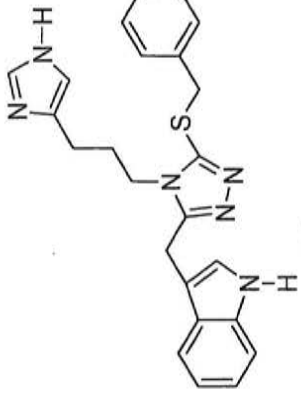
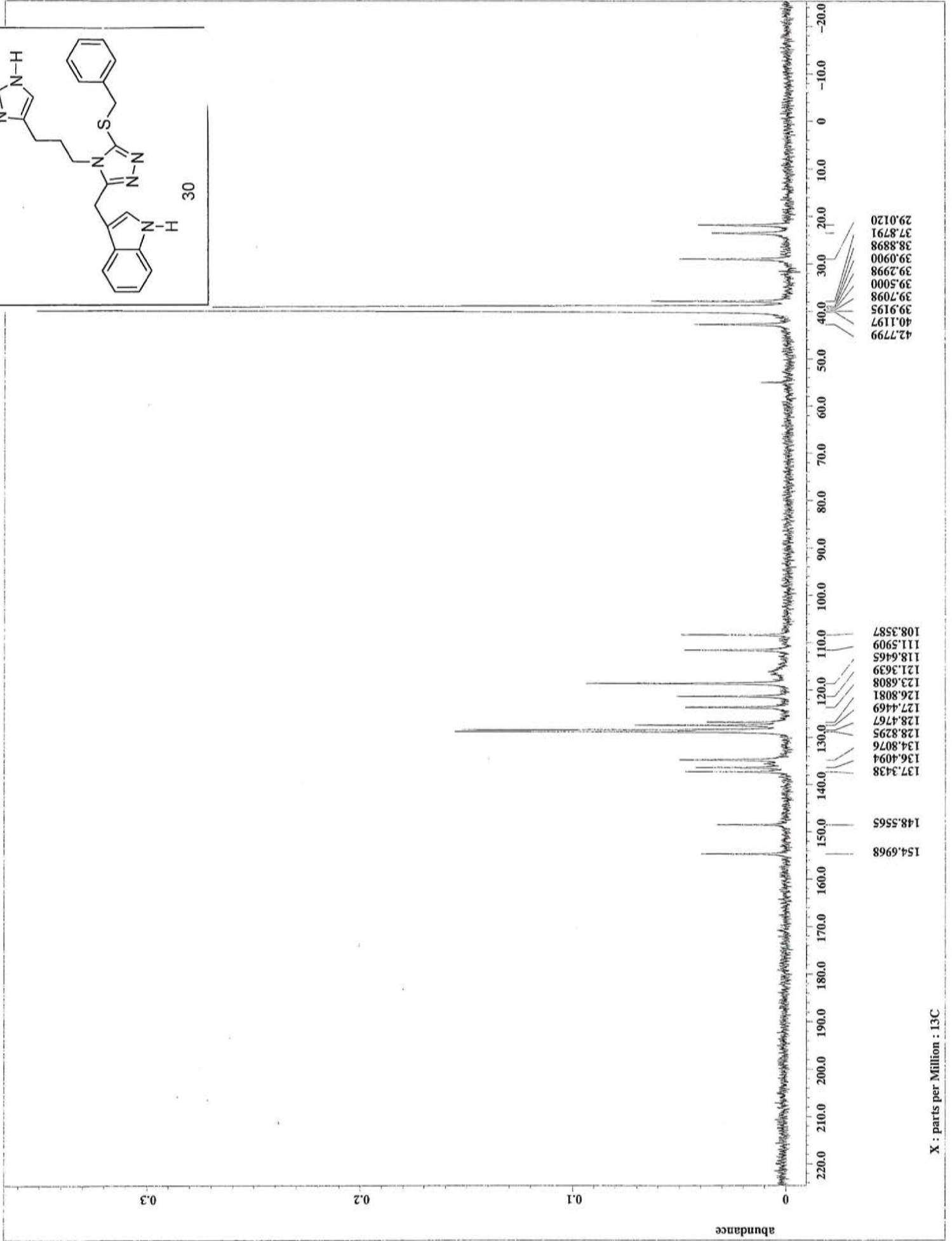
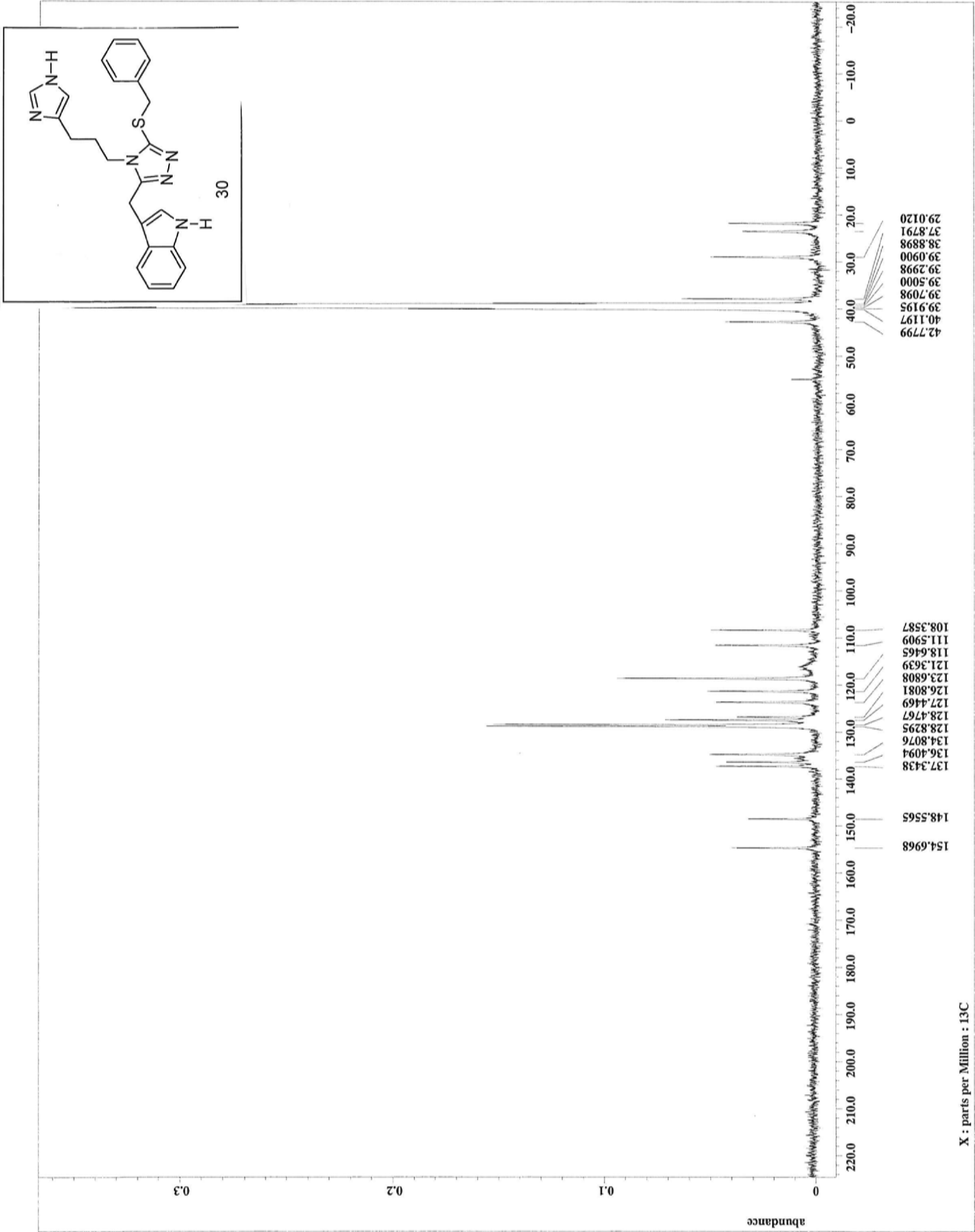


X : parts per Million : 1H

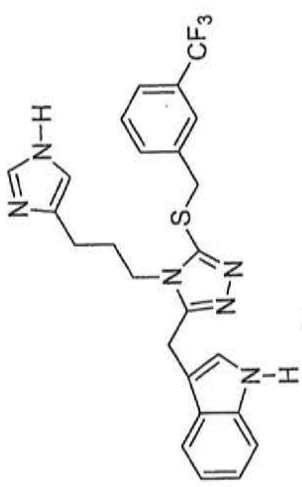


30

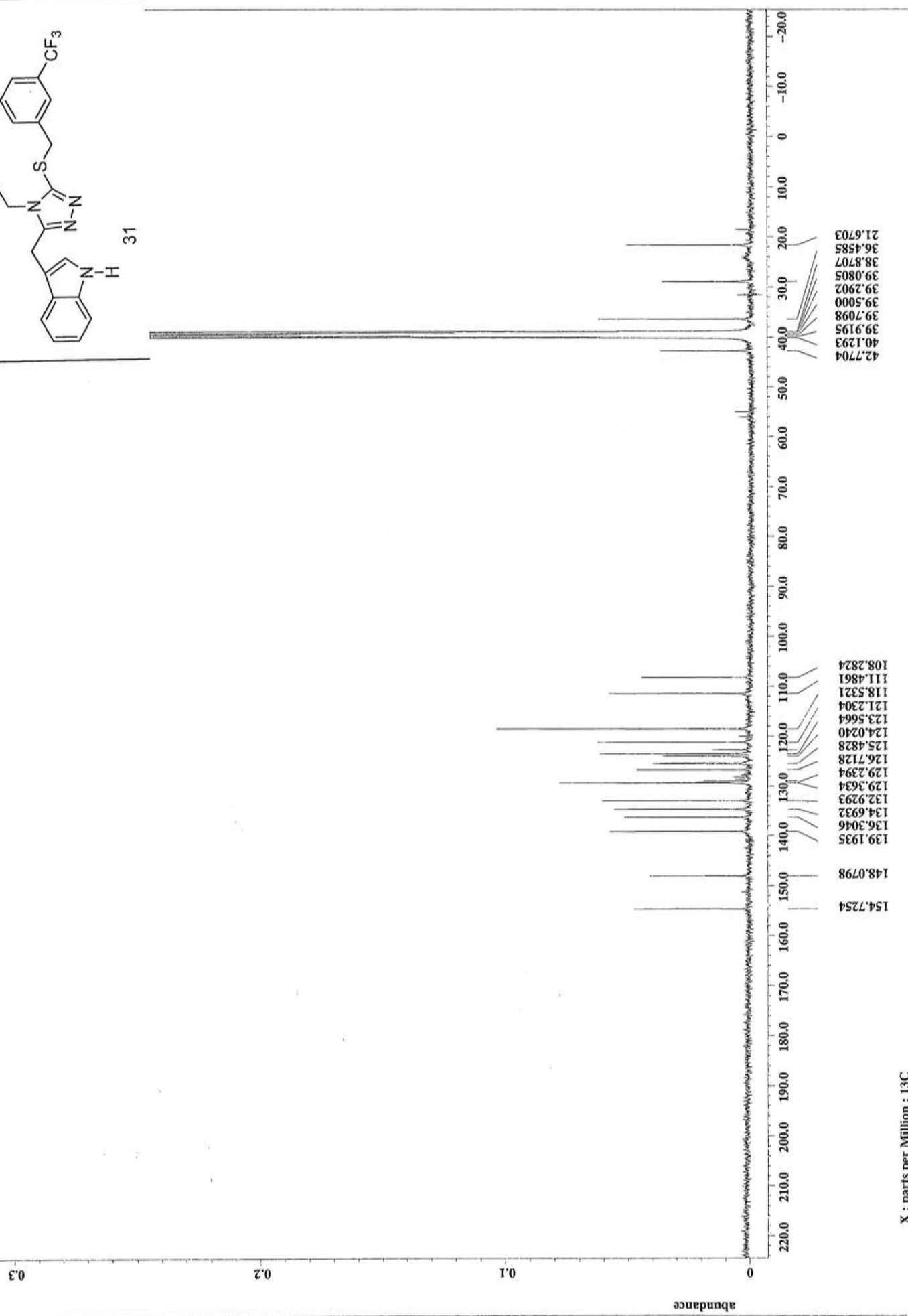




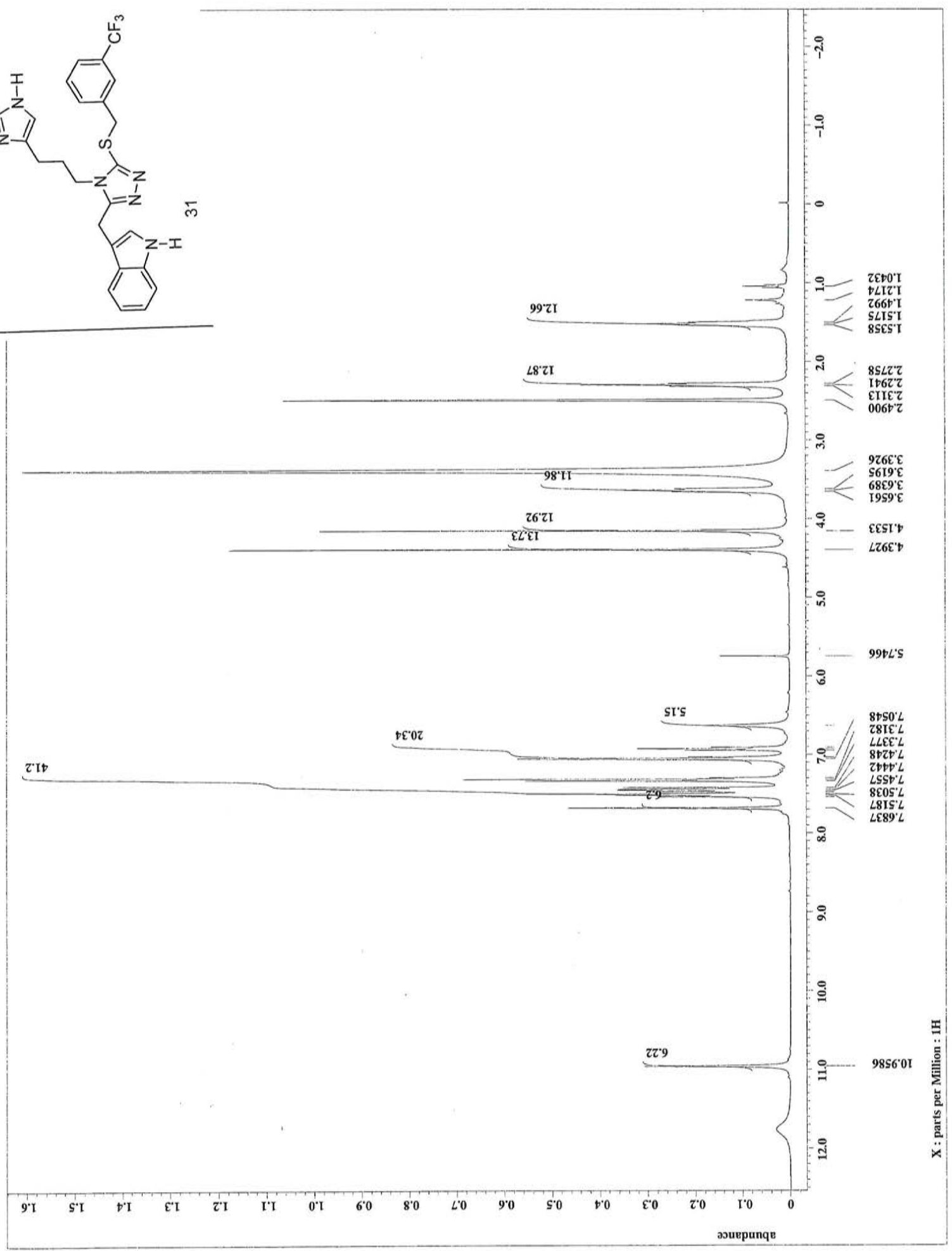
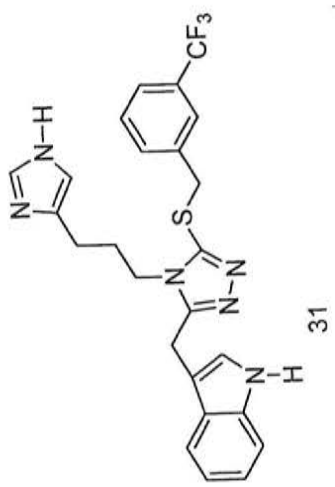
X : parts per Million : 13C

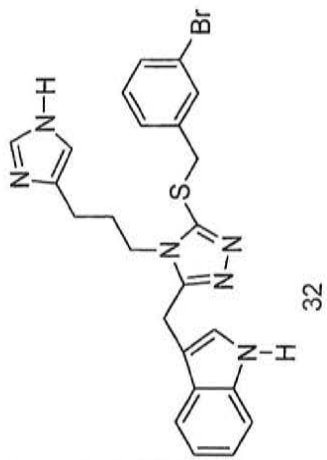


31

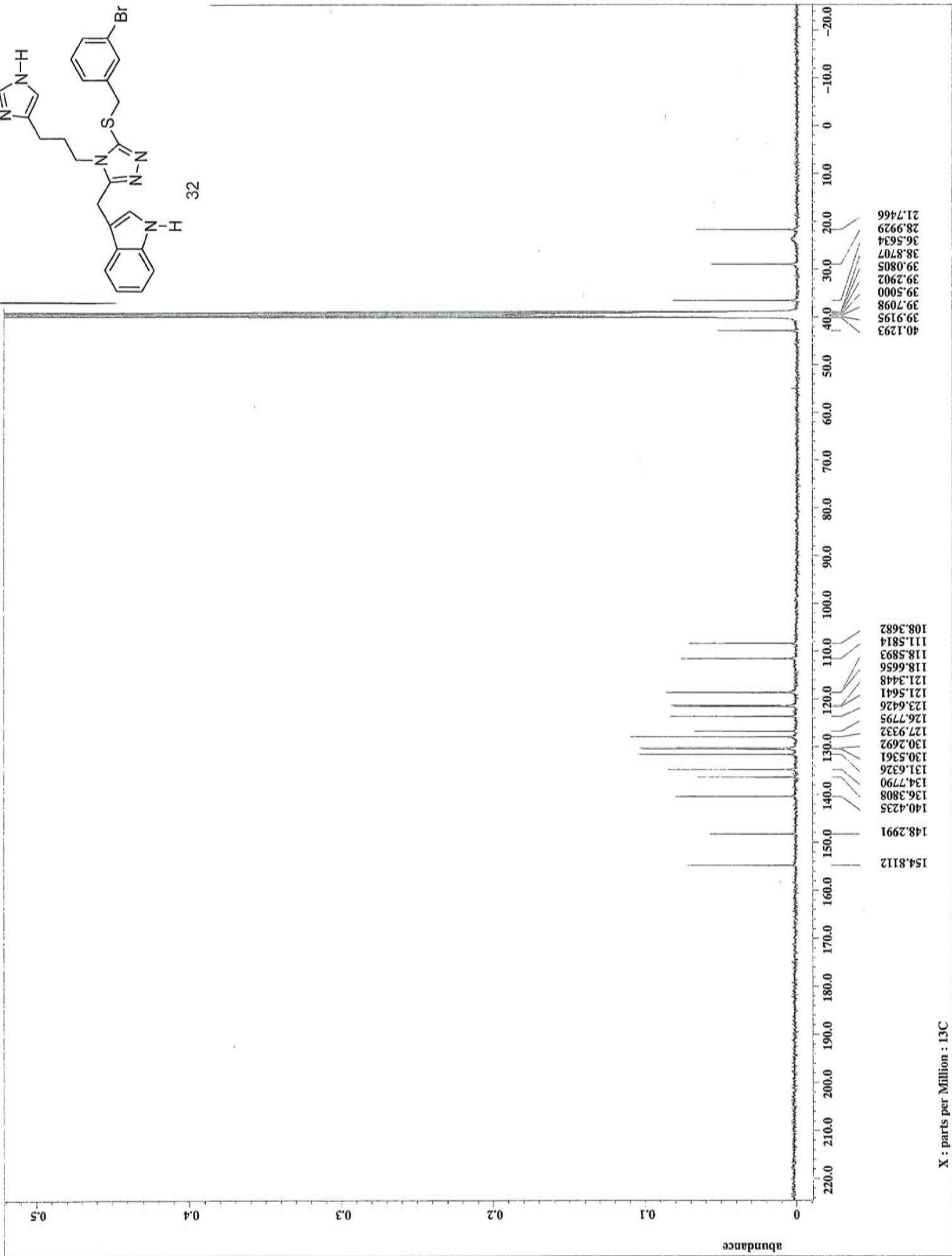


X : parts per Million : 13C





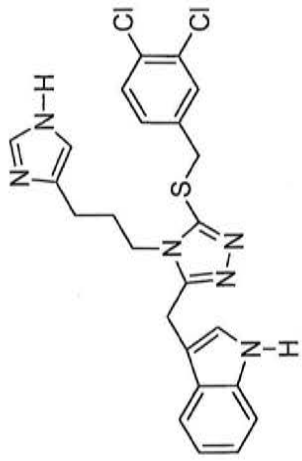
32



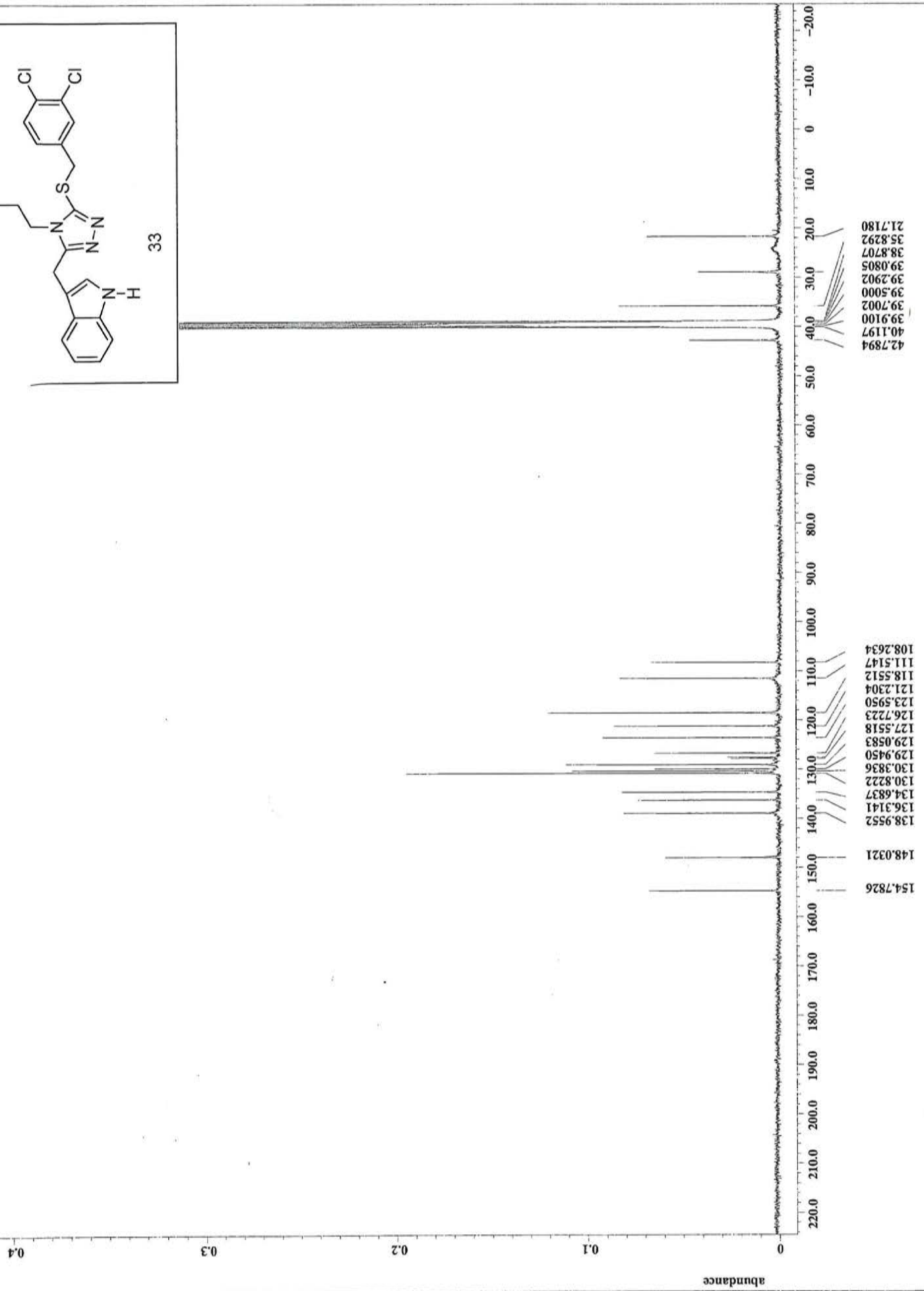
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39.7098
39.5000
39.2902
39.0805
38.8707
36.5634
28.9929
21.7466

154.8112
148.2991
140.4235
136.3808
134.7790
131.6326
130.5361
130.2692
127.9332
126.7795
123.6426
121.5641
121.3448
118.6656
118.5893
111.5814
108.3682

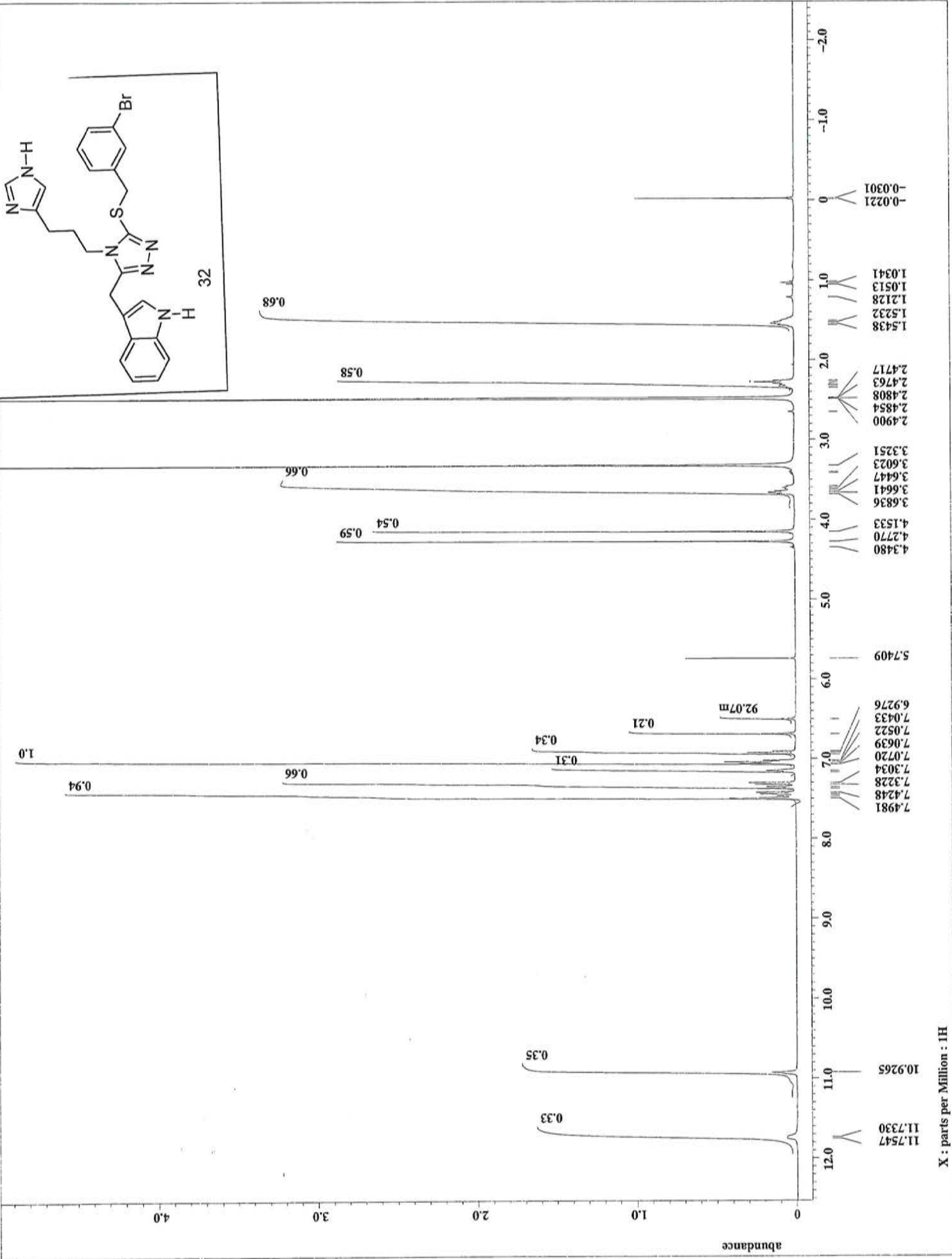
X : parts per Million : 13C



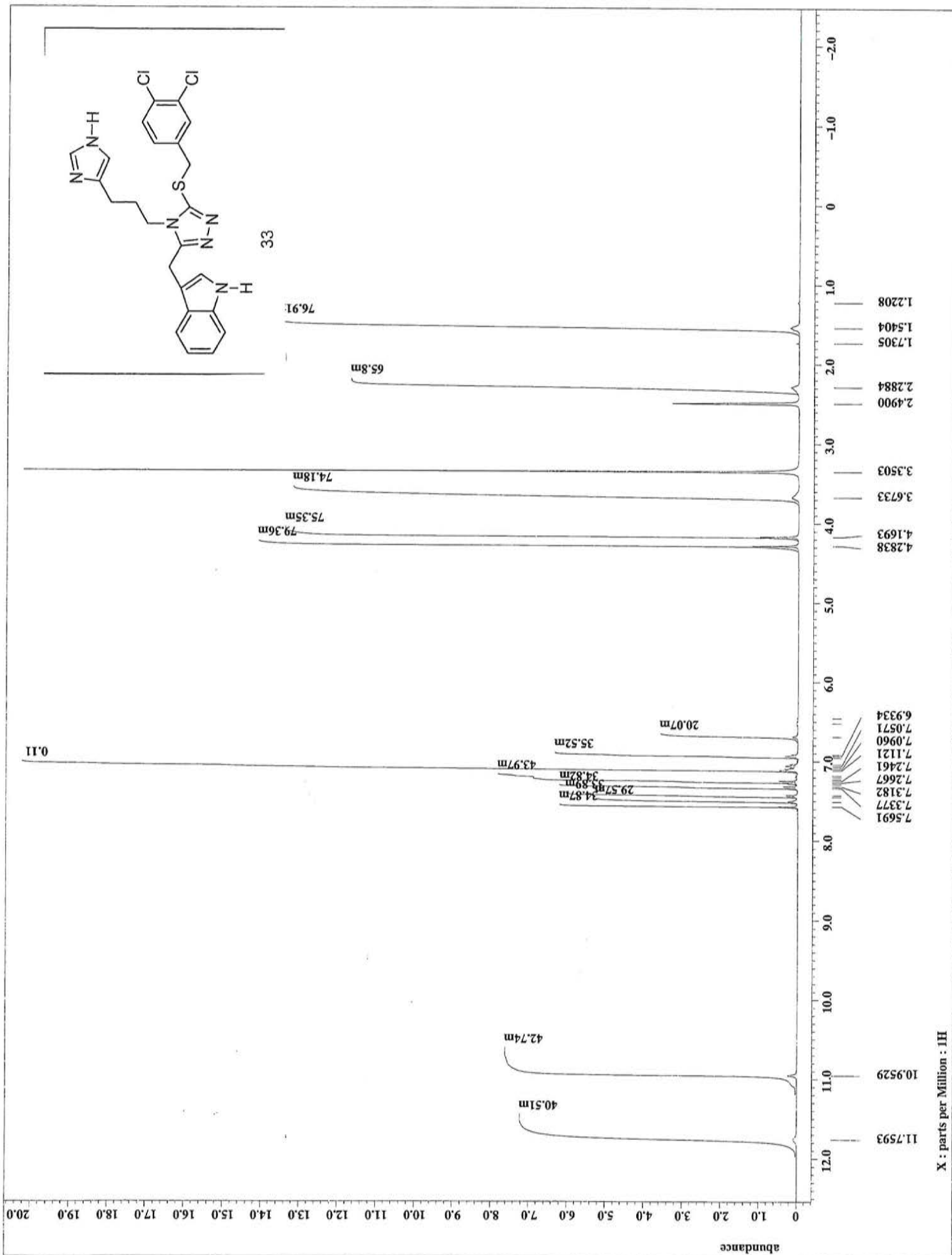
33

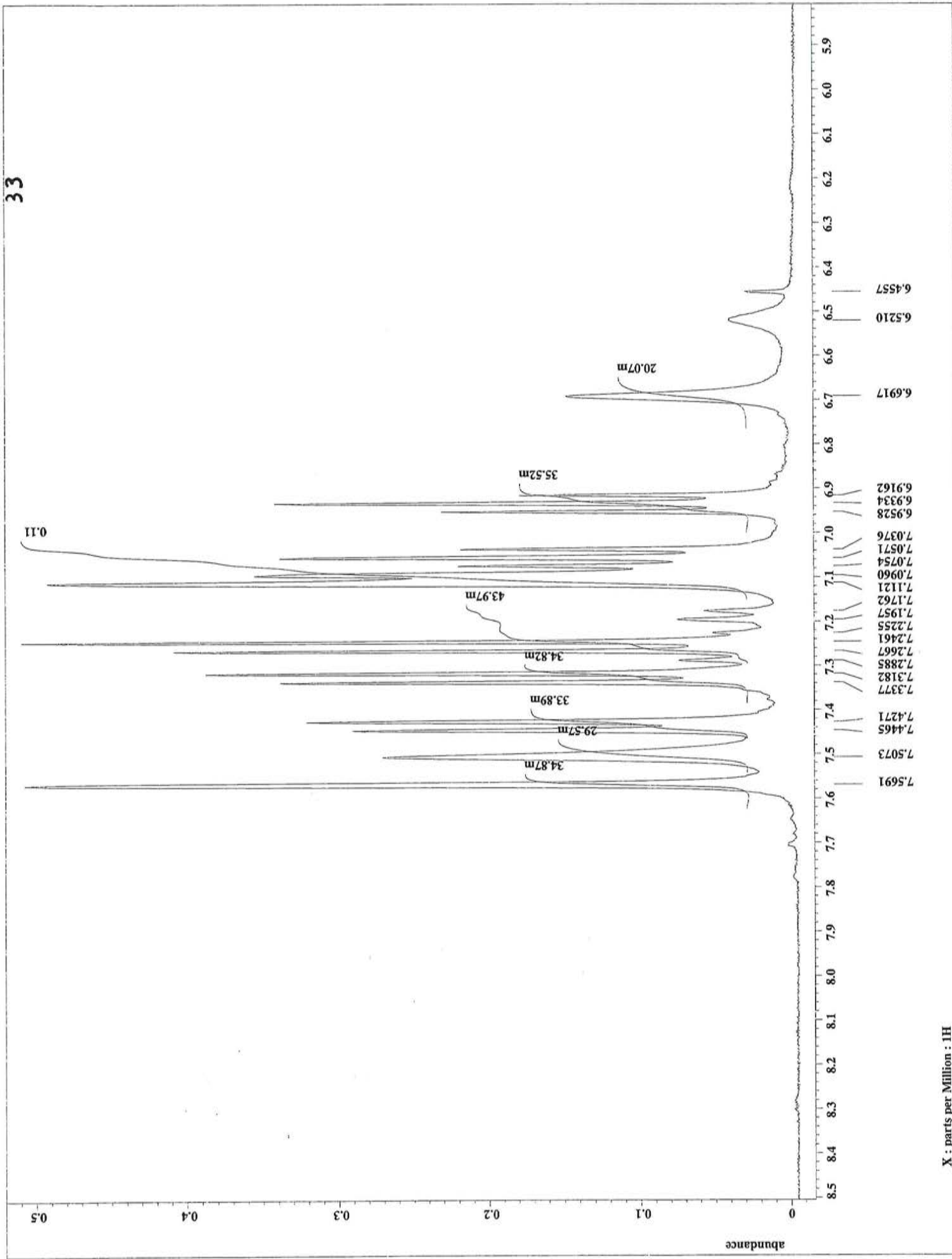


X : parts per Million : 13C

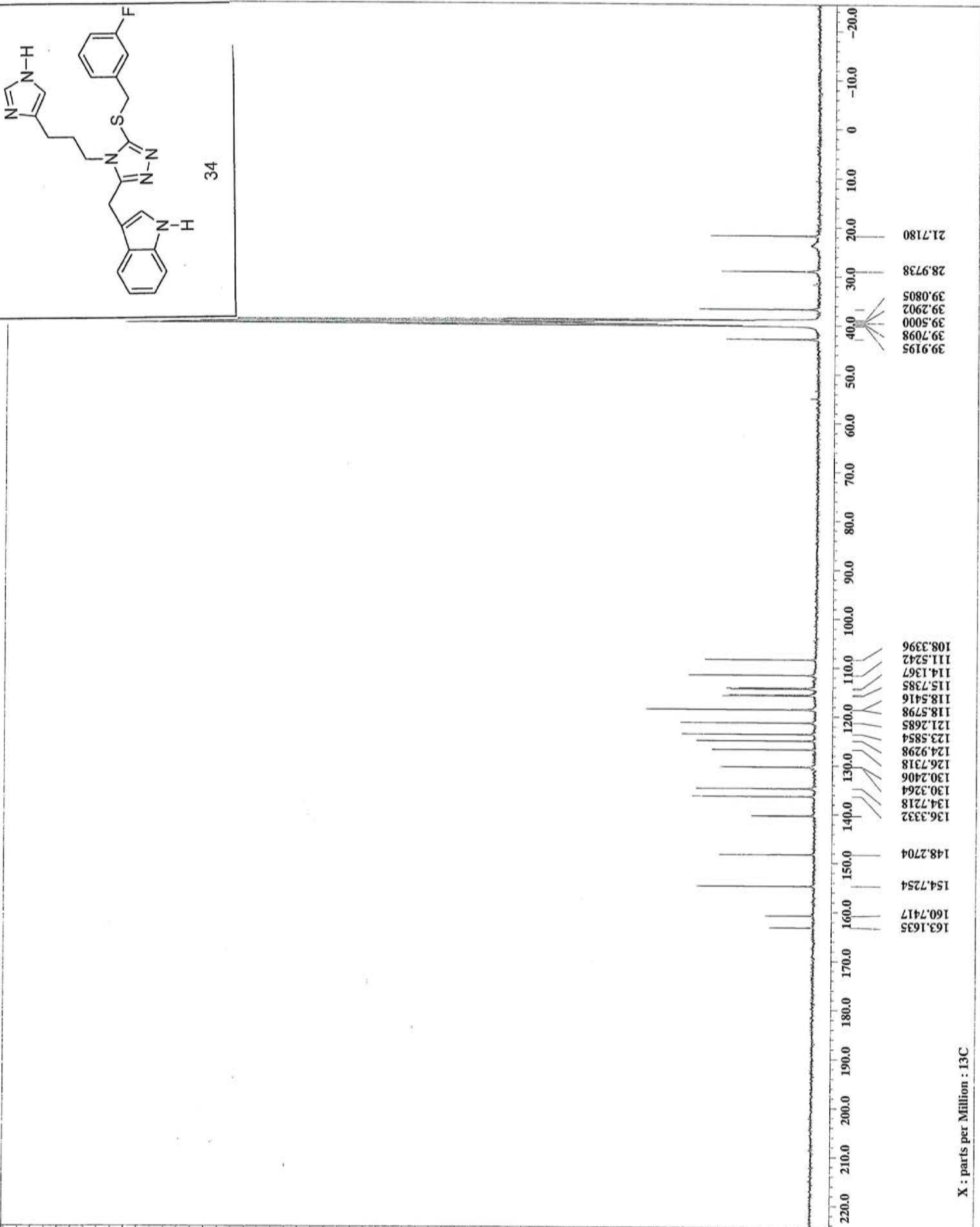


X : parts per Million : 1H

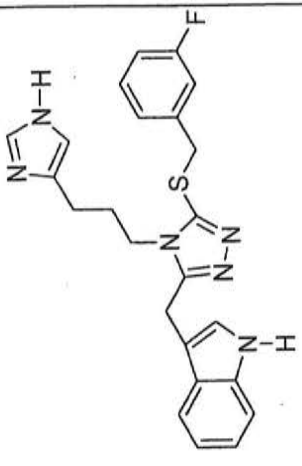




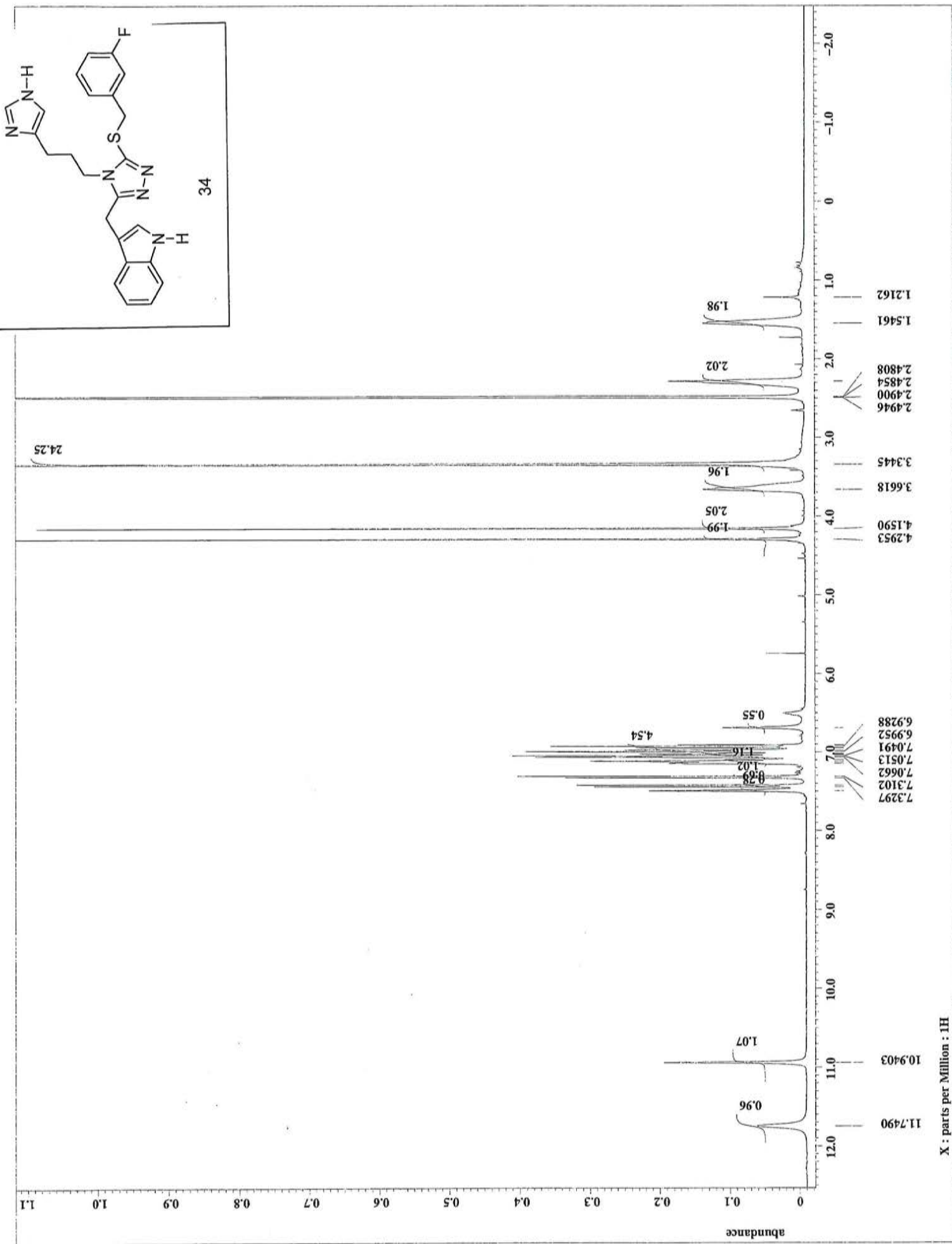
abundance



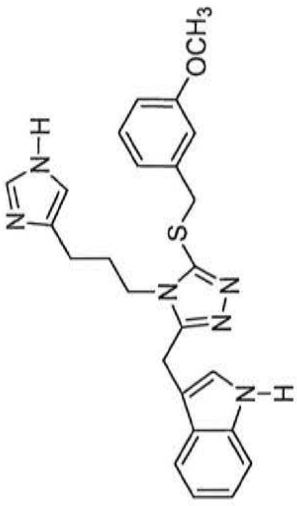
34



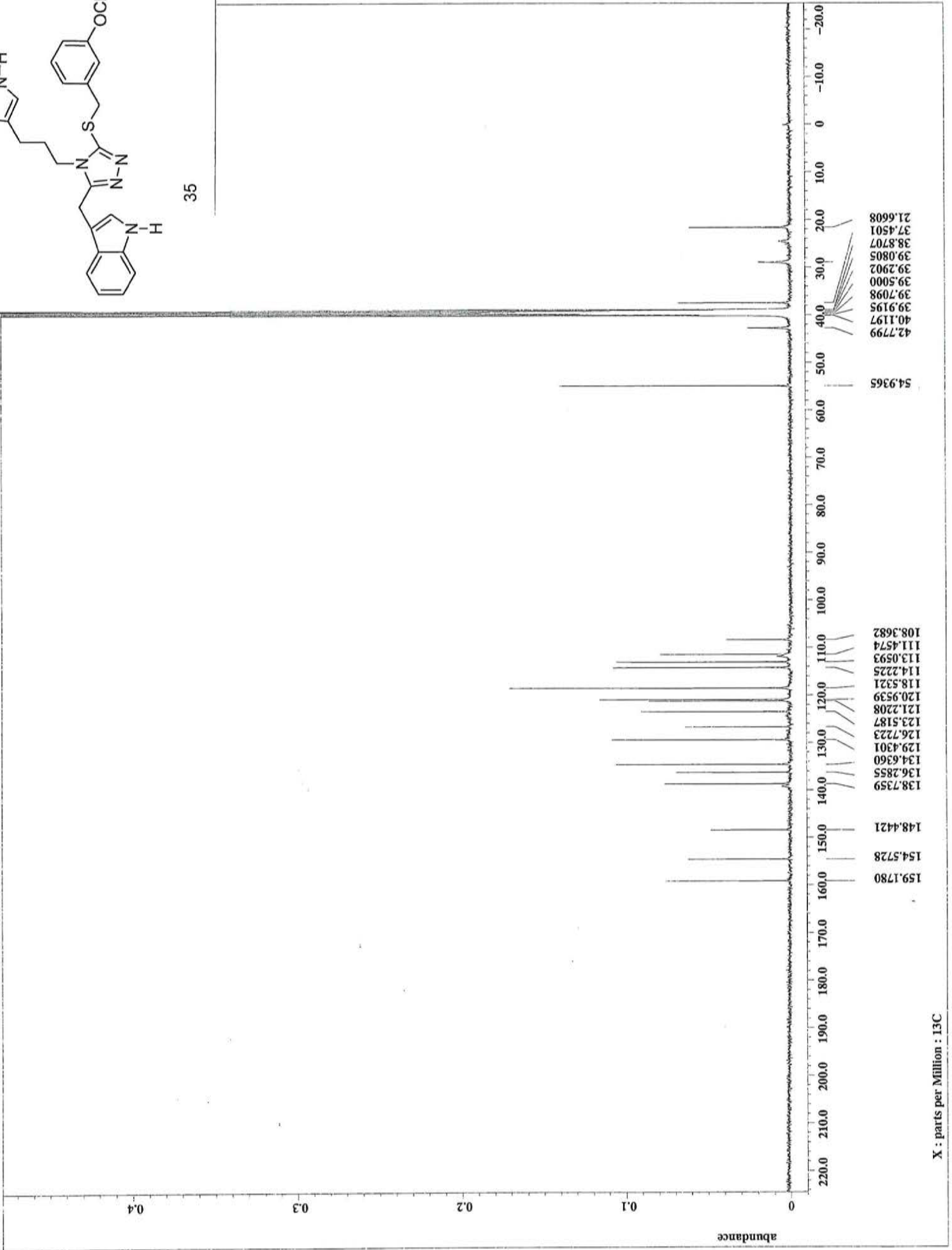
X : parts per Million : 13C

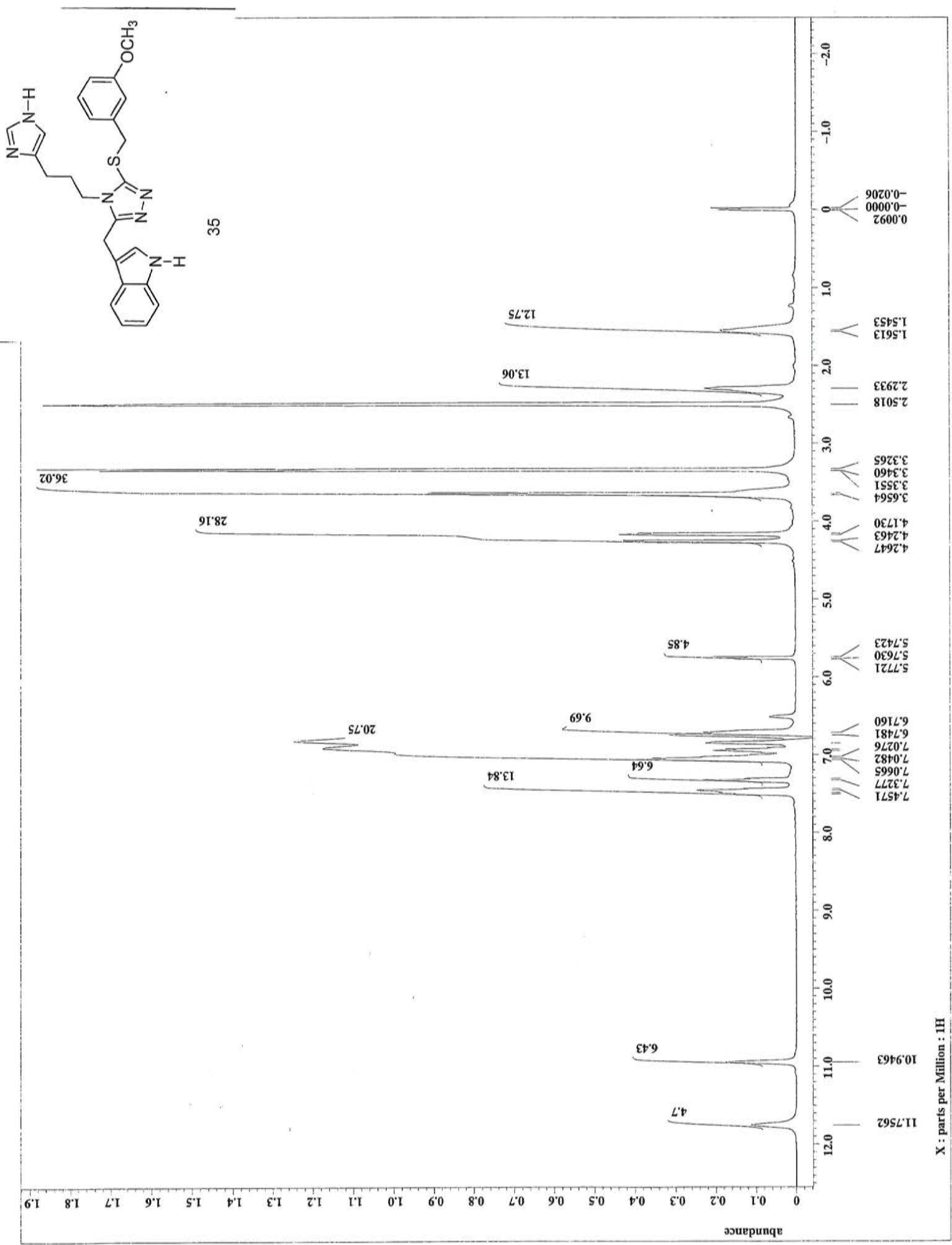


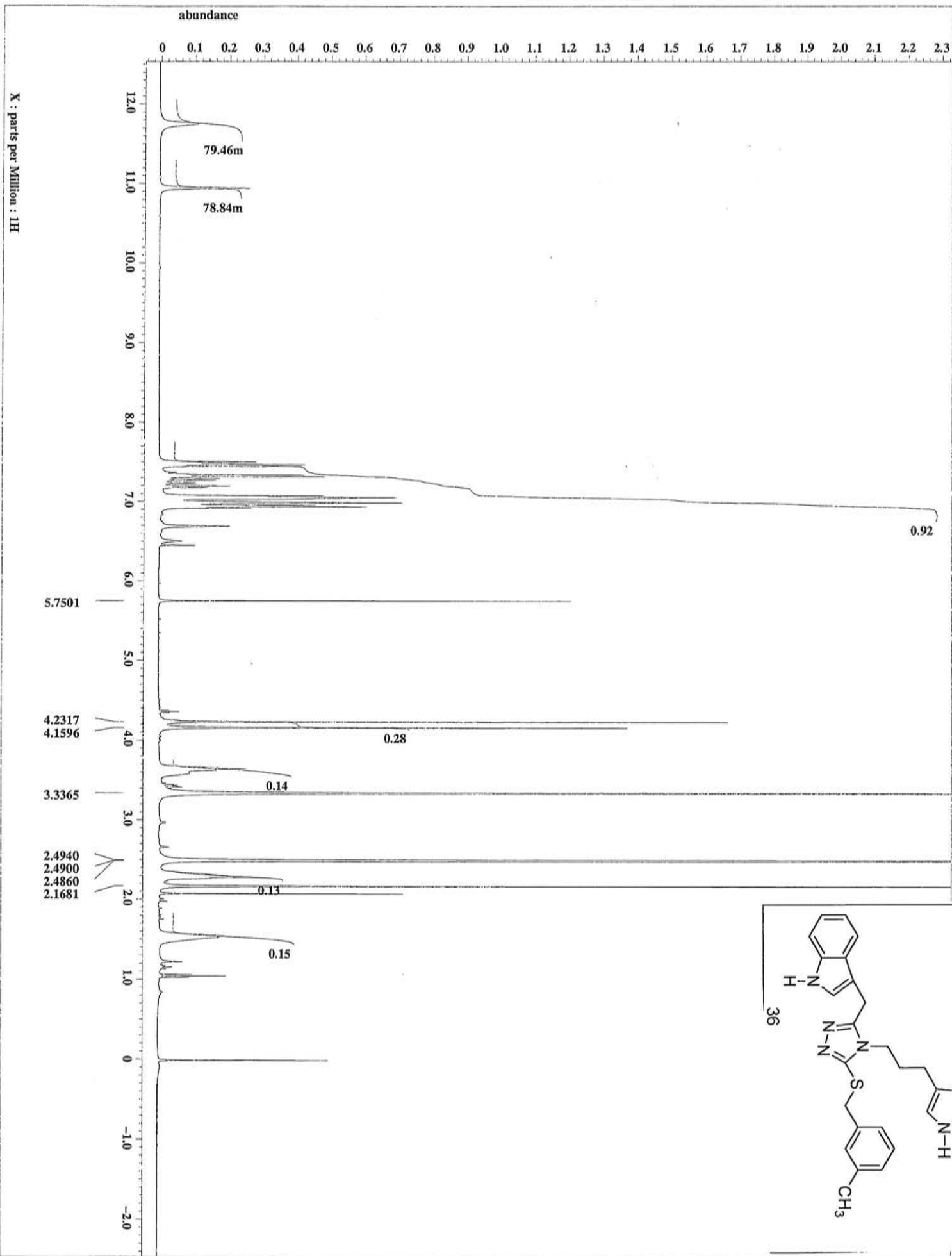
X : parts per Million : 1H

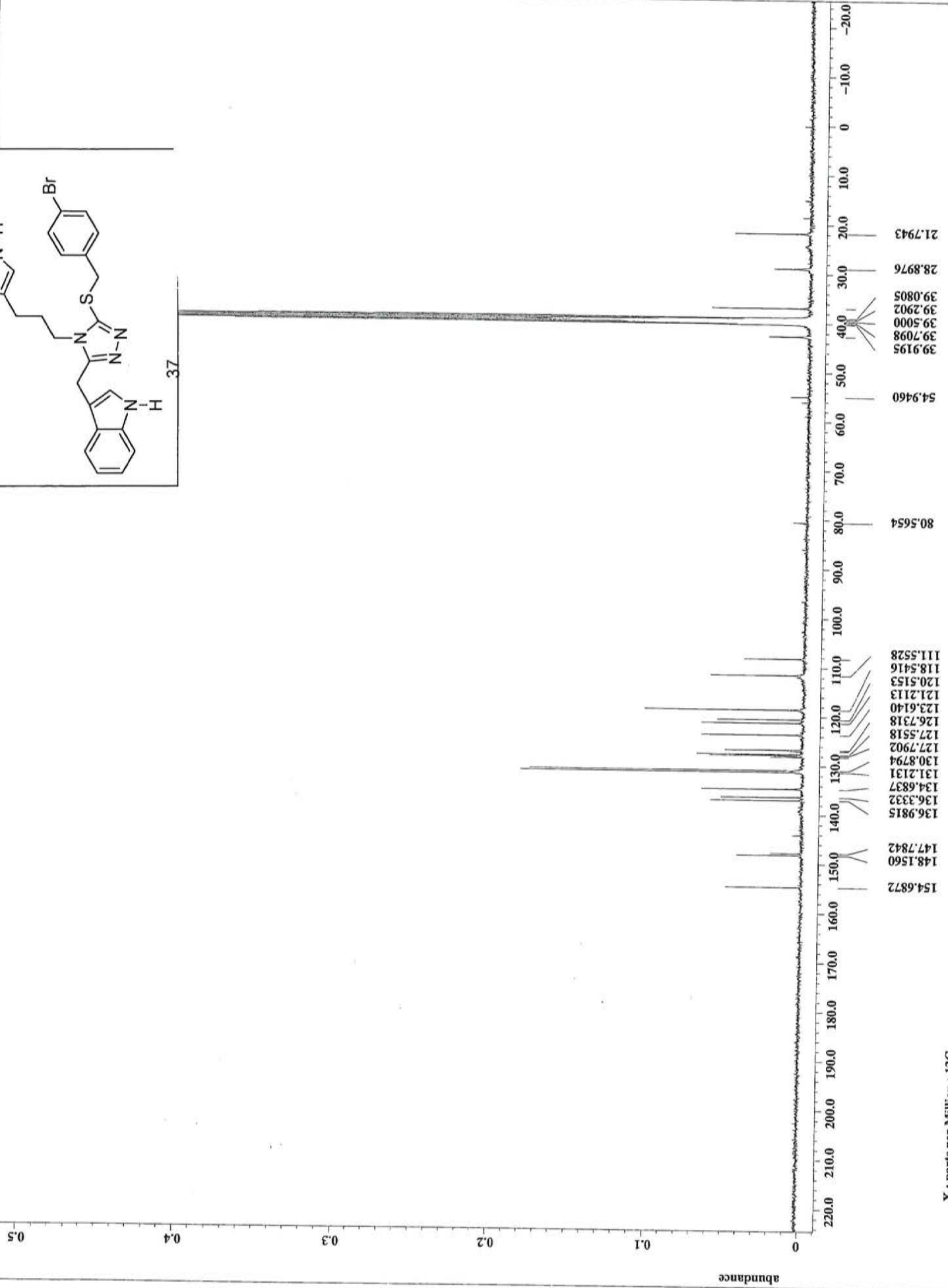
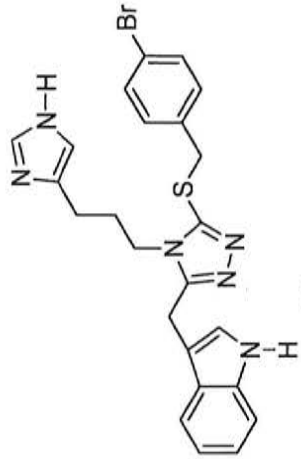


35

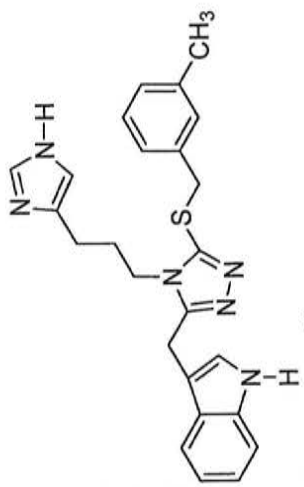




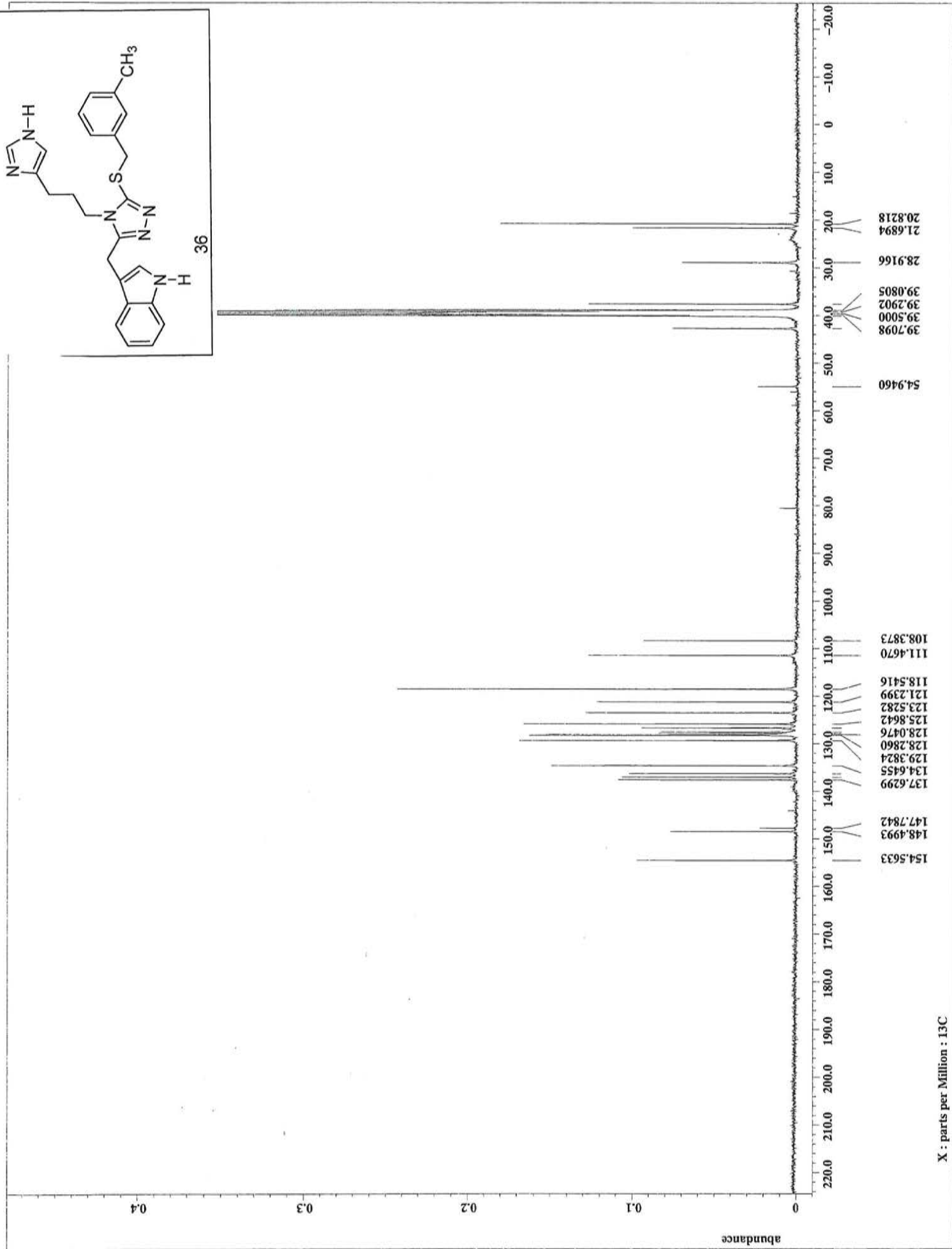




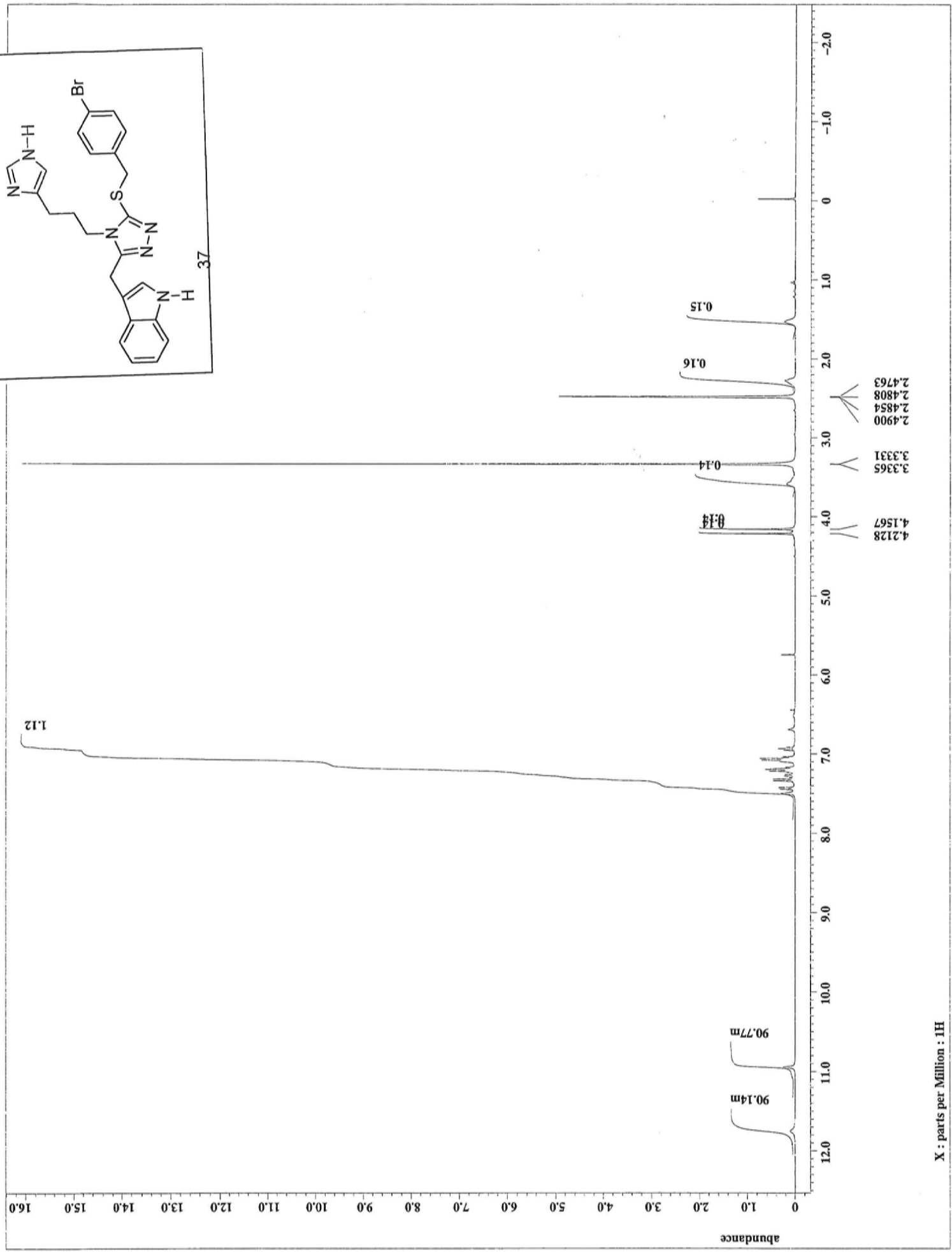
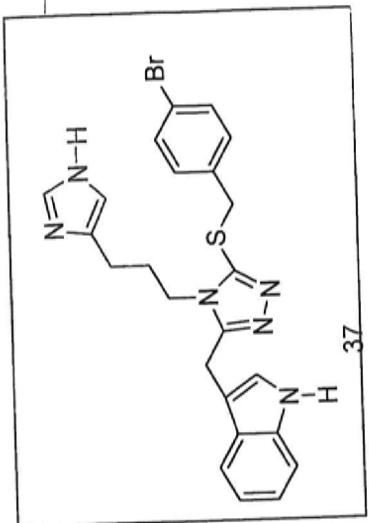
X : parts per Million : 13C



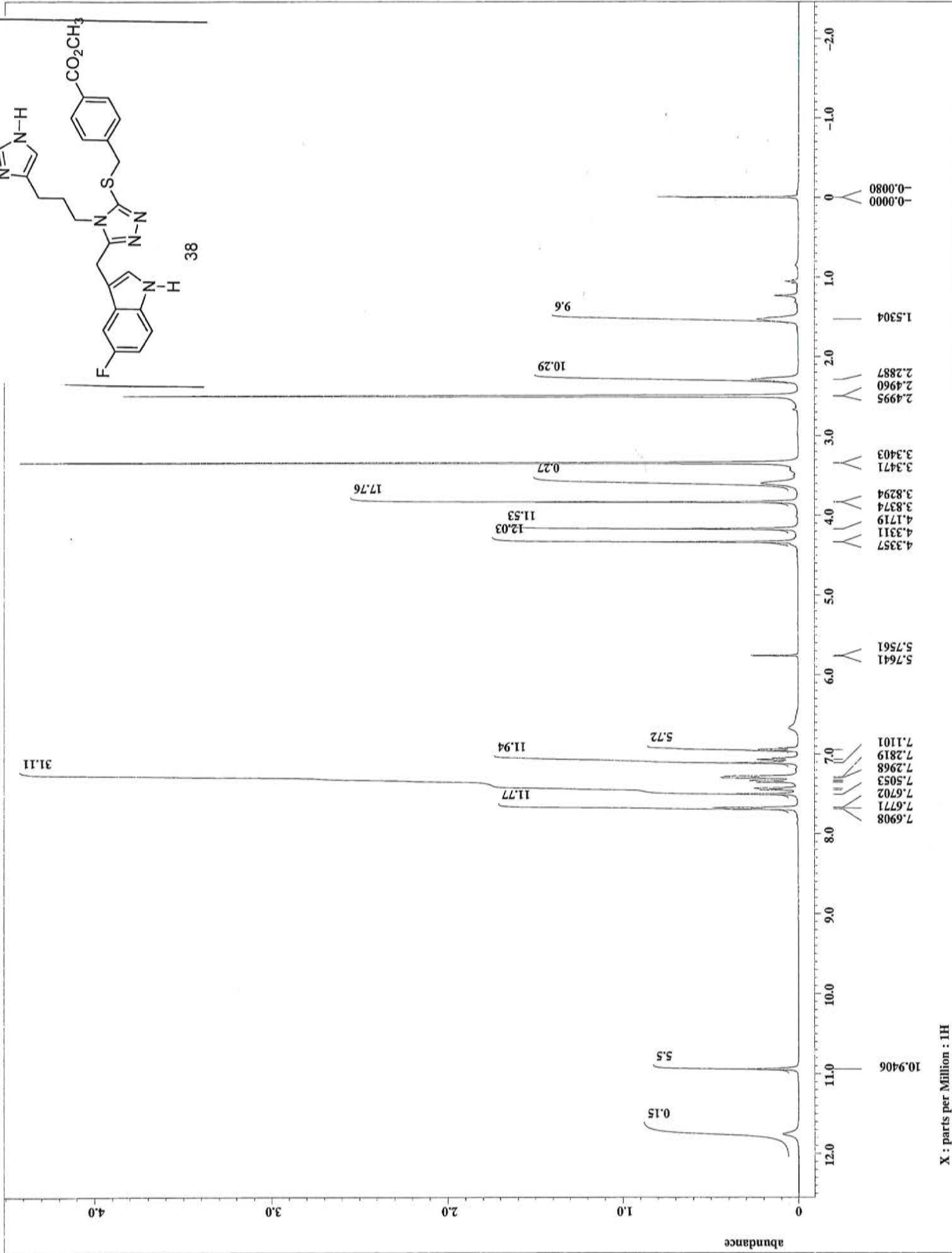
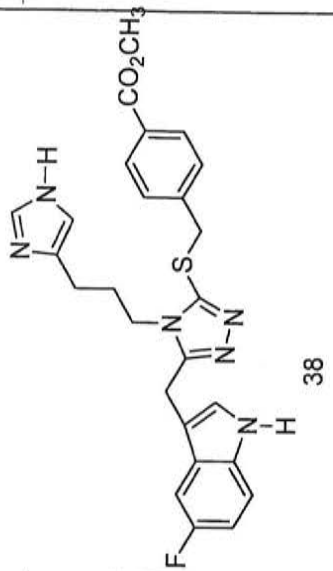
36

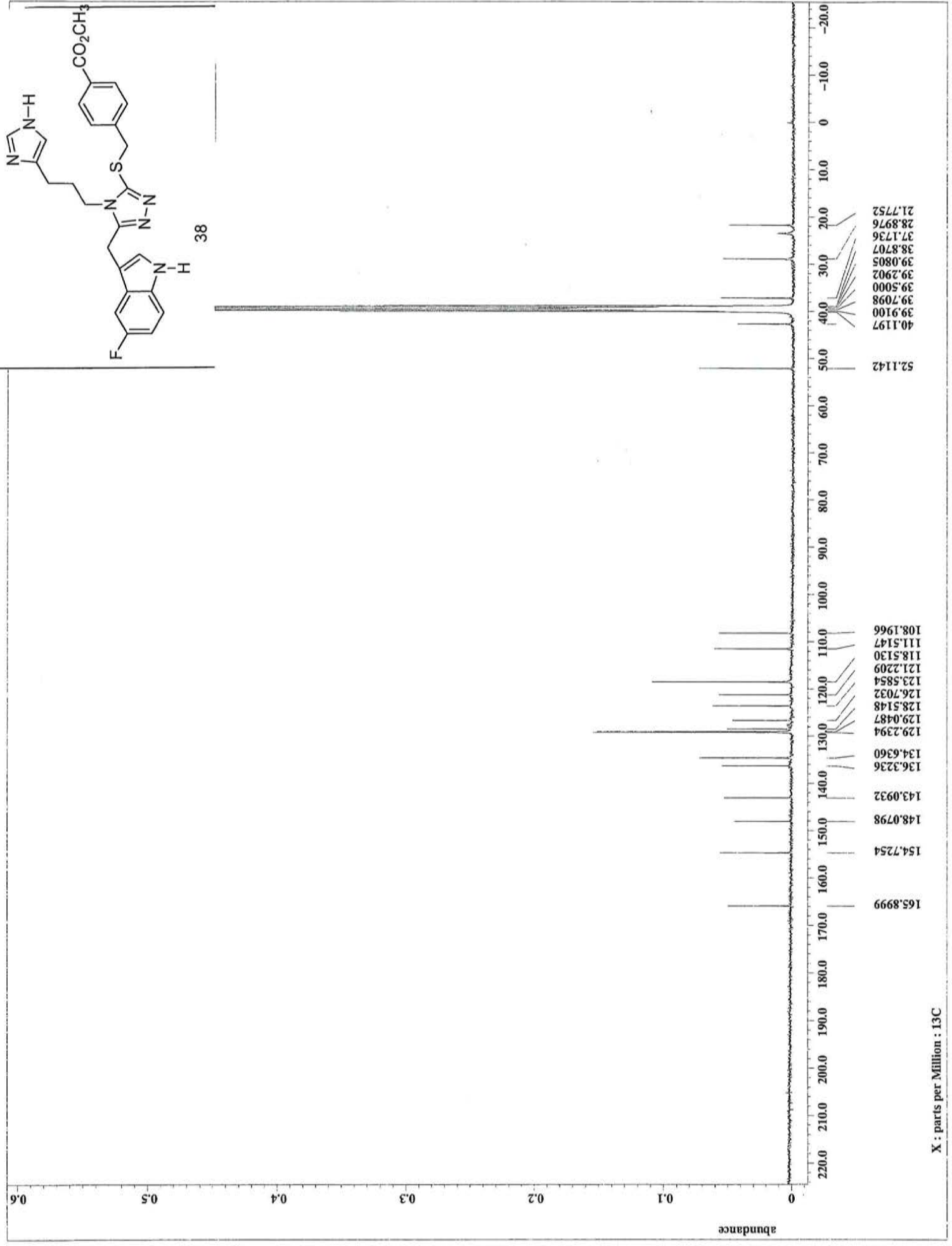
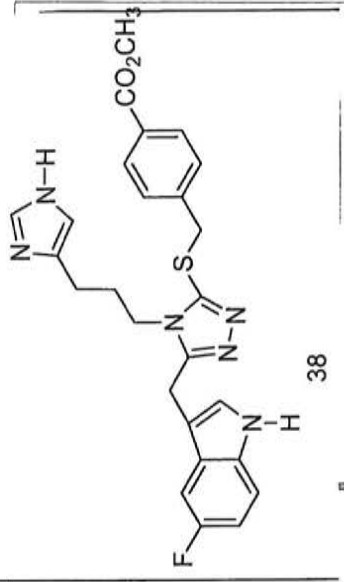


X : parts per Million : 13C

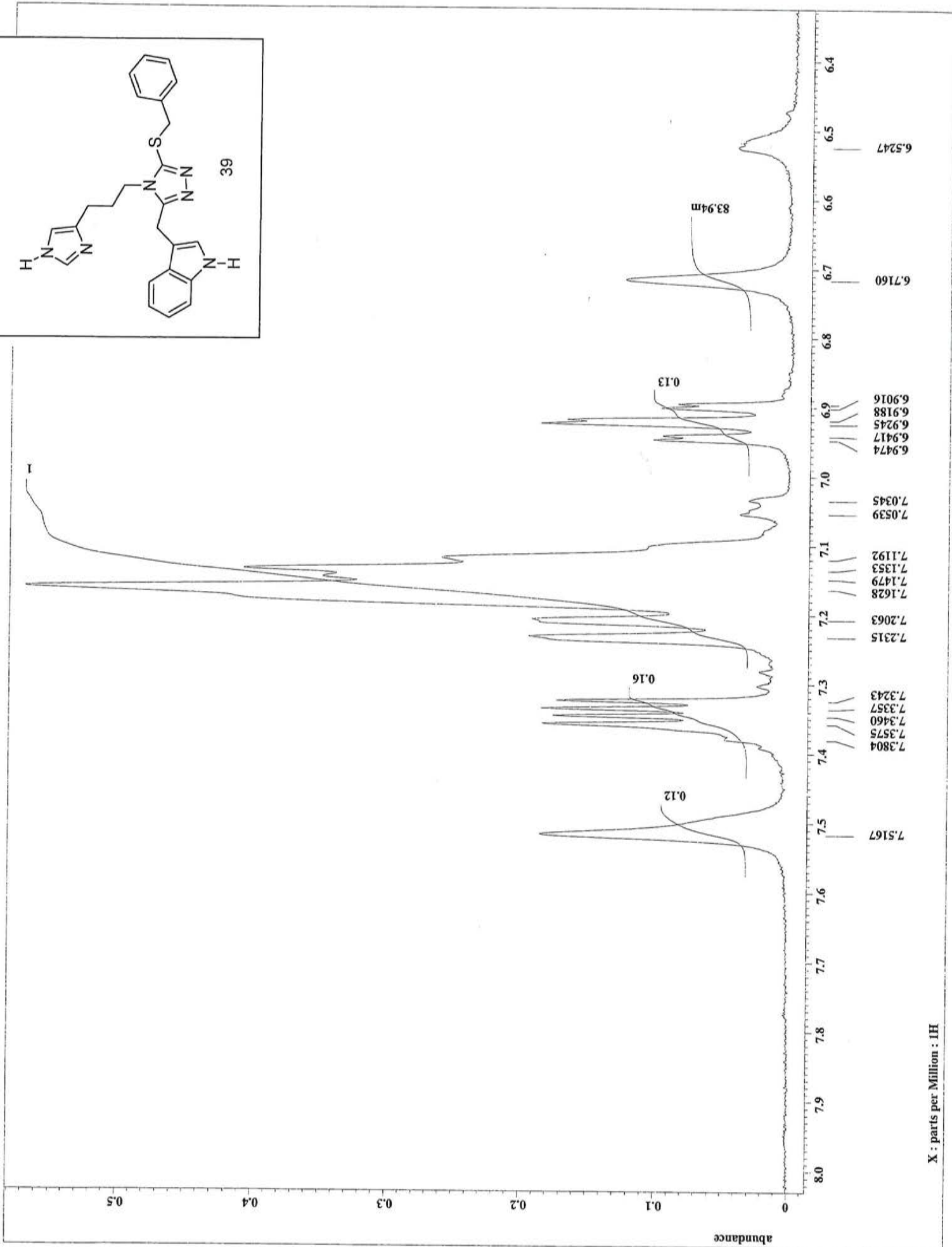
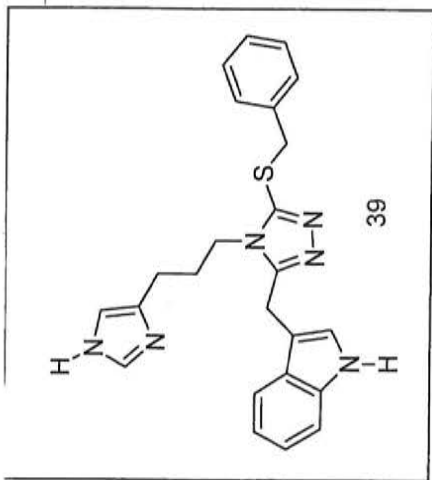


X : parts per Million : 1H

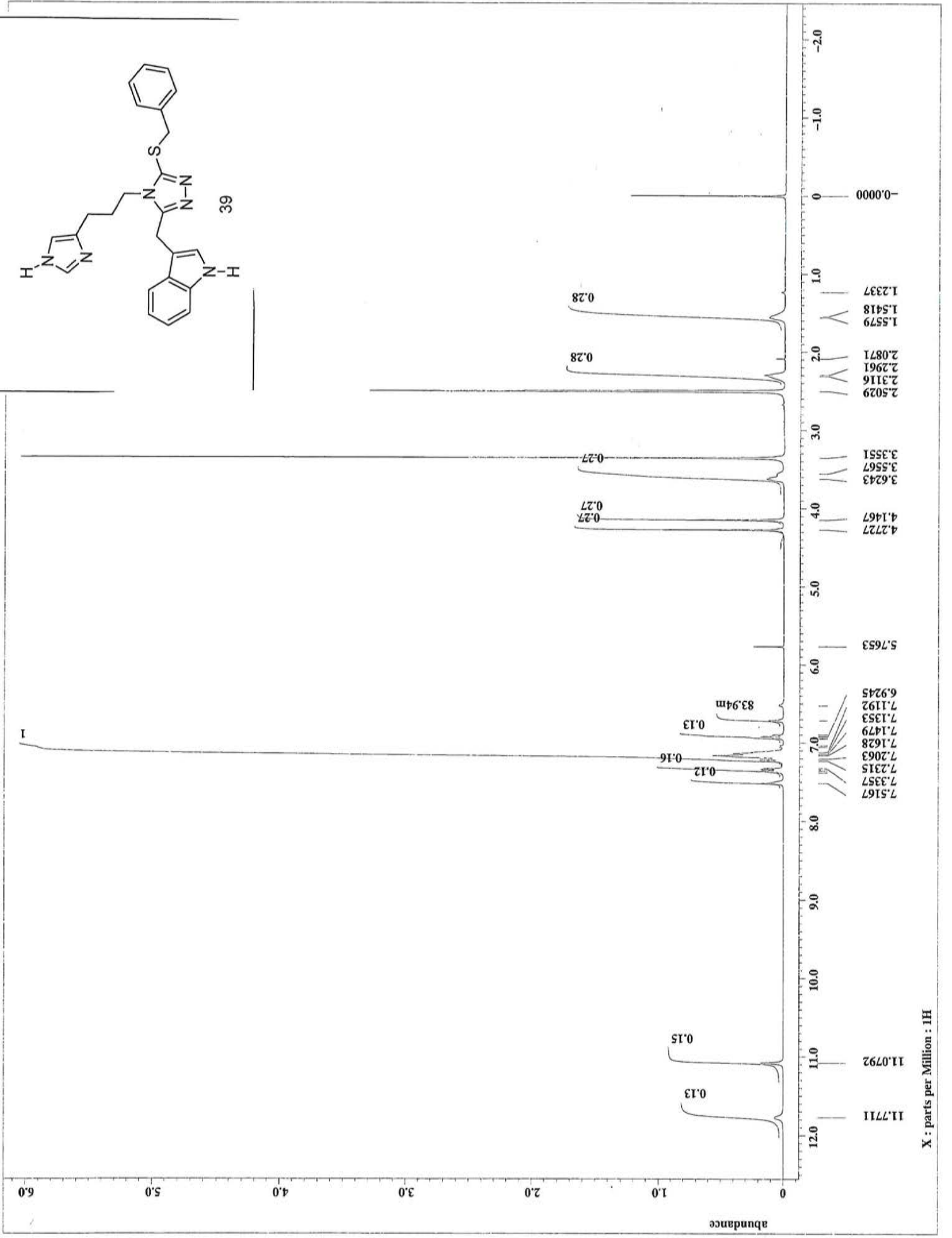
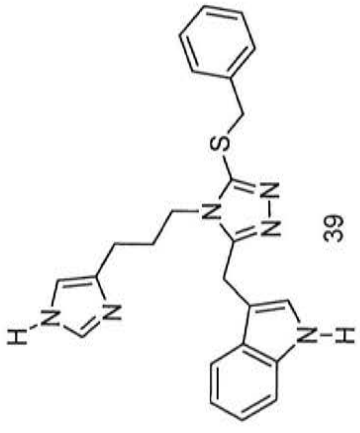


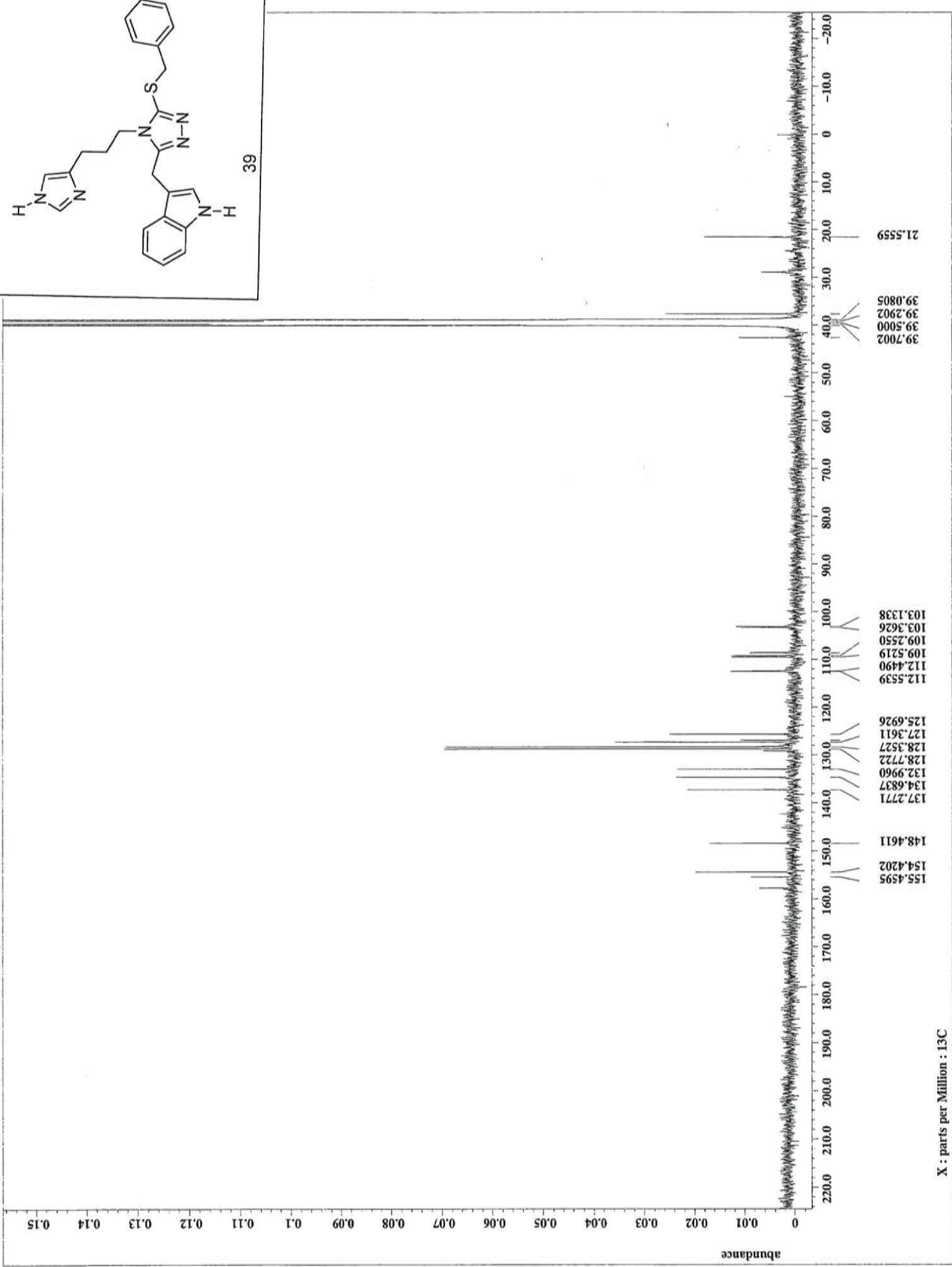
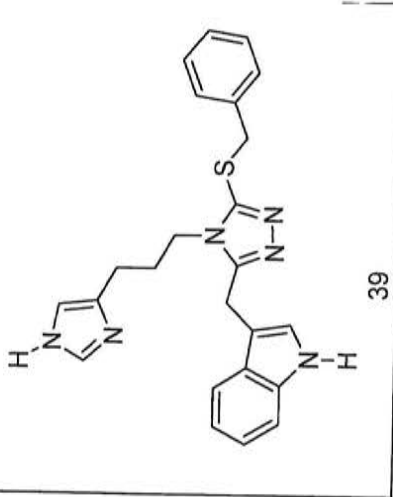


X : parts per Million : 13C

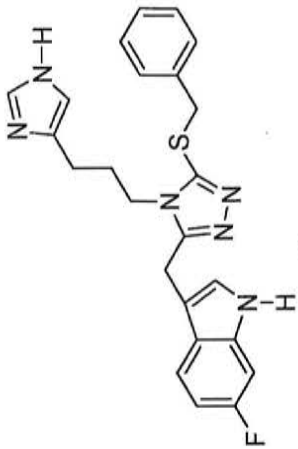


X : parts per Million : 1H





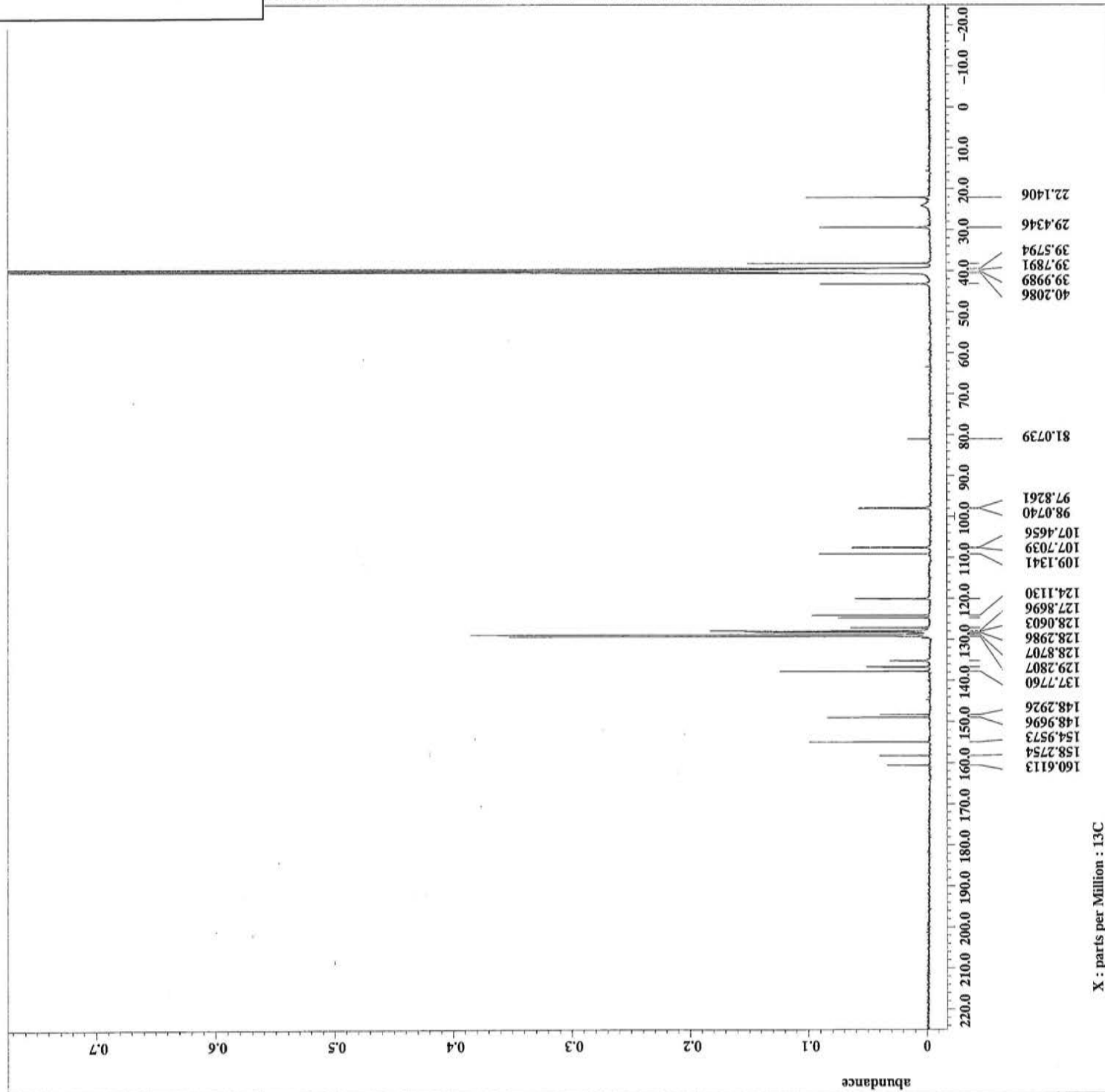
X : parts per Million : 13C



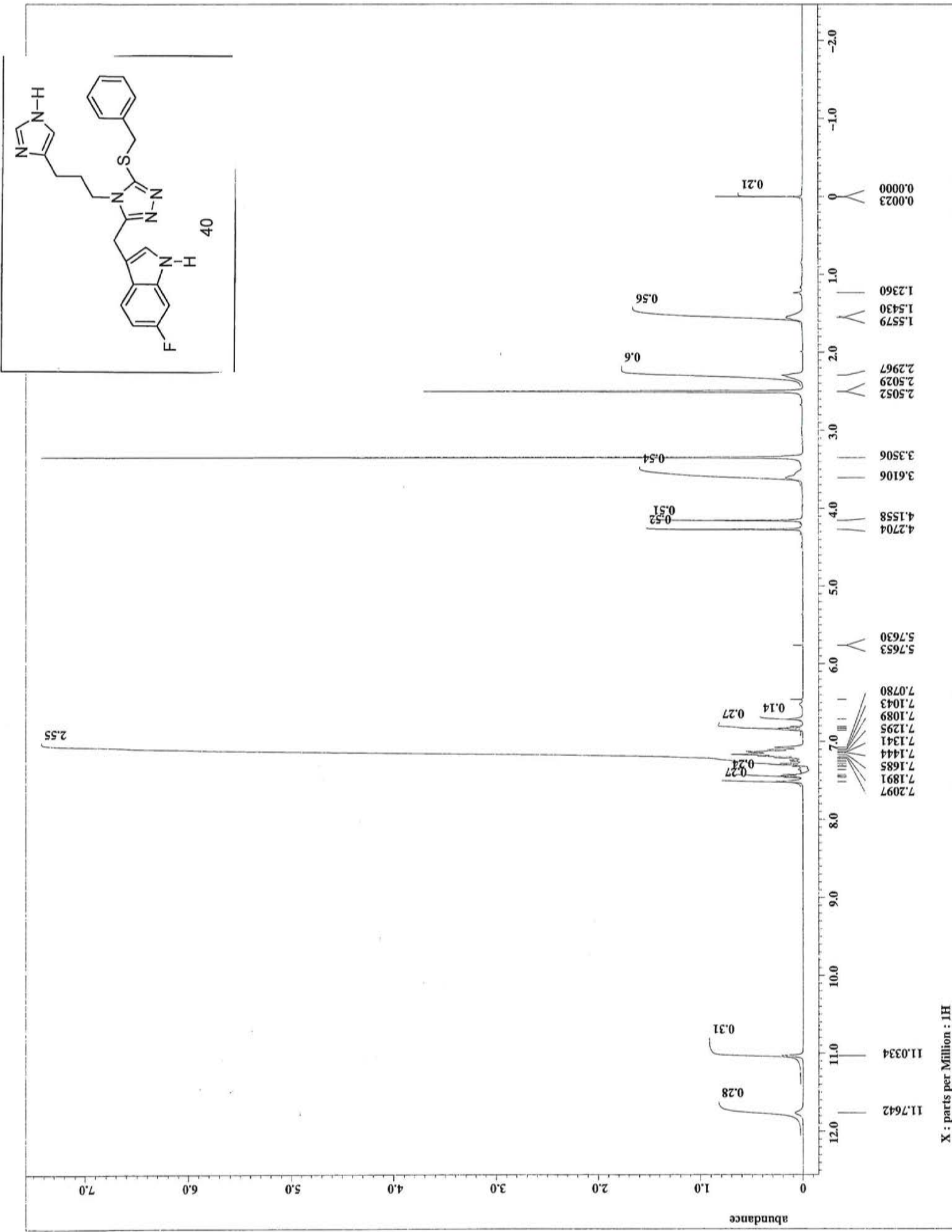
40

NOVA AREA

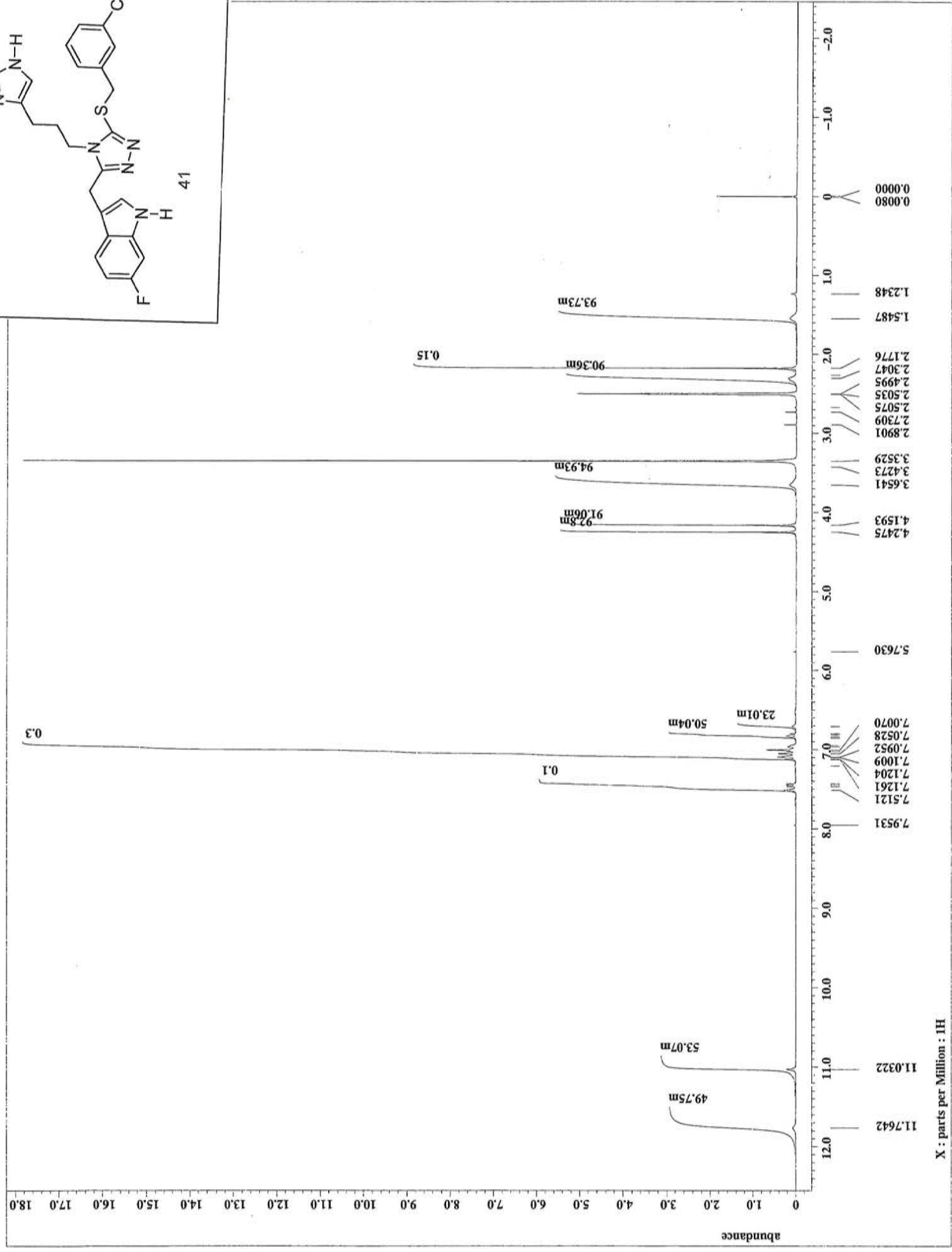
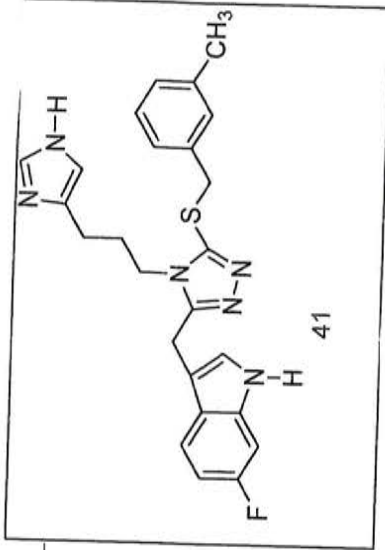
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 Dim_units = [ppm]
 Dimensions = X
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 Spectrometer = JNM-ECS400
 Field_strength = 9.389766 [T] (400 [MHz])
 X_acq_duration = 1.04333312 [s]
 X_domain = 13C
 X_freq = 100.52530333 [MHz]
 X_offset = 100 [ppm]
 X_points = 32768
 X_prescans = 4
 X_resolution = 0.95846665 [Hz]
 X_sweep = 31.40703518 [kHz]
 Irr_domain = 1H
 Irr_freq = 399.78219838 [MHz]
 Irr_offset = 5 [ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 12000
 Total_scans = 12000
 X_90_width = 12.84 [us]
 X_acq_time = 1.04333312 [s]
 X_angle = 30 [deg]
 X_atn = 9 [dB]
 X_pulse = 4.28 [us]
 Irr_atn_dec = 27 [dB]
 Irr_atn_noe = 27 [dB]
 Irr_noise = WALTZ
 Decoupling = TRUE
 Initial_wait = 1 [s]
 Nce = TRUE
 Noe_time = 2 [s]
 Recvr_gain = 60
 Relaxation_delay = 2 [s]
 Repetition_time = 3.04333312 [s]
 Temp_get = 19.5 [dC]



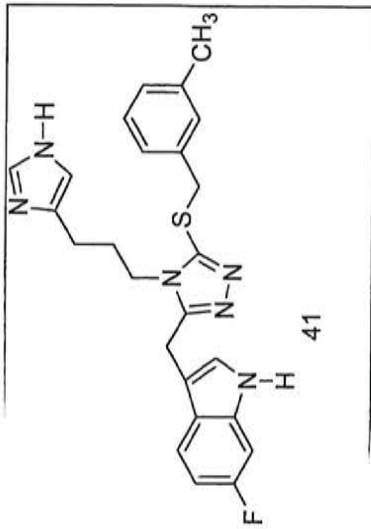
X : parts per Million : 13C



X : parts per Million : 1H



X : parts per Million : 1H



0.4

0.3

0.2

0.1

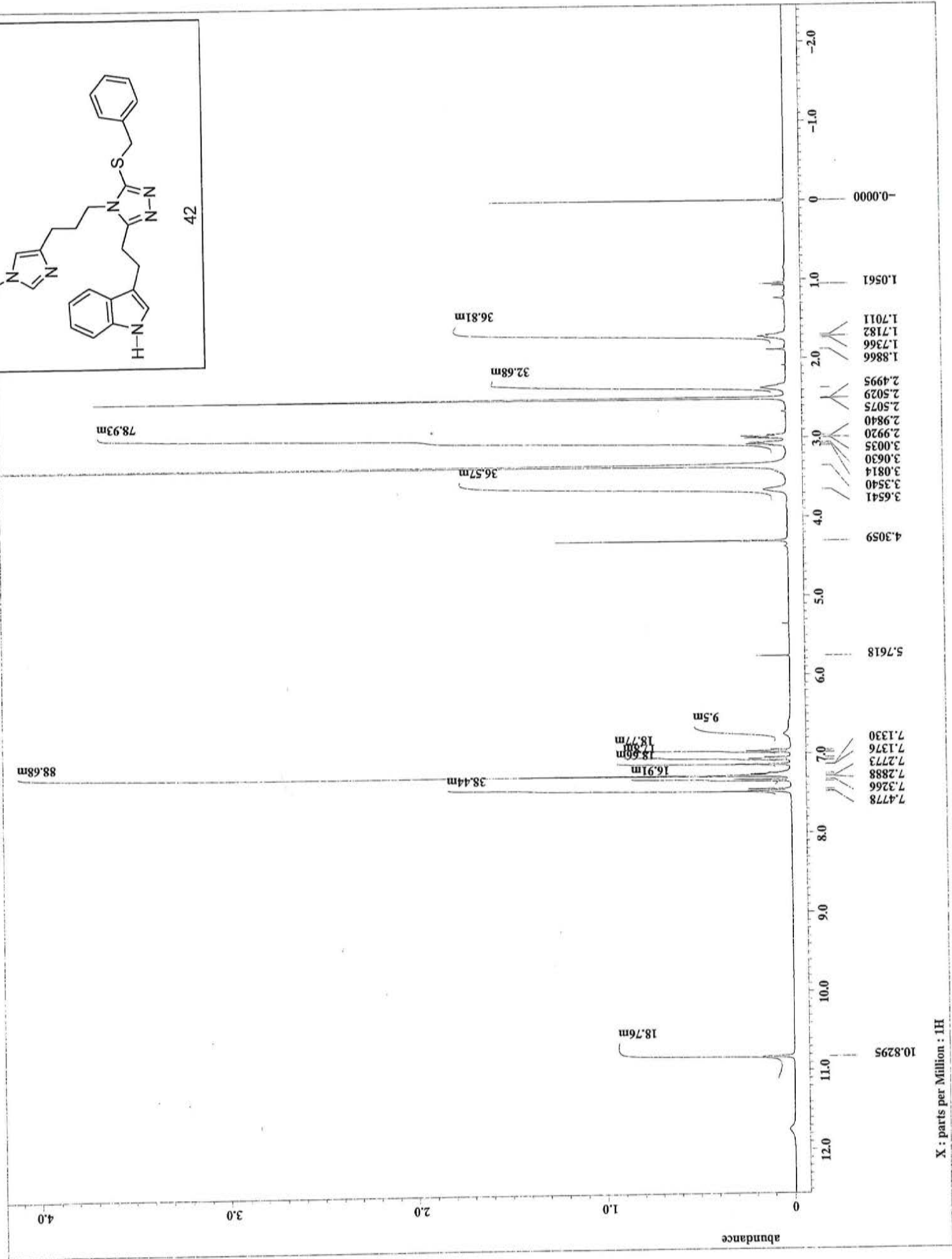
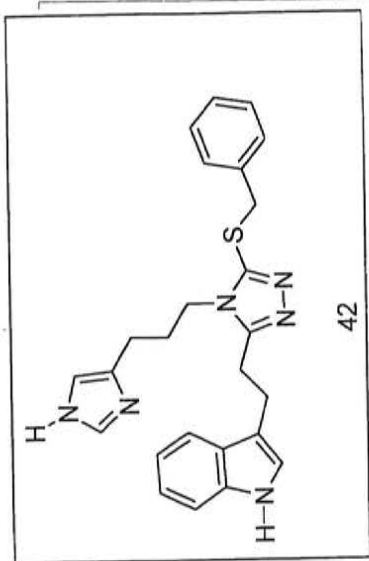
0

abundance

220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0

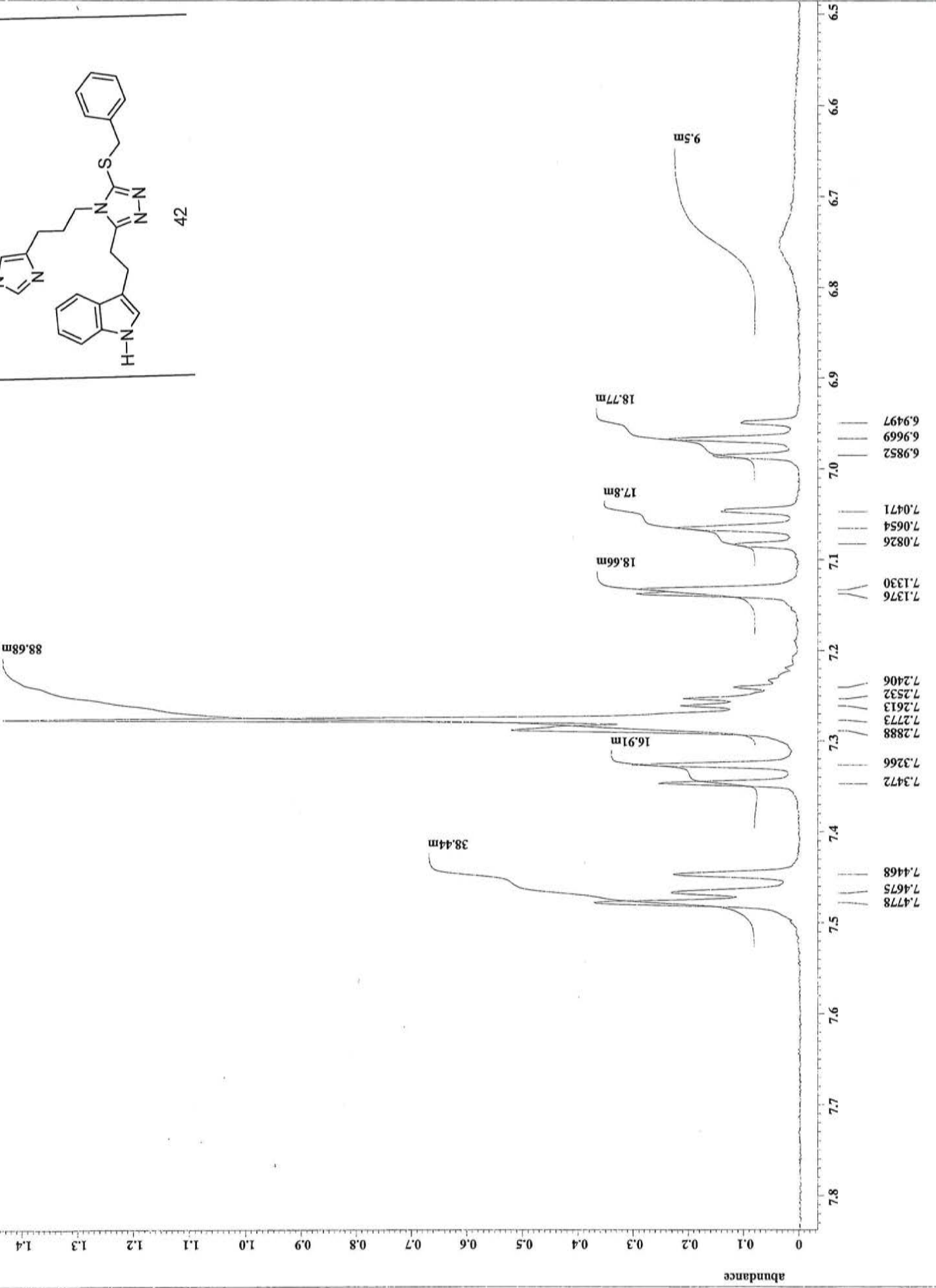
- 21.6227
- 20.8599
- 38.8707
- 39.0805
- 39.2902
- 39.5000
- 39.7002
- 39.9100
- 40.1197
- 97.6228
- 97.3653
- 107.0429
- 107.2813
- 108.7306
- 123.6522
- 125.9119
- 127.6281
- 128.1239
- 128.3336
- 129.4301
- 134.7504
- 137.1055
- 137.7061
- 148.6518
- 154.4965
- 157.8336
- 160.1601

X : parts per Million : 13C

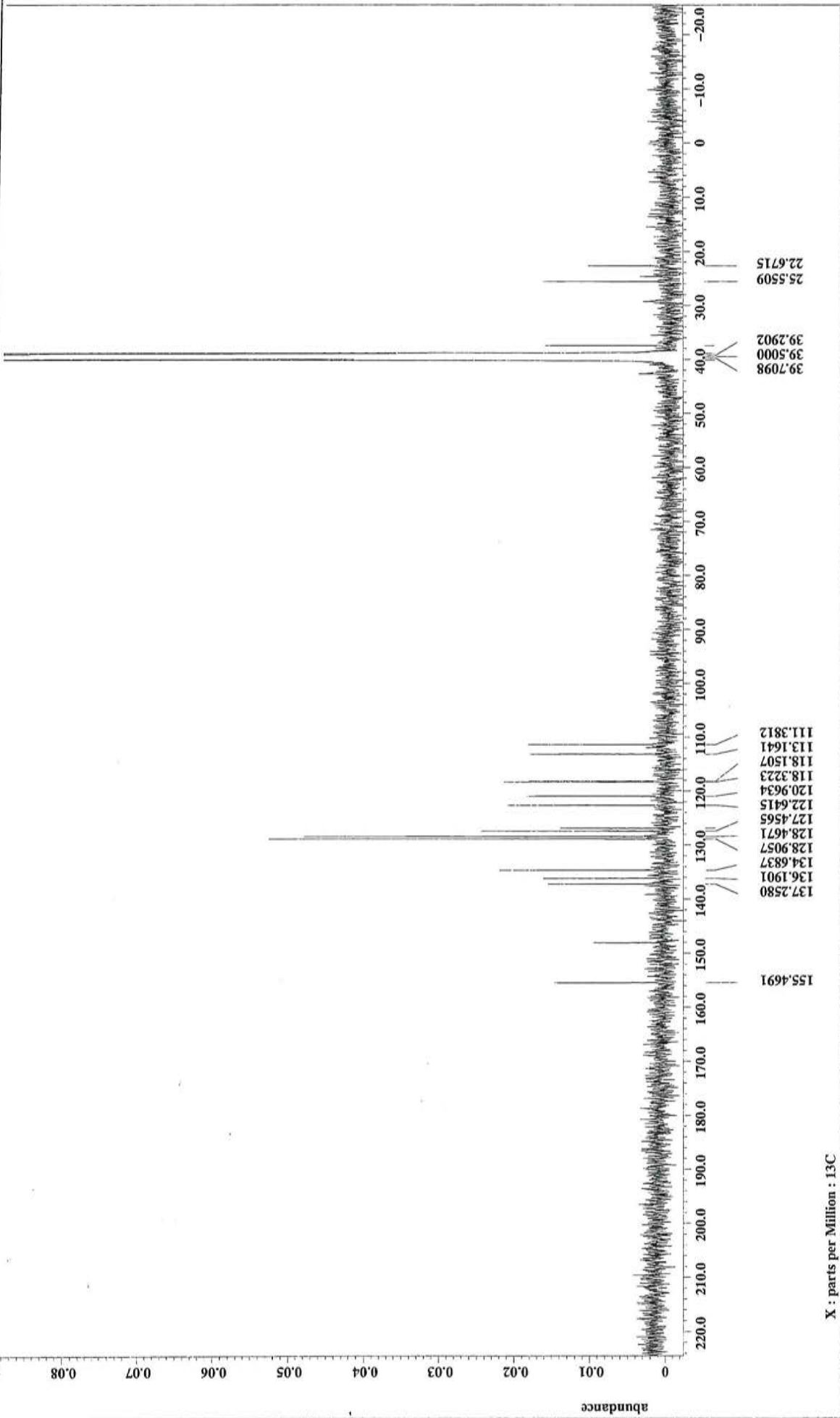
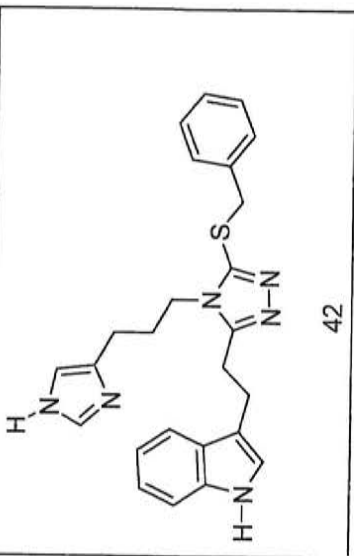


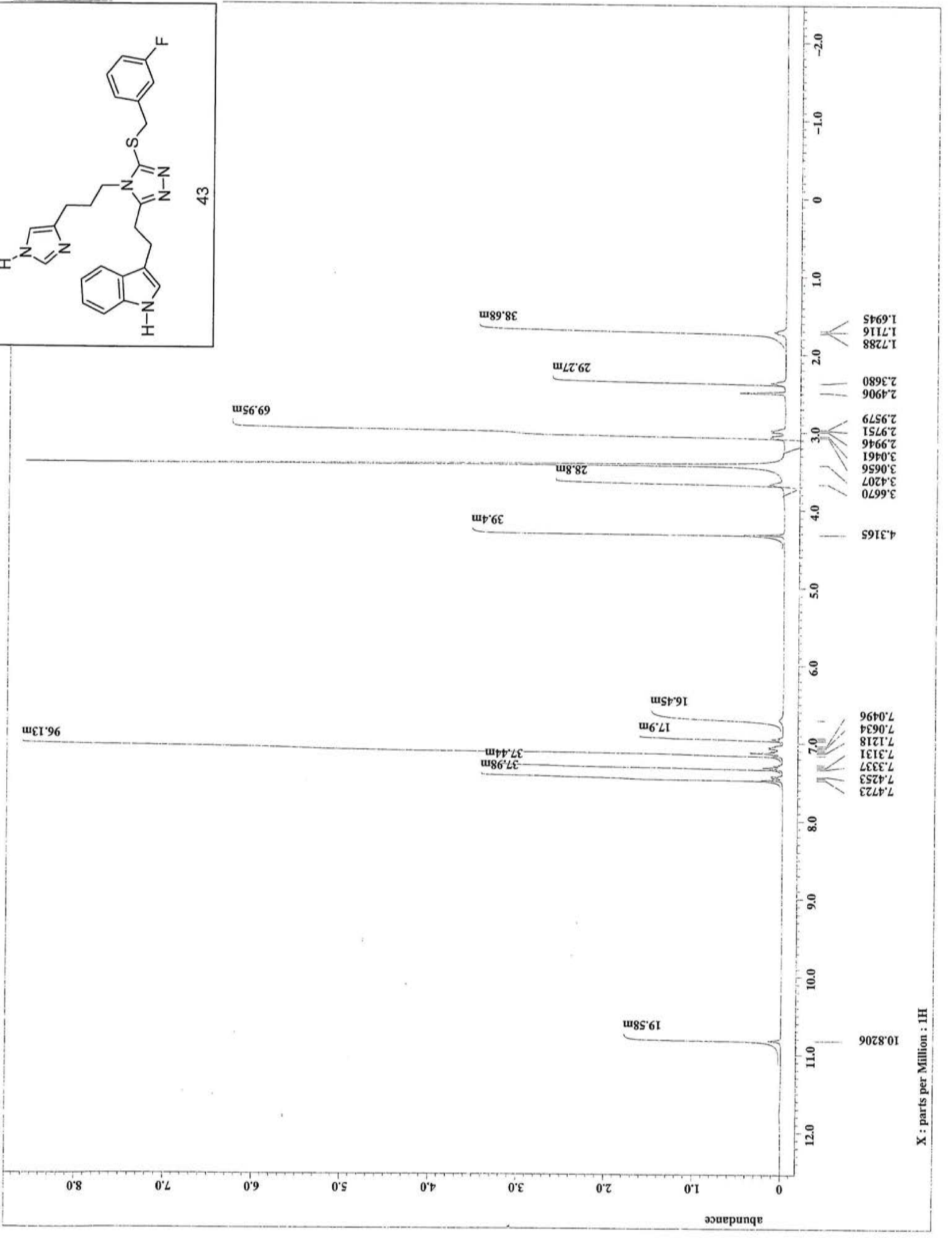
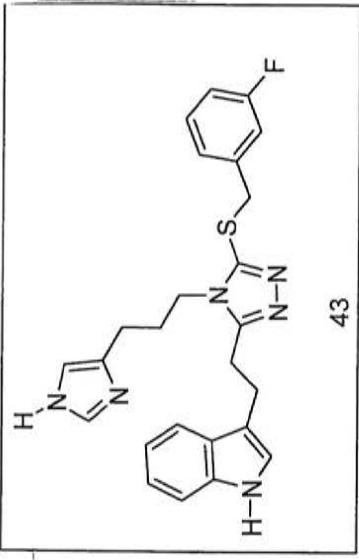
X : parts per Million : 1H

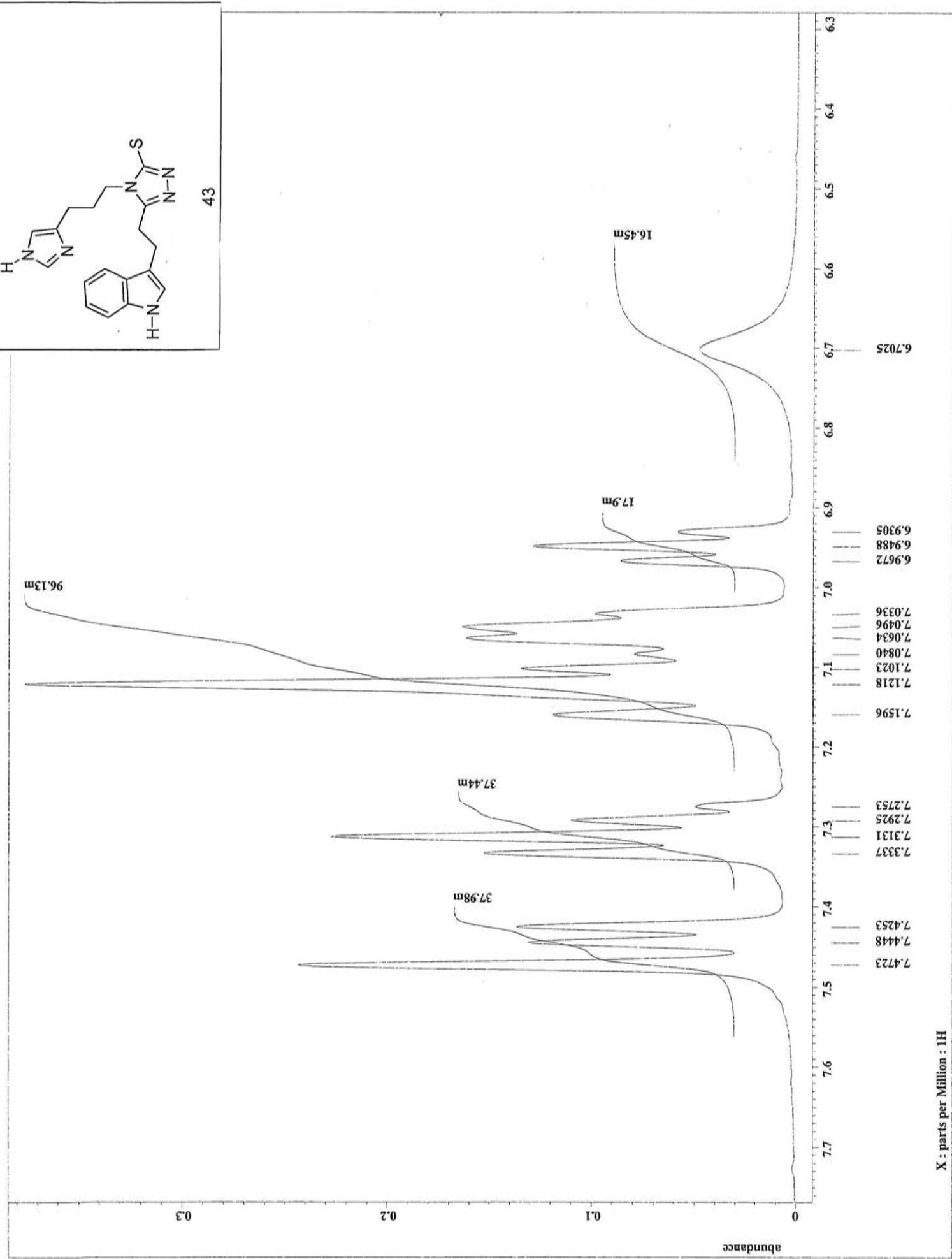
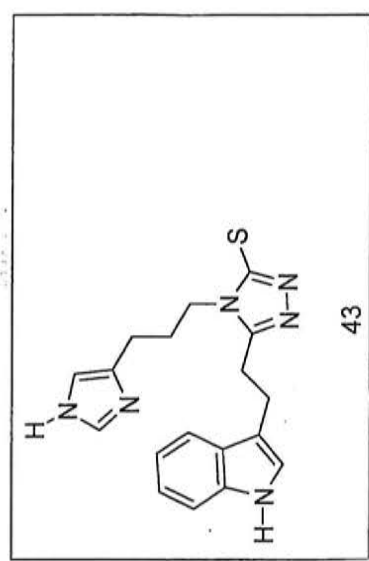
X : parts per Million : 1H



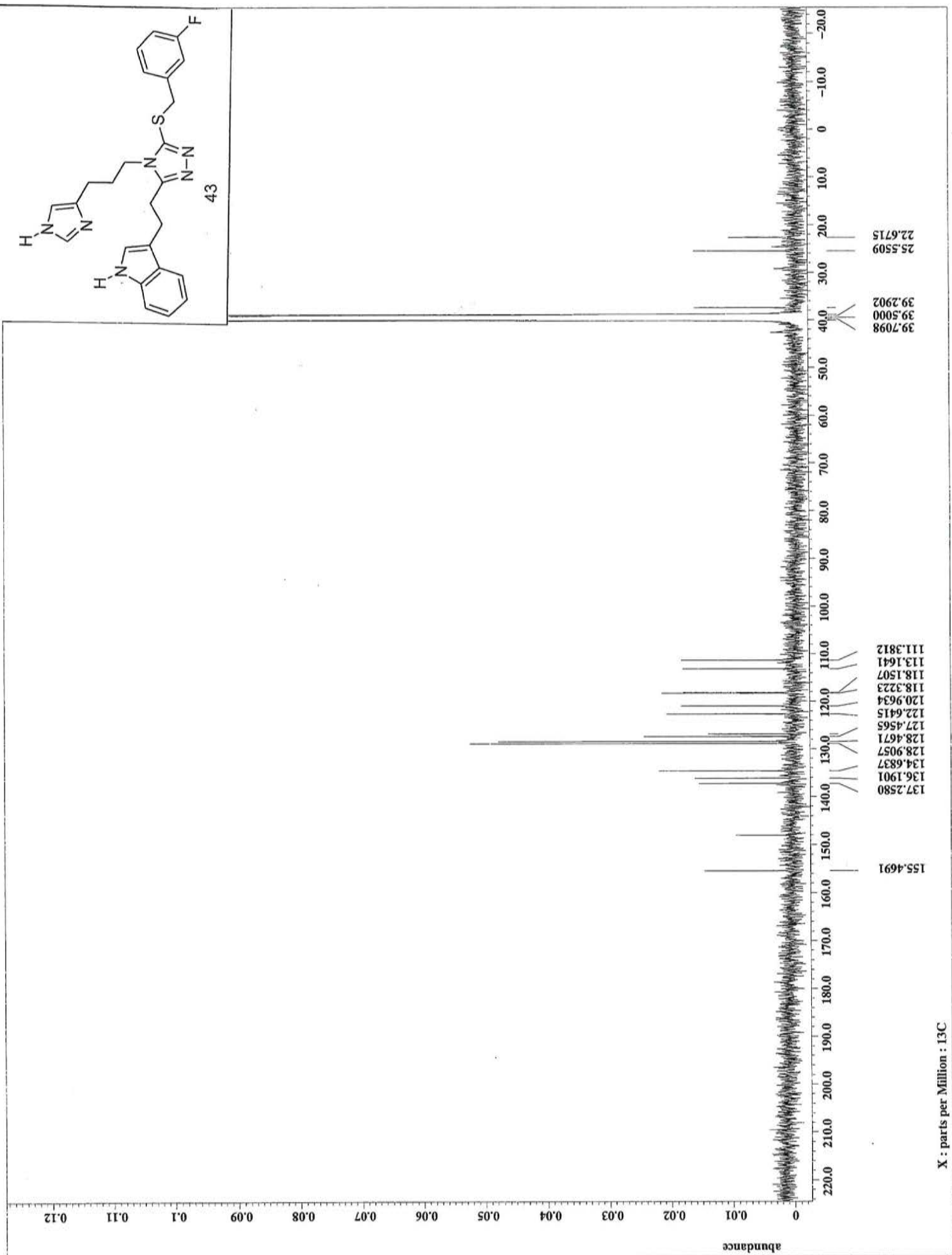
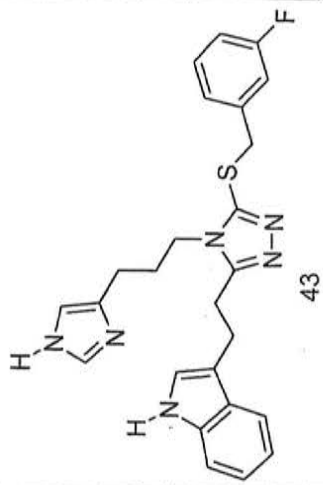
42



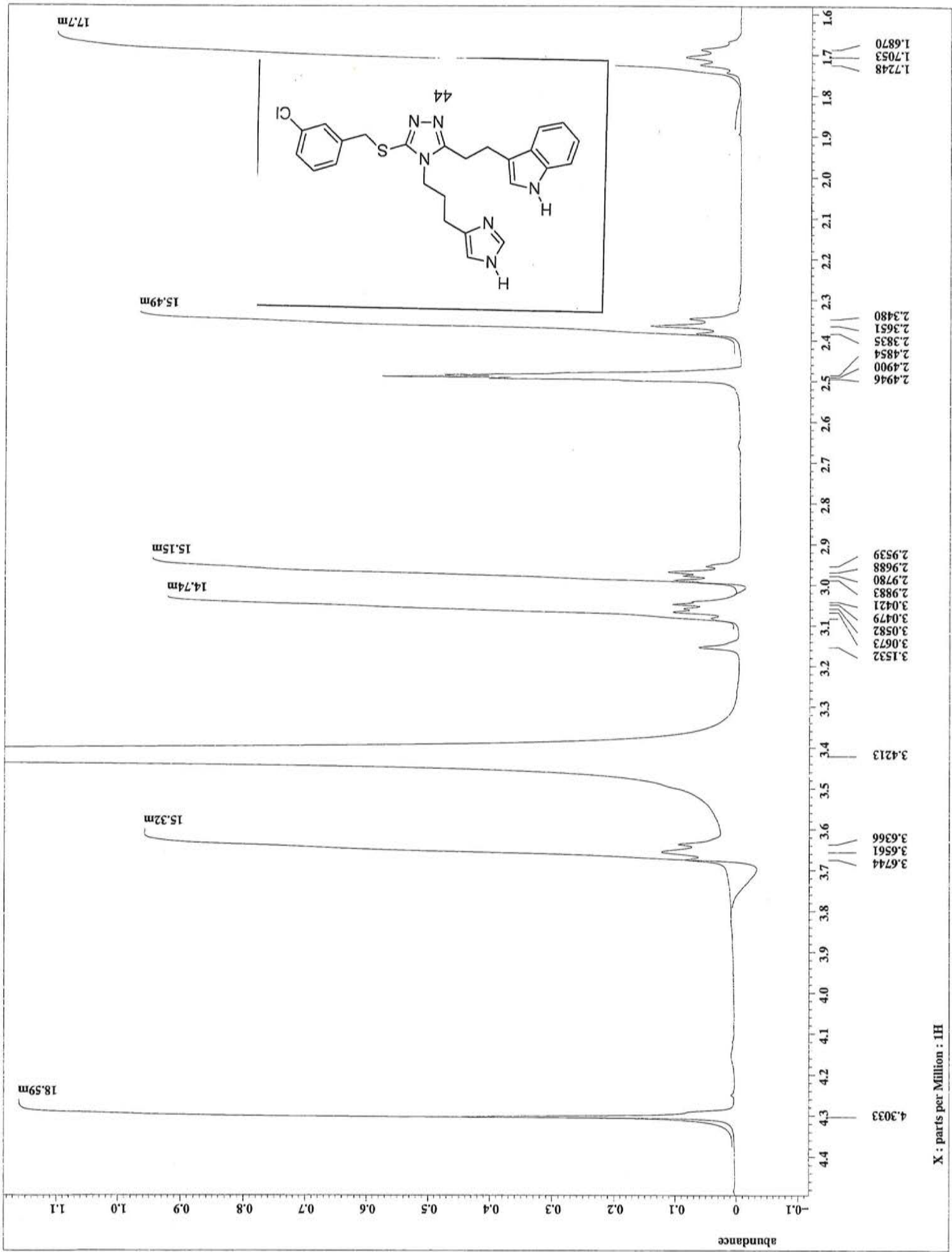




X : parts per Million : 1H



750 300



- 1.6870
- 1.7053
- 1.7248
- 1.7
- 1.8
- 1.9
- 2.0
- 2.1
- 2.2
- 2.3
- 2.3480
- 2.3651
- 2.3835
- 2.4854
- 2.4900
- 2.4946
- 2.5
- 2.6
- 2.7
- 2.8
- 2.9
- 2.9539
- 2.9688
- 2.9780
- 2.9883
- 3.0421
- 3.0479
- 3.0582
- 3.0673
- 3.1532
- 3.2
- 3.3
- 3.4
- 3.4213
- 3.5
- 3.6
- 3.6366
- 3.6561
- 3.6744
- 3.7
- 3.8
- 3.9
- 4.0
- 4.1
- 4.2
- 4.3
- 4.3033
- 4.4

X : parts per Million : 1H

abundance

17.7m

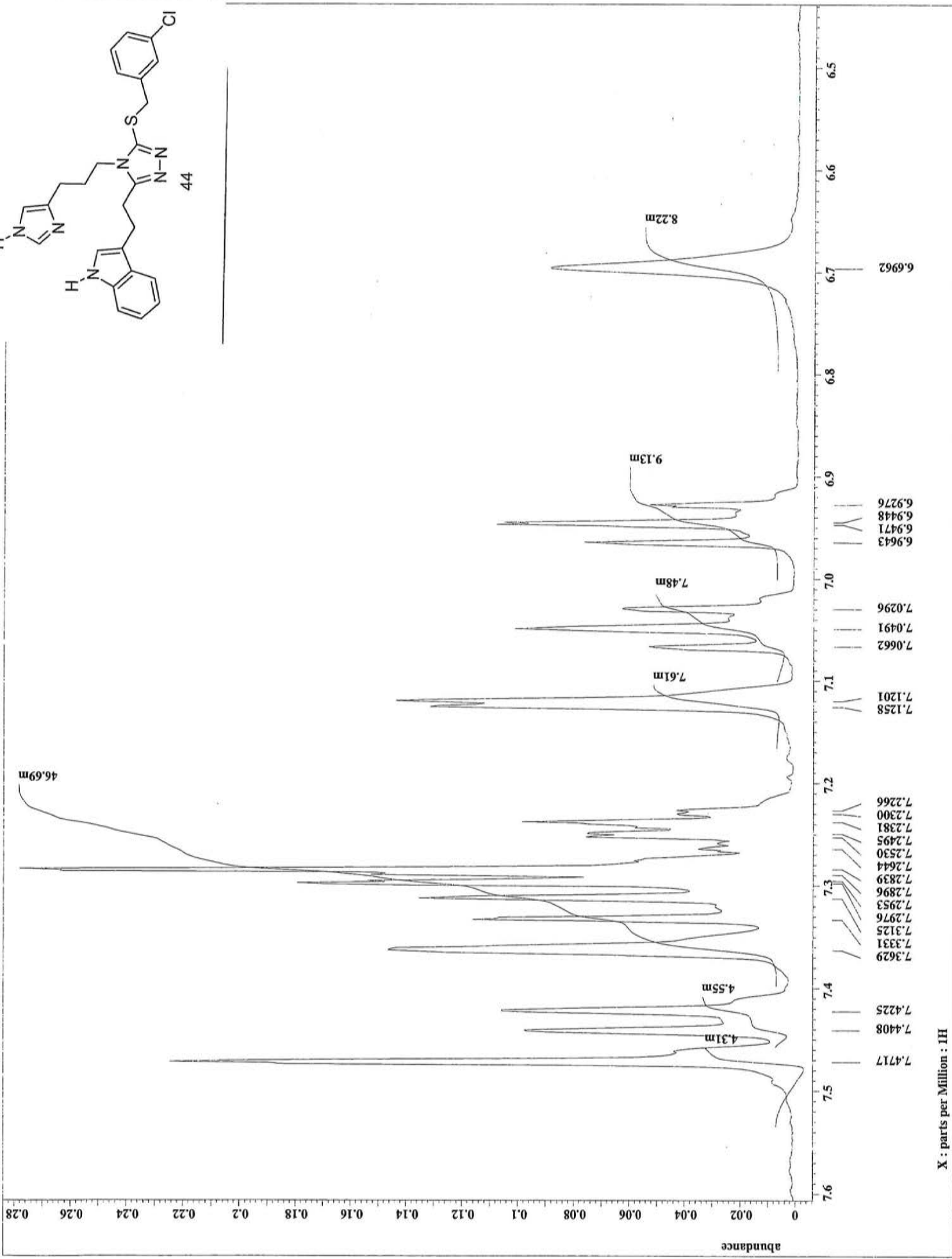
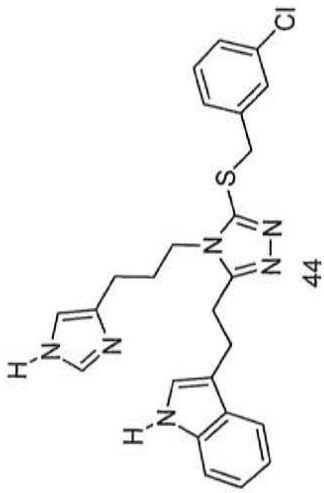
15.49m

15.15m

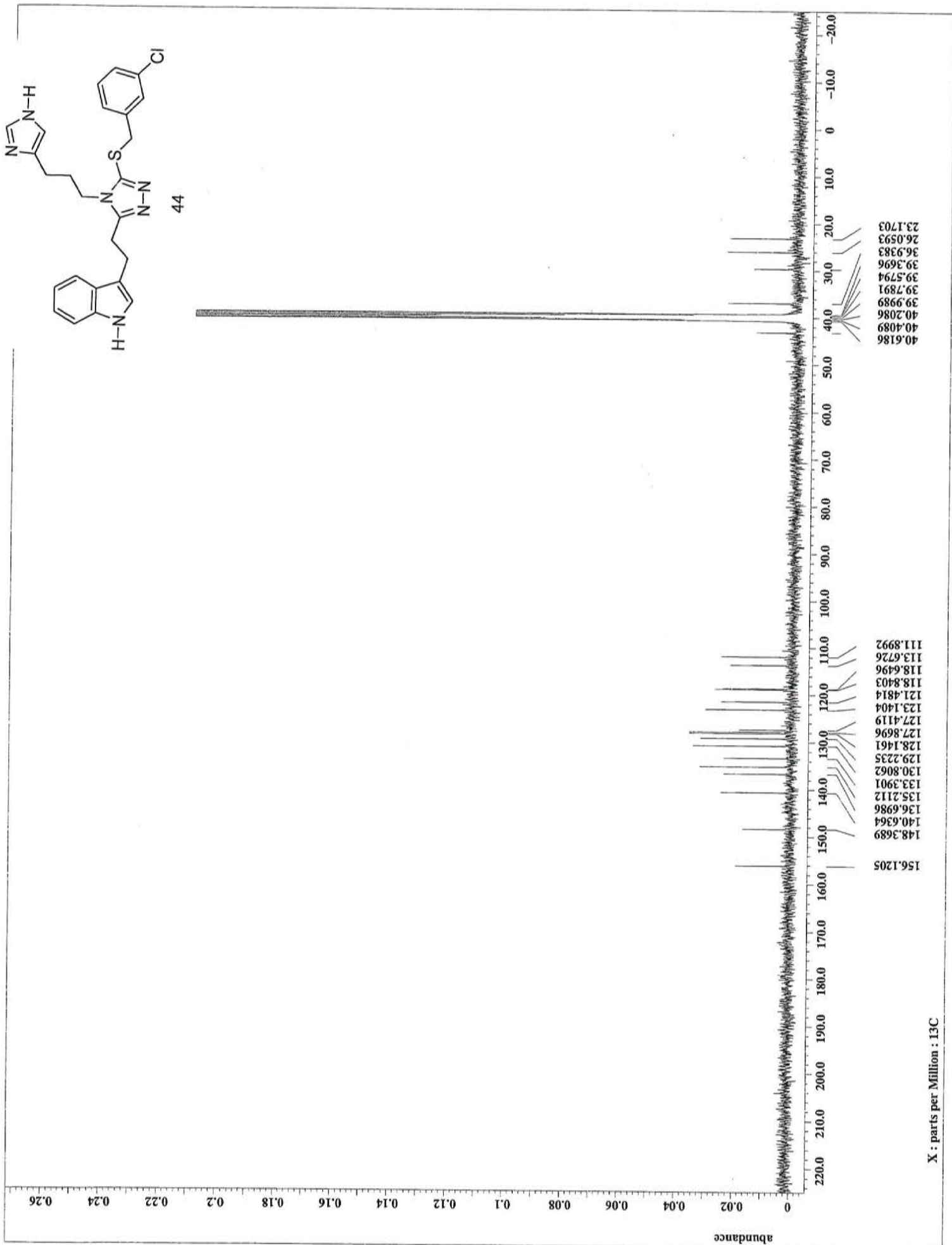
14.74m

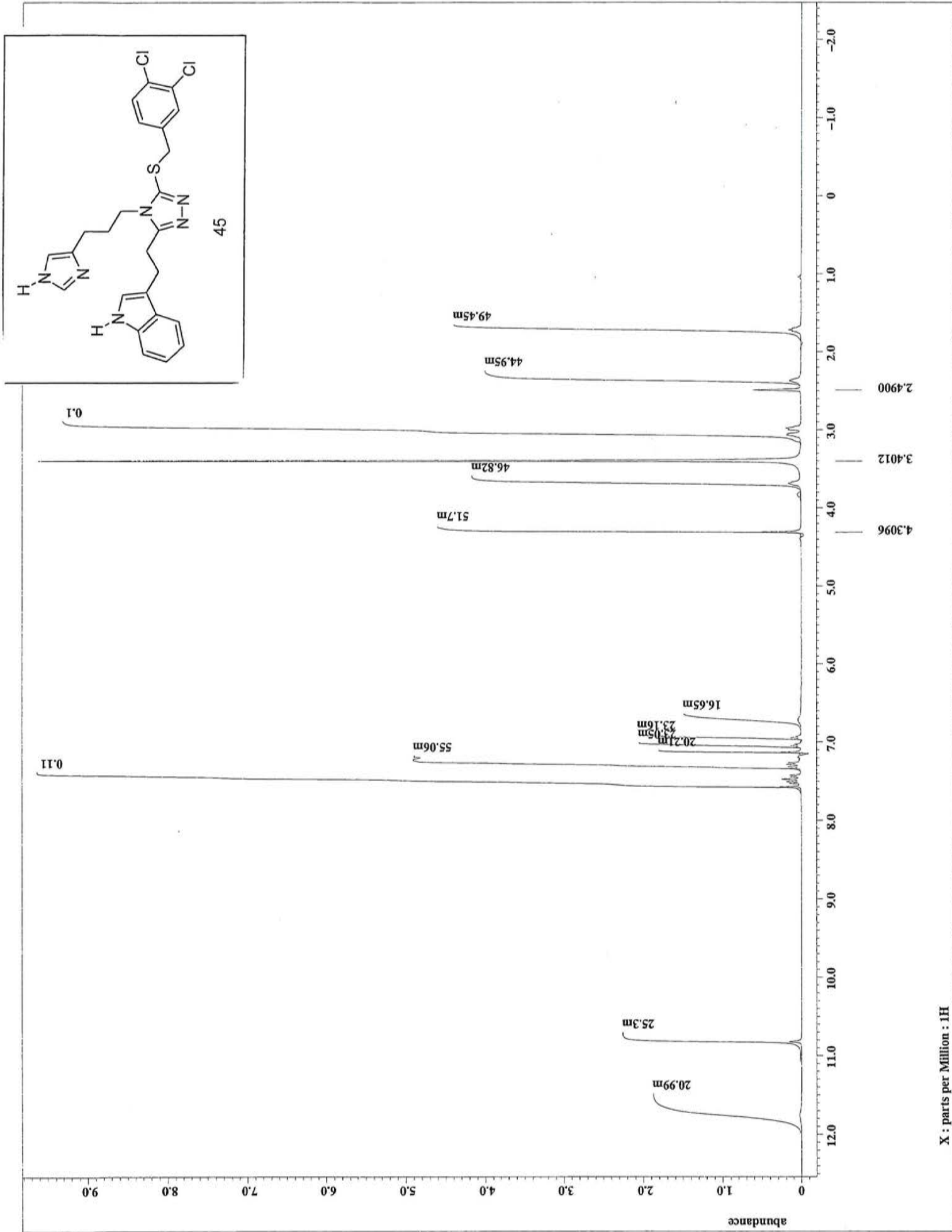
15.32m

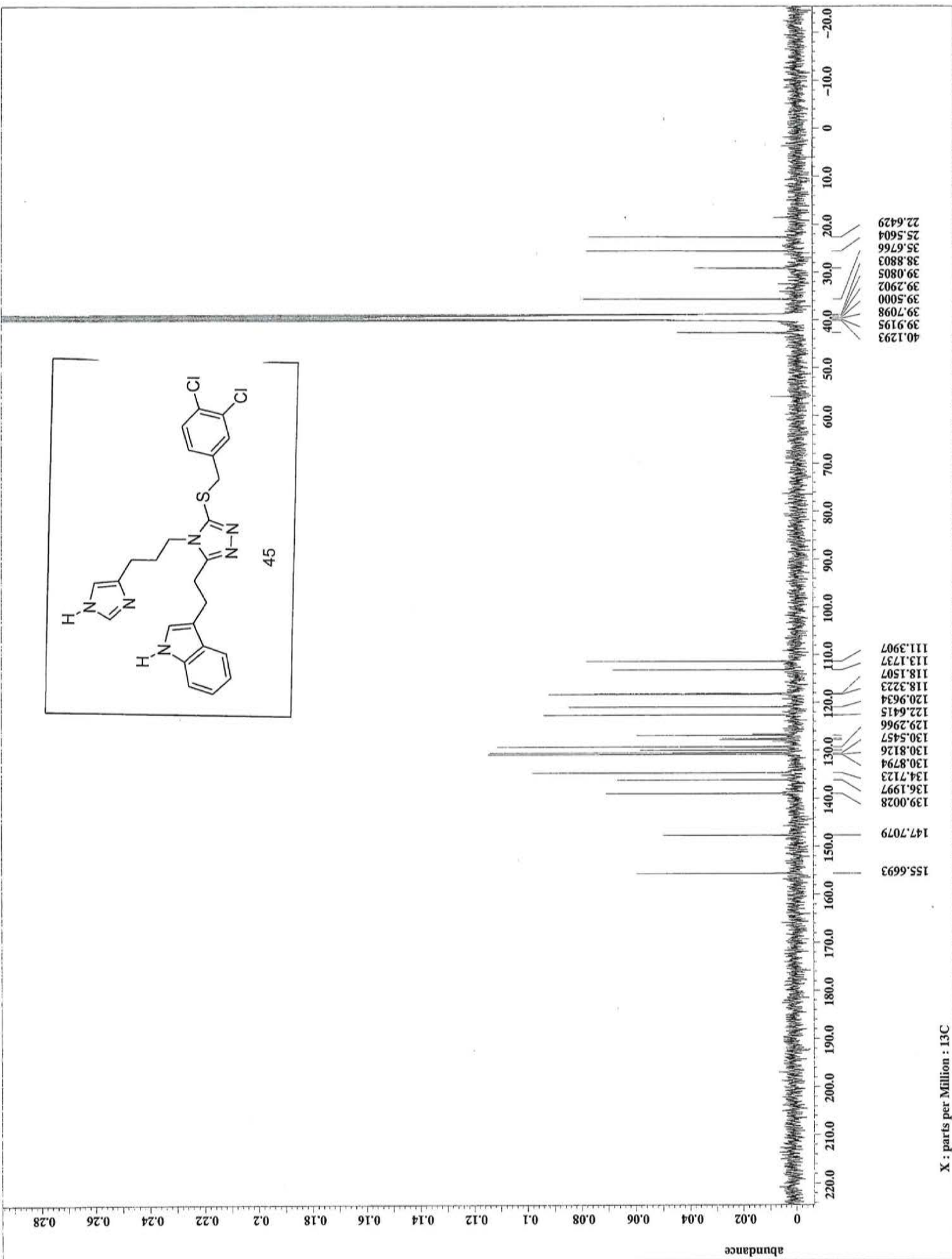
18.59m

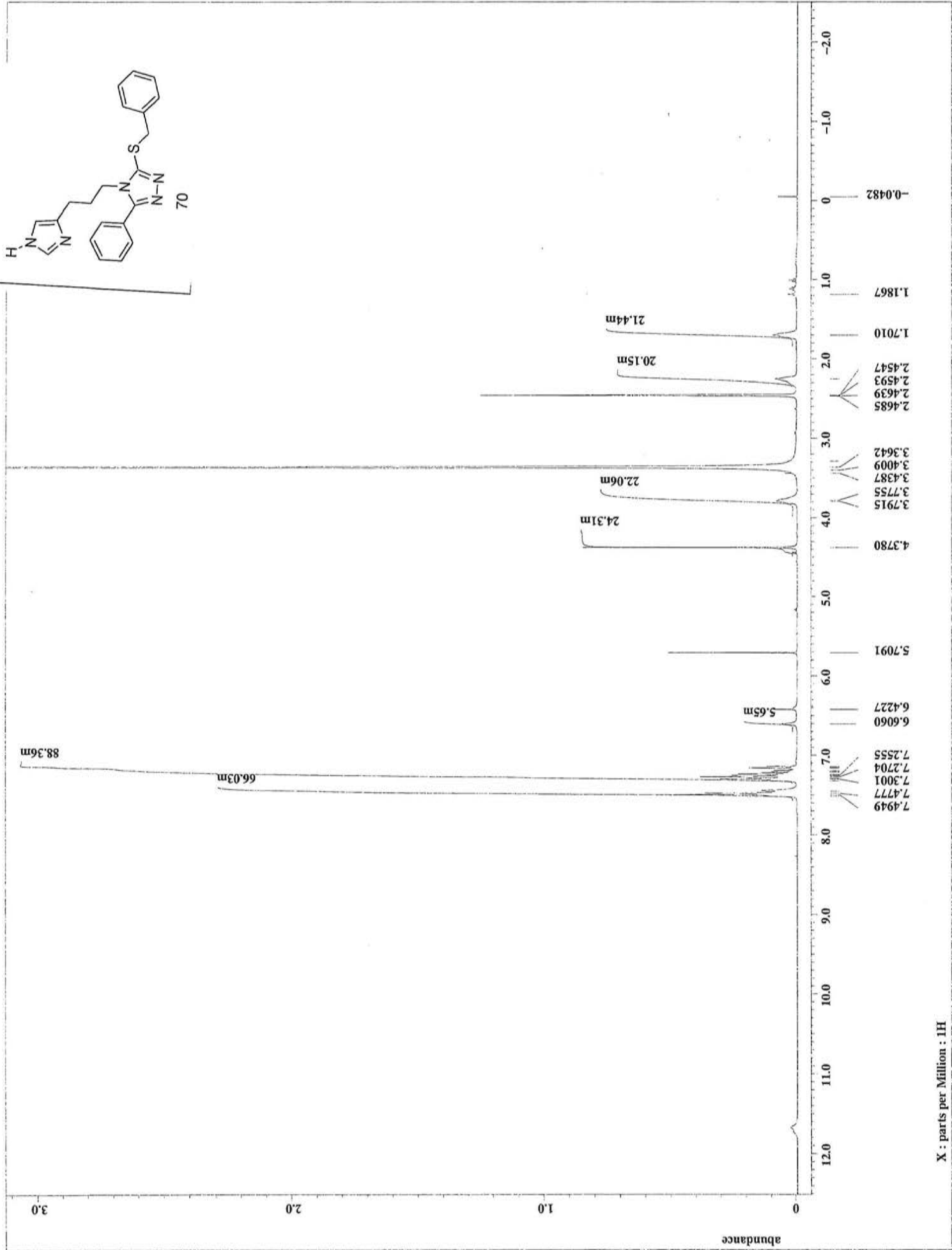


X : parts per Million : 1H

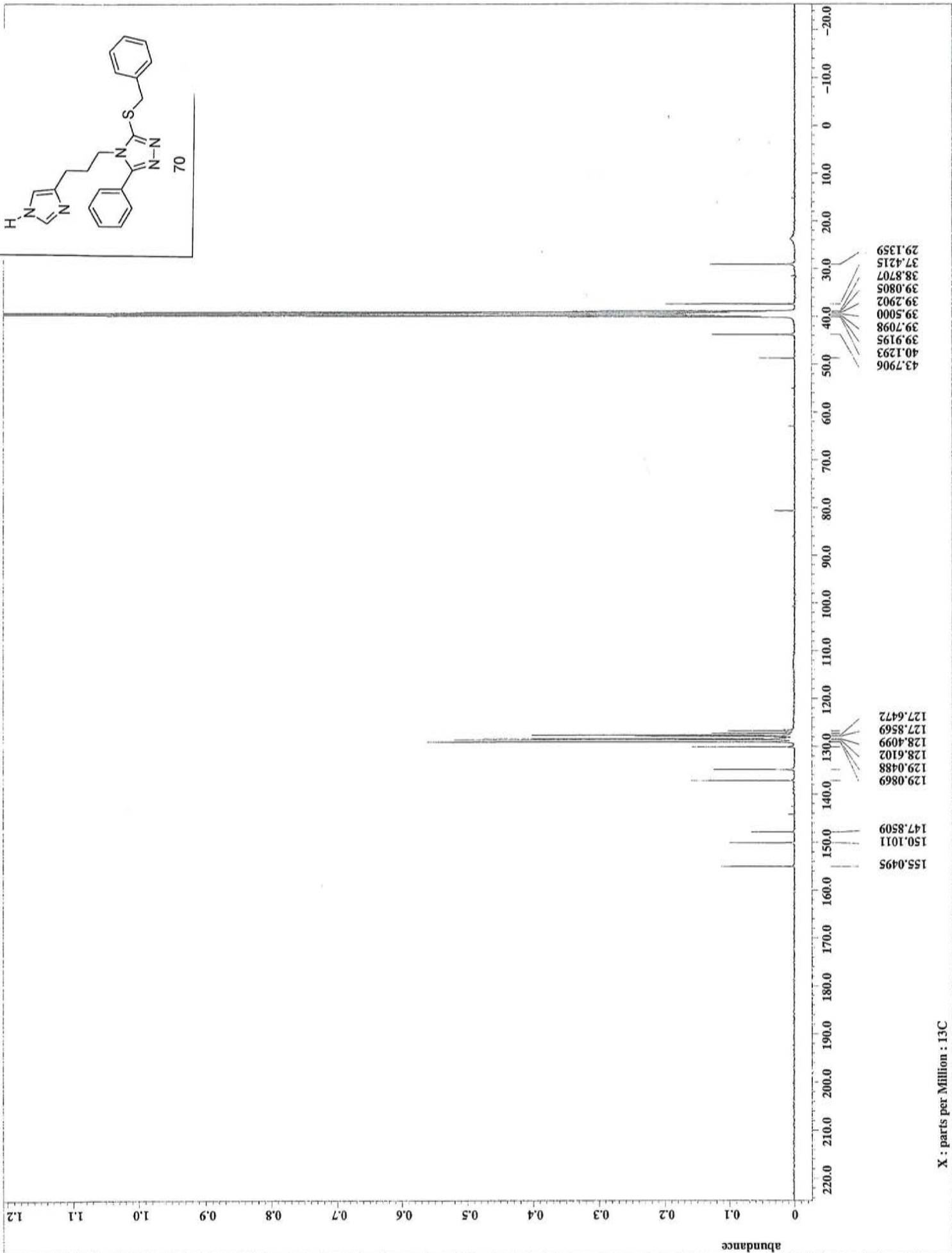


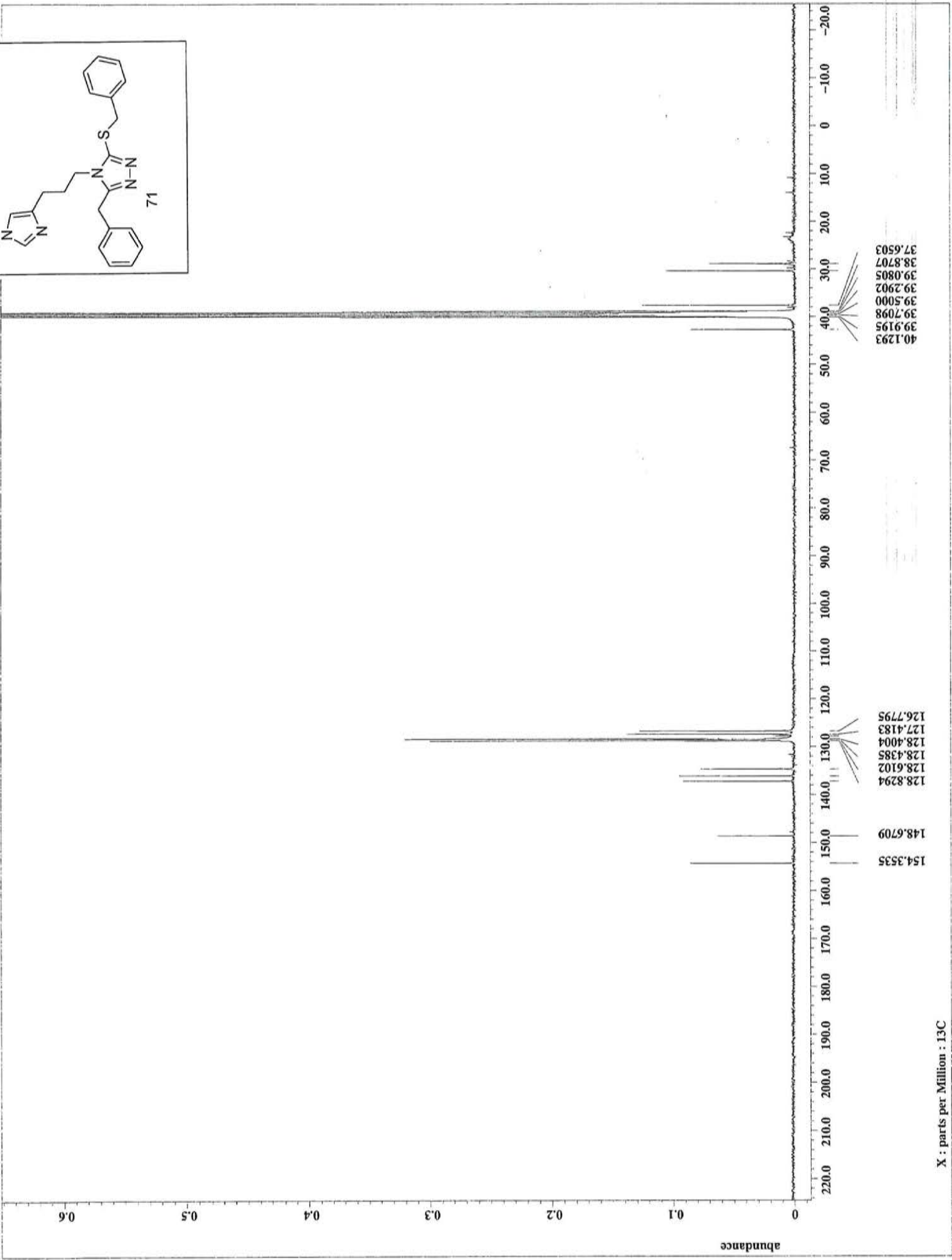
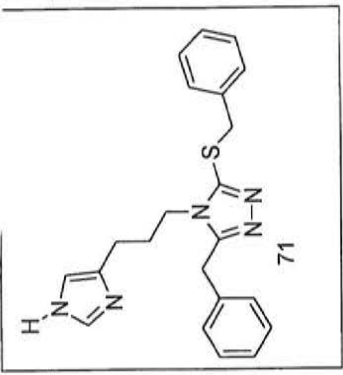


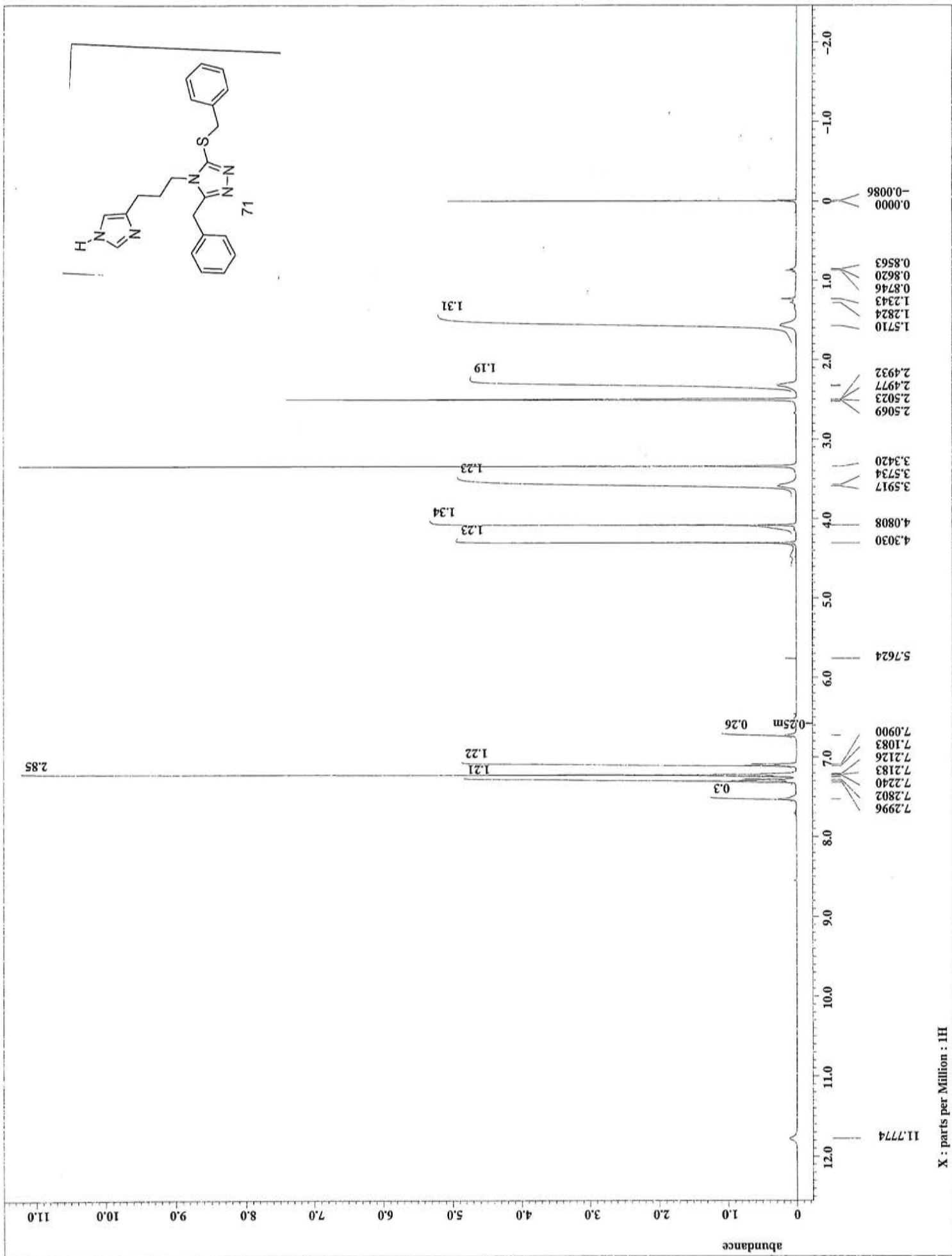




X : parts per Million : 1H







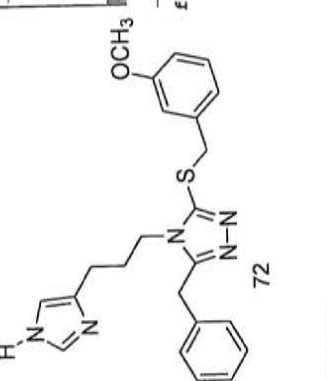
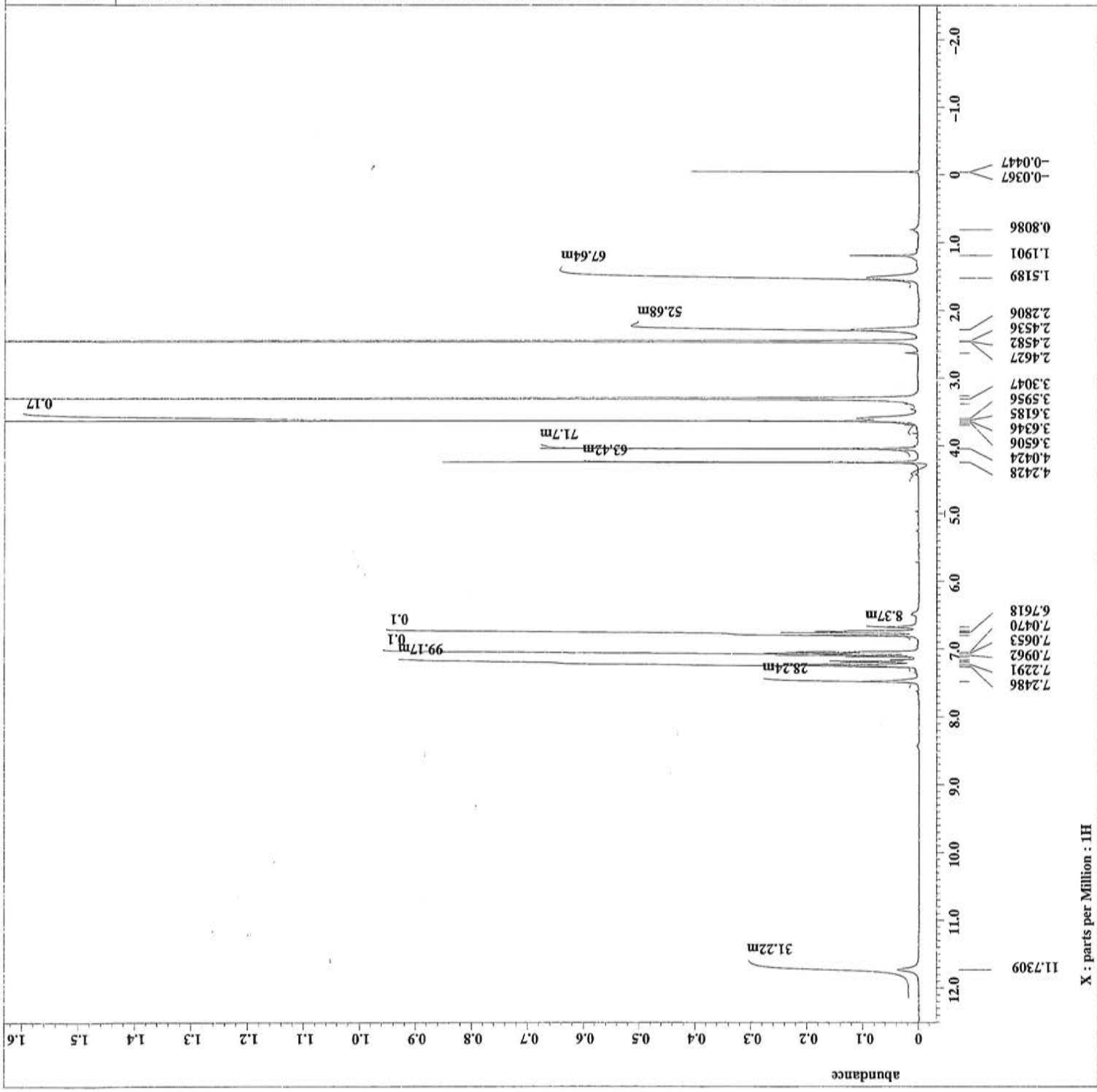
Filer
 Authc
 Exper
 Sampl
 Solv
 Creat
 Revis
 Curre

72

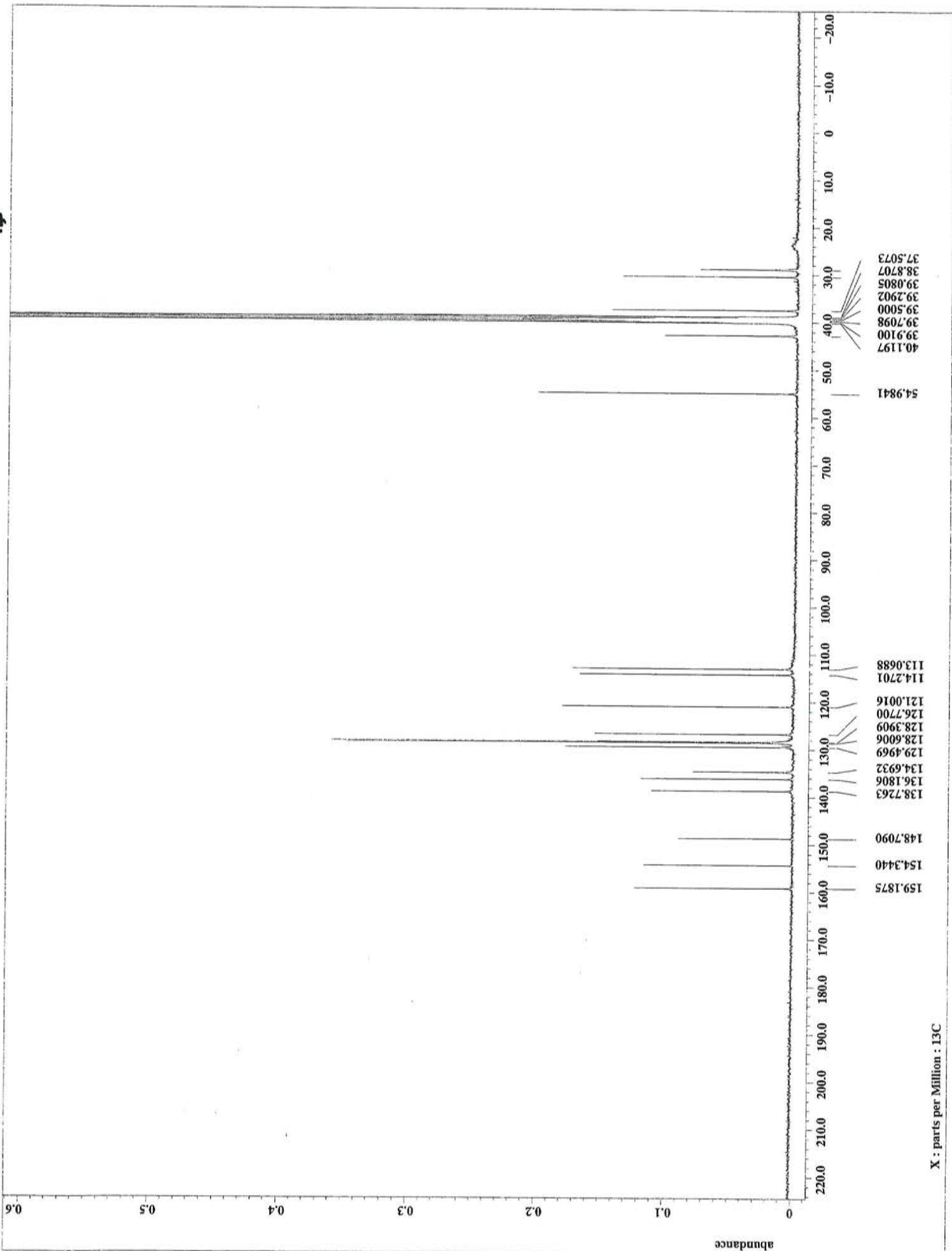
Data_format = 1D COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
 Dimensions = X
 Site = ECS 400
 Spectrometer = JNM-ECS400

Field_strength = 9.389766[T] (400 [MHz])
 X_acq_duration = 2.18365952[s]
 X_domain = 1H
 X_freq = 399.78219838 [MHz]
 X_offset = 5 [ppm]
 X_points = 16384
 X_prescans = 1
 X_resolution = 0.45794685 [Hz]
 X_sweep = 7.5030012 [kHz]
 Irr_domain = 1H
 Irr_freq = 399.78219838 [MHz]
 Irr_offset = 5 [ppm]
 Tri_domain = 1H
 Tri_freq = 399.78219838 [MHz]
 Tri_offset = 5 [ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 64
 Total_scans = 64

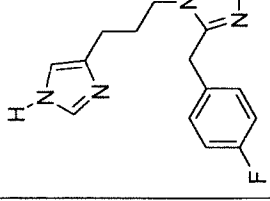
X_90_width = 10.65 [us]
 X_acq_time = 2.18365952[s]
 X_angle = 45 [deg]
 X_atn = 6 [dB]
 X_pulse = 5.325 [us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1 [s]
 Recvr_gain = 46
 Relaxation_delay = 4 [s]
 Repetition_time = 6.18365952[s]
 Temp_get = 19 [dC]



X : parts per Million : 1H

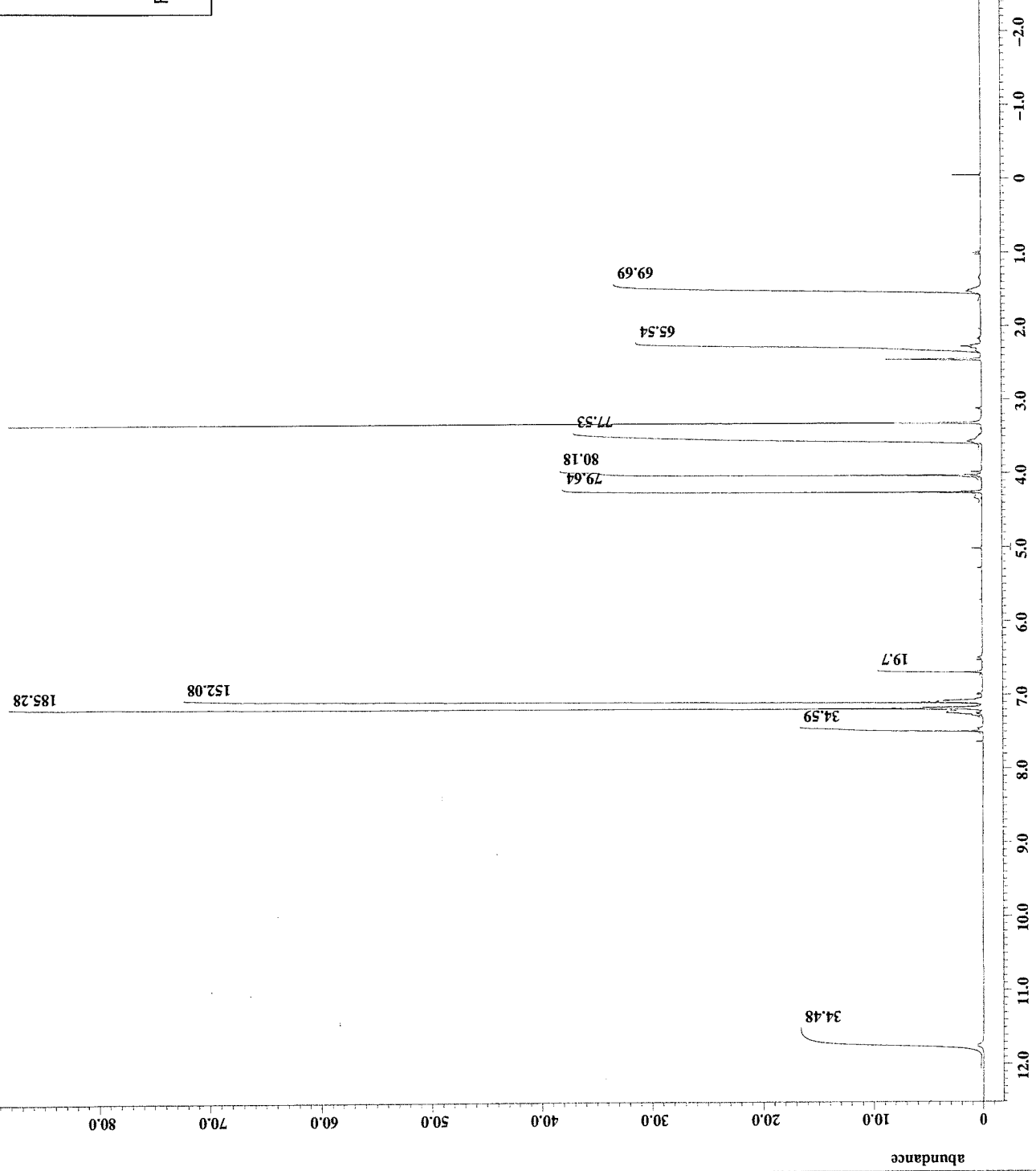


X : parts per Million : 13C



Current_time = 18-JUL-2024 09:30:07
 08:48:55
 09:29:35

Comment = single_pulse
 Data_format = 1D COMPLEX
 Dim_size = 13107
 Dim_title = 1H
 Dim_units = [ppm]
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 Site = ECS 400
 Spectrometer = JNM-ECS400
 Field_strength = 9.399766 [T] (400 [MHz])
 X_acq_duration = 2.18365952 [s]
 X_domain = 1H
 X_freq = 399.78219838 [MHz]
 X_offset = 5 [ppm]
 X_points = 16384
 X_prescans = 1
 X_resolution = 0.45794685 [Hz]
 X_sweep = 7.5030012 [KHz]
 Irr_domain = 1H
 Irr_freq = 399.78219838 [MHz]
 Irr_offset = 5 [ppm]
 Tri_domain = 1H
 Tri_freq = 399.78219838 [MHz]
 Tri_offset = 5 [ppm]
 Clipped = TRUE
 Mod_return = 1
 Scans = 8
 Total_scans = 8
 X_90_width = 10.65 [us]
 X_acq_time = 2.18365952 [s]
 X_angle = 45 [deg]
 X_atn = 6 [dB]
 X_pulse = 5.325 [us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_preset = FALSE
 Initial_wait = 1 [s]
 Recvr_gain = 50
 Relaxation_delay = 5 [s]
 Repetition_time = 7.18365952 [s]
 Temp_get = 20 [dC]



X : parts per Million : 1H

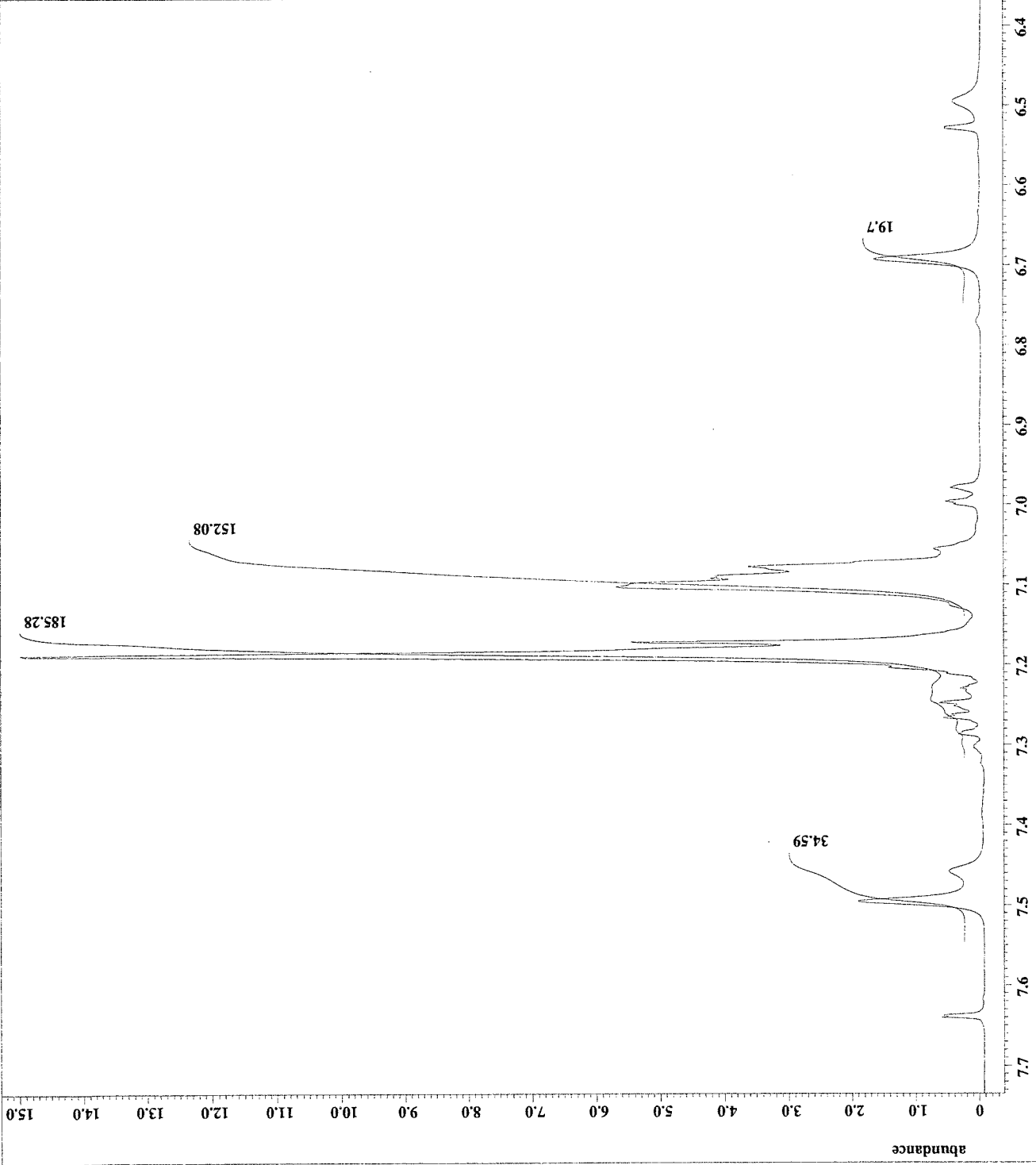
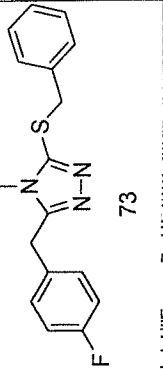


File no
Author
Experi
Sample
Solver
Creati
Revisi
Current_time

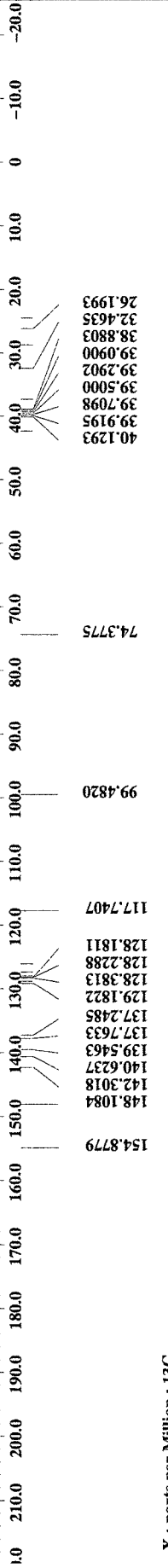
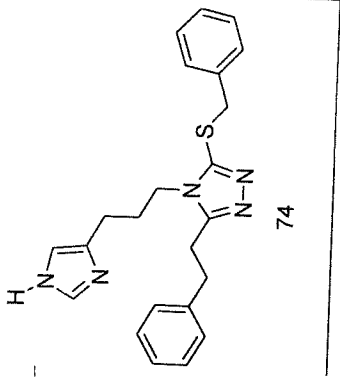
73

= 18-JUL-2024 09:30:36

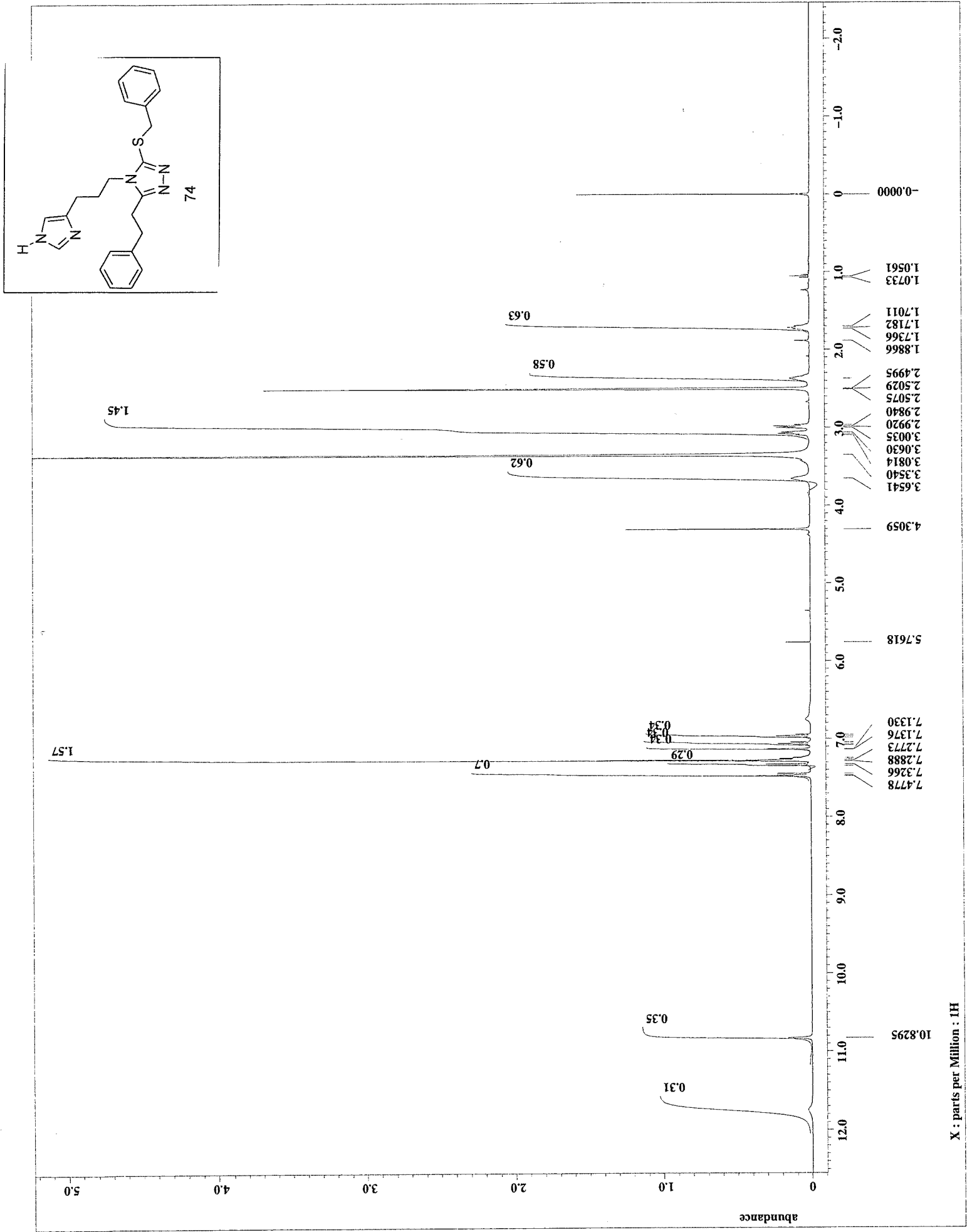
Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838 [MHz]
X_offset = 5 [ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685 [Hz]
X_sweep = 7.5030012 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Tri_domain = 1H
Tri_freq = 399.78219838 [MHz]
Tri_offset = 5 [ppm]
Clipped = TRUE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 10.65 [us]
X_acq_time = 2.18365952 [s]
X_angle = 45 [deg]
X_atn = 6 [dB]
X_pulse = 5.325 [us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1 [s]
Recvr_gain = 50
Relaxation_delay = 5 [s]
Repetition_time = 7.18365952 [s]
Temp_get = 20 [dC]



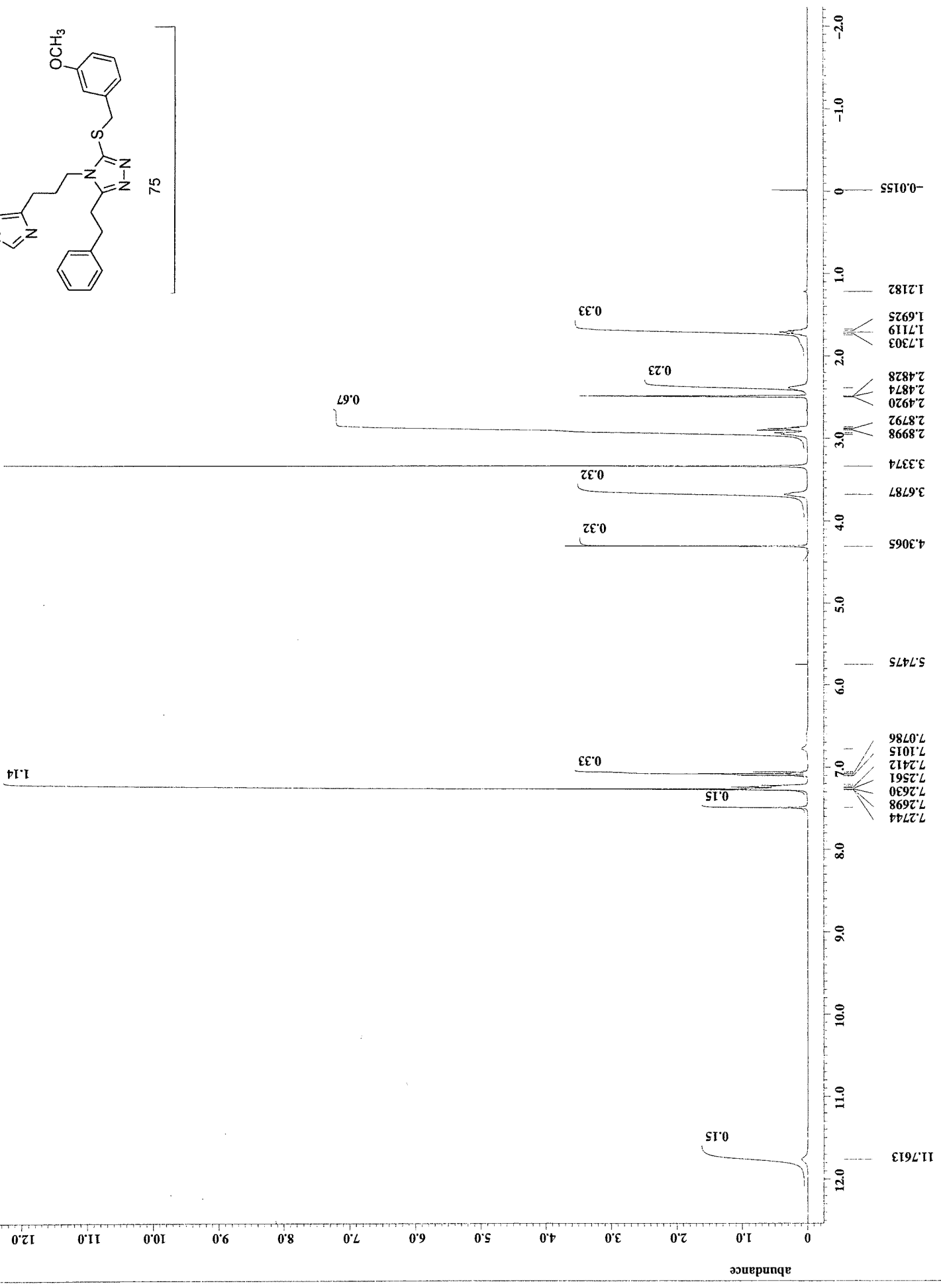
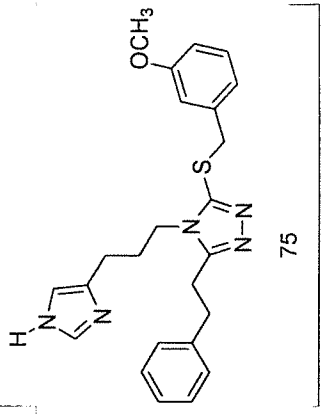
X : parts per Million : 1H

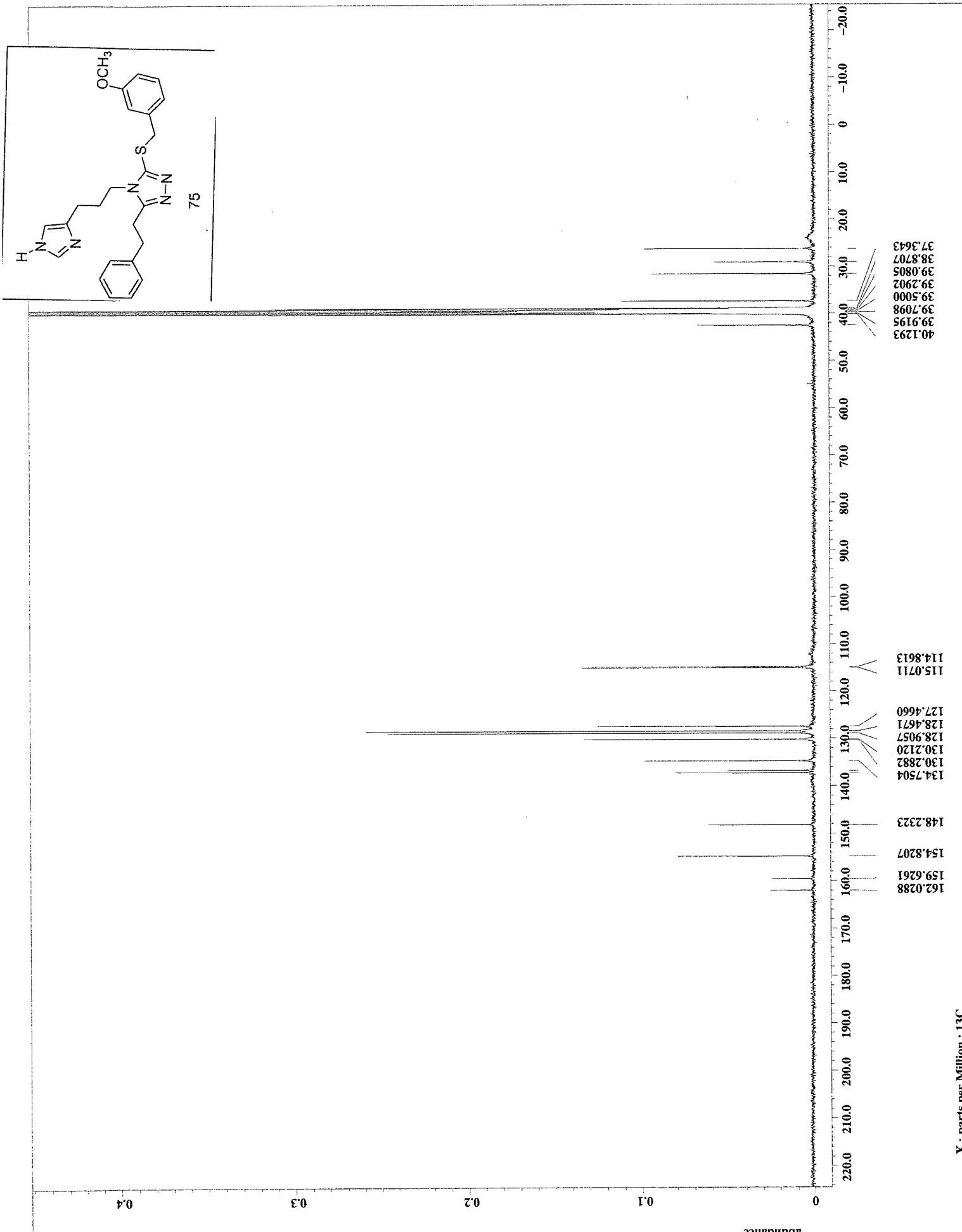


X : parts per Million : 13C

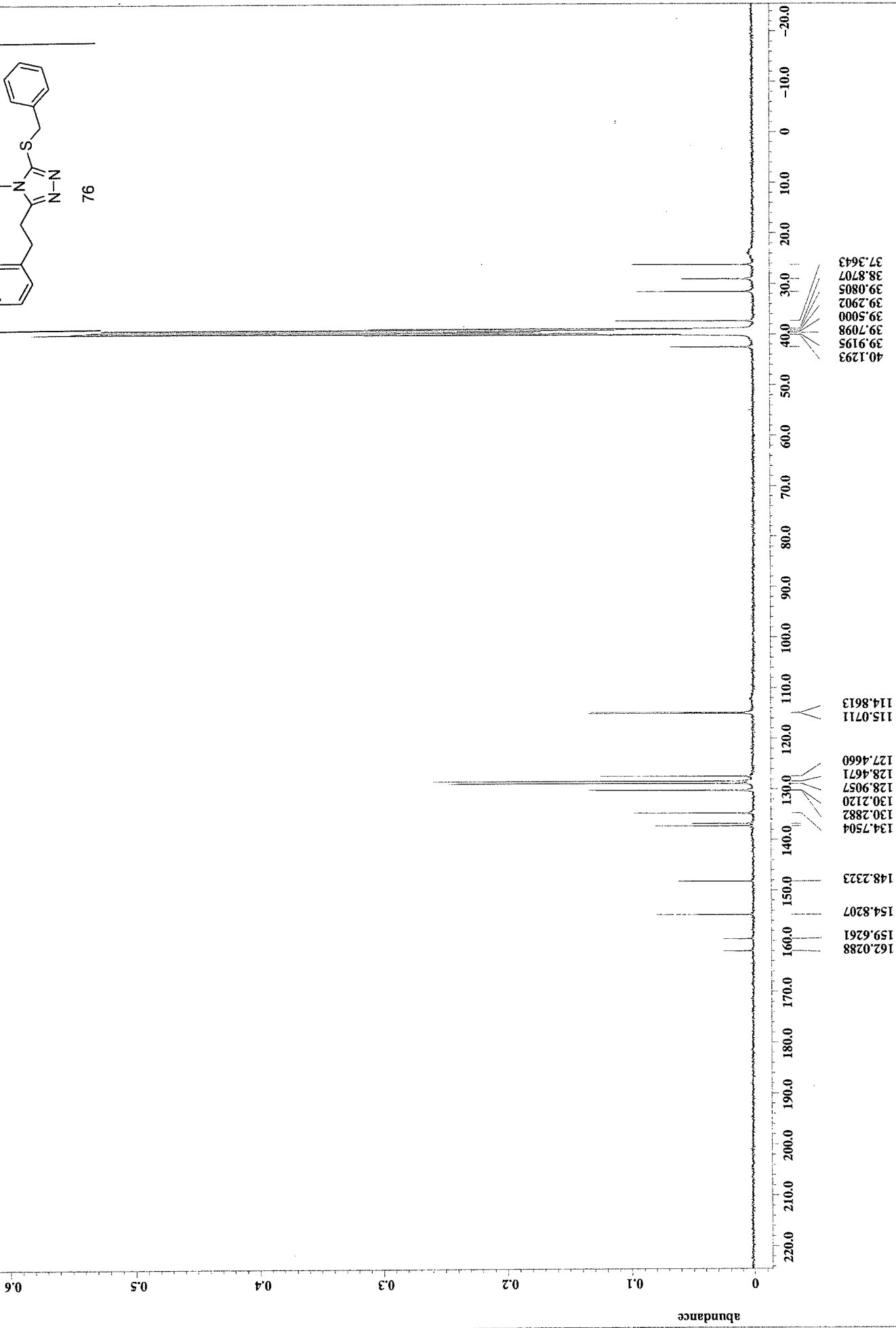
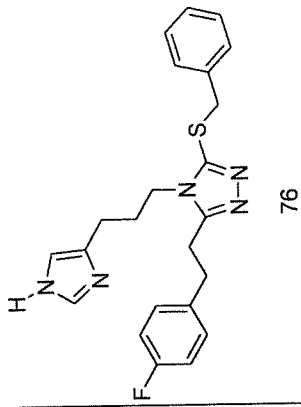


X : parts per Million : 1H

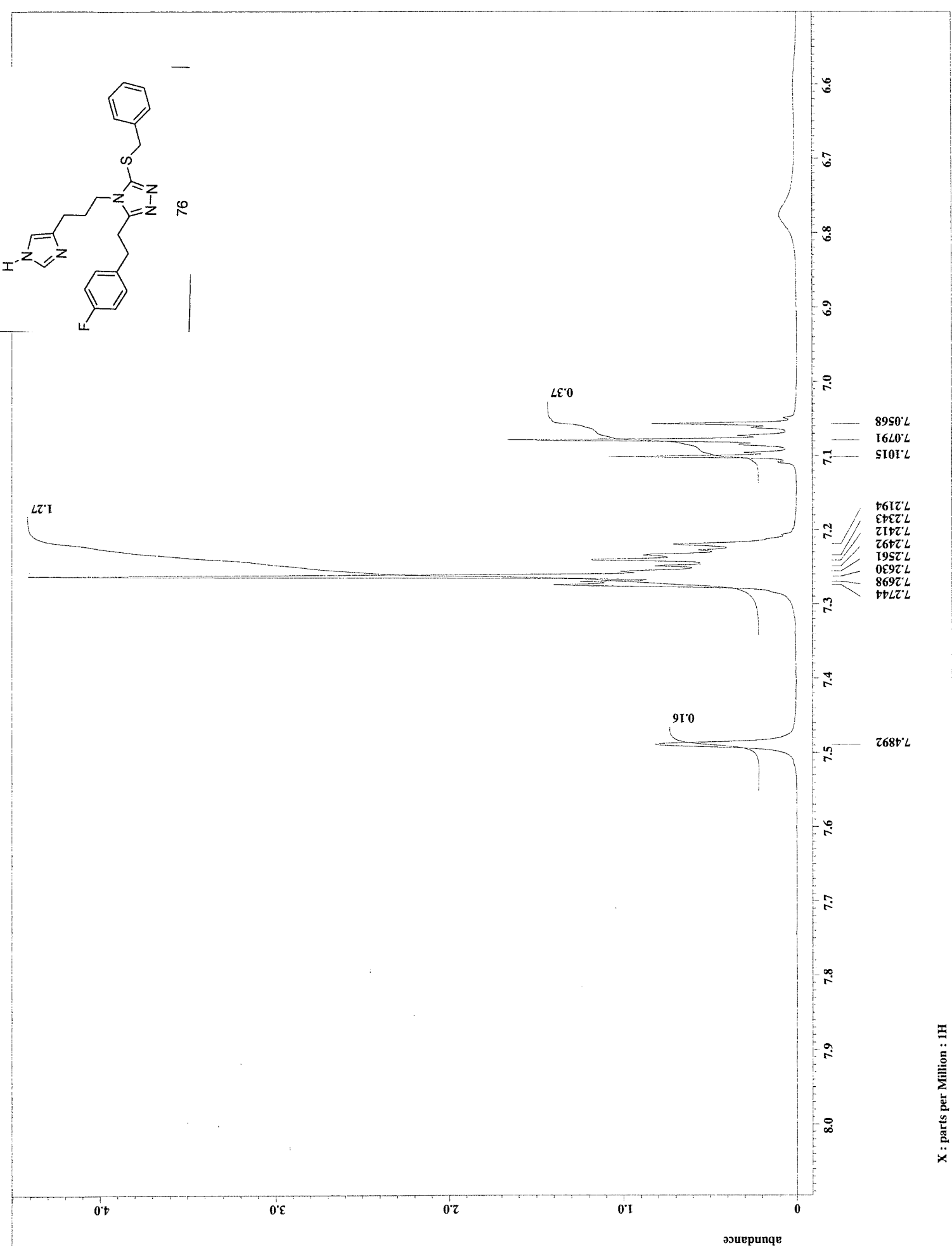


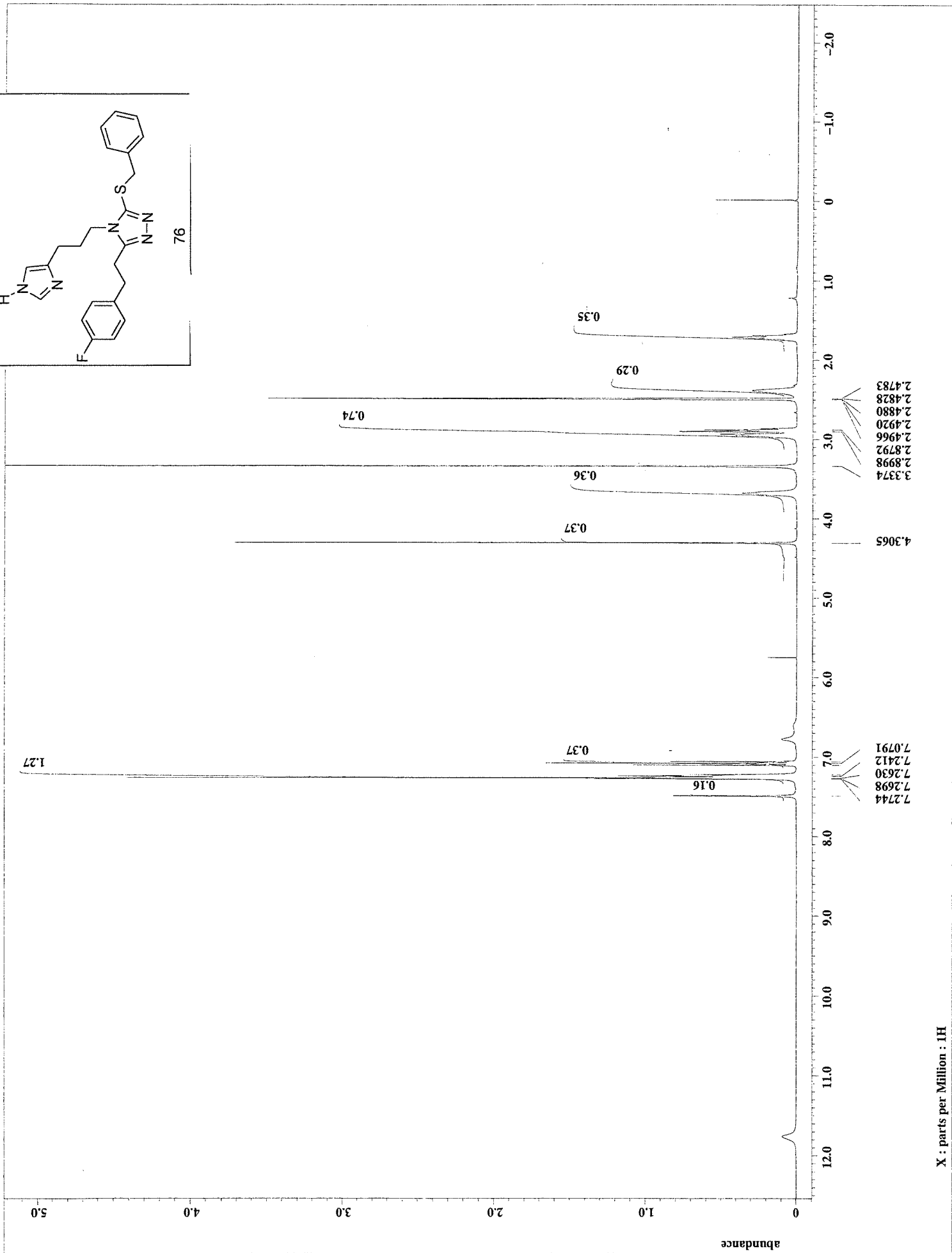
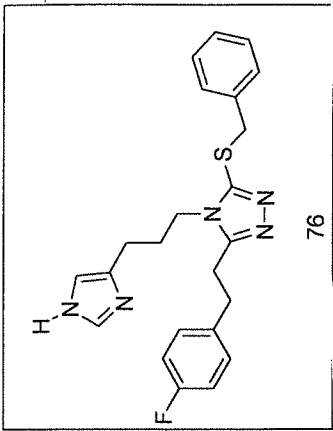


X : parts per Million : 13C

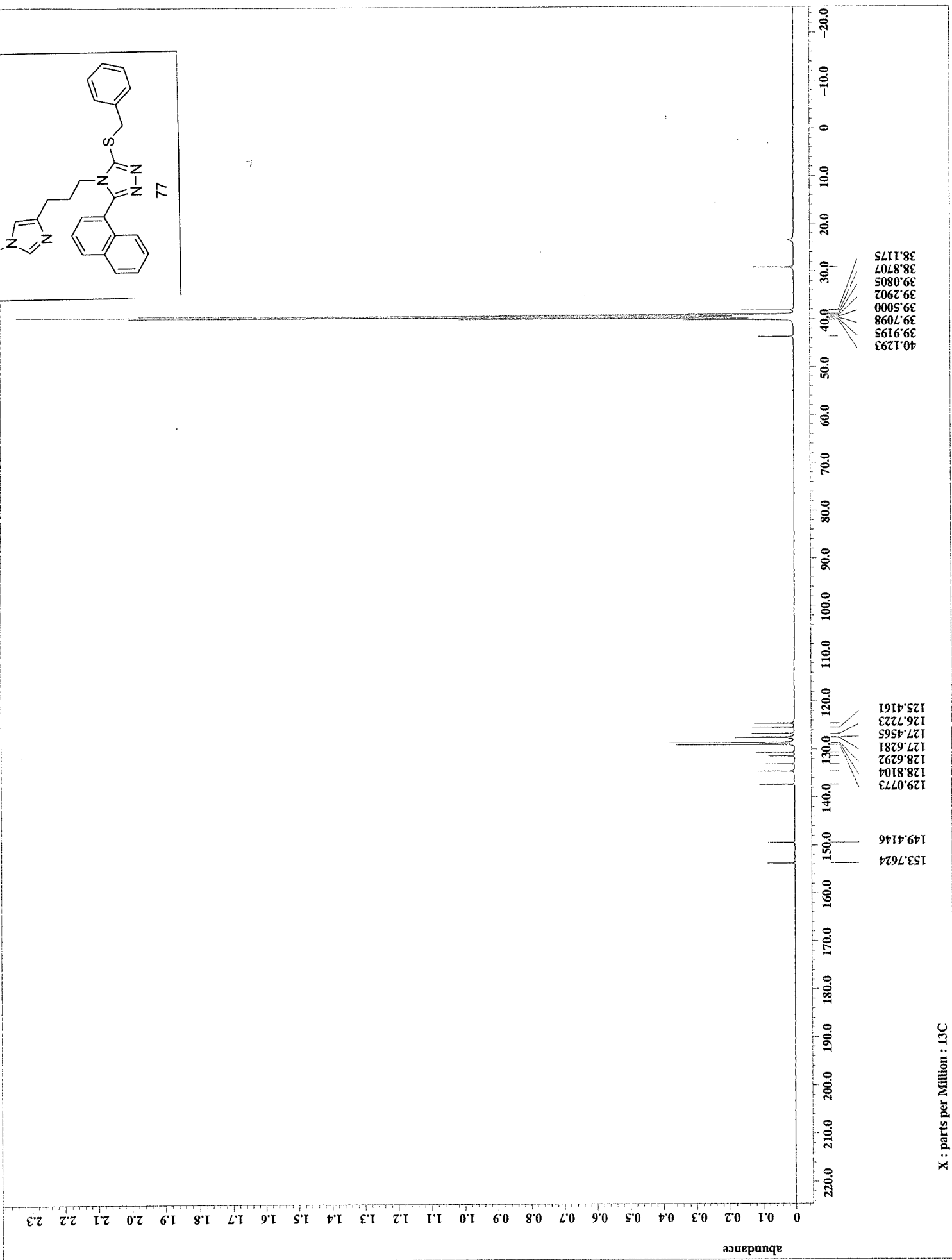
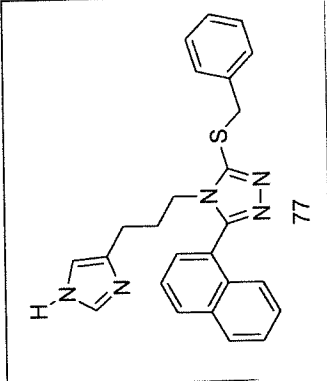


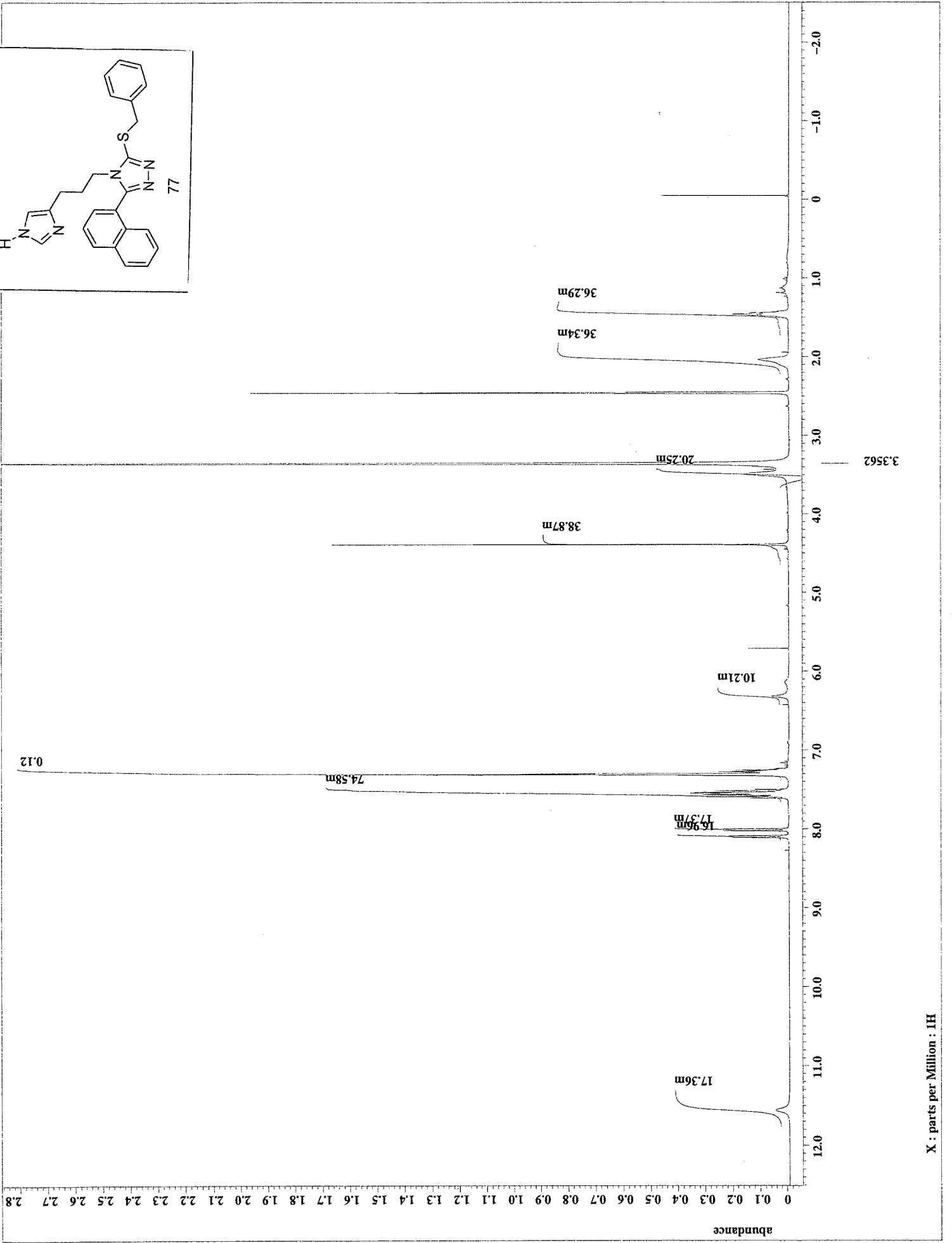
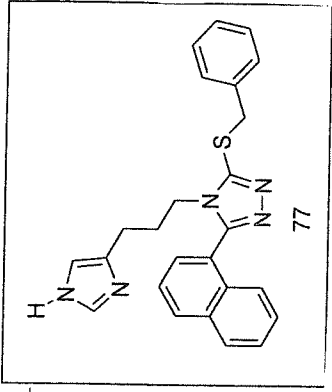
X : parts per Million : 13C



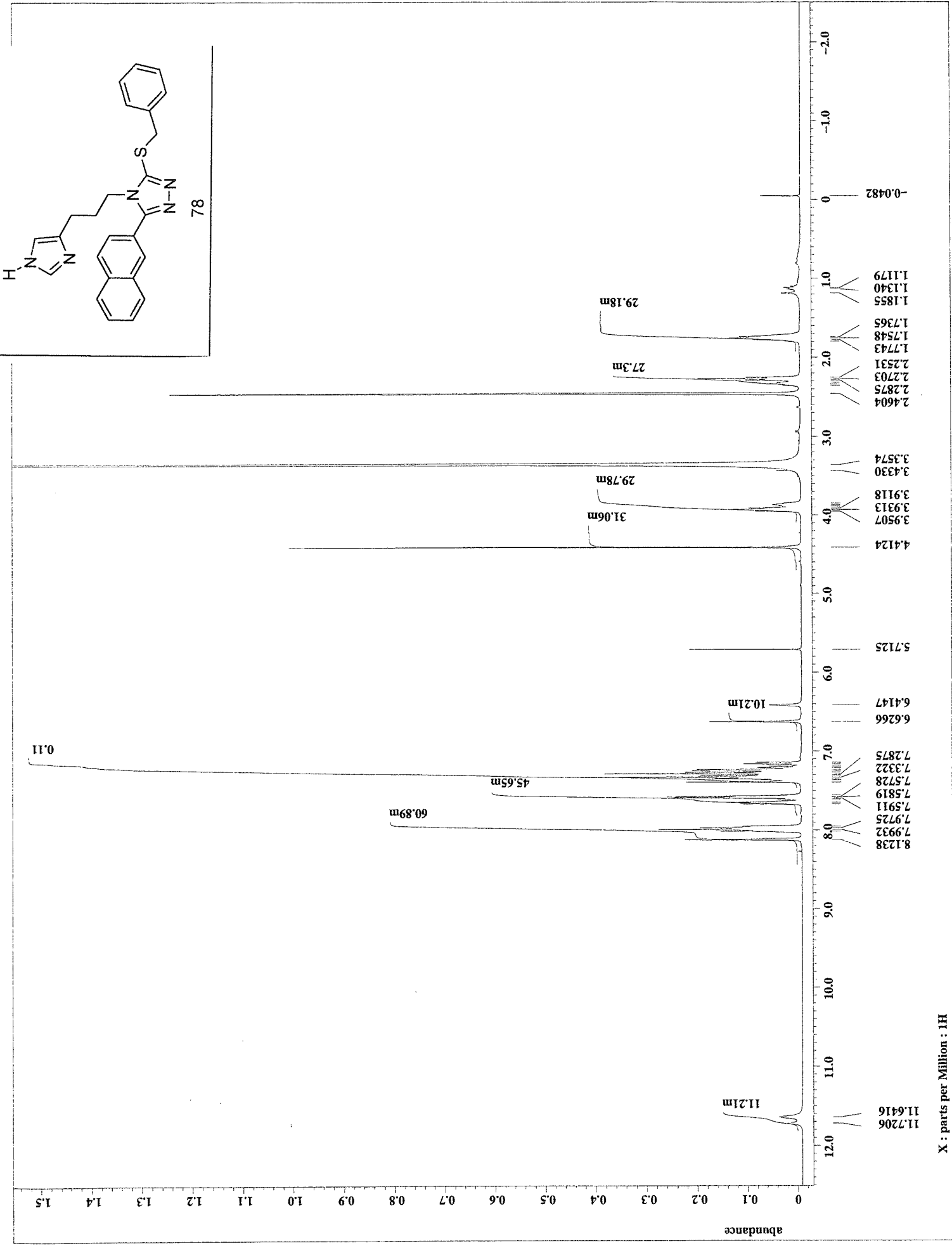


X : parts per Million : 1H

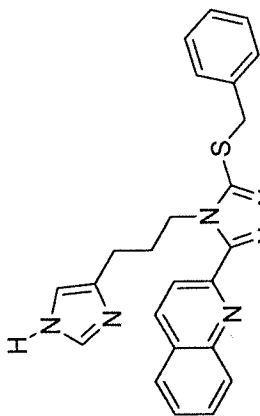




X : parts per Million : 1H



X : parts per Million : 1H



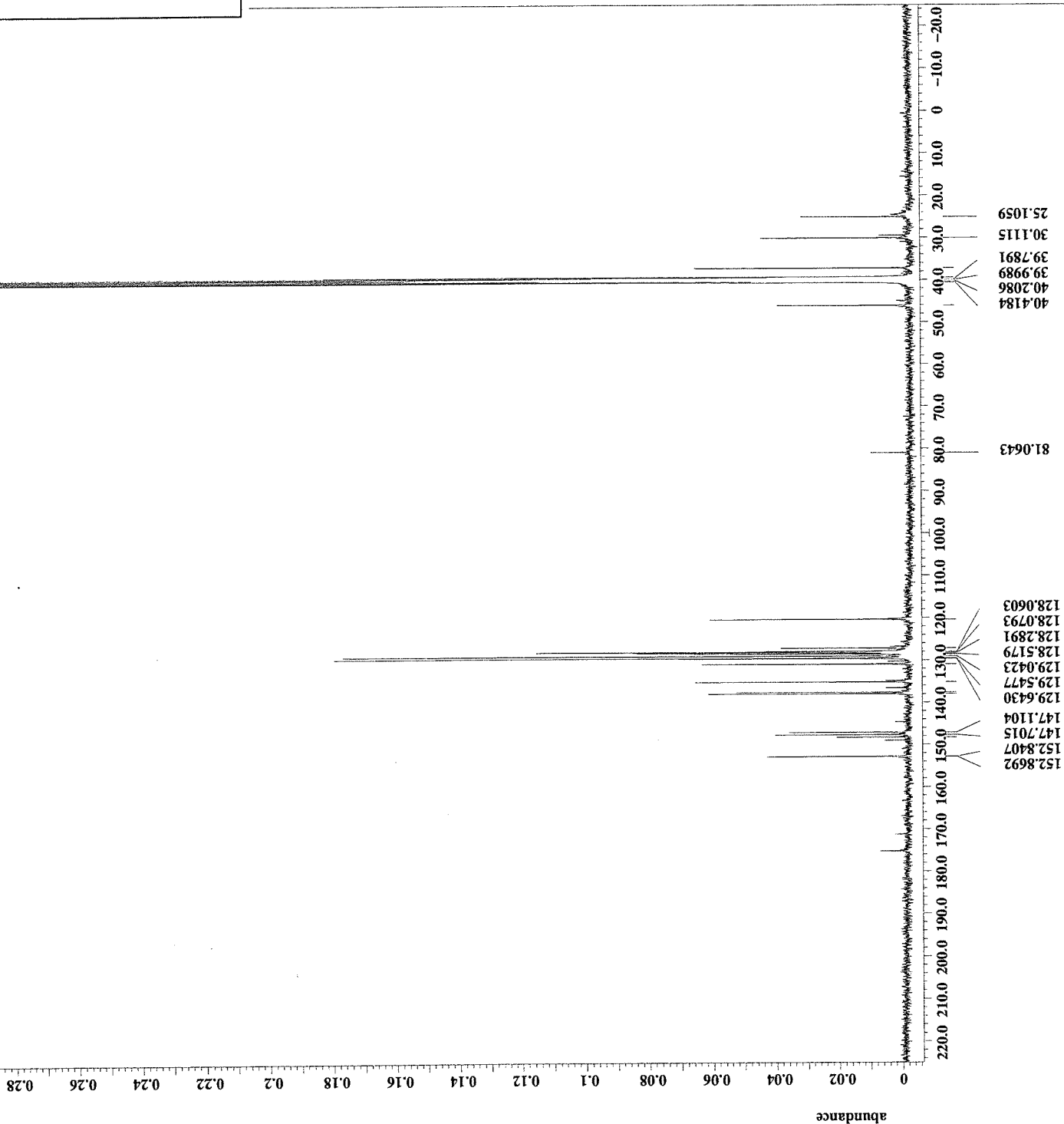
79

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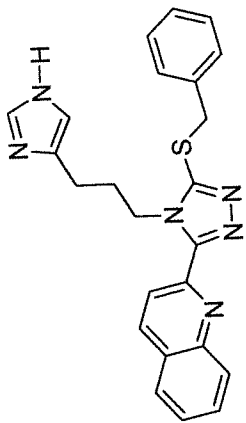
Dim_title      = 13C
Dim_units      = [ppm]
Dimensions     = X
Site           = ECS 400
Spectrometer   = JNM-ECS400

Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 1.04333312[s]
X_domain       = 13C
X_freq         = 100.52530333 [MHz]
X_offset       = 100 [ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 0.95846665 [Hz]
X_sweep        = 31.40703518 [kHz]
Irr_domain     = 1H
Irr_freq       = 399.78219838 [MHz]
Irr_offset     = 5 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 12000
Total_scans    = 12000

X_90_width     = 12.84 [us]
X_acq_time     = 1.04333312 [s]
X_angle        = 30 [deg]
X_atn          = 9 [dB]
X_pulse        = 4.28 [us]
Irr_atn_dec   = 27 [dB]
Irr_atn_noe   = 27 [dB]
Irr_noise      = WALTZ
Decoupling     = TRUE
Initial_wait   = 1 [s]
Noe            = TRUE
Noe_time       = 2 [s]
Recvr_gain     = 60
Relaxation_delay = 2 [s]
Repetition_time = 3.04333312 [s]
Temp_get       = 18.7 [dC]
  
```



X : parts per Million : 13C



N-5.jdf

3C

79

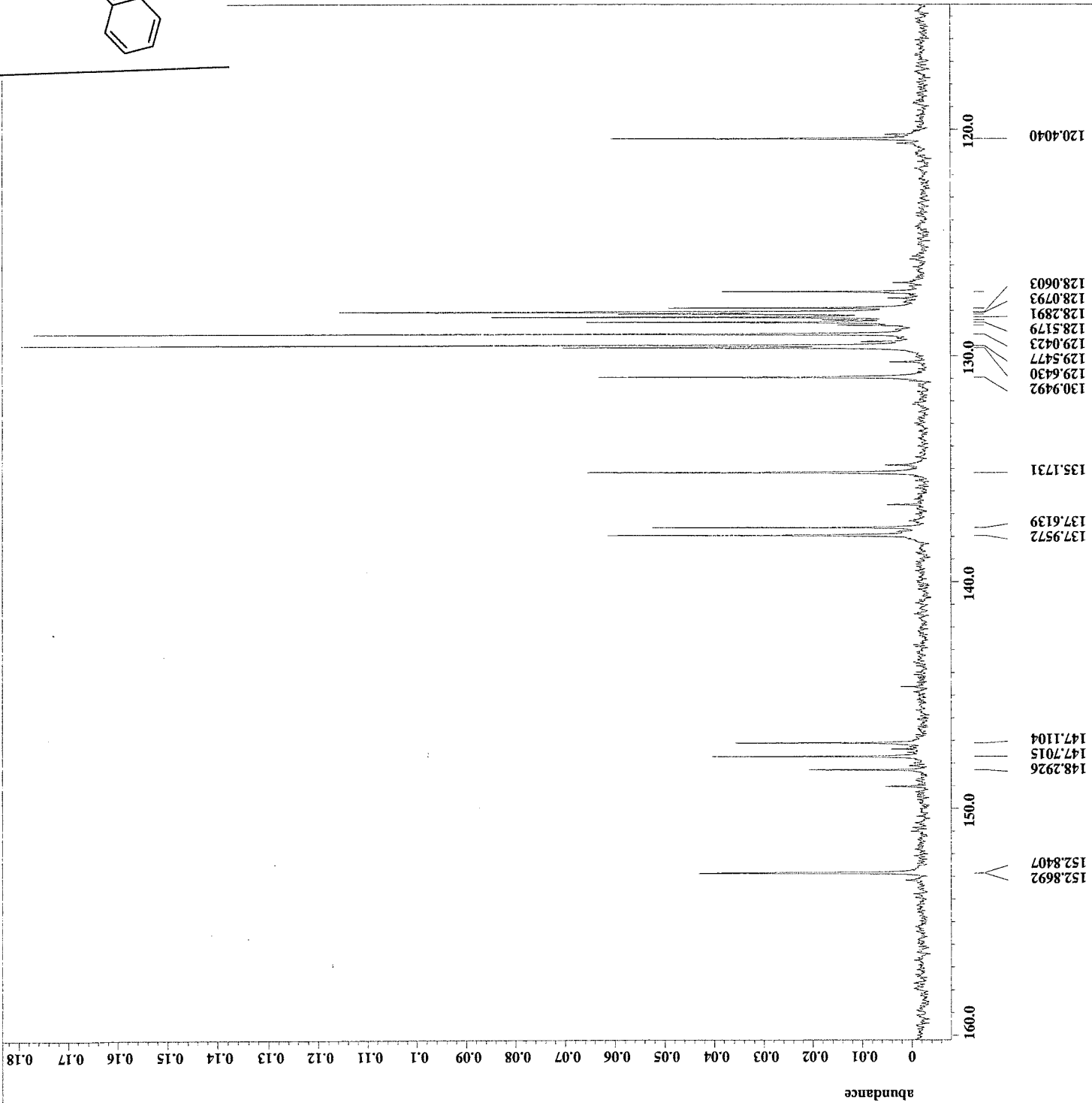
current_time = 16-JUL-2024 09:39:56
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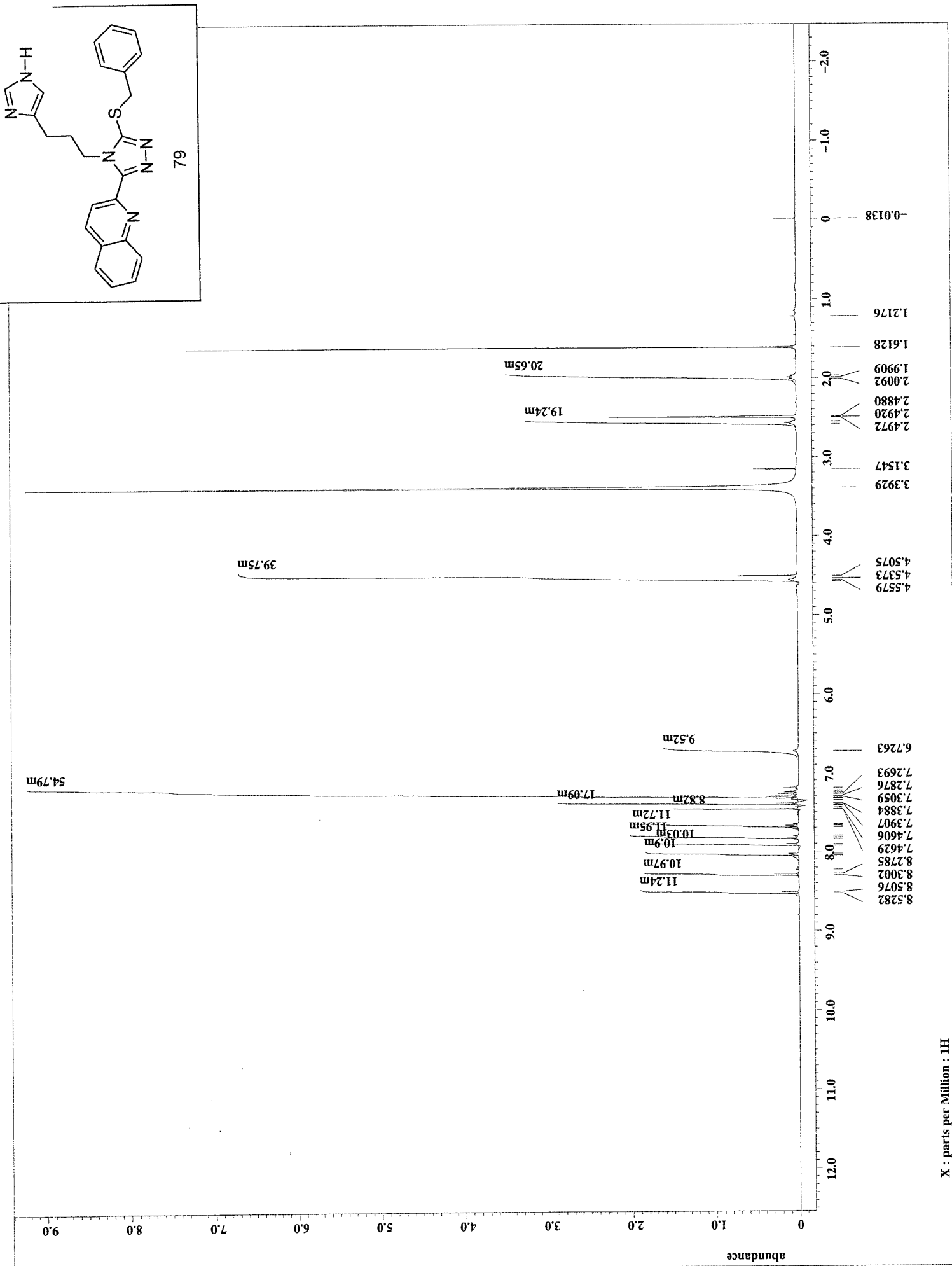
Comment
Data_format = ID COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400

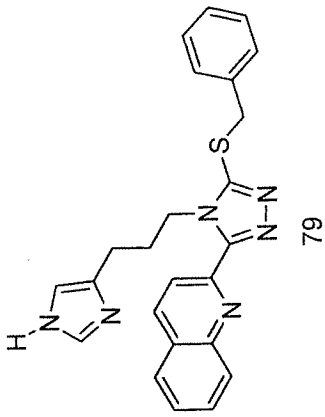
Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665 [Hz]
X_sweep = 31.40703518 [kHz]
Irr_domain = 1H.40703518 [kHz]
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 12000
Total_scans = 12000

X_90_width = 12.84 [us]
X_acq_time = 1.04333312 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 4.28 [us]
Irr_atn_dec = 27 [dB]
Irr_atn_noe = 27 [dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1 [s]
Noe_time = TRUE
Noe_time = 2 [s]
Recvr_gain = 60
Relaxation_delay = 2 [s]
Repetition_time = 3.04333312 [s]
Temp_get = 18.7 [dC]
  
```

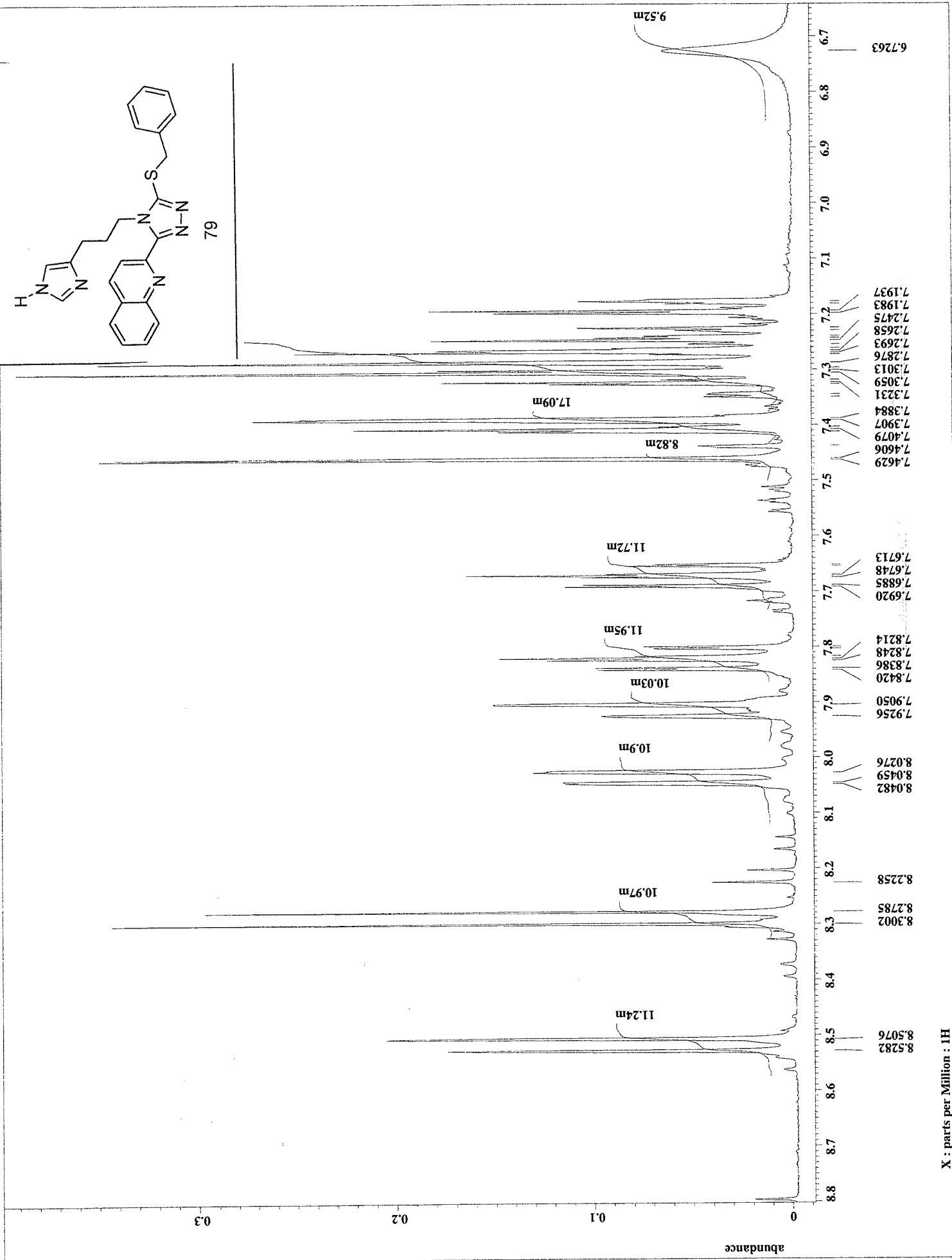


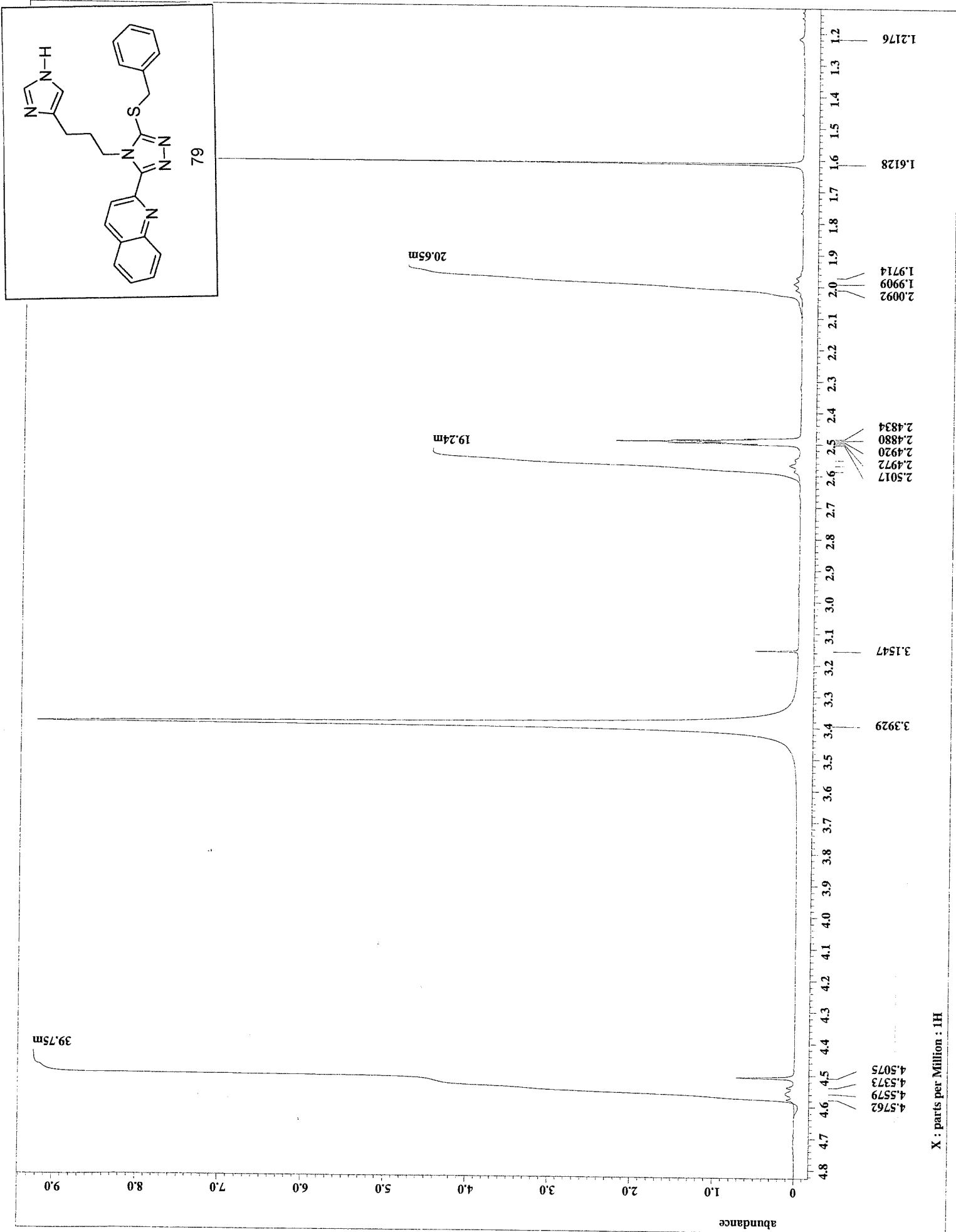
X : parts per Million : 13C



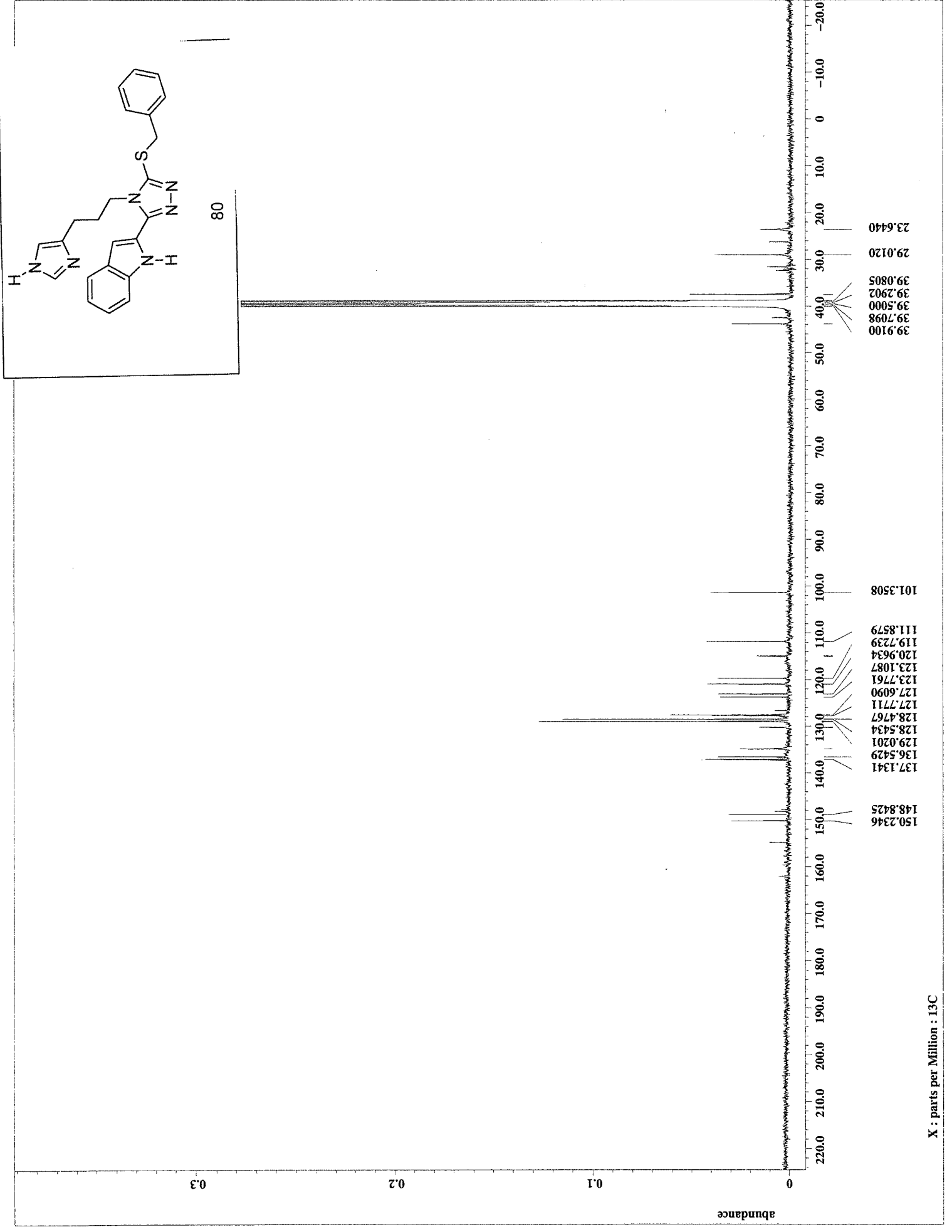


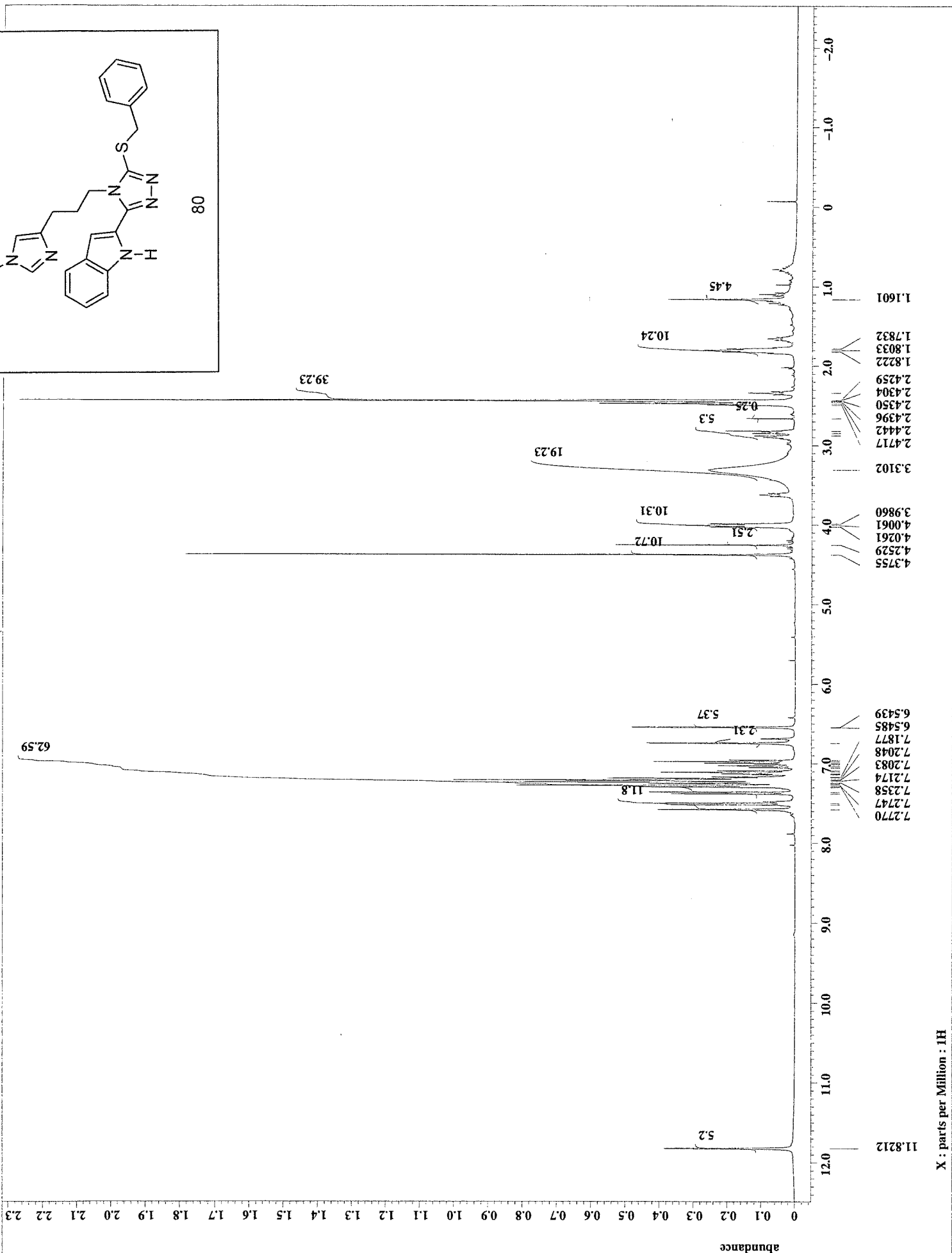
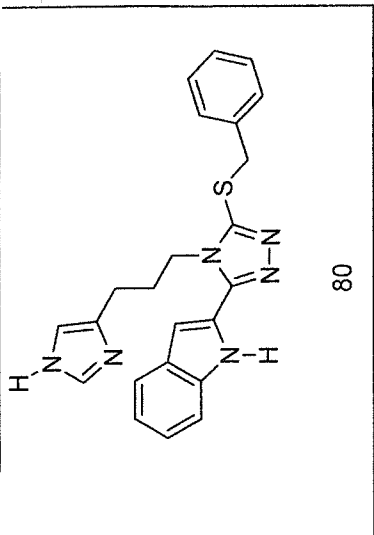
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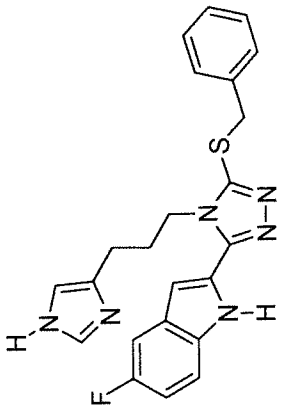


X : parts per Million : 1H

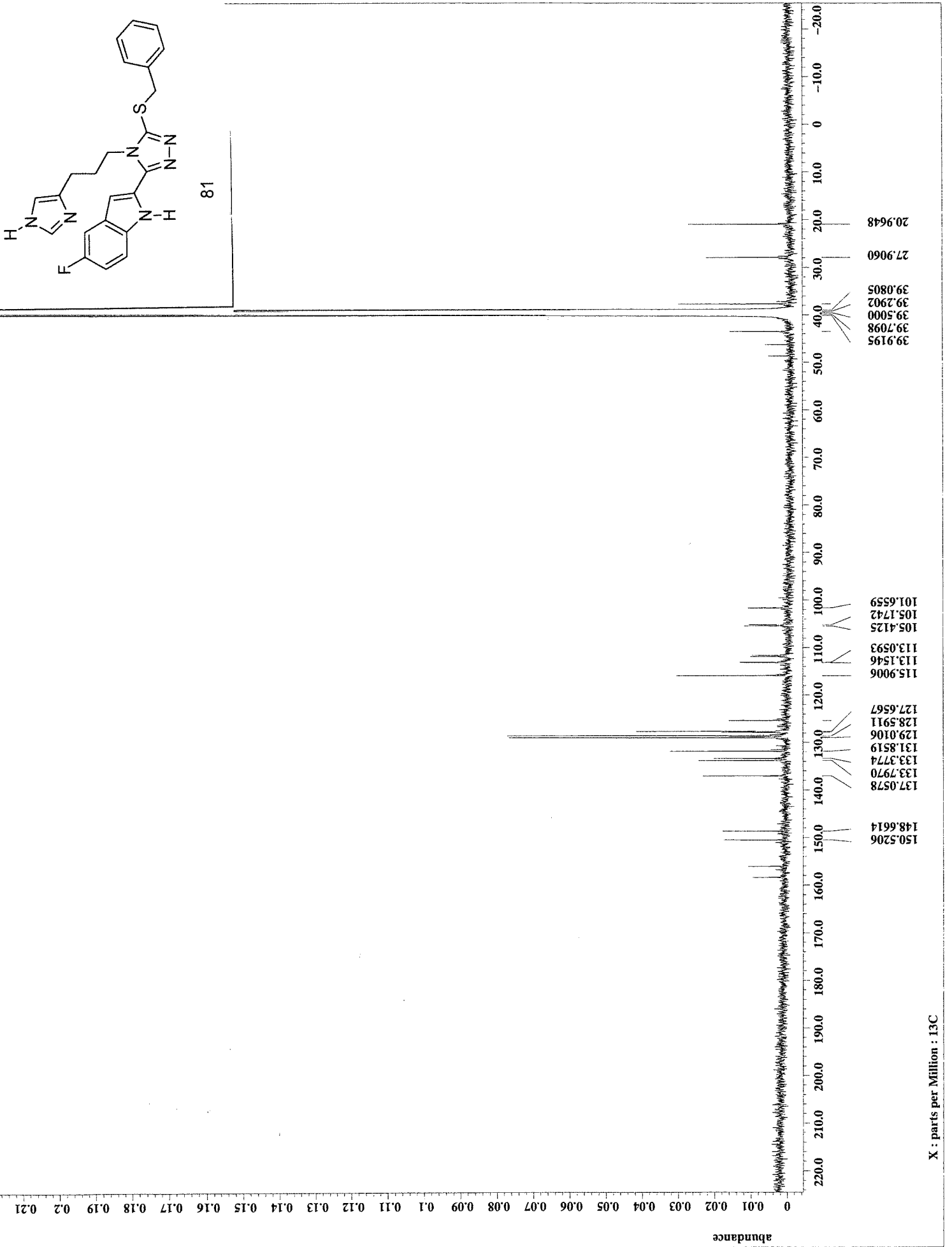




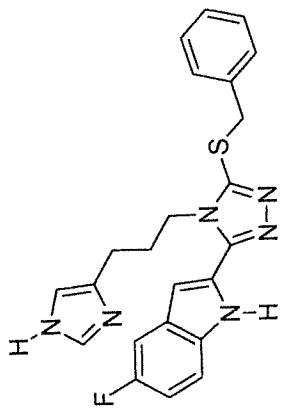
X : parts per Million : 1H



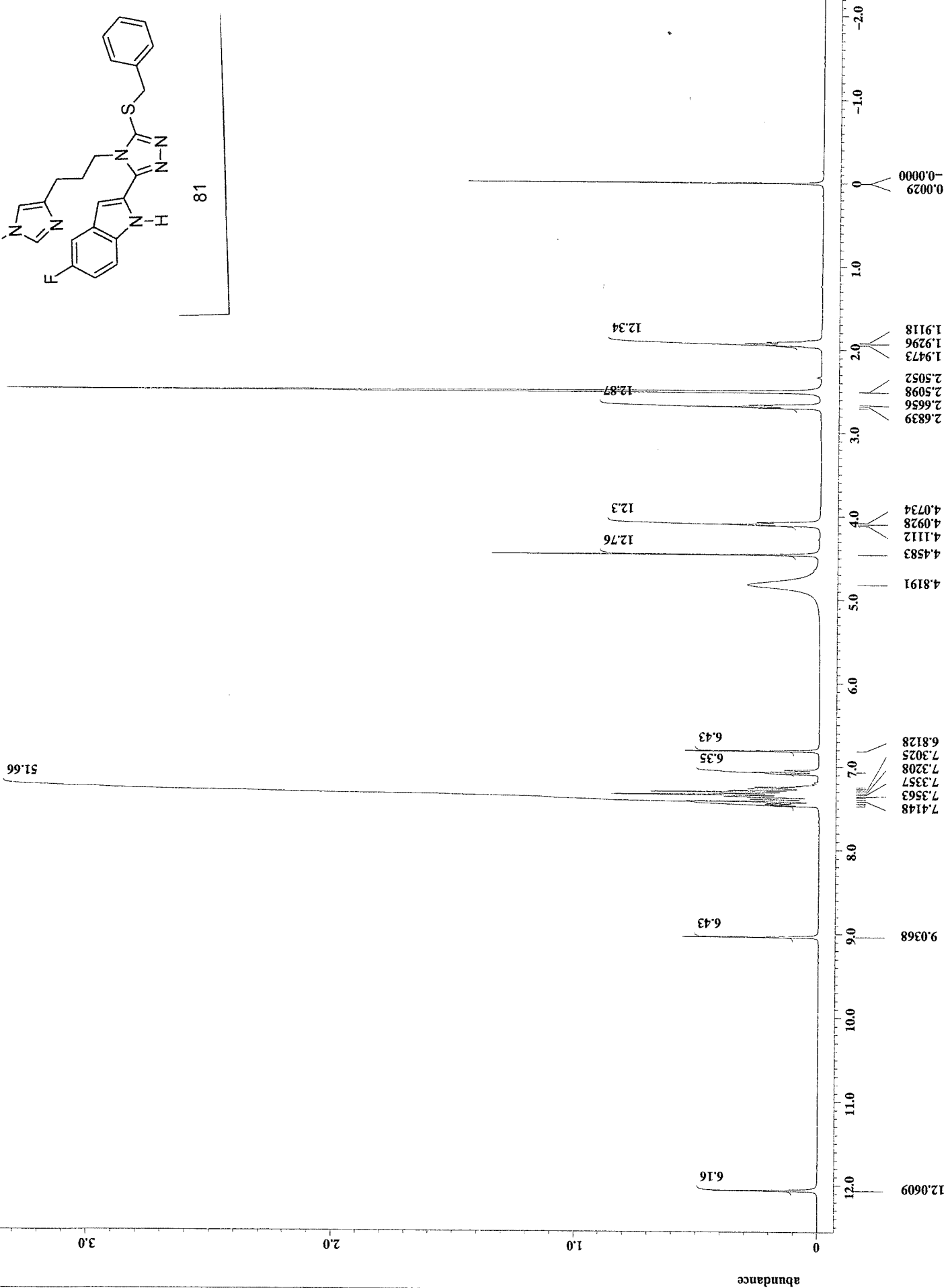
81



X : parts per Million : 13C

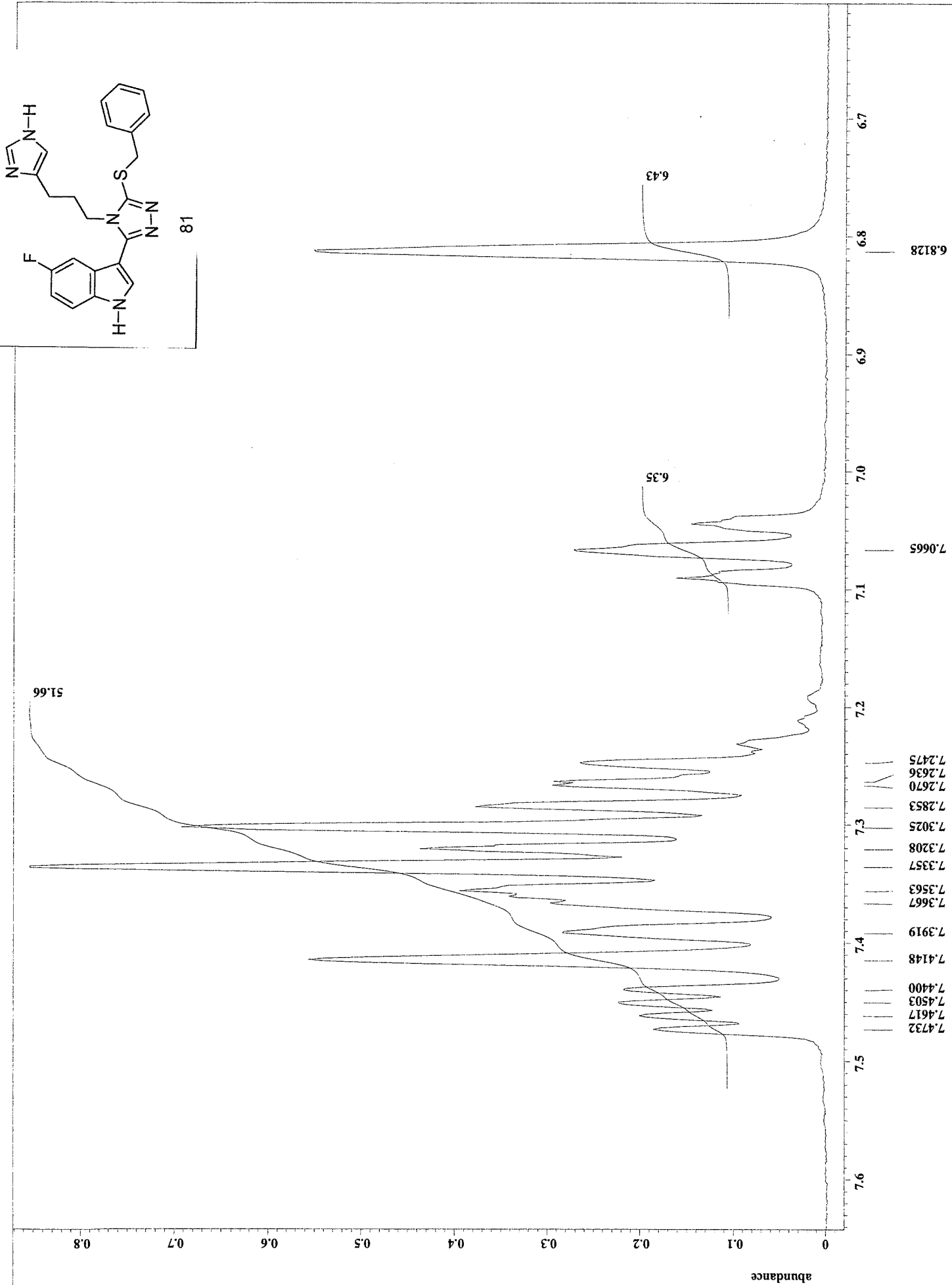


81

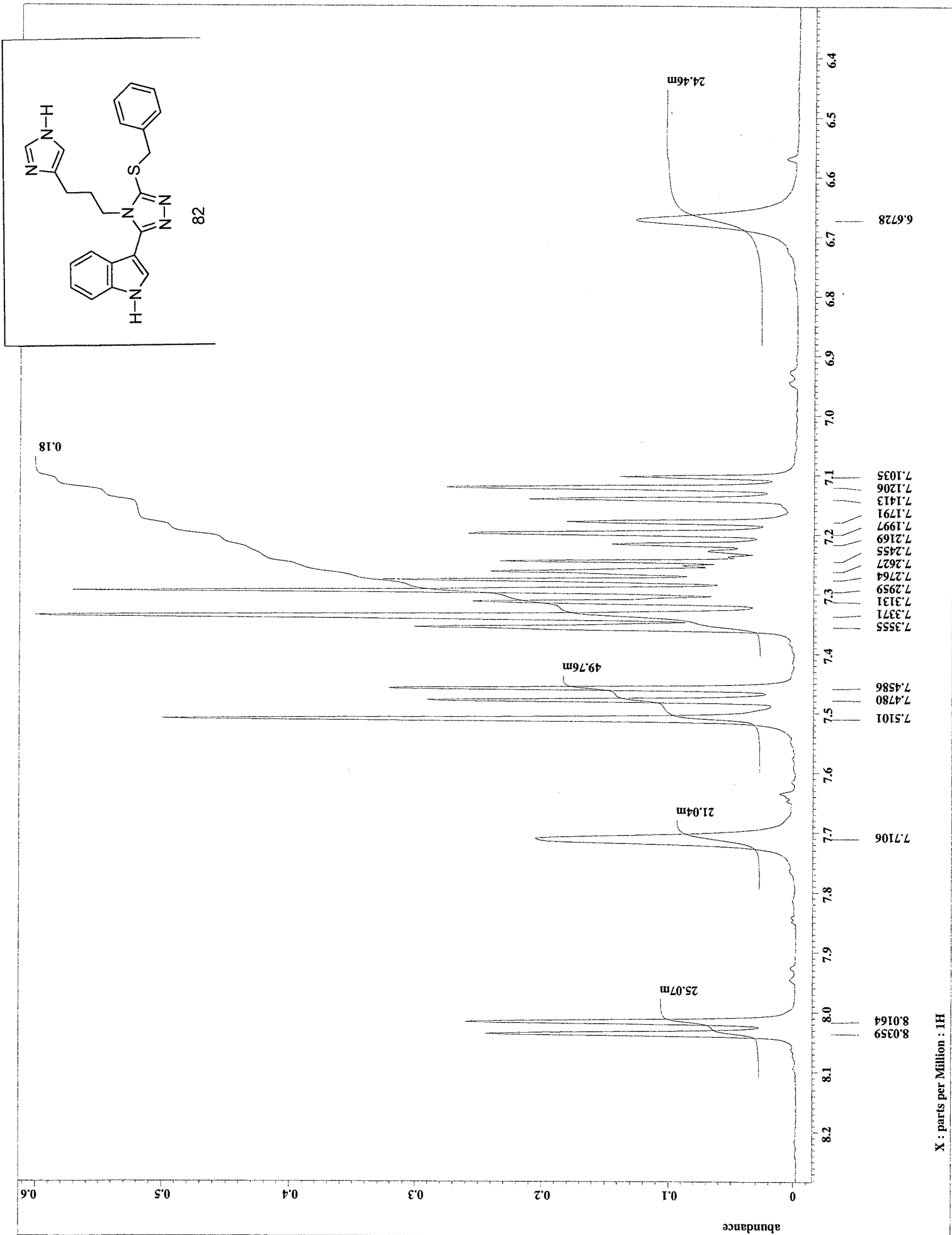


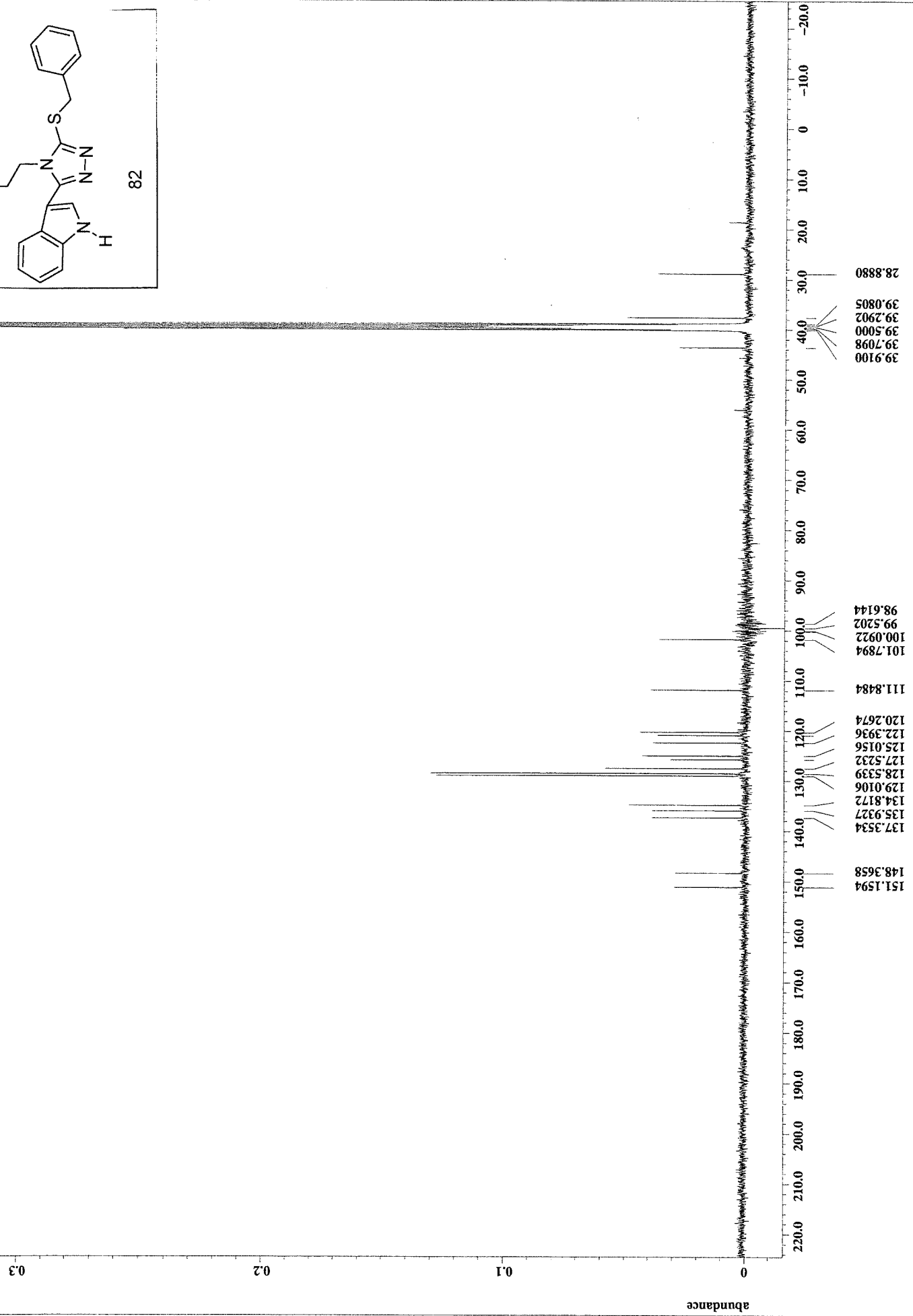
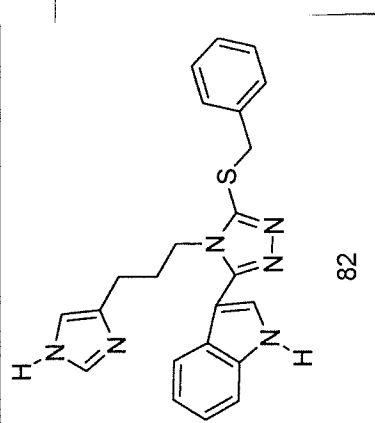
H : parts per Million : H

abundance

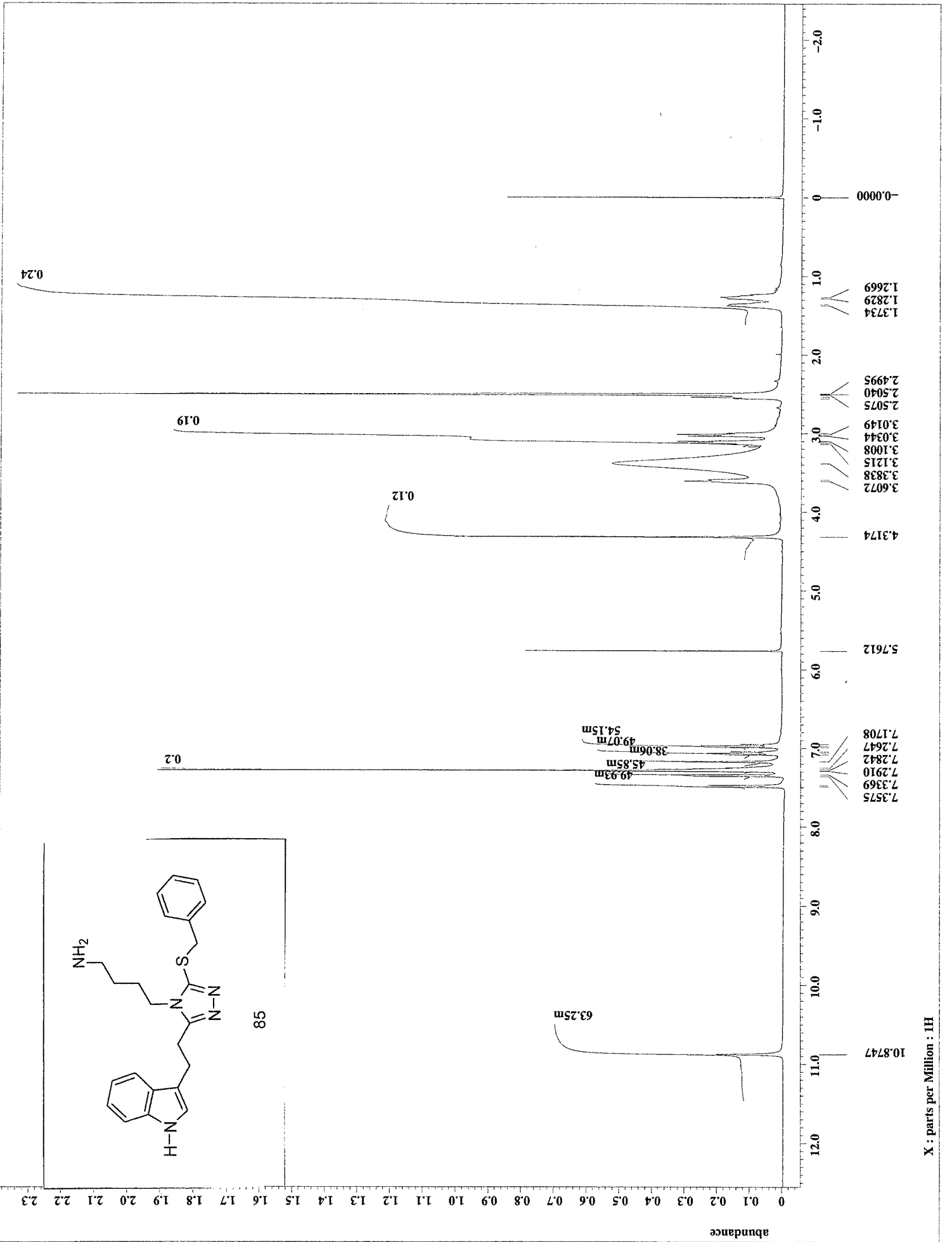


X : parts per Million : 1H

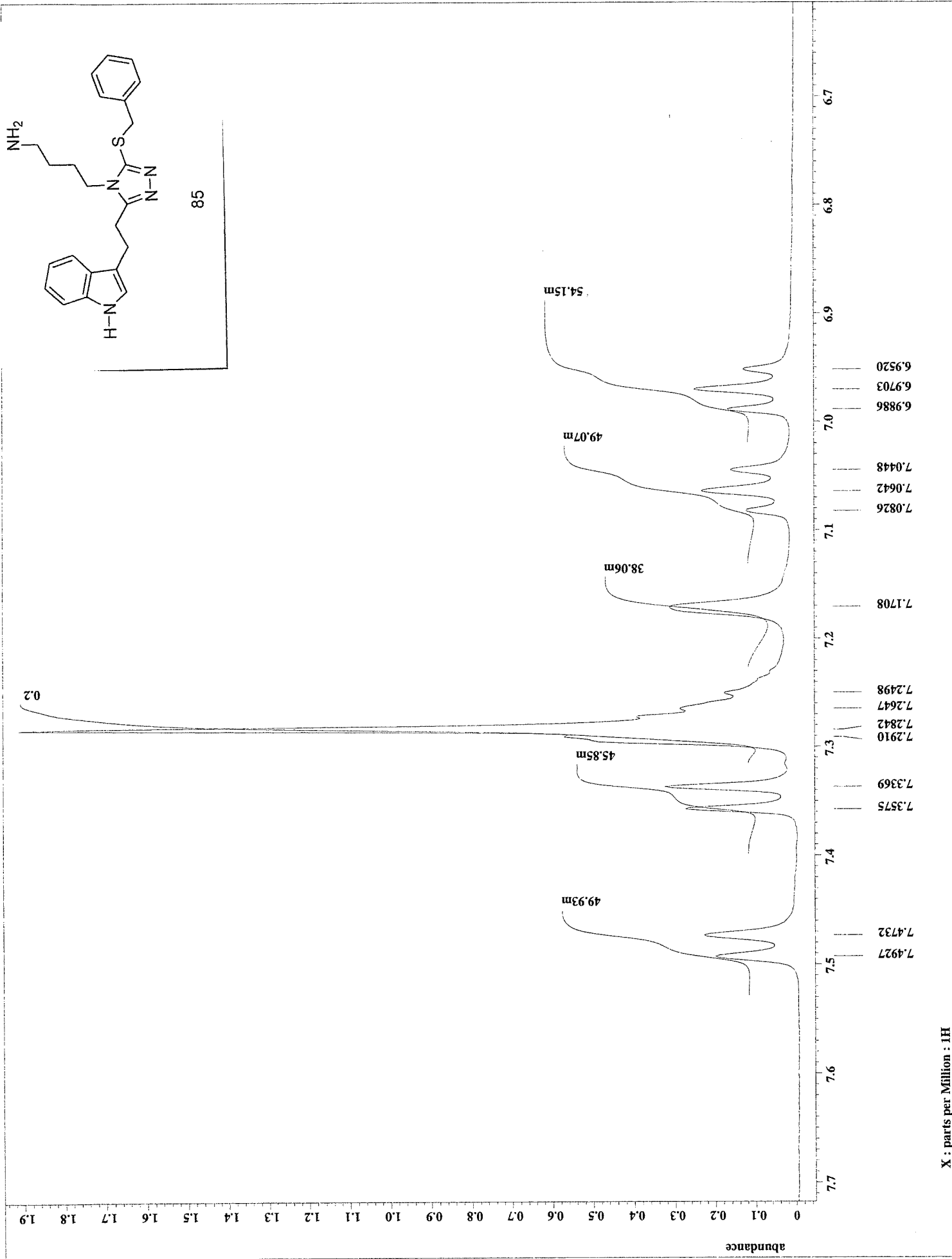




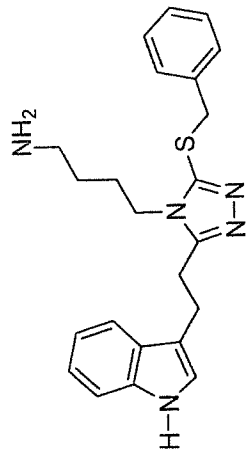
X : parts per Million : 13C



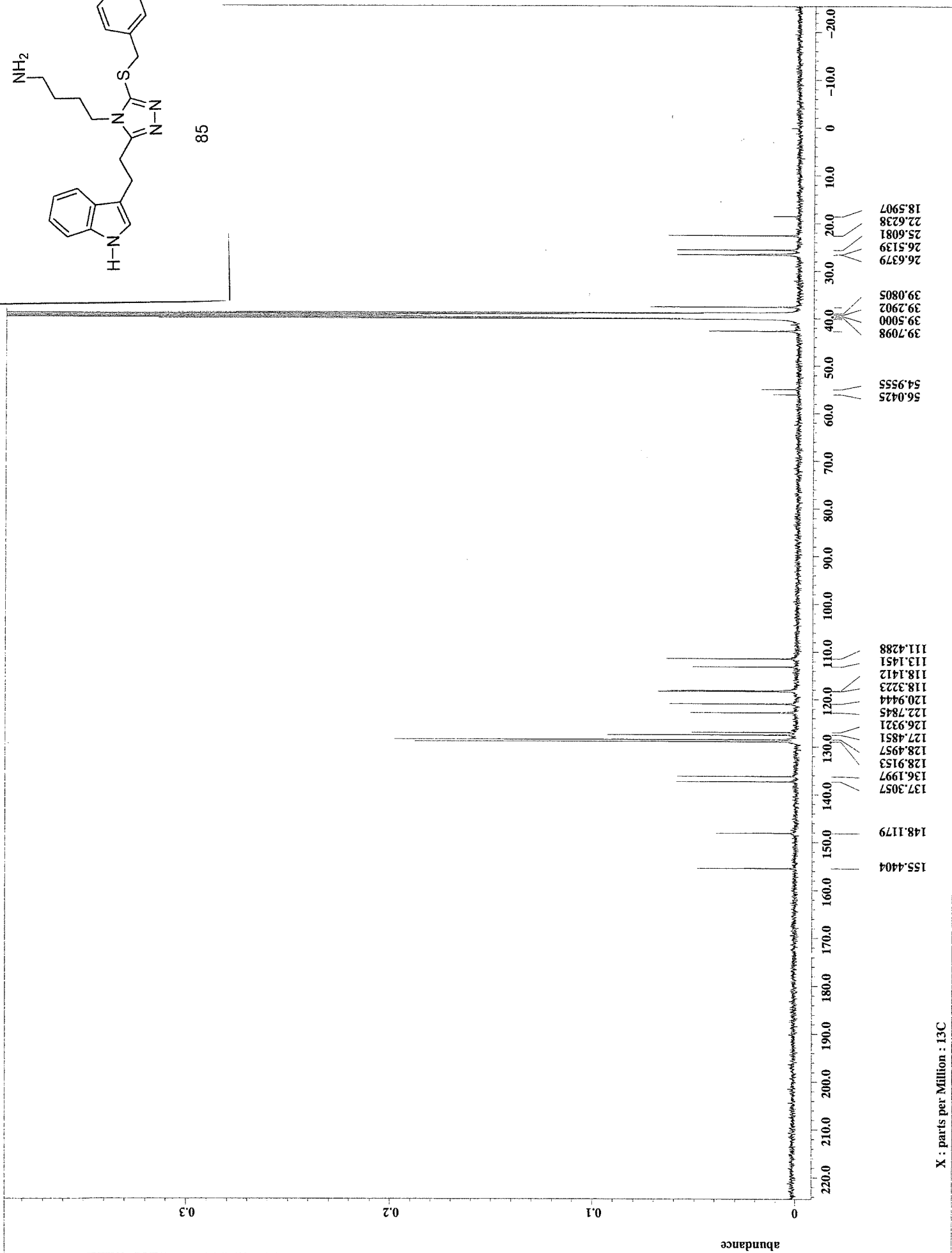
X : parts per Million : 1H

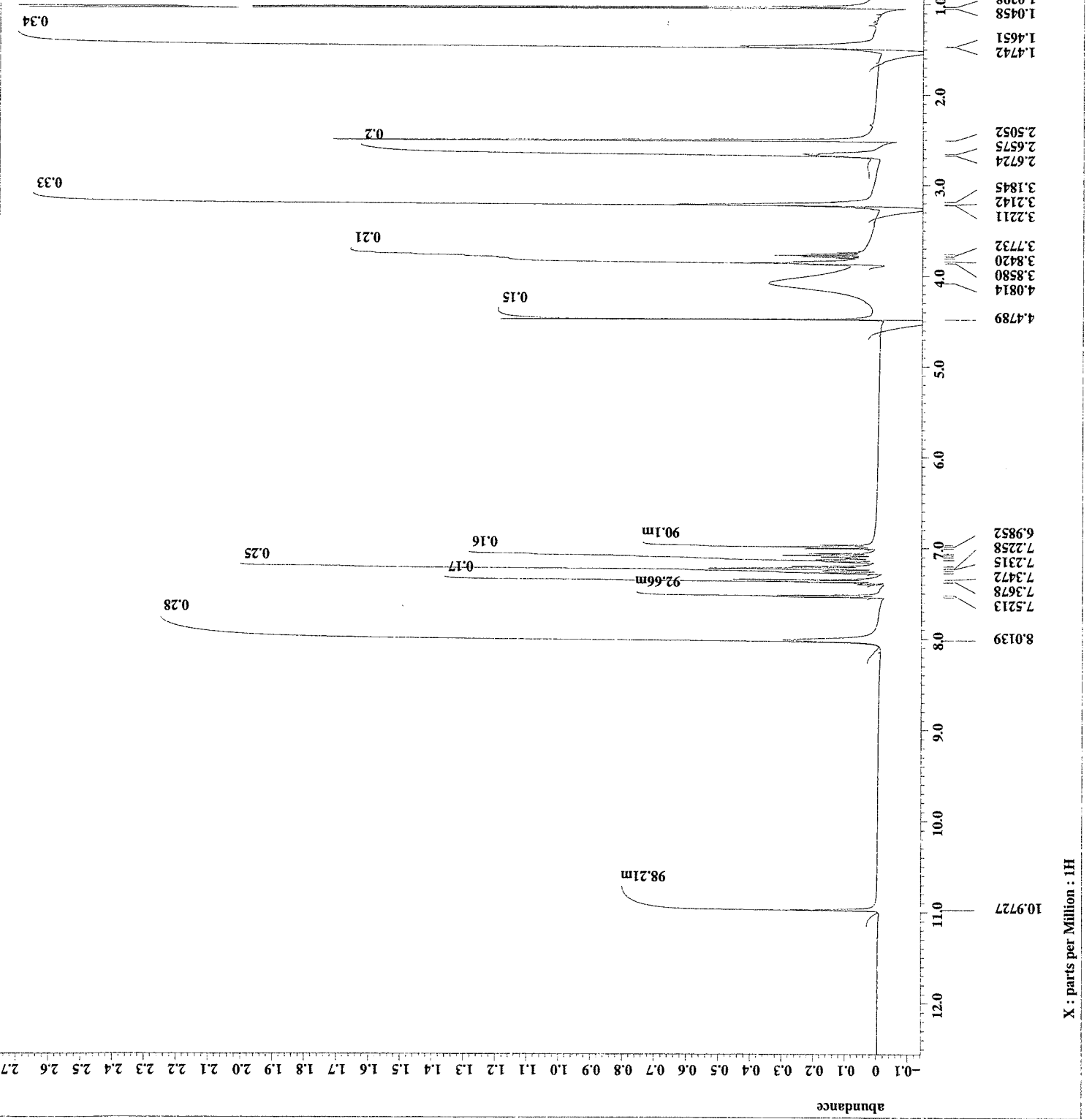
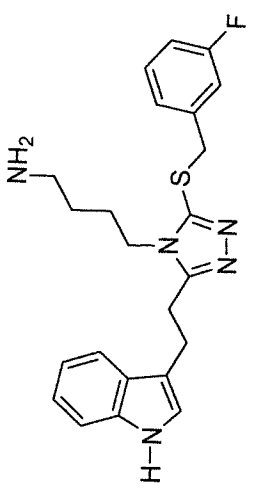


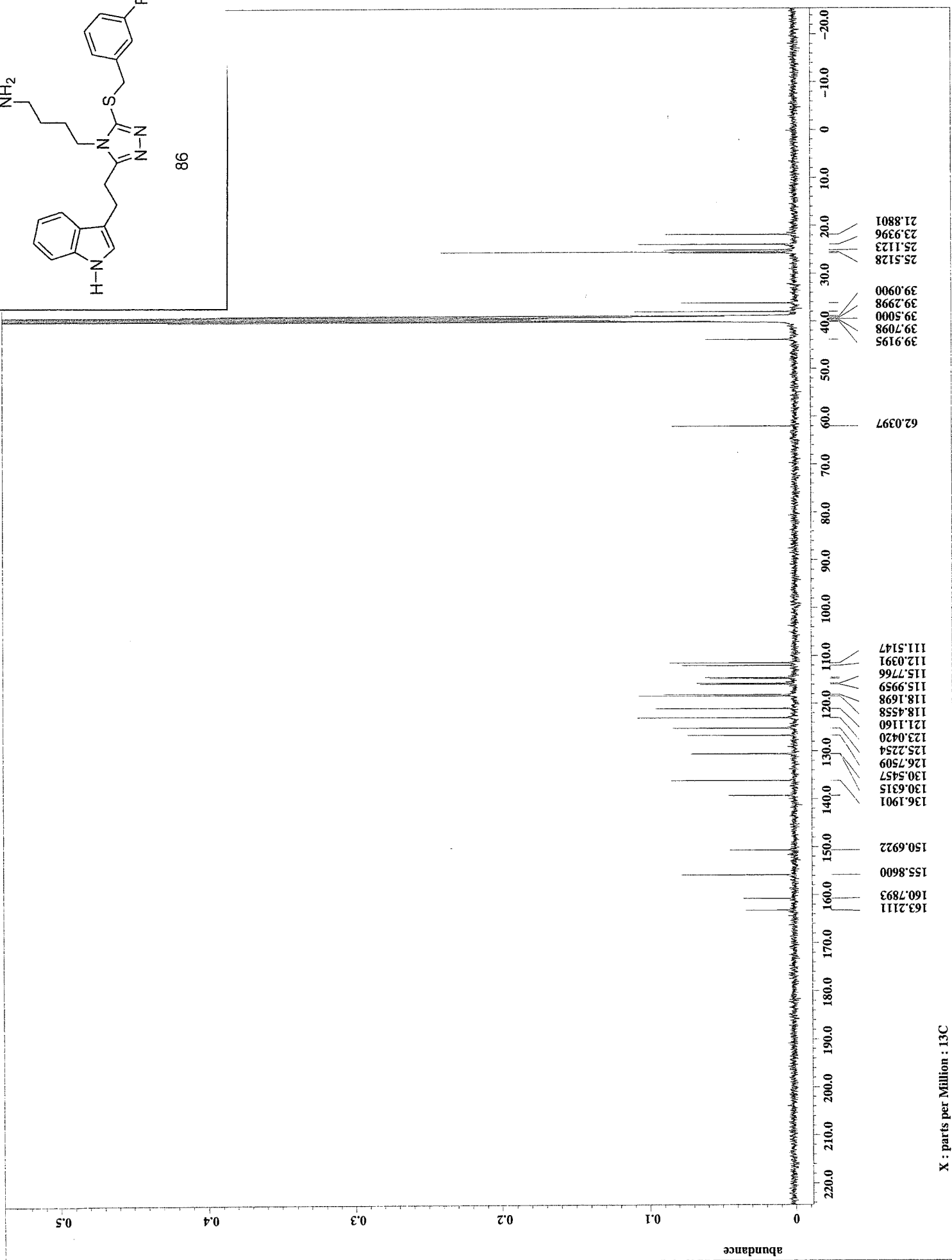
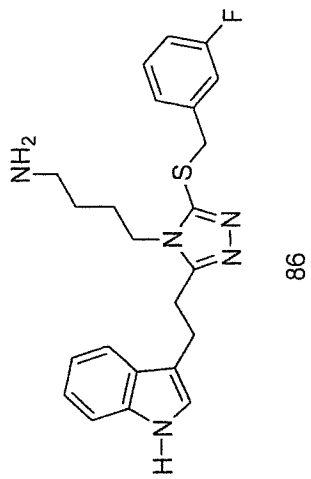
X : parts per Million : 1H



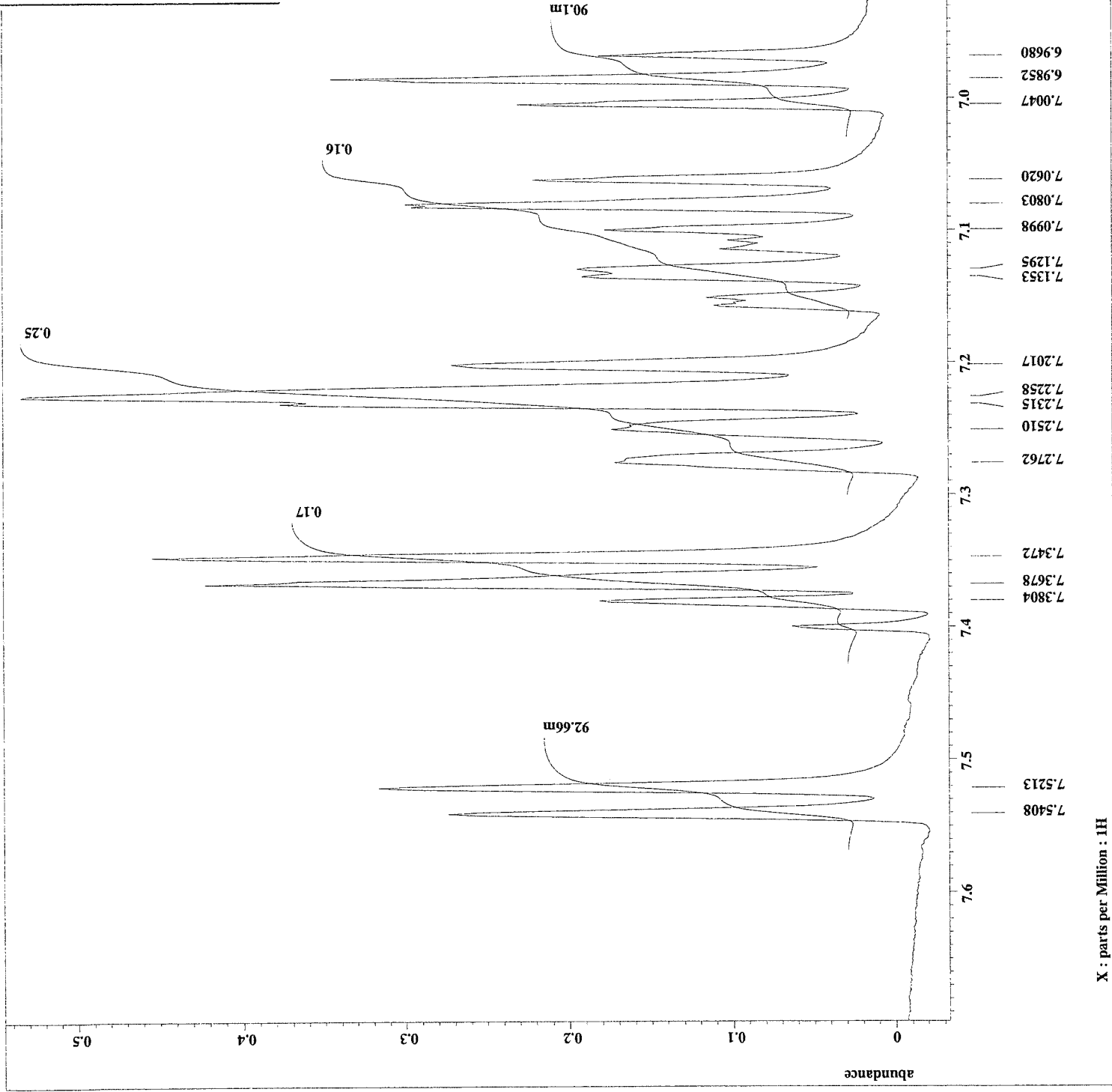
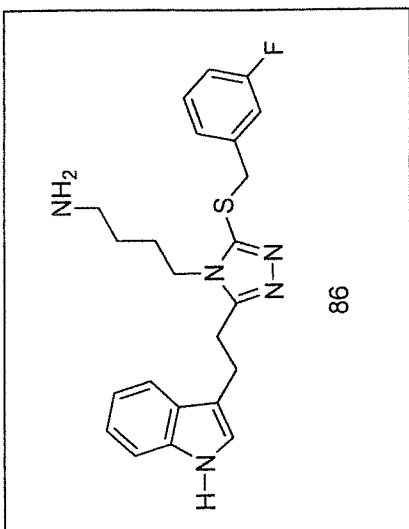
85



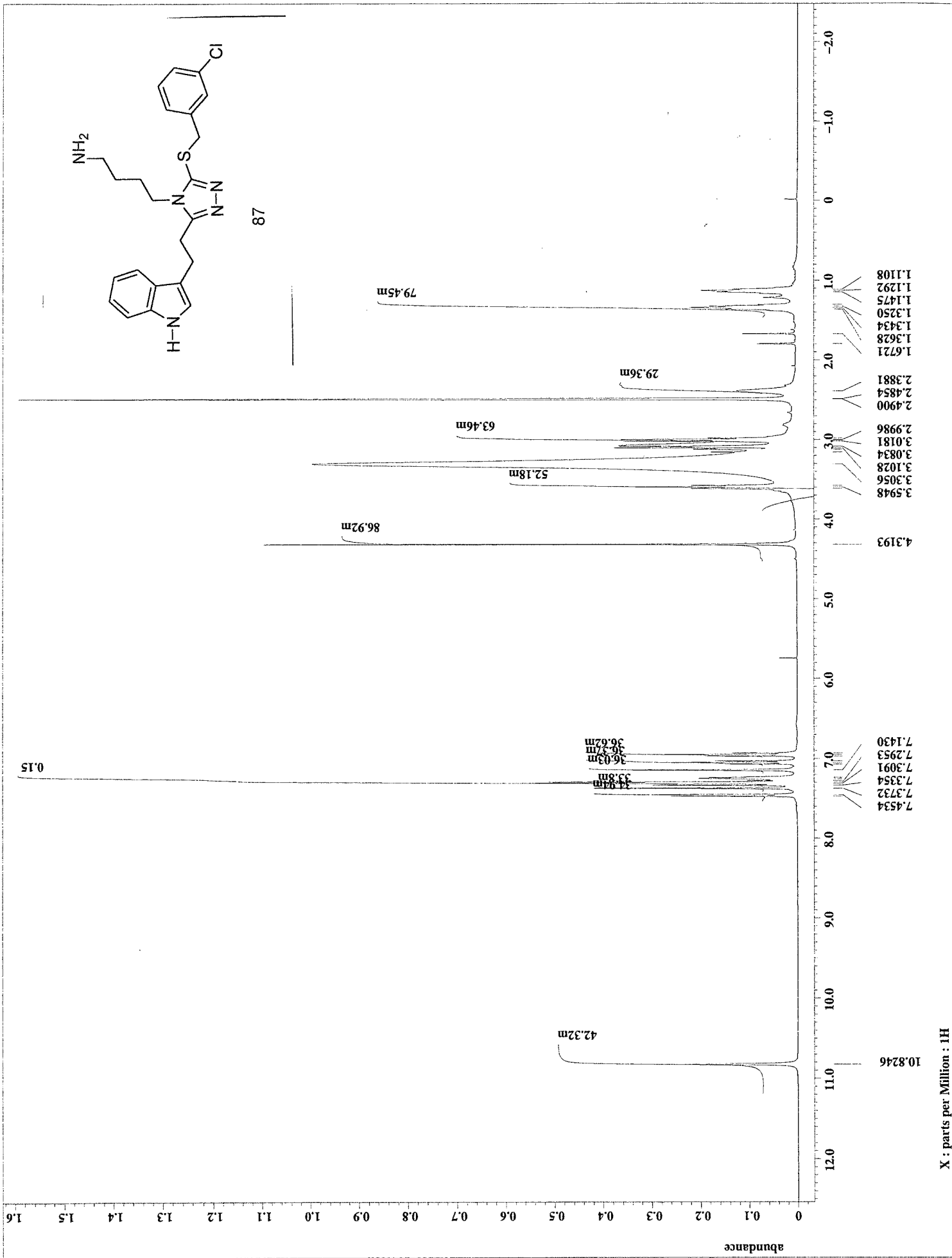




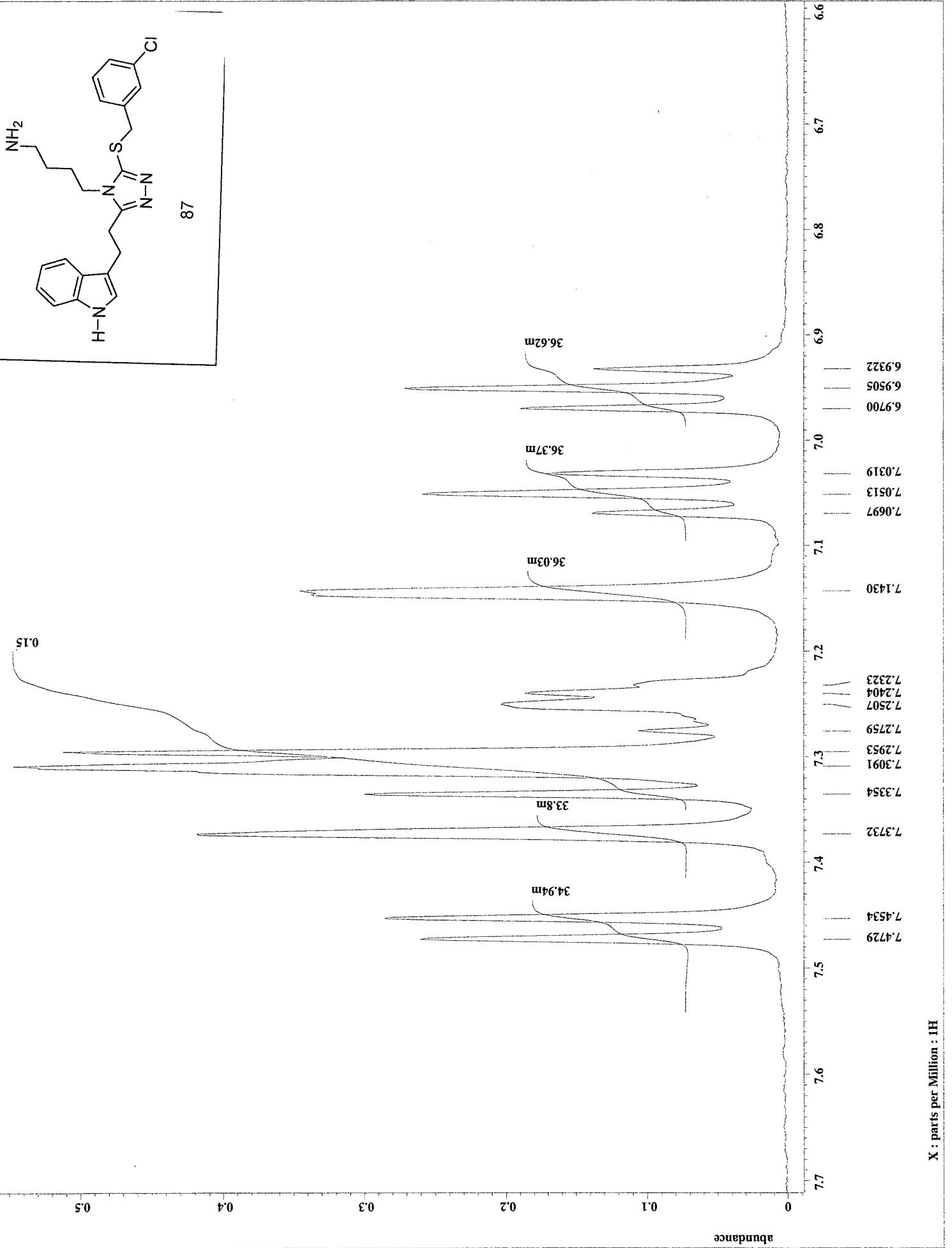
X : parts per Million : 13C



X : parts per Million : 1H

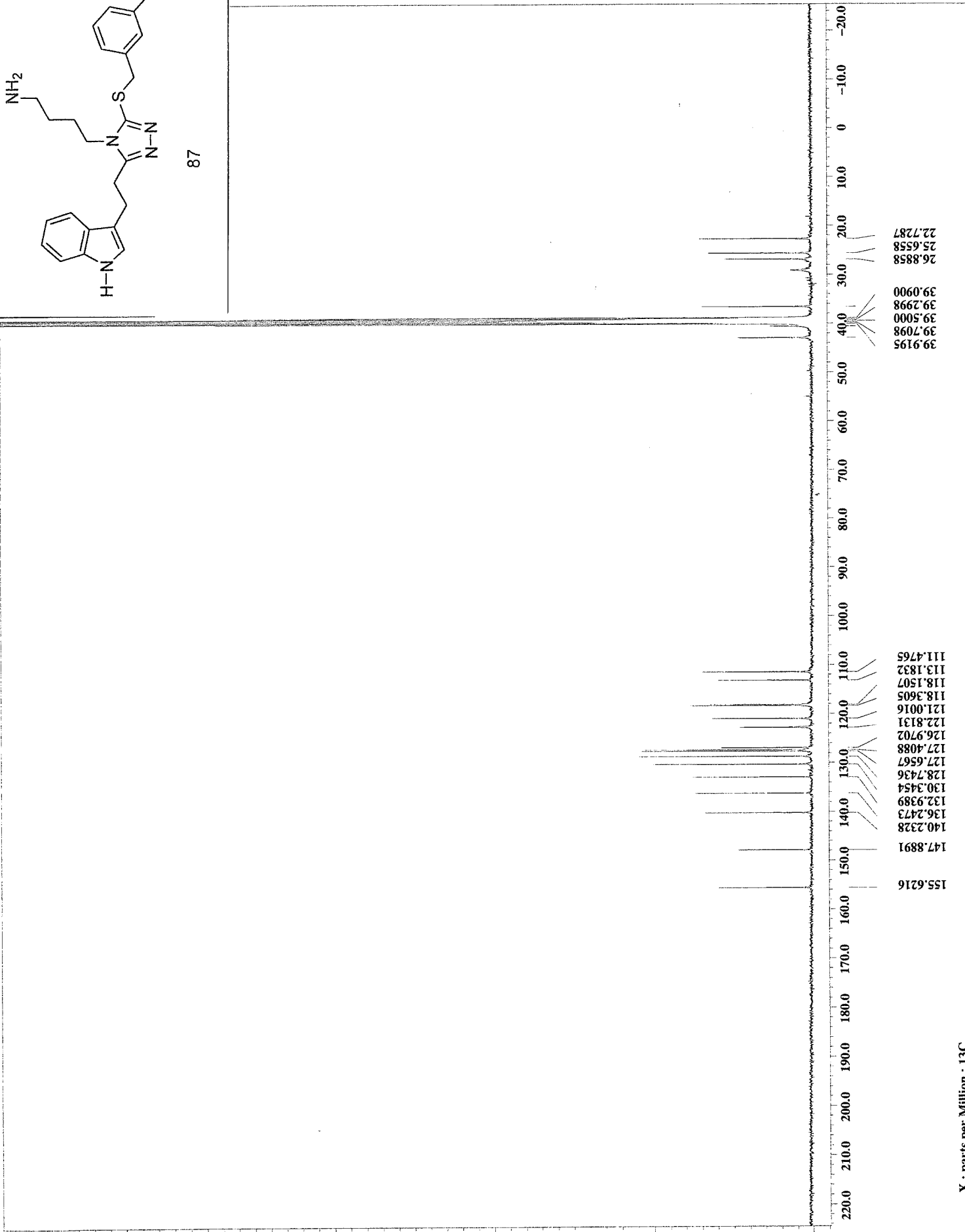


X : parts per Million : 1H

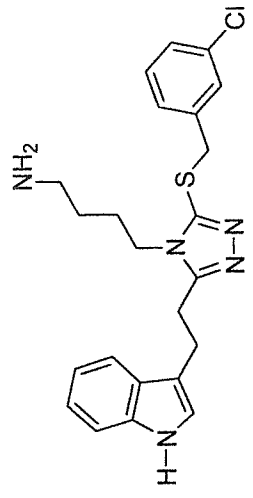


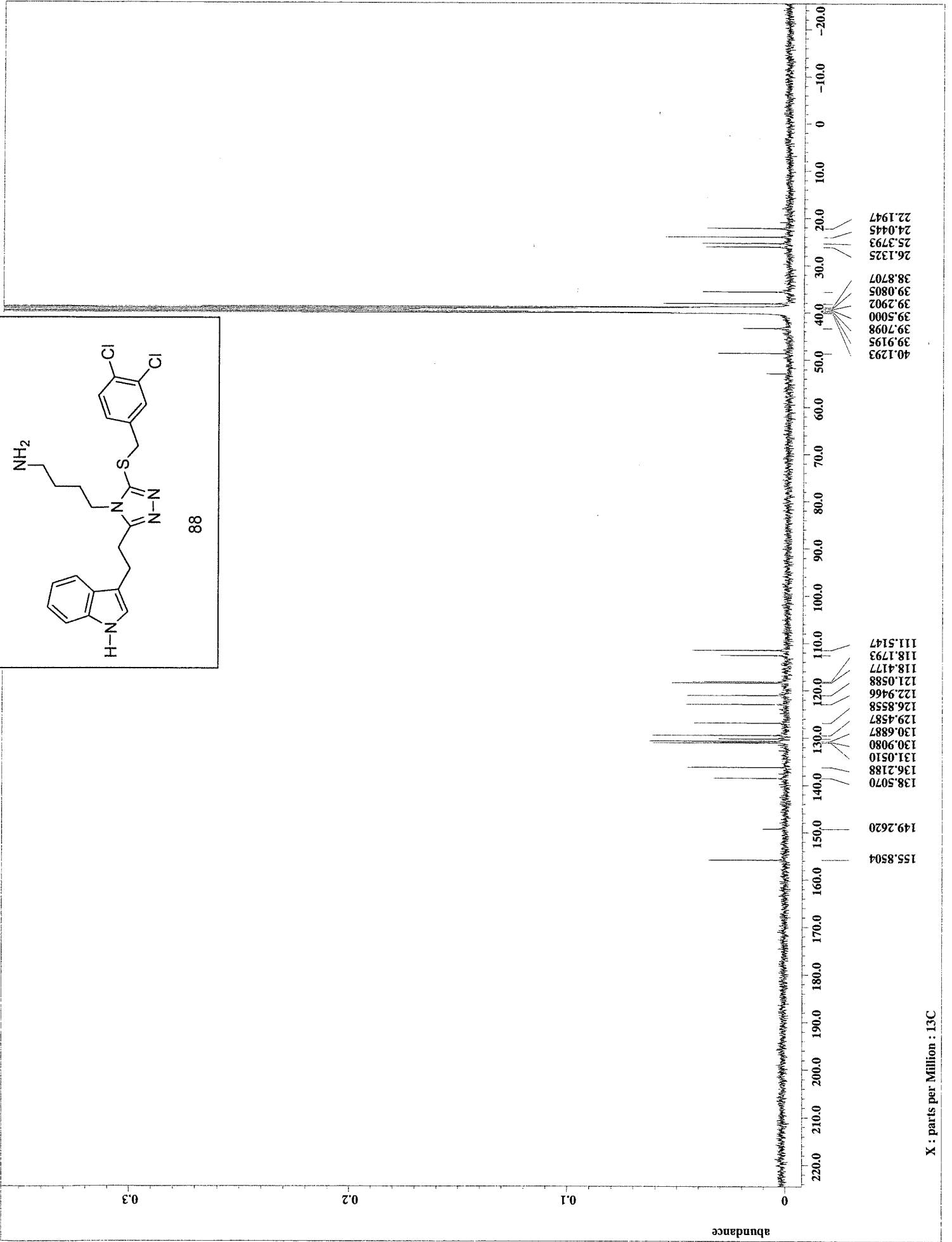
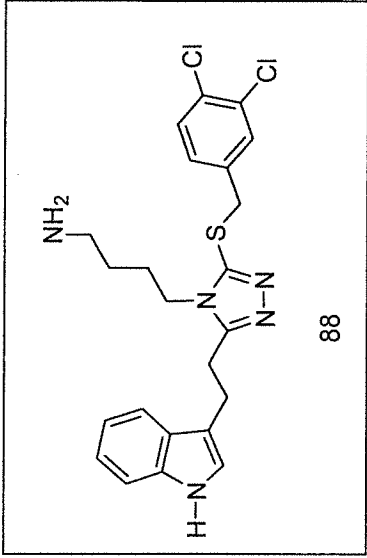
X : parts per Million : 1H

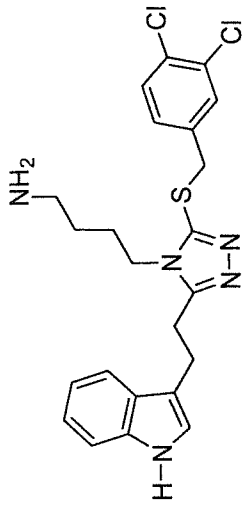
abundance



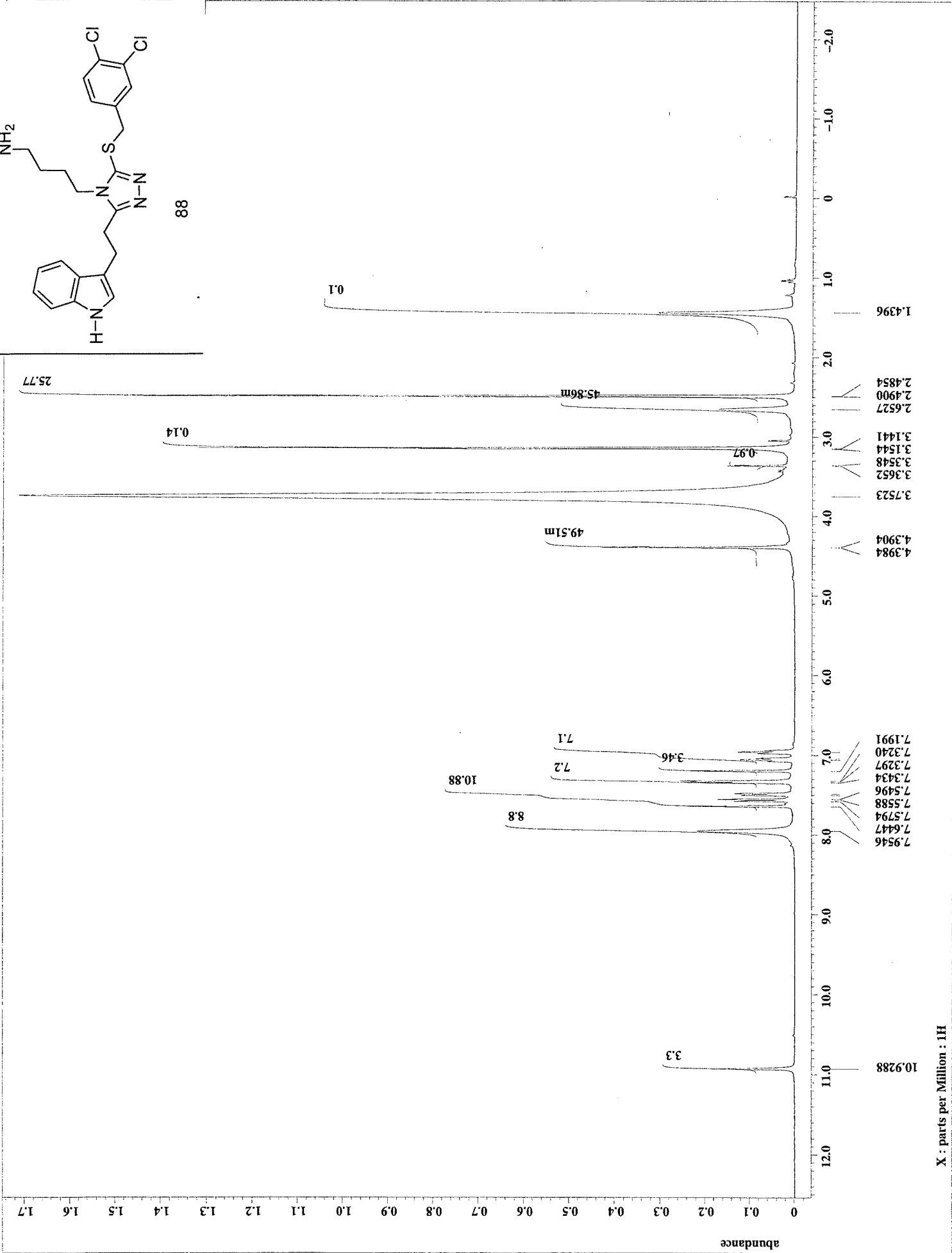
87



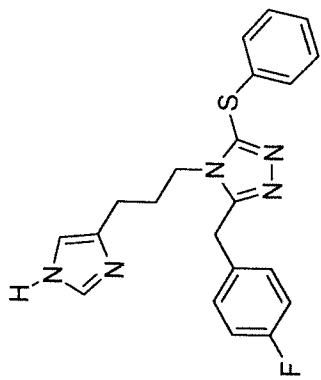




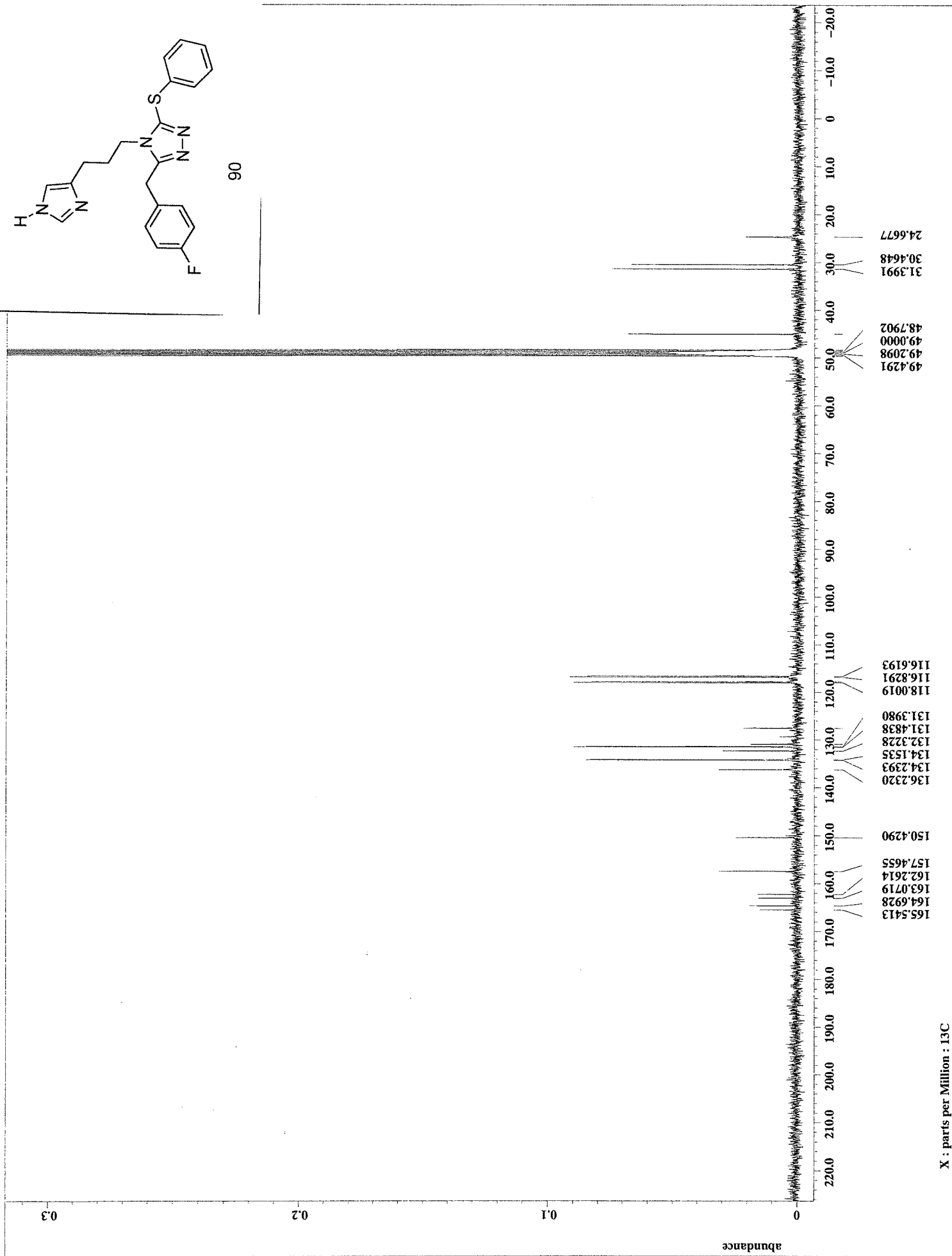
88

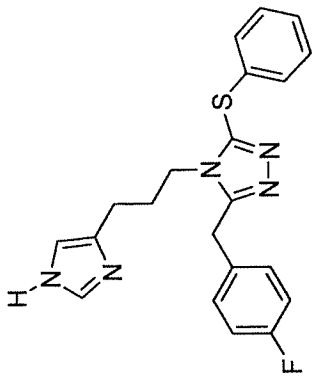


X : parts per Million : 1H

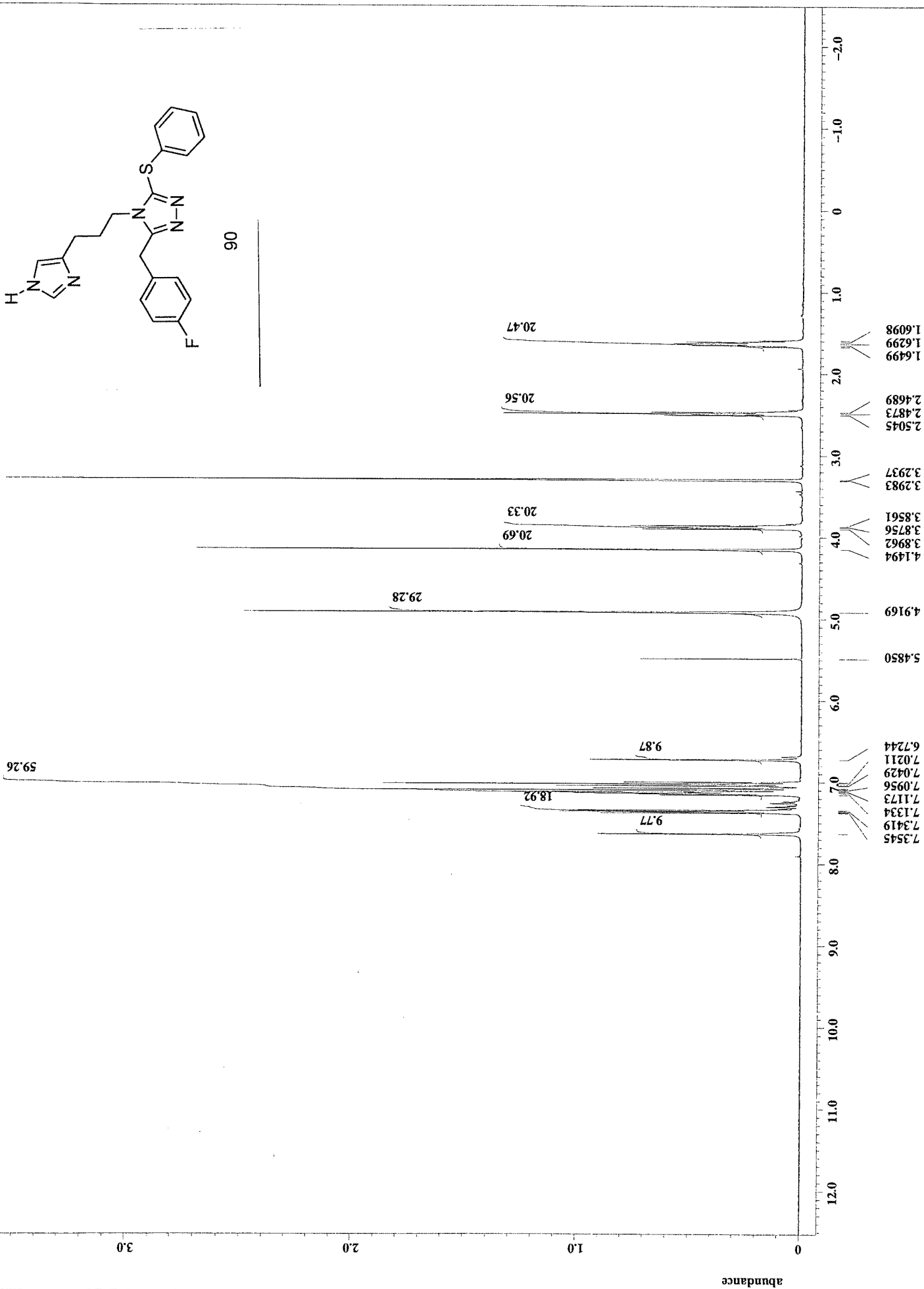


90

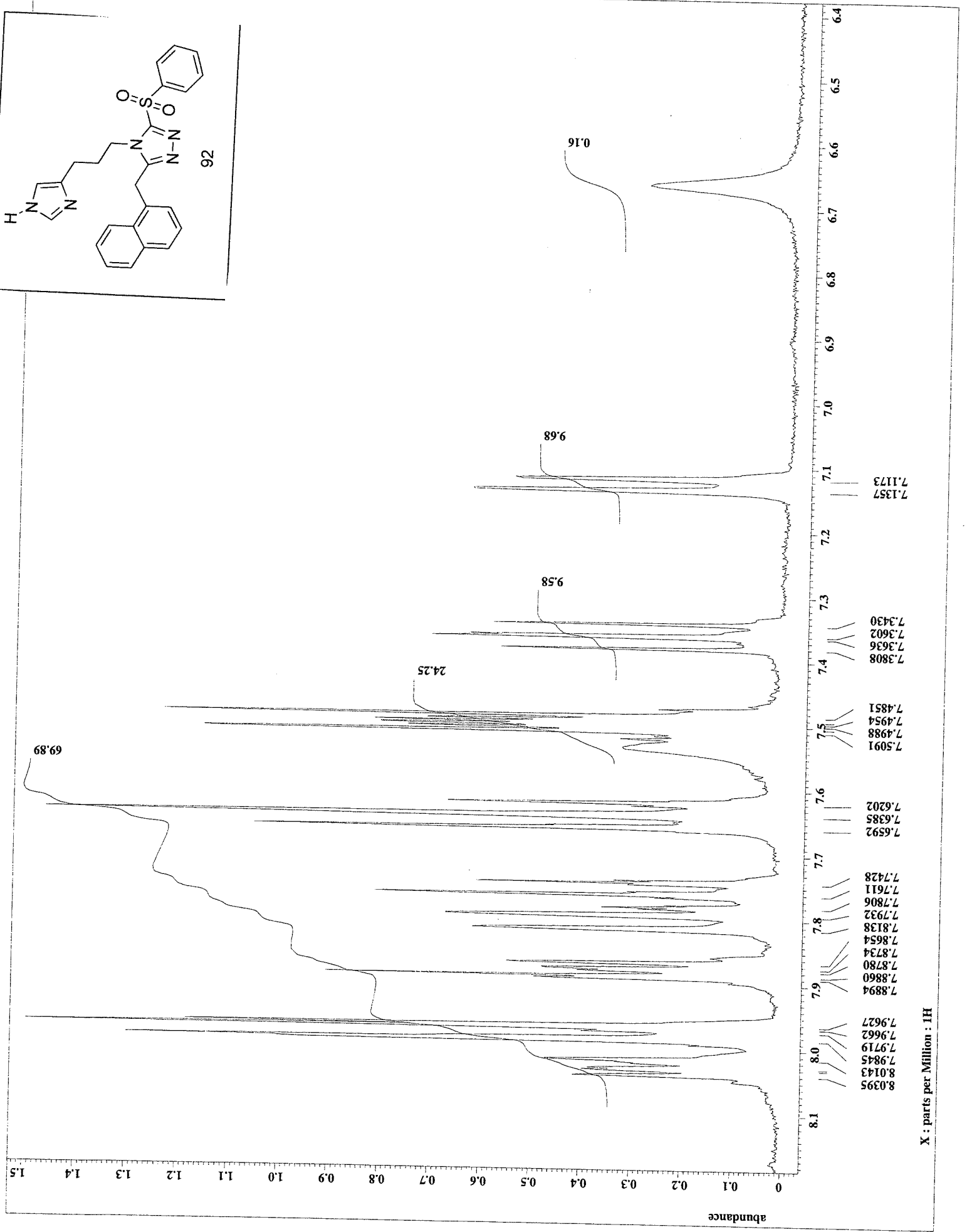
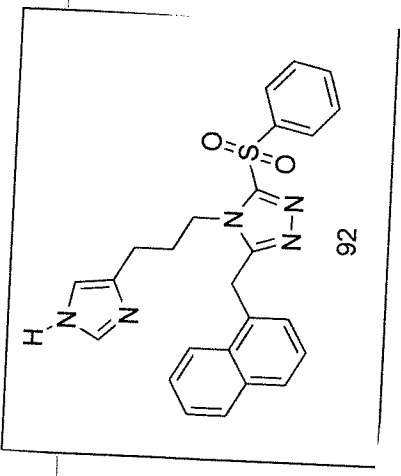




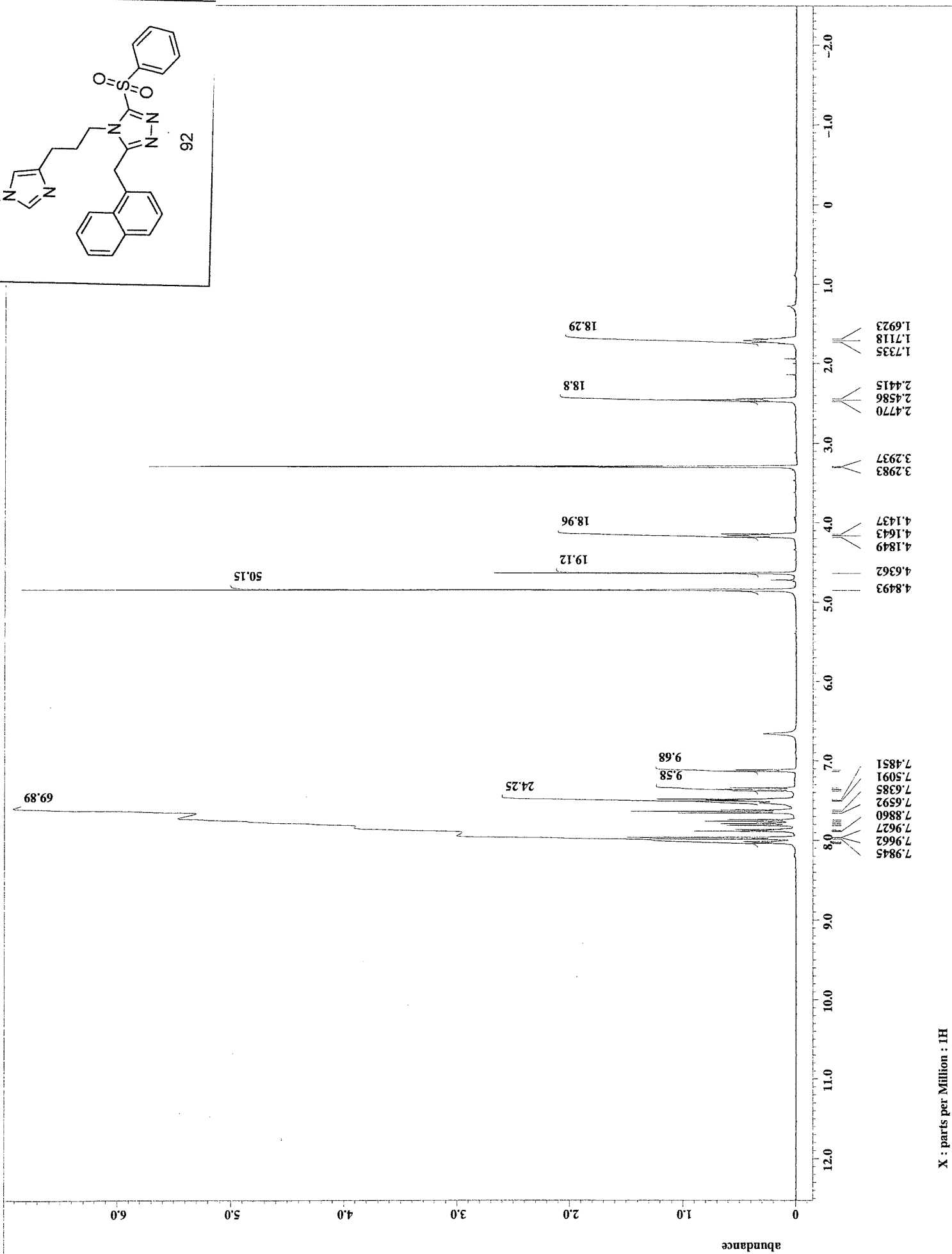
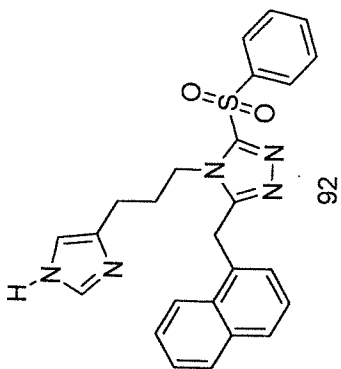
06

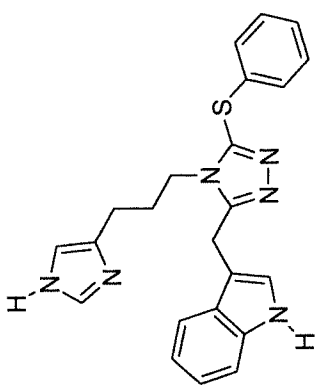


X : parts per Million : 1H

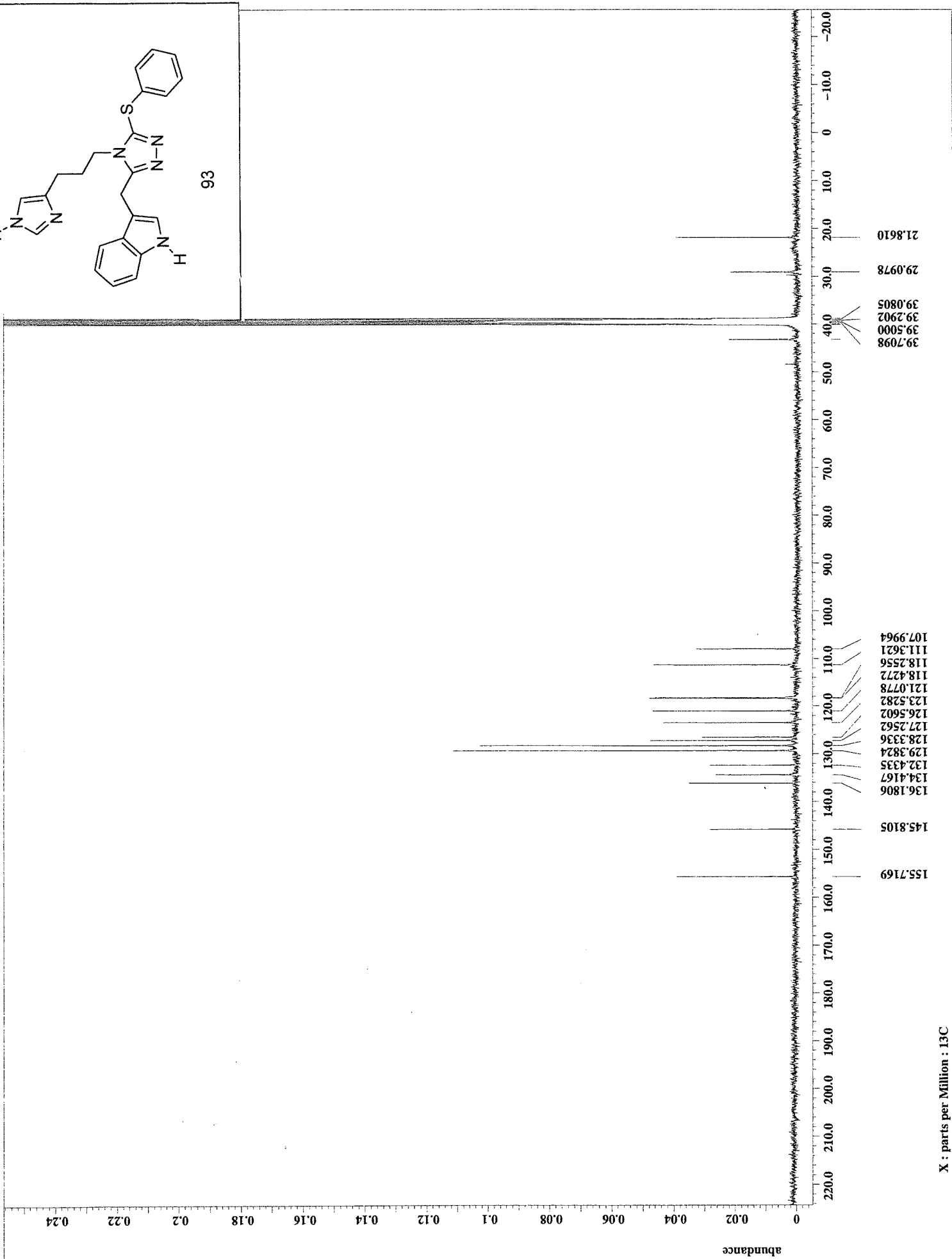


X : parts per Million : 1H

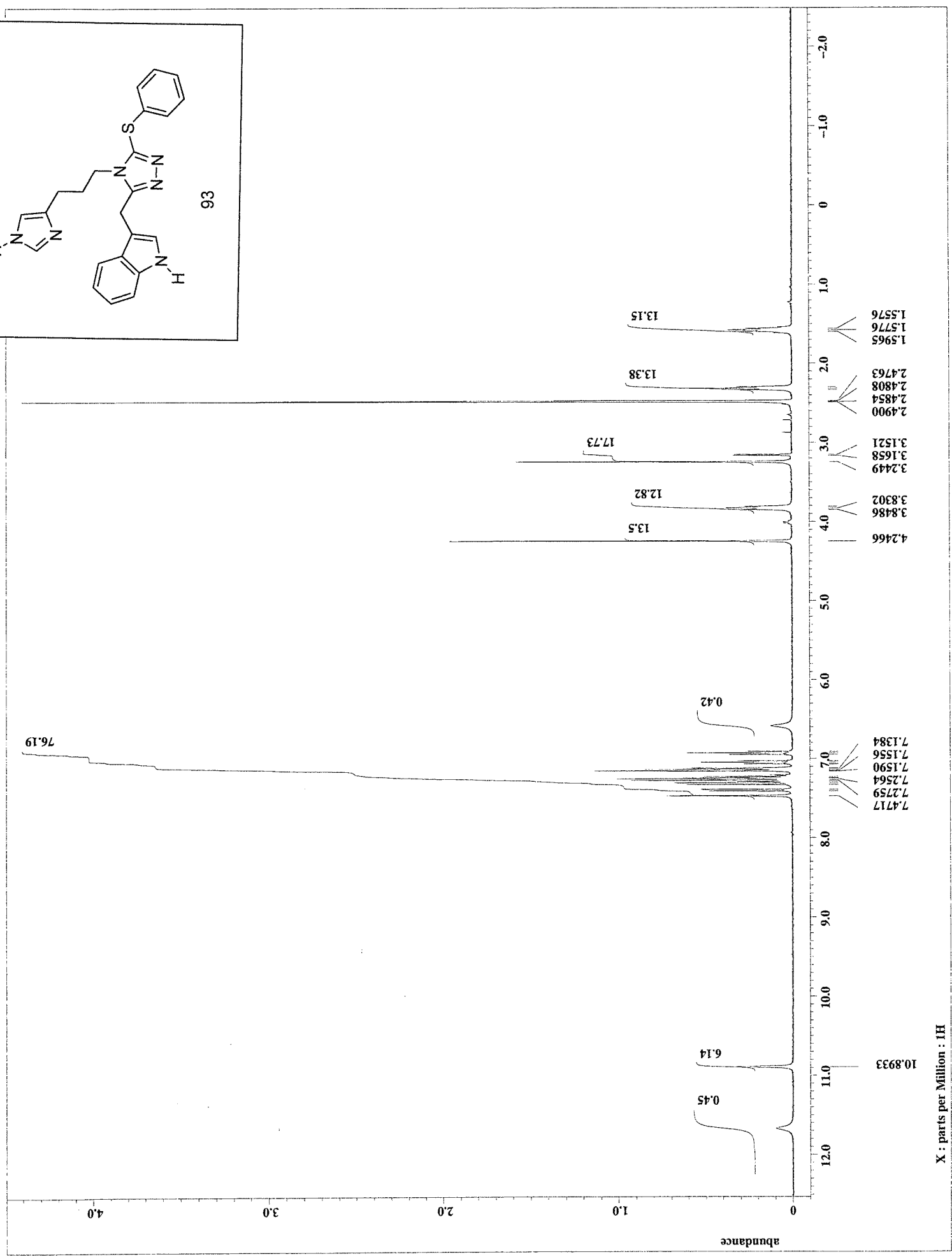
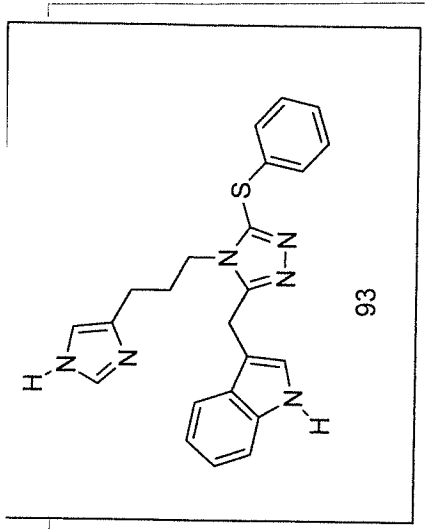


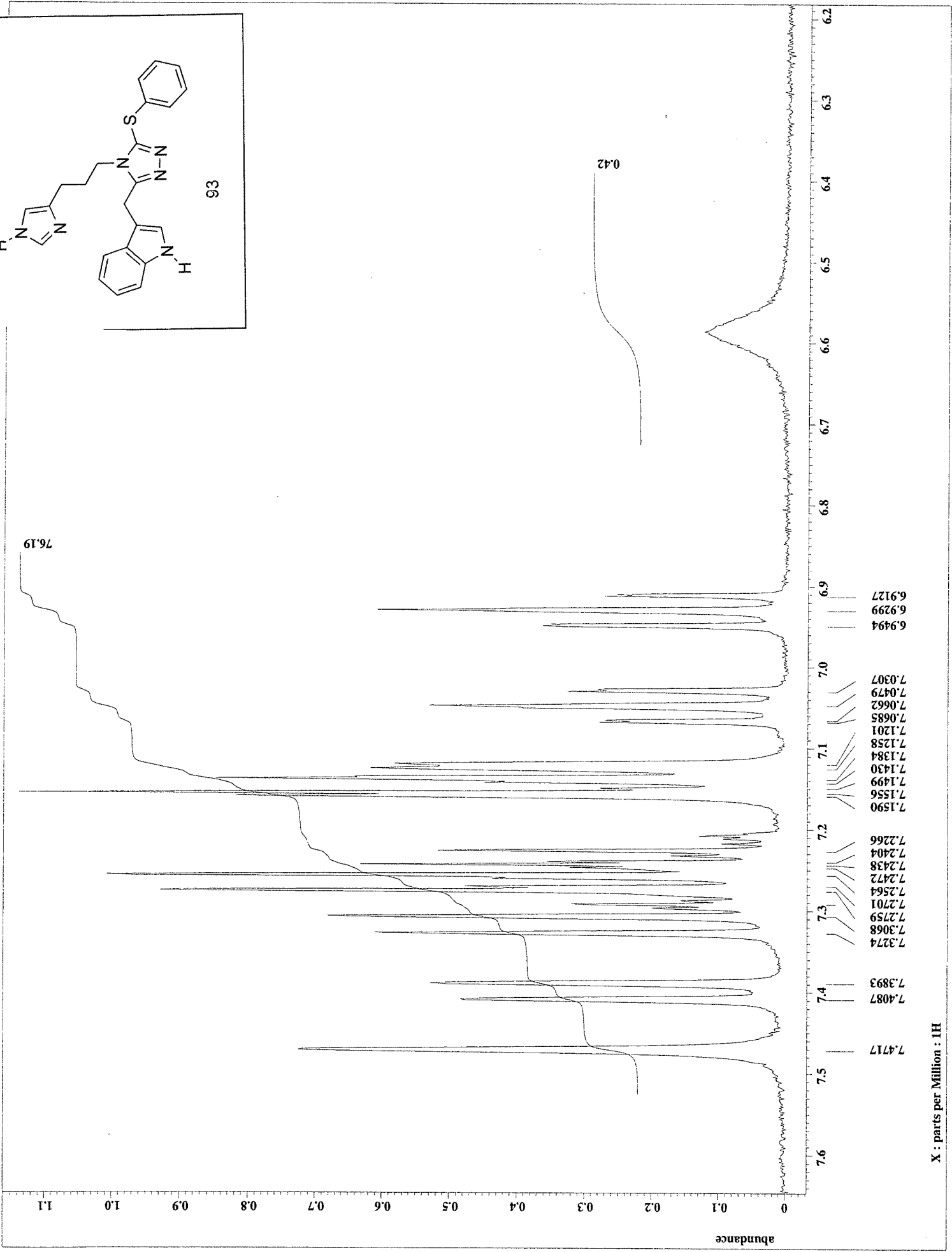
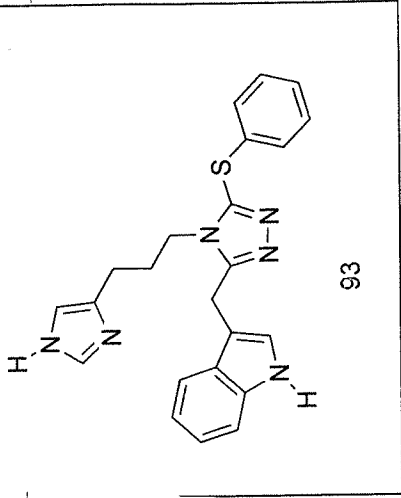


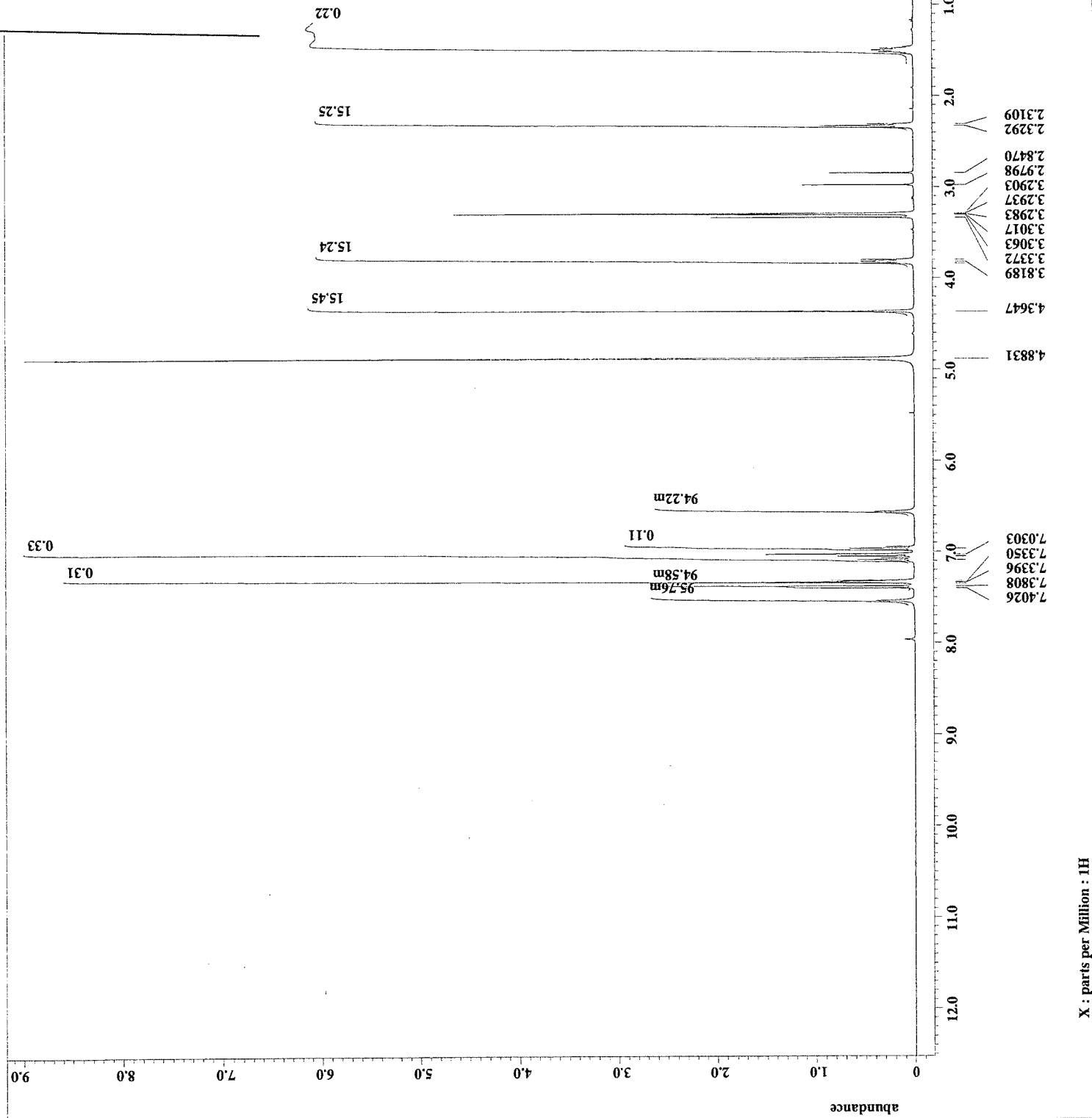
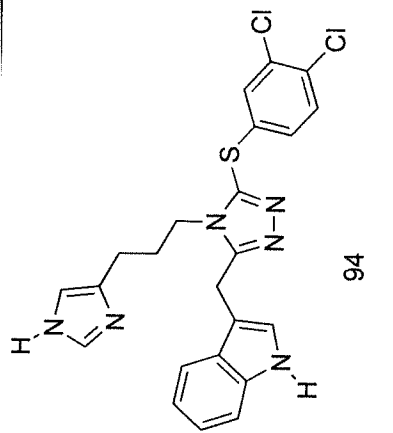
93



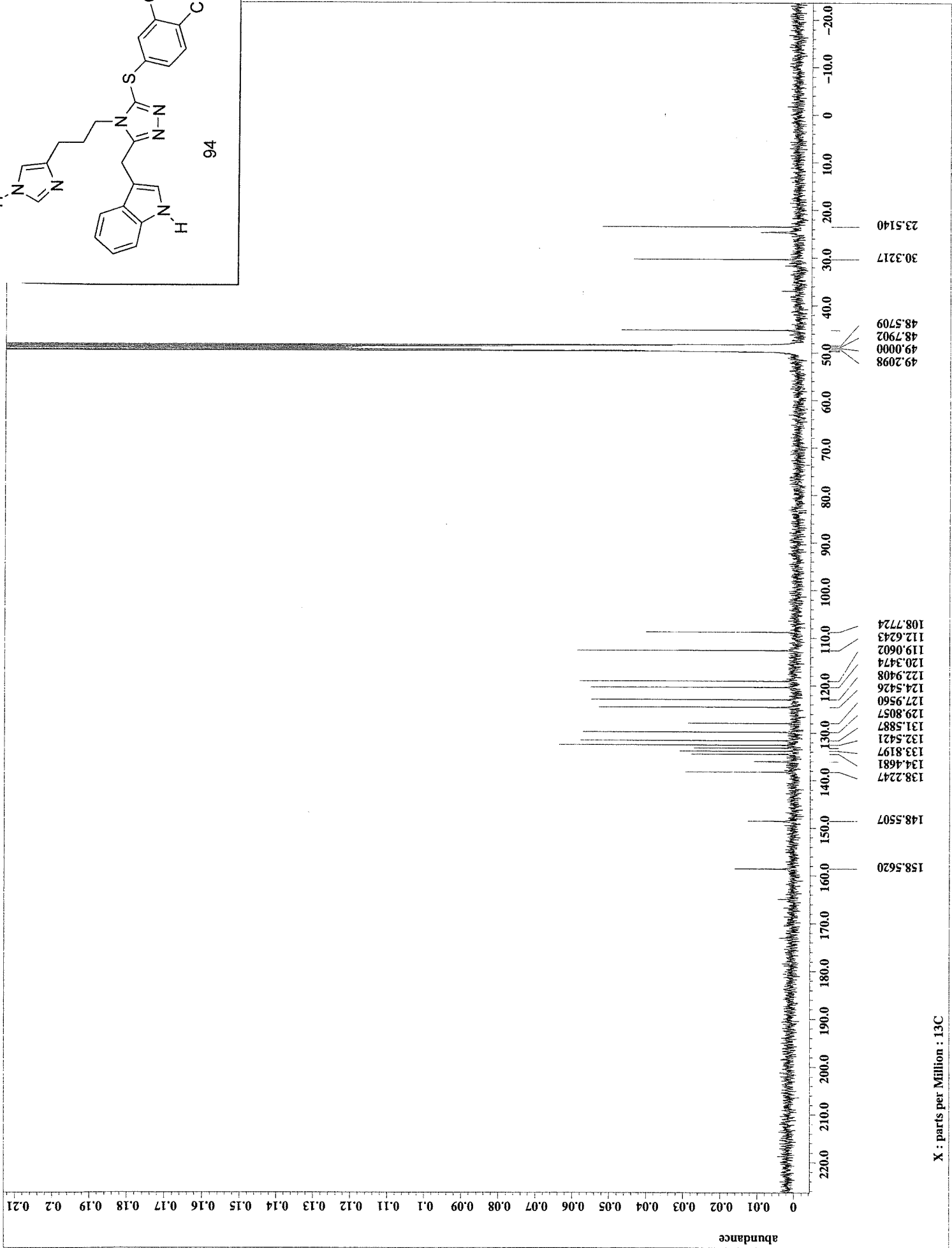
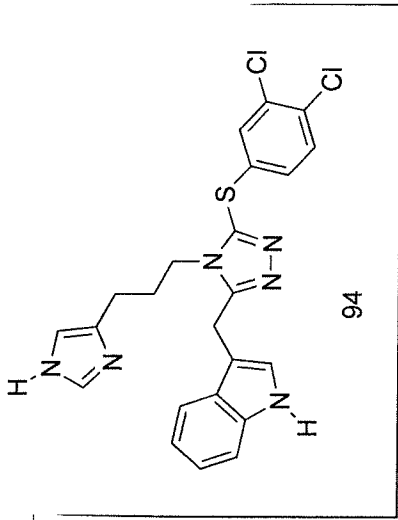
X : parts per Million : 13C



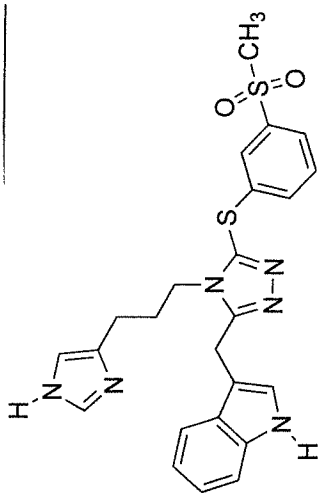




X : parts per Million : 1H



X : parts per Million : 13C



95

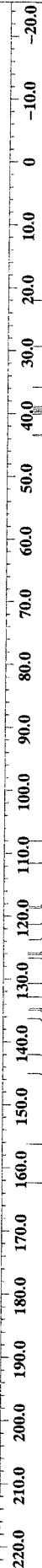
0.3

0.2

0.1

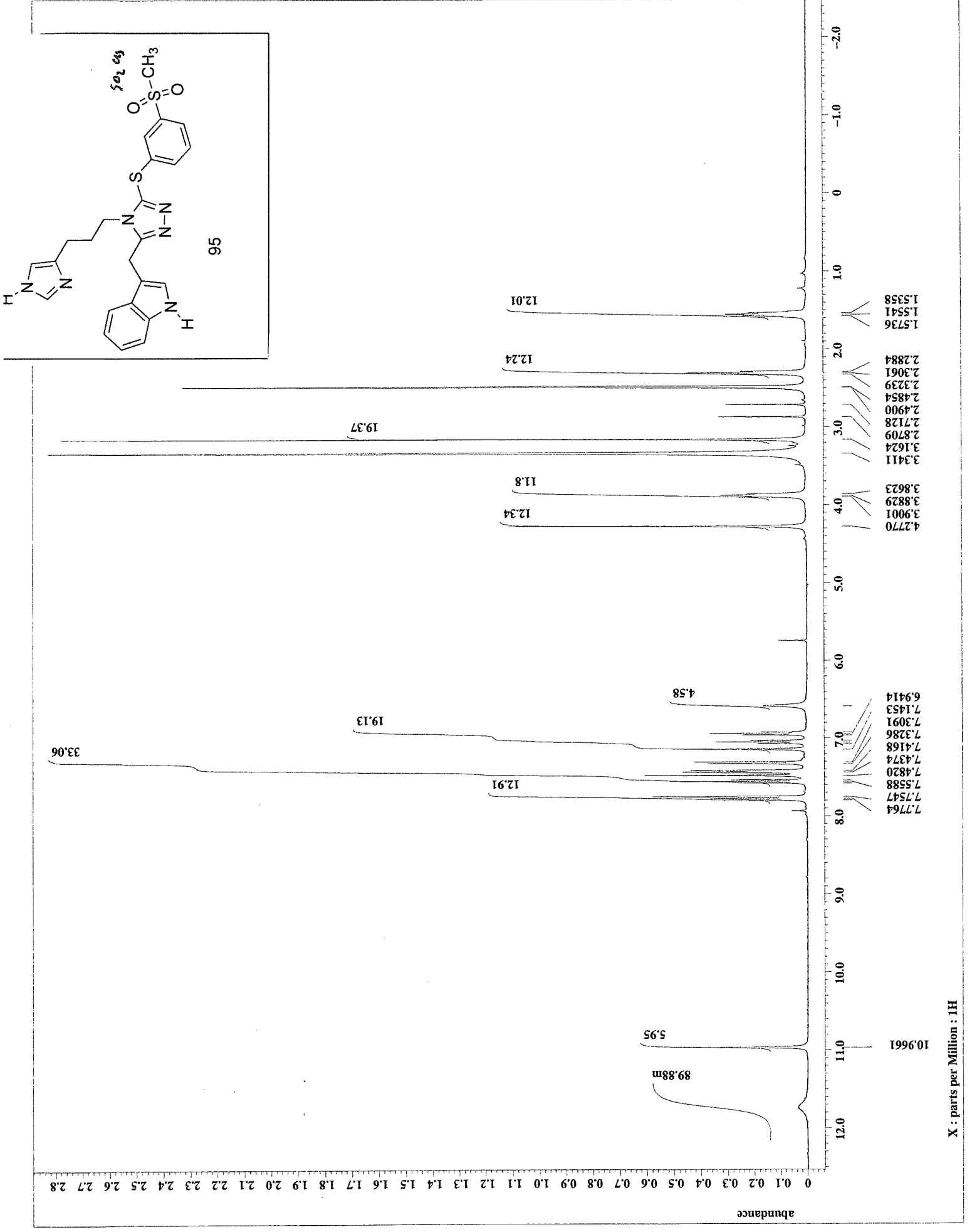
0

abundance

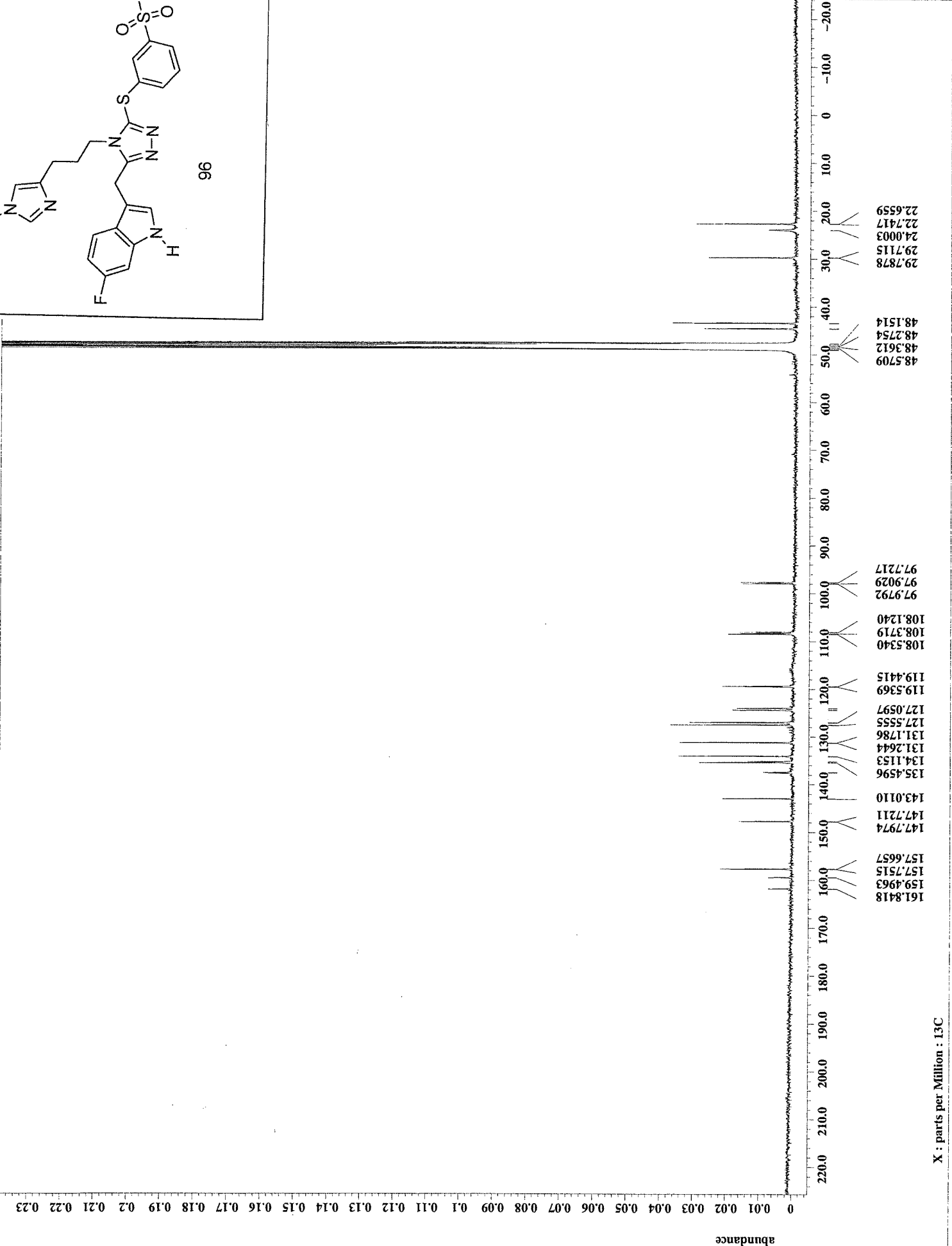
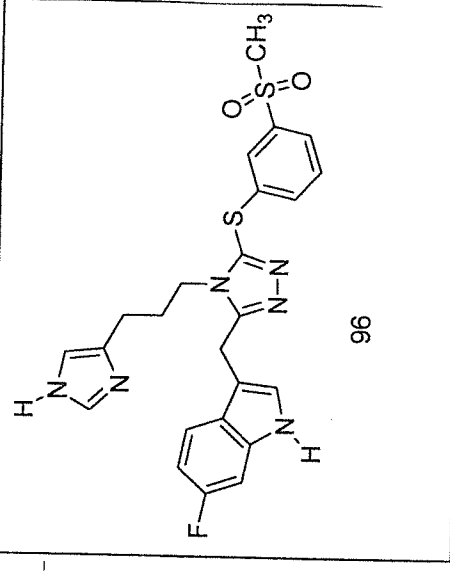


- 21.9850
- 29.2980
- 38.8803
- 39.0900
- 39.2902
- 39.5000
- 39.7098
- 39.9195
- 40.1293
- 43.2852
- 108.0345
- 111.5242
- 118.4081
- 118.6465
- 121.2685
- 123.7094
- 125.8260
- 126.0549
- 126.6651
- 130.7077
- 132.8435
- 134.6455
- 134.8839
- 136.2759
- 141.9681
- 145.0382
- 156.1937
- 162.3244

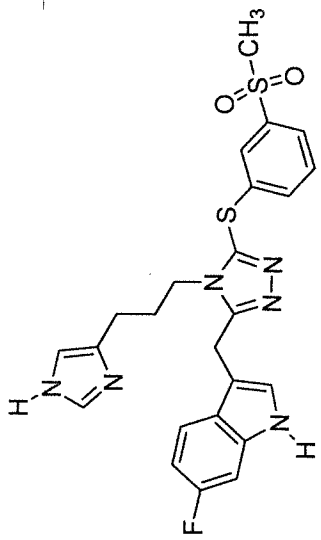
X : parts per Million : 13C



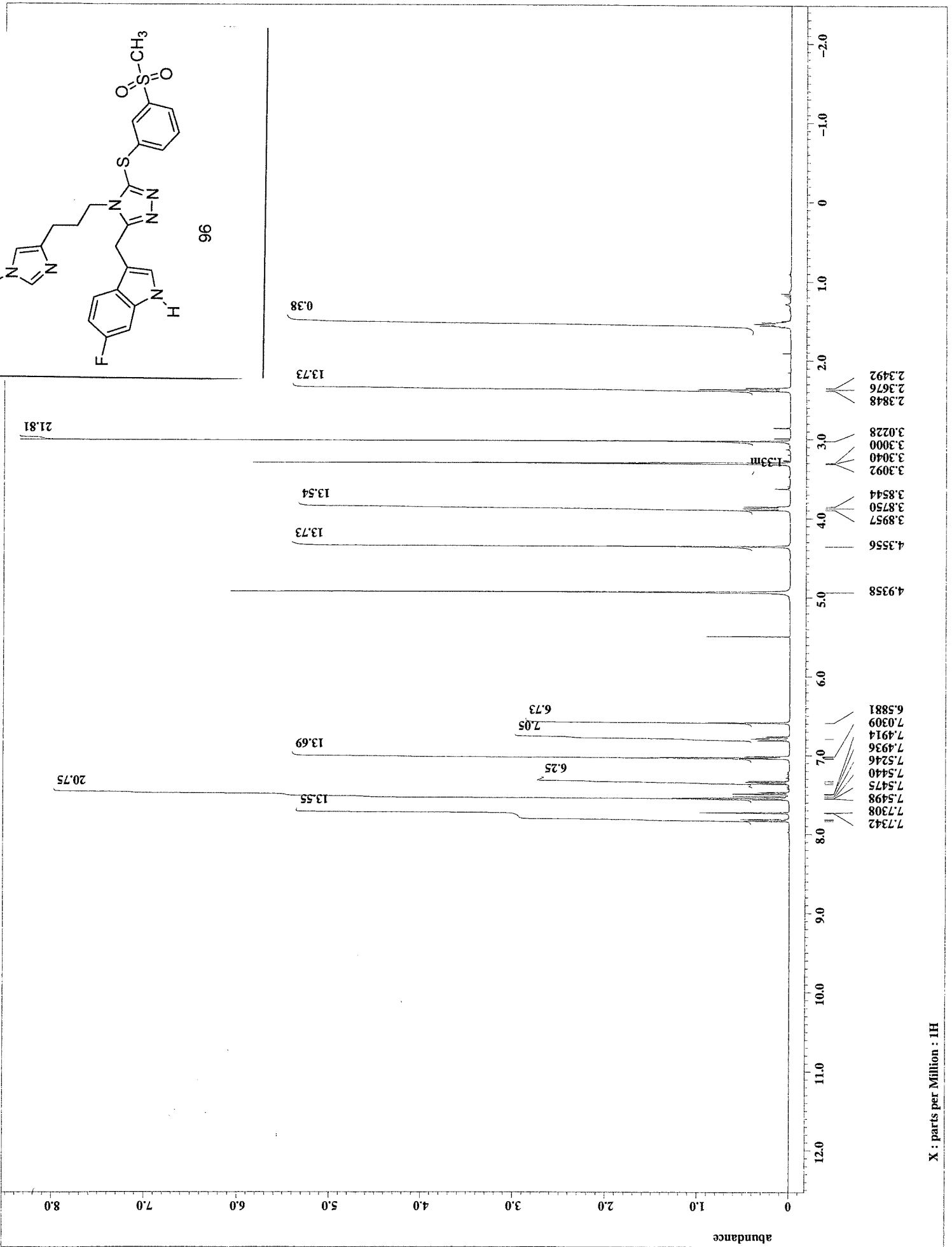
X : parts per Million : 1H



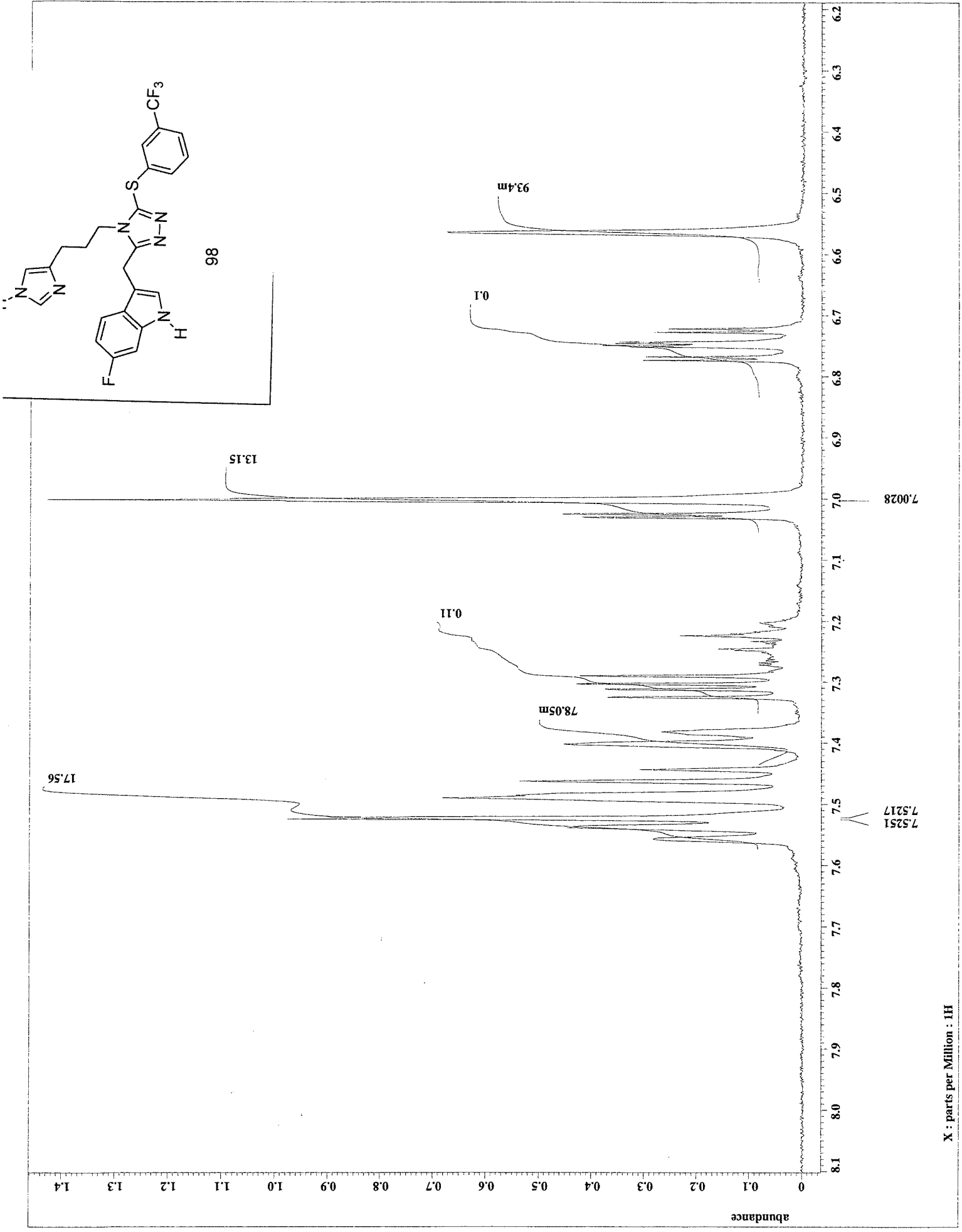
X : parts per Million : 13C



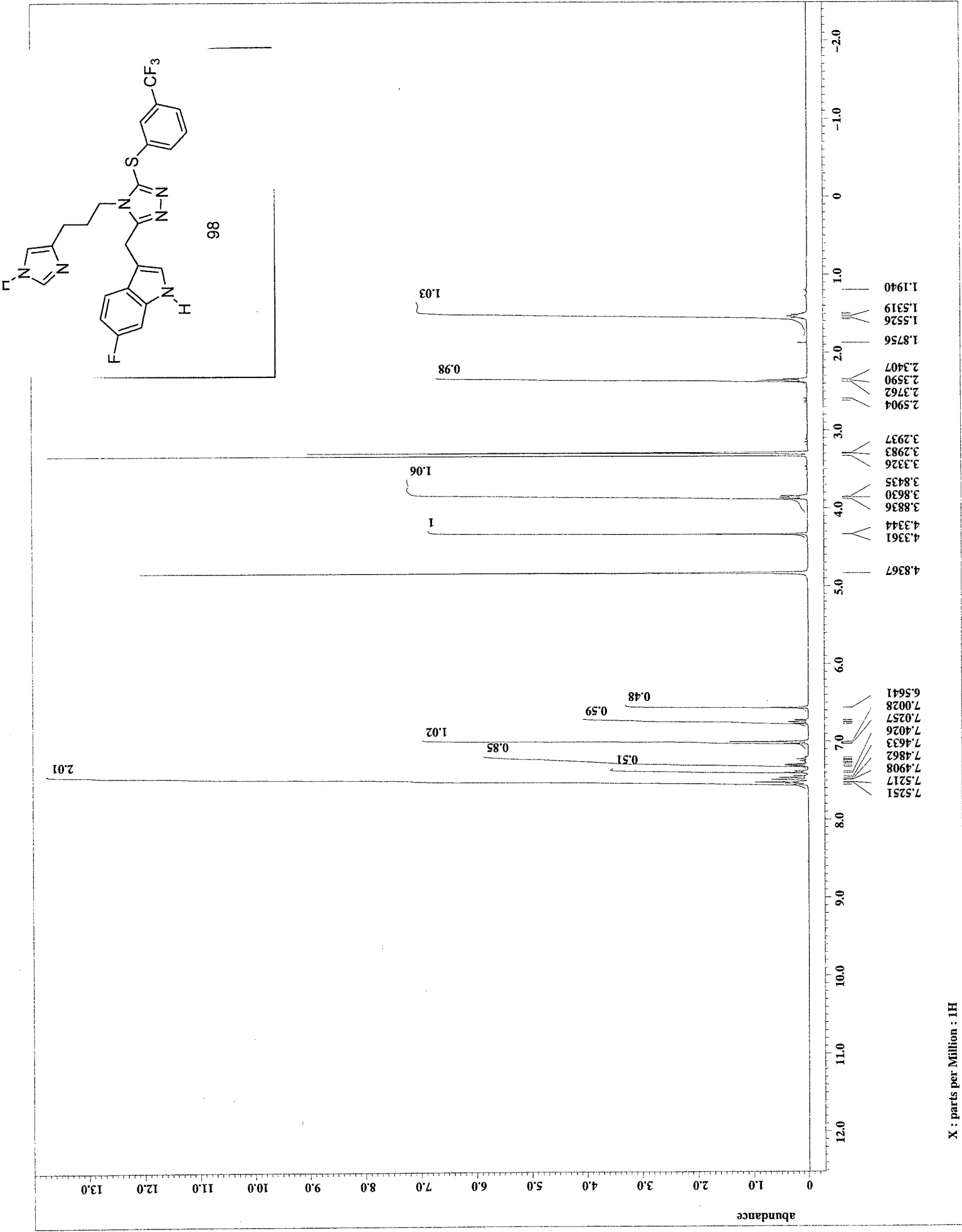
96



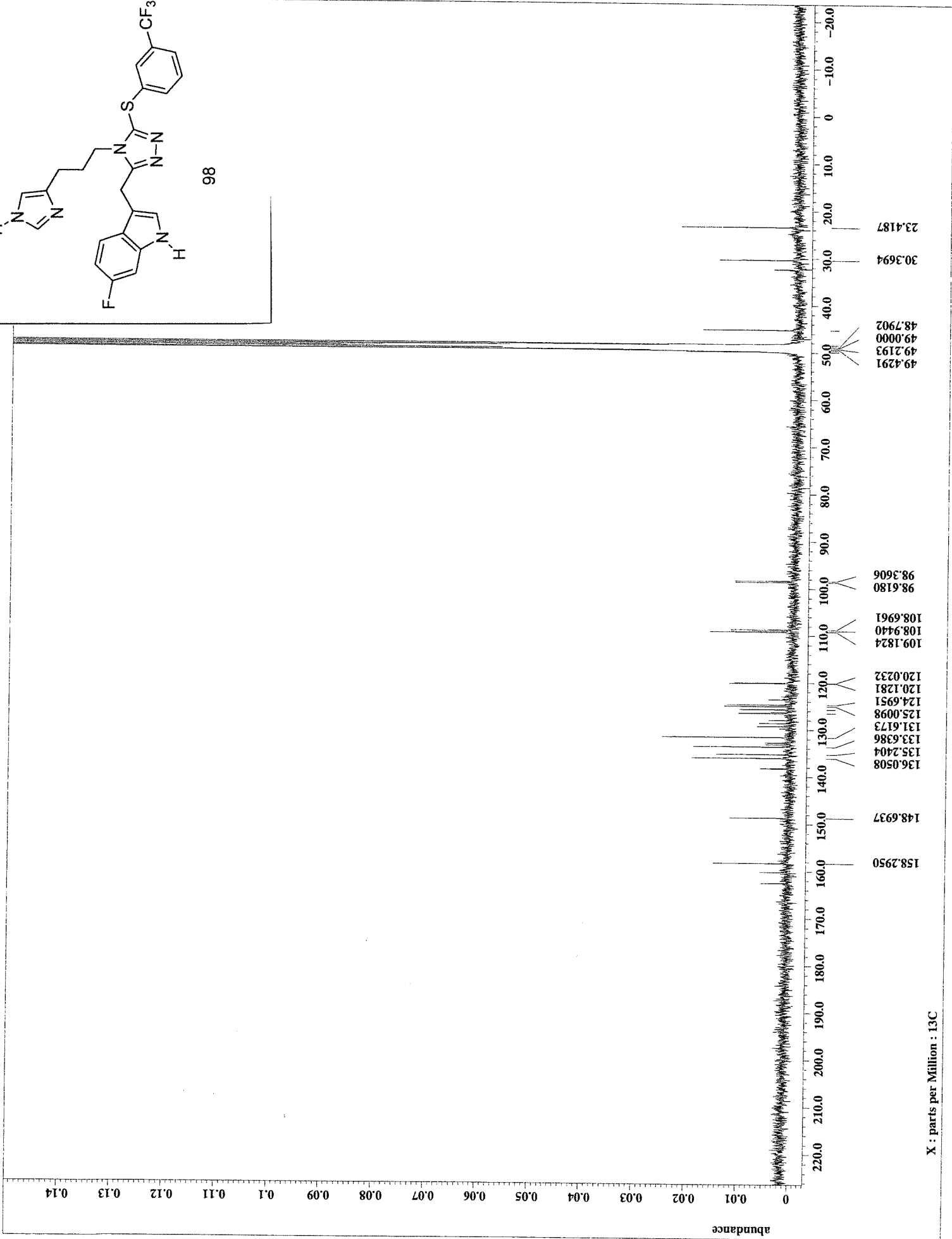
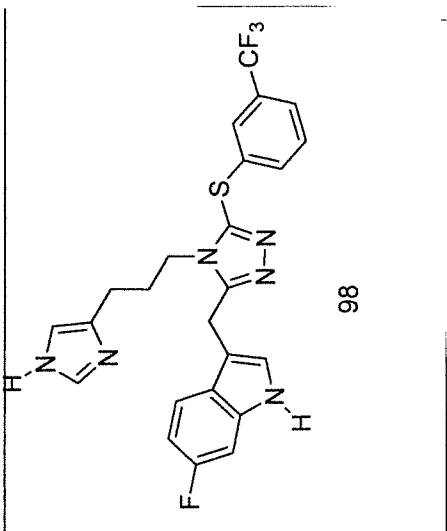
X : parts per Million : ^1H



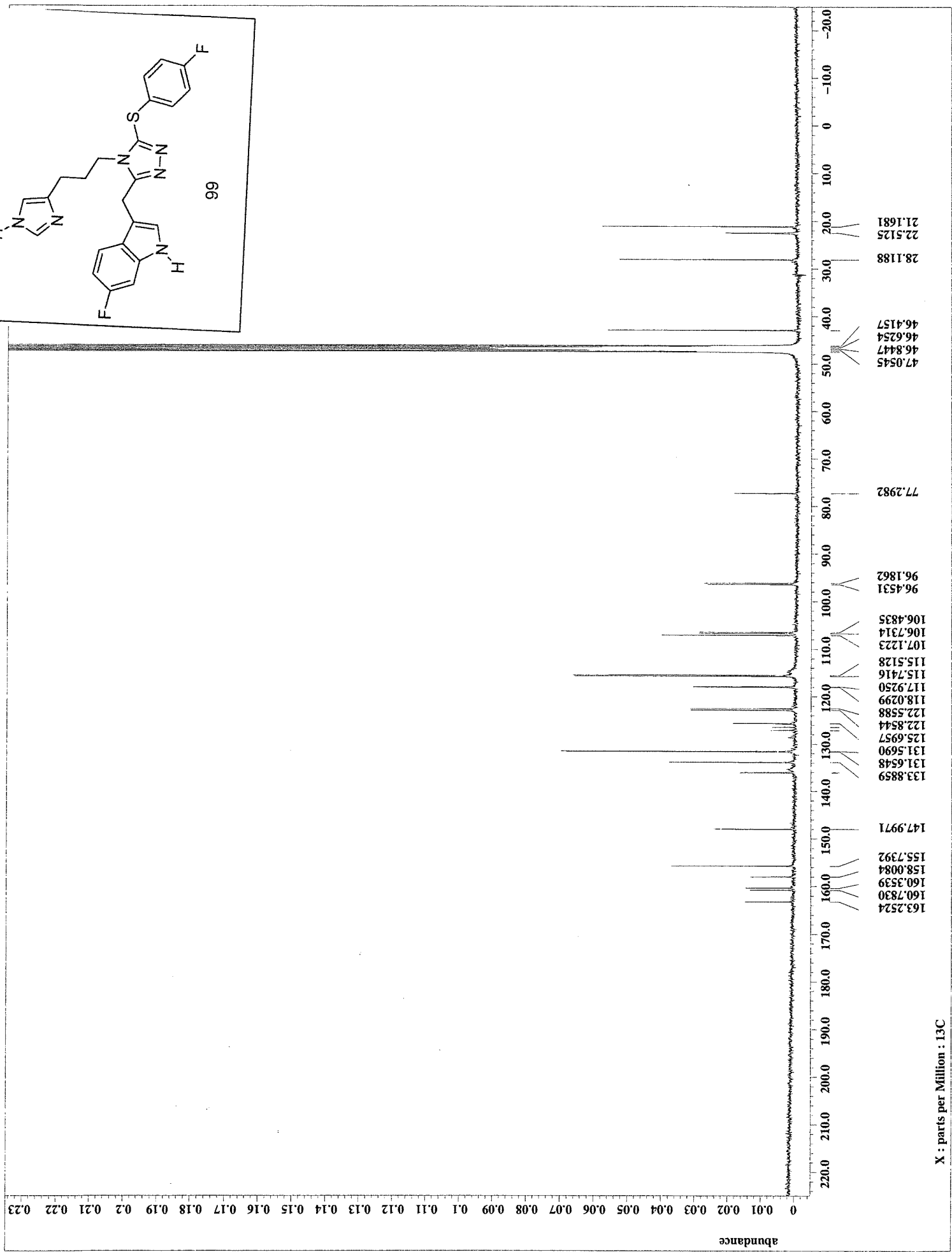
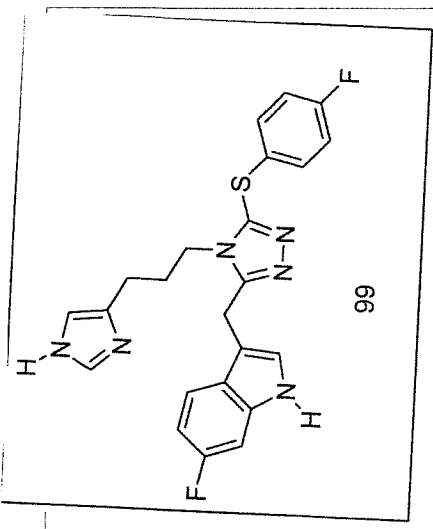
X : parts per Million : 1H



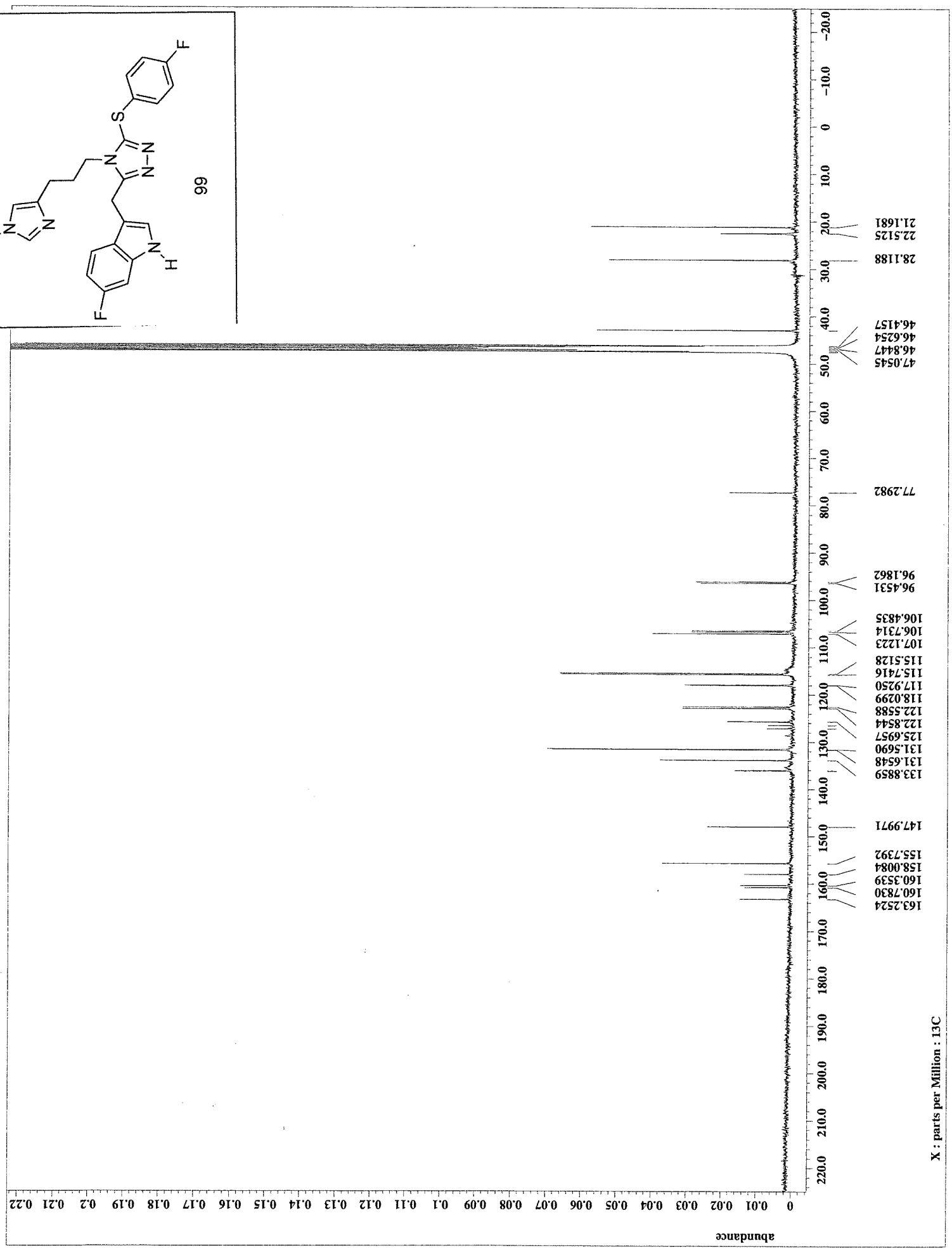
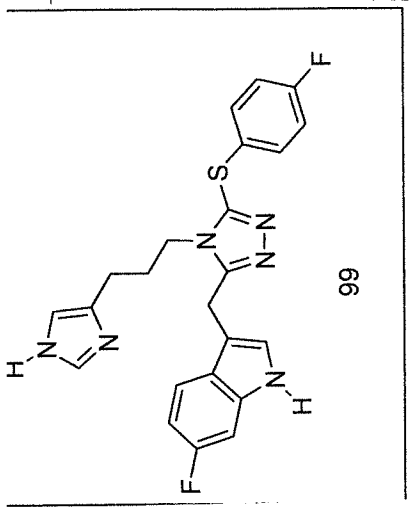
X : parts per Million : 1H

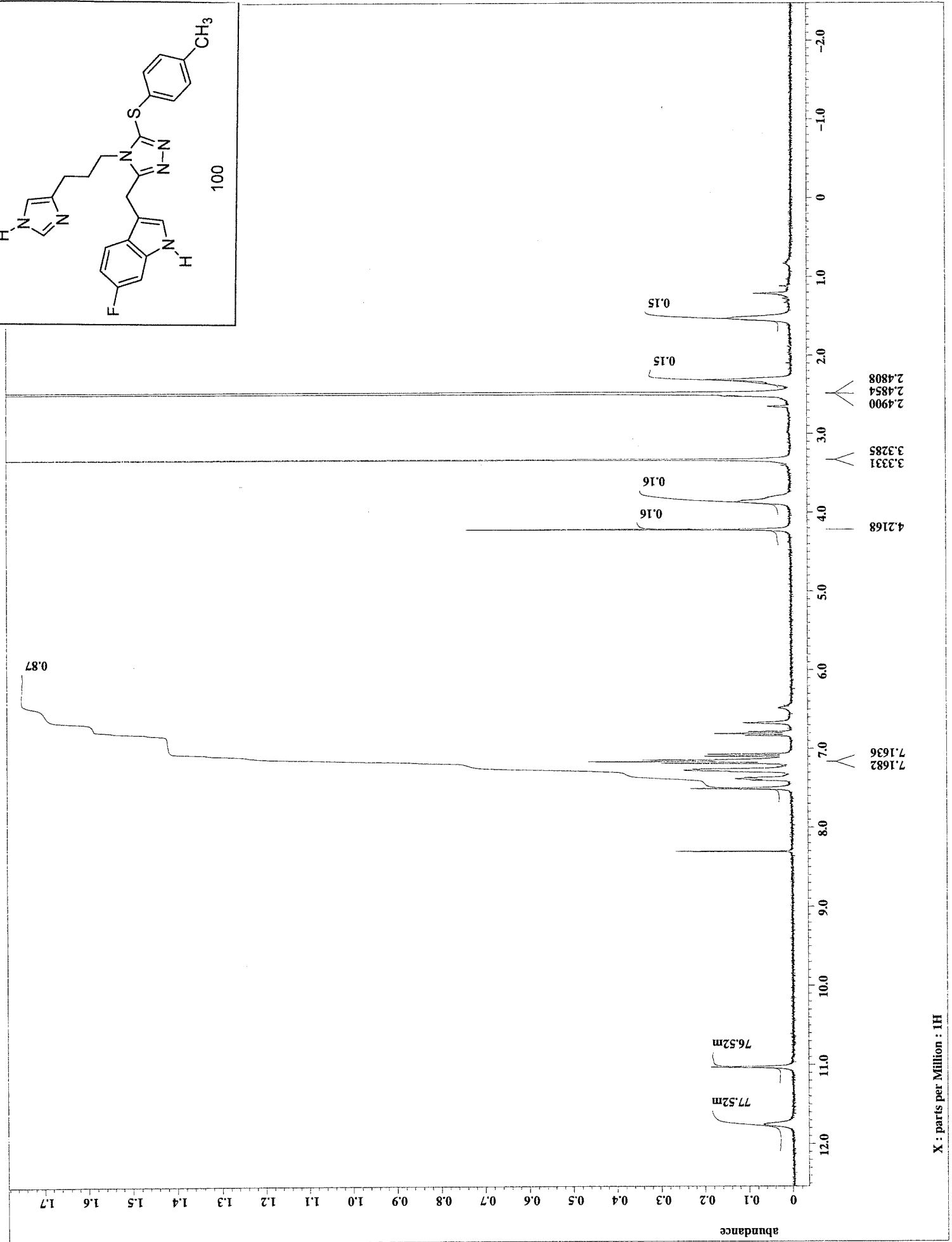
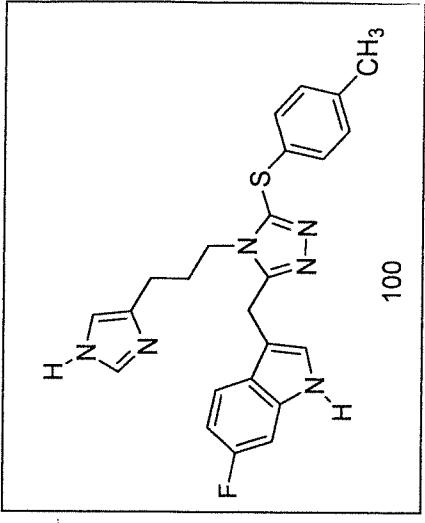


X : parts per Million : 13C

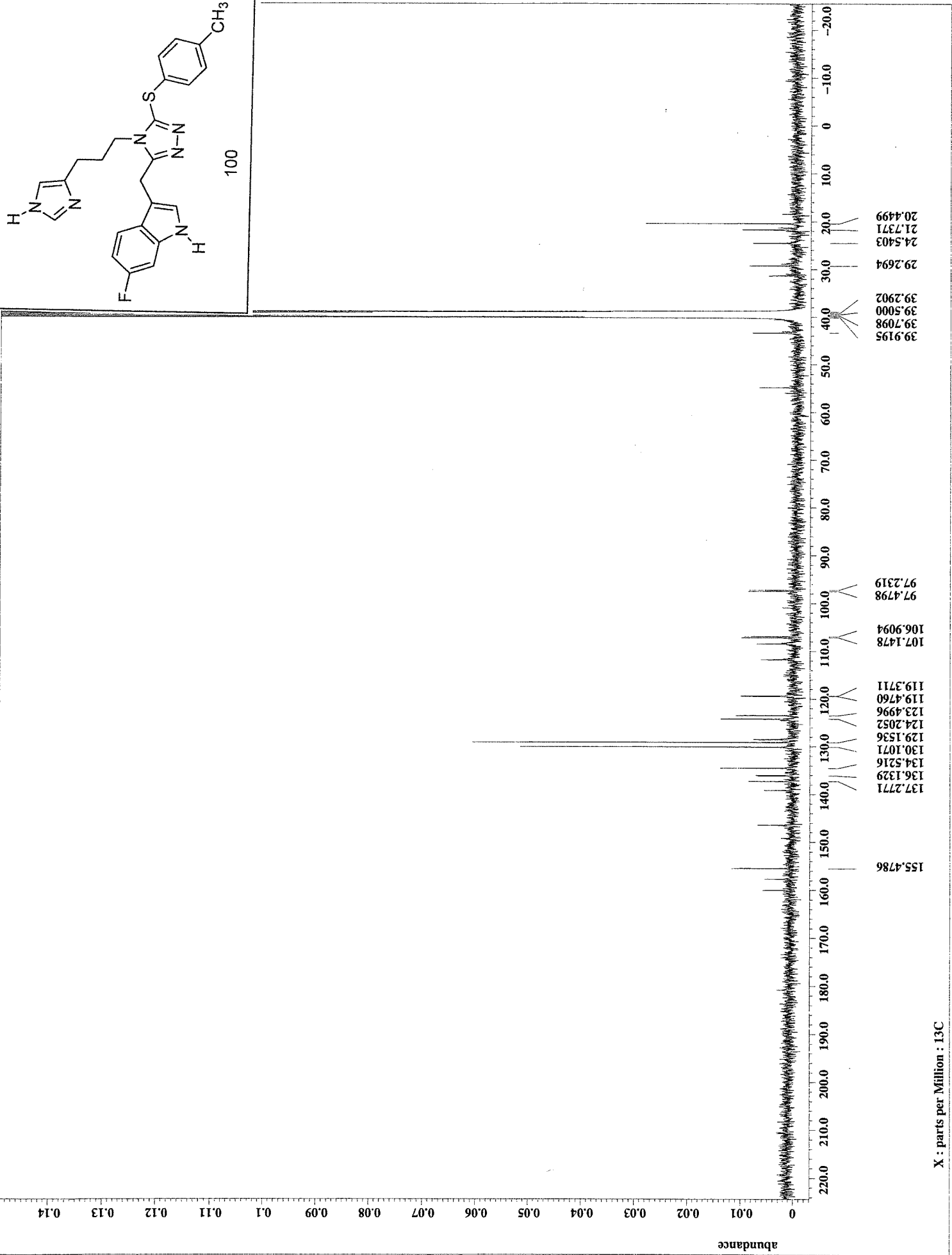
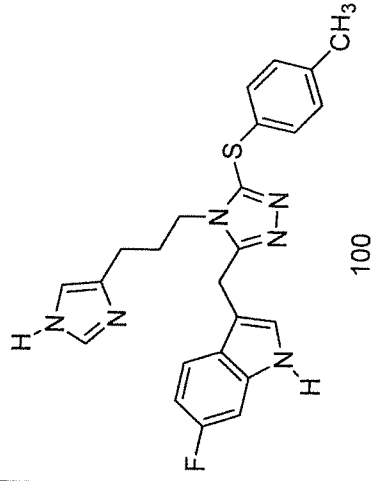


X : parts per Million : 13C

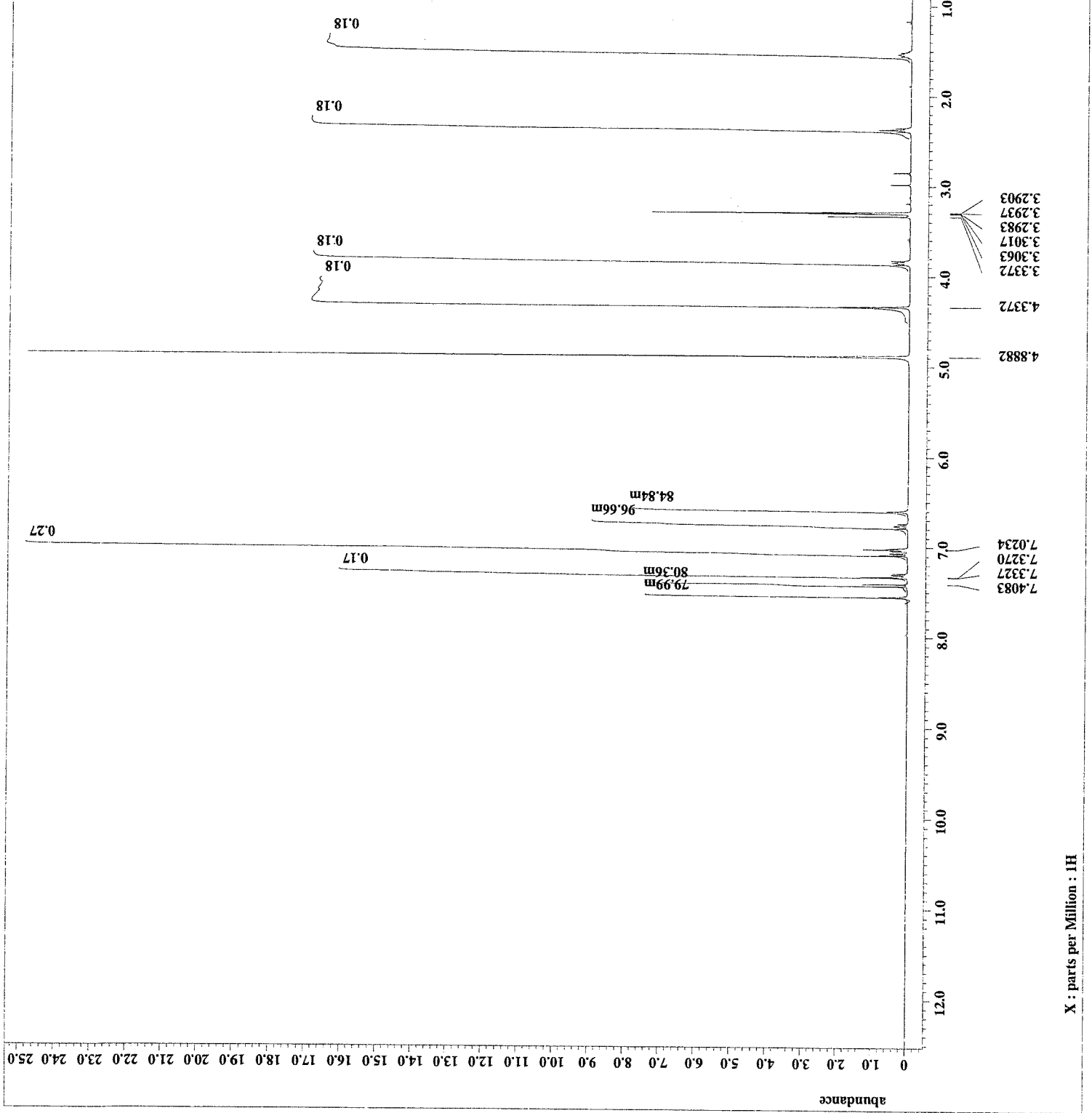
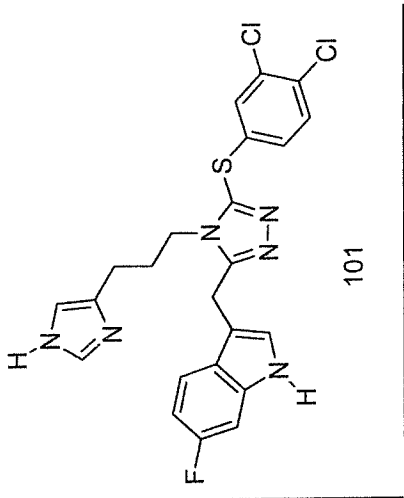


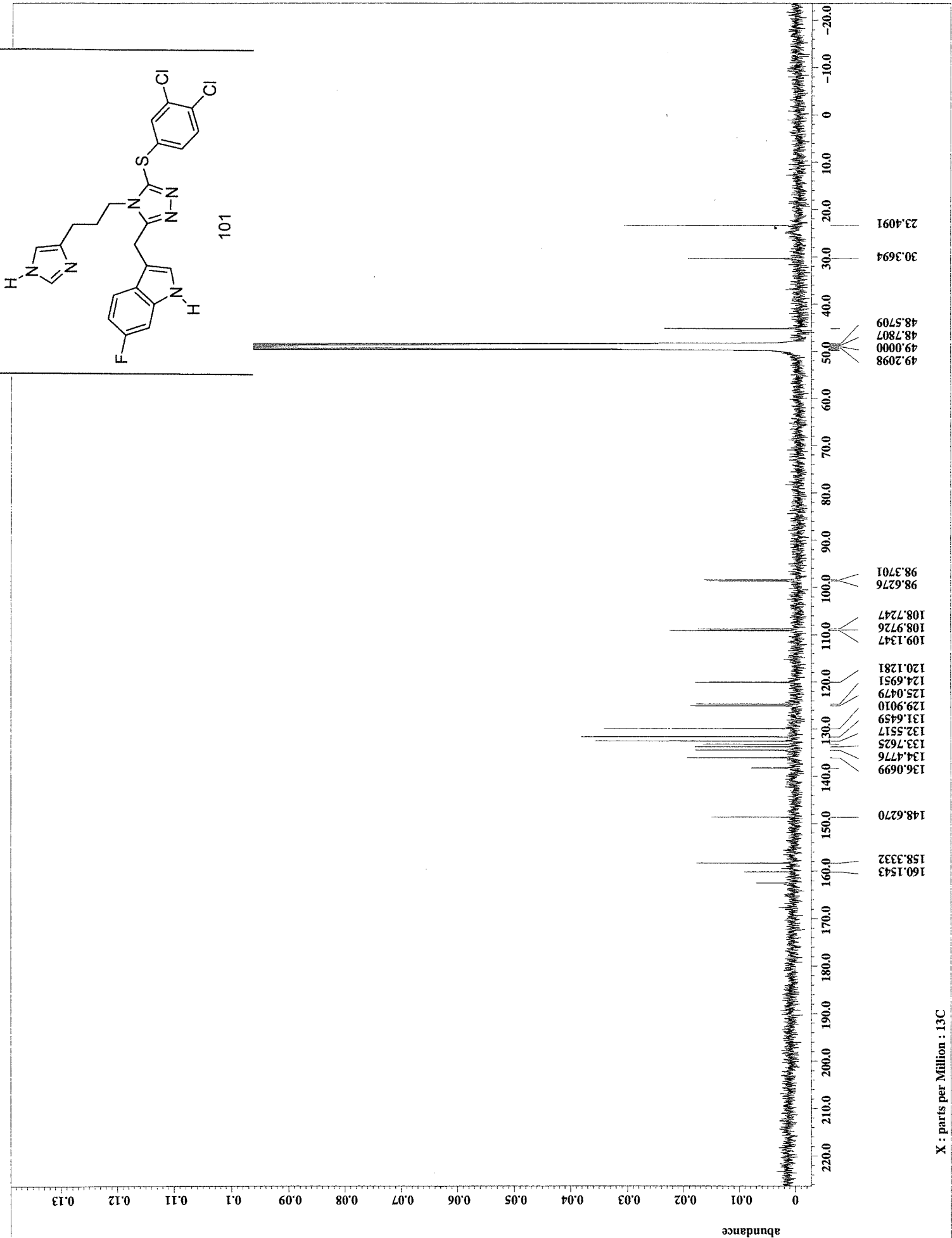


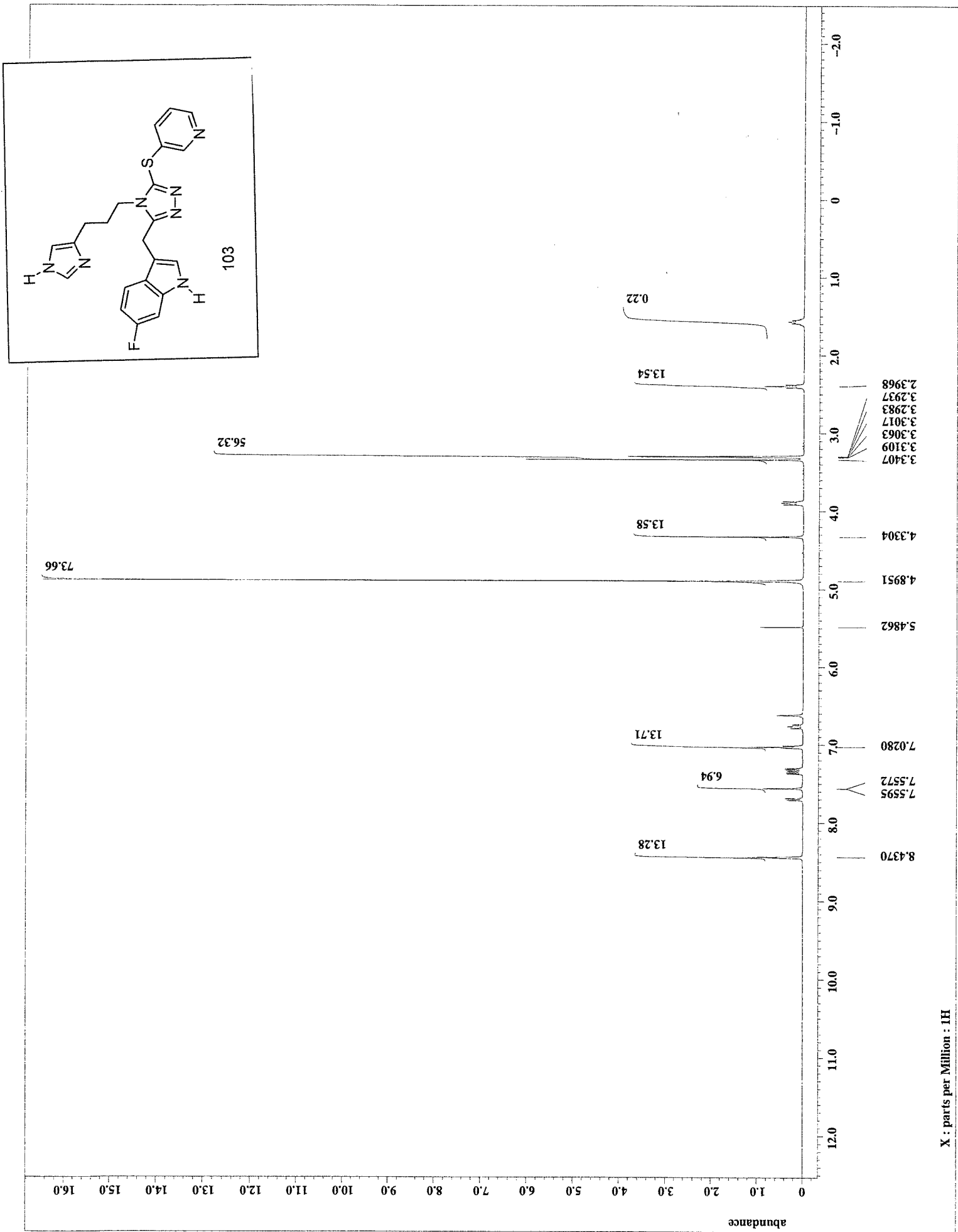
X : parts per Million : 1H



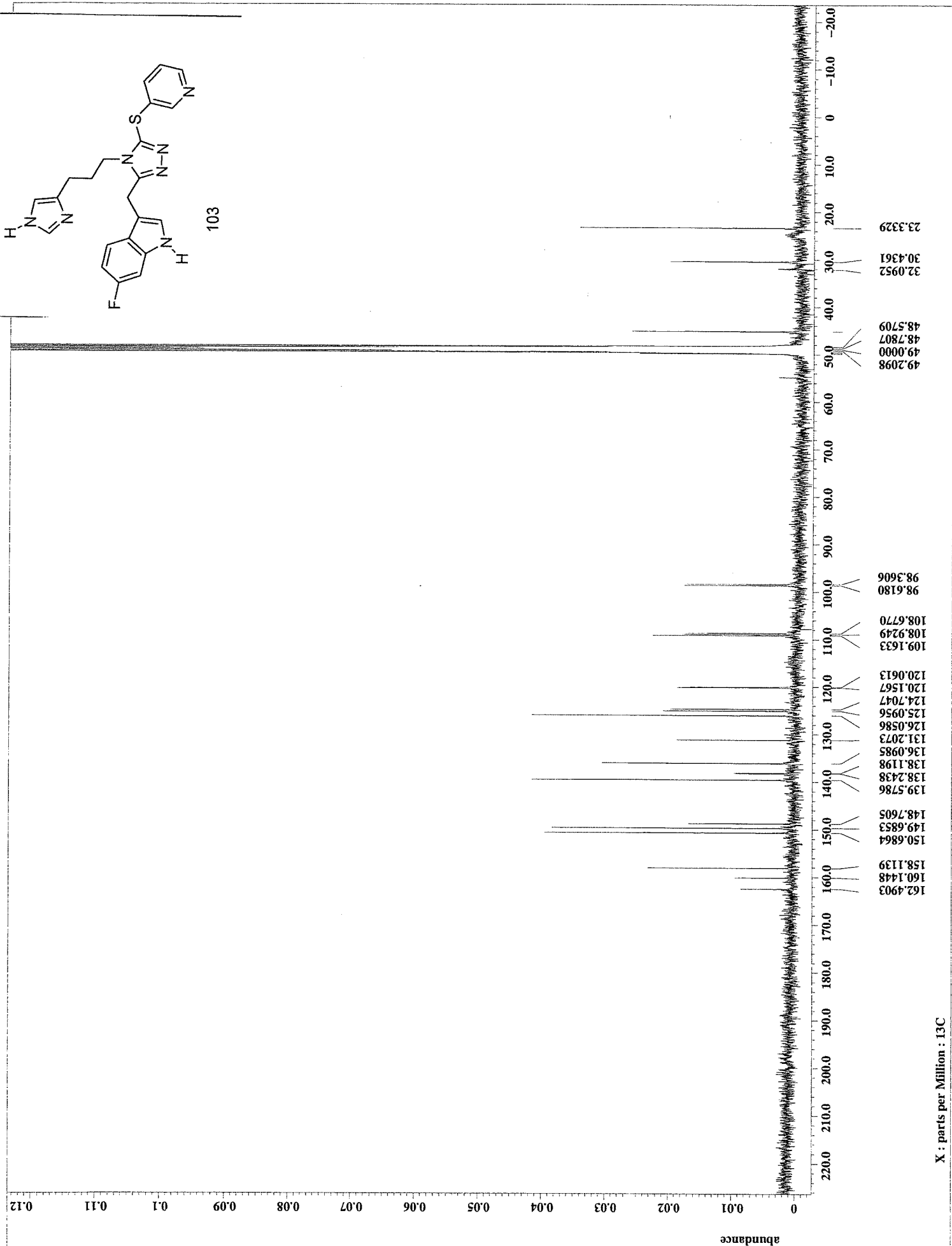
X : parts per Million : 13C



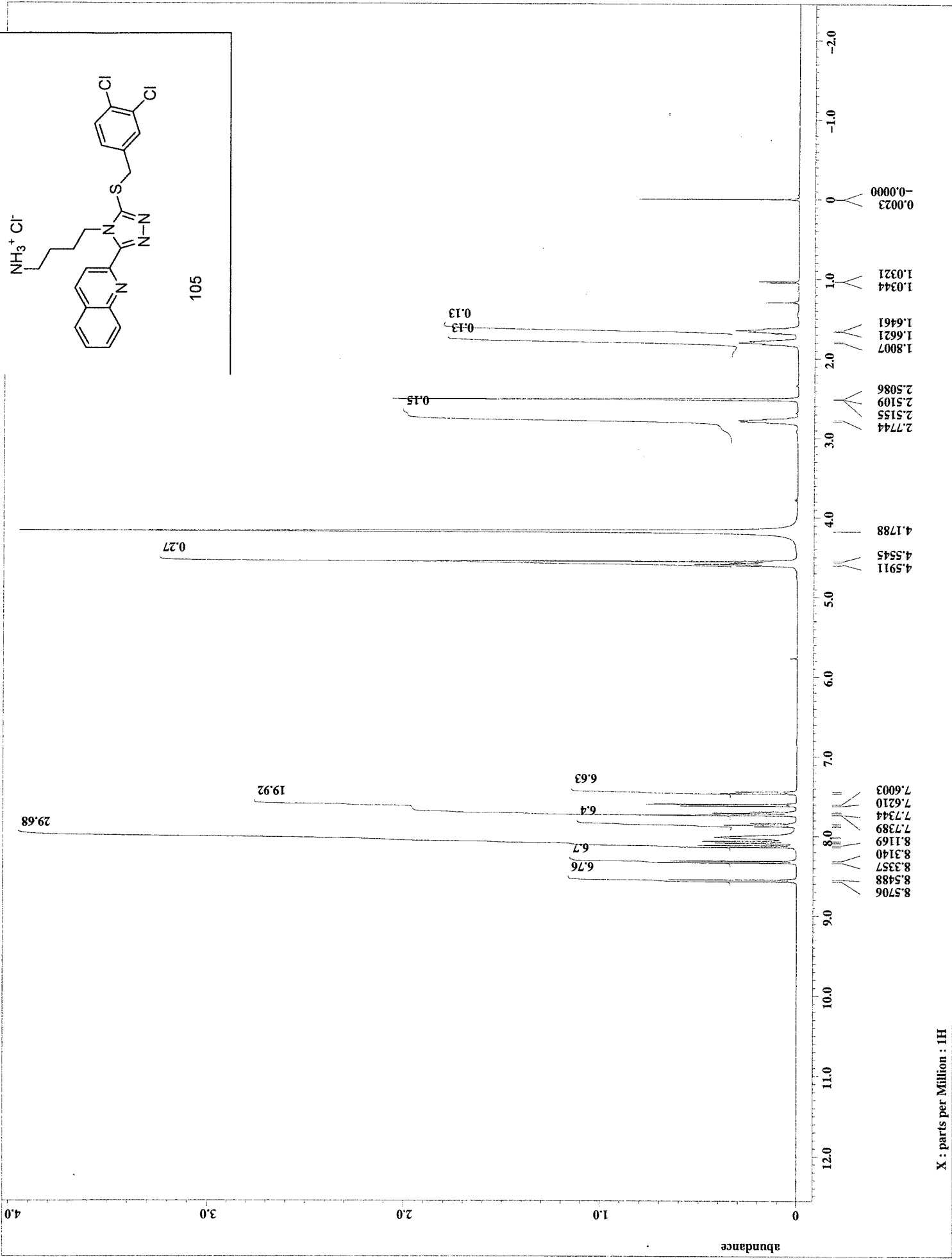




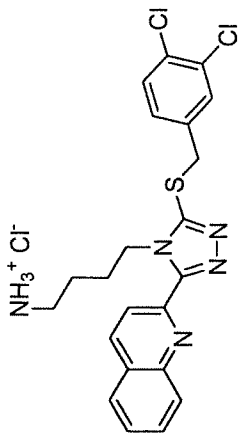
X : parts per Million : 1H



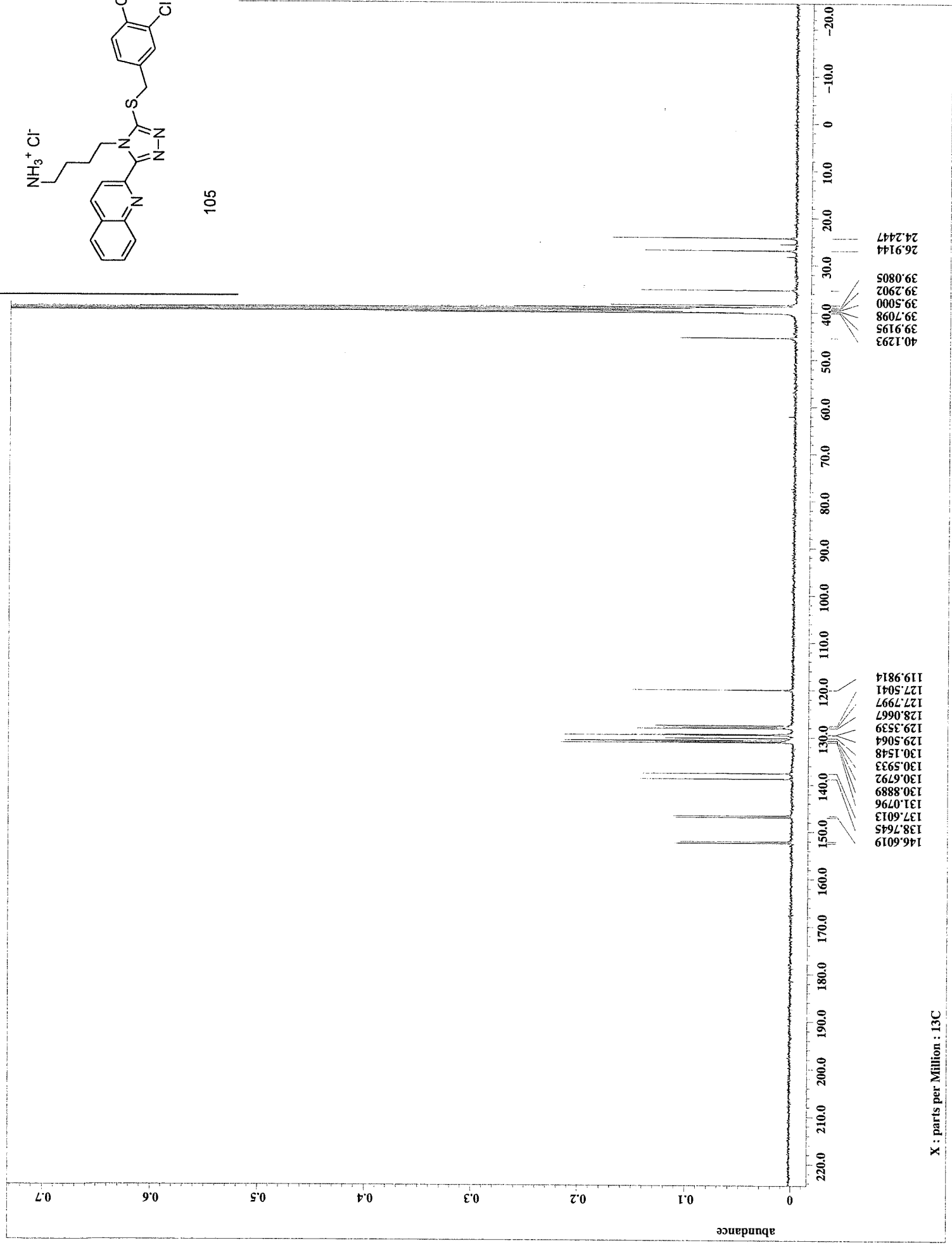
X : parts per Million : 13C



13C NMR

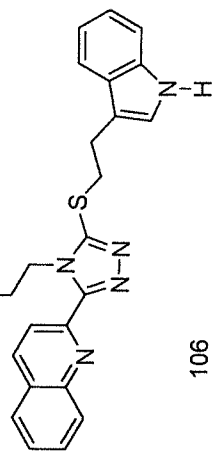


105

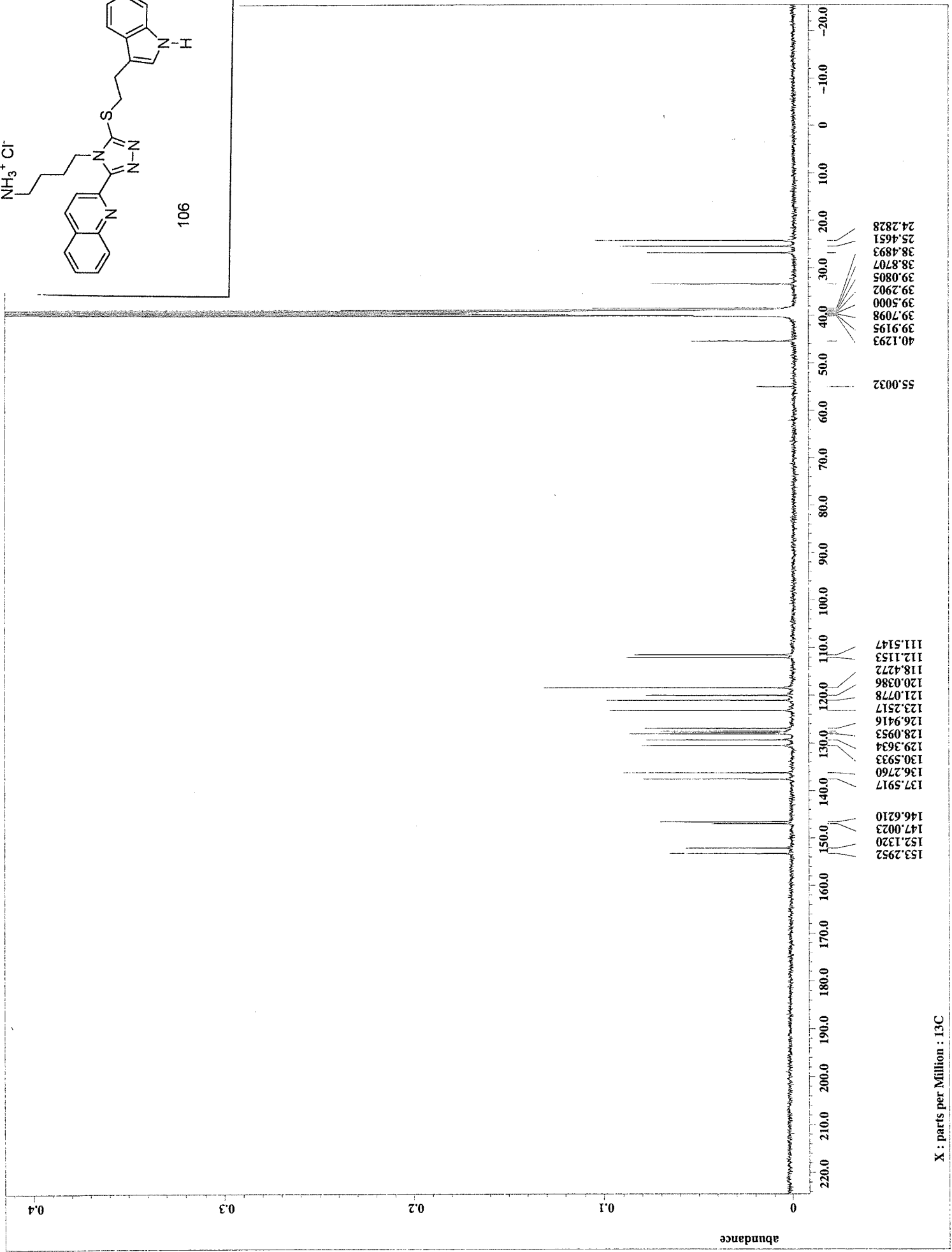


X : parts per Million : 13C

NH₃⁺ Cl⁻

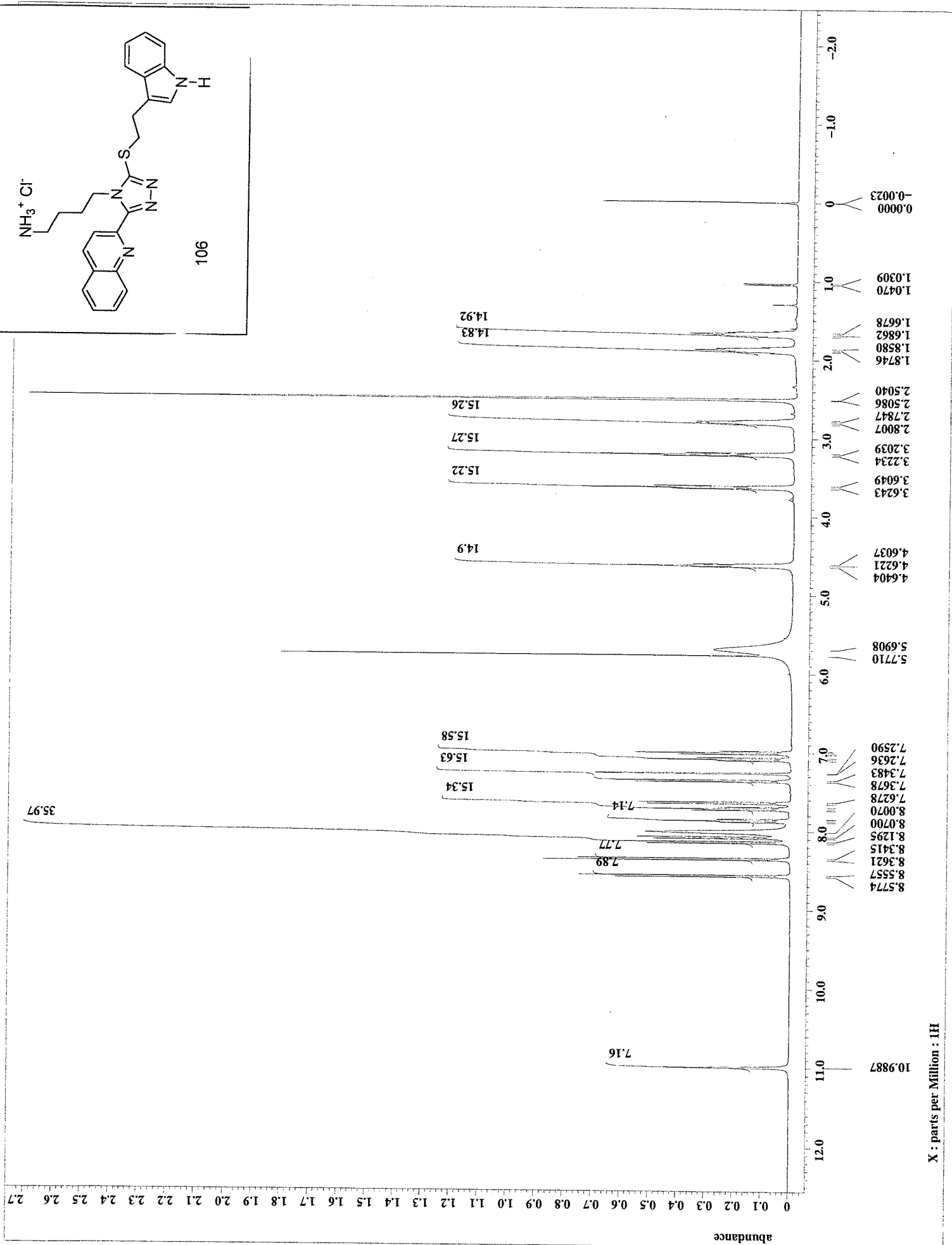


106

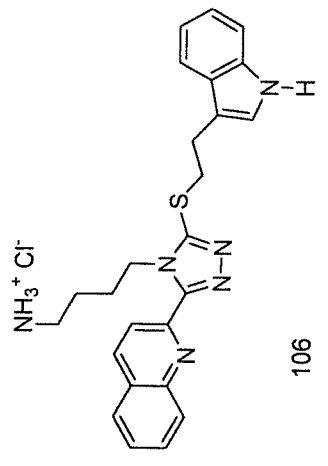


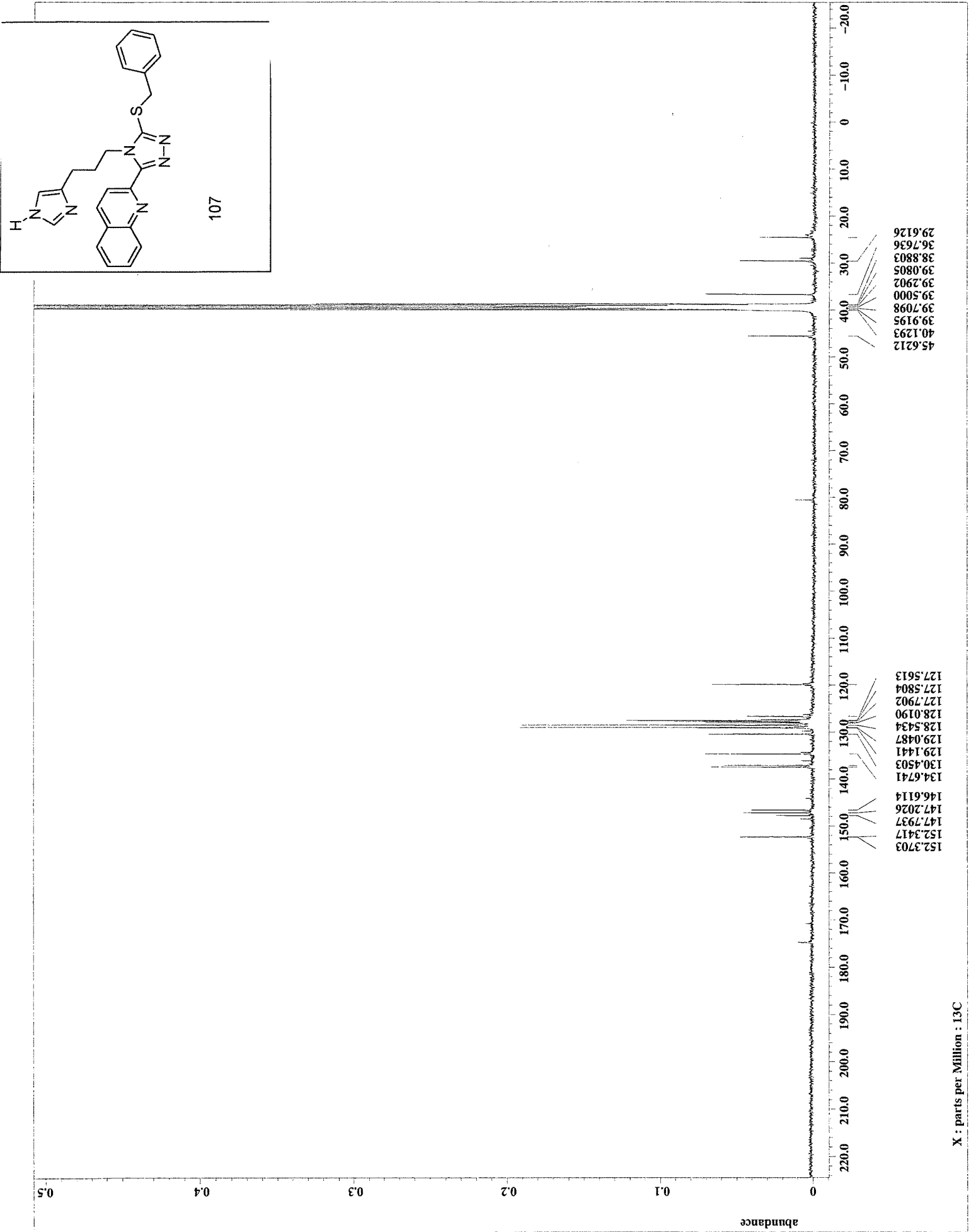
X : parts per Million : 13C

X : parts per Million : 1H



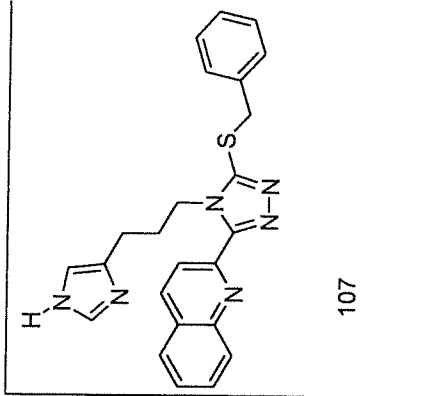
106



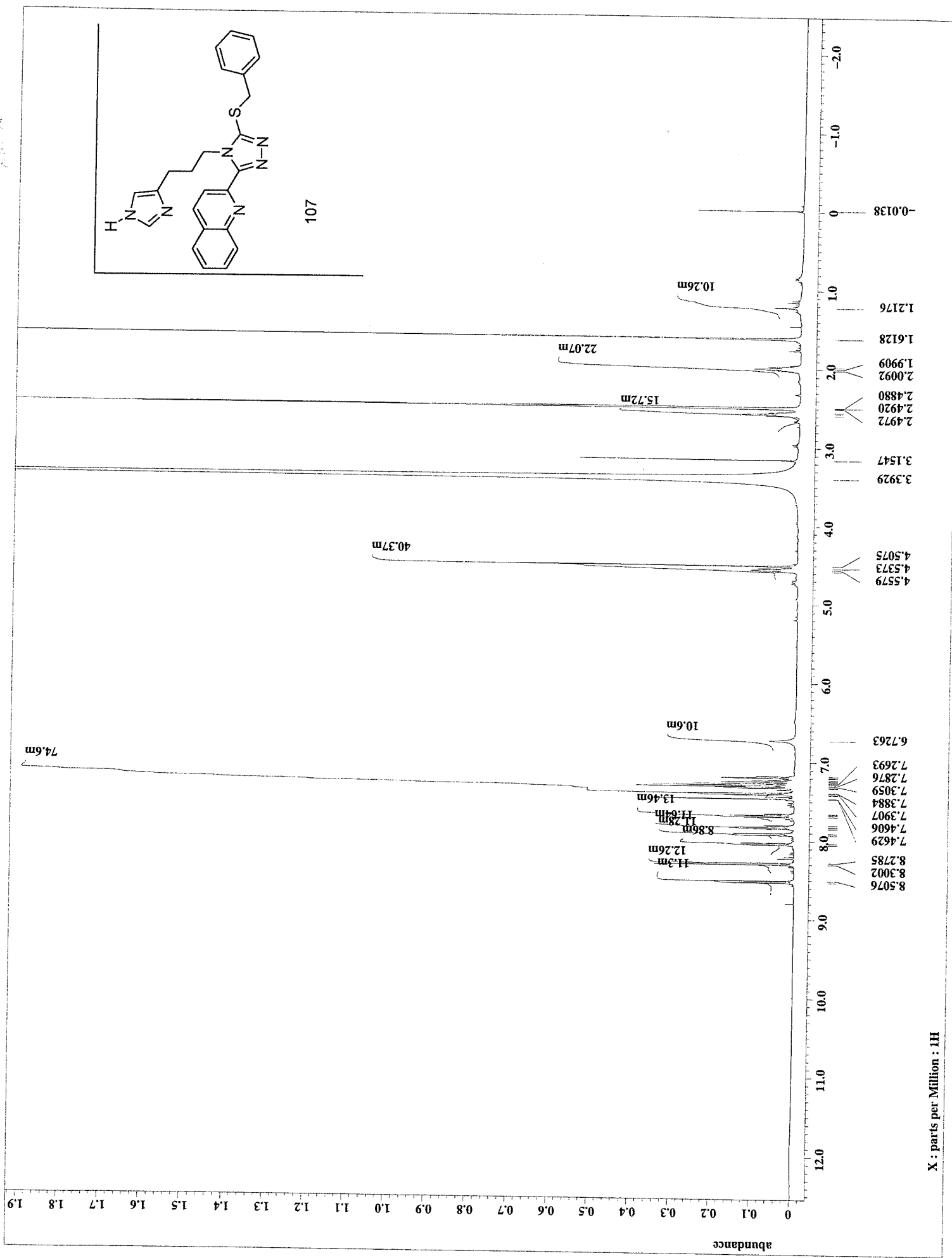


X : parts per Million : 13C

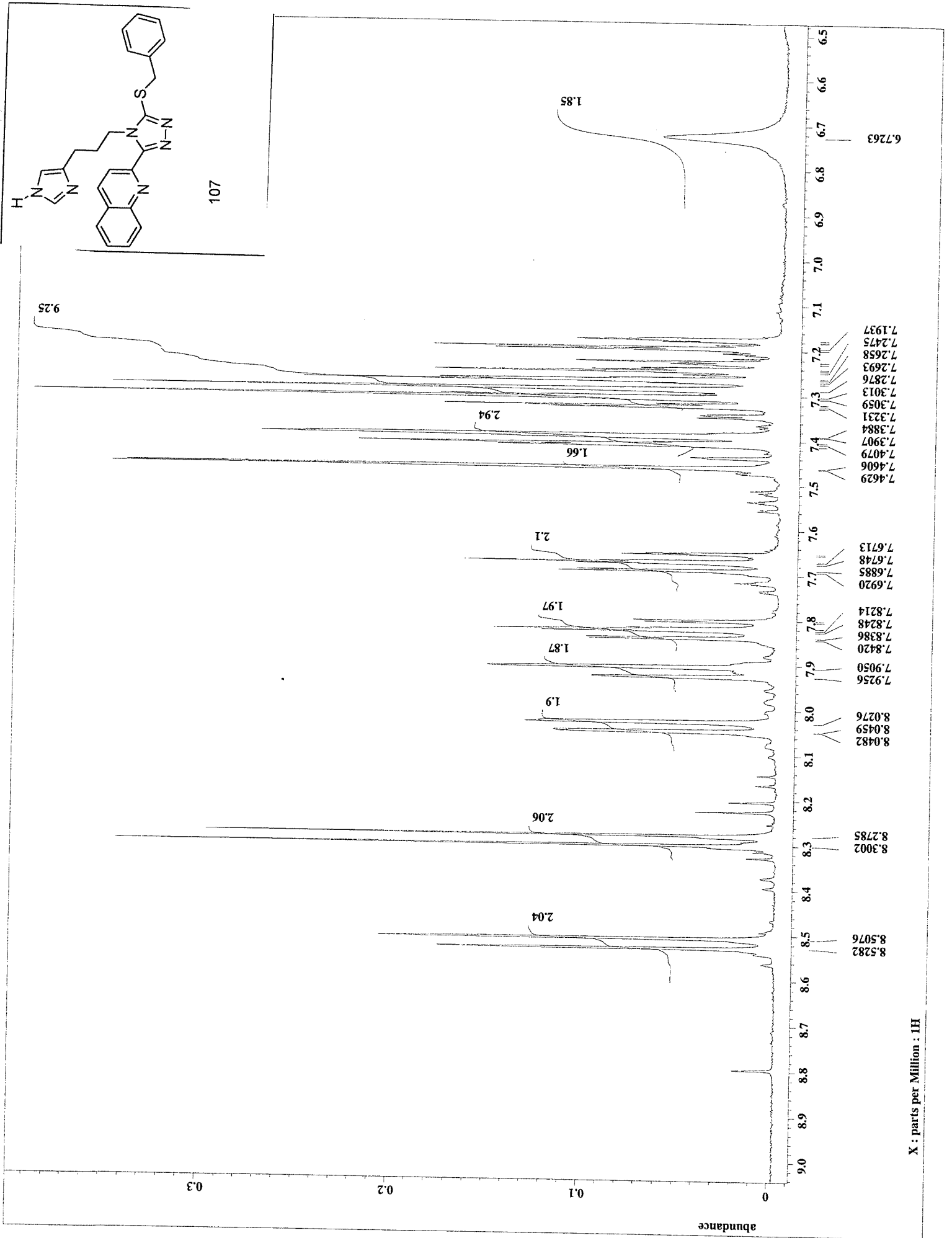
107



107



X : parts per Million : 1H



X : parts per Million : 1H



```

= AH.2.160_PROTON-13.jd
= ahospit
= single_pulse.ex2
= AH.2.160
= DMSO-D6
= 18-APR-2017 15:41:00
= 18-JUL-2024 10:21:32
= 18-JUL-2024 10:21:41
= 1D COMPLEX
= 13107
= 1H
= [ppm]
= X
= ECS 400
= JNM-ECS400
= 9.389766[T] (400[MHz])
= 2.18365952[s]
= 1H
= 399.78219838[MHz]
= 5[ppm]
= 16384
= 1
= 0.45794685[Hz]
= 7.5030012[kHz]
= 1H
= 399.78219838[MHz]
= 5[ppm]
= 1H
= 399.78219838[MHz]
= 5[ppm]
= FALSE
= 1
= 16
= 10.68[us]
= 2.18365952[s]
= 45[deg]
= 6[db]
= 5.34[us]
= Off
= Off
= FALSE
= Dante presat
= Initial wait
= 1[s]
= 48
= 4[s]
= 6.18365952[s]
= 460.0[dC]

```

```

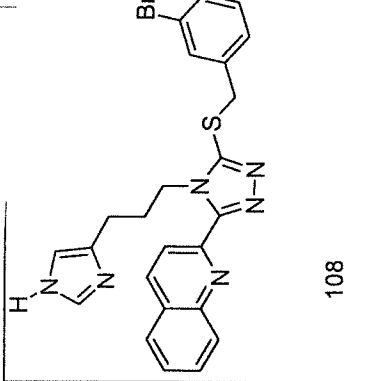
File name
Author
Experiment
Sample_id
Solvent
Creation_time
Revision_time
B[Current_time]
Data_format
Dim_size
Dim_title
Dim_units
Dimensions
Site
Spectrometer

```

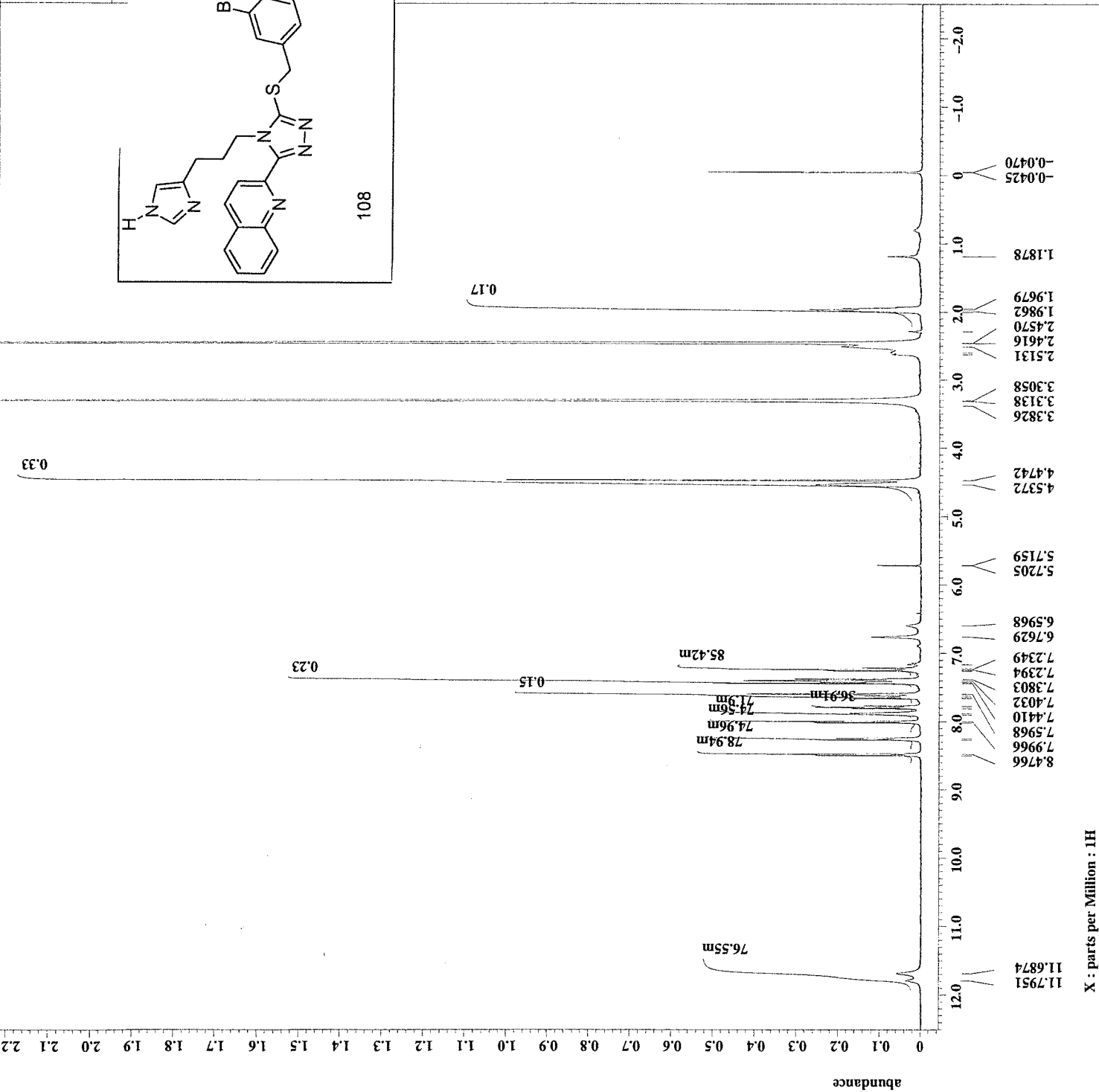
```

Field_strength
X_acq_duration
X_domain
X_freq
X_offset
X_points
X_prescans
X_resolution
X_sweep
Irr_domain
Irr_freq
Irr_offset
Tri_domain
Tri_freq
Tri_offset
Clipped
Mod_return
Scans
Total_scans
X_90_width
X_acq_time
X_angle
X_atn
X_pulse
Irr_mode
Tri_mode
Dante_presat
Initial_wait
Recvr_gain
Relaxation_delay
Repetition_time
Temp_get

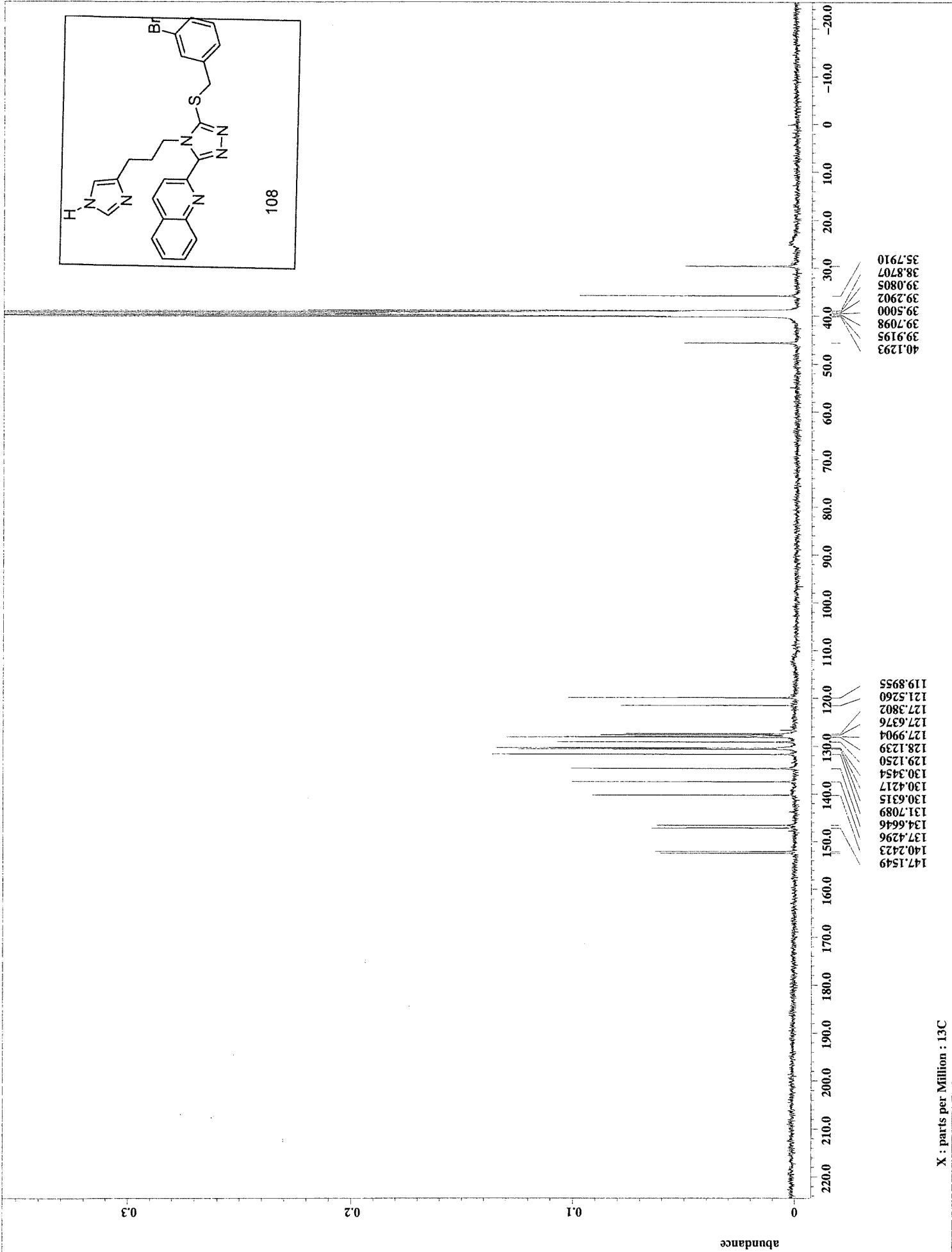
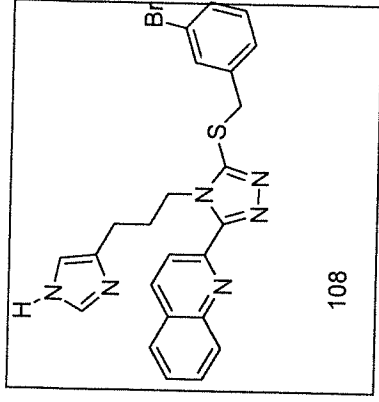
```



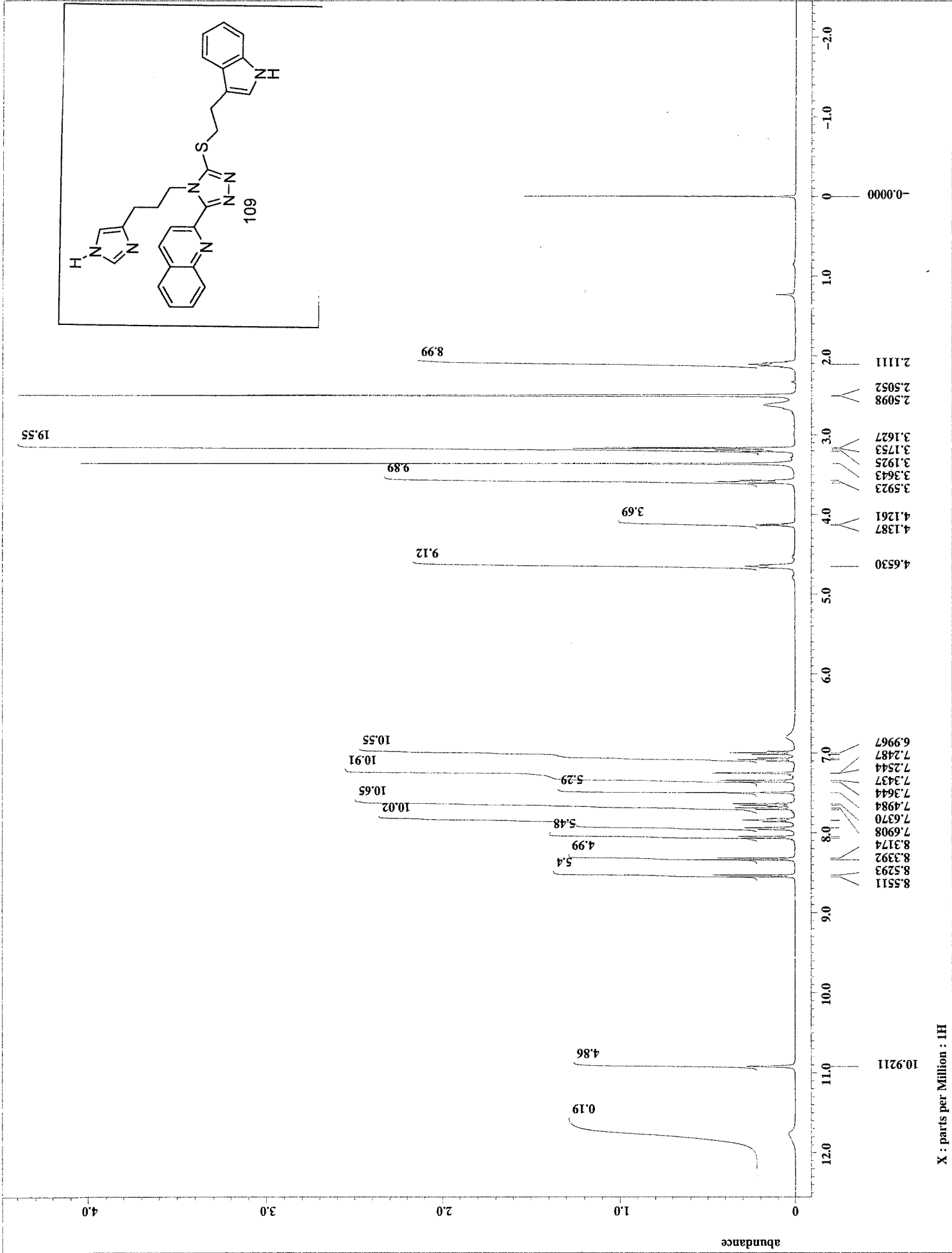
108



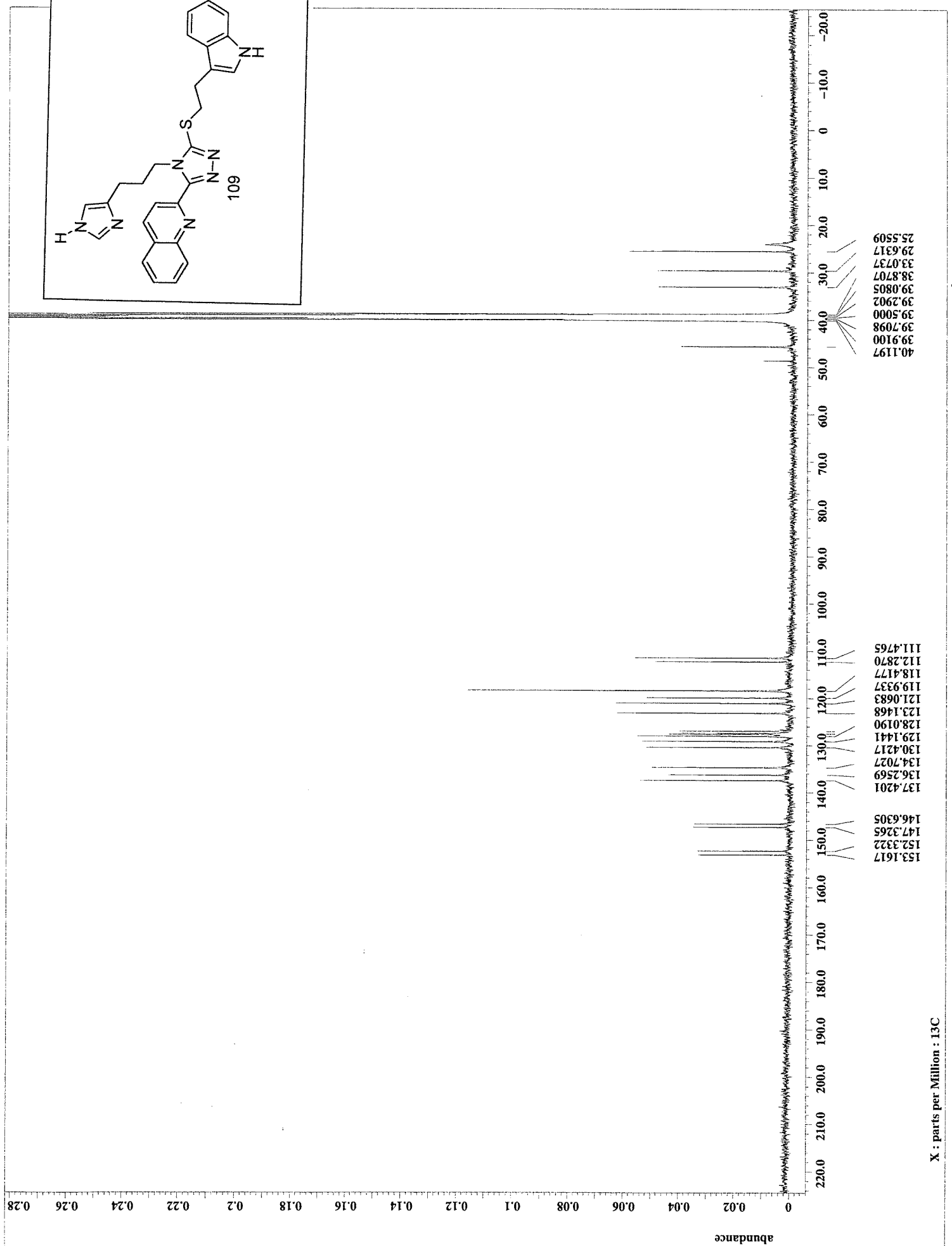
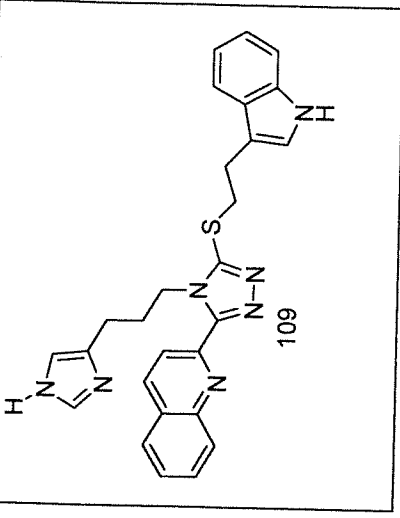
X : parts per Million : 1H



ANALYSIS



X : parts per Million : 1H



X : parts per Million : 13C

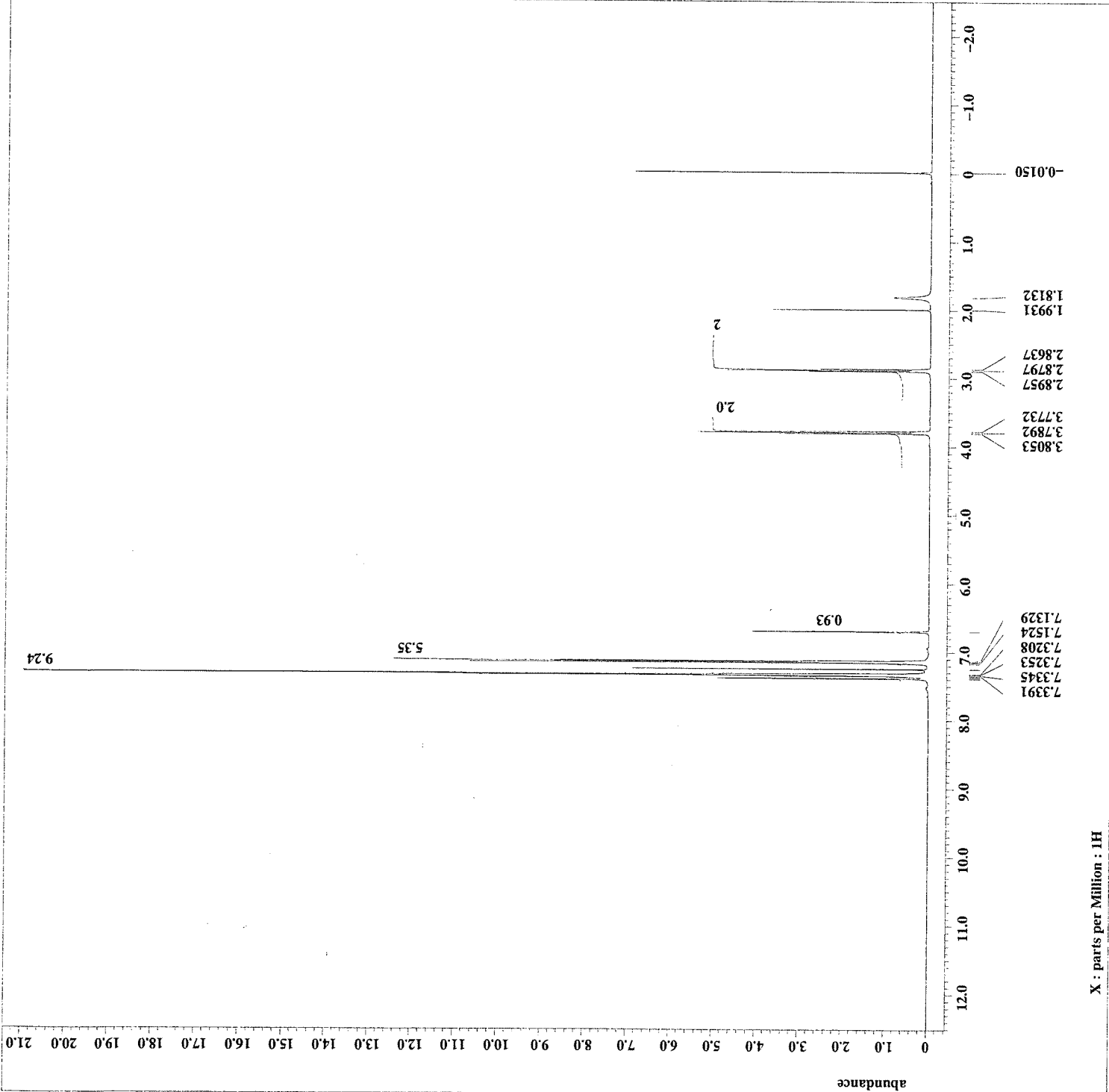
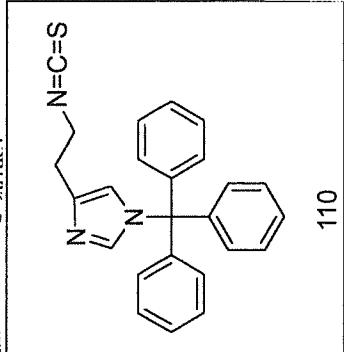
```

Filename = AWC-S2-58-3-4.jdf
Author = mcrider
Experiment = single_pulse.ex2
Sample_id = S#552083
Solvent = CHLOROFORM-D
Creation_time = 29-JUN-2018 13:54:54
Revision_time = 7-MAY-2024 08:50:41
Current_time = 7-MAY-2024 08:50:56

Comment = single_pulse
Data_format = 1D_COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400

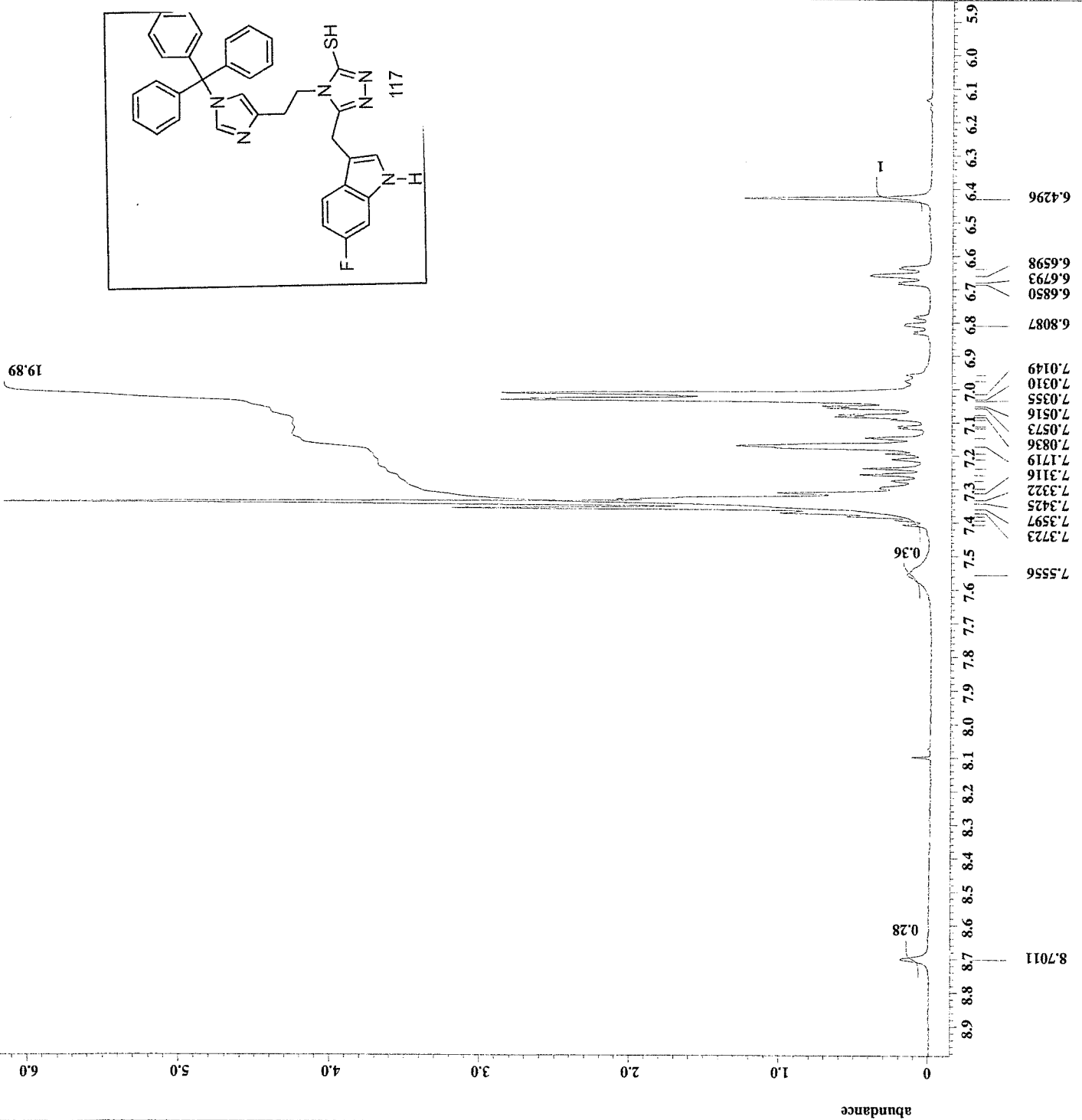
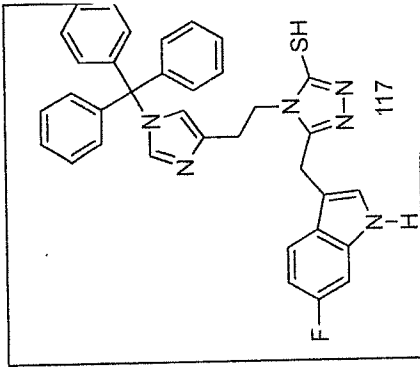
Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685[Hz]
X_sweep = 7.5030012[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = TRUE
Mod_return = 1
Scans = 8
Total_scans = 8

X_90_width = 10.65[us]
X_acq_time = 2.18365952[s]
X_angle = 45[deg]
X_atn = 6[dB]
X_pulse = 5.225[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 50
Relaxation_delay = 5[s]
Repetition_time = 7.18365952[s]
Temp_cat = 20[degC]
  
```





File name = LG-I-35-1 IN CH2CL2-5
Author = Delta
Experiment = single_pulse.exe
Sample_id = S#432422
Solvent = DMSO-D6
Creation_time = 12-JUN-2019 10:30:26
Revision_time = 6-MAY-2024 11:09:05
Current_time = 6-MAY-2024 11:09:18
Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838 [MHz]
X_offset = 5 [ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685 [Hz]
X_sweep = 7.5030012 [KHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Tri_domain = 1H
Tri_freq = 399.78219838 [MHz]
Tri_offset = 5 [ppm]
Clipped = TRUE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 11.365 [us]
X_acq_time = 2.18365952 [s]
X_angle = 45 [deg]
X_atn = 6 [dB]
X_pulse = 5.6825 [us]
Irr_mode = Off
Tri_mode = Off
Dante_preatt = FALSE
Initial_wait = 1 [s]
Recvr_gain = 50
Relaxation_delay = 5 [s]
Repetition_time = 7.18365952 [s]
Temp_get = 19.6 [dC]



X : parts per Million : 1H

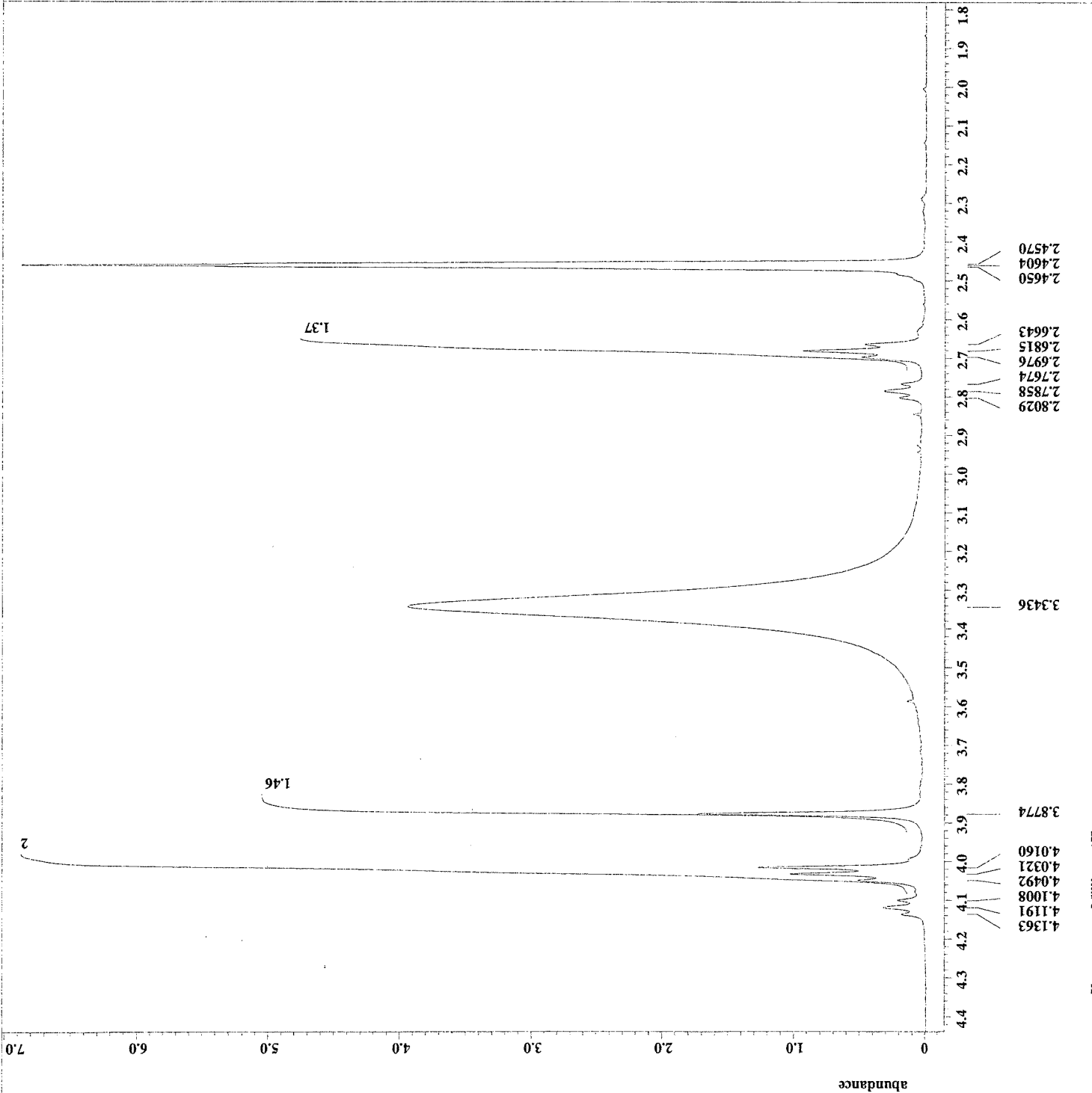
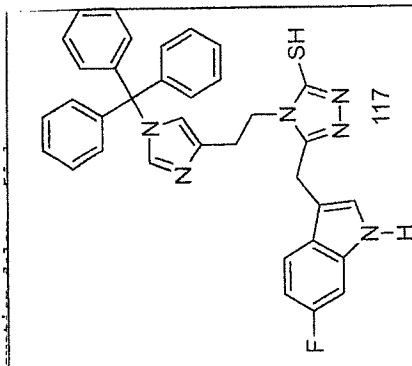
ADJEO

= LG-I-35-1 IN CH2CL2-4
 = Delta
 = single_pulse.ex2
 = S#432422
 = DMSO-D6
 = 12-JUN-2019 10:30:26
 = 6-MAY-2024 11:05:42
 = 6-MAY-2024 11:05:55

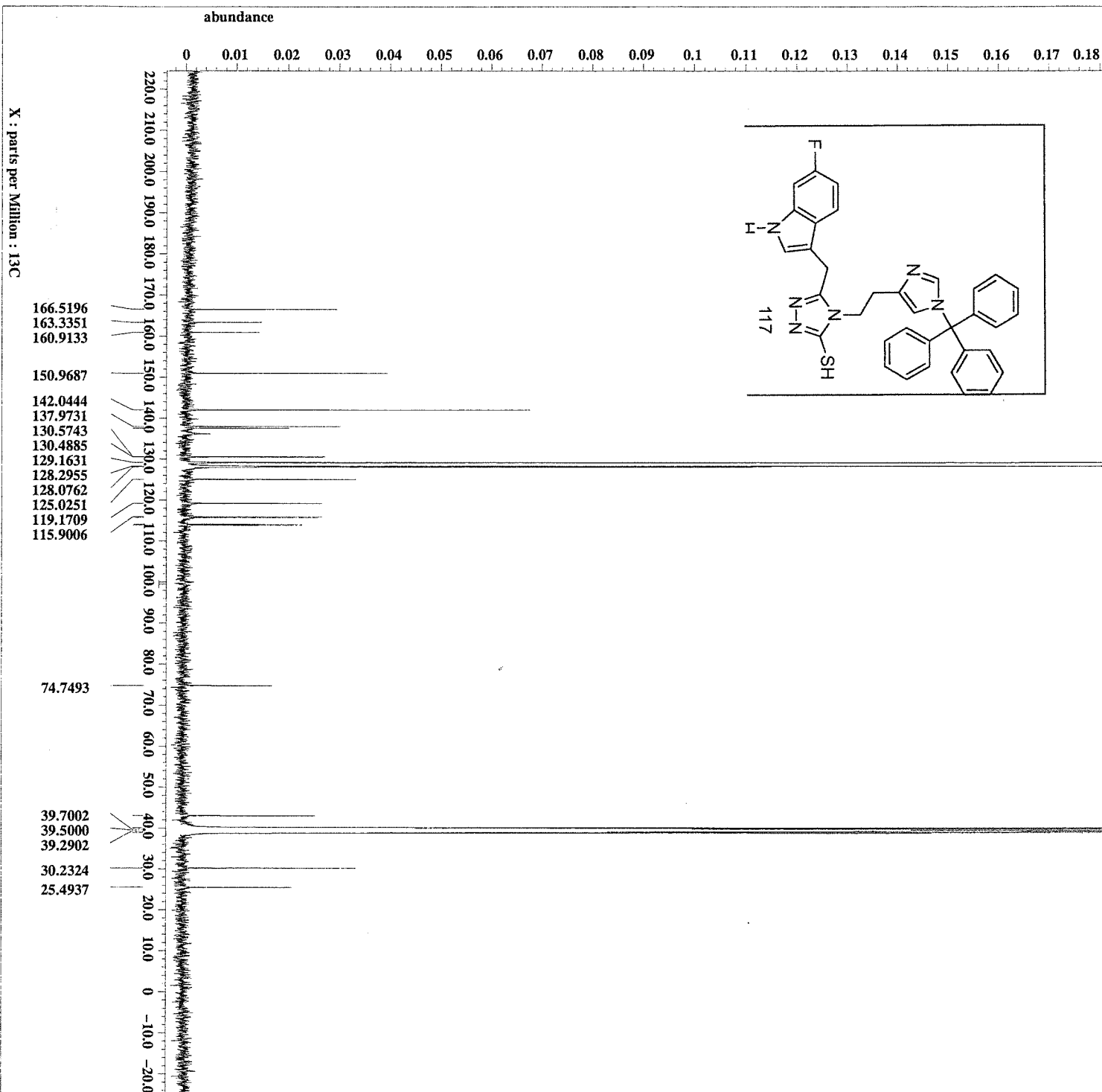
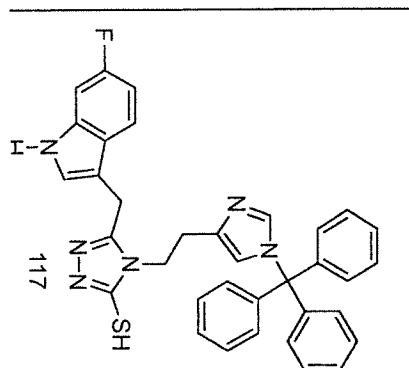
= single_pulse
 = ID COMPLEX
 = 13107
 = 1H
 = [ppm]
 = X
 = ECS 400
 = JNM-ECS400

Field_strength = 9.389766 [T] (400 [MHz])
 X_acq_duration = 2.18365952 [s]
 X_domain = 1H
 X_freq = 399.78219838 [MHz]
 X_offset = 5 [ppm]
 X_points = 16384
 X_prescans = 1
 X_resolution = 0.45794685 [Hz]
 X_sweep = 7.5030012 [kHz]
 Irr_domain = 1H
 Irr_freq = 399.78219838 [MHz]
 Irr_offset = 5 [ppm]
 Tri_domain = 1H
 Tri_freq = 399.78219838 [MHz]
 Clipped = TRUE
 Mod_return = 1
 Scans = 8
 Total_scans = 8

X_90_width = 11.365 [us]
 X_acq_time = 2.18365952 [s]
 X_angle = 45 [deg]
 X_atn = 6 [dB]
 X_pulse = 5.6825 [us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1 [s]
 Recvr_gain = 50



X : parts per Million : 1H



X : parts per Million : 13C

Filename = LG-m-F_SH_CARBON-5.fid
Author =
Experiment = single_pulse_dec
Sample_id = LG-m-F_SH
Solvent = DMSO-D6
Creation_time = 30-NOV-2018 01:27:06
Revision_time = 3-MAY-2024 10:48:52
Current_time = 3-MAY-2024 10:49:43

Data_format = 1D_COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400

Field_strength = 9.389766 [T] (400 [MHz])
X_acq_duration = 1.0433312 [s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665 [Hz]
X_sweep = 31.40703518 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 12000
Total_scans = 12000

X_90_width = 10.4 [us]
X_acq_time = 1.0433312 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 3.46566667 [us]
Irr_atn_dec = 24.2 [dB]
Irr_atn_noe = 24.2 [dB]
Irr_noise = VOLTZ
Decoupling = TRUE
Initial_wait = 1 [s]
Noe = TRUE
Noe_time = 2 [s]
Recvr_gain = 58
Relaxation_delay = 2 [s]
Repetition_time = 3.0433312 [s]
Temp_get = 17.6 [dC]

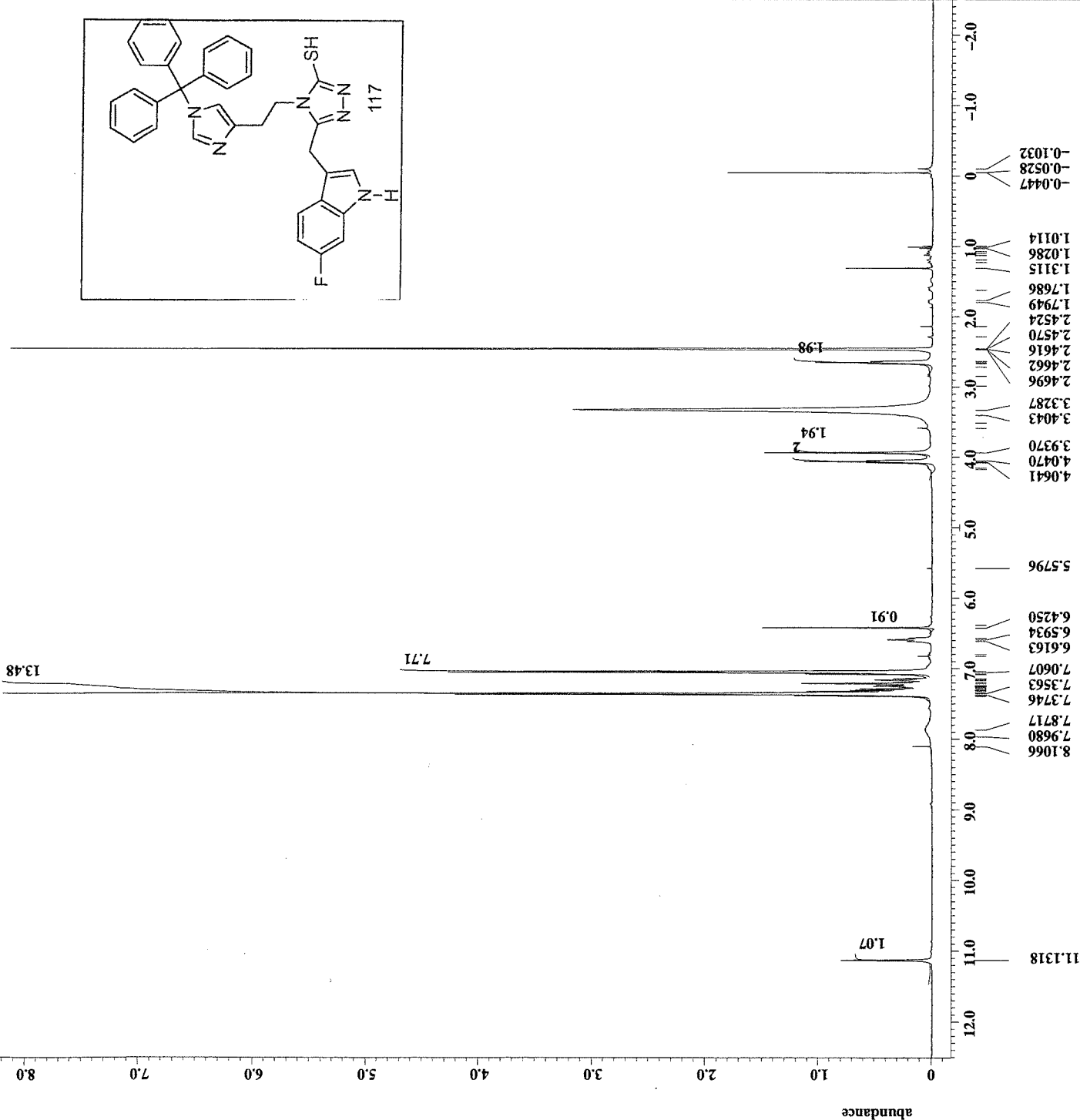
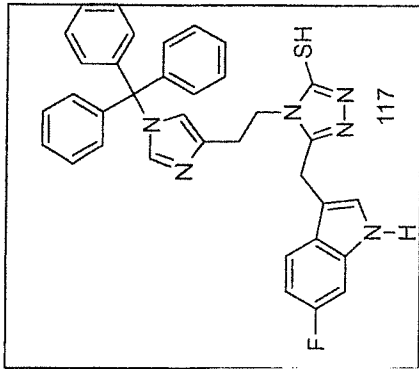
= LG-I-62-1-3.jdf
 = mcrider
 = single_pulse.ex2
 = S#362129
 = DMSO-D6
 = 27-JUN-2019 08:26:29
 = 2-MAY-2024 08:55:14
 = 2-MAY-2024 08:56:08

= single_pulse
 = 1D COMPLEX
 = 13107
 = 1H
 = [ppm]
 = X
 = ECS 400
 = JNM-ECS400

= 9.389766 [T] (400 [MHz])
 = 2.18365952 [s]
 = 1H
 = 399.78219838 [MHz]
 = 5 [ppm]
 = 16384
 = 1
 = 0.45794685 [Hz]
 = 7.5030012 [kHz]
 = 1H
 = 399.78219838 [MHz]
 = 5 [ppm]
 = 1H
 = 399.78219838 [MHz]
 = 5 [ppm]
 = TRUE
 = 1
 = 8

= 11.365 [us]
 = 2.18365952 [s]
 = 45 [deg]
 = 6 [dB]
 = 5.6825 [us]
 = Off
 = Off
 = FALSE
 = 1 [s]
 = 50
 = 5 [s]
 = 7.18365952 [s]
 = 19.2 [DC]

X_90_width
 X_acq_time
 X_angle
 X_atn
 X_pulse
 Irr_mode
 Irr_mode
 Dantle_presat
 Initial_wait
 Recvr_gain
 Relaxation_delay
 Repetition_time
 Temp_get





= KI 18A-7recrystal0911
 = Delta
 = single_pulse.ex2
 = S#327147
 = DMSO-D6
 = 11-SEP-2018 07:42:23
 = 7-MAY-2024 08:43:54
 = 7-MAY-2024 08:44:05

= single_pulse
 = 1D COMPLEX
 = 13107
 = 1H
 = [ppm]
 = X
 = ECS 400
 = JNM-ECS400

= 9.389766[T] (400 [MHz])
 = 2.18365952[s]
 = 1H
 = 399.78219838 [MHz]
 = 5 [ppm]
 = 16384
 = 1

= 0.45794685 [Hz]
 = 7.5030012 [kHz]
 = 1H
 = 399.78219838 [MHz]
 = 5 [ppm]
 = 399.78219838 [MHz]
 = 5 [ppm]
 = TRUE
 = 1
 = 8

= 10.65 [us]
 = 2.18365952 [s]
 = 45 [deg]
 = 6 [dB]
 = 5.325 [us]
 = Off
 = Off

= FALSE
 = 1 [s]
 = 50
 = 5 [s]
 = 7.18365952 [s]
 = 19.3 [dC]

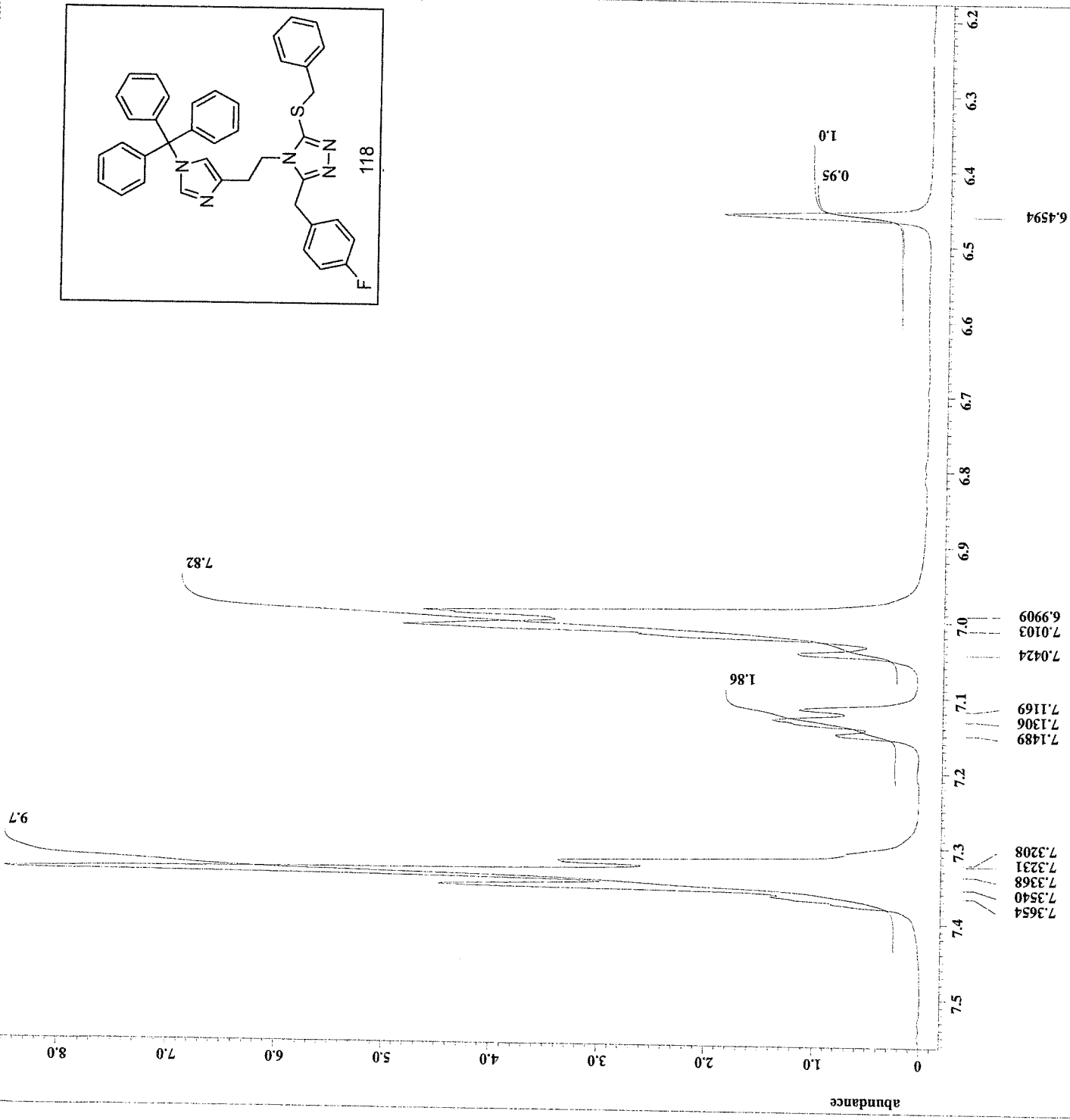
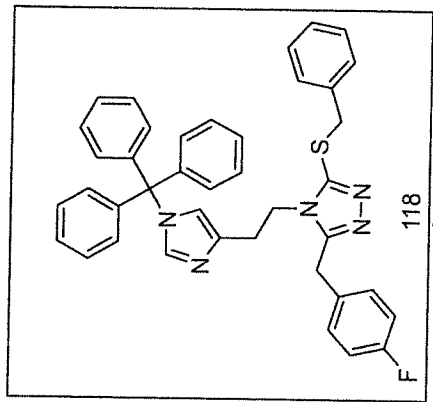
= single_pulse
 = 1D COMPLEX
 = 13107
 = 1H
 = [ppm]
 = X
 = ECS 400
 = JNM-ECS400

= 9.389766[T] (400 [MHz])
 = 2.18365952[s]
 = 1H
 = 399.78219838 [MHz]
 = 5 [ppm]
 = 16384
 = 1

= 0.45794685 [Hz]
 = 7.5030012 [kHz]
 = 1H
 = 399.78219838 [MHz]
 = 5 [ppm]
 = 399.78219838 [MHz]
 = 5 [ppm]
 = TRUE
 = 1
 = 8

= 10.65 [us]
 = 2.18365952 [s]
 = 45 [deg]
 = 6 [dB]
 = 5.325 [us]
 = Off
 = Off

= FALSE
 = 1 [s]
 = 50
 = 5 [s]
 = 7.18365952 [s]
 = 19.3 [dC]



X : parts per Million : 1H

= KI_18A-7recrystal0911
 = Delta
 = single_pulse.ex2
 = #327147
 = DMSO-D6
 = 11-SEP-2018 07:42:23
 = 7-MAY-2024 08:44:35
 = 7-MAY-2024 08:45:03

= single_pulse
 = 1D COMPLEX
 = 13107
 = 1H
 = [ppm]
 = X
 = ECS 400
 = JNM-ECS400

= 9.389766[T] (400 [MHz])
 = 2.18365952[s]
 = 1H
 = 399.78219838 [MHz]
 = 5 [ppm]
 = 16384
 = 1

= 0.45794685 [Hz]
 = 7.5030012 [kHz]
 = 1H
 = 399.78219838 [MHz]
 = 5 [ppm]
 = TRUE
 = 1
 = 8

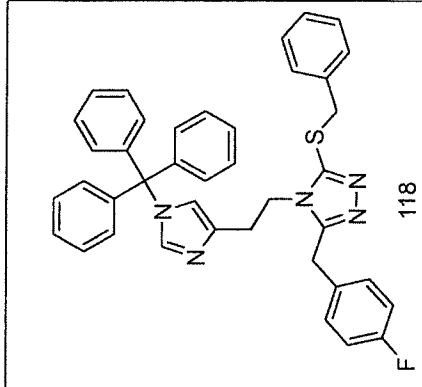
= 10.65 [us]
 = 2.18365952 [s]
 = 45 [deg]
 = 6 [dB]
 = 5.325 [us]
 = Off
 = Off
 = FALSE
 = 1 [fs]
 = 50
 = 5 [s]
 = 7.18365952 [s]
 = 19.3 [dC]

= 10.65 [us]
 = 2.18365952 [s]
 = 45 [deg]
 = 6 [dB]
 = 5.325 [us]
 = Off
 = Off
 = FALSE
 = 1 [fs]
 = 50
 = 5 [s]
 = 7.18365952 [s]
 = 19.3 [dC]

= 10.65 [us]
 = 2.18365952 [s]
 = 45 [deg]
 = 6 [dB]
 = 5.325 [us]
 = Off
 = Off
 = FALSE
 = 1 [fs]
 = 50
 = 5 [s]
 = 7.18365952 [s]
 = 19.3 [dC]

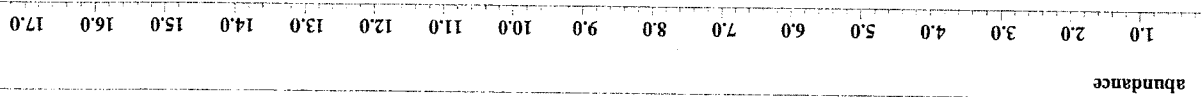
= 10.65 [us]
 = 2.18365952 [s]
 = 45 [deg]
 = 6 [dB]
 = 5.325 [us]
 = Off
 = Off
 = FALSE
 = 1 [fs]
 = 50
 = 5 [s]
 = 7.18365952 [s]
 = 19.3 [dC]

= 10.65 [us]
 = 2.18365952 [s]
 = 45 [deg]
 = 6 [dB]
 = 5.325 [us]
 = Off
 = Off
 = FALSE
 = 1 [fs]
 = 50
 = 5 [s]
 = 7.18365952 [s]
 = 19.3 [dC]



9.7

7.82



1.0080

3.9794
3.9622
3.7732
3.3058
2.7090
2.6930
2.6758
2.4582
2.4536

7.3540
7.3368
7.3231
7.3208
7.0103
6.9909
6.4594

X : parts per Million : 1H

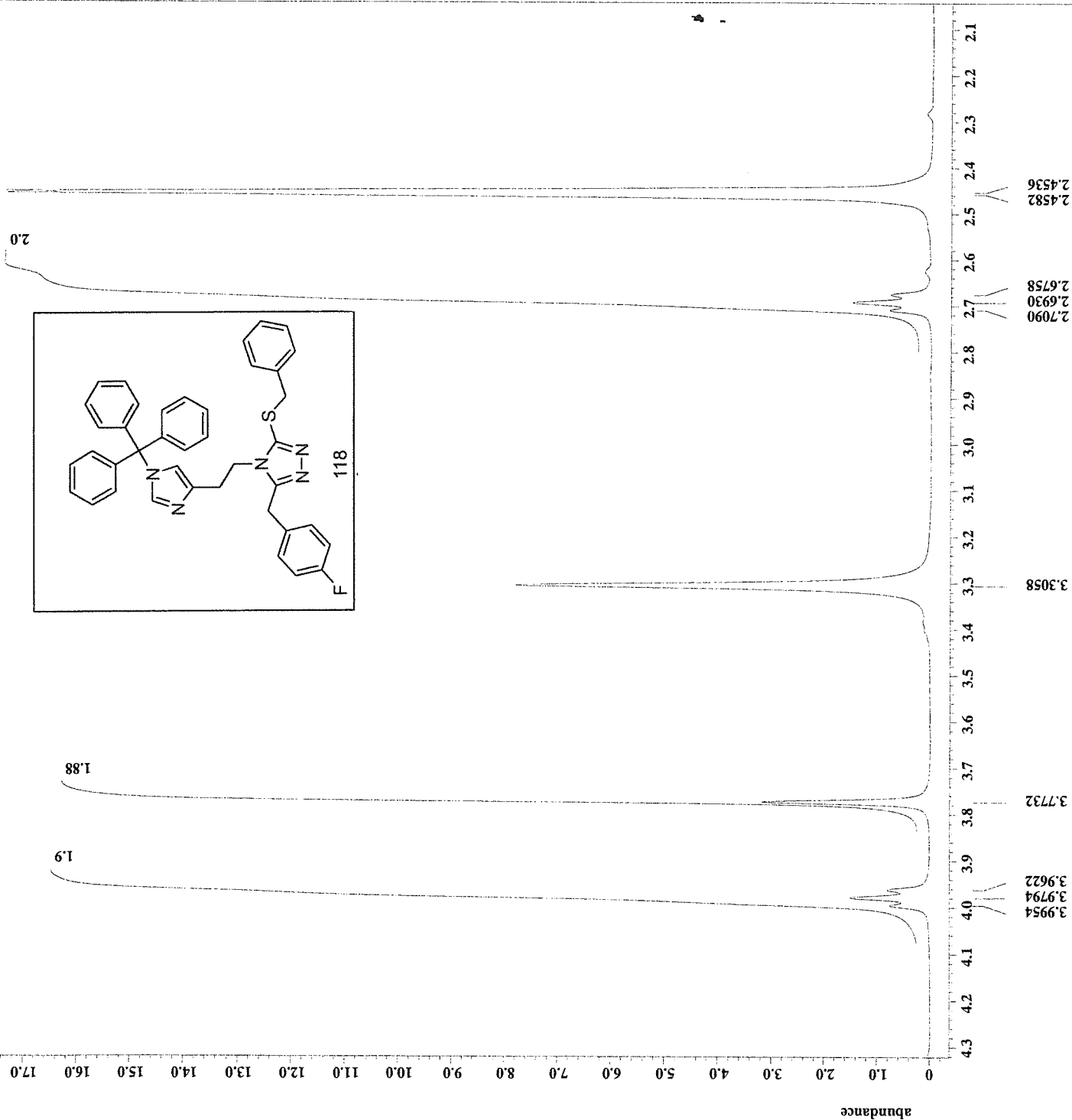


File = KI 18A-7recrystal0911
Name = Delta
Exp = single_pulse.ex2
ID = S#327147
Sol = DMSO-D6
Time = 11-SEP-2018 07:42:23
Rev = 7-MAY-2024 08:44:35
Cur = 7-MAY-2024 08:44:43

Comment = single_pulse
Data = 1D COMPLEX
Dim = 13107
Title = 1H
Units = [ppm]
Dim = X
Site = ECS 400
Spect = JNM-ECS400

Field = 9.389766 [T] (400 [MHz])
Acq = 2.18365952 [s]
X = 1H
Freq = 399.78219838 [MHz]
X = 5 [ppm]
Points = 16384
X = 1
Res = 0.45794685 [Hz]
X = 7.5030012 [kHz]
Sweep = 1H
X = 399.78219838 [MHz]
Freq = 5 [ppm]
X = 1H
Tri = 399.78219838 [MHz]
X = 5 [ppm]
Offset = TRUE
Mod = 1
Return = 8
Total = 8

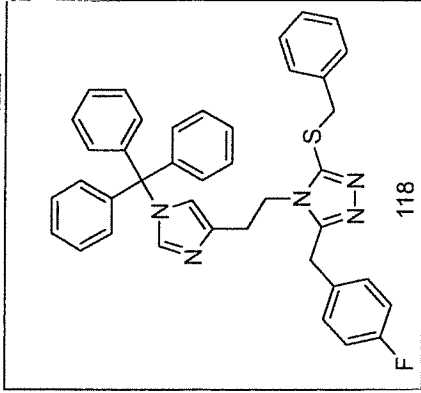
X = 10.65 [us]
X = 2.18365952 [s]
X = 45 [deg]
X = 6 [dB]
X = 5.325 [us]
X = Off
X = Off
X = FALSE
X = 1 [s]
X = 50
X = 7.18365952 [s]
X = 19.3 [dc]



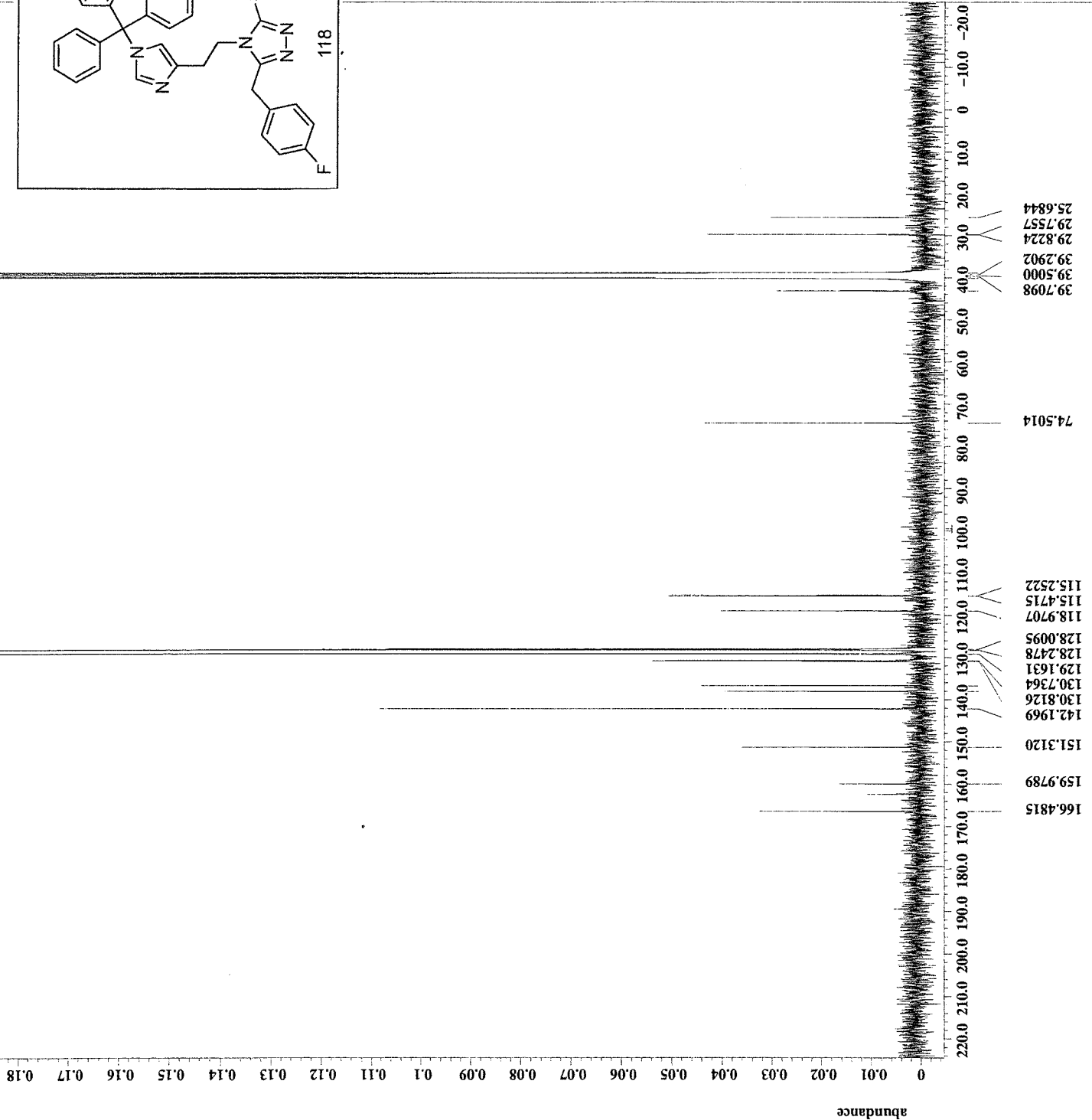
X : parts per Million : 1H

JEOL

= XI_18-7recrystalC0911
= Delta
= single_pulse_dec
= XI_18-7recrystalC0911
= DMSO-D6
= 11-SEP-2018 11:31:24
= 7-MAY-2024 10:39:13
= 7-MAY-2024 10:39:33
= 1D COMPLEX
= 26214
= 13C
= [ppm]
= X
= ECS 400
= JNM-ECS400



Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Mod_return = FALSE
Scans = 1
Total_scans = 3000
X_90_width = 13.22[us]
X_acq_time = 1.04333312[s]
X_angle = 30[deg]
X_atn = 9[db]
X_pulse = 4.40666667[us]
Irr_atn_dec = 27[db]
Irr_atn_noe = 27[db]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe_time = TRUE
Noe = 2[s]
Recvr_gain = 60
Relaxation_delay = 2[s]
Repetition_time = 3.04333312[s]
Temp_get = 20[dc]

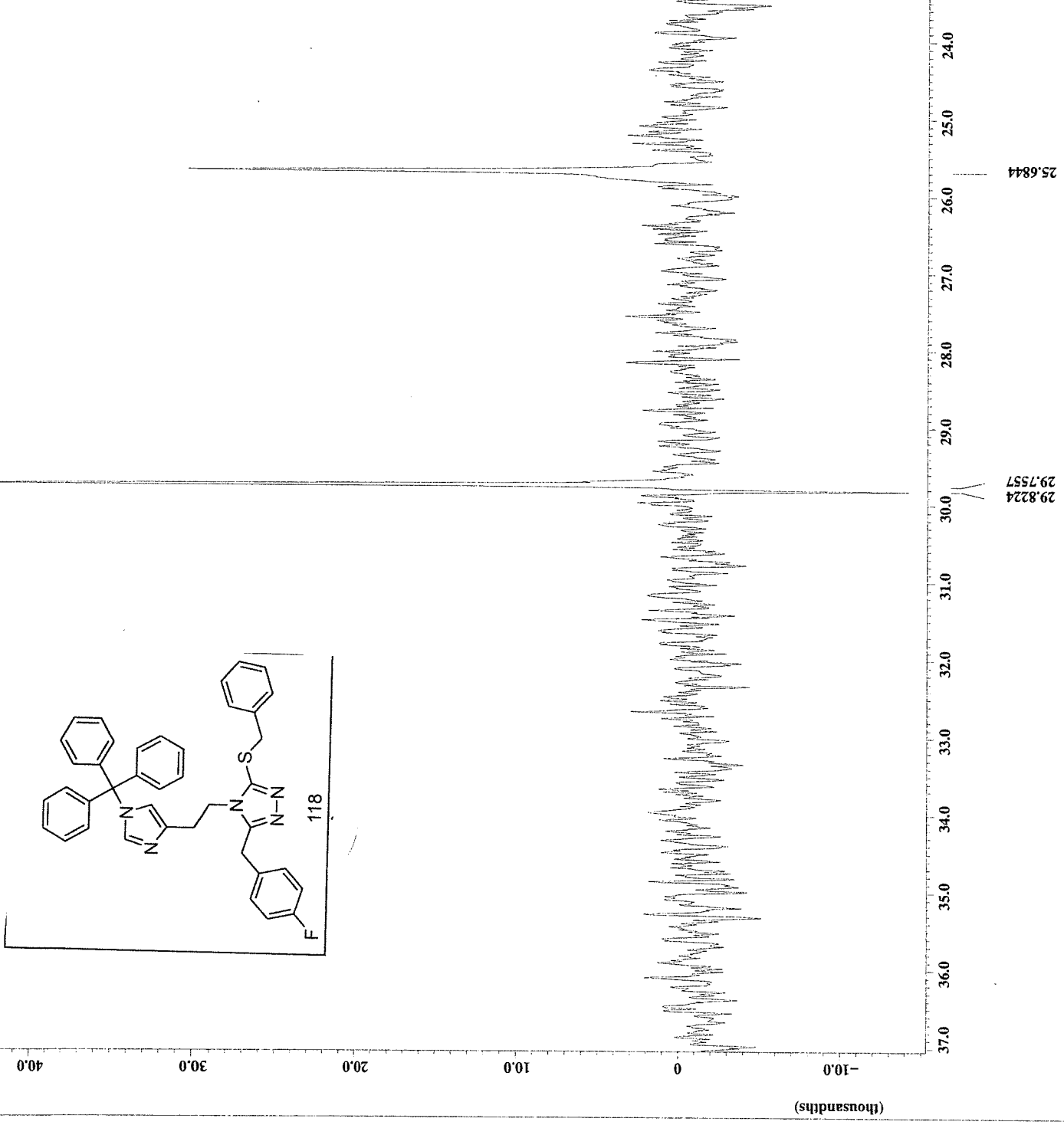
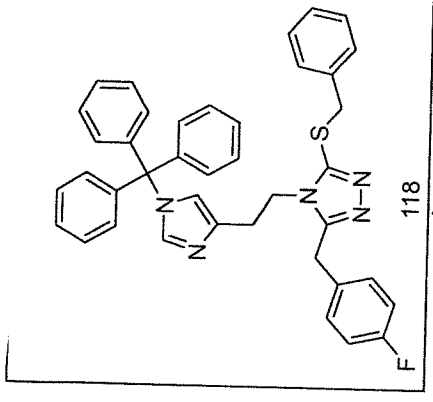


X : parts per Million : 13C

JEOL

```

= KI_18-7recrystalC0911
= Delta
= single_pulse_dec
= KI_18-7recrystalC0911
= DMSO-D6
= 11-SEP-2018 11:31:24
= 7-MAY-2024 10:39:13
= 7-MAY-2024 10:41:17
= 1D COMPLEX
= 26214
= 13C
= [ppm]
= X
= ECS 400
= JNM-ECS400
= 9.389766[T] (400[MHz])
= 1.04333312[s]
= 13C
= 100.52530333[MHz]
= 100[ppm]
= 32768
= 4
= 0.95846665[Hz]
= 1H
= 31.40703518[kHz]
= 399.78219838[MHz]
= 5[ppm]
= FALSE
= 1
= 3000
= 3000
= 13.22[us]
= 1.04333312[s]
= 30[deg]
= 9[dB]
= 4.40666667[us]
= 27[dB]
= WALTZ
= TRUE
= 1[s]
= TRUE
= 2[s]
= 60
= 2[s]
= 3.04333312[s]
= 20[dc]
  
```



JEOL

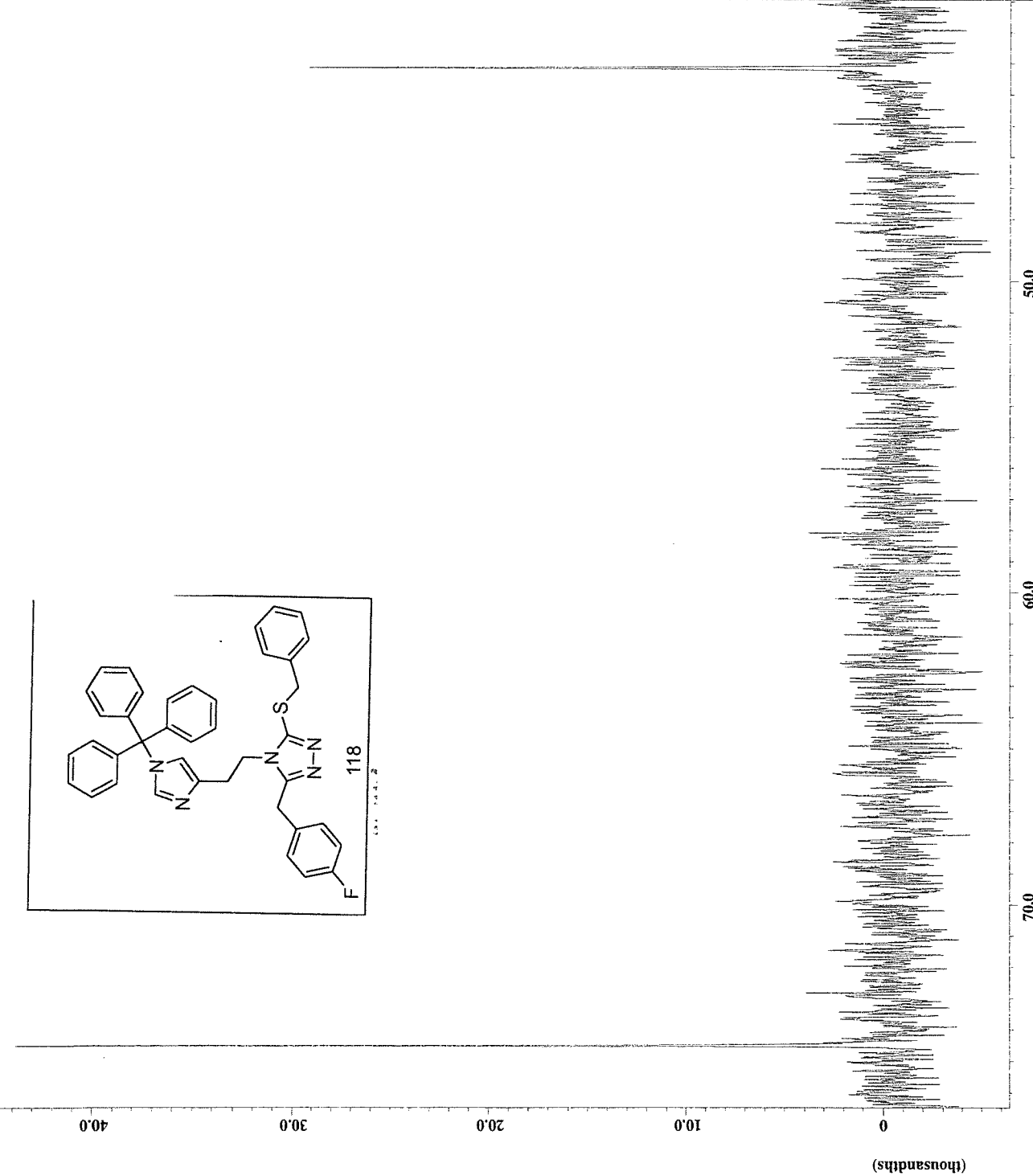
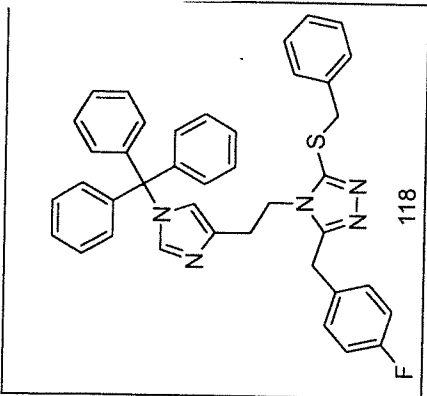
```

= KI_18-7recrystalC0911
= Delta
= single_pulse_dec
= KI_18-7recrystalC0911
= DMSO-D6
= 11-SEP-2018 11:31:24
= 7-MAY-2024 10:39:13
= 7-MAY-2024 10:40:56

Data format
= 1D COMPLEX
Dim_size
= 26214
Dim_title
= 13C
Dim_units
= [ppm]
Dimensions
= X
Site
= ECS 400
Spectrometer
= JNM-ECS400

Field_strength
= 9.389766[T] (400[MHz])
X_acq_duration
= 1.04333312[s]
X_domain
= 13C
X_freq
= 100.52530333[MHz]
X_offset
= 100[ppm]
X_points
= 32768
X_prescans
= 4
X_resolution
= 0.95846665[Hz]
X_sweep
= 31.40703518[KHz]
Irr_domain
= 1H
Irr_freq
= 399.78219838[MHz]
Irr_offset
= 5[ppm]
Clipped
= FALSE
Mod_return
= 1
Scans
= 3000
Total_scans
= 3000

X_90_width
= 13.22[us]
X_acq_time
= 1.04333312[s]
X_angle
= 30[deg]
X_atn
= 9[db]
X_pulse
= 4.40666667[us]
Irr_atn_dec
= 27[db]
Irr_atn_noe
= 27[db]
Irr_noise
= WALTZ
Decoupling
= TRUE
Initial_wait
= 1[s]
Noe_time
= TRUE
Noe_time
= 2[s]
Recvr_gain
= 60
Relaxation_delay
= 2[s]
Repetition_time
= 3.04333312[s]
Temp_get
= 20[dc]
  
```



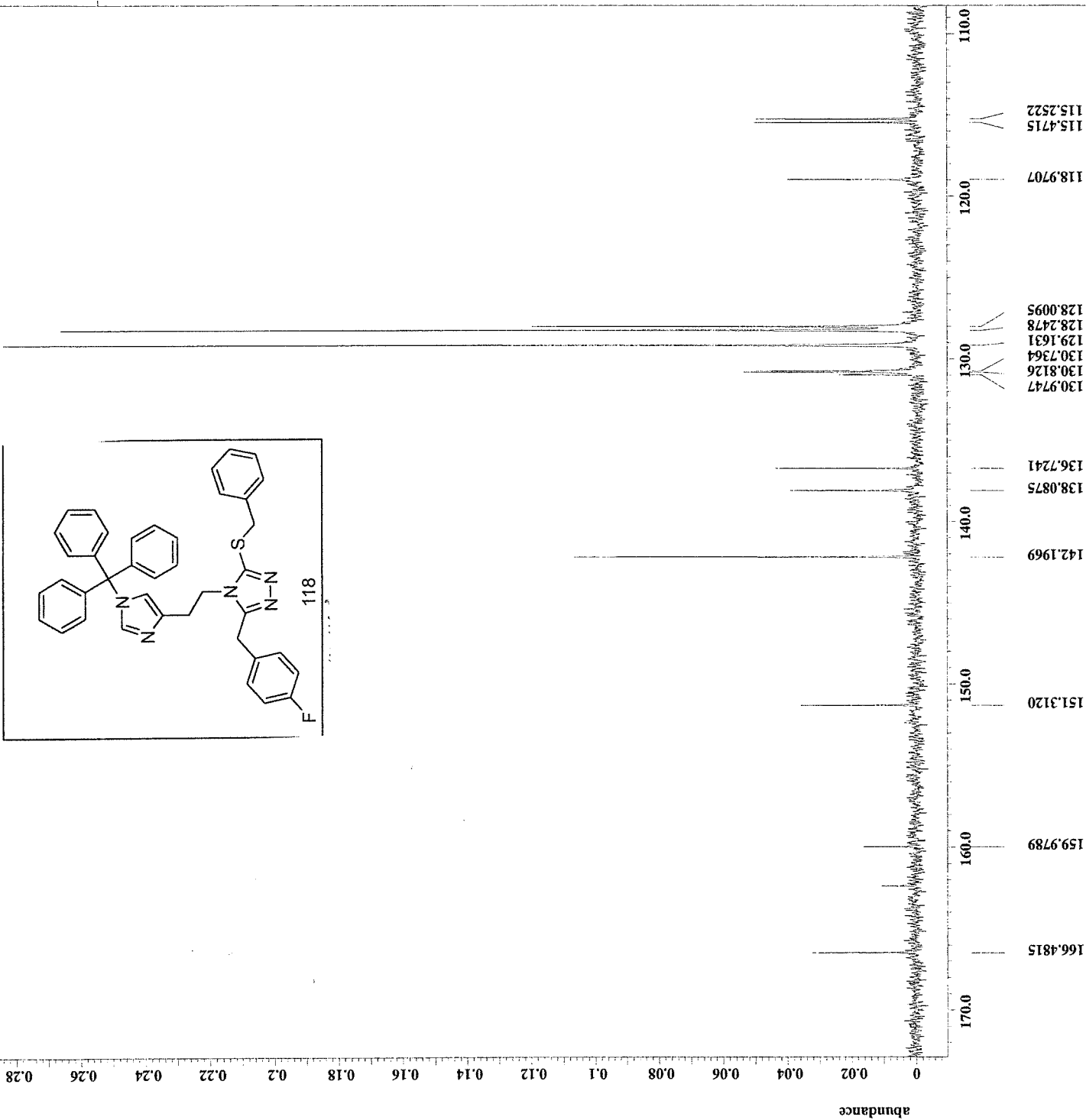
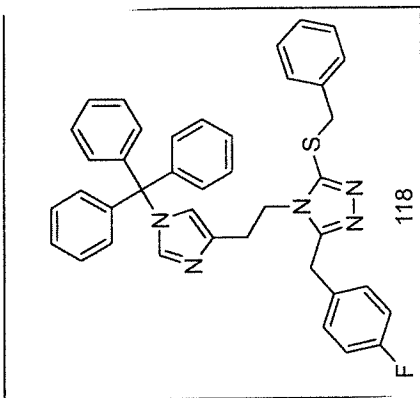
74.5014

43.1517

AJEOL

```

= KI_18-7recrystalC0911
= Delta
= single_pulse_dec
= KI_18-7recrystalC0911
= DMSO-D6
= 11-SEP-2018 11:31:24
= 7-MAY-2024 10:39:13
= 7-MAY-2024 10:40:16
= 1D_COMPLEX
= 26214
= 13C
= [ppm]
= X
= ECS 400
= JNM-ECS400
= 9.389766[M] (400[MHz])
= 1.04333312[s]
= 13C
= 100.52530333[MHz]
= 100[ppm]
= 32768
= 4
= 0.95846665[Hz]
= 31.40703518[KHz]
= 1H
= 399.78219838[MHz]
= 5[ppm]
= FALSE
= 1
= 3000
= 3000
= 13.22[us]
= 1.04333312[s]
= 30[deg]
= 9[dB]
= 4.40666667[us]
= 27[dB]
= WALTZ
= TRUE
= 1[s]
= TRUE
= 2[s]
= 60
= 2[s]
= 3.04333312[s]
= 20[dc]
  
```



X : parts per Million : 13C

AJEOL

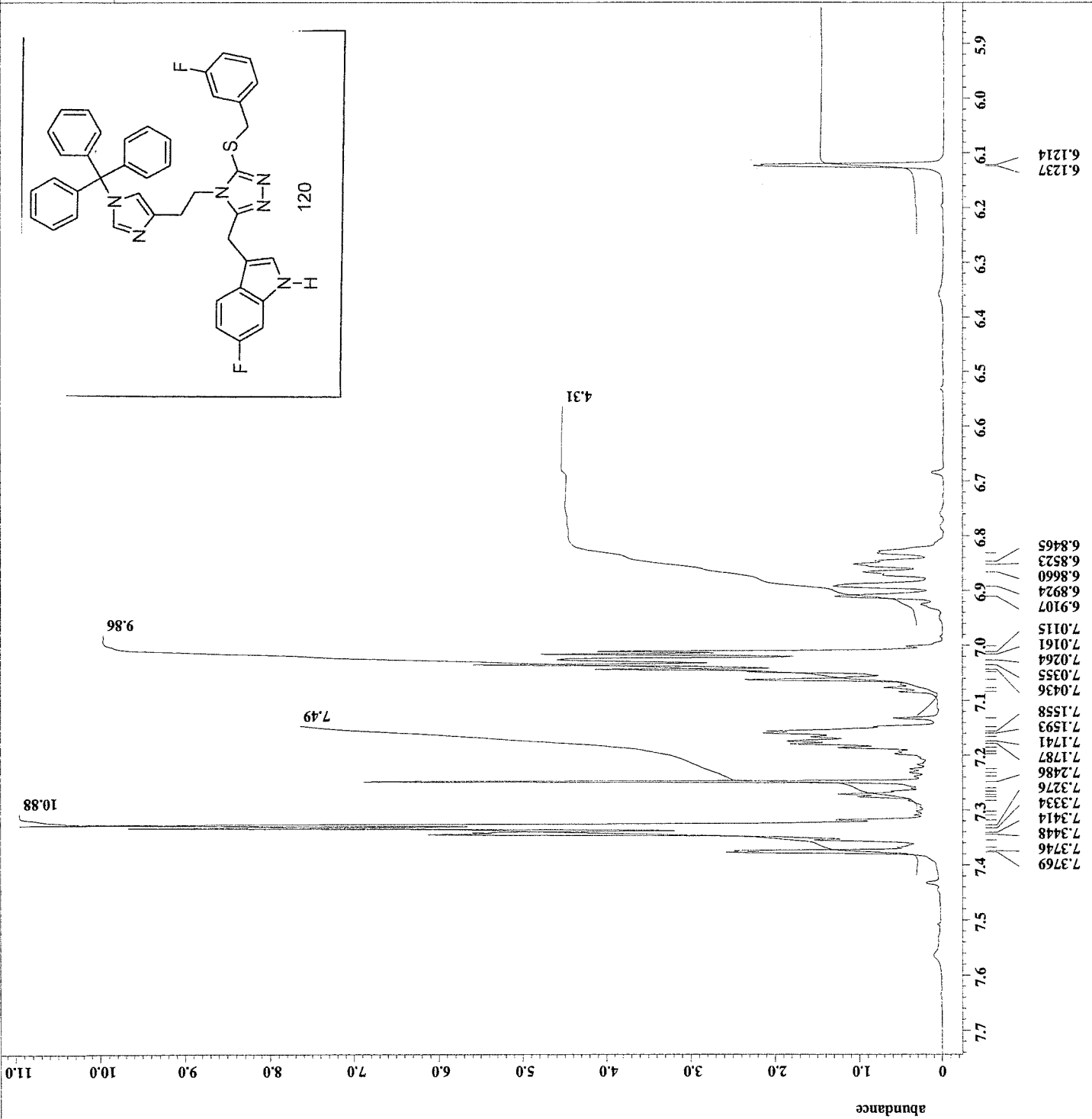
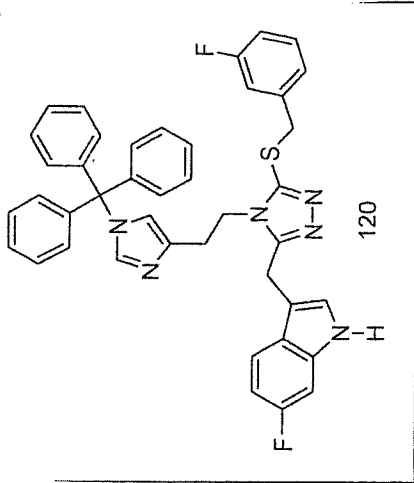
```

Filename = LG-mf-SBz-4.jdf
Author = mcrider
Experiment = single_pulse.ex2
Sample_id = S#546630
Solvent = CHLOROFORM-D
Creation_time = 18-DEC-2018 13:47:00
Revision_time = 3-MAY-2024 10:59:17
Current_time = 3-MAY-2024 11:00:12

Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400

Field_strength = 9.389766[Ti] (400[MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685[Hz]
X_sweep = 7.5030012[KHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = TRUE
Mod_return = 1
Scans = 8
Total_scans = 8

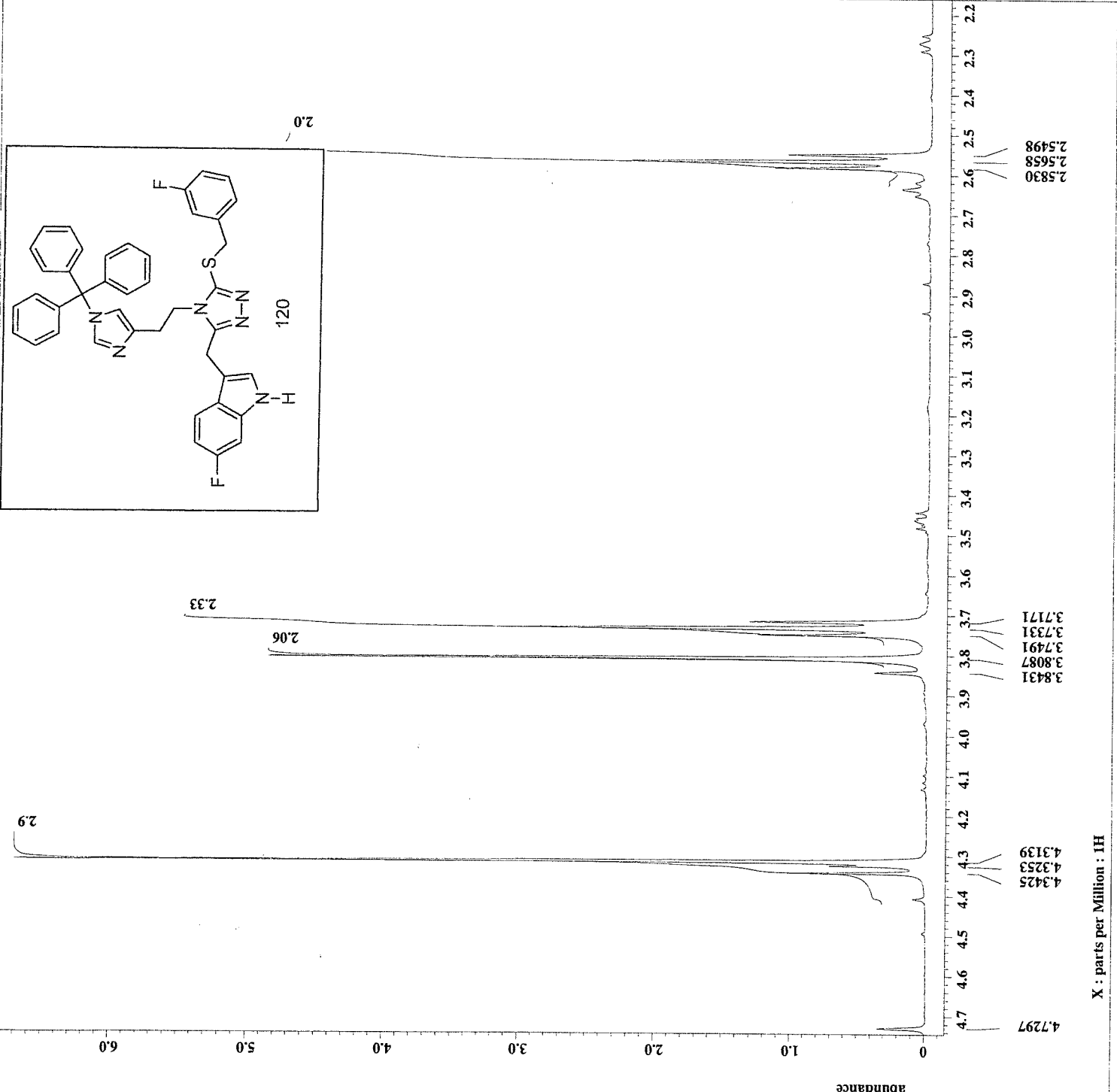
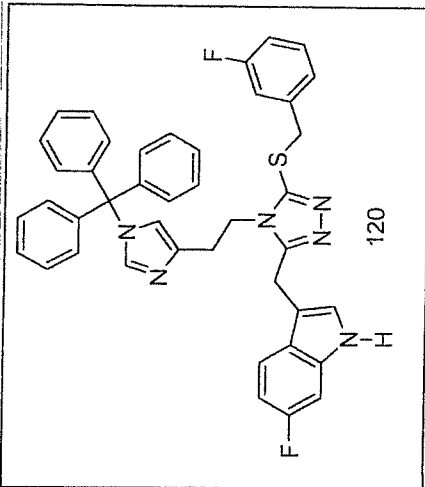
X_90_width = 11.365[us]
X_acq_time = 2.18365952[s]
X_angle = 45[deg]
X_atn = 6[dB]
X_pulse = 5.6825[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 50
Relaxation_delay = 5[s]
Repetition_time = 7.18365952[s]
Temp_get = 19[dc]
  
```



AJEOL

```

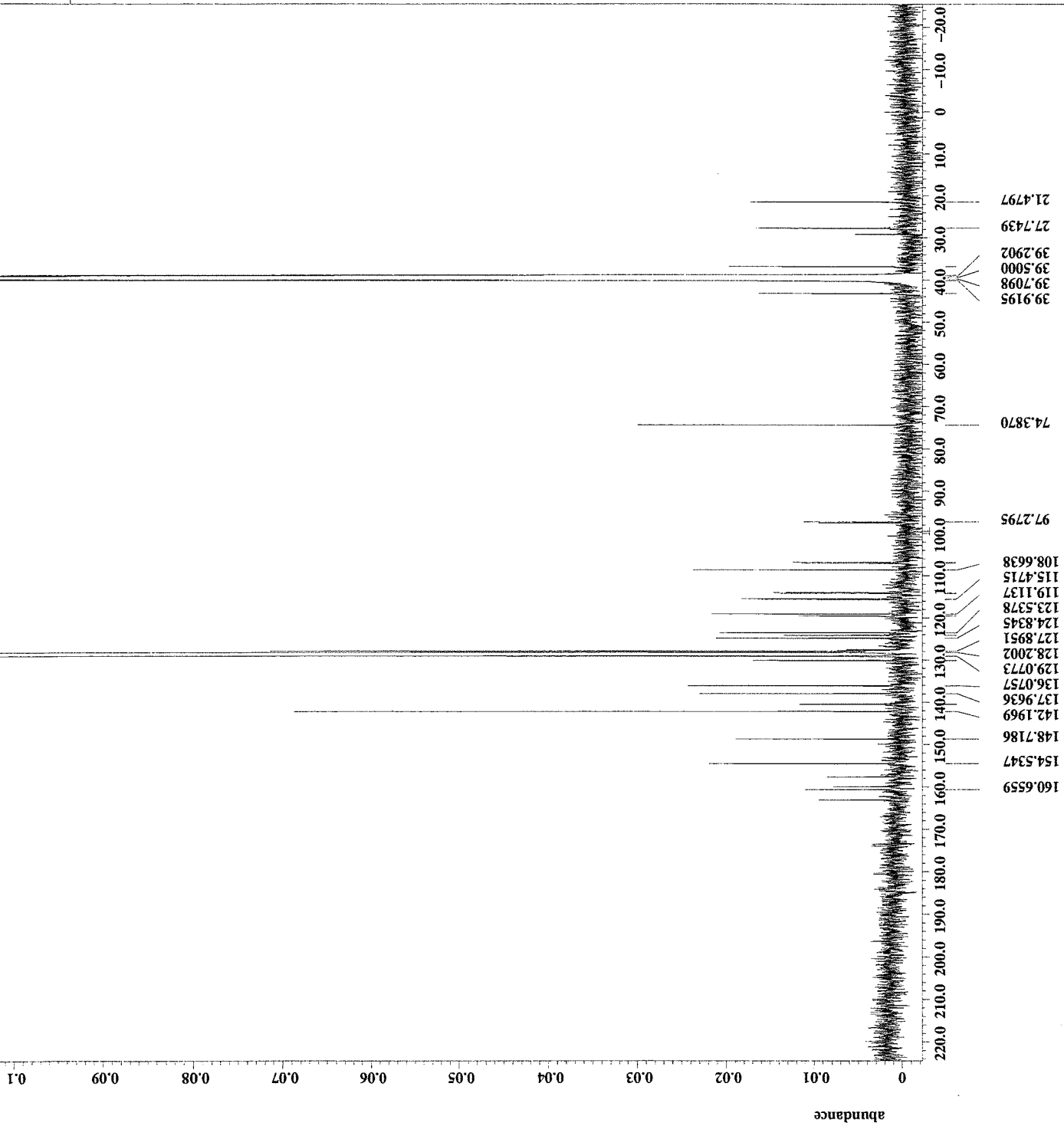
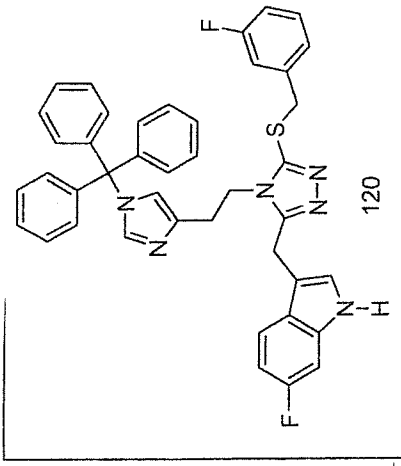
= LG-mf-SBz-4.jdf
= mcrider
= single_pulse.ex2
= S#546630
= CHLOROFORM-D
= 18-DEC-2018 13:47:00
= 3-MAY-2024 10:59:17
= 3-MAY-2024 10:59:23
= single_pulse
= 1D COMPLEX
= 13107
= 1H
= [ppm]
= X
= ECS 400
= JNM-ECS400
= 9.389766[T] (400[MHz])
= 2.18365952[s]
= 1H
= 399.78219838[MHz]
= 5[ppm]
= 16384
= 1
= 0.45794685[Hz]
= 7.5030012[kHz]
= 1H
= 399.78219838[MHz]
= 5[ppm]
= 1H
= 399.78219838[MHz]
= 5[ppm]
= TRUE
= 1
= 8
= 11.365[us]
= 2.18365952[s]
= 45[deg]
= 6[db]
= 5.6825[us]
= Off
= Off
= FALSE
= 1[s]
= 50
= 5[s]
= 7.18365952[s]
= 19[dc]
  
```



X : parts per Million : 1H



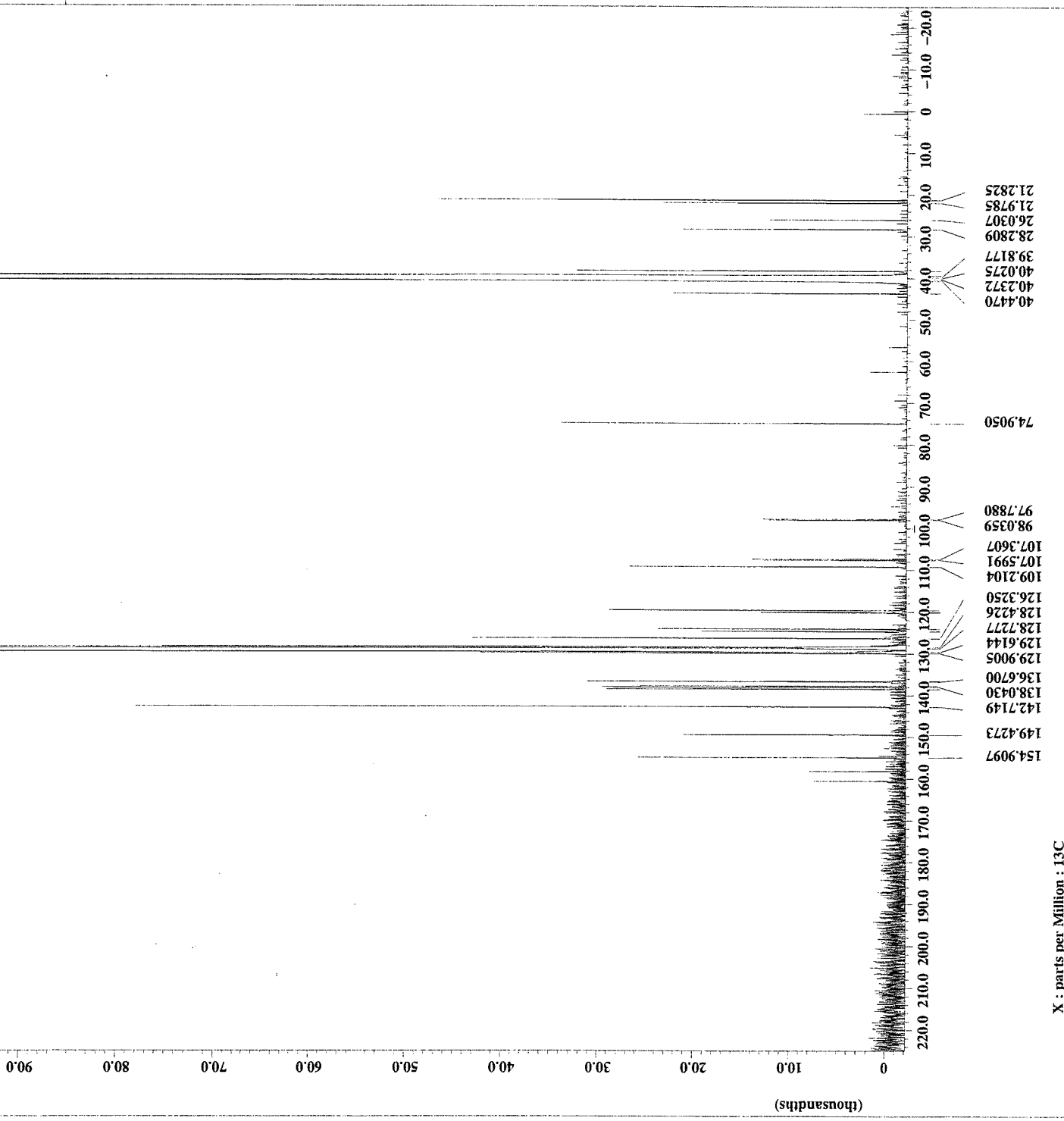
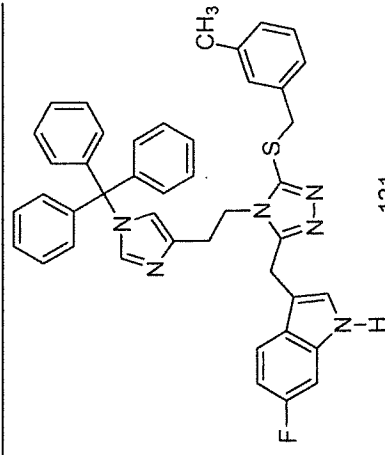
Filename = LG-I-65-1_CARBON-4.jd
Author = Delta
Experiment = single_pulse_dec
Sample_id = LG-I-65-1
Solvent = DMSO-D6
Creation_time = 17-SEP-2019 01:12:54
Revision_time = 6-MAY-2024 14:25:44
Current_time = 6-MAY-2024 14:26:17
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[MHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 12000
Total_scans = 12000
X_90_width = 10.466[us]
X_acq_time = 1.04333312[s]
X_angle = 30[deg]
X_atn = 10.3[dB]
X_pulse = 3.48866667[us]
Irr_atn_dec = 24[dB]
Irr_atn_noe = 24[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 60
Relaxation_delay = 2[s]
Repetition_time = 3.04333312[s]
Temp_get = 21[degC]



X : parts per Million : 13C



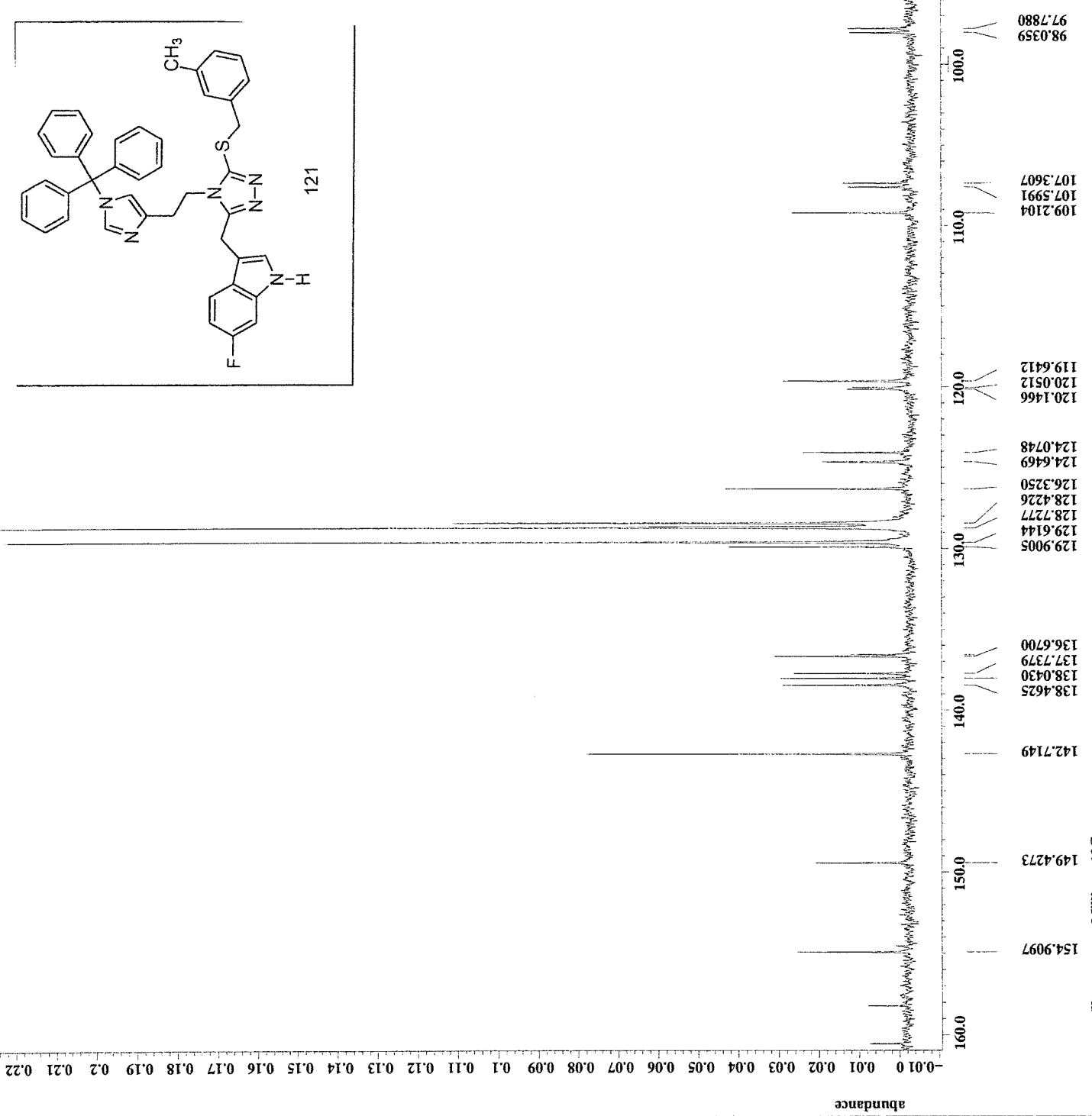
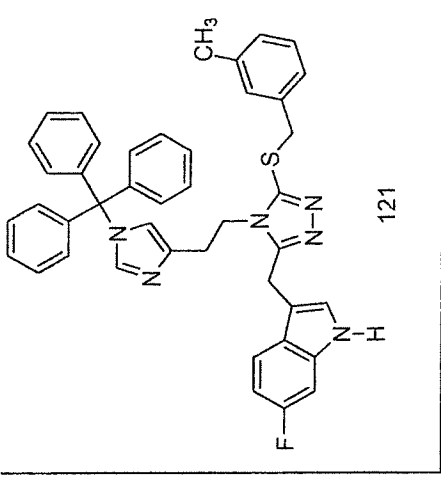
Filename = KI-6Findole-S-3MeBz_C
Author = mcrider
Experiment = single_pulse_dec
Sample_id = KI-6Findole-S-3MeBz
Solvent = DMSO-D6
Creation_time = 3-APR-2019 20:24:27
Revision_time = 7-MAY-2024 10:32:43
Current_time = 7-MAY-2024 10:33:12
Data_format = 1D_COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665 [Hz]
X_sweep = 31.40703518 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Clipped = TRUE
Mod_return = 1
Scans = 10000
Total_scans = 10000
X_90_width = 10.4 [us]
X_acq_time = 1.04333312 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 3.46666667 [us]
Irr_atn_dec = 24.2 [dB]
Irr_atn_noe = 24.2 [dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1 [s]
Noe_time = TRUE
Noe = 21eJ
Recvr_gain = 60
Relaxation_delay = 2 [s]
Repetition_time = 3.04333312 [s]
=====



X : parts per Million : 13C



File name = KI-6Findole-S-3MeBz_C
Author = mcridder
Experiment = single_pulse_dec
Sample_id = KI-6Findole-S-3MeBz
Solvent = DMSO-D6
Creation time = 3-APR-2019 20:24:27
Revision time = 7-MAY-2024 10:32:43
Current_time = 7-MAY-2024 10:33:42
Data format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766 [T] (400 [MHz])
X_acq_duration = 1.04333312 [s]
X_acmain = 13C
X_freq = 100.52530333 [MHz]
X_offset = 100 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665 [Hz]
X_sweep = 31.40703518 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Clipped = TRUE
Mod_return = 1
Scans = 10000
Total_scans = 10000
X_90_width = 10.4 [us]
X_acq_time = 1.04333312 [s]
X_angle = 30 [deg]
X_atn = 9 [dB]
X_pulse = 3.46666667 [us]
Irr_atn_dec = 24.2 [dB]
Irr_atn_noe = 24.2 [dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1 [s]
Noe = TRUE
Noe_time = 2 [s]
Recvr_gain = 60
Relaxation_delay = 2 [s]
Repetition_time = 3.04333312 [s]
Temp_get = 20.6 [dC]



X : parts per Million : 13C



= AMC-S2-56A-4.jdf
 = mcrider
 = single_pulse.ex2
 = S#358446
 = DMSO-D6
 = 9-JUN-2018 08:48:55
 = 13-MAY-2024 14:17:56
 = 13-MAY-2024 14:18:26
 = single_pulse
 = 1D COMPLEX
 = 13107
 = 1H
 = [ppm]
 = X
 = ECS 400
 = JNM-ECS400

= 9.389766[T] (400 [MHz])
 = 2.18365952[s]
 = 1H
 = 399.78219838 [MHz]
 = 5 [ppm]
 = 16384
 = 1
 = 0.45794685 [Hz]
 = 7.5030012 [kHz]
 = 1H
 = 399.78219838 [MHz]
 = 5 [ppm]
 = 1H
 = 399.78219838 [MHz]
 = 5 [ppm]
 = TRUE
 = 1
 = 8
 = 8
 = 10.65 [us]
 = 2.18365952 [s]
 = 45 [deg]
 = 6 [dB]
 = 5.325 [us]
 = Off
 = Off
 = FALSE
 = 1 [s]
 = 50
 = 5 [s]
 = 7.18365952 [s]
 = 20 [dc]

= 9.389766 [T] (400 [MHz])
 = 2.18365952 [s]
 = 1H
 = 399.78219838 [MHz]
 = 5 [ppm]
 = 16384
 = 1
 = 0.45794685 [Hz]
 = 7.5030012 [kHz]
 = 1H
 = 399.78219838 [MHz]
 = 5 [ppm]
 = 1H
 = 399.78219838 [MHz]
 = 5 [ppm]
 = TRUE
 = 1
 = 8
 = 8
 = 10.65 [us]
 = 2.18365952 [s]
 = 45 [deg]
 = 6 [dB]
 = 5.325 [us]
 = Off
 = Off
 = FALSE
 = 1 [s]
 = 50
 = 5 [s]
 = 7.18365952 [s]
 = 20 [dc]

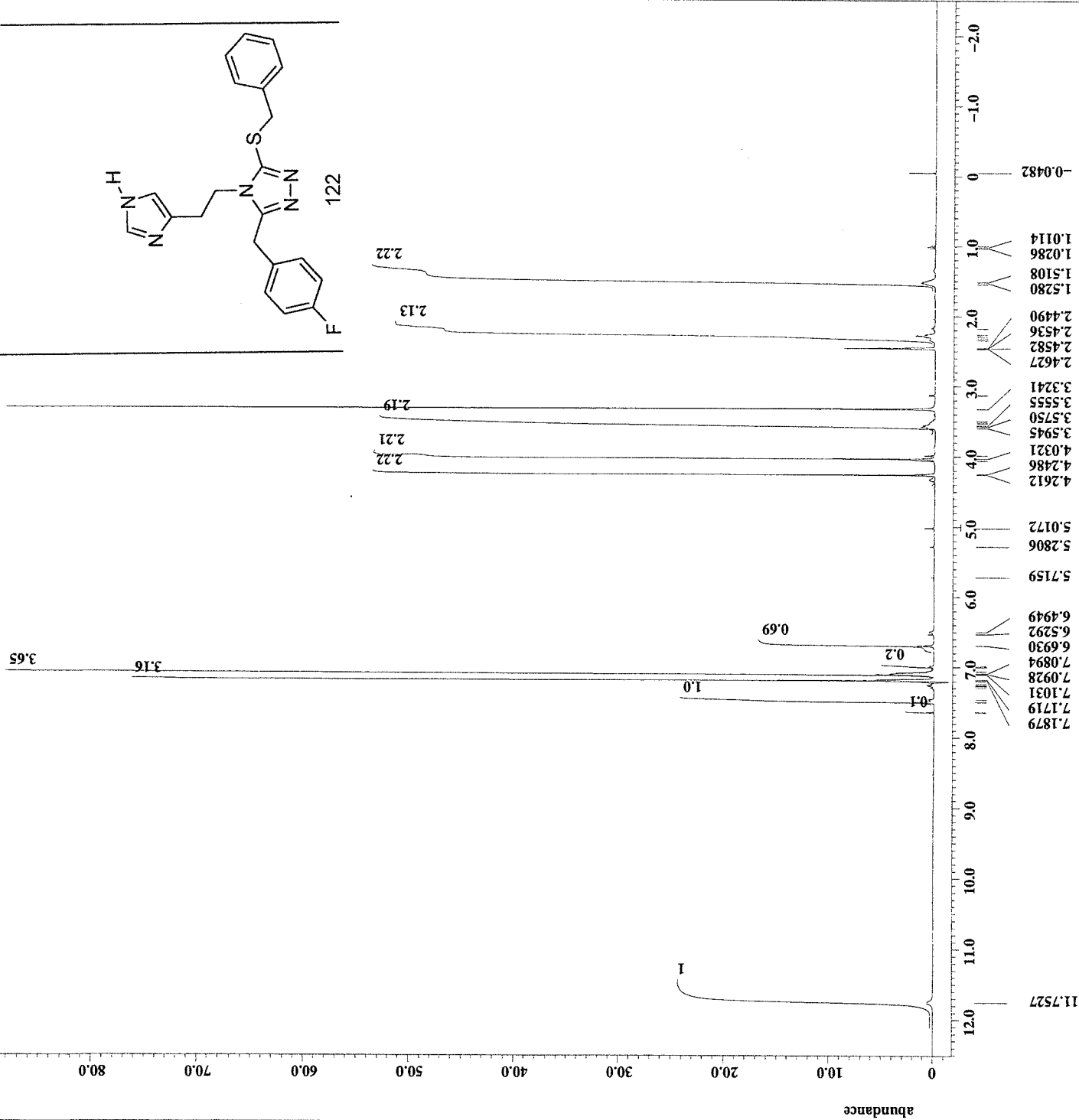
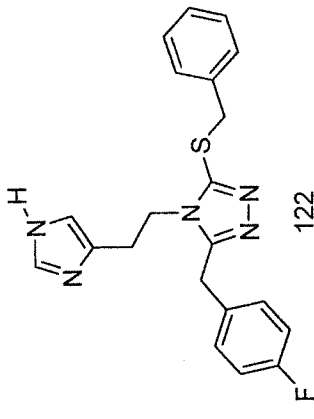
= 9.389766 [T] (400 [MHz])
 = 2.18365952 [s]
 = 1H
 = 399.78219838 [MHz]
 = 5 [ppm]
 = 16384
 = 1
 = 0.45794685 [Hz]
 = 7.5030012 [kHz]
 = 1H
 = 399.78219838 [MHz]
 = 5 [ppm]
 = 1H
 = 399.78219838 [MHz]
 = 5 [ppm]
 = TRUE
 = 1
 = 8
 = 8
 = 10.65 [us]
 = 2.18365952 [s]
 = 45 [deg]
 = 6 [dB]
 = 5.325 [us]
 = Off
 = Off
 = FALSE
 = 1 [s]
 = 50
 = 5 [s]
 = 7.18365952 [s]
 = 20 [dc]

= 9.389766 [T] (400 [MHz])
 = 2.18365952 [s]
 = 1H
 = 399.78219838 [MHz]
 = 5 [ppm]
 = 16384
 = 1
 = 0.45794685 [Hz]
 = 7.5030012 [kHz]
 = 1H
 = 399.78219838 [MHz]
 = 5 [ppm]
 = 1H
 = 399.78219838 [MHz]
 = 5 [ppm]
 = TRUE
 = 1
 = 8
 = 8
 = 10.65 [us]
 = 2.18365952 [s]
 = 45 [deg]
 = 6 [dB]
 = 5.325 [us]
 = Off
 = Off
 = FALSE
 = 1 [s]
 = 50
 = 5 [s]
 = 7.18365952 [s]
 = 20 [dc]

= 9.389766 [T] (400 [MHz])
 = 2.18365952 [s]
 = 1H
 = 399.78219838 [MHz]
 = 5 [ppm]
 = 16384
 = 1
 = 0.45794685 [Hz]
 = 7.5030012 [kHz]
 = 1H
 = 399.78219838 [MHz]
 = 5 [ppm]
 = 1H
 = 399.78219838 [MHz]
 = 5 [ppm]
 = TRUE
 = 1
 = 8
 = 8
 = 10.65 [us]
 = 2.18365952 [s]
 = 45 [deg]
 = 6 [dB]
 = 5.325 [us]
 = Off
 = Off
 = FALSE
 = 1 [s]
 = 50
 = 5 [s]
 = 7.18365952 [s]
 = 20 [dc]

= 9.389766 [T] (400 [MHz])
 = 2.18365952 [s]
 = 1H
 = 399.78219838 [MHz]
 = 5 [ppm]
 = 16384
 = 1
 = 0.45794685 [Hz]
 = 7.5030012 [kHz]
 = 1H
 = 399.78219838 [MHz]
 = 5 [ppm]
 = 1H
 = 399.78219838 [MHz]
 = 5 [ppm]
 = TRUE
 = 1
 = 8
 = 8
 = 10.65 [us]
 = 2.18365952 [s]
 = 45 [deg]
 = 6 [dB]
 = 5.325 [us]
 = Off
 = Off
 = FALSE
 = 1 [s]
 = 50
 = 5 [s]
 = 7.18365952 [s]
 = 20 [dc]

= 9.389766 [T] (400 [MHz])
 = 2.18365952 [s]
 = 1H
 = 399.78219838 [MHz]
 = 5 [ppm]
 = 16384
 = 1
 = 0.45794685 [Hz]
 = 7.5030012 [kHz]
 = 1H
 = 399.78219838 [MHz]
 = 5 [ppm]
 = 1H
 = 399.78219838 [MHz]
 = 5 [ppm]
 = TRUE
 = 1
 = 8
 = 8
 = 10.65 [us]
 = 2.18365952 [s]
 = 45 [deg]
 = 6 [dB]
 = 5.325 [us]
 = Off
 = Off
 = FALSE
 = 1 [s]
 = 50
 = 5 [s]
 = 7.18365952 [s]
 = 20 [dc]



X : parts per Million : 1H

AJEOL

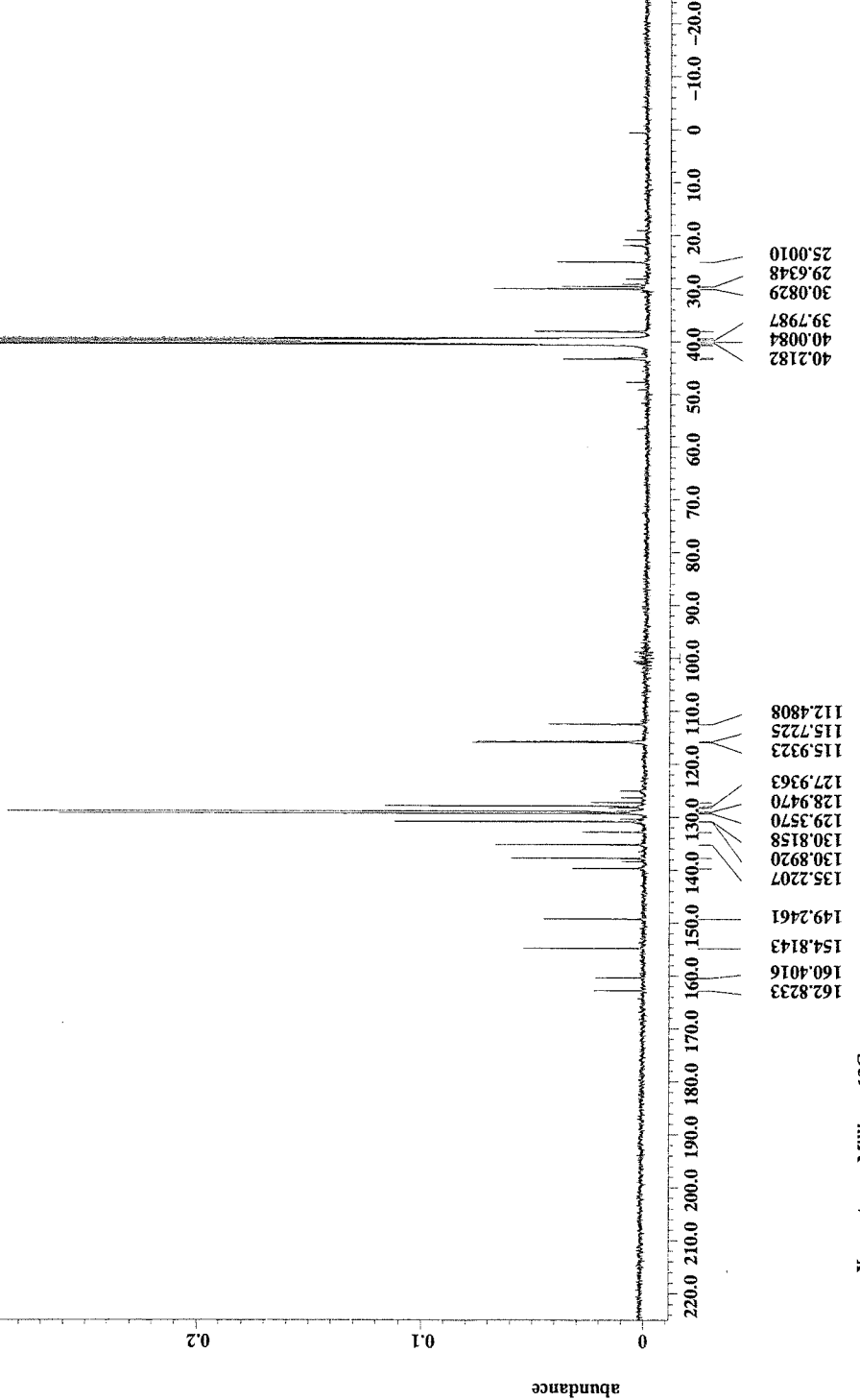
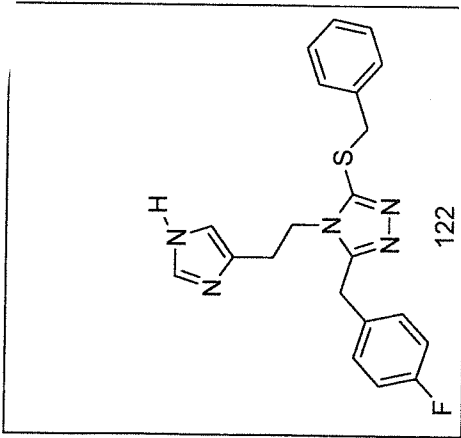
```

Filename = AMC-S2-56A_CARBON-4.J
Author = mcridler
Experiment = single_pulse_dec
Sample_id = AMC-S2-56A
Solvent = DMSO-D6
Creation_time = 9-JUN-2018 21:37:18
Revision_time = 13-MAY-2024 13:36:23
Current_time = 13-MAY-2024 13:36:47

Data_format = 1D_COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400

Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[MHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = TRUE
Mod_return = 1
Scans = 15000
Total_scans = 15000

X_90_width = 13.22[us]
X_acq_time = 1.04333312[s]
X_angle = 30[deg]
X_atn = 9[db]
X_pulse = 4.40666667[us]
Irr_atn_dec = 27[db]
Irr_atn_noe = 27[db]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe_time = TRUE
Noe_time = 2[s]
Recvr_gain = 60
Relaxation_delay = 2[s]
Repetition_time = 3.04333312[s]
Temp_get = 20.7[dc]
  
```



X : parts per Million : 13C

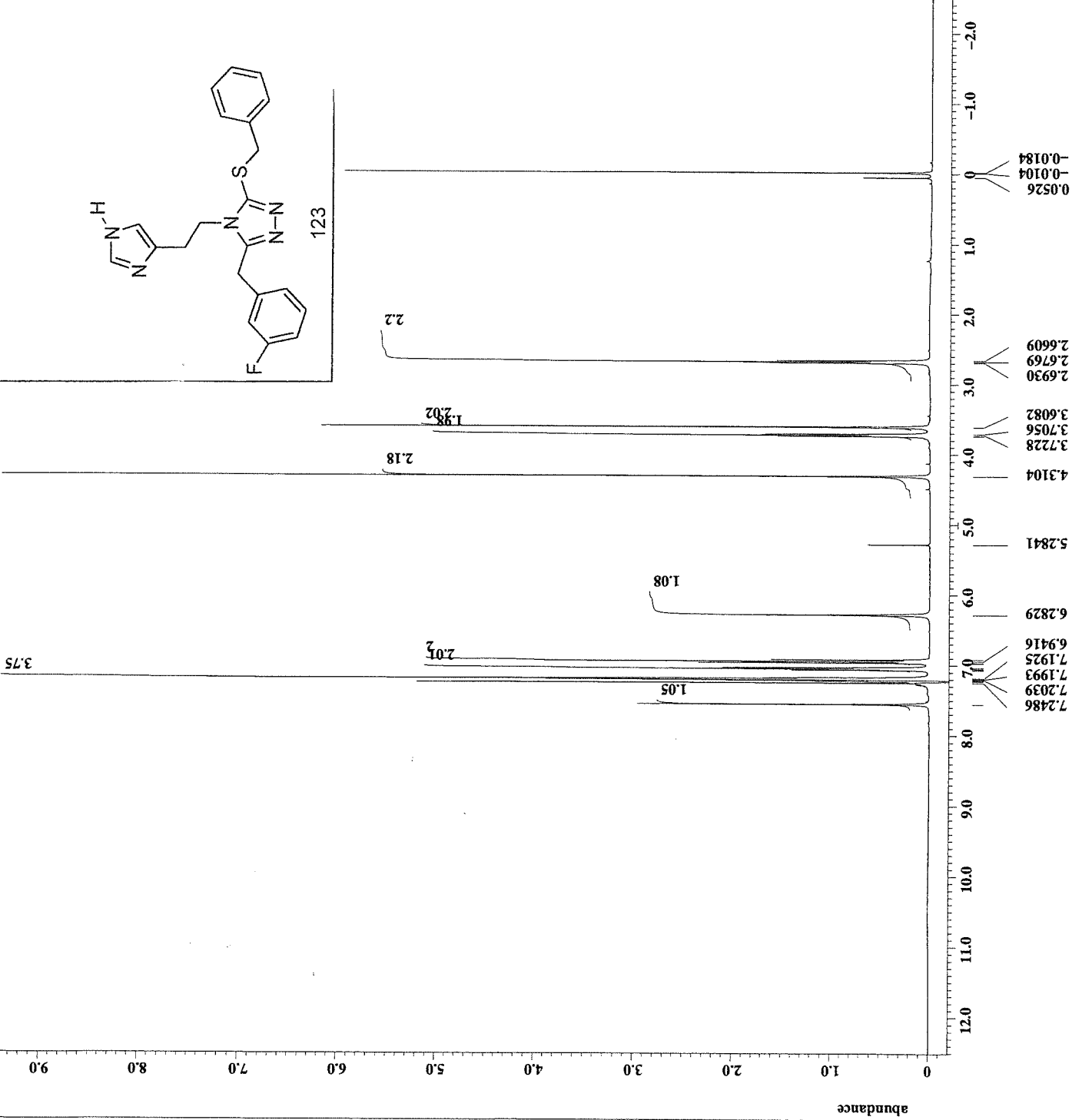
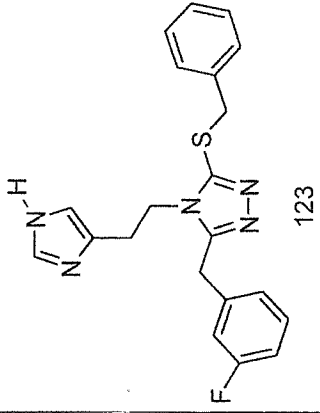
```

= KI-18-8-detryl1 2-4.
= mcrider
= single_pulse.ex2
= S#575857
= CHLOROFORM-D
= 26-OCT-2018 14:38:20
= 10-JAN-2019 15:48:27
= 2-MAY-2024 13:58:52

= single_pulse
= ID COMPLEX
= 13107
= 1H
= [ppm]
= X
= ECS 400
= JNM-ECS400

Field_strength = 9.389766[T] (400 [MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838 [MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685 [Hz]
X_sweep = 7.5030012 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838 [MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8

X_90_width = 11.365 [us]
X_acq_time = 2.18365952 [s]
X_angle = 45 [deg]
X_atn = 6 [dB]
X_pulse = 5.6825 [us]
Irr_mode = Off
Tri_mode = Off
Dance_preset = FALSE
Initial_wait = 1 [s]
Recvr_gain = 50
Relaxation_delay = 5 [s]
Repetition_time = 7.18365952 [s]
Temp_get = 18.6 [dC]
  
```



AJEOL

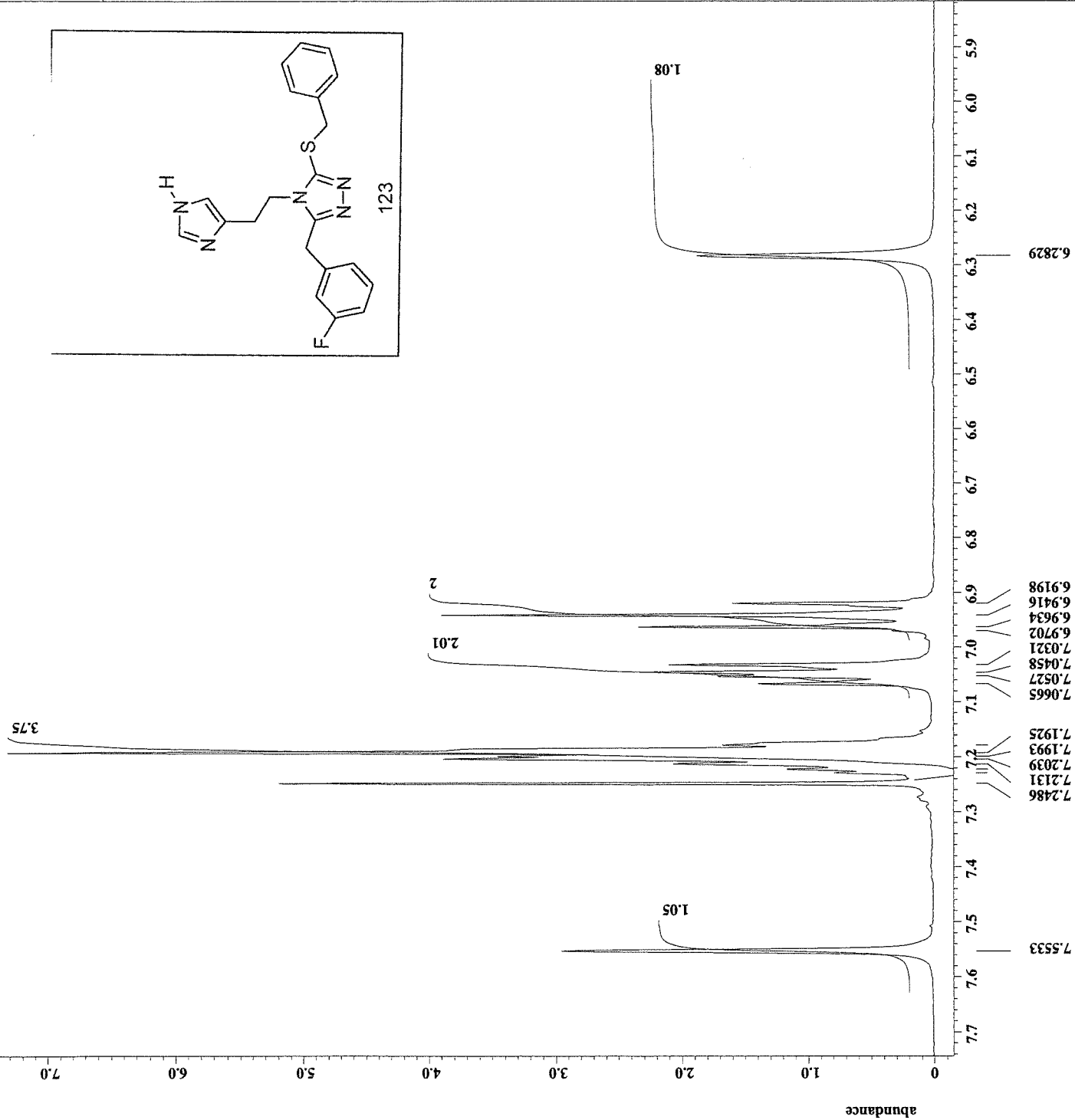
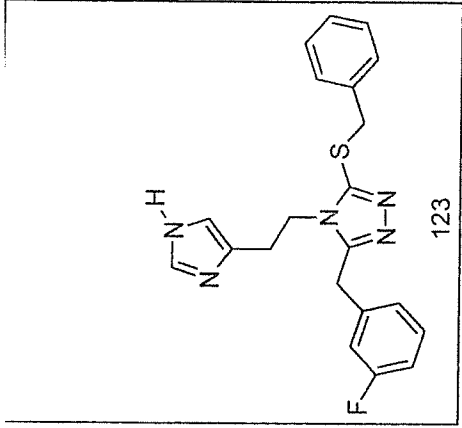
```

Filename = KI-18-8-detrityl 2-4.
Author = mcrider
Experiment = single_pulse.ex2
Sample_id = S#575857
Solvent = CHLOROFORM-D
Creation_time = 26-OCT-2018 14:38:20
Revision_time = 10-JAN-2019 15:48:27
Current_time = 2-MAY-2024 13:59:27

Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400

Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685[Hz]
X_sweep = 7.5030012[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Total_scans = 8

X_90_width = 11.365[us]
X_acq_time = 2.18365952[s]
X_angle = 45[deg]
X_atn = 6[db]
X_pulse = 5.6825[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 50
Relaxation_delay = 5[s]
Repetition_time = 7.18365952[s]
Temp_get = 18.6[degC]
  
```



X : parts per Million : 1H


```

= KI-18-8-detrityl_2_CA
= mcrider
= single_pulse_dec
= KI-18-8-detrityl_2
= CHLOROFORM-D
= 26-OCT-2018 15:59:59
= 2-MAY-2024 13:57:12
= 2-MAY-2024 13:57:33

= 1D COMPLEX
= 26214
= 13C
= [ppm]
= X
= ECS 400
= JNM-ECS400

= 9.389766[T] (400[MHz])
= 1.04333312[s]
= 13C
= 100.52530333[MHz]
= 32768
= 4
= 0.95846665[Hz]
= 31.40703518[MHz]
= 1H
= 399.78219838[MHz]
= 5[ppm]
= FALSE
= 1
= 1500
= 1500

= 10.4[us]
= 1.04333312[s]
= 30[deg]
= 9[dB]
= 3.46666667[us]
= 24.2[dB]
= 24.2[dB]
= WALTZ
= TRUE
= 1[s]
= TRUE
= 2[s]
= 60
= Relaxation_delay = 2[s]
= Repetition_time = 3.04333312[s]
= Temp_get = 19[degC]
  
```

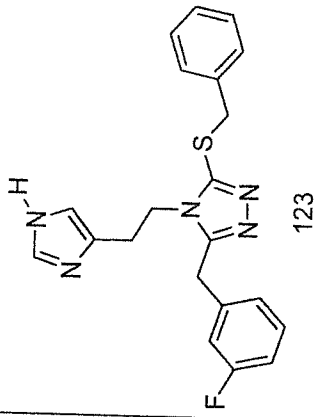
```

File name
Author
Experiment
Sample_id
Solvent
Creation time
Revision time
Current_time

Data_format
Dim_size
Dim_title
Dim_units
Dimensions
Site
Spectrometer

Field_strength
X_acq_duration
X_domain
X_freq
X_offset
X_points
X_prescans
X_resolution
X_sweep
Irr_domain
Irr_freq
Irr_offset
Clipped
Mod_return
Scans
Total_scans

X_90_width
X_acq_time
X_angle
X_atn
X_pulse
Irr_atn_dec
Irr_atn_noe
Irr_noise
Decoupling
Initial_wait
Noe
Noe_time
Recvr_gain
Relaxation_delay
Repetition_time
Temp_get
  
```

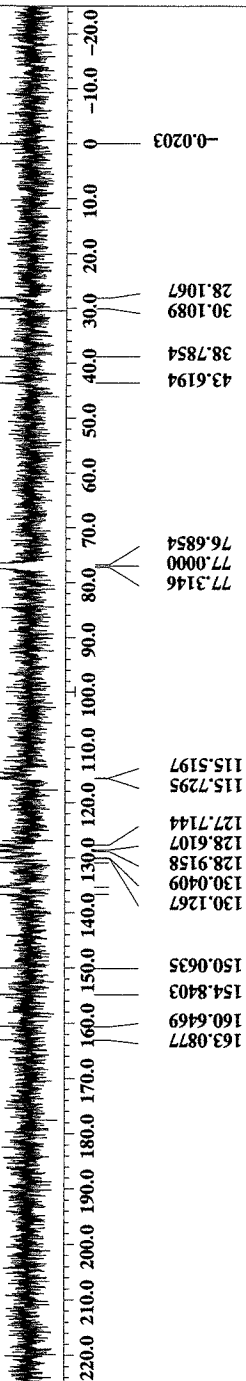


0.3

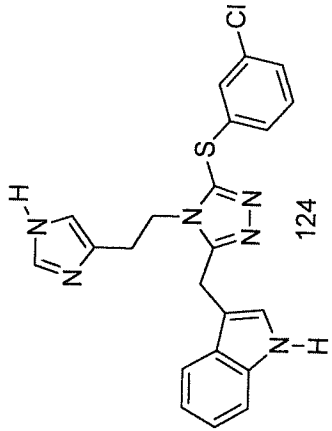
0.2

0.1

abundance



X : parts per Million : 13C



124

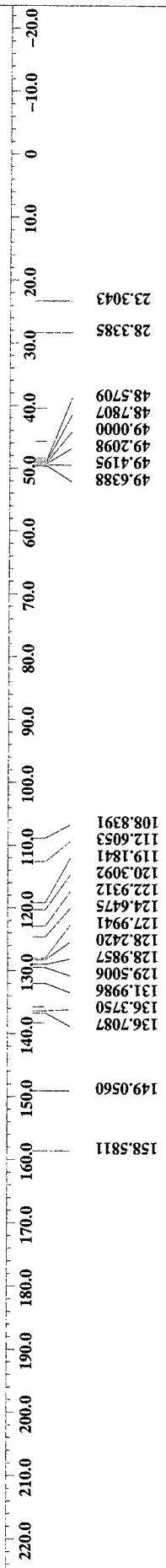
0.3

0.2

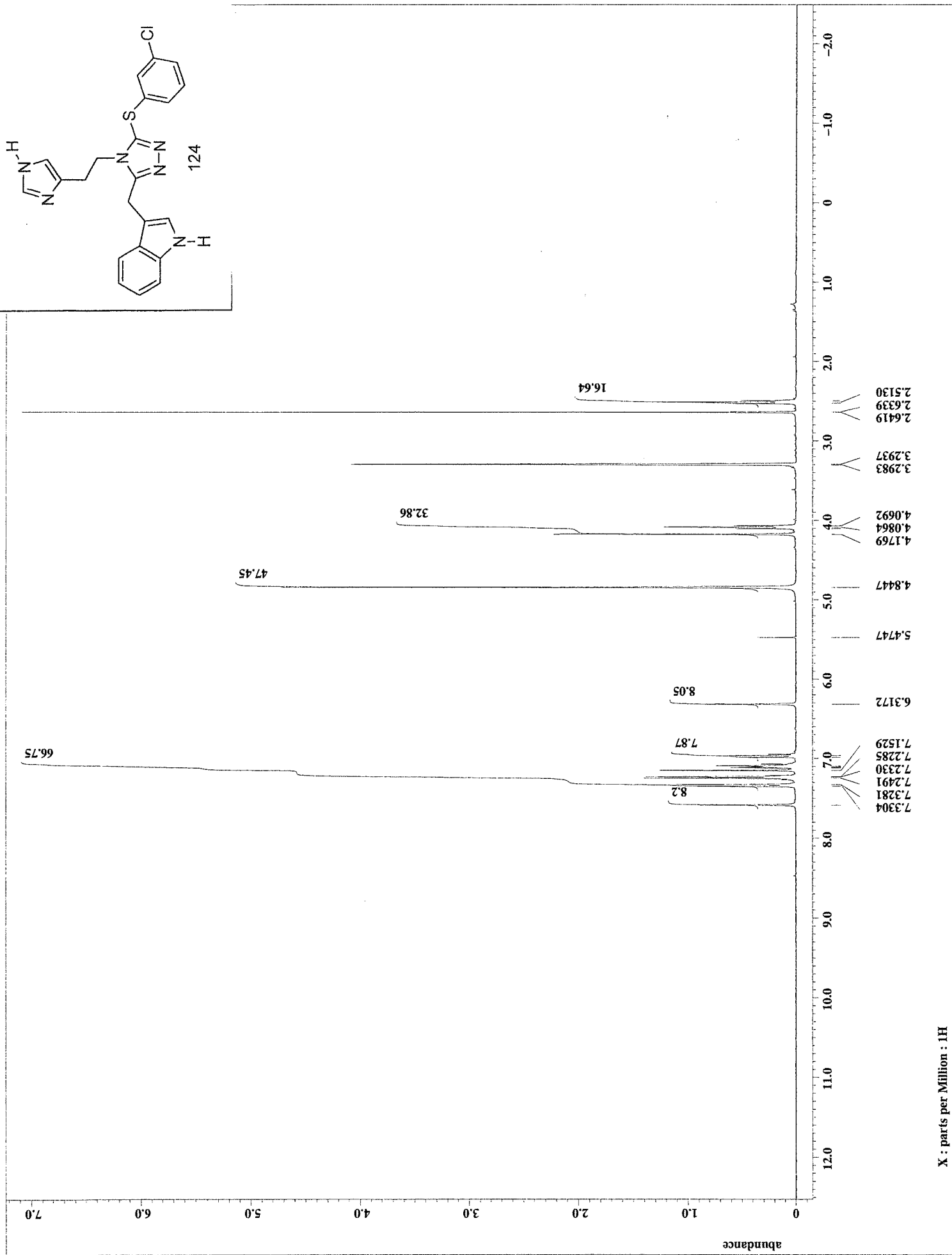
0.1

0

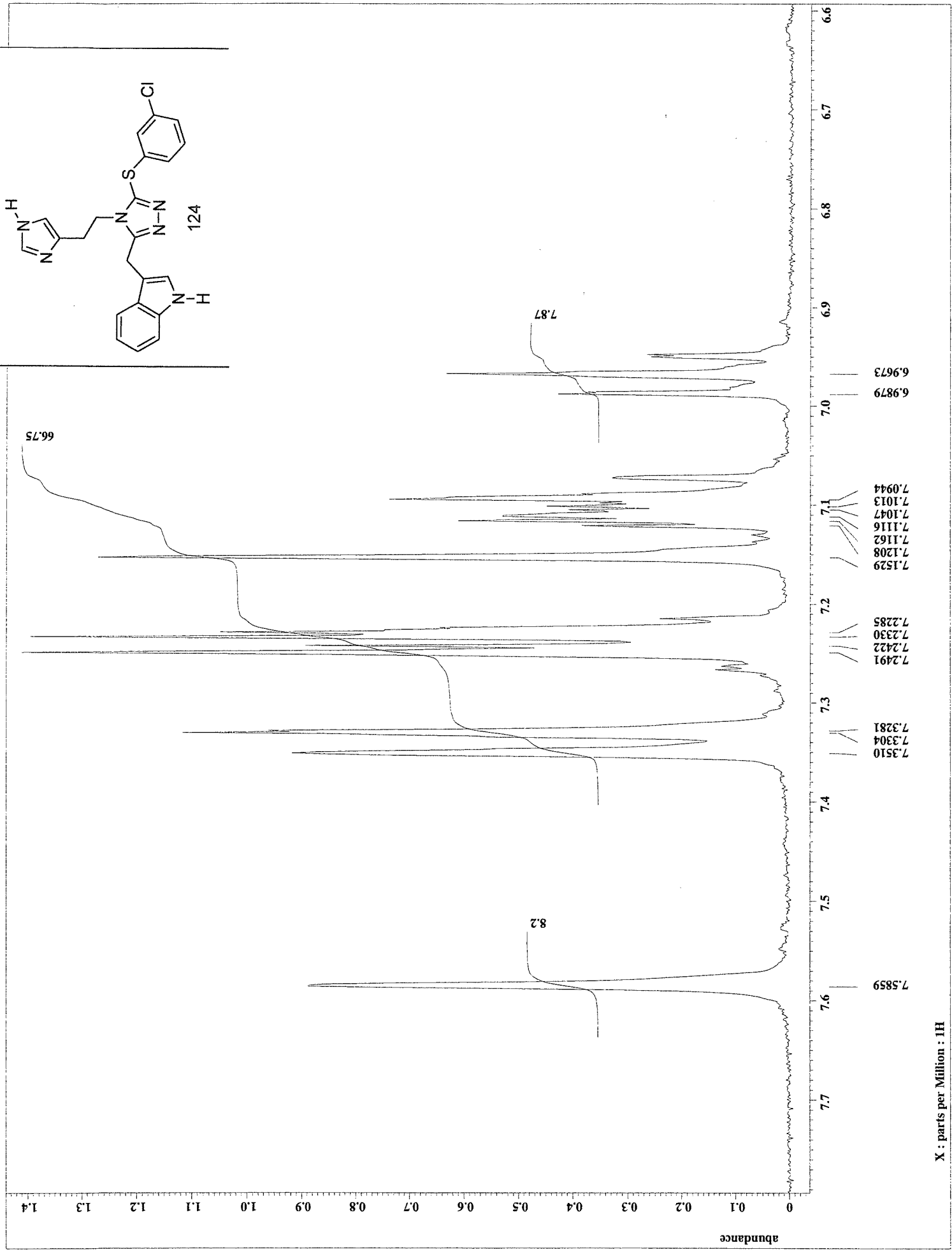
abundance



X : parts per Million : 13C



X : parts per Million : 1H



X : parts per Million : 1H



```

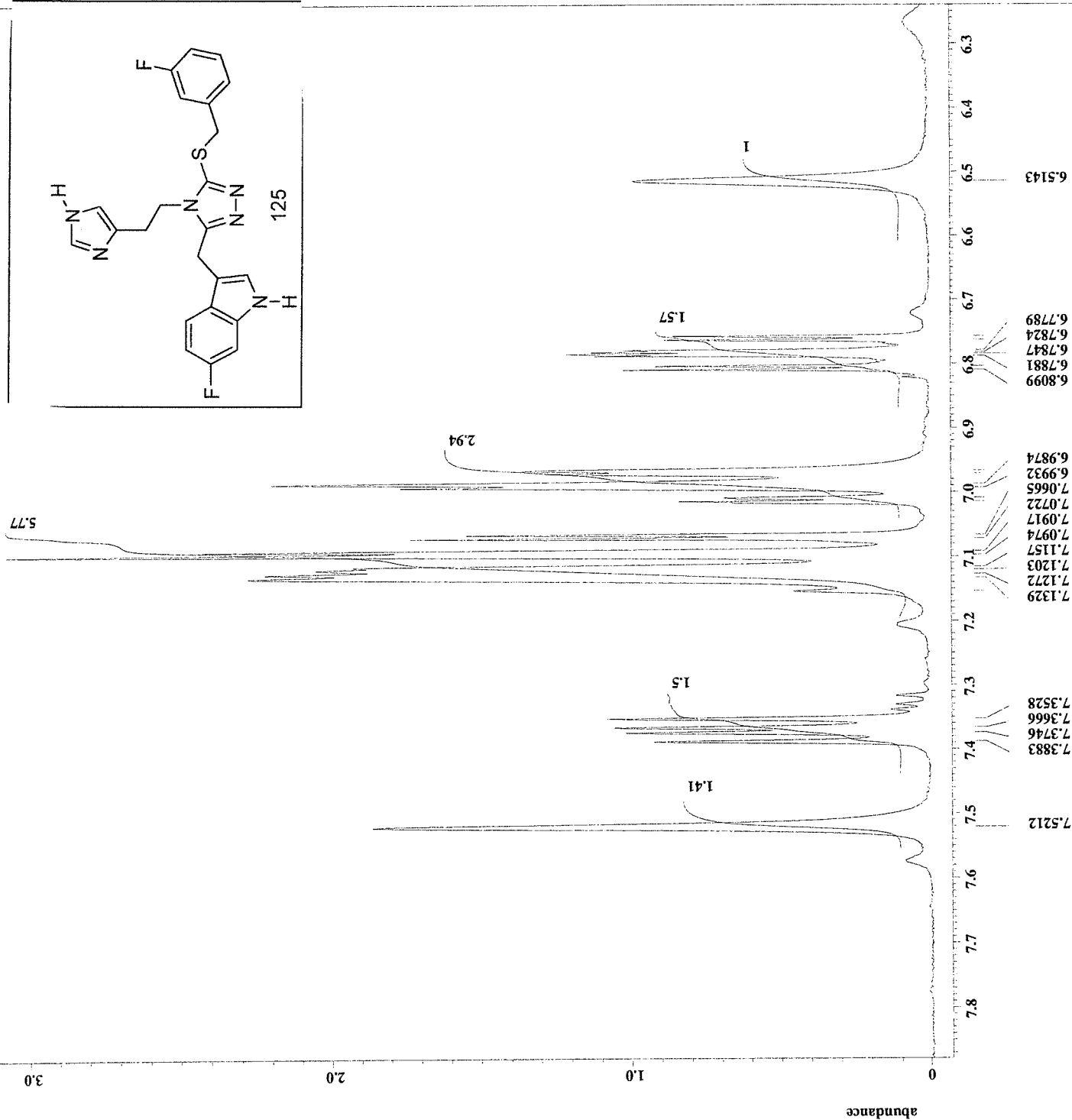
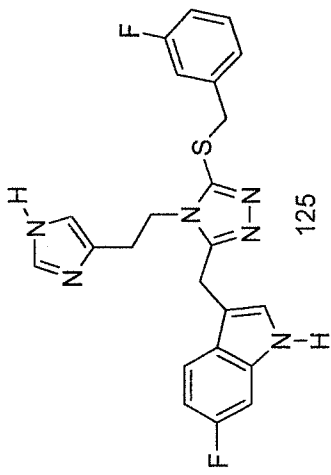
= LG-I-67-1-6.jdf
= mcridex
= single_pulse.ex2
= S#587616
= DMSO-D6
= 23-SEP-2019 14:38:20
= 6-MAY-2024 09:44:29
= 6-MAY-2024 09:44:38
= single_pulse
= 1D_COMPLEX
= 13107
= 1H
= [ppm]
= X
= ECS 400
= JNM-ECS400
= 9.389766[T] (400[MHz])
= 2.18365952[s]
= 1H
= 399.78219838 [MHz]
= 5[ppm]
= 16384
= 1
= 0.45794685 [Hz]
= 7.5030012 [kHz]
= 1H
= 399.78219838 [MHz]
= 5[ppm]
= 1H
= 399.78219838 [MHz]
= 5[ppm]
= TRUE
= 1
= 8
= 13.581 [us]
= 2.18365952[s]
= 45 [deg]
= 6[d8]
= 6.7905 [us]
= Off
= Off
= FALSE
= Dante_preset
= Initial_wait
= 1[s]
= 50
= Relaxation_delay
= 5[s]
= Repetition_time
= 7.18365952[s]
= Temp_get
= 19.8 [dC]

```

```

Filename
Author
Experiment
Sample_id
Solvent
Creation_time
Revision_time
Current_time
Comment
Data_format
Dim_size
Dim_title
Dim_units
Dimensions
Site
Spectrometer
Field_strength
X_acq_duration
X_domain
X_freq
X_offset
X_points
X_prescans
X_resolution
X_sweep
Irr_domain
Irr_freq
Irr_offset
Tri_domain
Tri_freq
Tri_offset
Clipped
Mod_return
Scans
Total_scans
X_90_width
X_acq_time
X_angle
X_atn
X_pulse
Irr_mode
Tri_mode
Dante_preset
Initial_wait
Recvr_gain
Relaxation_delay
Repetition_time
Temp_get

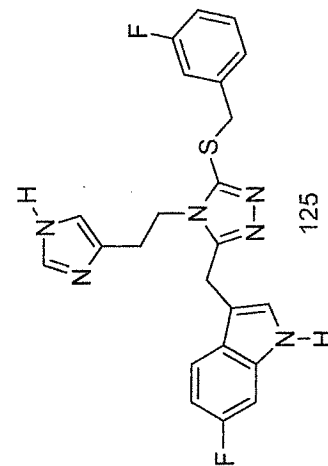
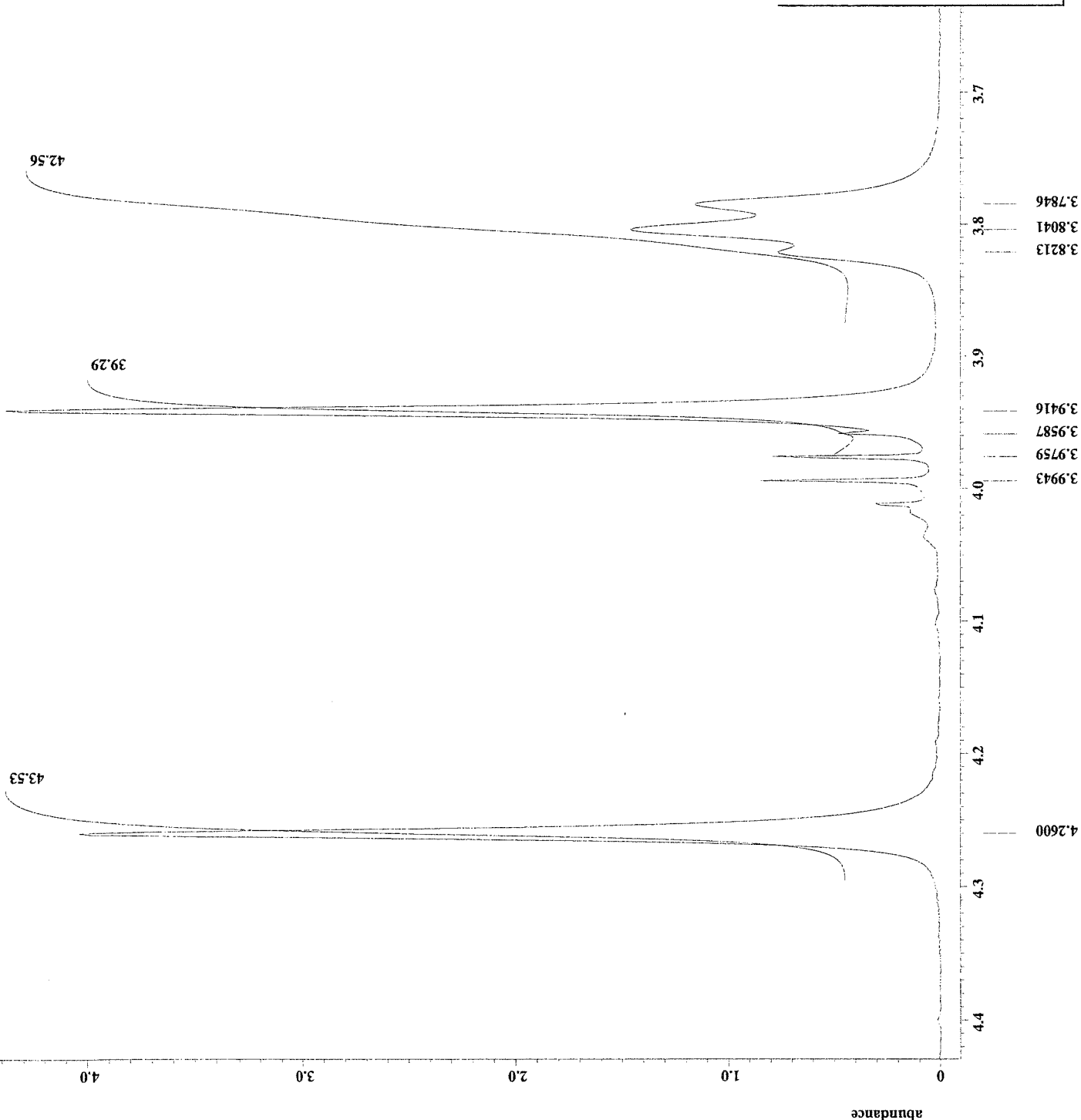
```



X : parts per Million : 1H



File name = LG-I-67-1-3.jdf
Author = mcrider
Experiment = single_pulse.ex2
Sample_id = S#587616
Solvent = DMSO-D6
Creation_time = 23-SEP-2019 14:38:20
Revision_time = 6-MAY-2024 09:40:26
Current_time = 6-MAY-2024 09:40:34
Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685[Hz]
X_sweep = 7.5030012[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = TRUE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 13.581[us]
X_acq_time = 2.18365952[s]
X_angle = 45[deg]
X_atn = 6[db]
X_pulse = 6.7905[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]



X : parts per Million : 1H

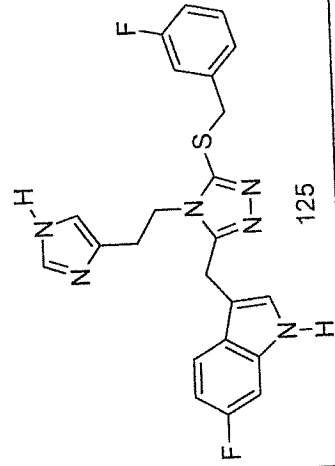
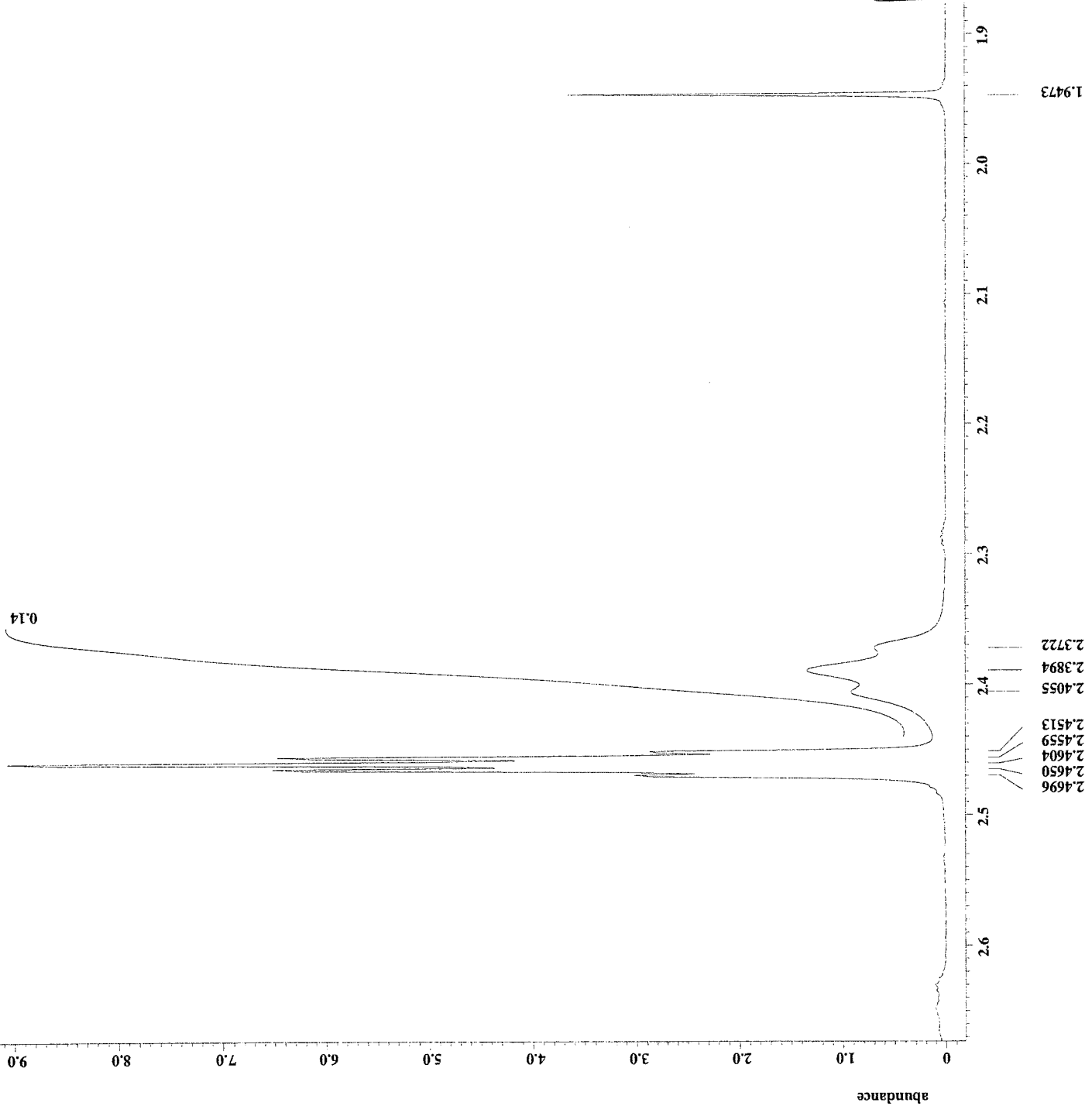


File = LG-I-67-1-5.jdf
Author = mcrider
Experiment = single_pulse.ex2
Sample_id = S#587616
Solvent = DMSO-D6
Creation_time = 23-SEP-2019 14:38:20
Revision_time = 6-MAY-2024 03:42:22
Current_time = 6-MAY-2024 03:42:28

Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400

Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685[Hz]
X_sweep = 7.5030012[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = TRUE
Mod_return = 1
Scans = 8
Total_scans = 8

X_90_width = 13.581[us]
X_acq_time = 2.18365952[s]
X_angle = 45[deg]
X_atn = 6[db]
X_pulse = 6.7905[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 50
Relaxation_delay = 5[s]
Repetition_time = 7.18365952[s]
Temp_get = 19.8[dc]



X : parts per Million : 1H



```

= 6F indole mCH3 detrit
= mcrider
= single_pulse.ex2
= S#531596
= DMSO-D6
= 14-APR-2019 13:13:52
= 7-MAY-2024 10:30:20
= 7-MAY-2024 10:30:39
= single_pulse
= 1D COMPLEX
= 13107
= 1H
= [ppm]
= X
= ECS 400
= JNM-ECS400

```

```

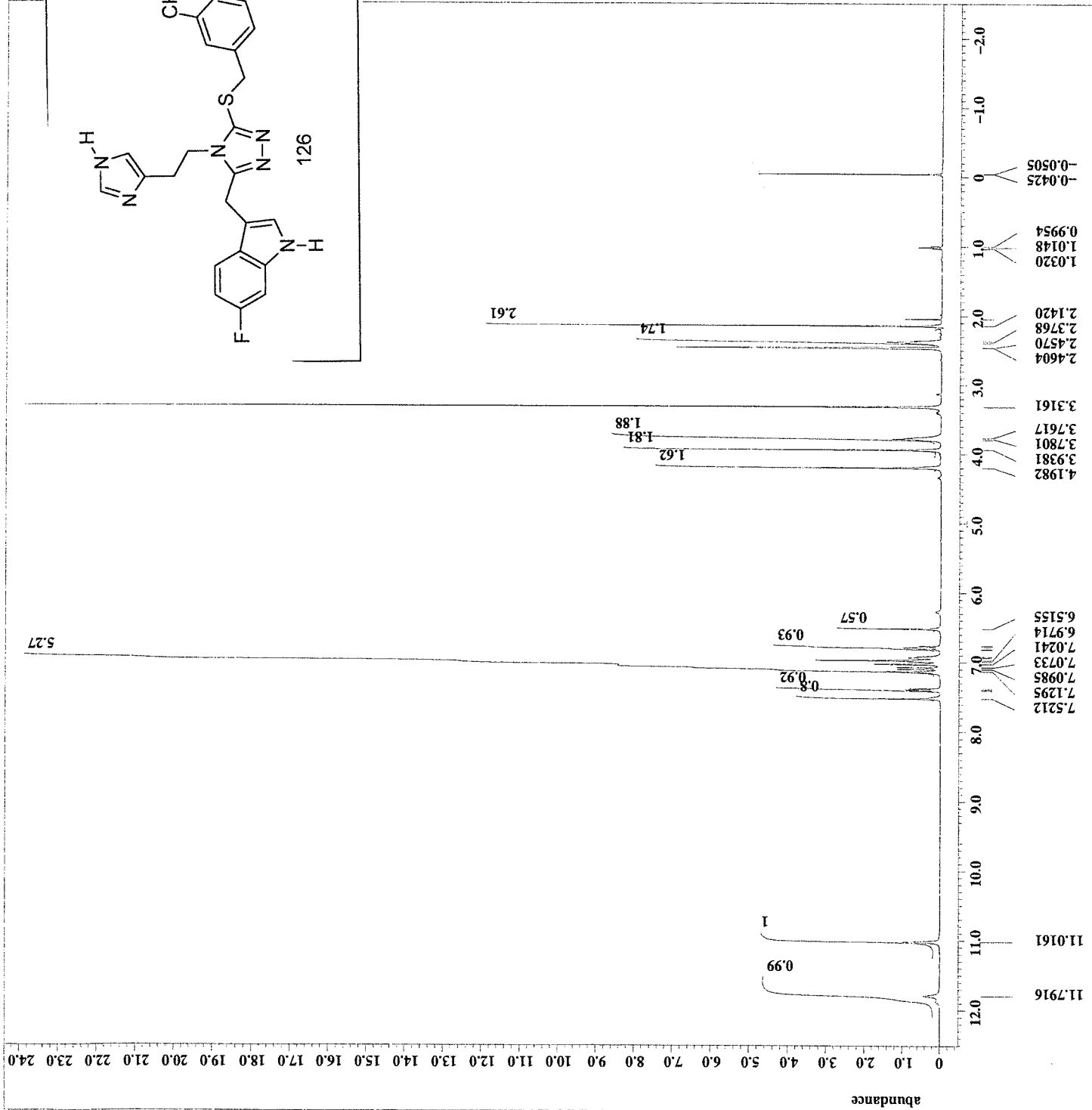
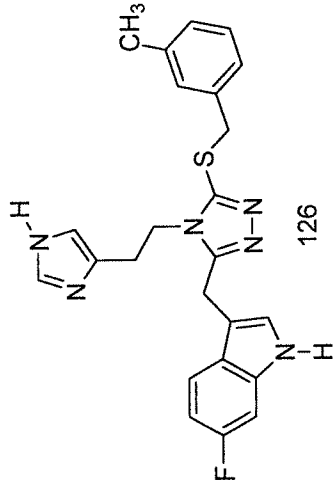
lename
thor
periment
pfile_id
lvent
sation_time
rison_time
rent_time
ment
a_format
l_size
l_title
l_units
nsions
e
spectrumeter

```

```

Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838 [MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685 [Hz]
X_sweep = 7.5030012 [KHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838 [MHz]
Tri_offset = 5[ppm]
Clipped = TRUE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 11.365[us]
X_acq_time = 2.18365952[s]
X_angle = 45[deg]
X_atn = 6[dB]
X_pulse = 5.6825[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 50
Relaxation_delay = 5[s]
Repetition_time = 7.18365952[s]
Temp_get = 19.5[dc]

```



X : parts per Million : 1H

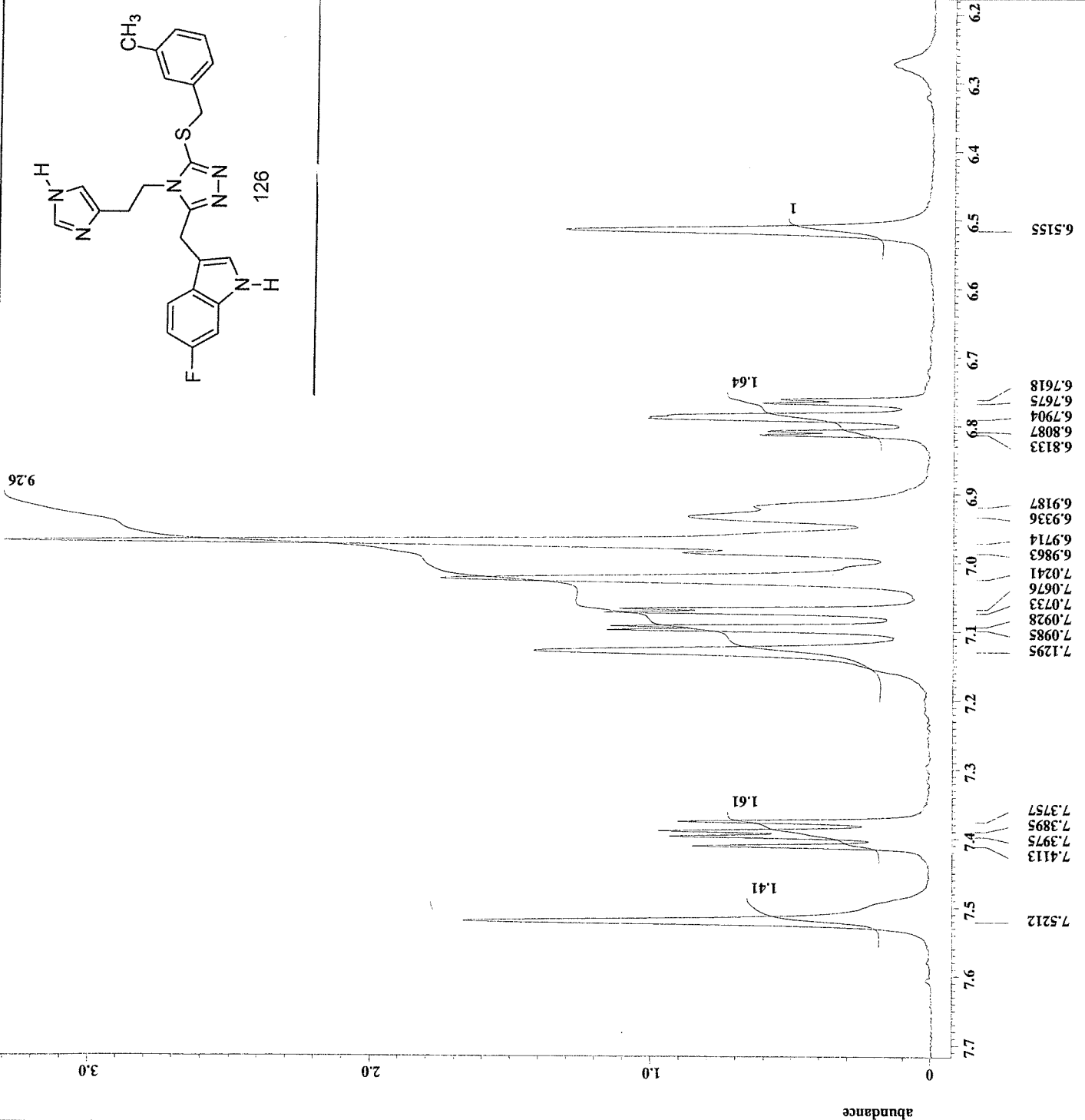
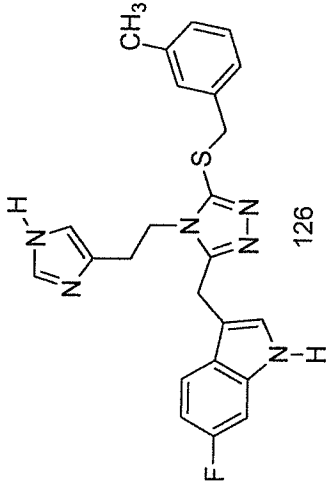


Filename = 6F indole mCH3 detrit
Author = mcridder
Experiment = single_pulse.ex2
Sample_id = S#531596
Solvent = DMSO-D6
Creation_time = 14-APR-2019 13:13:52
Revision_time = 7-MAY-2024 10:28:26
Current_time = 7-MAY-2024 10:28:36

Comment = single_pulse
Data_format = ID COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400

Field_strength = 9.389766 [T] (400 [MHz])
X_acq_duration = 2.18365952 [s]
X_domain = 1H
X_freq = 399.78219838 [MHz]
X_offset = 5 [ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685 [Hz]
X_sweep = 7.5030012 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5 [ppm]
Tri_domain = 1H
Tri_freq = 399.78219838 [MHz]
Tri_offset = 5 [ppm]
Clipped = TRUE
Mod_return = 1
Scans = 8
Total_scans = 8

X_90_width = 11.365 [us]
X_acq_time = 2.18365952 [s]
X_angle = 45 [deg]
X_atn = 6 [dB]
X_pulse = 5.6825 [us]
Irr_mode = Off
Tri_mode = Off
Dante_preset = FALSE
Initial_wait = 1 [s]
Recvr_gain = 50
Relaxation_delay = 5 [s]
Repetition_time = 7.18365952 [s]
Temp_get = 19.5 [dC]



X : parts per Million : 1H

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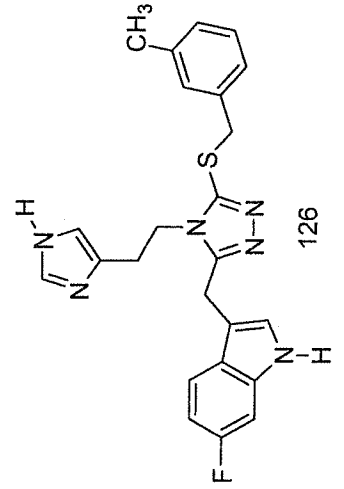
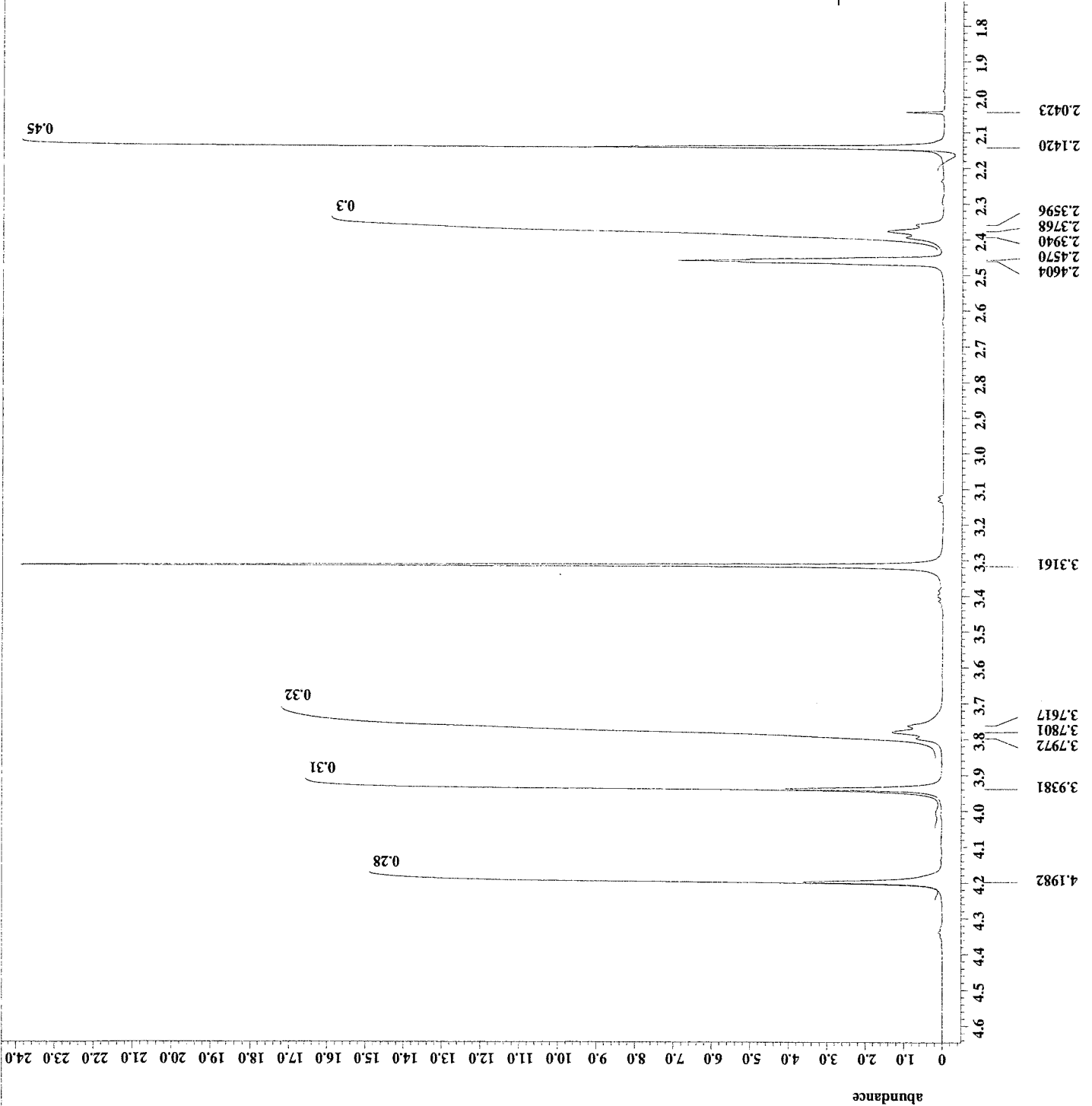
Filename = 6F indole mCH3 detrit
Author = mcrider
Experiment = single_pulse.ex2
Sample_id = S#531596
Solvent = DMSO-D6
Creation_time = 14-APR-2019 13:13:52
Revision_time = 7-MAY-2024 10:26:39
Current_time = 7-MAY-2024 10:26:52

Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400

Field_strength = 9.389766[T] (400[Mhz])
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838 [MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685 [Hz]
X_sweep = 7.5030012 [kHz]
Irr_domain = 1H
Irr_freq = 399.78219838 [MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838 [MHz]
Tri_offset = 5[ppm]
Clipped = TRUE
Mod_return = 1
Scans = 8
Total_scans = 8

X_90_width = 11.365[us]
X_acq_time = 2.18365952[s]
X_angle = 45[deg]
X_atn = 6[db]
X_pulse = 5.6825[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 50
Relaxation_delay = 5[s]
Repetition_time = 7.18365952[s]

NAME: 6F
P1: 10.5[sec]



X : parts per Million : 1H