

# Supporting Information

Foldamer scaffolds suggest distinct structures are associated with alternative gains-of-function in a preamyloid toxin

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Running Title: Foldamer manipulation of IAPP gains-of-function  
Keywords: Structure activity relationship, amylin, foldamer

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## METHODS

**Materials.** Thioflavin T (ThT) was purchased from Acros Organics (Fair Lawn, NJ), lipids from[dioleoylphosphatidylglycerol (DOPG) and dioleoylphosphatidylcholine (DOPC)] from Avanti Polar Lipids, Inc. (Alabaster, AL, USA), 96-well plates (black, w/flat bottom) from Greiner Bio-One (Monroe, NC, USA), silica plates (w/UV254, aluminum backed, 200 micron) and silica gel (standard grade, particle size = 40-63 micron, 230 × 400 mesh) from Sorbent Technologies (Atlanta, GA, USA). All the solvents were purchased from Sigma Aldrich (St. Louis, MI) or VWR (Bridgeport, NJ, USA) and used without further purification. 2,6-dichloro-3-nitropyridine, alkyl iodides, alkyl alcohols, triethylamine (dry), 2-chloro-1-methylpyridinium iodide, *tert*-butyl bromoacetate, trifluoroacetic acid (TFA), and triethylsilane (TES) were purchased from Sigma Aldrich (St. Louis, MI, USA). Islet amyloid polypeptide (IAPP) was purchased from Genscript (Piscataway, NJ, USA) and Elim Biopharmaceuticals (Hayward, CA, USA) with ≥98% purity and used after in-house repurification described below.

**Preparation of IAPP.** IAPP (~2 mg) was solubilized in 7 M guanidinium hydrochloride (1 mL). The solution was filtered (0.2 micron) and transferred to C-18 spin column, washed twice with water (400 µL each) followed by 10% acetonitrile in water, 0.1% formic acid (v/v) and then eluted into 200 µL of 50% acetonitrile in water, 0.1% formic acid (v/v). The concentration of IAPP (oxidized form) was calculated using absorbance measurements at 280 nm ( $\epsilon = 1400 \text{ M}^{-1}\text{cm}^{-1}$ ). The IAPP solution was divided into several aliquots (20-50 µL, 1-2 mM), lyophilized, and stored as a white solid at -80 °C. Fresh stock solution of IAPP was prepared in water for each experiment.

**Unilamellar vesicles.** Unless otherwise stated, LUVs used in this work were prepared from a 1:1 mixture of DOPG/DOPC. The lyophilized mixture was hydrated in 100 mM KCl, 50 mM sodium phosphate, and pH 7.4 for 20 minutes. A 20 mg/mL solution of lipid in buffer was passed 21 times

through a polycarbonate membrane (pore diameter ( $d$ ) = 100 nm). The phospholipid content of the final material was measured using a total phosphorous assay<sup>1</sup>.

**Kinetic assay.** Amyloid reactions were conducted in buffer containing liposome (630  $\mu\text{M}$  lipid, LUVs, DOPG:DOPC, 1:1, 100 nm) and 1  $\mu\text{M}$  ThT in a black 96-well plate. This was followed by addition of small molecule dissolved in DMSO (final DMSO concentration = 0.5%, v/v). Fiber formation was initiated by addition of IAPP stock solution. The final volume in each well was 200  $\mu\text{L}$ . Kinetics of fibrillation was monitored by ThT fluorescence (Ex 450 nm and Em 485 nm) using a FluoDia T70 fluorescence plate reader (Photon Technology International, Edison, NJ, USA). The data were blank subtracted and renormalized to the maximum intensity of reactions containing only IAPP. Each kinetic trace was fit to a sigmoidal form:

$$I = \frac{(b_2 + m_2 t) + (b_1 + m_1 t) e^{\frac{t-50}{\tau}}}{1 + e^{\frac{t-50}{\tau}}} \quad (1)$$

where  $I$  is the fluorescence intensity,  $t$  is time, and  $b$ ,  $m$ , and  $\tau$  are dependent fitting variables. All samples were run at least in triplicate and error bars shown in the text represent  $\pm$  one standard deviation.

**Liposome leakage assay.** The kinetics of liposome leakage induced by IAPP was monitored on QuantaMaster C-61 fluorescence spectrometer (Photon Technology International, Edison, NJ) at 25 °C. The excitation and emission were observed at 480 nm and 526 nm respectively with 3 nm slit widths. The stock solution of IAPP used in the measurements was kept in water at a concentration of 1-2 mM. The stock solution of water soluble quencher, DPX (*p*-xylene-bis-pyridinium bromide) was prepared in buffer (100 mM KCl, 50 mM NaPi, pH 7.4) at a concentration of 100 mM. The small molecules used in leakage assay were dissolved in DMSO

with a concentration range 10-20 mM. The final concentration of dye encapsulating liposome, DPX, human IAPP, and small molecules were 200, 6000, 4, and 4  $\mu$ M respectively. The final buffer concentration was corrected using higher concentration of buffer to keep the osmolality balanced. The final concentration of DMSO used in the assay was less than 0.4%. The control sample contained everything except IAPP. To determine the leakage rate constant, first the fluorescence was normalized and corrected by subtracting it from normalized fluorescence of control reaction. The corrected fluorescence was fit using equation given below (using Matlab). All the experiments were performed in triplicate and the error values presented are standard deviations.

$$a * \exp(-b * x) + c \quad (2)$$

a = amplitude from 100% unleaked to 0% leaked

c = final fraction of unleaked liposome

y = change in fluorescence

b = leakage rate constant.

**NMR (small molecules).** The NMR spectra of small molecules were recorded on 400, 500, and 600 MHz Agilent spectrometers. The deuterated solvents used for O-tert butyl ester protected and deprotected (O-COOH) oligoquinolines were  $\text{CDCl}_3$  and  $(\text{CD}_3)_2\text{SO}$  respectively. Splitting patterns which were difficult to interpret, recorded as multiplet (m) or broad (b).

**Mol. wt. determination (small molecules).** Mass spectra were obtained using either MALDI-TOF Voyager DE Pro (Yale, CBIC center) or University of Illinois Mass Spec. Facility. High-

resolution electrospray ionization mass spectra were obtained using the Waters Synapt G2-Si ESI MS mass spectrometer.

**HPLC purification (small molecules).** HPLC purification of small molecules was carried out on Varian ProStar using VYDAC reverse-phase columns (4.6 × 100 mm, 1 mL/min, analytical; 10 × 100 mm, 3 mL/min, semiprep.). The mobile phase was composed of A: 5% ACN, 95% H<sub>2</sub>O, 0.1% TFA(v/v) and B: 95% ACN, 5% H<sub>2</sub>O, and 0.08% TFA (v/v). The solvent gradient used for compound purification was: 0-100% solvent B in solvent A for 10 min at a flow rate of 3.0 mL/min followed by 100% solvent B for 25 min (1 mL/min for analytical). The solvent elution was monitored at 220 nm.

**Cell culture.** Rat insulinoma INS-1 cells (832/13, Dr. Gary W. Cline, Department of Internal Medicine, Yale University) were cultured at 37°C and 5% CO<sub>2</sub> in phenol red free RPMI 1640 media supplemented with 10% fetal bovine serum, 1% penicillin/streptomycin (Life Technologies, Carlsbad, CA, USA), and 2% INS-1 stock solution (500 mM HEPES, 100 mM L-glutamine, 100 mM sodium pyruvate, and 2.5 mM β-mercaptoethanol). Cells were passaged upon reaching ~95% confluence (0.25% Trypsin-EDTA, Life Technologies), propagated, and/or used in experiments. Cells used in experiments were pelleted and resuspended in fresh media with no Trypsin-EDTA.

**Cell viability Assay.** Cell viability was measured colourimetrically using the Cell-Titer Blue (CTB, Promega, Madison, WI, USA) fluorescence-based assay. Cells were plated at a density 50000 cells/well in 96-well plates (BD Biosciences, San Diego, CA, USA). Peptide was directly introduced to each well after 48 h of culture and then further incubated for an additional 48 h. For time dependent experiments, cells were incubated with peptide for the specified time points. After the incubation period, 30 μL CTB reagent was added to each well and incubated at 37°C and 5% CO<sub>2</sub> for 2.5 – 3.5 h. Fluorescence of the resorufin product was measured on a FluoDia T70

fluorescence plate reader (Photon Technology International, Birmingham, NJ, USA). All wells included the same amount of water to account for different concentrations of peptide added to sample wells. Wells that included water vehicle but not peptide served as the negative control (0% toxic), and wells containing 10% DMSO were the positive control (100% toxic). Percent toxicity was calculated using the following equation:

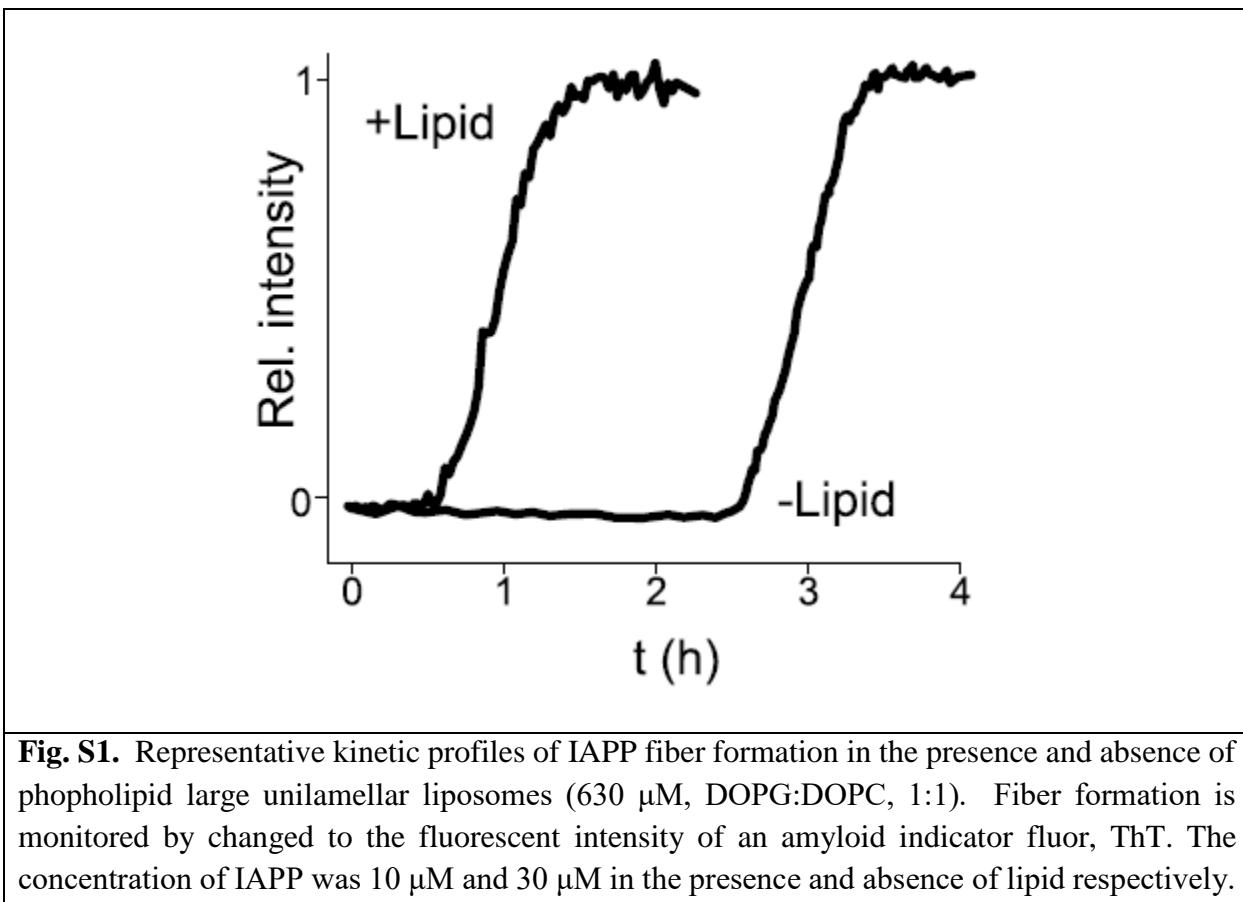
$$\% \text{Toxicity} = 100 - [100 \times \left( \frac{\langle S \rangle - \langle P \rangle}{\langle N \rangle - \langle P \rangle} \right)] \quad (3)$$

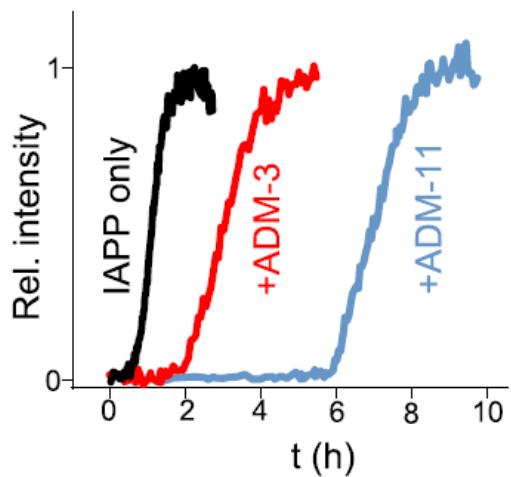
Each independent variable is the average of eight plate replicates from the negative control ( $\langle N \rangle$ ), positive control ( $\langle P \rangle$ ), and samples ( $\langle S \rangle$ ). Results presented for viability experiments are an average of three such experiments conducted independently on different days. Error bars represent the standard error of the mean.

**Fluorescence correlation spectroscopy.** FCS measurements were made on a laboratory-built instrument based around an inverted microscope using an Olympus IX71 microscope (Olympus, Tokyo, Japan), as described previously<sup>2</sup>. Briefly, a continuous-emission 488-nm diode-pumped solid-state 50 mW laser was set to 5–20 mW output power and further adjusted with neutral density filters to 18 mW of power just prior to entering the microscope. Fluorescence was collected through the objective and separated from the excitation laser using a Z488rdc long-pass dichroic and an HQ600/200m bandpass filter (Chroma, Bellows Falls, VT, USA). Fluorescence was focused onto the aperture of a 50 mm optical fiber coupled to an avalanche photodiode (Perkin Elmer, Waltham, MA, USA). A digital correlator (Flex03LQ-12; Correlator.com, Bridgewater, NJ, USA) was used to generate autocorrelation curves.

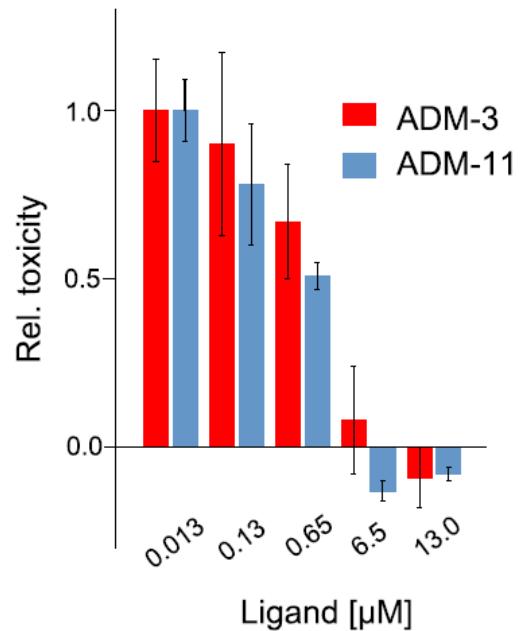
Measurements were made in 8-well chambered coverglasses (Nunc, Rochester, NY, USA) which were plasma treated followed by precoating with polylysine-conjugated polyethylene glycol (PEG-PLL), to prevent ADM-116 and/or IAPP from adsorbing to chamber surfaces. Low density PEG coating was preformed by preparing a 100 mg/mL solution of PEG (MW= 2KDa, NANOCs, Boston, MA, USA) in Poly-L-Lysine hydrobromide (Sigma Aldrich, St. Louis, MI, USA). Reaction was performed for 6 h in dark at r.t., followed by overnight dialysis. Chambers were incubated overnight with PEG-PLL solution, rinsed thoroughly with Millipore water, and stored in water before use. ADM-116<sub>F</sub> (25 nM)(Synthesis and characterisation of ADM-116<sub>F</sub> is presented elsewhere)<sup>3</sup> was added to buffer solutions (20 mM KCl, 50 mM sodium phosphate, pH 7.4) containing either IAPP (1 μM) or to a mixture of IAPP (1 μM) and liposomes (25 μM, DOPG:DOPC, 1:1, 100 nm). The mixture of IAPP and liposome was pre-incubated for 30 mins prior to the addition of ADM-116<sub>F</sub>. The autocorrelation curves were collected at regular intervals (10 min), and each autocorrelation curve was collected over 10 s and repeated 30 times. The data has been analysed as a function of count rates with QuickFit 3.0<sup>4</sup>.

## Supplementary Figures

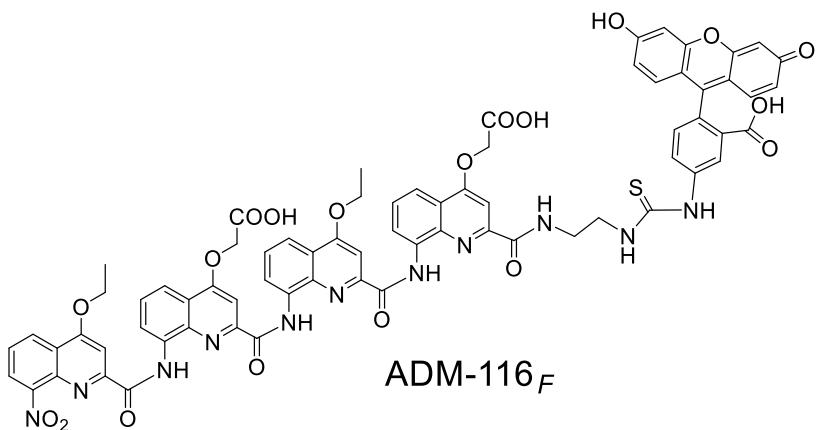
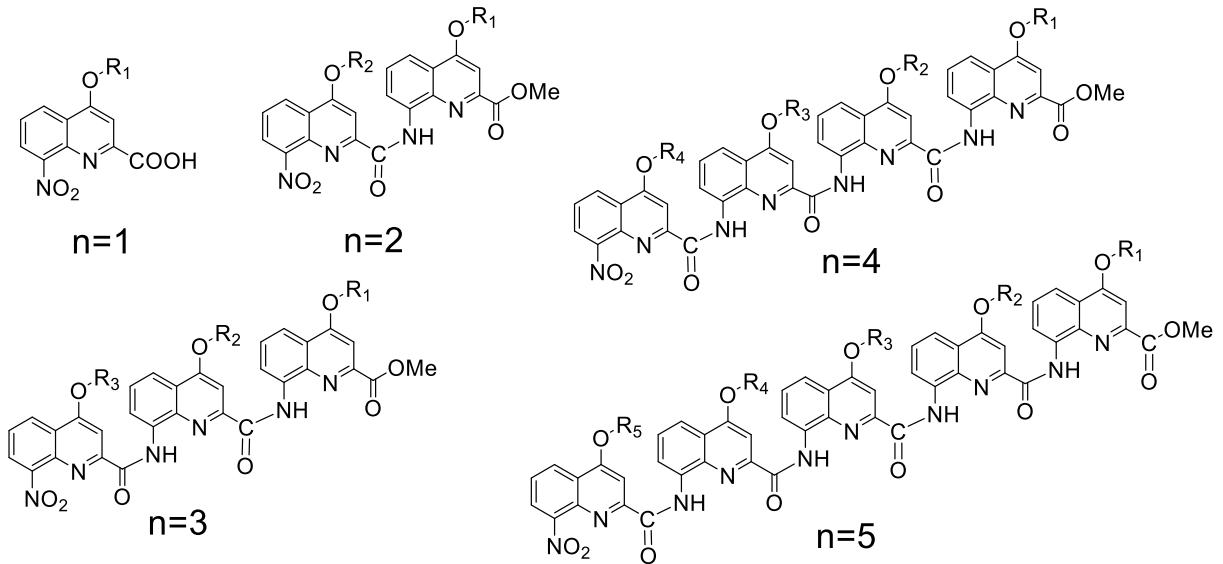




**Fig. S2.** Representative kinetic profiles of lipid catalysed IAPP fibrillation in the absence (black) and presence of ADM-3 (red) or ADM-11 (cyan) at equimolar ratio. [IAPP] = 10  $\mu$ M, (DOPG:DOPC, 1:1, d = 100 nm) = 630  $\mu$ M.



**Fig. S3.** Dose dependence of rescue of INS-1 cells from IAPP mediated toxicity by ADM-3 (red) and ADM-11 (cyan). INS-1 cells were incubated with 13 μM IAPP and oligopyridylamides at the indicated molar ratios for 48 h before measuring cell viability using CTB (cell titer blue) assay.

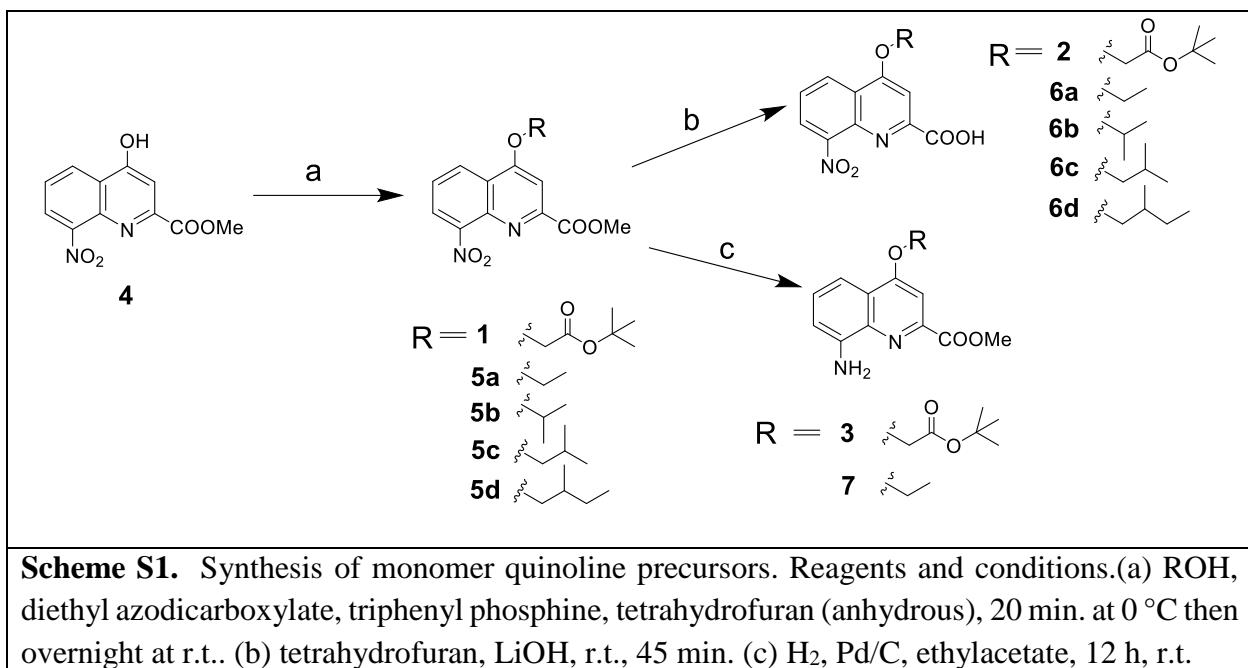


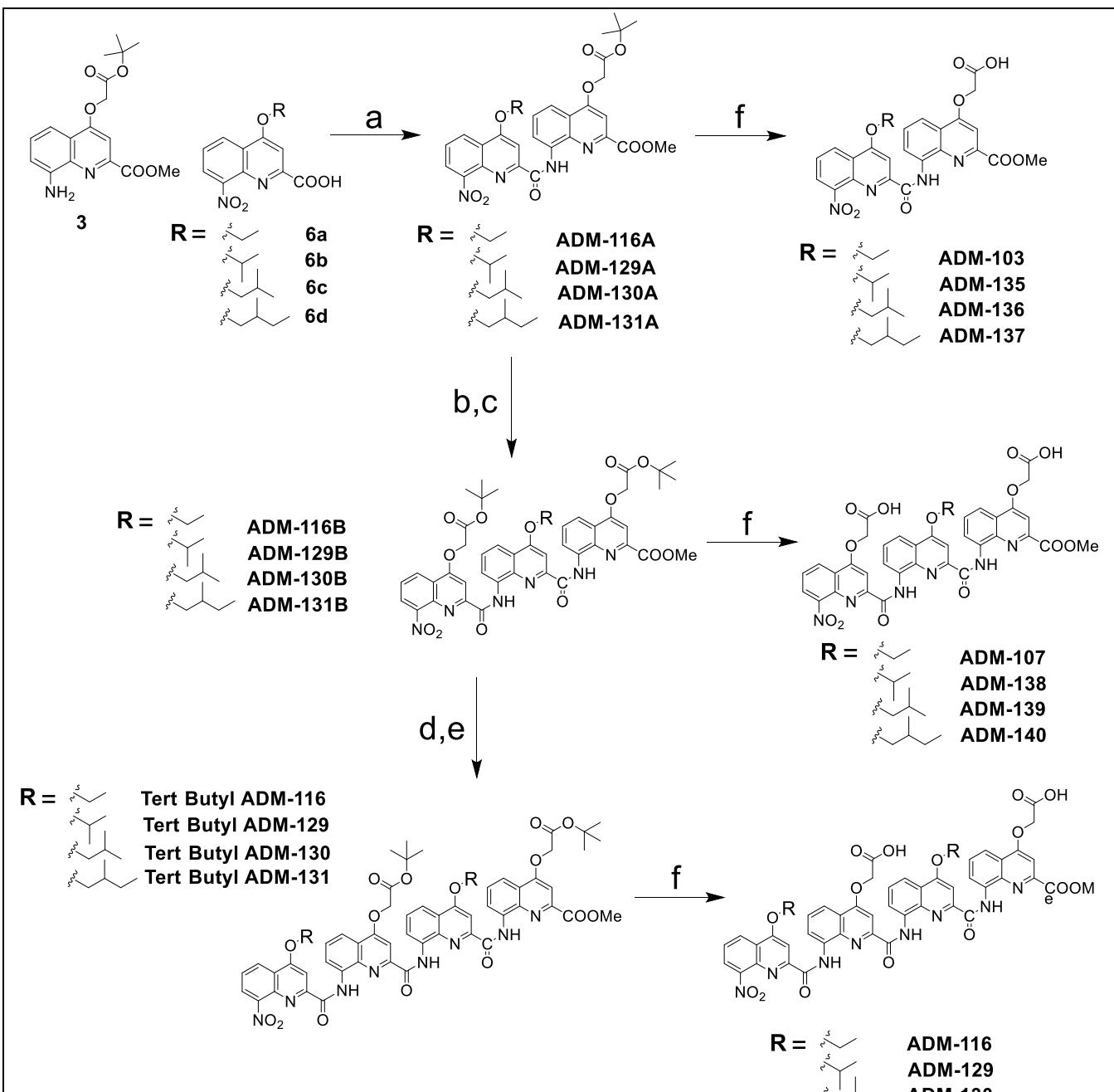
Compound	n	R <sub>1</sub>	R <sub>2</sub>	R <sub>3</sub>	R <sub>4</sub>	R <sub>5</sub>
ADM101	1					
ADM102	1					
ADM143	1					
ADM144	1					
ADM145	1					
ADM103	2					
ADM135	2					
ADM136	2					
ADM137	2					

	ADM104	2						
	ADM105	2						
	ADM106	3						
	ADM107	3						
	ADM138	3						
	ADM139	3						
	ADM140	3						
	ADM108	3						
	ADM109	3						
	ADM110	3						
	ADM111	4						
	ADM112	4						
	ADM113	4						
	ADM114	4						
	ADM115	4						
	ADM116	4						
	ADM117	4						
	ADM-141	4						
	ADM-142	4						
	ADM118	5						
	ADM119	5						
	ADM120	5						
	ADM121	5						
	ADM122	5						
	ADM123	5						
	ADM124	5						
	ADM125	5						
	ADM126	5						
	ADM129	4						

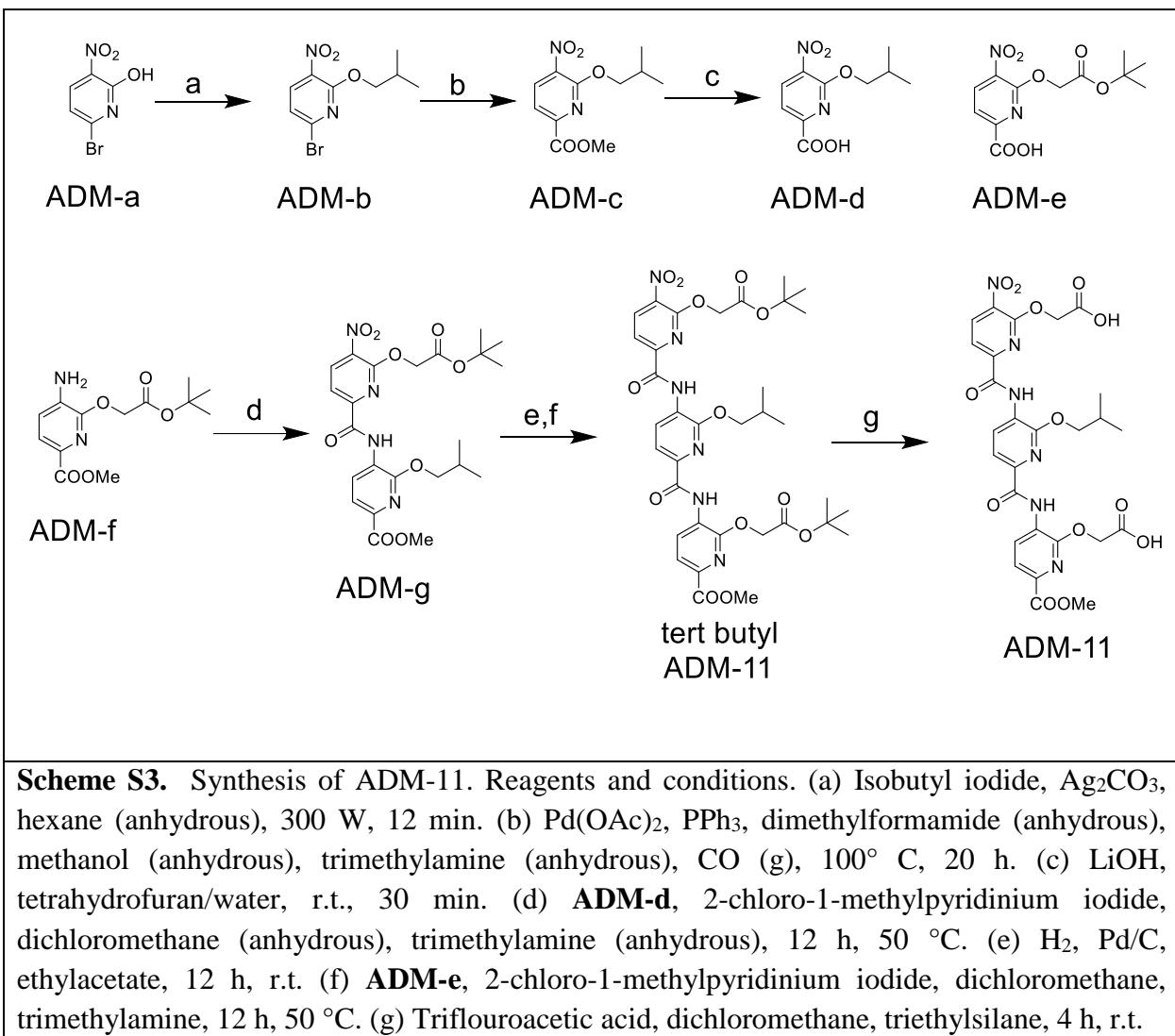
	ADM130	4					
	ADM131	4					

**Table S1.** Chemical structure of the oligoquinolines used in the study.





**Scheme S2.** Synthesis of the oligoquinolines with various side chain functionalities. Reagents and conditions. (a) 2-chloro-1-methylpyridinium iodide, dichloromethane (anhydrous), trimethylamine (anhydrous), 12 h, 50 °C. (b) H<sub>2</sub>, Pd/C, ethylacetate, 24 h, r.t. (c) **6a**, 2-chloro-1-methylpyridinium iodide, dichloromethane, trimethylamine, 12 h, 50 °C. (d) H<sub>2</sub>, Pd/C, ethylacetate, 12 h, r.t. (e) **6a/6b/6c/6d**, 2-chloro-1-methylpyridinium iodide, dichloromethane (anhydrous), trimethylamine (anhydrous), 12 h, 50 °C. (f) Trifluoroacetic acid, dichloromethane, triethylsilane, 4 h, r.t.



Compound	% yield
5a	82
5b	79
5c	85
5d	86
6a	93
6b	91
6c	92
6d	94

**Table S2.** % yield for the monomeric analogs of O-alkylated quinolines (Scheme S1).

**Synthesis of 1, 2, 3, 4, 5, and 6 have been reported elsewhere** (Kumar et. al. Chem. Biol. 2014)

**Synthesis of 5b, 5c, and 5d.**

To a solution of 4 (5 g, 20.15 mmol) in tetrahydrofuran (dry, 50 mL), triphenylphosphine (6.85 g, 30.2 mmol, 1.5 eq.) and alcohol (30.2 mmol, 1.5 eq.) were added under inert atmosphere and stirred for 10 min at 0 °C. To this mixture, diisopropyl azodicarboxylate (5.2 mL, 26.2 mmol, 1.3 eq.) was added dropwise over a period of 20 min at 0 °C under inert atmosphere. The reaction mixture was stirred for another 30 min and then at room temperature overnight. The volatiles were removed on rotovap and column chromatography (0 to 25% ethyl acetate in hexane, v/v) afforded the desired product as yellow solid (see Table S2 for % yield).

**5b**

<sup>1</sup>H NMR (400 MHz, Chloroform-*d*) δ 8.49 – 8.39 (m, 1H), 8.12 – 8.04 (td, *J* = 7.9, 7.4, 1.6 Hz, 2H), 7.64 – 7.63 (s, 1H), 7.63 – 7.57 (m, 1H), 4.02 – 4.00 (d, *J* = 0.7 Hz, 3H), 1.53 – 1.47 (d, *J* = 6.1 Hz, 7H). MS (MALDI-TOF) calcd for C<sub>14</sub>H<sub>14</sub>N<sub>2</sub>O<sub>5</sub> [(M+H)<sup>+</sup>], 290.28, obsd: 290.81.

**5c**

<sup>1</sup>H NMR (600 MHz, Chloroform-*d*) δ 8.51 – 8.46 (dd, *J* = 8.4, 1.4 Hz, 1H), 8.13 – 8.07 (m, 1H), 7.69 – 7.63 (m, 2H), 4.12 – 4.07 (d, *J* = 6.5 Hz, 2H), 4.05 – 4.02 (s, 3H), 2.02 – 1.85 (dt, *J* = 13.6, 6.8 Hz, 1H), 1.29 – 1.23 (d, *J* = 6.3 Hz, 6H), 1.20 – 1.09 (d, *J* = 6.8 Hz, 6H). MS (MALDI-TOF) calcd for C<sub>15</sub>H<sub>16</sub>N<sub>2</sub>O<sub>5</sub> [(M+H)<sup>+</sup>], 304.30, obsd: 304.83.

**5d**

<sup>1</sup>H NMR (600 MHz, Chloroform-*d*) δ 8.48 – 8.43 (dd, *J* = 8.5, 1.4 Hz, 1H), 8.10 – 8.06 (dd, *J* = 7.5, 1.4 Hz, 1H), 7.68 – 7.65 (m, 1H), 7.65 – 7.63 (s, 1H), 4.22 – 4.08 (m, 3H), 4.05 – 4.01 (s, 3H), 1.74 – 1.61 (m, 1H), 1.30 – 1.22 (m, 2H), 1.16 – 1.13 (d, *J* = 6.8 Hz, 3H), 1.04 – 1.00 (t, *J* = 7.5 Hz, 3H). MS (MALDI-TOF) calcd for C<sub>16</sub>H<sub>18</sub>N<sub>2</sub>O<sub>5</sub> [(M+H)<sup>+</sup>], 318.33, obsd: 318.34.

**Synthesis of 5a** (Reported elsewhere as compound 5)<sup>3</sup>

**Synthesis of 6a, 6b, 6c, and 6d.**

To a solution of 5 (2.0 g, 7.2 mmol) in tetrahydrofuran (100 mL), lithium hydroxide (0.2 N) in water (55 mL) was added and the solution was stirred for 45 min. Acetic acid (conc.) was then added with constant stirring to bring down the pH to ~4. To this reaction mixture, dichloromethane (200 mL) was added and the organic layer was successively washed once with water (20 mL) and brine (20 mL), dried over sodium sulfate, filtered and evaporated to afford 6 as a yellow solid (1.21g, 85%) (see Table S2 for % yield).

**6a** (Reported elsewhere as compound 6)<sup>3</sup>

**6b (ADM-143)**

<sup>1</sup>H NMR (600 MHz, Chloroform-*d*) δ 8.56 – 8.49 (dd, *J* = 8.5, 1.4 Hz, 1H), 8.23 – 8.18 (dd, *J* = 7.4, 1.5 Hz, 1H), 7.73 – 7.72 (s, 1H), 7.71 – 7.68 (dd, *J* = 8.7, 7.6 Hz, 1H), 5.07 – 5.00 (p, *J* = 6.1 Hz, 1H), 1.16 – 1.05 (d, *J* = 6.6 Hz, 6H). MS (MALDI-TOF) (m/z): calculated for C<sub>13</sub>H<sub>12</sub>N<sub>2</sub>O<sub>5</sub> [(M+H)+]: 276.25, found 276.71.

**6c (ADM-144)**

<sup>1</sup>H NMR (400 MHz, Chloroform-*d*) δ 8.55 – 8.48 (dd, *J* = 8.5, 1.4 Hz, 1H), 8.22 – 8.17 (dd, *J* = 7.5, 1.4 Hz, 1H), 7.74 – 7.68 (m, 2H), 4.19 – 4.02 (d, *J* = 6.5 Hz, 2H), 2.37 – 2.25 (dq, *J* = 13.4, 6.7 Hz, 1H), 1.16 – 1.10 (d, *J* = 6.7 Hz, 6H). MS (MALDI-TOF) (m/z): calculated for C<sub>14</sub>H<sub>14</sub>N<sub>2</sub>O<sub>5</sub> [(M+H)+]: 290.28, found 290.53.

**6d (ADM-145)**

<sup>1</sup>H NMR (400 MHz, Chloroform-*d*) δ 8.62 – 8.46 (dd, *J* = 8.4, 1.4 Hz, 1H), 8.30 – 8.18 (dd, *J* = 7.6, 1.4 Hz, 1H), 7.82 – 7.60 (m, 2H), 4.27 – 4.11 (m, 2H), 1.73 – 1.59 (ddd, *J* = 13.4, 7.5, 5.7 Hz,

1H), 1.31 – 1.19 (m, 2H), 1.18 – 1.10 (d,  $J$  = 6.8 Hz, 3H), 1.06 – 0.98 (t,  $J$  = 7.5 Hz, 3H). MS (MALDI-TOF) (m/z): calculated for C<sub>15</sub>H<sub>16</sub>N<sub>2</sub>O<sub>5</sub> [(M+H)+]: 304.30, found 304.54.

### **Standard protocol for reduction of nitro-oligoquinolines.**

To a solution of nitroquinoline (0.1-0.5 mmol) in tetrahydrofuran (10 mL), Pd/C (10% wt.) was added and the reaction started with constant stirring at room temperature in the atmosphere of H<sub>2</sub> (g). The progress of the reaction was monitored by TLC. Generally, the reduction reactions were completed in 4-6 h. The reaction mixture was filtered and dried which result in a yellow solid with quantitative yield. The product was used in the next step without further characterization.

### **Standard protocol for amide coupling.**

To a solution of **2** (1.2 mmol) in anhydrous dichloromethane (10 mL), triethylamine (4.0 mmol) and 2-chloromethyl-1-methyl pyridinium iodide (1.2 mmol) were added and the reaction was refluxed for 20 min. at 50 °C under inert atmosphere. To this solution, amino-oligoquinoline (1.0 mmol) was added and reaction started with constant stirring at 50 °C under inert atmosphere. The reaction mixture was stirred for 4 h. after which the volatiles were removed on rotovap. Flash chromatography (0 to 35% ethylacetate in hexane, v/v) yielded the desired product as a yellow to brown solid.

### **Standard protocol for deprotection of oligoquinolines.**

To a solution of oligoquinoline (0.04 mmol), a cocktail solution (2 mL, dichlormethane: trifluoroacetic acid: triethylsilane, 80:15:5, v/v) was added and the solution was stirred at room temperature for 4 h. The reaction mixture was dried and washed with cold diethyl ether (4 × 3 mL) that results in a yellow to brown solid.

Compound	% yield
ADM101	71
ADM102	73
ADM103	73
ADM104	69
ADM105	71
ADM106	66
ADM107	67
ADM108	68
ADM109	70
ADM110	71
ADM111	72
ADM112	67
ADM113	69
ADM114	68
ADM115	67
ADM117	69
ADM118	72
ADM119	69
ADM120	73
ADM121	71

ADM122	65
ADM123	70
ADM124	68
ADM125	66
ADM126	72
ADM127	59
ADM128	62
ADM129	67
ADM130	73
ADM131	74
ADM135	85
ADM136	88
ADM137	79
ADM138	80
ADM139	84
ADM140	81
ADM141	82
ADM142	78
<b>Table S3.</b> Combined yield (O- <i>tert</i> butyl protected and deprotected) for the oligoquinolines used in the study.	

**O-*tert* butyl analog of ADM-103** (Reported earlier as compound 8)<sup>3</sup>

**O-*tert* butyl analog of ADM-104** (Reported earlier as compound 11)<sup>3</sup>

**O-*tert* butyl analog of ADM-105** (Reported earlier as O-*tert* butyl analog of OQ2)<sup>5</sup>

### **O-*tert* butyl analog of ADM-106**

<sup>1</sup>H NMR (400 MHz, Chloroform-*d*) δ 12.24 – 12.20 (s, 1H), 12.15 – 12.12 (s, 1H), 9.05 – 8.98 (ddd, *J* = 14.0, 7.7, 1.2 Hz, 2H), 8.47 – 8.40 (dd, *J* = 8.4, 1.4 Hz, 1H), 8.16 – 8.09 (dd, *J* = 8.4, 1.3 Hz, 1H), 8.03 – 7.97 (dd, *J* = 8.5, 1.3 Hz, 1H), 7.93 – 7.88 (s, 1H), 7.78 – 7.72 (m, 2H), 7.72 – 7.67 (t, *J* = 8.0 Hz, 1H), 7.60 – 7.55 (dd, *J* = 7.6, 1.4 Hz, 1H), 7.42 – 7.37 (dd, *J* = 8.4, 7.5 Hz, 1H), 6.73 – 6.61 (s, 1H), 4.96 – 4.87 (s, 2H), 4.64 – 4.57 (s, 2H), 4.55 – 4.44 (q, *J* = 7.0 Hz, 2H), 3.46 – 3.39 (s, 3H), 1.71 – 1.66 (t, *J* = 7.0 Hz, 3H), 1.54 – 1.50 (d, *J* = 7.6 Hz, 19H). MS (MALDI-TOF) calcd for C<sub>45</sub>H<sub>44</sub>N<sub>6</sub>O<sub>13</sub> (M+H<sup>+</sup>), 876.88, obsd: 876.61.

**O-*tert* butyl analog of ADM-107** (Reported earlier as compound 9)<sup>3</sup>

### **O-*tert* butyl analog of ADM-108**

<sup>1</sup>H NMR (400 MHz, Chloroform-*d*) δ 12.23 – 12.21 (s, 1H), 12.21 – 12.19 (s, 1H), 9.07 – 9.00 (dd, *J* = 7.6, 1.2 Hz, 1H), 9.00 – 8.94 (dd, *J* = 7.7, 1.3 Hz, 1H), 8.61 – 8.54 (dd, *J* = 8.4, 1.5 Hz, 1H), 8.17 – 8.11 (dd, *J* = 8.5, 1.3 Hz, 1H), 7.96 – 7.89 (dd, *J* = 8.5, 1.3 Hz, 1H), 7.85 – 7.82 (s, 1H), 7.77 – 7.75 (s, 1H), 7.75 – 7.67 (td, *J* = 8.1, 6.9 Hz, 2H), 7.63 – 7.58 (dd, *J* = 7.6, 1.5 Hz, 1H), 7.44 – 7.37 (m, 1H), 6.80 – 6.76 (s, 1H), 4.98 – 4.96 (s, 2H), 4.95 – 4.93 (s, 2H), 4.14 – 4.11 (dd, *J* = 7.1, 4.4 Hz, 2H), 3.48 – 3.44 (s, 3H), 1.61 – 1.59 (s, 9H), 1.59 – 1.58 (s, 3H), 1.56 – 1.54 (s, 9H). MS (MALDI-TOF) calcd for C<sub>45</sub>H<sub>44</sub>N<sub>6</sub>O<sub>13</sub> (M+H<sup>+</sup>), 876.88, obsd: 875.51.

**O-*tert* butyl analog of ADM-109** (Reported earlier as compound 9)<sup>3</sup>

**O-*tert* butyl analog of ADM-110** (Reported earlier as O-*tert* butyl analog of OQ3)<sup>3</sup>

**O-*tert* butyl analog of ADM-111** (Reported earlier as O-*tert* butyl analog of OQ4)<sup>5</sup>

**O-*tert* butyl analog of ADM-112**

<sup>1</sup>H NMR (400 MHz, Chloroform-*d*) δ 12.33 – 12.26 (s, 1H), 11.89 – 11.82 (s, 1H), 11.70 – 11.64 (s, 1H), 9.23 – 9.10 (dd, *J* = 7.8, 1.3 Hz, 1H), 8.71 – 8.56 (dd, *J* = 8.4, 1.5 Hz, 1H), 8.44 – 8.36 (dd, *J* = 7.8, 1.3 Hz, 1H), 8.18 – 8.14 (dd, *J* = 7.7, 1.3 Hz, 1H), 8.12 – 8.06 (ddd, *J* = 8.5, 6.1, 1.3 Hz, 2H), 7.95 – 7.90 (dd, *J* = 8.4, 1.3 Hz, 1H), 7.89 – 7.86 (s, 1H), 7.83 – 7.76 (m, 1H), 7.71 – 7.62 (m, 2H), 7.51 – 7.45 (m, 1H), 7.41 – 7.39 (s, 1H), 7.37 – 7.29 (t, *J* = 8.0 Hz, 1H), 6.85 – 6.79 (s, 1H), 6.65 – 6.60 (s, 1H), 5.08 – 4.95 (s, 2H), 4.74 – 4.66 (s, 2H), 4.68 – 4.59 (s, 2H), 4.58 – 4.47 (q, *J* = 7.0 Hz, 2H), 3.50 – 3.38 (s, 3H), 1.76 – 1.67 (t, *J* = 6.9 Hz, 3H), 1.65 – 1.60 (s, 9H), 1.57 – 1.50 (d, *J* = 6.6 Hz, 18H). MS (MALDI-TOF) calcd for C<sub>61</sub>H<sub>60</sub>N<sub>8</sub>O<sub>17</sub> (M+H<sup>+</sup>), 1176.40, obsd: 1176.40.

**O-*tert* butyl analog of ADM-113**

<sup>1</sup>H NMR (400 MHz, Chloroform-*d*) δ 12.28 – 12.23 (s, 1H), 11.90 – 11.85 (s, 1H), 11.66 – 11.61 (s, 1H), 9.17 – 9.10 (dd, *J* = 7.7, 1.2 Hz, 1H), 8.66 – 8.59 (dd, *J* = 8.3, 1.4 Hz, 1H), 8.35 – 8.28 (dd, *J* = 7.7, 1.3 Hz, 1H), 8.21 – 8.13 (dd, *J* = 7.8, 1.3 Hz, 1H), 8.10 – 8.03 (dd, *J* = 8.4, 1.2 Hz, 1H), 8.05 – 7.96 (m, 3H), 7.81 – 7.72 (m, 2H), 7.70 – 7.55 (m, 2H), 7.50 – 7.41 (t, *J* = 8.0 Hz, 1H), 7.36 – 7.27 (t, *J* = 8.1 Hz, 1H), 6.81 – 6.76 (s, 1H), 6.72 – 6.67 (s, 1H), 5.02 – 4.97 (d, *J* = 1.8 Hz, 2H), 4.96 – 4.91 (s, 2H), 4.70 – 4.65 (s, 2H), 4.19 – 4.08 (q, *J* = 6.9 Hz, 2H), 3.46 – 3.41 (s, 3H), 1.62 – 1.56 (d, *J* = 3.0 Hz, 18H), 1.55 – 1.50 (s, 9H), 0.91 – 0.81 (m, 3H). MS (MALDI-TOF) calcd for C<sub>61</sub>H<sub>60</sub>N<sub>8</sub>O<sub>17</sub> (M+H<sup>+</sup>), 1176.40, obsd: 1175.89.

**O-*tert* butyl analog of ADM-114**

<sup>1</sup>H NMR (400 MHz, Chloroform-*d*) δ 12.36 – 12.25 (s, 1H), 11.91 – 11.83 (s, 1H), 11.71 – 11.60 (s, 1H), 9.15 – 9.05 (dd, *J* = 7.7, 1.4 Hz, 1H), 8.71 – 8.61 (dd, *J* = 8.3, 1.5 Hz, 1H), 8.47 – 8.36

(dd,  $J = 7.7$ , 1.3 Hz, 1H), 8.20 – 8.12 (dd,  $J = 7.6$ , 1.3 Hz, 1H), 8.11 – 8.05 (dd,  $J = 8.4$ , 1.3 Hz, 1H), 8.05 – 7.93 (m, 2H), 7.76 – 7.74 (s, 1H), 7.68 – 7.59 (m, 2H), 7.56 – 7.49 (tt,  $J = 7.0$ , 1.3 Hz, 1H), 7.46 – 7.30 (td,  $J = 16.3$ , 7.9 Hz, 3H), 6.88 – 6.84 (s, 1H), 6.63 – 6.60 (d,  $J = 1.2$  Hz, 1H), 5.05 – 4.97 (s, 2H), 4.97 – 4.90 (s, 2H), 4.72 – 4.53 (d,  $J = 10.5$  Hz, 2H), 4.25 – 4.12 (d,  $J = 7.3$  Hz, 2H), 3.53 – 3.28 (d,  $J = 1.5$  Hz, 3H), 1.64 – 1.56 (dd,  $J = 5.3$ , 1.4 Hz, 19H), 1.54 – 1.49 (d,  $J = 1.2$  Hz, 9H). 0.95 – 0.87 (m, 3H). MS (MALDI-TOF) calcd for  $C_{61}H_{60}N_8O_{17}$  ( $M+H^+$ ), 1176.40, obsd: 1175.79.

### **O-*tert* butyl analog of ADM-115**

$^1H$  NMR (400 MHz, Chloroform-*d*)  $\delta$  12.30 – 12.21 (s, 1H), 11.92 – 11.84 (s, 1H), 11.68 – 11.60 (s, 1H), 9.20 – 9.07 (dd,  $J = 7.7$ , 1.2 Hz, 1H), 8.67 – 8.57 (dd,  $J = 8.3$ , 1.4 Hz, 1H), 8.35 – 8.28 (dd,  $J = 7.7$ , 1.3 Hz, 1H), 8.22 – 8.13 (dd,  $J = 7.8$ , 1.3 Hz, 1H), 8.09 – 8.05 (dd,  $J = 8.4$ , 1.2 Hz, 1H), 8.03 – 7.97 (m, 3H), 7.77 – 7.76 (s, 1H), 7.69 – 7.64 (dd,  $J = 7.6$ , 1.5 Hz, 1H), 7.62 – 7.56 (t,  $J = 8.0$  Hz, 1H), 7.49 – 7.43 (t,  $J = 8.0$  Hz, 1H), 7.39 – 7.37 (s, 1H), 7.35 – 7.29 (t,  $J = 8.1$  Hz, 1H), 6.80 – 6.77 (s, 1H), 6.70 – 6.67 (s, 1H), 5.04 – 4.96 (m, 2H), 4.96 – 4.90 (s, 2H), 4.72 – 4.61 (s, 2H), 4.21 – 4.09 (q,  $J = 6.9$  Hz, 2H), 3.48 – 3.37 (s, 3H), 1.62 – 1.56 (m, 21H), 1.54 – 1.52 (s, 9H). MS (MALDI-TOF) calcd for  $C_{61}H_{60}N_8O_{17}$  ( $M+H^+$ ), 1176.40, obsd: 1175.65.

**O-*tert* butyl analog of ADM-116** (Reported earlier as compound 10)<sup>3</sup>

**O-*tert* butyl analog of ADM-117** (Reported earlier as compound 13)<sup>3</sup>

**O-*tert* butyl analog of ADM-118** (Reported earlier as O-*tert* butyl analog of OQ5)<sup>5</sup>

### **O-*tert* butyl analog of ADM-119**

$^1H$  NMR (400 MHz, Chloroform-*d*)  $\delta$  11.97 – 11.91 (s, 1H), 11.73 – 11.72 (s, 1H), 11.72 – 11.71 (s, 1H), 11.57 – 11.52 (s, 1H), 8.57 – 8.52 (dd,  $J = 8.3$ , 1.5 Hz, 1H), 8.52 – 8.46 (dt,  $J = 7.8$ , 1.4 Hz, 2H), 8.24 – 8.21 (dd,  $J = 5.1$ , 1.3 Hz, 1H), 8.21 – 8.18 (d,  $J = 1.2$  Hz, 1H), 8.16 – 8.12 (dd,  $J$

$\delta$  = 8.4, 1.3 Hz, 1H), 8.09 – 8.04 (ddd,  $J$  = 8.5, 2.7, 1.3 Hz, 1H), 7.97 – 7.92 (m, 1H), 7.74 – 7.63 (dt,  $J$  = 13.7, 8.0 Hz, 2H), 7.60 – 7.51 (m, 2H), 7.49 – 7.46 (s, 1H), 7.46 – 7.38 (m, 4H), 6.78 – 6.76 (s, 1H), 6.76 – 6.72 (s, 1H), 6.54 – 6.50 (s, 1H), 5.09 – 5.01 (d,  $J$  = 3.1 Hz, 2H), 4.78 – 4.60 (m, 6H), 3.67 – 3.54 (dd,  $J$  = 11.9, 7.0 Hz, 2H), 3.25 – 3.14 (s, 3H), 1.83 – 1.74 (t,  $J$  = 6.9 Hz, 3H), 1.69 – 1.66 (s, 9H), 1.66 – 1.62 (s, 9H), 1.55 – 1.54 (s, 9H), 1.53 – 1.51 (s, 9H). MS (MALDI-TOF) calcd for  $C_{77}H_{76}N_{10}O_{21}$  ( $M+H^+$ ), 1476.52, obsd: 1476.79.

### **O-*tert* butyl analog of ADM-120**

$^1H$  NMR (400 MHz, Chloroform-*d*)  $\delta$  11.94 – 11.89 (s, 1H), 11.73 – 11.71 (s, 1H), 11.70 – 11.69 (s, 1H), 11.56 – 11.52 (s, 1H), 8.64 – 8.59 (dd,  $J$  = 8.3, 1.4 Hz, 1H), 8.54 – 8.49 (dd,  $J$  = 7.7, 1.2 Hz, 1H), 8.48 – 8.42 (dd,  $J$  = 7.7, 1.3 Hz, 1H), 8.23 – 8.14 (m, 3H), 8.07 – 8.00 (tdd,  $J$  = 8.5, 4.3, 1.4 Hz, 4H), 7.96 – 7.91 (dd,  $J$  = 8.4, 1.3 Hz, 1H), 7.71 – 7.62 (td,  $J$  = 7.9, 5.7 Hz, 2H), 7.58 – 7.50 (ddt,  $J$  = 18.6, 9.0, 2.5 Hz, 2H), 7.49 – 7.47 (s, 1H), 7.48 – 7.31 (s, 1H), 6.78 – 6.75 (s, 1H), 6.73 – 6.71 (s, 1H), 6.53 – 6.49 (s, 1H), 5.06 – 4.98 (d,  $J$  = 4.0 Hz, 2H), 4.74 – 4.69 (d,  $J$  = 6.4 Hz, 2H), 4.66 – 4.61 (d,  $J$  = 4.1 Hz, 2H), 4.51 – 4.44 (m, 2H), 3.90 – 3.81 (m, 2H), 3.19 – 3.16 (s, 3H), 1.82 – 1.76 (t,  $J$  = 7.0 Hz, 3H), 1.66 – 1.63 (s, 9H), 1.63 – 1.61 (s, 9H), 1.54 – 1.51 (s, 9H), 1.52 – 1.49 (s, 9H). MS (MALDI-TOF) calcd for  $C_{77}H_{76}N_{10}O_{21}$  ( $M+H^+$ ), 1476.52, obsd: 1476.77.

### **O-*tert* butyl analog of ADM-121**

$^1H$  NMR (400 MHz, Chloroform-*d*) major enantiomer:  $\delta$  12.00 – 11.97 (s, 1H), 11.81 – 11.77 (s, 1H), 11.75 – 11.72 (s, 1H), 11.57 – 11.52 (s, 1H), 8.71 – 8.62 (dd,  $J$  = 8.3, 1.5 Hz, 1H), 8.59 – 8.50 (ddd,  $J$  = 11.0, 7.6, 1.3 Hz, 2H), 8.21 – 8.14 (ddd,  $J$  = 8.6, 3.3, 1.4 Hz, 2H), 8.14 – 8.09 (ddd,  $J$  = 7.7, 4.6, 1.3 Hz, 2H), 8.05 – 8.03 (d,  $J$  = 1.3 Hz, 3H), 8.03 – 8.01 (d,  $J$  = 1.5 Hz, 3H), 7.74 – 7.65 (td,  $J$  = 7.9, 3.6 Hz, 2H), 7.55 – 7.53 (s, 2H), 7.46 – 7.43 (s, 1H), 6.80 – 6.76 (s, 1H), 6.76 – 6.73 (s, 1H), 6.52 – 6.47 (s, 1H), 5.07 – 5.05 (d,  $J$  = 2.7 Hz, 3H), 4.68 – 4.54 (m, 2H), 4.33 – 4.13 (m,

3H), 3.81 – 3.59 (m, 2H), 3.26 – 3.09 (s, 3H), 1.64 – 1.62 (d,  $J$  = 1.3 Hz, 18H), 1.55 – 1.53 (s, 9H), 1.53 – 1.49 (s, 9H). MS (MALDI-TOF) calcd for  $C_{77}H_{76}N_{10}O_{21}$  ( $M+H^+$ ), 1476.52, obsd: 1476.23.

### **O-*tert* butyl analog of ADM-122**

$^1H$  NMR (400 MHz, Chloroform-*d*)  $\delta$  11.99 – 11.95 (s, 1H), 11.77 – 11.74 (s, 1H), 11.73 – 11.71 (s, 1H), 11.55 – 11.49 (s, 1H), 8.64 – 8.58 (dd,  $J$  = 8.4, 1.5 Hz, 1H), 8.55 – 8.50 (dd,  $J$  = 7.7, 1.4 Hz, 1H), 8.49 – 8.44 (m, 1H), 8.22 – 8.17 (dd,  $J$  = 7.6, 1.3 Hz, 1H), 8.17 – 8.14 (dd,  $J$  = 7.8, 1.2 Hz, 1H), 8.13 – 8.08 (m, 1H), 8.07 – 8.06 (d,  $J$  = 1.1 Hz, 1H), 8.05 – 7.98 (m, 5H), 7.95 – 7.89 (dd,  $J$  = 8.4, 1.3 Hz, 1H), 7.73 – 7.67 (t,  $J$  = 8.1 Hz, 1H), 7.66 – 7.61 (t,  $J$  = 8.0 Hz, 1H), 7.59 – 7.48 (ddt,  $J$  = 15.1, 7.1, 1.5 Hz, 2H), 6.83 – 6.79 (s, 1H), 6.72 – 6.68 (s, 1H), 6.53 – 6.48 (s, 1H), 5.05 – 5.03 (d,  $J$  = 2.1 Hz, 2H), 4.51 – 4.42 (m, 5H), 3.91 – 3.82 (m, 4H), 3.24 – 3.10 (s, 3H), 2.10 – 1.95 (m, 3H), 1.69 – 1.57 (m, 41H). MS (MALDI-TOF) calcd for  $C_{77}H_{76}N_{10}O_{21}$  ( $M+H^+$ ), 1476.52, obsd: 1477.78.

### **O-*tert* butyl analog of ADM-123**

$^1H$  NMR (400 MHz, Chloroform-*d*)  $\delta$  11.96 – 11.91 (s, 1H), 11.77 – 11.74 (s, 1H), 11.73 – 11.68 (s, 1H), 11.55 – 11.49 (s, 1H), 8.63 – 8.58 (dd,  $J$  = 8.4, 1.5 Hz, 1H), 8.52 – 8.48 (m, 1H), 8.47 – 8.42 (m, 1H), 8.22 – 8.14 (ddd,  $J$  = 10.9, 7.6, 1.3 Hz, 2H), 8.14 – 8.09 (dd,  $J$  = 8.4, 1.3 Hz, 1H), 8.04 – 7.99 (dd,  $J$  = 8.3, 1.5 Hz, 1H), 7.99 – 7.94 (dd,  $J$  = 8.5, 1.3 Hz, 1H), 7.94 – 7.90 (dd,  $J$  = 8.6, 1.2 Hz, 1H), 7.70 – 7.62 (q,  $J$  = 8.2 Hz, 1H), 7.59 – 7.50 (m, 2H), 7.47 – 7.33 (m, 6H), 6.75 – 6.73 (s, 1H), 6.72 – 6.70 (s, 1H), 6.60 – 6.57 (s, 1H), 5.08 – 4.98 (dd,  $J$  = 8.9, 3.1 Hz, 4H), 4.75 – 4.61 (m, 4H), 4.16 – 4.04 (m, 2H), 3.21 – 3.17 (s, 3H), 1.66 – 1.63 (s, 9H), 1.63 – 1.60 (s, 18H), 1.60 – 1.55 (t,  $J$  = 7.0 Hz, 3H), 1.54 – 1.50 (s, 9H). MS (MALDI-TOF) calcd for  $C_{77}H_{76}N_{10}O_{21}$  ( $M+H^+$ ), 1476.52, obsd: 1477.80.

### **O-*tert* butyl analog of ADM-124**

<sup>1</sup>H NMR (400 MHz, Chloroform-*d*) δ 12.02 – 11.95 (s, 1H), 11.80 – 11.76 (s, 1H), 11.76 – 11.72 (s, 1H), 11.58 – 11.53 (s, 1H), 8.60 – 8.56 (dd, *J* = 8.3, 1.5 Hz, 1H), 8.55 – 8.51 (dd, *J* = 7.6, 1.3 Hz, 2H), 8.24 – 8.21 (dd, *J* = 7.7, 1.3 Hz, 1H), 8.20 – 8.16 (dd, *J* = 8.4, 1.2 Hz, 1H), 8.16 – 8.11 (ddd, *J* = 8.4, 3.8, 1.3 Hz, 2H), 8.10 – 8.02 (m, 2H), 7.88 – 7.81 (dd, *J* = 8.4, 1.3 Hz, 1H), 7.75 – 7.64 (dt, *J* = 12.7, 8.0 Hz, 2H), 7.52 – 7.50 (s, 1H), 7.44 – 7.42 (s, 1H), 7.41 – 7.34 (m, 3H), 6.81 – 6.79 (s, 1H), 6.78 – 6.75 (s, 1H), 6.54 – 6.48 (s, 1H), 5.12 – 5.01 (d, *J* = 2.8 Hz, 2H), 4.76 – 4.63 (m, 4H), 4.61 – 4.47 (m, 2H), 4.32 – 4.09 (m, 2H), 3.24 – 3.15 (s, 3H), 1.87 – 1.73 (t, *J* = 7.0 Hz, 3H), 1.71 – 1.60 (d, *J* = 7.3 Hz, 12H), 1.60 – 1.48 (d, *J* = 9.9 Hz, 27H). MS (MALDI-TOF) calcd for C<sub>73</sub>H<sub>70</sub>N<sub>10</sub>O<sub>19</sub> (M+H<sup>+</sup>), 1391.41, obsd: 1391.72.

**O-*tert* butyl analog of ADM-125** (Reported earlier as compound *tert* butyl of ADM-116)<sup>3</sup>

**O-*tert* butyl analog of ADM-126** (Reported earlier as compound *tert* butyl of ADM-116)<sup>3</sup>

### **ADM-129A**

<sup>1</sup>H NMR (400 MHz, Chloroform-*d*) δ 11.89 – 11.84 (s, 1H), 9.14 – 9.07 (dd, *J* = 7.8, 1.3 Hz, 1H), 8.55 – 8.48 (dd, *J* = 8.4, 1.4 Hz, 1H), 8.21 – 8.13 (dd, *J* = 7.5, 1.4 Hz, 1H), 8.12 – 8.05 (dd, *J* = 8.4, 1.3 Hz, 1H), 7.97 – 7.92 (s, 1H), 7.72 – 7.59 (m, 2H), 7.57 – 7.52 (s, 1H), 5.14 – 5.02 (m, 1H), 4.87 – 4.82 (s, 2H), 4.25 – 4.17 (s, 3H), 1.57 – 1.54 (d, *J* = 6.1 Hz, 6H), 1.53 – 1.50 (s, 9H). MS (MALDI-TOF) calcd for C<sub>30</sub>H<sub>30</sub>N<sub>4</sub>O<sub>9</sub> (M+H<sup>+</sup>), 590.59, obsd: 590.43.

### **ADM-129B**

<sup>1</sup>H NMR (400 MHz, Chloroform-*d*) δ 12.26 – 12.21 (s, 1H), 12.19 – 12.14 (s, 1H), 9.06 – 8.97 (ddd, *J* = 9.3, 7.7, 1.3 Hz, 2H), 8.57 – 8.49 (dd, *J* = 8.4, 1.4 Hz, 1H), 8.07 – 7.97 (ddd, *J* = 11.5, 8.4, 1.3 Hz, 2H), 7.87 – 7.80 (d, *J* = 6.7 Hz, 2H), 7.80 – 7.71 (t, *J* = 8.1 Hz, 1H), 7.68 – 7.59 (m, 2H), 7.48 – 7.39 (dd, *J* = 8.4, 7.6 Hz, 1H), 6.72 – 6.67 (s, 1H), 5.16 – 5.00 (p, *J* = 6.1 Hz, 1H),

4.97 – 4.93 (s, 2H), 4.65 – 4.58 (s, 2H), 3.45 – 3.40 (s, 3H), 1.59 – 1.57 (s, 9H), 1.56 – 1.54 (d,  $J$  = 6.0 Hz, 6H), 1.53 – 1.51 (s, 9H). MS (MALDI-TOF) calcd for C<sub>46</sub>H<sub>46</sub>N<sub>6</sub>O<sub>13</sub> (M+H<sup>+</sup>), 890.31, obsd: 890.25.

### **O-*tert* butyl analog of ADM-129**

<sup>1</sup>H NMR (400 MHz, Chloroform-*d*) δ 12.37 – 12.31 (s, 1H), 11.96 – 11.86 (s, 1H), 11.77 – 11.60 (s, 1H), 9.16 – 9.08 (dd,  $J$  = 7.7, 1.2 Hz, 1H), 8.60 – 8.53 (dd,  $J$  = 8.3, 1.5 Hz, 1H), 8.41 – 8.35 (dd,  $J$  = 7.7, 1.3 Hz, 1H), 8.26 – 8.20 (dd,  $J$  = 7.8, 1.3 Hz, 1H), 8.11 – 8.07 (dd,  $J$  = 8.4, 1.3 Hz, 1H), 8.03 – 8.00 (d,  $J$  = 1.6 Hz, 2H), 7.80 – 7.77 (s, 1H), 7.76 – 7.68 (m, 1H), 7.66 – 7.57 (m, 1H), 7.55 – 7.50 (m, 1H), 7.49 – 7.46 (s, 1H), 7.40 – 7.35 (m, 1H), 6.92 – 6.88 (s, 1H), 6.64 – 6.61 (s, 1H), 5.16 – 5.03 (p,  $J$  = 6.0 Hz, 1H), 4.97 – 4.93 (s, 2H), 4.80 – 4.69 (m, 2H), 4.69 – 4.56 (d,  $J$  = 13.6 Hz, 2H), 3.48 – 3.39 (s, 3H), 1.64 – 1.58 (s, 10H), 1.55 – 1.51 (s, 9H), 1.31 – 1.24 (d,  $J$  = 15.1 Hz, 12H). MS (MALDI-TOF) calcd for C<sub>59</sub>H<sub>58</sub>N<sub>8</sub>O<sub>15</sub> (M+H<sup>+</sup>), 1119.15, obsd: 1120.11.

### **ADM-130A**

<sup>1</sup>H NMR (400 MHz, Chloroform-*d*) δ 11.87 – 11.80 (s, 1H), 9.19 – 9.03 (dd,  $J$  = 7.8, 1.3 Hz, 1H), 8.55 – 8.48 (dd,  $J$  = 8.4, 1.4 Hz, 1H), 8.21 – 8.15 (dd,  $J$  = 7.5, 1.4 Hz, 1H), 8.10 – 8.04 (dd,  $J$  = 8.4, 1.3 Hz, 1H), 7.97 – 7.88 (s, 1H), 7.70 – 7.65 (m, 1H), 7.65 – 7.61 (m, 1H), 7.56 – 7.51 (s, 1H), 4.88 – 4.79 (s, 2H), 4.24 – 4.18 (s, 2H), 4.18 – 4.12 (m, 3H), 2.39 – 2.24 (dt,  $J$  = 13.3, 6.6 Hz, 1H), 1.53 – 1.48 (s, 9H), 1.18 – 1.10 (d,  $J$  = 6.7 Hz, 6H). MS (MALDI-TOF) calcd for C<sub>32</sub>H<sub>34</sub>N<sub>4</sub>O<sub>9</sub> (M+H<sup>+</sup>), 604.21, obsd: 604.14.

### **ADM-130B**

<sup>1</sup>H NMR (400 MHz, Chloroform-*d*) δ 12.28 – 12.20 (s, 1H), 12.19 – 12.12 (s, 1H), 9.10 – 8.96 (ddd,  $J$  = 7.6, 6.2, 1.3 Hz, 2H), 8.59 – 8.48 (dd,  $J$  = 8.4, 1.5 Hz, 1H), 8.10 – 7.94 (ddd,  $J$  = 16.9, 8.4, 1.3 Hz, 2H), 7.89 – 7.80 (d,  $J$  = 4.6 Hz, 2H), 7.79 – 7.73 (t,  $J$  = 8.1 Hz, 1H), 7.70 – 7.60 (m,

2H), 7.47 – 7.41 (dd,  $J$  = 8.4, 7.6 Hz, 1H), 6.73 – 6.66 (s, 1H), 4.98 – 4.90 (s, 2H), 4.65 – 4.58 (s, 2H), 4.20 – 4.12 (d,  $J$  = 6.5 Hz, 2H), 3.49 – 3.36 (s, 3H), 2.39 – 2.25 (hept,  $J$  = 6.6 Hz, 1H), 1.61 – 1.56 (s, 9H), 1.55 – 1.51 (s, 9H), 1.19 – 1.14 (d,  $J$  = 6.7 Hz, 6H). MS (MALDI-TOF) calcd for C<sub>47</sub>H<sub>48</sub>N<sub>6</sub>O<sub>13</sub> (M+H<sup>+</sup>), 904.32, obsd: 904.29.

### **O-*tert* butyl analog of ADM-130**

<sup>1</sup>H NMR (400 MHz, Chloroform-*d*) δ 12.34 – 12.19 (s, 1H), 11.91 – 11.79 (s, 1H), 11.71 – 11.59 (s, 1H), 9.17 – 9.10 (dd,  $J$  = 7.7, 1.2 Hz, 1H), 8.60 – 8.52 (dd,  $J$  = 8.4, 1.4 Hz, 1H), 8.42 – 8.34 (dd,  $J$  = 7.7, 1.3 Hz, 1H), 8.24 – 8.18 (dd,  $J$  = 7.7, 1.3 Hz, 1H), 8.12 – 8.07 (dd,  $J$  = 8.4, 1.3 Hz, 1H), 8.04 – 7.96 (m, 3H), 7.78 – 7.76 (s, 1H), 7.76 – 7.71 (t,  $J$  = 8.0 Hz, 1H), 7.65 – 7.57 (m, 2H), 7.45 – 7.43 (s, 1H), 7.38 – 7.36 (d,  $J$  = 2.5 Hz, 1H), 6.90 – 6.86 (s, 1H), 6.66 – 6.58 (s, 1H), 4.96 – 4.91 (s, 2H), 4.71 – 4.58 (m, 2H), 4.40 – 4.13 (m, 2H), 3.90 – 3.84 (m, 2H), 3.47 – 3.39 (s, 3H), 2.52 – 2.41 (dq,  $J$  = 13.4, 6.7 Hz, 1H), 1.64 – 1.56 (s, 9H), 1.56 – 1.50 (s, 9H), 1.20 – 1.14 (d,  $J$  = 6.7 Hz, 6H). MS (MALDI-TOF) calcd for C<sub>61</sub>H<sub>62</sub>N<sub>8</sub>O<sub>15</sub> (M+H<sup>+</sup>), 1146.43, obsd: 1145.90.

### **ADM-131A**

<sup>1</sup>H NMR (600 MHz, Chloroform-*d*) δ 11.88 – 11.81 (s, 1H), 9.15 – 9.06 (dd,  $J$  = 7.7, 1.2 Hz, 1H), 8.54 – 8.46 (dd,  $J$  = 8.4, 1.4 Hz, 1H), 8.22 – 8.15 (dd,  $J$  = 7.5, 1.4 Hz, 1H), 8.11 – 8.05 (dd,  $J$  = 8.4, 1.3 Hz, 1H), 7.97 – 7.92 (s, 1H), 7.71 – 7.61 (m, 2H), 7.56 – 7.51 (s, 1H), 4.87 – 4.81 (s, 2H), 4.27 – 4.23 (dd,  $J$  = 9.0, 5.9 Hz, 1H), 4.22 – 4.21 (s, 3H), 4.19 – 4.16 (dd,  $J$  = 9.0, 6.5 Hz, 1H), 2.15 – 2.05 (m, 1H), 1.71 – 1.62 (m, 2H), 1.52 – 1.50 (s, 9H), 1.17 – 1.09 (d,  $J$  = 6.7 Hz, 3H), 1.05 – 0.98 (t,  $J$  = 7.5 Hz, 3H). MS (MALDI-TOF) calcd for C<sub>32</sub>H<sub>34</sub>N<sub>4</sub>O<sub>9</sub> (M+H<sup>+</sup>), 618.21, obsd: 618.23.

### **ADM-131B**

<sup>1</sup>H NMR (400 MHz, Chloroform-*d*) δ 12.26 – 12.21 (s, 1H), 12.19 – 12.13 (s, 1H), 9.09 – 8.98 (ddd,  $J$  = 7.9, 6.7, 1.3 Hz, 2H), 8.57 – 8.50 (dd,  $J$  = 8.4, 1.5 Hz, 1H), 8.09 – 7.97 (m, 2H), 7.87 –

7.81 (d,  $J = 7.1$  Hz, 2H), 7.78 – 7.73 (t,  $J = 8.1$  Hz, 1H), 7.67 – 7.62 (m, 2H), 7.48 – 7.41 (dd,  $J = 8.4, 7.5$  Hz, 1H), 6.73 – 6.67 (s, 1H), 4.97 – 4.94 (s, 2H), 4.64 – 4.60 (s, 2H), 4.24 – 4.13 (m, 2H), 3.47 – 3.38 (s, 3H), 1.61 – 1.57 (s, 13H), 1.43–1.34 (m, 7H), 1.18 – 1.13 (d,  $J = 6.8$  Hz, 3H), 1.07 – 0.96 (t,  $J = 7.4$  Hz, 3H). MS (MALDI-TOF) calcd for  $C_{48}H_{50}N_6O_{13}$  ( $M+H^+$ ), 918.34, obsd: 918.37.

### O-*tert* butyl analog of ADM-131

$^1H$  NMR (400 MHz, Chloroform-*d*)  $\delta$  12.30 – 12.25 (s, 1H), 11.89 – 11.83 (s, 1H), 11.71 – 11.62 (s, 1H), 9.21 – 9.08 (dd,  $J = 7.7, 1.3$  Hz, 1H), 8.63 – 8.49 (dd,  $J = 8.3, 1.5$  Hz, 1H), 8.45 – 8.34 (dd,  $J = 7.6, 1.3$  Hz, 1H), 8.24 – 8.16 (dd,  $J = 7.8, 1.3$  Hz, 1H), 8.13 – 8.05 (dd,  $J = 8.4, 1.3$  Hz, 1H), 8.04 – 7.95 (ddd,  $J = 9.9, 8.5, 1.3$  Hz, 2H), 7.78 – 7.76 (s, 1H), 7.76 – 7.71 (t,  $J = 8.0$  Hz, 1H), 7.65 – 7.56 (m, 2H), 7.46 – 7.43 (s, 1H), 7.42 – 7.33 (m, 2H), 6.93 – 6.84 (s, 1H), 6.65 – 6.60 (s, 1H), 4.98 – 4.90 (s, 2H), 4.70 – 4.59 (d,  $J = 12.8$  Hz, 2H), 4.16 – 4.04 (q,  $J = 7.2$  Hz, 2H), 4.03 – 3.83 (dt,  $J = 31.4, 8.8$  Hz, 2H), 3.47 – 3.40 (s, 3H), 2.33 – 2.18 (hept,  $J = 8.8, 7.8$  Hz, 1H), 2.15 – 2.04 (m, 1H), 1.62 – 1.58 (s, 9H), 1.54 – 1.50 (s, 9H), 1.29 – 1.22 (q,  $J = 7.0$  Hz, 7H), 1.19 – 1.10 (m, 6H), 1.09 – 1.02 (m, 4H). MS (MALDI-TOF) calcd for  $C_{63}H_{66}N_8O_{15}$  ( $M+H^+$ ), 1174.46, obsd: 1173.83.

**ADM-102** (Reported earlier as compound OQ1)<sup>5</sup>

**ADM-103**

<sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ 11.65 – 11.60 (s, 1H), 9.06 – 8.99 (dd, *J* = 7.8, 1.3 Hz, 1H), 8.52 – 8.45 (dd, *J* = 8.4, 1.4 Hz, 1H), 8.45 – 8.39 (dd, *J* = 7.5, 1.4 Hz, 1H), 7.99 – 7.95 (dd, *J* = 8.5, 1.3 Hz, 2H), 7.89 – 7.85 (s, 1H), 7.85 – 7.81 (dd, *J* = 8.4, 7.4 Hz, 1H), 7.78 – 7.72 (m, 1H), 7.55 – 7.53 (s, 1H), 5.17 – 5.15 (s, 2H), 4.58 – 4.45 (d, *J* = 7.0 Hz, 2H), 4.06 – 4.05 (s, 3H), 1.55 – 1.51 (t, *J* = 6.9 Hz, 3H). HRMS-ESI (m/z): calculated for C<sub>25</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub><sup>+</sup> [(M+H)+]: 521.1303, found 521.1306.

**ADM-104**

<sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>) δ 11.67 – 11.61 (s, 1H), 9.05 – 8.99 (d, *J* = 7.7 Hz, 1H), 8.60 – 8.53 (d, *J* = 8.4 Hz, 1H), 8.52 – 8.44 (d, *J* = 7.4 Hz, 1H), 7.97 – 7.92 (m, 1H), 7.92 – 7.88 (d, *J* = 8.0 Hz, 1H), 7.89 – 7.86 (s, 1H), 7.77 – 7.72 (t, *J* = 8.0 Hz, 1H), 7.62 – 7.59 (s, 1H), 5.33 – 5.25 (s, 2H), 4.48 – 4.38 (q, *J* = 7.0 Hz, 2H), 4.13 – 4.00 (s, 3H), 1.56 – 1.46 (t, *J* = 6.9 Hz, 3H). HRMS-ESI (m/z): calculated for C<sub>25</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub><sup>+</sup> [(M+H)+]: 521.1303, found 521.1311.

**ADM-105** (Reported earlier as compound OQ2)<sup>5</sup>

**ADM-106**

<sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ 13.94 – 12.78 (br, s, 2H), 11.98 – 11.97 (s, 1H), 11.97 – 11.95 (s, 1H), 9.03 – 8.96 (dd, *J* = 7.7, 1.2 Hz, 1H), 8.89 – 8.83 (d, *J* = 7.6 Hz, 1H), 8.46 – 8.40 (dd, *J* = 8.2, 1.6 Hz, 1H), 8.08 – 8.02 (dd, *J* = 8.4, 1.3 Hz, 1H), 7.88 – 7.86 (s, 2H), 7.85 – 7.80 (t, *J* = 8.0 Hz, 1H), 7.75 – 7.72 (d, *J* = 5.4 Hz, 2H), 7.64 – 7.60 (dd, *J* = 7.5, 1.5 Hz, 1H), 7.60 – 7.55 (t, *J* = 7.9 Hz, 1H), 6.68 – 6.59 (s, 2H), 5.21 – 5.12 (s, 2H), 4.83 – 4.69 (s, 2H), 4.63 – 4.52 (q, *J* = 7.0 Hz, 2H), 3.38 – 3.36 (s, 3H), 1.62 – 1.56 (t, *J* = 6.9 Hz, 3H). HRMS-ESI (m/z): calculated for C<sub>37</sub>H<sub>29</sub>N<sub>6</sub>O<sub>13</sub><sup>+</sup> [(M+H)+]: 765.1787, found 765.1789.

### **ADM-107**

<sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ 13.95 – 12.86 (s, 3H), 11.97 – 11.95 (s, 1H), 11.95 – 11.93 (s, 1H), 9.02 – 8.98 (dd, *J* = 7.7, 1.2 Hz, 1H), 8.94 – 8.90 (dd, *J* = 7.6, 1.3 Hz, 1H), 8.50 – 8.45 (dd, *J* = 8.2, 1.5 Hz, 1H), 8.02 – 7.97 (dd, *J* = 8.4, 1.3 Hz, 1H), 7.91 – 7.89 (dd, *J* = 8.4, 1.3 Hz, 1H), 7.88 – 7.86 (s, 1H), 7.83 – 7.81 (s, 1H), 7.81 – 7.75 (dt, *J* = 9.9, 8.0 Hz, 2H), 7.68 – 7.65 (dd, *J* = 7.5, 1.6 Hz, 1H), 7.65 – 7.59 (t, *J* = 7.8 Hz, 1H), 6.72 – 6.71 (s, 1H), 5.34 – 5.28 (s, 2H), 4.95 – 4.91 (s, 2H), 4.58 – 4.48 (q, *J* = 7.0 Hz, 2H), 3.33 – 3.29 (s, 3H), 1.57 – 1.52 (t, *J* = 6.9 Hz, 3H). HRMS-ESI (m/z): calculated for C<sub>37</sub>H<sub>29</sub>N<sub>6</sub>O<sub>13</sub><sup>+</sup> [(M+H)<sup>+</sup>]: 765.1787, found 765.1785.

### **ADM-108**

<sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 13.96 – 13.00 (s, 3H), 12.05 – 12.00 (s, 1H), 11.96 – 11.91 (s, 1H), 9.04 – 8.96 (dd, *J* = 7.7, 1.3 Hz, 1H), 8.88 – 8.81 (dd, *J* = 7.6, 1.3 Hz, 1H), 8.53 – 8.42 (dd, *J* = 8.3, 1.5 Hz, 1H), 8.06 – 8.00 (dd, *J* = 8.5, 1.3 Hz, 1H), 7.88 – 7.86 (s, 1H), 7.84 – 7.80 (dd, *J* = 8.4, 1.7 Hz, 2H), 7.76 – 7.75 (s, 1H), 7.73 – 7.68 (m, 2H), 7.64 – 7.58 (t, *J* = 8.0 Hz, 1H), 6.73 – 6.70 (s, 1H), 5.33 – 5.29 (s, 2H), 5.28 – 5.25 (s, 2H), 4.22 – 4.10 (q, *J* = 7.0 Hz, 2H), 3.38 – 3.31 (s, 3H), 1.51 – 1.39 (t, *J* = 6.9 Hz, 3H). HRMS-ESI (m/z): calculated for C<sub>37</sub>H<sub>29</sub>N<sub>6</sub>O<sub>13</sub><sup>+</sup> [(M+H)<sup>+</sup>]: 765.1787, found 765.1786.

### **ADM-109**

ADM-109 is a racemic mixture of two enantiomers (right and left hand) under the NMR conditions (in DMSO-*d*<sub>6</sub>).

<sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ 12.27 – 12.24 (s, 1H), 12.19 – 12.16 (s, 1H), 12.06 – 12.03 (s, 1H), 11.97 – 11.94 (s, 1H), 8.99 – 8.90 (dd, *J* = 25.2, 7.6 Hz, 2H), 8.85 – 8.80 (d, *J* = 7.6 Hz, 1H), 8.79 – 8.75 (d, *J* = 7.8 Hz, 1H), 8.46 – 8.41 (d, *J* = 8.2 Hz, 1H), 8.06 – 8.01 (d, *J* = 8.4 Hz, 1H), 8.01 – 7.97 (d, *J* = 8.4 Hz, 1H), 7.89 – 7.85 (s, 1H), 7.85 – 7.76 (m, 4H), 7.74 – 7.70 (s, 3H), 7.70

– 7.63 (m, 2H), 7.58 – 7.55 (s, 1H), 6.72 – 6.66 (d,  $J$  = 13.5 Hz, 2H), 4.88 – 4.85 (s, 2H), 4.61 – 4.54 (q,  $J$  = 7.0 Hz, 2H), 4.44 – 4.37 (q,  $J$  = 7.0 Hz, 2H), 4.19 – 4.10 (dq,  $J$  = 13.6, 6.9 Hz, 4H), 1.61 – 1.56 (t,  $J$  = 7.0 Hz, 3H), 1.55 – 1.51 (t,  $J$  = 6.9 Hz, 3H), 1.48 – 1.43 (m, 6H). HRMS-ESI (m/z): calculated for  $C_{37}H_{31}N_6O_{11}^+$  [(M+H)+]: 735.2045, found 735.2050.

**ADM-110** (Reported earlier as compound OQ3)<sup>5</sup>

**ADM-111** (Reported earlier as compound OQ4)<sup>5</sup>

**ADM-112**

<sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ 13.88 – 12.63 (s, 3H), 12.03 – 12.00 (s, 1H), 11.62 – 11.59 (s, 1H), 11.47 – 11.44 (s, 1H), 9.10 – 9.02 (d,  $J$  = 7.4 Hz, 1H), 8.56 – 8.48 (d,  $J$  = 7.9 Hz, 1H), 8.34 – 8.28 (d,  $J$  = 7.4 Hz, 1H), 8.07 – 8.02 (d,  $J$  = 7.4 Hz, 1H), 8.00 – 7.96 (d,  $J$  = 8.1 Hz, 1H), 7.95 – 7.92 (d,  $J$  = 8.4 Hz, 1H), 7.91 – 7.87 (d,  $J$  = 8.4 Hz, 1H), 7.85 – 7.81 (m, 1H), 7.80 – 7.78 (s, 1H), 7.78 – 7.74 (m, 1H), 7.69 – 7.65 (m, 1H), 7.64 – 7.60 (m, 1H), 7.53 – 7.47 (t,  $J$  = 8.0 Hz, 1H), 7.30 – 7.27 (s, 1H), 6.83 – 6.77 (s, 1H), 6.62 – 6.57 (s, 1H), 5.36 – 5.18 (m, 2H), 4.99 – 4.95 (d,  $J$  = 5.2 Hz, 2H), 4.95 – 4.80 (m, 2H), 4.69 – 4.53 (m, 2H), 1.72 – 1.67 (t,  $J$  = 6.9 Hz, 3H). HRMS-ESI (m/z): calculated for  $C_{49}H_{37}N_8O_{17}^+$  [(M+H)+]: 1009.2271, found 1009.2231.

**ADM-113**

<sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 13.94 – 12.88 (br, s, 3H), 12.19 – 12.13 (s, 1H), 11.78 – 11.73 (s, 1H), 11.57 – 11.51 (s, 1H), 9.02 – 8.92 (dd,  $J$  = 11.9, 7.6 Hz, 2H), 8.41 – 8.32 (d,  $J$  = 7.5 Hz, 1H), 8.05 – 7.93 (t,  $J$  = 7.7 Hz, 2H), 7.77 – 7.72 (d,  $J$  = 3.0 Hz, 1H), 7.48 – 7.36 (m, 2H), 7.31 – 7.21 (d,  $J$  = 8.7 Hz, 1H), 7.12 – 7.04 (dd,  $J$  = 9.8, 5.9 Hz, 1H), 7.04 – 6.96 (d,  $J$  = 2.1 Hz, 2H), 6.90 – 6.83 (s, 1H), 6.84 – 6.75 (s, 1H), 6.68 – 6.60 (s, 1H), 5.94 – 5.87 (d,  $J$  = 8.3 Hz, 1H), 4.98 – 4.84 (m, 4H), 4.25 – 4.11 (m, 4H), 1.60 – 1.45 (t,  $J$  = 7.0 Hz, 3H). HRMS-ESI (m/z): calculated for  $C_{49}H_{37}N_8O_{17}^+$  [(M+H)+]: 1009.2271, found 1009.2275.

### **ADM-114**

<sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ 12.13 – 12.04 (s, 1H), 11.68 – 11.60 (s, 1H), 11.48 – 11.40 (s, 1H), 9.04 – 8.96 (dd, *J* = 7.5, 1.3 Hz, 1H), 8.61 – 8.53 (dd, *J* = 8.2, 1.5 Hz, 1H), 8.40 – 8.32 (dd, *J* = 7.4, 1.4 Hz, 1H), 8.01 – 7.97 (dd, *J* = 7.7, 1.3 Hz, 1H), 7.95 – 7.86 (m, 3H), 7.80 – 7.72 (m, 4H), 7.68 – 7.63 (t, *J* = 7.9 Hz, 1H), 7.49 – 7.45 (t, *J* = 8.0 Hz, 1H), 7.28 – 7.21 (s, 1H), 6.87 – 6.80 (s, 1H), 6.61 – 6.53 (s, 1H), 5.31 – 5.19 (m, 4H), 4.96 – 4.76 (m, 2H), 4.34 – 4.15 (dt, *J* = 63.9, 7.9 Hz, 2H), 1.53 – 1.48 (t, *J* = 7.0 Hz, 3H). HRMS-ESI (m/z): calculated for C<sub>49</sub>H<sub>37</sub>N<sub>8</sub>O<sub>17</sub><sup>+</sup> [(M+H)+]: 1009.2271, found 1009.2281.

### **ADM-115**

<sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 12.19 – 12.08 (s, 1H), 11.79 – 11.72 (s, 1H), 11.56 – 11.49 (s, 1H), 8.97 – 8.93 (d, *J* = 7.4 Hz, 1H), 8.40 – 8.32 (dd, *J* = 7.6, 1.4 Hz, 1H), 7.99 – 7.95 (m, 1H), 7.92 – 7.86 (m, 1H), 7.83 – 7.80 (s, 2H), 7.75 – 7.73 (s, 1H), 7.46 – 7.38 (td, *J* = 8.1, 2.8 Hz, 2H), 7.11 – 7.04 (m, 1H), 7.01 – 6.96 (s, 2H), 6.89 – 6.83 (s, 1H), 6.66 – 6.59 (s, 2H), 6.55 – 6.47 (d, *J* = 8.3 Hz, 1H), 5.93 – 5.88 (d, *J* = 8.3 Hz, 1H), 4.98 – 4.85 (m, 4H), 4.24 – 4.12 (d, *J* = 7.1 Hz, 4H), 1.57 – 1.49 (t, *J* = 6.9 Hz, 3H). HRMS-ESI (m/z): calculated for C<sub>49</sub>H<sub>37</sub>N<sub>8</sub>O<sub>17</sub><sup>+</sup> [(M+H)+]: 1009.2271, found 1009.2268.

**ADM-116** (Reported earlier as compound ADM-116)<sup>3</sup>

### **ADM-117**

<sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ 12.07 – 12.00 (s, 1H), 11.73 – 11.66 (s, 1H), 11.40 – 11.35 (s, 1H), 9.07 – 9.02 (d, *J* = 7.5 Hz, 1H), 8.59 – 8.54 (d, *J* = 8.1 Hz, 1H), 8.46 – 8.41 (m, 1H), 8.25 – 8.18 (d, *J* = 7.6 Hz, 1H), 8.08 – 8.03 (d, *J* = 7.6 Hz, 1H), 8.01 – 7.95 (d, *J* = 8.4 Hz, 1H), 7.87 – 7.85 (s, 1H), 7.85 – 7.83 (s, 1H), 7.82 – 7.81 (s, 1H), 7.73 – 7.70 (t, *J* = 6.7 Hz, 1H), 7.70 – 7.68

(d,  $J = 1.9$  Hz, 1H), 7.68 – 7.66 (s, 1H), 7.46 – 7.42 (d,  $J = 7.9$  Hz, 1H), 7.23 – 7.19 (s, 1H), 6.82 – 6.78 (s, 1H), 6.62 – 6.59 (s, 1H), 5.32 – 5.17 (dd,  $J = 15.1, 8.0$  Hz, 4H), 5.01 – 4.93 (d,  $J = 4.2$  Hz, 2H), 4.59 – 4.51 (q,  $J = 7.0$  Hz, 2H), 1.63 – 1.56 (t,  $J = 6.9$  Hz, 3H), 1.56 – 1.50 (t,  $J = 6.9$  Hz, 3H). HRMS-ESI (m/z): calculated for  $C_{49}H_{39}N_8O_{15}^+$  [(M+H)+]: 979.2535, found 979.2537.

**ADM-118** (Reported earlier as compound OQ5)<sup>5</sup>

**ADM-119**

<sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ 11.68 – 11.62 (s, 1H), 11.49 – 11.47 (s, 1H), 11.47 – 11.45 (s, 1H), 11.34 – 11.28 (s, 1H), 8.52 – 8.46 (dt,  $J = 8.2, 1.7$  Hz, 1H), 8.46 – 8.39 (d,  $J = 7.5$  Hz, 1H), 8.40 – 8.33 (d,  $J = 7.5$  Hz, 1H), 8.12 – 8.06 (d,  $J = 7.5$  Hz, 1H), 8.03 – 7.95 (dd,  $J = 14.6, 8.2$  Hz, 2H), 7.94 – 7.85 (dd,  $J = 12.3, 7.7$  Hz, 2H), 7.83 – 7.77 (d,  $J = 7.7$  Hz, 2H), 7.77 – 7.70 (t,  $J = 8.0$  Hz, 1H), 7.62 – 7.57 (t,  $J = 7.8$  Hz, 1H), 7.57 – 7.55 (dd,  $J = 7.5, 1.6$  Hz, 1H), 7.54 – 7.50 (t,  $J = 8.0$  Hz, 1H), 7.46 – 7.37 (t,  $J = 8.0$  Hz, 1H), 7.36 – 7.28 (d,  $J = 1.9$  Hz, 1H), 7.22 – 7.18 (s, 1H), 6.76 – 6.72 (s, 1H), 6.71 – 6.65 (s, 1H), 6.49 – 6.42 (s, 1H), 5.19 – 5.15 (s, 2H), 4.88 – 4.78 (s, 6H), 4.73 – 4.58 (m, 2H), 3.11 – 3.04 (s, 3H), 1.79 – 1.66 (m, 3H). HRMS-ESI (m/z): calculated for  $C_{61}H_{45}N_{10}O_{21}^+$  [(M+H)+]: 1253.2755, found 1253.2756.

**ADM-120**

<sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>) δ 13.99 – 12.95 (br, s, 4H), 11.69 – 11.63 (s, 1H), 11.55 – 11.50 (s, 1H), 11.49 – 11.44 (s, 1H), 11.31 – 11.24 (s, 1H), 8.61 – 8.52 (dd,  $J = 8.0, 1.8$  Hz, 1H), 8.46 – 8.41 (d,  $J = 7.6$  Hz, 1H), 8.41 – 8.35 (d,  $J = 7.5$  Hz, 1H), 8.14 – 8.06 (d,  $J = 7.6$  Hz, 1H), 8.04 – 7.98 (d,  $J = 8.1$  Hz, 1H), 7.98 – 7.88 (m, 3H), 7.85 – 7.73 (m, 3H), 7.68 – 7.58 (m, 2H), 7.55 – 7.48 (t,  $J = 8.0$  Hz, 1H), 7.47 – 7.41 (t,  $J = 8.0$  Hz, 1H), 7.36 – 7.28 (s, 1H), 7.28 – 7.21 (s, 1H), 6.82 – 6.75 (s, 1H), 6.73 – 6.65 (s, 1H), 6.56 – 6.46 (s, 1H), 5.27 – 5.18 (s, 2H), 5.01 – 4.82 (dq,  $J$

= 31.9, 16.6, 16.1 Hz, 5H), 4.71 – 4.51 (m, 2H), 3.17 – 3.04 (s, 3H), 1.78 – 1.67 (t,  $J$  = 6.9 Hz, 3H). HRMS-ESI (m/z): calculated for  $C_{61}H_{45}N_{10}O_{21}^+$  [(M+H)+]: 1253.2755, found 1253.2760.

### ADM-121

$^1H$  NMR (500 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  11.75 – 11.68 (s, 1H), 11.60 – 11.56 (s, 1H), 11.55 – 11.50 (s, 1H), 11.35 – 11.30 (s, 1H), 8.63 – 8.55 (dd,  $J$  = 6.7, 3.0 Hz, 1H), 8.53 – 8.49 (d,  $J$  = 7.6 Hz, 1H), 8.45 – 8.39 (d,  $J$  = 7.5 Hz, 1H), 8.10 – 8.06 (d,  $J$  = 7.6 Hz, 1H), 8.05 – 7.98 (dd,  $J$  = 15.1, 8.2 Hz, 2H), 7.95 – 7.91 (d,  $J$  = 8.2 Hz, 1H), 7.90 – 7.87 (d,  $J$  = 7.5 Hz, 1H), 7.86 – 7.82 (t,  $J$  = 7.9 Hz, 1H), 7.82 – 7.78 (t,  $J$  = 8.0 Hz, 1H), 7.78 – 7.74 (d,  $J$  = 8.3 Hz, 1H), 7.68 – 7.62 (q,  $J$  = 4.3 Hz, 2H), 7.58 – 7.52 (t,  $J$  = 8.1 Hz, 1H), 7.46 – 7.39 (t,  $J$  = 8.0 Hz, 1H), 7.33 – 7.29 (s, 1H), 7.28 – 7.22 (s, 1H), 6.83 – 6.77 (s, 1H), 6.73 – 6.68 (s, 1H), 6.50 – 6.46 (s, 1H), 5.35 – 5.20 (m, 4H), 5.05 – 4.96 (d,  $J$  = 16.3 Hz, 1H), 4.95 – 4.84 (m, 2H), 4.83 – 4.70 (d,  $J$  = 16.2 Hz, 1H), 4.40 – 4.31 (dt,  $J$  = 14.1, 7.2 Hz, 1H), 4.28 – 4.15 (m, 1H), 3.16 – 3.08 (s, 3H), 1.63 – 1.52 (t,  $J$  = 6.9 Hz, 3H).

HRMS-ESI (m/z): calculated for  $C_{61}H_{45}N_{10}O_{21}^+$  [(M+H)+]: 1253.2755, found 1253.2758.

### ADM-122

$^1H$  NMR (500 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  11.74 – 11.64 (s, 1H), 11.54 – 11.41 (d,  $J$  = 8.5 Hz, 2H), 11.31 – 11.20 (s, 1H), 8.59 – 8.54 (m, 1H), 8.46 – 8.41 (d,  $J$  = 7.4 Hz, 1H), 8.40 – 8.33 (d,  $J$  = 7.2 Hz, 1H), 8.15 – 8.08 (d,  $J$  = 7.5 Hz, 1H), 8.02 – 7.96 (d,  $J$  = 8.2 Hz, 1H), 7.96 – 7.87 (dd,  $J$  = 7.9, 3.8 Hz, 3H), 7.85 – 7.71 (m, 3H), 7.69 – 7.63 (t,  $J$  = 7.8 Hz, 1H), 7.64 – 7.57 (dd,  $J$  = 7.7, 1.6 Hz, 1H), 7.54 – 7.48 (t,  $J$  = 7.9 Hz, 1H), 7.47 – 7.40 (t,  $J$  = 7.9 Hz, 1H), 7.28 – 7.19 (d,  $J$  = 10.9 Hz, 2H), 6.80 – 6.77 (s, 1H), 6.77 – 6.72 (s, 1H), 6.53 – 6.50 (s, 1H), 5.29 – 5.18 (d,  $J$  = 4.4 Hz, 4H), 4.97 – 4.90 (s, 2H), 4.36 – 4.18 (m, 4H), 3.15 – 3.07 (s, 3H), 1.60 – 1.55 (m, 3H). HRMS-ESI (m/z): calculated for  $C_{61}H_{45}N_{10}O_{21}^+$  [(M+H)+]: 1253.2755, found 1253.2761.

### **ADM-123**

<sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 13.92 – 12.98 (s, 4H), 11.69 – 11.60 (s, 1H), 11.55 – 11.50 (s, 1H), 11.51 – 11.43 (s, 1H), 11.32 – 11.24 (s, 1H), 8.60 – 8.50 (dd, *J* = 7.4, 2.2 Hz, 1H), 8.45 – 8.38 (m, 1H), 8.38 – 8.28 (dd, *J* = 7.5, 1.4 Hz, 1H), 8.16 – 8.07 (m, 1H), 8.03 – 7.97 (td, *J* = 8.3, 1.3 Hz, 2H), 7.97 – 7.92 (dd, *J* = 7.7, 1.3 Hz, 1H), 7.87 – 7.77 (m, 3H), 7.76 – 7.69 (t, *J* = 8.0 Hz, 1H), 7.69 – 7.60 (m, 2H), 7.59 – 7.52 (t, *J* = 8.1 Hz, 1H), 7.47 – 7.39 (t, *J* = 8.1 Hz, 1H), 7.27 – 7.21 (d, *J* = 7.5 Hz, 2H), 6.82 – 6.79 (s, 1H), 6.69 – 6.65 (s, 1H), 6.57 – 6.52 (s, 1H), 5.35 – 5.20 (m, 4H), 5.08 – 4.86 (m, 4H), 4.24 – 4.11 (p, *J* = 9.4 Hz, 2H), 3.14 – 3.08 (s, 3H), 1.59 – 1.47 (t, *J* = 6.9 Hz, 3H). HRMS-ESI (m/z): calculated for C<sub>61</sub>H<sub>45</sub>N<sub>10</sub>O<sub>21</sub><sup>+</sup> [(M+H)<sup>+</sup>]: 1253.2755, found 1253.2756.

### **ADM-124**

<sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>) δ 14.13 – 12.77 (s, 3H), 11.69 – 11.60 (s, 1H), 11.54 – 11.48 (s, 1H), 11.49 – 11.42 (s, 1H), 11.36 – 11.22 (s, 1H), 8.52 – 8.41 (m, 2H), 8.40 – 8.31 (d, *J* = 7.5 Hz, 1H), 8.02 – 7.98 (d, *J* = 7.6 Hz, 1H), 7.98 – 7.95 (d, *J* = 8.4 Hz, 1H), 7.94 – 7.90 (d, *J* = 8.3 Hz, 1H), 7.88 – 7.84 (d, *J* = 8.3 Hz, 1H), 7.84 – 7.79 (m, 1H), 7.79 – 7.76 (d, *J* = 8.0 Hz, 1H), 7.76 – 7.70 (t, *J* = 8.0 Hz, 1H), 7.70 – 7.65 (d, *J* = 8.2 Hz, 1H), 7.56 – 7.50 (m, 2H), 7.50 – 7.44 (t, *J* = 8.0 Hz, 1H), 7.38 – 7.33 (t, *J* = 8.0 Hz, 1H), 7.33 – 7.30 (s, 1H), 7.19 – 7.16 (s, 1H), 6.74 – 6.70 (s, 1H), 6.67 – 6.63 (s, 1H), 6.44 – 6.38 (s, 1H), 5.29 – 5.13 (m, 2H), 4.98 – 4.89 (d, *J* = 16.1 Hz, 1H), 4.88 – 4.79 (m, 2H), 4.75 – 4.61 (m, 2H), 4.62 – 4.52 (m, 1H), 4.35 – 4.23 (dq, *J* = 9.6, 7.0 Hz, 1H), 4.18 – 4.08 (dq, *J* = 9.5, 6.8 Hz, 1H), 3.10 – 2.97 (s, 3H), 1.75 – 1.62 (t, *J* = 6.9 Hz, 3H), 1.58 – 1.44 (t, *J* = 6.9 Hz, 3H). HRMS-ESI (m/z): calculated for C<sub>61</sub>H<sub>47</sub>N<sub>10</sub>O<sub>19</sub><sup>+</sup> [(M+H)<sup>+</sup>]: 1223.3031, found 1223.3027.

**ADM-125** (Reported earlier as compound ADM-1116)<sup>3</sup>

**ADM-126** (Reported earlier as compound ADM-116I)<sup>3</sup>

**ADM-129**

<sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ 12.16 – 12.08 (s, 1H), 11.73 – 11.67 (s, 1H), 11.53 – 11.47 (s, 1H), 9.04 – 8.96 (d, *J* = 7.5 Hz, 1H), 8.53 – 8.47 (d, *J* = 8.3 Hz, 1H), 8.40 – 8.33 (d, *J* = 7.5 Hz, 1H), 8.06 – 7.97 (d, *J* = 7.5 Hz, 1H), 7.95 – 7.92 (d, *J* = 8.3 Hz, 1H), 7.91 – 7.86 (dd, *J* = 8.3, 5.1 Hz, 2H), 7.79 – 7.74 (t, *J* = 8.0 Hz, 1H), 7.74 – 7.71 (d, *J* = 11.9 Hz, 2H), 7.71 – 7.67 (t, *J* = 7.9 Hz, 1H), 7.58 – 7.53 (t, *J* = 7.9 Hz, 1H), 7.49 – 7.44 (t, *J* = 8.0 Hz, 1H), 7.36 – 7.32 (s, 1H), 6.90 – 6.80 (s, 1H), 6.60 – 6.51 (s, 1H), 5.25 – 5.15 (tt, *J* = 12.3, 5.5 Hz, 3H), 5.15 – 5.05 (d, *J* = 17.1 Hz, 1H), 4.91 – 4.78 (tt, *J* = 12.3, 5.0 Hz, 2H), 4.77 – 4.64 (d, *J* = 16.8 Hz, 1H), 3.36 – 3.34 (s, 3H), 1.83 – 1.78 (d, *J* = 6.0 Hz, 3H), 1.55 – 1.51 (d, *J* = 5.9 Hz, 3H), 1.45 – 1.39 (m, 9H). HRMS-ESI (m/z): calculated for C<sub>51</sub>H<sub>43</sub>N<sub>8</sub>O<sub>15</sub><sup>+</sup> [(M+H)+]: 1007.2842, found 1007.2838.

**ADM-130**

<sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 12.11 – 12.01 (s, 1H), 11.70 – 11.60 (s, 1H), 11.50 – 11.43 (s, 1H), 9.07 – 8.95 (d, *J* = 7.6 Hz, 1H), 8.60 – 8.51 (dd, *J* = 8.2, 1.6 Hz, 1H), 8.42 – 8.32 (d, *J* = 7.5 Hz, 1H), 8.03 – 7.98 (d, *J* = 7.7 Hz, 1H), 7.96 – 7.94 (d, *J* = 3.5 Hz, 1H), 7.94 – 7.92 (d, *J* = 3.5 Hz, 1H), 7.91 – 7.87 (d, *J* = 8.4 Hz, 1H), 7.82 – 7.79 (d, *J* = 8.0 Hz, 1H), 7.78 – 7.75 (d, *J* = 7.1 Hz, 2H), 7.70 – 7.65 (dd, *J* = 7.5, 1.6 Hz, 1H), 7.64 – 7.58 (t, *J* = 7.9 Hz, 1H), 7.52 – 7.45 (t, *J* = 8.1 Hz, 1H), 7.35 – 7.26 (s, 1H), 6.85 – 6.79 (s, 1H), 6.63 – 6.55 (s, 1H), 5.38 – 5.10 (m, 2H), 4.97 – 4.71 (m, 2H), 4.47 – 4.22 (dt, *J* = 46.9, 8.8 Hz, 2H), 4.12 – 3.83 (dt, *J* = 60.1, 8.2 Hz, 2H), 2.46 – 2.36 (dq, *J* = 13.3, 6.9 Hz, 1H), 2.29 – 2.18 (dt, *J* = 13.3, 6.6 Hz, 1H), 1.31 – 1.22 (t, *J* = 7.1 Hz, 6H), 1.18 – 1.09 (t, *J* = 6.3 Hz, 6H). HRMS-ESI (m/z): calculated for C<sub>59</sub>H<sub>53</sub>N<sub>8</sub>O<sub>16</sub><sup>+</sup> [(M+H)+]: 1035.3155, found 1035.3151.

### **ADM-131**

<sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ 12.06 – 12.03 (s, 1H), 11.64 – 11.61 (s, 1H), 11.48 – 11.45 (s, 1H), 9.03 – 8.98 (dd, *J* = 7.6, 1.3 Hz, 1H), 8.55 – 8.50 (dd, *J* = 8.2, 1.5 Hz, 1H), 8.41 – 8.36 (d, *J* = 7.5 Hz, 1H), 8.01 – 7.86 (m, 4H), 7.82 – 7.71 (td, *J* = 16.6, 16.0, 7.9 Hz, 3H), 7.68 – 7.63 (dd, *J* = 7.4, 1.4 Hz, 1H), 7.62 – 7.56 (m, 1H), 7.51 – 7.45 (t, *J* = 8.0 Hz, 1H), 7.33 – 7.29 (s, 1H), 6.84 – 6.81 (s, 1H), 6.61 – 6.58 (s, 1H), 5.33 – 5.26 (d, *J* = 16.2 Hz, 1H), 5.23 – 5.17 (d, *J* = 16.4 Hz, 1H), 4.97 – 4.91 (d, *J* = 16.2 Hz, 1H), 4.86 – 4.80 (d, *J* = 16.3 Hz, 1H), 4.49 – 4.40 (dd, *J* = 22.2, 6.9 Hz, 1H), 4.40 – 4.29 (dt, *J* = 34.1, 7.4 Hz, 1H), 4.16 – 4.10 (t, *J* = 7.3 Hz, 1H), 4.09 – 4.03 (t, *J* = 7.8 Hz, 1H), 4.00 – 3.94 (t, *J* = 7.5 Hz, 1H), 3.93 – 3.87 (d, *J* = 7.8 Hz, 1H), 2.25 – 2.17 (dt, *J* = 13.4, 6.9 Hz, 1H), 2.07 – 1.94 (q, *J* = 6.5 Hz, 1H), 1.85 – 1.75 (m, 1H), 1.72 – 1.61 (m, 1H), 1.57 – 1.49 (dq, *J* = 10.7, 6.5, 5.7 Hz, 1H), 1.44 – 1.37 (dt, *J* = 14.1, 7.3 Hz, 1H), 1.27 – 1.22 (dd, *J* = 6.9, 3.3 Hz, 3H), 1.16 – 1.08 (m, 9H). HRMS-ESI (m/z): calculated for C<sub>55</sub>H<sub>51</sub>N<sub>8</sub>O<sub>15</sub><sup>+</sup> [(M+H)<sup>+</sup>]: 1063.3468, found 1063.3462.

### **ADM-135**

<sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ 11.70 – 11.65 (s, 1H), 9.10 – 9.00 (dd, *J* = 7.7, 1.2 Hz, 1H), 8.54 – 8.49 (dd, *J* = 8.4, 1.4 Hz, 1H), 8.47 – 8.44 (dd, *J* = 7.5, 1.3 Hz, 1H), 8.02 – 7.99 (dd, *J* = 8.4, 1.3 Hz, 1H), 7.95 – 7.93 (s, 1H), 7.88 – 7.84 (m, 1H), 7.81 – 7.76 (t, *J* = 8.1 Hz, 1H), 7.55 – 7.54 (s, 1H), 5.30 – 5.20 (hept, *J* = 6.1 Hz, 1H), 5.13 – 5.05 (s, 2H), 4.16 – 3.94 (s, 3H), 1.52 – 1.50 (d, *J* = 6.0 Hz, 7H). MS (MALDI-TOF) calcd for C<sub>26</sub>H<sub>22</sub>N<sub>4</sub>O<sub>9</sub> (M+H<sup>+</sup>), 535.1465, obsd: 535.1459.

### **ADM-136**

<sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ 13.85 – 12.87 (s, 1H), 11.67 – 11.64 (s, 1H), 9.08 – 9.00 (dd, *J* = 7.8, 1.2 Hz, 1H), 8.57 – 8.51 (dd, *J* = 8.4, 1.3 Hz, 1H), 8.46 – 8.42 (dd, *J* = 7.5, 1.3 Hz, 1H), 8.02

– 7.95 (dd,  $J = 8.4$ , 1.3 Hz, 1H), 7.91 – 7.89 (s, 1H), 7.88 – 7.84 (t,  $J = 7.9$  Hz, 1H), 7.79 – 7.75 (t,  $J = 8.1$  Hz, 1H), 7.57 – 7.53 (s, 1H), 5.17 – 5.12 (s, 2H), 4.28 – 4.25 (d,  $J = 6.4$  Hz, 2H), 4.08 – 4.04 (s, 3H), 2.28 – 2.21 (dq,  $J = 13.3$ , 6.6 Hz, 1H), 1.13 – 1.09 (d,  $J = 6.7$  Hz, 7H). MS (MALDI-TOF) calcd for  $C_{27}H_{24}N_4O_9$  ( $M+H^+$ ), 549.1622, obsd: 549.1617.

### **ADM-137**

$^1H$  NMR (600 MHz, DMSO- $d_6$ )  $\delta$  11.70 – 11.65 (s, 1H), 9.09 – 9.01 (d,  $J = 7.7$  Hz, 1H), 8.58 – 8.51 (d,  $J = 8.3$  Hz, 1H), 8.50 – 8.45 (d,  $J = 7.4$  Hz, 1H), 8.07 – 7.98 (d,  $J = 8.4$  Hz, 1H), 7.96 – 7.93 (s, 1H), 7.92 – 7.87 (t,  $J = 7.9$  Hz, 1H), 7.81 – 7.75 (t,  $J = 8.1$  Hz, 1H), 7.56 – 7.51 (s, 1H), 5.16 – 4.98 (s, 2H), 4.40 – 4.35 (dd,  $J = 9.3$ , 5.8 Hz, 1H), 4.34 – 4.29 (dd,  $J = 9.3$ , 6.3 Hz, 1H), 4.11 – 4.05 (s, 3H), 2.08 – 2.02 (dt,  $J = 13.1$ , 6.5 Hz, 1H), 1.73 – 1.62 (tt,  $J = 13.1$ , 7.3 Hz, 1H), 1.46 – 1.33 (dp,  $J = 14.9$ , 7.5 Hz, 1H), 1.15 – 1.10 (d,  $J = 6.7$  Hz, 3H), 1.02 – 0.97 (t,  $J = 7.5$  Hz, 3H). MS (MALDI-TOF) calcd for  $C_{28}H_{26}N_4O_9$  ( $M+H^+$ ), 563.1778, obsd: 563.1769.

### **ADM-138**

$^1H$  NMR (600 MHz, DMSO- $d_6$ )  $\delta$  12.26 – 12.22 (s, 1H), 12.20 – 12.16 (s, 1H), 8.96 – 8.92 (d,  $J = 7.6$  Hz, 1H), 8.87 – 8.84 (d,  $J = 7.5$  Hz, 1H), 7.98 – 7.95 (d,  $J = 8.4$  Hz, 1H), 7.94 – 7.91 (d,  $J = 8.4$  Hz, 1H), 7.82 – 7.80 (s, 1H), 7.80 – 7.76 (t,  $J = 8.0$  Hz, 2H), 7.52 – 7.50 (s, 1H), 7.26 – 7.20 (d,  $J = 8.1$  Hz, 1H), 7.08 – 7.04 (t,  $J = 7.9$  Hz, 1H), 6.70 – 6.67 (s, 1H), 6.04 – 5.97 (d,  $J = 7.4$  Hz, 1H), 5.30 – 5.19 (hept,  $J = 6.1$  Hz, 1H), 5.05 – 5.00 (s, 2H), 4.96 – 4.90 (s, 2H), 4.78 – 4.70 (s, 2H), 1.53 – 1.51 (d,  $J = 6.0$  Hz, 6H). MS (MALDI-TOF) calcd for  $C_{38}H_{30}N_6O_{13}$  ( $M+H^+$ ), 779.1949, obsd: 779.1945.

### **ADM-139**

<sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ 14.02 – 12.57 (s, 2H), 11.98 – 11.95 (s, 1H), 11.96 – 11.93 (s, 1H), 9.03 – 9.00 (d, *J* = 7.5 Hz, 1H), 8.95 – 8.89 (d, *J* = 7.6 Hz, 1H), 8.50 – 8.47 (dd, *J* = 8.2, 1.6 Hz, 1H), 8.06 – 8.00 (dd, *J* = 8.3, 3.0 Hz, 1H), 7.94 – 7.88 (d, *J* = 8.3 Hz, 1H), 7.88 – 7.85 (d, *J* = 2.6 Hz, 1H), 7.84 – 7.82 (d, *J* = 3.5 Hz, 1H), 7.82 – 7.80 (d, *J* = 8.2 Hz, 1H), 7.80 – 7.76 (t, *J* = 8.0 Hz, 1H), 7.68 – 7.65 (dd, *J* = 7.5, 1.6 Hz, 1H), 7.65 – 7.60 (t, *J* = 7.8 Hz, 1H), 6.73 – 6.70 (s, 1H), 5.31 – 5.27 (d, *J* = 3.5 Hz, 2H), 4.94 – 4.90 (s, 2H), 4.30 – 4.25 (d, *J* = 6.4 Hz, 2H), 2.32 – 2.22 (dh, *J* = 13.6, 6.7 Hz, 1H), 1.16 – 1.10 (d, *J* = 6.7 Hz, 6H). MS (MALDI-TOF) calcd for C<sub>39</sub>H<sub>32</sub>N<sub>6</sub>O<sub>13</sub> (M+H<sup>+</sup>), 793.2106, obsd: 793.2102.

### **ADM-140**

<sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ 11.98 – 11.96 (s, 1H), 11.96 – 11.94 (s, 1H), 9.04 – 8.99 (d, *J* = 7.5 Hz, 1H), 8.94 – 8.90 (dd, *J* = 7.7, 1.2 Hz, 1H), 8.50 – 8.46 (dd, *J* = 8.2, 1.5 Hz, 1H), 8.03 – 8.01 (dd, *J* = 8.3, 1.1 Hz, 1H), 7.92 – 7.89 (m, 1H), 7.88 – 7.86 (s, 1H), 7.86 – 7.84 (s, 1H), 7.84 – 7.80 (t, *J* = 8.0 Hz, 1H), 7.80 – 7.76 (t, *J* = 8.0 Hz, 1H), 7.68 – 7.65 (dd, *J* = 7.5, 1.5 Hz, 1H), 7.65 – 7.61 (t, *J* = 7.8 Hz, 1H), 6.73 – 6.70 (s, 1H), 5.32 – 5.29 (s, 2H), 4.96 – 4.89 (s, 2H), 4.38 – 4.33 (dd, *J* = 9.2, 5.9 Hz, 1H), 4.32 – 4.27 (dd, *J* = 9.2, 6.4 Hz, 1H), 1.71 – 1.61 (tt, *J* = 13.1, 7.4 Hz, 1H), 1.44 – 1.35 (m, 1H), 1.32 – 1.29 (s, 1H), 1.22 – 1.18 (s, 1H), 1.13 – 1.10 (d, *J* = 6.7 Hz, 3H), 1.00 – 0.97 (t, *J* = 7.5 Hz, 3H). MS (MALDI-TOF) calcd for C<sub>40</sub>H<sub>34</sub>N<sub>6</sub>O<sub>13</sub> (M+H<sup>+</sup>), 807.2262, obsd: 807.2257.

### **ADM-141**

<sup>1</sup>H NMR (400 MHz, Chloroform-*d*) δ 12.36 – 12.25 (s, 1H), 11.91 – 11.83 (s, 1H), 11.69 – 11.61 (s, 1H), 9.14 – 9.05 (dd, *J* = 7.7, 1.3 Hz, 1H), 8.70 – 8.61 (dd, *J* = 8.4, 1.6 Hz, 1H), 8.45 – 8.38 (dd, *J* = 7.6, 1.3 Hz, 1H), 8.19 – 8.13 (dd, *J* = 7.7, 1.3 Hz, 1H), 8.11 – 8.06 (dd, *J* = 8.4, 1.3 Hz, 1H), 8.05 – 7.94 (m, 3H), 7.77 – 7.73 (s, 1H), 7.66 – 7.59 (m, 2H), 7.43 – 7.34 (m, 4H), 7.26 –

7.23 (d,  $J = 1.4$  Hz, 1H), 6.91 – 6.80 (s, 1H), 6.63 – 6.59 (d,  $J = 1.4$  Hz, 1H), 5.03 – 4.98 (s, 2H), 4.96 – 4.91 (s, 2H), 4.70 – 4.57 (d,  $J = 9.9$  Hz, 2H), 4.22 – 4.15 (d,  $J = 7.5$  Hz, 2H), 3.48 – 3.37 (d,  $J = 1.4$  Hz, 3H), 1.52 – 1.50 (d, 6H). HRMS-ESI (m/z): calculated for  $C_{49}H_{39}N_8O_{15}^+ [(M+H)^+]$ : 979.2535, found 979.2541.

### **ADM-142**

$^1H$  NMR (600 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  13.51 – 13.31 (d,  $J = 34.9$  Hz, 2H), 12.26 – 12.23 (s, 1H), 11.70 – 11.69 (s, 1H), 11.68 – 11.67 (s, 2H), 8.98 – 8.93 (d,  $J = 7.5$  Hz, 1H), 8.44 – 8.35 (d,  $J = 7.6$  Hz, 1H), 7.94 – 7.89 (t,  $J = 9.6$  Hz, 2H), 7.89 – 7.86 (d,  $J = 7.7$  Hz, 1H), 7.84 – 7.81 (d,  $J = 8.4$  Hz, 1H), 7.80 – 7.77 (m, 2H), 7.76 – 7.75 (s, 2H), 7.49 – 7.39 (t,  $J = 8.0$  Hz, 1H), 7.24 – 7.20 (d,  $J = 8.2$  Hz, 1H), 7.13 – 7.11 (s, 1H), 7.04 – 7.00 (t,  $J = 7.7$  Hz, 1H), 6.88 – 6.84 (s, 1H), 6.62 – 6.59 (s, 1H), 6.00 – 5.91 (d,  $J = 7.5$  Hz, 1H), 5.32 – 5.20 (s, 3H), 4.97 – 4.82 (s, 2H), 4.78 – 4.63 (s, 2H), 4.57 – 4.38 (s, 2H), 1.66 – 1.63 (t,  $J = 7.0$  Hz, 3H), 1.53 – 1.50 (t,  $J = 6.9$  Hz, 3H). HRMS-ESI (m/z): calculated for  $C_{49}H_{39}N_8O_{15}^+ [(M+H)^+]$ : 979.2535, found 979.2539.

**The synthetic routes for the synthesis of ADM-b, ADM-c, ADM-d, ADM-g, tert butyl ADM-11, and ADM-11 was reported somewhere else<sup>6</sup>.**

### **ADM-b**

$^1H$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.09 – 8.03 (d,  $J = 8.2$  Hz, 1H), 7.15 – 7.08 (d,  $J = 8.2$  Hz, 1H), 4.22 – 4.18 (d,  $J = 6.6$  Hz, 2H), 2.19 – 2.00 (dp,  $J = 13.3, 6.7$  Hz, 1H), 1.41 – 1.32 (d,  $J = 6.3$  Hz, 6H). HRMS-ESI (m/z): calculated for  $C_{59}H_{53}N_8O_{16}^+ [(M)^+]$ : 1129.3574, found 1129.3578.

### **ADM-c**

$^1H$  NMR (400 MHz, Chloroform-*d*)  $\delta$  8.31 – 8.25 (d,  $J = 8.0$  Hz, 1H), 7.79 – 7.73 (d,  $J = 8.0$  Hz, 1H), 4.37 – 4.28 (d,  $J = 6.5$  Hz, 2H), 4.02 – 3.91 (s, 3H), 2.23 – 2.06 (dpd,  $J = 13.4, 6.7, 3.0$  Hz, 1H), 1.05 – 1.02 (d,  $J = 6.8$  Hz, 6H).  $^{13}C$  NMR (126 MHz, Chloroform-*d*)  $\delta$  19.03, 27.89, 53.04,

74.22, 117.51, 135.33, 137.55, 148.63, 156.00, 163.82 HRMS-ESI (m/z): calculated for  $C_{59}H_{53}N_8O_{16}^+$  [(M+H)+]: 1129.3574, found 1129.3578.

### **ADM-d**

$^1H$  NMR (400 MHz, Chloroform-*d*)  $\delta$  9.64 – 8.72 (s, 1H), 8.42 – 8.34 (d, *J* = 8.0 Hz, 1H), 7.96 – 7.86 (d, *J* = 8.0 Hz, 1H), 4.33 – 4.25 (d, *J* = 6.5 Hz, 2H), 2.27 – 2.05 (m, 1H), 1.09 – 1.04 (d, *J* = 6.8 Hz, 6H).  $^{13}C$  NMR (126 MHz, Chloroform-*d*)  $\delta$  18.97, 43.52, 74.72, 117.19, 136.42, 137.52, 146.68, 155.76, 163.54. HRMS-ESI (m/z): calculated for  $C_{10}H_{12}N_2O_5^+$  [(M)<sup>+</sup>]: 239.0746, found 239.0742.

### **ADM-g**

$^1H$  NMR (400 MHz, Chloroform-*d*)  $\delta$  10.43 – 10.33 (s, 1H), 8.95 – 8.88 (d, *J* = 8.1 Hz, 1H), 8.45 – 8.38 (d, *J* = 8.0 Hz, 1H), 7.97 – 7.93 (d, *J* = 8.0 Hz, 1H), 7.89 – 7.84 (d, *J* = 8.1 Hz, 1H), 5.03 – 4.95 (s, 2H), 4.48 – 4.40 (d, *J* = 6.2 Hz, 2H), 3.94 – 3.91 (s, 3H), 2.29 – 2.18 (dq, *J* = 13.2, 6.6 Hz, 1H), 1.49 – 1.45 (s, 10H), 1.12 – 1.07 (d, *J* = 6.7 Hz, 6H).  $^{13}C$  NMR (101 MHz, Chloroform-*d*)  $\delta$  19.08, 27.82, 28.05, 52.49, 63.51, 74.49, 82.37, 115.21, 121.13, 125.67, 126.28, 128.31, 136.65, 138.61, 149.63, 151.34, 155.54, 160.78, 164.85, 167.15. HRMS-ESI (m/z): calculated for  $C_{23}H_{28}N_4O_9^+$  [(M+H)+]: 503.1856, found 503.1852.

### **Tert butyl ADM-11**

$^1H$  NMR (400 MHz, Chloroform-*d*)  $\delta$  10.42 – 10.38 (s, 1H), 10.09 – 10.04 (s, 1H), 8.99 – 8.93 (dd, *J* = 8.1, 4.0 Hz, 2H), 8.55 – 8.47 (d, *J* = 8.1 Hz, 1H), 8.11 – 8.05 (d, *J* = 8.1 Hz, 1H), 8.00 – 7.94 (d, *J* = 8.1 Hz, 1H), 7.89 – 7.84 (d, *J* = 8.1 Hz, 1H), 5.10 – 5.06 (s, 2H), 5.01 – 4.98 (s, 2H), 4.50 – 4.44 (d, *J* = 6.8 Hz, 2H), 3.93 – 3.91 (s, 3H), 2.42 – 2.29 (hept, *J* = 6.7 Hz, 1H), 1.50 – 1.46 (s, 9H), 1.41 – 1.37 (s, 9H), 1.16 – 1.10 (d, *J* = 6.7 Hz, 6H).  $^{13}C$  NMR (151 MHz, cdcl<sub>3</sub>)  $\delta$  19.43, 27.96, 28.06, 52.40, 63.48, 63.99, 64.07, 73.56, 82.20, 83.22, 116.86, 117.34, 121.29, 125.89, 127.04, 128.32, 129.65, 132.98, 137.26, 137.80, 140.46, 149.43, 151.22, 151.89, 154.37, 160.14,

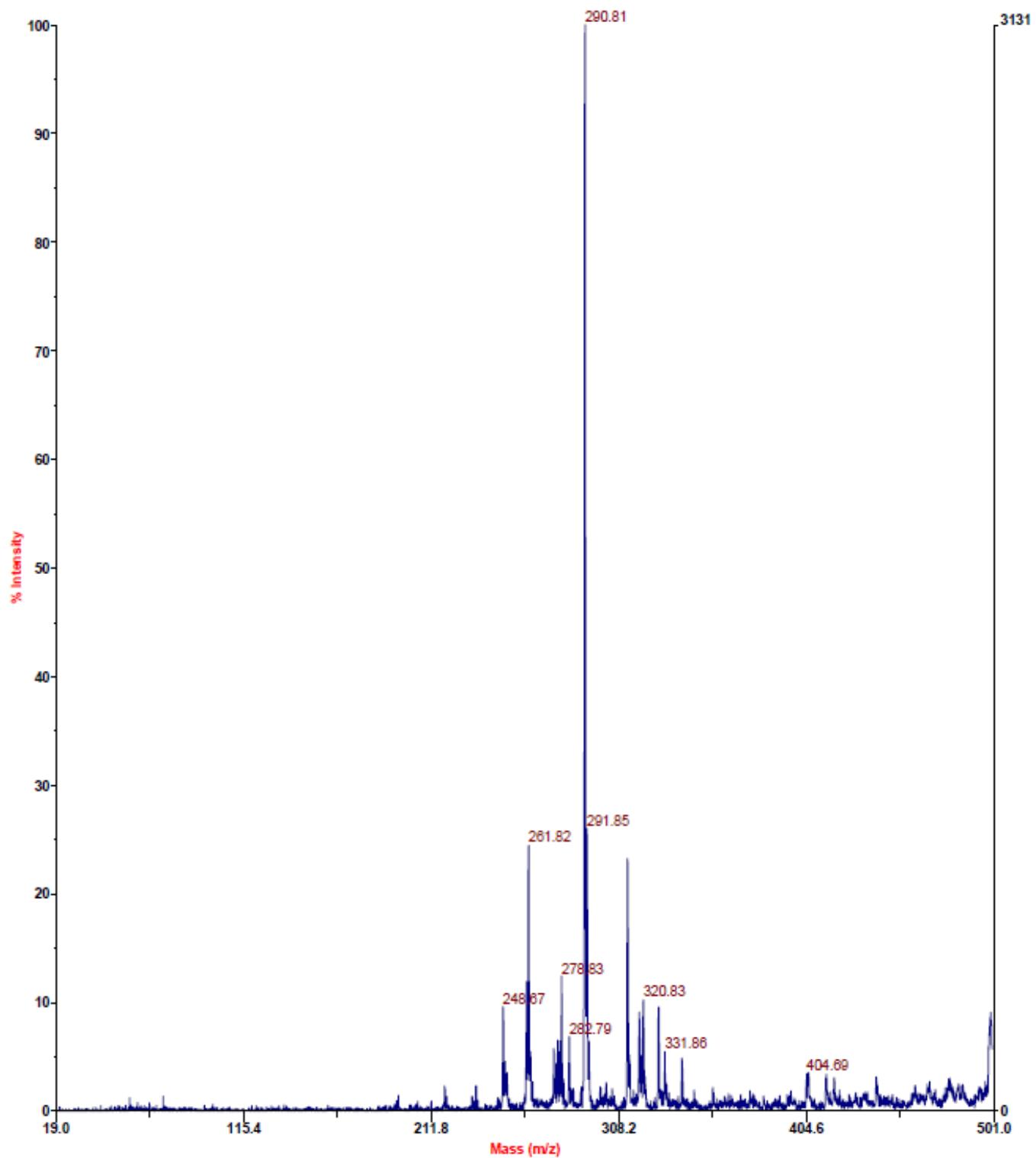
162.54, 165.02, 165.84, 167.32. HRMS-ESI (m/z): calculated for C<sub>35</sub>H<sub>42</sub>N<sub>6</sub>O<sub>13</sub><sup>+</sup> [(M)<sup>+</sup>]: 753.2810, found 753.2810.

**ADM-11**

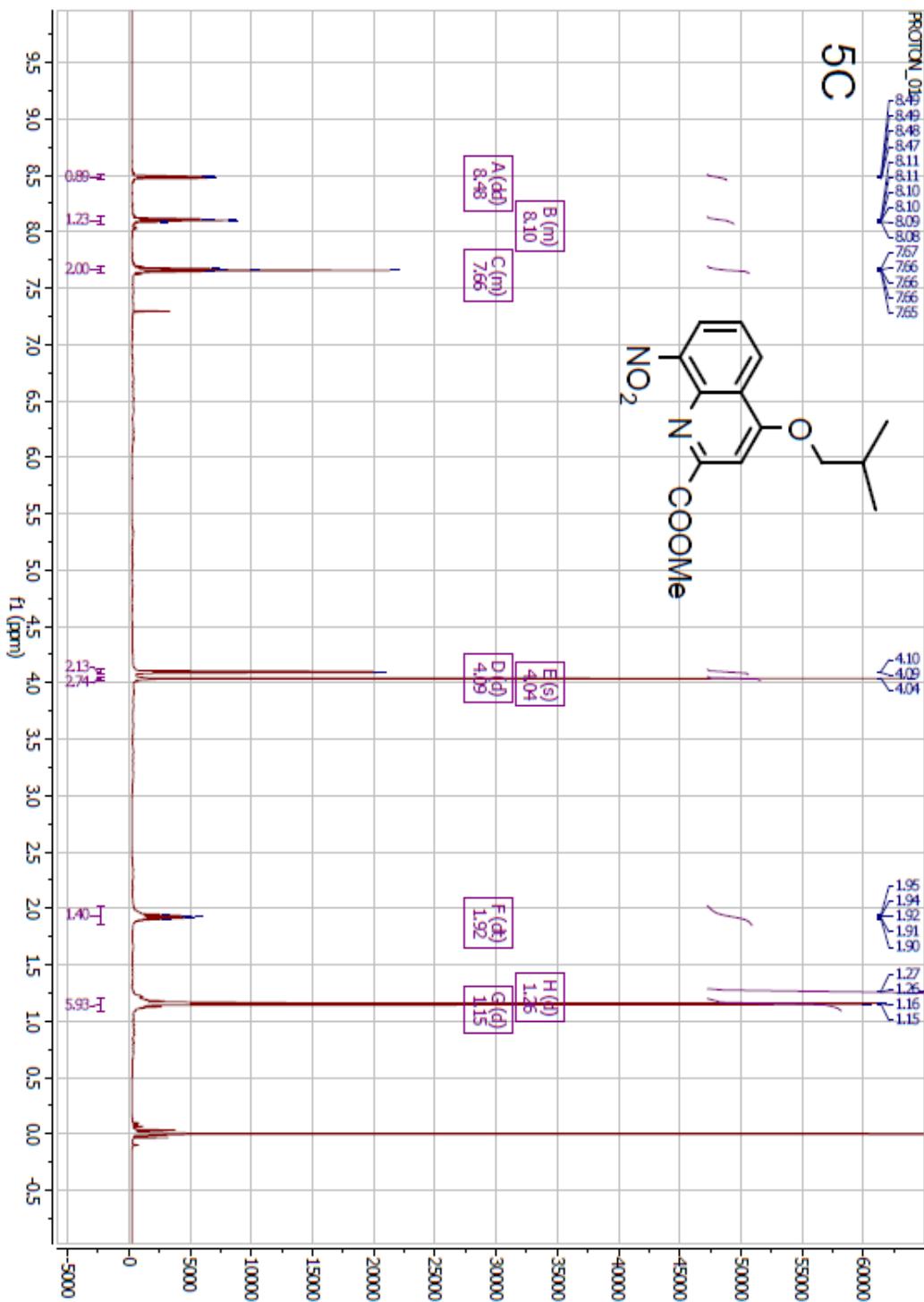
<sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>) δ 13.49 – 13.04 (s, 3H), 10.29 – 10.23 (d, J = 11.4 Hz, 1H), 10.00 – 9.97 (s, 1H), 8.78 – 8.70 (dd, J = 13.7, 6.5 Hz, 2H), 8.70 – 8.64 (d, J = 8.0 Hz, 1H), 7.97 – 7.89 (d, J = 8.0 Hz, 1H), 7.84 – 7.78 (m, 1H), 7.77 – 7.73 (d, J = 8.0 Hz, 1H), 5.22 – 5.14 (s, 2H), 5.04 – 5.03 (s, 2H), 4.33 – 4.29 (d, J = 6.9 Hz, 2H), 3.80 – 3.76 (d, J = 2.4 Hz, 4H), 2.32 – 2.22 (dt, J = 13.5, 6.7 Hz, 1H), 1.04 – 0.99 (d, J = 6.6 Hz, 6H). HRMS-ESI (m/z): calculated for C<sub>27</sub>H<sub>26</sub>N<sub>6</sub>O<sub>13</sub><sup>+</sup> [(M)<sup>+</sup>]: 641.1558, found 641.1552.



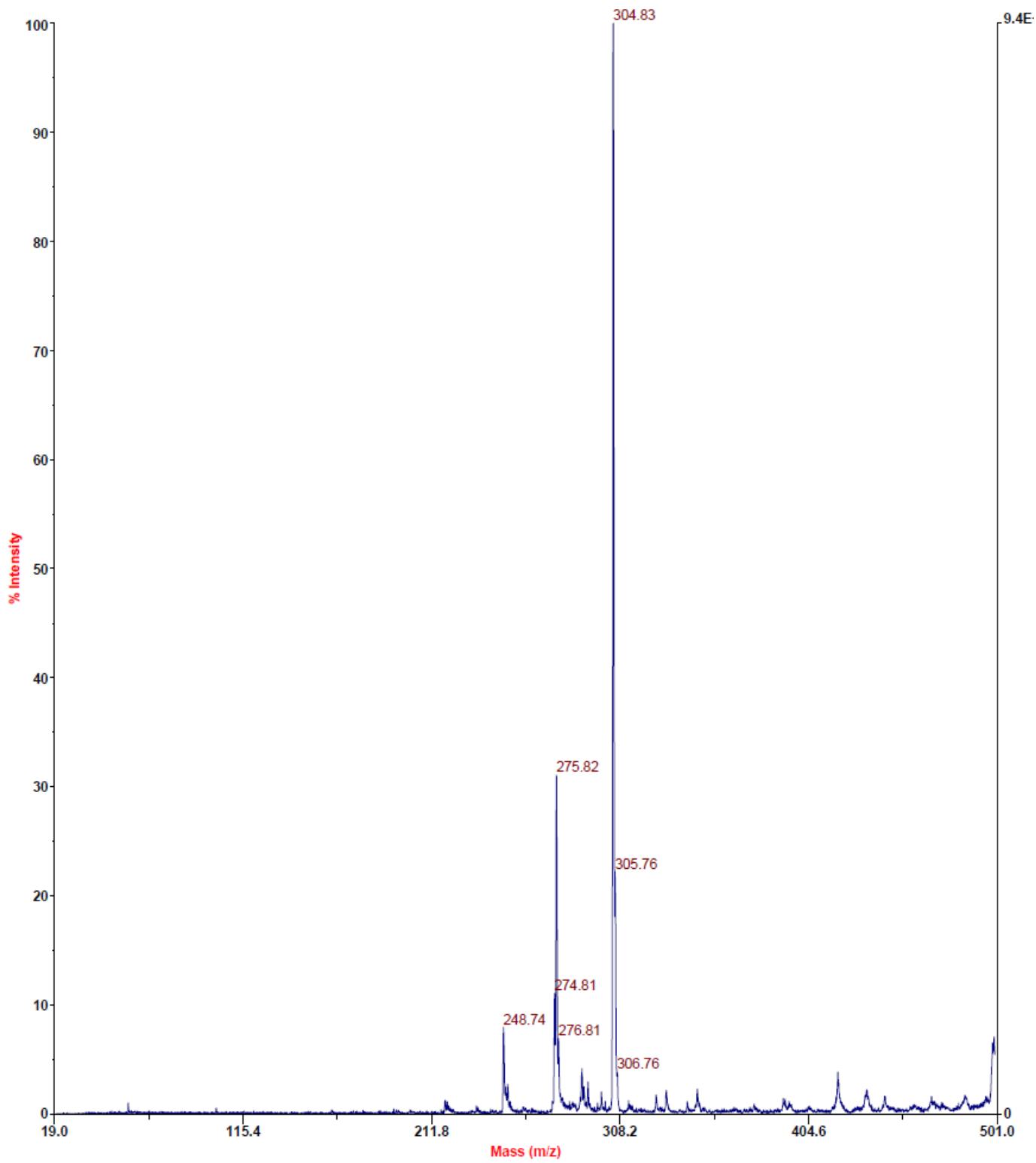
**Fig.**  $^1\text{H}$  NMR of 5B.



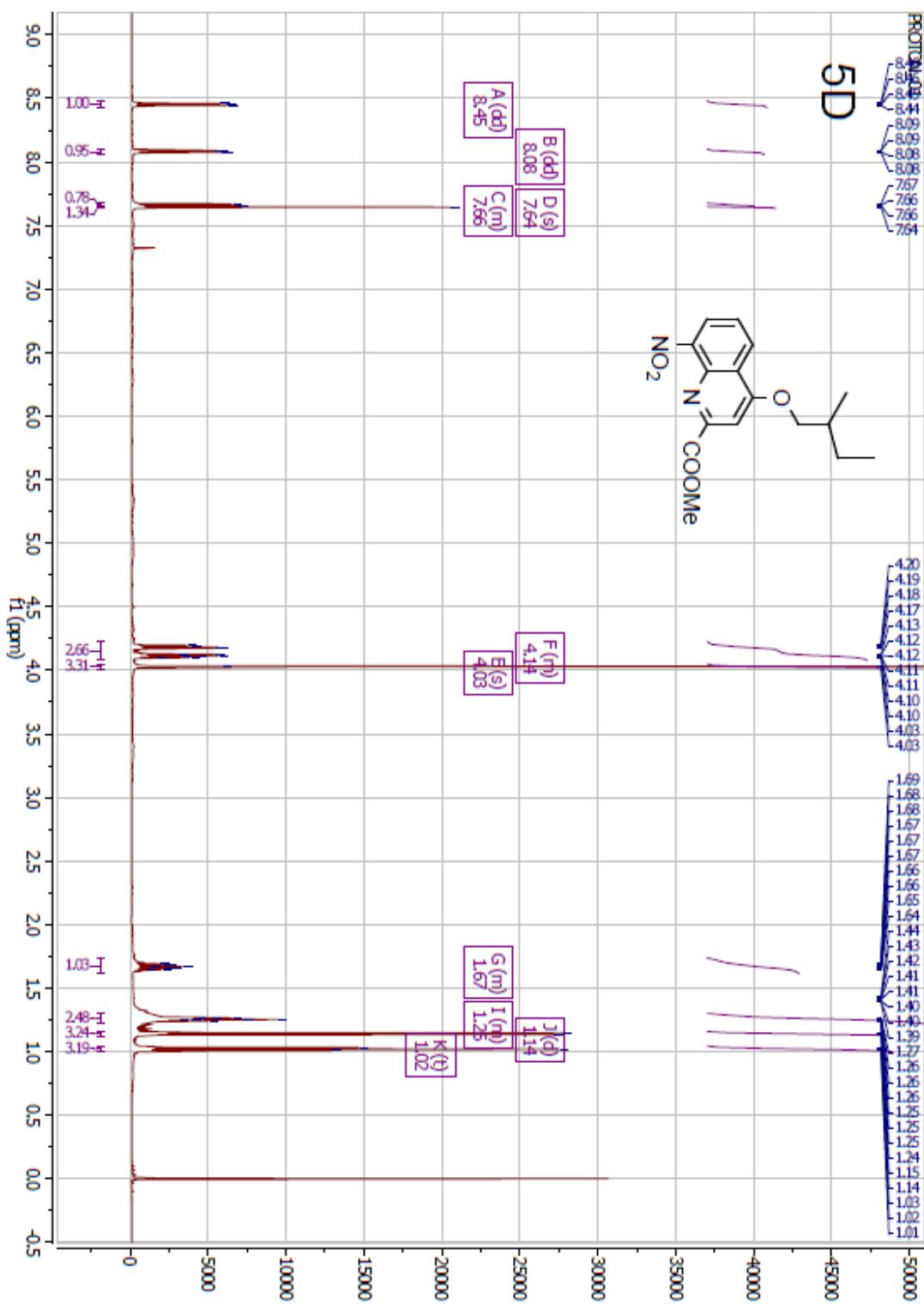
**Fig.** MALDI-TOF of 5B.



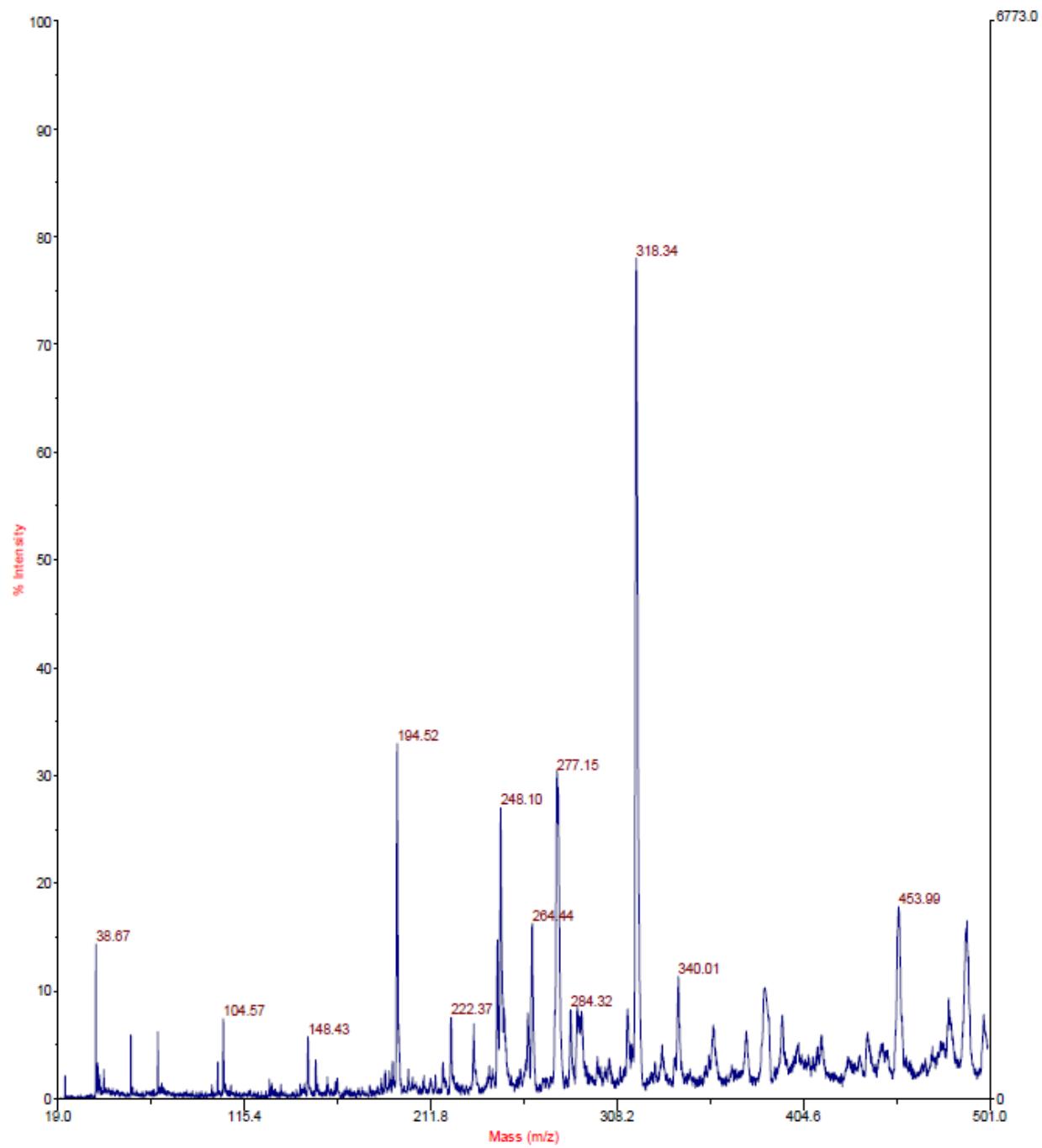
**Fig.** <sup>1</sup>H NMR of 5C.



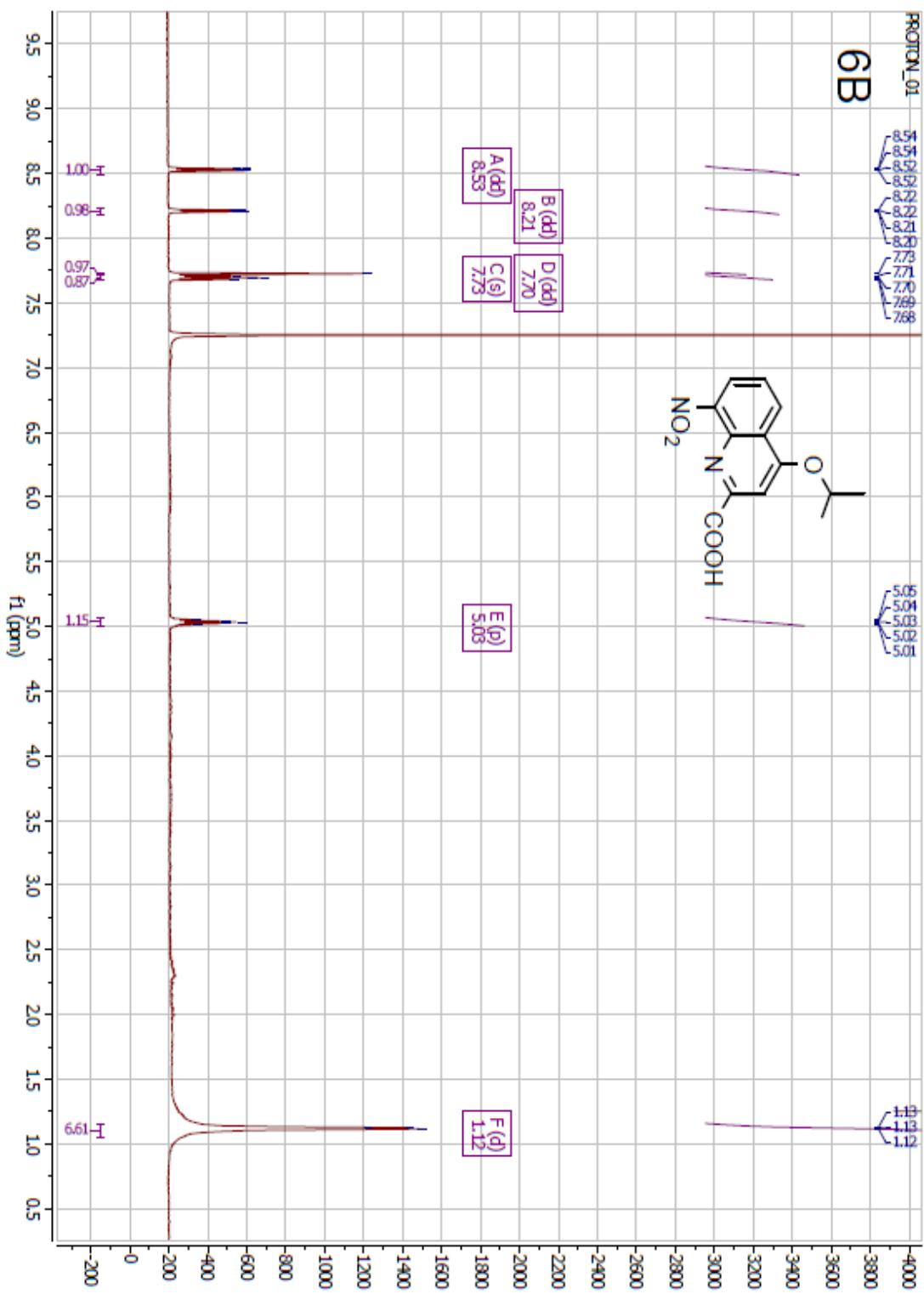
**Fig.** MALDI-TOF of 5C.



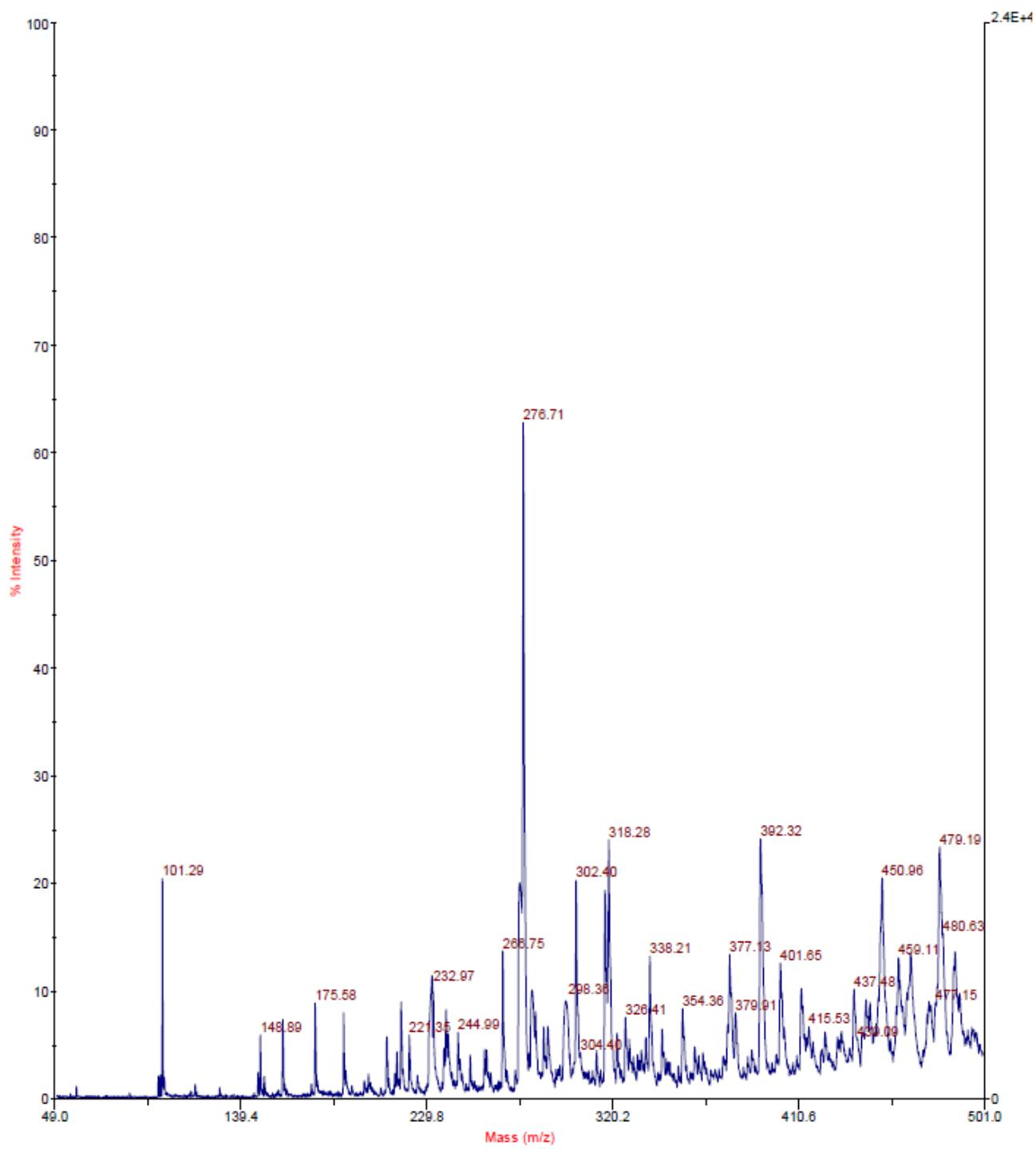
**Fig.**  $^1\text{H}$  NMR of 5D.



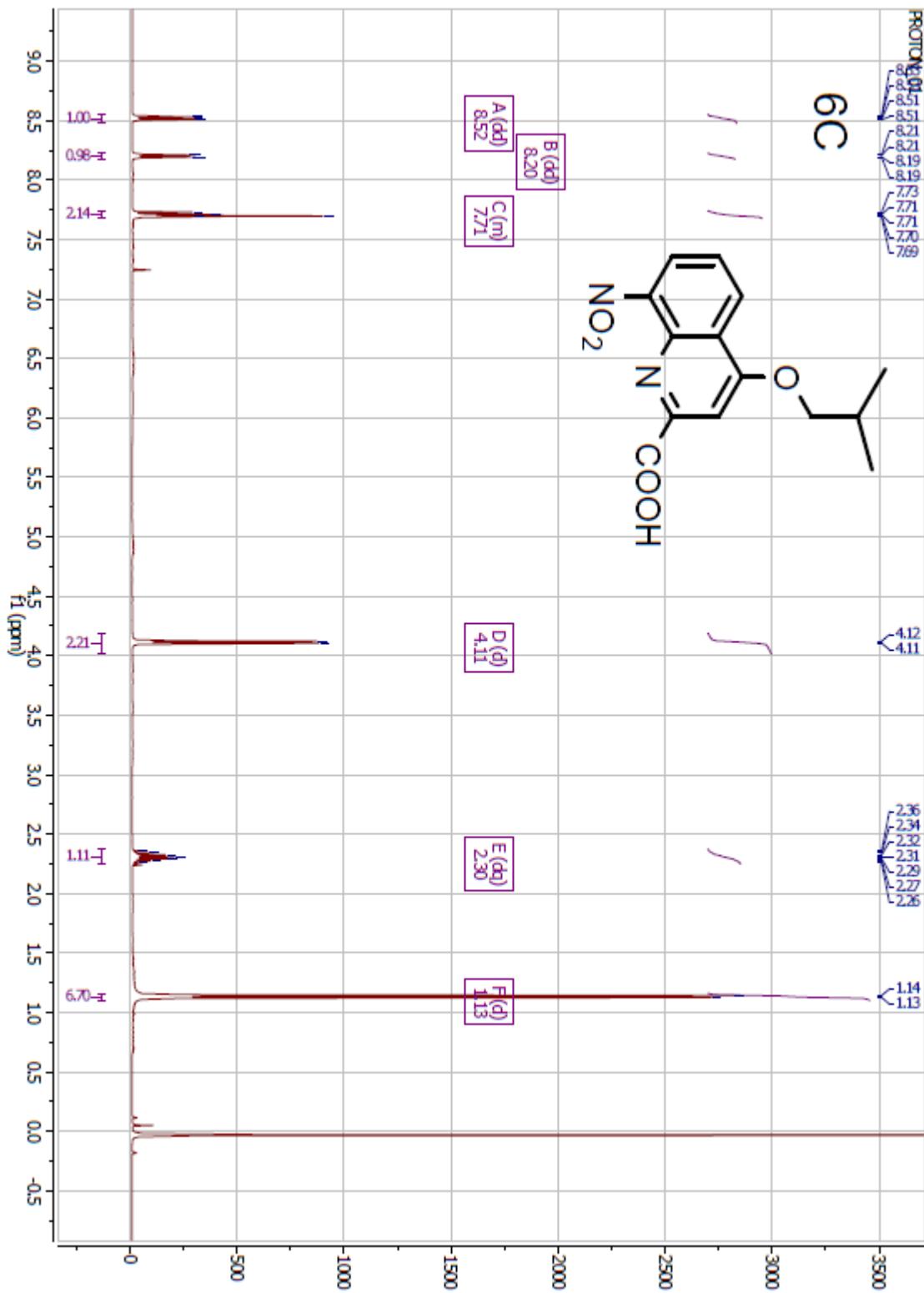
**Fig.** MALDI-TOF of 5D.



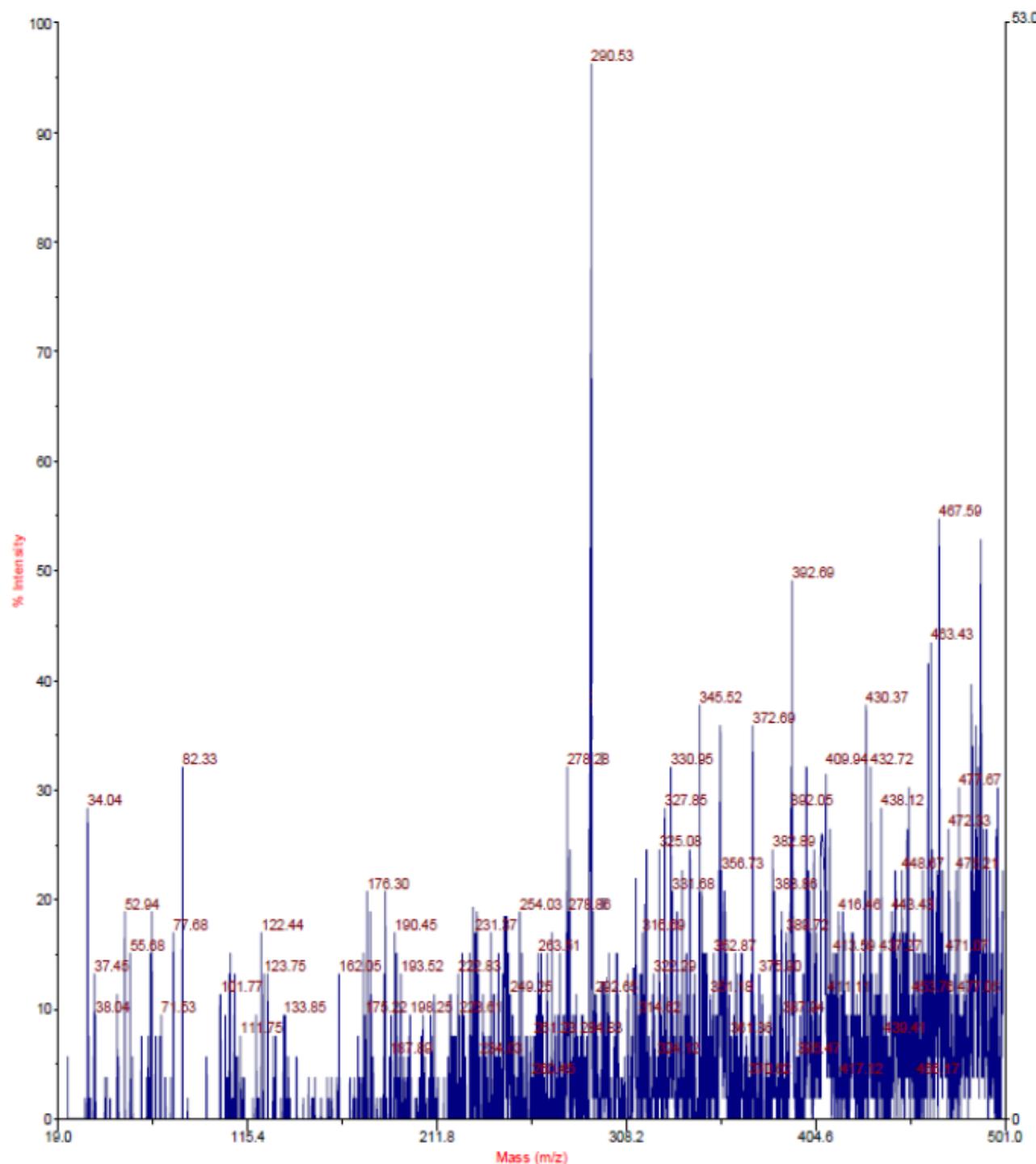
**Fig.** <sup>1</sup>H NMR of 6B (ADM-143).



**Fig.** MALDI-TOF of 6B (ADM-143).



**Fig.**  $^1\text{H}$  NMR of 6C (ADM-144).



**Fig.** MALDI-TOF of 6C (ADM-144).

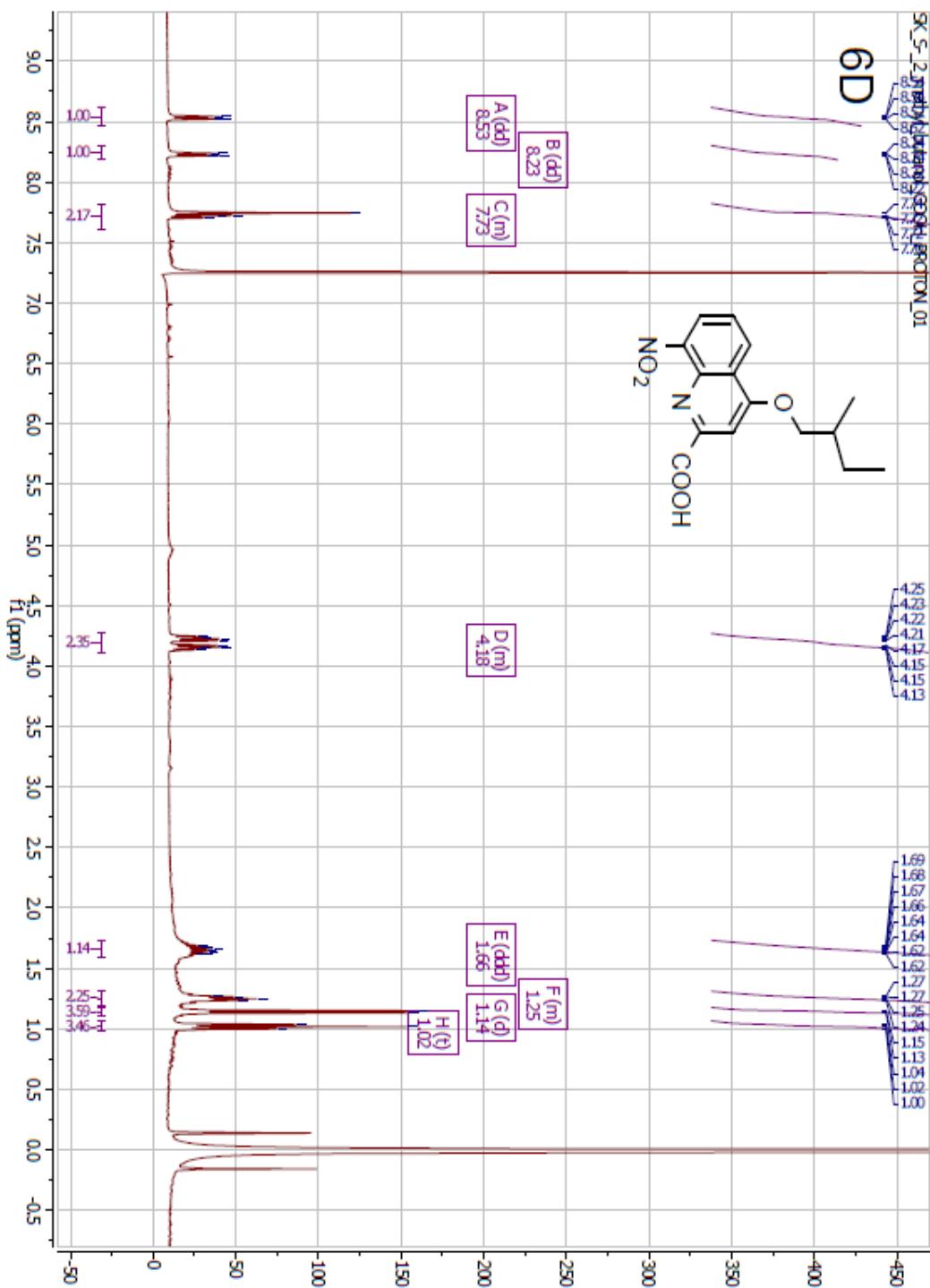
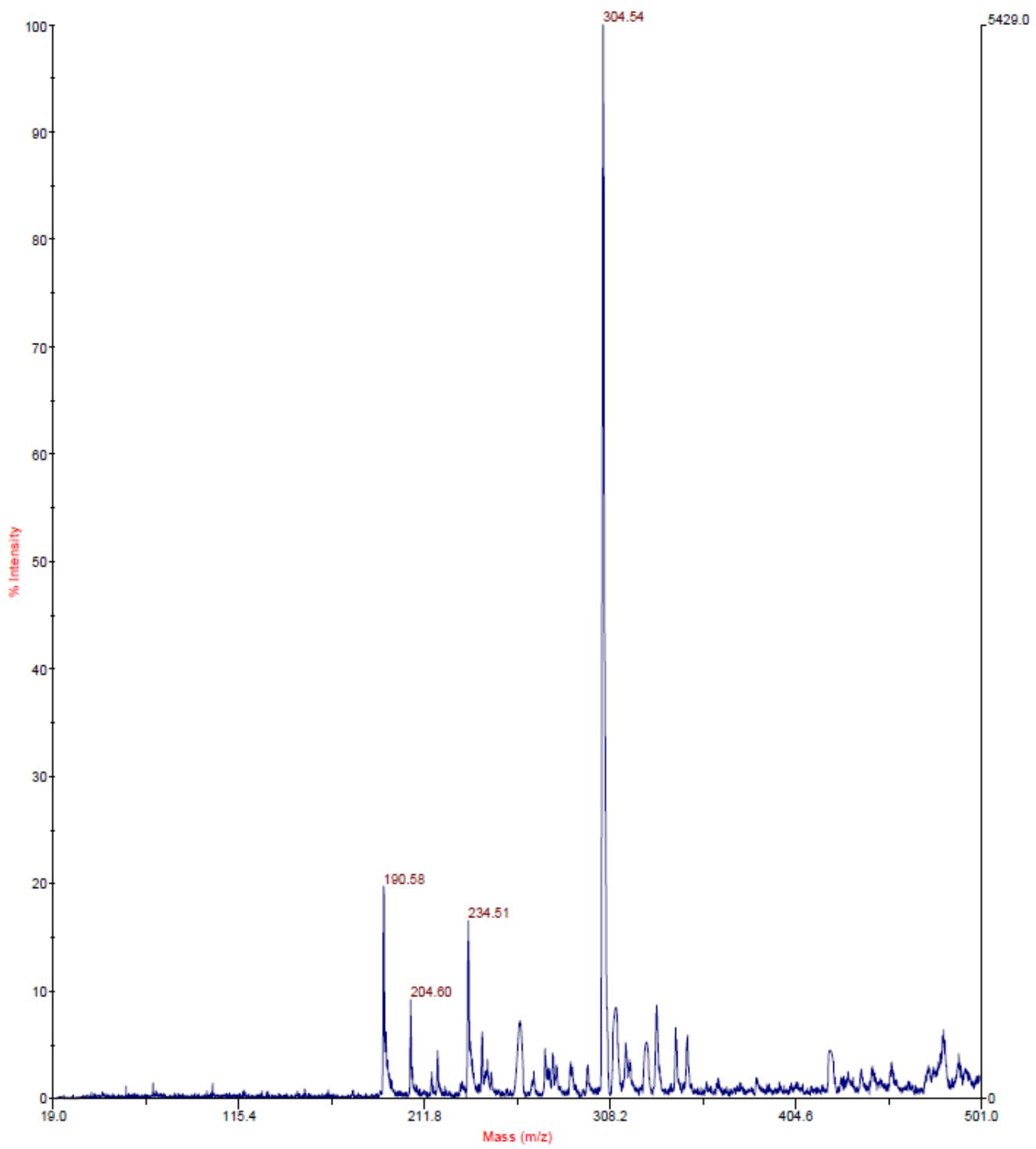
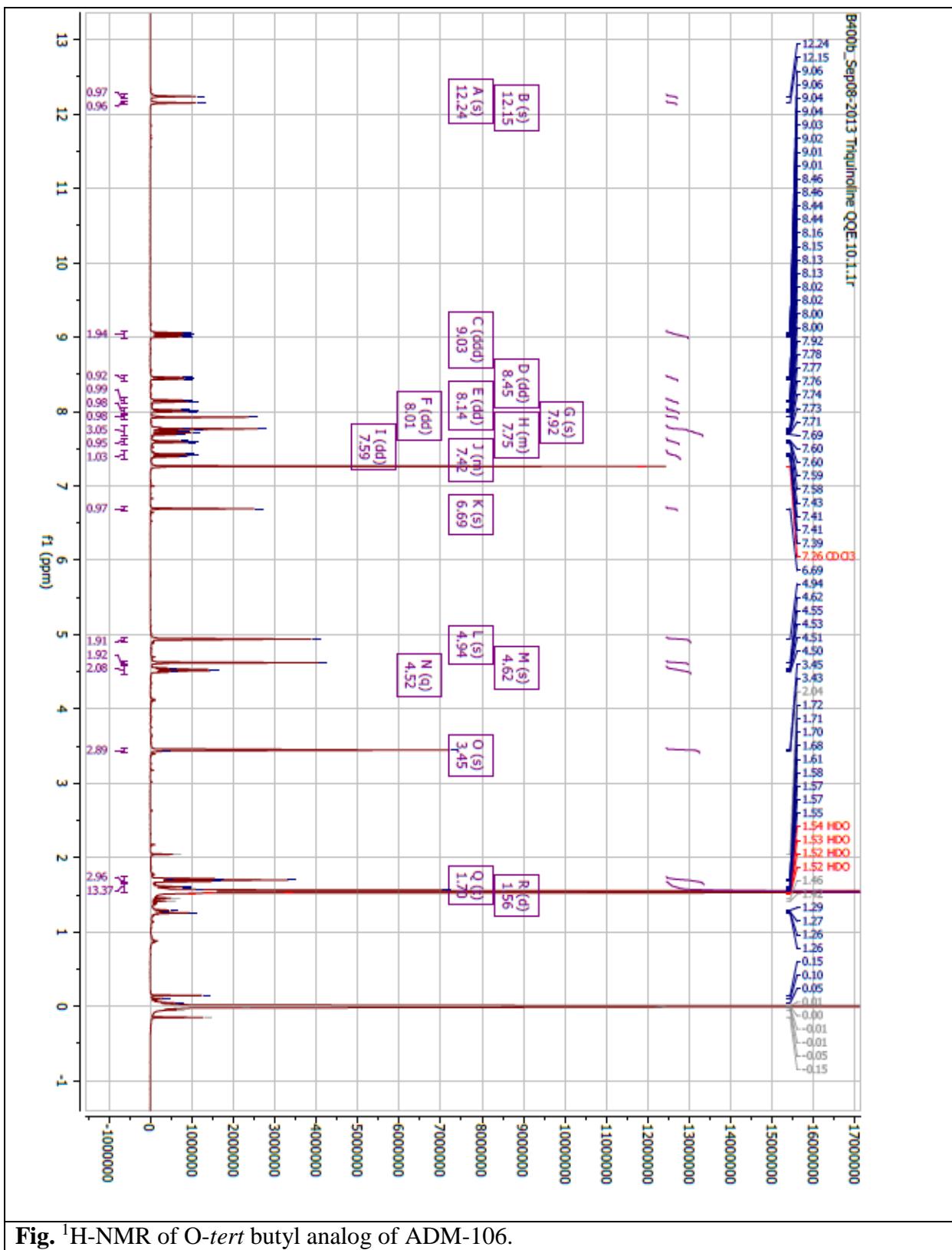


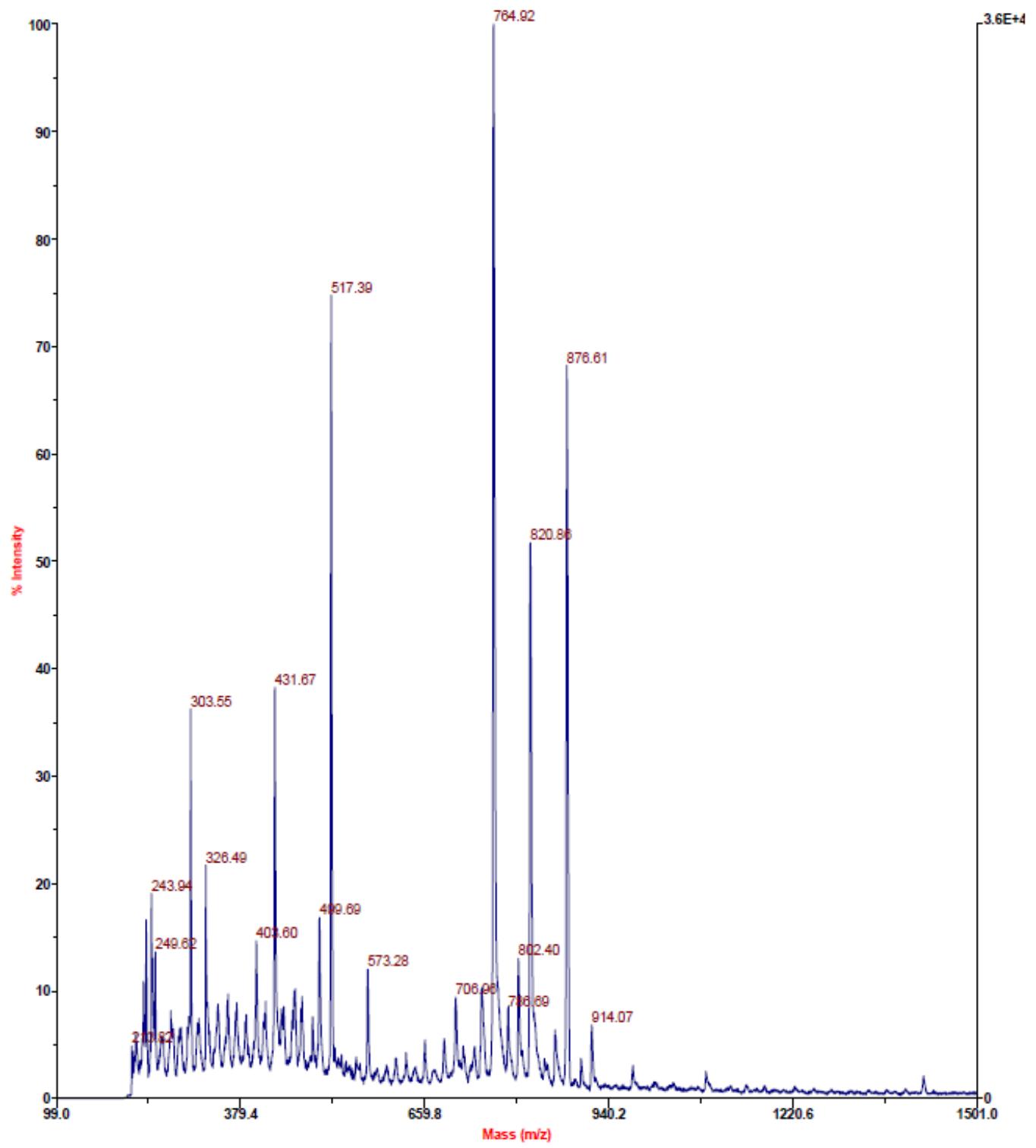
Fig.  $^1\text{H}$  NMR of 6D (ADM-145).



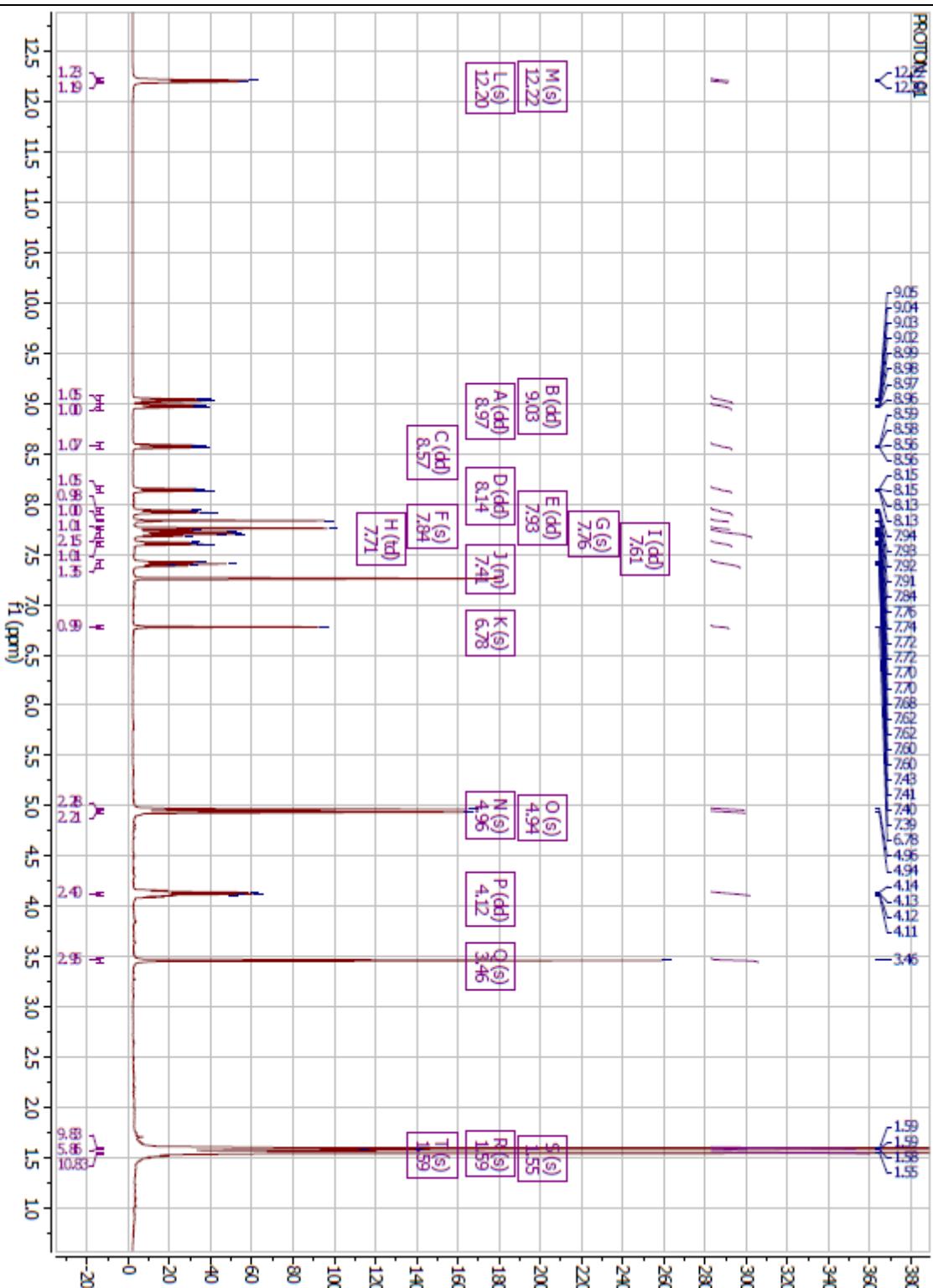
**Fig.** MALDI-TOF of 6D (ADM-145).



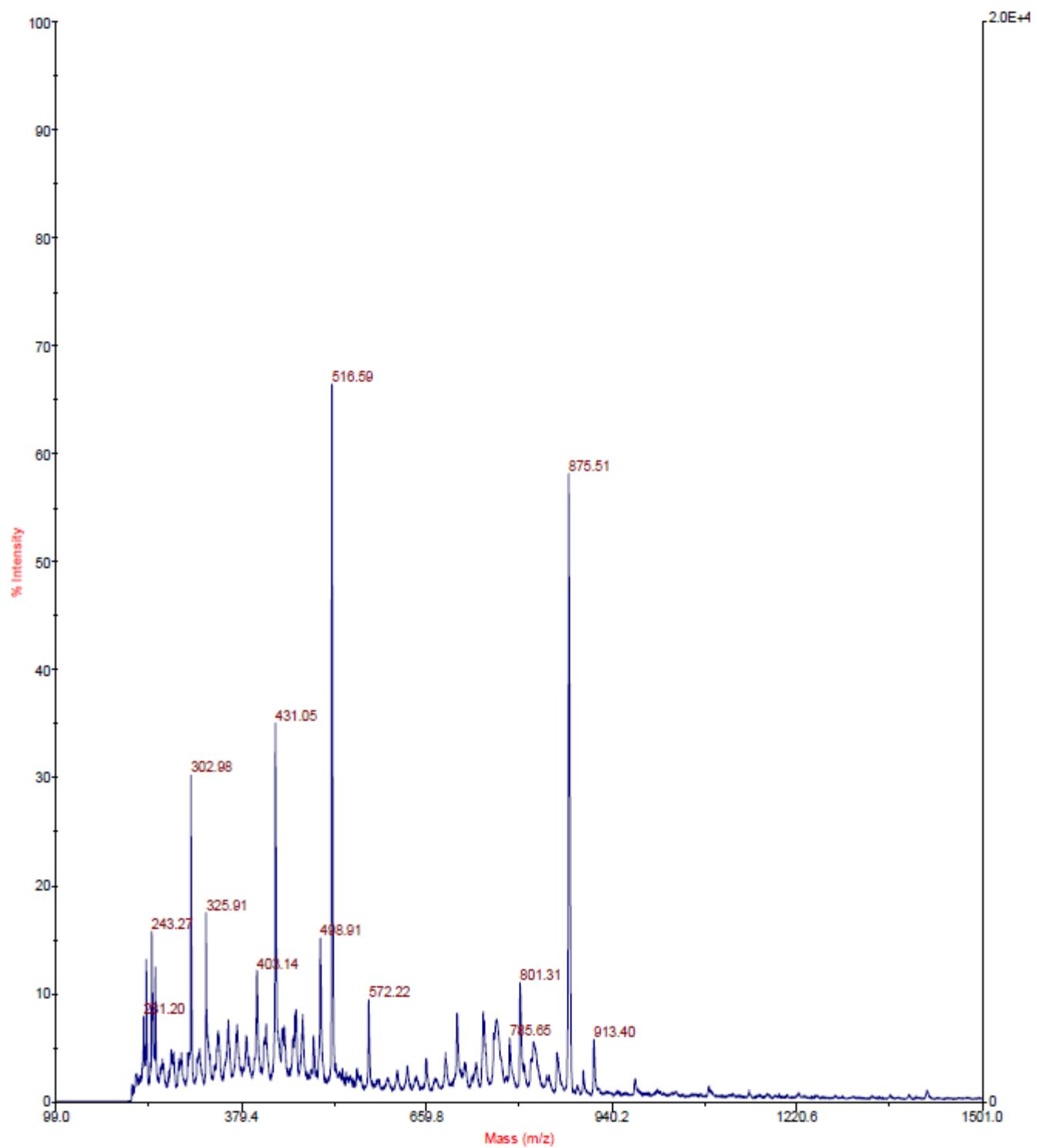
**Fig.**  $^1\text{H}$ -NMR of O-*tert* butyl analog of ADM-106.



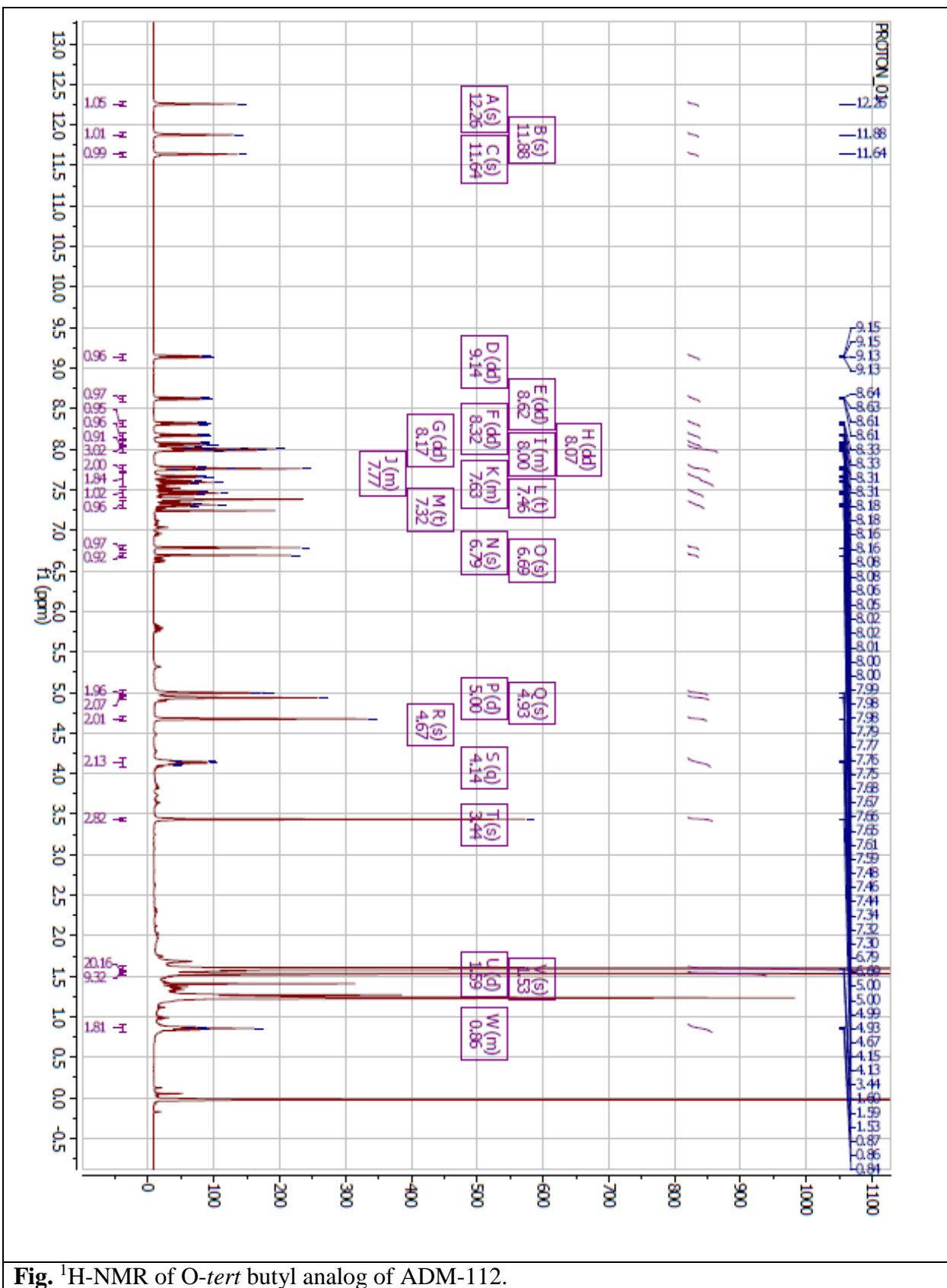
**Fig.** MALDI-TOF of O-*tert* butyl analog of ADM-106.



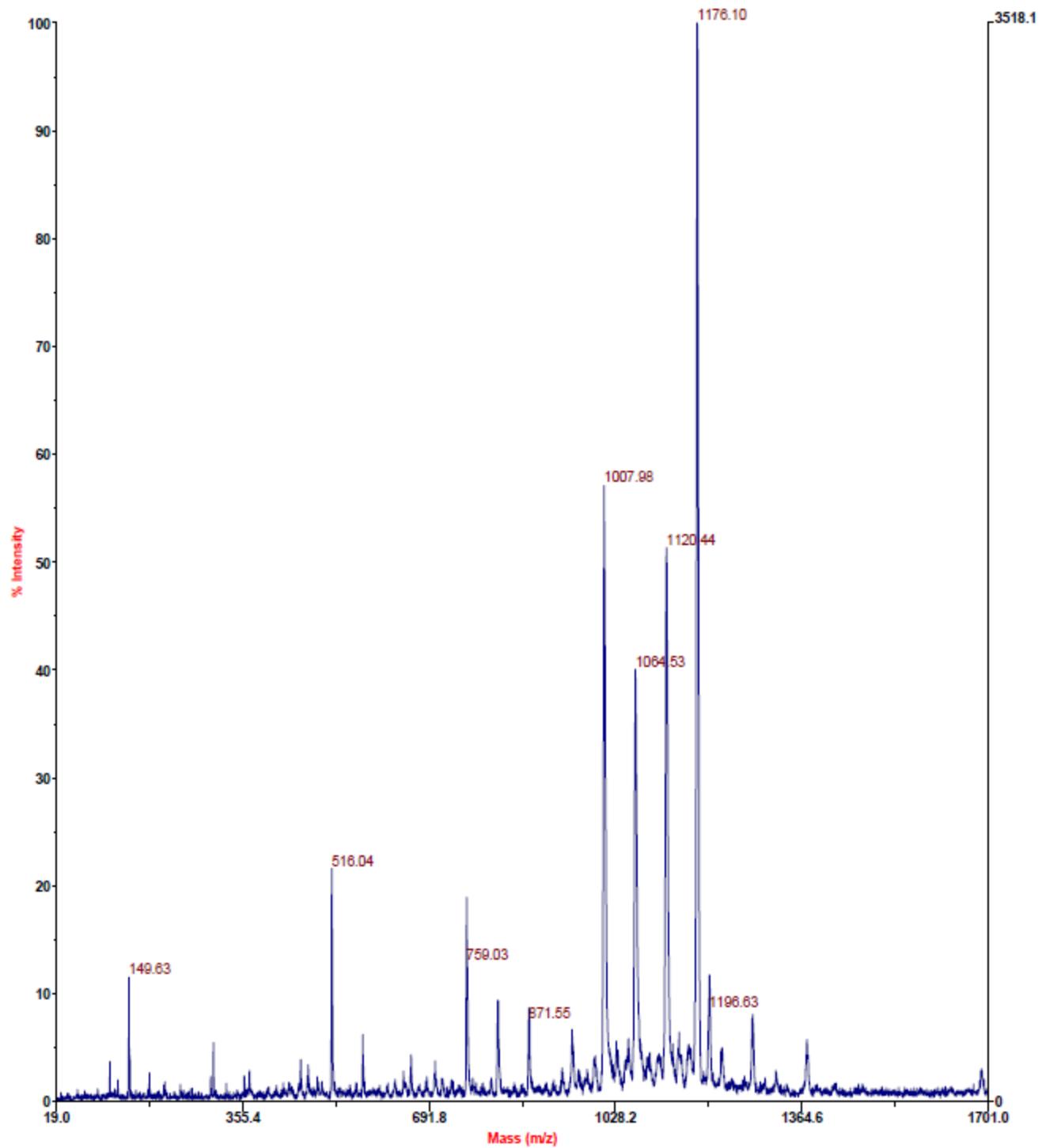
**Fig.**  $^1\text{H}$ -NMR of O-*tert* butyl analog of ADM-108.



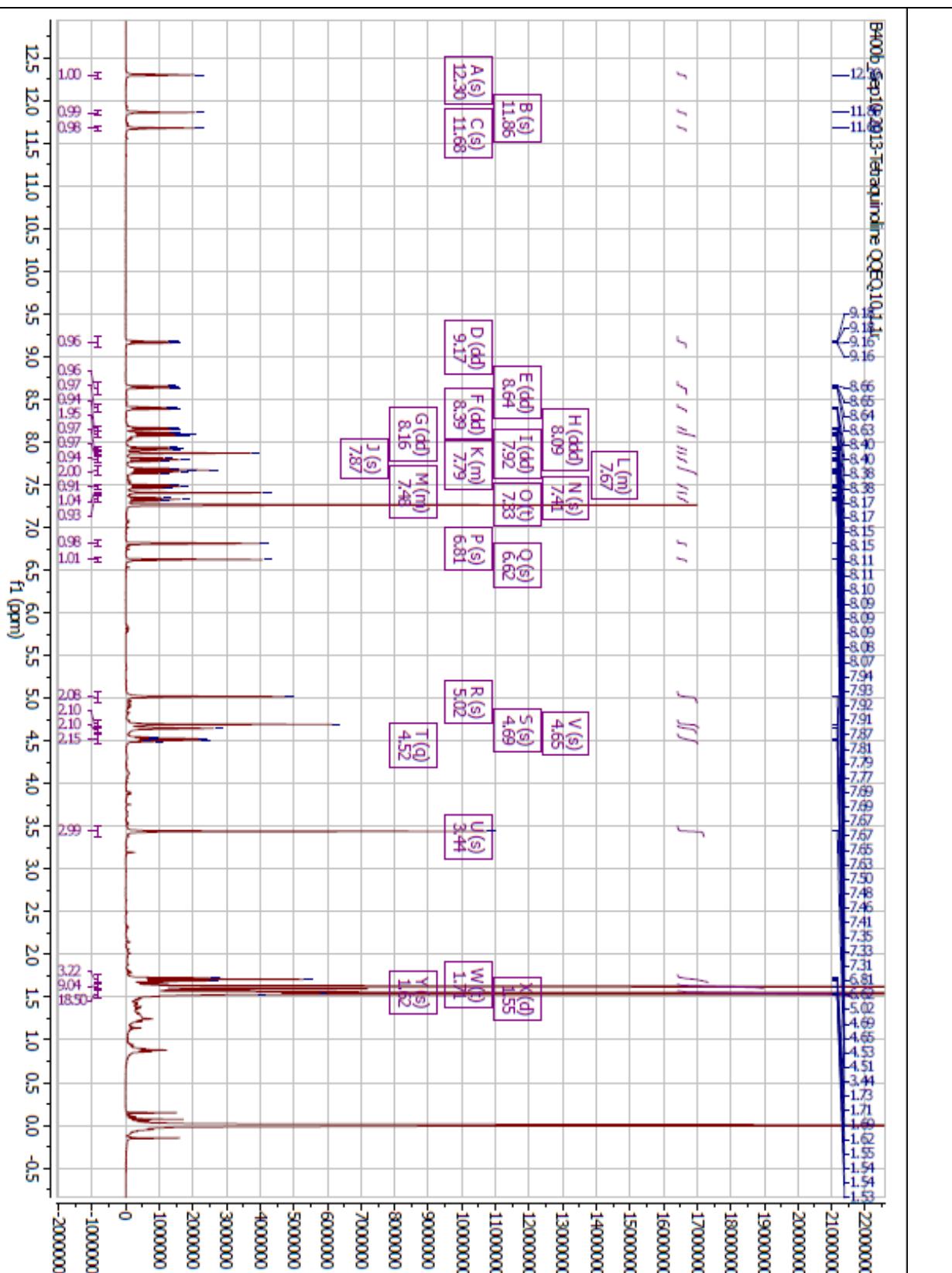
**Fig.** MALDI-TOF of O-*tert* butyl analog of ADM-108.



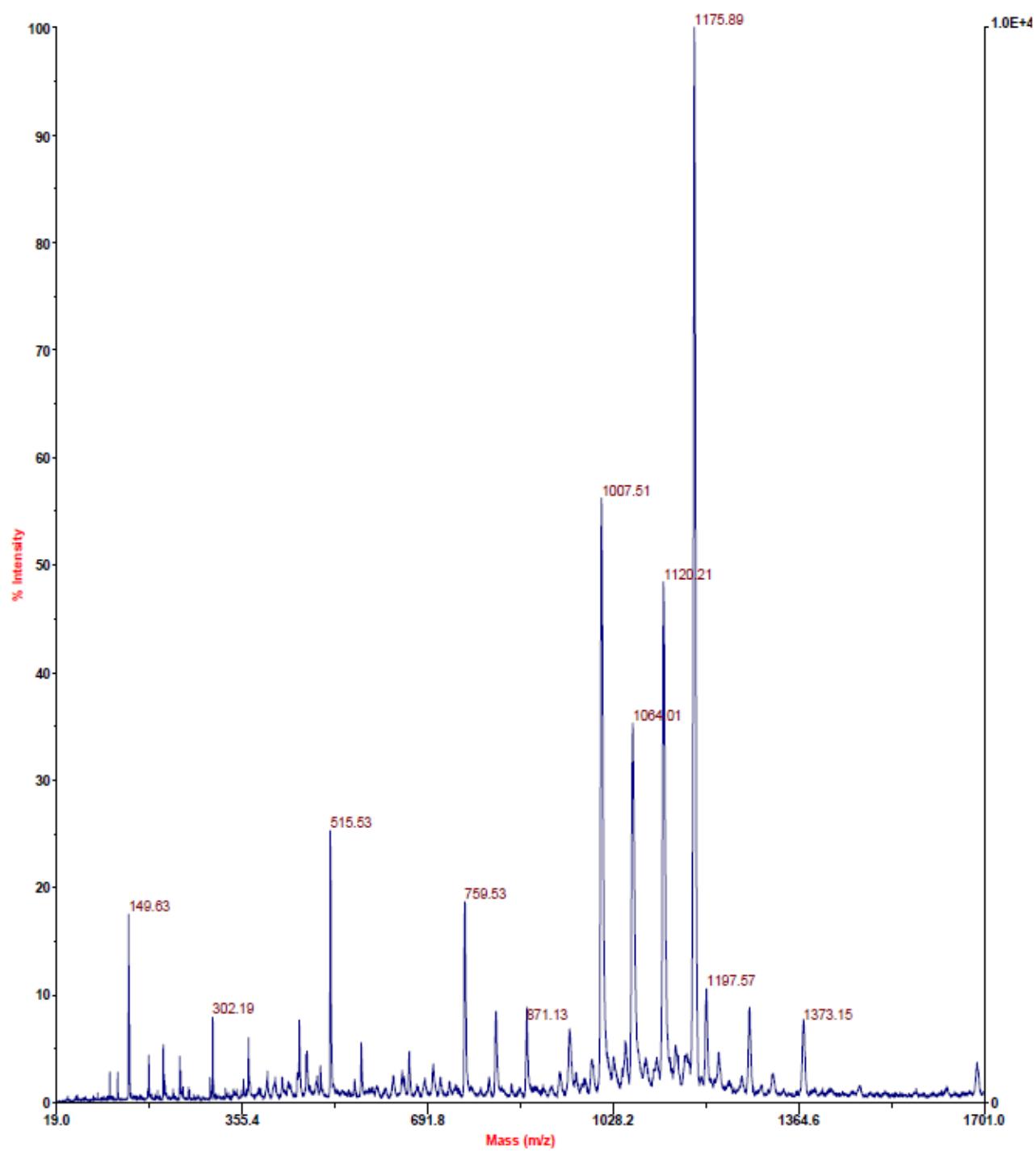
**Fig.**  $^1\text{H}$ -NMR of O-*tert* butyl analog of ADM-112.



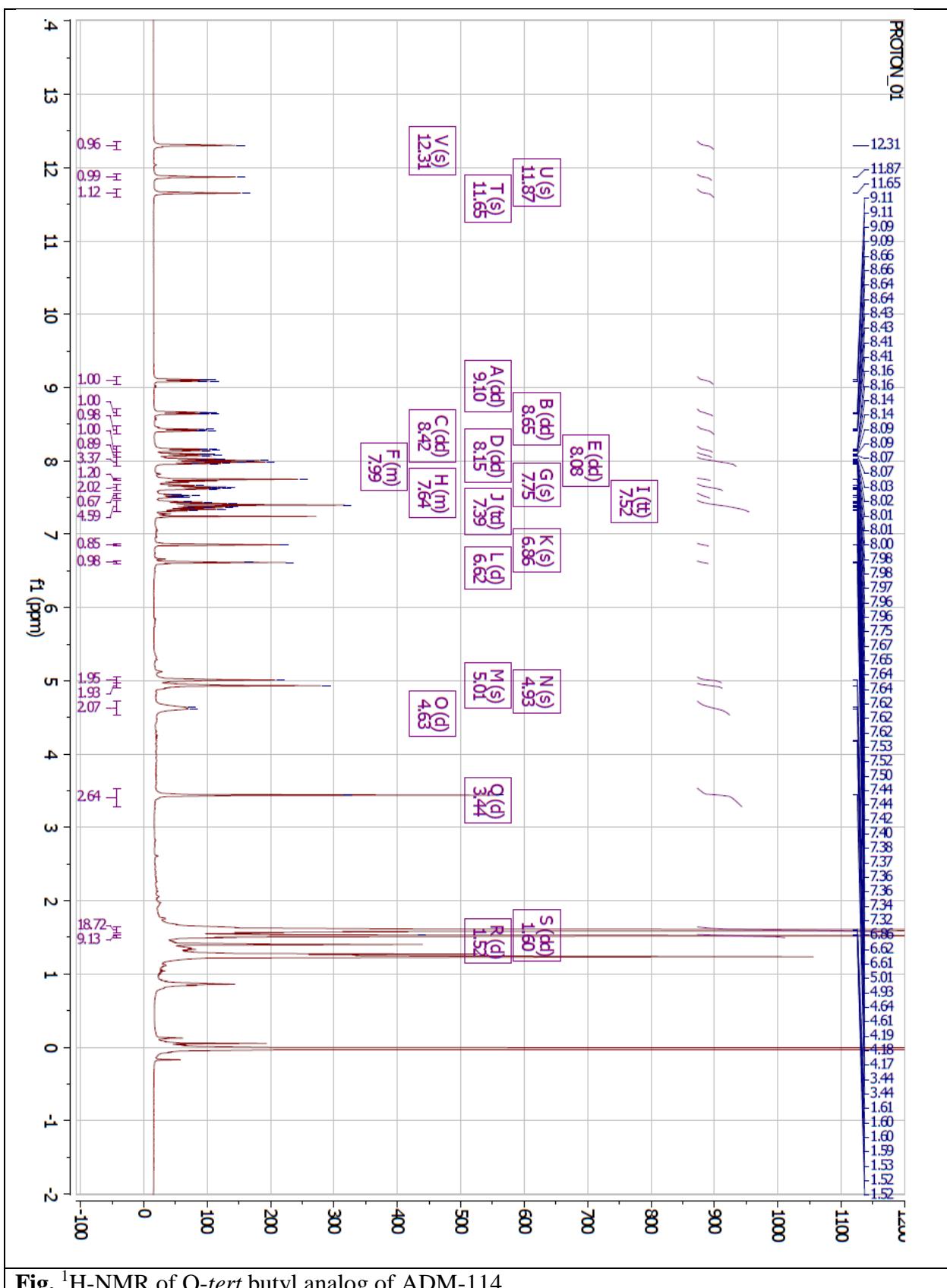
**Fig.** MALDI-TOF of O-*tert* butyl analog of ADM-112.



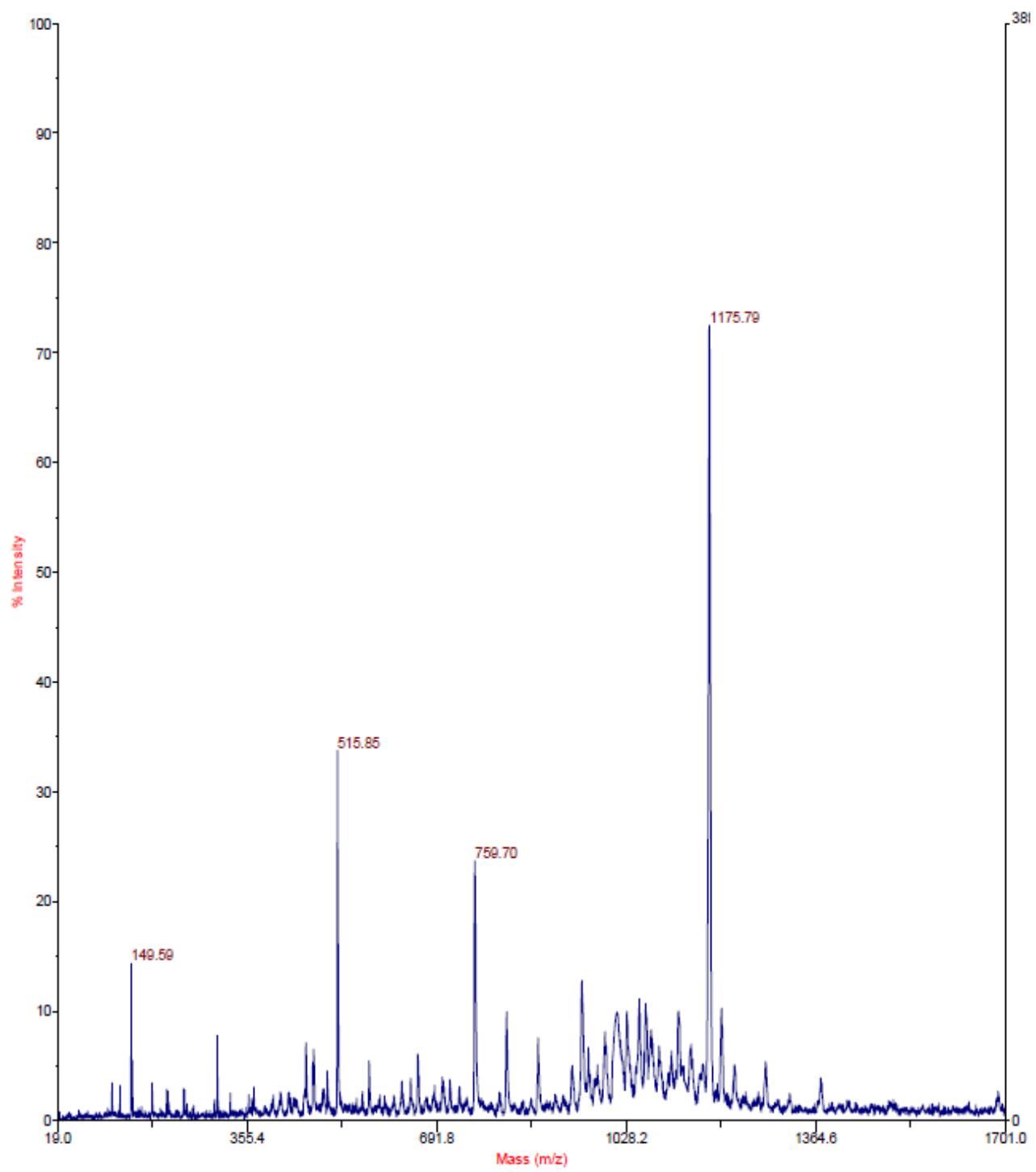
**Fig.**  $^1\text{H}$ -NMR of O-*tert* butyl analog of ADM-113.



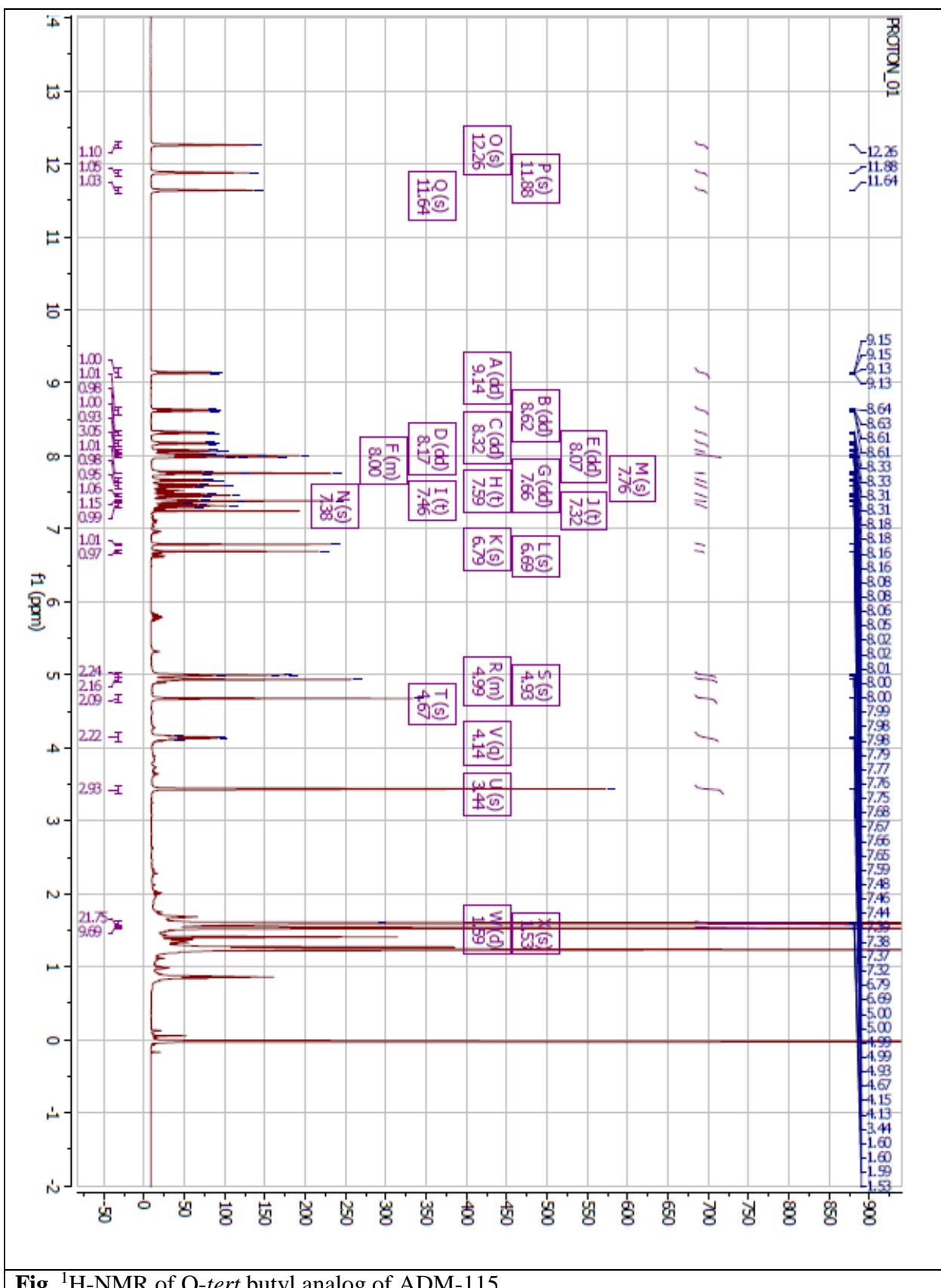
**Fig.** MALDI-TOF of O-*tert* butyl analog of ADM-113.



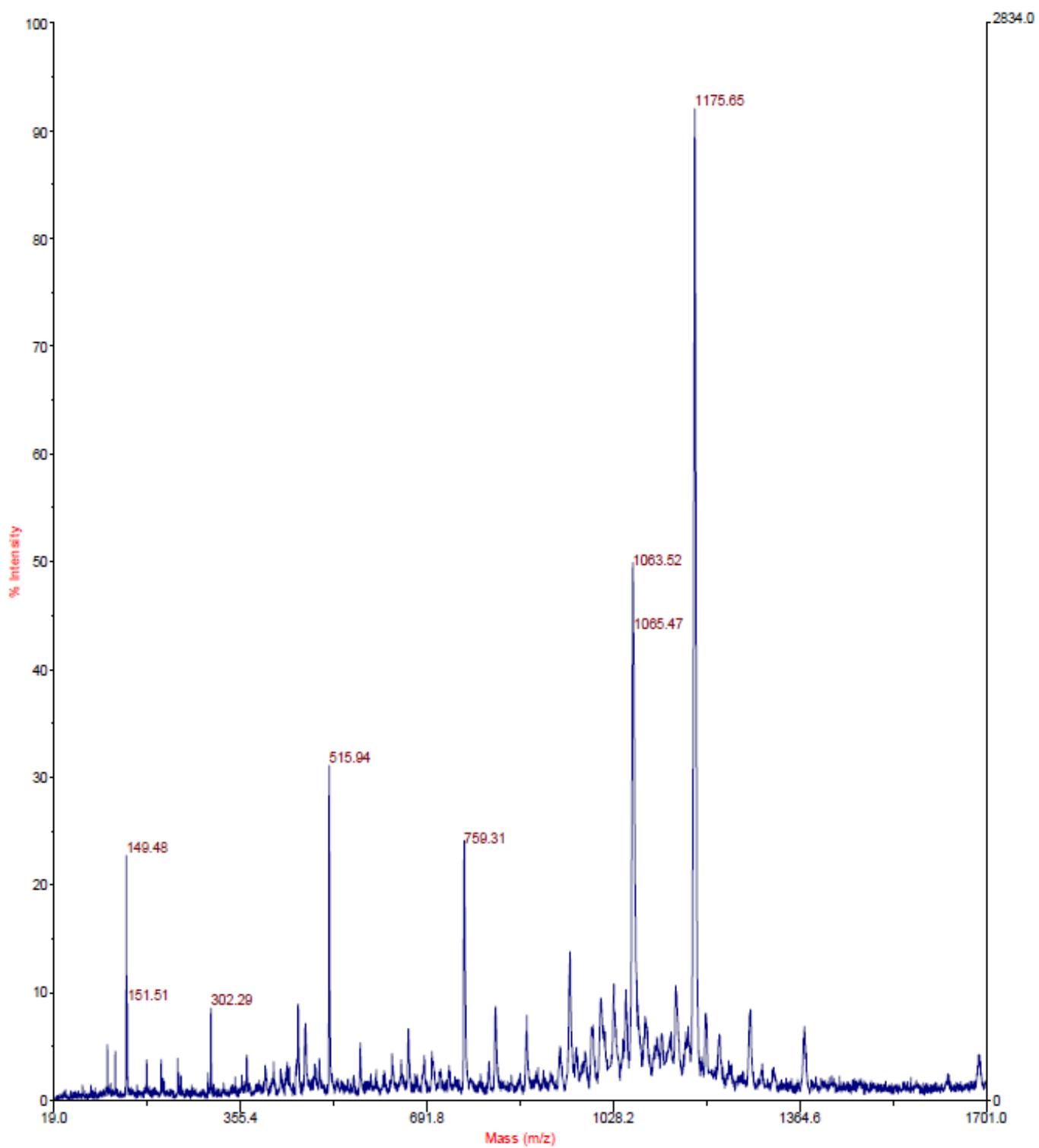
**Fig.**  $^1\text{H}$ -NMR of O-*tert* butyl analog of ADM-114.



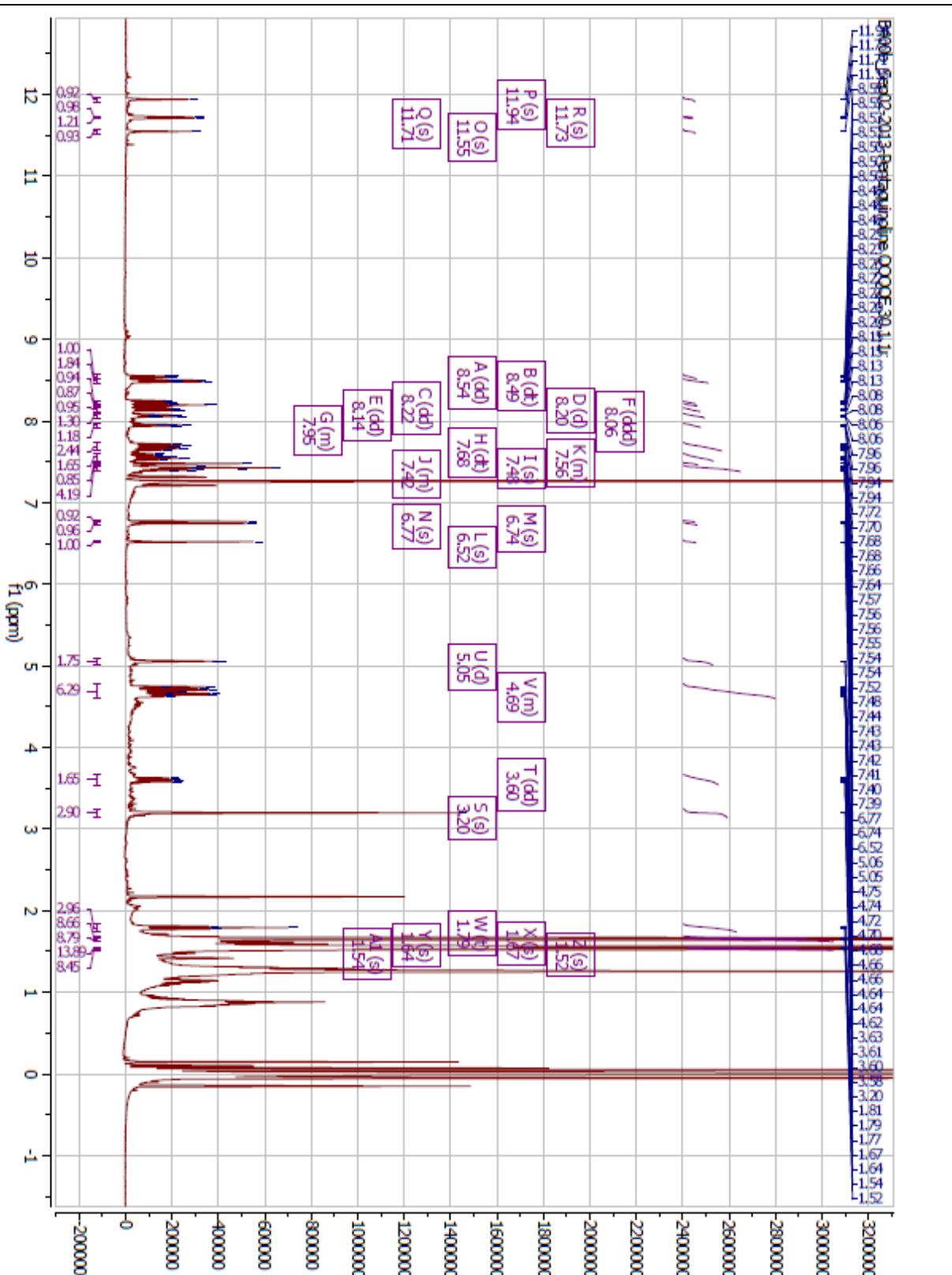
**Fig.** MALDI-TOF of O-*tert* butyl analog of ADM-114.



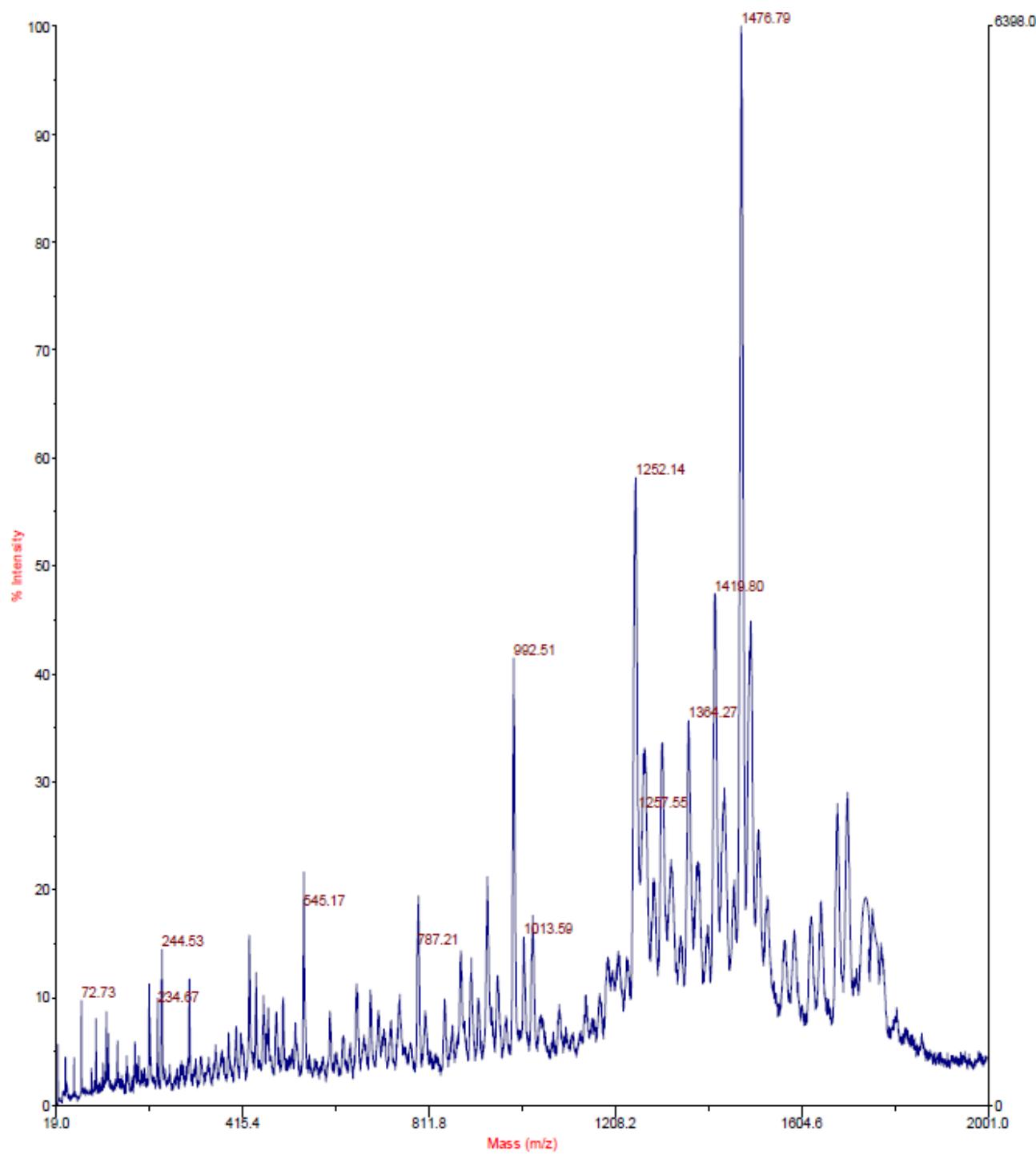
**Fig.**  $^1\text{H}$ -NMR of O-*tert* butyl analog of ADM-115.



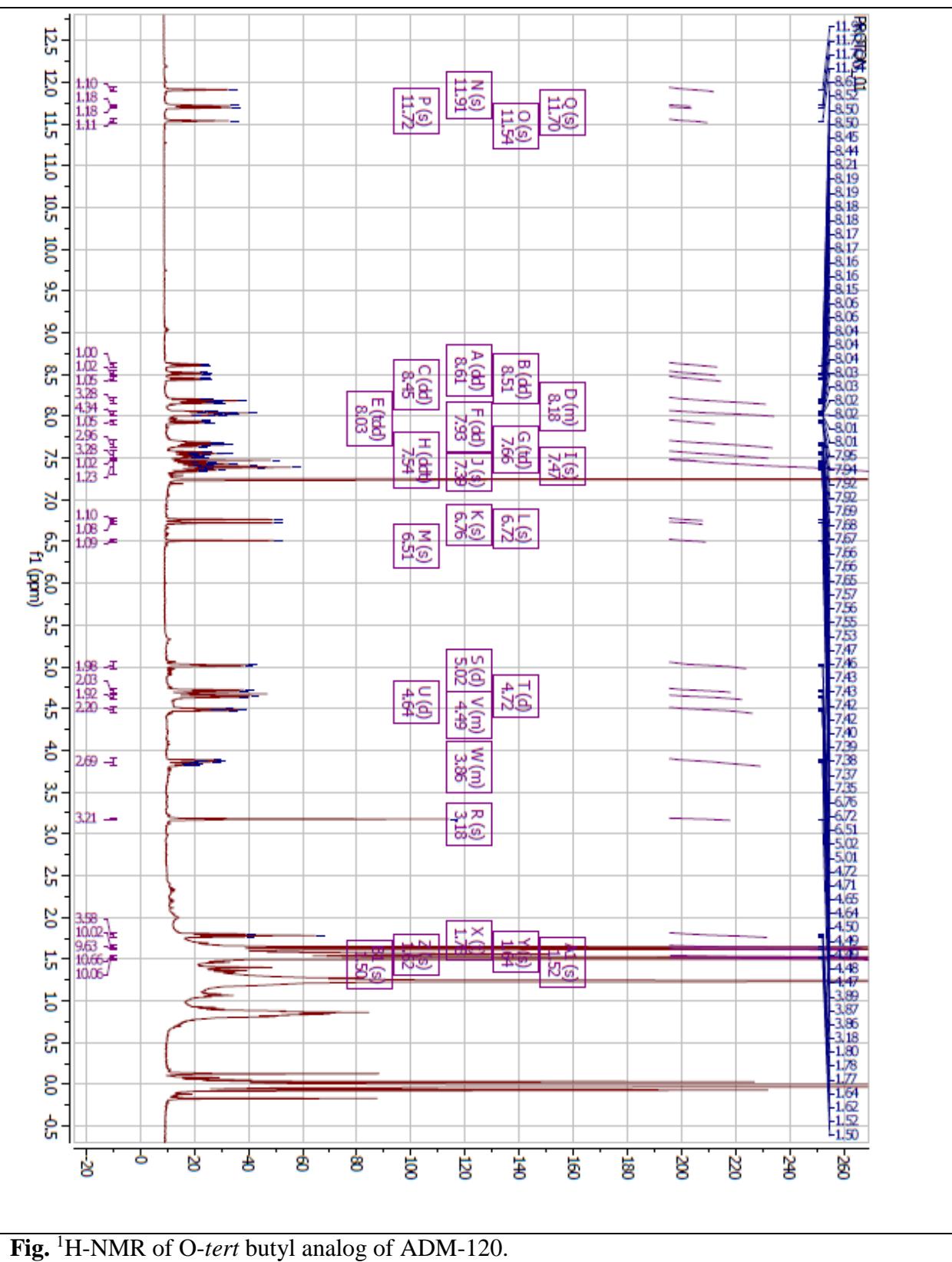
**Fig.** MALDI-TOF of O-*tert* butyl analog of ADM-115.



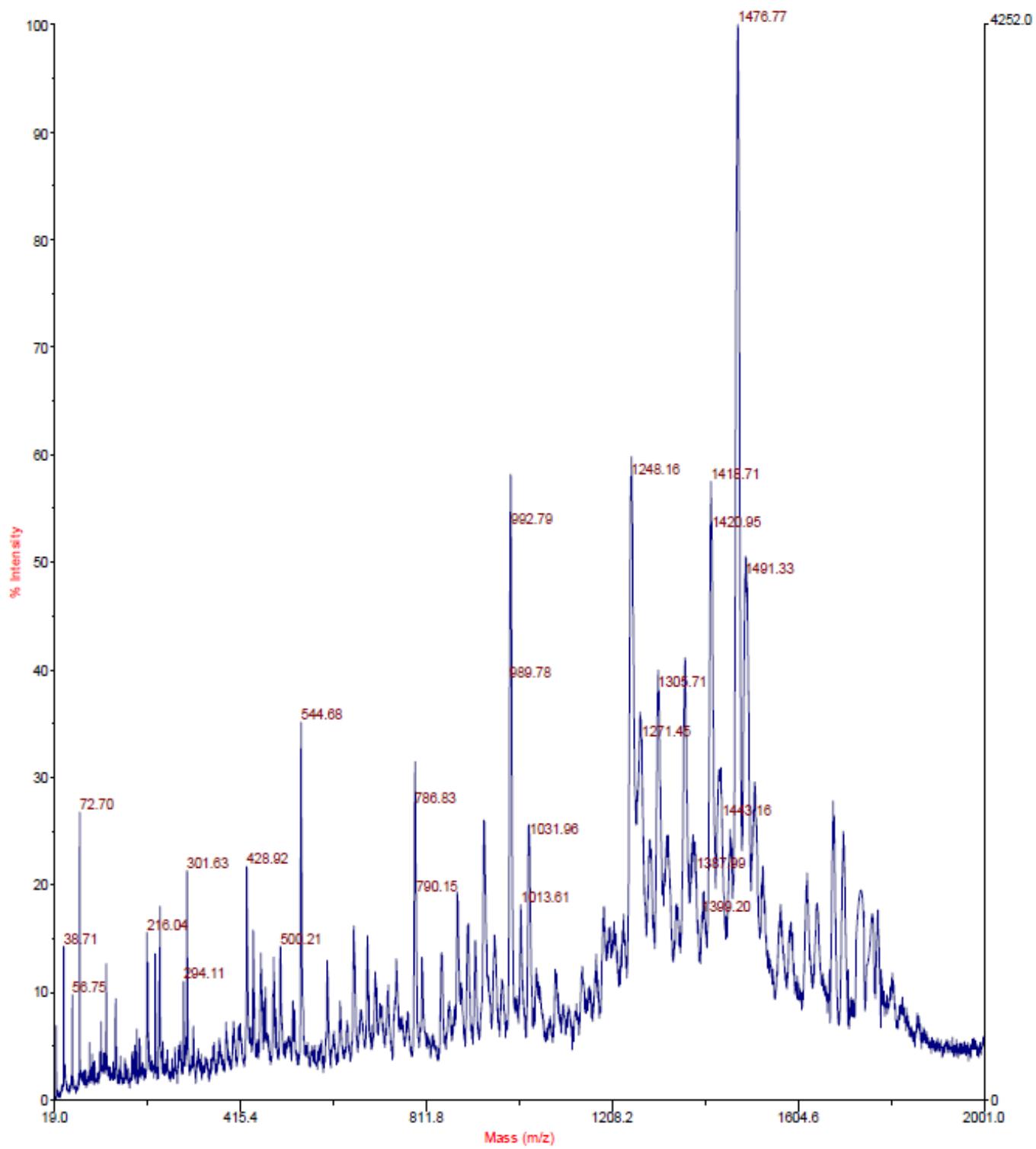
**Fig.**  $^1\text{H}$ -NMR of O-*tert* butyl analog of ADM-119.



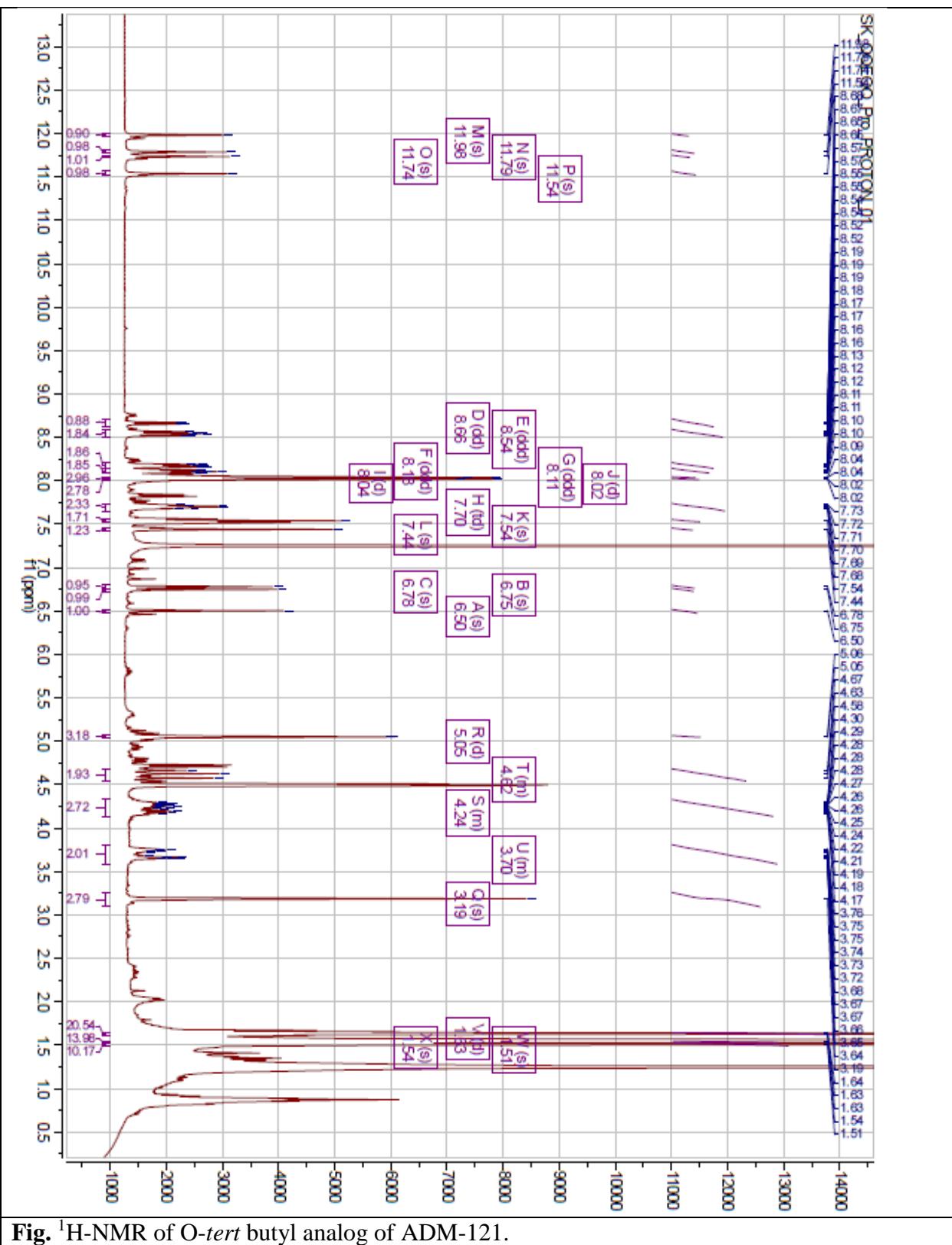
**Fig.** MALDI-TOF of O-*tert* butyl analog of ADM-119.



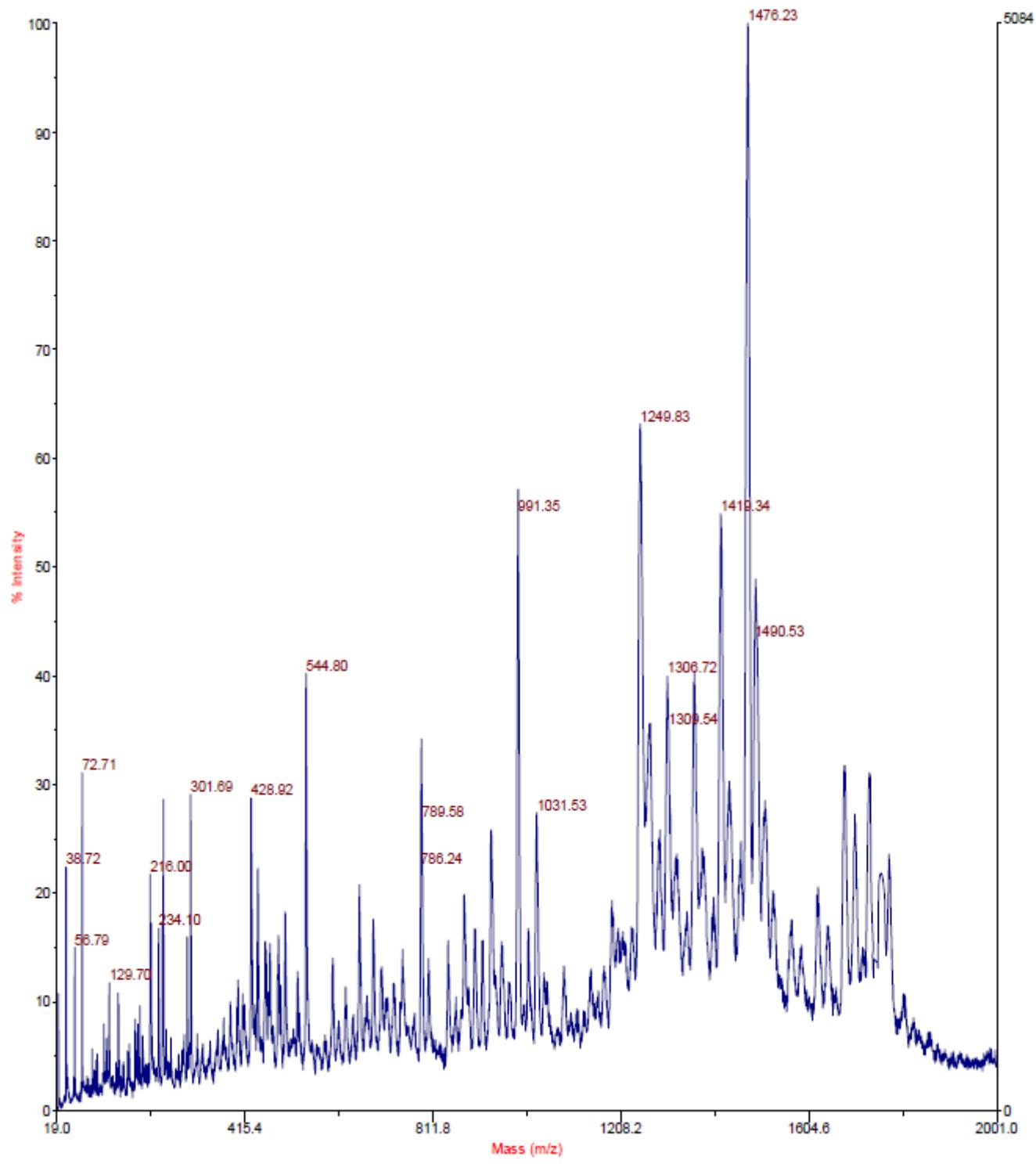
**Fig.**  $^1\text{H}$ -NMR of O-*tert* butyl analog of ADM-120.



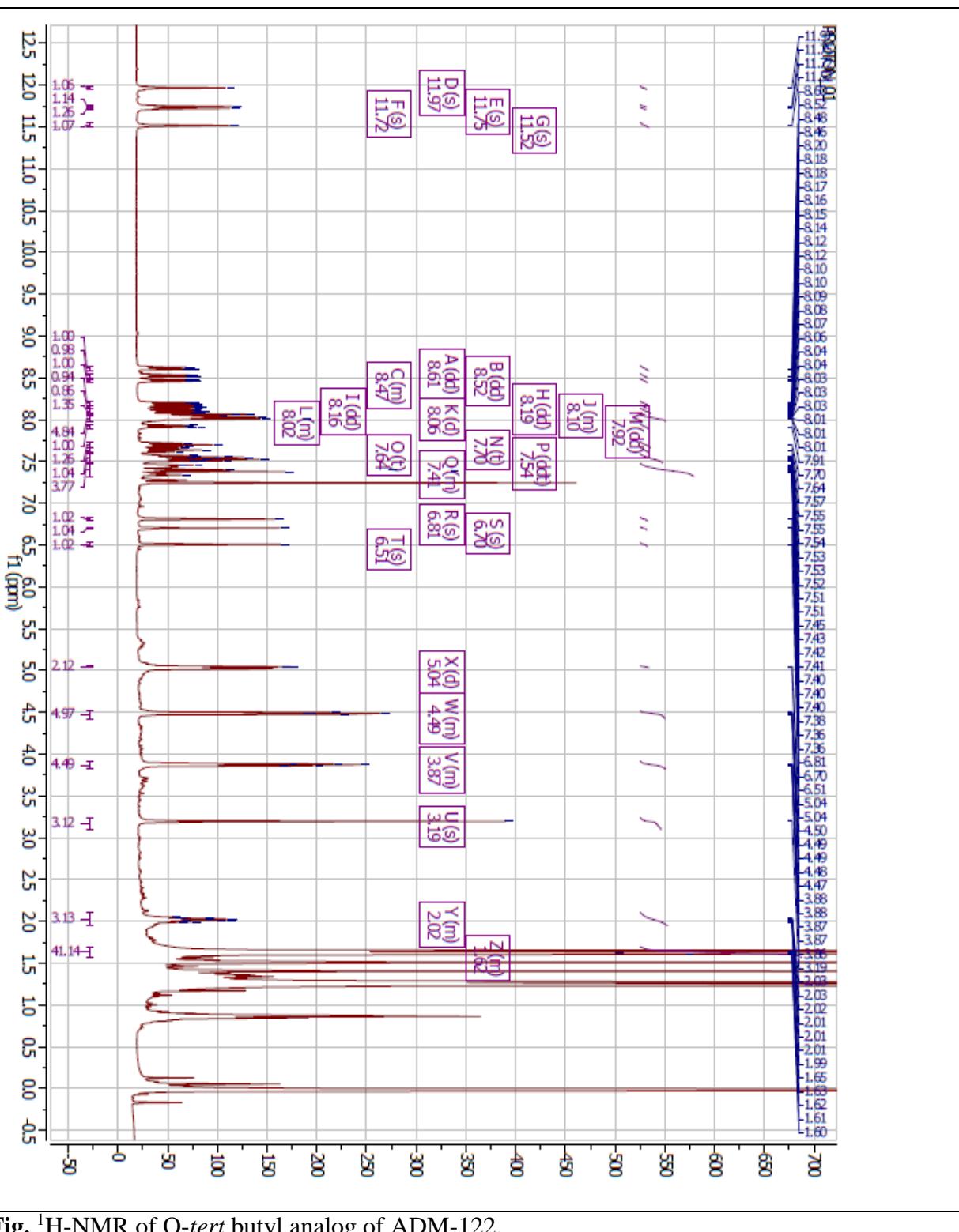
**Fig.** MALDI-TOF of O-*tert* butyl analog of ADM-120.



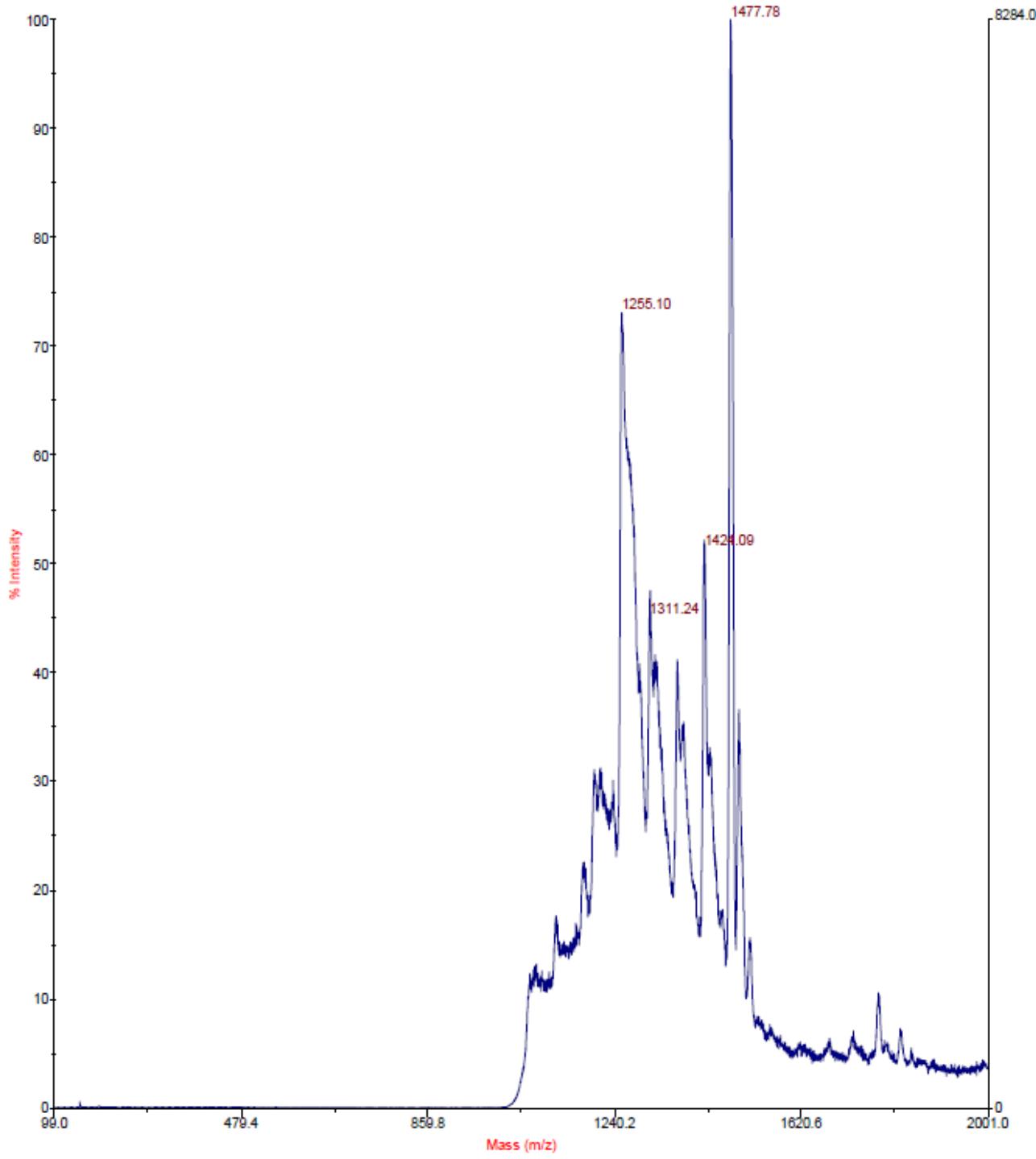
**Fig.**  $^1\text{H}$ -NMR of O-*tert* butyl analog of ADM-121.



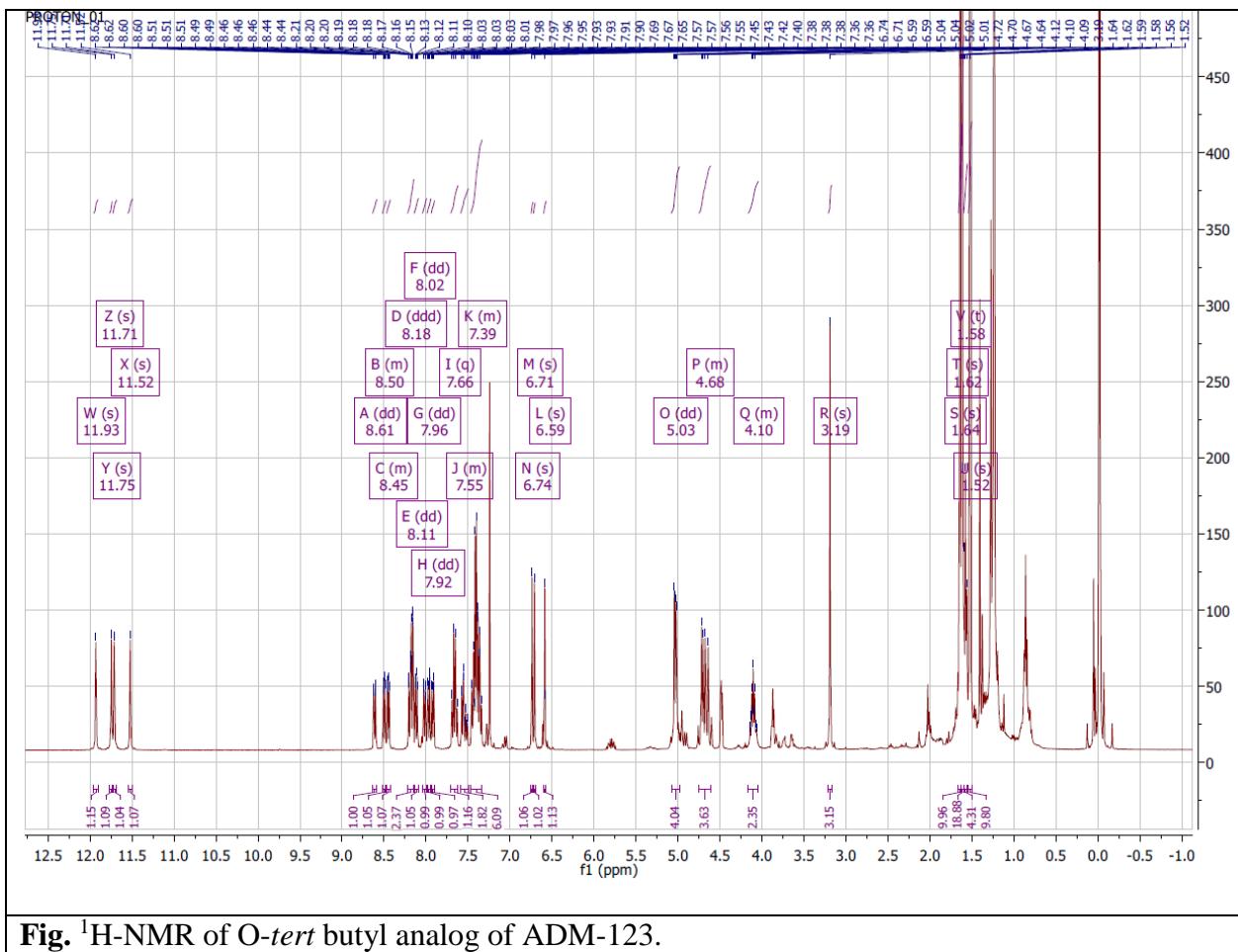
**Fig.** MALDI-TOF of O-*tert* butyl analog of ADM-121.



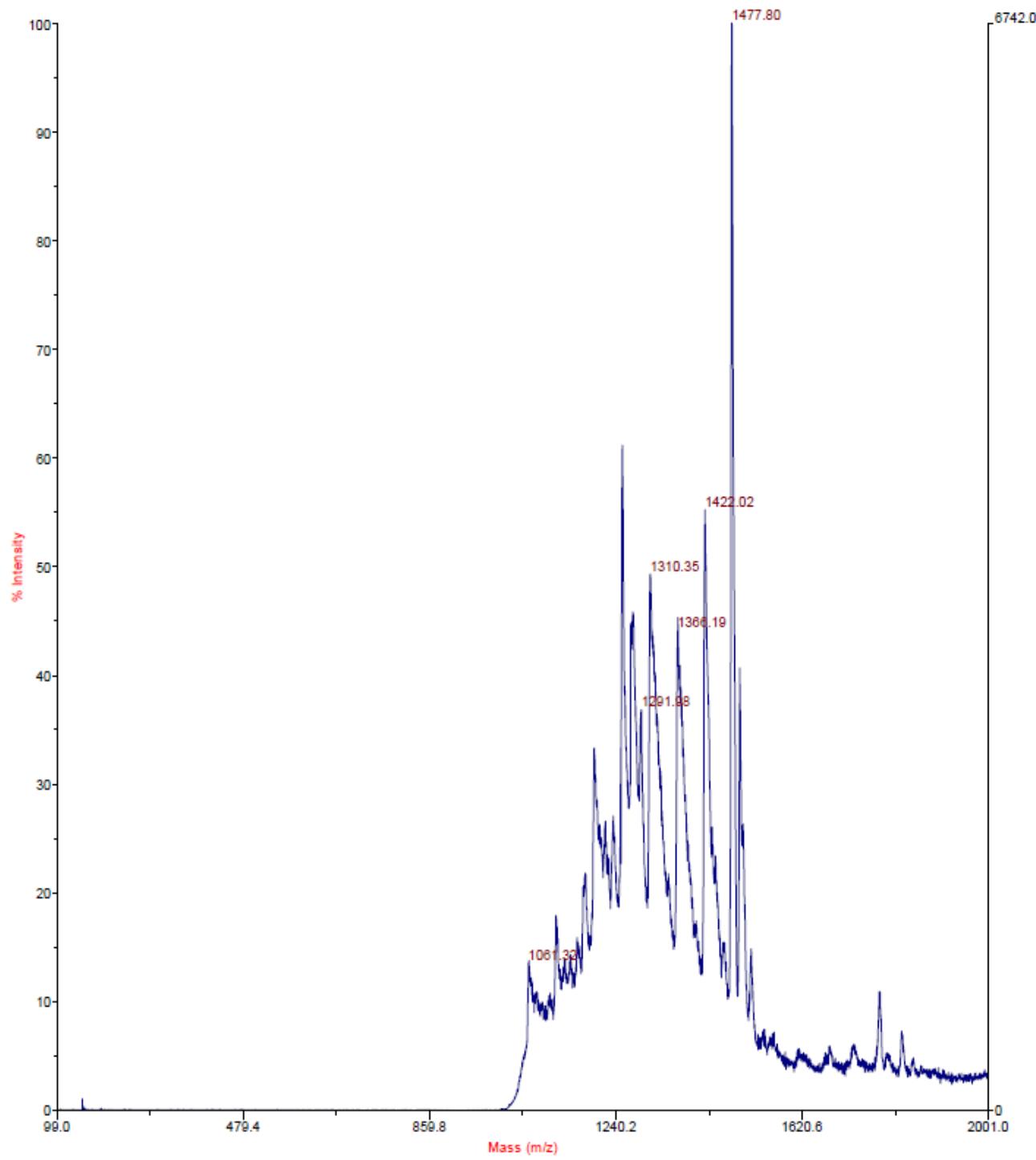
**Fig.**  $^1\text{H-NMR}$  of O-*tert* butyl analog of ADM-122.



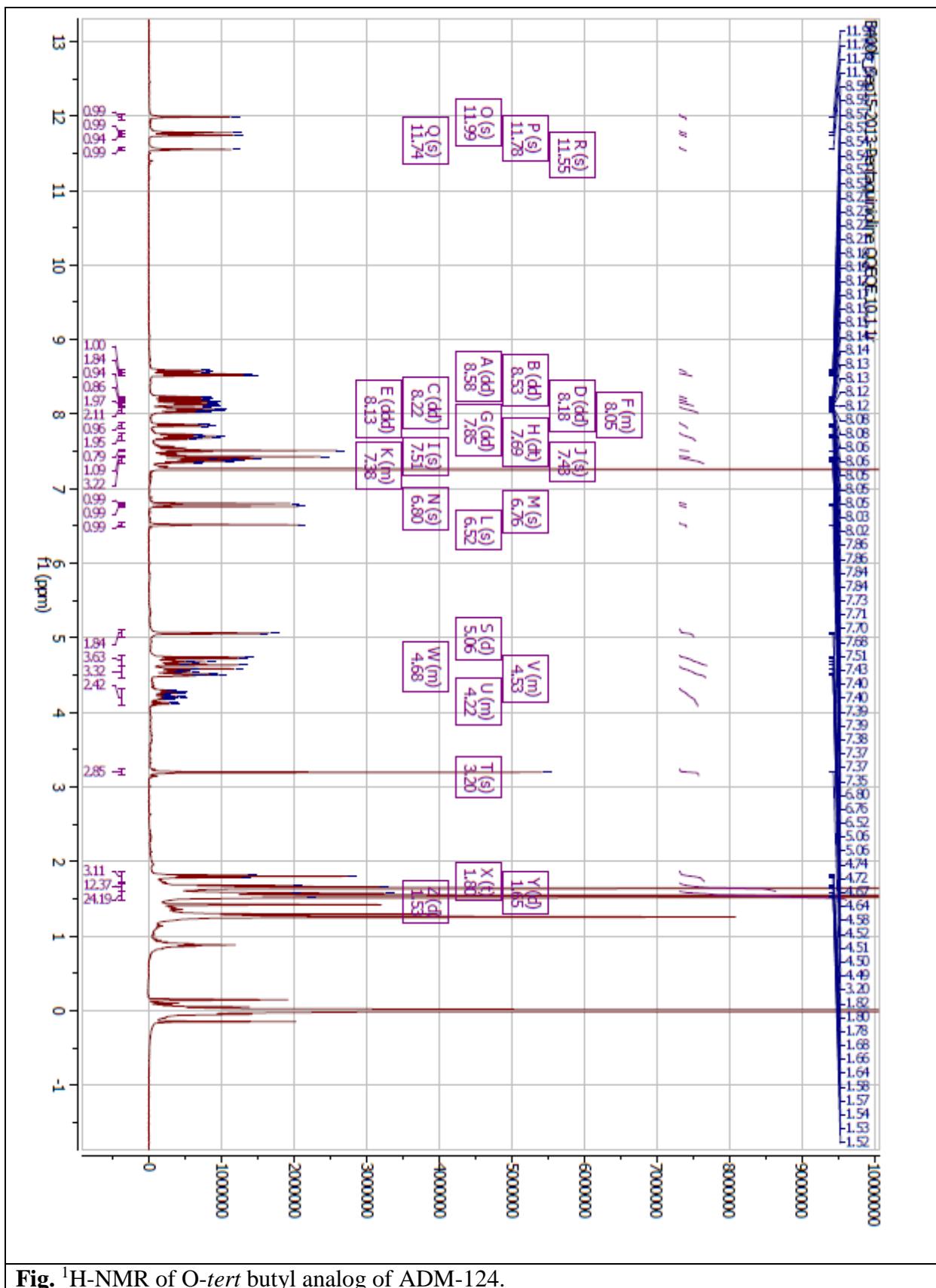
**Fig.** MALDI-TOF of O-*tert* butyl analog of ADM-122.



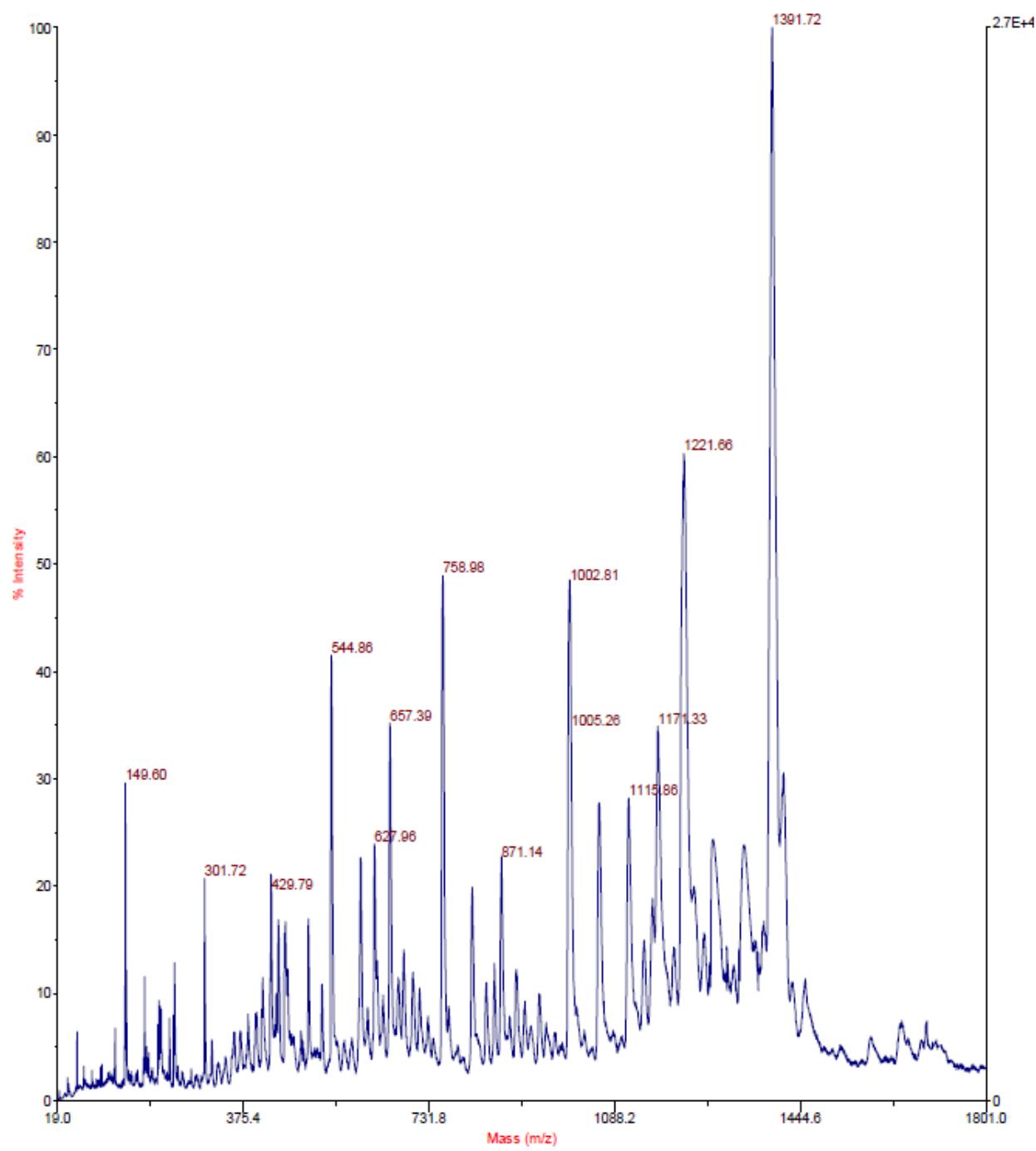
**Fig.**  $^1\text{H}$ -NMR of O-*tert* butyl analog of ADM-123.



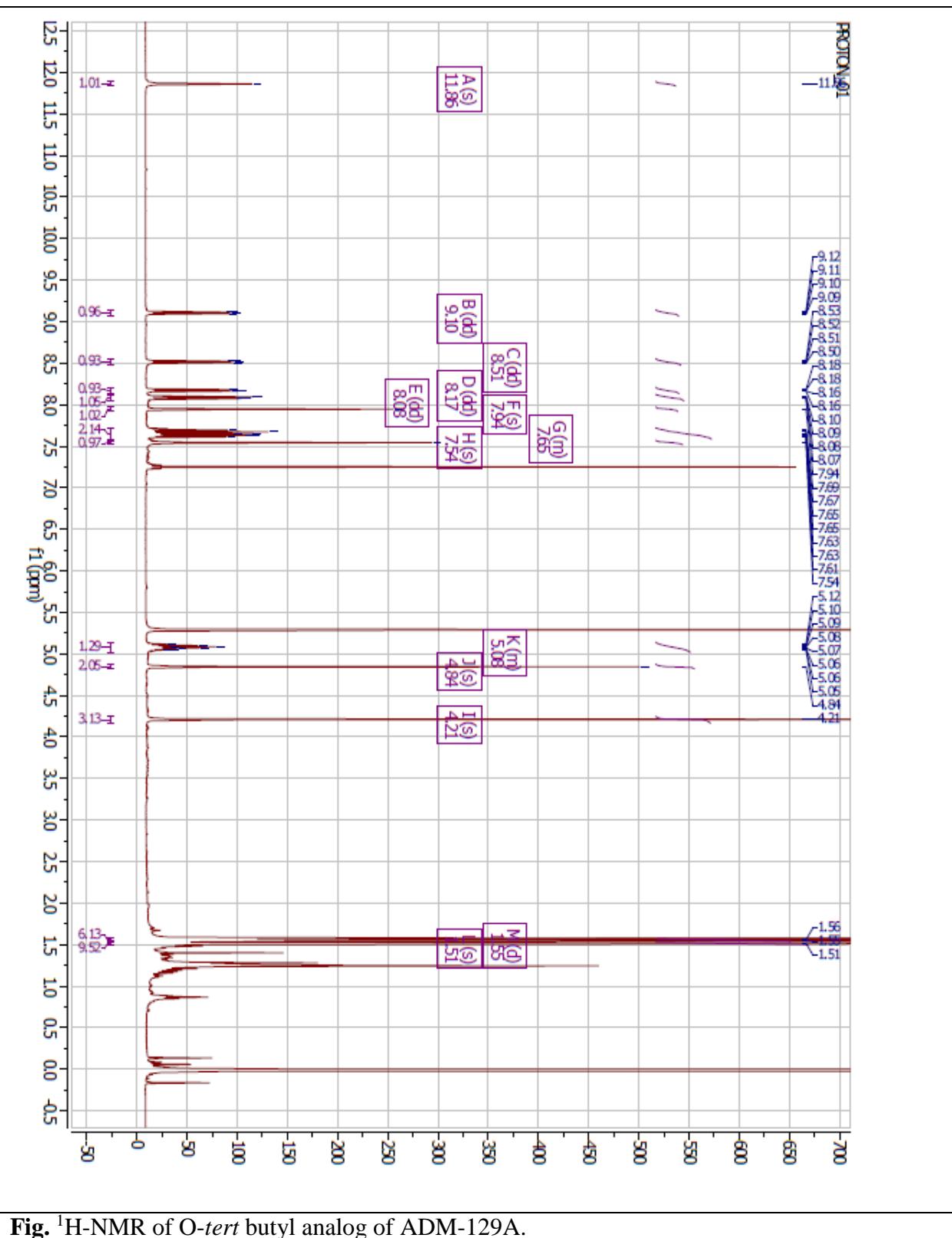
**Fig.** MALDI-TOF of O-*tert* butyl analog of ADM-123.



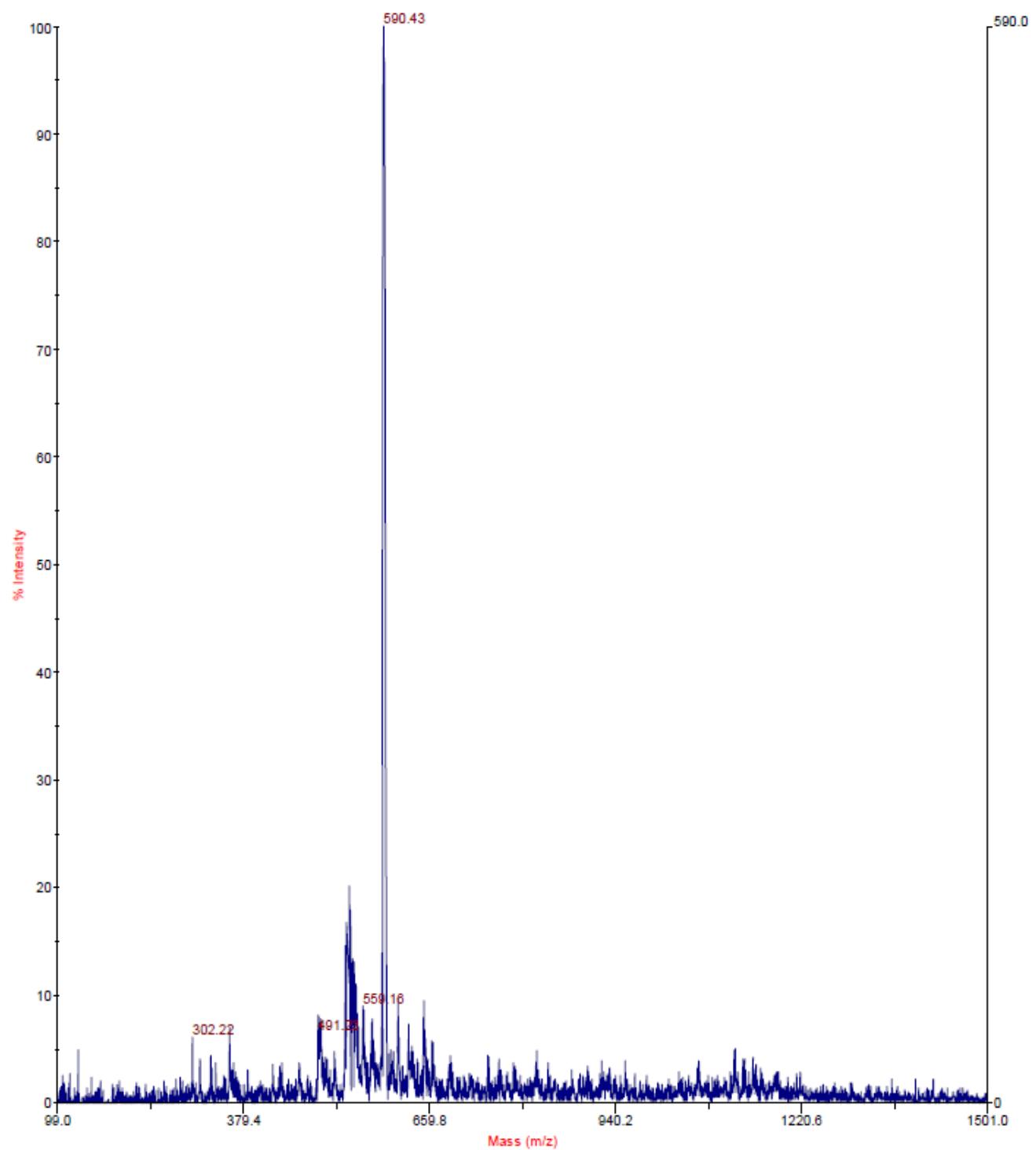
**Fig.**  $^1\text{H}$ -NMR of O-*tert* butyl analog of ADM-124.



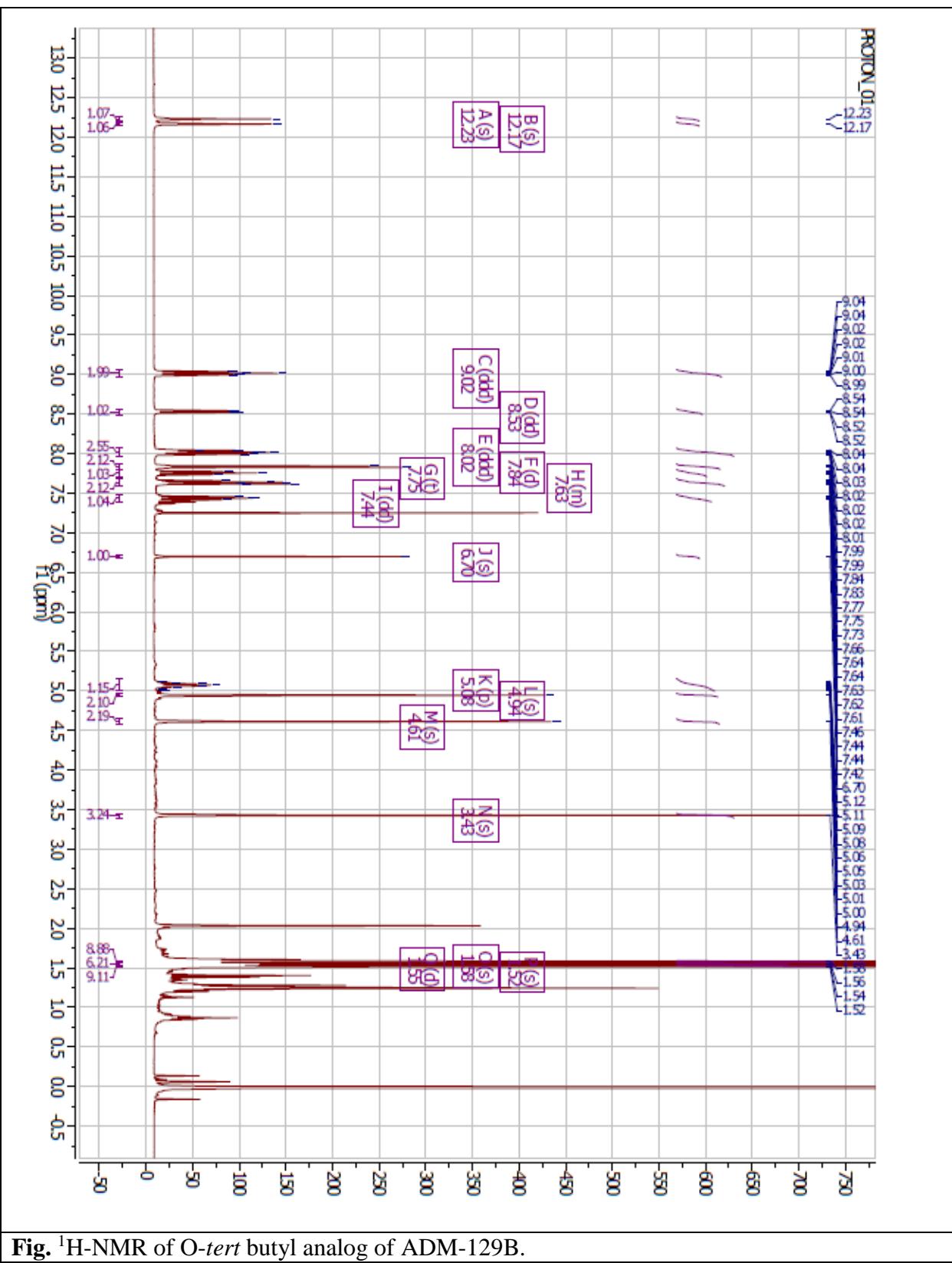
**Fig.** MALDI-TOF of O-*tert* butyl analog of ADM-124.



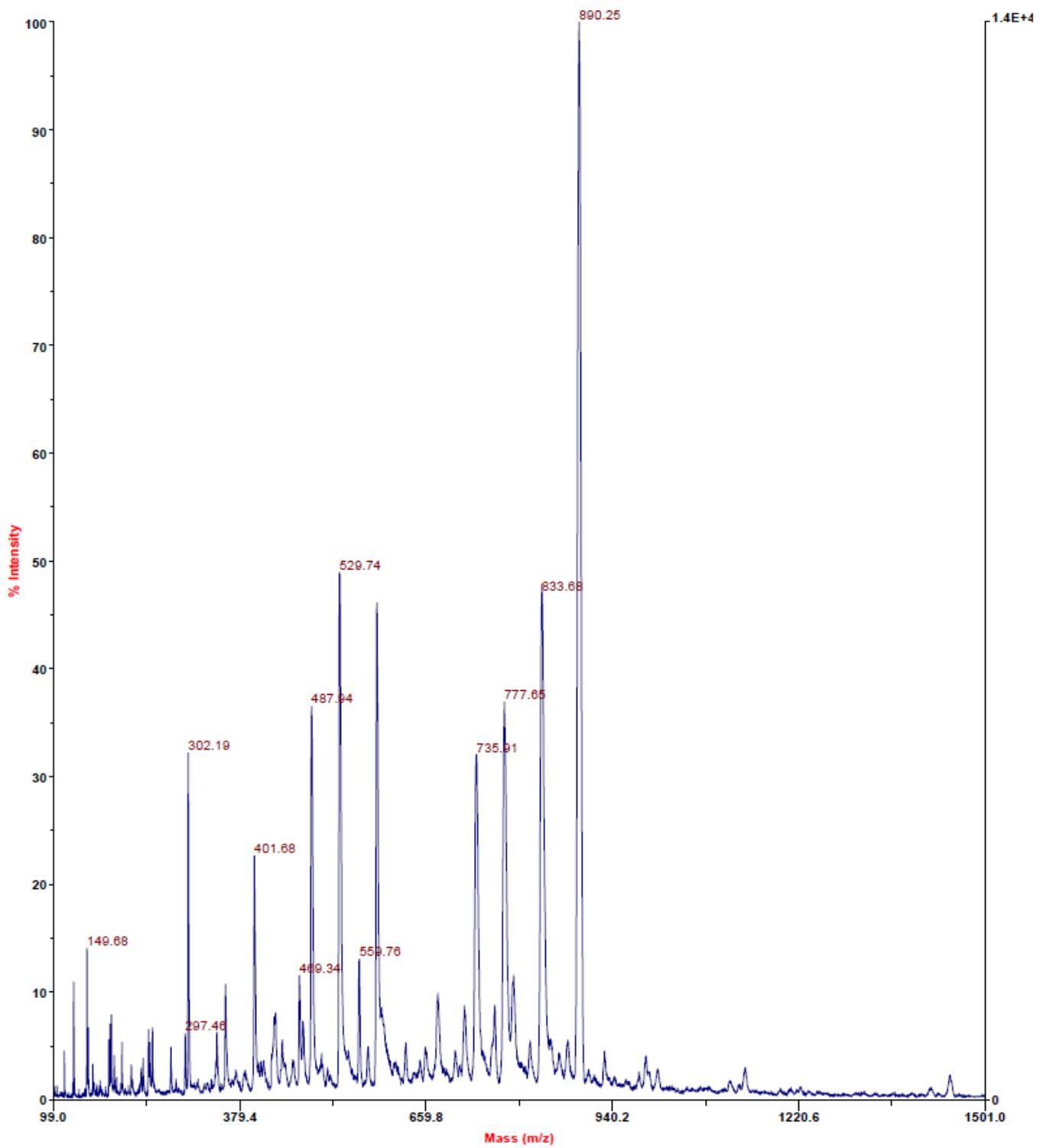
**Fig.** <sup>1</sup>H-NMR of O-*tert* butyl analog of ADM-129A.



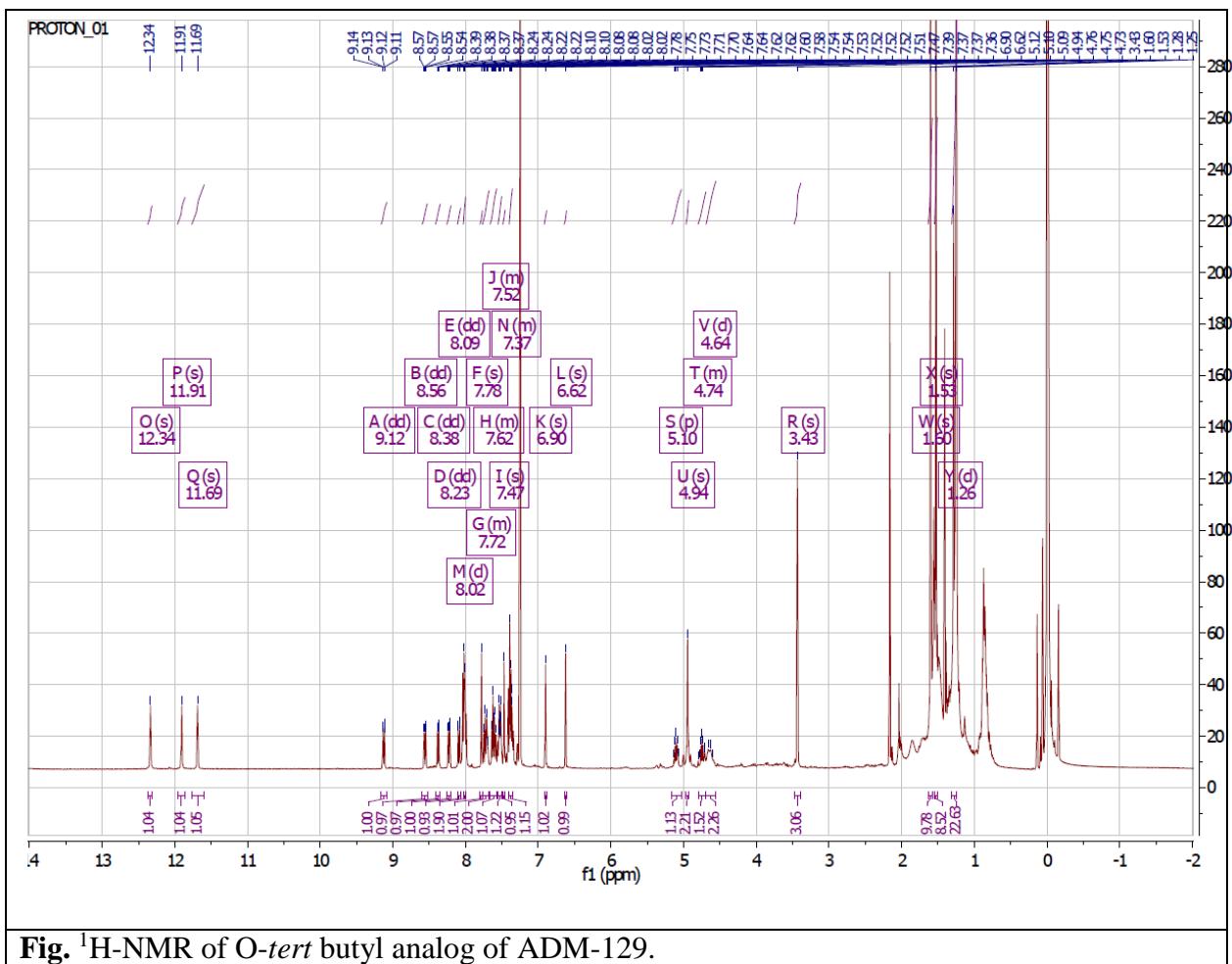
**Fig.** MALDI-TOF of O-*tert* butyl analog of ADM-129A.

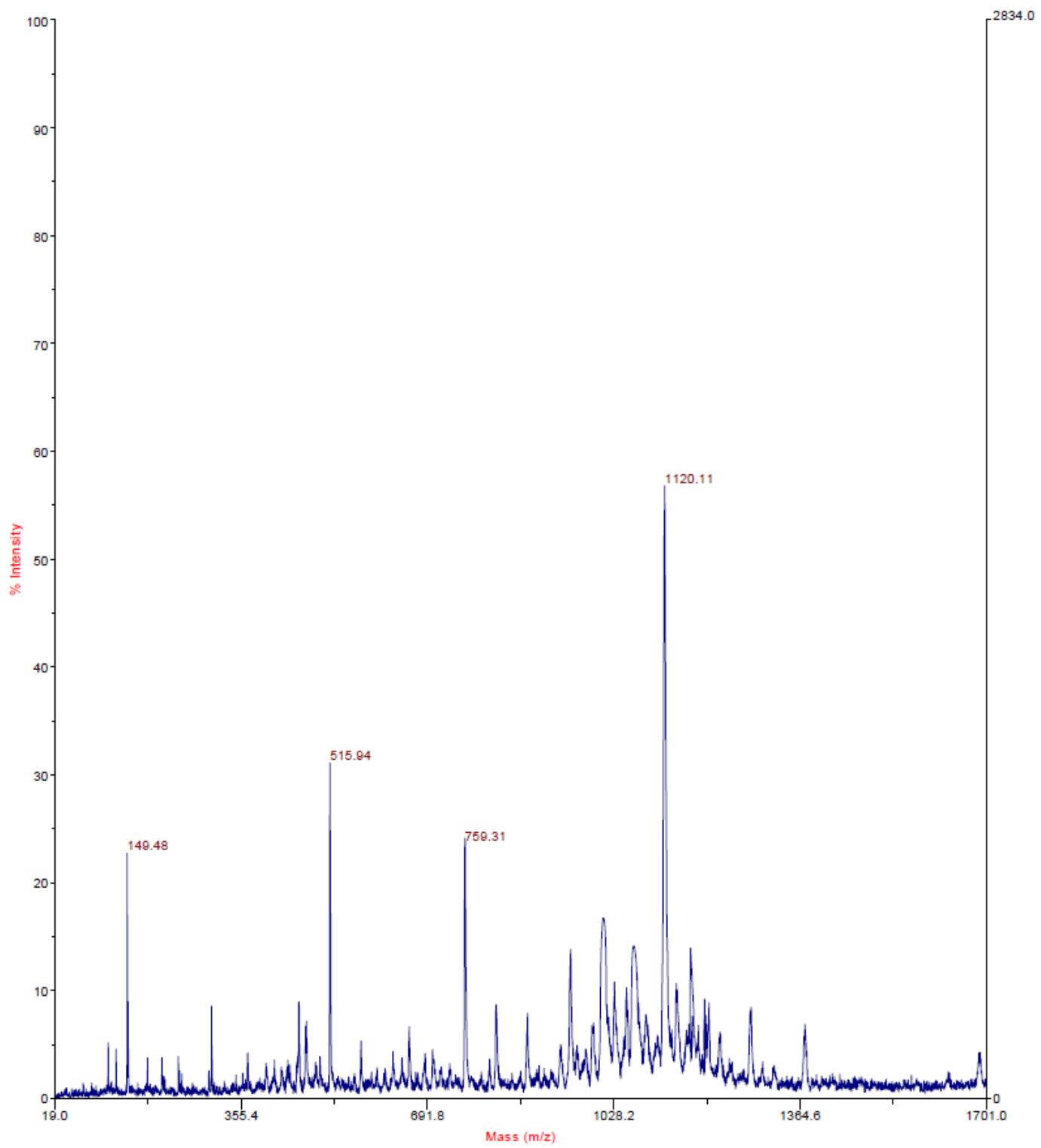


**Fig.**  $^1\text{H}$ -NMR of O-*tert* butyl analog of ADM-129B.

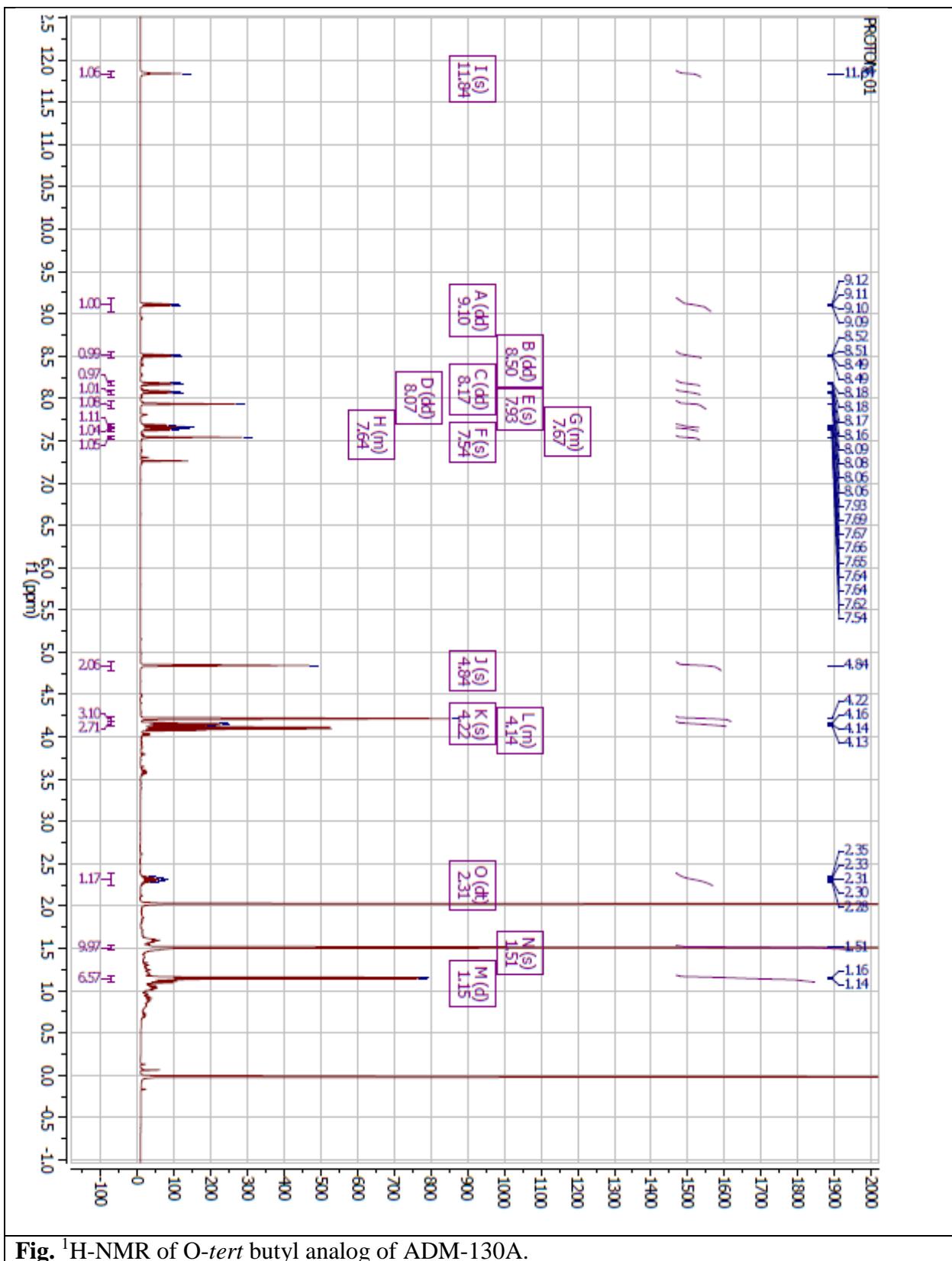


**Fig.** MALDI-TOF of O-*tert* butyl analog of ADM-129B.

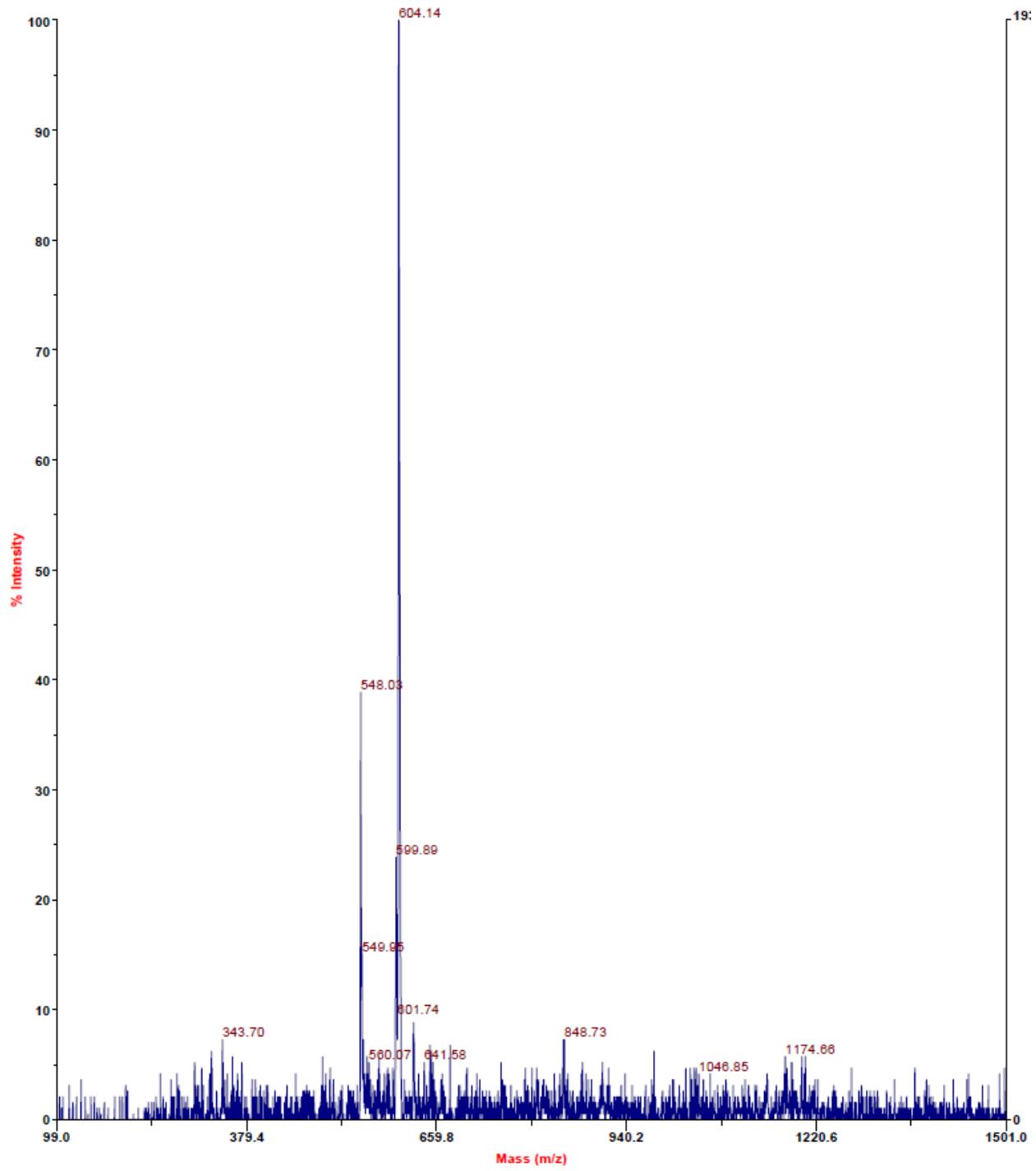




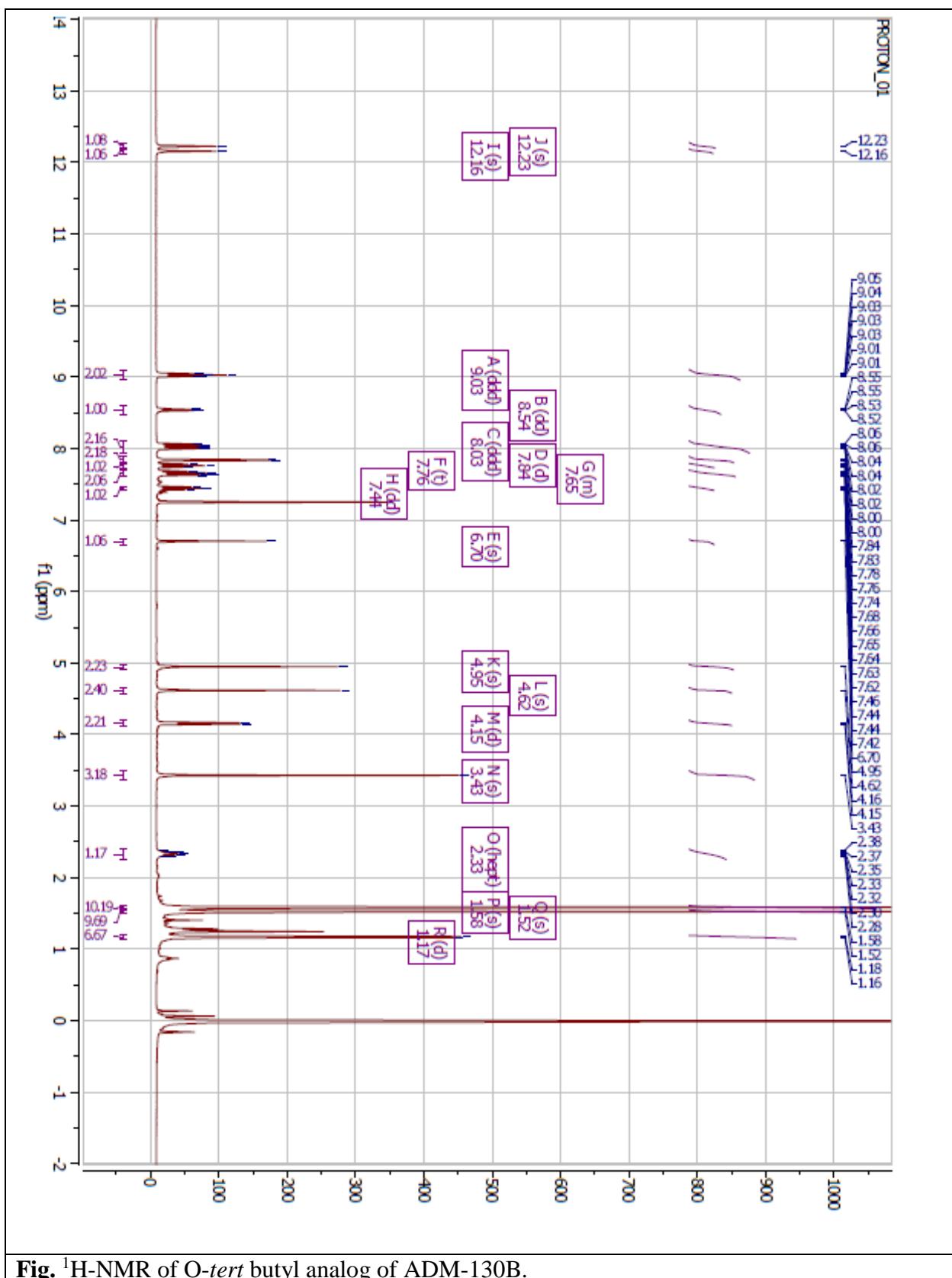
**Fig.** MALDI-TOF of O-*tert* butyl analog of ADM-129.



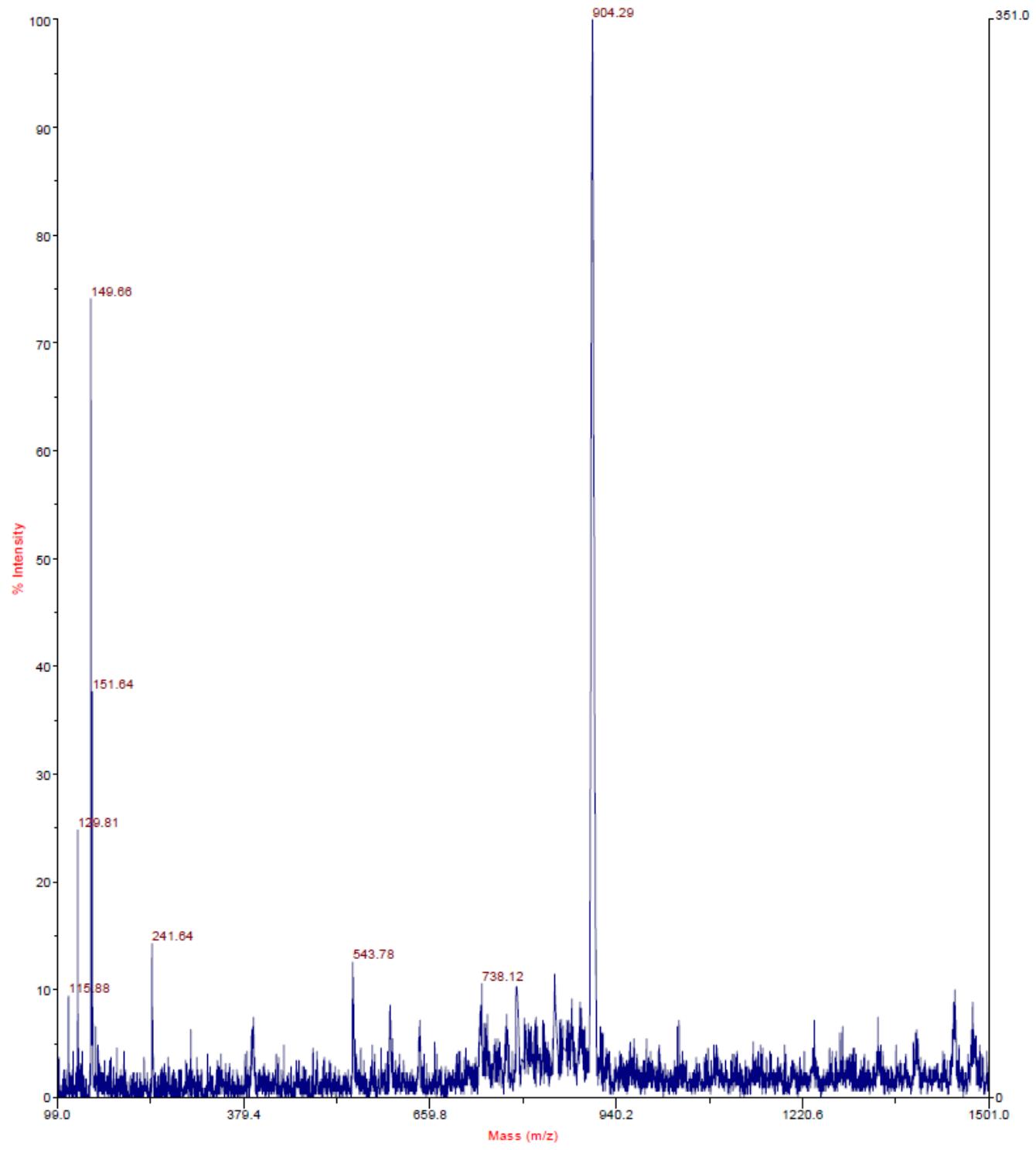
**Fig.**  $^1\text{H}$ -NMR of O-*tert* butyl analog of ADM-130A.



**Fig.** MALDI-TOF of O-*tert* butyl analog of ADM-130A.



**Fig.**  $^1\text{H}$ -NMR of O-*tert* butyl analog of ADM-130B.



**Fig.** MALDI-TOF of O-*tert* butyl analog of ADM-130B.

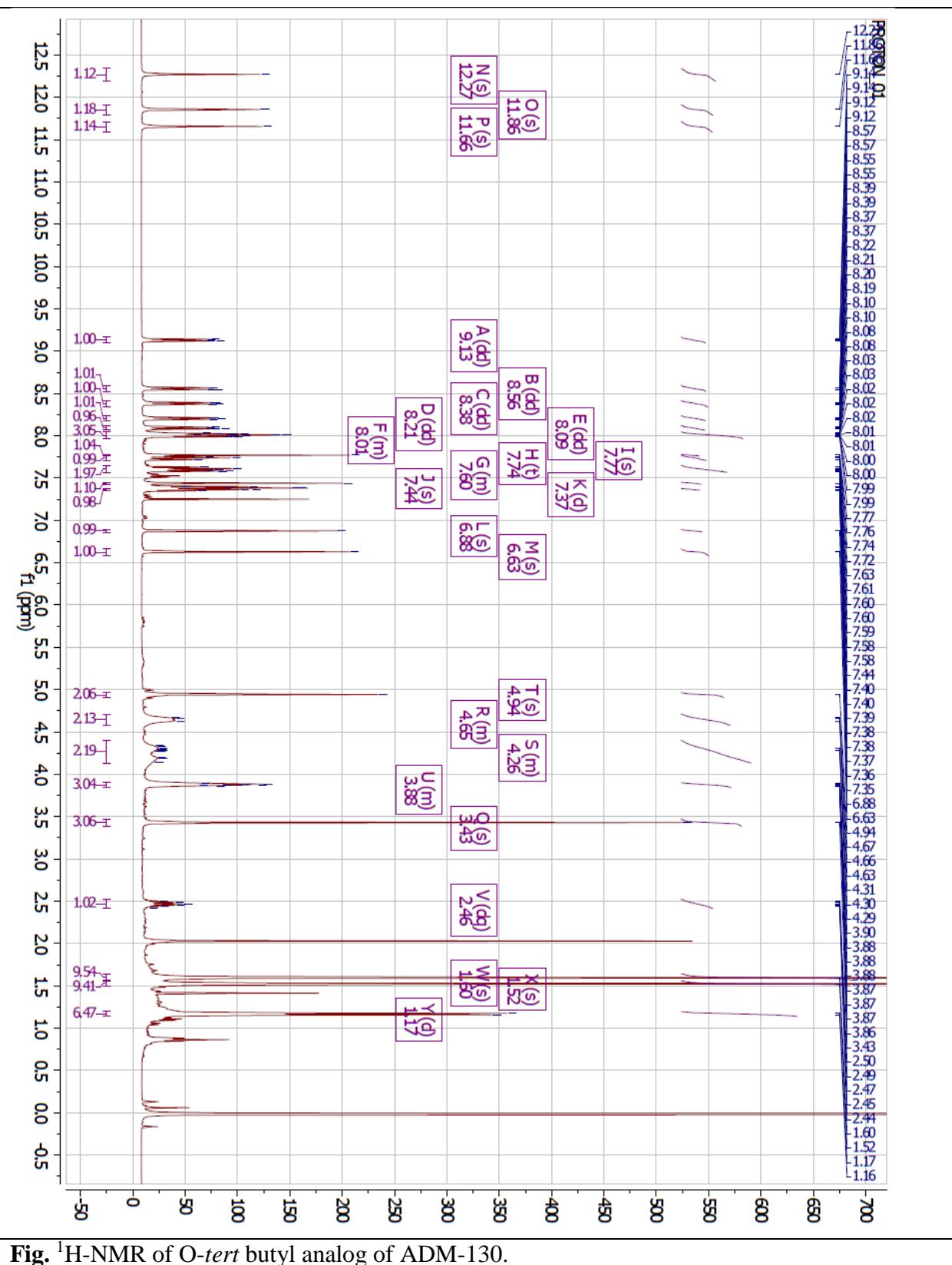
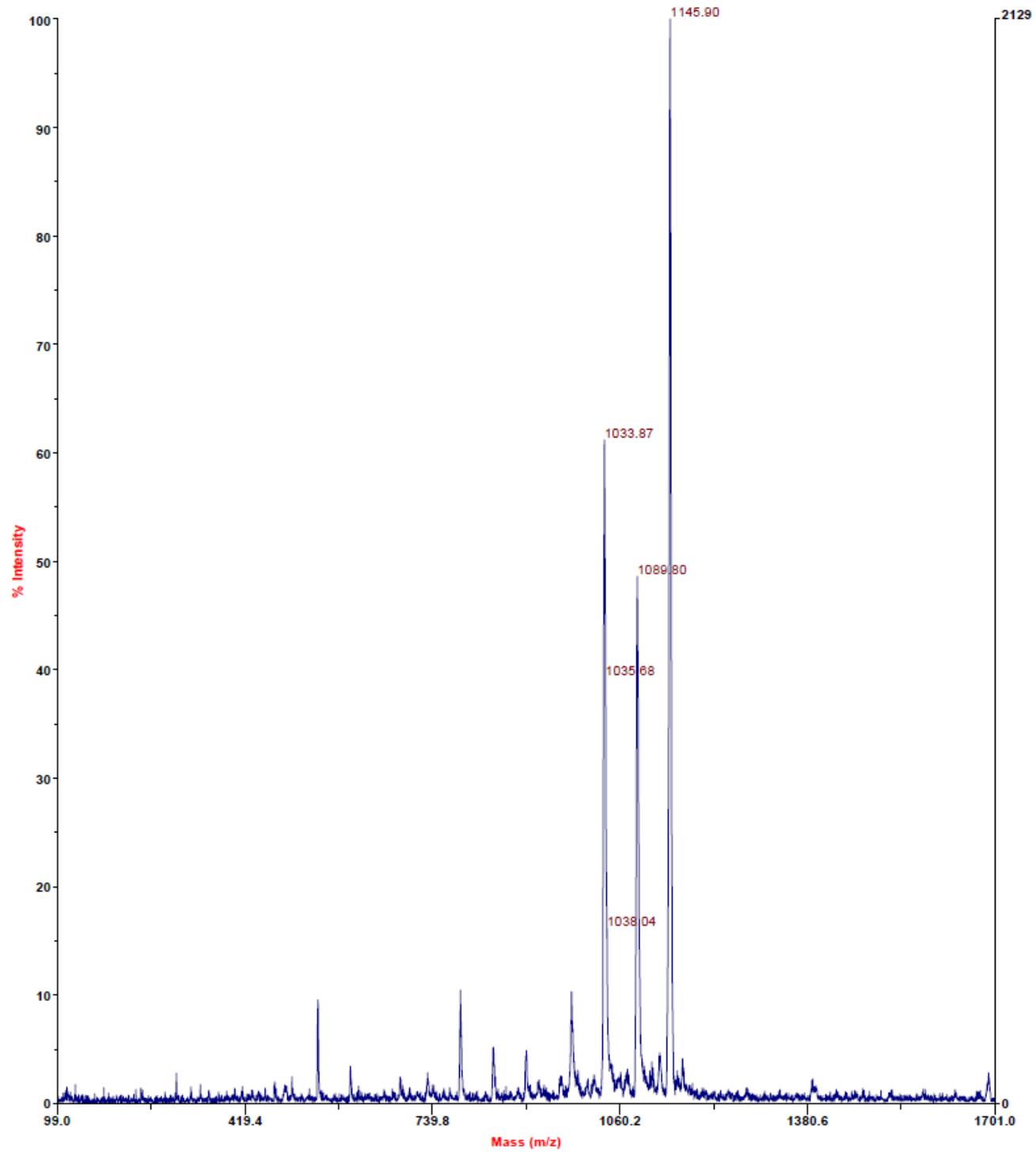
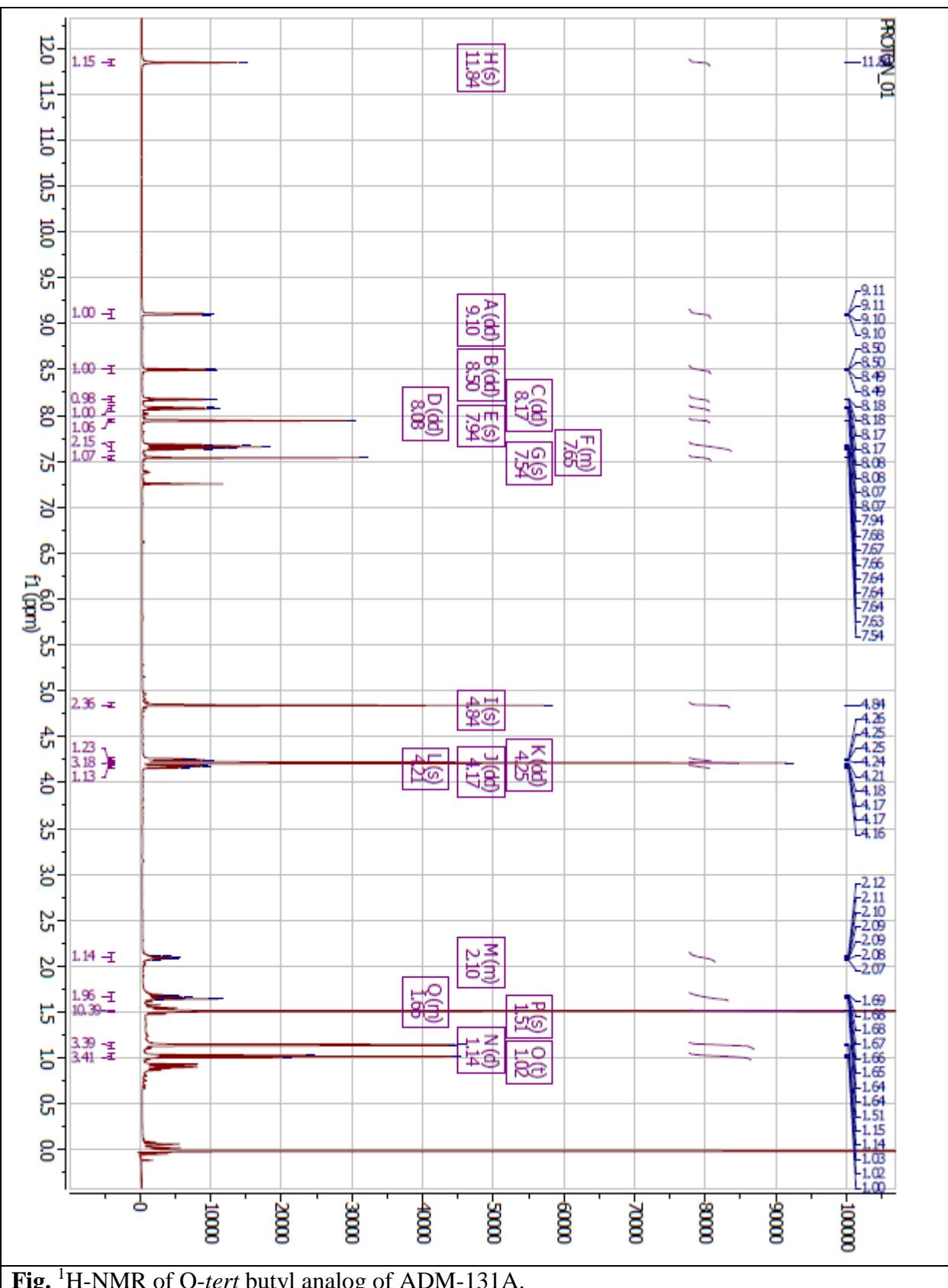


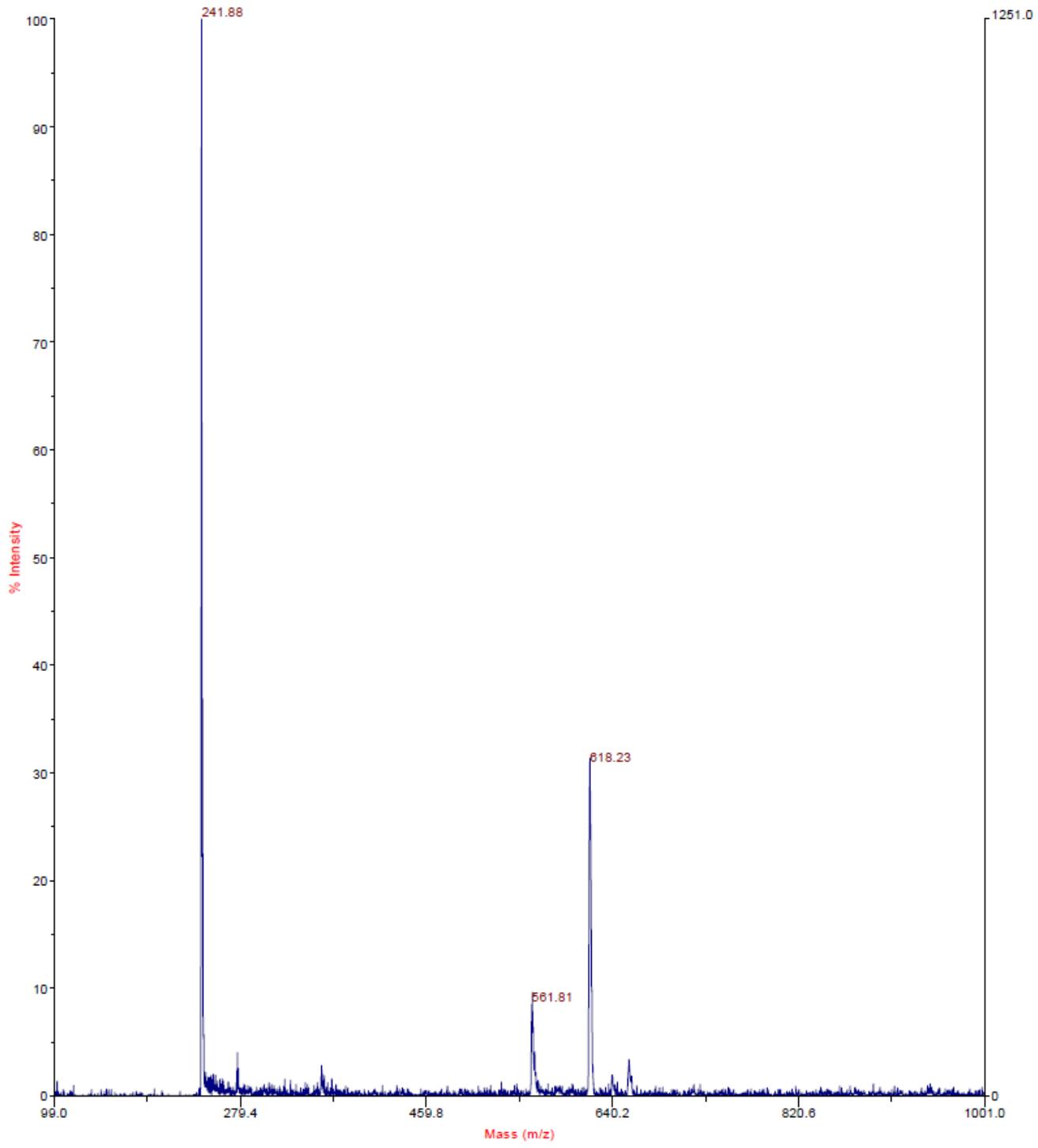
Fig.  $^1\text{H}$ -NMR of *O*-*tert* butyl analog of ADM-130.



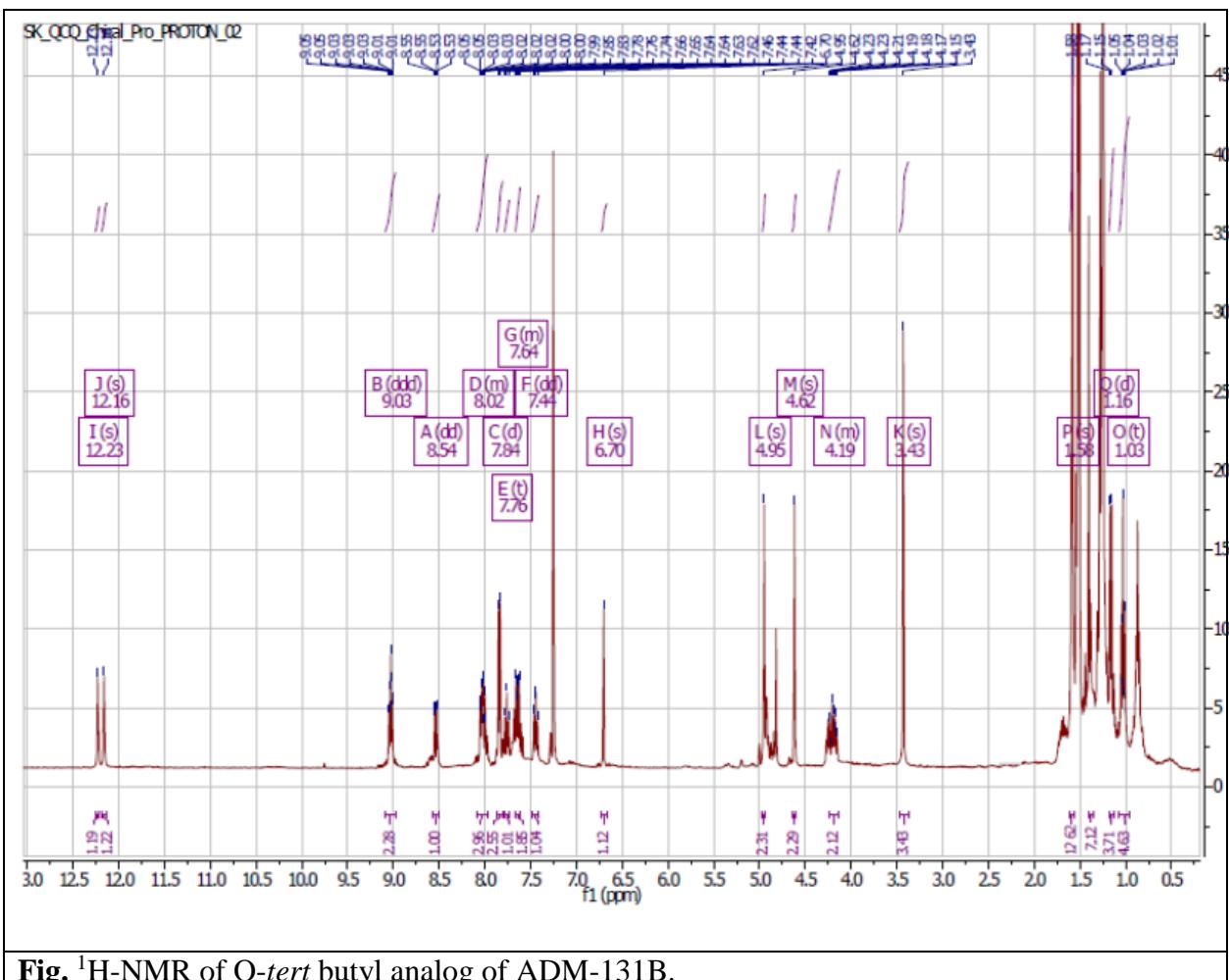
**Fig.** MALDI-TOF of O-*tert* butyl analog of ADM-130.



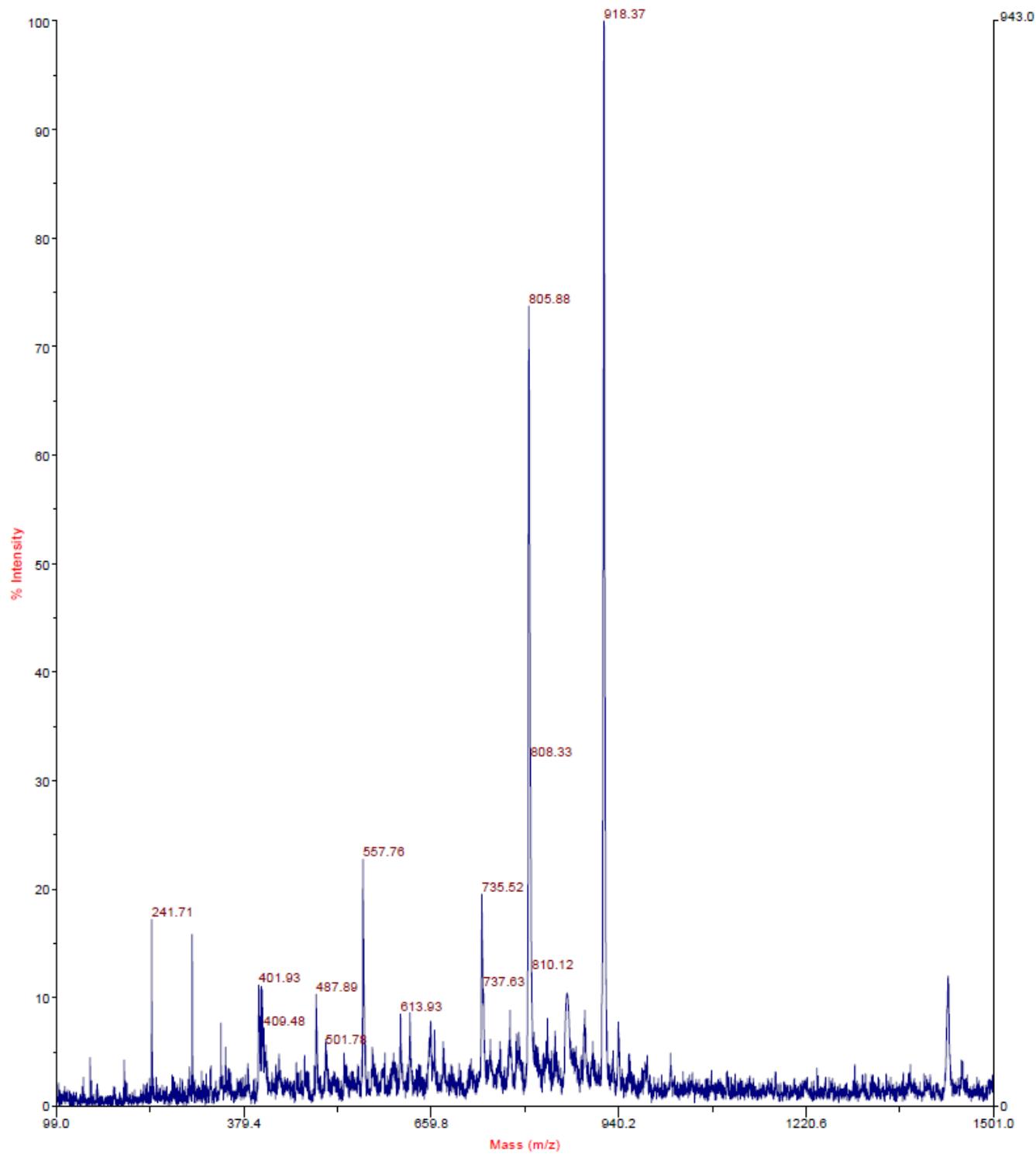
**Fig.**  $^1\text{H}$ -NMR of O-tert butyl analog of ADM-131A.



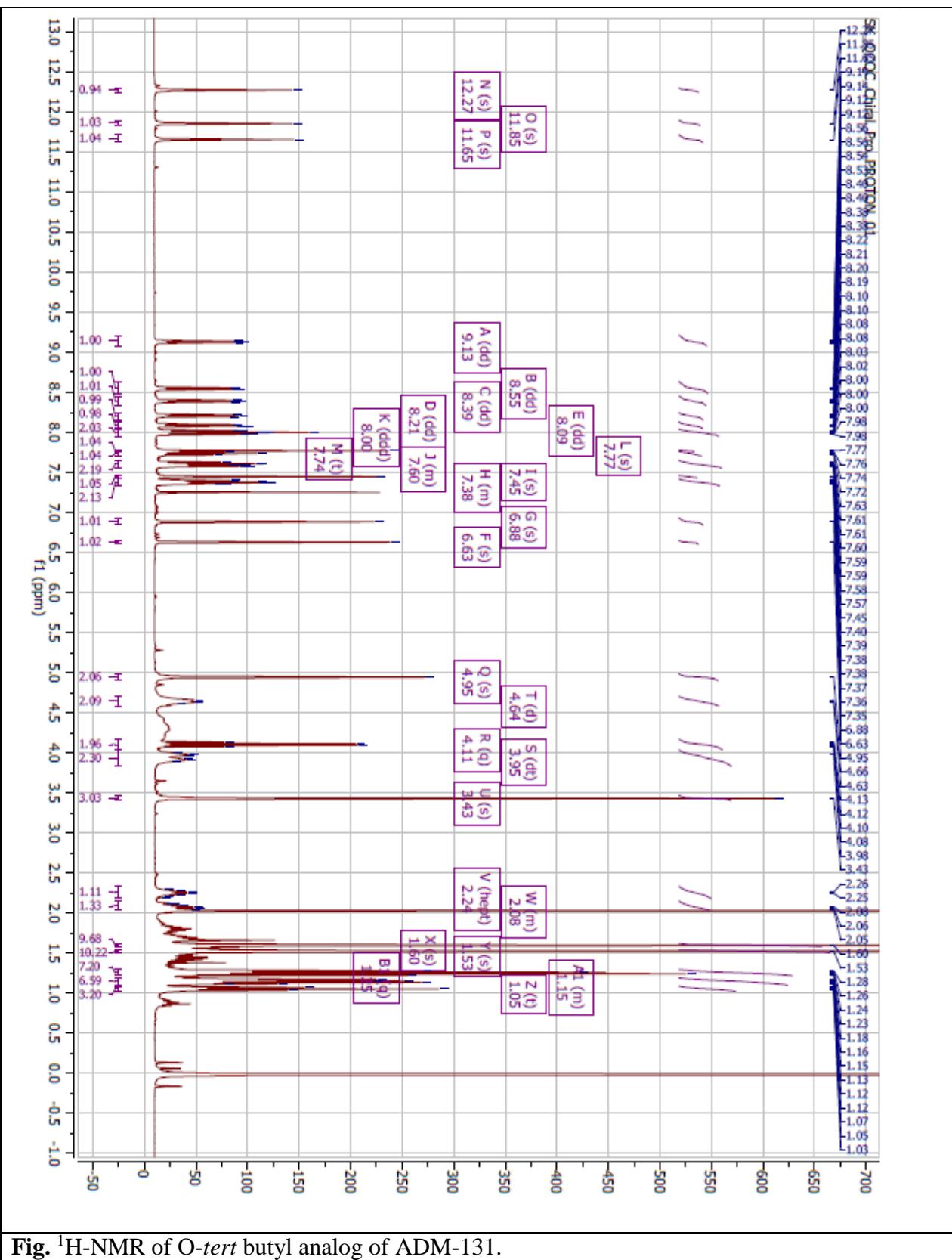
**Fig.** MALDI-TOF of O-*tert* butyl analog of ADM-131A.



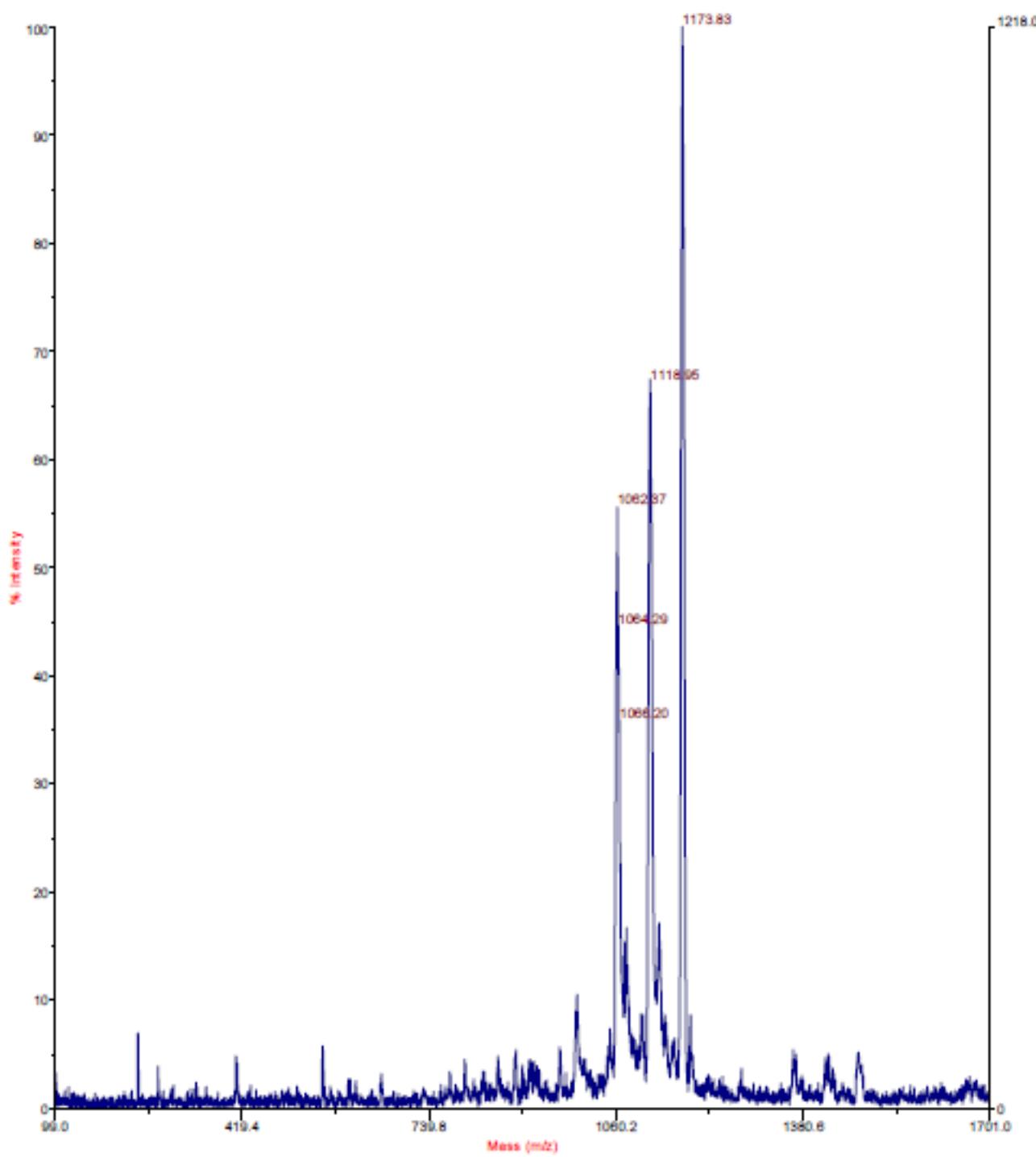
**Fig.**  $^1\text{H}$ -NMR of O-*tert* butyl analog of ADM-131B.



**Fig.** MALDI-TOF of O-*tert* butyl analog of ADM-131B.



**Fig.** <sup>1</sup>H-NMR of O-tert butyl analog of ADM-131.



**Fig.** MALDI-TOF of O-*tert* butyl analog of ADM-131.

# ADM-102

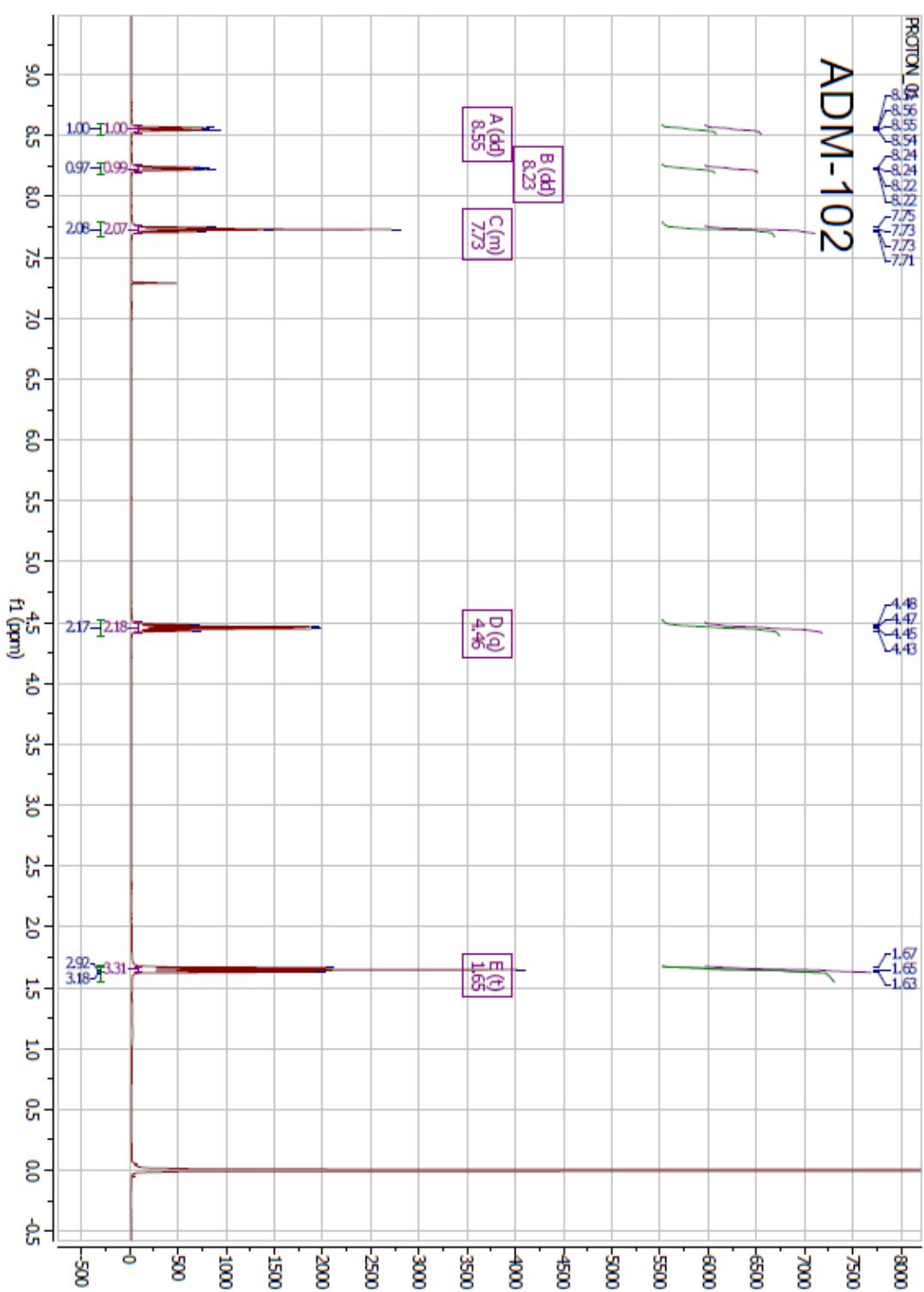
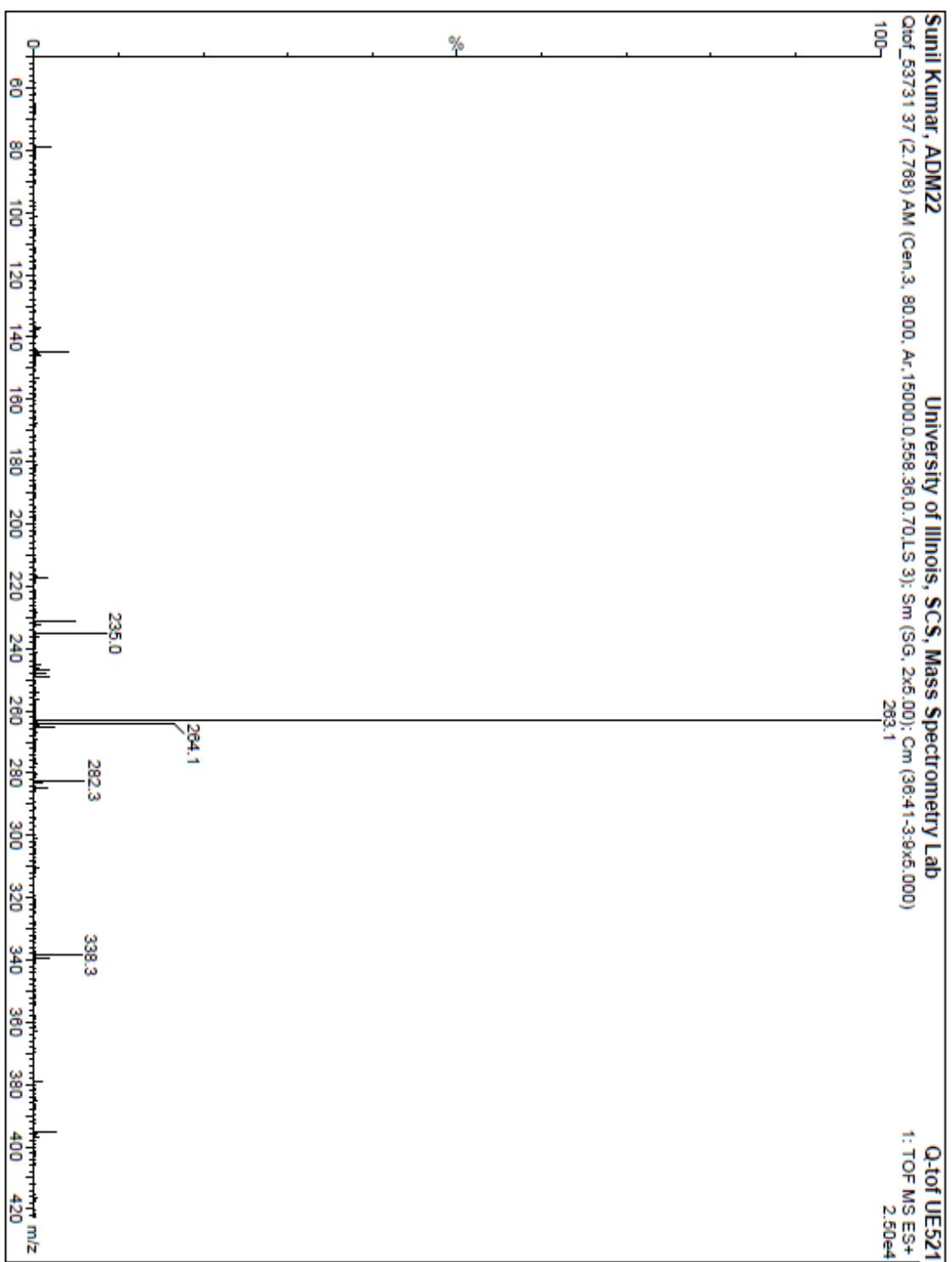
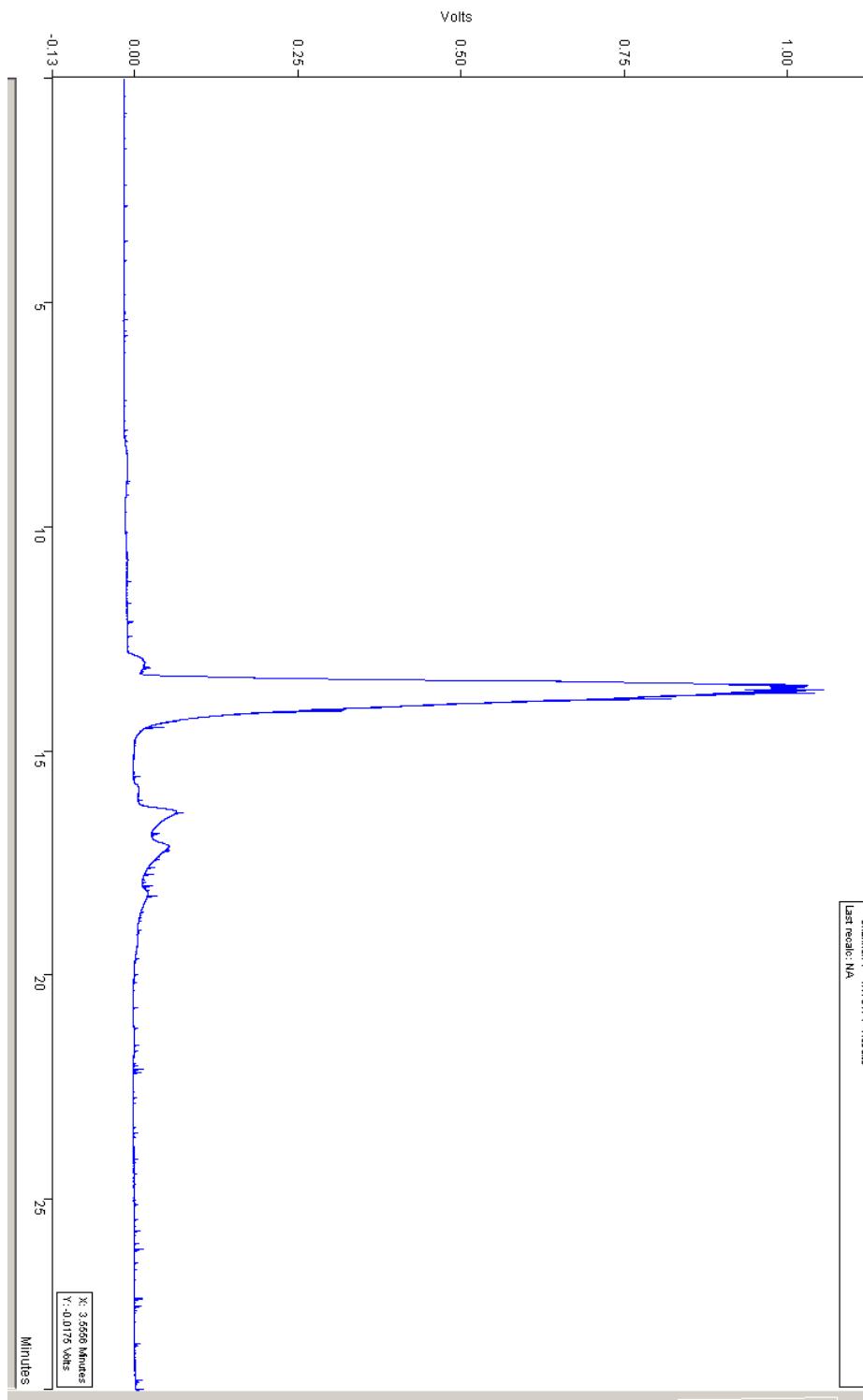


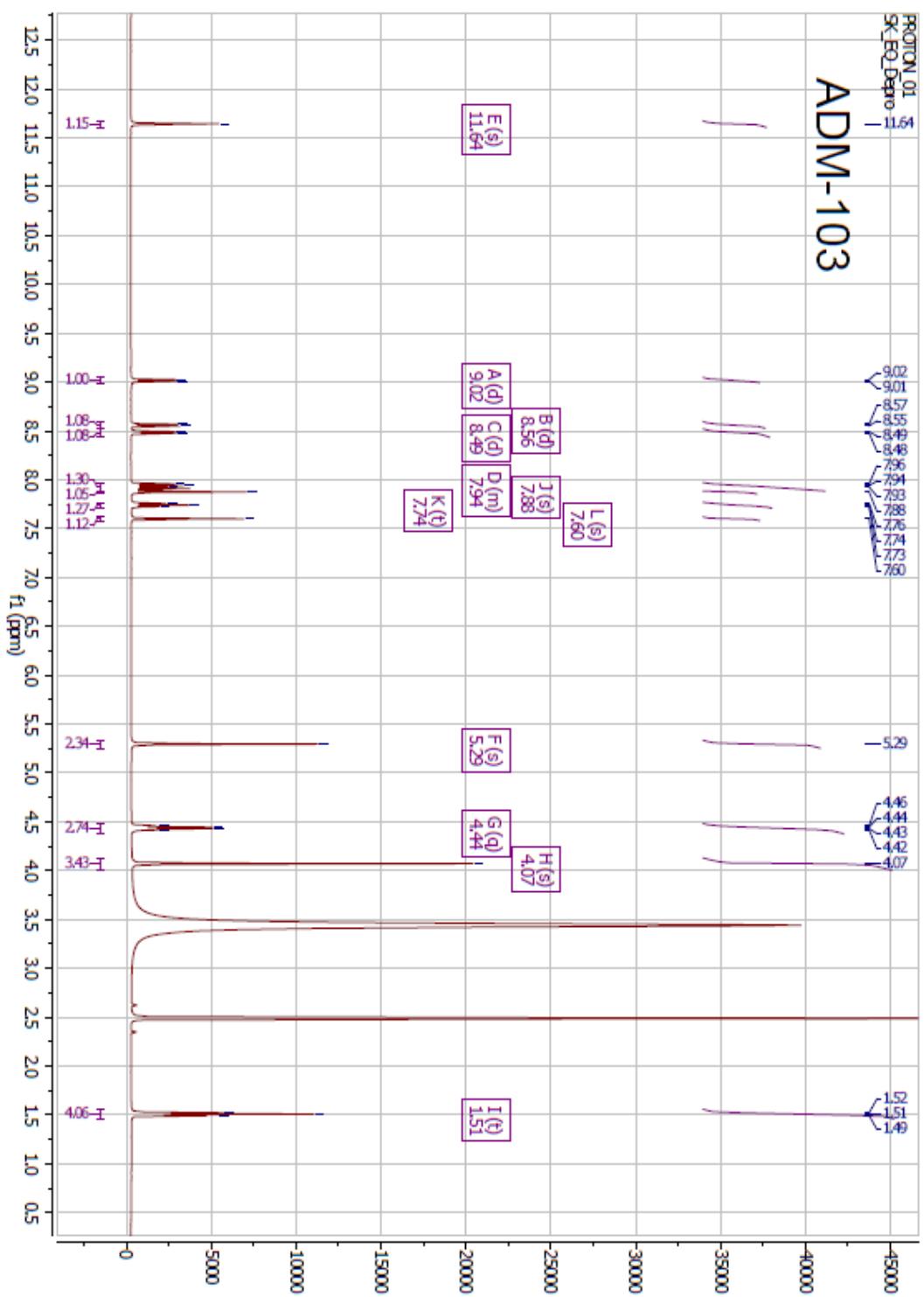
Fig.  $^1\text{H}$ -NMR of ADM-102.



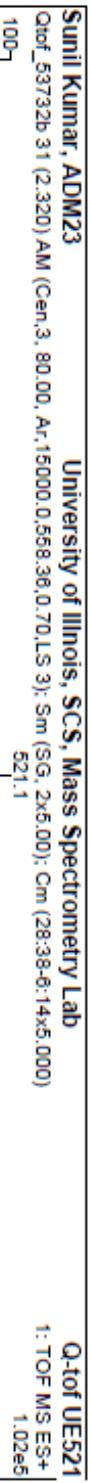
**Fig.** ESI-MS of ADM-102.



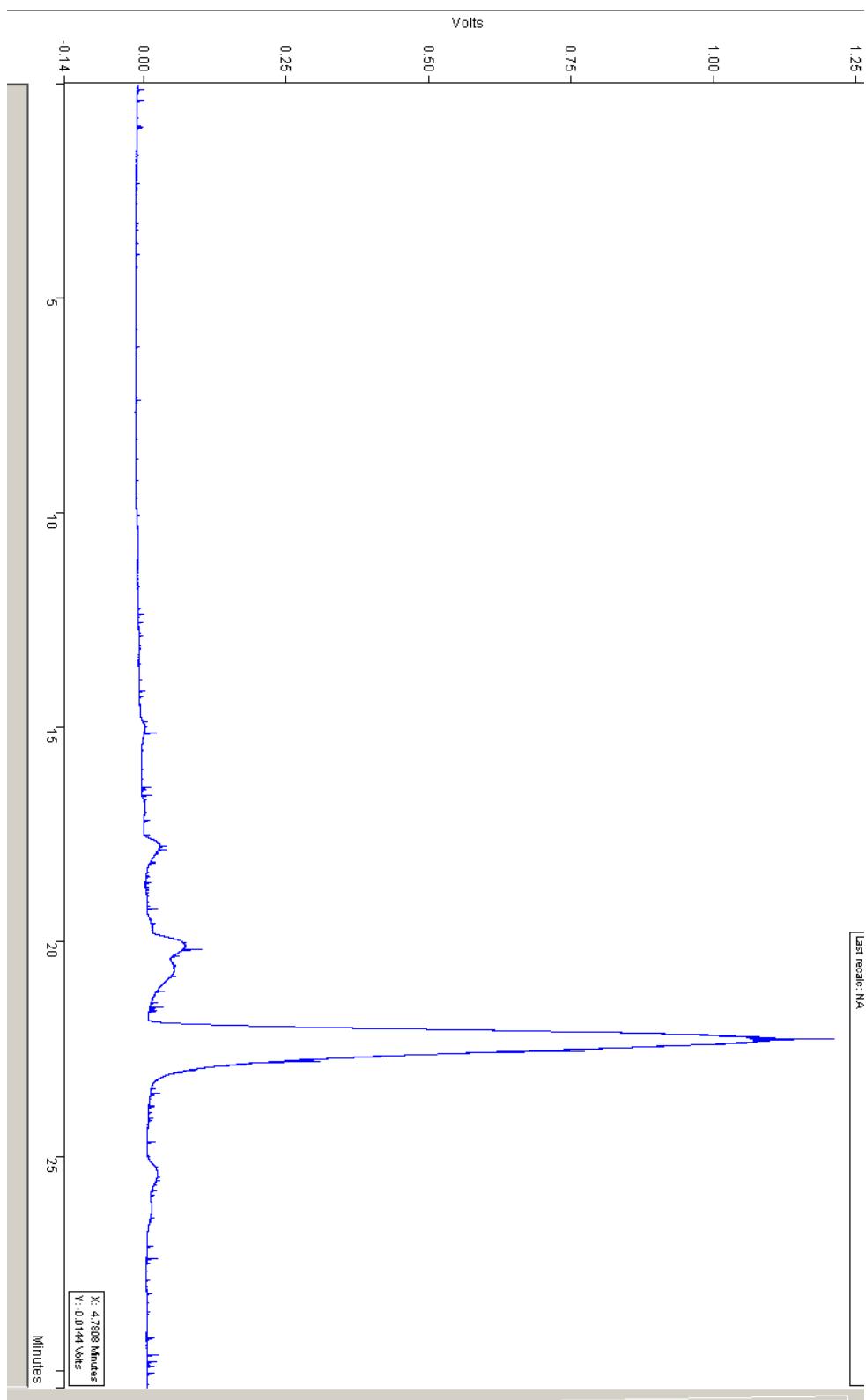
**Fig.** RP-HPLC of ADM-102.



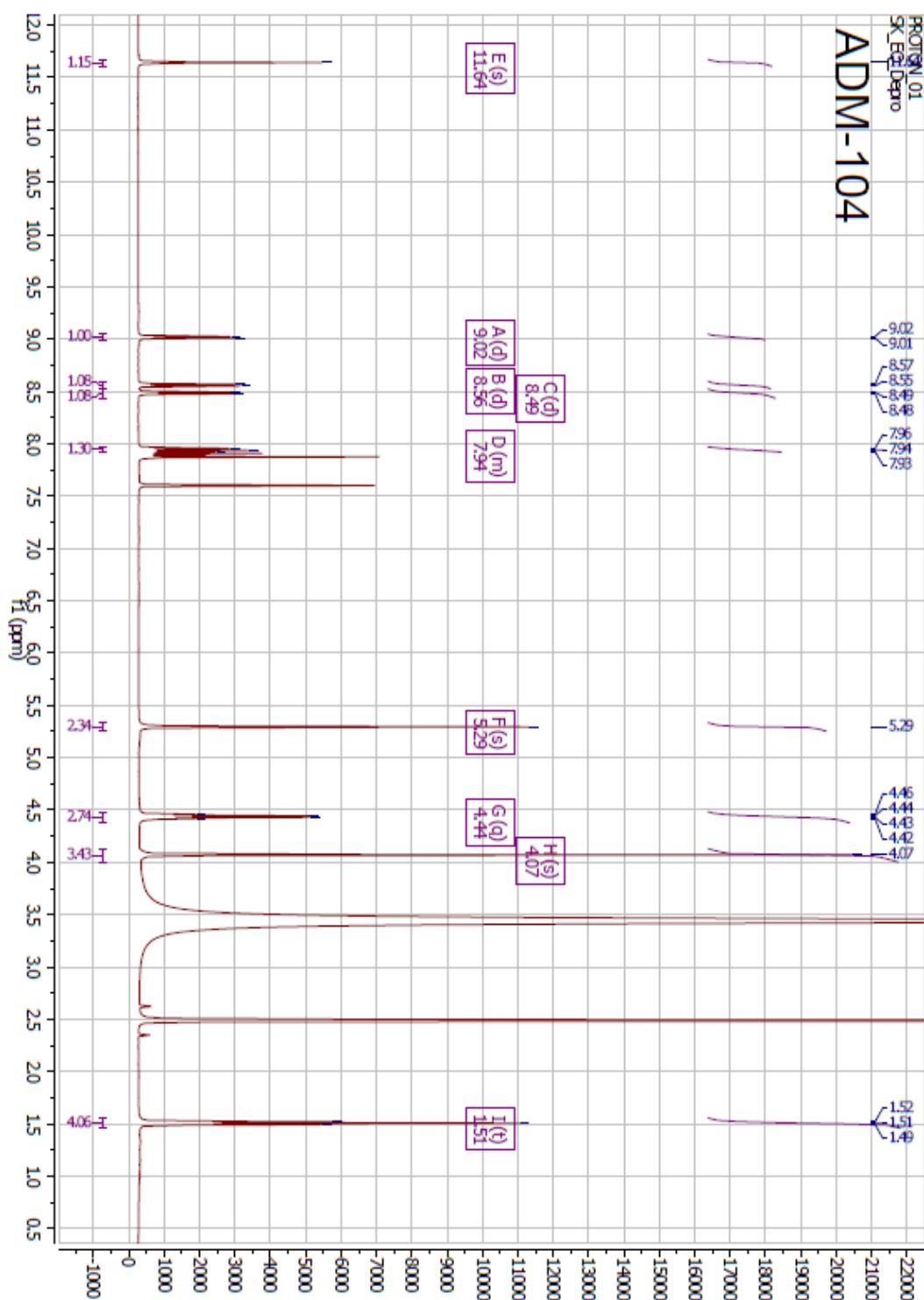
**Fig.**  $^1\text{H}$ -NMR of ADM-103.



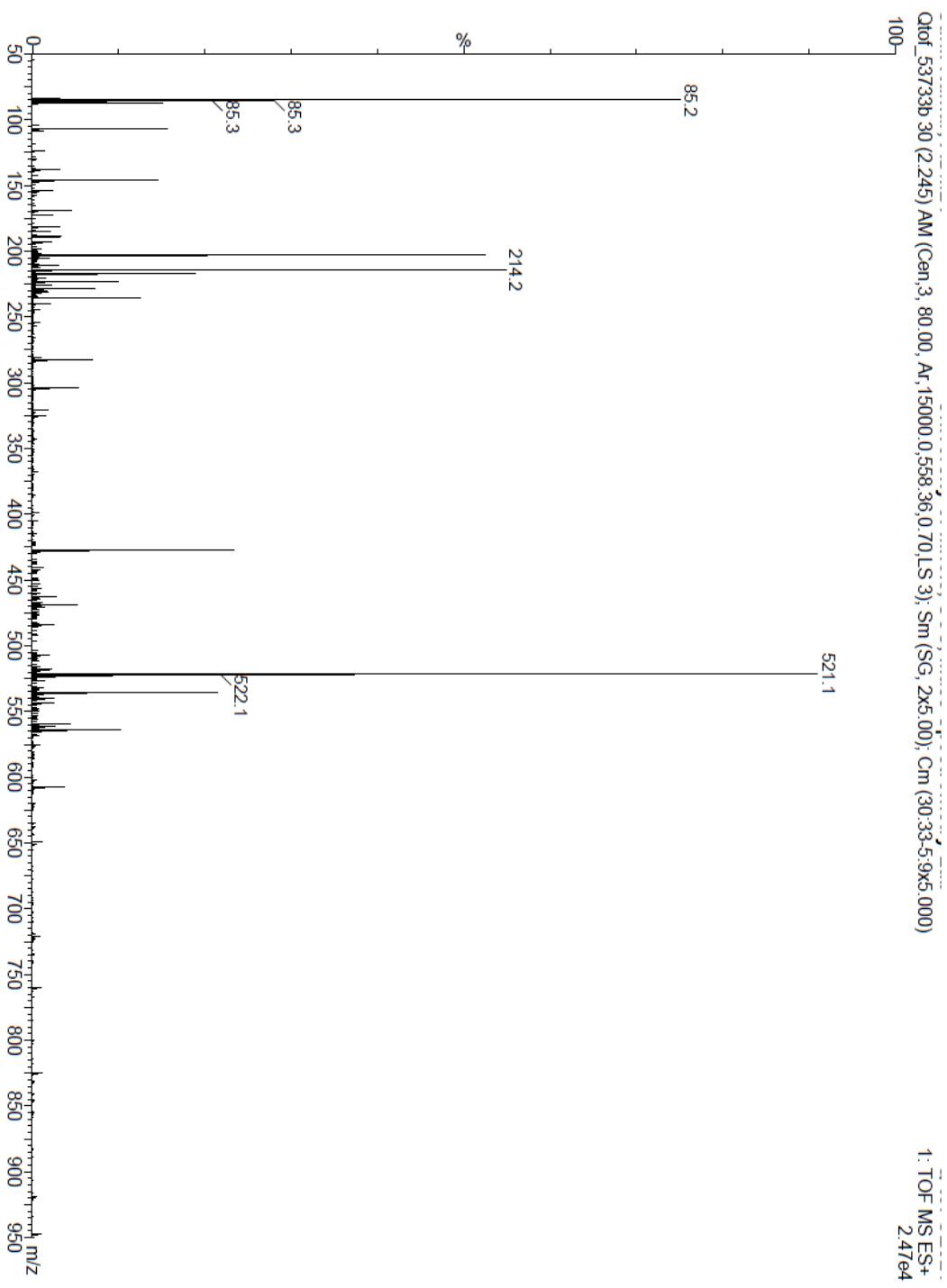
**Fig.** ESI-MS of ADM-103.



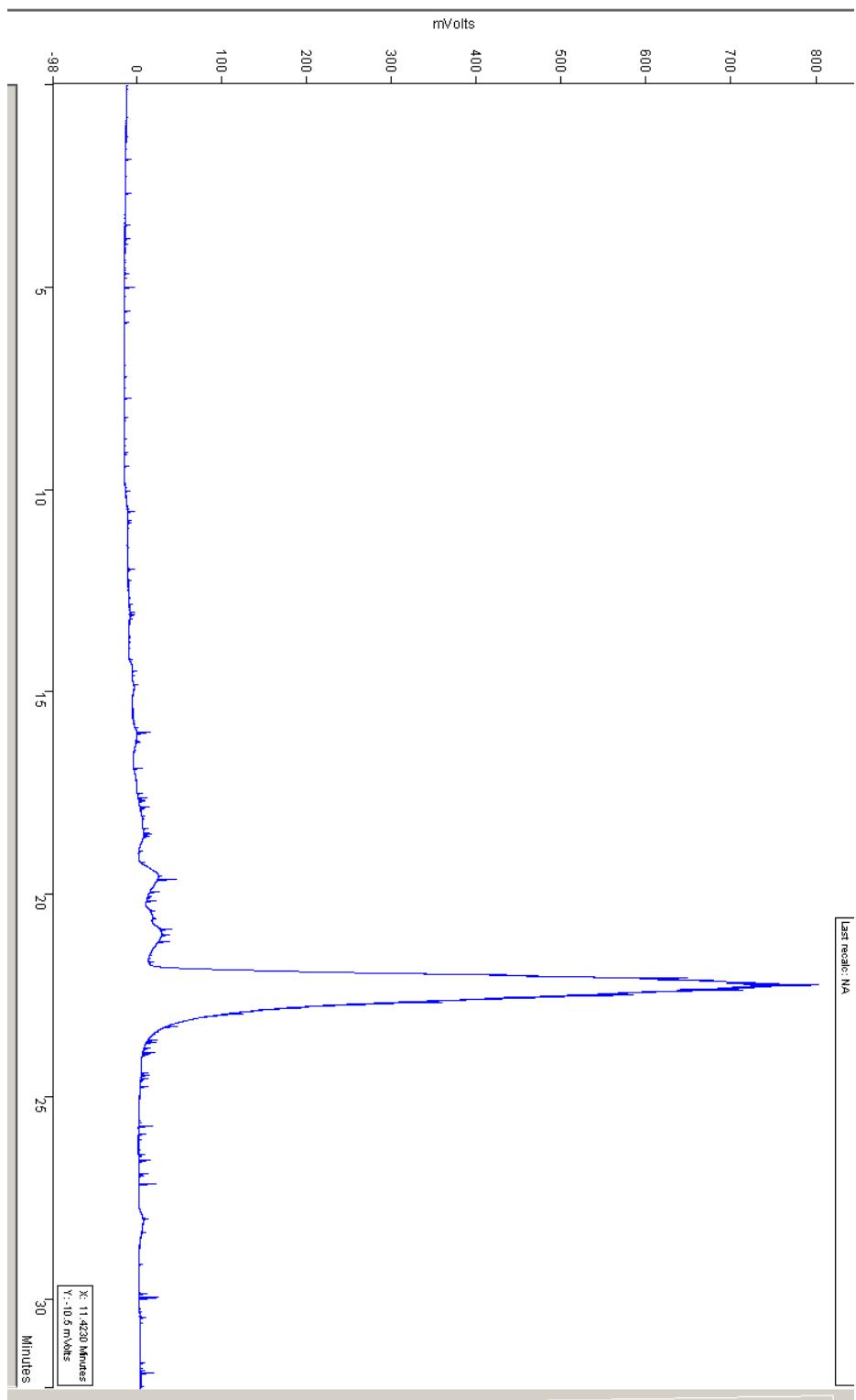
**Fig.** RP-HPLC of ADM-103.



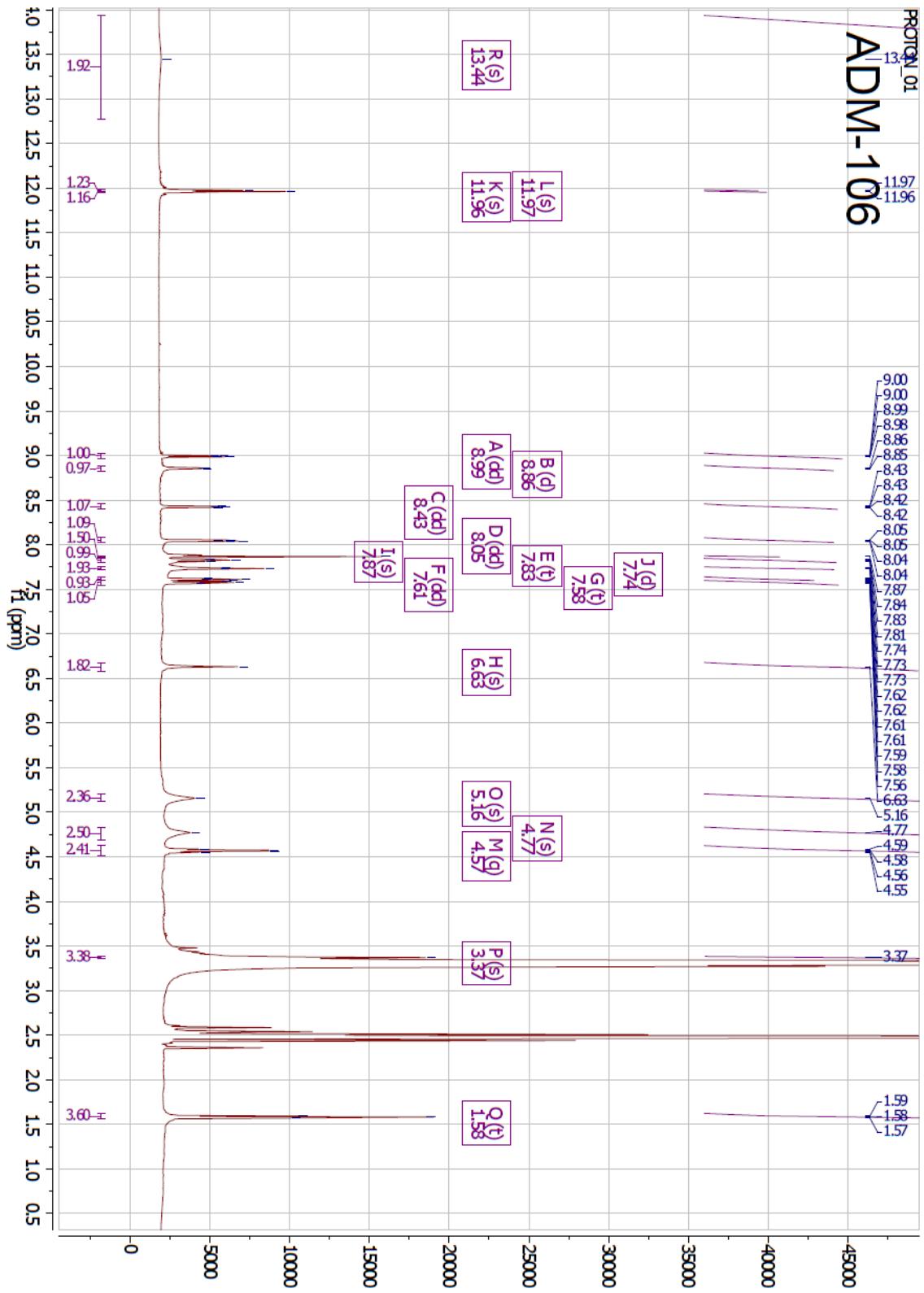
**Fig.**  $^1\text{H}$ -NMR of ADM-104.



**Fig.** ESI-MS of ADM-104.



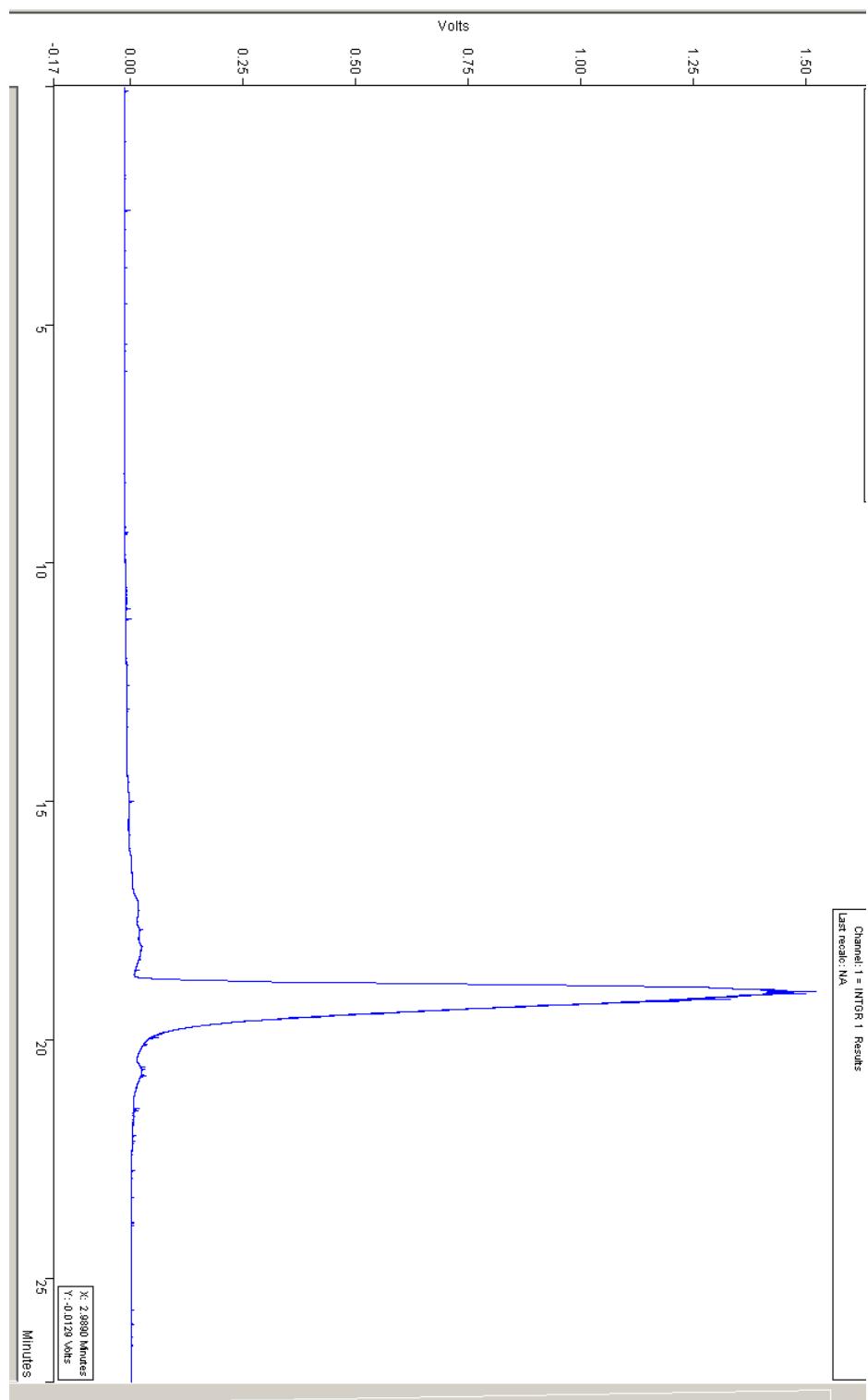
**Fig.** RP-HPLC of ADM-104.



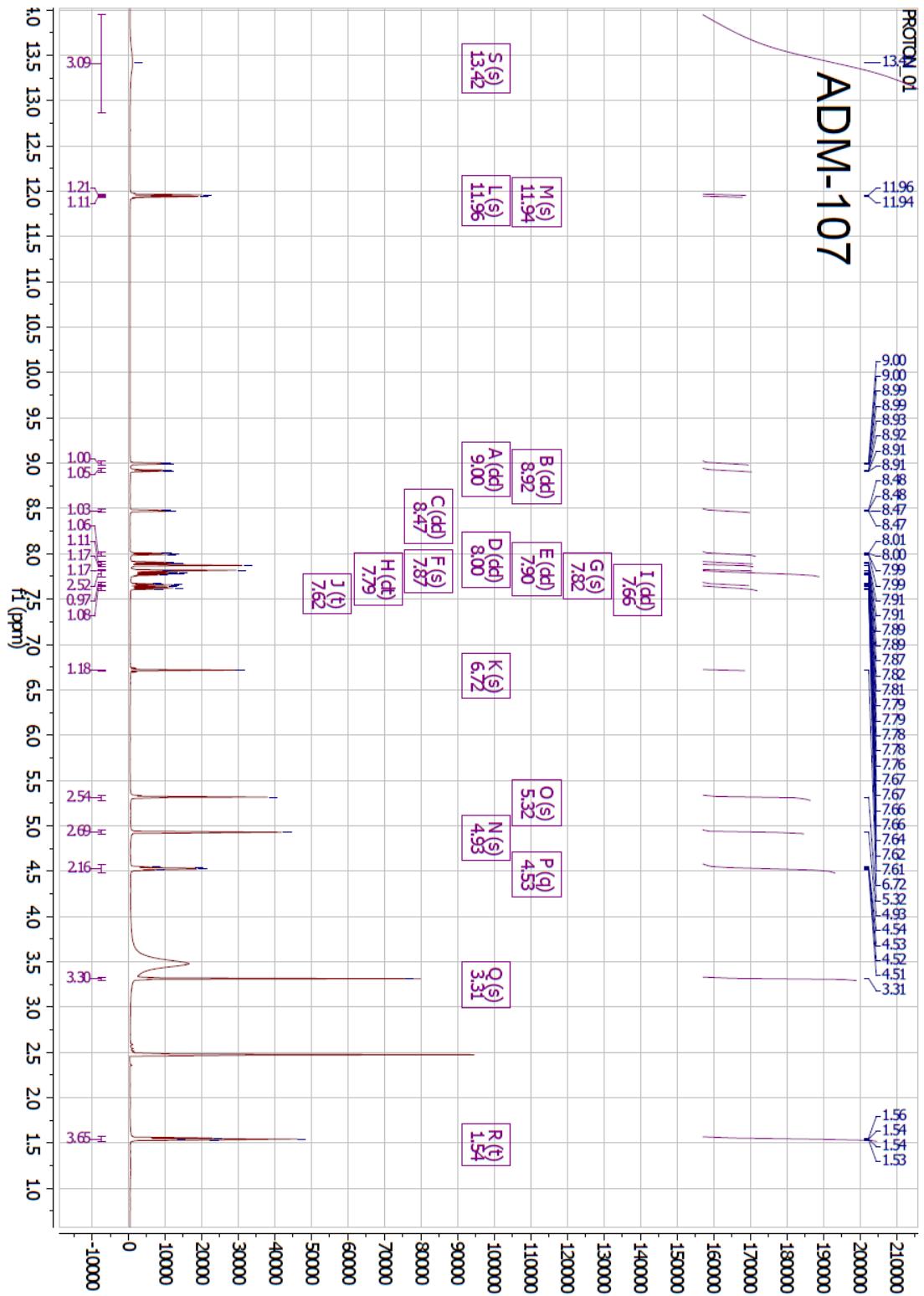
**Fig.**  $^1\text{H}$ -NMR of ADM-106.



**Fig.** ESI-MS of ADM-106.



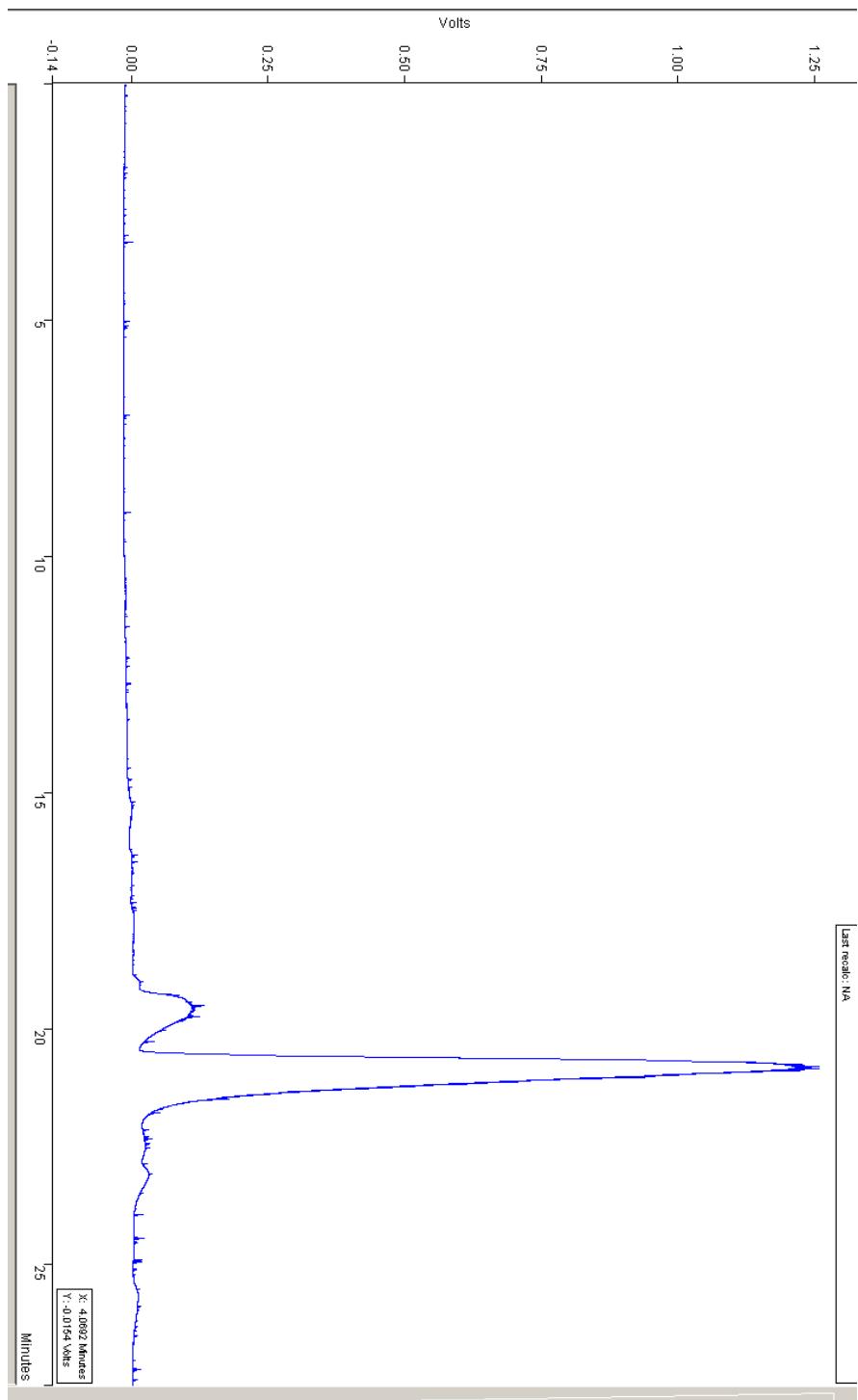
**Fig.** RP-HPLC of ADM-106.



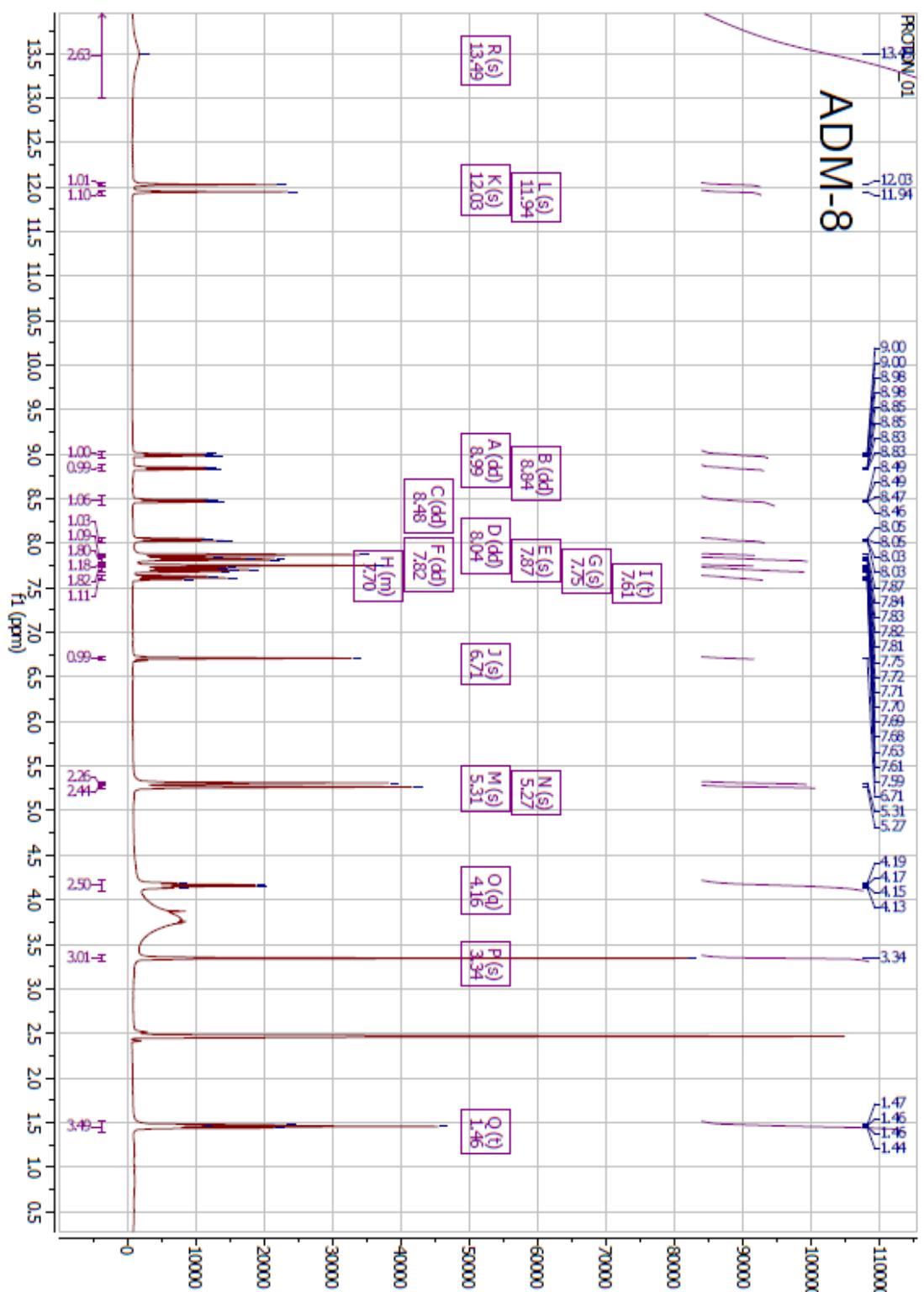
**Fig.**  $^1\text{H}$ -NMR of ADM-107.



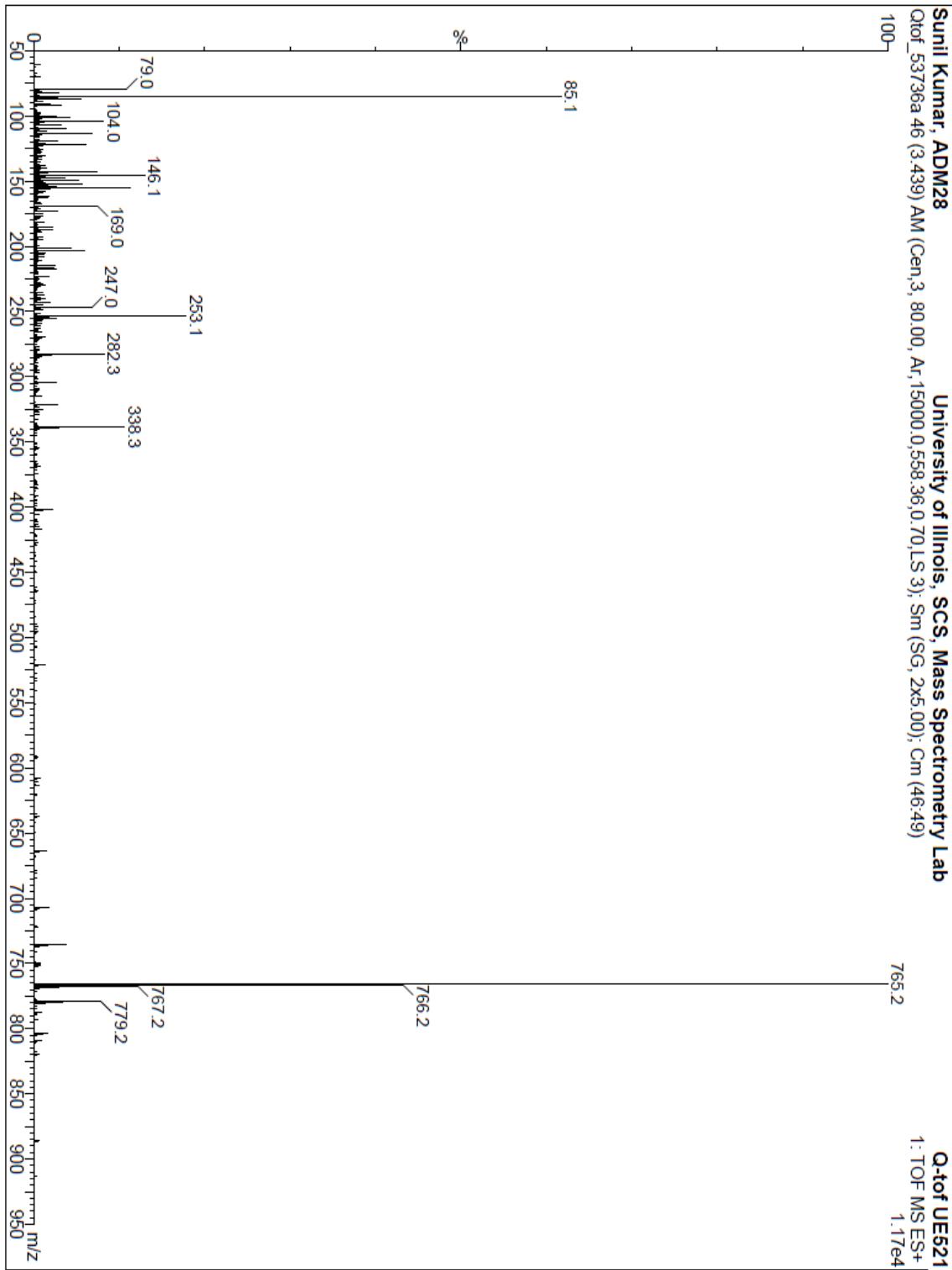
**Fig.** ESI-MS of ADM-107.



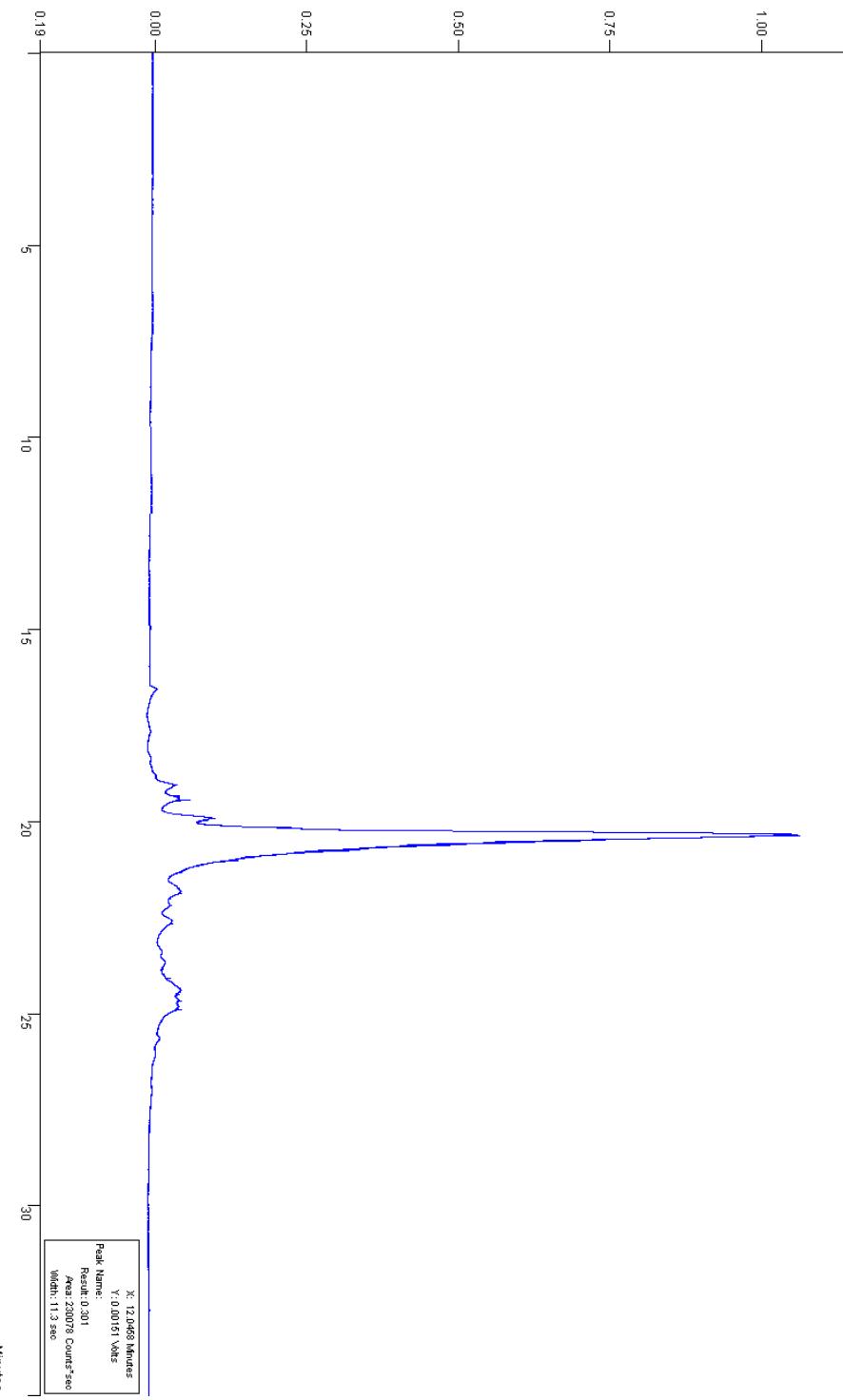
**Fig.** RP-HPLC of ADM-107.



**Fig.** <sup>1</sup>H-NMR of ADM-108.

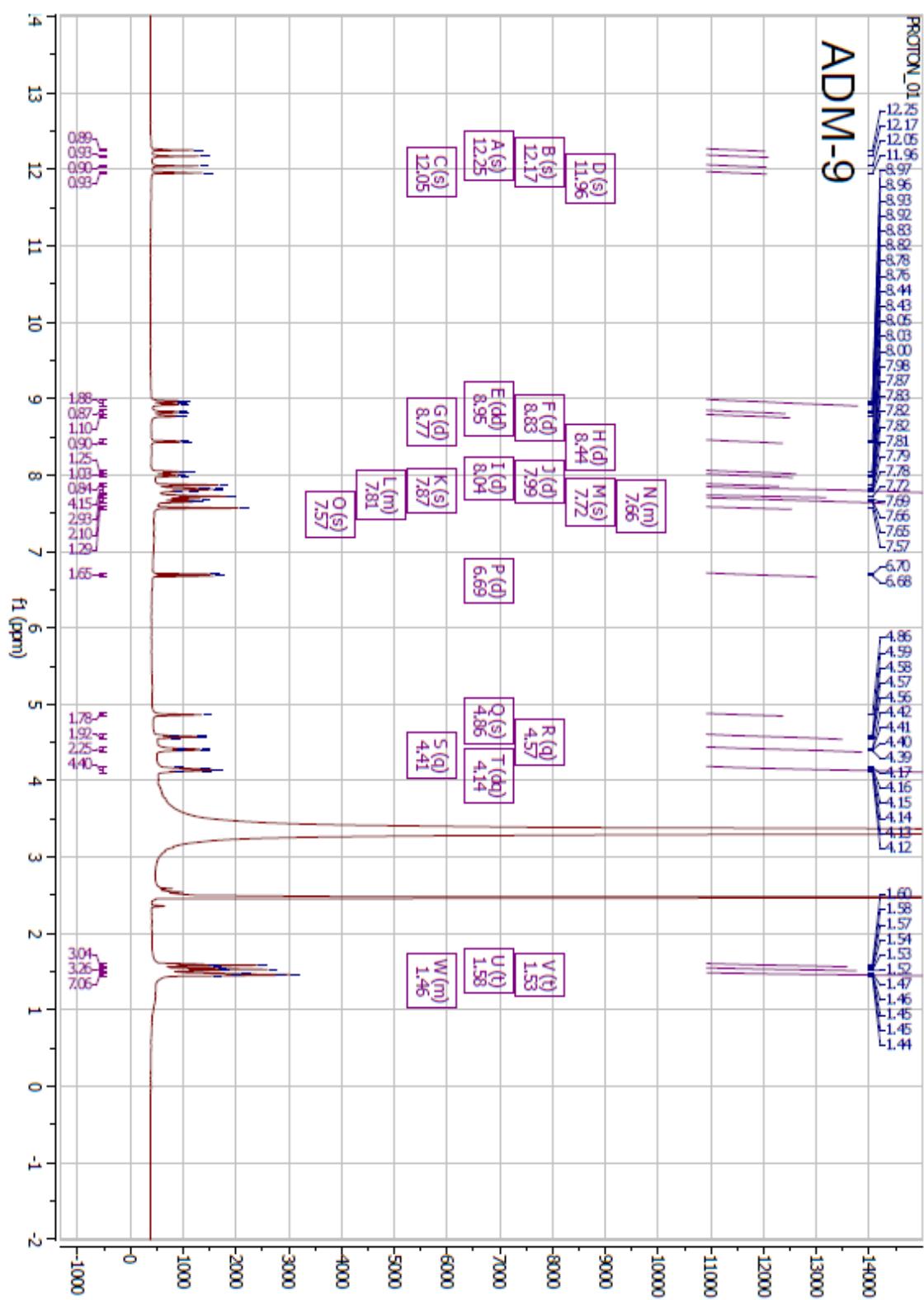


**Fig.** ESI-MS of ADM-108.

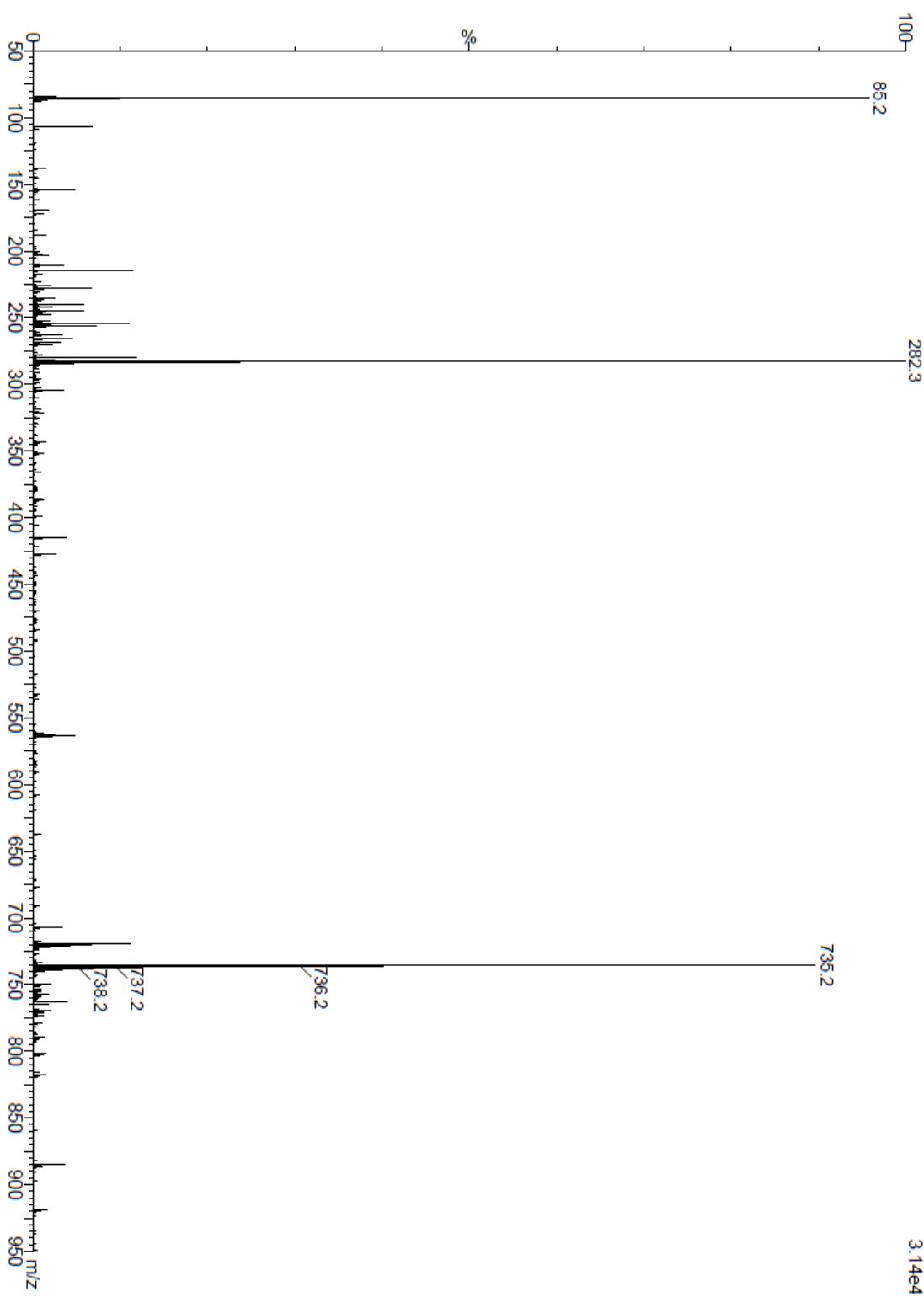


**Fig.** RP-HPLC of ADM-108.

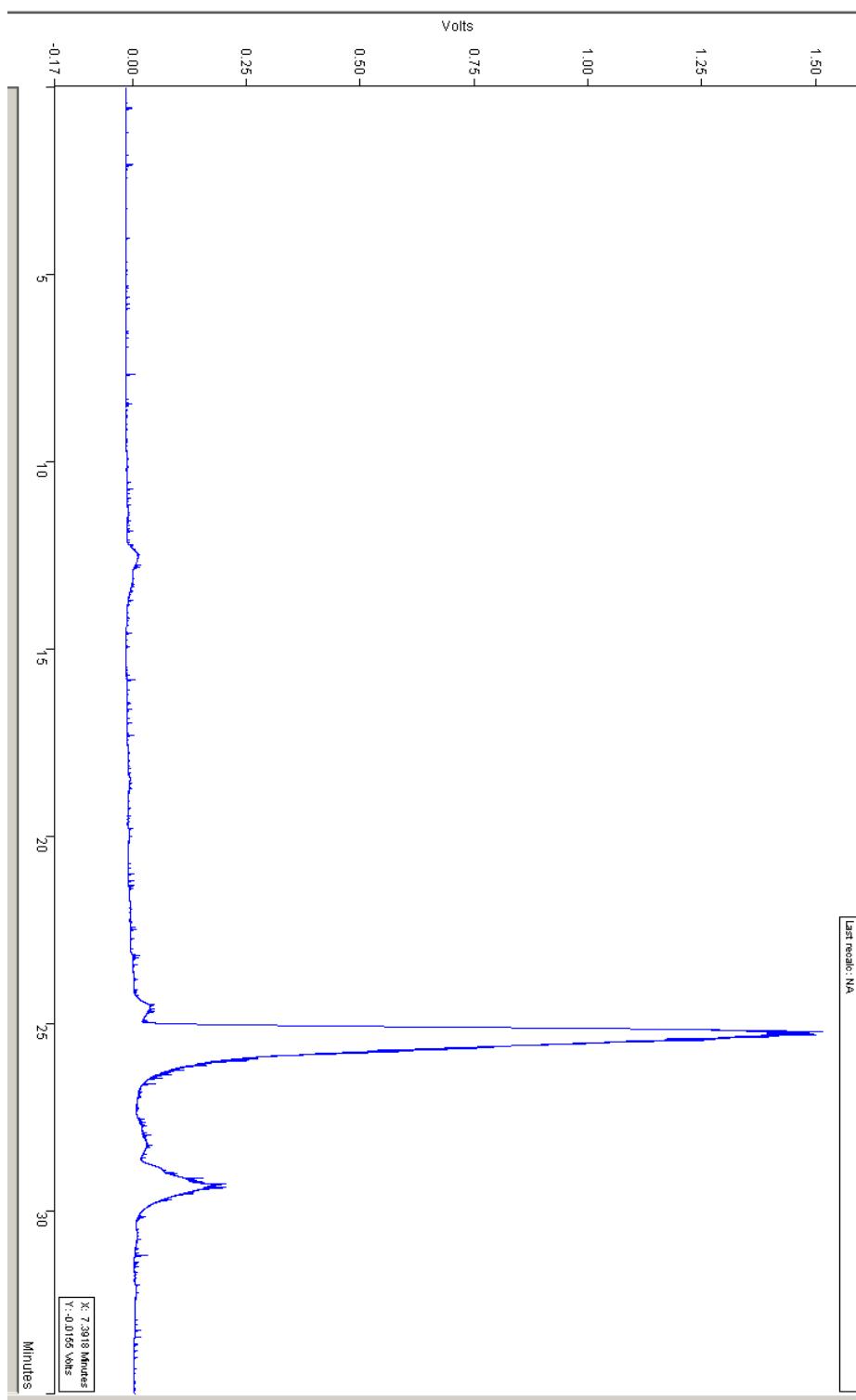
**ADM-9**



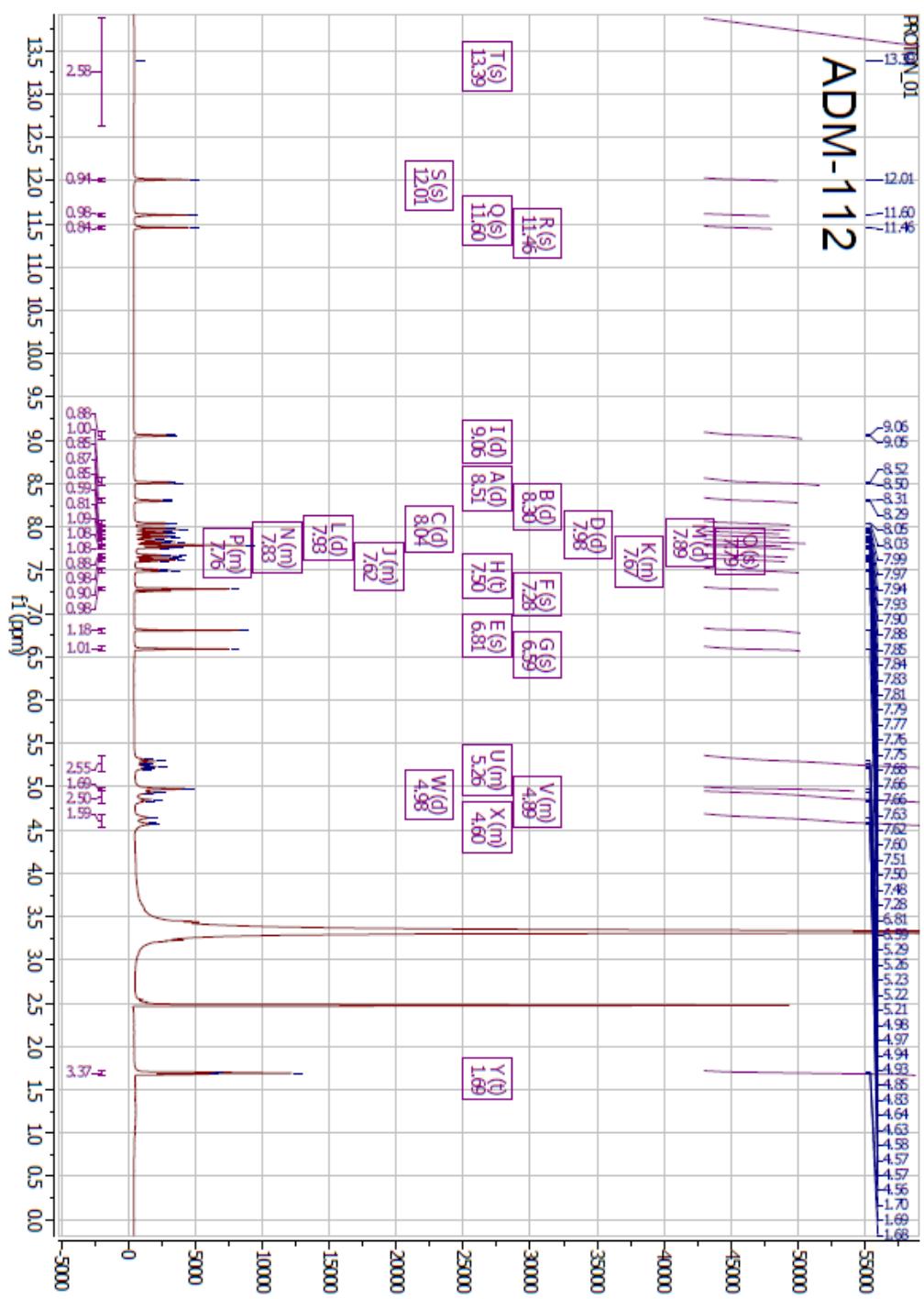
**Fig.**  $^1\text{H}$ -NMR of ADM-109.



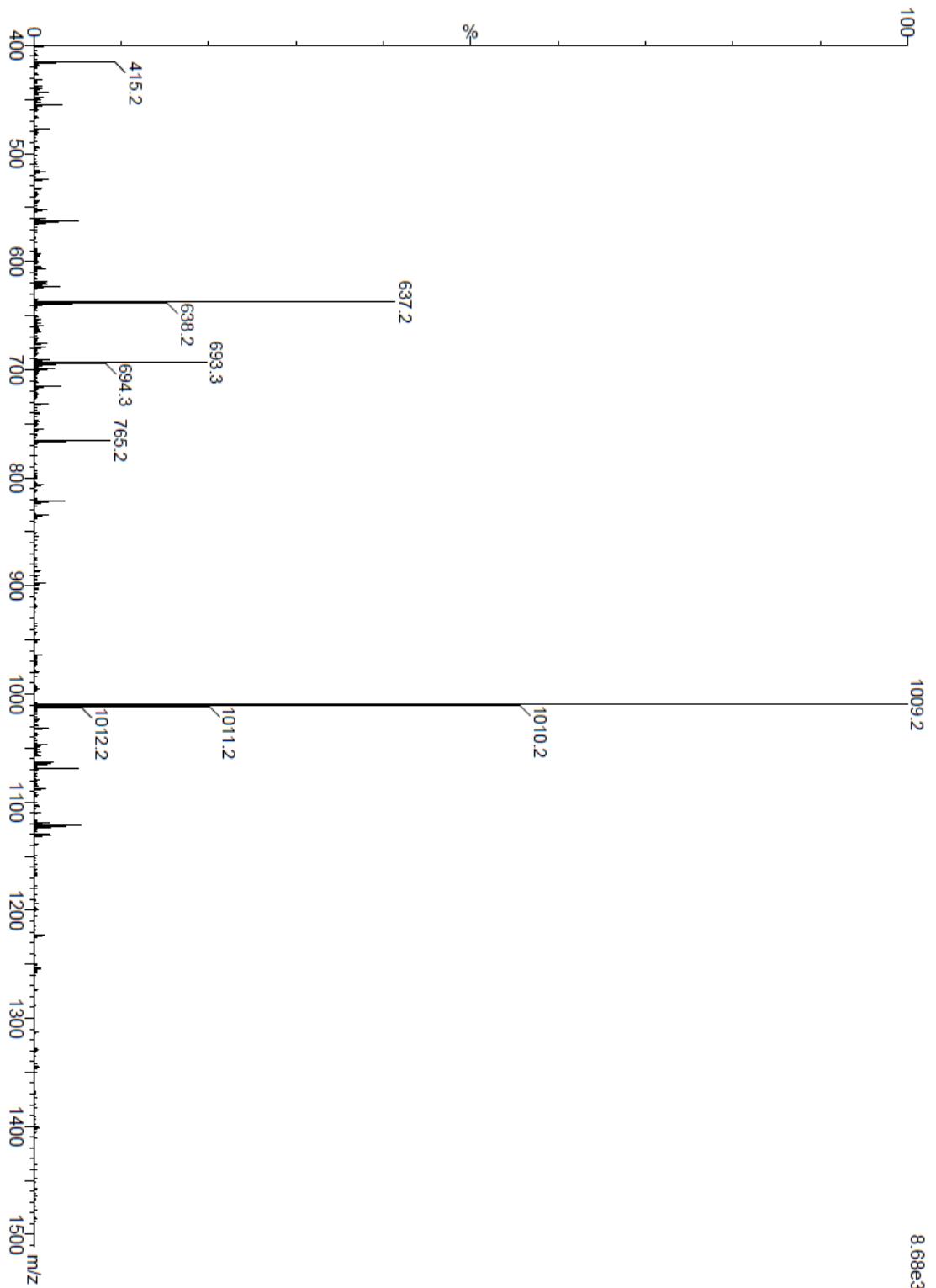
**Fig.** ESI-MS of ADM-109.



**Fig.** RP-HPLC of ADM-109.



**Fig.**  $^1\text{H}$ -NMR of ADM-112.



**Fig.** ESI-MS of ADM-112.

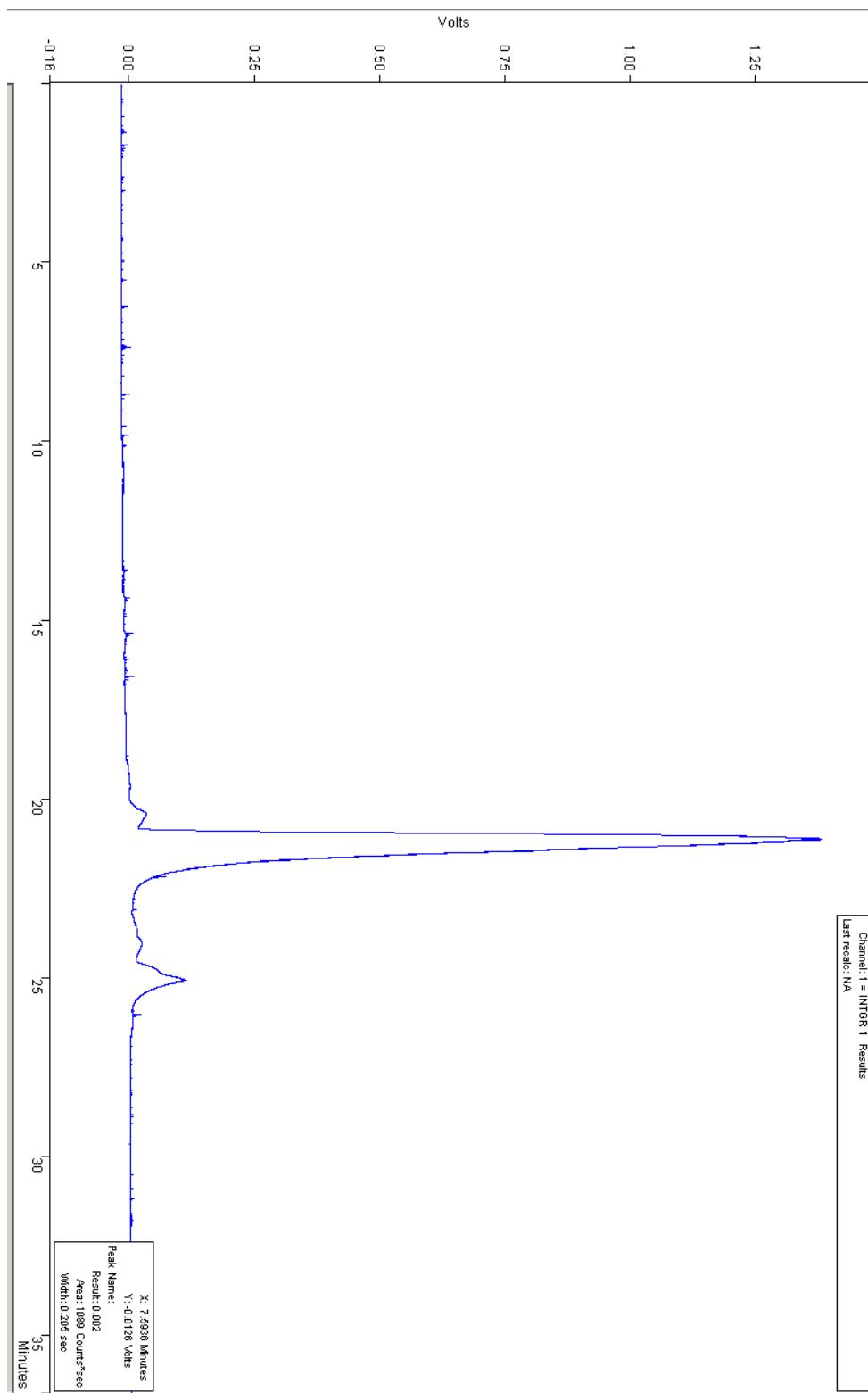


Fig. RP-HPLC of ADM-112.

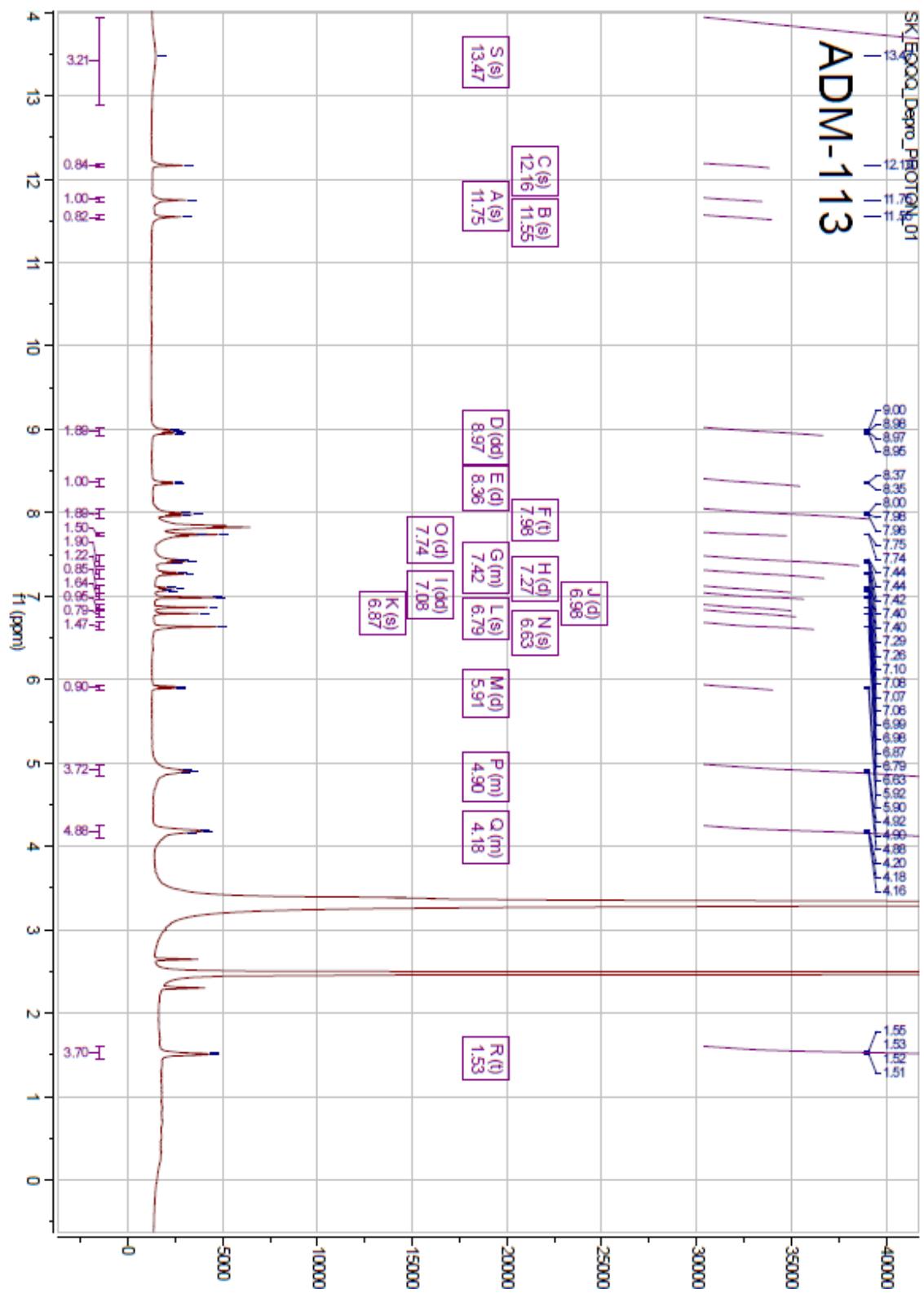
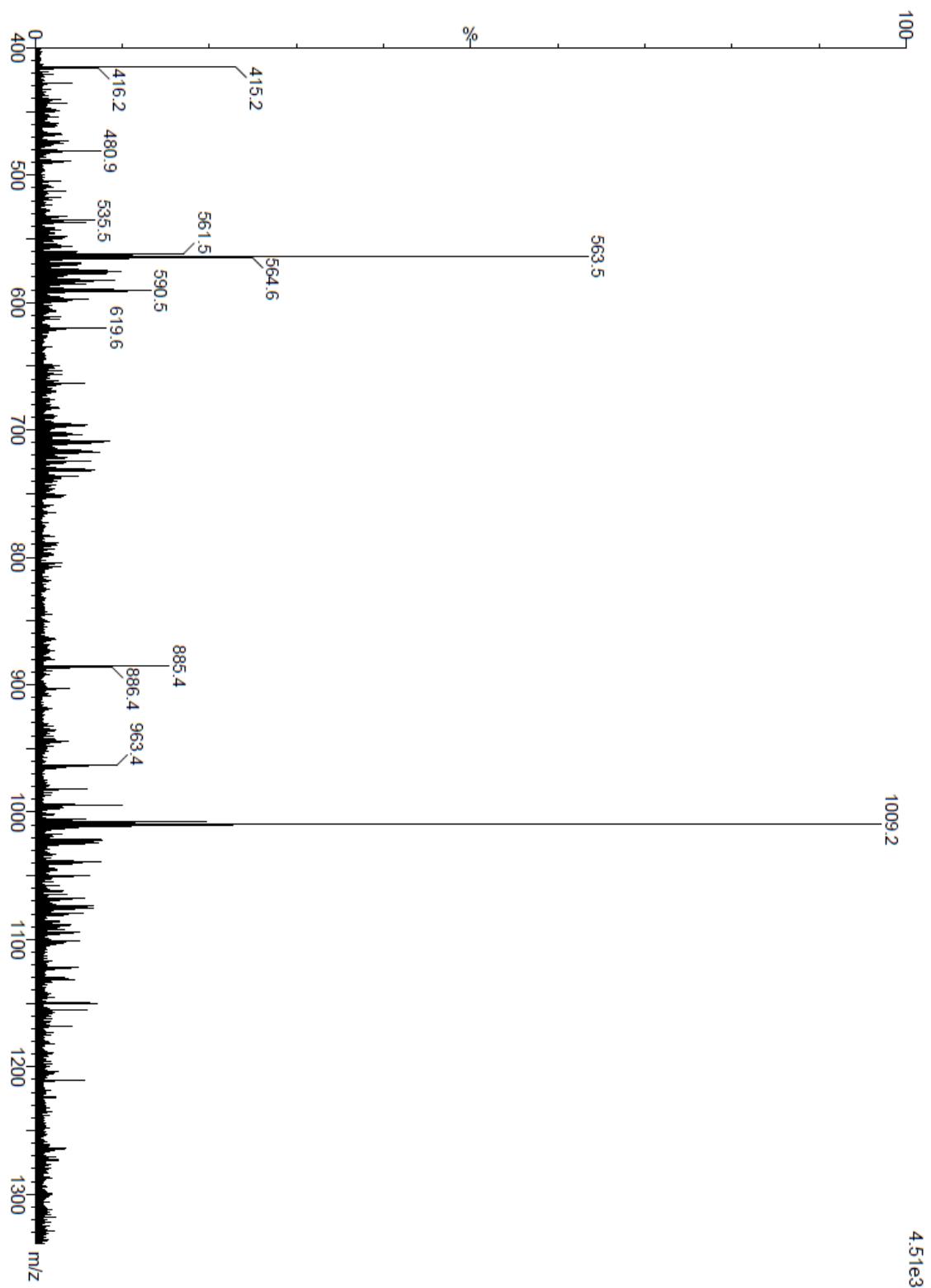
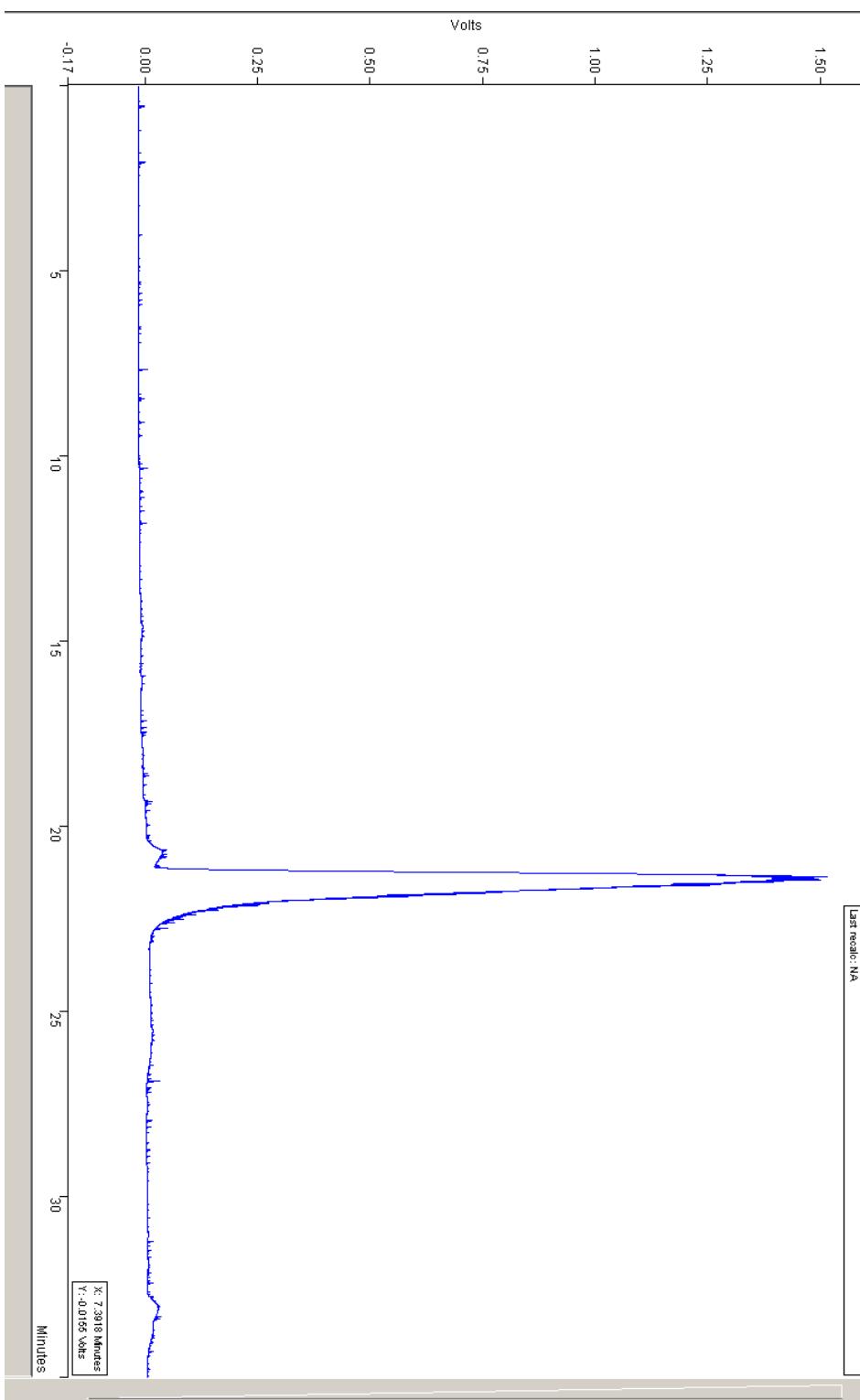


Fig.  $^1\text{H}$ -NMR of ADM-113.



**Fig.** ESI-MS of ADM-113.



**Fig.** RP-HPLC of ADM-113.

# ADM-114

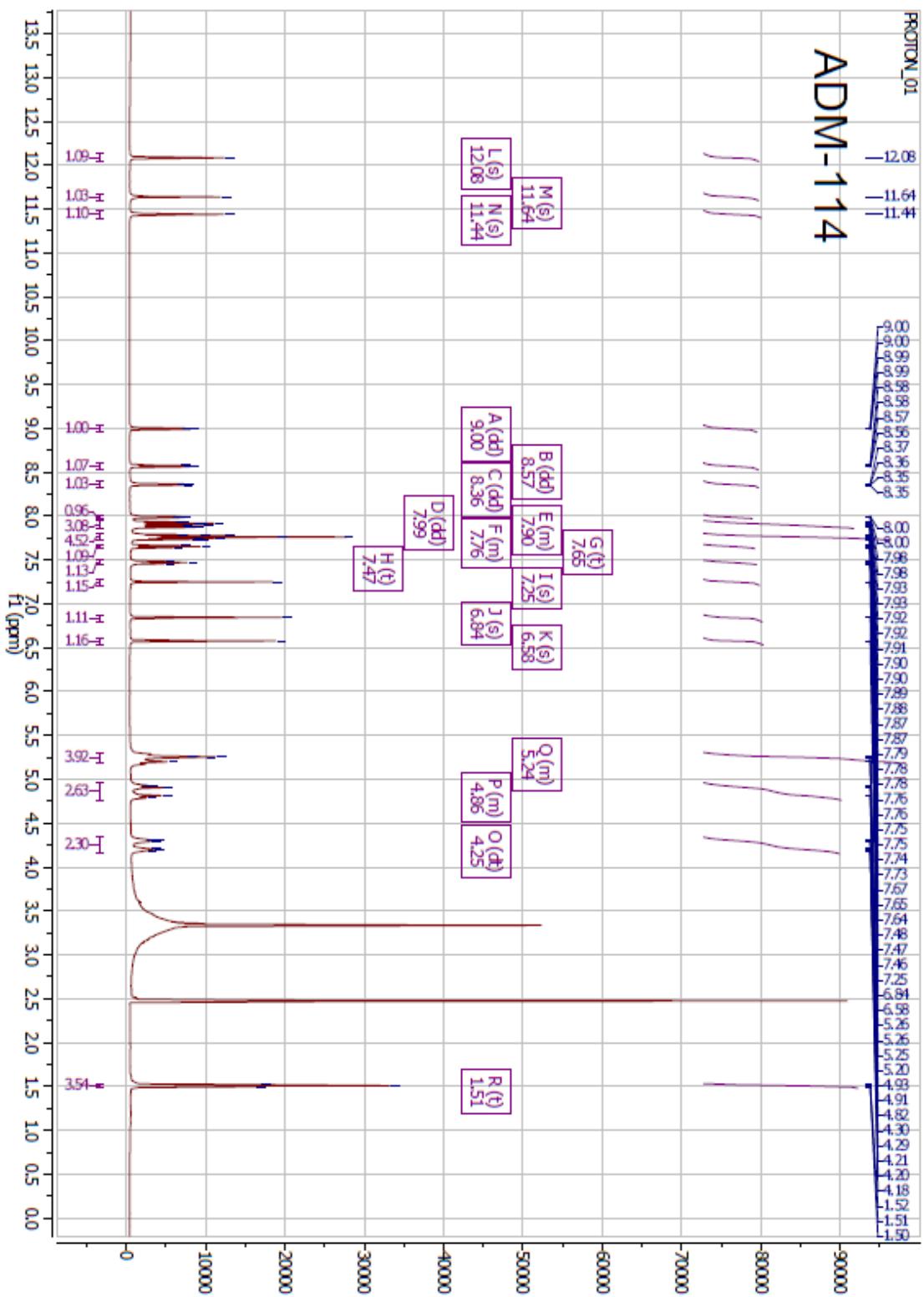
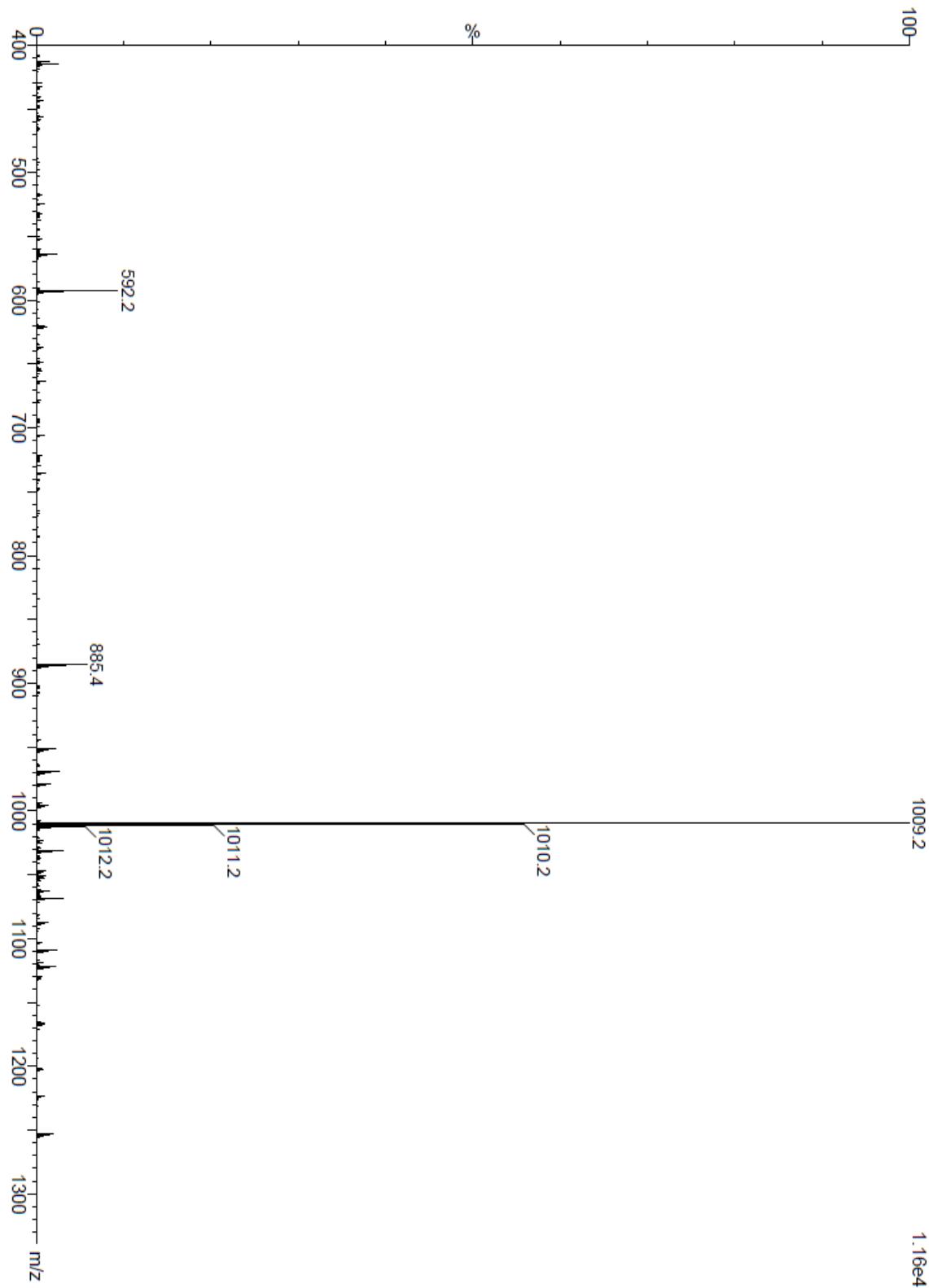
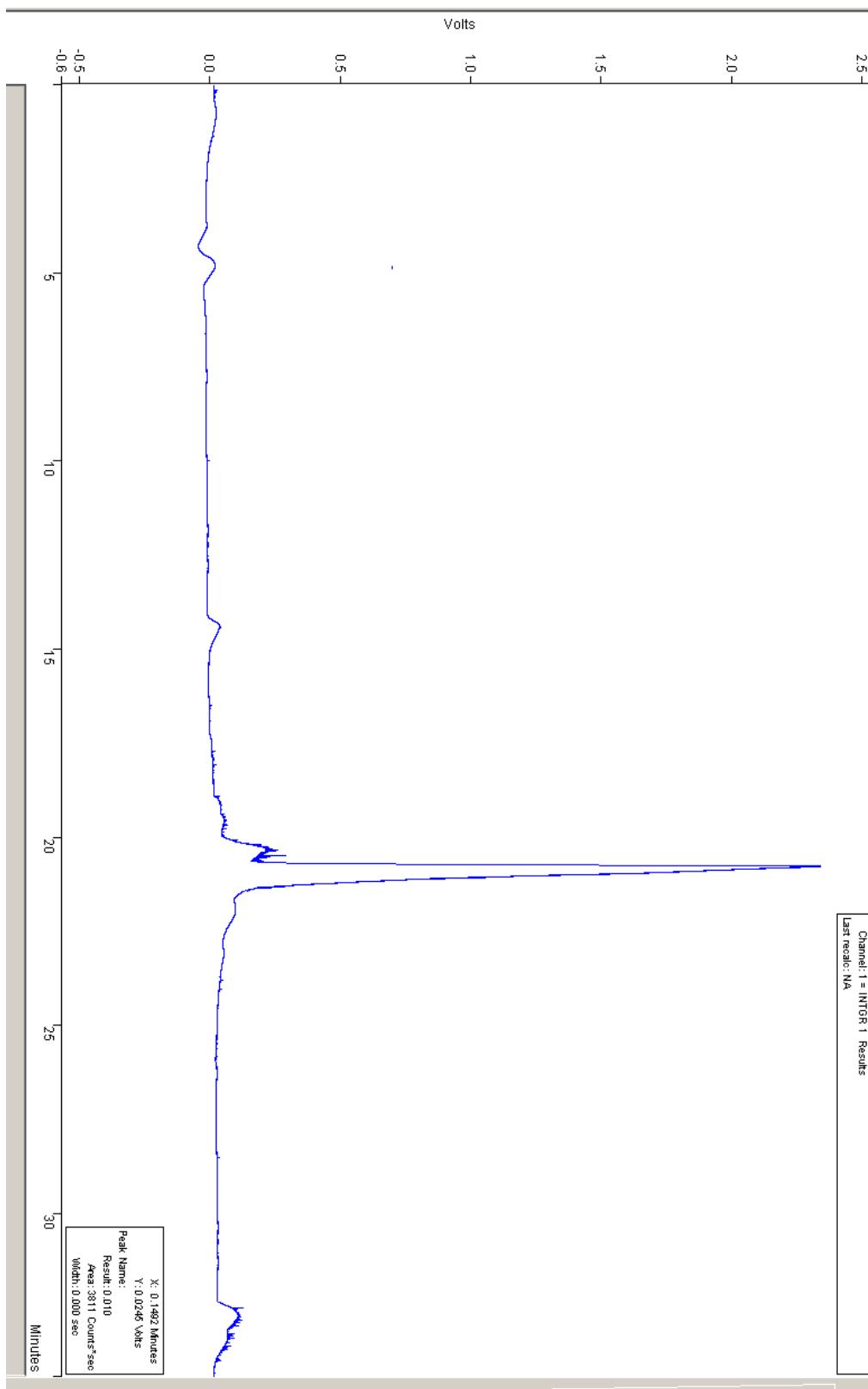


Fig. <sup>1</sup>H-NMR of ADM-114.



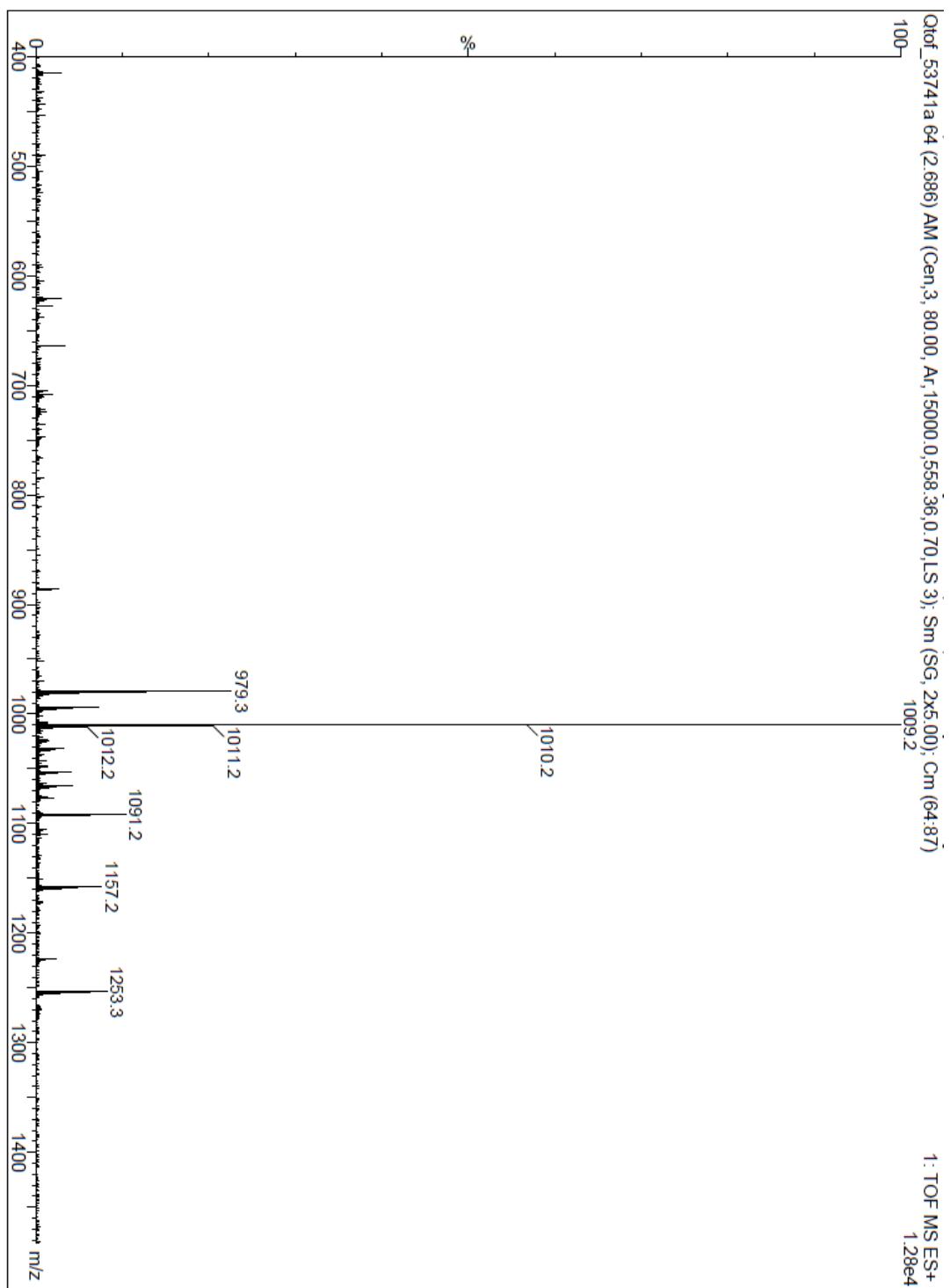
**Fig.** ESI-MS of ADM-114.



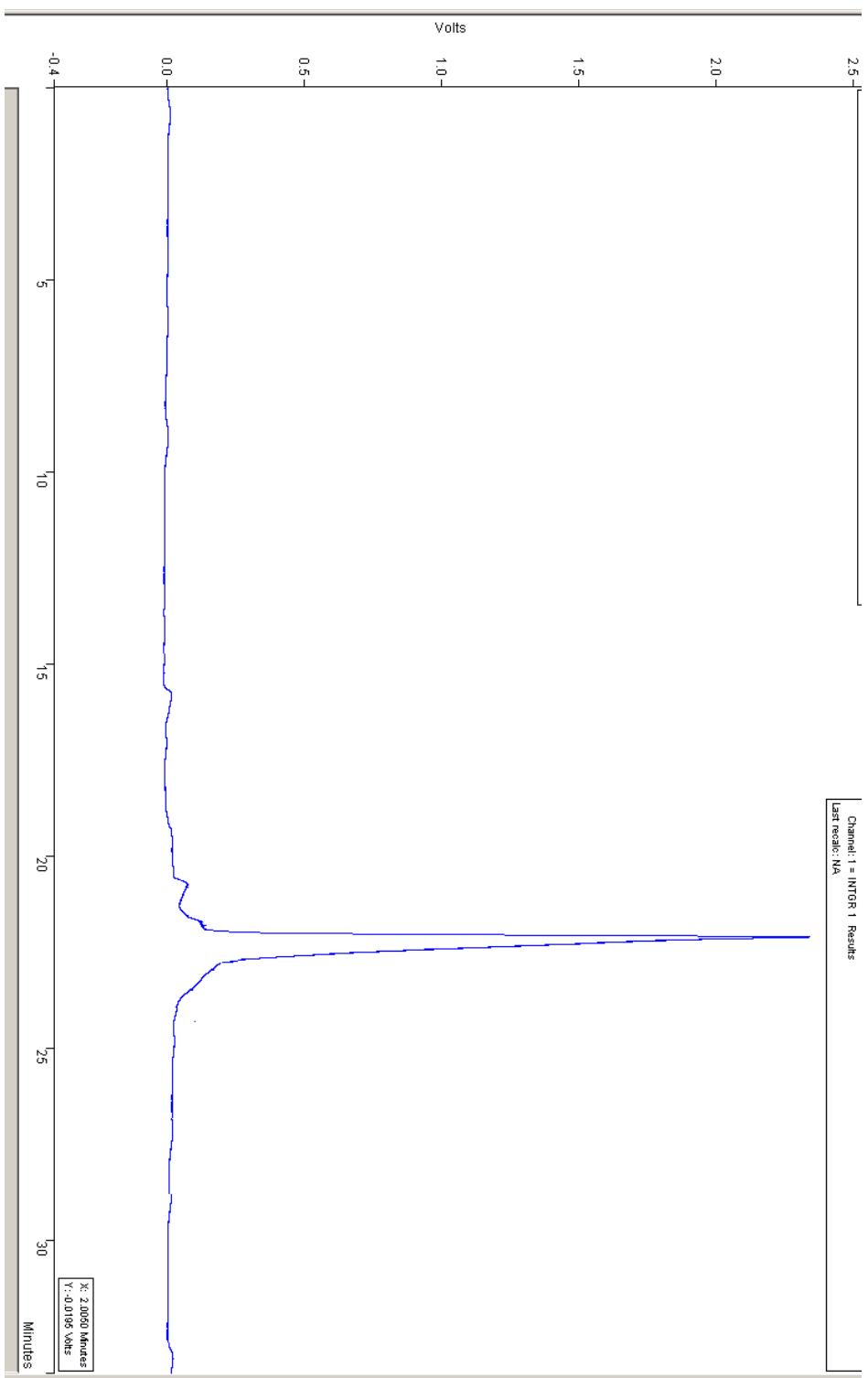
**Fig.** RP-HPLC of ADM-114.



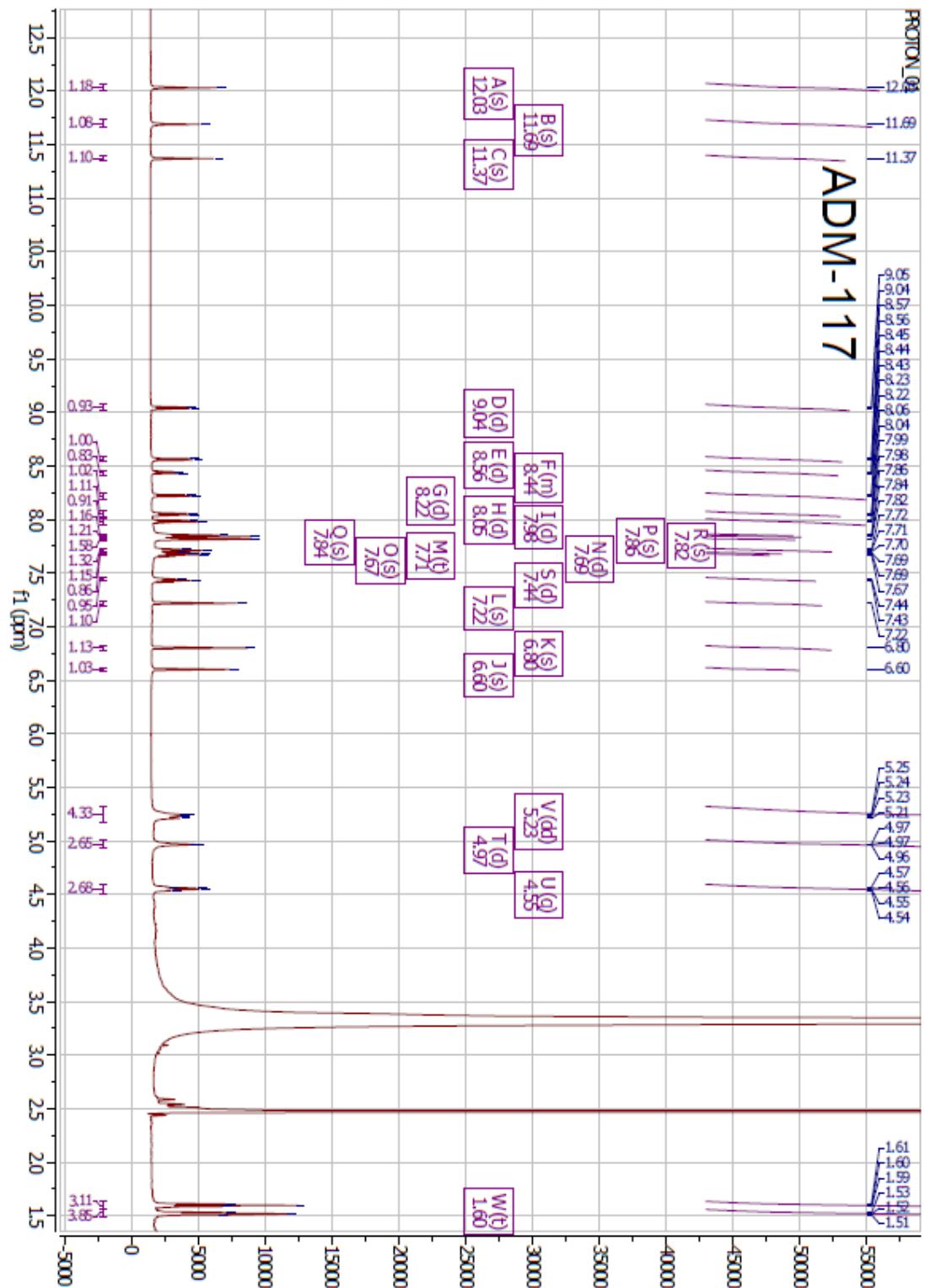
Fig.  $^1\text{H}$ -NMR of ADM-115.

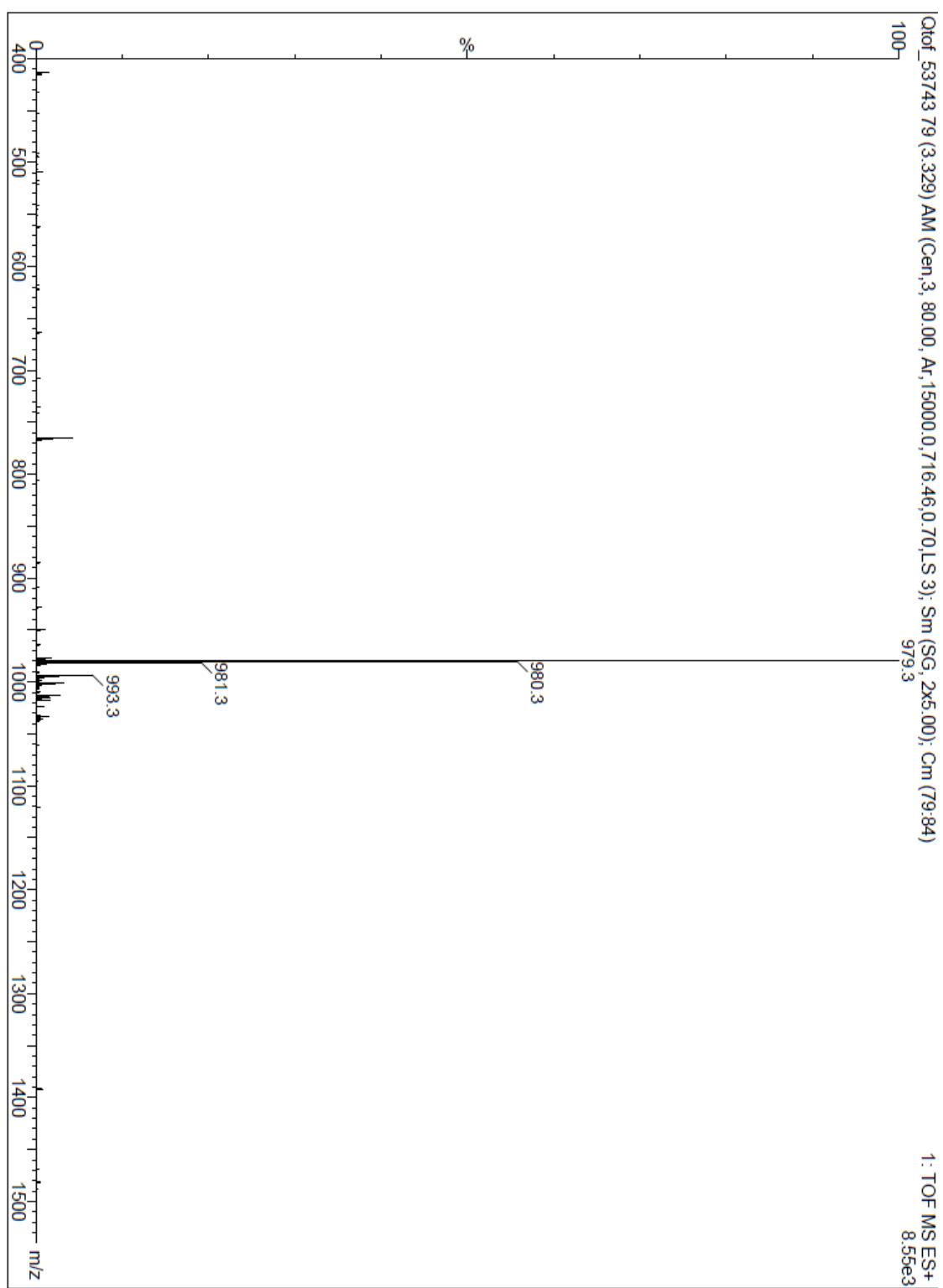


**Fig.** ESI-MS of ADM-115.

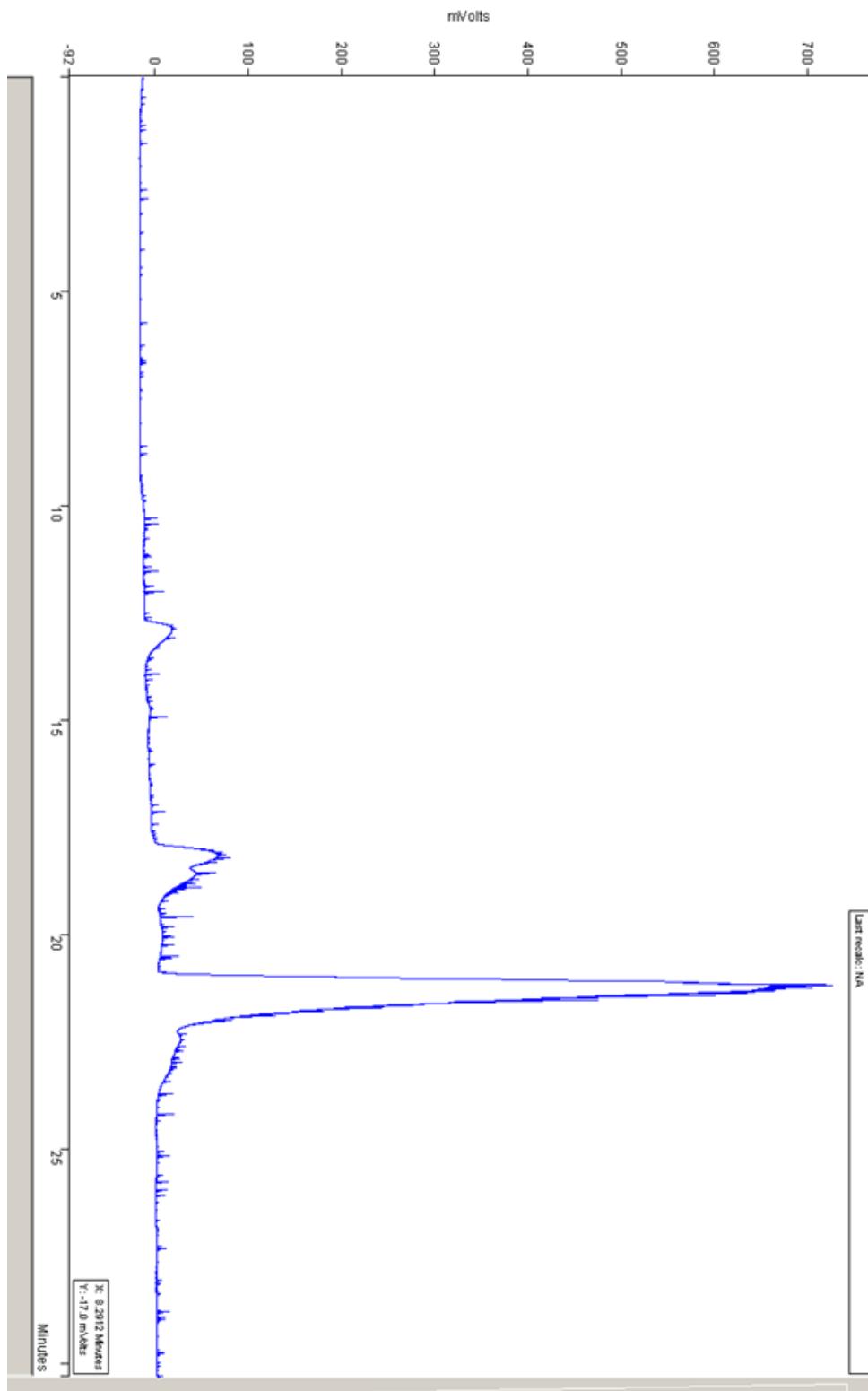


**Fig.** RP-HPLC of ADM-115.





**Fig.** ESI-MS of ADM-117.



**Fig.** RP-HPLC of ADM-117.

# ADM-119

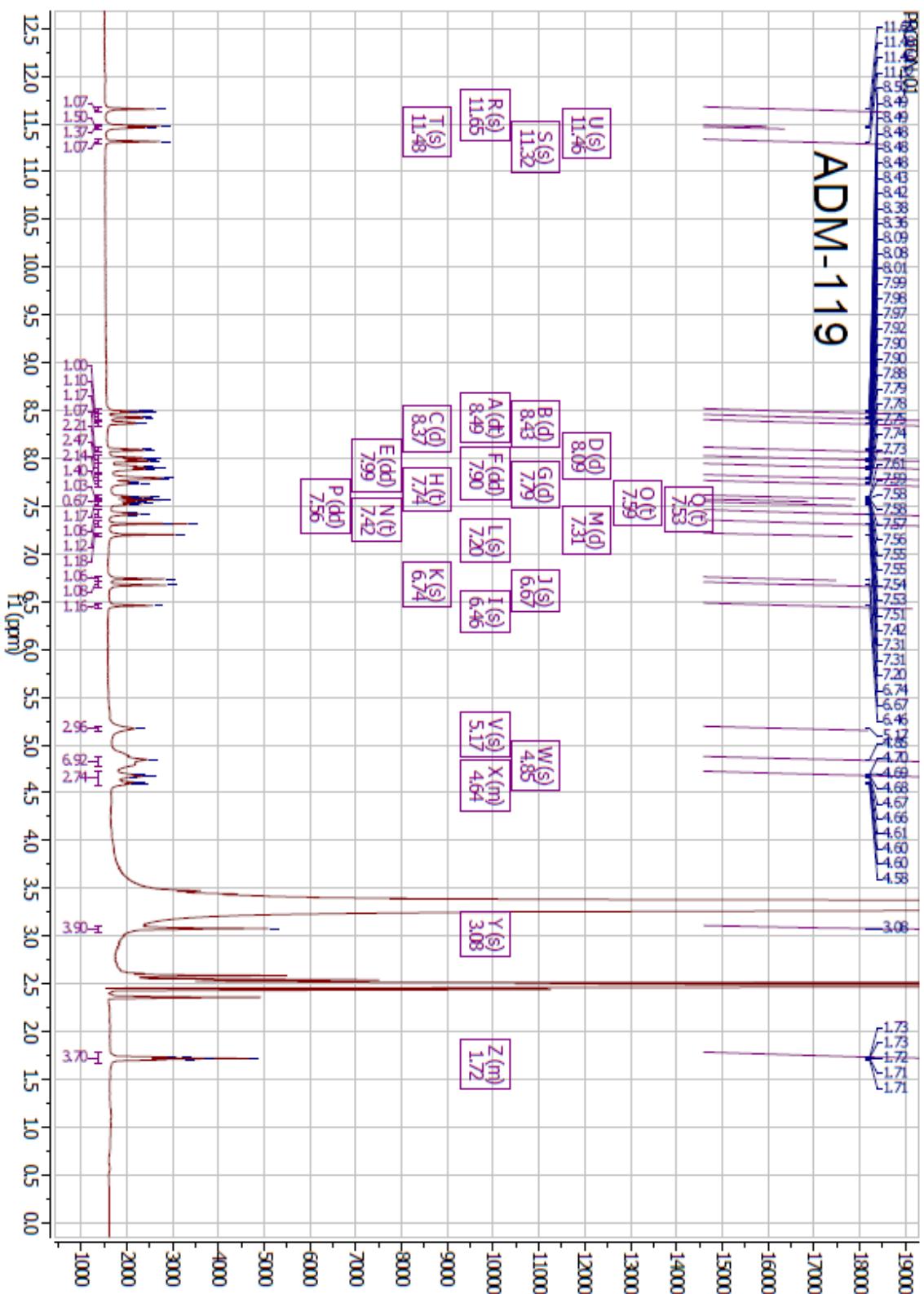
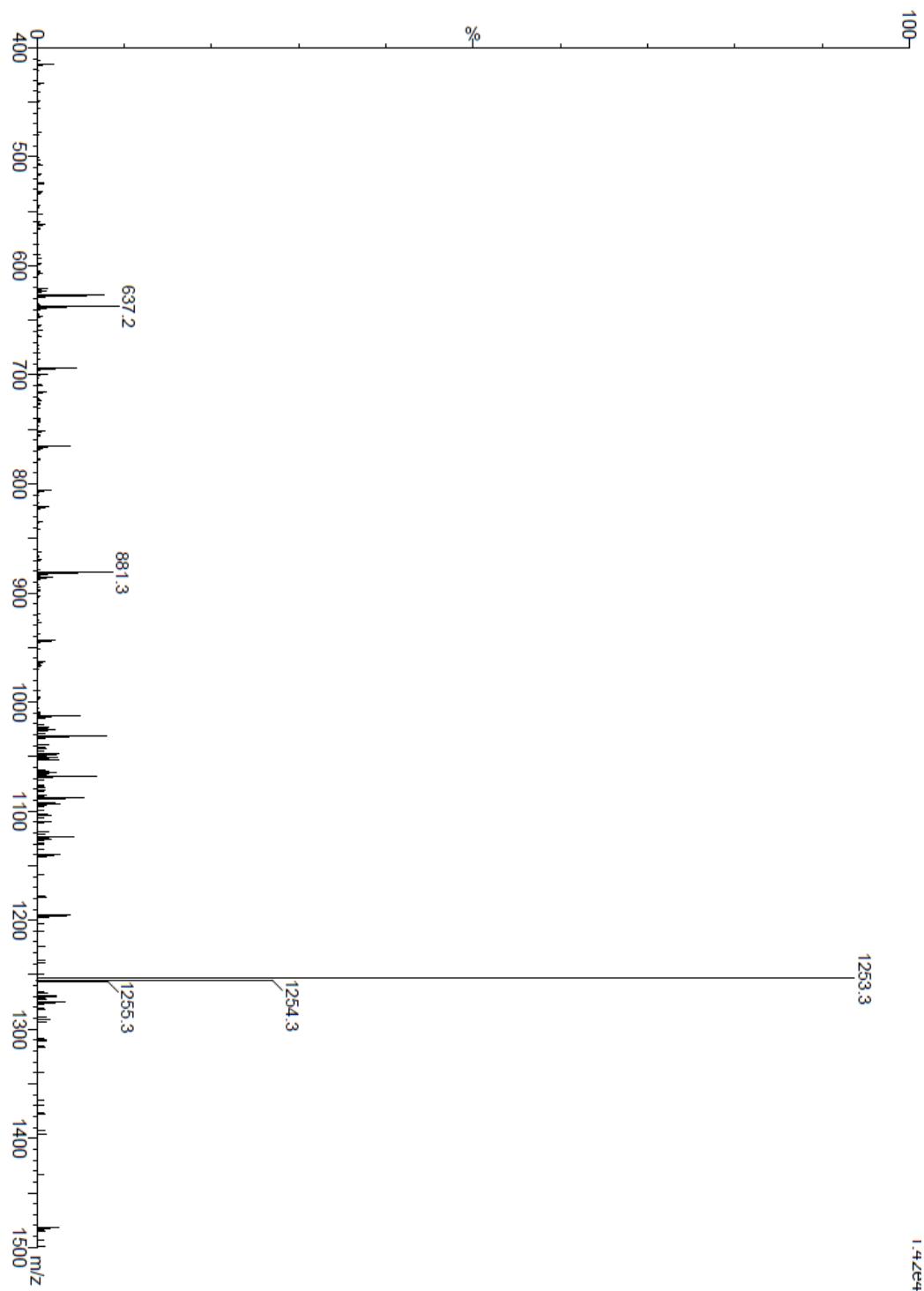
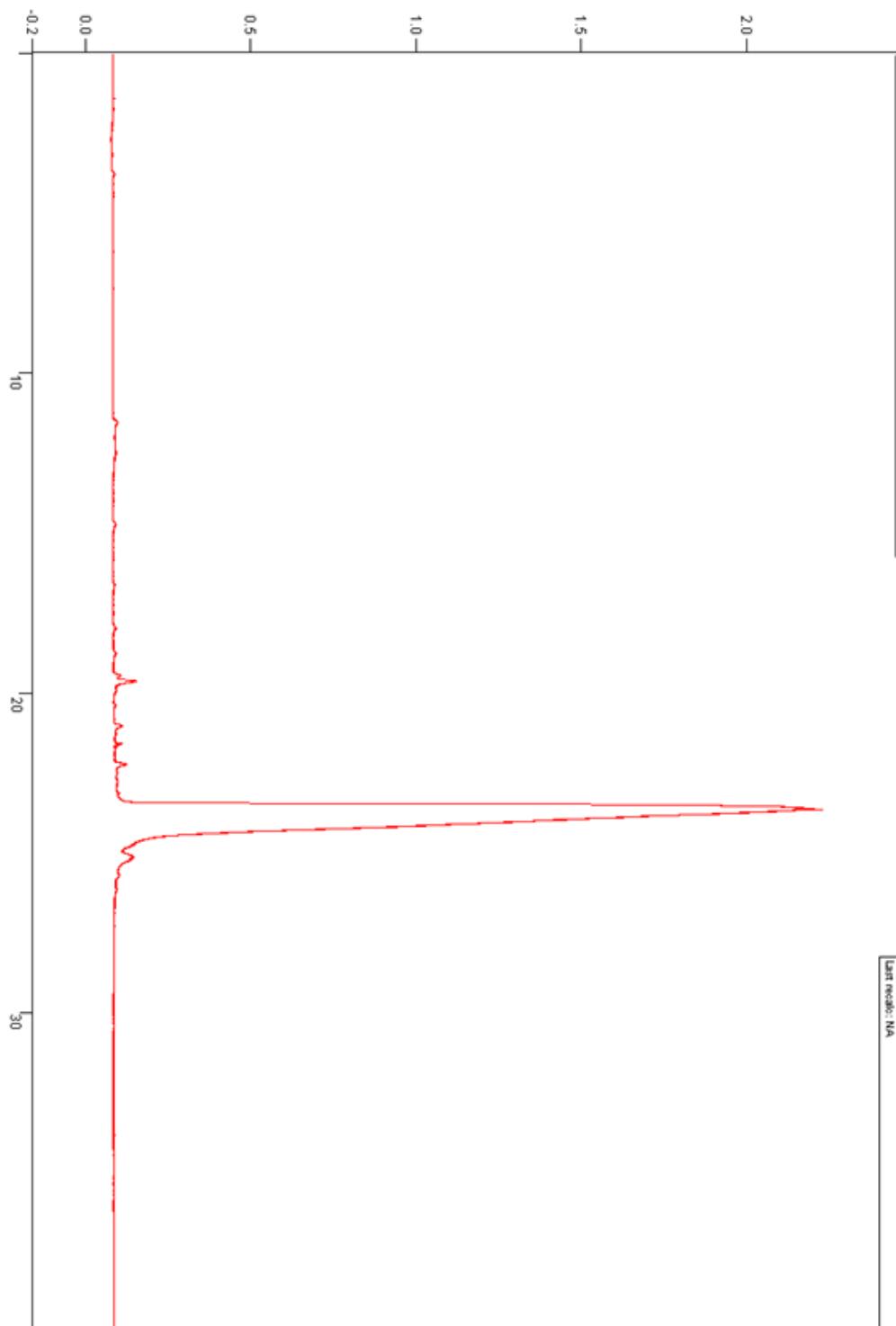


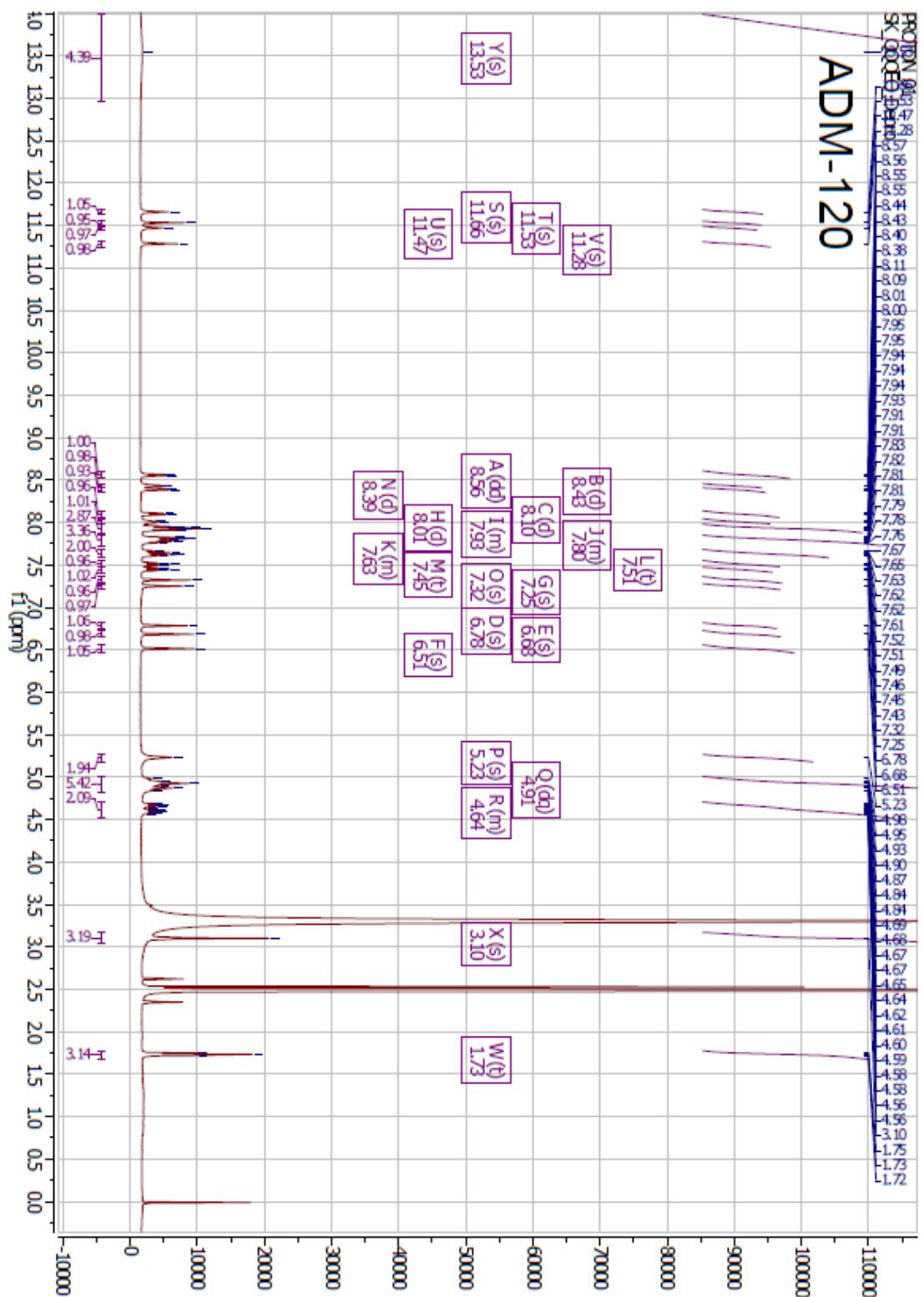
Fig.  $^1\text{H}$ -NMR of ADM-119.



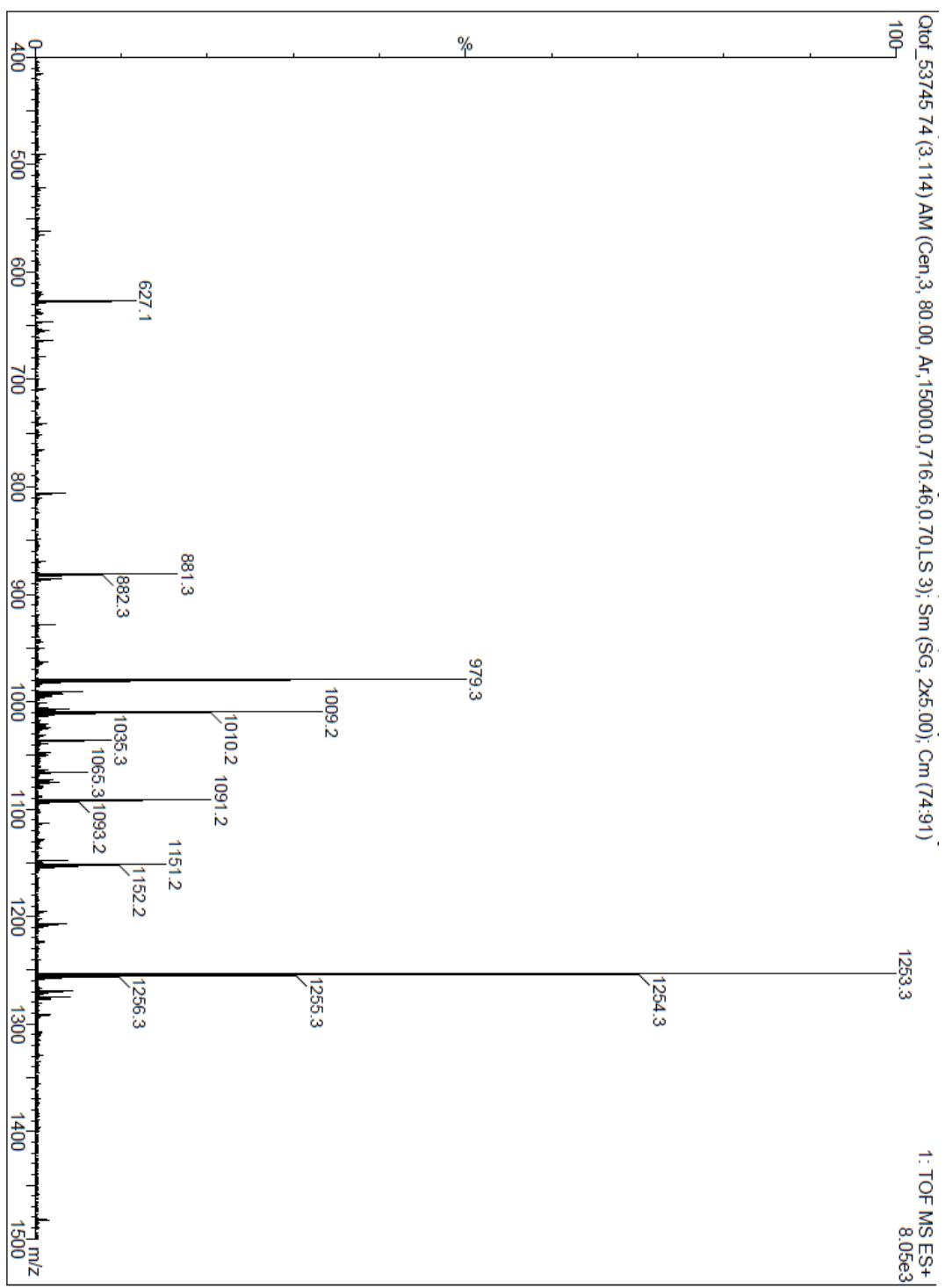
**Fig.** ESI-MS of ADM-119.



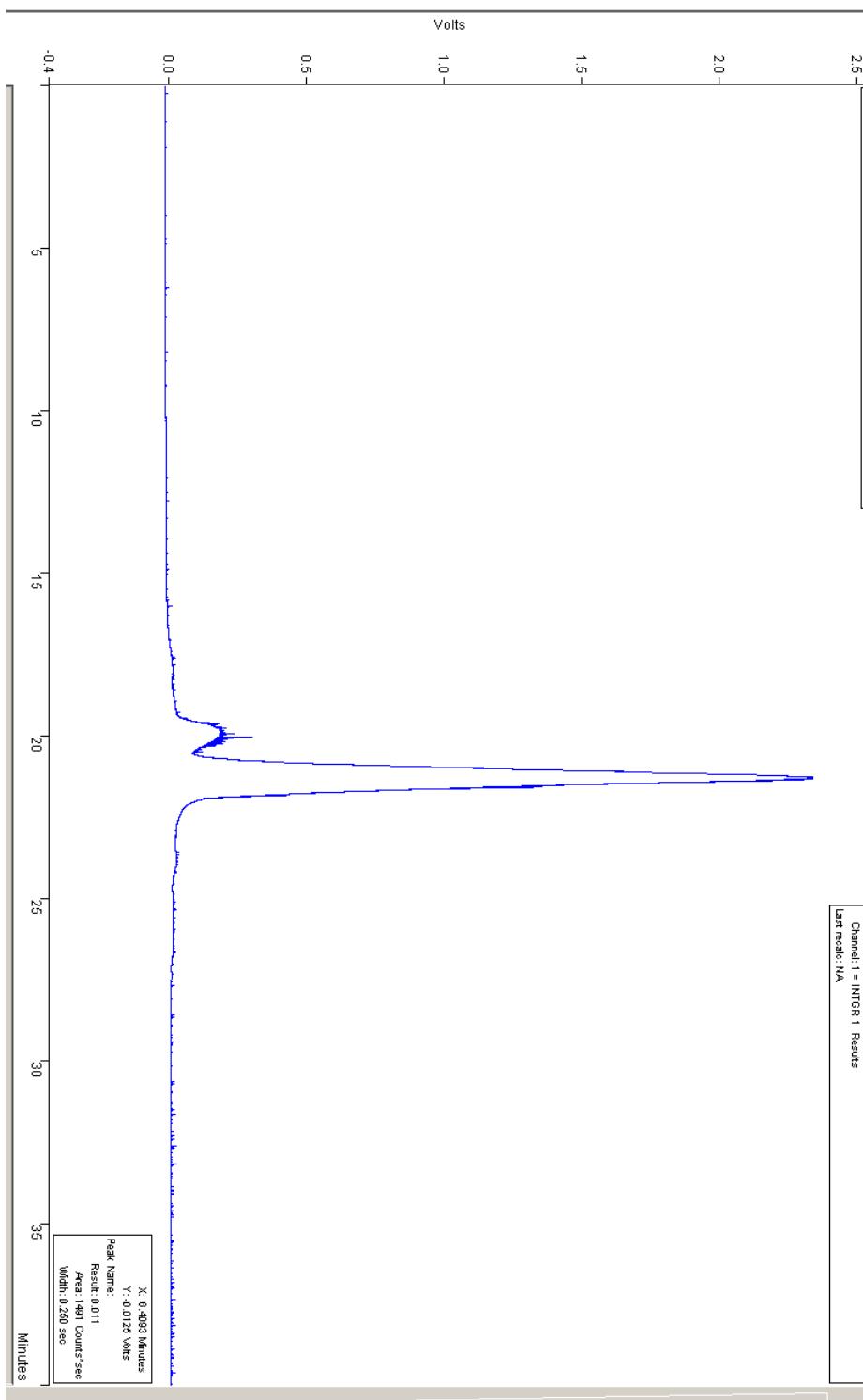
**Fig.** RP-HPLC of ADM-119.



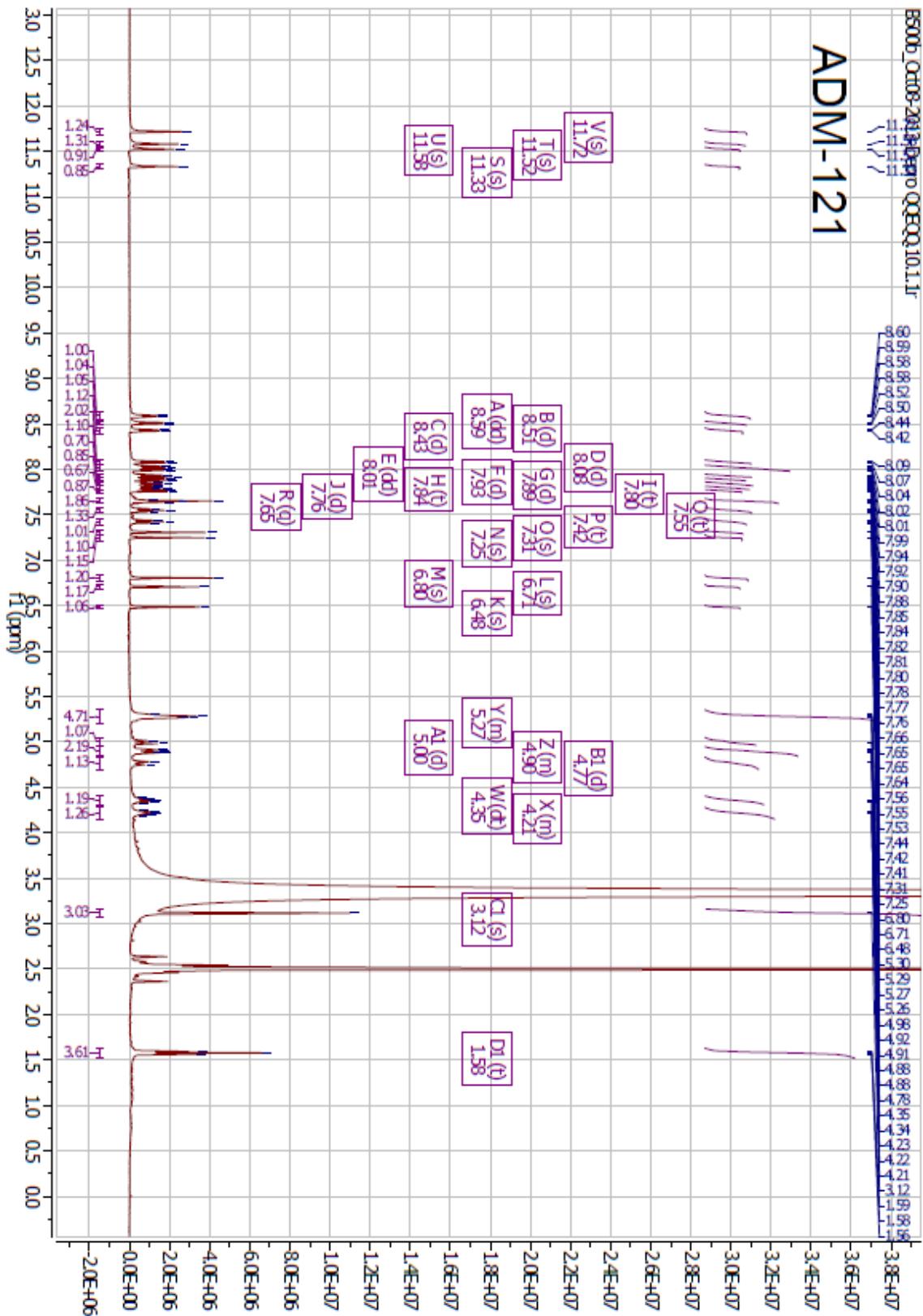
**Fig.**  $^1\text{H}$ -NMR of ADM-120.



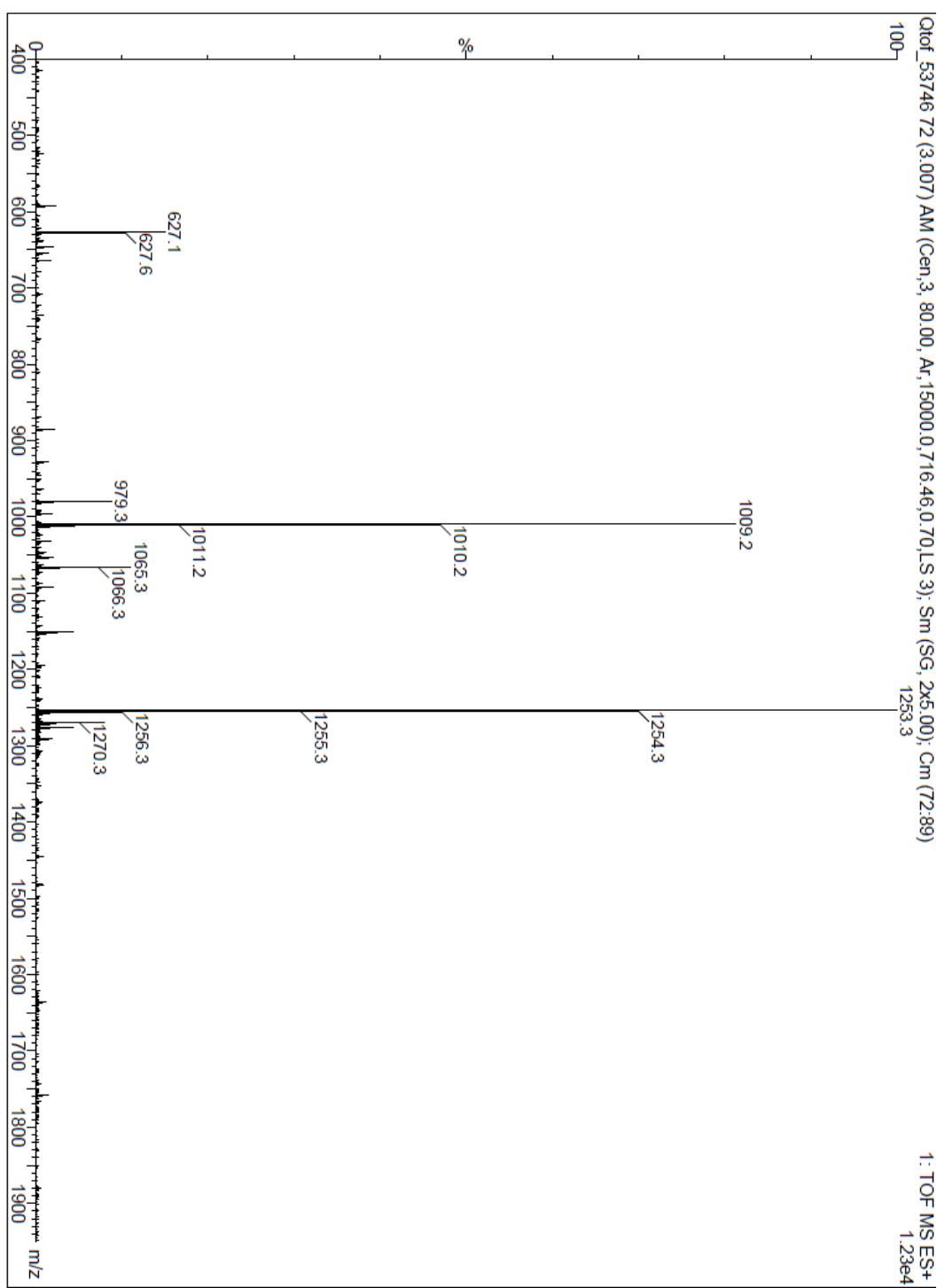
**Fig.** ESI-MS of ADM-120.



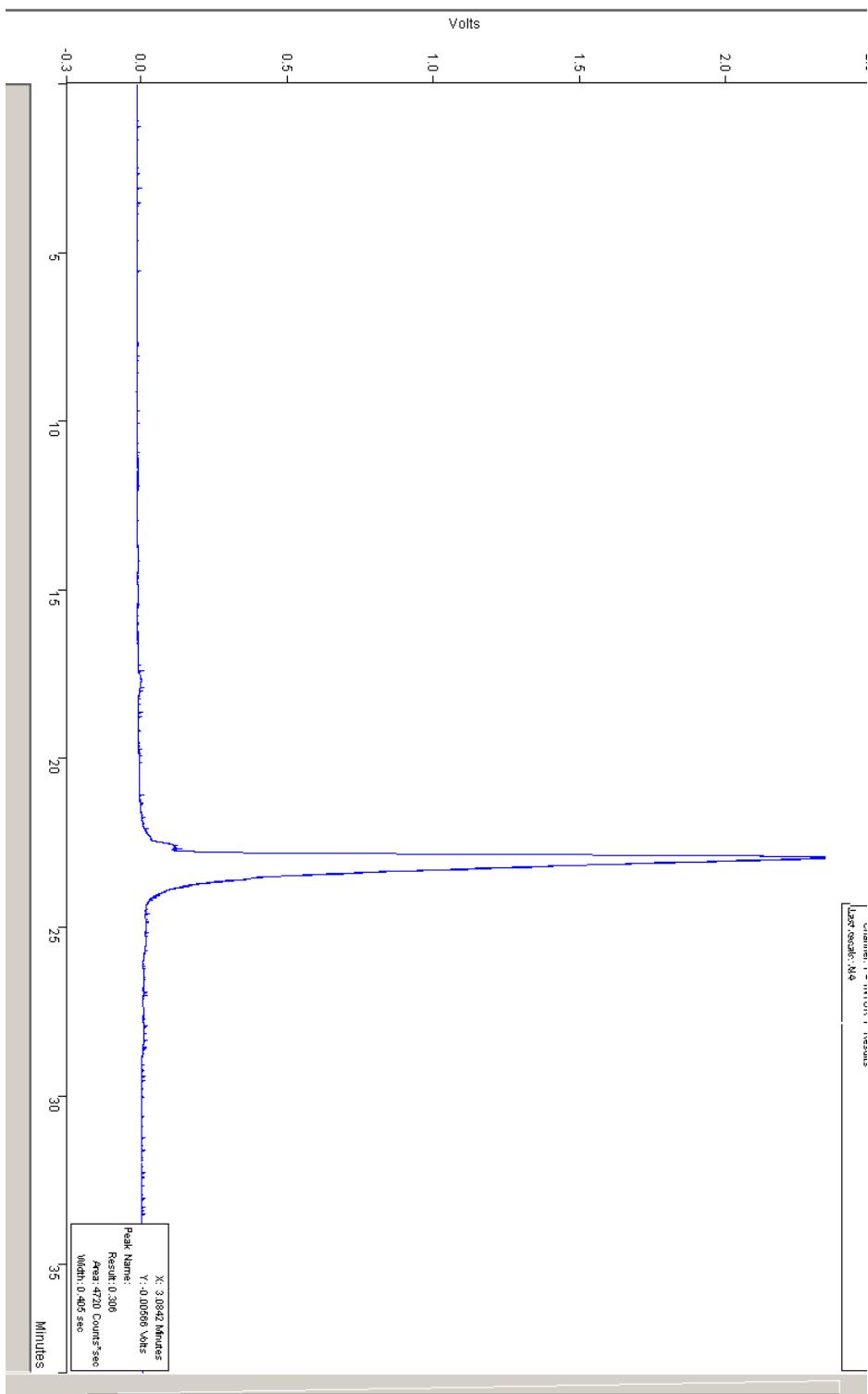
**Fig.** RP-HPLC of ADM-120.



**Fig.**  $^1\text{H}$ -NMR of ADM-121.

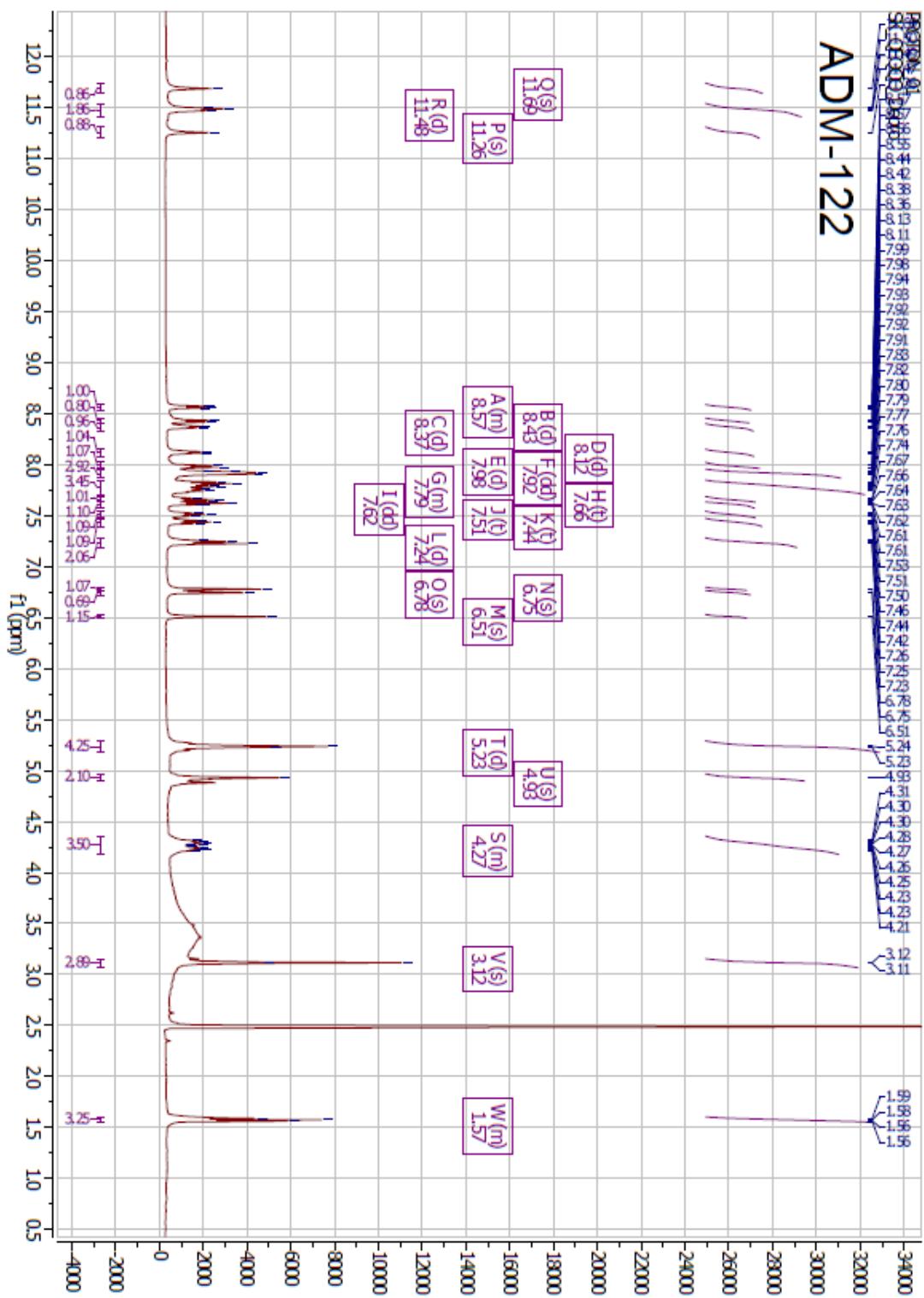


**Fig.** ESI-MS of ADM-121.

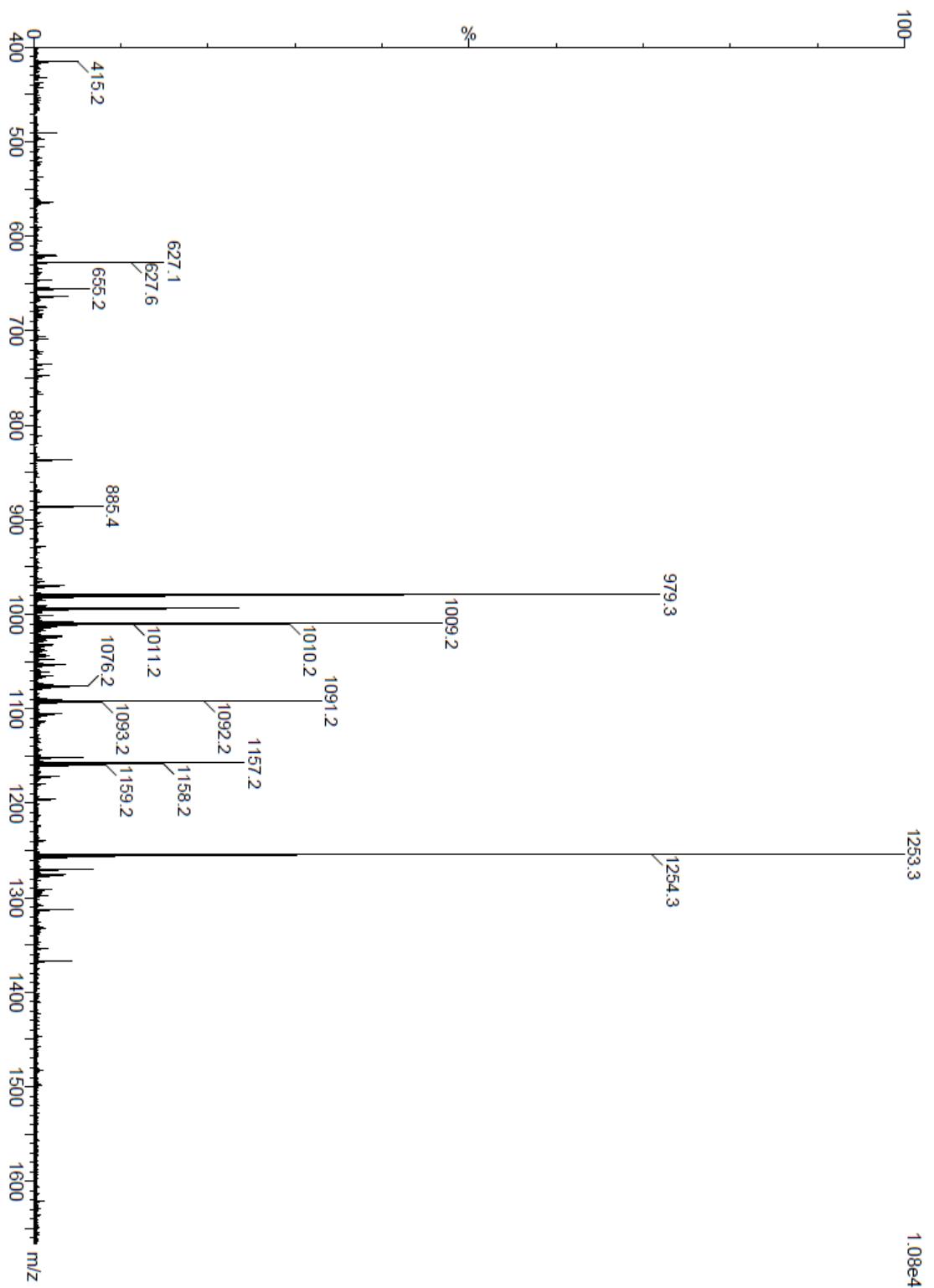


**Fig.** RP-HPLC of ADM-121.

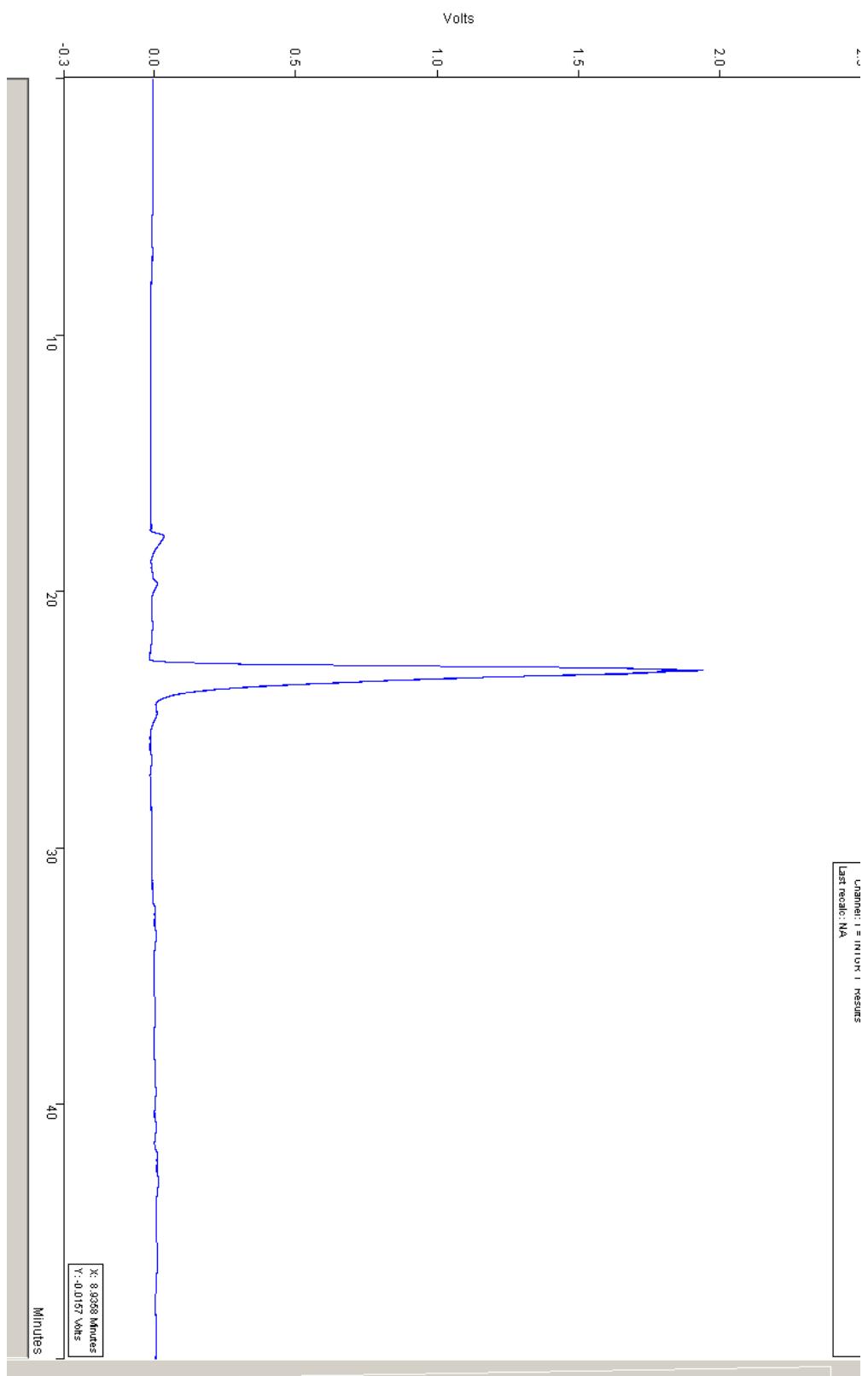
## ADM-122



**Fig.**  $^1\text{H}$ -NMR of ADM-122.



**Fig.** ESI-MS of ADM-122.



**Fig.** RP-HPLC of ADM-122.

# ADM-123

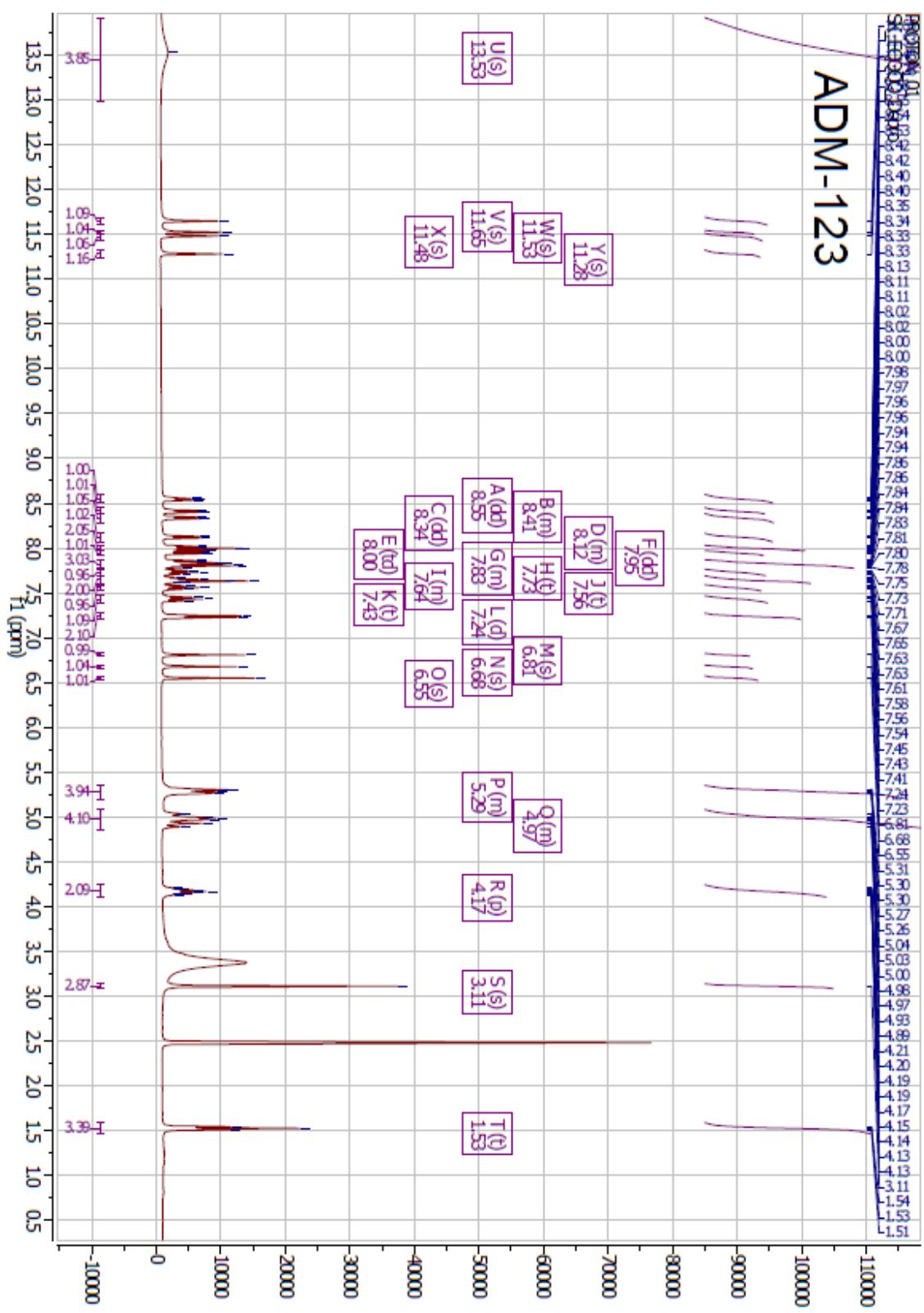
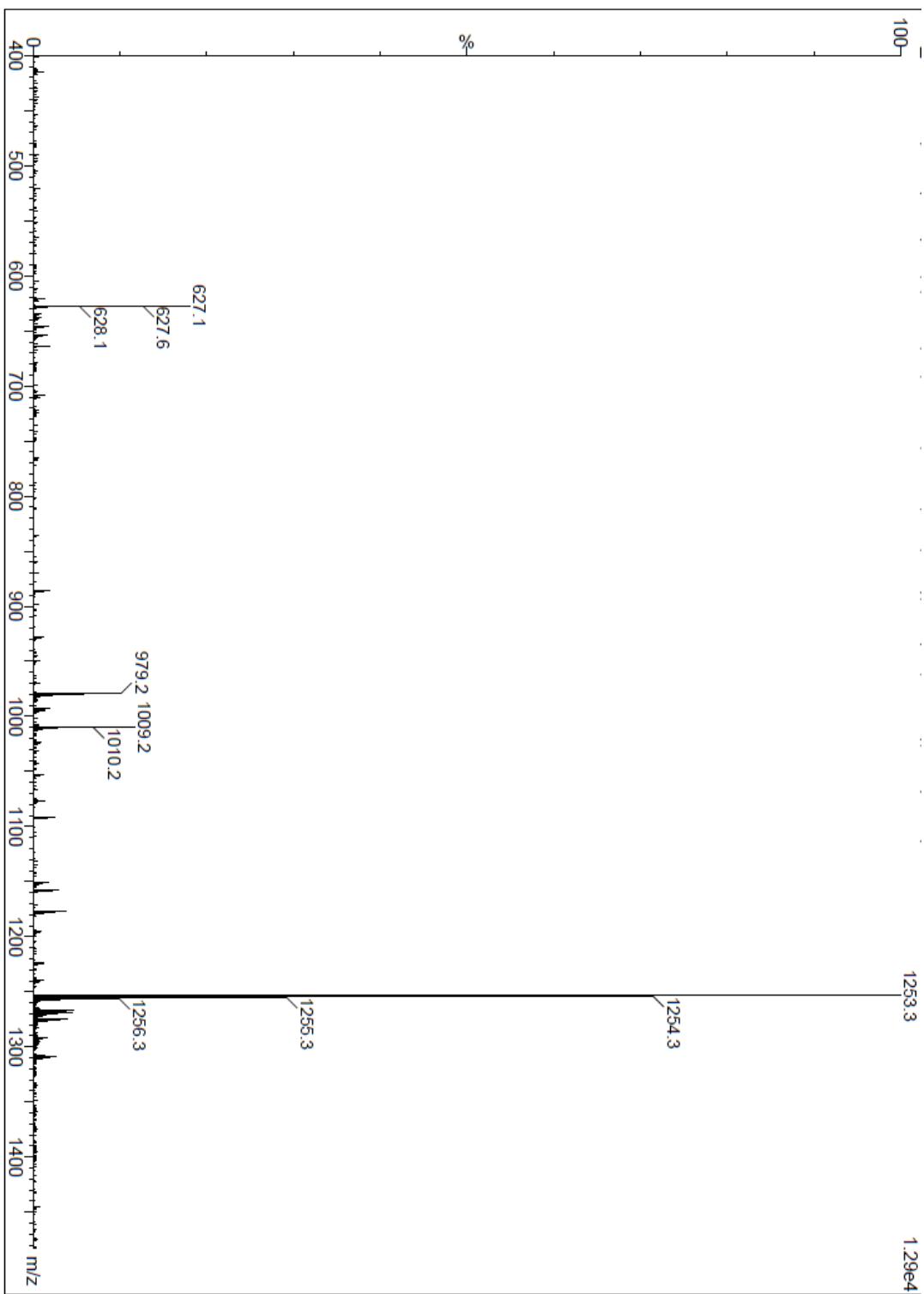
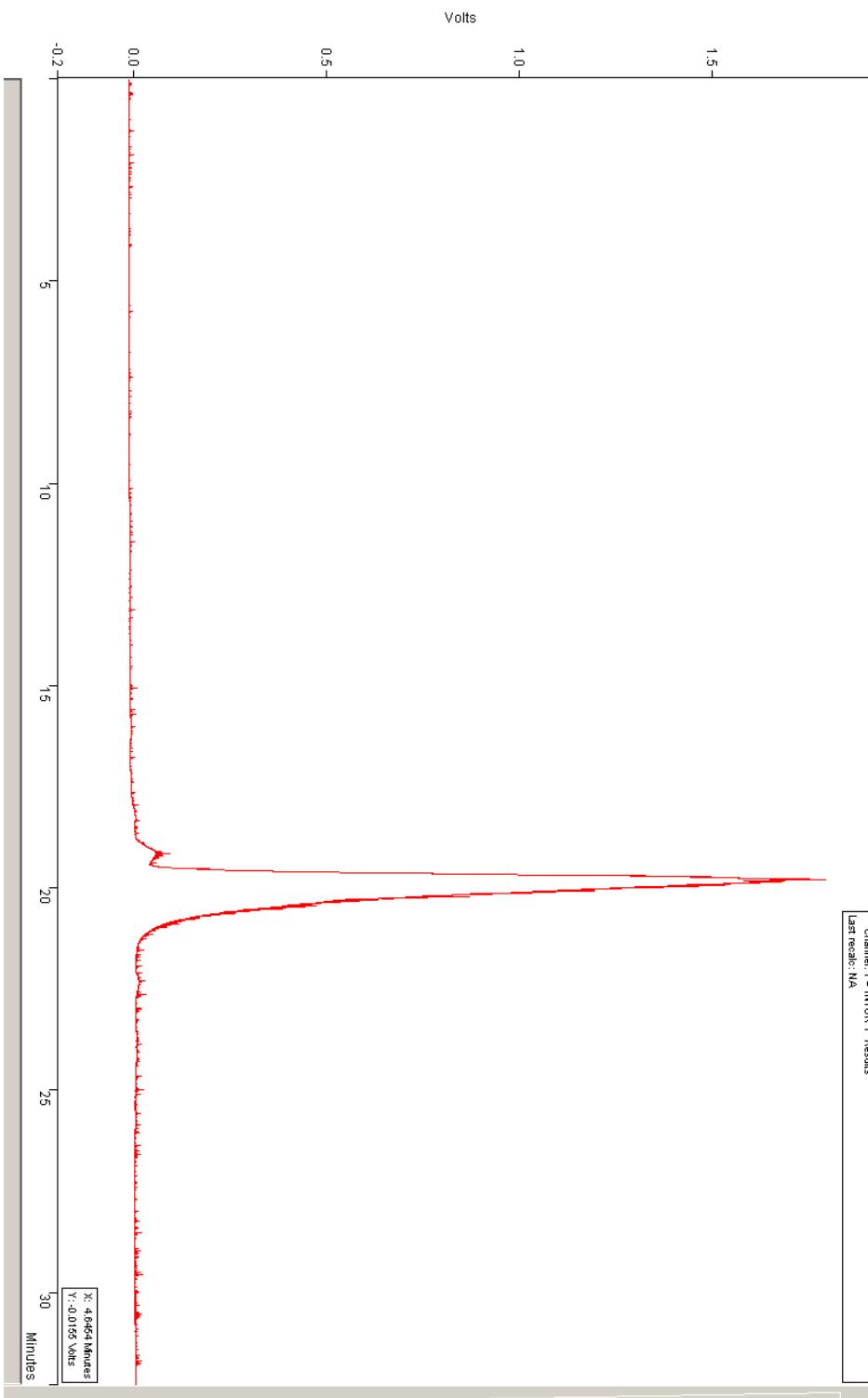


Fig.  $^1\text{H}$ -NMR of ADM-123.



**Fig.** ESI-MS of ADM-123.



**Fig.** RP-HPLC of ADM-123.

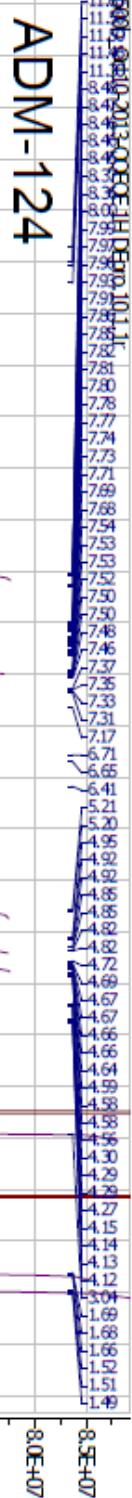
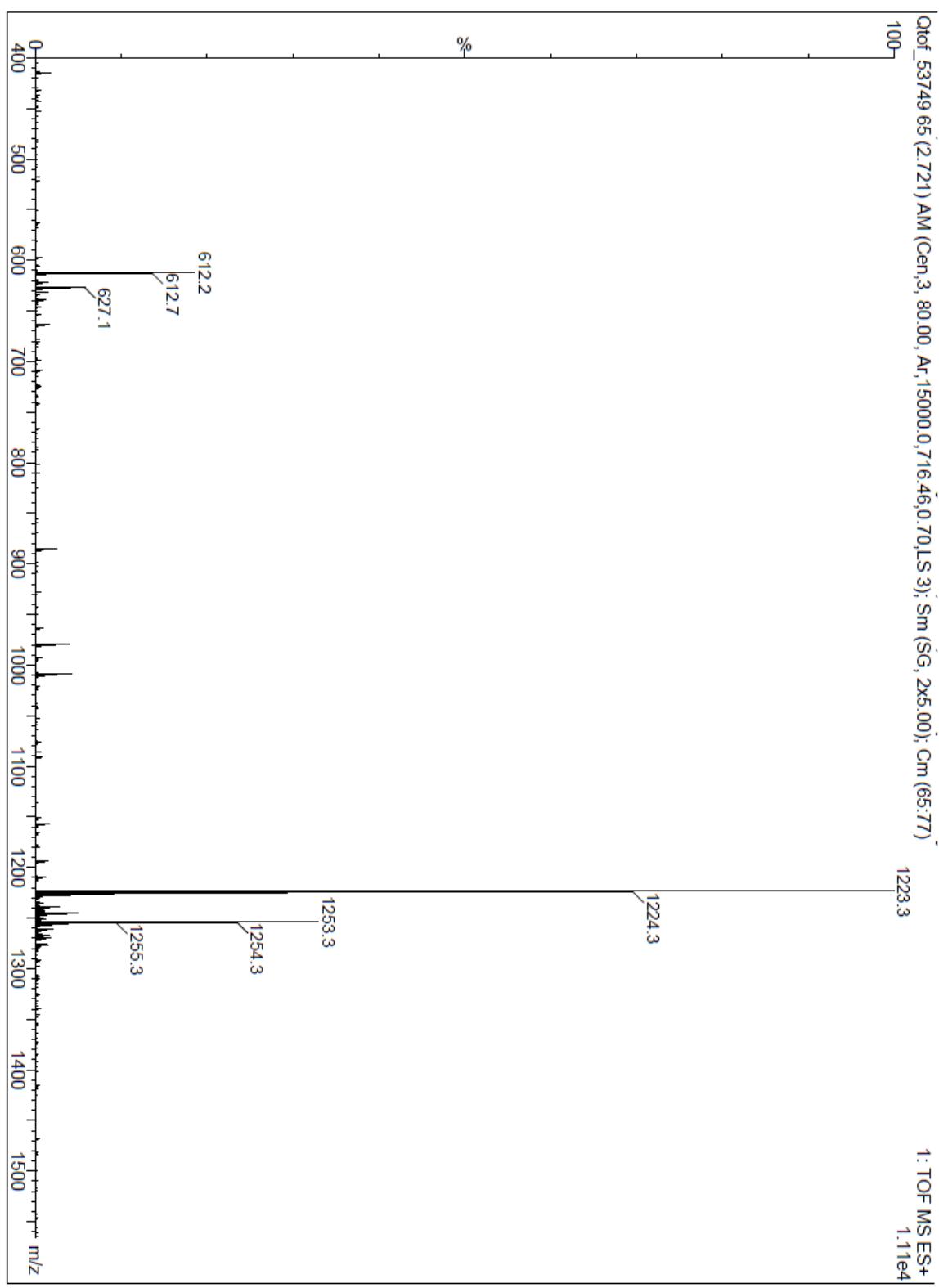
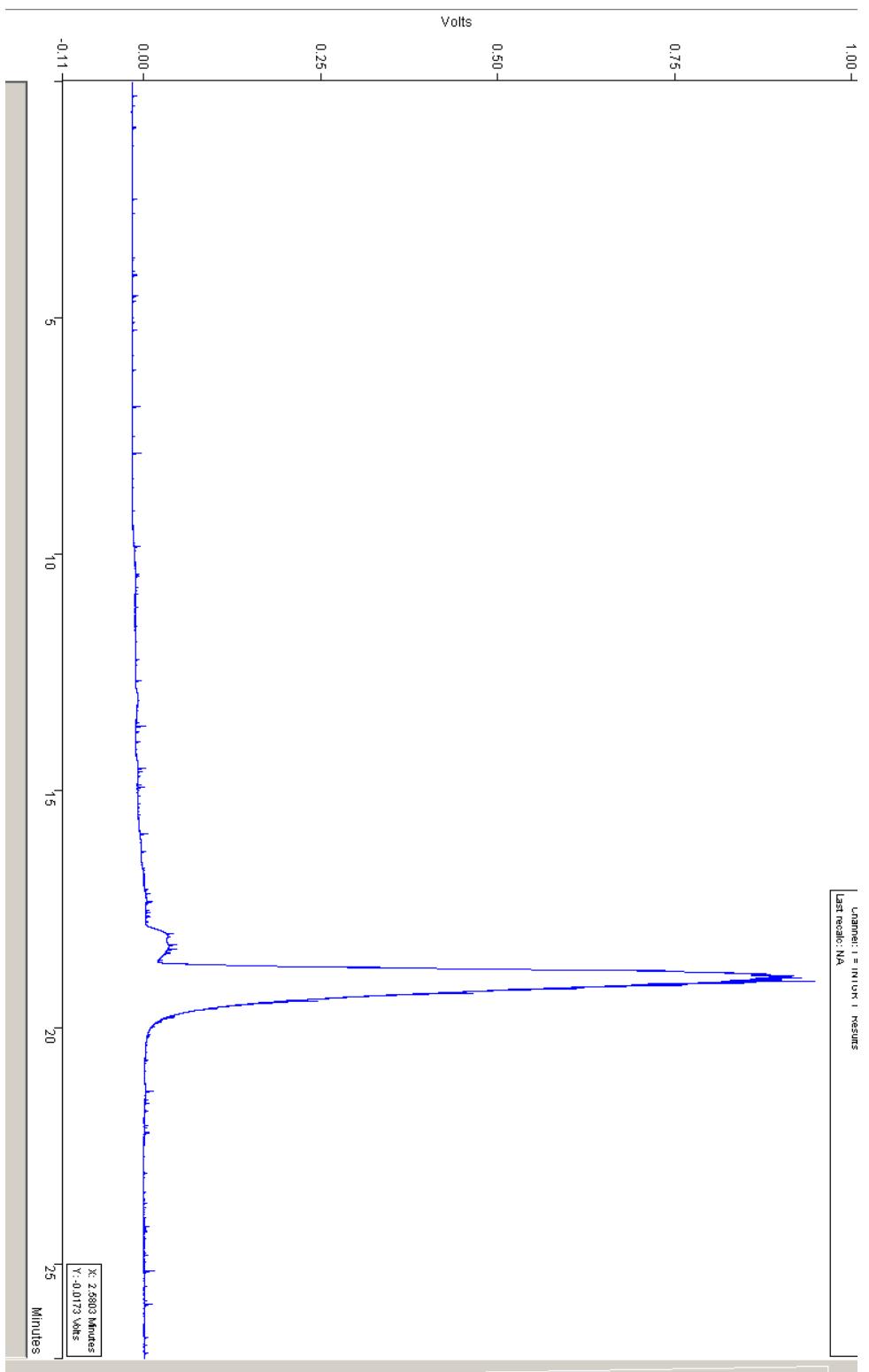


Fig.  $^1\text{H}$ -NMR of ADM-124.



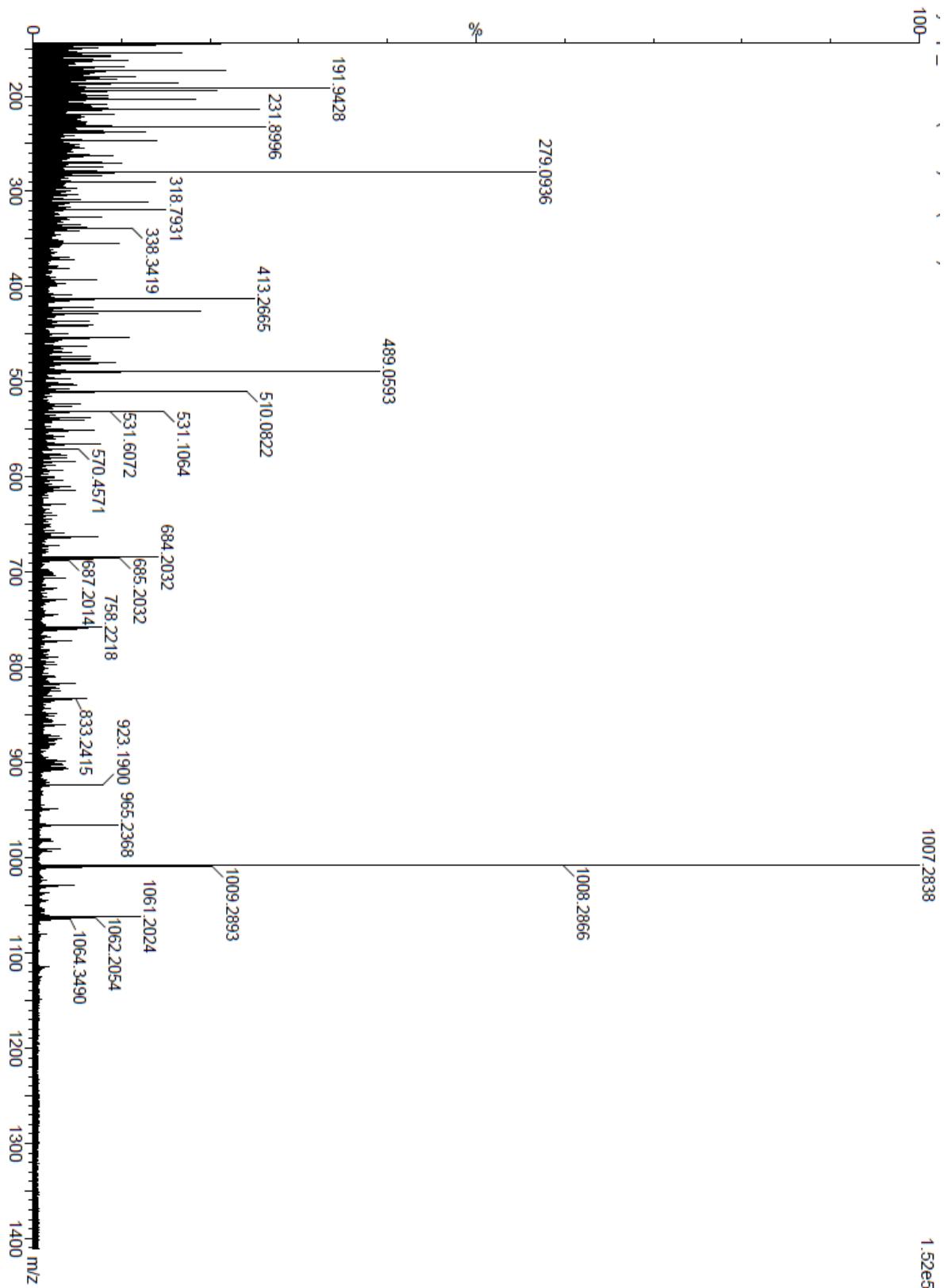
**Fig.** ESI-MS of ADM-124.



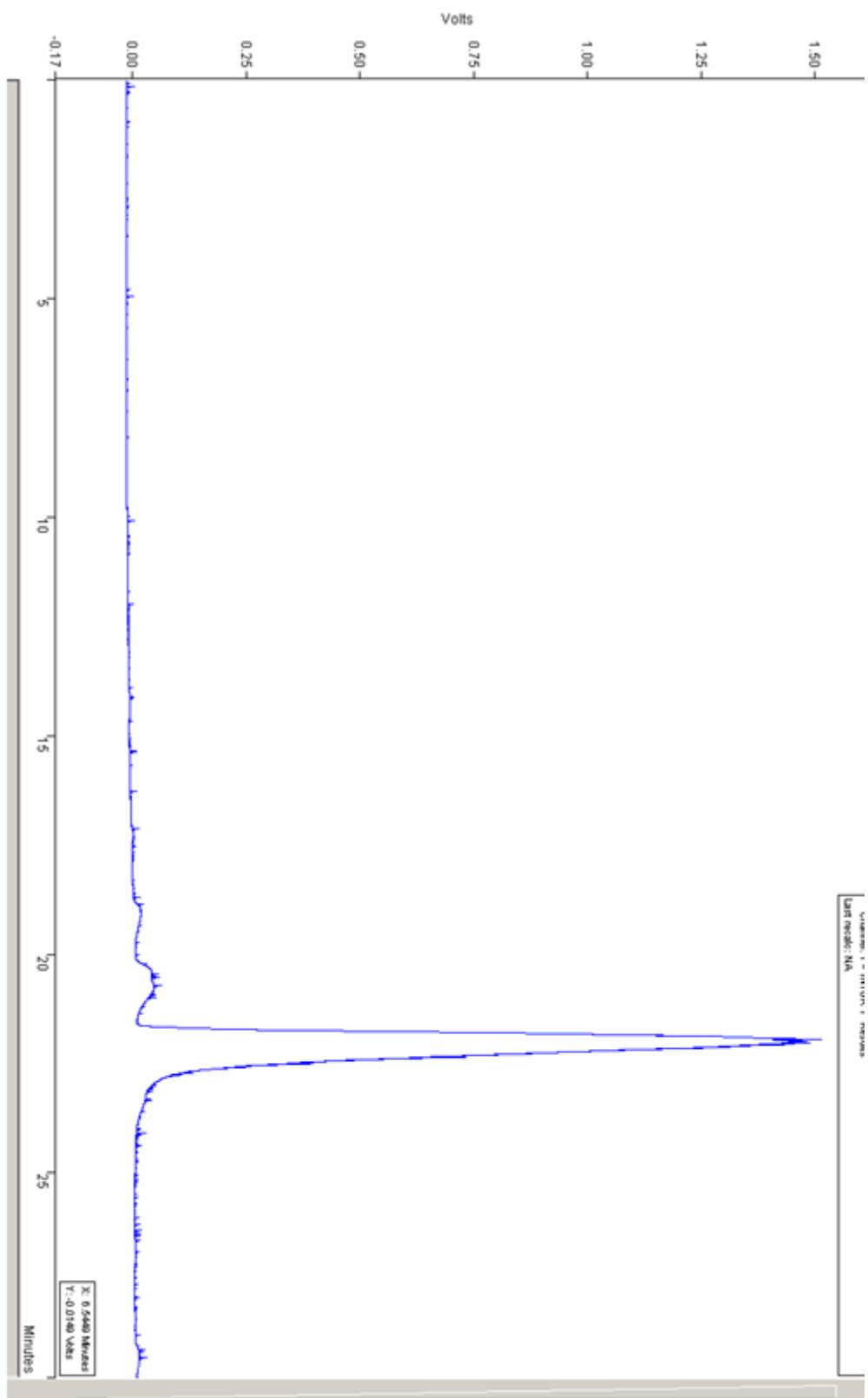
**Fig.** RP-HPLC of ADM-124.



Fig.  $^1\text{H}$ -NMR of ADM-129.



**Fig.** ESI-MS of ADM-129.



**Fig.** RP-HPLC of ADM-129.

# ADM-130

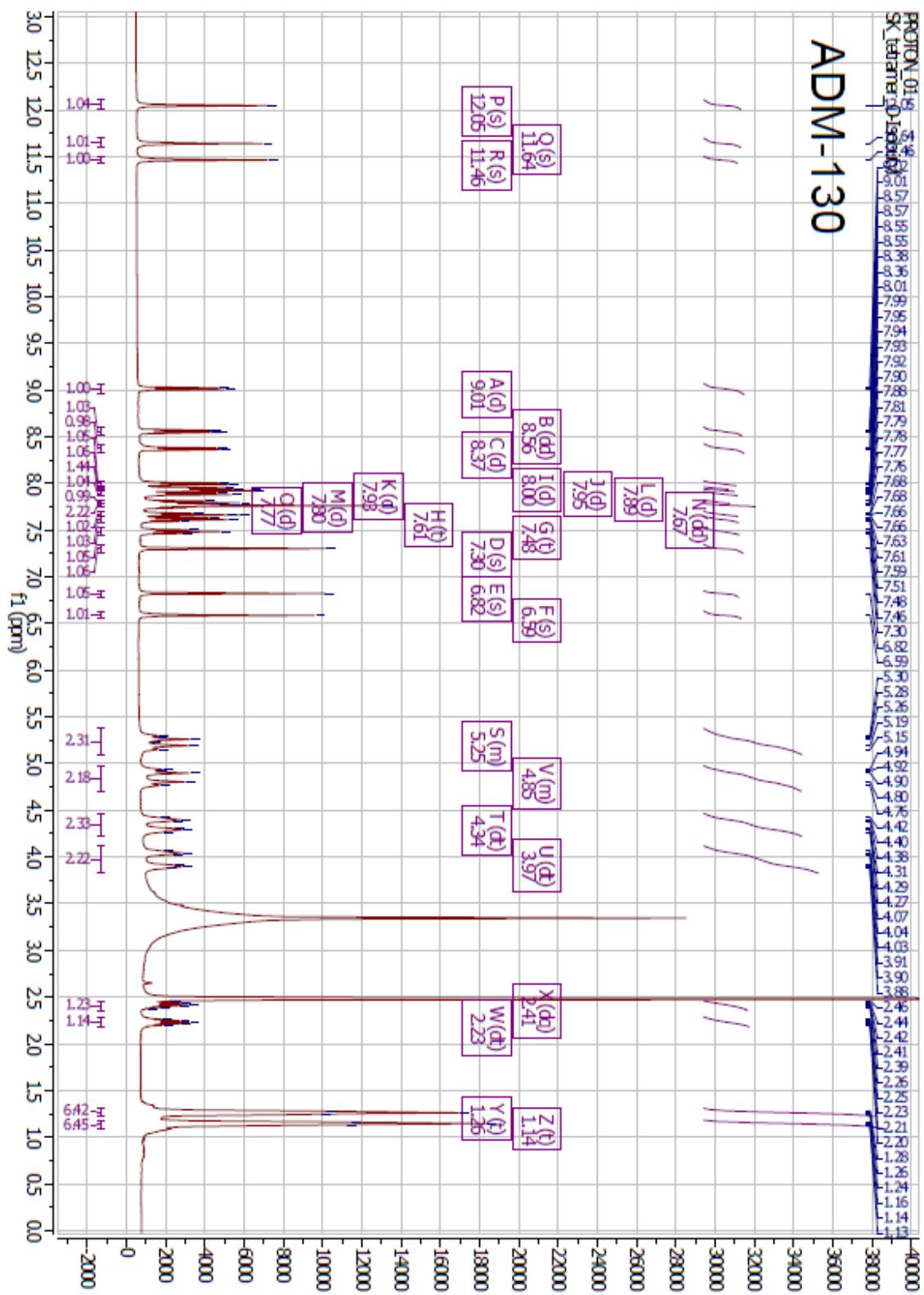
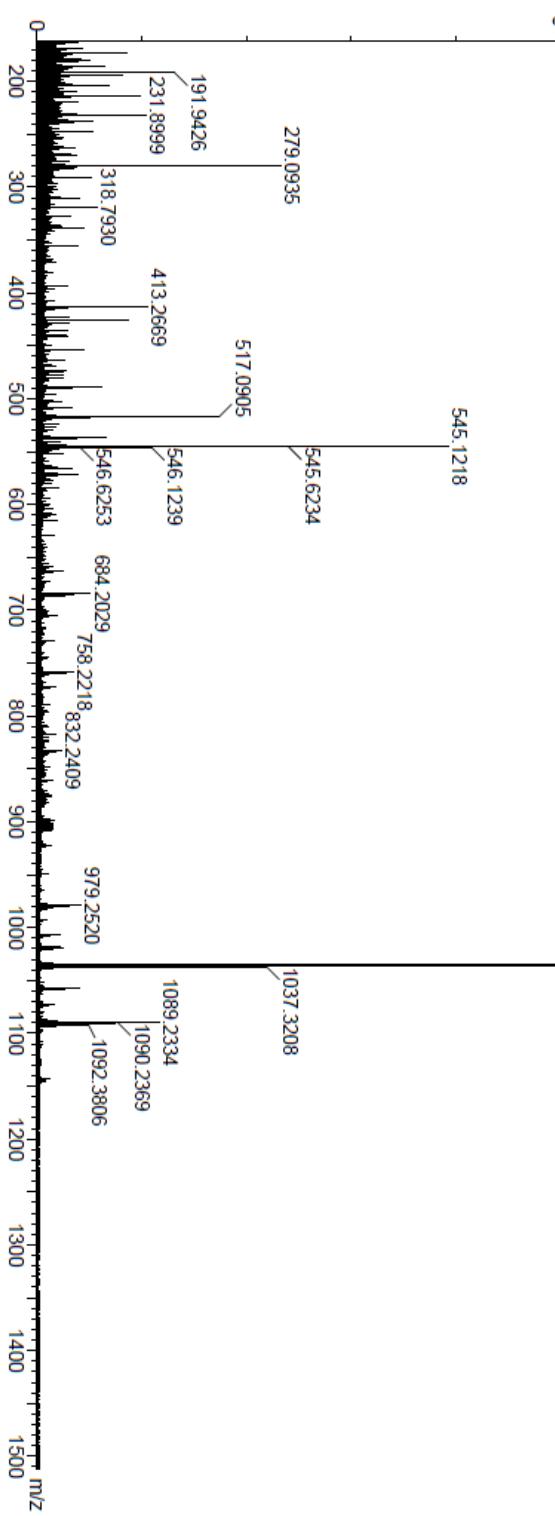


Fig. <sup>1</sup>H-NMR of ADM-130.

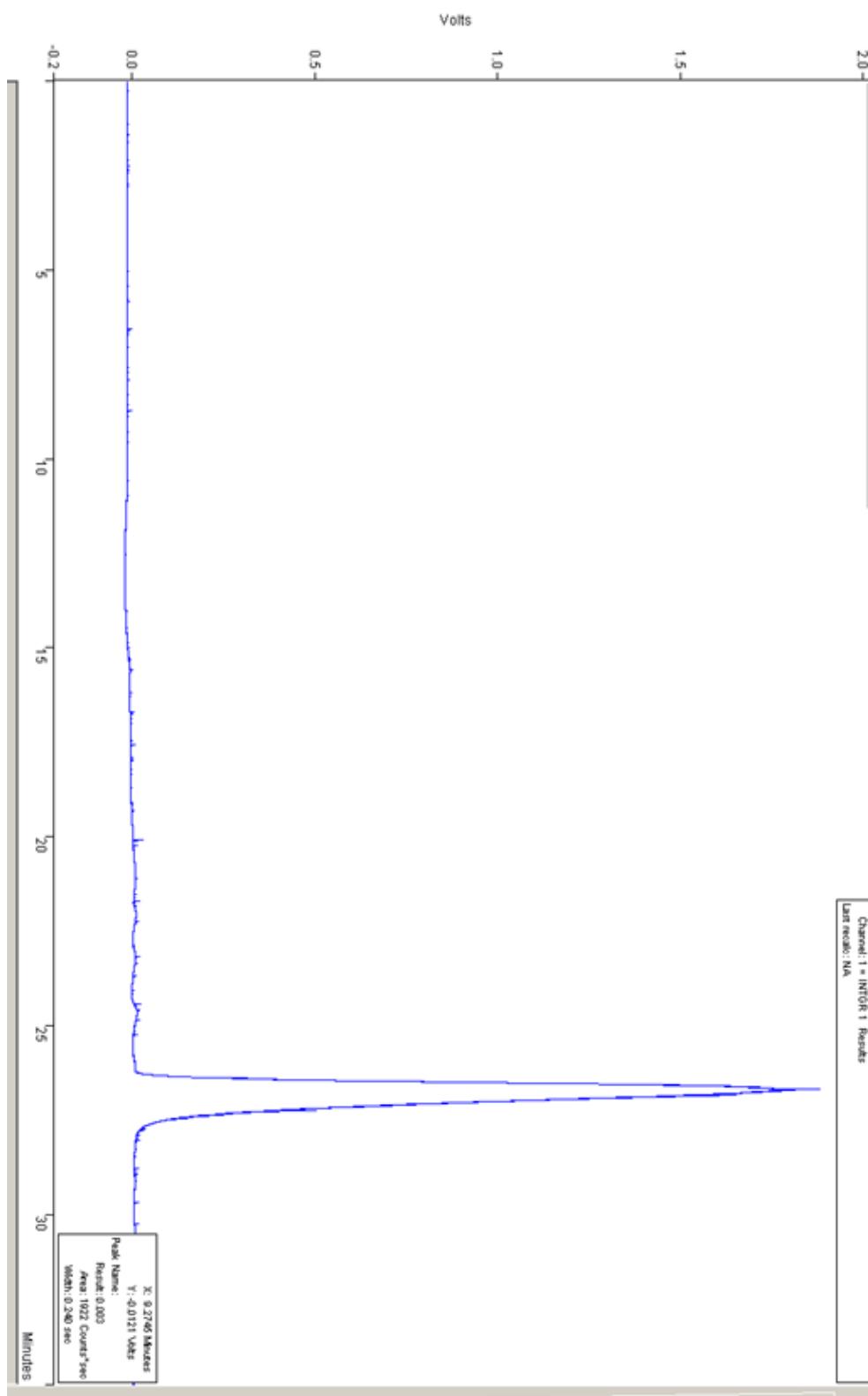
Syapt\_10867 (1.229) Cm (45.71)

1035.3151

1: TOF MS ES+  
5.32e5



**Fig.** ESI-MS of ADM-130.



**Fig.** RP-HPLC of ADM-130.

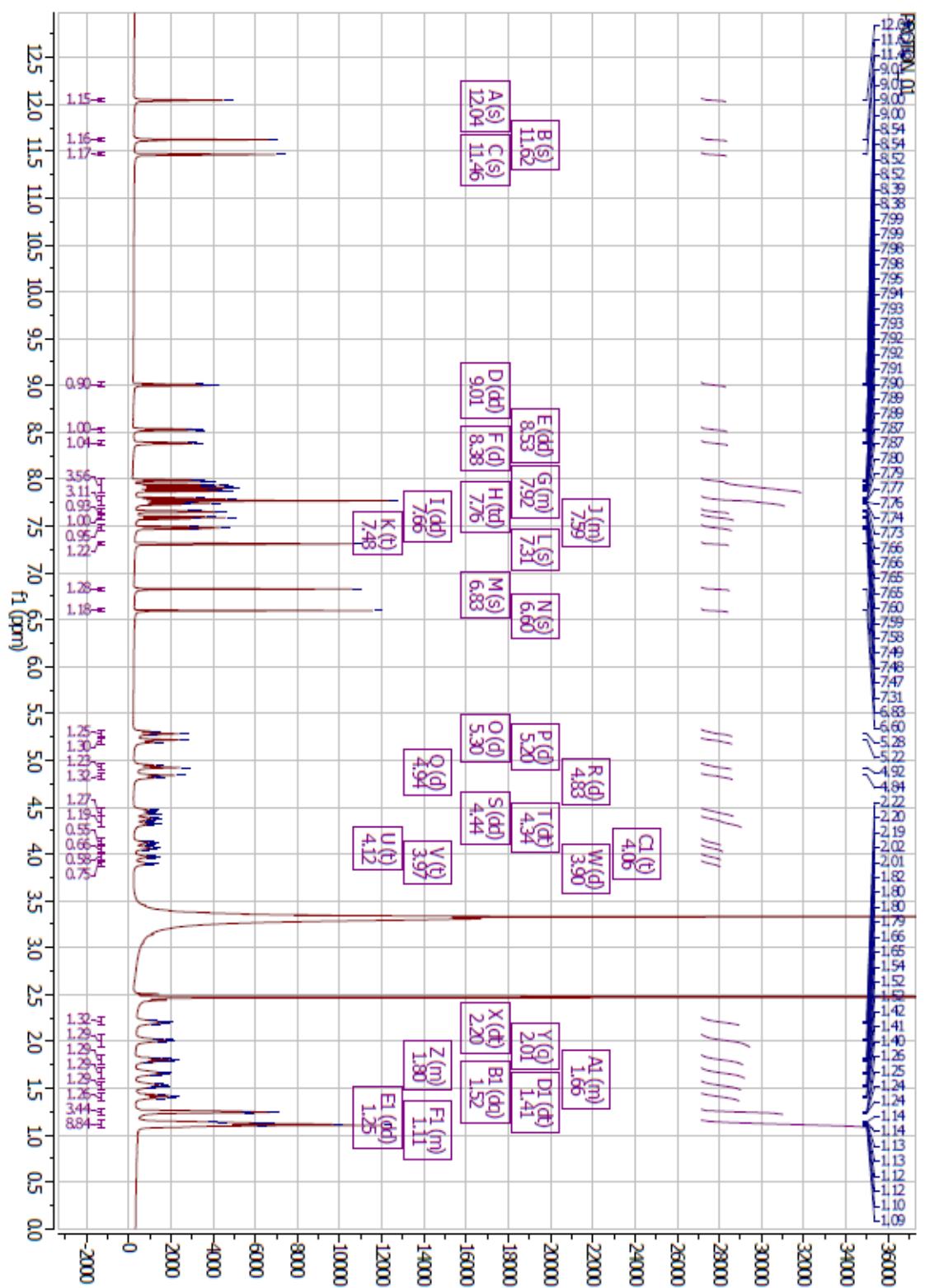
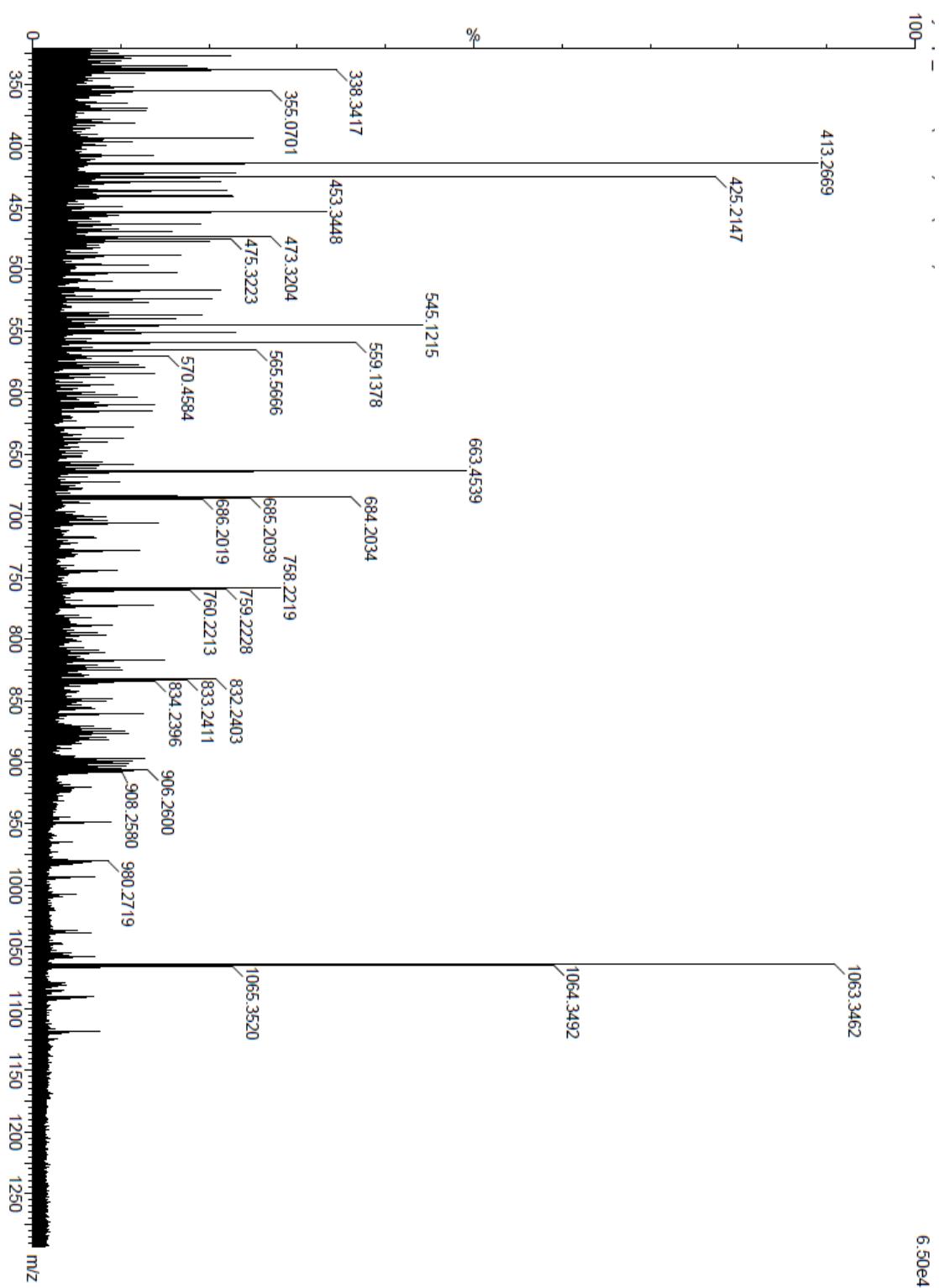
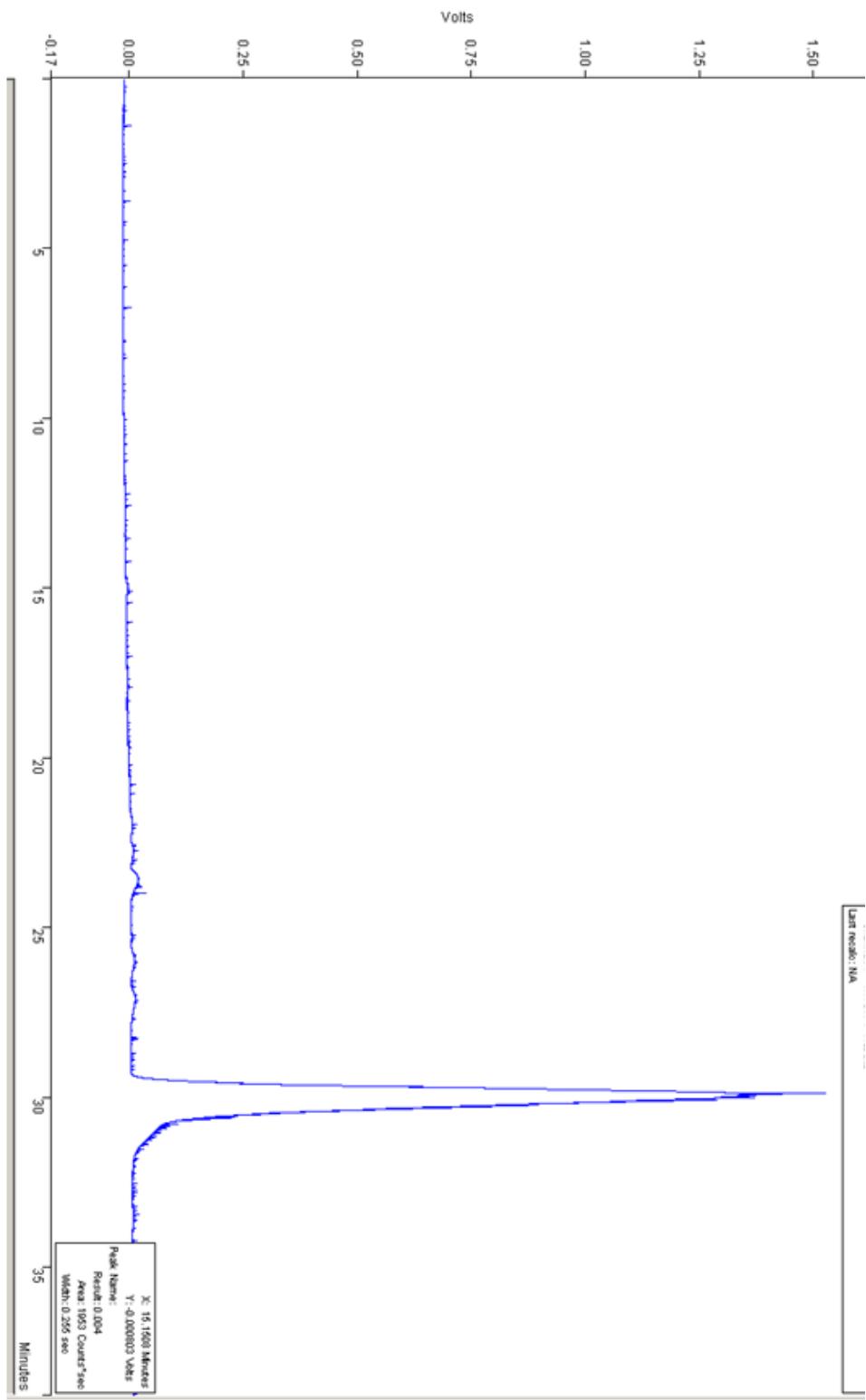


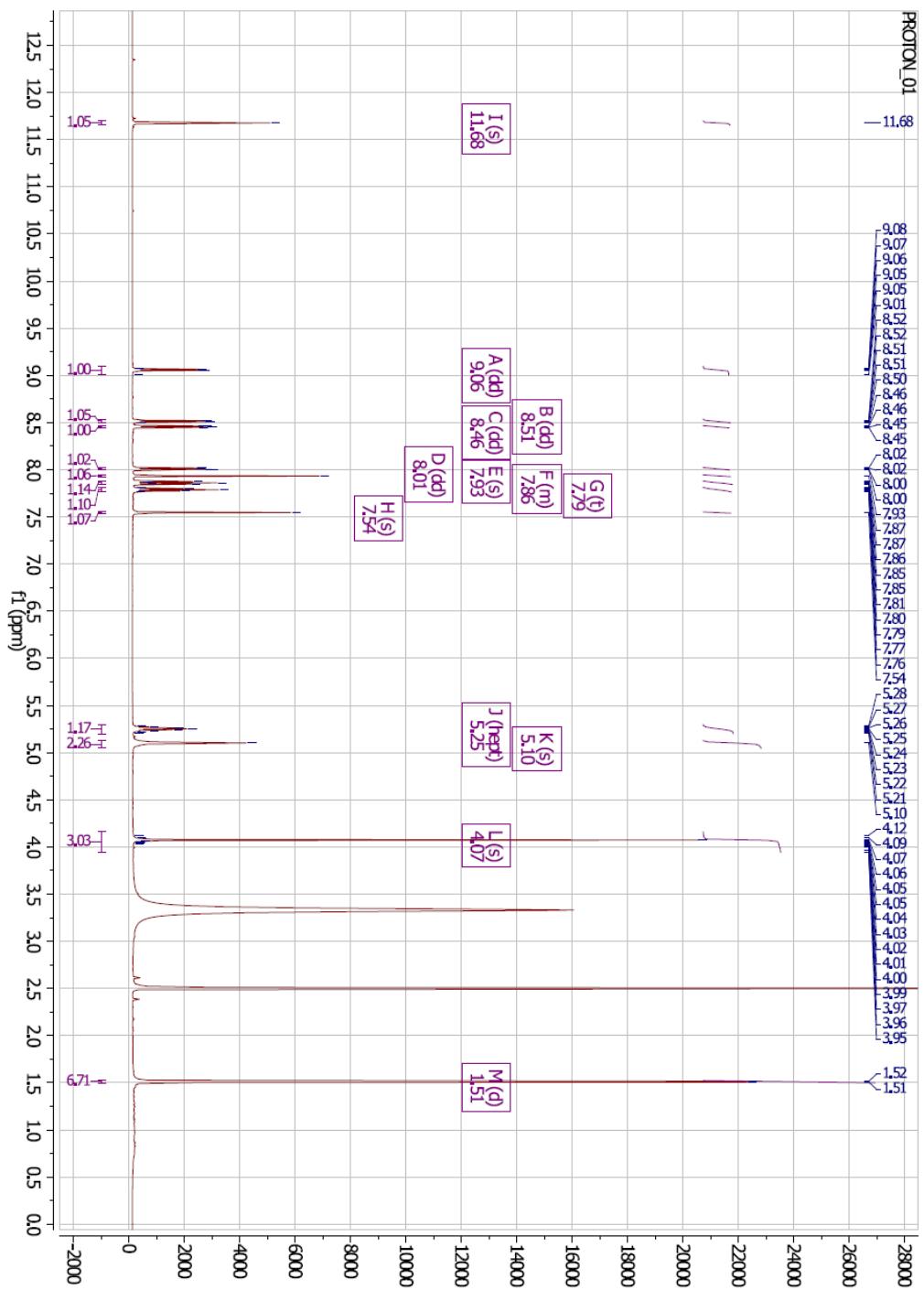
Fig.  $^1\text{H}$ -NMR of ADM-131.



**Fig.** ESI-MS of ADM-131.



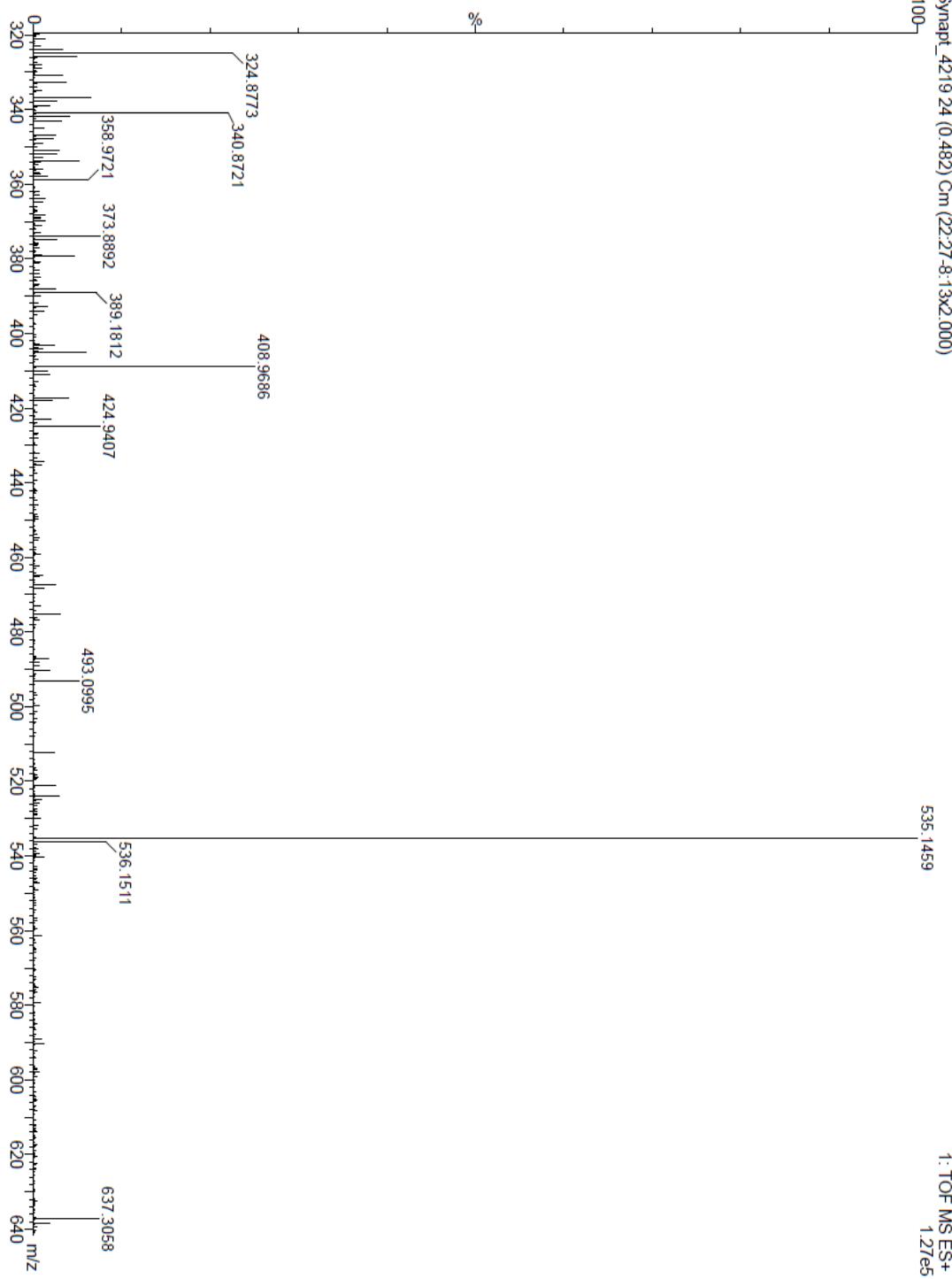
**Fig.** RP-HPLC of ADM-131.



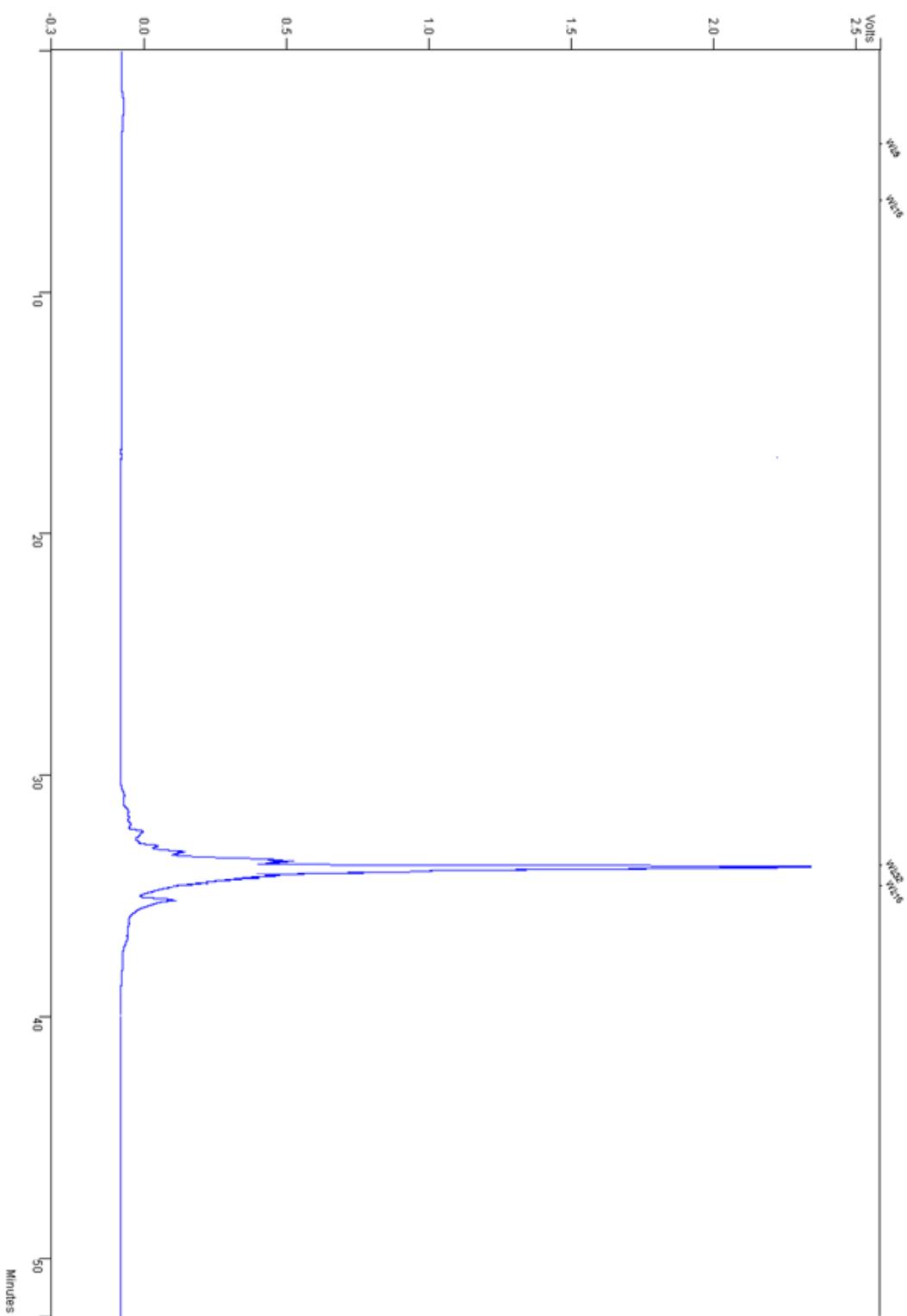
**Fig.**  $^1\text{H}$ -NMR of ADM-135.

Kumar, Sunil ADM-135  
Synapt\_4219 24 (0.482) Cm (22:27:8:13x2.000)

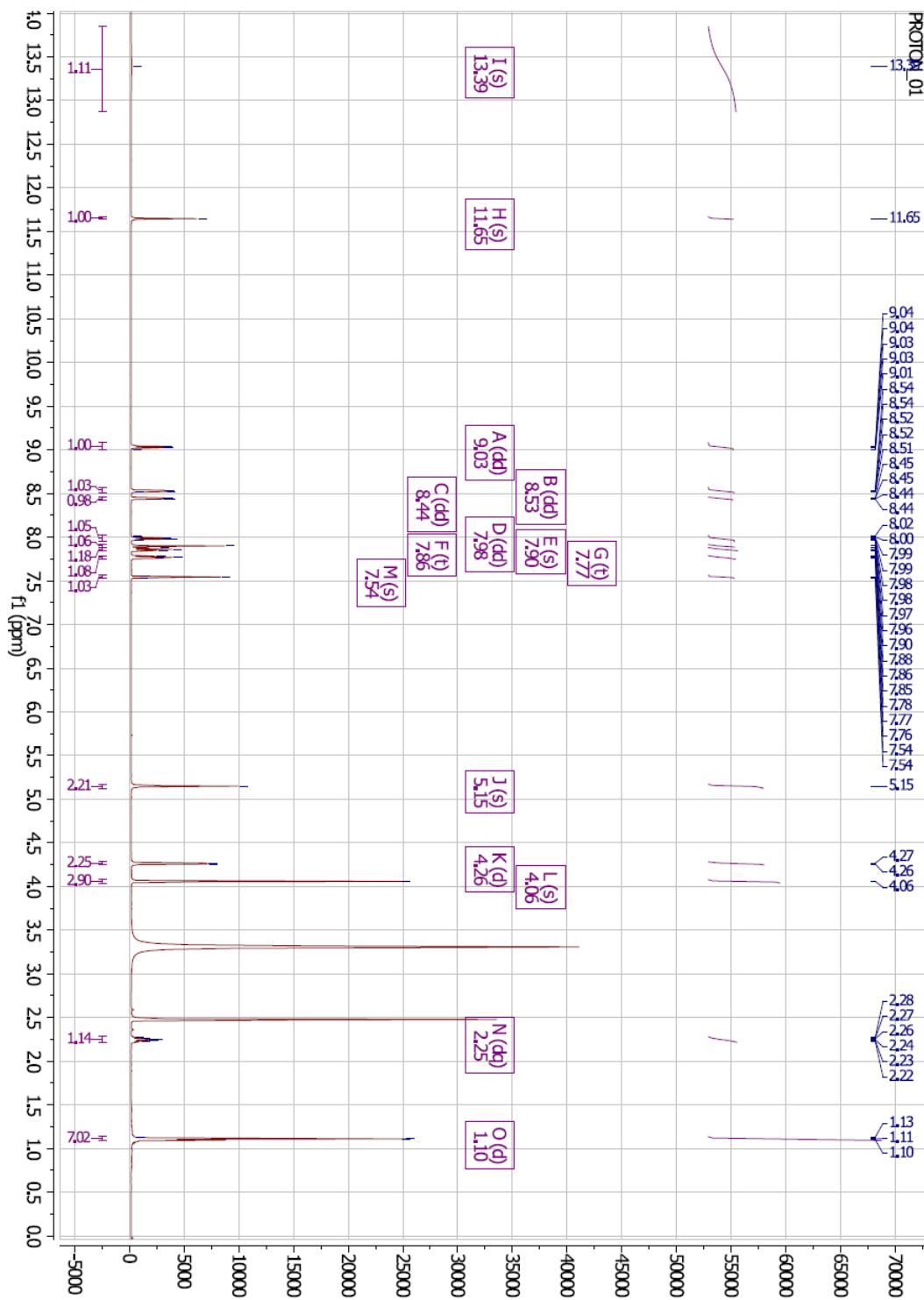
SYNAPT G2-S#UGA305  
1: TOF MSE<sub>S+</sub>  
1.27e5



**Fig.** ESI-MS of ADM-135.



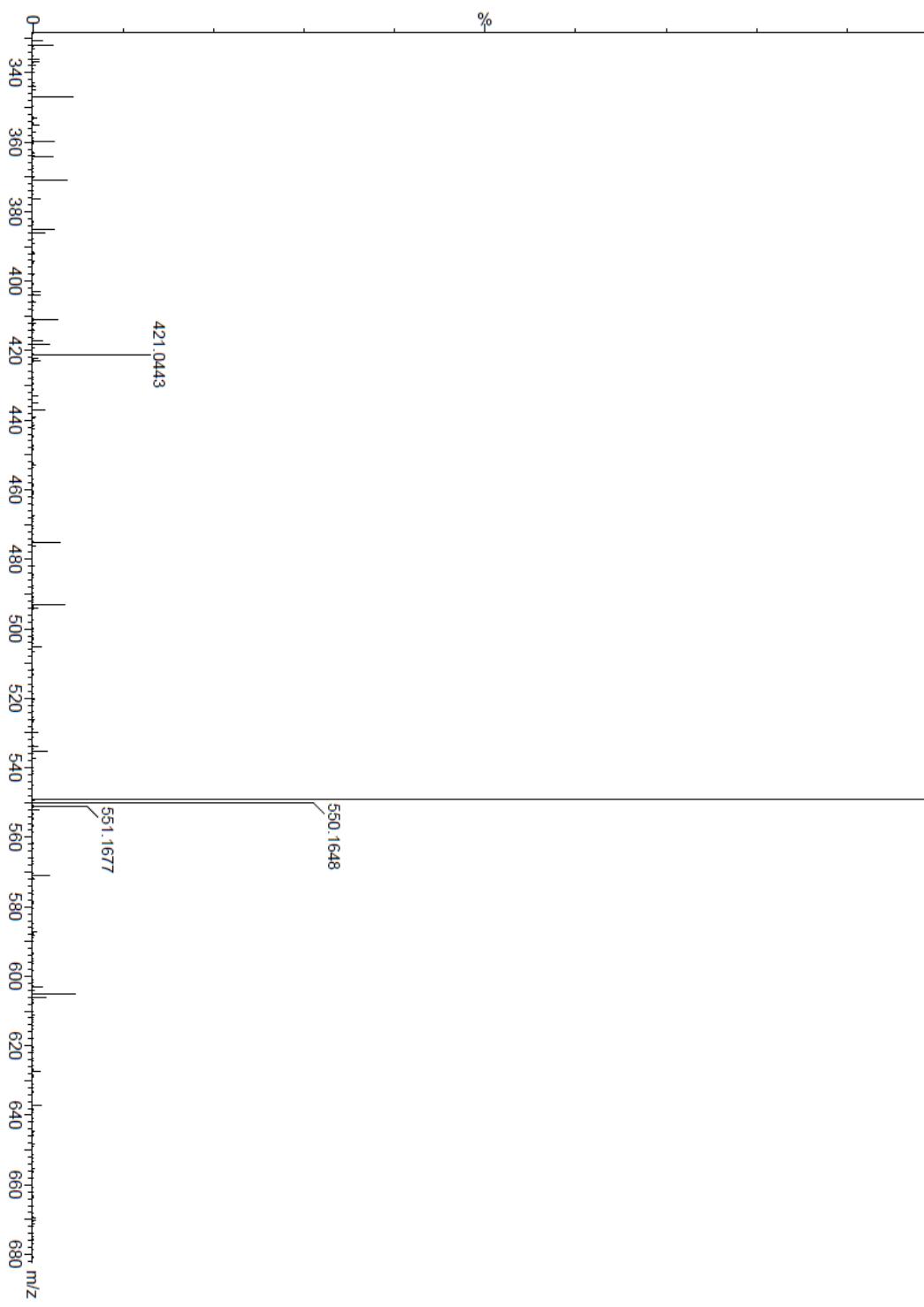
**Fig.** RP-HPLC of ADM-135.



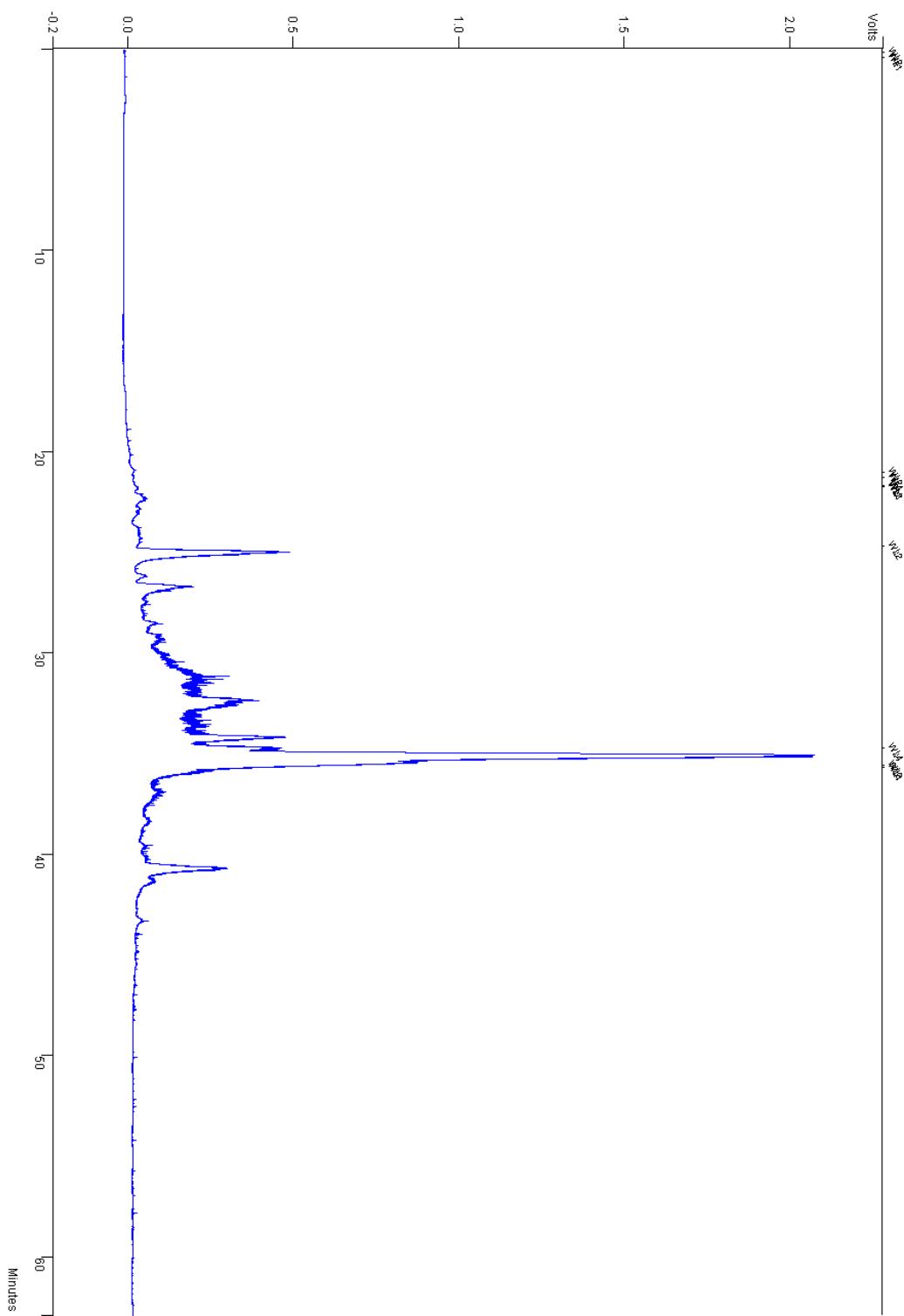
**Fig.**  $^1\text{H}$ -NMR of ADM-136.

Kumar, Sunil ADM-136  
Synapt\_4220 23 (0.465) Cm (22.27.6.13x2.000)

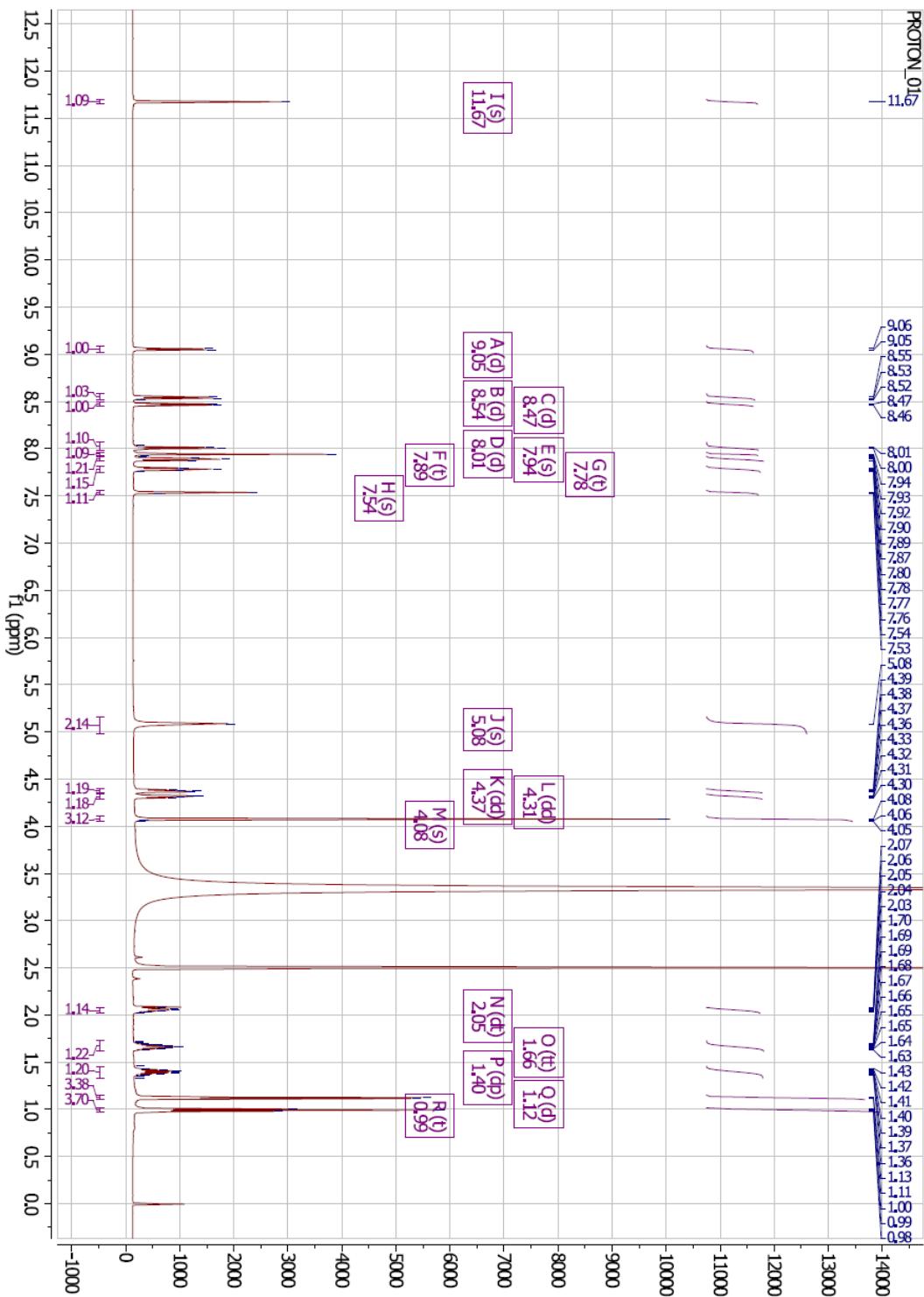
SYNAPTG2-Si#UGA305  
1: TOF MS ES+  
3.80e5



**Fig.** ESI-MS of ADM-136.



**Fig.** RP-HPLC trace of ADM-136.

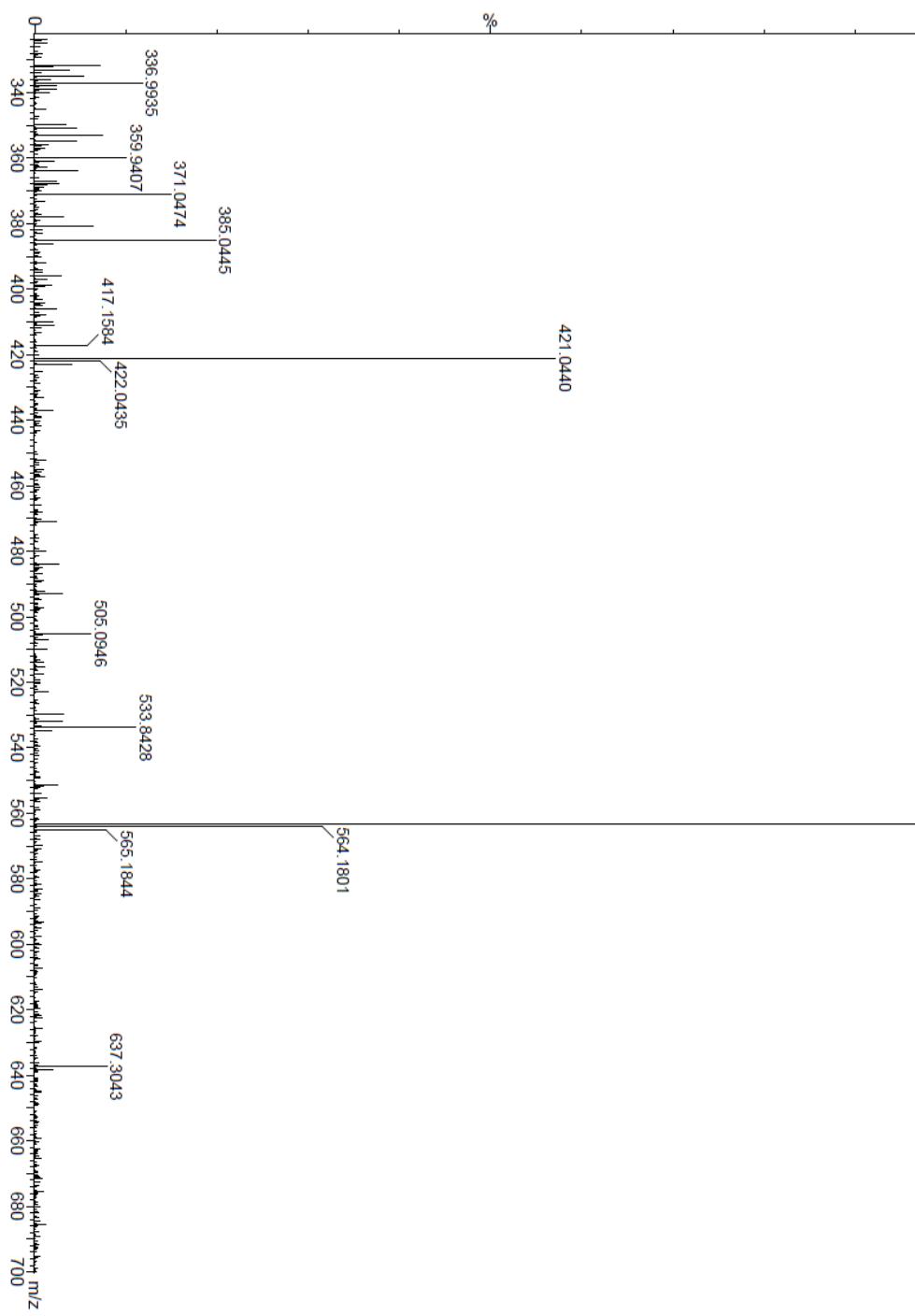


**Fig.** <sup>1</sup>H-NMR of ADM-137.

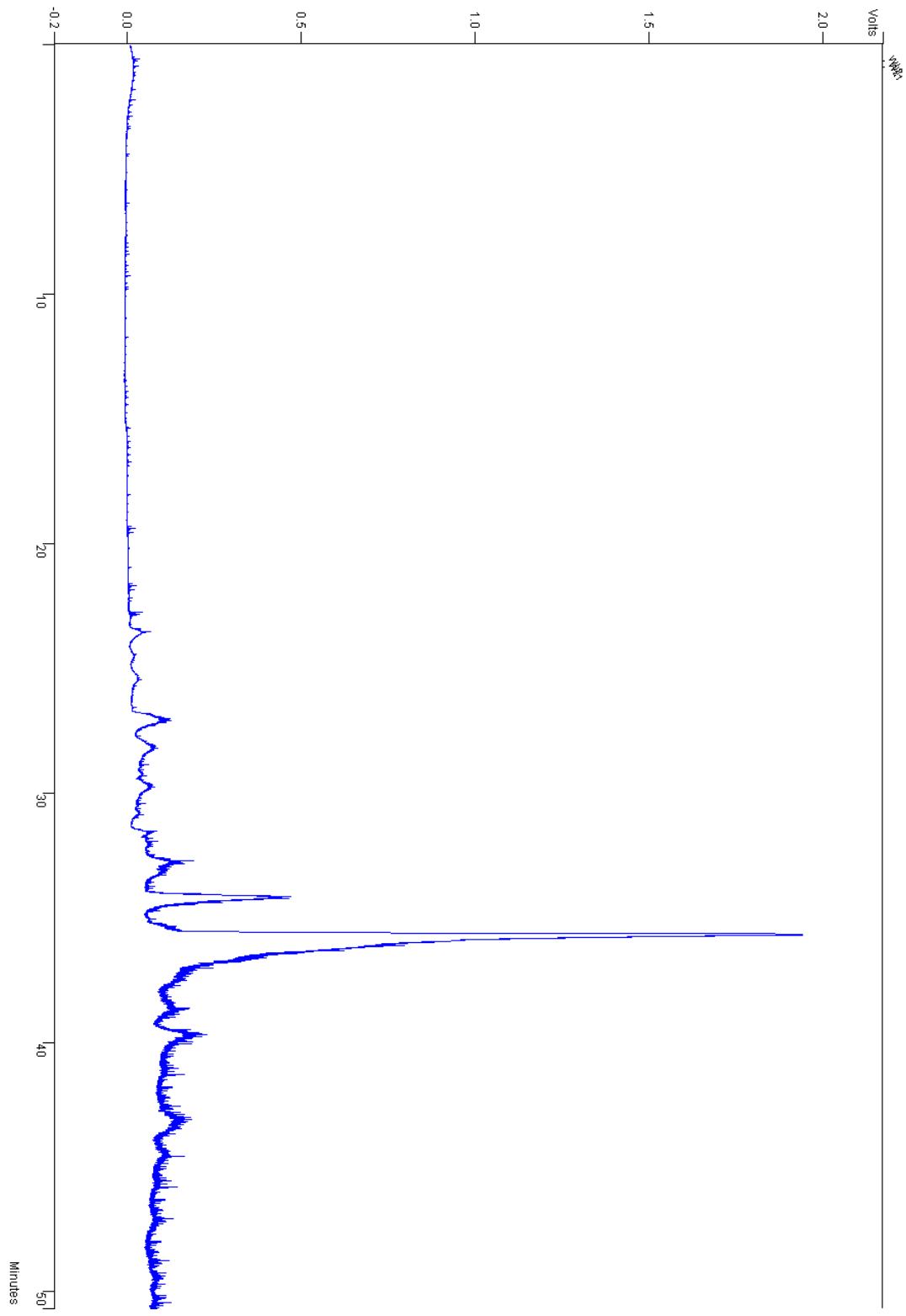
Kumar\_Sunil ADM-137  
Synapt\_4221 24 (0.482) Cm (24:28:6:10x2,000)

563.1769

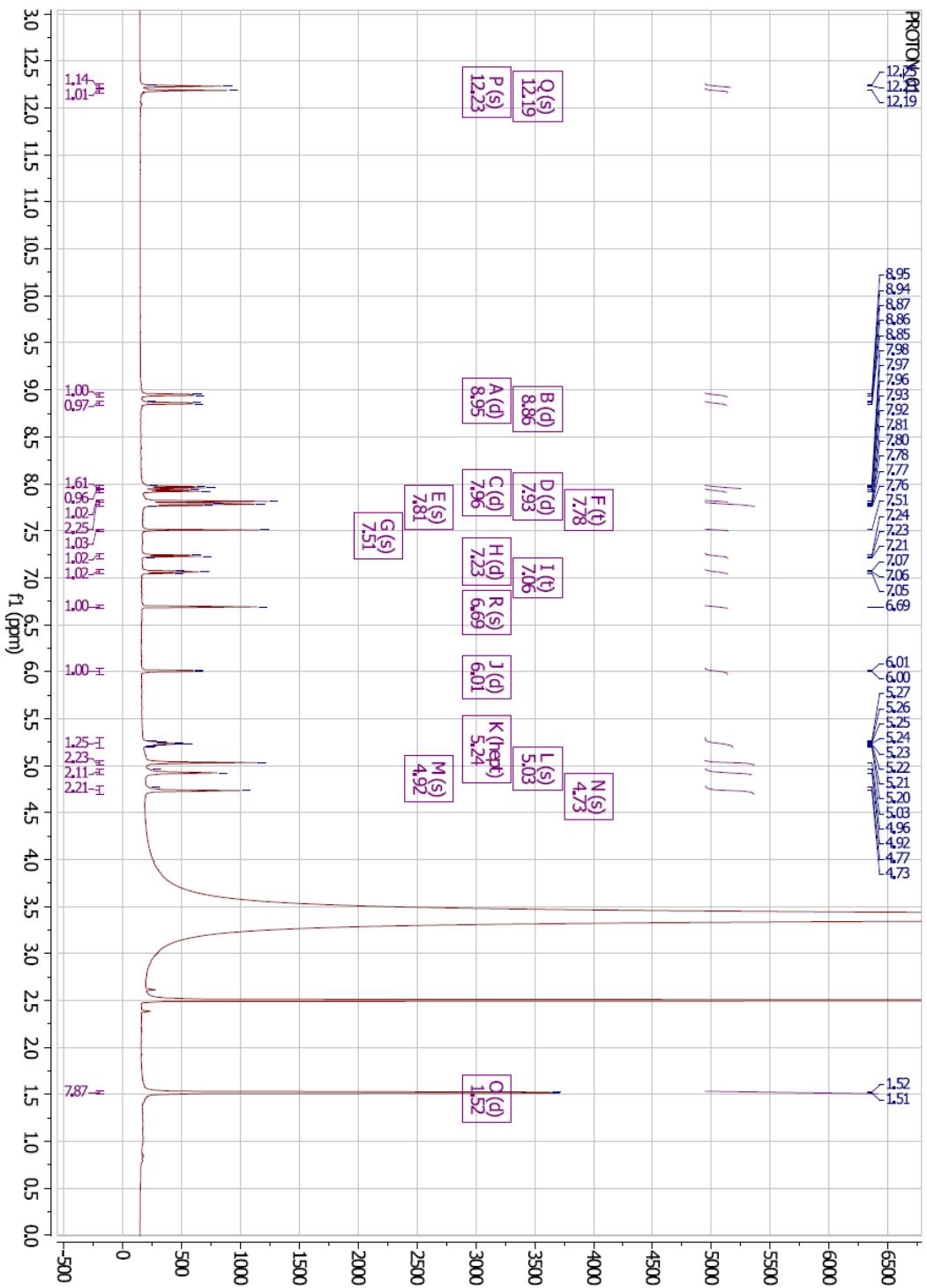
SYNAPTOG2-SI#UGA305  
1: TOF MS ES+  
6.71e4



**Fig.** ESI-MS of ADM-137.



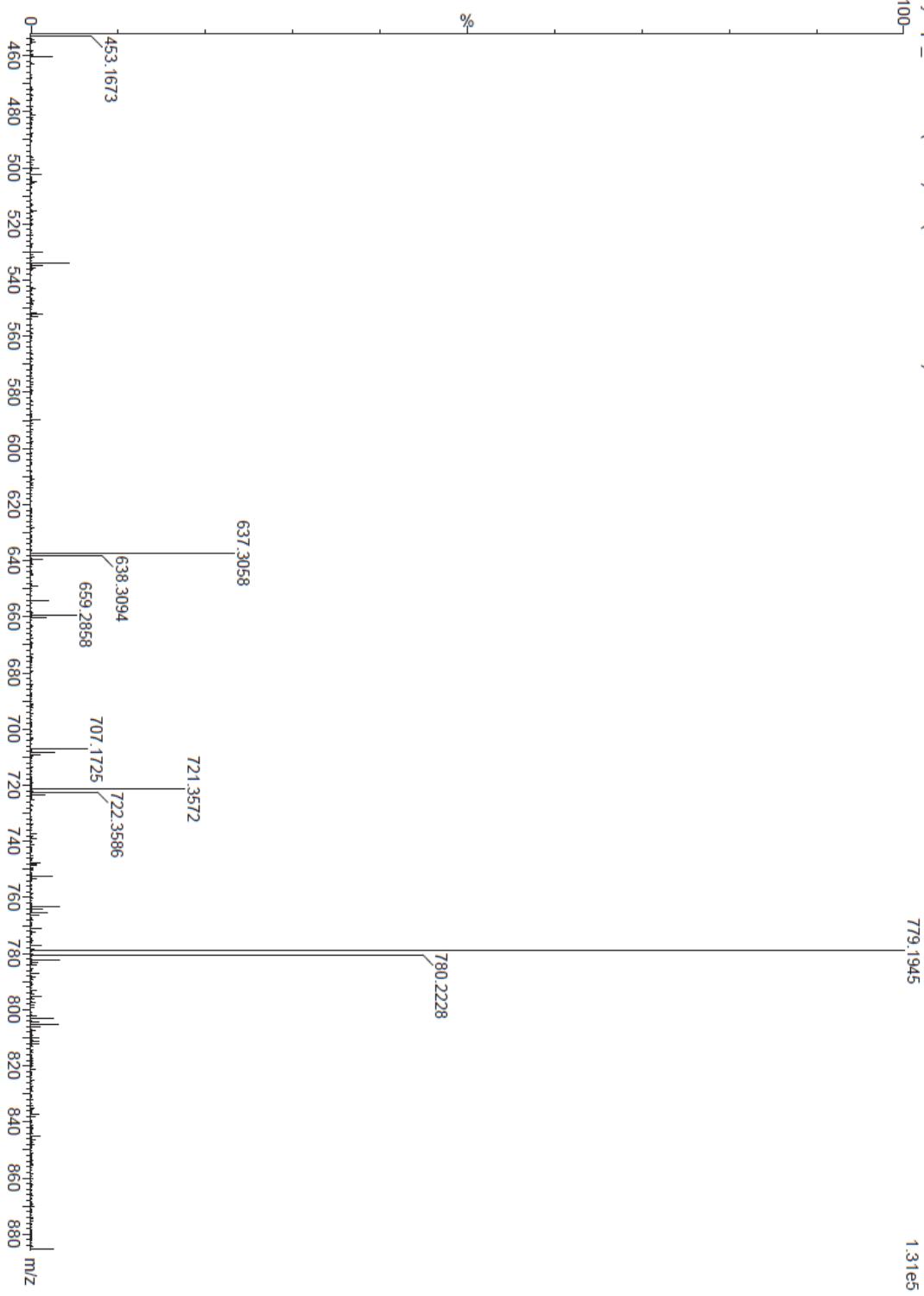
**Fig.** RP-HPLC of ADM-137.



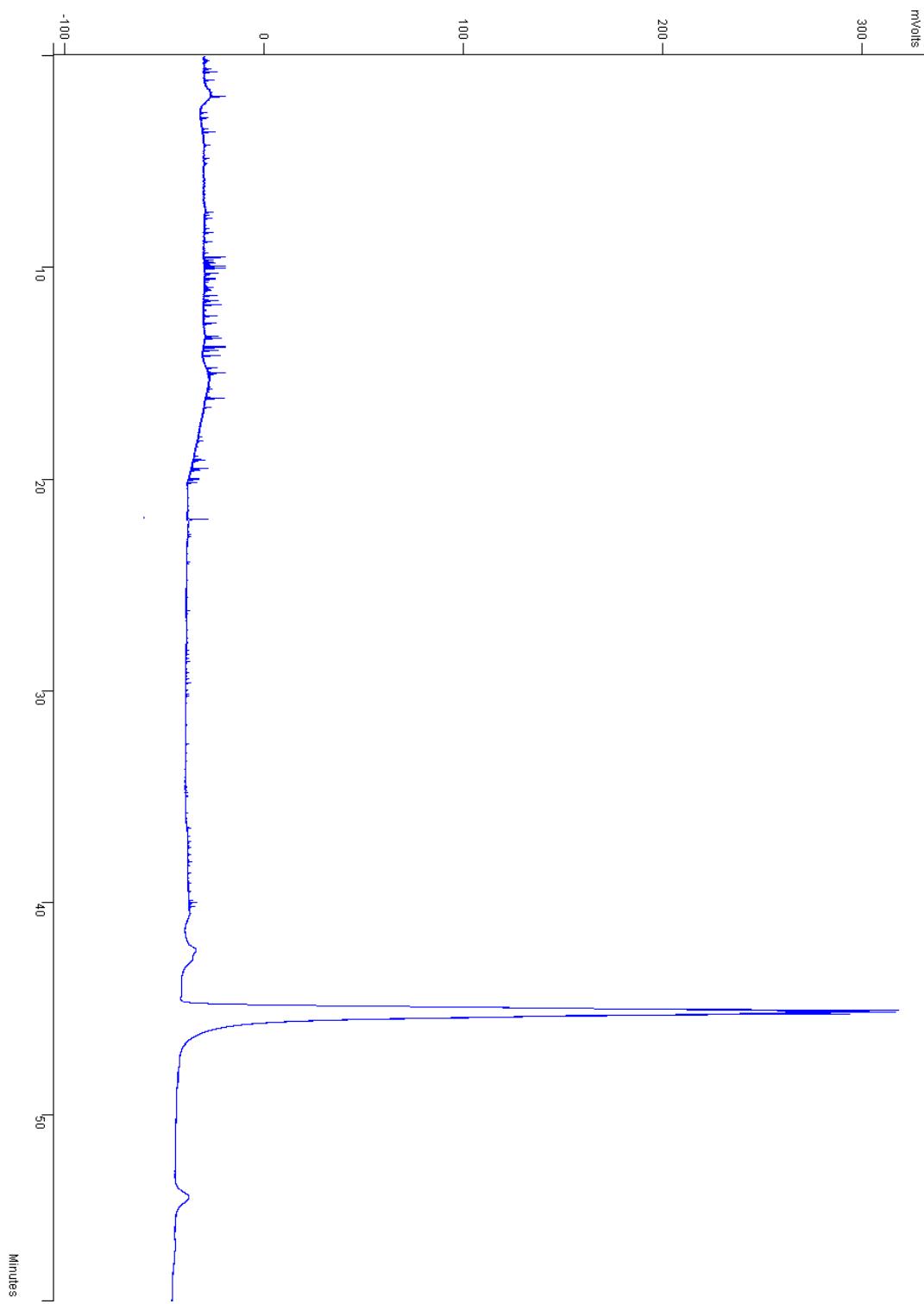
**Fig.**  $^1\text{H}$ -NMR of ADM-138.

Kumar, Sunil ADM-138  
Synapt\_4222a 24 (0.482) Cm (24:25:9:12:2.000)  
779.1945

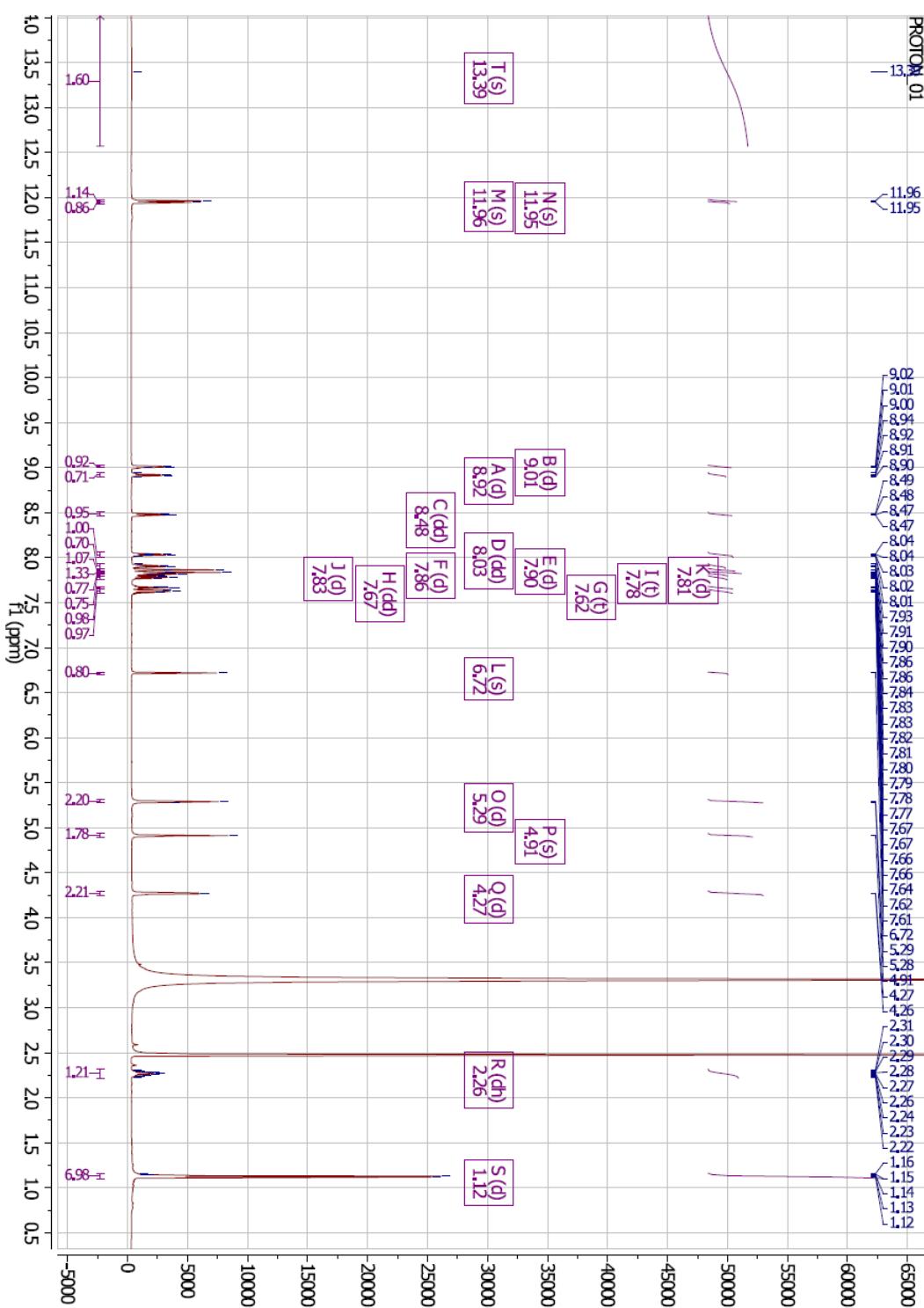
SYNAPTG2-S#UGA305  
1: TOF MS ES+  
1.31e5



**Fig.** ESI-MS of ADM-138.



**Fig.** RP-HPLC of ADM-138.

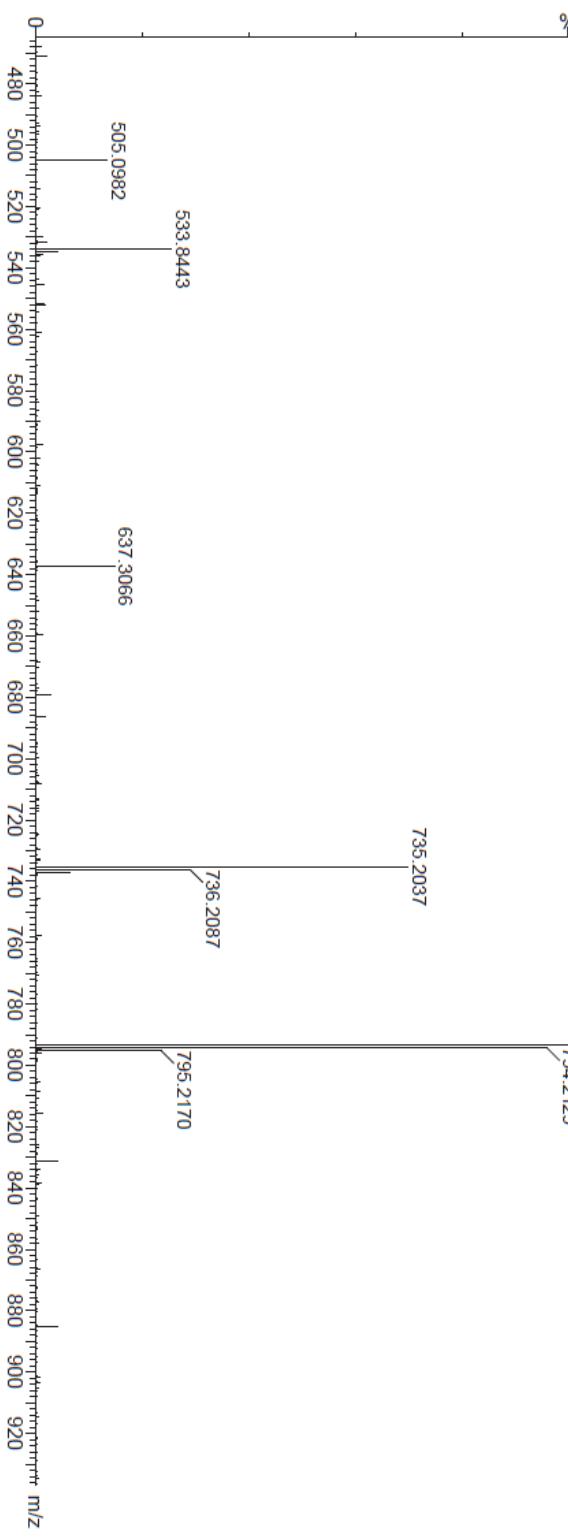


**Fig.**  $^1\text{H}$ -NMR of ADM-139.

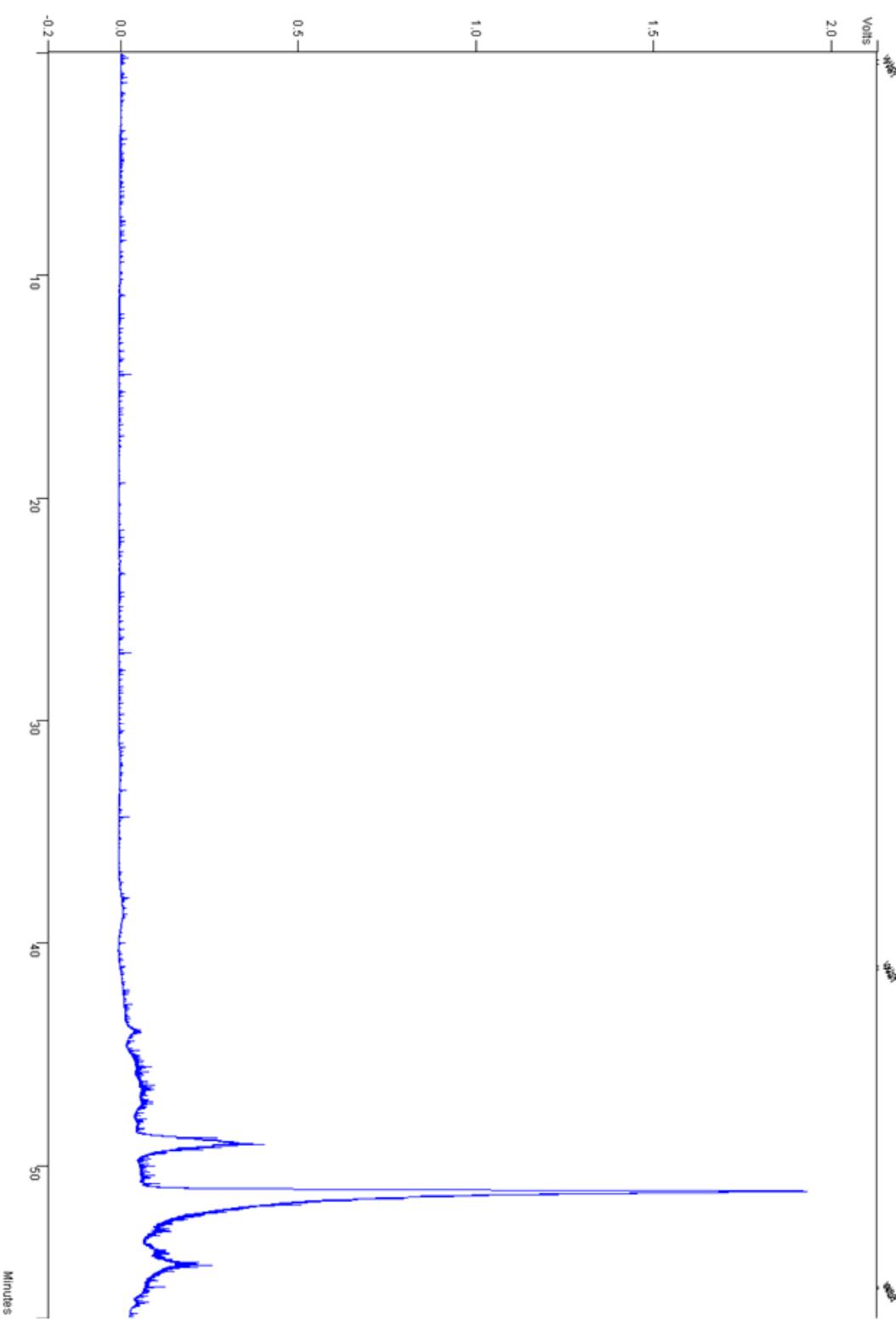
Kumar, Sunil ADM-139  
Synapt\_4223 23 (0.465) Cm (22.26.5:13x2.000)

793.2102

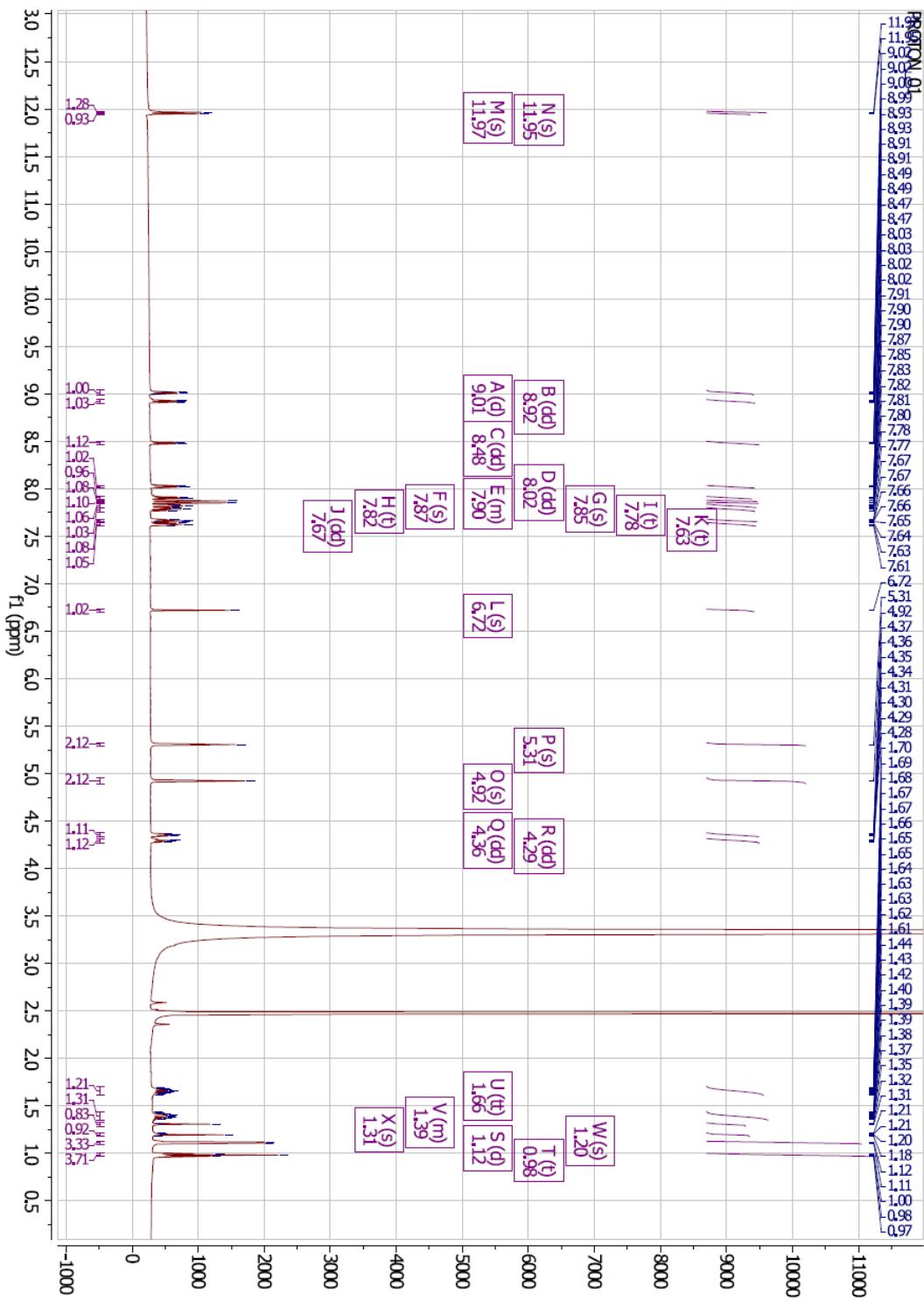
SYNAPTOG2-Si#UGA305  
1: TOF MS ES+  
6.18e4



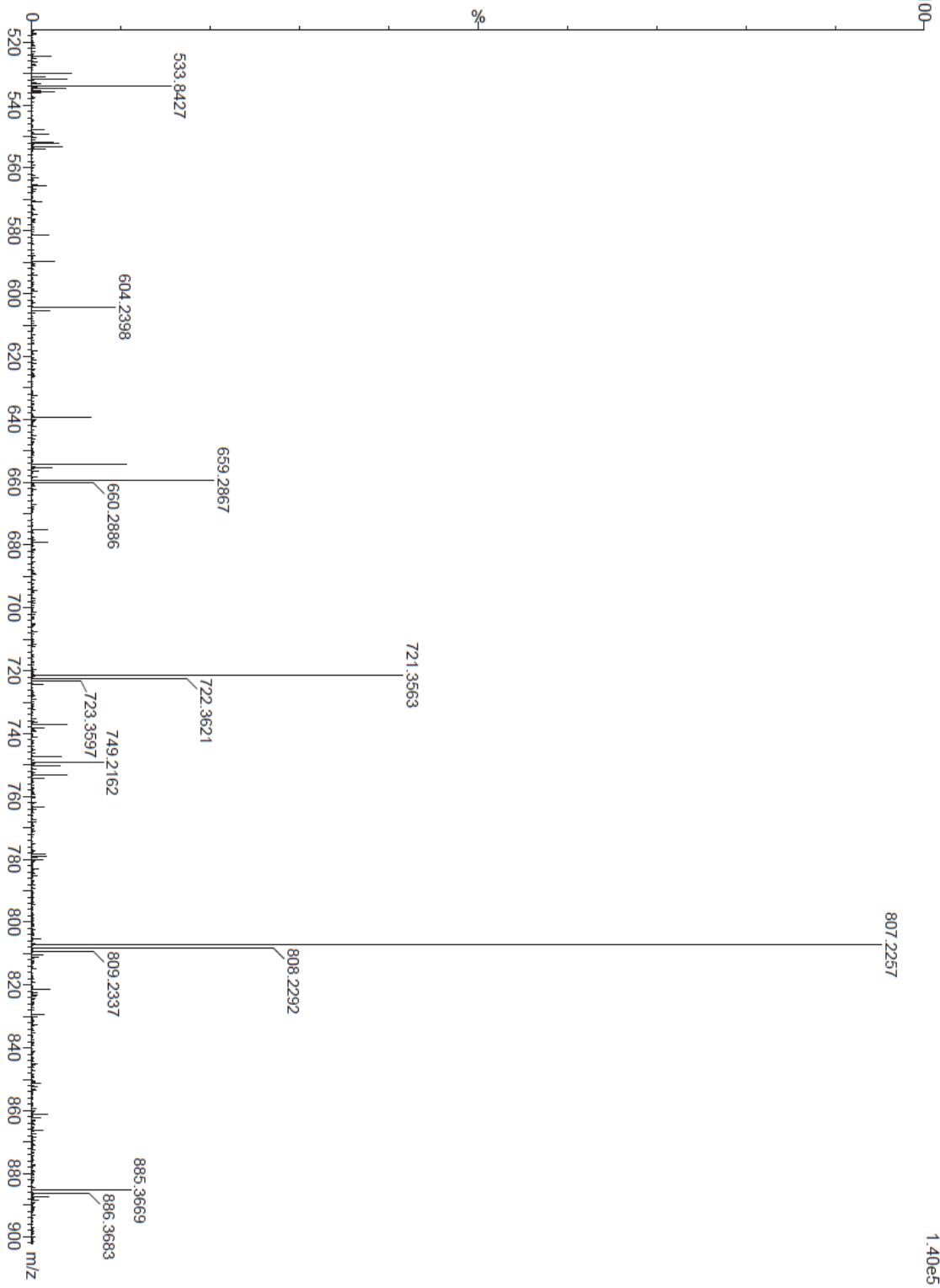
**Fig.** ESI-MS of ADM-139.



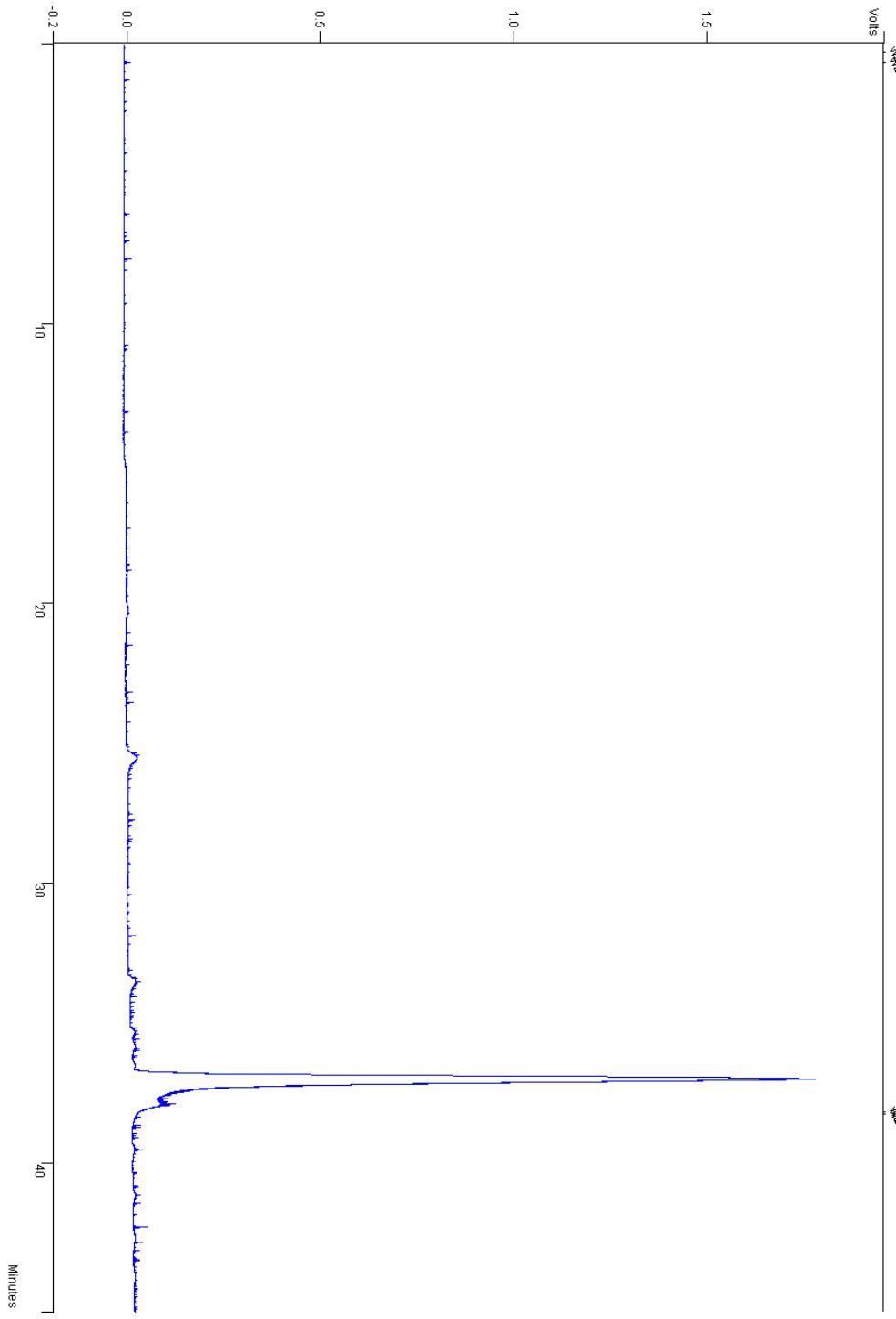
**Fig.** RP-HPLC of ADM-139.



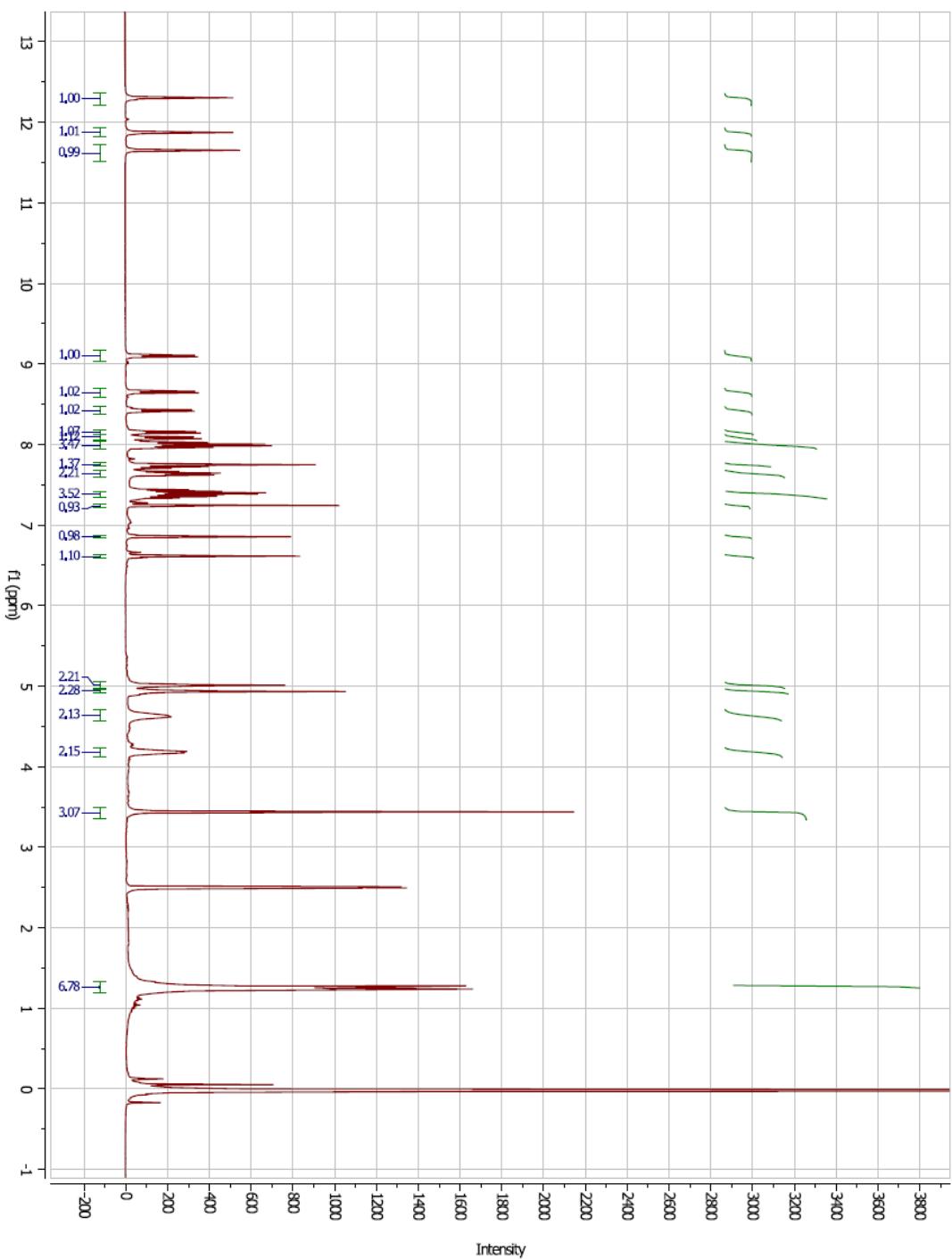
**Fig.**  $^1\text{H}$ -NMR of ADM-140.



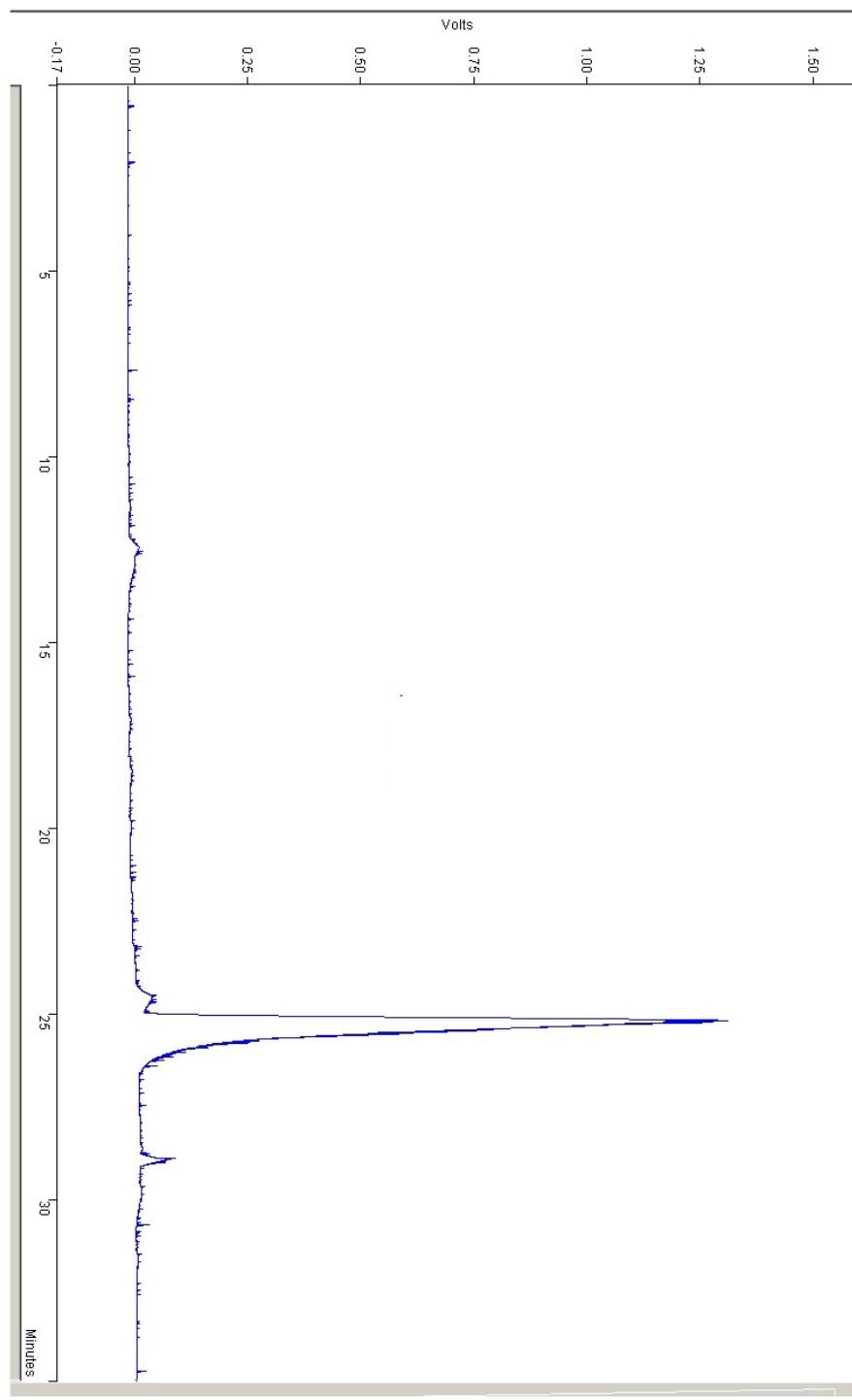
**Fig.** ESI-MS of ADM-140.



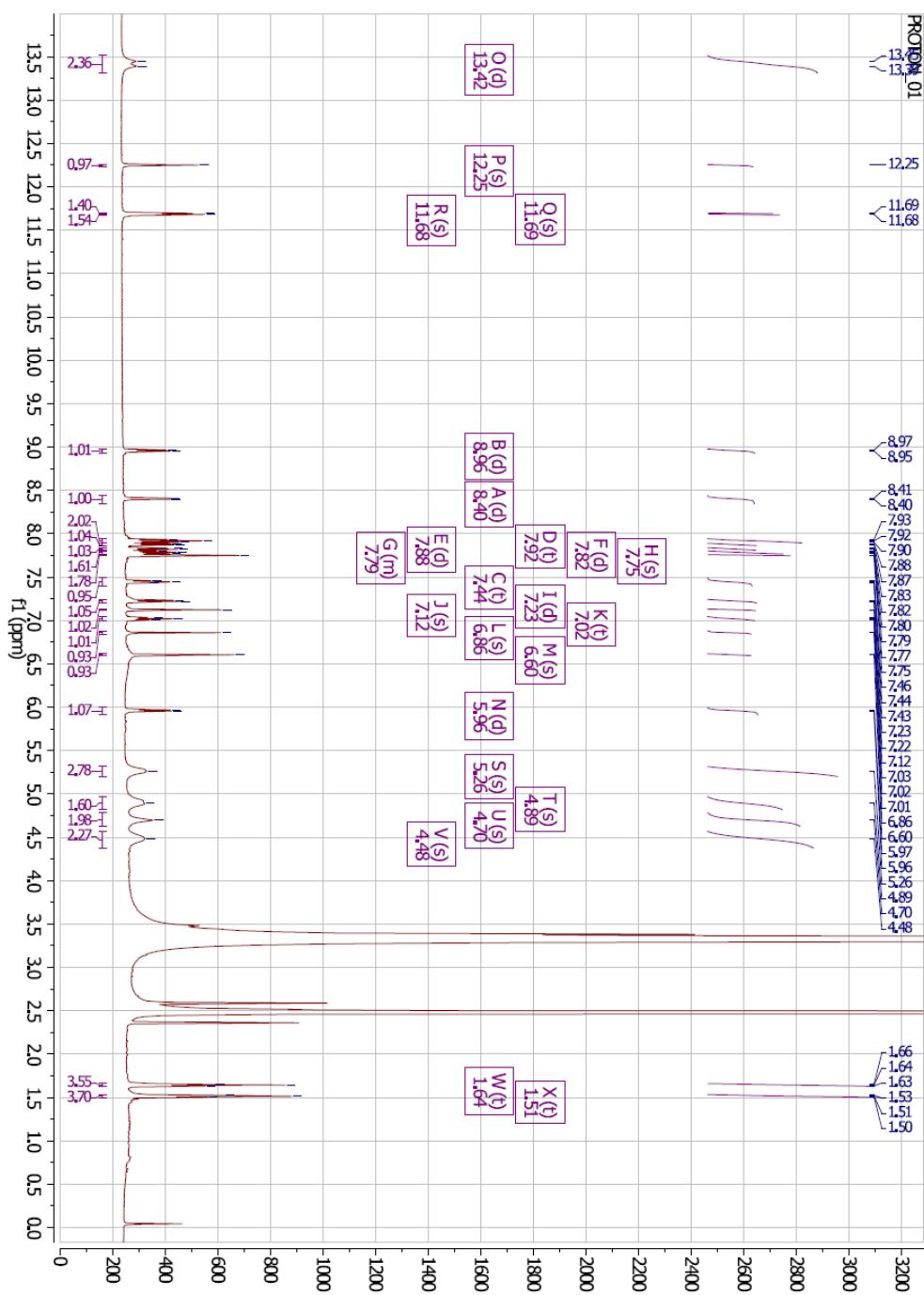
**Fig.** RP-HPLC of ADM-140.



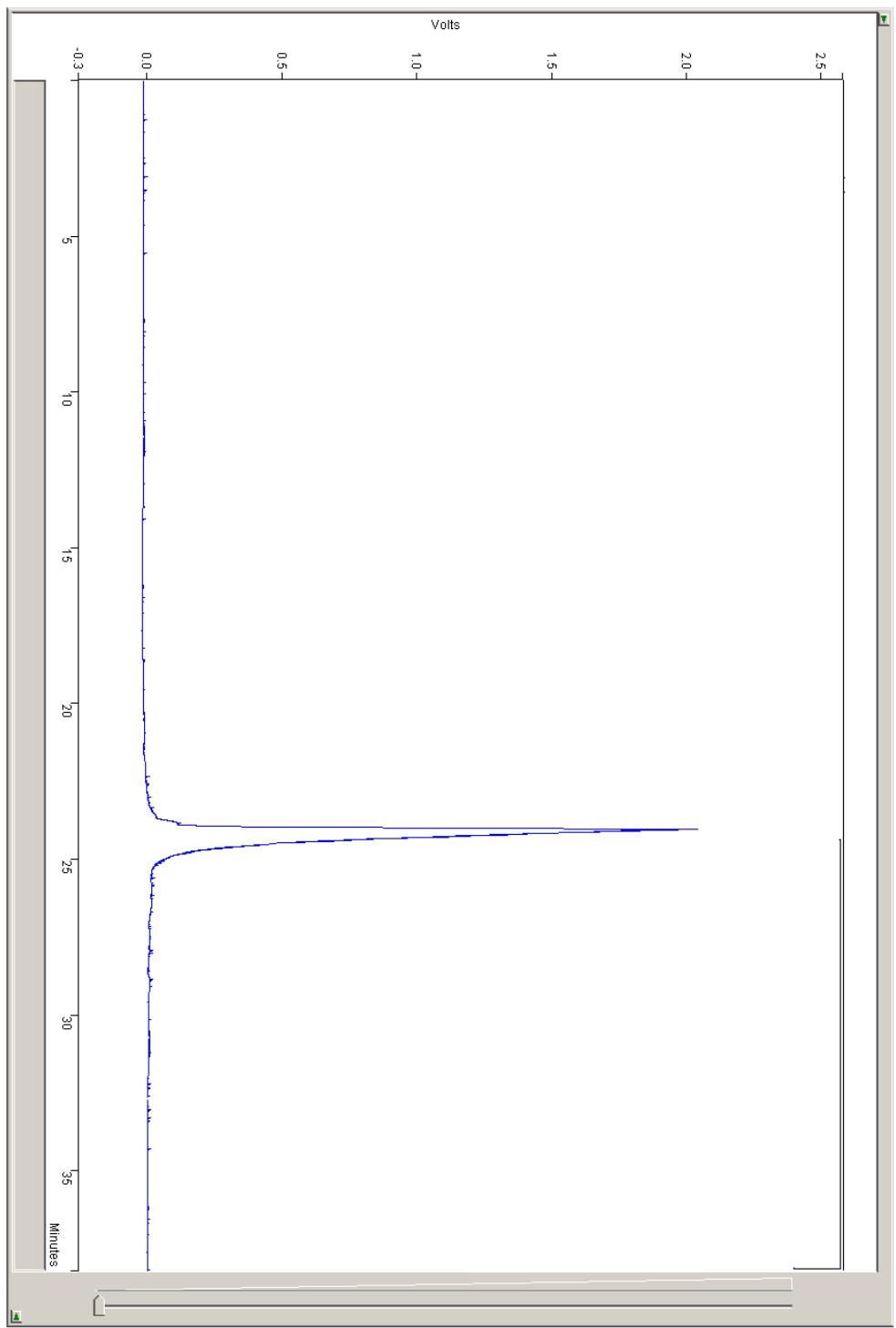
**Fig.**  ${}^1\text{H}$ -NMR of ADM-141.



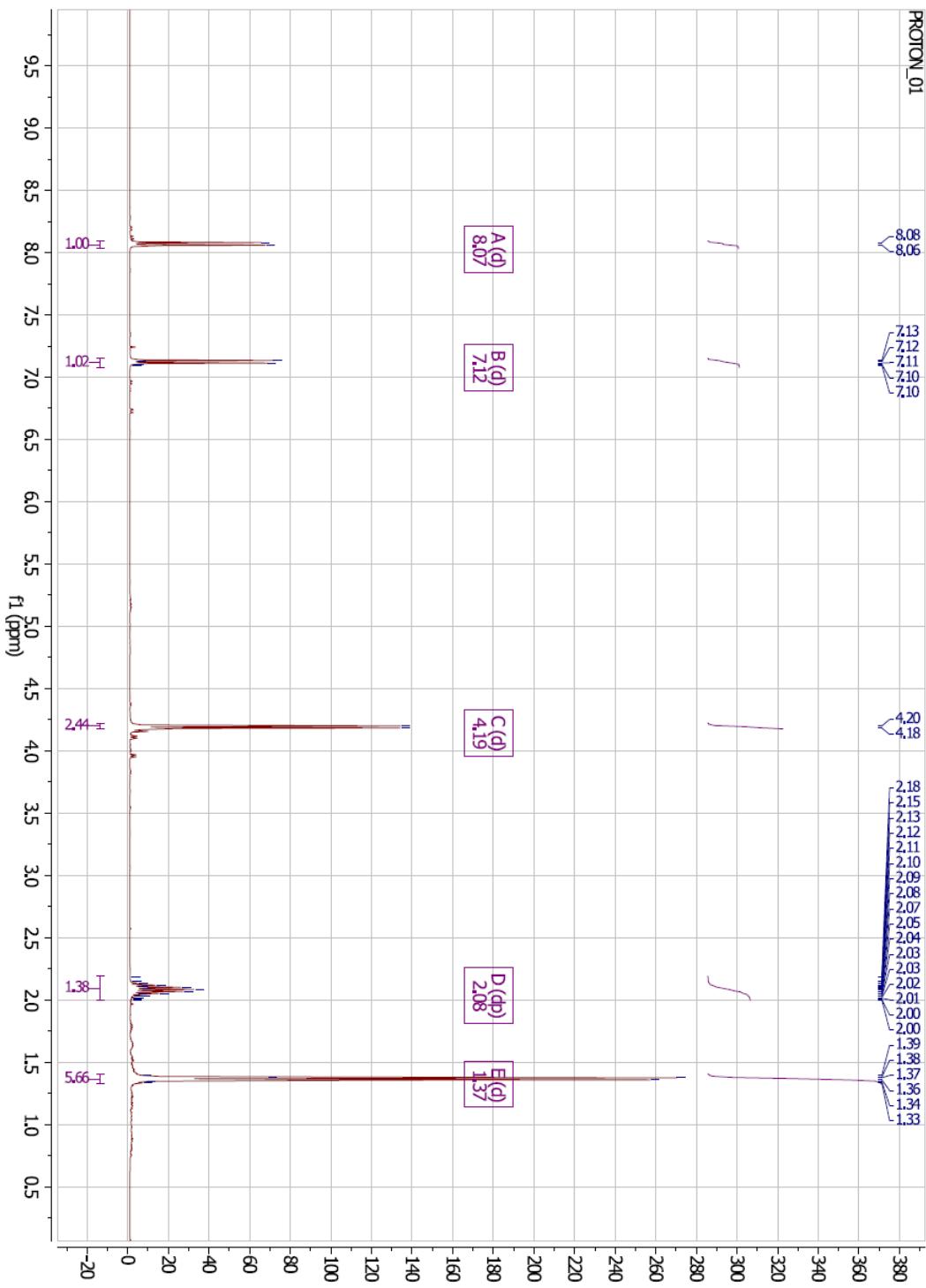
**Fig.**  $^1\text{H-NMR}$  of ADM-141.



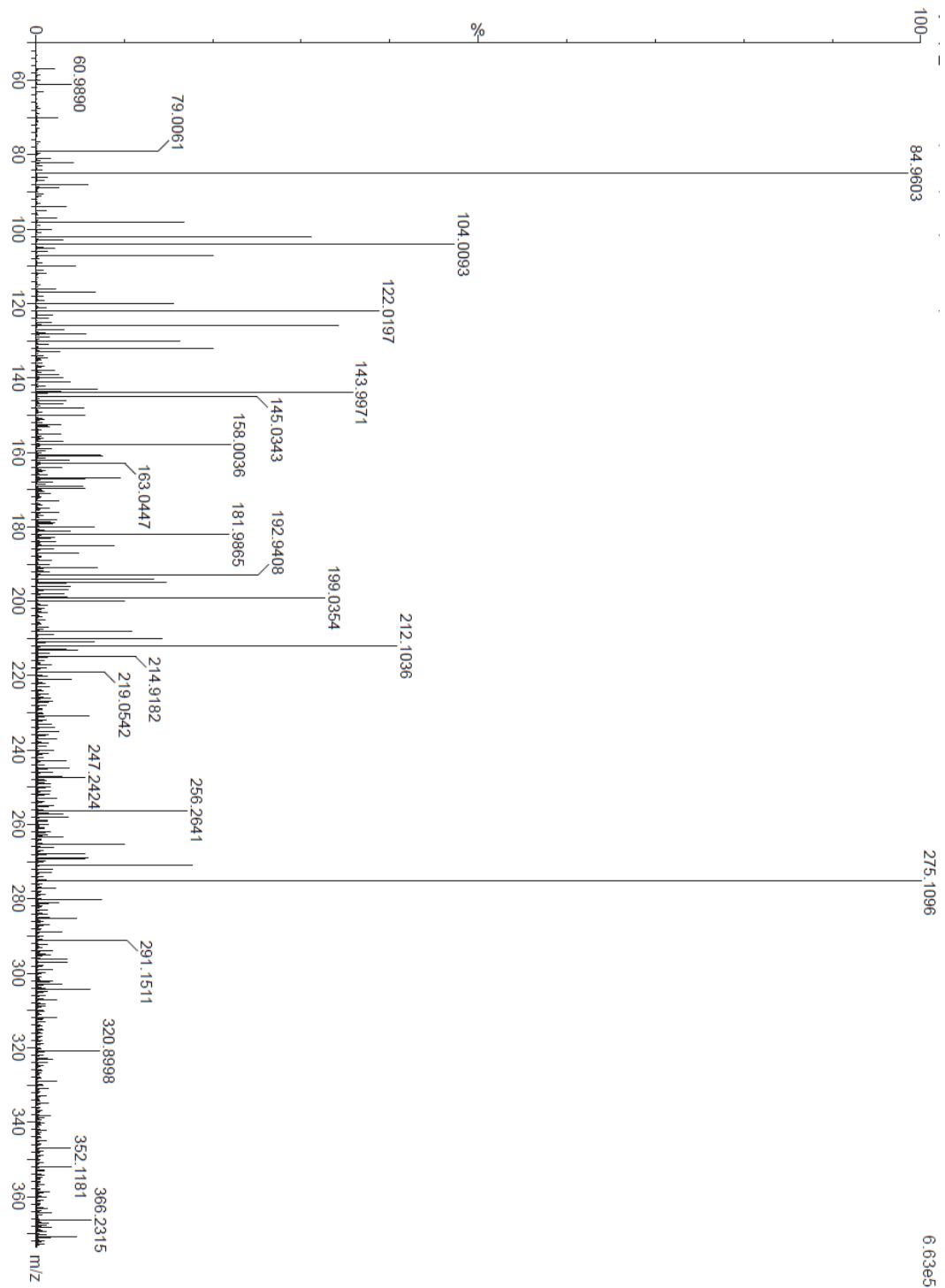
**Fig.** <sup>1</sup>H-NMR of ADM-142.



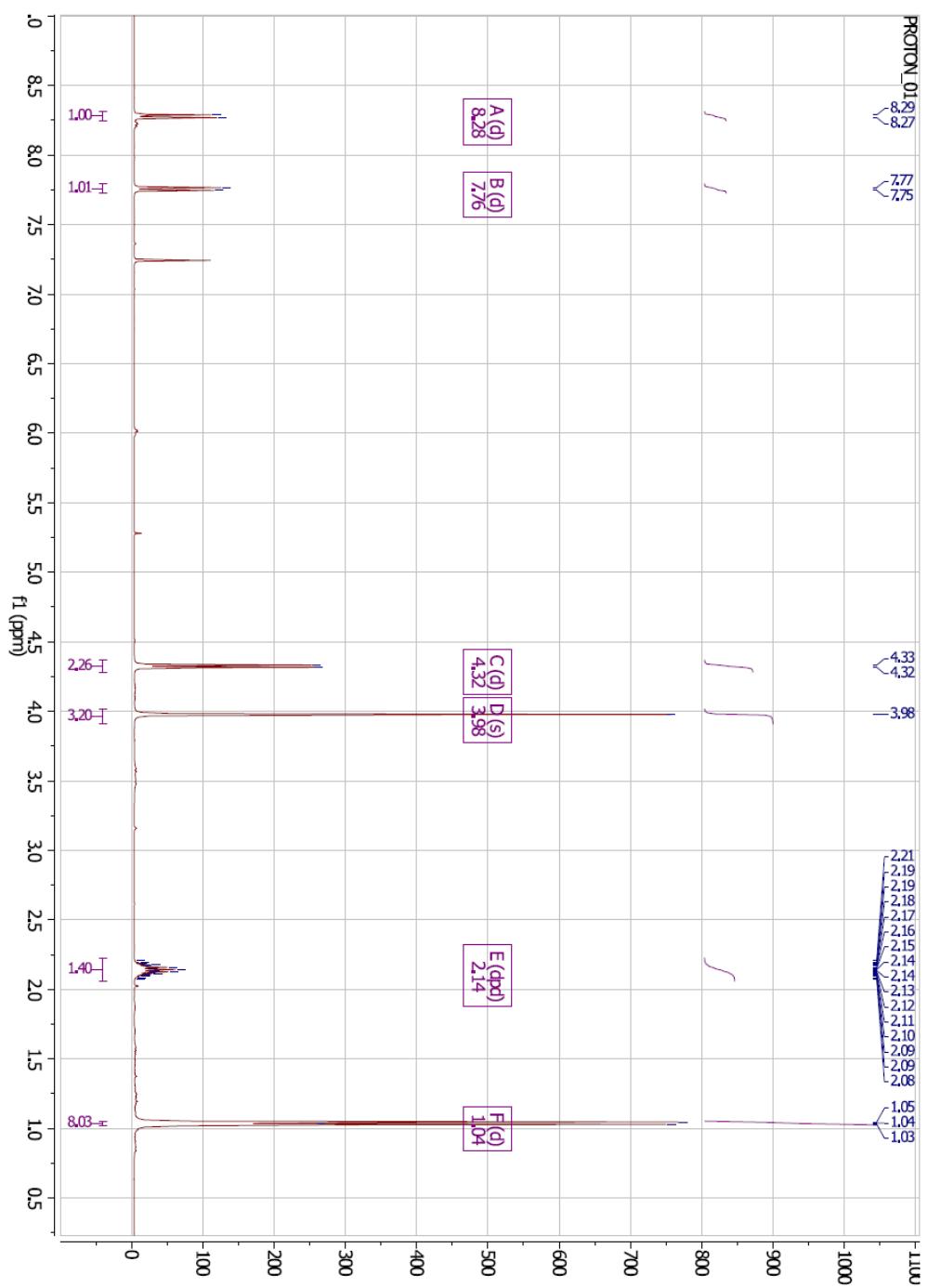
**Fig.** RP-HPLC of ADM-142.



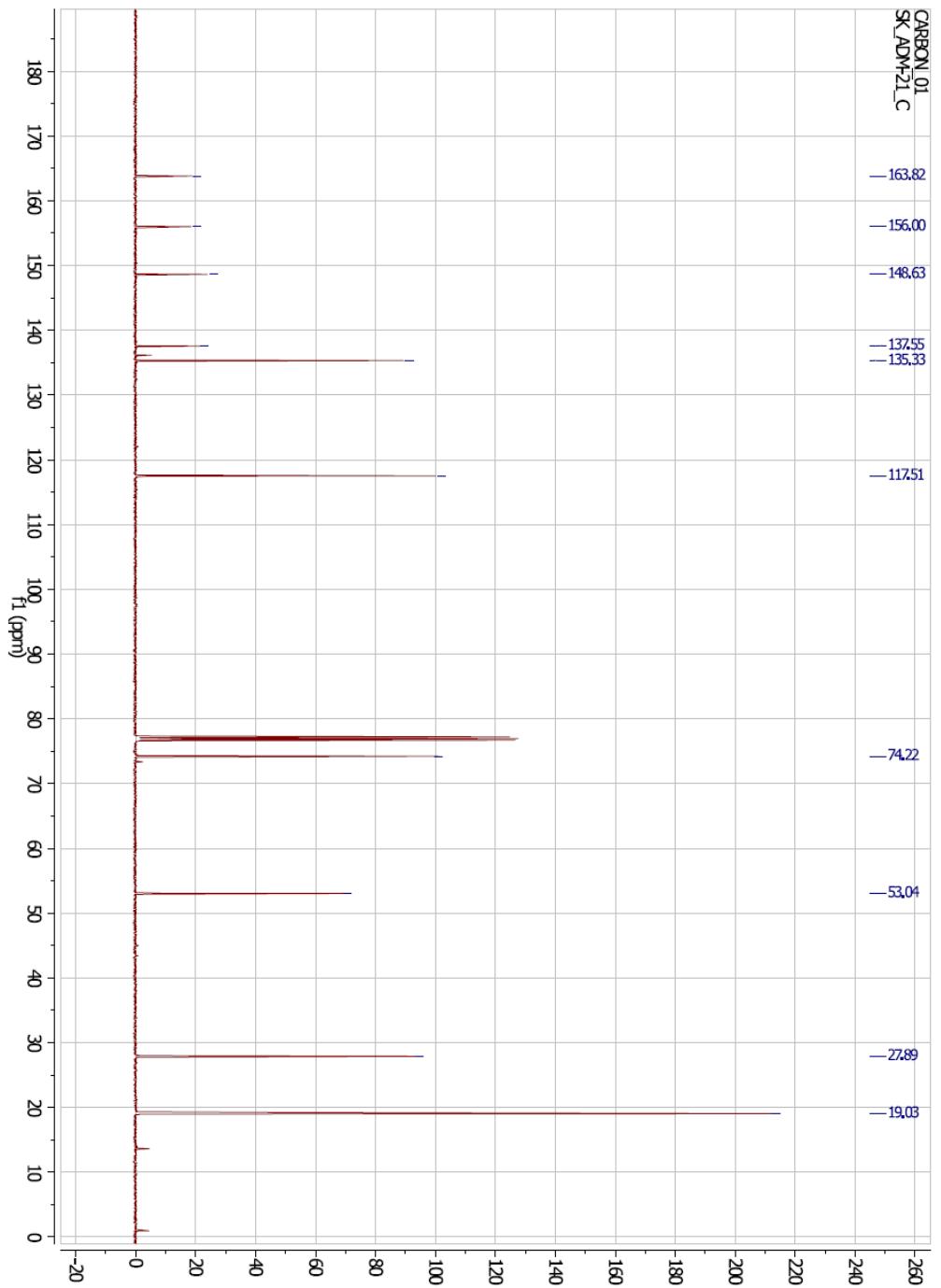
**Fig.**  $^{13}\text{H}$ -NMR of tert butyl ADM-b.



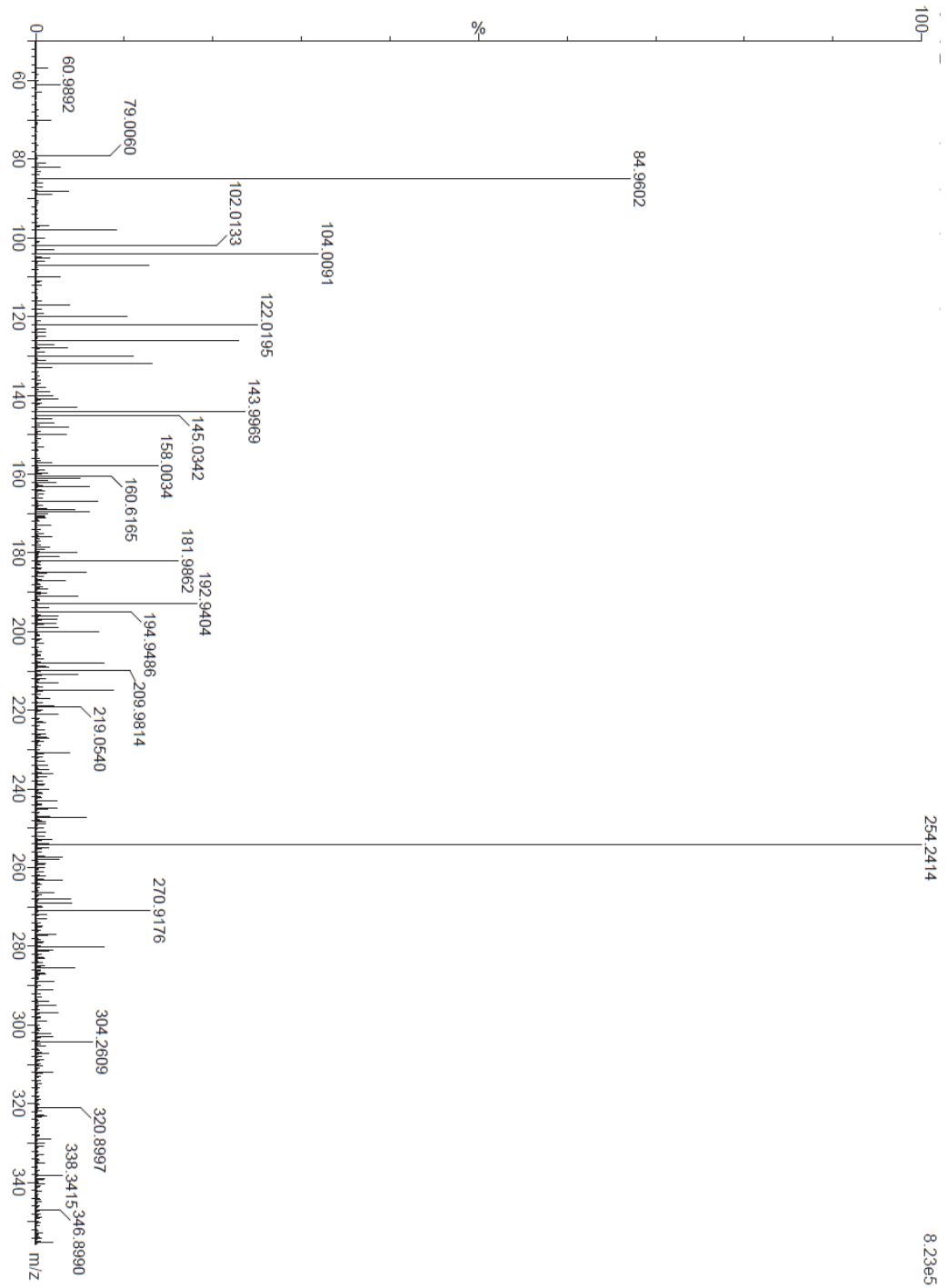
**Fig.** ESI-MS of ADM-b.



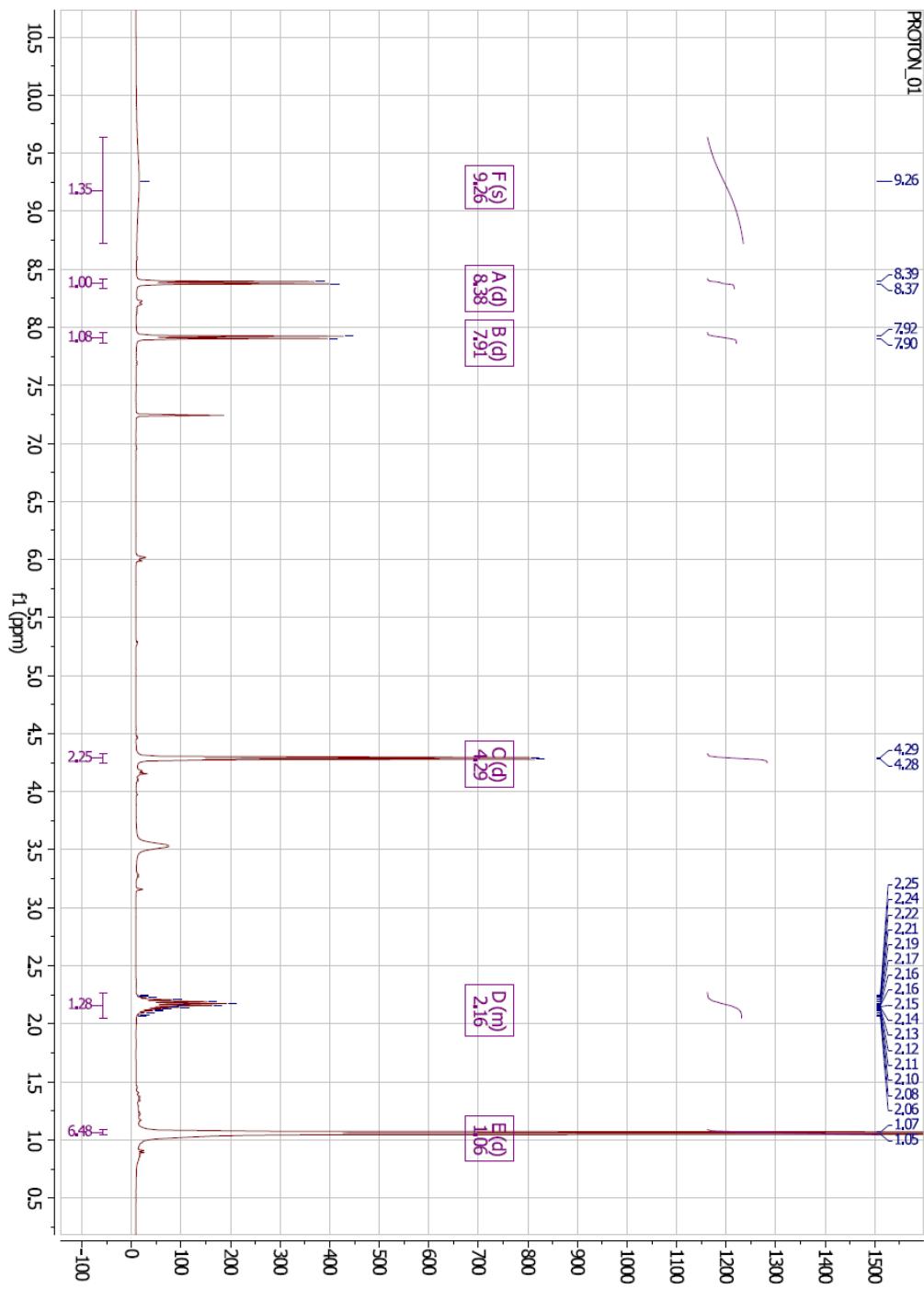
**Fig.**  $^{13}\text{C}$ -NMR of tert butyl ADM-c.



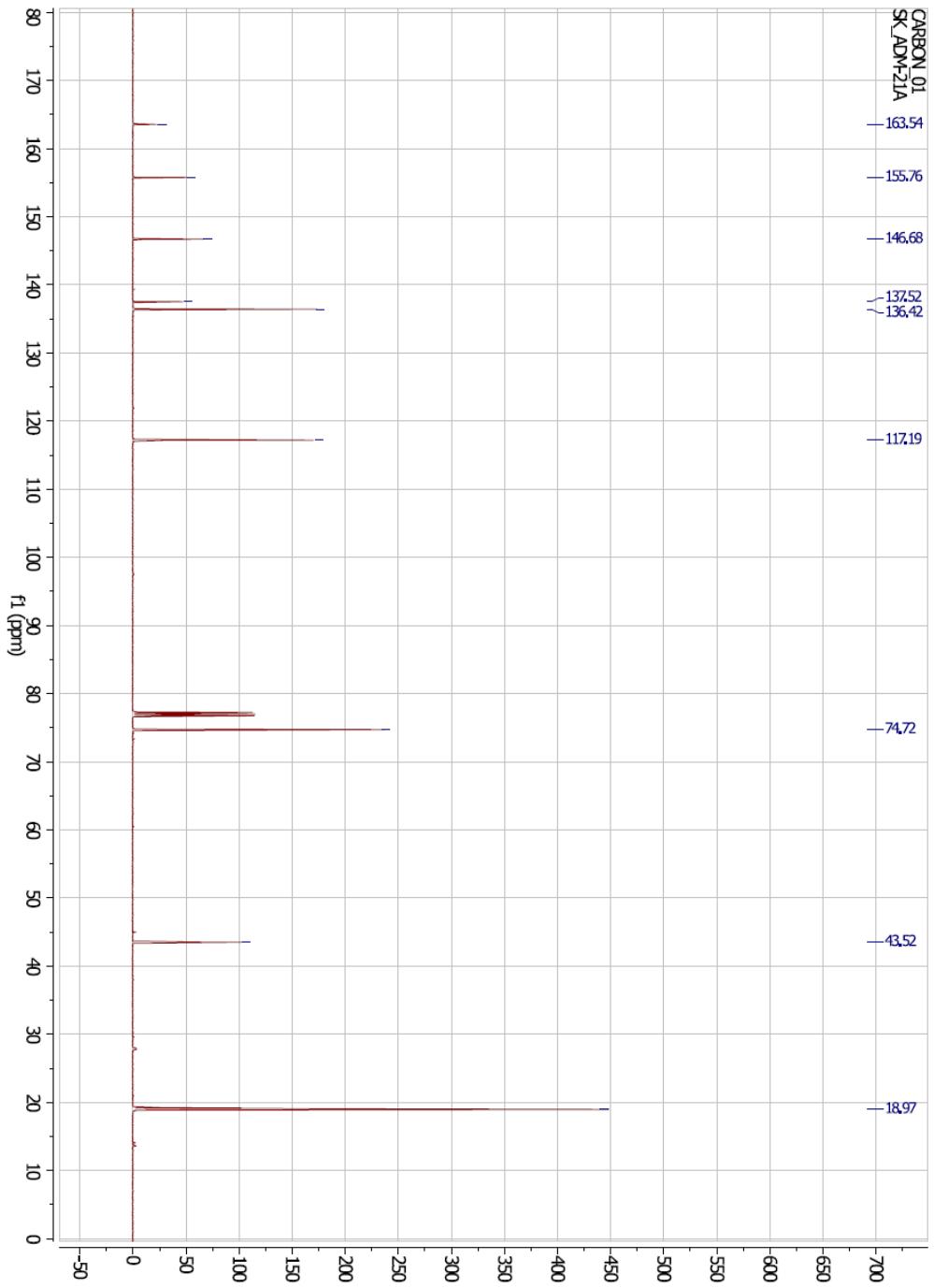
**Fig.**  $^{13}\text{C}$ -NMR of tert butyl ADM-c.



**Fig.** ESI-MS of ADM-c.



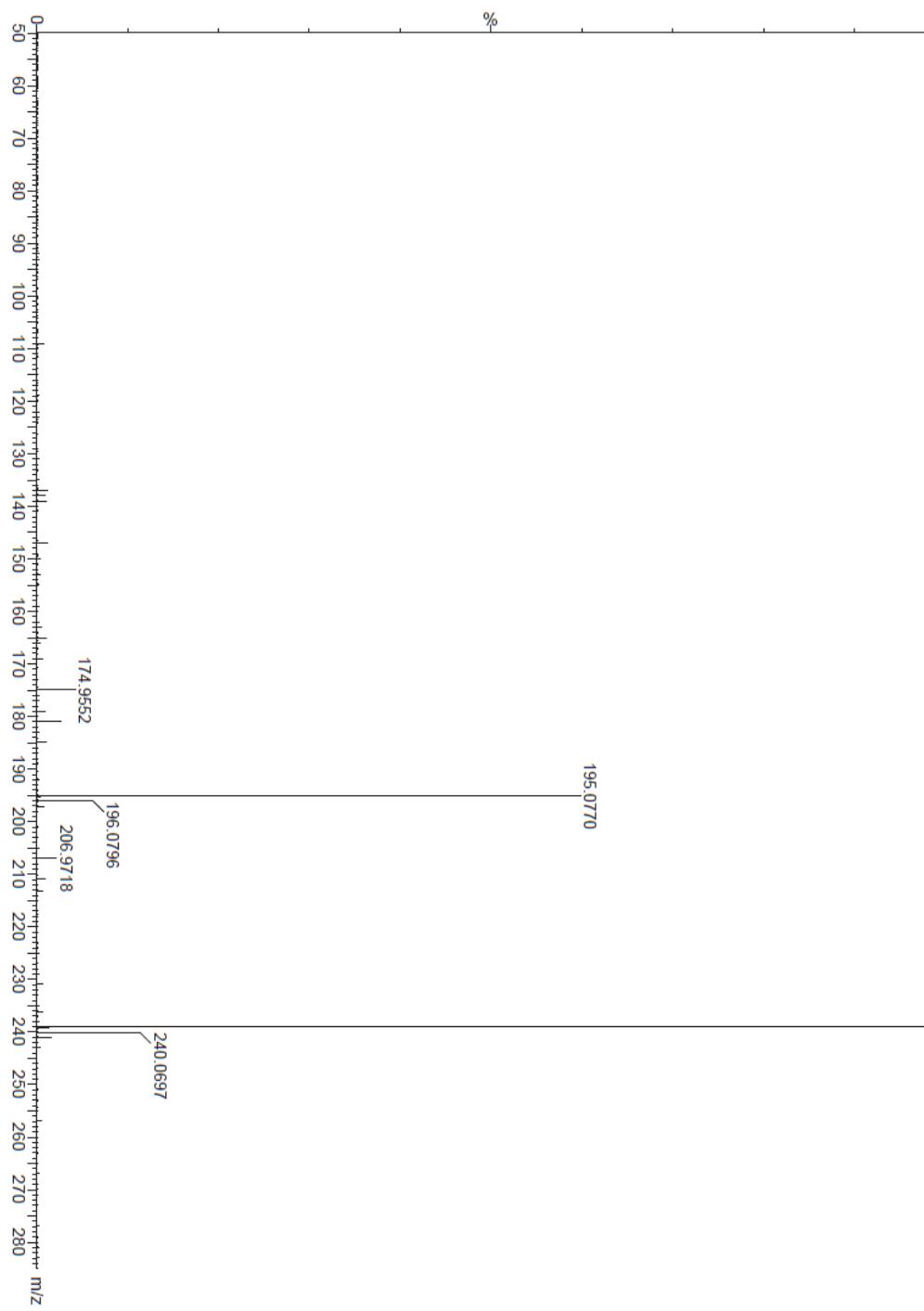
**Fig.**  $^1\text{H}$ -NMR of tert butyl ADM-d.



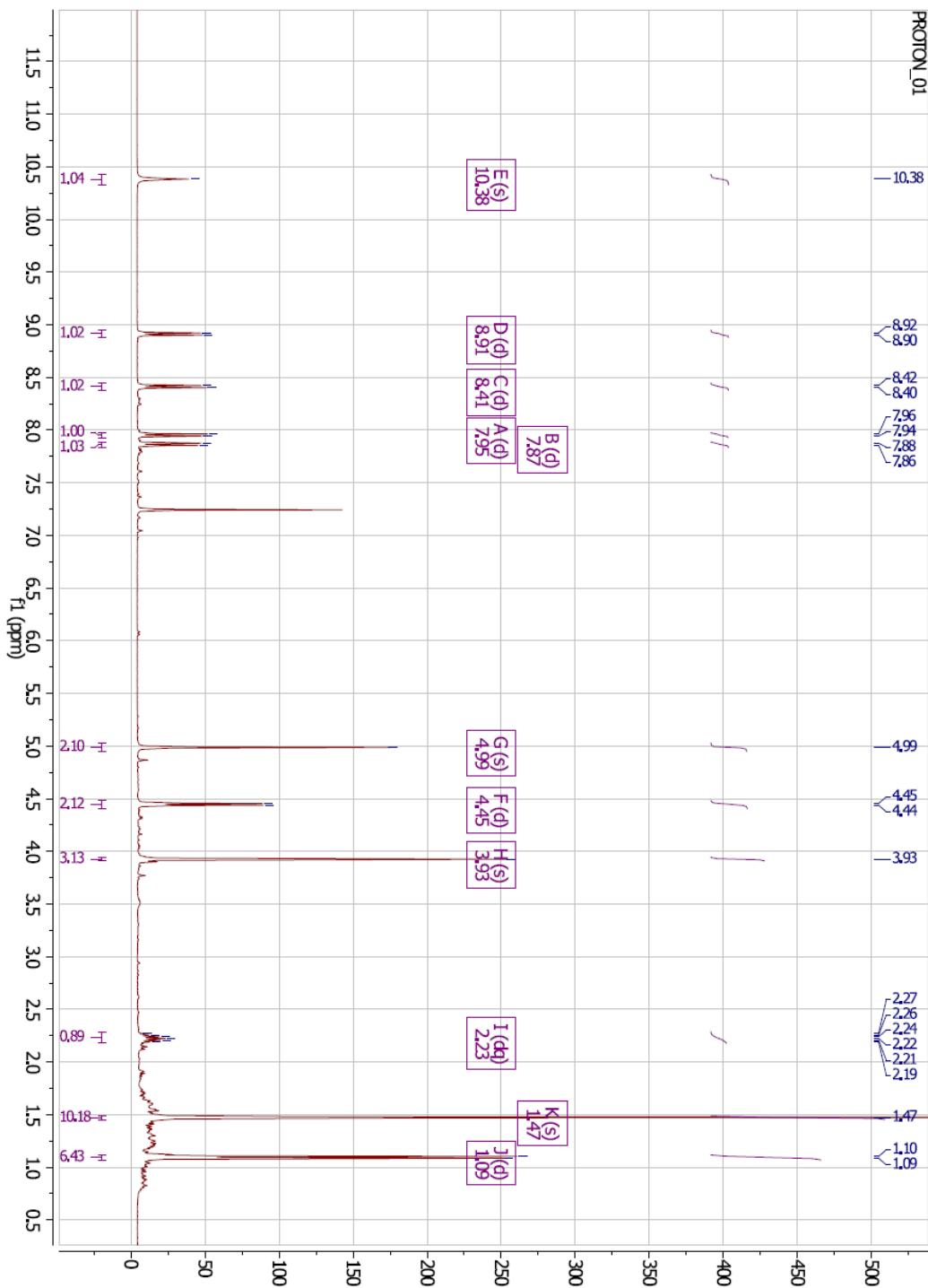
**Fig.**  $^{13}\text{C}$ -NMR of tert butyl ADM-d.

Kumar, Sunil ADM-21A  
Synapt\_4867n 25 (0.519) Cm (25-12)

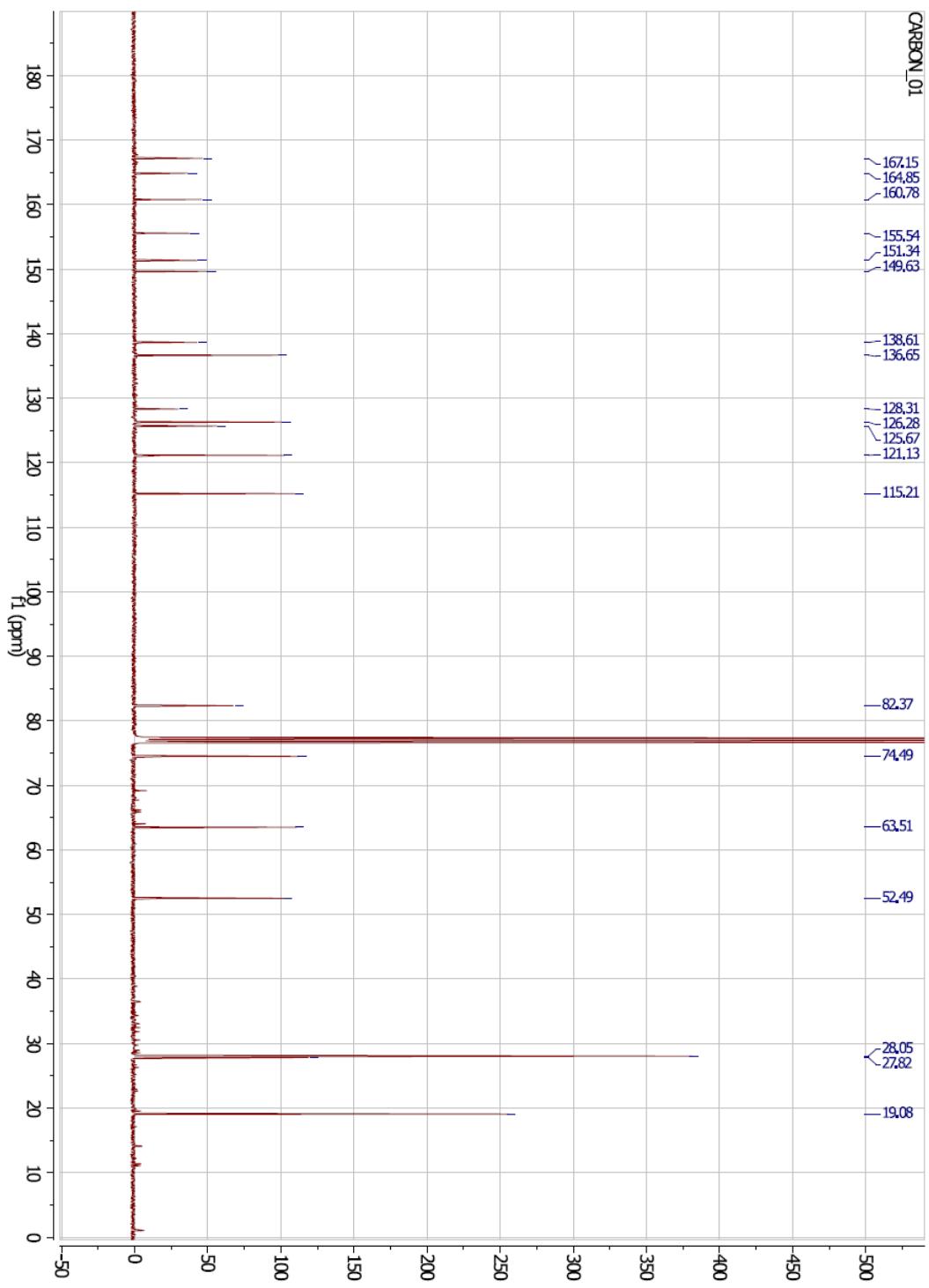
SYNAPTG2-Si#UGA305  
1: TOF MS ES-  
1.44e6



**Fig.** ESI-MS of ADM-d.



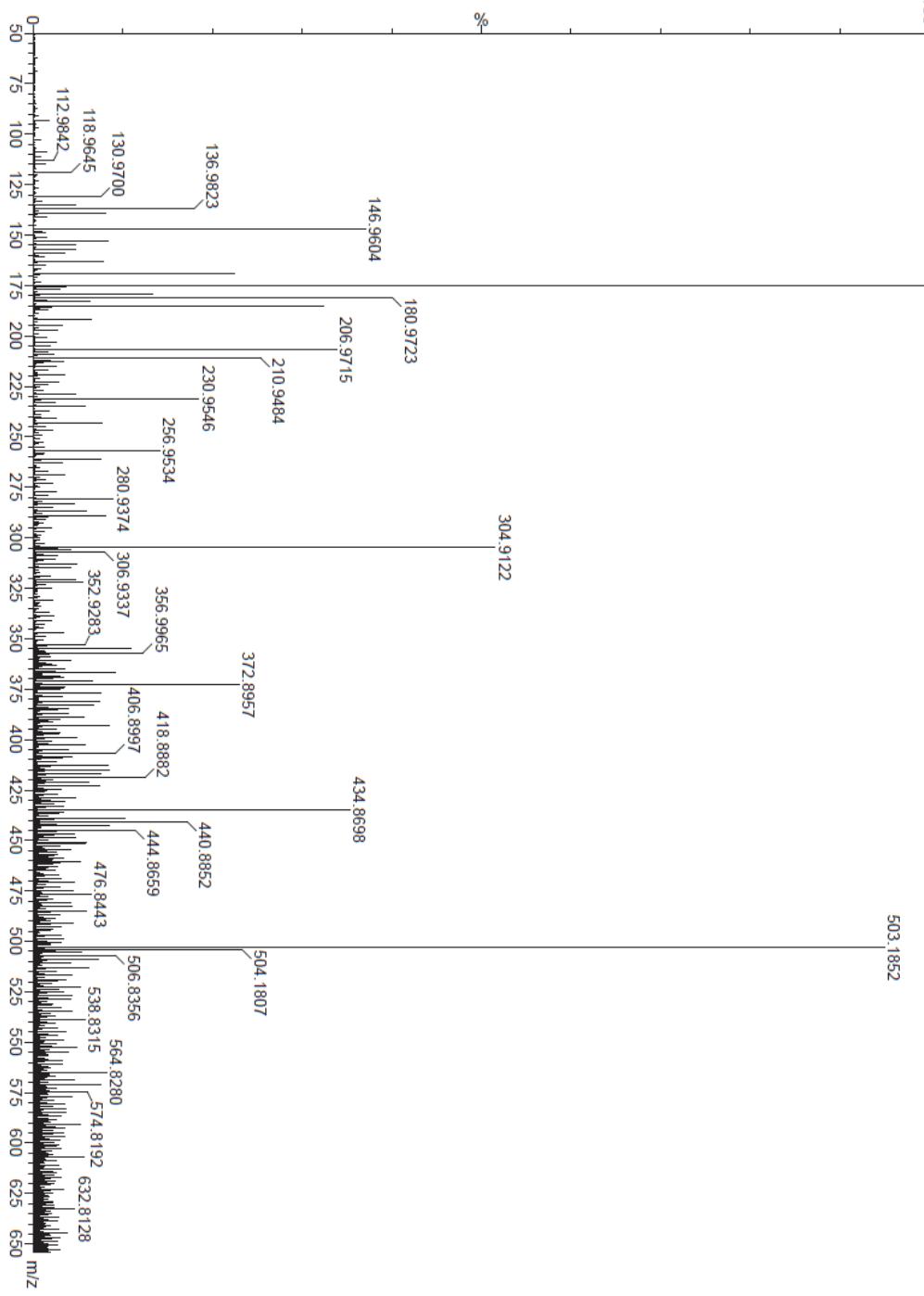
**Fig.**  $^1\text{H}$ -NMR of tert butyl ADM-g.



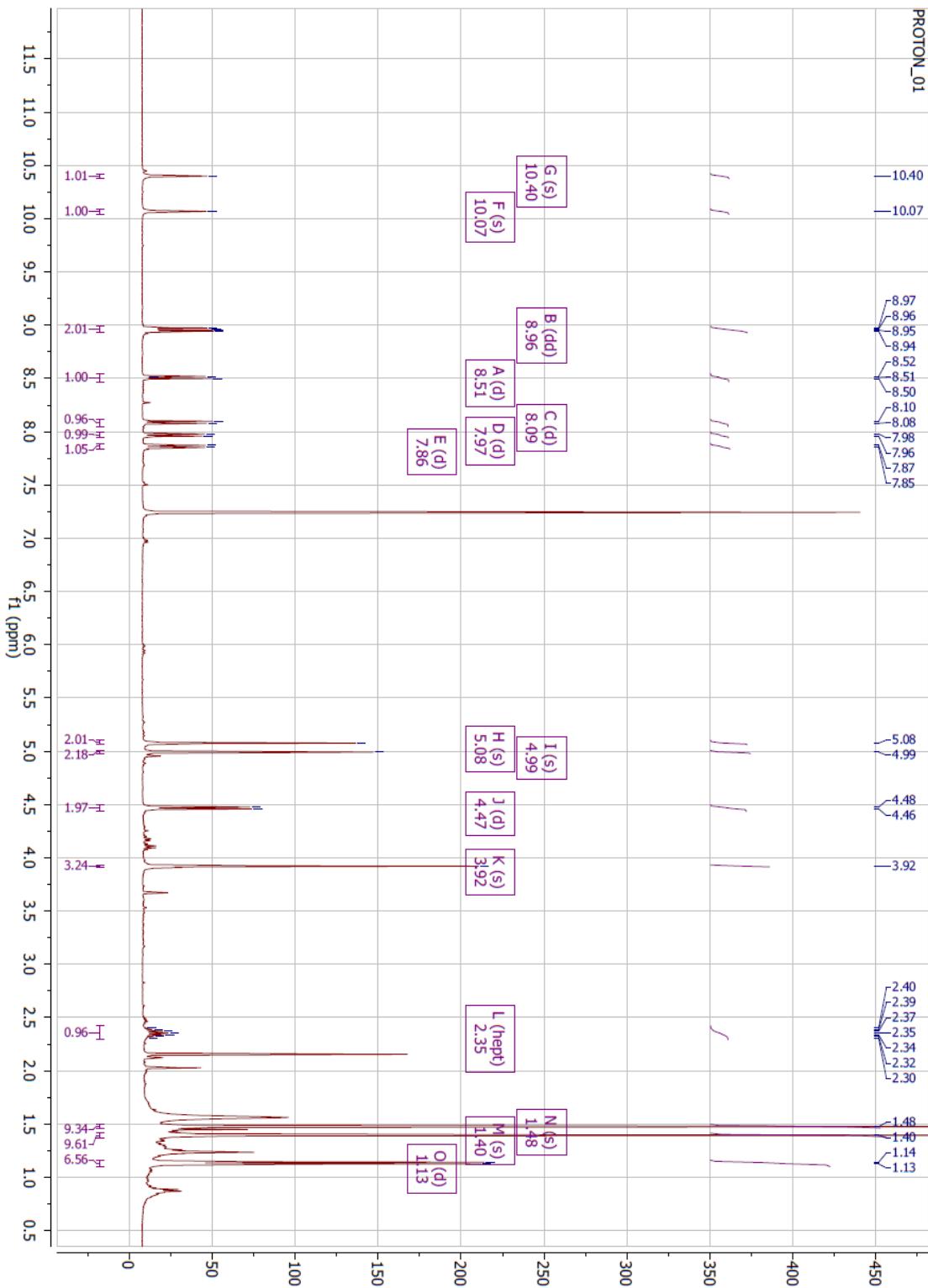
**Fig.**  $^{13}\text{C}$ -NMR of tert butyl ADM-g.

Kumar, Sunil ADM-30A  
Synapt\_4877n 22 (0.448) Cm (22.24.9.11)  
174.9550

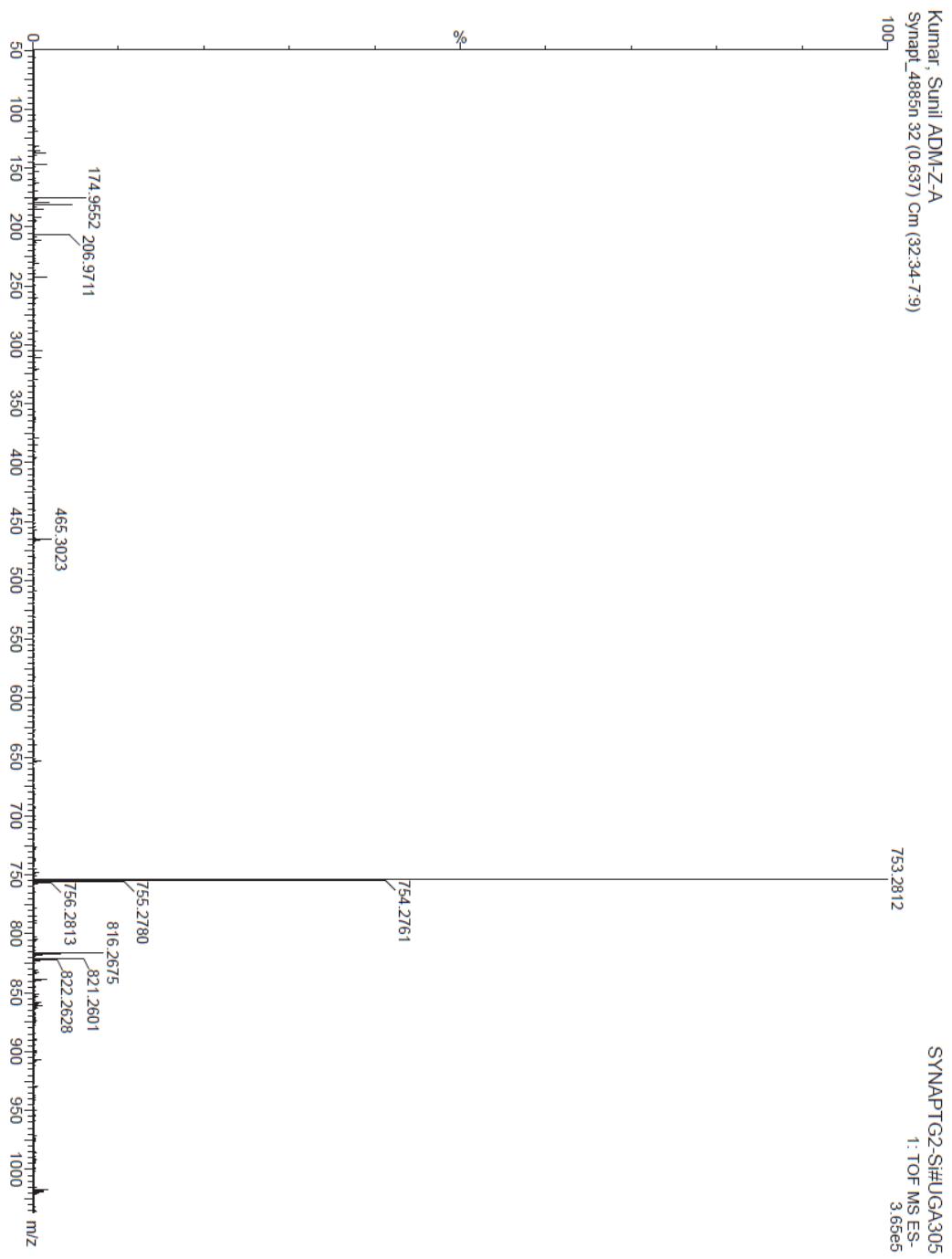
SYNAPTG2-S#UGA305  
1: TOF MS ES-  
6.33e5



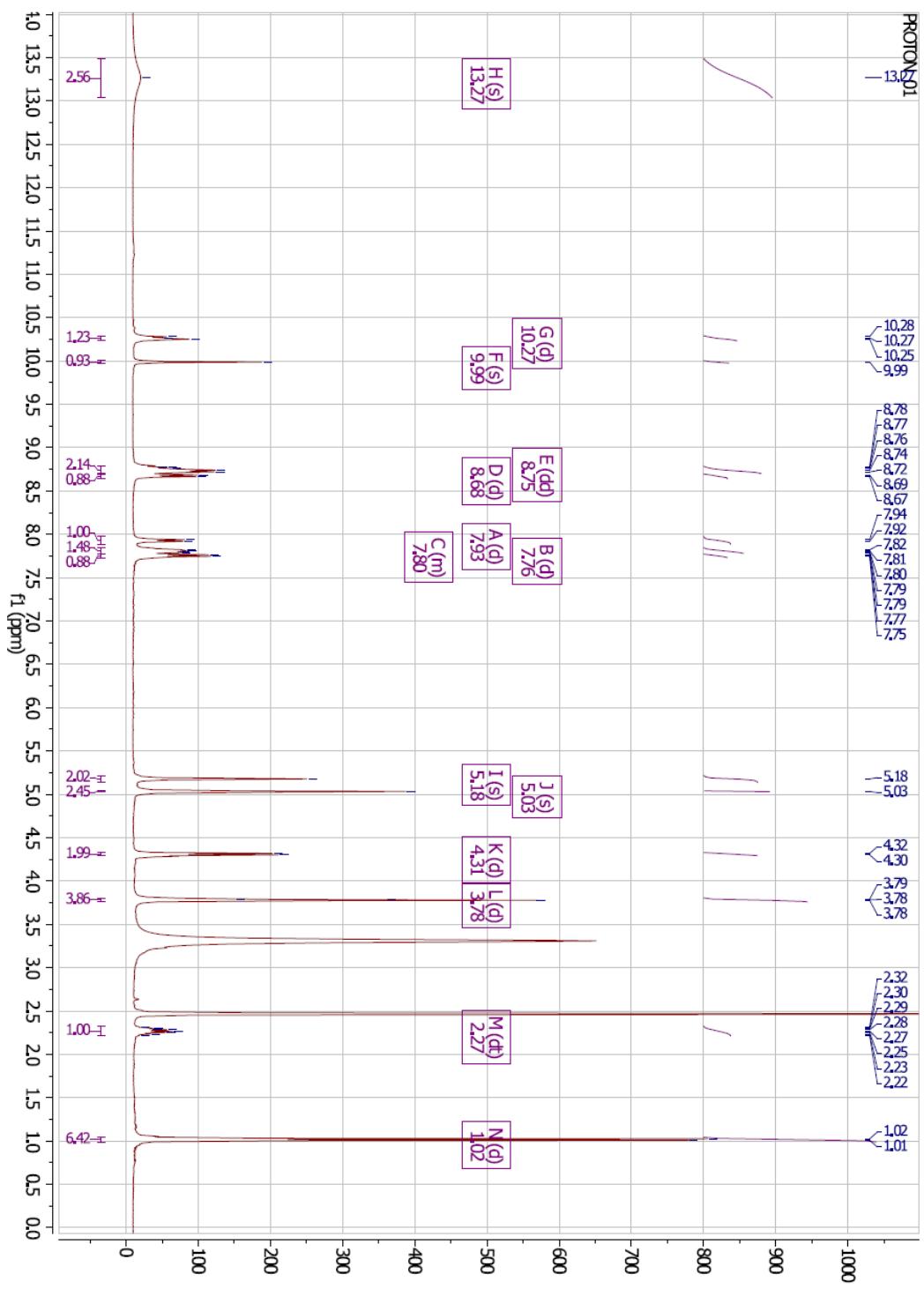
**Fig.** ESI-MS of ADM-g.



**Fig.**  $^1\text{H}$ -NMR of tert butyl ADM-11.



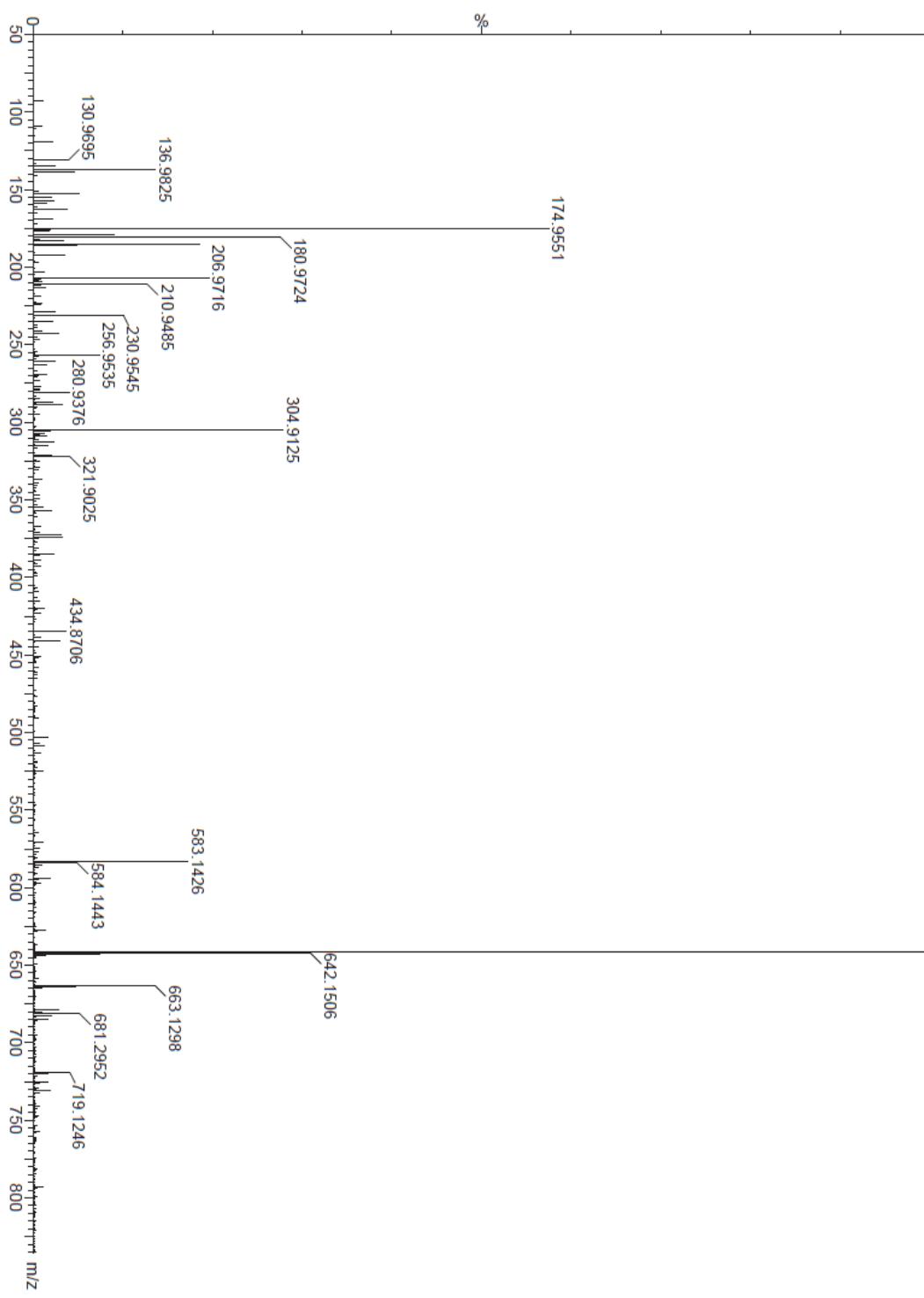
**Fig.** ESI-MS of tert butyl ADM-11.



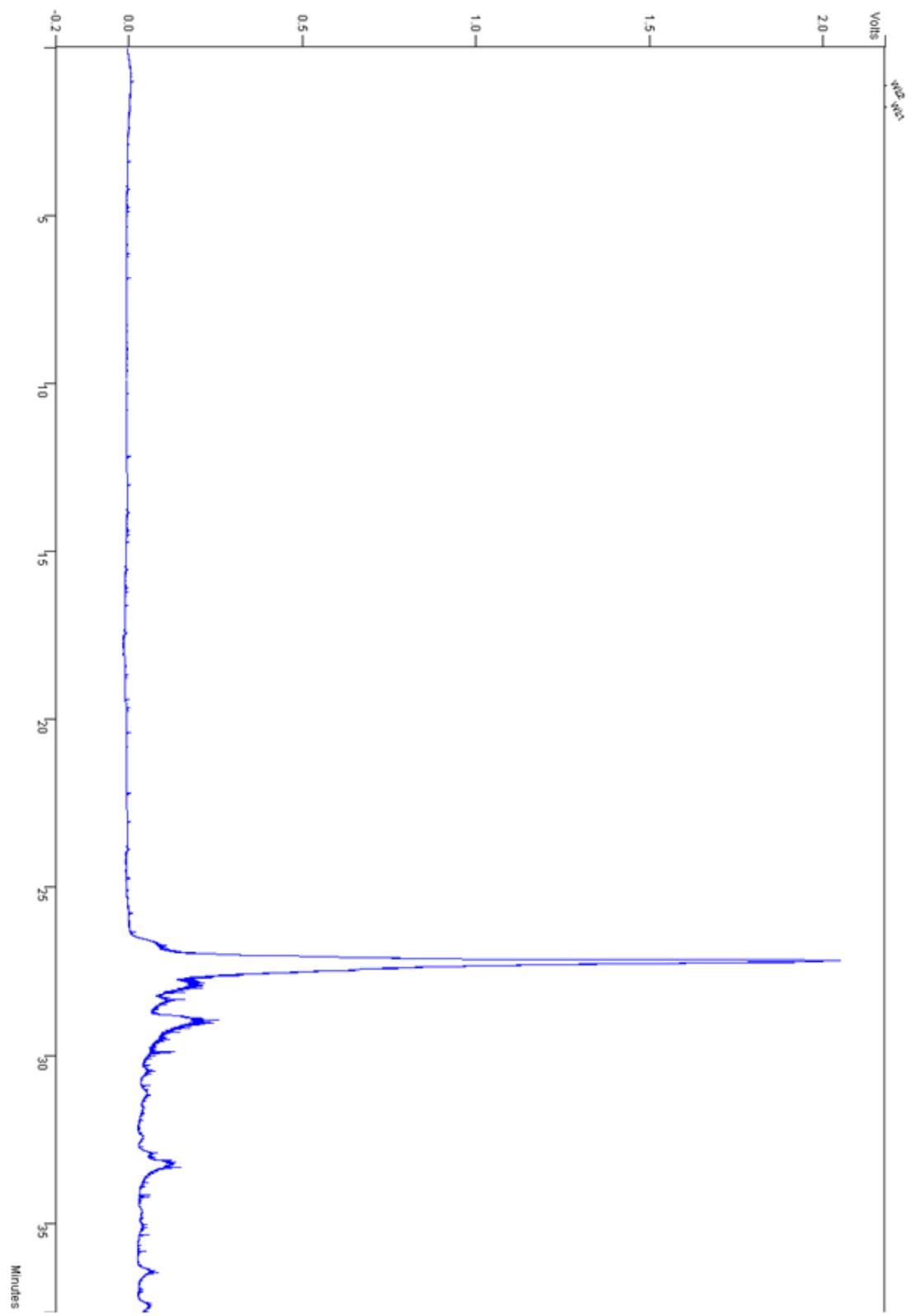
**Fig.**  $^1\text{H}$ -NMR of ADM-11.

Kumar, Sunil ADM-Z  
Synapt\_4884n 24 (0.482) Cm (24:25:4:9)  
100

SYNAPTG2-Si#UGA305  
1: TOF MS ES-  
3.49e5



**Fig.** ESI-MS of ADM-11.



**Fig.** RP-HPLC trace of ADM-11.

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