

SUPPLEMENTARY INFORMATION Part 2

Synthesis of models of the BC ring systems of MPC1001 and MPC1001F†

Shuai Dong,^{a,b} Kiran Indukuri,^b Derrick L. J. Clive^{b*} and Jin-Ming Gao^{a*}

*^aShaanxi Key Laboratory of Natural Products & Chemical Biology, College of Science,
Northwest A&F University, Yangling 712100, Shaanxi, P. R. China*

^bChemistry Department, University of Alberta, Edmonton, Alberta T6G 2G2, Canada

E-mail address: derrick.clive@ualberta.ca

E-mail address: jinminggao@nwsuaf.edu.cn

(2 <i>S</i>)-2-{[(Benzyloxy)carbonyl]amino}butanedioic acid	S3
1,4-Di- <i>tert</i> -Butyl (2 <i>S</i>)-2-{[(Benzyloxy)carbonyl]amino}butanedioate	S4
NMR spectra of 13	S6
NMR spectra of 14	S8
NMR spectra of 19	S10
NMR spectra of 20	S12
NMR spectra of 21	S14
NMR spectra of 22 (less polar isomer)	S16
NMR spectra of 22 (more polar isomer)	S18
NMR spectra of 23	S20
NMR spectra of 24	S22
NMR spectra of 24 (ROESY	S24
NMR spectra of 24 (ROESY expansion)	S25
NMR spectra of 25	S26
NMR spectra of 27	S28

NMR spectra of 28	S30
NMR spectra of 29	S32
NMR spectra of 31	S34
NMR spectra of 32	S36
NMR spectra of 32a	S38
NMR spectra of 33	S40
NMR spectra of 33 (ROESY)	S42
NMR spectra of 33a	S43
NMR spectra of 33a (ROESY)	S45
NMR spectra of 34	S46
NMR spectra of 34a	S48
NMR spectra of 35	S50
NMR spectra of 37	S51
NMR spectra of 37a	S53
NMR spectra of 38	S55
NMR spectra of 38a	S57
NMR spectra of 39	S59
NMR spectra of 40	S61



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Recorded on: **mr400, Apr 21 2016**
Pulse Sequence: **s2pul**

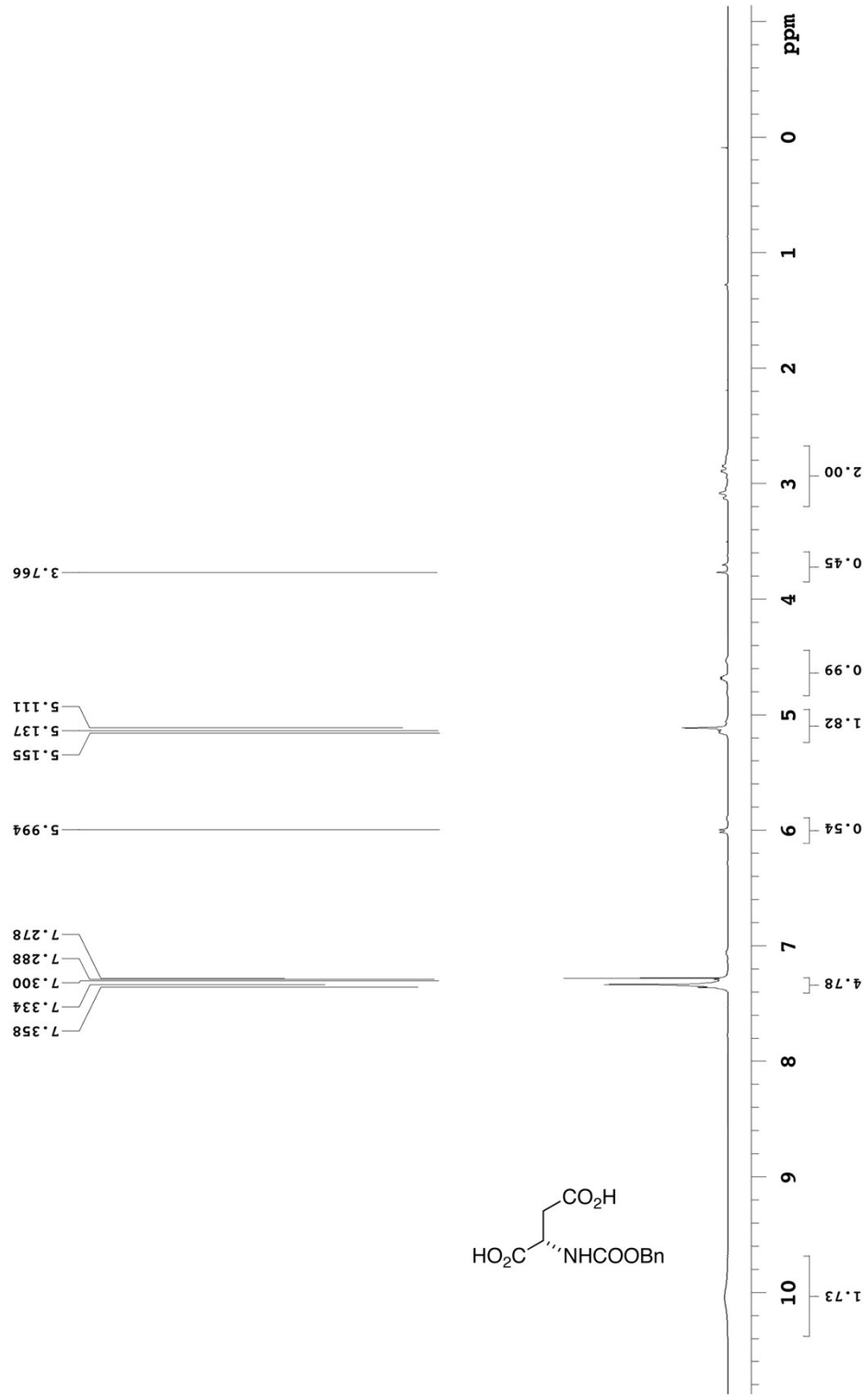
Sweep Width(Hz): **4807.69**
Digital Res (Hz/pt): **0.07**

Acquisition Time(s): **5**
Hz per mm(Hz/mm): **20.03**

Relaxation Delay(s): **0.1**
Completed Scans **16**

ADS-3

399.978 MHz H1 1D in cdcl3 (ref. to CDC13 @ 7.26 ppm), temp 25.9 C -> actual temp = 27.0 C, onenmr probe



File: /mnt/d600/home14/civenmr/nmrdata/dongshuai/2016.04/ADS-3



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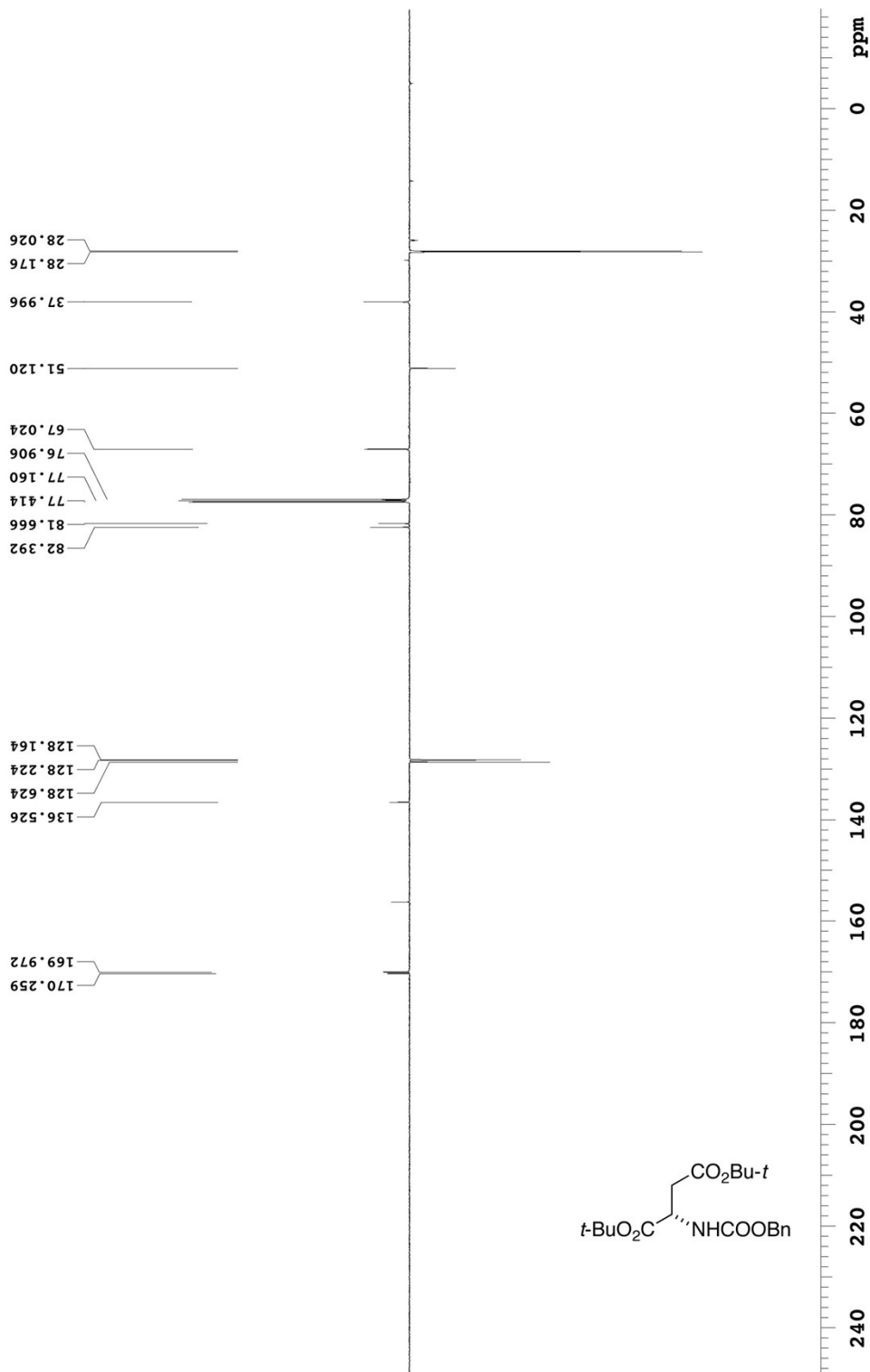
Recorded on: u500, Apr 14 2015
Pulse Sequence: APT_ad

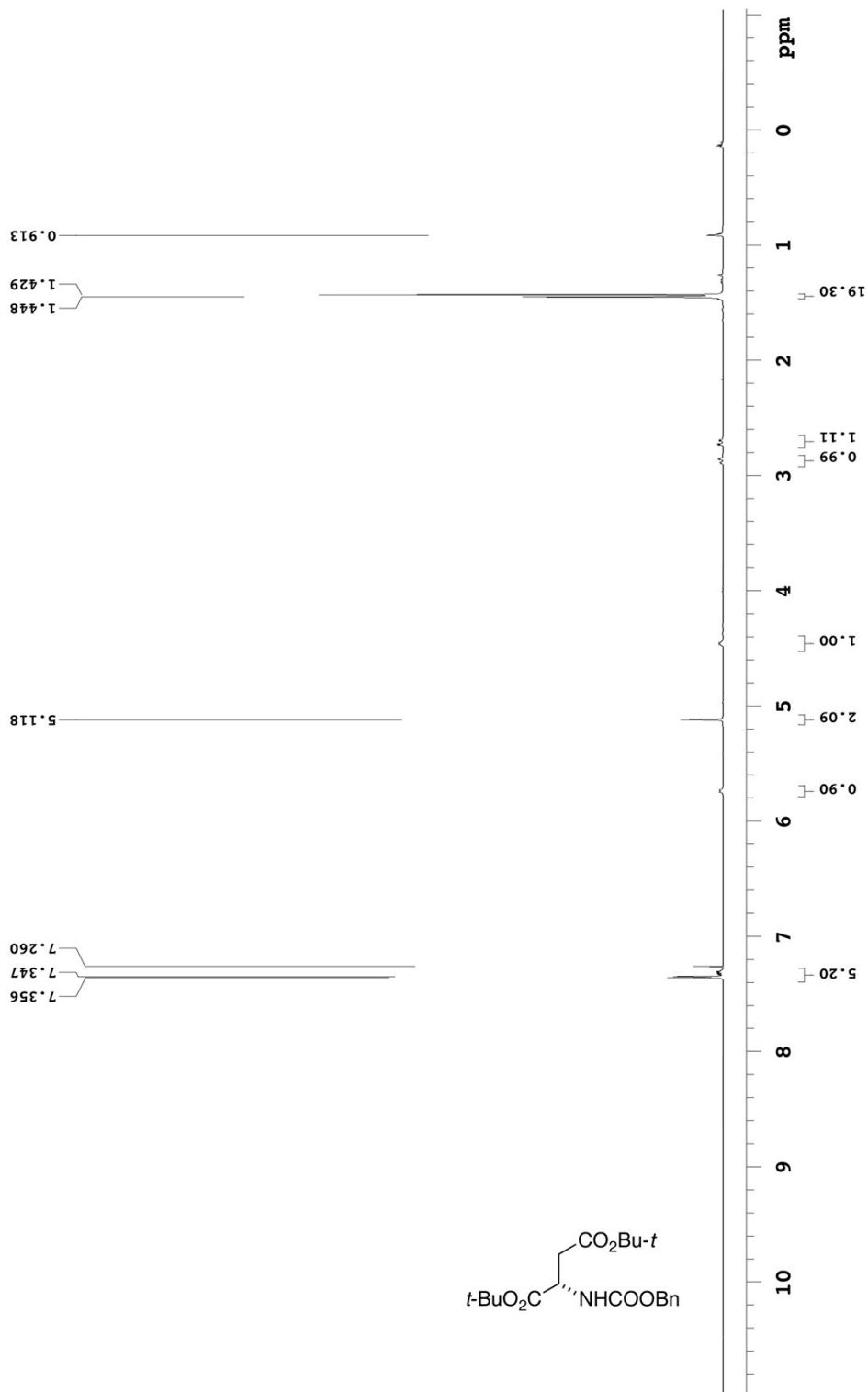
Sweep Width(Hz): 33783.8
Digital Res (Hz/pt): 0.26

Acquisition Time(s): 2
Hz per mm(Hz/mm): 140.76

Relaxation Delay(s): 0.5
Completed Scans: 512

shuai, ADS-101_BK2_PAGE85
125.690 MHz C13[H1] APT_ad in cdcl3 (ref. to CDCl3 @ 77.06 ppm), temp 27.7 C -> actual temp = 27.0 C, coldldual probe
C & CH2 same, CH & CH3 opposite side of solvent signal



CC(C)(C)OC(=O)C[C@H](CNC(=O)OCC1=CC=CC=C1)C(=O)OCC2=CC=CC=C2

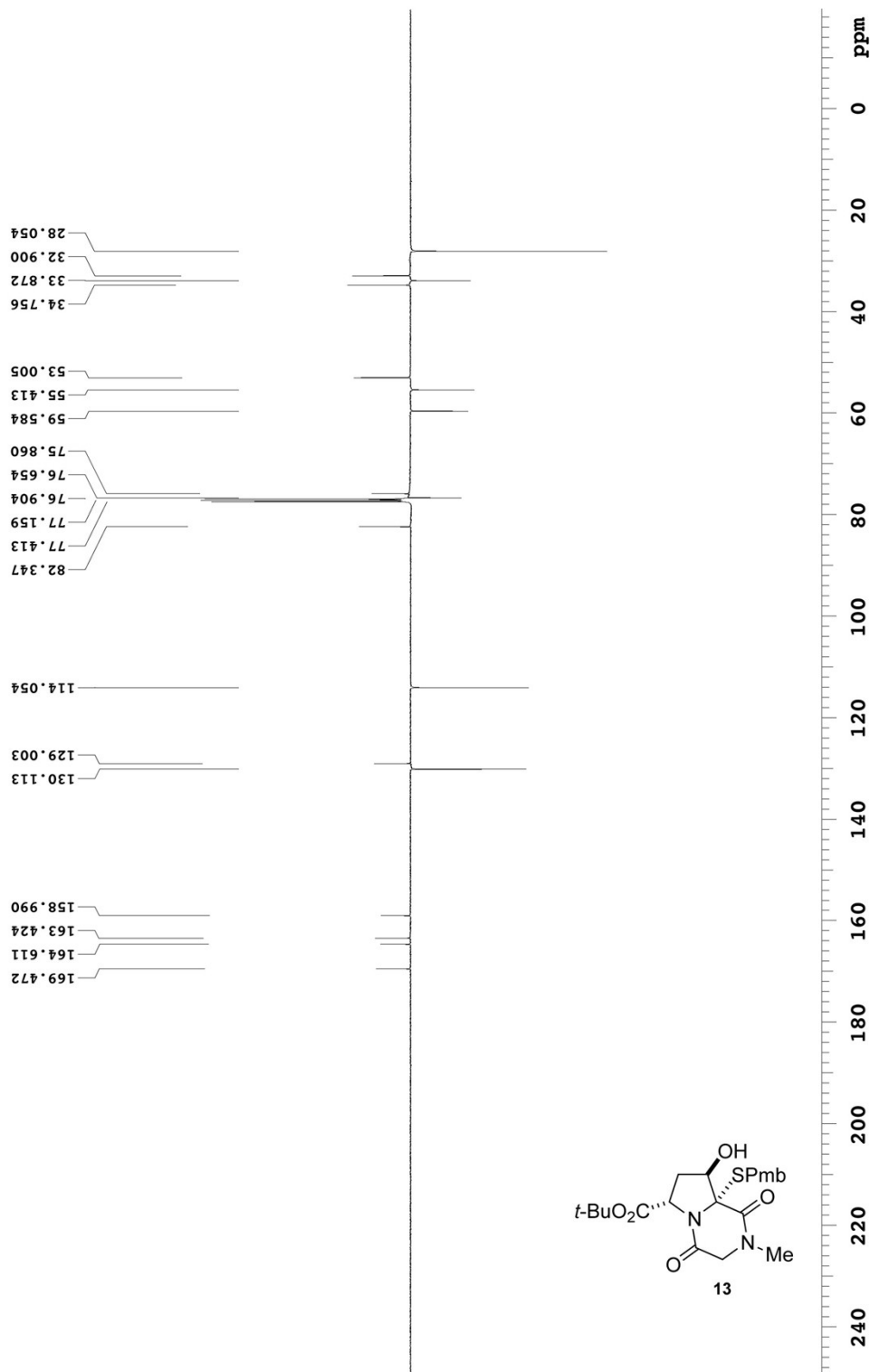


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Recorded on: **u500, Mar 18 2015** Sweep Width(Hz): **33783.8** Acquisition Time(s): **2** Relaxation Delay(s): **0.5**
Pulse Sequence: **APT_ad** Digital Res. (Hz/pt): **0.26** Hz per mm(Hz/mm): **140.76** Completed Scans: **512**

shuai, ADS-83_BK2_PAGE9
125.690 MHz C13[H1] APT_ad in cdcl3 (ref. to CDCl3 @ 77.06 ppm), temp 27.7 C -> actual temp = 27.0 C, coldlual probe
C & CH2 same, CH & CH3 opposite side of solvent signal



Recorded on: **ibd5, Mar 18 2015**
Pulse Sequence: **s2pul**

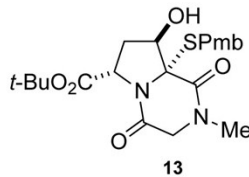
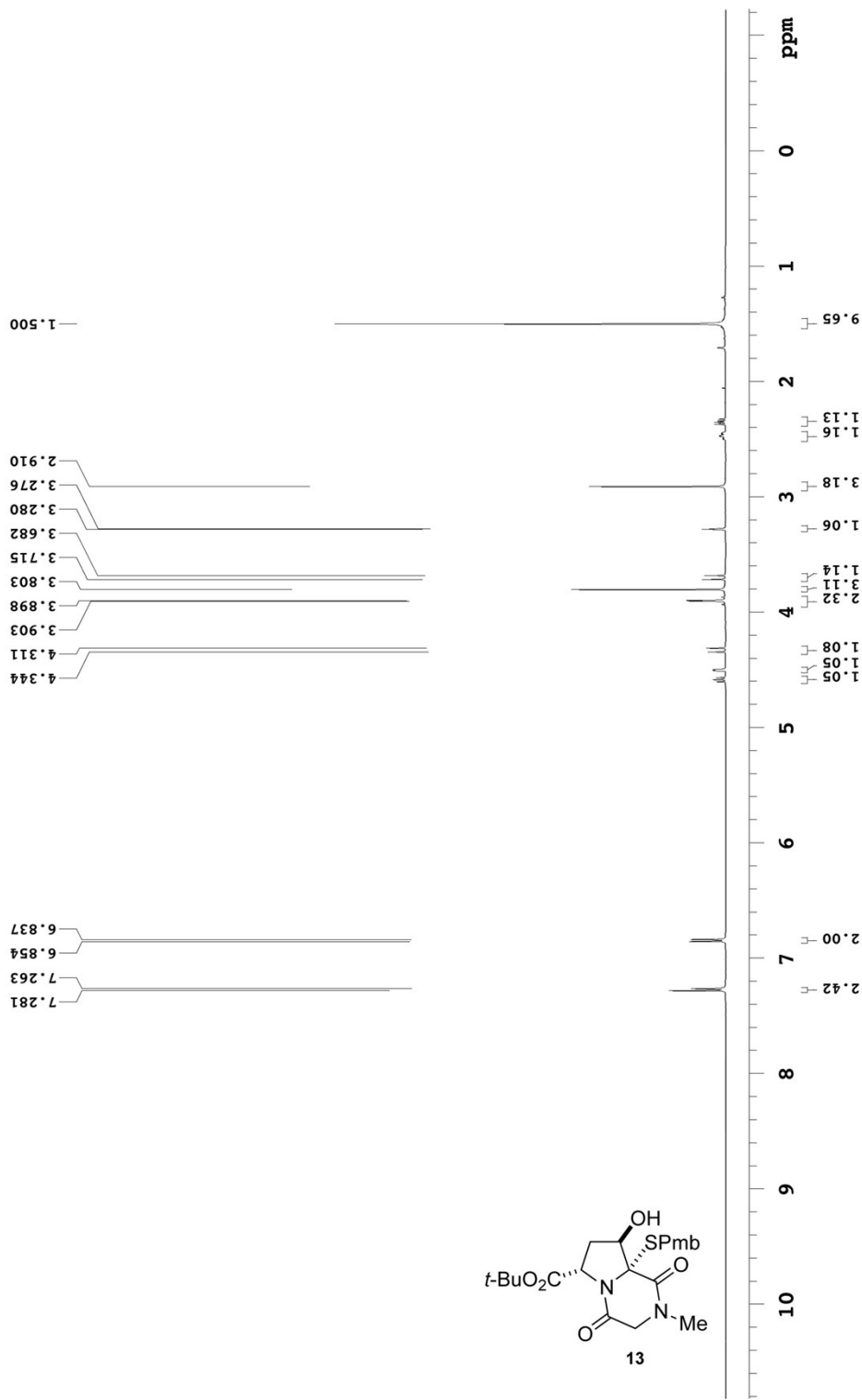
Sweep Width(Hz): **6000.6**
Digital Res.(Hz/pt): **0.09**

Acquisition Time(s): **5**
Hz per mm(Hz/mm): **25**

Relaxation Delay(s): **0.1**
Completed Scans **16**

ADS-83 BK2 PAGE9

498.118 MHz ¹H 1D in cdcl₃ (ref. to CDC13 @ 7.26 ppm), temp 26.4 C -> actual temp = 27.0 C, autoxtdb probe





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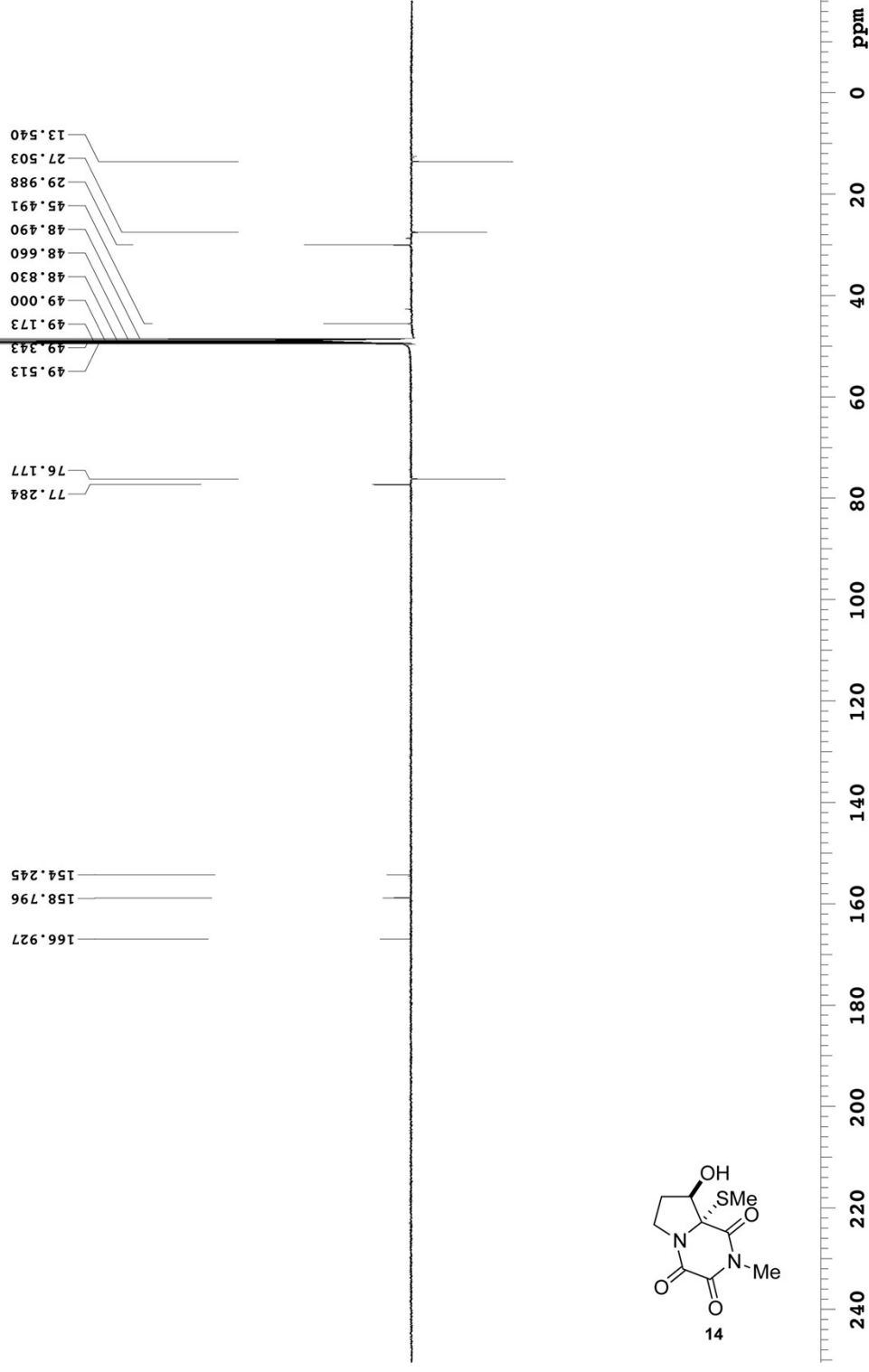
Recorded on: u500, Mar 31 2016
Pulse Sequence: APT_ad

Sweep Width(Hz): 33783.8
Digital Res (Hz/pt): 0.26

Acquisition Time(s): 2
Relaxation Delay(s): 1
Completed Scans: 2000

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shuai, ADS_BK6_PAGE47
125.691 MHz C13[1H] APT_ad in cd3od (ref. to CD3OD @ 49.0 ppm), temp 27.7 C -> actual temp = 27.0 C, coldludal probe
C & CH2 same, CH & CH3 opposite side of solvent signal





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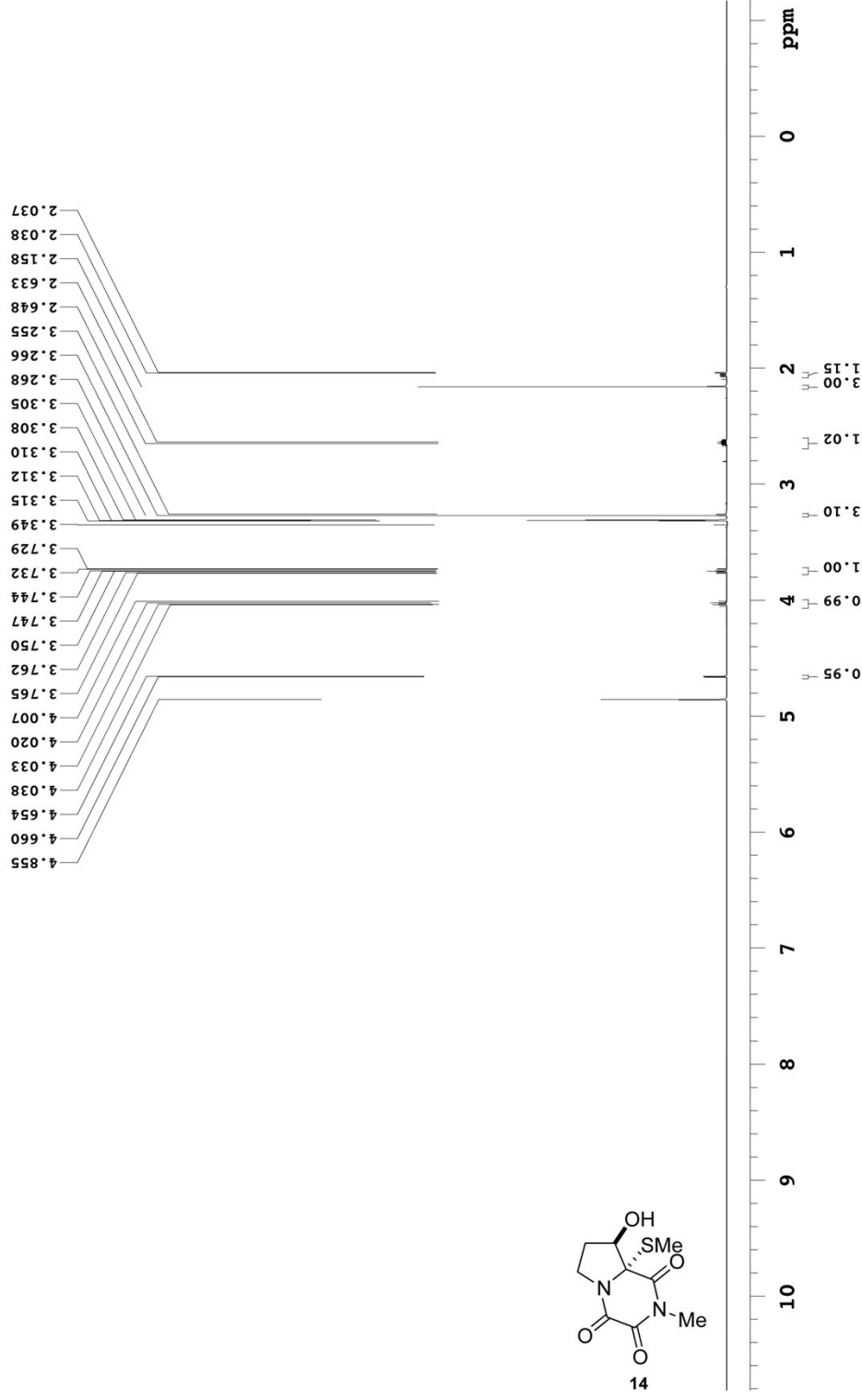
Recorded on: **v700, Mar 30 2016**
Pulse Sequence: **PRESAT**

Sweep Width(Hz): **8389.26**
Digital Res. (Hz/pt): **0.13**

Acquisition Time(s): **3**
Hz per mm(Hz/mm): **34.95**

Relaxation Delay(s): **0.1**
Completed Scans **16**

shuai, ADS_BK6_PAGE47
699.765 MHz HT PRESAT in cd3od (ref. to CD3OD @ 3.30 ppm), temp 27.5 C -> actual temp = 27.0 C, coldid probe





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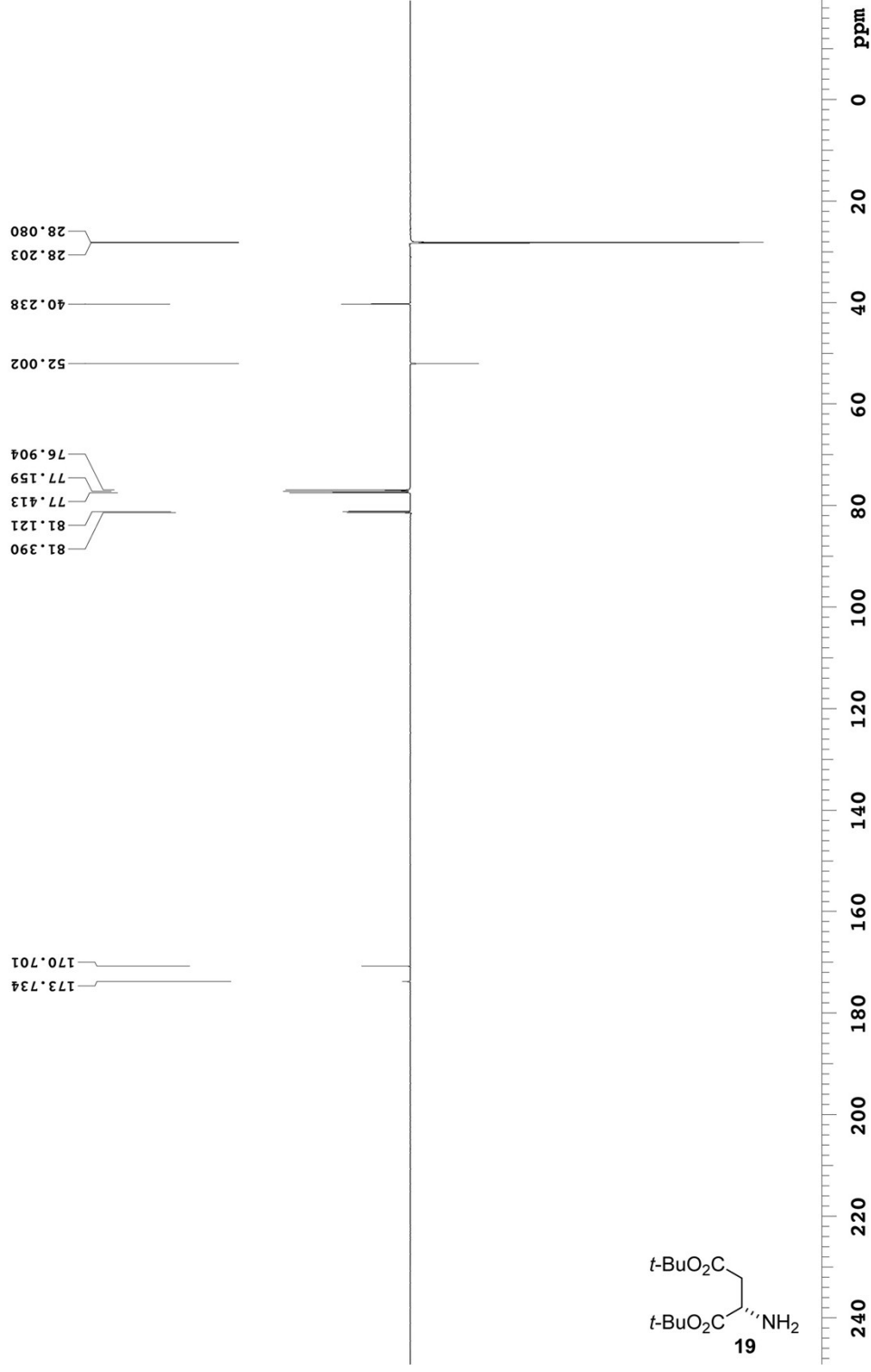
Recorded on: **u500, Feb 26 2015**
Pulse Sequence: **APT_ad**

Sweep Width(Hz): **33783.8**
Digital Res (Hz/pt): **0.26**

Acquisition Time(s): **2**
Hz per mm(Hz/mm): **140.76**

Relaxation Delay(s): **0.5**
Completed Scans: **512**

shuai, ADS-5_BK1_ATP
125.690 MHz C13[H1] APT_ad in cdcl3 (ref. to CDCl3 @ 77.06 ppm), temp 27.7 C -> actual temp = 27.0 C, cold dual probe
C & CH2 same, CH & CH3 opposite side of solvent signal

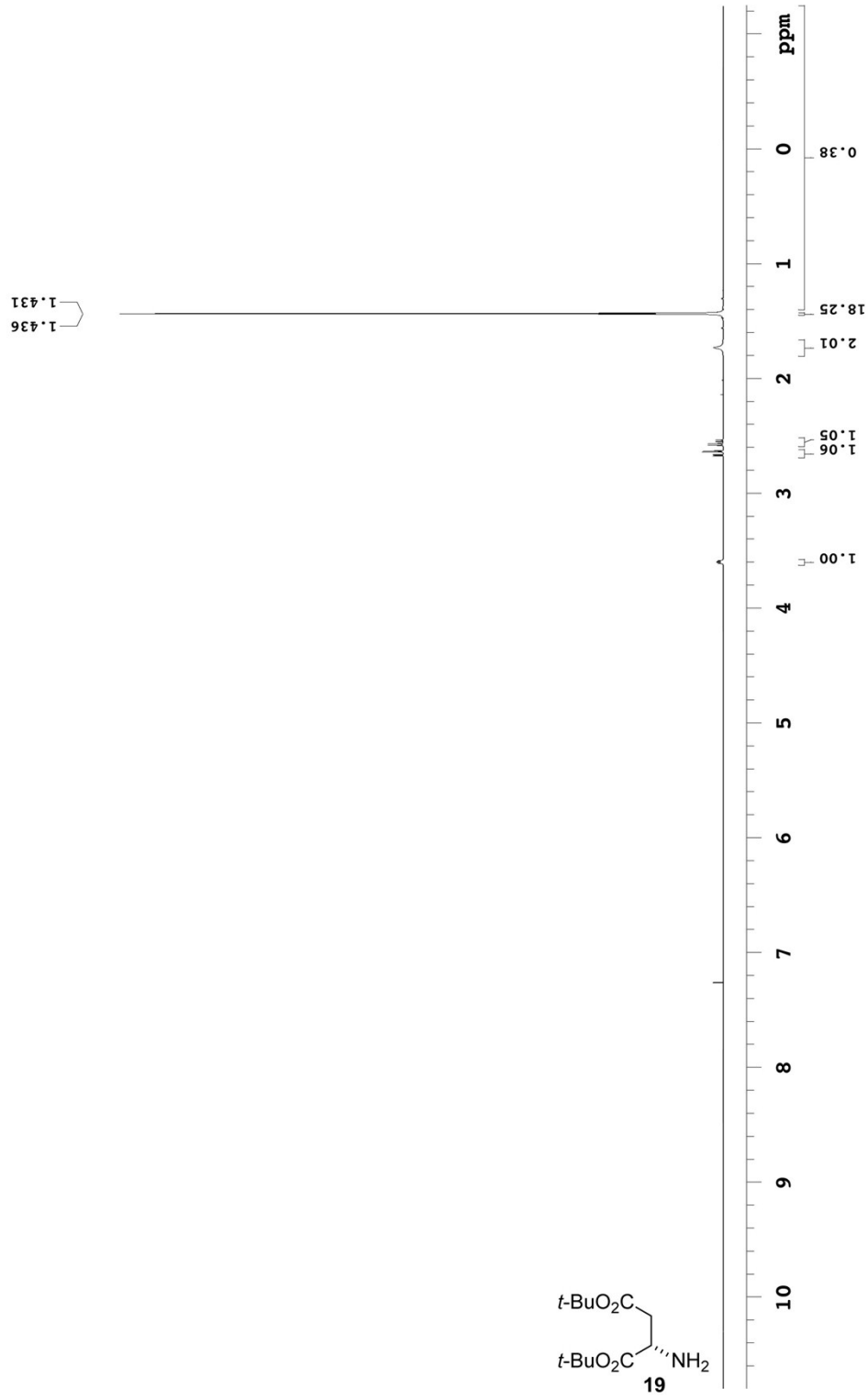




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Recorded on: ibds, Feb 26 2015	Sweep Width(Hz): 6000.6	Acquisition Time(s): 5	Relaxation Delay(s): 0.1
Pulse Sequence: s2pul	Digital Res (Hz/pt): 0.09	Hz per mm(Hz/mm): 25	Completed Scans: 16

498.118 MHz ¹H 1D in cdcl₃ (ref. to CDC13 @ 7.26 ppm), temp 26.4 C -> actual temp = 27.0 C, autotxdtb probe



File: /mnt/d600/home14/ciivenmr/nmrdata/dongshuai/2015.02/ADS-5_H



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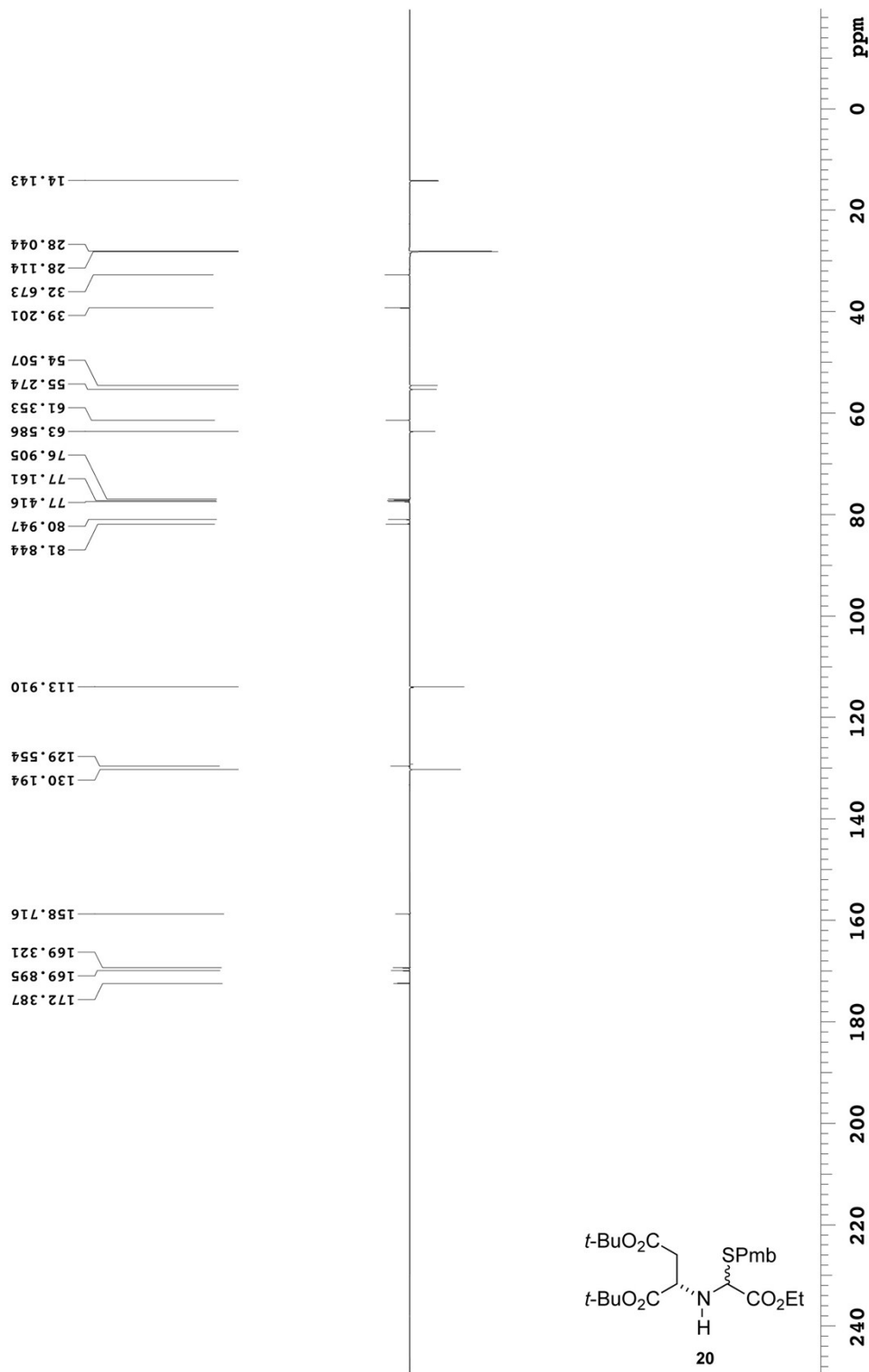
Recorded on: u500, Feb 28 2015
Pulse Sequence: APT_ad

Sweep Width(Hz): 33783.8
Digital Res. (Hz/pt): 0.26

Acquisition Time(s): 2
Hz per mm(Hz/mm): 140.76

Relaxation Delay(s): 0.5
Completed Scans: 512

shuai, ADS-72_BK1_PAGE186
125.690 MHz C13[1H] APT_ad in cdcl3 (ref. to CDCl3 @ 77.06 ppm), temp 27.7 C -> actual temp = 27.0 C, coldlual probe
C & CH2 same, CH & CH3 opposite side of solvent signal





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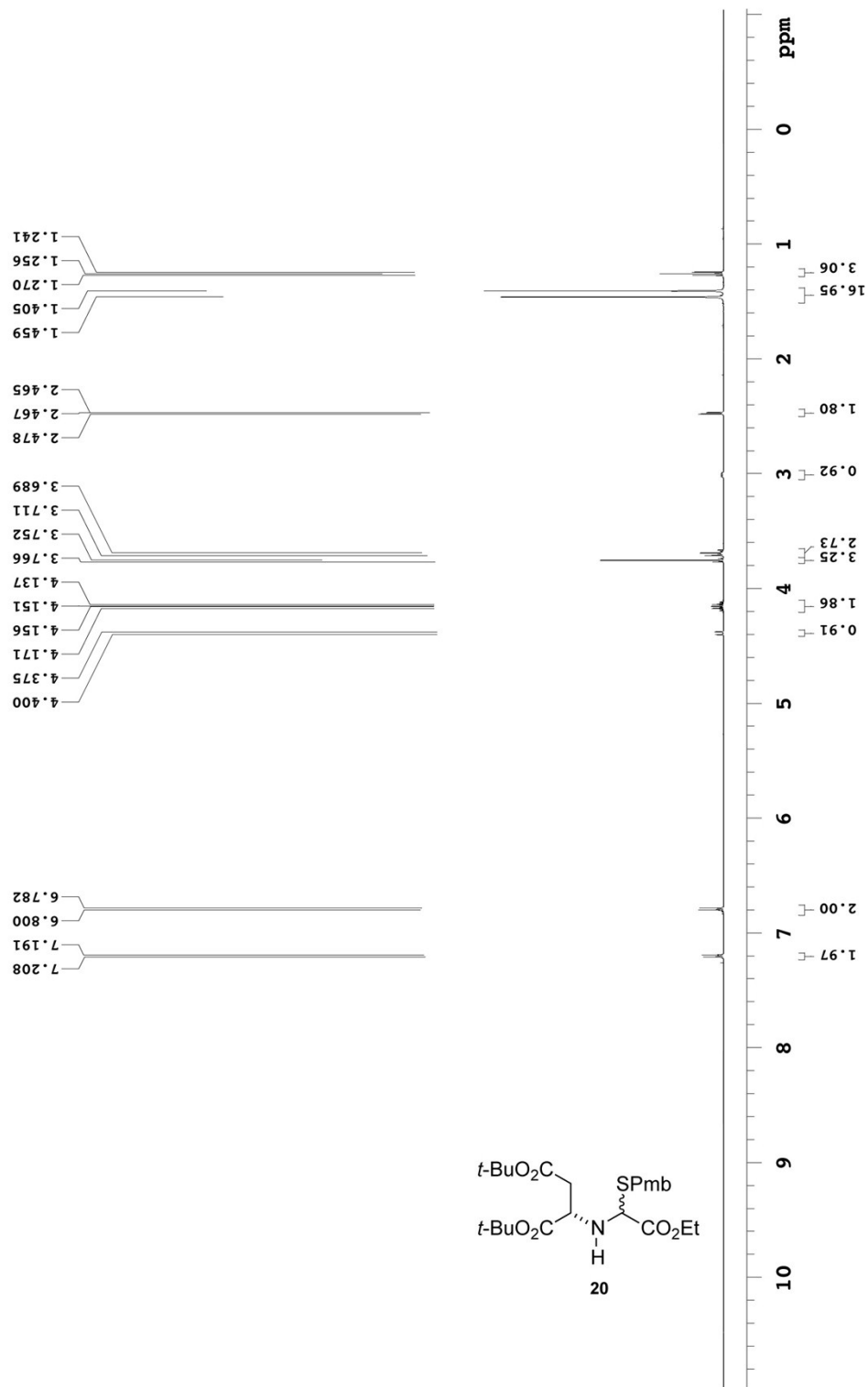
Recorded on: u500, Feb 27 2015
Pulse Sequence: PRESAT

Sweep Width(Hz): 6009.62
Digital Res (Hz/pt): 0.18

Acquisition Time(s): 5
Hz per mm(Hz/mm): 25.04

Relaxation Delay(s): 0.1
Completed Scans: 16

shuai, ADS-72_BK1_PAGE186
499.806 MHz ¹H PRESAT in cdcl₃ (ref. to CDCl₃ @ 7.26 ppm), temp 27.7 C -> actual temp = 27.0 C, coldludal probe





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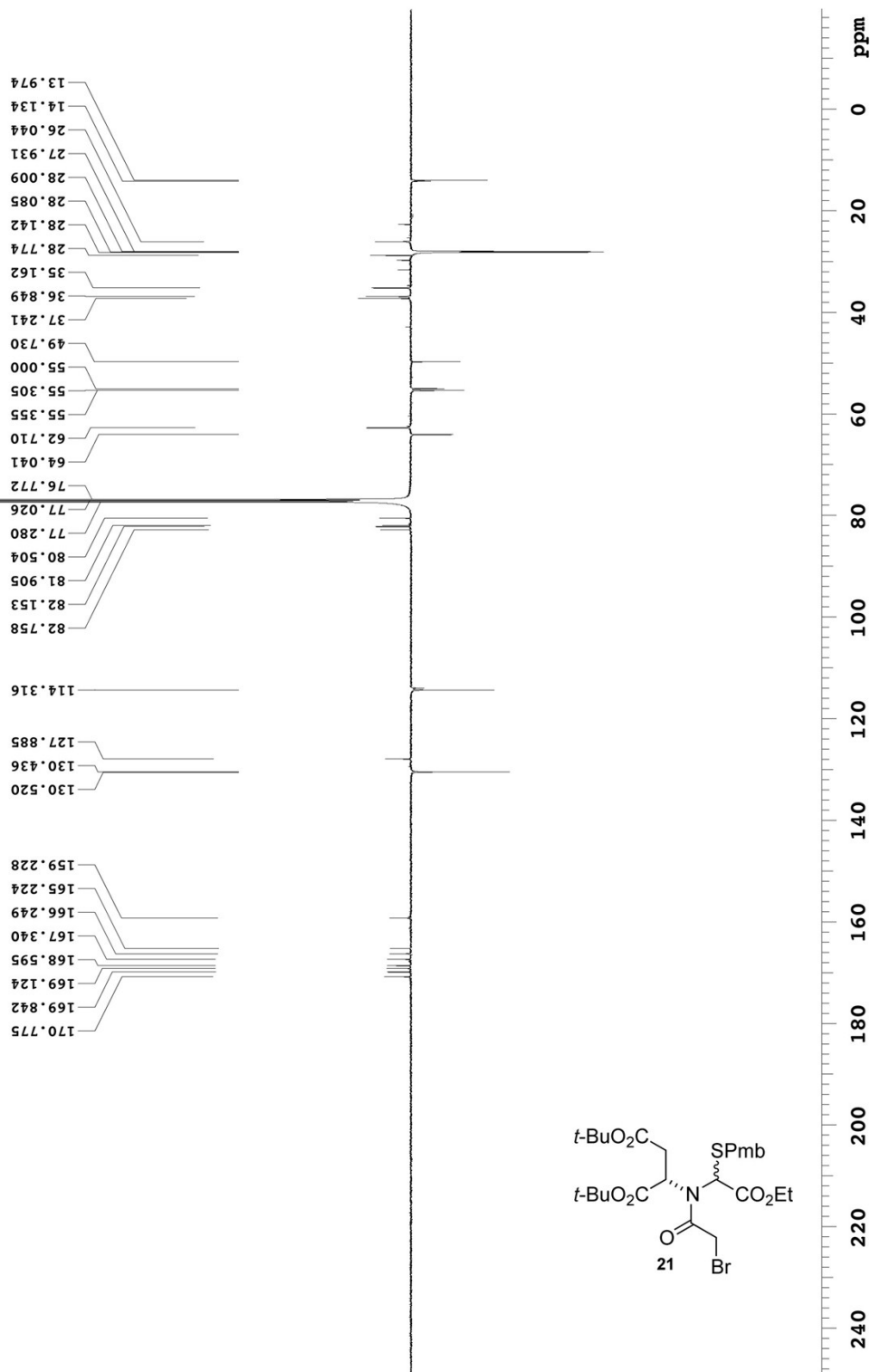
Recorded on: u500, Dec 6 2014
Pulse Sequence: APT_ad

Sweep Width(Hz): 33783.8
Digital Res (Hz/pt): 0.26

Acquisition Time(s): 2.5
Hz per mm(Hz/mm): 140.76

Relaxation Delay(s): 0.1
Completed Scans: 5000

shuai, ADS-28 BK1, PAGE63
125.690 MHz C13[H1] APT_ad in cdcl3 (ref. to CDCl3 @ 77.06 ppm), temp 27.7 C -> actual temp = 27.0 C, coldlual probe
C & CH2 same, CH & CH3 opposite side of signal





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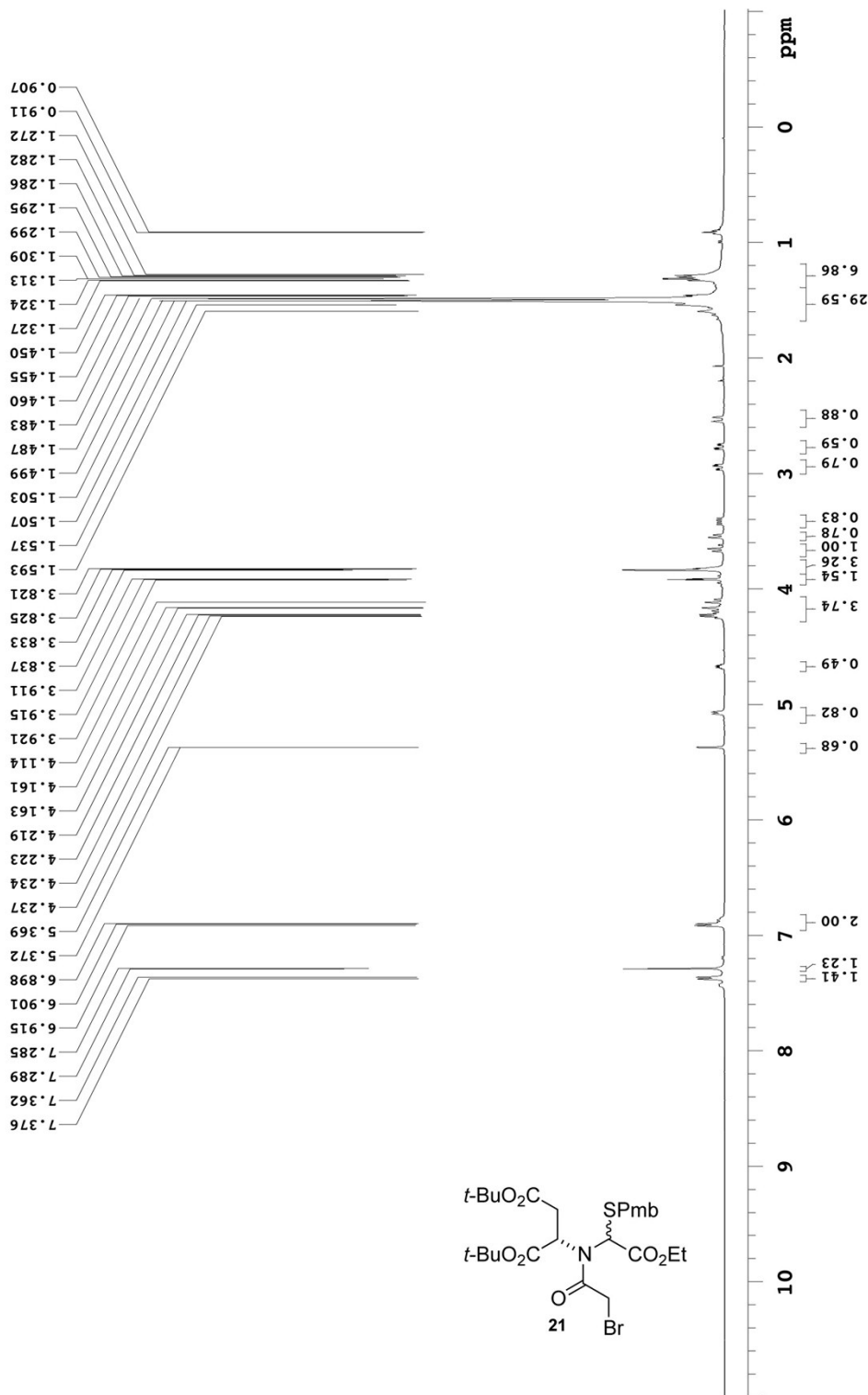
Recorded on: u500, Dec 6 2014
Pulse Sequence: PRESAT

Sweep Width(Hz): 6009.62
Digital Res (Hz/pt): 0.18

Acquisition Time(s): 5
Hz per mm(Hz/mm): 25.04

Relaxation Delay(s): 0.1
Completed Scans: 32

shuai, ADS-28_BK1_PAGE63
499.806 MHz H1 PRESAT in cdcl3 (ref. to CDCl3 @ 7.26 ppm), temp 27.7 C -> actual temp = 27.0 C, coldlual probe





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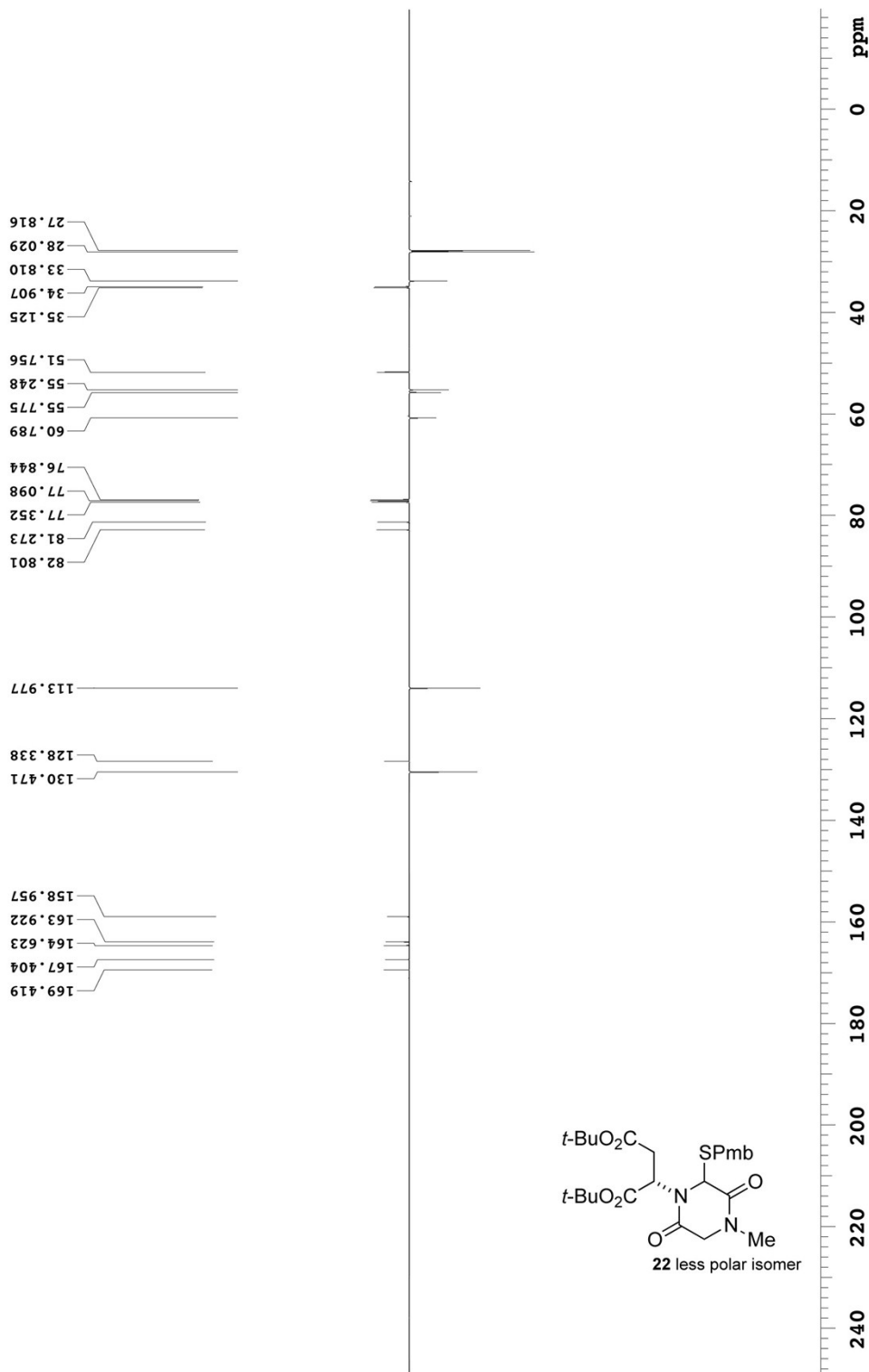
Recorded on: u500, Jan 16 2015
Pulse Sequence: APT_ad

Sweep Width(Hz): 33783.8
Digital Res (Hz/pt): 0.26

Acquisition Time(s): 2
Hz per mm(Hz/mm): 140.76

Relaxation Delay(s): 0.5
Completed Scans: 512

shuai, ADS-50_BK1_PAGE119
125.690 MHz C13[1H] APT_ad in cdcl3 (ref. to CDCl3 @ 77.06 ppm), temp 27.7 C -> actual temp = 27.0 C, coldlual probe
C & CH2 same, CH & CH3 opposite side of solvent signal





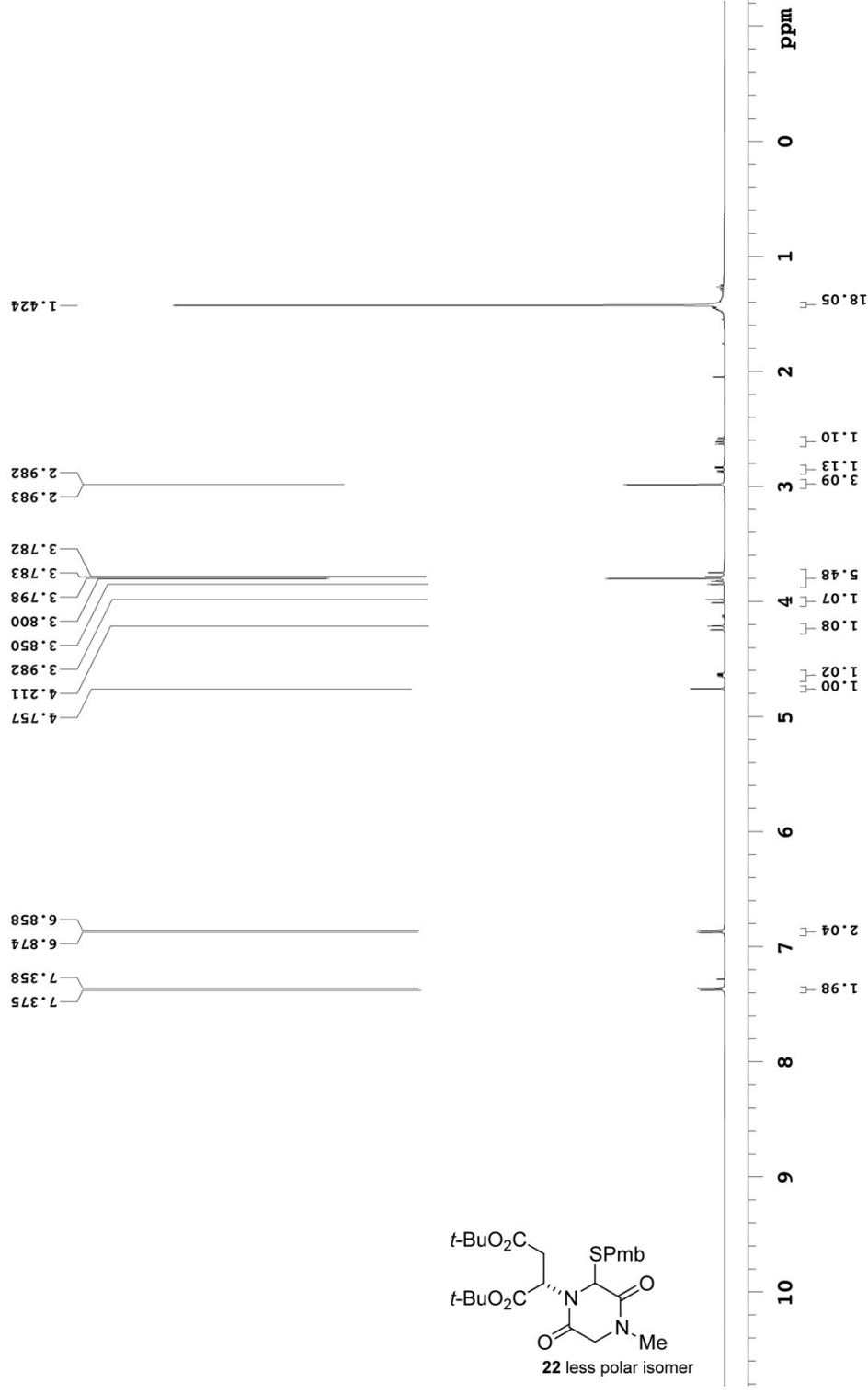
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Recorded on: **ibds, Mar 5 2015** Sweep Width(Hz): **6000.6** Acquisition Time(s): **5** Relaxation Delay(s): **0.1**
Pulse Sequence: **s2pul** Digital Res (Hz/pt): **0.09** Hz per mm(Hz/mm): **25** Completed Scans: **16**

ISOMERB BK1 PAGE193

498.118 MHz H1 1D in cdcl3 (ref. to CDC13 @ 7.26 ppm), temp 26.4 C -> actual temp = 27.0 C, autotxdtb probe



File: /mnt/d600/home14/ciivenmr/nmrdata/spectra_for_shuai/2015.03.05.i5_ISOMERB_BK1_PAGE193_16.38_H1_1D



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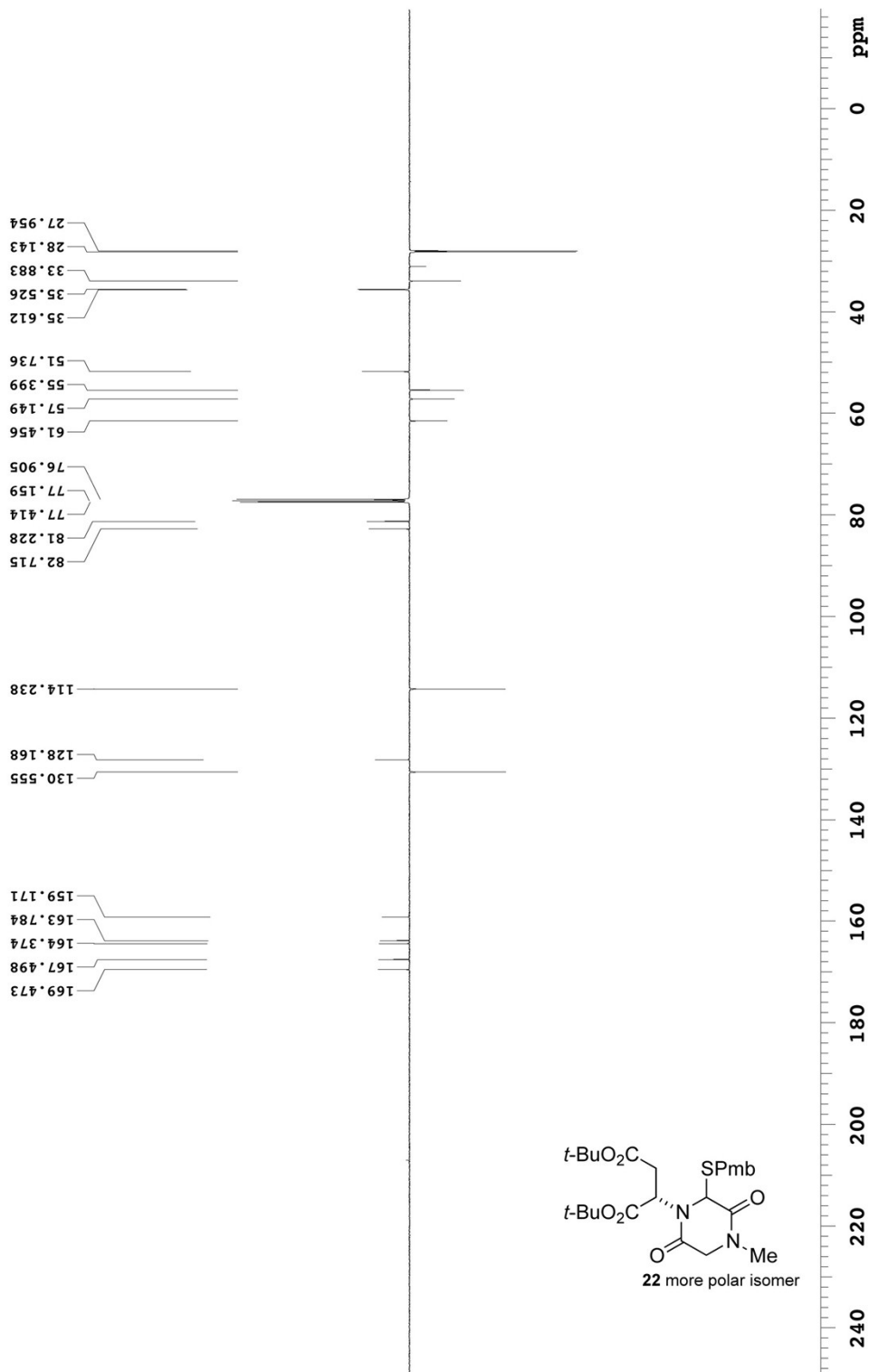
Recorded on: u500, Mar 6 2015
Pulse Sequence: APT_ad

Sweep Width(Hz): 33783.8
Digital Res. (Hz/pt): 0.26

Acquisition Time(s): 2
Hz per mm(Hz/mm): 140.76

Relaxation Delay(s): 0.5
Completed Scans: 512

shuai, ISOMERA_BK1_PAGE193
125.690 MHz C13[1H] APT_ad in cdcl3 (ref. to CDCl3 @ 77.06 ppm), temp 27.7 C -> actual temp = 27.0 C, coldlual probe
C & CH2 same, CH & CH3 opposite side of solvent signal





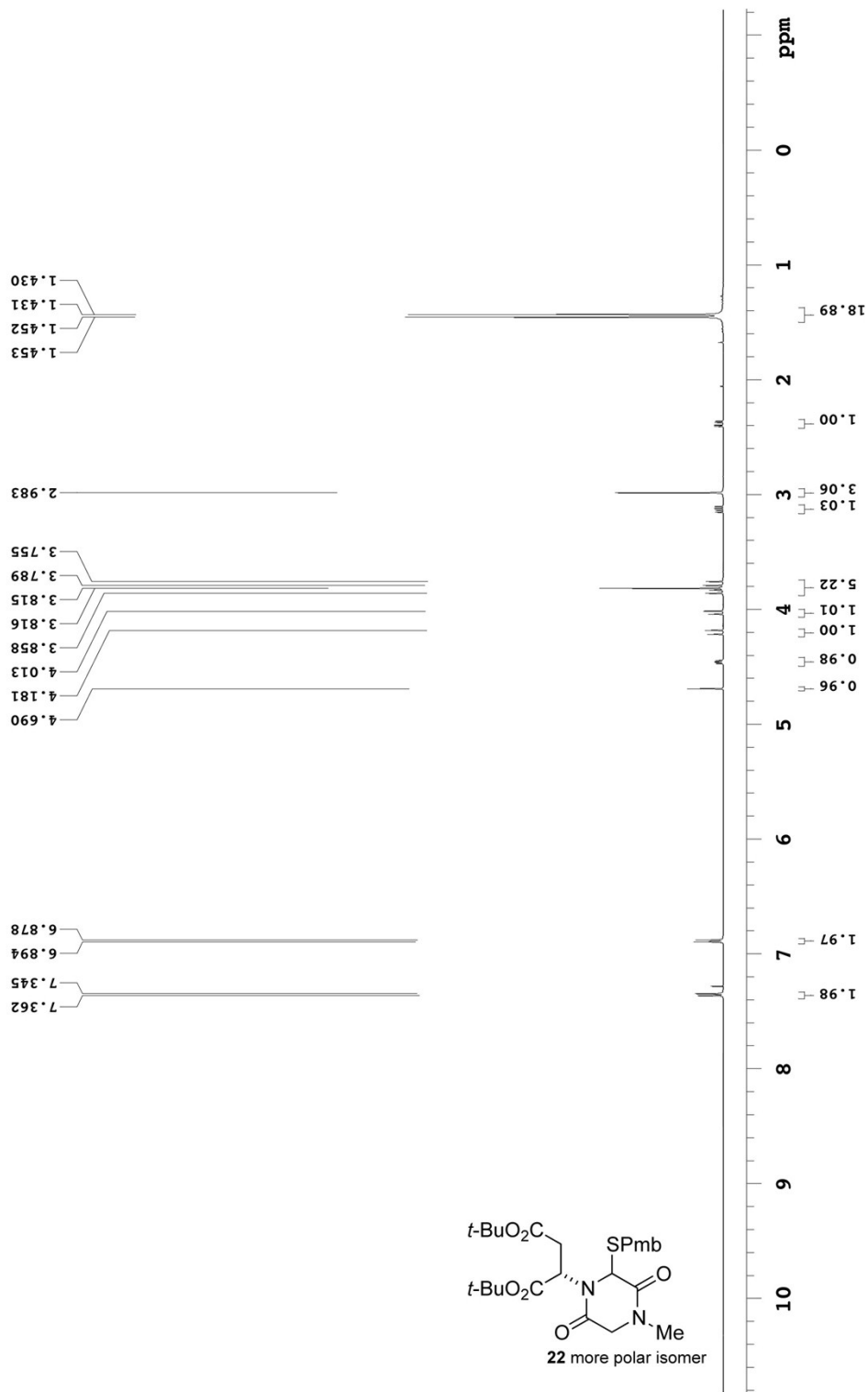
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ISOMERA BK1 PAGE193

498.118 MHz ¹H 1D in cdcl₃ (ref. to CDC13 @ 7.26 ppm), temp 26.4 C -> actual temp = 27.0 C, autotxdtb probe

Recorded on: **ibds, Mar 5 2015** Sweep Width(Hz): **6000.6** Acquisition Time(s): **5** Relaxation Delay(s): **0.1**
Pulse Sequence: **s2pul** Digital Res (Hz/pt): **0.09** Hz per mm(Hz/mm): **25** Completed Scans: **16**



File: /mnt/d600/home14/ciivenmr/nmrdata/spectra_for_shuai/2015.03.05.i5_ISOMERA_BK1_PAGE193_16.32_H1_1D



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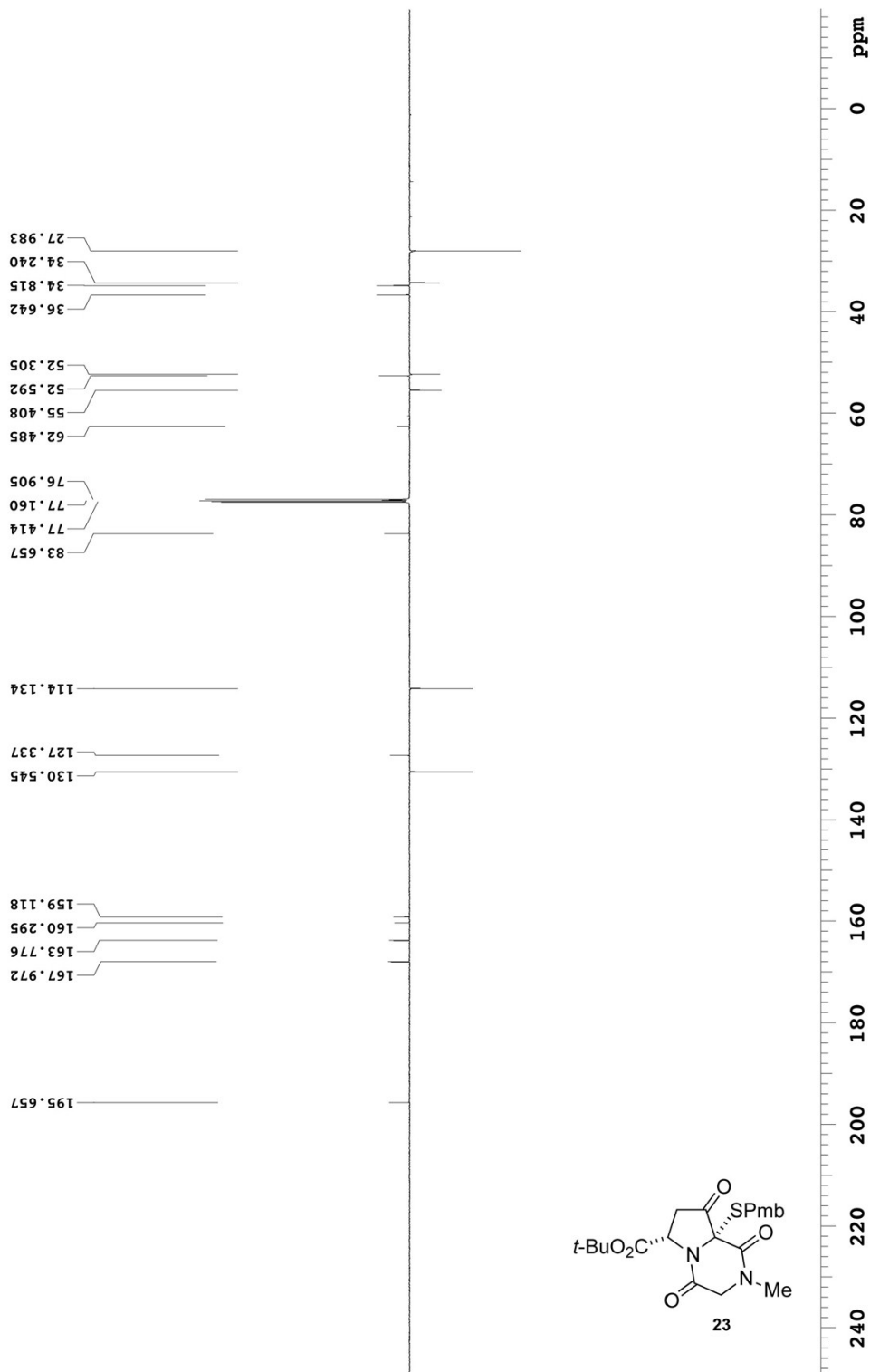
Recorded on: u500, Feb 12 2015
Pulse Sequence: APT_ad

Sweep Width(Hz): 33783.8
Digital Res. (Hz/pt): 0.26

Acquisition Time(s): 2
Hz per mm(Hz/mm): 140.76

Relaxation Delay(s): 0.5
Completed Scans: 512

shuai, ADS-58_BK1_PAGE153
125.690 MHz C13[1H] APT_ad in cdcl3 (ref. to CDCl3 @ 77.06 ppm), temp 27.7 C -> actual temp = 27.0 C, coldlual probe
C & CH2 same, CH & CH3 opposite side of solvent signal





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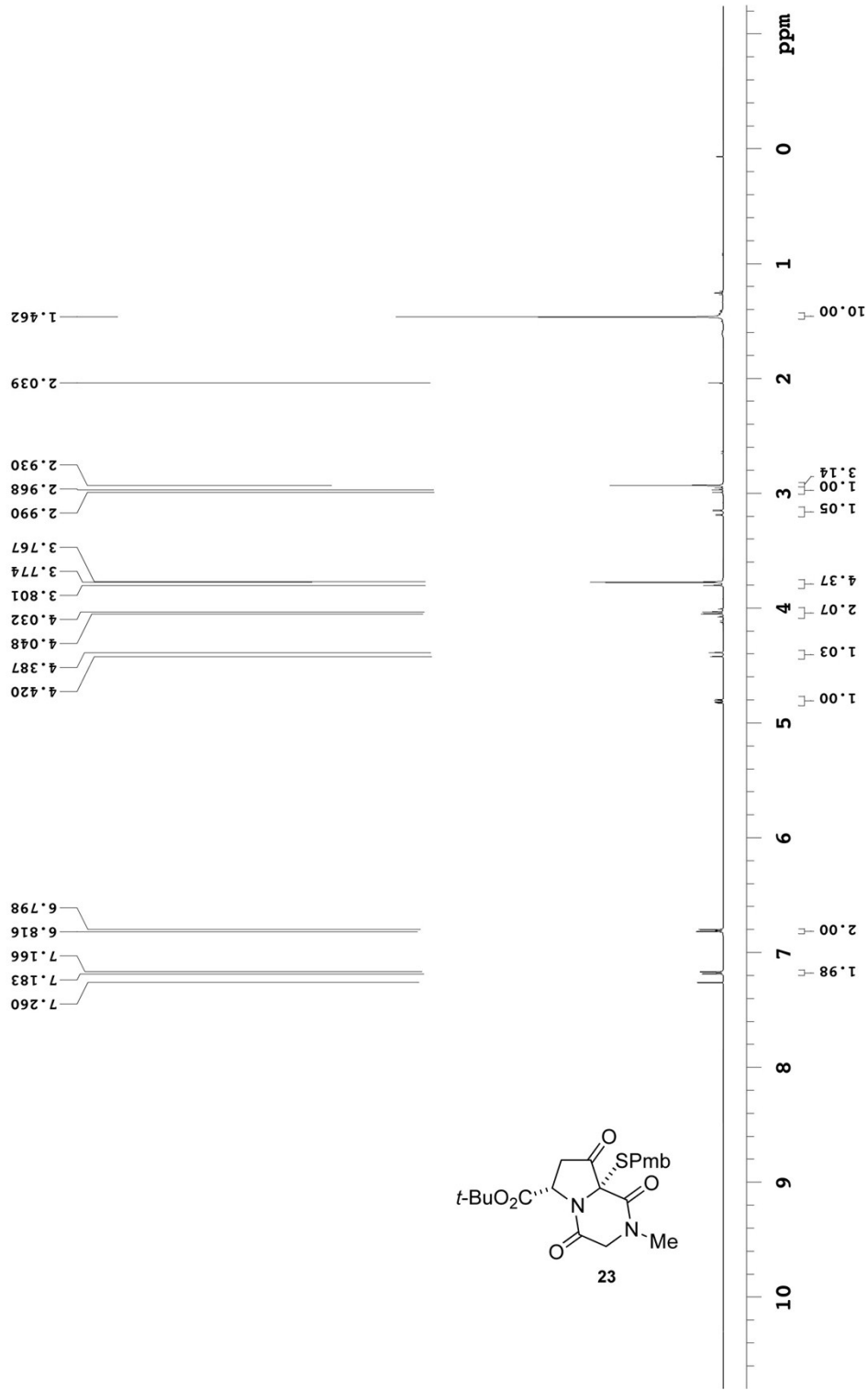
Recorded on: **ibd5, Feb 12 2015**
Pulse Sequence: **s2pul**

Sweep Width(Hz): **6000.6**
Digital Res. (Hz/pt): **0.09**

Acquisition Time(s): **5**
Hz per mm(Hz/mm): **25**

Relaxation Delay(s): **0.1**
Completed Scans: **16**

498.118 MHz H1 1D in cdcl3 (ref. to CDC13 @ 7.26 ppm), temp 26.4 C -> actual temp = 27.0 C, autotdb probe





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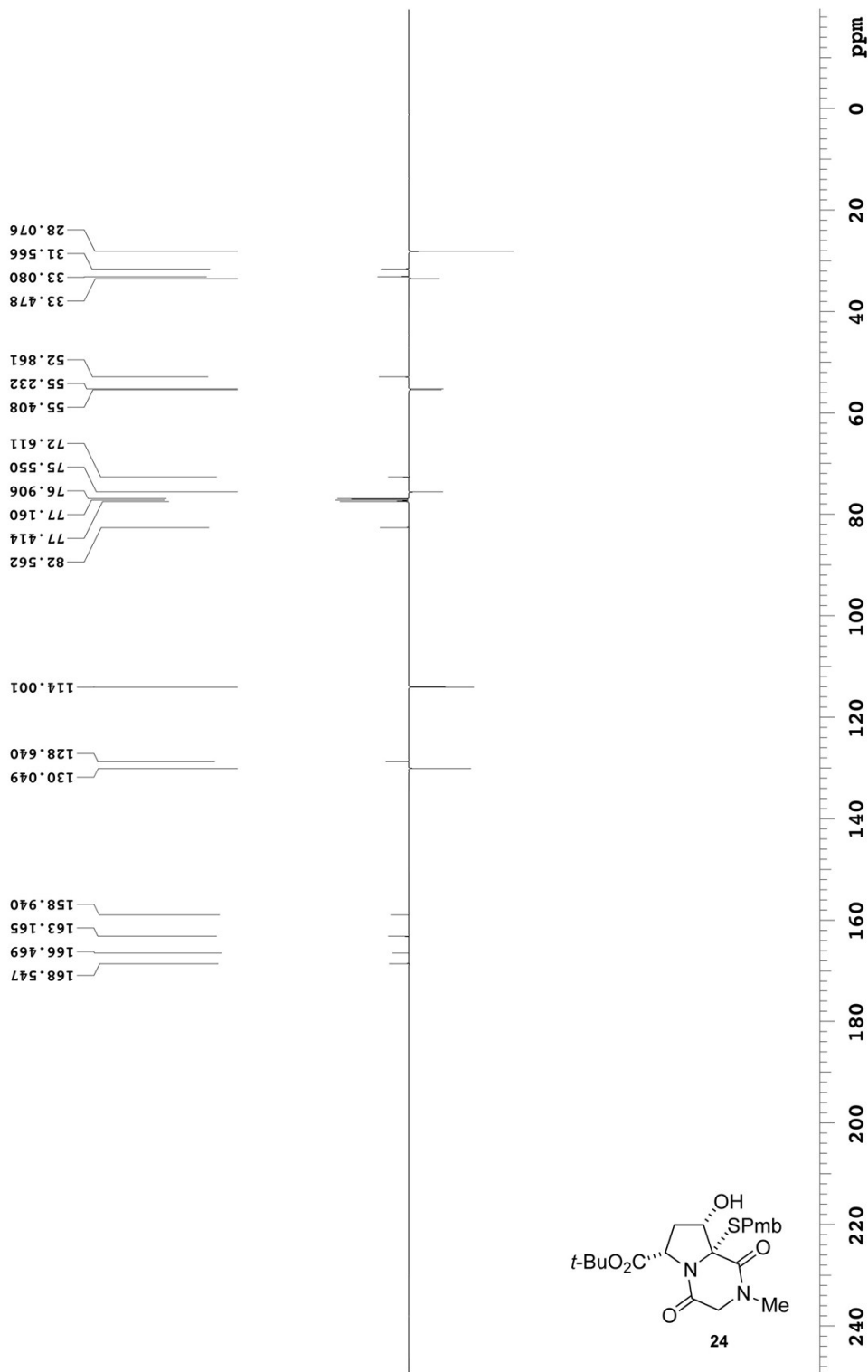
Recorded on: u500, Mar 12 2015
Pulse Sequence: APT_ad

Sweep Width(Hz): 33783.8
Digital Res. (Hz/pt): 0.26

Acquisition Time(s): 2
Hz per mm(Hz/mm): 140.76

Relaxation Delay(s): 0.5
Completed Scans: 512

shuai, ADS-81_BK2_PAGE3
125.690 MHz C13[1H] APT_ad in cdcl3 (ref. to CDCl3 @ 77.06 ppm), temp 27.7 C -> actual temp = 27.0 C, coldlual probe
C & CH2 same, CH & CH3 opposite side of solvent signal





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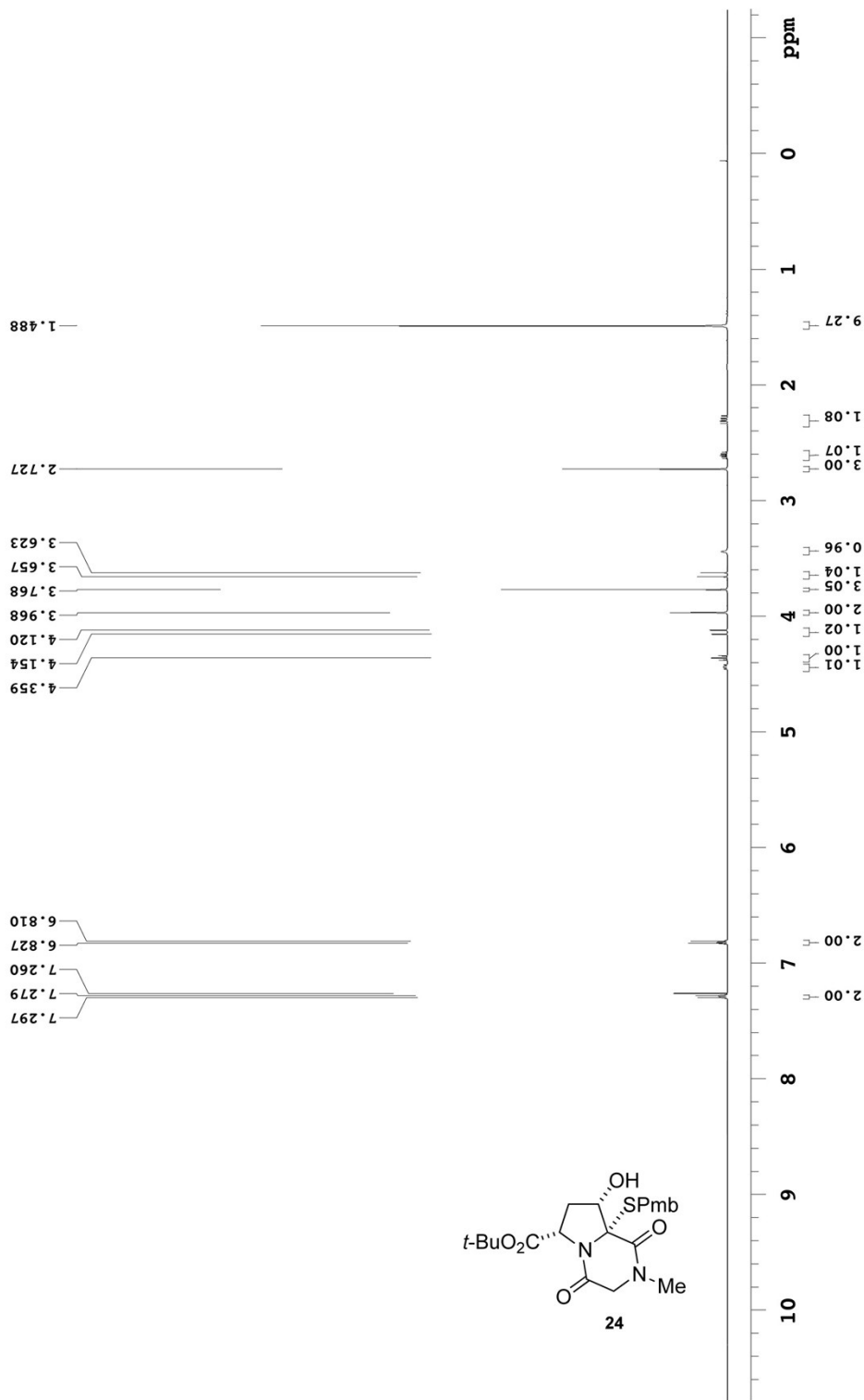
Recorded on: **ibd5, Mar 12 2015**
Pulse Sequence: **s2pul**

Sweep Width(Hz): **6000.6**
Digital Res. (Hz/pt): **0.09**

Acquisition Time(s): **5**
Relaxation Delay(s): **0.1**
Completed Scans: **16**

ADS-81 BK2 PAGE3

498.118 MHz H1 1D in cdcl3 (ref. to CDC13 @ 7.26 ppm), temp 26.4 C -> actual temp = 27.0 C, autotxdtb probe

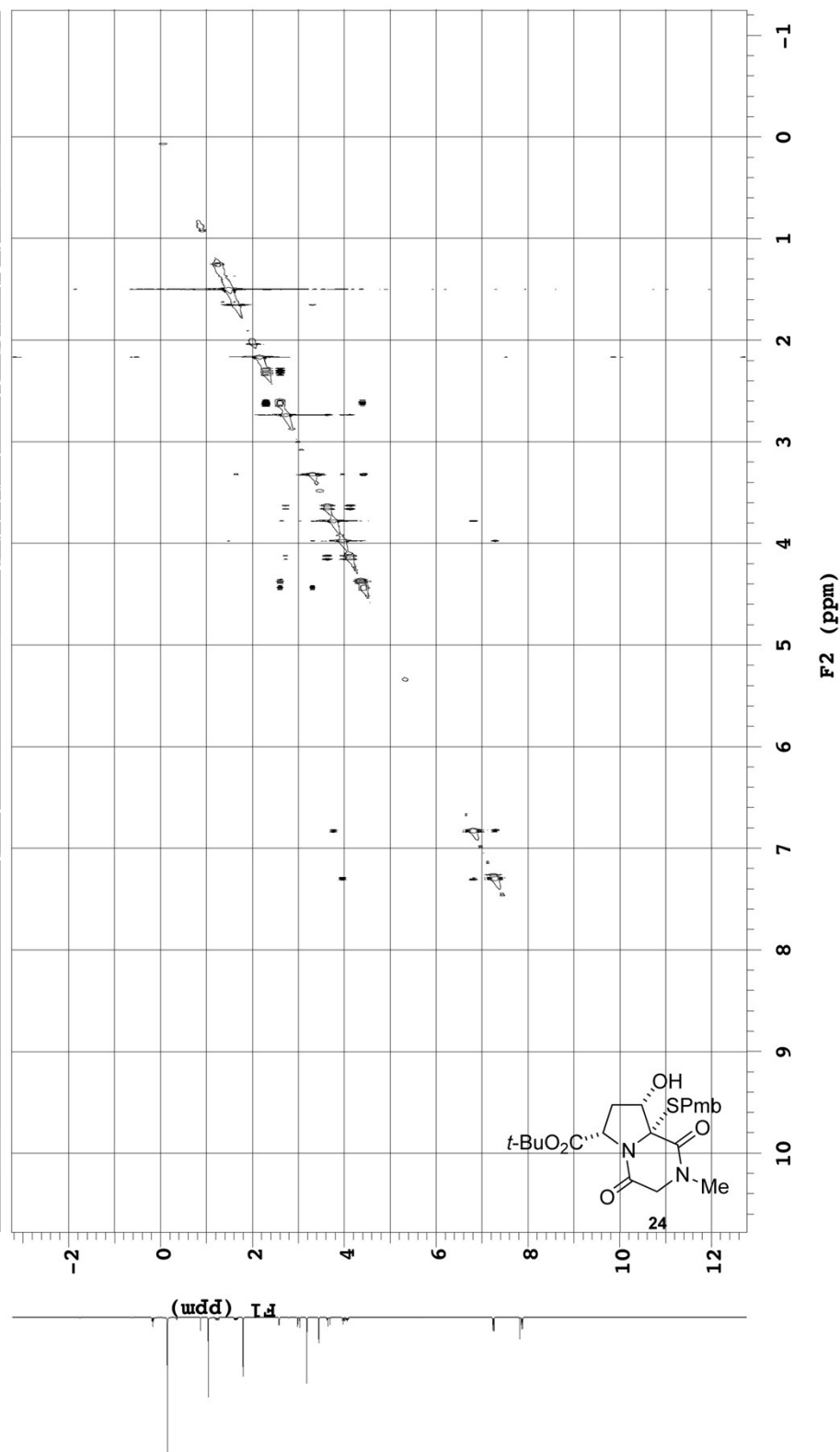




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Recorded on: **u500, Feb 5 2015** Sweep Width F2(F1) (Hz): **6009.621 8012.82** Acquisition Time(s): **1** Relaxation Delay(s): **1**
Pulse Sequence: **ROESY** Digital Res. F2(F1) (Hz/ppm): **1.471 15.65** Hz per mm F2(F1) (Hz/mm): **25.60 155.31** No. of Scans/Increments: **161 170**

shuai, ADS-59_BK1_PAGE147
499.806 MHz ¹H ROESY in cdcl₃ (ref. to CDC13 @ 7.26 ppm), temp 27.7 C -> actual temp = 27.0 C, cold dual probe





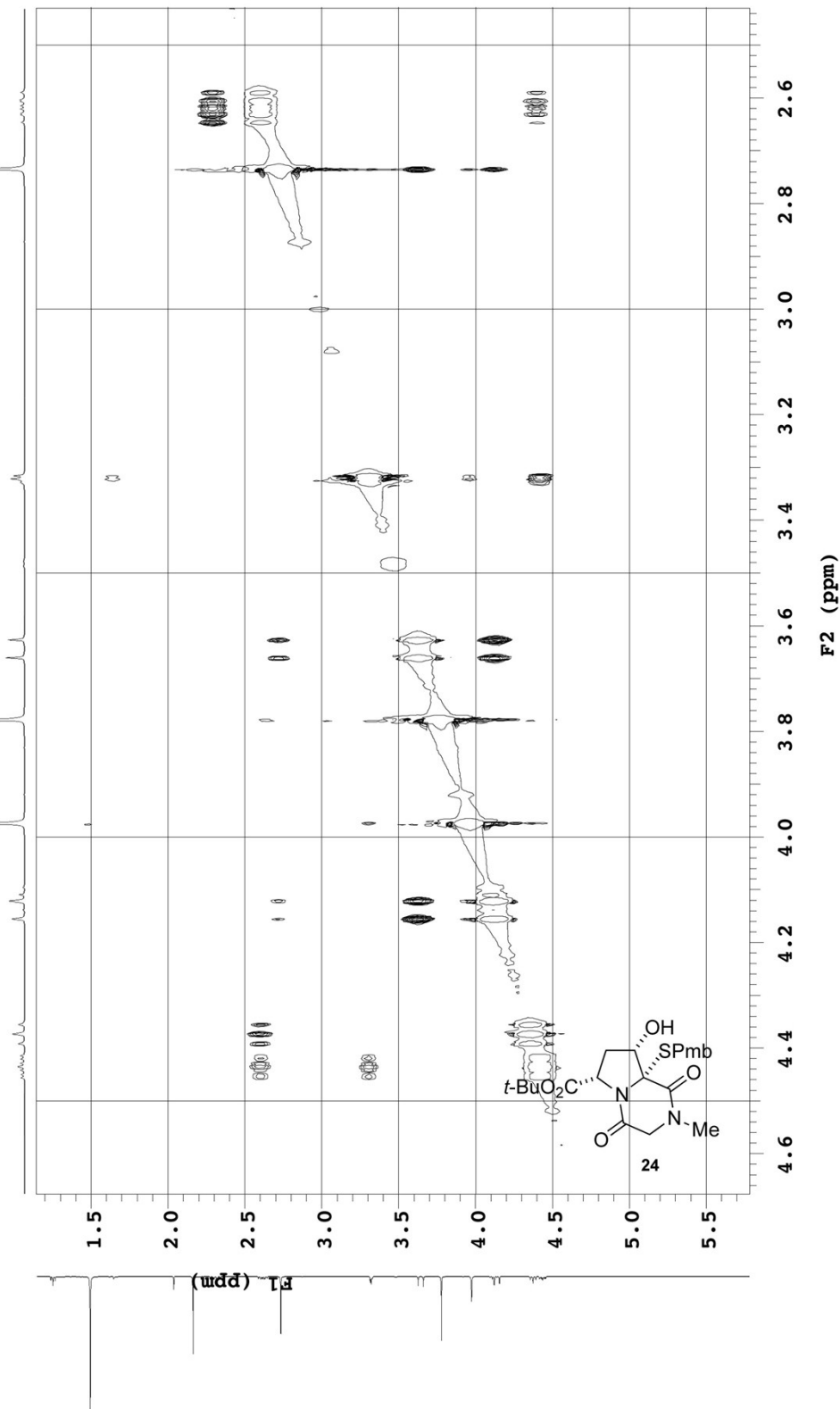
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Recorded on: **u500, Feb 5 2015** Sweep Width F2(F1) (Hz): **6009.621 8012.82** Acquisition Time(s): **1** Relaxation Delay(s): **1**
Pulse Sequence: **ROESY** Digital Res. F2(F1) (Hz/ppm): **1.471 15.65** Hz per mm F2(F1) (Hz/mm): **4.781 16.02** No. of Scans/Increments: **161 170**

shuai, ADS-59_BK1_PAGE147

499.806 MHz ¹H ROESY in cdcl₃ (ref. to CDC13 @ 7.26 ppm), temp 27.7 C -> actual temp = 27.0 C, cold dual probe



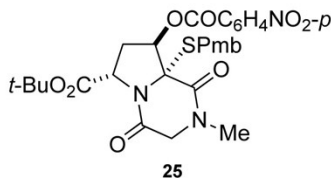
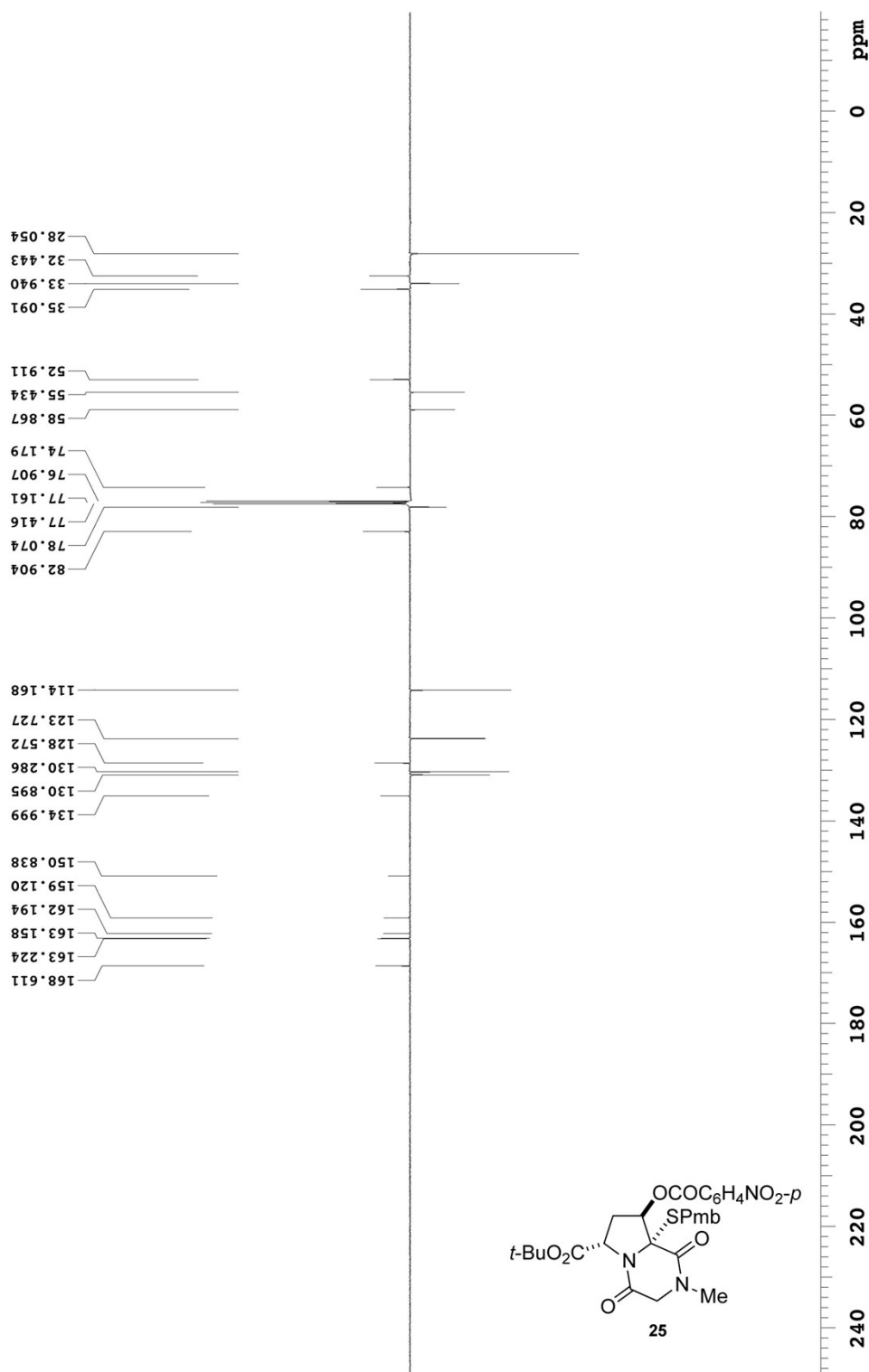
Recorded on: u500, Mar 17 2015
Pulse Sequence: APT_ad

Sweep Width(Hz): **33783.8**
Digital Res.(Hz/pt): **0.26**

Acquisition Time(s): **2**
Hz per mm(Hz/mm): **140.76**

Relaxation Delay(s): **0.5**
Completed Scans **512**

shual, ADS-82, BK2_PAGES
125.690 MHz C13[H1] APT-ad in cdcl3 (ref. to CDCl3 @ 77.06 ppm), temp 27.7 C -> actual temp = 27.0 C, coldlual probe
C & CH2 same, CH & CH3 opposite side of solvent signal





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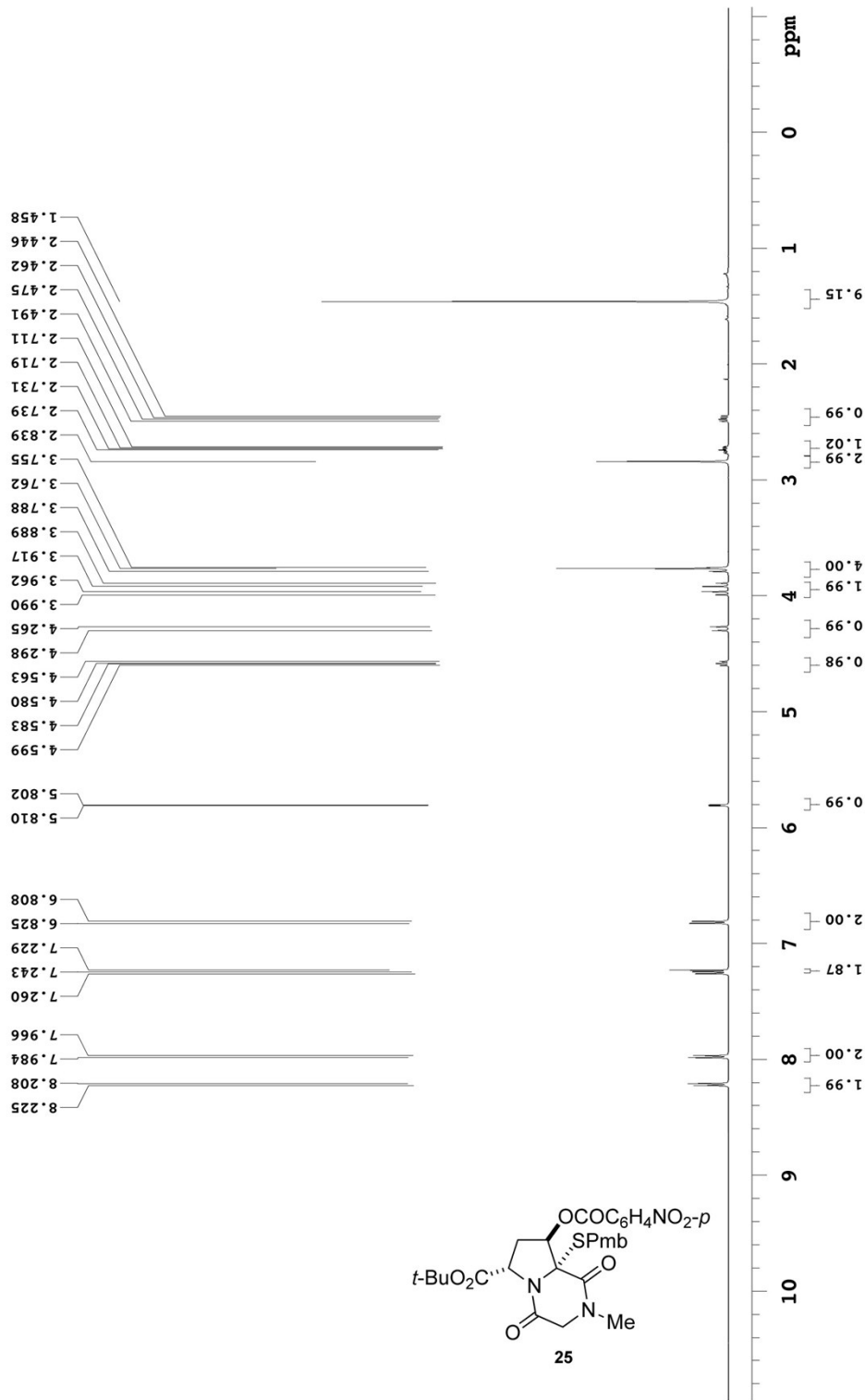
Recorded on: u500, Mar 17 2015
Pulse Sequence: PRESAT

Sweep Width(Hz): 6009.62
Digital Res. (Hz/pt): 0.18

Acquisition Time(s): 5
Hz per mm(Hz/mm): 25.04

Relaxation Delay(s): 0.1
Completed Scans: 16

shuai, ADS-82_BK2_PAGES
499.806 MHz HT PRESAT in cdcl3 (ref. to CDCl3 @ 7.26 ppm), temp 27.7 C -> actual temp = 27.0 C, coldlual probe





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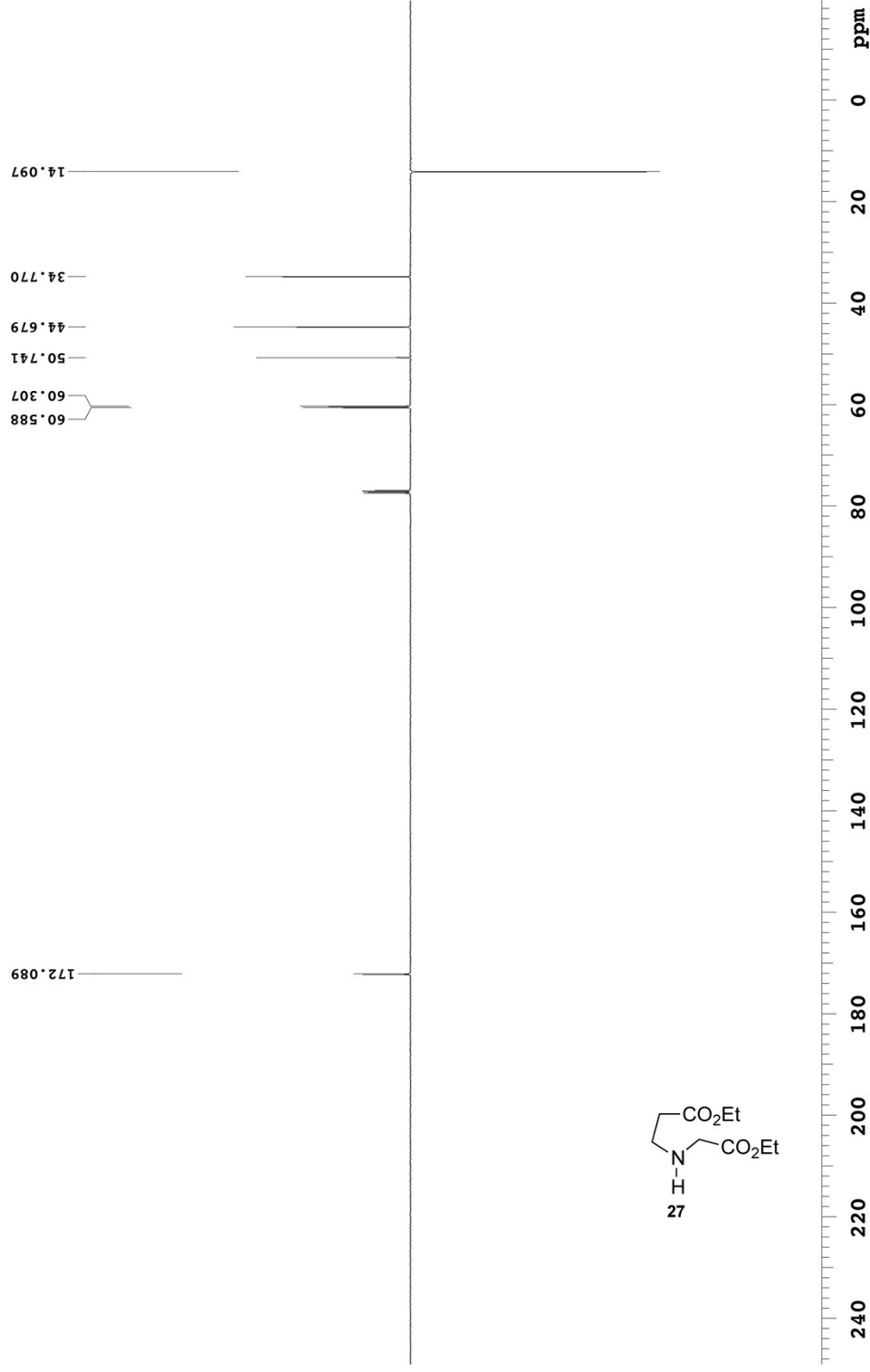
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Recorded on: **u500, Jul 23 2015**
Pulse Sequence: **APT_ad**

Sweep Width(Hz): **33783.8**
Digital Res. (Hz/pt): **0.26**

Acquisition Time(s): **2**
Relaxation Delay(s): **0.5**
Completed Scans: **128**

Kiran, IK-01-P39
125.690 MHz C13[1H] APT_ad in cdcl3 (ref. to CDCl3 @ 77.06 ppm), temp 27.7 C -> actual temp = 27.0 C, cold dual probe
C & CH2 same, CH & CH3 opposite side of solvent signal



File: /mnt/d600/home14/civenmr/nmrdata/spectra_for_shuai/rou2/2015.07.23.u5_IK-01-P39_loc8_15.18_C13_APT_ad



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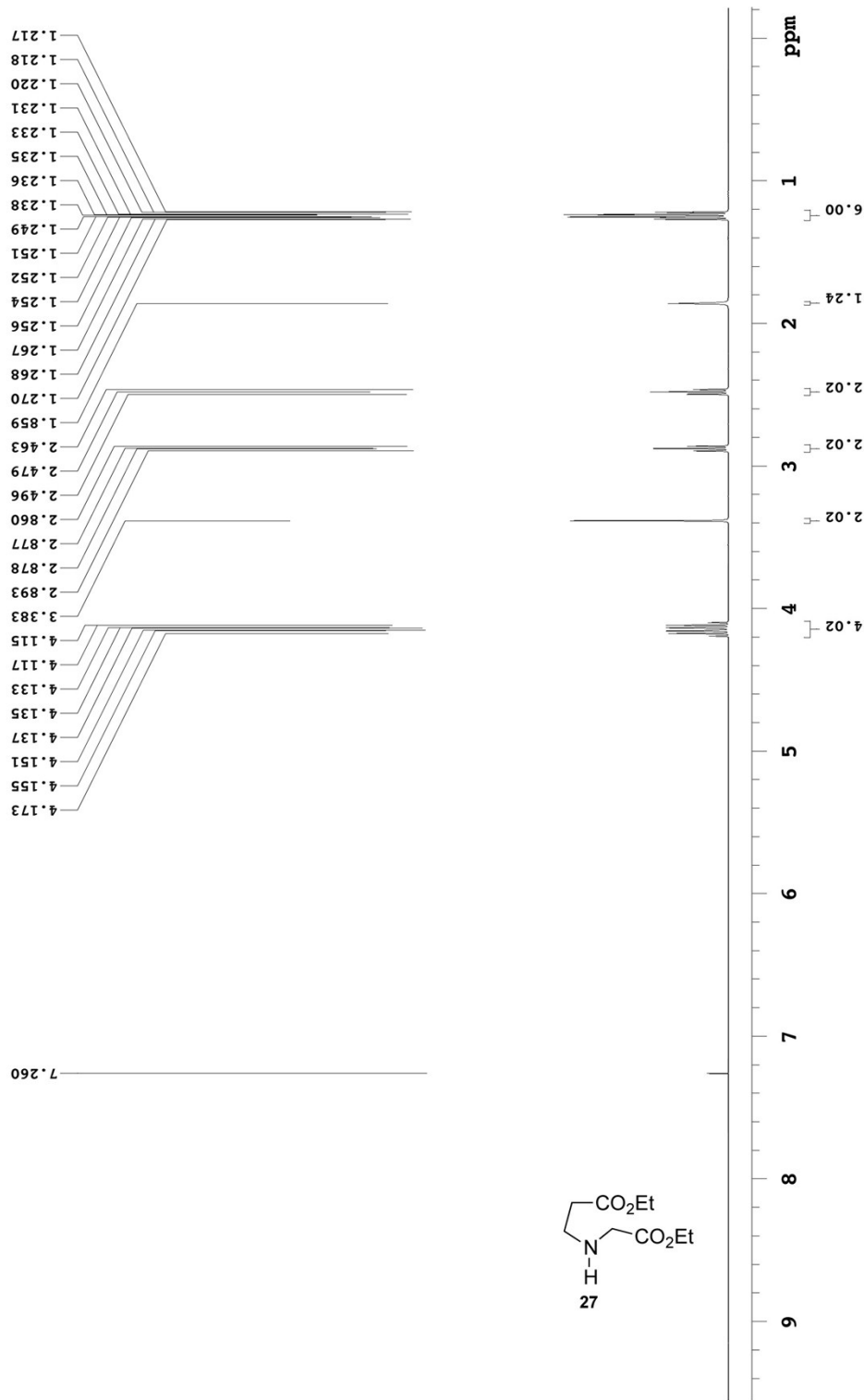
Recorded on: 1400, Jul 24 2015
Pulse Sequence: s2pul

Sweep Width(Hz): 4801.92
Digital Res (Hz/pt): 0.07

Acquisition Time(s): 4.998
Hz per mm(Hz/mm): 16.28

Relaxation Delay(s): 0.1
Completed Scans 16

IK-01-P39
399.794 MHz H1 1D in cdcl3 (ref. to CDC13 @ 7.26 ppm), temp 26.5 C -> actual temp = 27.0 C, autotxdtb probe





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Agilent Technologies

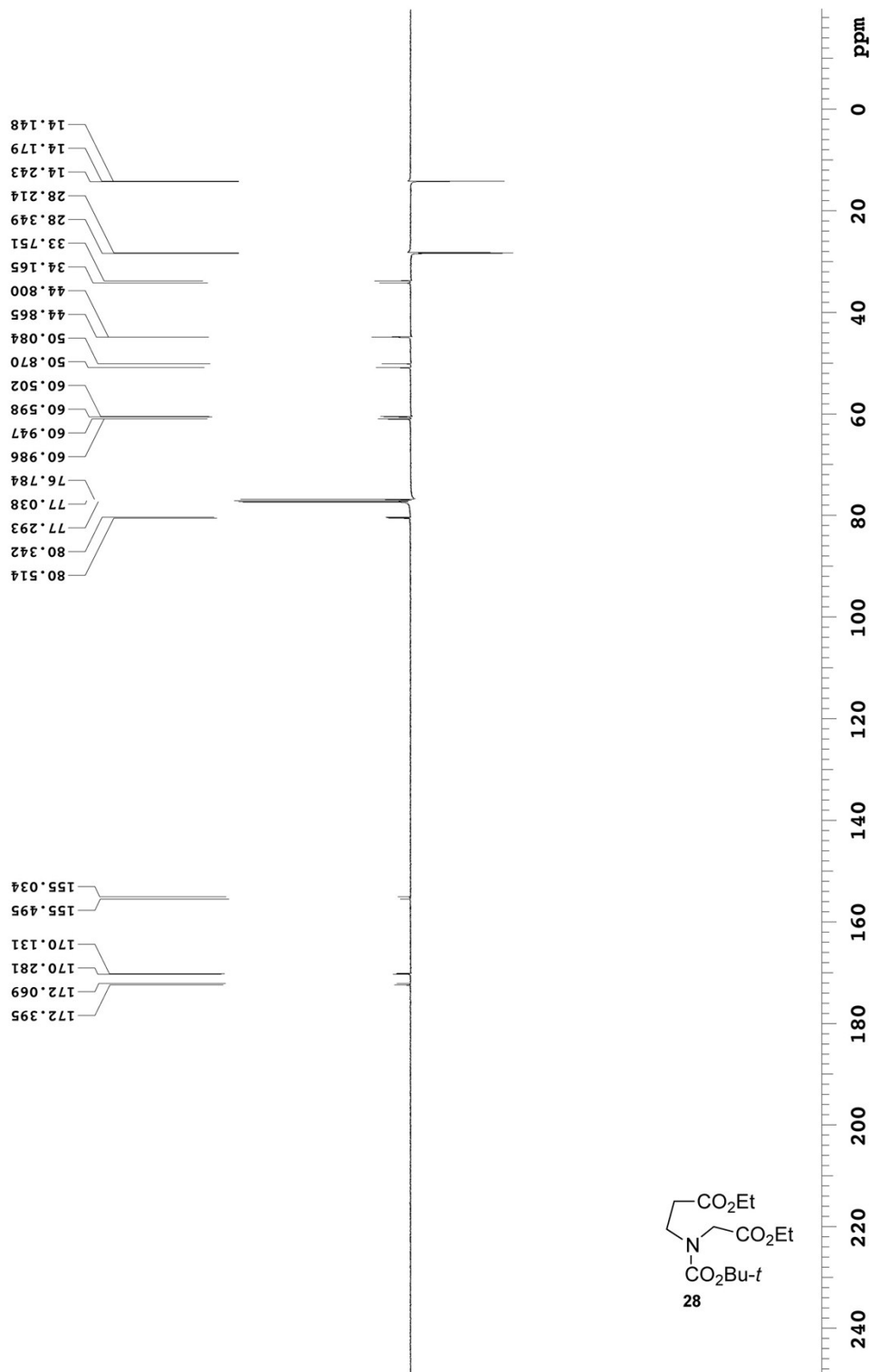
Recorded on: u500, Jul 24 2015
Pulse Sequence: APT_ad

Sweep Width(Hz): 33783.8
Digital Res (Hz/pt): 0.26

Acquisition Time(s): 2
Hz per mm(Hz/mm): 140.76

Relaxation Delay(s): 0.5
Completed Scans: 192

Kiran, IK-01-P47
125.690 MHz C13[1H] APT_ad in cdcl3 (ref. to CDCl3 @ 77.06 ppm), temp 27.7 C -> actual temp = 27.0 C, cold dual probe
C & CH2 same, CH & CH3 opposite side of solvent signal





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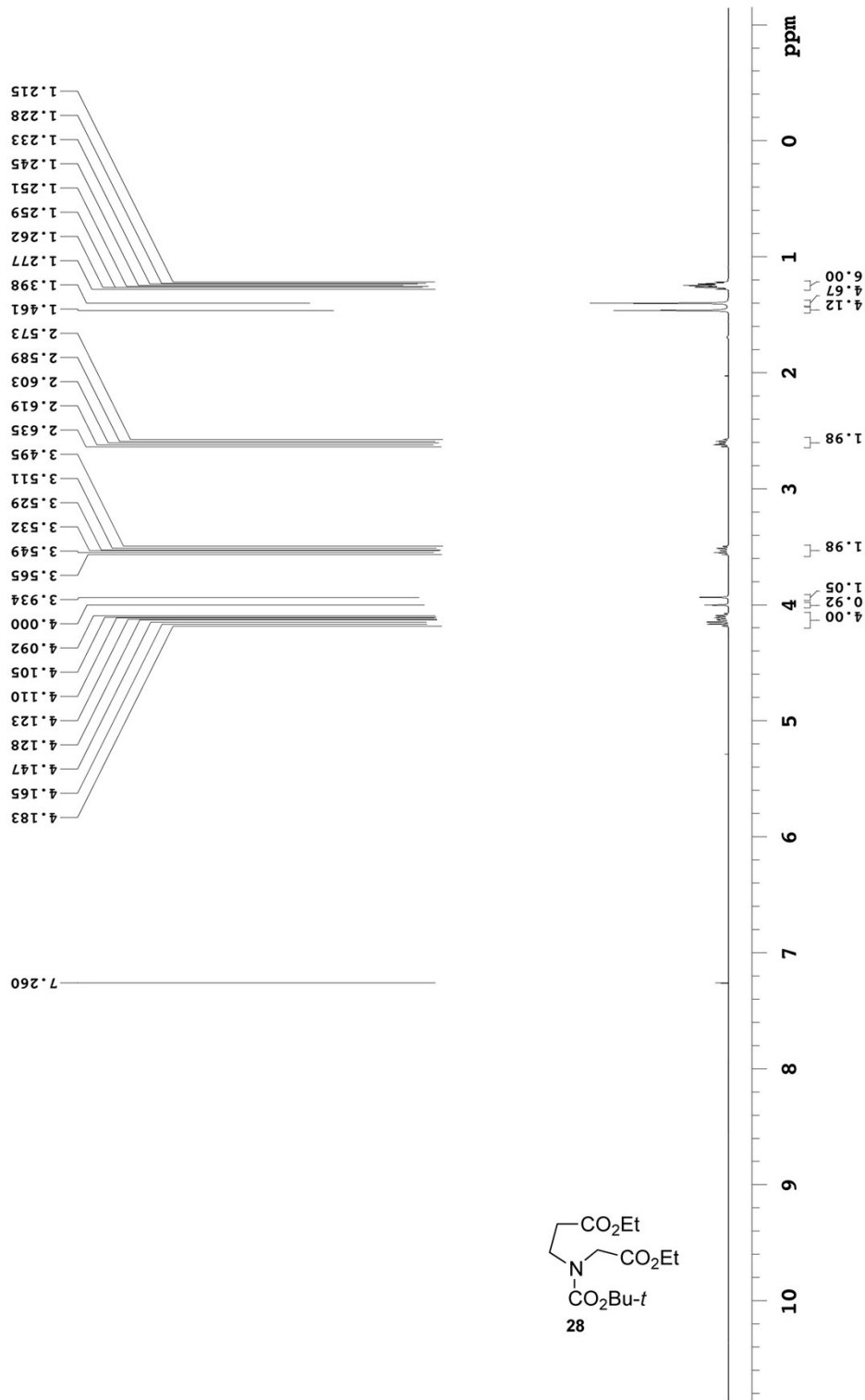
Recorded on: 1400, Jul 24 2015
Pulse Sequence: s2pul

Sweep Width(Hz): 4801.92
Digital Res. (Hz/pt): 0.07

Acquisition Time(s): 4.998
Hz per mm(Hz/mm): 20.01

Relaxation Delay(s): 0.1
Completed Scans: 16

IK-01-P47
399.794 MHz H1 1D in cdcl3 (ref. to CDC13 @ 7.26 ppm), temp 26.5 C -> actual temp = 27.0 C, autotxdtb probe





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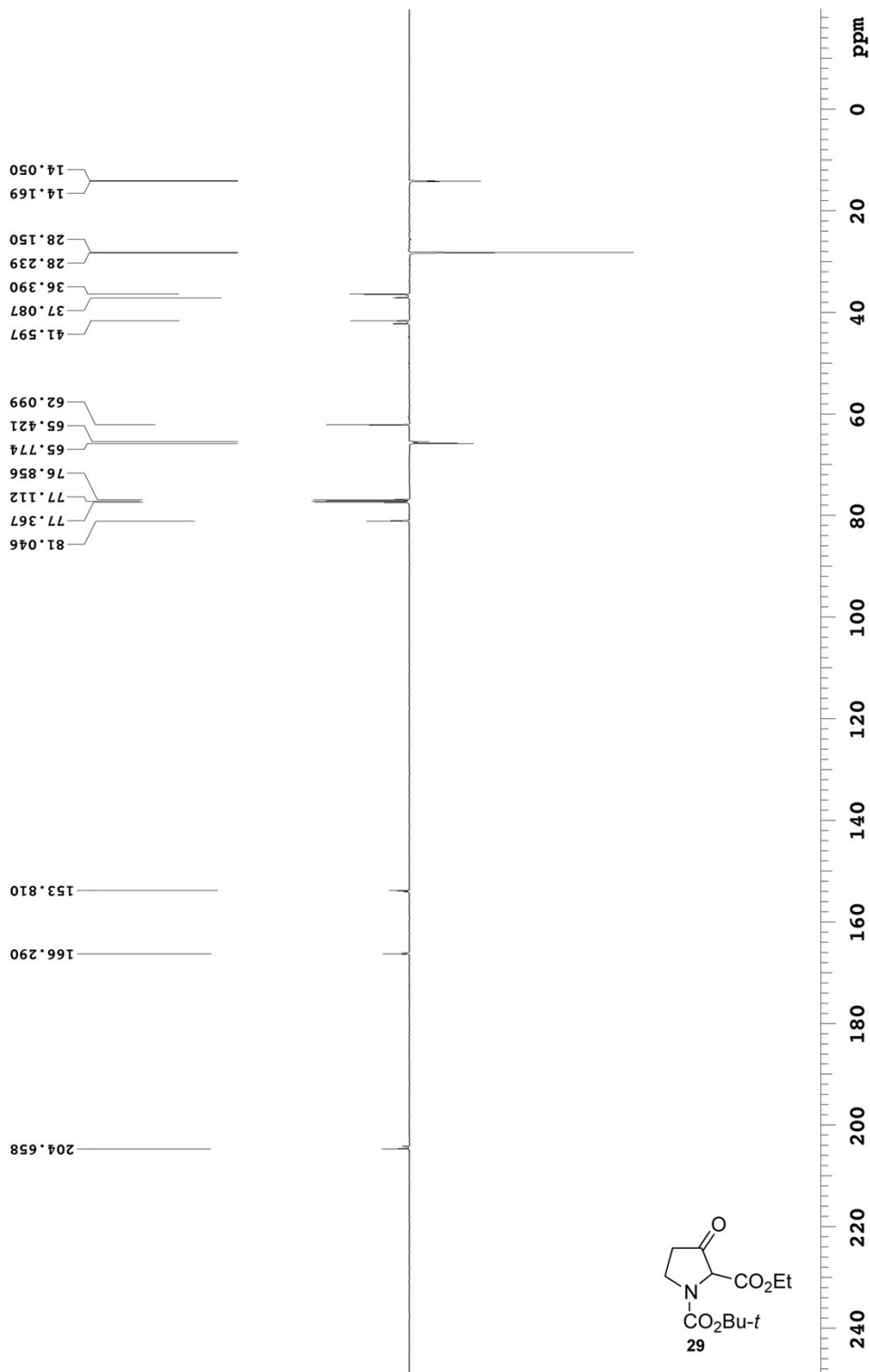
Recorded on: u500, Jul 27 2015
Pulse Sequence: APT_ad

Sweep Width(Hz): 33783.8
Digital Res (Hz/pt): 0.26

Acquisition Time(s): 2
Hz per mm(Hz/mm): 140.76

Relaxation Delay(s): 0.5
Completed Scans: 648

Kiran, IK-01-P51
125.690 MHz C13[H1] APT_ad in cdcl3 (ref. to CDCl3 @ 77.06 ppm), temp 27.7 C -> actual temp = 27.0 C, cold dual probe
C & CH2 same, CH & CH3 opposite side of solvent signal





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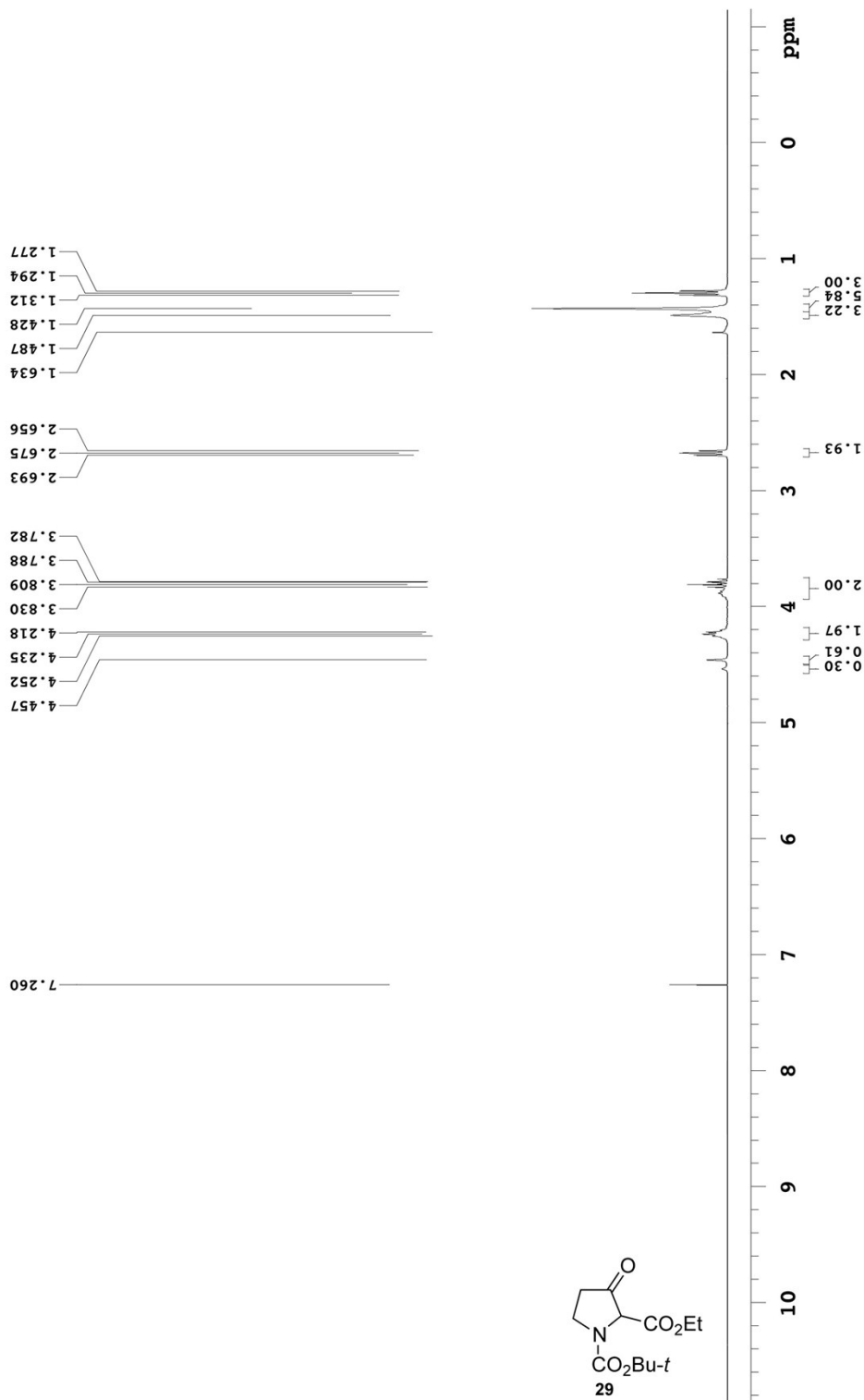
Recorded on: 1400, Jul 27 2015
Pulse Sequence: s2pul

Sweep Width(Hz): 4801.92
Digital Res (Hz/pt): 0.07

Acquisition Time(s): 4.998
Hz per mm(Hz/mm): 20.01

Relaxation Delay(s): 0.1
Completed Scans: 16

IK-01-P51
399.794 MHz H1 1D in cdcl3 (ref. to CDC13 @ 7.26 ppm), temp 26.5 C -> actual temp = 27.0 C, autotxdtb probe



File: /mnt/d600/home14/ciivenmr/nmrdata/spectra_for_shuai/rou2/2015.07.27.14_IK-01-P51_H1_1D



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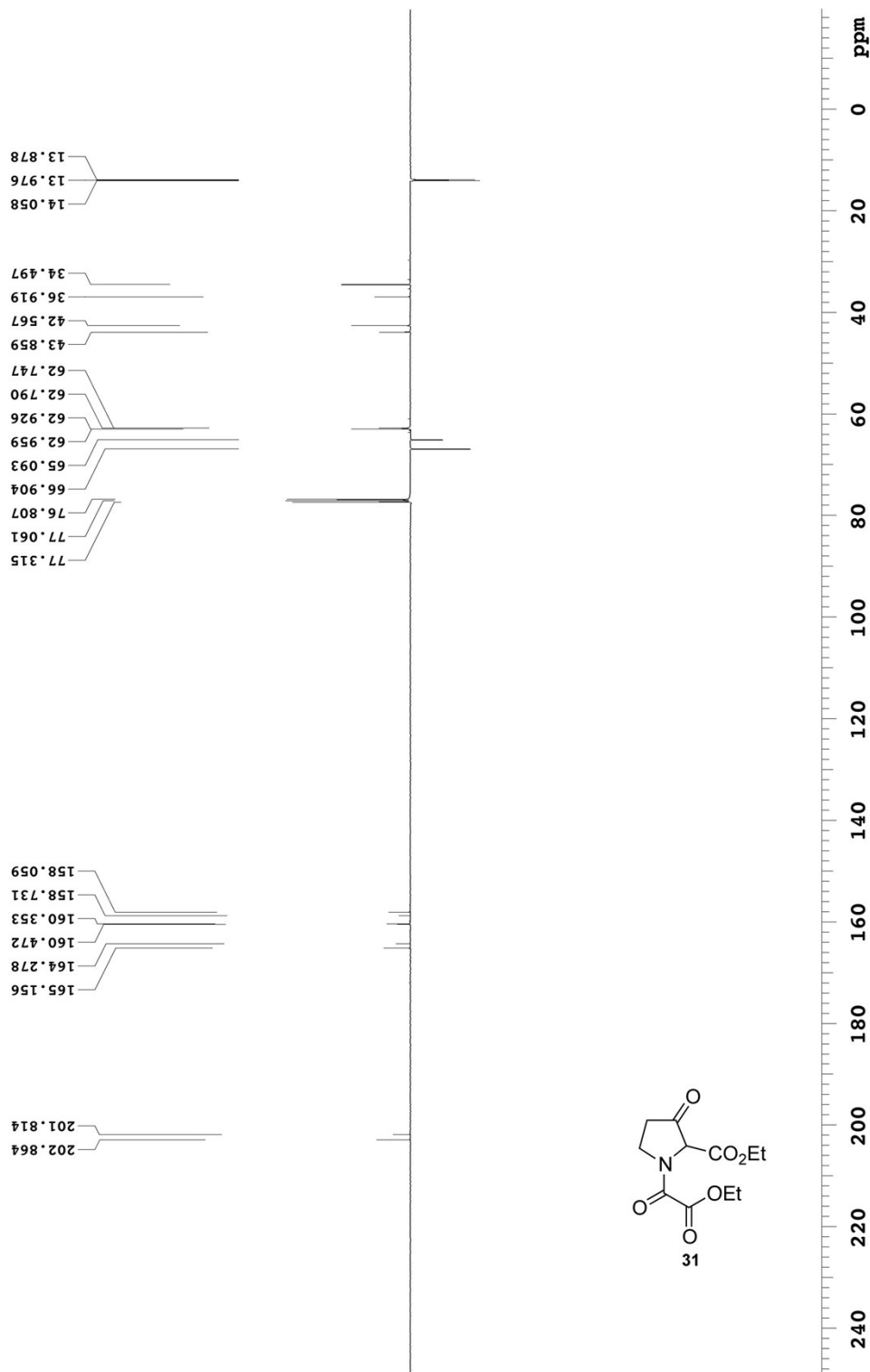
Recorded on: **u500, Aug 10 2015**
Pulse Sequence: **APT_ad**

Sweep Width(Hz): **33783.8**
Digital Res (Hz/pt): **0.26**

Acquisition Time(s): **2**
Hz per mm(Hz/mm): **140.76**

Relaxation Delay(s): **0.5**
Completed Scans: **648**

Kiran, IK-01-P83-A
125.690 MHz C13[H1] APT_ad in cdcl3 (ref. to CDCl3 @ 77.06 ppm), temp 27.7 C -> actual temp = 27.0 C, coldldual probe
C & CH2 same, CH & CH3 opposite side of solvent signal





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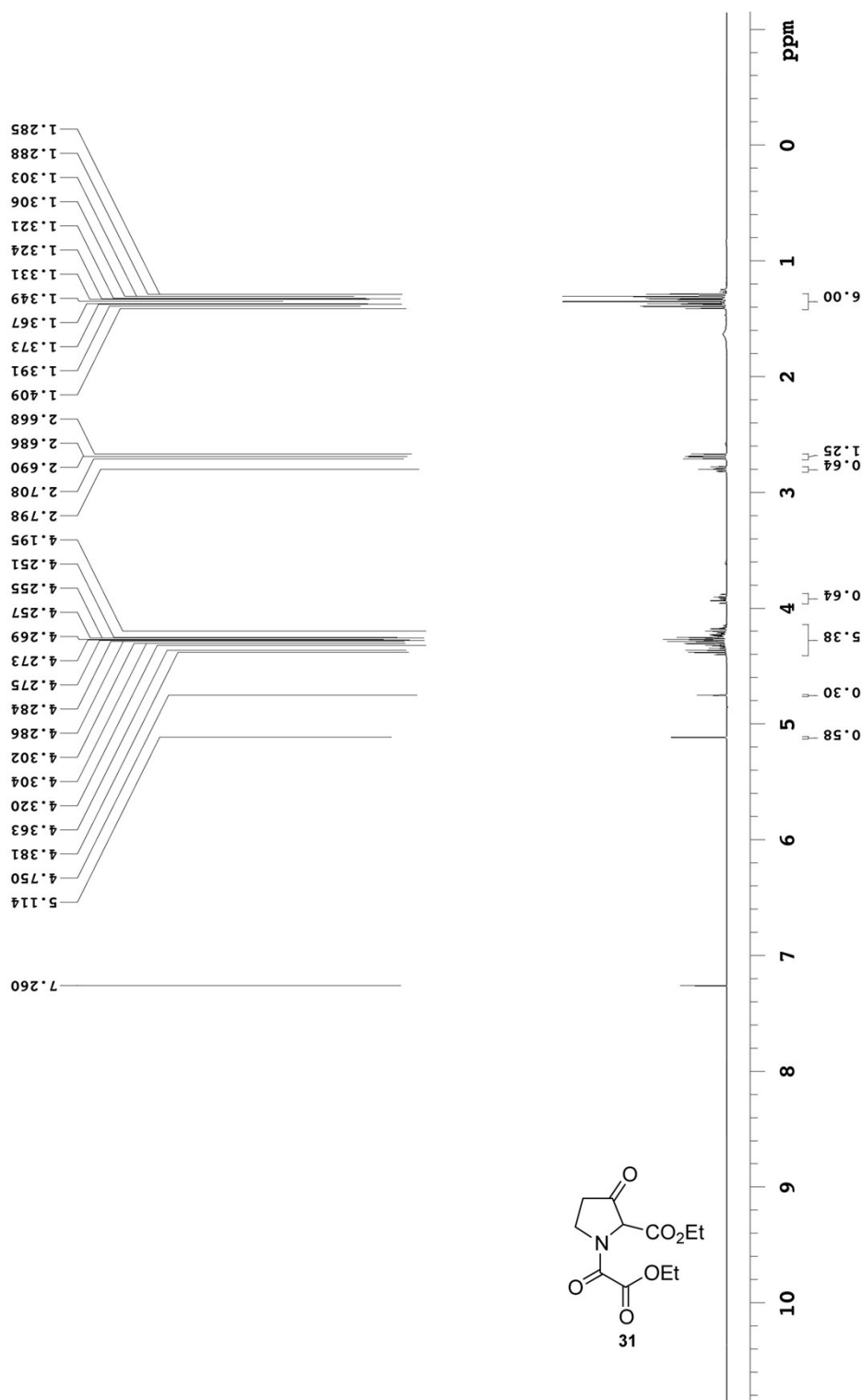
Recorded on: 1400, Aug 10 2015
Pulse Sequence: s2pul

Sweep Width(Hz): 4801.92
Digital Res (Hz/pt): 0.07

Acquisition Time(s): 4.998
Hz per mm(Hz/mm): 20.01

Relaxation Delay(s): 0.1
Completed Scans: 16

IK-01-P83-A
399.794 MHz H1 1D in cdcl3 (ref. to CDC13 @ 7.26 ppm), temp 26.5 C -> actual temp = 27.0 C, autotxdtb probe





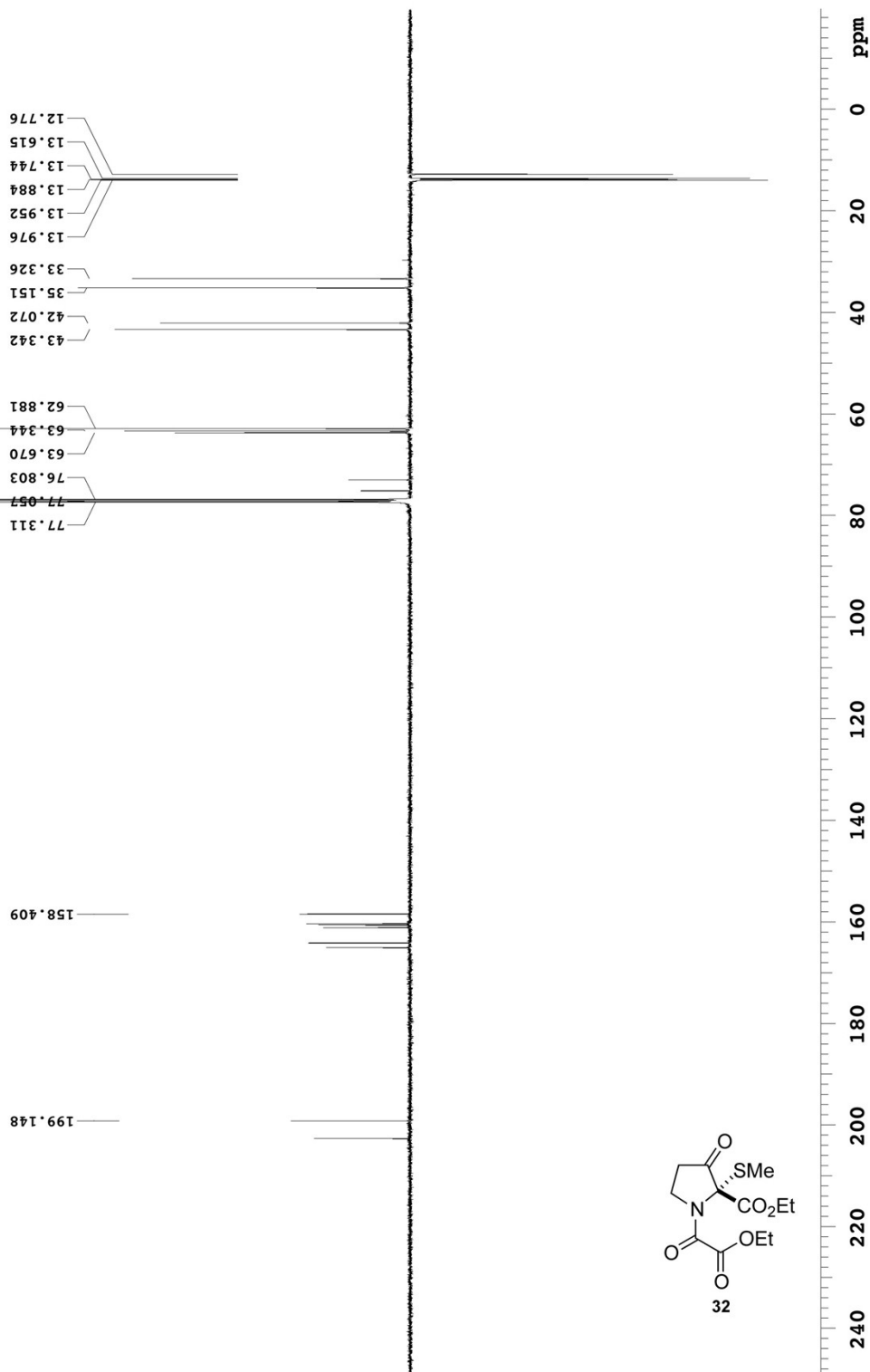
Agilent Technologies

Recorded on: u500, Sep 4 2015
Pulse Sequence: APT_ad

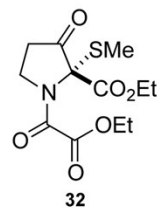
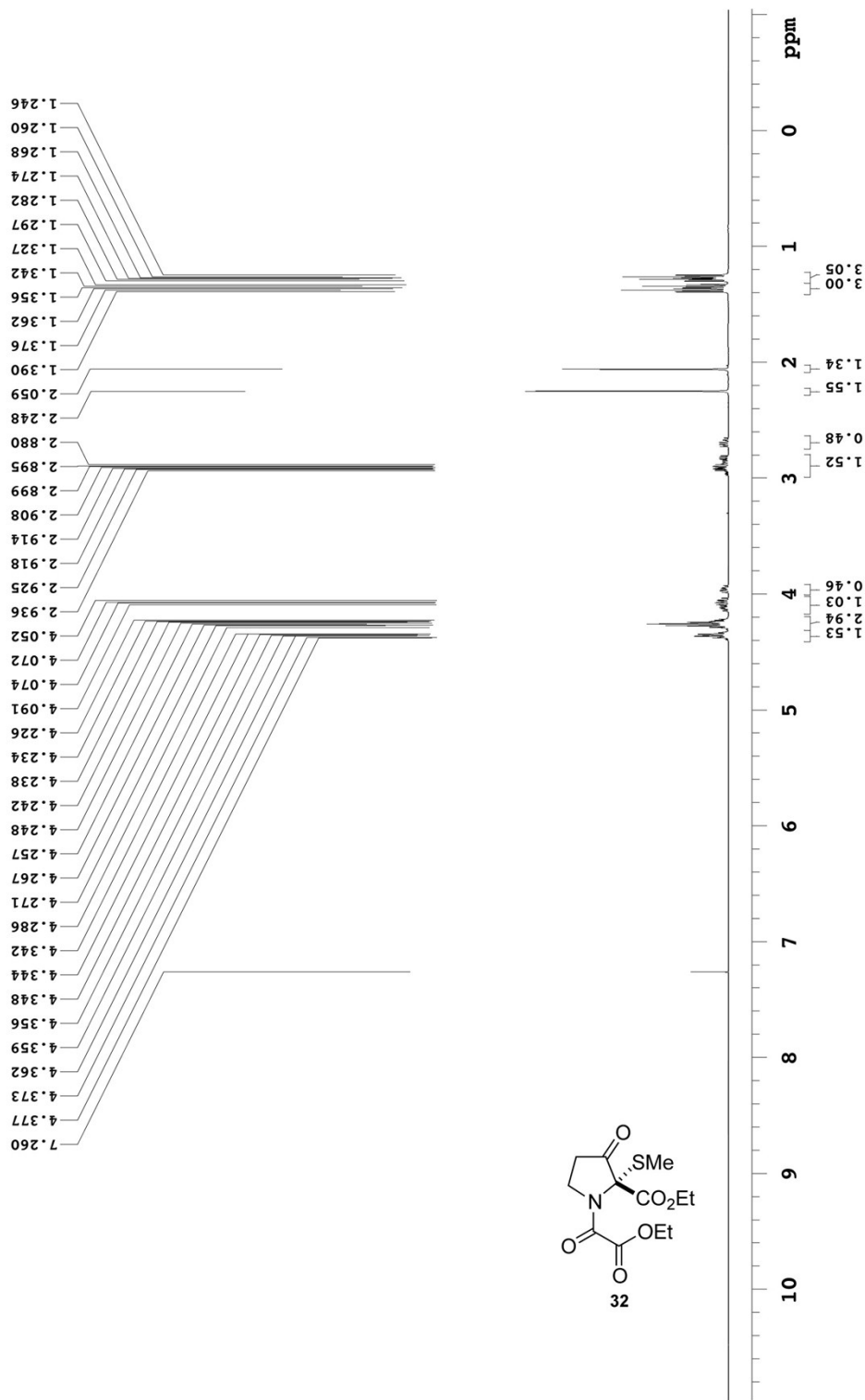
Sweep Width(Hz): 33783.8
Digital Res (Hz/pt): 0.26

Acquisition Time(s): 2
Relaxation Delay(s): 0.5
Completed Scans: 512

Kiran, JK-01-P135
125.690 MHz C13[H1] APT_ad in cdcl3 (ref. to CDCl3 @ 77.06 ppm), temp 27.7 C -> actual temp = 27.0 C, cold dual probe
C & CH2 same, CH & CH3 opposite side of solvent signal



Kiran, IK-01-P135
499.806 MHz H¹ PRESAT in cdcl₃ (ref. to CDC13 @ 7.26 ppm), temp 27.7 C -> actual temp = 27.0 C, coldludal probe





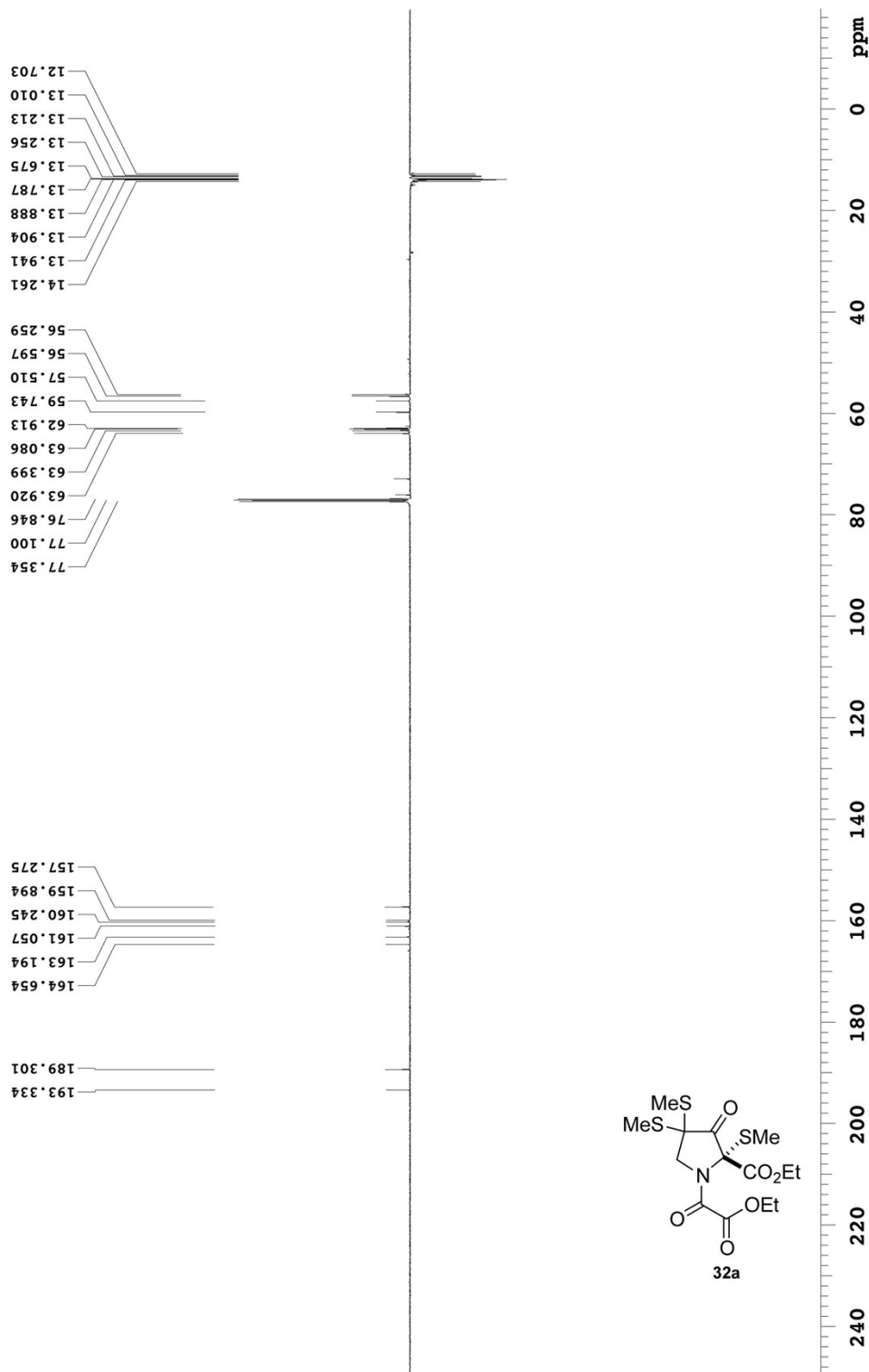
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Recorded on: u500, Sep 17 2015
Pulse Sequence: APT_ad

Sweep Width(Hz): 33783.8
Digital Res (Hz/pt): 0.26

Relaxation Delay(s): 0.5
Completed Scans: 256

Kiran, IK-01-P147A
125.690 MHz C13[H1] APT_ad in cdcl3 (ref. to CDCl3 @ 77.06 ppm), temp 27.7 C -> actual temp = 27.0 C, cold dual probe
C & CH2 same, CH & CH3 opposite side of solvent signal





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Recorded on: **u500, Sep 17 2015**
Pulse Sequence: **PRESAT**

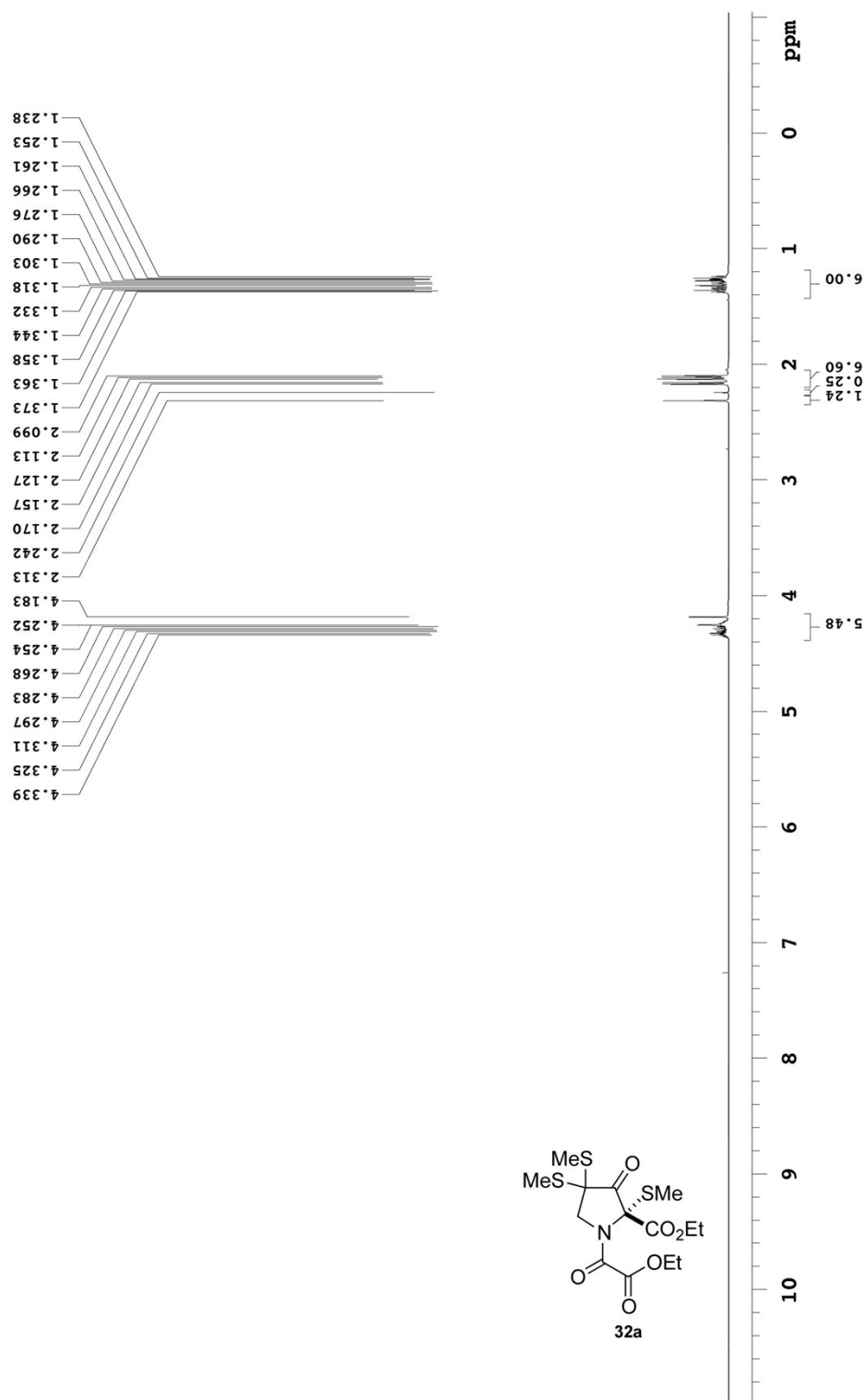
Sweep Width(Hz): **6009.62**
Digital Res. (Hz/pt): **0.18**

Acquisition Time(s): **5**
Hz per mm(Hz/mm): **25.04**

Relaxation Delay(s): **0.1**
Completed Scans: **16**

Kiran, IK-01-P147A

499.806 MHz ¹H1 PRESAT in cdcl₃ (ref. to CDCl₃ @ 7.26 ppm), temp 27.7 C -> actual temp = 27.0 C, coldlual probe





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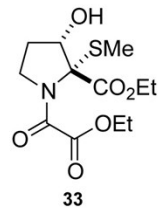
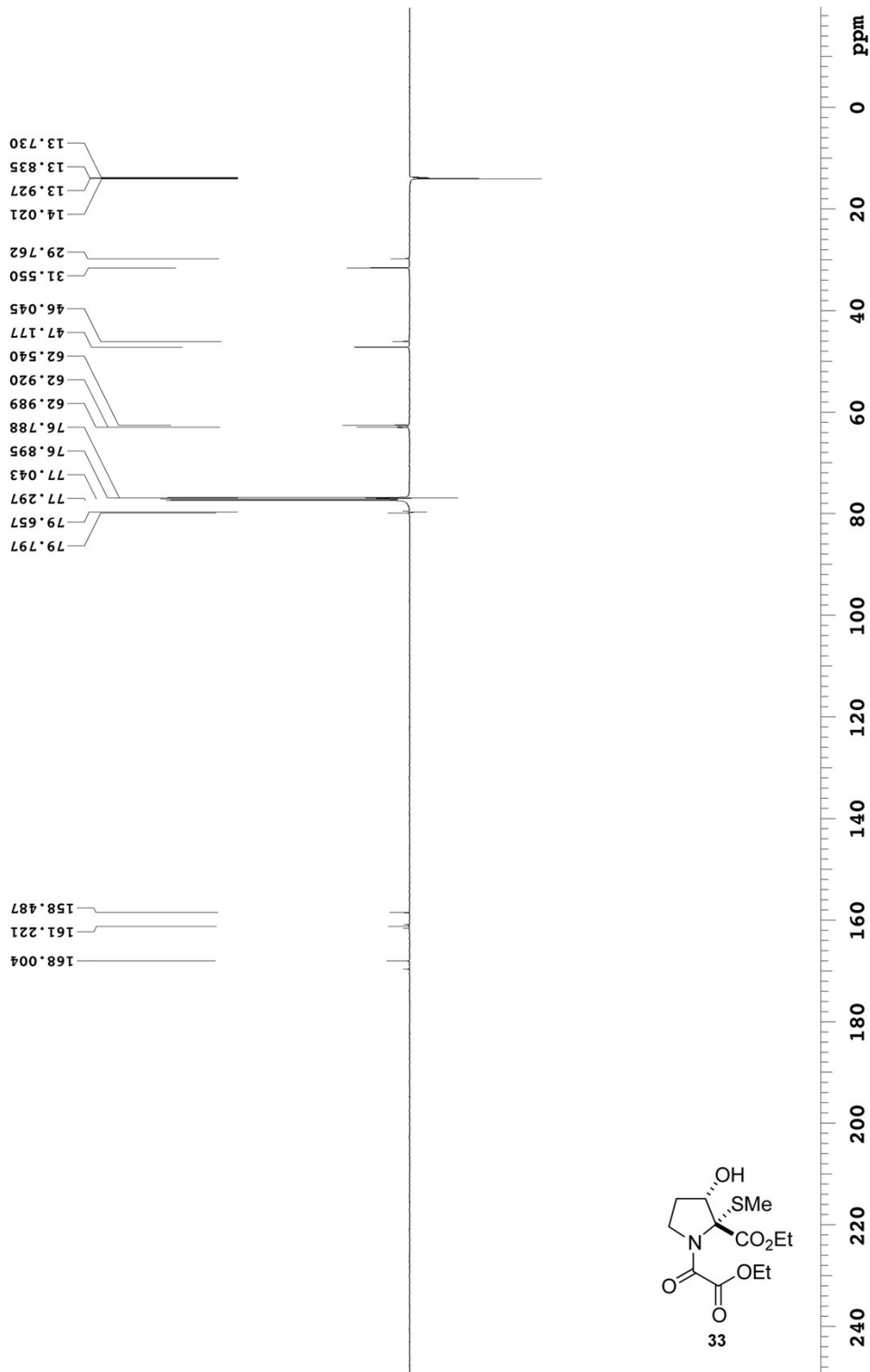
Recorded on: u500, Sep 18 2015
Pulse Sequence: APT_ad

Sweep Width(Hz): 33783.8
Digital Res (Hz/pt): 0.26

Acquisition Time(s): 2
Hz per mm(Hz/mm): 140.76

Relaxation Delay(s): 0.5
Completed Scans: 2012

Kiran, IK-01-P165
125.690 MHz C13[H1] APT_ad in cdcl3 (ref. to CDCl3 @ 77.06 ppm), temp 27.7 C -> actual temp = 27.0 C, cold dual probe
C & CH2 same, CH & CH3 opposite side of solvent signal



File: /mnt/d600/home14/ciivenmr/nmrdata/spectra_for_shuai/rou2/2015.09.18.u5_IK-01-P165_loc11_0623_C13_APT_ad



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Recorded on: **ibds, Sep 8 2015**
Pulse Sequence: **s2pul**

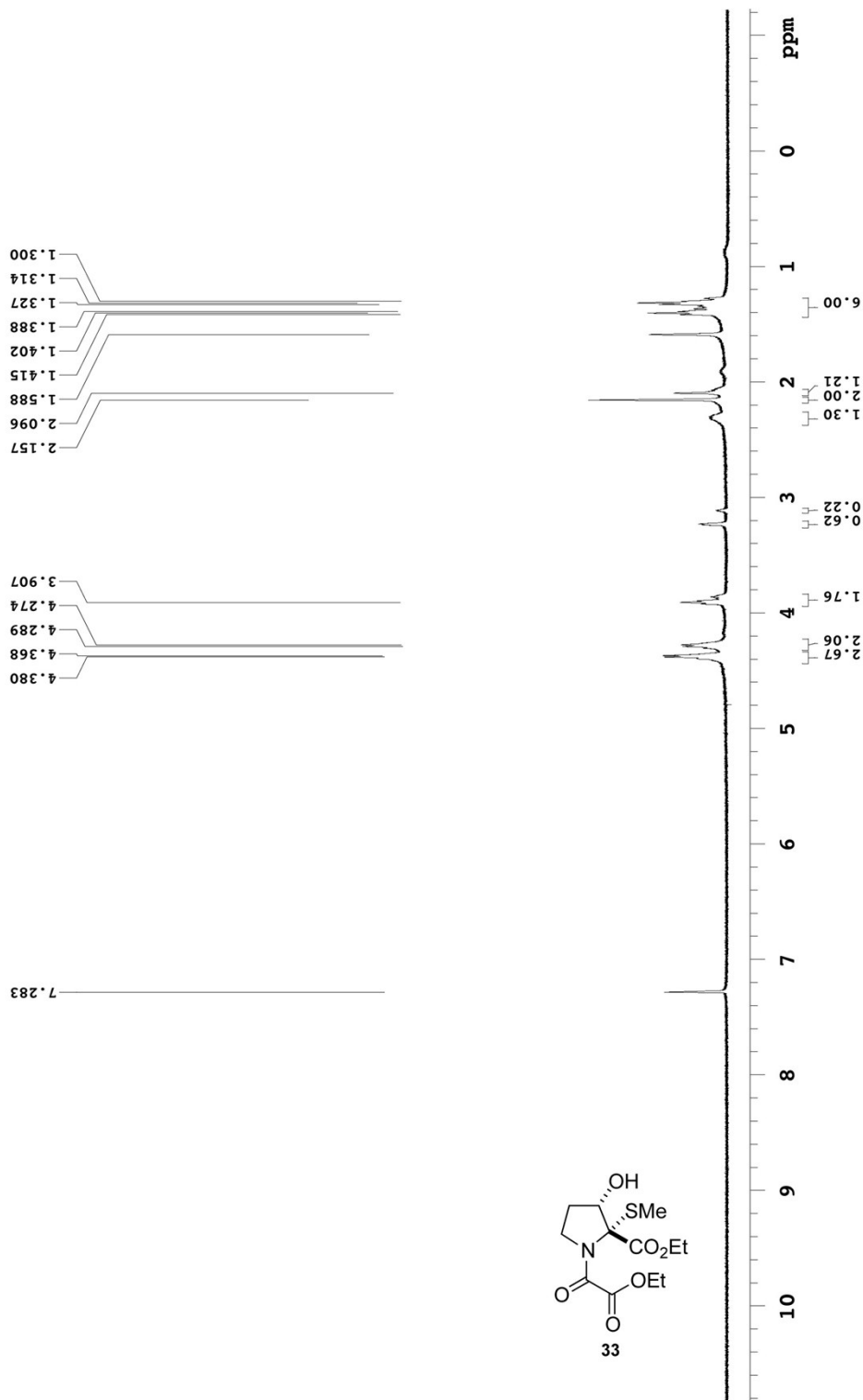
Sweep Width(Hz): **6000.6**
Digital Res. (Hz/pt): **0.09**

Acquisition Time(s): **5**
Hz per mm(Hz/mm): **25**

Relaxation Delay(s): **0.1**
Completed Scans **16**

IK-01-P143A

498.118 MHz H1 1D in cdcl3 (ref. to CDC13 @ 7.26 ppm), temp 26.4 C -> actual temp = 27.0 C, autotxdtb probe

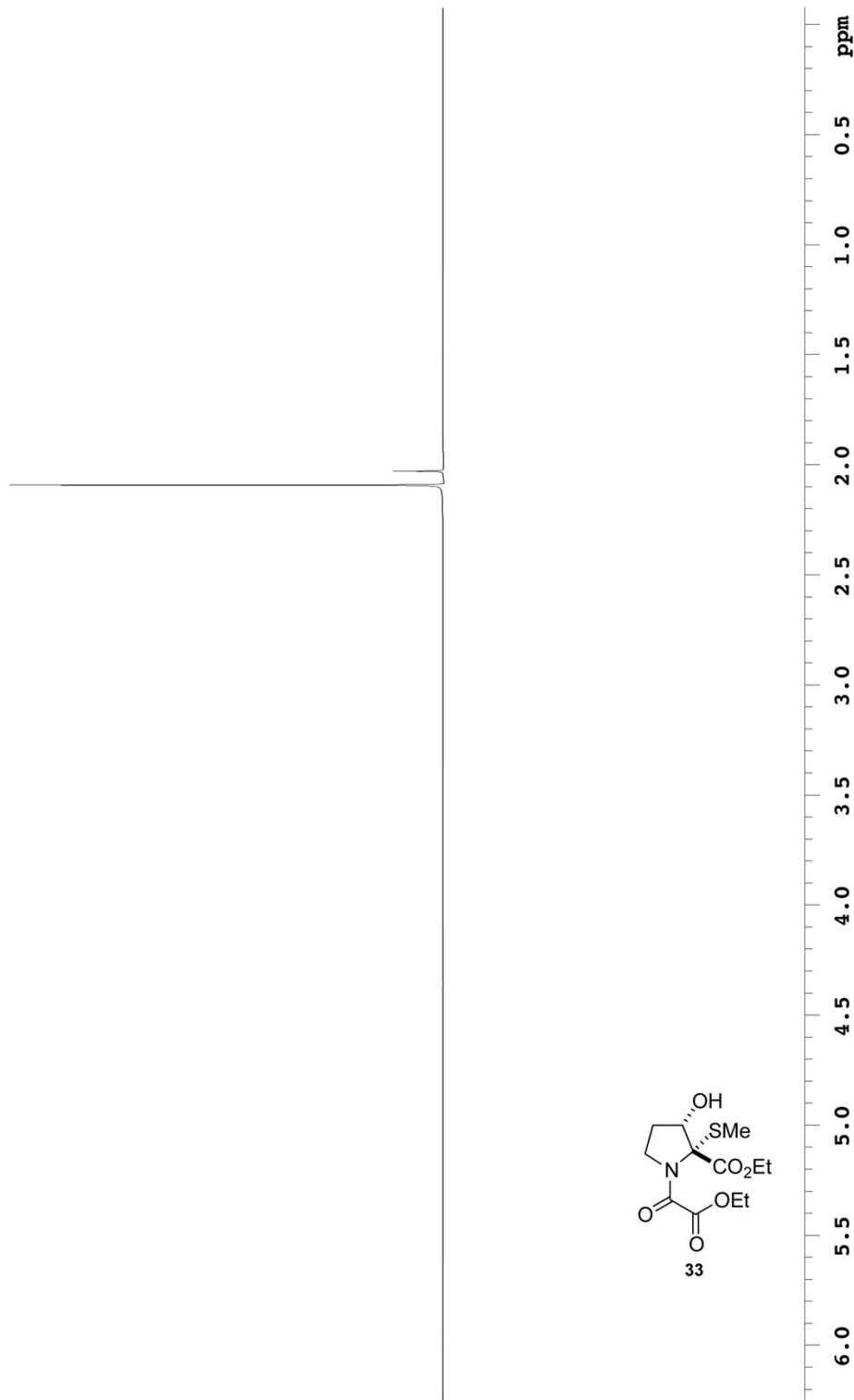




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Recorded on: ibds, Dec 4 2015	Sweep Width(Hz): 6000.6	Acquisition Time(s): 3	Relaxation Delay(s): 2
Pulse Sequence: ROESY1D	Digital Res (Hz/pt): 0.09	Hz per mm(Hz/mm): 13.14	Completed Scans: 64

498.118 MHz ¹H ROESY1D in cdcl₃ (ref. to CDC18 @ 7.26 ppm), temp 26.4 C -> actual temp = 27.0 C, autotxdb probe



File: /mnt/d600/home14/civenmr/nmrdata/spectra_for_shuai/rou2/2015.12.04.15_K02-P115U-Major-TROESY_H1_ROESY1D

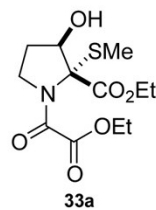
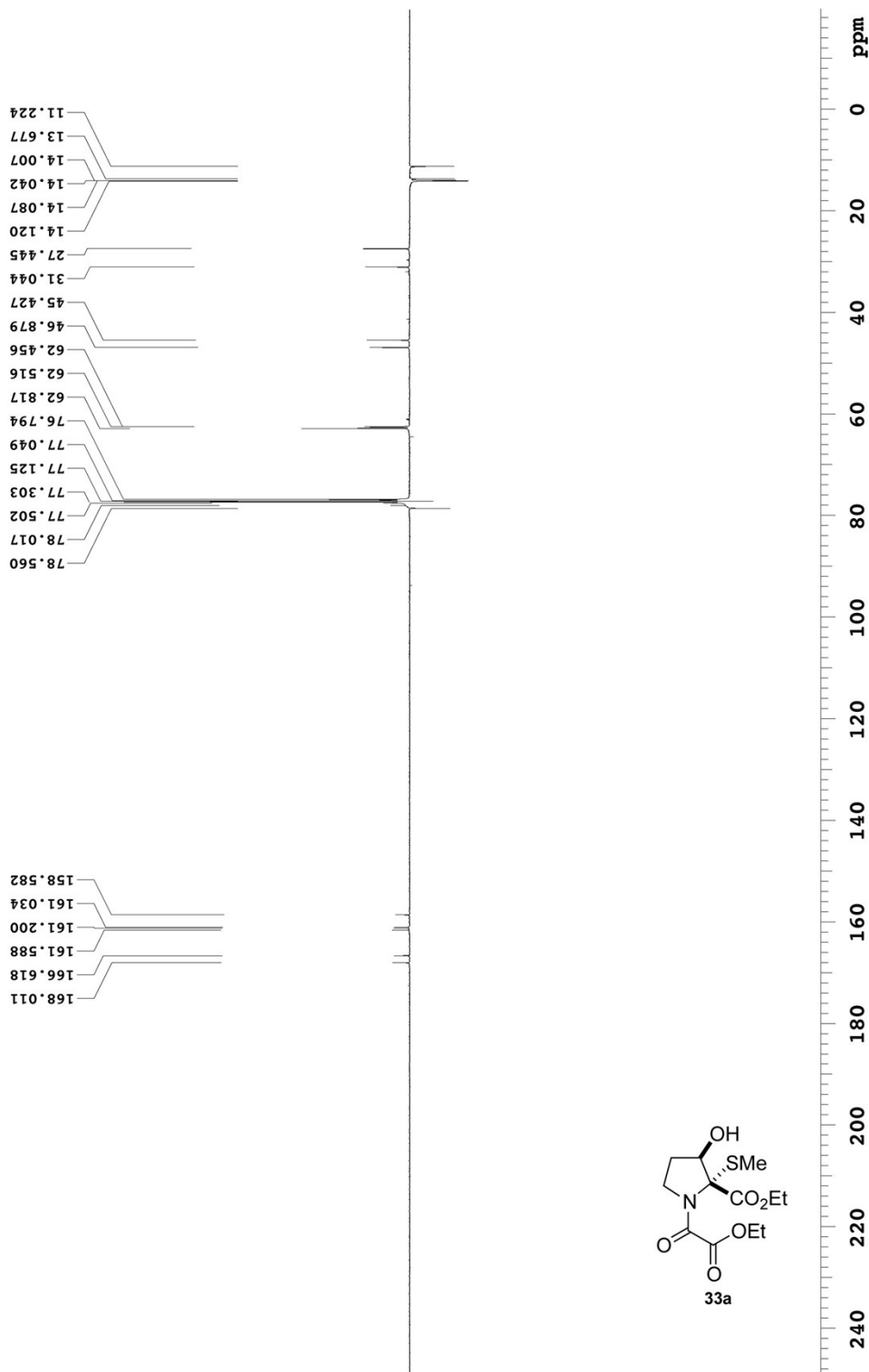


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Recorded on: u500, Sep 5 2015
Pulse Sequence: APT_ad
Sweep Width(Hz): 33783.8
Digital Res (Hz/pt): 0.26
Acquisition Time(s): 2
Hz per mm(Hz/mm): 140.76
Relaxation Delay(s): 0.5
Completed Scans: 2012

Kiran, IK-01-P143
125.690 MHz C13[H1] APT_ad in cdcl3 (ref. to CDCl3 @ 77.06 ppm), temp 27.7 C -> actual temp = 27.0 C, cold dual probe
C & CH2 same, CH & CH3 opposite side of solvent signal





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Recorded on: **u500, Sep 5 2015**
Pulse Sequence: **PRESAT**

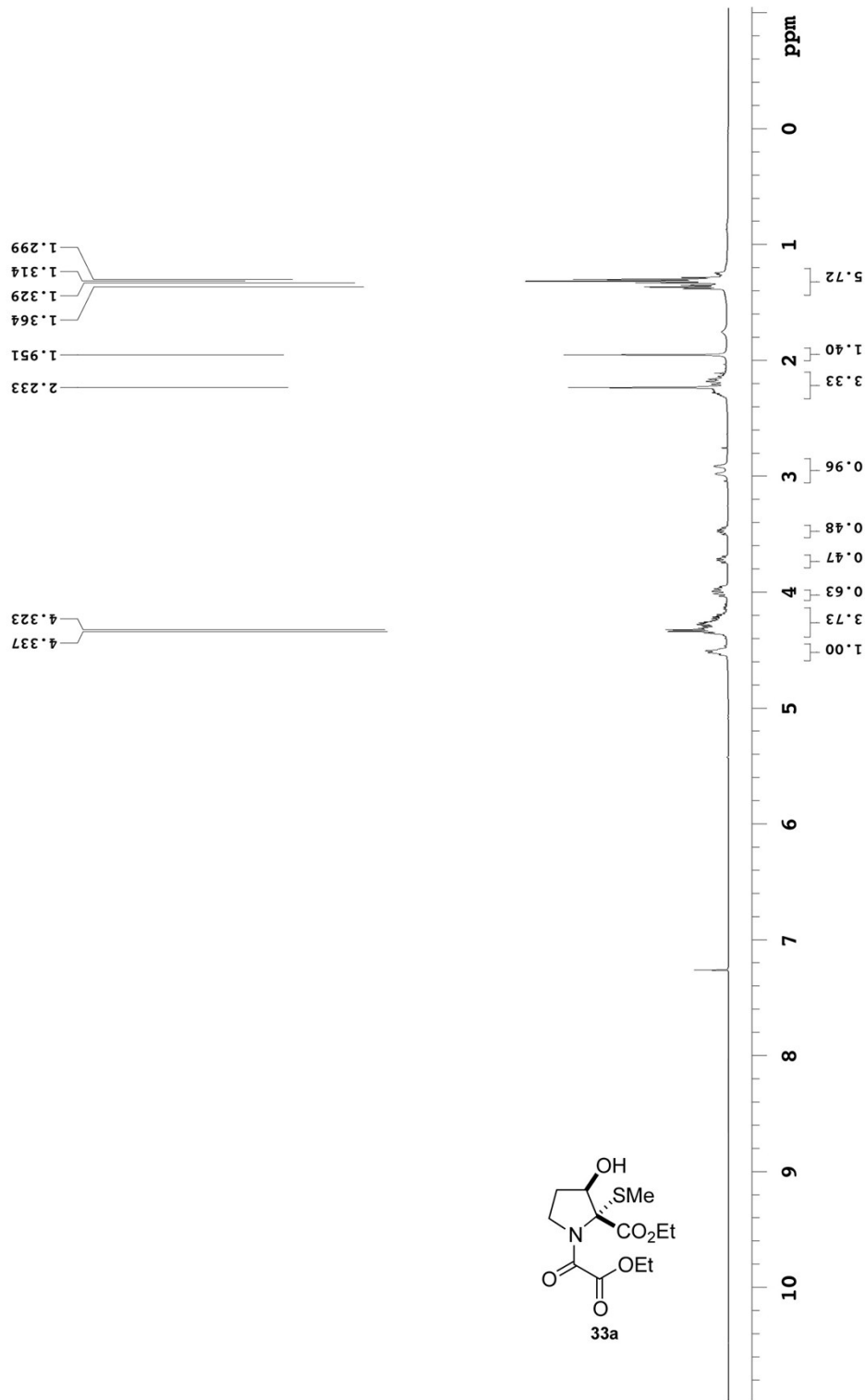
Sweep Width(Hz): **6009.62**
Digital Res. (Hz/pt): **0.18**

Acquisition Time(s): **5**
Hz per mm(Hz/mm): **25.04**

Relaxation Delay(s): **0.1**
Completed Scans **32**

Kiran, IK-01-P143

499.806 MHz ¹H PRESAT in cdcl₃ (ref. to CDCl₃ @ 7.26 ppm), temp 27.7 C -> actual temp = 27.0 C, coldludal probe



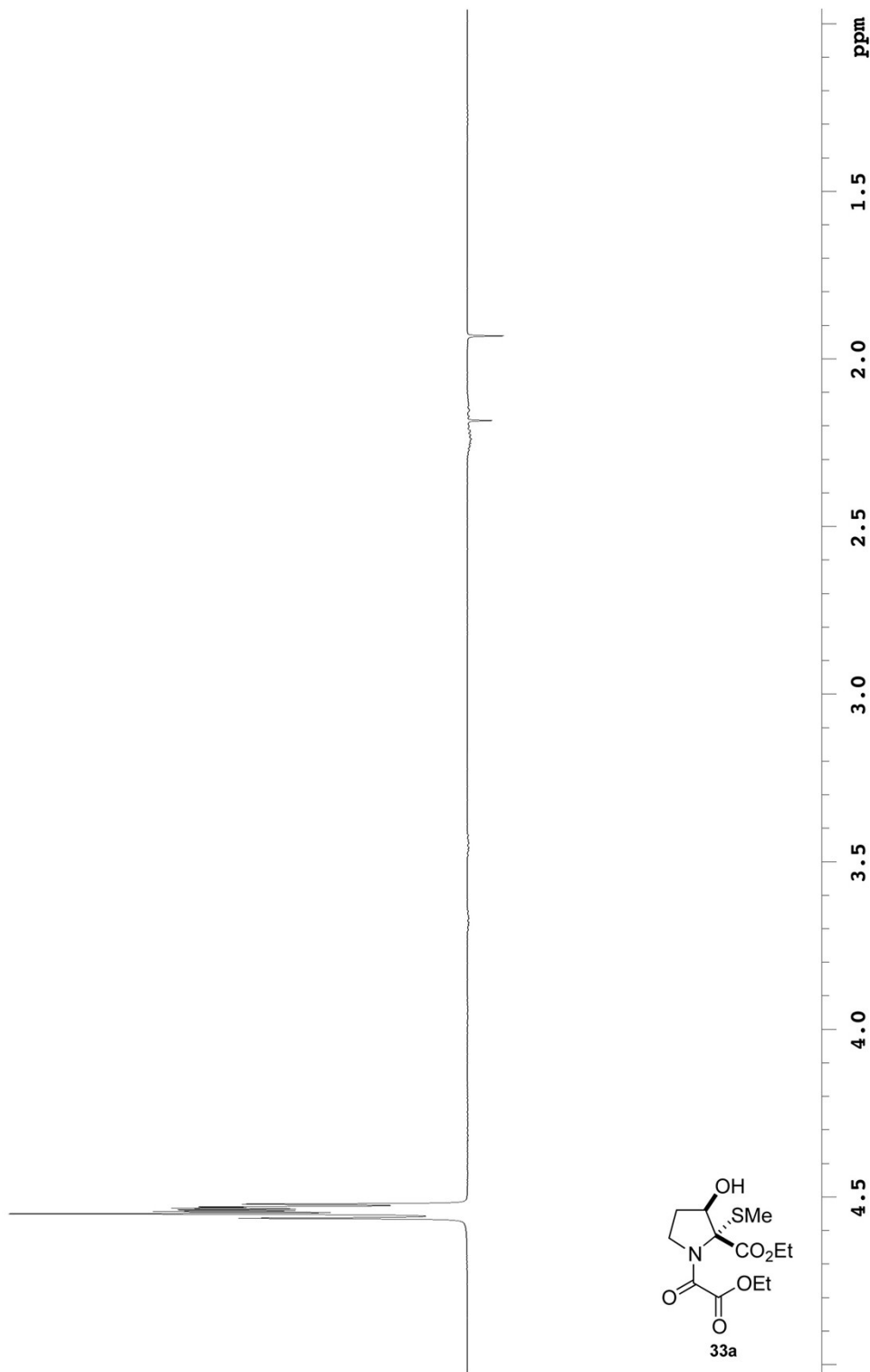
File: /mnt/d500/home14/ciivenmr/nmrdata/spectra_for_shuai/rou2/2015.09.05.u5_IK-01-P143_loc12_21.44_H1_1D



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Recorded on:	ibds, Dec 4 2015	Sweep Width(Hz):	6000.6	Acquisition Time(s):	3	Relaxation Delay(s):	2
Pulse Sequence:	ROESY1D	Digital Res. (Hz/pt):	0.09	Hz per mm(Hz/mm):	8.45	Completed Scans	64

IK-02-P115L-Minor-TROESY
498.118 MHz ¹H ROESY1D in cdcl₃ (ref. to CDCl₃ @ 7.26 ppm), temp 26.4 C -> actual temp = 27.0 C, autotxdb probe



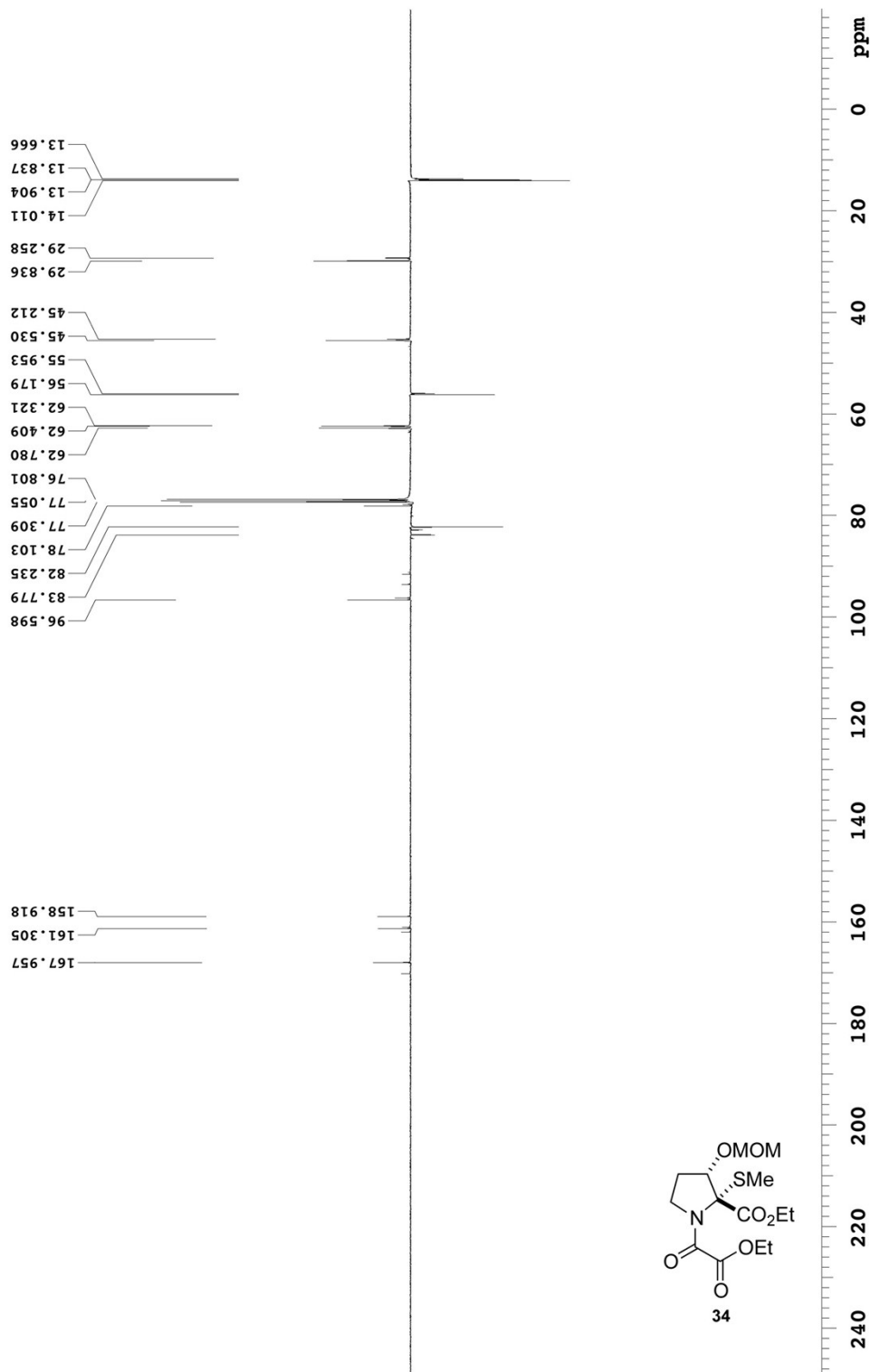
File: /mnt/d600/home14/ciivenmr/nmrdata/spectra_for_shuai/rou2/2015.12.04.15_IK-02-P115L-Minor-TROESY-¹H1_ROESY1D



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Recorded on: u500, Dec 1 2015	Sweep Width(Hz): 33783.8	Acquisition Time(s): 2	Relaxation Delay(s): 0.5
Pulse Sequence: APT_ad	Digital Res (Hz/pt): 0.26	Hz per mm(Hz/mm): 140.76	Completed Scans: 648

Kiran, JK-02-P117
125.690 MHz C13[H1] APT_ad in cdcl3 (ref. to CDCl3 @ 77.06 ppm), temp 27.7 C -> actual temp = 27.0 C, coldldual probe
C & CH2 same, CH & CH3 opposite side of solvent signal



File: /mnt/d600/home14/civenmr/nmrdata/spectra_for_shuai/rou2/2015.12.01.u5_JK-02-P117_loc10_15.16_C13_APT_ad

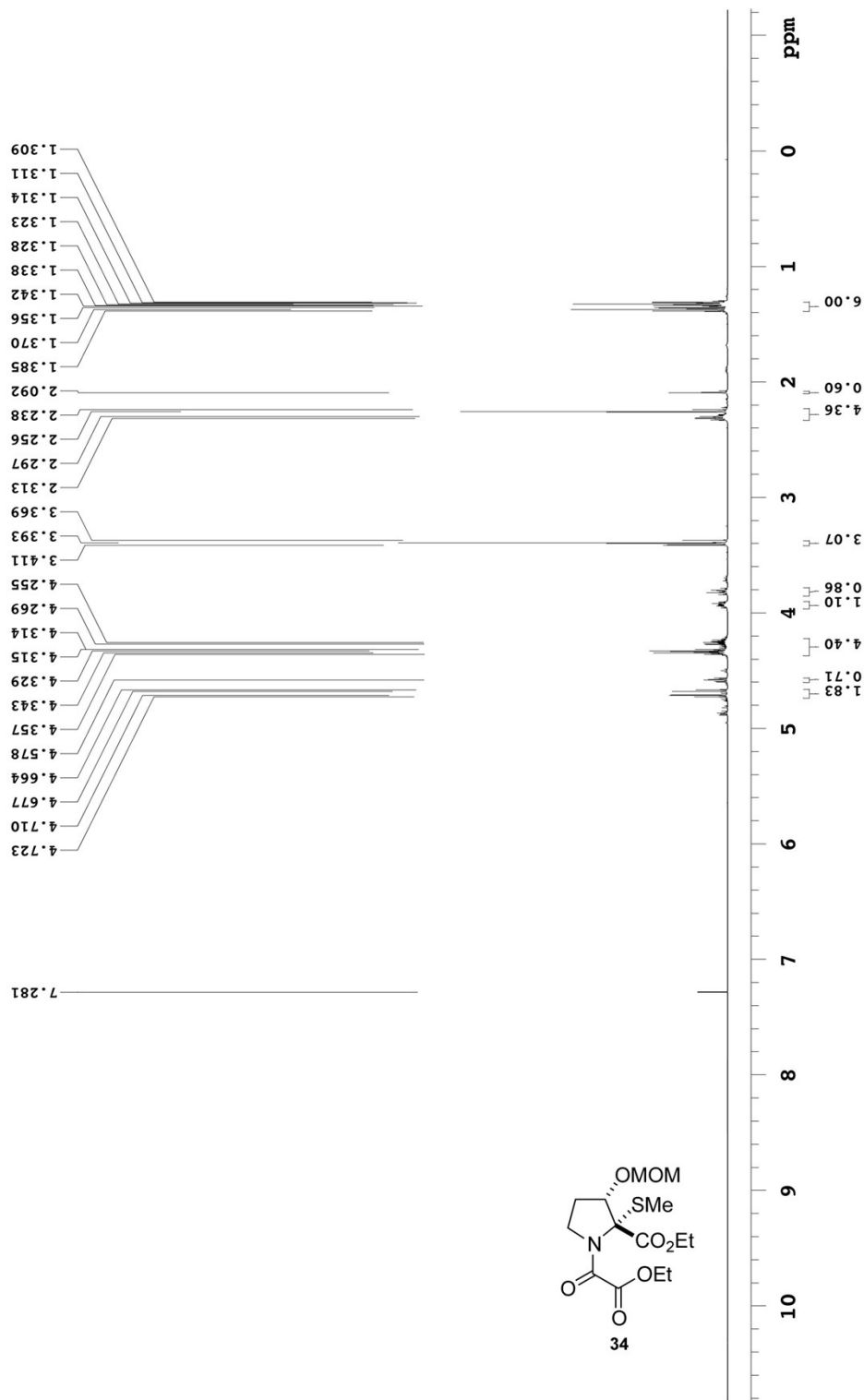


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Recorded on: **ibds, Dec 1 2015** Sweep Width(Hz): **6000.6** Acquisition Time(s): **5** Relaxation Delay(s): **0.1**
Pulse Sequence: **s2pul** Digital Res (Hz/pt): **0.09** Hz per mm(Hz/mm): **25** Completed Scans: **16**

lk-02-P117
498.118 MHz H1 1D in cdcl3 (ref. to CDC13 @ 7.26 ppm), temp 26.4 C -> actual temp = 27.0 C, autotxdtb probe





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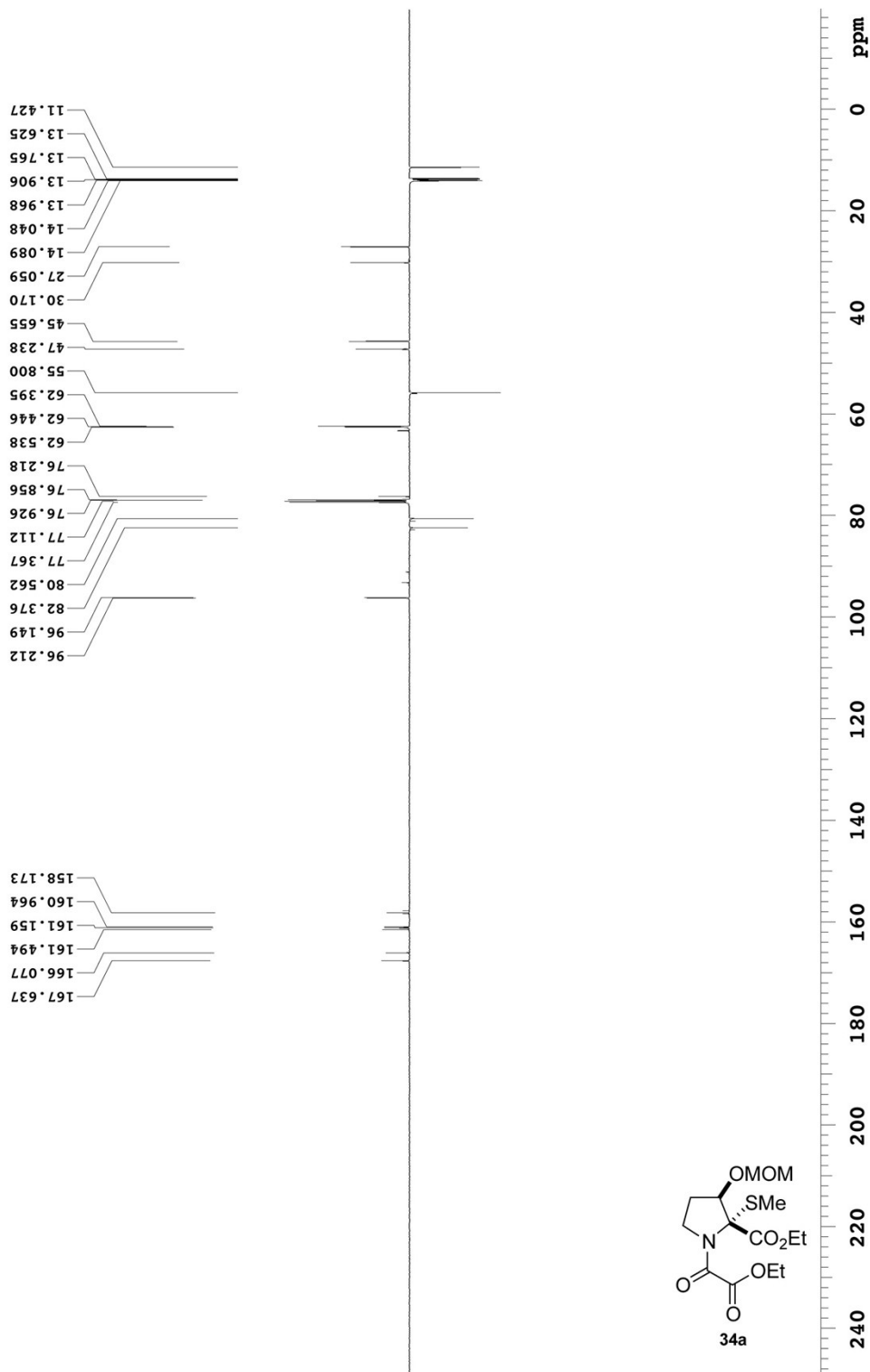
Recorded on: u500, Dec 8 2015
Pulse Sequence: APT_ad

Sweep Width(Hz): 33783.8
Digital Res (Hz/pt): 0.26

Acquisition Time(s): 2
Hz per mm(Hz/mm): 140.76

Relaxation Delay(s): 0.5
Completed Scans: 648

Kiran, IK-02-P137
125.690 MHz C13[H1] APT_ad in cdcl3 (ref. to CDCl3 @ 77.06 ppm), temp 27.7 C -> actual temp = 27.0 C, coldlual probe
C & CH2 same, CH & CH3 opposite side of solvent signal





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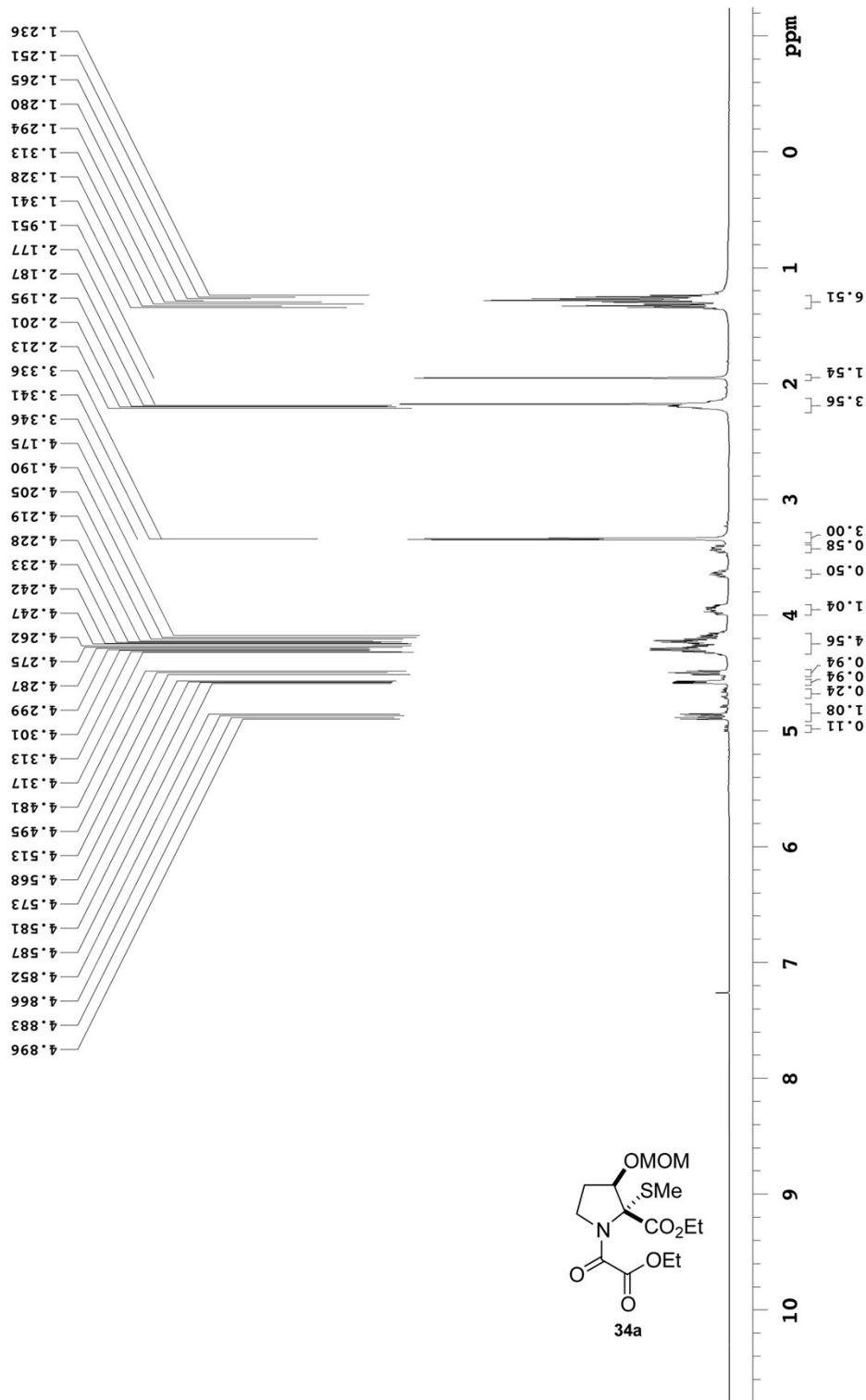
Recorded on: **ibds, Dec 8 2015**
Pulse Sequence: **s2pul**

Sweep Width(Hz): **6000.6**
Digital Res (Hz/pt): **0.09**

Acquisition Time(s): **5**
Hz per mm(Hz/mm): **25**

Relaxation Delay(s): **0.1**
Completed Scans **16**

IK-02-P137
498.118 MHz H1 1D in cdcl3 (ref. to CDC13 @ 7.26 ppm), temp 26.4 C -> actual temp = 27.0 C, autotxdtb probe



File: /mnt/d600/home14/ciivenmr/nmrdata/spectra_for_shuai/rou2/2015.12.08.15_IK-02-P137_H1_1D



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Recorded on: **mr400, Feb 8 2016**
Pulse Sequence: **s2pul**

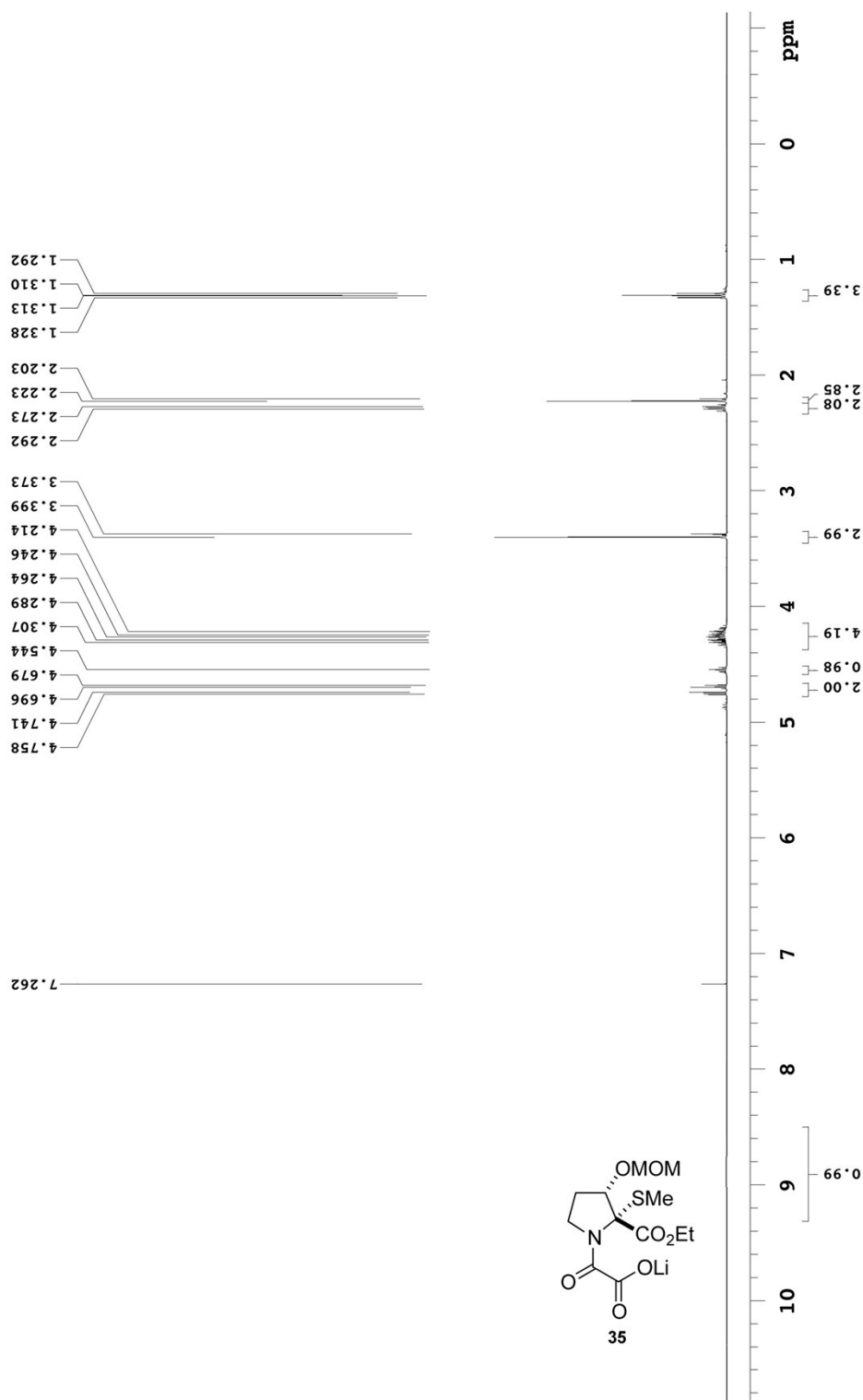
Sweep Width(Hz): **4807.69**
Digital Res (Hz/pt): **0.07**

Acquisition Time(s): **5**
Hz per mm(Hz/mm): **20.03**

Relaxation Delay(s): **0.1**
Completed Scans: **6**

ADS BK5 PAGE95

399.984 MHz H1 1D in cdcl3 (ref. to CDC13 @ 7.26 ppm), temp 25.9 C -> actual temp = 27.0 C, onenmr probe





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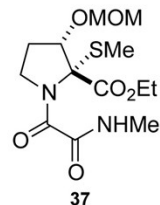
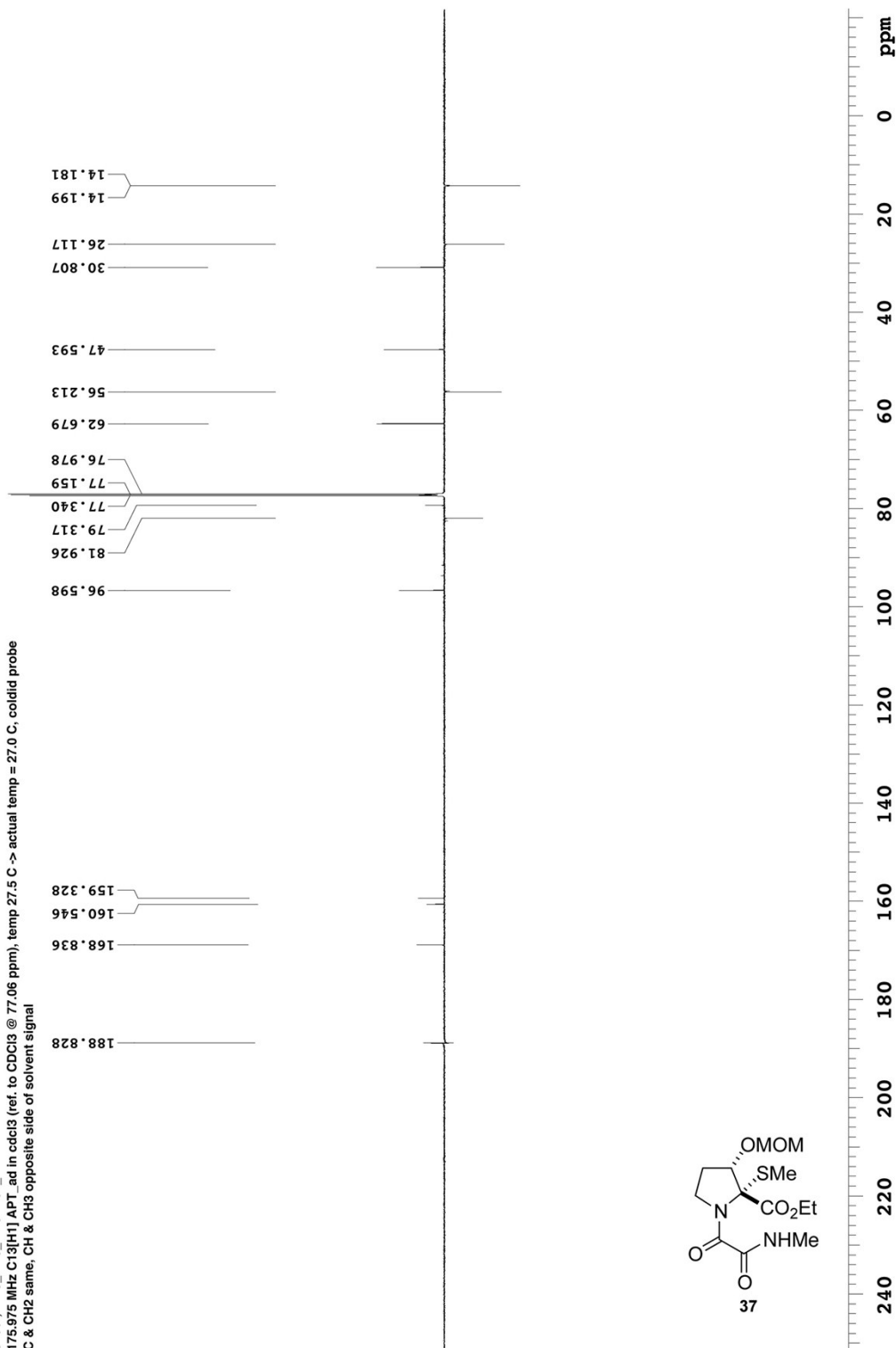
Recorded on: **V700, Mar 12 2016**
 Pulse Sequence: **APT_ad**

Sweep Width(Hz): **48076.9**
 Digital Res (Hz/pt): **0.37**

Acquisition Time(s): **2**
 Hz per mm(Hz/mm): **200.32**

Relaxation Delay(s): **0.5**
 Completed Scans: **2692**

shuai, ADS_BKS_PAGE201_Fr1
 175.975 MHz C13[H1] APT_ad in cdcl3 (ref. to CDCl3 @ 77.06 ppm), temp 27.5 C -> actual temp = 27.0 C, coldid probe
 C & CH2 same, CH & CH3 opposite side of solvent signal





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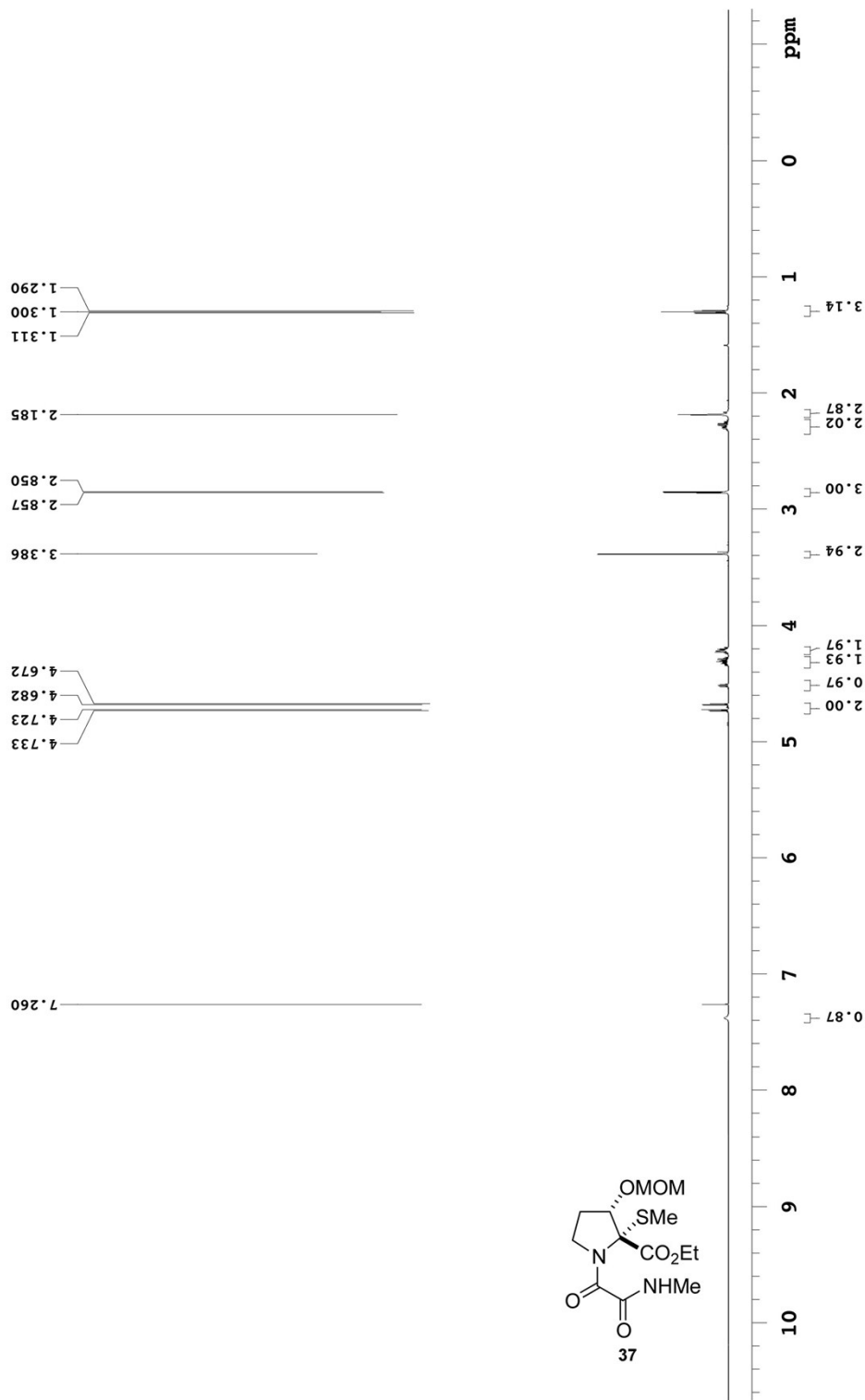
Recorded on: **V700, Mar 12 2016**
Pulse Sequence: **PRESAT**

Sweep Width(Hz): **8389.26**
Digital Res (Hz/pt): **0.13**

Acquisition Time(s): **5**
Hz per mm(Hz/mm): **34.95**

Relaxation Delay(s): **0.1**
Completed Scans: **16**

shuai, ADS_BK5_PAGE201_F1
699.762 MHz ¹H1 PRESAT in cdcl3 (ref. to CDCl3 @ 7.26 ppm), temp 27.5 C -> actual temp = 27.0 C, coldid probe





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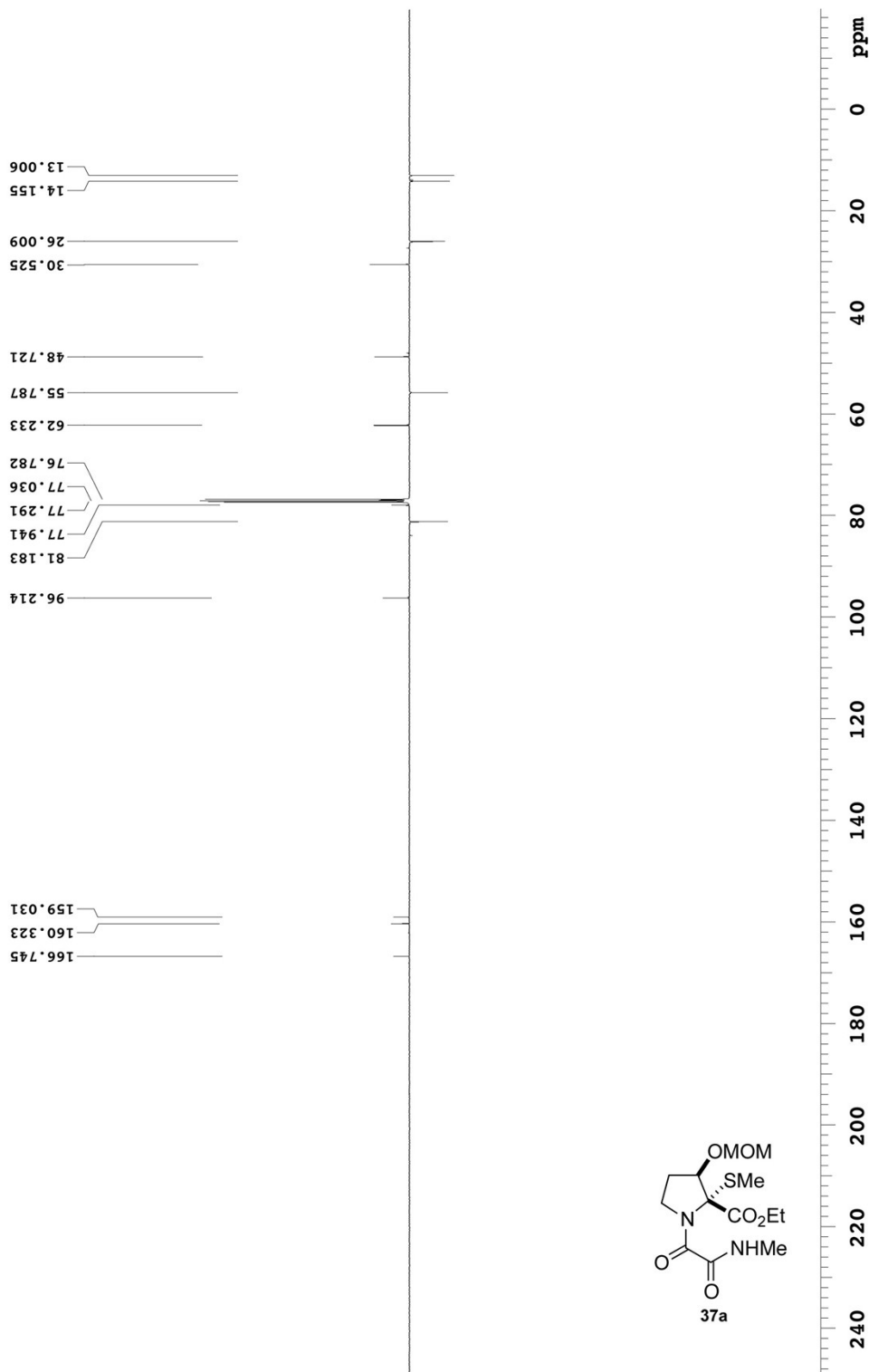
Recorded on: u500, Feb 25 2016
Pulse Sequence: APT_ad

Sweep Width(Hz): 33783.8
Digital Res (Hz/pt): 0.26

Acquisition Time(s): 2
Hz per mm(Hz/mm): 140.76

Relaxation Delay(s): 0.5
Completed Scans: 2012

shuai, ADS_BK5_PAGE149
125.690 MHz C13[1H] APT_ad in cdcl3 (ref. to CDCl3 @ 77.06 ppm), temp 27.7 C -> actual temp = 27.0 C, coldddual probe
C & CH2 same, CH & CH3 opposite side of solvent signal





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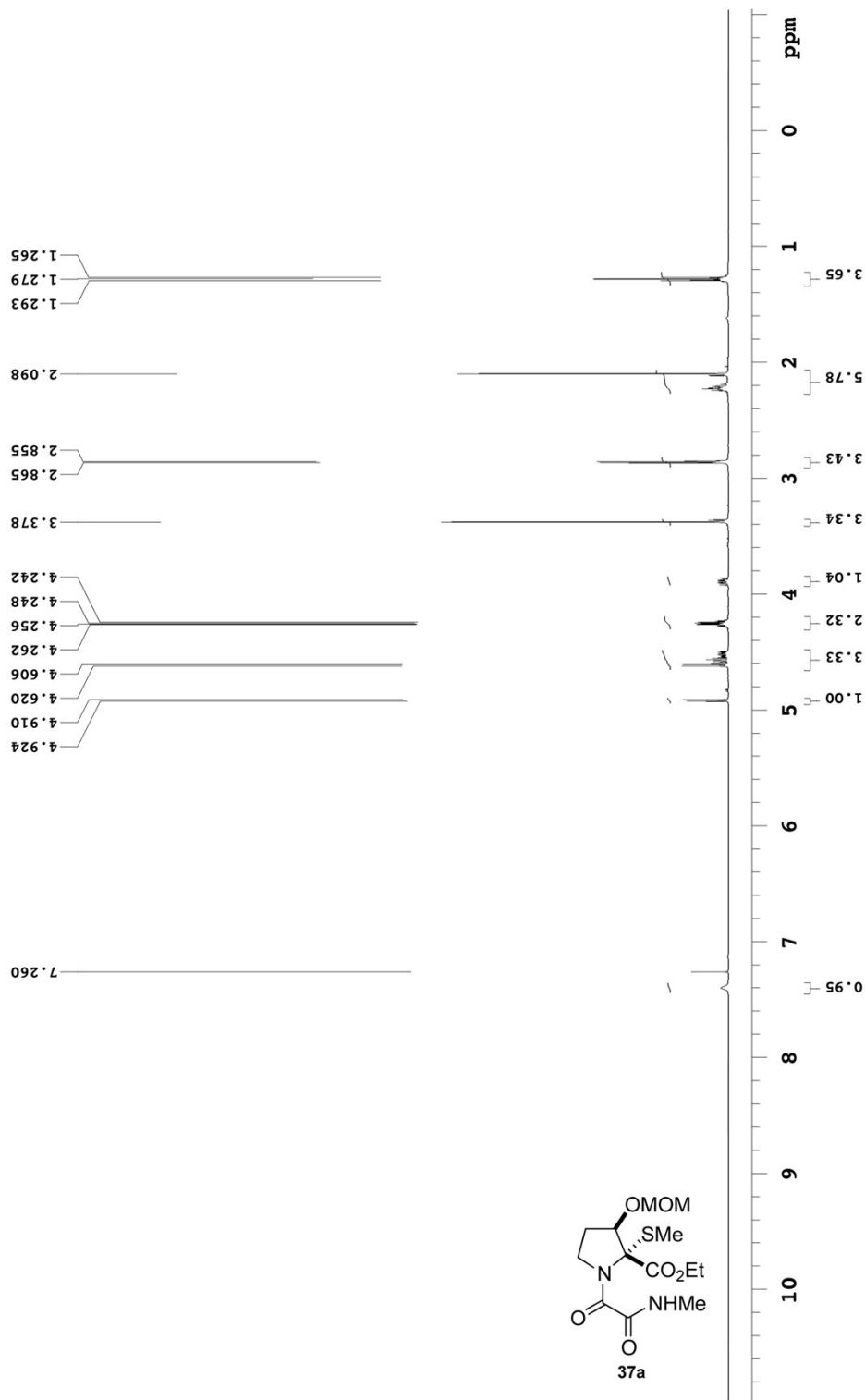
Recorded on: u500, Feb 25 2016
Pulse Sequence: PRESAT

Sweep Width(Hz): 6009.62
Digital Res. (Hz/pt): 0.18

Acquisition Time(s): 5
Hz per mm(Hz/mm): 25.04

Relaxation Delay(s): 0.1
Completed Scans: 16

shuai, ADS_BK5_PAGE149
499.806 MHz HT PRESAT in cdcl3 (ref. to CDCl3 @ 7.26 ppm), temp 27.7 C -> actual temp = 27.0 C, coldlual probe





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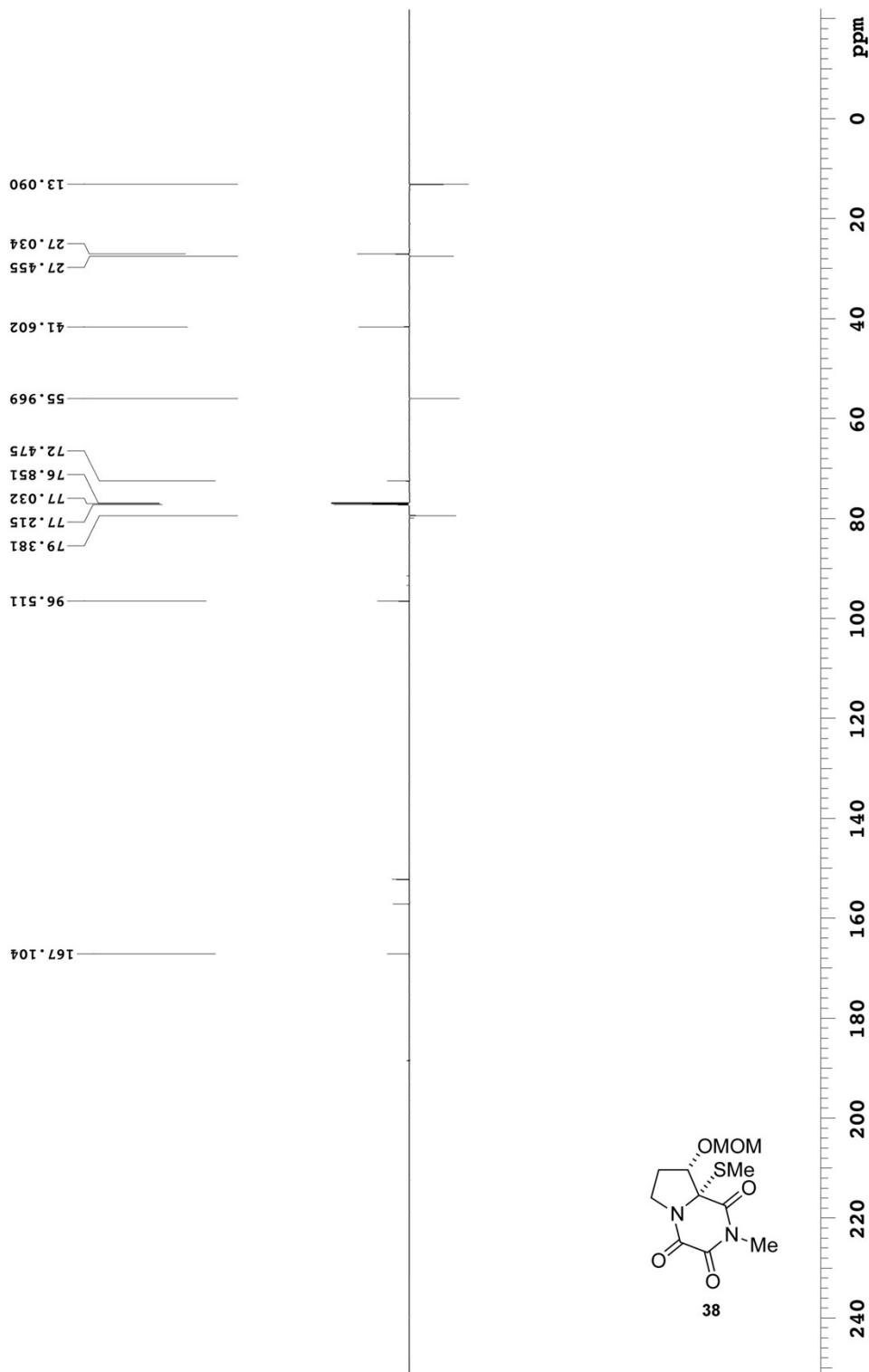
Recorded on: **V700, Mar 18 2016**
Pulse Sequence: **APT_ad**

Sweep Width(Hz): **48076.9**
Digital Res (Hz/pt): **0.37**

Acquisition Time(s): **2**
Hz per mm(Hz/mm): **200.32**

Relaxation Delay(s): **0.5**
Completed Scans: **1328**

shuai, ADS_BK6_PAGE7
175.975 MHz C13{H1} APT_ad in cdcl3 (ref. to CDCl3 @ 77.06 ppm), temp 27.5 C -> actual temp = 27.0 C, coldid probe
C & CH2 same, CH & CH3 opposite side of solvent signal



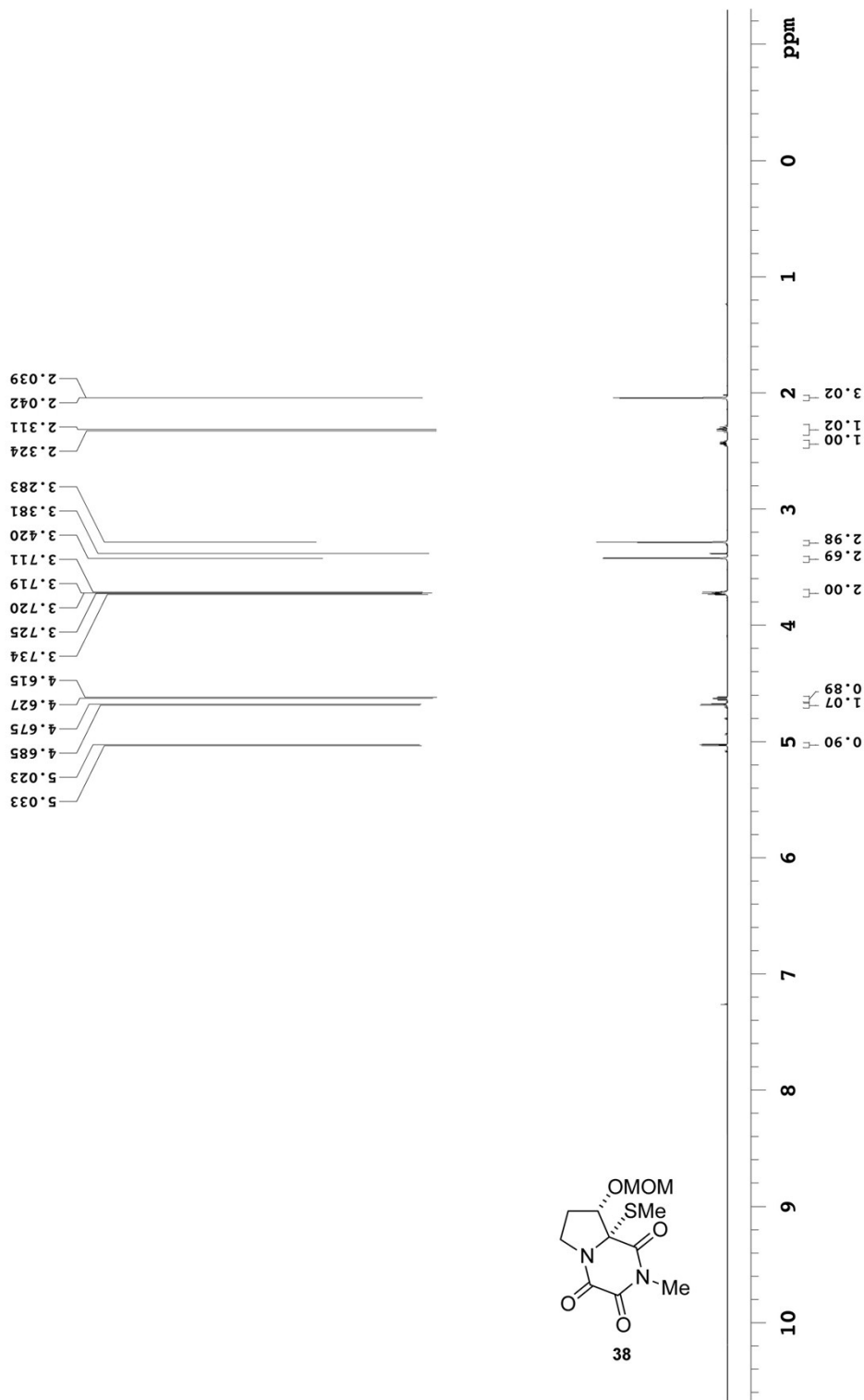


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Recorded on: **V700, Mar 17 2016** Sweep Width(Hz): **8389.26** Acquisition Time(s): **5** Relaxation Delay(s): **0.1**
Pulse Sequence: **PRESAT** Digital Res (Hz/pt): **0.13** Hz per mm(Hz/mm): **34.95** Completed Scans: **16**

shuai, ADS_BK6_PAGE7
699.762 MHz ¹H1 PRESAT in cdc13 (ref. to CDC13 @ 7.26 ppm), temp 27.5 C -> actual temp = 27.0 C, coldid probe





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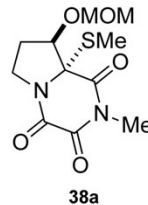
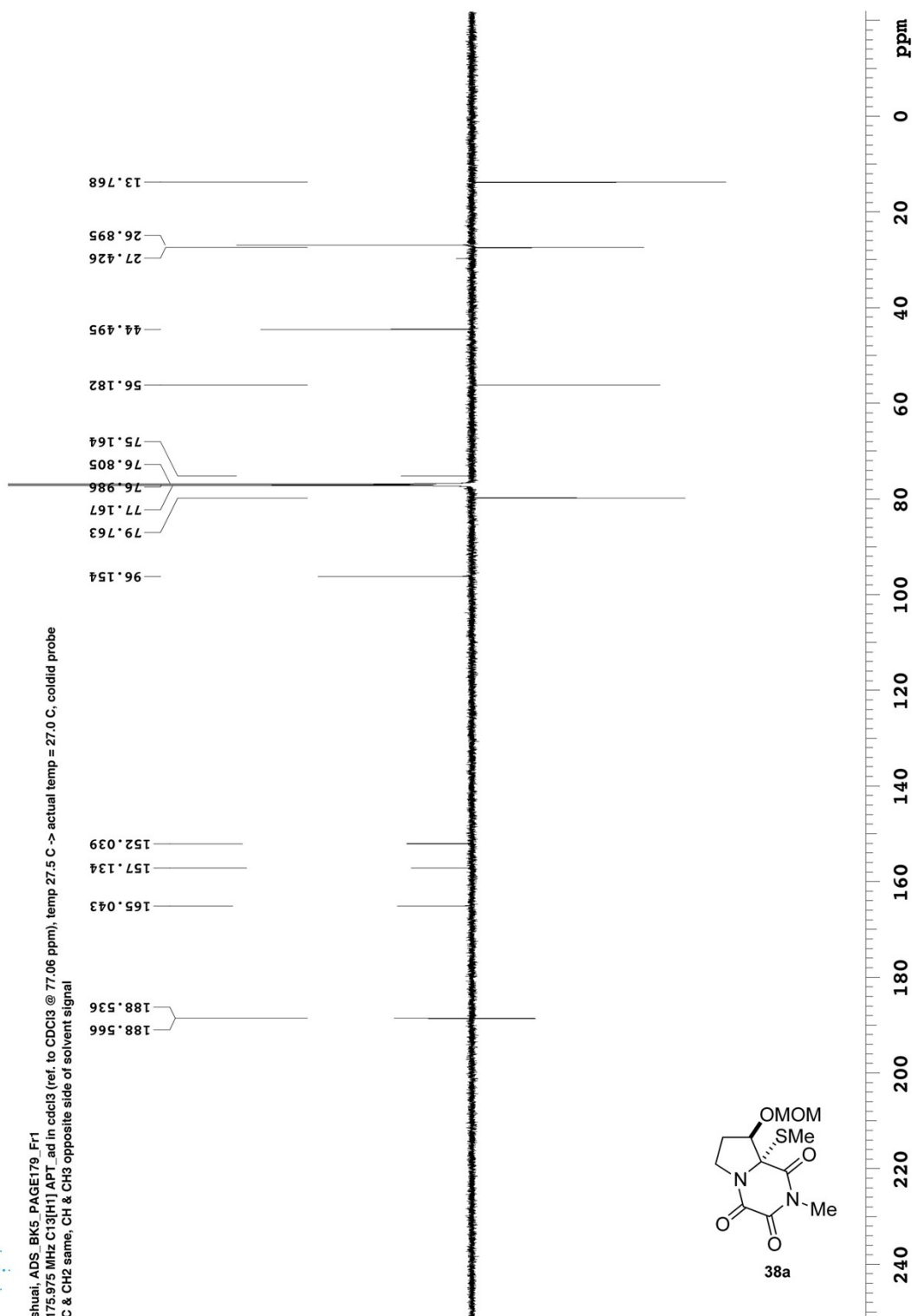
shuai. ADS_BK5_PAGE179_Fr1
1775.975 MHz C13[H1] APT_ad in cdc13 (ref. to CDC13 @ 77.06 ppm), temp 27.5 C -> actual temp = 27.0 C, coldid probe
C & CH2 same, CH & CH3 opposite side of solvent signal

Relaxation Delay(s): **0.5**
Completed Scans **2692**

Acquisition Time(s): **2**
Hz per mm(Hz/mm): **200.32**

Sweep Width(Hz): **48076.9**
Digital Res.(Hz/pt): **0.37**

Recorded on: v700, Mar 12 2016
Pulse Sequence: APT_ad





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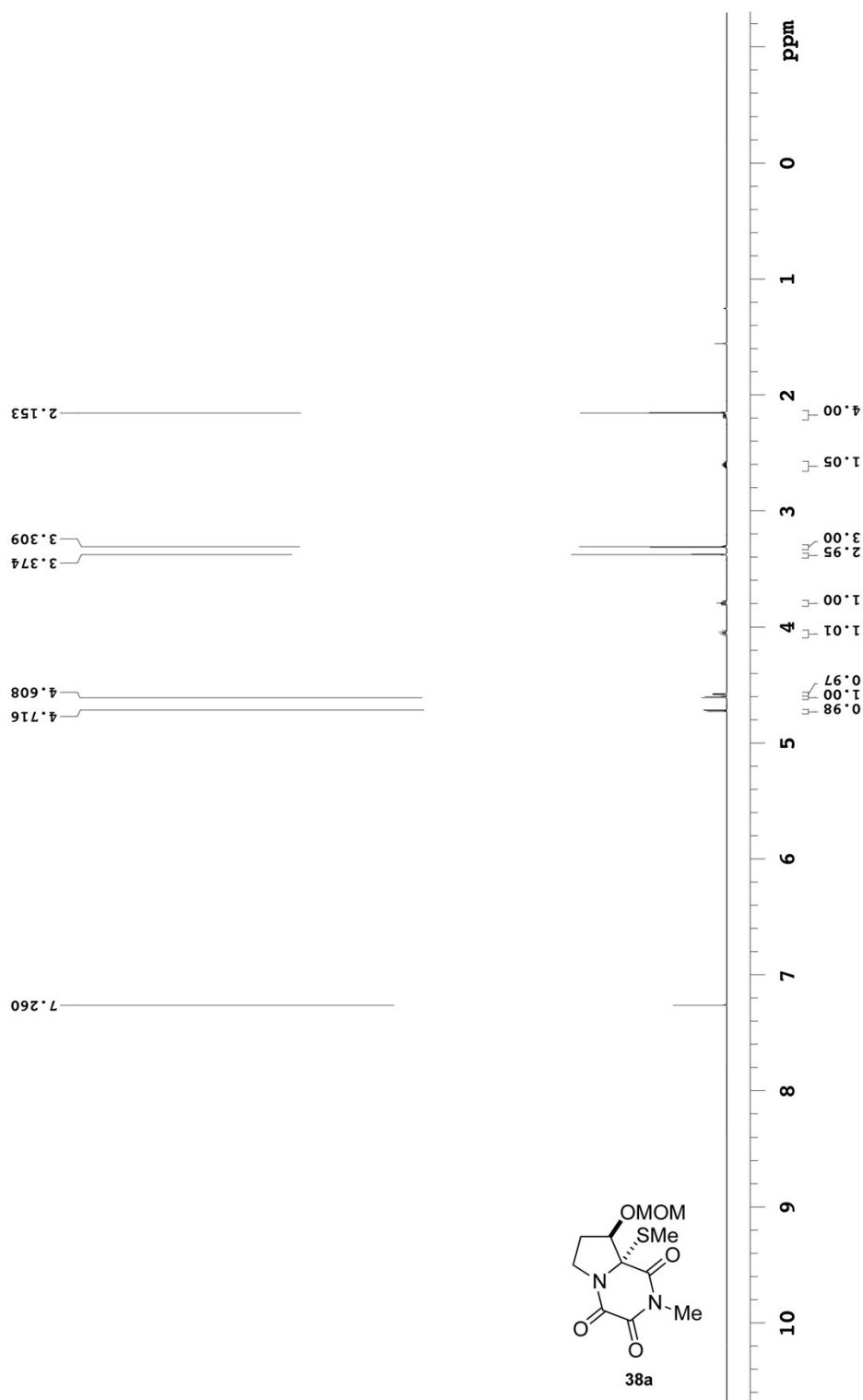
Recorded on: **v700, Mar 12 2016**
Pulse Sequence: **PRESAT**

Sweep Width(Hz): **8389.26**
Digital Res (Hz/pt): **0.13**

Acquisition Time(s): **5**
Hz per mm(Hz/mm): **34.95**

Relaxation Delay(s): **0.1**
Completed Scans **16**

shuai, ADS_BK5_PAGE179_Fr1
699.762 MHz H1 PRESAT in cdcl3 (ref. to CDCl3 @ 7.26 ppm), temp 27.5 C -> actual temp = 27.0 C, coldid probe



File: /mnt/d500/home14/ciivenmr/nmrdata/spectra_for_shuai/rou2/2016.03.12.v7_ADS_BK5_PAGE179_Fr1_loc5_12.51_H1_1D



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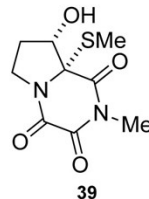
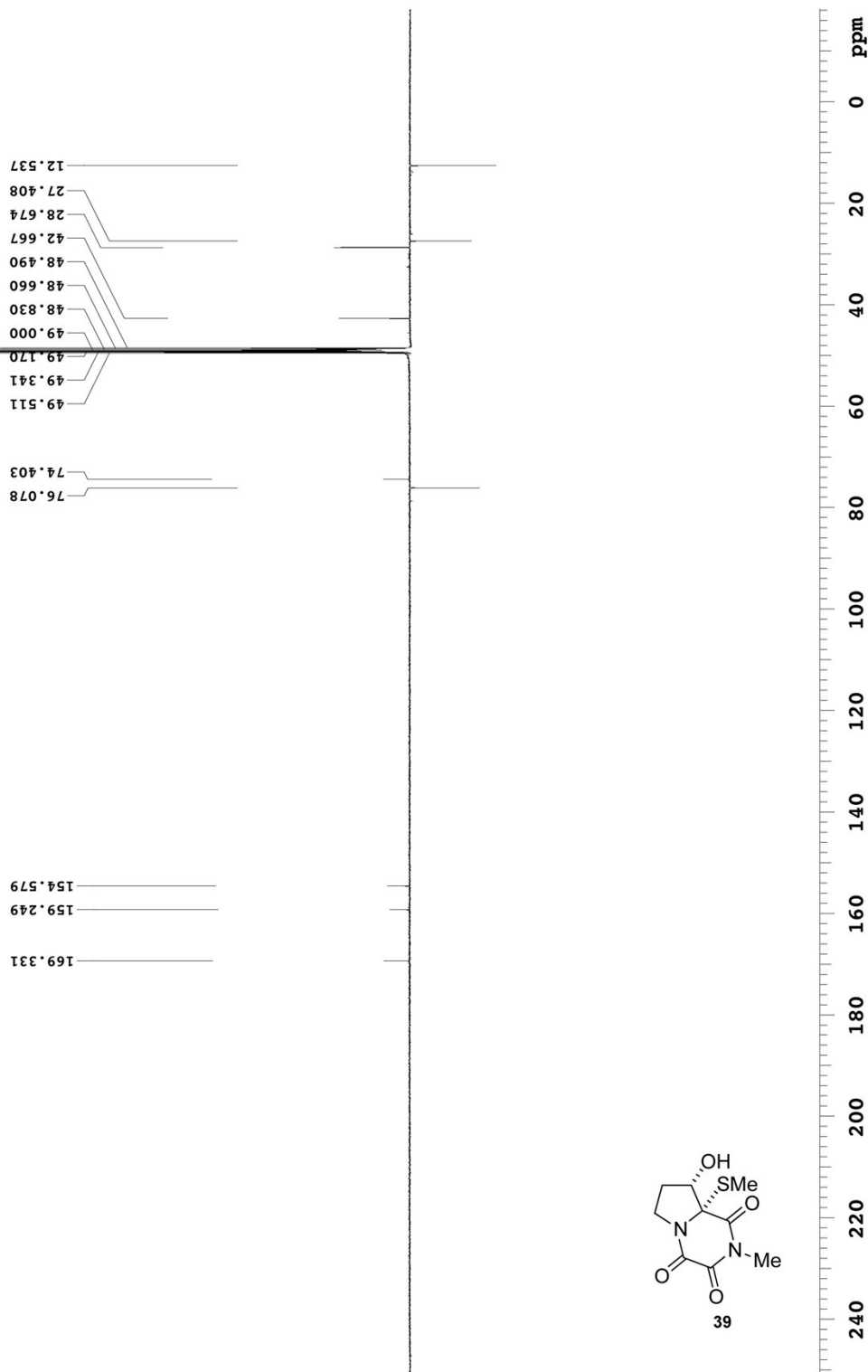
Agilent Technologies

Recorded on: u500, Mar 31 2016
Pulse Sequence: APT_ad

Sweep Width(Hz): 33783.8
Digital Res (Hz/pt): 0.26

Acquisition Time(s): 2
Relaxation Delay(s): 0.5
Completed Scans: 2012

shuai, ADS_BK6_PAGE45
125.691 MHz C13[1H] APT_ad in cd3od (ref. to CD3OD @ 49.0 ppm), temp 27.7 C -> actual temp = 27.0 C, coldlual probe
C & CH2 same, CH & CH3 opposite side of solvent signal





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Recorded on: **v700, Mar 30 2016**
Pulse Sequence: **PRESAT**

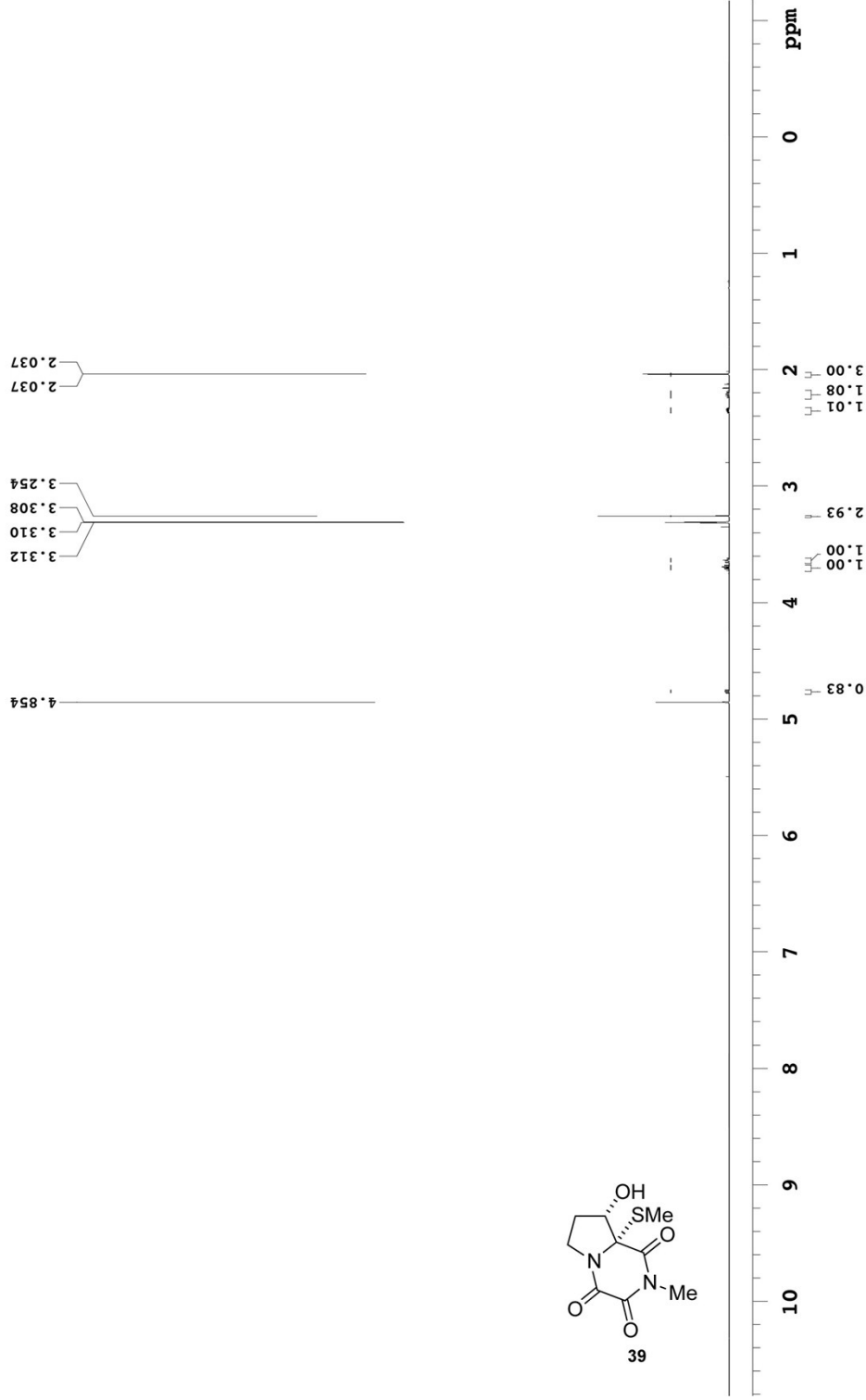
Sweep Width(Hz): **8389.26**
Digital Res (Hz/pt): **0.13**

Acquisition Time(s): **3**
Hz per mm(Hz/mm): **34.95**

Relaxation Delay(s): **0.1**
Completed Scans **16**

shuai, ADS_BK6_PAGE45

699.765 MHz HT PRESAT in cd3od (ref. to CD3OD @ 3.30 ppm), temp 27.5 C -> actual temp = 27.0 C, coldid probe





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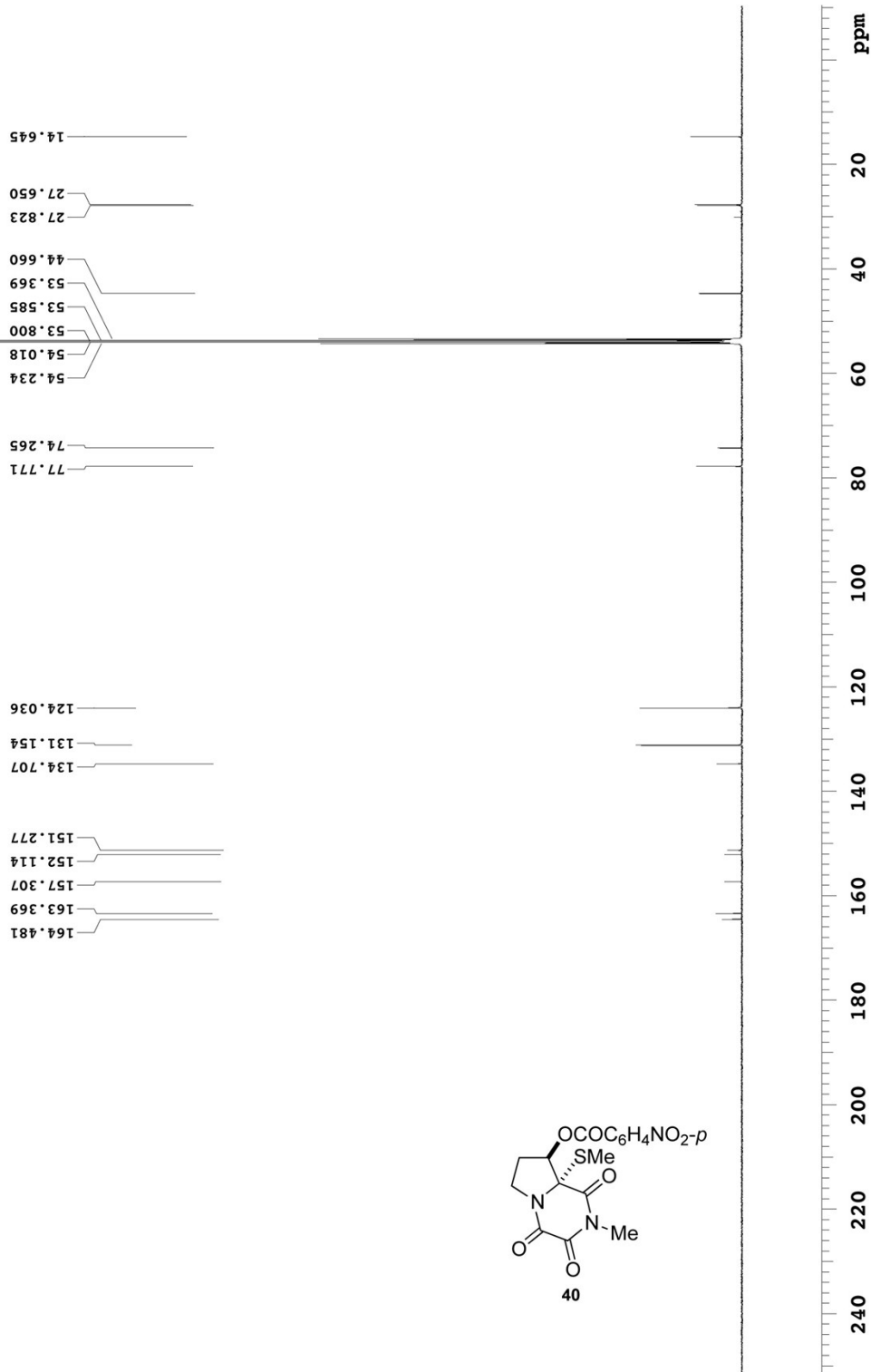
Recorded on: u500, Apr 5 2016
Pulse Sequence: s2pul

Sweep Width(Hz): 32894.7
Digital Res (Hz/pt): 0.25

Acquisition Time(s): 2.5
Hz per mm(Hz/mm): 137.06

Relaxation Delay(s): 0
Completed Scans: 628

shuai, ADS_BK6_PAGE57
125.691 MHz C13[H1] 1D in cd2cl2 (ref. to CD2Cl2 @ 53.8 ppm), temp 27.7 C -> actual temp = 27.0 C, coldludal probe





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Recorded on: u500, Apr 5 2016
Pulse Sequence: PRESAT

Sweep Width(Hz): 6009.62
Digital Res (Hz/pt): 0.09

Acquisition Time(s): 5
Hz per mm(Hz/mm): 25.04

Relaxation Delay(s): 0.1
Completed Scans: 16

shuai, ADS_BK6_PAGE57
499.807 MHz HT PRESAT in cd2cl2 (ref. to CD2Cl2 @ 5.32 ppm), temp 27.7 C -> actual temp = 27.0 C, coldlual probe

