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## Supporting information for

# Docking study and biological evaluation of pyrrolidine-based iminosugars as pharmacological chaperones for Gaucher disease

Atsushi Kato,*[a] Izumi Nakagome,[b] Kasumi Sato,[a] Arisa Yamamoto,[a] Isao Adachi,[a] Robert J. Nash,[c] George W. J. Fleet,[d] Yoshihiro Natori,[e] Yasuka Watanabe,[e] Tatsushi Imahori,[e] Yuichi Yoshimura,[e] Hiroki Takahata,[e] Shuichi Hirono*[b]

[a] Department of Hospital Pharmacy, University of Toyama, 2630 Sugitani, Toyama 930-0194, Japan

[b] School of Pharmaceutical Sciences, Kitasato University, Tokyo 108-8641, Japan

[c] Institute of Biological, Environmental and Rural Sciences / Phytoquest Limited, Plas Gogerddan, A berystwyth, Ceredigion, SY23 3EB, United Kingdom

[d] Chemistry Research Laboratory, Department of Chemistry, University of Oxford, Oxford, OX1 3TA, United Kingdom

[e] Faculty of Pharmaceutical Sciences, Tohoku Pharmaceutical University, Sendai 981-8558, Japan

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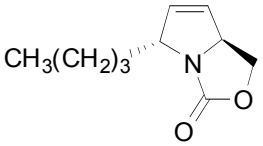
## General experimental:

### Typical Procedure for Negishi Coupling

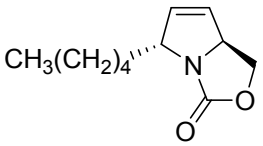
### (5*R*,7a*S*)-5-Butyl-1,7a-dihydropyrrolo[1,2-c]oxazol-3(5H)-one (2a)

89% yield; $[\alpha]_D^{22}$= -167.6 (*c* 0.42, $CHCl_3$). *Lit. ent*-**2a**[2] : $[\alpha]_D^{24}$ = +175.4 (*c* 1.08, $CHCl_3$).



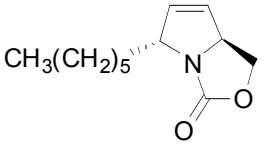
### (5*R*,7a*S*)-5-Pentyl-1,7a-dihydropyrrolo[1,2-c]oxazol-3(5H)-one (2b)

75 % yield; $[\alpha]_D^{18}$= -140.6 (*c* 0.49, $CHCl_3$). *Lit. ent*-**2b**[2] : $[\alpha]_D^{24}$ = +170.9 (*c* 1.00, $CHCl_3$).



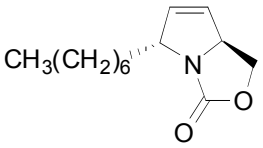
### (5*R*,7a*S*)-5-Hexyl-1,7a-dihydropyrrolo[1,2-c]oxazol-3(5H)-one (2c)

65% yield; $[\alpha]_D^{25}$= -196.8 (*c* 0.40, $CHCl_3$). *Lit. ent*-**2c**[2] : $[\alpha]_D^{24}$ = +170.9 (*c* 1.00, $CHCl_3$).



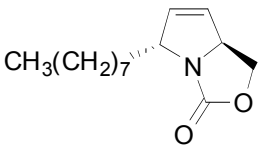
### (5R,7aS)-5-Heptyl-1,7a-dihydropyrrolo[1,2-c]oxazol-3(5H)-one (2d)

68 % yield; $[\alpha]_D^{27}$= -151.1 (*c* 1.09, $CHCl_3$). *Lit. ent*-**2d**[2] : $[\alpha]_D^{25}$ = +154.4 (*c* 1.09, $CHCl_3$).



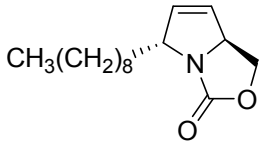
### (5*R*,7a*S*)-5-Octyl-1,7a-dihydropyrrolo[1,2-c]oxazol-3(5H)-one (2e)

65 % yield; $[\alpha]_D^{23}$= -139.1 (*c* 1.0, $CHCl_3$). *Lit. ent*-**2e**[2] : $[\alpha]_D^{25}$ = +140.1 (*c* 1.07, $CHCl_3$).



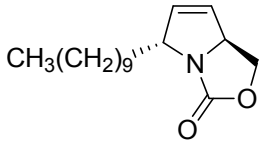
### (5*R*,7a*S*)-5-Nonyl-1,7a-dihydropyrrolo[1,2-c]oxazol-3(5H)-one (2f)

57 % yield; $[\alpha]_D^{27}$= -126.6 (*c* 1.16, $CHCl_3$). *Lit. ent*-**2f**[2] : $[\alpha]_D^{25}$ = +138.1 (*c* 1.75, $CHCl_3$).



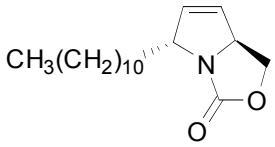
**(5*R*,7a*S*)-5-Decyl-1,7a-dihydropyrrolo[1,2-c]oxazol-3(5H)-one (2g)**

65 % yield; $[\alpha]_D^{27}$= -136.0 (*c* 1.19, $CHCl_3$). *Lit. ent*-**2g**[2] : $[\alpha]_D^{24}$ = +123.0 (*c* 0.97, $CHCl_3$).



**(5*R*,7a*S*)-5-Undecyl-1,7a-dihydropyrrolo[1,2-c]oxazol-3(5H)-one (2h)**

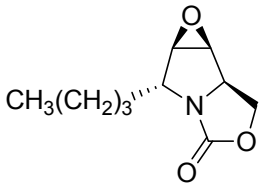
63% yield; $[\alpha]_D^{25}$ = -111.1 (*c* 0.40, $CHCl_3$). *Lit. ent*-**2h**[2] : $[\alpha]_D^{25}$ = +115.6 (*c* 0.74, $CHCl_3$).



**Typical procedure for epoxidation**

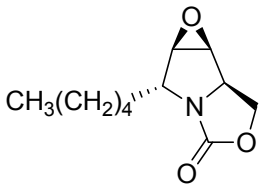
**(1a*S*,1b*R*,6*R*,6a*R*)-6-Butyltetrahydrooxireno[2',3':3,4]pyrrolo[1,2-c]oxazol-4(1aH)-one (3a)**

92% yield; $[\alpha]_D^{29}$ = -40.8 (*c* 0.95, $CHCl_3$). *Lit. ent*-**3a**[2] : $[\alpha]_D^{22}$ = +48.2 (*c* 0.12, $CHCl_3$).



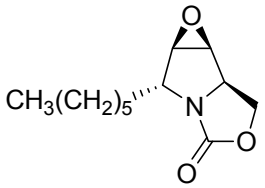
**(1a*S*,1b*R*,6*R*,6a*R*)-6-Pentyltetrahydrooxireno[2',3':3,4]pyrrolo[1,2-c]oxazol-4(1aH)-one (3b)**

90% yield; $[\alpha]_D^{23}$ = -55.0 (*c* 0.34, $CHCl_3$). *Lit. ent*-**3b**[2] : $[\alpha]_D^{24}$ = +40.4 (*c* 1.18, $CHCl_3$).



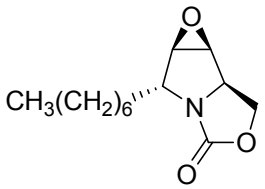
**(1a*S*,1b*R*,6*R*,6a*R*)-6-Hexyltetrahydrooxireno[2',3':3,4]pyrrolo[1,2-c]oxazol-4(1aH)-one (3c)**

99% yield; $[\alpha]_D^{22}$ = -58.8 (*c* 0.18, $CHCl_3$). *Lit. ent*-**3c**[2] : $[\alpha]_D^{22}$ = +37.1 (*c* 0.15, $CHCl_3$).



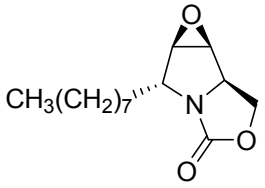
**(1a*S*,1b*R*,6*R*,6a*R*)-6-Heptyltetrahydrooxireno[2',3':3,4]pyrrolo[1,2-c]oxazol-4(1aH)-one (3d)**

99 % yield; $[\alpha]_D^{26}$ = -38.4 (*c* 1.12, $CHCl_3$). *Lit. ent*-**3d**[2] : $[\alpha]_D^{22}$ = +42.2 (*c* 0.16, $CHCl_3$).



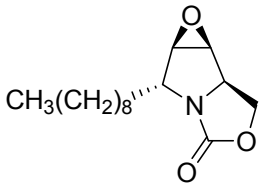
**(1a*S*,1b*R*,6*R*,6a*R*)-6-Octyltetrahydrooxireno[2',3':3,4]pyrrolo[1,2-c]oxazol-4(1aH)-one (3e)**

85 % yield; $[\alpha]_D^{19}$ = -43.4 (*c* 0.41, $CHCl_3$). *Lit. ent*-**3e**[2] : $[\alpha]_D^{22}$ = +41.9 (*c* 0.98, $CHCl_3$).



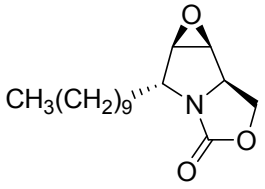
**(1a*S*,1b*R*,6*R*,6a*R*)-6-Nonyltetrahydrooxireno[2',3':3,4]pyrrolo[1,2-c]oxazol-4(1aH)-one (3f)**

89 % yield**;** $[\alpha]_D^{27}$ = -34.3 (*c* 1.14, $CHCl_3$). *Lit. ent*-**3f**[2] : $[\alpha]_D^{25}$ = +34.0 (*c* 1.06, $CHCl_3$).



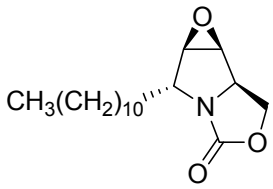
**(1a*S*,1b*R*,6*R*,6a*R*)-6-Decyltetrahydrooxireno[2',3':3,4]pyrrolo[1,2-c]oxazol-4(1aH)-one (3g)**

86 % yield; $[\alpha]_D^{27}$ = -30.7 (*c* 1.10, $CHCl_3$). *Lit. ent*-**3g**[2] : $[\alpha]_D^{22}$ = +27.8 (*c* 0.48, $CHCl_3$).



**(1a*S*,1b*R*,6*R*,6a*R*)-6-Undcyltetrahydrooxireno[2',3':3,4]pyrrolo[1,2-c]oxazol-4(1aH)-one (3h)**

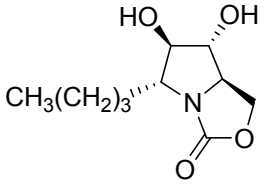
86% yield; $[\alpha]_D^{25}$ = -32.5 (*c* 0.66, $CHCl_3$). *Lit. ent*-**3h**[2] : $[\alpha]_D^{25}$ = +31.1 (*c* 1.09, $CHCl_3$).



**Typical Procedure for the preparation of a diol.**

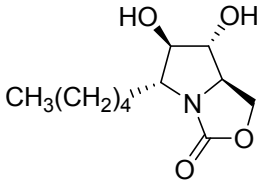
**(5*R*,6*R*,7*R*,7a*R*)-6,7-Dihydroxy-5-Butyltetrahydropyrrolo[1,2-c]oxazol-3(1H)-one (4a)**

52 % yield; $[\alpha]_D^{29}$= -23.7 (*c* 0.9, $CHCl_3$). *Lit. ent*-**4a**[2] : $[\alpha]_D^{23}$ = +22.2 (*c* 0.46, $CHCl_3$).



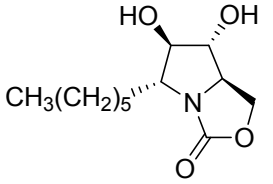
**(5*R*,6*R*,7*R*,7a*R*)-6,7-Dihydroxy-5-Pentyltetrahydropyrrolo[1,2-c]oxazol-3(1H)-one (4b)**

96 % yield, $[\alpha]_D^{27}$= -17.7 ( *c* 0.78 $CHCl_3$). *Lit. ent*-**4b**[2] : $[\alpha]_D^{20}$ = +20.4 (*c* 0.25, $CHCl_3$).



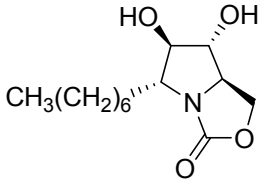
**(5*R*,6*R*,7*R*,7a*R*)-6,7-Dihydroxy-5-Hexyltetrahydropyrrolo[1,2-c]oxazol-3(1H)-one (4c)**

85 % yield, $[\alpha]_D^{26}$ = -14.7 (*c* 1.04, $CHCl_3$). *Lit. ent*-**4c**[2] : $[\alpha]_D^{24}$ = +11.6 (*c* 1.07, $CHCl_3$).



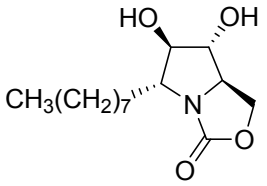
**(5*R*,6*R*,7*R*,7a*R*)-6,7-Dihydroxy-5-Heptyltetrahydropyrrolo[1,2-c]oxazol-3(1H)-one (4d)**

69 % yield, $[\alpha]_D^{27}$ = -14.6 (*c* 1.23, $CHCl_3$). *Lit. ent*-**4d**[2] : $[\alpha]_D^{20}$ = +11.0 (*c* 0.67, $CHCl_3$).



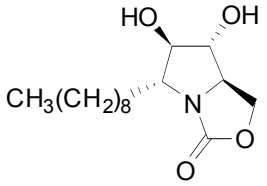
**(5*R*,6*R*,7*R*,7a*R*)-6,7-Dihydroxy-5-Octyltetrahydropyrrolo[1,2-c]oxazol-3(1H)-one (4e)**

94 % yield, $[\alpha]_D^{25}$ = -18.4 (*c* 0.30, $CHCl_3$). *Lit. ent*-**4e**[2] : $[\alpha]_D^{22}$ = +15.3 (*c* 0.80, $CHCl_3$).



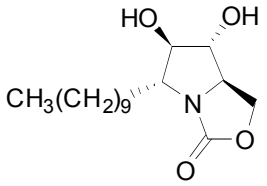
**(5*R*,6*R*,7*R*,7a*R*)-6,7-Dihydroxy-5-Nonyltetrahydropyrrolo[1,2-c]oxazol-3(1H)-one (4f)**

75 % yield, $[\alpha]_D^{28}$ = -15.5 (*c* 1.10, $CHCl_3$). *Lit. ent*-**4f**[2] : $[\alpha]_D^{24}$ = +17.6 (*c* 1.09, $CHCl_3$).



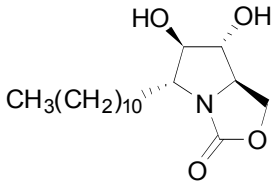
**(5*R*,6*R*,7*R*,7a*R*)-6,7-Dihydroxy-5-Decyltetrahydropyrrolo[1,2-c]oxazol-3(1H)-one (4g)**

65 % yield, $[\alpha]_D^{27}$= -9.0 (*c* 0.69, $CHCl_3$). *Lit. ent*-**4g**[2] : $[\alpha]_D^{22}$ = +15.5 (*c* 0.57, $CHCl_3$).



**(5*R*,6*R*,7*R*,7a*R*)-6,7-Dihydroxy-5-Undecyltetrahydropyrrolo[1,2-c]oxazol-3(1H)-one (4h)**

60% yield, $[\alpha]_D^{26}$= -13.4 (*c* 1.05, $CHCl_3$). *Lit. ent*-**4h**[2] : $[\alpha]_D^{24}$ = +12.9 (*c* 1.02, $CHCl_3$).

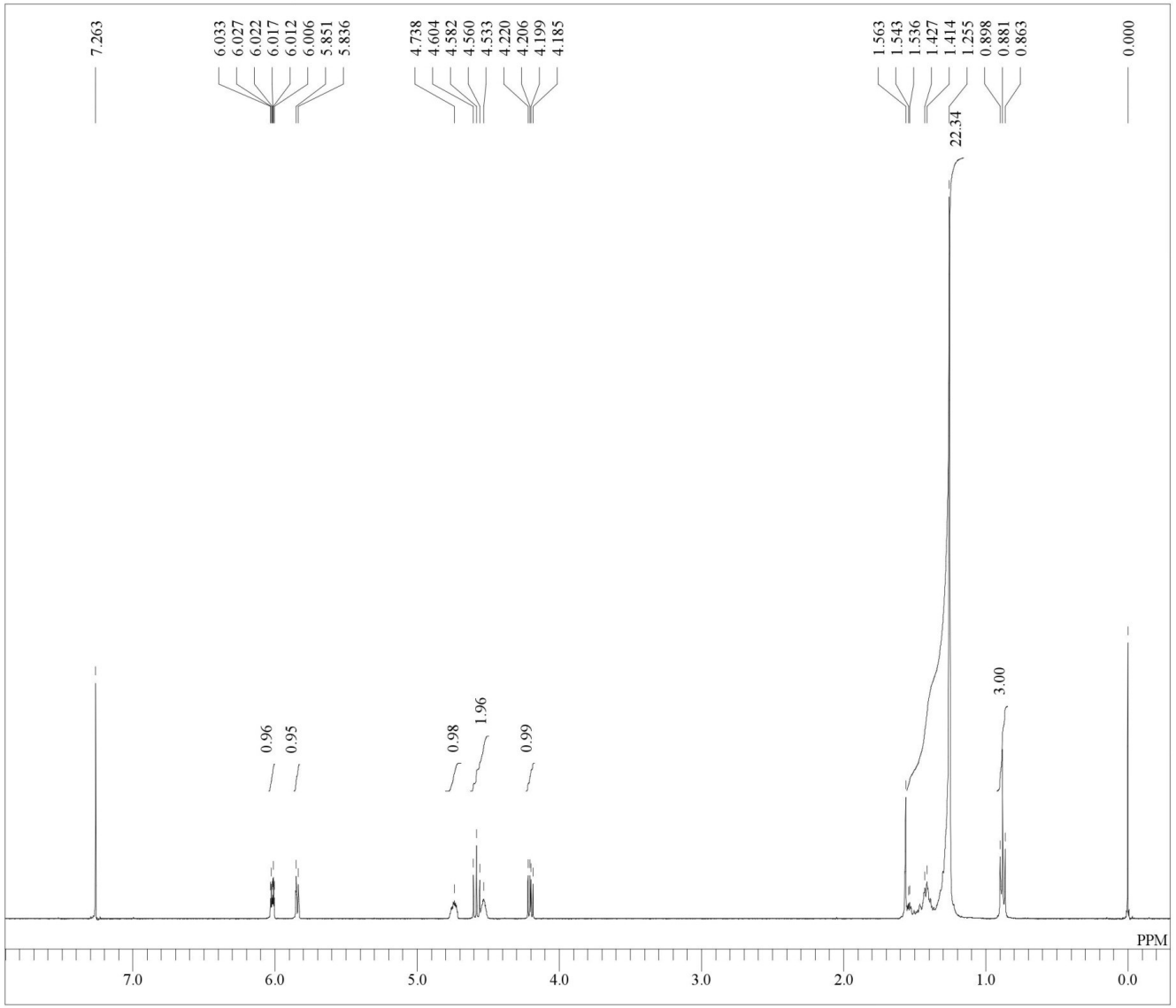


References

1) *Bioorg. Med. Chem. Lett*. **2011**, *21*, 738-741.

2) *J. Med. Chem.* **2012**, *55*, 10347-10362.

2i (1H-NMR)

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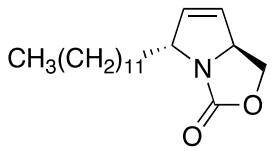
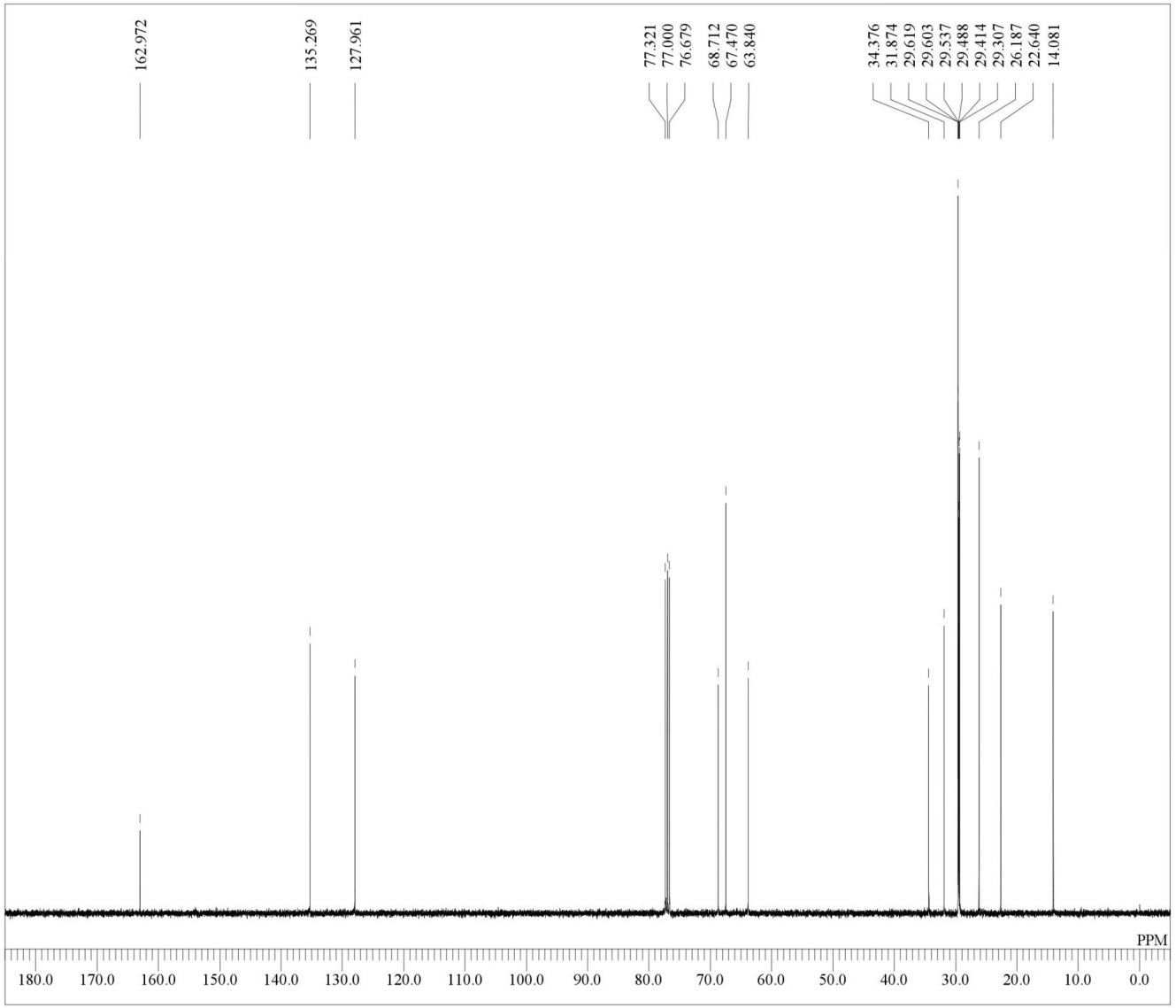



**2i**

2i (13C-NMR)




| | |
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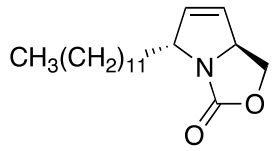
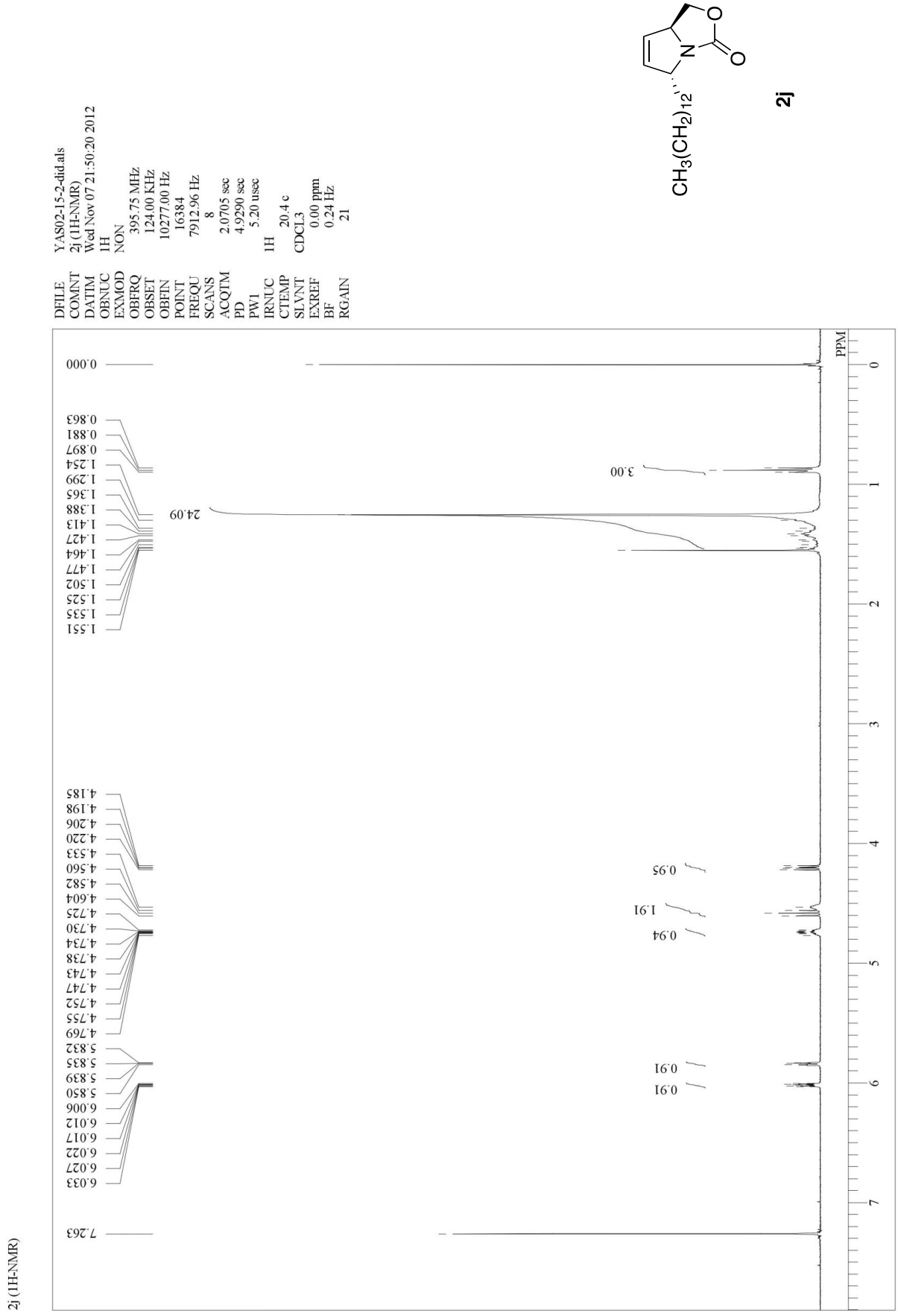



**2i**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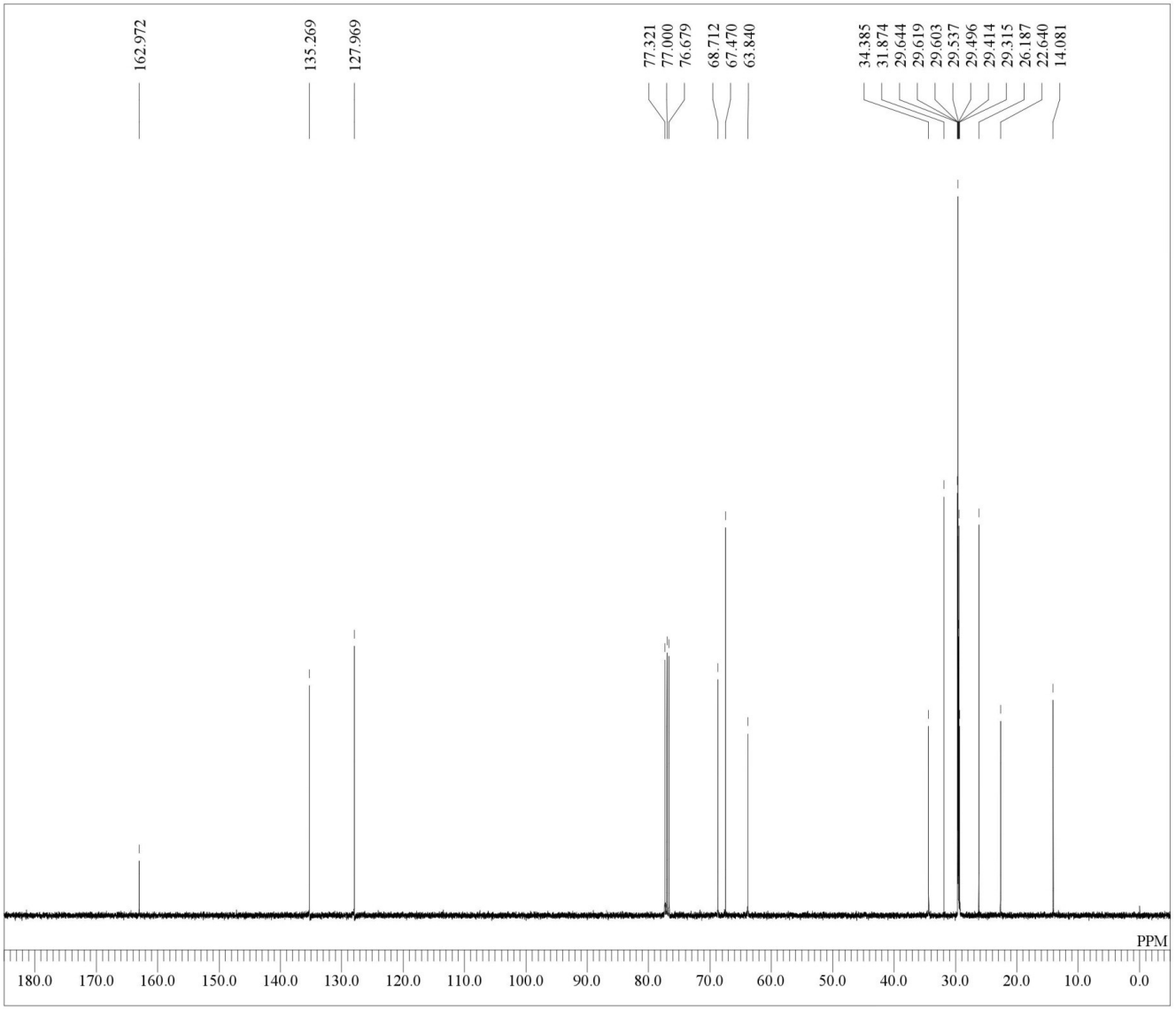
2j (1H-NMR)

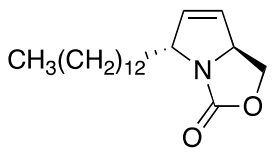

O
O
N
CH3(CH2)12

**2j**

2j (13C-NMR)

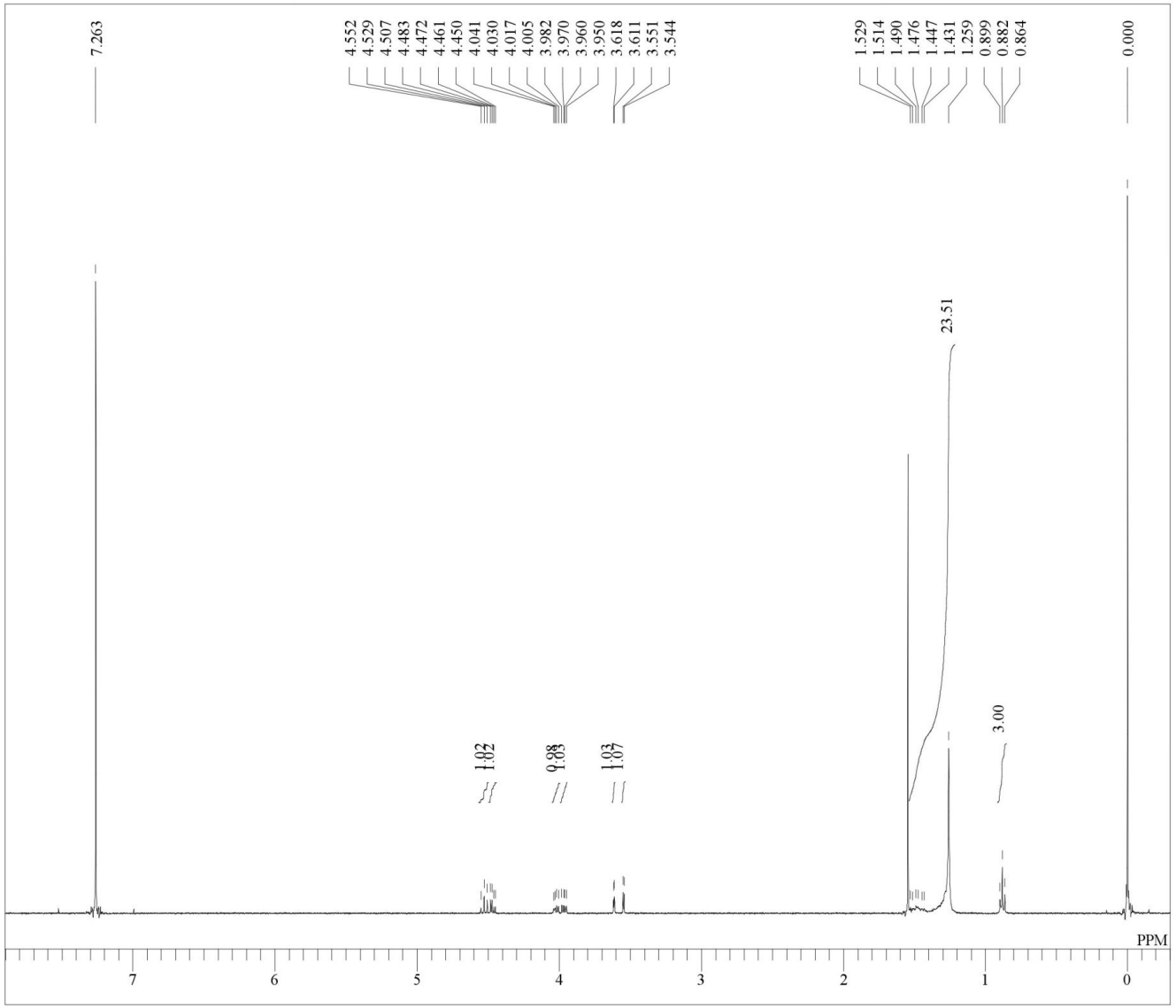



| | |
|---|---|
| DFILE | YAS02-15-C13-did.als |
| COMNT | 2j (13C-NMR) |
| DATIM | Thu Nov 22 17:39:24 2012 |
| OBNUC | 13C |
| EXMOD | BCM |
| OBFRQ | 99.45 MHz |
| OBSET | 94.00 KHz |
| OBFIN | 10309.00 Hz |
| POINT | 32768 |
| FREQU | 26845.64 Hz |
| SCANS | 664 |
| ACQTM | 1.2206 sec |
| PD | 1.7790 sec |
| PW1 | 5.20 usec |
| IRNUC | 1H |
| CTEMP | 21.8 c |
| SLVNT | CDCL3 |
| EXREF | 77.00 ppm |
| BF | 0.24 Hz |
| RGAIN | 23 |

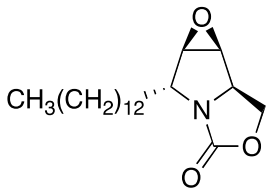



**2j**

3i (1H-NMR)

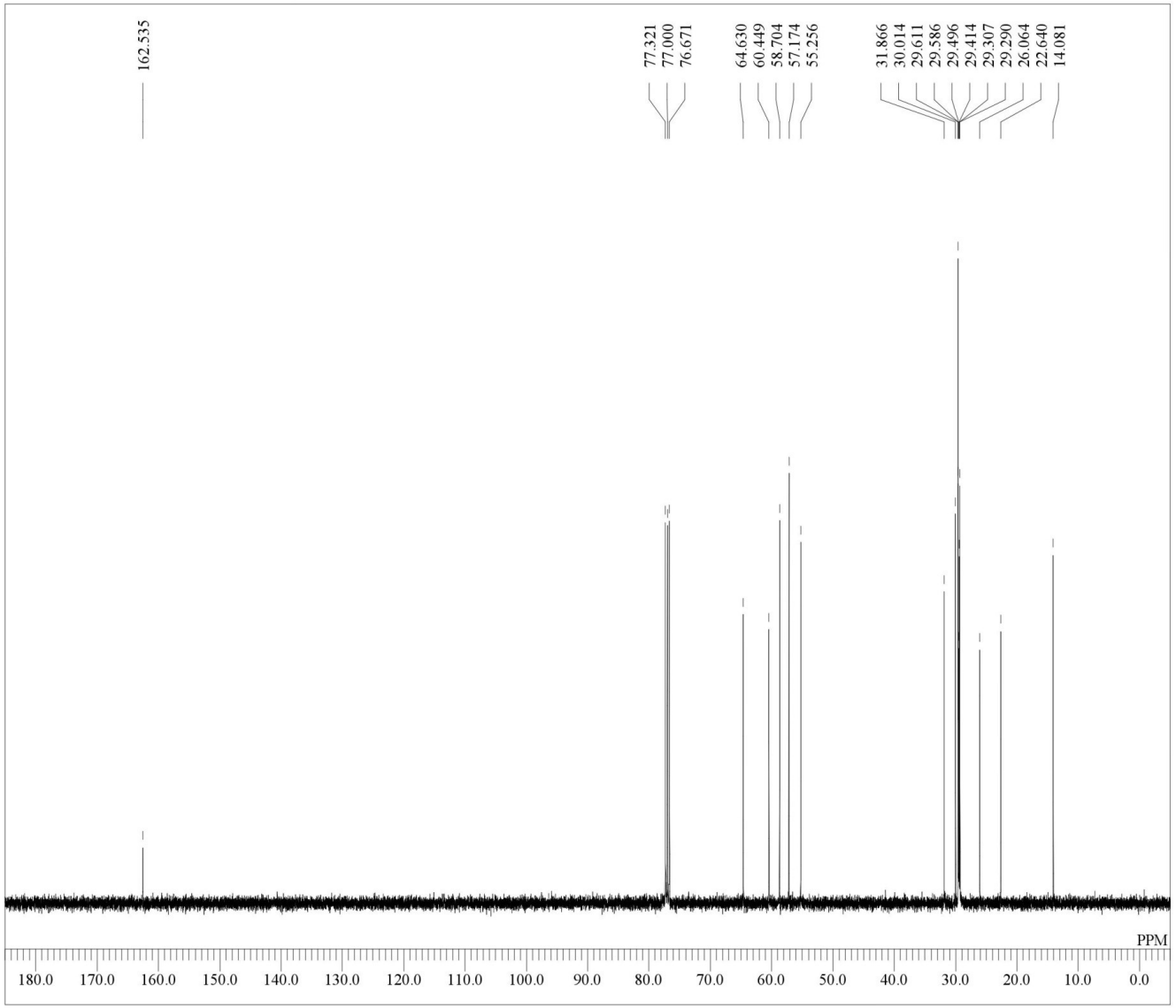



DFILE YAS02-14-did.als
COMNT 3i (1H-NMR)
DATIM Wed Oct 31 17:35:57 2012
OBNUC 1H
EXMOD NON
OBFRQ 395.75 MHz
OBSET 124.00 KHz
OBFIN 10277.00 Hz
POINT 16384
FREQU 7912.96 Hz
SCANS 8
ACQTM 2.0705 sec
PD 4.9290 sec
PW1 5.20 usec
IRNUC 1H
CTEMP 20.9 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.24 Hz
RGAIN 24

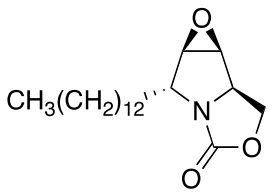



**3i**

3i (13C-NMR)

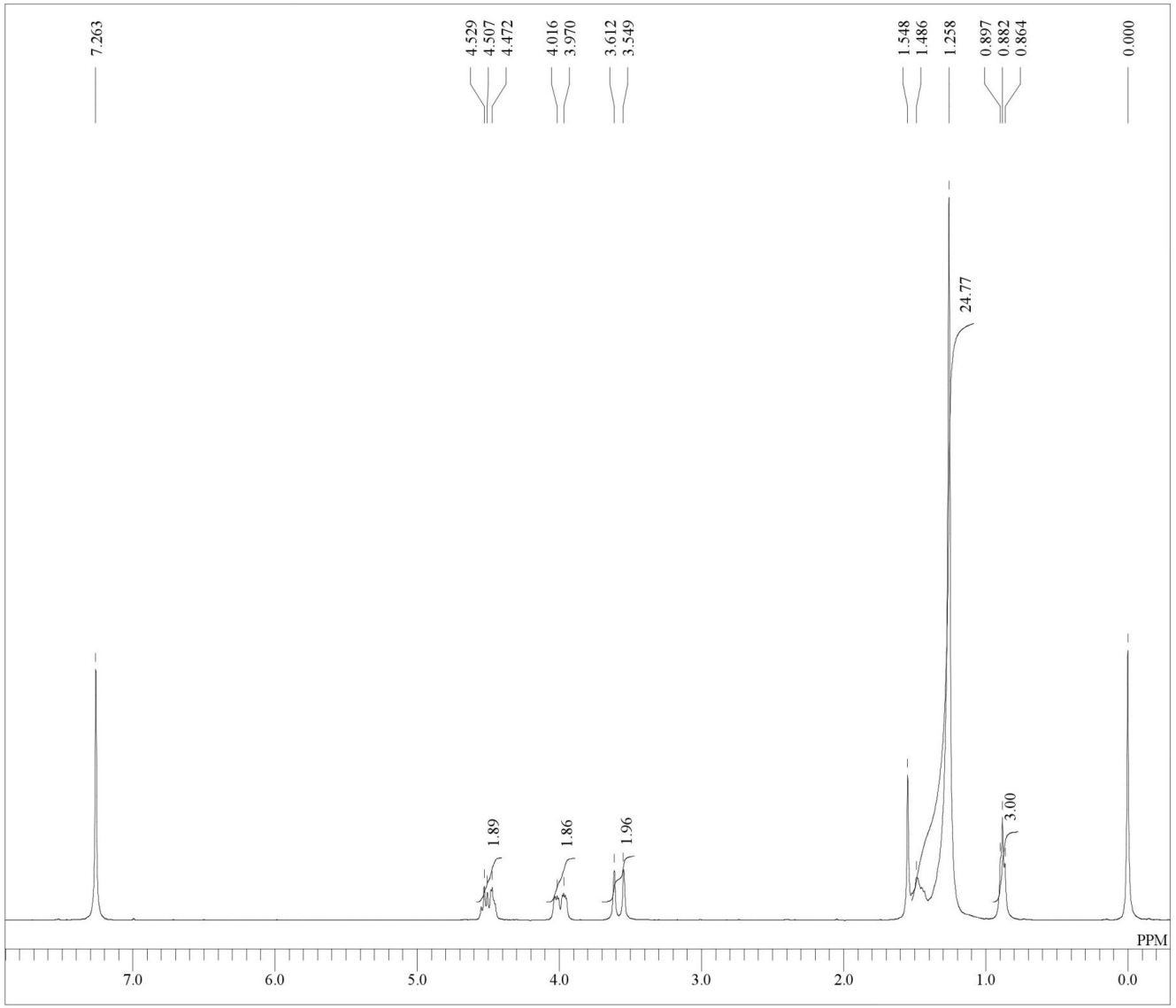



| | |
|---|---|
| DFILE | YAS02-14-2-C13-did.als |
| COMNT | 3i (13C-NMR) |
| DATIM | Wed Jan 16 12:19:31 2013 |
| OBNUC | 13C |
| EXMOD | BCM |
| OBFRQ | 99.45 MHz |
| OBSET | 94.00 KHz |
| OBFIN | 10309.00 Hz |
| POINT | 32768 |
| FREQU | 26845.64 Hz |
| SCANS | 480 |
| ACQTM | 1.2206 sec |
| PD | 1.7790 sec |
| PW1 | 5.20 usec |
| IRNUC | 1H |
| CTEMP | 22.1 c |
| SLVNT | CDCL3 |
| EXREF | 77.00 ppm |
| BF | 0.24 Hz |
| RGAIN | 23 |

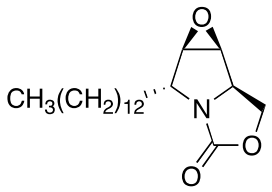



**3i**

3j (1H-NMR)

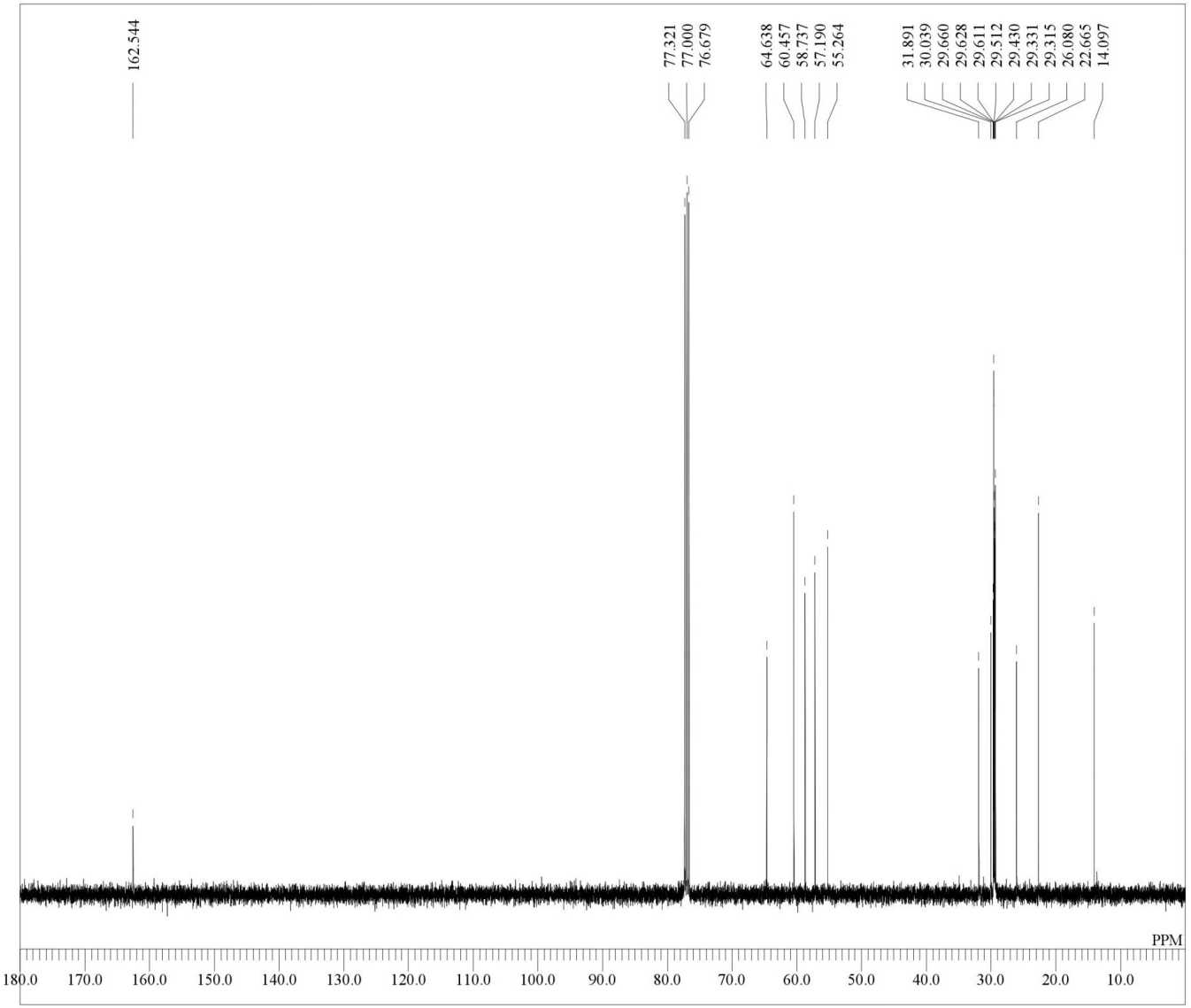



DFILE YAS02-17-1-did.als
COMNT 3j (1H-NMR)
DATIM Fri Nov 09 19:25:06 2012
OBNUC 1H
EXMOD NON
OBFRQ 395.75 MHz
OBSET 124.00 KHz
OBFIN 10277.00 Hz
POINT 16384
FREQU 7912.96 Hz
SCANS 8
ACQTM 2.0705 sec
PD 4.9290 sec
PW1 5.20 usec
IRNUC 1H
CTEMP 21.0 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 4.20 Hz
RGAIN 21

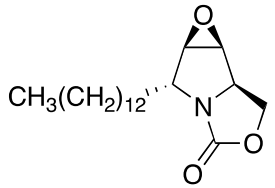



**3j**

3j (13C-NMR)

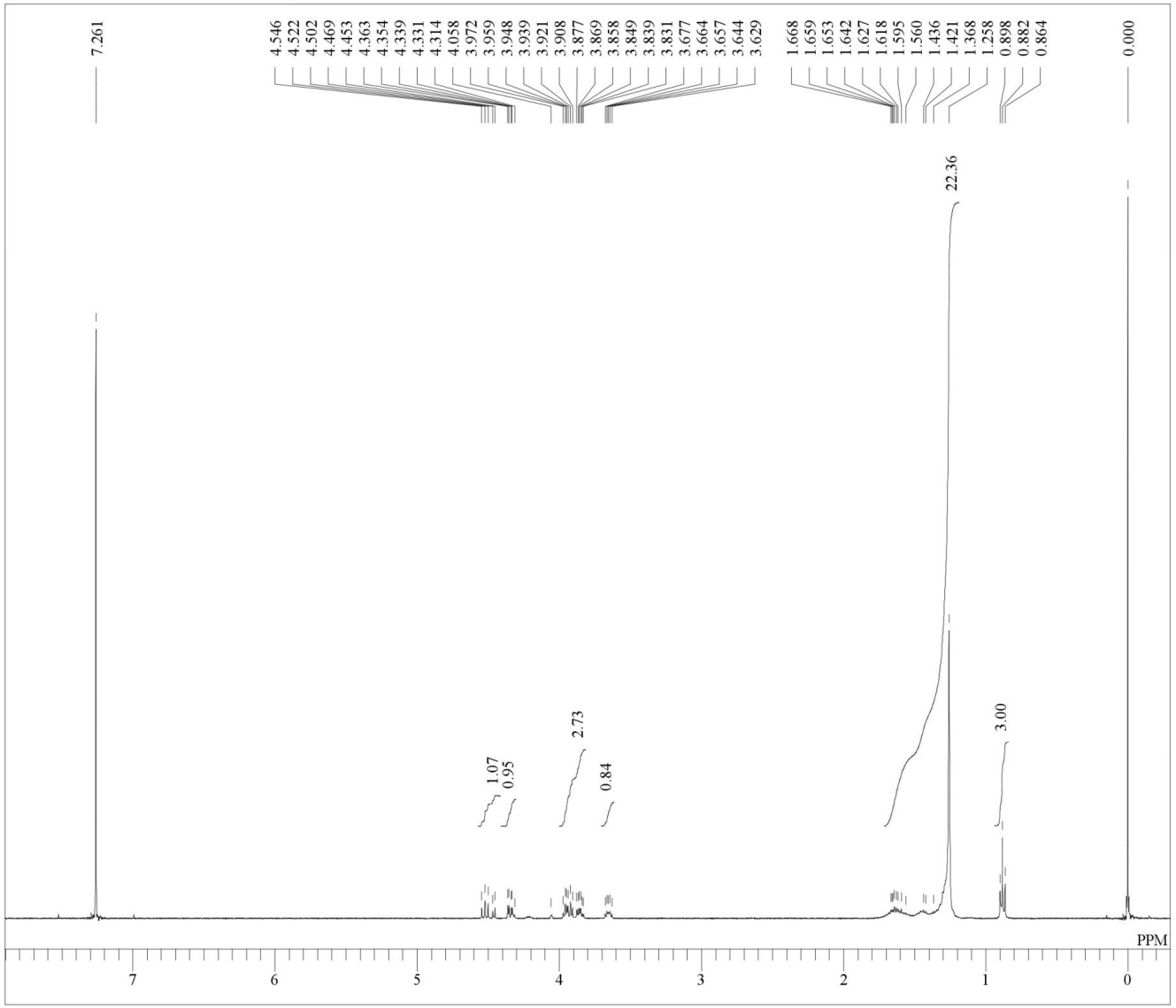



| | |
|---|---|
| DFILE | YAS02-17-13C-did.als |
| COMNT | 3j (13C-NMR) |
| DATIM | Tue Jan 22 16:10:39 2013 |
| OBNUC | 13C |
| EXMOD | BCM |
| OBFRQ | 99.45 MHz |
| OBSET | 94.00 KHz |
| OBFIN | 10309.00 Hz |
| POINT | 32768 |
| FREQU | 26845.64 Hz |
| SCANS | 640 |
| ACQTM | 1.2206 sec |
| PD | 1.7790 sec |
| PW1 | 5.20 usec |
| IRNUC | 1H |
| CTEMP | 21.8 c |
| SLVNT | CDCL3 |
| EXREF | 77.00 ppm |
| BF | 0.24 Hz |
| RGAIN | 23 |

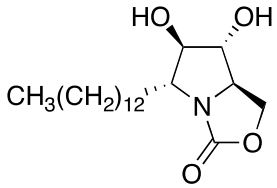



**3j**

4i (1H-NMR)

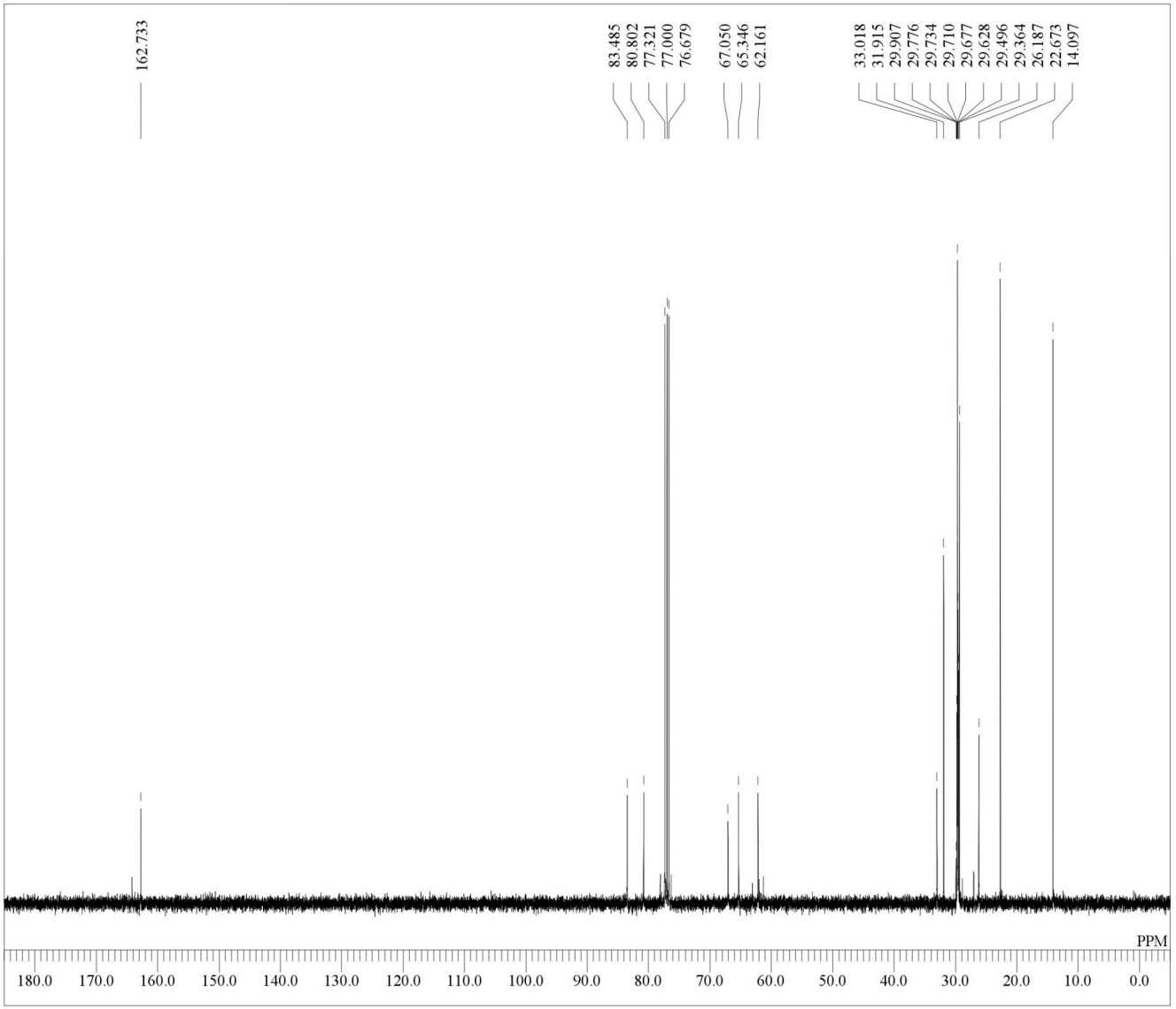



DFILE YAS02-16-1-did.als
COMNT 4i (1H-NMR)
DATIM Wed Nov 07 21:41:43 2012
OBNUC 1H
EXMOD NON
OBFRQ 395.75 MHz
OBSET 124.00 KHz
OBFIN 10277.00 Hz
POINT 16384
FREQU 7912.96 Hz
SCANS 8
ACQTM 2.0705 sec
PD 4.9290 sec
PW1 5.20 usec
IRNUC 1H
CTEMP 21.3 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.24 Hz
RGAIN 22

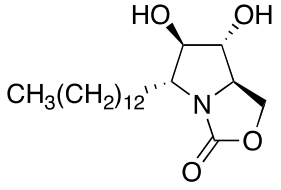



**4i**

4i (13C-NMR)

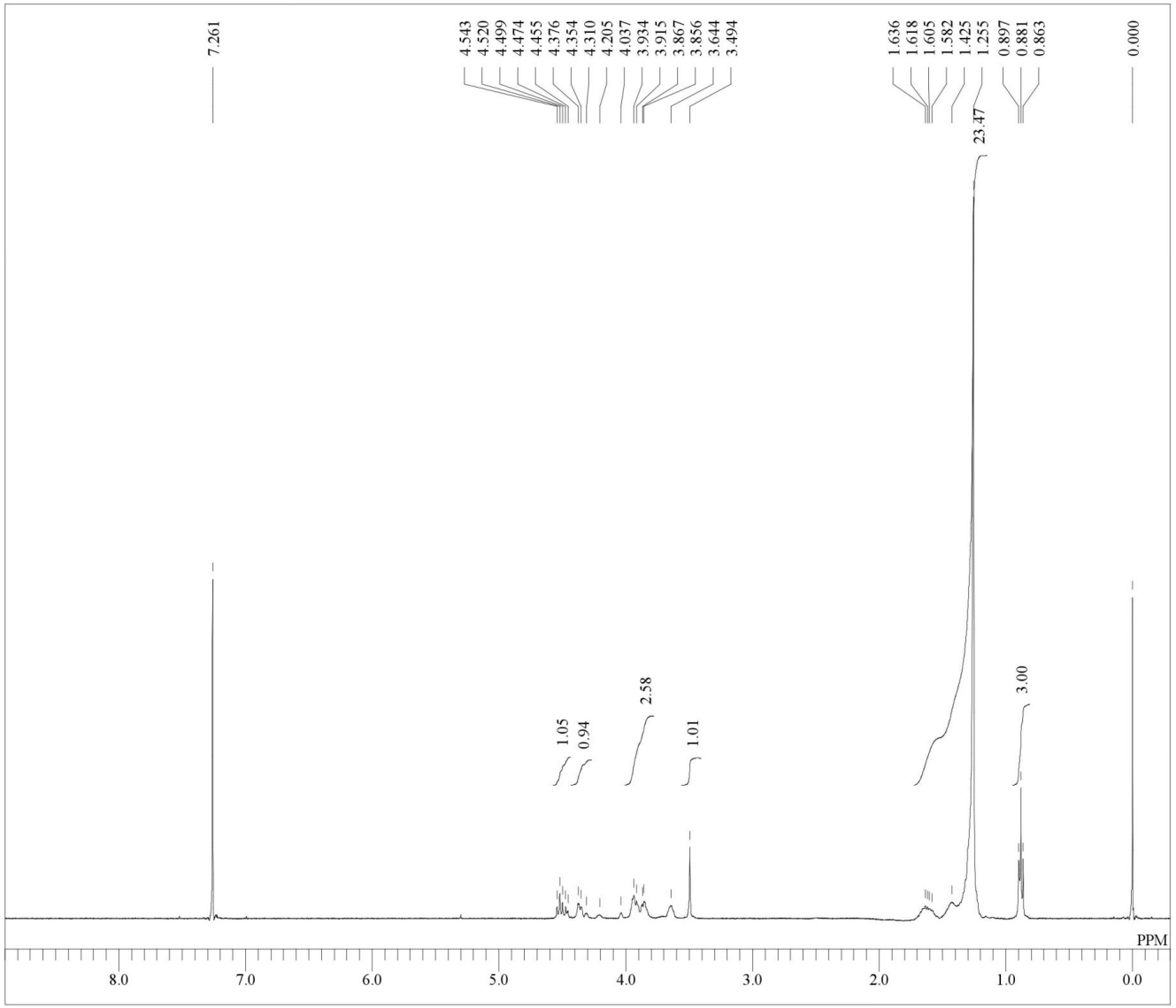



| | |
|---|---|
| DFILE | YAS02-16-13C-did.als |
| COMNT | 4i (13C-NMR) |
| DATIM | Wed Feb 27 15:11:47 2013 |
| OBNUC | 13C |
| EXMOD | BCM |
| OBFRQ | 99.45 MHz |
| OBSET | 94.00 KHz |
| OBFIN | 10309.00 Hz |
| POINT | 32768 |
| FREQU | 26845.64 Hz |
| SCANS | 424 |
| ACQTM | 1.2206 sec |
| PD | 1.7790 sec |
| PW1 | 5.20 usec |
| IRNUC | 1H |
| CTEMP | 21.3 c |
| SLVNT | CDCL3 |
| EXREF | 77.00 ppm |
| BF | 0.24 Hz |
| RGAIN | 23 |

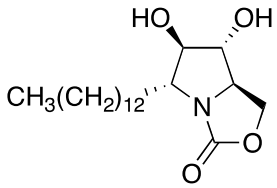



**4i**

4j (1H-NMR)

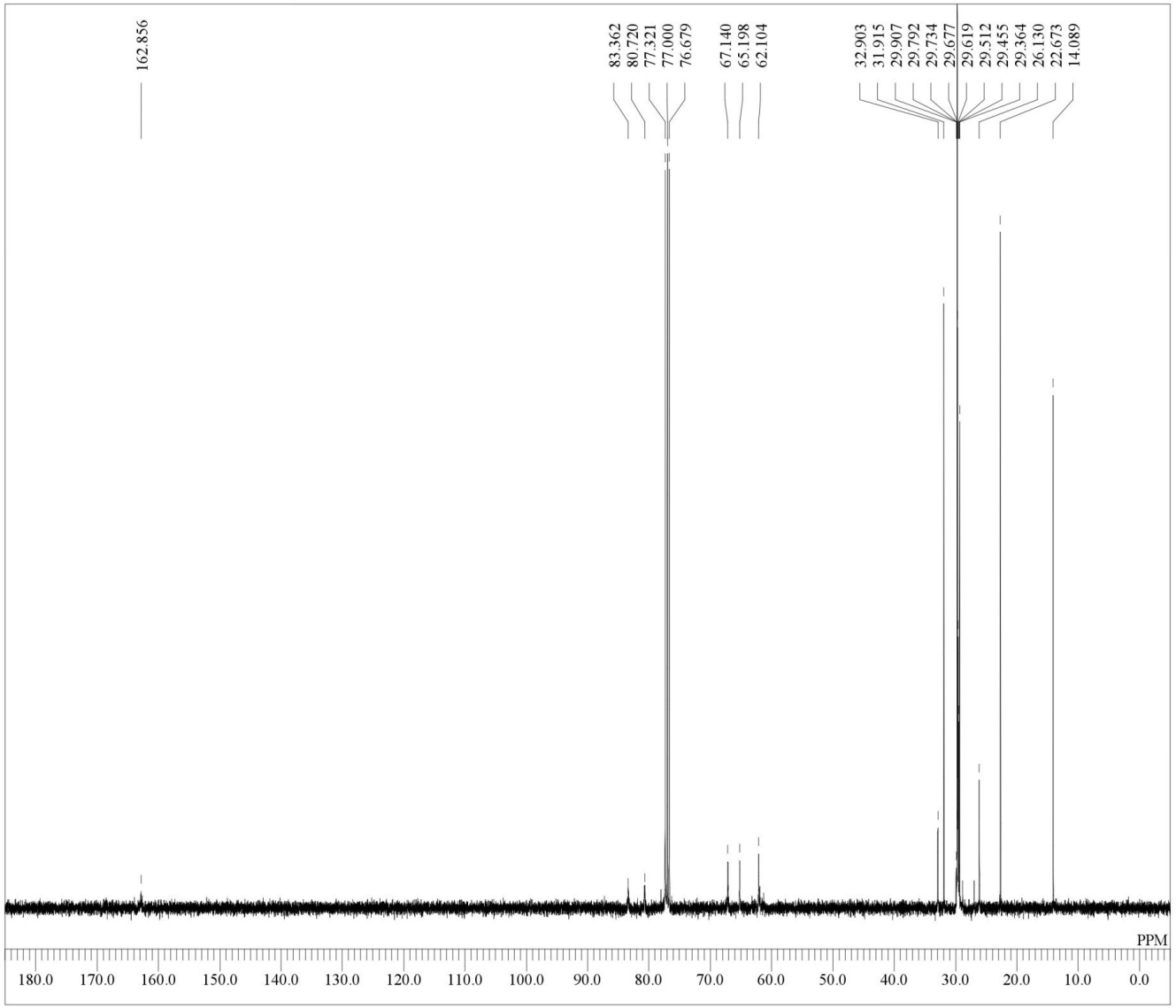



| | |
|---|---|
| DFILE | YAS02-18-3-did.als |
| COMNT | 4j (1H-NMR) |
| DATIM | Wed Nov 14 18:50:18 2012 |
| OBNUC | 1H |
| EXMOD | NON |
| OBFRQ | 395.75 MHz |
| OBSET | 124.00 KHz |
| OBFIN | 10277.00 Hz |
| POINT | 16384 |
| FREQU | 7912.96 Hz |
| SCANS | 8 |
| ACQTM | 2.0705 sec |
| PD | 4.9290 sec |
| PW1 | 5.20 usec |
| IRNUC | 1H |
| CTEMP | 20.8 c |
| SLVNT | CDCL3 |
| EXREF | 0.00 ppm |
| BF | 0.24 Hz |
| RGAIN | 19 |

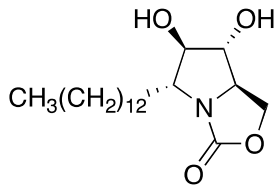



**4j**

4j (13C-NMR)

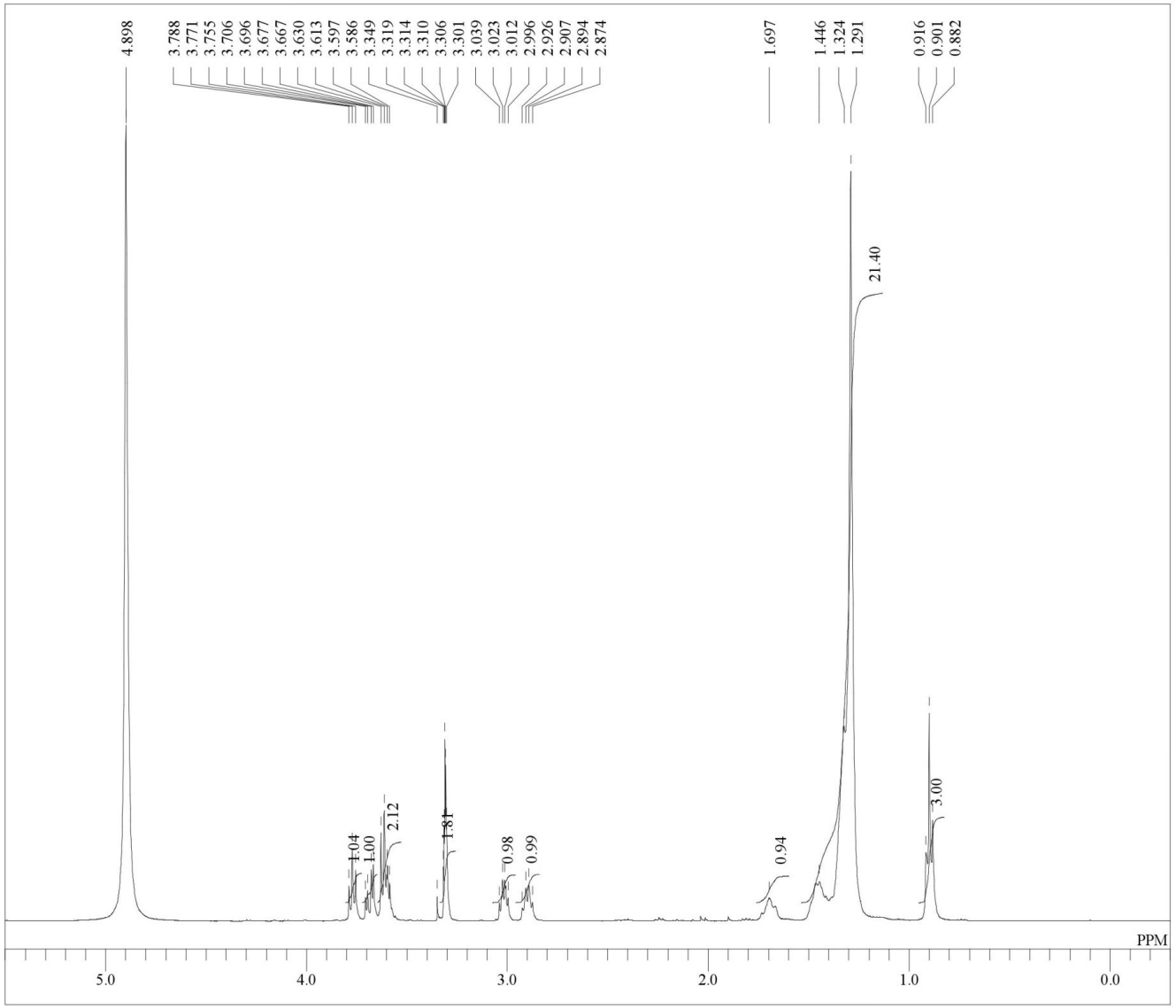



| | |
|---|---|
| DFILE | YAS02-18-13C-did.als |
| COMNT | 4j (13C-NMR) |
| DATIM | Tue Jan 22 10:22:52 2013 |
| OBNUC | 13C |
| EXMOD | BCM |
| OBFRQ | 99.45 MHz |
| OBSET | 94.00 KHz |
| OBFIN | 10309.00 Hz |
| POINT | 32768 |
| FREQU | 26845.64 Hz |
| SCANS | 960 |
| ACQTM | 1.2206 sec |
| PD | 1.7790 sec |
| PW1 | 5.20 usec |
| IRNUC | 1H |
| CTEMP | 21.3 c |
| SLVNT | CDCL3 |
| EXREF | 77.00 ppm |
| BF | 0.24 Hz |
| RGAIN | 23 |

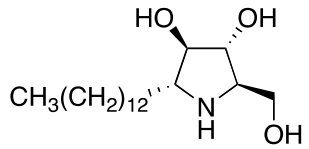



**4j**

5i (1H-NMR)

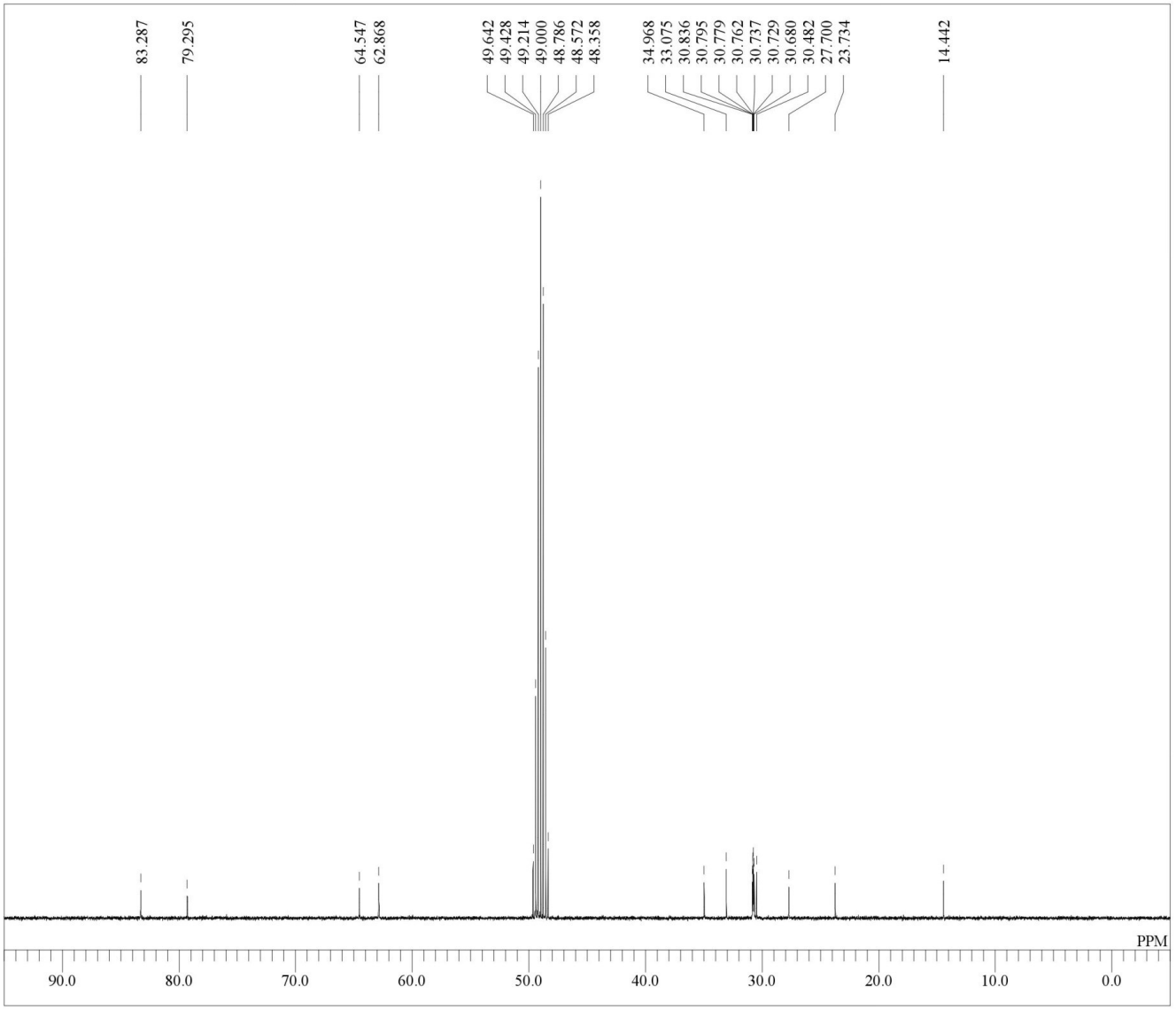



DFILE YAS02-19-2-did.als
COMNT 5i (1H-NMR)
DATIM Tue Nov 13 18:31:33 2012
OBNUC 1H
EXMOD NON
OBFRQ 395.75 MHz
OBSET 124.00 KHz
OBFIN 10277.00 Hz
POINT 16384
FREQU 7912.96 Hz
SCANS 8
ACQTM 2.0705 sec
PD 4.9290 sec
PW1 5.20 usec
IRNUC 1H
CTEMP 19.1 c
SLVNT CD3OD
EXREF 3.31 ppm
BF 0.24 Hz
RGAIN 13

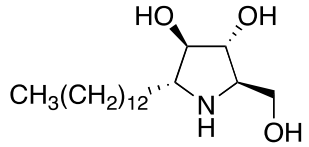



**5i**

5i (13C-NMR)

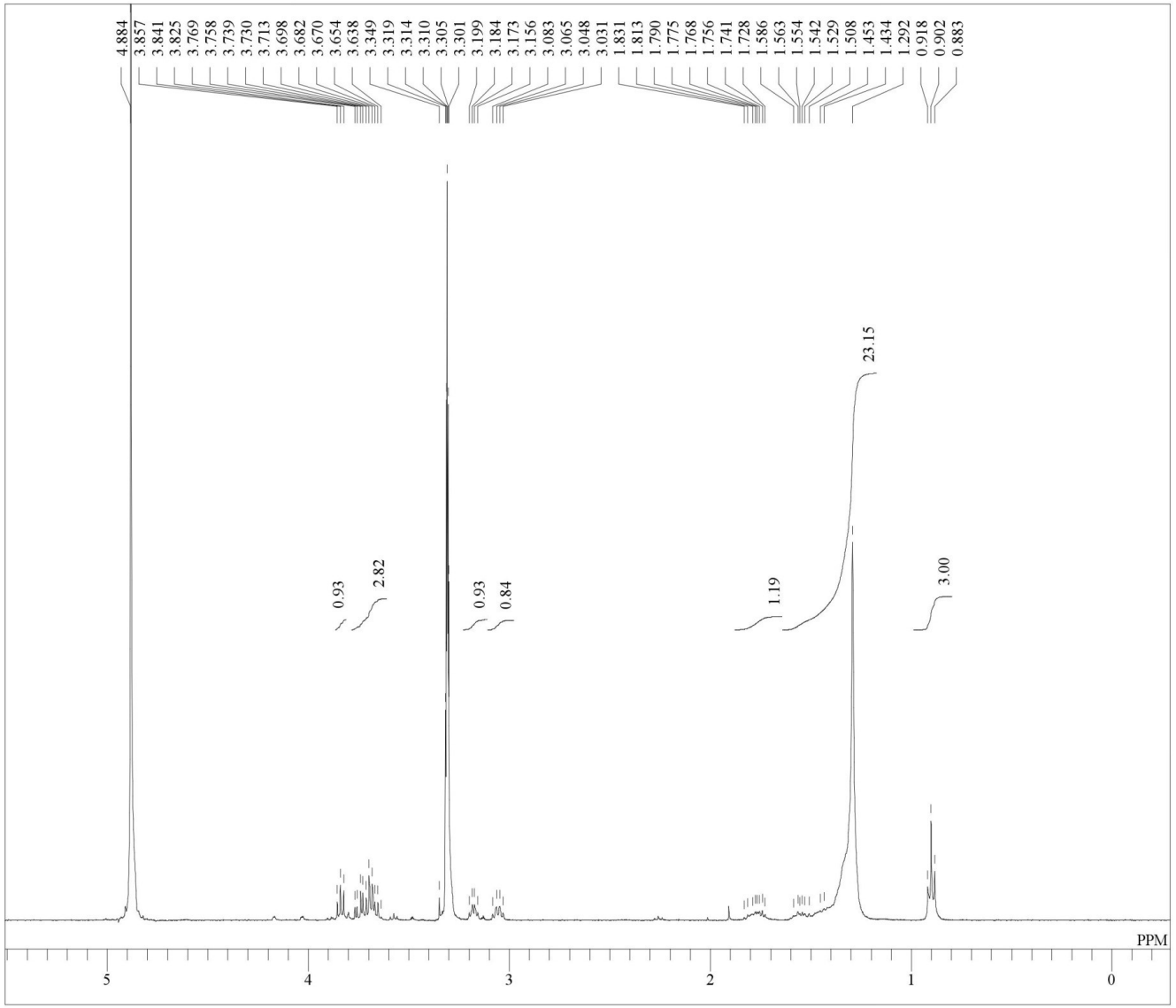



| | |
|---|---|
| DFILE | YAS02-19-C13-did.als |
| COMNT | 5i (13C-NMR) |
| DATIM | Tue Nov 13 18:54:08 2012 |
| OBNUC | 13C |
| EXMOD | BCM |
| OBFRQ | 99.45 MHz |
| OBSET | 94.00 KHz |
| OBFIN | 10309.00 Hz |
| POINT | 32768 |
| FREQU | 26845.64 Hz |
| SCANS | 380 |
| ACQTM | 1.2206 sec |
| PD | 1.7790 sec |
| PW1 | 5.20 usec |
| IRNUC | 1H |
| CTEMP | 21.3 c |
| SLVNT | CD3OD |
| EXREF | 49.00 ppm |
| BF | 0.24 Hz |
| RGAIN | 22 |

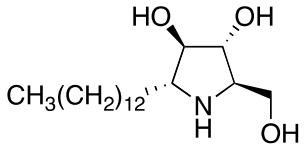



**5i**

5j (1H-NMR)

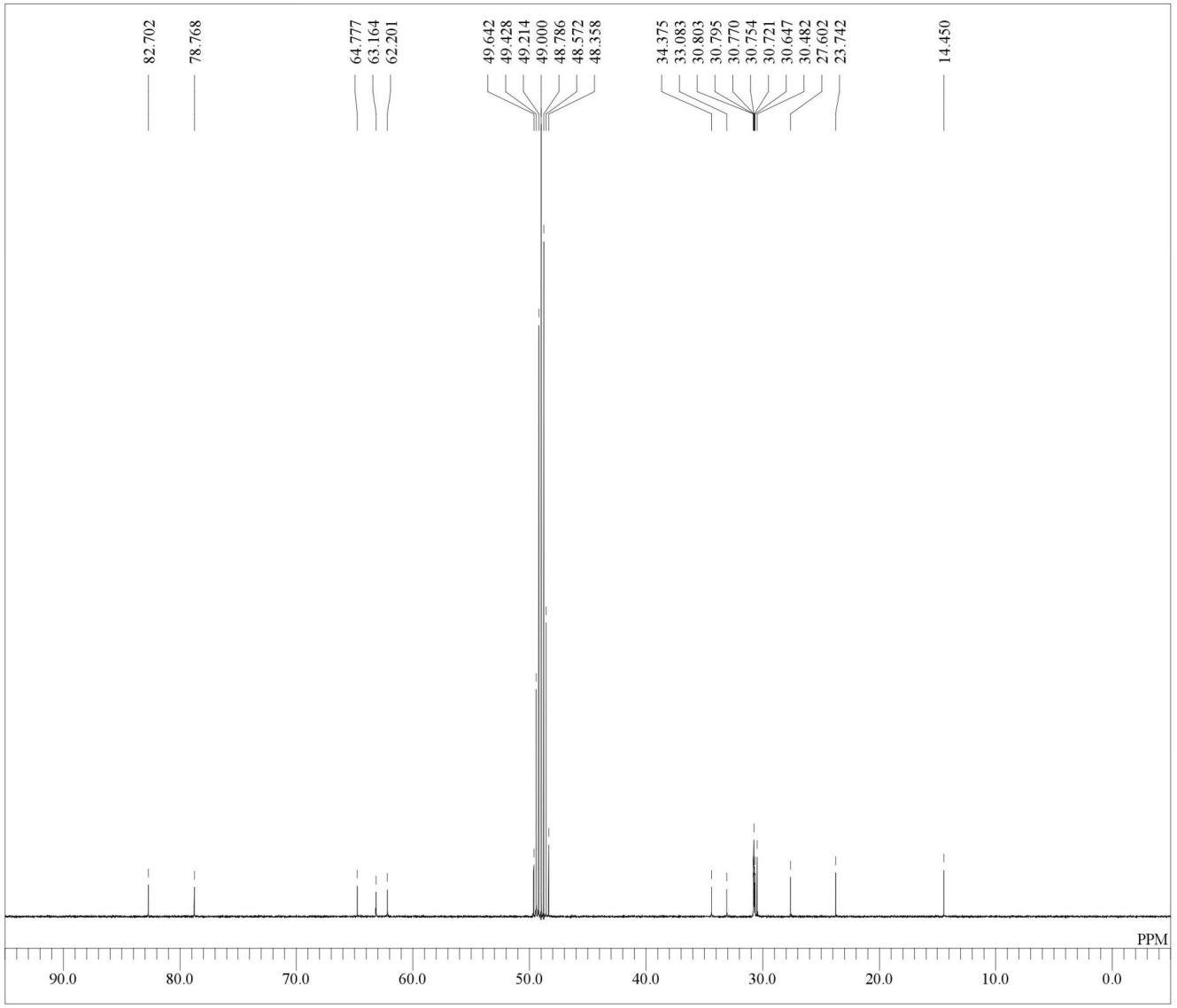



| | |
|---|---|
| DFILE | YAS02-20-did.als |
| COMNT | 5j (1H-NMR) |
| DATIM | Thu Nov 15 18:53:44 2012 |
| OBNUC | 1H |
| EXMOD | NON |
| OBFRQ | 395.75 MHz |
| OBSET | 124.00 KHz |
| OBFIN | 10277.00 Hz |
| POINT | 16384 |
| FREQU | 7912.96 Hz |
| SCANS | 8 |
| ACQTM | 2.0705 sec |
| PD | 4.9290 sec |
| PW1 | 5.20 usec |
| IRNUC | 1H |
| CTEMP | 20.6 c |
| SLVNT | CD3OD |
| EXREF | 3.31 ppm |
| BF | 0.24 Hz |
| RGAIN | 18 |

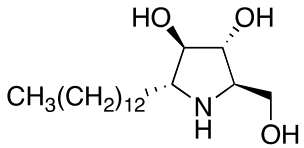



**5j**

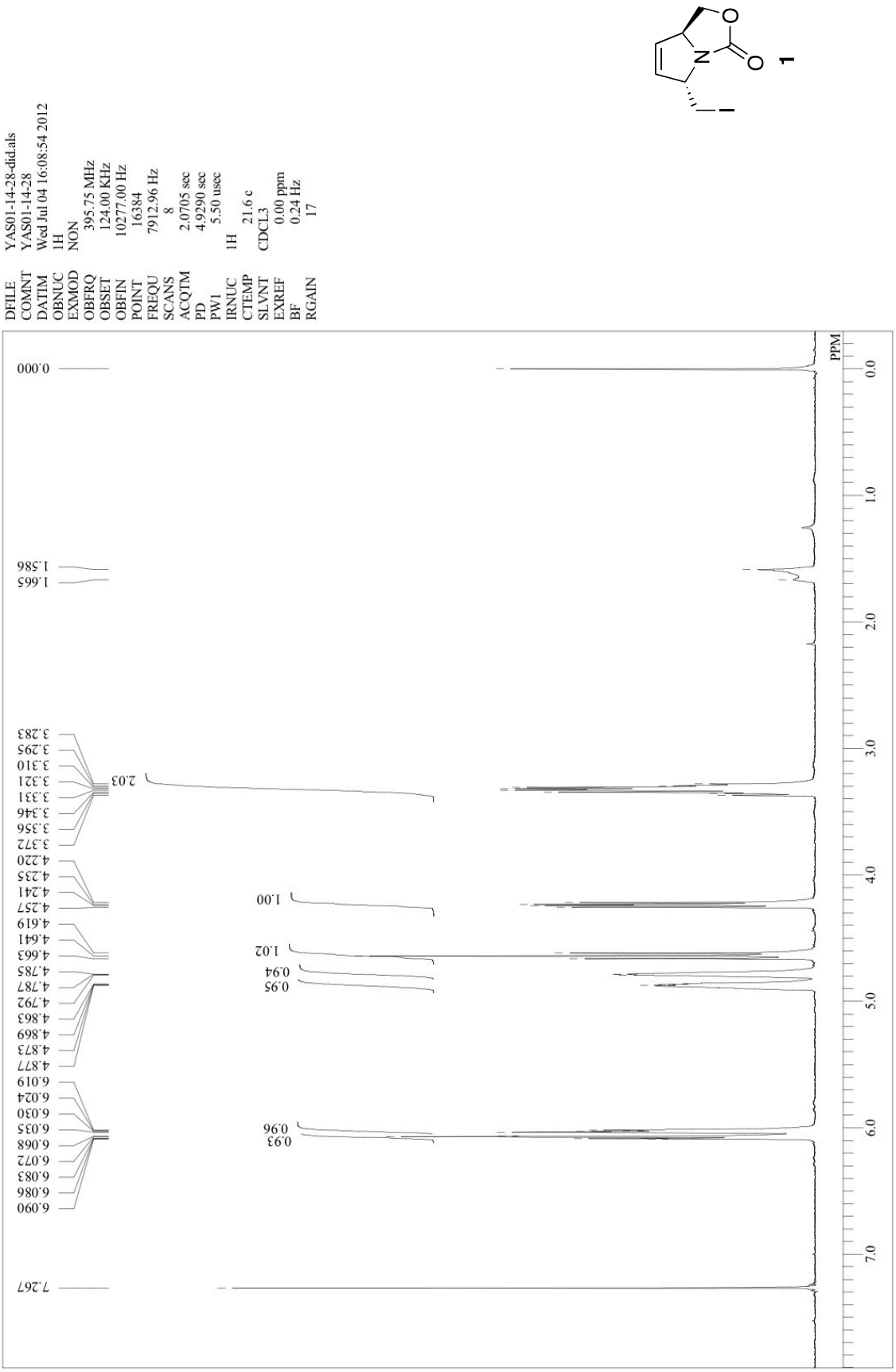
5j (13C-NMR)

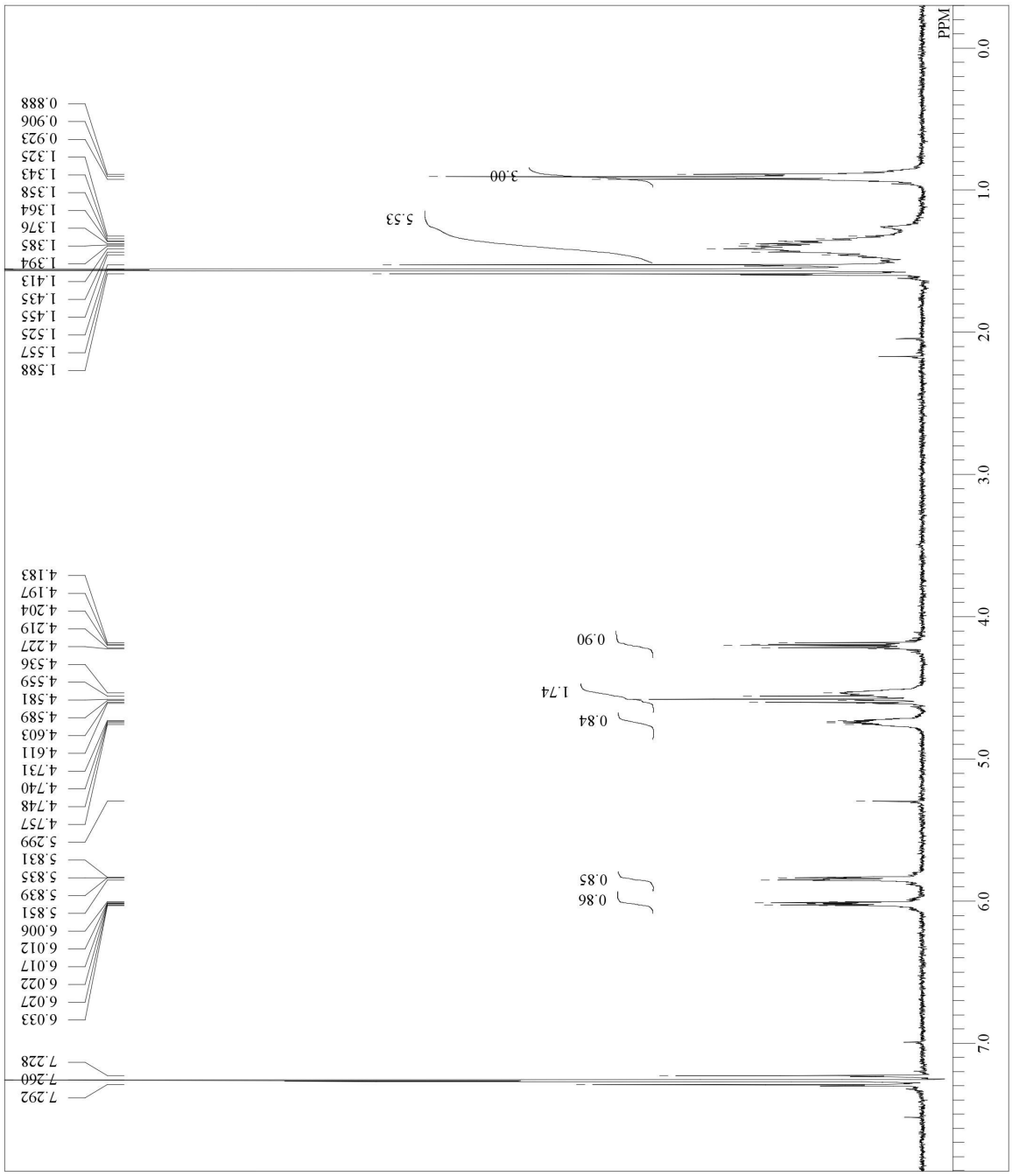



| | |
|---|---|
| DFILE | YAS02-20-2-C13-did.als |
| COMNT | 5j (13C-NMR) |
| DATIM | Mon Nov 19 12:59:34 2012 |
| OBNUC | 13C |
| EXMOD | BCM |
| OBFRQ | 99.45 MHz |
| OBSET | 94.00 KHz |
| OBFIN | 10309.00 Hz |
| POINT | 32768 |
| FREQU | 26845.64 Hz |
| SCANS | 800 |
| ACQTM | 1.2206 sec |
| PD | 1.7790 sec |
| PW1 | 5.20 usec |
| IRNUC | 1H |
| CTEMP | 21.4 c |
| SLVNT | CD3OD |
| EXREF | 49.00 ppm |
| BF | 0.24 Hz |
| RGAIN | 22 |




**5j**


DFILE YAS01-14-28-did.als
COMNT YAS01-14-28
DATIM Wed Jul 04 16:08:54 2012
OBNUC 1H
EXMOD NON
OBFRQ 395.75 MHz
OBSET 124.00 KHz
OBFIN 10277.00 Hz
POINT 16384
FREQU 7912.96 Hz
SCANS 8
ACQTM 2.0705 sec
PD 4.9290 sec
PW1 5.50 usec
IRNUC 1H
CTEMP 21.6 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.24 Hz
RGAIN 17
0.000
1.586
1.665
2.03
3.283
3.295
3.310
3.321
3.331
3.346
3.356
3.372
4.220
4.235
4.241
4.257
1.00
4.619
4.641
4.663
1.02
4.785
4.787
4.792
0.95
0.94
4.863
4.869
4.873
4.877
6.019
6.024
6.030
6.035
6.068
6.072
6.083
6.086
6.090
0.93
0.96
7.267
PPM
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0


DFILE KEM_1_29_1_PRODUCT-T.als
COMNT KEM_1_28_1_PRODUCT
DATIM Wed Jul 02 16:34:38 2008
OBNUC 1H
EXMOD NON
OBFRQ 395.75 MHz
OBSET 124.00 KHz
OBFIN 10277.00 Hz
POINT 16384
FREQU 7912.96 Hz
SCANS 8
ACQTM 2.0705 sec
PD 4.9290 sec
PW1 5.20 usec
IRNUC 1H
CTEMP 23.1 c
SLVNT CDCL3
EXREF 7.26 ppm
BF 0.24 Hz
RGAIN 22
PPM
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
0.86
0.85
0.90
1.74
0.84
3.00
5.53
7.292
7.260
7.228
6.033
6.027
6.022
6.017
6.012
6.006
5.851
5.839
5.835
5.831
5.299
4.757
4.748
4.740
4.731
4.611
4.603
4.589
4.581
4.559
4.536
4.227
4.219
4.204
4.197
4.183
1.588
1.557
1.525
1.455
1.435
1.413
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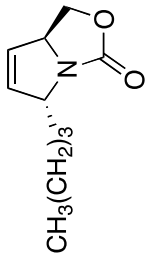
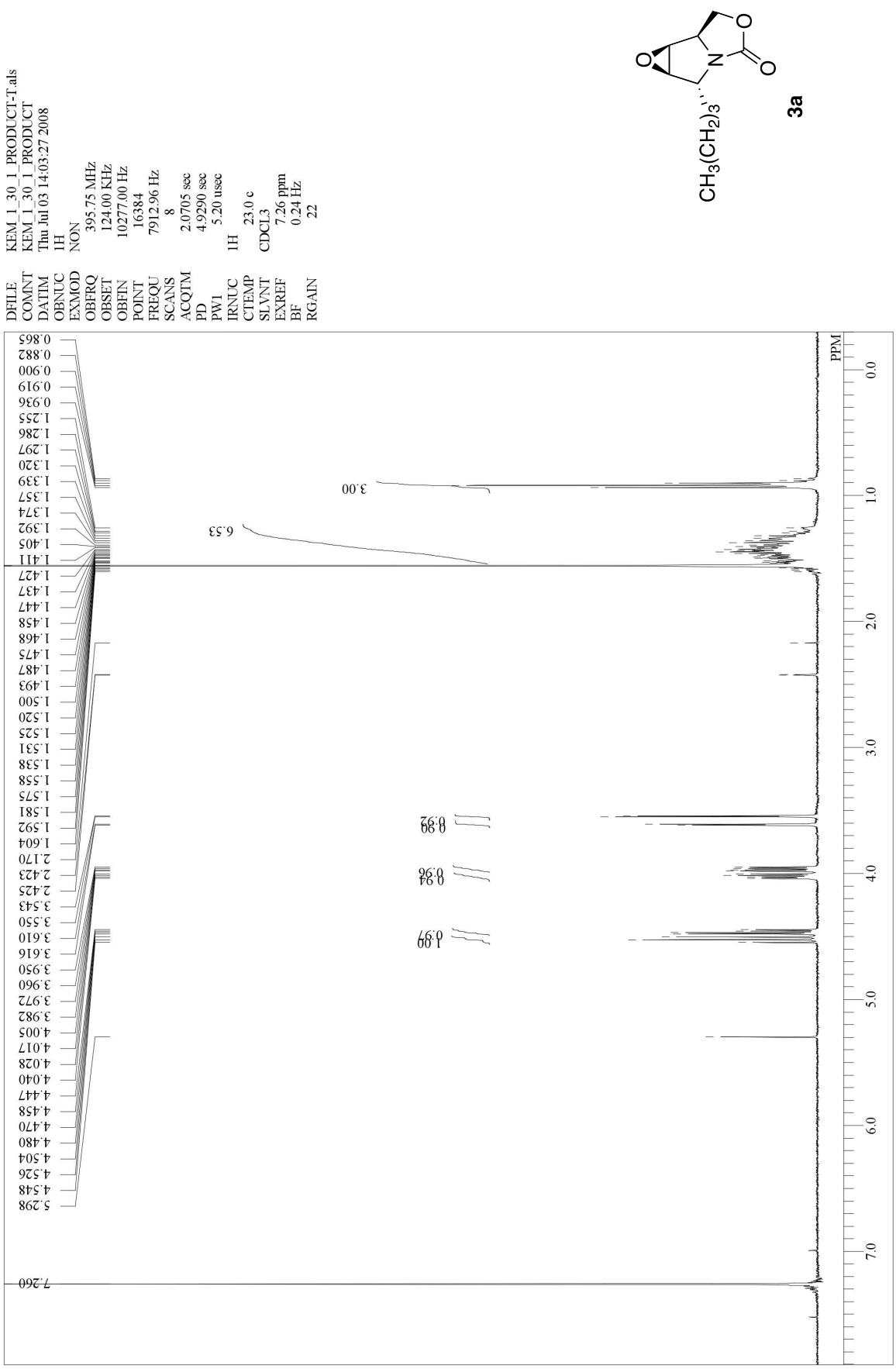
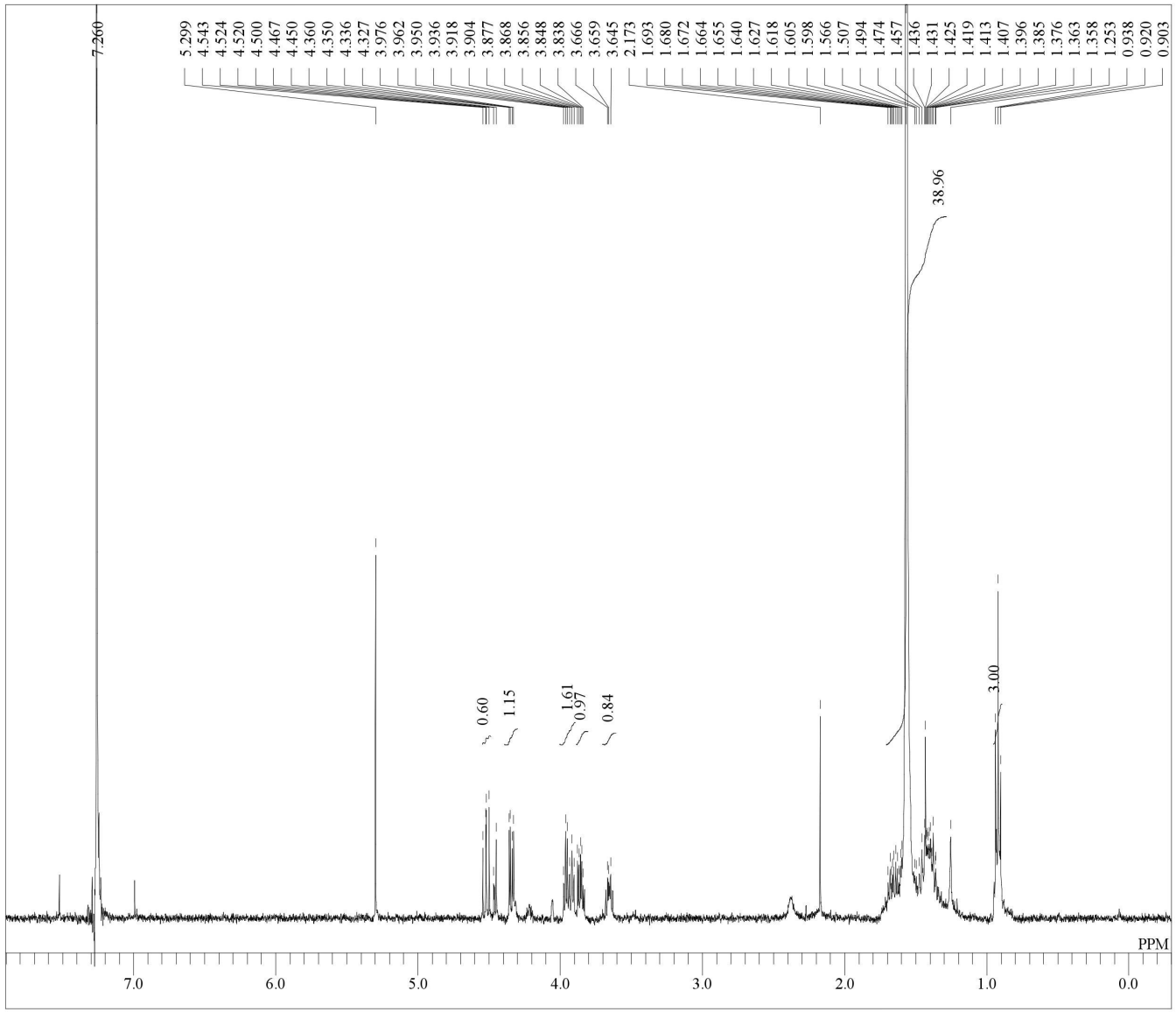
1.385
1.376
1.364
1.358
1.343
1.325
0.923
0.906
0.888

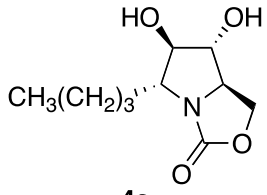

O
O
N
CH3(CH2)3

**2a**

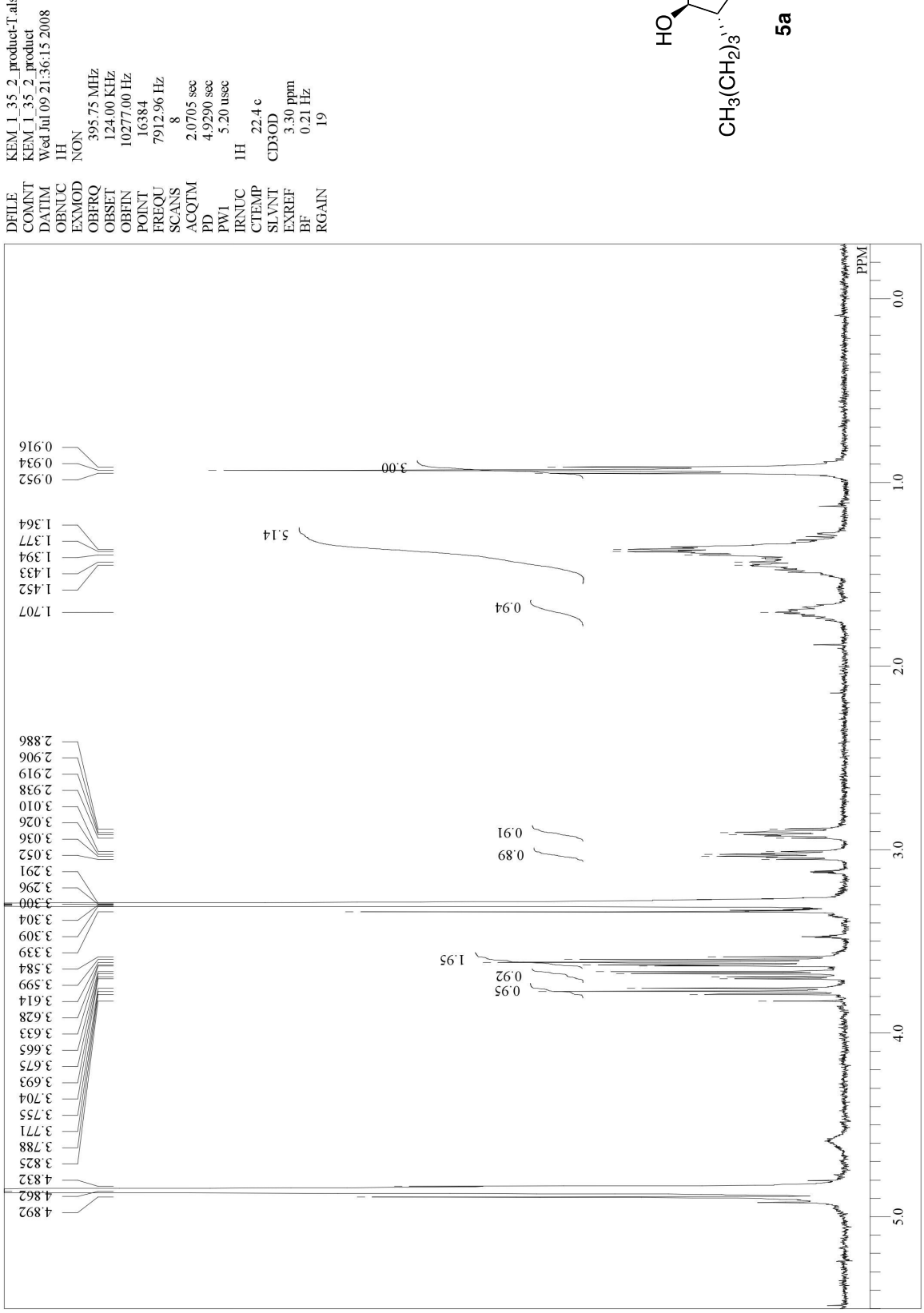

DFILE KEM_1_30_1_PRODUCT-T.als
COMNT KEM_1_30_1_PRODUCT
DATIM Thu Jul 03 14:03:27 2008
OBNUC 1H
EXMOD NON
OBFRQ 395.75 MHz
OBSET 124.00 KHz
OBFIN 10277.00 Hz
POINT 16384
FREQU 7912.96 Hz
SCANS 8
ACQTM 2.0705 sec
PD 4.9290 sec
PW1 5.20 usec
IRNUC 1H
CTEMP 23.0 c
SLVNT CDCL3
EXREF 7.26 ppm
BF 0.24 Hz
RGAIN 22
7.260
5.298
4.548
4.526
4.504
4.480
4.470
4.458
4.447
4.040
4.028
4.017
4.005
3.982
3.972
3.960
3.950
3.616
3.610
3.550
3.543
2.425
2.423
2.170
1.604
1.592
1.581
1.575
1.558
1.538
1.531
1.525
1.520
1.500
1.493
1.487
1.475
1.468
1.458
1.447
1.437
1.427
1.411
1.405
1.392
1.374
1.357
1.339
1.320
1.297
1.286
1.255
0.936
0.919
0.900
0.882
0.865
6.53
3.00
1.00
0.97
0.94
0.96
0.89
0.92
PPM
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
CH3(CH2)3
O
O
N
O
3a




| | |
|---|---|
| DFILE | KEM_1_33_1_PRODUCT-T.als |
| COMNT | KEM_1_33_1_PRODUCT |
| DATIM | Tue Jul 08 16:28:06 2008 |
| OBNUC | 1H |
| EXMOD | NON |
| OBFRQ | 395.75 MHz |
| OBSET | 124.00 KHz |
| OBFIN | 10277.00 Hz |
| POINT | 16384 |
| FREQU | 7912.96 Hz |
| SCANS | 8 |
| ACQTM | 2.0705 sec |
| PD | 4.9290 sec |
| PW1 | 5.20 usec |
| IRNUC | 1H |
| CTEMP | 22.8 c |
| SLVNT | CDCL3 |
| EXREF | 7.26 ppm |
| BF | 0.24 Hz |
| RGAIN | 24 |

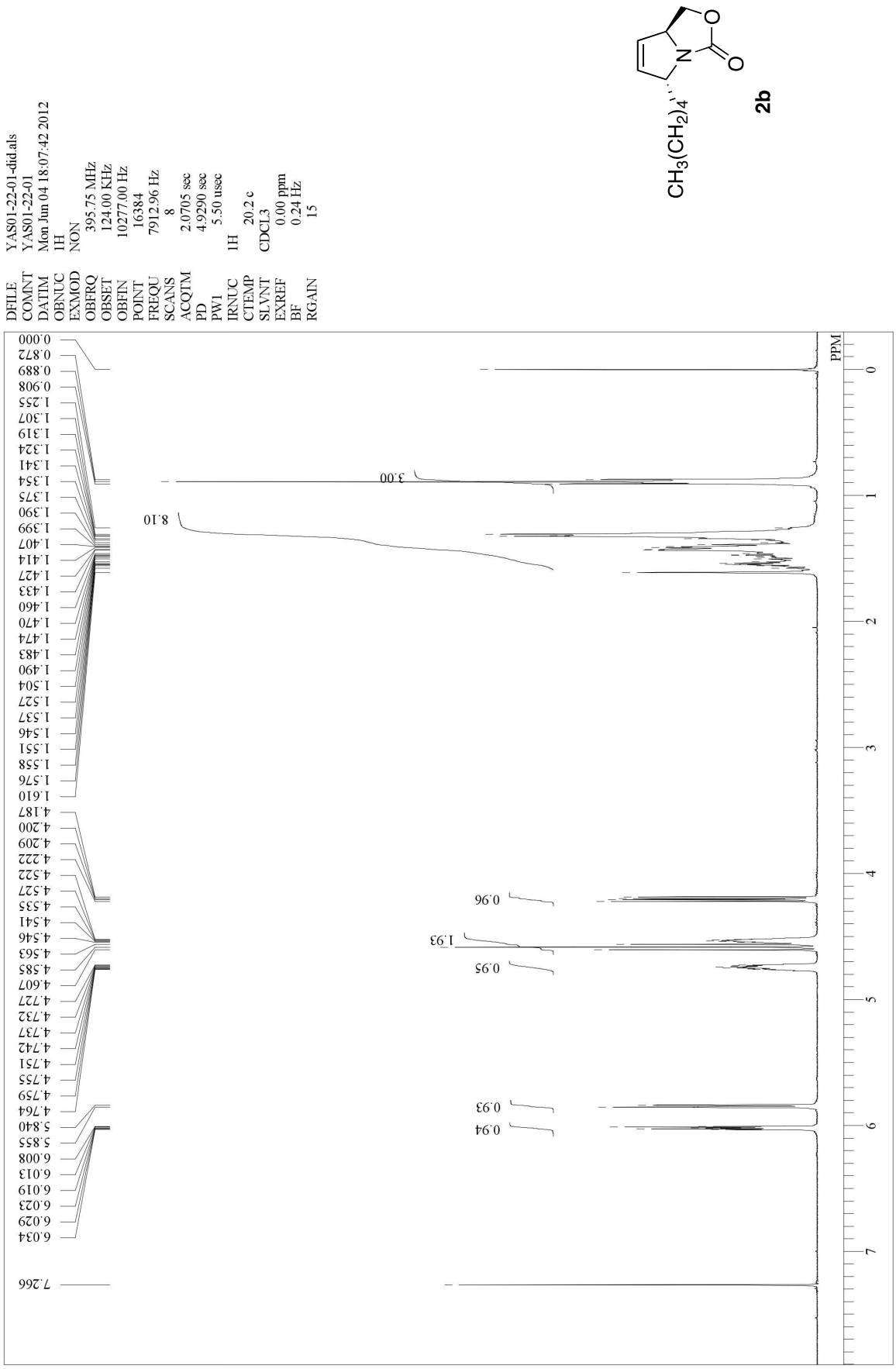



**4a**


DFILE KEM_1_35_2_product-T.als
COMNT KEM_1_35_2_product
DATIM Wed Jul 09 21:36:15 2008
OBNUC 1H
EXMOD NON
OBFRQ 395.75 MHz
OBSET 124.00 KHz
OBFIN 10277.00 Hz
POINT 16384
FREQU 7912.96 Hz
SCANS 8
ACQTM 2.0705 sec
PD 4.9290 sec
PW1 5.20 usec
IRNUC 1H
CTEMP 22.4 c
SLVNT CD3OD
EXREF 3.30 ppm
BF 0.21 Hz
RGAIN 19
4.892
4.862
4.832
3.825
3.788
3.771
3.755
3.704
3.693
3.675
3.665
3.633
3.628
3.614
3.599
3.584
3.339
3.309
3.304
3.300
3.296
3.291
3.052
3.036
3.026
3.010
2.938
2.919
2.906
2.886
1.707
1.452
1.433
1.394
1.377
1.364
0.952
0.934
0.916
3.00
5.14
0.94
0.91
0.89
1.95
0.95
0.92
PPM
5.0
4.0
3.0
2.0
1.0
0.0

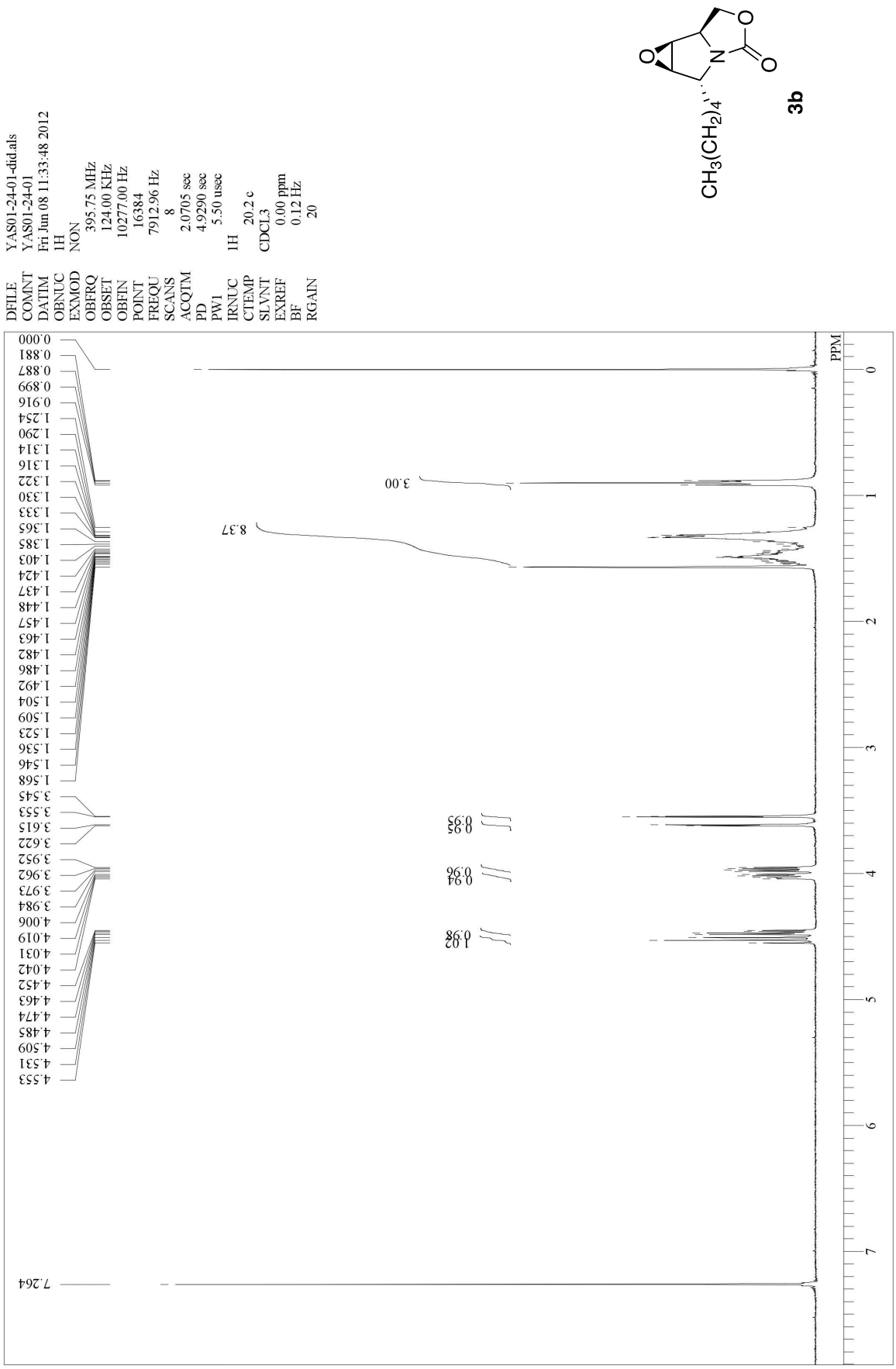

OH
HO
N
H
OH
$CH_3(CH_2)_3$

**5a**


DFILE YAS01-22-01-did.als
COMNT YAS01-22-01
DATIM Mon Jun 04 18:07:42 2012
OBNUC 1H
EXMOD NON
OBFRQ 395.75 MHz
OBSET 124.00 KHz
OBFIN 10277.00 Hz
POINT 16384
FREQU 7912.96 Hz
SCANS 8
ACQTM 2.0705 sec
PD 4.9290 sec
PW1 5.50 usec
IRNUC 1H
CTEMP 20.2 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.24 Hz
RGAIN 15
7.266
6.034
6.029
6.023
6.019
6.013
6.008
5.855
5.840
4.764
4.759
4.755
4.751
4.742
4.737
4.732
4.727
4.607
4.585
4.563
4.546
4.541
4.535
4.527
4.522
4.222
4.209
4.200
4.187
1.610
1.576
1.558
1.551
1.546
1.537
1.527
1.504
1.490
1.483
1.474
1.470
1.460
1.433
1.427
1.414
1.407
1.399
1.390
1.375
1.354
1.341
1.324
1.319
1.307
1.255
0.908
0.889
0.872
0.000
8.10
3.00
0.96
1.93
0.95
0.93
0.94
PPM
0
1
2
3
4
5
6
7

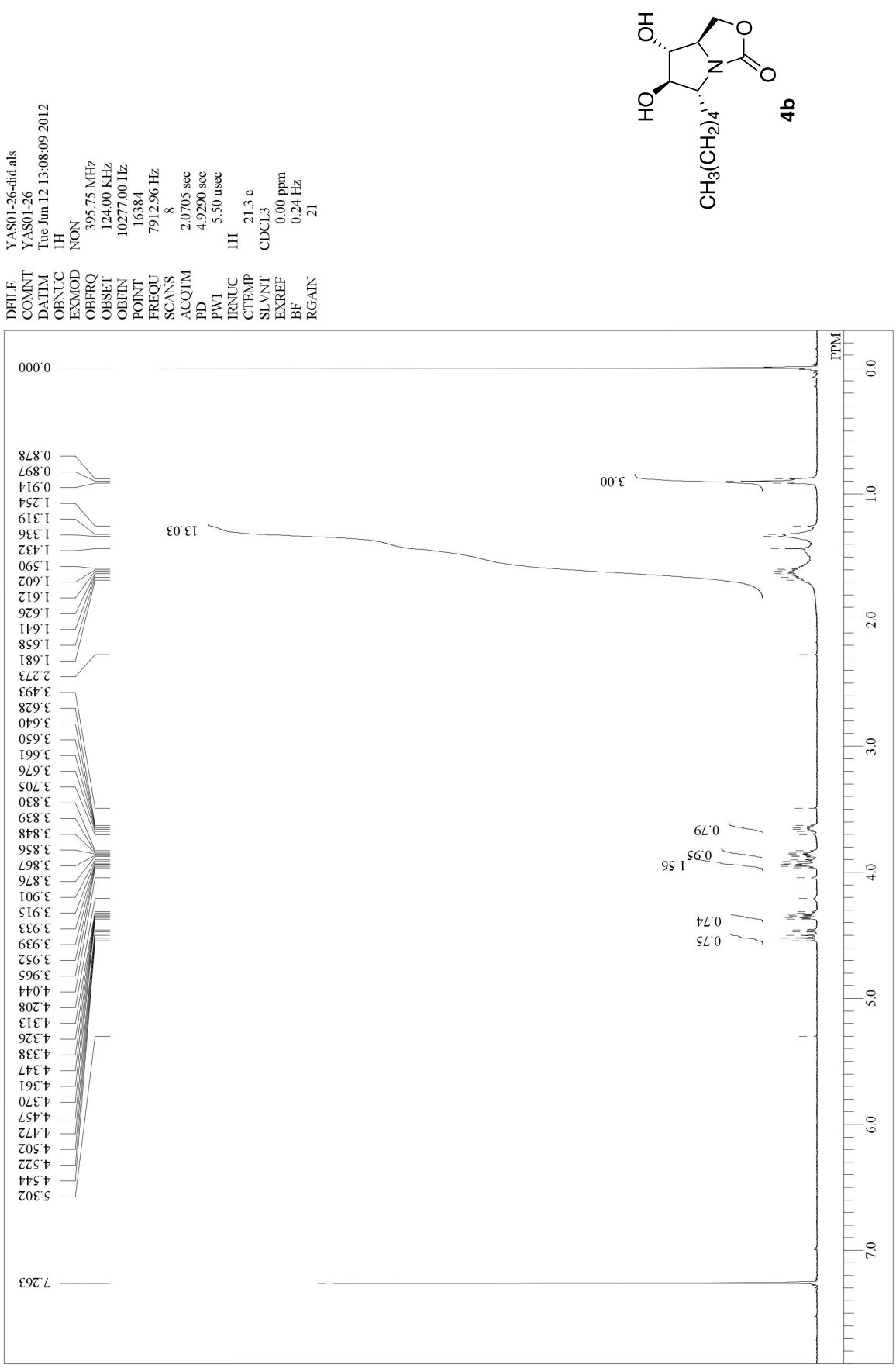

CH3(CH2)4
O
O
N
O

**2b**


DFILE YAS01-24-01-did.als
COMNT YAS01-24-01
DATIM Fri Jun 08 11:33:48 2012
OBNUC 1H
EXMOD NON
OBFRQ 395.75 MHz
OBSET 124.00 KHz
OBFIN 10277.00 Hz
POINT 16384
FREQU 7912.96 Hz
SCANS 8
ACQTM 2.0705 sec
PD 4.9290 sec
PW1 5.50 usec
IRNUC 1H
CTEMP 20.2 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 20
7.264
4.553
4.531
4.509
4.485
4.474
4.463
4.452
4.042
4.031
4.019
4.006
3.984
3.973
3.962
3.952
3.622
3.615
3.553
3.545
1.568
1.546
1.536
1.523
1.509
1.504
1.492
1.486
1.482
1.463
1.457
1.448
1.437
1.424
1.403
1.385
1.365
1.333
1.330
1.322
1.316
1.314
1.290
1.254
0.916
0.899
0.887
0.881
0.000
8.37
3.00
0.95
0.94
1.02
PPM
0
1
2
3
4
5
6
7

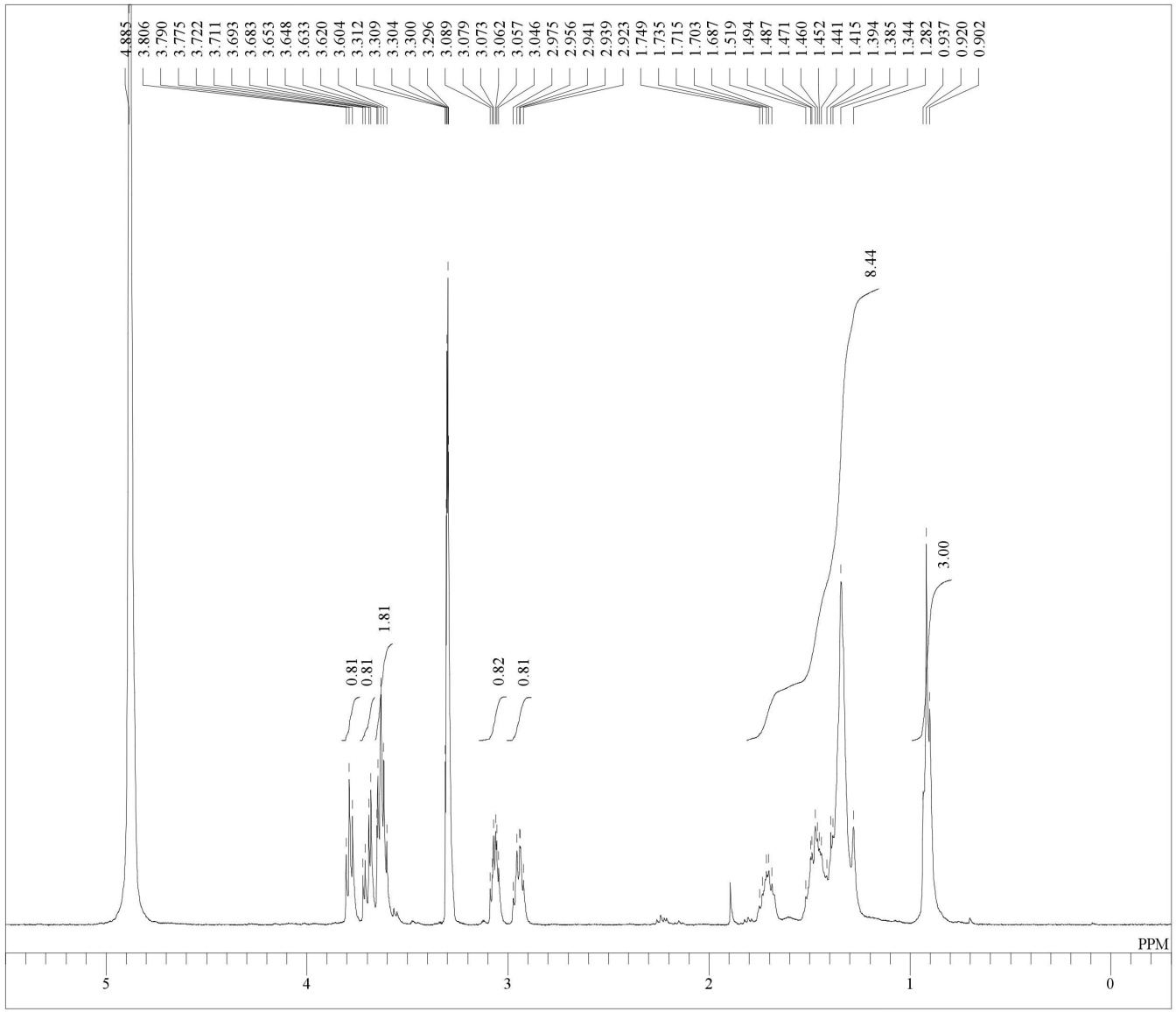

O
O
N
O
O
CH3(CH2)4

**3b**

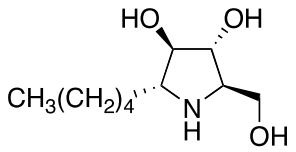

DFILE YAS01-26-did.als
COMNT YAS01-26
DATIM Tue Jun 12 13:08:09 2012
OBNUC 1H
EXMOD NON
OBFRQ 395.75 MHz
OBSET 124.00 KHz
OBFIN 10277.00 Hz
POINT 16384
FREQU 7912.96 Hz
SCANS 8
ACQTM 2.0705 sec
PD 4.9290 sec
PW1 5.50 usec
IRNUC 1H
CTEMP 21.3 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.24 Hz
RGAIN 21
0.000
7.263
5.302
4.544
4.522
4.502
4.472
4.457
4.370
4.361
4.347
4.338
4.326
4.313
4.208
4.044
3.965
3.952
3.939
3.933
3.915
3.901
3.876
3.867
3.856
3.848
3.839
3.830
3.705
3.676
3.661
3.650
3.640
3.628
3.493
2.273
1.681
1.658
1.641
1.626
1.612
1.602
1.590
1.432
1.336
1.319
1.254
0.914
0.897
0.878
13.03
3.00
0.79
1.56
0.95
0.75
0.74
PPM
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0


OH
HO
O
O
N
CH3(CH2)4

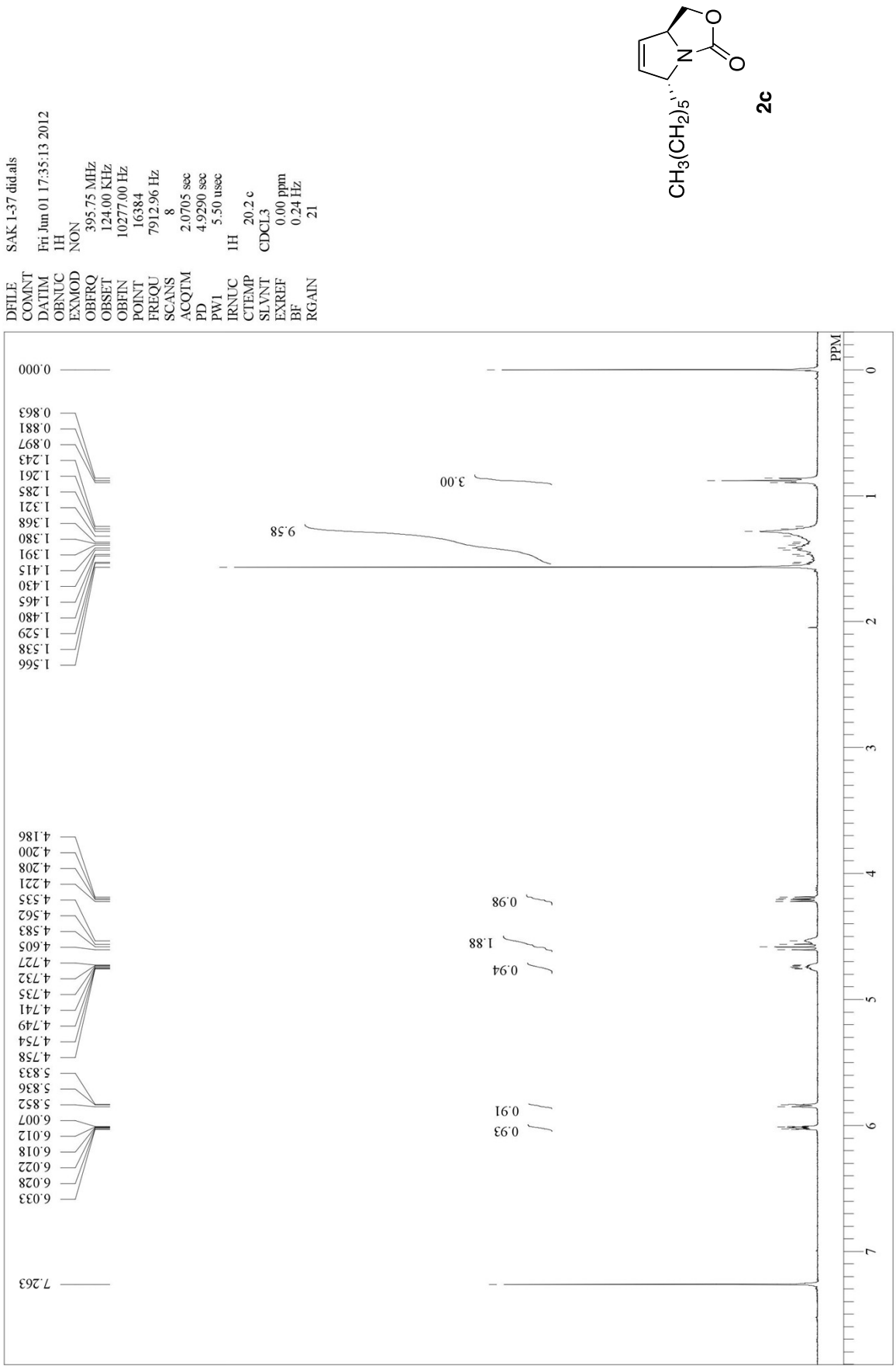
**4b**




| | |
|---|---|
| DFILE | YAS01-27-02-did.als |
| COMNT | YAS01-27-02 |
| DATIM | Wed Jun 20 10:52:11 2012 |
| OBNUC | 1H |
| EXMOD | NON |
| OBFRQ | 395.75 MHz |
| OBSET | 124.00 KHz |
| OBFIN | 10277.00 Hz |
| POINT | 16384 |
| FREQU | 7912.96 Hz |
| SCANS | 8 |
| ACQTM | 2.0705 sec |
| PD | 4.9290 sec |
| PW1 | 5.50 usec |
| IRNUC | 1H |
| CTEMP | 20.8 c |
| SLVNT | CD3OD |
| EXREF | 3.30 ppm |
| BF | 0.24 Hz |
| RGAIN | 16 |

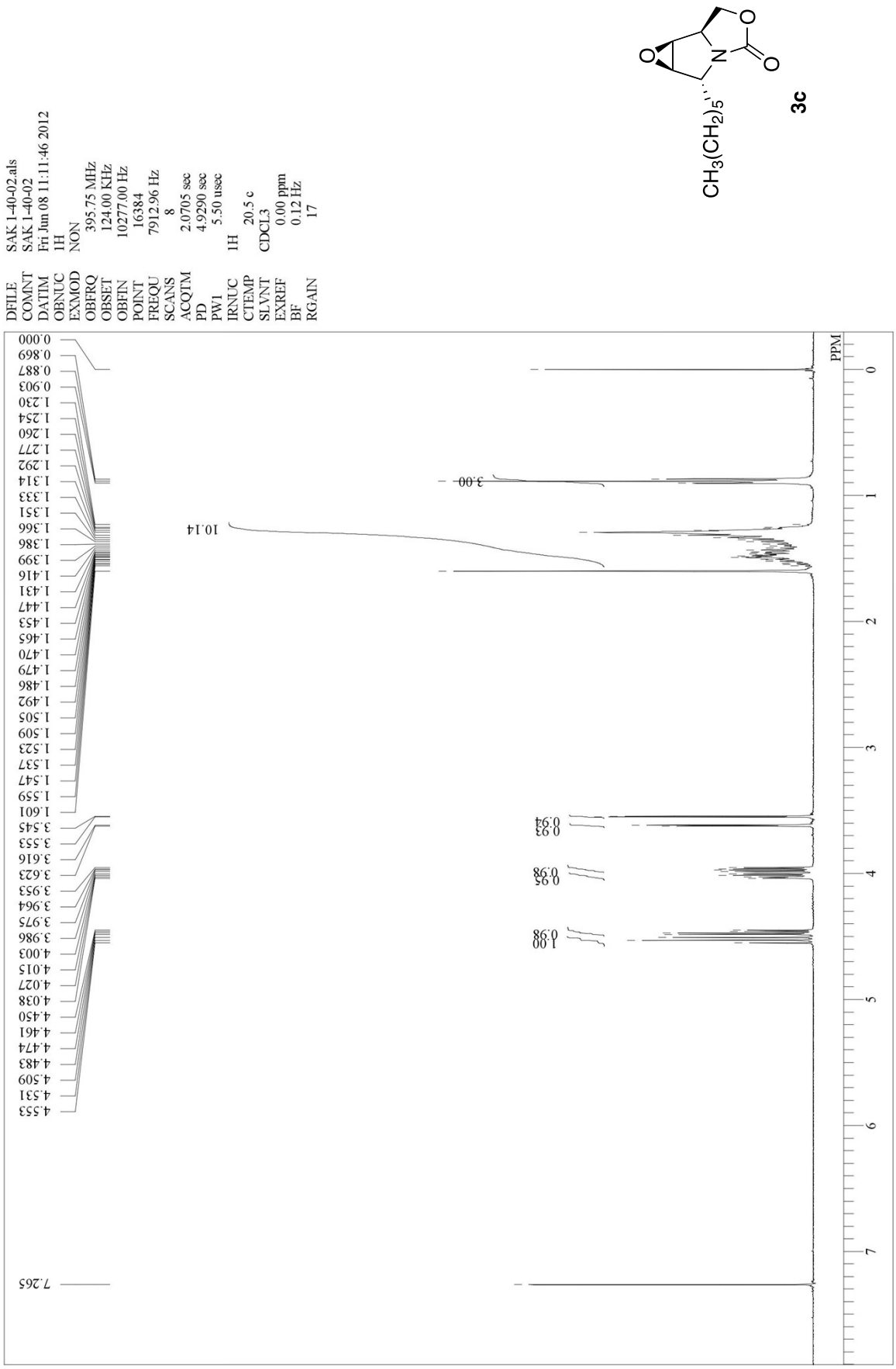



**5b**


DFILE SAK 1-37 did.als
COMNT
DATIM Fri Jun 01 17:35:13 2012
OBNUC 1H
EXMOD NON
OBFRQ 395.75 MHz
OBSET 124.00 KHz
OBFIN 10277.00 Hz
POINT 16384
FREQU 7912.96 Hz
SCANS 8
ACQTM 2.0705 sec
PD 4.9290 sec
PW1 5.50 usec
IRNUC 1H
CTEMP 20.2 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.24 Hz
RGAIN 21
0.000
0.863
0.881
0.897
1.243
1.261
1.285
1.321
1.368
1.380
1.391
1.415
1.430
1.465
1.480
1.529
1.538
1.566
3.00
9.58
0.98
1.88
0.94
0.93
0.91
4.186
4.200
4.208
4.221
4.535
4.562
4.583
4.603
4.727
4.732
4.735
4.741
4.749
4.754
4.758
5.833
5.836
5.852
6.007
6.012
6.018
6.022
6.028
6.033
7.263
PPM
0
1
2
3
4
5
6
7

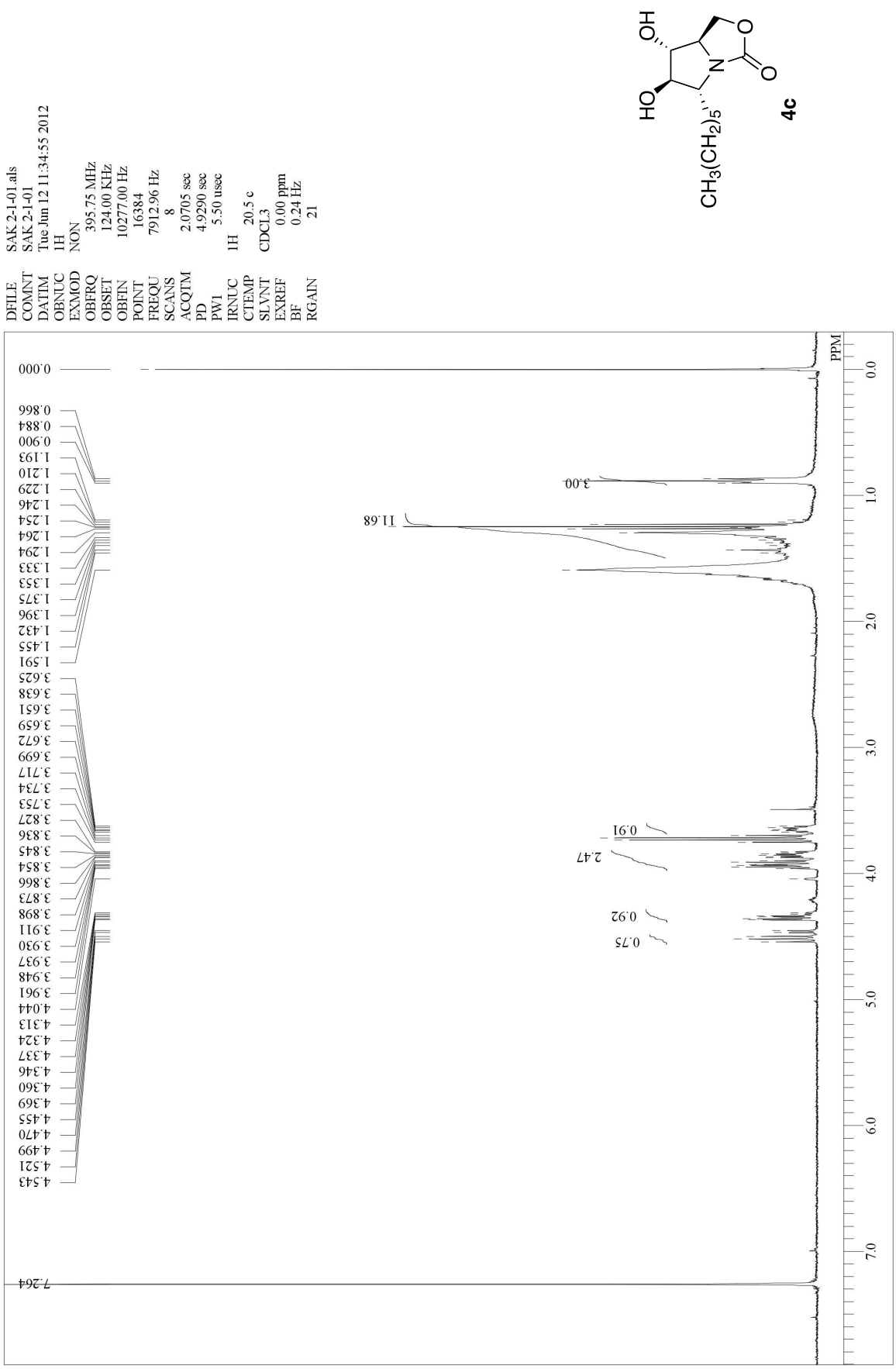

CH3(CH2)5
O
O
N
O

**2c**


DFILE SAK 1-40-02.als
COMNT SAK 1-40-02
DATIM Fri Jun 08 11:11:46 2012
OBNUC 1H
EXMOD NON
OBFRQ 395.75 MHz
OBSET 124.00 KHz
OBFIN 10277.00 Hz
POINT 16384
FREQU 7912.96 Hz
SCANS 8
ACQTM 2.0705 sec
PD 4.9290 sec
PW1 5.50 usec
IRNUC 1H
CTEMP 20.5 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 17
PPM
7.265
10.14
3.00
1.00
0.98
0.95
0.98
0.93
0.94

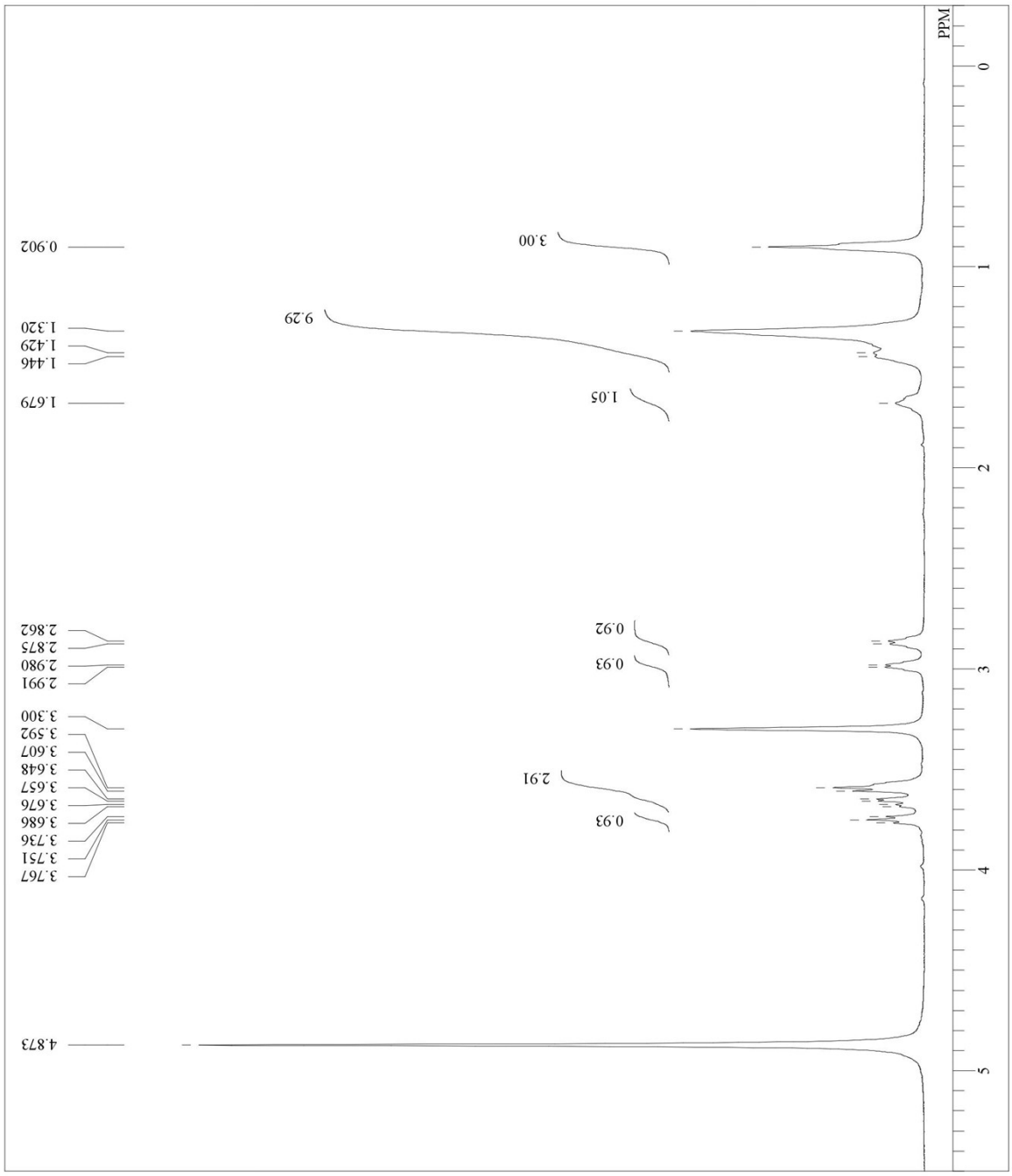

O
O
N
O
CH3(CH2)5

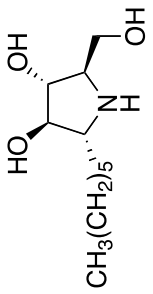
**3c**


DFILE SAK 2-1-01.als
COMNT SAK 2-1-01
DATIM Tue Jun 12 11:34:55 2012
OBNUC 1H
EXMOD NON
OBFRQ 395.75 MHz
OBSET 124.00 KHz
OBFIN 10277.00 Hz
POINT 16384
FREQU 7912.96 Hz
SCANS 8
ACQTM 2.0705 sec
PD 4.9290 sec
PW1 5.50 usec
IRNUC 1H
CTEMP 20.5 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.24 Hz
RGAIN 21
PPM
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
0.000
0.866
0.884
0.900
1.193
1.210
1.229
1.246
1.254
1.264
1.294
1.333
1.353
1.375
1.396
1.432
1.455
1.591
3.625
3.638
3.651
3.659
3.672
3.699
3.717
3.734
3.753
3.827
3.836
3.845
3.854
3.866
3.873
3.898
3.911
3.930
3.937
3.948
3.961
4.044
4.313
4.324
4.337
4.346
4.360
4.369
4.455
4.470
4.499
4.521
4.543
7.264
11.68
3.00
0.91
2.47
0.92
0.75

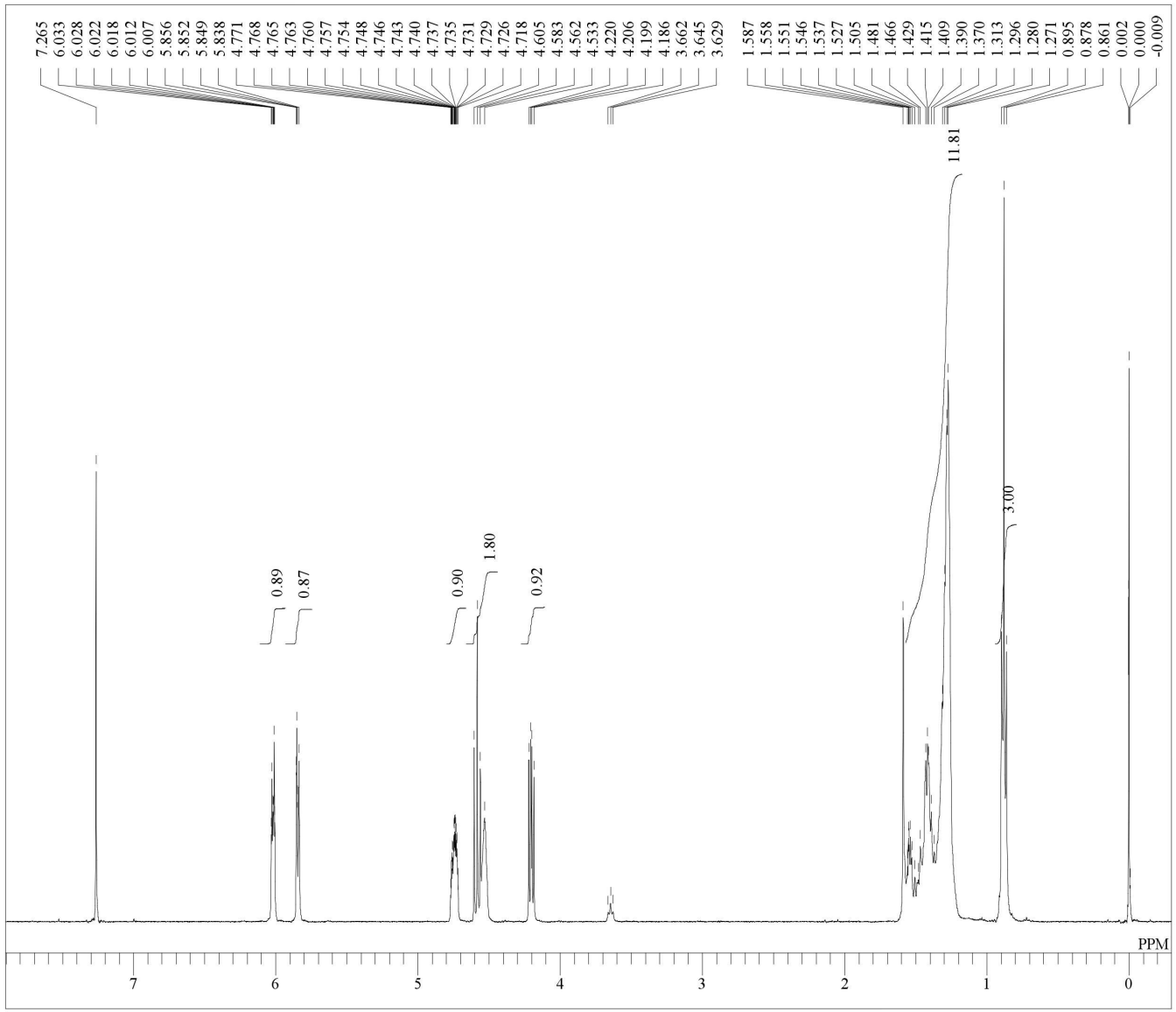

OH
HO
O
N
O
CH3(CH2)5

**4c**

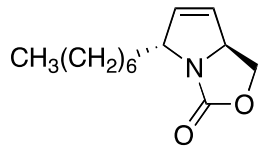

DFILE SAK 2-3-02 did.als
COMNT SAK 2-3-02
DATIM Fri Jun 15 14:01:05 2012
OBNUC 1H
EXMOD NON
OBFRQ 395.75 MHz
OBSET 124.00 KHz
OBFIN 10277.00 Hz
POINT 16384
FREQU 7912.96 Hz
SCANS 8
ACQTM 2.0705 sec
PD 4.9290 sec
PW1 5.50 usec
IRNUC 1H
CTEMP 21.3 c
SLVNT CD3OD
EXREF 3.30 ppm
BF 0.42 Hz
RGAIN 15
4.873
3.767
3.751
3.736
3.686
3.676
3.657
3.648
3.607
3.592
3.300
2.991
2.980
2.875
2.862
1.679
1.446
1.429
1.320
0.902
3.00
9.29
1.05
0.92
0.93
2.91
0.93
PPM
0
1
2
3
4
5


OH
OH
HO
N
H
CH3(CH2)5

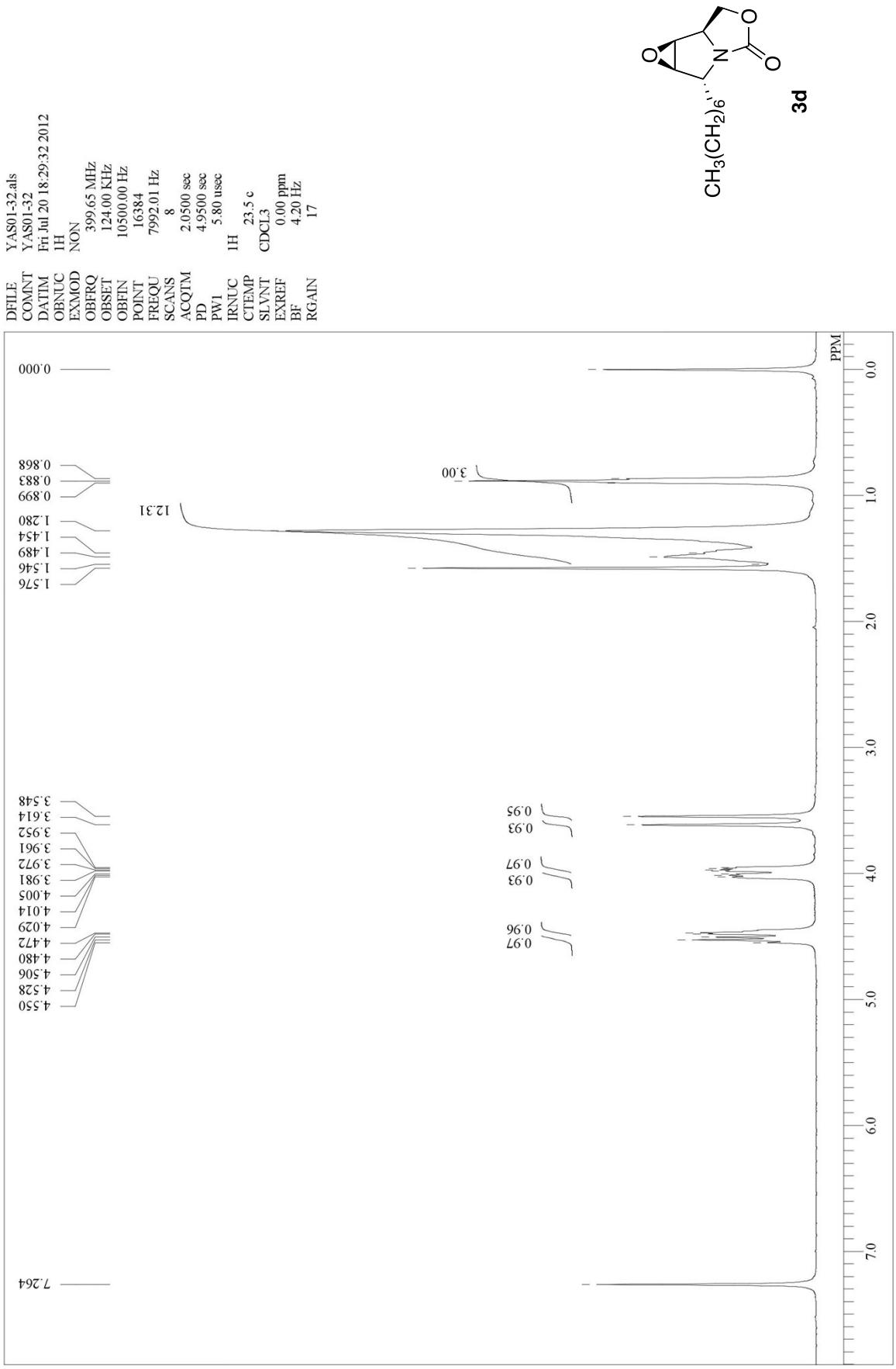
**5c**




| | |
|---|---|
| DFILE | YAS01-30-1.als |
| COMNT | YAS01-30-1 |
| DATIM | Tue Jul 10 18:10:10 2012 |
| OBNUC | 1H |
| EXMOD | NON |
| OBFRQ | 395.75 MHz |
| OBSET | 124.00 KHz |
| OBFIN | 10277.00 Hz |
| POINT | 16384 |
| FREQU | 7912.96 Hz |
| SCANS | 8 |
| ACQTM | 2.0705 sec |
| PD | 4.9290 sec |
| PW1 | 5.50 usec |
| IRNUC | 1H |
| CTEMP | 20.9 c |
| SLVNT | CDCL3 |
| EXREF | 0.00 ppm |
| BF | 0.24 Hz |
| RGAIN | 15 |

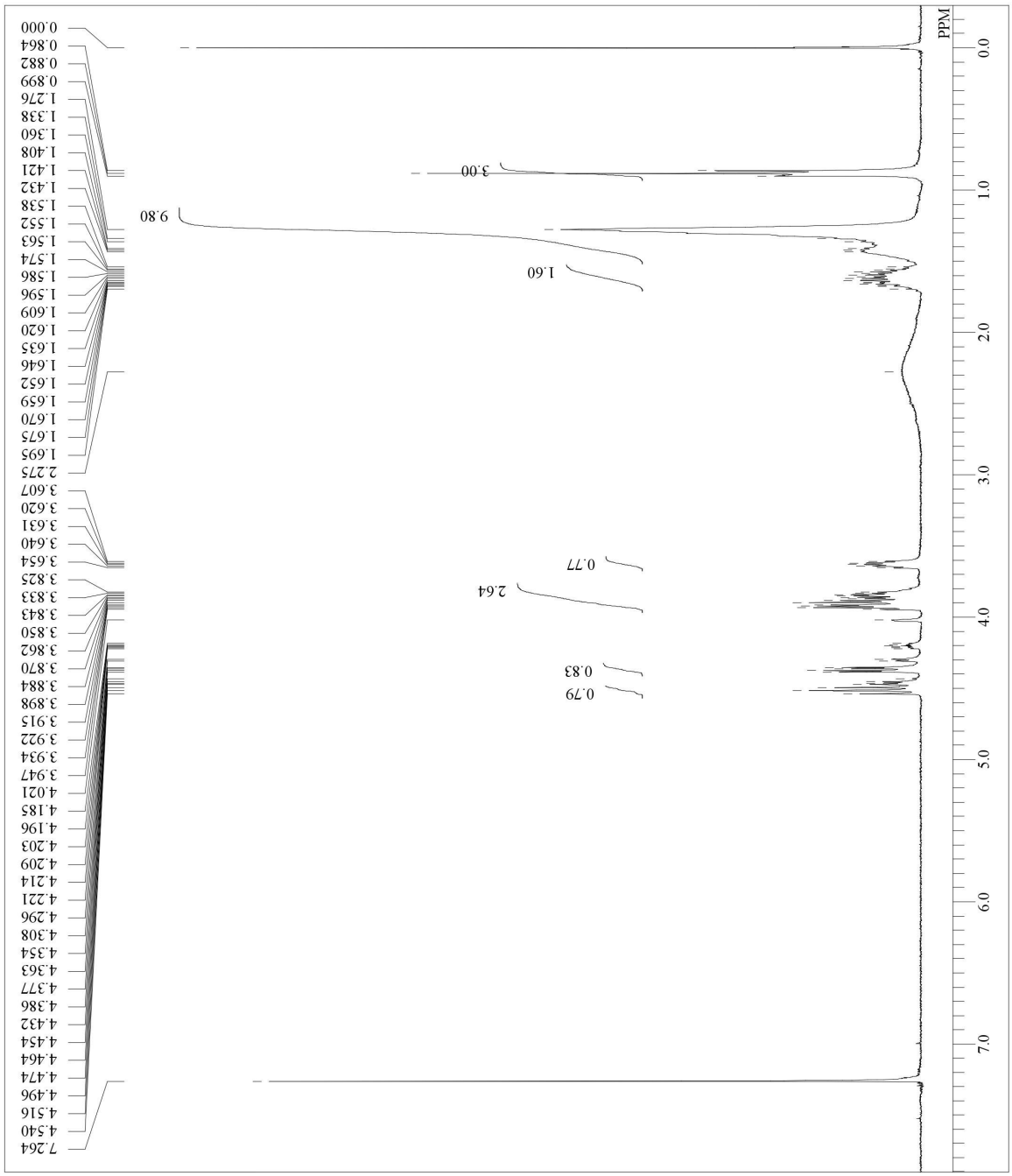


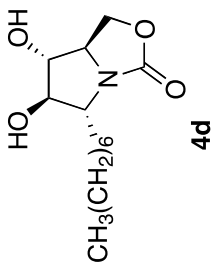

**2d**


DFILE YAS01-32.als
COMNT YAS01-32
DATIM Fri Jul 20 18:29:32 2012
OBNUC 1H
EXMOD NON
OBFRQ 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 16384
FREQU 7992.01 Hz
SCANS 8
ACQTM 2.0500 sec
PD 4.9500 sec
PW1 5.80 usec
IRNUC 1H
CTEMP 23.5 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 4.20 Hz
RGAIN 17
0.000
7.264
4.550
4.528
4.506
4.480
4.472
4.029
4.014
4.005
3.981
3.972
3.961
3.952
3.614
3.548
1.576
1.546
1.489
1.454
1.280
12.31
0.899
0.883
0.868
3.00
0.97
0.96
0.93
0.97
0.93
0.95
PPM
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0

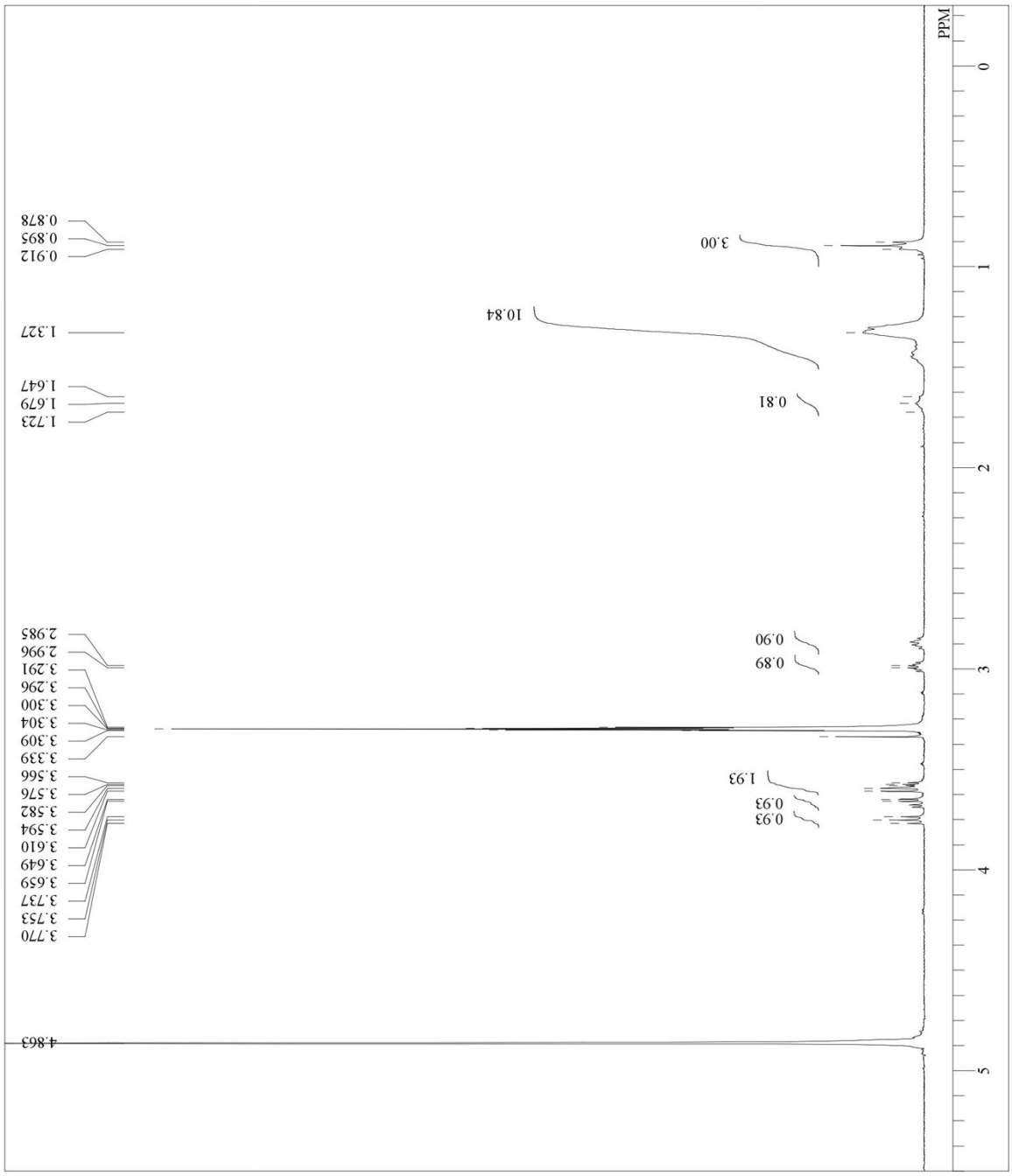

O
O
N
O
O
CH3(CH2)6

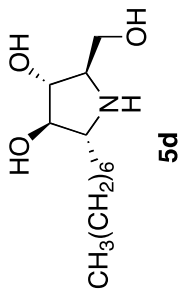
**3d**


DFILE YAS01-40-did.als
COMNT YAS01-40
DATIM Wed Aug 01 17:08:36 2012
OBNUC 1H
EXMOD NON
OBFRQ 395.75 MHz
OBSET 124.00 KHz
OBFIN 10277.00 Hz
POINT 16384
FREQU 7912.96 Hz
SCANS 8
ACQTM 2.0705 sec
PD 4.9290 sec
PW1 5.50 usec
IRNUC 1H
CTEMP 21.8 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.24 Hz
RGAIN 19
9.80
3.00
1.60
0.77
2.64
0.83
0.79
PPM
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0

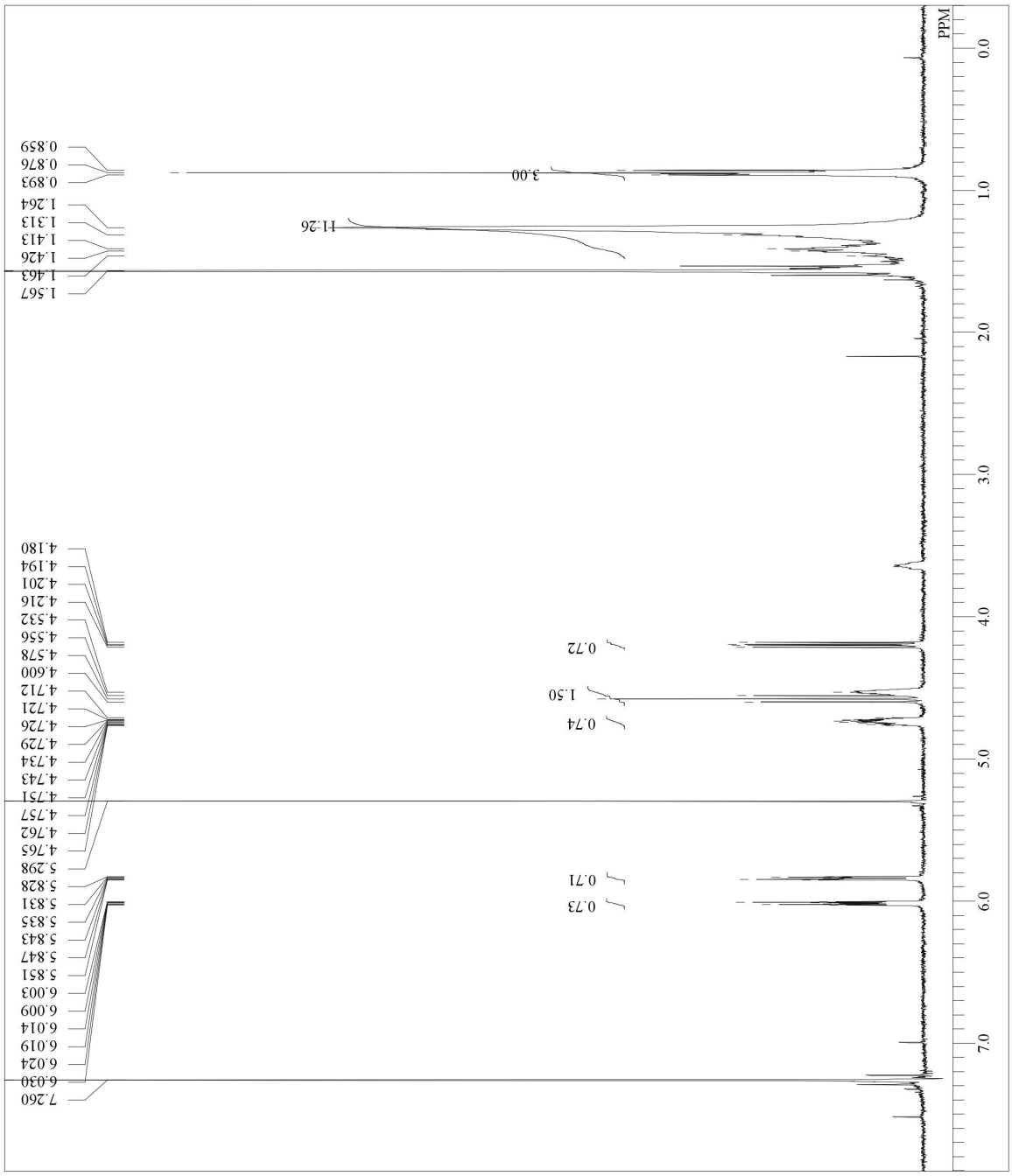

OH
HO
N
O
O
CH3(CH2)6

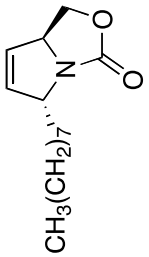
**4d**


DFILE YAS02-02-did.als
COMNT YAS02-02
DATIM Tue Aug 28 18:43:21 2012
OBNUC 1H
EXMOD NON
OBFRQ 395.75 MHz
OBSET 124.00 KHz
OBFIN 10277.00 Hz
POINT 16384
FREQU 7912.96 Hz
SCANS 8
ACQTM 2.0705 sec
PD 4.9290 sec
PW1 5.50 usec
IRNUC 1H
CTEMP 21.7 c
SLVNT CD3OD
EXREF 3.30 ppm
BF 0.24 Hz
RGAIN 18
4.863
3.770
3.753
3.737
3.659
3.649
3.610
3.594
3.582
3.576
3.566
3.339
3.309
3.304
3.300
3.296
3.291
2.996
2.985
1.723
1.679
1.647
1.327
0.912
0.895
0.878
3.00
10.84
0.81
0.90
0.89
1.93
0.93
0.93
PPM
0
1
2
3
4
5

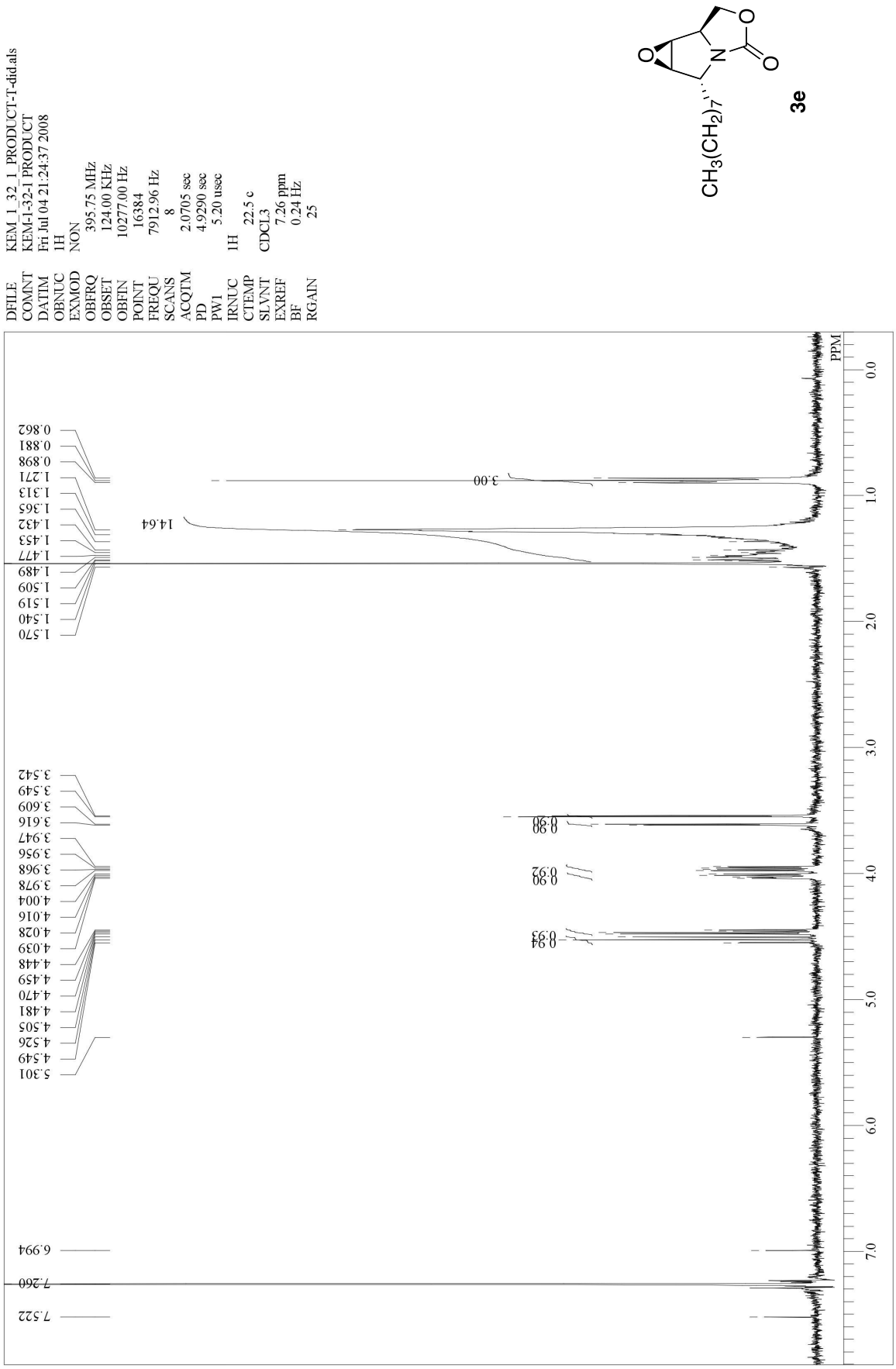

OH
HO
N
H
OH
CH3(CH2)6

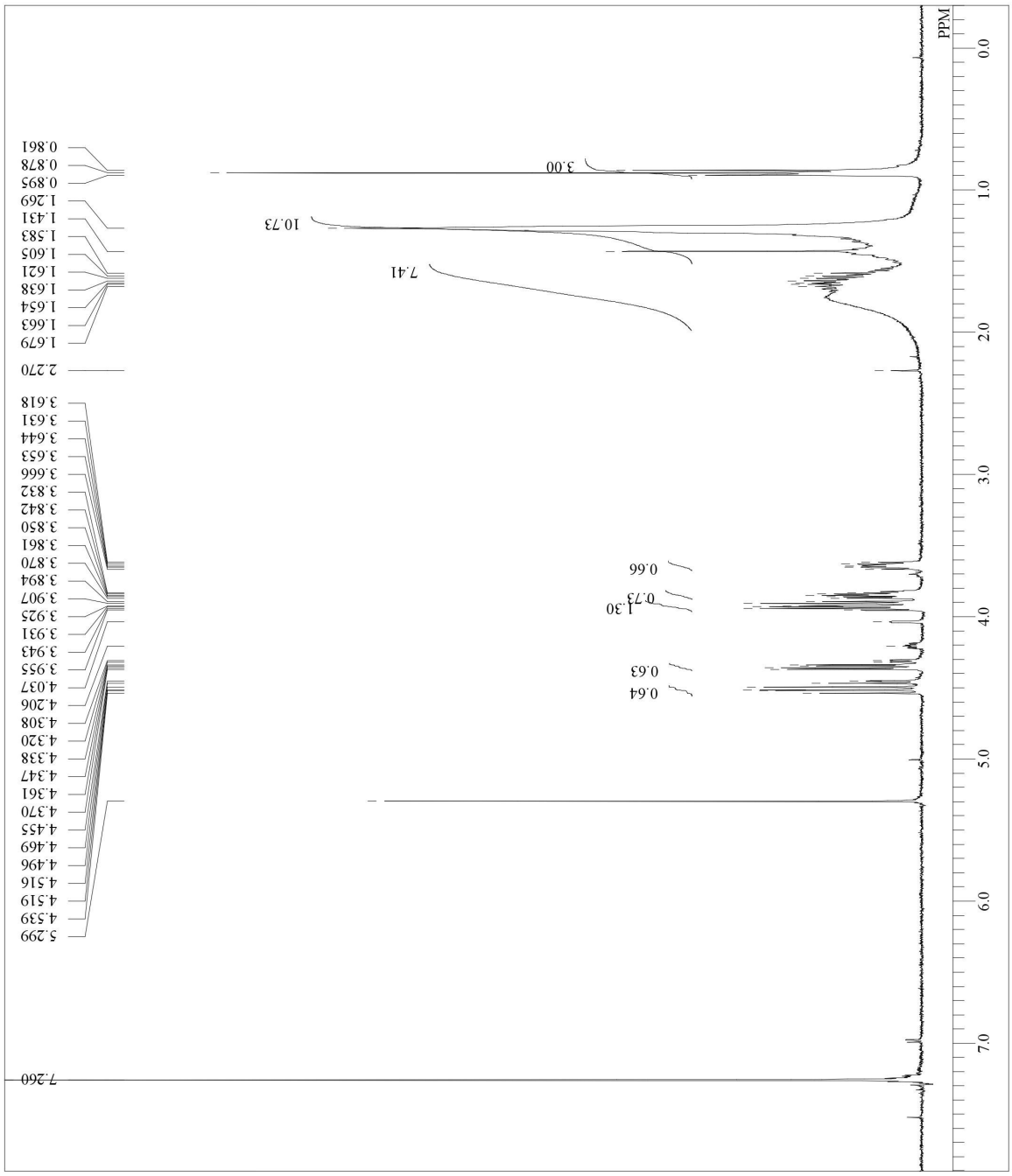
**5d**

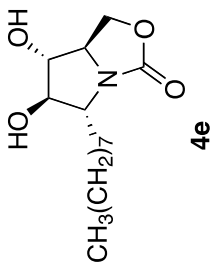

DFILE KEM_1_31_1_PRODUCT-T-did.als
COMNT KEM_1_31_1_PRODUCT
DATIM Thu Jul 03 22:19:26 2008
OBNUC 1H
EXMOD NON
OBFRQ 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 16384
FREQU 7992.01 Hz
SCANS 8
ACQTM 2.0500 sec
PD 4.9500 sec
PW1 5.40 usec
IRNUC 1H
CTEMP 24.9 c
SLVNT CDCL3
EXREF 7.26 ppm
BF 0.24 Hz
RGAIN 21
PPM
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
0.72
1.50
0.74
0.73
0.71
3.00
11.26
0.859
0.876
0.893
1.264
1.313
1.413
1.426
1.463
1.567
4.180
4.194
4.201
4.216
4.532
4.556
4.578
4.600
4.712
4.721
4.726
4.729
4.734
4.743
4.751
4.757
4.762
4.765
5.298
5.828
5.831
5.835
5.843
5.847
5.851
6.003
6.009
6.014
6.019
6.024
6.030
7.260


CH3(CH2)7
O
O
N

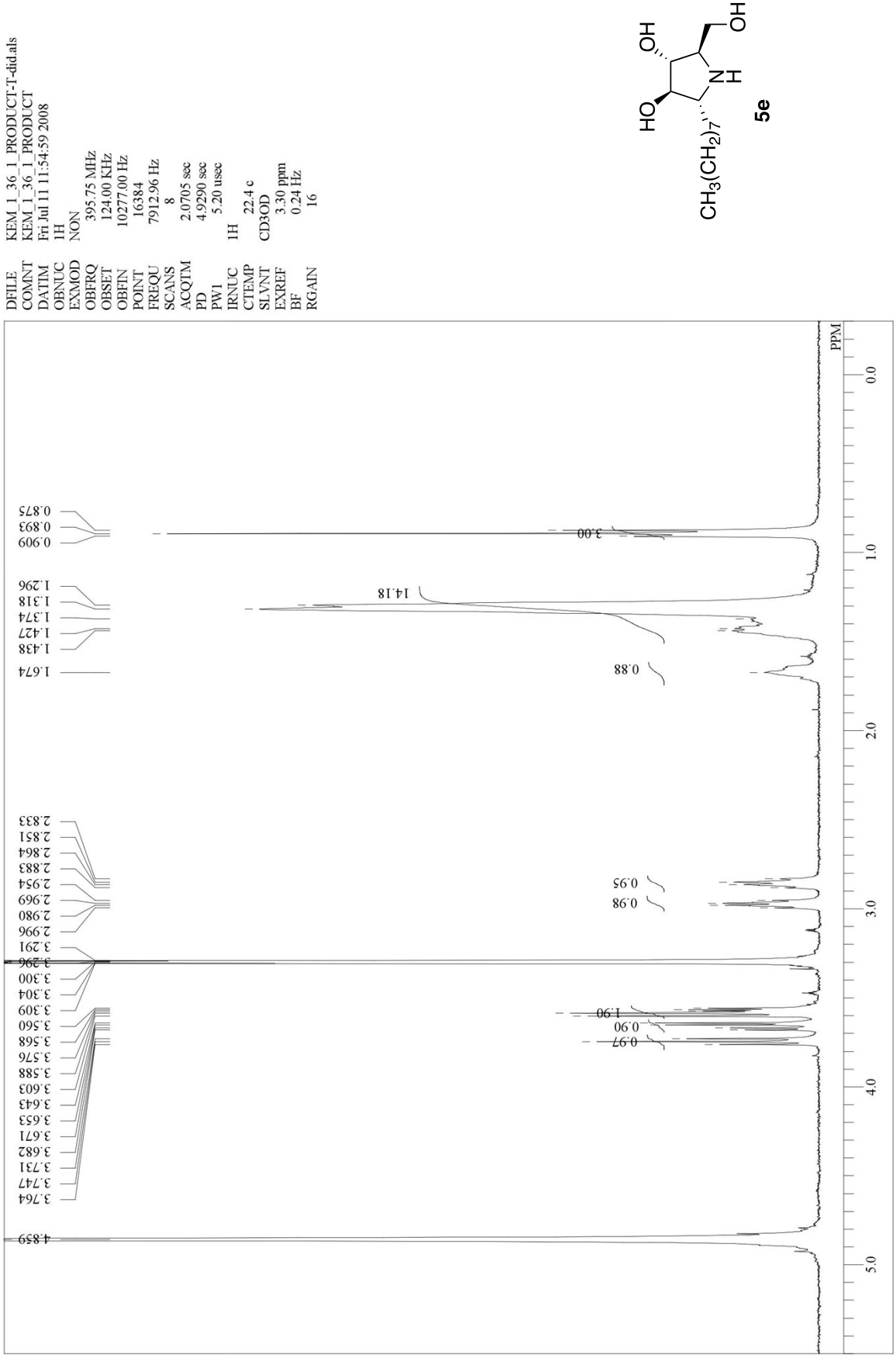
**2e**


DFILE KEM_1_32_1_PRODUCT-T-did.als
COMNT KEM-1-32-1 PRODUCT
DATIM Fri Jul 04 21:24:37 2008
OBNUC 1H
EXMOD NON
OBFRQ 395.75 MHz
OBSET 124.00 KHz
OBFIN 10277.00 Hz
POINT 16384
FREQU 7912.96 Hz
SCANS 8
ACQTM 2.0705 sec
PD 4.9290 sec
PW1 5.20 usec
IRNUC 1H
CTEMP 22.5 c
SLVNT CDCL3
EXREF 7.26 ppm
BF 0.24 Hz
RGAIN 25
CH3(CH2)7
3e
PPM


DFILE KEM_1_34_1_PRODUCT-T.als
COMNT KEM_1_34_1_PRODUCT
DATIM Wed Jul 09 14:50:37 2008
OBNUC 1H
EXMOD NON
OBFRQ 395.75 MHz
OBSET 124.00 KHz
OBFIN 10277.00 Hz
POINT 16384
FREQU 7912.96 Hz
SCANS 8
ACQTM 2.0705 sec
PD 4.9290 sec
PW1 5.20 usec
IRNUC 1H
CTEMP 22.7 c
SLVNT CDCL3
EXREF 7.26 ppm
BF 0.24 Hz
RGAIN 20
7.260
5.299
4.539
4.519
4.516
4.496
4.469
4.455
4.370
4.361
4.347
4.338
4.320
4.308
4.206
4.037
3.955
3.943
3.931
3.925
3.907
3.894
3.870
3.861
3.850
3.842
3.832
3.666
3.653
3.644
3.631
3.618
2.270
1.679
1.663
1.654
1.638
1.621
1.605
1.583
1.431
1.269
0.895
0.878
0.861
3.00
10.73
7.41
0.66
1.30
0.73
0.64
0.63
PPM
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

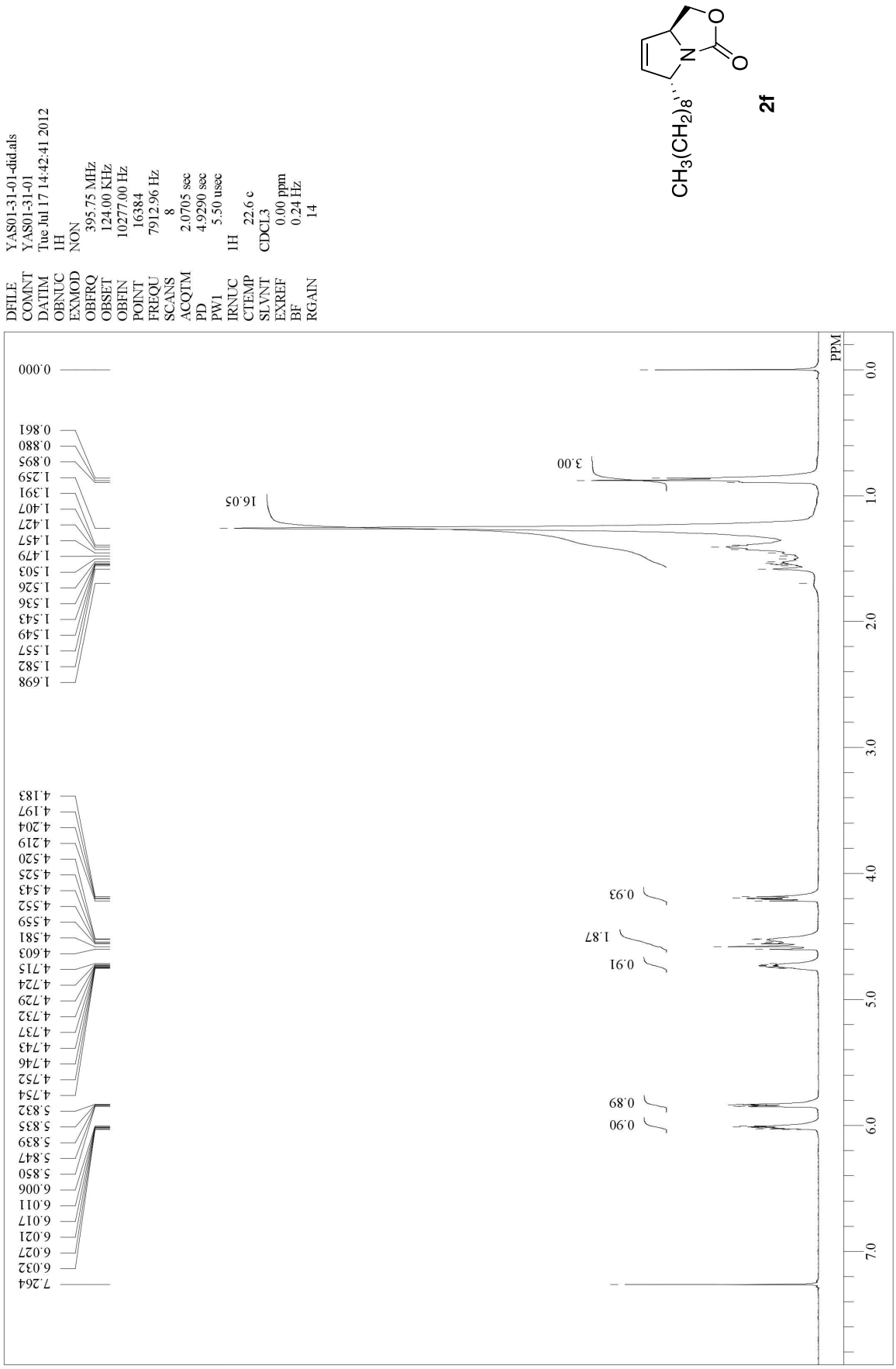

OH
HO
N
O
O
CH3(CH2)7

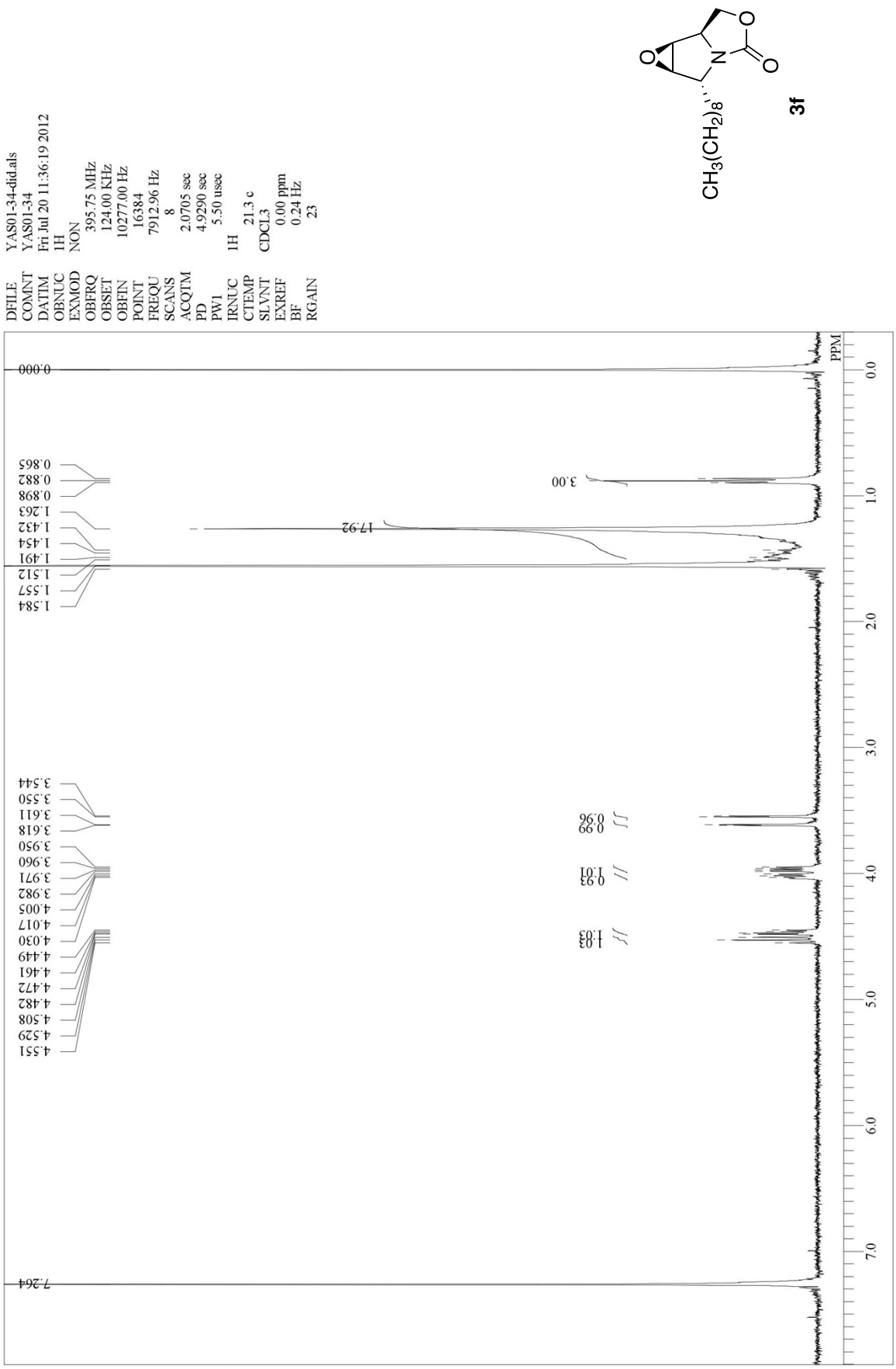
**4e**


DFILE KEM_1_36_1_PRODUCT-T-did.als
COMNT KEM_1_36_1_PRODUCT
DATIM Fri Jul 11 11:54:59 2008
OBNUC 1H
EXMOD NON
OBFRQ 395.75 MHz
OBSET 124.00 KHz
OBFIN 10277.00 Hz
POINT 16384
FREQU 7912.96 Hz
SCANS 8
ACQTM 2.0705 sec
PD 4.9290 sec
PW1 5.20 usec
IRNUC 1H
CTEMP 22.4 c
SLVNT CD3OD
EXREF 3.30 ppm
BF 0.24 Hz
RGAIN 16
PPM
0.0
1.0
2.0
3.0
4.0
5.0
0.875
0.893
0.909
1.296
1.318
1.374
1.427
1.438
1.674
2.833
2.851
2.864
2.883
2.954
2.969
2.980
2.996
3.291
3.296
3.300
3.304
3.309
3.560
3.568
3.576
3.588
3.603
3.643
3.653
3.671
3.682
3.731
3.747
3.764
4.859
3.00
14.18
0.88
0.95
0.98
1.90
0.90
0.97


OH
OH
HO
N
H
CH3(CH2)7

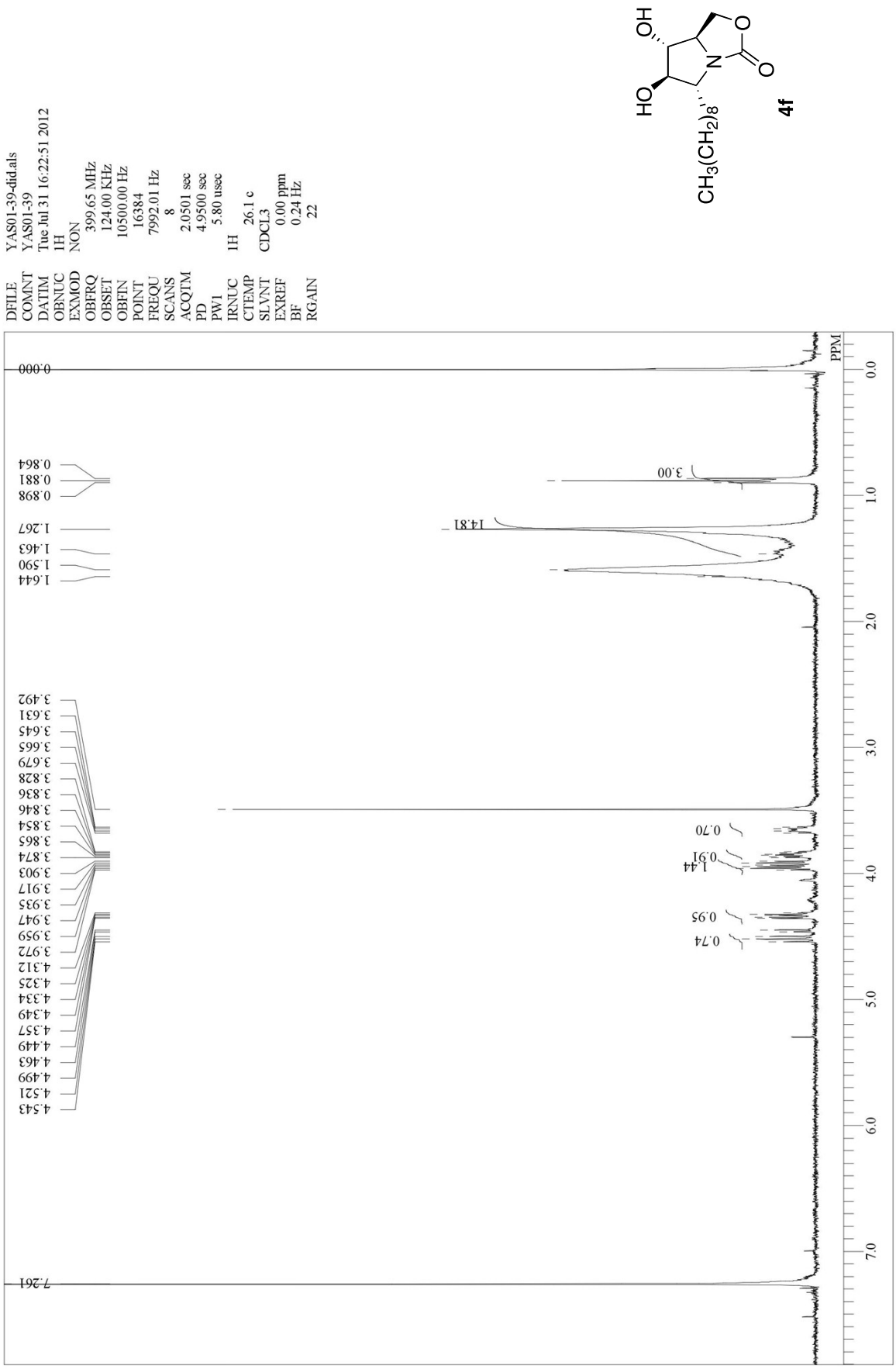
**5e**


DFILE YAS01-31-01-did.als
COMNT YAS01-31-01
DATIM Tue Jul 17 14:42:41 2012
OBNUC 1H
EXMOD NON
OBFRQ 395.75 MHz
OBSET 124.00 KHz
OBFIN 10277.00 Hz
POINT 16384
FREQU 7912.96 Hz
SCANS 8
ACQTM 2.0705 sec
PD 4.9290 sec
PW1 5.50 usec
IRNUC 1H
CTEMP 22.6 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.24 Hz
RGAIN 14
0.000
0.861
0.880
0.895
1.259
1.391
1.407
1.427
1.457
1.479
1.503
1.526
1.536
1.543
1.549
1.557
1.582
1.698
4.183
4.197
4.204
4.219
4.520
4.525
4.543
4.552
4.559
4.581
4.603
4.715
4.724
4.729
4.732
4.737
4.743
4.746
4.752
4.754
5.832
5.835
5.839
5.847
5.850
6.006
6.011
6.017
6.021
6.027
6.032
7.264
16.05
3.00
0.93
1.87
0.91
0.89
0.90
PPM
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
CH3(CH2)8
O
O
N
O
2f


DFILE YAS01-34-did.als
COMNT YAS01-34
DATIM Fri Jul 20 11:36:19 2012
OBNUC 1H
EXMOD NON
OBFRQ 395.75 MHz
OBSET 124.00 KHz
OBFIN 10277.00 Hz
POINT 16384
FREQU 7912.96 Hz
SCANS 8
ACQTM 2.0705 sec
PD 4.9290 sec
PW1 5.50 usec
IRNUC 1H
CTEMP 21.3 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.24 Hz
RGAIN 23
0.000
0.865
0.882
0.898
1.263
1.432
1.454
1.491
1.512
1.557
1.584
3.00
17.92
3.544
3.550
3.611
3.618
3.950
3.960
3.971
3.982
4.005
4.017
4.030
4.449
4.461
4.472
4.482
4.508
4.529
4.551
7.264
0.96
0.99
1.01
0.93
1.03
PPM
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0

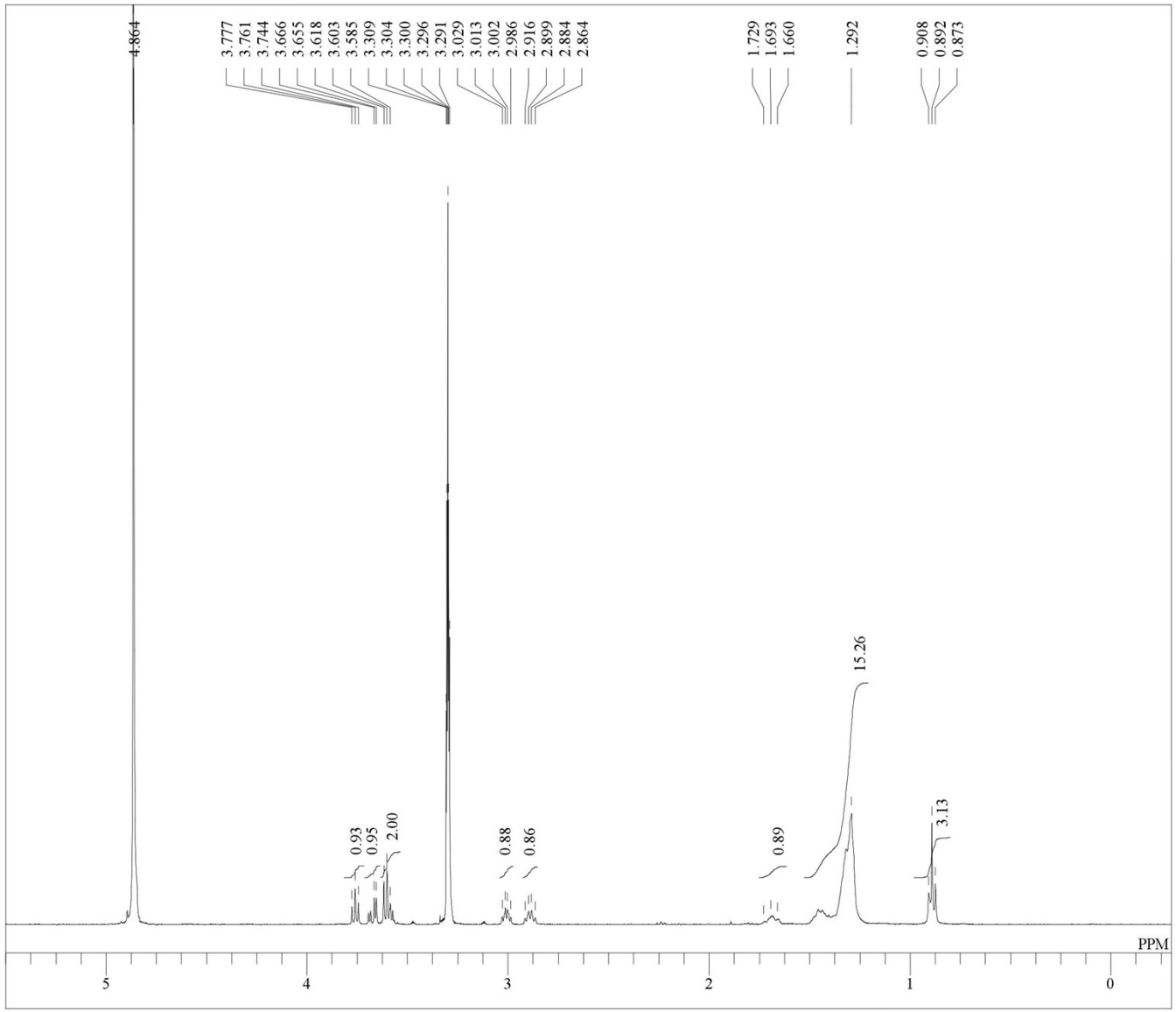

O
O
N
O
CH3(CH2)8

**3f**

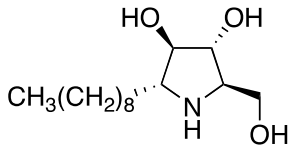

DFILE YAS01-39-did.als
COMNT YAS01-39
DATIM Tue Jul 31 16:22:51 2012
OBNUC 1H
EXMOD NON
OBFRQ 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 16384
FREQU 7992.01 Hz
SCANS 8
ACQTM 2.0501 sec
PD 4.9500 sec
PW1 5.80 usec
IRNUC 1H
CTEMP 26.1 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.24 Hz
RGAIN 22
PPM
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
0.000
7.261
4.543
4.521
4.499
4.463
4.449
4.357
4.349
4.334
4.325
4.312
3.972
3.959
3.947
3.935
3.917
3.903
3.874
3.865
3.854
3.846
3.836
3.828
3.679
3.665
3.645
3.631
3.492
1.644
1.590
1.463
1.267
0.898
0.881
0.864
3.00
14.81
0.70
1.44
0.91
0.74
0.95


OH
HO
N
O
O
CH3(CH2)8

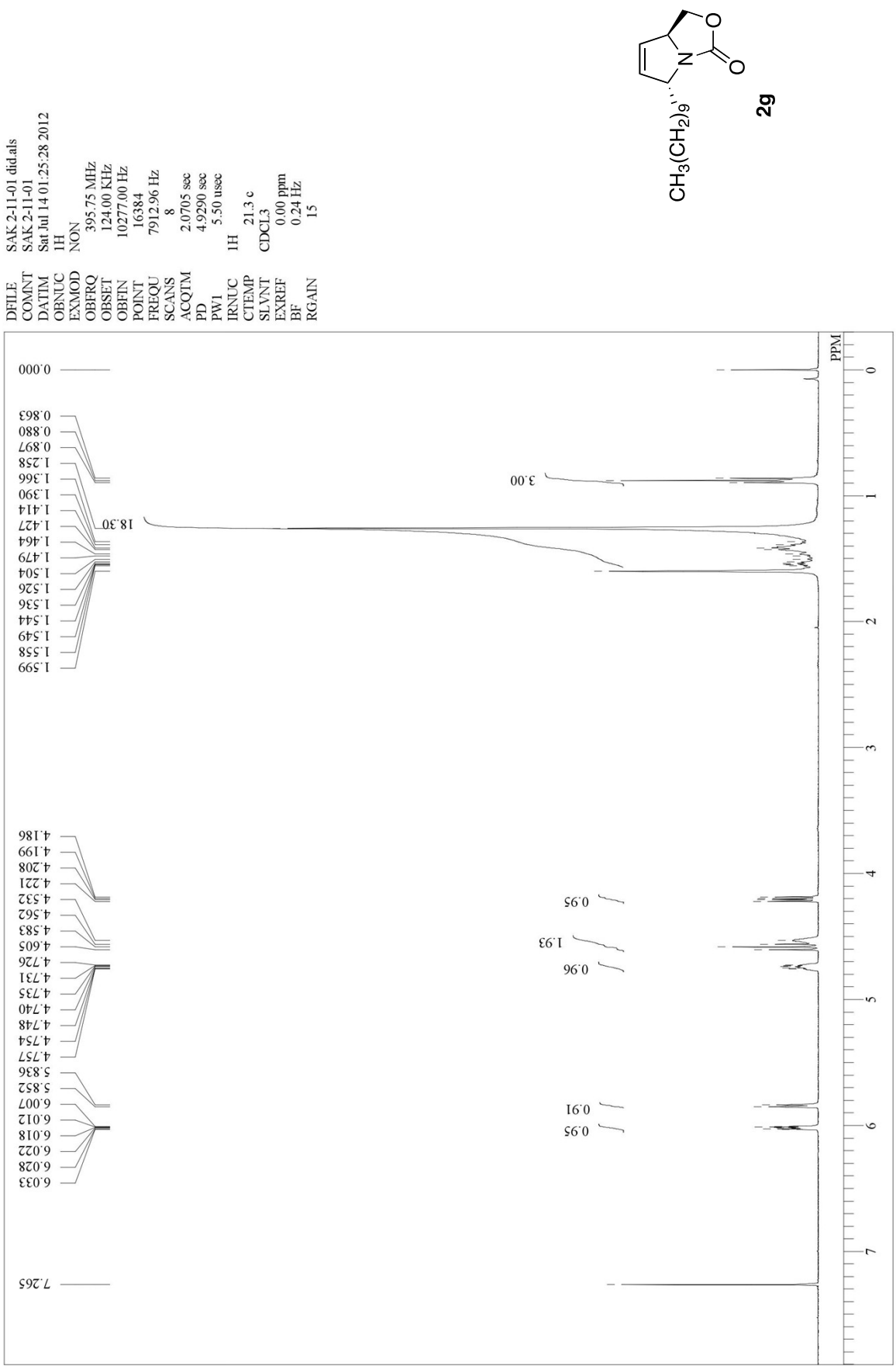
**4f**




| | |
|---|---|
| DFILE | YAS02-01-2-did.als |
| COMNT | YAS02-01-2 |
| DATIM | Thu Aug 30 09:46:53 2012 |
| OBNUC | 1H |
| EXMOD | NON |
| OBFRQ | 395.75 MHz |
| OBSET | 124.00 KHz |
| OBFIN | 10277.00 Hz |
| POINT | 16384 |
| FREQU | 7912.96 Hz |
| SCANS | 8 |
| ACQTM | 2.0705 sec |
| PD | 4.9290 sec |
| PW1 | 5.50 usec |
| IRNUC | 1H |
| CTEMP | 21.6 c |
| SLVNT | CD3OD |
| EXREF | 3.30 ppm |
| BF | 0.24 Hz |
| RGAIN | 18 |

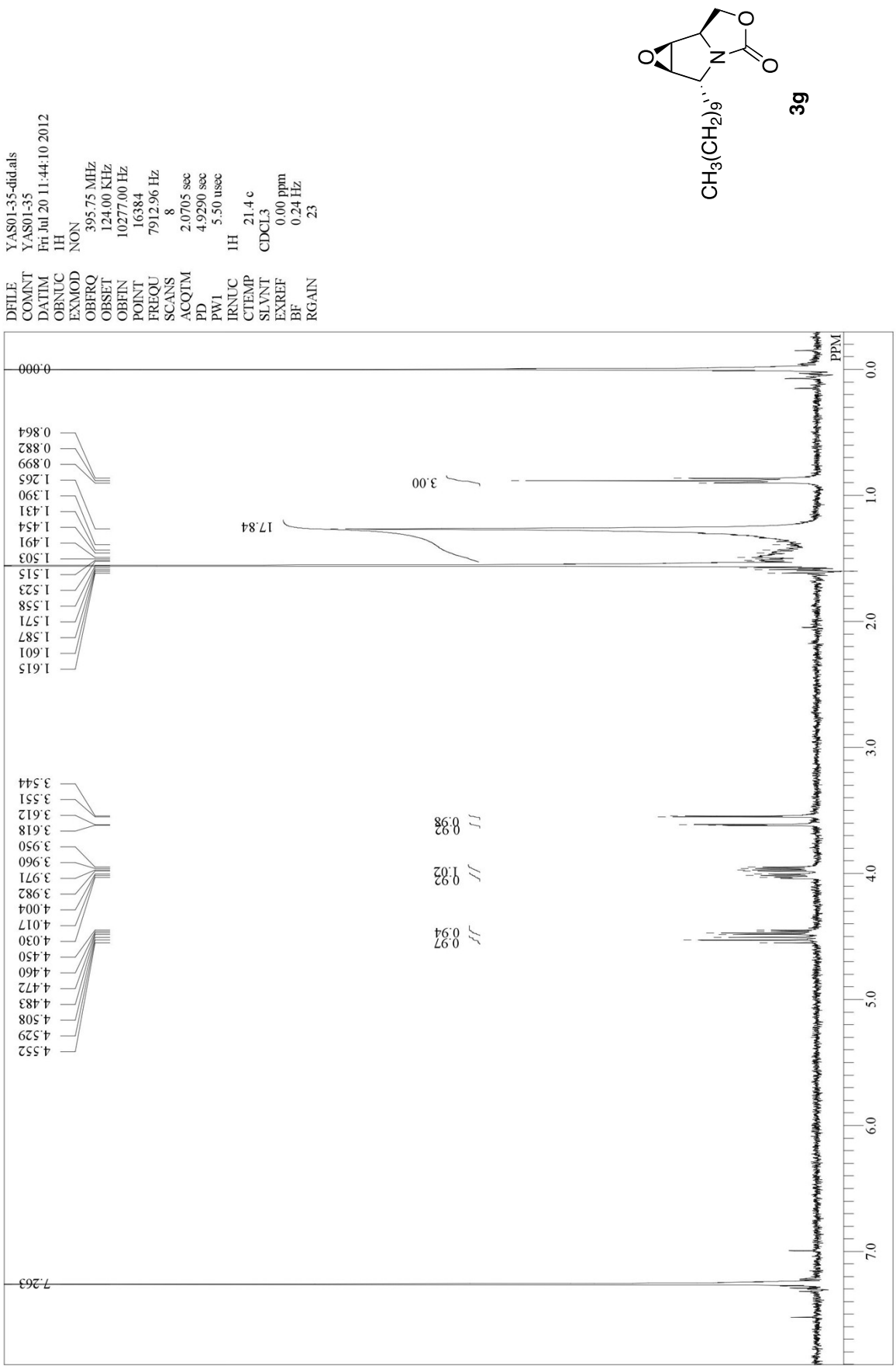



**5f**


DFILE SAK 2-11-01 did.als
COMNT SAK 2-11-01
DATIM Sat Jul 14 01:25:28 2012
OBNUC 1H
EXMOD NON
OBFRQ 395.75 MHz
OBSET 124.00 KHz
OBFIN 10277.00 Hz
POINT 16384
FREQU 7912.96 Hz
SCANS 8
ACQTM 2.0705 sec
PD 4.9290 sec
PW1 5.50 usec
IRNUC 1H
CTEMP 21.3 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.24 Hz
RGAIN 15
0.000
0.863
0.880
0.897
1.258
1.366
1.390
1.414
1.427
1.464
1.479
1.504
1.526
1.536
1.544
1.549
1.558
1.599
18.30
3.00
4.186
4.199
4.208
4.221
4.532
4.562
4.583
4.605
4.726
4.731
4.735
4.740
4.748
4.754
4.757
5.836
5.852
6.007
6.012
6.018
6.022
6.028
6.033
7.265
0.95
0.91
0.96
1.93
0.95
PPM
0
1
2
3
4
5
6
7

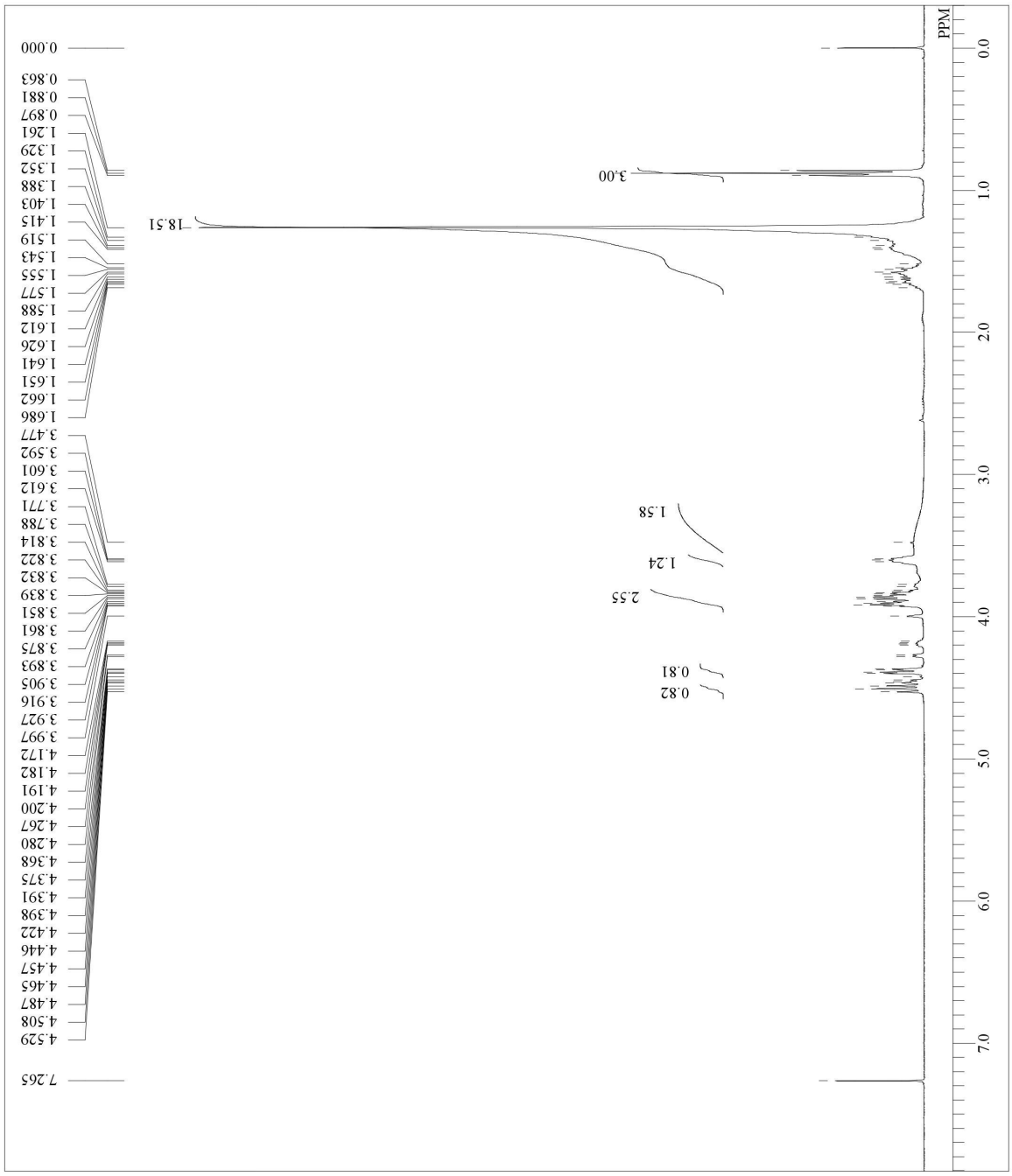

O
N
O
CH3(CH2)9

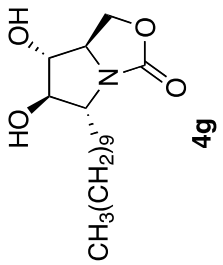
**2g**

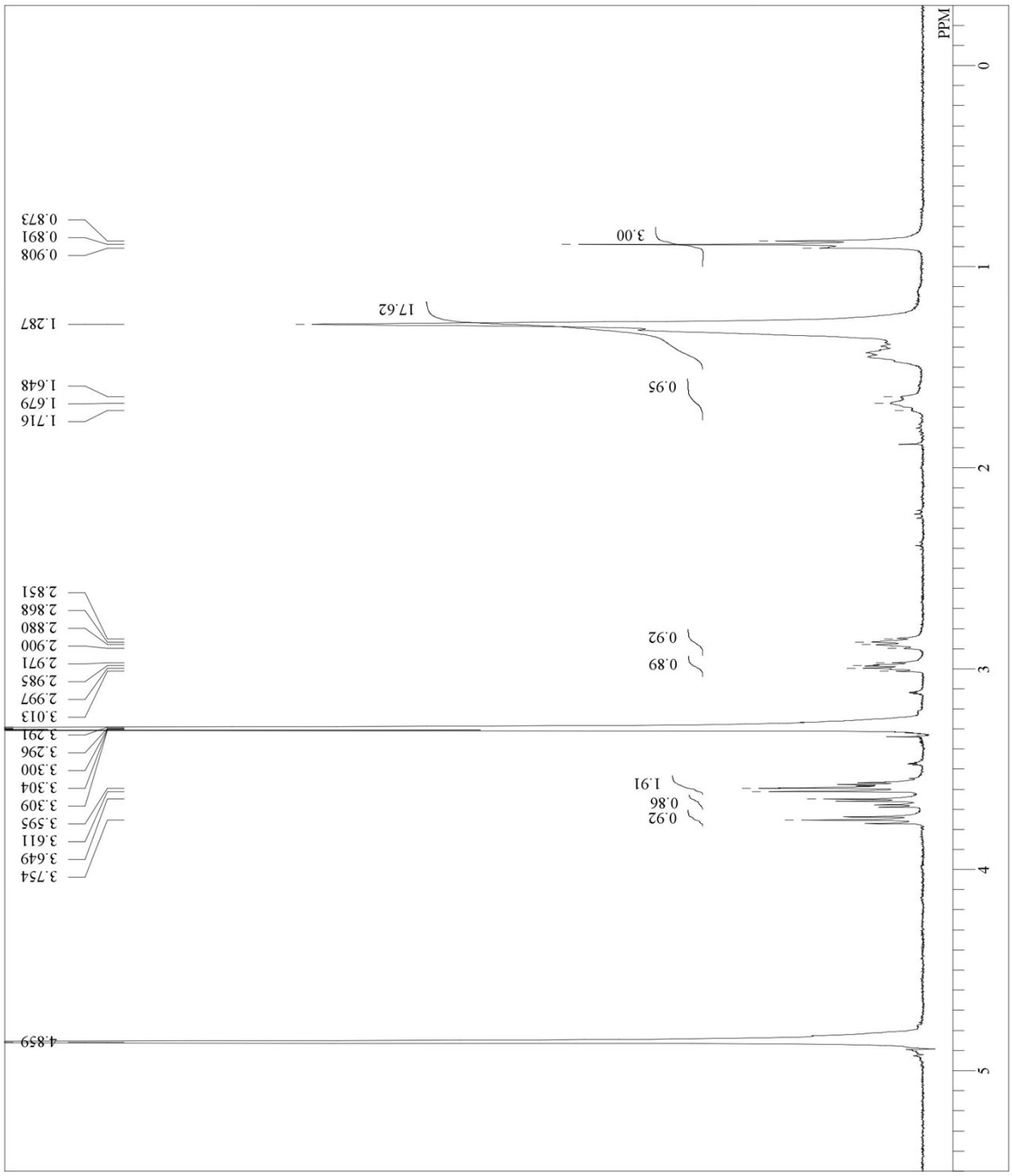

DFILE YAS01-35-did.als
COMNT YAS01-35
DATIM Fri Jul 20 11:44:10 2012
OBNUC 1H
EXMOD NON
OBFRQ 395.75 MHz
OBSET 124.00 KHz
OBFIN 10277.00 Hz
POINT 16384
FREQU 7912.96 Hz
SCANS 8
ACQTM 2.0705 sec
PD 4.9290 sec
PW1 5.50 usec
IRNUC 1H
CTEMP 21.4 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.24 Hz
RGAIN 23
PPM
7.263
4.552
4.529
4.508
4.483
4.472
4.460
4.450
4.030
4.017
4.004
3.982
3.971
3.960
3.950
3.618
3.612
3.551
3.544
1.615
1.601
1.587
1.571
1.558
1.523
1.515
1.503
1.491
1.454
1.431
1.390
1.265
0.899
0.882
0.864
0.000
17.84
3.00
0.97
0.94
0.92
1.02
0.92
0.98

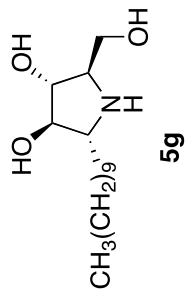

O
O
N
O
CH3(CH2)9

**3g**

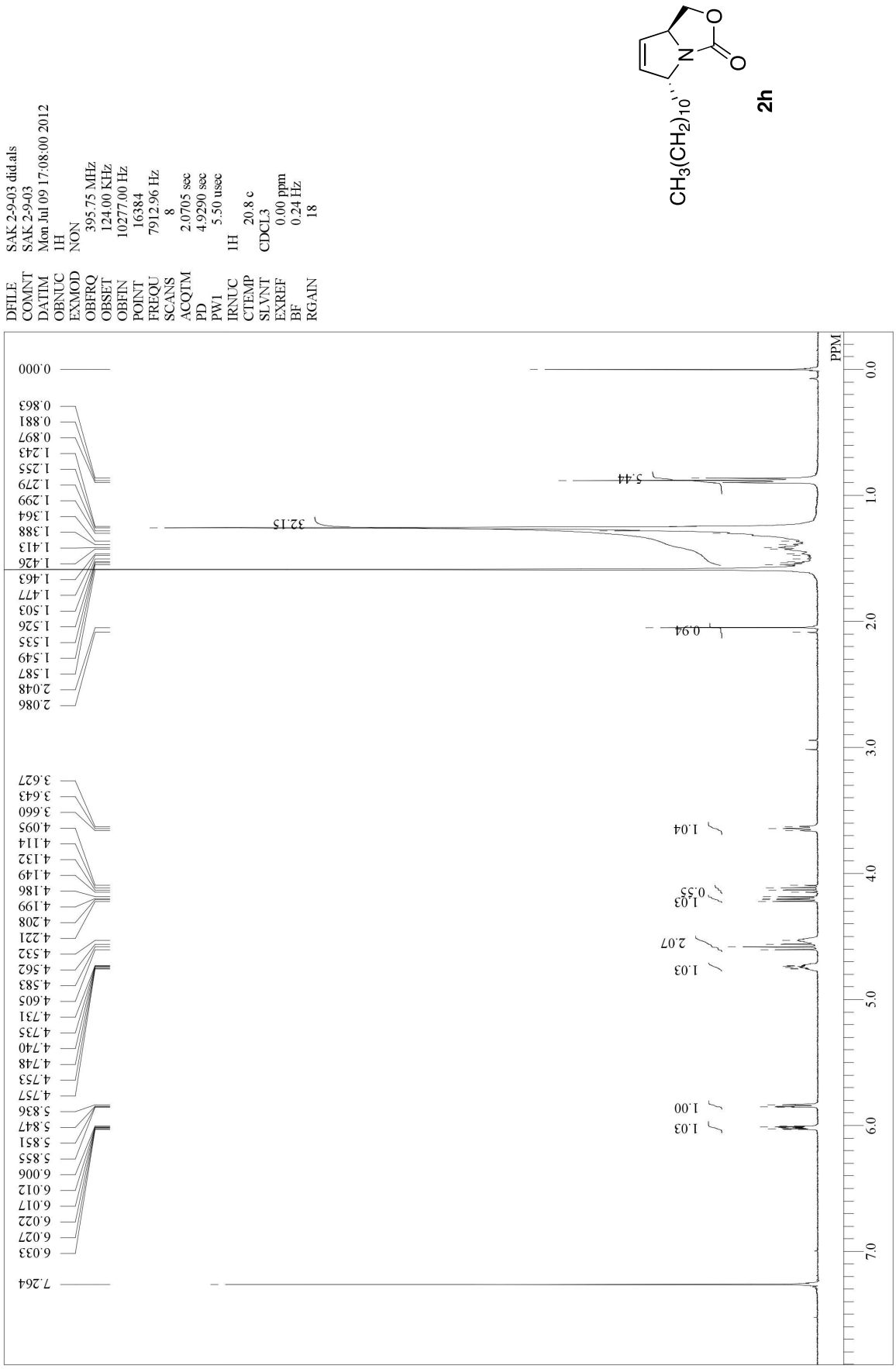

DFILE YAS01-36-did.als
COMNT YAS01-36
DATIM Tue Jul 31 10:46:35 2012
OBNUC 1H
EXMOD NON
OBFRQ 395.75 MHz
OBSET 124.00 KHz
OBFIN 10277.00 Hz
POINT 16384
FREQU 7912.96 Hz
SCANS 8
ACQTM 2.0705 sec
PD 4.9290 sec
PW1 5.50 usec
IRNUC 1H
CTEMP 21.8 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.24 Hz
RGAIN 14
7.265
4.529
4.508
4.487
4.465
4.457
4.446
4.422
4.398
4.391
4.375
4.368
4.280
4.267
4.200
4.191
4.182
4.172
3.997
3.927
3.916
3.905
3.893
3.875
3.861
3.851
3.839
3.832
3.822
3.814
3.788
3.771
3.612
3.601
3.592
3.477
1.686
1.662
1.651
1.641
1.626
1.612
1.588
1.577
1.555
1.543
1.519
1.415
1.403
1.388
1.352
1.329
1.261
0.897
0.881
0.863
0.000
18.51
3.00
1.58
1.24
2.55
0.82
0.81
PPM
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0


OH
HO
O
N
O
CH3(CH2)9
4g


DFILE YAS01-41-did.als
COMNT YAS01-41
DATIM Mon Aug 27 15:05:21 2012
OBNUC 1H
EXMOD NON
OBFRQ 395.75 MHz
OBSET 124.00 KHz
OBFIN 10277.00 Hz
POINT 16384
FREQU 7912.96 Hz
SCANS 8
ACQTM 2.0705 sec
PD 4.9290 sec
PW1 5.50 usec
IRNUC 1H
CTEMP 22.2 c
SLVNT CD3OD
EXREF 3.30 ppm
BF 0.24 Hz
RGAIN 18
PPM
0.873
0.891
0.908
1.287
1.648
1.679
1.716
2.851
2.868
2.880
2.900
2.971
2.985
2.997
3.013
3.291
3.296
3.300
3.304
3.309
3.595
3.611
3.649
3.754
4.859
0.92
0.86
1.91
0.89
0.92
0.95
17.62
3.00

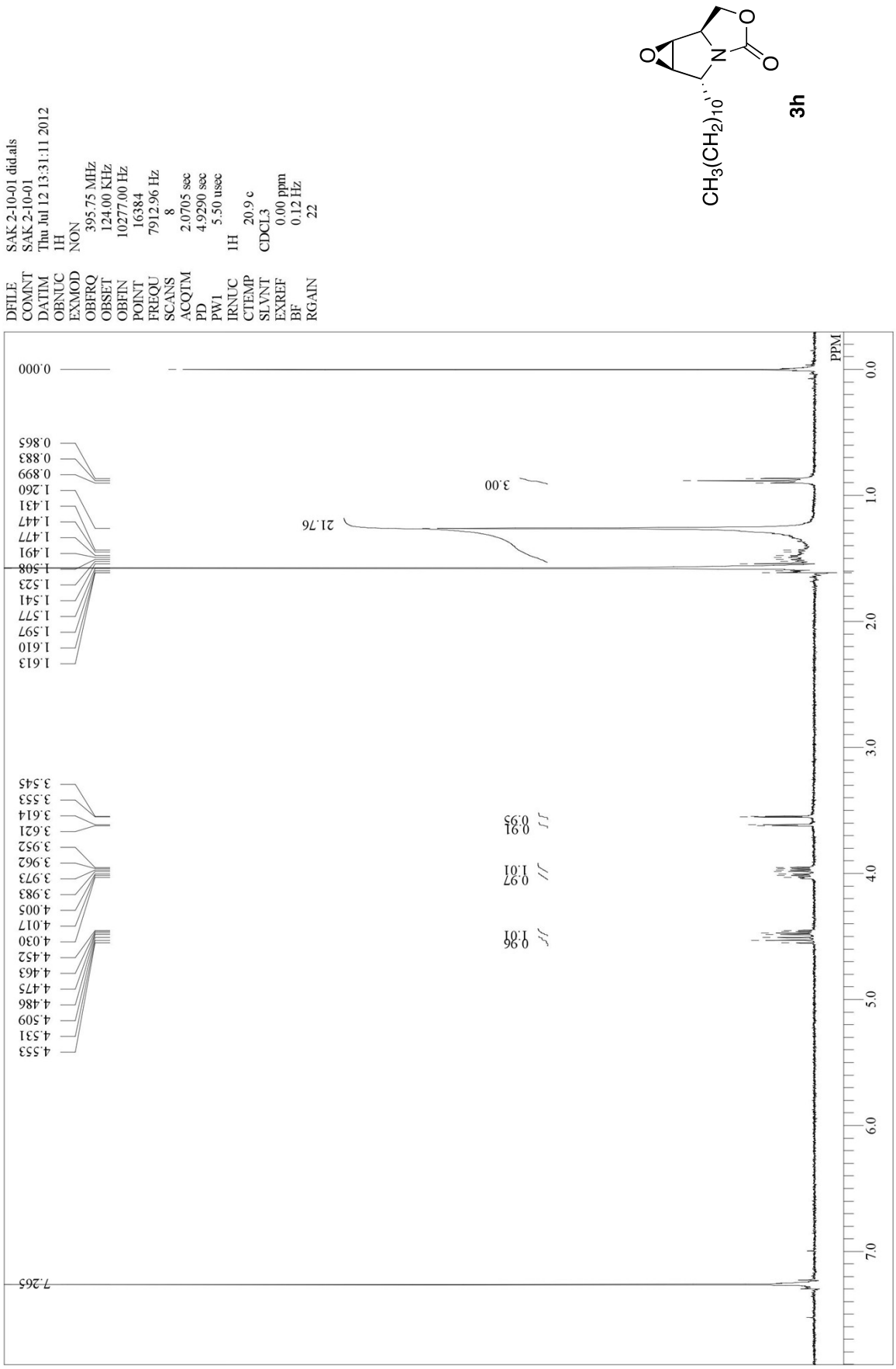

OH
OH
HO
N
H
CH3(CH2)9

**5g**


DFILE SAK 2-9-03 did.als
COMNT SAK 2-9-03
DATIM Mon Jul 09 17:08:00 2012
OBNUC 1H
EXMOD NON
OBFRQ 395.75 MHz
OBSET 124.00 KHz
OBFIN 10277.00 Hz
POINT 16384
FREQU 7912.96 Hz
SCANS 8
ACQTM 2.0705 sec
PD 4.9290 sec
PW1 5.50 usec
IRNUC 1H
CTEMP 20.8 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.24 Hz
RGAIN 18
PPM
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
0.000
0.863
0.881
0.897
1.243
1.255
1.279
1.299
1.364
1.388
1.413
1.426
1.463
1.477
1.503
1.526
1.535
1.549
1.587
2.048
2.086
3.627
3.643
3.660
4.095
4.114
4.132
4.149
4.186
4.199
4.208
4.221
4.532
4.562
4.583
4.603
4.731
4.735
4.740
4.748
4.753
4.757
5.836
5.847
5.851
5.855
6.006
6.012
6.017
6.022
6.027
6.033
7.264
32.15
5.44
0.94
1.04
0.55
1.03
2.07
1.03
1.00
1.03

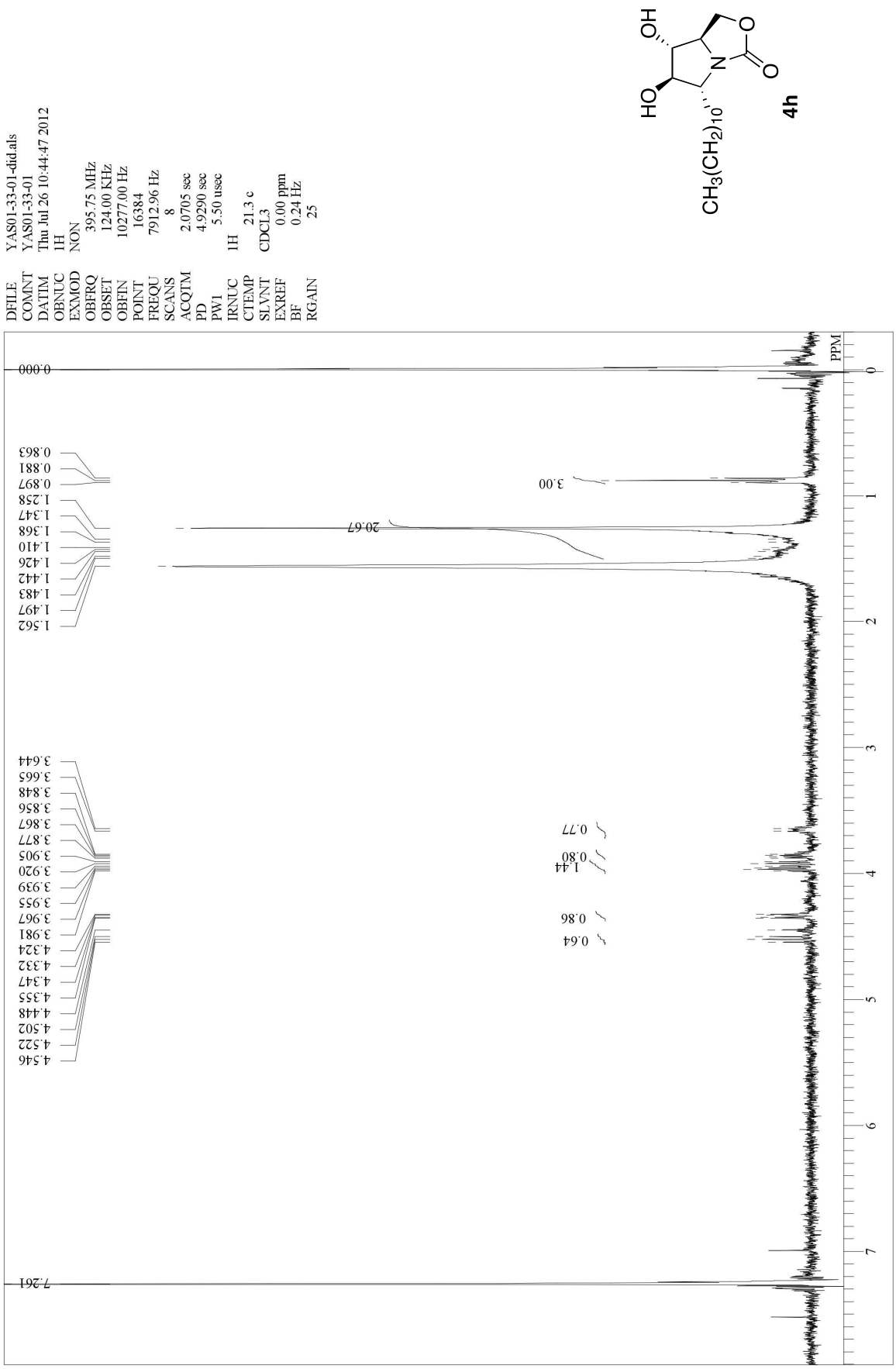

CH3(CH2)10
O
O
N
O

**2h**


DFILE SAK 2-10-01 did.als
COMNT SAK 2-10-01
DATIM Thu Jul 12 13:31:11 2012
OBNUC 1H
EXMOD NON
OBFRQ 395.75 MHz
OBSET 124.00 KHz
OBFIN 10277.00 Hz
POINT 16384
FREQU 7912.96 Hz
SCANS 8
ACQTM 2.0705 sec
PD 4.9290 sec
PW1 5.50 usec
IRNUC 1H
CTEMP 20.9 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 22
0.000
0.865
0.883
0.899
1.260
1.431
1.447
1.477
1.491
1.508
1.523
1.541
1.577
1.597
1.610
1.613
3.545
3.553
3.614
3.621
3.952
3.962
3.973
3.983
4.005
4.017
4.030
4.452
4.463
4.475
4.486
4.509
4.531
4.553
7.265
21.76
3.00
0.91
0.95
0.97
1.01
0.96
1.01
PPM
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0

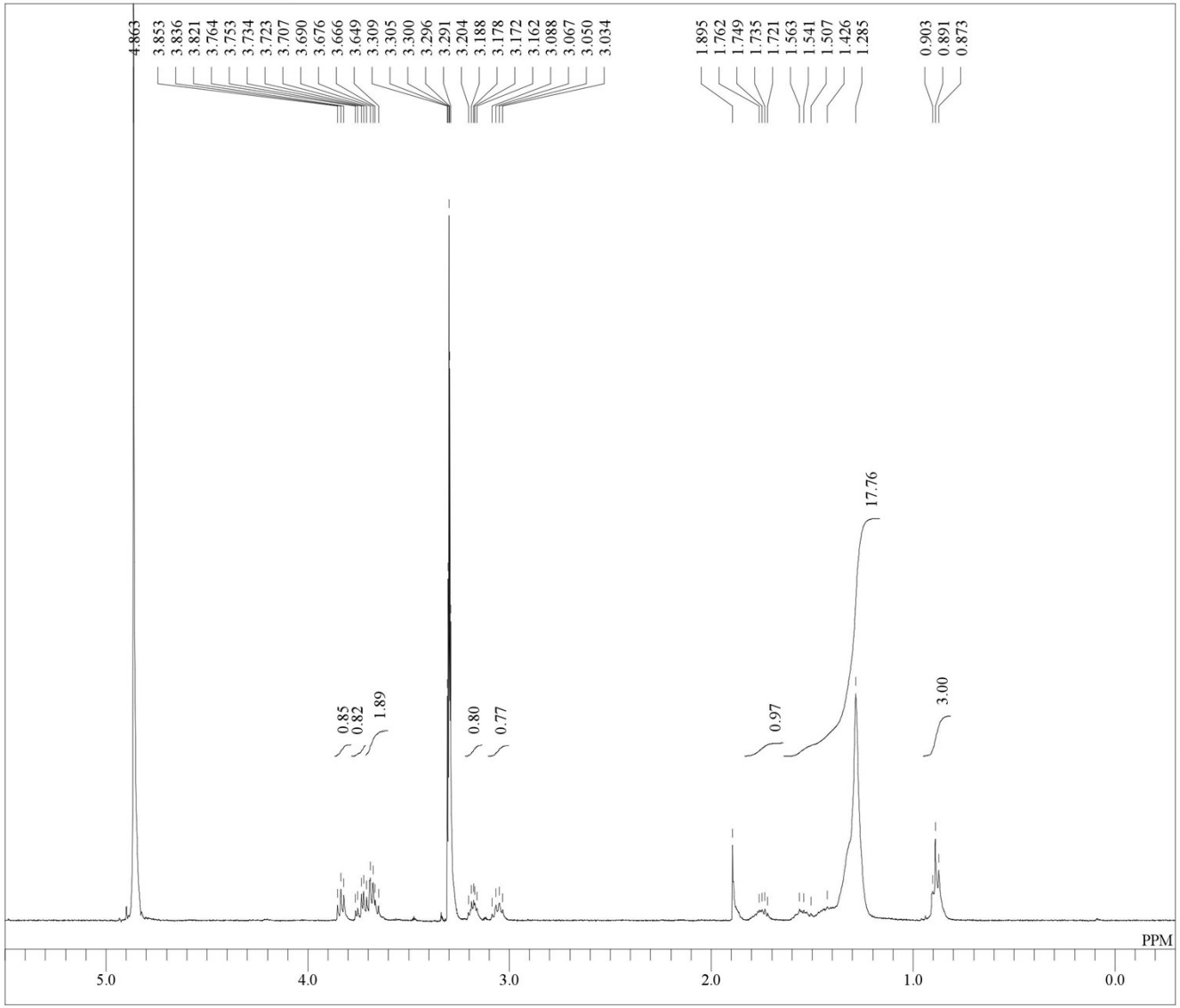

O
O
N
O
CH3(CH2)10

**3h**

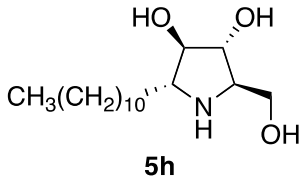

DFILE YAS01-33-01-did.als
COMNT YAS01-33-01
DATIM Thu Jul 26 10:44:47 2012
OBNUC 1H
EXMOD NON
OBFRQ 395.75 MHz
OBSET 124.00 KHz
OBFIN 10277.00 Hz
POINT 16384
FREQU 7912.96 Hz
SCANS 8
ACQTM 2.0705 sec
PD 4.9290 sec
PW1 5.50 usec
IRNUC 1H
CTEMP 21.3 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.24 Hz
RGAIN 25
PPM
7.261
4.546
4.522
4.502
4.448
4.355
4.347
4.332
4.324
3.981
3.967
3.955
3.939
3.920
3.905
3.877
3.867
3.856
3.848
3.665
3.644
1.562
1.497
1.483
1.442
1.426
1.410
1.368
1.347
1.258
0.897
0.881
0.863
0.000
3.00
20.67
1.44
0.80
0.77
0.86
0.64


OH
HO
O
N
O
CH3(CH2)10

**4h**




| | |
|---|---|
| DFILE | YAS01-38-02-did.als |
| COMNT | YAS01-38-01 |
| DATIM | Tue Jul 31 10:41:17 2012 |
| OBNUC | 1H |
| EXMOD | NON |
| OBFRQ | 395.75 MHz |
| OBSET | 124.00 KHz |
| OBFIN | 10277.00 Hz |
| POINT | 16384 |
| FREQU | 7912.96 Hz |
| SCANS | 8 |
| ACQTM | 2.0705 sec |
| PD | 4.9290 sec |
| PW1 | 5.50 usec |
| IRNUC | 1H |
| CTEMP | 22.0 c |
| SLVNT | CD3OD |
| EXREF | 3.30 ppm |
| BF | 0.01 Hz |
| RGAIN | 17 |




**5h**