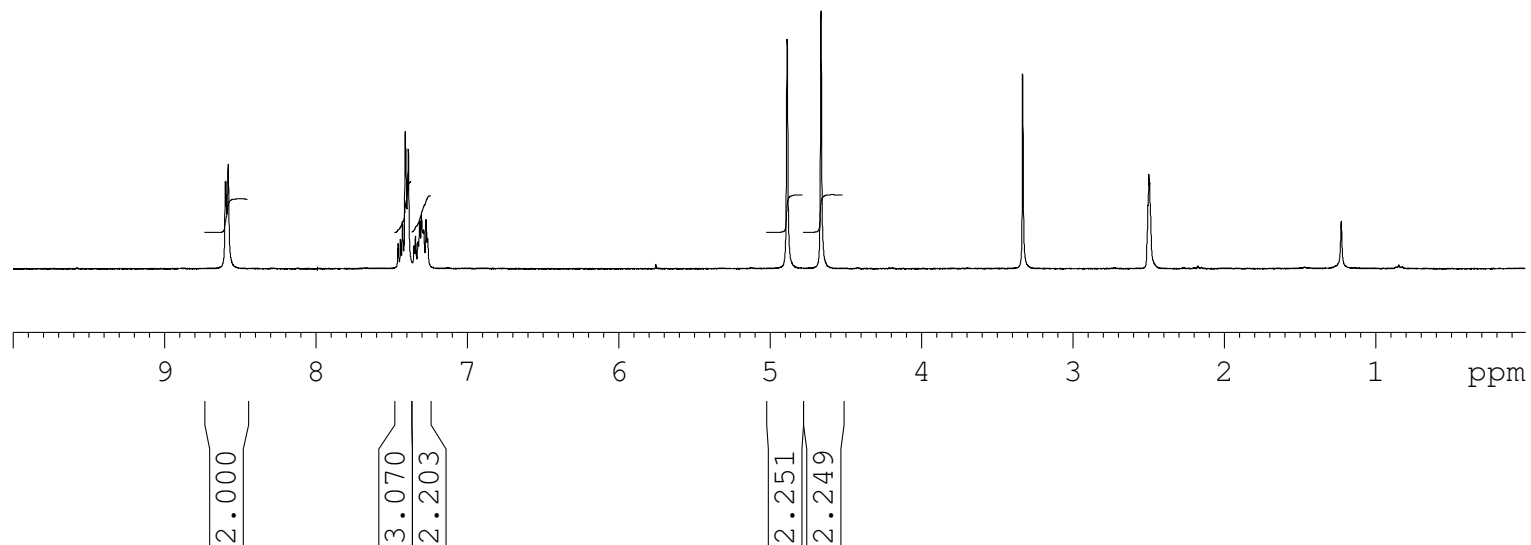
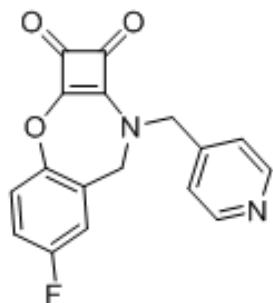
4.886
 4.662

3.330

2.497
 2.491

1.225

dc-3-134-101



Current Data Parameters

NAME dc-3-134-101
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20100604
 Time 10.33
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT DMSO
 NS 16
 DS 0
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 645.1
 DW 104.400 usec
 DE 54.00 usec
 TE 296.2 K
 D1 1.00000000 sec
 TD0 1

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

NUC1 1H
 P1 9.75 usec
 PL1 0.00 dB
 SFO1 300.1324000 MHz

F2 - Processing parameters

SI 32768
 SF 300.1300024 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

Elemental Composition Report

Multiple Mass Analysis: 2 mass(es) processed

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 80.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

29 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-17 H: 0-12 N: 0-2 O: 0-3 F: 0-1 Na: 0-1

File name: dc-3-134-101

Notebook Ref: 25561

IU Database#: 25561

Instrument: LCT KC366

Test name: Accurate Mass

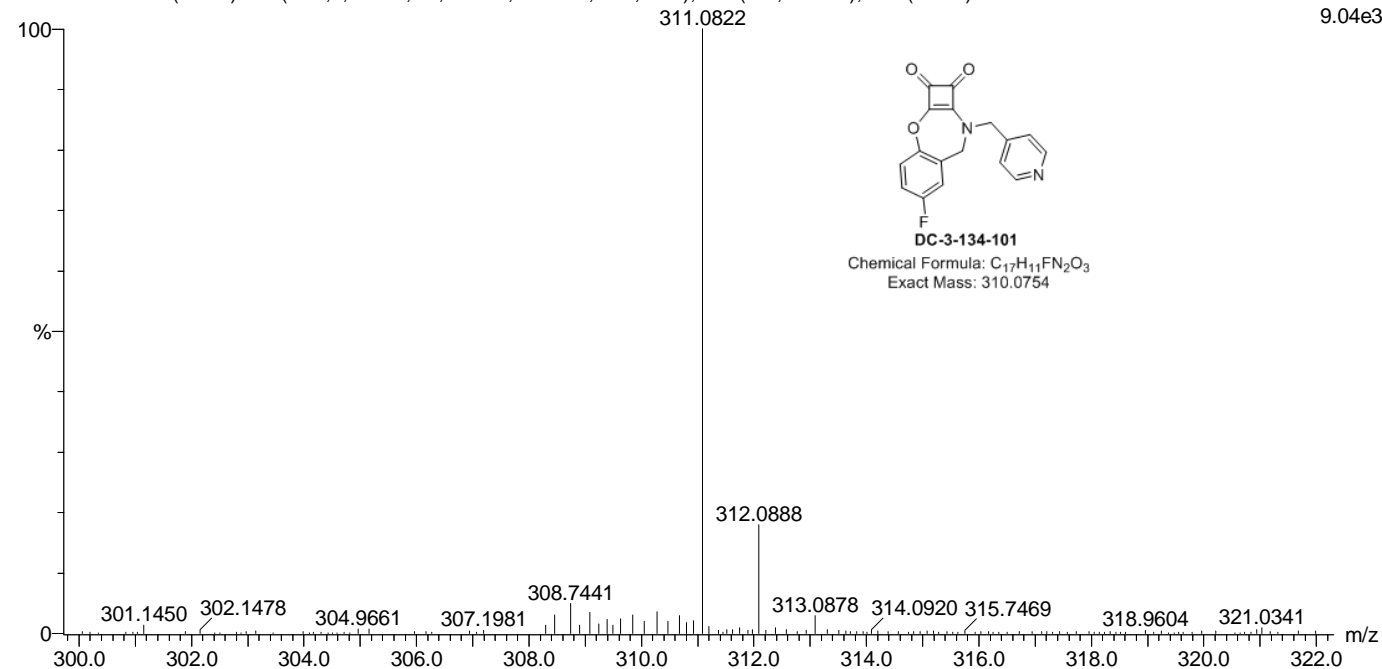
15-Jun-2010 16:24:54

Method: ESI-TOF

Base Peak Mass: 311.08215332

dc-3-134-101 70 (1.753) AM (Cen,8, 90.00, Ar,5000.0,1222.14,0.70,LS 7); Sm (SG, 2x4.00); Cm (70:82)

1: TOF MS ES+
9.04e3



Minimum: 70.00
 Maximum: 100.00

-1.5
 80.0

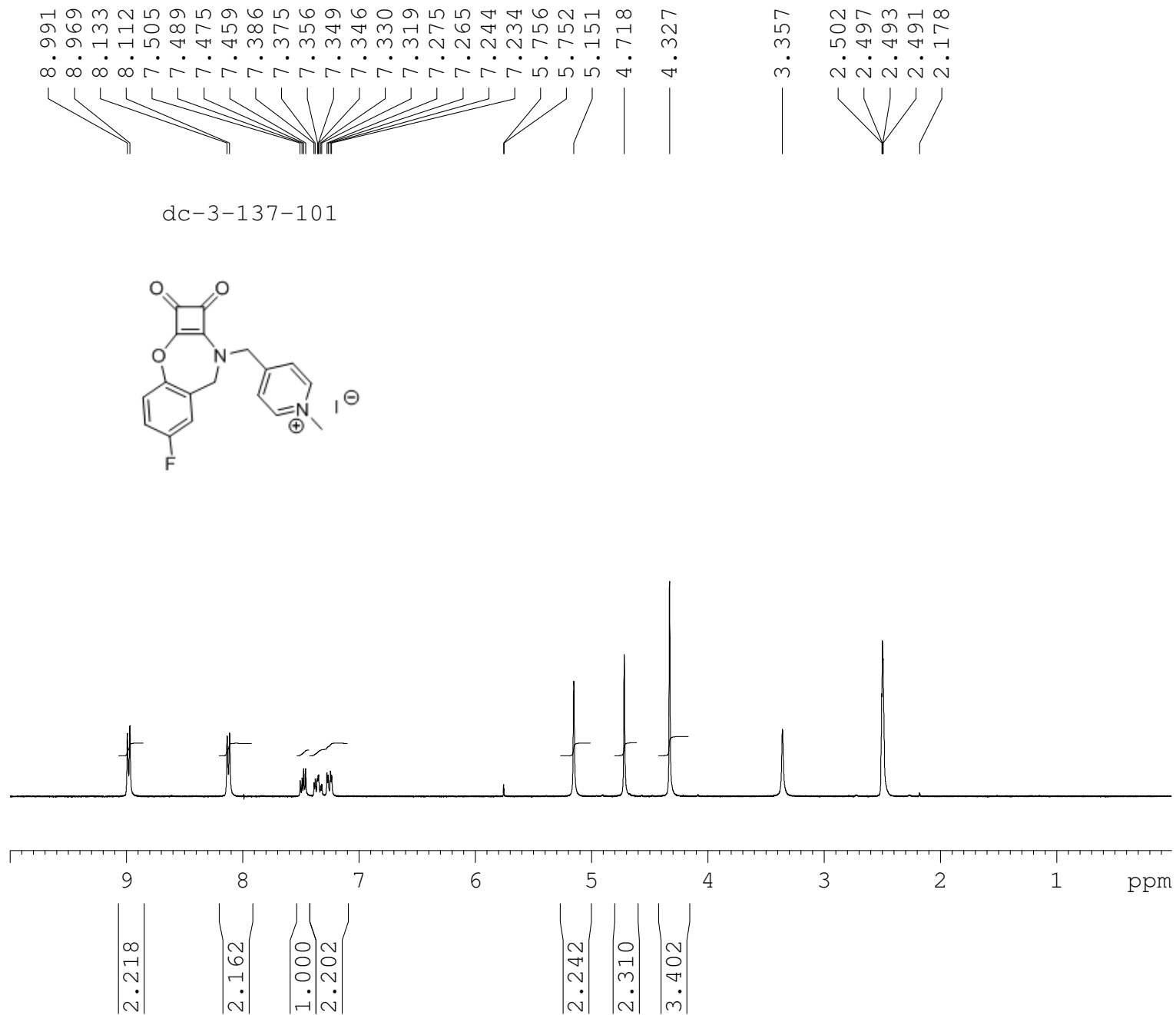
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
311.0822	100.00	311.0832	-1.0	-3.2	12.5	12.2	C17 H12 N2 O3 F

Current Data Parameters
 NAME dc-3-137-101
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100604
 Time 10.28
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT DMSO
 NS 16
 DS 0
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 724.1
 DW 104.400 usec
 DE 54.00 usec
 TE 296.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.75 usec
 PL1 0.00 dB
 SFO1 300.1324000 MHz

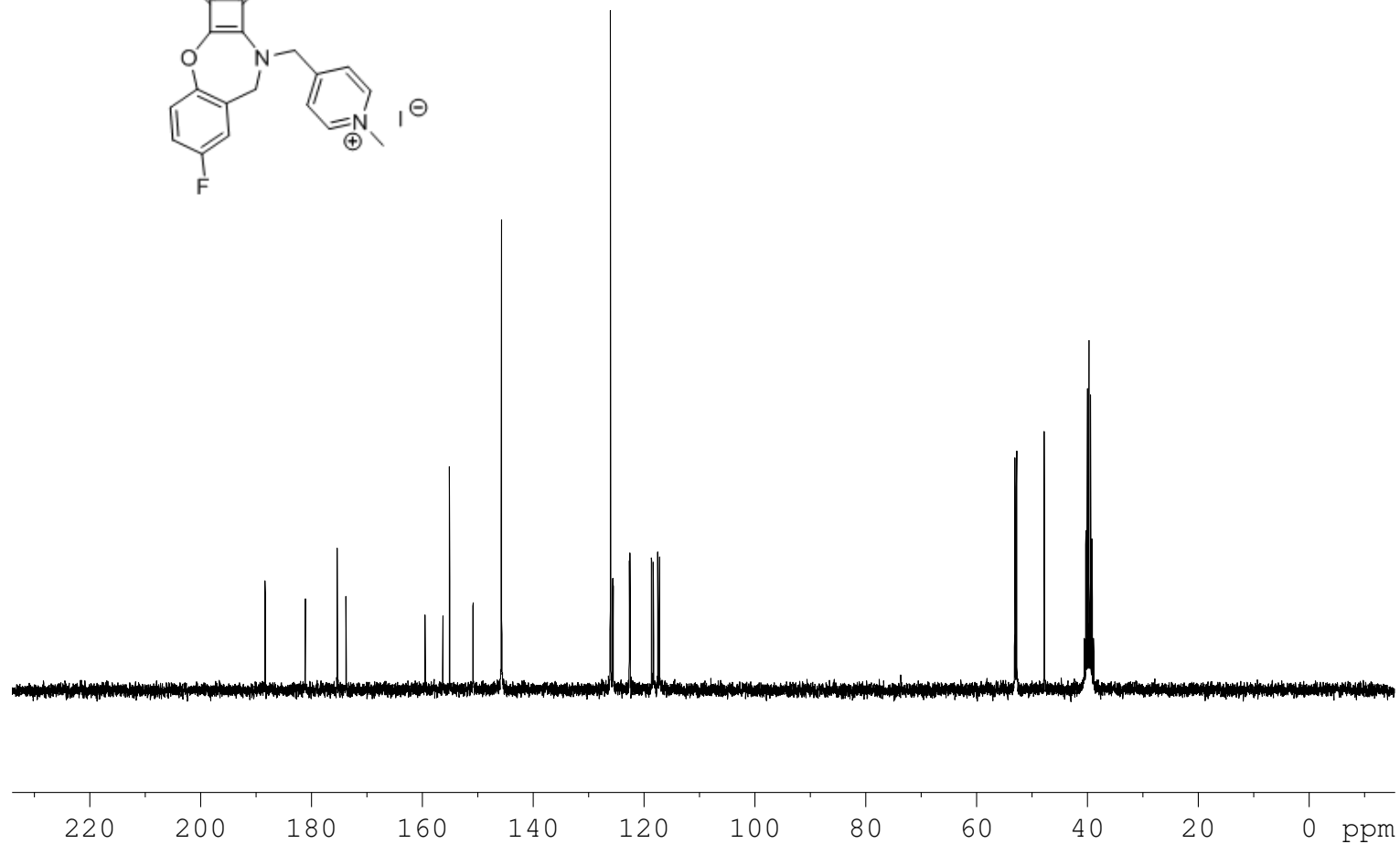
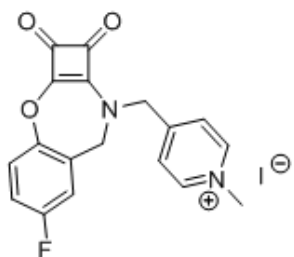
F2 - Processing parameters
 SI 32768
 SF 300.1300024 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00



188.327
 181.085
 175.319
 173.723
 159.471
 156.255
 155.048
 150.815
 150.782
 145.680
 126.020
 125.622
 125.515
 122.593
 122.478
 118.584
 118.258
 117.467
 117.160

DC-3-137-carbon-2

53.021
 52.711
 47.720
 40.487
 40.208
 39.929
 39.651
 39.374
 39.096
 38.818



Current Data Parameters
 NAME DC-3-137-carbon-
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100730
 Time 15.48
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zgdc
 TD 65536
 SOLVENT DMSO
 NS 250
 DS 0
 SWH 18832.393 Hz
 FIDRES 0.287360 Hz
 AQ 1.7400308 sec
 RG 3251
 DW 26.550 usec
 DE 6.00 usec
 TE 295.2 K
 D1 1.00000000 sec
 d11 0.03000000 sec
 TD0 1

==== CHANNEL f1 ====
 NUC1 13C
 P1 11.80 usec
 PL1 0.00 dB
 SFO1 75.4760200 MHz

==== CHANNEL f2 ====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 95.00 usec
 PL2 0.00 dB
 PL12 18.00 dB
 SFO2 300.1312005 MHz

Elemental Composition Report

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 80.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

29 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-18 H: 0-14 N: 0-2 O: 0-3 F: 0-1 Na: 0-1

File name: dc-3-137-101

Instrument: LCT KC366

Method: ESI-TOF

dc-3-137-101-rerun5 42 (1.053) AM (Cen.8, 90.00, Ar,5000.0,922.36,0.70,LS 7); Sm (SG, 2x4.00); Cm (42)

Notebook Ref: 25562

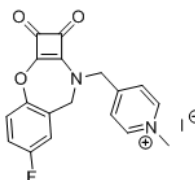
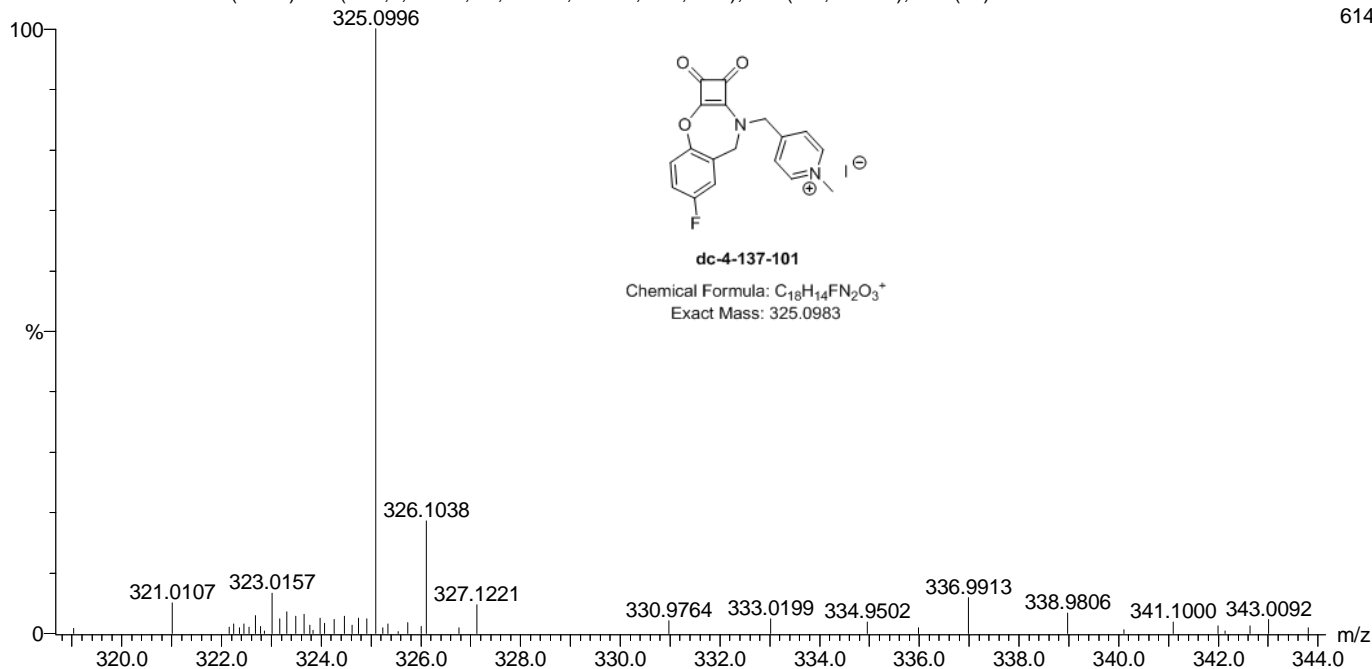
Test name: Accurate Mass

Base Peak Mass: 325.09957886

IU Database#: 25562

15-Jun-2010 17:19:02

1: TOF MS ES+
614



dc-4-137-101

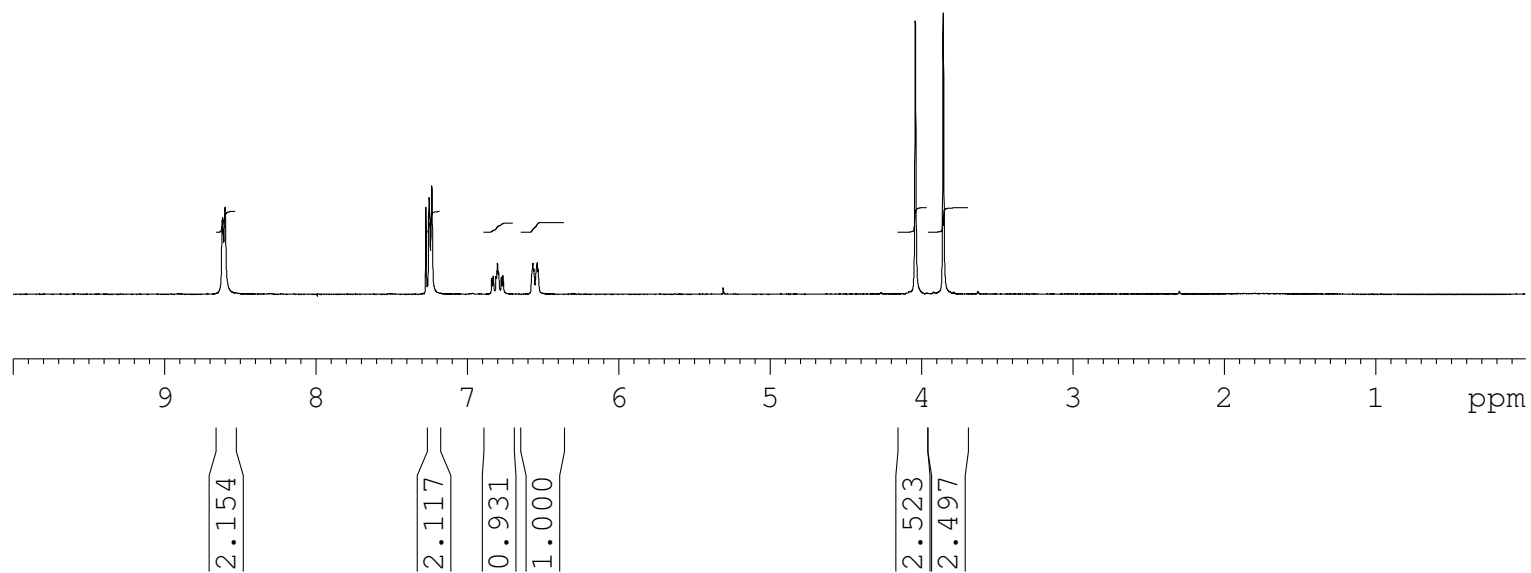
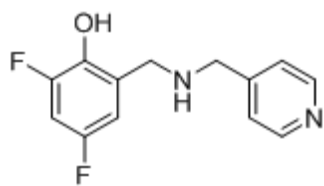
Chemical Formula: C₁₈H₁₄FN₂O₃⁺
 Exact Mass: 325.0983

Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
325.0996	100.00	325.0988	0.8	2.5	12.5	3.7	C18 H14 N2 O3 F

8.616
 8.600
 7.274
 7.270
 7.252
 7.234
 6.838
 6.828
 6.809
 6.800
 6.793
 6.774
 6.764
 6.566
 6.560
 6.538
 6.532
 5.309
 5.305

4.039
 3.855

dc-4-23-101



Current Data Parameters
 NAME dc-4-23-101
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100628
 Time 11.43
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 362
 DW 104.400 usec
 DE 54.00 usec
 TE 296.2 K
 D1 1.00000000 sec
 TD0 1

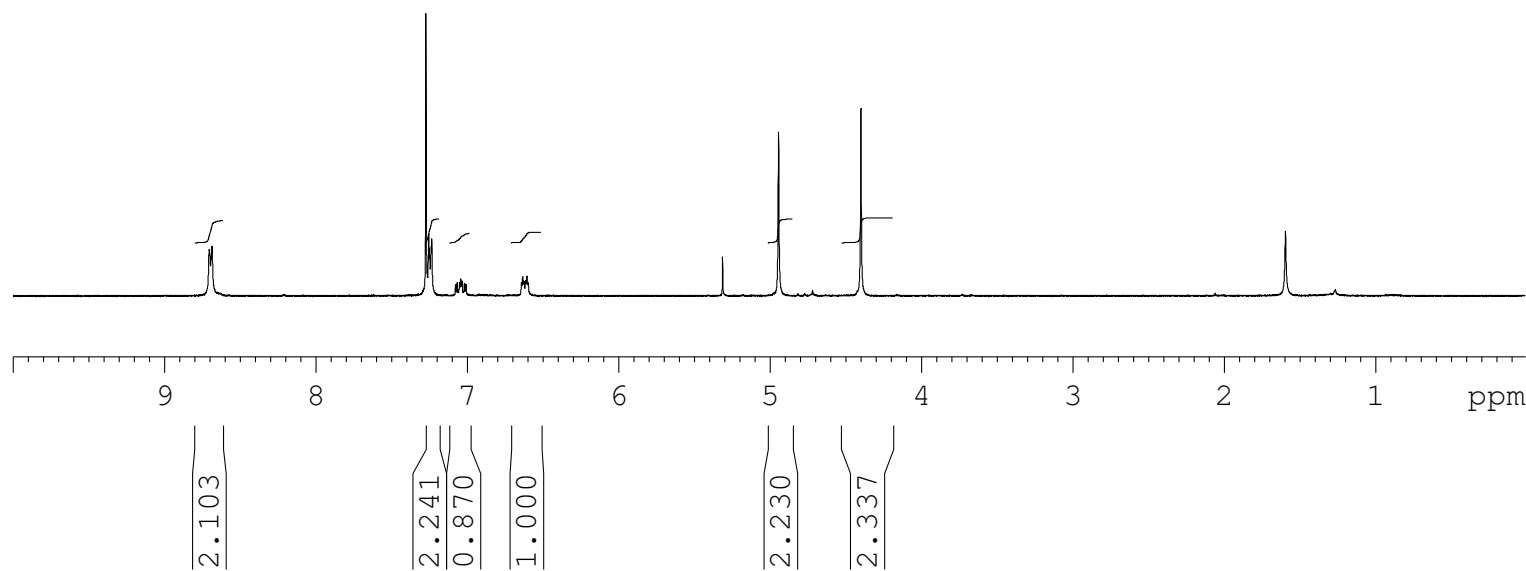
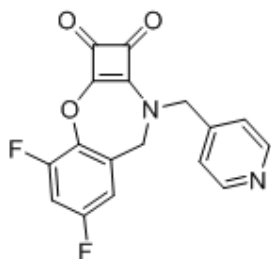
==== CHANNEL f1 ====
 NUC1 1H
 P1 9.75 usec
 PL1 0.00 dB
 SFO1 300.1324000 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300024 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

8.705
 8.686
 7.273
 7.254
 7.234
 7.076
 7.066
 7.050
 7.044
 7.034
 7.018
 7.008
 6.641
 6.633
 6.624
 6.614
 6.605
 6.597
 5.312
 4.943
 4.399

1.593

dc-4-25-101



Current Data Parameters
 NAME dc-4-25-101
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100629
 Time 15.46
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 1149.4
 DW 104.400 usec
 DE 54.00 usec
 TE 295.2 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 ====
 NUC1 1H
 P1 9.75 usec
 PL1 0.00 dB
 SFO1 300.1324000 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300024 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

Elemental Composition Report

Tolerance = 100.0 PPM / DBE: min = -1.5, max = 80.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

28 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-17 H: 0-11 N: 0-2 O: 0-3 F: 0-2

File name: dc-4-25-101

Instrument: LCT KC366

Method: ESI-TOF

dc-4-25-101 115 (2.887) AM (Cen,8, 80.00, Ar,5000.0,1222.14,0.70,LS 7); Sm (SG, 2x4.00); Cm (115:117)

Notebook Ref: 25942

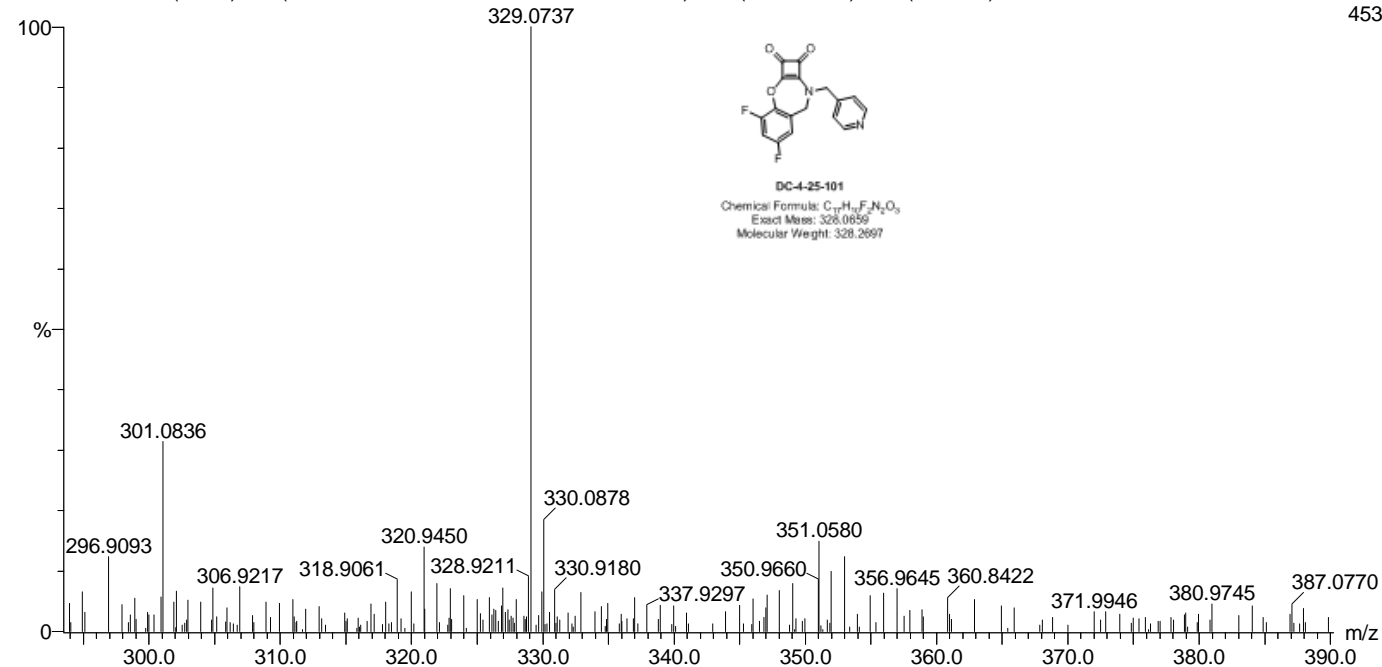
Test name: Accurate Mass

Base Peak Mass: 329.0736943

IU Database#: 25942

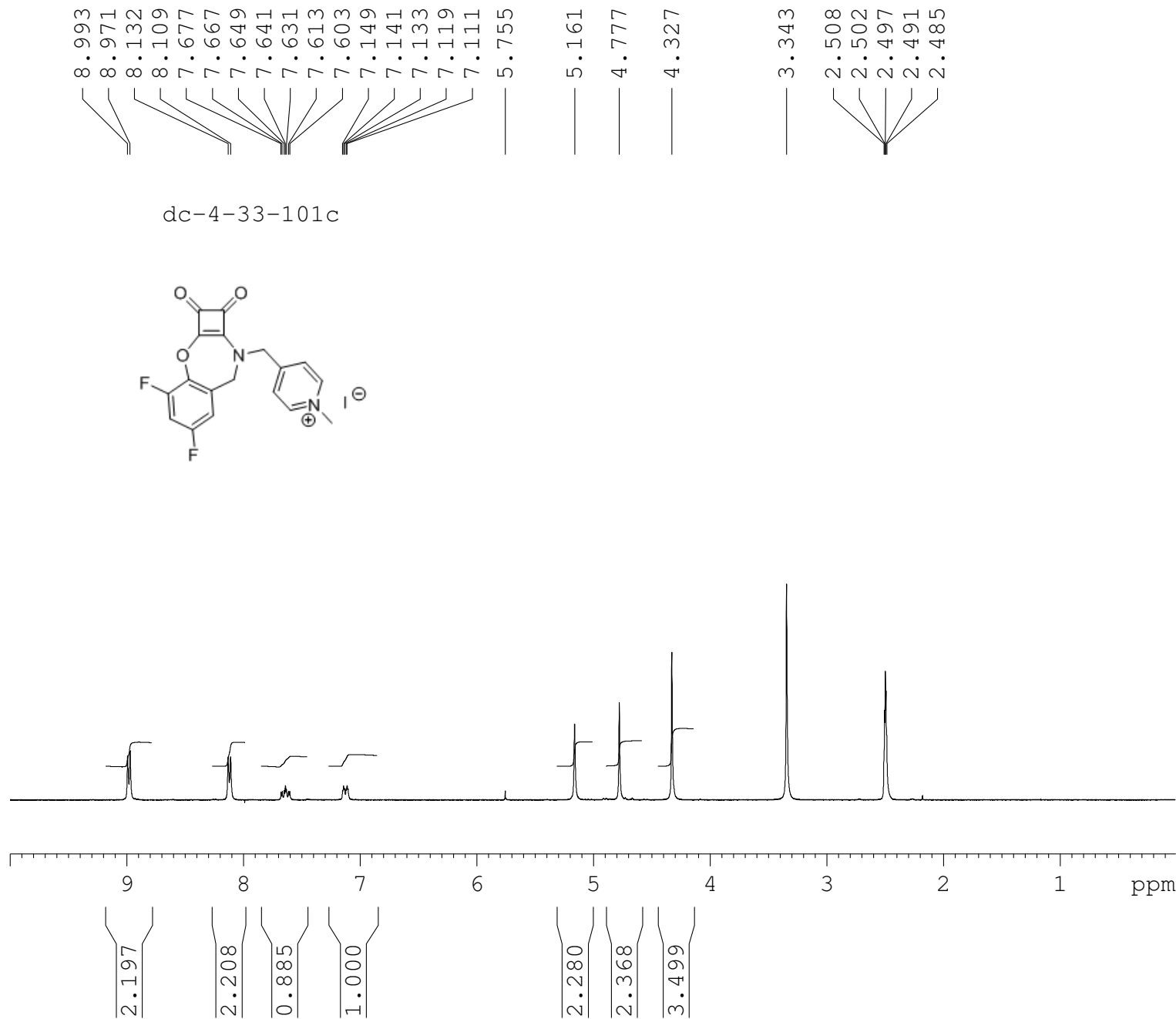
09-Jul-2010 14:37:47

1: TOF MS ES+
453



Minimum: 60.00 -1.5
 Maximum: 100.00 5.0 100.0 80.0

Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
329.0737	100.00	329.0738	-0.1	-0.3	12.5	0.7	C17 H11 N2 O3 F2

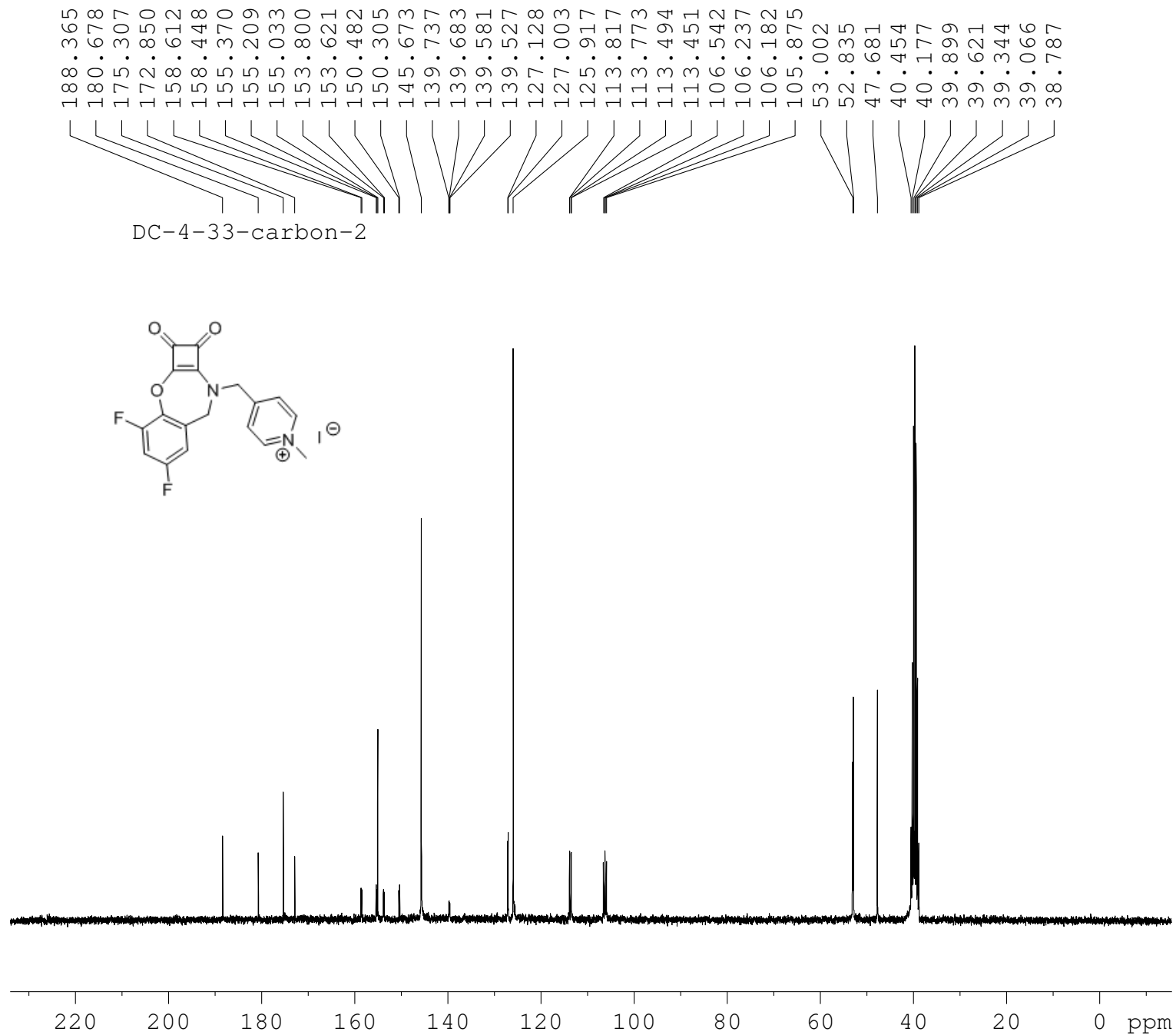


Current Data Parameters
 NAME dc-4-33-101c
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100709
 Time 10.49
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT D2O
 NS 32
 DS 0
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 1024
 DW 104.400 usec
 DE 54.00 usec
 TE 296.2 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 ====
 NUC1 1H
 P1 9.75 usec
 PL1 0.00 dB
 SFO1 300.1324000 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300024 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME DC-4-33-carbon-2
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100731
 Time 17.53
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zgdc
 TD 65536
 SOLVENT DMSO
 NS 2400
 DS 0
 SWH 18832.393 Hz
 FIDRES 0.287360 Hz
 AQ 1.7400308 sec
 RG 5792.6
 DW 26.550 usec
 DE 6.00 usec
 TE 295.2 K
 D1 1.00000000 sec
 d11 0.03000000 sec
 TD0 1

==== CHANNEL f1 ====
 NUC1 13C
 P1 11.80 usec
 PL1 0.00 dB
 SFO1 75.4760200 MHz

==== CHANNEL f2 ====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 95.00 usec
 PL2 0.00 dB
 PL12 18.00 dB
 SFO2 300.1312005 MHz

Elemental Composition Report

Multiple Mass Analysis: 2 mass(es) processed

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 80.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

28 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-18 H: 0-13 N: 0-2 O: 0-3 F: 0-2

File name: dc-4-33-101

Instrument: LCT KC366

Method: ESI-TOF

dc-4-33-101b 30 (0.752) AM (Cen,8, 80.00, Ar,5000.0,1222.14,0.70,LS 6); Sm (SG, 2x6.00); Cm (29:30)

Notebook Ref: 26284

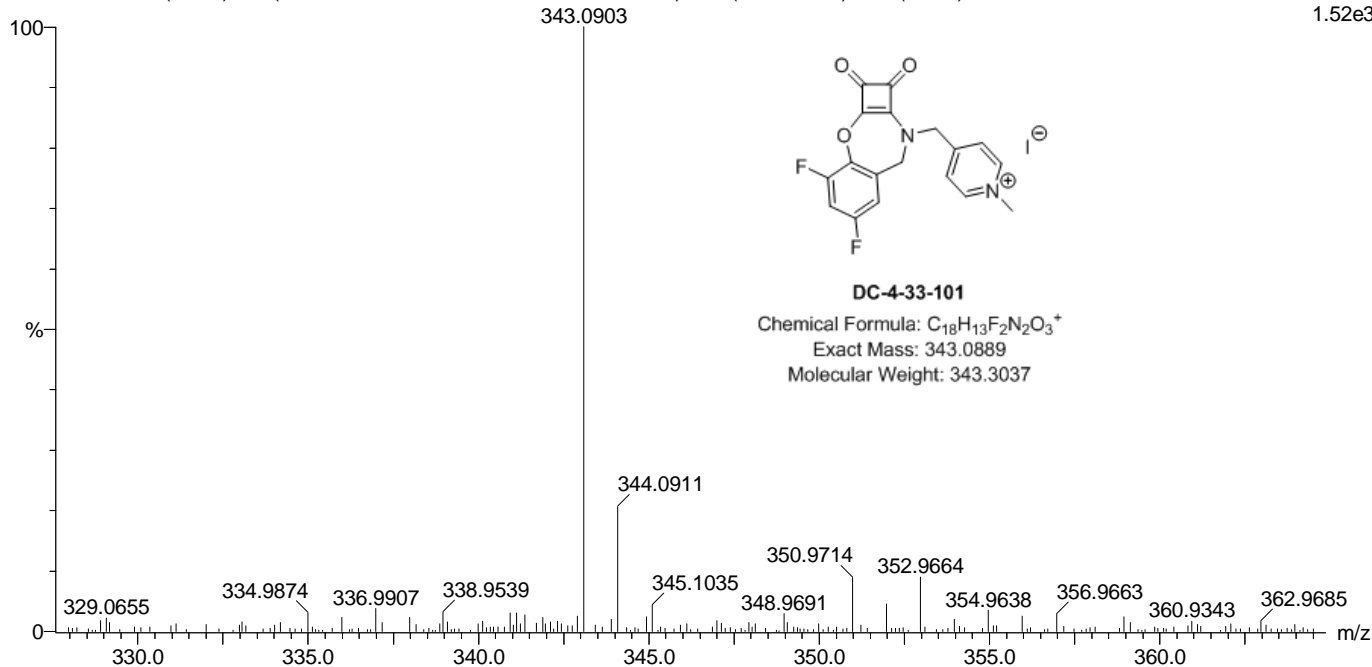
Test name: Accurate Mass

Base Peak Mass: 343.09027100

IU Database#: 26284

30-Jul-2010 12:34:30

1: TOF MS ES+
1.52e3



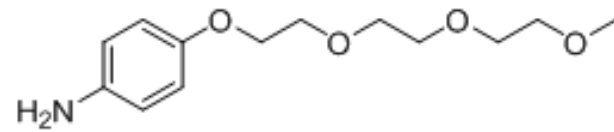
Minimum: 50.00
 Maximum: 100.00

-1.5
 80.0

Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
343.0903	100.00	343.0894	0.9	2.6	12.5	4.6	C18 H13 N2 O3 F2

7.266
6.765
6.758
6.743
6.736
6.724
6.645
6.634
6.626
6.612
6.604
4.063
4.048
4.030
3.824
3.807
3.791
3.743
3.737
3.730
3.726
3.724
3.718
3.708
3.689
3.679
3.670
3.667
3.660
3.654
3.645
3.636
3.586
3.561
3.552
3.543
3.531
3.459
3.373
3.294

DC-2-46-101



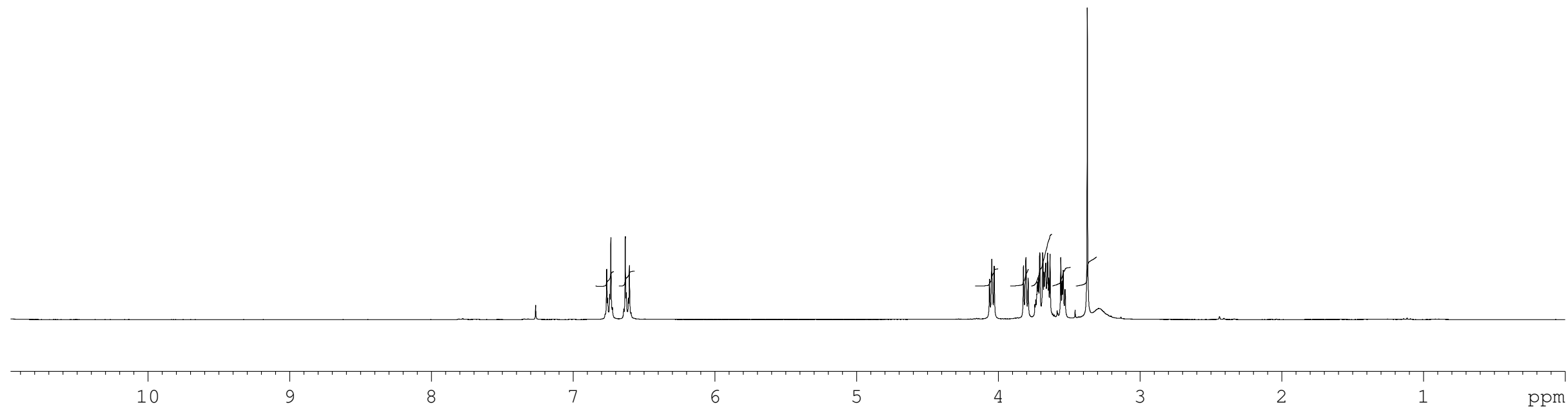
DC-2-46-101

Current Data Parameters
NAME DC-2-46-101
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100211
Time 10.11
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDC13
NS 16
DS 0
SWH 3591.954 Hz
FIDRES 0.109618 Hz
AQ 4.5613556 sec
RG 90.5
DW 139.200 usec
DE 54.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 9.75 usec
PL1 0.00 dB
SFO1 300.1315007 MHz

F2 - Processing parameters
SI 32768
SF 300.1300042 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



1.943
2.000

2.306
2.287
6.957
2.505
3.925

Elemental Composition Report

Tolerance = 15.0 PPM / DBE: min = -1.5, max = 80.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

25 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-24 H: 0-26 N: 0-1 O: 0-7 Na: 0-1

File name: dc-2-59-101

Instrument: LCT KC366

Method: ESI-TOF

dc-2-59-101 23 (0.586) AM (Cen,6, 90.00, Ar,6000.0,1222.14,0.70,LS 4); Sm (SG, 2x6.00); Cm (23)

Notebook Ref:

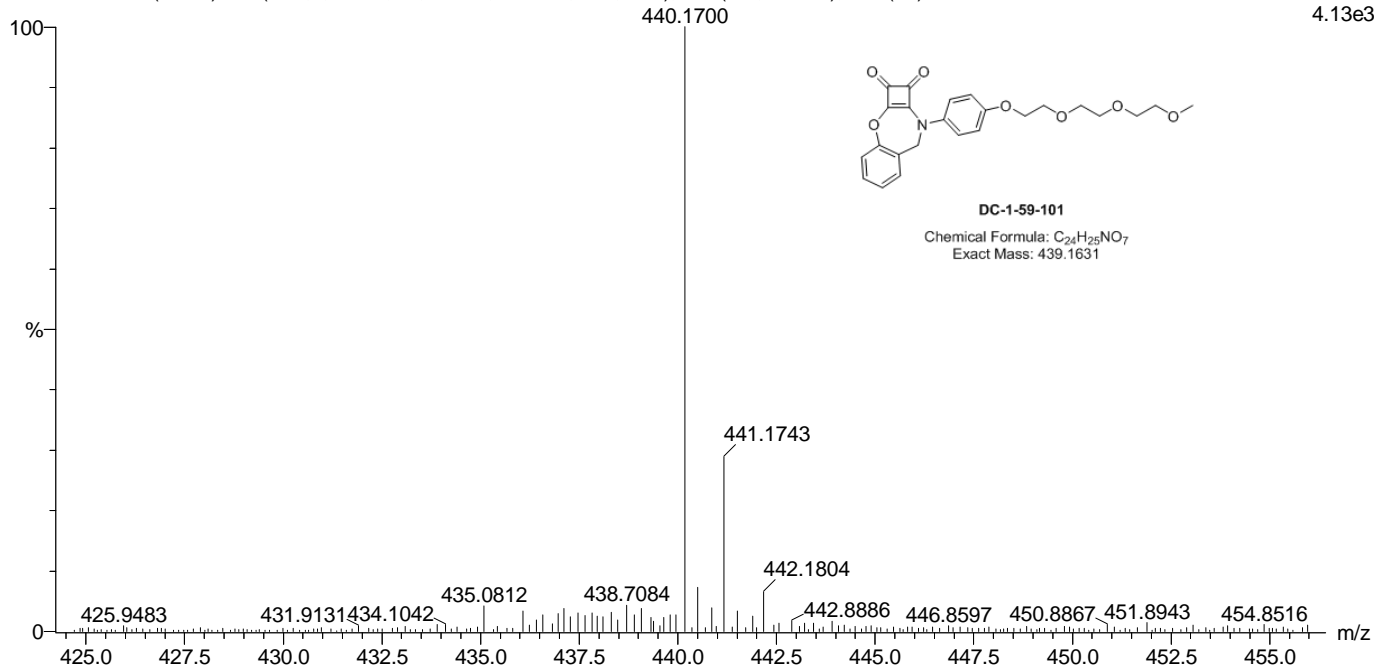
Test name: Accurate Mass

Base Peak Mass: 440.16995239

IU Database#:

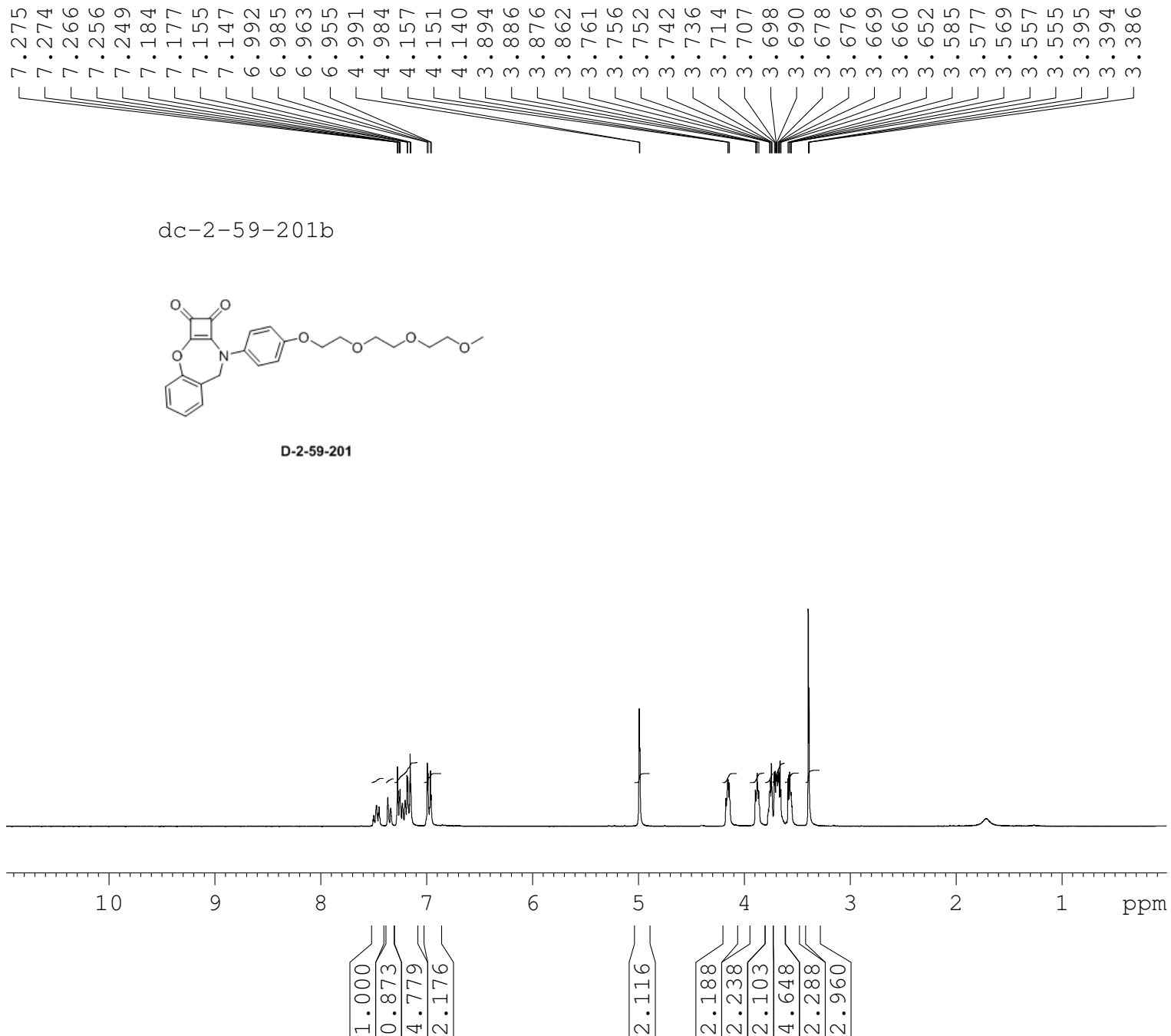
26-Feb-2010 12:12:41

1: TOF MS ES+
4.13e3



Minimum: 80.00
 Maximum: 100.00

Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
440.1700	100.00	440.1709	-0.9	-2.0	12.5	5.8	C ₂₄ H ₂₆ N O ₇



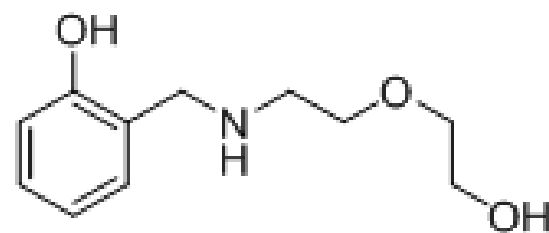
Current Data Parameters
 NAME dc-2-59-201b
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100814
 Time 10.50
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT CDC13
 NS 8
 DS 0
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 362
 DW 104.400 usec
 DE 54.00 usec
 TE 294.2 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 ====
 NUC1 1H
 P1 9.75 usec
 PL1 0.00 dB
 SFO1 300.1324000 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300024 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

DC-2-61-101b



DC-2-61-101b

7.266
7.187
7.182
7.160
7.156
7.135
7.130
6.993
6.990
6.970
6.840
6.836
6.813
6.809
6.798
6.794
6.773
6.769
6.749
6.745
5.293
4.002
3.751
3.745
3.737
3.732
3.721
3.692
3.619
3.603
3.586
3.576
3.565
3.561
3.552
3.547
2.875
2.858
2.841

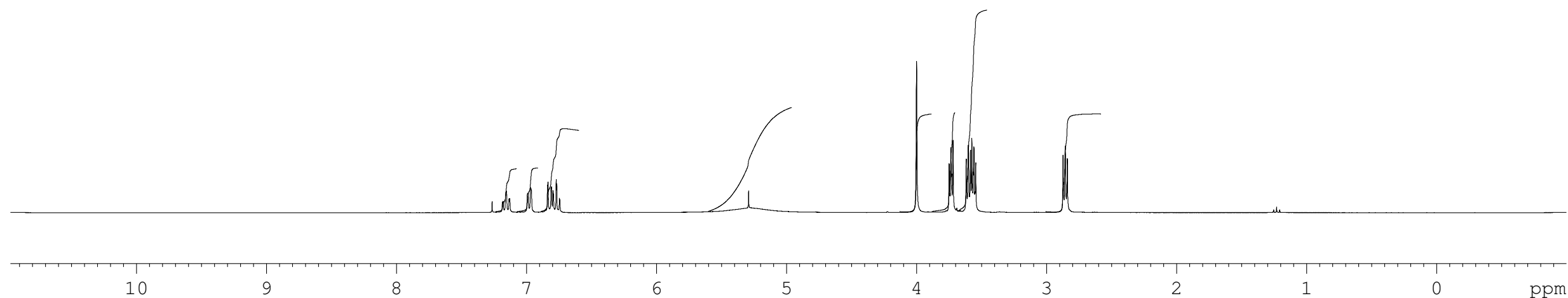
1.231

Current Data Parameters
 NAME DC-2-61-101b
 EXPNO 1
 PROCNO 1

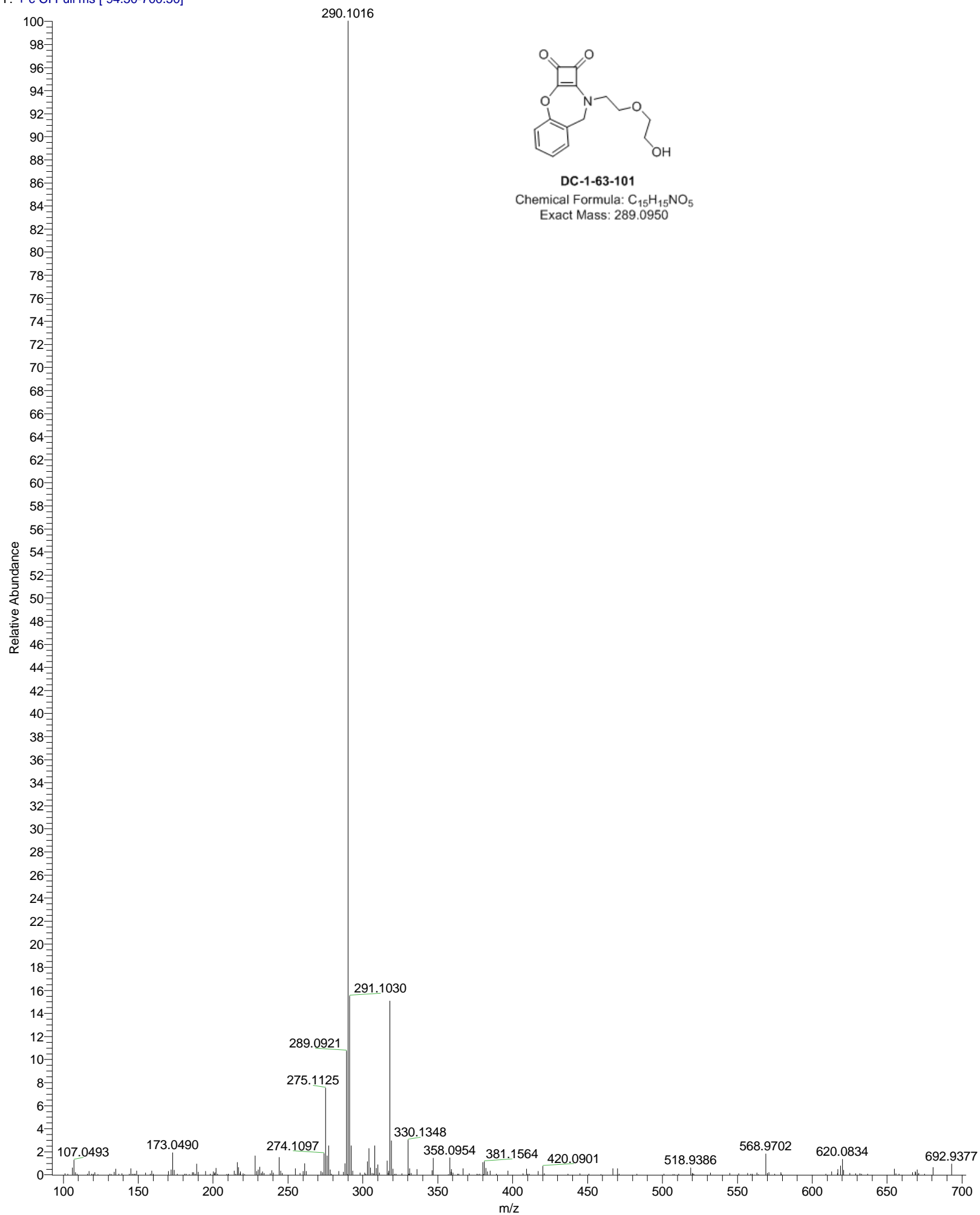
F2 - Acquisition Parameters
 Date_ 20100216
 Time 14.13
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT DMSO
 NS 16
 DS 0
 SWH 3591.954 Hz
 FIDRES 0.109618 Hz
 AQ 4.5613556 sec
 RG 80.6
 DW 139.200 usec
 DE 54.00 usec
 TE 299.2 K
 D1 1.00000000 sec
 TD0 1

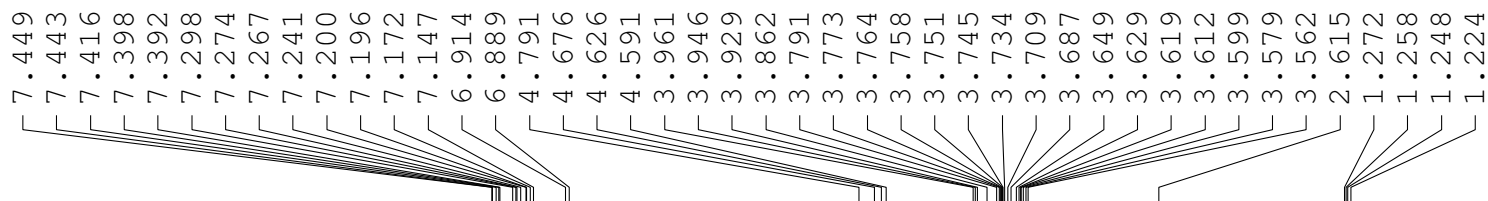
==== CHANNEL f1 =====
 NUC1 1H
 P1 9.75 usec
 PL1 0.00 dB
 SFO1 300.1315007 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300042 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

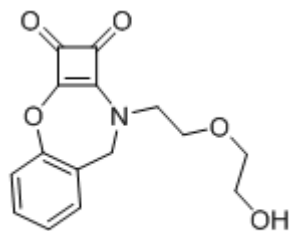


1.000
1.020
1.899
2.435
2.285
2.322
4.715
2.283

dc-2-63-101-c1 #88-91 RT: 4.14-4.28 AV: 4 NL: 3.19E7
T: + c CI Full ms [94.50-700.50]



dc-2-63-101b



dc-2-63-101b

Current Data Parameters
 NAME dc-2-63-101b
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100814
 Time 10.55
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 362
 DW 104.400 usec
 DE 54.00 usec
 TE 294.2 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 ====
 NUC1 1H
 P1 9.75 usec
 PL1 0.00 dB
 SFO1 300.1324000 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300024 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

