Electronic Supplementary Material (ESI) for RSC Adv.

Supporting Information to

Rapid, effective deprotection of *tert*-butoxycarbonyl (Boc) amino acids and peptides at high temperatures using a thermally stable Ionic Liquid.

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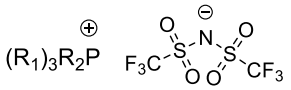
General: Compounds were purchased in their purest commercial quality. All materials were used as obtained, unless and otherwise indicated. Column chromatography for recovery of Ionic Liquid was performed using silica gel (300-400 mesh) with Hexane/EtOAc as eluent. ^{1}H NMR, ^{13}C NMR, ^{19}F NMR and ^{31}P NMR experiments were performed on 500 MHz a JEOL Eclipse Plus 500 instrument. Chemical shifts were recorded with reference to residual solvent peaks (D_2O residue = 4.79 ppm, $CDCl_3$ residue = 7.26 ppm. ESI Mass spectroscopy was performed with Thermo Finnigan LXQ linear Ion Trap mass spectrometer, when required.



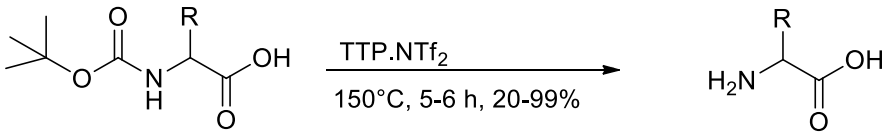
R_1= Hexyl, R_2 = Tetradecyl

Trihexyl tetradecyl phosphonium bis(trifluoromethane)sulfonimide

($TTP.NTf_2$)

General Procedures for Experiments

Preparation of TTP-NTf_2: To a solution of (40 g, 77 mmol) trihexyl tetradecylphosphonium chloride, (graciously donated by CYTEC, West Paterson, NJ, USA) in methanol (20 mL) was added (24.32 g, 84.71 mmol) $LiNTf_2$. Additional methanol was added to obtain a clear solution. The solution was slightly warm at the beginning and was stirred overnight. Methanol was removed under reduced pressure and ~200 mL CH_2Cl_2 was added to the round bottom flask. The organic layer containing the ionic liquid was transferred to the separating funnel and LiCl was extracted with (3x100 mL) deionized water. The organic layer was concentrated under reduced pressure at and dried in vacuum oven (maintained at 40 °C) over P_2O_5 for at least 36 h before use. The products were characterized by ^{1}H NMR, ^{13} C NMR, ^{19}F and ^{31}P NMR.



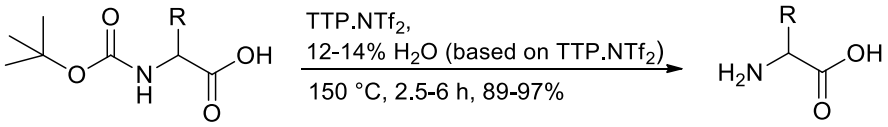
1-13 1A-13 A

R = H, Me, *i*Pr, iso-Bu, s-Bu, Bzl, pyrrolidine, thiomethylethyl, 1-hydroxyethyl, 3-(1H-imidazol-4-yl), 4-amino-butyl, carboxymethyl, carboxyethyl.

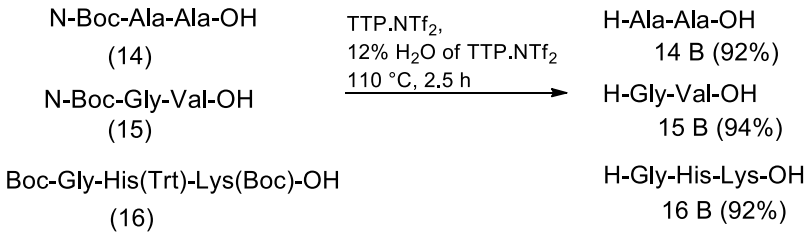
Method A (Neat Reaction in TTP-NTf_2) A mixture of (0.25 g, 0.32-1.43 mmol) N-Boc protected amino acid/peptides and TTP-NTf_2 (7 g, 9.16 mmol) was stirred (~150 rpm) for 5-6 h at 150 °C in a round bottom flask (50 mL) equipped with a reflux condenser. Completion of reaction was monitored by TLC using ethyl acetate/methanol (95:5) and ninhydrin as staining agent. On cooling, the reaction mixture was

transferred into separating funnel with 3x10 mL (CH_2Cl_2/water 1:1). In addition, CH_2Cl_2 (100 mL) and water (50 – 80 mL, depending on the substrate) was added to the separating funnel. The layers were allowed to separate after shaking and the organic layer (containing the ionic liquid) was removed. To the aqueous layer (containing the amino acids) fresh CH_2Cl_2 (2x 75mL) was added to ensure removal of any trace of ionic liquid remaining. The aqueous layer was evaporated to dryness to obtain the product. In most of the cases, this gave us the purified amino acid, but otherwise a final washing with ~ 5 mL isopropanol (using centrifuge) proved very effective. All the products were characterized by ^{1}H NMR, ^{13}C NMR. ESI-MS was done in some cases.

The peptides were added to TTP-NTf_2 and heated at 120 °C for 3 h (Scheme not shown). However, incomplete conversions and product decompositions were observed (14A-16A).

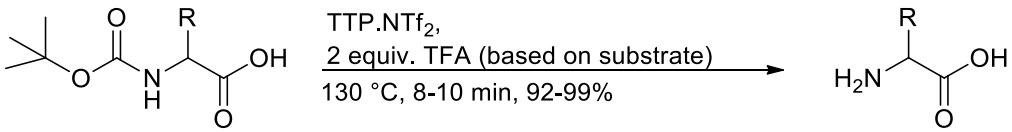


1-13 1B-13B

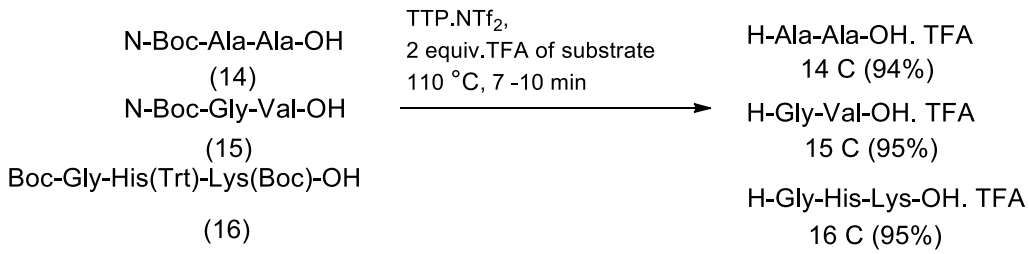


Method B (TTP-NTf_2 and water) To a mixture of (0.25 g, 0.32-1.43 mmol) N-Boc protected amino acid/peptides and TTP-NTf_2 (7 g, 9.16 mmol) was added deionized water 12-14% (based on TTP.NTf_2). The resulting mixture was stirred (~200 rpm) for 2.5-6 h at 150 °C (for amino acids) and 2.5 h at 110 °C (for peptides). The remaining work-up is similar to method A. All the products were characterized by ^{1}H NMR, ^{13}C NMR. ESI-MS was done in some cases.

L-Histidine and L-Lysine tends to form emulsions especially for method B. They were centrifuged for 5 min at around 5000 rpm (The Drucker Co., Model 614 B) to obtain the purified compound. For peptides, the water was generally removed at ~ 40-45 °C under reduced pressure.



1-13 1C-13C



Method C (TTP-NTf_2 and TFA) To a stirring mixture of (0.25 g, 0.32-1.43 mmol) N-Boc protected amino acid/peptides and TTP-NTf_2 (7 g, 9.16 mmol) was added TFA (2 equiv, based on substrate). The resulting mixture was stirred (~150 rpm) for 7-10 min at 100 °C (for peptides) and 130 °C (for amino acids). The remaining procedure is similar to method A.

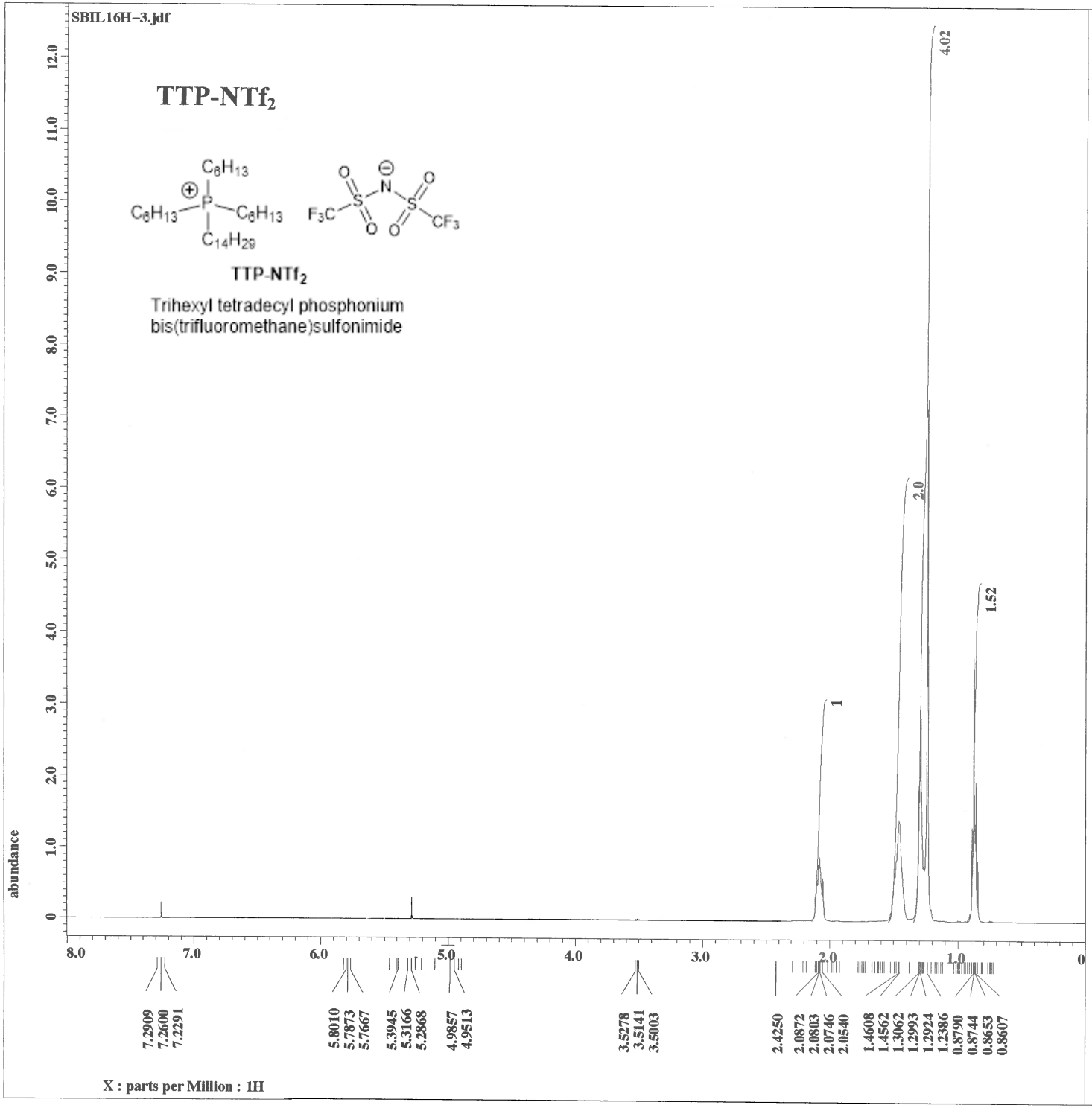
For peptides, the water was removed by either freeze drying or simply air drying at higher flow using an inverted funnel at room temperature. All the products were characterized by ^{1}H NMR, ^{13}C NMR. ESI-MS was done in some cases.

SBIL16H-3.jdf

TTP-NTf_2

TTP-NTf_2

Trihexyl tetradecyl phosphonium
bis(trifluoromethane)sulfonimide



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7.2291	3.5278
5.8010	3.5141
5.7873	3.5003
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5.3945	2.0872
5.3166	2.0803
5.2868	2.0746
	2.0540

1.4608	1.2386
1.4562	0.8790
1.3062	0.8744
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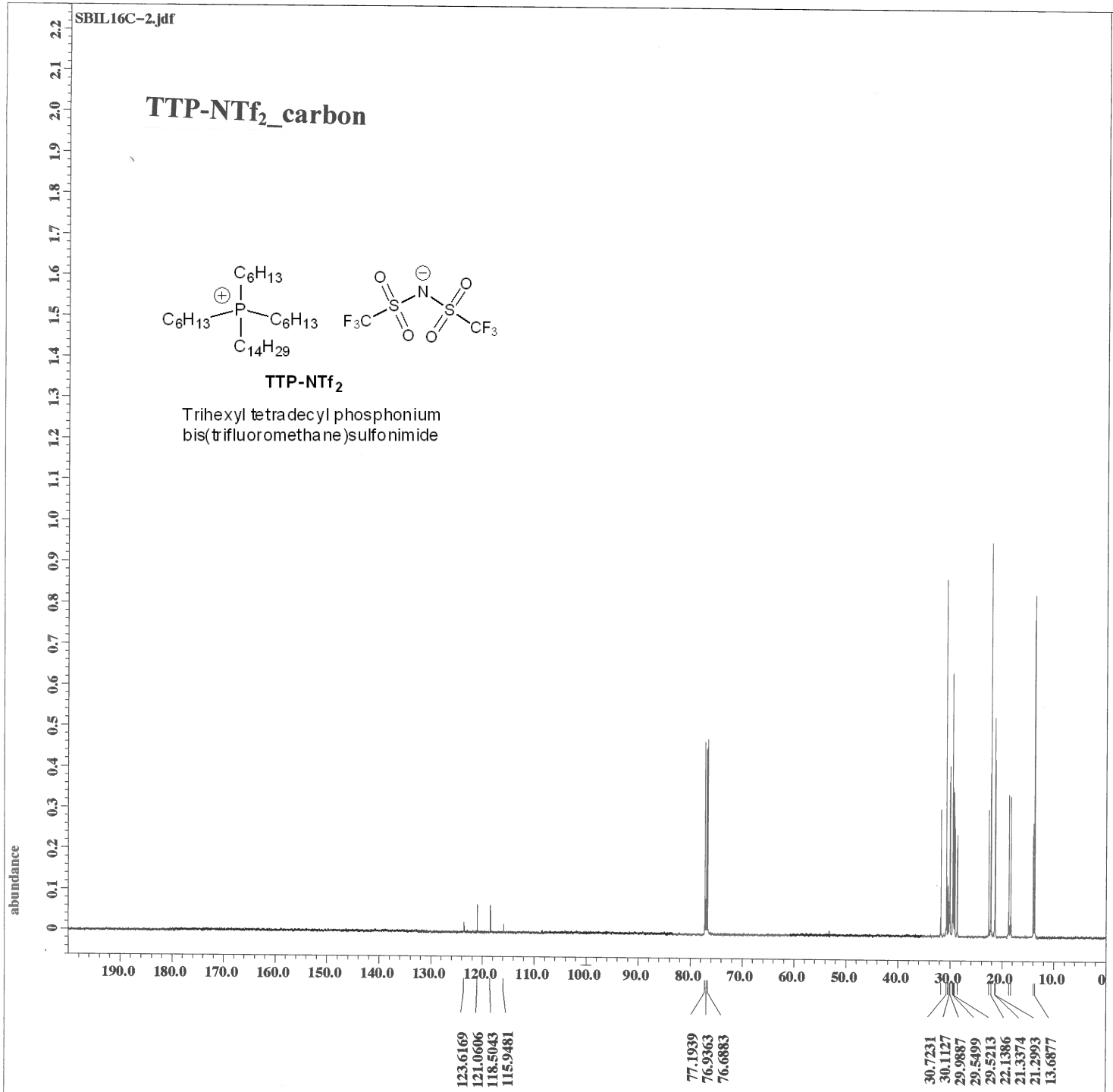
SBIL16C-2.jdf

TTP-NTf$_2$_carbon

TTP-NTf$_2$

Trihexyl tetradecyl phosphonium
bis(trifluoromethane)sulfonimide



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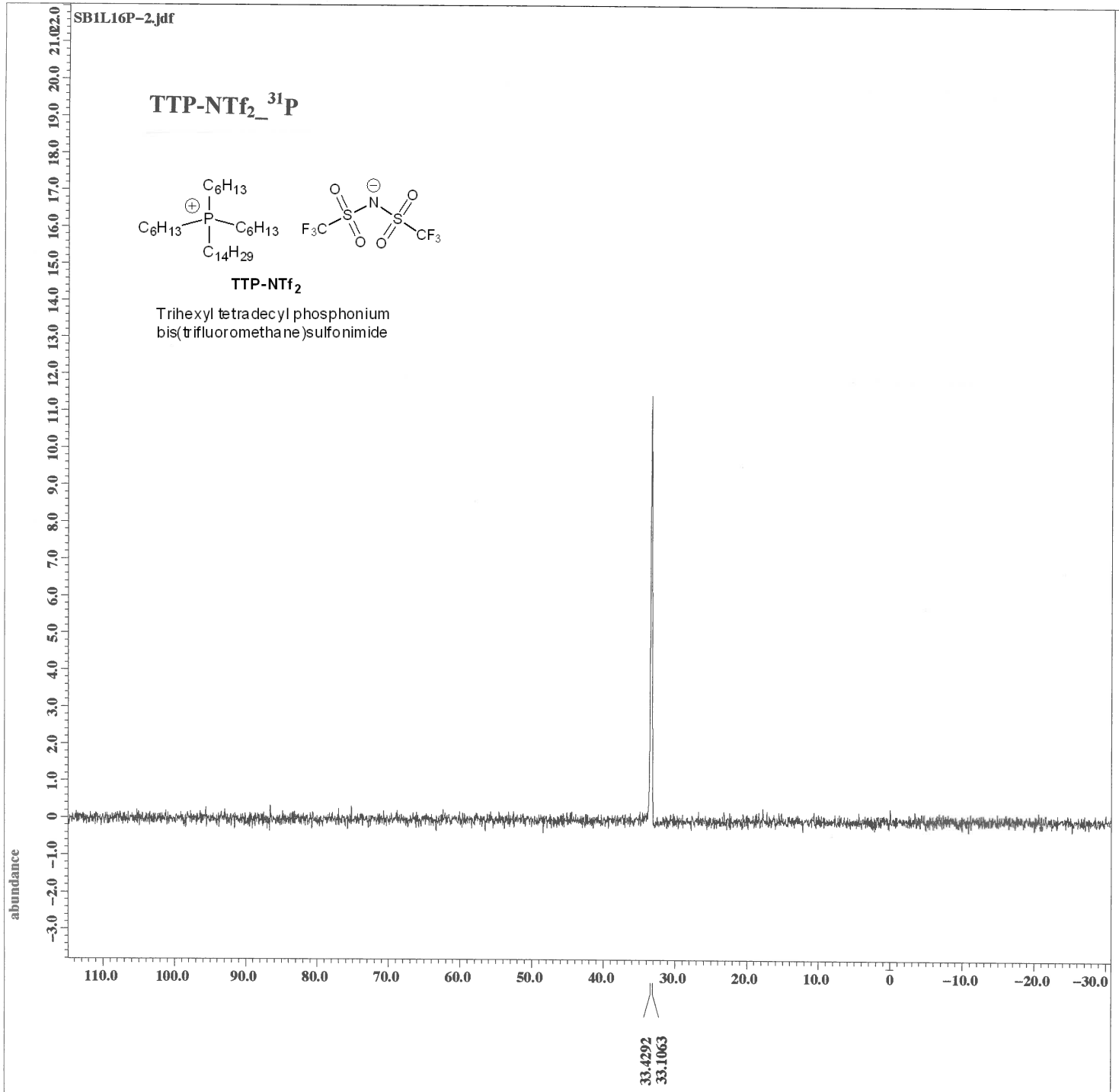
SB1L16P-2.jdf

TTP-NTf$_2$_^{31}P

TTP-NTf$_2$

Trihexyl tetradecyl phosphonium
bis(trifluoromethane)sulfonimide

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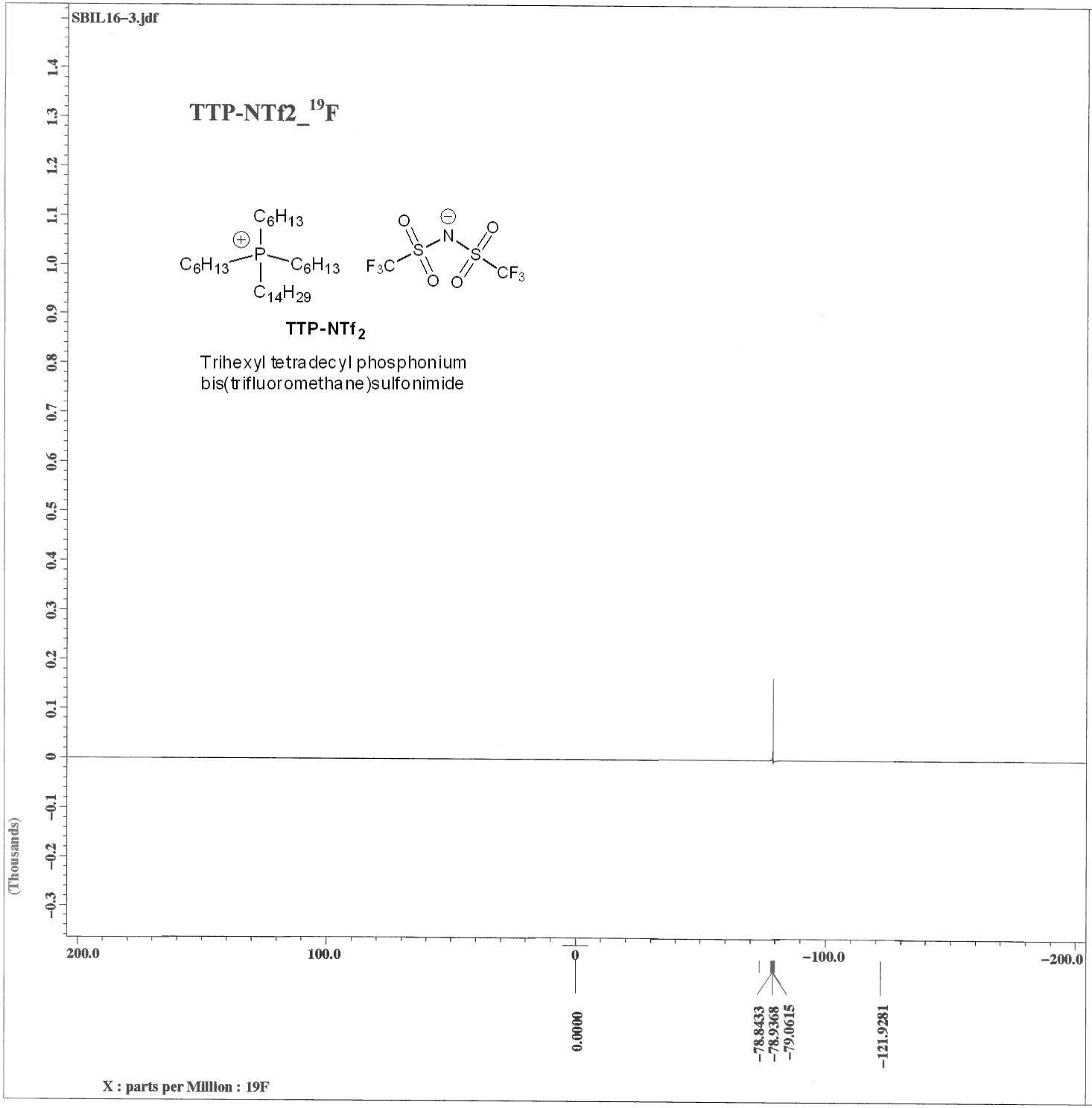
SBIL16-3.jdf

TTP-NTf2_^{19}F

TTP-NTf$_2$

Trihexyl tetradecyl phosphonium
bis(trifluoromethane)sulfonimide



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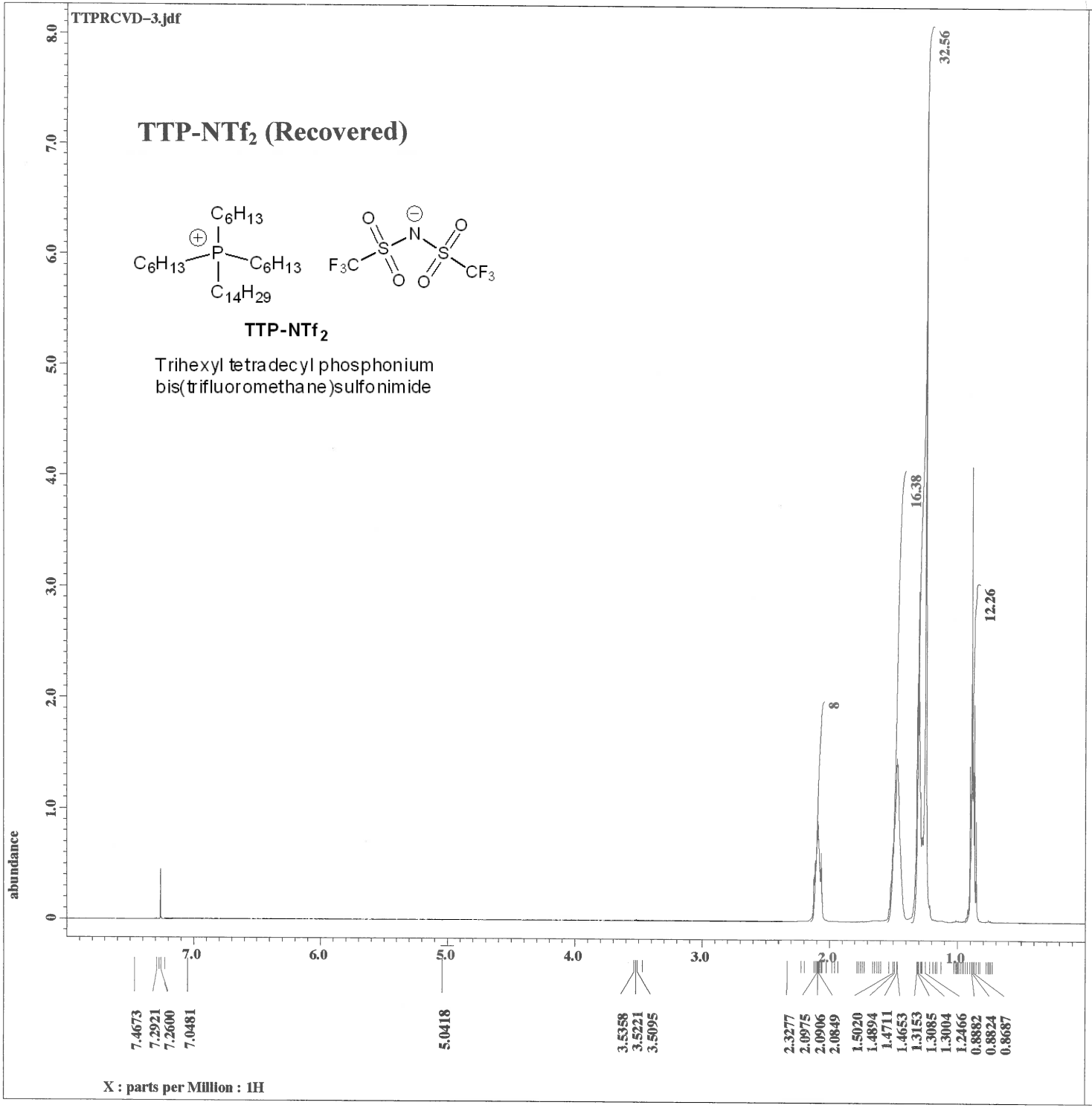
TTPRCVD-3.jdf

TTP-NTf_2 (Recovered)

TTP-NTf_2

Trihexyl tetradecyl phosphonium
bis(trifluoromethane)sulfonimide



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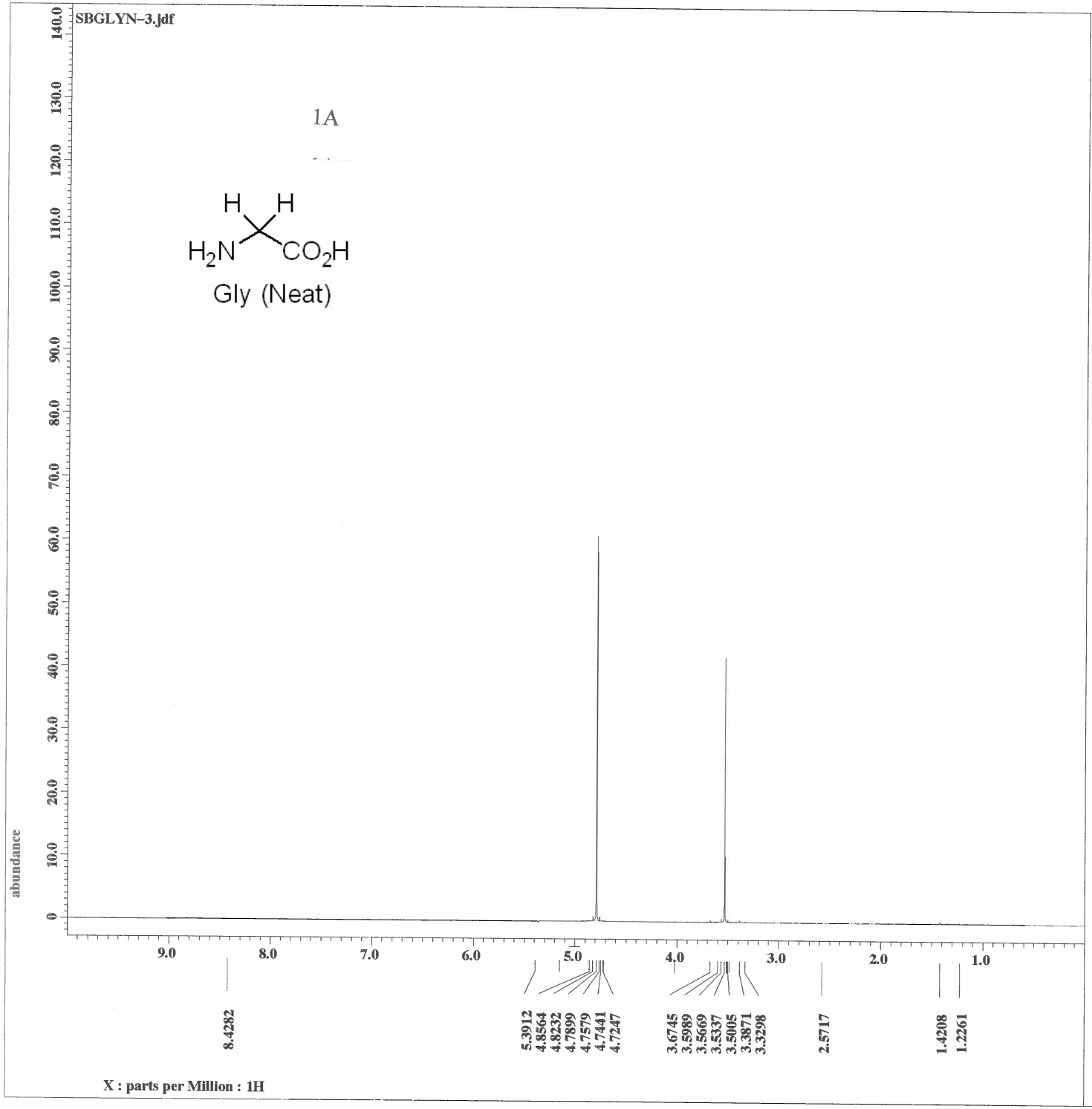
SBGLYN-3.jdf

1A

Gly (Neat)



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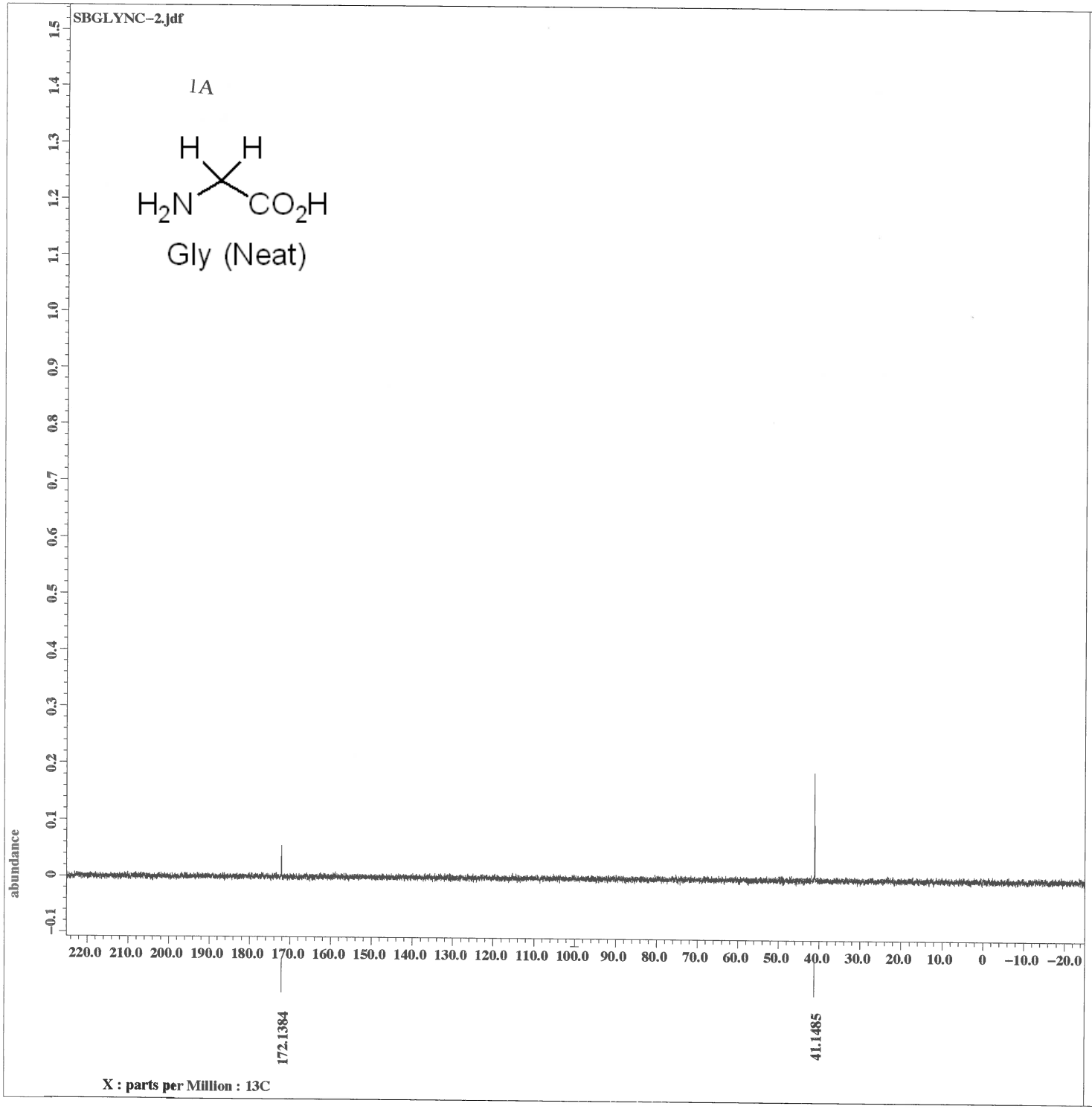
SBGLYNC-2.jdf

1A

Gly (Neat)



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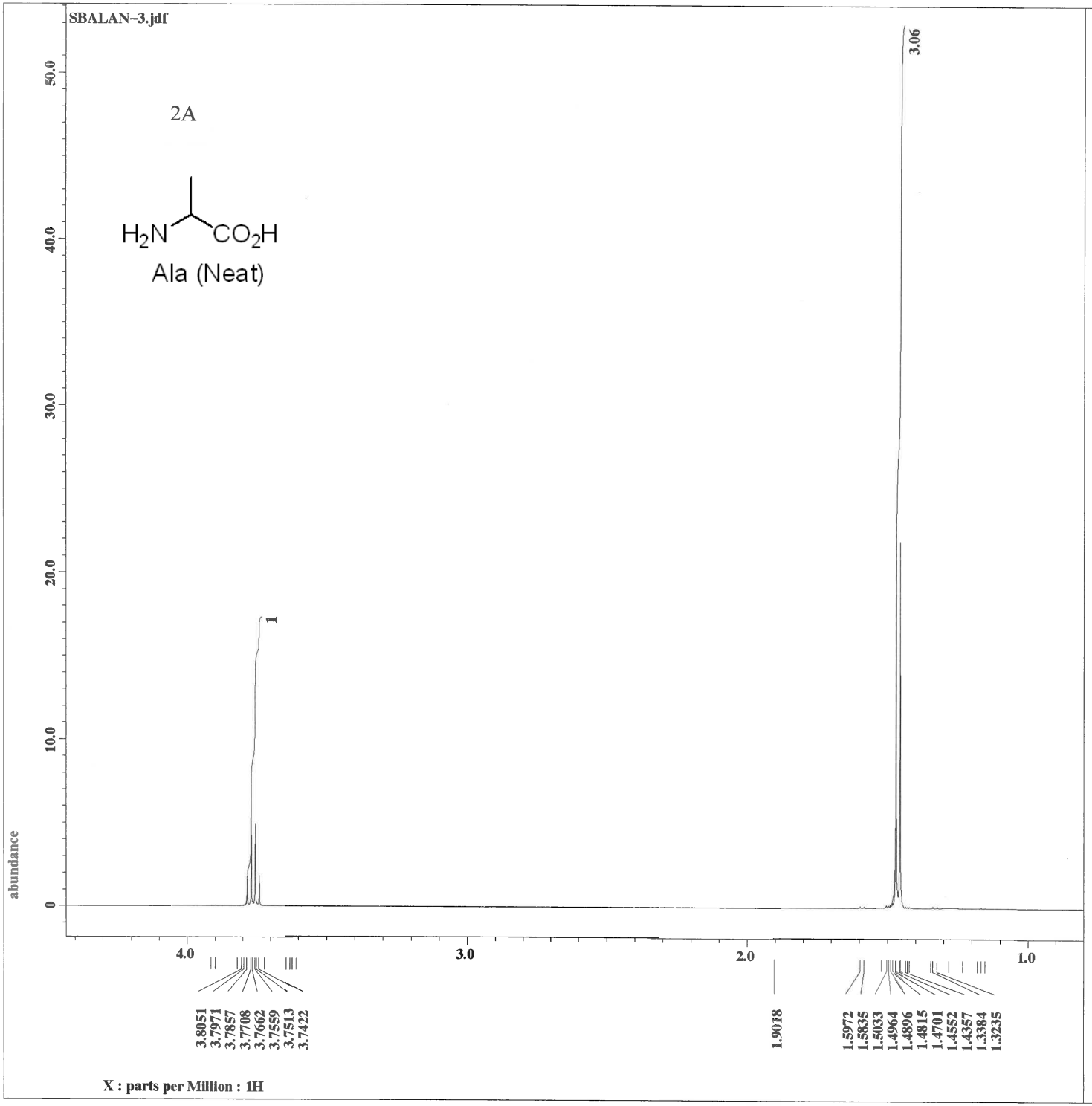
SBALAN-3.jdf

2A

Ala (Neat)



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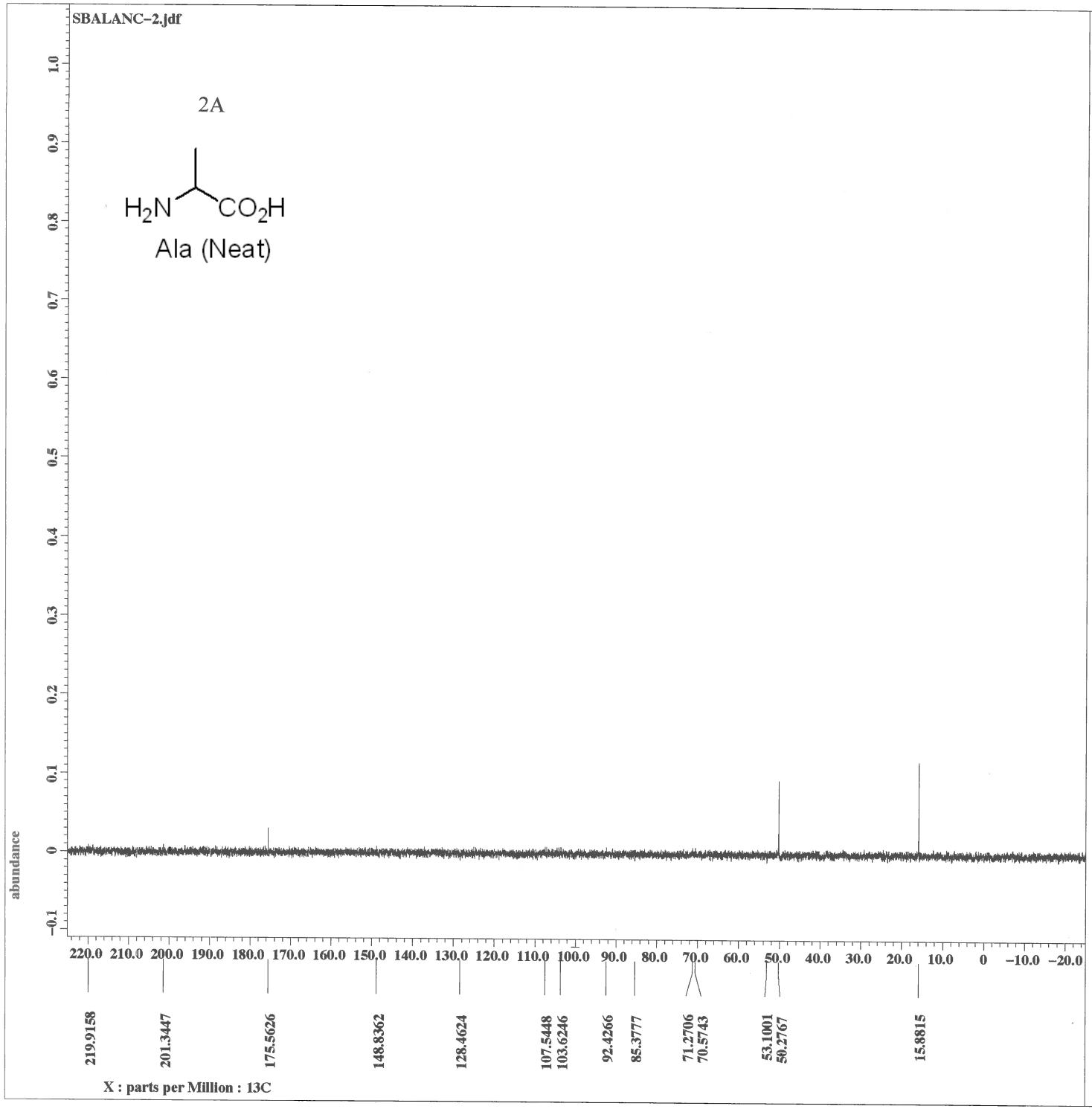
X_90_width	= 12.54[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 4[dB]
X_pulse	= 6.27[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 46
Relaxation_delay	= 10[s]
Repetition_time	= 11.74587904[s]
Temp_get	= 22[dC]

SBALANC-2.jdf

2A

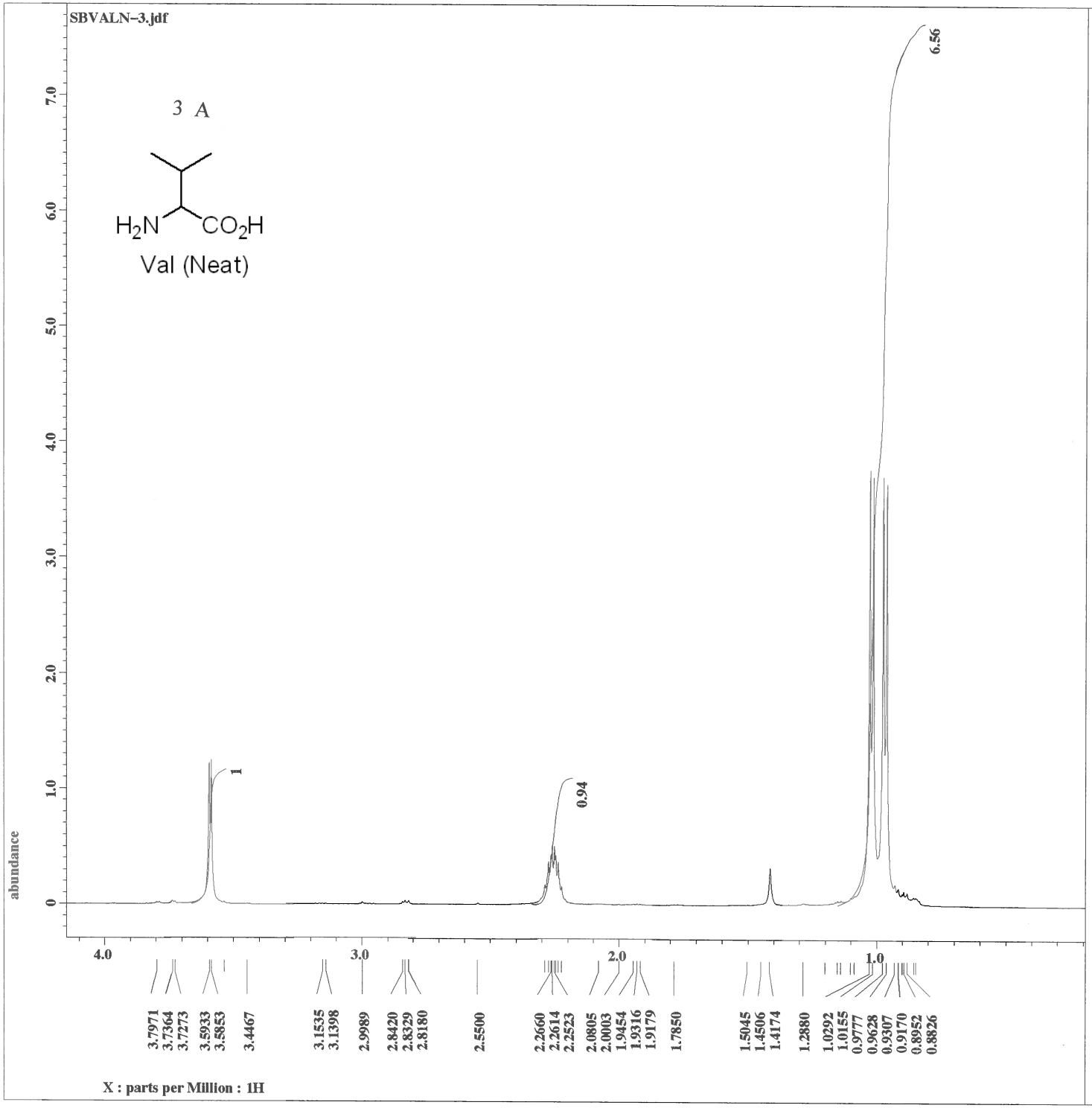
Ala (Neat)



Filename	= SBALANC-2.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= S#352979
Solvent	= D2O
Creation_time	= 23-SEP-2015 22:37:29
Revision_time	= 23-SEP-2015 09:53:49
Current_time	= 23-SEP-2015 09:54:01
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 0.83361792[s]
X_domain	= 13C
X_freq	= 125.76529768[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.19959034[Hz]
X_sweep	= 39.3081761[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 10
Scans	= 280
Total_scans	= 280
X_90_width	= 10.73[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 9[dB]
X_pulse	= 3.57666667[us]
Irr_atn_dec	= 20[dB]
Irr_atn_noe	= 20[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 0.2[s]
Recvr_gain	= 50
Relaxation_delay	= 0.2[s]
Repetition_time	= 1.03361792[s]
Temp_get	= 22.4[dC]

SBVALN-3.jdf

Val (Neat)

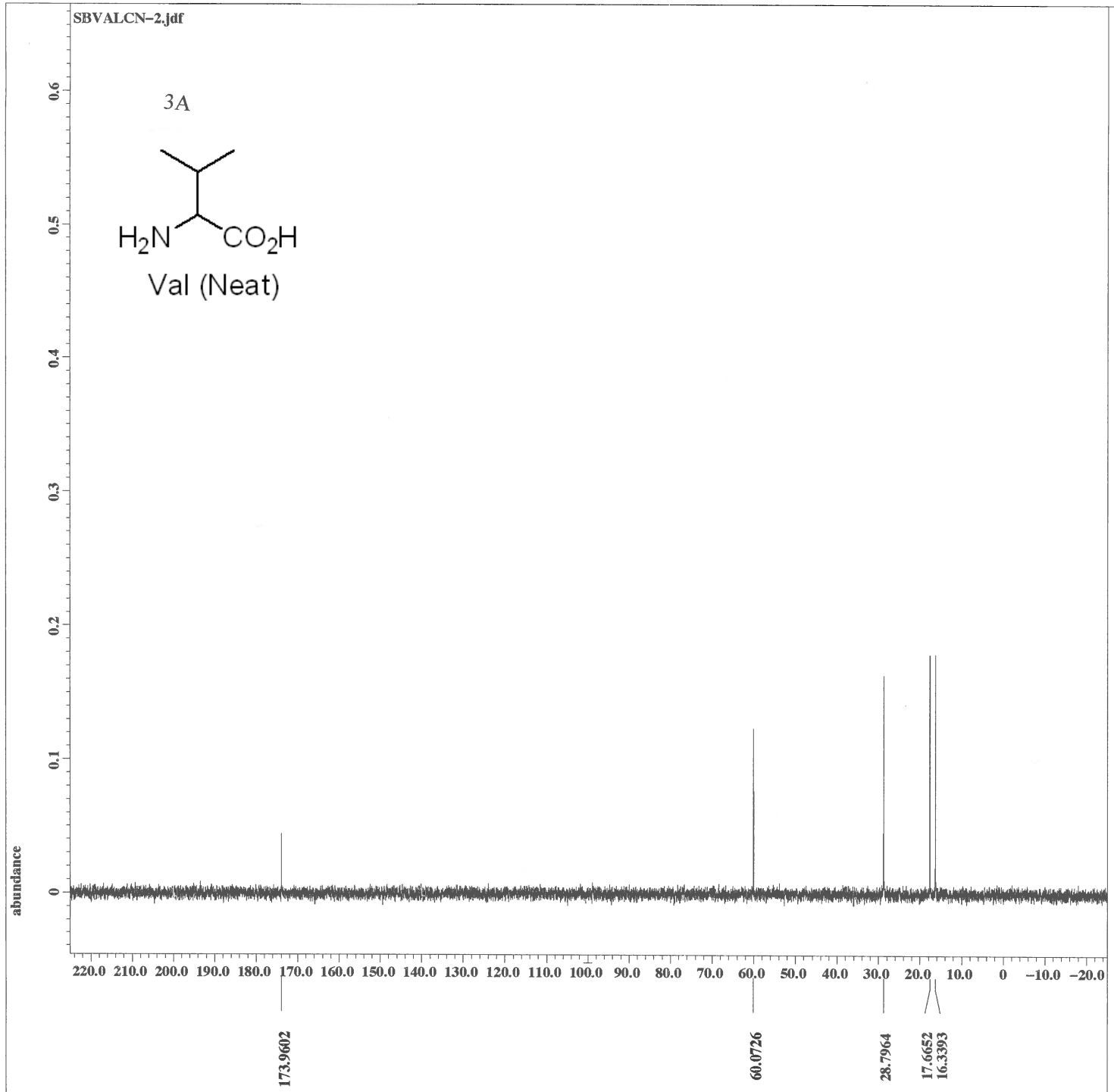


Filename	= SBVALN-3.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= S#338198
Solvent	= D2O
Creation_time	= 23-SEP-2015 22:10:56
Revision_time	= 23-SEP-2015 09:28:38
Current_time	= 23-SEP-2015 09:29:28
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 1.74587904[s]
X_domain	= 1H
X_freq	= 500.15991521[MHz]
X_offset	= 5.0[ppm]
X_points	= 16384
X_prescans	= 0
X_resolution	= 0.57277737[Hz]
X_sweep	= 9.38438438[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Tri_domain	= 1H
Tri_freq	= 500.15991521[MHz]
Tri_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 10
Total_scans	= 10
X_90_width	= 12.54[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 4[dB]
X_pulse	= 6.27[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 36
Relaxation_delay	= 10[s]
Repetition_time	= 11.74587904[s]
Temp_get	= 21.9[dC]

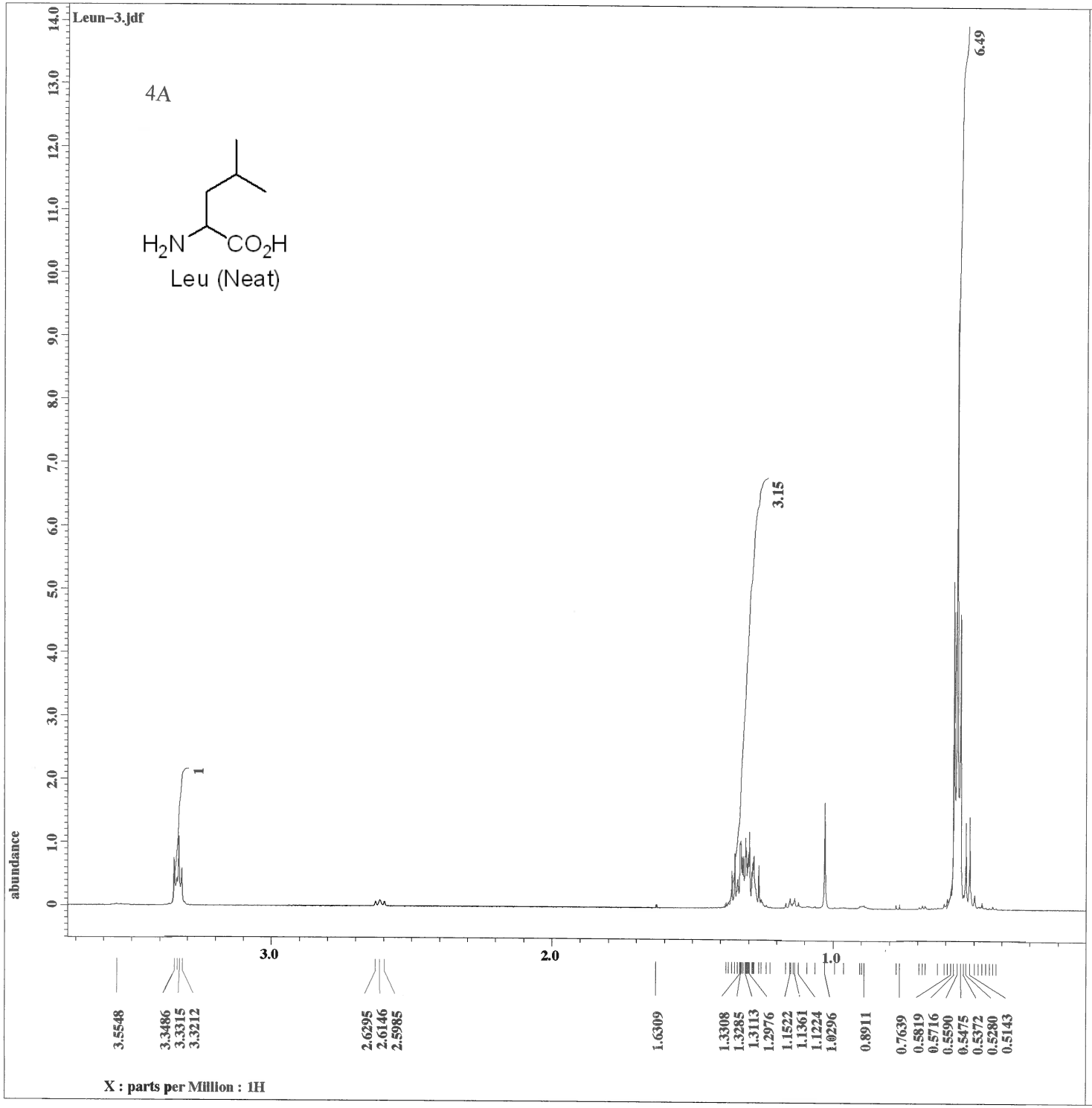
SBVALCN-2.jdf

3A

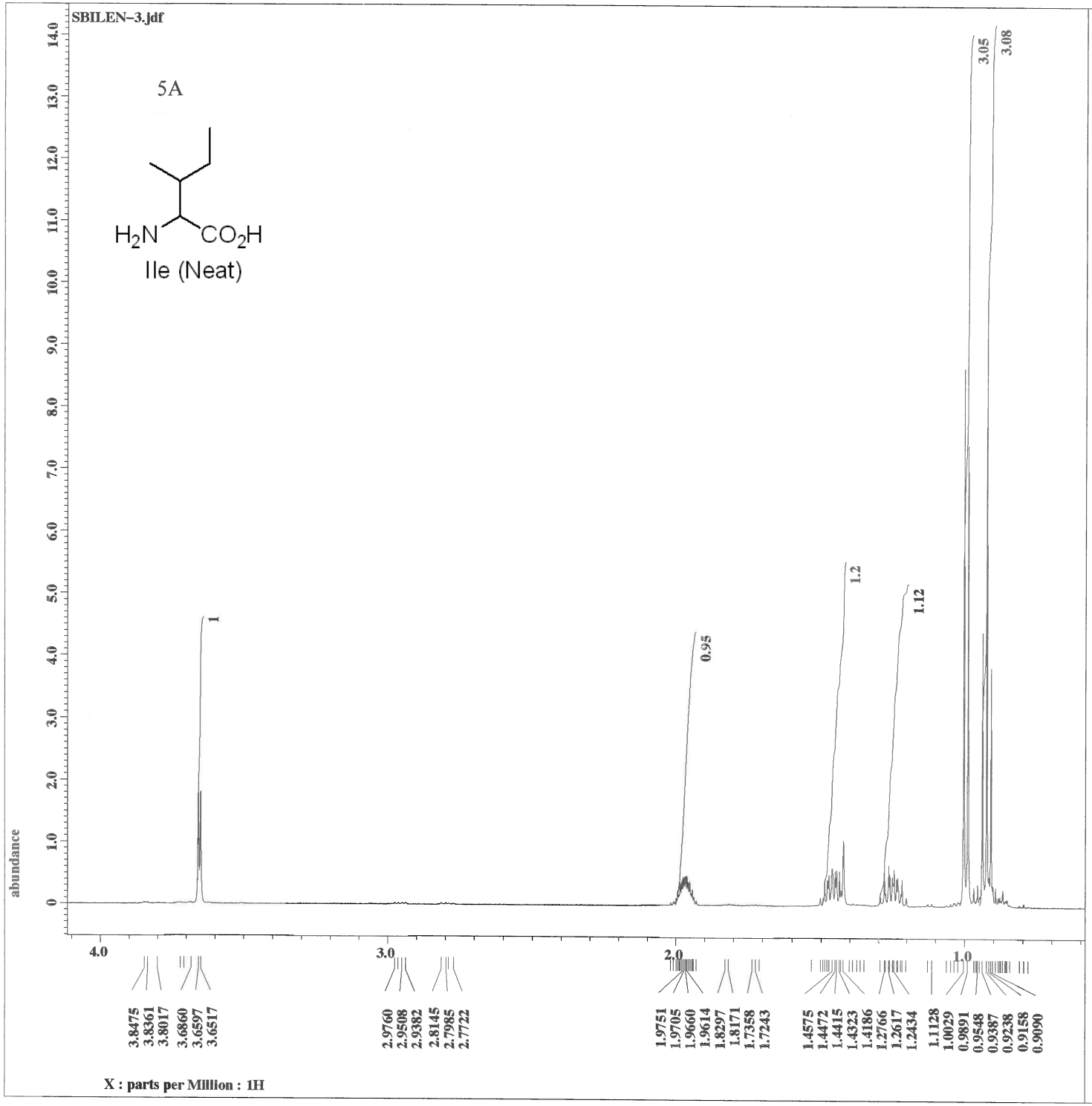
Val (Neat)



Filename	= SBVALCN-2.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= S#340420
Solvent	= D2O
Creation_time	= 23-SEP-2015 22:16:54
Revision_time	= 23-SEP-2015 09:33:18
Current_time	= 23-SEP-2015 09:35:42
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 0.83361792[s]
X_domain	= 13C
X_freq	= 125.76529768[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.19959034[Hz]
X_sweep	= 39.3081761[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 10
Scans	= 300
Total_scans	= 300
X_90_width	= 10.73[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 9[dB]
X_pulse	= 3.57666667[us]
Irr_atn_dec	= 20[dB]
Irr_atn_noe	= 20[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 0.2[s]
Recvr_gain	= 50
Relaxation_delay	= 0.2[s]
Repetition_time	= 1.03361792[s]
Temp_get	= 22.4[dC]



Filename	= Leun-3.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= S#728776
Solvent	= D2O
Creation_time	= 24-SEP-2015 09:03:05
Revision_time	= 23-SEP-2015 20:20:02
Current_time	= 23-SEP-2015 20:21:18
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 1.74587904[s]
X_domain	= 1H
X_freq	= 500.15991521[MHz]
X_offset	= 5.0[ppm]
X_points	= 16384
X_prescans	= 0
X_resolution	= 0.57277737[Hz]
X_sweep	= 9.38438438[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Tri_domain	= 1H
Tri_freq	= 500.15991521[MHz]
Tri_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 16
Total_scans	= 16
X_90_width	= 12.54[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 4[dB]
X_pulse	= 6.27[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 48
Relaxation_delay	= 10[s]
Repetition_time	= 11.74587904[s]
Temp_get	= 22[dC]

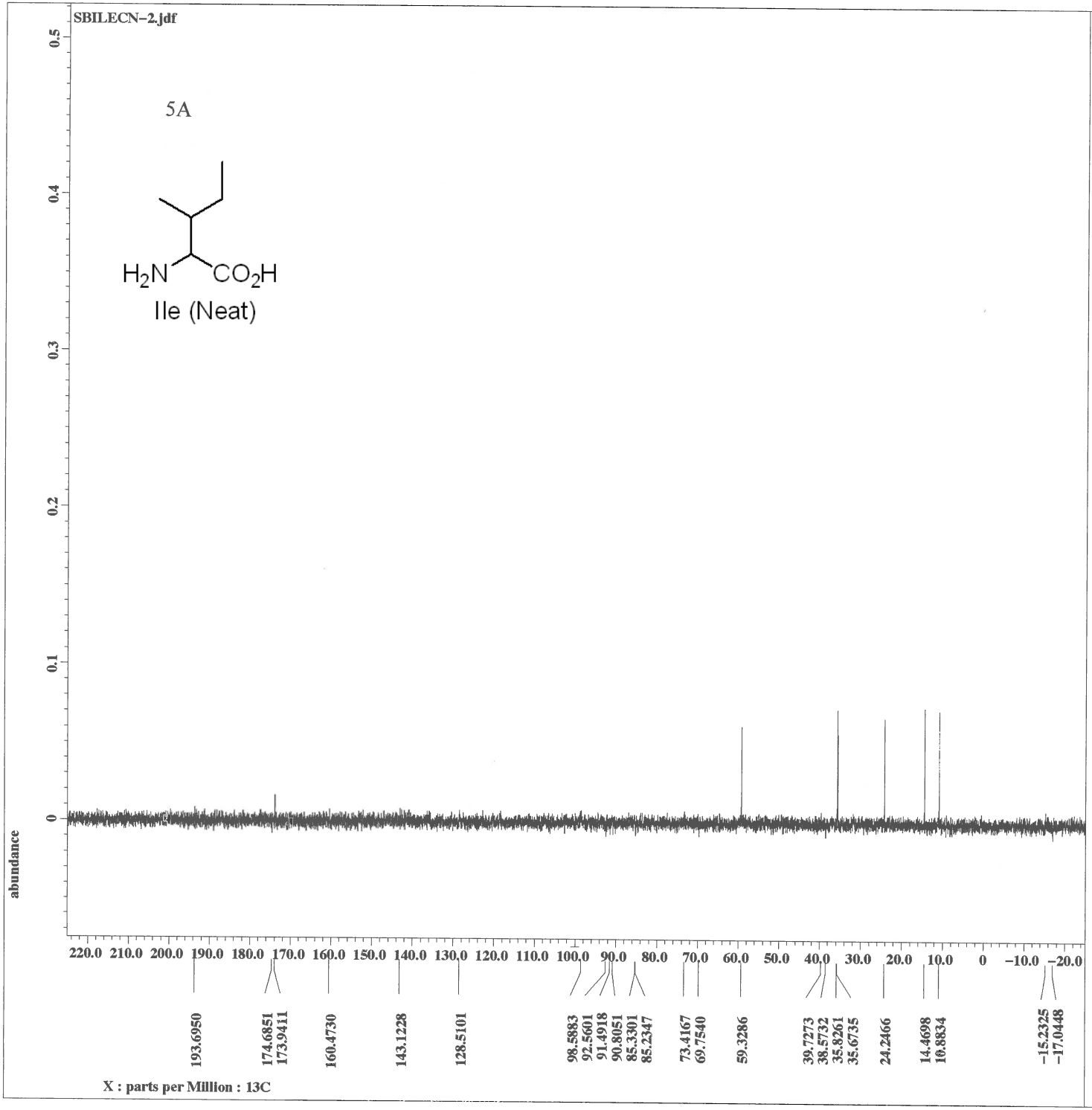



```
Filename          = SBILEN-3.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#472655
Solvent           = D2O
Creation_time     = 24-SEP-2015 01:54:38
Revision_time     = 23-SEP-2015 13:14:31
Current_time      = 23-SEP-2015 13:15:21

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = JNM-ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.74587904[s]
X_domain          = 1H
X_freq            = 500.15991521[MHz]
X_offset          = 5.0[ppm]
X_points          = 16384
X_prescans        = 0
X_resolution      = 0.57277737[Hz]
X_sweep           = 9.38438438[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Tri_domain        = 1H
Tri_freq          = 500.15991521[MHz]
Tri_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 12.54[us]
X_acq_time        = 1.74587904[s]
X_angle           = 45[deg]
X_atn             = 4[dB]
X_pulse           = 6.27[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 44
Relaxation_delay  = 10[s]
Repetition_time   = 11.74587904[s]
Temp_get          = 22[dC]
```

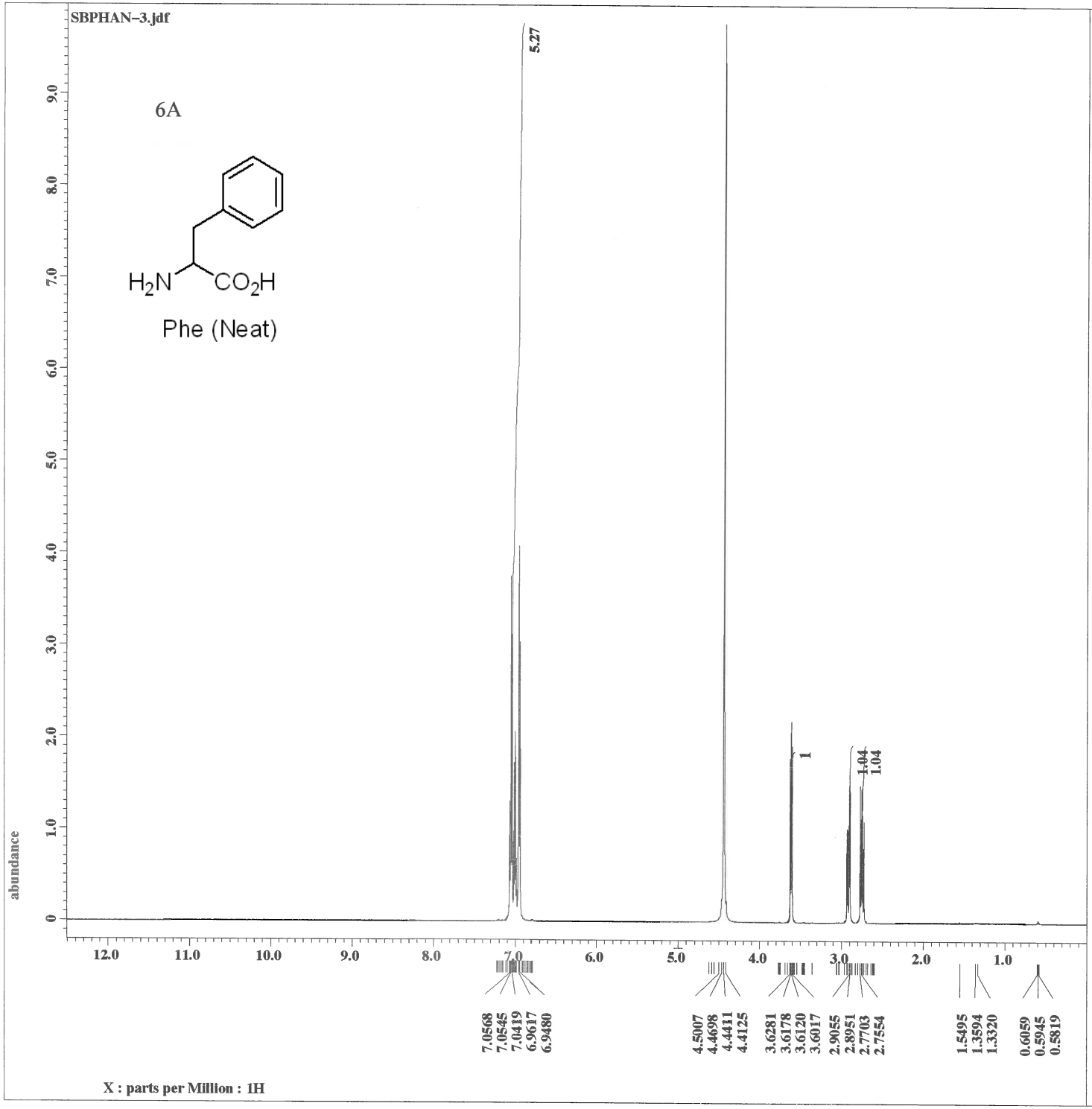
SBILECN-2.jdf

5A

Ile (Neat)




```
Filename          = SBILECN-2.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#475404
Solvent           = D2O
Creation_time     = 24-SEP-2015 02:02:00
Revision_time     = 23-SEP-2015 13:18:17
Current_time      = 23-SEP-2015 13:18:27

Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = JNM-ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 0.83361792[s]
X_domain          = 13C
X_freq            = 125.76529768[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 1.19959034[Hz]
X_sweep           = 39.3081761[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 10
Scans             = 340
Total_scans       = 340

X_90_width        = 10.73[us]
X_acq_time        = 0.83361792[s]
X_angle           = 30[deg]
X_atn             = 9[dB]
X_pulse           = 3.57666667[us]
Irr_atn_dec       = 20[dB]
Irr_atn_noe       = 20[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 0.1[s]
Recvr_gain        = 50
Relaxation_delay  = 0.1[s]
Repetition_time   = 0.93361792[s]
Temp_get          = 22.4[dC]
```

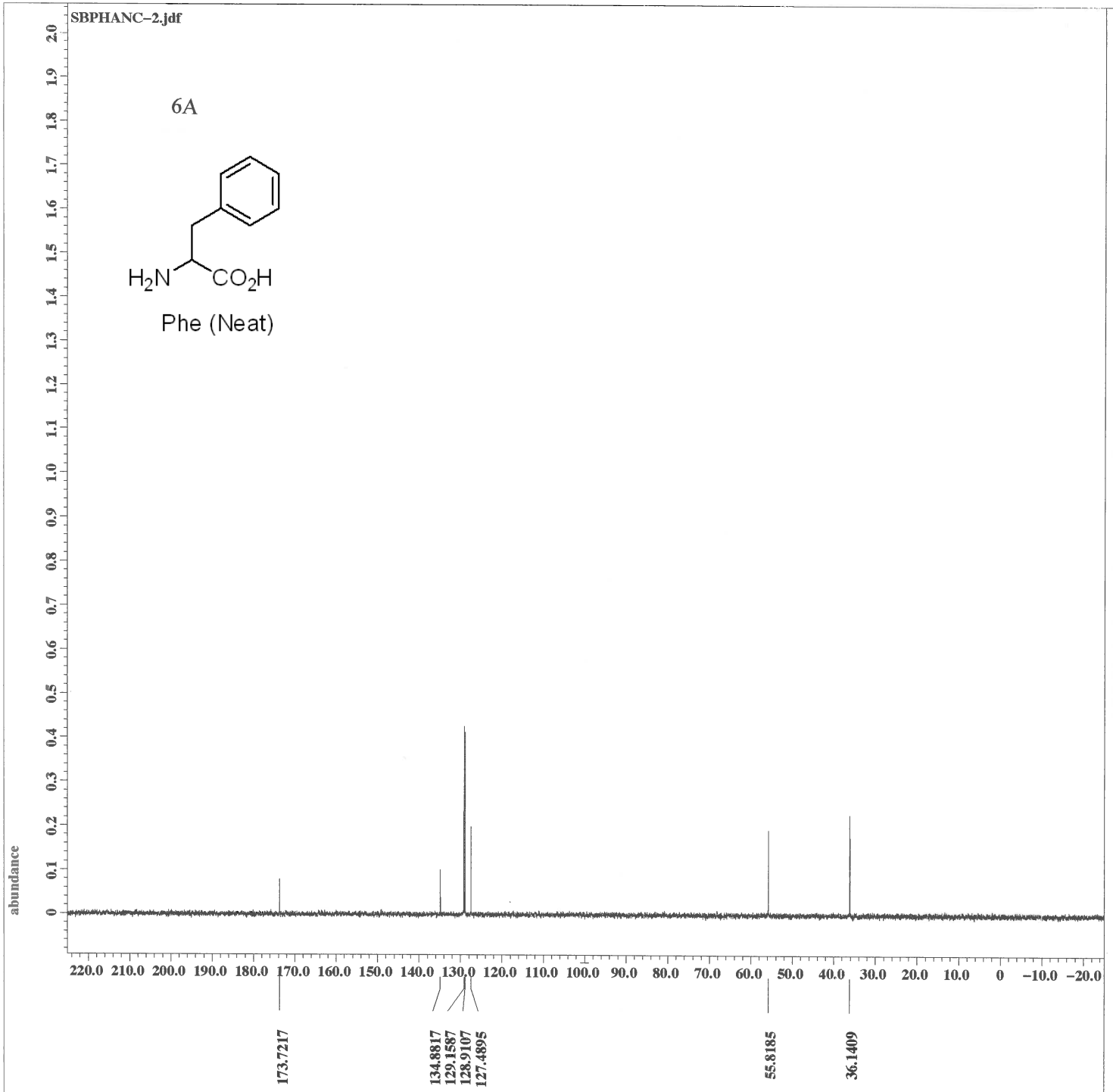



```
Filename          = SBPHAN-3.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#347797
Solvent           = D2O
Creation_time     = 24-SEP-2015 22:26:34
Revision_time     = 24-SEP-2015 09:44:03
Current_time      = 24-SEP-2015 09:44:42

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = JNM-ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.74587904[s]
X_domain          = 1H
X_freq            = 500.15991521[MHz]
X_offset          = 5.0[ppm]
X_points          = 16384
X_prescans        = 0
X_resolution      = 0.57277737[Hz]
X_sweep           = 9.38438438[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Tri_domain        = 1H
Tri_freq          = 500.15991521[MHz]
Tri_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 12.54[us]
X_acq_time        = 1.74587904[s]
X_angle           = 45[deg]
X_atn             = 4[dB]
X_pulse           = 6.27[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 36
Relaxation_delay  = 10[s]
Repetition_time   = 11.74587904[s]
Temp_get          = 21.7[dC]
```

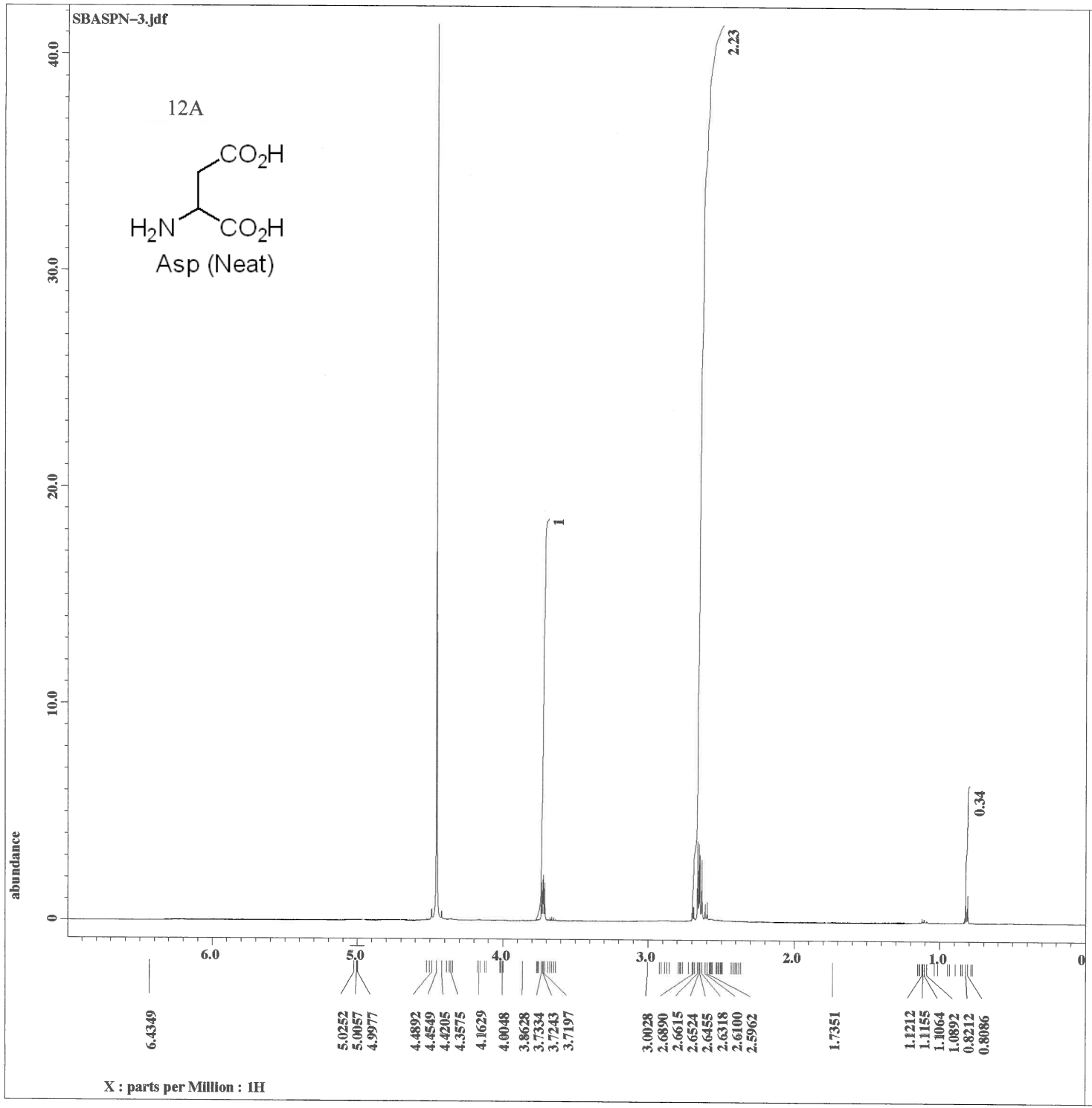
SBPHANC-2.jdf

6A

Phe (Neat)



Filename	= SBPHANC-2.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= S#349860
Solvent	= D2O
Creation_time	= 24-SEP-2015 22:30:47
Revision_time	= 24-SEP-2015 09:46:43
Current_time	= 24-SEP-2015 09:46:50
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 0.83361792[s]
X_domain	= 13C
X_freq	= 125.76529768[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.19959034[Hz]
X_sweep	= 39.3081761[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 10
Scans	= 190
Total_scans	= 190
X_90_width	= 10.73[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 9[dB]
X_pulse	= 3.57666667[us]
Irr_atn_dec	= 20[dB]
Irr_atn_noe	= 20[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 0.2[s]
Recvr_gain	= 50
Relaxation_delay	= 0.2[s]
Repetition_time	= 1.03361792[s]
Temp_get	= 22.1[dC]

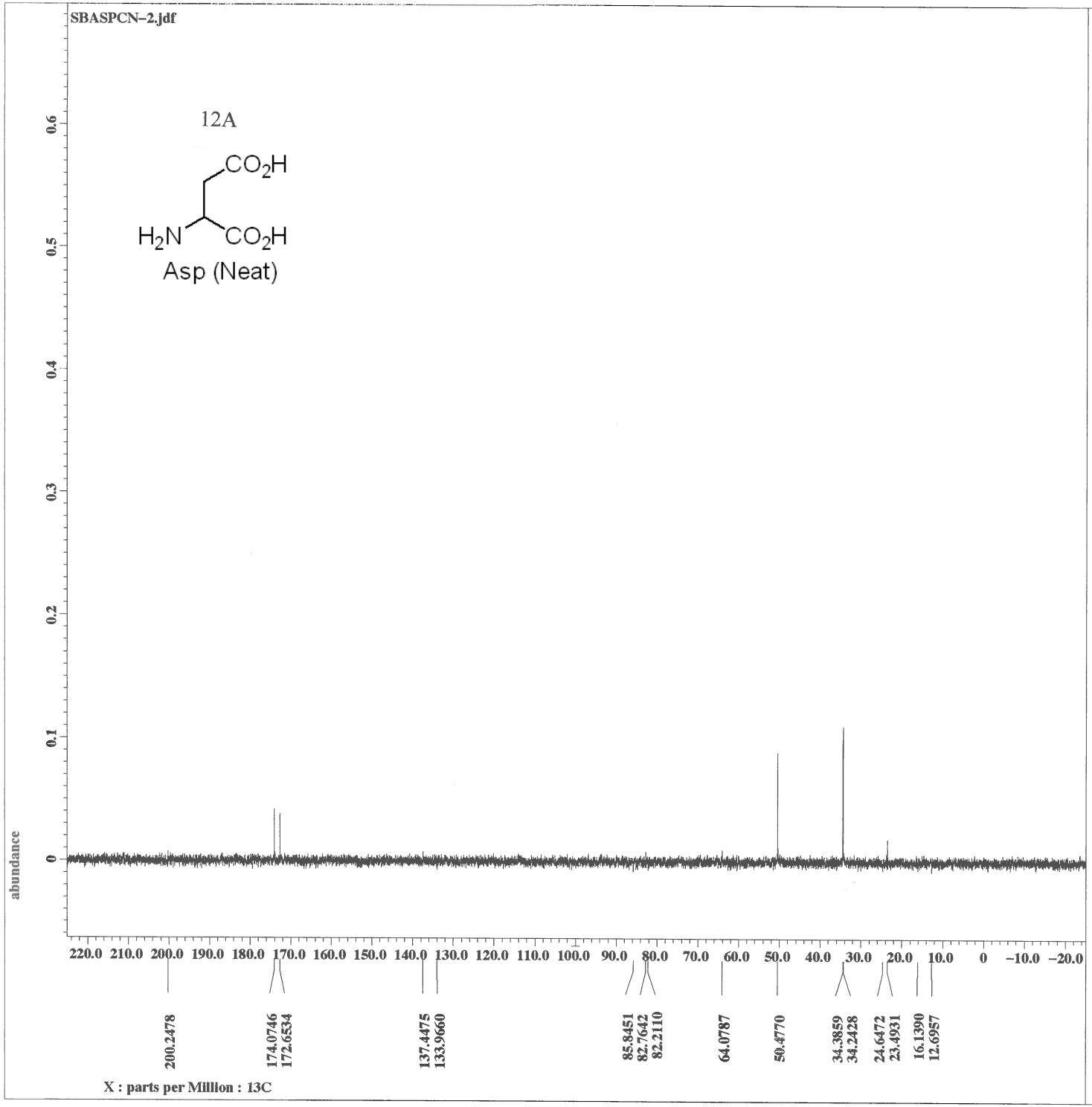


Filename	= SBASPN-3.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= S#481740
Solvent	= D2O
Creation_time	= 24-SEP-2015 02:09:34
Revision_time	= 23-SEP-2015 13:26:50
Current_time	= 23-SEP-2015 13:27:30
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 1.74587904[s]
X_domain	= 1H
X_freq	= 500.15991521[MHz]
X_offset	= 5.0[ppm]
X_points	= 16384
X_prescans	= 0
X_resolution	= 0.57277737[Hz]
X_sweep	= 9.38438438[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Tri_domain	= 1H
Tri_freq	= 500.15991521[MHz]
Tri_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 7
Total_scans	= 7
X_90_width	= 12.54[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 4[dB]
X_pulse	= 6.27[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 42
Relaxation_delay	= 10[s]
Repetition_time	= 11.74587904[s]
Temp_get	= 22[dC]

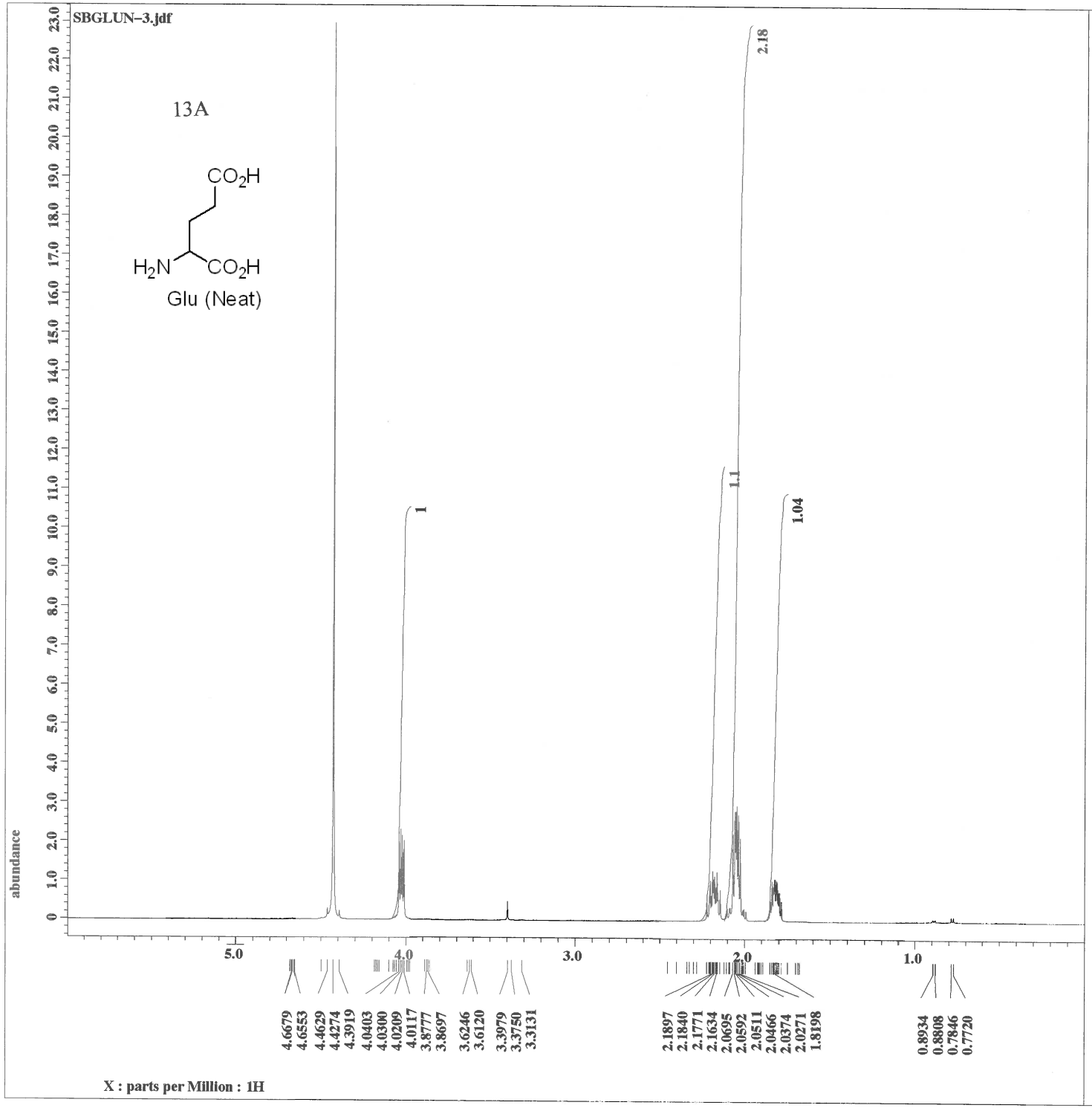
SBASPCN-2.jdf

12A

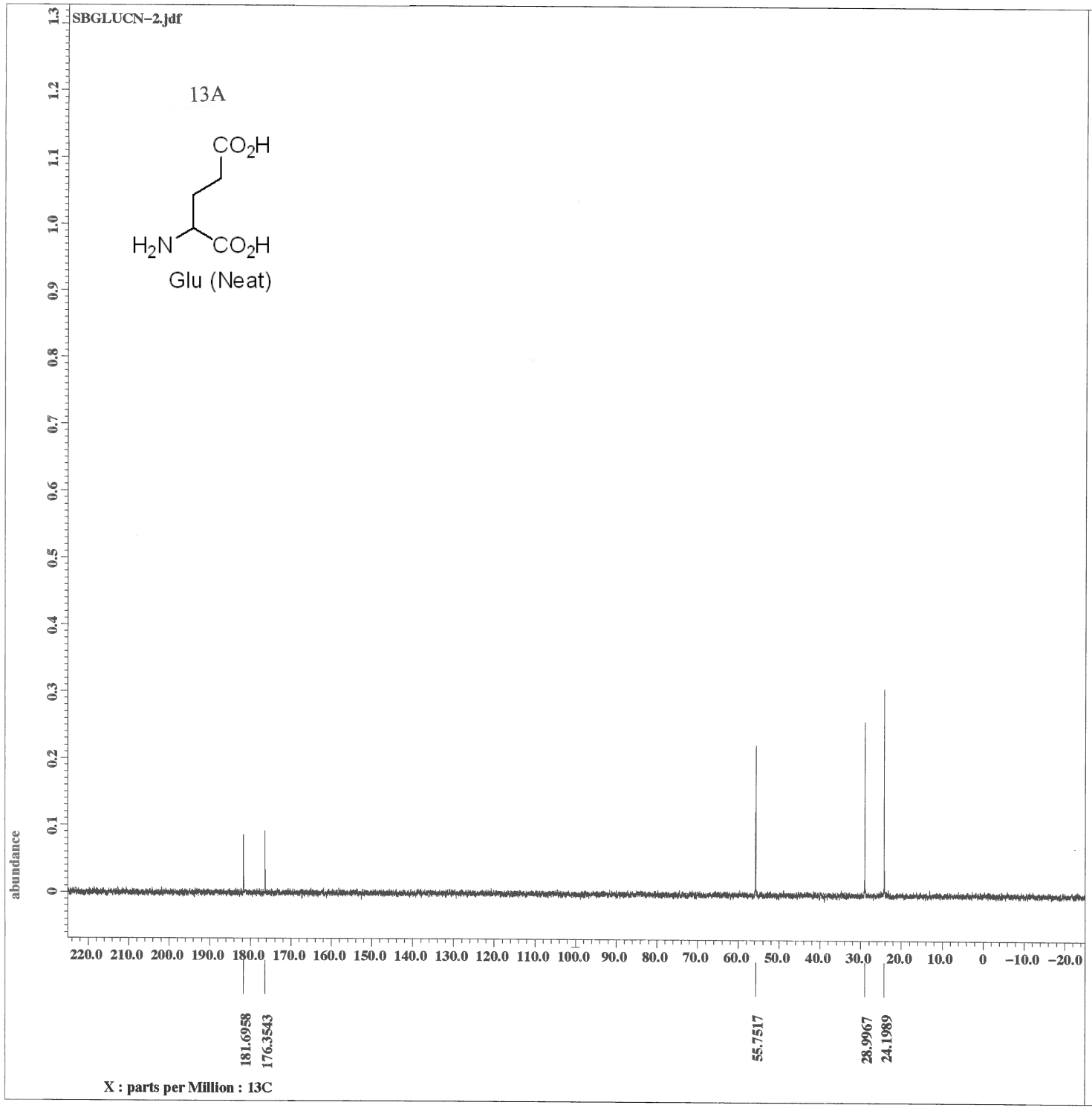
Asp (Neat)



Filename	= SBASPCN-2.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= S#483593
Solvent	= D2O
Creation_time	= 24-SEP-2015 02:17:04
Revision_time	= 23-SEP-2015 13:33:04
Current_time	= 23-SEP-2015 13:33:16
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 0.83361792[s]
X_domain	= 13C
X_freq	= 125.76529768[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.19959034[Hz]
X_sweep	= 39.3081761[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 10
Scans	= 430
Total_scans	= 430
X_90_width	= 10.73[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 9[dB]
X_pulse	= 3.57666667[us]
Irr_atn_dec	= 20[dB]
Irr_atn_noe	= 20[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 0.1[s]
Recvr_gain	= 50
Relaxation_delay	= 0.1[s]
Repetition_time	= 0.93361792[s]
Temp_get	= 22.5[dC]



Filename	= SBGLUN-3.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= S#715952
Solvent	= D2O
Creation_time	= 24-SEP-2015 08:40:44
Revision_time	= 23-SEP-2015 19:57:41
Current_time	= 23-SEP-2015 19:58:39
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 1.74587904[s]
X_domain	= 1H
X_freq	= 500.15991521[MHz]
X_offset	= 5.0[ppm]
X_points	= 16384
X_prescans	= 0
X_resolution	= 0.57277737[Hz]
X_sweep	= 9.38438438[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Tri_domain	= 1H
Tri_freq	= 500.15991521[MHz]
Tri_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 11
Total_scans	= 11
X_90_width	= 12.54[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 4[dB]
X_pulse	= 6.27[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 38
Relaxation_delay	= 10[s]
Repetition_time	= 11.74587904[s]
Temp_get	= 21.9[dC]

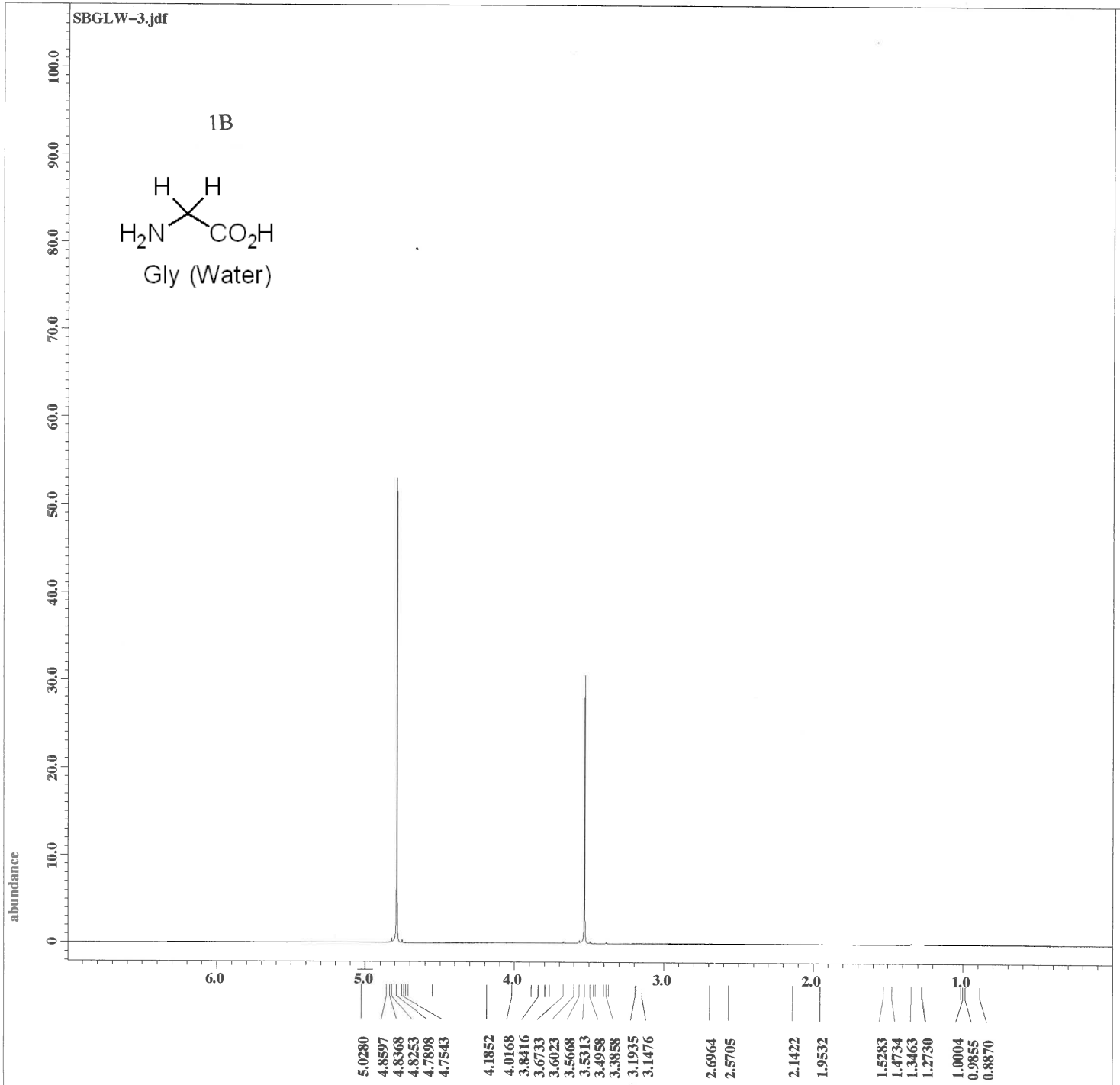


Filename	= SBGLUCN-2.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= S#720106
Solvent	= D2O
Creation_time	= 24-SEP-2015 08:50:35
Revision_time	= 23-SEP-2015 20:06:32
Current_time	= 23-SEP-2015 20:08:52
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 0.83361792[s]
X_domain	= 13C
X_freq	= 125.76529768[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.19959034[Hz]
X_sweep	= 39.3081761[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 10
Scans	= 350
Total_scans	= 350
X_90_width	= 10.73[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 9[dB]
X_pulse	= 3.57666667[us]
Irr_atn_dec	= 20[dB]
Irr_atn_noe	= 20[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 0.2[s]
Recvr_gain	= 50
Relaxation_delay	= 0.2[s]
Repetition_time	= 1.03361792[s]
Temp_get	= 22.4[dC]

SBGLW-3.jdf

1B

Gly (Water)

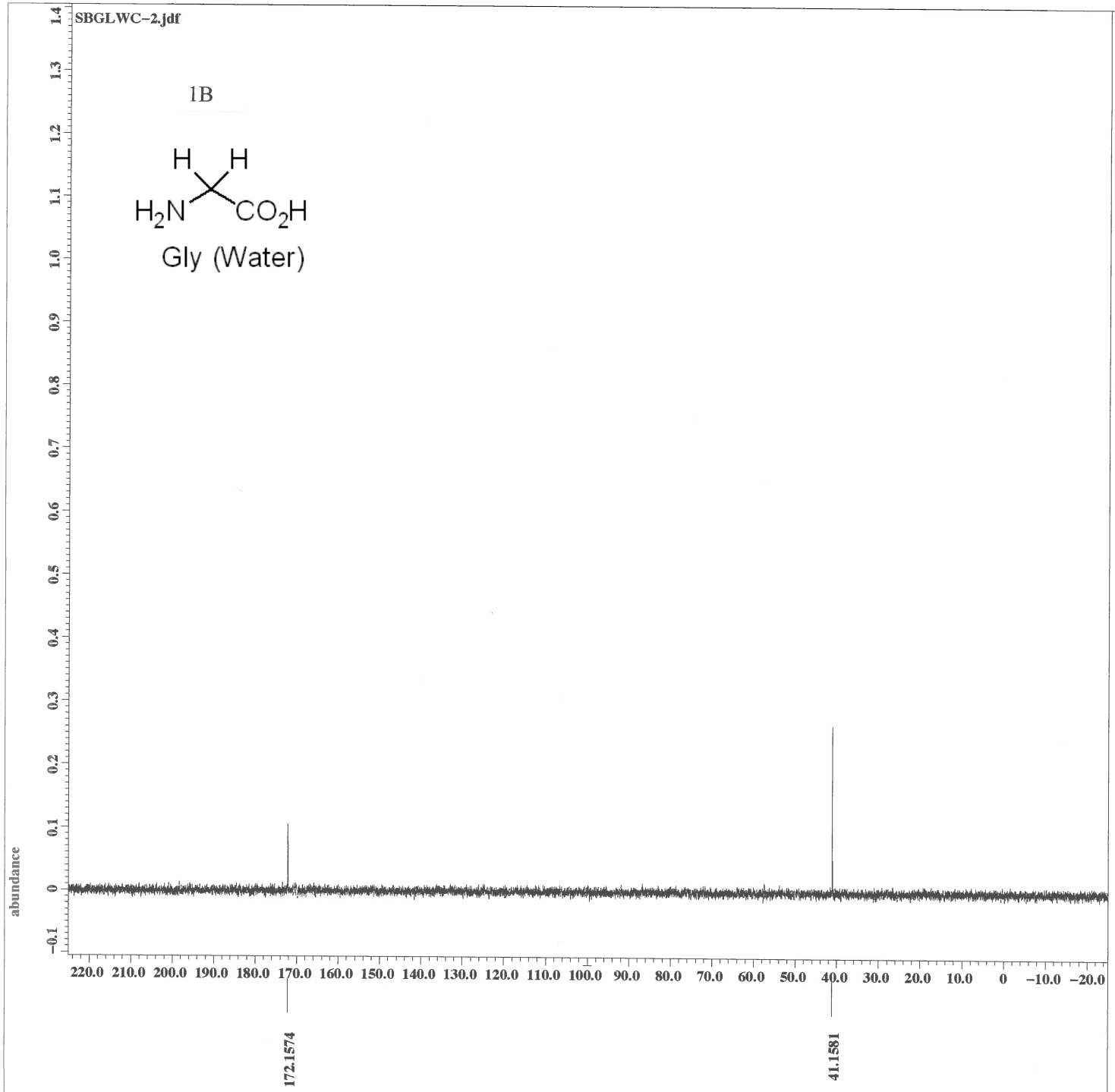


Filename	= SBGLW-3.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= S#356998
Solvent	= D2O
Creation_time	= 5-SEP-2015 22:41:36
Revision_time	= 5-SEP-2015 10:00:29
Current_time	= 5-SEP-2015 10:02:25
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 1.74587904[s]
X_domain	= 1H
X_freq	= 500.15991521[MHz]
X_offset	= 5.0[ppm]
X_points	= 16384
X_prescans	= 0
X_resolution	= 0.57277737[Hz]
X_sweep	= 9.38438438[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Tri_domain	= 1H
Tri_freq	= 500.15991521[MHz]
Tri_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 10
Total_scans	= 10
X_90_width	= 12.54[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 4[dB]
X_pulse	= 6.27[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 40
Relaxation_delay	= 10[s]
Repetition_time	= 11.74587904[s]
Temp_get	= 21[dC]

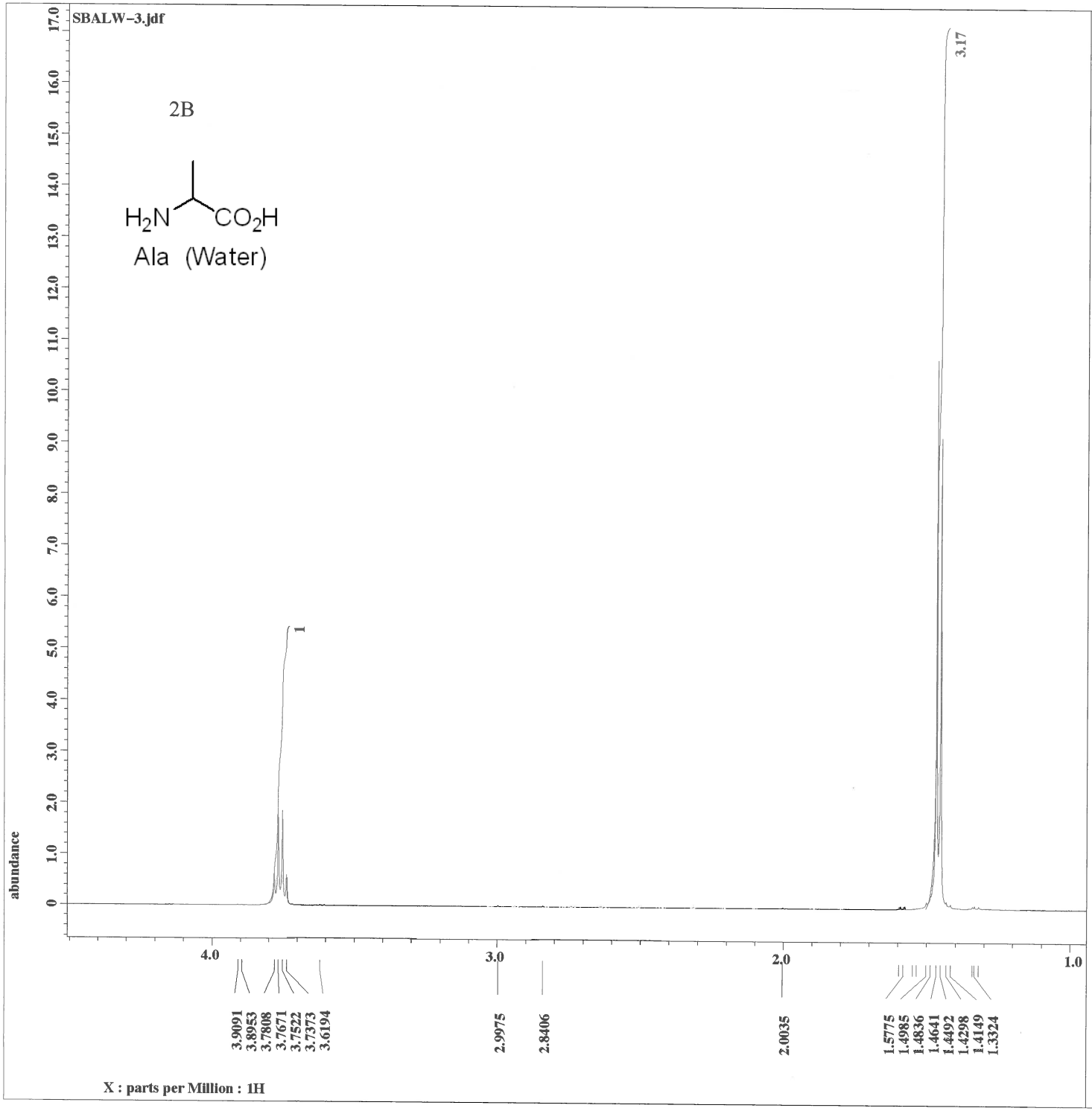
SBGLWC-2.jdf

1B

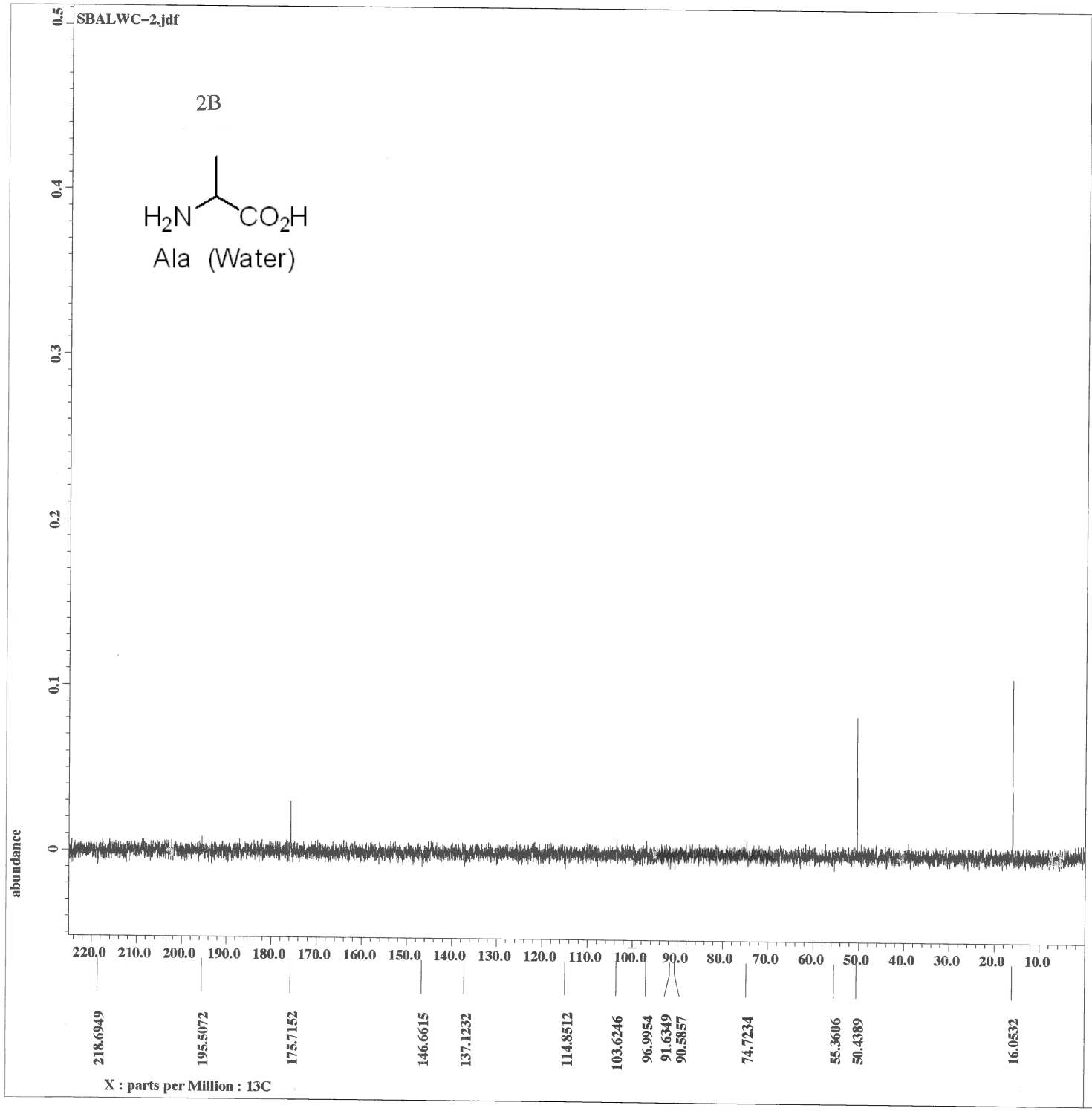
Gly (Water)



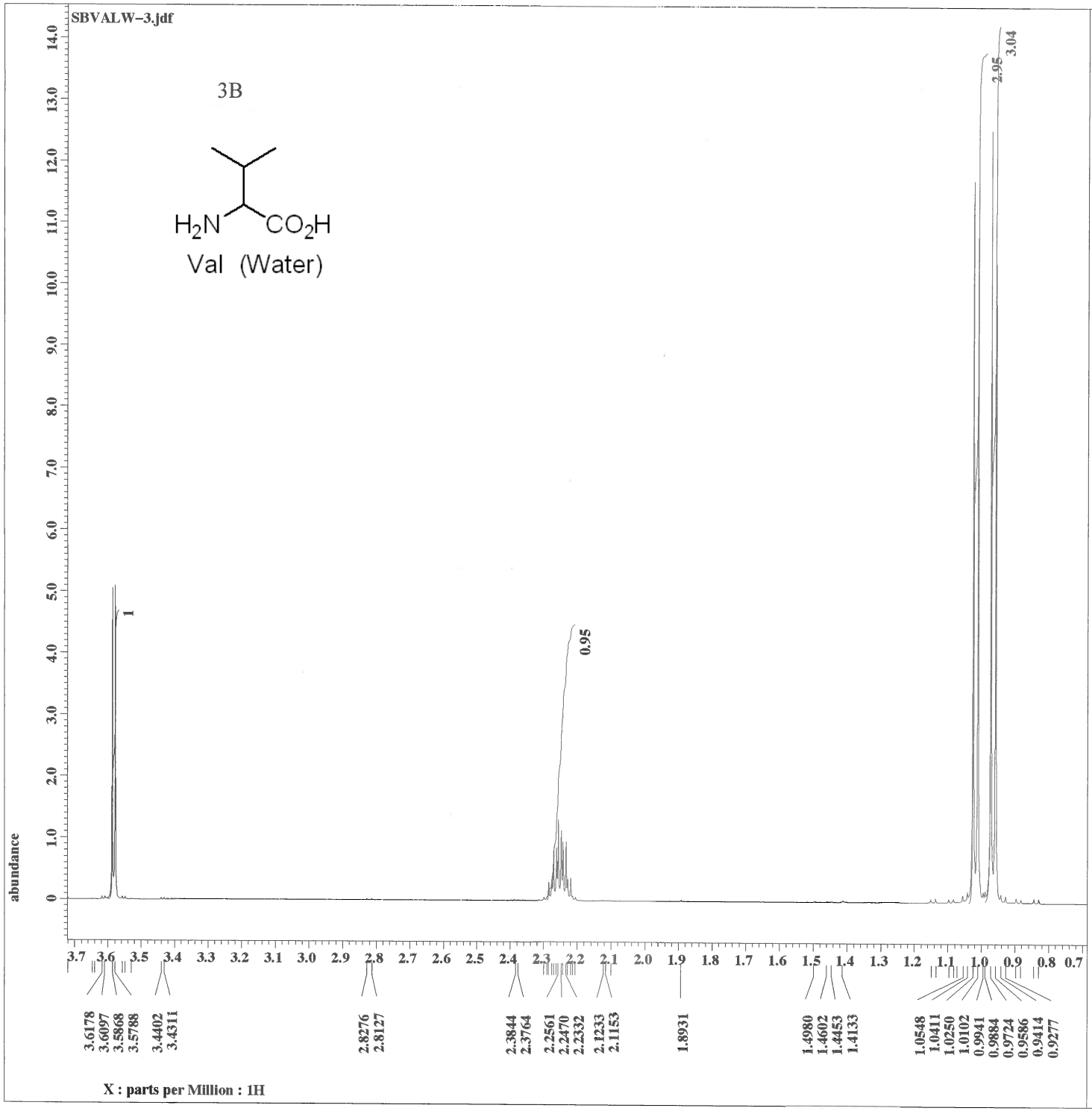
Filename	= SBGLWC-2.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= S#359532
Solvent	= D2O
Creation_time	= 5-SEP-2015 22:49:11
Revision_time	= 5-SEP-2015 10:05:57
Current_time	= 5-SEP-2015 10:06:07
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 0.83361792[s]
X_domain	= 13C
X_freq	= 125.76529768[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.19959034[Hz]
X_sweep	= 39.3081761[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 10
Scans	= 130
Total_scans	= 130
X_90_width	= 10.73[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 9[dB]
X_pulse	= 3.57666667[us]
Irr_atn_dec	= 20[dB]
Irr_atn_noe	= 20[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 2[s]
Recvr_gain	= 50
Relaxation_delay	= 2[s]
Repetition_time	= 2.83361792[s]
Temp_get	= 21.5[dC]




```
Filename          = SBALW-4.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#346045
Solvent           = D2O
Creation_time     =  7-SEP-2015 22:23:24
Revision_time     =  7-SEP-2015 09:43:11
Current_time      =  7-SEP-2015 09:43:12

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = JNM-ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.74587904[s]
X_domain          = 1H
X_freq            = 500.15991521[MHz]
X_offset          = 5.0[ppm]
X_points          = 16384
X_prescans        = 0
X_resolution      = 0.57277737[Hz]
X_sweep           = 9.38438438[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Tri_domain        = 1H
Tri_freq          = 500.15991521[MHz]
Tri_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 12
Total_scans       = 12

X_90_width        = 12.54[us]
X_acq_time        = 1.74587904[s]
X_angle           = 45[deg]
X_atn             = 4[dB]
X_pulse           = 6.27[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 46
Relaxation_delay  = 10[s]
Repetition_time   = 11.74587904[s]
Temp_get          = 21.3[dC]
```




```
Filename          = SBALWC-2.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#348239
Solvent           = D2O
Creation_time     =  7-SEP-2015 22:39:24
Revision_time     =  7-SEP-2015 09:57:35
Current_time      =  7-SEP-2015 09:57:47

Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = JNM-ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 0.83361792[s]
X_domain          = 13C
X_freq            = 125.76529768[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 1.19959034[Hz]
X_sweep           = 39.3081761[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 10
Scans             = 320
Total_scans       = 320

X_90_width        = 10.73[us]
X_acq_time        = 0.83361792[s]
X_angle           = 30[deg]
X_atn             = 9[dB]
X_pulse           = 3.57666667[us]
Irr_atn_dec       = 20[dB]
Irr_atn_noe       = 20[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 50
Relaxation_delay  = 2[s]
Repetition_time   = 2.83361792[s]
Temp_get          = 21.7[dC]
```

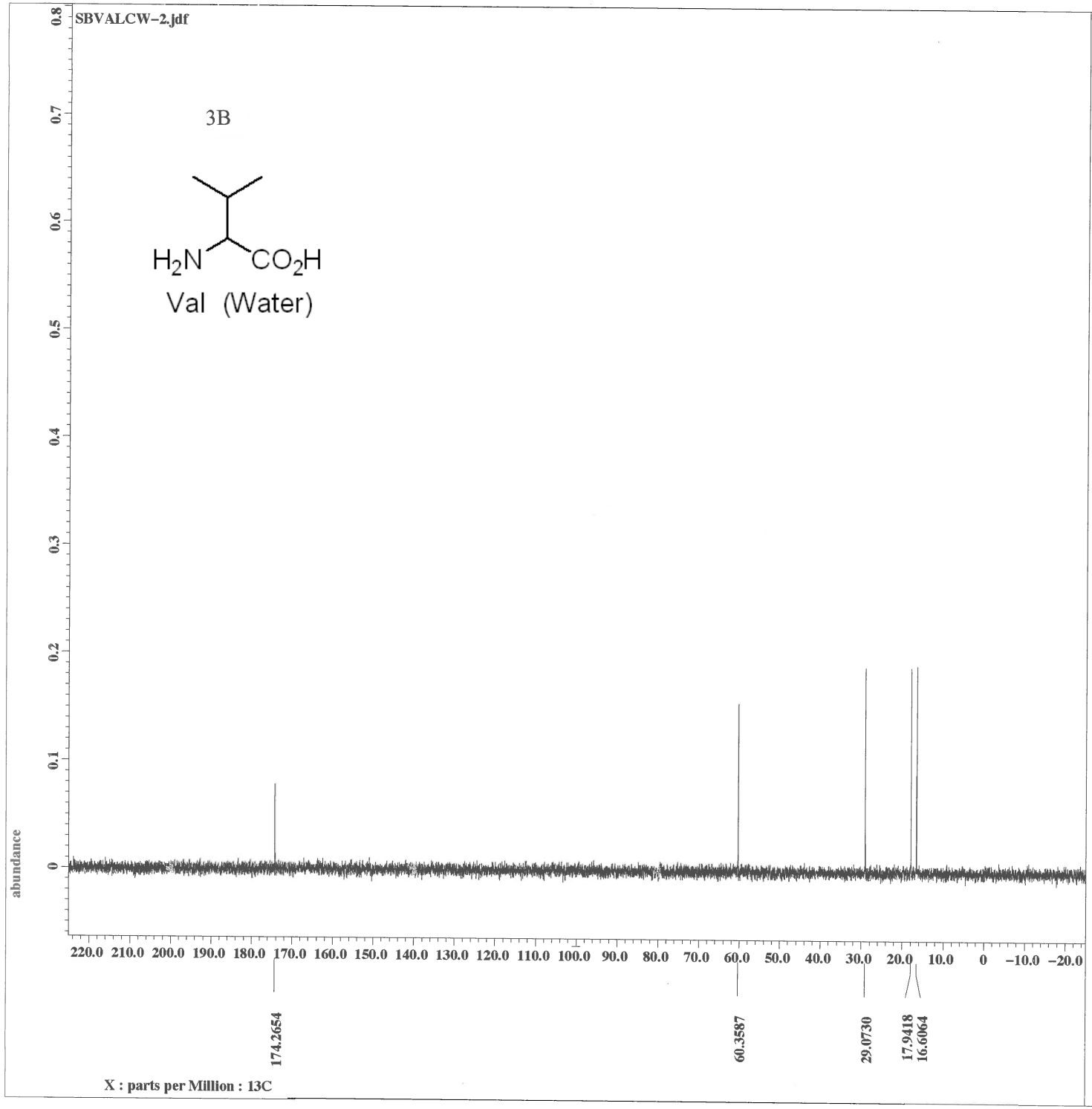



```
Filename          = SBVALW-3.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#344123
Solvent           = D2O
Creation_time     =  5-SEP-2015 22:20:08
Revision_time     =  5-SEP-2015 09:43:45
Current_time      =  5-SEP-2015 09:44:35

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = JNM-ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.74587904[s]
X_domain          = 1H
X_freq            = 500.15991521[MHz]
X_offset          = 5.0[ppm]
X_points          = 16384
X_prescans        = 0
X_resolution      = 0.57277737[Hz]
X_sweep           = 9.38438438[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Tri_domain        = 1H
Tri_freq          = 500.15991521[MHz]
Tri_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 10
Total_scans       = 10

X_90_width        = 12.54[us]
X_acq_time        = 1.74587904[s]
X_angle           = 45[deg]
X_atn             = 4[dB]
X_pulse           = 6.27[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 40
Relaxation_delay  = 10[s]
Repetition_time   = 11.74587904[s]
Temp_get          = 21.1[dC]
```

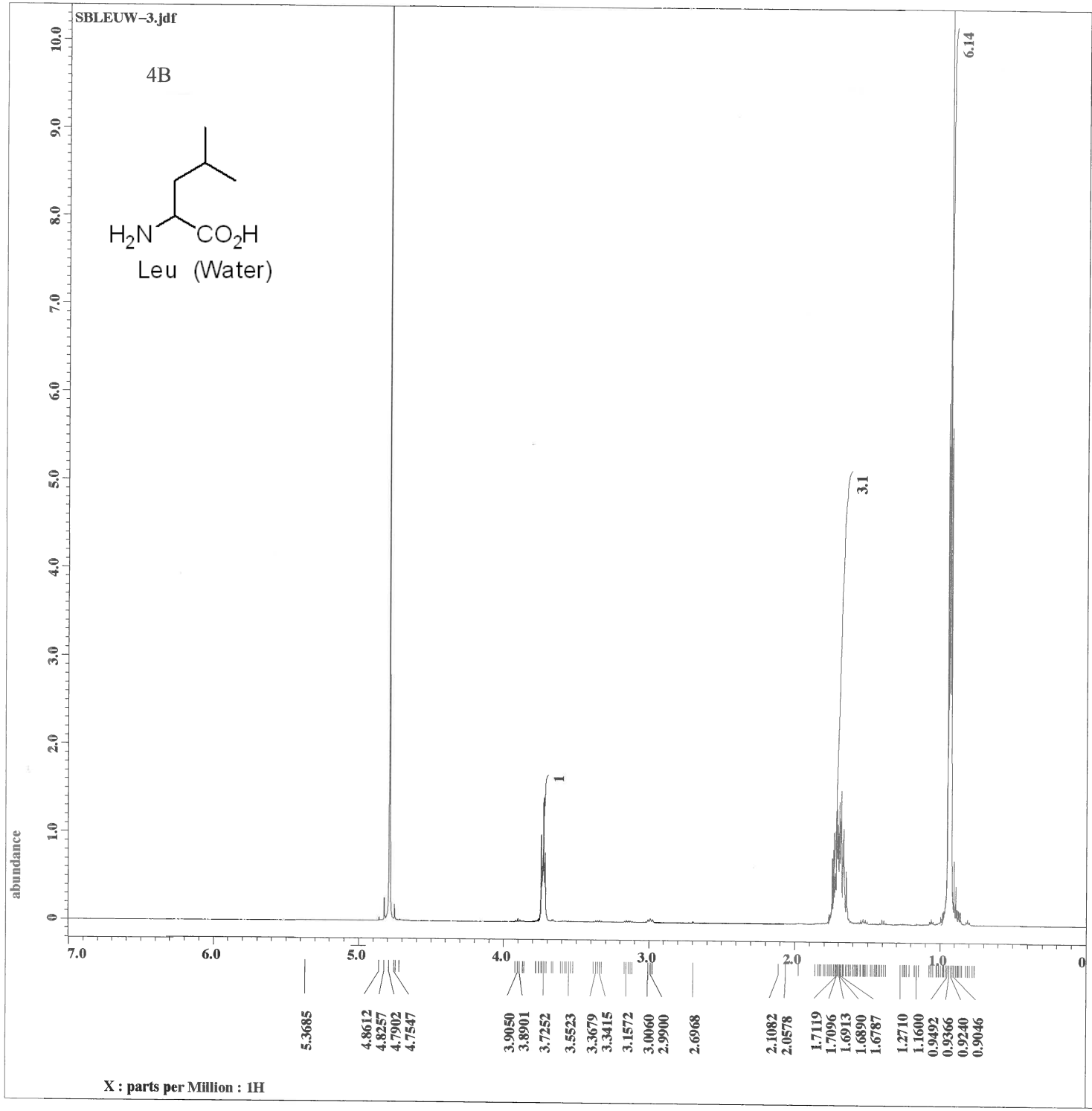
SBVALCW-2.jdf

3B

Val (Water)



Filename	= SBVALCW-2.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= S#346395
Solvent	= D2O
Creation_time	= 5-SEP-2015 22:31:32
Revision_time	= 5-SEP-2015 09:48:54
Current_time	= 5-SEP-2015 09:49:24
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 0.83361792[s]
X_domain	= 13C
X_freq	= 125.76529768[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.19959034[Hz]
X_sweep	= 39.3081761[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 10
Scans	= 220
Total_scans	= 220
X_90_width	= 10.73[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 9[dB]
X_pulse	= 3.57666667[us]
Irr_atn_dec	= 20[dB]
Irr_atn_noe	= 20[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 2[s]
Recvr_gain	= 50
Relaxation_delay	= 2[s]
Repetition_time	= 2.83361792[s]
Temp_get	= 21.5[dC]

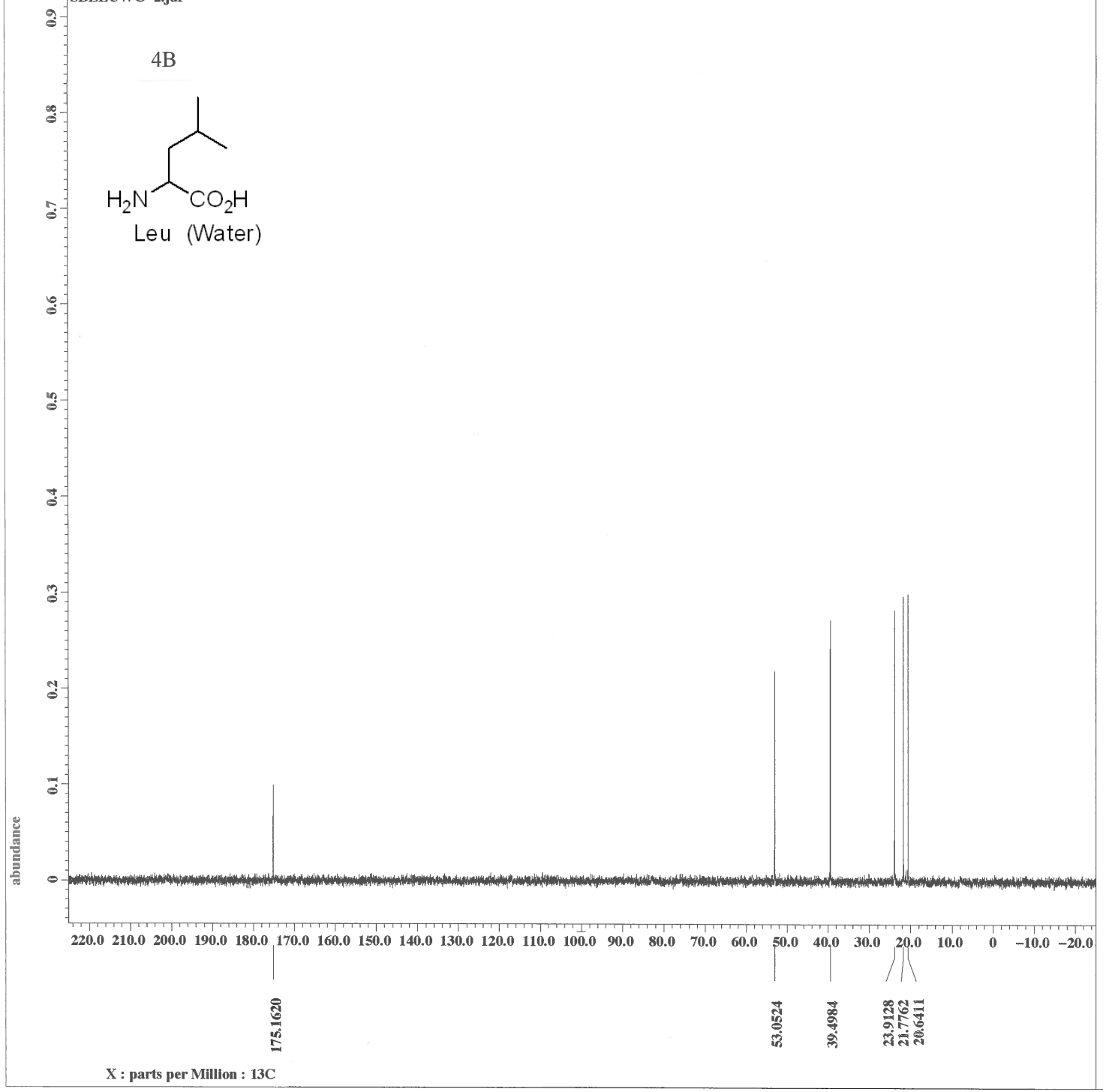



```
Filename          = SBLEUW-3.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#685358
Solvent           = D2O
Creation_time     =  9-SEP-2015 07:49:56
Revision_time     =  8-SEP-2015 19:10:20
Current_time      =  8-SEP-2015 19:10:57

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = JNM-ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.74587904[s]
X_domain          = 1H
X_freq            = 500.15991521[MHz]
X_offset          = 5.0[ppm]
X_points          = 16384
X_prescans        = 0
X_resolution      = 0.57277737[Hz]
X_sweep           = 9.38438438[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Tri_domain        = 1H
Tri_freq          = 500.15991521[MHz]
Tri_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 10
Total_scans       = 10

X_90_width        = 12.54[us]
X_acq_time        = 1.74587904[s]
X_angle           = 45[deg]
X_atn             = 4[dB]
X_pulse           = 6.27[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 34
Relaxation_delay  = 10[s]
Repetition_time   = 11.74587904[s]
Temp_get          = 21.3[dC]
```

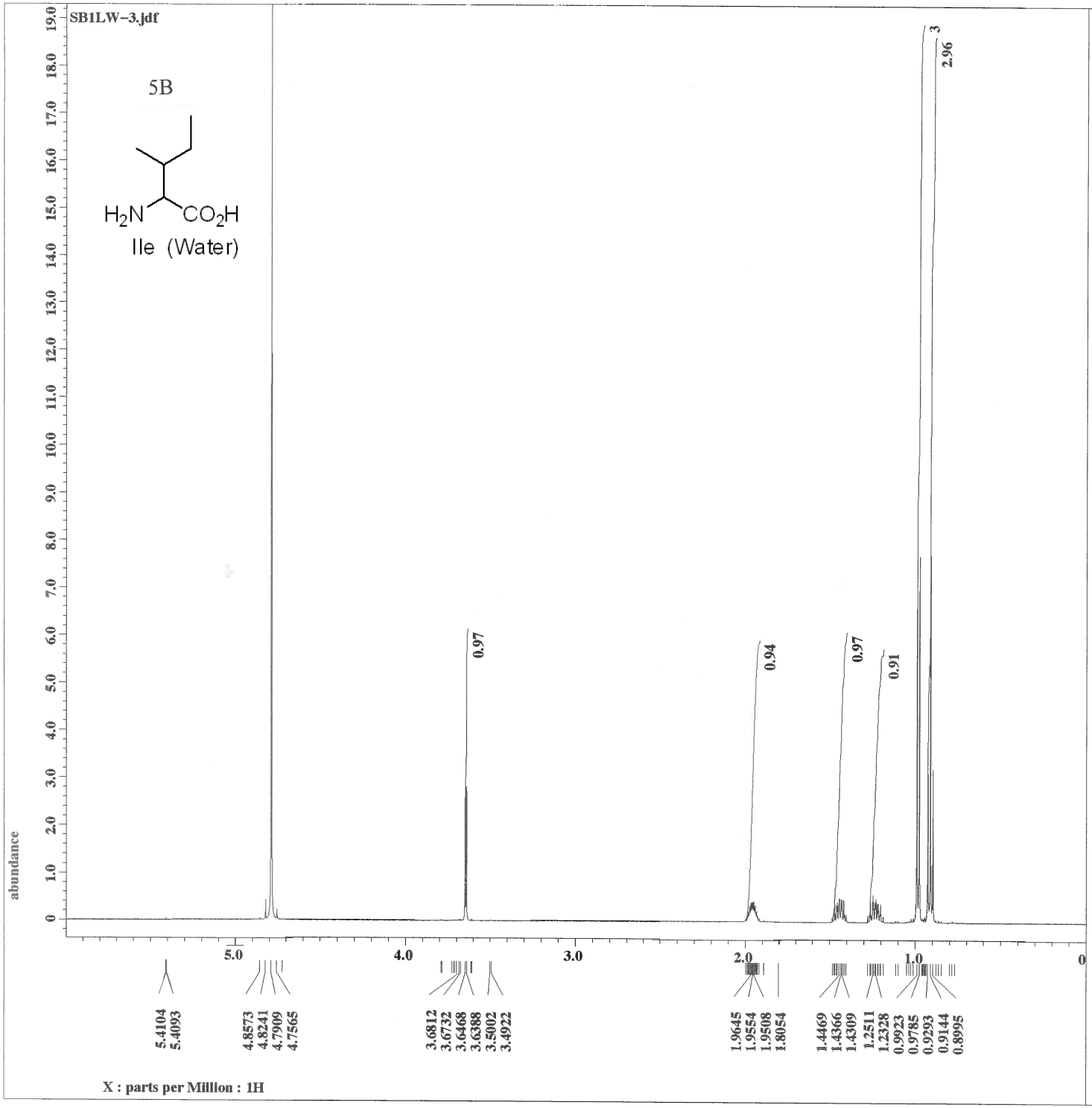
SBLEUWC-2.jdf

4B

Leu (Water)



Filename	= SBLEUWC-2.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= S#688161
Solvent	= D2O
Creation_time	= 9-SEP-2015 07:57:40
Revision_time	= 8-SEP-2015 19:14:22
Current_time	= 8-SEP-2015 19:14:59
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 0.83361792[s]
X_domain	= 13C
X_freq	= 125.76529768[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.19959034[Hz]
X_sweep	= 39.3081761[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 10
Scans	= 310
Total_scans	= 310
X_90_width	= 10.73[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 9[dB]
X_pulse	= 3.57666667[us]
Irr_atn_dec	= 20[dB]
Irr_atn_noe	= 20[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 0.5[s]
Recvr_gain	= 50
Relaxation_delay	= 0.5[s]
Repetition_time	= 1.33361792[s]
Temp_get	= 21.8[dC]

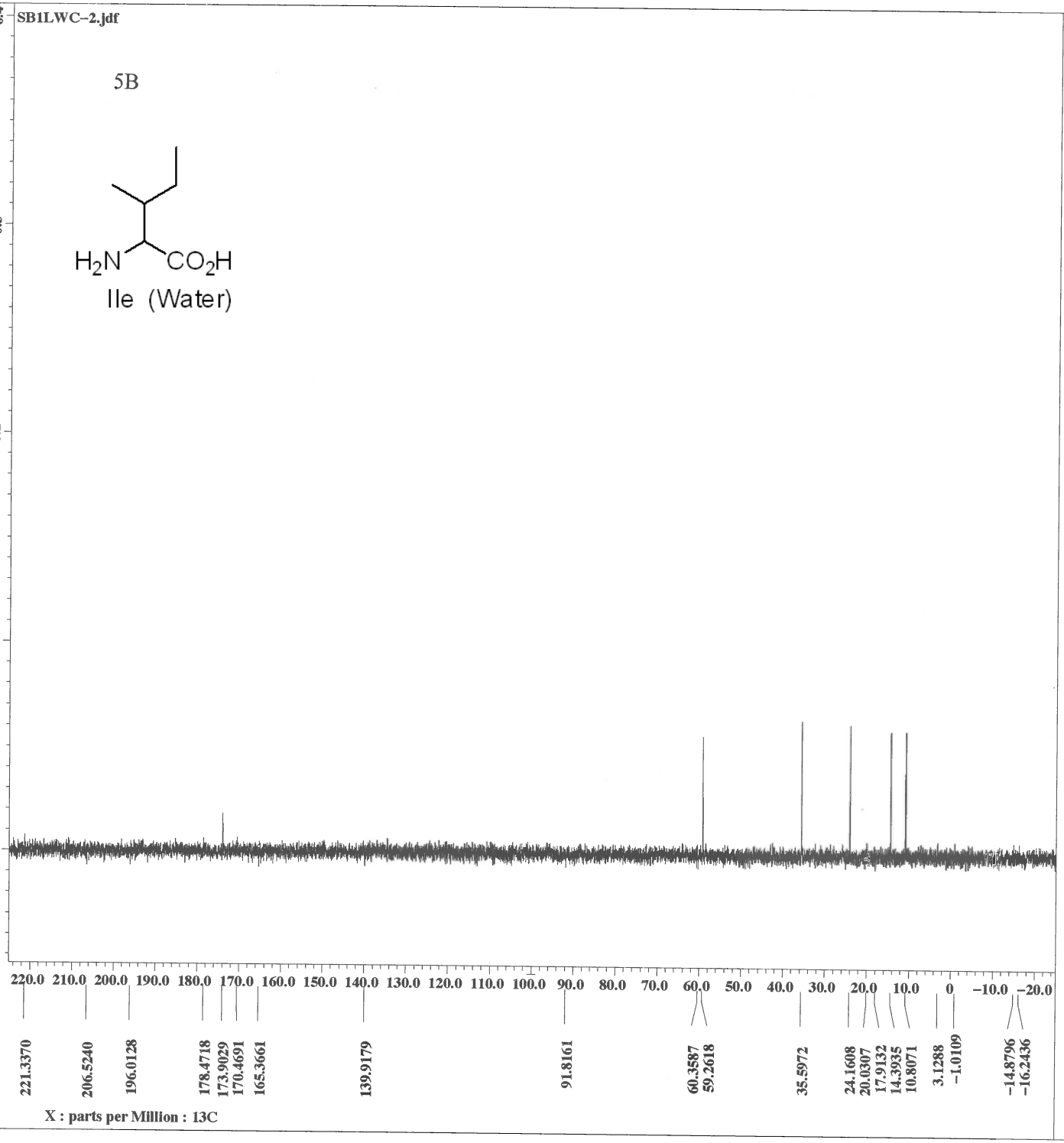



```
Filename          = SB1LW-3.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#640441
Solvent           = D2O
Creation_time     =  8-SEP-2015 06:34:04
Revision_time     =  7-SEP-2015 17:58:14
Current_time      =  7-SEP-2015 17:58:59

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = JNM-ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.74587904[s]
X_domain          = 1H
X_freq            = 500.15991521[MHz]
X_offset          = 5.0[ppm]
X_points          = 16384
X_prescans        = 0
X_resolution      = 0.57277737[Hz]
X_sweep           = 9.38438438[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Tri_domain        = 1H
Tri_freq          = 500.15991521[MHz]
Tri_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 12
Total_scans       = 12

X_90_width        = 12.54[us]
X_acq_time        = 1.74587904[s]
X_angle           = 45[deg]
X_atn             = 4[dB]
X_pulse           = 6.27[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 46
Relaxation_delay  = 10[s]
Repetition_time   = 11.74587904[s]
Temp_get          = 20.9[dC]
```

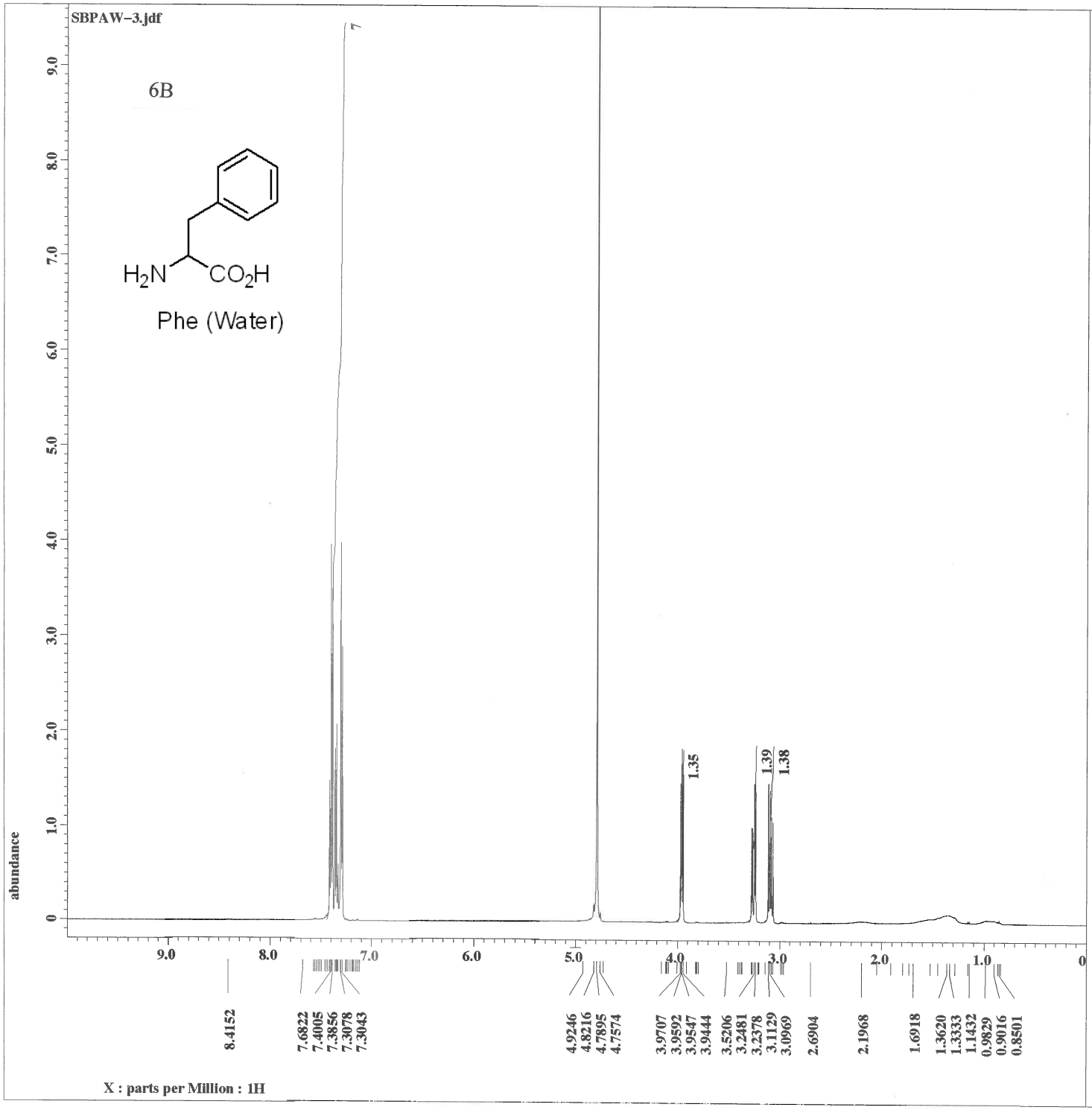
SB1LWC-2.jdf

5B

Ile (Water)



Filename	= SB1LWC-2.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= S#642712
Solvent	= D2O
Creation_time	= 8-SEP-2015 06:50:00
Revision_time	= 7-SEP-2015 18:07:13
Current_time	= 7-SEP-2015 18:07:28
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 0.83361792[s]
X_domain	= 13C
X_freq	= 125.76529768[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.19959034[Hz]
X_sweep	= 39.3081761[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 10
Scans	= 490
Total_scans	= 490
X_90_width	= 10.73[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 9[dB]
X_pulse	= 3.57666667[us]
Irr_atn_dec	= 20[dB]
Irr_atn_noe	= 20[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 1[s]
Recvr_gain	= 50
Relaxation_delay	= 1[s]
Repetition_time	= 1.83361792[s]
Temp_get	= 21.6[dC]

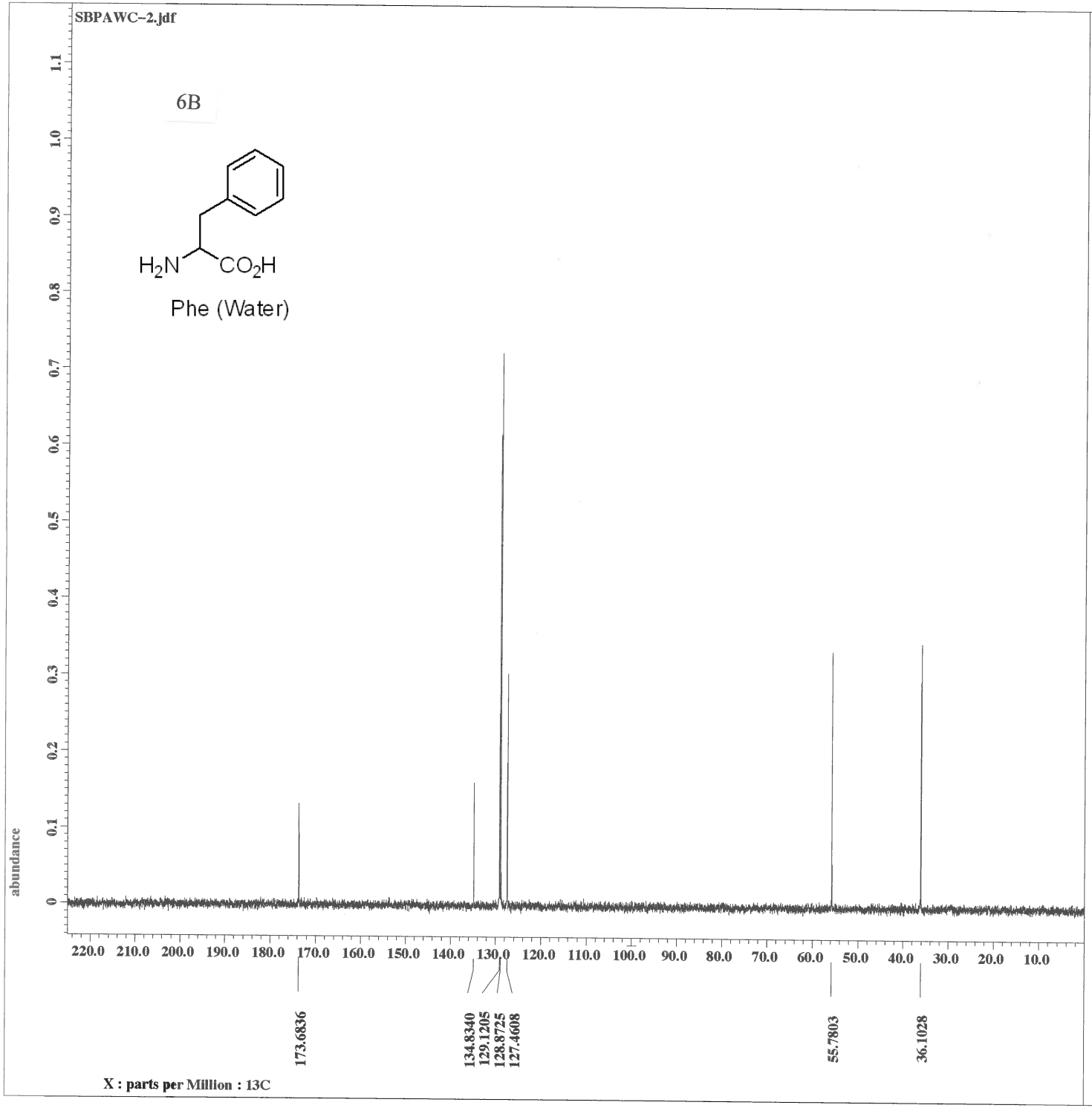


Filename	= SBPAW-3.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= S#695842
Solvent	= D2O
Creation_time	= 9-SEP-2015 08:06:28
Revision_time	= 8-SEP-2015 19:25:33
Current_time	= 8-SEP-2015 19:26:16
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 1.74587904[s]
X_domain	= 1H
X_freq	= 500.15991521[MHz]
X_offset	= 5.0[ppm]
X_points	= 16384
X_prescans	= 0
X_resolution	= 0.57277737[Hz]
X_sweep	= 9.38438438[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Tri_domain	= 1H
Tri_freq	= 500.15991521[MHz]
Tri_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 10
Total_scans	= 10
X_90_width	= 12.54[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 4[dB]
X_pulse	= 6.27[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 34
Relaxation_delay	= 10[s]
Repetition_time	= 11.74587904[s]
Temp_get	= 21.3[dC]

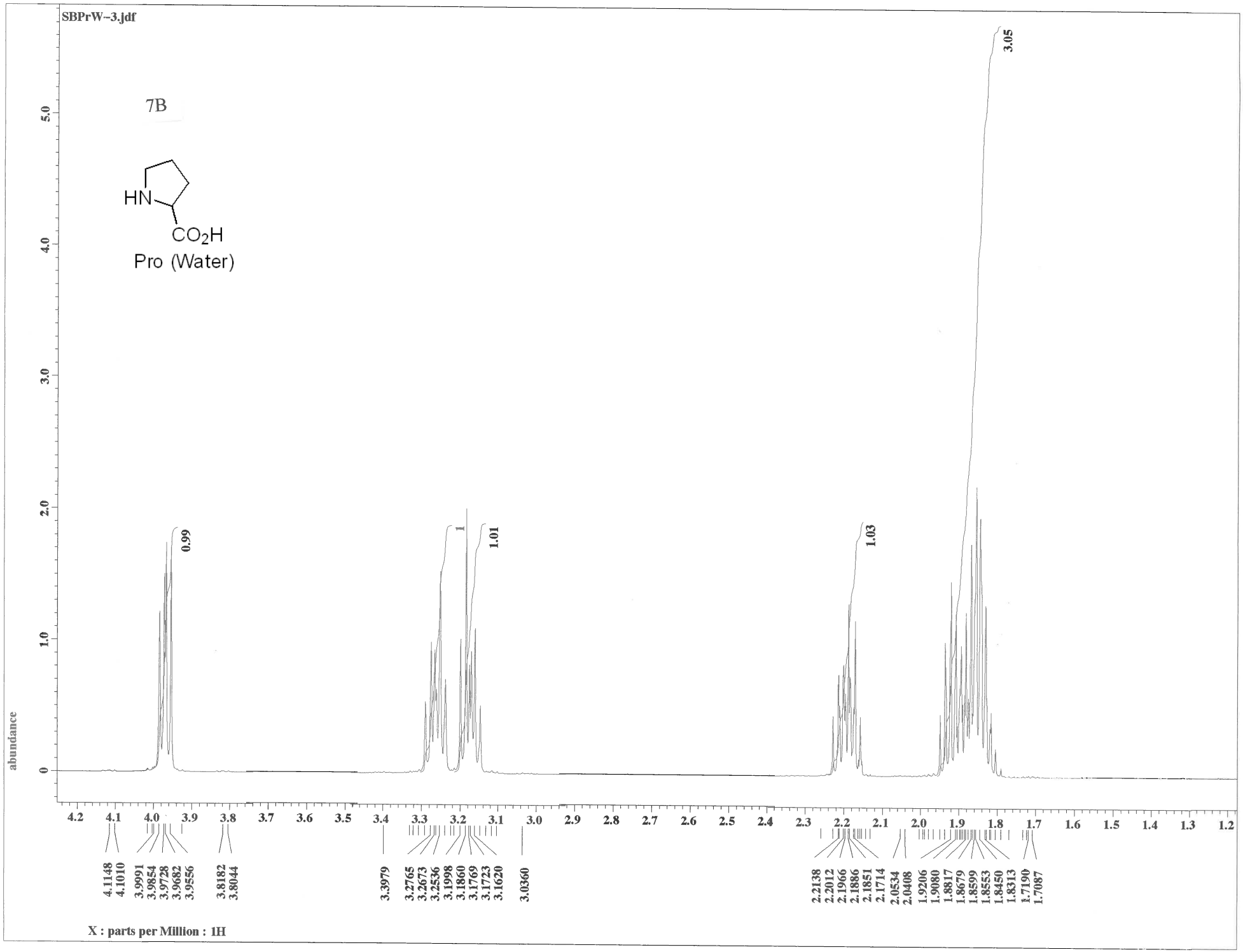
SBPAWC-2.jdf

6B

Phe (Water)



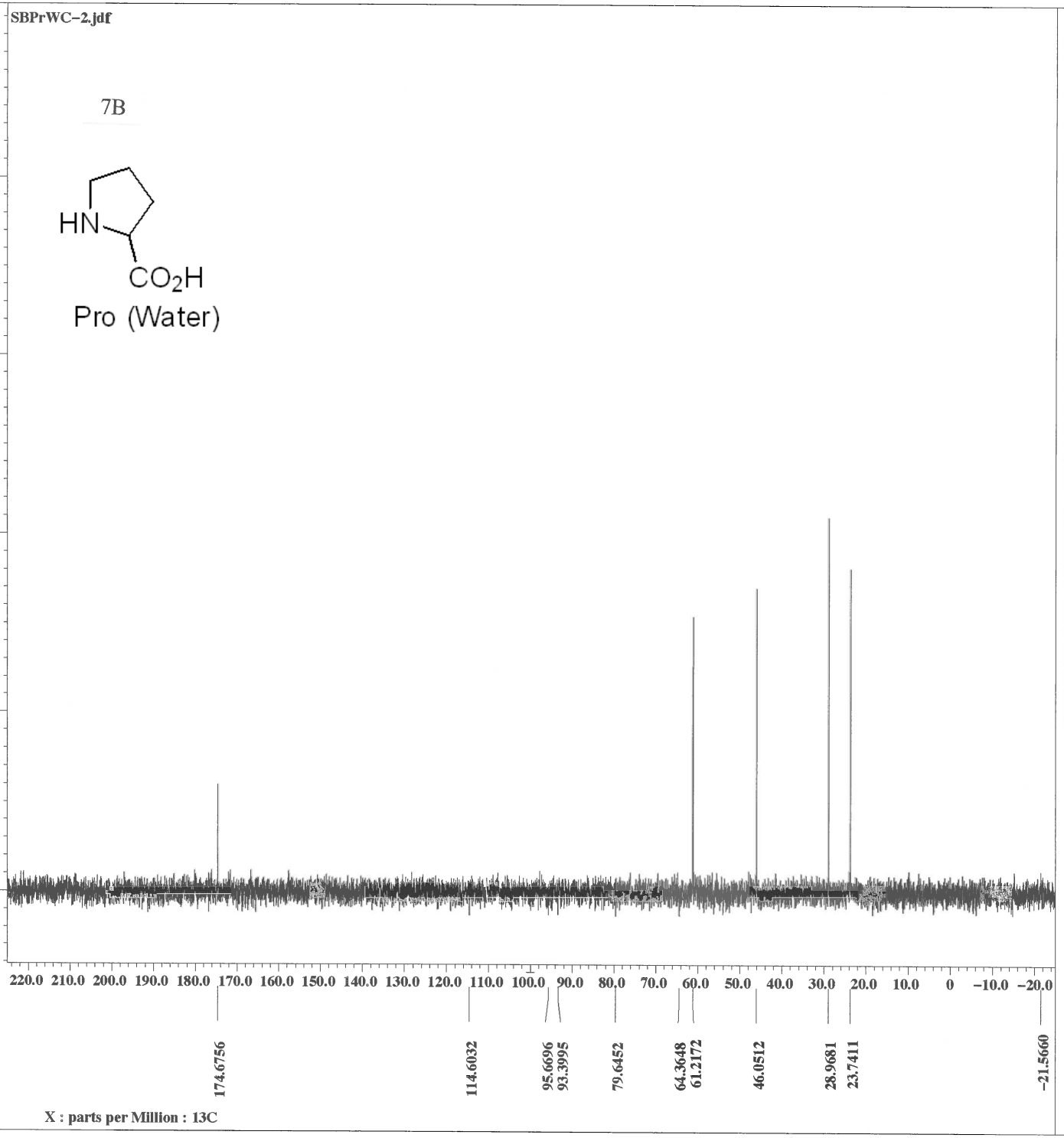
Filename	= SBPAWC-2.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= S#698167
Solvent	= D2O
Creation_time	= 9-SEP-2015 08:12:34
Revision_time	= 8-SEP-2015 19:29:24
Current_time	= 8-SEP-2015 19:29:33
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 0.83361792[s]
X_domain	= 13C
X_freq	= 125.76529768[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.19959034[Hz]
X_sweep	= 39.3081761[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 10
Scans	= 230.0
Total_scans	= 230.0
X_90_width	= 10.73[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 9[dB]
X_pulse	= 3.57666667[us]
Irr_atn_dec	= 20[dB]
Irr_atn_noe	= 20[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 0.5[s]
Recvr_gain	= 50
Relaxation_delay	= 0.5[s]
Repetition_time	= 1.33361792[s]
Temp_get	= 21.7[dC]


SBPrW-3.jdf
7B
HN
CO2H
Pro (Water)
abundance
X : parts per Million : 1H
0.99
1
1.01
1.03
3.05
4.1148
4.1010
3.9991
3.9854
3.9728
3.9682
3.9556
3.8182
3.8044
3.3979
3.2765
3.2673
3.2536
3.1998
3.1860
3.1769
3.1723
3.1620
3.0360
2.2138
2.2012
2.1966
2.1886
2.1851
2.1714
2.0534
2.0408
1.9206
1.9080
1.8817
1.8679
1.8599
1.8553
1.8450
1.8313
1.7190
1.7087

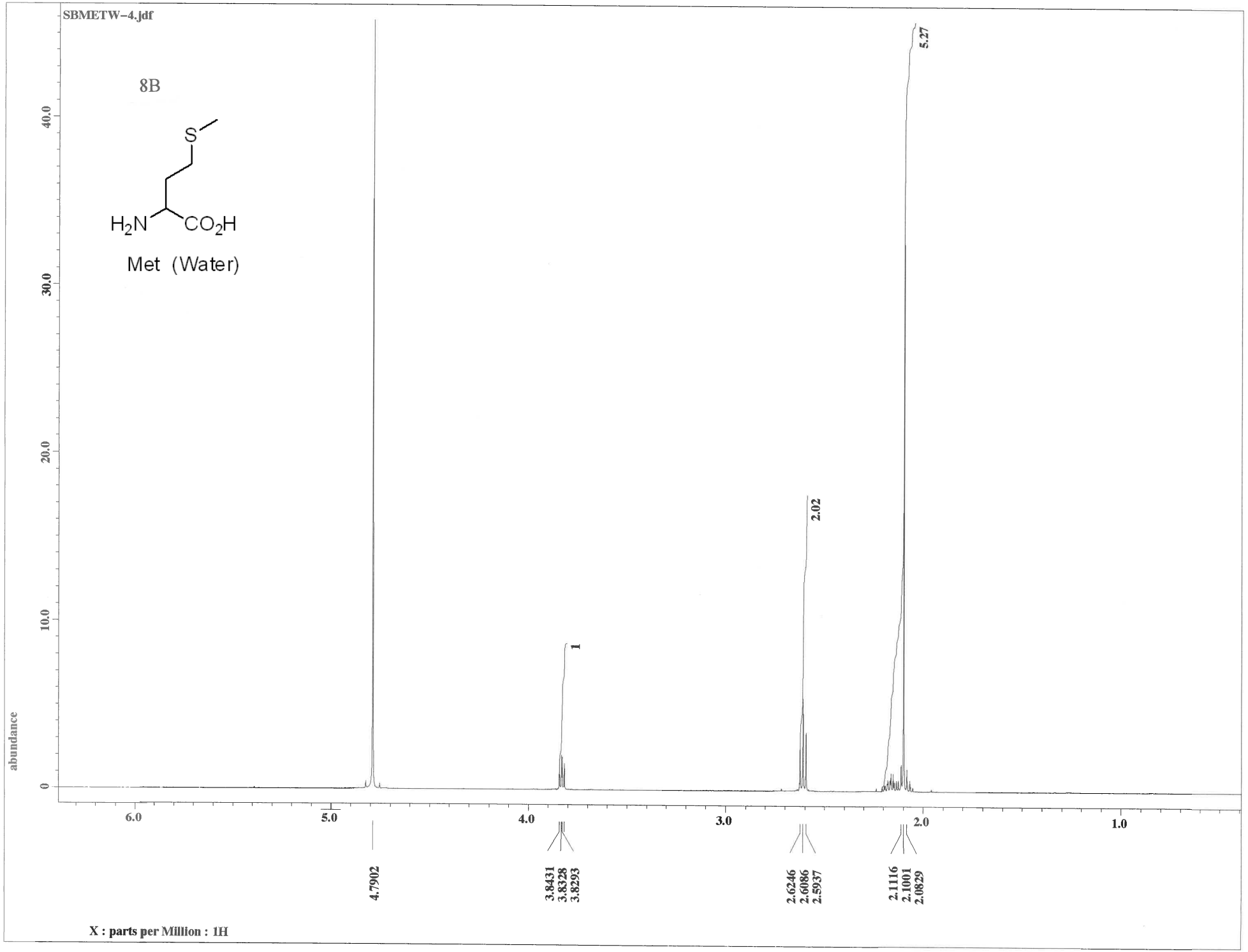
SBPrWC-2.jdf

7B

Pro (Water)



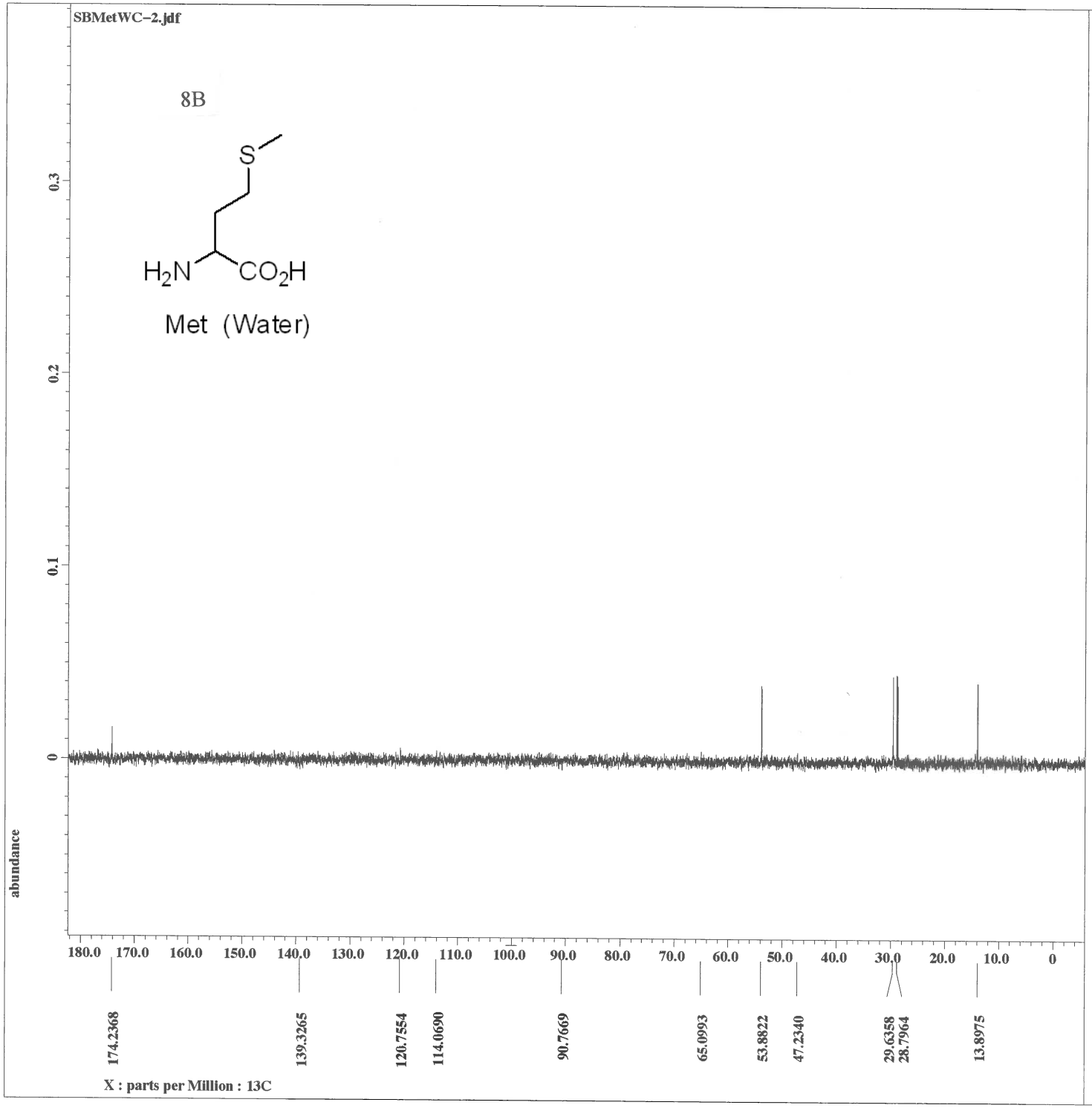
Filename	= SBPrWC-2.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= S#697198
Solvent	= D2O
Creation_time	= 5-SEP-2015 08:12:28
Revision_time	= 4-SEP-2015 19:29:27
Current_time	= 4-SEP-2015 19:31:06
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 0.83361792[s]
X_domain	= 13C
X_freq	= 125.76529768[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.19959034[Hz]
X_sweep	= 39.3081761[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 10
Scans	= 140
Total_scans	= 140
X_90_width	= 10.73[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 9[dB]
X_pulse	= 3.57666667[us]
Irr_atn_dec	= 20[dB]
Irr_atn_noe	= 20[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 2[s]
Recvr_gain	= 50
Relaxation_delay	= 2[s]
Repetition_time	= 2.83361792[s]
Temp_get	= 21[dC]


SBMETW-4.jdf
8B
S
H2N
CO2H
Met (Water)
abundance
40.0
30.0
20.0
10.0
0
6.0
5.0
4.0
3.0
2.0
1.0
5.27
2.02
1
4.7902
3.8431
3.8328
3.8293
2.6246
2.6086
2.5937
2.1116
2.1001
2.0829
X : parts per Million : 1H

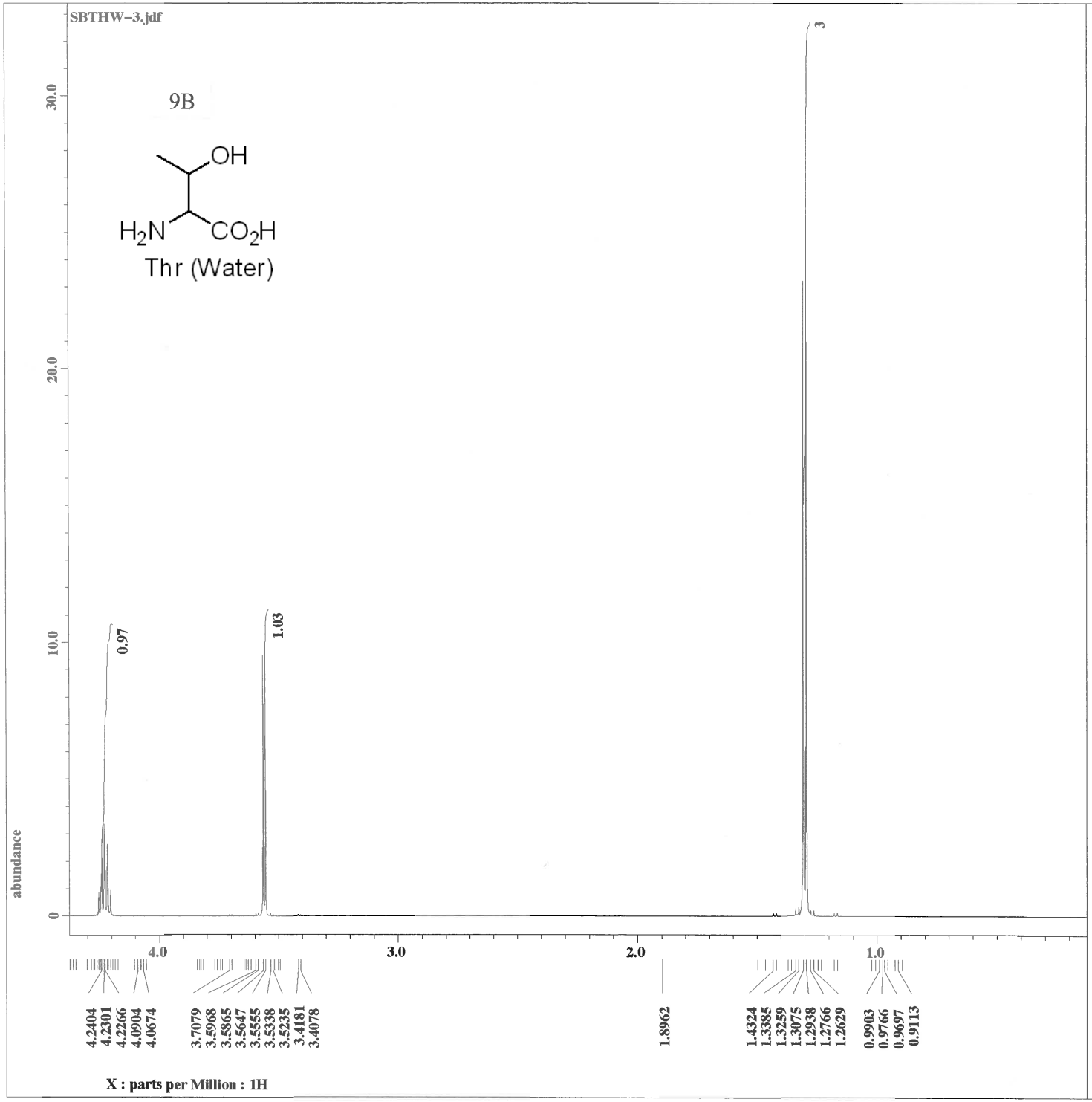
SBMetWC-2.jdf

8B

Met (Water)



Filename	= SBMetWC-2.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= S#703584
Solvent	= D2O
Creation_time	= 5-SEP-2015 08:56:06
Revision_time	= 4-SEP-2015 20:13:30
Current_time	= 4-SEP-2015 20:13:59
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 0.83361792[s]
X_domain	= 13C
X_freq	= 125.76529768[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.19959034[Hz]
X_sweep	= 39.3081761[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 10
Scans	= 840
Total_scans	= 840
X_90_width	= 10.73[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 9[dB]
X_pulse	= 3.57666667[us]
Irr_atn_dec	= 20[dB]
Irr_atn_noe	= 20[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 2[s]
Recvr_gain	= 50
Relaxation_delay	= 2[s]
Repetition_time	= 2.83361792[s]
Temp_get	= 21.5[dC]

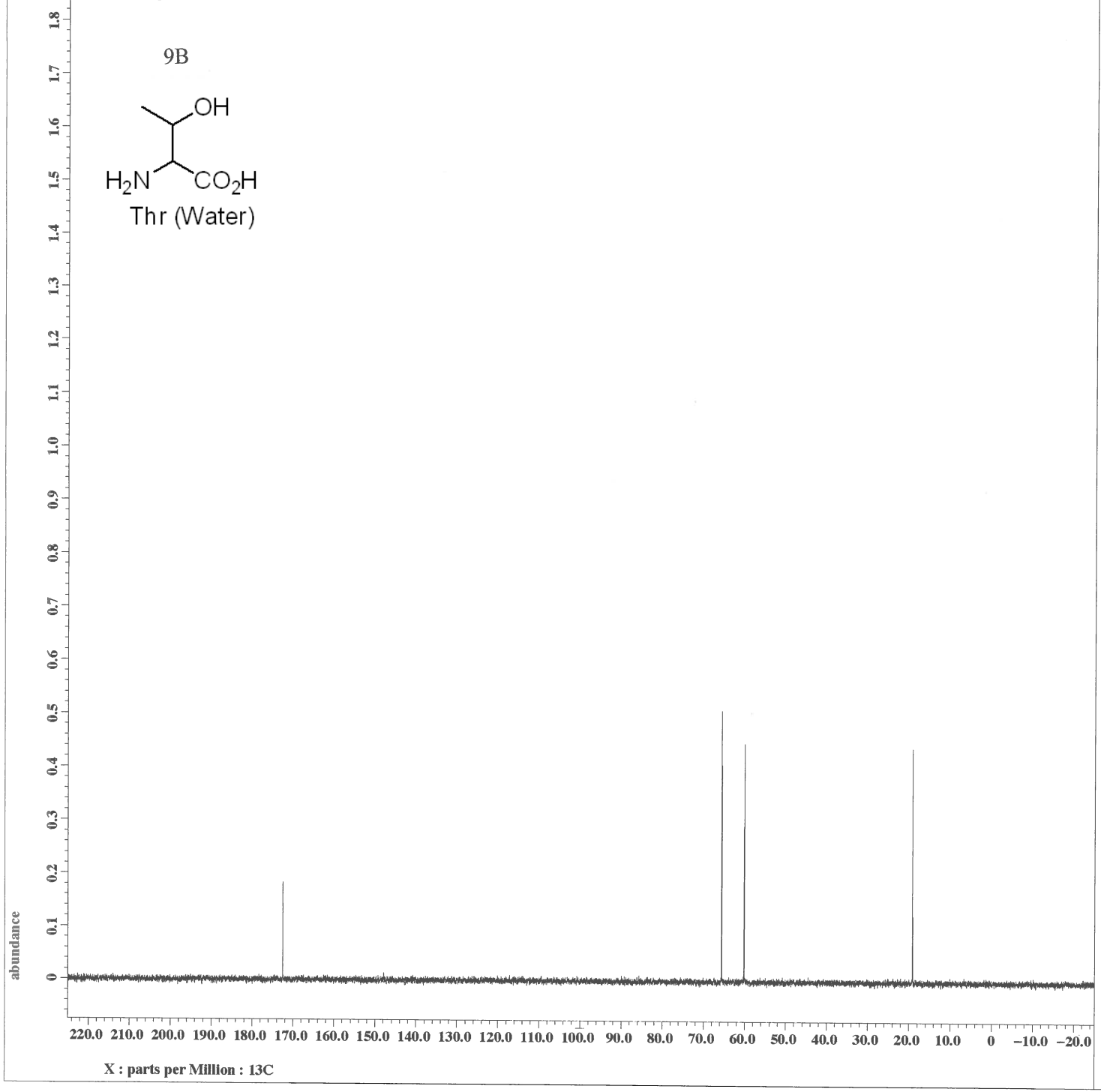



```
Filename          = SBTHW-3.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#655485
Solvent           = D2O
Creation_time     =  8-SEP-2015 07:00:19
Revision_time     =  7-SEP-2015 18:19:41
Current_time      =  7-SEP-2015 18:20:31

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = JNM-ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.74587904[s]
X_domain          = 1H
X_freq            = 500.15991521[MHz]
X_offset          = 5.0[ppm]
X_points          = 16384
X_prescans        = 0
X_resolution      = 0.57277737[Hz]
X_sweep           = 9.38438438[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Tri_domain        = 1H
Tri_freq          = 500.15991521[MHz]
Tri_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 16
Total_scans       = 16

X_90_width        = 12.54[us]
X_acq_time        = 1.74587904[s]
X_angle           = 45[deg]
X_atn             = 4[dB]
X_pulse           = 6.27[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 36
Relaxation_delay  = 10[s]
Repetition_time   = 11.74587904[s]
Temp_get          = 21.2[dC]
```

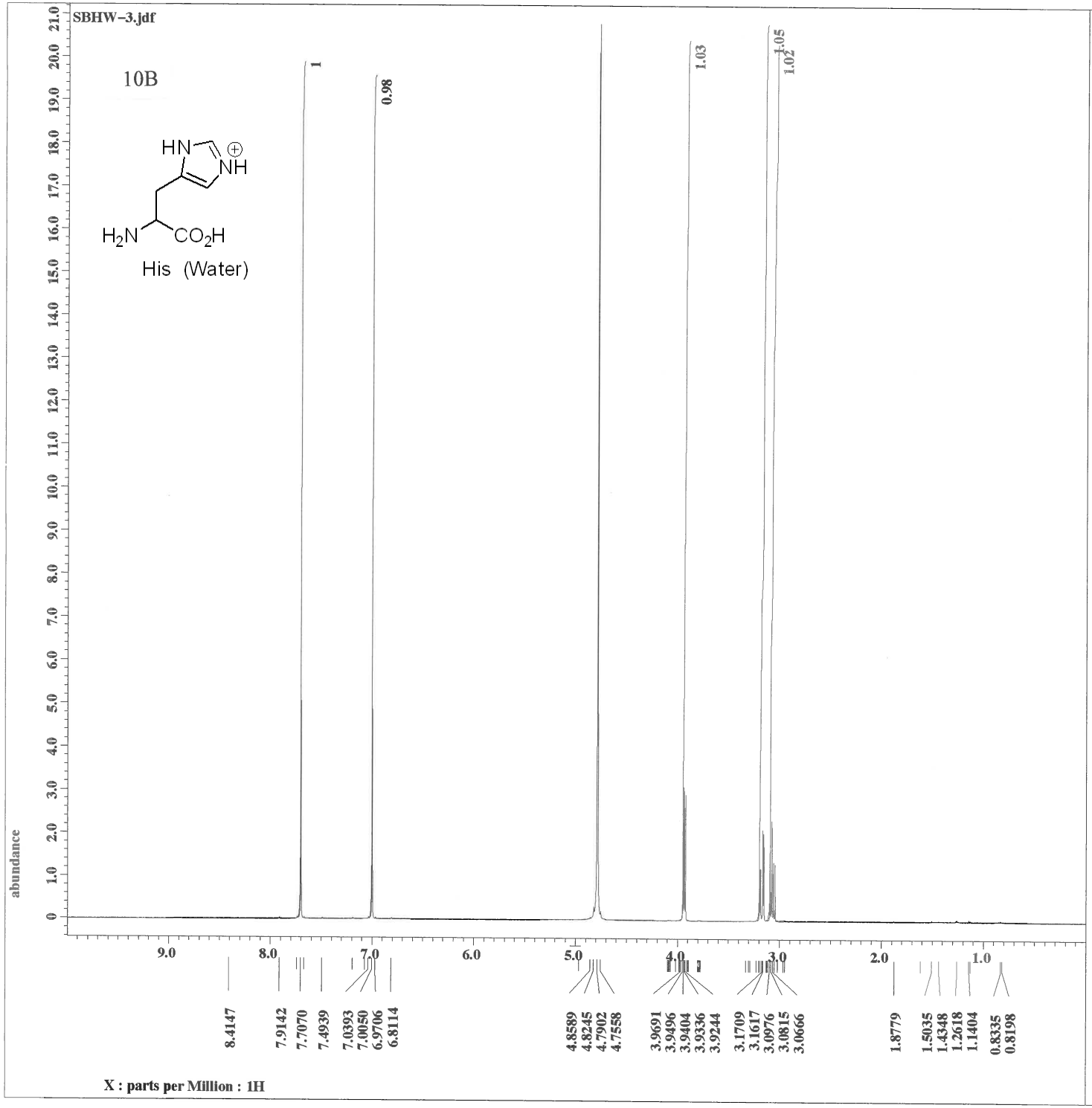
SBTHWC-2.jdf

9B

Thr (Water)




```
Filename          = SBTHWC-2.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#658391
Solvent           = D2O
Creation_time     =  8-SEP-2015 07:07:34
Revision_time     =  7-SEP-2015 18:23:57
Current_time      =  7-SEP-2015 18:24:24

Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = JNM-ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 0.83361792[s]
X_domain          = 13C
X_freq            = 125.76529768[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 1.19959034[Hz]
X_sweep           = 39.3081761[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 10
Scans             = 210
Total_scans       = 210

X_90_width        = 10.73[us]
X_acq_time        = 0.83361792[s]
X_angle           = 30[deg]
X_atn             = 9[dB]
X_pulse           = 3.57666667[us]
Irr_atn_dec       = 20[dB]
Irr_atn_noe       = 20[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 1[s]
Recvr_gain        = 50
Relaxation_delay  = 1[s]
Repetition_time   = 1.83361792[s]
Temp_get          = 21.7[dC]
```

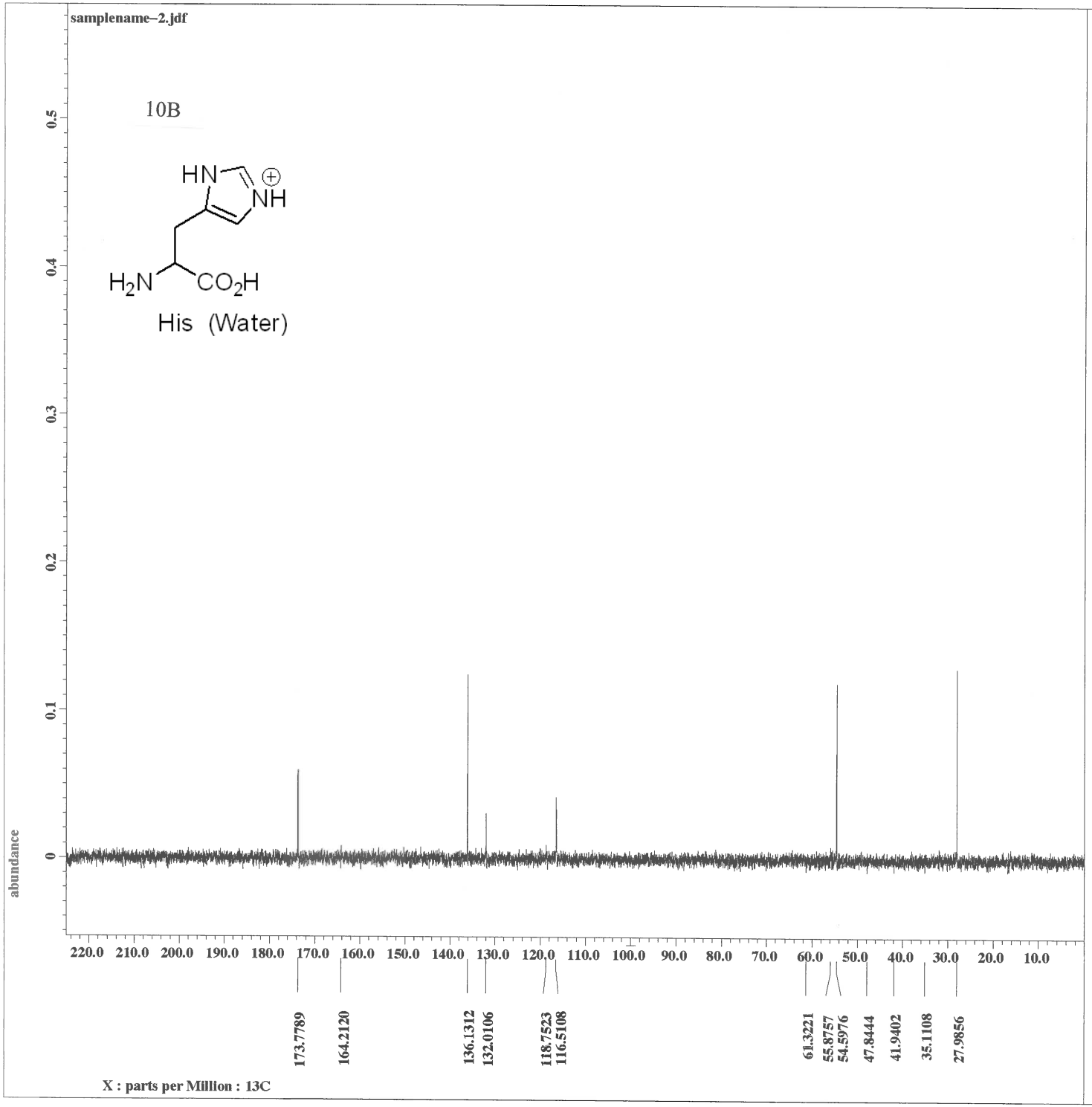


Filename	= SBHW-3.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= S#327296
Solvent	= D2O
Creation_time	= 7-SEP-2015 21:52:53
Revision_time	= 7-SEP-2015 09:11:18
Current_time	= 7-SEP-2015 09:11:59
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 1.74587904[s]
X_domain	= 1H
X_freq	= 500.15991521[MHz]
X_offset	= 5.0[ppm]
X_points	= 16384
X_prescans	= 0
X_resolution	= 0.57277737[Hz]
X_sweep	= 9.38438438[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Tri_domain	= 1H
Tri_freq	= 500.15991521[MHz]
Tri_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 11
Total_scans	= 11
X_90_width	= 12.54[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 4[dB]
X_pulse	= 6.27[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 44
Relaxation_delay	= 10[s]
Repetition_time	= 11.74587904[s]
Temp_get	= 21[dC]

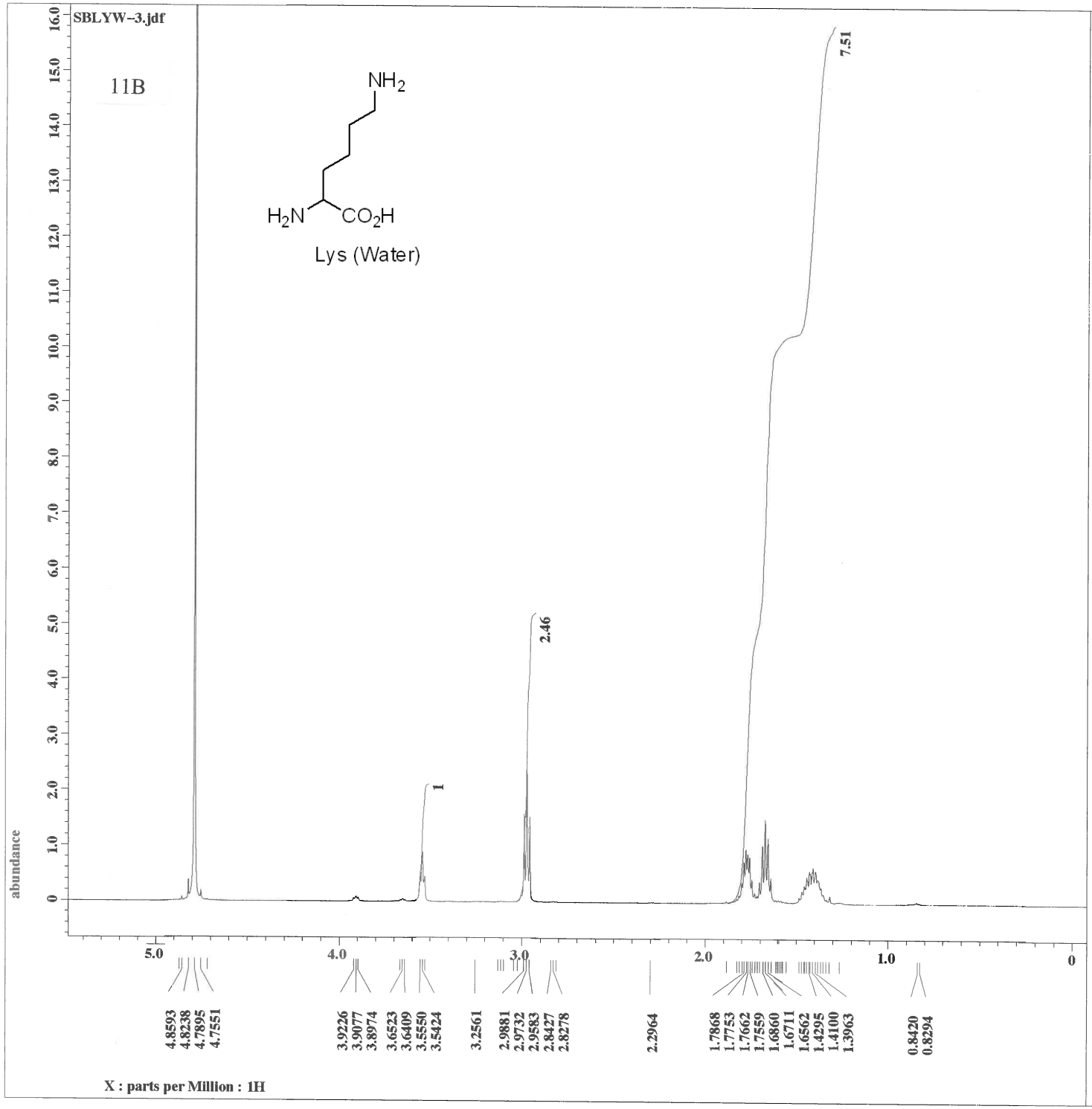
samplename-2.jdf

10B

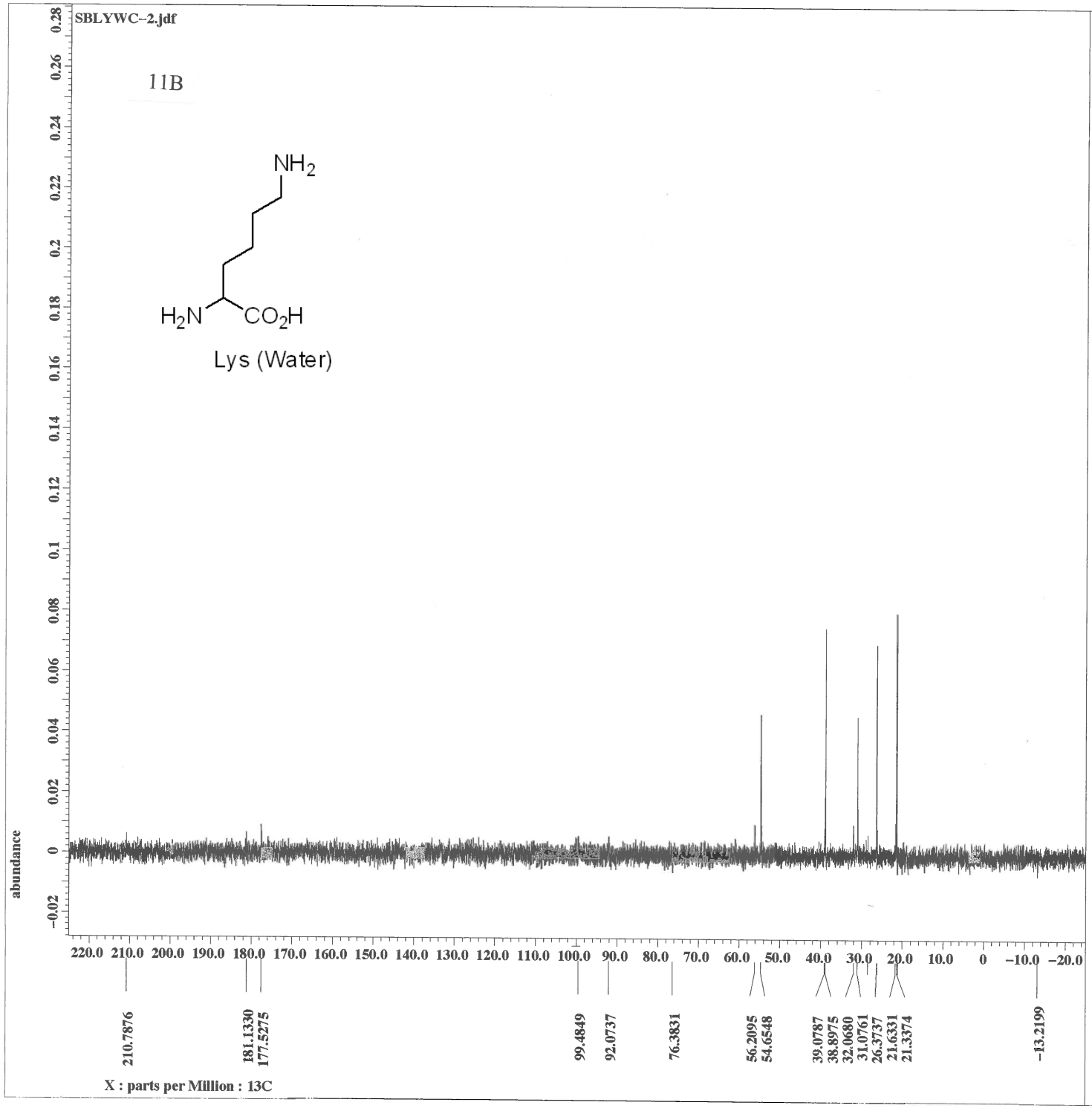
His (Water)



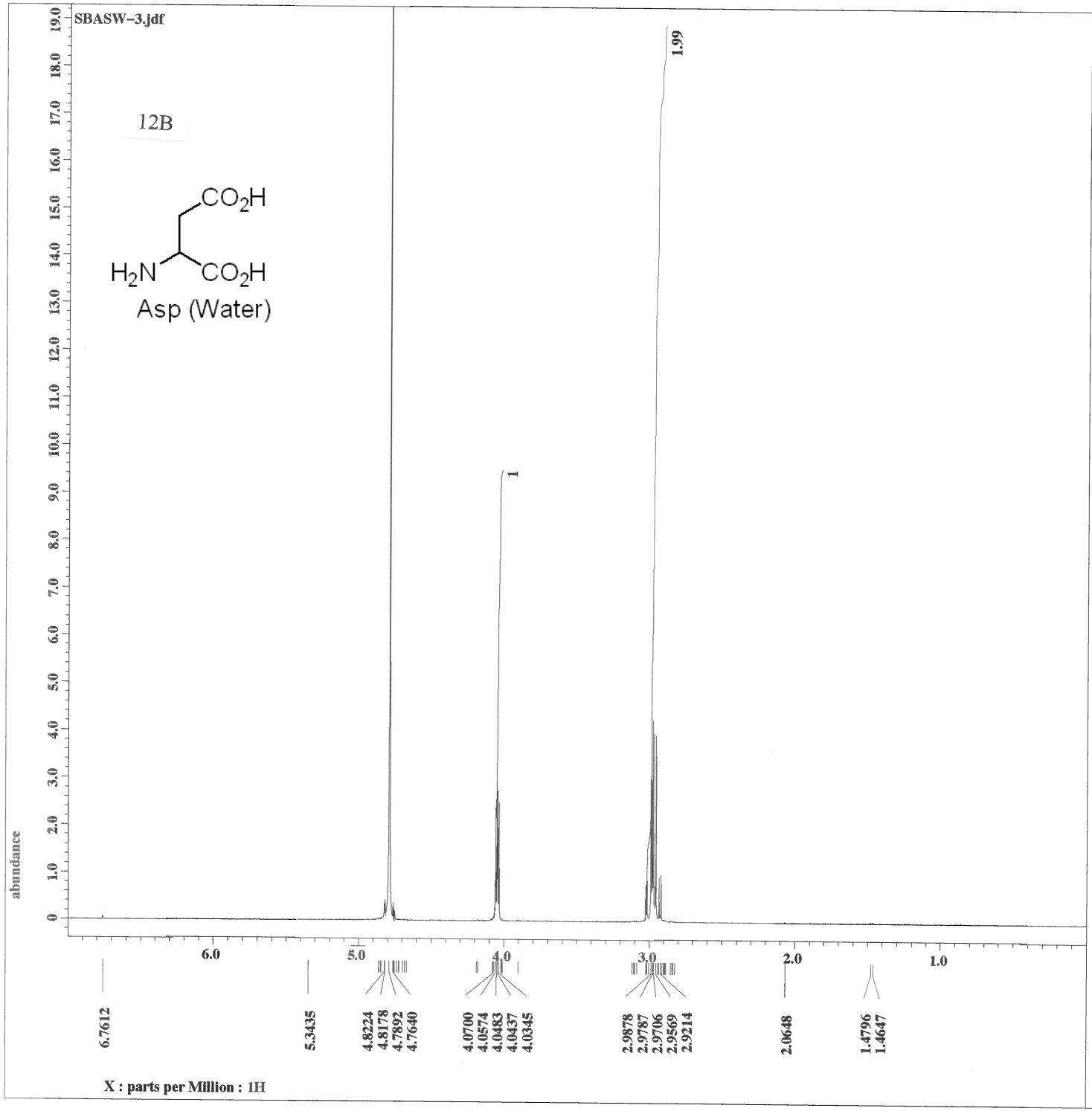
Filename	= samplename-2.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= S#329812
Solvent	= D2O
Creation_time	= 7-SEP-2015 22:11:03
Revision_time	= 7-SEP-2015 09:28:13
Current_time	= 7-SEP-2015 09:29:02
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 0.83361792[s]
X_domain	= 13C
X_freq	= 125.76529768[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.19959034[Hz]
X_sweep	= 39.3081761[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 10
Scans	= 370
Total_scans	= 370
X_90_width	= 10.73[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 9[dB]
X_pulse	= 3.57666667[us]
Irr_atn_dec	= 20[dB]
Irr_atn_noe	= 20[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 2[s]
Recvr_gain	= 50
Relaxation_delay	= 2[s]
Repetition_time	= 2.83361792[s]
Temp_get	= 21.8[dC]




```
Filename          = SBLYW-3.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#329649
Solvent           = D2O
Creation_time     =  9-SEP-2015 21:56:20
Revision_time     =  9-SEP-2015 09:17:02
Current_time      =  9-SEP-2015 09:18:13

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = JNM-ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.74587904[s]
X_domain          = 1H
X_freq            = 500.15991521[MHz]
X_offset          = 5.0[ppm]
X_points          = 16384
X_prescans        = 0
X_resolution      = 0.57277737[Hz]
X_sweep           = 9.38438438[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Tri_domain        = 1H
Tri_freq          = 500.15991521[MHz]
Tri_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 11
Total_scans       = 11

X_90_width        = 12.54[us]
X_acq_time        = 1.74587904[s]
X_angle           = 45[deg]
X_atn             = 4[dB]
X_pulse           = 6.27[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 42
Relaxation_delay  = 10[s]
Repetition_time   = 11.74587904[s]
Temp_get          = 21.3[dC]
```




```
Filename          = SBLYWC-2.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#331949
Solvent           = D2O
Creation_time     =  9-SEP-2015 22:12:00
Revision_time     =  9-SEP-2015 09:28:36
Current_time      =  9-SEP-2015 09:29:30

Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = JNM-ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 0.83361792[s]
X_domain          = 13C
X_freq            = 125.76529768[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 1.19959034[Hz]
X_sweep           = 39.3081761[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 10
Scans             = 670
Total_scans       = 670

X_90_width        = 10.73[us]
X_acq_time        = 0.83361792[s]
X_angle           = 30[deg]
X_atn             = 9[dB]
X_pulse           = 3.57666667[us]
Irr_atn_dec       = 20[dB]
Irr_atn_noe       = 20[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 0.5[s]
Recvr_gain        = 50
Relaxation_delay  = 0.5[s]
Repetition_time   = 1.33361792[s]
Temp_get          = 21.7[dC]
```

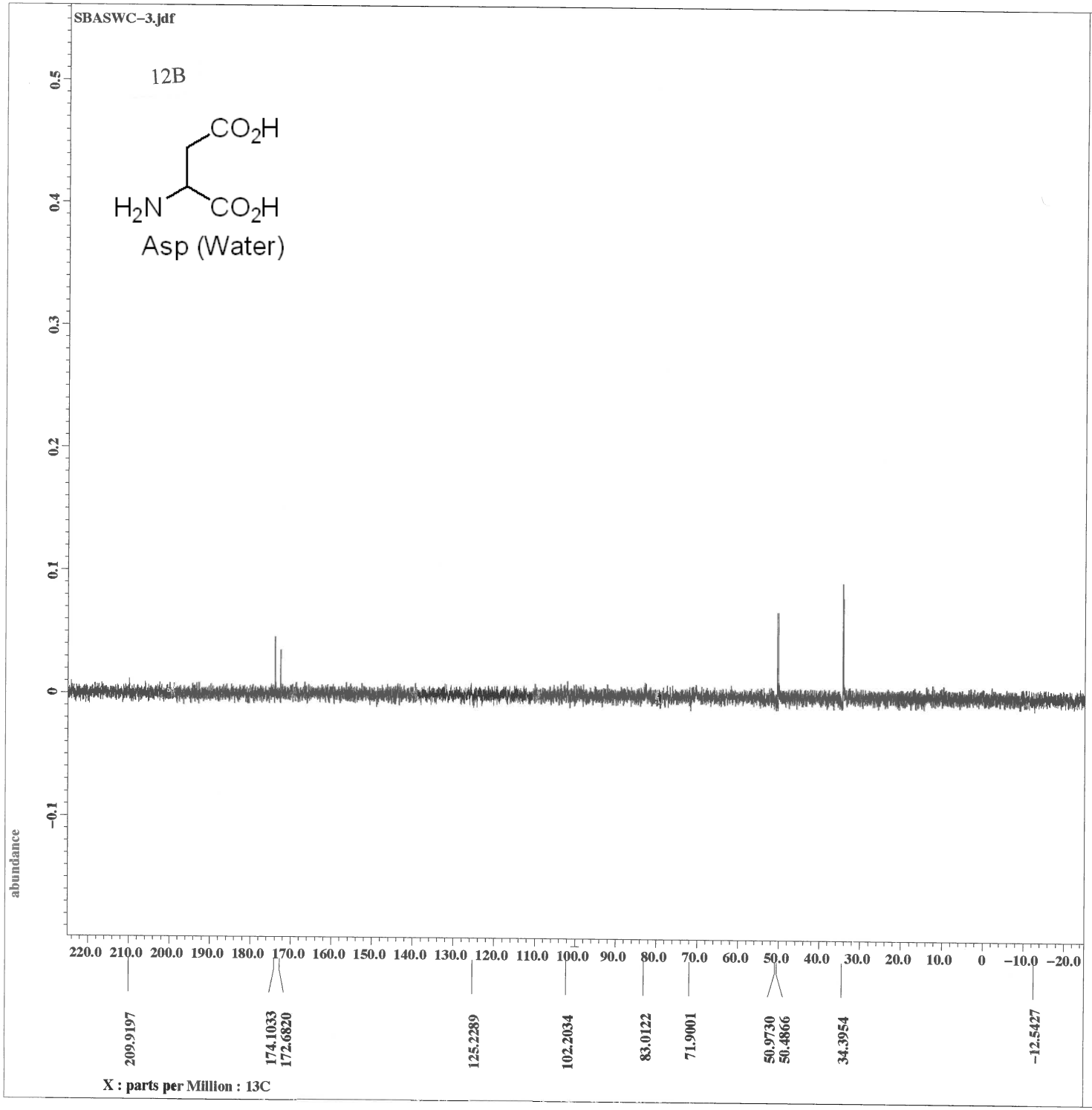



```
Filename          = SBASW-3.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#340075
Solvent           = D2O
Creation_time     =  8-SEP-2015 22:12:54
Revision_time     =  8-SEP-2015 09:31:32
Current_time      =  8-SEP-2015 09:32:03

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = JNM-ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.74587904[s]
X_domain          = 1H
X_freq            = 500.15991521[MHz]
X_offset          = 5.0[ppm]
X_points          = 16384
X_prescans        = 0
X_resolution      = 0.57277737[Hz]
X_sweep           = 9.38438438[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Tri_domain        = 1H
Tri_freq          = 500.15991521[MHz]
Tri_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 9
Total_scans       = 9

X_90_width        = 12.54[us]
X_acq_time        = 1.74587904[s]
X_angle           = 45[deg]
X_atn             = 4[dB]
X_pulse           = 6.27[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 46
Relaxation_delay  = 10[s]
Repetition_time   = 11.74587904[s]
Temp_get          = 21.4[dC]
```

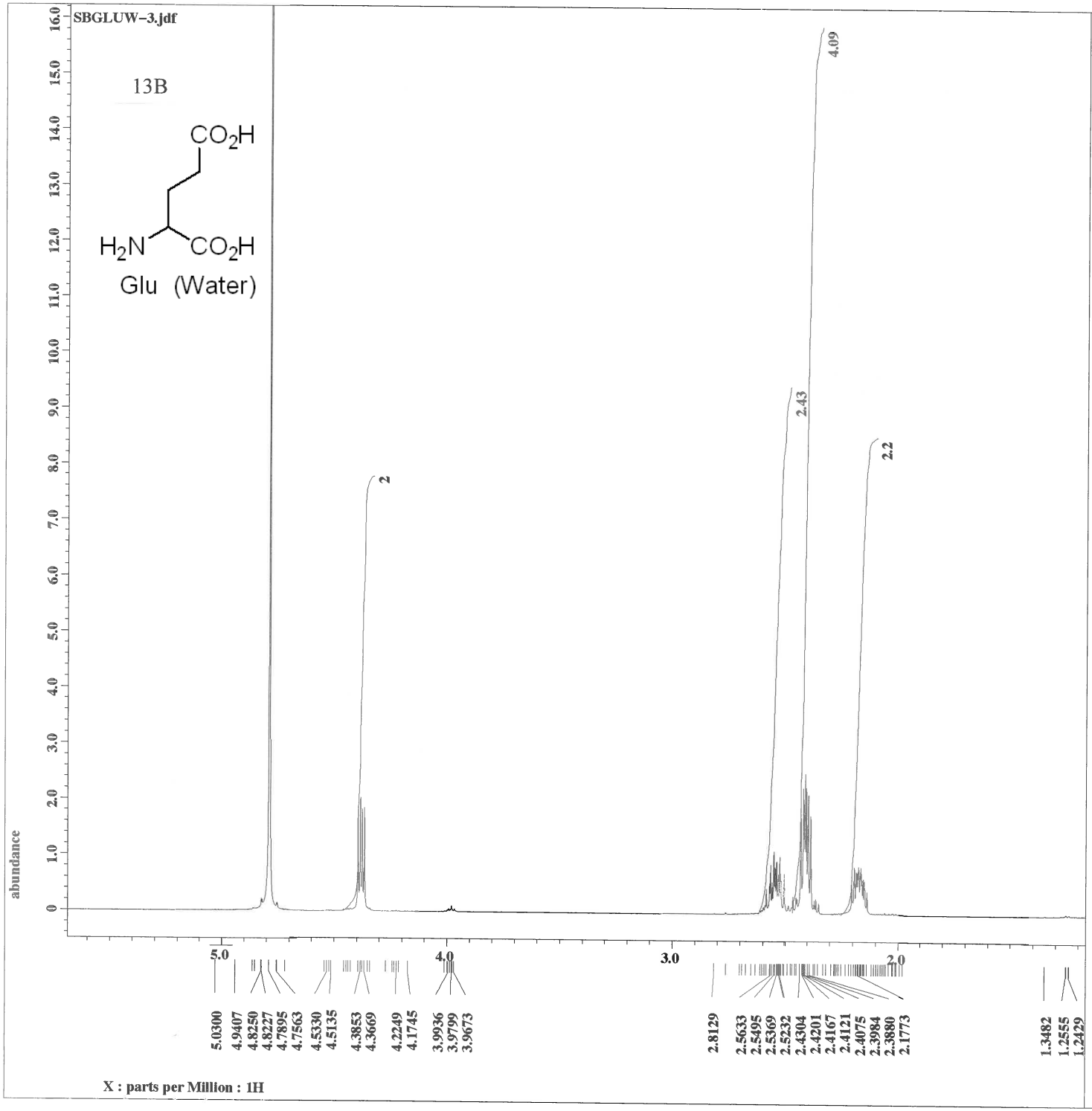
SBASWC-3.jdf

12B

Asp (Water)



Filename	= SBASWC-3.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= S#341913
Solvent	= D2O
Creation_time	= 8-SEP-2015 22:20:09
Revision_time	= 8-SEP-2015 09:37:27
Current_time	= 8-SEP-2015 09:37:49
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 0.83361792[s]
X_domain	= 13C
X_freq	= 125.76529768[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.19959034[Hz]
X_sweep	= 39.3081761[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 10
Scans	= 210
Total_scans	= 210
X_90_width	= 10.73[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 9[dB]
X_pulse	= 3.57666667[us]
Irr_atn_dec	= 20[dB]
Irr_atn_noe	= 20[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 1[s]
Recvr_gain	= 50
Relaxation_delay	= 1[s]
Repetition_time	= 1.83361792[s]
Temp_get	= 21.8[dC]

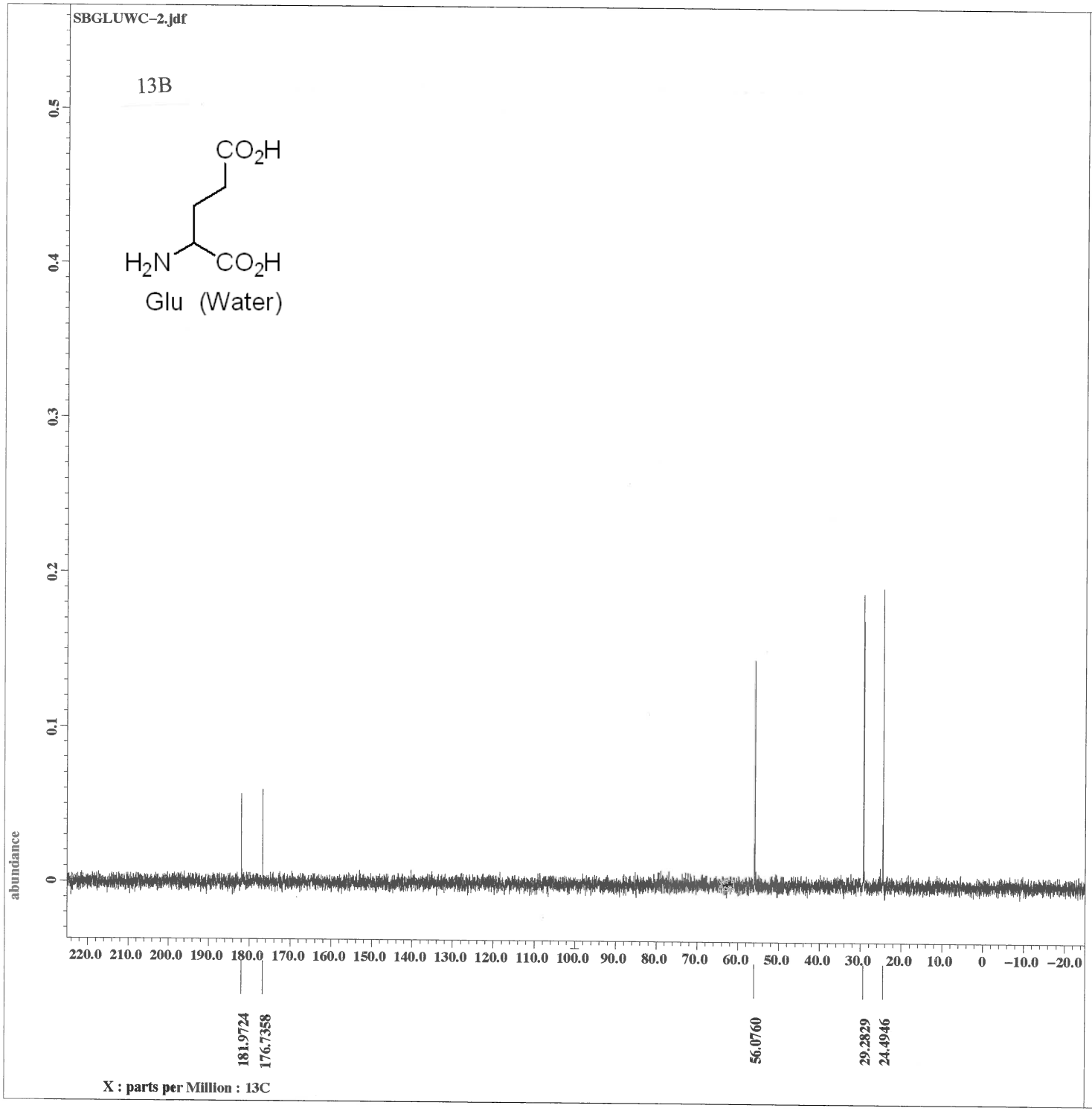


Filename	= SBGLUW-3.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= S#349238
Solvent	= D2O
Creation_time	= 8-SEP-2015 22:29:20
Revision_time	= 8-SEP-2015 09:48:51
Current_time	= 8-SEP-2015 09:49:45
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 1.74587904[s]
X_domain	= 1H
X_freq	= 500.15991521[MHz]
X_offset	= 5.0[ppm]
X_points	= 16384
X_prescans	= 0
X_resolution	= 0.57277737[Hz]
X_sweep	= 9.38438438[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Tri_domain	= 1H
Tri_freq	= 500.15991521[MHz]
Tri_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 13
Total_scans	= 13
X_90_width	= 12.54[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 4[dB]
X_pulse	= 6.27[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 40
Relaxation_delay	= 10[s]
Repetition_time	= 11.74587904[s]
Temp_get	= 21.3[dC]

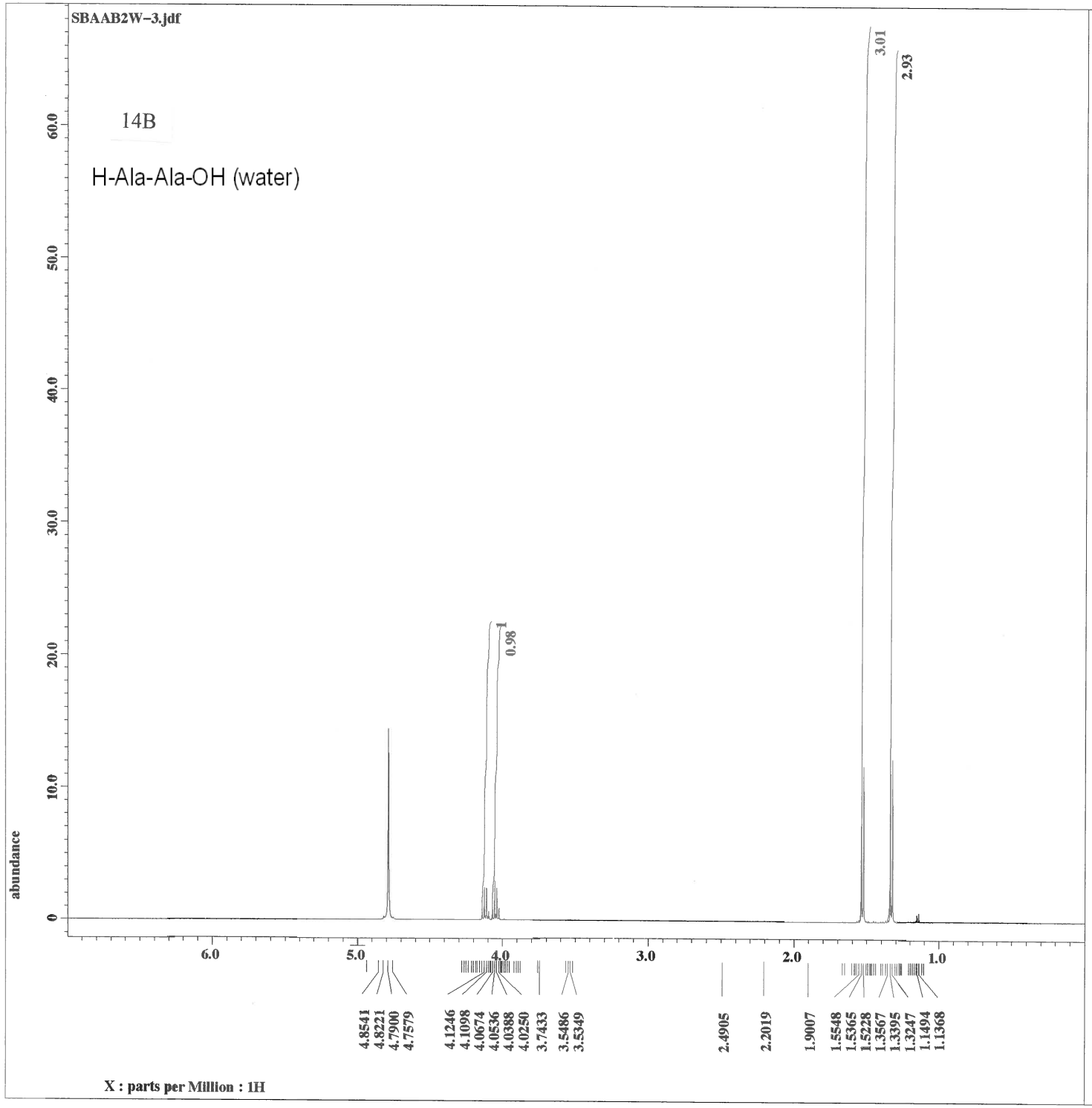
SBGLUWC-2.jdf

13B

Glu (Water)



Filename	= SBGLUWC-2.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= S#351786
Solvent	= D2O
Creation_time	= 8-SEP-2015 22:37:02
Revision_time	= 8-SEP-2015 09:53:35
Current_time	= 8-SEP-2015 09:53:52
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 0.83361792[s]
X_domain	= 13C
X_freq	= 125.76529768[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.19959034[Hz]
X_sweep	= 39.3081761[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 10
Scans	= 310
Total_scans	= 310
X_90_width	= 10.73[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 9[dB]
X_pulse	= 3.57666667[us]
Irr_atn_dec	= 20[dB]
Irr_atn_noe	= 20[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 0.5[s]
Recvr_gain	= 50
Relaxation_delay	= 0.5[s]
Repetition_time	= 1.33361792[s]
Temp_get	= 21.7[dC]

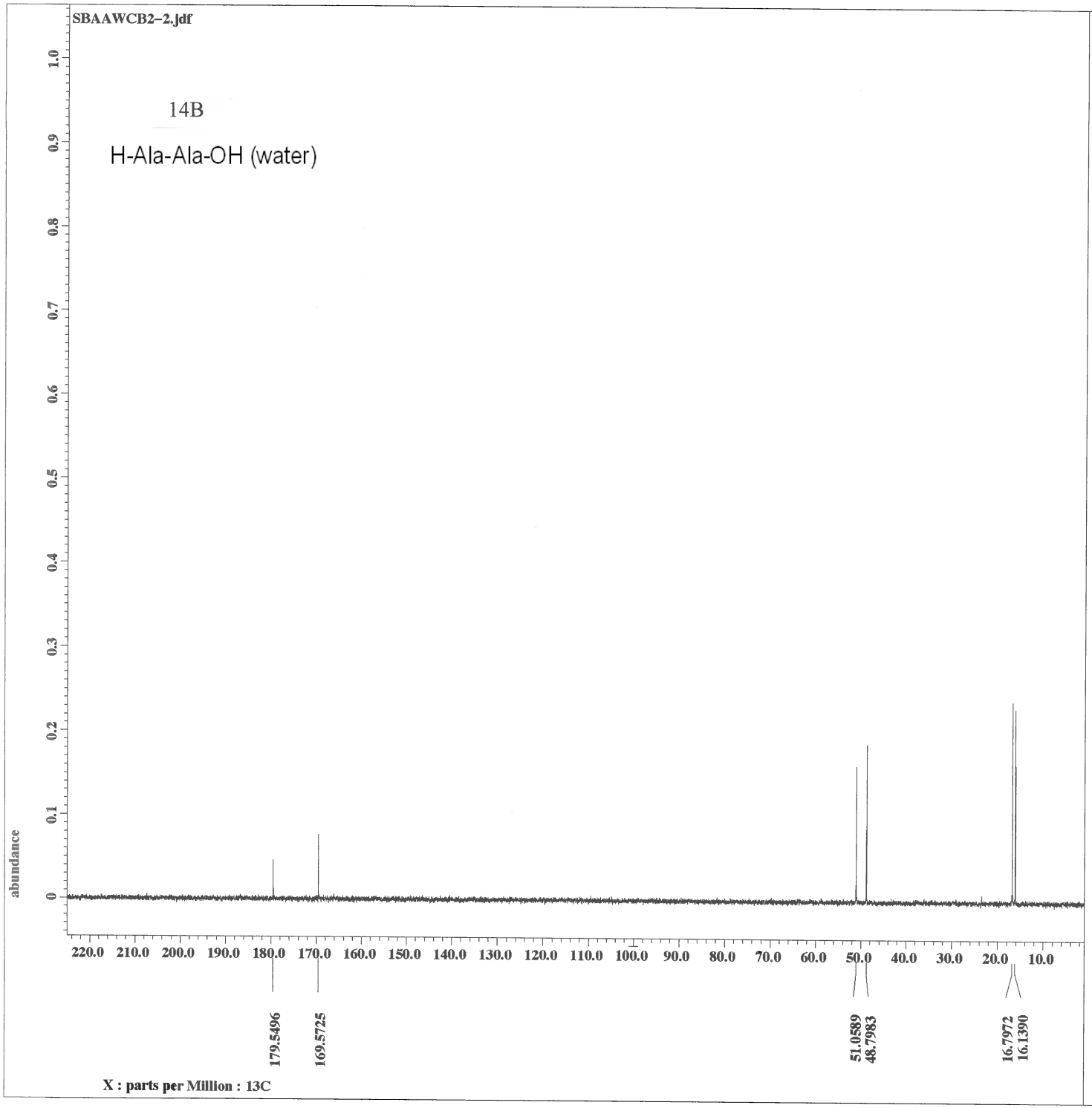



```
Filename          = SBAAB2W-3.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#703714
Solvent           = D2O
Creation_time     = 16-SEP-2015 08:21:00
Revision_time     = 15-SEP-2015 19:40:30
Current_time      = 15-SEP-2015 19:41:17

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = JNM-ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.74587904[s]
X_domain          = 1H
X_freq            = 500.15991521[MHz]
X_offset          = 5.0[ppm]
X_points          = 16384
X_prescans        = 0
X_resolution      = 0.57277737[Hz]
X_sweep           = 9.38438438[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Tri_domain        = 1H
Tri_freq          = 500.15991521[MHz]
Tri_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 16
Total_scans       = 16

X_90_width        = 12.54[us]
X_acq_time        = 1.74587904[s]
X_angle           = 45[deg]
X_atn             = 4[dB]
X_pulse           = 6.27[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 36
Relaxation_delay  = 10[s]
Repetition_time   = 11.74587904[s]
Temp_get          = 21.2[dC]
```

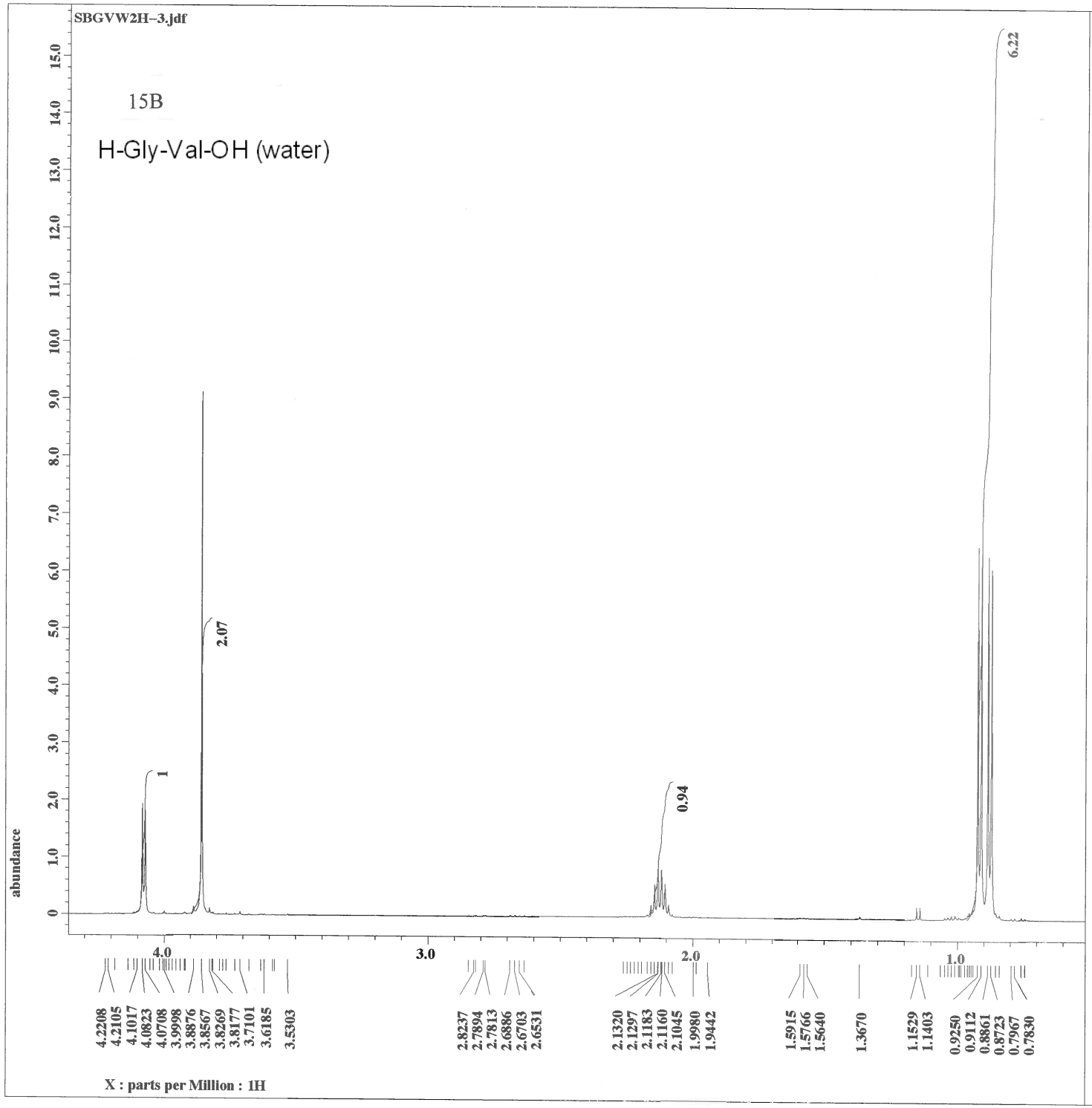
SBAAWCB2-2.jdf

14B

H-Ala-Ala-OH (water)



Filename	= SBAAWCB2-2.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= S#706822
Solvent	= D2O
Creation_time	= 16-SEP-2015 08:36:56
Revision_time	= 15-SEP-2015 19:53:44
Current_time	= 15-SEP-2015 19:54:11
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 0.83361792[s]
X_domain	= 13C
X_freq	= 125.76529768[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.19959034[Hz]
X_sweep	= 39.3081761[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 10
Scans	= 860
Total_scans	= 860
X_90_width	= 10.73[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 9[dB]
X_pulse	= 3.57666667[us]
Irr_atn_dec	= 20[dB]
Irr_atn_noe	= 20[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 0.2[s]
Recvr_gain	= 50
Relaxation_delay	= 0.2[s]
Repetition_time	= 1.03361792[s]
Temp_get	= 21.6[dC]

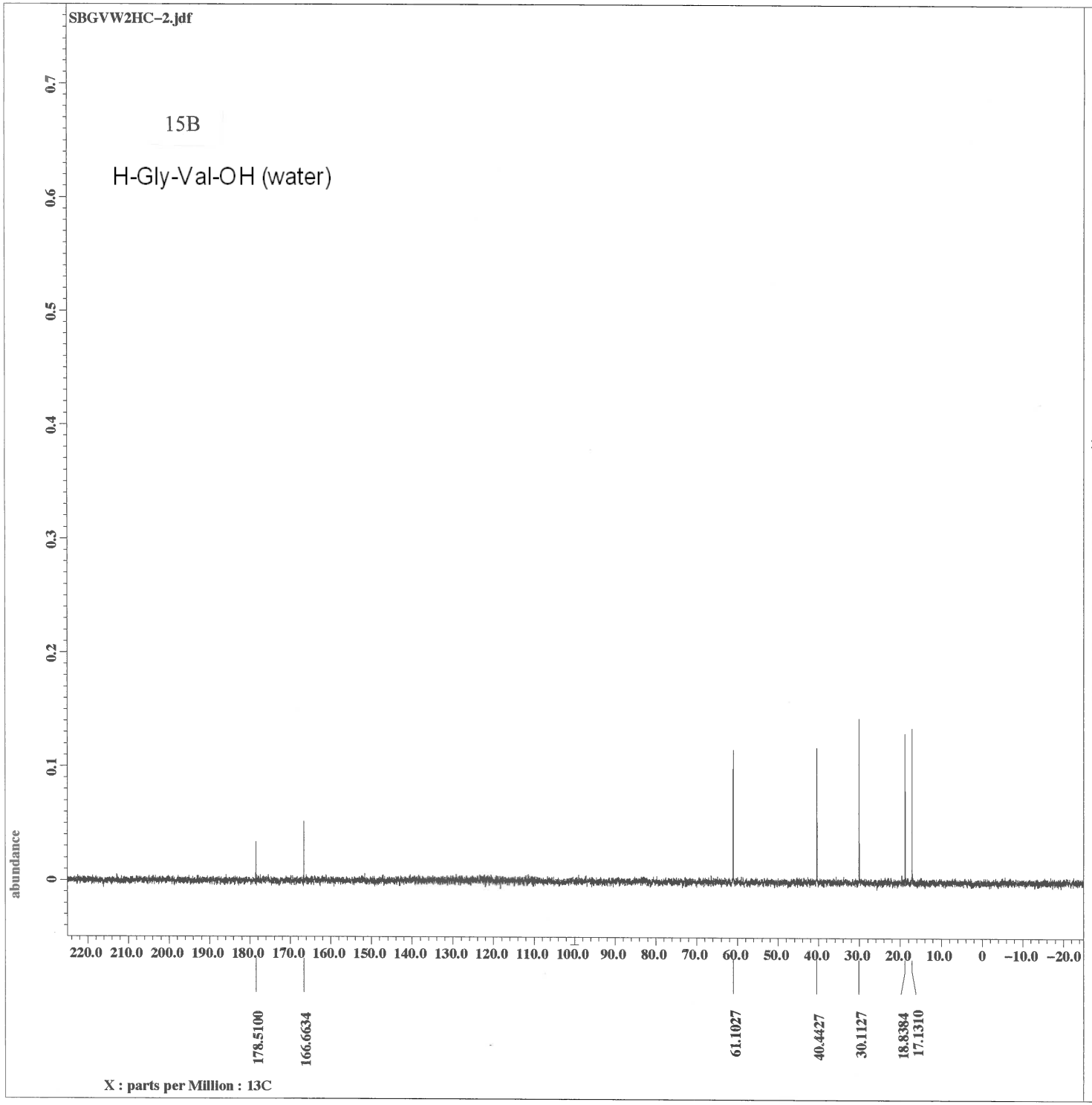



```
Filename          = SBGVW2H-3.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#384210
Solvent           = D2O
Creation_time     = 19-SEP-2015 23:28:27
Revision_time     = 19-SEP-2015 10:47:55
Current_time      = 19-SEP-2015 10:48:48

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = JNM-ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.74587904[s]
X_domain          = 1H
X_freq            = 500.15991521[MHz]
X_offset          = 5.0[ppm]
X_points          = 16384
X_prescans        = 0
X_resolution      = 0.57277737[Hz]
X_sweep           = 9.38438438[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Tri_domain        = 1H
Tri_freq          = 500.15991521[MHz]
Tri_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 15
Total_scans       = 15

X_90_width        = 12.54[us]
X_acq_time        = 1.74587904[s]
X_angle           = 45[deg]
X_atn             = 4[dB]
X_pulse           = 6.27[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 40
Relaxation_delay  = 10[s]
Repetition_time   = 11.74587904[s]
Temp_get          = 21.1[dC]
```

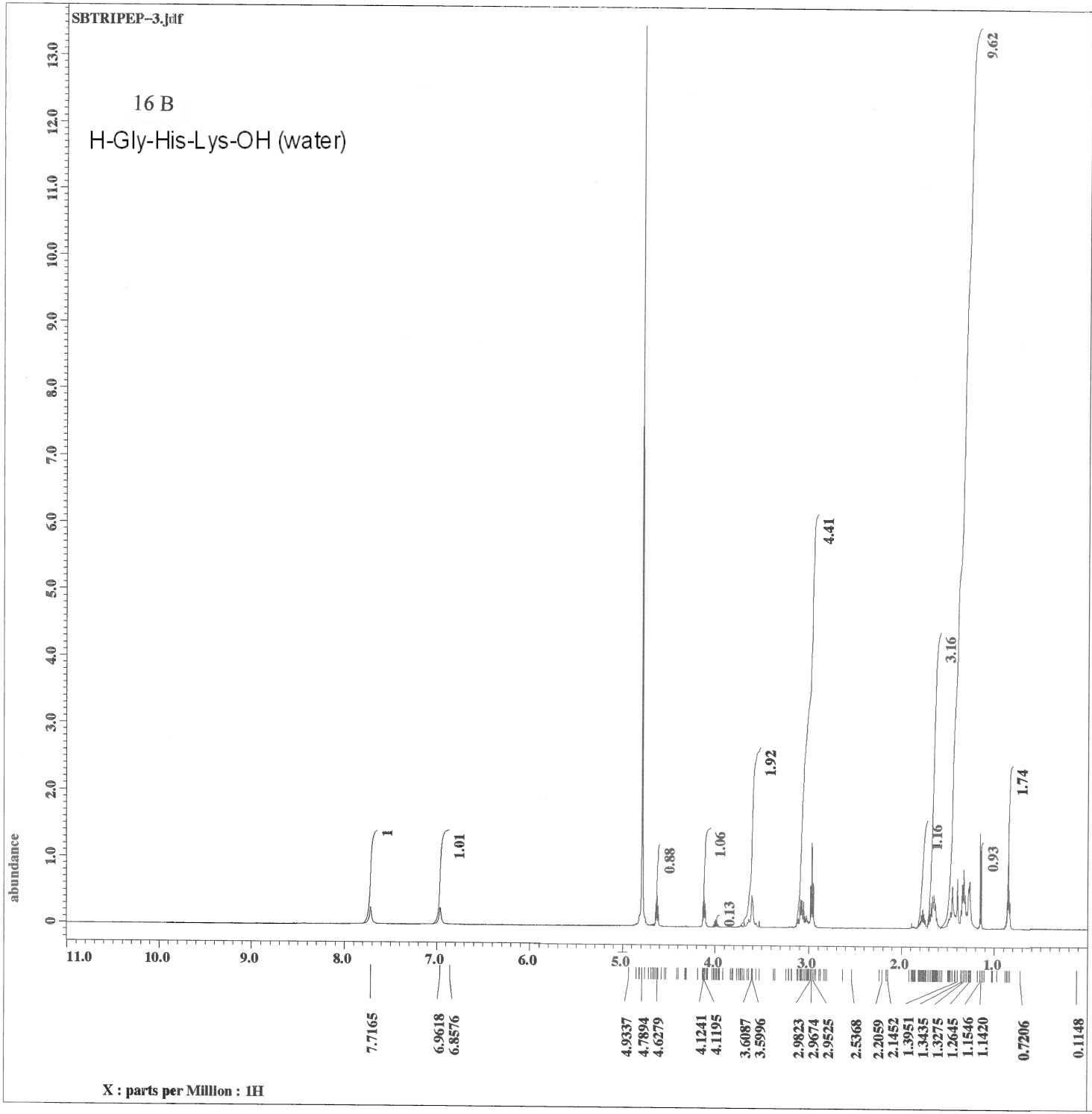
SBGVW2HC-2.jdf

15B

H-Gly-Val-OH (water)



Filename	= SBGVW2HC-2.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= S#387286
Solvent	= D2O
Creation_time	= 19-SEP-2015 23:42:05
Revision_time	= 19-SEP-2015 10:58:46
Current_time	= 19-SEP-2015 10:58:54
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 0.83361792[s]
X_domain	= 13C
X_freq	= 125.76529768[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.19959034[Hz]
X_sweep	= 39.3081761[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 10
Scans	= 720
Total_scans	= 720
X_90_width	= 10.73[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 9[dB]
X_pulse	= 3.57666667[us]
Irr_atn_dec	= 20[dB]
Irr_atn_noe	= 20[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 0.2[s]
Recvr_gain	= 50
Relaxation_delay	= 0.2[s]
Repetition_time	= 1.03361792[s]
Temp_get	= 21.6[dC]

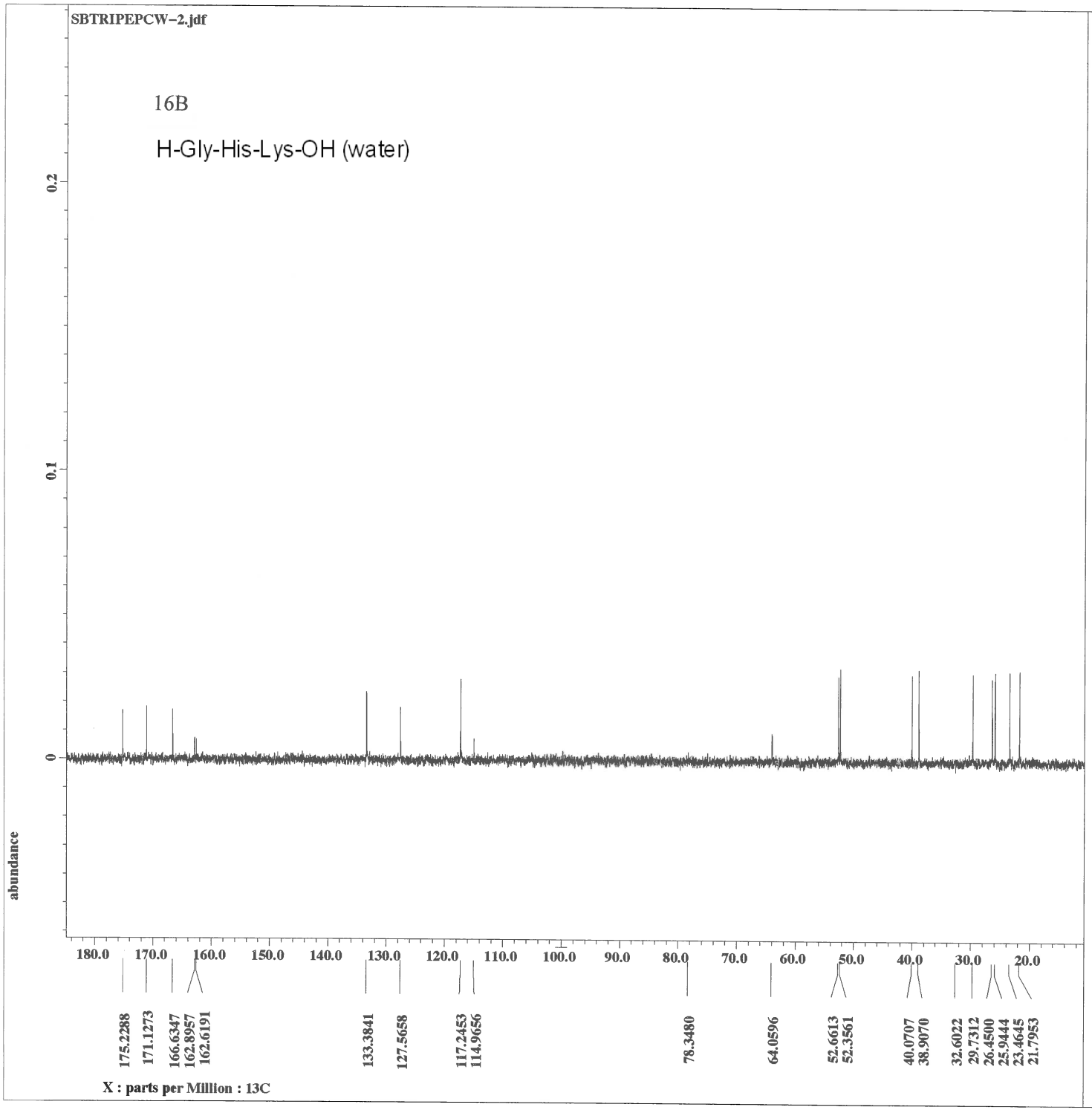



```
Filename          = SBTRIPEP-3.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#714036
Solvent           = D2O
Creation_time     = 22-SEP-2015 08:38:26
Revision_time     = 21-SEP-2015 19:59:17
Current_time      = 21-SEP-2015 19:59:49

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = JNM-ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.74587904[s]
X_domain          = 1H
X_freq            = 500.15991521[MHz]
X_offset          = 5.0[ppm]
X_points          = 16384
X_prescans        = 0
X_resolution      = 0.57277737[Hz]
X_sweep           = 9.38438438[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Tri_domain        = 1H
Tri_freq          = 500.15991521[MHz]
Tri_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 16
Total_scans       = 16

X_90_width        = 12.54[us]
X_acq_time        = 1.74587904[s]
X_angle           = 45[deg]
X_atn             = 4[dB]
X_pulse           = 6.27[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 36
Relaxation_delay  = 10[s]
Repetition_time   = 11.74587904[s]
Temp_get          = 22.6[dC]
```

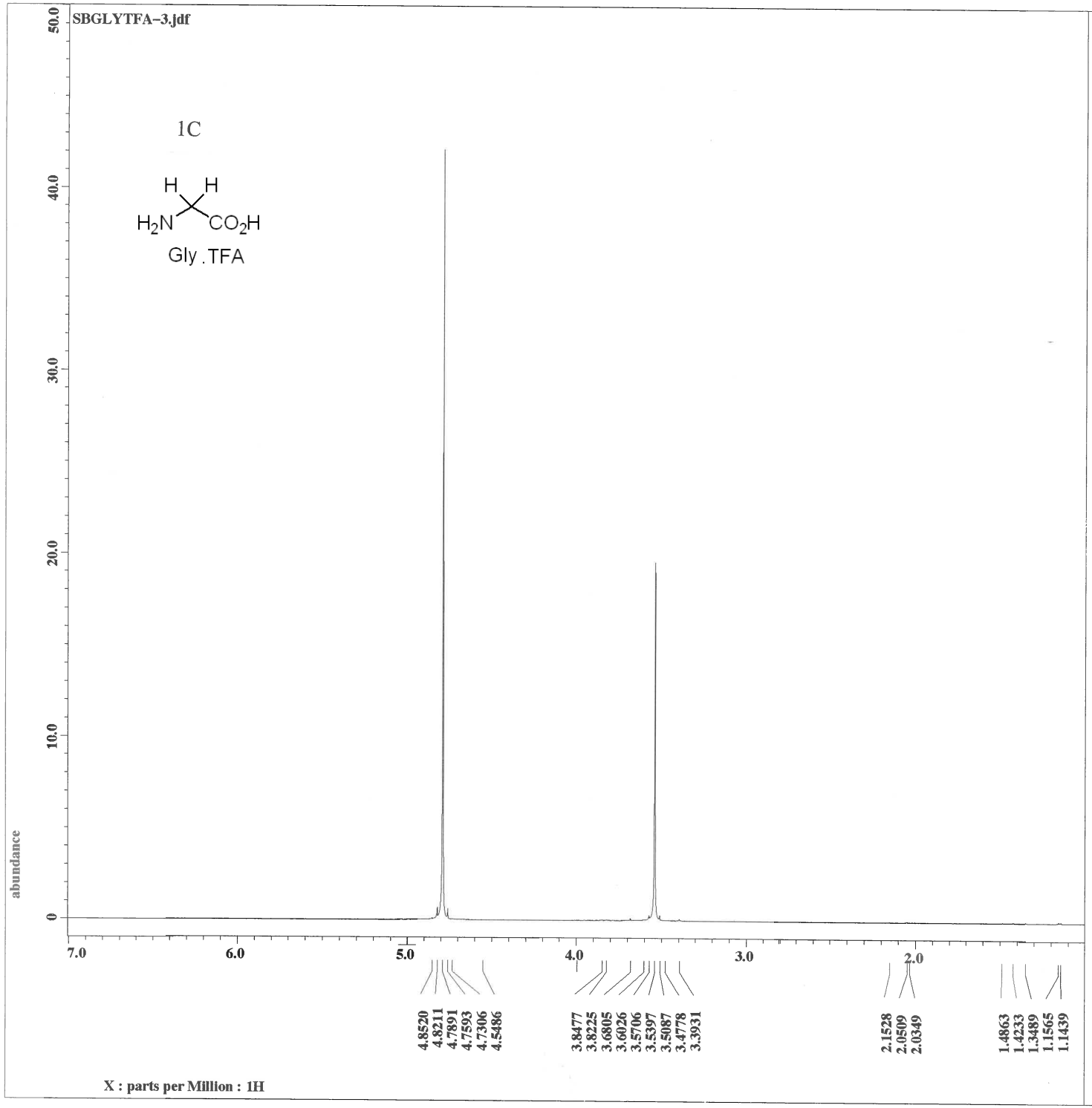
SBTRIPEPCW-2.jdf

16B

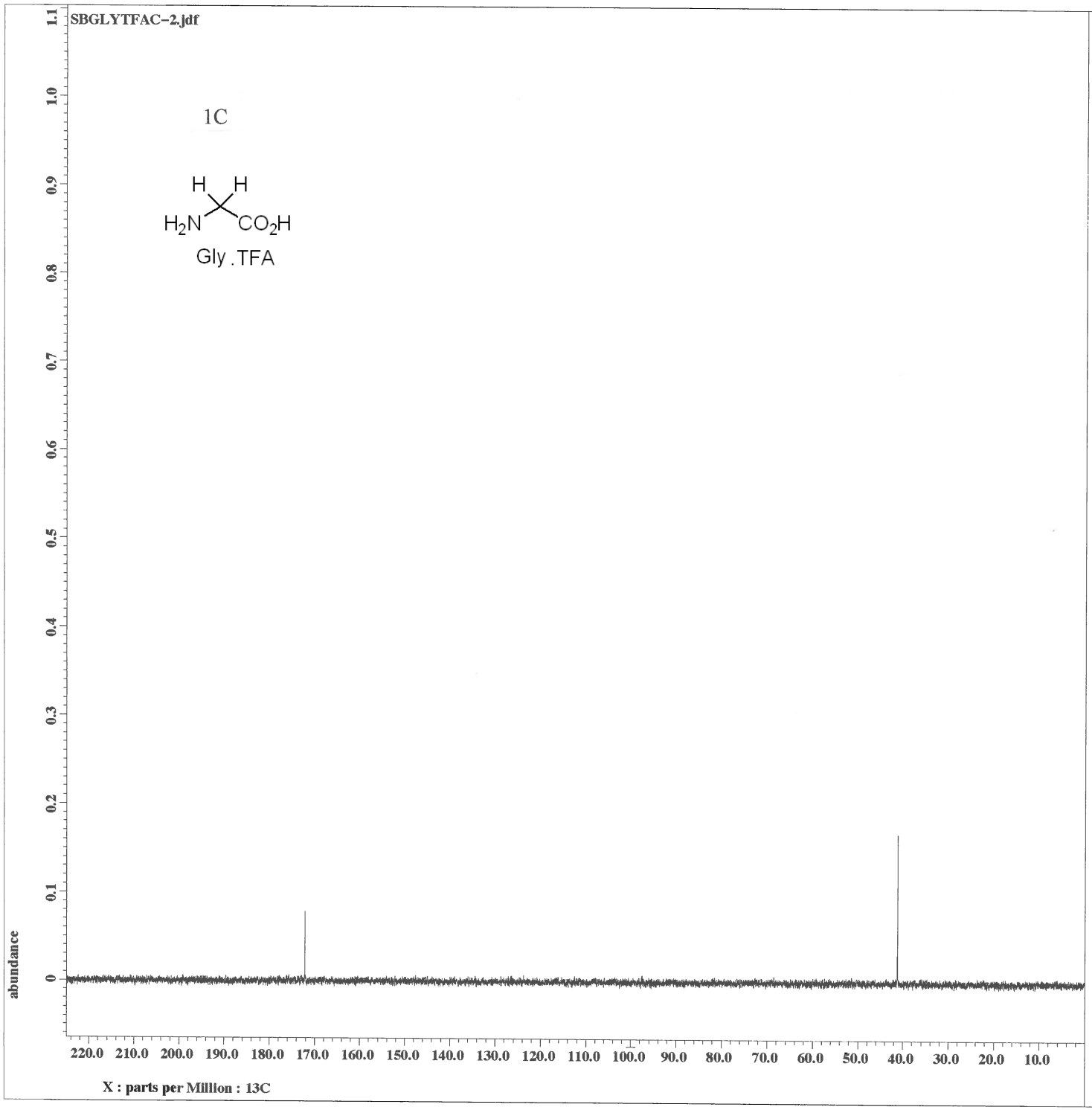
H-Gly-His-Lys-OH (water)



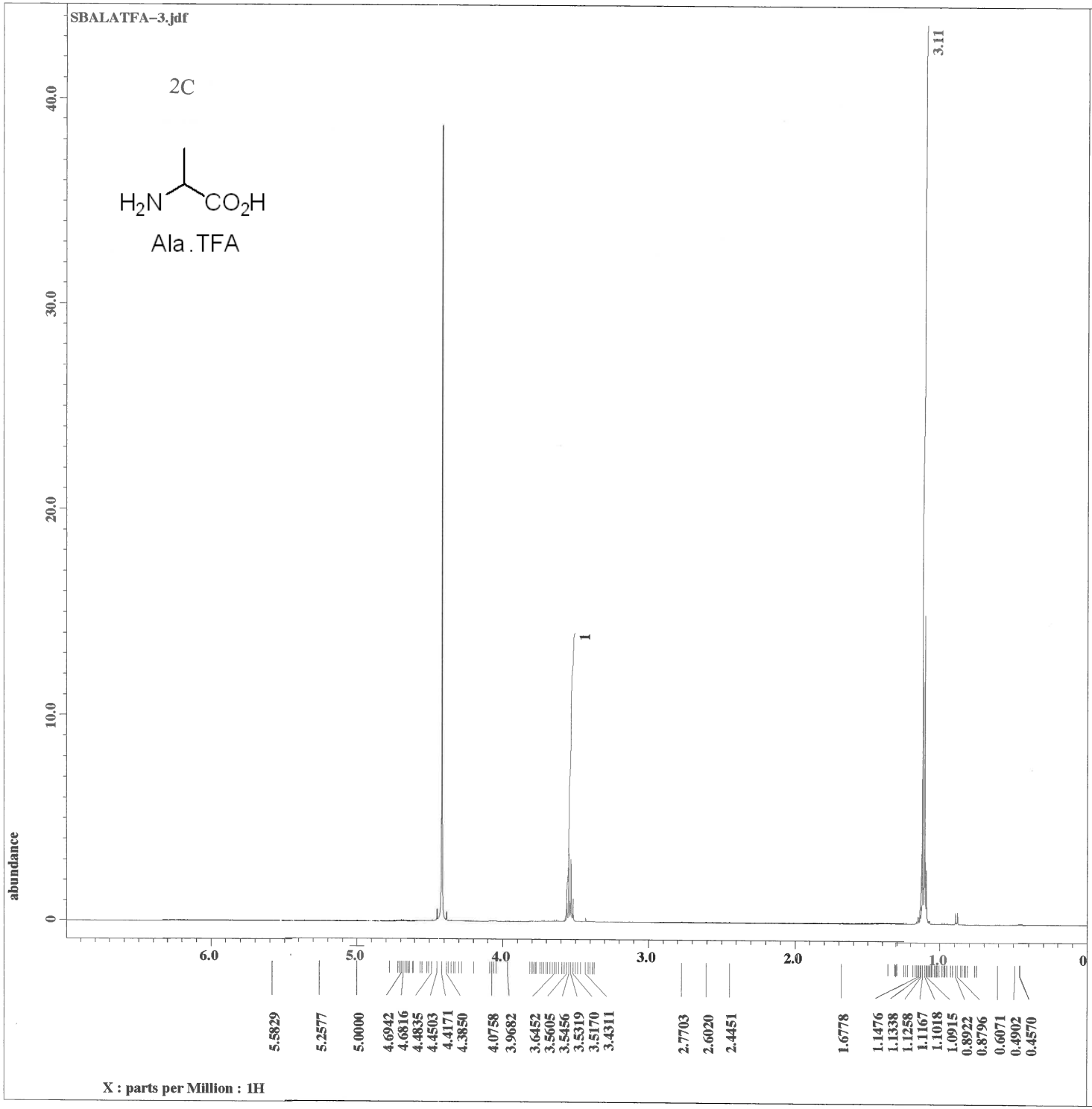
Filename	= SBTRIPEPCW-2.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= S#359807
Solvent	= D2O
Creation_time	= 23-SEP-2015 23:21:05
Revision_time	= 23-SEP-2015 10:37:13
Current_time	= 23-SEP-2015 10:37:39
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 0.83361792[s]
X_domain	= 13C
X_freq	= 125.76529768[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.19959034[Hz]
X_sweep	= 39.3081761[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 10
Scans	= 2150
Total_scans	= 2150
X_90_width	= 10.73[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 9[dB]
X_pulse	= 3.57666667[us]
Irr_atn_dec	= 20[dB]
Irr_atn_noe	= 20[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 0.2[s]
Recvr_gain	= 50
Relaxation_delay	= 0.2[s]
Repetition_time	= 1.03361792[s]
Temp_get	= 22.5[dC]



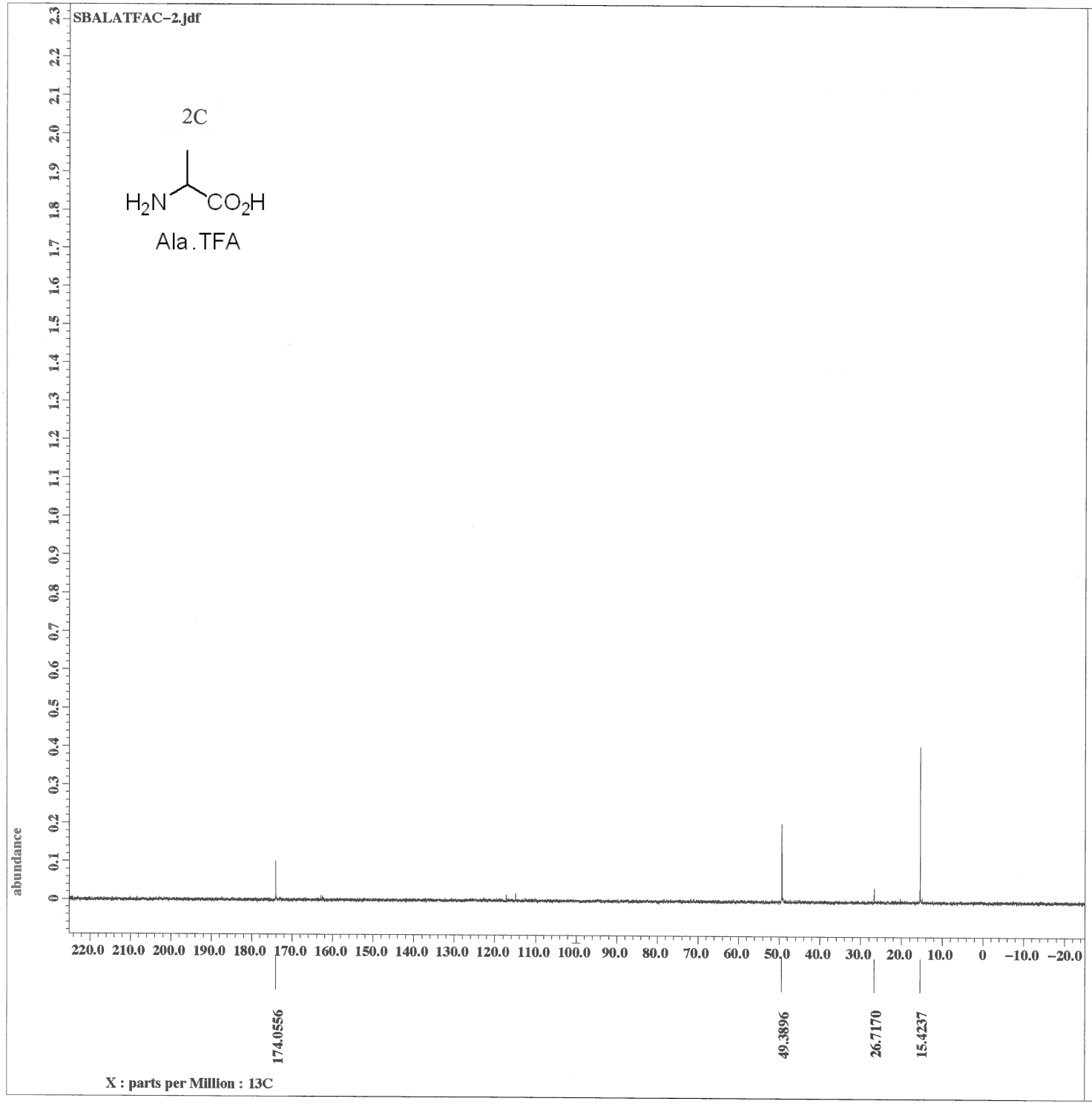

```
Filename          = SBGLYTFA-3.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#684782
Solvent           = D2O
Creation_time     = 10-SEP-2015 07:48:33
Revision_time     =  9-SEP-2015 19:06:33
Current_time      =  9-SEP-2015 19:07:56

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = JNM-ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.74587904[s]
X_domain          = 1H
X_freq            = 500.15991521[MHz]
X_offset          = 5.0[ppm]
X_points          = 16384
X_prescans        = 0
X_resolution      = 0.57277737[Hz]
X_sweep           = 9.38438438[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Tri_domain        = 1H
Tri_freq          = 500.15991521[MHz]
Tri_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 12.54[us]
X_acq_time        = 1.74587904[s]
X_angle           = 45[deg]
X_atn             = 4[dB]
X_pulse           = 6.27[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 42
Relaxation_delay  = 10[s]
Repetition_time   = 11.74587904[s]
Temp_get          = 21.3[dC]
```



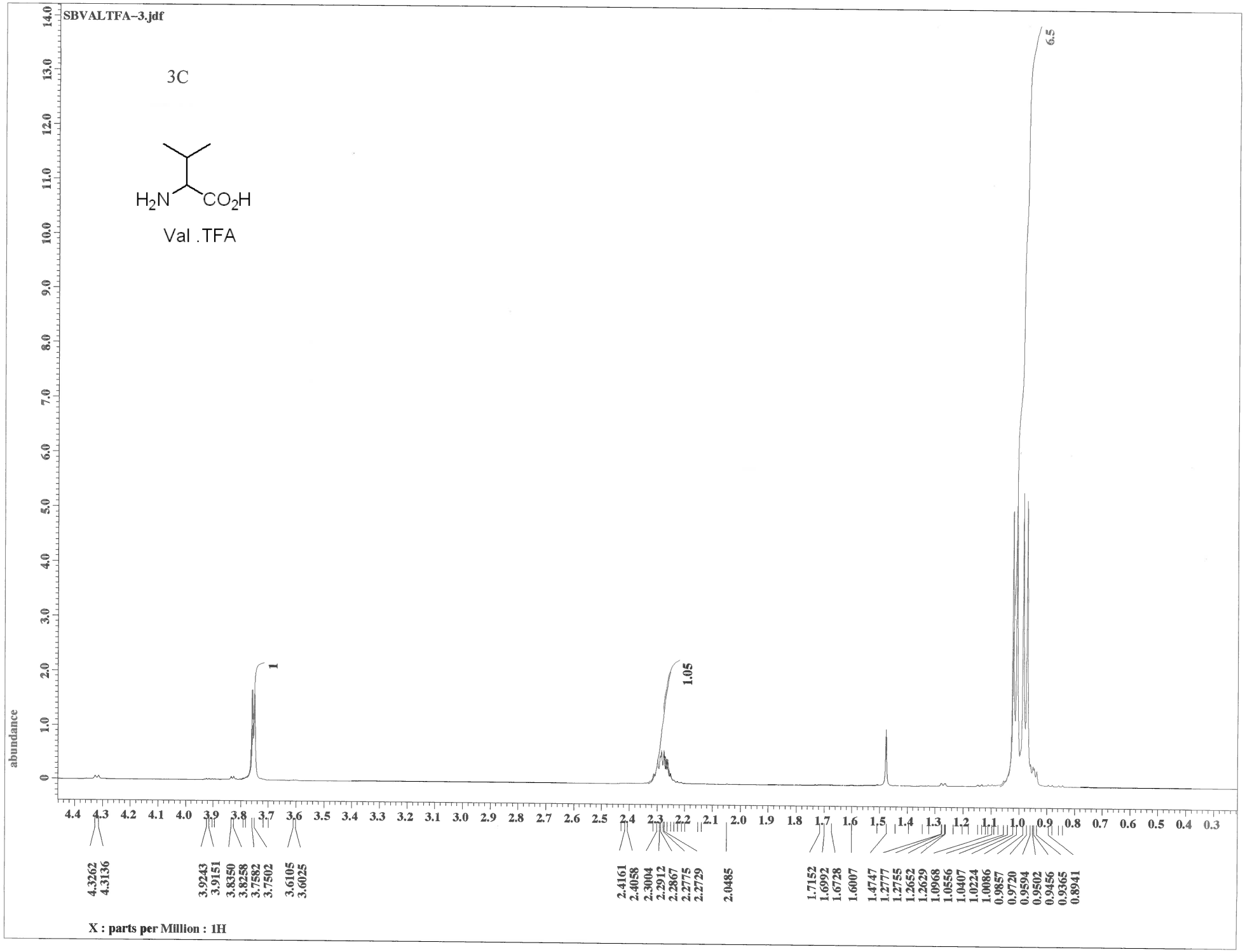

```
Filename          = SBGLYTFAC-2.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#687420
Solvent           = D2O
Creation_time     = 10-SEP-2015 07:56:49
Revision_time     =  9-SEP-2015 19:13:06
Current_time      =  9-SEP-2015 19:15:19

Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = JNM-ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 0.83361792[s]
X_domain          = 13C
X_freq            = 125.76529768[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 1.19959034[Hz]
X_sweep           = 39.3081761[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 10
Scans             = 420
Total_scans       = 420

X_90_width        = 10.73[us]
X_acq_time        = 0.83361792[s]
X_angle           = 30[deg]
X_atn             = 9[dB]
X_pulse           = 3.57666667[us]
Irr_atn_dec       = 20[dB]
Irr_atn_noe       = 20[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 0.2[s]
Recvr_gain        = 50
Relaxation_delay  = 0.2[s]
Repetition_time   = 1.03361792[s]
Temp_get          = 21.8[dC]
```




```
Filename          = SBALATFA-3.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#729523
Solvent           = D2O
Creation_time     = 11-SEP-2015 09:02:52
Revision_time     = 10-SEP-2015 20:20:43
Current_time      = 10-SEP-2015 20:21:35

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = JNM-ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.74587904[s]
X_domain          = 1H
X_freq            = 500.15991521[MHz]
X_offset          = 5.0[ppm]
X_points          = 16384
X_prescans        = 0
X_resolution      = 0.57277737[Hz]
X_sweep           = 9.38438438[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Tri_domain        = 1H
Tri_freq          = 500.15991521[MHz]
Tri_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 11
Total_scans       = 11

X_90_width        = 12.54[us]
X_acq_time        = 1.74587904[s]
X_angle           = 45[deg]
X_atn             = 4[dB]
X_pulse           = 6.27[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 34
Relaxation_delay  = 10[s]
Repetition_time   = 11.74587904[s]
Temp_get          = 21.2[dC]
```

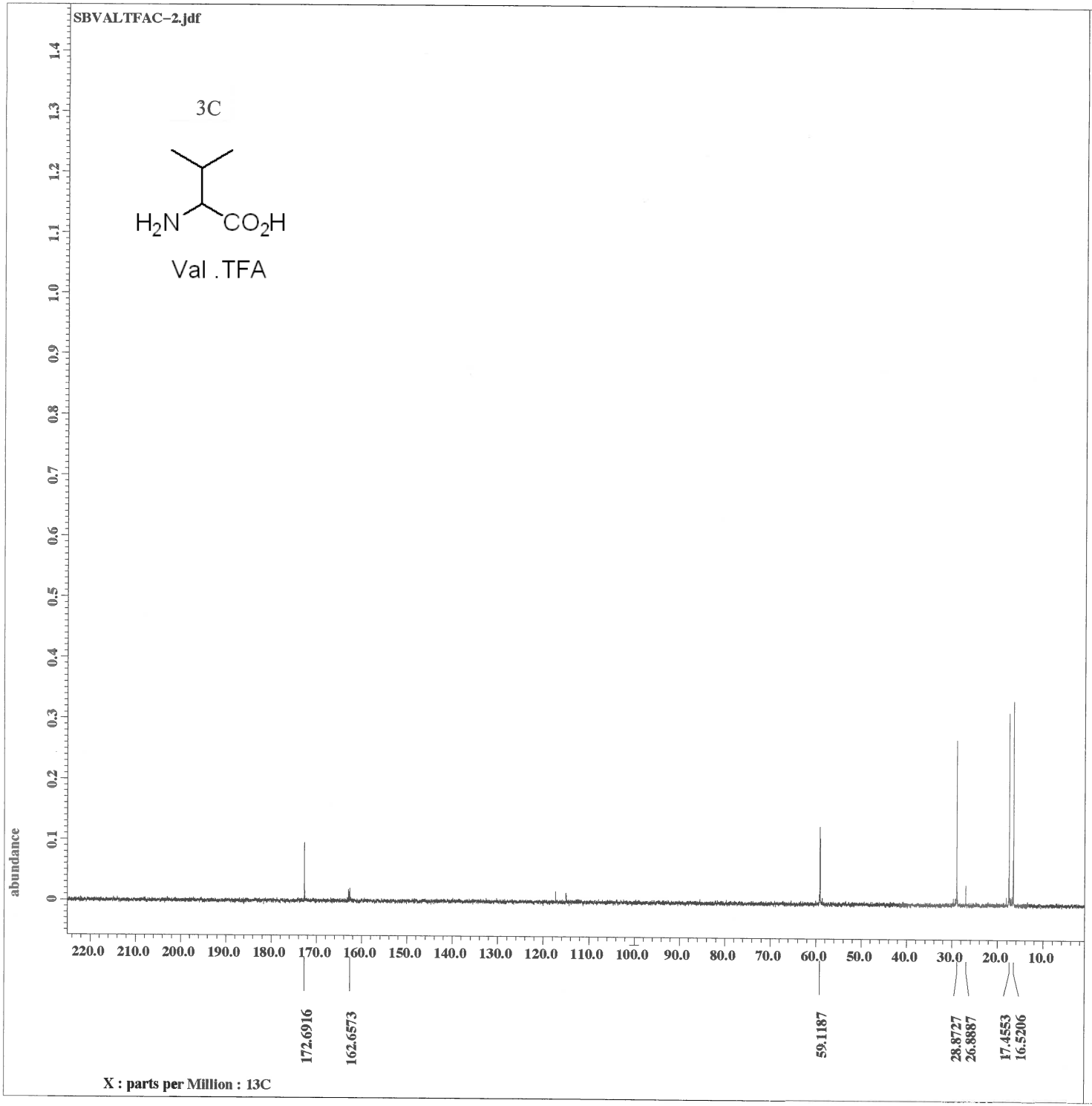


Filename	= SBALATFAC-2.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= S#731862
Solvent	= D2O
Creation_time	= 11-SEP-2015 09:10:54
Revision_time	= 10-SEP-2015 20:27:27
Current_time	= 10-SEP-2015 20:28:06
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 0.83361792[s]
X_domain	= 13C
X_freq	= 125.76529768[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.19959034[Hz]
X_sweep	= 39.3081761[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 10
Scans	= 420
Total_scans	= 420
X_90_width	= 10.73[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 9[dB]
X_pulse	= 3.57666667[us]
Irr_atn_dec	= 20[dB]
Irr_atn_noe	= 20[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 0.2[s]
Recvr_gain	= 50
Relaxation_delay	= 0.2[s]
Repetition_time	= 1.03361792[s]
Temp_get	= 21.6[dC]

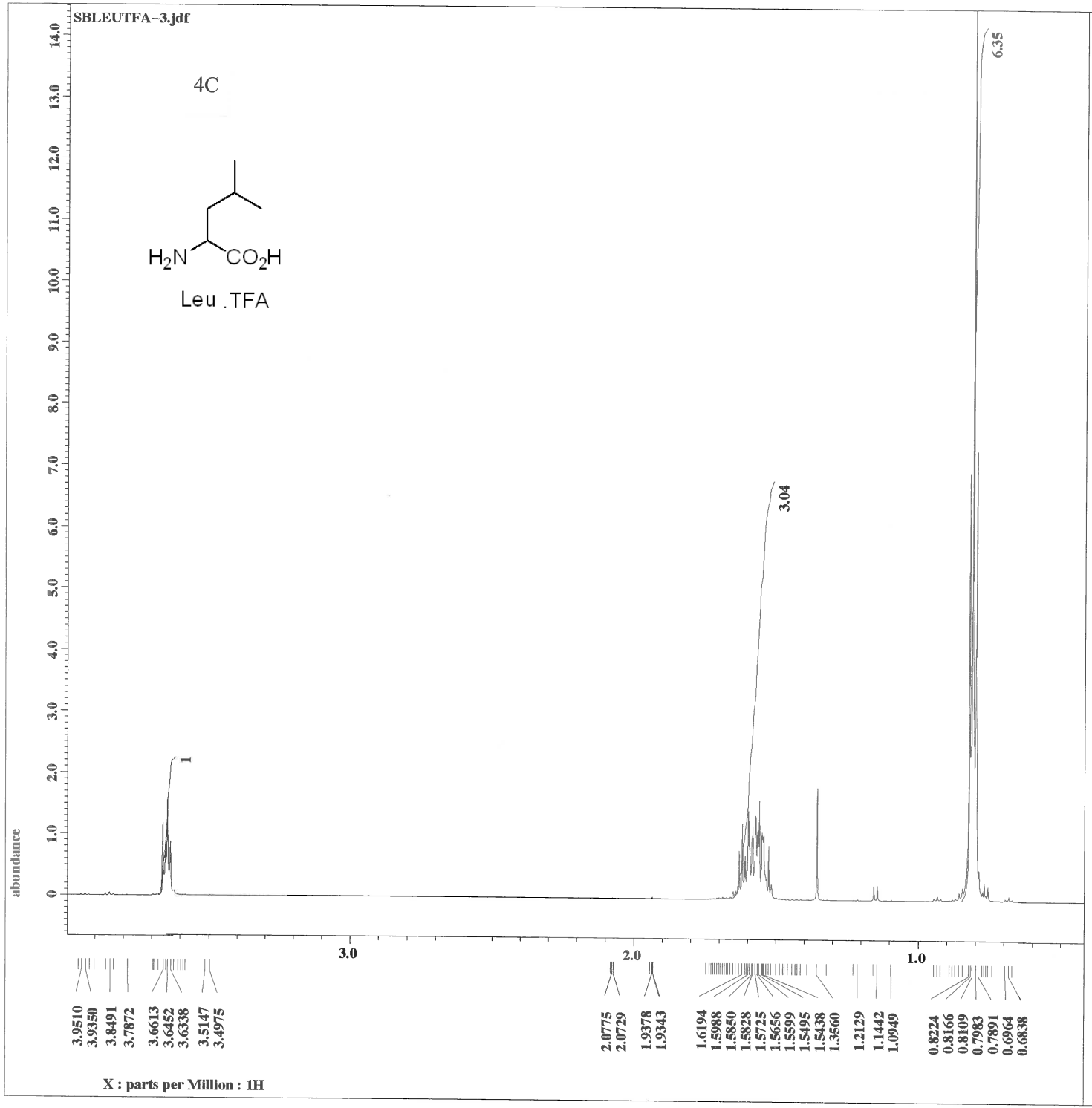

SBVALTFA-3.jdf
3C
H_2N CO_2H
Val .TFA
6.5
1
1.05
abundance
4.3262
4.3136
3.9243
3.9151
3.8350
3.8258
3.7582
3.7502
3.6105
3.6025
2.4161
2.4058
2.3004
2.2912
2.2867
2.2775
2.2729
2.0485
1.7152
1.6992
1.6728
1.6007
1.4747
1.2777
1.2755
1.2652
1.2629
1.0968
1.0556
1.0407
1.0224
1.0086
0.9857
0.9720
0.9594
0.9502
0.9456
0.9365
0.8941
X : parts per Million : 1H

SBVALTFAC-2.jdf

Val .TFA



Filename	= SBVALTFAC-2.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= S#697773
Solvent	= D2O
Creation_time	= 10-SEP-2015 08:16:46
Revision_time	= 9-SEP-2015 19:33:43
Current_time	= 9-SEP-2015 19:34:23
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 0.83361792[s]
X_domain	= 13C
X_freq	= 125.76529768[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.19959034[Hz]
X_sweep	= 39.3081761[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 10
Scans	= 640
Total_scans	= 640
X_90_width	= 10.73[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 9[dB]
X_pulse	= 3.57666667[us]
Irr_atn_dec	= 20[dB]
Irr_atn_noe	= 20[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 0.1[s]
Recvr_gain	= 50
Relaxation_delay	= 0.1[s]
Repetition_time	= 0.93361792[s]
Temp_get	= 21.7[dC]



Filename	= SBLEUTFA-3.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= S#720720
Solvent	= D2O
Creation_time	= 11-SEP-2015 08:47:59
Revision_time	= 10-SEP-2015 20:06:27
Current_time	= 10-SEP-2015 20:08:03
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 1.74587904[s]
X_domain	= 1H
X_freq	= 500.15991521[MHz]
X_offset	= 5.0[ppm]
X_points	= 16384
X_prescans	= 0
X_resolution	= 0.57277737[Hz]
X_sweep	= 9.38438438[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Tri_domain	= 1H
Tri_freq	= 500.15991521[MHz]
Tri_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 10
Total_scans	= 10
X_90_width	= 12.54[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 4[dB]
X_pulse	= 6.27[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 34
Relaxation_delay	= 10[s]
Repetition_time	= 11.74587904[s]
Temp_get	= 21.2[dC]

SBLEUTFAC-2.jdf

4C

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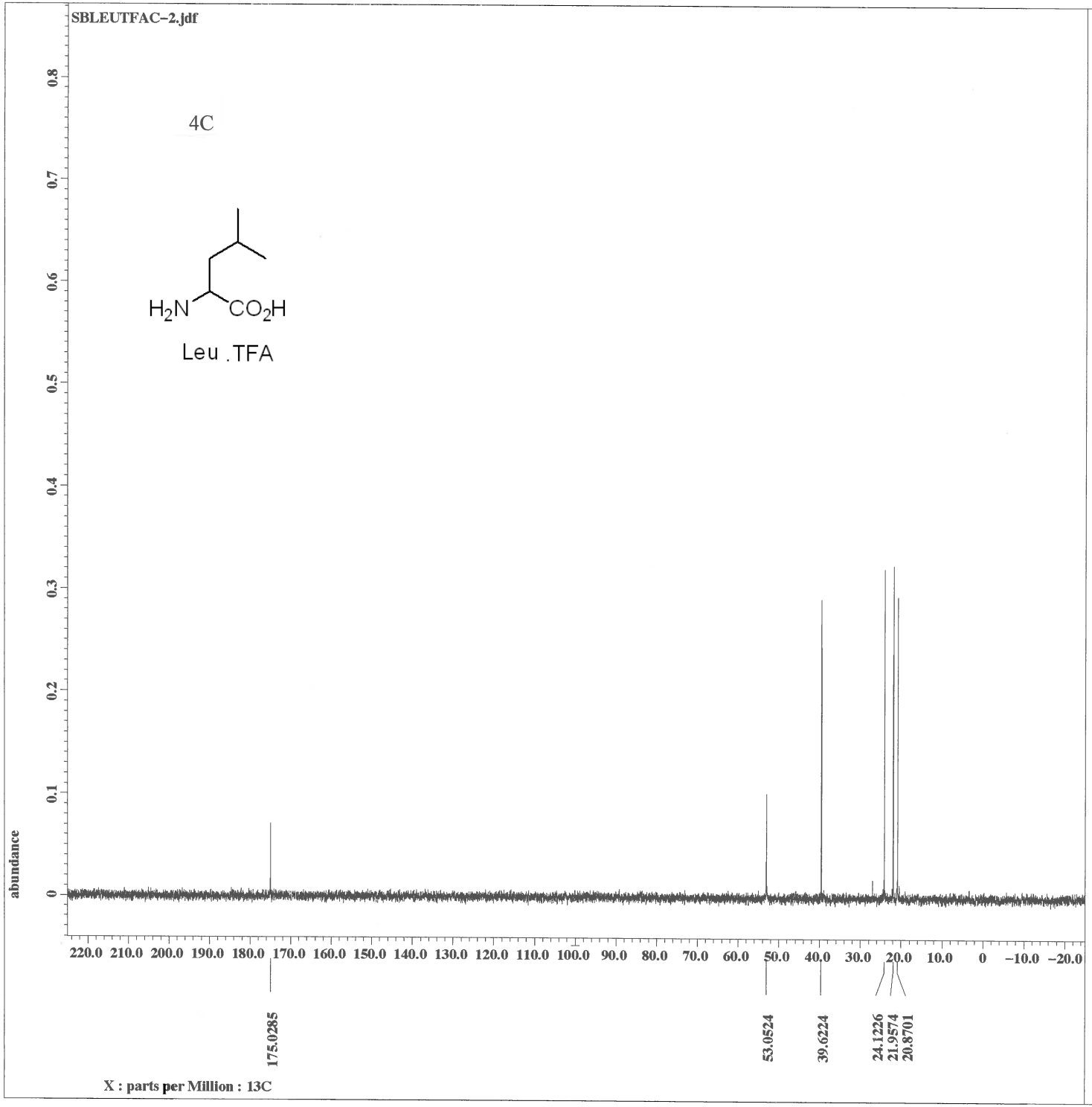
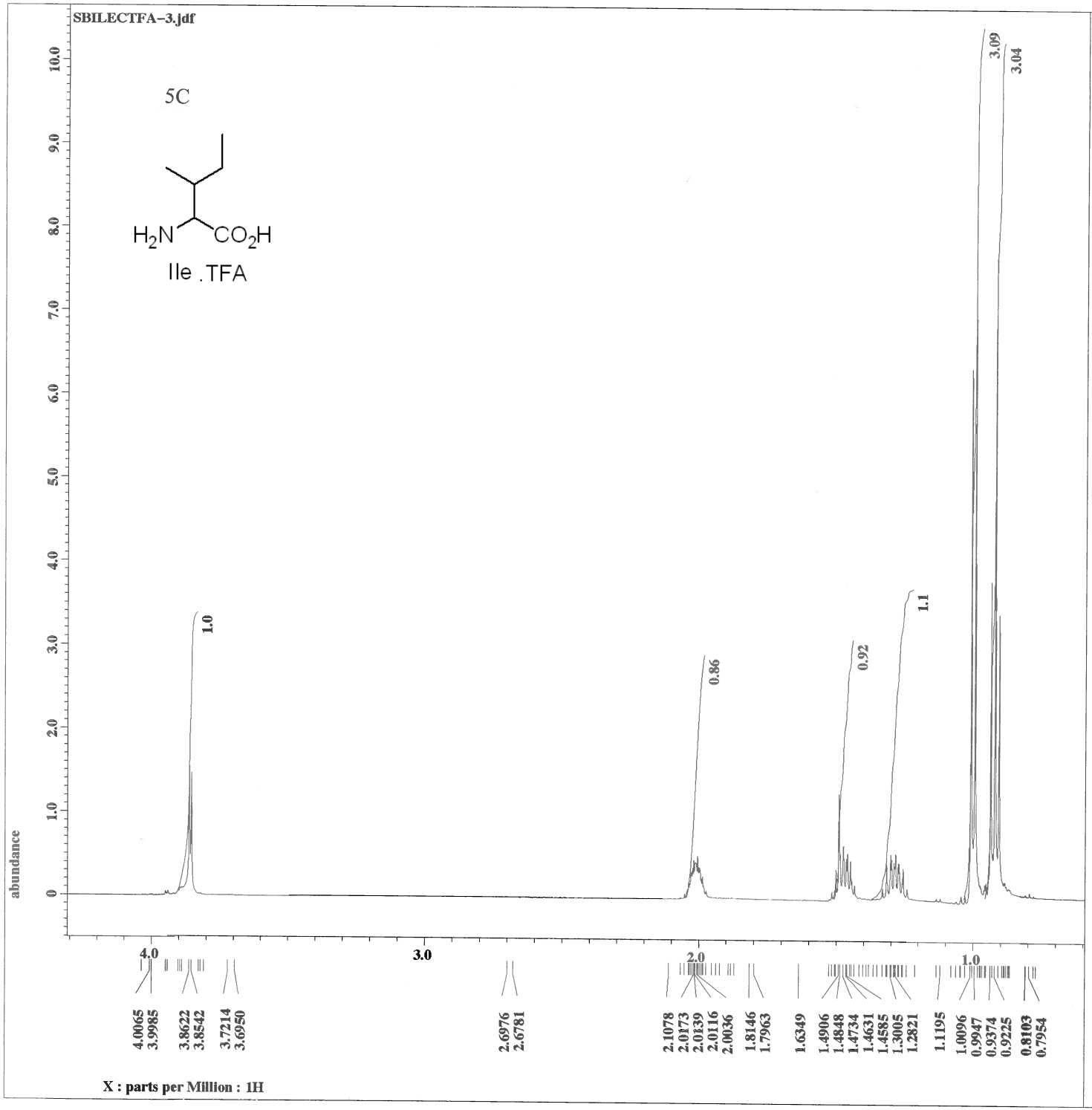


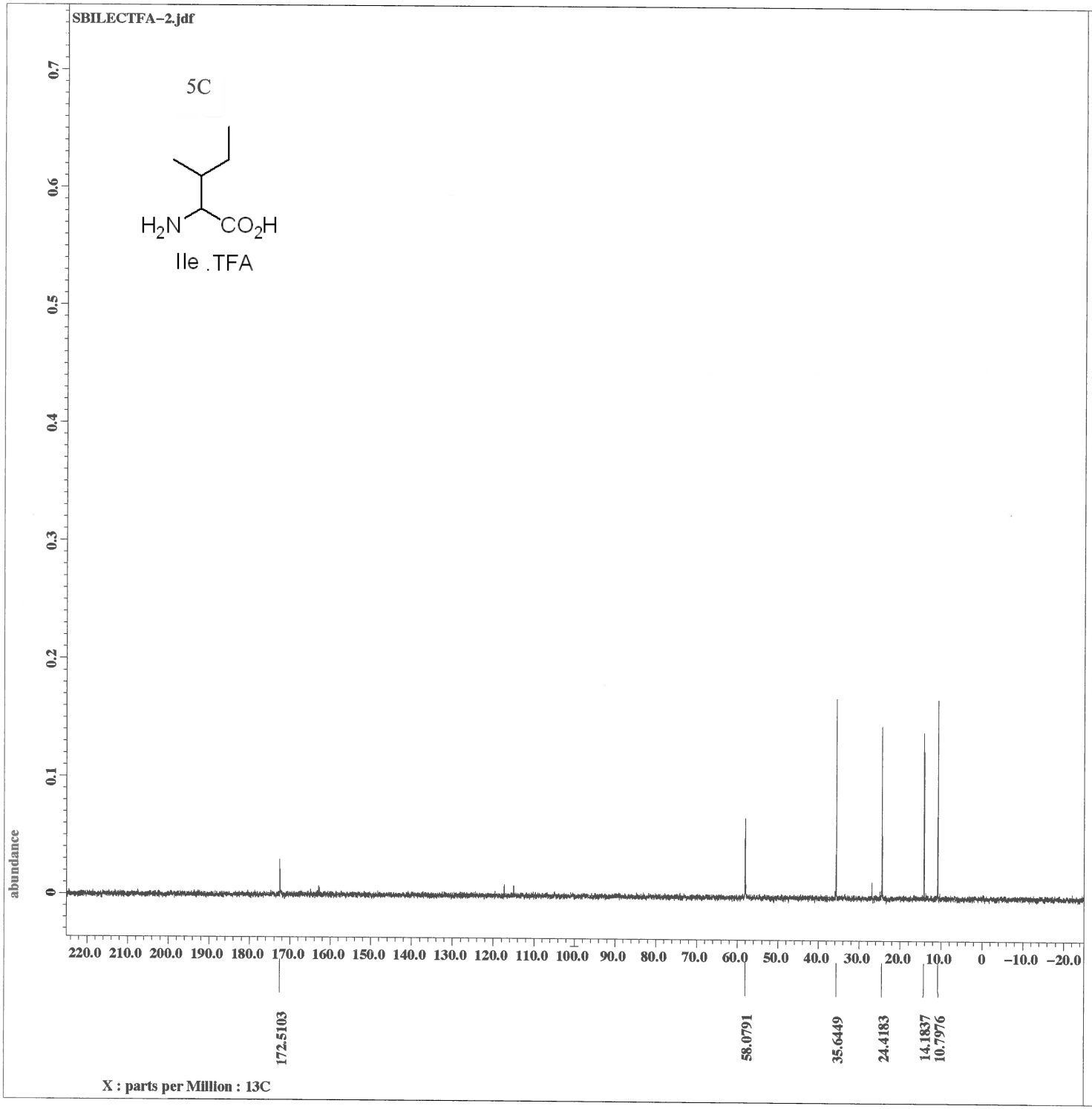
Filename	= SBLEUTFAC-2.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= S#723009
Solvent	= D2O
Creation_time	= 11-SEP-2015 08:54:15
Revision_time	= 10-SEP-2015 20:11:01
Current_time	= 10-SEP-2015 20:11:43
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 0.83361792[s]
X_domain	= 13C
X_freq	= 125.76529768[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.19959034[Hz]
X_sweep	= 39.3081761[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 10
Scans	= 310
Total_scans	= 310
X_90_width	= 10.73[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 9[dB]
X_pulse	= 3.57666667[us]
Irr_atn_dec	= 20[dB]
Irr_atn_noe	= 20[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 0.2[s]
Recvr_gain	= 50
Relaxation_delay	= 0.2[s]
Repetition_time	= 1.03361792[s]
Temp_get	= 21.6[dC]



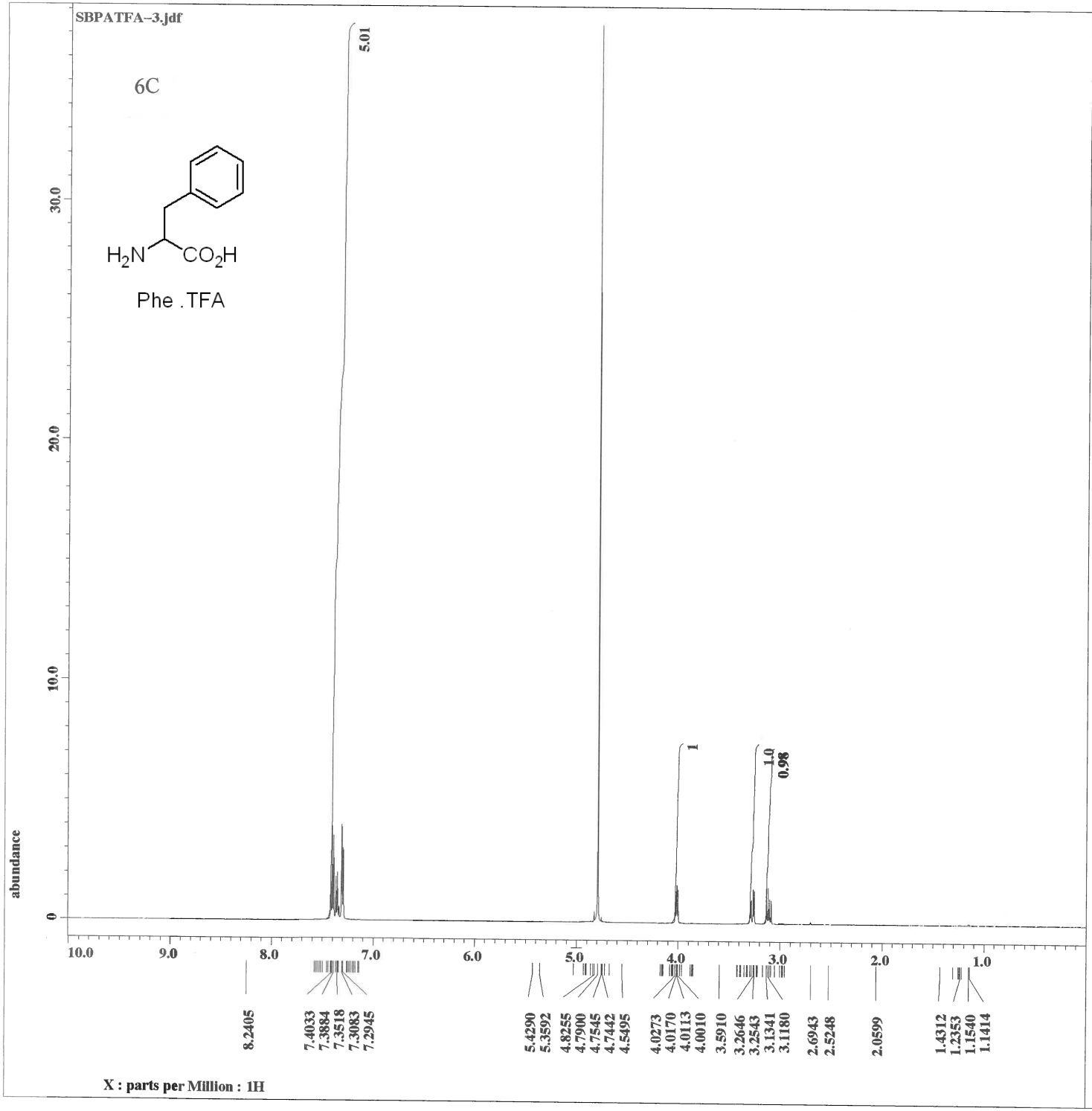
Filename	= SBILECTFA-4.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= S#728966
Solvent	= D2O
Creation_time	= 27-SEP-2015 09:02:20
Revision_time	= 26-SEP-2015 20:23:54
Current_time	= 26-SEP-2015 20:23:56
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 1.74587904[s]
X_domain	= 1H
X_freq	= 500.15991521[MHz]
X_offset	= 5.0[ppm]
X_points	= 16384
X_prescans	= 0
X_resolution	= 0.57277737[Hz]
X_sweep	= 9.38438438[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Tri_domain	= 1H
Tri_freq	= 500.15991521[MHz]
Tri_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 10
Total_scans	= 10
X_90_width	= 12.54[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 4[dB]
X_pulse	= 6.27[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 36
Relaxation_delay	= 10[s]
Repetition_time	= 11.74587904[s]
Temp_get	= 21.6[dC]

SBILECTFA-2.jdf

Ile .TFA



Filename	= SBILECTFA-2.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= S#731232
Solvent	= D2O
Creation_time	= 27-SEP-2015 09:27:10
Revision_time	= 26-SEP-2015 20:43:10
Current_time	= 26-SEP-2015 20:45:11
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 0.83361792[s]
X_domain	= 13C
X_freq	= 125.76529768[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.19959034[Hz]
X_sweep	= 39.3081761[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 10
Scans	= 1390
Total_scans	= 1390
X_90_width	= 10.73[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 9[dB]
X_pulse	= 3.57666667[us]
Irr_atn_dec	= 20[dB]
Irr_atn_noe	= 20[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 0.2[s]
Recvr_gain	= 50
Relaxation_delay	= 0.2[s]
Repetition_time	= 1.03361792[s]
Temp_get	= 22.1[dC]

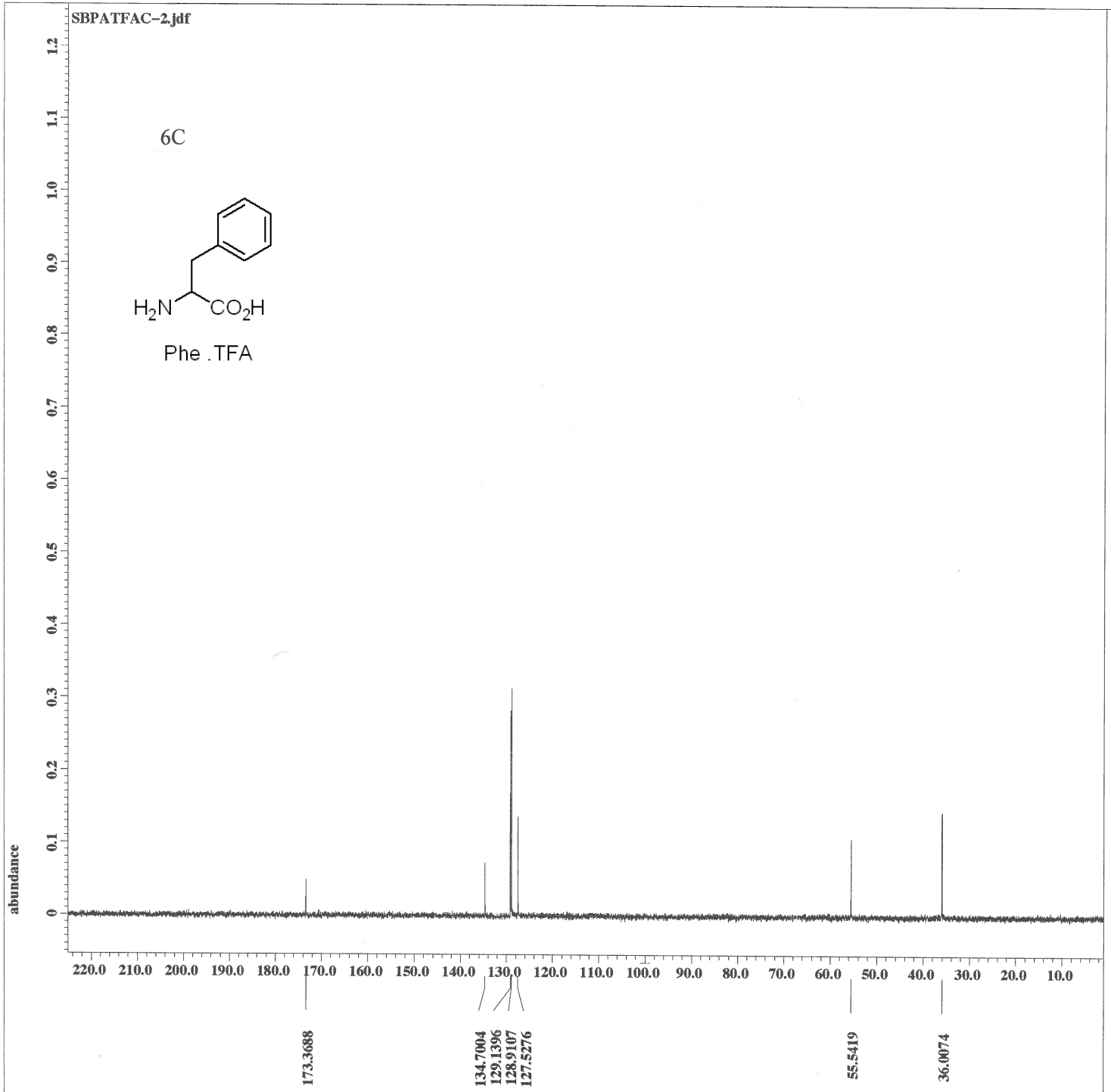


Filename	= SBPATFA-3.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= S#398428
Solvent	= D2O
Creation_time	= 19-SEP-2015 23:52:20
Revision_time	= 19-SEP-2015 11:10:44
Current_time	= 19-SEP-2015 11:11:11
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 1.74587904[s]
X_domain	= 1H
X_freq	= 500.15991521[MHz]
X_offset	= 5.0[ppm]
X_points	= 16384
X_prescans	= 0
X_resolution	= 0.57277737[Hz]
X_sweep	= 9.38438438[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Tri_domain	= 1H
Tri_freq	= 500.15991521[MHz]
Tri_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 16
Total_scans	= 16
X_90_width	= 12.54[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 4[dB]
X_pulse	= 6.27[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 40
Relaxation_delay	= 10[s]
Repetition_time	= 11.74587904[s]
Temp_get	= 21.2[dC]

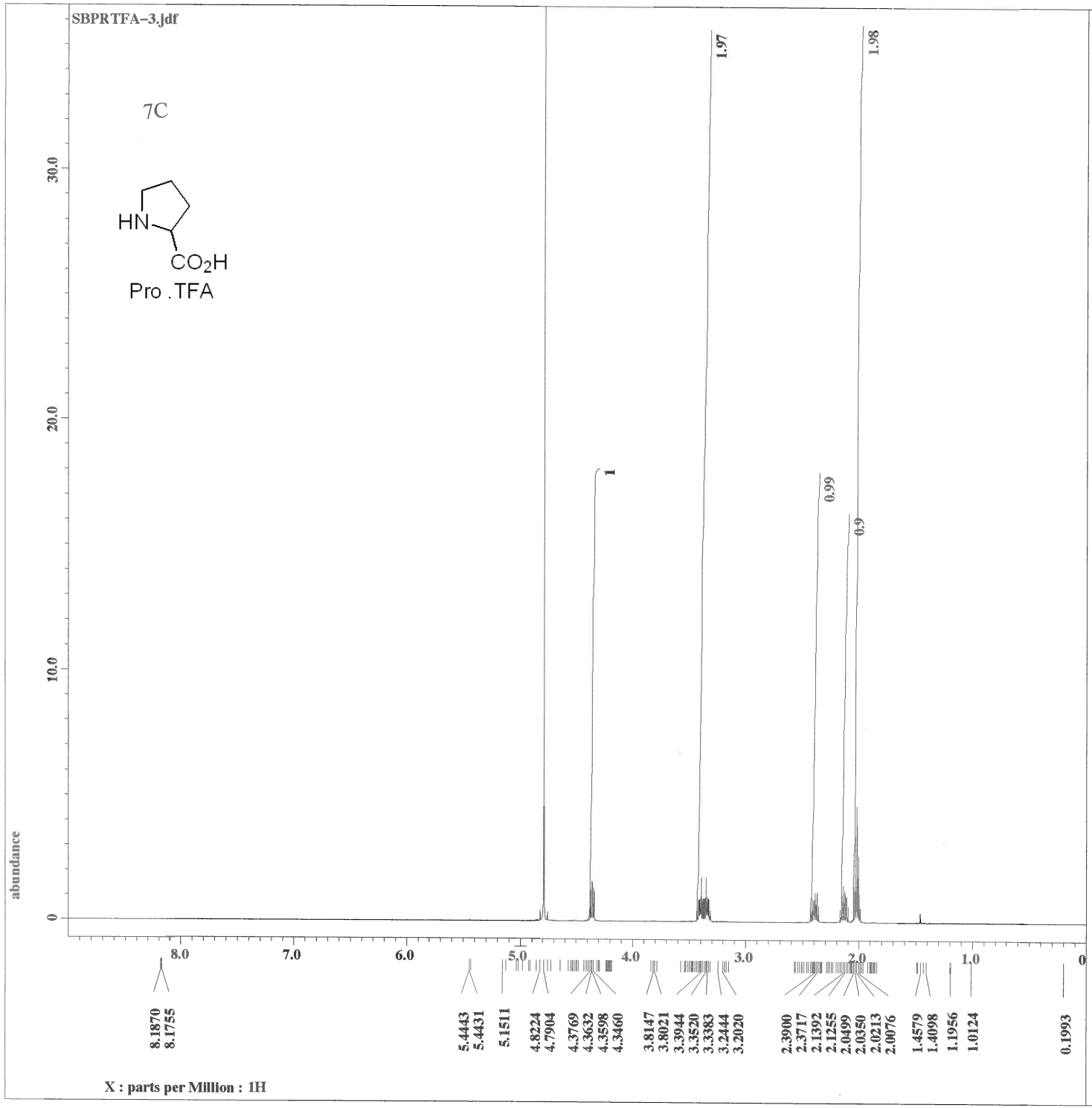
SBPATFAC-2.jdf

6C

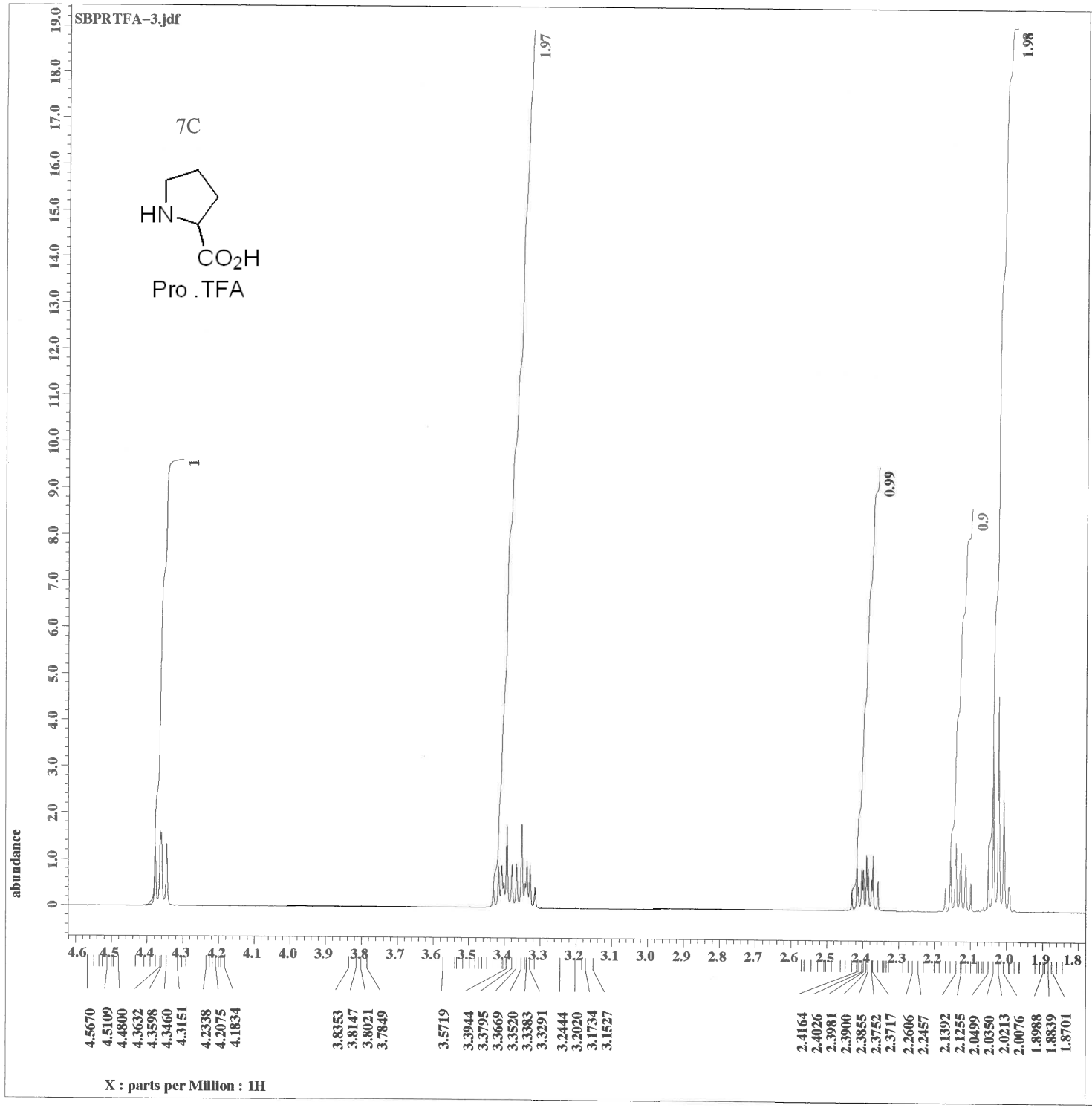
Phe .TFA



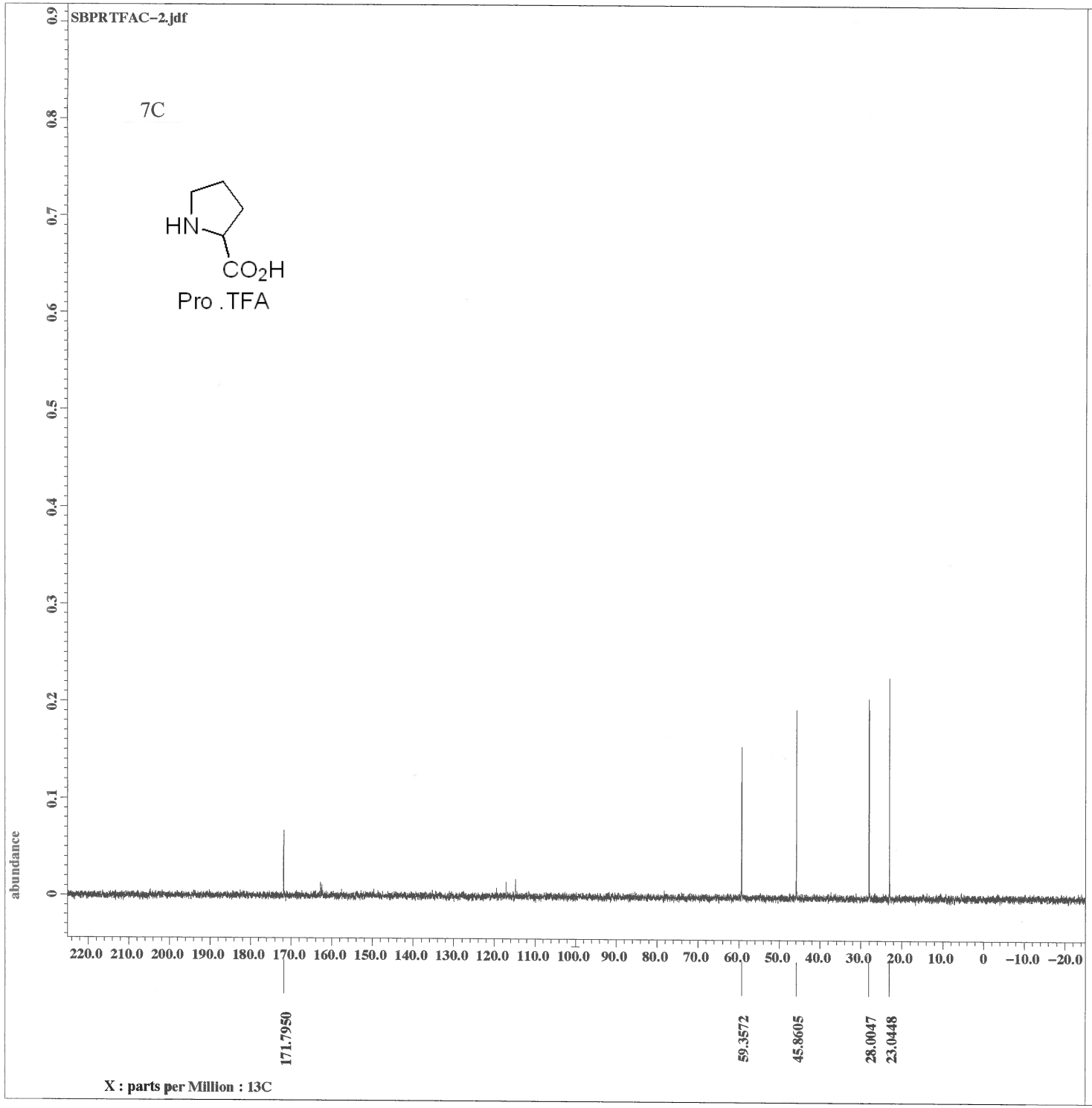
Filename	= SBPATFAC-2.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= S#401375
Solvent	= D2O
Creation_time	= 20-SEP-2015 00:01:27
Revision_time	= 19-SEP-2015 11:17:31
Current_time	= 19-SEP-2015 11:17:59
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 0.83361792[s]
X_domain	= 13C
X_freq	= 125.76529768[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.19959034[Hz]
X_sweep	= 39.3081761[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 10
Scans	= 480
Total_scans	= 480
X_90_width	= 10.73[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 9[dB]
X_pulse	= 3.57666667[us]
Irr_atn_dec	= 20[dB]
Irr_atn_noe	= 20[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 0.2[s]
Recvr_gain	= 50
Relaxation_delay	= 0.2[s]
Repetition_time	= 1.03361792[s]
Temp_get	= 21.7[dC]



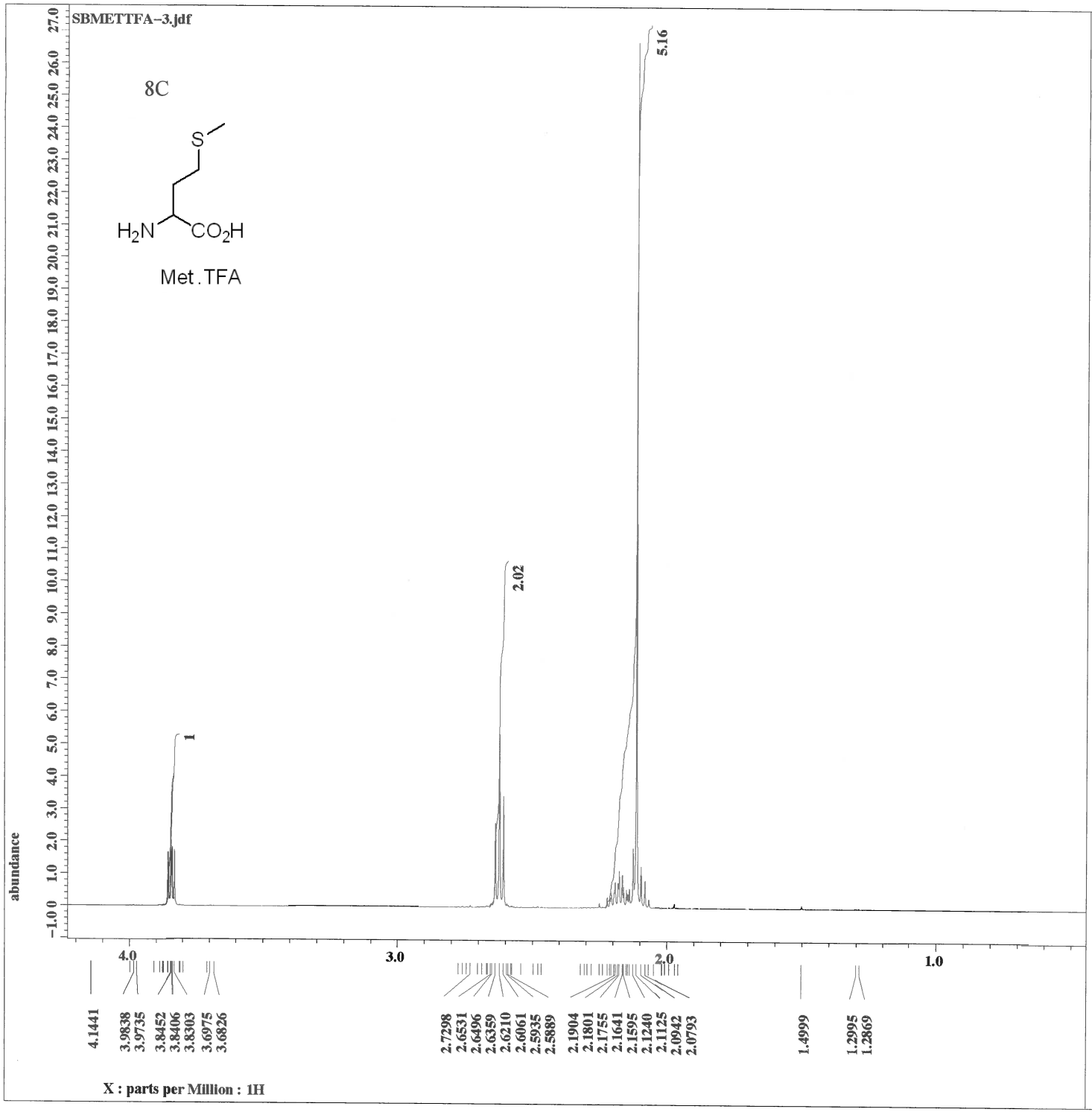
Filename	= SBPRTFA-3.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= S#364521
Solvent	= D2O
Creation_time	= 10-SEP-2015 22:55:29
Revision_time	= 10-SEP-2015 10:14:36
Current_time	= 10-SEP-2015 10:16:13
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 1.74587904[s]
X_domain	= 1H
X_freq	= 500.15991521[MHz]
X_offset	= 5.0[ppm]
X_points	= 16384
X_prescans	= 0
X_resolution	= 0.57277737[Hz]
X_sweep	= 9.38438438[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Tri_domain	= 1H
Tri_freq	= 500.15991521[MHz]
Tri_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 16
Total_scans	= 16
X_90_width	= 12.54[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 4[dB]
X_pulse	= 6.27[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 36
Relaxation_delay	= 10[s]
Repetition_time	= 11.74587904[s]
Temp_get	= 21.1[dC]




```
Filename          = SBPRTFA-3.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#364521
Solvent           = D2O
Creation_time     = 10-SEP-2015 22:55:29
Revision_time     = 10-SEP-2015 10:14:36
Current_time      = 10-SEP-2015 10:16:47

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = JNM-ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.74587904[s]
X_domain          = 1H
X_freq            = 500.15991521[MHz]
X_offset          = 5.0[ppm]
X_points          = 16384
X_prescans        = 0
X_resolution      = 0.57277737[Hz]
X_sweep           = 9.38438438[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Tri_domain        = 1H
Tri_freq          = 500.15991521[MHz]
Tri_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 16
Total_scans       = 16

X_90_width        = 12.54[us]
X_acq_time        = 1.74587904[s]
X_angle           = 45[deg]
X_atn             = 4[dB]
X_pulse           = 6.27[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 36
Relaxation_delay  = 10[s]
Repetition_time   = 11.74587904[s]
Temp_get          = 21.1[dC]
```



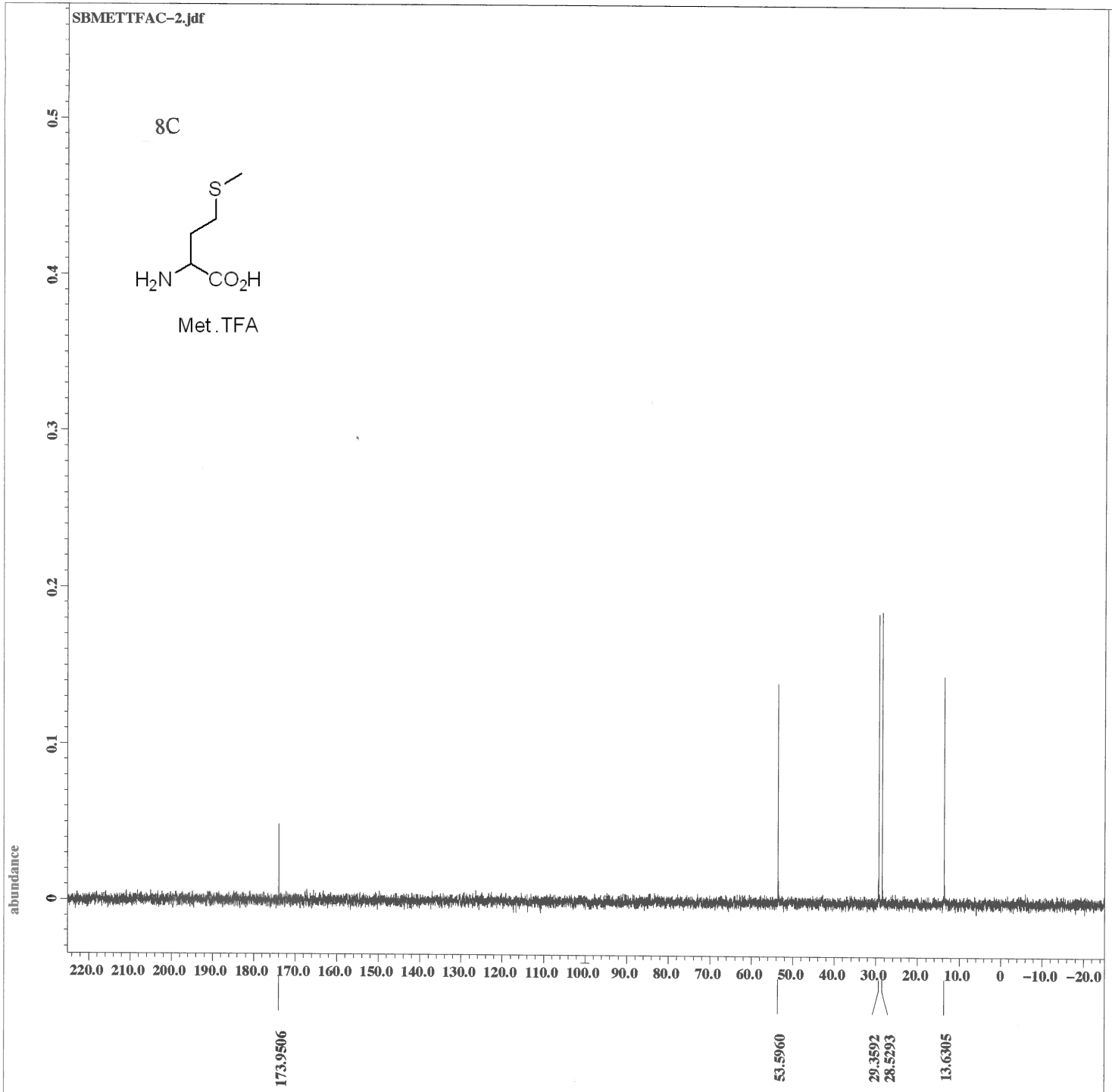
Filename	= SBPRTFAC-2.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= S#368427
Solvent	= D2O
Creation_time	= 10-SEP-2015 23:06:02
Revision_time	= 10-SEP-2015 10:22:49
Current_time	= 10-SEP-2015 10:23:29
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 0.83361792[s]
X_domain	= 13C
X_freq	= 125.76529768[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.19959034[Hz]
X_sweep	= 39.3081761[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 10
Scans	= 470
Total_scans	= 470
X_90_width	= 10.73[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 9[dB]
X_pulse	= 3.57666667[us]
Irr_atn_dec	= 20[dB]
Irr_atn_noe	= 20[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 0.2[s]
Recvr_gain	= 50
Relaxation_delay	= 0.2[s]
Repetition_time	= 1.03361792[s]
Temp_get	= 21.5[dC]



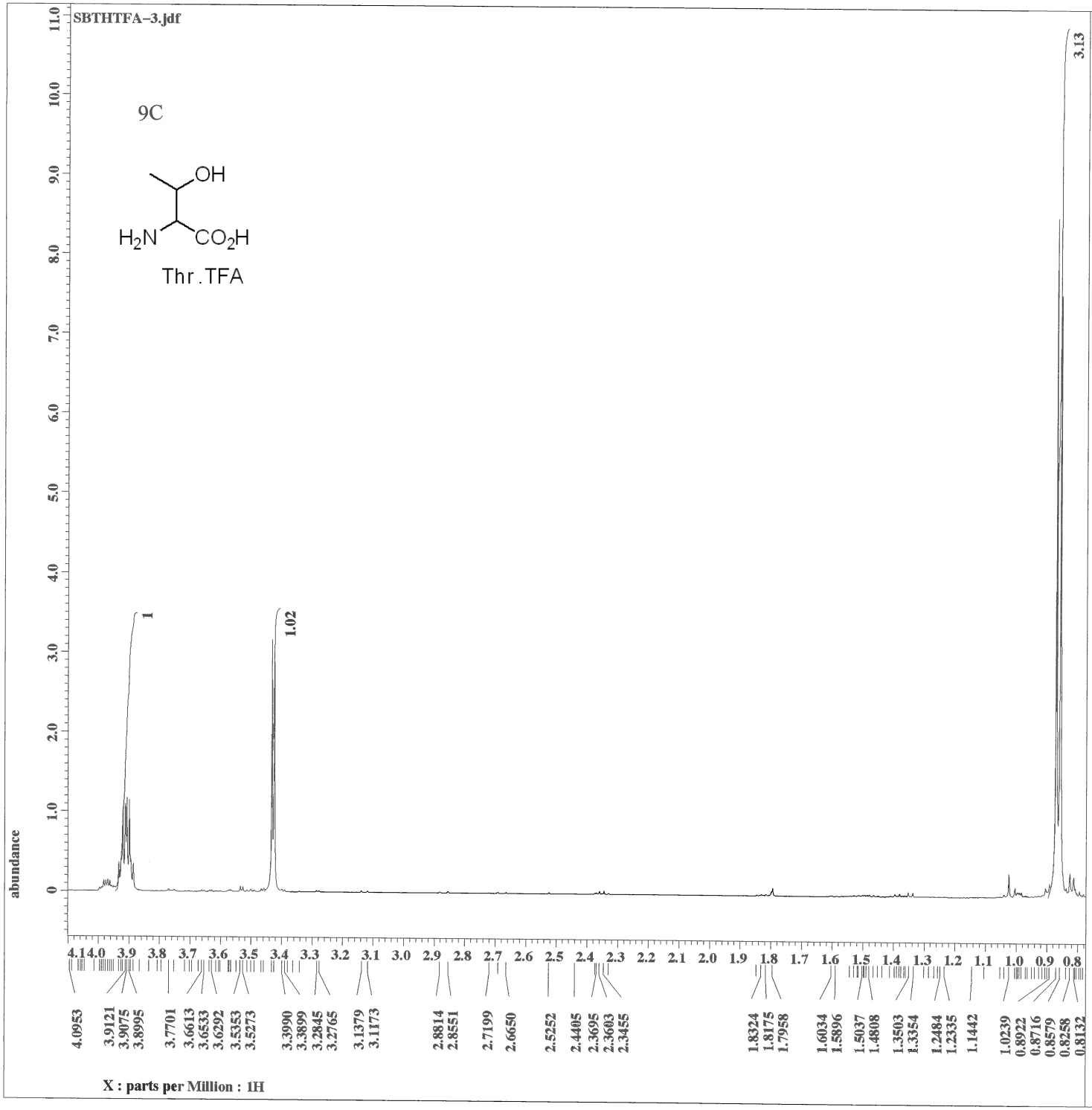
Filename	= SBMETTFA-3.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= S#666579
Solvent	= D2O
Creation_time	= 16-SEP-2015 07:18:08
Revision_time	= 15-SEP-2015 18:36:19
Current_time	= 15-SEP-2015 18:37:13
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 1.74587904[s]
X_domain	= 1H
X_freq	= 500.15991521[MHz]
X_offset	= 5.0[ppm]
X_points	= 16384
X_prescans	= 0
X_resolution	= 0.57277737[Hz]
X_sweep	= 9.38438438[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Tri_domain	= 1H
Tri_freq	= 500.15991521[MHz]
Tri_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 11
Total_scans	= 11
X_90_width	= 12.54[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 4[dB]
X_pulse	= 6.27[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 38
Relaxation_delay	= 10[s]
Repetition_time	= 11.74587904[s]
Temp_get	= 21.2[dC]

SBMETTFAC-2.jdf

Met.TFA



Filename	= SBMETTFAC-2.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= S#669006
Solvent	= D2O
Creation_time	= 16-SEP-2015 07:26:52
Revision_time	= 15-SEP-2015 18:43:06
Current_time	= 15-SEP-2015 18:43:22
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 0.83361792[s]
X_domain	= 13C
X_freq	= 125.76529768[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.19959034[Hz]
X_sweep	= 39.3081761[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 10
Scans	= 500
Total_scans	= 500
X_90_width	= 10.73[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 9[dB]
X_pulse	= 3.57666667[us]
Irr_atn_dec	= 20[dB]
Irr_atn_noe	= 20[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 0.1[s]
Recvr_gain	= 50
Relaxation_delay	= 0.1[s]
Repetition_time	= 0.93361792[s]
Temp_get	= 21.6[dC]

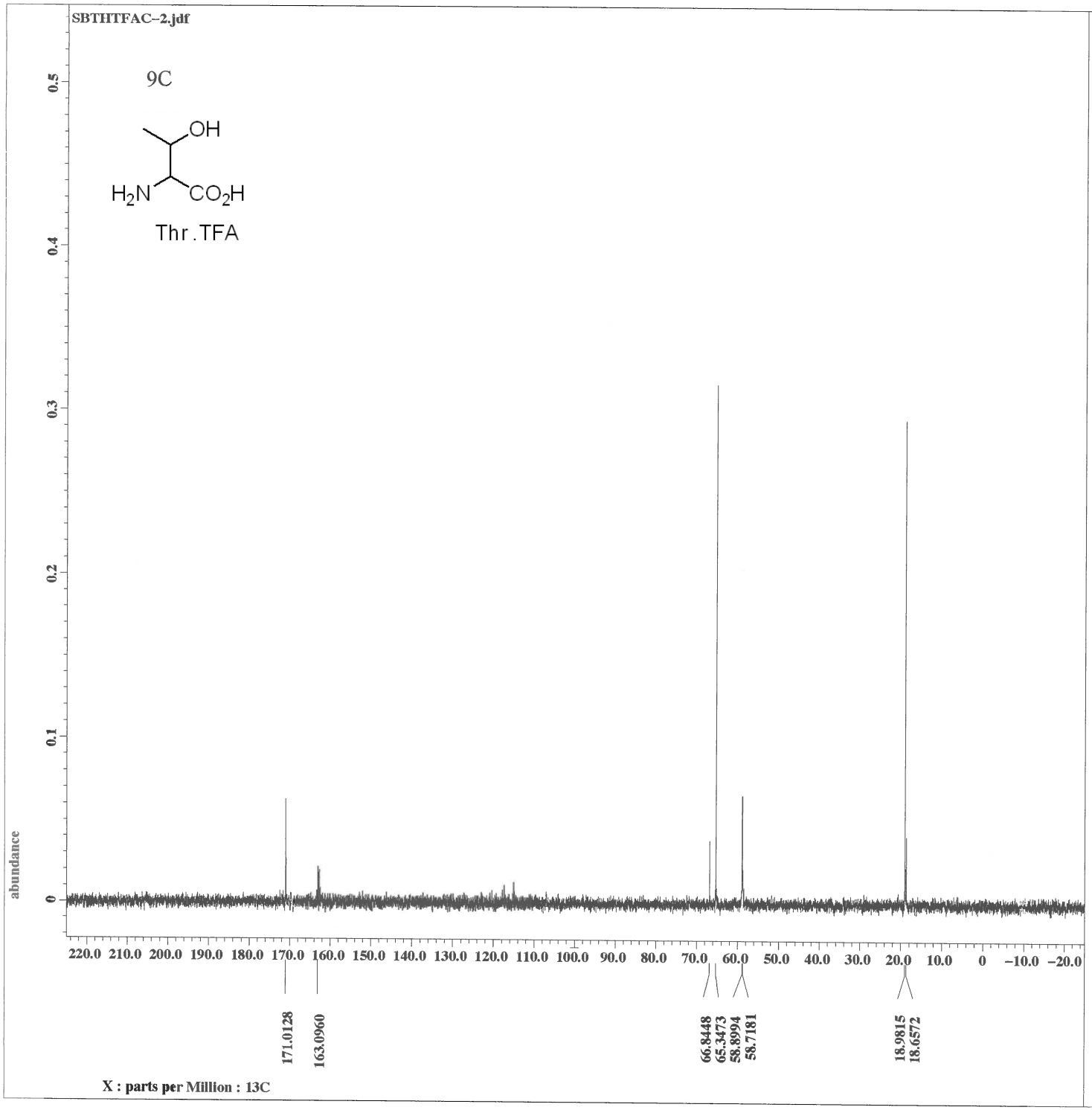


Filename	= SBTHTFA-3.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= S#508822
Solvent	= D2O
Creation_time	= 10-SEP-2015 02:54:48
Revision_time	= 9-SEP-2015 14:12:32
Current_time	= 9-SEP-2015 14:13:28
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 1.74587904[s]
X_domain	= 1H
X_freq	= 500.15991521[MHz]
X_offset	= 5.0[ppm]
X_points	= 16384
X_prescans	= 0
X_resolution	= 0.57277737[Hz]
X_sweep	= 9.38438438[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Tri_domain	= 1H
Tri_freq	= 500.15991521[MHz]
Tri_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 10
Total_scans	= 10
X_90_width	= 12.54[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 4[dB]
X_pulse	= 6.27[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 32
Relaxation_delay	= 10[s]
Repetition_time	= 11.74587904[s]
Temp_get	= 21.5[dC]

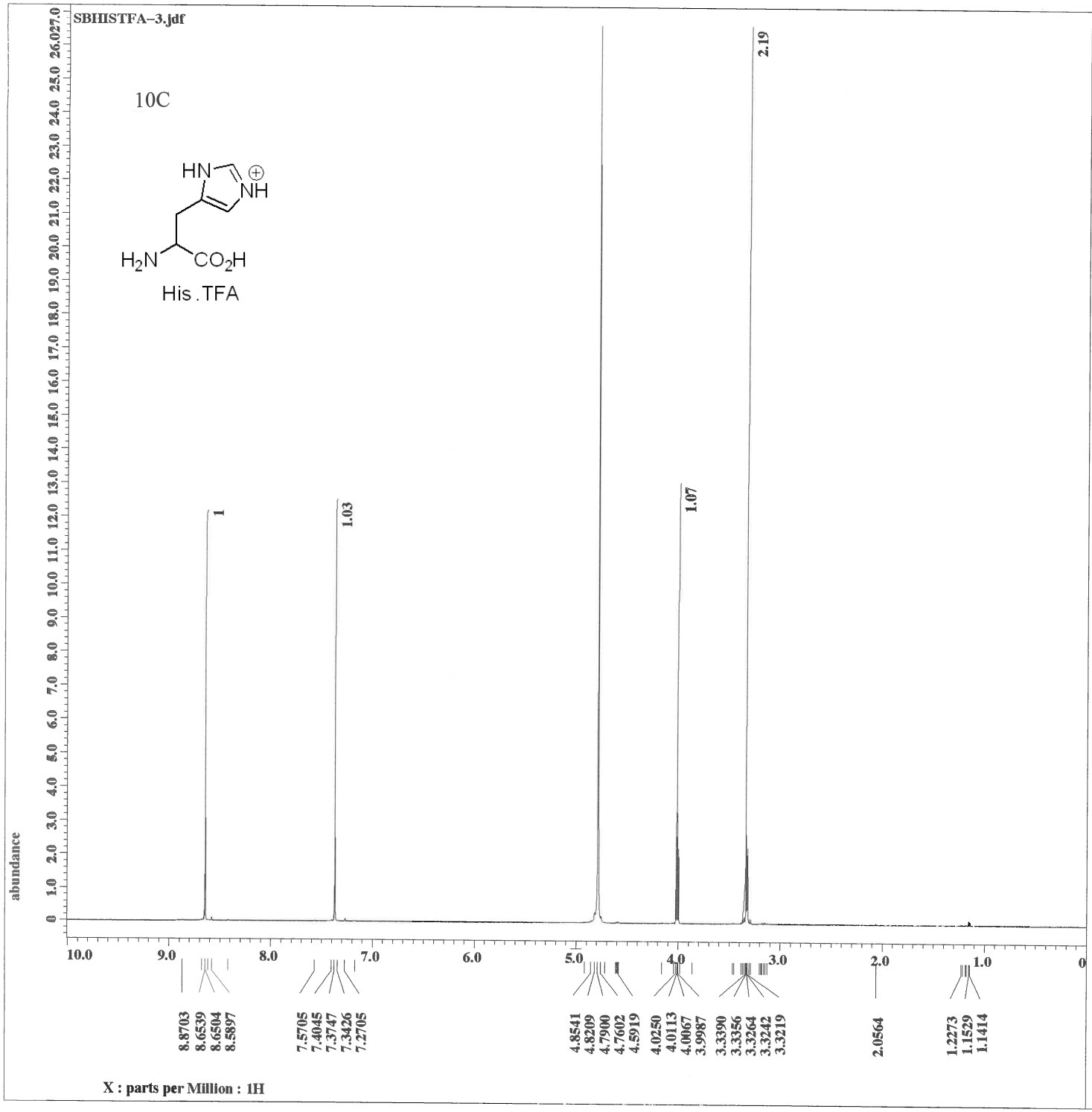
SBTHTFAC-2.jdf

9C

Thr.TFA



Filename	= SBTHTFAC-2.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= S#518113
Solvent	= D2O
Creation_time	= 10-SEP-2015 03:14:26
Revision_time	= 9-SEP-2015 14:31:07
Current_time	= 9-SEP-2015 14:31:47
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 0.83361792[s]
X_domain	= 13C
X_freq	= 125.76529768[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.19959034[Hz]
X_sweep	= 39.3081761[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 10
Scans	= 410.0
Total_scans	= 410.0
X_90_width	= 10.73[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 9[dB]
X_pulse	= 3.57666667[us]
Irr_atn_dec	= 20[dB]
Irr_atn_noe	= 20[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 0.2[s]
Recvr_gain	= 50
Relaxation_delay	= 0.2[s]
Repetition_time	= 1.03361792[s]
Temp_get	= 21.9[dC]

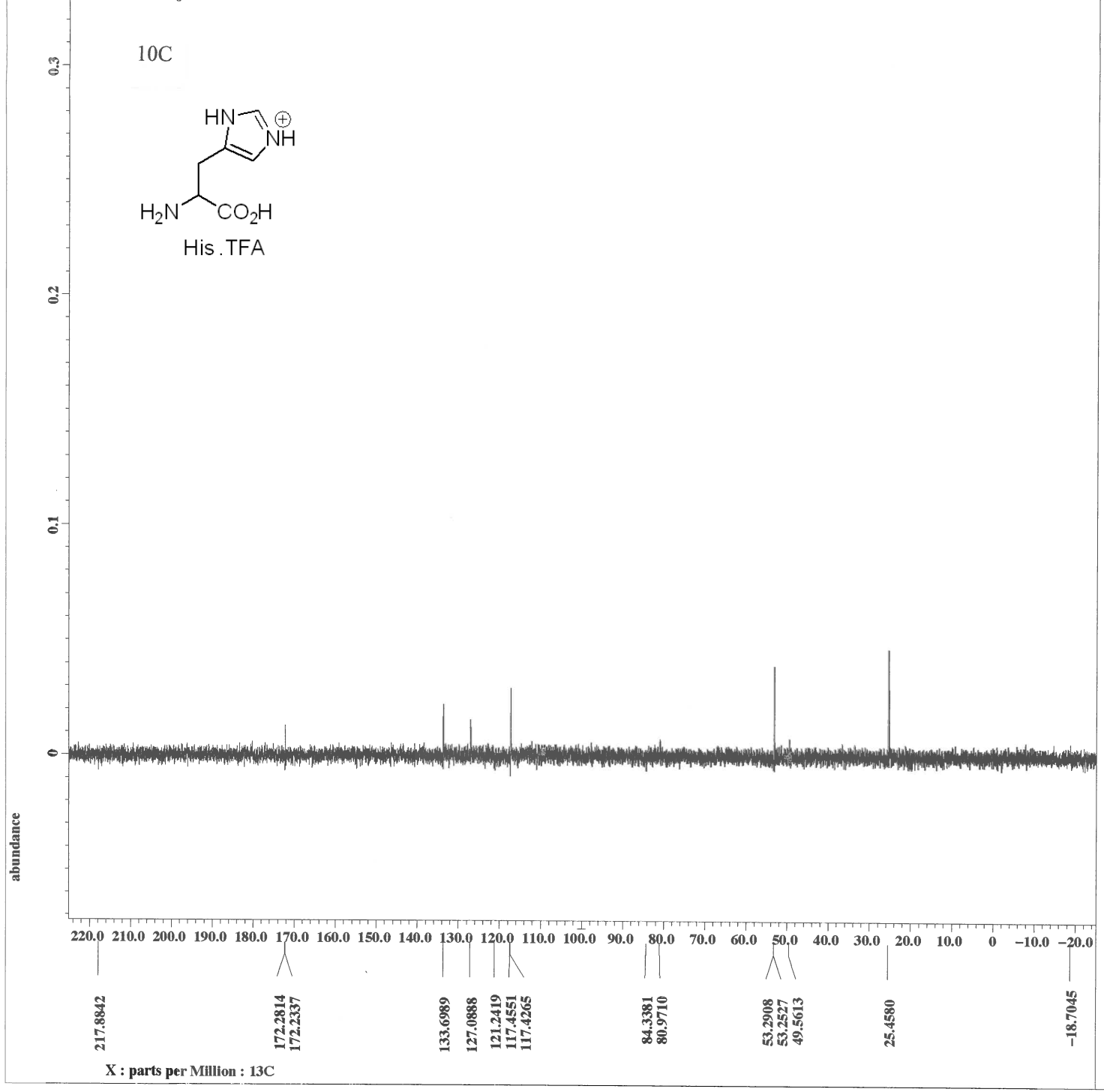



```
Filename          = SBHISTFA-3.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#653572
Solvent           = D2O
Creation_time     = 16-SEP-2015 06:55:52
Revision_time     = 15-SEP-2015 18:14:40
Current_time      = 15-SEP-2015 18:15:28

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = JNM-ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.74587904[s]
X_domain          = 1H
X_freq            = 500.15991521[MHz]
X_offset          = 5.0[ppm]
X_points          = 16384
X_prescans        = 0
X_resolution      = 0.57277737[Hz]
X_sweep           = 9.38438438[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Tri_domain        = 1H
Tri_freq          = 500.15991521[MHz]
Tri_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 10
Total_scans       = 10

X_90_width        = 12.54[us]
X_acq_time        = 1.74587904[s]
X_angle           = 45[deg]
X_atn             = 4[dB]
X_pulse           = 6.27[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 48
Relaxation_delay  = 10[s]
Repetition_time   = 11.74587904[s]
Temp_get          = 21.1[dC]
```

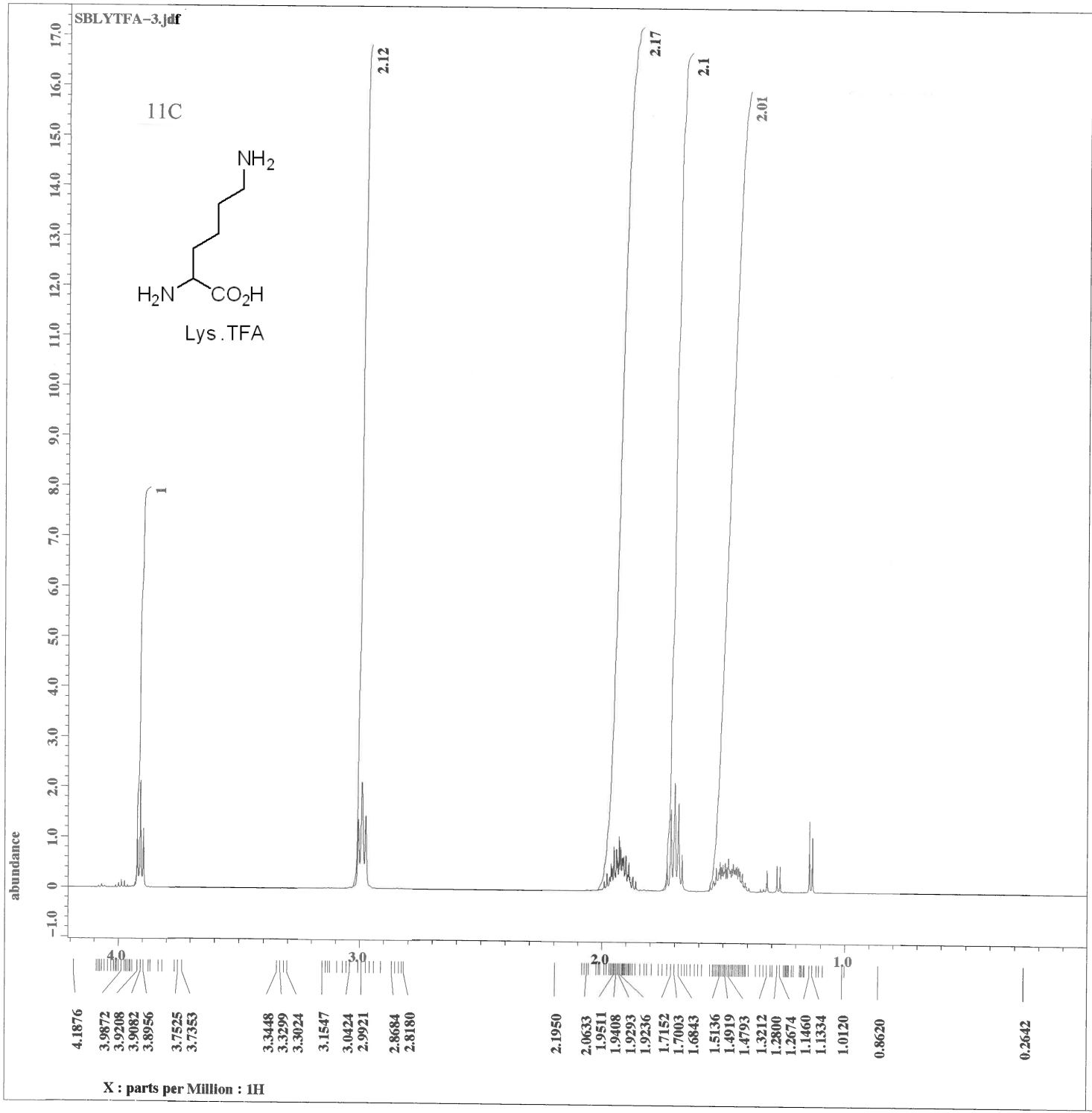
SBHISCTFA-3.jdf

10C

His . TFA



Filename	= SBHISCTFA-3.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= S#655640
Solvent	= D2O
Creation_time	= 16-SEP-2015 07:06:50
Revision_time	= 15-SEP-2015 18:23:26
Current_time	= 15-SEP-2015 18:23:42
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 0.83361792[s]
X_domain	= 13C
X_freq	= 125.76529768[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.19959034[Hz]
X_sweep	= 39.3081761[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 10
Scans	= 580
Total_scans	= 580
X_90_width	= 10.73[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 9[dB]
X_pulse	= 3.57666667[us]
Irr_atn_dec	= 20[dB]
Irr_atn_noe	= 20[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 0.2[s]
Recvr_gain	= 50
Relaxation_delay	= 0.2[s]
Repetition_time	= 1.03361792[s]
Temp_get	= 21.6[dC]

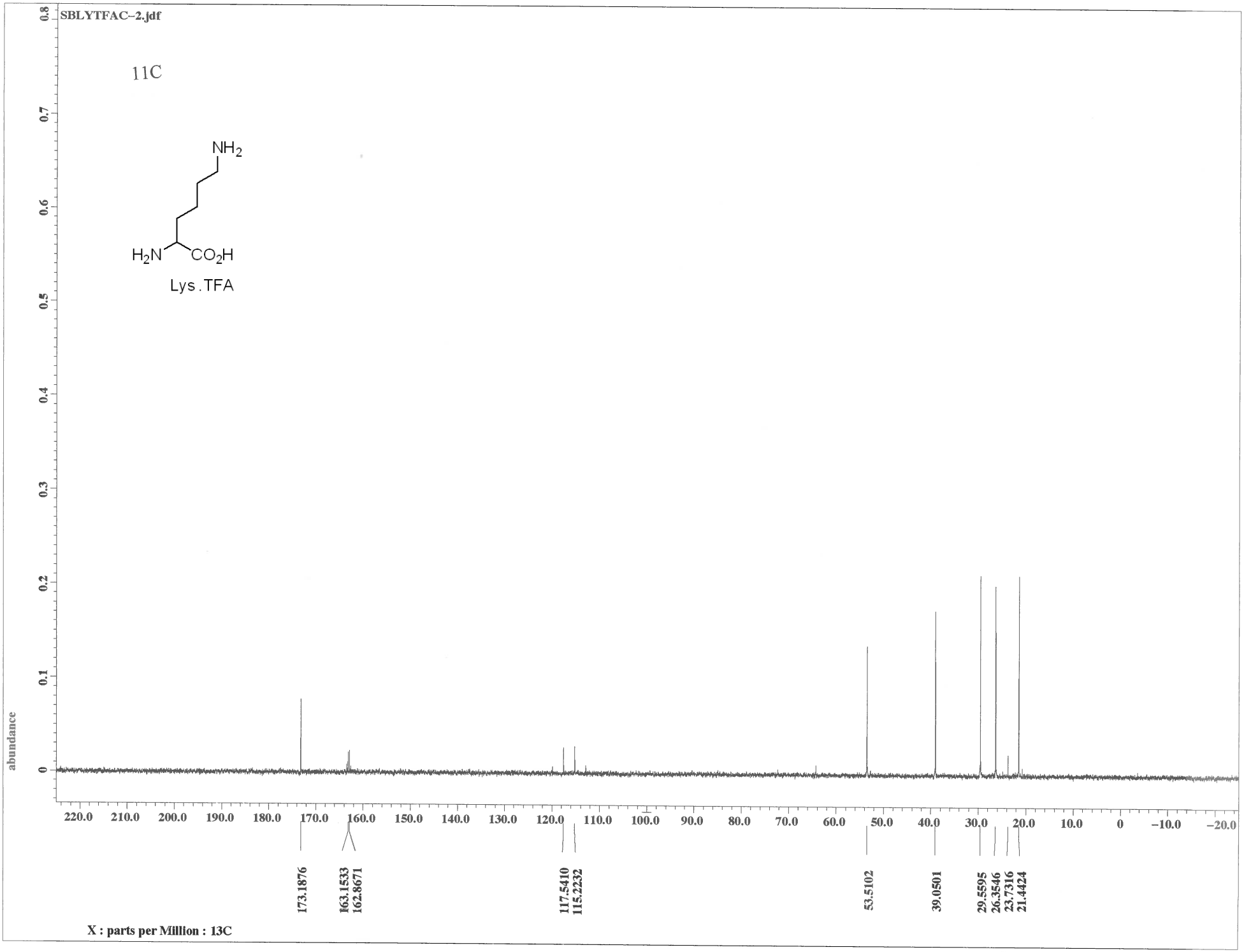


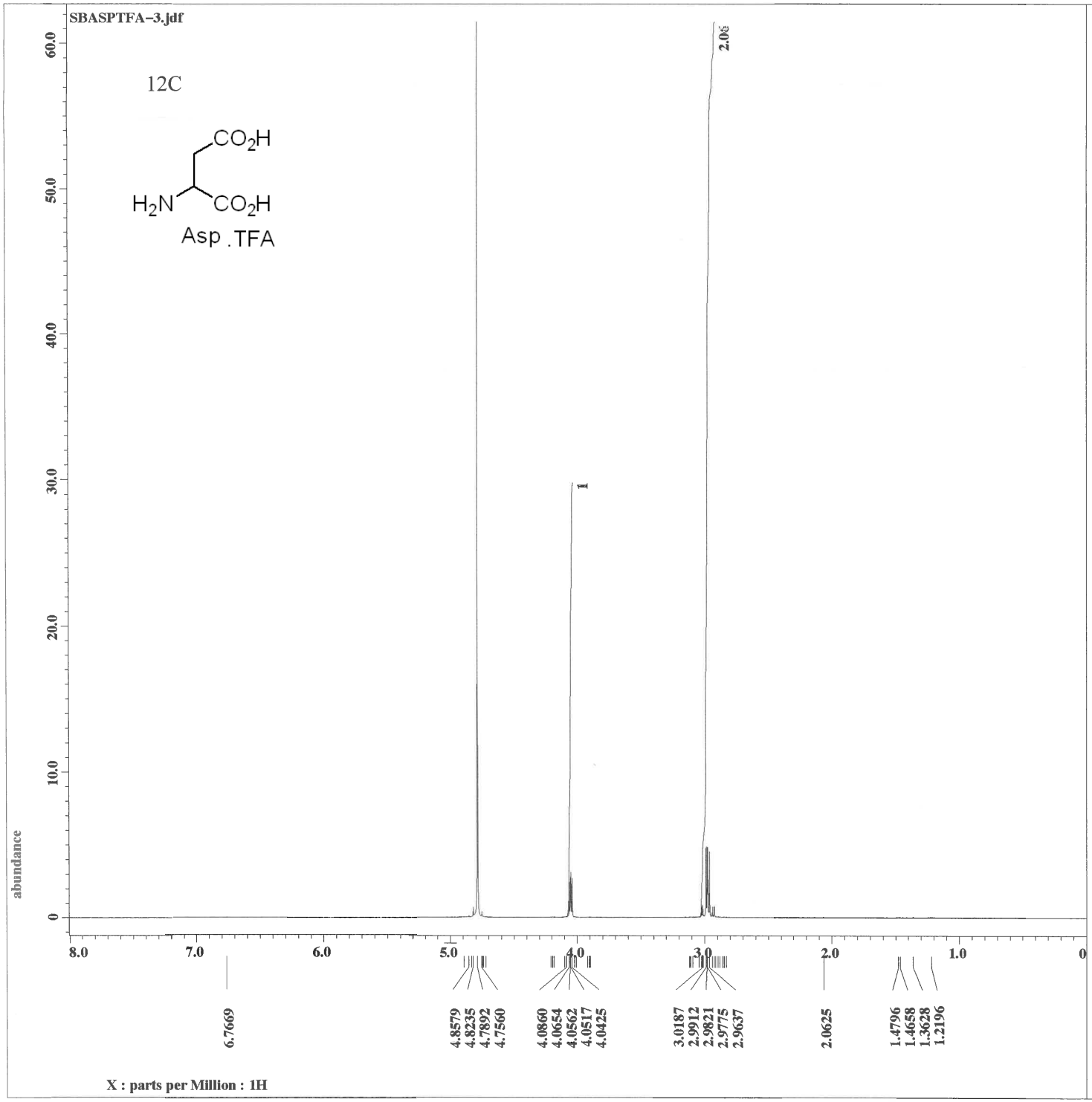
Filename	= SBLYTFA-3.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= S#499730
Solvent	= CHLOROFORM-D
Creation_time	= 10-SEP-2015 02:40:37
Revision_time	= 9-SEP-2015 13:59:25
Current_time	= 9-SEP-2015 14:00:27
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 1.74587904[s]
X_domain	= 1H
X_freq	= 500.15991521[MHz]
X_offset	= 5.0[ppm]
X_points	= 16384
X_prescans	= 0
X_resolution	= 0.57277737[Hz]
X_sweep	= 9.38438438[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Tri_domain	= 1H
Tri_freq	= 500.15991521[MHz]
Tri_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 11
Total_scans	= 11
X_90_width	= 12.54[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 4[dB]
X_pulse	= 6.27[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 34
Relaxation_delay	= 10[s]
Repetition_time	= 11.74587904[s]
Temp_get	= 21.6[dC]

SBLYTFAC–2.jdf

11C

Lys . TFA



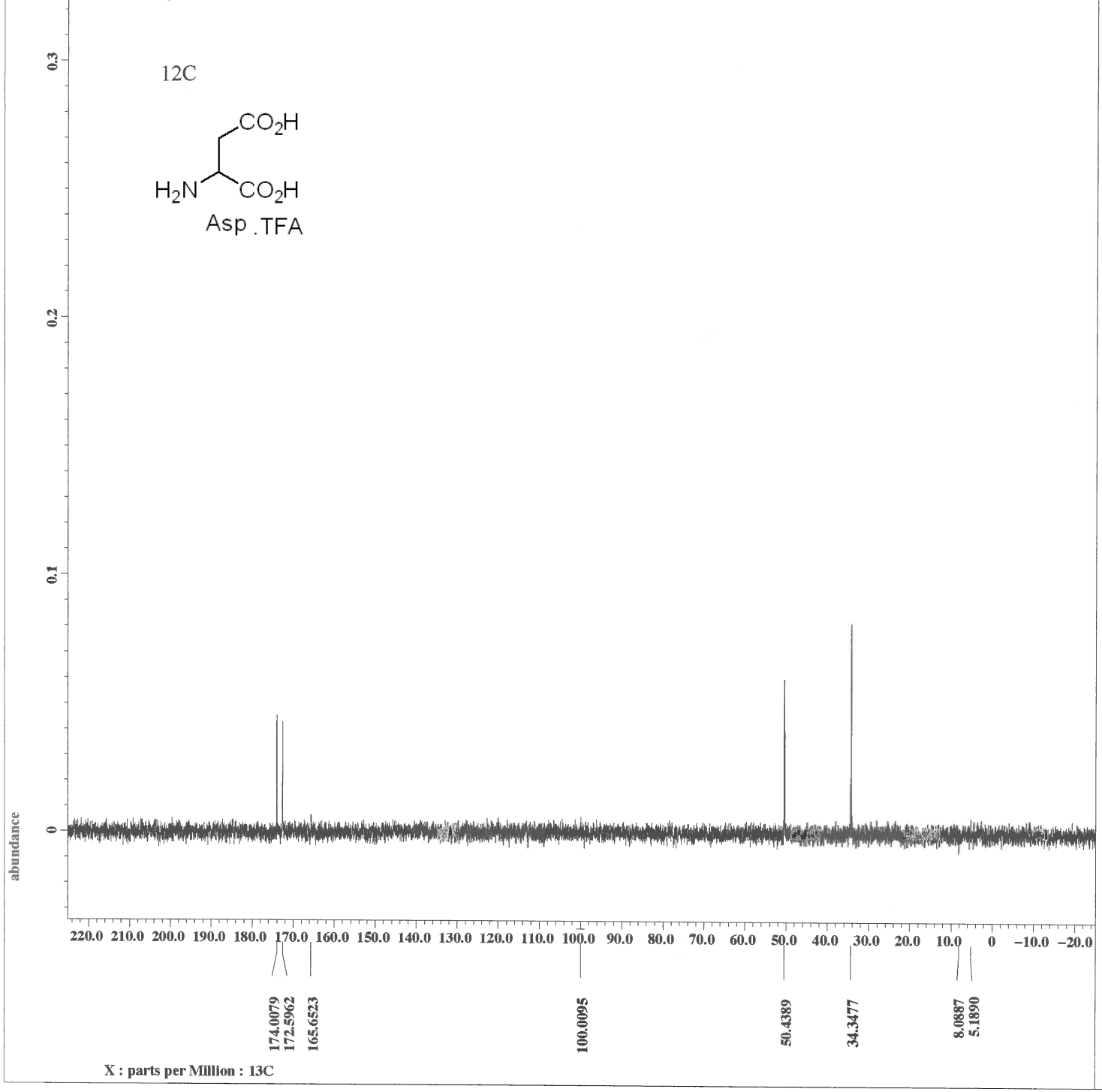



```
Filename          = SBASPTFA-3.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#381529
Solvent           = D2O
Creation_time     = 12-SEP-2015 23:22:32
Revision_time     = 12-SEP-2015 10:41:13
Current_time      = 12-SEP-2015 10:41:33

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = JNM-ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.74587904[s]
X_domain          = 1H
X_freq            = 500.15991521[MHz]
X_offset          = 5.0[ppm]
X_points          = 16384
X_prescans        = 0
X_resolution      = 0.57277737[Hz]
X_sweep           = 9.38438438[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Tri_domain        = 1H
Tri_freq          = 500.15991521[MHz]
Tri_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 9
Total_scans       = 9

X_90_width        = 12.54[us]
X_acq_time        = 1.74587904[s]
X_angle           = 45[deg]
X_atn             = 4[dB]
X_pulse           = 6.27[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 44
Relaxation_delay  = 10[s]
Repetition_time   = 11.74587904[s]
Temp_get          = 21.3[dC]
```

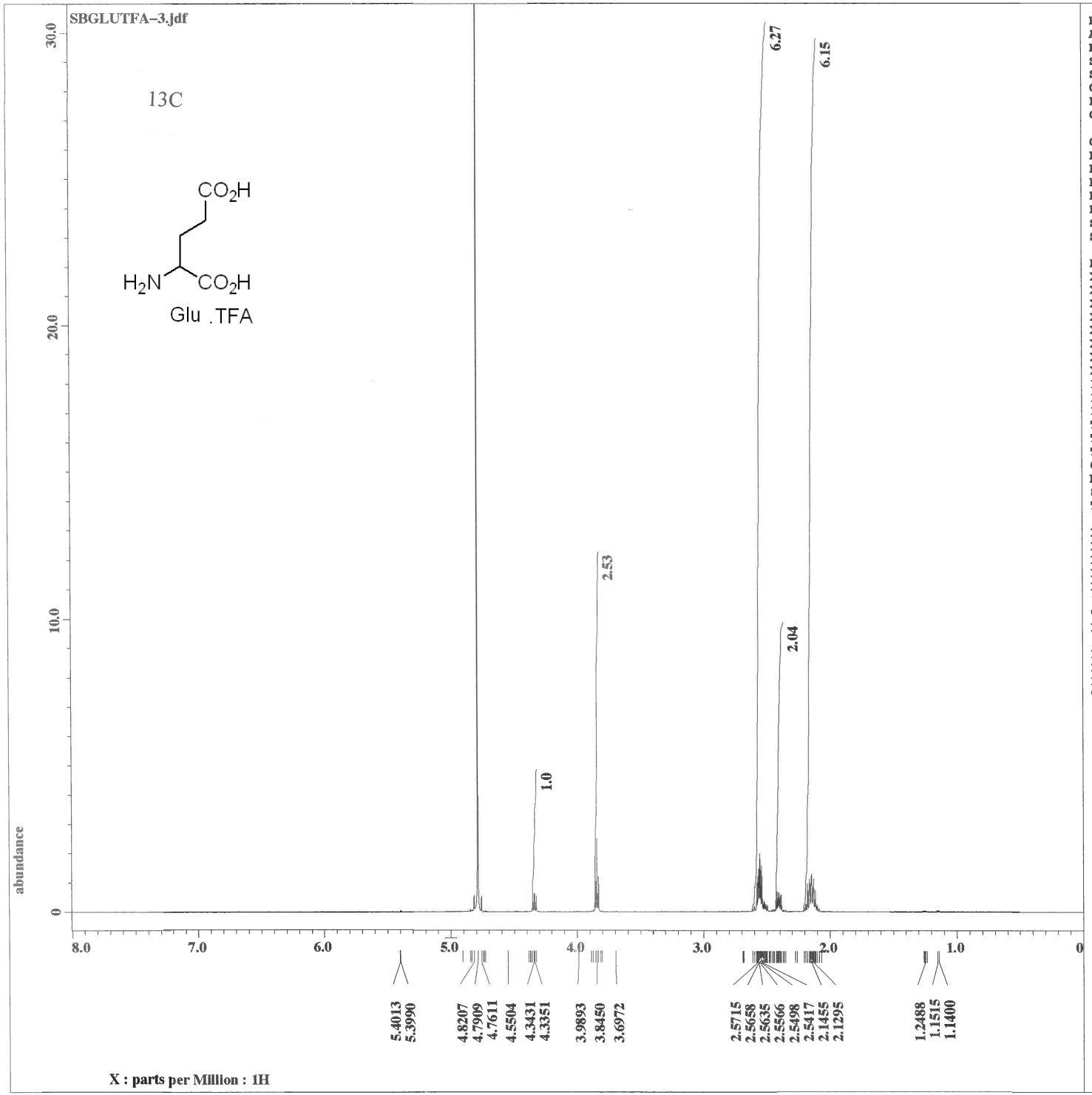
SBASPTFA-2.jdf

12C

Asp .TFA

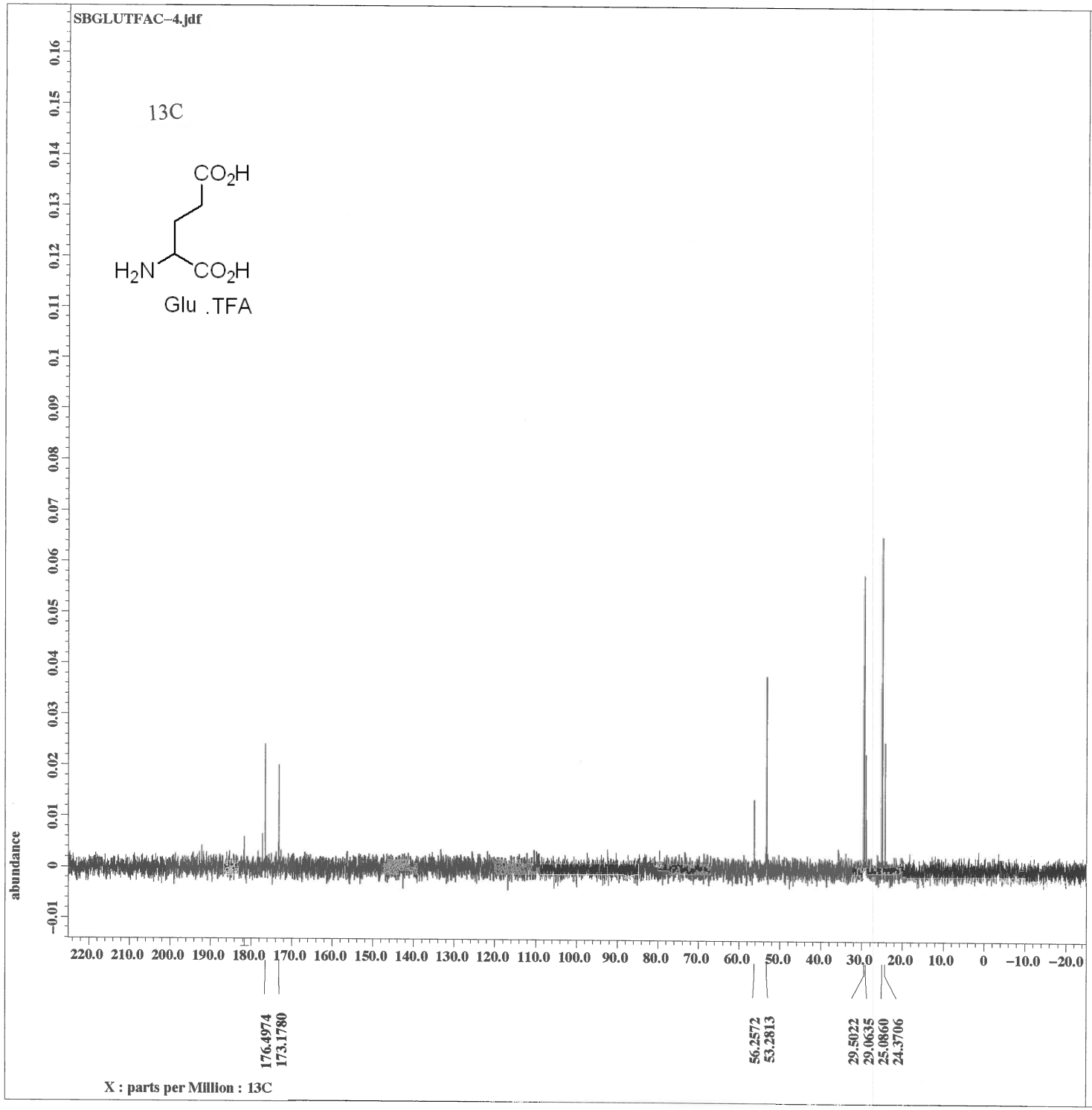


Filename	= SBASPTFA-2.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= S#383772
Solvent	= D2O
Creation_time	= 12-SEP-2015 23:35:29
Revision_time	= 12-SEP-2015 10:51:56
Current_time	= 12-SEP-2015 10:52:27
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 0.83361792[s]
X_domain	= 13C
X_freq	= 125.76529768[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.19959034[Hz]
X_sweep	= 39.3081761[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 10
Scans	= 690
Total_scans	= 690
X_90_width	= 10.73[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 9[dB]
X_pulse	= 3.57666667[us]
Irr_atn_dec	= 20[dB]
Irr_atn_noe	= 20[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 0.2[s]
Recvr_gain	= 50
Relaxation_delay	= 0.2[s]
Repetition_time	= 1.03361792[s]
Temp_get	= 21.9[dC]

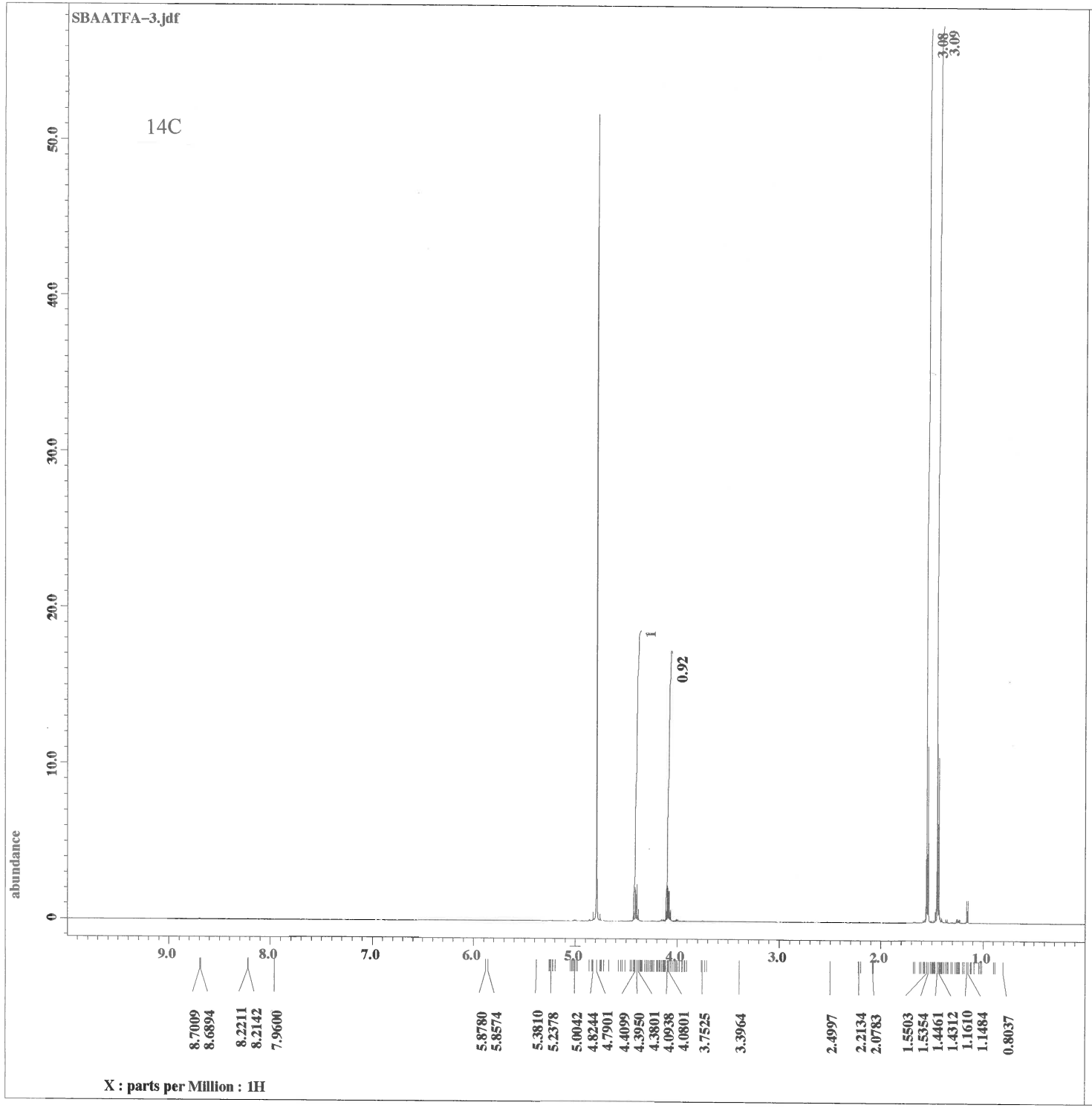



```
Filename          = SBGLUTFA-3.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#317982
Solvent           = D2O
Creation_time     = 20-SEP-2015 21:38:18
Revision_time     = 20-SEP-2015 09:04:47
Current_time      = 20-SEP-2015 09:05:23

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = JNM-ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.74587904[s]
X_domain          = 1H
X_freq            = 500.15991521[MHz]
X_offset          = 5.0[ppm]
X_points          = 16384
X_prescans        = 0
X_resolution      = 0.57277737[Hz]
X_sweep           = 9.38438438[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Tri_domain        = 1H
Tri_freq          = 500.15991521[MHz]
Tri_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 16
Total_scans       = 16

X_90_width        = 12.54[us]
X_acq_time        = 1.74587904[s]
X_angle           = 45[deg]
X_atn             = 4[dB]
X_pulse           = 6.27[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 46
Relaxation_delay  = 10[s]
Repetition_time   = 11.74587904[s]
Temp_get          = 21.2[dC]
```

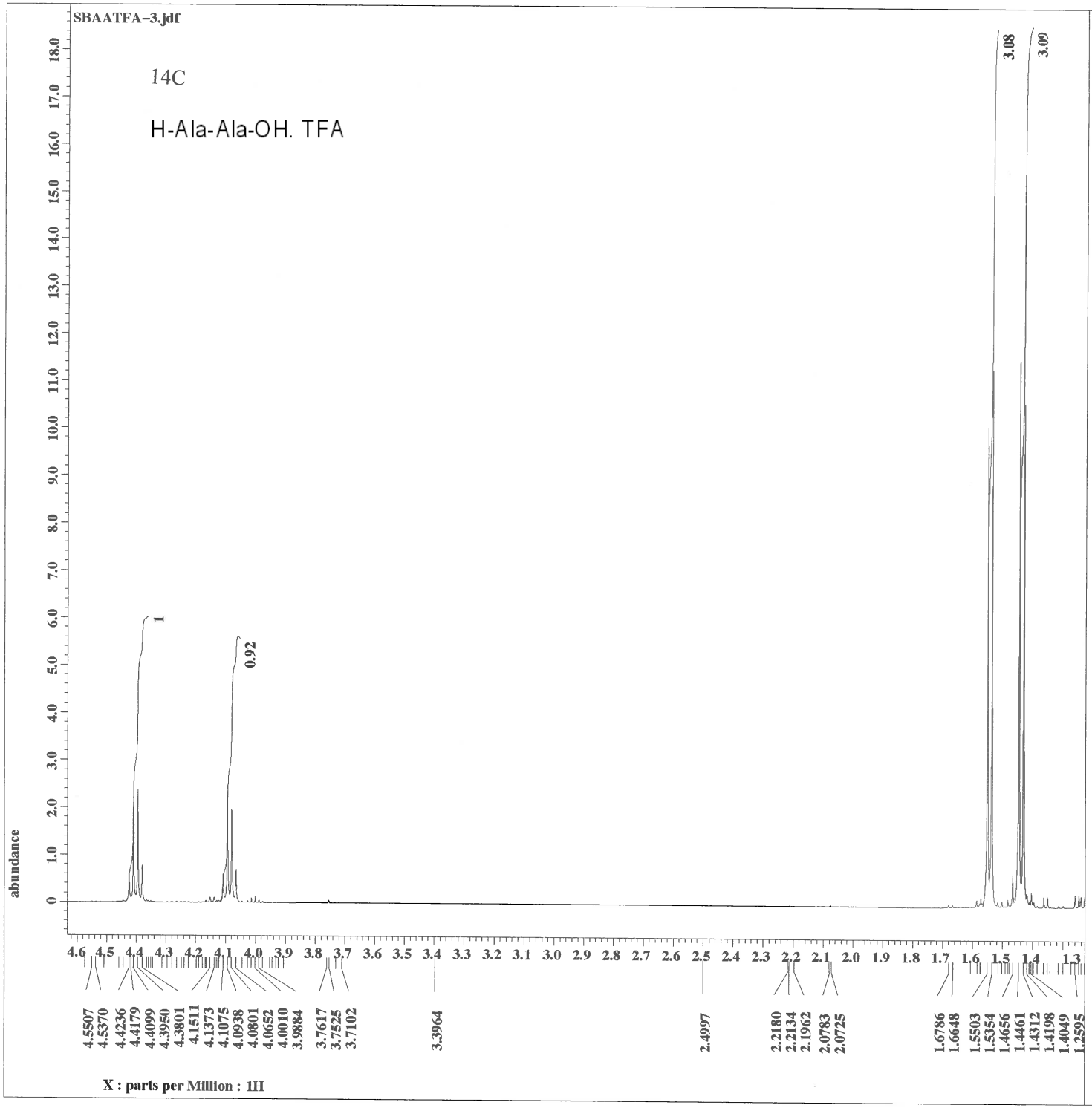
SBGLUTFAC-4.jdf



Filename	= SBGLUTFAC-4.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= S#321121
Solvent	= D2O
Creation_time	= 20-SEP-2015 22:07:54
Revision_time	= 20-SEP-2015 09:26:46
Current_time	= 20-SEP-2015 09:27:30
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 0.83361792[s]
X_domain	= 13C
X_freq	= 125.76529768[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.19959034[Hz]
X_sweep	= 39.3081761[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 10
Scans	= 1650
Total_scans	= 1650
X_90_width	= 10.73[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 9[dB]
X_pulse	= 3.57666667[us]
Irr_atn_dec	= 20[dB]
Irr_atn_noe	= 20[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 0.2[s]
Recvr_gain	= 50
Relaxation_delay	= 0.2[s]
Repetition_time	= 1.03361792[s]
Temp_get	= 21.7[dC]




```
Filename          = SBAATFA-3.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#373771
Solvent           = D2O
Creation_time     = 21-SEP-2015 23:10:09
Revision_time     = 21-SEP-2015 10:28:55
Current_time      = 21-SEP-2015 10:29:18

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = JNM-ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.74587904[s]
X_domain          = 1H
X_freq            = 500.15991521[MHz]
X_offset          = 5.0[ppm]
X_points          = 16384
X_prescans        = 0
X_resolution      = 0.57277737[Hz]
X_sweep           = 9.38438438[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Tri_domain        = 1H
Tri_freq          = 500.15991521[MHz]
Tri_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 10
Total_scans       = 10

X_90_width        = 12.54[us]
X_acq_time        = 1.74587904[s]
X_angle           = 45[deg]
X_atn             = 4[dB]
X_pulse           = 6.27[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 36
Relaxation_delay  = 10[s]
Repetition_time   = 11.74587904[s]
Temp_get          = 23.3[dC]
```

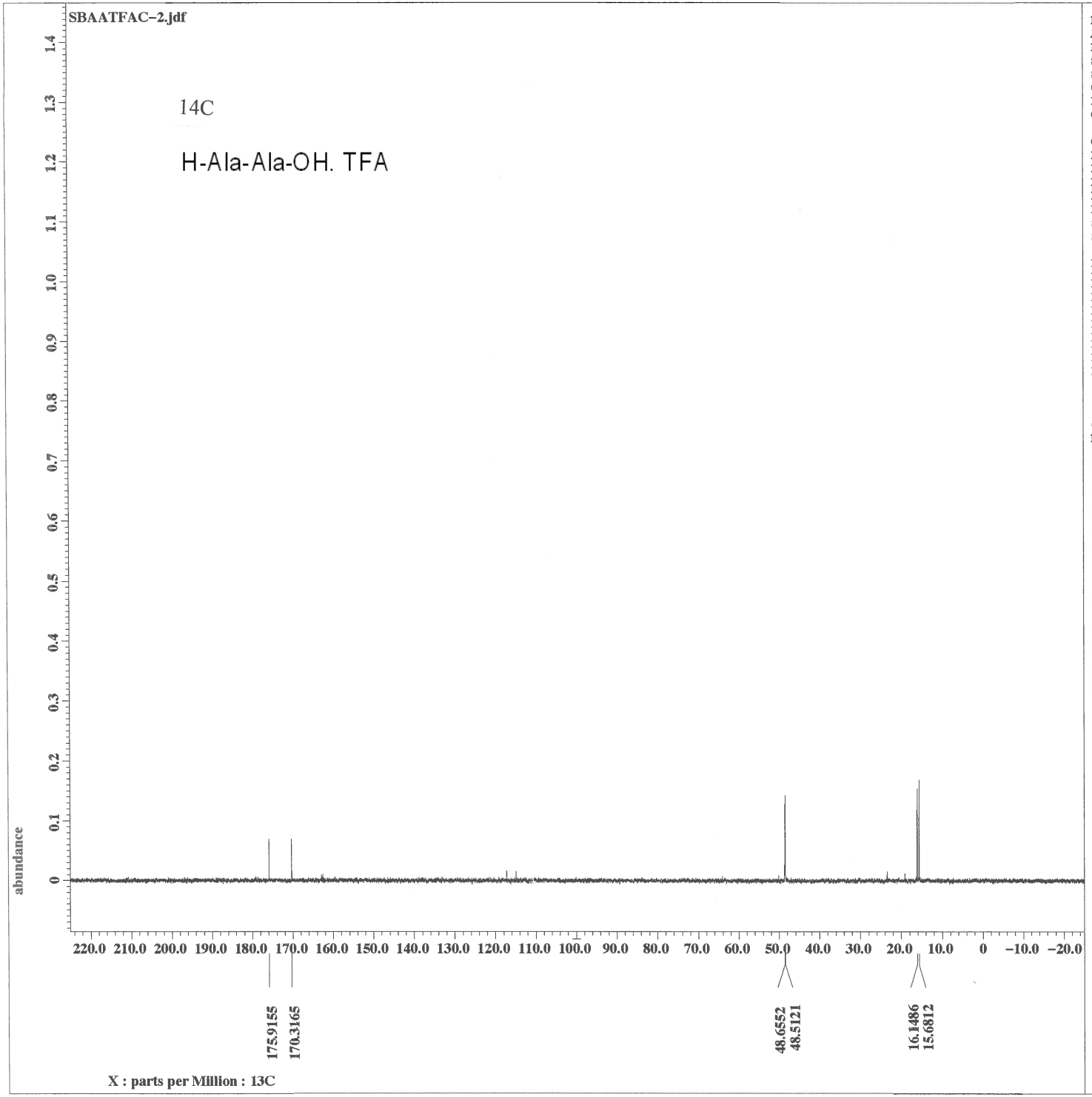



```
Filename          = SBAATFA-3.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#373771
Solvent           = D2O
Creation_time     = 21-SEP-2015 23:10:09
Revision_time     = 21-SEP-2015 10:28:55
Current_time      = 21-SEP-2015 10:29:50

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = JNM-ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 1.74587904[s]
X_domain          = 1H
X_freq            = 500.15991521[MHz]
X_offset          = 5.0[ppm]
X_points          = 16384
X_prescans        = 0
X_resolution      = 0.57277737[Hz]
X_sweep           = 9.38438438[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Tri_domain        = 1H
Tri_freq          = 500.15991521[MHz]
Tri_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 10
Total_scans       = 10

X_90_width        = 12.54[us]
X_acq_time        = 1.74587904[s]
X_angle           = 45[deg]
X_atn             = 4[dB]
X_pulse           = 6.27[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 36
Relaxation_delay  = 10[s]
Repetition_time   = 11.74587904[s]
Temp_get          = 23.3[dC]
```

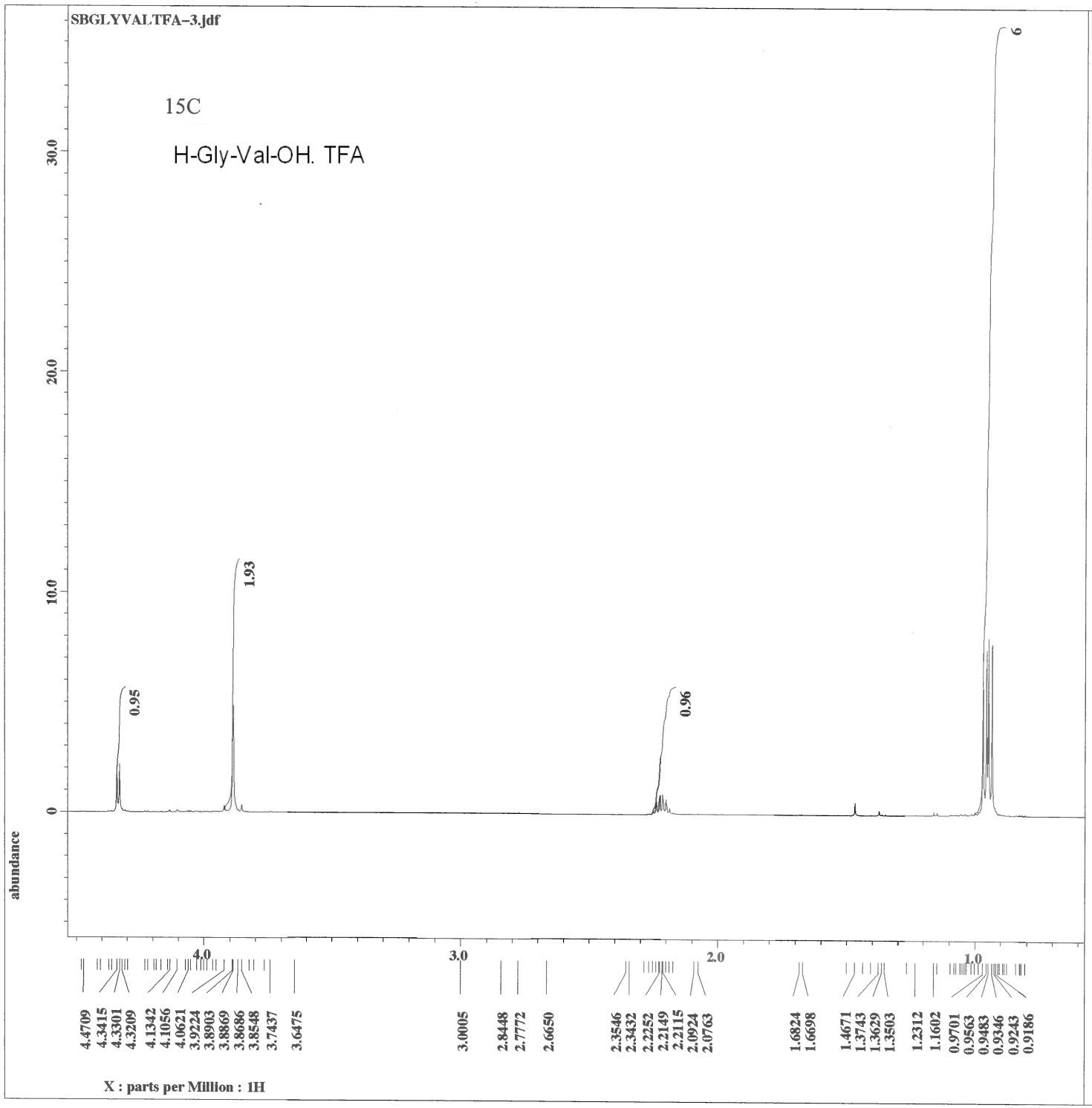
SBAATFAC-2.jdf

14C

H-Ala-Ala-OH. TFA



Filename	= SBAATFAC-2.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= S#376071
Solvent	= D2O
Creation_time	= 21-SEP-2015 23:20:23
Revision_time	= 21-SEP-2015 10:36:39
Current_time	= 21-SEP-2015 10:37:01
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 0.83361792[s]
X_domain	= 13C
X_freq	= 125.76529768[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.19959034[Hz]
X_sweep	= 39.3081761[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 10
Scans	= 540
Total_scans	= 540
X_90_width	= 10.73[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 9[dB]
X_pulse	= 3.57666667[us]
Irr_atn_dec	= 20[dB]
Irr_atn_noe	= 20[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 0.2[s]
Recvr_gain	= 50
Relaxation_delay	= 0.2[s]
Repetition_time	= 1.03361792[s]
Temp_get	= 23.7[dC]

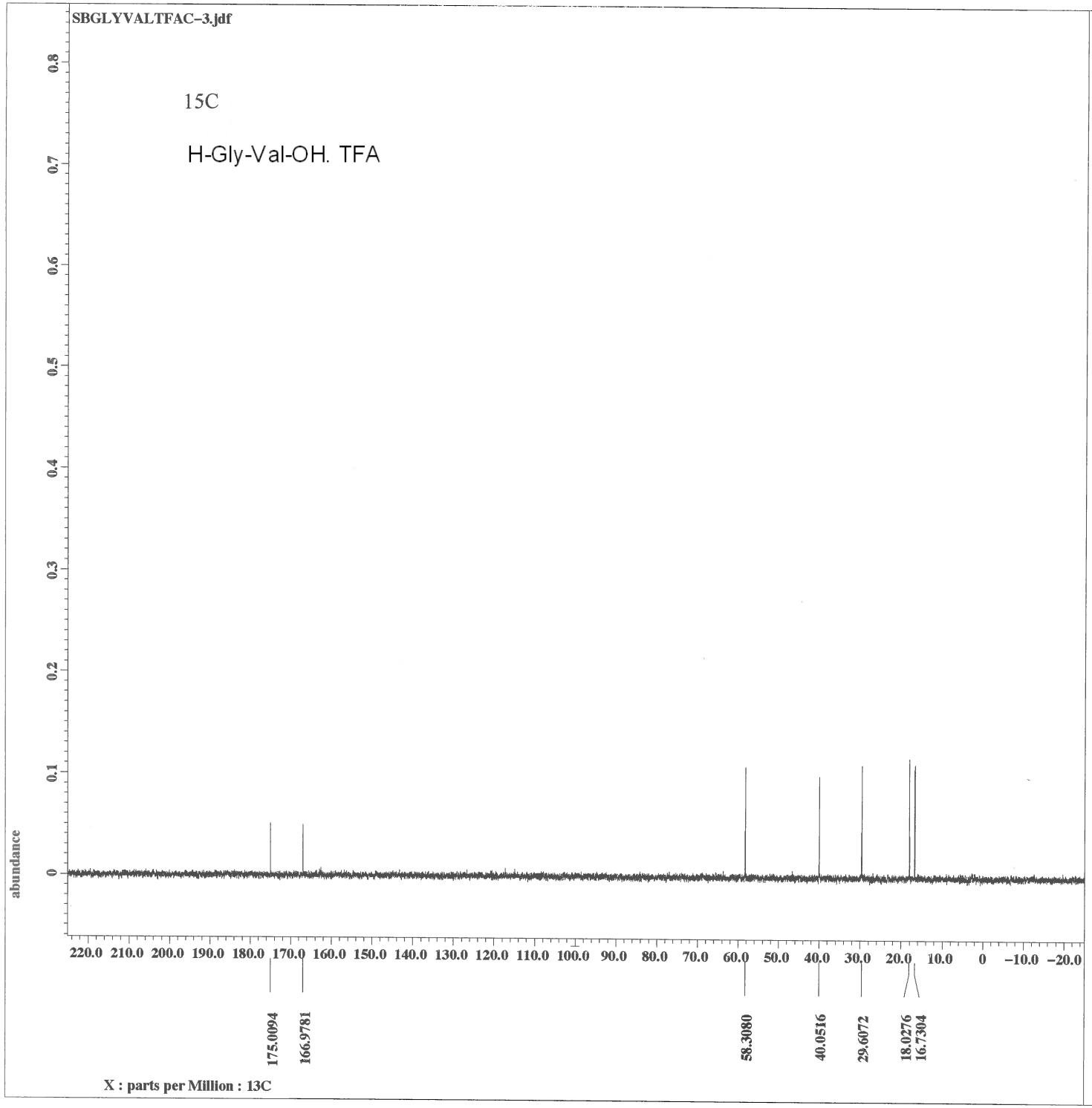


Filename	= SBGLYVALTFA-3.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= S#701195
Solvent	= D2O
Creation_time	= 22-SEP-2015 08:16:04
Revision_time	= 21-SEP-2015 19:35:40
Current_time	= 21-SEP-2015 19:37:13
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 1.74587904[s]
X_domain	= 1H
X_freq	= 500.15991521[MHz]
X_offset	= 5.0[ppm]
X_points	= 16384
X_prescans	= 0
X_resolution	= 0.57277737[Hz]
X_sweep	= 9.38438438[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Tri_domain	= 1H
Tri_freq	= 500.15991521[MHz]
Tri_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 11
Total_scans	= 11
X_90_width	= 12.54[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 4[dB]
X_pulse	= 6.27[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 38
Relaxation_delay	= 10[s]
Repetition_time	= 11.74587904[s]
Temp_get	= 22.6[dC]

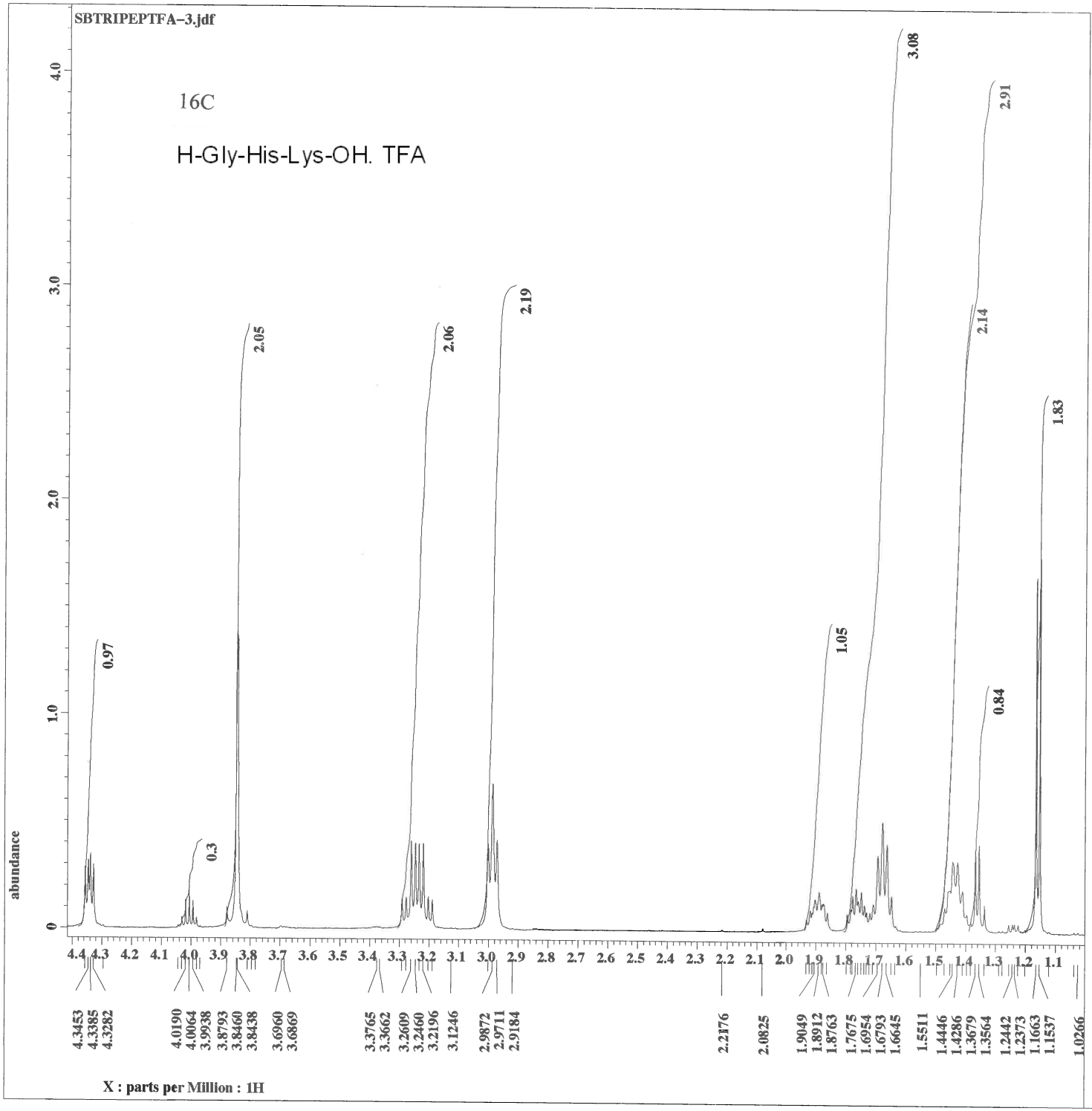
SBGLYVALTFAC-3.jdf

15C

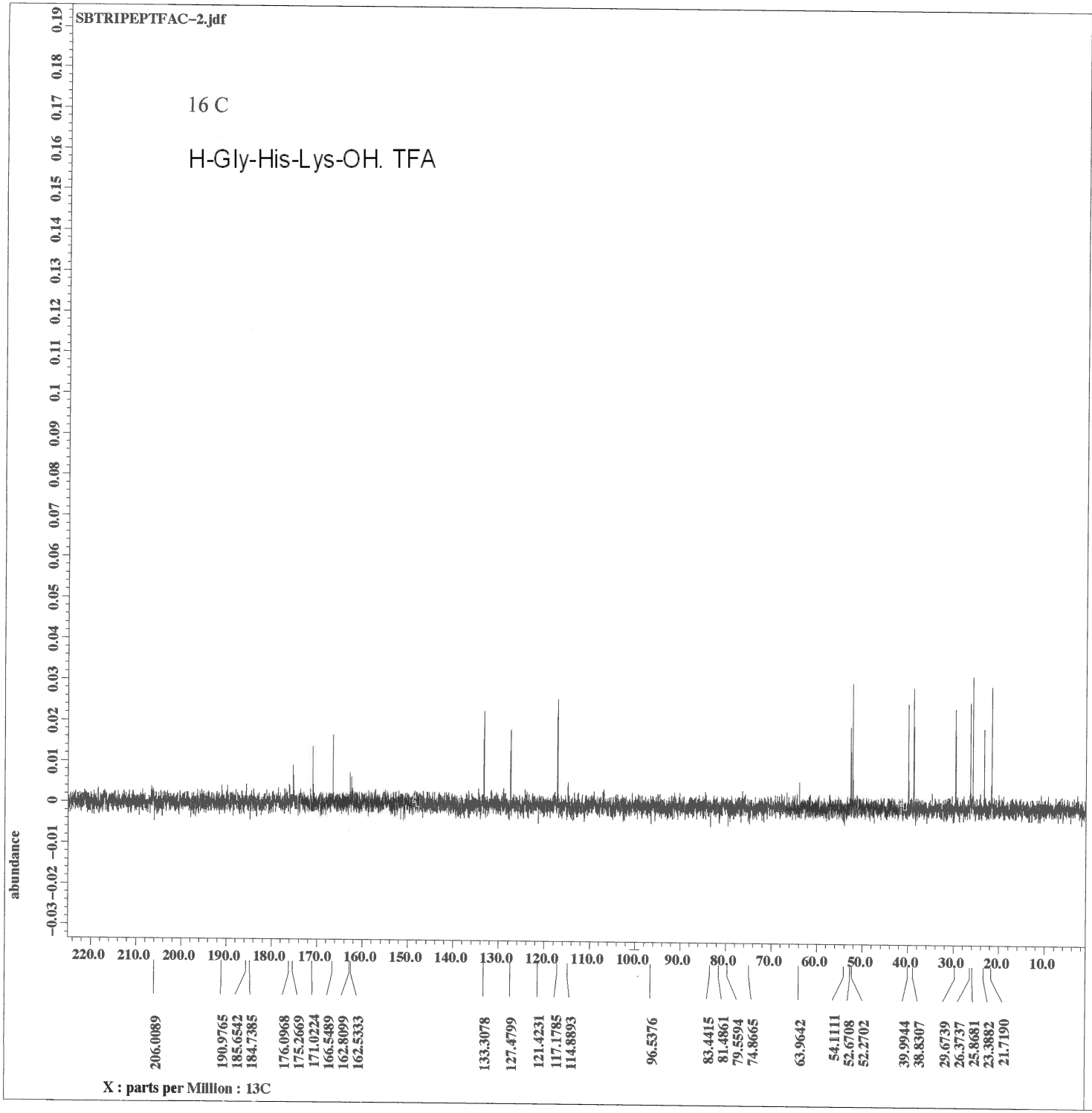
H-Gly-Val-OH. TFA



Filename	= SBGLYVALTFAC-3.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= S#703778
Solvent	= D2O
Creation_time	= 22-SEP-2015 08:27:39
Revision_time	= 21-SEP-2015 19:43:48
Current_time	= 21-SEP-2015 19:44:09
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 0.83361792[s]
X_domain	= 13C
X_freq	= 125.76529768[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.19959034[Hz]
X_sweep	= 39.3081761[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 10
Scans	= 580
Total_scans	= 580
X_90_width	= 10.73[us]
X_acq_time	= 0.83361792[s]
X_angle	= 30[deg]
X_atn	= 9[dB]
X_pulse	= 3.57666667[us]
Irr_atn_dec	= 20[dB]
Irr_atn_noe	= 20[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 0.2[s]
Recvr_gain	= 50
Relaxation_delay	= 0.2[s]
Repetition_time	= 1.03361792[s]
Temp_get	= 23[dC]



Filename	= SBTRIPEPTFA-3.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= S#522951
Solvent	= D2O
Creation_time	= 23-SEP-2015 03:20:00
Revision_time	= 22-SEP-2015 14:42:01
Current_time	= 22-SEP-2015 14:43:02
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 500
Spectrometer	= JNM-ECA500
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 1.74587904[s]
X_domain	= 1H
X_freq	= 500.15991521[MHz]
X_offset	= 5.0[ppm]
X_points	= 16384
X_prescans	= 0
X_resolution	= 0.57277737[Hz]
X_sweep	= 9.38438438[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Tri_domain	= 1H
Tri_freq	= 500.15991521[MHz]
Tri_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 16
Total_scans	= 16
X_90_width	= 12.54[us]
X_acq_time	= 1.74587904[s]
X_angle	= 45[deg]
X_atn	= 4[dB]
X_pulse	= 6.27[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 40
Relaxation_delay	= 10[s]
Repetition_time	= 11.74587904[s]
Temp_get	= 22.5[dC]




```
Filename          = SBTRIPEPTFAC-2.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#526053
Solvent           = D2O
Creation_time     = 23-SEP-2015 03:39:32
Revision_time     = 22-SEP-2015 14:55:42
Current_time      = 22-SEP-2015 14:56:50

Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = JNM-ECA500

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 0.83361792[s]
X_domain          = 13C
X_freq            = 125.76529768[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 1.19959034[Hz]
X_sweep           = 39.3081761[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 10
Scans             = 1070
Total_scans       = 1070

X_90_width        = 10.73[us]
X_acq_time        = 0.83361792[s]
X_angle           = 30[deg]
X_atn             = 9[dB]
X_pulse           = 3.57666667[us]
Irr_atn_dec       = 20[dB]
Irr_atn_noe       = 20[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 0.2[s]
Recvr_gain        = 50
Relaxation_delay  = 0.2[s]
Repetition_time   = 1.03361792[s]
Temp_get          = 22.9[dC]
```