

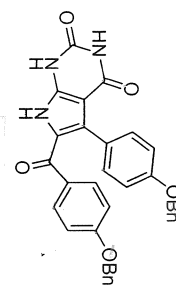
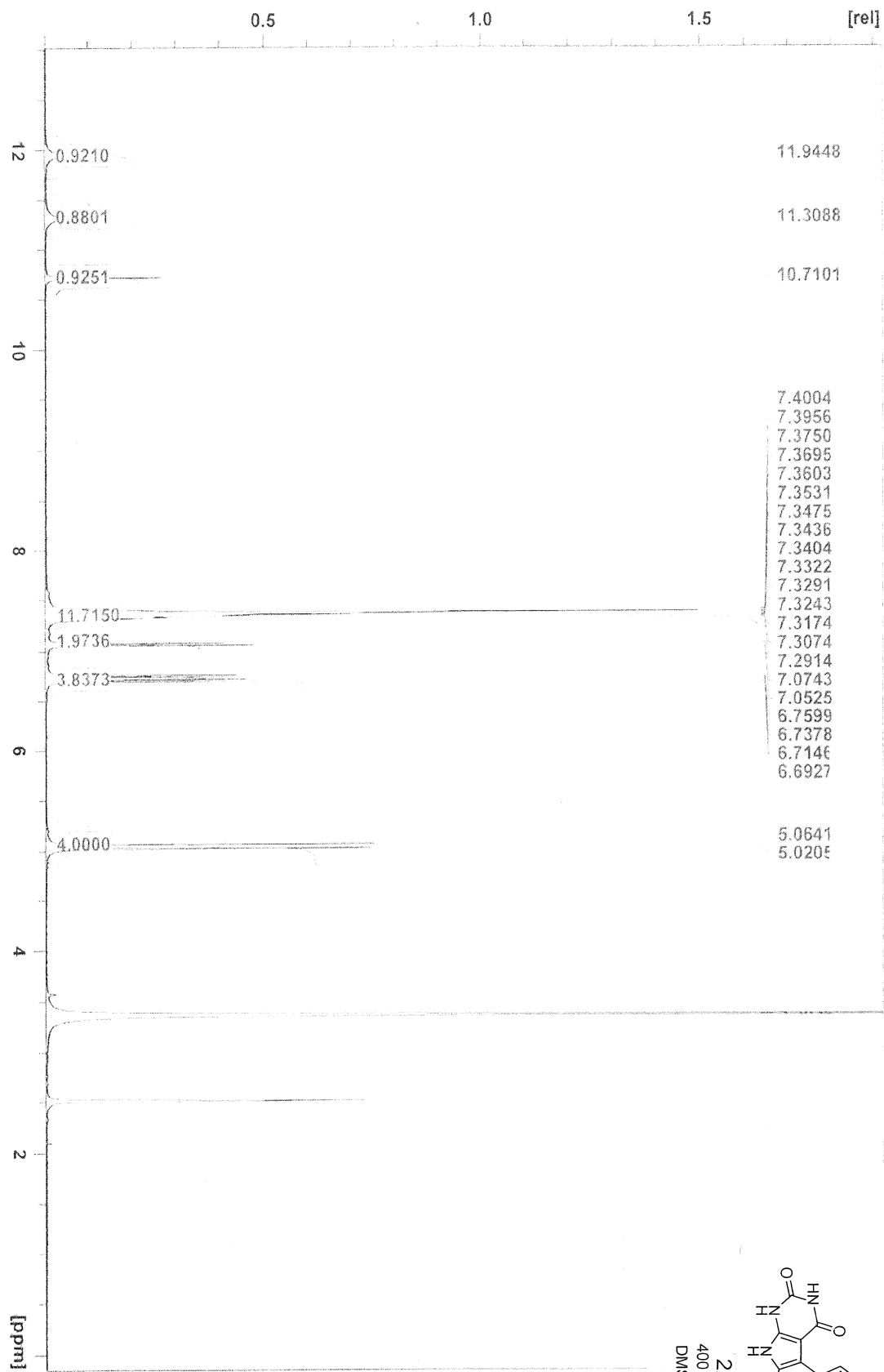
Supporting Information

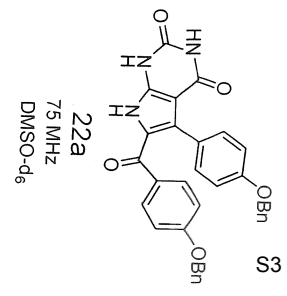
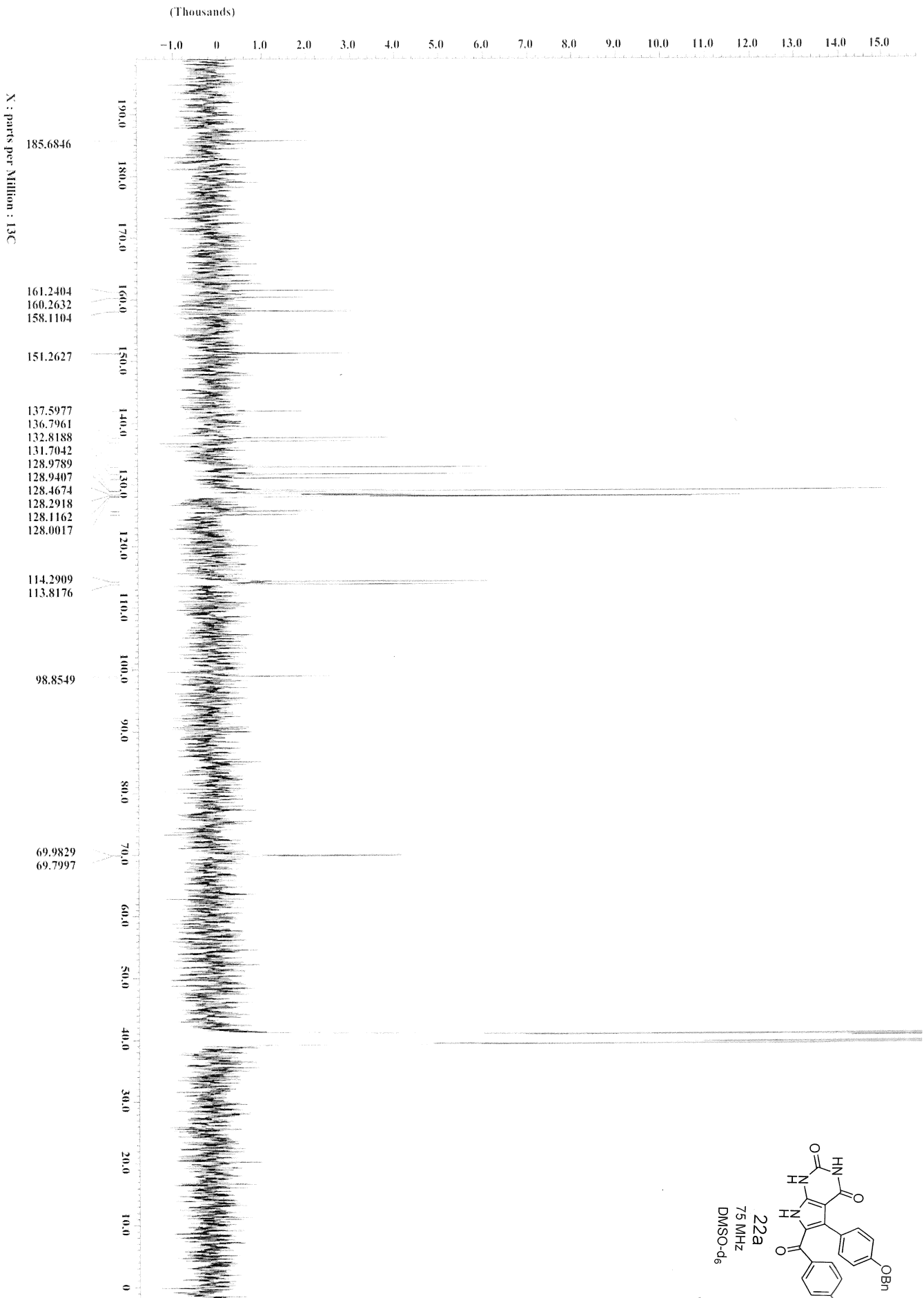
Exploring Natural Product Chemistry and Biology with Multicomponent Reactions. 5. Discovery of a Novel Tubulin-Targeting Scaffold Derived from the Rigidin Family of Marine Alkaloids

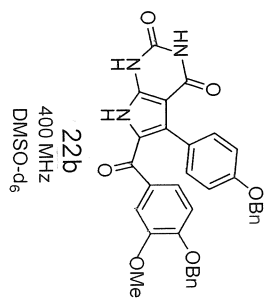
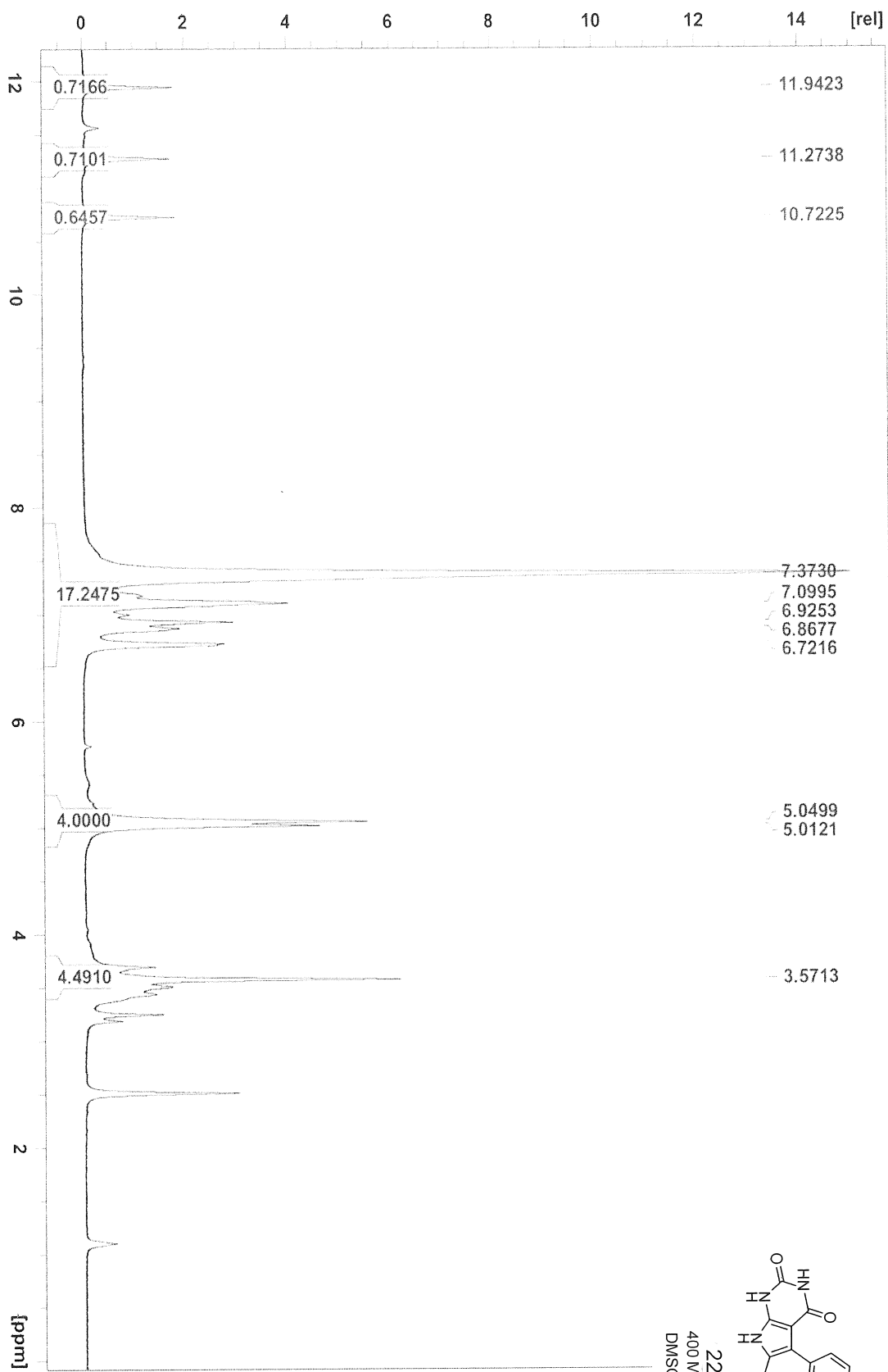
Liliya V. Frolova,^{*} Igor V. Magedov, Anntherese E. Romero, Menuka Karki, Isaiah Otero, Kathryn Hayden, Nikolai Evdokimov, Laetitia Moreno Y. Banuls, Shiva K. Rastogi, W. Ross Smith, Shi-Long Lu, Robert Kiss, Charles B. Shuster, Ernest Hamel, Tania Betancourt, Snezna Rogelj, and Alexander Kornienko^{*}

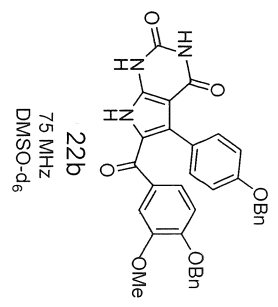
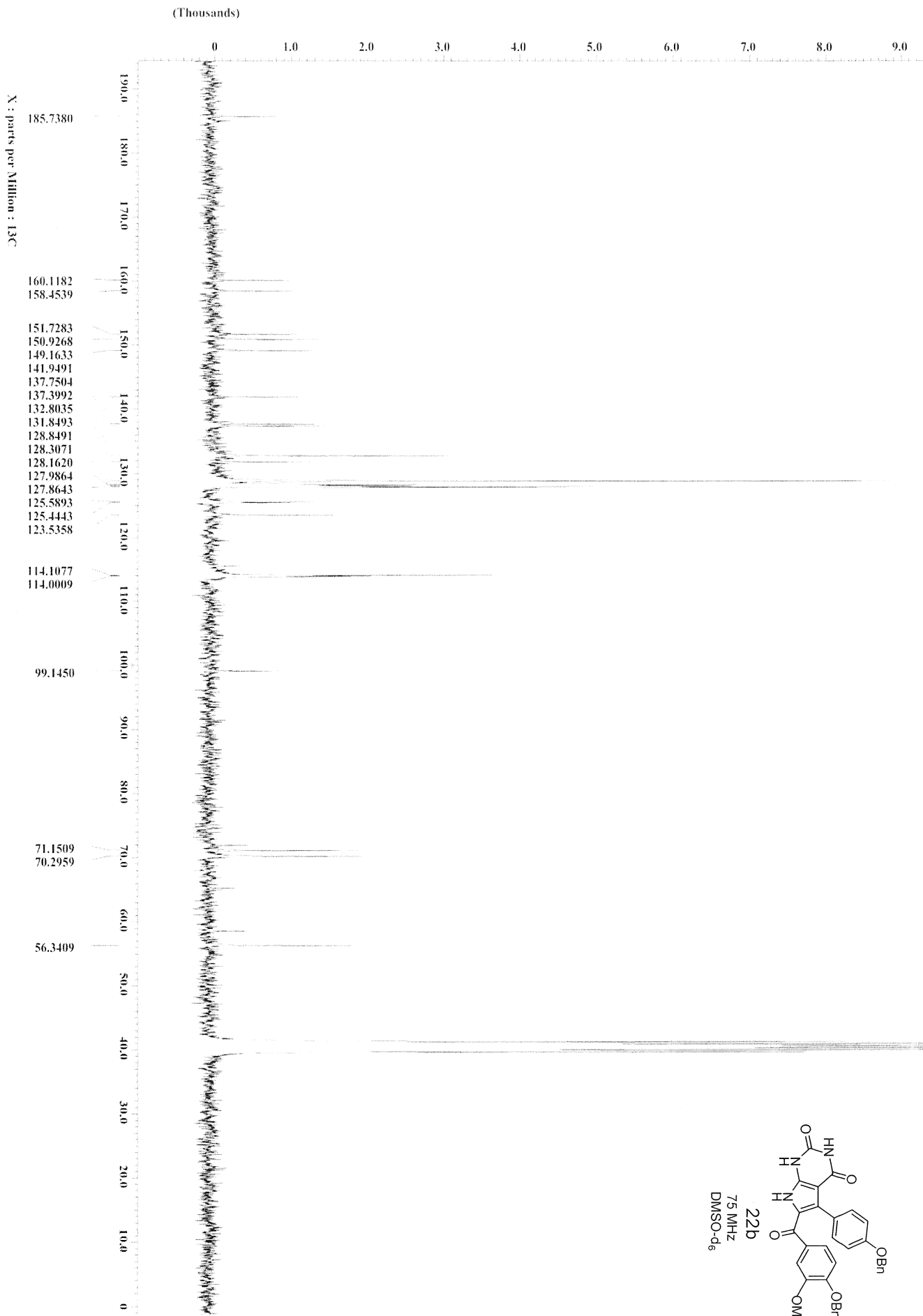
Departments of Chemistry and Biology, New Mexico Institute of Mining and Technology, Socorro, NM 87801, USA, Department of Biology, New Mexico State University, Las Cruces, NM 88003, USA, Laboratoire de Toxicologie and Laboratoire de Chimie Analytique, Toxicologie et Chimie Physique Appliquée, Institut de Pharmacie, Université Libre de Bruxelles, Brussels, Belgium, Departments of Otolaryngology, Dermatology and Pathology, University of Colorado, Anschutz Medical Campus, Aurora, CO 80045, USA, Screening Technologies Branch, Developmental Therapeutics Program, Division of Cancer Treatment and Diagnosis, National Cancer Institute, Frederick National Laboratory of Cancer Research, National Institutes of Health, Frederick, MD 21702, USA, Department of Chemistry and Biochemistry, Texas State University – San Marcos, San Marcos, TX 78666, USA.

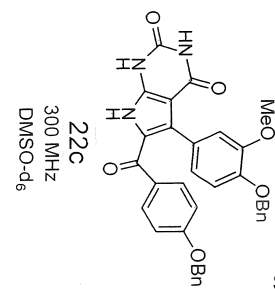
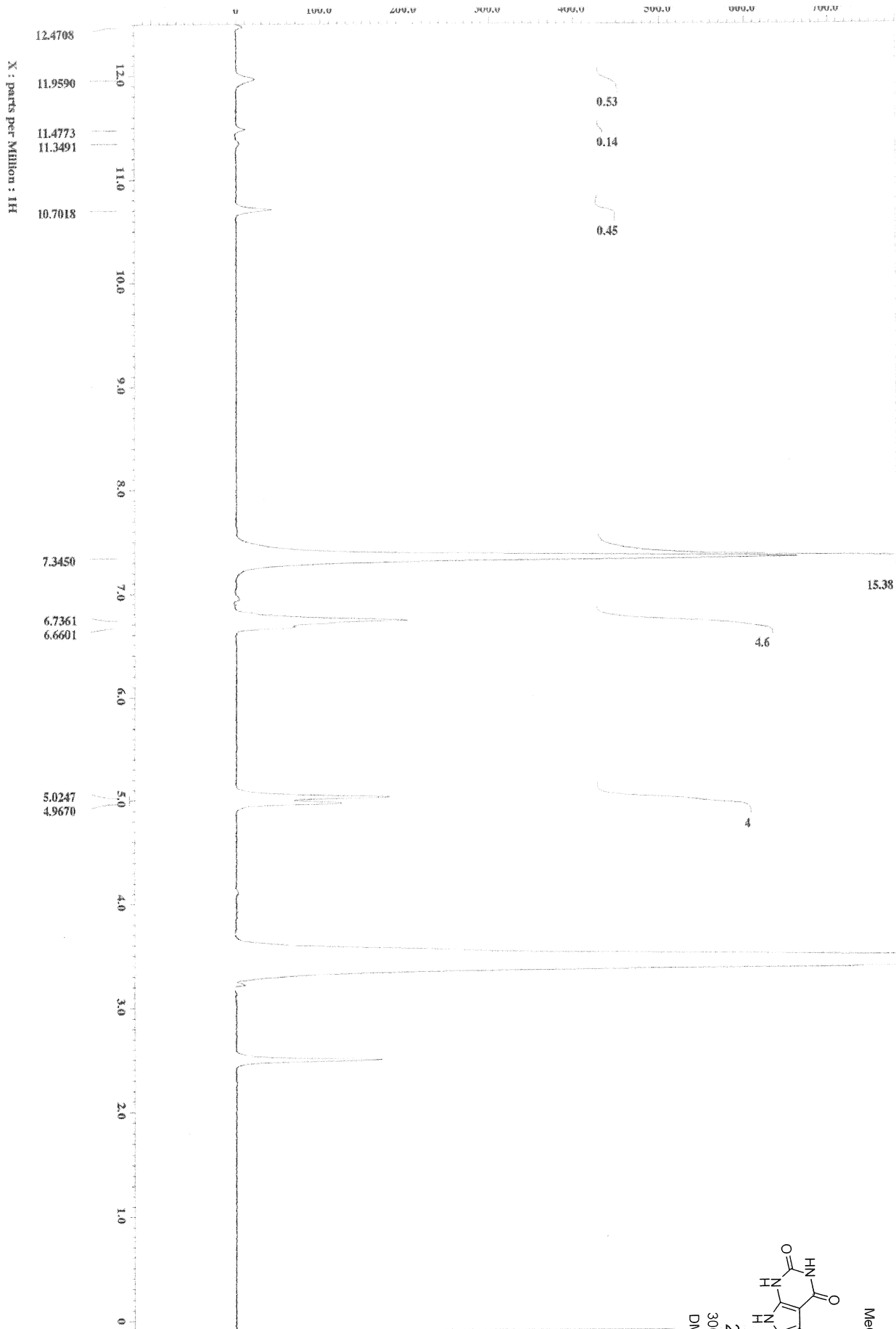
Copies of ¹H and ¹³C NMR Spectra for All New Compounds



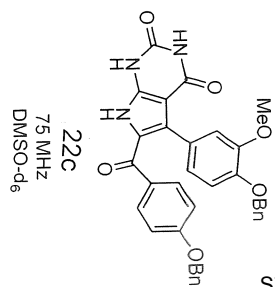
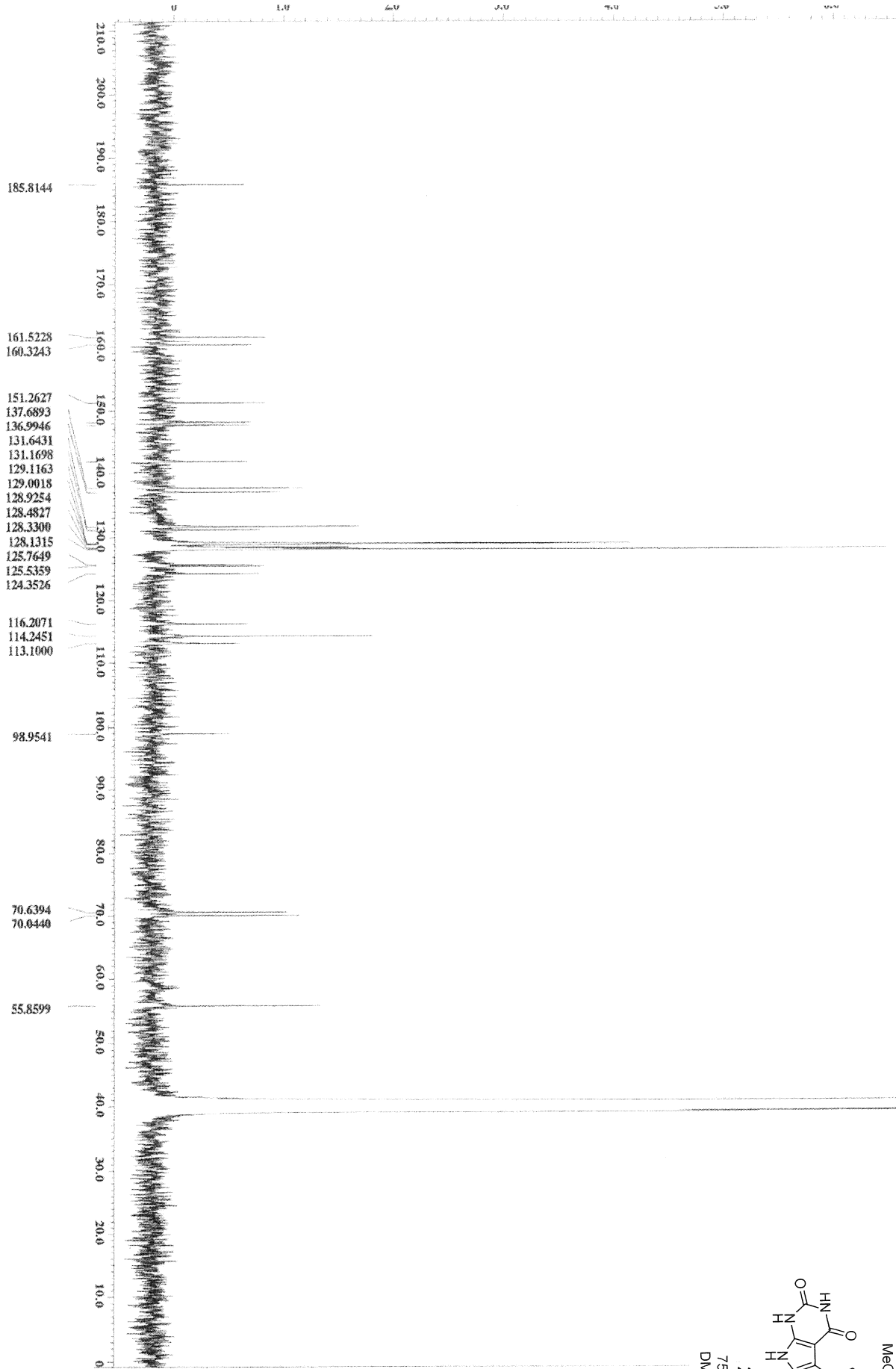


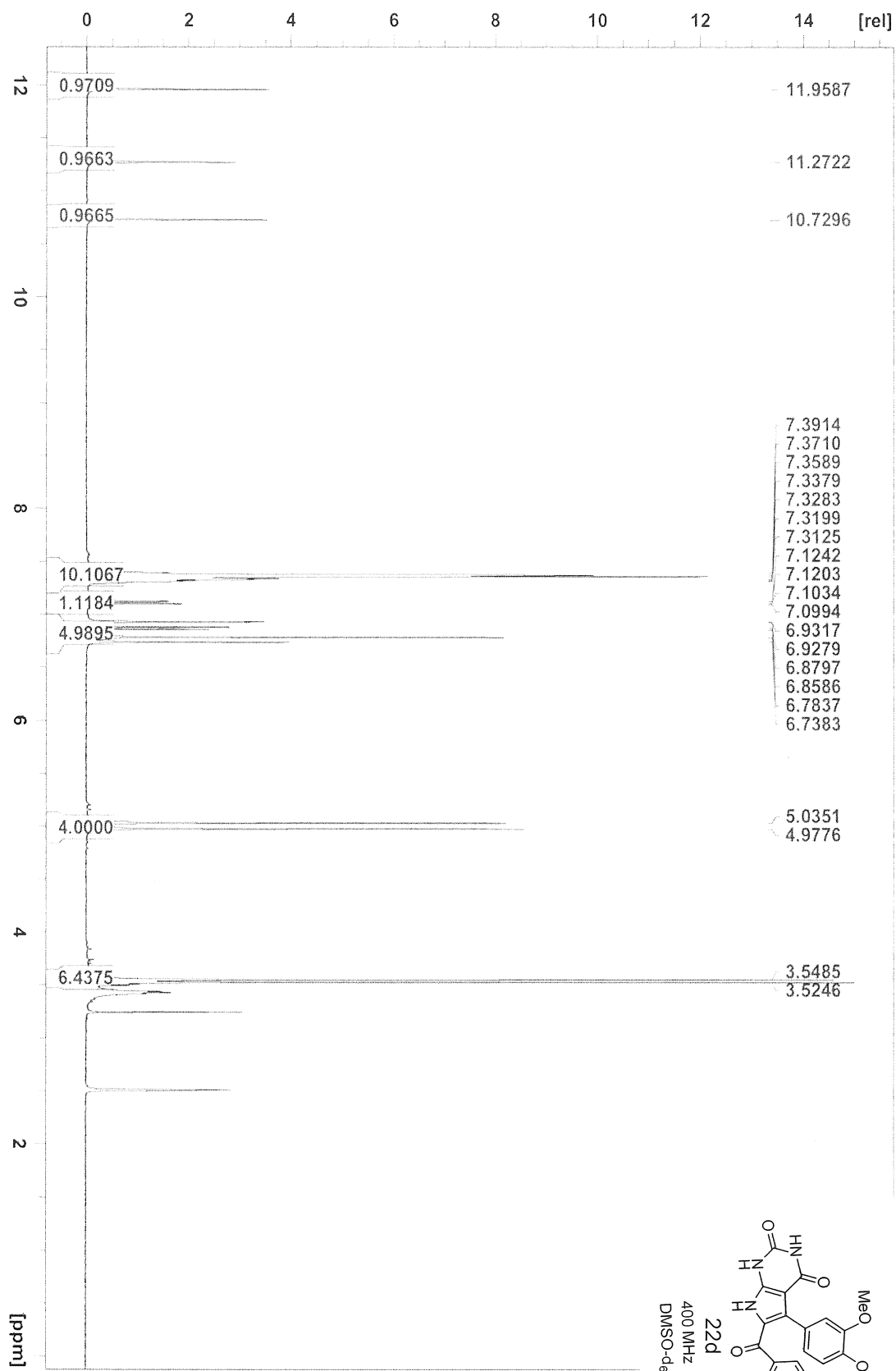


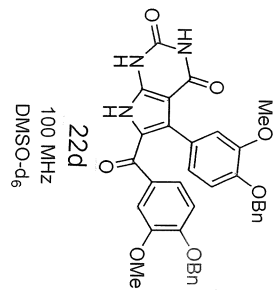
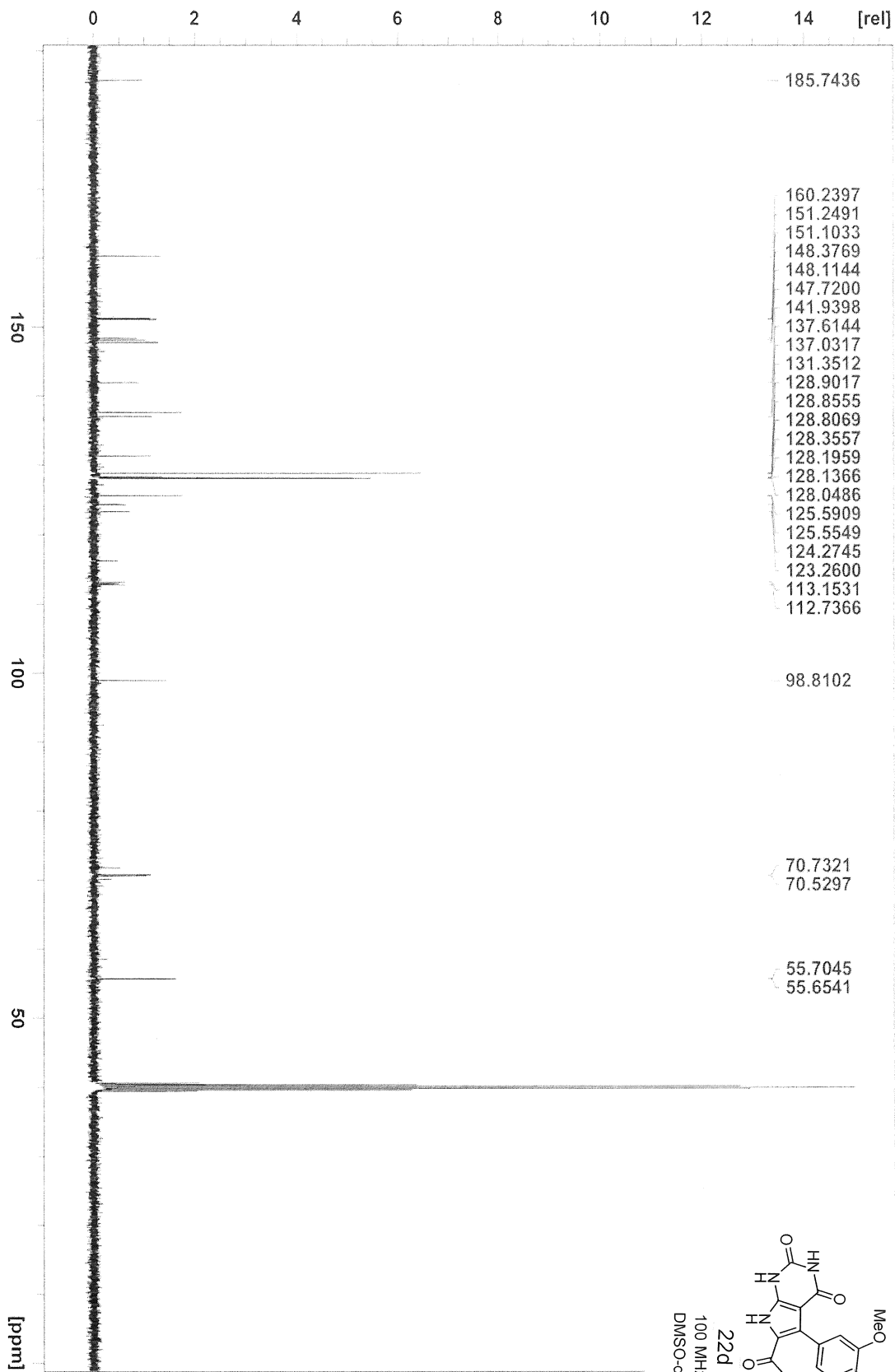


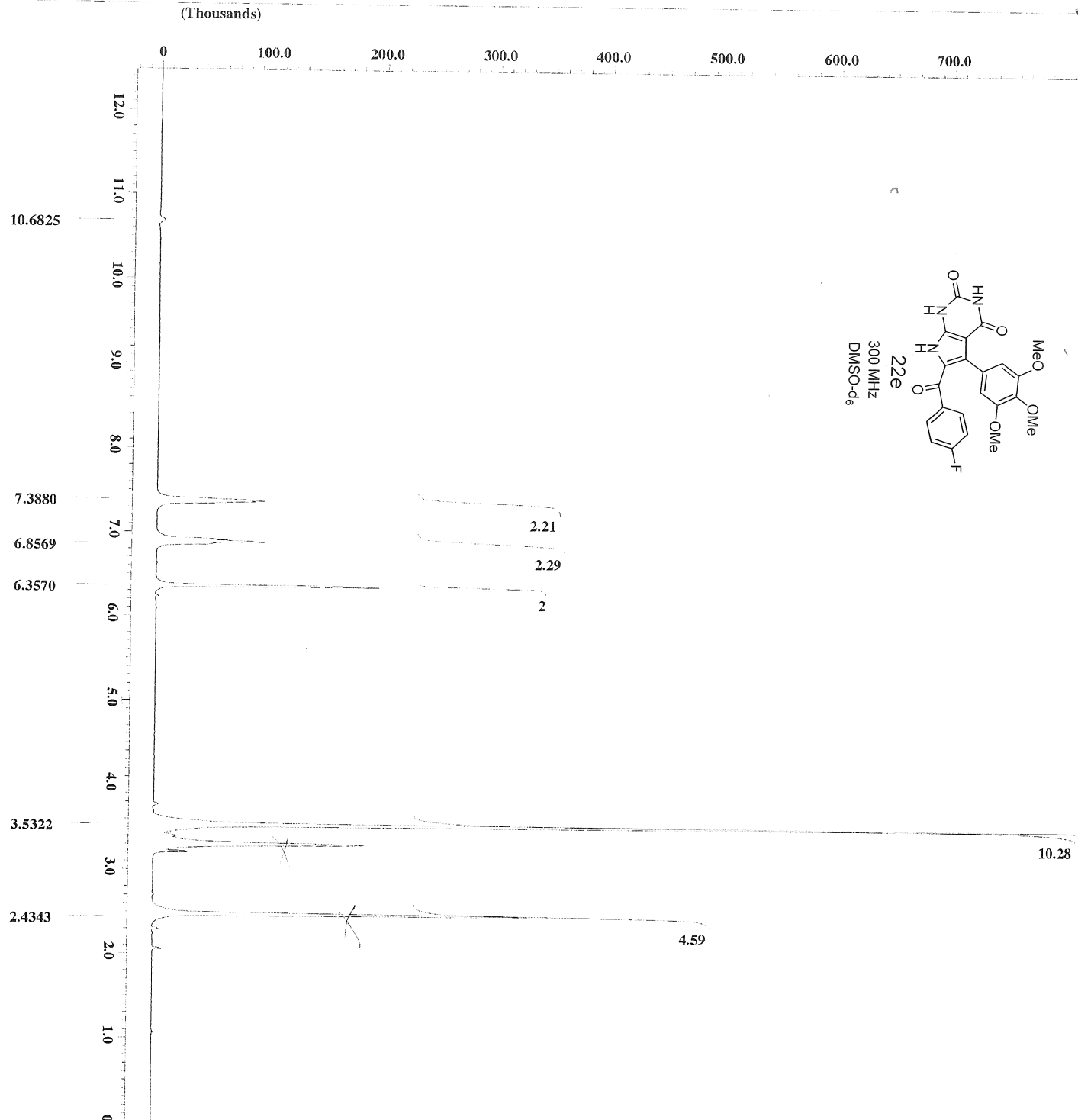
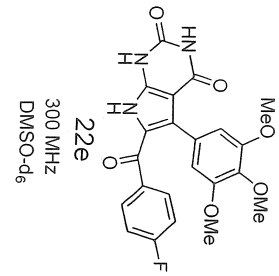


X : parts per Million : 13C









```

Filename      = 1d_spectrum-f-fp-5-j.d
Author       = alex
Experiment   = single_pulse.exp
Sample_id    = S#779403
Solvent      = DMSO-D6
Creation time = 19-JAN-2011 20:14:35
Revision time = 25-JAN-2011 11:30:33
Current_time  = 25-JAN-2011 11:30:37

Comment
Data_format  = Single Pulse Experiment
Dim_size     = 16384
Dim_title    = 1H
Dim_units    = [ppm]
Dimensions   = X
Site         = Eclipse+ 300
Spectrometer = DELTA_NMR

Field_strength = 7.0586013[T] (300[MHz]
X_acq_duration = 3.6339712[s]
X_domain       = 1H
X_freq         = 300.52965592[MHz]
X_offset      = 5[ppm]
X_points      = 16384
X_prescans    = 0
X_resolution  = 0.27518105[Hz]
X_sweep       = 4.50856628[KHz]
Clipped       = FALSE
Mod_return    = 1
Scans         = 50
Total_scans   = 50

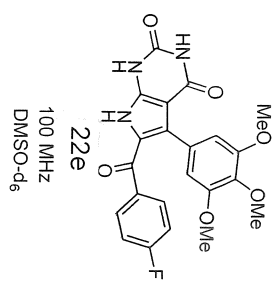
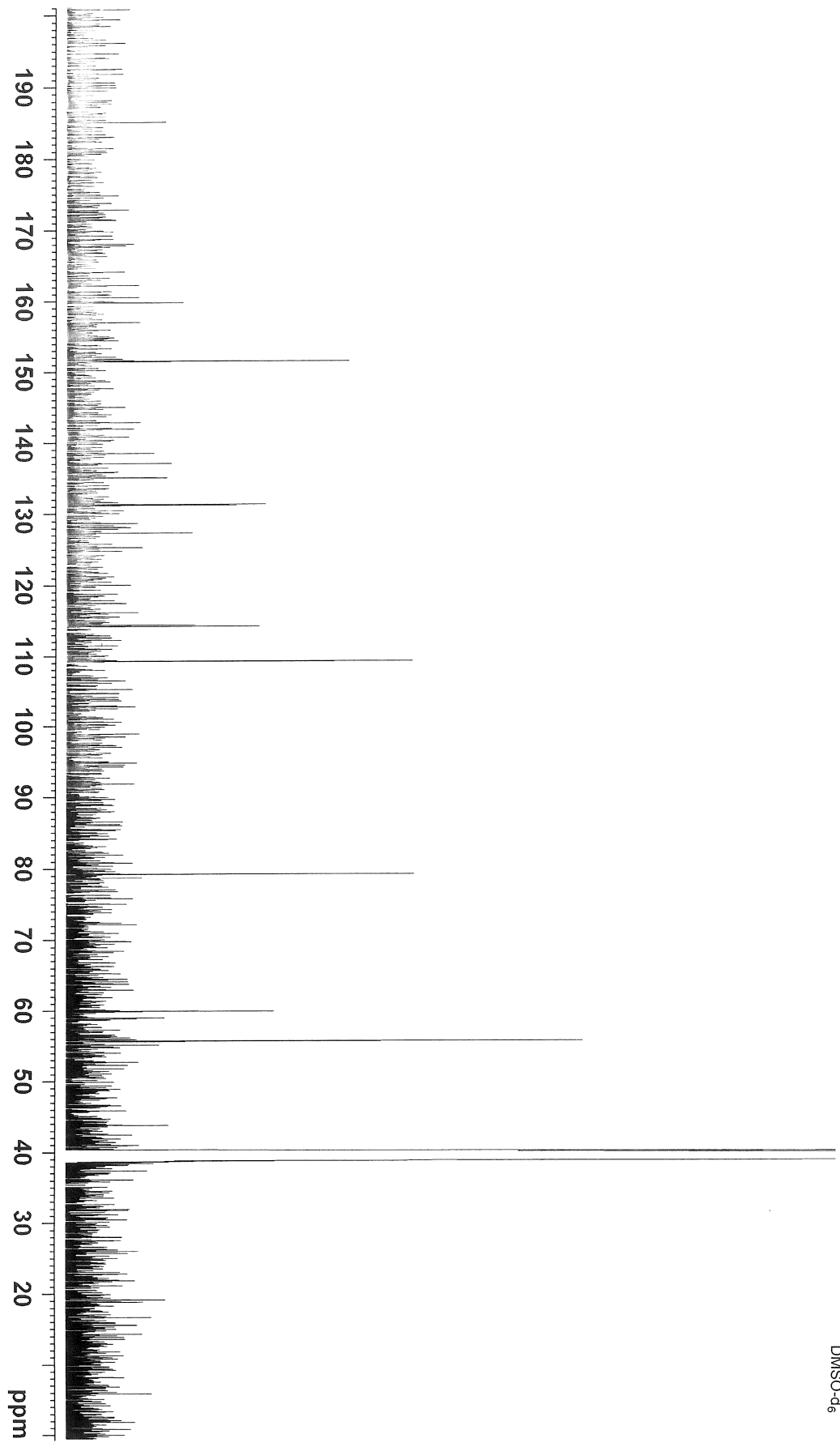
X_90_width    = 16[us]
X_acq_time    = 3.6339712[s]
X_angle       = 45[deg]
X_pulse       = 8[us]
X_pulse       = 8[us]
Initial_wait  = 1[s]
Phase_preset  = 3[us]
Recvr_gain    = 15
Relaxation_delay = 4[s]
Temp_get      = 23.7[dc]
Unblank_time  = 2[us]
    
```

X : parts per Million : 1H

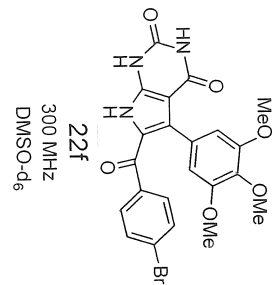
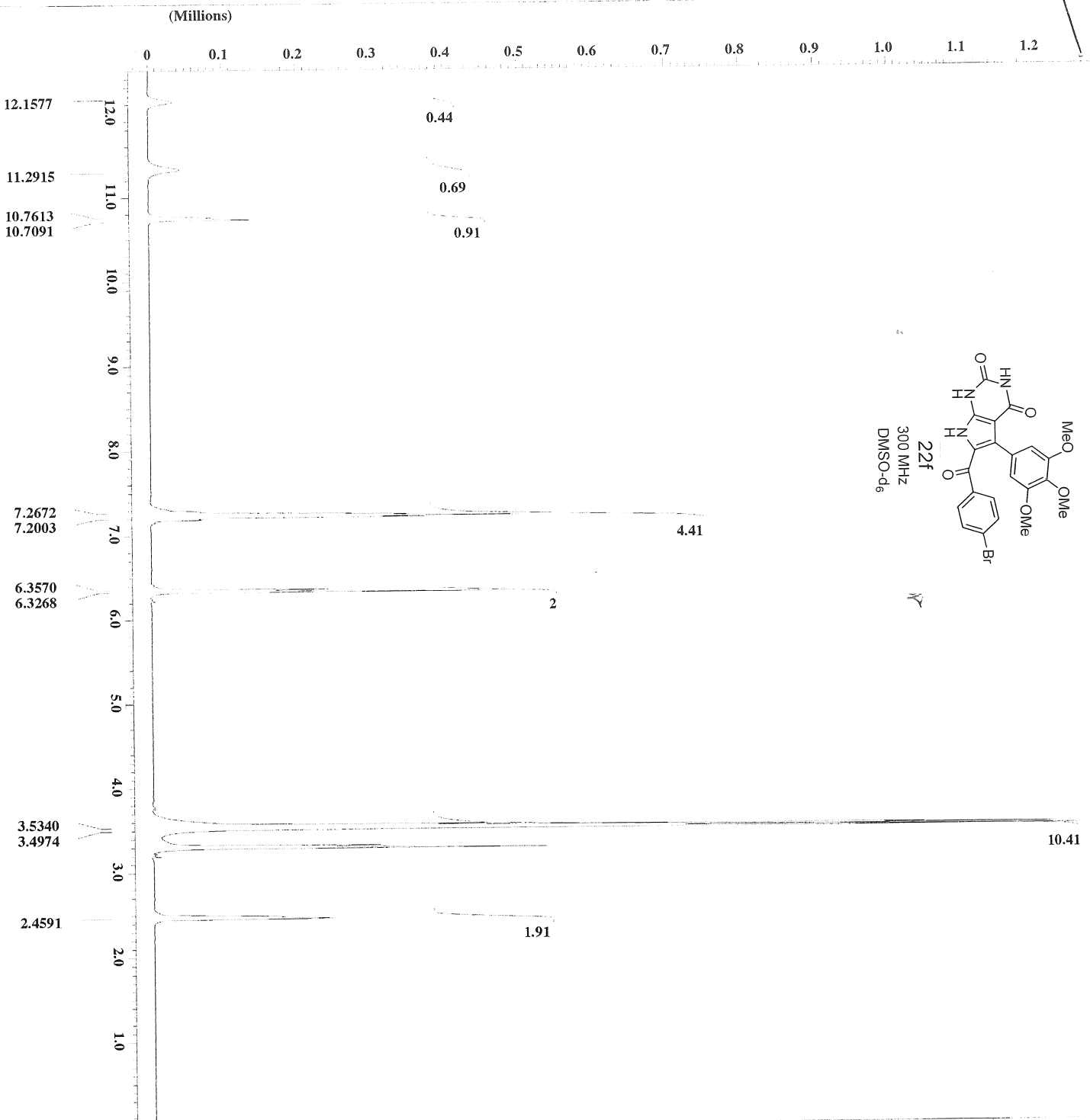
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AK_A5_13C_DMSOd6

- 185.07
- 159.75
- 151.49
- 138.56
- 137.12
- 135.11
- 131.26
- 127.40
- 114.24
- 109.26
- 79.20
- 59.88
- 55.71
- 55.67



X : parts per Million : 1H



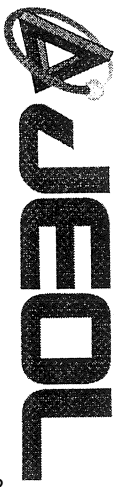
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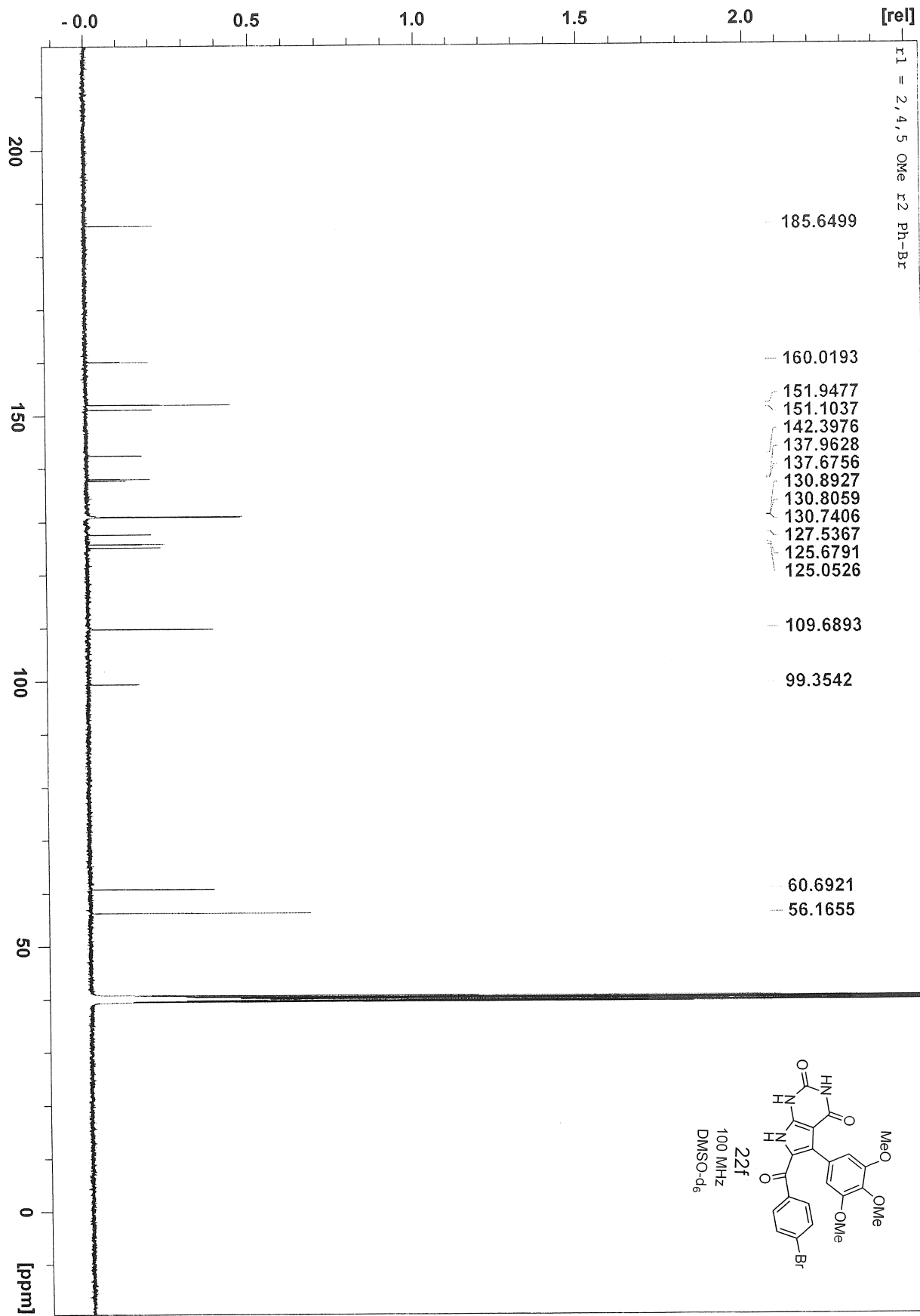
Filename = 1d_spectrum-Br-FP-8.j
Author = alex
Experiment = single_pulse.exp
Sample_id = S#640724
Solvent = DMSO-d6
Creation_time = 18-JAN-2011 17:46:46
Revision_time = 25-JAN-2011 11:28:01
Current_time = 25-JAN-2011 11:28:04

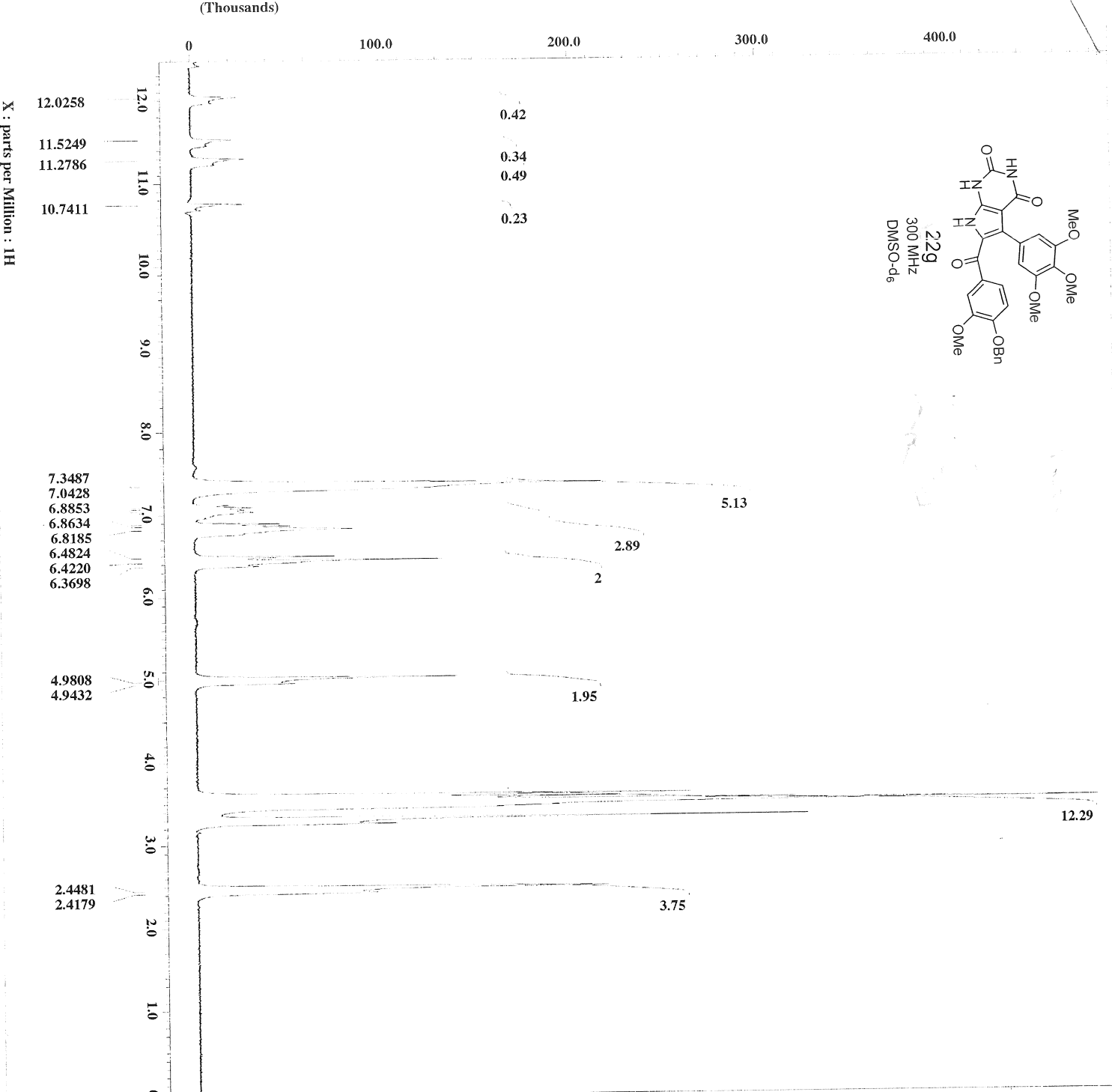
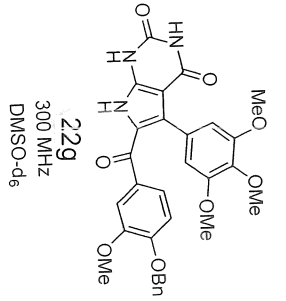
Comment = Single Pulse Experiment
Data_format = 1D REAL
Dim_size = 16384
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Spectrometer = Eclipse+ 300
Site = DELTA_NMR

Field_strength = 7.0586013[M] (300)MHz
X_acq_duration = 3.6339712[s]
X_domain = 1H
X_freq = 300.5296592[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.27518105[Hz]
X_sweep = 4.50856628[kHz]
Clipped = FALSE
Mod_return = 1
Scans = 50
Total_scans = 50

X_90_width = 16[us]
X_acq_time = 3.6339712[s]
X_angle = 45[deg]
X_pulse = 8[us]
Initial_wait = 1[s]
Phase_preset = 3[us]
Recvr_gain = 15
Relaxation_delay = 4[s]
Temp_get = 24.2[dc]
Unblank_time = 2[us]
  
```







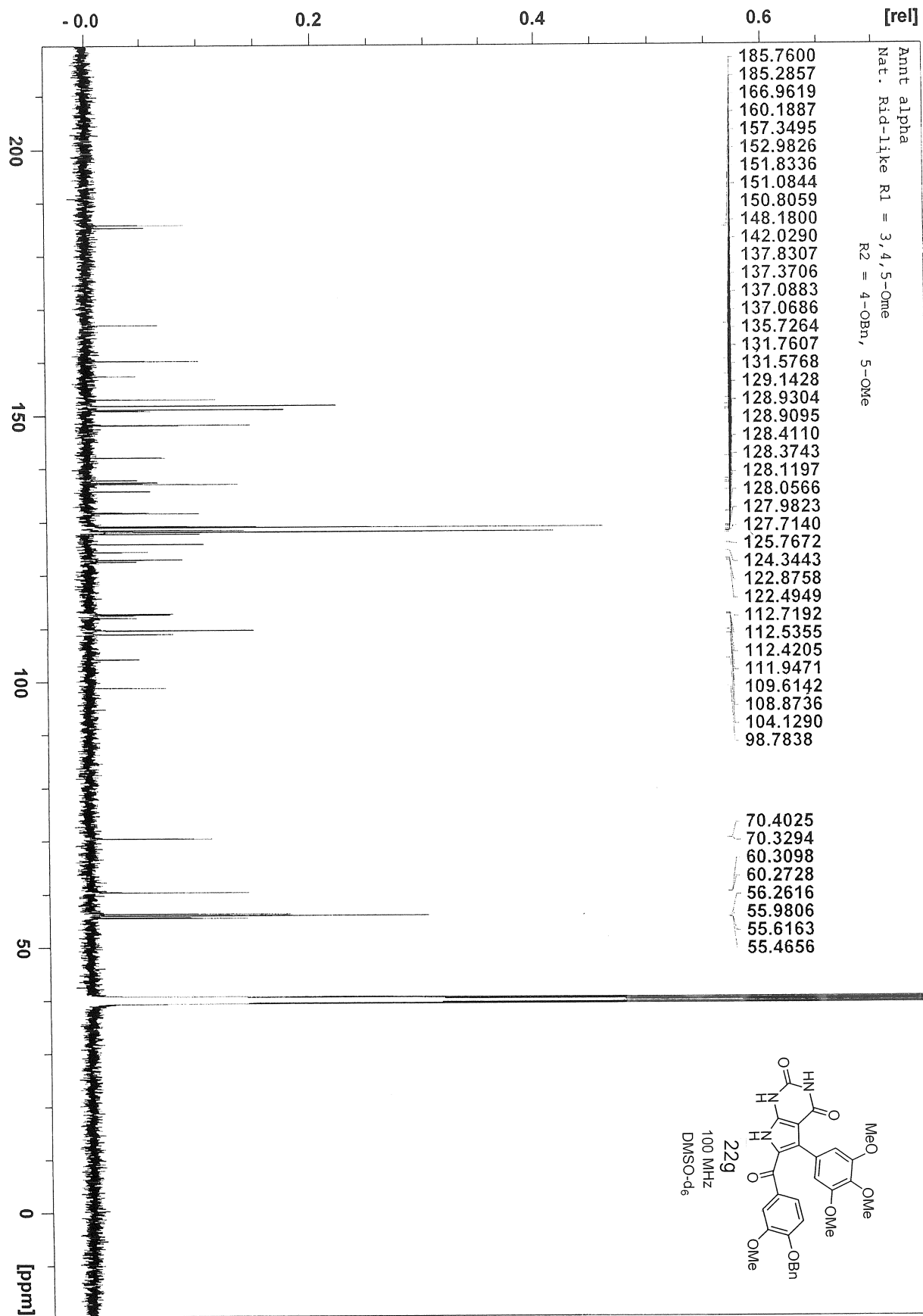
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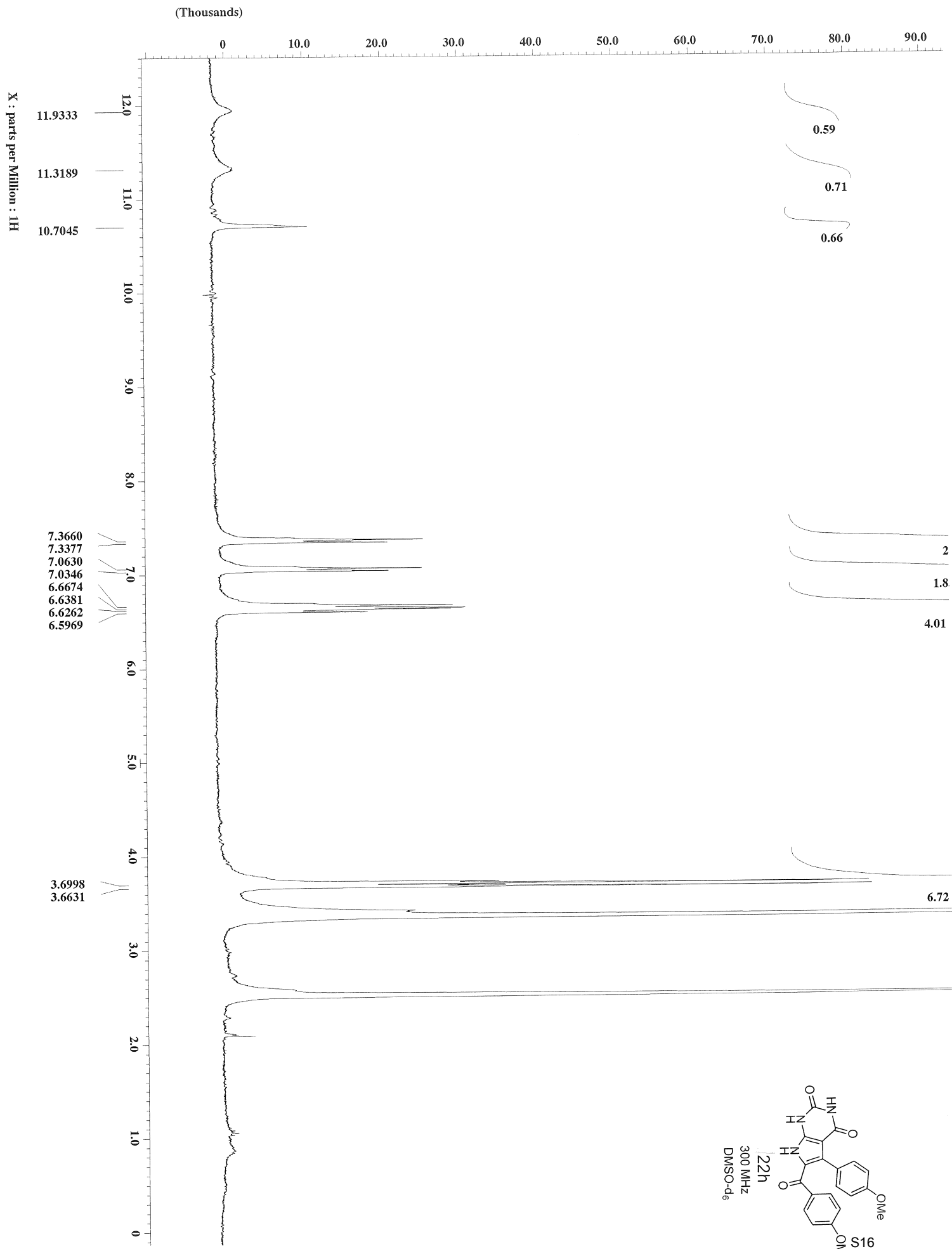
Filename = id_spectrum-ANNT-06FP
Author = alex
Experiment = single_pulse.exp
Sample_id = S#778727
Solvent = DMSO-d6
Creation_time = 10-JAN-2011 21:33:28
Revision_time = 25-JAN-2011 11:22:16
Current_time = 25-JAN-2011 11:22:25

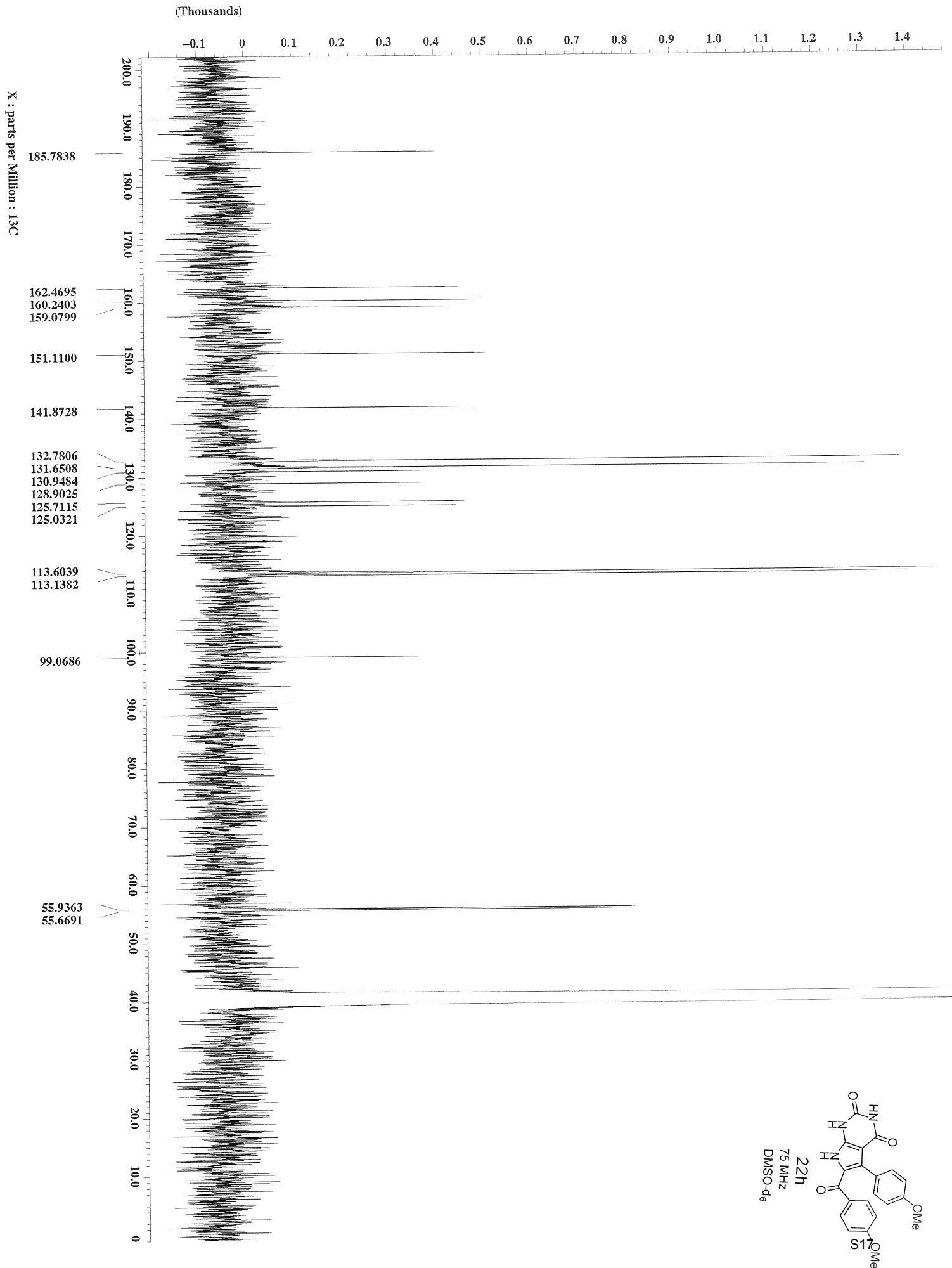
Comment = Single Pulse Experiment
Data_format = 1D REAL
Dim_size = 16384
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = X
Spectrometer = DELTA_NMR

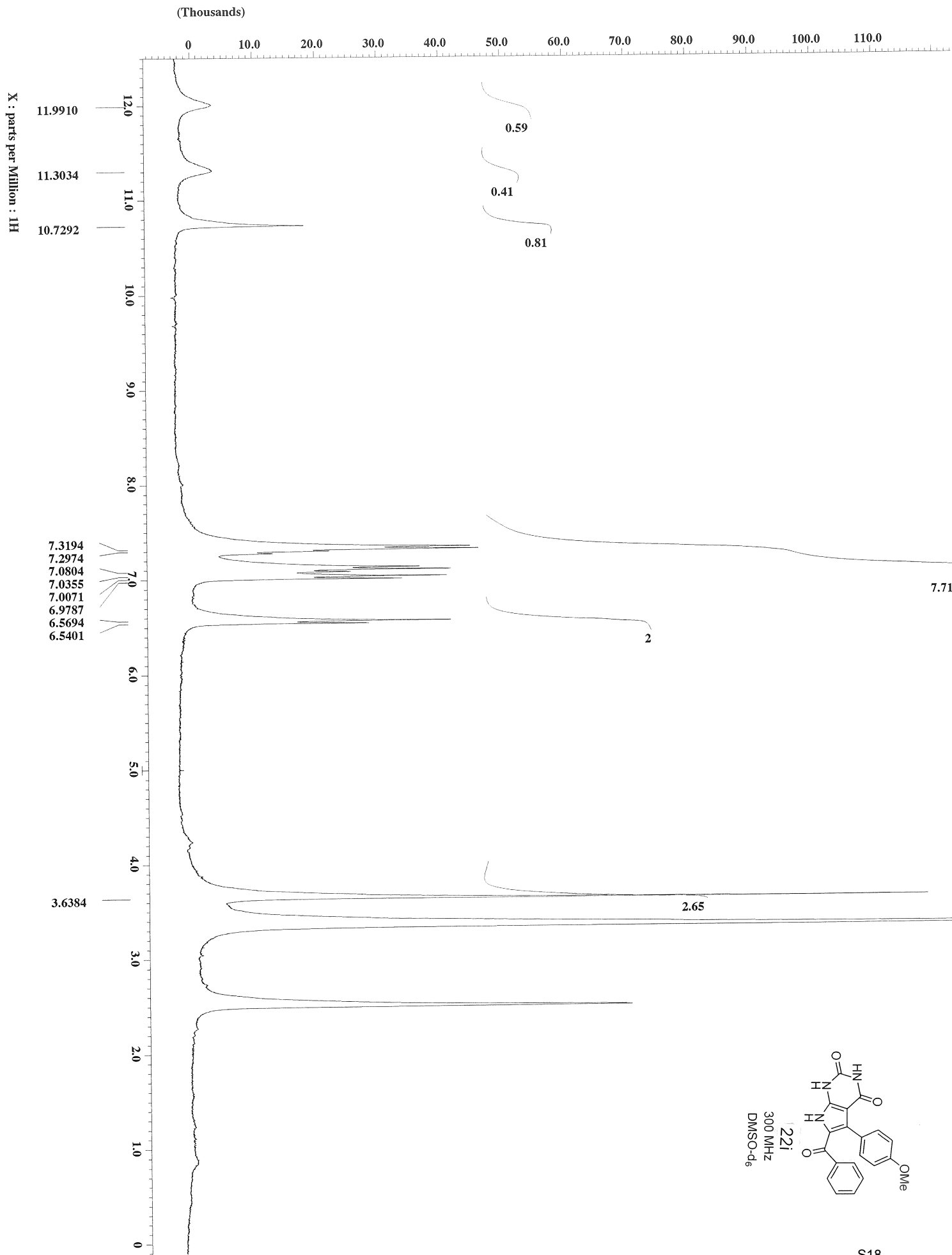
Field_strength = 7.0586013 [T] (300) [MHz]
X_acq_duration = 3.6339712 [s]
X_domain = 1H
X_freq = 300.52965592 [MHz]
X_offset = 51 [ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.27518105 [Hz]
X_sweep = 4.5085628 [kHz]
Clipped = FALSE
Mod_return = 1
Scans = 24
Total_scans = 24

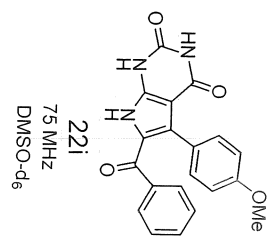
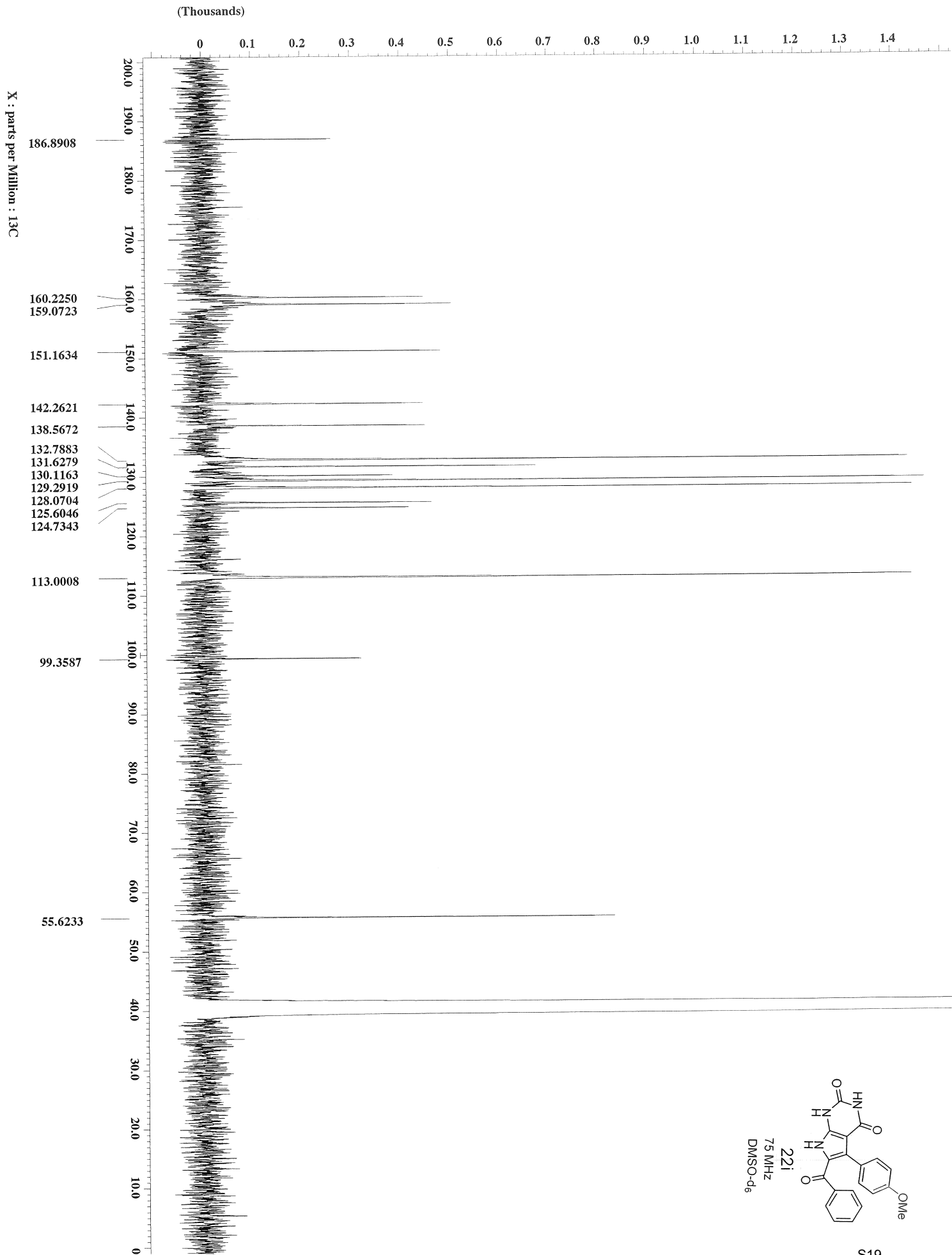
X_90_width = 16 [us]
X_acq_time = 3.6339712 [s]
X_angle = 45 [deg]
X_pulse = 8 [us]
Initial_wait = 1 [s]
Phase_preset = 3 [us]
Recvr_gain = 15
Relaxation_delay = 4 [s]
Temp_get = 21.2 [degC]
Unblank_time = 2 [us]
    
```











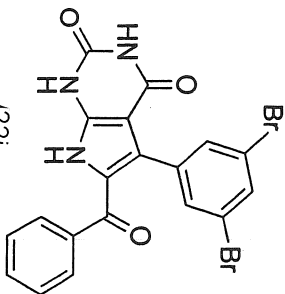
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Filename = 1d_spectrum-355.jdf
Author = alex
Experiment = single_pulse.exp
Sample_id = S#359108
Solvent = DMSO-D6
Creation time = 8-MAR-2011 09:55:33
Revision time = 8-MAR-2011 10:09:40
Current_time = 8-MAR-2011 10:09:45

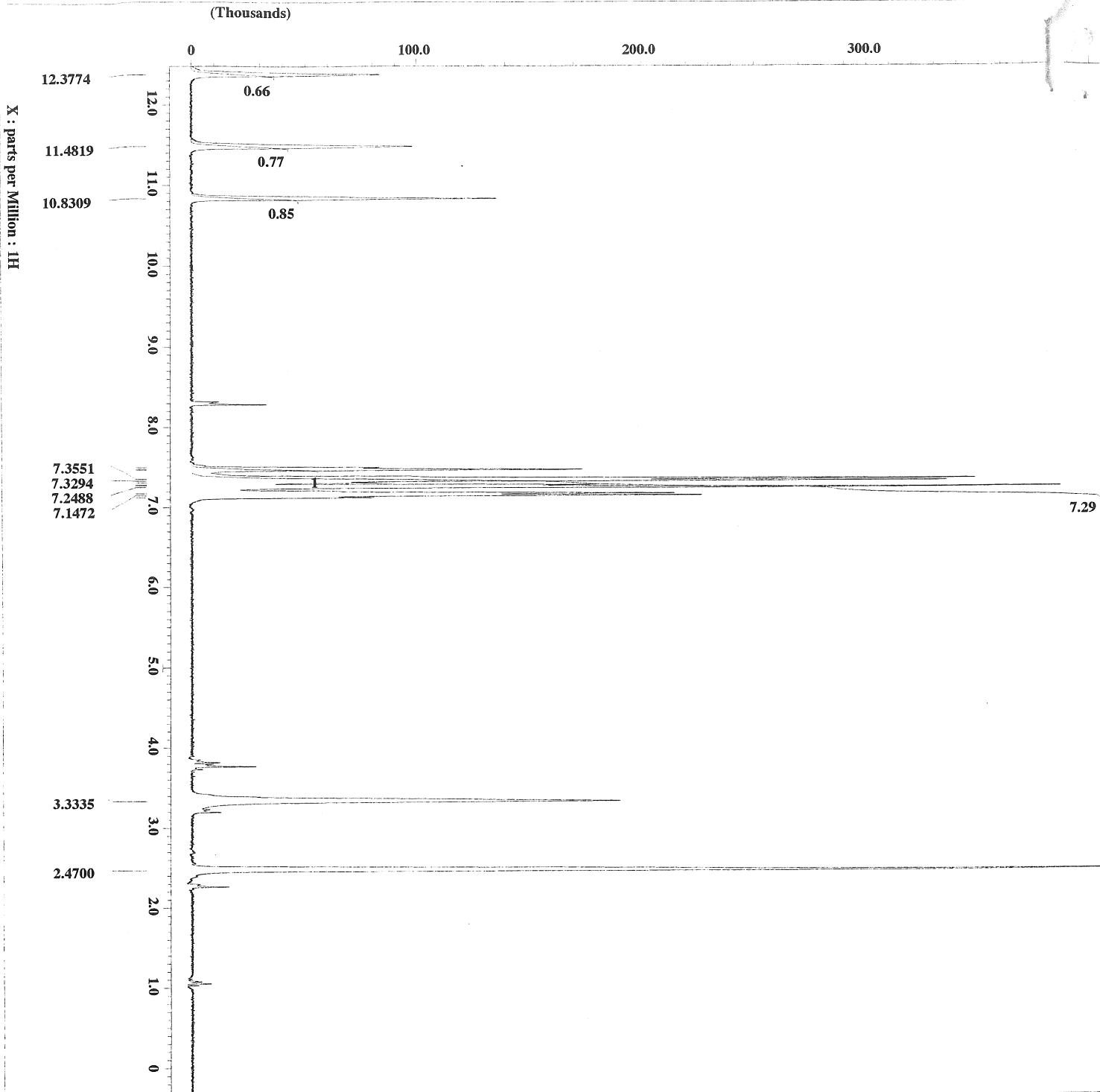
Comment = Single Pulse Experiment
Data format = ID REAL
Dim size = 16384
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = Eclipset 300
Spectrometer = DELTA_NMR

Field strength = 7.0586013[TG] (300)MHz
X_acq_duration = 3.6339712[s]
X_domain = 1H
X_freq = 300.52965592[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.27518105[Hz]
X_sweep = 4.50856628[kHz]
Clipped = FALSE
Mod_return = 1
Scans = 32
Total_scans = 32

X_90_width = 16[us]
X_acq_time = 3.6339712[s]
X_angle = 45[deg]
X_pulse = 8[us]
Initial_wait = 1[s]
Phase_preset = 3[us]
Recvr_gain = 15
Relaxation_delay = 4[s]
Temp_get = 18.5[dc]
Tmbank_time = 2[us]
    
```



300 MHz, DMSO-d₆




```

Filename = id_13c_spectrum-160.f
Author = alex
Experiment = single pulse_dec
Sample_id = S#673647
Solvent = DMSO-d6
Creation_time = 9-MAR-2011 06:44:47
Revision_time = 9-MAR-2011 10:34:45
Current_time = 9-MAR-2011 10:35:02
  
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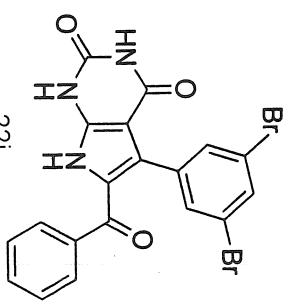
```

Comment = Single Pulse with Bro
Data_format = ID COMPLEX
Dim_size = 32768
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Eclipse+ = 300
Site = DELTA_NMR
Spectrometer =
  
```

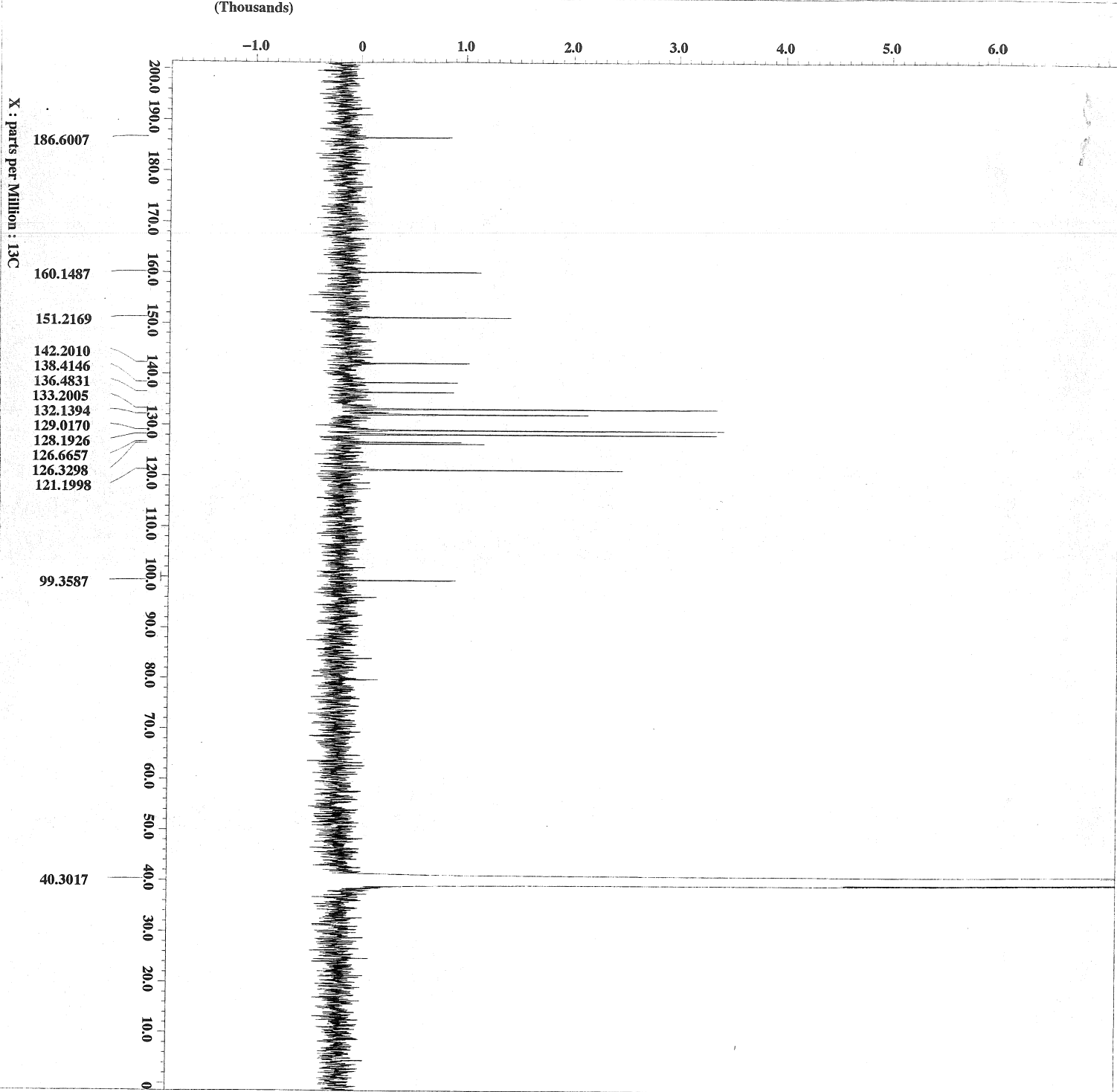
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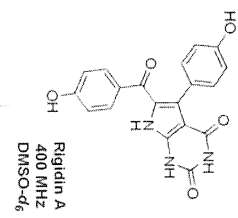
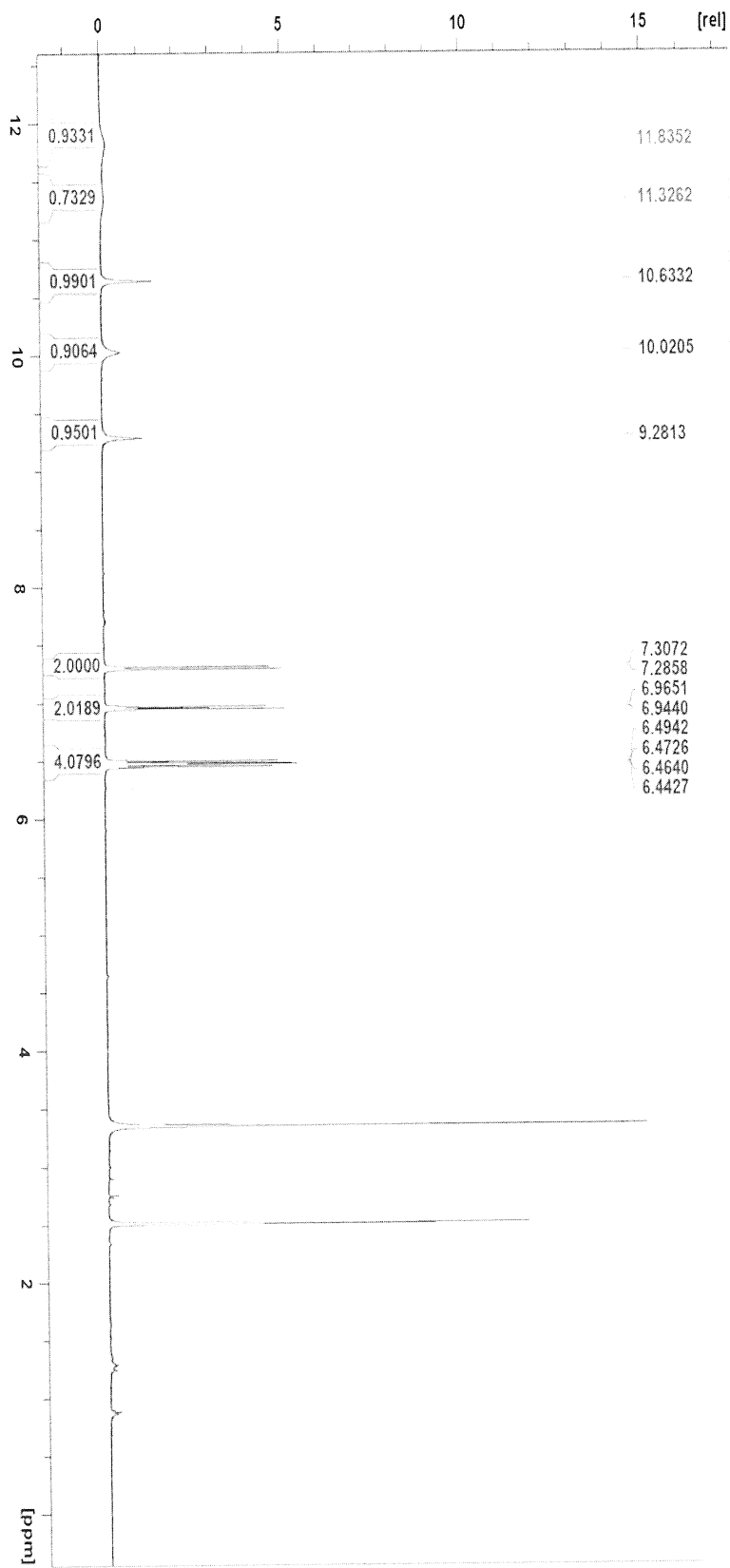
Field_strength = 7.0586013 [T] (300 [MHz]
X_acq_duration = 1.7334272 [s]
X_domain = 13C
X_freq = 75.56823426 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.57689184 [Hz]
X_sweep = 18.90359168 [kHz]
Irr_domain = 1H
Irr_freq = 300.52965592 [MHz]
Irr_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16000
Total_scans = 16000

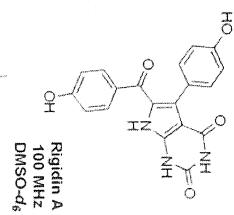
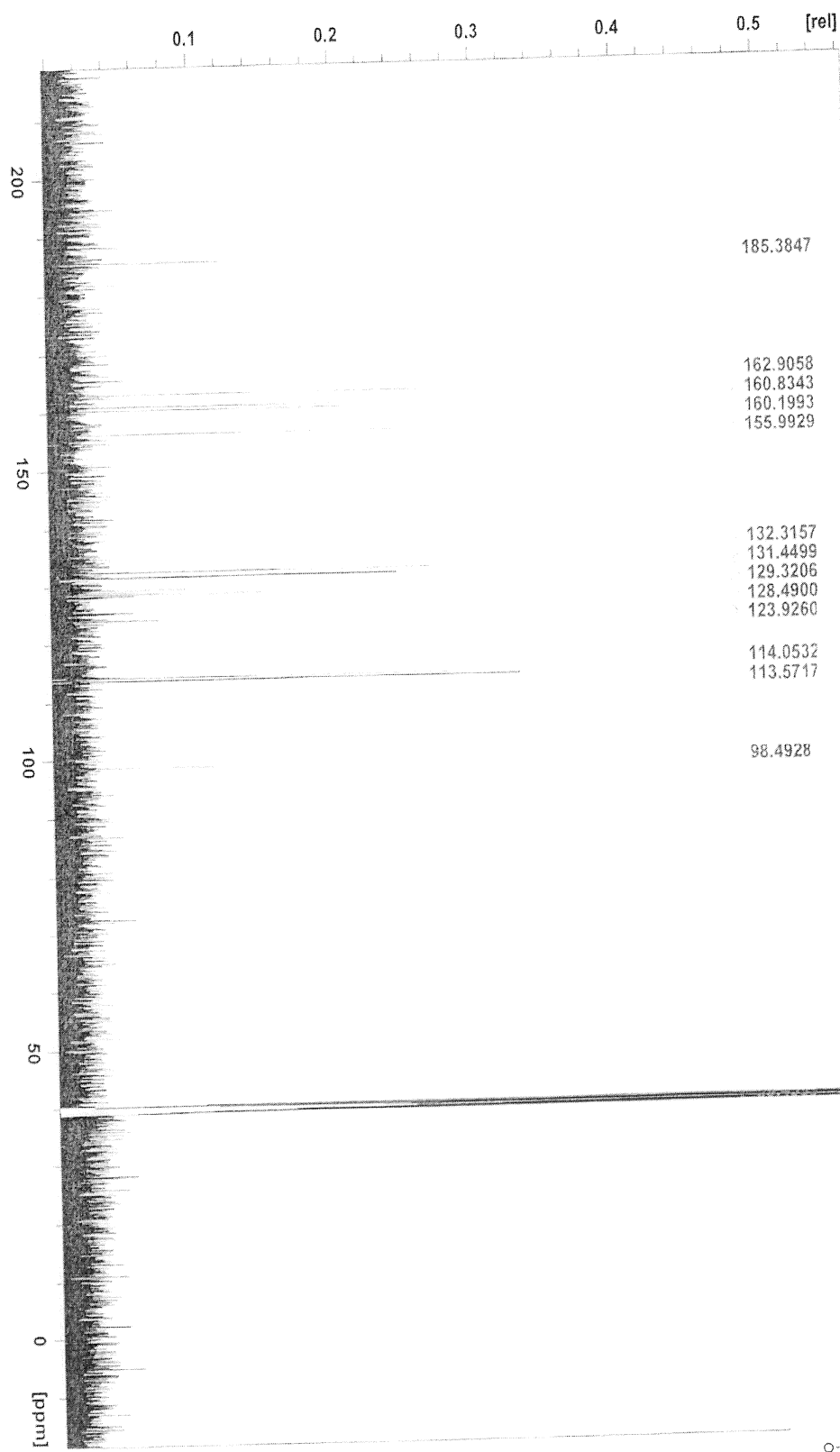
X_90_width = 8.1 [us]
X_acq_time = 1.7334272 [s]
X_angle = 30 [deg]
X_pulse = 2.7 [us]
Initial_wait = 1 [s]
Phase_preset = 3 [us]
Recvr_gain = 15
Relaxation_delay = 1 [s]
Temp_get = 17.6 [dc]
Unblank_time = 2 [us]
  
```

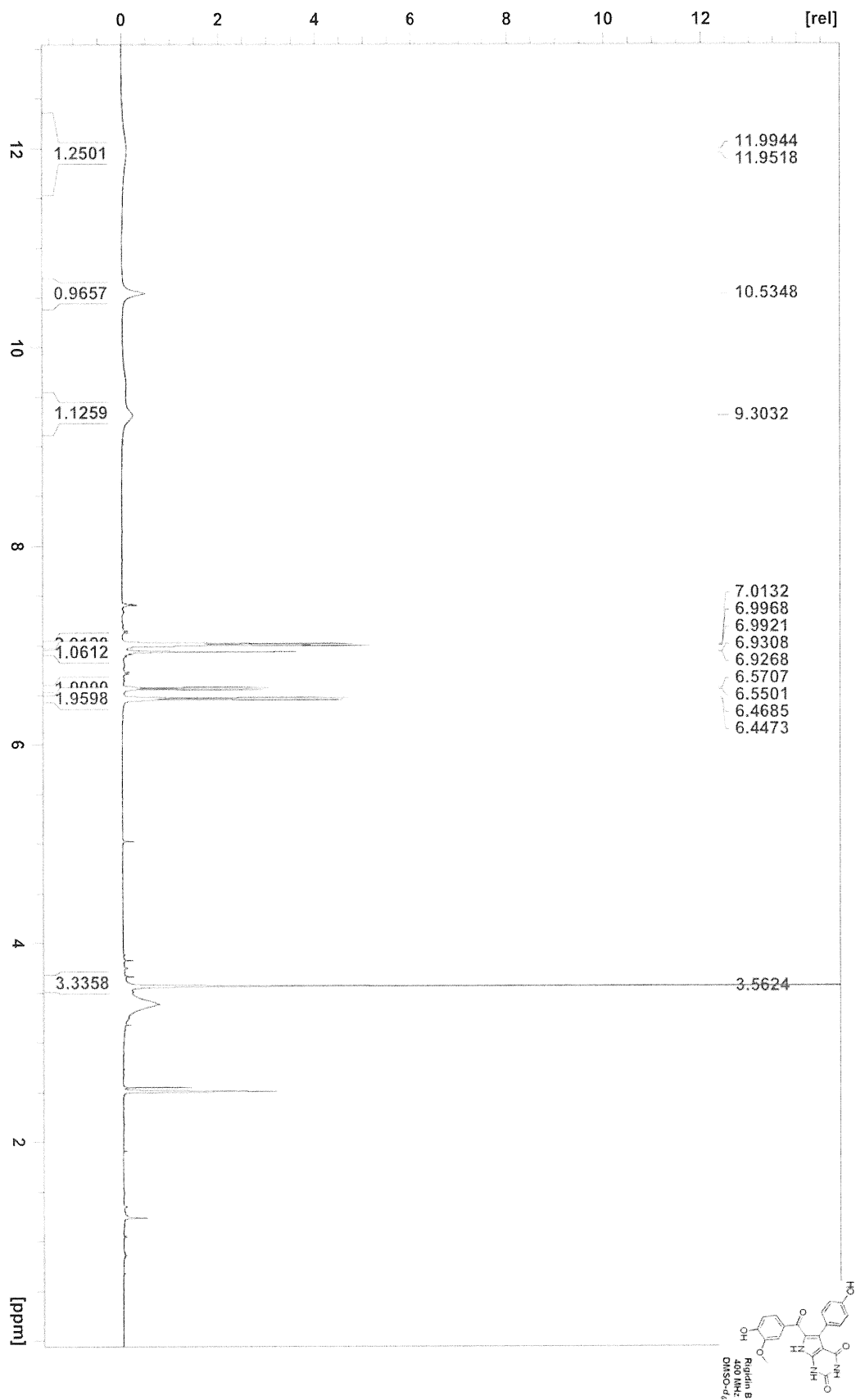


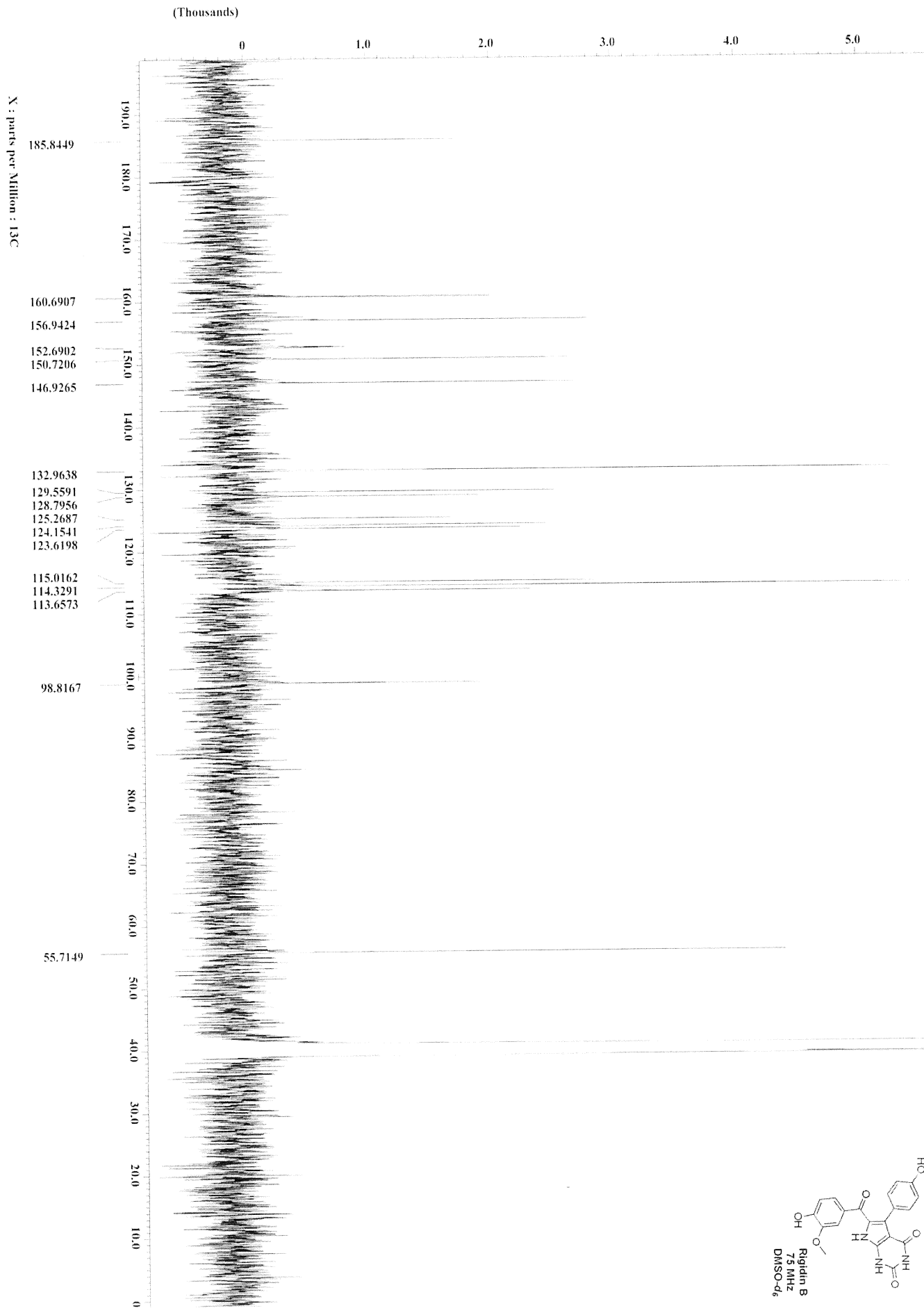
75 MHz, DMSO-d₆

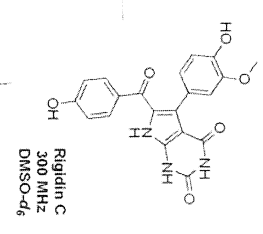
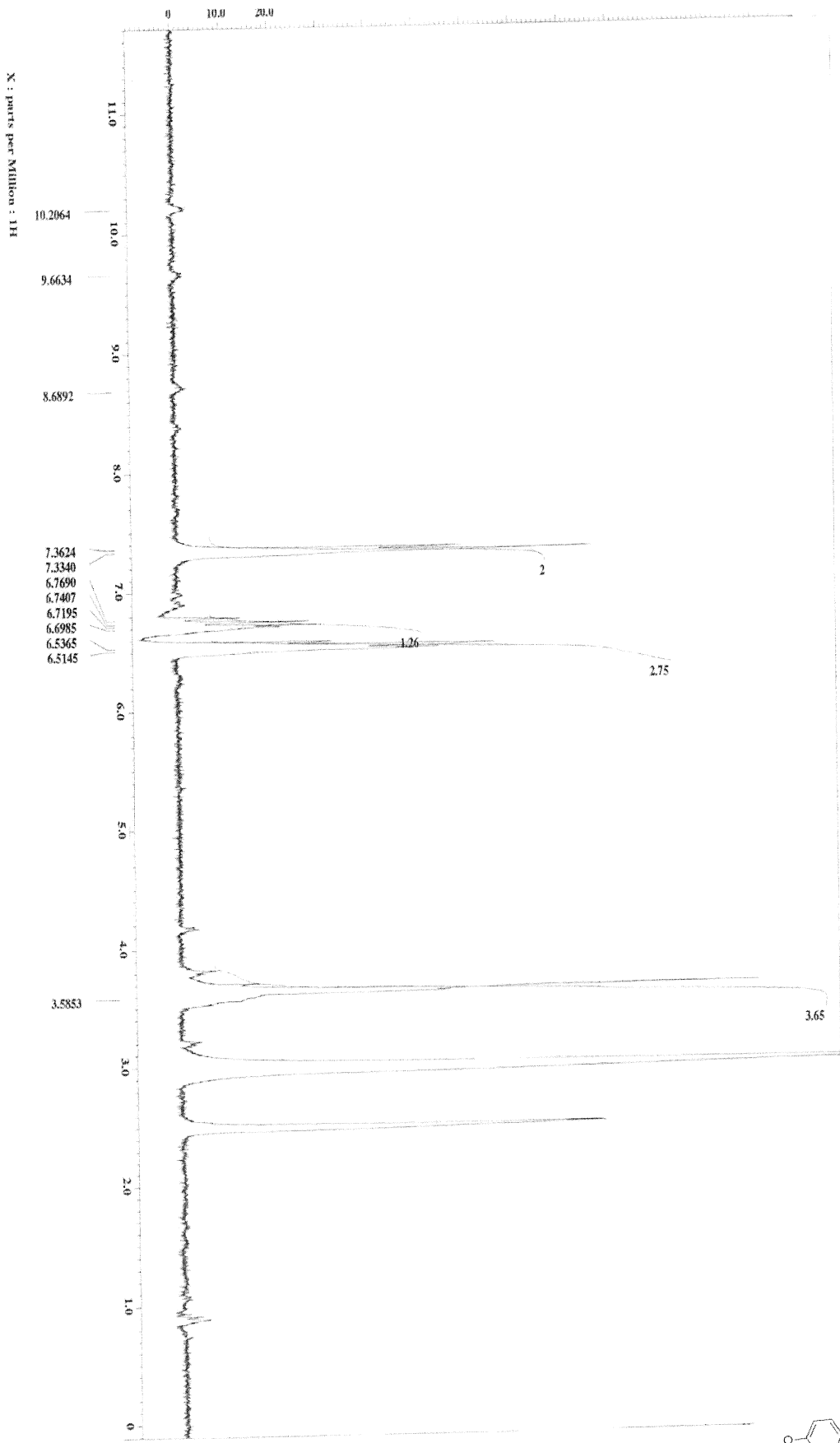


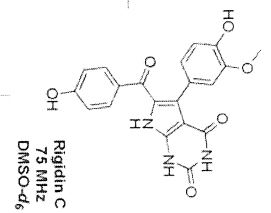
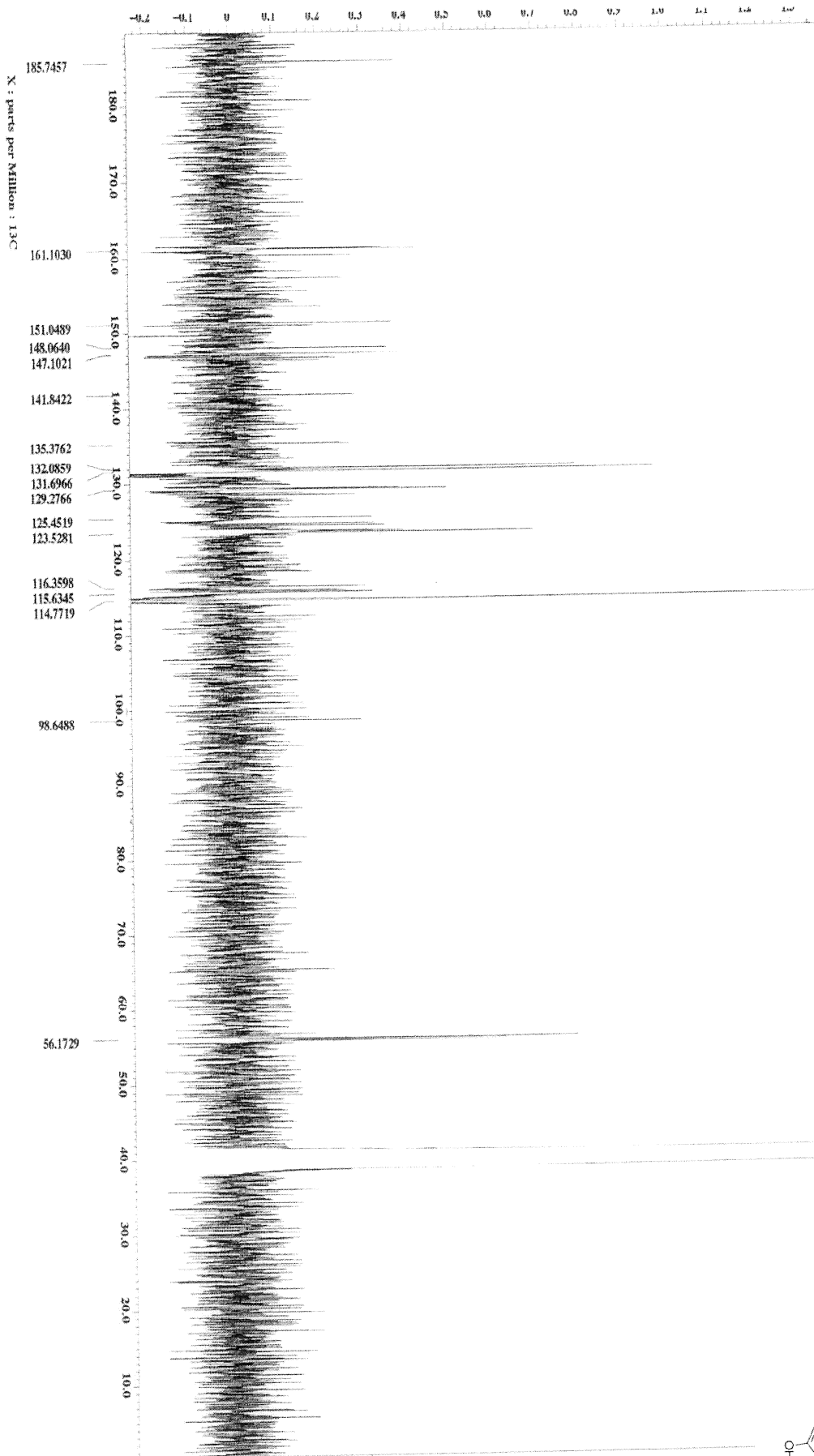


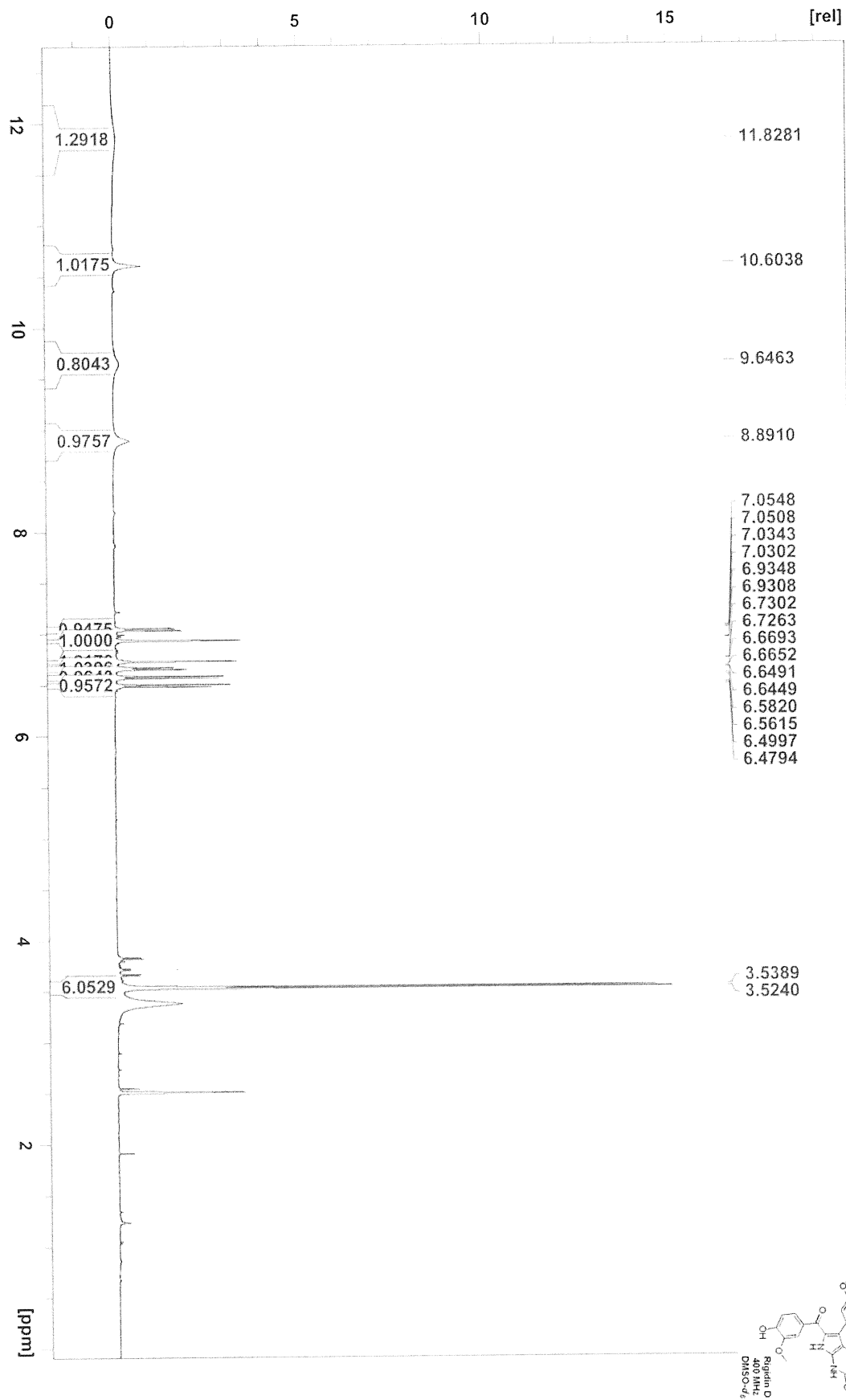


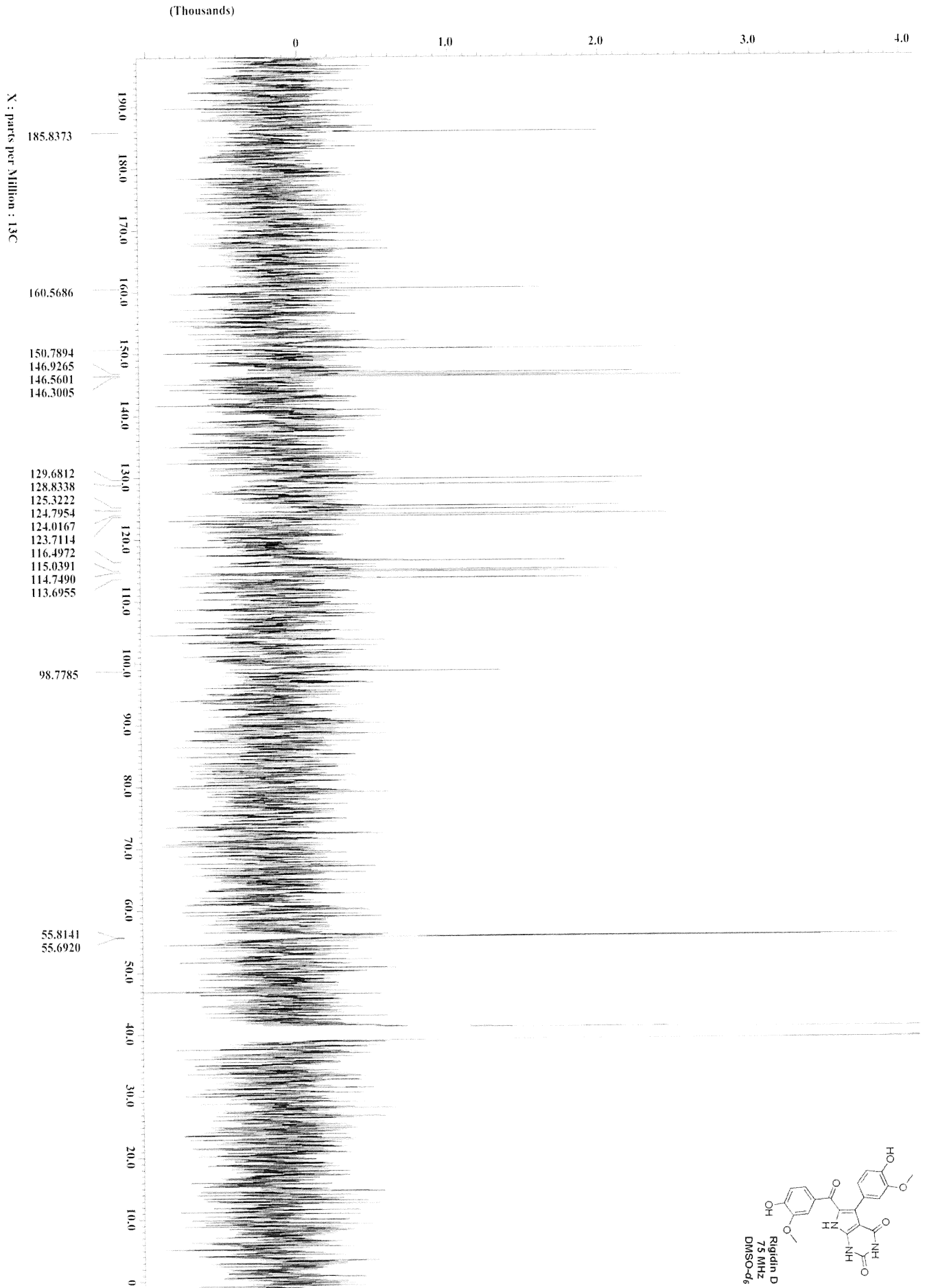












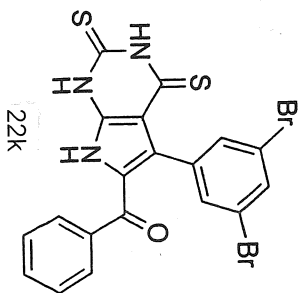
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Filename = 1d_spectrum-388.jdf
Author = alex
Experiment = single_pulse.exp
Sample_id = S#376136
Solvent = DMSO-d6
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Revision_time = 14-APR-2011 10:38:07
Current_time = 14-APR-2011 10:38:18

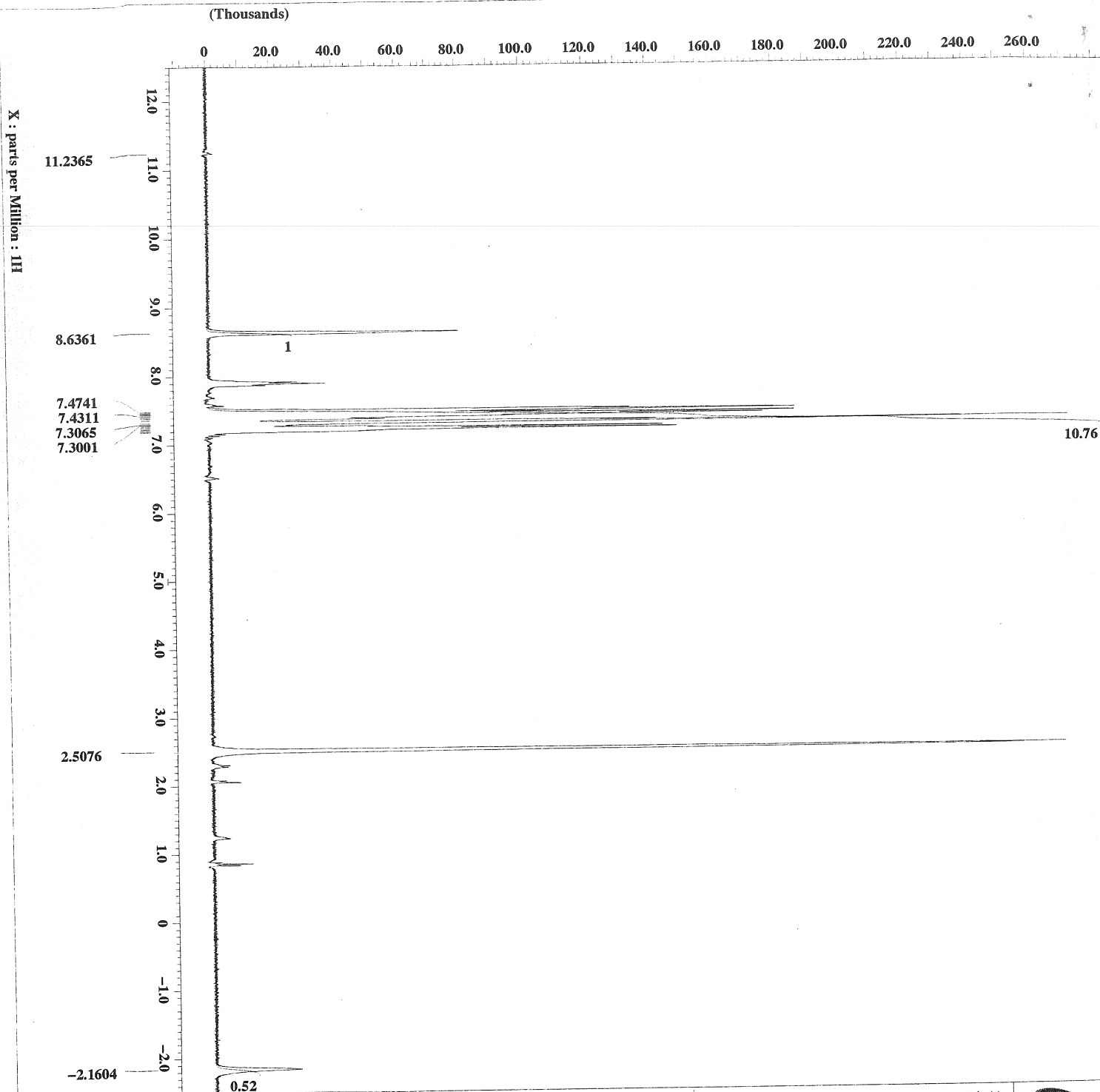
Comment = Single Pulse Experiment
Data_format = 1d_REAL
Dim_size = 16384
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Eclipse+ 300
Site = DELTA_NMR
Spectrometer

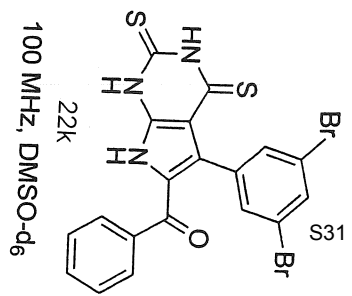
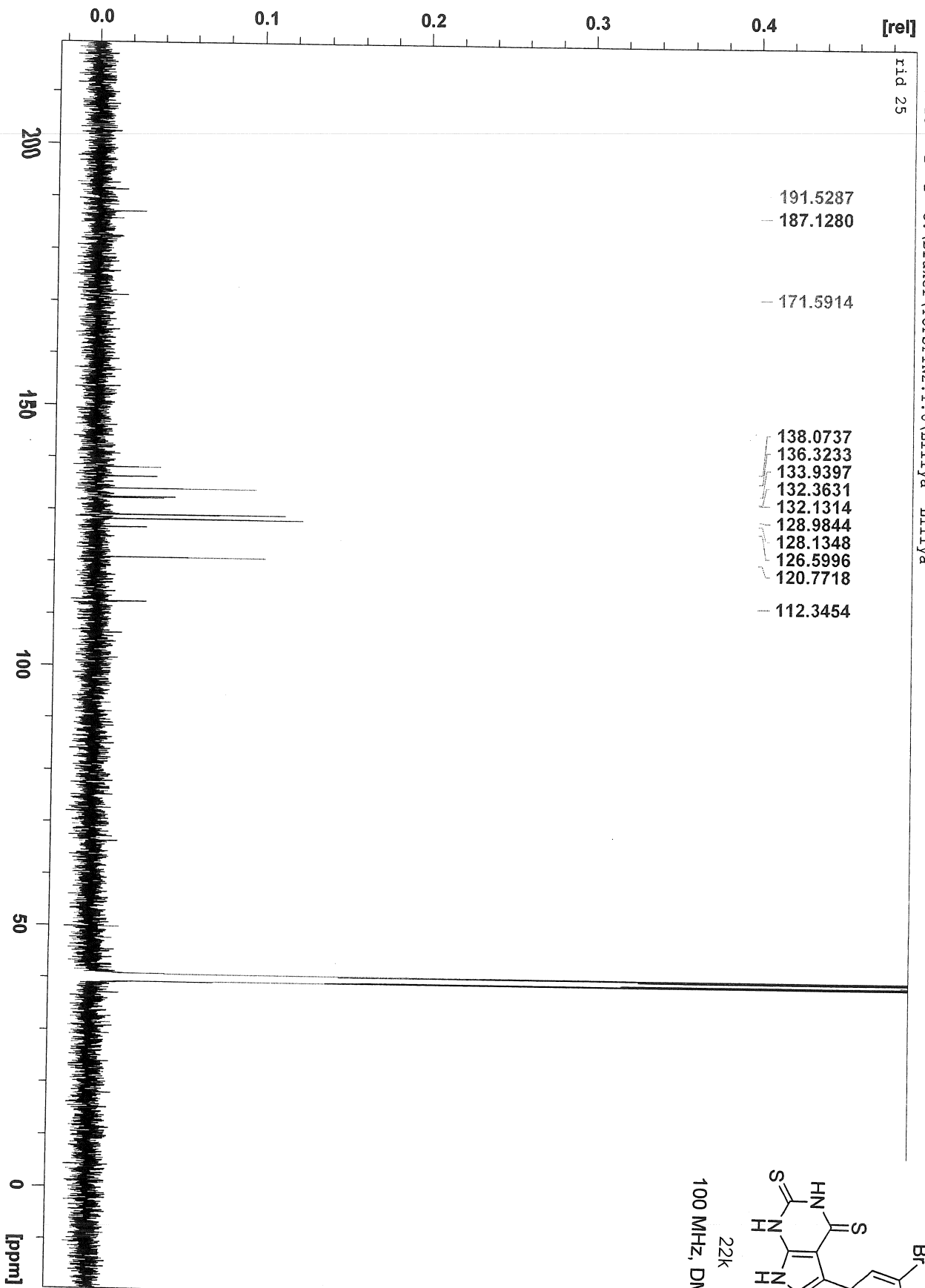
Field_strength = 7.0586013[E] (300[MHz]
X_acq_duration = 3.6339712[s]
X_domain = 1H
X_freq = 300.52965592[MHz]
X_offset = 51ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.27518105[Hz]
X_sweep = 4.50856628[kHz]
Clipped = FALSE
Mod_return = 1
Scans = 32
Total_scans = 32

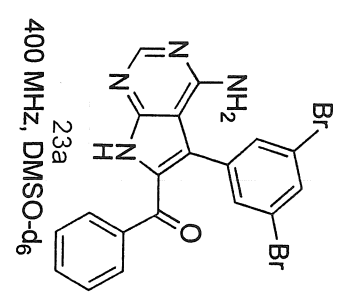
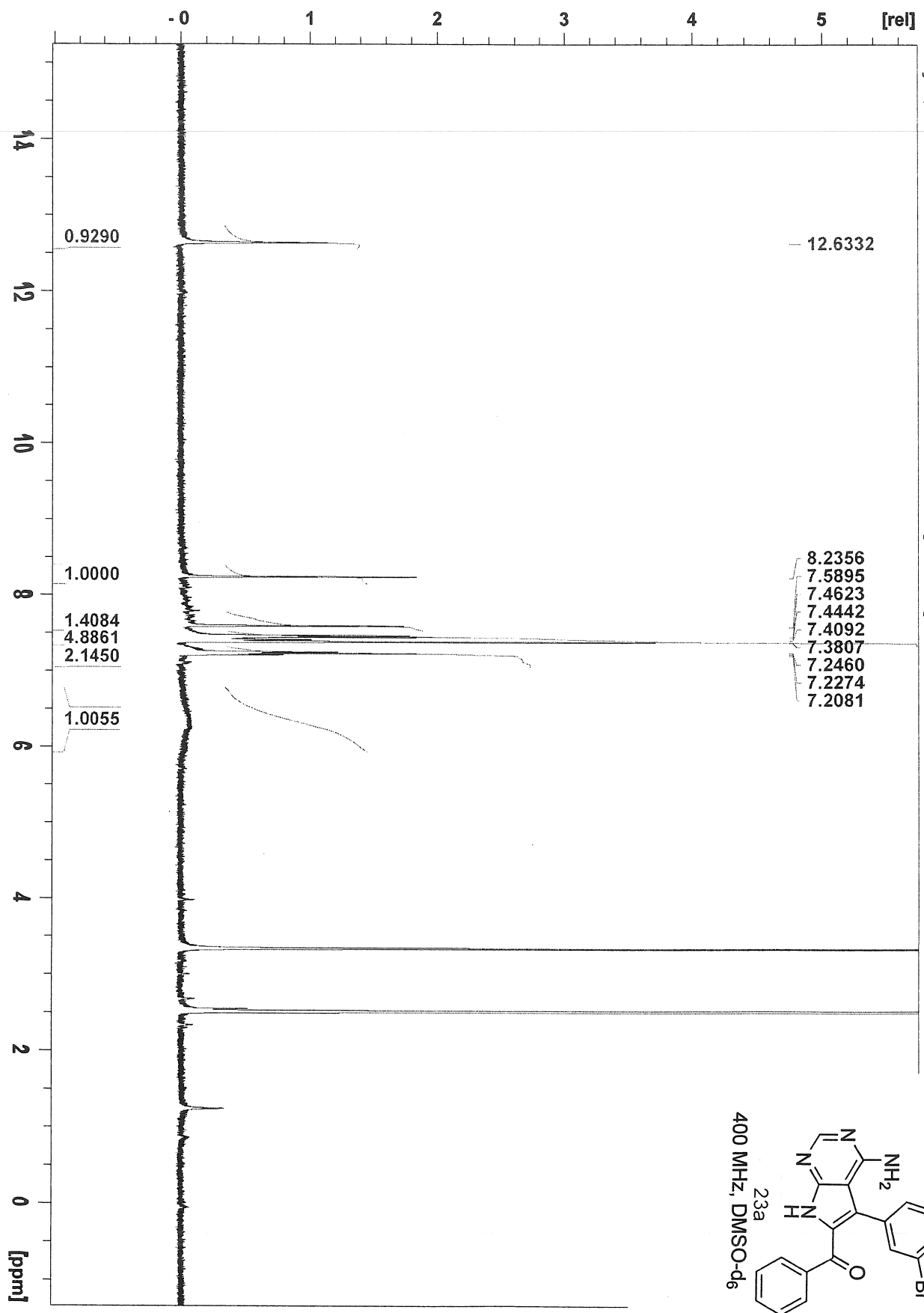
X_90_width = 16[us]
X_acq_time = 3.6339712[s]
X_angle = 45[deg]
X_pulse = 8[us]
Initial_wait = 1[us]
Phase_preset = 3[us]
Recvr_gain = 15
Relaxation_delay = 4[us]
Temp_get = 24.1[dc]
Unblank_time = 2[us]
    
```

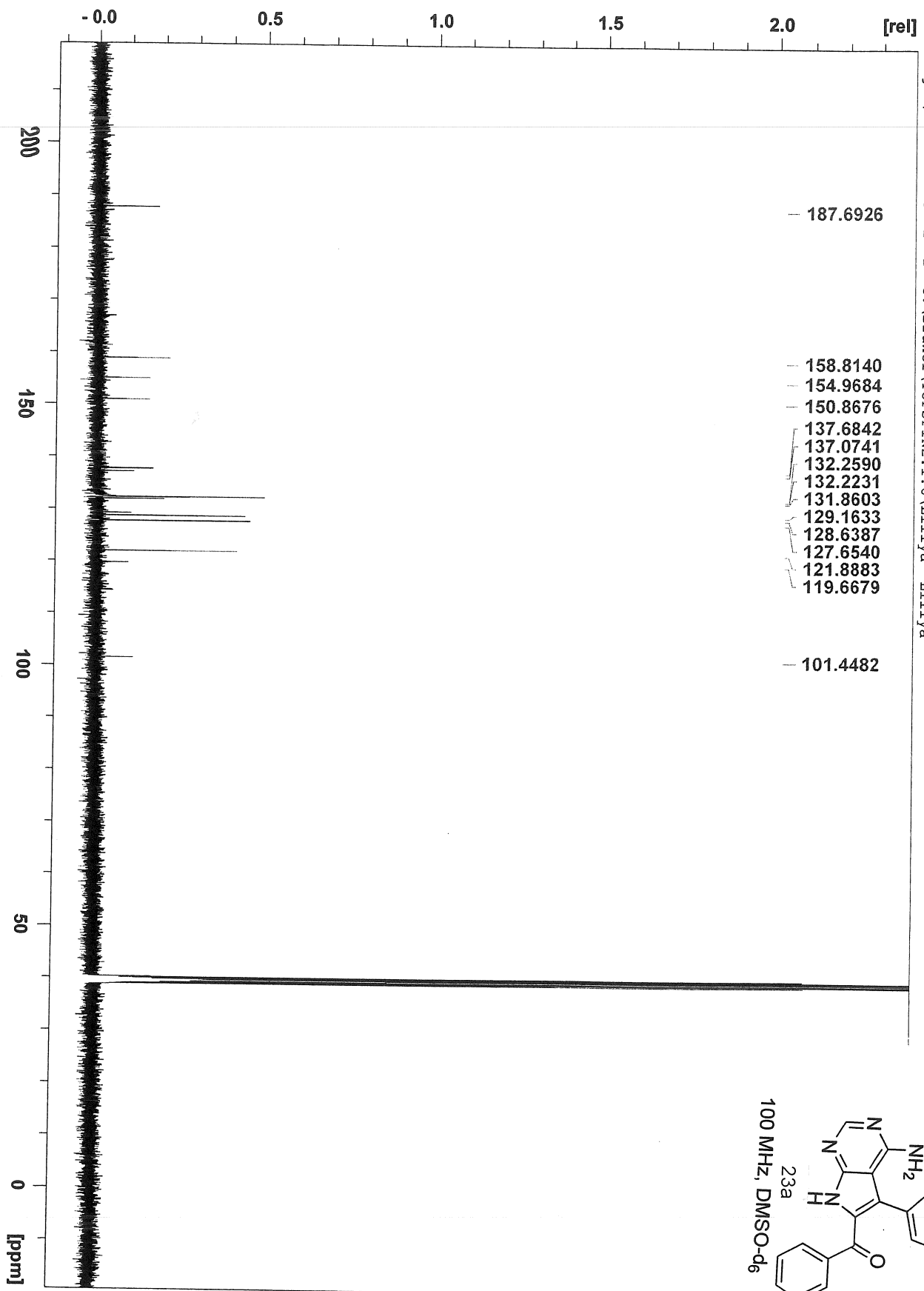


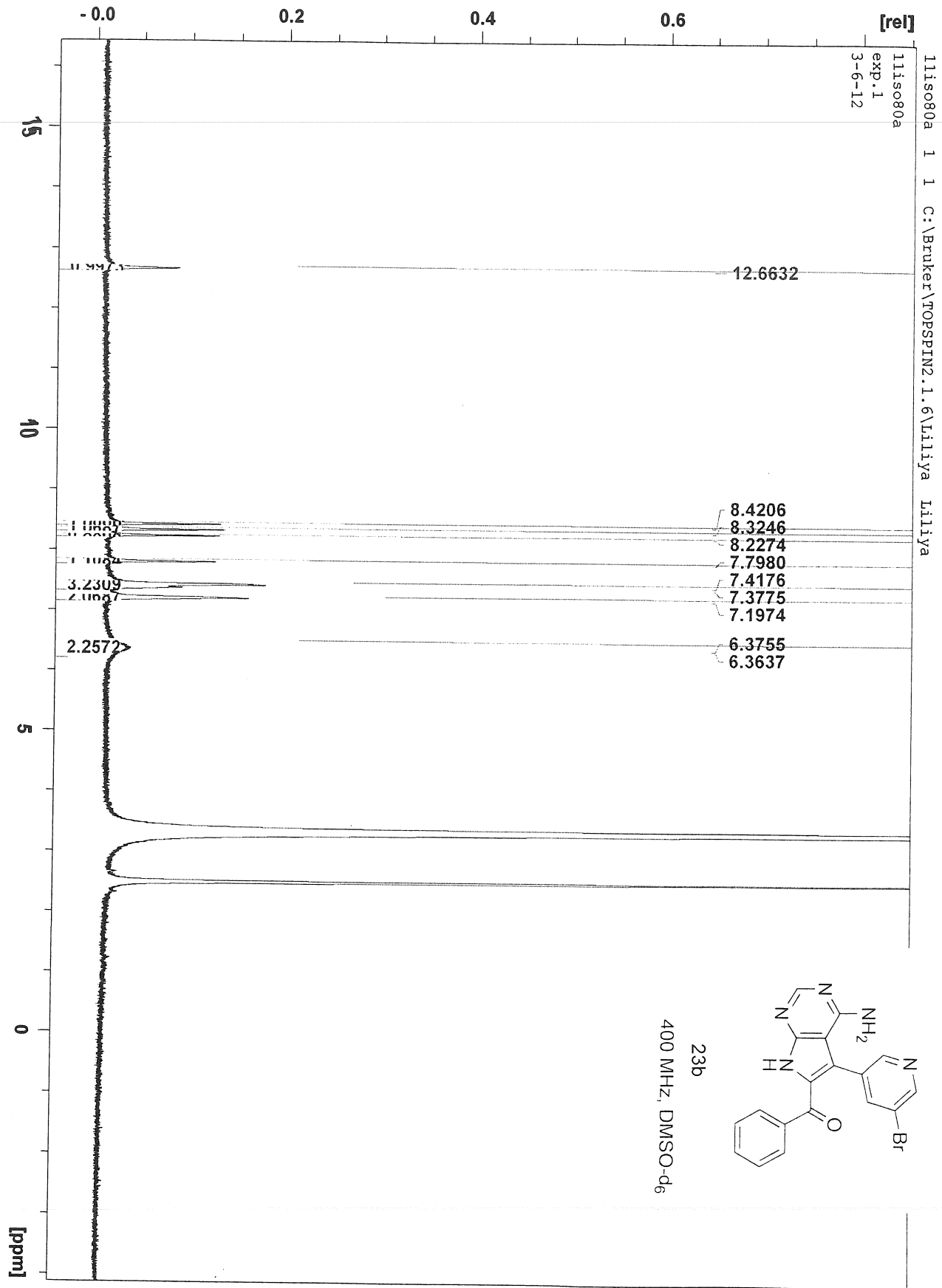
300 MHz, DMSO-d₆

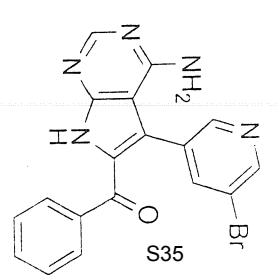
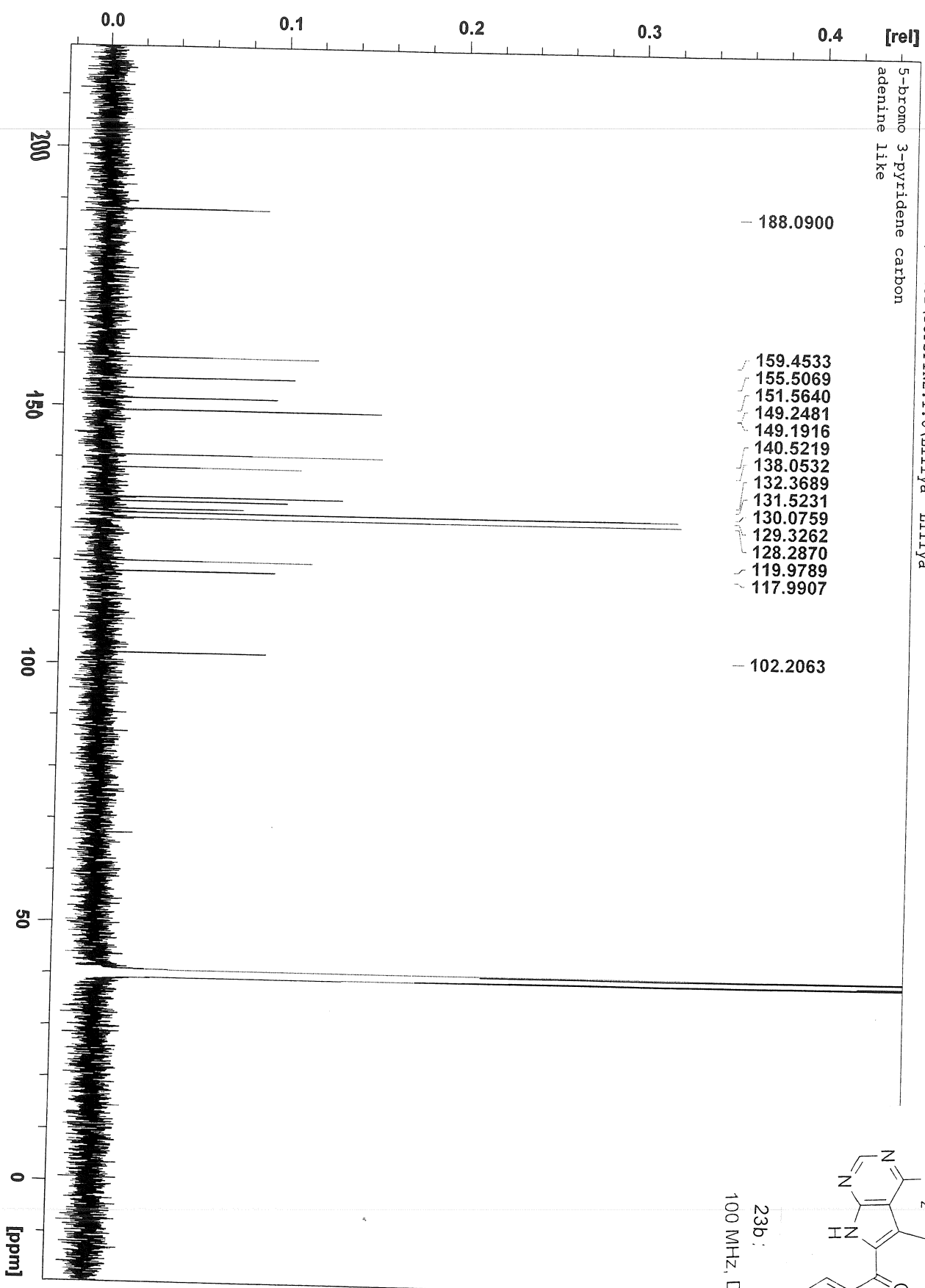


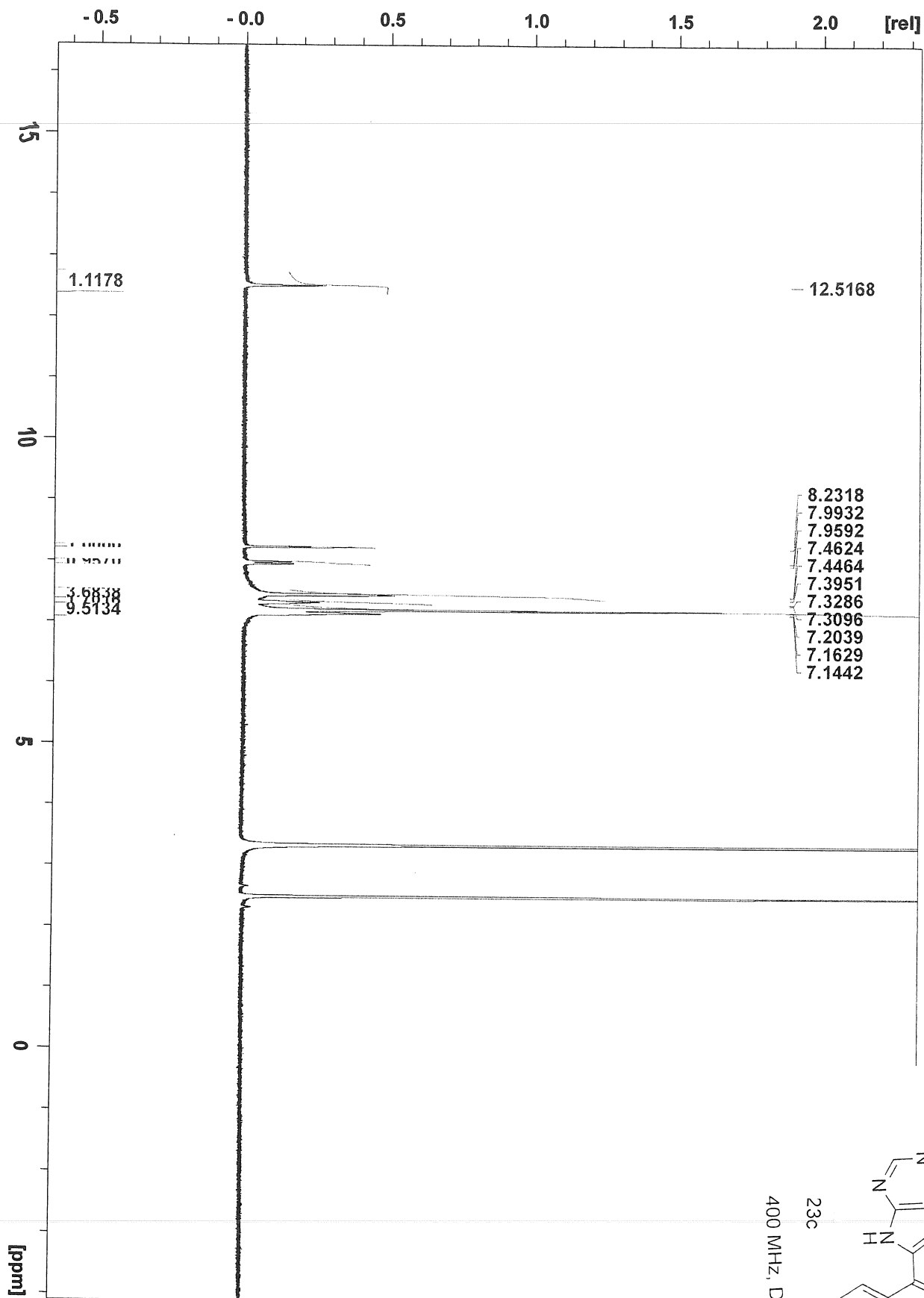




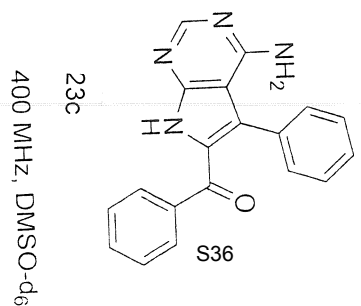


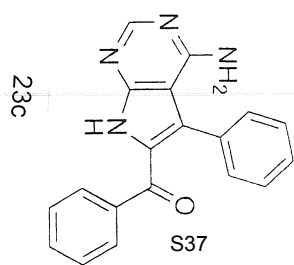
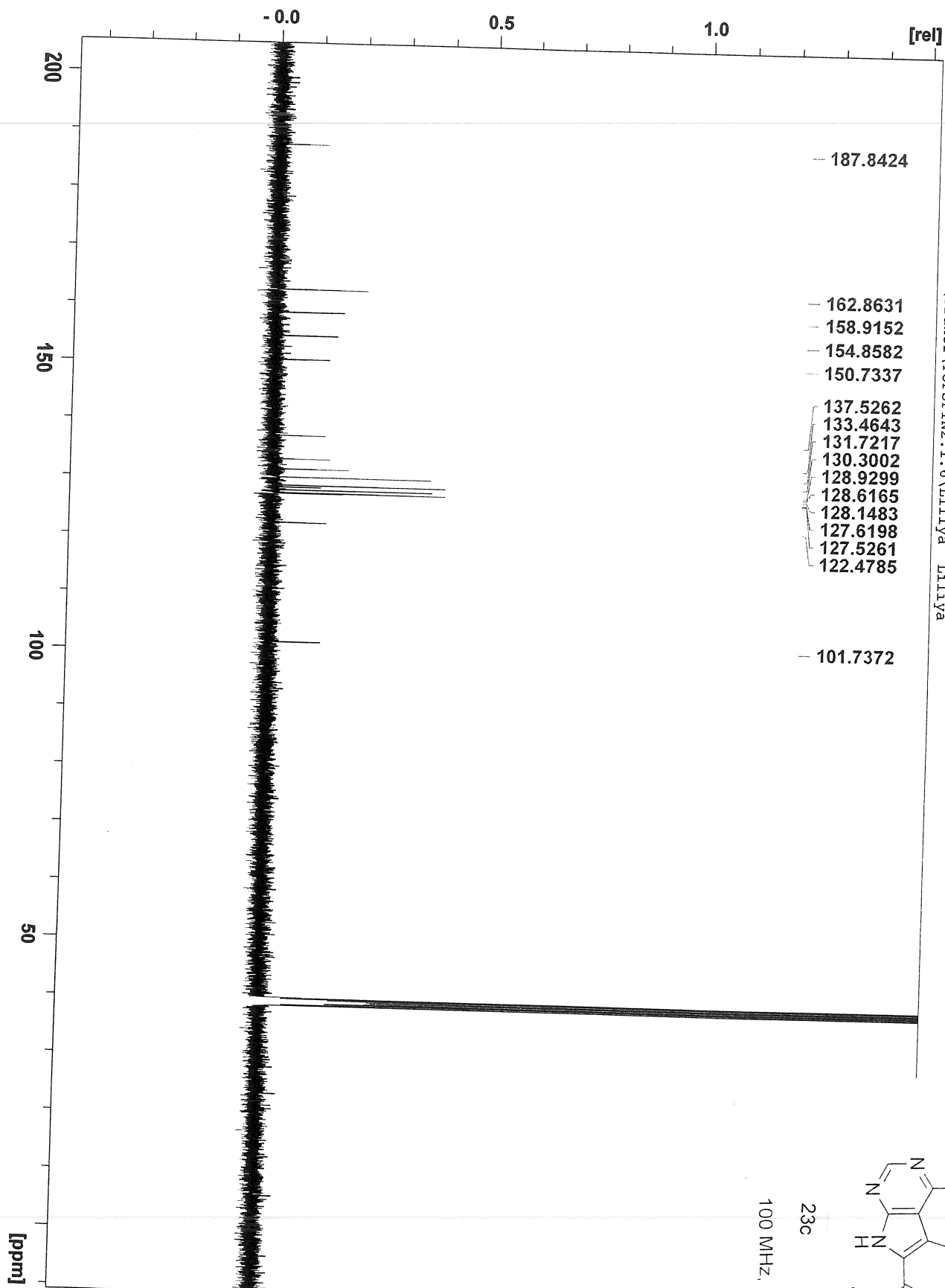


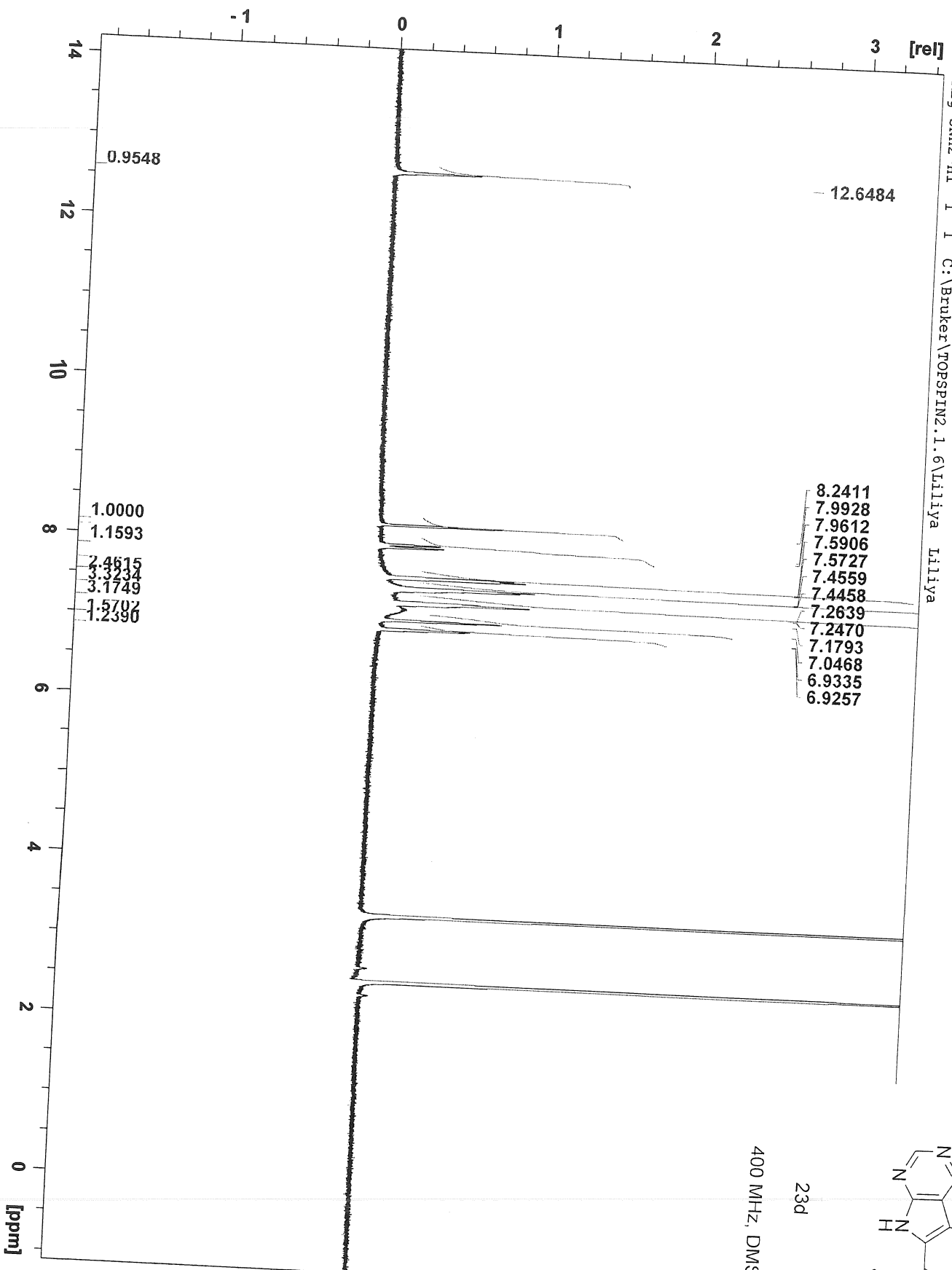




Rig-PhNH2 1 1 C:\Bruker\TOPSPIN2.1.6\Lillya Lillya



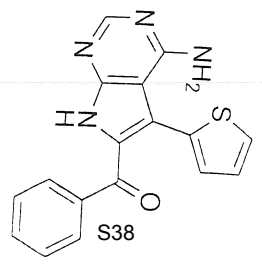


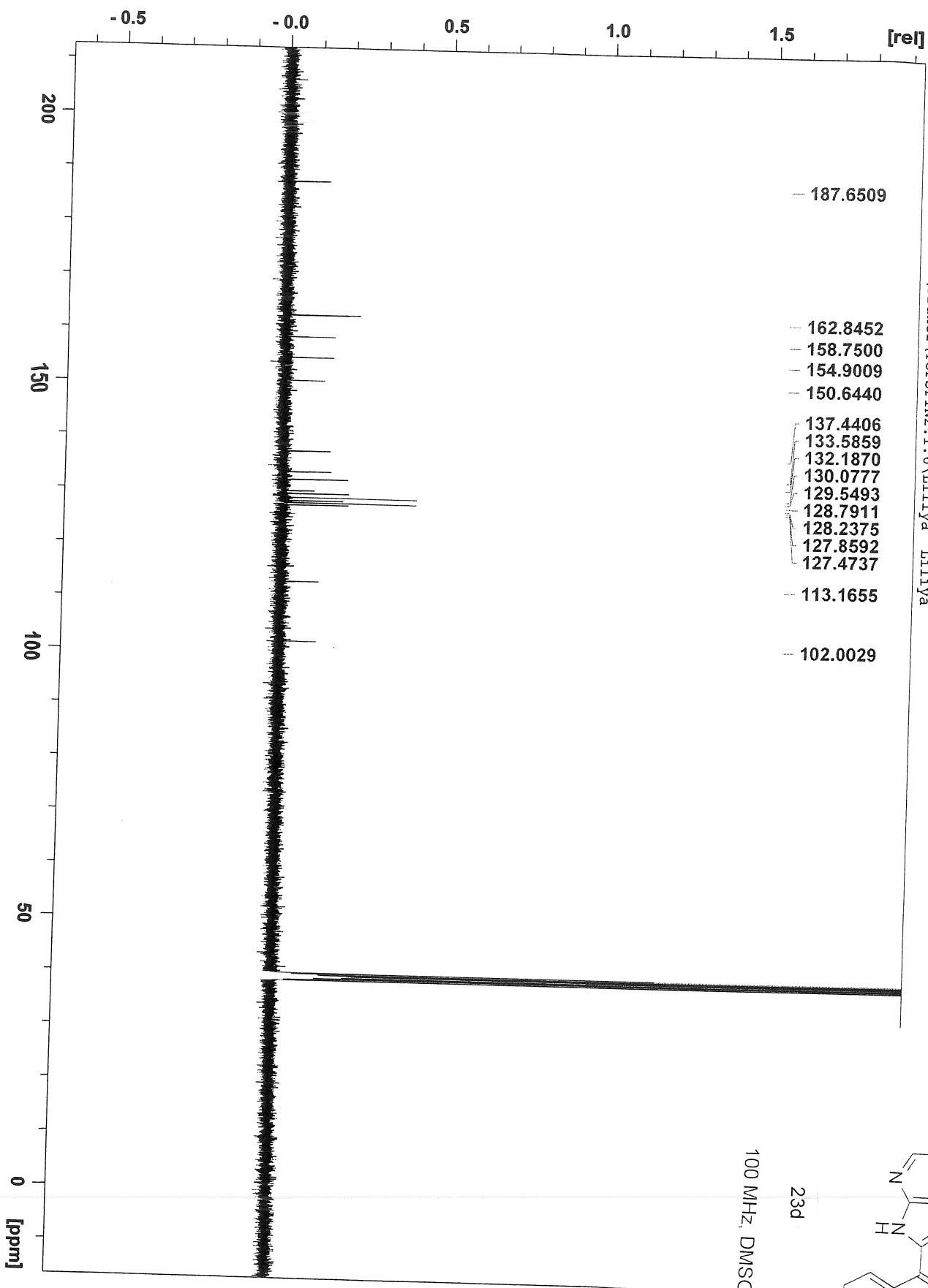


Rlg-SNH2-H1 1 1 C:\Bruker\TOPSPIN2.1.6\Lillya Lillya

400 MHz, DMSO-d₆

23d

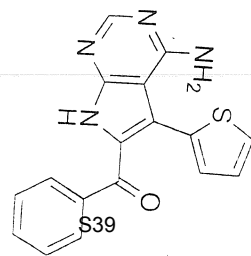


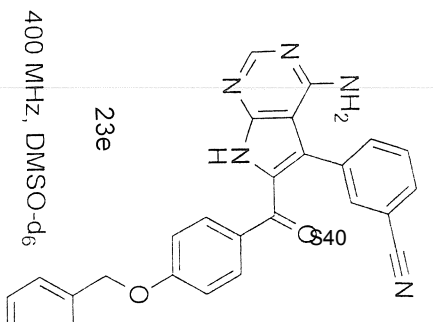
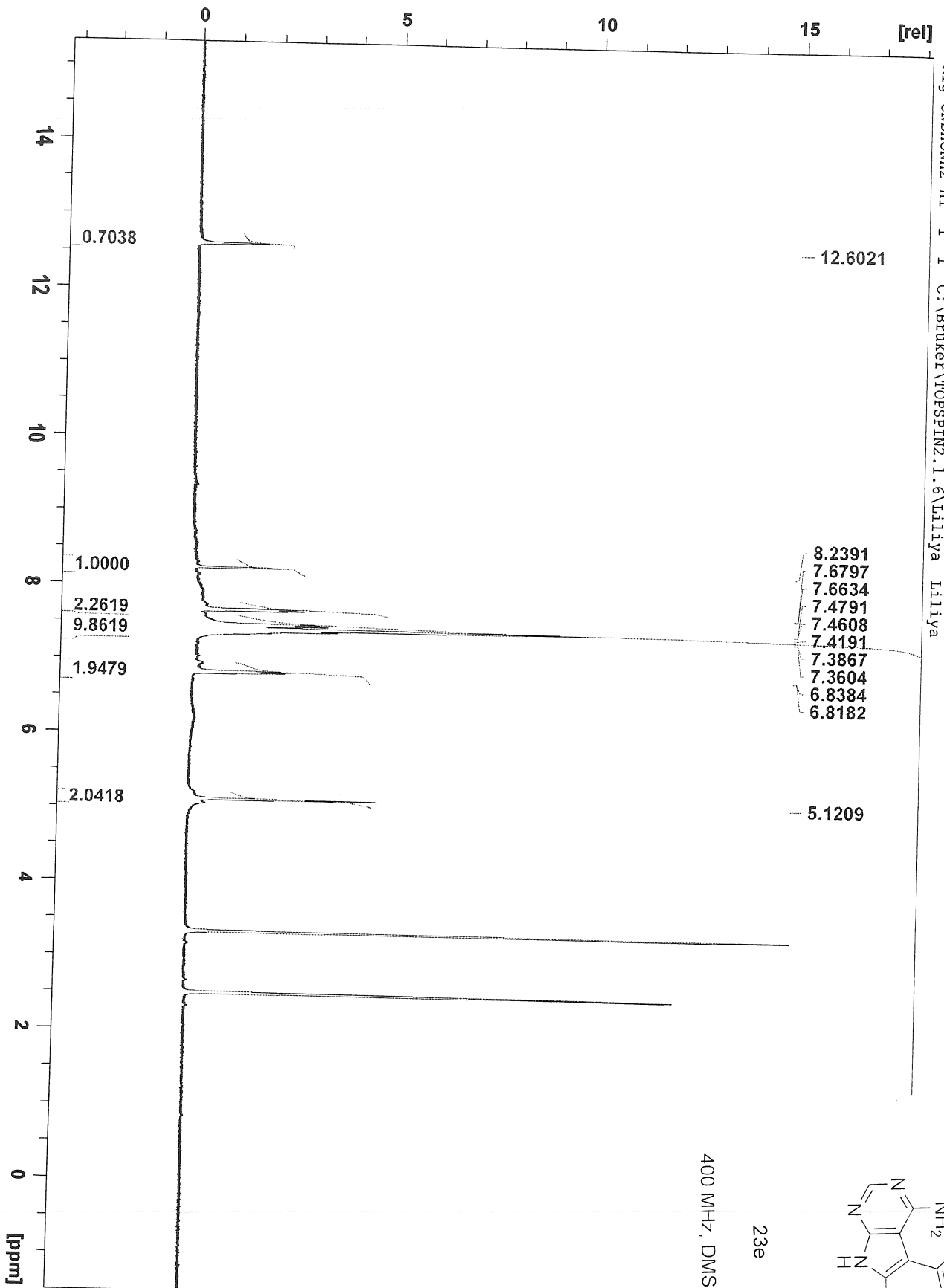


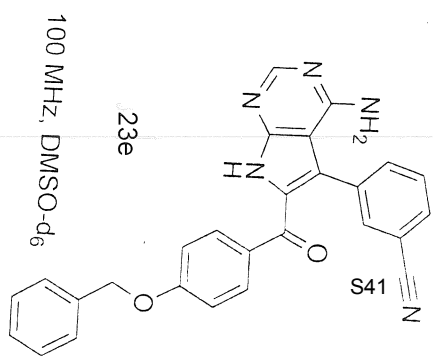
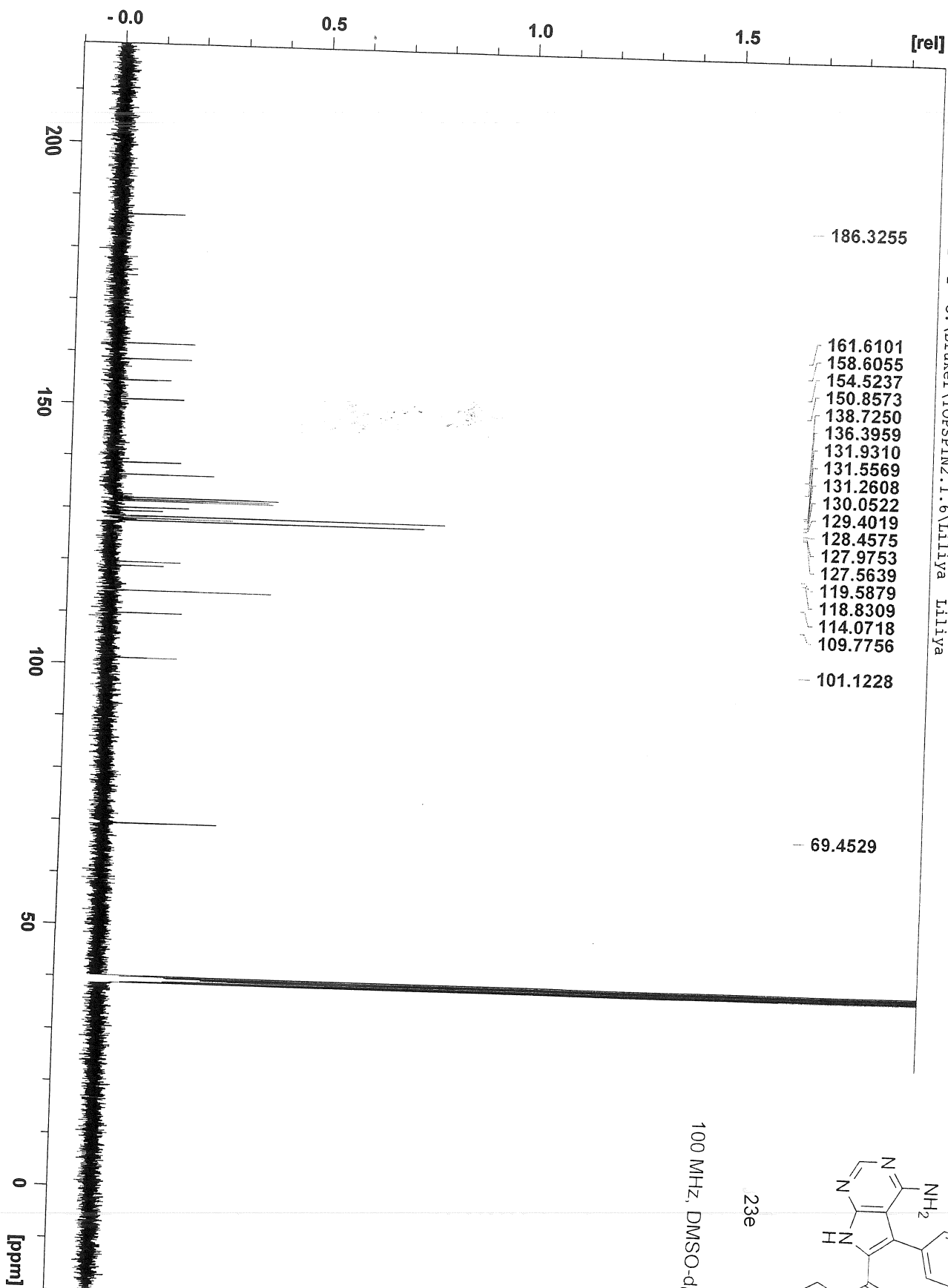
R19-SNH2-C13 1 1 C:\Bruker\TOPSPIN2.1.6\Liliya Liliya

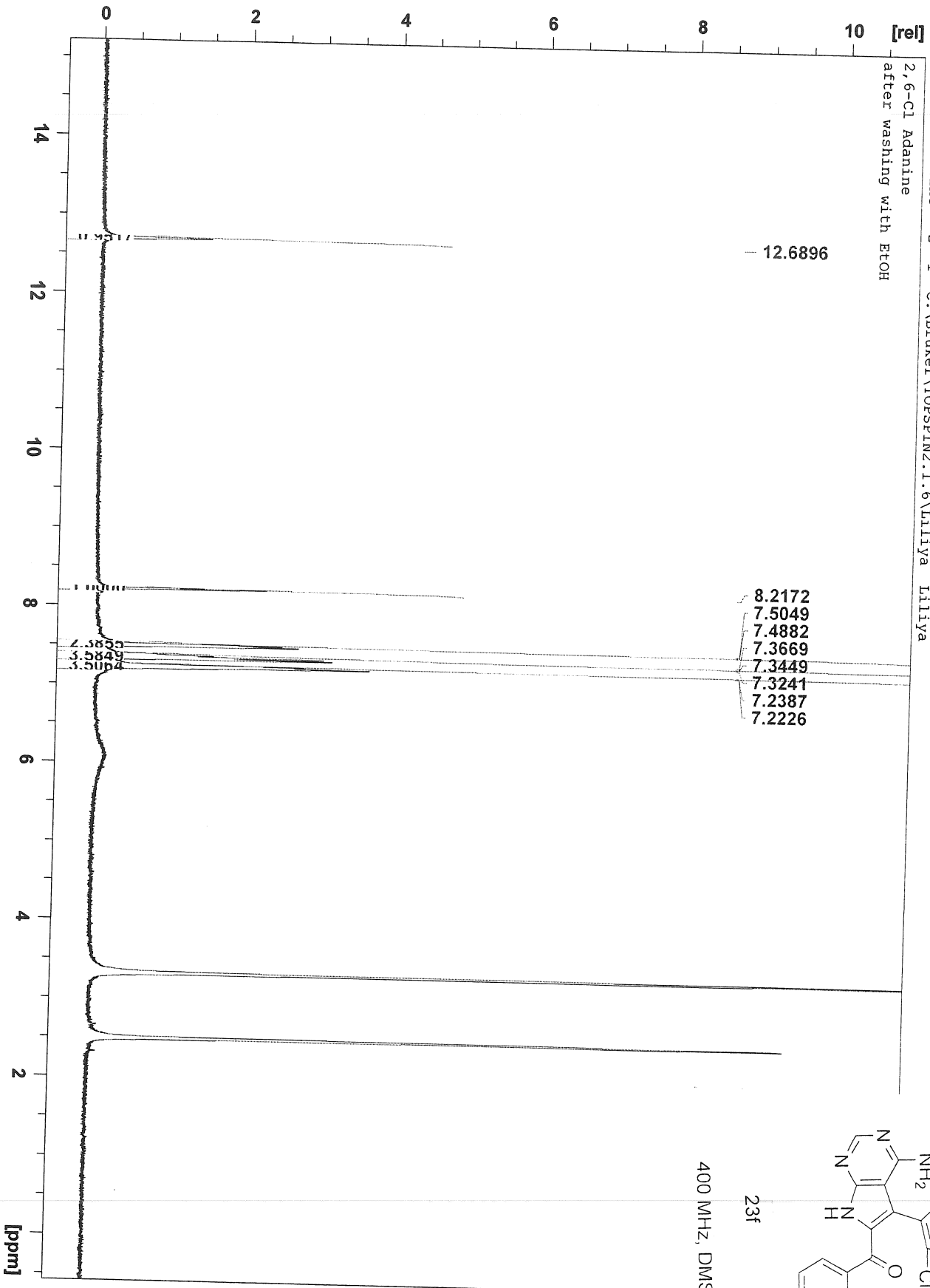
100 MHz, DMSO-d₆

23d

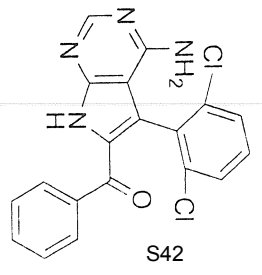








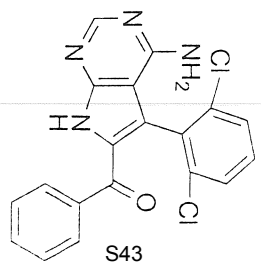
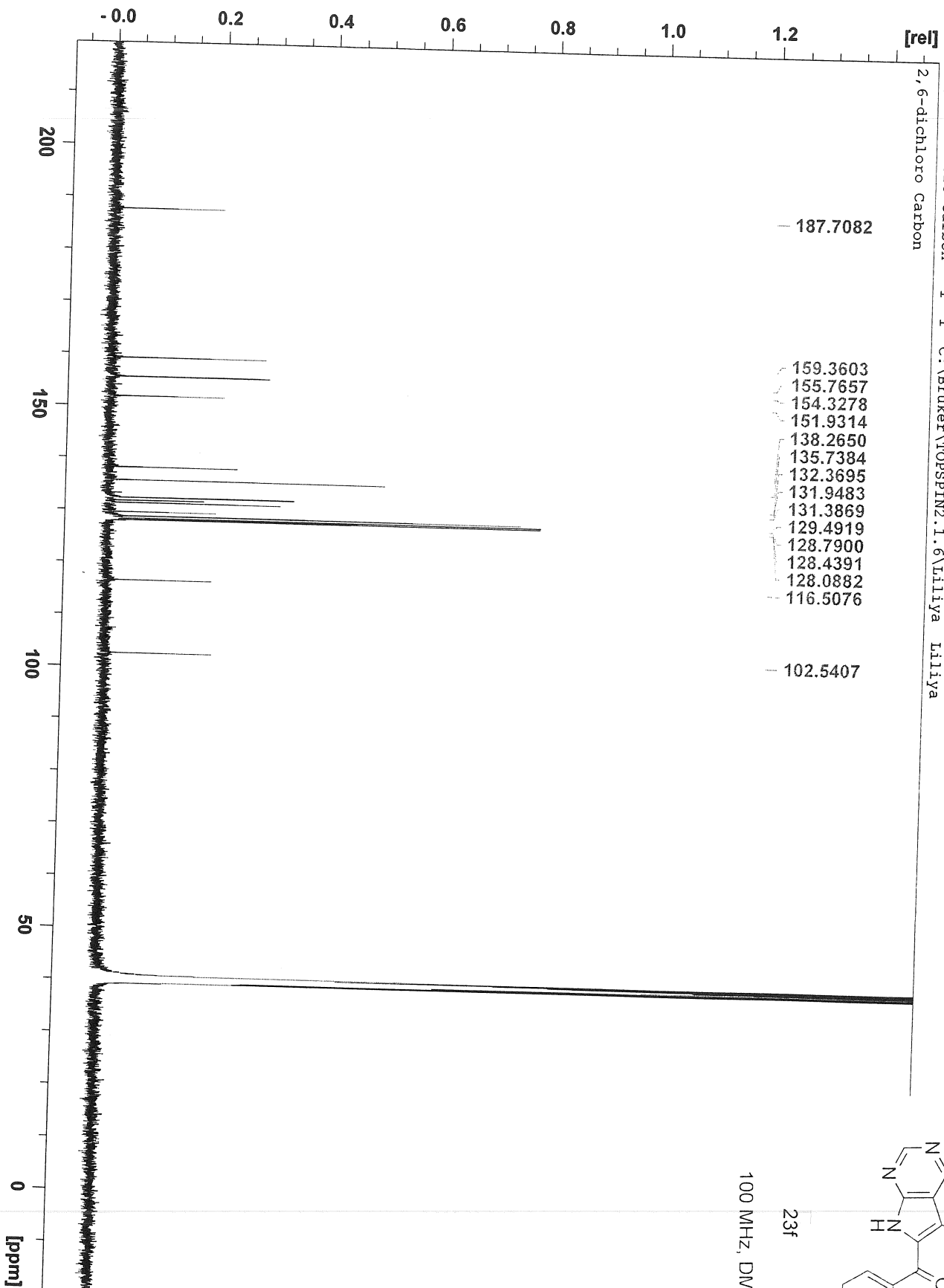
"2,6-Cl Adanine" 2 1 C:\Bruker\TOPSPIN2.1.6\Liliya Liliya
 2,6-Cl Adanine
 after washing with EtOH



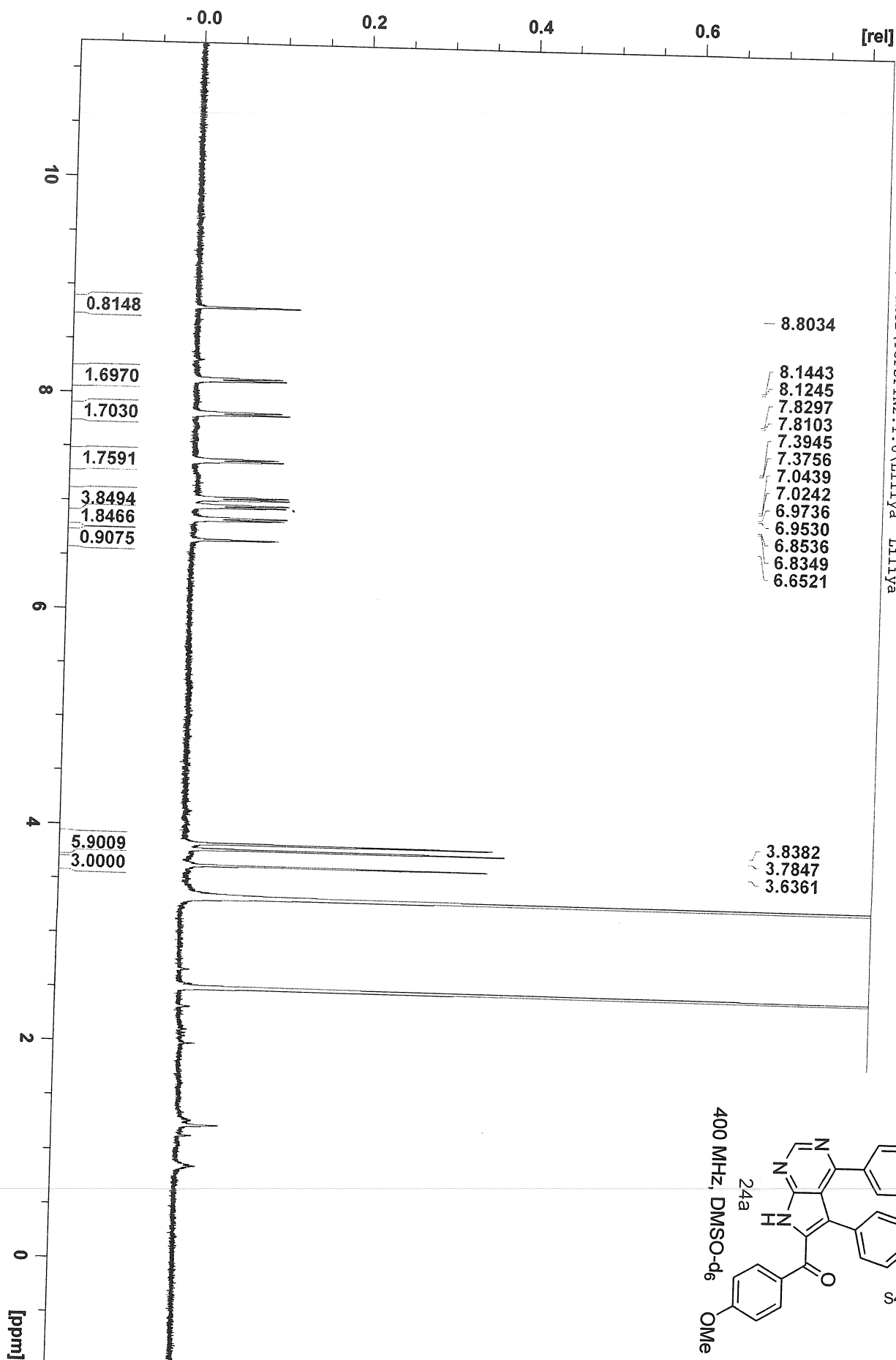
400 MHz, DMSO-d₆

23f

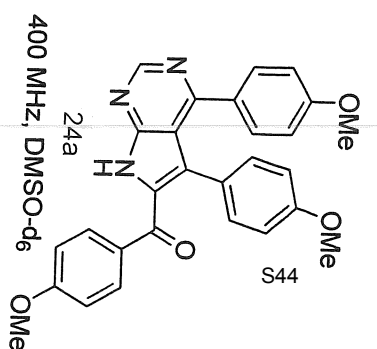
[ppm]

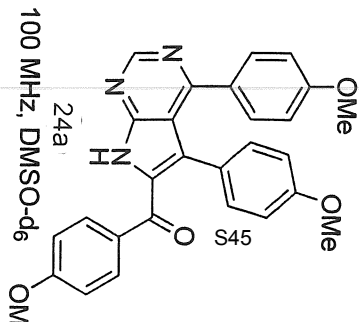
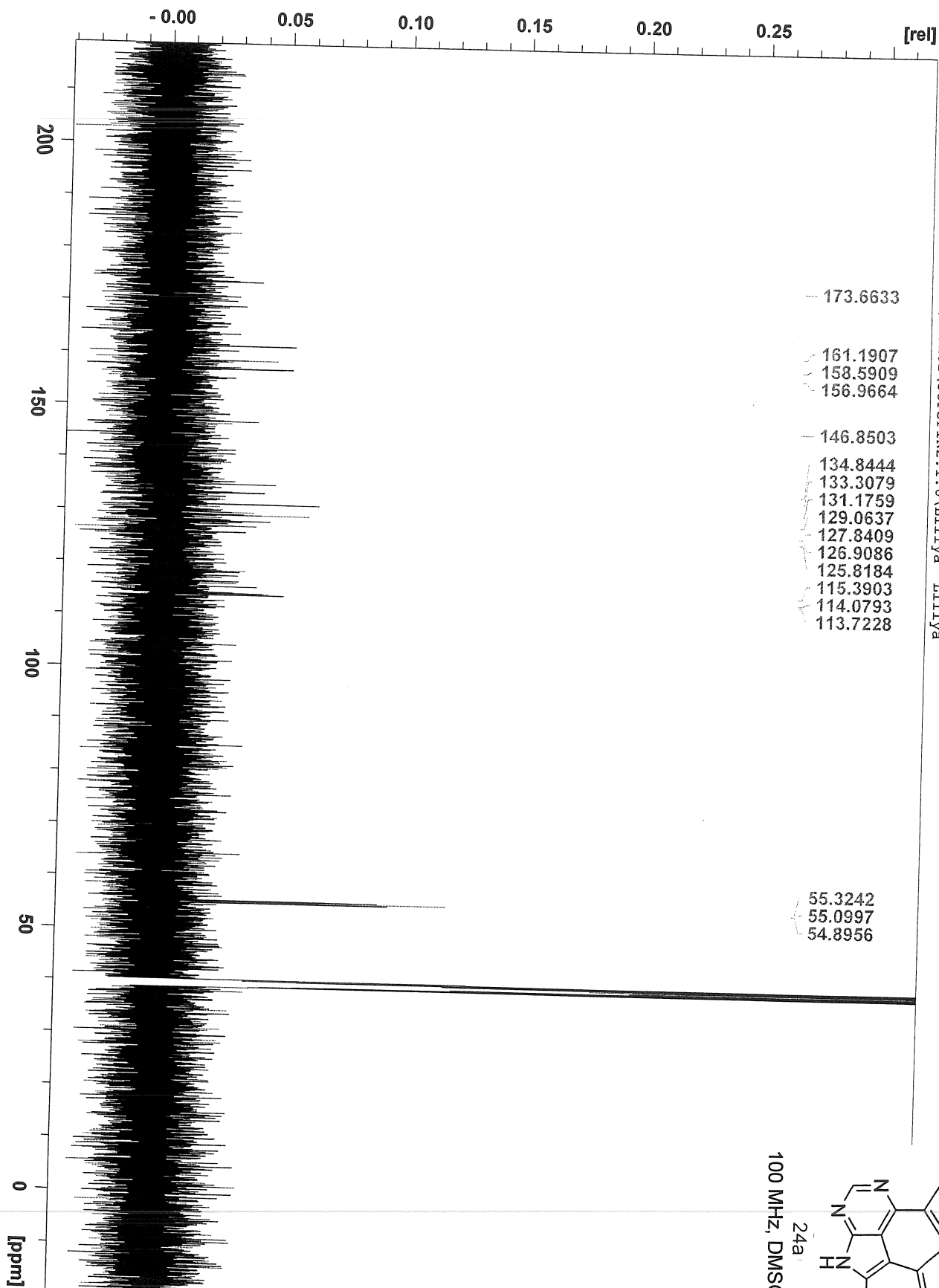


100 MHz, DMSO-d₆

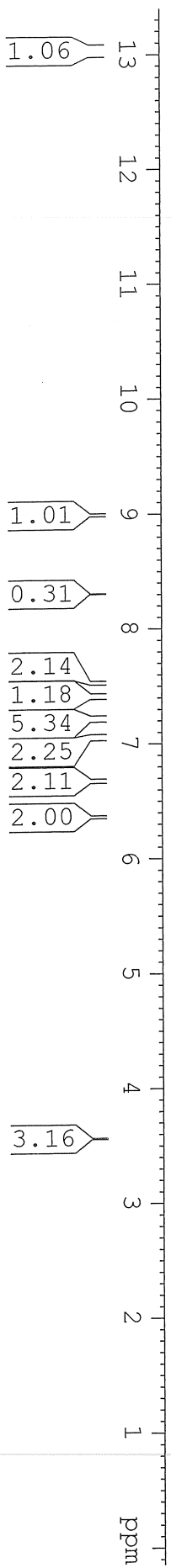


Rid-OCH3-cl 2 1 C:\Bruker\TOPSPIN2.1.6\Lillya Lillya





Rid-OCH3-c1-C13 2 1 C:\Bruker\TOPSPIN2.1.6\Liliya Liliya



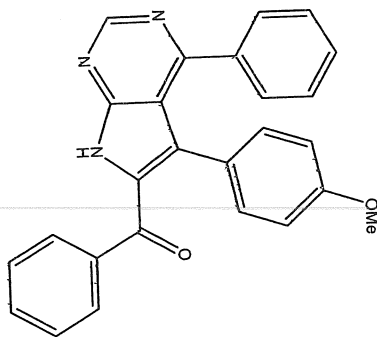
13.0370

- 8.9936
- 8.3063
- 7.5414
- 7.5382
- 7.5342
- 7.5255
- 7.5206
- 7.5173
- 7.4340
- 7.4176
- 7.4154
- 7.4131
- 7.4000
- 7.3968
- 7.2573
- 7.2416
- 7.2390
- 7.2349
- 7.2230
- 7.2212
- 7.2071
- 7.2021
- 7.1988
- 7.0725
- 7.0679
- 7.0543
- 7.0520
- 7.0340
- 6.6842
- 6.6788
- 6.6676
- 6.6621
- 6.3760
- 6.3706
- 6.3593
- 6.3540
- 3.5661
- 3.3241
- 2.5046
- 2.5000
- 2.4954

rsk_1143_MCR-0_DMSO-D6

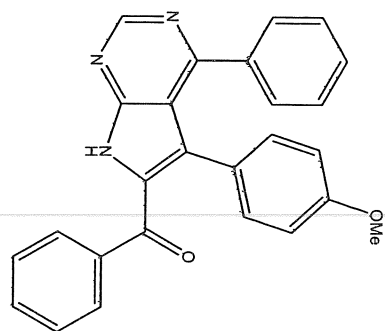
400 MHz, DMSO-d₆

24b



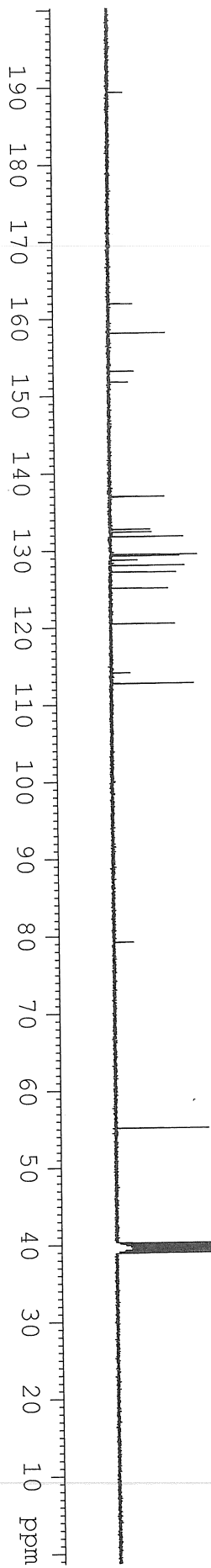
— 189.8013

- 162.3490
- 158.5138
- 153.5810
- 152.1714
- 137.3912
- 133.1411
- 132.1862
- 129.8670
- 129.7078
- 129.1525
- 128.4532
- 127.5862
- 125.4992
- 120.8911
- 114.5258
- 113.1409

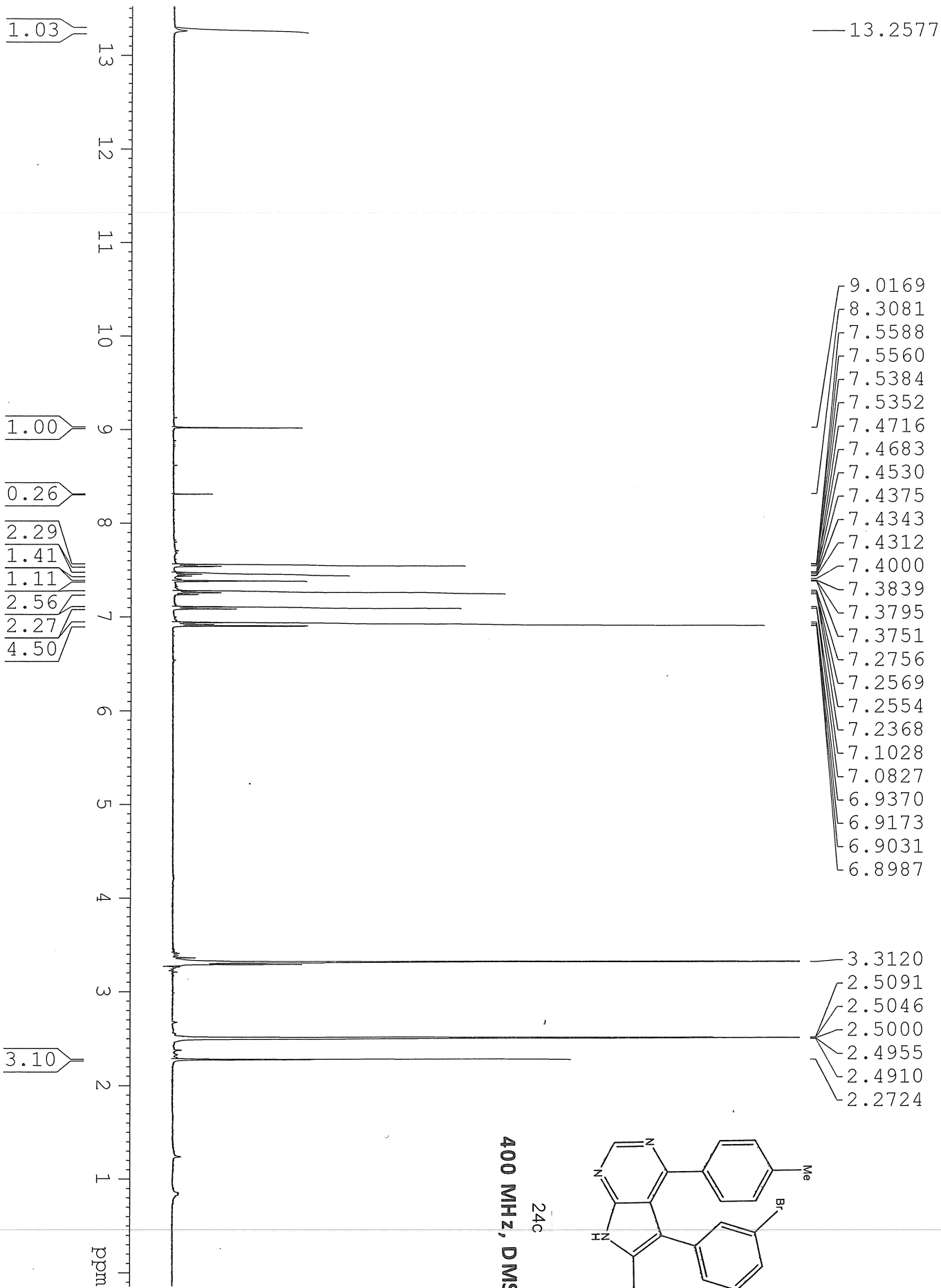


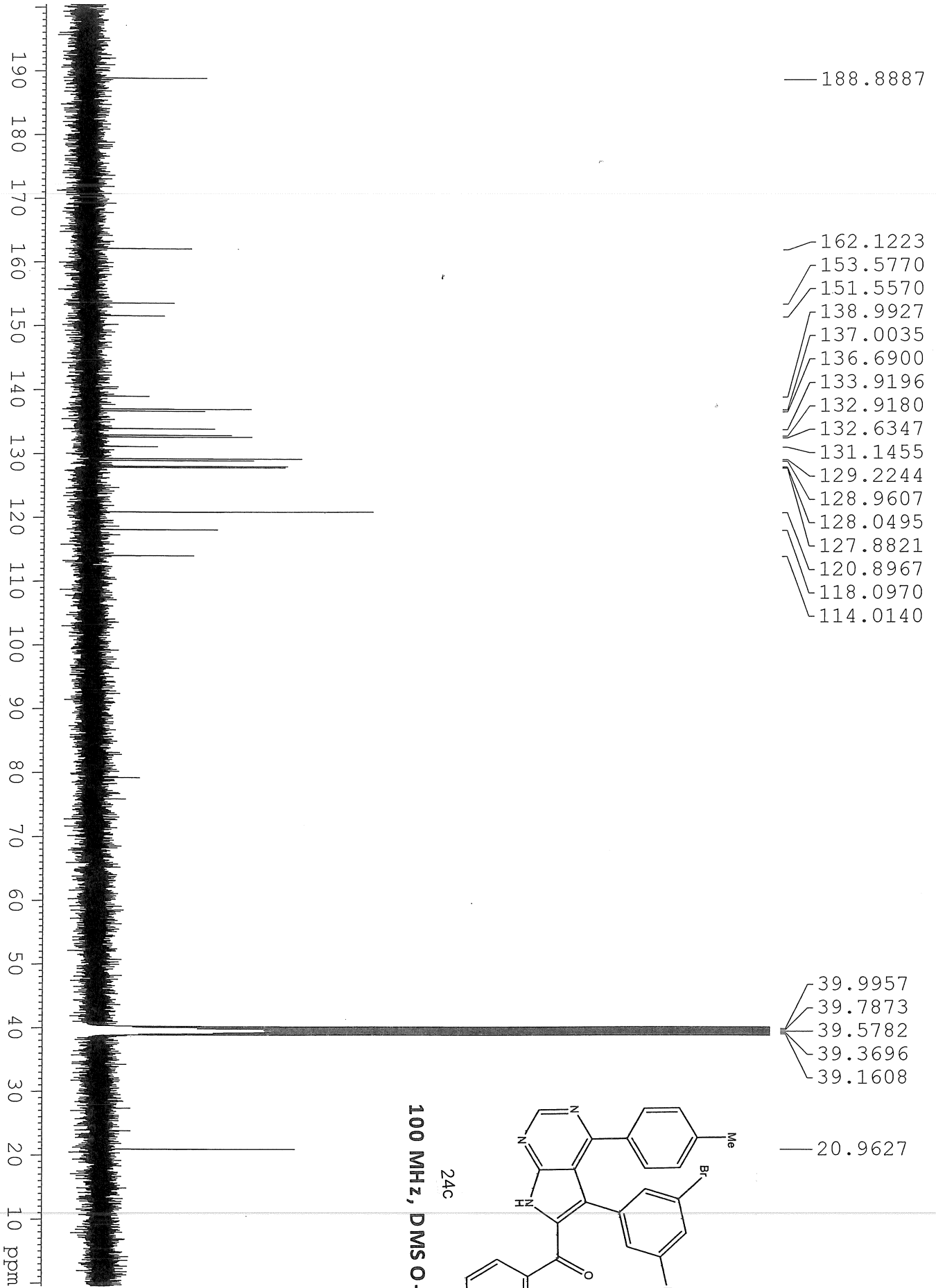
24b

100 MHz, DMSO-d₆

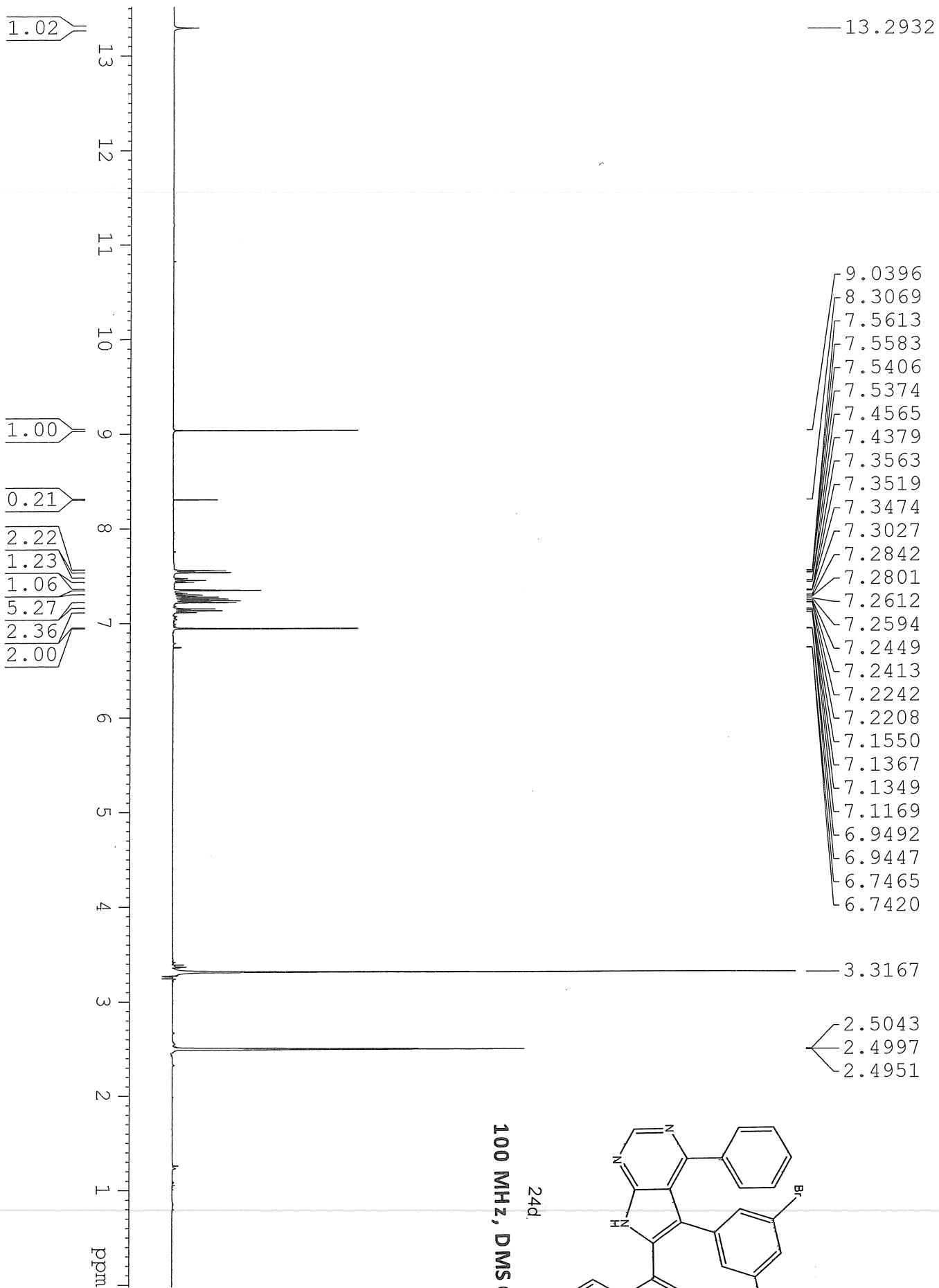


rsk_1044_MCRI_DMSOd6





rsk_1144_MCR-3_DMSO-D6



MCR-3-DMSO-d6-C

— 189.2983

— 162.4297

— 153.9944

— 152.0325

— 137.4065

— 137.1427

— 133.4908

— 133.3650

— 133.0714

— 131.7069

— 129.6402

— 129.4424

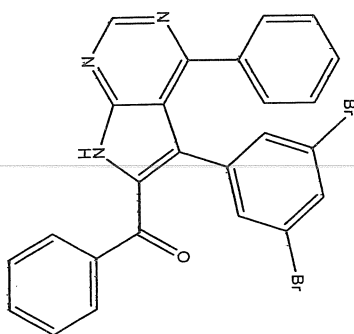
— 128.4761

— 127.7521

— 121.3436

— 118.4190

— 114.4671

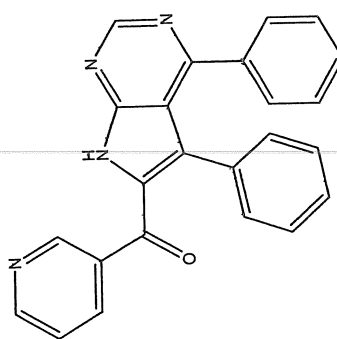


24d

400 MHz, DMSO-d₆

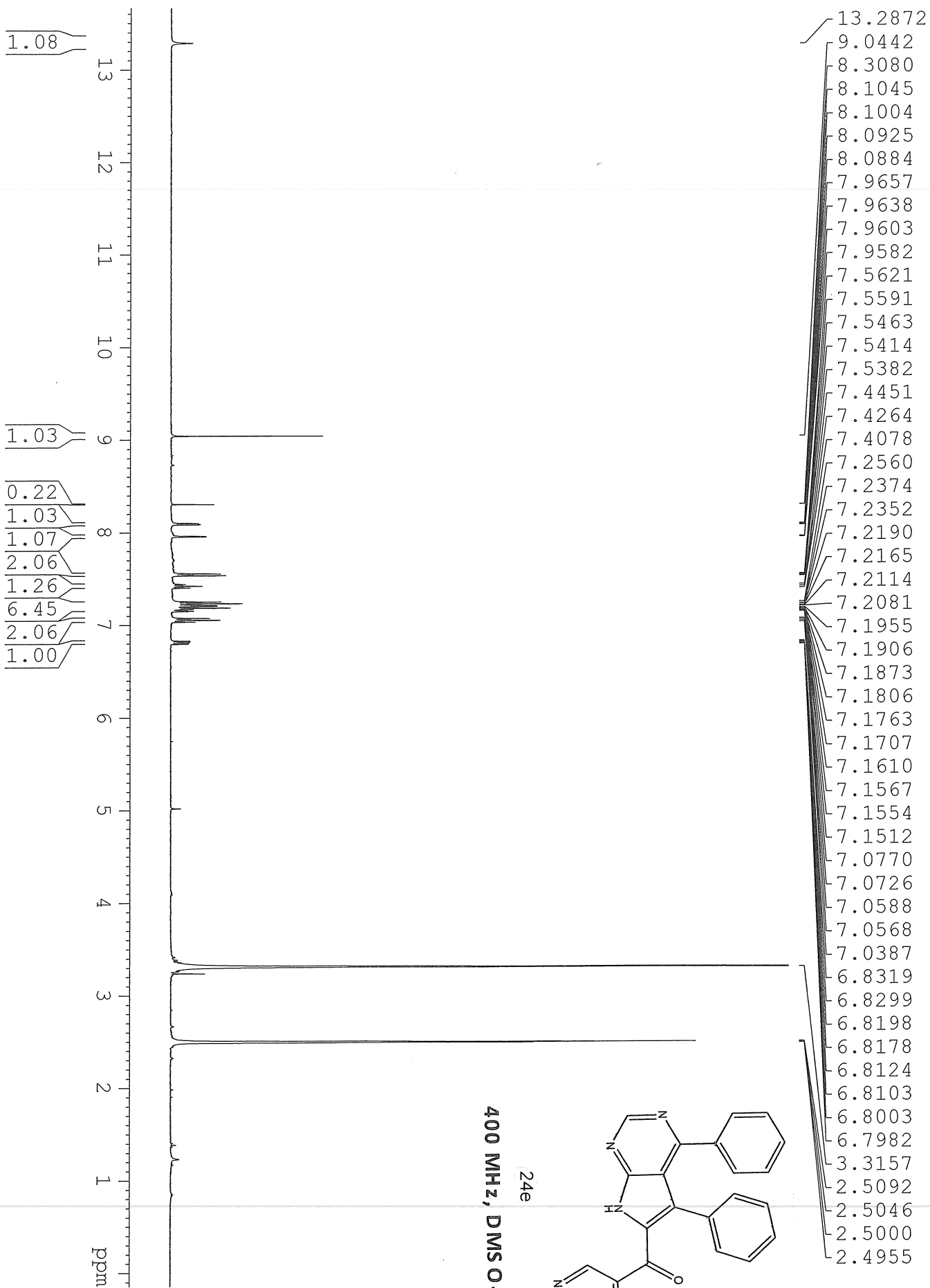


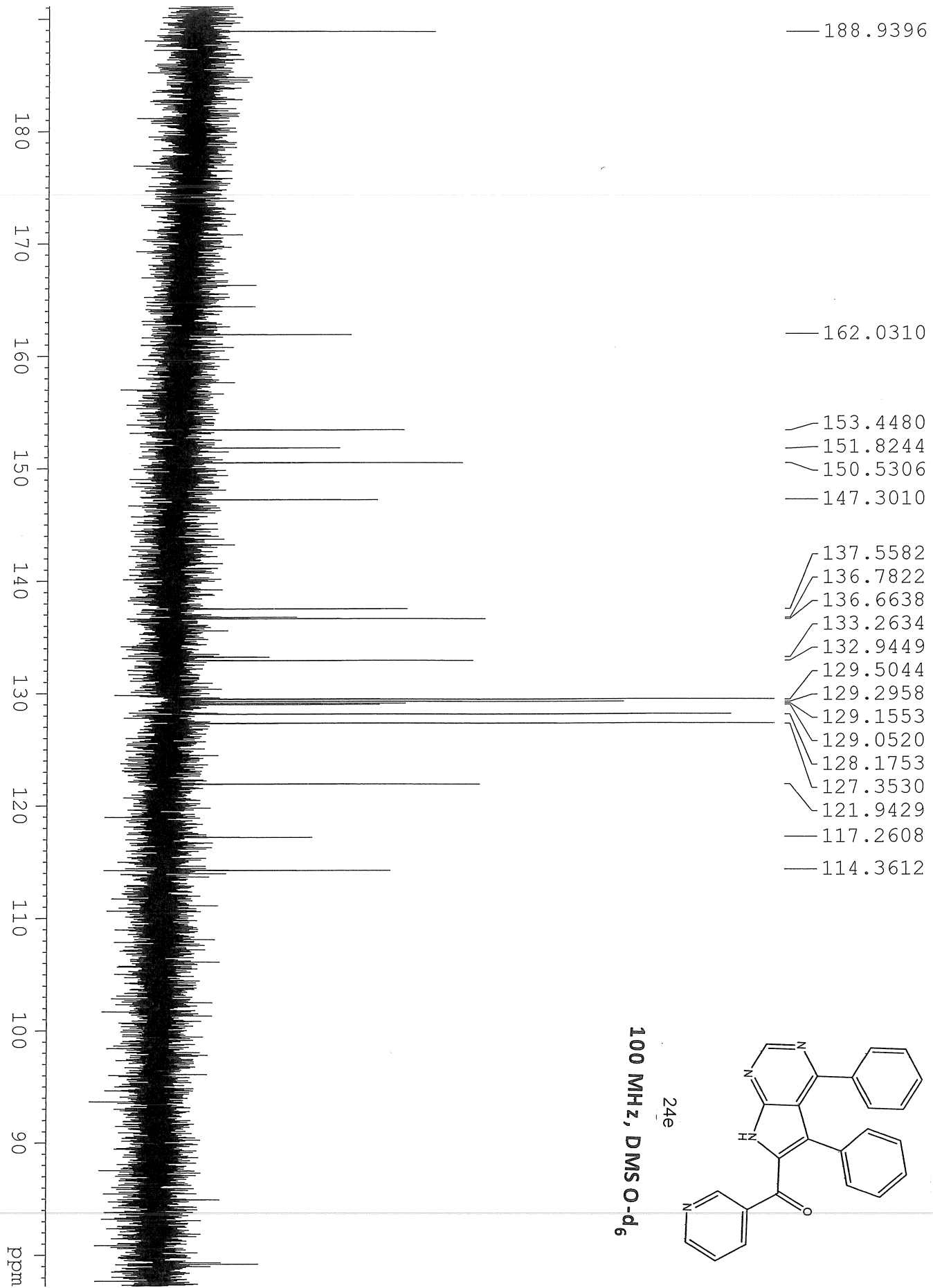
rsk_1044_MCR_4a_DMSOd6



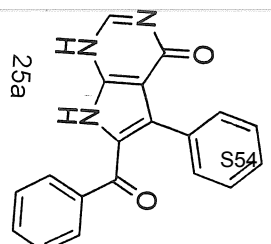
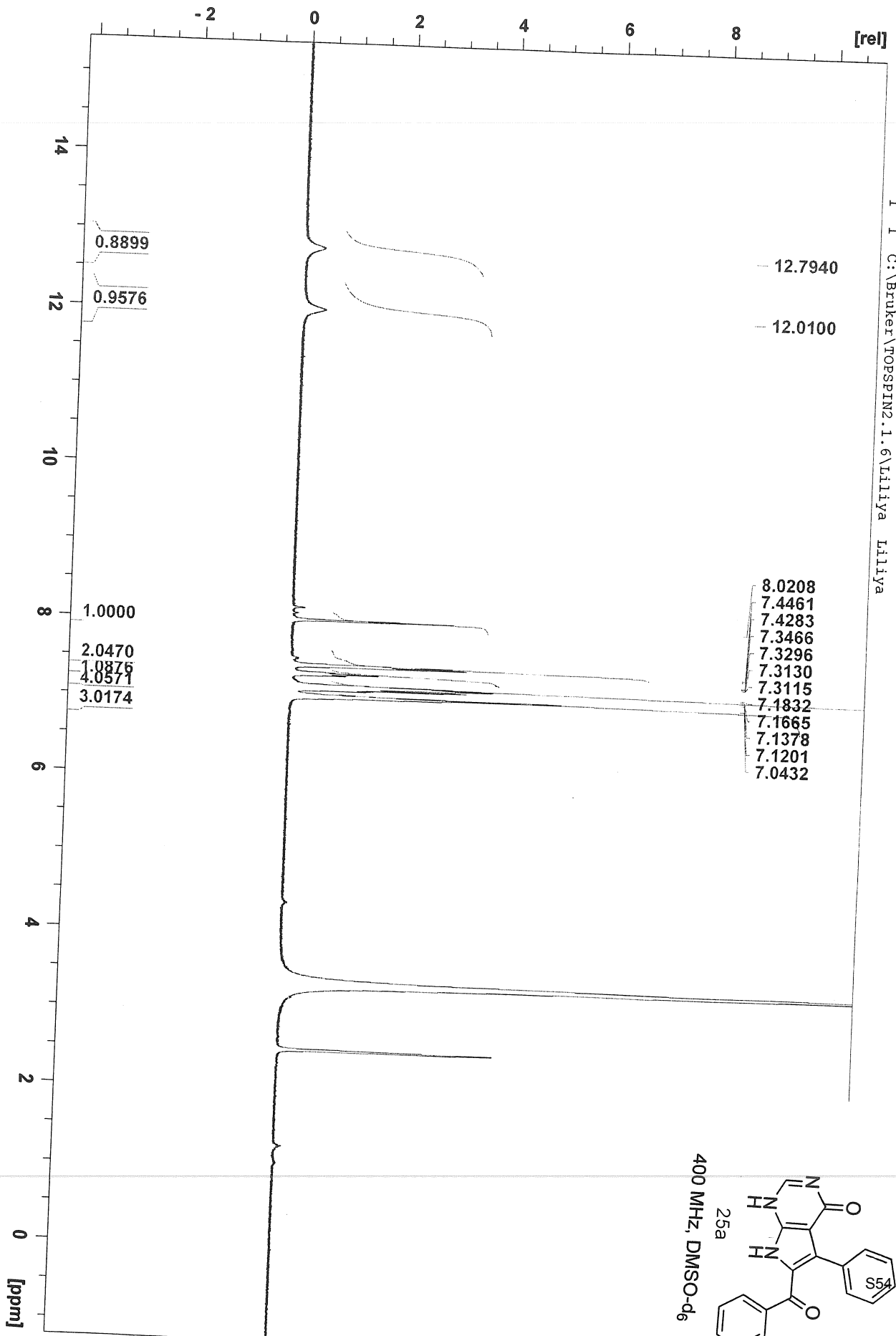
24e

400 MHz, DMSO-d₆

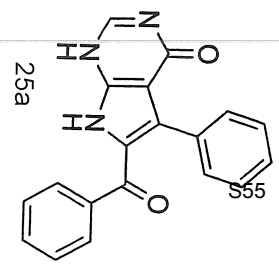
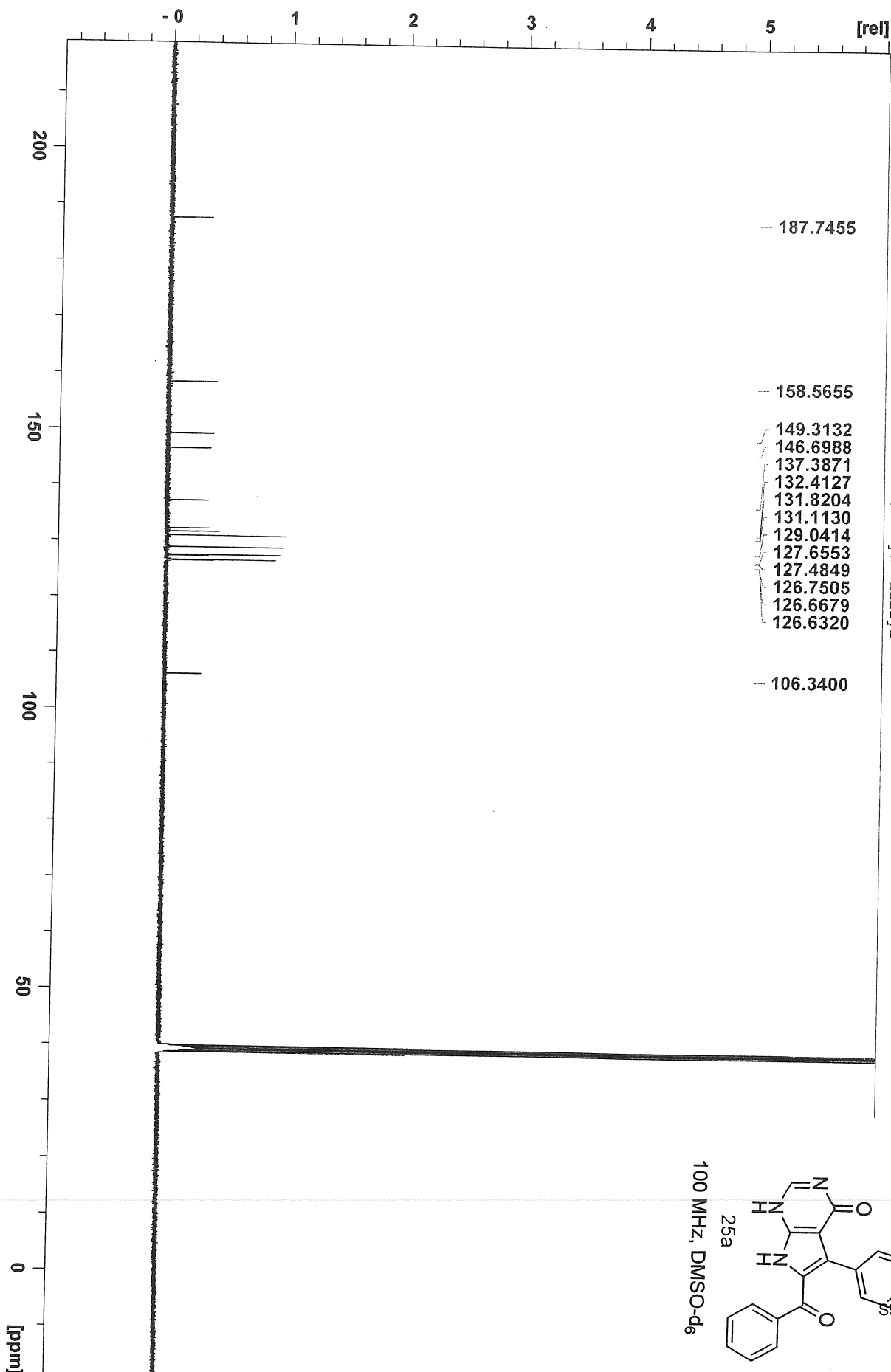


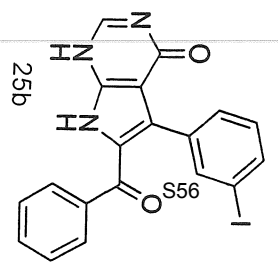
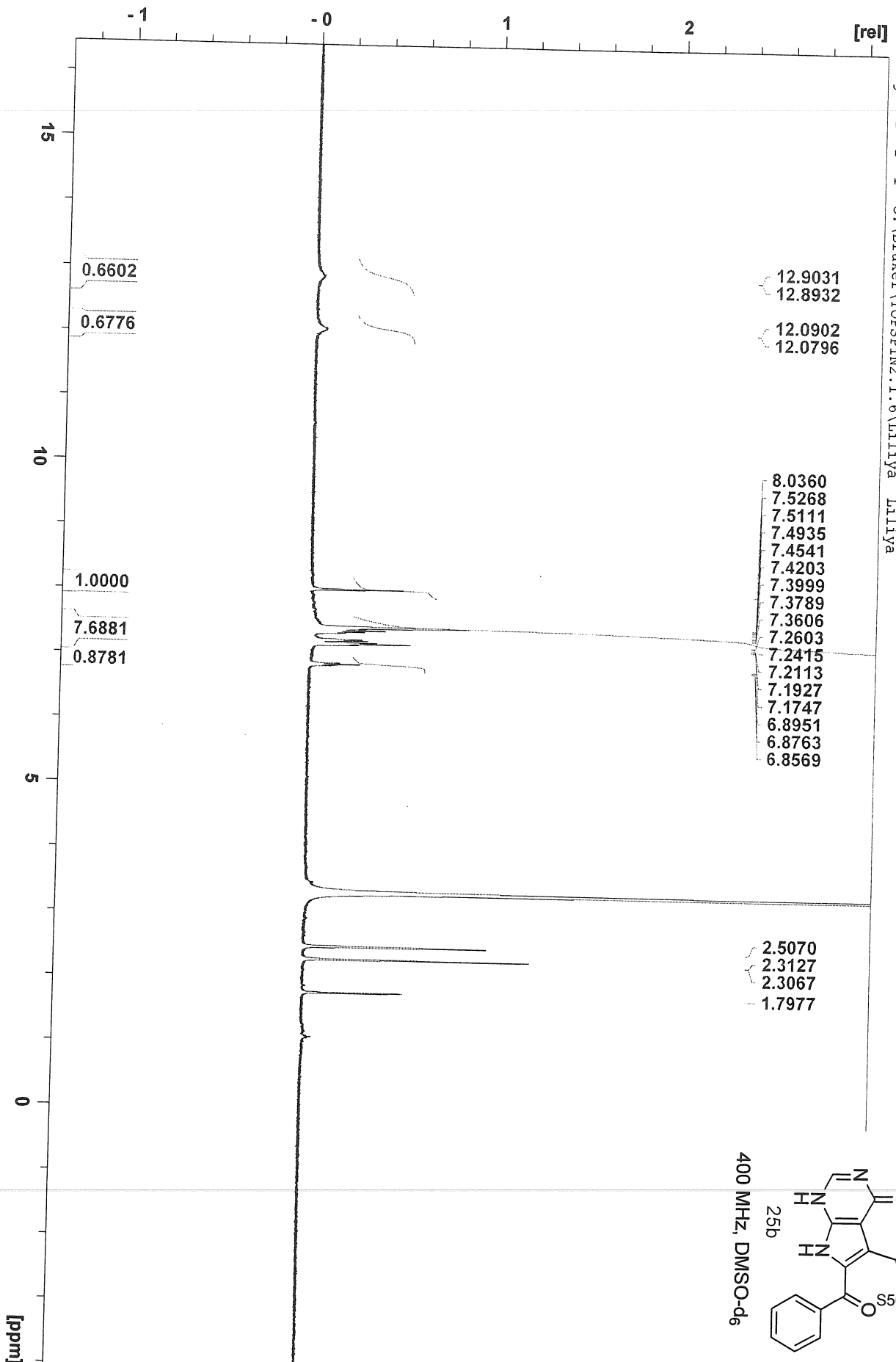


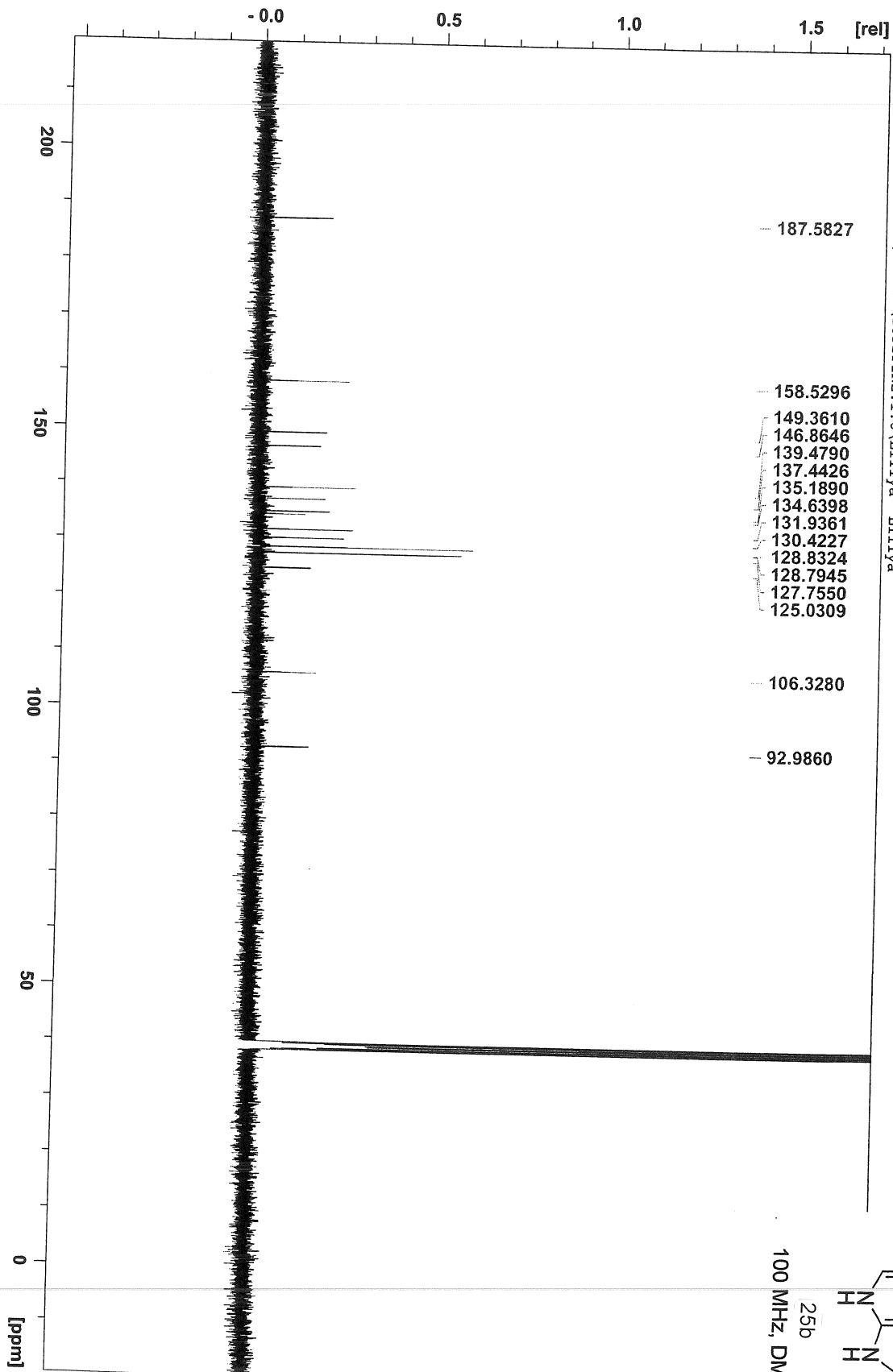
MCR1_DMSOd6



400 MHz, DMSO-d₆

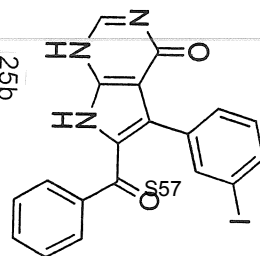






100 MHz, DMSO-d₆

25b



R1d-I-C13 4 1 C:\Bruker\TOPSPIN2.1.6\Liliya Liliya

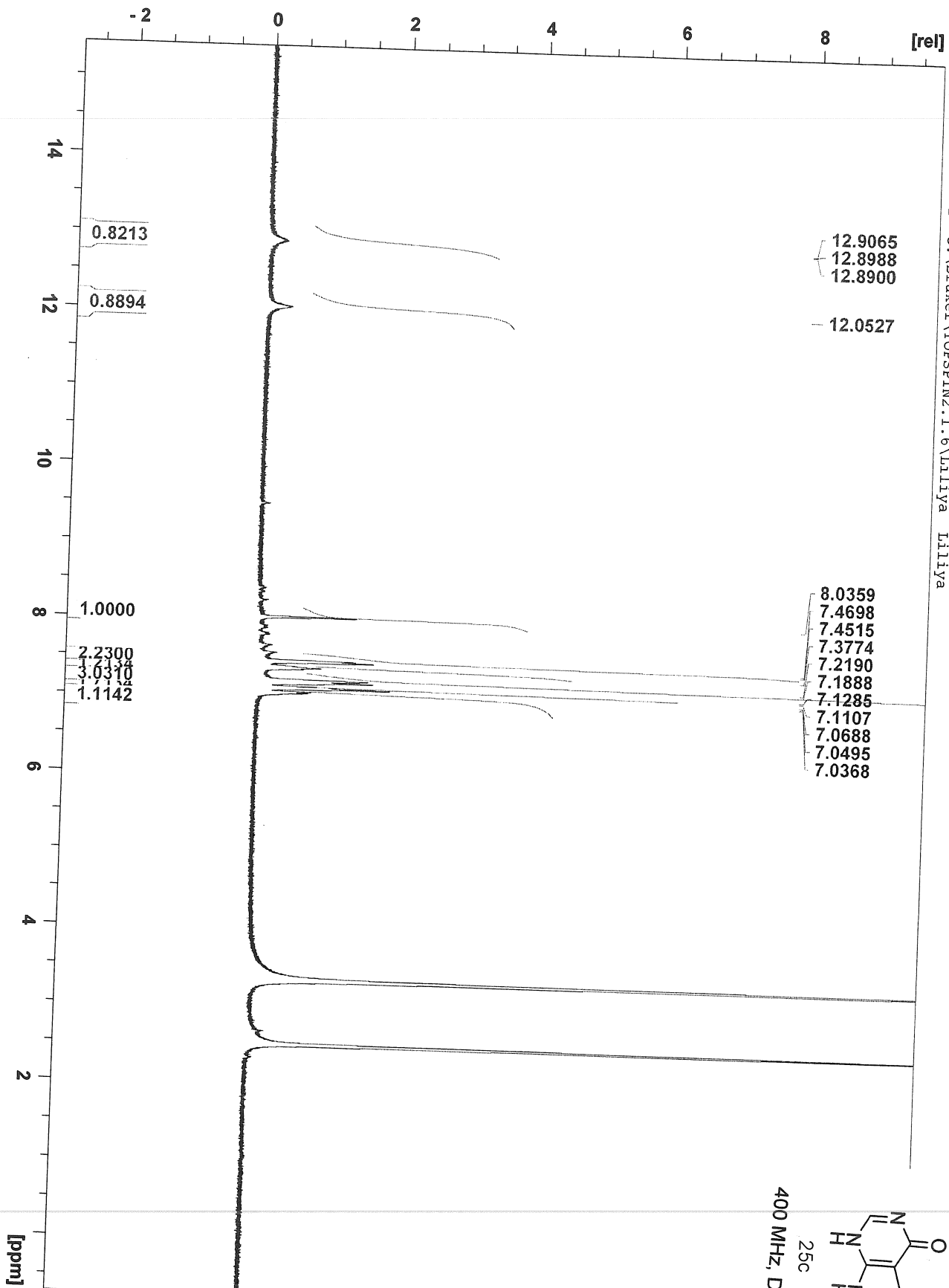
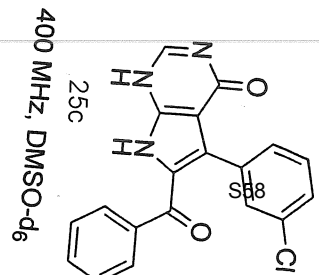
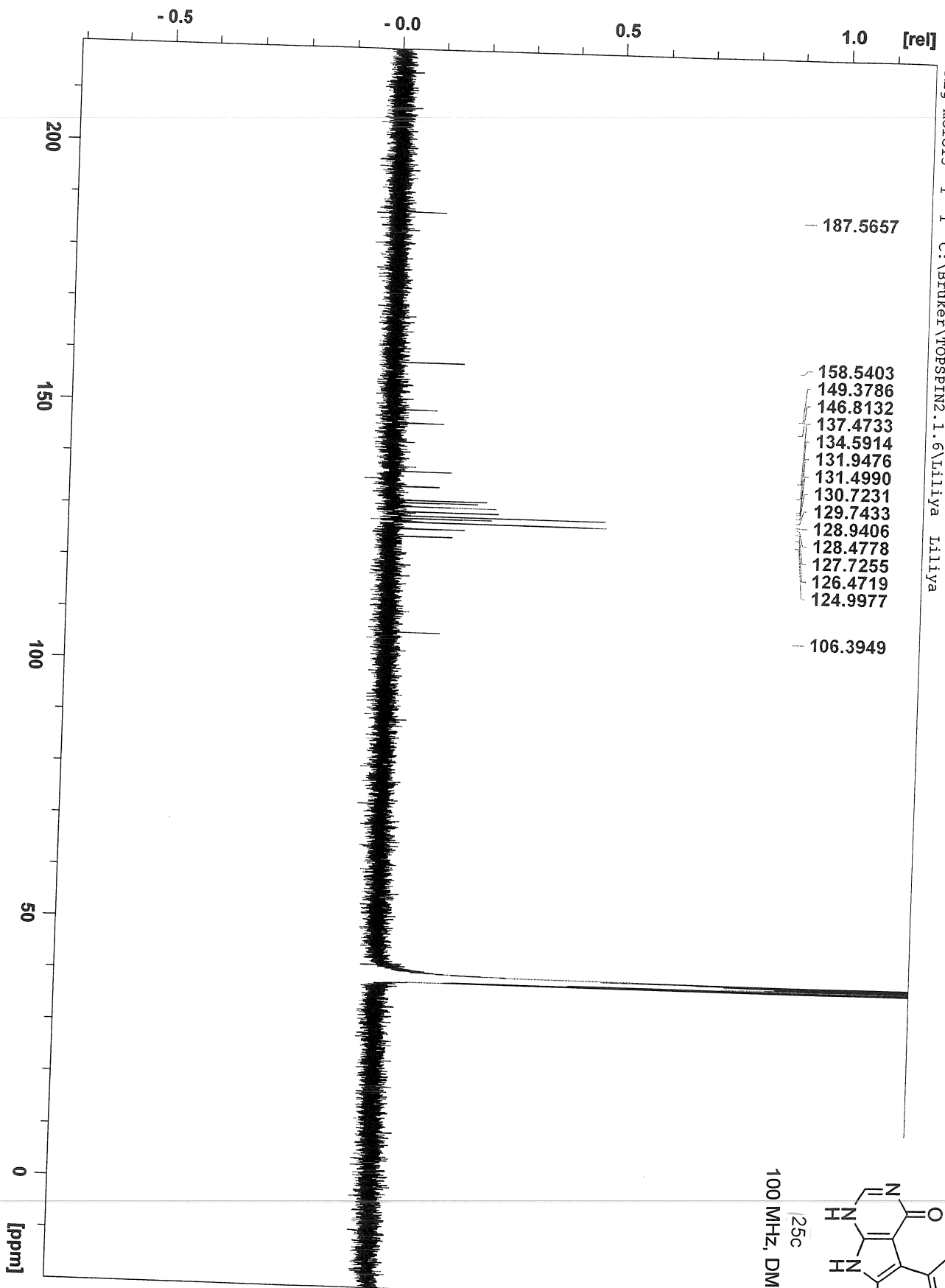


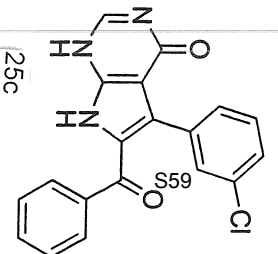
Fig-MC1H1 1 1 C:\Bruker\TOPSPIN2.1.6\Lillya Lillya

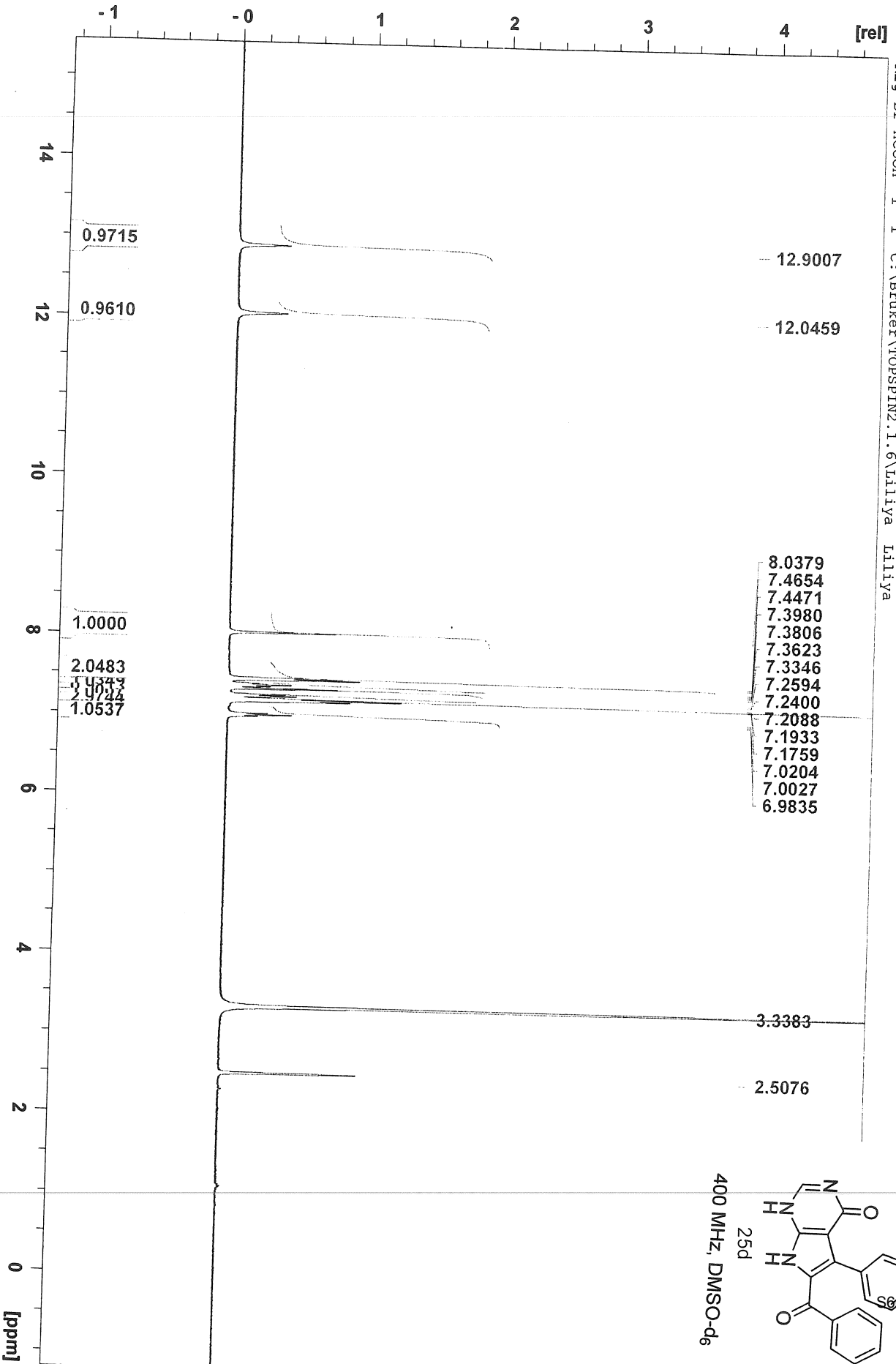




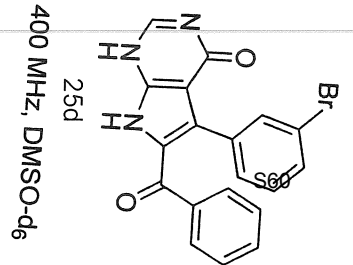
R19-mC1C13 1 1 C:\Bruker\TOPSPIN2.1.6\lillya lillya

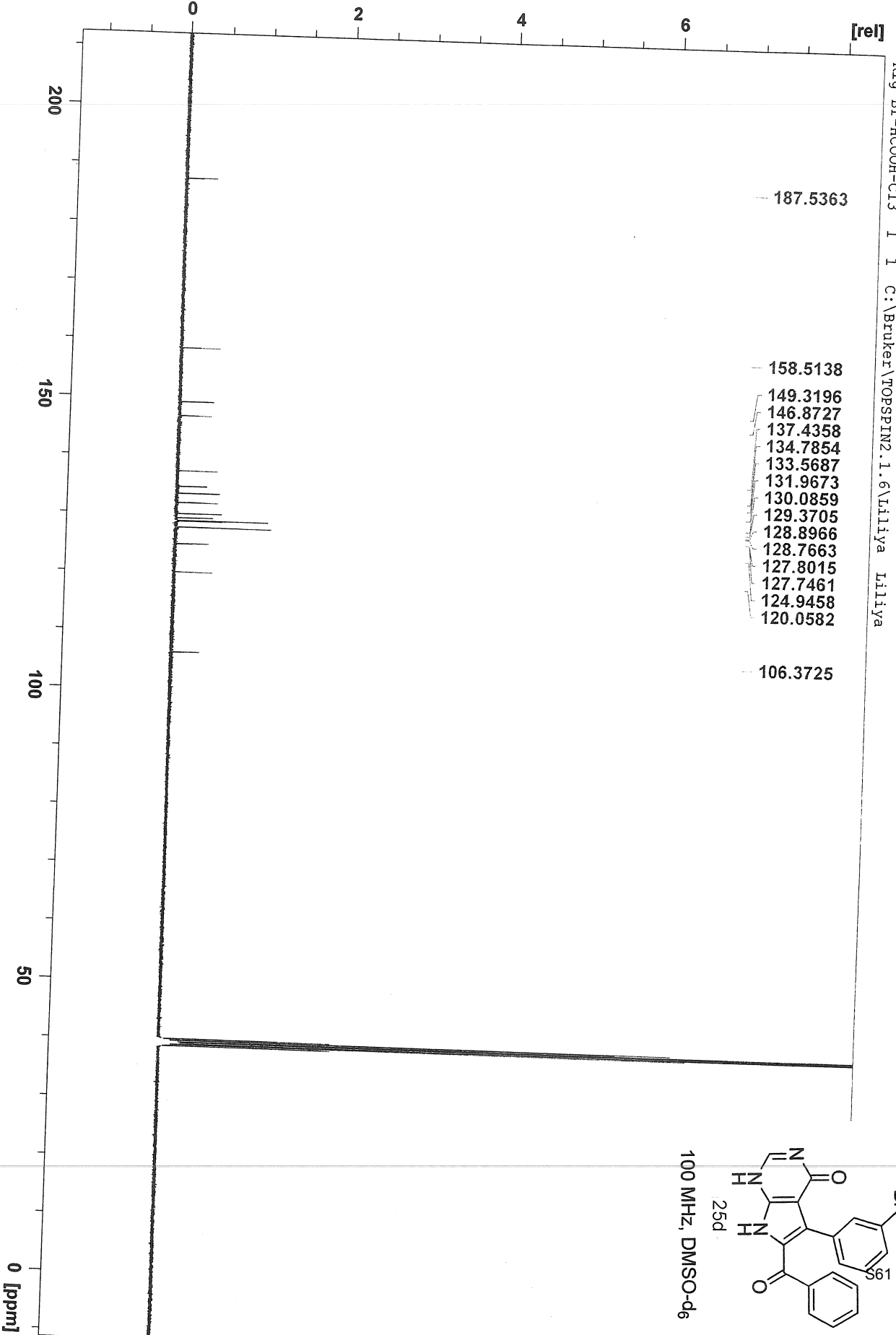
100 MHz, DMSO-d₆



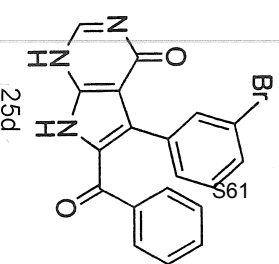


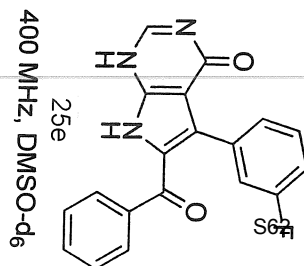
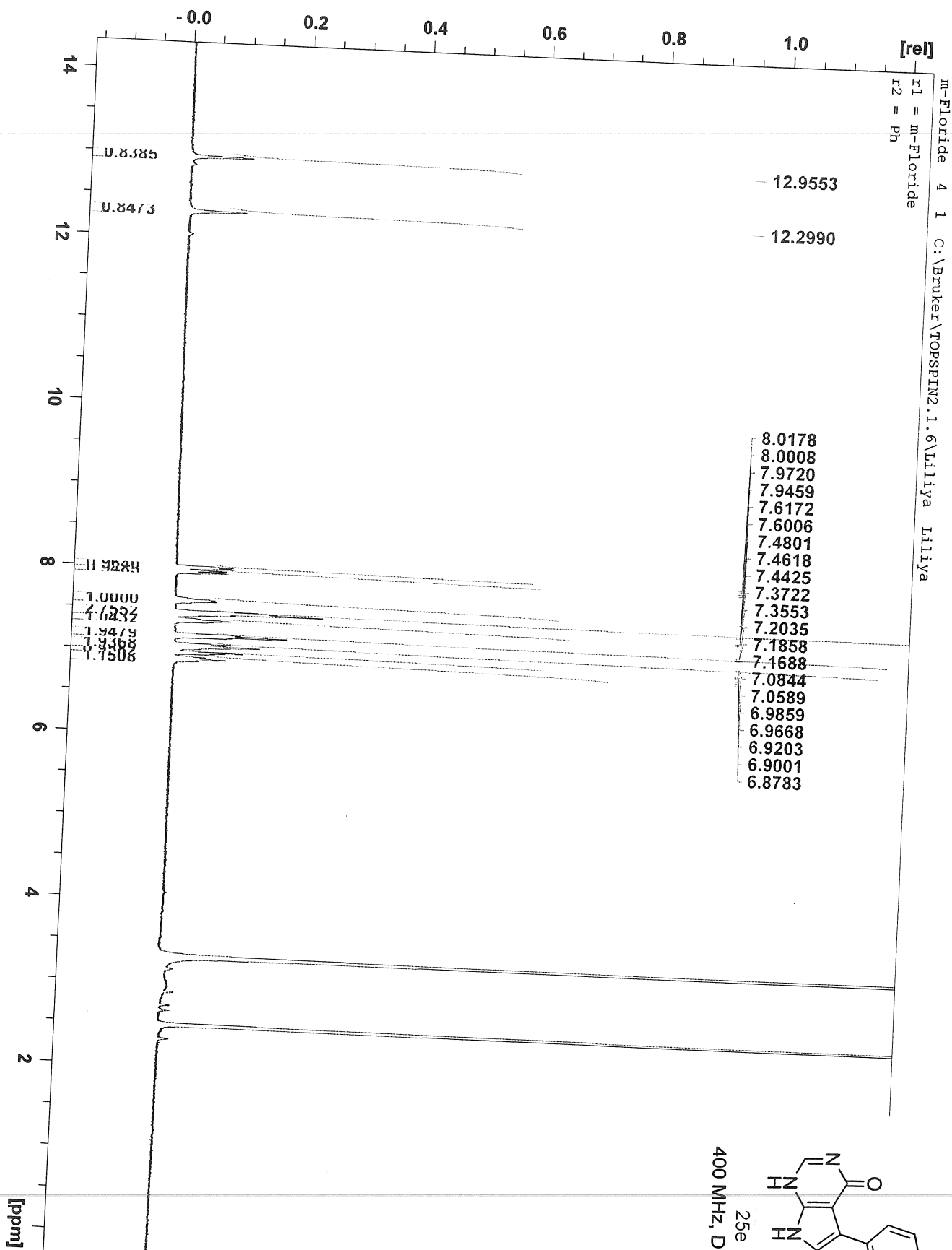
Rlg-Br-HCOOH 1 1 C:\Bruker\TOPSPIN2.1.6\lilya Lilya

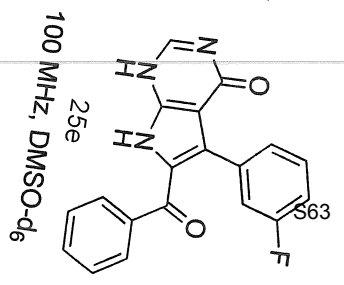
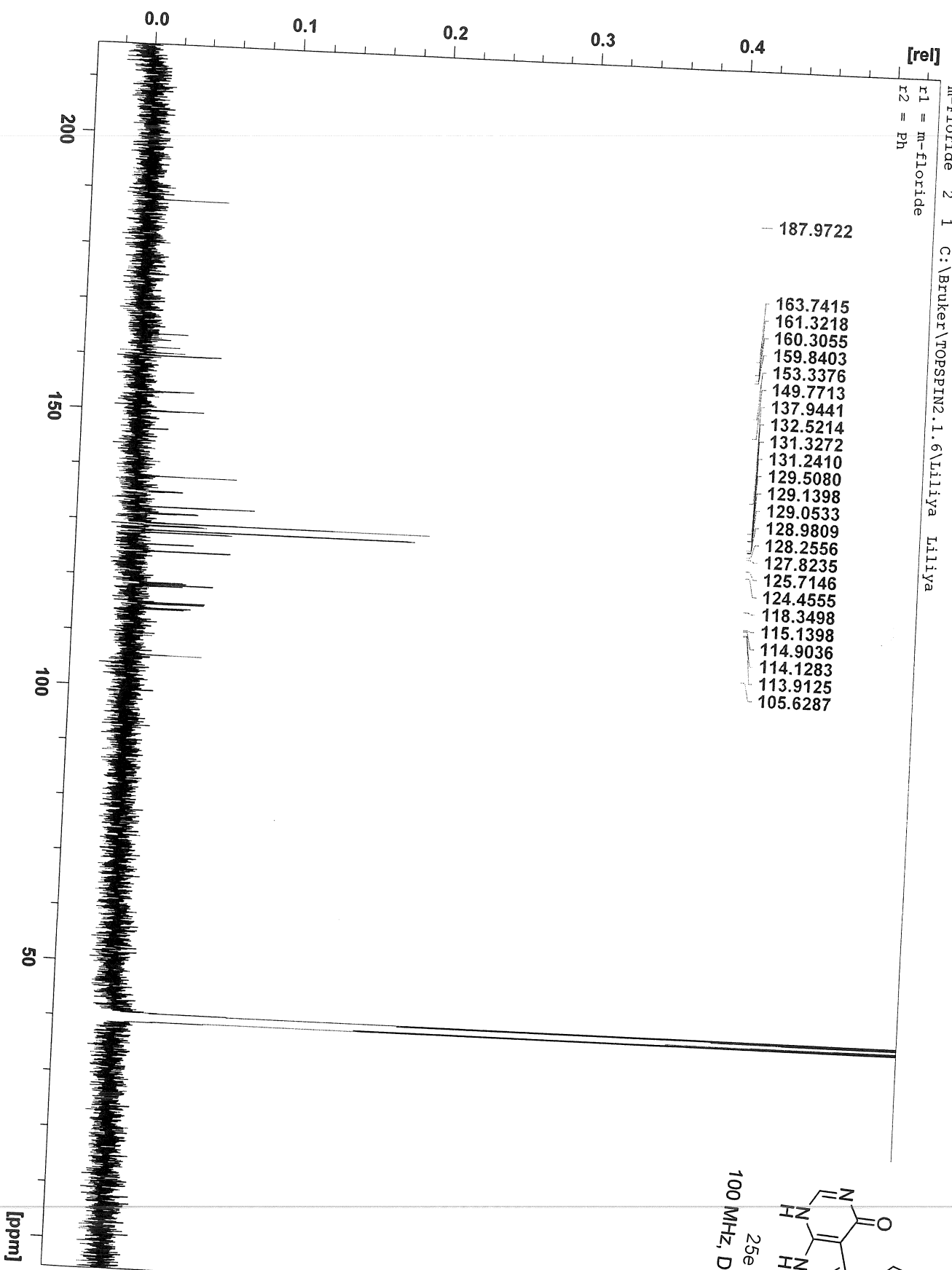


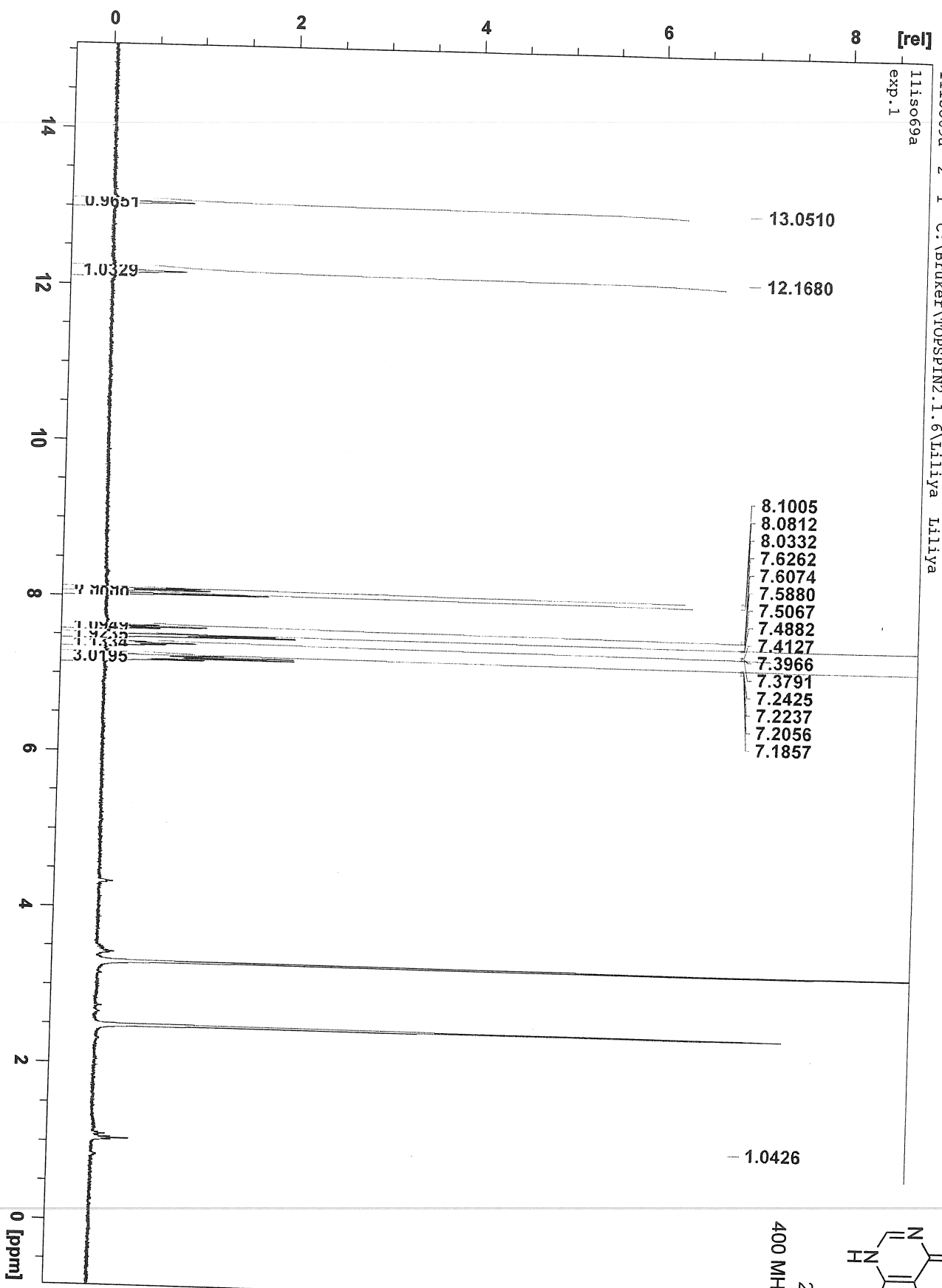


Rtg-Br-HCOOH-C13 1 1 C:\Bruker\TOPSPIN2.1.6\LiLiya LiLiya

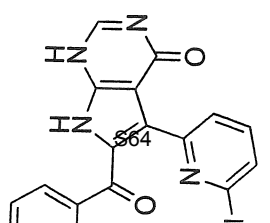




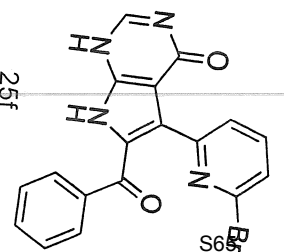
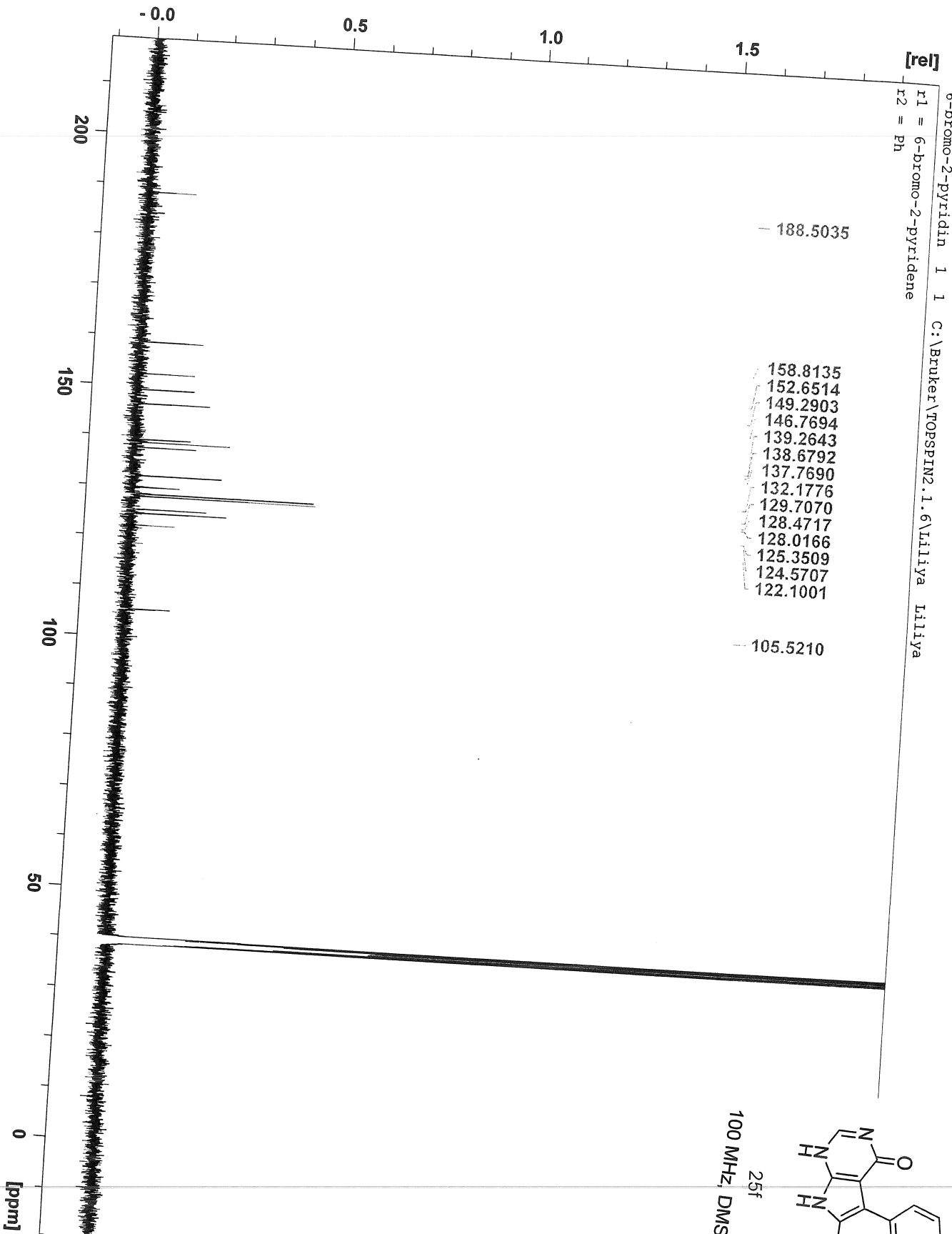




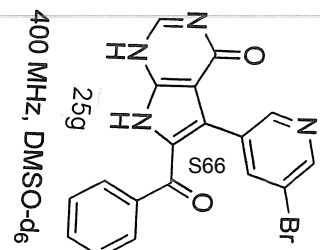
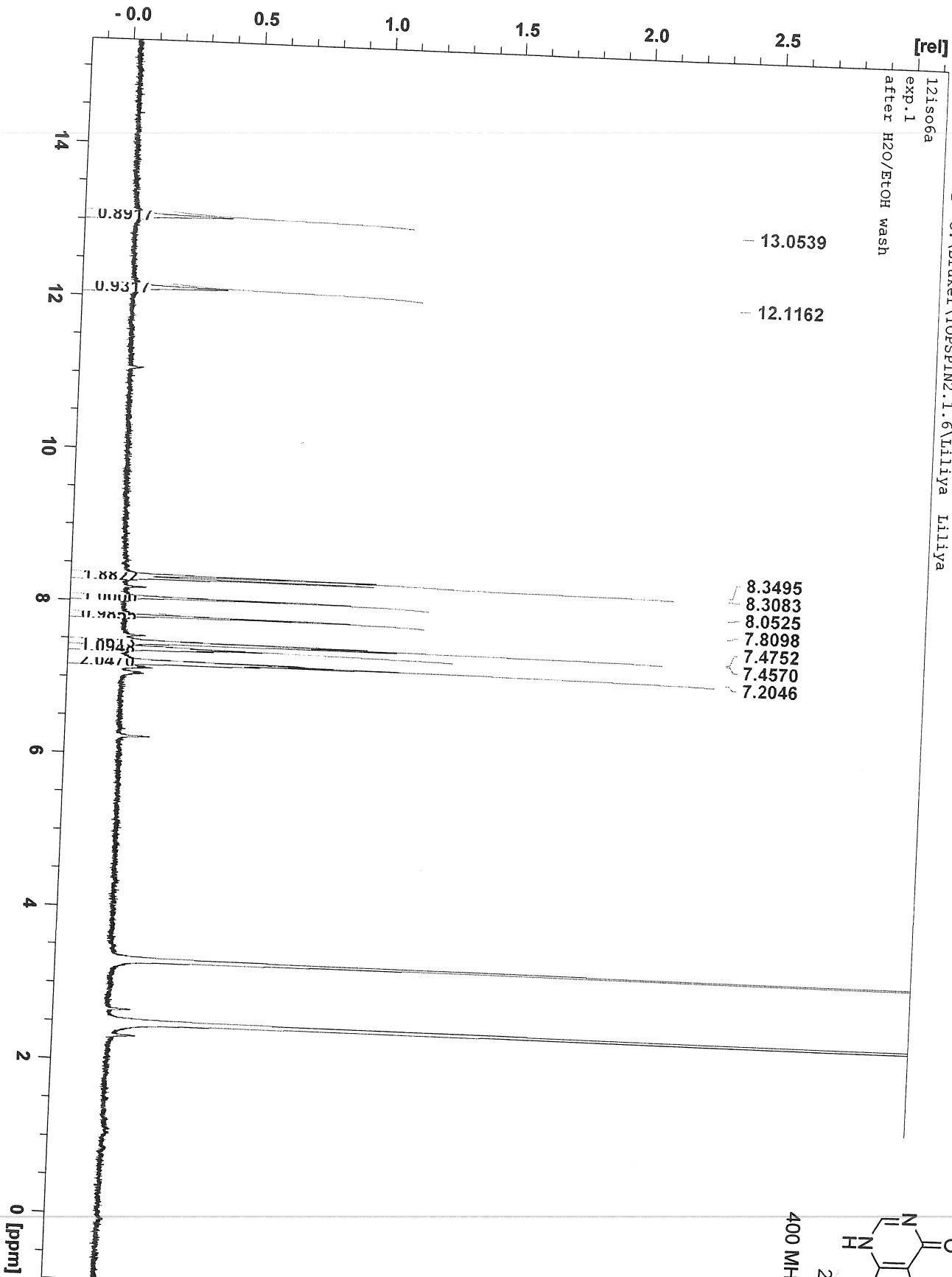
400 MHz, DMSO-d₆, 25°C



6-bromo-2-pyridin 1 1 C:\Bruker\TOPSPIN2.1.6\Lillya Lillya
r1 = 6-bromo-2-pyridine
r2 = Ph



100 MHz, DMSO-d₆



```

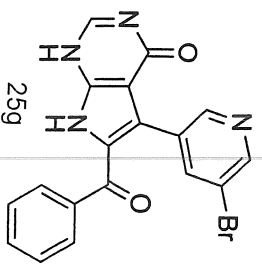
Filename = 1d_13c_spectrum-159.j
Author = alex
Experiment = single_pulse_dec
Sample_id = S#666288
Solvent = DMSO-d6
Creation time = 4-MAR-2011 06:32:32
Revision time = 4-MAR-2011 10:15:01
Current_time = 4-MAR-2011 10:15:34

Comment
Data_format = Single Pulse with Bro
ID_REAL = 1D REAL
Dim_size = 32768
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = X
Spectrometer = Eclipse+ 300
= DELTA_NMR

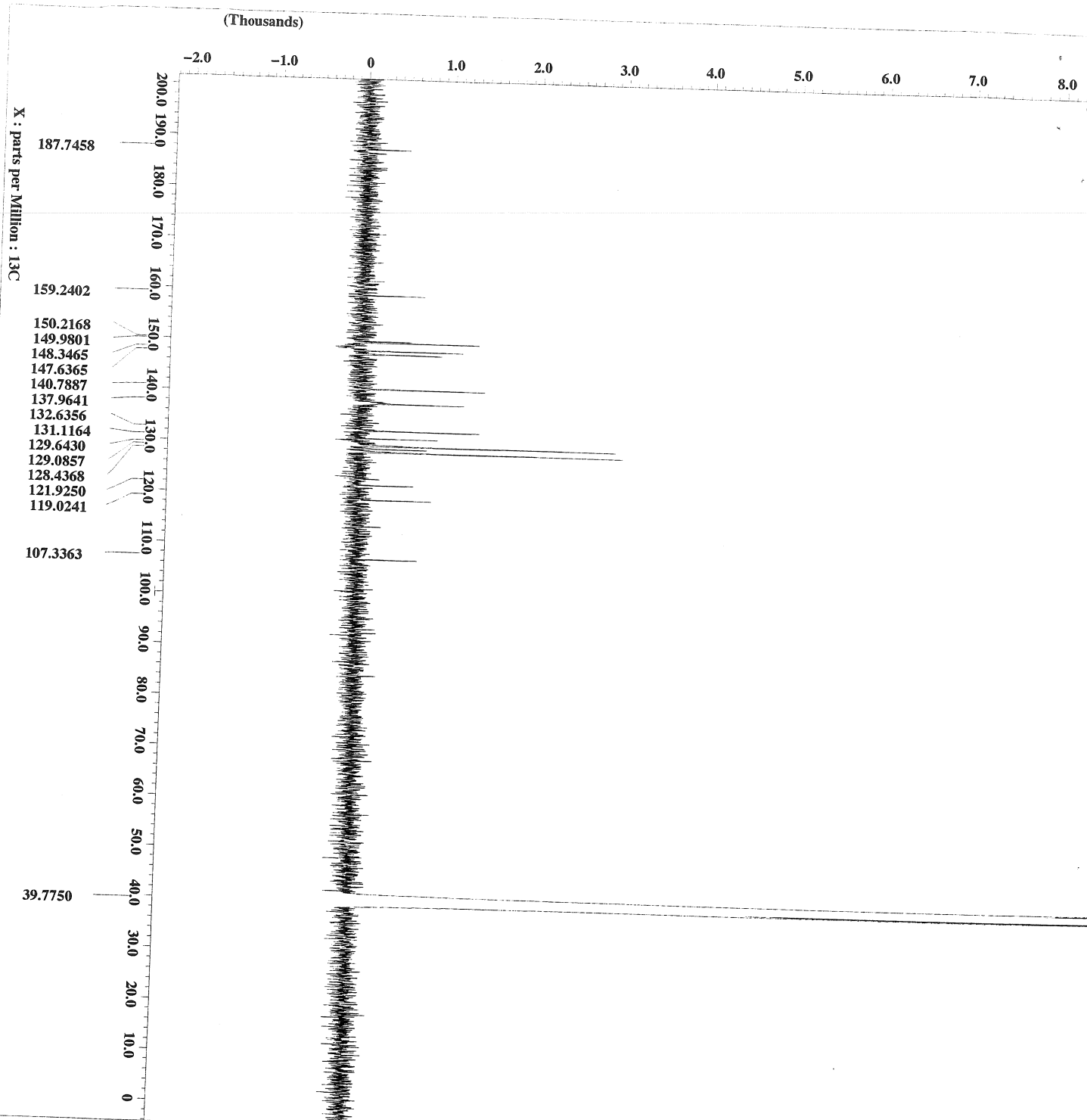
Field strength = 7.0586013[M] (300)[MHz]
X_acq_duration = 1.7338272[s]
X_domain = 13C
X_freq = 75.56823426[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.57689184[MHz]
X_sweep = 18.90359168[kHz]
Irr_domain = 1H
Irr_freq = 300.52965592[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16000
Total_scans = 16000

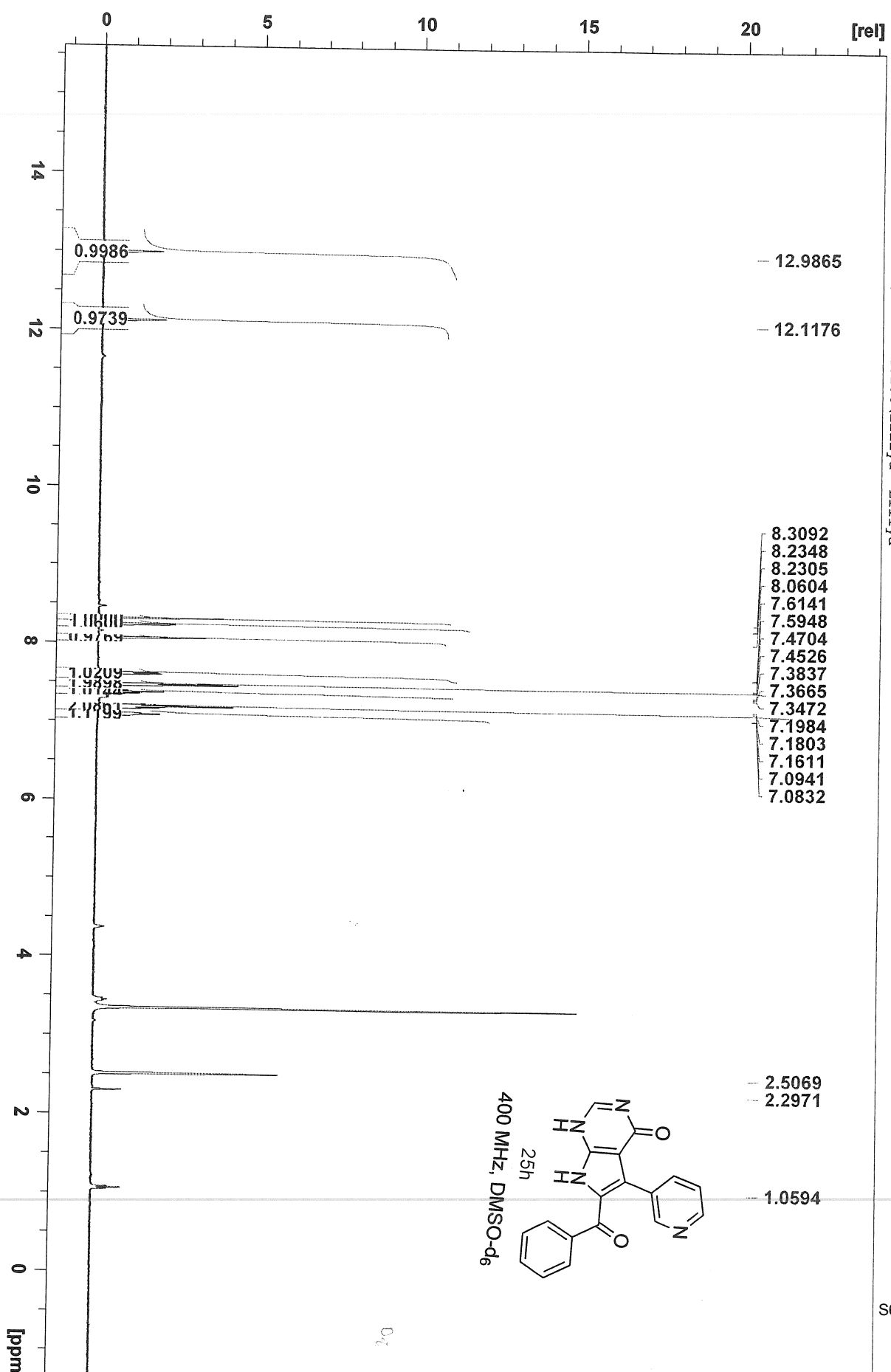
X_90_width = 8.1[us]
X_acq_time = 1.7338272[s]
X_angle = 30[deg]
X_pulse = 2.7[us]
Initial_wait = 1[s]
Phase_preset = 1[us]
Recvr_gain = 15
Relaxation_delay = 1[s]
Temp_get = 20.7[deg]
Unblank_time = 2[us]

```

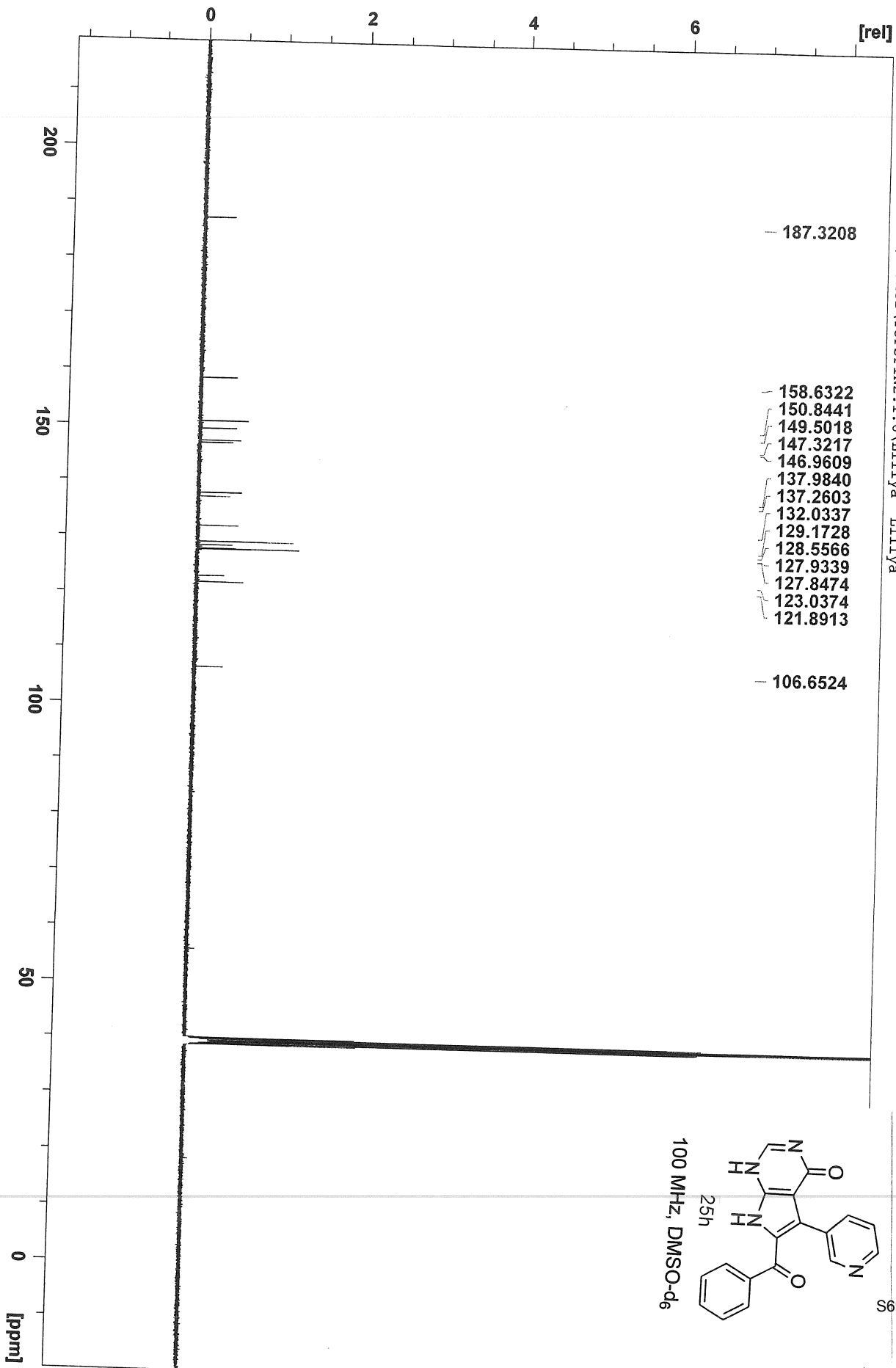


75 MHz, DMSO-d₆





R1d-N 22 1 C:\Bruker\TOPSPIN2.1.6\lillyya Lillyya



Rig-N-C13 1 1 C:\Bruker\TOPSPIN2.1.6\LiLiya LiLiya

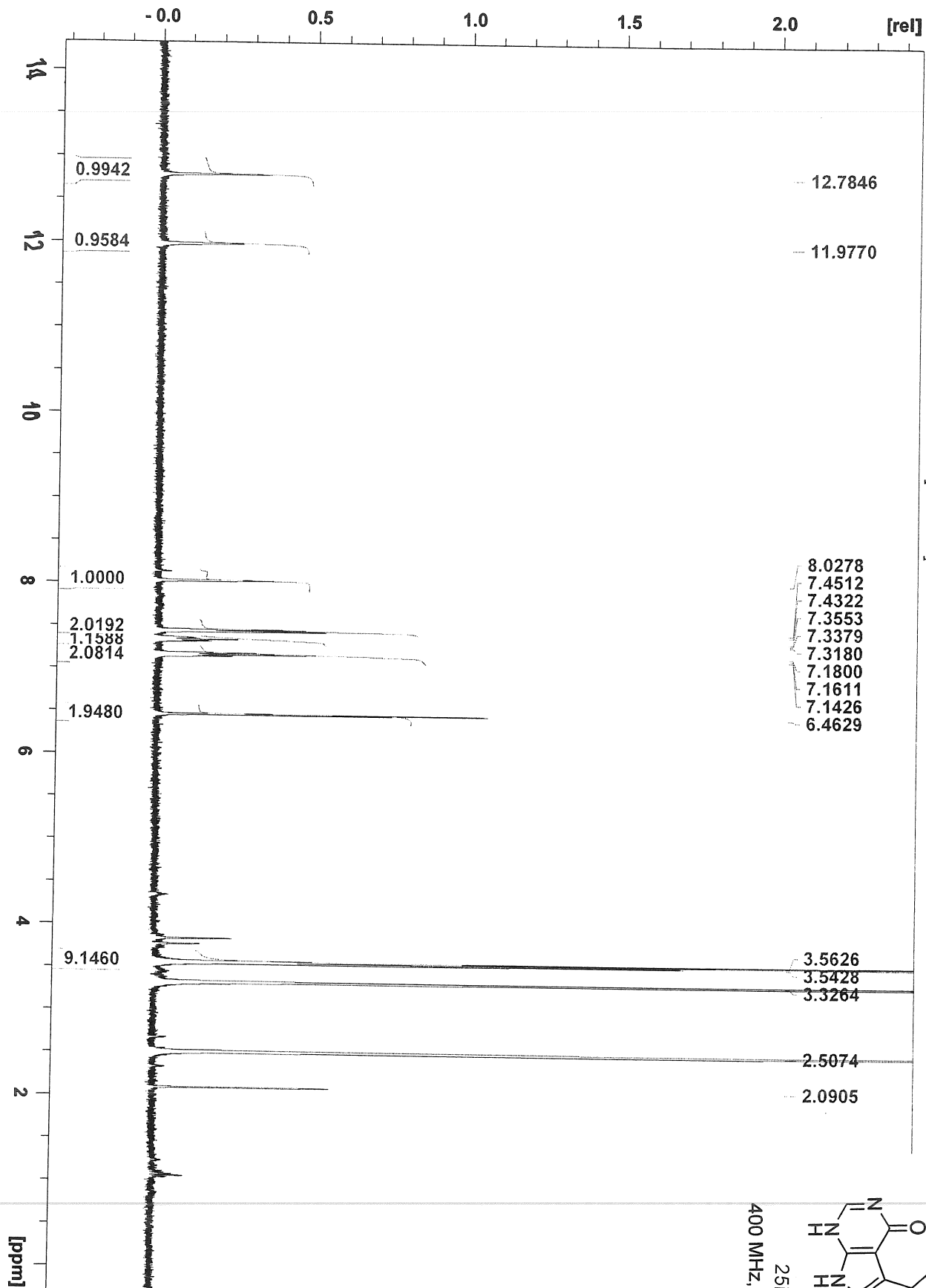
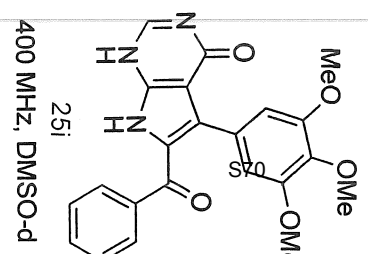
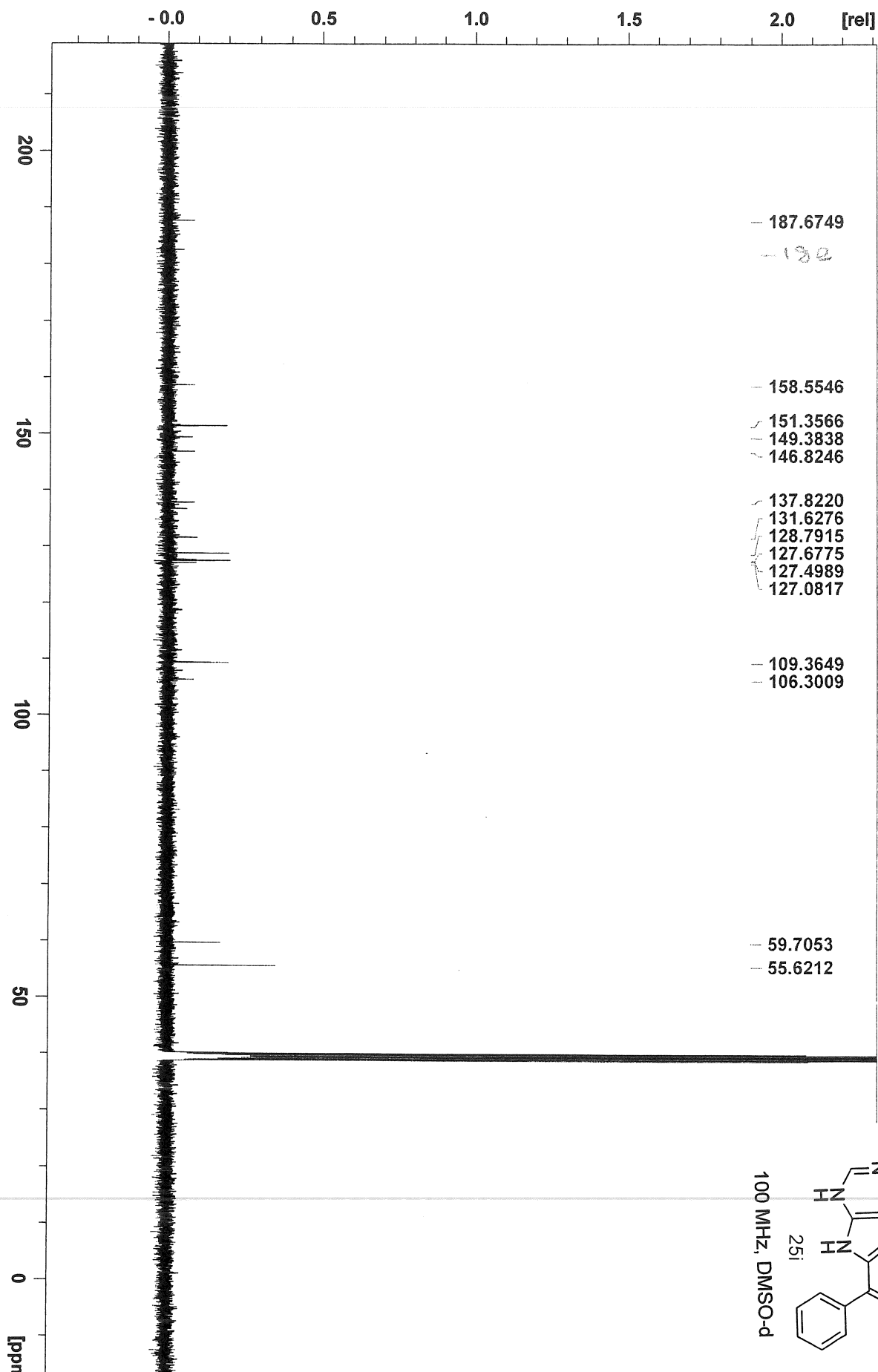
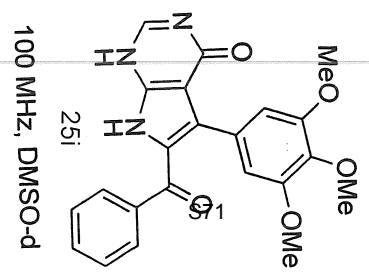


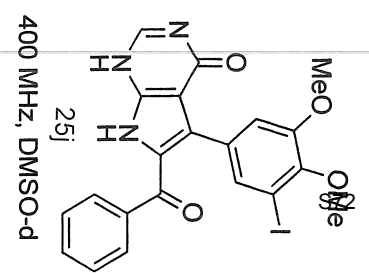
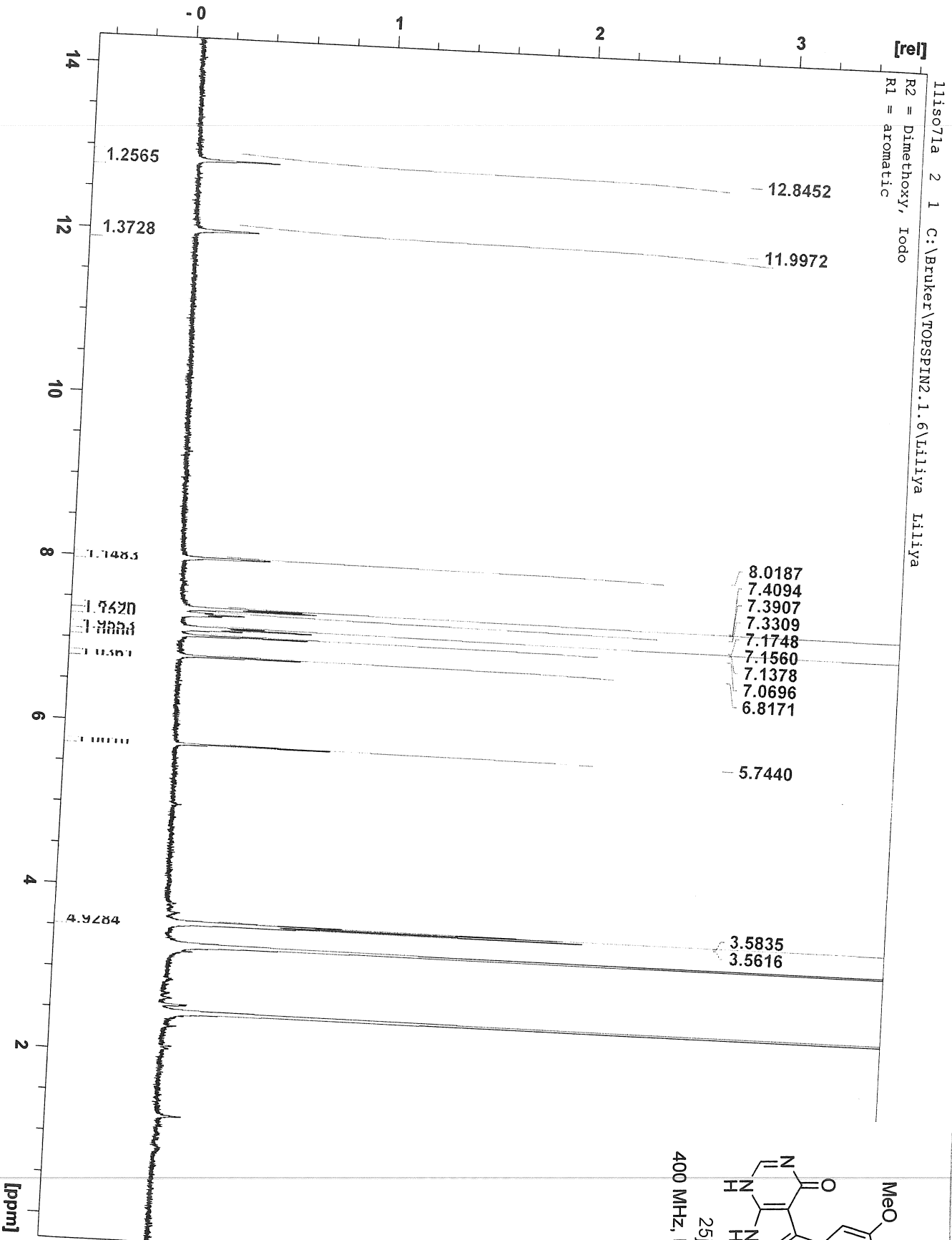
Fig-3CH3O 2 1 C:\Bruker\TOPSPIN2.1.6\Liliya Liliya

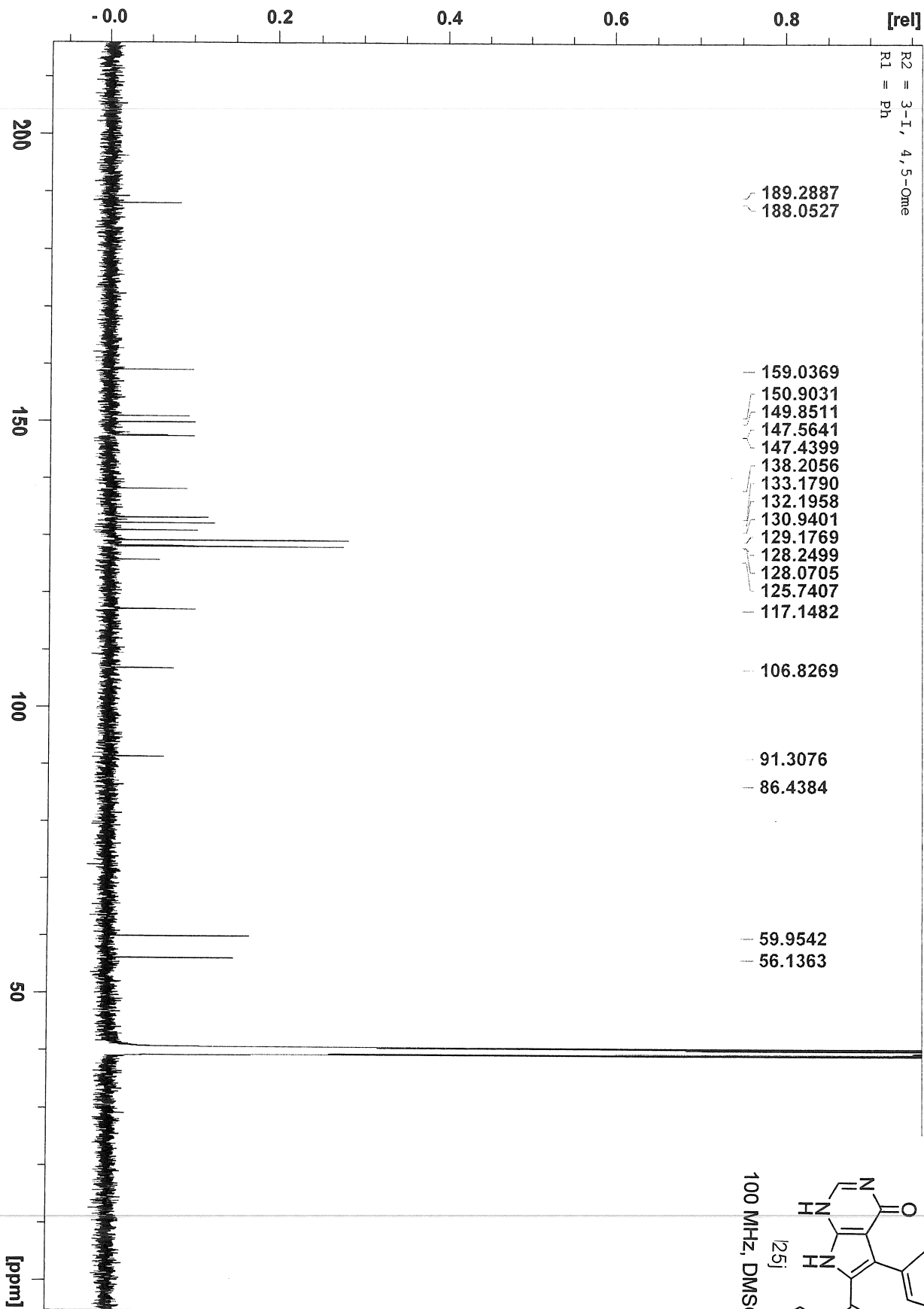




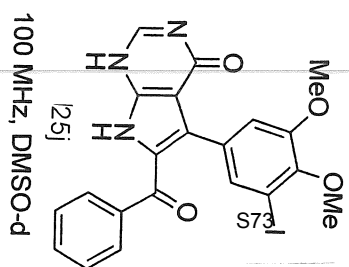
Rid8-30CH3-C13 4 1 C:\Bruker\TOPSPIN2.1.6\LiLiya LiLiya

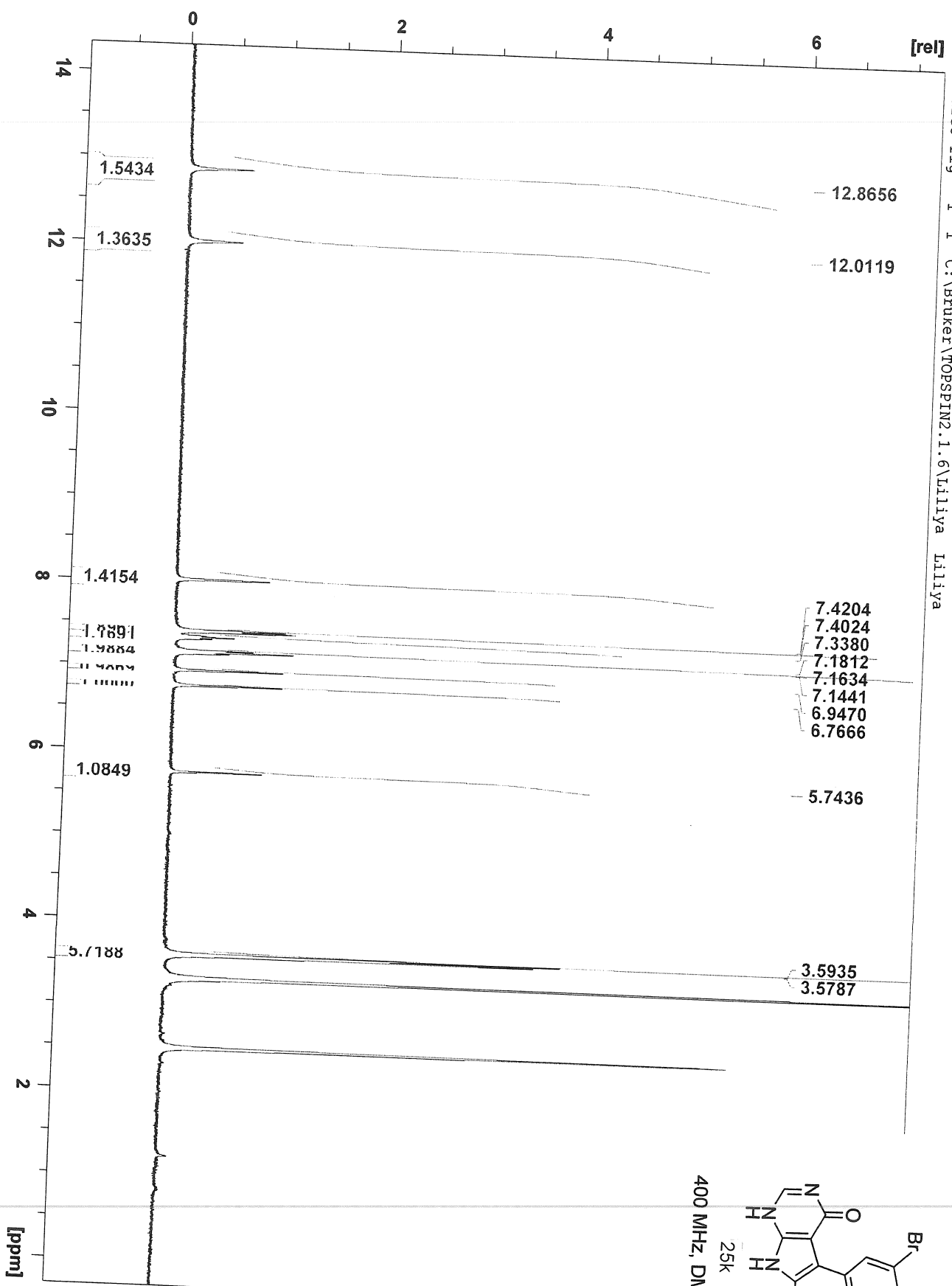




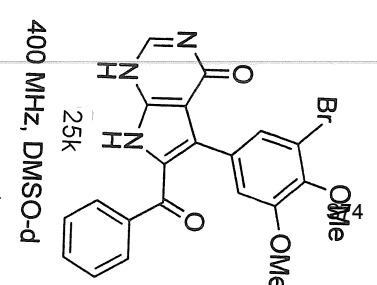


"3-I, 4,5-Ome" 1 1 C:\Bruker\TOPSPIN2.1.6\Liliya Liliya





"marco rig" 1 1 C:\Bruker\TOPSPIN2.1.6\Liliya Liliya



marco rig
exp3
2-16-12

188.00

159.03

152.02

149.85

147.46

144.96

138.24

132.21

130.22

129.24

128.29

128.05

127.39

125.82

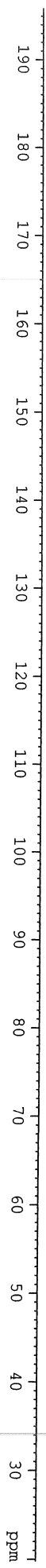
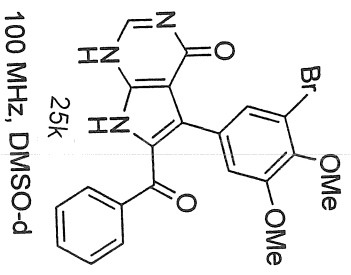
116.33

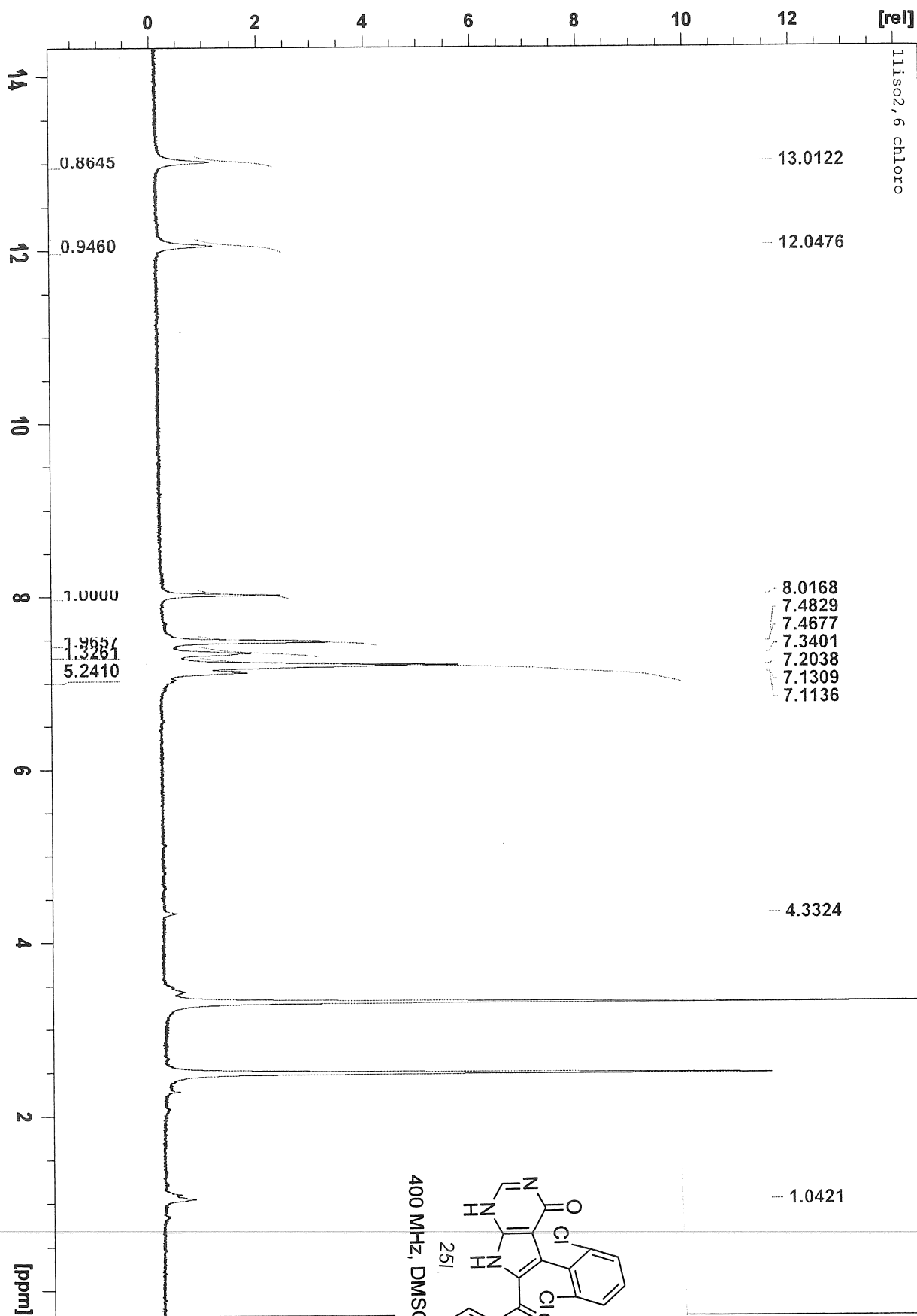
115.51

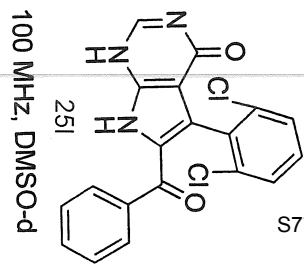
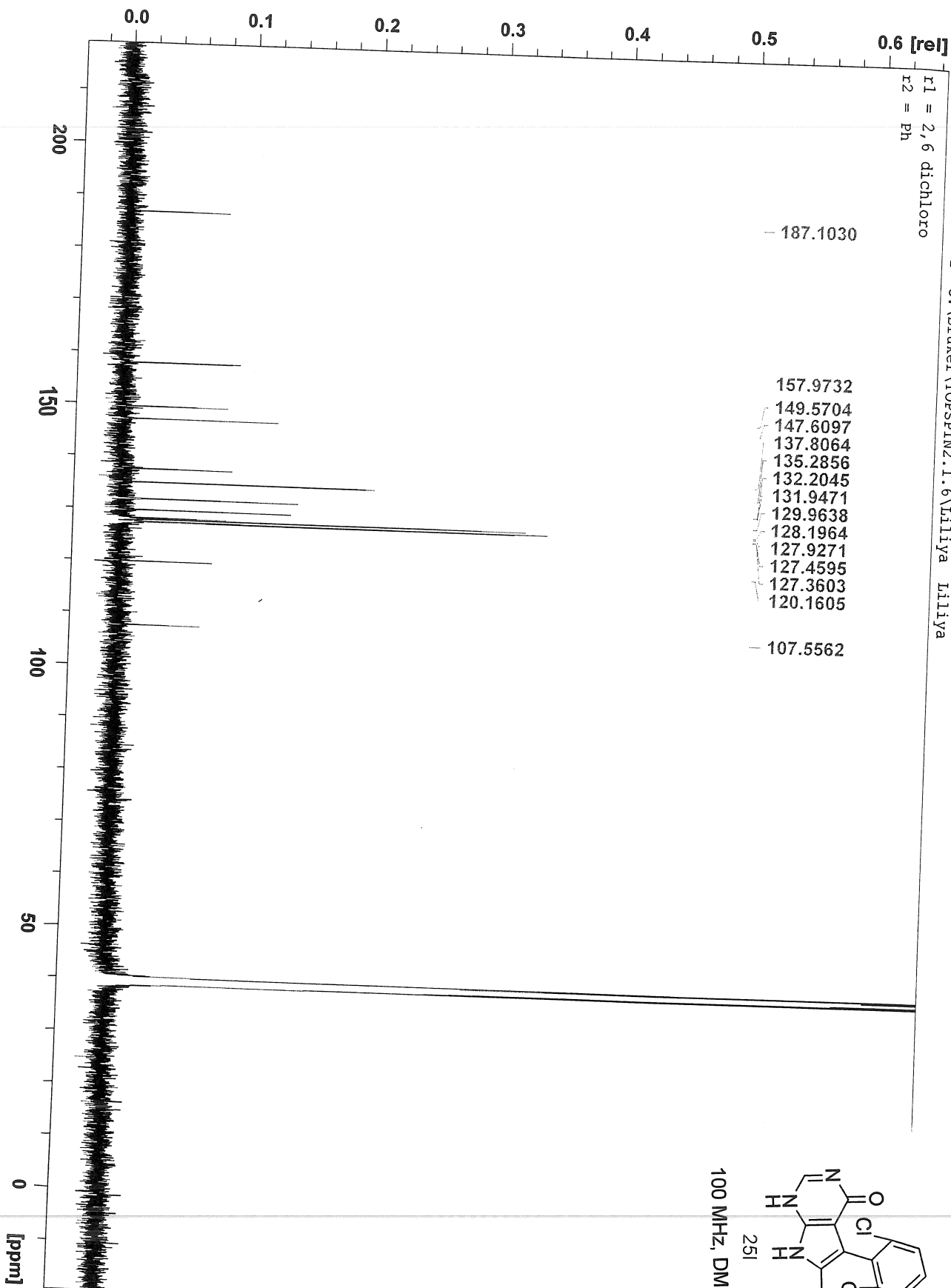
106.87

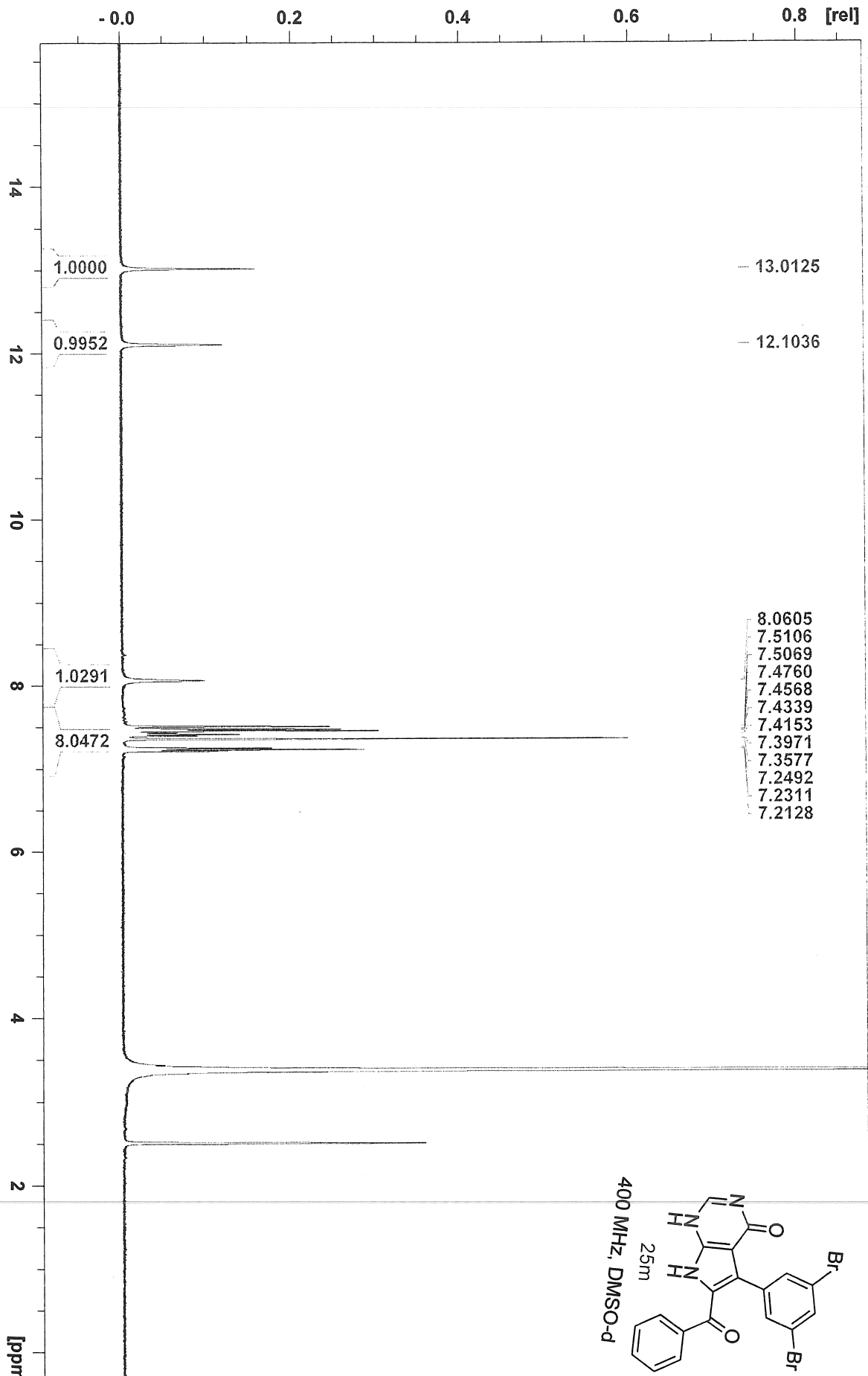
60.18

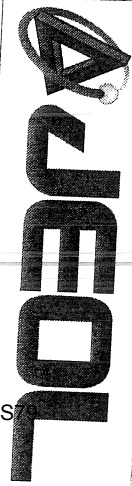
56.25











```

Filename = id_13c_spectrum-162.j
Author = alex
Experiment = single_pulse_dec
Sample_id = S#580883
Solvent = DMSO-D6
Creation_time = 13-MAR-2011 04:10:15
Revision_time = 13-MAR-2011 11:59:17
Current_time = 13-MAR-2011 11:59:37

```

```

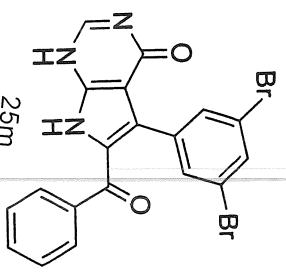
Comment = Single Pulse with Bro
Data_format = 1D REAL
Dim_size = 32768
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = Eclipse+ 300
Spectrometer = DELTA_NMR

```

```

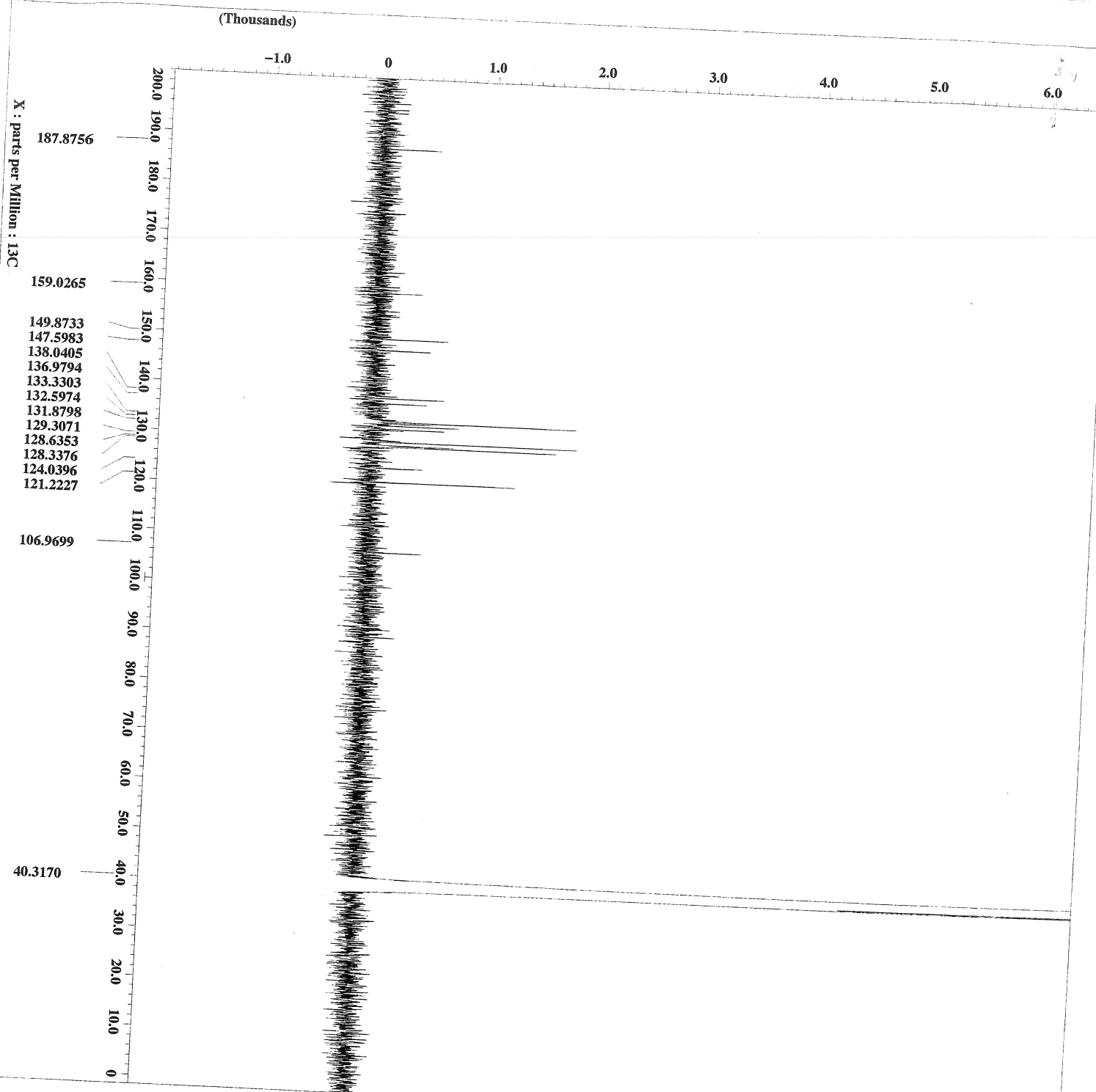
Field_strength = 7.05860131[T] (300)[MHz]
X_acq_duration = 1.7334272[ls]
X_domain = 13C
X_freq = 75.56823426[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.57689184[Hz]
X_sweep = 18.90359168[kHz]
Irr_domain = 1H
Irr_freq = 300.52965592[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 16000
Total_scans = 16000
X_90_width = 8.1[us]
X_acq_time = 1.7334272[ls]
X_angle = 30[deg]
X_pulse = 2.7[us]
Initial_wait = 1[ls]
Phase_preset = 3[us]
Recvr_gain = 15
Relaxation_delay = 1[ls]
Temp_get = 22.6[deg]
Undrftk_time = 2[us]

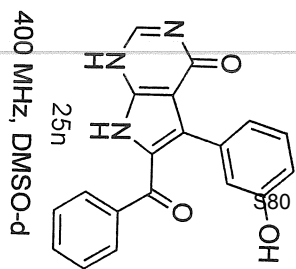
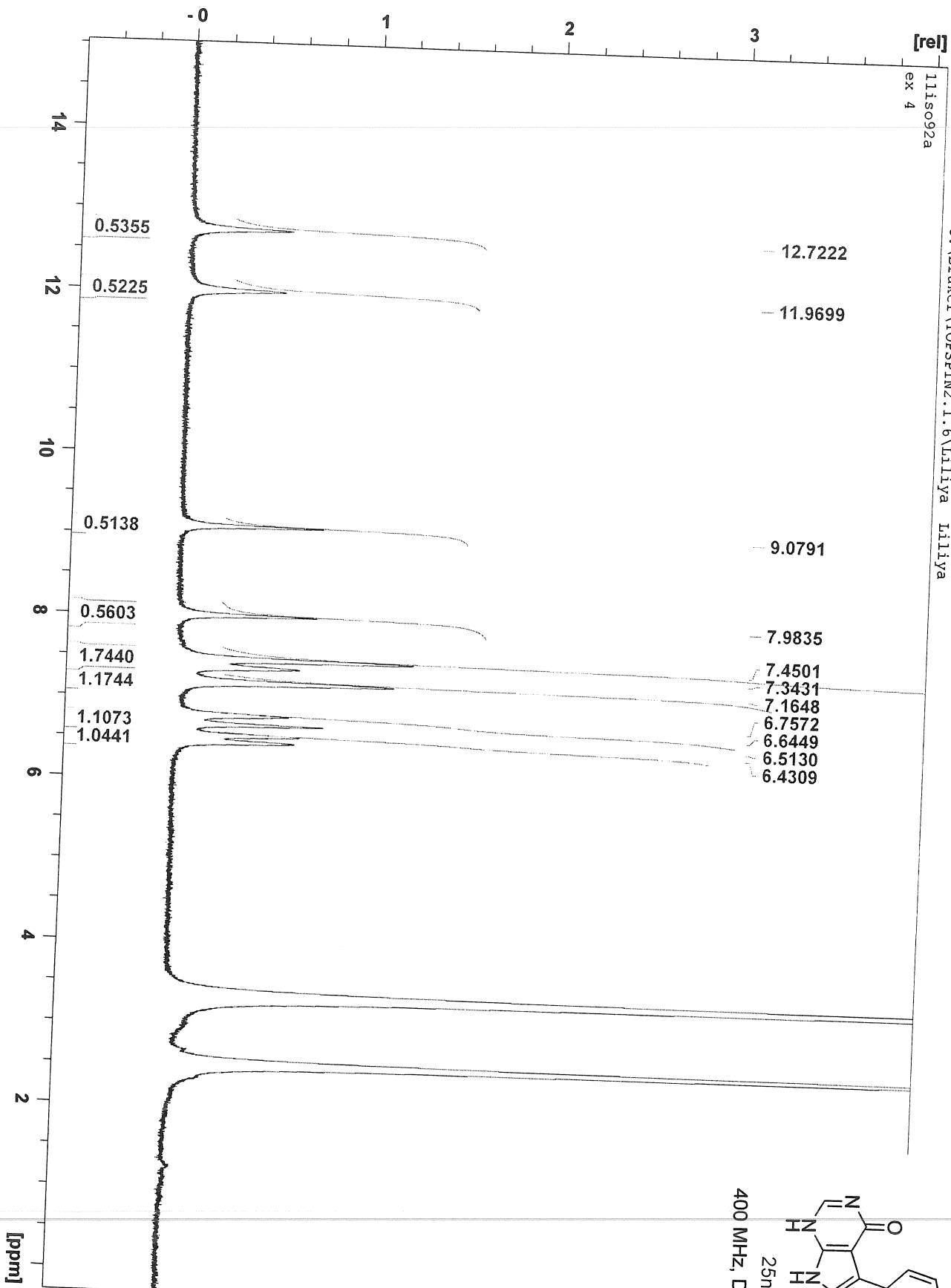
```

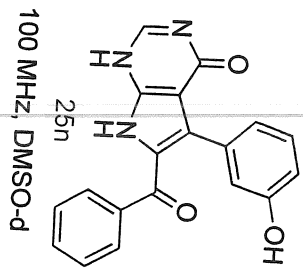
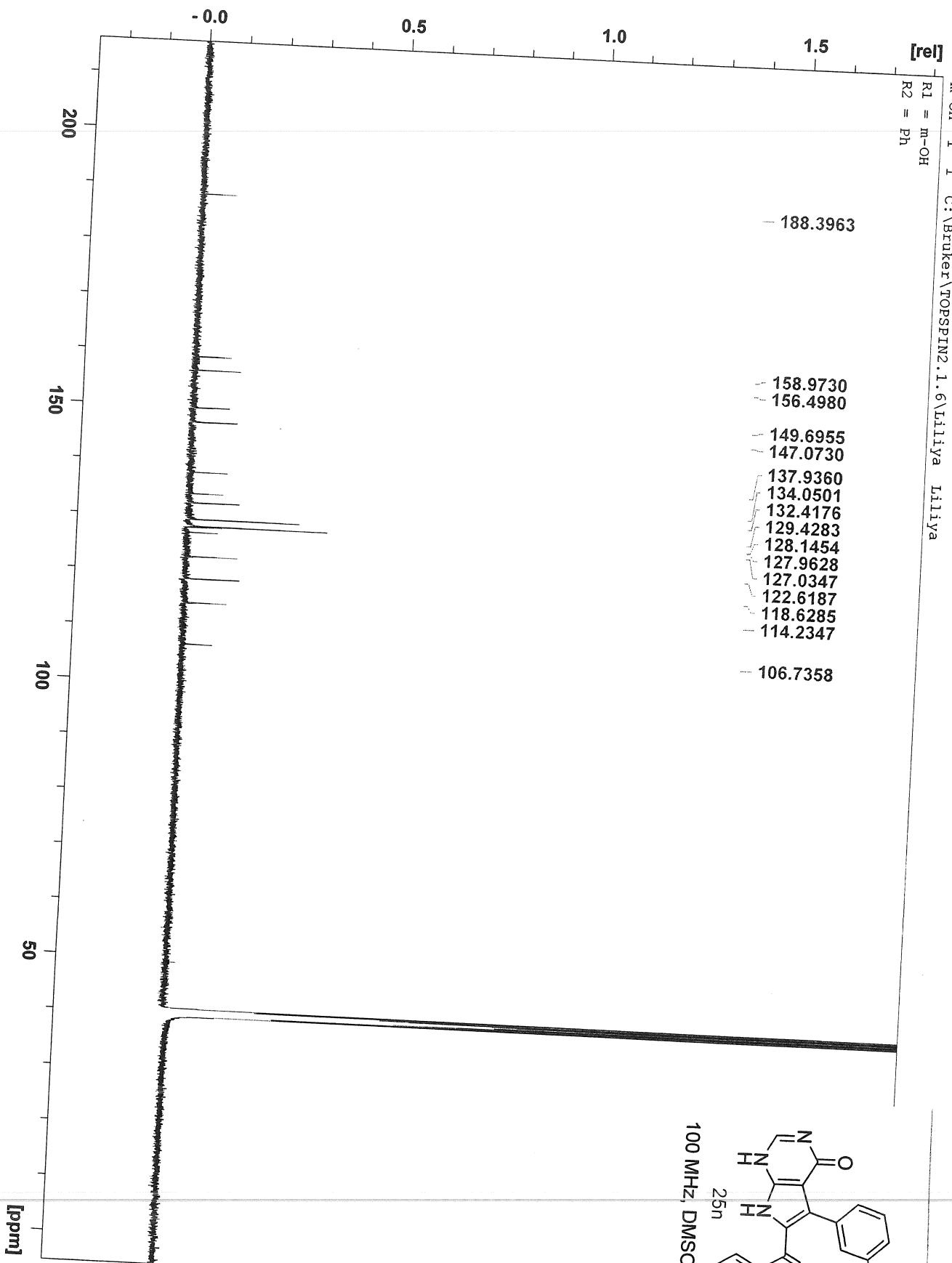


75 MHz, DMSO-d

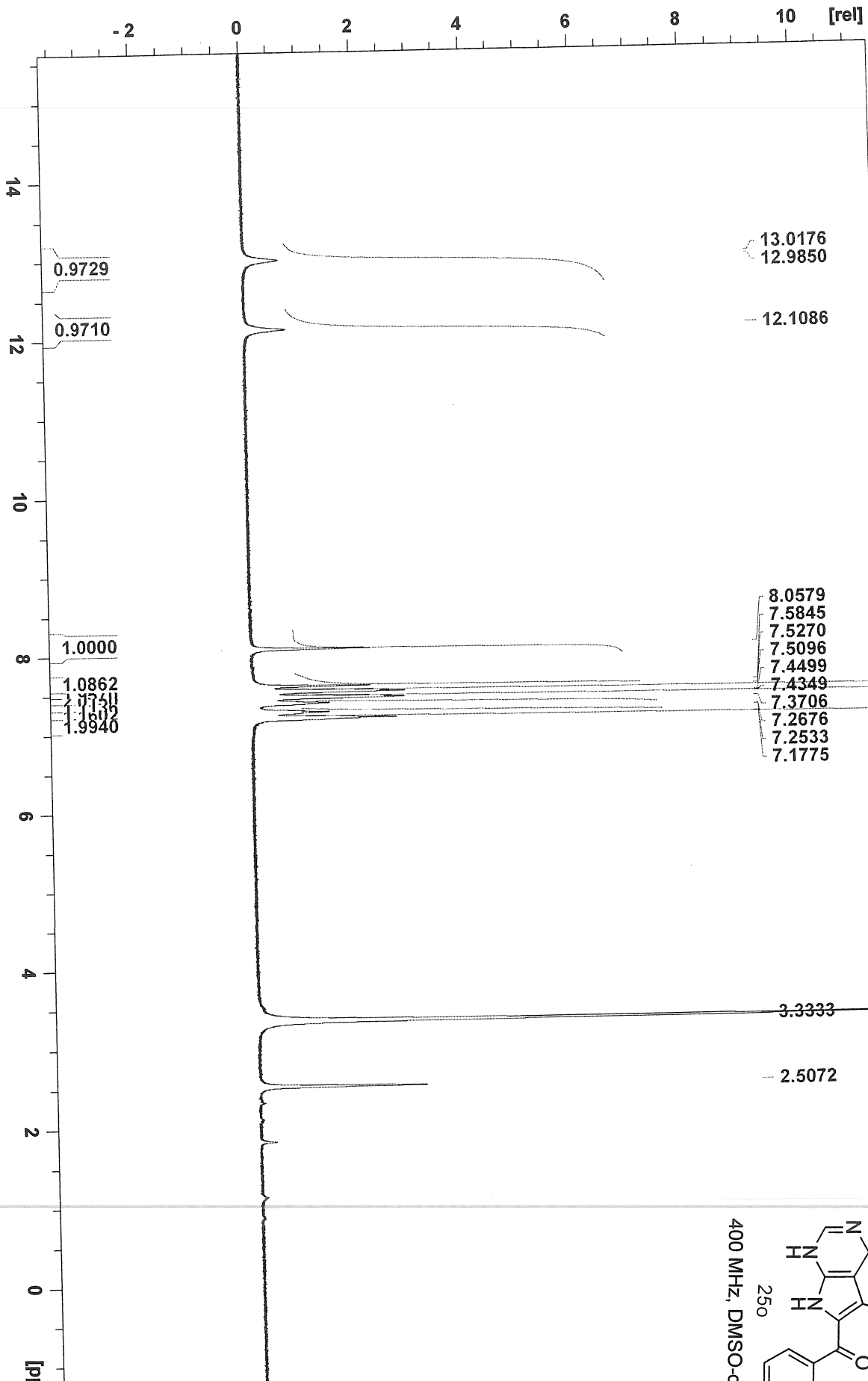
25m



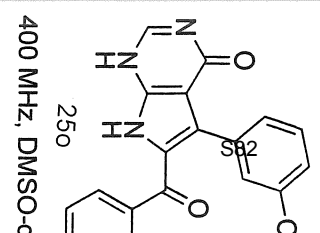


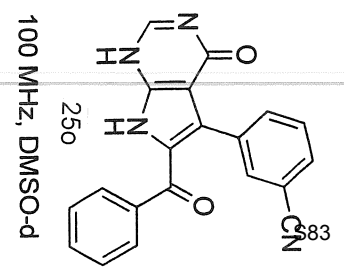
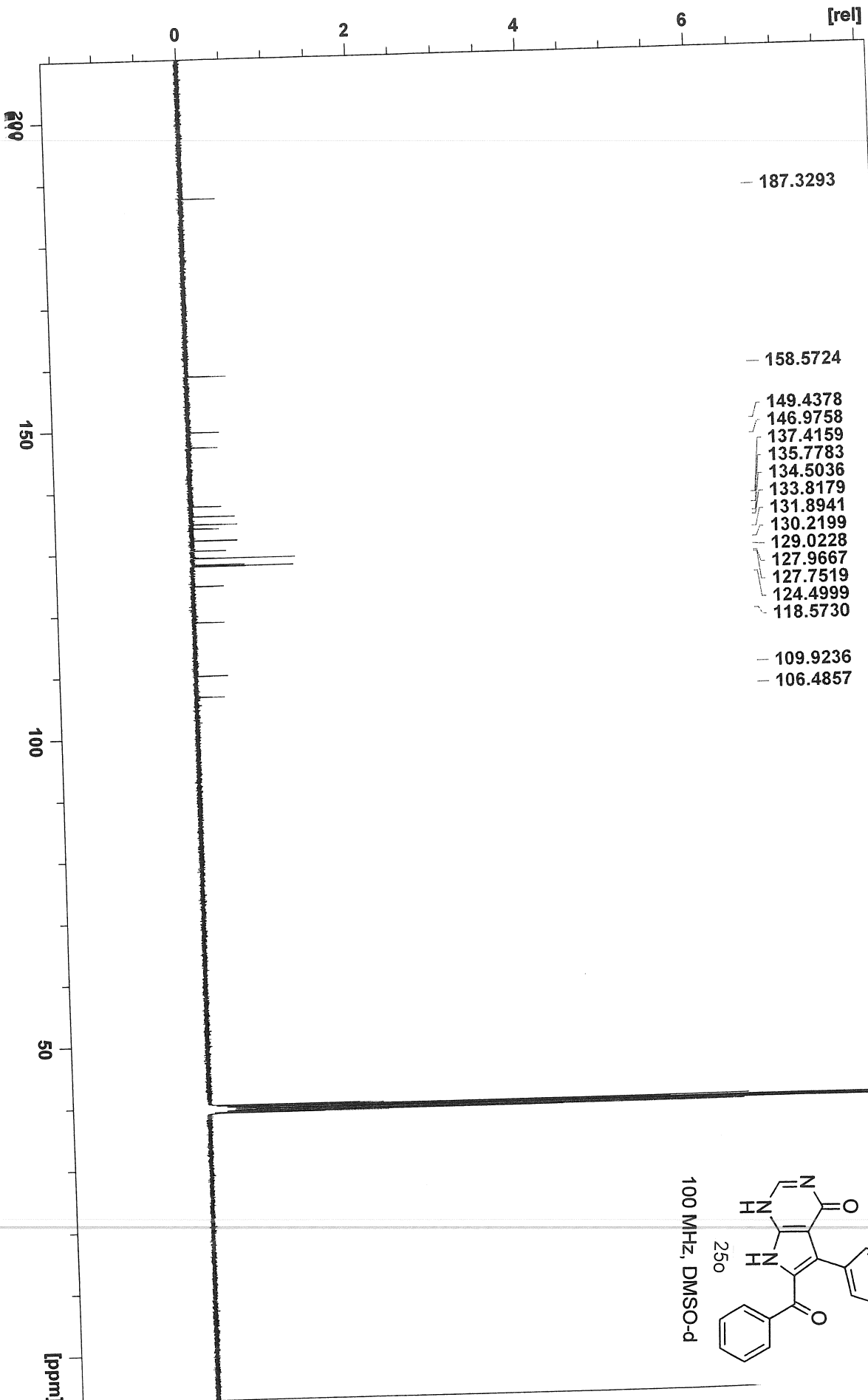


m-OH 1 1 C:\Bruker\TOPSPIN2.1.6\Lillya Lillya
 R1 = m-OH
 R2 = Ph

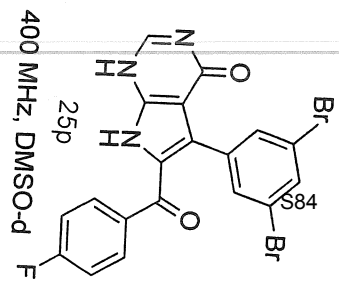
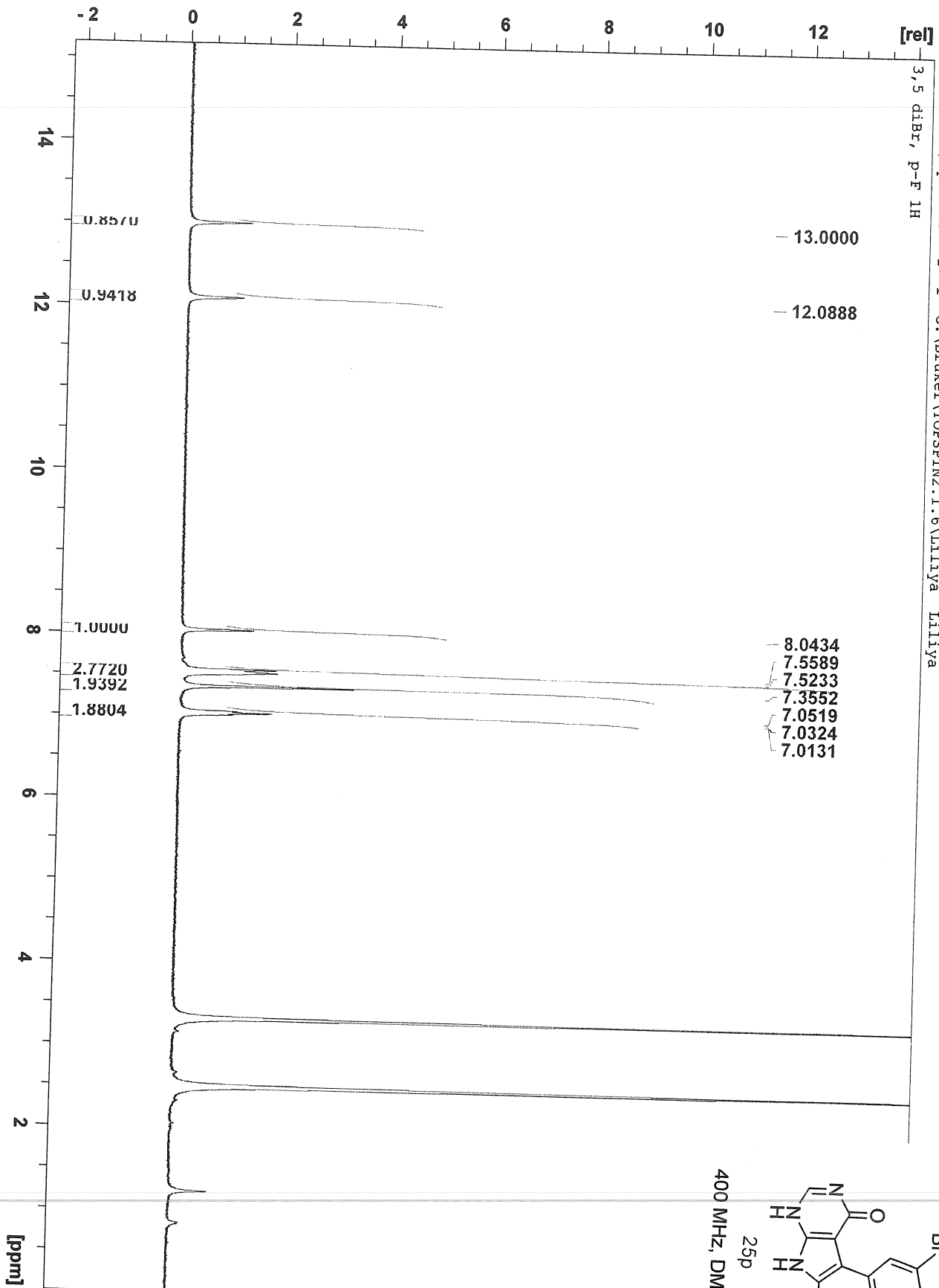


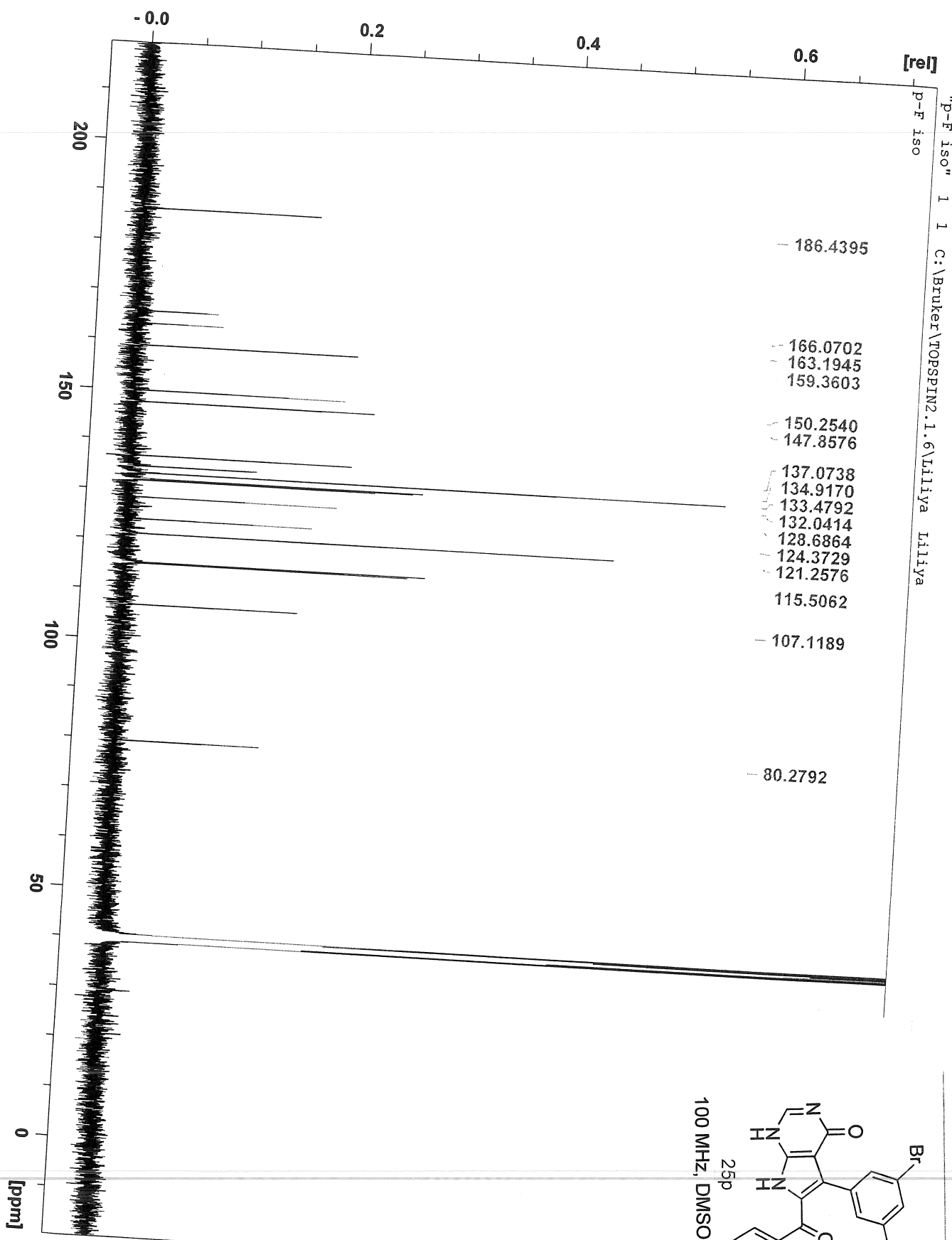
Rig-CN-H2O 1 1 C:\Bruker\TOPSPIN2.1.6\lillya lillya



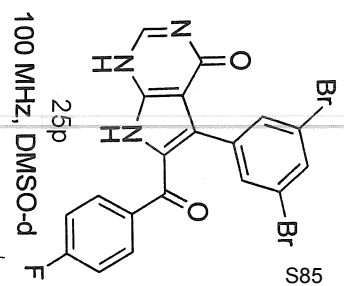


Rig-CN-H2O-C13 1 1 C:\Bruker\TOPSPIN2.1.6\lilija lilija





"p-F iso" 1 1 C:\Bruker\TOPSPIN2.1.6\Lillya Lillya
p-F iso





```

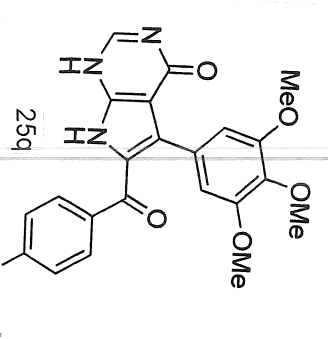
Filename = 1d_spectrwm-331.jdf 03
Author = alex
Experiment = single_pulse.exp
Sample id = S#372562
Solvent = DMSO-d6
Creation_time = 14-APR-2011 10:17:45
Revision_time = 14-APR-2011 10:30:48
Current_time = 14-APR-2011 10:31:01
  
```

```

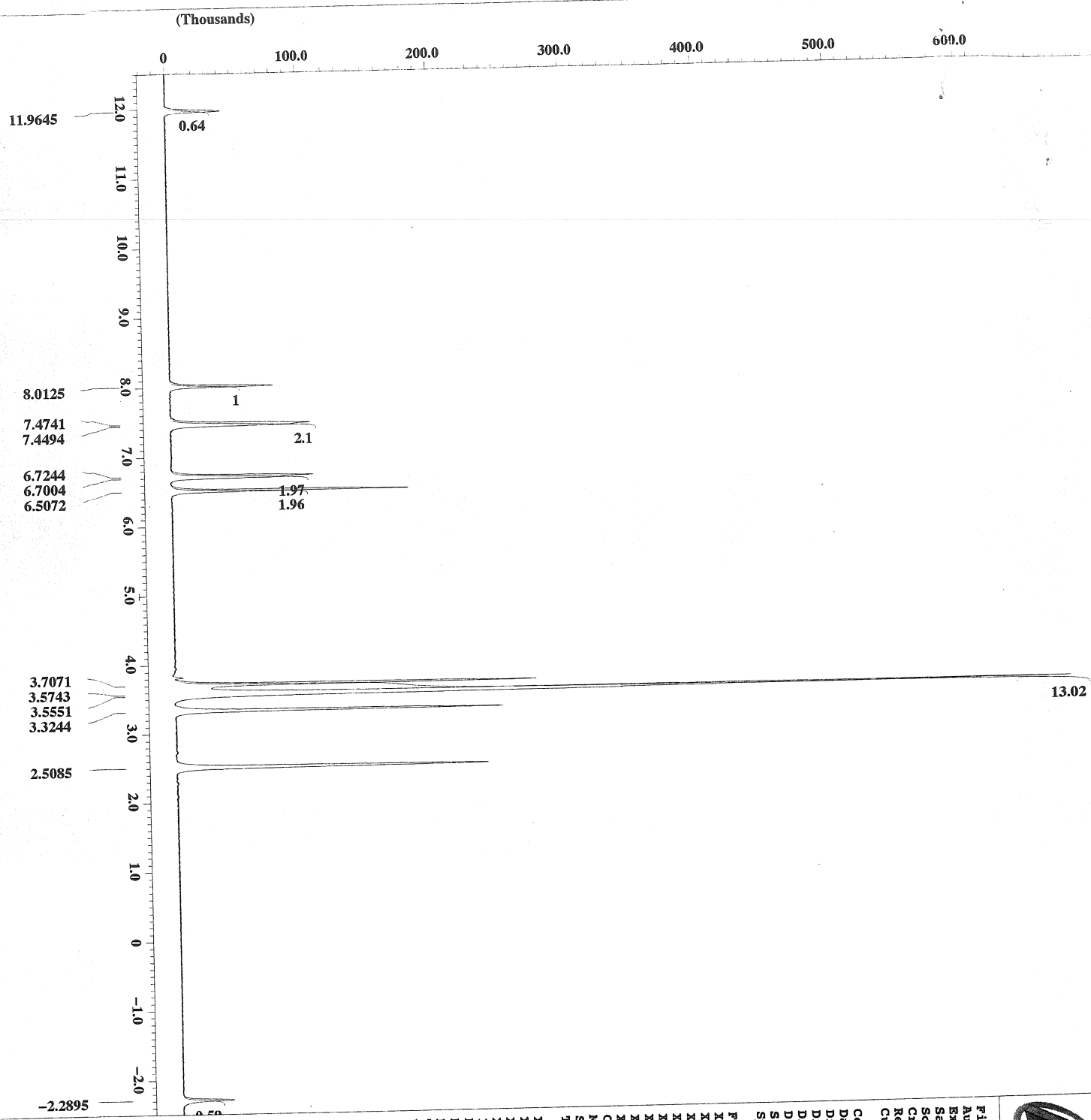
Comment = Single Pulse Experiment
Data format = ID RENTL
Dim size = 16384
Dim title = 1H
Dim units = [ppm]
Dimensions = X Eclipse+ 300
Site = DELTA_NMR
Spectrometer =
  
```

```

Field strength = 7.0586013[T] (300)[MHZ]
X_acq_duration = 3.6339712[rs]
X_domain = 1H
X_freq = 300.52965592[MHZ]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 0
X_resolution = 0.27518105[Hz]
X_sweep = FALSE
X_return = 1
Mod return = 32
Scans = 32
Total_scans = 32
X_90_width = 16[us]
X_acq_time = 3.6339712[rs]
X_angle = 45[deg]
X_pulse = 8[us]
Initial wait = 1[rs]
Phase preset = 3[us]
Recvr_gain = 15
Relaxation_delay = 4[rs]
Temp_get = 24.1[dc]
Unblank_time = 2[us]
  
```



X : parts per Million : 1H



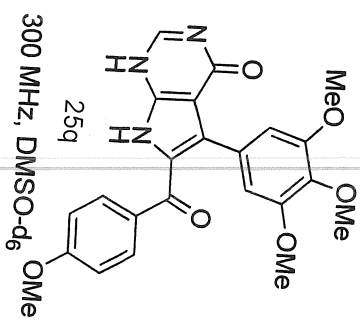
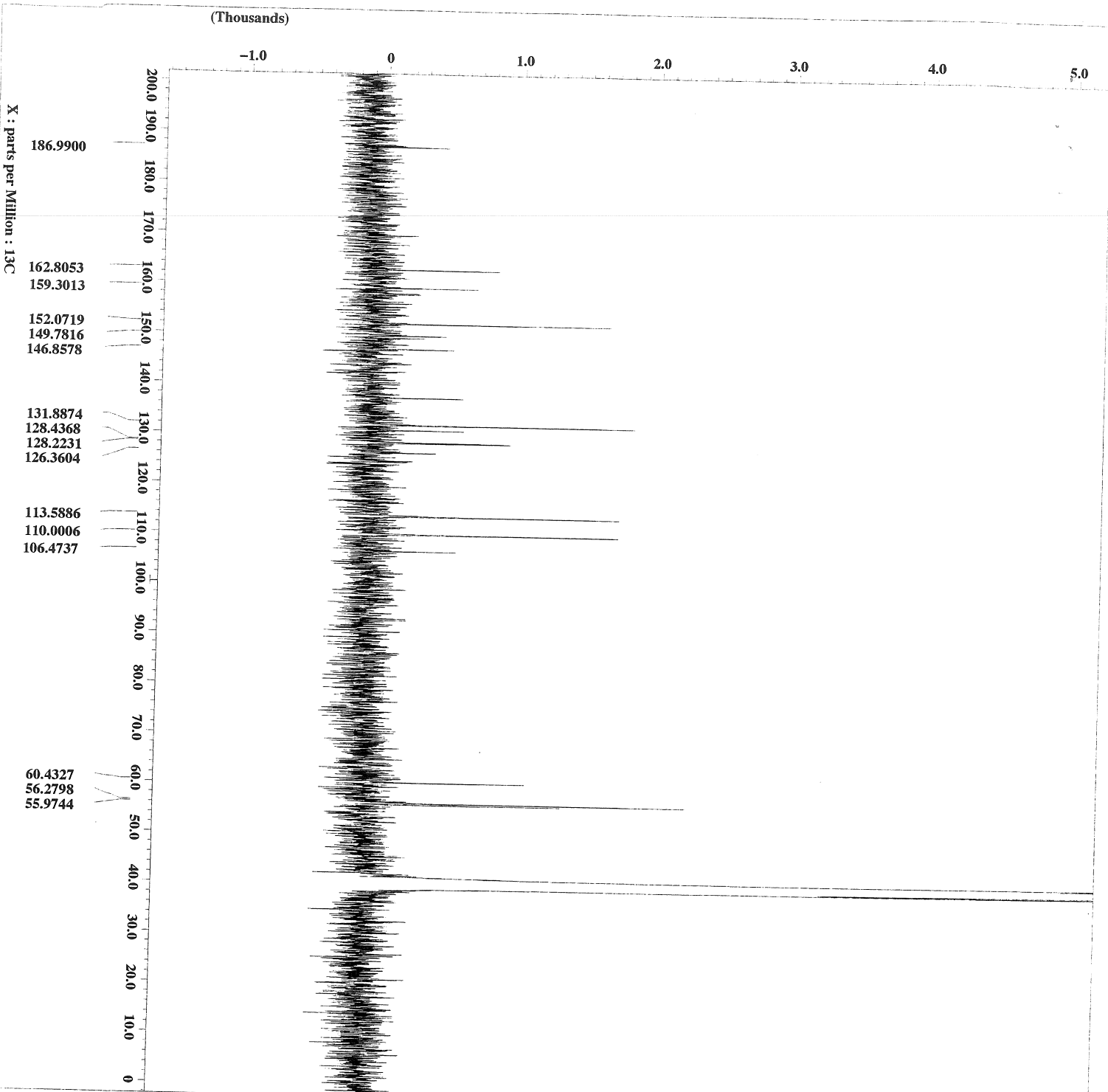
```

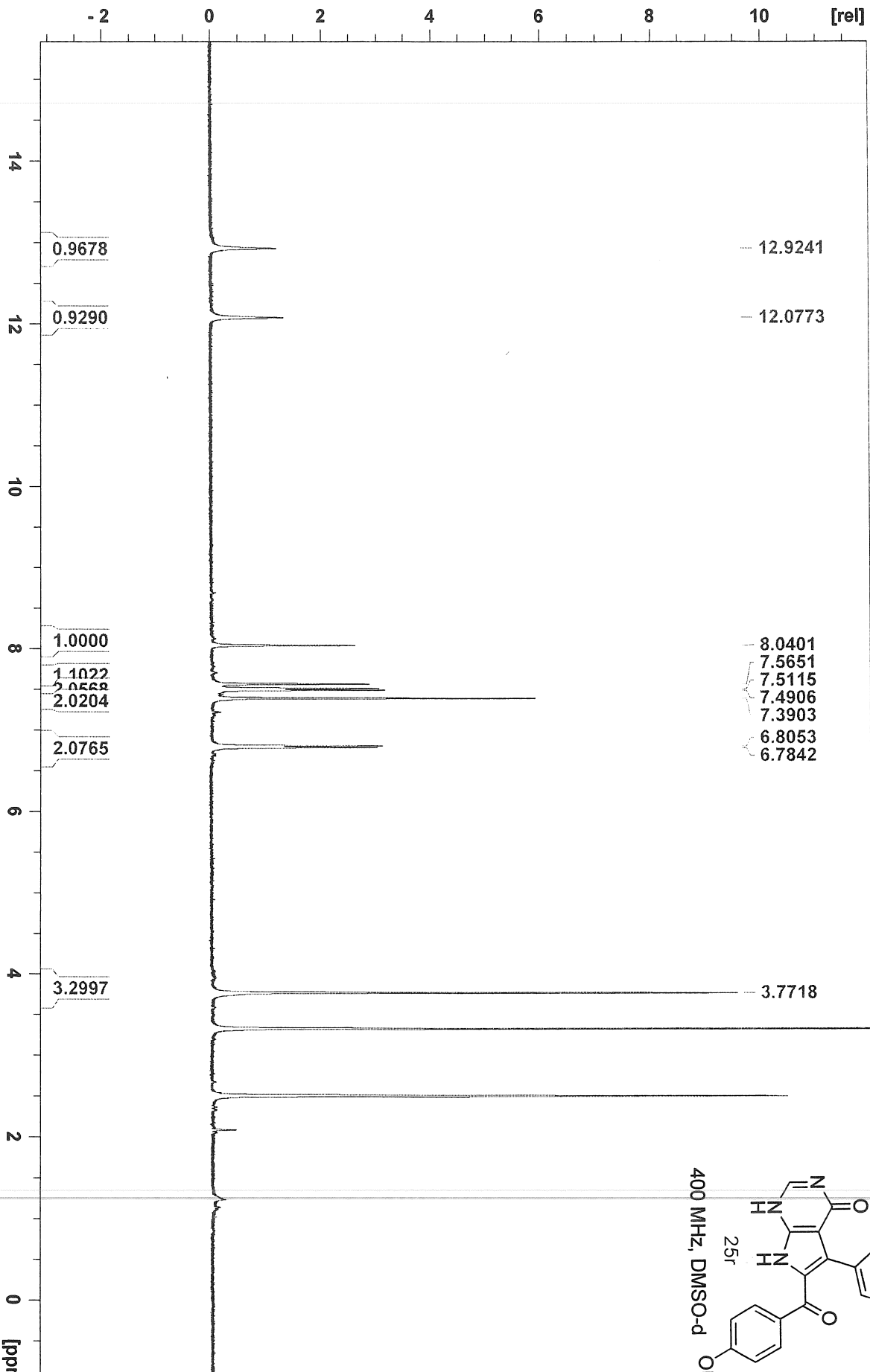
Filename = 1d_13c_spectrum-163.j
Author = alex
Experiment = single_pulse_dec
Sample_id = S649359
Solvent = DMSO-D6
Creation time = 15-APR-2011 09:06:20
Revision time = 15-APR-2011 12:59:20
Current_time = 15-APR-2011 12:59:33

Comment
Data_format = Single Pulse with Bro
ID_COMPLX = ID COMPLEX
Dim_size = 32768
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = Eclipse+ 300
Spectrometer = DELTA_NMR

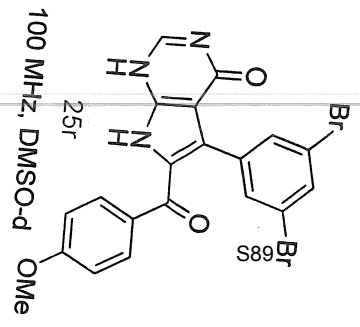
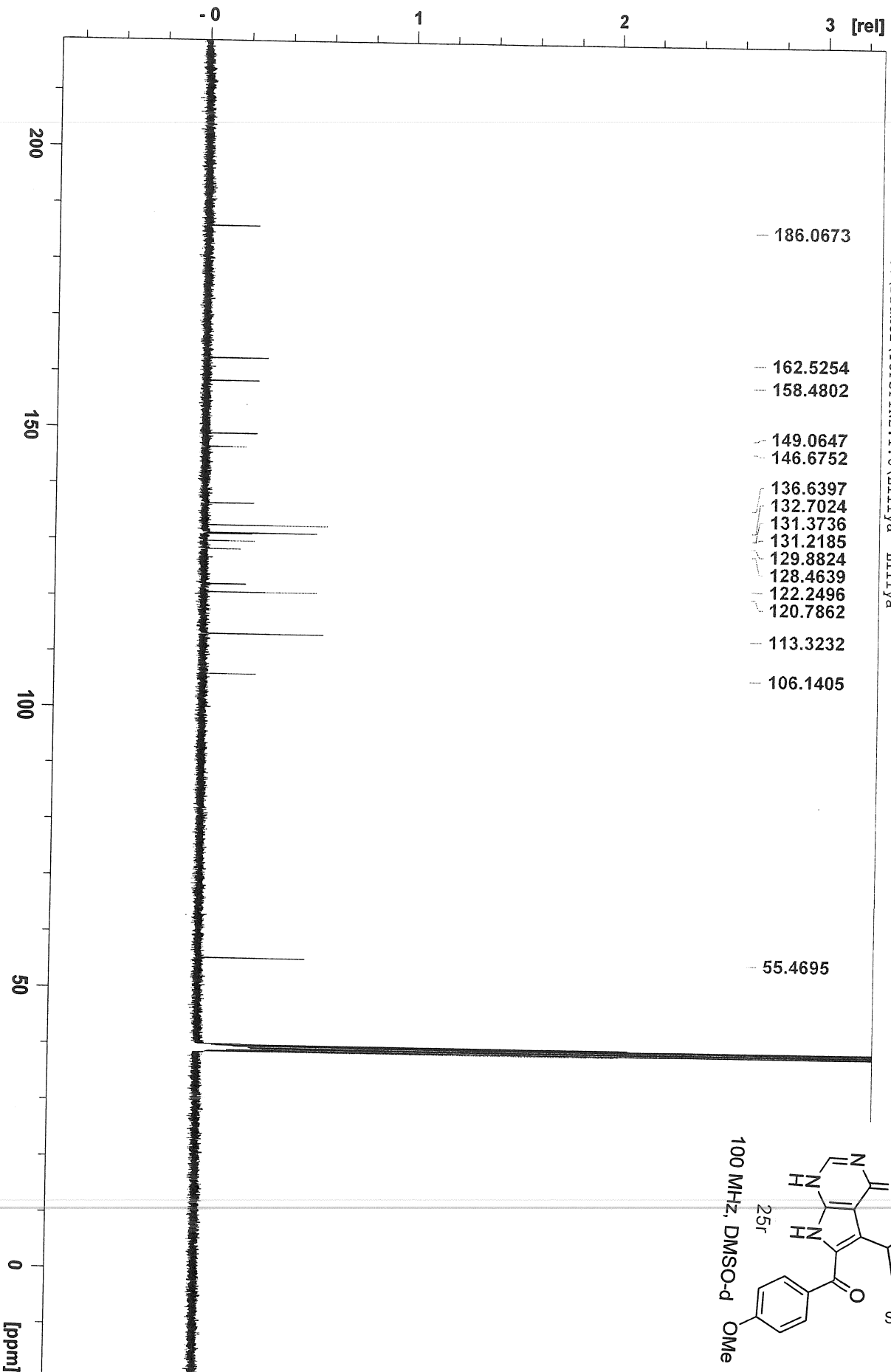
Field_strength = 7.0586013[T] (300[MHz]
X_acq_duration = 1.7334272[ls]
X_domain = 13C
X_freq = 75.56823426[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.57689184[Hz]
X_sweep = 18.90359168[kHz]
Irr_domain = 1H
Irr_freq = 300.52965592[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 20000
Total_scans = 20000

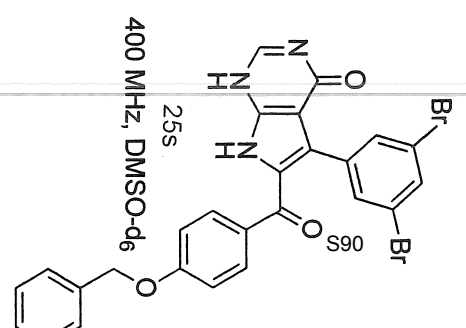
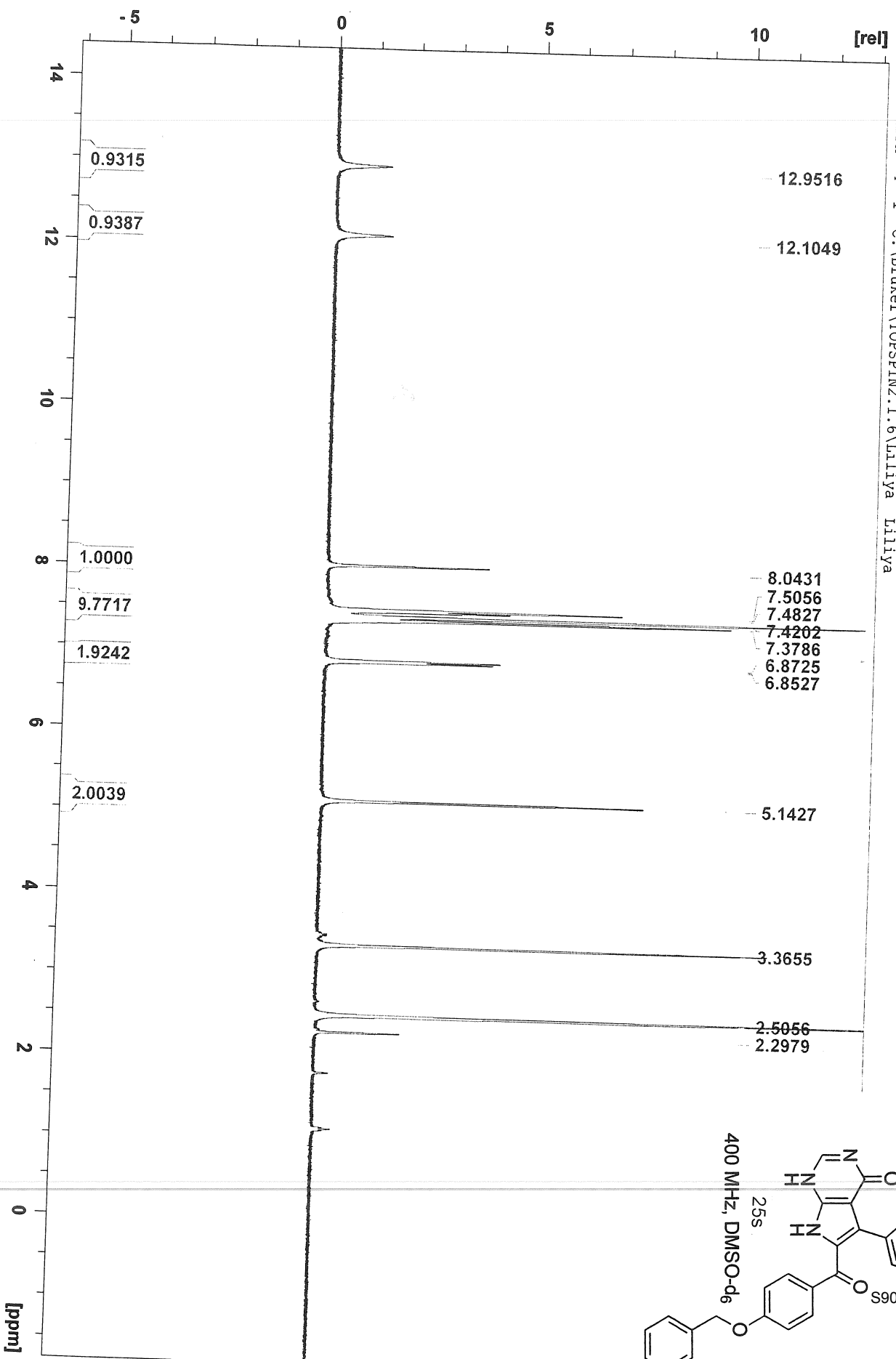
X_90_width = 8.1[us]
X_acq_time = 1.7334272[ls]
X_angle = 30[deg]
X_pulse = 2.7[us]
Initial wait = 1[ls]
Phase_preset = 3[us]
Recvr_gain = 15
Relaxation_delay = 1[ls]
Temp_get = 26[dc]
Unblank time = 2[us]
  
```

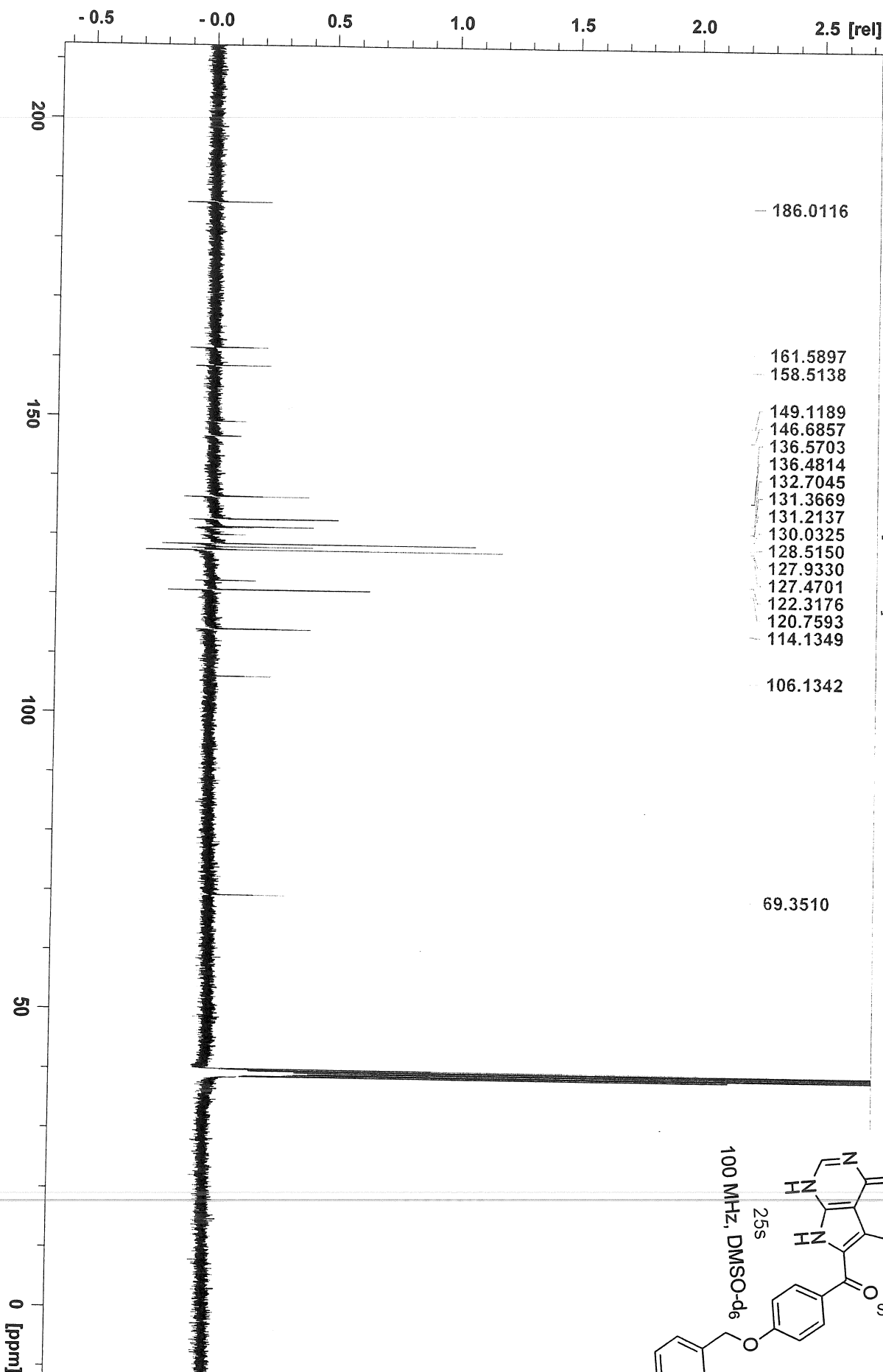




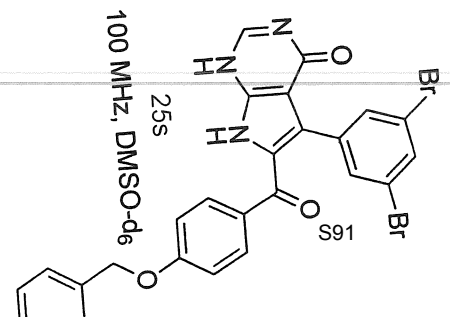
Rid8-OCH3-H1 1 1 C:\Bruker\TOPSPIN2.1.6\Liliya Liliya

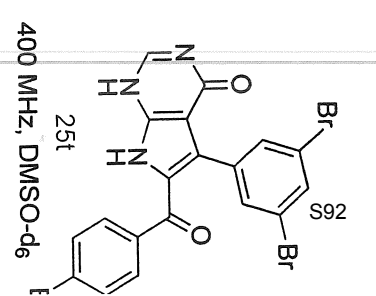
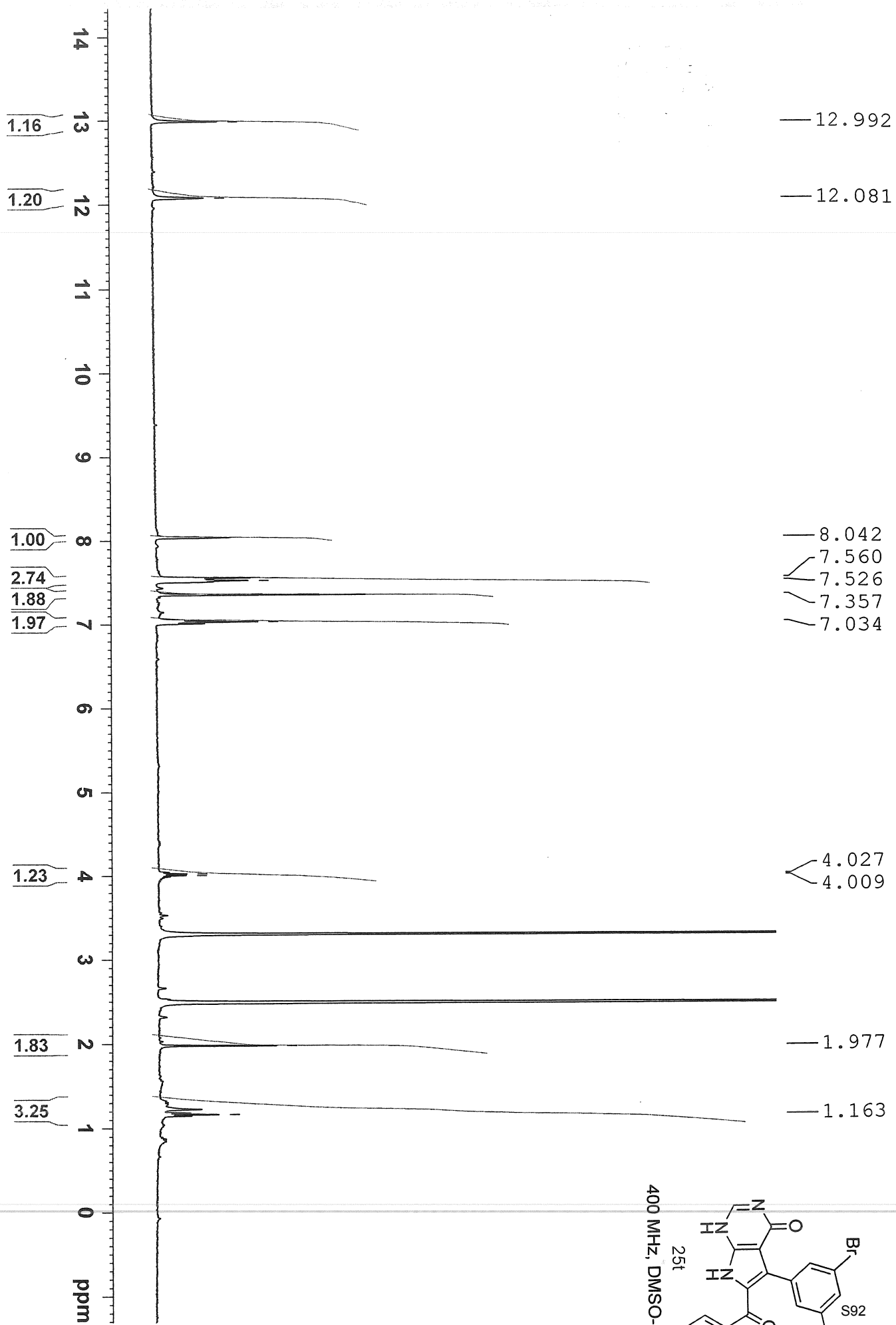


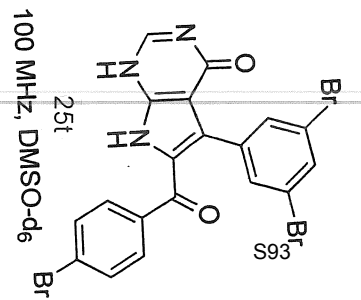
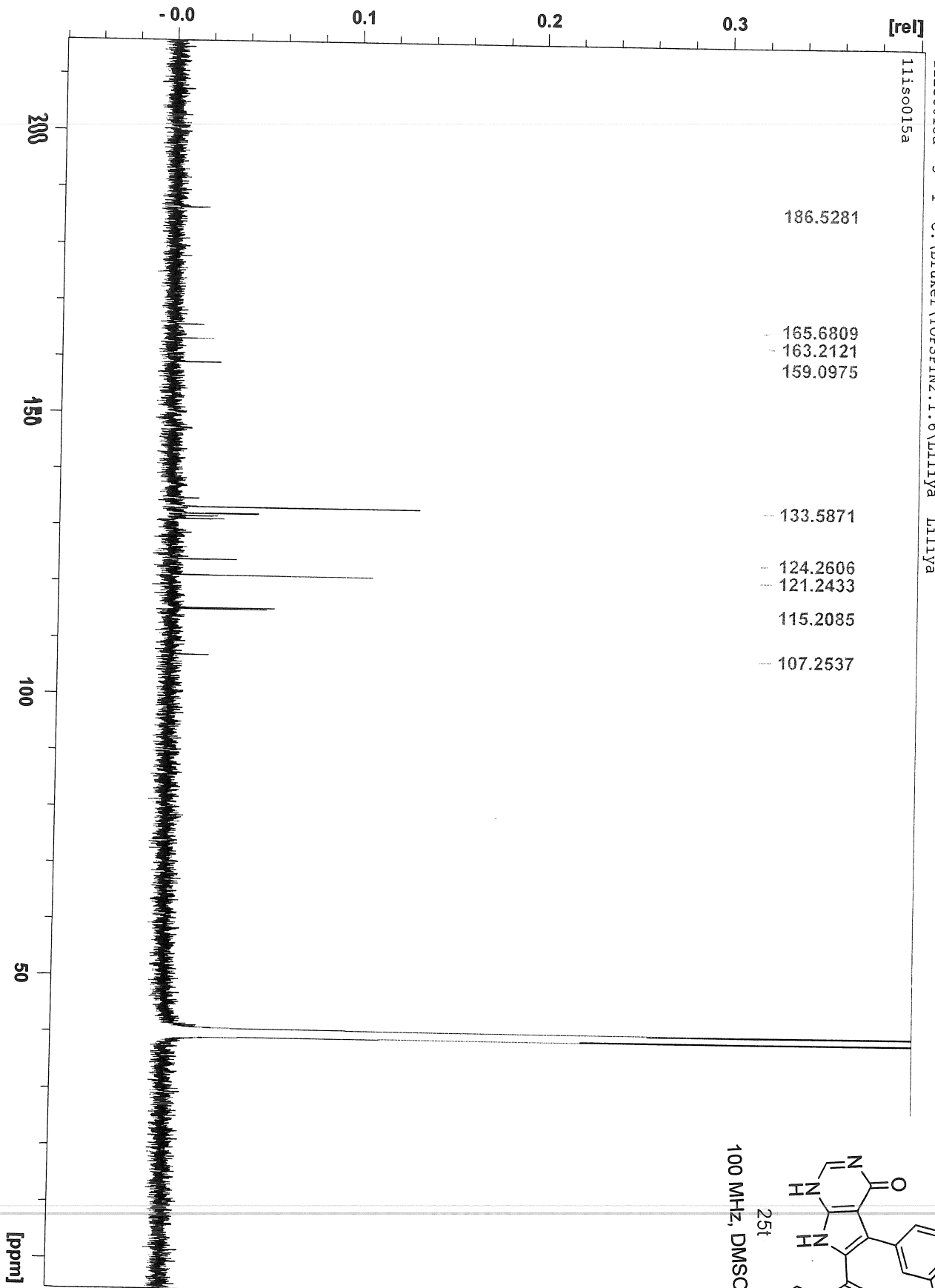


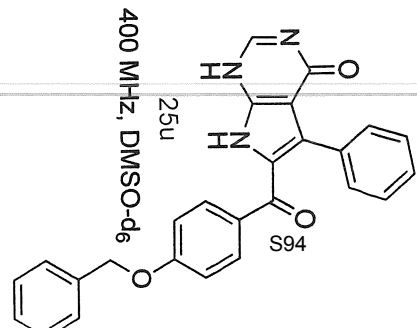
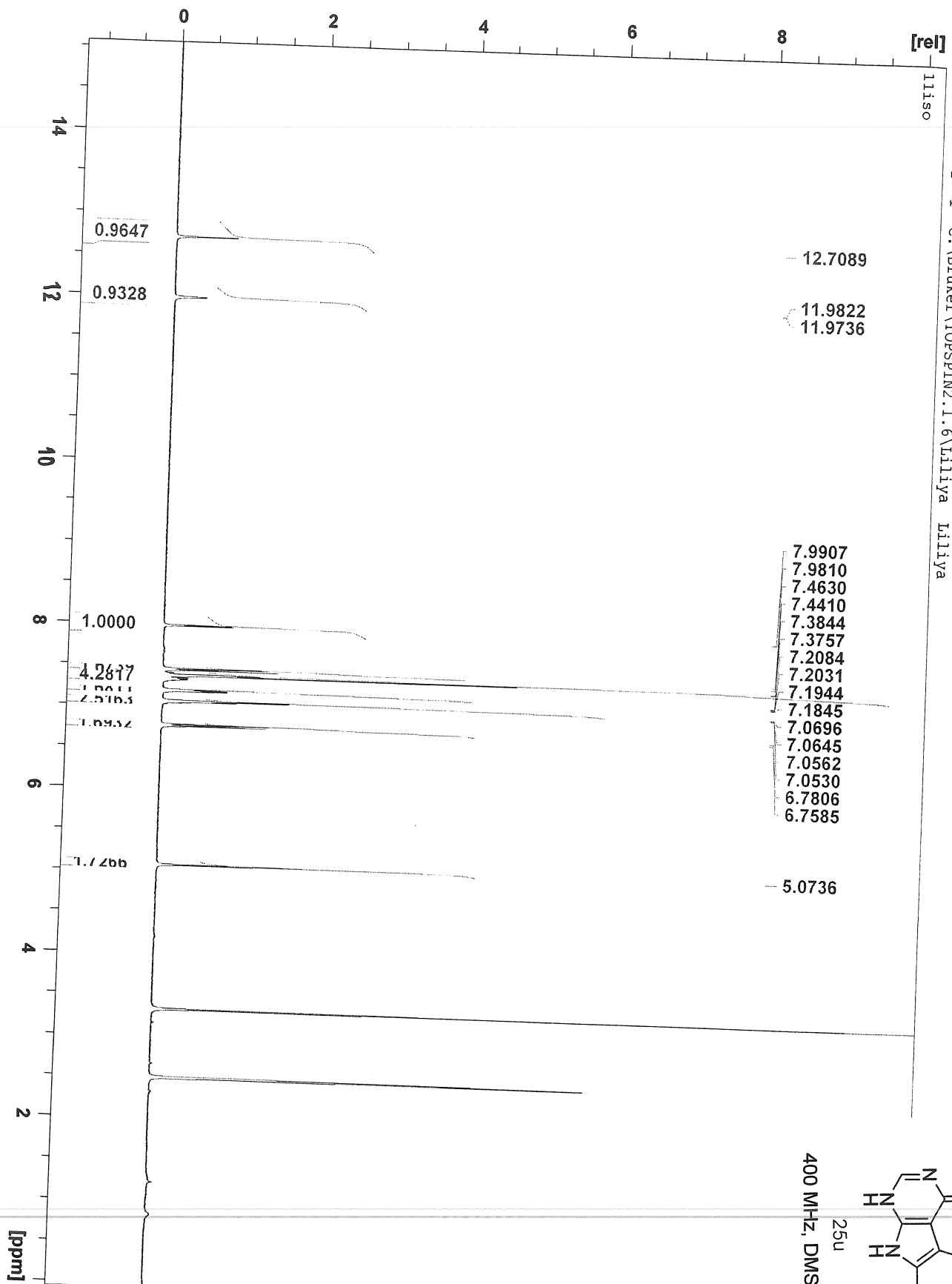


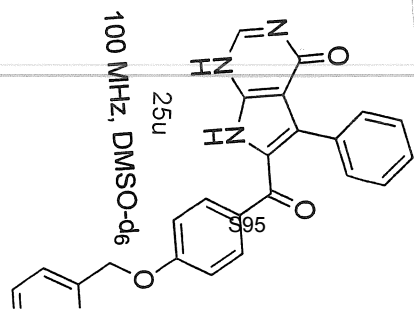
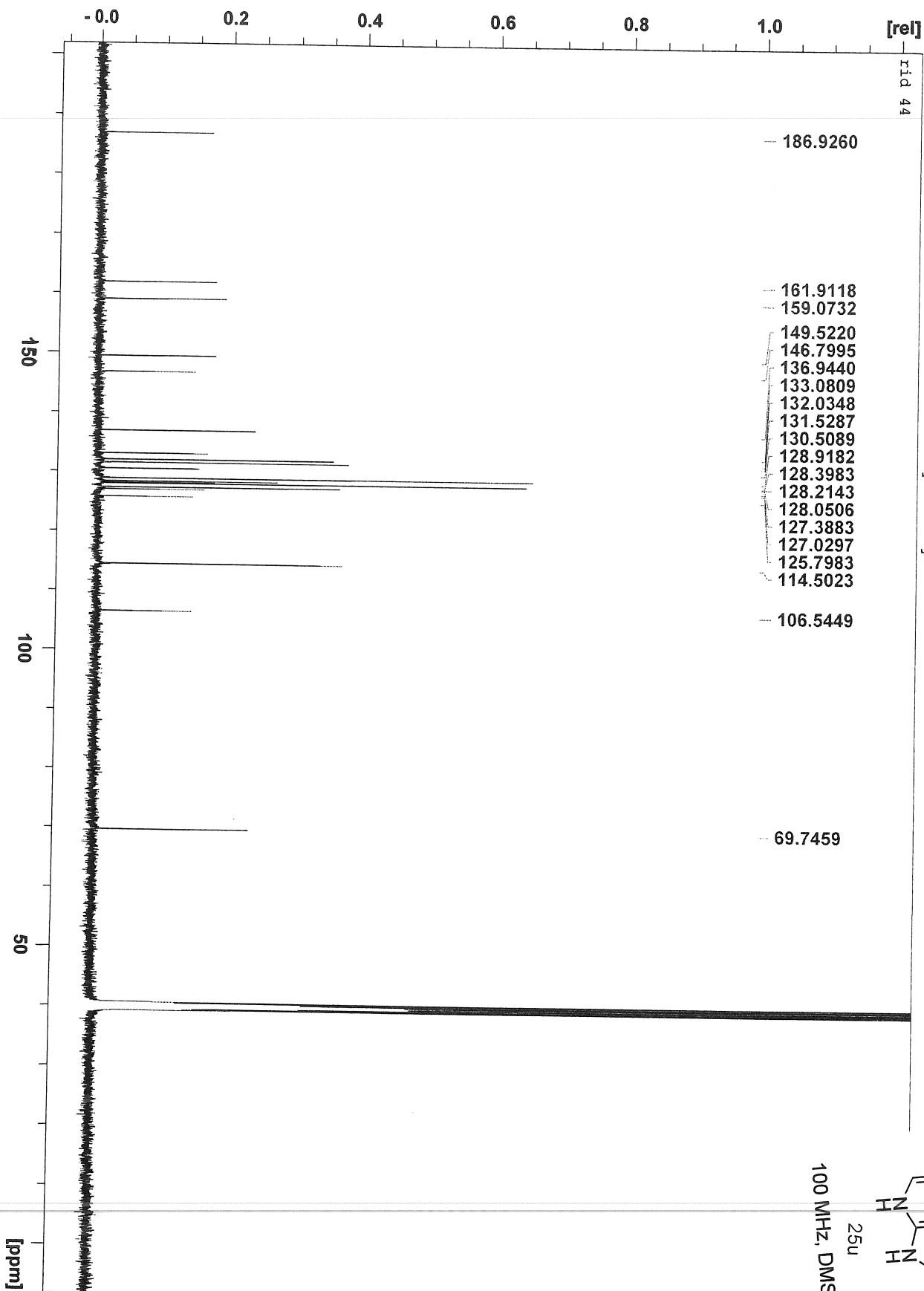
Rid-CH2Ph-C13-2 4 1 C:\Bruker\TOPSPIN2.1.6\Liliya Liliya

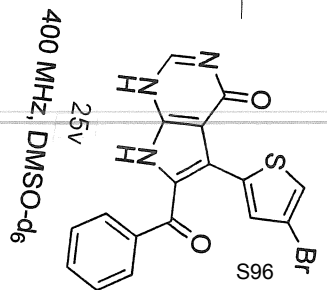
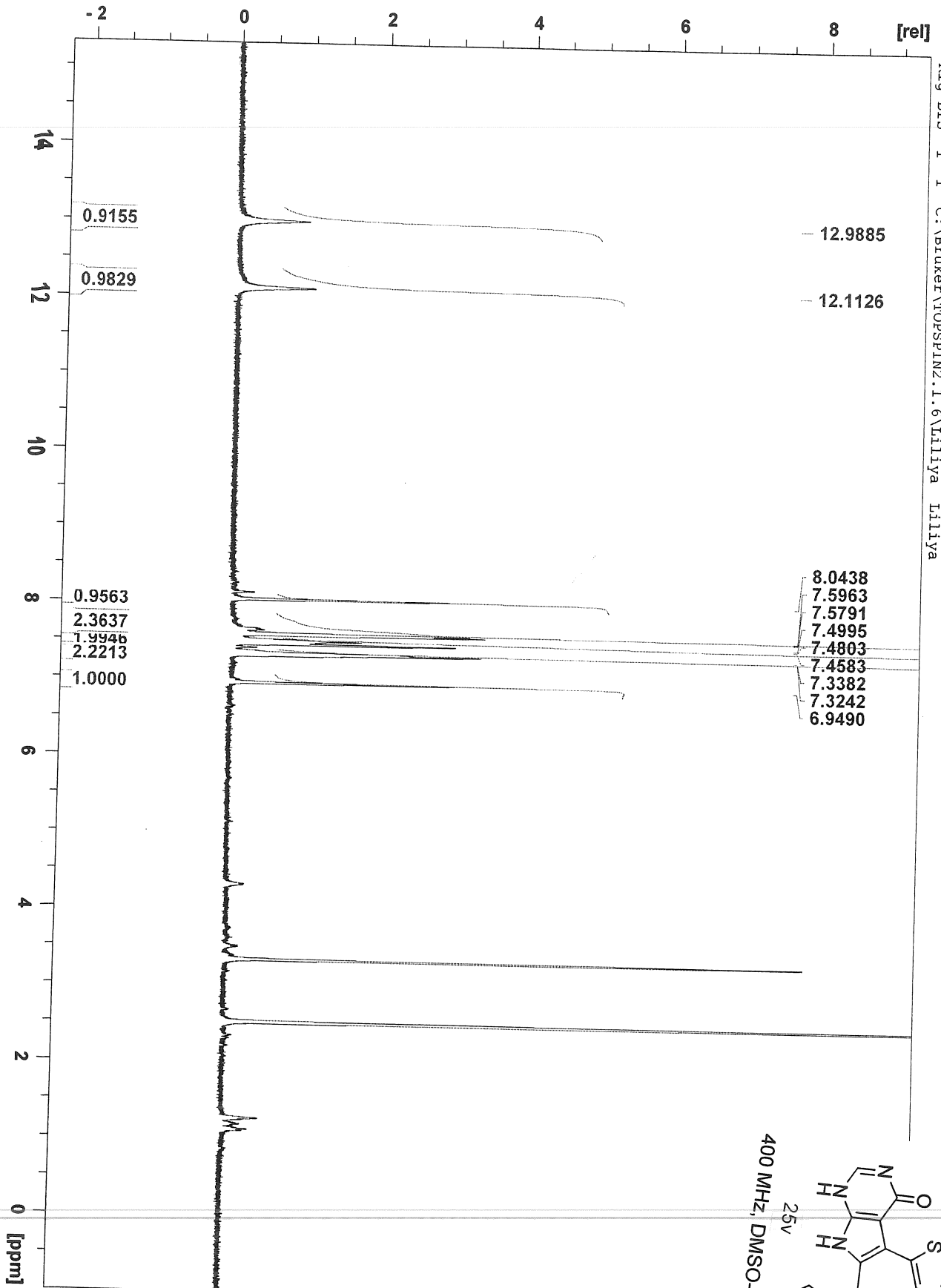


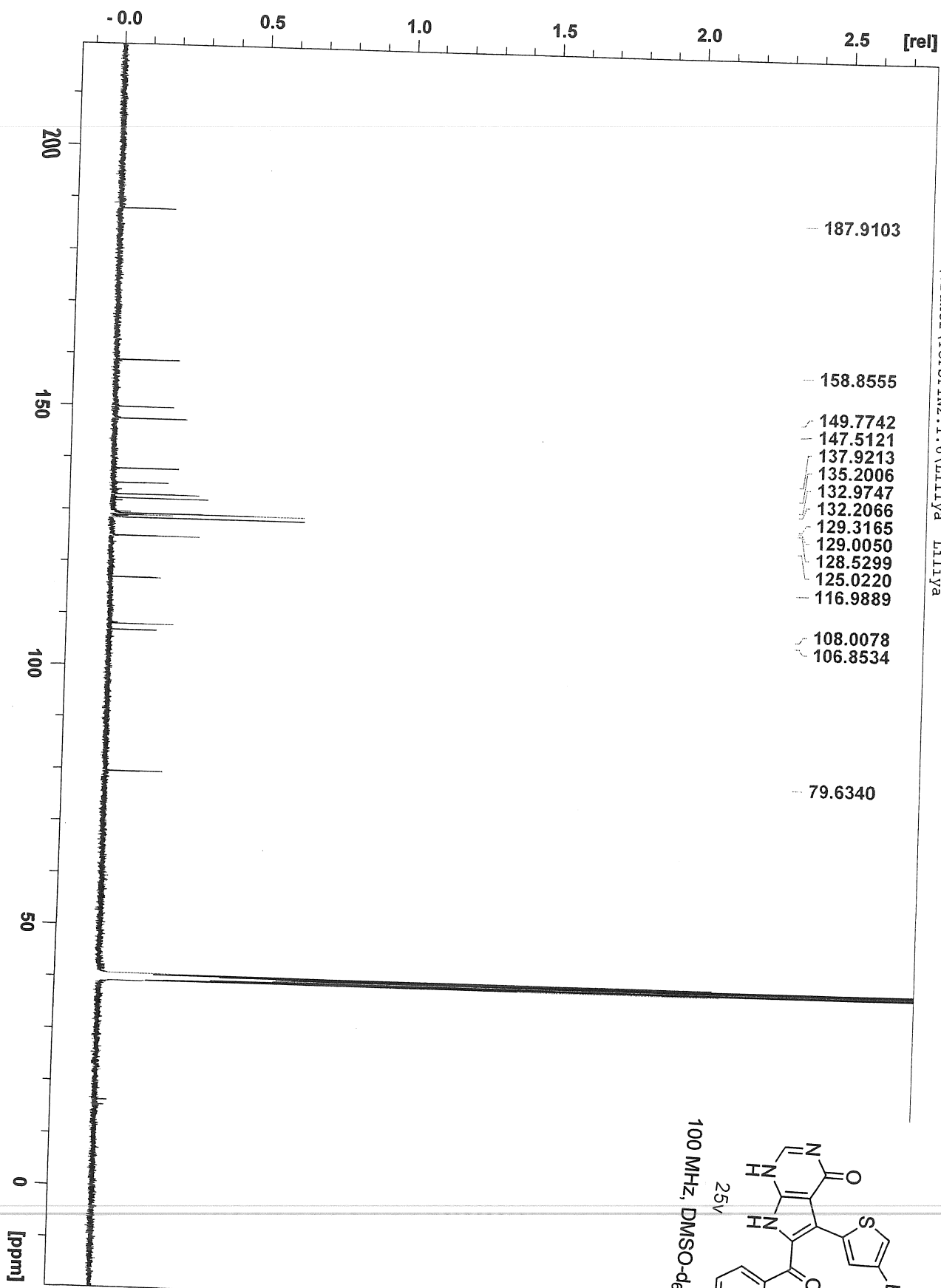


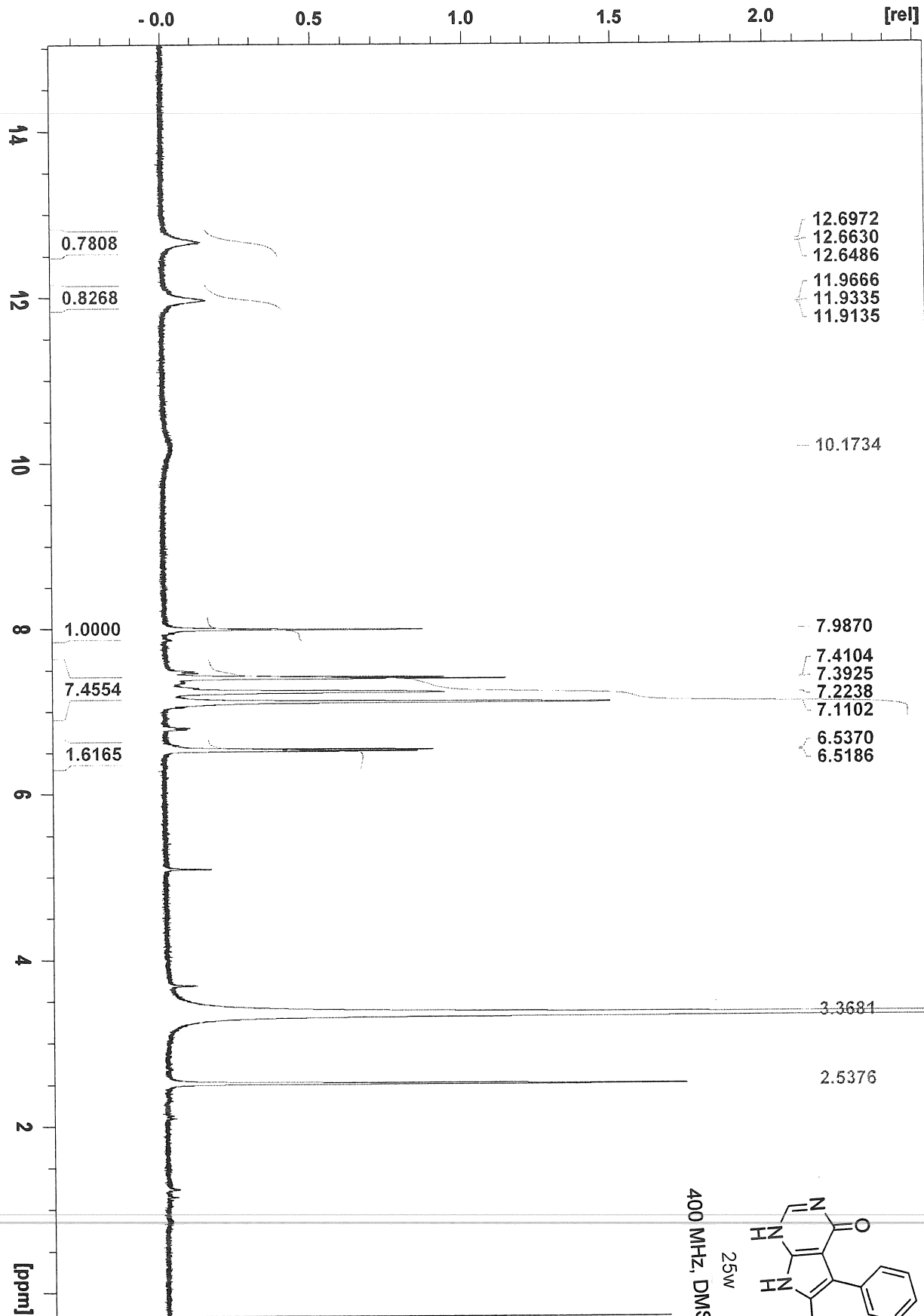




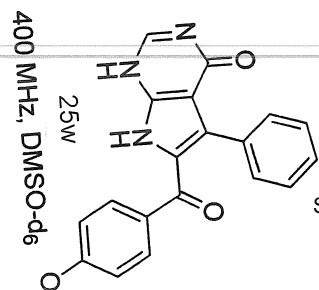


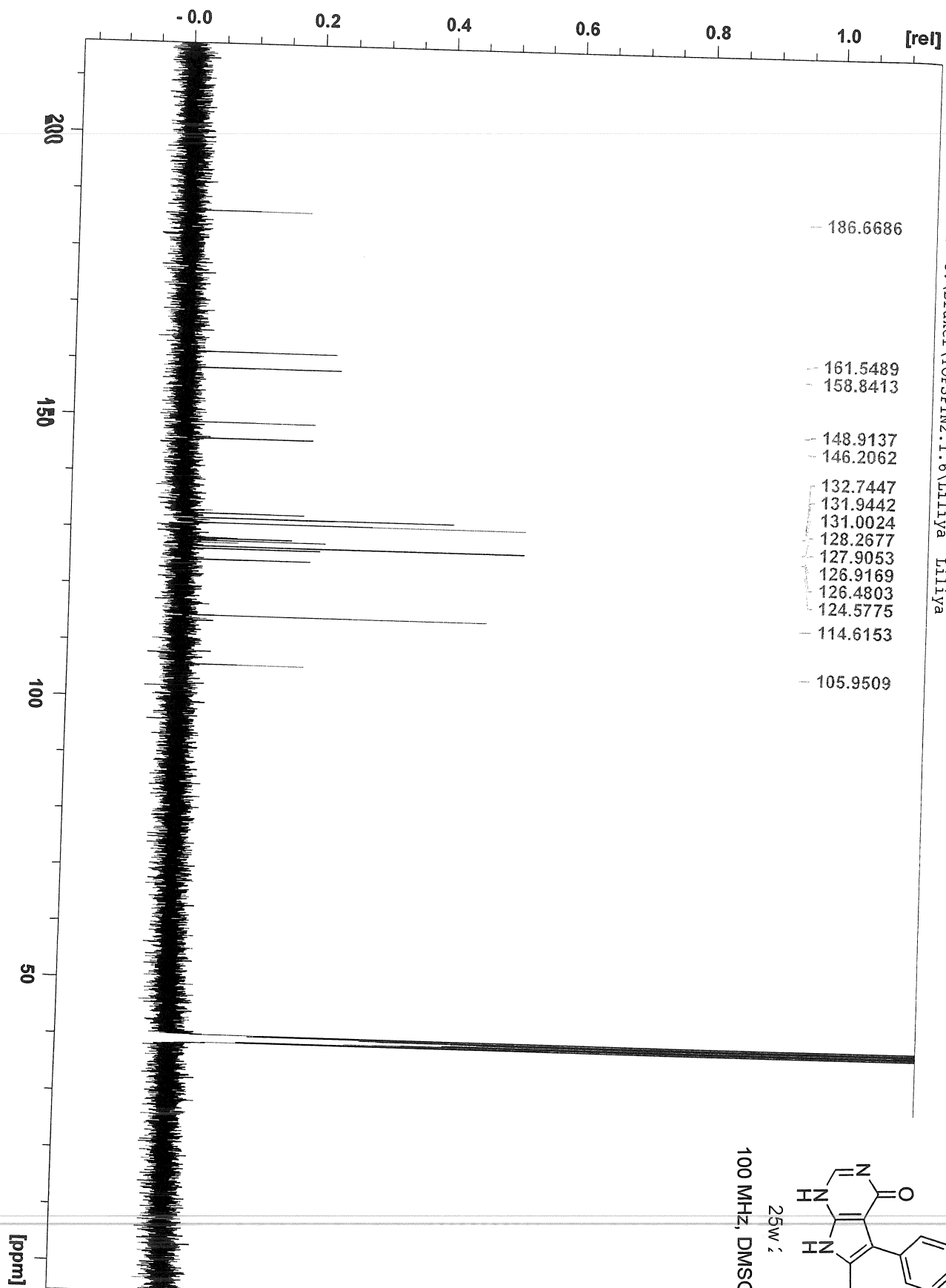




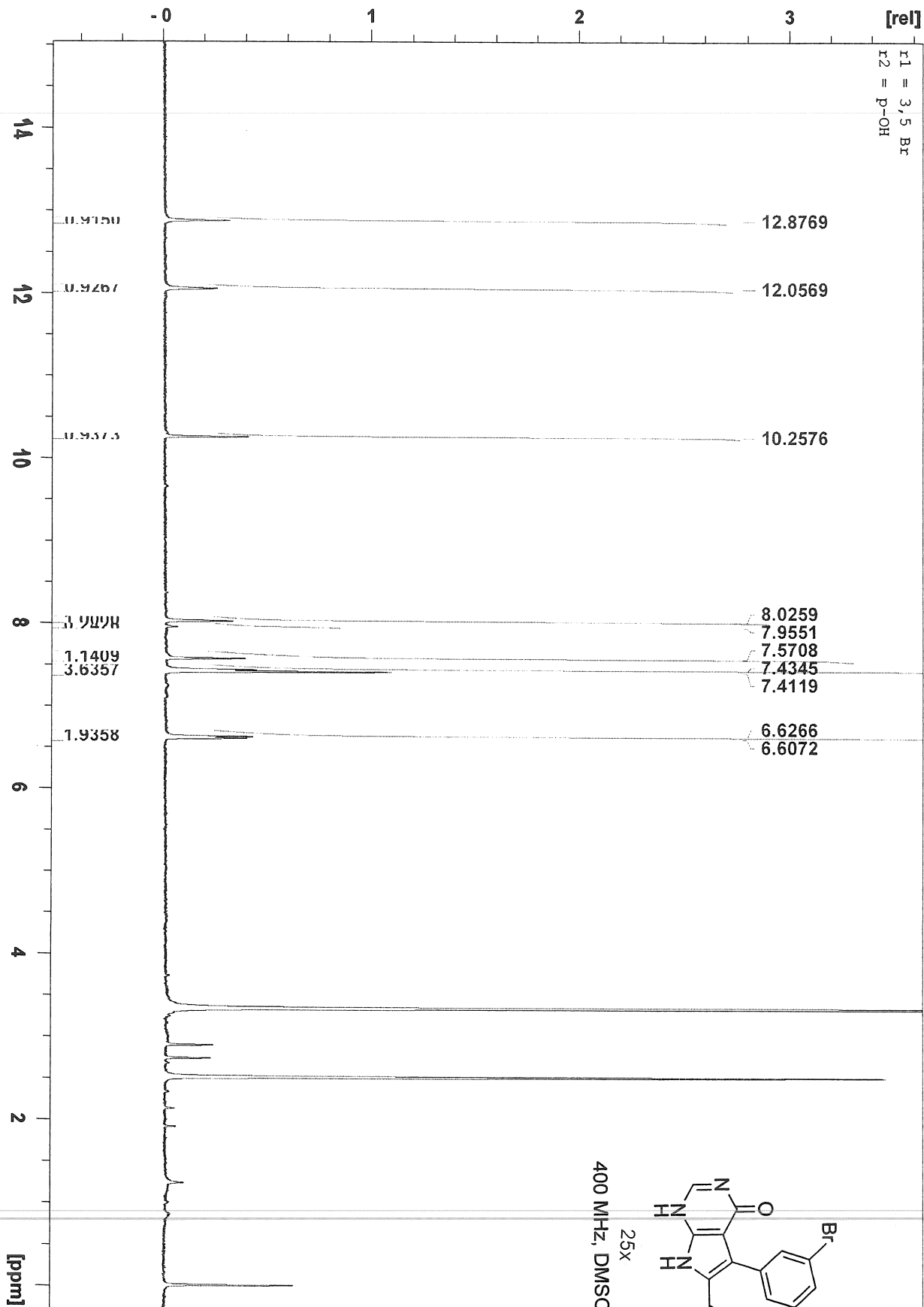


R1g35-OH-H1 2 1 C:\Bruker\TOPSPIN2.1.6\lillya Lillya

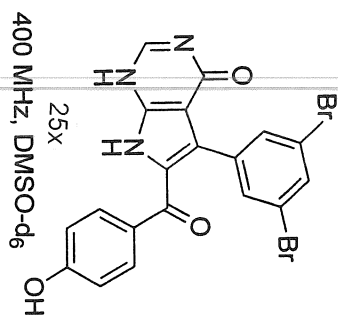


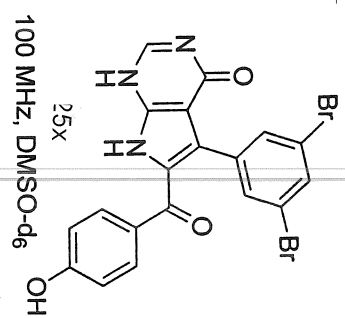
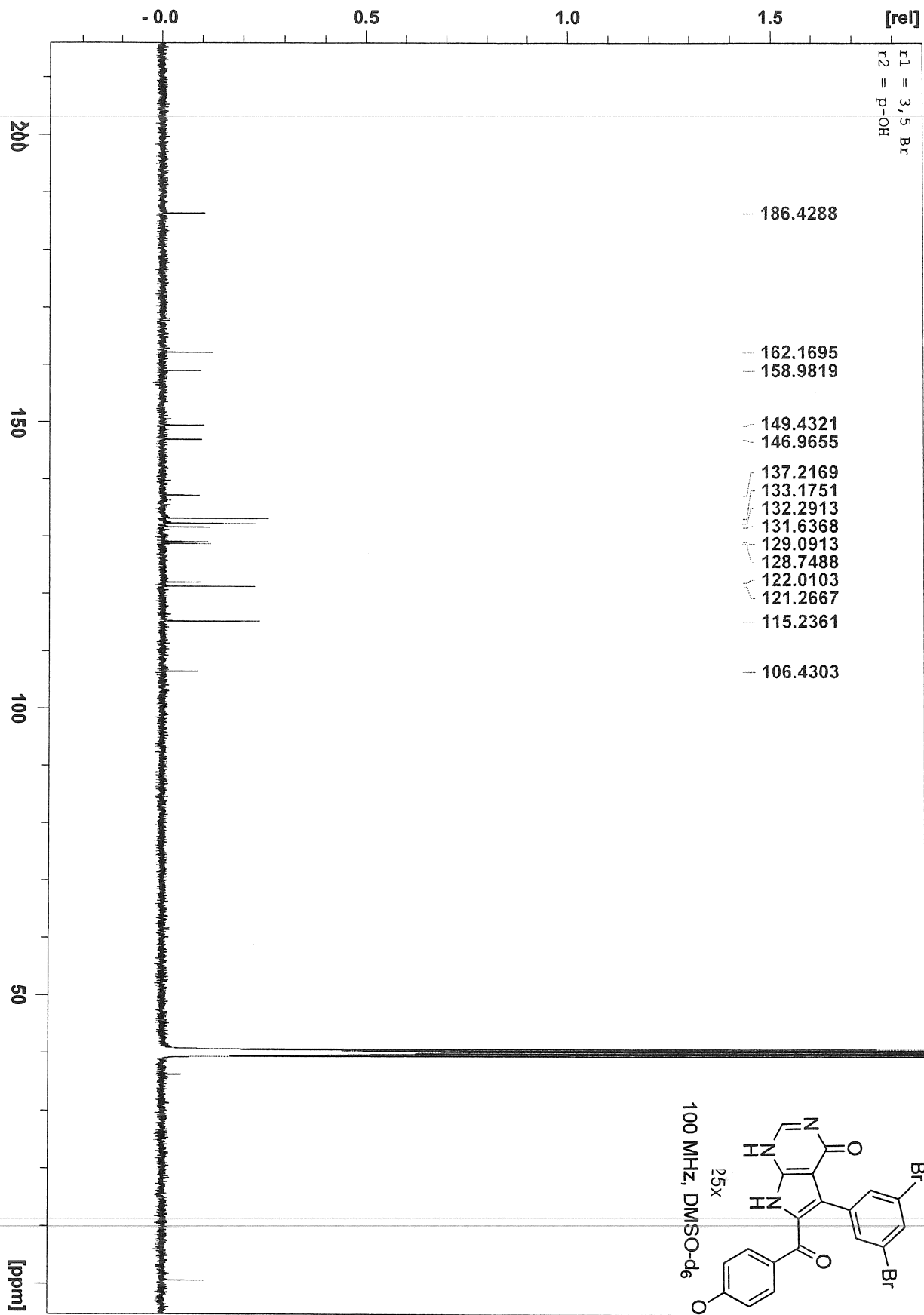


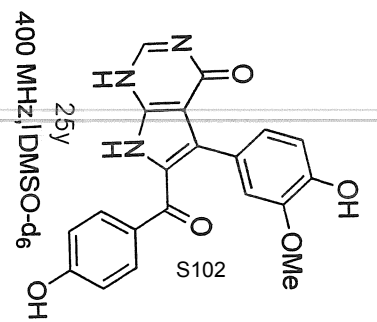
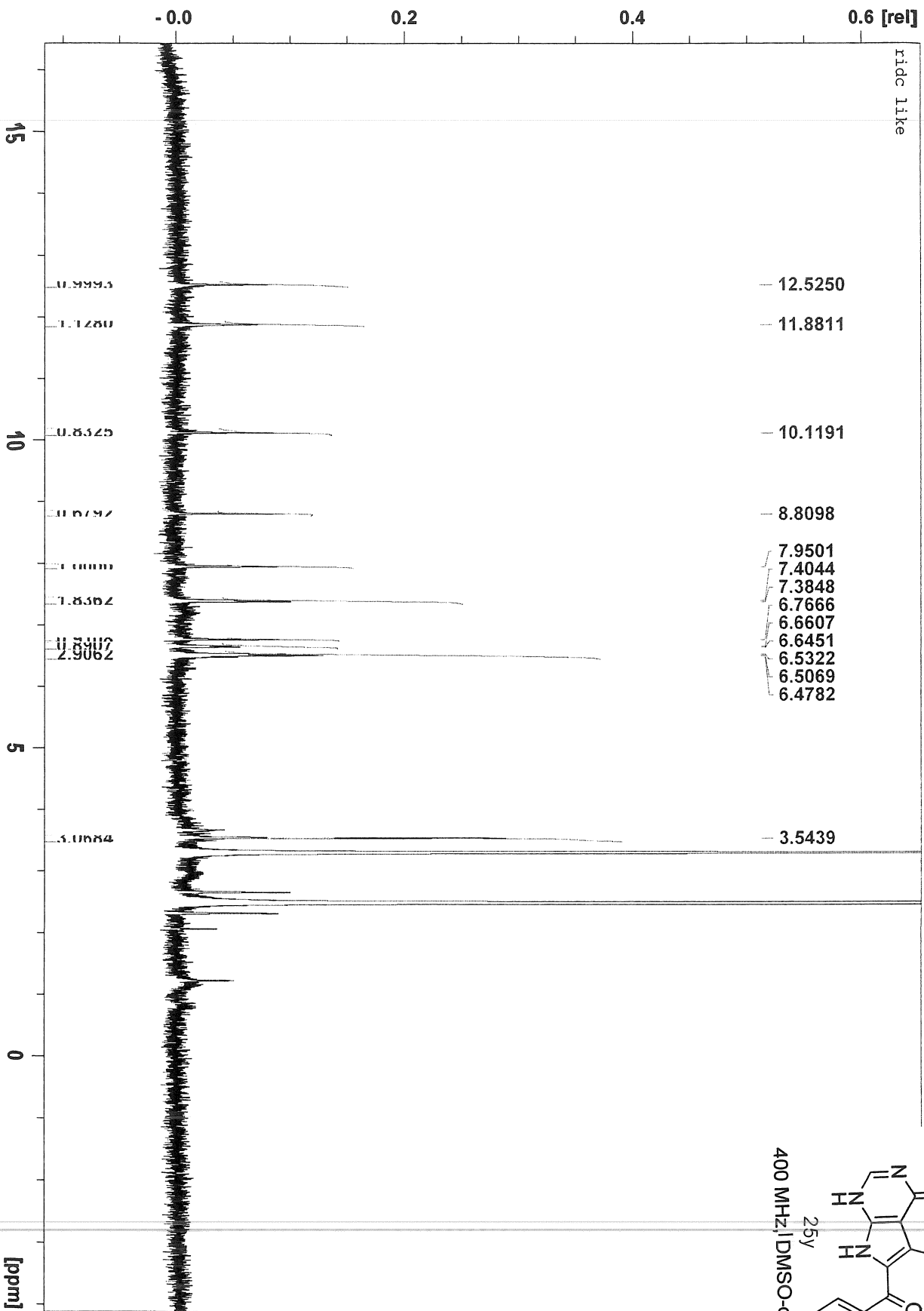
Rig35-OH-C13 2 1 C:\Bruker\TOPSPIN2.1.6\lilija lilija

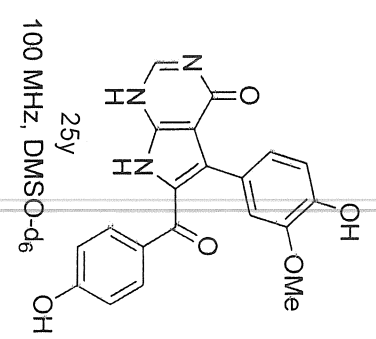
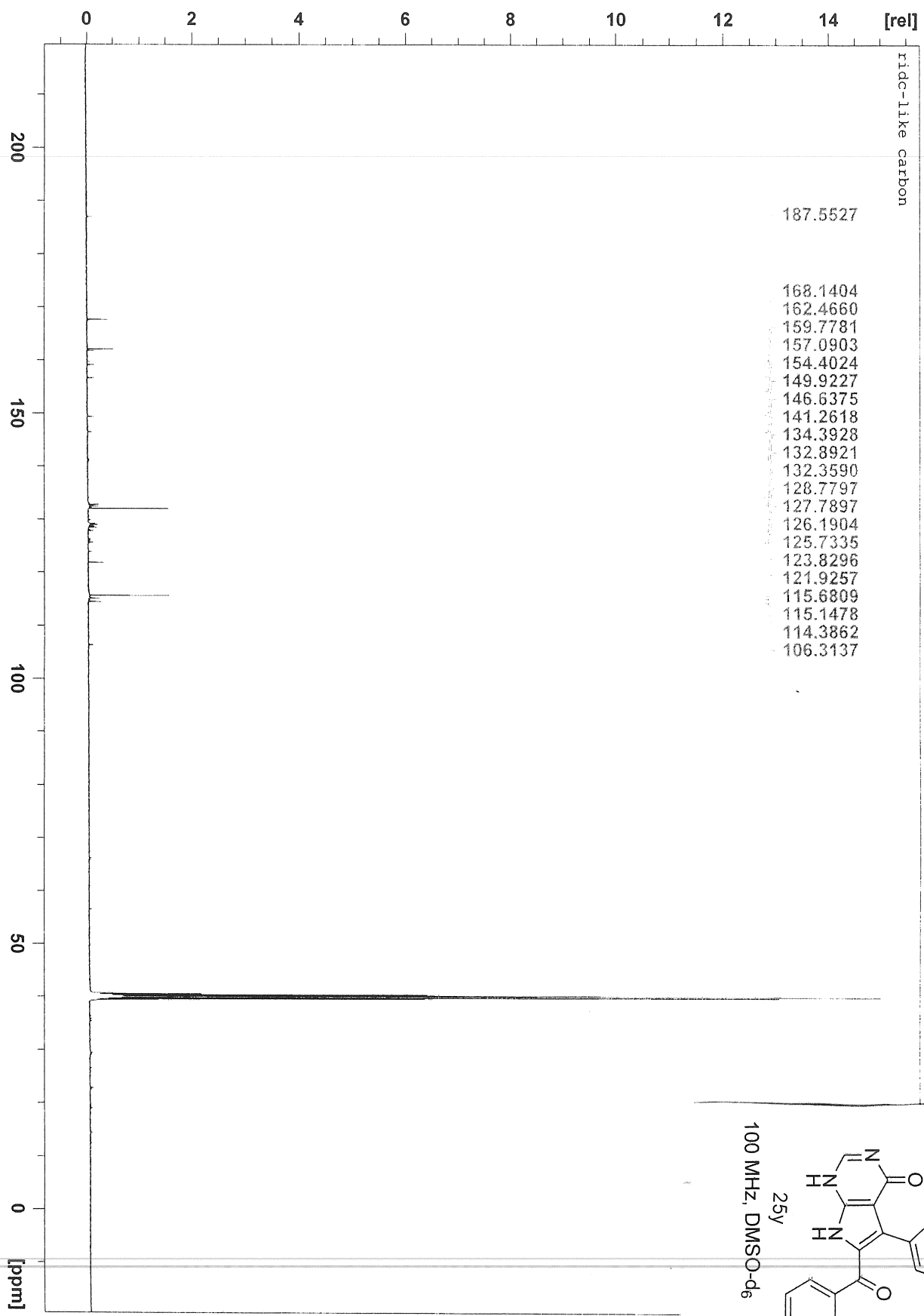


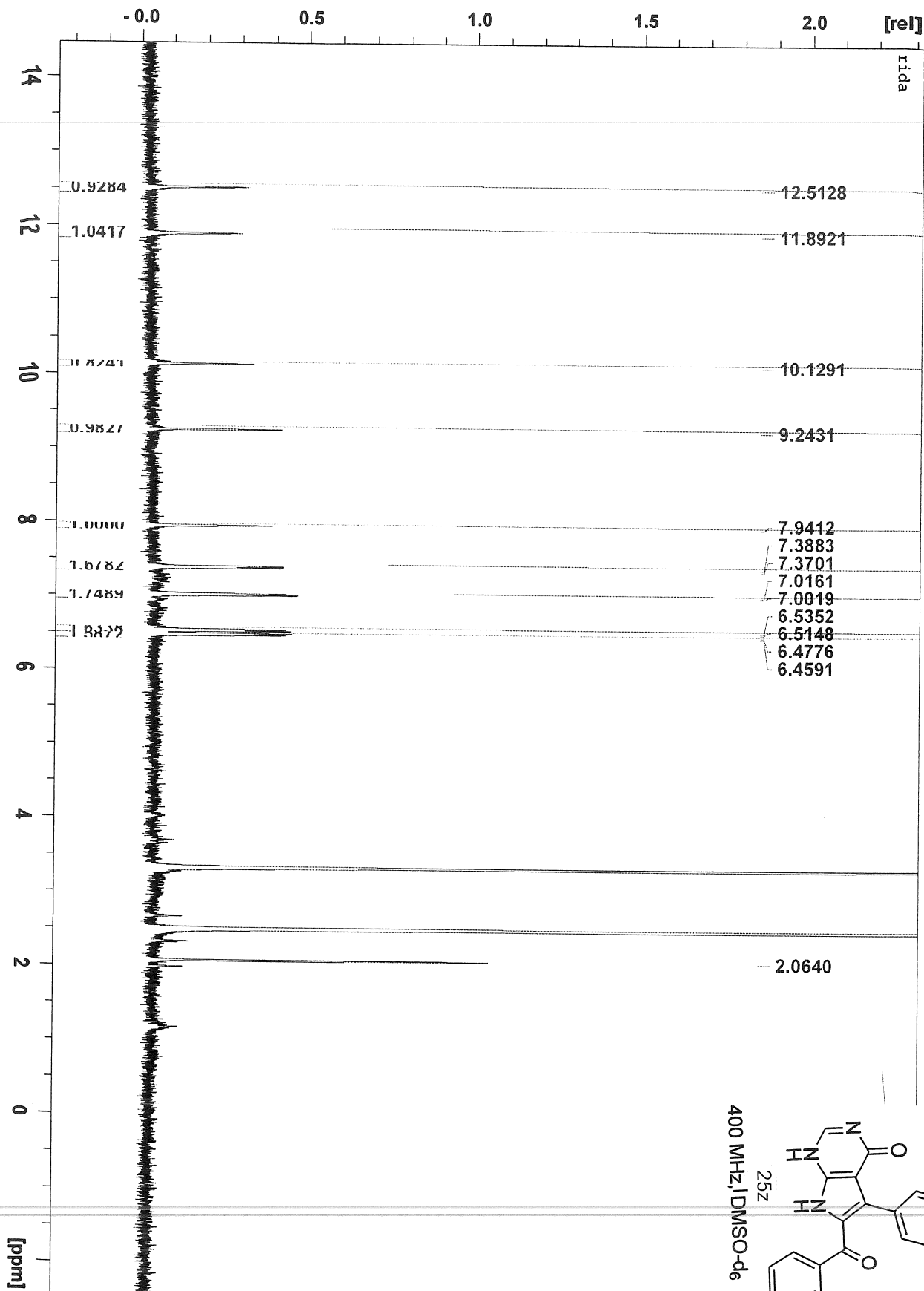
"3,5 Br, p-OH" 1 1 C:\Bruker\TOPSPIN2.1.6\Lillya Lillya
 r1 = 3,5 Br
 r2 = p-OH

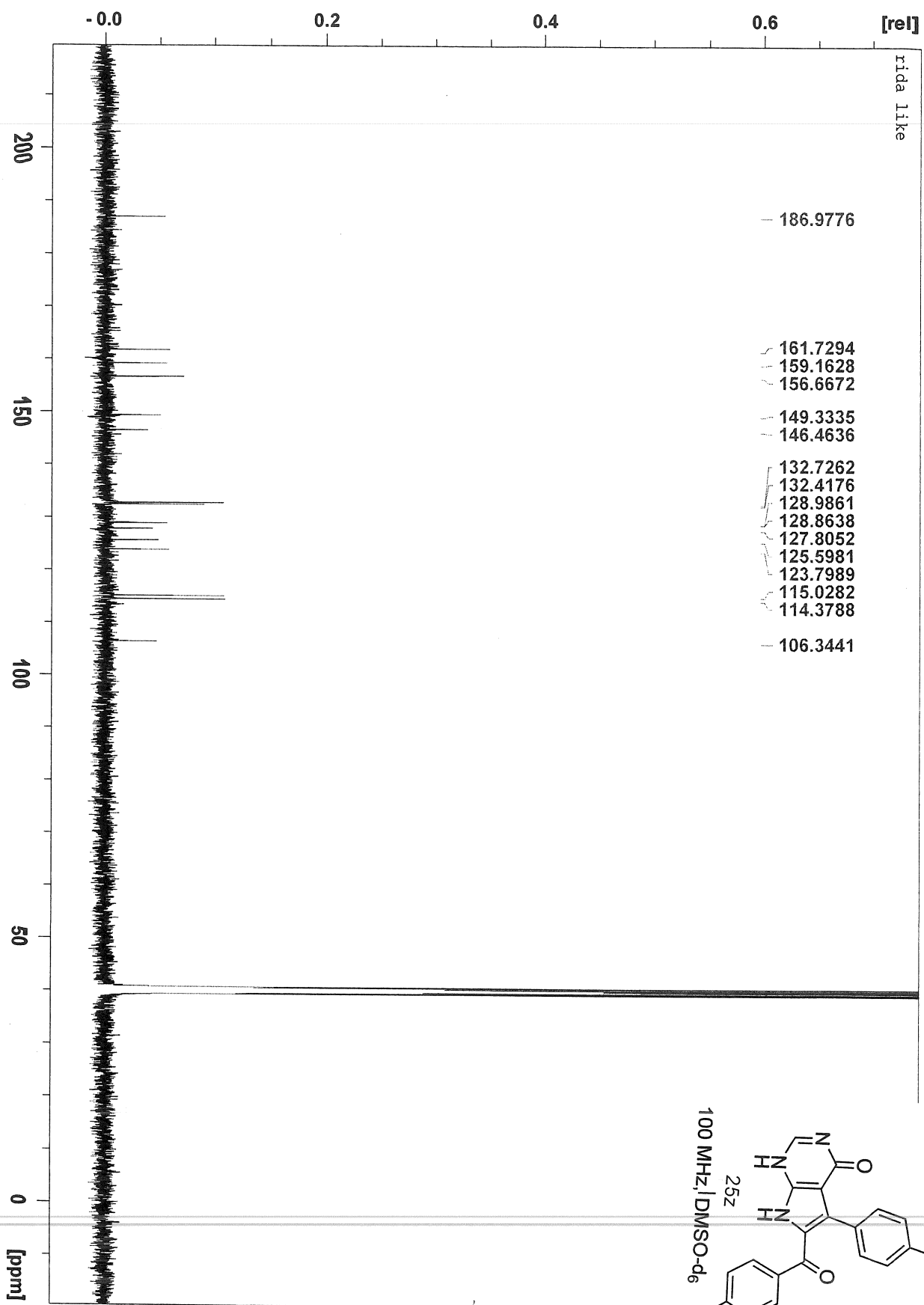












"rida like- c13" 2 1 C:\Bruker\TOPSPIN2.1.6\liliya liliya

rida like

