

Supplementary Information

Unexpected Discovery of Dichloroacetate Derived Adenosine Triphosphate Competitors Targeting Pyruvate Dehydrogenase Kinase to Inhibit Cancer Proliferation

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Cell culture

MCF-7 and A549 were cultured in DMEM or DMEM/F12 (1:1) supplemented with 10% fetal bovine serum and 1% penicillin/streptomycin in 5% CO₂ at 37 °C. Cells from exponentially growing cultures were used for all the experiments. The MCF-10a was cultured in DMEM/F12 (500 mL) supplemented with 5% horse serum (25 mL), *epidermal growth factor* (100 µL, 100 mg/mL), hydrocortizone (250 µL, 1 mg/mL), cholera toxin (50 µL, 1 mg/mL), insulin (500 µL, 10 mg/mL). The prepared compounds were dissolved in DMSO at 40 mM as stocking solution, while DCA was dissolved in PBS containing 1% DMSO at desired concentrations.

IncuCyte Zoom live cells image for the growth of the cancer cells

The growth behaviors of the cancer cells after treating with the inhibitors was studied using IncuCyte Zoom live cells images (Essen BioScience Company). The MCF-7 (2000/well) and A549 (3000/well) were seeded into each well of a 96-well plate for 24 h, then DCA, 15, 26 and 39 at the desired concentrations were added into each well, followed by another 72 h incubation. Cell images were recorded every three hours, and cells without adding others drugs were served as control.

Cell cytotoxic assay

Cytotoxic activity was assessed by MTT assay. A suspension of cells (2000/well for MCF-7, 3000/well for A549 and 2000/well for MCF-10a) were seeded in 96-well plates and cultured for 24 h. Two working compound solutions, namely 400 µM and 20 µM, were prepared by diluting the 40 mM compound stock solutions in PBS buffer containing 1% DMSO. The working solutions (10 µL/well) were added to the corresponding plates, and the plates were incubated for 72 h. Then, 10 µL of MTT solution (5 mg/mL) was added to each well. After 4 h of incubation at 37 °C, the solvent was removed and 100 µL DMSO was added to each well, with the aid of gentle shaking to dissolve the formazan crystals. The absorbance of the wells was read at 570 nm. After the potent compounds (**15**, **26** and **39**) were identified, dose-response studies were undertaken to determine the exact IC₅₀ values of these compounds. Eight different concentrations of **15**, **26** and **39** ranging from 600 µM-3.125 µM (PBS buffer containing 1% DMSO) were added into the 96-well plate. The OD values were read in the SpectraMax M Series Muti-mode Microplate Reader, and the results were expressed as IC₅₀ values, which were the mean values derived from three independent experiments.

Lactate measurement

A suspension of MCF-7 cells (2×10^5 / well) were seeded in 6-well plates and cultured overnight. Then DCA (100 mM), **39** (200 µM, 100 µM and 50 µM), **15** (400 µM) and **26** (400 µM) were added to the corresponding wells, and the plates were incubated for 12 h. Then, the medium was removed to EP tubes, which were centrifuged for 5 min (6000 r/min). At last 1 mL medium was collected, the lactate production was evaluated by Nova Bioprofile Flex analyzer. (Nova Biomedical).

PDK kinase activity assay

PDK1 kinase activity was measured by the Kinase-Glo® Luminescent Kinase Assays (Promega). Reagents: PDK1 800 µM (in 50 mM K₃PO₄, 250 mM KCl, 2 mM MgCl₂, pH

= 7.4); Assay buffer (10 X, 250 mM Tris-HCl, 10 mM EDTA, 5 mM EGTA, 10 mM DTT, 50 mM MgCl₂), peptide 10 mM (amino acid sequences: RYHGHMSMSP, which is a fragment around S293 of PDC), ATP 10 mM.

Procedures:

1. Added 25 μ L of dd water and 5 μ L assay buffer (10 X) to 96-well plate, and marked as well 1#, 2#, 3#, 4#, 5# and 6#.
2. Then 5 μ L of 1% DMSO PBS buffer was added to wells 1# and 6#, and 5 μ L of DCA (10 mM), **15**, **26** and **39** (500 μ M) to wells 2#, 3#, 4#, 5#.
3. Then 5 μ L ATP (10 μ M) and 5 μ L peptide (40 μ M) were added to wells 1#, 2#, 3#, 4#, 5# and 6#.
4. Then 5 μ L PDK1 (10 μ M) was added to wells 1#, 2#, 3#, 4# and 5#, and 5 μ L protein buffer to well 6#. Mix the plate and incubate at 37 °C for 30 min.
5. To each wells, 50 μ L of the appropriate kinase-Glo reagent was added. The plate was mixed, and incubated for another 10 min at room temperature.
6. Luminescence signal was recorded.
7. The experiment was repeated for three times.

Western Blot Analysis

1 μ L PDC protein (4 μ g/ μ L) was added into the 35 mL dd H₂O and 5 μ L of kinase reaction buffer (10 X, 250 mM Tris-HCl, 10 mM EDTA, 5 mM EGTA, 10 mM DTT, 50 mM MgCl₂), then 5 μ L DCA (10 mM), **15** (500 μ M), **26** (500 μ M) and **39** (500 μ M) were added to the corresponding groups, the control group was added 5 μ L 1% DMSO PBS buffer. Then 5 μ L ATP (10 nM) were added to each group. The mixture were incubated at 37 °C for 30 min. Then equal amounts of PDC protein was loaded for separation. After electrophoresis, proteins were transferred to a nitrocellulose membrane, blocked with PBS containing 5% skimmed milk powder for 1 h at room temperature, then respective primary antibody (Abcam, Cambridge, UK) were added, and the mixture incubated for 2 h at room temperature. After washing, secondary antibody was added and incubated for 1 h at room temperature. Bands were scanned by the MYECL Imager (Thermo Fisher Scientific).

TMRM assay

MCF-7 cells were cultured on 24-well plate at a density of 2×10^5 cells/mL and allowed to grow overnight at 37 °C. Cells were treated with 10 mM DCA, 60 μ M **15** and **26**, and 40 μ M **39** for 12 h at 37 °C. A solution of TMRM (50 nM) was added and incubation was carried out at 37 °C for 20 min in dark. The cells were washed 3 times with PBS, and live cell imaging was performed in PBS media.

JC-1 assay for flow cytometry analysis

MCF-7 cells were cultured on a six well plate at a density of 5×10^5 cells/mL and allowed to grow overnight at 37 °C. Cells were treated with DCA at 10 mM or 20 μ M, and 20 μ M of **15**, **26** and **39** for 8 h at 37 °C. A solution of JC-1 reagent (10 g/mL in PBS buffer) was added and incubation was carried out at 37 °C for 15 min. Then the culture medium was removed. The cells were washed 3 times with PBS and trypsinized for 15 min at 37 °C. The cells were isolated and washed 3 times by centrifugation (1200 rpm for 5 min at 4 °C). The resulting cell pellet was resuspended in 100 μ L PBS and analyzed by BD FACS Calibur flow cytometry.

JC-1 assay for image

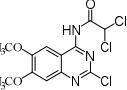
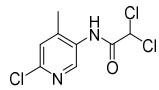
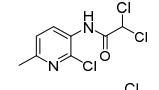
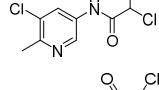
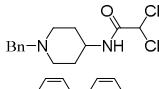
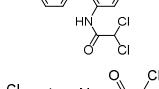
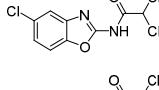
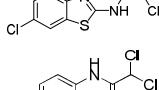
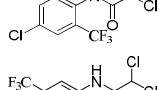
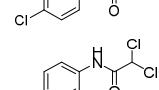
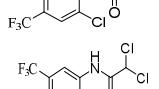
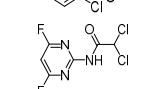
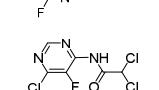
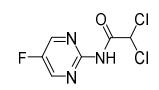
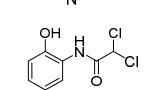
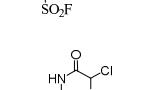
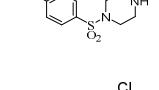
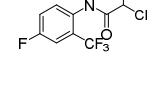
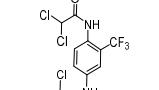
MCF-7 cells were cultured on 24-well plate at a density of 2×10^5 cells/mL and allowed to grow overnight at 37 °C. Cells were treated with DCA (10 mM and 20 μ M), **15**, **26** and **39** (20 μ M) for 8 h at 37 °C. A solution of JC-1 reagent (10 g/mL in PBS buffer) was added and incubation was carried out at 37 °C for 20 min. The cells were washed 3 times with PBS, and live cell imaging was performed in PBS buffer.

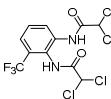
Statistical analysis

Data are reported as Mean \pm SD. Statistical analysis was performed using GraphPad Prism version 6.0 for Windows. * $p < 0.05$ is considered as statistically significant.

Table S1: Cytotoxic assay for the prepared compounds against A549 and MCF-7

Compounds	Structure	Purity (%) ^a	Inhibition rate (%)				-logP _{app} ^c	ClogP
			A549		MCF-7			
			40 (μM)	2 (μM)	40 (μM)	2 (μM)		
5		95.12	17.93	NI ^b	16.62	NI	4.94	2.65
6		94.72	8.06	NI	13.64	NI	5.03	2.81
7		95.39	8.82	NI	15.85	NI	4.90	2.80
8		97.09	6.43	NI	22.68	NI	4.92	3.15
9		95.37	16.94	NI	24.17	NI	4.90	2.65
10		96.21	10.05	NI	20.76	NI	5.06	1.80
11		97.01	5.21	NI	21.51	NI	5.15	2.65
12		97.77	4.07	NI	11.19	NI	4.87	1.80
13		96.35	0.63	NI	12.37	NI	4.89	2.82
14		96.61	12.38	NI	11.81	NI	4.88	2.64
15		95.78	80.67	6.09	67.47	NI	5.22	1.43
17		96.42	8.23	NI	2.63	NI	5.15	1.55
19		96.68	5.47	NI	8.89	NI	5.27	1.80
22		94.95	12.43	8.35	6.16	NI	5.06	2.24
23		96.07	10.08	5.81	10.13	NI	5.37	1.91
24		97.20	5.31	NI	10.49	NI	5.06	3.11
26		96.71	73.89	8.45	65.15	NI	5.45	0.93

27		95.25	36.66	8.19	54.47	NI	5.45	3.69
28		95.95	12.25	NI	15.80	NI	5.03	2.50
29		96.09	15.26	NI	13.03	NI	4.95	2.30
30		95.42	37.09	NI	23.50	NI	5.39	3.15
32		97.11	3.55	NI	5.00	NI	4.97	2.09
34		95.05	11.58	NI	NI	NI	4.72	3.35
35		95.57	5.63	NI	NI	NI	5.70	3.39
36		96.13	8.72	NI	NI	NI	5.03	4.04
38		95.33	11.21	NI	5.87	NI	NT	3.17
39		98.64	97.81	NI	94.05	NI	5.04	4.42
40		95.47	1.09	NI	23.27	NI	NT	3.77
41		97.11	34.58	NI	32.97	NI	NT	3.77
43		95.55	1.45	NI	26.05	NI	5.41	0.89
44		96.32	5.32	NI	20.87	NI	5.58	1.46
45		95.02	1.23	NI	21.38	NI	5.53	4.60
46		95.93	1.22	NI	26.20	NI	5.24	3.16
47		95.31	0.45	NI	26.22	NI	5.44	1.85
50		96.23	NI	NI	NT ^d	NT	NT	2.60
52		97.64	33.2%	NI	NT	NT	NT	2.85

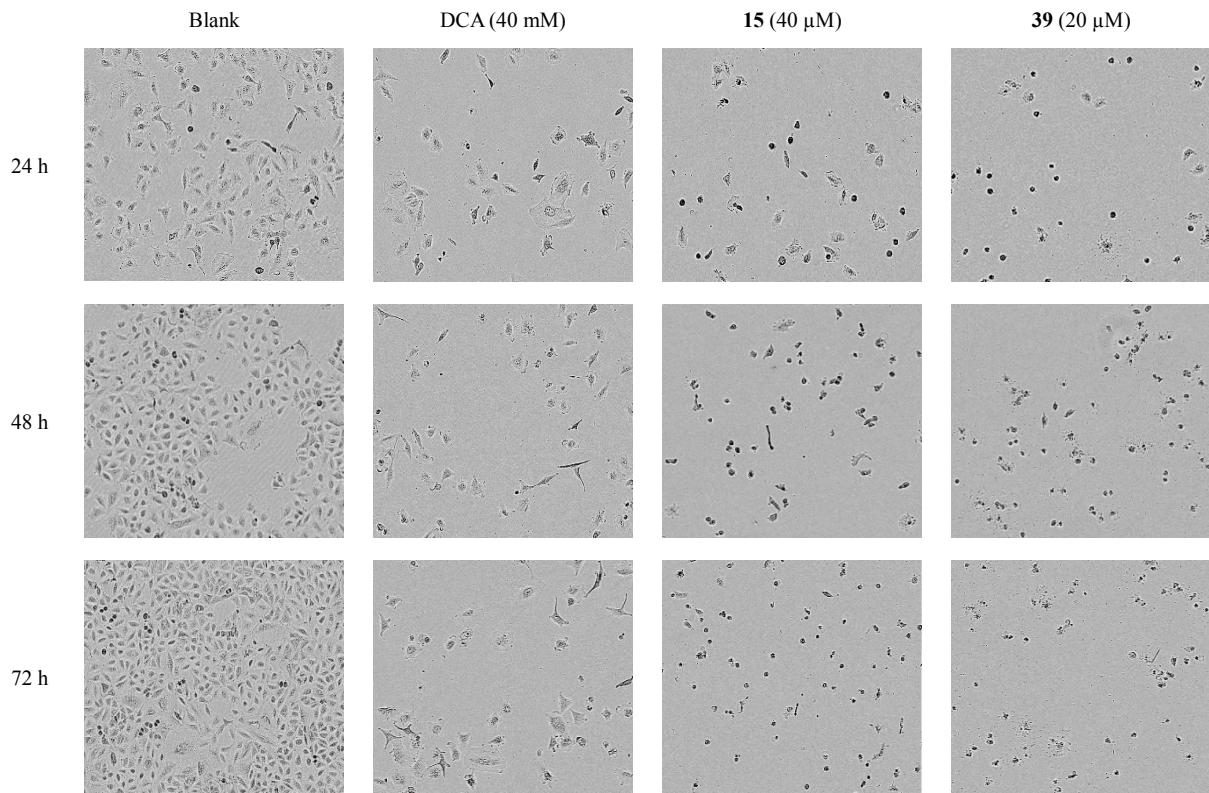
53		95.83	12.1%	NI	NT	NT	NT	2.64
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^a All tested compounds exhibited purities of > 95 % as analyzed by HPLC (Agilent HPLC 1260, USA). ^b NI = no inhibition; ^c The permeability data (-logP_{app}) were determined by using the PAMPA assay (Pion Inc, USA); ^d NT = not test

Figure S1

Cell growth behavior after treatments of the DCA, **15**, **26** and **39**.

For A549



For MCF-7

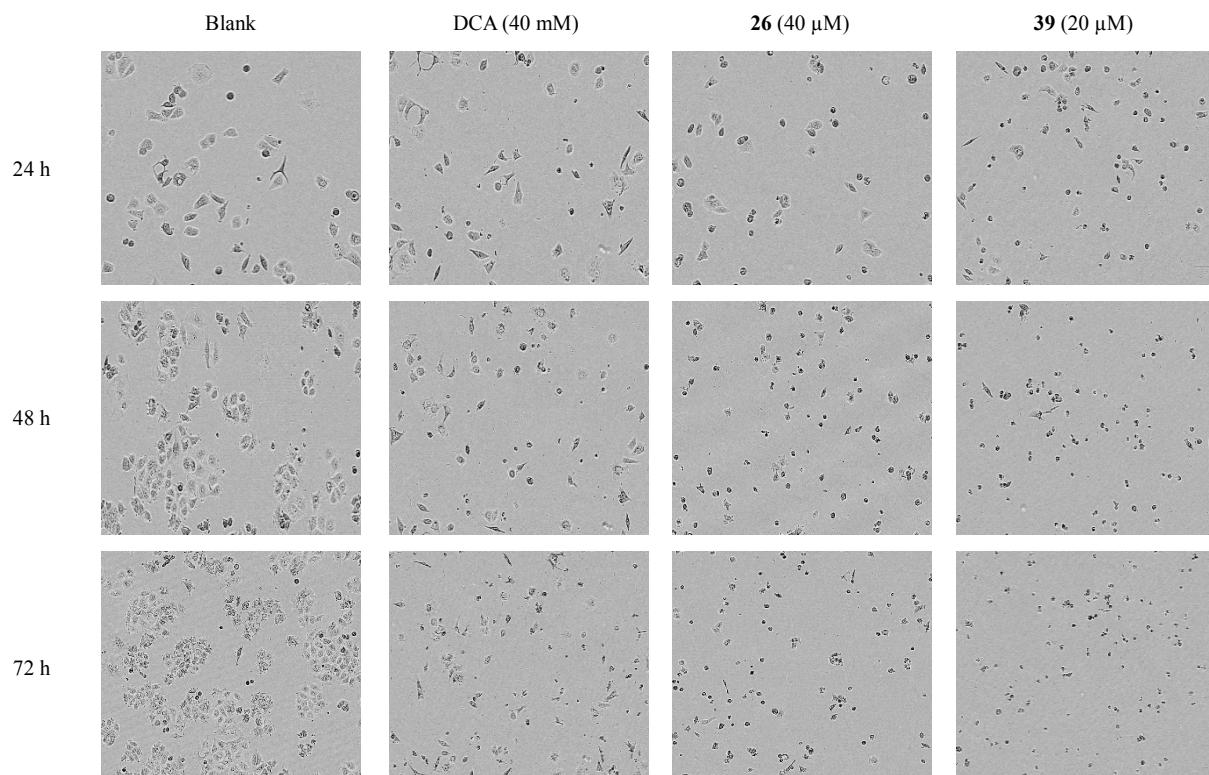


Figure S2

The exact IC₅₀ values for **15**, **26** **39** and DCA against the cancer cells proliferation

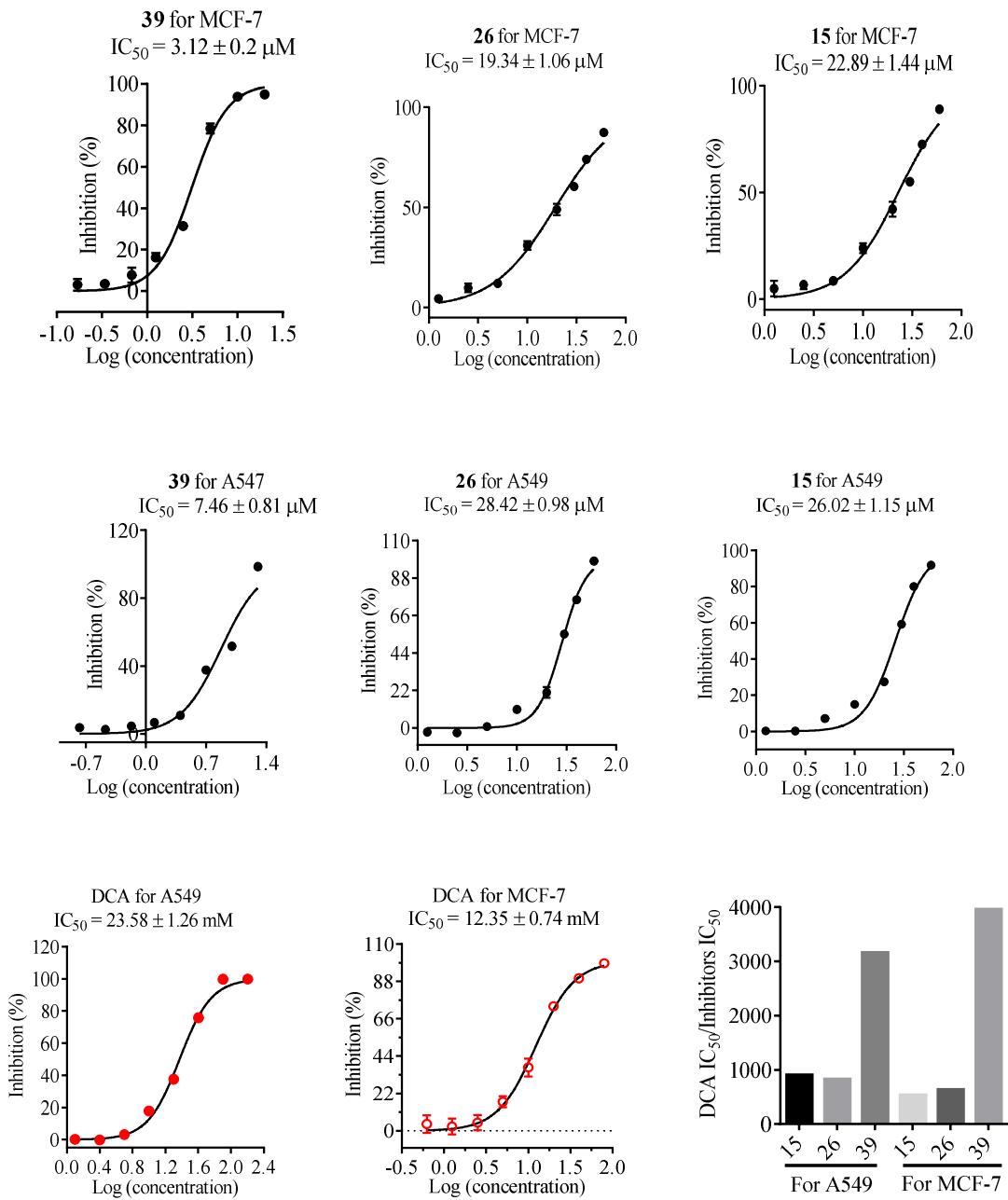
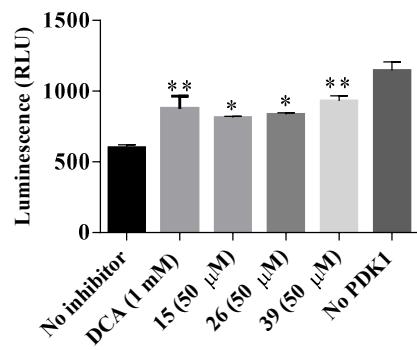
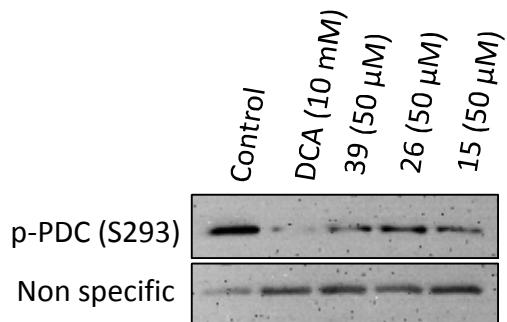


Figure S3



DCA at 1 mM, and compounds **15**, **26** and **39** at 50 μ M reduced the phosphorylation level of peptide fragment around Ser 293 site of PDC. * $P < 0.05$, versus no inhibitor control group.

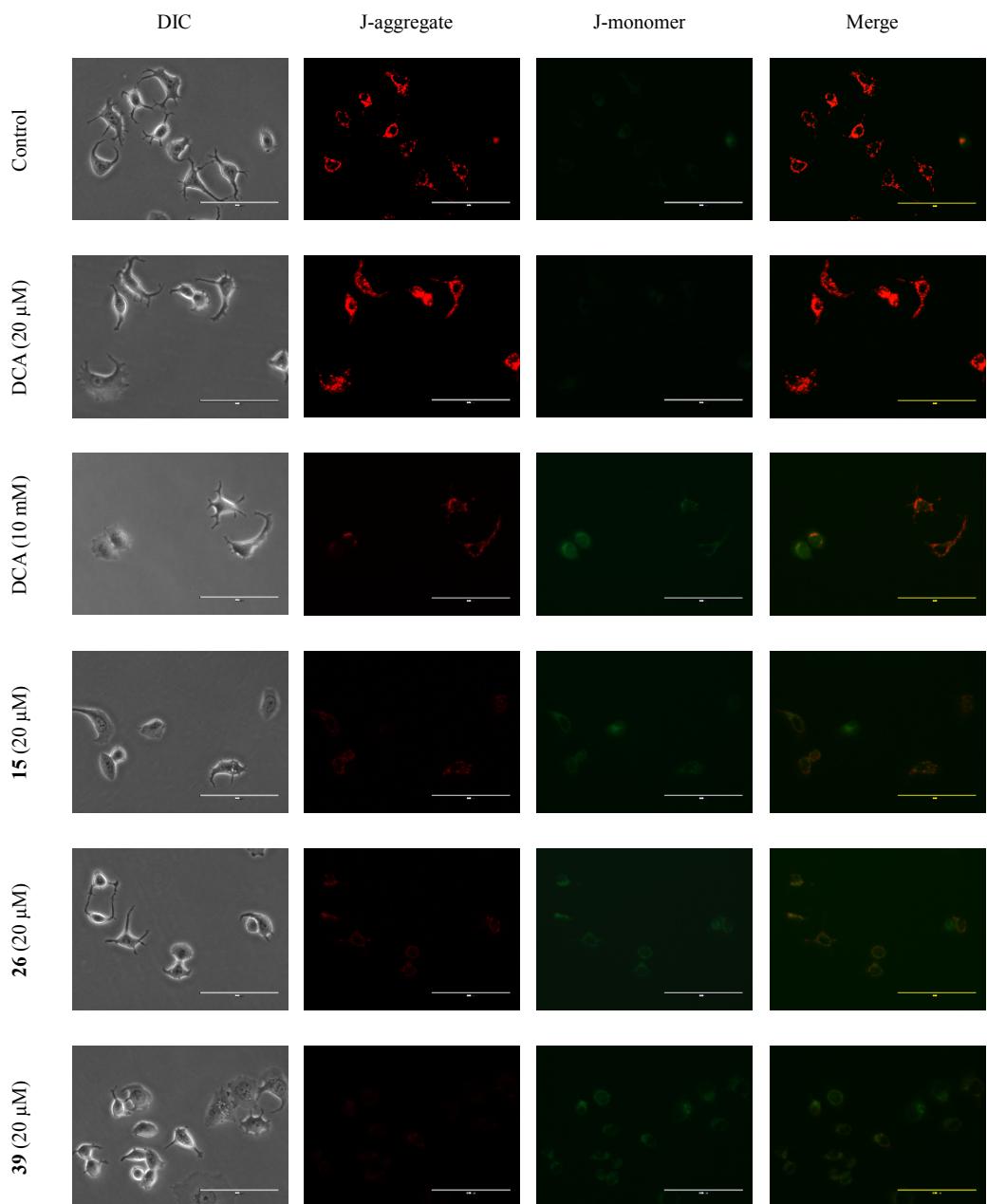
Figure S4



DCA, **15**, **26** and **39** inhibit the phosphorylation of PDC by PDK.

Figure S5

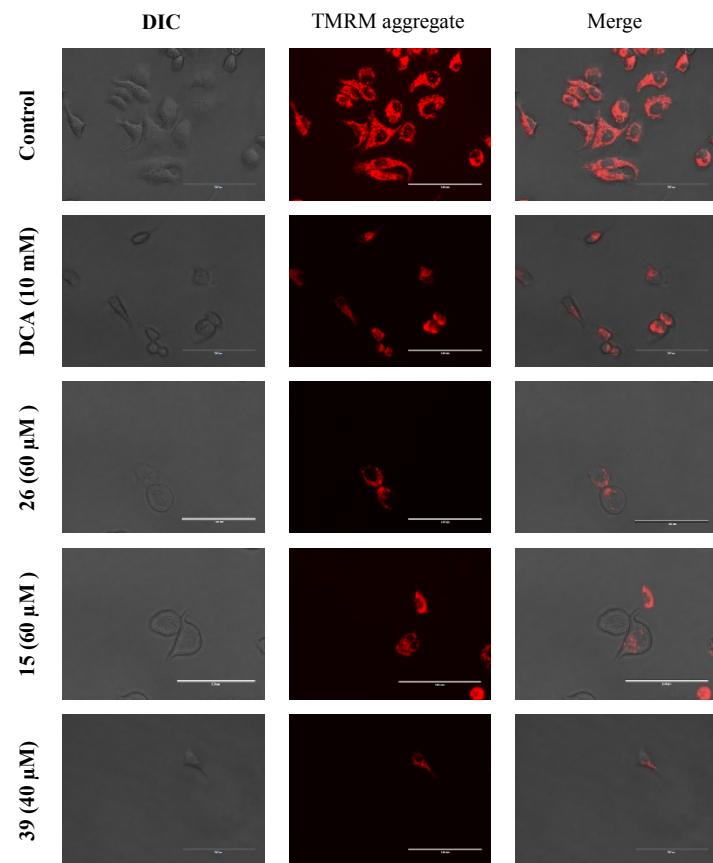
Changes in the mitochondria membrane potential (MMP) after treatment of DCA, compounds **15**, **26** and **39** measured by the JC-1 assay.



Control: Treatment of MCF-7 cells without any inhibitor. Green fluorescence, depolarized (J-monomer) mitochondria; red fluorescence, hyperpolarized (J-aggregates). DIC: Differential Interference Contrast.

Figure S6

Depolarization of MMP after treatment of DCA, compounds **15**, **26** and **39** measured by TMRM live cell imaging assay



Compared with control group, DCA could depolarized mitochondrial membrane potential (MMP) of MCF-7 cell at very high concentration (10 mM). Note that **39** significantly depolarized the MMP at a concentration of 40 μ M.

Synthesis of the DCA analogues

Synthesis of the 2,2-dichloro-N-(5-chloropyridin-2-yl)acetamide (5): A mixture of 5-chloropyridin-2-amine (1.29 g, 10 mmol) and Et₃N (1.67 mL, 12 mmol) were stirred in the DCM (20 mL) at ice bath. Then 2, 2-dichloroacetyl chloride (1.06 mL, 11 mmol) was added with dropwise. After completion of the reaction, the mixture was extracted with saturated brine (3 x 30 mL), then the combined organic phase was dried over anhydrous sodium sulfate and subsequently the solvent was evaporated under reduced pressure. The residue was purified by silica gel column chromatography (eluent, petroleum/ethyl acetate, 10/1, V/V) to obtain the compound **5** (1.20 g) as pale yellow solid. m.p. 105-106 °C. Yield: 50.4 %. ¹H NMR (400 MHz, DMSO-*d*₆): δ 11.39 (s, 1H), 8.45 (dd, 1H, *J* = 0.4, 2.4 Hz), 8.07 (d, 1H, *J* = 8.8 Hz), 8.00 (dd, 1H, *J* = 2.4, 4.8 Hz), 6.67 (s, 1H) ppm; ¹³C NMR (100 MHz, DMSO-*d*₆): δ 162.49, 149.46, 146.96, 138.56, 126.65, 115.09, 66.80; HRMS (ESI) calcd. for C₇H₆Cl₃N₂O [M+H]⁺, 238.9546; found, 238.9570.

2,2-Dichloro-N-(3-chloro-5-(trifluoromethyl)pyridin-2-yl)acetamide (6): Compound **6** was prepared according to the procedure depicted for **1-5**, starting from 3-chloro-5-(trifluoromethyl)pyridin-2-amine (1.96 g, 10 mmol), Et₃N (1.67 mL, 12 mmol) and 2, 2-dichloroacetyl chloride (1.06 mL, 11 mmol). The product (1.72 g) was obtained as slight yellow solid. m.p. 127-129 °C. Yield: 56.0 %. ¹H NMR (400 MHz, DMSO-*d*₆): δ 11.31 (s, 1H), 8.88 (d, 1H, *J* = 0.8 Hz), 8.61 (d, 1H, *J* = 2 Hz), 6.78 (s, 1H) ppm; ¹³C NMR (100 MHz, DMSO-*d*₆): δ 162.28, 150.35, 144.32, 144.28, 136.99, 136.96, 126.86, 126.46, 125.26, 124.93, 124.60, 124.27, 124.15, 121.44, 66.56; HRMS (ESI) calcd. for C₈H₅Cl₃F₃N₂O [M+H]⁺, 306.9420; found, 306.9418.

N-(6-Bromopyridin-2-yl)-2,2-dichloroacetamide (7): m.p. 143-144 °C. ¹H NMR (400 MHz, DMSO-*d*₆): δ 11.57 (s, 1H), 8.04 (d, 1H, *J* = 8.4 Hz), 7.82 (t, 1H, *J* = 15.6 Hz), 7.45 (d, 1H, *J* = 7.6 Hz), 6.63 (s, 1H) ppm; ¹³C NMR (100 MHz, DMSO-*d*₆): δ 162.50, 150.97, 142.04, 139.16, 124.50, 112.90, 66.72; HRMS (ESI) calcd. for C₇H₆BrCl₂N₂O [M+H]⁺, 282.9041; found, 282.9069.

2,2-Dichloro-N-(6-chloro-5-methylpyridin-3-yl)acetamide (8): m.p. 137-138 °C. Yield: 64.0 %. ¹H NMR (400 MHz, DMSO-*d*₆): δ 10.42 (s, 1H), 8.15 (d, 1H, *J* = 1.6 Hz), 7.96 (d, 1H, *J* = 2 Hz), 6.83 (s, 1H) ppm; ¹³C NMR (100 MHz, DMSO-*d*₆): δ 162.93, 147.11, 141.66, 135.49, 133.69, 129.97, 66.64; HRMS (ESI) calcd. for C₈H₈Cl₃N₂O [M+H]⁺, 252.9702; found, 252.9734.

2,2-Dichloro-N-(6-chloropyridin-2-yl)acetamide (9): m.p. 135-136 °C. Yield: 79.2 %. ¹H NMR (400 MHz, DMSO-*d*₆): δ 11.54 (s, 1H), 8.02 (d, 1H, *J* = 8 Hz), 7.93 (t, 1H, *J* = 8 Hz), 7.32 (d, 1H, *J* = 7.6), 6.63 (s, 1H) ppm; ¹³C NMR (100 MHz, DMSO-*d*₆): δ 162.54, 150.78, 148.40, 142.40, 120.69, 112.62, 66.74; HRMS (ESI) calcd. for C₇H₆Cl₃N₂O [M+H]⁺, 238.9546; found, 238.9576.

2,2-Dichloro-N-(4-chloropyridin-3-yl)acetamide (10): m.p. 104-105 °C. Yield: 53.6 %. ¹H NMR (400 MHz, DMSO-*d*₆): δ 10.62 (s, 1H), 8.74 (s, 1H), 8.45 (d, 1H, *J* = 5.2 Hz), 7.68 (d, 1H, *J* = 5.2 Hz), 6.81 (s, 1H) ppm; ¹³C NMR (100 MHz, DMSO-*d*₆): δ 163.09,

148.49, 148.01, 138.15, 130.58, 124.99, 66.63; HRMS (ESI) calcd. for C₇H₆Cl₃N₂O [M+H]⁺, 238.9546; found, 238.9602.

2,2-Dichloro-N-(6-chloropyridin-3-yl)acetamide (11): m.p. 110-111 °C. Yield: 75.3 %. ¹H NMR (400 MHz, DMSO-d₆): δ 11.04 (s, 1H), 8.61 (d, 1H, J = 2.4 Hz), 8.10 (dd, 1H, J = 2.8, 8.4 Hz), 7.52 (d, 1H, J = 8.8 Hz), 6.64 (s, 1H) ppm; ¹³C NMR (100 MHz, DMSO-d₆): δ 162.50, 145.15, 141.21, 134.14, 130.74, 124.58, 67.08; HRMS (ESI) calcd. for C₇H₆Cl₃N₂O [M+H]⁺, 238.9546; found, 238.9552.

2,2-Dichloro-N-(2-chloropyridin-3-yl)acetamide (12): m.p. 96-97 °C. Yield: 80.7 %. ¹H NMR (400 MHz, DMSO-d₆): δ 10.48 (s, 1H), 8.31 (q, 1H), 8.13 (q, 1H), 7.50 (q, 1H), 6.84 (s, 1H) ppm; ¹³C NMR (100 MHz, DMSO-d₆): δ 162.97, 147.02, 144.39, 135.14, 130.70, 123.78, 66.64; HRMS (ESI) calcd. for C₇H₆Cl₃N₂O [M+H]⁺, 238.9546; found, 238.9552.

2,2-Dichloro-N-(4,6-dimethylpyridin-2-yl)acetamide (13): m.p. 109-110 °C. Yield: 78.3 %. ¹H NMR (400 MHz, DMSO-d₆): δ 11.07 (s, 1H), 7.71 (s, 1H), 6.91 (s, 1H), 6.66 (s, 1H), 2.37 (s, 3H), 2.29 (s, 3H) ppm; ¹³C NMR (100 MHz, DMSO-d₆): δ 162.14, 156.72, 150.18, 149.87, 121.00, 111.40, 66.90, 23.39, 20.89; HRMS (ESI) calcd. for C₉H₁₁Cl₂N₂O [M+H]⁺, 233.0248; found, 233.0335.

2,2-Dichloro-N-(4-chloropyridin-2-yl)acetamide (14): m.p. 111-112 °C. Yield: 75.6 %. ¹H NMR (400 MHz, DMSO-d₆): δ 11.49 (s, 1H), 8.38 (d, 1H, J = 5.6 Hz), 8.10 (d, 1H, J = 1.6 Hz), 7.36 (dd, 1H, J = 2, 5.2 Hz), 6.68 (s, 1H) ppm; ¹³C NMR (100 MHz, DMSO-d₆): δ 162.78, 151.94, 149.94, 144.53, 120.87, 113.56, 66.71; HRMS (ESI) calcd. for C₇H₆Cl₃N₂O [M+H]⁺, 238.9546; found, 238.9570.

2,2-Dichloro-N-(4,6-dimethylpyrimidin-2-yl)acetamide (17): m.p. 134-135 °C. Yield: 32.1 %. ¹H NMR (400 MHz, DMSO-d₆): δ 11.13 (s, 1H), 7.04 (s, 1H), 6.81 (s, 1H), 2.38 (s, 6H) ppm; ¹³C NMR (100 MHz, DMSO-d₆): δ 168.15, 156.40, 116.49, 67.08, 23.41; HRMS (ESI) calcd. for C₈H₁₀Cl₂N₃O [M+H]⁺, 234.0201; found, 234.0302.

2,2-Dichloro-N-(4-chloro-6-methylpyrimidin-2-yl)acetamide (19): m.p. 126-127 °C. Yield: 54.4 %. ¹H NMR (400 MHz, DMSO-d₆): δ 11.54 (s, 1H), 7.37 (s, 1H), 6.71 (s, 1H), 2.44 (s, 3H) ppm; ¹³C NMR (100 MHz, DMSO-d₆): δ 171.18, 161.44, 160.37, 156.39, 116.77, 66.94, 23.41; HRMS (ESI) calcd. for C₇H₇Cl₃N₃O [M+H]⁺, 253.9655; found, 253.9712.

2,2-Dichloro-N-(4-chloro-6-methoxypyrimidin-2-yl)acetamide (22): m.p. 142-143 °C. Yield: 53.4 %. ¹H NMR (400 MHz, DMSO-d₆): δ 11.51 (s, 1H), 6.91 (s, 1H), 6.74 (s, 1H), 3.96 (s, 3H) ppm; ¹³C NMR (100 MHz, DMSO-d₆): δ 171.27, 161.57, 160.11, 156.16, 102.80, 66.95, 54.97; HRMS (ESI) calcd. for C₇H₇Cl₃N₃O₂ [M+H]⁺, 269.9604; found, 269.9649.

2,2-Dichloro-N-(2-chloropyrimidin-5-yl)acetamide (23): m.p. 108-109 °C. Yield: 57.2 %. ¹H NMR (400 MHz, DMSO-d₆): δ 11.27 (s, 1H), 8.98 (s, 2H), 6.70 (s, 1H) ppm; ¹³C NMR

(100 MHz, DMSO-*d*₆): δ 162.82, 154.51, 151.09, 132.94, 66.79; HRMS (ESI) calcd. for C₆H₅Cl₃N₃O [M+H]⁺, 239.9498; found, 239.9504.

2,2-Dichloro-N-(6-chloro-2-(methylthio)pyrimidin-4-yl)acetamide (24): m.p. 146-147 °C. Yield: 53.4 %. ¹H NMR (400 MHz, DMSO-*d*₆): δ 11.87 (s, 1H), 7.73 (s, 1H), 6.63 (s, 1H), 2.53 (s, 3H) ppm; ¹³C NMR (100 MHz, DMSO-*d*₆): δ 172.29, 163.74, 161.02, 158.17, 104.67, 66.49, 13.72; HRMS (ESI) calcd. for C₇H₇Cl₃N₃OS [M+H]⁺, 285.9375; found, 285.9409.

2,2-Dichloro-N-(2-chloro-6,7-dimethoxyquinazolin-4-yl)acetamide (27): m.p. > 200 °C. Yield: 30.4 %. ¹H NMR (400 MHz, DMSO-*d*₆): δ 11.57 (s, 1H), 7.49 (s, 1H), 7.37 (s, 1H), 7.02 (s, 1H), 3.99 (s, 3H), 3.93 (s, 3H) ppm; ¹³C NMR (100 MHz, DMSO-*d*₆): δ 163.36, 156.95, 155.86, 153.12, 150.81, 150.15, 110.96, 106.35, 102.36, 67.01, 56.58, 56.23; HRMS (ESI) calcd. for C₁₂H₁₁Cl₃N₃O₃ [M+H]⁺, 349.9866; found, 349.9896.

2,2-Dichloro-N-(6-chloro-4-methylpyridin-3-yl)acetamide (28): m.p. 144-145 °C. Yield: 84.9 %. ¹H NMR (400 MHz, DMSO-*d*₆): δ 10.37 (s, 1H), 8.35 (s, 1H), 7.52 (s, 1H), 6.75 (s, 1H), 2.23 (s, 3H) ppm; ¹³C NMR (100 MHz, DMSO-*d*₆): δ 163.05, 147.50, 146.42, 146.20, 131.79, 125.55, 66.85, 17.04; HRMS (ESI) calcd. for C₈H₈Cl₃N₂O [M+H]⁺, 252.9702; found, 252.9722.

2,2-Dichloro-N-(2-chloro-6-methylpyridin-3-yl)acetamide (29): m.p. 112-113 °C. Yield: 69.1 %. ¹H NMR (400 MHz, DMSO-*d*₆): δ 10.40 (s, 1H), 7.96 (d, 1H, J = 7.2 Hz), 7.34 (d, 1H, J = 8 Hz), 6.80 (s, 1H), 2.46 (s, 3H) ppm; ¹³C NMR (100 MHz, DMSO-*d*₆): δ 162.87, 156.45, 143.55, 135.67, 127.90, 123.04, 66.64, 23.17; HRMS (ESI) calcd. for C₈H₈Cl₃N₂O [M+H]⁺, 252.9702; found, 252.9712.

2,2-dichloro-N-(5-chloro-6-methylpyridin-3-yl)acetamide (30): m.p. 128-129 °C. Yield: 73.0 %. ¹H NMR (400 MHz, DMSO-*d*₆): δ 10.97 (s, 1H), 8.44 (d, 1H, J = 2.4 Hz), 8.04 (d, 1H, J = 2.4 Hz), 6.64 (s, 1H), 2.34 (s, 3H) ppm; ¹³C NMR (100 MHz, DMSO-*d*₆): δ 162.45, 145.49, 138.62, 134.05, 132.49, 130.94, 67.08, 19.29; HRMS (ESI) calcd. for C₈H₈Cl₃N₂O [M+H]⁺, 252.9702; found, 252.9763.

N-([1,1'-Biphenyl]-2-yl)-2,2-dichloroacetamide (34): m.p. 103-104 °C. Yield: 78.6 %. ¹H NMR (400 MHz, DMSO-*d*₆): δ 10.04 (s, 1H), 7.49-7.46 (m, 1H), 7.46-7.41 (m, 3H), 7.40-7.37 (m, 3H), 7.37-7.35 (m, 1H), 6.54 (s, 1H) ppm; HRMS (ESI) calcd. for C₁₄H₁₂Cl₂NO [M+H]⁺, 280.0296; found, 280.0304.

2,2-Dichloro-N-(5-chlorobenzo[d]oxazol-2-yl)acetamide (35): m.p. 199-200 °C. Yield: 28.6 %. ¹H NMR (400 MHz, DMSO-*d*₆): δ 7.67-7.43 (m, 2H), 7.32 (d, 1H, J = 8 Hz), 6.69 (s, 1H) ppm; HRMS (ESI) calcd. for C₉H₆Cl₃N₂O₂ [M+H]⁺, 278.9495; found, 278.9491.

2,2-Dichloro-N-(6-chlorobenzo[d]thiazol-2-yl)acetamide (36): m.p. 177-178 °C. Yield: 56.2 %. ¹H NMR (400 MHz, DMSO-*d*₆): δ 8.08 (d, 1H, J = 2 Hz), 7.70 (d, 1H, J = 8.4 Hz), 7.42 (dd, 1H, J = 2, 8.4 Hz), 6.70 (s, 1H) ppm; ¹³C NMR (100 MHz, DMSO-*d*₆): δ 164.07,

159.34, 146.29, 133.02, 128.43, 126.95, 121.81, 121.62; HRMS (ESI) calcd. for C₉H₆Cl₃F₃N₂OS [M+H]⁺, 294.9266; found, 294.9267.

2,2-Dichloro-N-(4-chloro-3-(trifluoromethyl)phenyl)acetamide (38): m.p. 108-109 °C. Yield: 54.4 %. ¹H NMR (400 MHz, DMSO-d₆): δ 10.43 (s, 1H), 7.88 (d, 1H, J = 2 Hz), 7.82 (dd, 1H, J = 2, 19.2 Hz), 7.54 (d, 1H, J = 8.8 Hz), 6.73 (s, 1H) ppm.

2,2-Dichloro-N-(2-chloro-4-(trifluoromethyl)phenyl)acetamide (40): m.p. 79-81 °C. Yield: 78.9 %. ¹H NMR (400 MHz, DMSO-d₆): δ 10.53 (s, 1H), 7.98 (d, 2H, J = 7.6 Hz), 7.78 (dd, 1H, J = 1.2, 8.4 Hz), 6.89 (s, 1H) ppm; ¹³C NMR (100 MHz, DMSO-d₆): δ 162.90, 137.41, 128.02, 127.70, 127.52, 127.37, 127.09, 126.98, 126.44, 125.05, 124.94, 124.67, 121.98, 119.26 66.68.

2,2-Dichloro-N-(2-chloro-5-(trifluoromethyl)phenyl)acetamide (41): m.p. 90-91 °C. Yield: 59.2 %. ¹H NMR (400 MHz, DMSO-d₆): δ 10.54 (s, 1H), 8.08 (d, 1H, J = 1.6 Hz), 7.80 (d, 1H, J = 8.4 Hz), 7.65 (dd, 2H, J = 1.6, 8.4 Hz), 6.86 (s, 1H) ppm; ¹³C NMR (100 MHz, DMSO-d₆): δ 163.03, 134.53, 131.56, 131.21, 128.91, 128.58, 128.26, 127.93, 124.89, 124.16, 122.77, 122.73, 122.18, 119.48, 66.66.

2,2-Dichloro-N-(4,6-difluoropyrimidin-2-yl)acetamide (43): m.p. 115-116 °C. Yield: 37.2 %. ¹H NMR (400 MHz, DMSO-d₆): δ 11.89 (s, 1H), 7.08 (S, 1H), 6.65 (s, 1H) ppm; ¹³C NMR (100 MHz, DMSO-d₆): δ 173.43, 173.22, 161.40, 156.44, 156.22, 156.00, 89.02, 88.65, 88.27, 66.83; HRMS (ESI) calcd. for C₆H₄Cl₂F₂N₃O [M+H]⁺, 241.9699; found, 241.9689.

2,2-Dichloro-N-(6-chloro-5-fluoropyrimidin-4-yl)acetamide (44): m.p. 154-155 °C. Yield: 37.2 %. ¹H NMR (400 MHz, DMSO-d₆): δ 11.77 (s, 1H), 7.08 (S, 1H), 8.73 (d, 1H, J = 0.4 Hz), 6.79 (s, 1H) ppm; ¹³C NMR (100 MHz, DMSO-d₆): δ 162.03, 153.16, 153.05, 147.47, 147.31, 146.62, 146.51, 146.02, 143.33, 66.38; HRMS (ESI) calcd. for C₆H₄Cl₃FN₃O [M+H]⁺, 257.9404; found, 257.9406.

2,2-Dichloro-N-(5-fluoropyrimidin-2-yl)acetamide (45): m.p. 149-150 °C. Yield: 37.2 %. ¹H NMR (400 MHz, DMSO-d₆): δ 11.45 (s, 1H), 8.83 (s, 1H), 6.70 (s, 1H) ppm; ¹³C NMR (100 MHz, DMSO-d₆): δ 161.36, 156.16, 153.60, 153.14, 153.11, 146.68, 146.46, 67.02; HRMS (ESI) calcd. for C₆H₅Cl₂FN₃O [M+H]⁺, 223.9794; found, 223.9800.

3-(2,2-Dichloroacetamido)-4-hydroxybenzenesulfonyl fluoride (46): m.p. 119-120 °C. Yield: 66.7 %. ¹H NMR (400 MHz, DMSO-d₆): δ 10.72 (s, 1H), 8.50 (d, 1H, J = 2 Hz), 8.05-7.99 (m, 2H), 6.88 (s, 1H) ppm; ¹³C NMR (100 MHz, DMSO-d₆): δ 163.20, 135.46, 135.43, 132.27, 130.74, 130.49, 126.81, 125.08, 66.55; HRMS (ESI) calcd. for C₈H₇Cl₂FNO₄S [M+H]⁺, 301.9457; found, 301.9463.

2,2-Dichloro-N-(2-hydroxy-5-(piperazin-1-ylsulfonyl)phenyl)acetamide (47): m.p. 146-147 °C. Yield: 66.7 %. ¹H NMR (400 MHz, DMSO-d₆): δ 8.57 (s, 1H), 8.37 (d, 1H, J = 8.4 Hz), 8.12 (dd, 1H, J = 2, 8.4 Hz), 7.43 (d, 1H, J = 4 Hz), 6.27 (s, 1H), 3.39 (t, 4H, J = 4.2 Hz), 3.31 (t, 3H, J = 4.8 Hz), 3.01 (m, 1H) ppm; ¹³C NMR (100 MHz, DMSO-d₆): δ

163.05, 134.79, 131.14, 132.03, 131.04, 126.08, 124.72, 66.87, 55.01, 46.69, 44.68; HRMS (ESI) calcd. for $C_{12}H_{16}Cl_2N_3O_4S$ $[M+H]^+$, 368.0239; found, 368.0245.

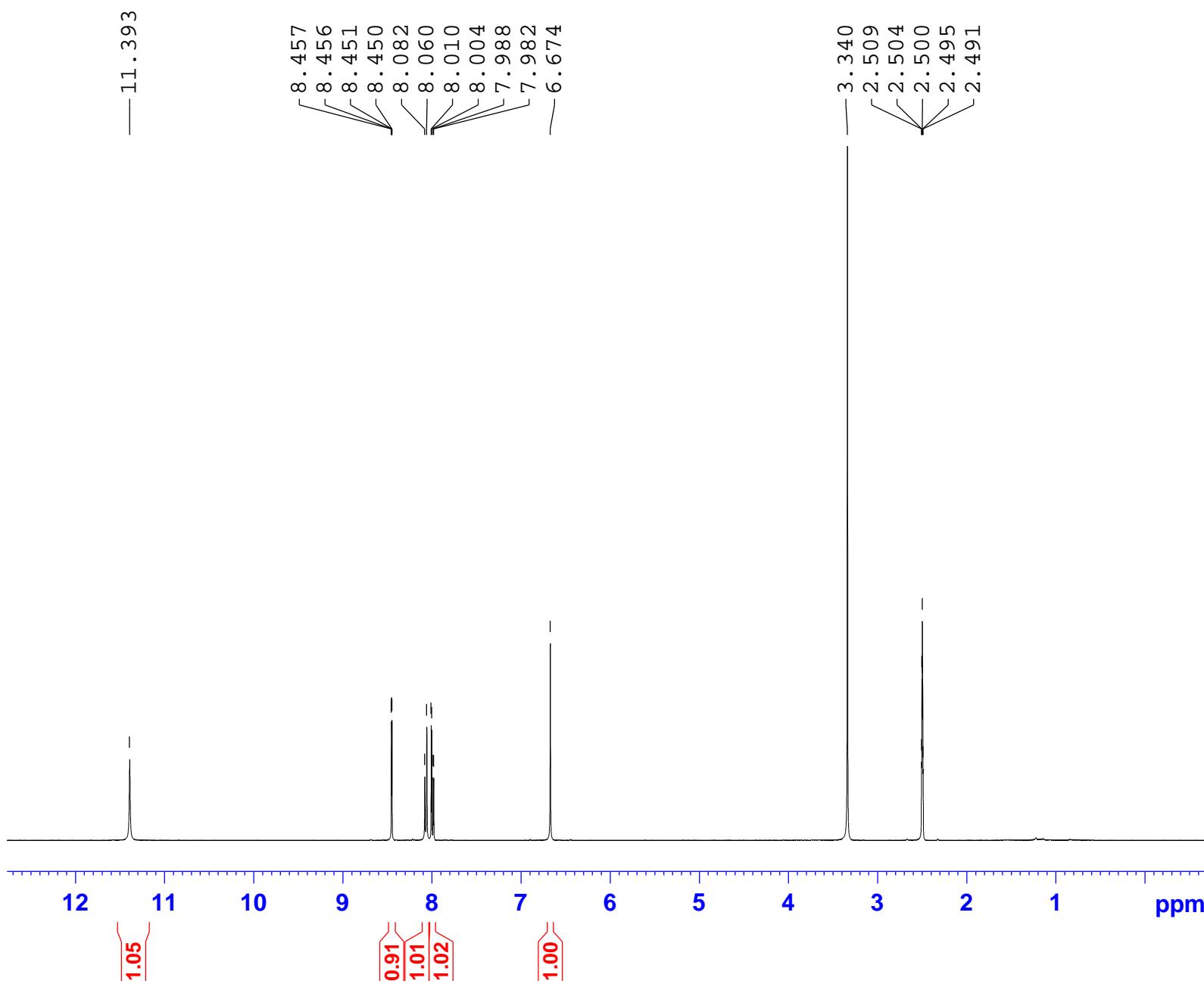
2,2-Dichloro-N-(4-fluoro-2-(trifluoromethyl)phenyl)acetamide (50): m.p. 120-121 °C. Yield: 66.7 %. 1H NMR (400 MHz, DMSO- d_6): δ 10.39 (s, 1H), 7.72 (m, 1H), 7.76 (m, 1H), 7.53 (m, 1H), 6.71 (s, 1H) ppm; ^{13}C NMR (100 MHz, DMSO- d_6): δ 164.09, 161.99, 159.54, 133.34, 133.26, 130.56, 130.54, 128.44, 128.36, 128.14, 128.05, 127.83, 127.74, 127.52, 127.44, 126.95, 126.92, 124.22, 124.20, 121.50, 120.97, 114.90, 114.49, 66.93.

***N,N'*-(2-(Trifluoromethyl)-1,4-phenylene)bis(2,2-dichloroacetamide) (52):** m.p. 161-162 °C. Yield: 54.2 %. 1H NMR (400 MHz, DMSO- d_6): δ 11.08 (s, 1H), 10.35 (s, 1H), 8.10 (d, 1H, J = 2.4 Hz), 7.90 (dd, 1H, J = 2.4, 8.8 Hz), 7.50 (d, 1H, J = 8.4 Hz), 6.71 (s, 1H), 6.64 (s, 1H) ppm; ^{13}C NMR (100 MHz, DMSO- d_6): δ 163.99, 162.79, 137.51, 131.67, 130.01, 127.47, 126.86, 126.26, 125.96, 124.75, 124.54, 122.03, 119.31, 117.93, 117.88, 117.77, 67.63, 66.98; HRMS (ESI) calcd. for $C_{11}H_8Cl_4N_2O_2F_3$ $[M+H]^+$, 396.9292; found, 396.9292.

***N,N'*-(3-(Trifluoromethyl)-1,2-phenylene)bis(2,2-dichloroacetamide) (53):** m.p. 203-204 °C. Yield: 39.2 %. 1H NMR (400 MHz, DMSO- d_6): δ 10.25 (s, 1H), 10.23 (s, 1H), 7.90 (d, 1H, J = 8 Hz), 7.73-7.62 (m, 2H), 6.69 (s, 1H), 6.66 (s, 1H) ppm; ^{13}C NMR (100 MHz, DMSO- d_6): δ 163.41, 163.07, 136.35, 130.16, 129.59, 128.46, 128.08, 127.76, 126.60, 124.80, 124.72, 122.08, 66.98, 66.75; HRMS (ESI) calcd. for $C_{11}H_8Cl_4N_2O_2F_3$ $[M+H]^+$, 396.9292; found, 396.9281.

1H NMR, ^{13}H NMR, HRMS and HPLC spectra

zsl-1-5-h



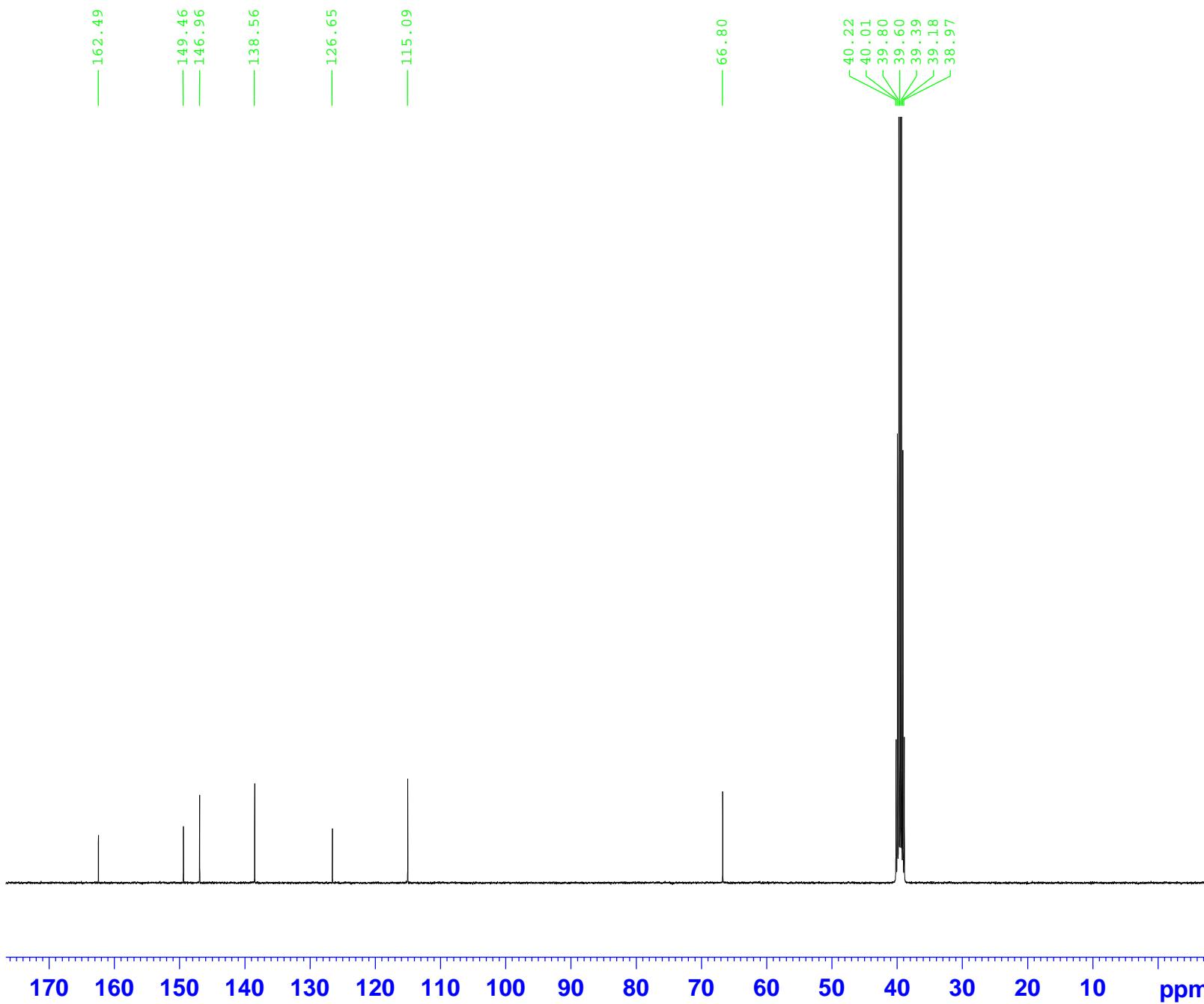
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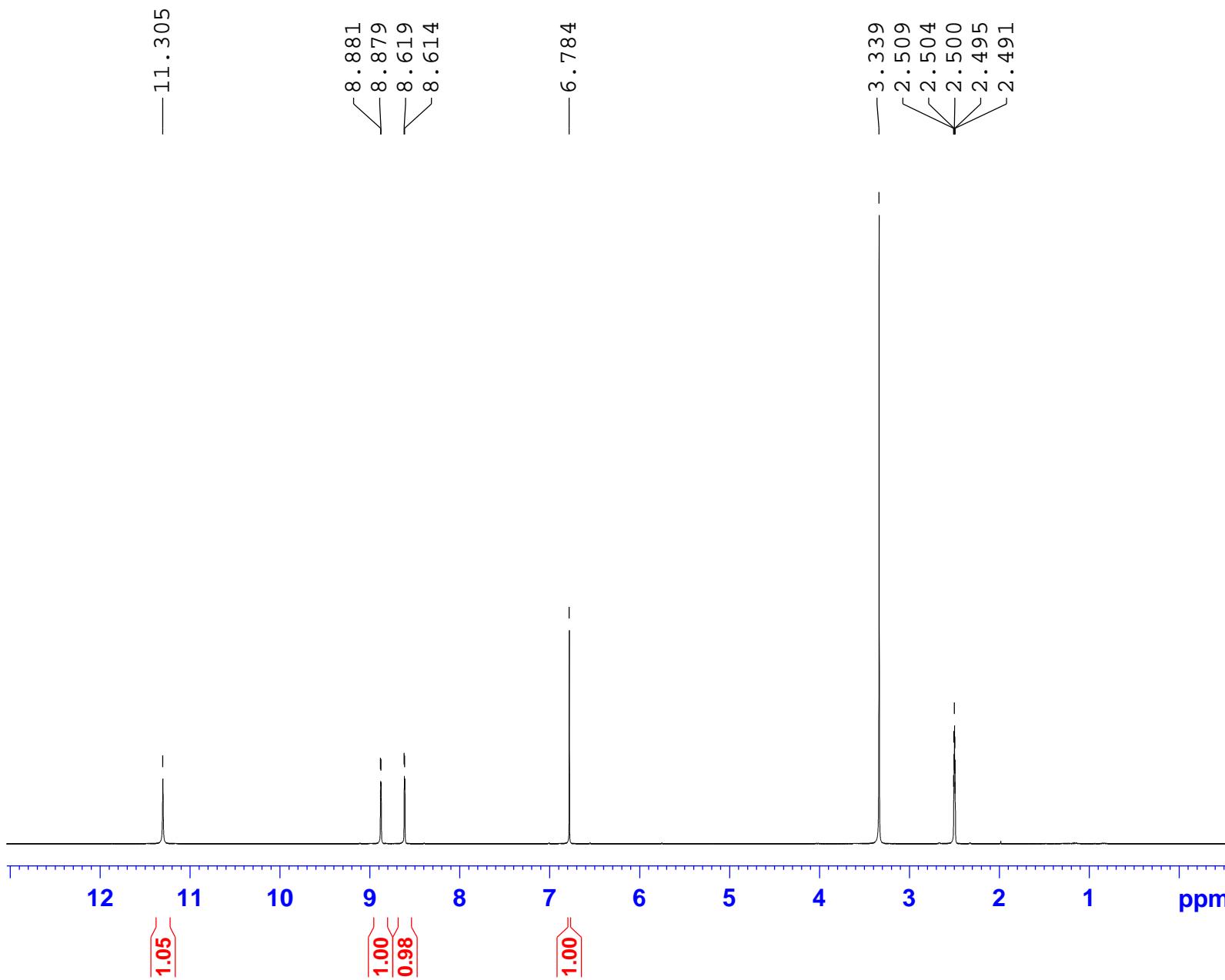
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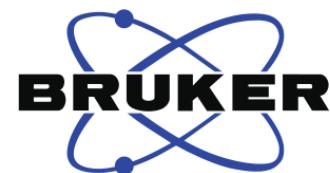
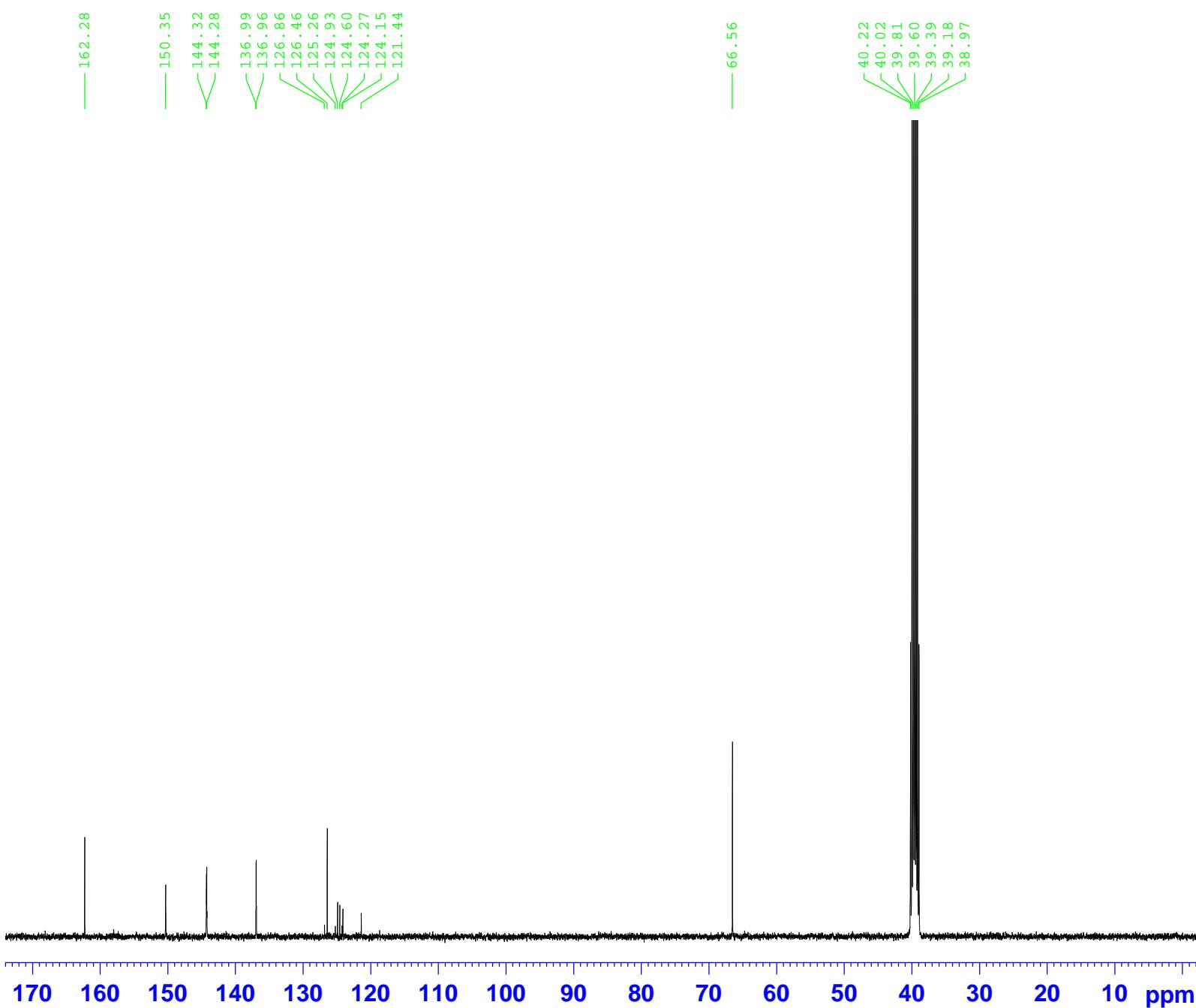
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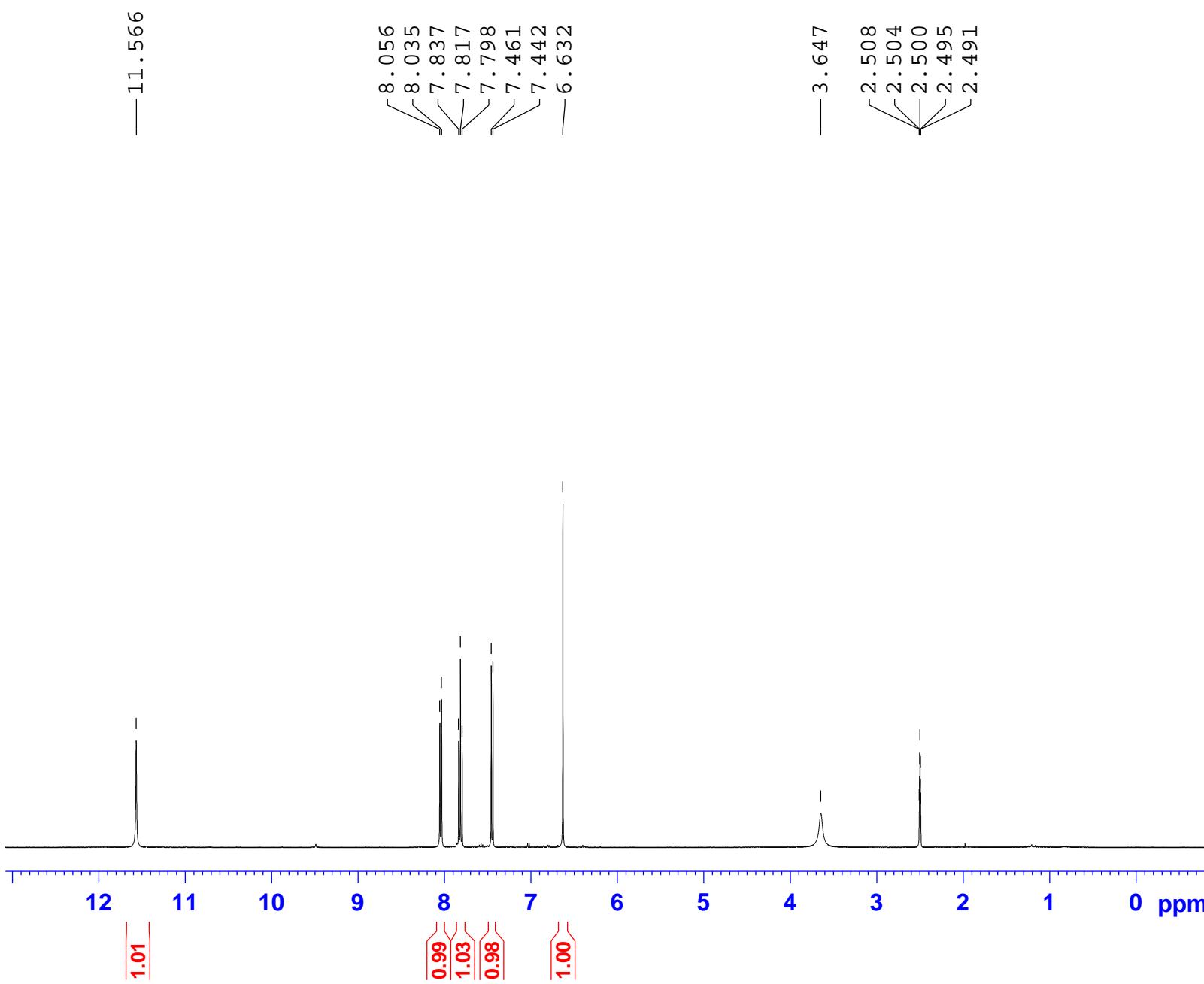
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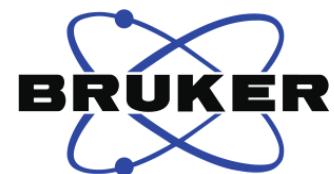
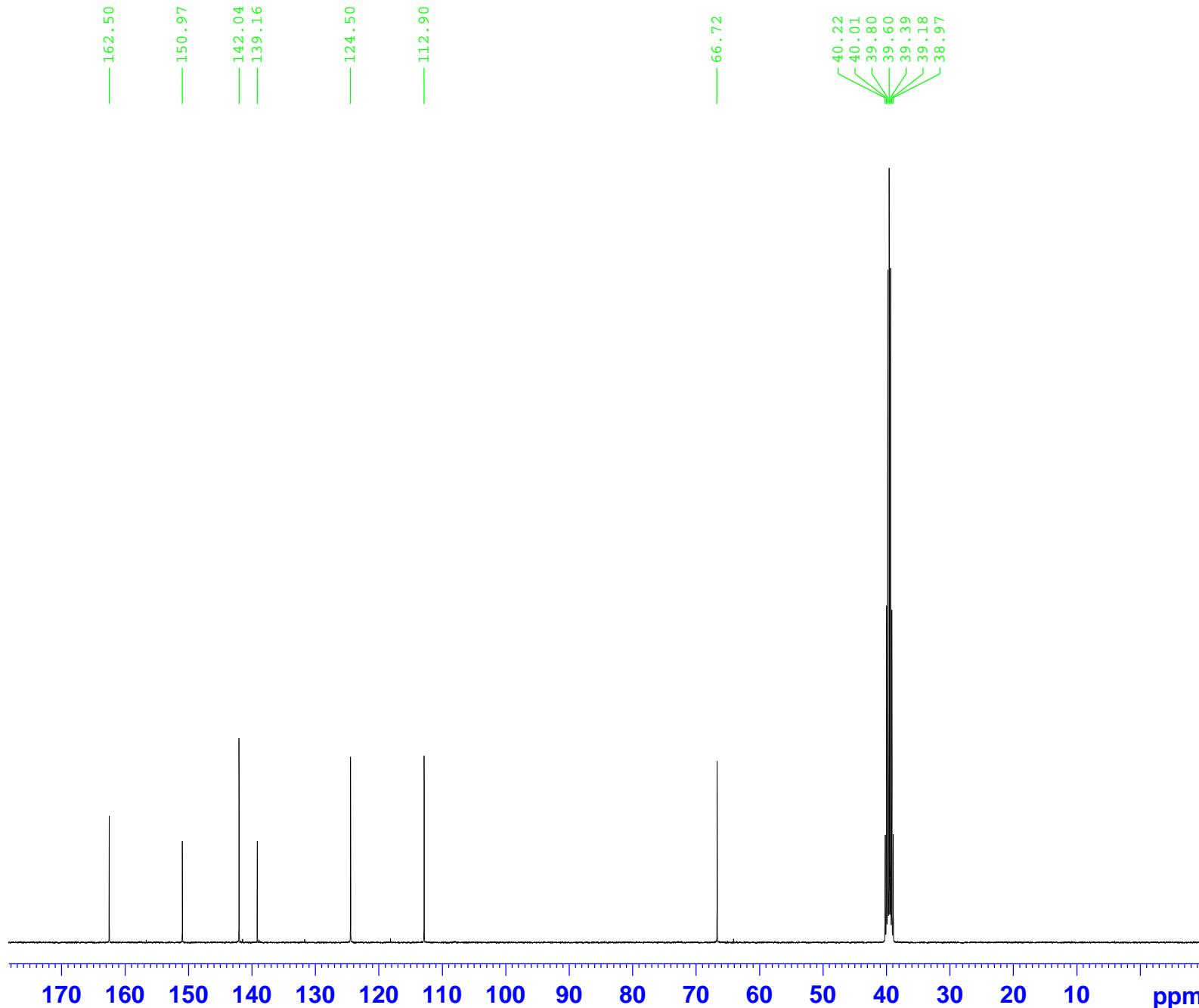
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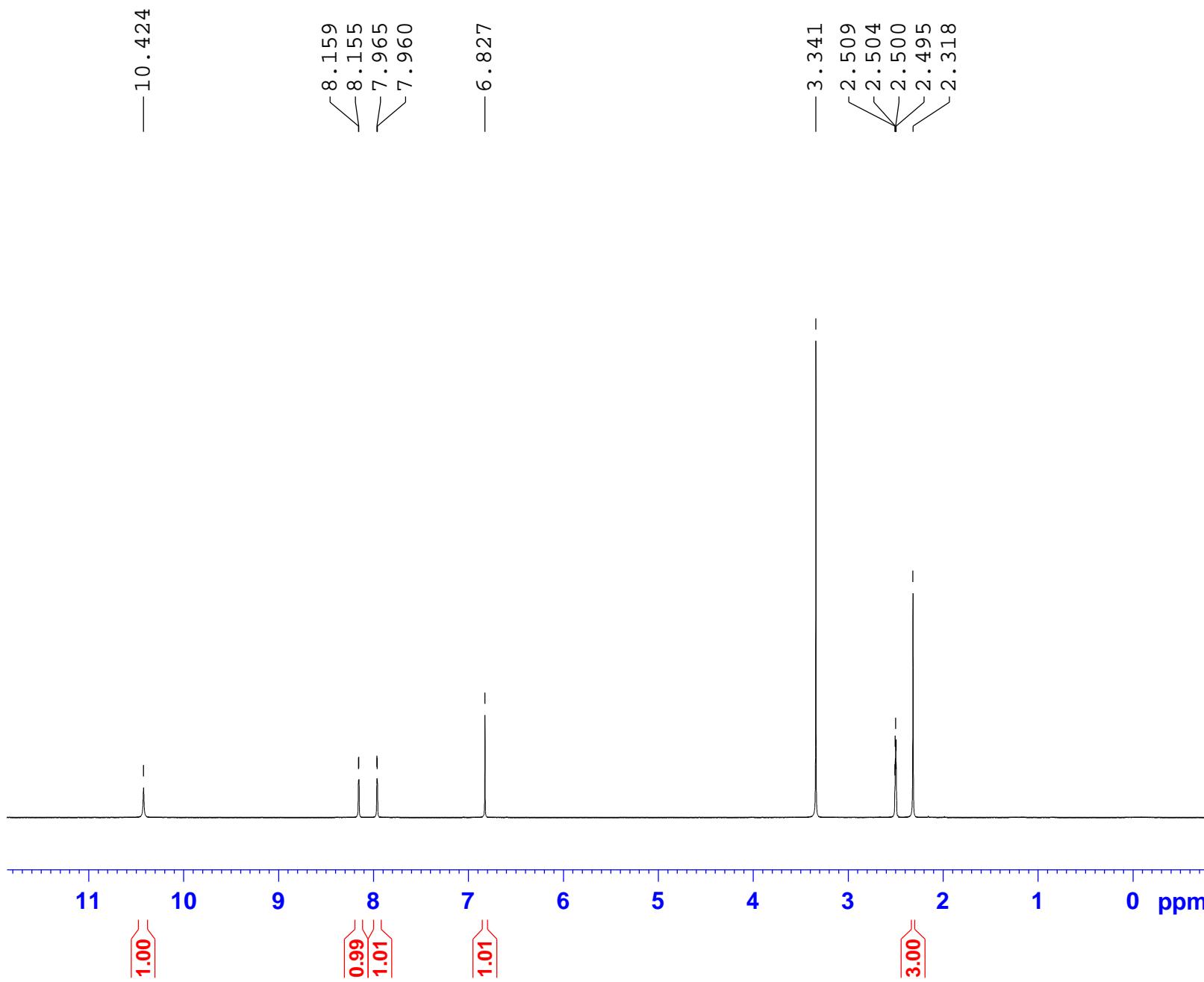
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TE 295.0 K
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SI 32768
SF 100.6128059 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

ZSL-1-8-H



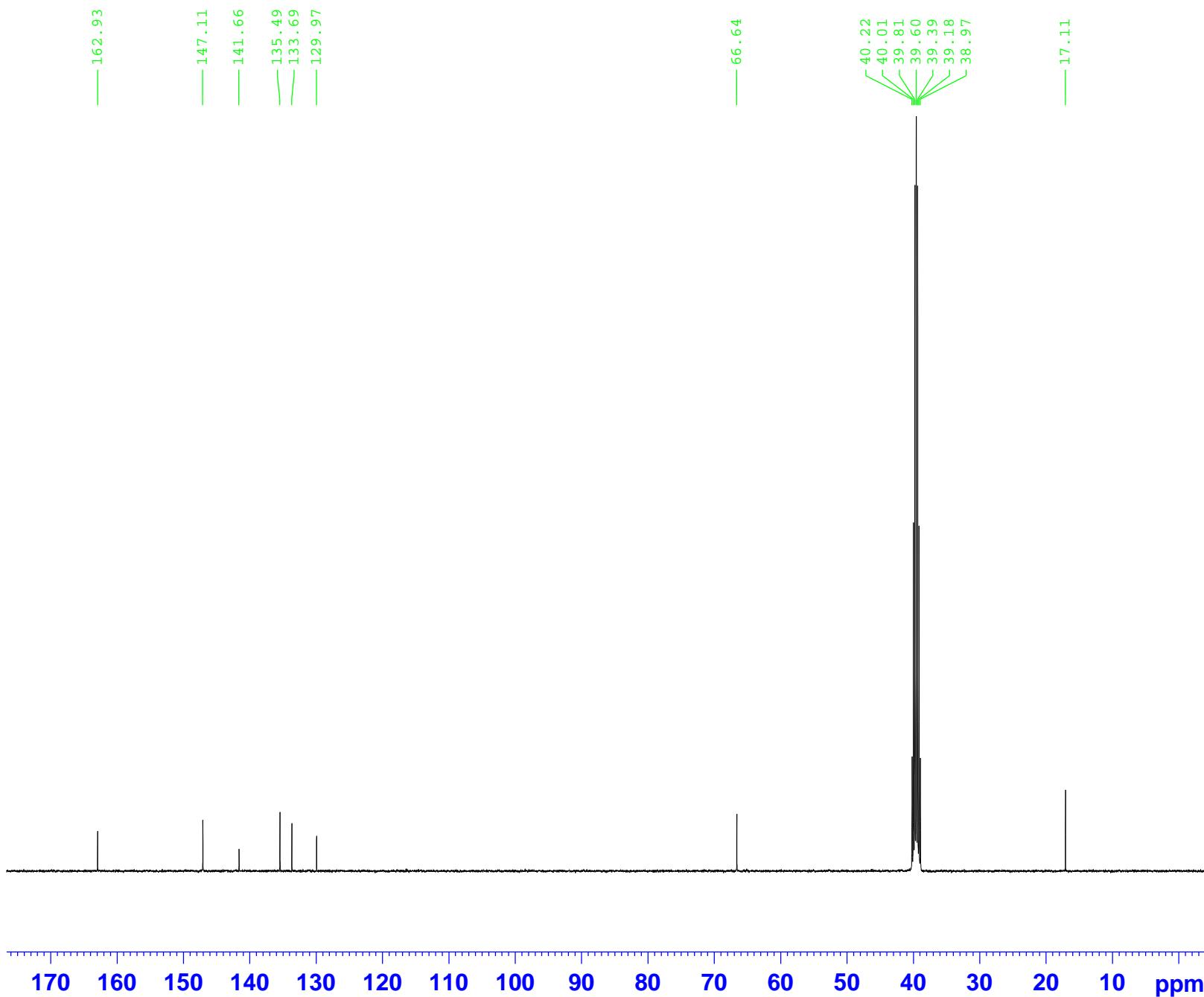
Current Data Parameters
NAME April11-2015
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date 20150411
Time 11.29
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 128.54
DW 62.400 usec
DE 6.50 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 9.50 usec
PLW1 15.80000019 W

F2 - Processing parameters
SI 65536
SF 400.1300035 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ZSL-1-8-C



Current Data Parameters
NAME Apr01-2015
EXPNO 10
PROCNO 1

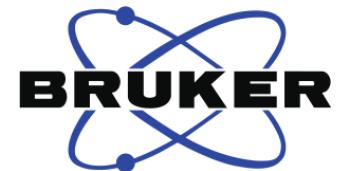
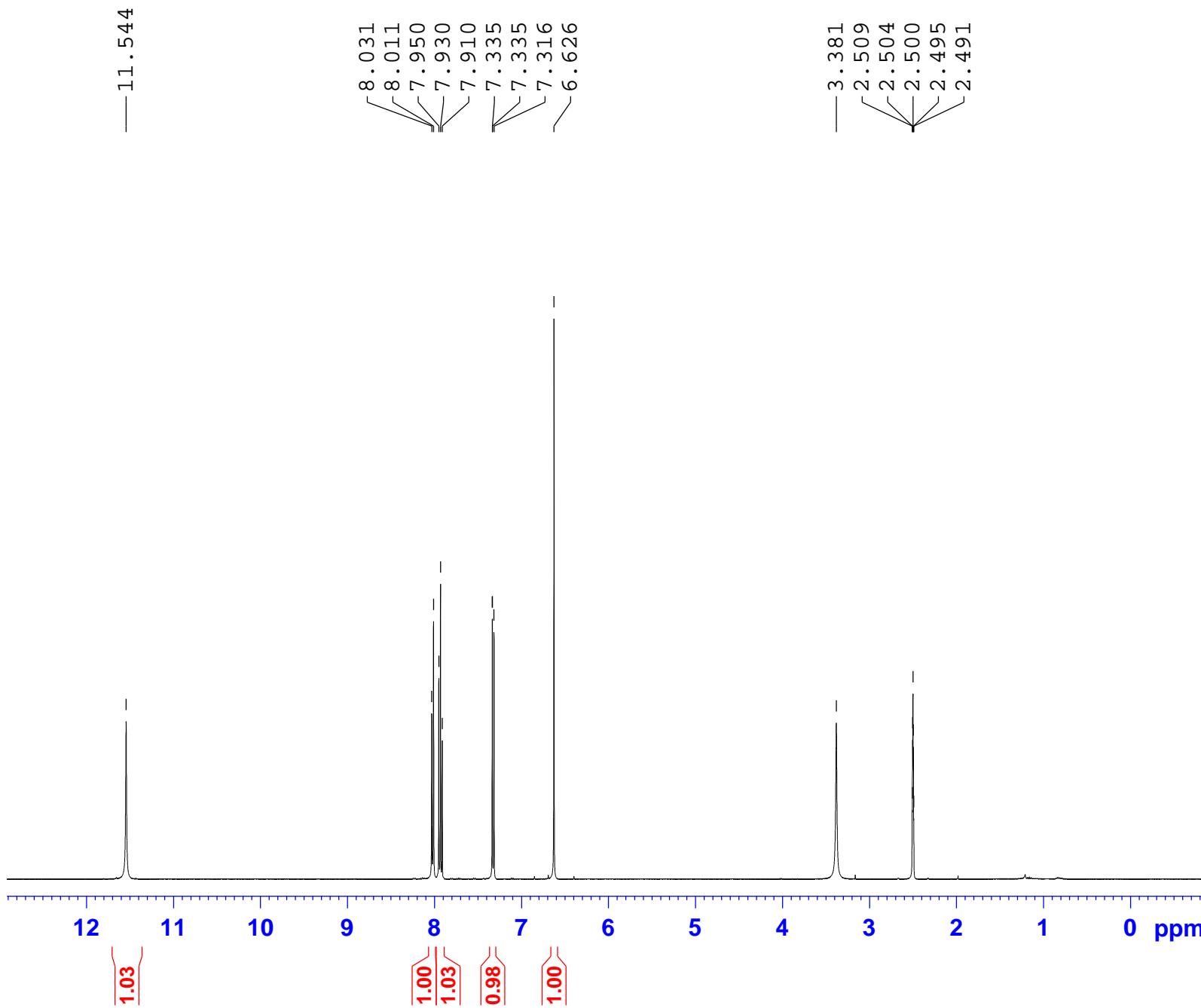
F2 - Acquisition Parameters
Date 20150401
Time 20.15
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 199.94
DW 20.800 usec
DE 6.50 usec
TE 295.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 9.50 usec
PLW1 66.50000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 18.00000000 W
PLW12 0.20056000 W
PLW13 0.16245000 W

F2 - Processing parameters
SI 32768
SF 100.6128060 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

ZSL-1-9-H



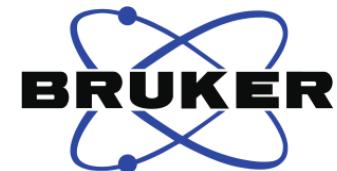
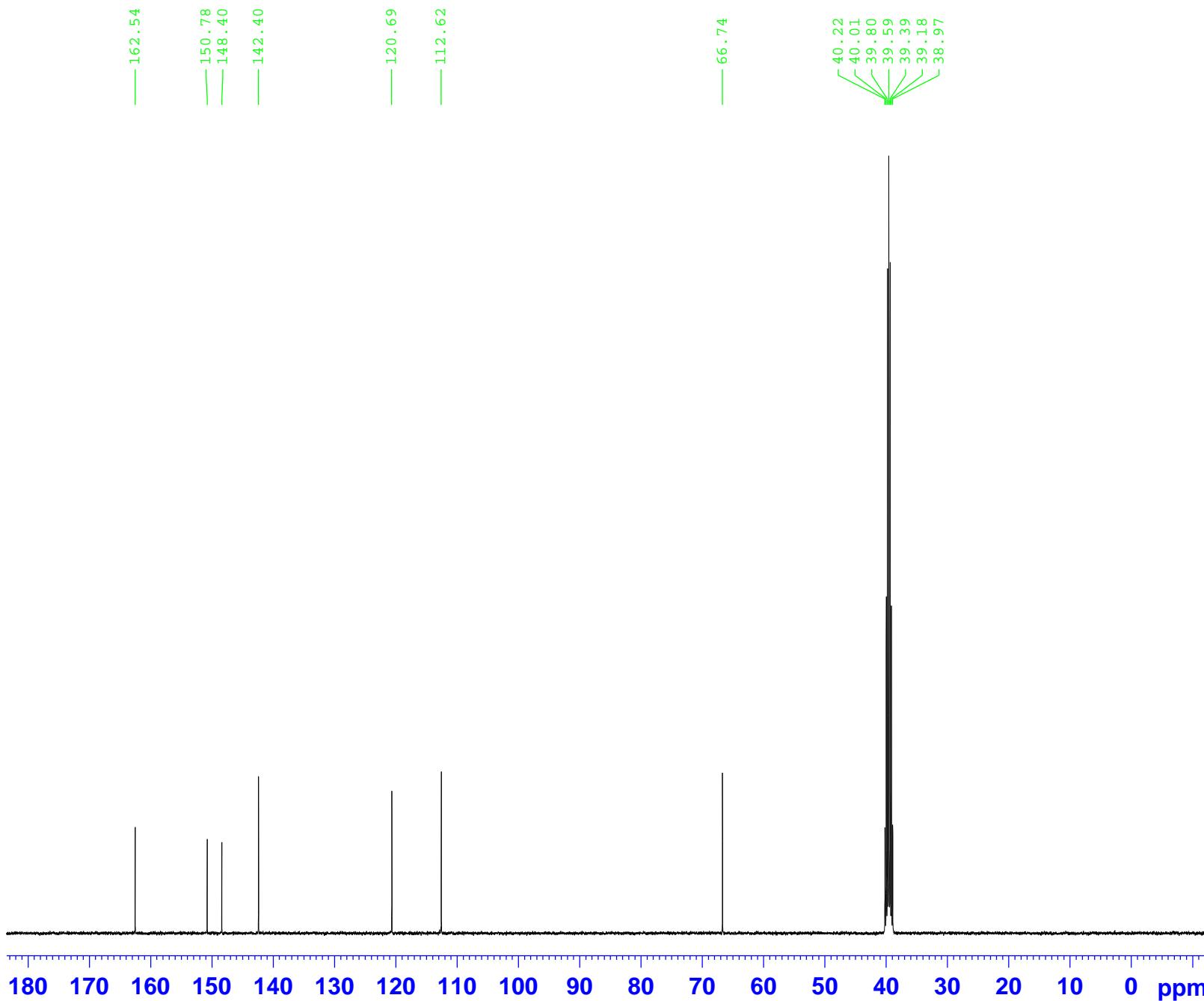
Current Data Parameters
NAME April1-2015
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150411
Time 12.25
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 112.04
DW 62.400 usec
DE 6.50 usec
TE 295.0 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 9.50 usec
PLW1 15.80000019 W

F2 - Processing parameters
SI 65536
SF 400.1300035 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ZSL-1-9-C



Current Data Parameters
NAME Apr02-2015
EXPNO 4
PROCNO 1

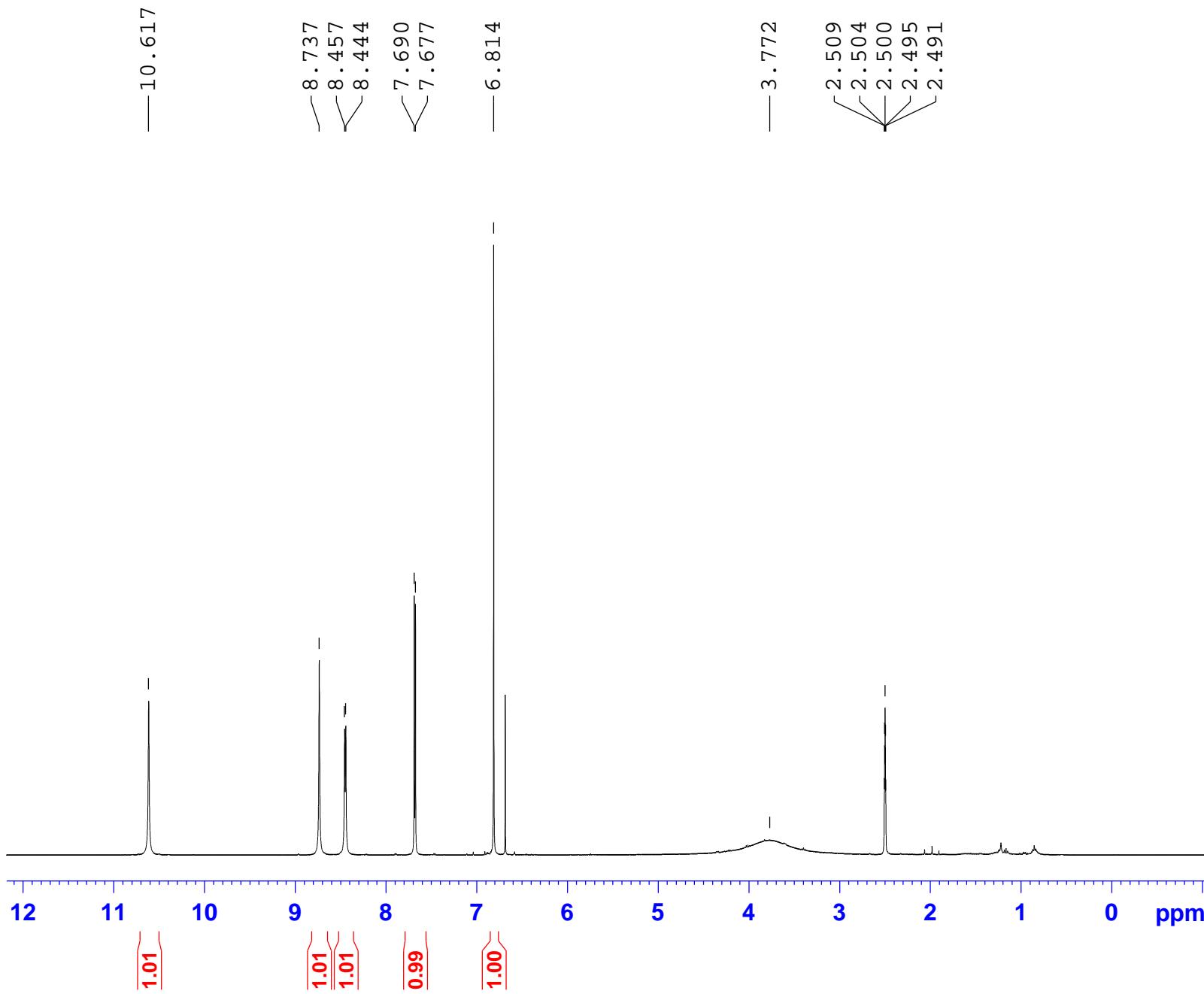
F2 - Acquisition Parameters
Date_ 20150402
Time 21.09
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 199.94
DW 20.800 usec
DE 6.50 usec
TE 295.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 9.50 usec
PLW1 66.50000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 18.00000000 W
PLW12 0.20056000 W
PLW13 0.16245000 W

F2 - Processing parameters
SI 32768
SF 100.6128060 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

ZSL-1-10-H



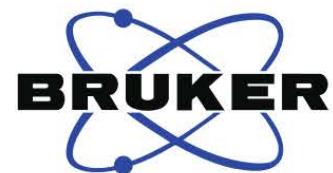
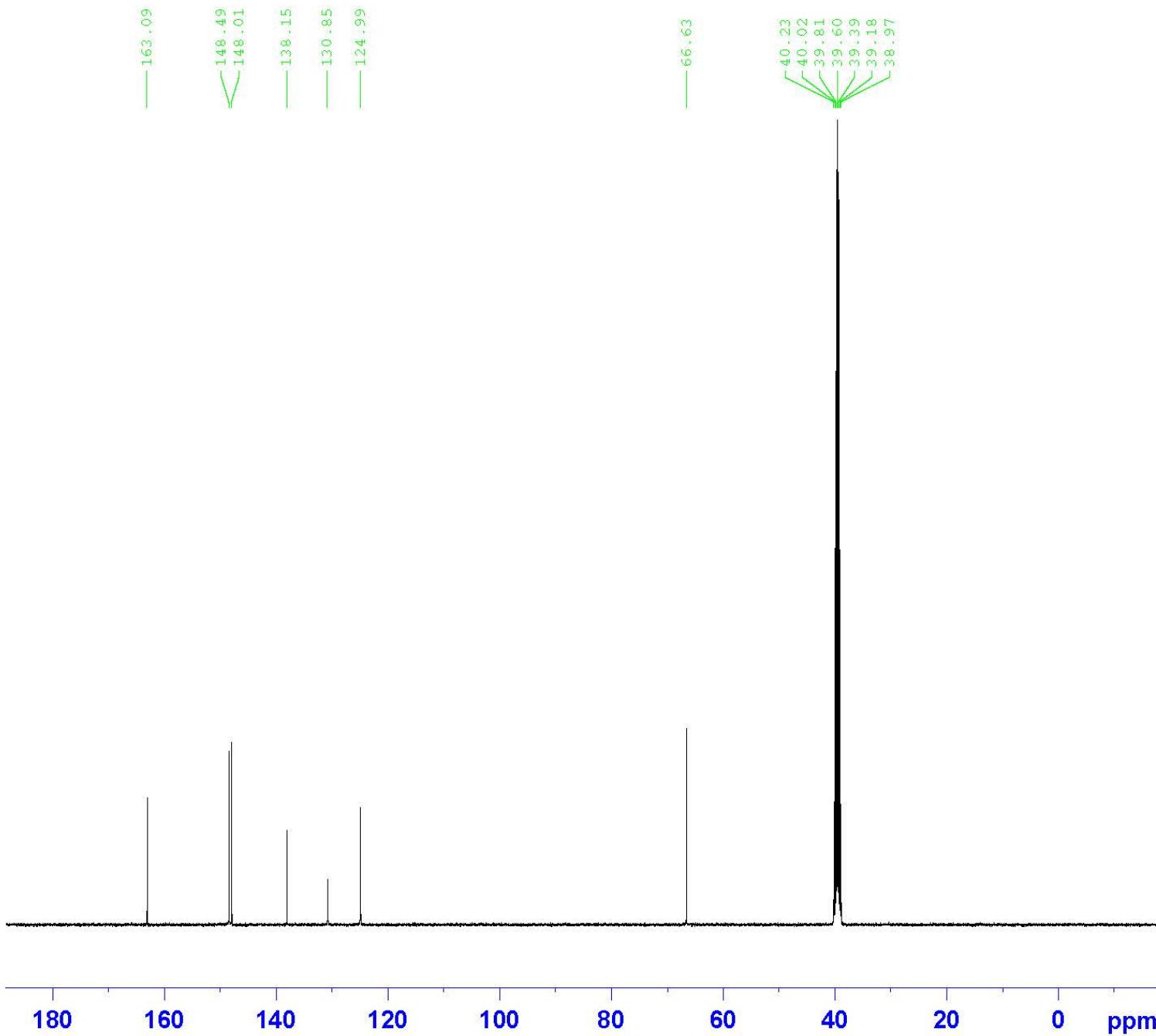
Current Data Parameters
NAME April1-2015
EXPNO 9
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150411
Time 12.37
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 78.4
DW 62.400 usec
DE 6.50 usec
TE 295.0 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 9.50 usec
PLW1 15.80000019 W

F2 - Processing parameters
SI 65536
SF 400.1300035 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

zsl-1-10-C



Current Data Parameters
NAME Apr04-2015
EXPNO 2
PROCNO 1

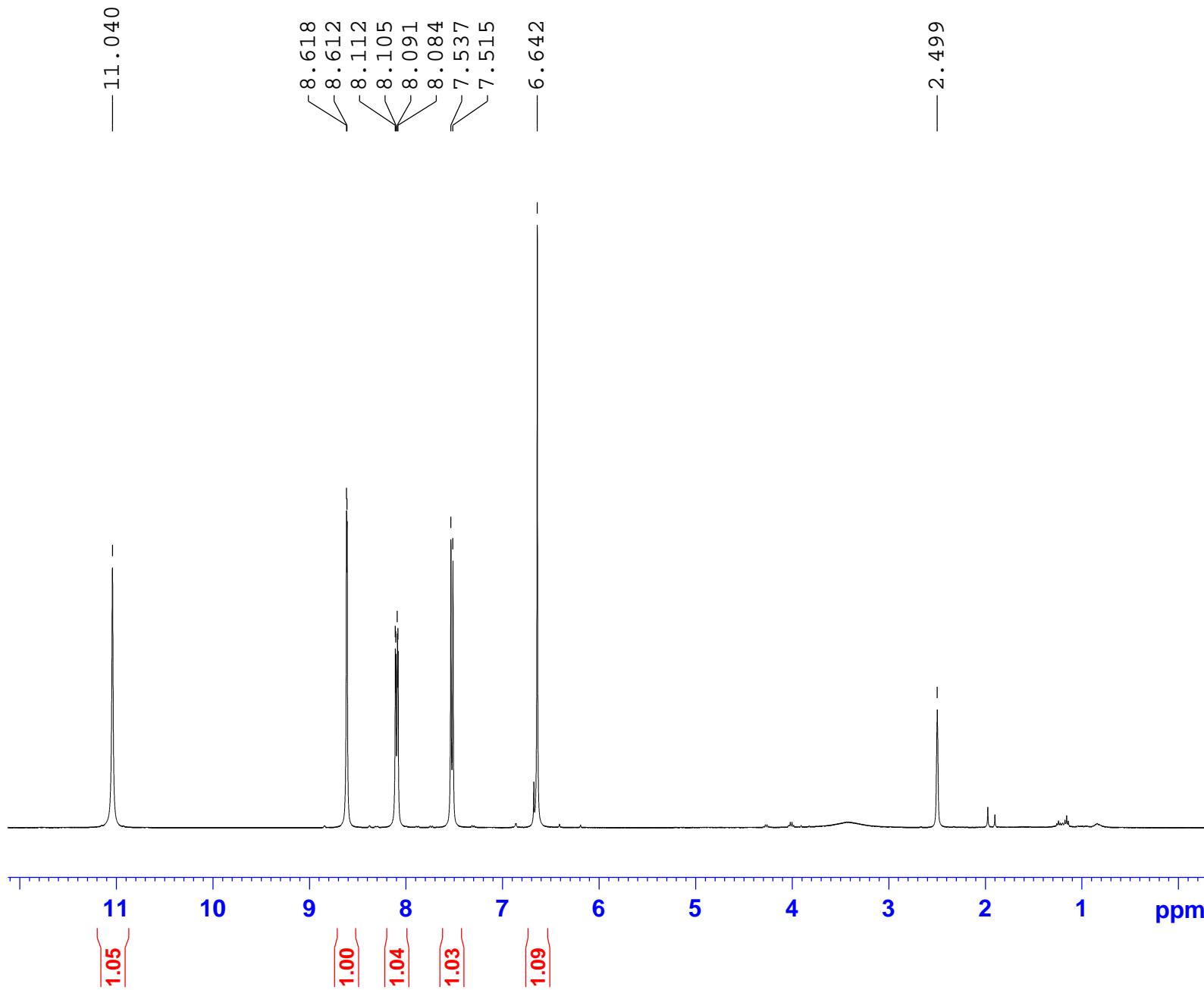
F2 - Acquisition Parameters
Date 20150404
Time 17.44
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 199.94
DW 20.800 usec
DE 6.50 usec
TE 295.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 ¹³C
P1 9.50 usec
PLW1 66.50000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 ¹H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 18.00000000 W
PLW12 0.20056000 W
PLW13 0.16245000 W

F2 - Processing parameters
SI 32768
SF 100.6128031 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

ZSL-1-11-H



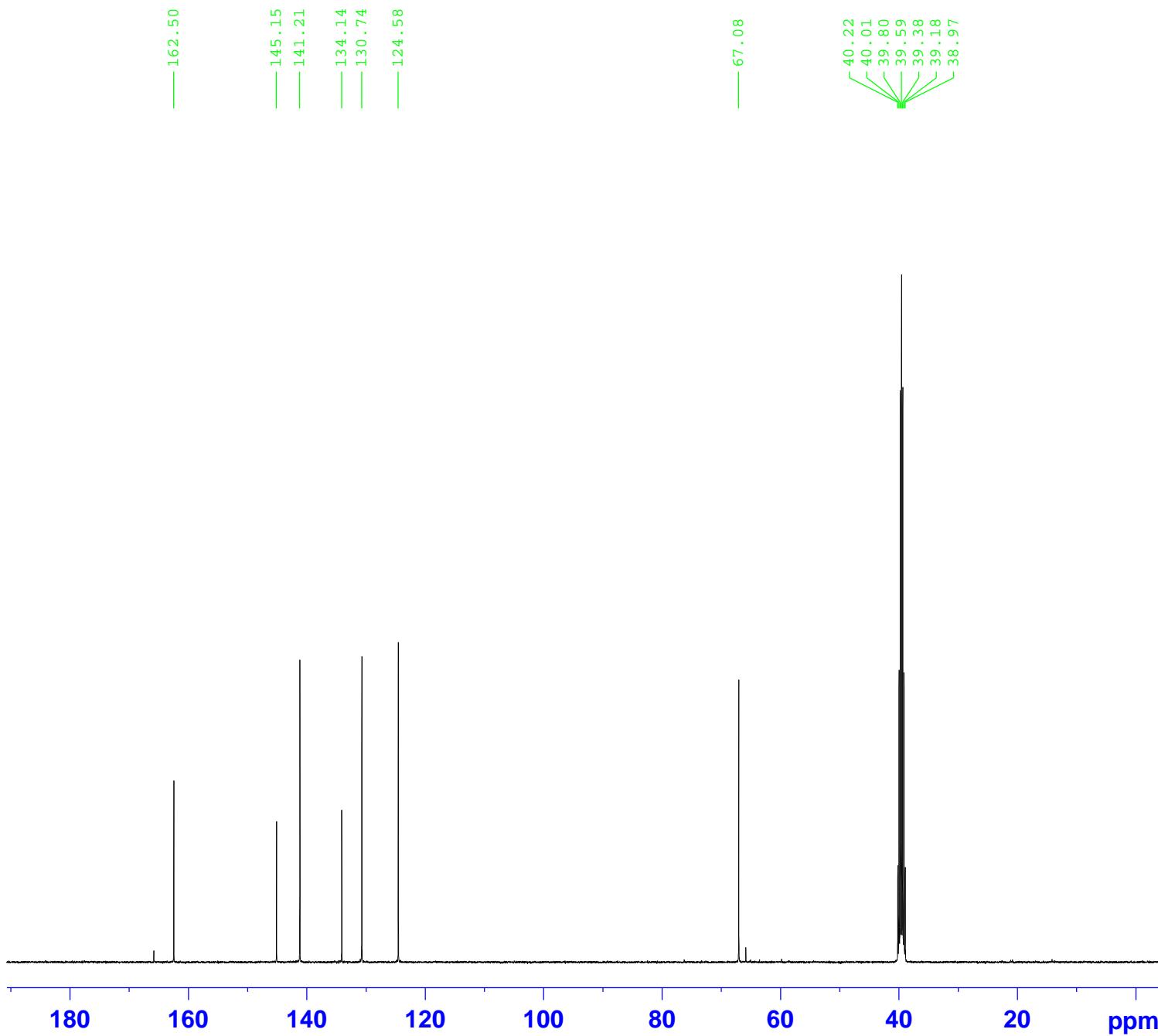
Current Data Parameters
NAME Apr11-2015
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150411
Time 17.56
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 78.4
DW 62.400 usec
DE 6.50 usec
TE 295.0 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 9.50 usec
PLW1 15.80000019 W

F2 - Processing parameters
SI 65536
SF 400.1300038 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ZSL-1-11-C



Current Data Parameters
NAME Apr11-2015
EXPNO 17
PROCNO 1

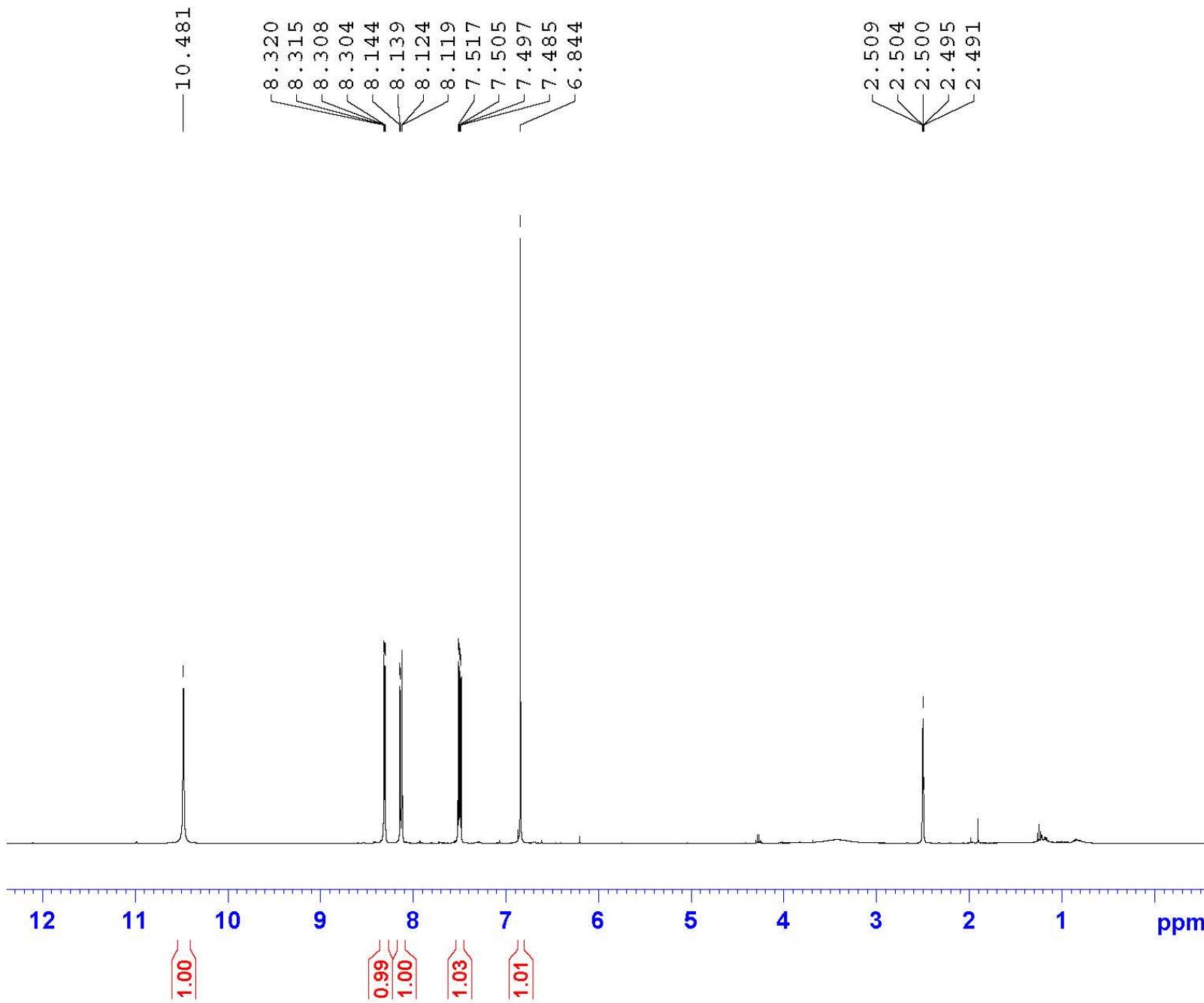
F2 - Acquisition Parameters
Date_ 20150412
Time 0.17
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zpgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 199.94
DW 20.800 usec
DE 6.50 usec
TE 295.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 9.50 usec
PLW1 66.50000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 18.00000000 W
PLW12 0.20056000 W
PLW13 0.16245000 W

F2 - Processing parameters
SI 32768
SF 100.6128057 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

ZSL-1-12-H



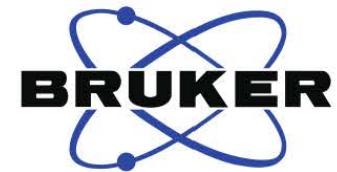
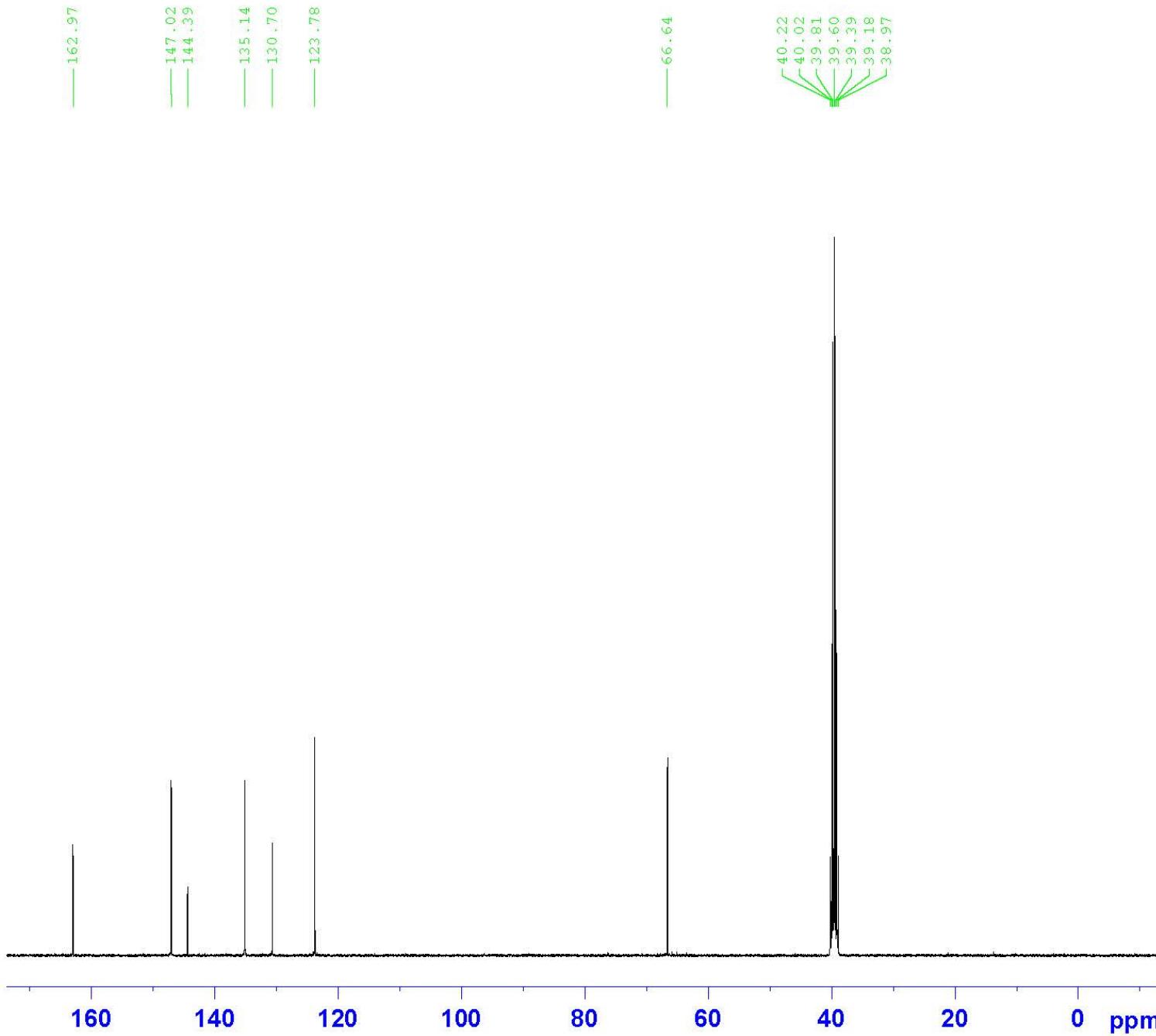
Current Data Parameters
NAME April1-2015
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150411
Time 18.00
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 88.59
DW 62.400 usec
DE 6.50 usec
TE 295.0 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 9.50 usec
PLW1 15.80000019 W

F2 - Processing parameters
SI 65536
SF 400.1300035 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ZSL-1-12-C



Current Data Parameters
NAME April1-2015
EXPNO 16
PROCNO 1

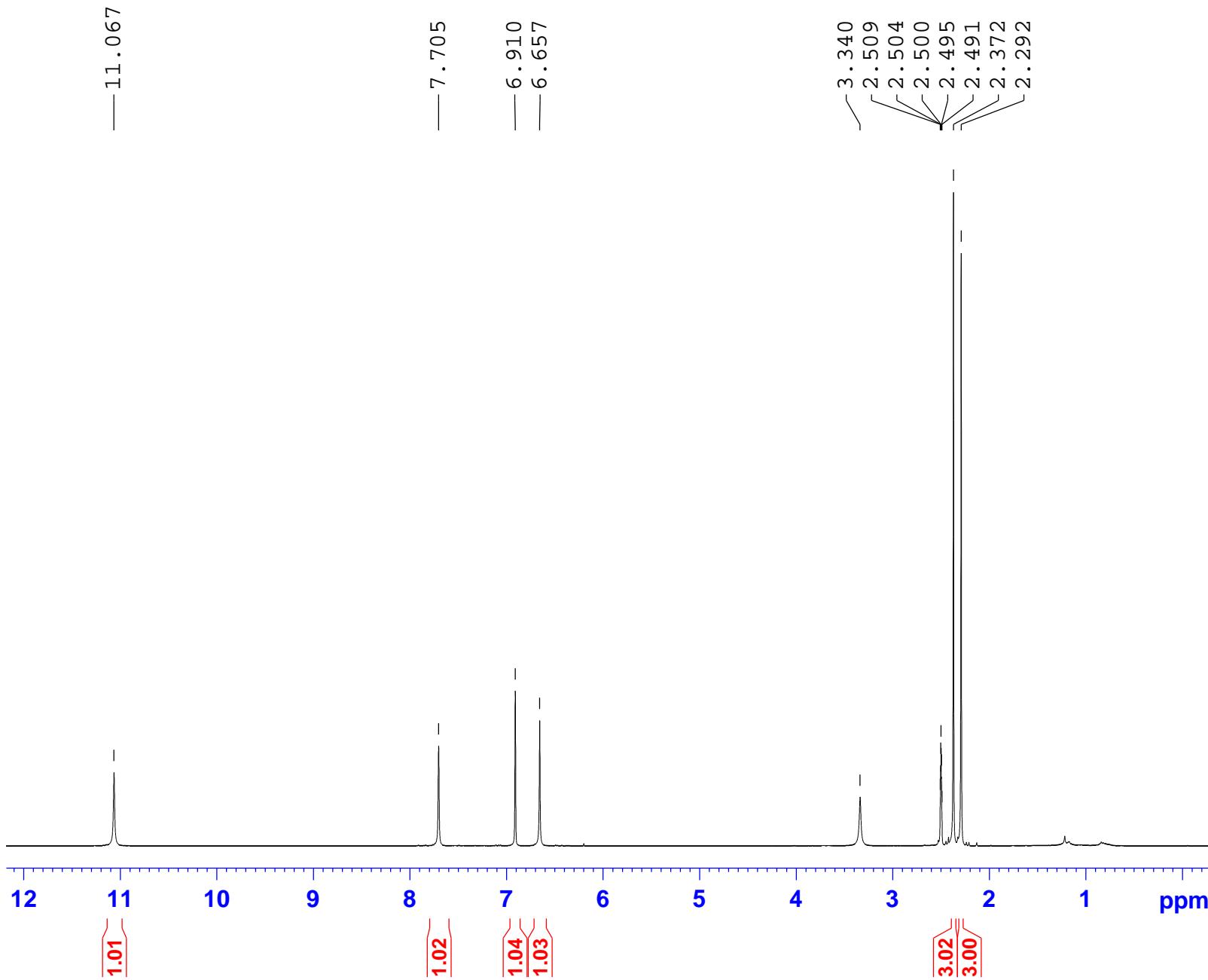
F2 - Acquisition Parameters
Date_ 20150411
Time 22.17
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 199.94
DW 20.800 usec
DE 6.50 usec
TE 295.0 K
D1 2.0000000 sec
D11 0.03000000 sec
TDO 1

===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 9.50 usec
PLW1 66.50000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 18.00000000 W
PLW12 0.20056000 W
PLW13 0.16245000 W

F2 - Processing parameters
SI 32768
SF 100.6128056 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

ZSL-1-13-H



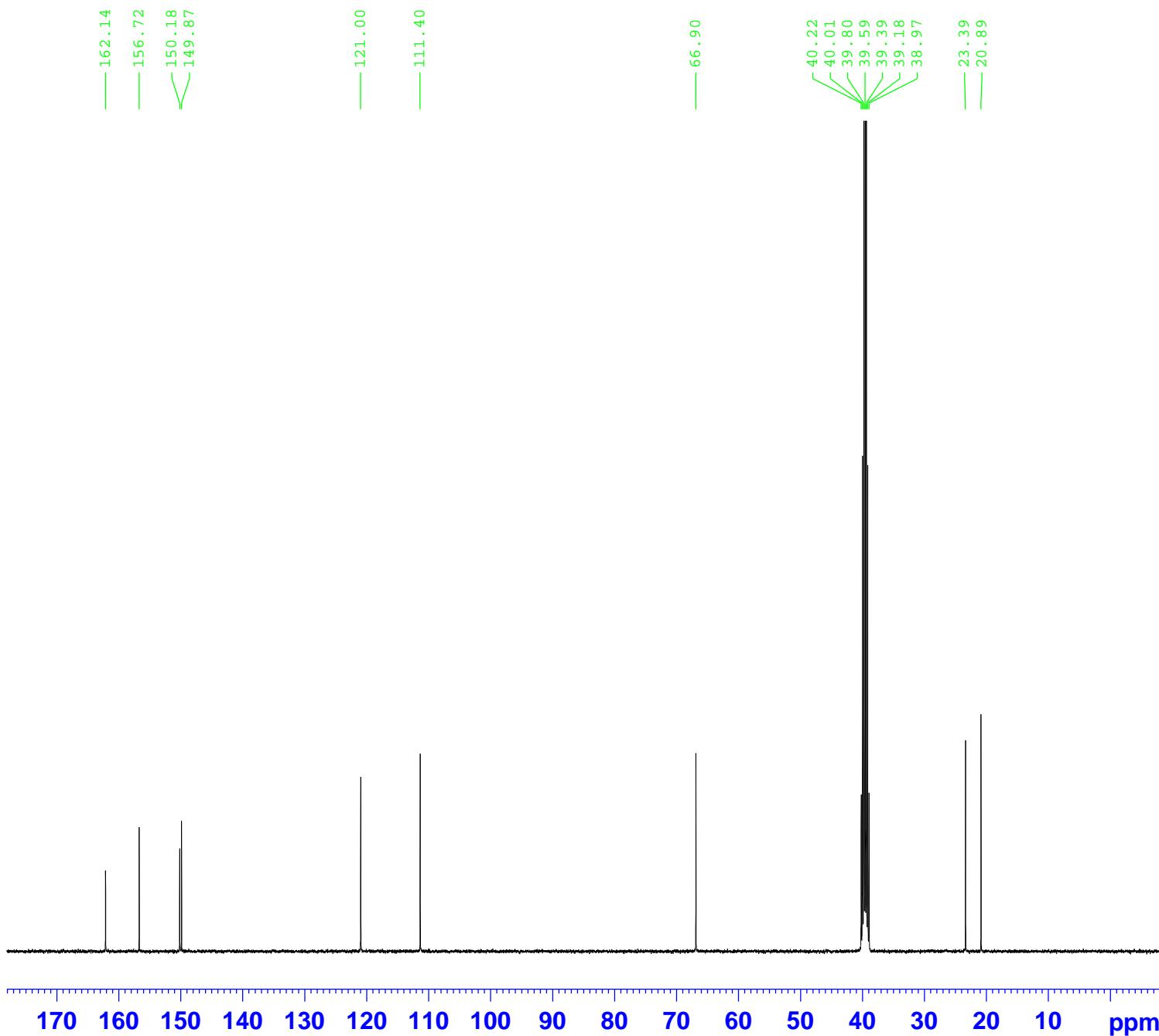
Current Data Parameters
NAME April11-2015
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date 20150411
Time 18.03
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 78.4
DW 62.400 usec
DE 6.50 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 ======
SFO1 400.1324710 MHz
NUC1 1H
P1 9.50 usec
PLW1 15.80000019 W

F2 - Processing parameters
SI 65536
SF 400.1300033 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ZSL-1-13-C



Current Data Parameters
NAME April11-2015
EXPNO 15
PROCNO 1

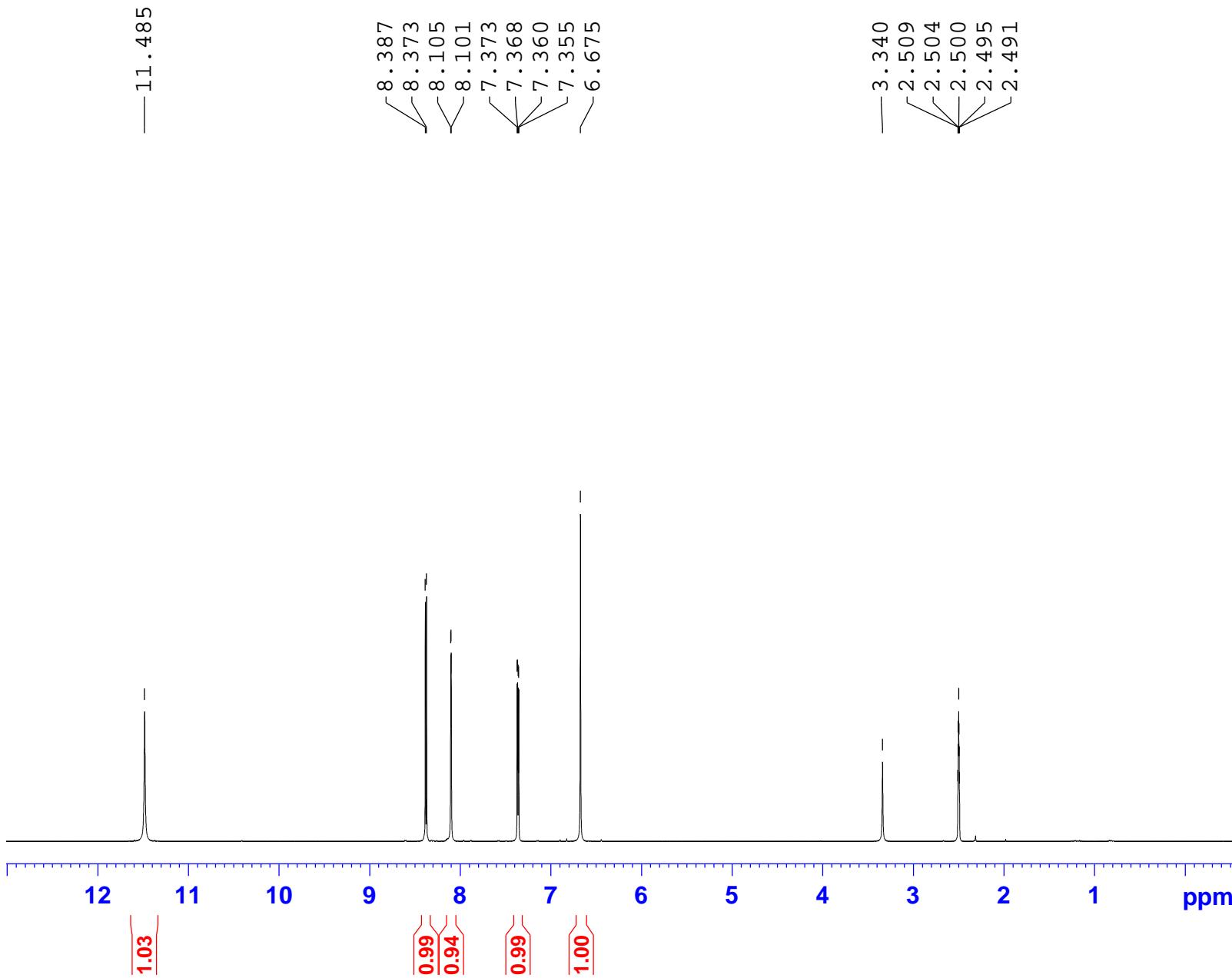
F2 - Acquisition Parameters
Date_ 20150411
Time 20.17
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 199.94
DW 20.800 usec
DE 6.50 usec
TE 295.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 9.50 usec
PLW1 66.50000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 18.00000000 W
PLW12 0.20056000 W
PLW13 0.16245000 W

F2 - Processing parameters
SI 32768
SF 100.6128060 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

ZSL-1-14-H



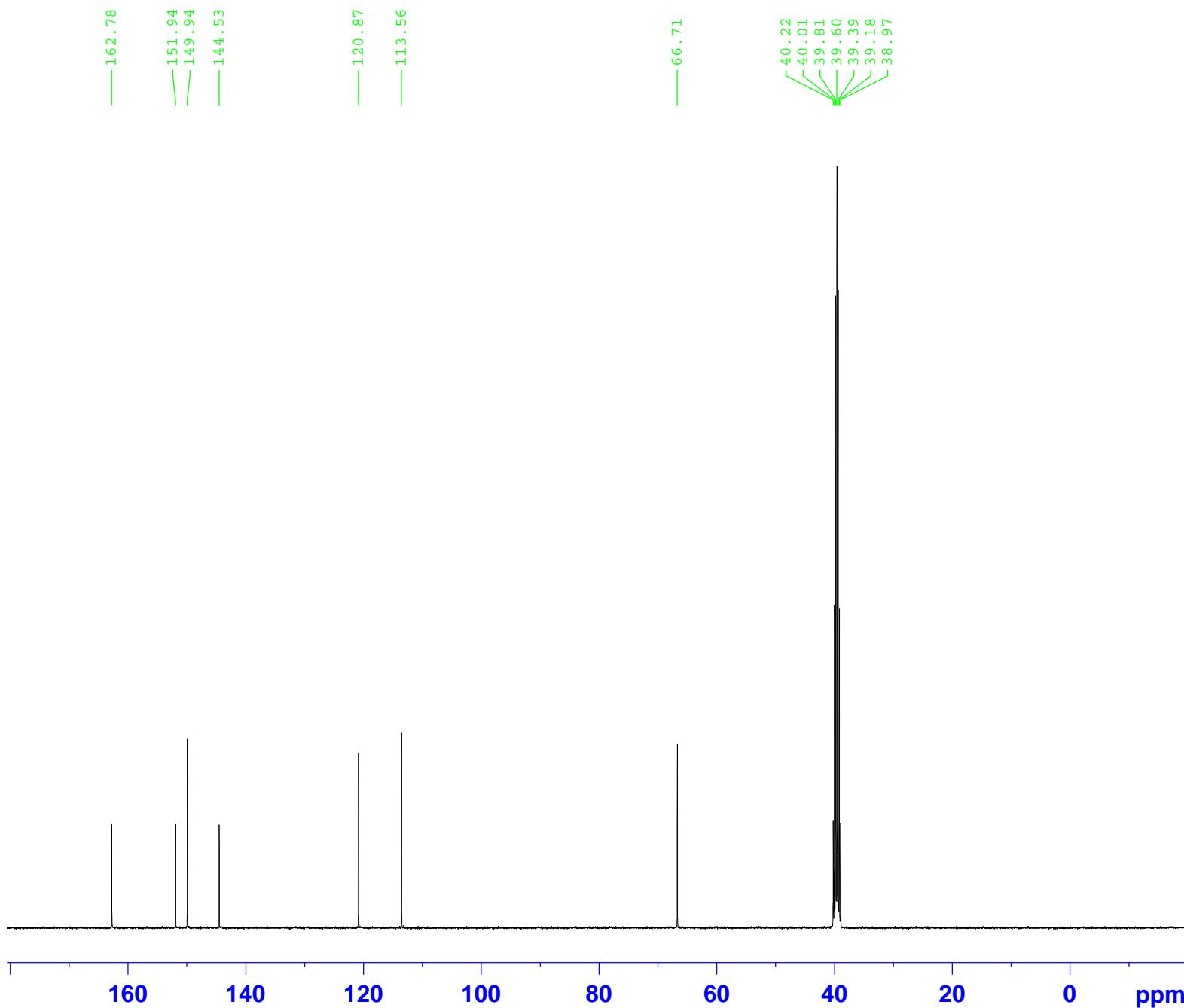
Current Data Parameters
NAME April12-2015
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150412
Time 10.09
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 112.04
DW 62.400 usec
DE 6.50 usec
TE 295.0 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 9.50 usec
PLW1 15.80000019 W

F2 - Processing parameters
SI 65536
SF 400.1300036 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ZSL-1-14-C



Current Data Parameters
NAME April12-2015
EXPNO 4
PROCNO 1

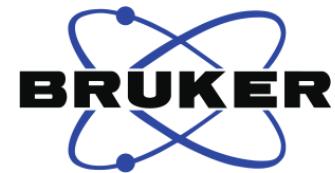
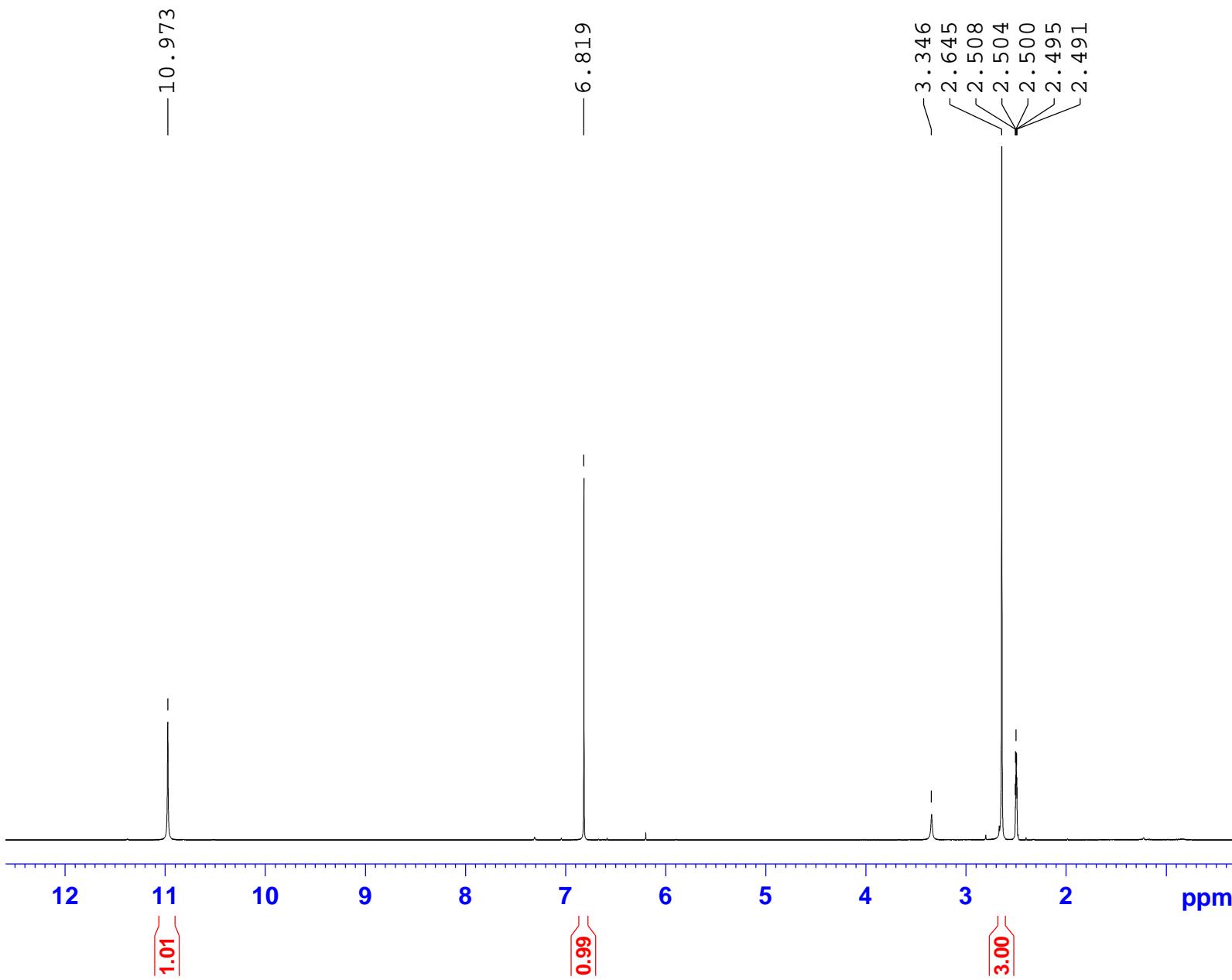
F2 - Acquisition Parameters
Date_ 20150412
Time 12.27
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zqpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 199.94
DW 20.800 usec
DE 6.50 usec
TE 295.0 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 9.50 usec
PLW1 66.50000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 18.00000000 W
PLW12 0.20056000 W
PLW13 0.16245000 W

F2 - Processing parameters
SI 32768
SF 100.6128060 MHz
WDW EM
SSB 0
LB 0 1.00 Hz
GB 0
PC 1.40

ZSL-1-15-H



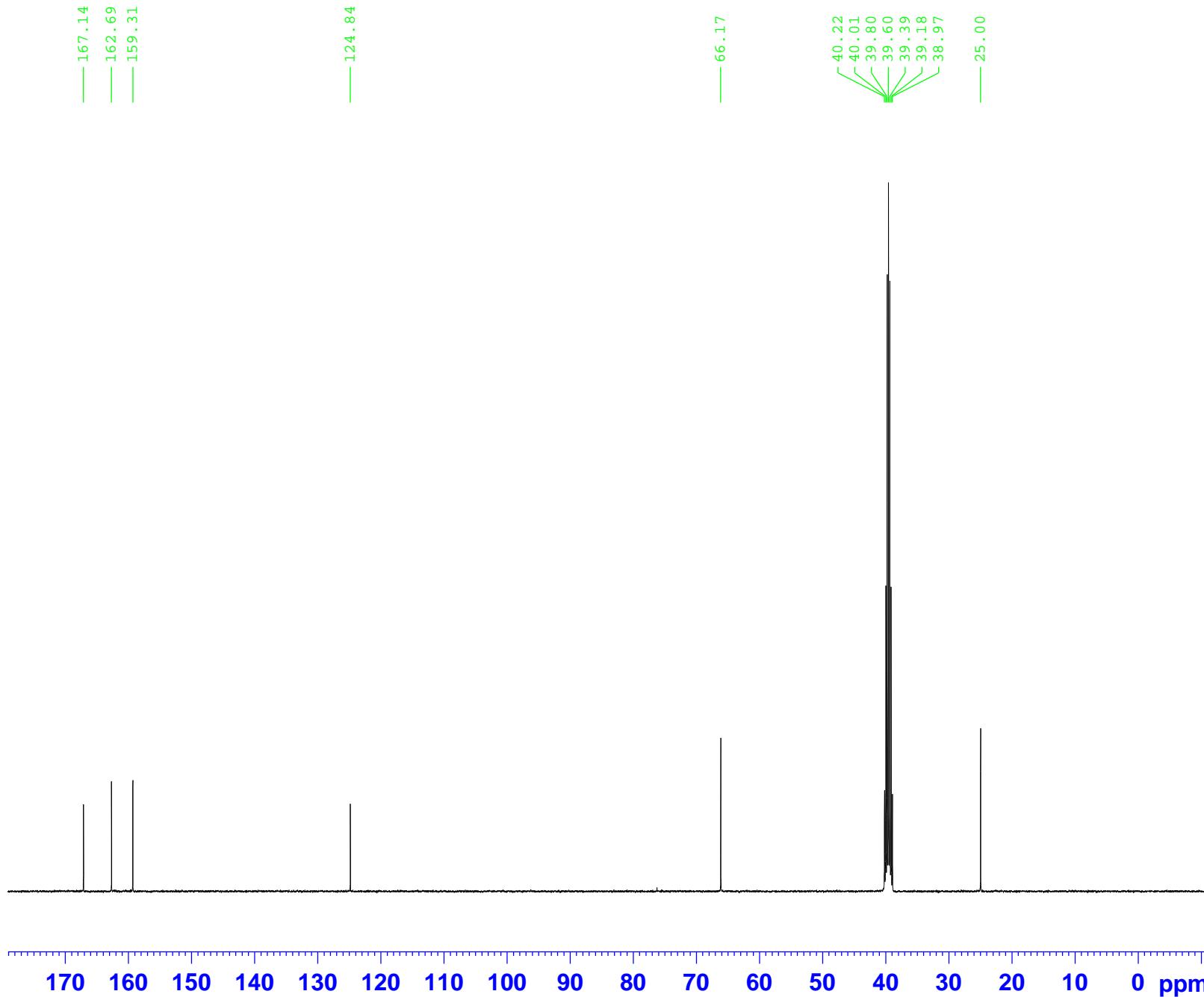
Current Data Parameters
NAME April12-2015
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150412
Time 10.13
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 112.04
DW 62.400 usec
DE 6.50 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 9.50 usec
PLW1 15.80000019 W

F2 - Processing parameters
SI 65536
SF 400.1300036 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ZSL-1-15-C



Current Data Parameters
NAME Apr12-2015
EXPNO 5
PROCNO 1

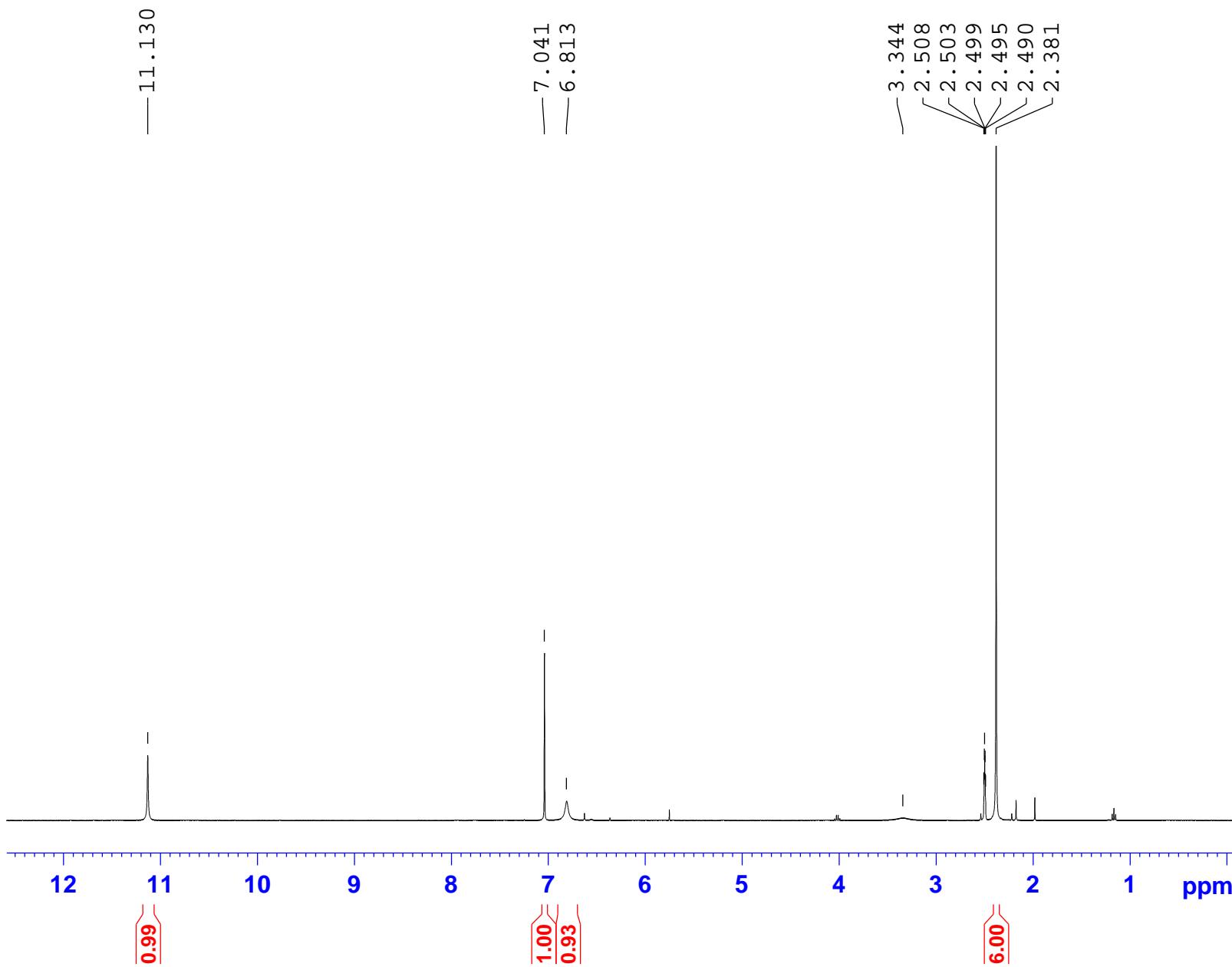
F2 - Acquisition Parameters
Date_ 20150412
Time 14.27
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 199.94
DW 20.800 usec
DE 6.50 usec
TE 295.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 9.50 usec
PLW1 66.50000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 18.00000000 W
PLW12 0.20056000 W
PLW13 0.16245000 W

F2 - Processing parameters
SI 32768
SF 100.6128065 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

ZSL-1-17-H



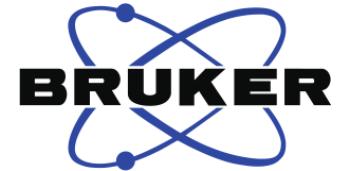
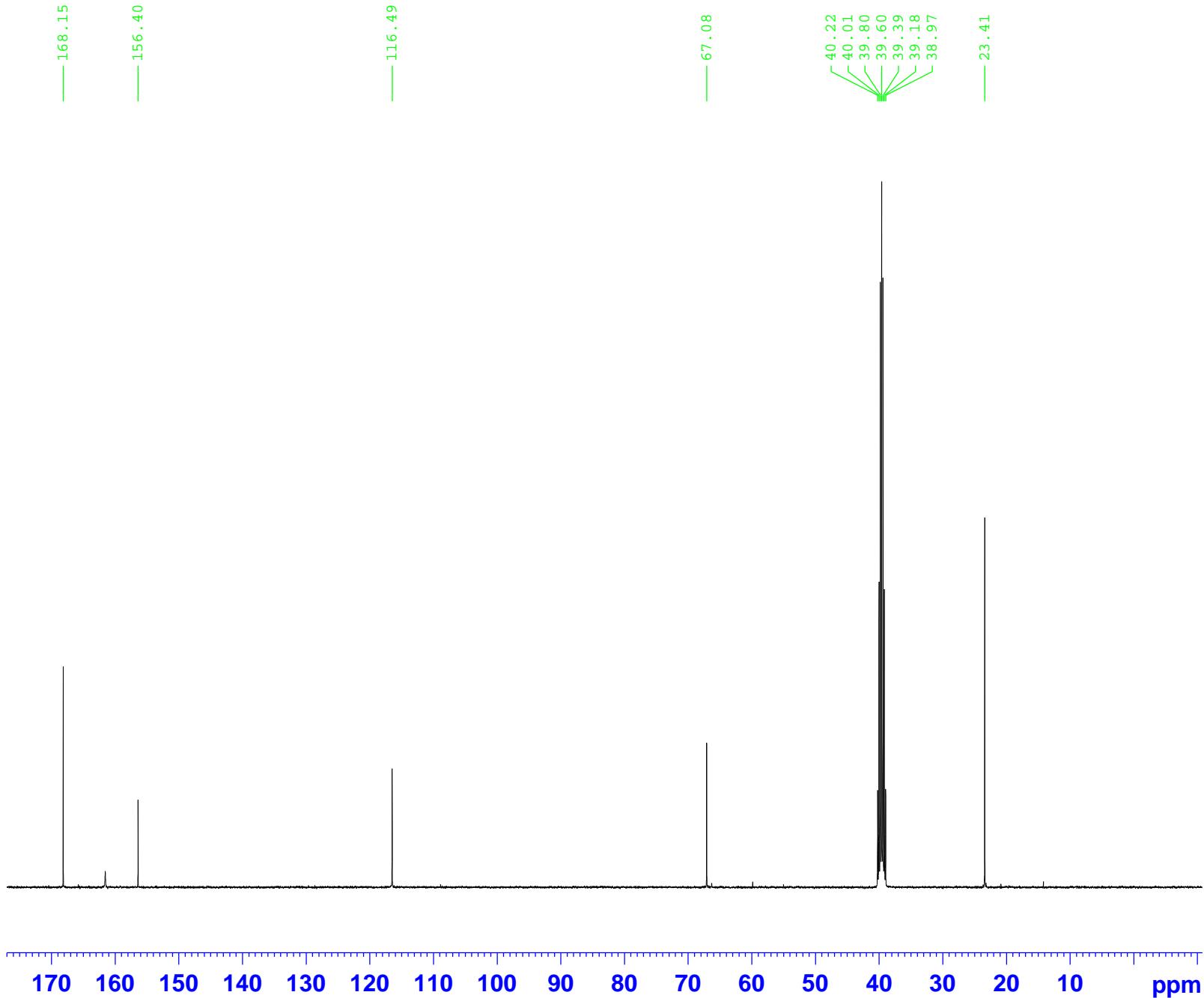
Current Data Parameters
NAME April12-2015
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150412
Time 10.17
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 78.4
DW 62.400 usec
DE 6.50 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 9.50 usec
PLW1 15.80000019 W

F2 - Processing parameters
SI 65536
SF 400.1300038 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ZSL-1-17-C



Current Data Parameters
NAME Apr12-2015
EXPNO 6
PROCNO 1

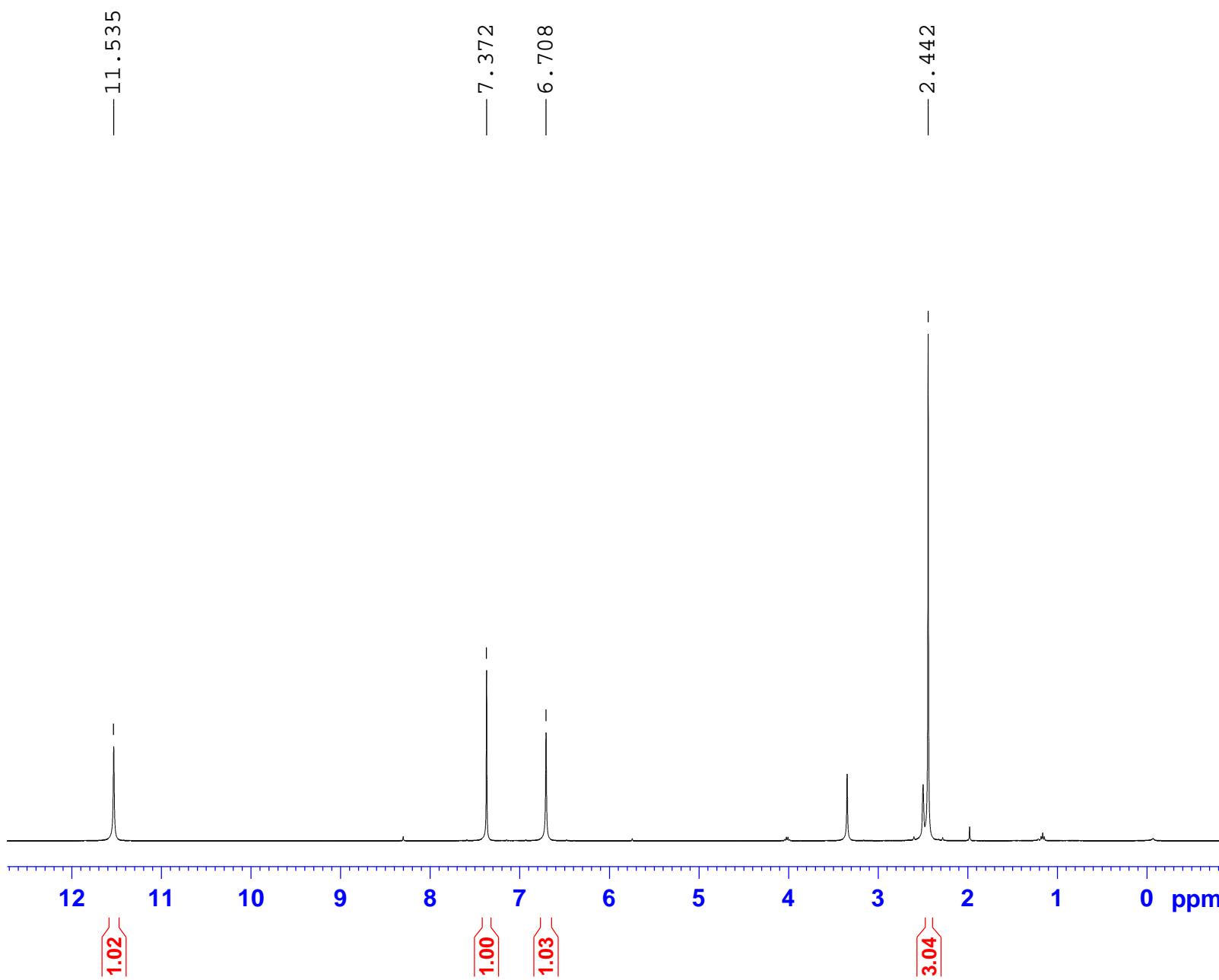
F2 - Acquisition Parameters
Date_ 20150412
Time 16.53
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 199.94
DW 20.800 usec
DE 6.50 usec
TE 295.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 9.50 usec
PLW1 66.50000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 18.00000000 W
PLW12 0.20056000 W
PLW13 0.16245000 W

F2 - Processing parameters
SI 32768
SF 100.6128060 MHz
WDW EM
SSB 0
LB 0 1.00 Hz
GB 0
PC 1.40

ZSL-1-19-H



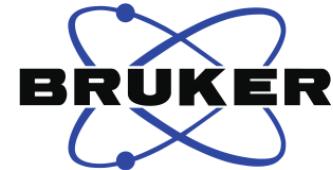
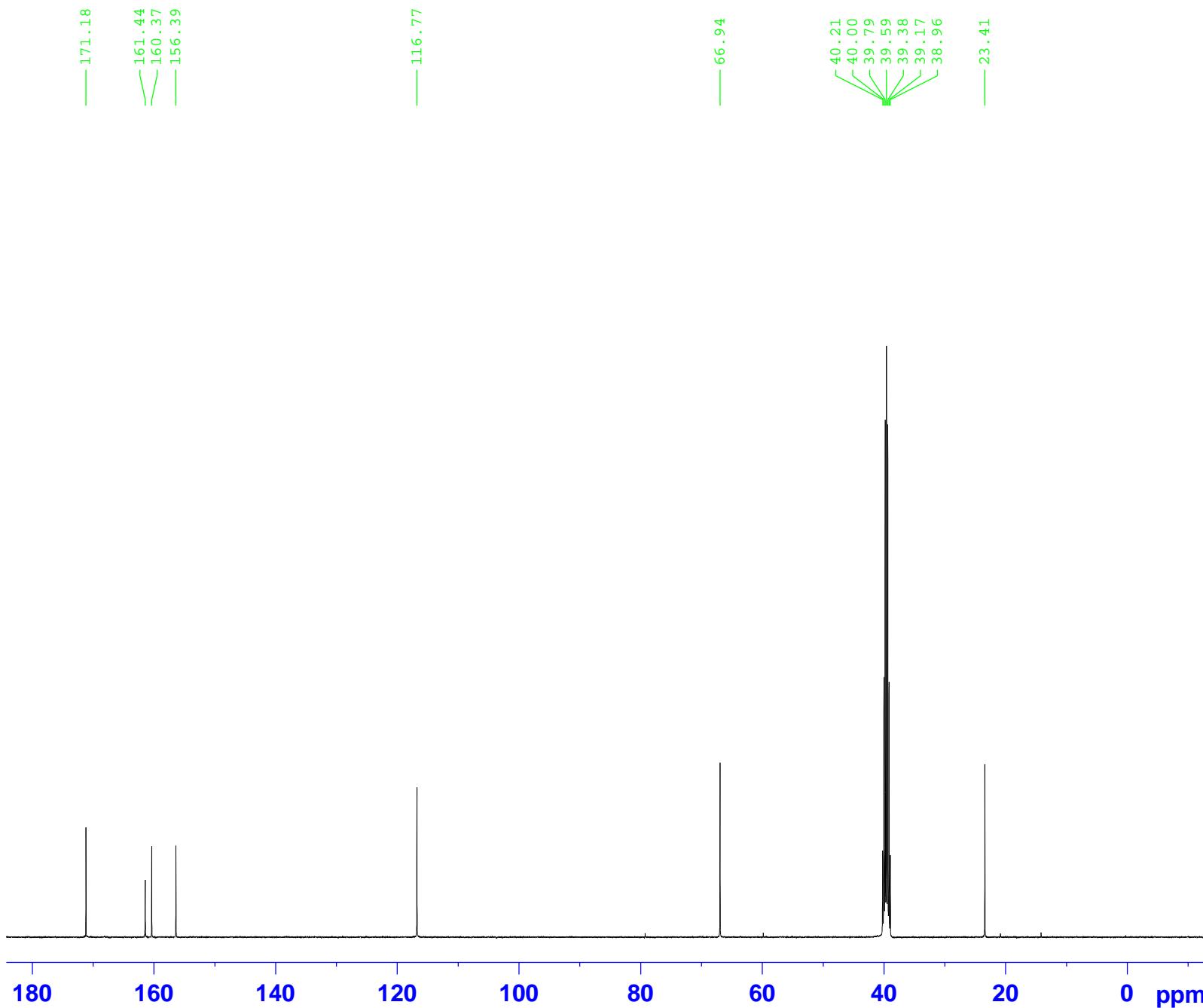
Current Data Parameters
NAME April13-2015
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters
Date 20150413
Time 22.24
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 71.13
DW 62.400 usec
DE 6.50 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 9.50 usec
PLW1 15.80000019 W

F2 - Processing parameters
SI 65536
SF 400.1300037 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ZSL-1-19-C



Current Data Parameters
NAME April13-2015
EXPNO 9
PROCNO 1

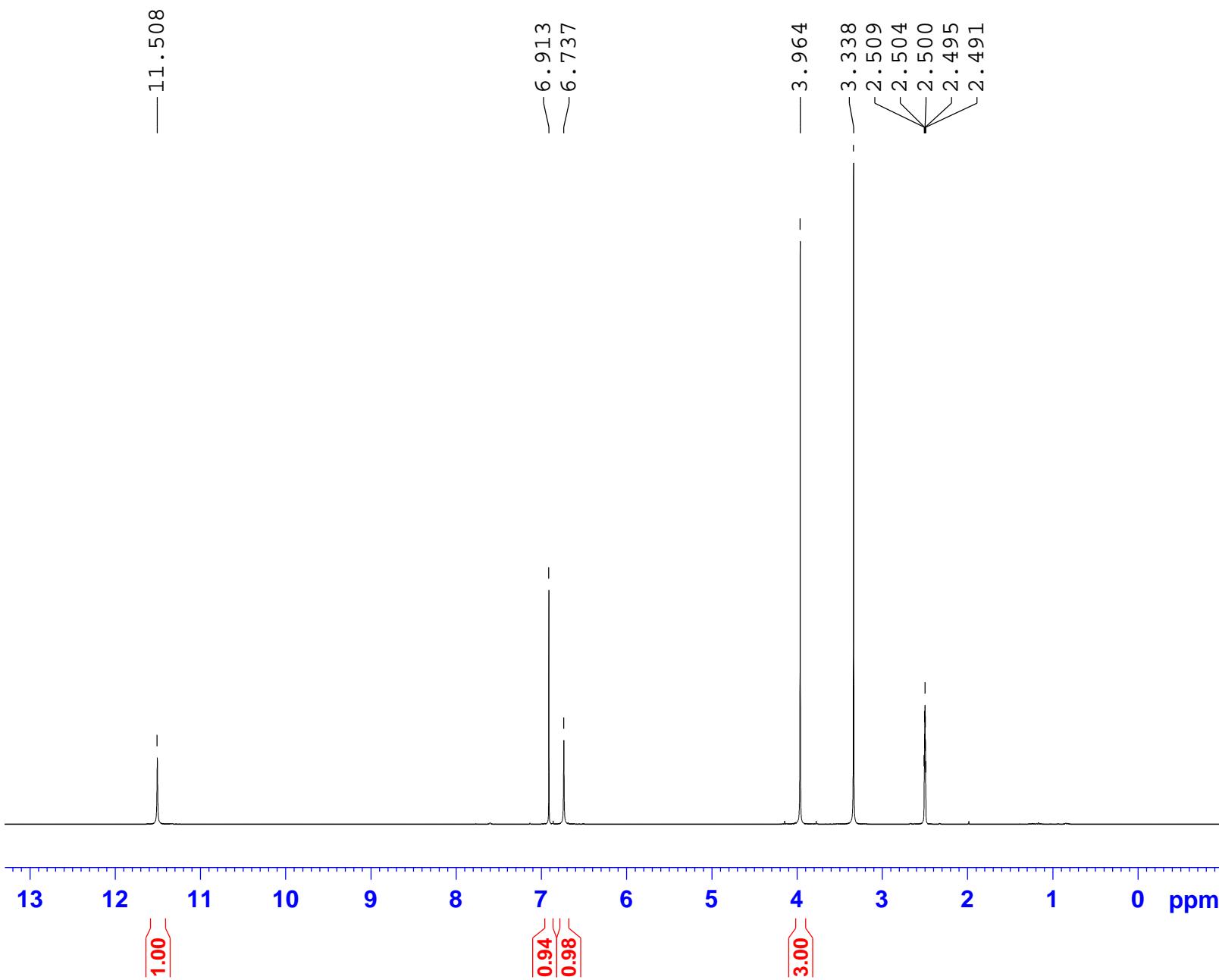
F2 - Acquisition Parameters
Date 20150414
Time 2.26
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 4096
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 199.94
DW 20.800 usec
DE 6.50 usec
TE 295.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 9.50 usec
PLW1 66.50000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 18.00000000 W
PLW12 0.20056000 W
PLW13 0.16245000 W

F2 - Processing parameters
SI 32768
SF 100.6128068 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

ZSL-1-22-H



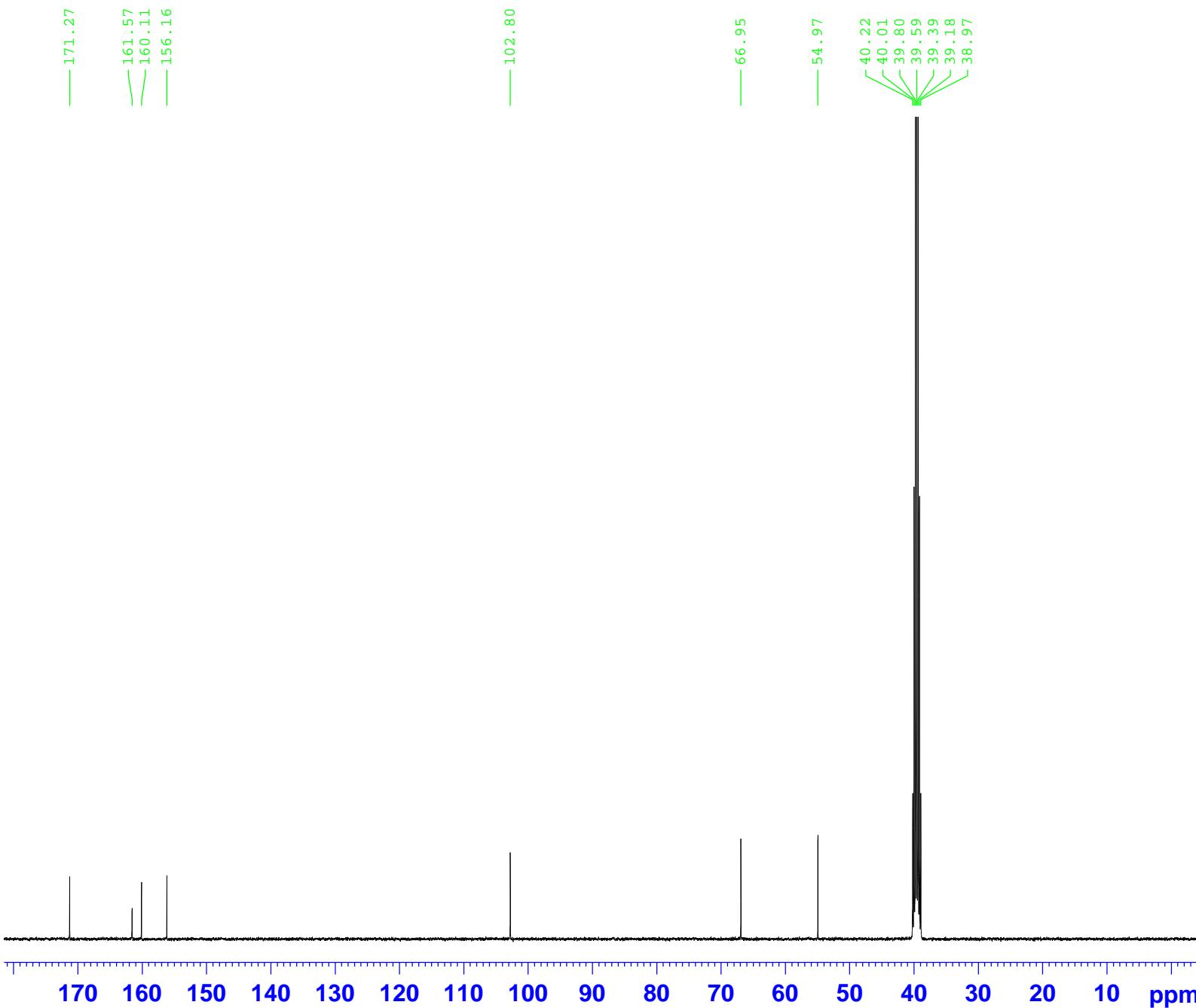
Current Data Parameters
NAME April12-2015
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150412
Time 17.22
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 112.04
DW 62.400 usec
DE 6.50 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 ======
SFO1 400.1324710 MHz
NUC1 1H
P1 9.50 usec
PLW1 15.80000019 W

F2 - Processing parameters
SI 65536
SF 400.1300035 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ZSL-1-22-C



Current Data Parameters
NAME April12-2015
EXPNO 10
PROCNO 1

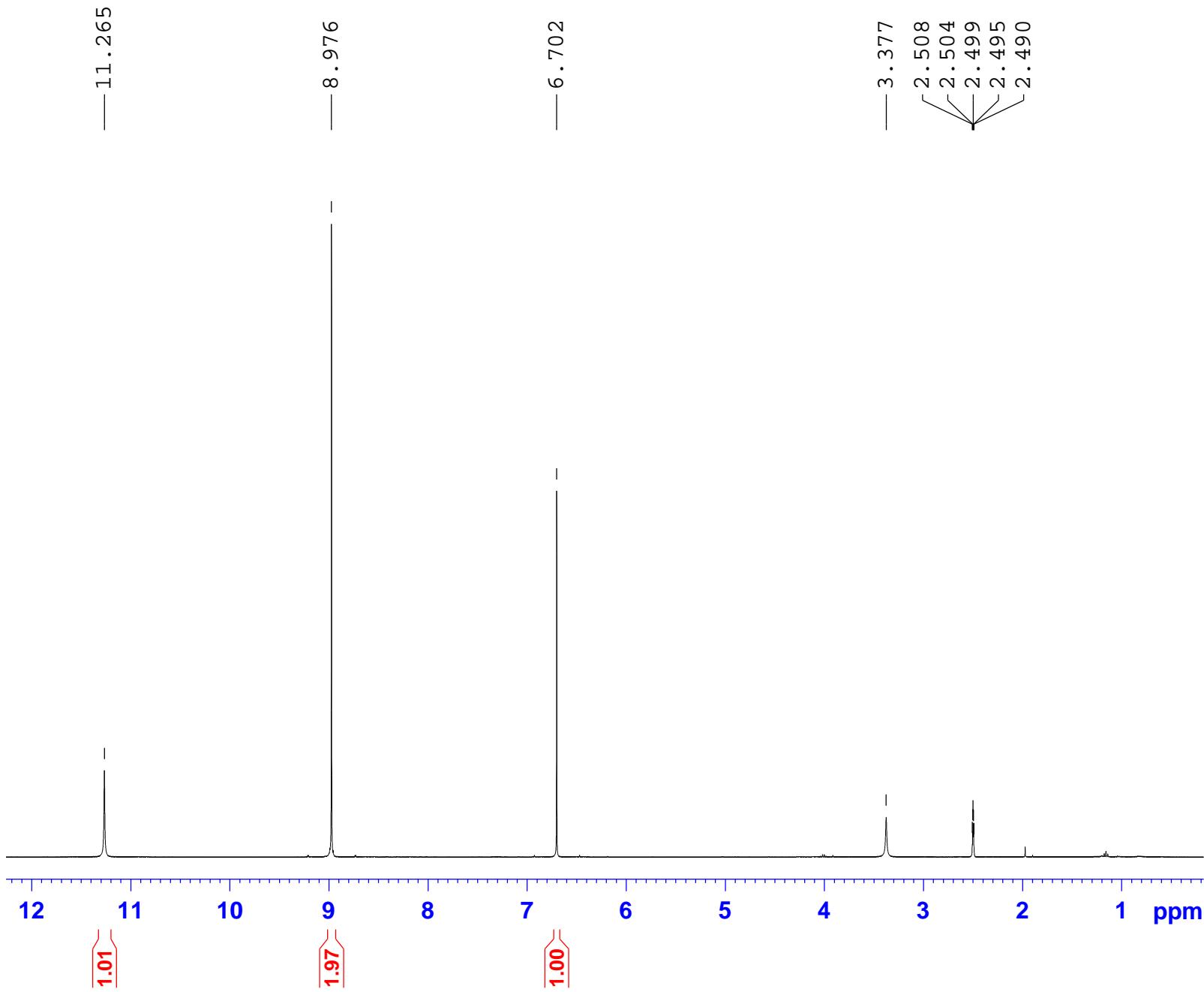
F2 - Acquisition Parameters
Date_ 20150412
Time 19.51
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 199.94
DW 20.800 usec
DE 6.50 usec
TE 295.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 9.50 usec
PLW1 66.50000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 18.00000000 W
PLW12 0.20056000 W
PLW13 0.16245000 W

F2 - Processing parameters
SI 32768
SF 100.6128059 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

ZSL-1-23-H



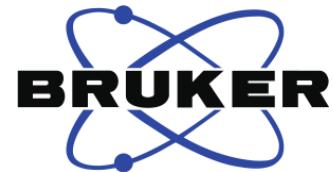
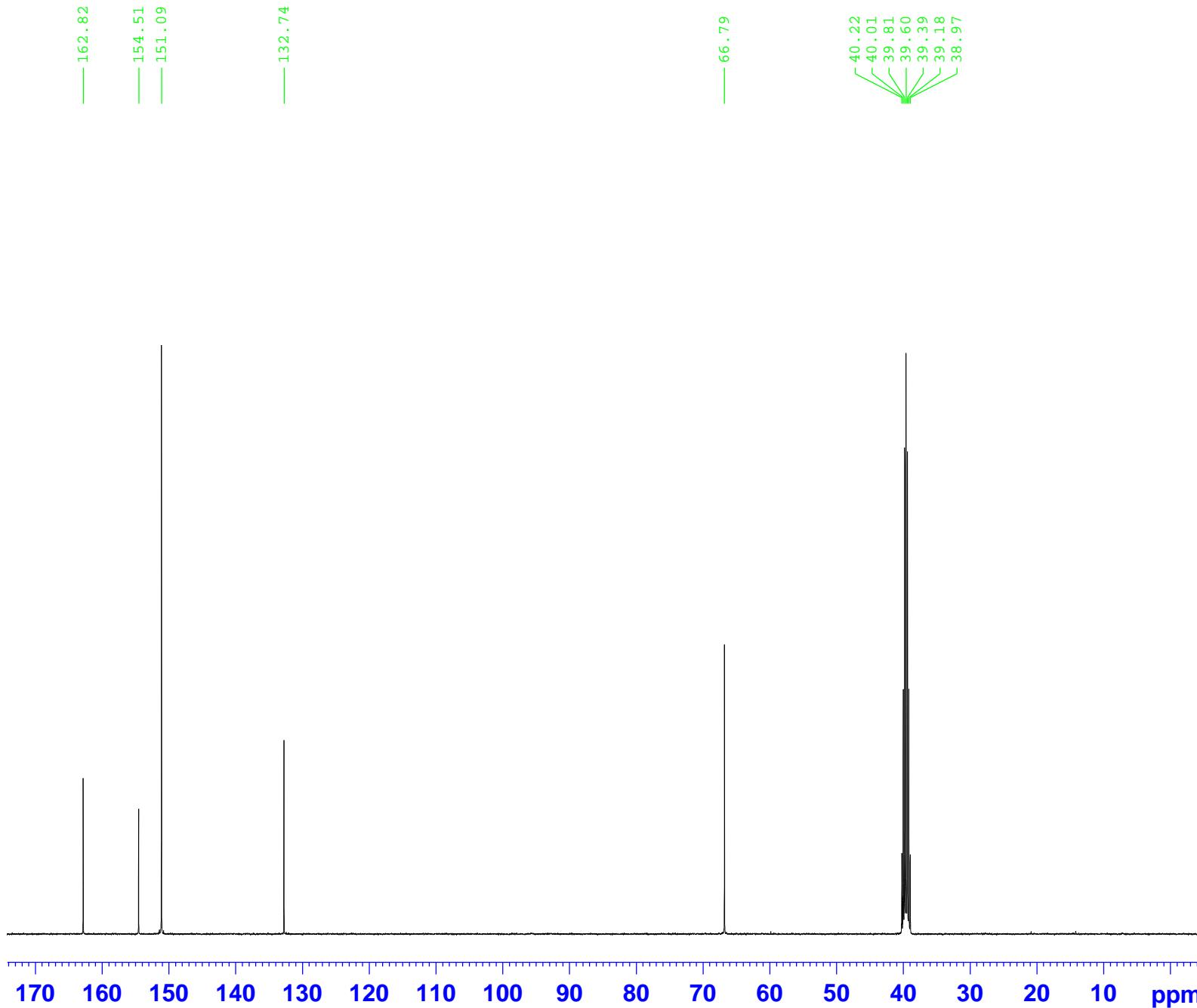
Current Data Parameters
NAME Apr12-2015
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150412
Time 17.26
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 78.4
DW 62.400 usec
DE 6.50 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 ======
SFO1 400.1324710 MHz
NUC1 1H
P1 9.50 usec
PLW1 15.80000019 W

F2 - Processing parameters
SI 65536
SF 400.1300038 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ZSL-1-23-C



Current Data Parameters
NAME April2-2015
EXPNO 11
PROCNO 1

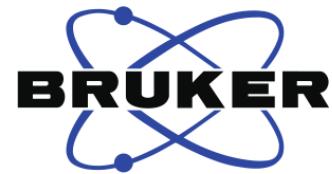
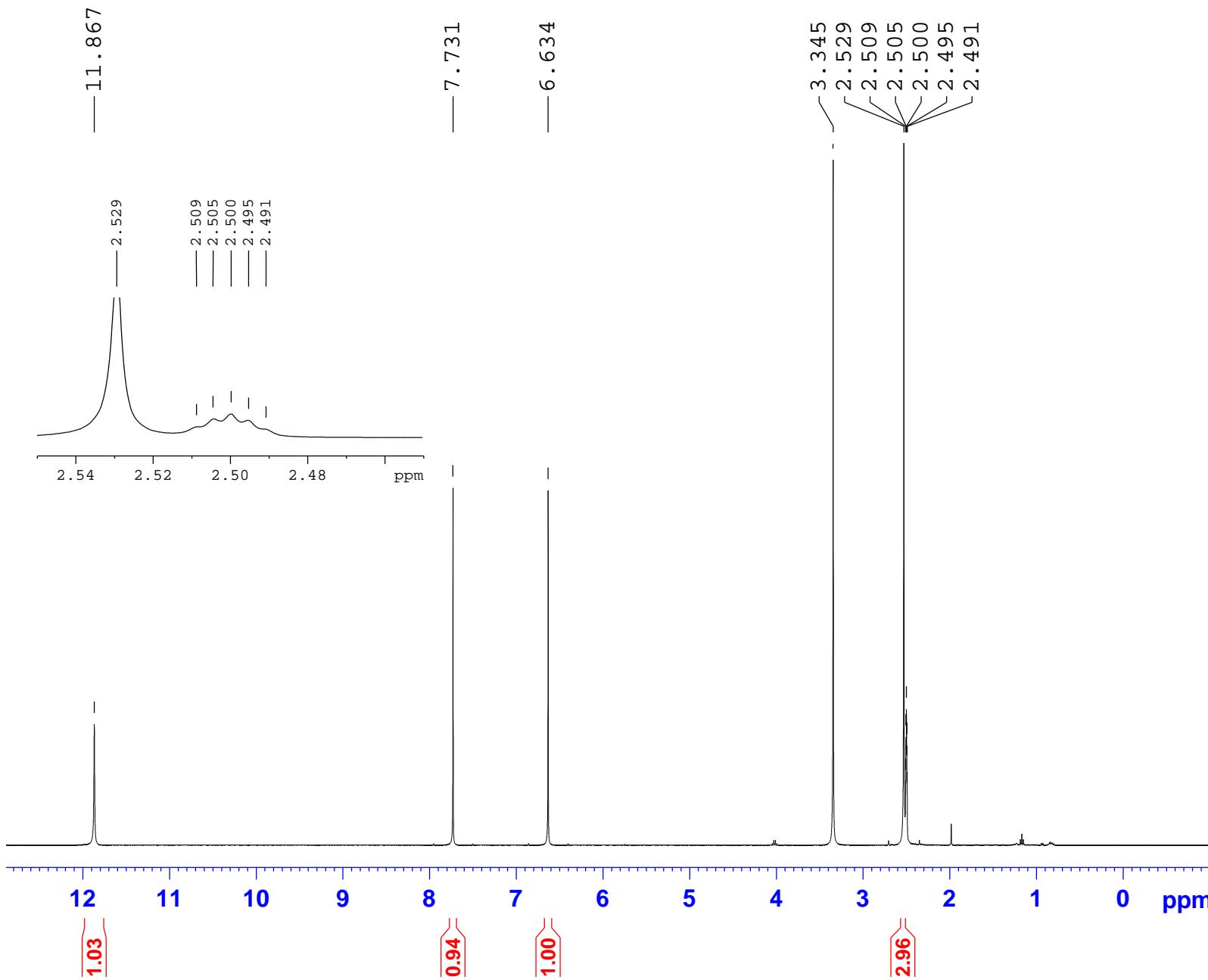
F2 - Acquisition Parameters
Date_ 20150412
Time 21.51
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zpgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 199.94
DW 20.800 usec
DE 6.50 usec
TE 295.0 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 9.50 usec
PLW1 66.50000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 18.00000000 W
PLW12 0.20056000 W
PLW13 0.16245000 W

F2 - Processing parameters
SI 32768
SF 100.6128046 MHz
WDW EM
SSB 0
LB 0 1.00 Hz
GB 0
PC 1.40

ZSL-1-24-H



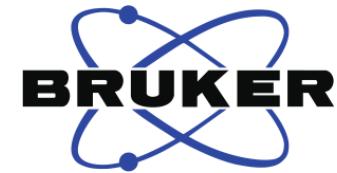
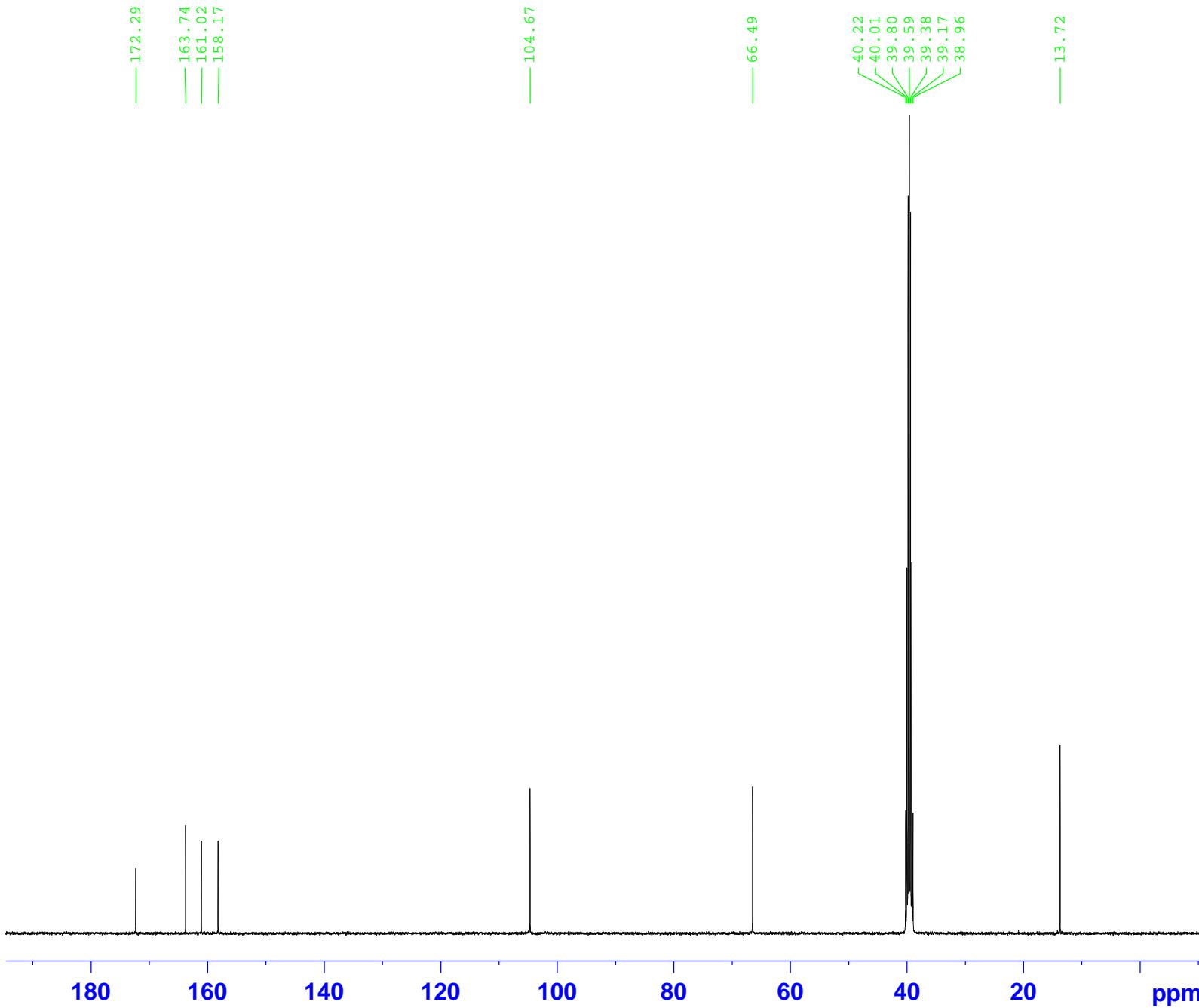
Current Data Parameters
NAME Apr12-2015
EXPNO 9
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150412
Time 17.30
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 98.76
DW 62.400 usec
DE 6.50 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 9.50 usec
PLW1 15.80000019 W

F2 - Processing parameters
SI 65536
SF 400.1300035 MHz
WDW EM
SSB 0
LB 0 0.30 Hz
GB 0
PC 1.00

ZSL-1-24-C



Current Data Parameters
NAME April12-2015
EXPNO 12
PROCNO 1

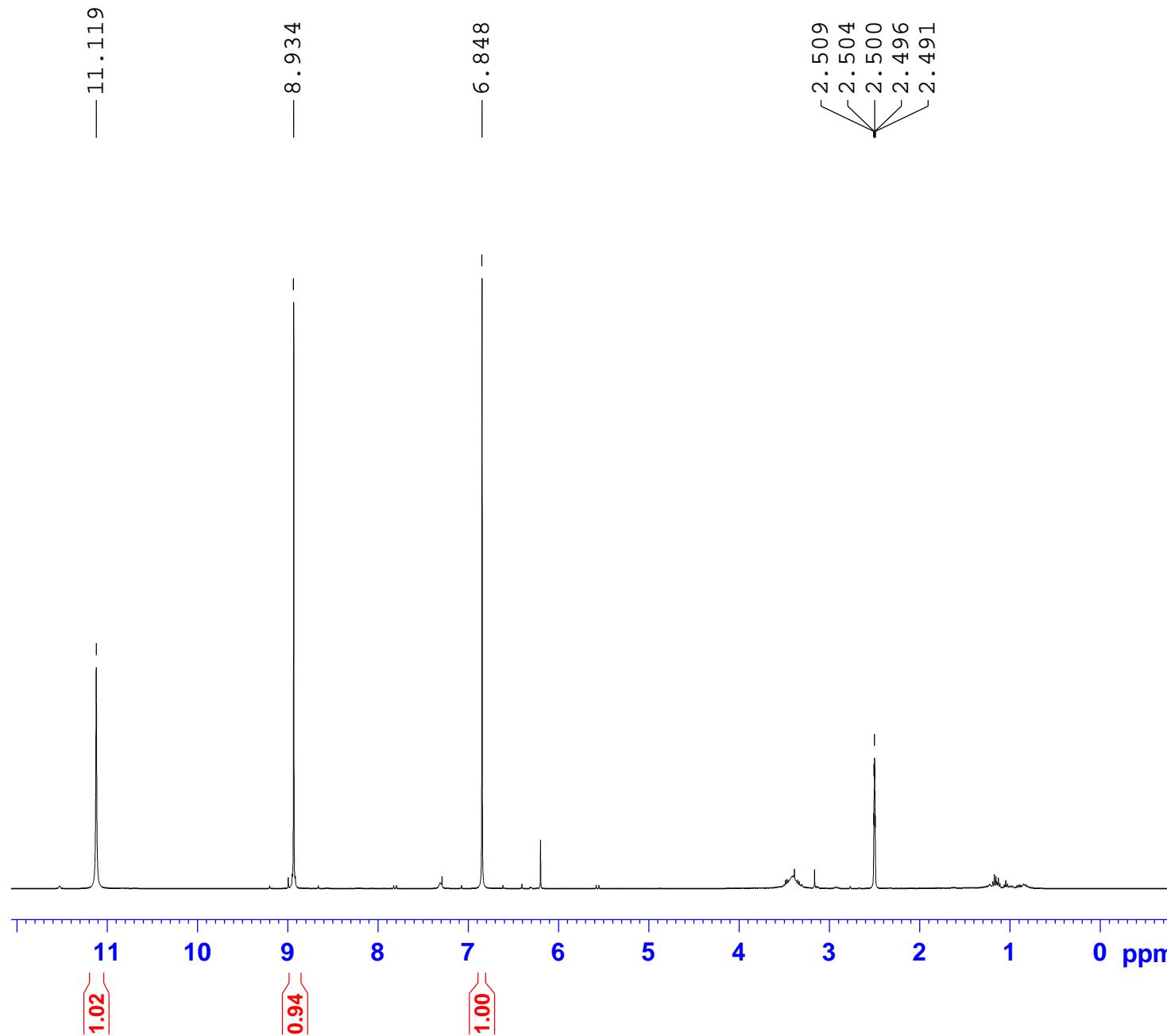
F2 - Acquisition Parameters
Date_ 20150412
Time 23.50
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 199.94
DW 20.800 usec
DE 6.50 usec
TE 295.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 9.50 usec
PLW1 66.50000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 18.00000000 W
PLW12 0.20056000 W
PLW13 0.16245000 W

F2 - Processing parameters
SI 32768
SF 100.6128062 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

ZSL-1-26-H



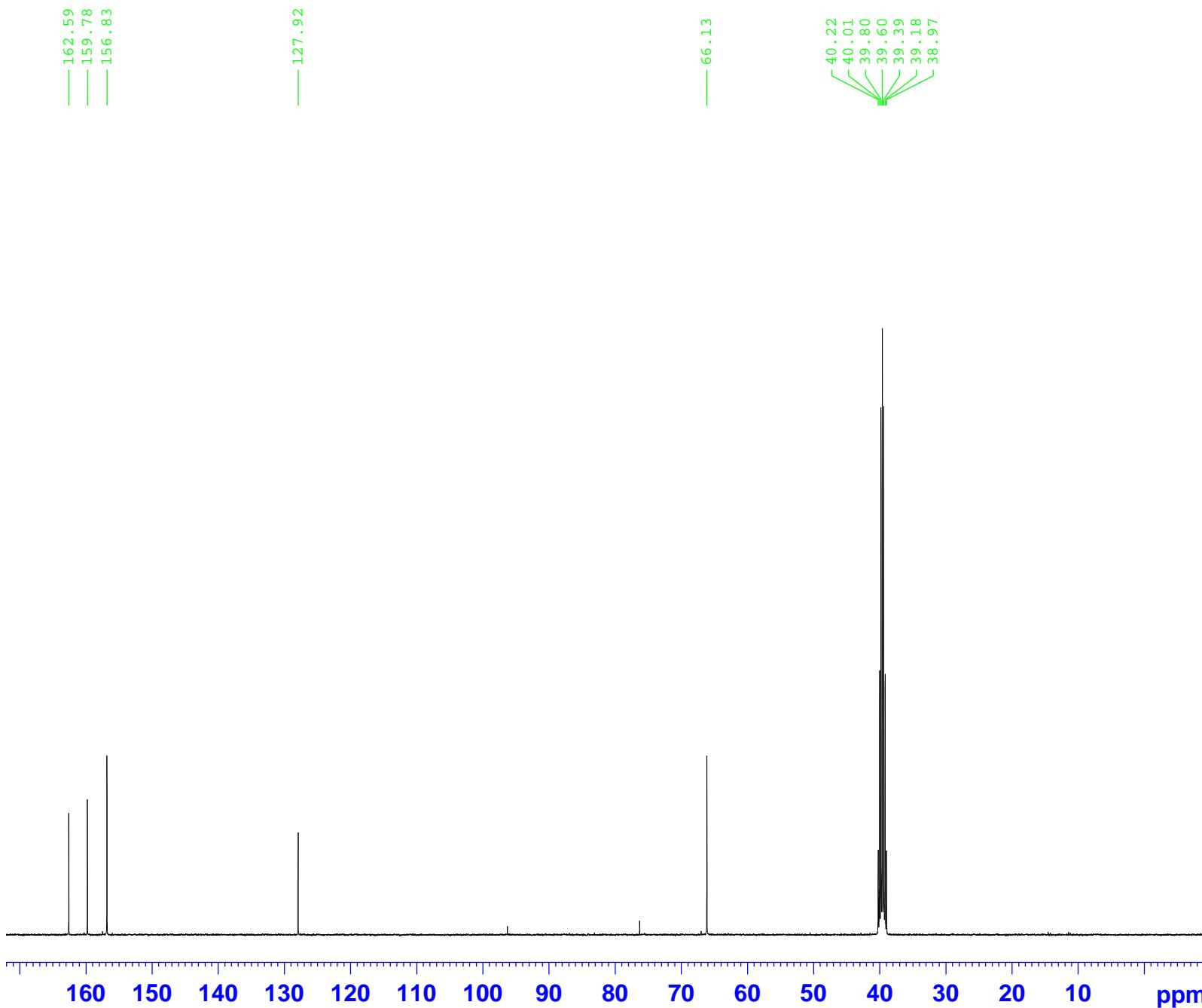
Current Data Parameters
NAME Apr14-2015
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150414
Time 11.32
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 98.76
DW 62.400 usec
DE 6.50 usec
TE 295.0 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 9.50 usec
PLW1 15.80000019 W

F2 - Processing parameters
SI 65536
SF 400.1300034 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ZSL-1-26-C



Current Data Parameters
NAME April14-2015
EXPNO 6
PROCNO 1

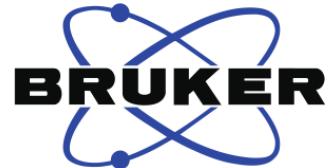
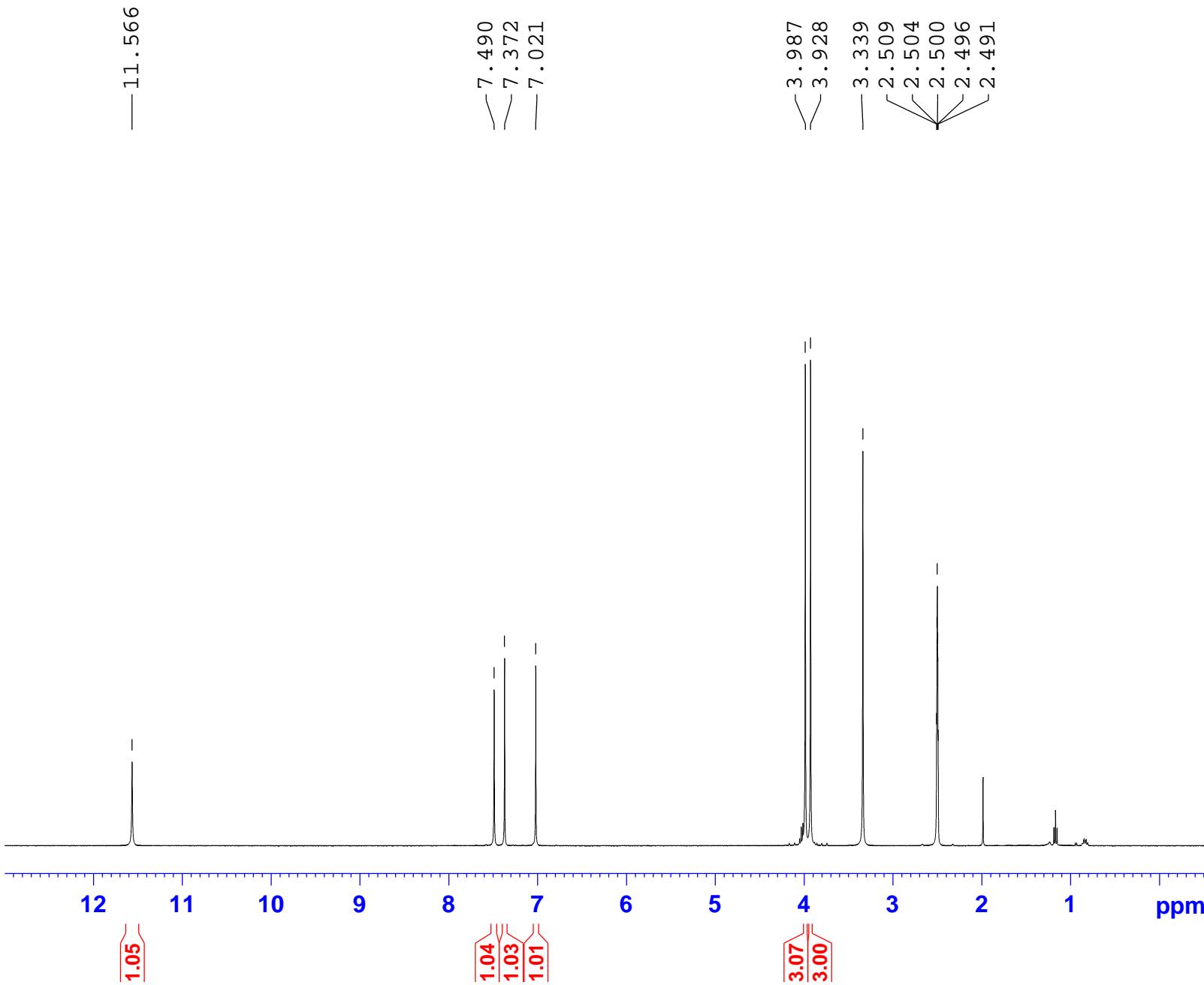
F2 - Acquisition Parameters
Date_ 20150414
Time 19.12
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 199.94
DW 20.800 usec
DE 6.50 usec
TE 295.0 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 9.50 usec
PLW1 66.50000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 18.00000000 W
PLW12 0.20056000 W
PLW13 0.16245000 W

F2 - Processing parameters
SI 32768
SF 100.6128059 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

ZSL-1-27-H



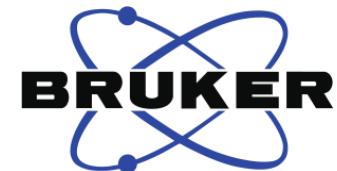
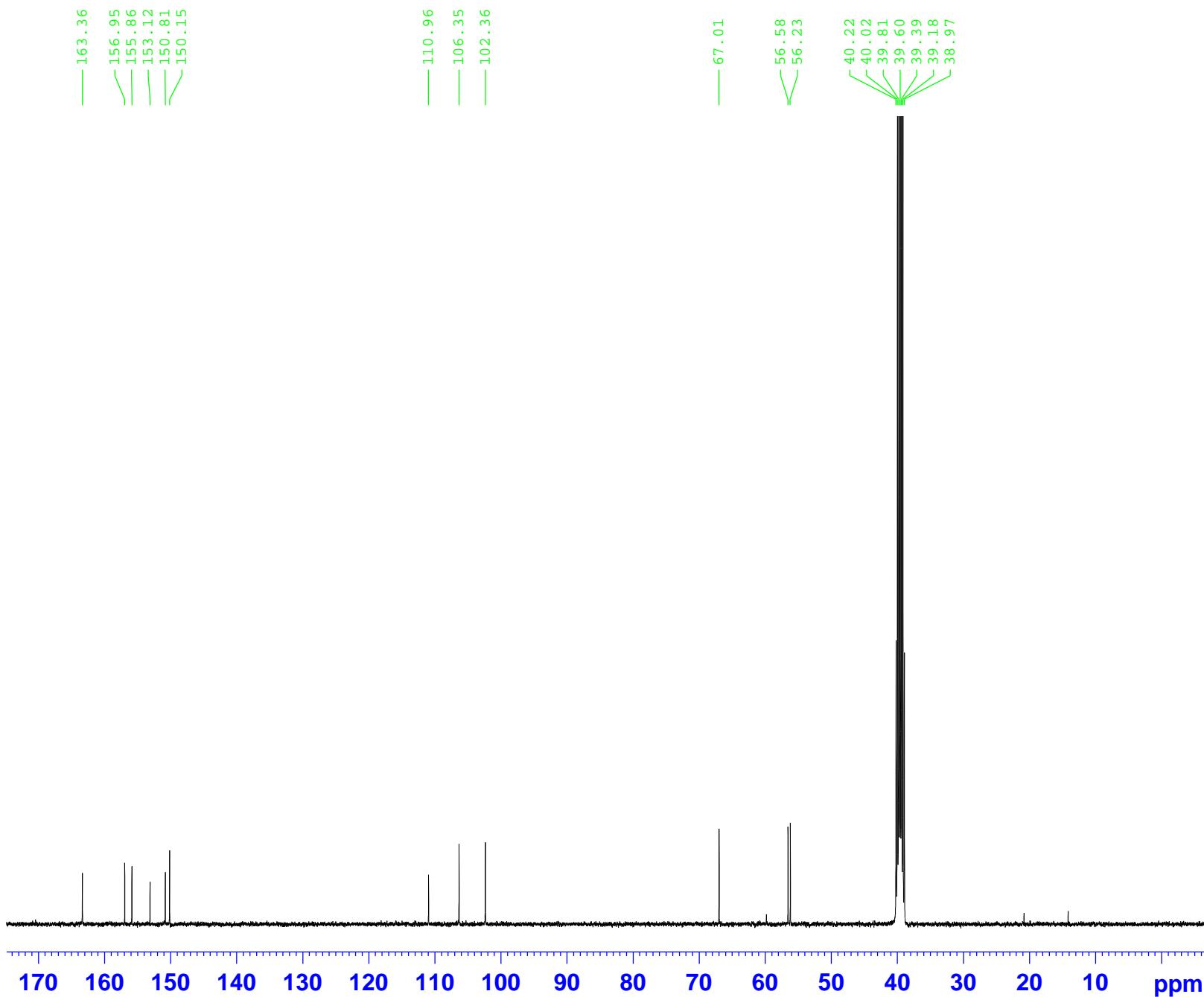
Current Data Parameters
NAME April14-2015
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150414
Time 11.28
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 128.54
DW 62.400 usec
DE 6.50 usec
TE 295.0 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 9.50 usec
PLW1 15.80000019 W

F2 - Processing parameters
SI 65536
SF 400.1300033 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ZSL-1-27-C



Current Data Parameters
NAME Apr14-2015
EXPNO 5
PROCNO 1

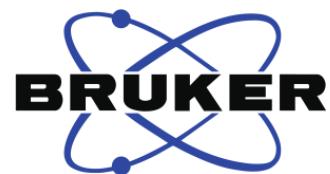
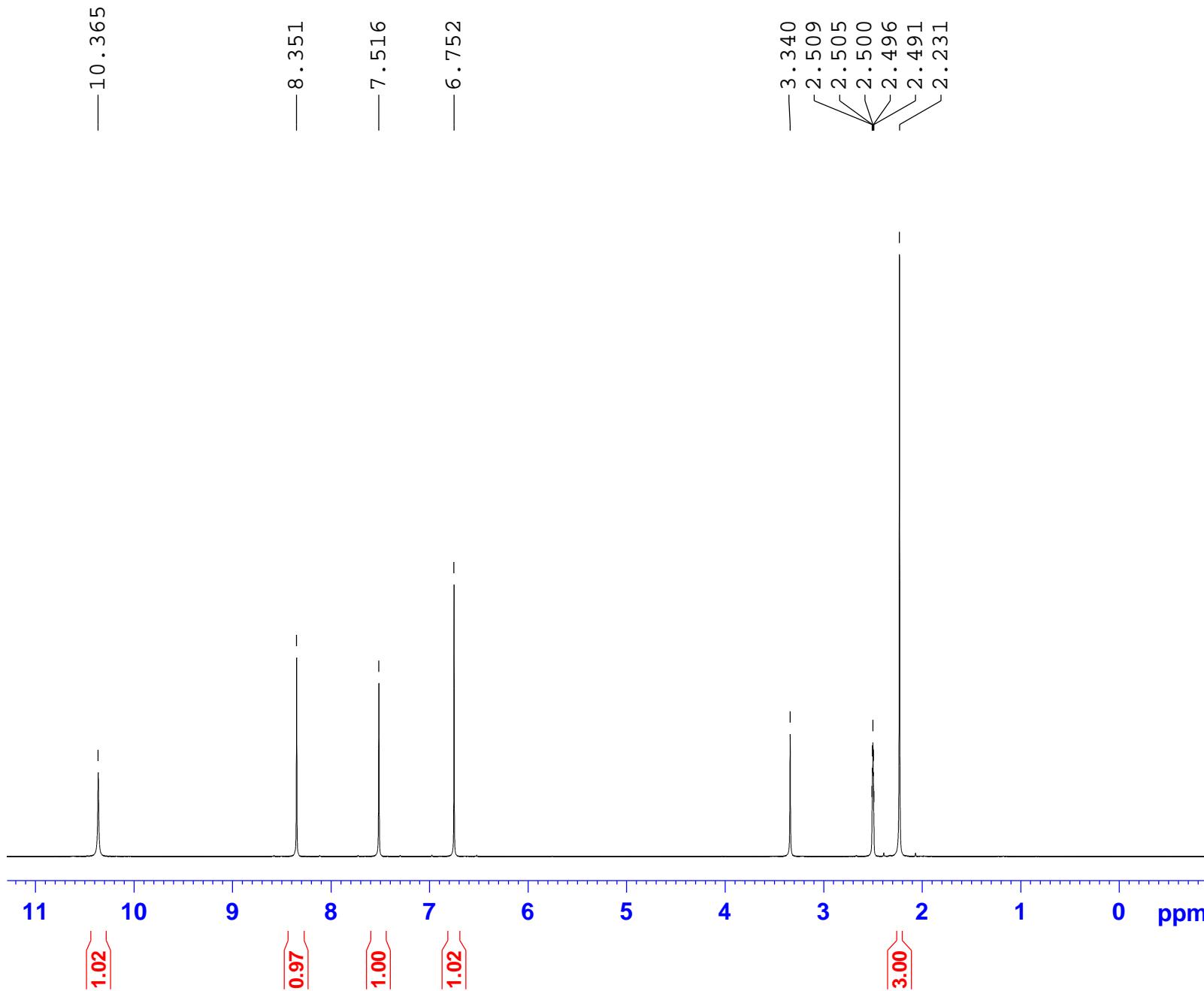
F2 - Acquisition Parameters
Date_ 20150414
Time 15.38
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 4096
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 199.94
DW 20.800 usec
DE 6.50 usec
TE 295.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 ¹³C
P1 9.50 usec
PLW1 66.50000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 ^{1H}
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 18.00000000 W
PLW12 0.20056000 W
PLW13 0.16245000 W

F2 - Processing parameters
SI 32768
SF 100.6128062 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

ZSL-1-28-H



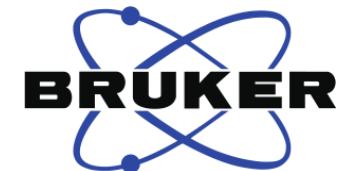
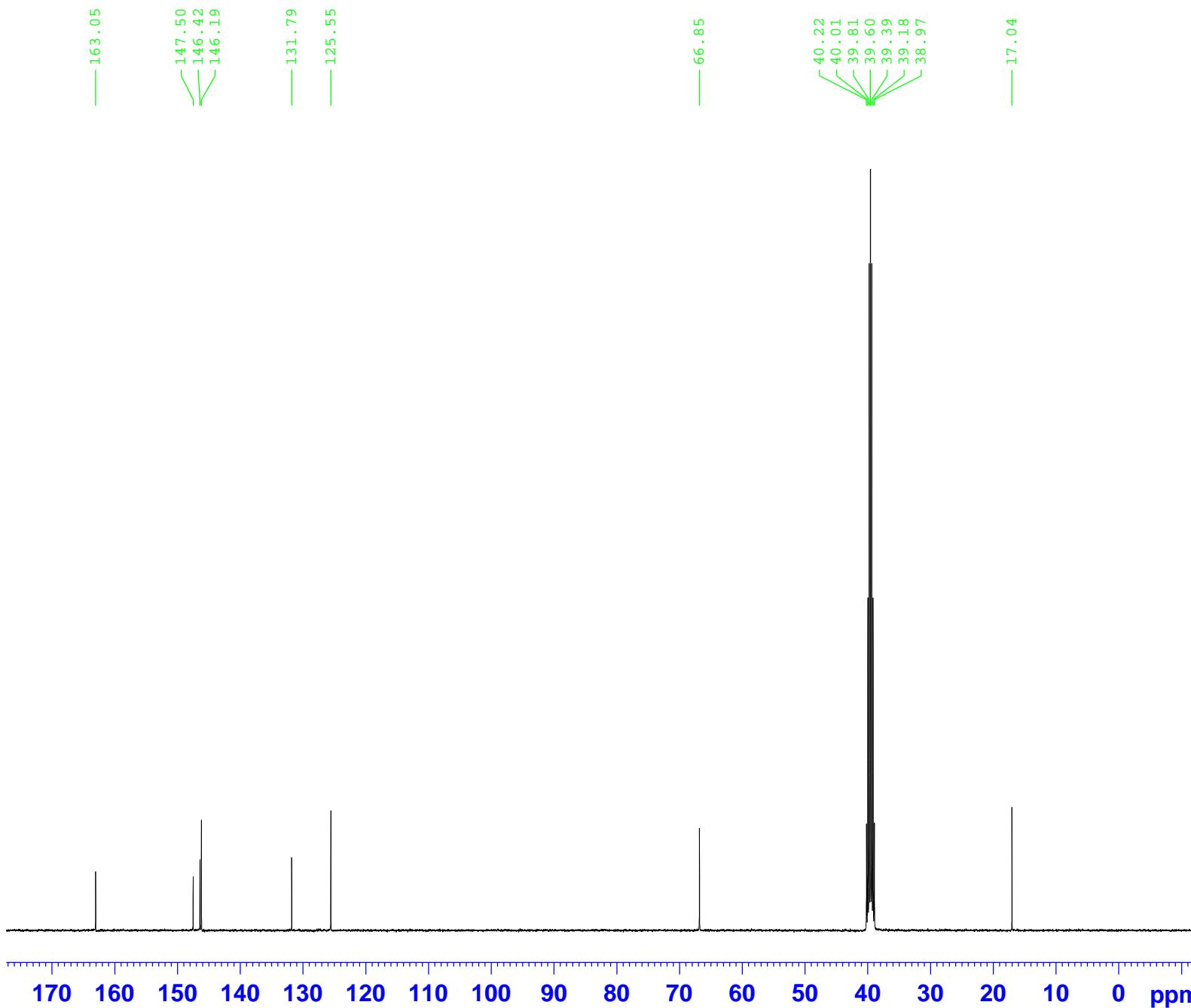
Current Data Parameters
NAME April15-2015
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150415
Time 8.40
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 98.76
DW 62.400 usec
DE 6.50 usec
TE 295.0 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 9.50 usec
PLW1 15.80000019 W

F2 - Processing parameters
SI 65536
SF 400.1300032 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ZSL-1-28-C



Current Data Parameters
NAME Apr15-2015
EXPNO 2
PROCNO 1

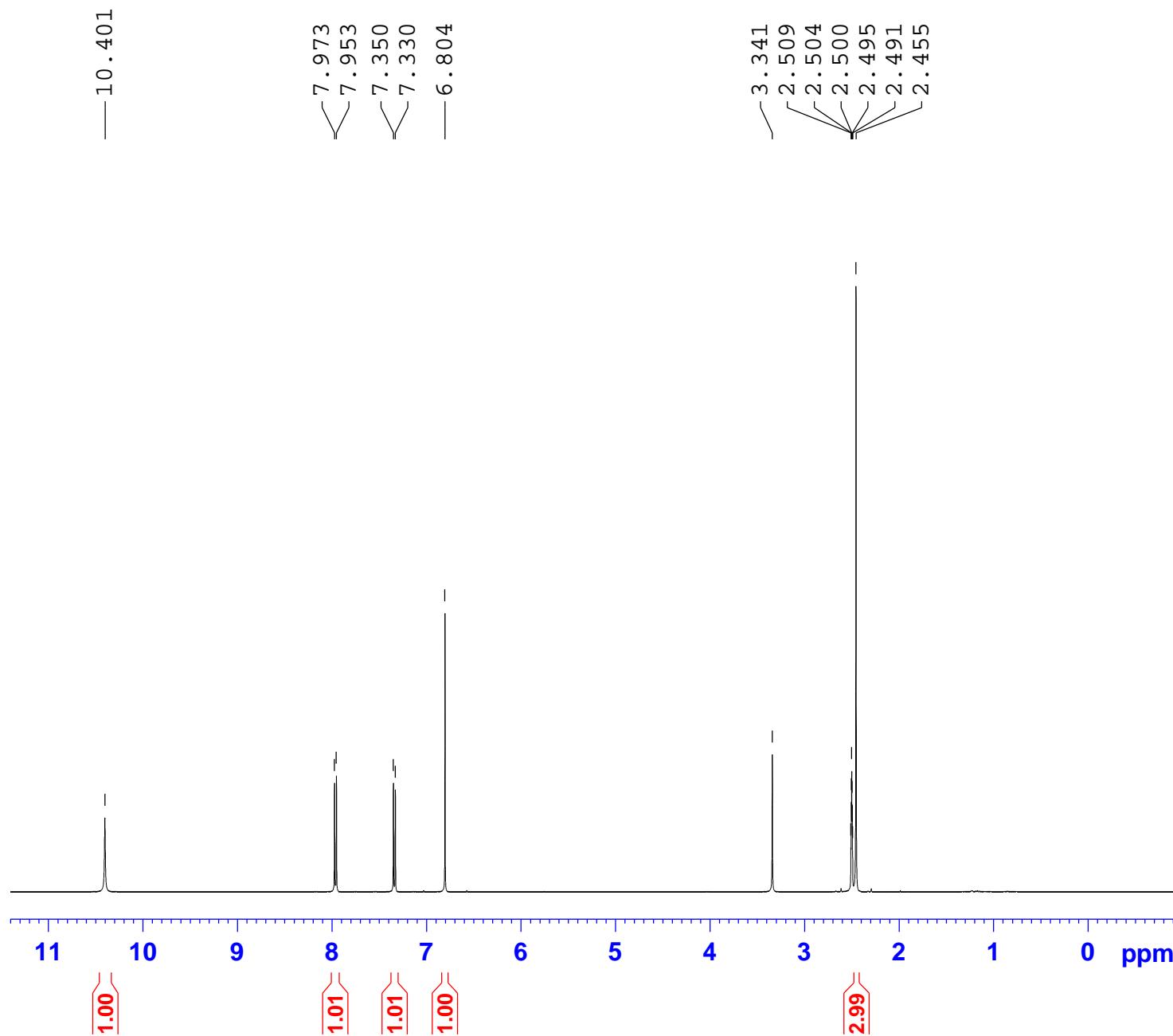
F2 - Acquisition Parameters
Date_ 20150415
Time 16.37
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 199.94
DW 20.800 usec
DE 6.50 usec
TE 295.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 9.50 usec
PLW1 66.50000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 18.00000000 W
PLW12 0.20056000 W
PLW13 0.16245000 W

F2 - Processing parameters
SI 32768
SF 100.6128065 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

ZSL-1-29-H



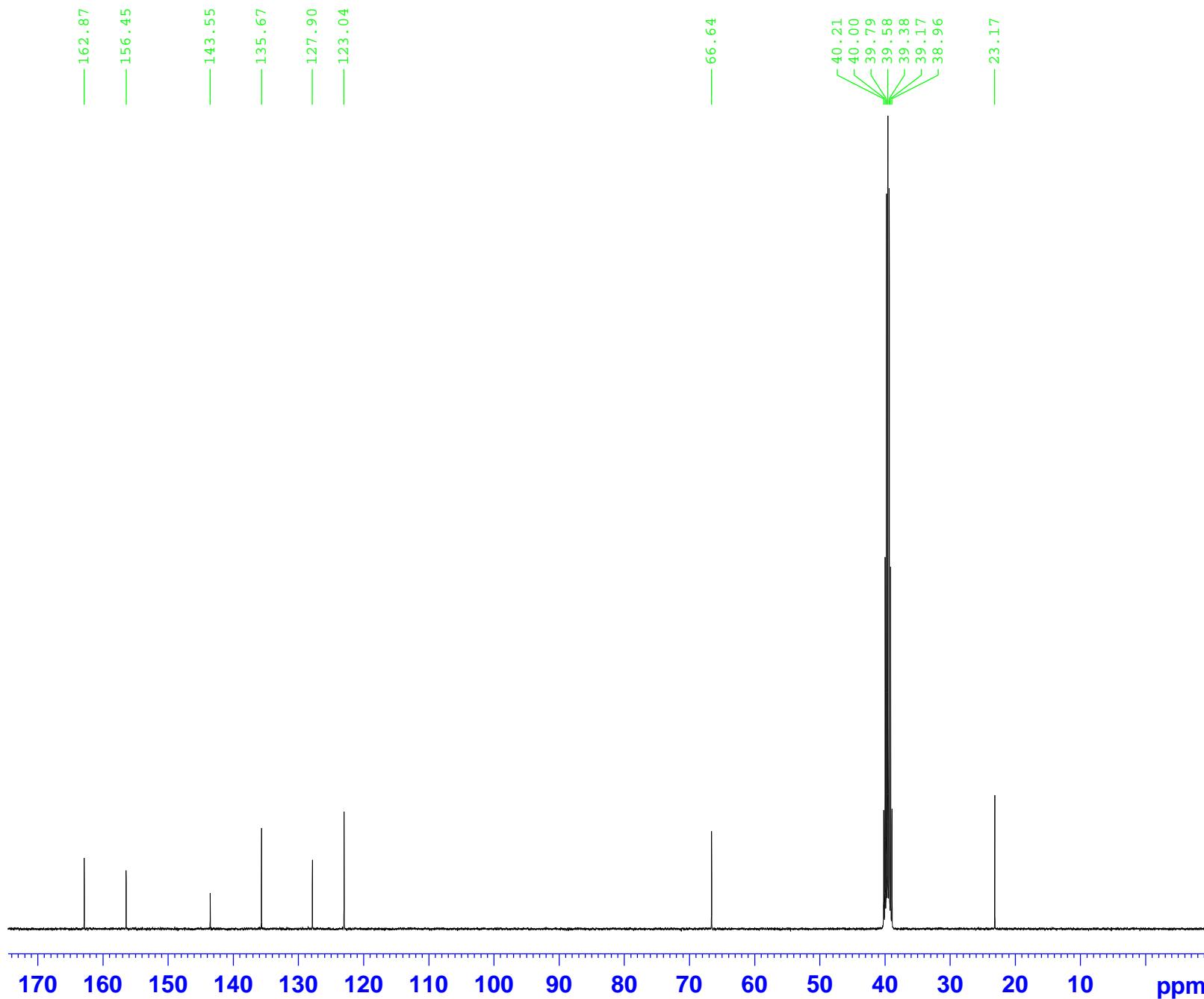
Current Data Parameters
NAME April16-2015
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date 20150416
Time 8.47
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 112.04
DW 62.400 usec
DE 6.50 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 400.1324710 MHz
NUC1 1H
P1 9.50 usec
PLW1 15.80000019 W

F2 - Processing parameters
SI 65536
SF 400.1300035 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ZSL-1-29-C



Current Data Parameters
NAME Apr16-2015
EXPNO 4
PROCNO 1

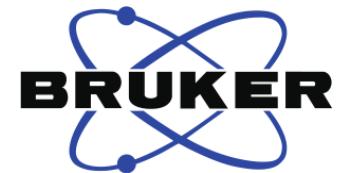
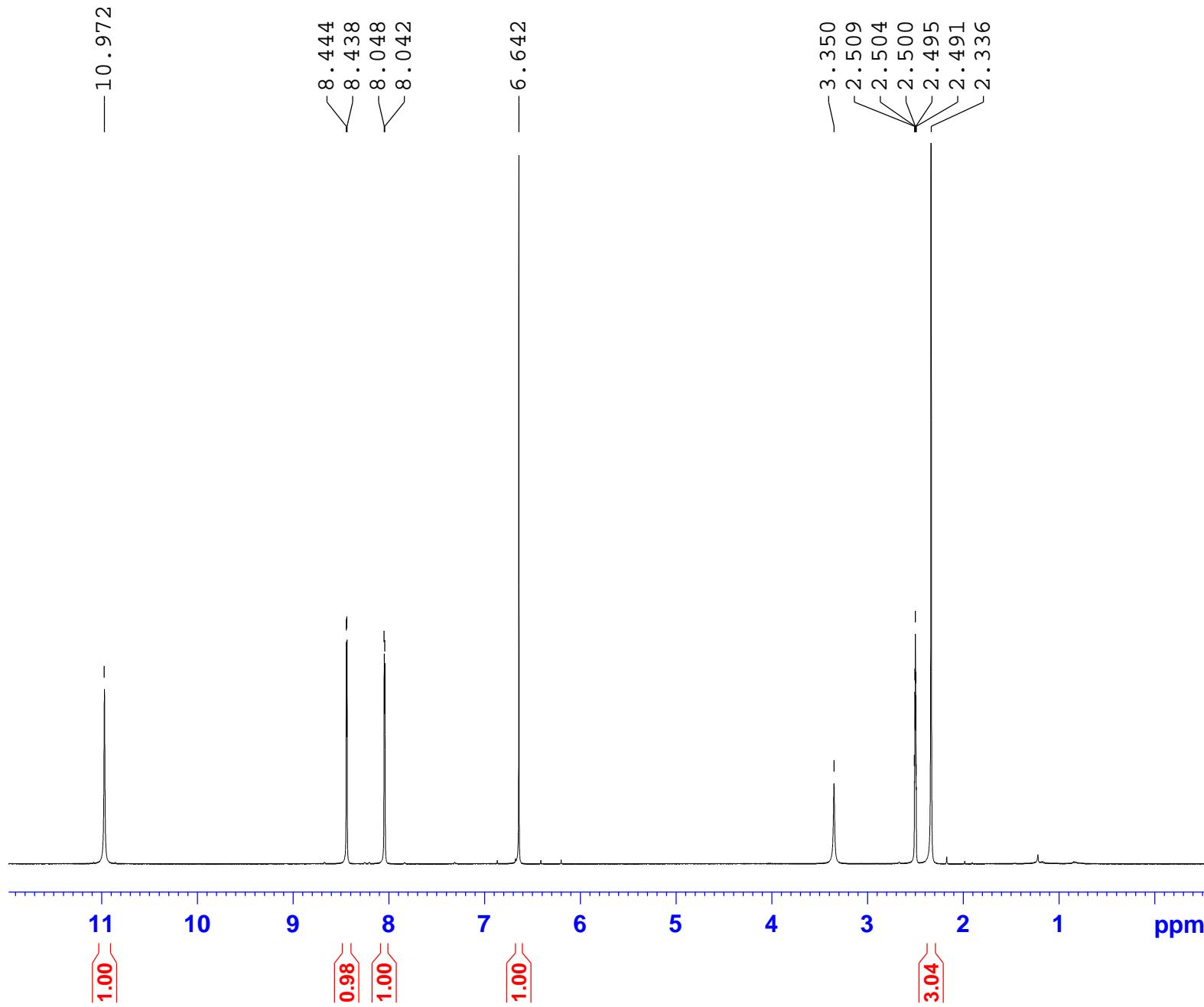
F2 - Acquisition Parameters
Date_ 20150416
Time 13.39
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 199.94
DW 20.800 usec
DE 6.50 usec
TE 295.0 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 ¹³C
P1 9.50 usec
PLW1 66.50000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 ¹H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 18.00000000 W
PLW12 0.20056000 W
PLW13 0.16245000 W

F2 - Processing parameters
SI 32768
SF 100.6128079 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

ZSL-1-30-H



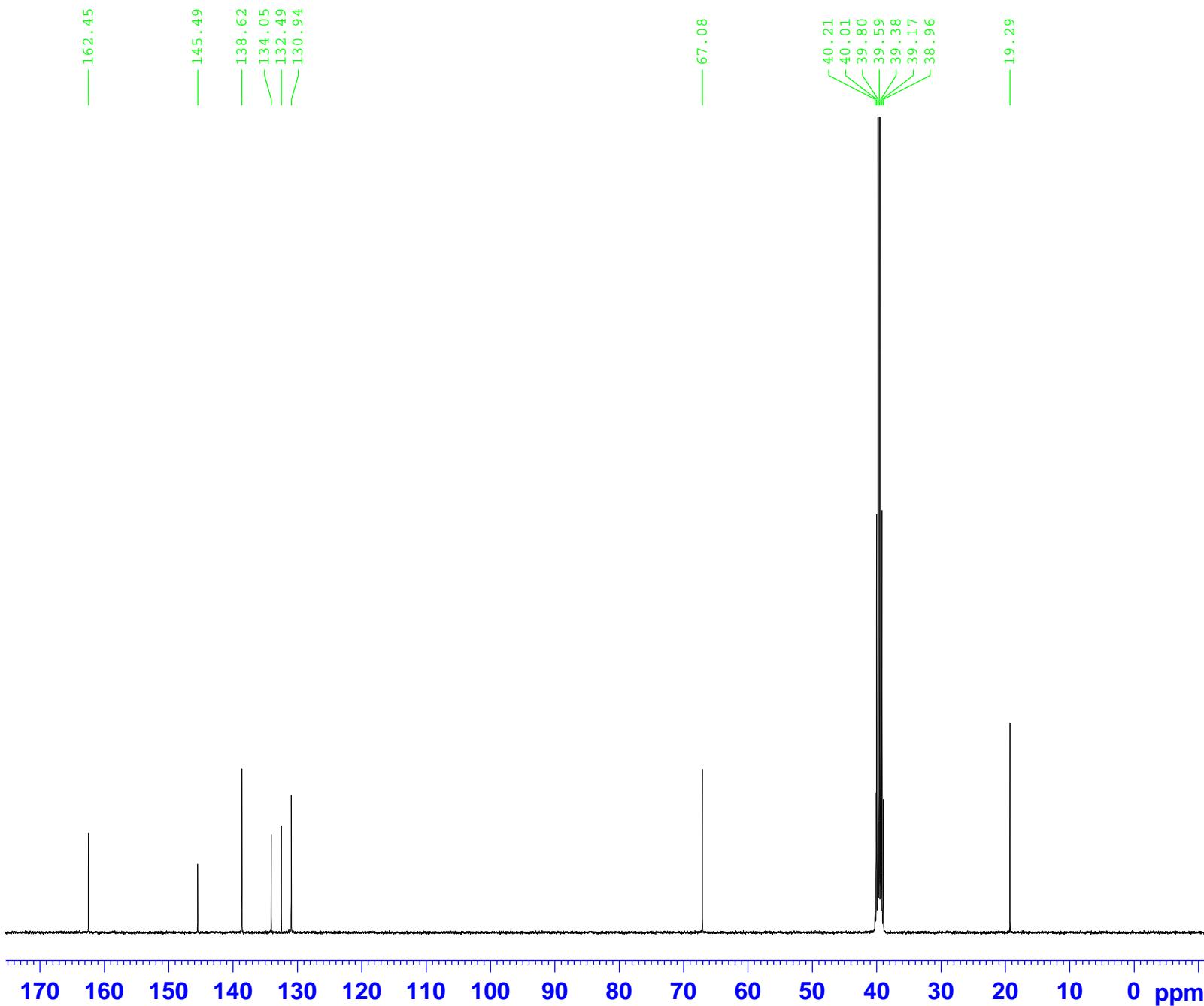
Current Data Parameters
NAME April16-2015
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150416
Time 8.51
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 98.76
DW 62.400 usec
DE 6.50 usec
TE 295.0 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 9.50 usec
PLW1 15.80000019 W

F2 - Processing parameters
SI 65536
SF 400.1300035 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ZSL-1-30-C



Current Data Parameters
NAME April16-2015
EXPNO 3
PROCNO 1

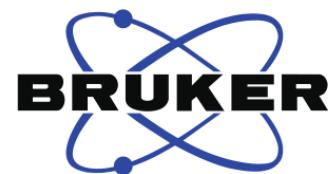
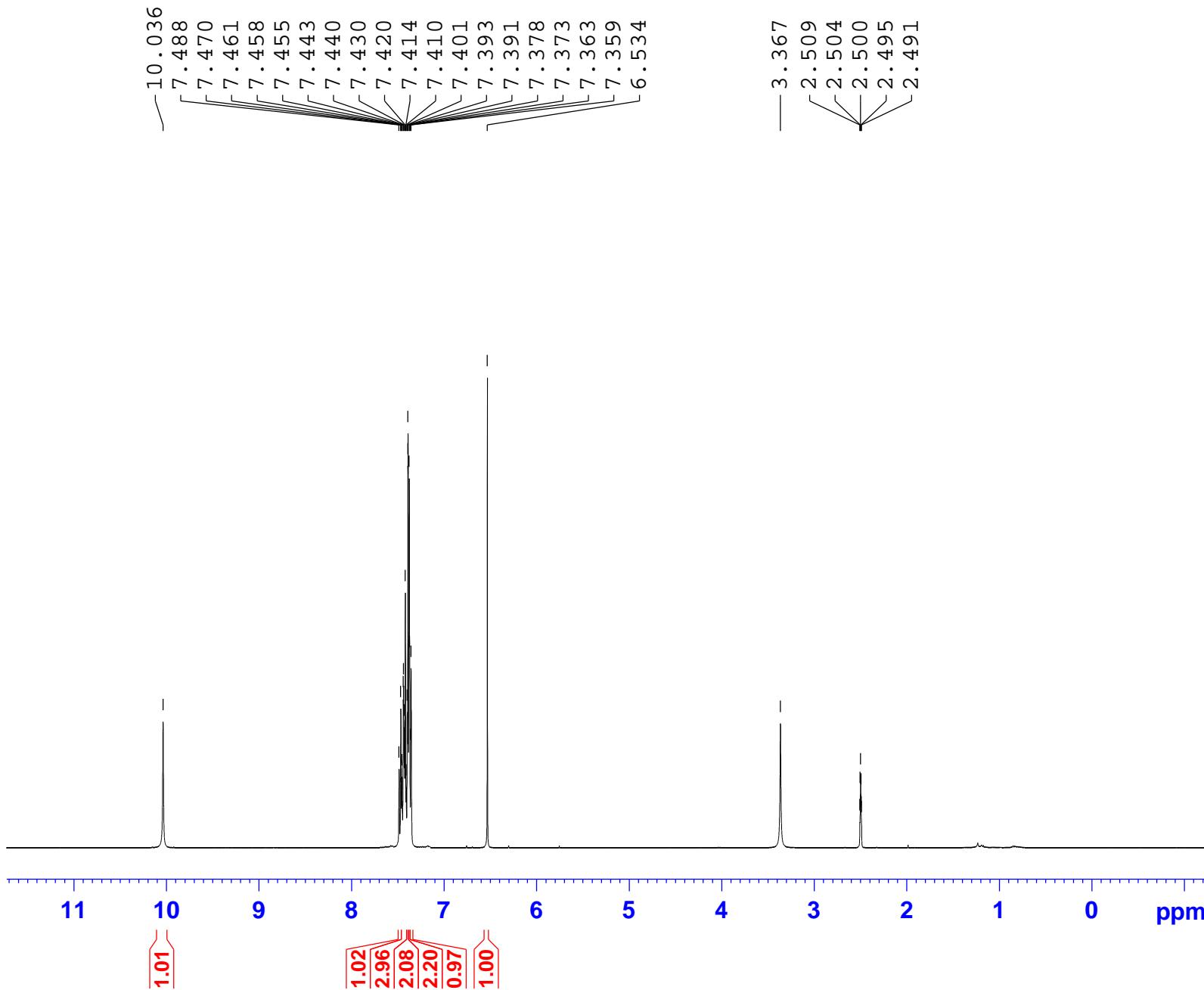
F2 - Acquisition Parameters
Date_ 20150416
Time 10.51
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 199.94
DW 20.800 usec
DE 6.50 usec
TE 295.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 9.50 usec
PLW1 66.50000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 18.00000000 W
PLW12 0.20056000 W
PLW13 0.16245000 W

F2 - Processing parameters
SI 32768
SF 100.6128071 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

ZSL-1-34-H



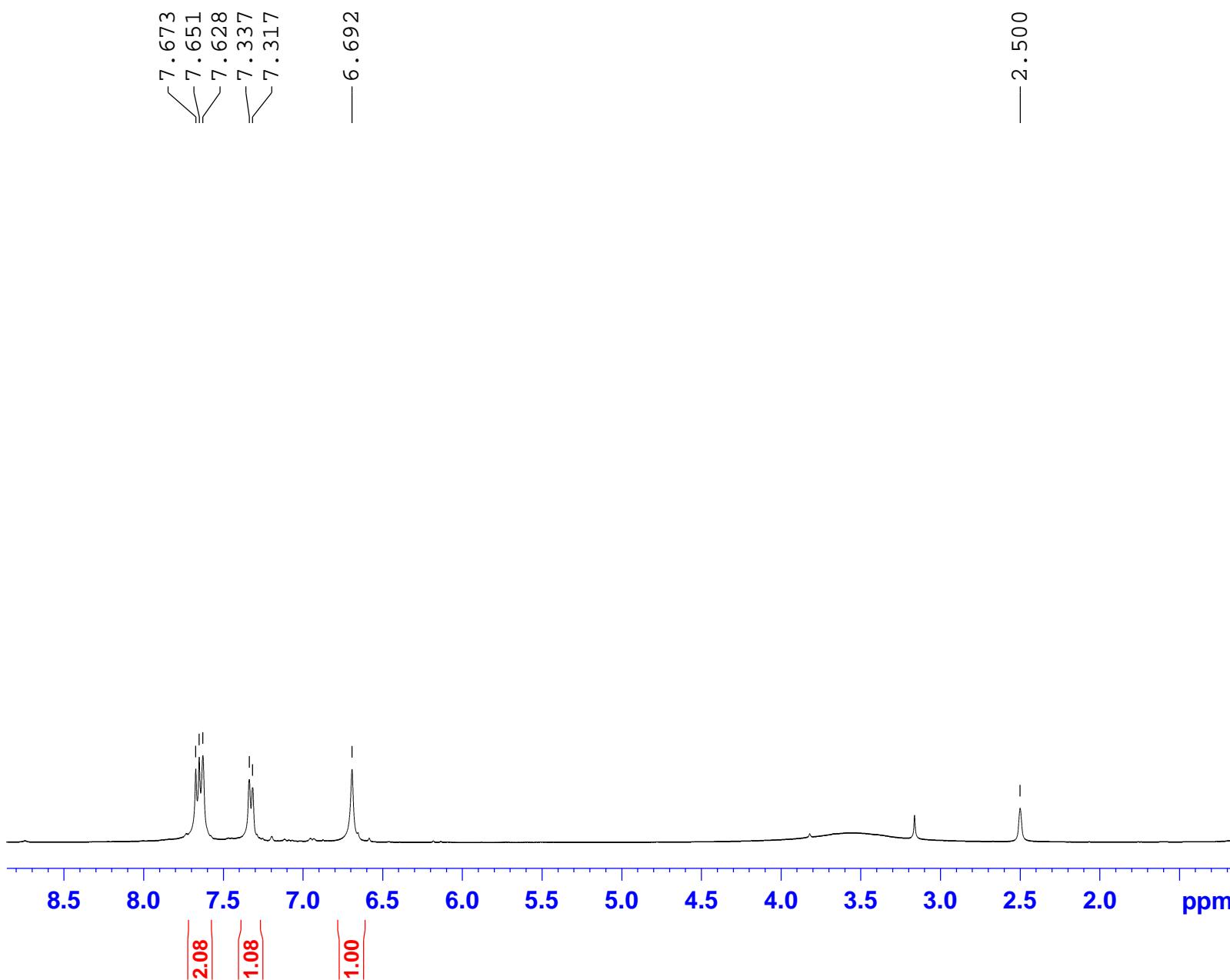
Current Data Parameters
NAME May29-2015
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150529
Time 12.19
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 54.6
DW 62.400 usec
DE 6.50 usec
TE 295.0 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 9.50 usec
PLW1 15.80000019 W

F2 - Processing parameters
SI 65536
SF 400.1300037 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

zsl-1-35-H



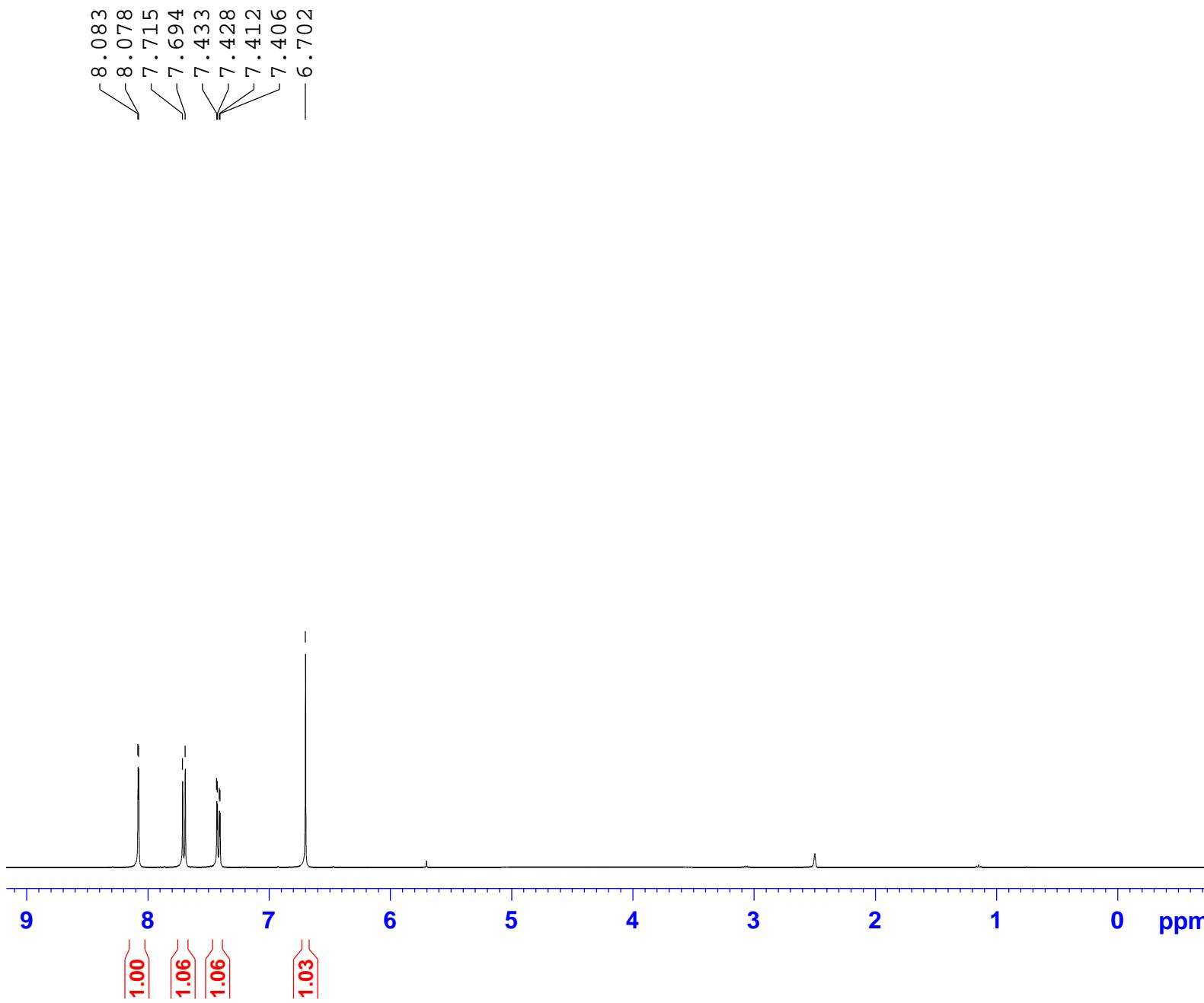
Current Data Parameters
NAME Oct27-2015
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20151027
Time 12.48
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.12
DW 62.400 usec
DE 6.50 usec
TE 295.0 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 ======
SFO1 400.1324710 MHz
NUC1 1H
P1 9.50 usec
PLW1 15.80000019 W

F2 - Processing parameters
SI 65536
SF 400.1300030 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

zsl-1-36-H



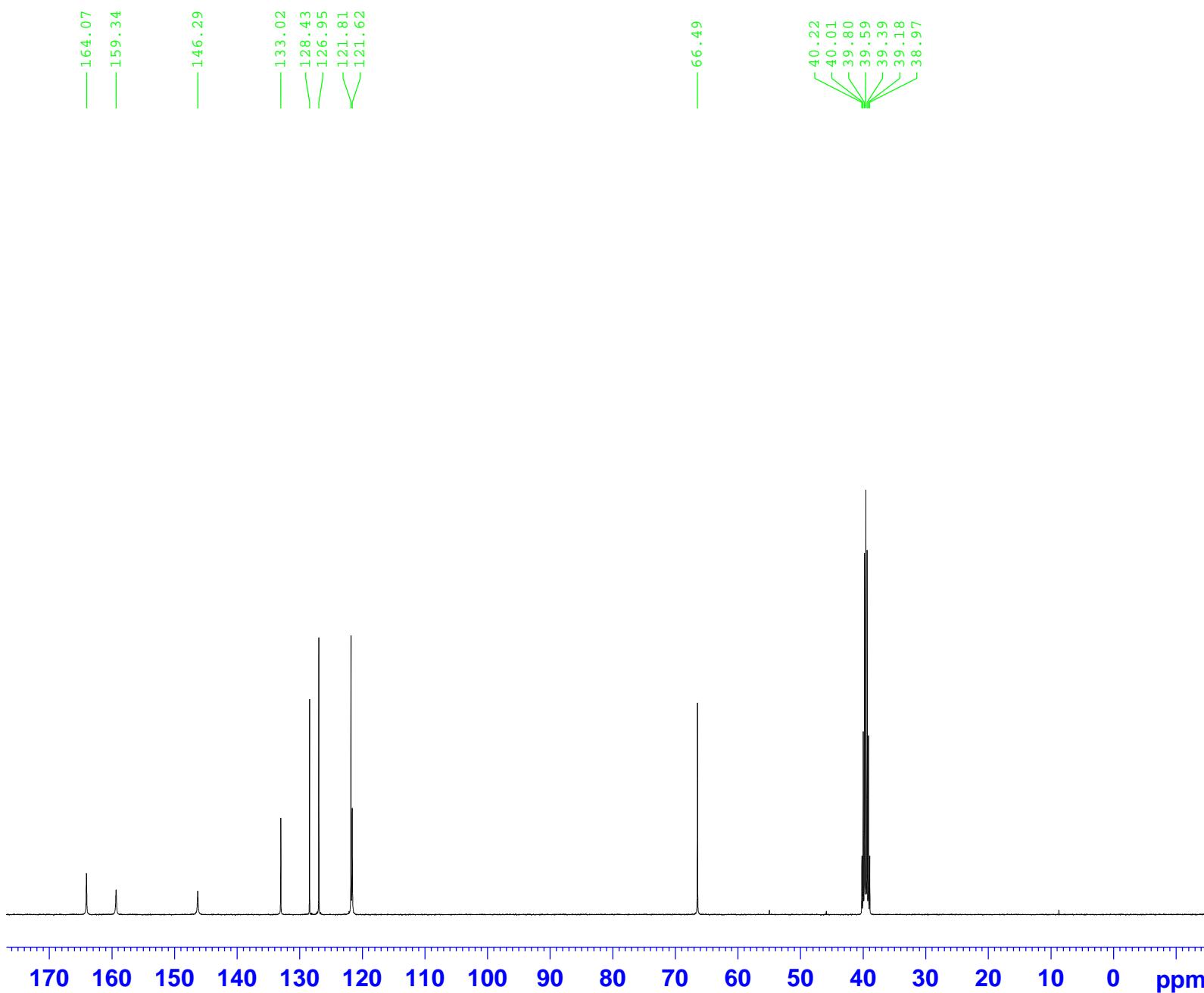
Current Data Parameters
NAME Oct27-2015
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20151027
Time 13.03
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.12
DW 62.400 usec
DE 6.50 usec
TE 295.0 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 9.50 usec
PLW1 15.80000019 W

F2 - Processing parameters
SI 65536
SF 400.1300031 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

zsl-1-36-C



Current Data Parameters
NAME Oct27-2015
EXPNO 6
PROCNO 1

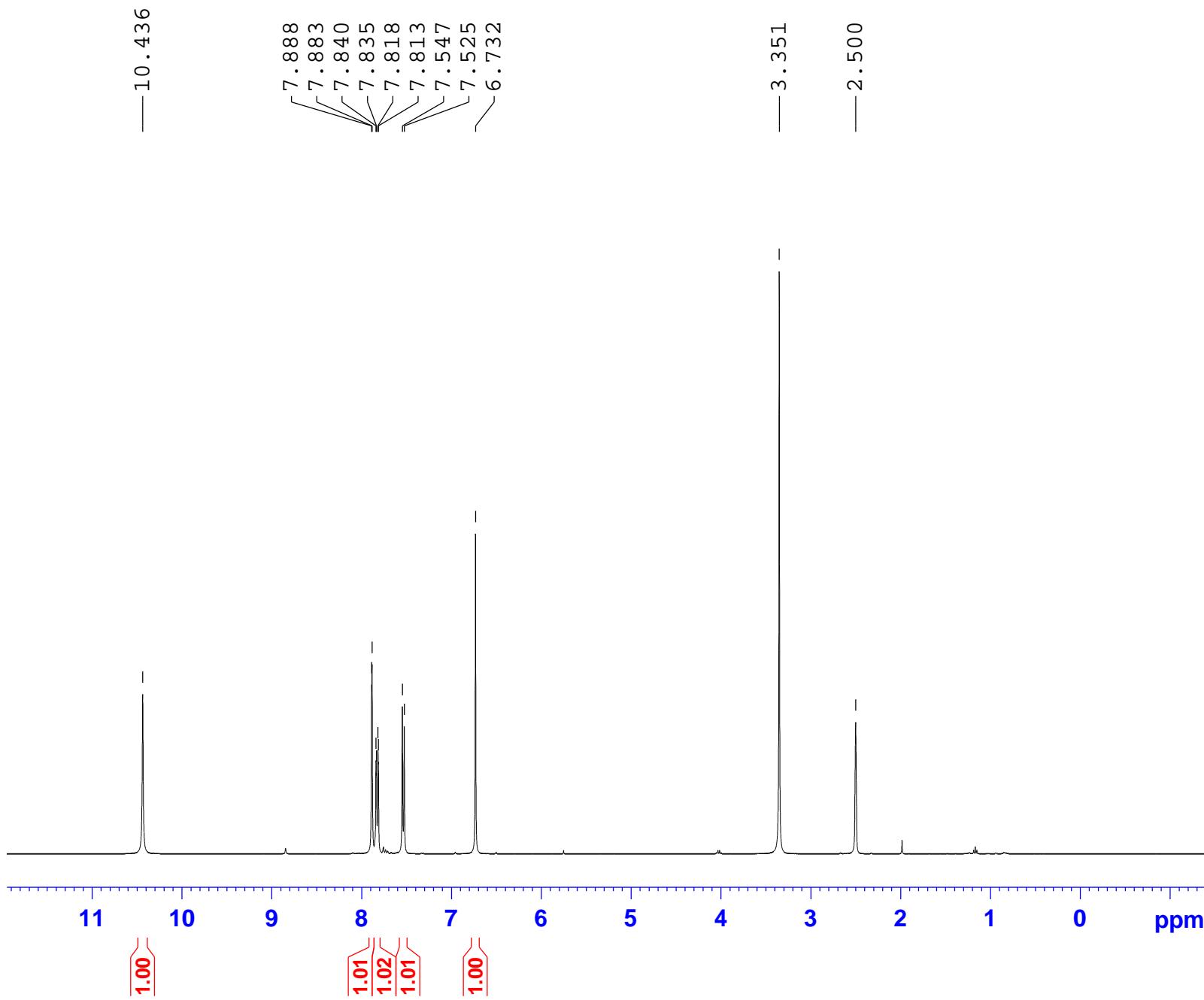
F2 - Acquisition Parameters
Date_ 20151027
Time 17.02
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 4096
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 199.94
DW 20.800 usec
DE 6.50 usec
TE 295.0 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 9.50 usec
PLW1 66.50000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 18.00000000 W
PLW12 0.20056000 W
PLW13 0.16245000 W

F2 - Processing parameters
SI 32768
SF 100.6128001 MHz
WDW EM
SSB 0
LB 0 1.00 Hz
GB 0
PC 1.40

ZSL-1-38-H



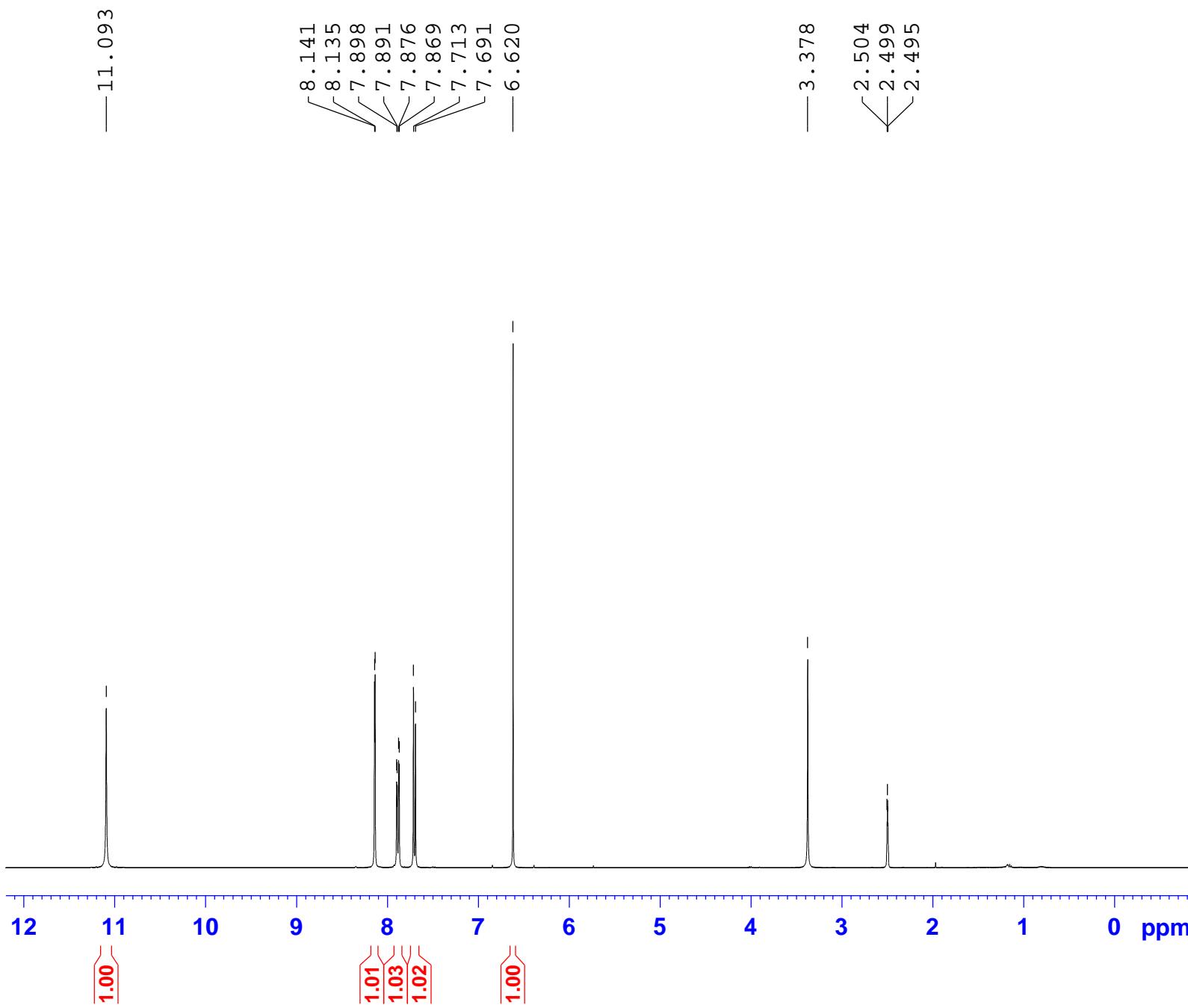
Current Data Parameters
NAME May29-2015
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150529
Time 11.16
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 98.76
DW 62.400 usec
DE 6.50 usec
TE 295.0 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 9.50 usec
PLW1 15.80000019 W

F2 - Processing parameters
SI 65536
SF 400.1300038 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ZSL-1-39-H



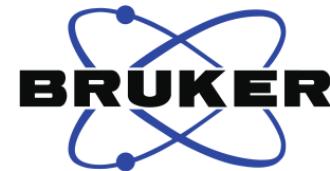
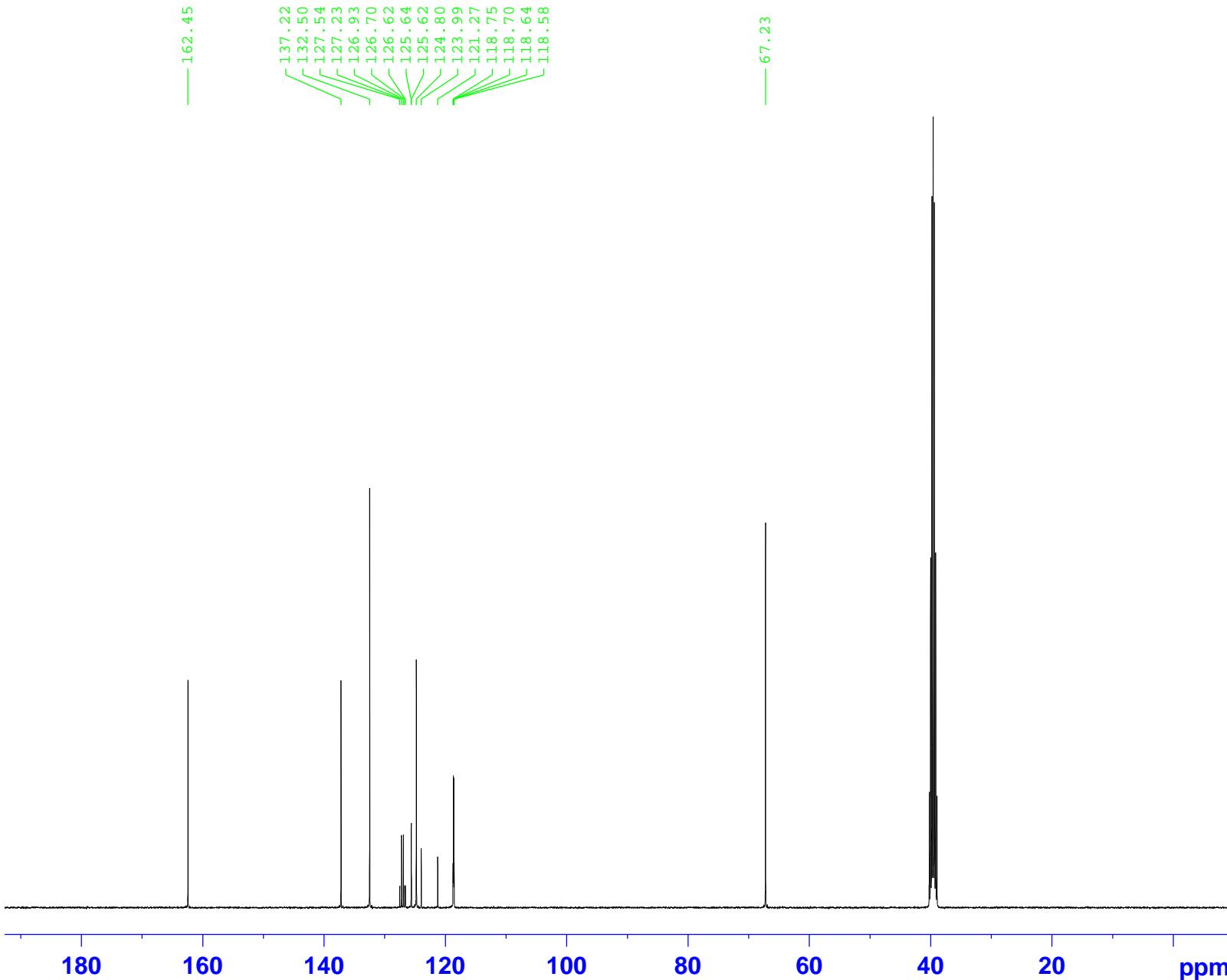
Current Data Parameters
NAME May29-2015
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150529
Time 11.12
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 71.13
DW 62.400 usec
DE 6.50 usec
TE 295.0 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 9.50 usec
PLW1 15.80000019 W

F2 - Processing parameters
SI 65536
SF 400.1300038 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ZSL-1-39-C



Current Data Parameters
NAME May31-2015
EXPNO 1
PROCNO 1

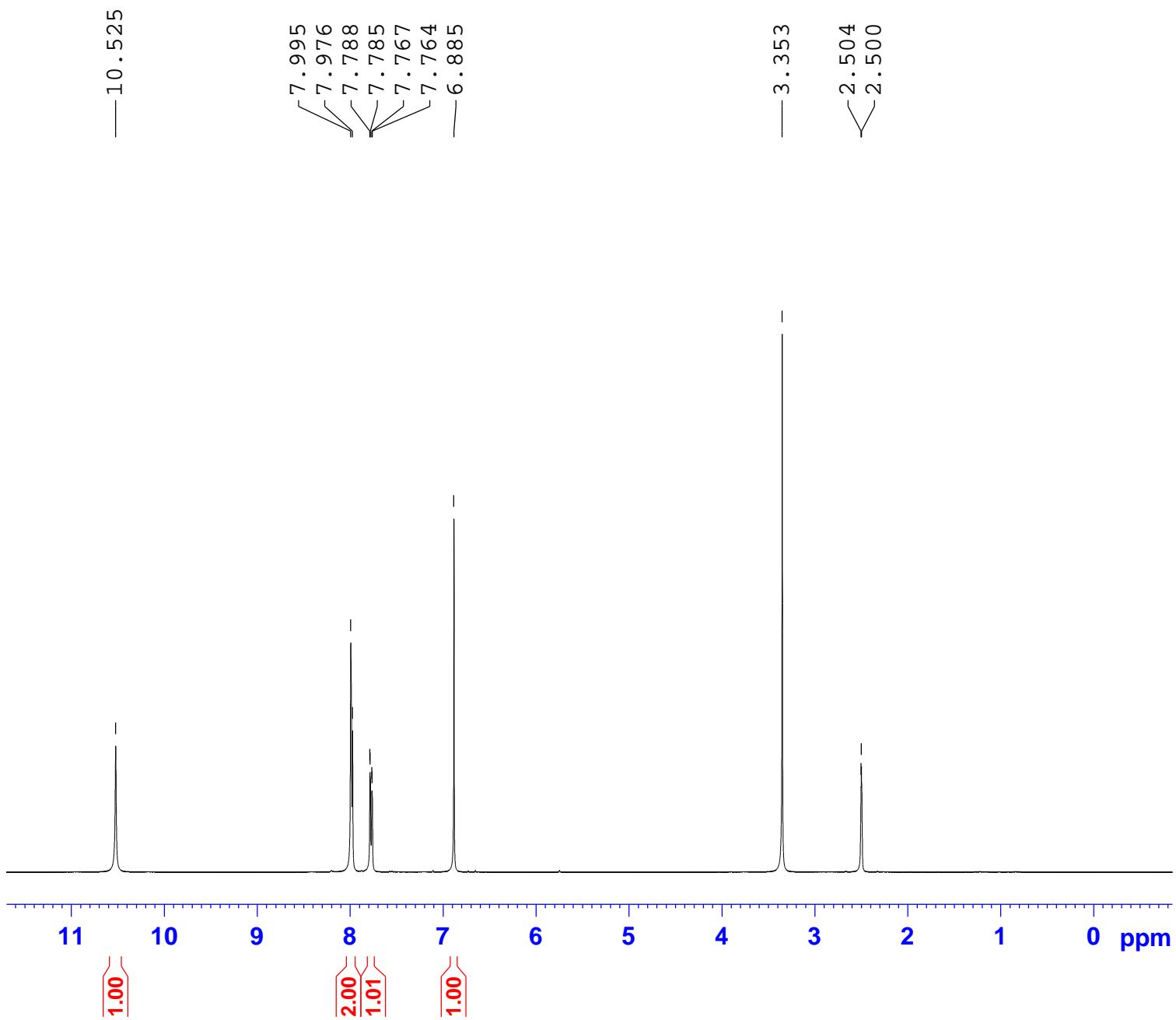
F2 - Acquisition Parameters
Date_ 20150531
Time 23.17
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 4096
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 199.94
DW 20.800 usec
DE 6.50 usec
TE 295.0 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 ¹³C
P1 9.50 usec
PLW1 66.50000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 ¹H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 18.00000000 W
PLW12 0.20056000 W
PLW13 0.16245000 W

F2 - Processing parameters
SI 32768
SF 100.6128043 MHz
WDW EM
SSB 0
LB 0 1.00 Hz
GB 0
PC 1.40

zsl-1-40-H



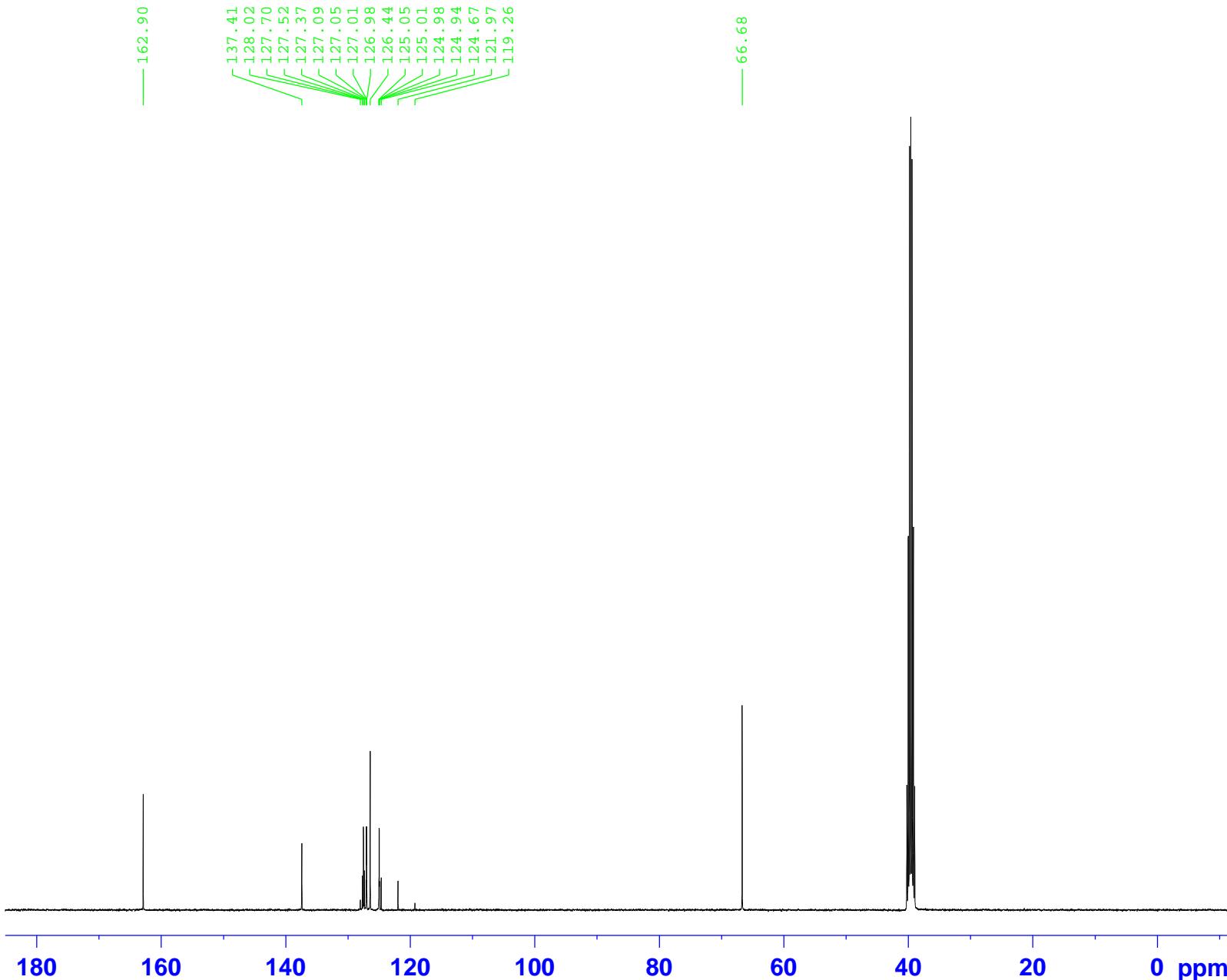
Current Data Parameters
NAME May29-2015
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150529
Time 10.32
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 64
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 98.76
DW 62.400 usec
DE 6.50 usec
TE 295.0 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 9.50 usec
PLW1 15.80000019 W

F2 - Processing parameters
SI 65536
SF 400.1300037 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ZSL-1-40-C



Current Data Parameters
NAME May30-2015
EXPNO 2
PROCNO 1

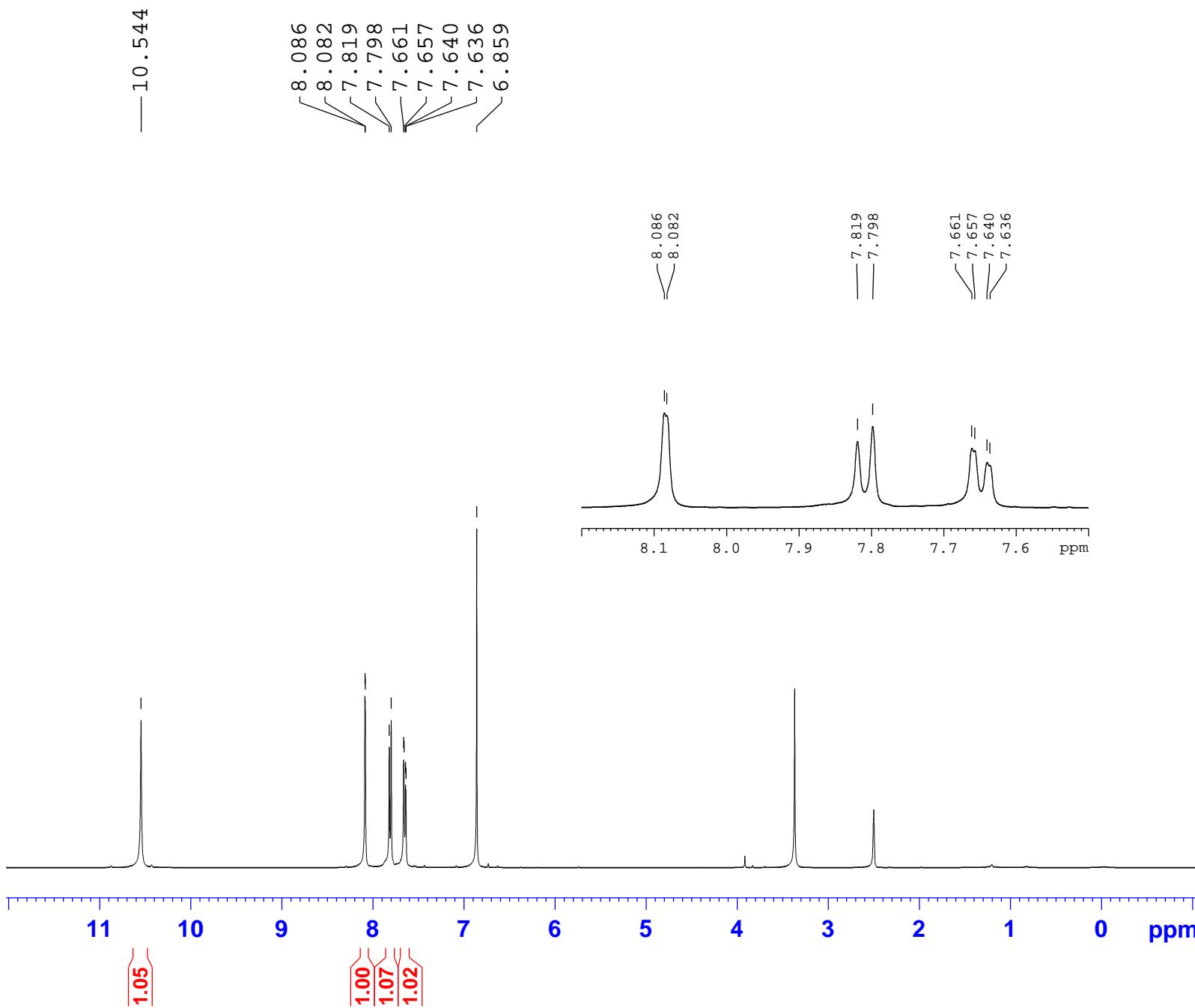
F2 - Acquisition Parameters
Date_ 20150530
Time 20.15
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 4096
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 199.94
DW 20.800 usec
DE 6.50 usec
TE 295.0 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 9.50 usec
PLW1 66.50000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPKG[2] waltz16
PCPD2 90.00 usec
PLW2 18.00000000 W
PLW12 0.20056000 W
PLW13 0.16245000 W

F2 - Processing parameters
SI 32768
SF 100.6128047 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

ZSL-1-41-H



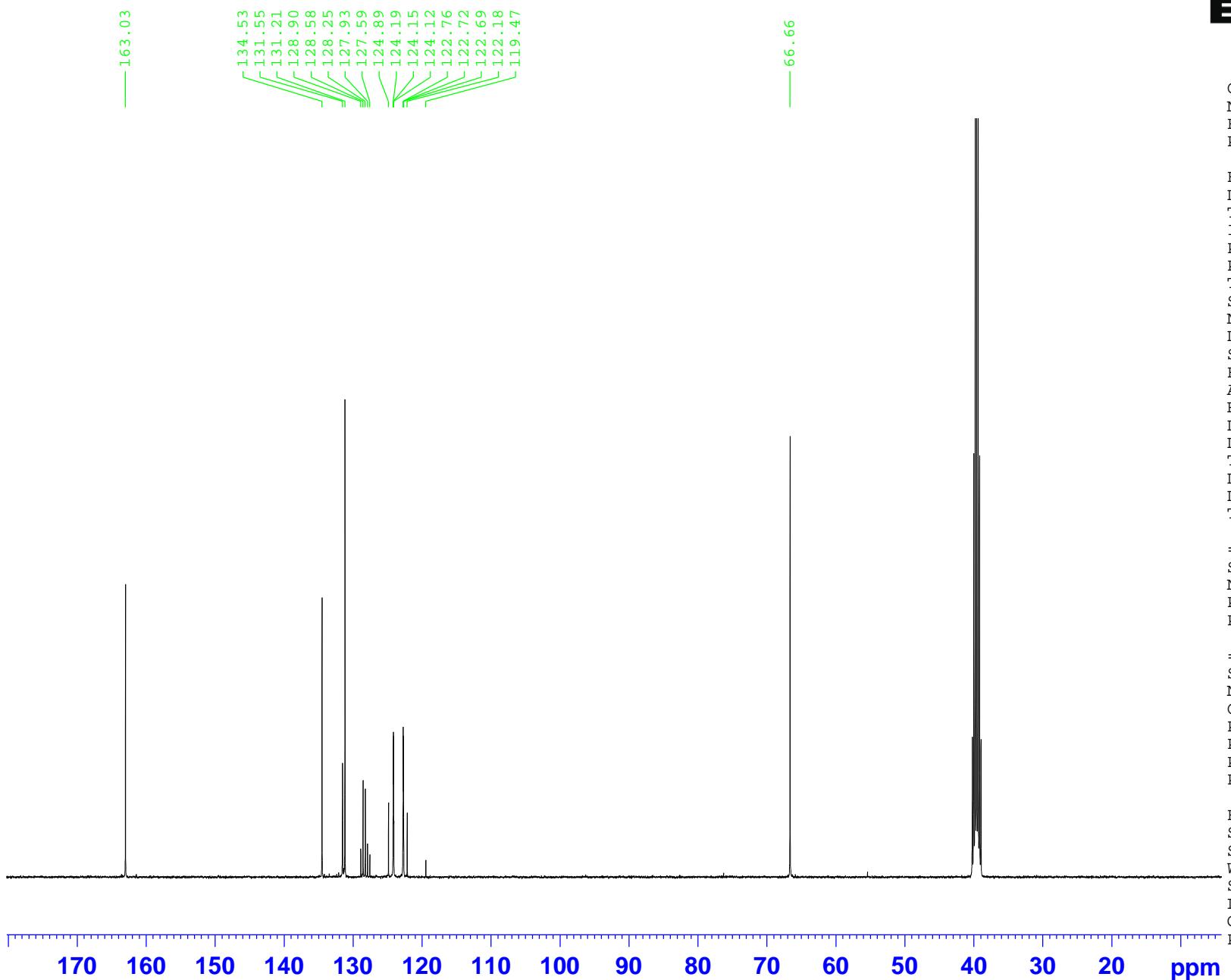
Current Data Parameters
NAME May28-2015
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150528
Time 22.00
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 71.13
DW 62.400 usec
DE 6.50 usec
TE 295.0 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 9.50 usec
PLW1 15.80000019 W

F2 - Processing parameters
SI 65536
SF 400.1300037 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ZSL-1-41-C



Current Data Parameters
NAME May30-2015
EXPNO 1
PROCNO 1

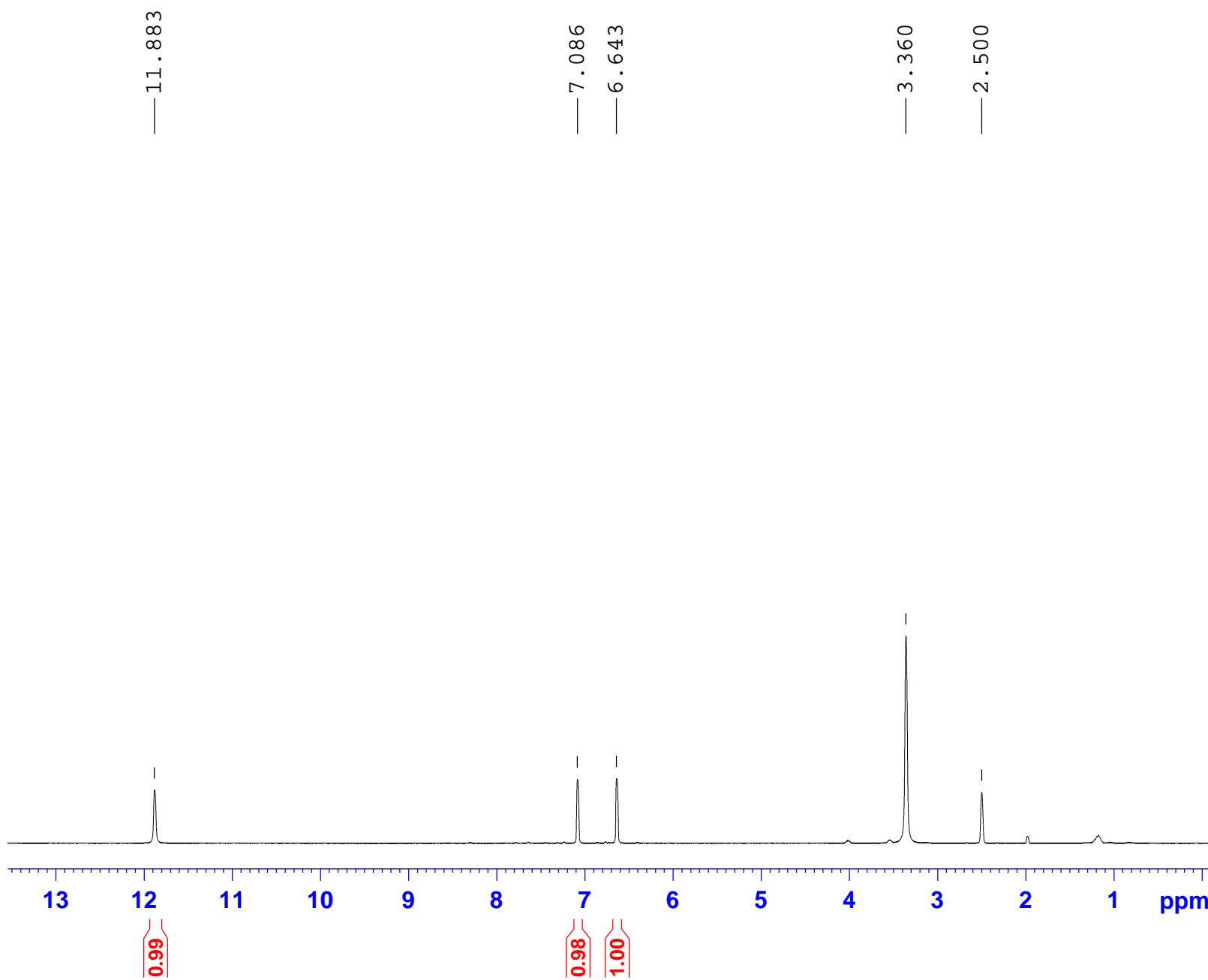
F2 - Acquisition Parameters
Date_ 20150530
Time 14.02
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zqpg30
TD 65536
SOLVENT DMSO
NS 4096
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 199.94
DW 20.800 usec
DE 6.50 usec
TE 295.0 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 ¹³C
P1 9.50 usec
PLW1 66.50000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 ¹H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 18.00000000 W
PLW12 0.20056000 W
PLW13 0.16245000 W

F2 - Processing parameters
SI 32768
SF 100.6128043 MHz
WDW EM
SSB 0 1.00 Hz
LB 0
GB
PC 1.40

ZSL-1-43-H



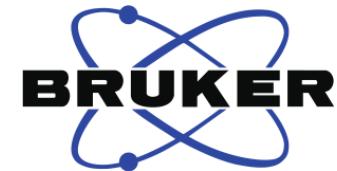
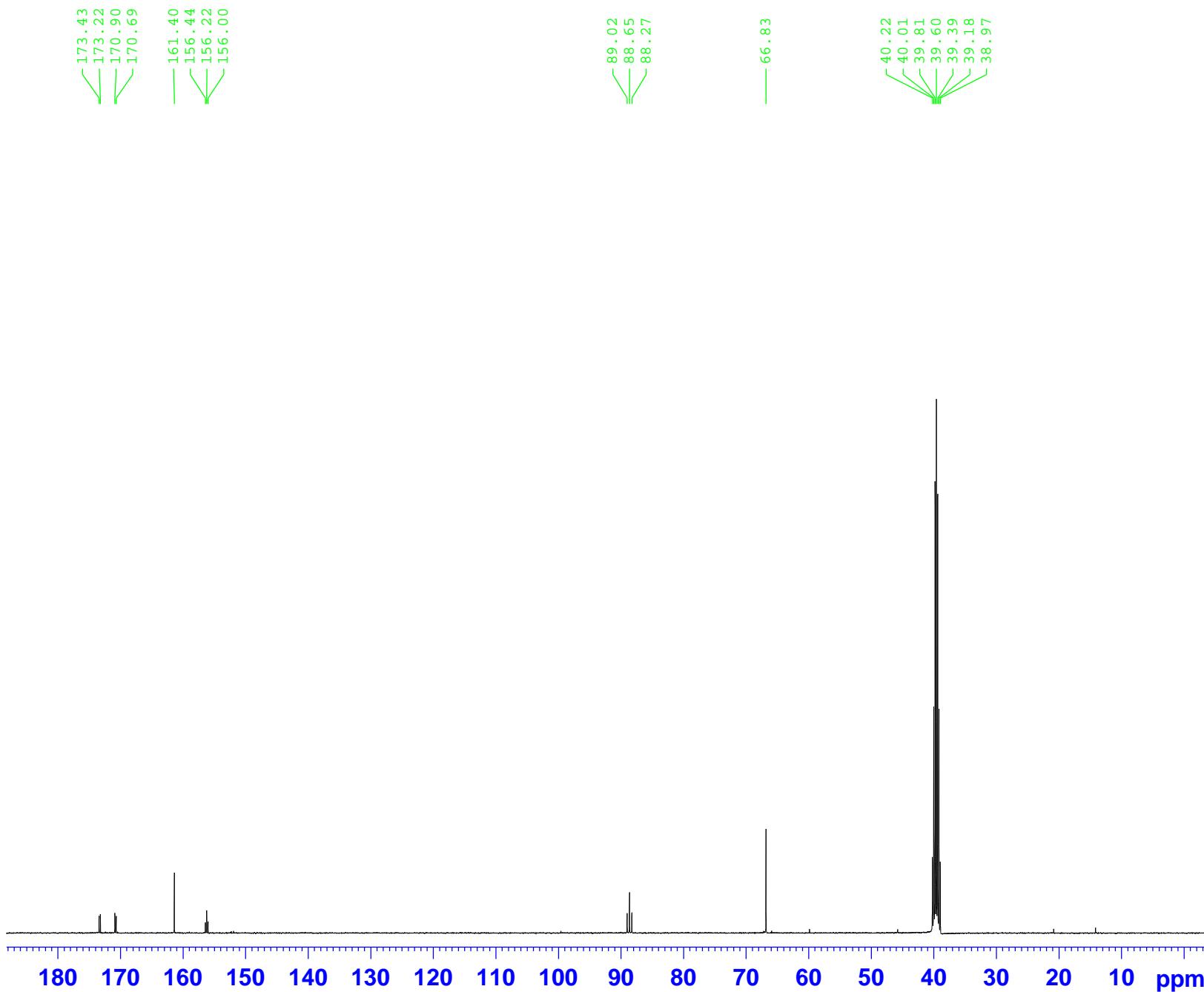
Current Data Parameters
NAME Mar31-2015
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150331
Time 11.48
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 88.59
DW 62.400 usec
DE 6.50 usec
TE 295.0 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 ======
SFO1 400.1324710 MHz
NUC1 1H
P1 9.50 usec
PLW1 15.80000019 W

F2 - Processing parameters
SI 65536
SF 400.1300045 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ZSL-1-43-C



Current Data Parameters
NAME Mar31-2015
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150331
Time 15.49
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 4096
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 199.94
DW 20.800 usec
DE 6.50 usec
TE 295.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 ¹³C
P1 9.50 usec
PLW1 66.50000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 ¹H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 18.00000000 W
PLW12 0.20056000 W
PLW13 0.16245000 W

F2 - Processing parameters
SI 32768
SF 100.6128032 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

ZSL-1-44-H

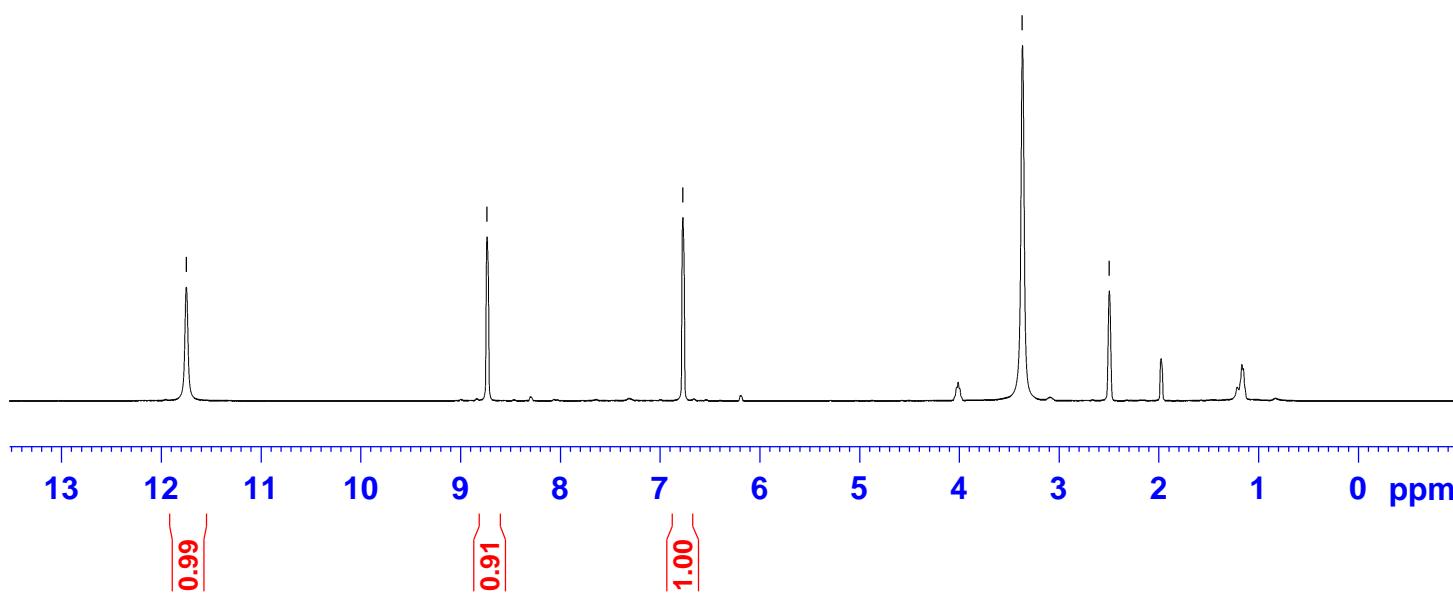
— 11.748

— 8.736

— 6.773

— 3.369

— 2.498



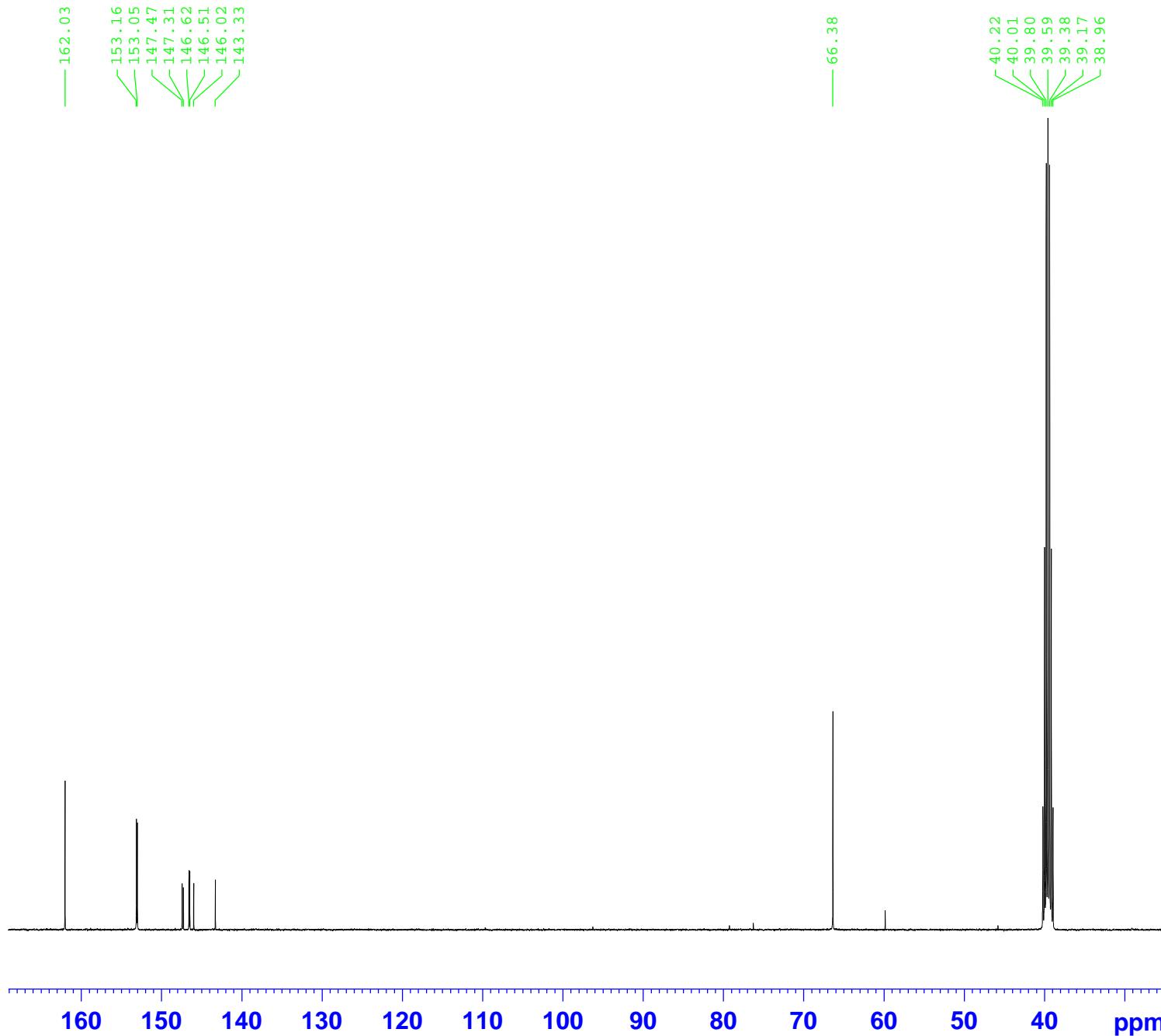
Current Data Parameters
NAME Mar30-2015
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150330
Time 20.27
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 88.59
DW 62.400 usec
DE 6.50 usec
TE 295.0 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 9.50 usec
PLW1 15.80000019 W

F2 - Processing parameters
SI 65536
SF 400.1300054 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ZSL-1-44-C



Current Data Parameters
NAME Mar30-2015
EXPNO 8
PROCNO 1

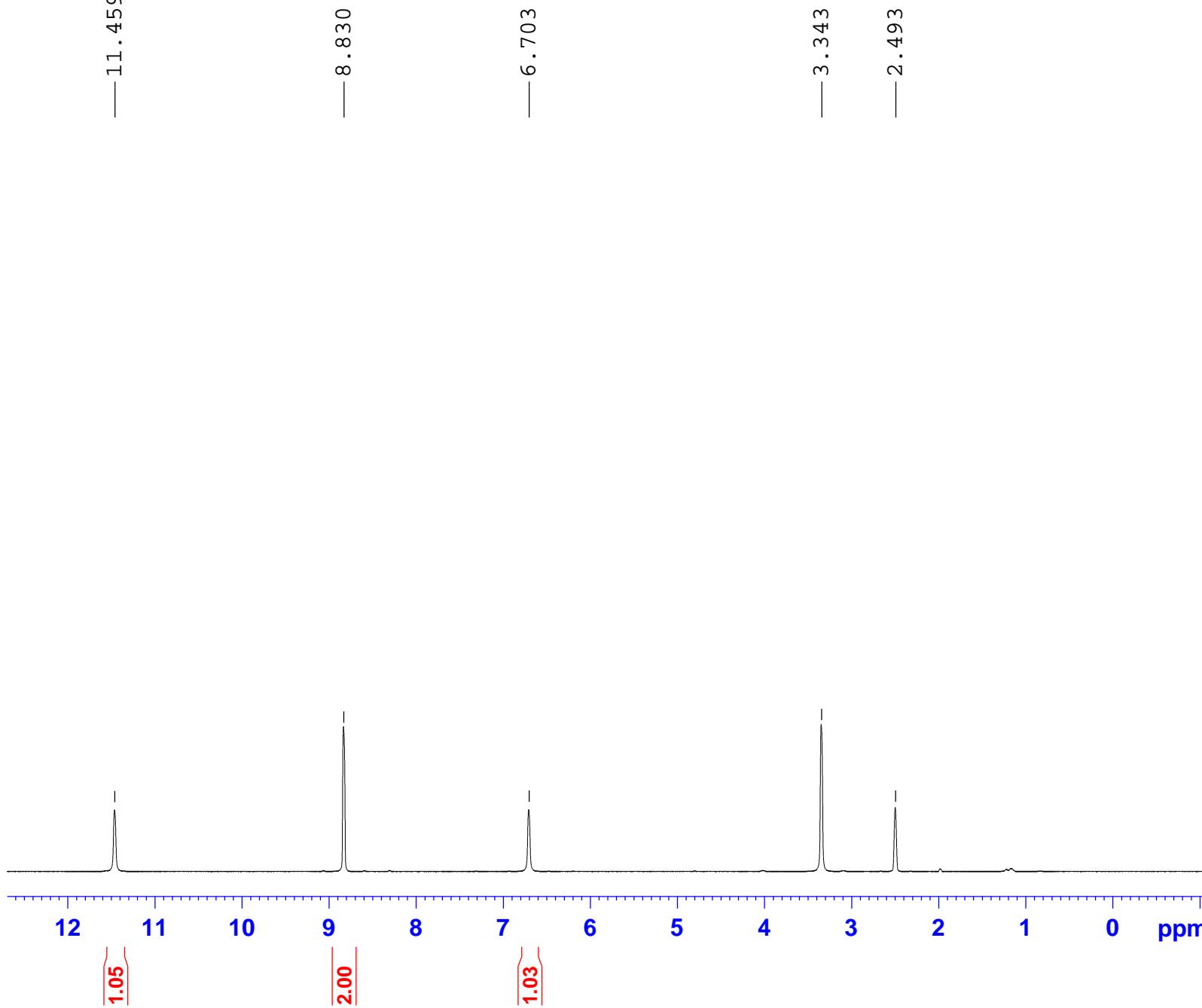
F2 - Acquisition Parameters
Date_ 20150331
Time 0.30
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zqpg30
TD 65536
SOLVENT DMSO
NS 4096
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 199.94
DW 20.800 usec
DE 6.50 usec
TE 295.0 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 ¹³C
P1 9.50 usec
PLW1 66.50000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 ¹H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 18.00000000 W
PLW12 0.20056000 W
PLW13 0.16245000 W

F2 - Processing parameters
SI 32768
SF 100.6128041 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

ZSL-1-45-H



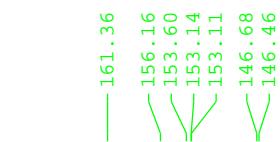
Current Data Parameters
NAME Mar30-2015
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date 20150330
Time 17.06
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 112.04
DW 62.400 usec
DE 6.50 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 ======
SFO1 400.1324710 MHz
NUC1 1H
P1 9.50 usec
PLW1 15.80000019 W

F2 - Processing parameters
SI 65536
SF 400.1300049 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ZSL-1-45-C



67.02

40.22
40.02
39.81
39.60
39.39
39.18
38.97



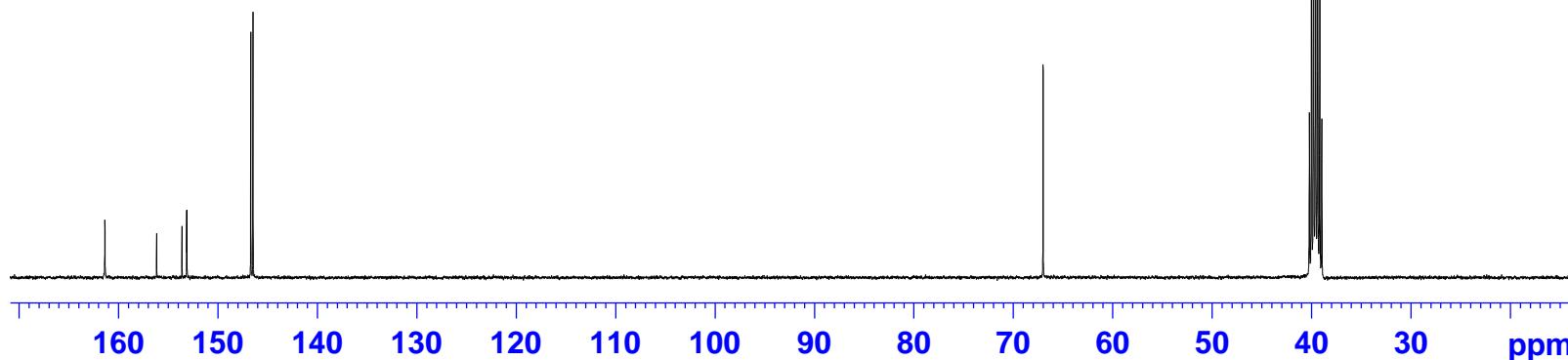
Current Data Parameters
NAME Mar30-2015
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150330
Time 19.12
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 199.94
DW 20.800 usec
DE 6.50 usec
TE 295.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

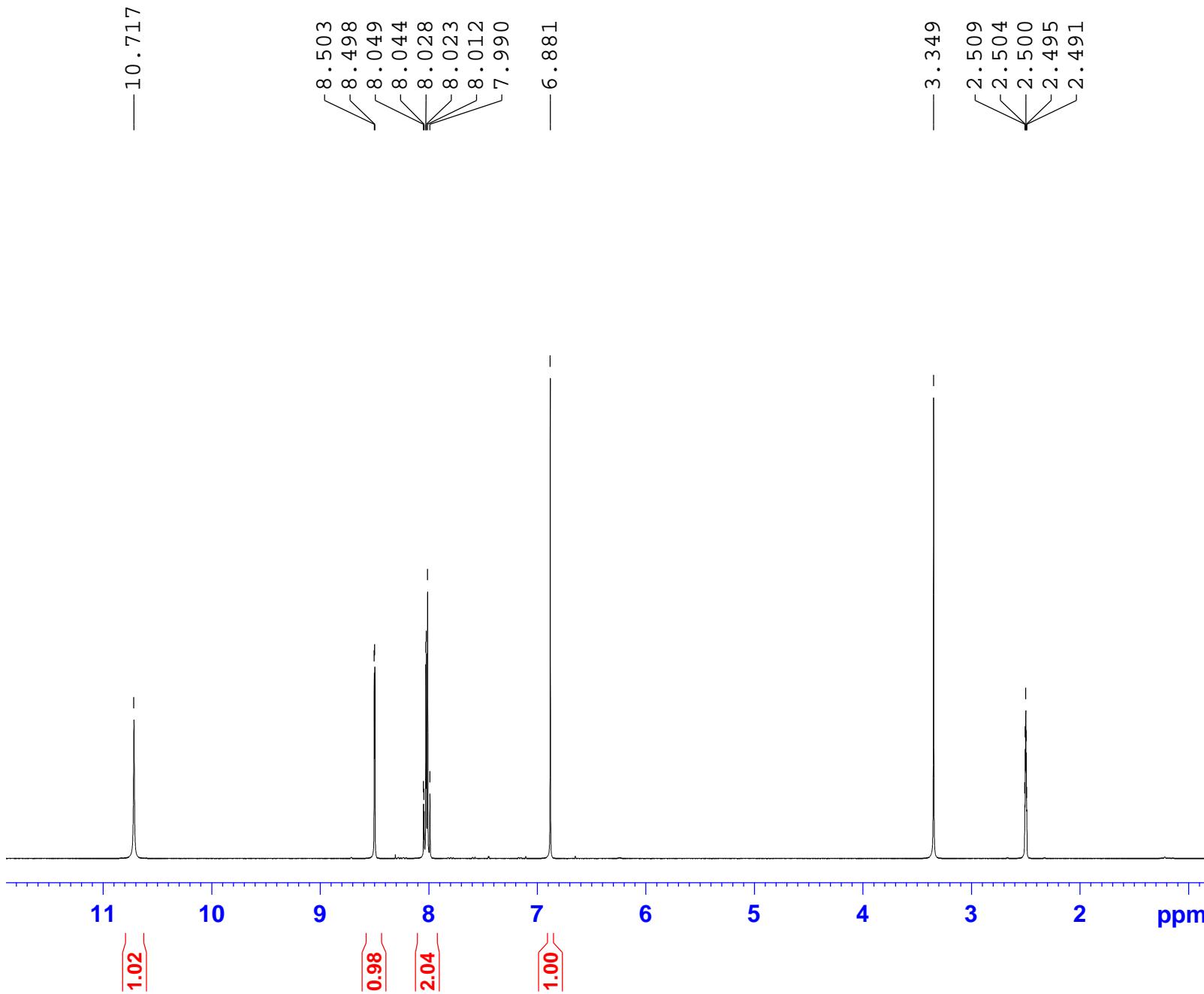
===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 9.50 usec
PLW1 66.50000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 18.00000000 W
PLW12 0.20056000 W
PLW13 0.16245000 W

F2 - Processing parameters
SI 32768
SF 100.6128047 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



ZSL-1-46-H



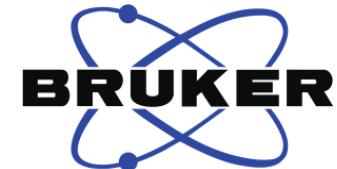
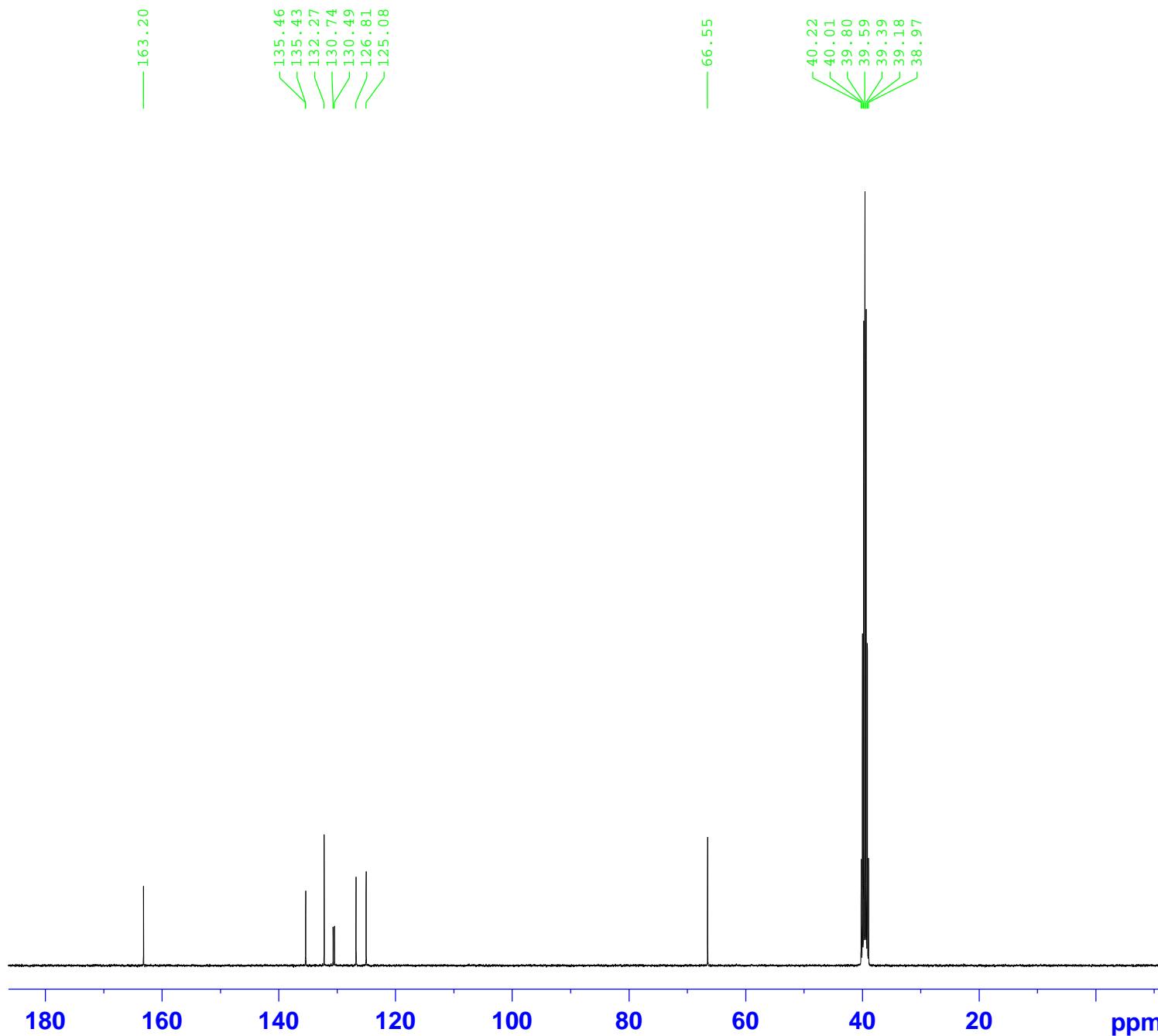
Current Data Parameters
NAME April1-2015
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150411
Time 12.29
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 128.54
DW 62.400 usec
DE 6.50 usec
TE 295.0 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 9.50 usec
PLW1 15.80000019 W

F2 - Processing parameters
SI 65536
SF 400.1300036 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ZSL-1-46-C



Current Data Parameters
NAME Apr02-2015
EXPNO 2
PROCNO 1

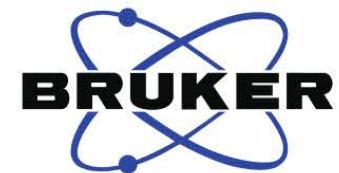
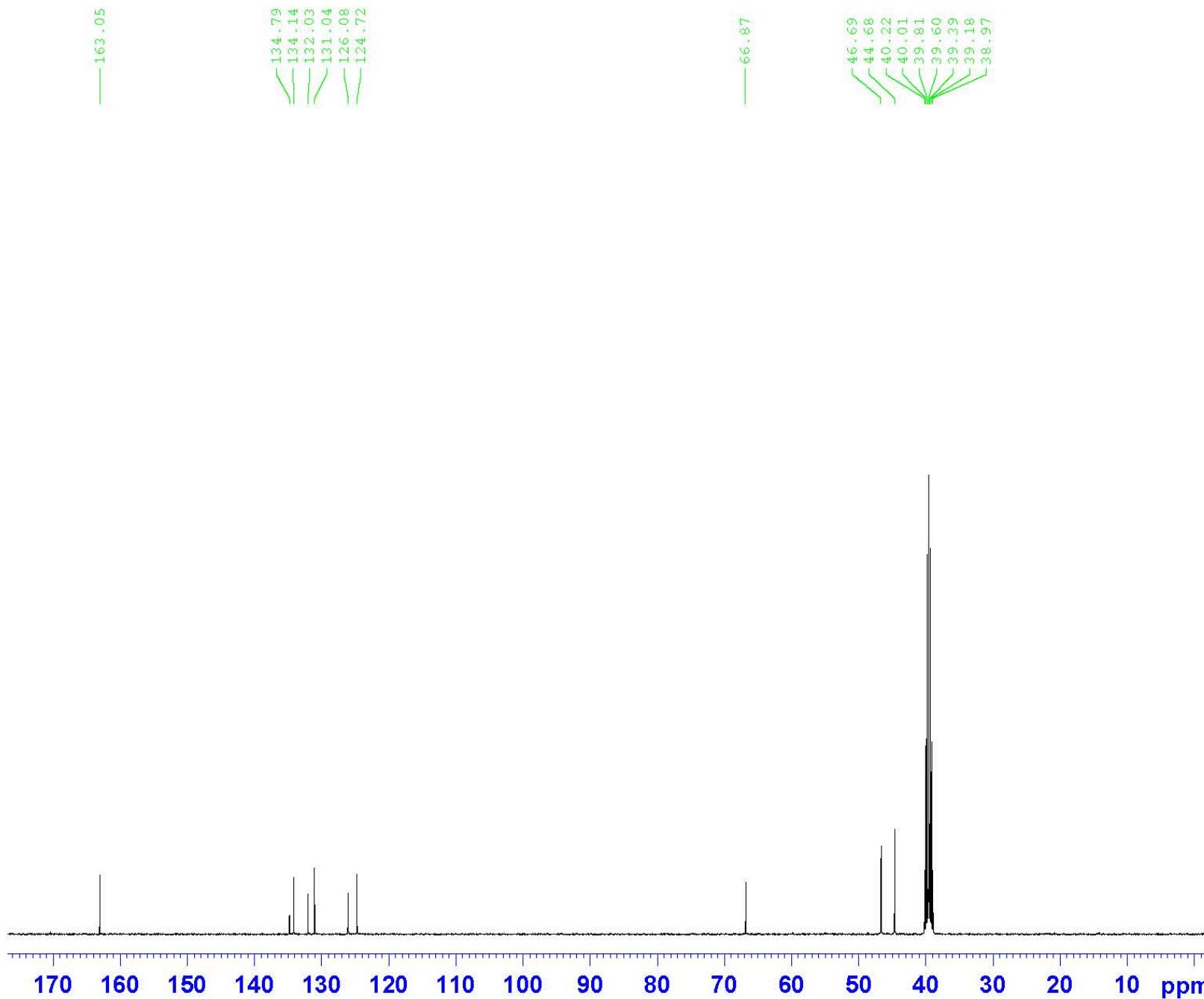
F2 - Acquisition Parameters
Date_ 20150402
Time 18.36
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 199.94
DW 20.800 usec
DE 6.50 usec
TE 295.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 9.50 usec
PLW1 66.50000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 18.00000000 W
PLW12 0.20056000 W
PLW13 0.16245000 W

F2 - Processing parameters
SI 32768
SF 100.6128061 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

ZSL-1-47-C



Current Data Parameters
NAME Apr05-2015
EXPNO 2
PROCNO 1

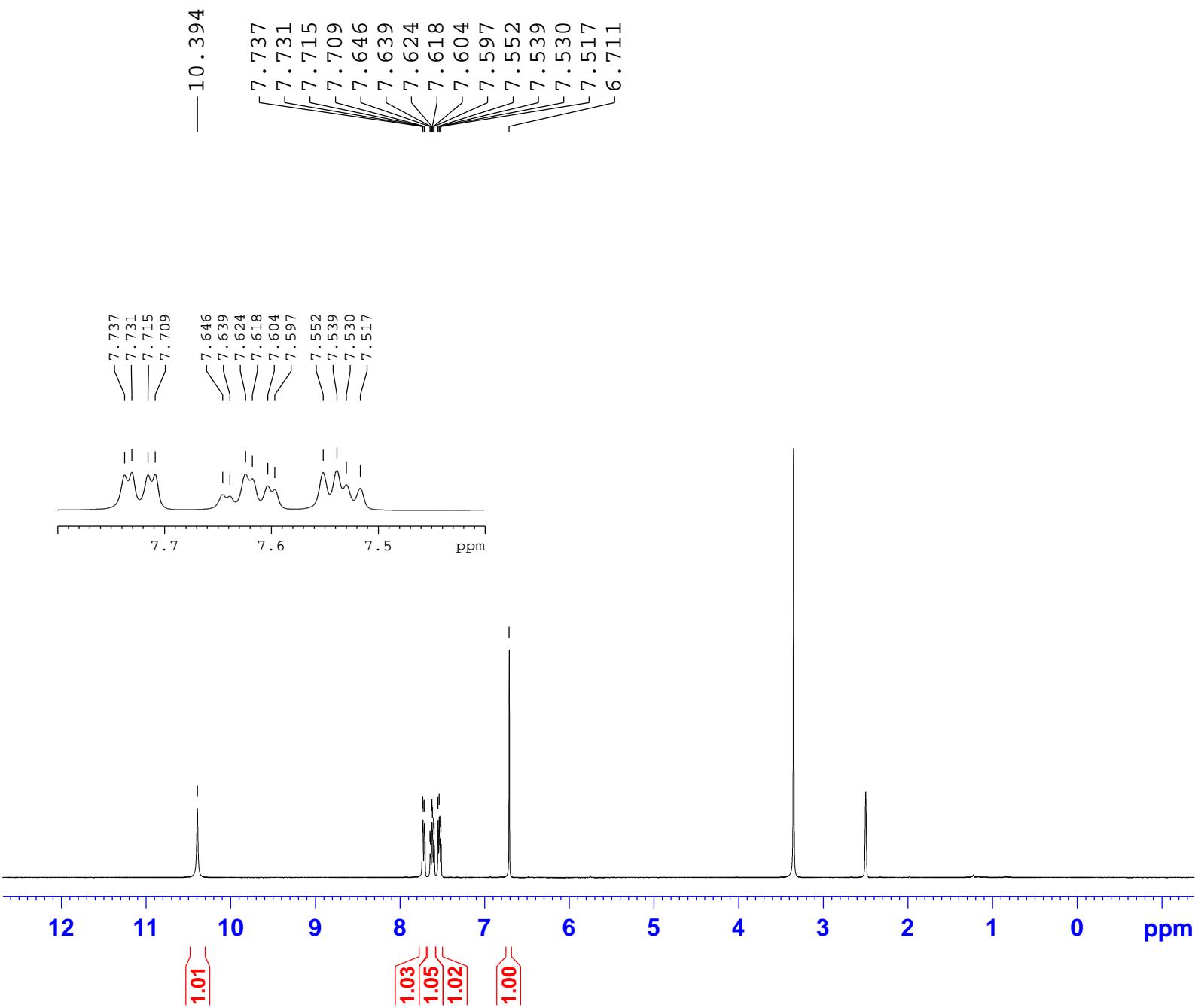
F2 - Acquisition Parameters
Date_ 20150405
Time 21.53
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgppg30
TD 65536
SOLVENT DMSO
NS 4096
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 199.94
DW 20.800 usec
DE 6.50 usec
TE 295.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 9.50 usec
PLW1 66.50000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG [2 waltz16
PCPD2 90.00 usec
PLW2 18.00000000 W
PLW12 0.20056000 W
PLW13 0.16245000 W

F2 - Processing parameters
SI 32768
SF 100.6128053 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

zsl-1-50-H



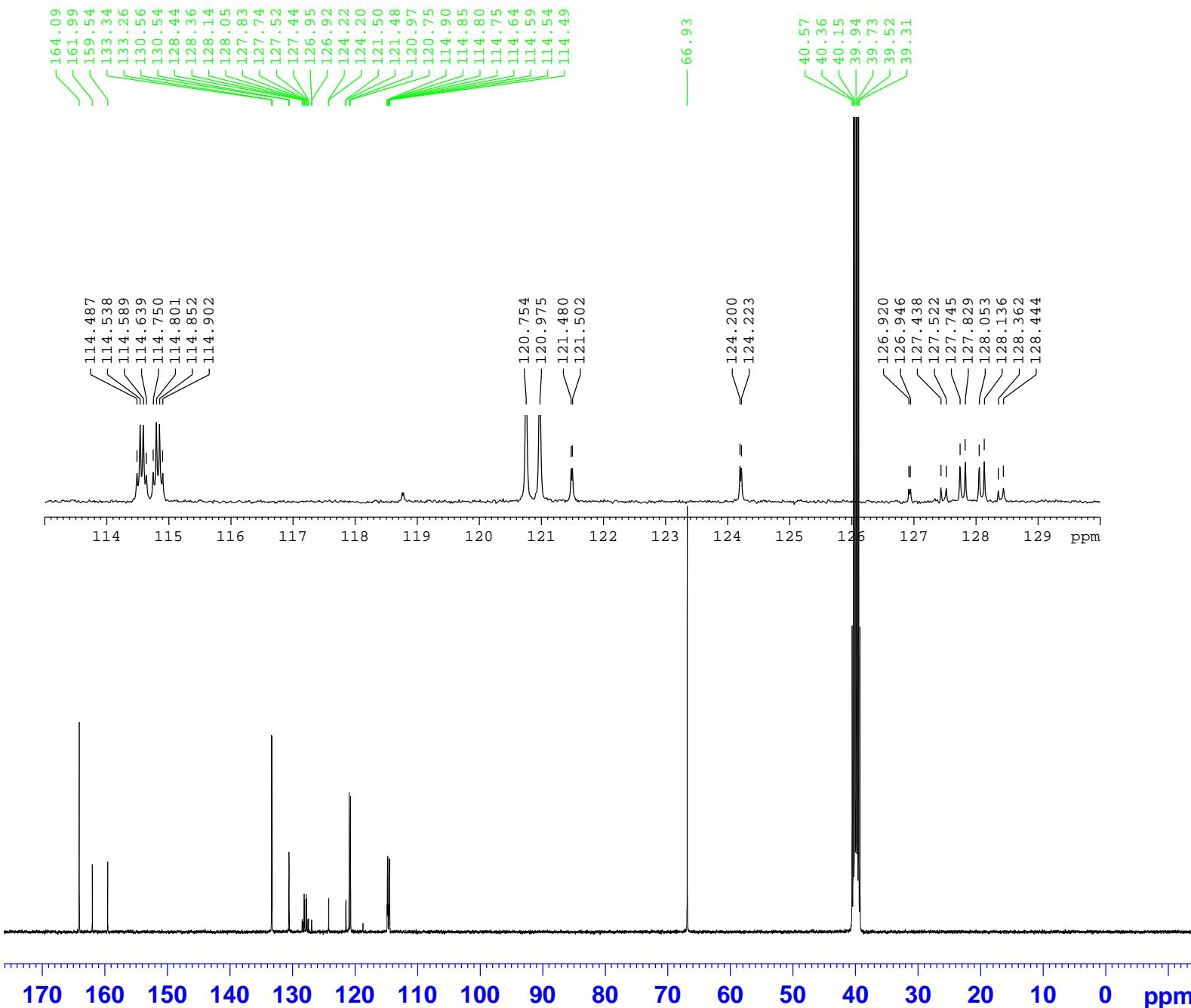
Current Data Parameters
NAME Jul25-2015
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150725
Time 21.18
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 98.76
DW 62.400 usec
DE 6.50 usec
TE 295.0 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 ======
SFO1 400.1324710 MHz
NUC1 1H
P1 9.50 usec
PLW1 15.80000019 W

F2 - Processing parameters
SI 65536
SF 400.1300038 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

zsl-1-50-C



Current Data Parameters
NAME Jul25-2015
EXPNO 3
PROCNO 1

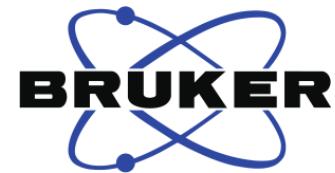
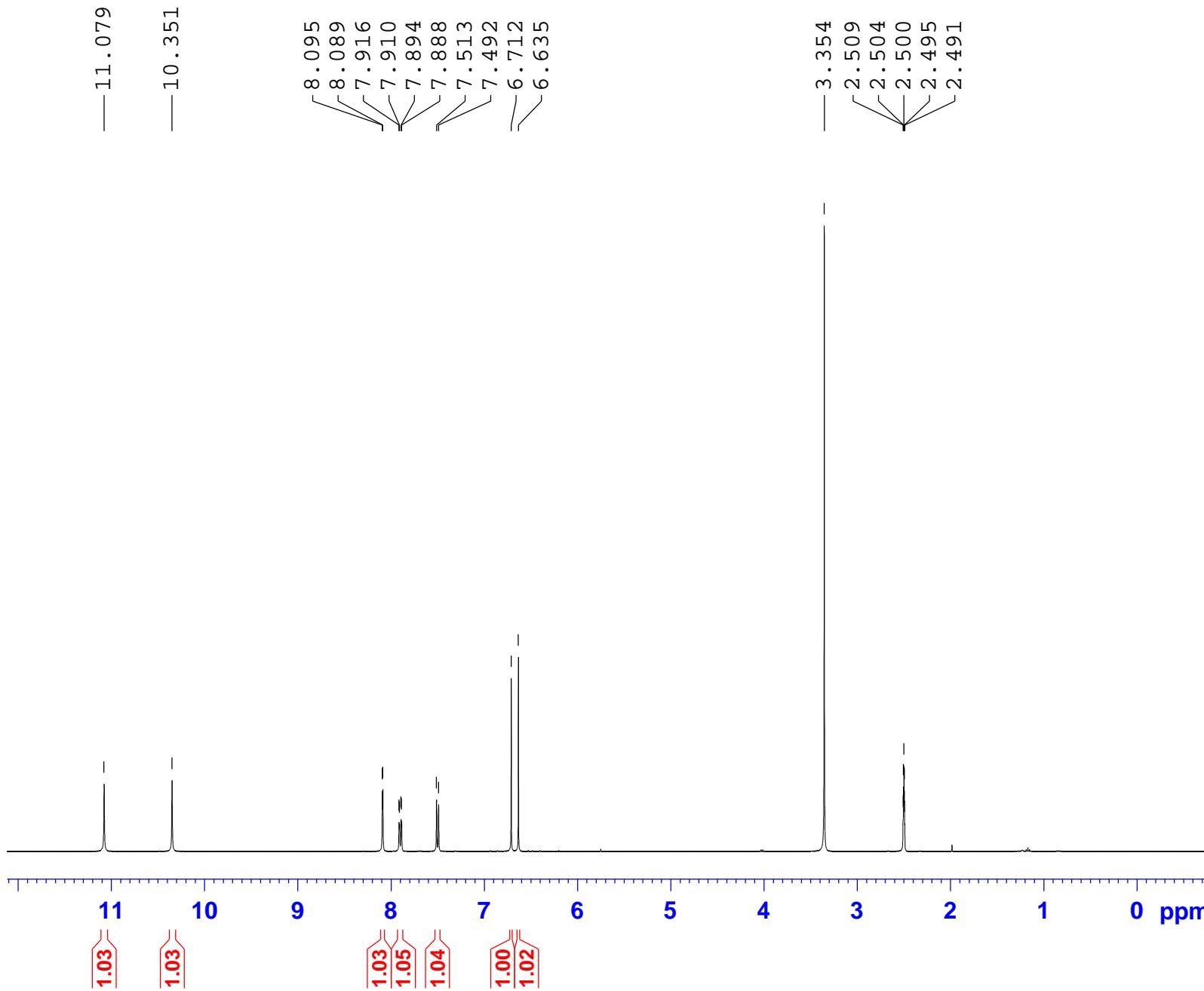
F2 - Acquisition Parameters
Date_ 20150726
Time 22.49
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 8192
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 199.94
DW 20.800 usec
DE 6.50 usec
TE 295.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 ¹³C
P1 9.50 usec
PLW1 66.50000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 ¹H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 18.00000000 W
PLW12 0.20056000 W
PLW13 0.16245000 W

F2 - Processing parameters
SI 32768
SF 100.6127700 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

zsl-1-52-H



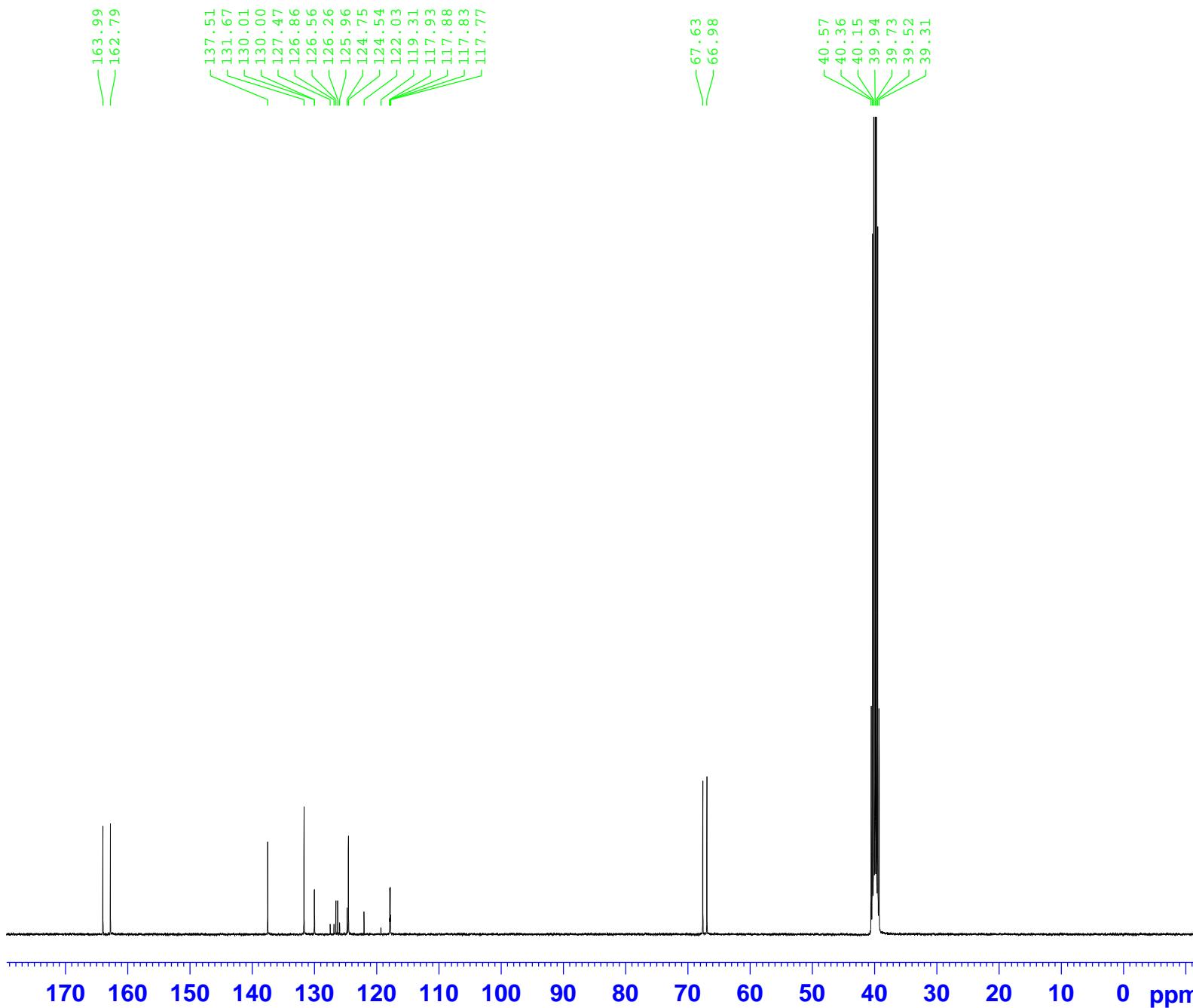
Current Data Parameters
NAME Jul27-2015
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150727
Time 15.51
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 98.76
DW 62.400 usec
DE 6.50 usec
TE 295.0 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 ======
SFO1 400.1324710 MHz
NUC1 1H
P1 9.50 usec
PLW1 15.80000019 W

F2 - Processing parameters
SI 65536
SF 400.1300036 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

zsl-1-52-C



Current Data Parameters
NAME Jul27-2015
EXPNO 3
PROCNO 1

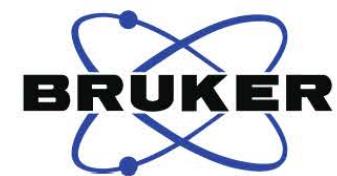
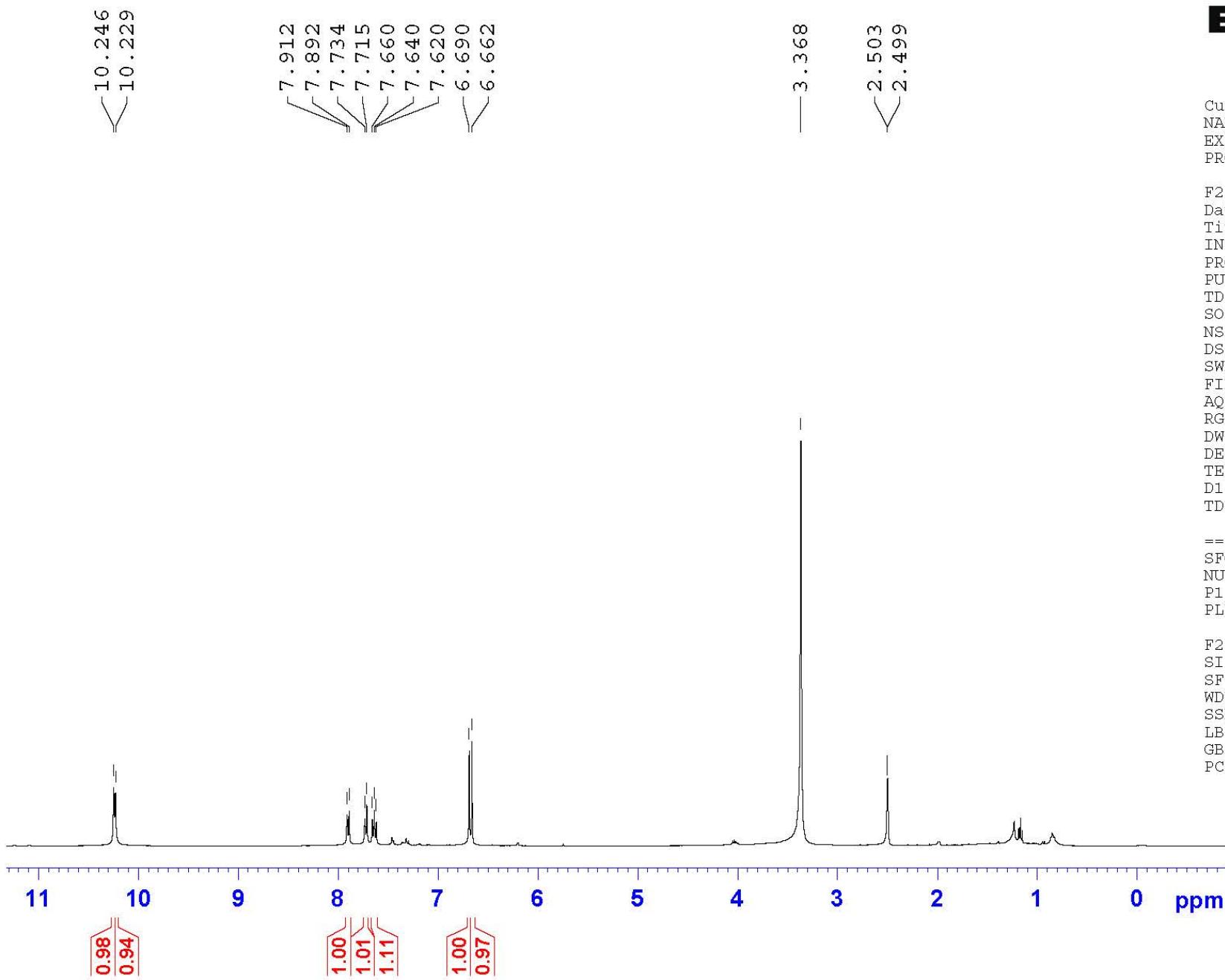
F2 - Acquisition Parameters
Date_ 20150727
Time 23.47
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 8192
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 199.94
DW 20.800 usec
DE 6.50 usec
TE 295.0 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 9.50 usec
PLW1 66.50000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 18.00000000 W
PLW12 0.20056000 W
PLW13 0.16245000 W

F2 - Processing parameters
SI 32768
SF 100.6127704 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

ZSL-1-53-H



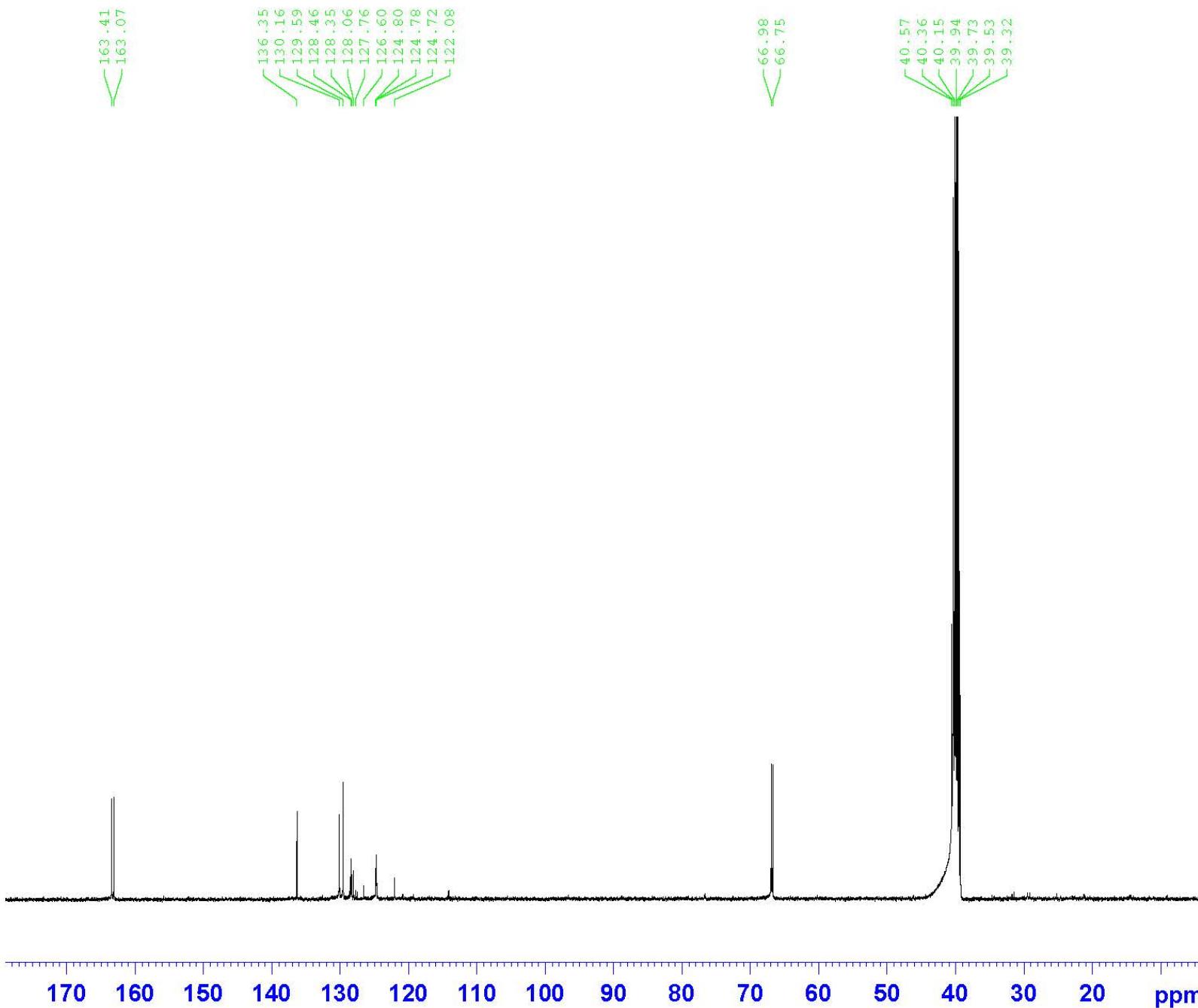
Current Data Parameters
NAME Jul28-2015
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150728
Time 16.54
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 78.4
DW 62.400 usec
DE 6.50 usec
TE 295.0 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 9.50 usec
PLW1 15.80000019 W

F2 - Processing parameters
SI 65536
SF 400.1300035 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

zsl-1-53-C



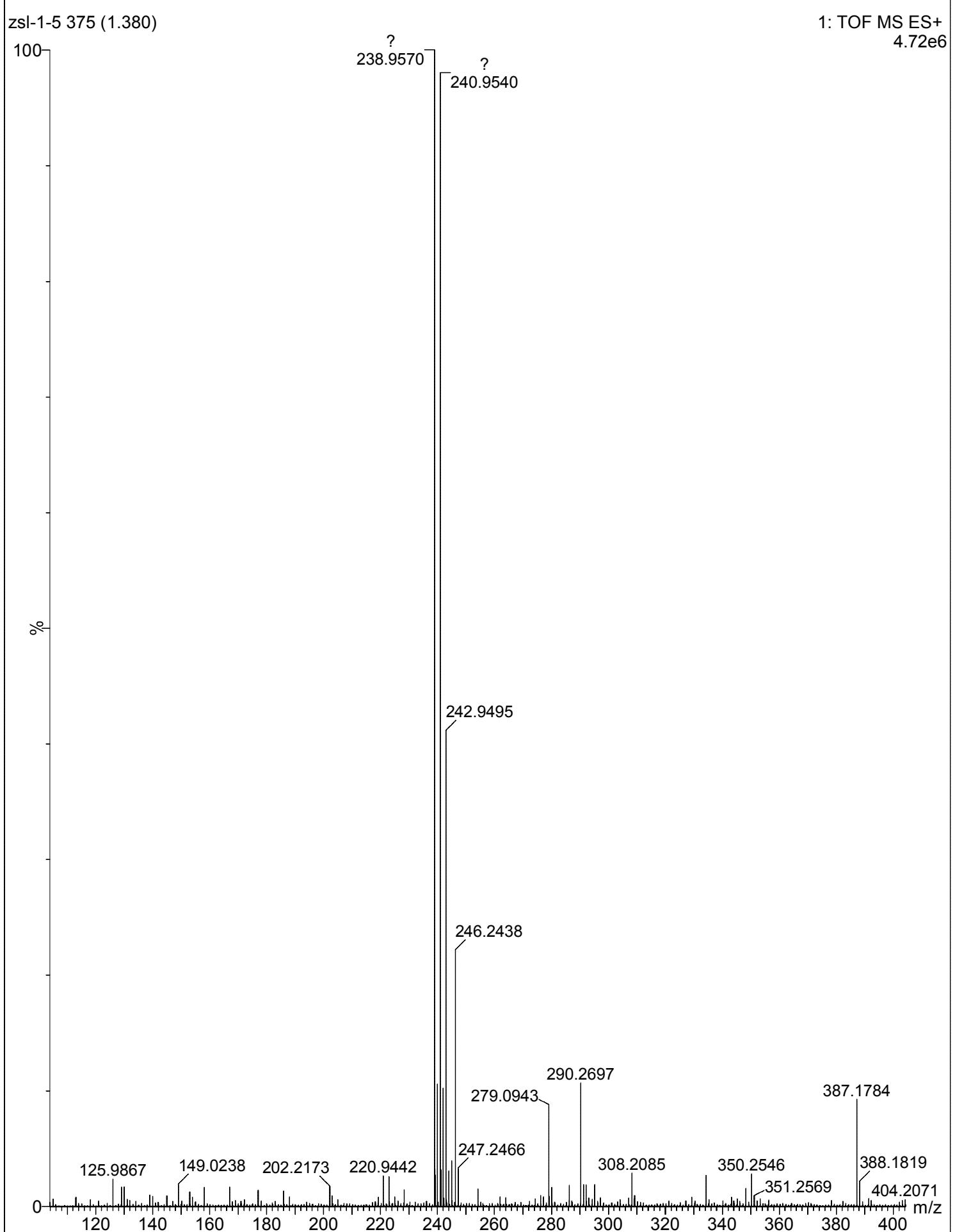
Current Data Parameters
NAME Jul28-2015
EXPNO 4
PROCNO 1

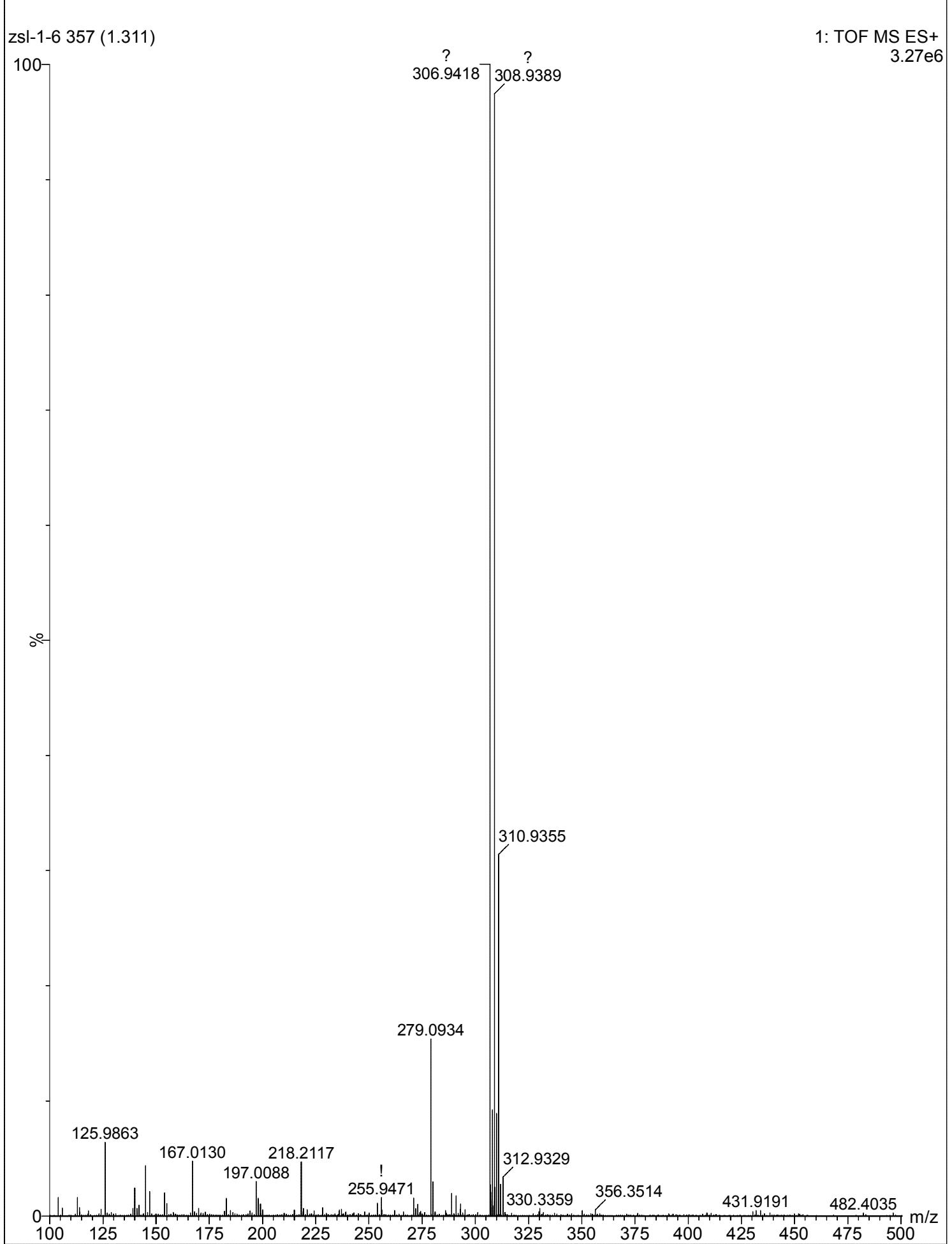
F2 - Acquisition Parameters
Date_ 20150729
Time 4.19
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 8192
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 199.94
DW 20.800 usec
DE 6.50 usec
TE 295.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

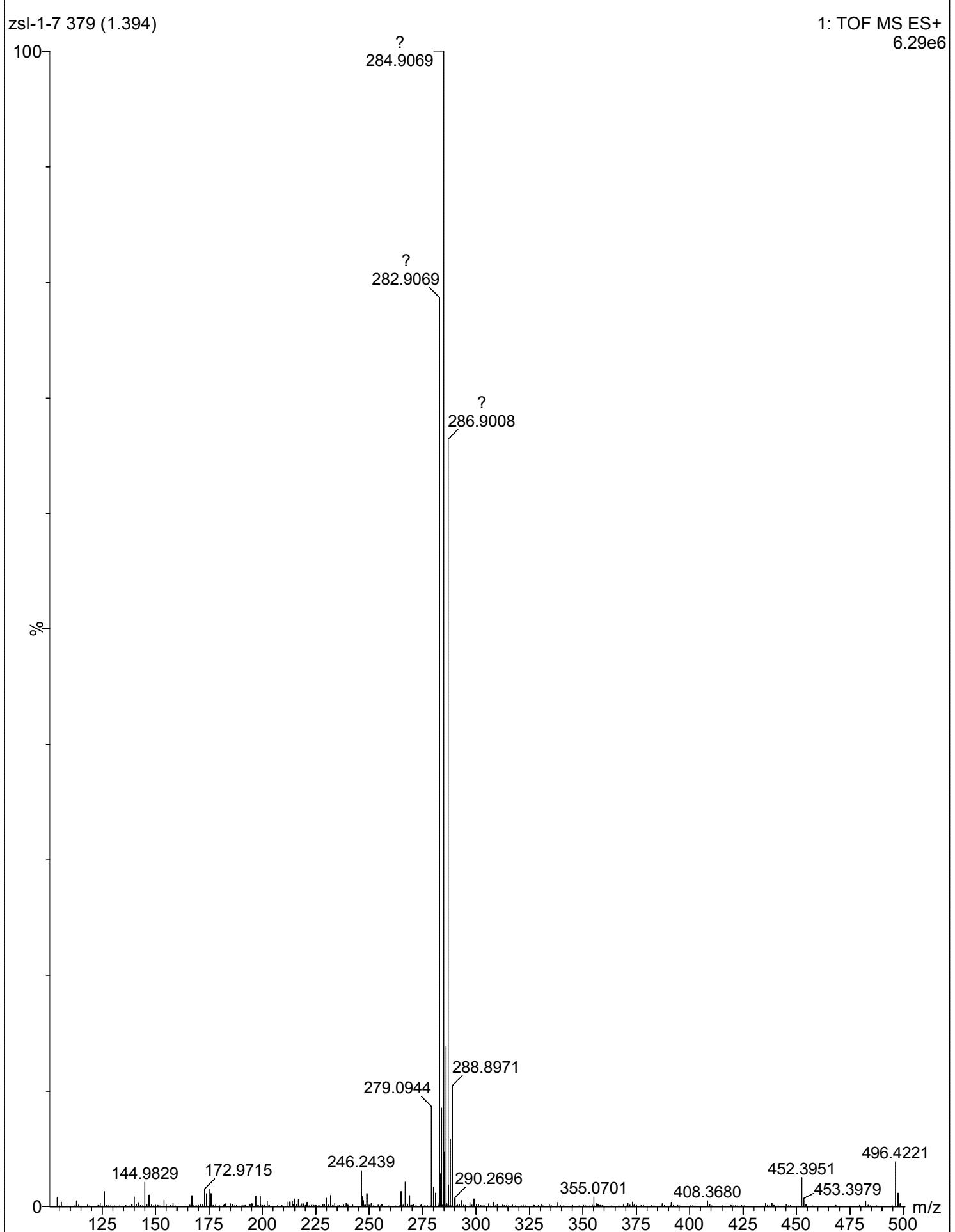
===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 9.50 usec
PLW1 66.50000000 W

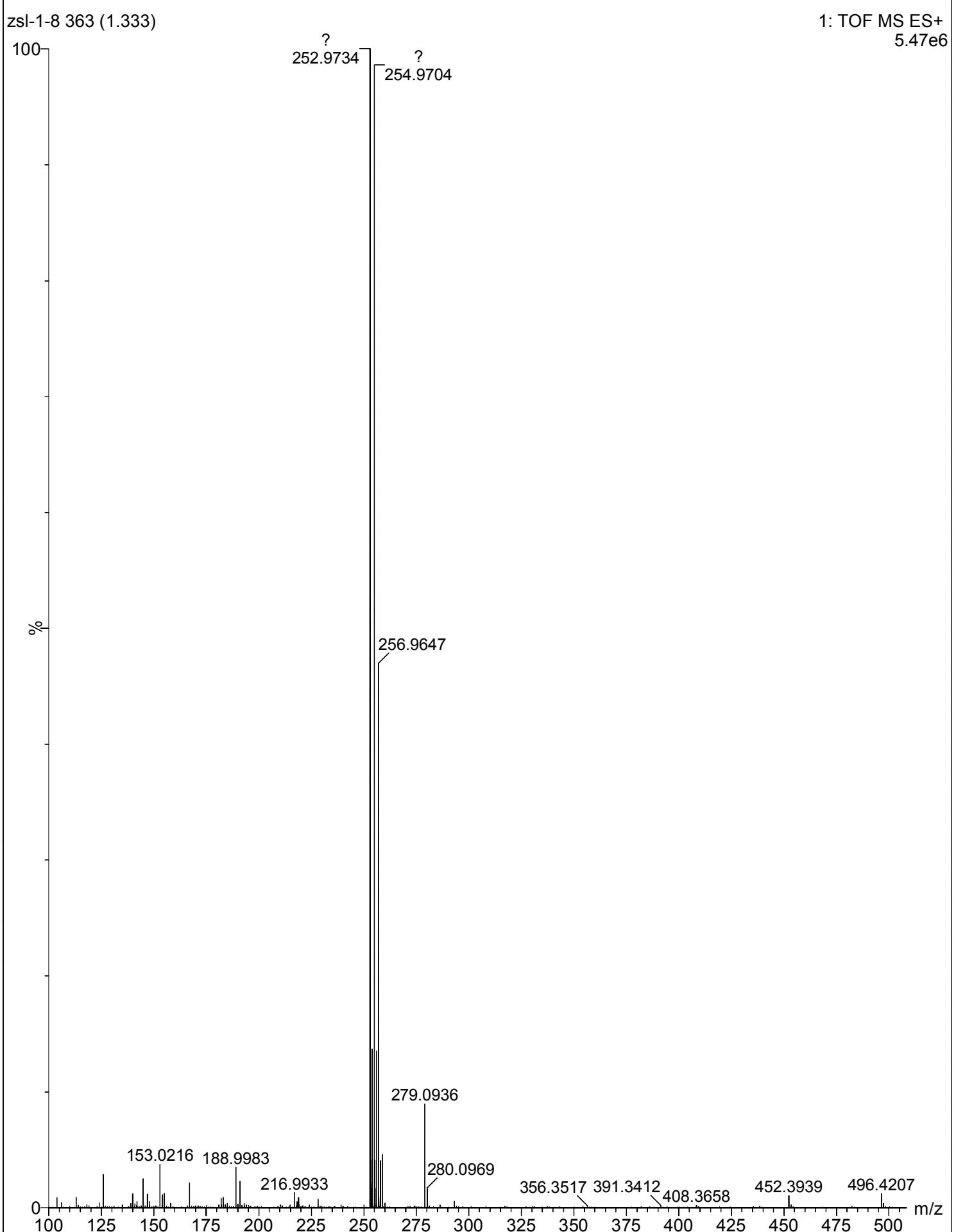
===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 18.00000000 W
PLW12 0.20056000 W
PLW13 0.16245000 W

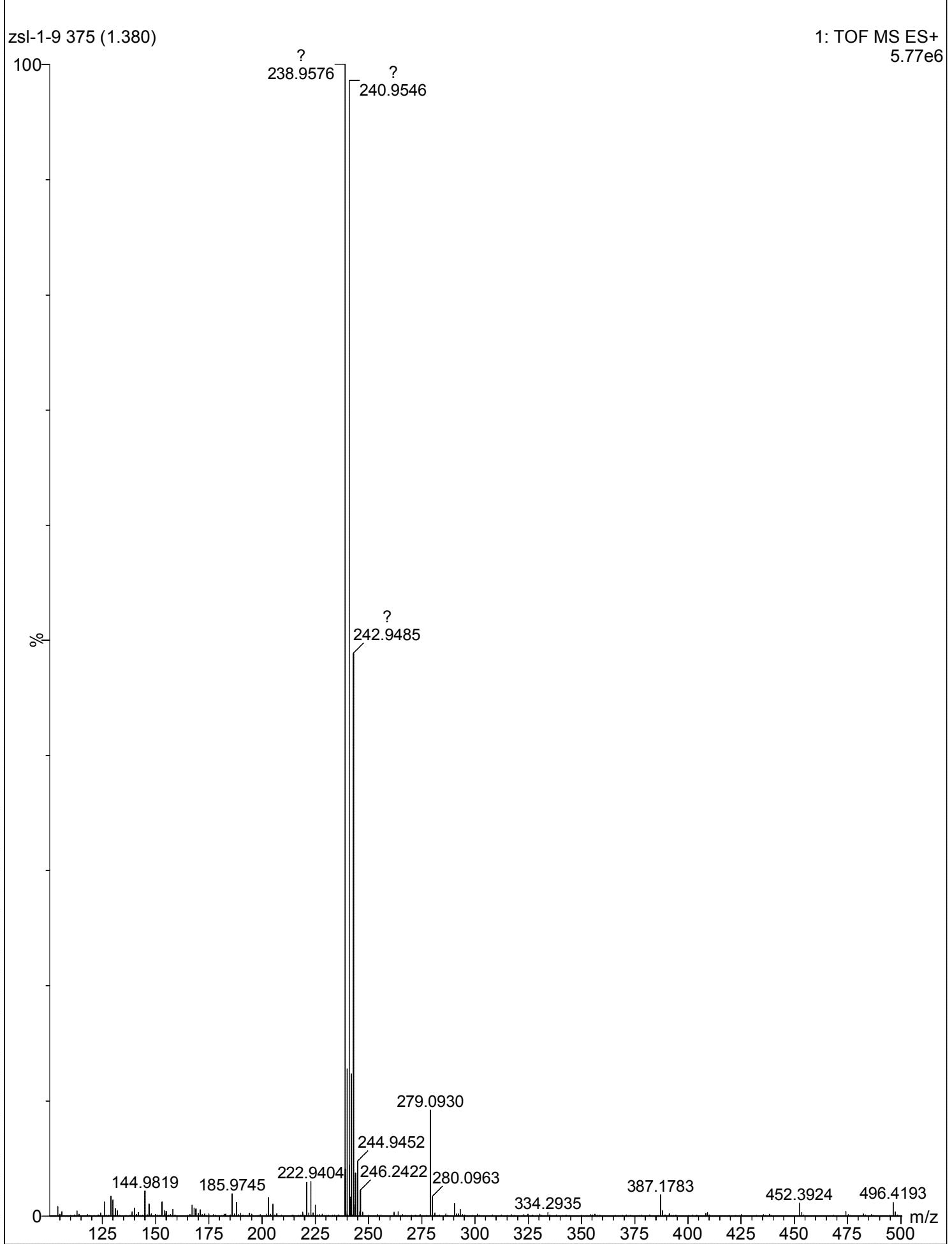
F2 - Processing parameters
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

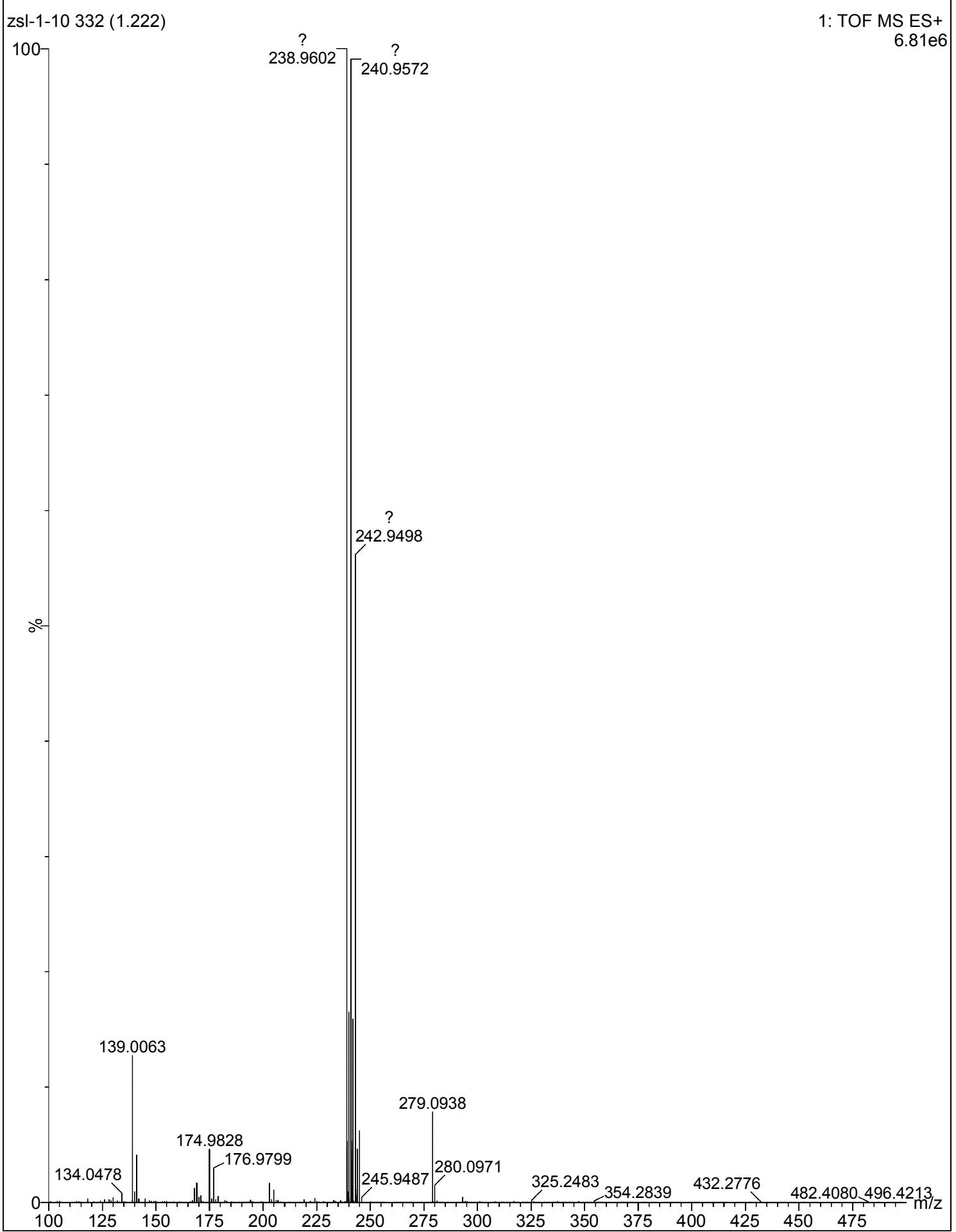


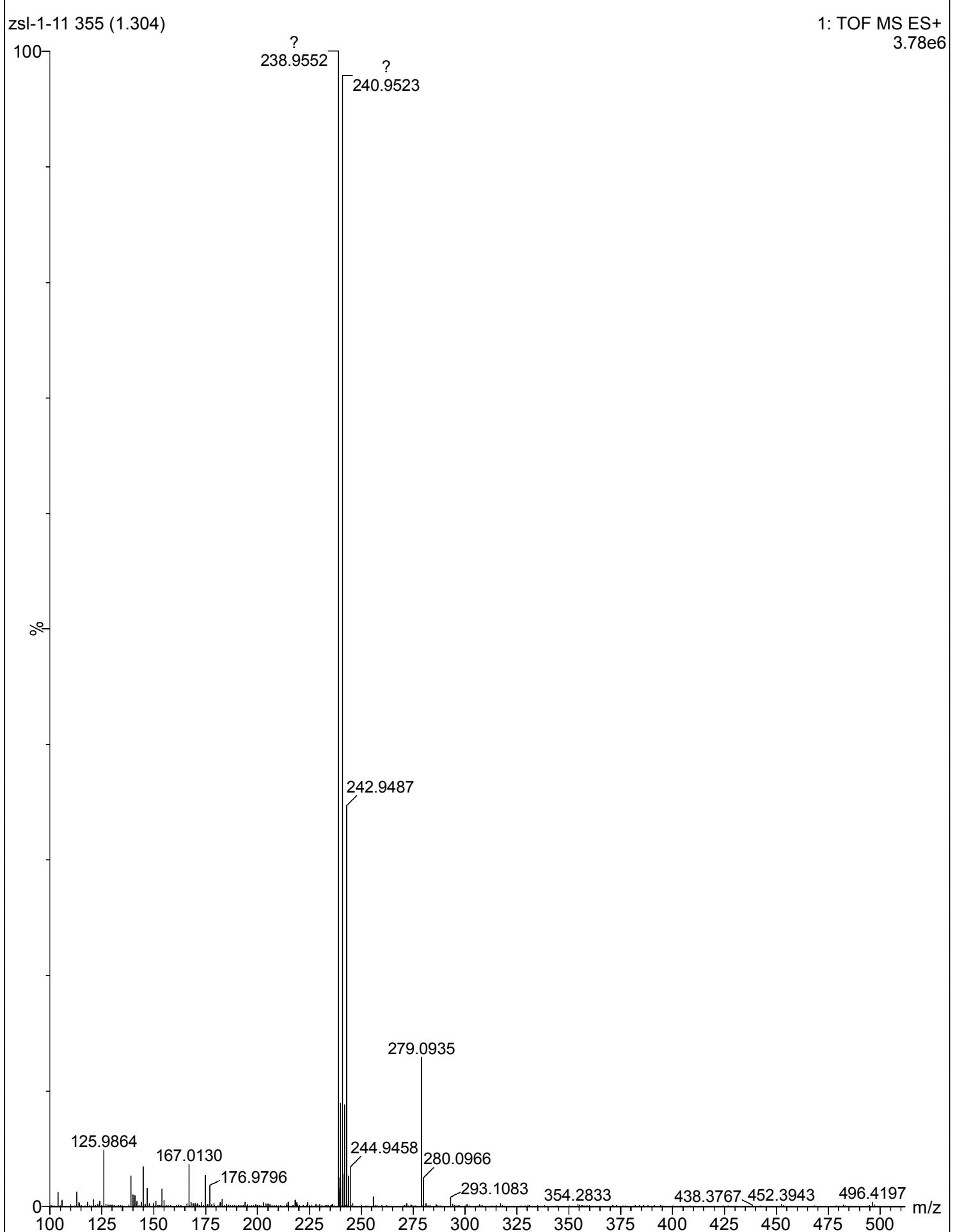


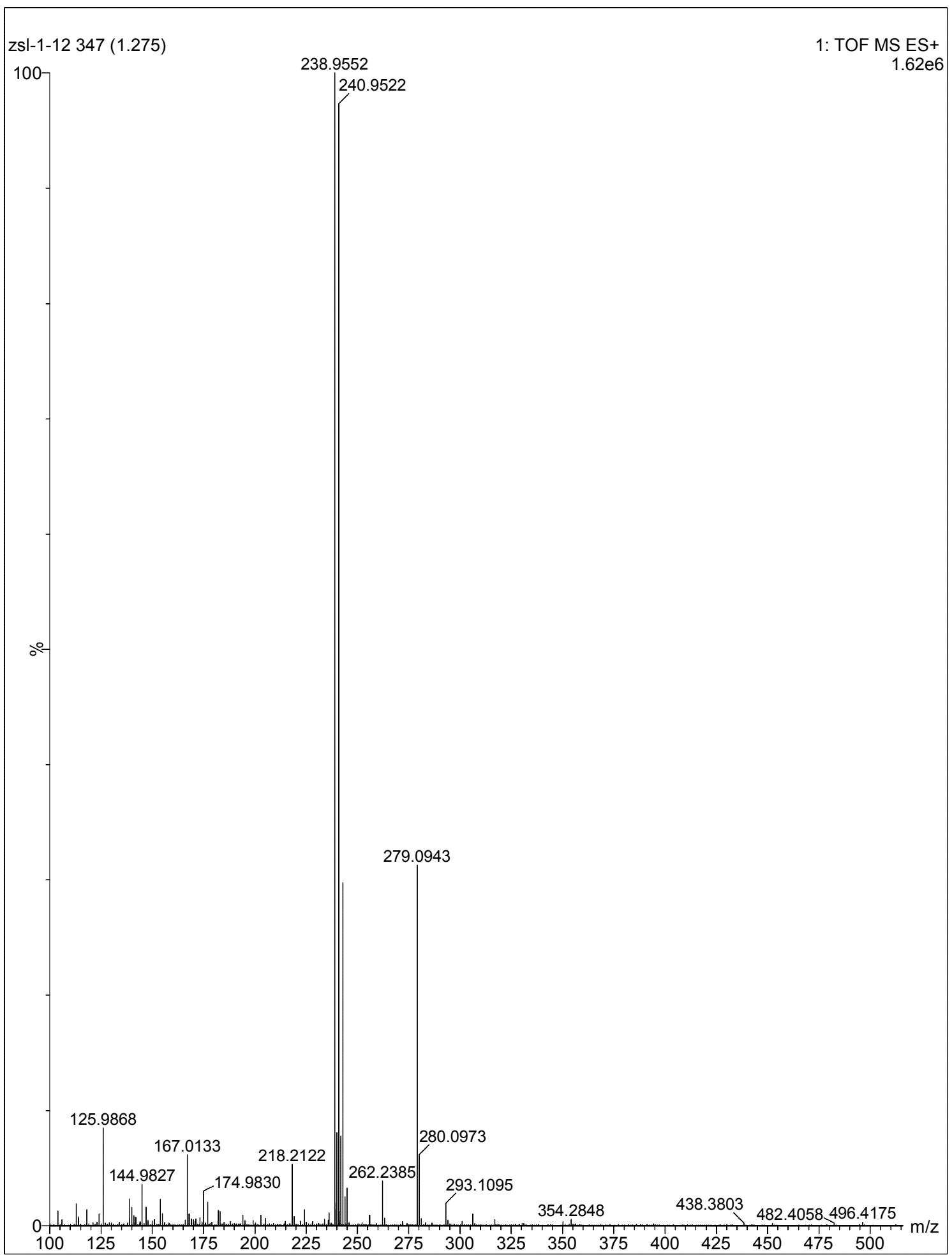


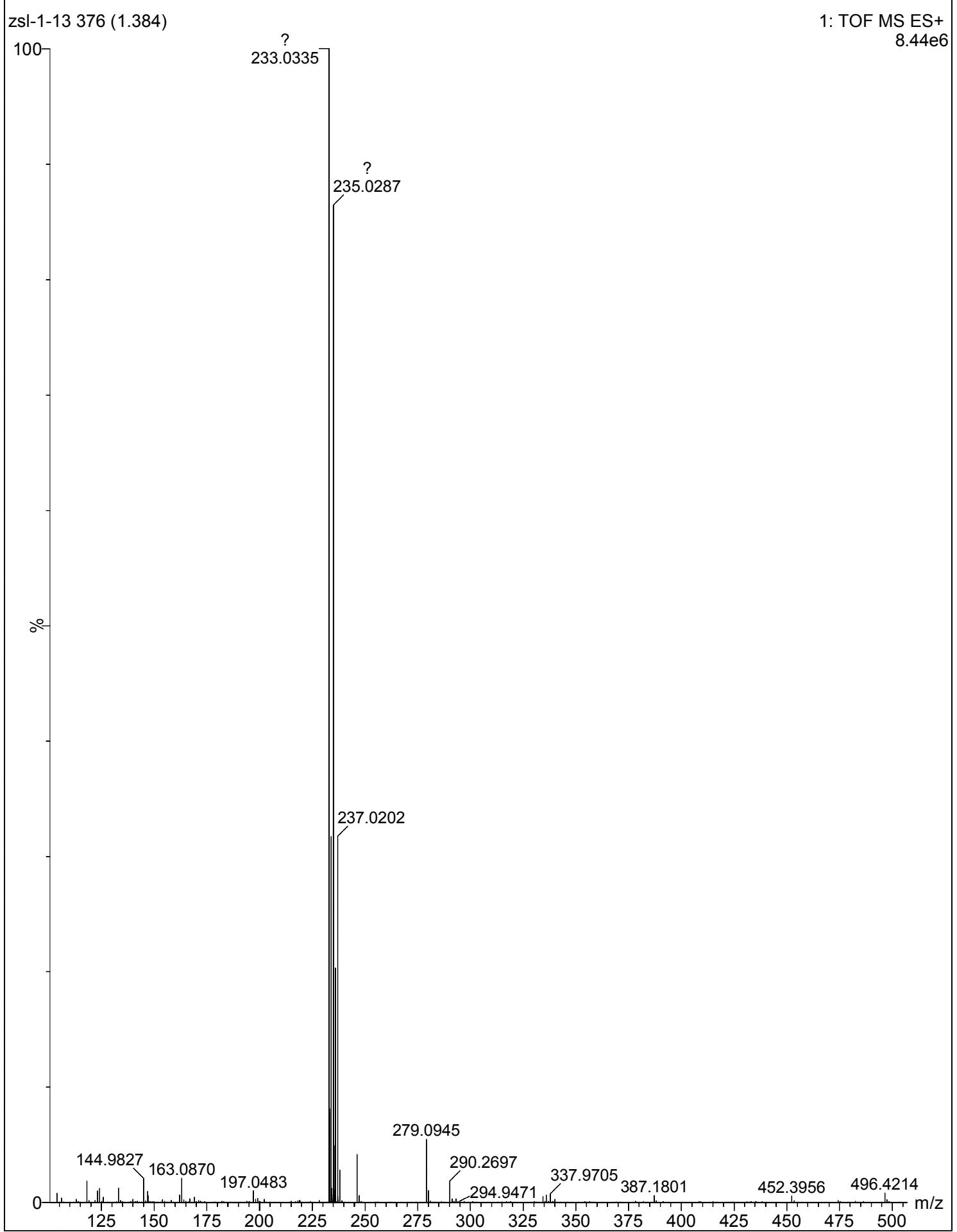


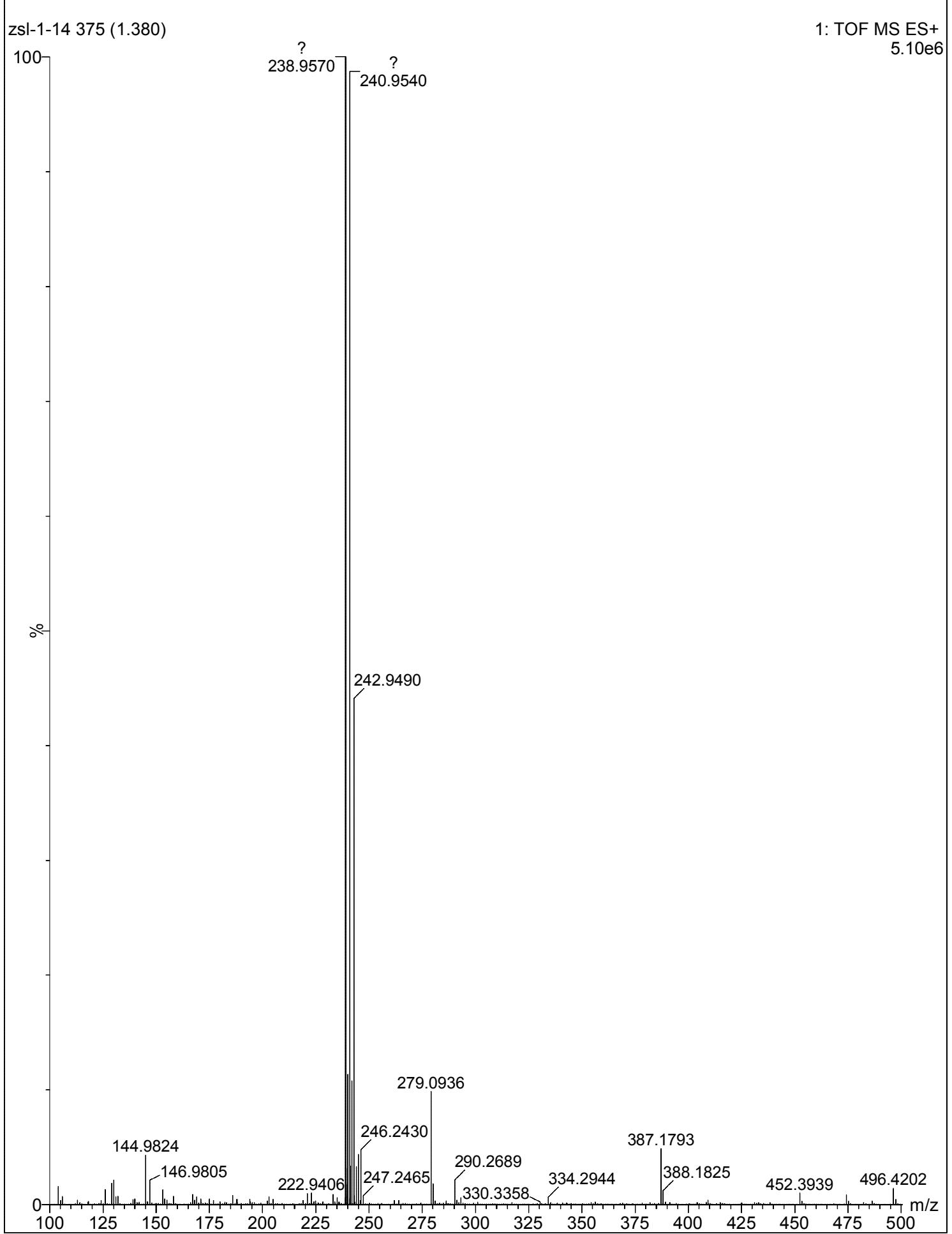


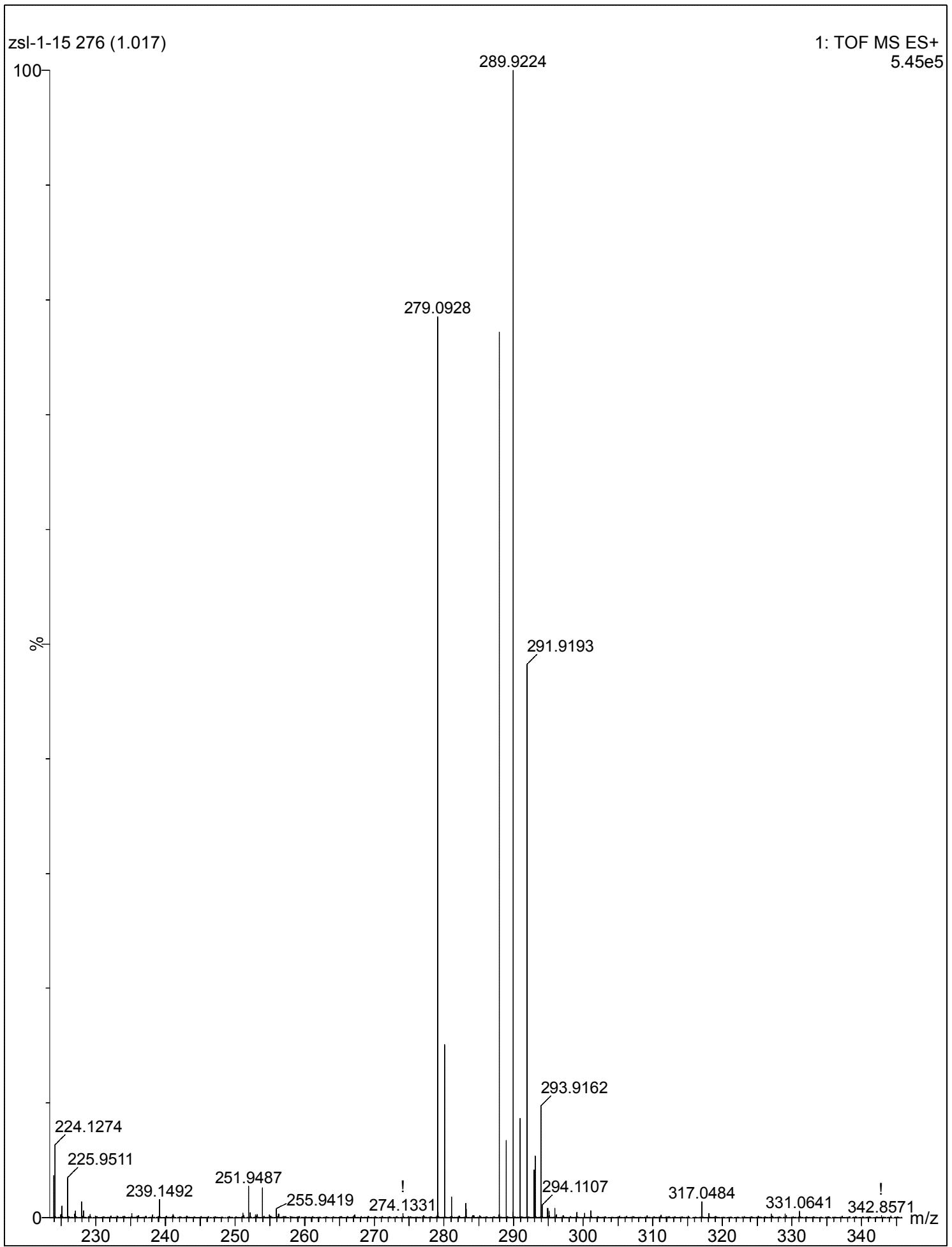


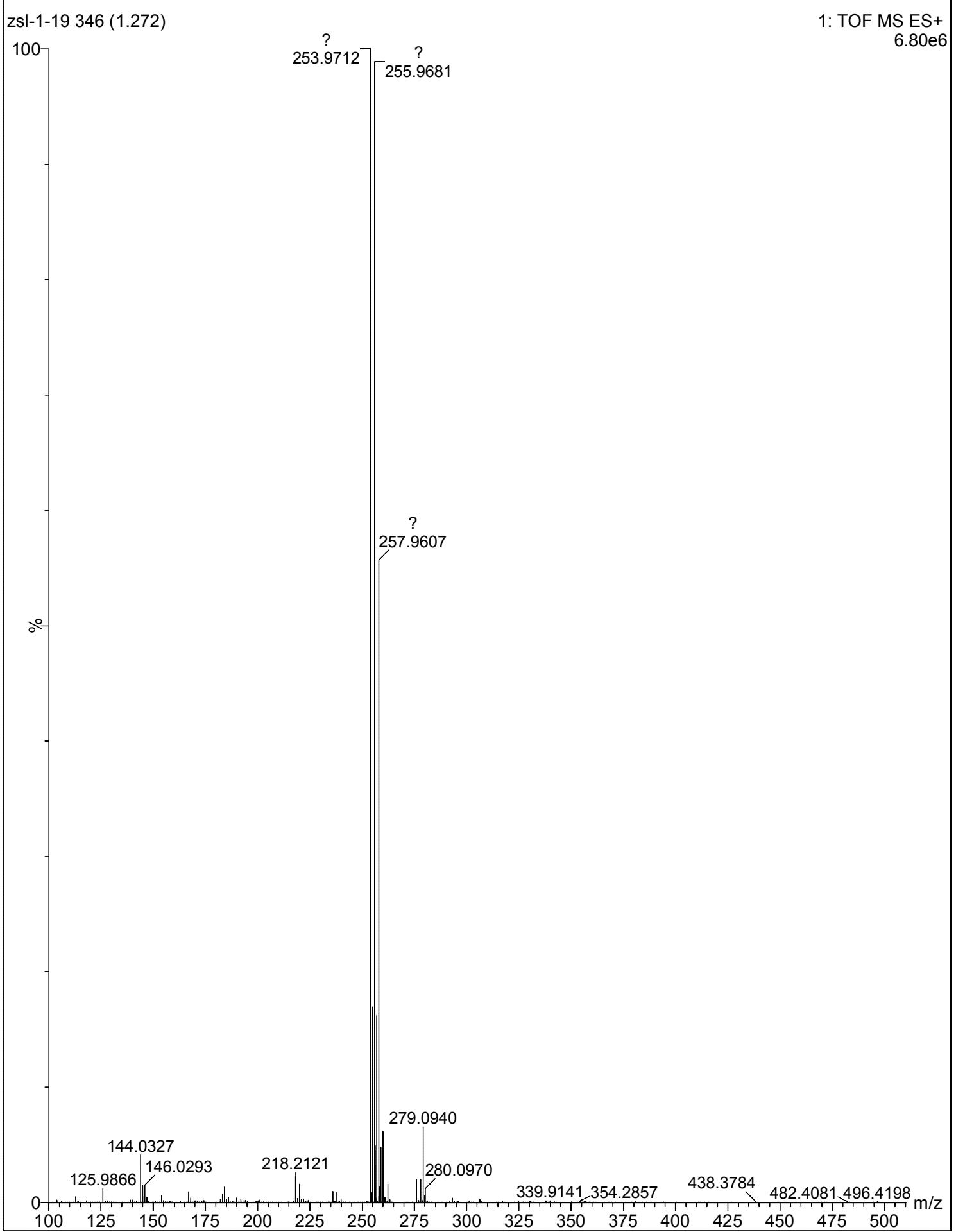


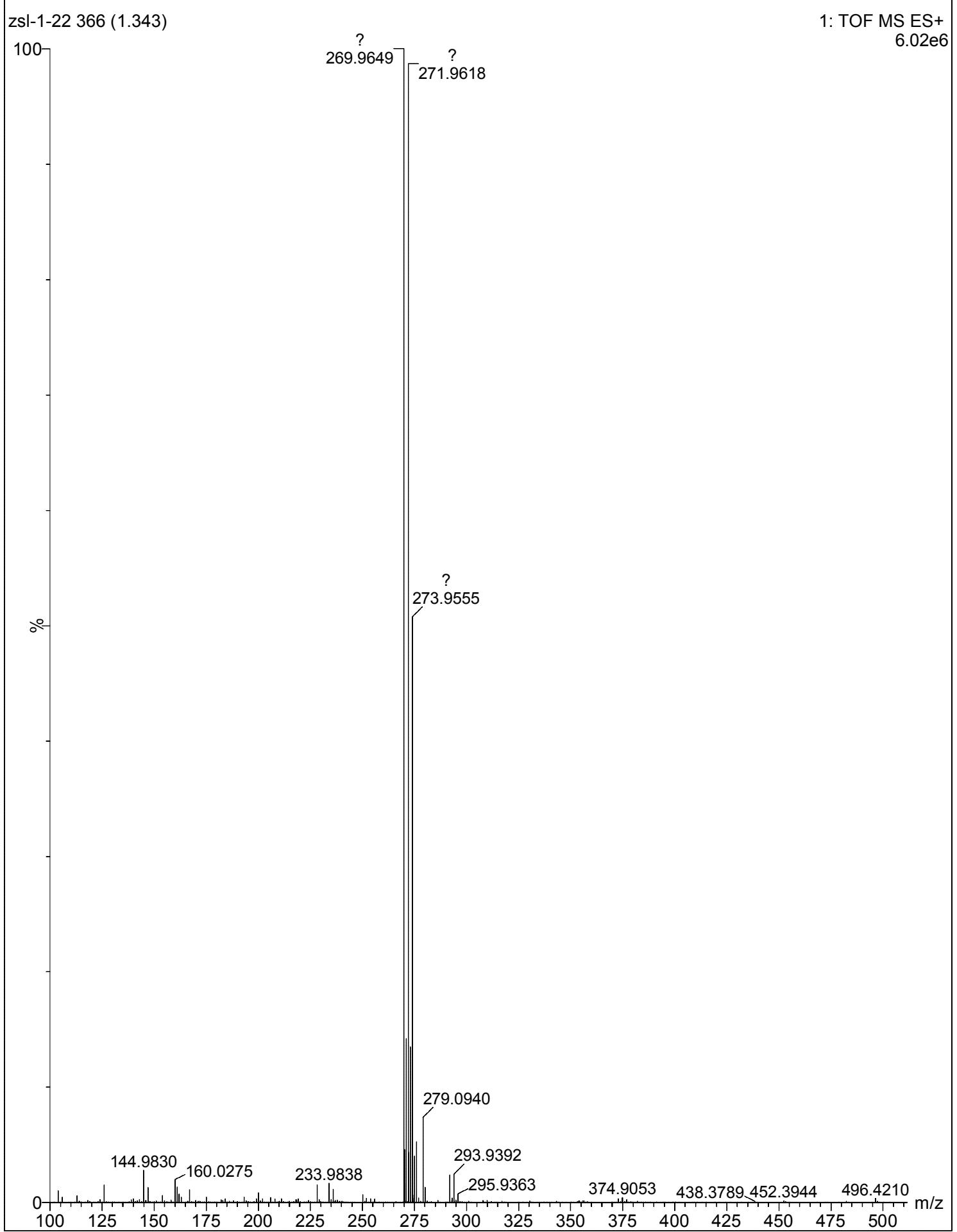


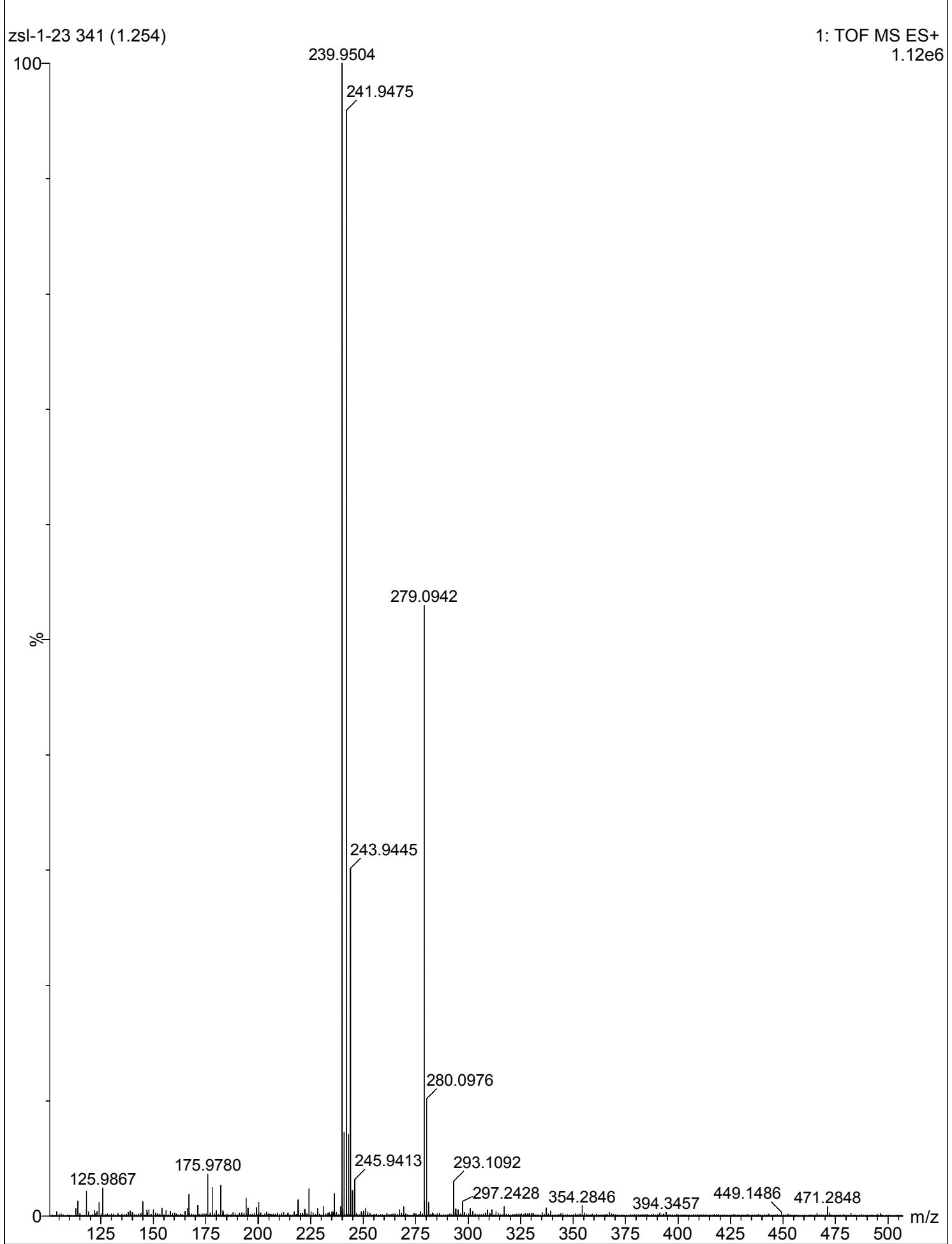


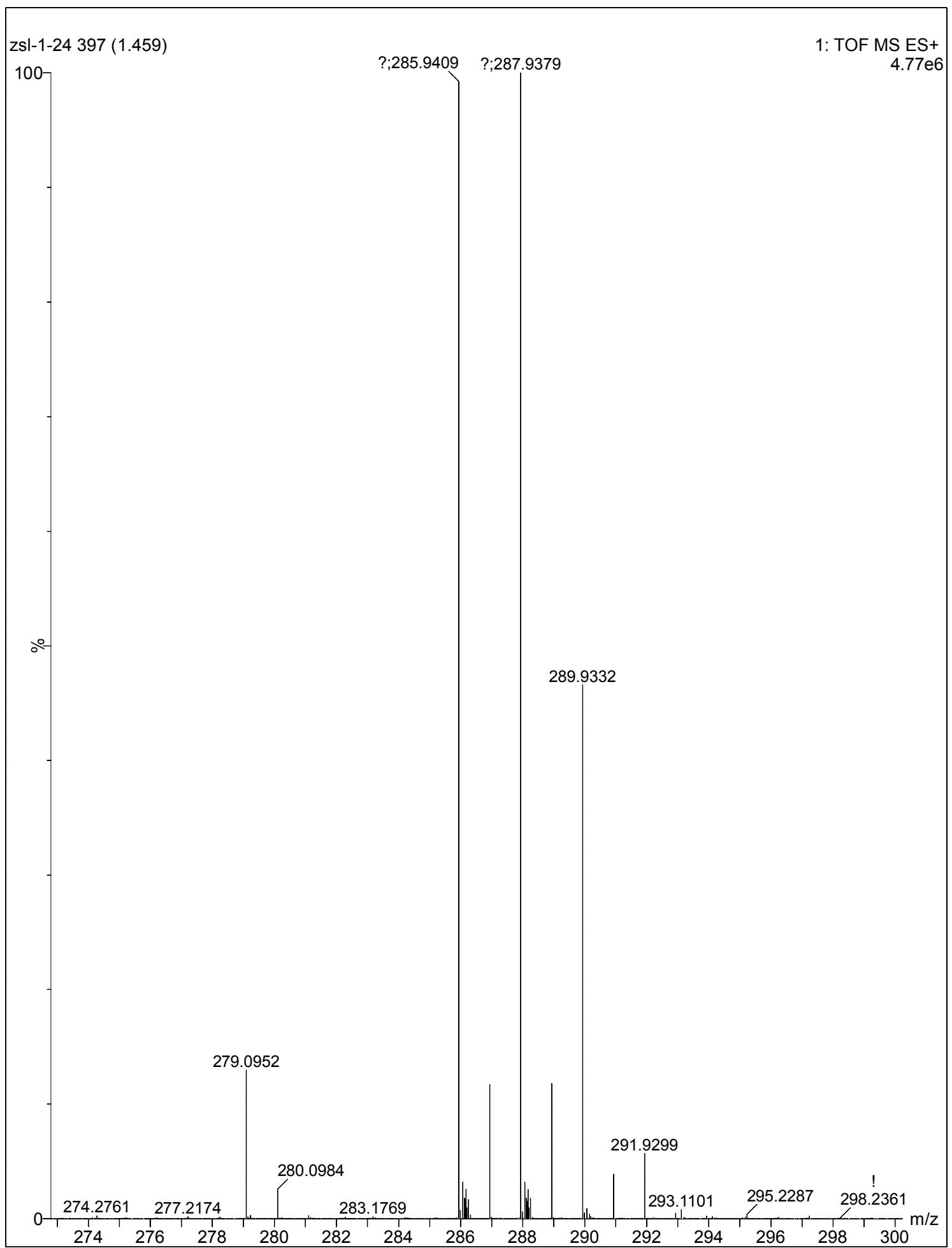


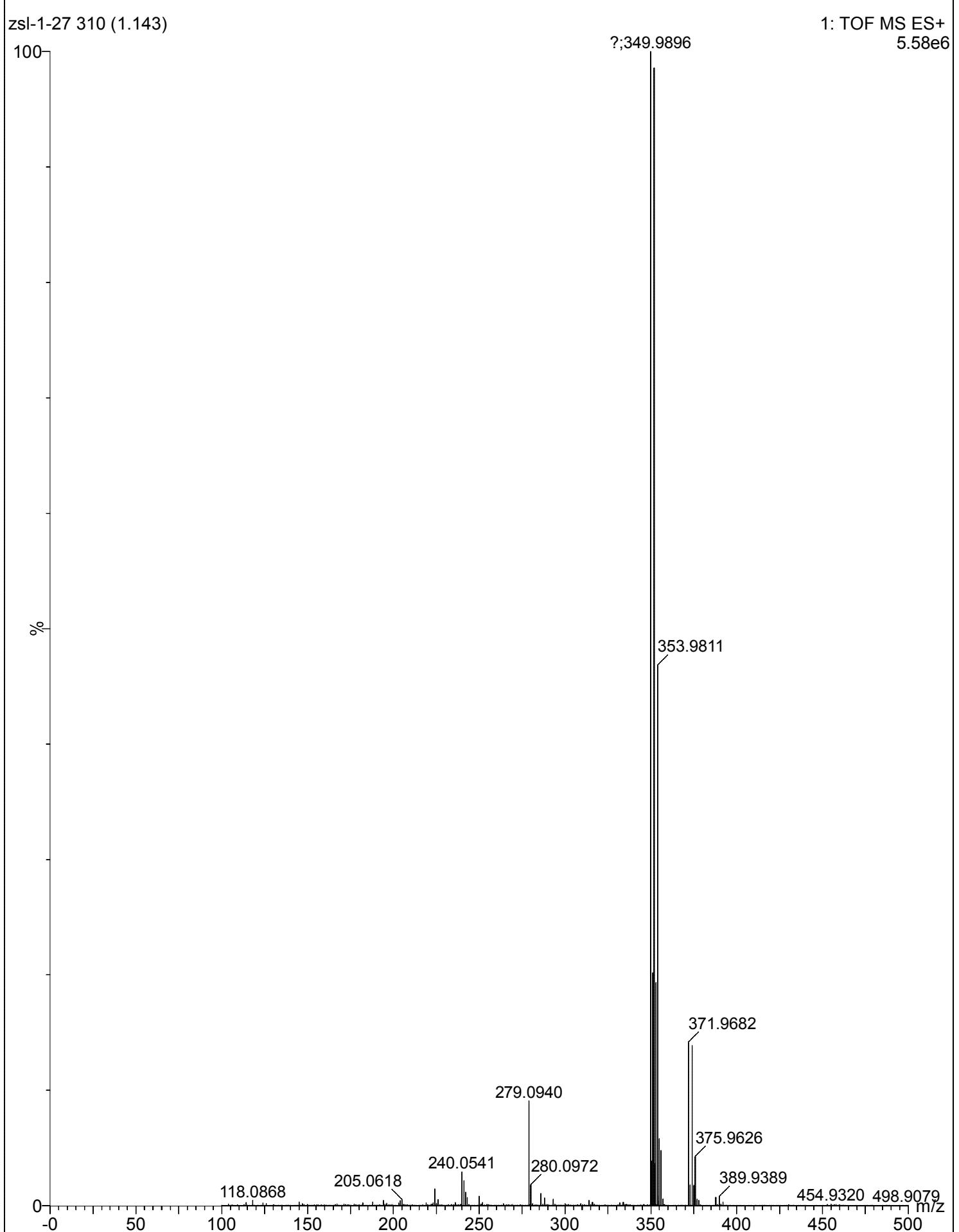


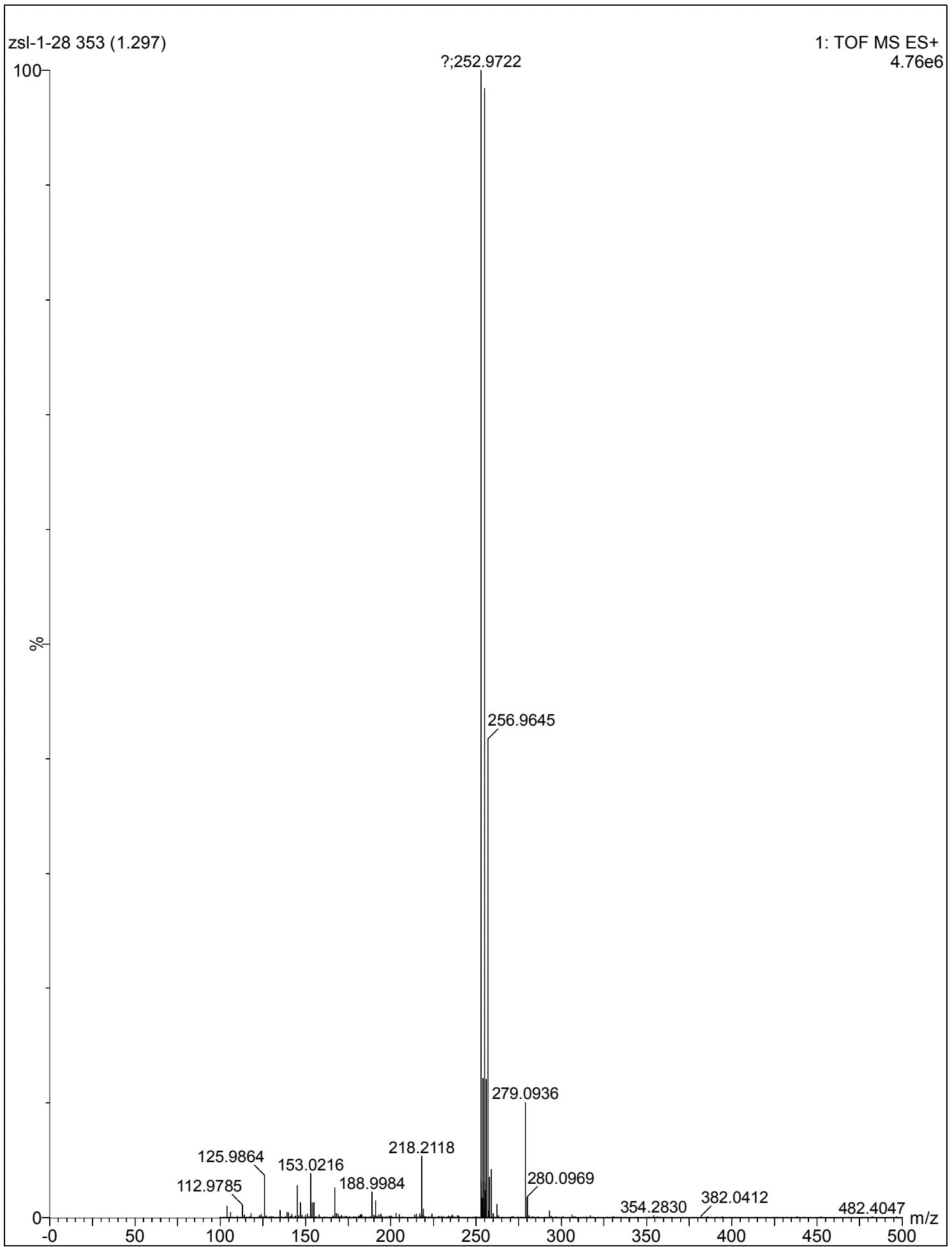


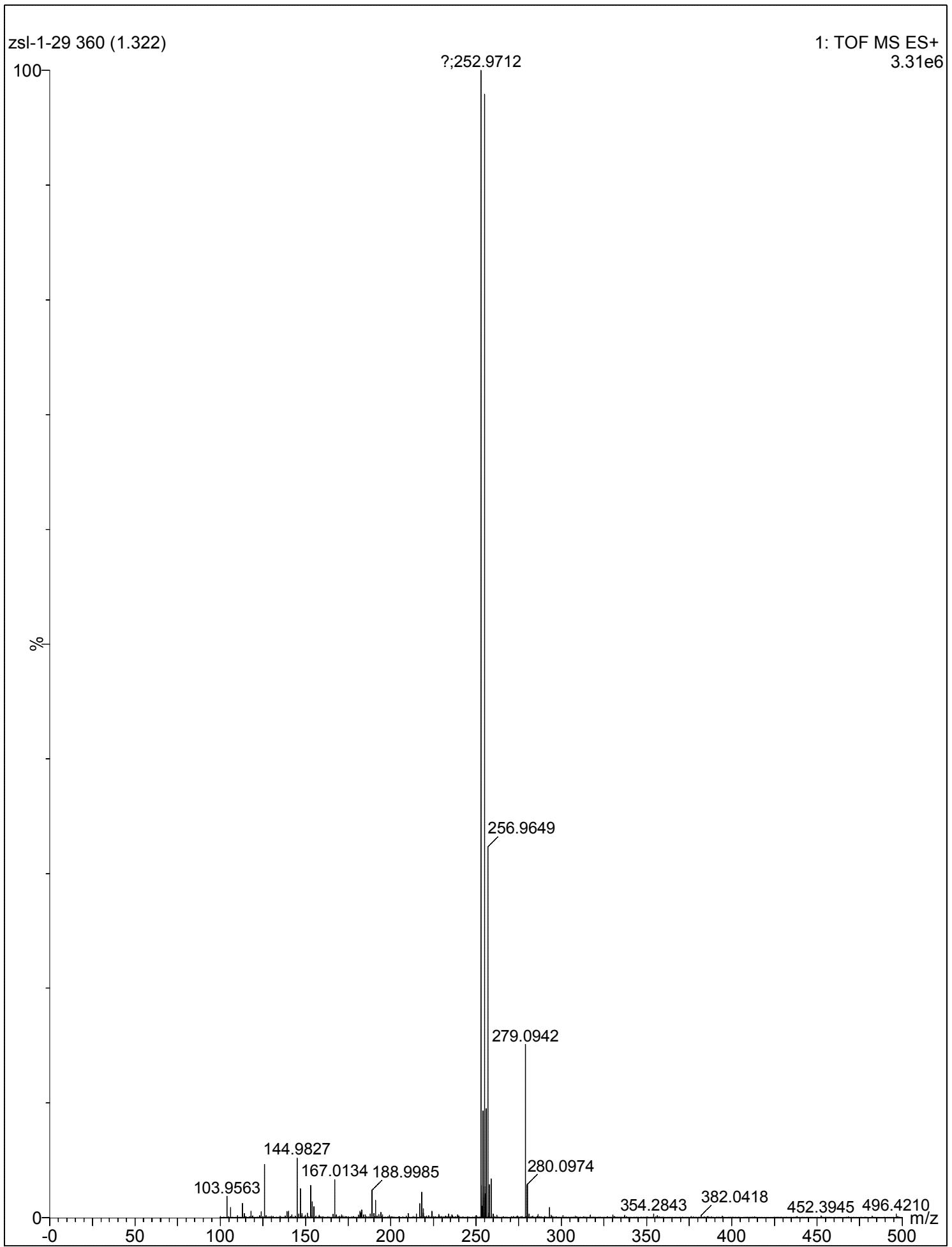


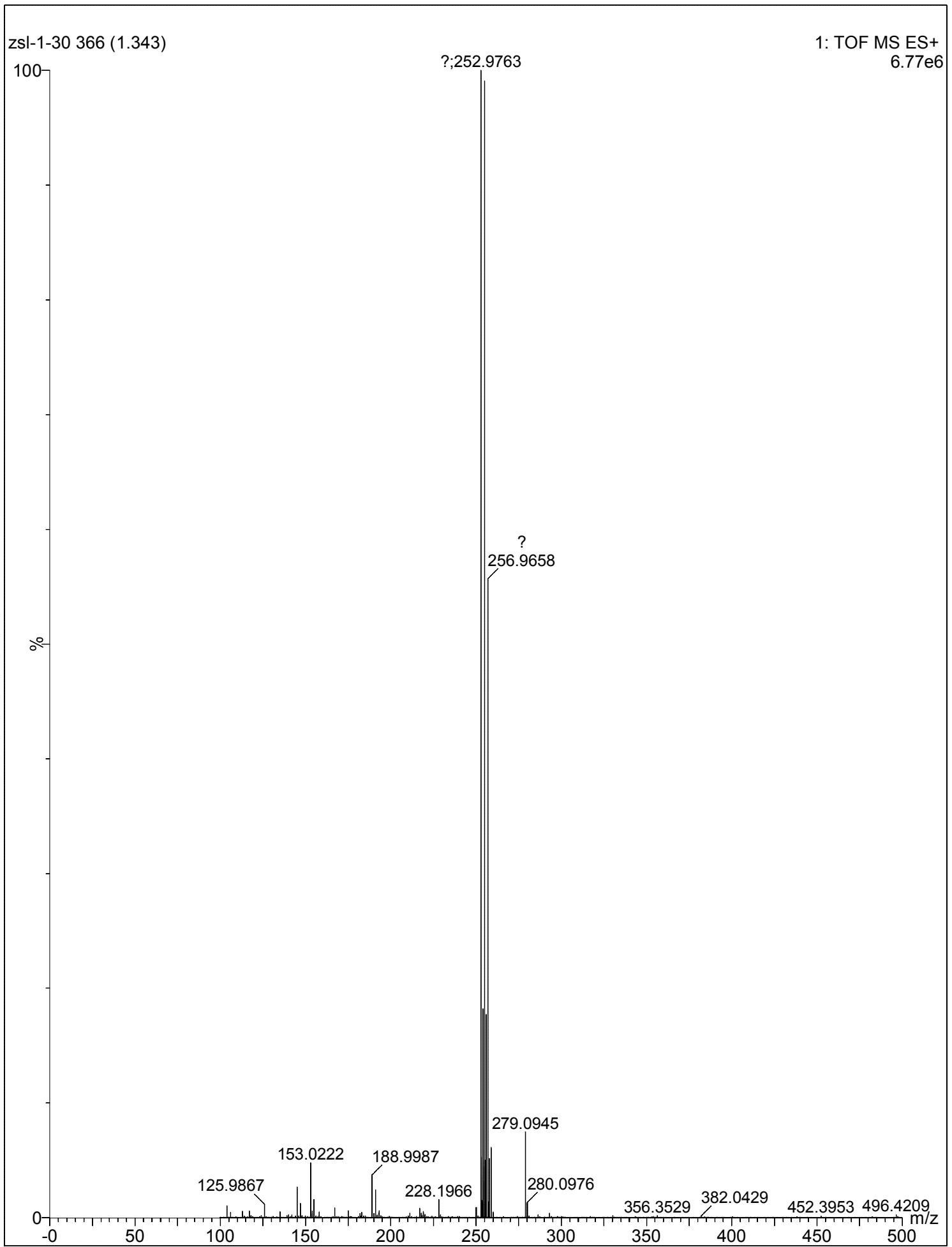


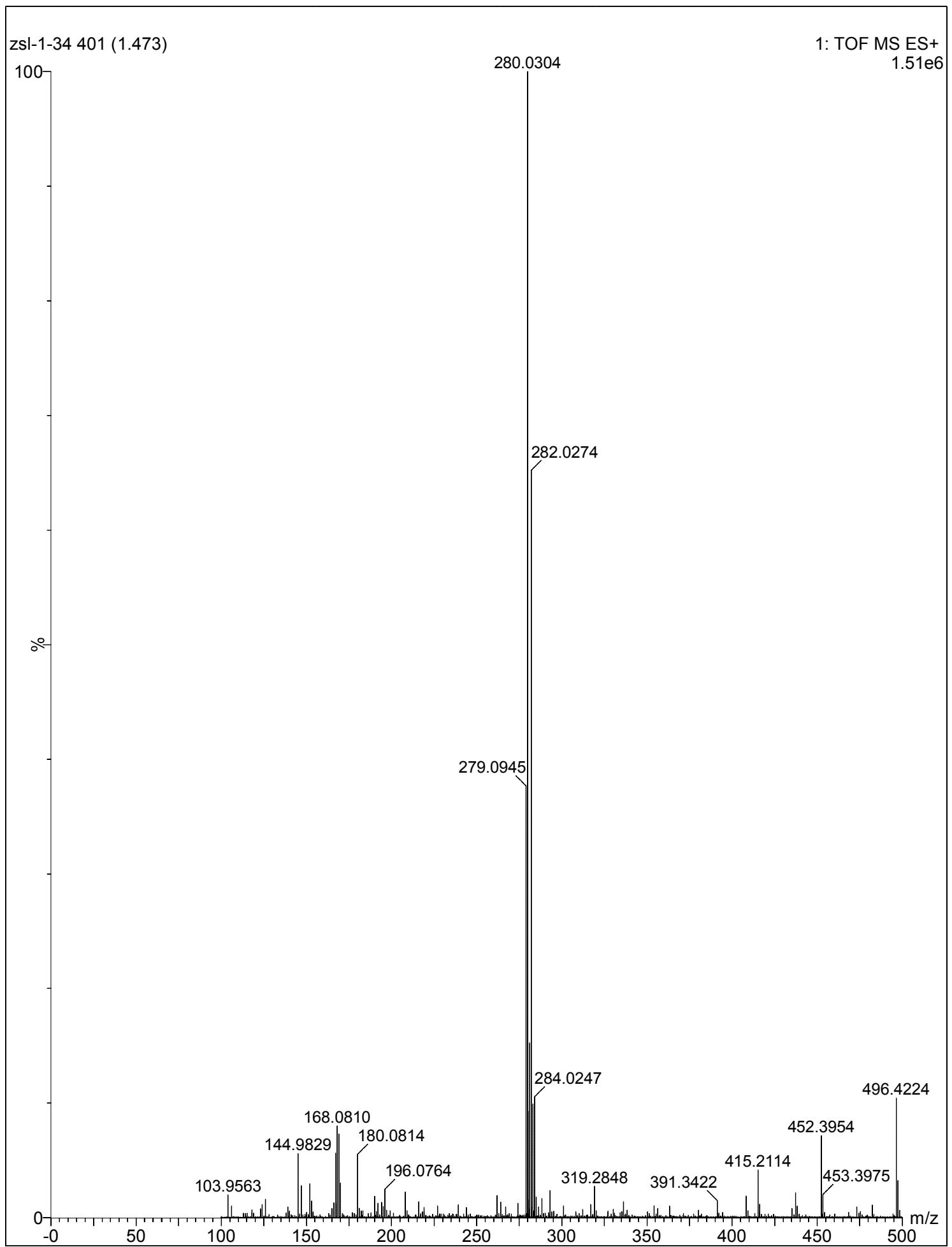


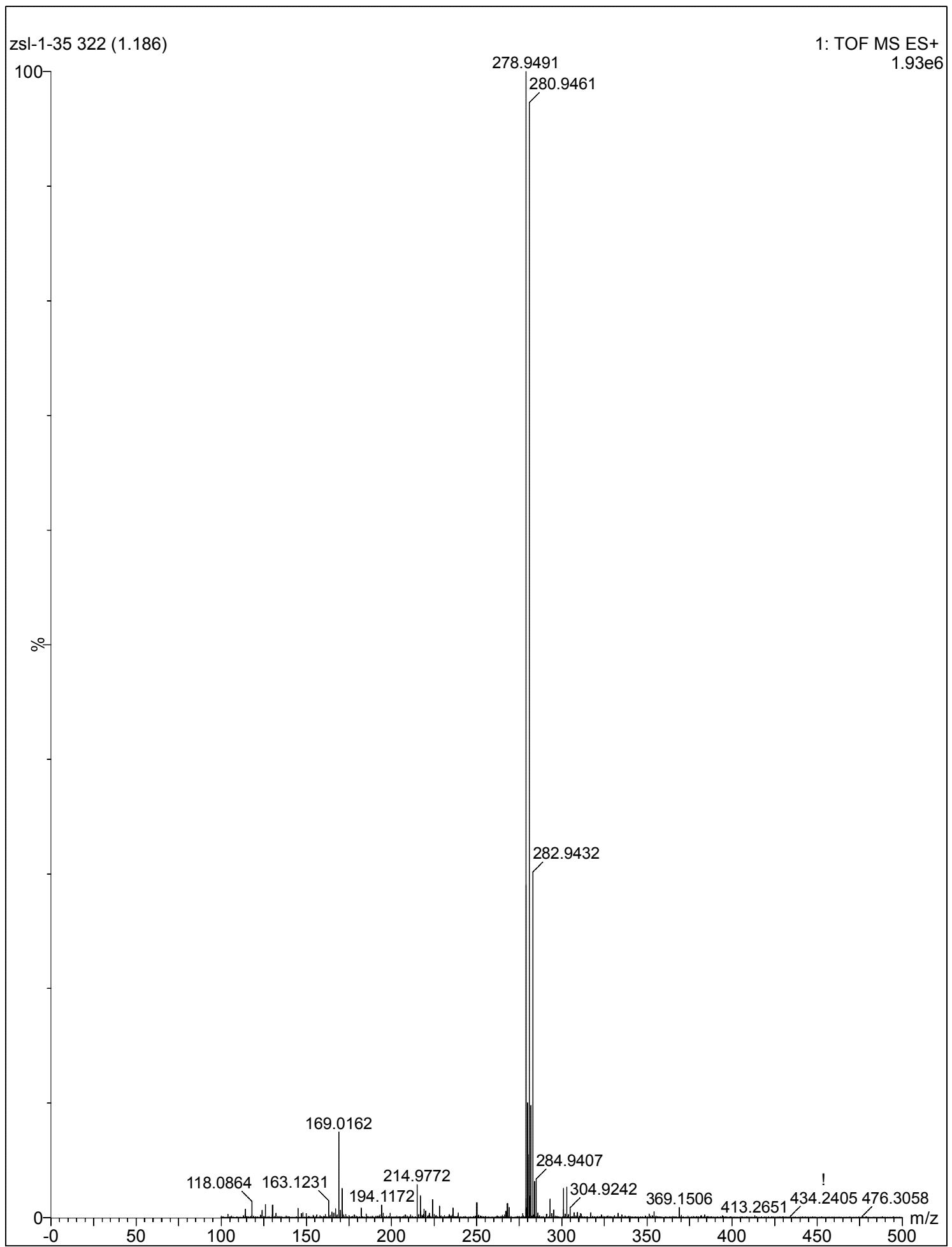


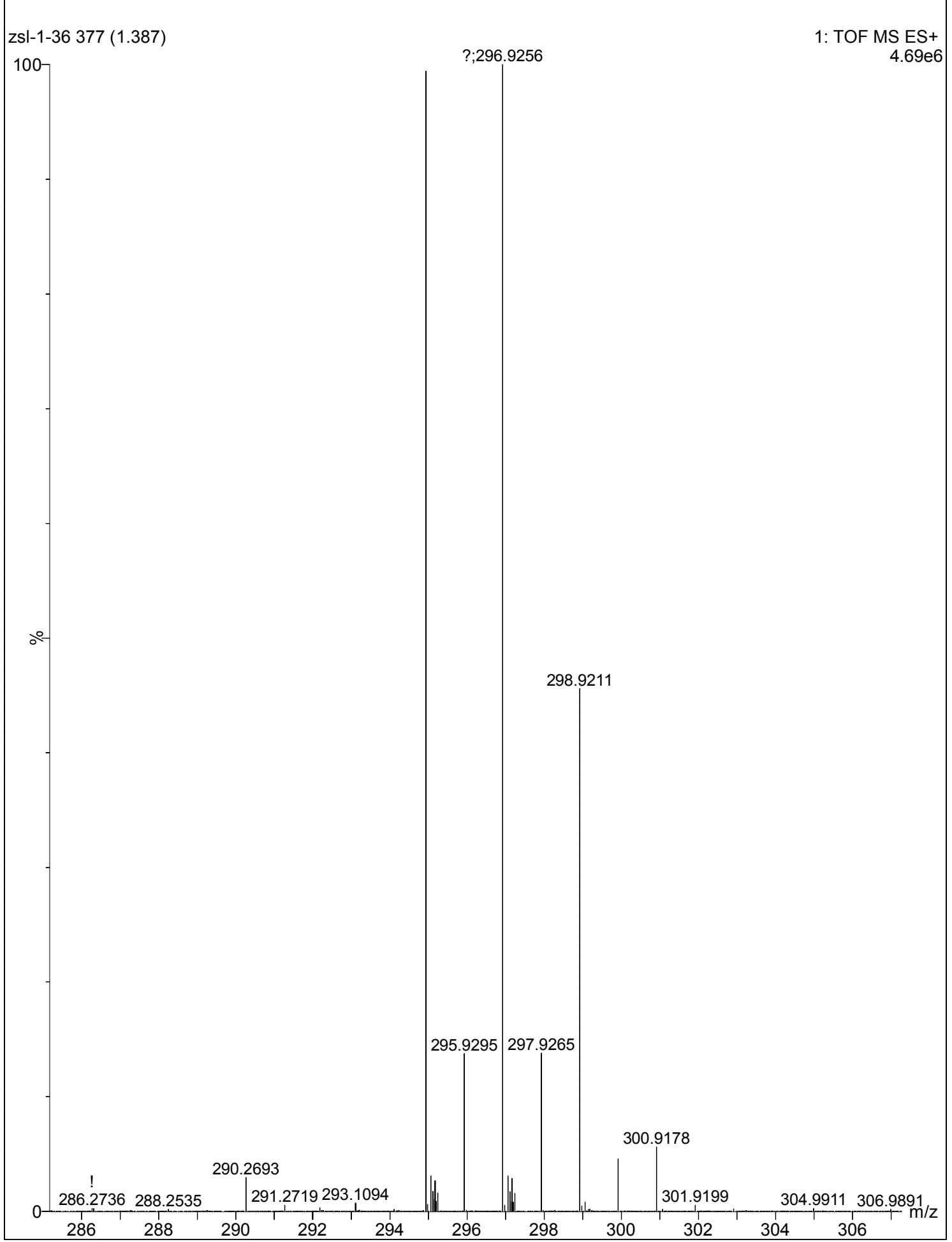


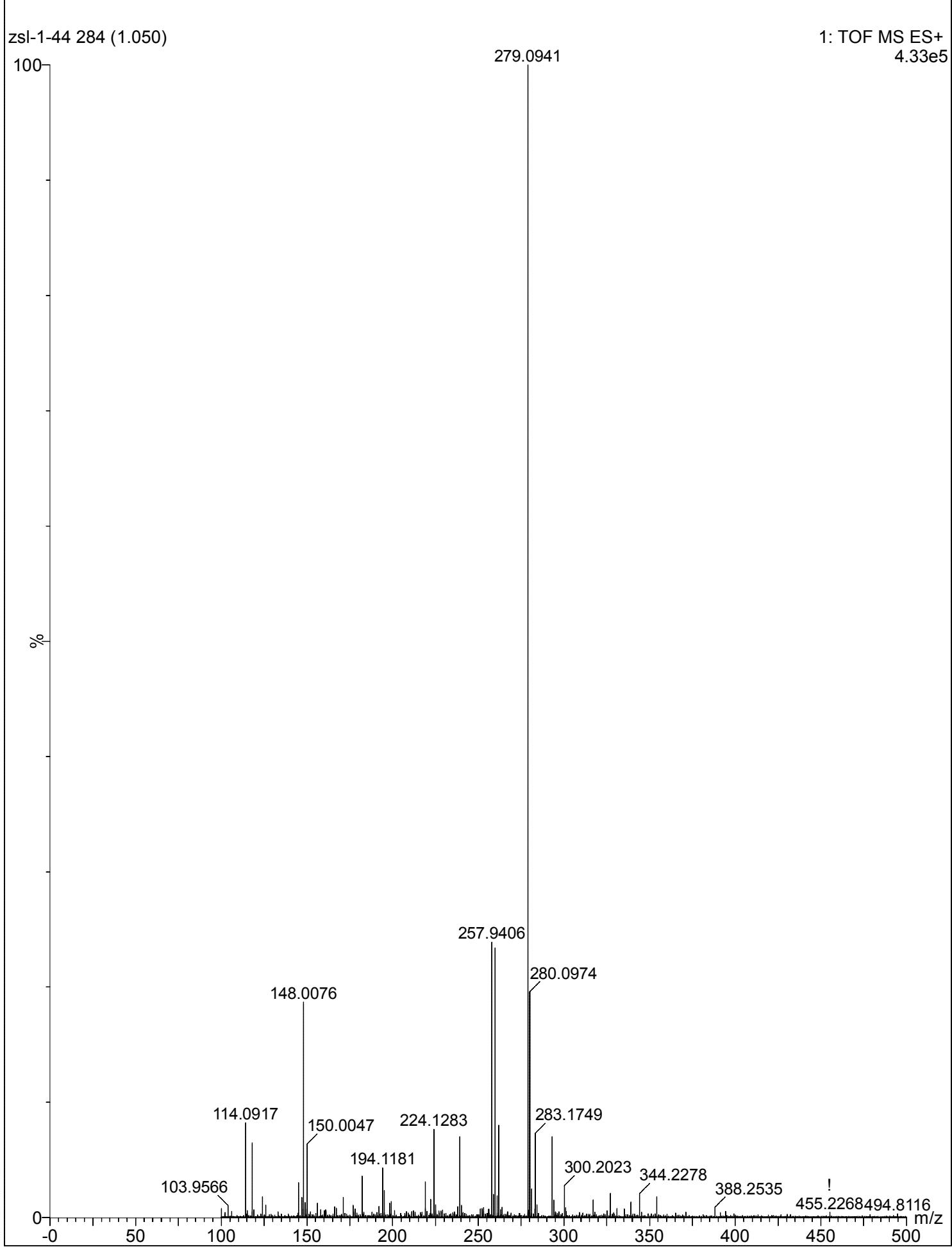


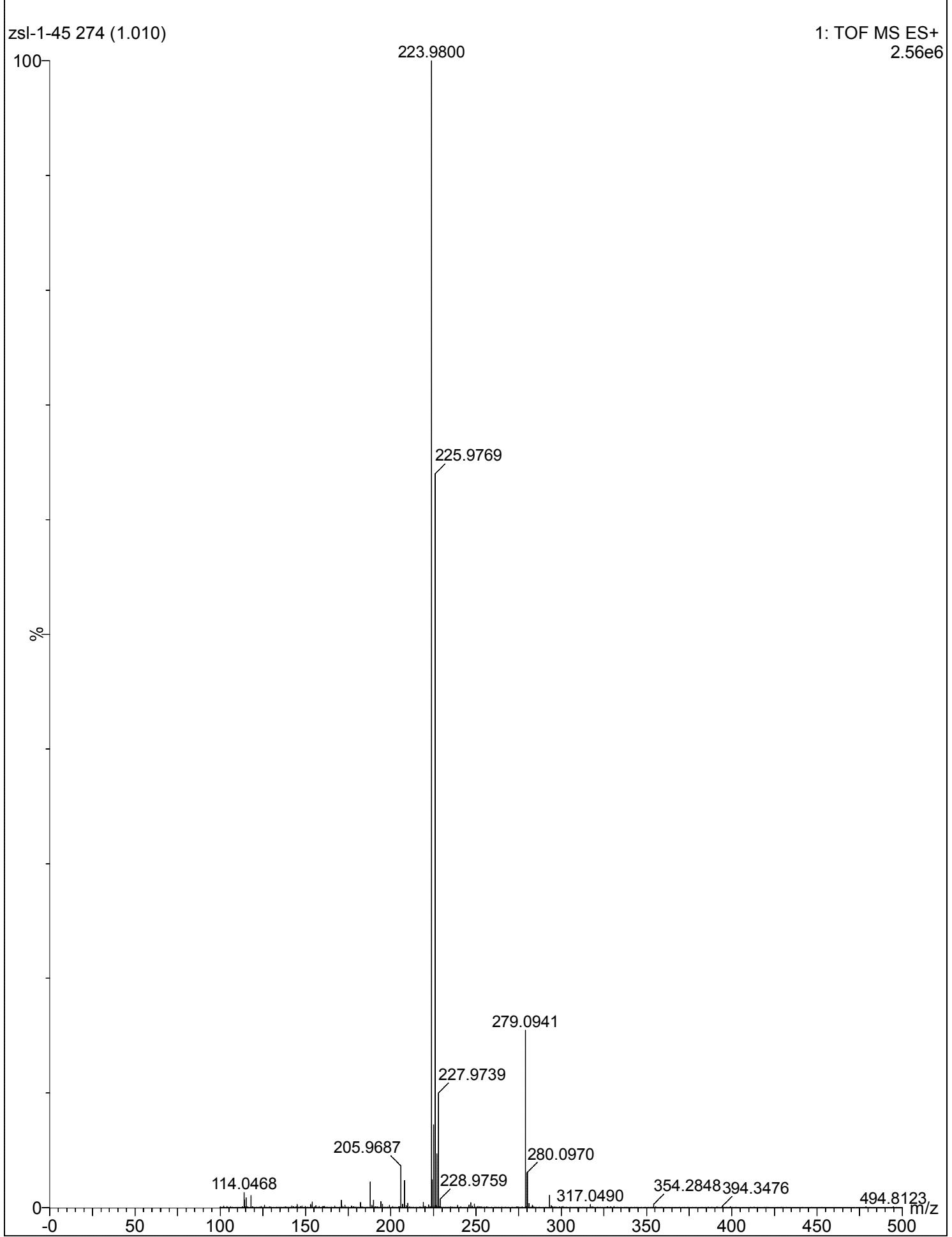






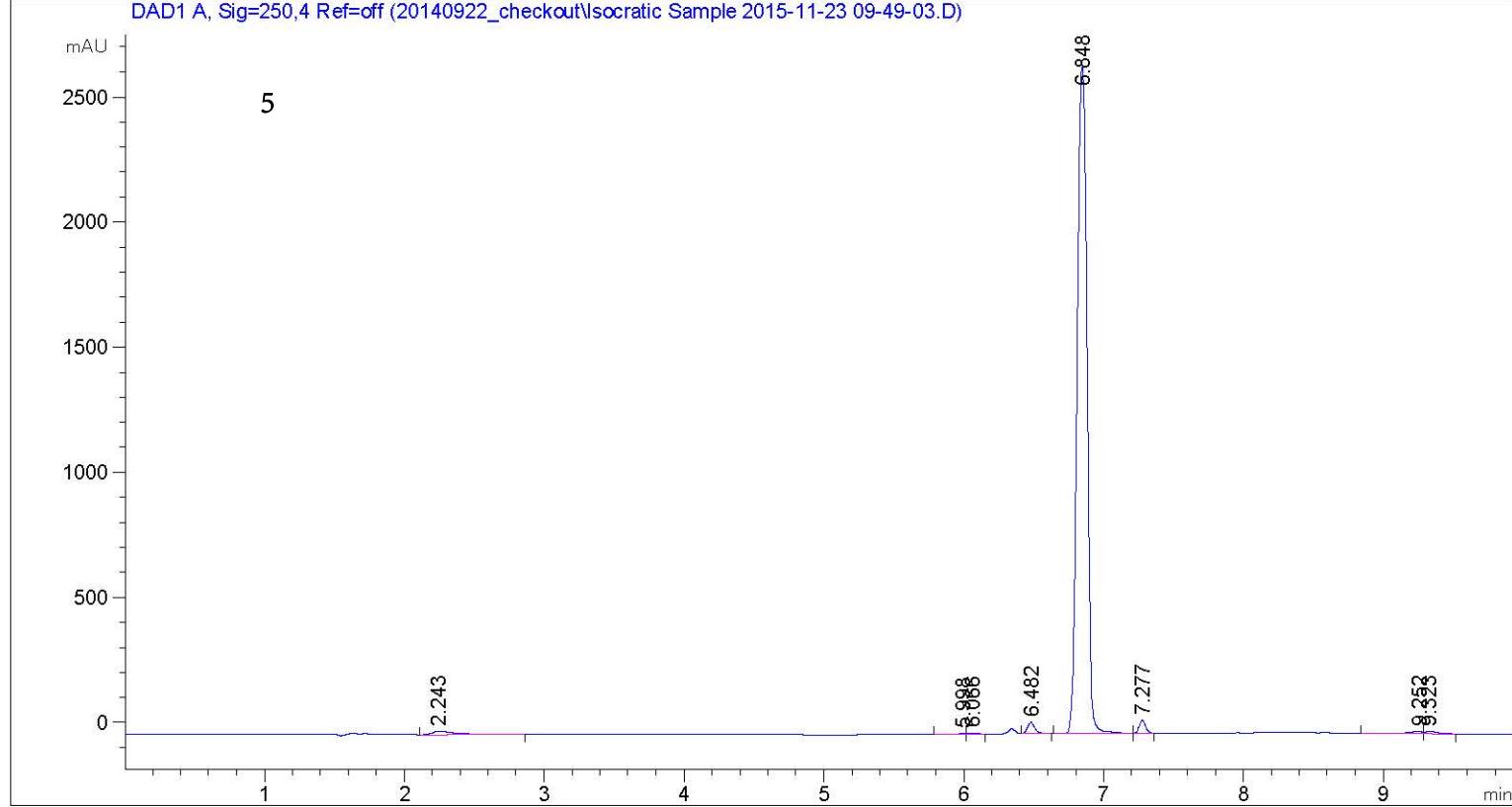






Sample Name: Isocratic Sample

```
=====
Acq. Operator   : SYSTEM
Sample Operator : SYSTEM
Acq. Instrument : HPLC                               Location : 1
Injection Date  : 11/23/2015 9:49:03 AM
                                                Inj Volume : No inj
Method          : C:\Chem32\1\Methods\DEF_LC.M
Last changed    : 11/23/2015 9:00:54 AM by SYSTEM
Additional Info : Peak(s) manually integrated
```



```
=====
                        Area Percent Report
=====
```

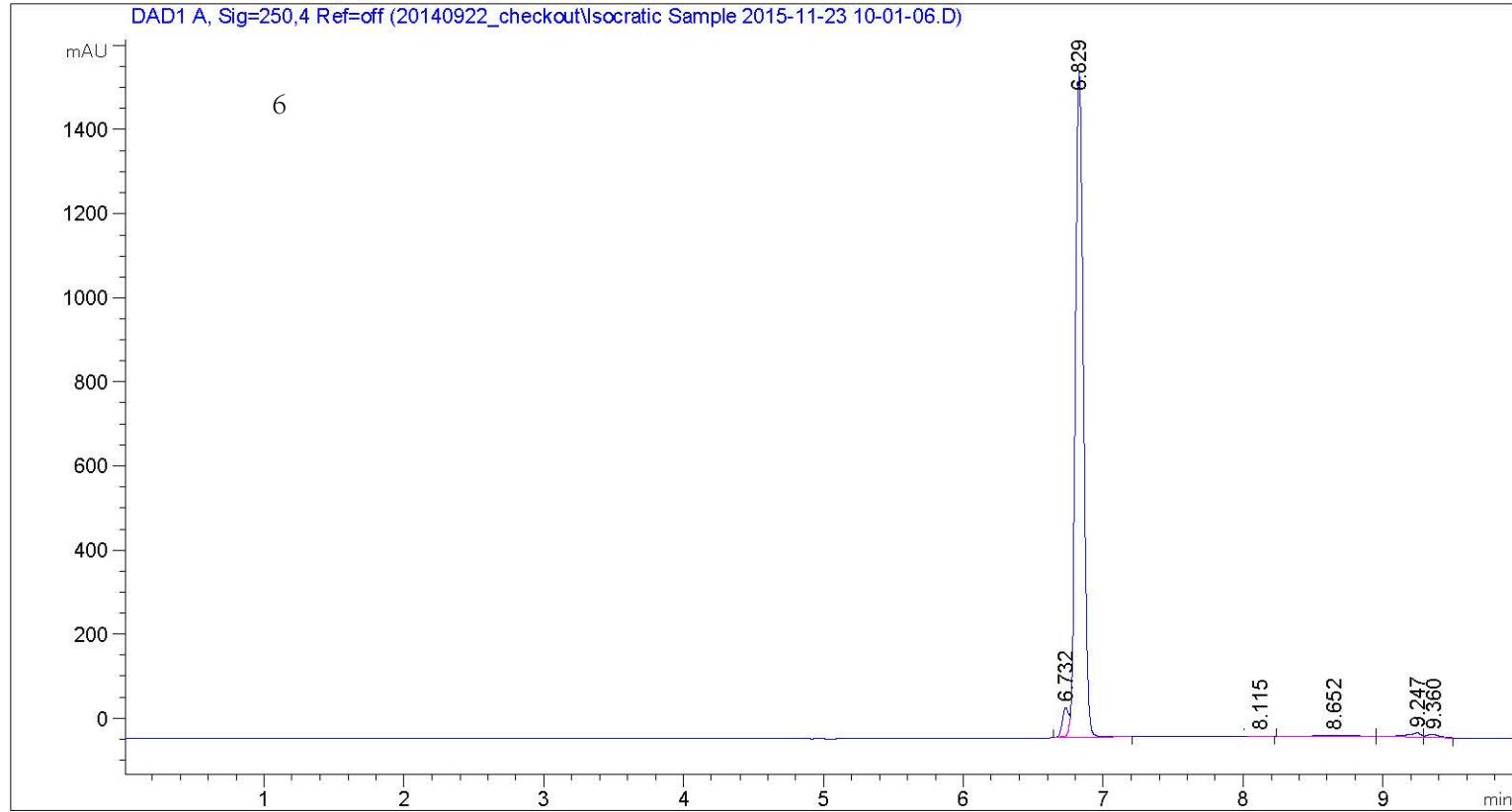
```
Sorted By      : Signal
Multiplier     : 1.0000
Dilution      : 1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: DAD1 A, Sig=250,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.243	BB	0.1698	174.03569	13.55296	1.2861
2	5.998	BV	0.0475	5.16811	1.60944	0.0382
3	6.066	BV	0.0520	18.65882	5.44193	0.1379
4	6.482	BV	0.0558	170.73572	45.49647	1.2617
5	6.848	BB	0.0803	1.28722e4	2668.57642	95.1248
6	7.277	BV	0.0513	166.49522	52.06132	1.2304
7	9.252	BV	0.1187	75.21325	8.07200	0.5558
8	9.323	BV	0.0890	49.40413	7.29242	0.3651
Totals			1.35319e4	2802.10296		

Sample Name: Isocratic Sample

=====
Acq. Operator : SYSTEM
Sample Operator : SYSTEM
Acq. Instrument : HPLC Location : 1
Injection Date : 11/23/2015 10:01:06 AM
Inj Volume : No inj
Method : C:\Chem32\1\Methods\DEF_LC.M
Last changed : 11/23/2015 9:00:54 AM by SYSTEM
Additional Info : Peak(s) manually integrated



=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

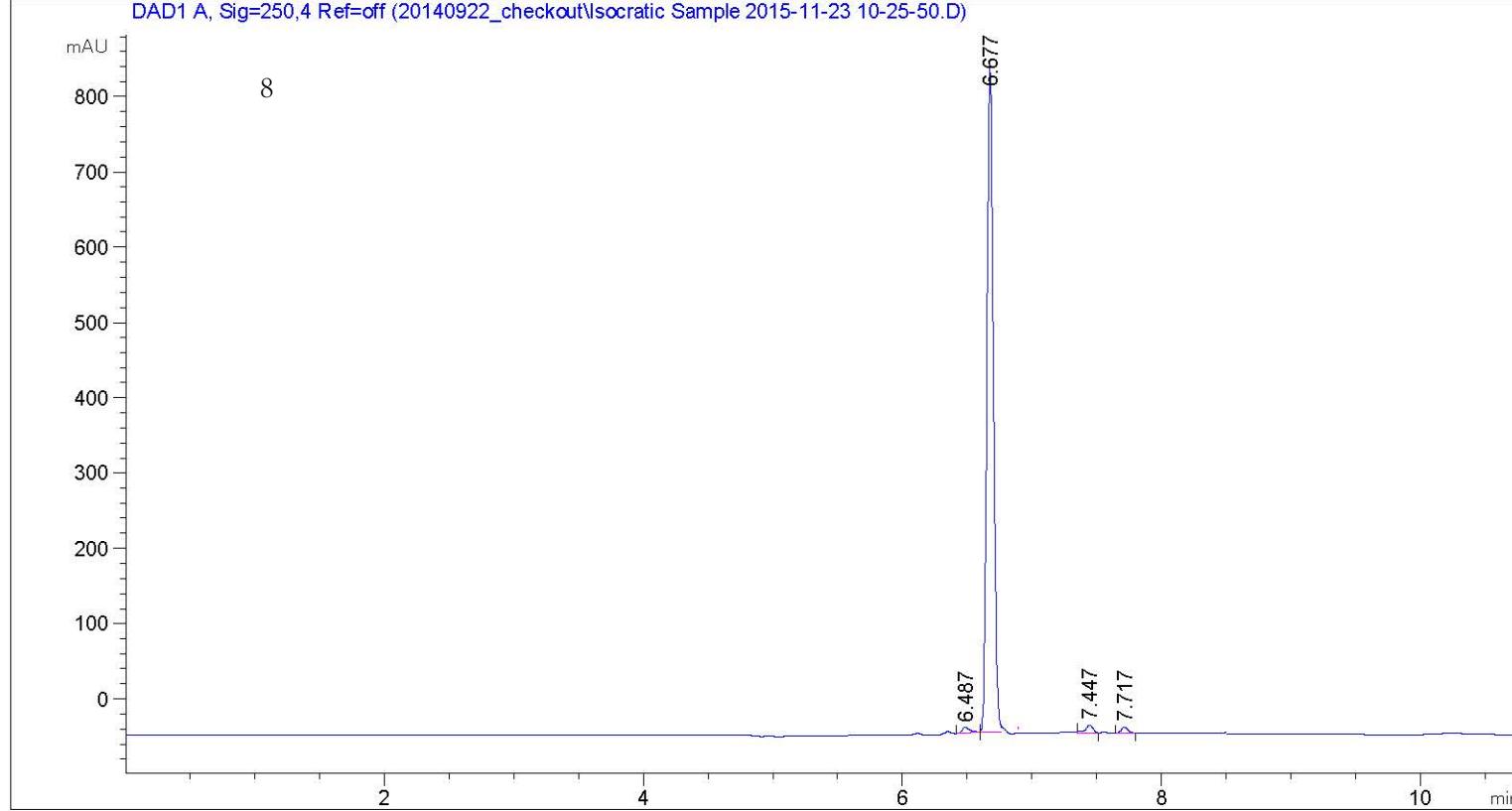
Signal 1: DAD1 A, Sig=250,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.732	BV E	0.0457	192.99501	66.86919	2.9140
2	6.829	VB R	0.0621	6273.55176	1587.80969	94.7232
3	8.115	BB	0.0738	5.12904	1.03541	0.0774
4	8.652	BB	0.3260	52.44033	2.52799	0.7918
5	9.247	BV	0.0901	64.97754	9.46888	0.9811
6	9.360	VB	0.0906	33.94433	5.30795	0.5125

Totals : 6623.03800 1673.01911

Sample Name: Isocratic Sample

=====
Acq. Operator : SYSTEM
Sample Operator : SYSTEM
Acq. Instrument : HPLC Location : 1
Injection Date : 11/23/2015 10:25:50 AM
Inj Volume : No inj
Method : C:\Chem32\1\Methods\DEF_LC.M
Last changed : 11/23/2015 9:00:54 AM by SYSTEM
Additional Info : Peak(s) manually integrated



=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

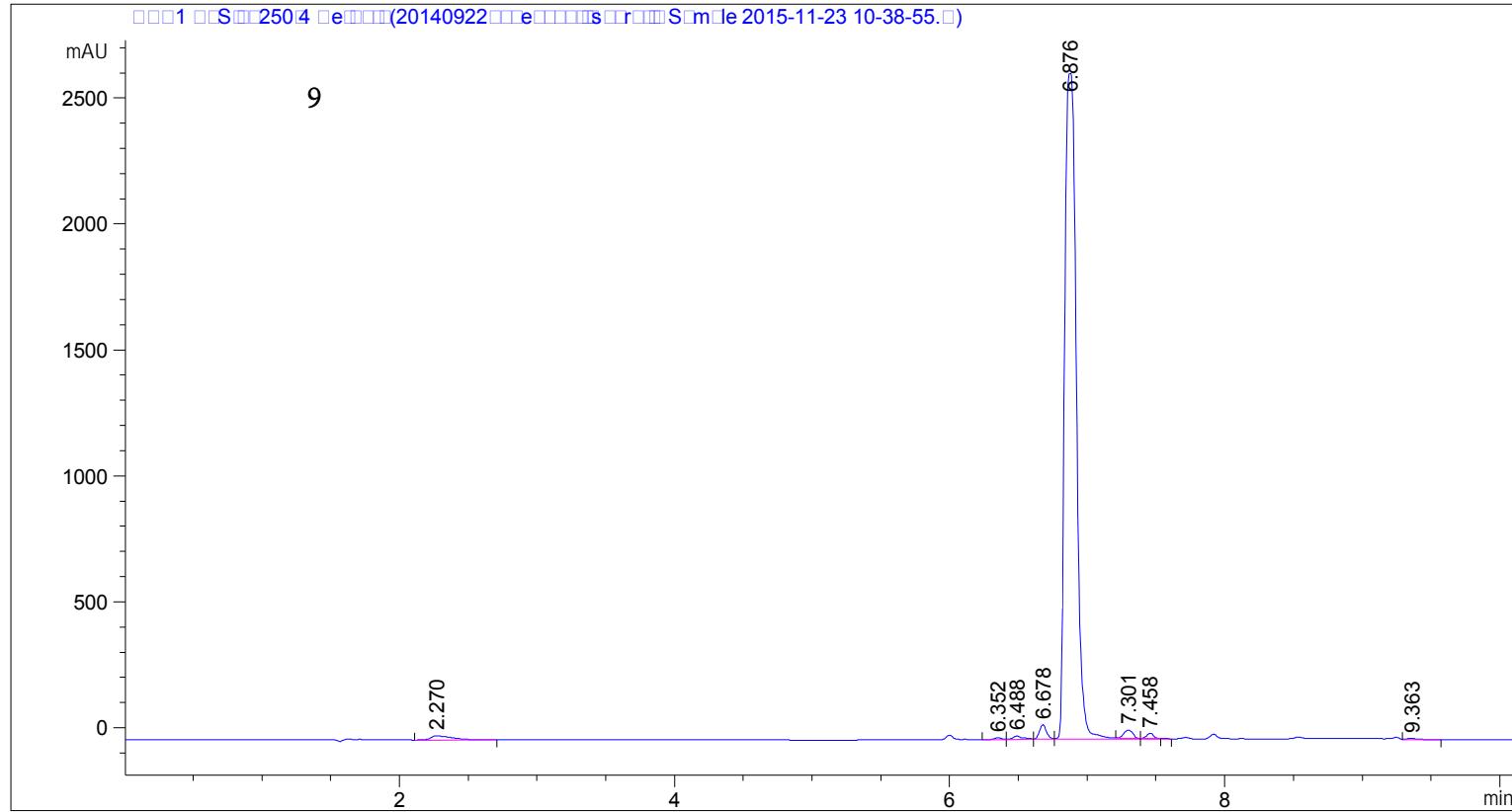
Signal 1: DAD1 A, Sig=250,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.487	BB	0.0660	34.06039	7.63676	0.9950
2	6.677	BV R	0.0545	3323.72900	882.31671	97.0928
3	7.447	VB	0.0569	39.54647	10.28591	1.1552
4	7.717	BB	0.0532	25.91555	7.71214	0.7570

Totals : 3423.25141 907.95152

Sample Name: Isocratic Sample

=====
 Acq. Operator : SYSTEM
 Sample Operator : SYSTEM
 Acq. Instrument : HPLC Location : 1
 Injection Date : 11/23/2015 10:38:55 AM
 Inj Volume : No inj
 Method : C:\Chem32\1\Methods\DEF_LC.M
 Last changed : 11/23/2015 9:00:54 AM by SYSTEM
 Additional Info : Peak(s) manually integrated



=====
 Area Percent Report
 =====

Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

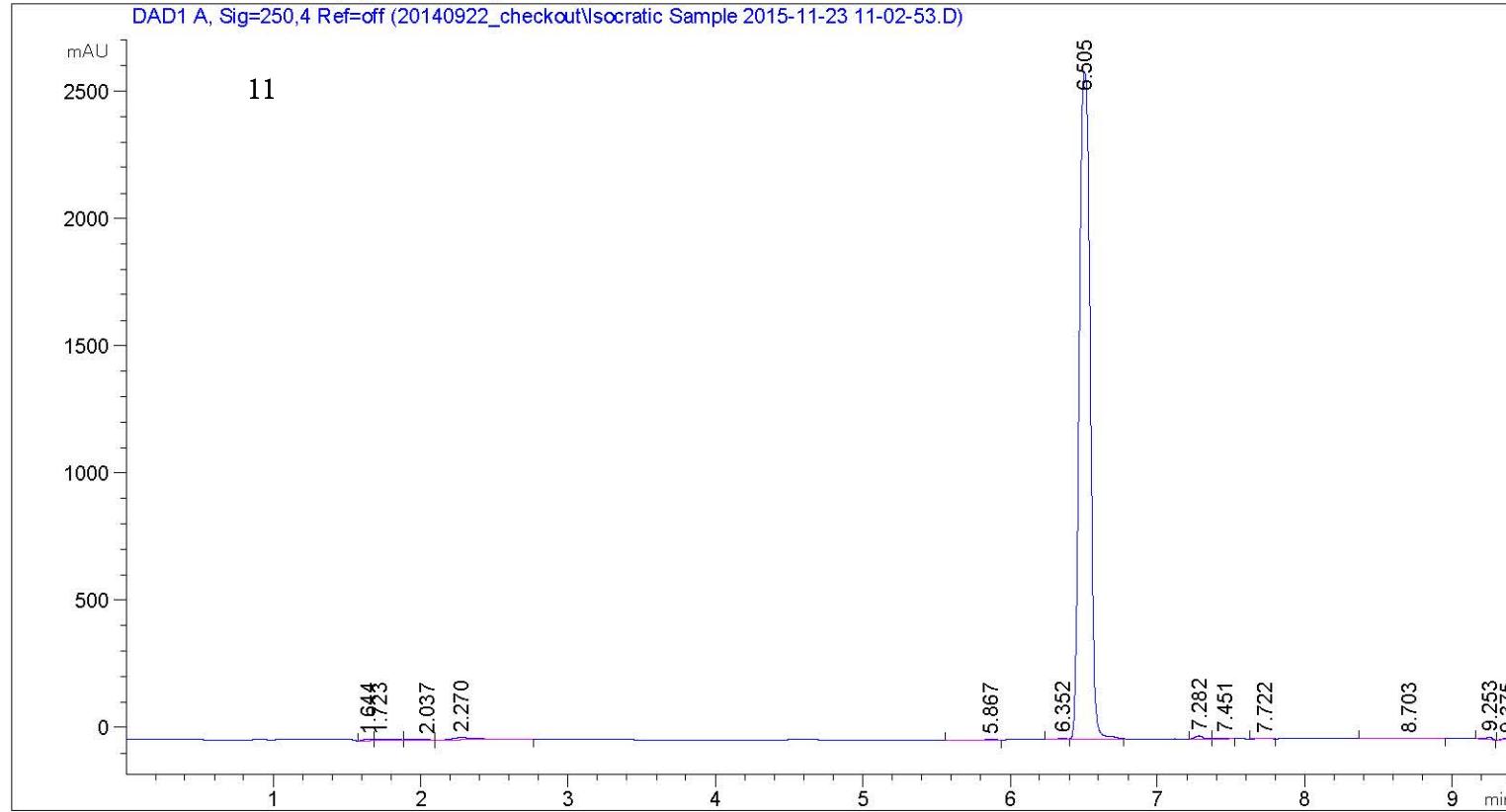
Signal 1: DAD1 A, Sig=250, 4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.270	BB	0.1517	192.66154	17.07070	1.1920
2	6.352	BV	0.0559	24.30444	6.76927	0.1504
3	6.488	VV	0.0767	70.43023	13.10474	0.4358
4	6.678	VV	0.0565	210.62202	57.80111	1.3032
5	6.876	VV R	0.0960	1.54147e4	2644.37476	95.3746
6	7.301	VV E	0.0755	149.64880	32.60897	0.9259
7	7.458	VV E	0.0556	78.04235	21.91191	0.4829
8	9.363	BB	0.1097	21.86939	3.28522	0.1353

Totals : 1.61623e4 2796.92668

Sample Name: Isocratic Sample

```
=====
Acq. Operator   : SYSTEM
Sample Operator : SYSTEM
Acq. Instrument : HPLC                               Location : 1
Injection Date  : 11/23/2015 11:02:53 AM
                                                Inj Volume : No inj
Method          : C:\Chem32\1\Methods\DEF_LC.M
Last changed    : 11/23/2015 9:00:54 AM by SYSTEM
Additional Info : Peak(s) manually integrated
```



```
=====
Area Percent Report
=====
```

```
Sorted By      : Signal
Multiplier     : 1.0000
Dilution      : 1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: DAD1 A, Sig=250,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.644	BV	0.0796	33.93282	6.86893	0.2468
2	1.723	VV	0.1173	54.18127	5.89222	0.3941
3	2.037	VB	0.1863	39.59730	3.29245	0.2880
4	2.270	BB	0.1684	122.54164	9.76694	0.8914
5	5.867	BB	0.0729	6.47753	1.24031	0.0471
6	6.352	BV E	0.0546	15.69003	4.50336	0.1141
7	6.505	VV R	0.0833	1.33357e4	2623.92944	97.0088
8	7.282	BV	0.0552	44.67350	12.65564	0.3250
9	7.451	VB	0.0596	15.31281	3.74989	0.1114

Sample Name: Isocratic Sample

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
10	7.722	BB	0.0541	7.35693	2.13847	0.0535
11	8.703	BB	0.2695	24.52579	1.37897	0.1784
12	9.253	BB	0.0483	32.28912	10.37633	0.2349
13	9.375	BBA	0.0947	14.62536	2.63551	0.1064

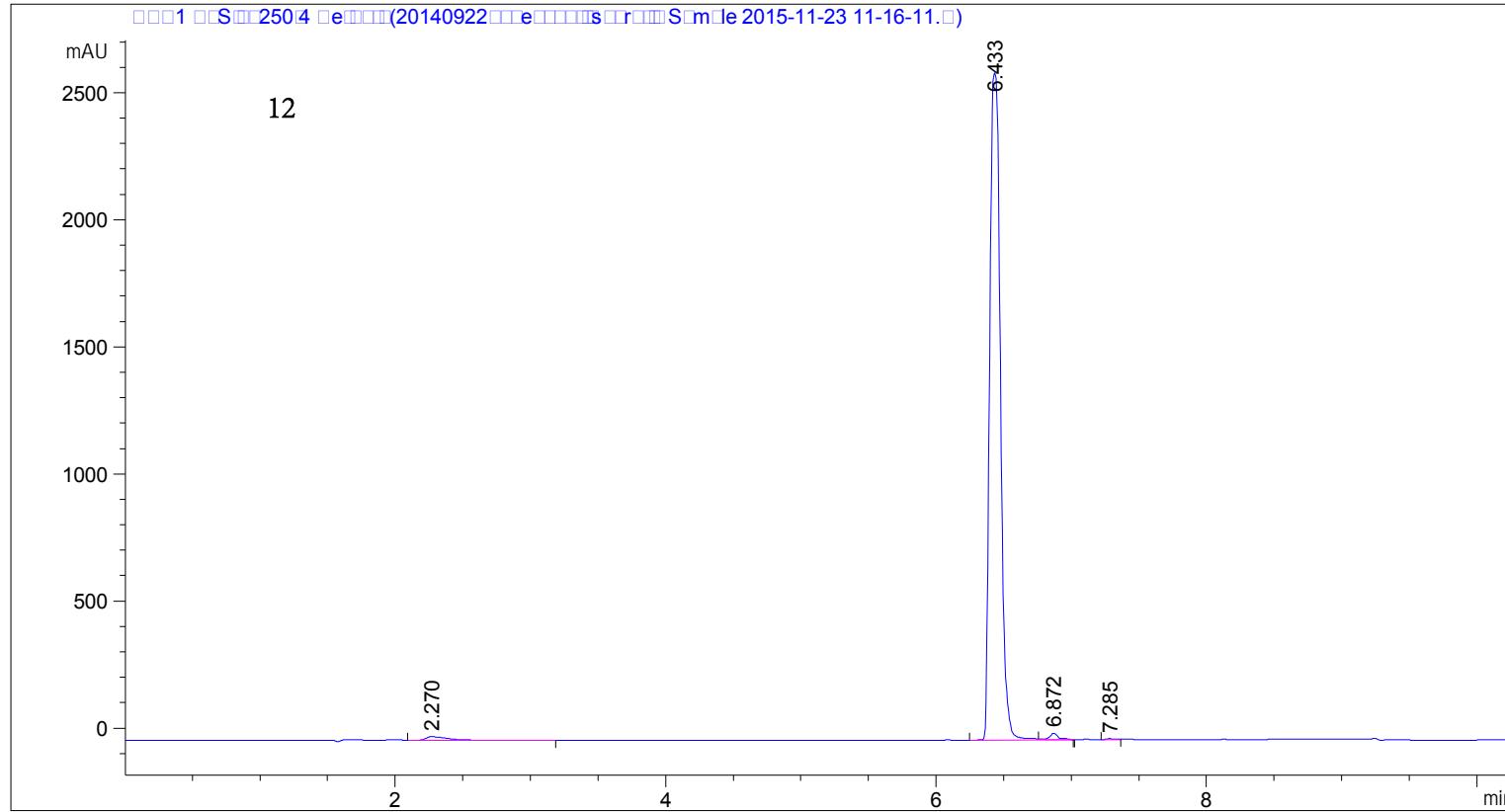
Totals : 1.37469e4 2688.42846

=====

*** End of Report ***

Sample Name: Isocratic Sample

```
=====
Acq. Operator : SYSTEM
Sample Operator : SYSTEM
Acq. Instrument : HPLC
Injection Date : 11/23/2015 11:16:11 AM
Location : 1
Inj Volume : No inj
Method : C:\Chem32\1\Methods\DEF_LC.M
Last changed : 11/23/2015 9:00:54 AM by SYSTEM
Additional Info : Peak(s) manually integrated
```



```
=====
Area Percent Report
=====
```

```
Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs
```

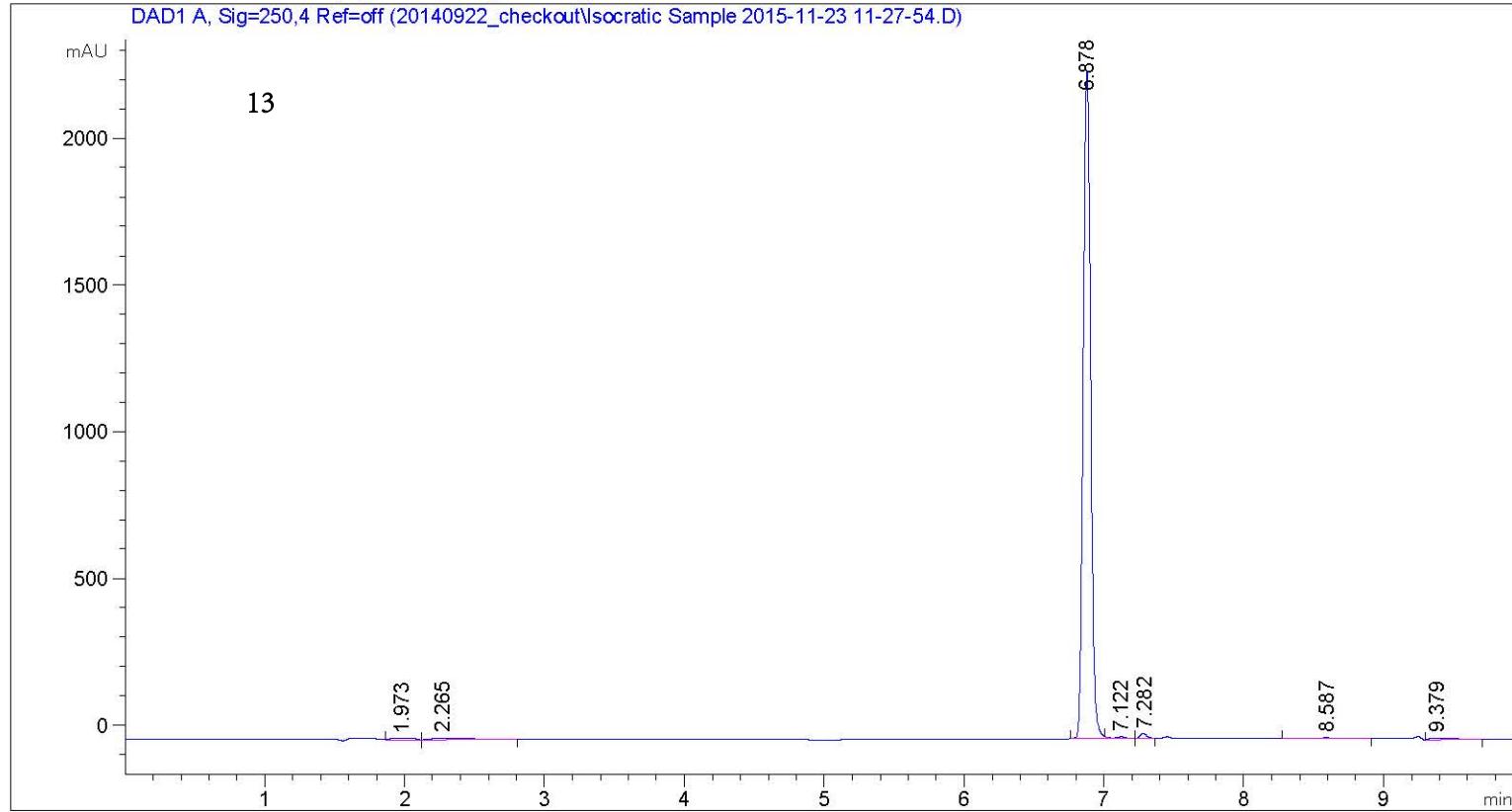
Signal 1: DAD1 A, Sig=250, 4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.270	BB	0.1712	201.20720	15.52212	1.3755
2	6.433	BVR	0.0896	1.43021e4	2625.41675	97.7728
3	6.872	VBE	0.0631	107.90790	25.63625	0.7377
4	7.285	BV	0.0640	16.67609	3.73960	0.1140

Totals : 1.46279e4 2670.31470

Sample Name: Isocratic Sample

```
=====
Acq. Operator   : SYSTEM
Sample Operator : SYSTEM
Acq. Instrument : HPLC                               Location : 1
Injection Date  : 11/23/2015 11:27:54 AM
                                                Inj Volume : No inj
Method          : C:\Chem32\1\Methods\DEF_LC.M
Last changed    : 11/23/2015 9:00:54 AM by SYSTEM
Additional Info : Peak(s) manually integrated
```



```
=====
                           Area Percent Report
=====
```

```
Sorted By      : Signal
Multiplier     : 1.0000
Dilution      : 1.0000
Use Multiplier & Dilution Factor with ISTDs
```

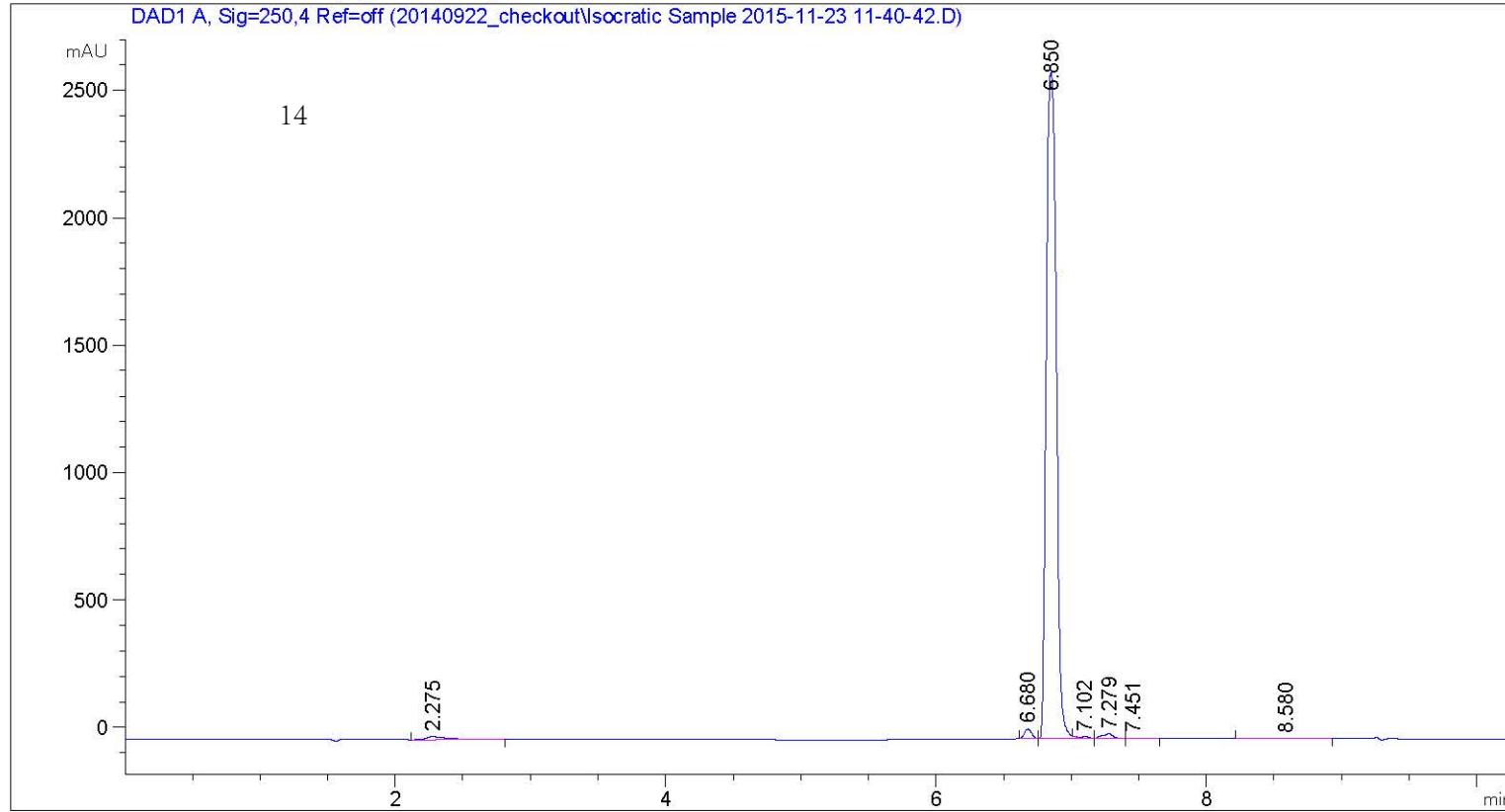
Signal 1: DAD1 A, Sig=250,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.973	VB	0.1808	62.23008	4.69128	0.7130
2	2.265	BB	0.1963	94.60788	6.25941	1.0840
3	6.878	BV R	0.0589	8408.97363	2288.50757	96.3478
4	7.122	VB E	0.0661	22.29380	4.80987	0.2554
5	7.282	BV	0.0526	52.15508	15.77667	0.5976
6	8.587	BB	0.1948	25.51794	1.78496	0.2924
7	9.379	BB	0.1582	61.95139	5.63868	0.7098

Totals : 8727.72980 2327.46845

Sample Name: Isocratic Sample

```
=====
Acq. Operator   : SYSTEM
Sample Operator : SYSTEM
Acq. Instrument : HPLC           Location : 1
Injection Date  : 11/23/2015 11:40:42 AM
                                Inj Volume : No inj
Method          : C:\Chem32\1\Methods\DEF_LC.M
Last changed    : 11/23/2015 9:00:54 AM by SYSTEM
Additional Info : Peak(s) manually integrated
```



```
=====
                        Area Percent Report
=====
```

```
Sorted By      : Signal
Multiplier     : 1.0000
Dilution      : 1.0000
Use Multiplier & Dilution Factor with ISTDs
```

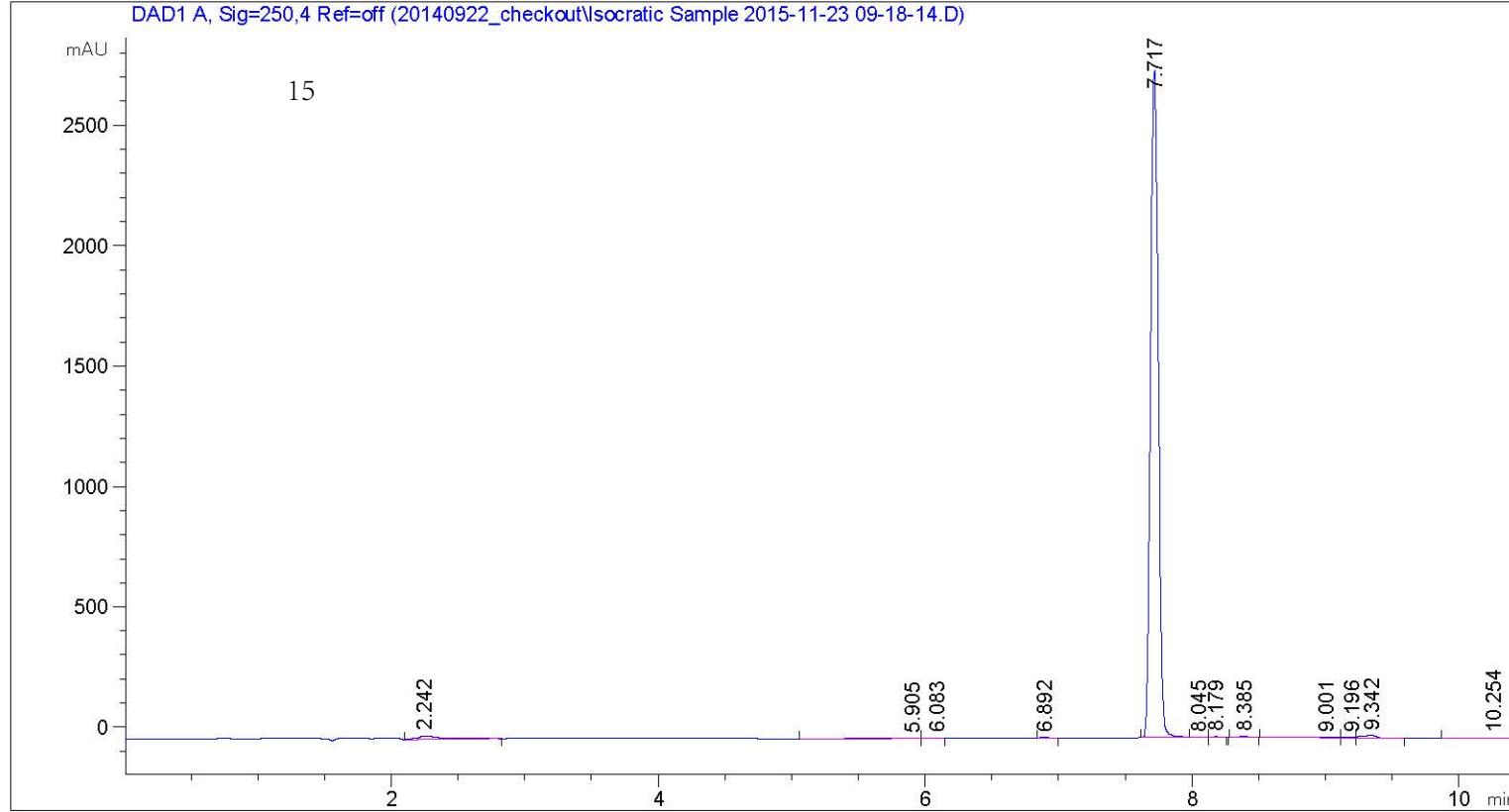
Signal 1: DAD1 A, Sig=250,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.275	BB	0.1680	150.24184	11.84628	1.0777
2	6.680	VB	0.0569	137.25691	39.18944	0.9846
3	6.850	BV R	0.0841	1.34674e4	2613.84839	96.6060
4	7.102	VV E	0.0674	28.71290	6.04468	0.2060
5	7.279	VV E	0.0802	116.34489	19.89294	0.8346
6	7.451	VB E	0.0620	15.06252	3.51379	0.1080
7	8.580	BB	0.2565	25.52819	1.38866	0.1831

Totals : 1.39406e4 2695.72418

Sample Name: Isocratic Sample

```
=====
Acq. Operator   : SYSTEM
Sample Operator : SYSTEM
Acq. Instrument : HPLC                               Location : 1
Injection Date  : 11/23/2015 9:18:14 AM
                                                Inj Volume : No inj
Method          : C:\Chem32\1\Methods\DEF_LC.M
Last changed    : 11/23/2015 9:00:54 AM by SYSTEM
Additional Info : Peak(s) manually integrated
```



```
=====
Area Percent Report
=====
```

```
Sorted By      : Signal
Multiplier     : 1.0000
Dilution      : 1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: DAD1 A, Sig=250,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.242	BB	0.1712	176.21985	13.59750	1.5132
2	5.905	BV	0.4540	47.52156	1.26006	0.4081
3	6.083	VB	0.0649	7.80441	1.79056	0.0670
4	6.892	VB	0.0559	7.11439	1.97917	0.0611
5	7.717	BV R	0.0650	1.11543e4	2770.62915	95.7817
6	8.045	VV E	0.0676	7.86546	1.71065	0.0675
7	8.179	VB E	0.0666	11.39242	2.62498	0.0978
8	8.385	BB	0.0655	21.60625	5.09020	0.1855
9	9.001	BV	0.2717	68.41373	3.44523	0.5875

Sample Name: Isocratic Sample

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
10	9.196	VV	0.0803	27.28393	4.80340	0.2343
11	9.342	VB	0.1072	92.52674	12.38306	0.7945
12	10.254	BBA	0.2581	23.50101	1.47302	0.2018

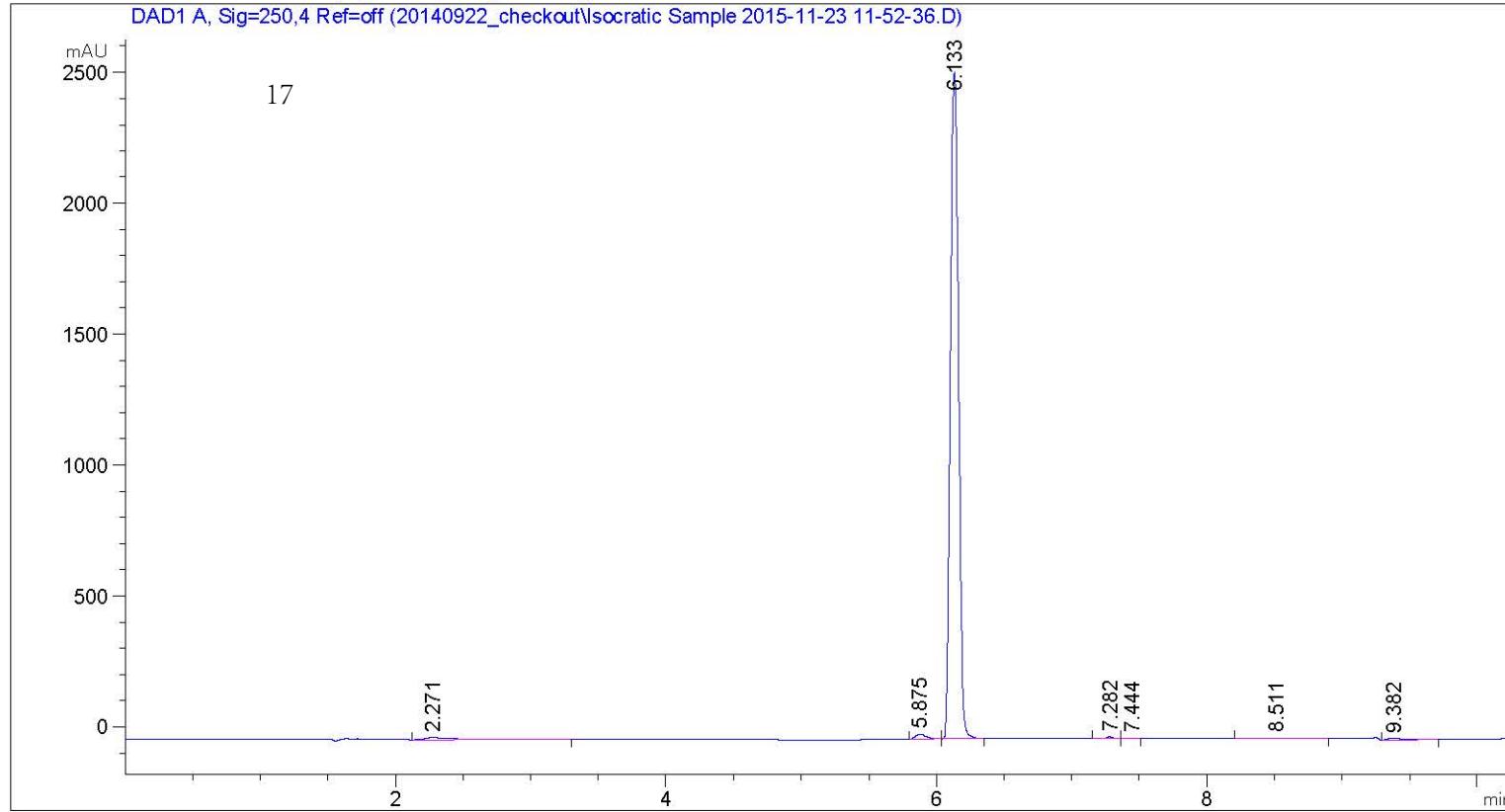
Totals : 1.16456e4 2820.78698

=====

*** End of Report ***

Sample Name: Isocratic Sample

```
=====
Acq. Operator   : SYSTEM
Sample Operator : SYSTEM
Acq. Instrument : HPLC                               Location : 1
Injection Date  : 11/23/2015 11:52:36 AM
                                                Inj Volume : No inj
Method          : C:\Chem32\1\Methods\DEF_LC.M
Last changed    : 11/23/2015 9:00:54 AM by SYSTEM
Additional Info : Peak(s) manually integrated
```



```
=====
Area Percent Report
=====
```

```
Sorted By      : Signal
Multiplier     : 1.0000
Dilution      : 1.0000
Use Multiplier & Dilution Factor with ISTDs
```

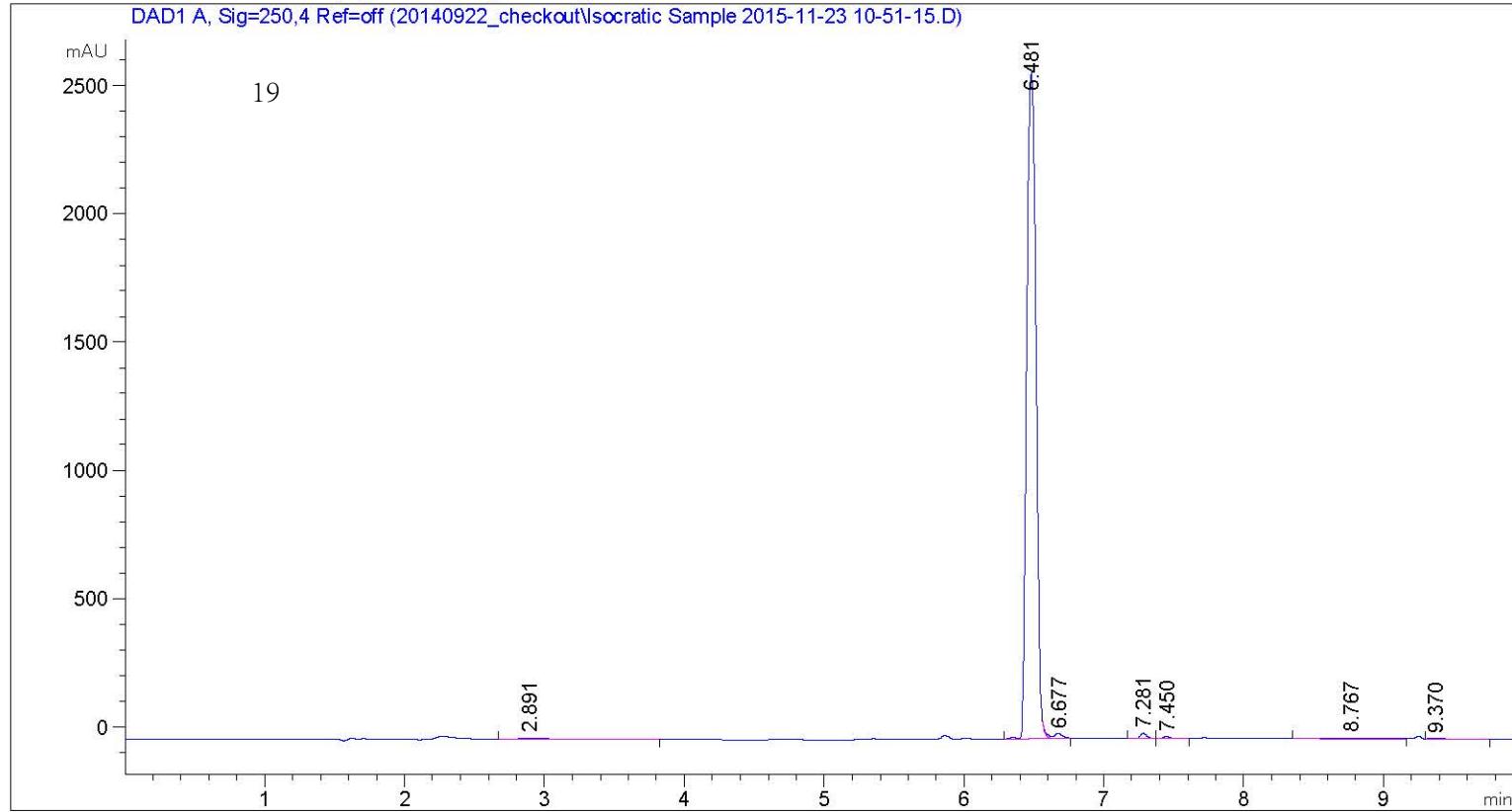
Signal 1: DAD1 A, Sig=250,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.271	BB	0.2220	163.89236	9.46781	1.4682
2	5.875	BB	0.0864	107.87881	18.96727	0.9664
3	6.133	BV	0.0713	1.07631e4	2545.05566	96.4217
4	7.282	BV	0.0626	28.21264	6.77204	0.2527
5	7.444	VB	0.0723	9.09362	1.76077	0.0815
6	8.511	BB	0.2142	24.41945	1.45173	0.2188
7	9.382	BB	0.1679	65.93641	5.66000	0.5907

Totals : 1.11625e4 2589.13529

Sample Name: Isocratic Sample

```
=====
Acq. Operator   : SYSTEM
Sample Operator : SYSTEM
Acq. Instrument : HPLC                               Location : 1
Injection Date  : 11/23/2015 10:51:15 AM
                                                Inj Volume : No inj
Method          : C:\Chem32\1\Methods\DEF_LC.M
Last changed    : 11/23/2015 9:00:54 AM by SYSTEM
Additional Info : Peak(s) manually integrated
```



```
=====
                           Area Percent Report
=====
```

```
Sorted By      : Signal
Multiplier     : 1.0000
Dilution      : 1.0000
Use Multiplier & Dilution Factor with ISTDs
```

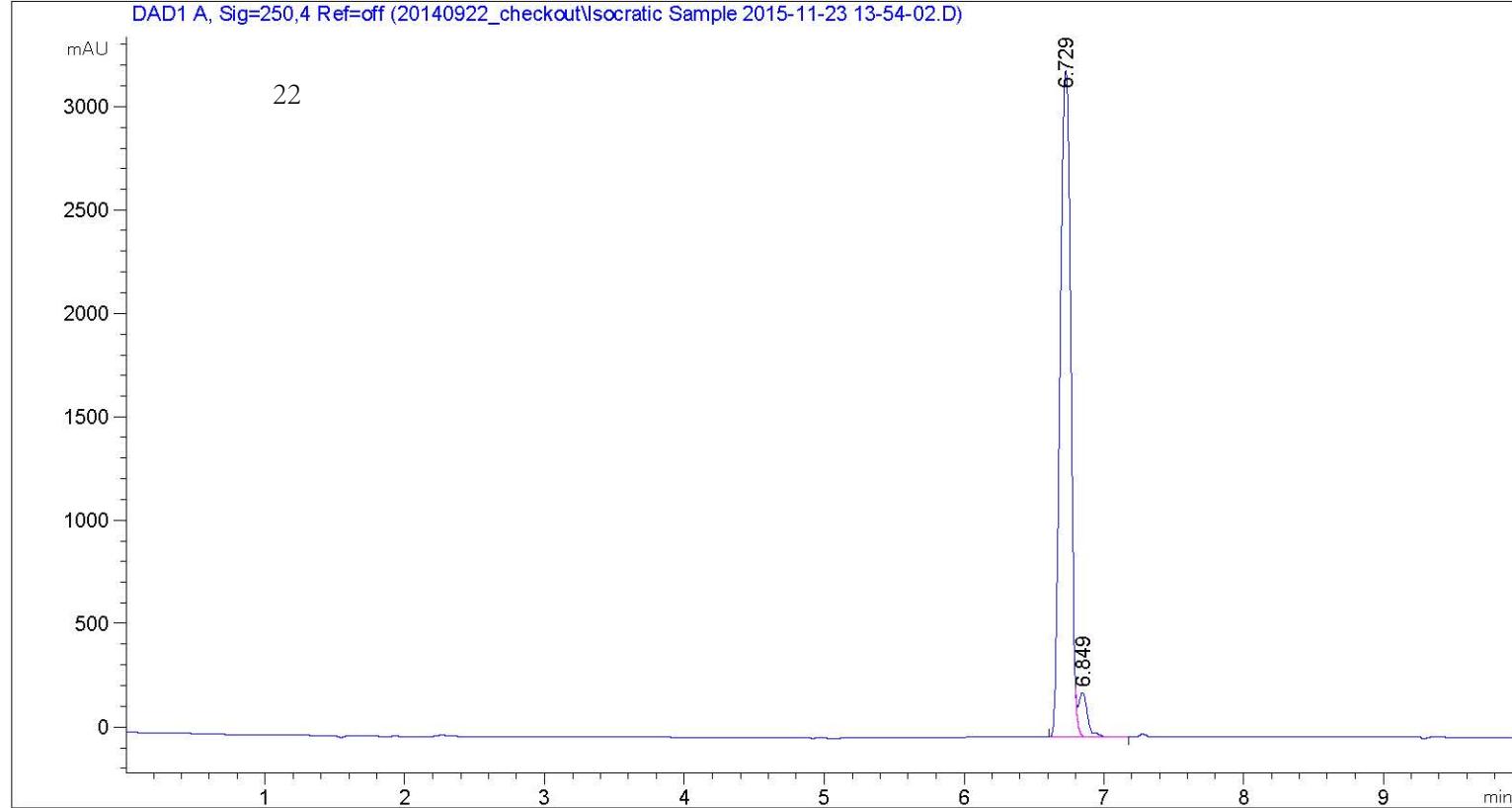
Signal 1: DAD1 A, Sig=250,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.891	BB	0.1448	50.82417	5.16587	0.4151
2	6.481	VV R	0.0751	1.18362e4	2596.46875	96.6819
3	6.677	VB E	0.0740	91.35598	17.19945	0.7462
4	7.281	BV	0.0529	71.95615	20.53755	0.5878
5	7.450	VB	0.0557	27.34380	7.29252	0.2234
6	8.767	BV	0.4619	130.93163	3.69045	1.0695
7	9.370	BB	0.1309	33.80587	3.98733	0.2761

Totals : 1.22424e4 2654.34191

Sample Name: Isocratic Sample

=====
Acq. Operator : SYSTEM
Sample Operator : SYSTEM
Acq. Instrument : HPLC Location : 1
Injection Date : 11/23/2015 1:54:03 PM
Inj Volume : No inj
Method : C:\Chem32\1\Methods\DEF_LC.M
Last changed : 11/23/2015 1:52:23 PM by SYSTEM
(modified after loading)
Additional Info : Peak(s) manually integrated



=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=250,4 Ref=off

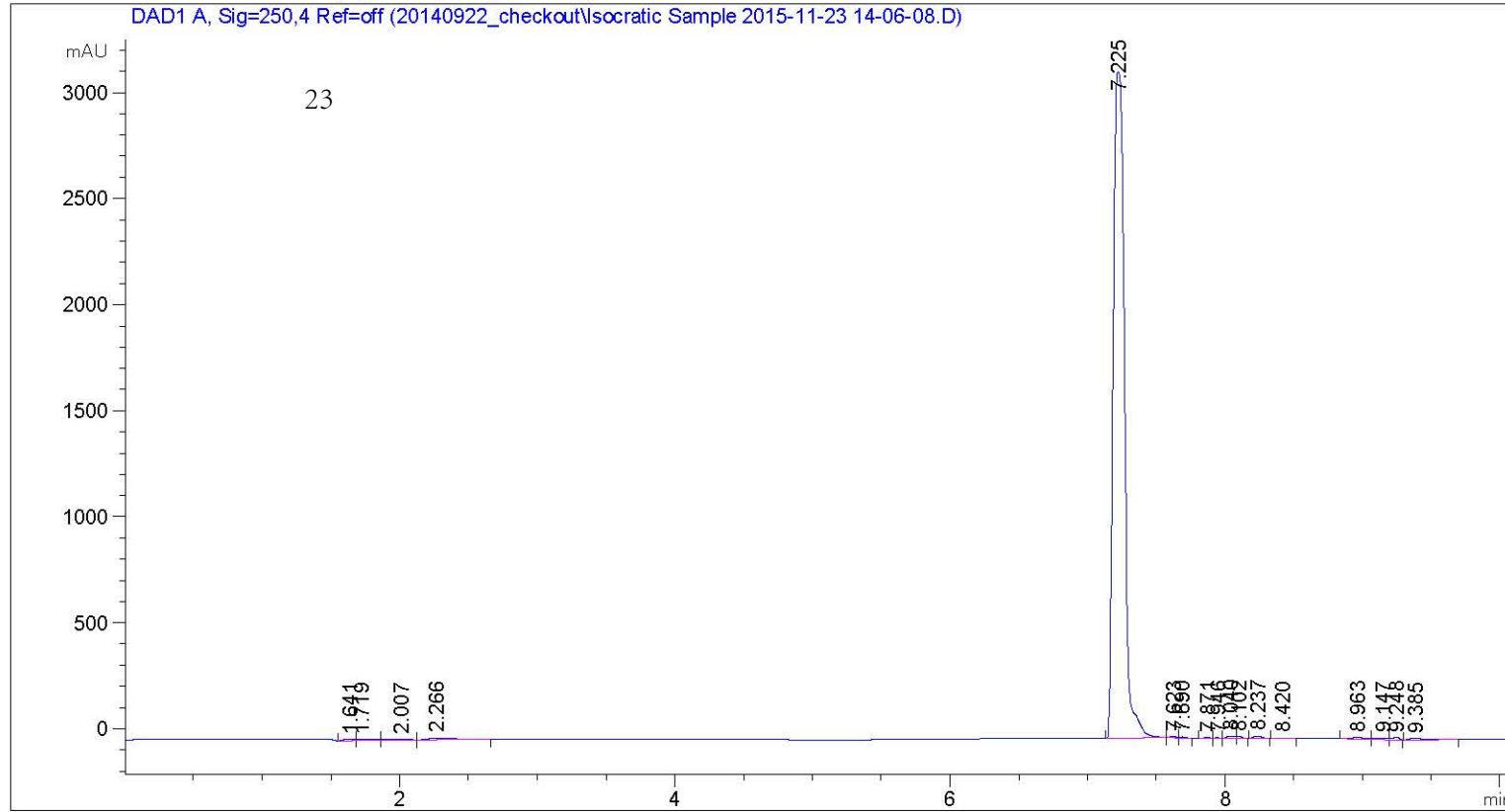
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.729	BV R	0.0847	1.68057e4	3228.26318	94.9564
2	6.849	VB E	0.0659	892.63202	208.72389	5.0436

Totals : 1.76983e4 3436.98708

=====
*** End of Report ***

Sample Name: Isocratic Sample

```
=====
Acq. Operator   : SYSTEM
Sample Operator : SYSTEM
Acq. Instrument : HPLC                               Location : 1
Injection Date  : 11/23/2015 2:06:08 PM
                                                Inj Volume : No inj
Method          : C:\Chem32\1\Methods\DEF_LC.M
Last changed    : 11/23/2015 1:52:23 PM by SYSTEM
Additional Info : Peak(s) manually integrated
```



```
=====
Area Percent Report
=====
```

```
Sorted By      : Signal
Multiplier     : 1.0000
Dilution      : 1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: DAD1 A, Sig=250,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.641	BV	0.0826	50.09356	8.51895	0.2738
2	1.719	VV	0.1120	63.14124	7.22389	0.3451
3	2.007	VB	0.1773	67.36708	4.64365	0.3682
4	2.266	BB	0.1643	112.82310	9.12488	0.6166
5	7.225	BB	0.0933	1.75799e4	3140.22949	96.0793
6	7.623	BV	0.0488	17.63625	5.59204	0.0964
7	7.690	VB	0.0527	16.54796	4.99190	0.0904
8	7.871	BV	0.0506	17.28793	5.22266	0.0945
9	7.946	VW	0.0502	12.77369	3.90231	0.0698

Sample Name: Isocratic Sample

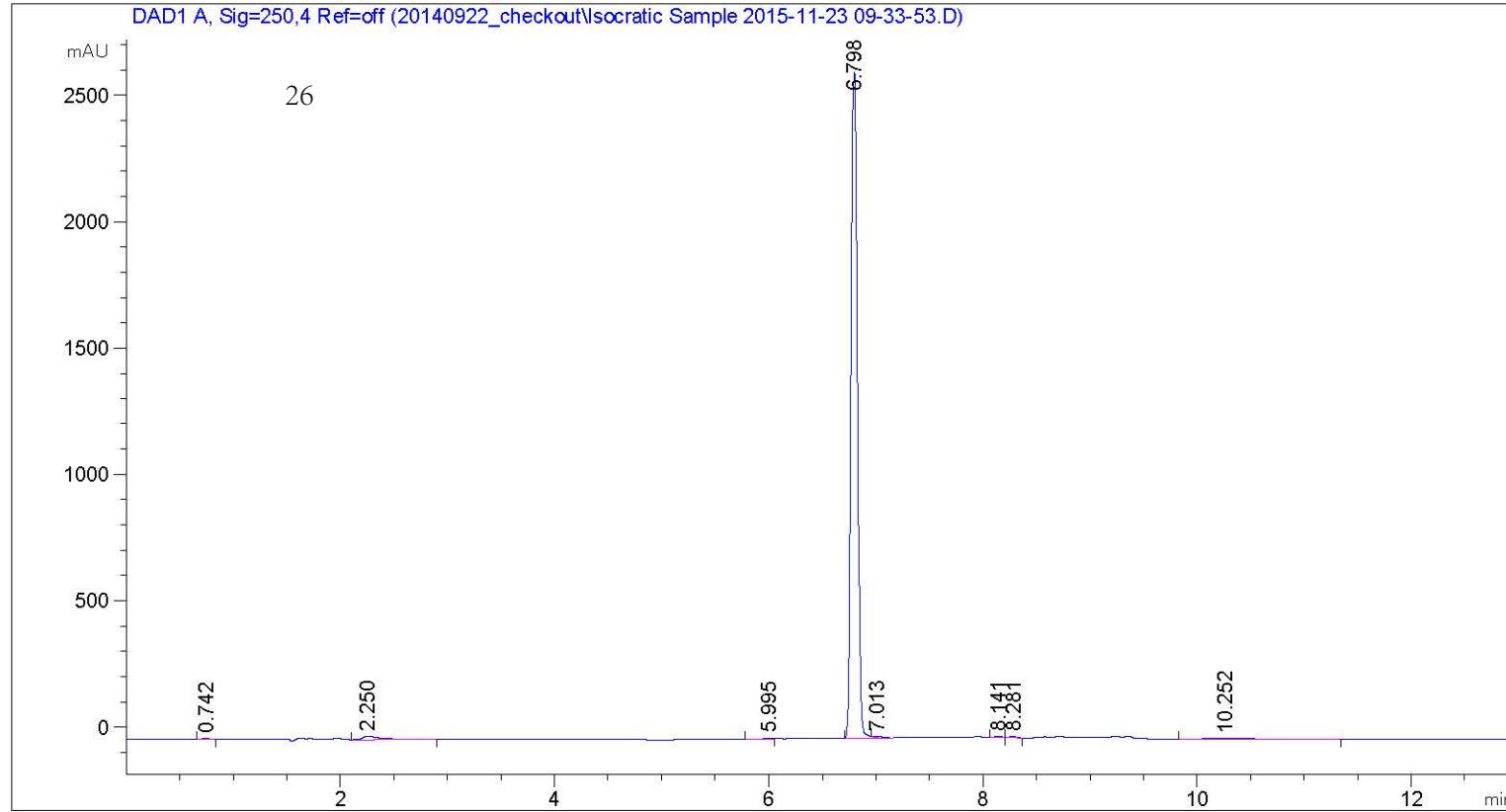
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
10	8.040	VV	0.0594	46.91190	12.06303	0.2564
11	8.102	VB	0.0463	20.32620	6.90995	0.1111
12	8.237	BB	0.0614	45.08829	11.59140	0.2464
13	8.420	BV	0.0919	8.37146	1.39647	0.0458
14	8.963	BV	0.0995	61.10505	8.74404	0.3340
15	9.147	VV	0.0959	57.01537	8.32851	0.3116
16	9.248	VB	0.0577	50.32167	12.83670	0.2750
17	9.385	BB	0.1683	70.57056	5.95506	0.3857

Totals : 1.82973e4 3257.27494

=====*** End of Report ***=====

Sample Name: Isocratic Sample

```
=====
Acq. Operator   : SYSTEM
Sample Operator : SYSTEM
Acq. Instrument : HPLC                               Location : 1
Injection Date  : 11/23/2015 9:33:53 AM
                                                Inj Volume : No inj
Method          : C:\Chem32\1\Methods\DEF_LC.M
Last changed    : 11/23/2015 9:00:54 AM by SYSTEM
Additional Info : Peak(s) manually integrated
```



```
=====
                           Area Percent Report
=====
```

```
Sorted By      : Signal
Multiplier     : 1.0000
Dilution      : 1.0000
Use Multiplier & Dilution Factor with ISTDs
```

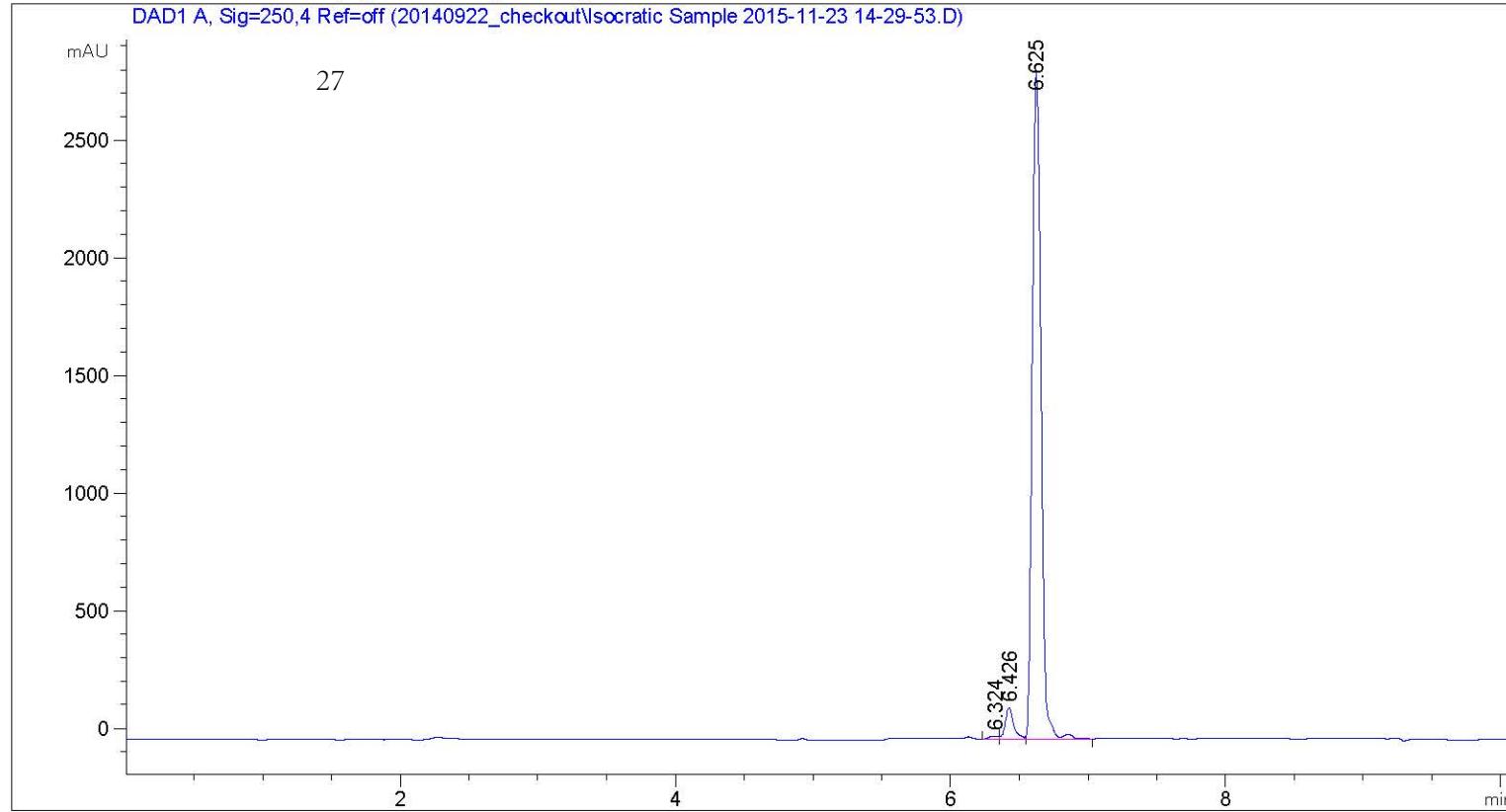
Signal 1: DAD1 A, Sig=250,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.742	BB	0.0541	9.61003	2.79853	0.0859
2	2.250	BB	0.1731	175.00810	13.16705	1.5636
3	5.995	BV	0.0580	11.83317	3.13857	0.1057
4	6.798	BV R	0.0680	1.08789e4	2645.26147	97.1991
5	7.013	VB E	0.0981	30.61336	4.35177	0.2735
6	8.141	BV	0.0743	17.17974	3.55785	0.1535
7	8.281	VB	0.0765	18.88062	3.64338	0.1687
8	10.252	BBA	0.3862	50.36755	1.71725	0.4500

Totals: 1.11924e4 2677.63588

Sample Name: Isocratic Sample

=====
Acq. Operator : SYSTEM
Sample Operator : SYSTEM
Acq. Instrument : HPLC Location : 1
Injection Date : 11/23/2015 2:29:53 PM
Inj Volume : No inj
Method : C:\Chem32\1\Methods\DEF_LC.M
Last changed : 11/23/2015 1:52:23 PM by SYSTEM
Additional Info : Peak(s) manually integrated



=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=250,4 Ref=off

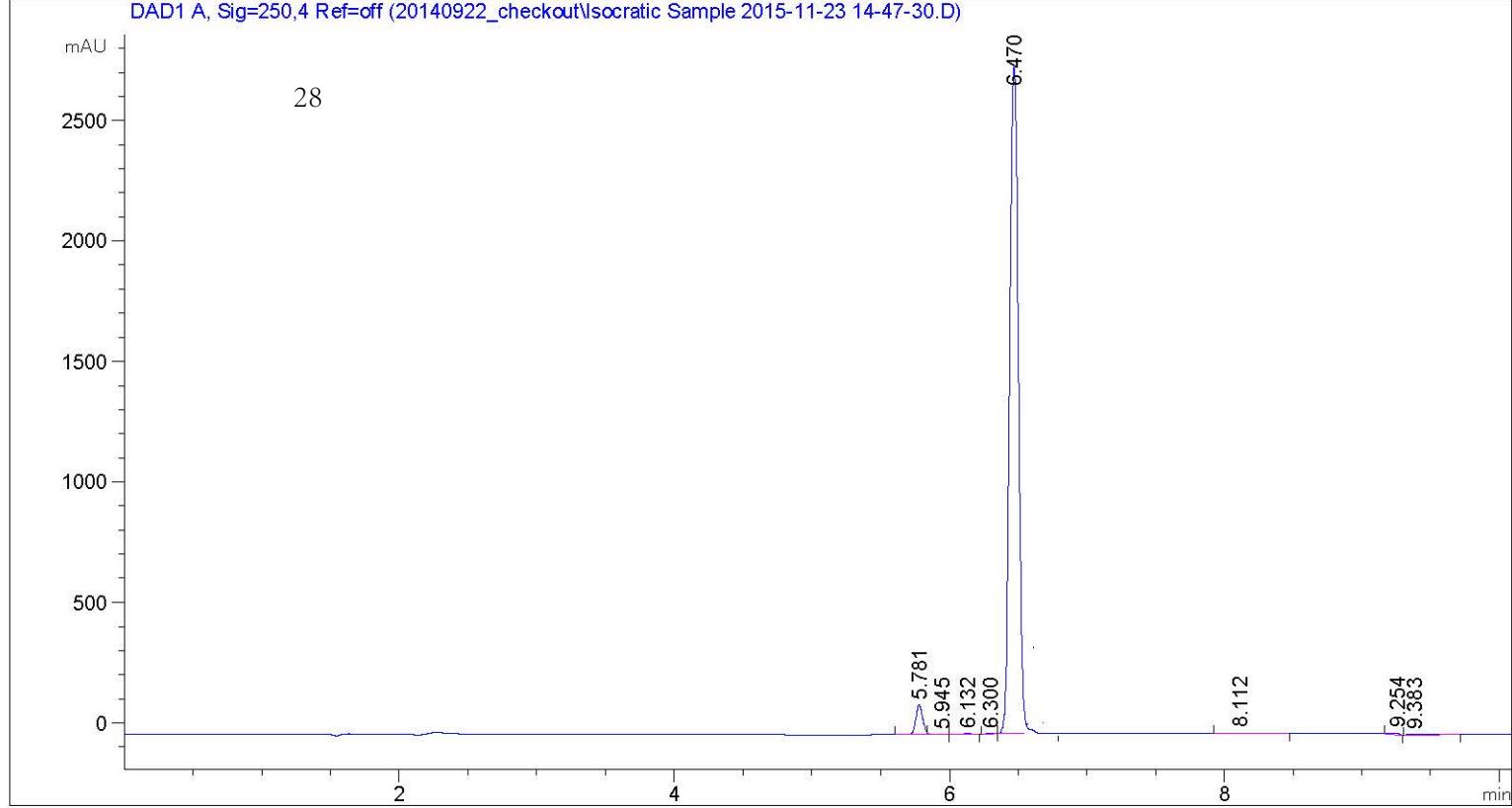
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.324	BV E	0.0820	64.28326	12.92804	0.4879
2	6.426	VV E	0.0627	562.25610	134.63994	4.2671
3	6.625	VV R	0.0712	1.25499e4	2836.61182	95.2450

Totals : 1.31764e4 2984.17980

=====
*** End of Report ***

Sample Name: Isocratic Sample

```
=====
Acq. Operator   : SYSTEM
Sample Operator : SYSTEM
Acq. Instrument : HPLC                               Location : 1
Injection Date  : 11/23/2015 2:47:30 PM
                                                Inj Volume : No inj
Method          : C:\Chem32\1\Methods\DEF_LC.M
Last changed    : 11/23/2015 1:52:23 PM by SYSTEM
Additional Info : Peak(s) manually integrated
```



```
=====
Area Percent Report
=====
```

```
Sorted By      : Signal
Multiplier     : 1.0000
Dilution      : 1.0000
Use Multiplier & Dilution Factor with ISTDs
```

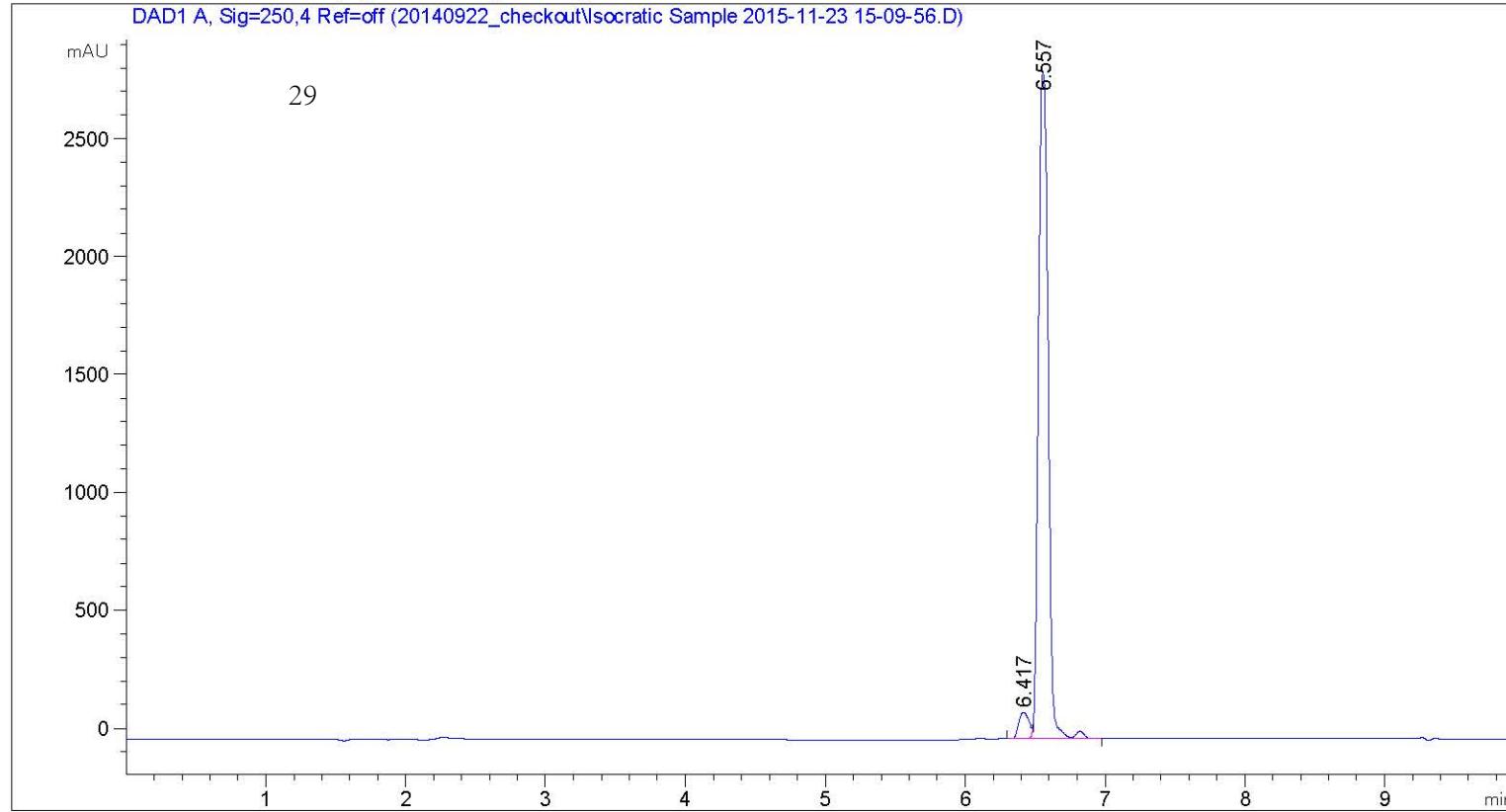
Signal 1: DAD1 A, Sig=250,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.781	BV R	0.0539	417.44977	122.06186	2.9553
2	5.945	VV E	0.0782	6.00018	1.05761	0.0425
3	6.132	VB E	0.0731	16.41354	3.35444	0.1162
4	6.300	BB	0.0582	6.17198	1.70788	0.0437
5	6.470	BV R	0.0708	1.35526e4	2774.21948	95.9458
6	8.112	VB	0.1578	26.97421	2.21905	0.1910
7	9.254	BB	0.0498	30.28040	8.88518	0.2144
8	9.383	BB	0.1715	69.37580	5.80218	0.4911

Totals: 1.41252e4 2919.30767

Sample Name: Isocratic Sample

=====
Acq. Operator : SYSTEM
Sample Operator : SYSTEM
Acq. Instrument : HPLC Location : 1
Injection Date : 11/23/2015 3:09:56 PM
Inj Volume : No inj
Method : C:\Chem32\1\Methods\DEF_LC.M
Last changed : 11/23/2015 1:52:23 PM by SYSTEM
Additional Info : Peak(s) manually integrated



=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=250,4 Ref=off

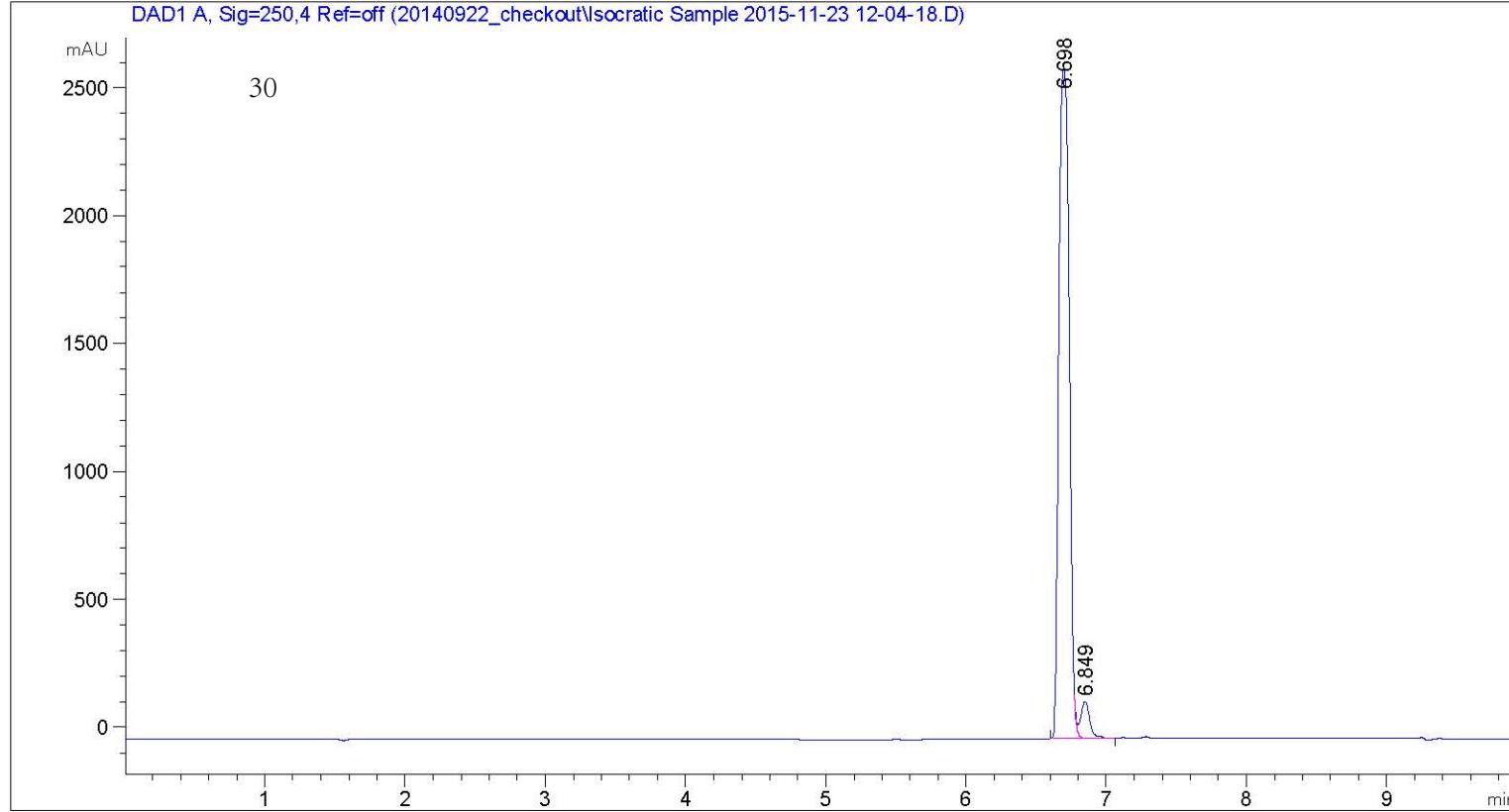
Peak	RetTime	Type	Width	Area	Height	Area %
#	[min]		[min]	[mAU*s]	[mAU]	%
1	6.417	BV E	0.0845	558.03223	111.35776	3.9022
2	6.557	VV R	0.0801	1.37424e4	2830.98901	96.0978

Totals : 1.43004e4 2942.34677

=====
*** End of Report ***

Sample Name: Isocratic Sample

=====
Acq. Operator : SYSTEM
Sample Operator : SYSTEM
Acq. Instrument : HPLC Location : 1
Injection Date : 11/23/2015 12:04:18 PM
Inj Volume : No inj
Method : C:\Chem32\1\Methods\DEF_LC.M
Last changed : 11/23/2015 9:00:54 AM by SYSTEM
Additional Info : Peak(s) manually integrated



=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=250,4 Ref=off

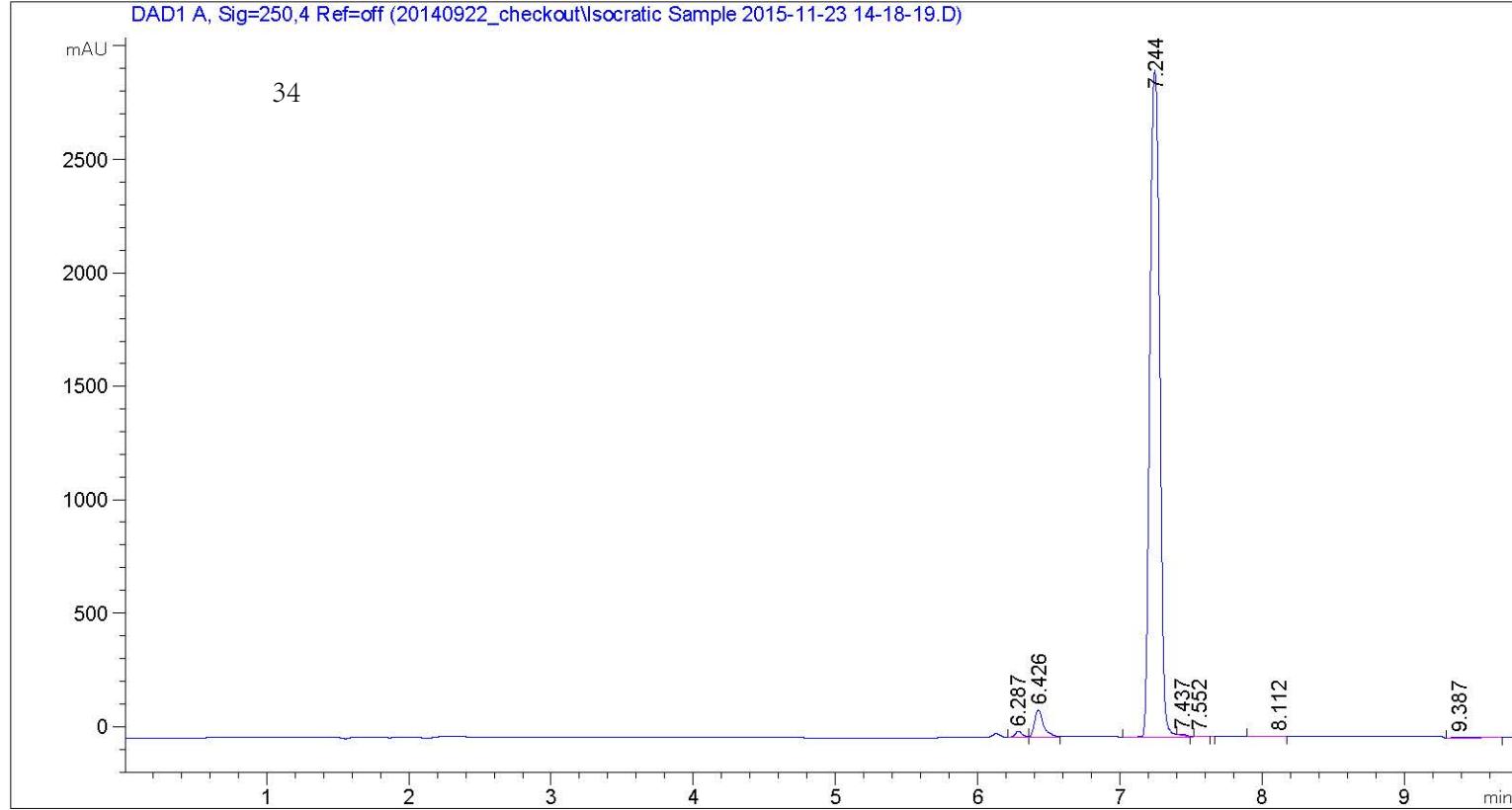
Peak	RetTime	Type	Width	Area	Height	Area %
#	[min]		[min]	[mAU*s]	[mAU]	%
1	6.698	BV R	0.0861	1.34351e4	2610.17627	95.4195
2	6.849	VB E	0.0665	644.94122	143.28596	4.5805

Totals : 1.40800e4 2753.46223

=====
*** End of Report ***

Sample Name: Isocratic Sample

```
=====
Acq. Operator   : SYSTEM
Sample Operator : SYSTEM
Acq. Instrument : HPLC           Location : 1
Injection Date  : 11/23/2015 2:18:19 PM
                                Inj Volume : No inj
Method          : C:\Chem32\1\Methods\DEF_LC.M
Last changed    : 11/23/2015 1:52:23 PM by SYSTEM
Additional Info : Peak(s) manually integrated
```



```
=====
                        Area Percent Report
=====
```

```
Sorted By      : Signal
Multiplier     : 1.0000
Dilution      : 1.0000
Use Multiplier & Dilution Factor with ISTDs
```

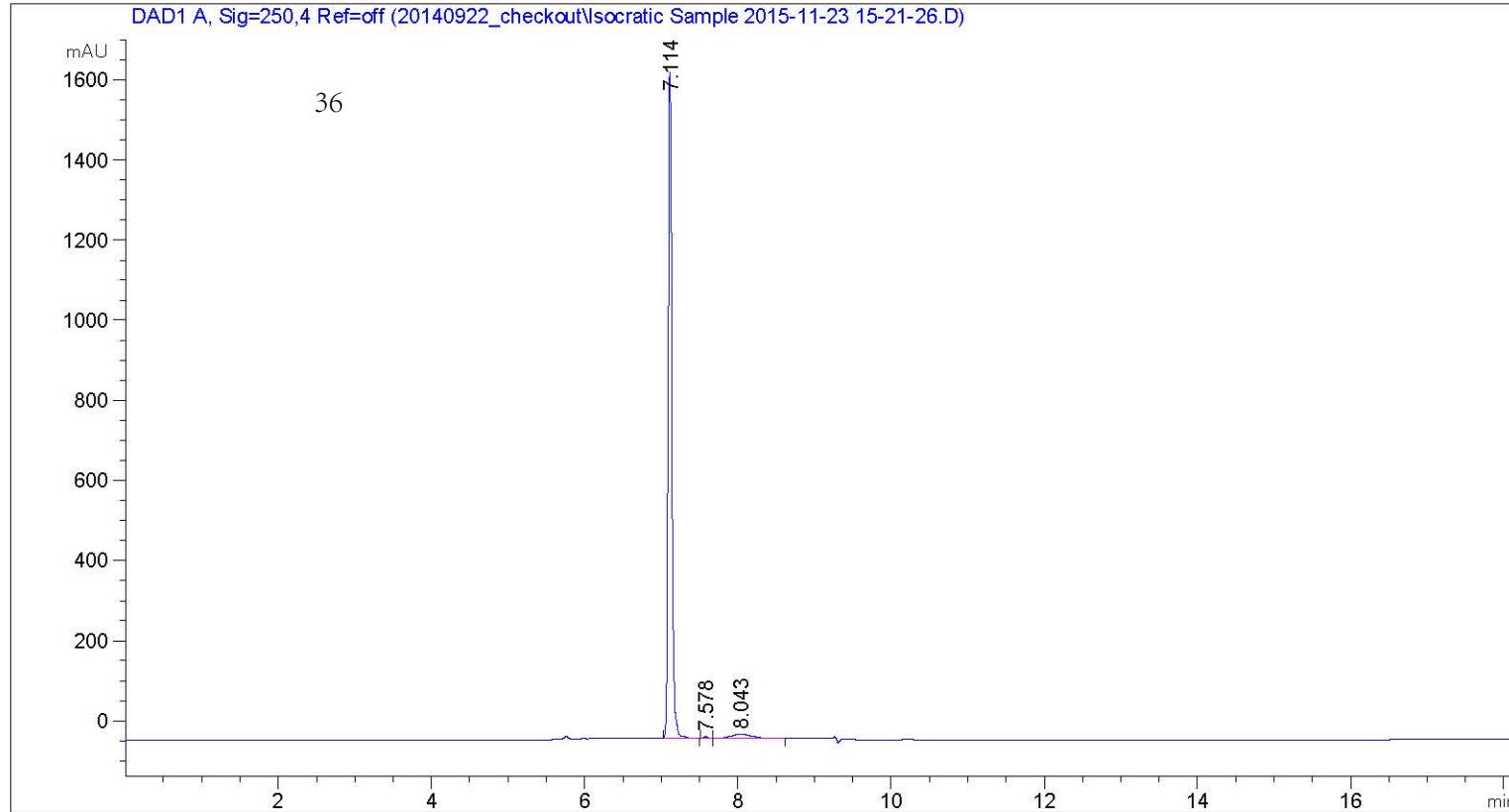
Signal 1: DAD1 A, Sig=250,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.287	BV	0.0566	94.36362	25.85353	0.6399
2	6.426	VV	0.0651	531.21619	121.27173	3.6021
3	7.244	BV R	0.0796	1.40167e4	2940.25439	95.0452
4	7.437	VV E	0.0516	10.89211	3.21137	0.0739
5	7.552	VB E	0.0549	5.34480	1.45390	0.0362
6	8.112	BV	0.1170	16.42403	1.85996	0.1114
7	9.387	BB	0.1699	72.45693	6.12934	0.4913

Totals : 1.47474e4 3100.03423

Sample Name: Isocratic Sample

=====
Acq. Operator : SYSTEM
Sample Operator : SYSTEM
Acq. Instrument : HPLC Location : 1
Injection Date : 11/23/2015 3:21:26 PM
Inj Volume : No inj
Method : C:\Chem32\1\Methods\DEF_LC.M
Last changed : 11/23/2015 1:52:23 PM by SYSTEM
Additional Info : Peak(s) manually integrated



=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=250,4 Ref=off

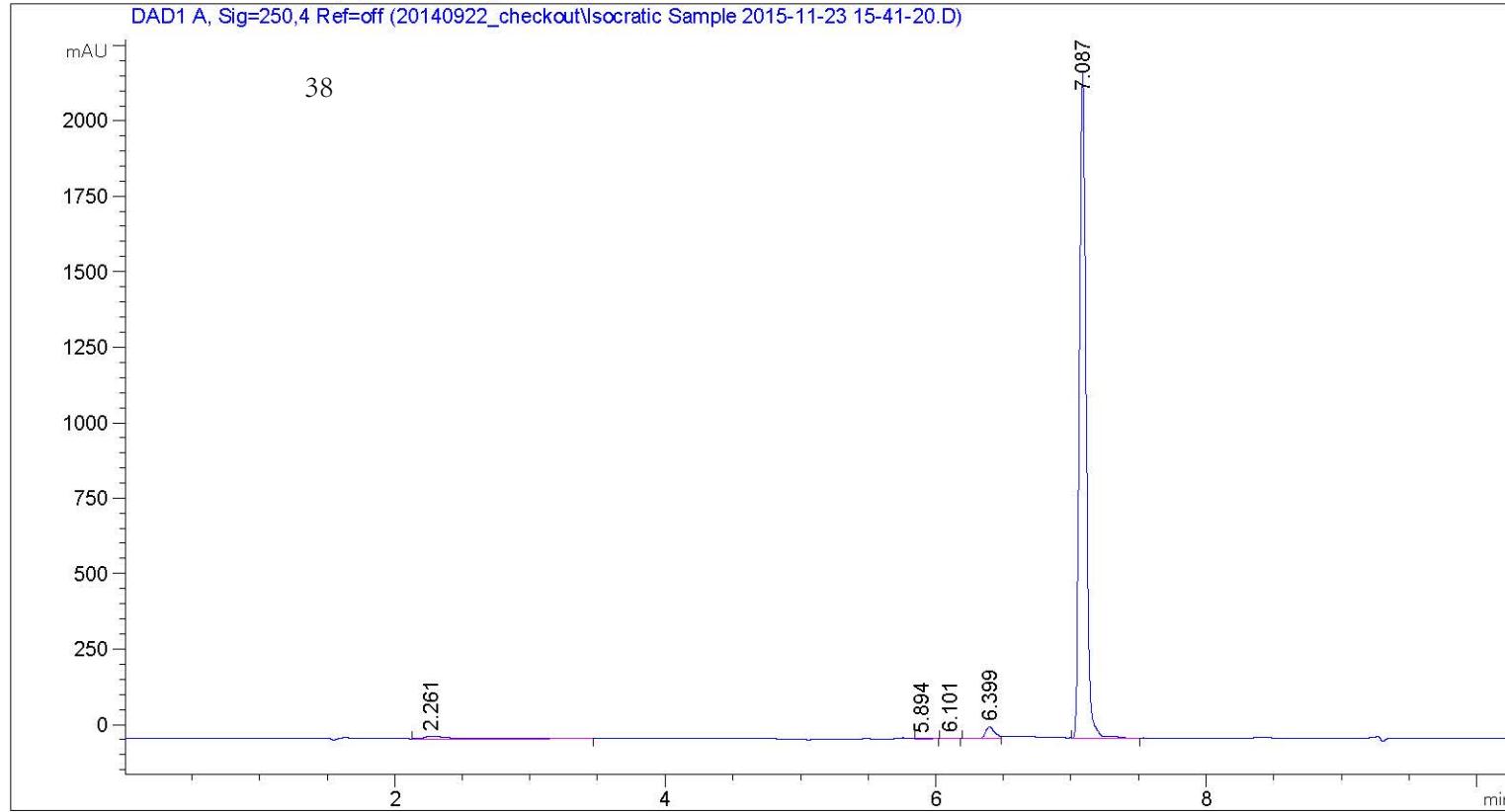
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.114	BB	0.0512	5631.18750	1674.93628	96.1264
2	7.578	BV	0.0617	16.34036	3.99914	0.2789
3	8.043	VB	0.3257	210.58186	9.91898	3.5947

Totals : 5858.10972 1688.85439

=====
*** End of Report ***

Sample Name: Isocratic Sample

```
=====
Acq. Operator   : SYSTEM
Sample Operator : SYSTEM
Acq. Instrument : HPLC                               Location : 1
Injection Date  : 11/23/2015 3:41:20 PM
                                                Inj Volume : No inj
Method          : C:\Chem32\1\Methods\DEF_LC.M
Last changed    : 11/23/2015 1:52:23 PM by SYSTEM
Additional Info : Peak(s) manually integrated
```



```
=====
                           Area Percent Report
=====
```

```
Sorted By      : Signal
Multiplier     : 1.0000
Dilution      : 1.0000
Use Multiplier & Dilution Factor with ISTDs
```

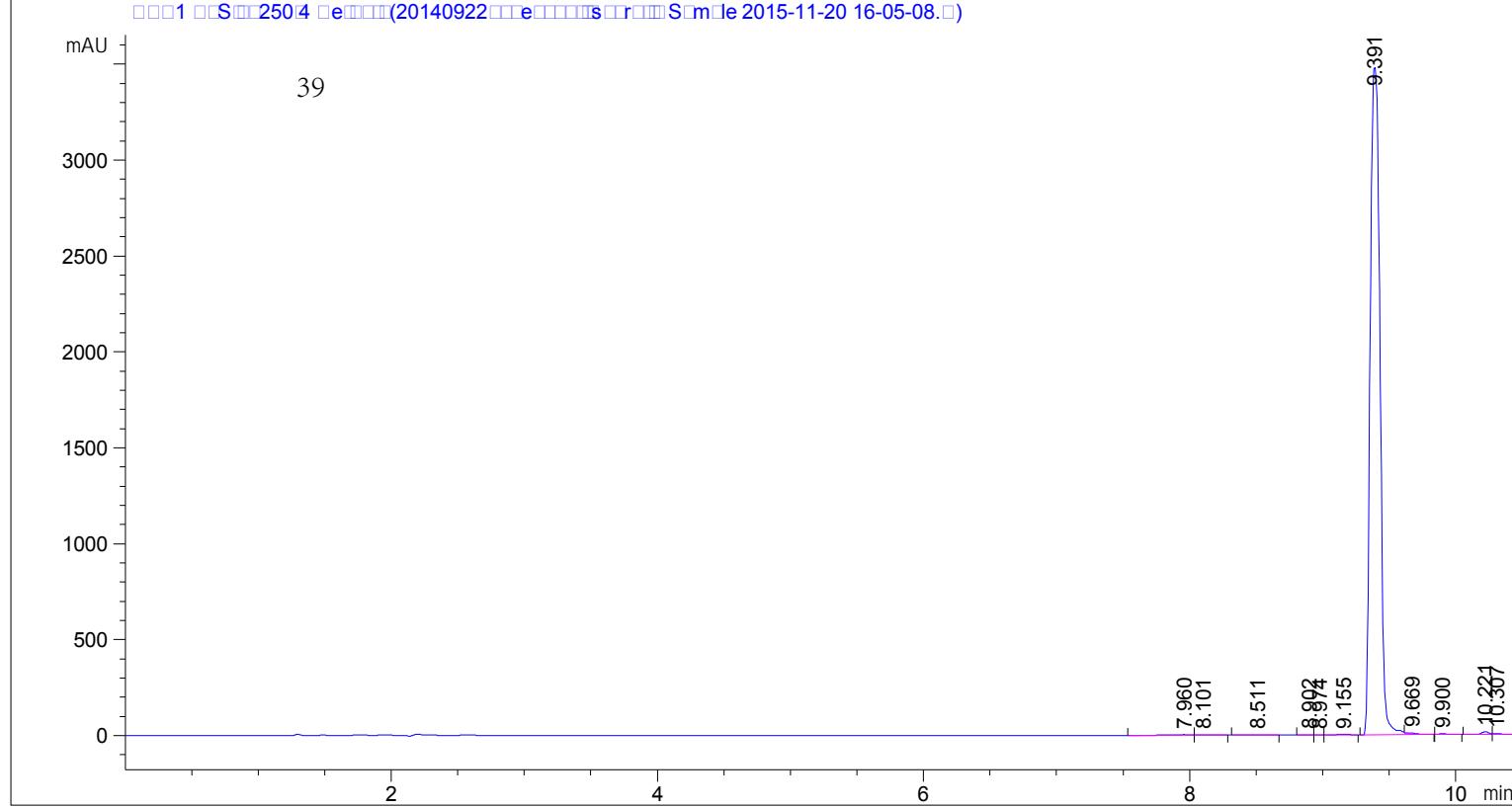
Signal 1: DAD1 A, Sig=250,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.261	BB	0.2598	175.52229	8.53958	2.2170
2	5.894	VB	0.0753	5.16739	1.01748	0.0653
3	6.101	BB	0.0576	7.33592	2.05491	0.0927
4	6.399	BV	0.0706	181.93294	38.86682	2.2980
5	7.087	BV R	0.0537	7547.06641	2208.18066	95.3271

Totals : 7917.02494 2258.65945

Sample Name: Isocratic Sample

```
=====
Acq. Operator : SYSTEM
Sample Operator : SYSTEM
Acq. Instrument : HPLC                               Location : 1
Injection Date : 11/20/2015 4:05:21 PM
Inj Volume : No inj
Acq. Method : C:\CHEM32\1\METHODS\Purity.M
Last changed : 11/20/2015 4:13:14 PM by SYSTEM
(modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\Purity.M
Last changed : 11/20/2015 4:16:52 PM by SYSTEM
Additional Info : Peak(s) manually integrated
```



```
=====
Area Percent Report
=====
```

```
Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: DAD1 A, Sig=250, 4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.960	BV	0.1667	38.58892	3.29221	0.2150
2	8.101	VB	0.1421	29.40253	3.00727	0.1638
3	8.511	BB	0.1191	12.58373	1.54421	0.0701
4	8.902	BV	0.0583	5.92203	1.56104	0.0330
5	8.974	VV	0.0563	6.29287	1.58632	0.0351
6	9.155	VB	0.1317	27.08353	3.04796	0.1509

Sample Name: Isocratic Sample

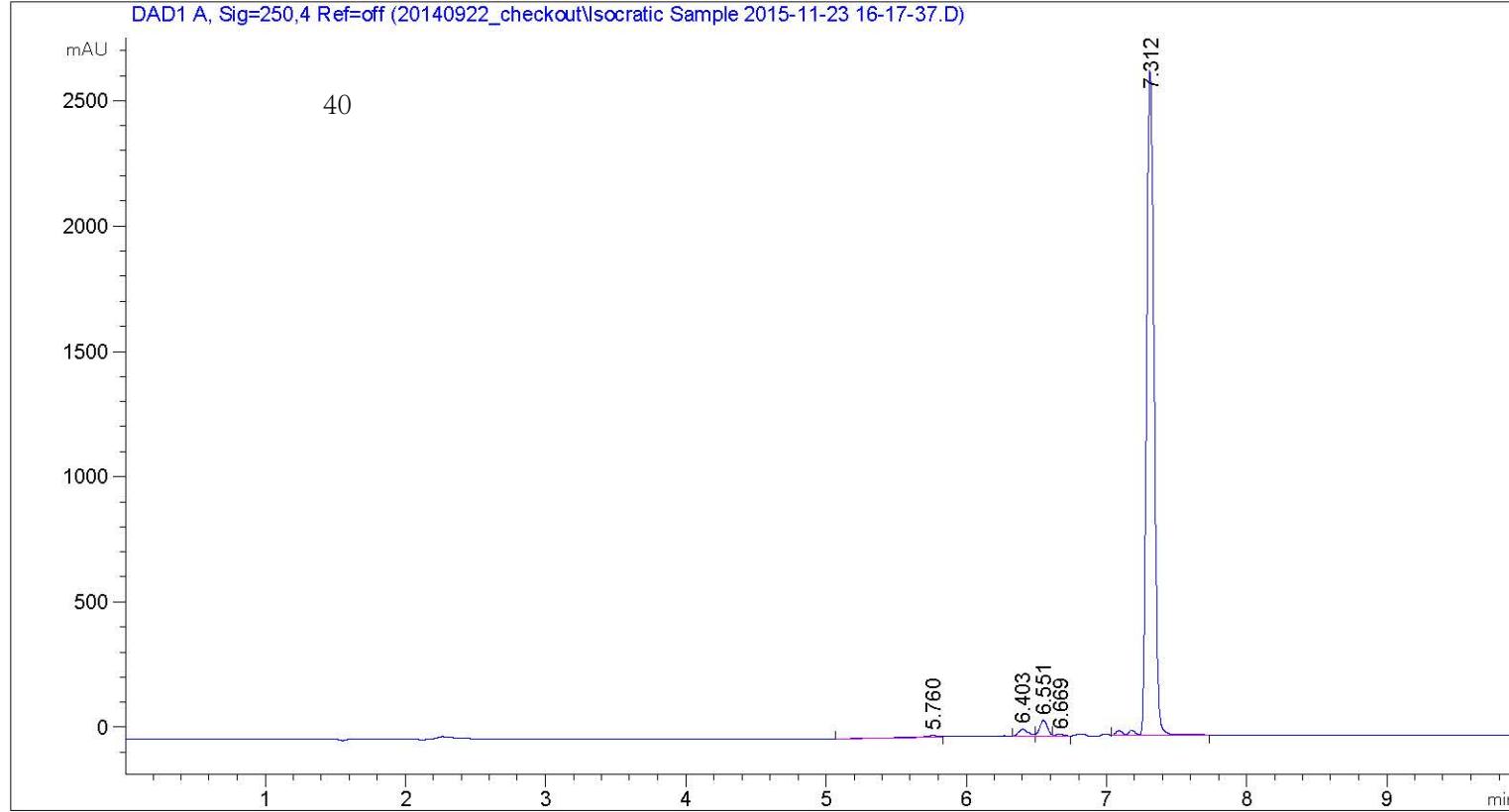
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
7	9. 391	BV R	0. 0853	1. 77025e4	3480. 91382	98. 6399
8	9. 669	VB E	0. 0722	27. 98109	5. 41967	0. 1559
9	9. 900	BB	0. 0618	21. 97360	5. 14826	0. 1224
10	10. 221	BV	0. 0587	55. 00555	14. 34767	0. 3065
11	10. 307	VBA	0. 0583	19. 25345	4. 85408	0. 1073

Totals : 1. 79466e4 3524. 72250

=====*** End of Report ***=====

Sample Name: Isocratic Sample

=====
Acq. Operator : SYSTEM
Sample Operator : SYSTEM
Acq. Instrument : HPLC Location : 1
Injection Date : 11/23/2015 4:17:37 PM
Inj Volume : No inj
Method : C:\Chem32\1\Methods\DEF_LC.M
Last changed : 11/23/2015 1:52:23 PM by SYSTEM
Additional Info : Peak(s) manually integrated



=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=250,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.760	BV	0.1394	86.97375	8.08938	0.8322
2	6.403	BV	0.0703	128.87801	27.71333	1.2332
3	6.551	VV R	0.0585	237.78137	62.40410	2.2753
4	6.669	VB E	0.0686	19.99117	4.80075	0.1913
5	7.312	VV R	0.0592	9977.14160	2656.33789	95.4680

Totals : 1.04508e4 2759.34545