

Supporting Information

for

Rapid regio- and multi-coupling reactivity of 2,3-dibromobenzofurans with atom-economic triarylbismuths under palladium catalysis

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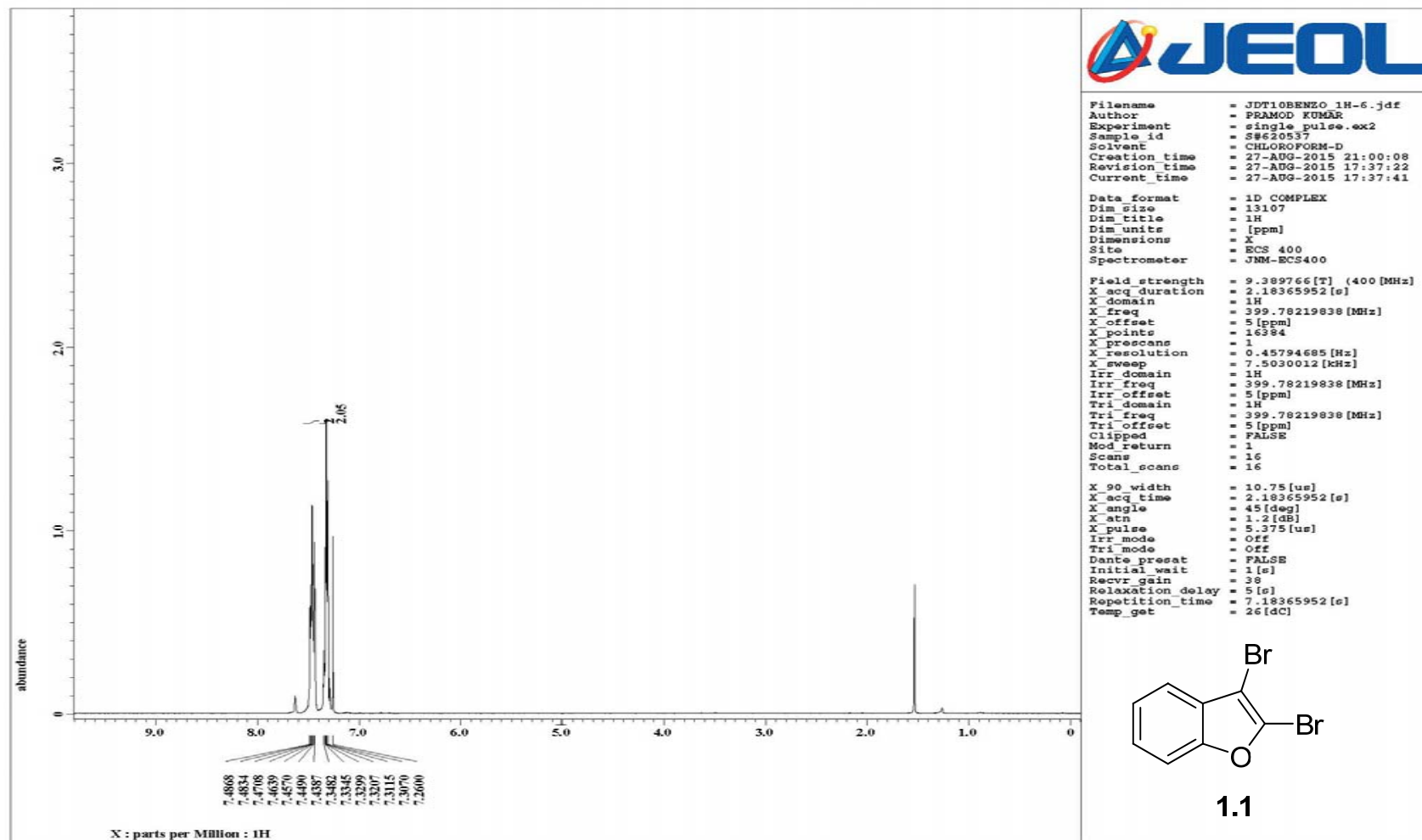
*Corresponding author

¹H, ¹³C NMR spectra of all compounds

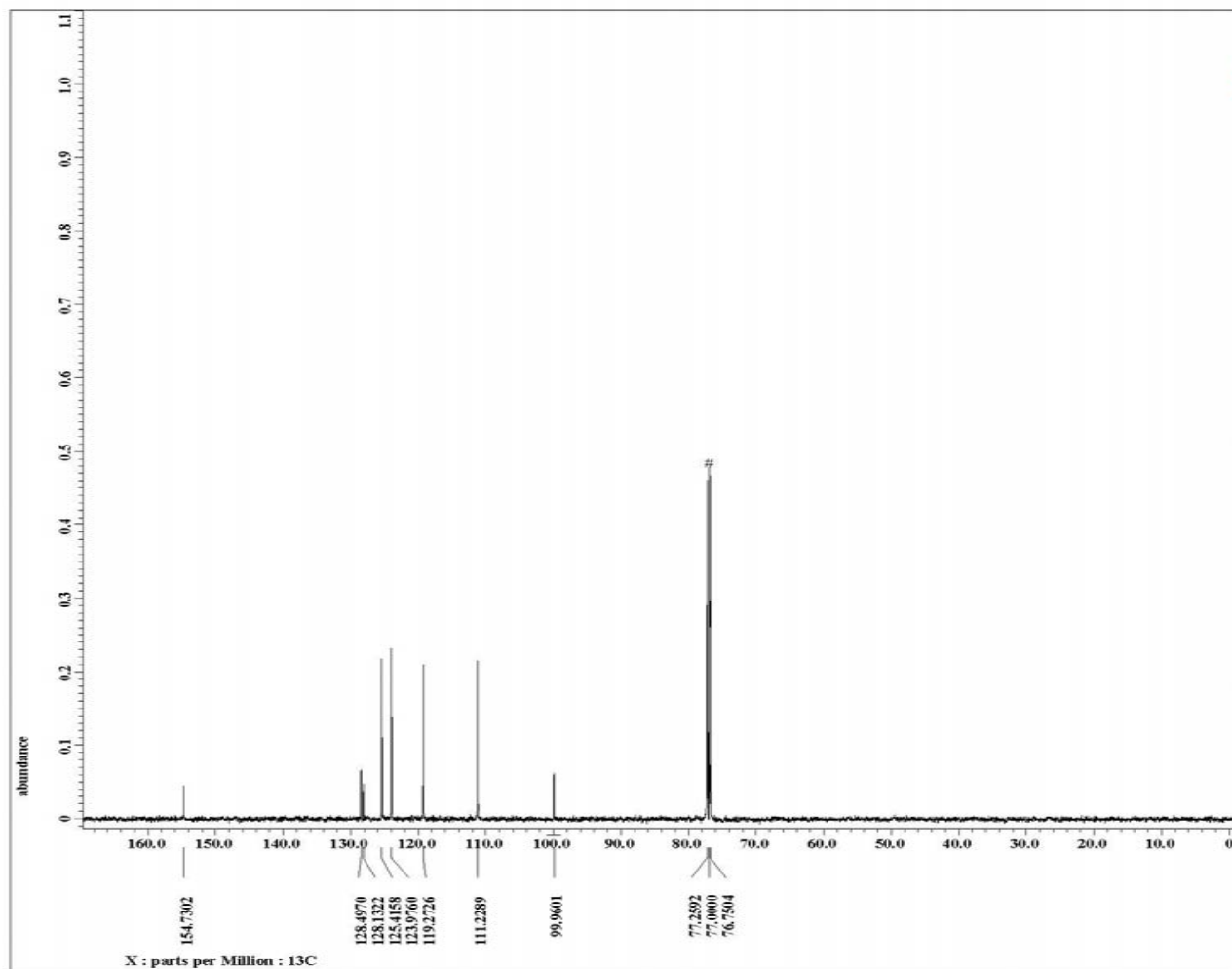
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1. ¹H, ¹³C Spectra of Compounds (1.1-1.6)



400 MHz ¹H NMR spectrum of compound **1.1**



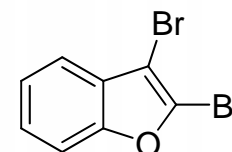
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Filename      = JDT461P_13C-6.jdf
Author       = N.Ahmed
Experiment   = single pulse dec
Sample id    = S8394501
Solvent      = CHLOROFORM-D
Creation time = 22-OCT-2012 10:01:50
Revision time = 27-AUG-2015 17:40:29
Current Time = 27-AUG-2015 17:42:13

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Dim size     = 26214
Dim title    = 13C
Dim units    = [ppm]
Dimensions   = X
Site         = ECX 500
Spectrometer = DELTA2_NMR

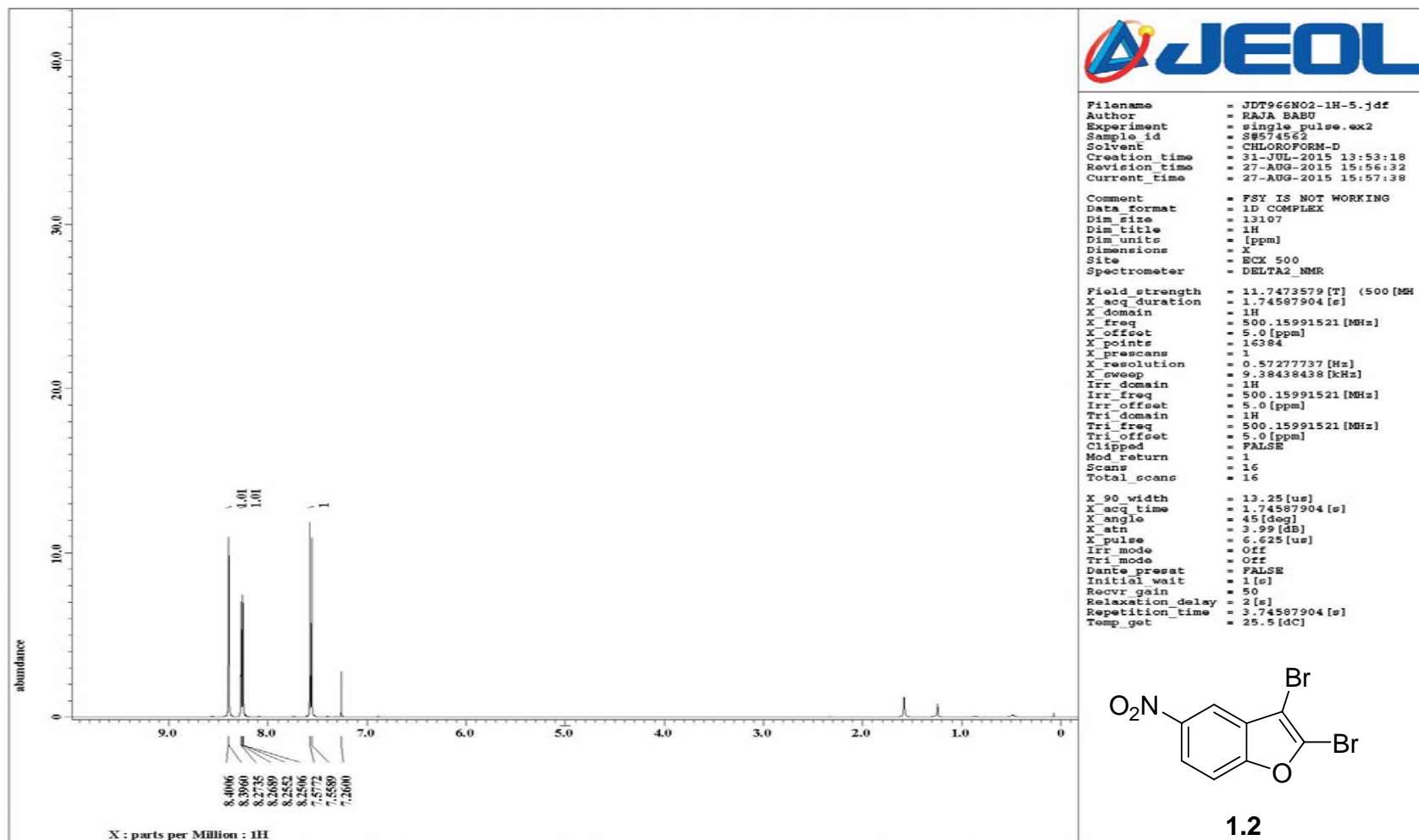
Field strength = 11.7473579 [T] (500 [MH]
X_acq duration = 0.82837504 [s]
X_domain       = 13C
X_freq         = 125.76529768 [MHz]
X_offset       = 100 [ppm]
X_points       = 22768
X_prescans     = 4
X_resolution   = 1.20718268 [Hz]
X_sweep        = 39.55696203 [kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521 [MHz]
Irr_offset     = 5.0 [ppm]
Clipped        = PALSE
Mod return     = 1
Scans          = 1000
Total_scans    = 1000

X_90 width     = 9.62 [us]
X_acq time     = 0.82837504 [s]
X_angle        = 30 [deg]
X_atn          = 7.1 [dB]
X_pulse        = 3.20666667 [us]
Irr_atn dec    = 19.5 [dB]
Irr_atn noe    = 21.5 [dB]
Irr_noise      = WALTZ
Decoupling     = TRUE
Initial wait   = 1 [s]
Noe            = TRUE
Noe time       = 1 [s]
Recvr gain     = 58
Relaxation delay = 1 [s]
Repetition time = 1.82837504 [s]
Temp_get       = 20.9 [dC]
  
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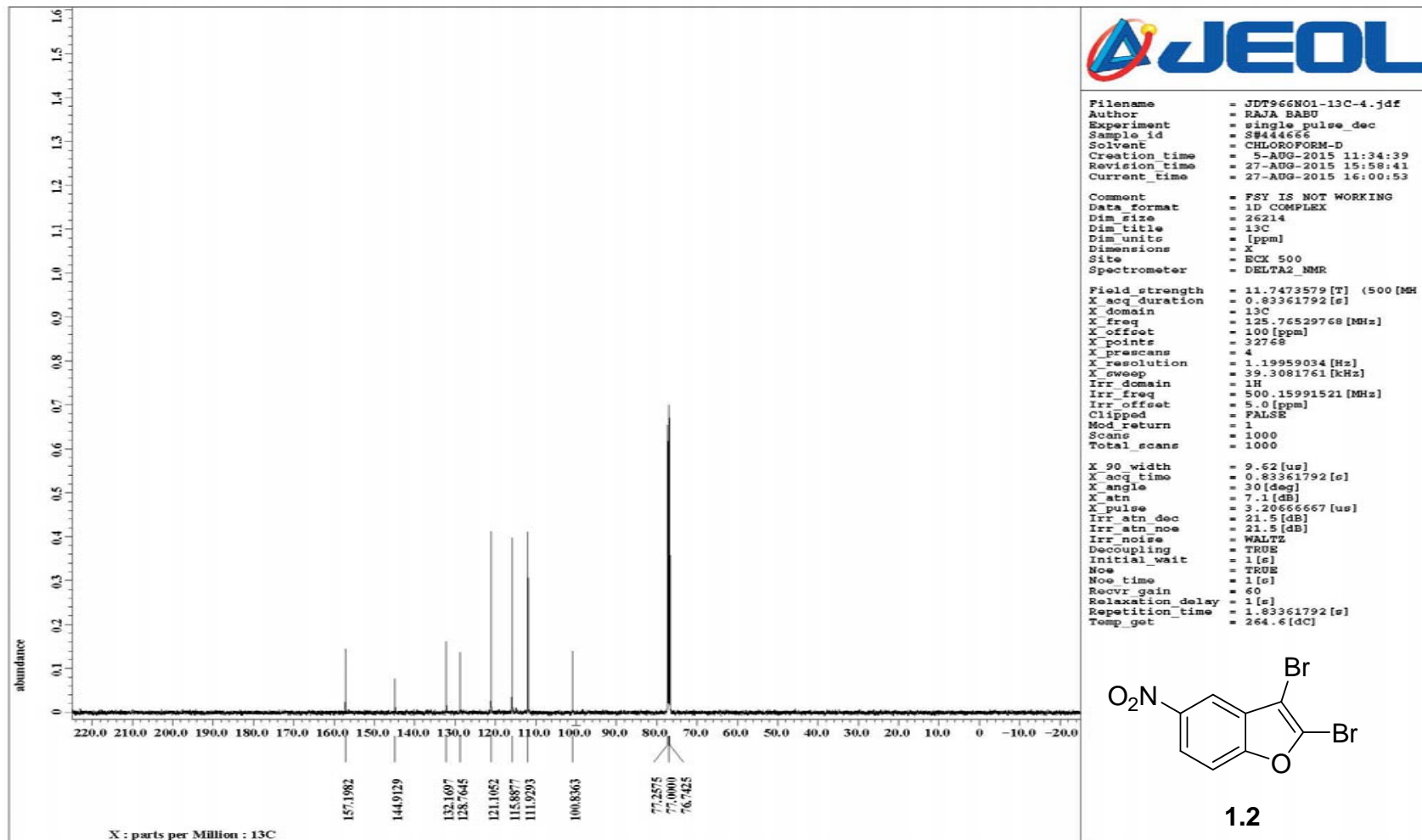


1.1

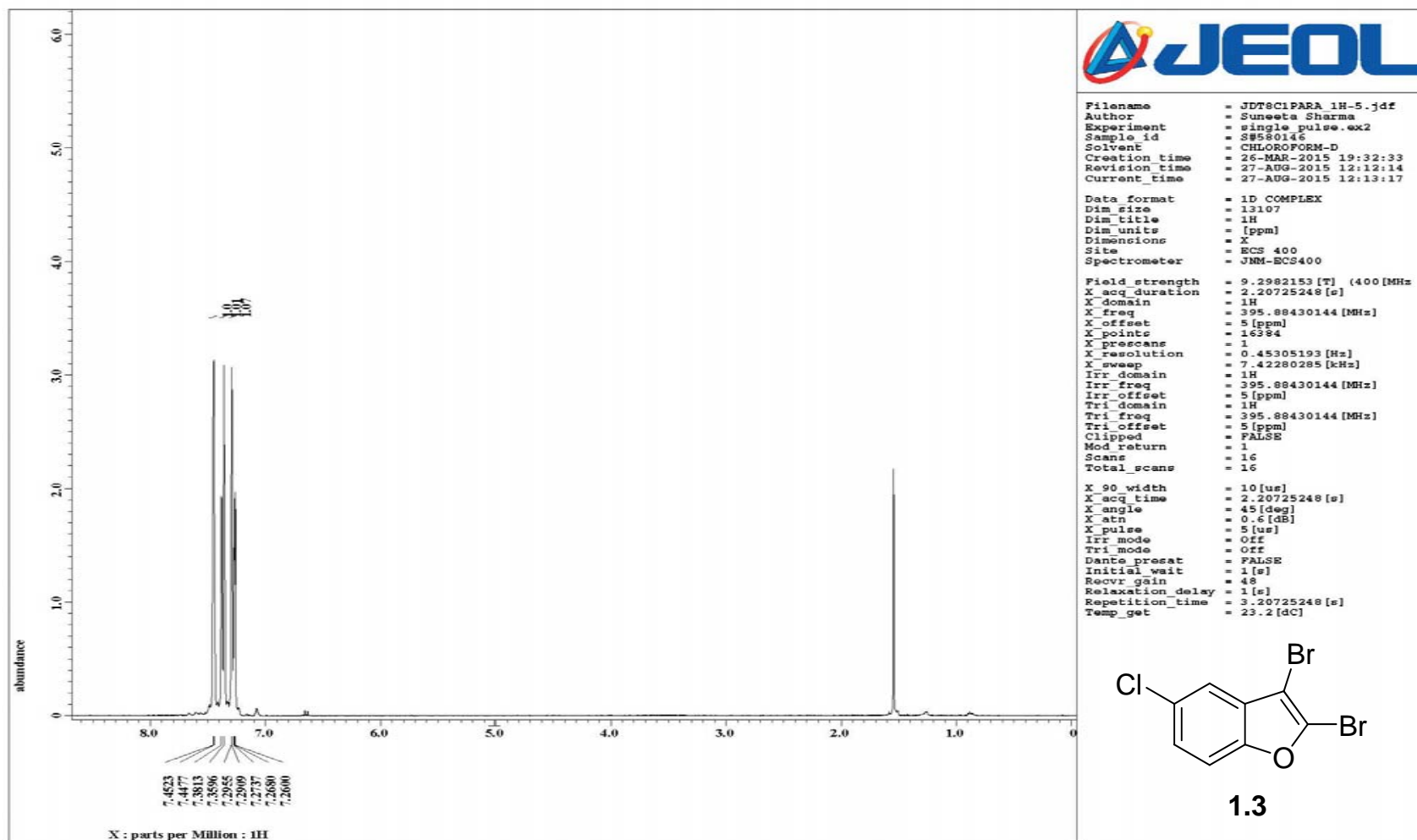
125 MHz ^{13}C NMR spectrum of compound 1.1



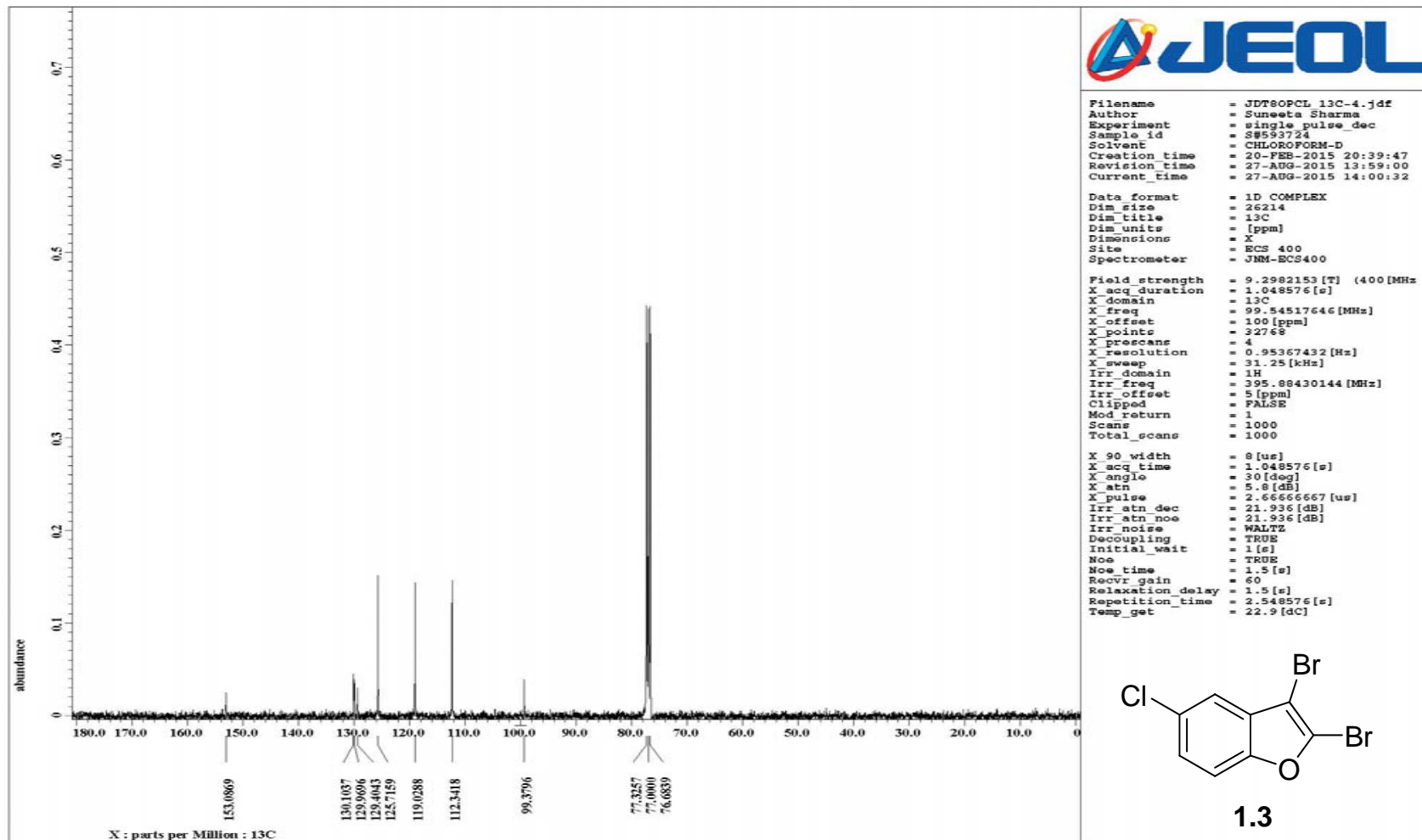
500 MHz ^1H NMR spectrum of compound **1.2**



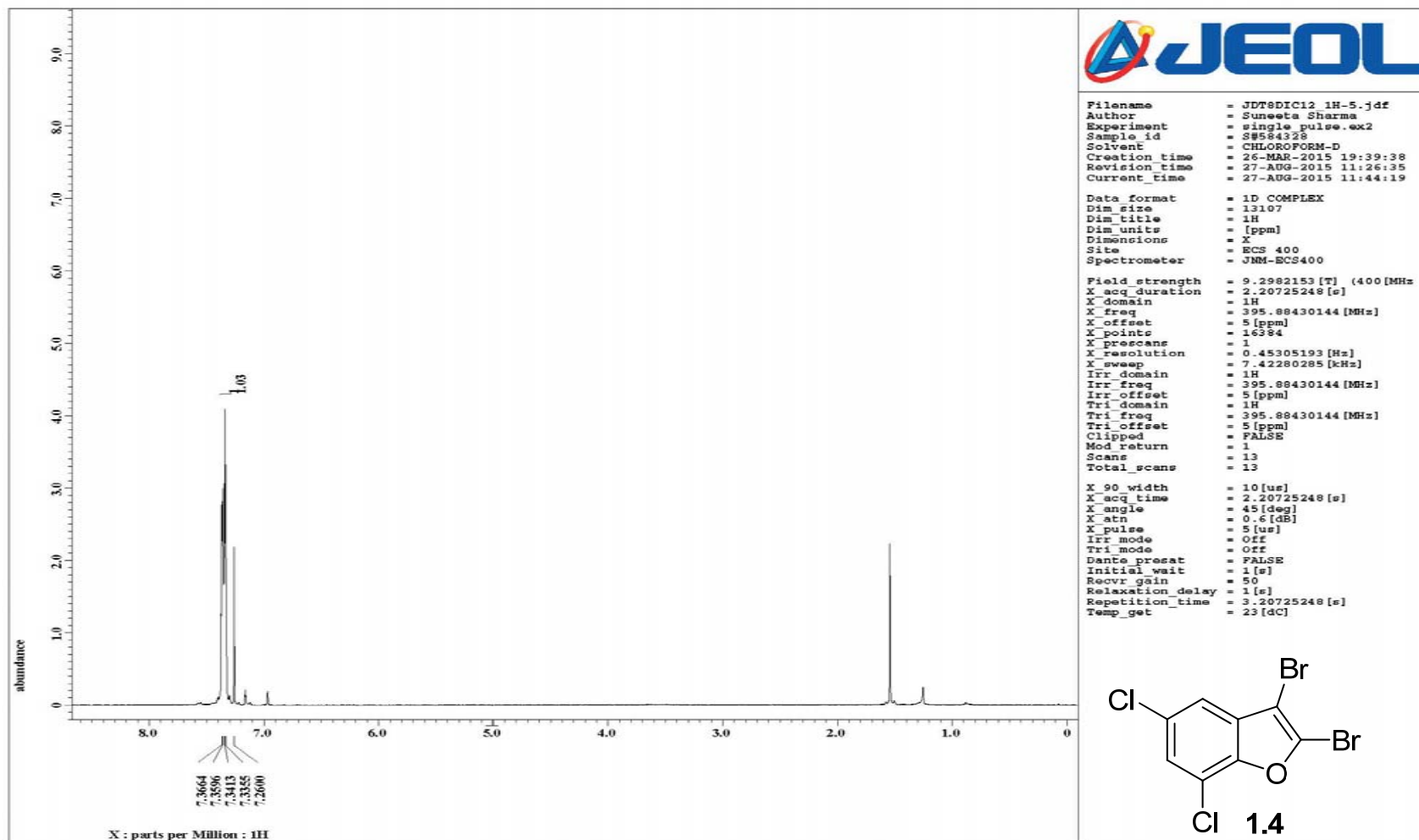
125 MHz ^{13}C NMR spectrum of compound 1.2



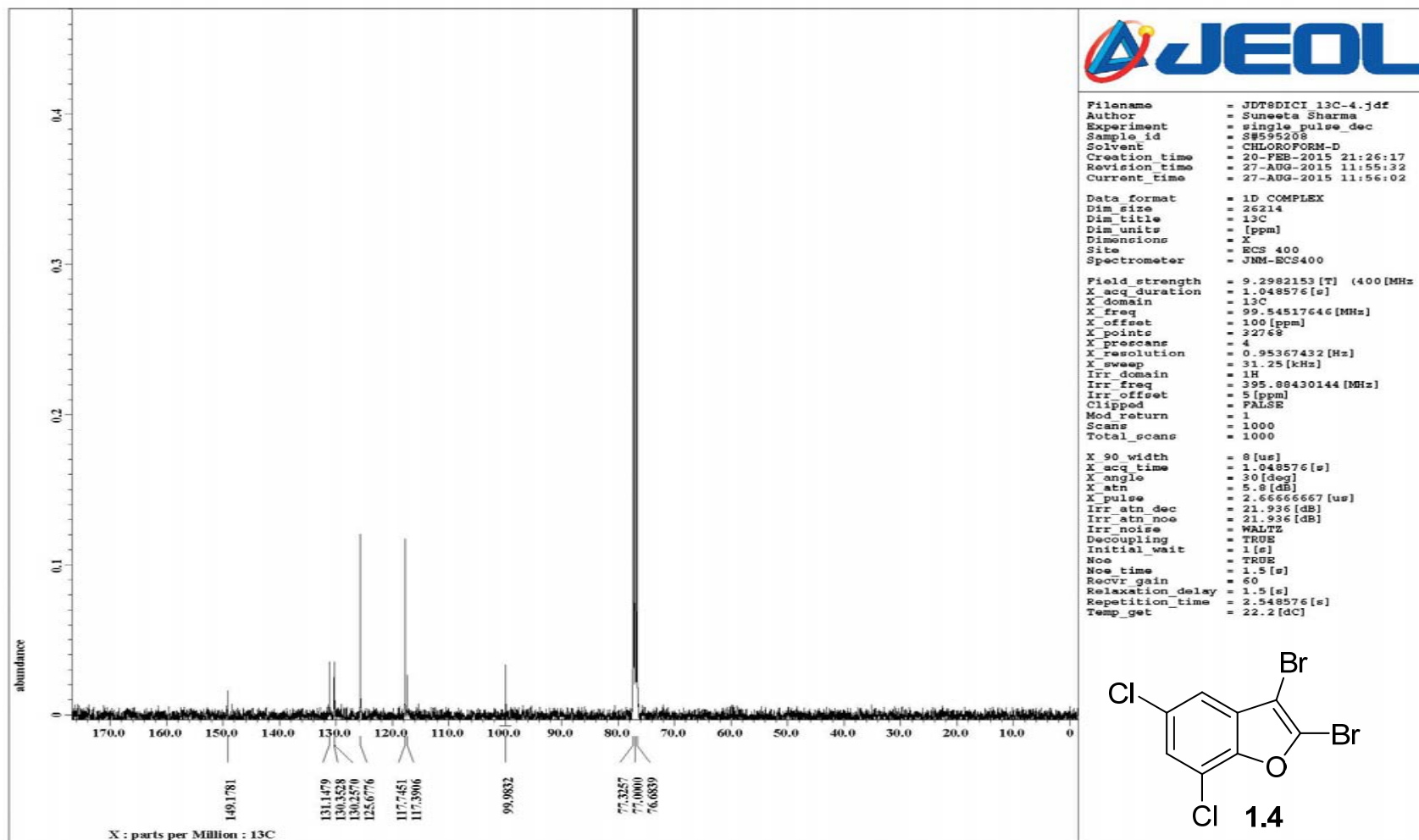
400 MHz ^1H NMR spectrum of compound **1.3**



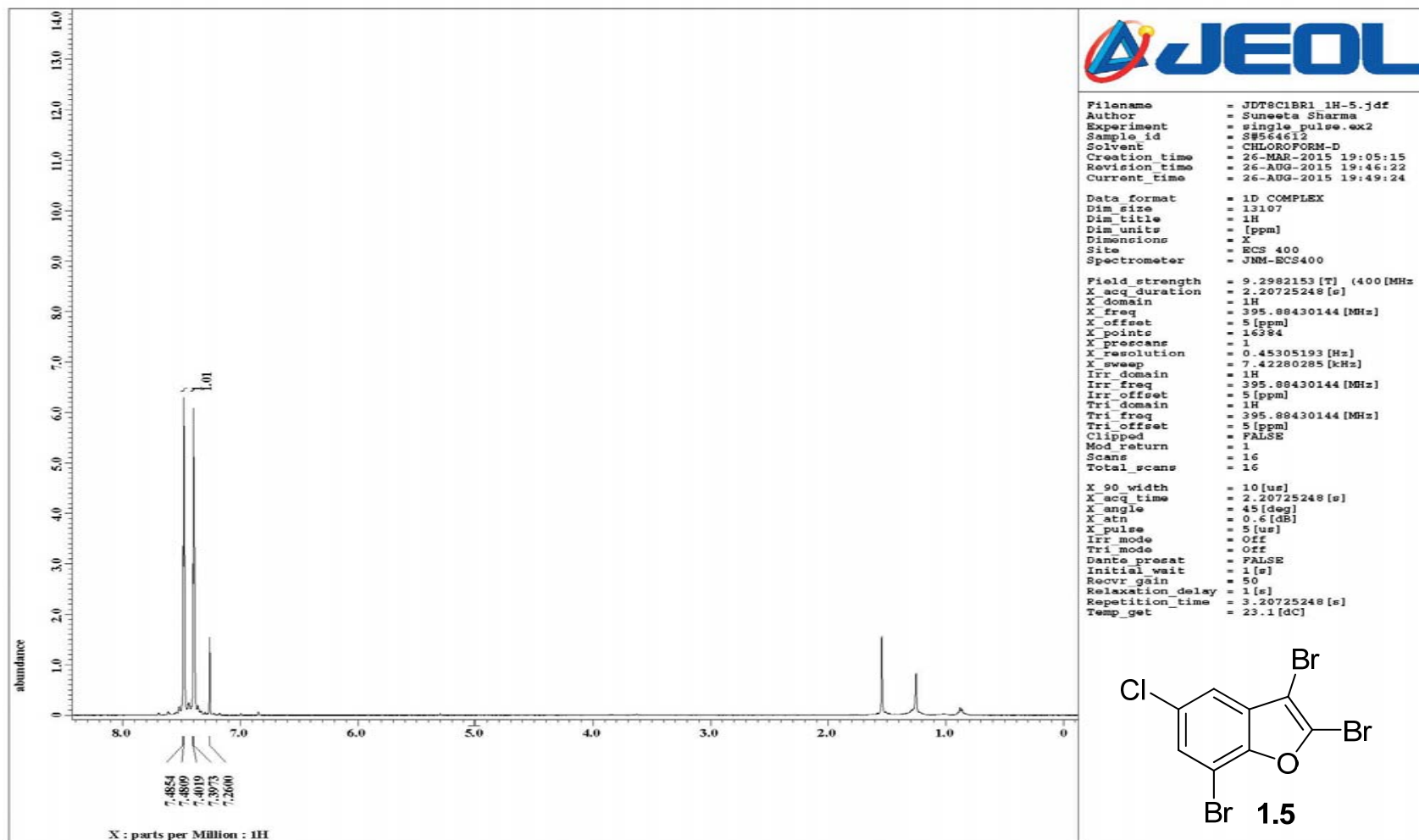
100 MHz ^{13}C NMR spectrum of compound 1.3



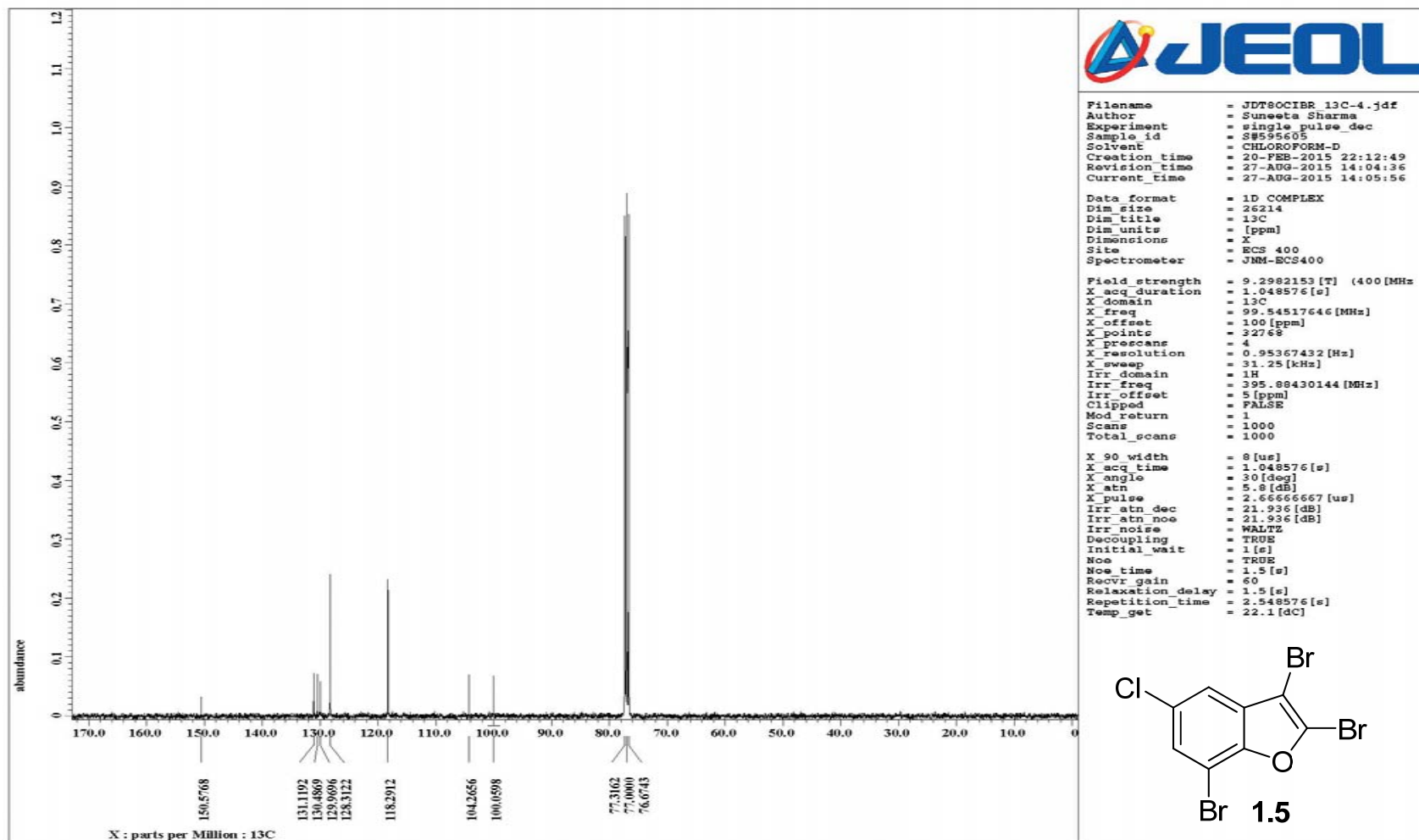
400 MHz ^1H NMR spectrum of compound **1.4**



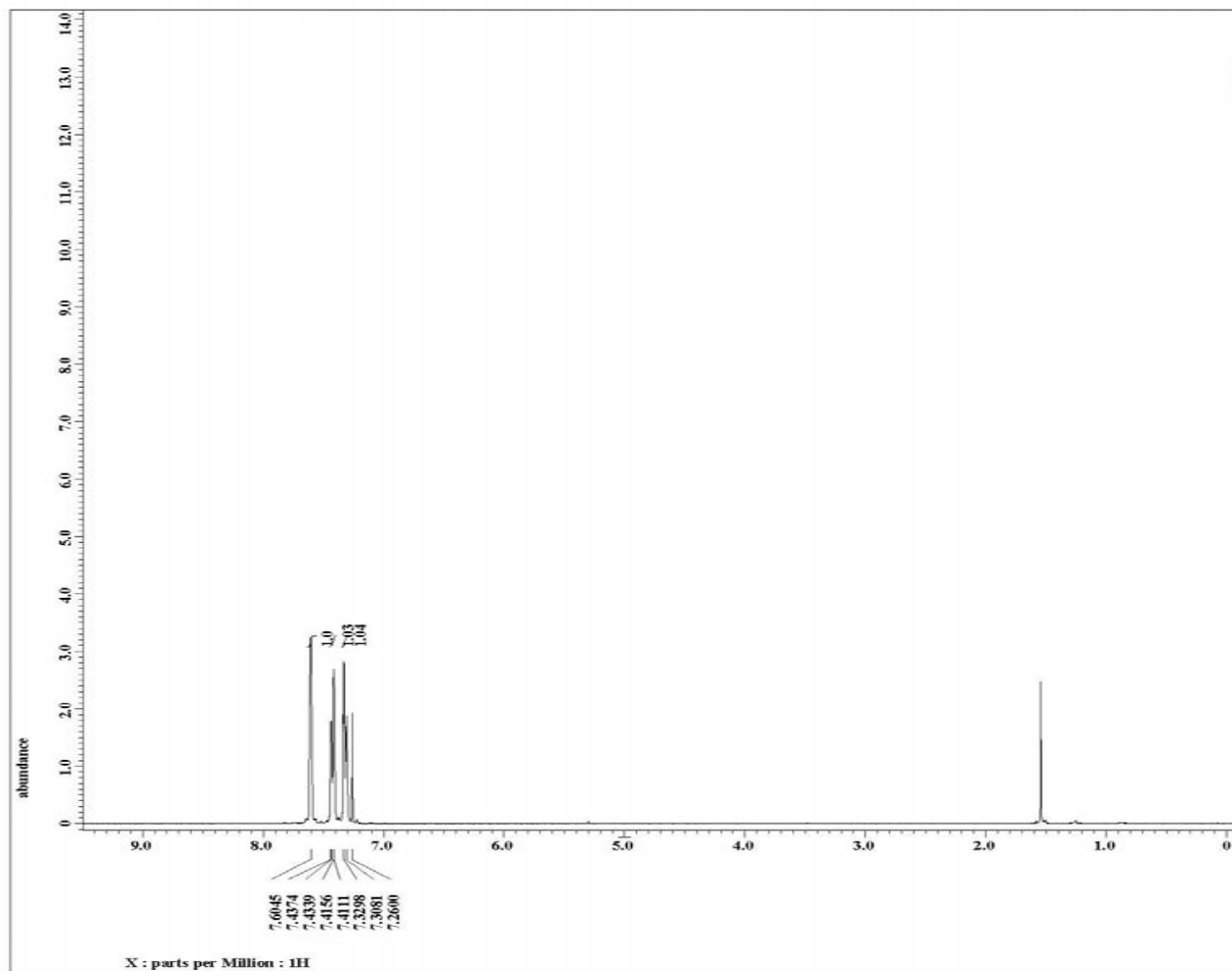
100 MHz ^{13}C NMR spectrum of compound **1.4**



400 MHz ^1H NMR spectrum of compound **1.5**



100 MHz ^{13}C NMR spectrum of compound 1.5



```

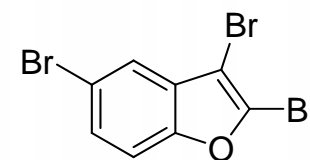
Filename      = JDTSTRBRA 1H-4.jdf
Author       = Suneeta Sharma
Experiment   = single pulse.ex2
Sample id    = S#576335
Solvent      = CHLOROFORM-D
Creation time = 26-MAR-2015 19:26:08
Revision time = 27-AUG-2015 16:36:31
Current Time = 27-AUG-2015 16:37:09

Data format   = 1D COMPLEX
Dim size      = 13107
Dim title     = 1H
Dim units     = [ppm]
Dimensions    = X
Site          = ECS 400
Spectrometer  = JNM-ECS400

Field strength = 9.2982153 [T] (400 [MHz])
X_acq duration = 2.20725248 [s]
X_domain      = 1H
X_freq        = 395.88430144 [MHz]
X_offset      = 5 [ppm]
X_points      = 16384
X_prescans    = 1
X_resolution  = 0.45305193 [Hz]
X_sweep       = 7.42280285 [kHz]
Irr_domain    = 1H
Irr_freq      = 395.88430144 [MHz]
Irr_offset    = 5 [ppm]
Tri_domain    = 1H
Tri_freq      = 395.88430144 [MHz]
Tri_offset    = 5 [ppm]
Clipped       = FALSE
Mod return    = 1
Scans         = 16
Total scans   = 16

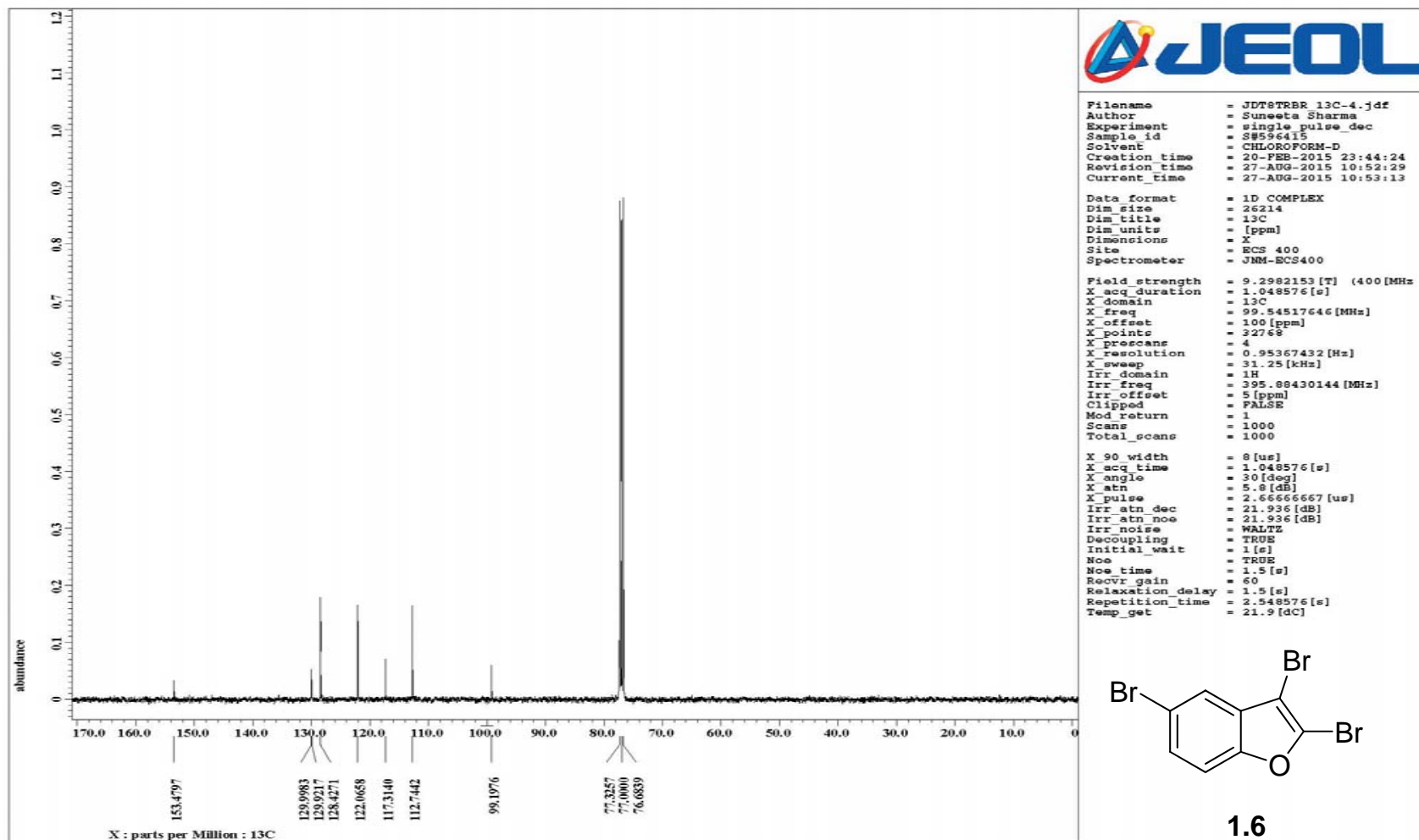
X_90 width    = 10 [us]
X_acq time    = 2.20725248 [s]
X_angle       = 45 [deg]
X_atn         = 0.6 [dB]
X_pulse       = 5 [us]
Irr_mode      = Off
Tri_mode      = Off
Dante preset  = FALSE
Initial wait  = 1 [s]
Recvr gain    = 50
Relaxation delay = 1 [s]
Repetition time = 3.20725248 [s]
Temp_get      = 23 [dC]

```



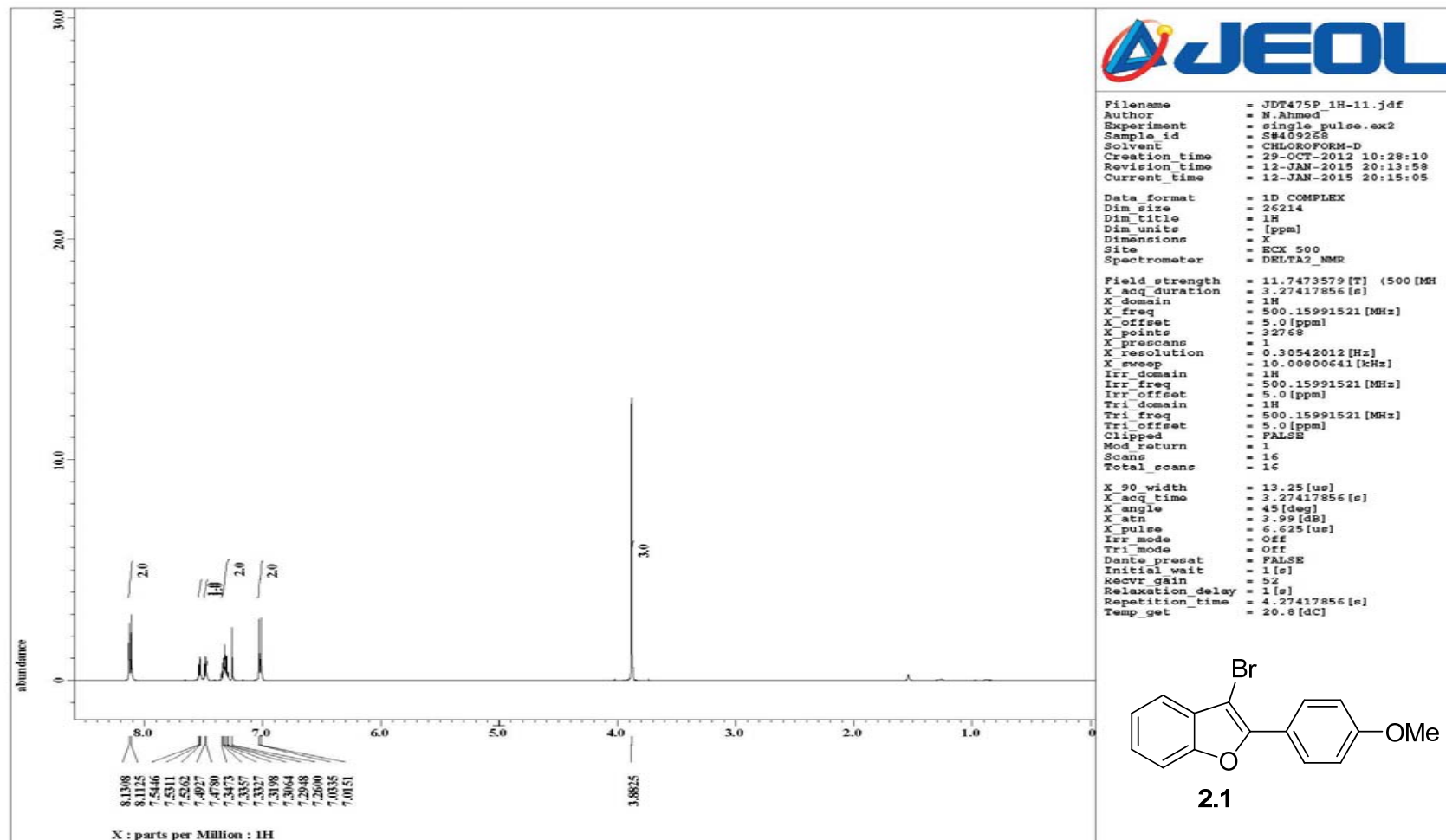
1.6

400 MHz ¹H NMR spectrum of compound **1.6**

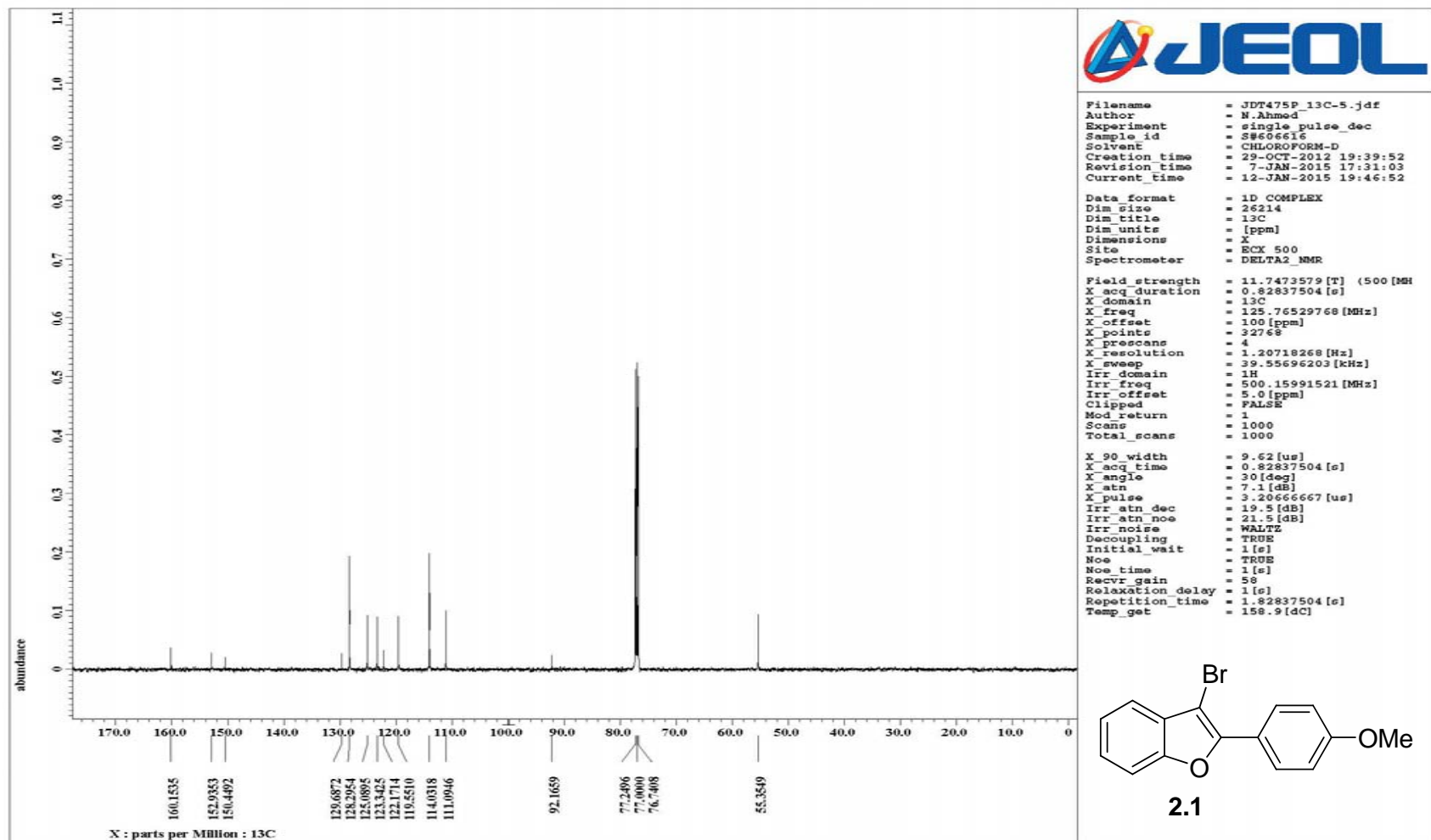


100 MHz ^{13}C NMR spectrum of compound **1.6**

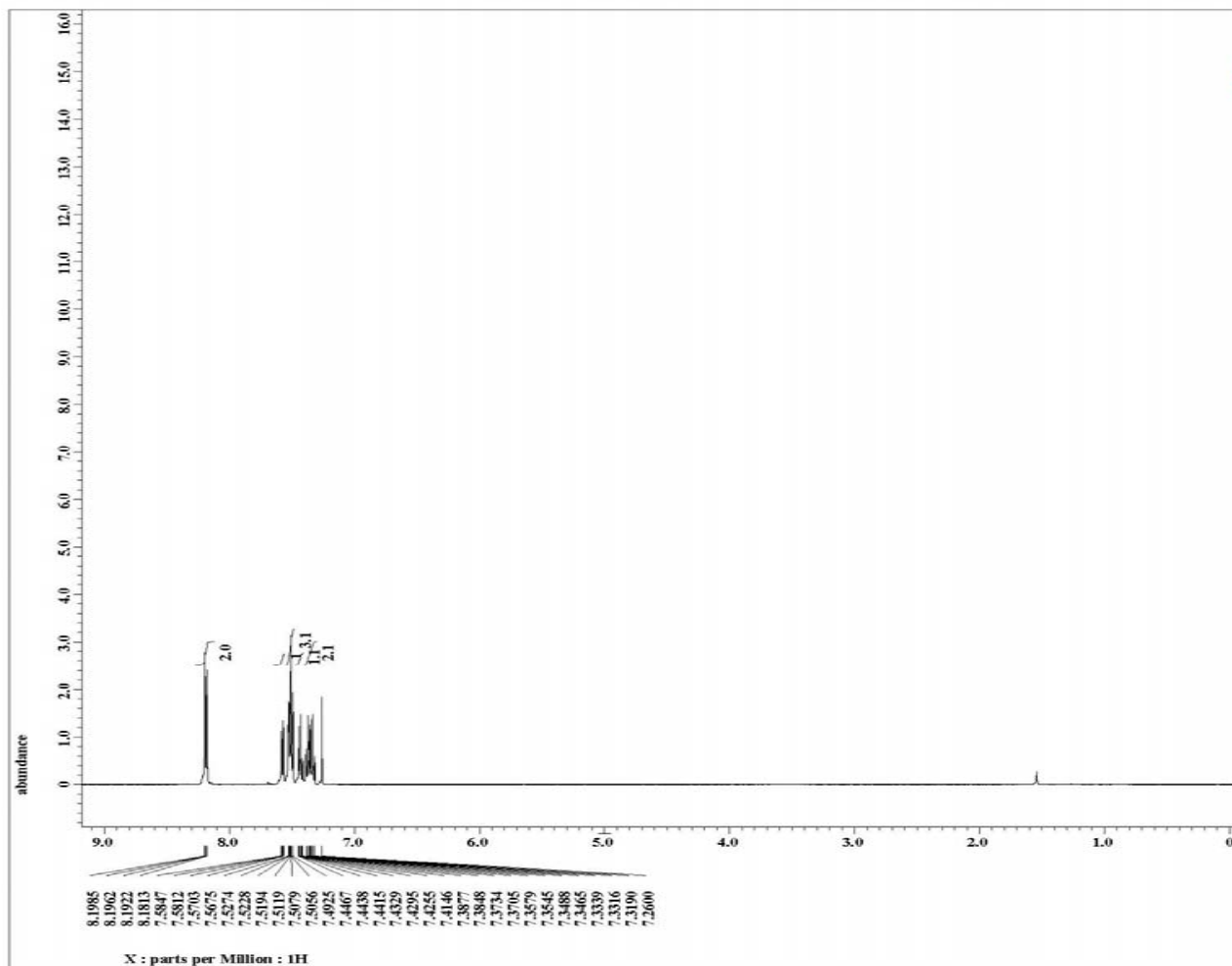
2. ^1H , ^{13}C Spectra of Compounds (2.1-2.27):



500 MHz ^1H NMR spectrum of compound **2.1**



125 MHz ^{13}C NMR spectrum of compound **2.1**



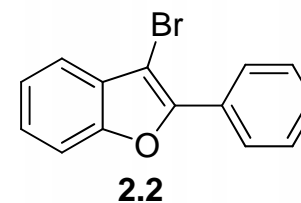
```

Filename      = JDT4112_1H-5.jdf
Author       = M.Ahmed
Experiment   = single pulse.ex2
Sample id    = S#423454
Solvent      = CHLOROFORM-D
Creation time = 20-DEC-2012 10:56:48
Revision time = 13-JAN-2015 17:45:53
Current Time  = 13-JAN-2015 17:46:31

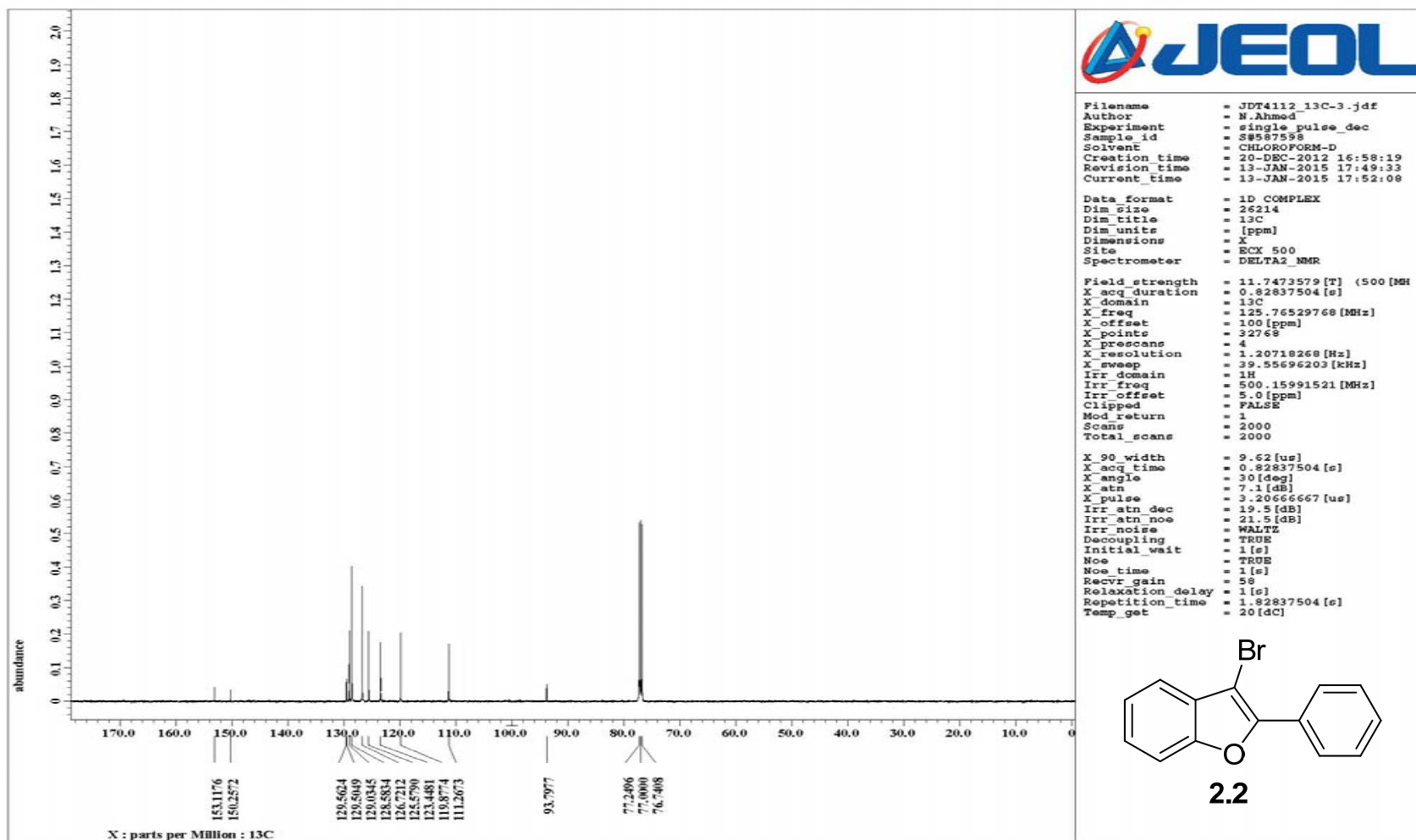
Data format  = 1D COMPLEX
Dim size     = 26214
Dim title    = 1H
Dim units    = [ppm]
Dimensions   = X
Site         = ECX 500
Spectrometer = DELTA2_NMR

Field strength = 11.7473579 [T] (500 [MH]
X_acq_duration = 3.49175808 [s]
X_domain       = 1H
X_freq         = 500.15991521 [MHz]
X_offset       = 5.0 [ppm]
X_points       = 32768
X_prescans     = 1
X_resolution   = 0.28638868 [Hz]
X_sweep        = 9.38438438 [kHz]
Irr_domain    = 1H
Irr_freq      = 500.15991521 [MHz]
Irr_offset     = 5.0 [ppm]
Tri_domain    = 1H
Tri_freq      = 500.15991521 [MHz]
Tri_offset    = 5.0 [ppm]
Clipped       = FALSE
Mod_return    = 1
Scans         = 16
Total_scans   = 16

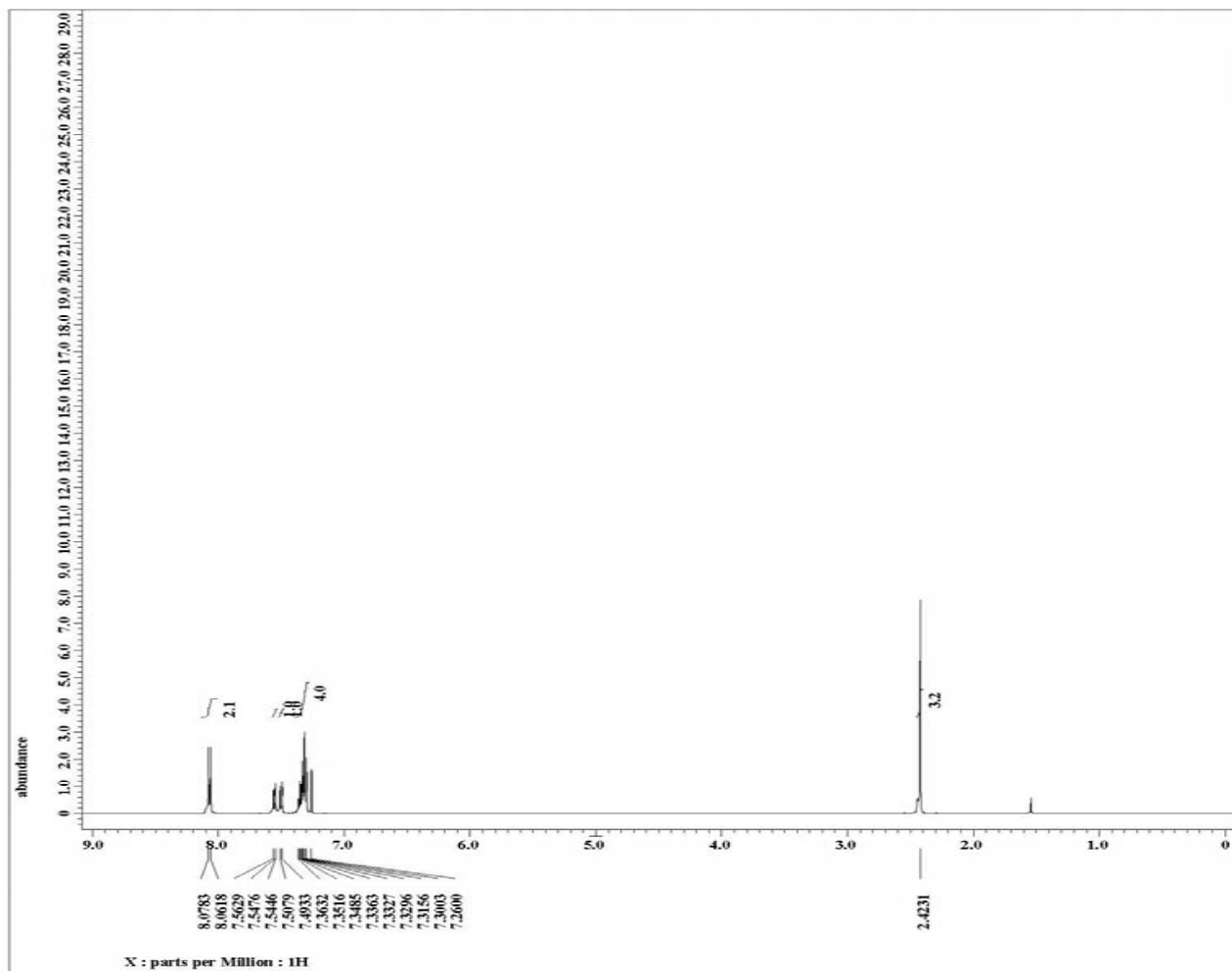
X_90_width    = 13.25 [us]
X_acq_time     = 3.49175808 [s]
X_angle        = 45 [deg]
X_atn          = 3.99 [dB]
X_pulse        = 6.625 [us]
Irr_mode       = Off
Dante_preset   = FALSE
Initial_wait   = 1 [s]
Recvr_gain     = 50
Relaxation_delay = 1 [s]
Repetition_time = 4.49175808 [s]
Temp_get       = 20.3 [dC]
  
```



500 MHz ^1H NMR spectrum compound **2.2**



125 MHz ^{13}C NMR spectrum of compound **2.2**



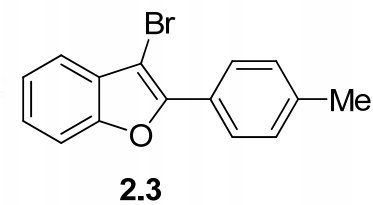
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Filename      = JDT4105P_1H-7.jdf
Author       = M.Ahmed
Experiment   = single pulse.ex2
Sample id    = S#529837
Solvent      = CHLOROFORM-D
Creation time = 21-NOV-2012 13:33:24
Revision time = 12-JAN-2015 19:58:48
Current time  = 12-JAN-2015 19:59:37

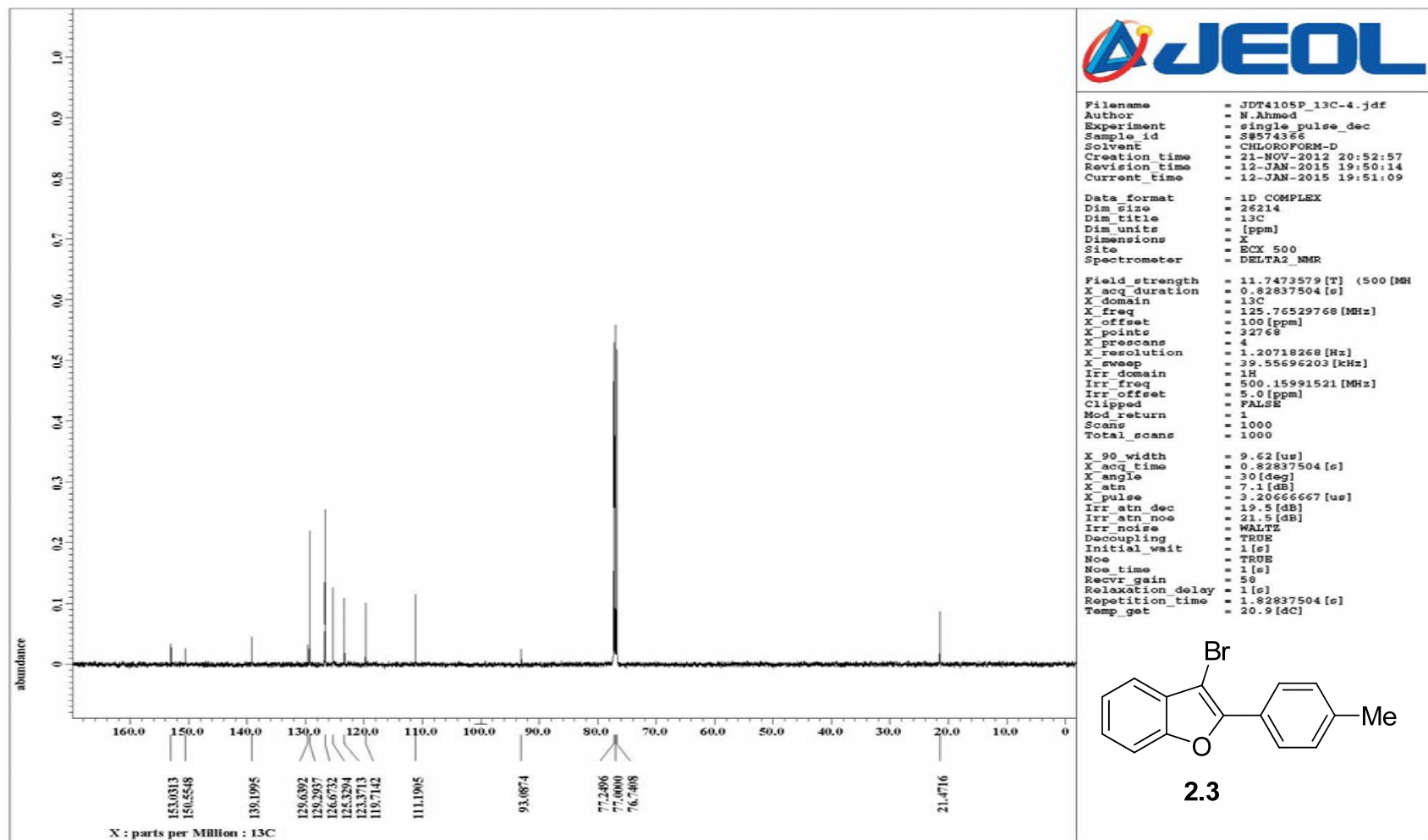
Data format  = 1D COMPLEX
Dim size     = 26214
Dim title    = 1H
Dim units    = [ppm]
Dimensions   = X
Site         = ECX 500
Spectrometer = DELTA2_NMR

Field strength = 11.7473579 [T] (500 [MH]
X_acq_duration = 3.27417856 [s]
X_domain       = 1H
X_freq         = 500.15991521 [MHz]
X_offset       = 5.0 [ppm]
X_points       = 32768
X_prescans     = 1
X_resolution   = 0.30542012 [Hz]
X_sweep        = 10.00800641 [kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521 [MHz]
Irr_offset     = 5.0 [ppm]
Tri_domain     = 1H
Tri_freq       = 500.15991521 [MHz]
Tri_offset     = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 16
Total_scans    = 16

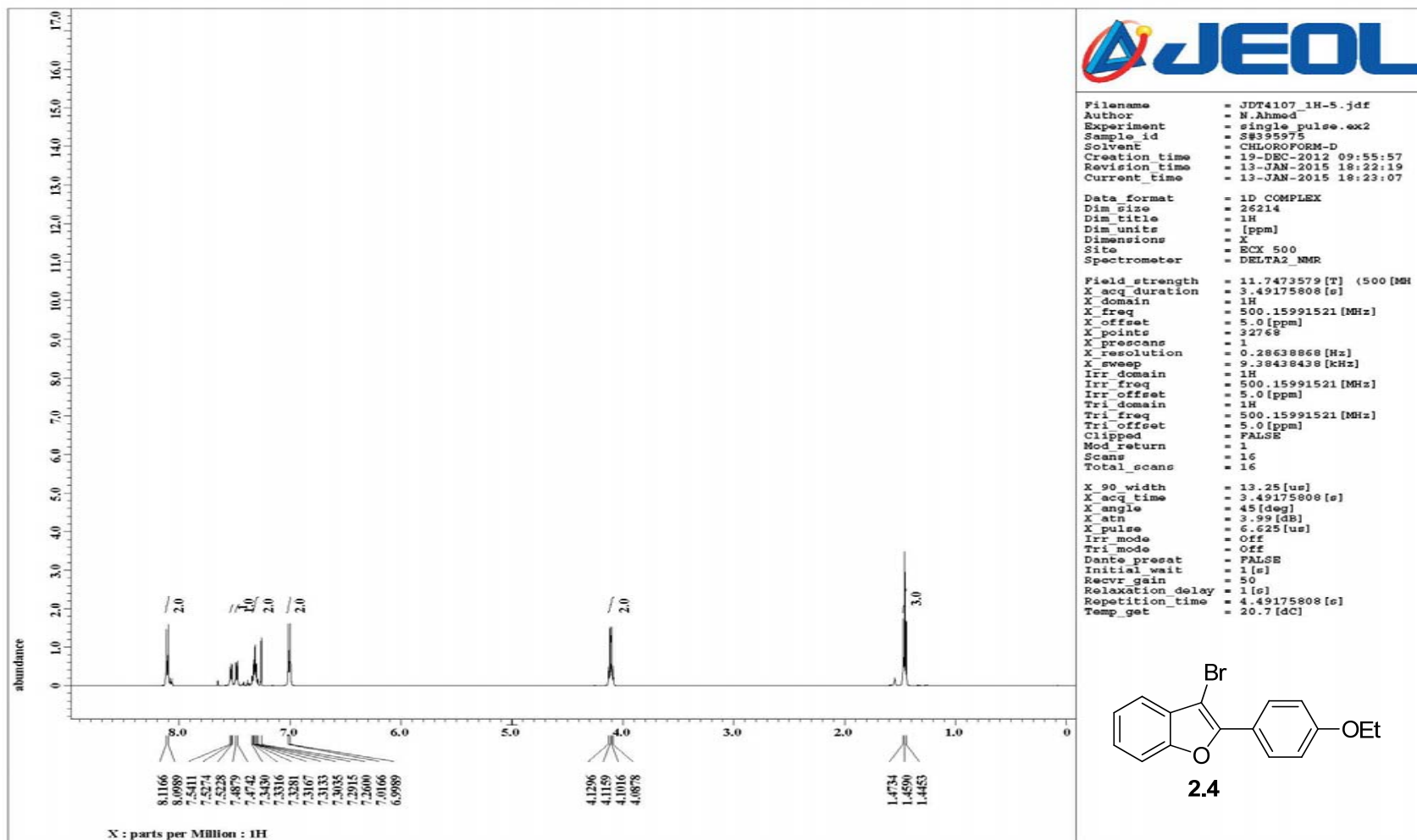
X_90_width    = 13.25 [us]
X_acq_time    = 3.27417856 [s]
X_angle       = 45 [deg]
X_atn         = 3.99 [dB]
X_pulse       = 6.625 [us]
Irr_mode      = Off
Dante_preset  = FALSE
Initial_wait  = 1 [s]
Recvr_gain    = 52
Relaxation_delay = 1 [s]
Repetition_time = 4.27417856 [s]
Temp_get      = 20.1 [dC]
  
```



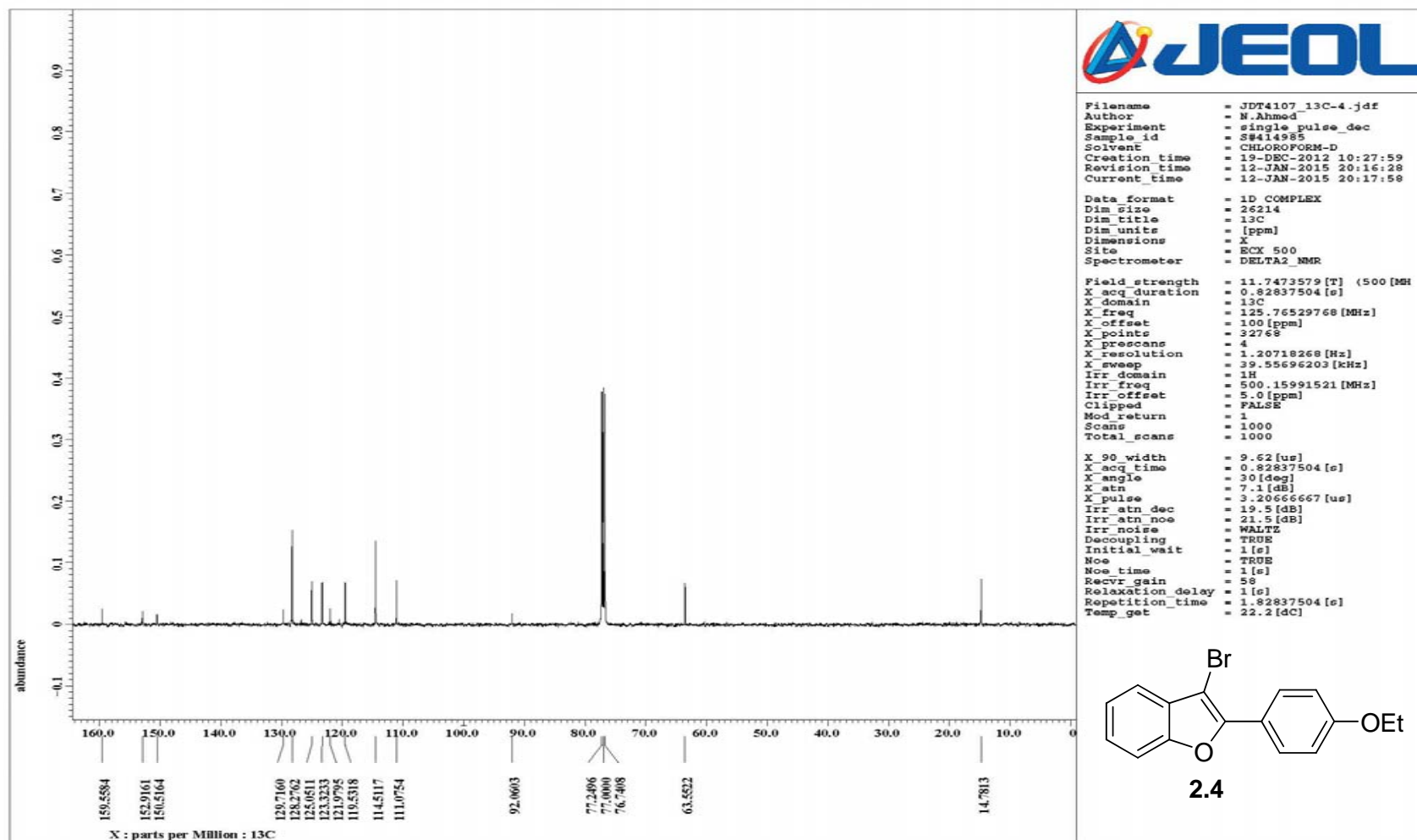
500 MHz ^1H NMR spectrum of compound **2.3**



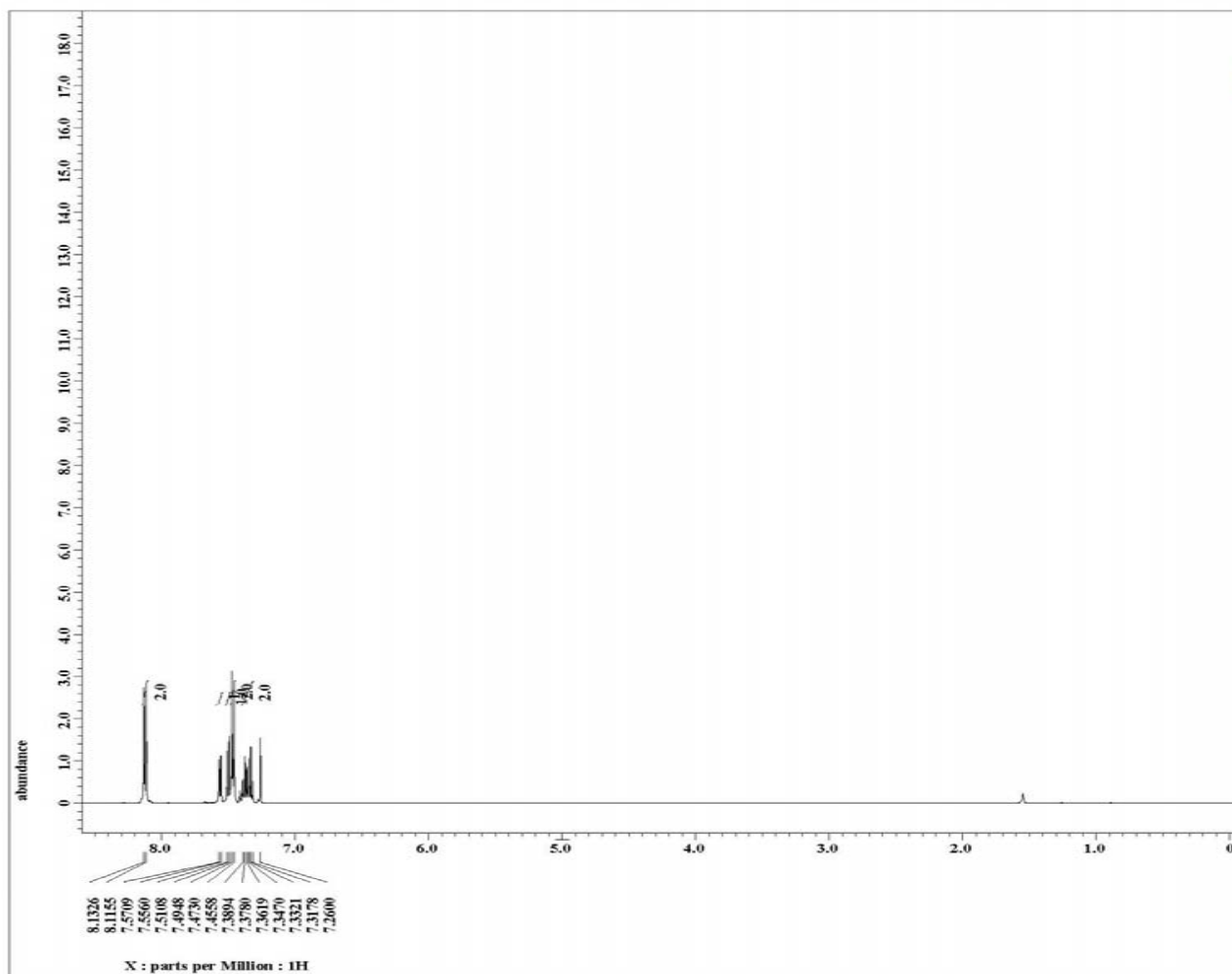
125 MHz ^{13}C NMR spectrum of compound **2.3**



500 MHz ^1H NMR spectrum of compound **2.4**



125 MHz ^{13}C NMR spectrum of compound **2.4**



```

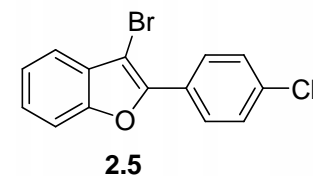
Filename      = JDT4108_1H-5.jdf
Author       = M.Ahmed
Experiment   = single_pulse.ex2
Sample id    = S#395881
Solvent      = CHLOROFORM-D
Creation time = 19-DEC-2012 09:48:54
Revision time = 13-JAN-2015 18:30:11
Current time  = 13-JAN-2015 18:37:05

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Dim units     = [ppm]
Dimensions    = X
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Spectrometer  = DELTA2_NMR

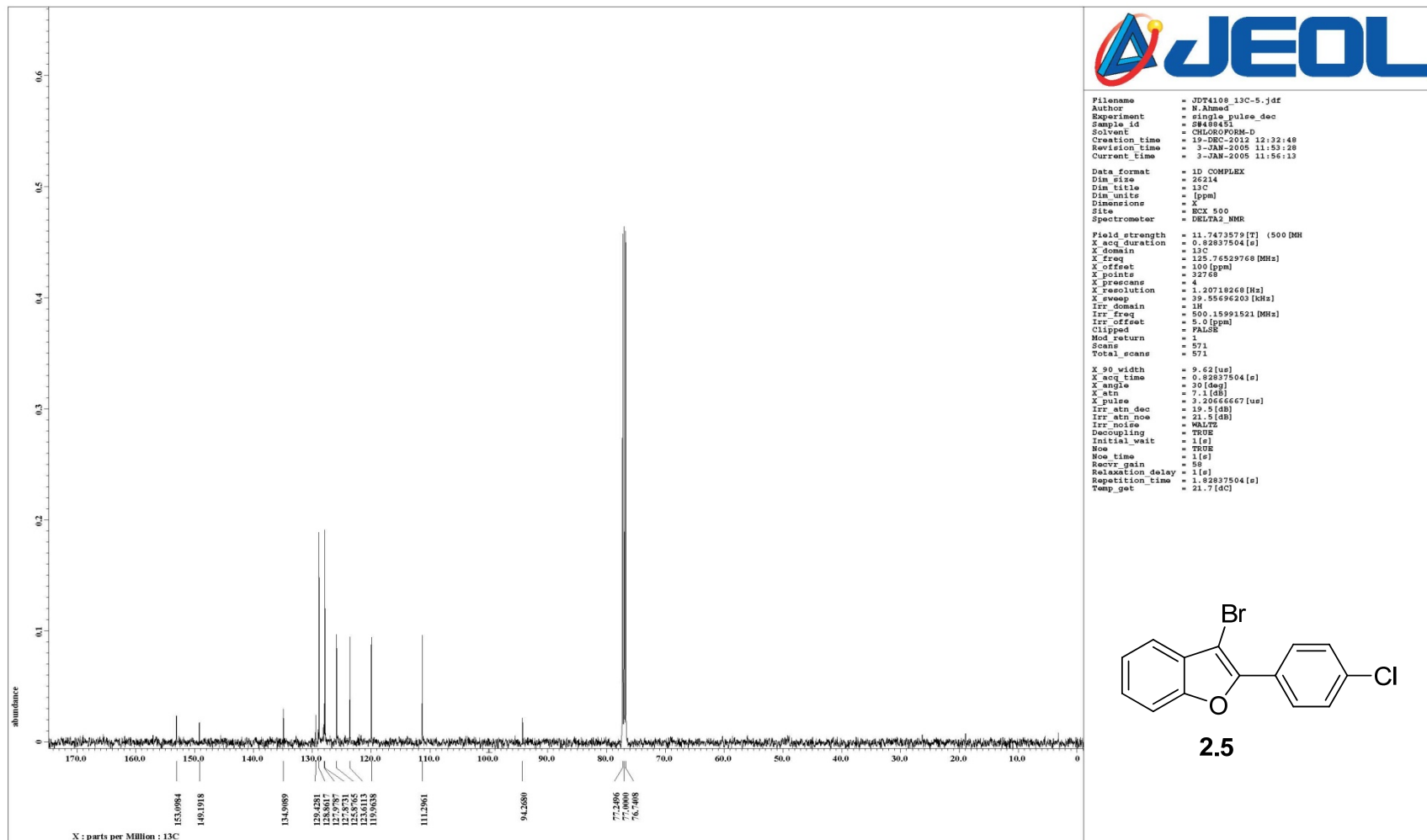
Field strength = 11.7473579 [T] (500 [MH
X_acq duration = 3.49175808 [s]
X_domain       = 1H
X_freq         = 500.15991521 [MHz]
X_offset       = 5.0 [ppm]
X_points       = 22768
X_prescans     = 1
X_resolution   = 0.28638868 [Hz]
X_sweep        = 9.38438438 [kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521 [MHz]
Irr_offset     = 5.0 [ppm]
Tri_domain     = 1H
Tri_freq       = 500.15991521 [MHz]
Tri_offset     = 5.0 [ppm]
Clipped        = FALSE
Mod return     = 1
Scans          = 16
Total_scans    = 16

X_90 width    = 13.25 [us]
X_acq time     = 3.49175808 [s]
X_angle       = 45 [deg]
X_atn         = 3.99 [dB]
X_pulse       = 6.625 [us]
Irr_mode      = Off
Tri_mode      = Off
Dante preset  = FALSE
Initial wait  = 1 [s]
Recvr gain    = 52
Relaxation delay = 1 [s]
Repetition_time = 4.49175808 [s]
Temp_get      = 20.1 [dc]

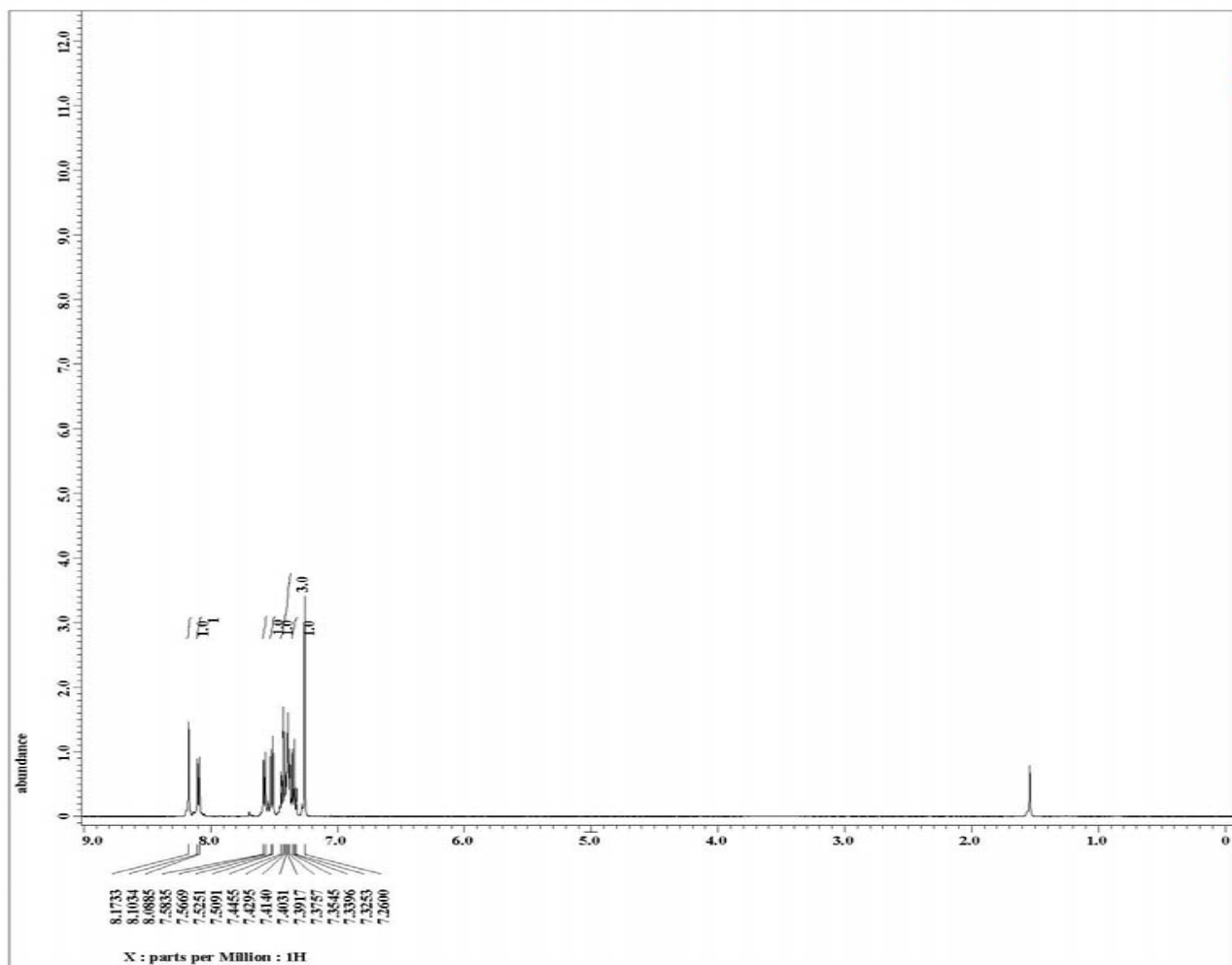
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500 MHz ^1H NMR spectrum of compound **2.5**



125 MHz ^{13}C NMR spectrum of compound **2.5**



```

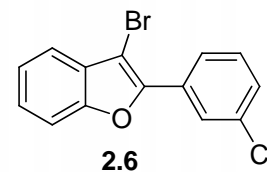
Filename      = JDT4109_1H-5.jdf
Author       = N.Ahmed
Experiment    = single_pulse.ex2
Sample_id    = S#395759
Solvent      = CHLOROFORM-D
Creation time = 19-DEC-2012 09:42:16
Revision time = 13-JAN-2015 18:56:07
Current time  = 13-JAN-2015 18:56:23

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Dim size     = 26214
Dim title    = 1H
Dim units    = [ppm]
Dimensions   = X
Site        = ECX 500
Spectrometer = DELTA2_NMR

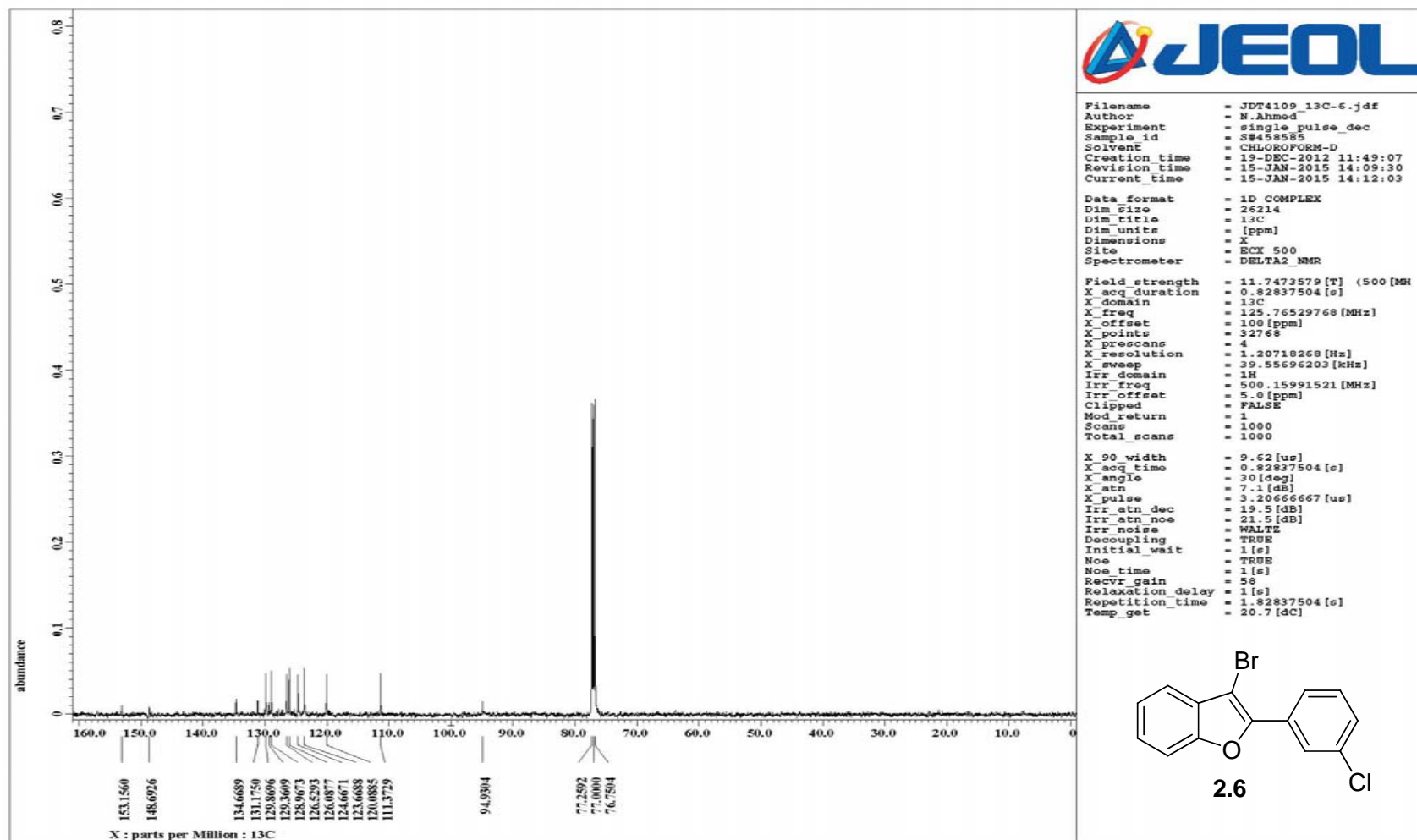
Field strength = 11.7473579 [T] (500 [MH]
X_acq duration = 3.49175808 [s]
X_domain      = 1H
X_freq       = 500.15991521 [MHz]
X_offset     = 5.0 [ppm]
X_points     = 32768
X_prescans   = 1
X_resolution = 0.28638868 [Hz]
X_sweep      = 9.38438438 [kHz]
Irr_domain   = 1H
Irr_freq     = 500.15991521 [MHz]
Irr_offset   = 5.0 [ppm]
Tri_domain   = 1H
Tri_freq     = 500.15991521 [MHz]
Tri_offset   = 5.0 [ppm]
Clipped      = FALSE
Mod return   = 1
Scans        = 16
Total_scans  = 16

X_90 width   = 13.25 [us]
X_acq time   = 3.49175808 [s]
X_angle      = 45 [deg]
X_atn        = 3.99 [dB]
X_pulse      = 6.625 [us]
Irr_mode     = Off
Tri_mode     = Off
Dante presat = FALSE
Initial wait = 1 [s]
Recvr gain   = 60
Relaxation delay = 1 [s]
Repetition_time = 4.49175808 [s]
Temp_get     = 20.3 [dC]

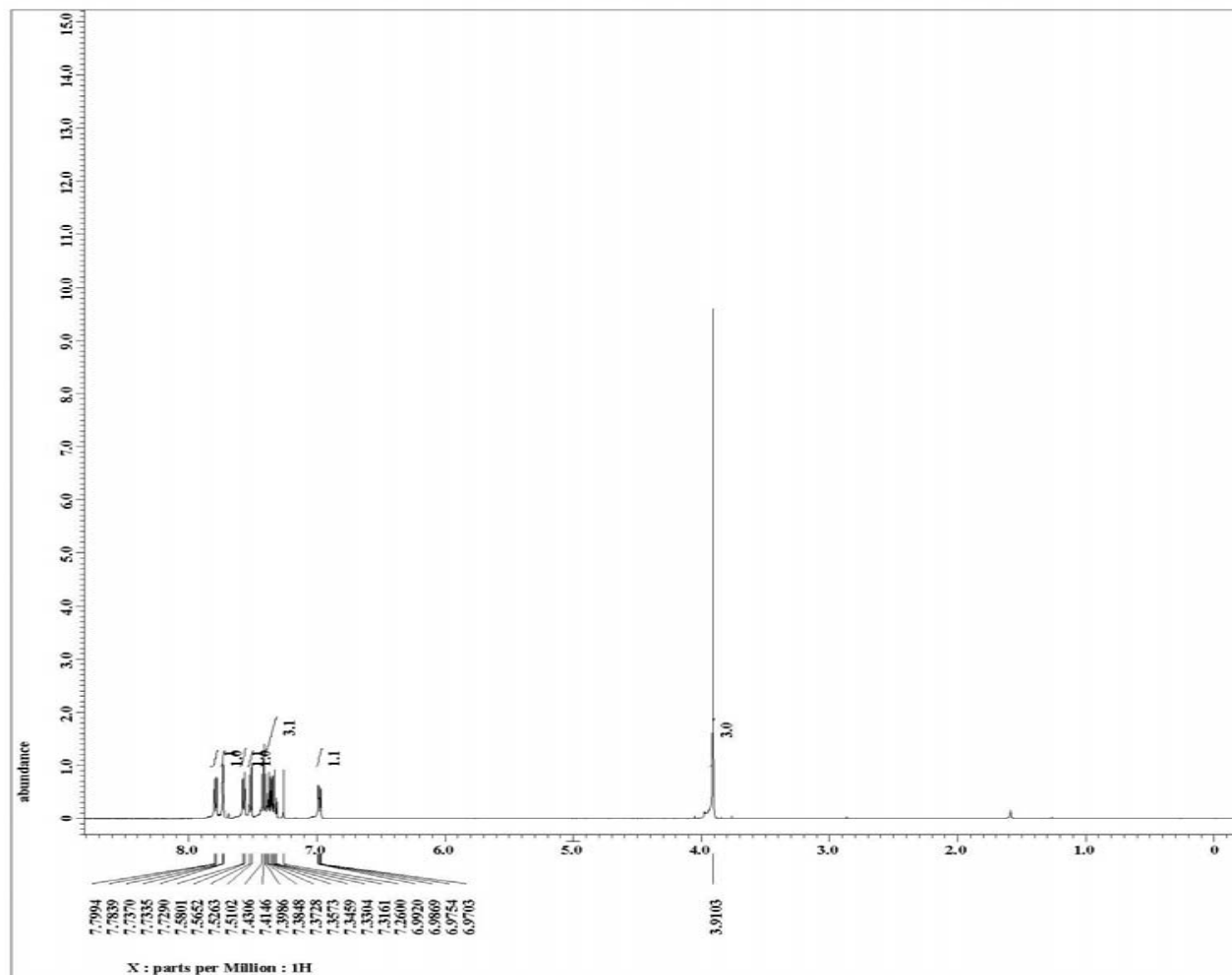
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500 MHz ¹H NMR spectrum of compound **2.6**



125 MHz ^{13}C NMR spectrum of compound **2.6**



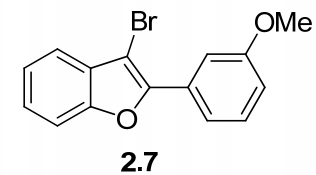
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Filename      = JDT4110_1H-13.jdf
Author       = M.Ahmed
Experiment   = single pulse.ex2
Sample id    = S#423390
Solvent      = CHLOROFORM-D
Creation time = 20-DEC-2012 10:49:47
Revision time = 9-FEB-2015 00:38:59
Current time  = 9-FEB-2015 00:39:23

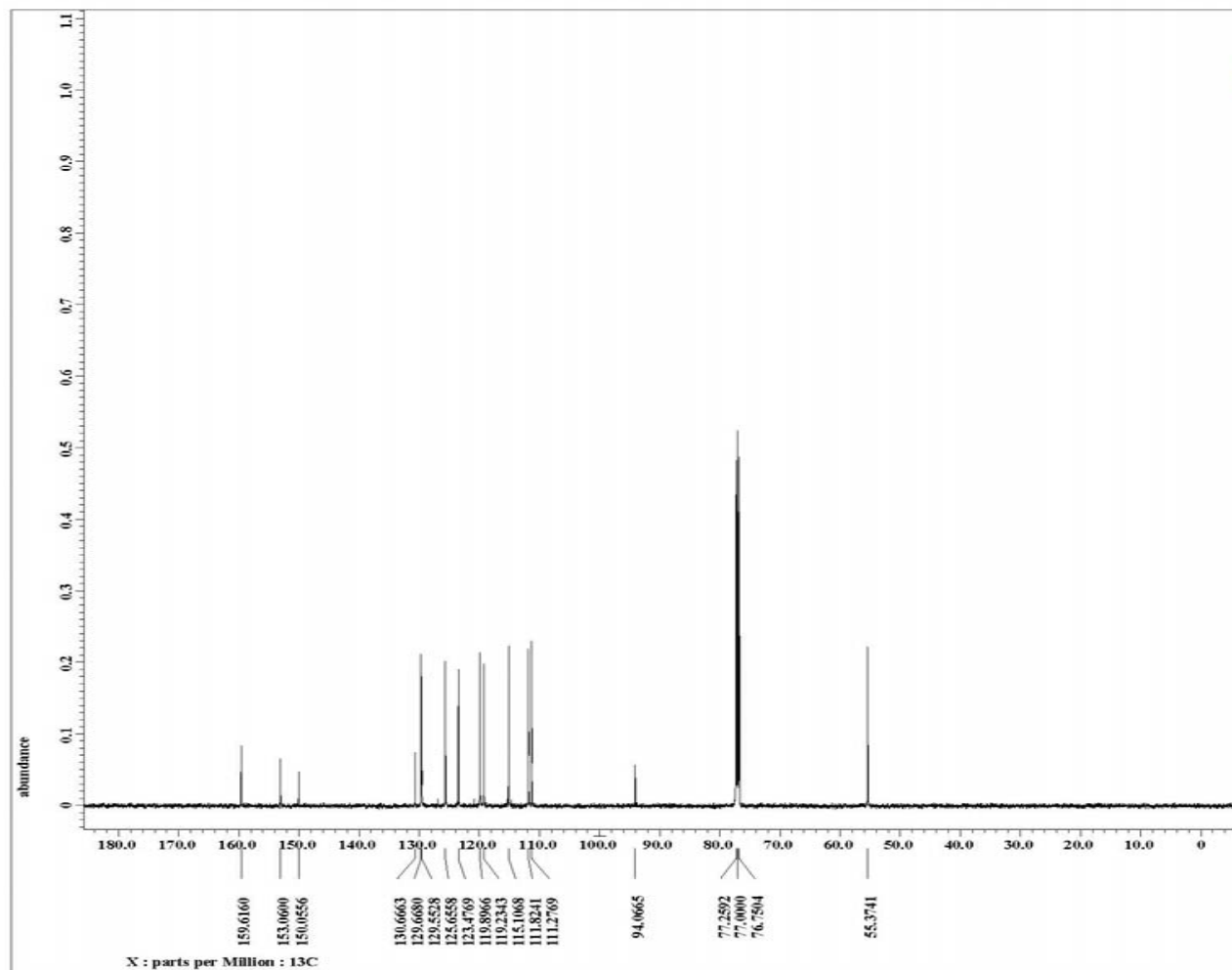
Data format  = 1D COMPLEX
Dim size     = 26214
Dim title    = 1H
Dim units    = [ppm]
Dimensions   = X
Site         = ECX 500
Spectrometer = DELTA2_NMR

Field strength = 11.7473579 [T] (500 [MH]
X_acq_duration = 3.49175808 [s]
X_domain      = 1H
X_freq        = 500.15991521 [MHz]
X_offset      = 5.0 [ppm]
X_points      = 32768
X_prescans    = 1
X_resolution  = 0.28638868 [Hz]
X_sweep       = 9.38438438 [kHz]
Irr_domain    = 1H
Irr_freq      = 500.15991521 [MHz]
Irr_offset    = 5.0 [ppm]
Tri_domain    = 1H
Tri_freq      = 500.15991521 [MHz]
Tri_offset    = 5.0 [ppm]
Clipped       = FALSE
Mod return    = 1
Scans         = 16
Total_scans   = 16

X_90_width    = 13.25 [us]
X_acq_time    = 3.49175808 [s]
X_angle       = 45 [deg]
X_atn         = 3.99 [dB]
X_pulse       = 6.625 [us]
Irr_mode      = Off
Tri_mode      = Off
Dante_preset = FALSE
Initial_wait  = 1 [s]
Recvr_gain    = 46
Relaxation_delay = 1 [s]
Repetition_time = 4.49175808 [s]
Temp_get      = 20.2 [dC]
  
```



500 MHz ^1H NMR spectrum of compound **2.7**



```

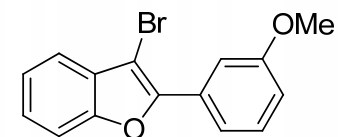
Filename      = JDT4110_13C-8.jdf
Author       = M.Ahmed
Experiment   = single pulse_dec
Sample id    = S#587482
Solvent      = CHLOROFORM-D
Creation time = 20-DEC-2012 15:51:18
Revision time = 9-FEB-2015 00:40:42
Current time  = 9-FEB-2015 00:41:12

Data format  = 1D COMPLEX
Dim size     = 26214
Dim title    = 13C
Dim units    = [ppm]
Dimensions   = X
Site         = ECX 500
Spectrometer = DELTA2_NMR

Field strength = 11.7473579 [T] (500 [MH]
X_acq_duration = 0.82837504 [s]
X_domain       = 13C
X_freq         = 125.76529768 [MHz]
X_offset       = 100 [ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.20718268 [Hz]
X_sweep        = 39.55696203 [kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521 [MHz]
Irr_offset     = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 2000
Total_scans    = 2000

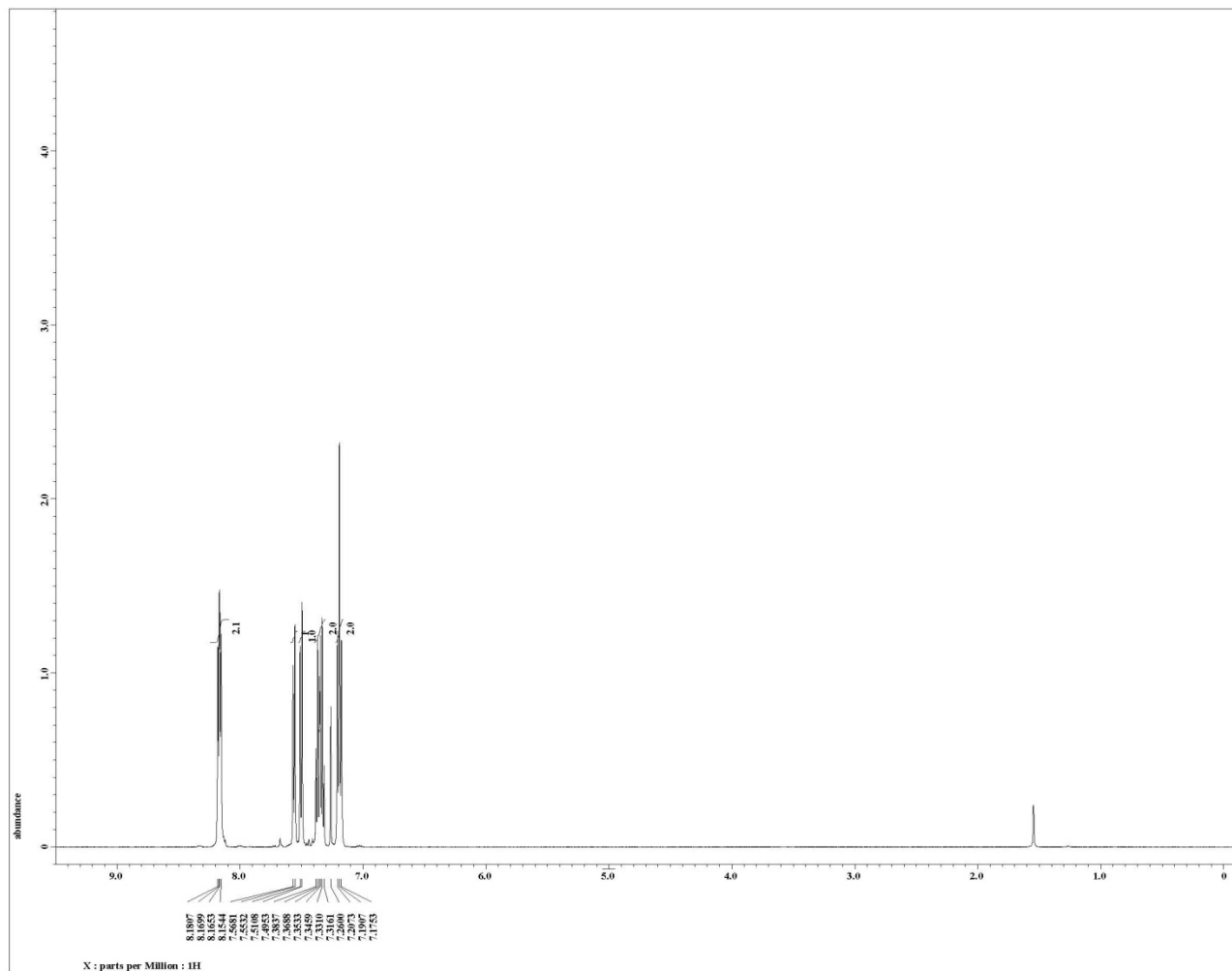
X_90_width     = 9.62 [us]
X_acq_time     = 0.82837504 [s]
X_angle        = 30 [deg]
X_atn          = 7.1 [dB]
X_pulse        = 3.20666667 [us]
Irr_atn_dec    = 19.5 [dB]
Irr_atn_noe    = 21.5 [dB]
Irr_noise      = WALTZ
Decoupling     = TRUE
Initial_wait   = 1 [s]
Noe            = TRUE
Noe_time       = 1 [s]
Recvr_gain     = 58
Relaxation_delay = 1 [s]
Repetition_time = 1.82837504 [s]
Temp_get       = 20.4 [dC]

```



2.7

125 MHz ^{13}C NMR spectrum of compound **2.7**



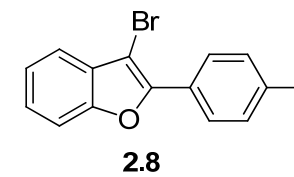
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Filename      = JDT4111 1H-10.jds
Author       = N.Ahmed
Experiment   = single_pulse.ex2
Sample Id    = SW42357
Solvent      = CDCl3/CF3COOH-D
Creation time = 20-DEC-2012 11:04:13
Revision time = 3-JAN-2005 08:49:17
Current time  = 3-JAN-2005 08:51:25

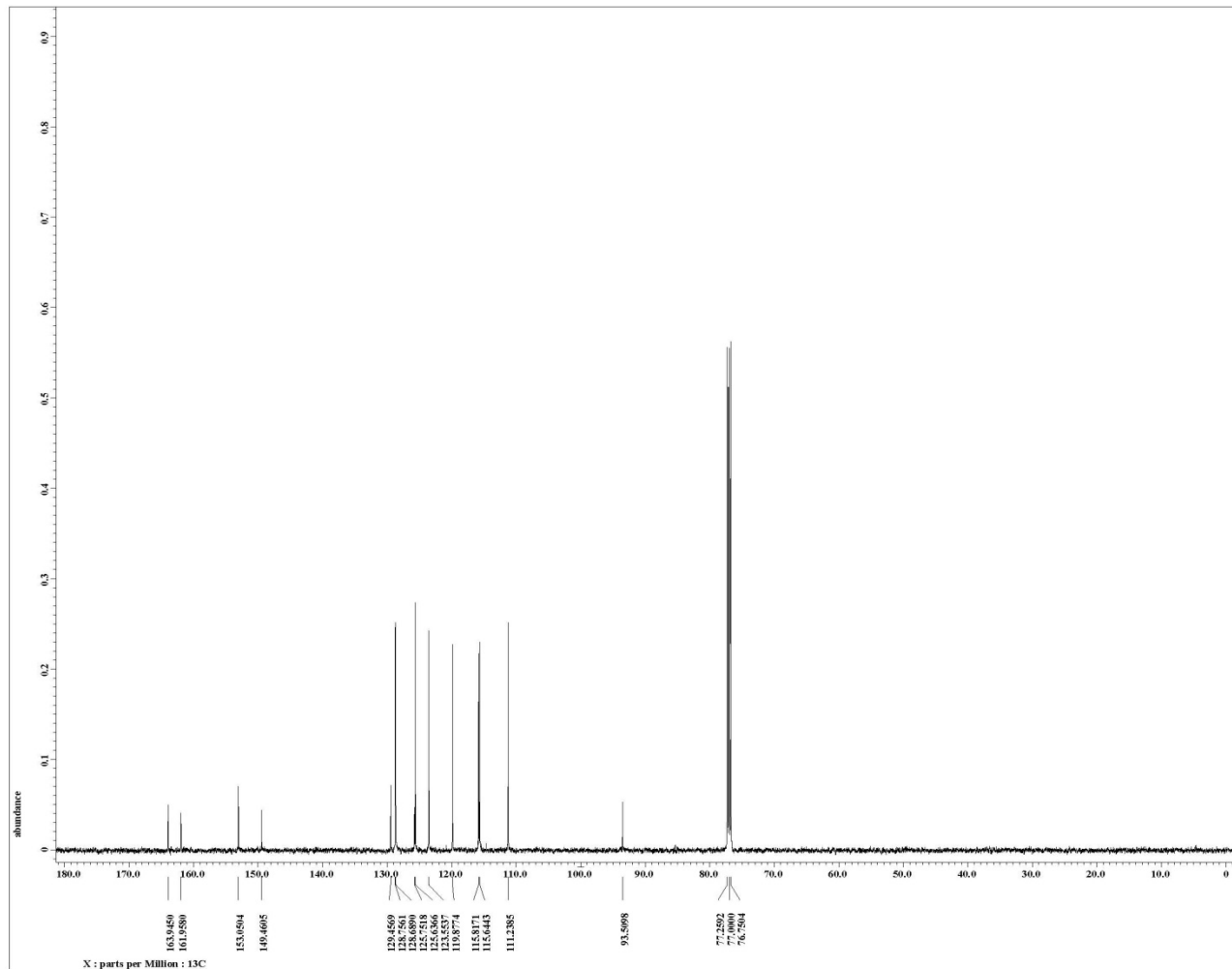
Data format  = 1D COMPLEX
Dim_size     = 26214
Dim_title    = 1H
Dim_units    = [ppm]
Dimensions   = X
Site         = EX5 500
Spectrometer = DELTA2 NMR

Field strength = 11.7473579 [T] (500 [MH]
X_acq_duration = 3.49175808 [s]
X_domain       = 1H
X_freq         = 500.15991521 [MHz]
X_offset       = 5.0 [ppm]
X_points       = 32768
X_prescans     = 1
X_resolution   = 0.28638868 [Hz]
X_sweep        = 9.38438438 [kHz]
IRF_domain    = 1H
IRF_freq       = 500.15991521 [MHz]
IRF_offset     = 5.0 [ppm]
Tri_domain    = 1H
Tri_freq      = 500.15991521 [MHz]
Tri_offset    = 5.0 [ppm]
Clipped       = FALSE
Mod_return    = 1
Scans         = 16
Total_scans   = 16

X_90_width    = 13.25 [us]
X_acq_time    = 3.49175808 [s]
X_angle       = 45 [deg]
X_atn         = 3.99 [dB]
X_pulse       = 6.825 [us]
IRF_mode      = Off
Tri_mode      = Off
Dante_preat   = FALSE
Initial_wait  = 1 [s]
Recvr_gain    = 50
Relaxation_delay = 1 [s]
Repetition_time = 4.49175808 [s]
Temp_get      = 20.2 [dC]
  
```



500 MHz ^1H NMR spectrum of compound **2.8**



```

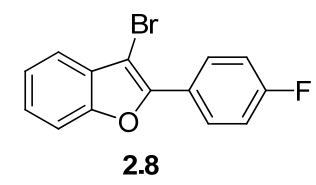
Filename      = JDT4111_13C-7.jdf
Author       = N.Ahmed
Experiment   = single_pulse_dec
Sample Id    = SW587685
Solvent      = CHLOROFORM-D
Creation time = 20-DEC-2012 16:05:19
Revision time = 3-JAN-2005 09:32:36
Current time  = 3-JAN-2005 09:34:05

Data format  = 1D_COMPLEX
Dim_size     = 26214
Dim_title    = 13C
Dim_units    = [ppm]
Dimensions   = X
Size         = EXC 500
Spectrometer = DELTA2_NMR

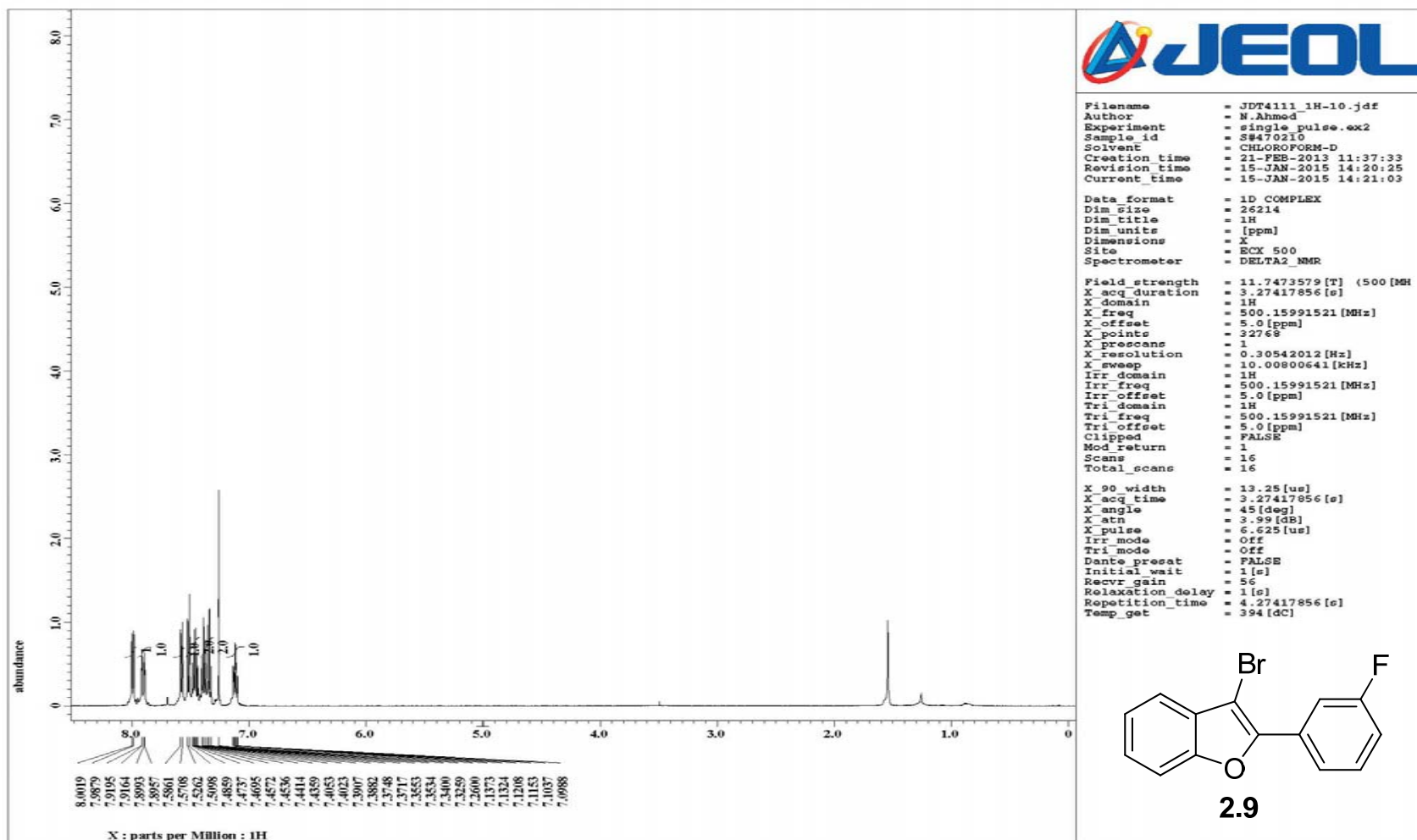
Field strength = 11.7473579 [T] (500 [MH]
X_acq_duration = 0.82837504 [s]
X_domain       = 13C
X_freq         = 125.76529768 [MHz]
X_offset       = 100 [ppm]
X_points       = 32768
X_preamplifier = 4
X_resolution   = 1.20718268 [Hz]
X_sweep        = 39.55696203 [kHz]
IRF_domain    = 18
IRF_freq       = 500.15991521 [MHz]
IRF_offset     = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 2000
Total_scans    = 2000

X_90_width    = 9.62 [us]
X_acq_time    = 0.82837504 [s]
X_angle       = 30 [deg]
X_atn         = 7.1 [dB]
X_pulse       = 3.20666667 [us]
IRF_atn_dec   = 19.5 [dB]
IRF_atn_noe   = 21.5 [dB]
IRF_noise     = WALTZ
Decoupling    = TRUE
Initial_wait  = 1 [s]
Noe           = TRUE
Noe_time      = 1 [s]
Recvr_gain    = 55
Relaxation_delay = 1 [s]
Repetition_time = 1.82837504 [s]
Temp_get      = 20.3 [dC]

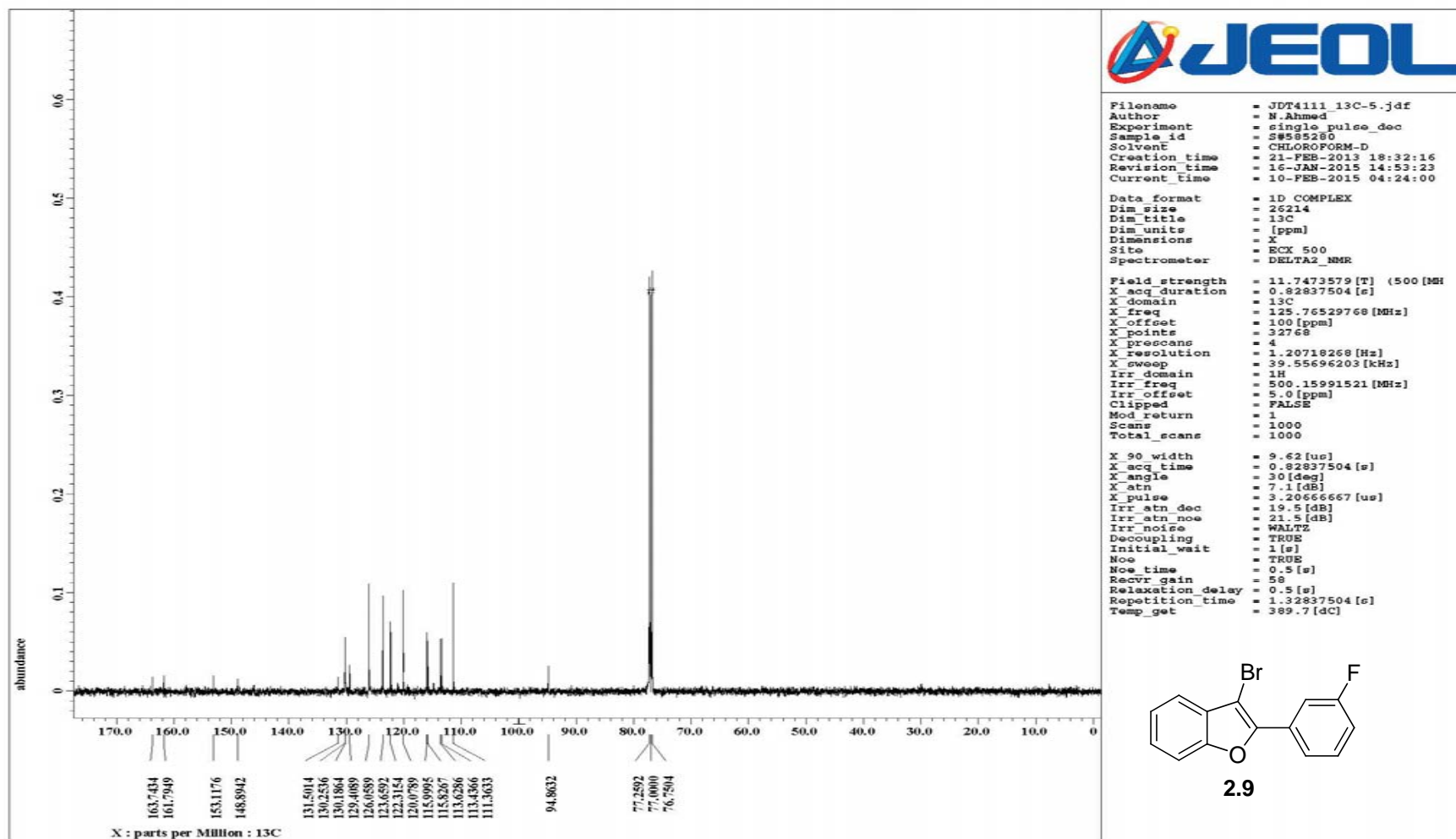
```



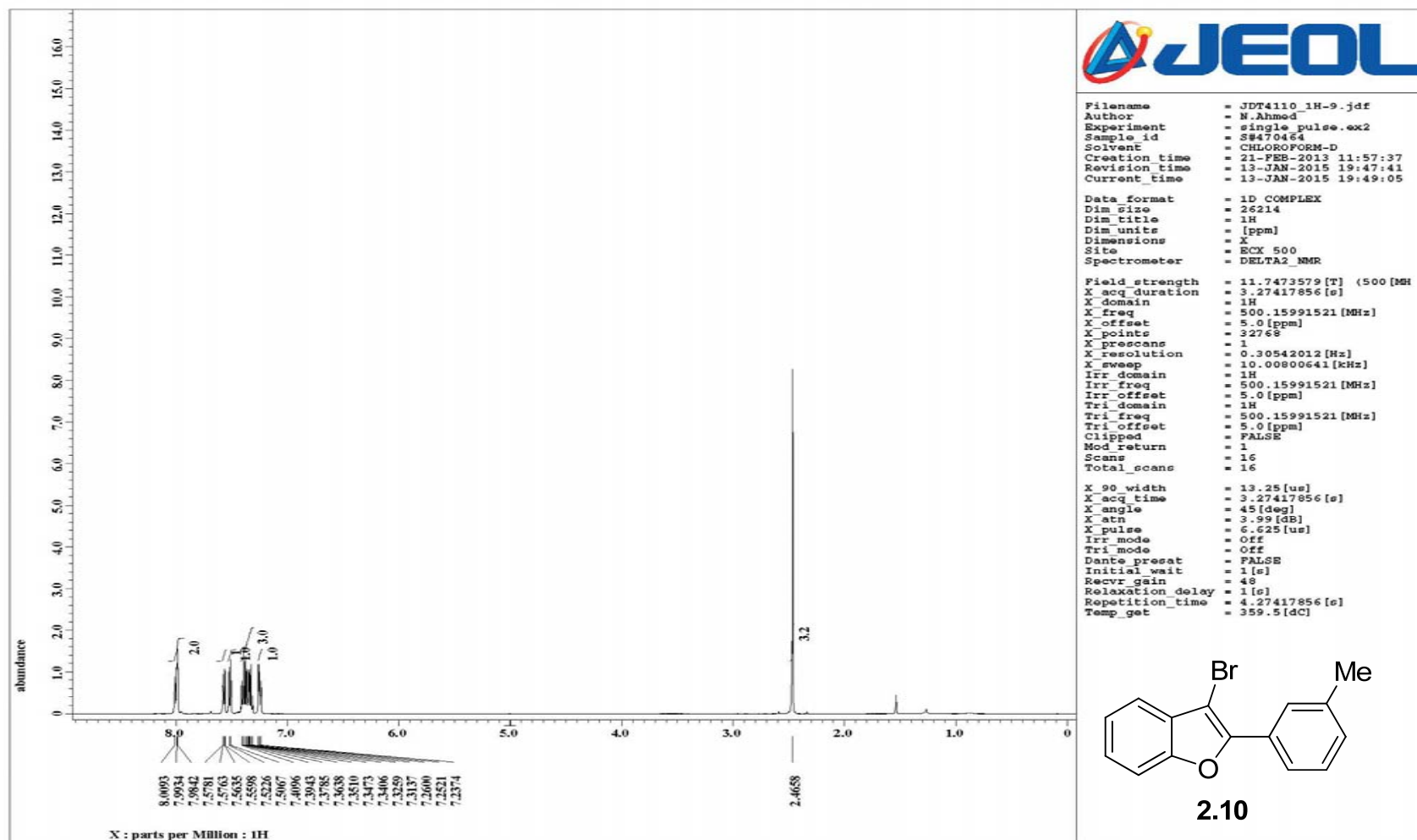
125 MHz ¹³C NMR spectrum of compound 2.8



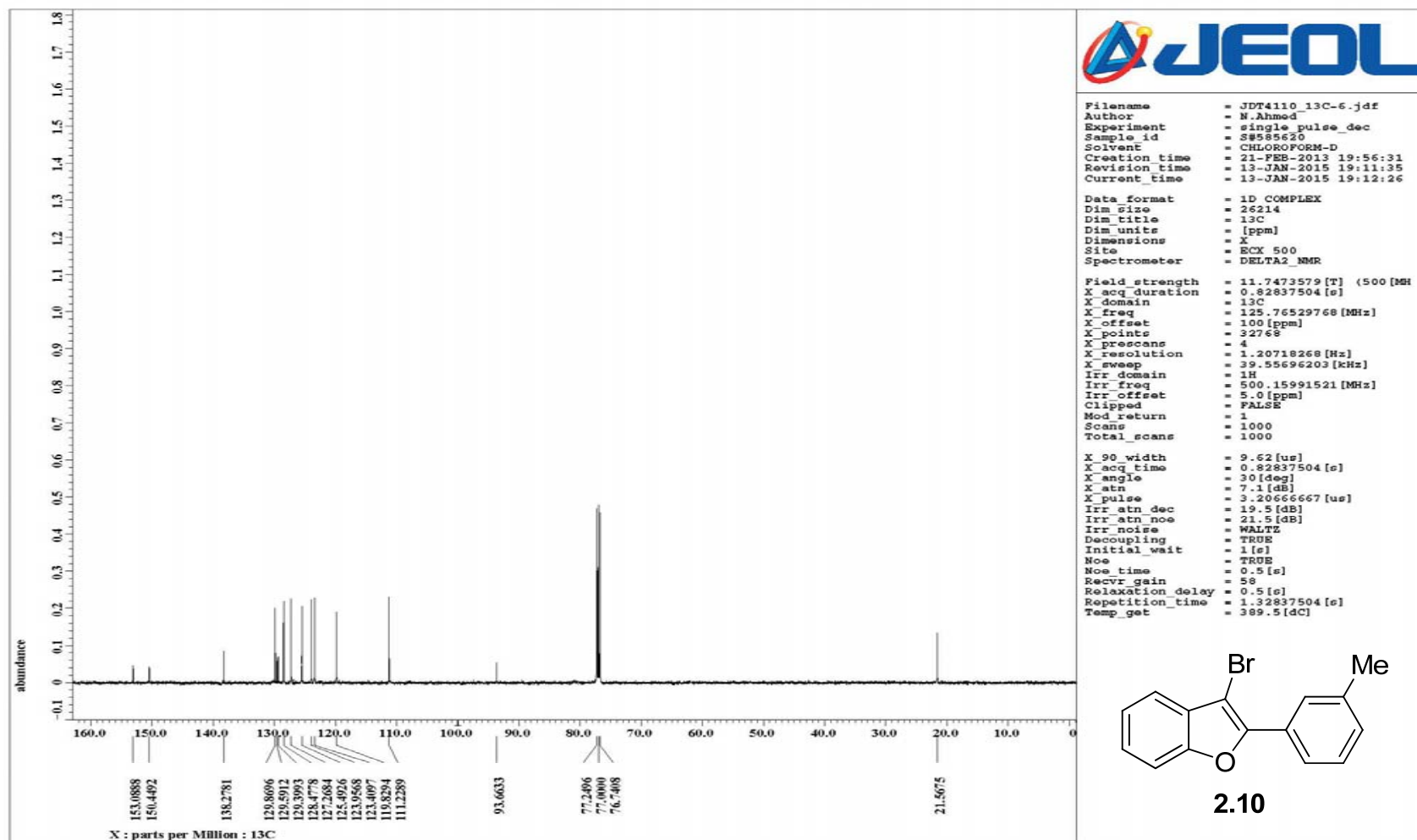
500 MHz ^1H NMR spectrum of compound **2.9**



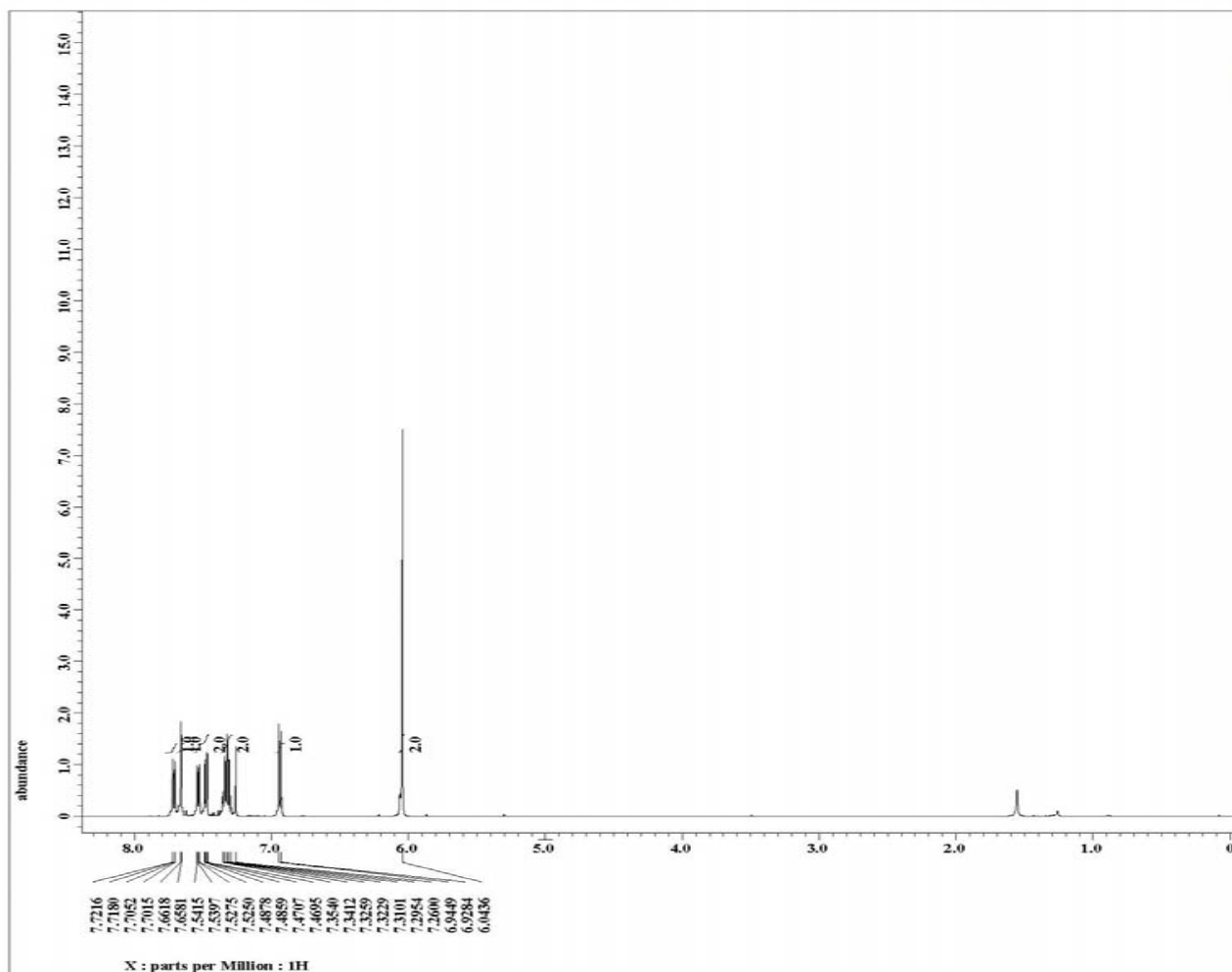
125 MHz ^{13}C NMR spectrum of compound **2.9**



500 MHz ¹H NMR spectrum of compound **2.10**



125 MHz ^{13}C NMR spectrum of compound **2.10**



```

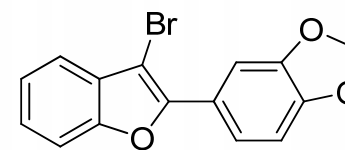
Filename      = JDT4122_1H-5.jdf
Author       = M.Ahmed
Experiment   = single_pulse.ex2
Sample id    = S#470371
Solvent      = CHLOROFORM-D
Creation time = 21-FEB-2013 11:51:09
Revision time = 16-JAN-2015 16:02:22
Current time  = 16-JAN-2015 16:03:22

Data format  = 1D COMPLEX
Dim Size     = 26214
Dim title    = 1H
Dim units    = [ppm]
Dimensions   = X
Site         = ECX 500
Spectrometer = DELTA2_NMR

Field strength = 11.7473579 [T] (500 [MH]
X_acq duration = 3.27417856 [s]
X_domain       = 1H
X_freq         = 500.15991521 [MHz]
X_offset       = 5.0 [ppm]
X_points       = 32768
X_prescans     = 1
X_resolution   = 0.30542012 [Hz]
X_sweep        = 10.00800641 [kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521 [MHz]
Irr_offset     = 5.0 [ppm]
Tri_domain     = 1H
Tri_freq       = 500.15991521 [MHz]
Tri_offset     = 5.0 [ppm]
Clipped        = FALSE
Mod return     = 1
Scans          = 16
Total_scans    = 16

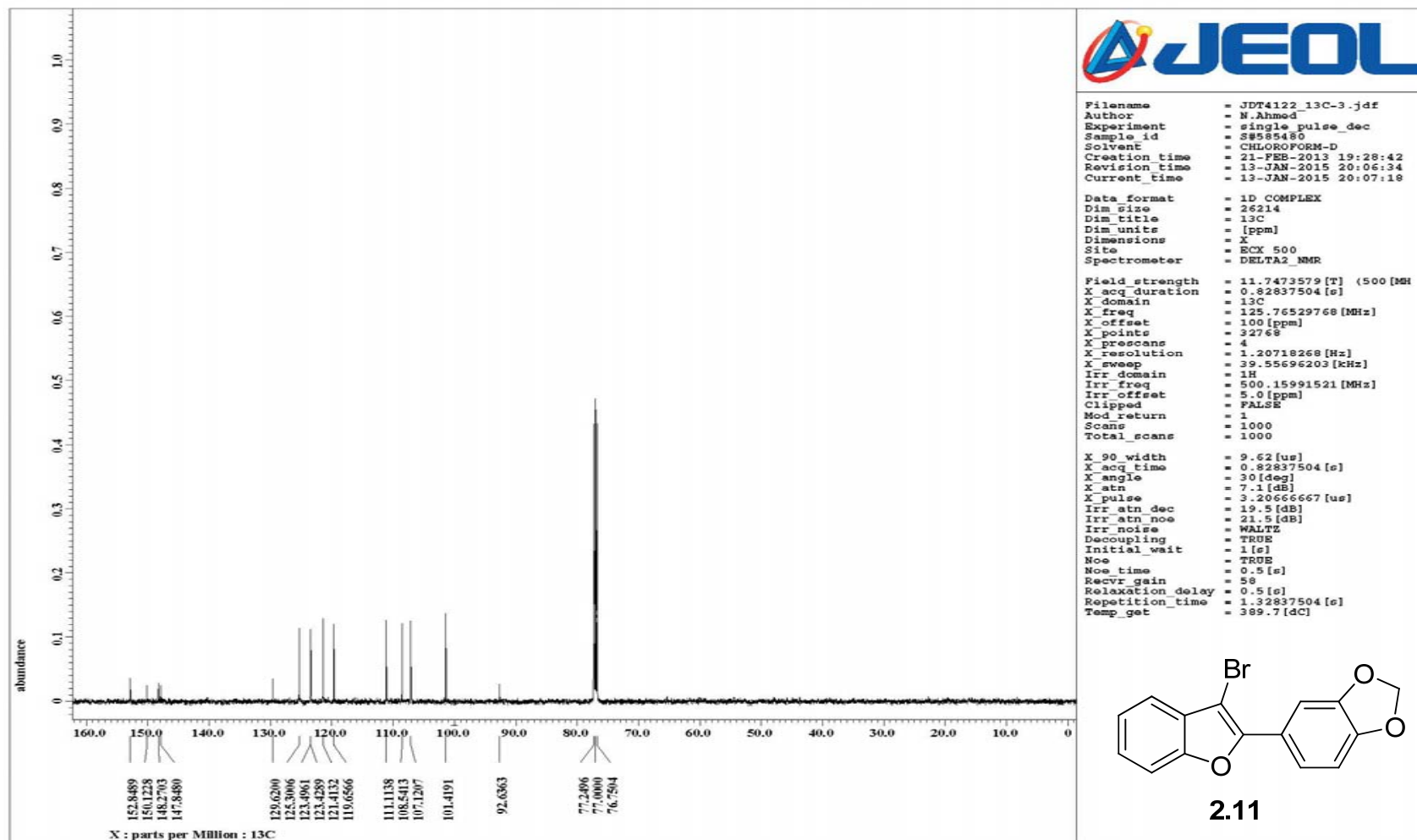
X_90 width     = 13.25 [us]
X_acq time     = 3.27417856 [s]
X_angle        = 45 [deg]
X_atn          = 3.99 [dB]
X_pulse        = 6.625 [us]
Irr_mode       = Off
Tri_mode       = Off
Dante preset   = FALSE
Initial wait   = 1 [s]
Recvr gain     = 52
Relaxation delay = 1 [s]
Repetition_time = 4.27417856 [s]
Temp_get       = 172.7 [dC]

```

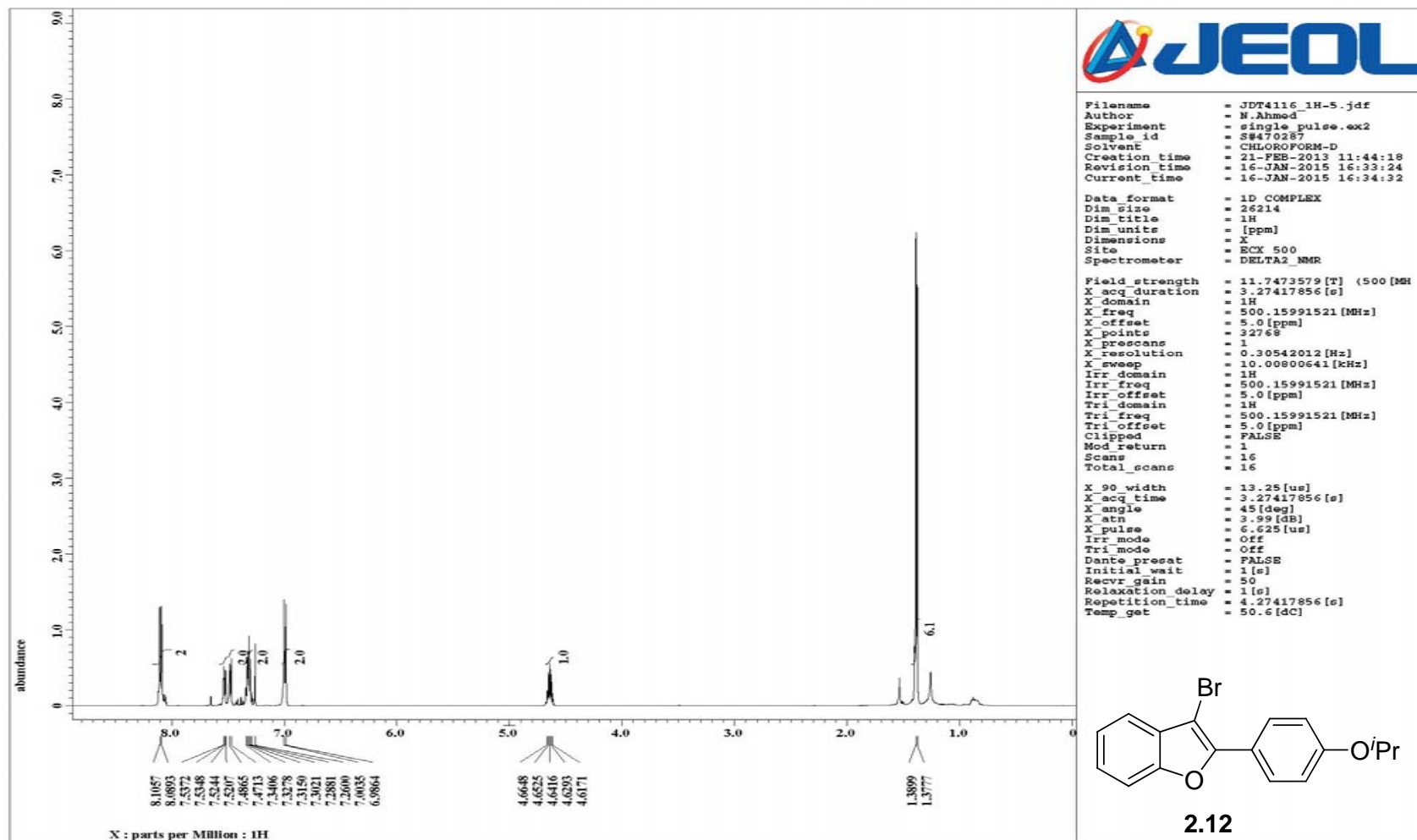


2.11

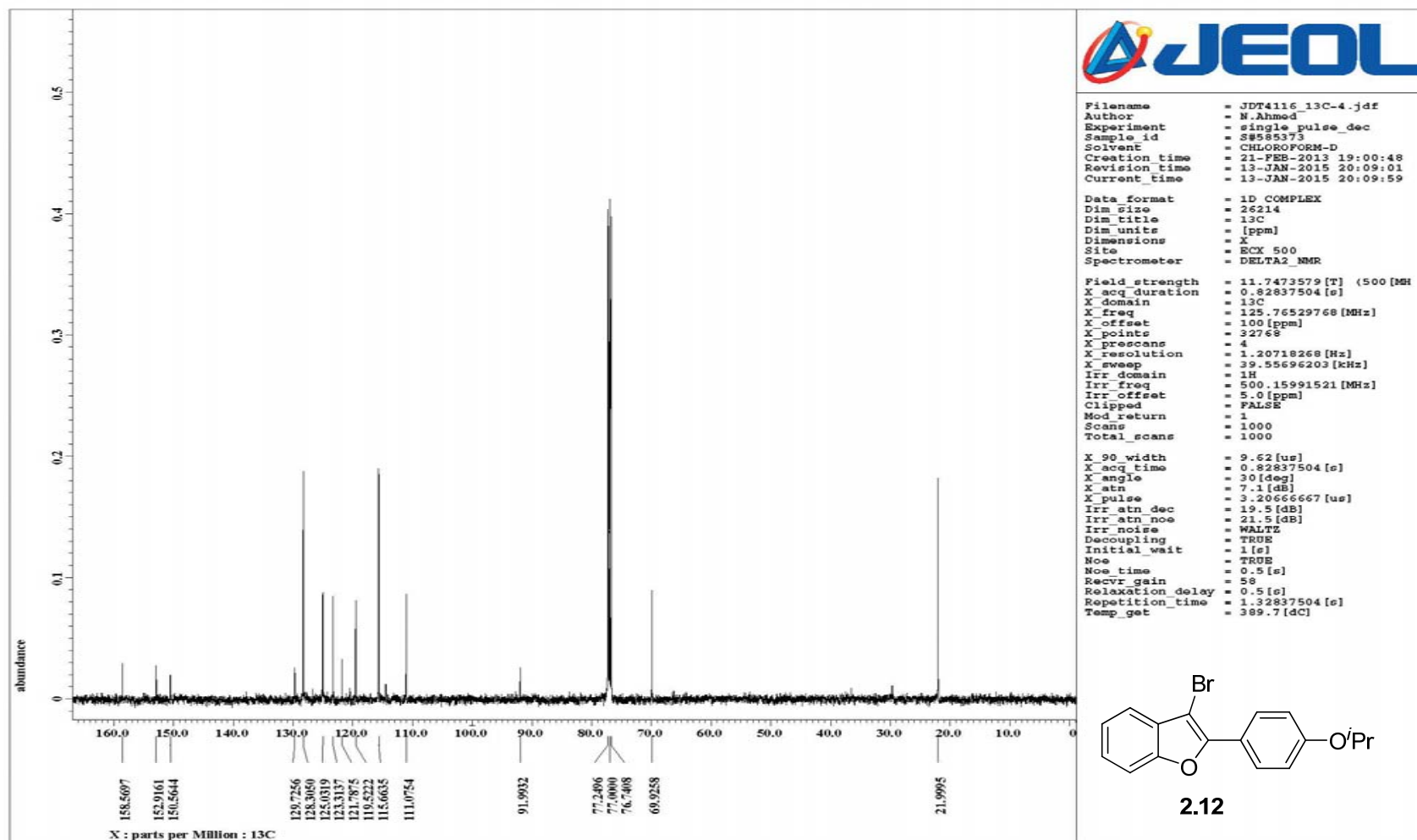
500 MHz ^1H NMR spectrum of compound **2.11**



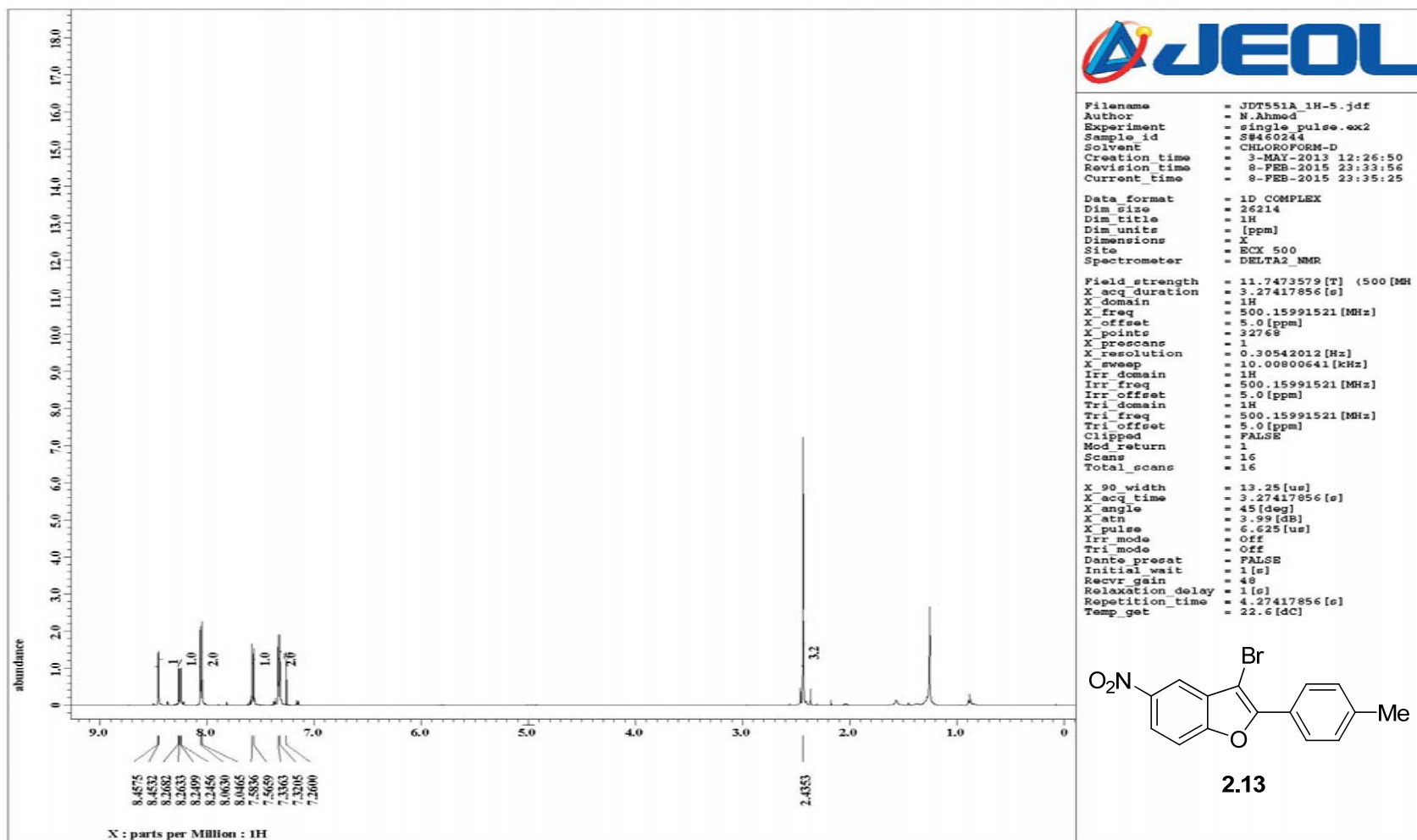
125 MHz ^{13}C NMR spectrum of compound **2.11**



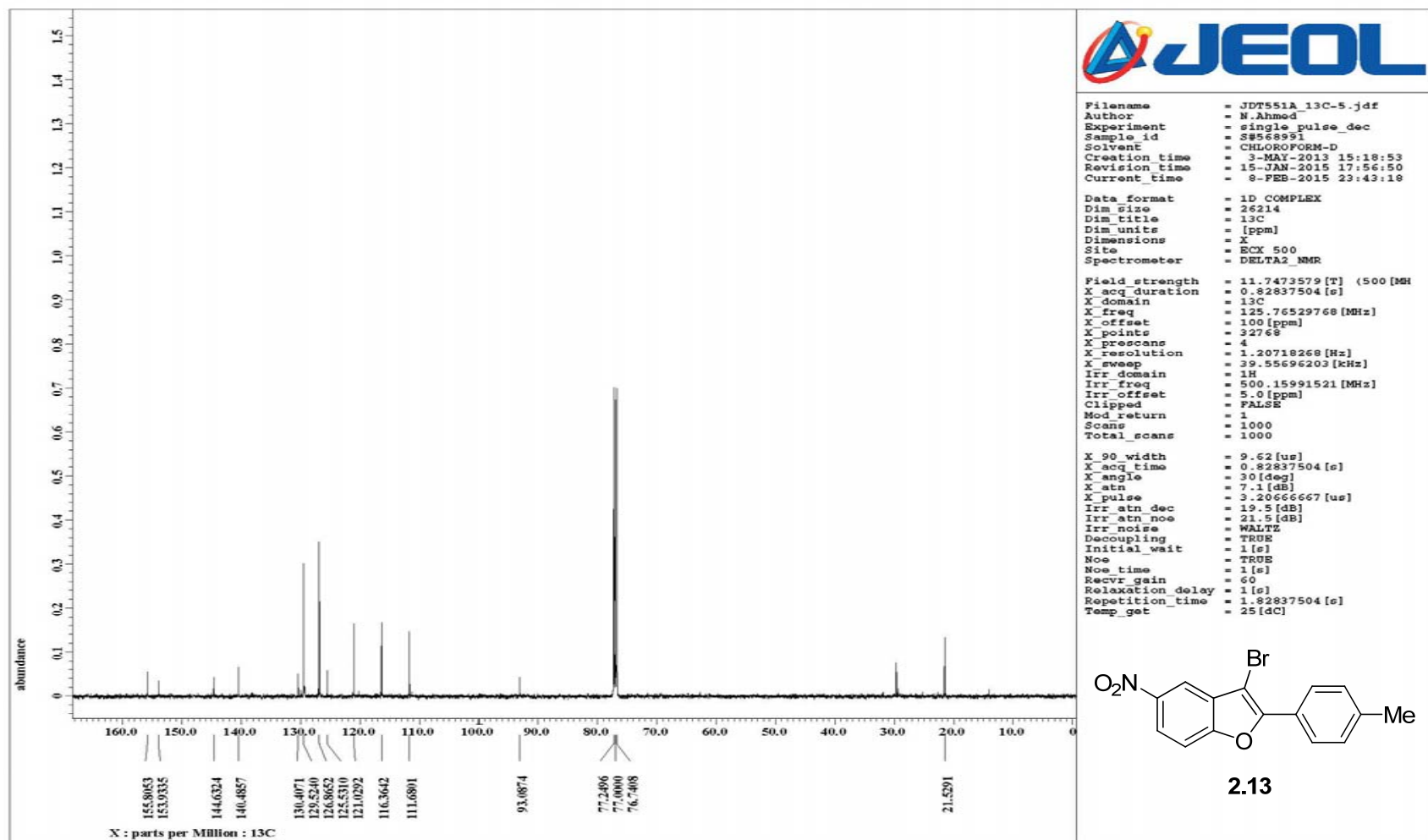
500 MHz ^1H NMR spectrum of compound **2.12**



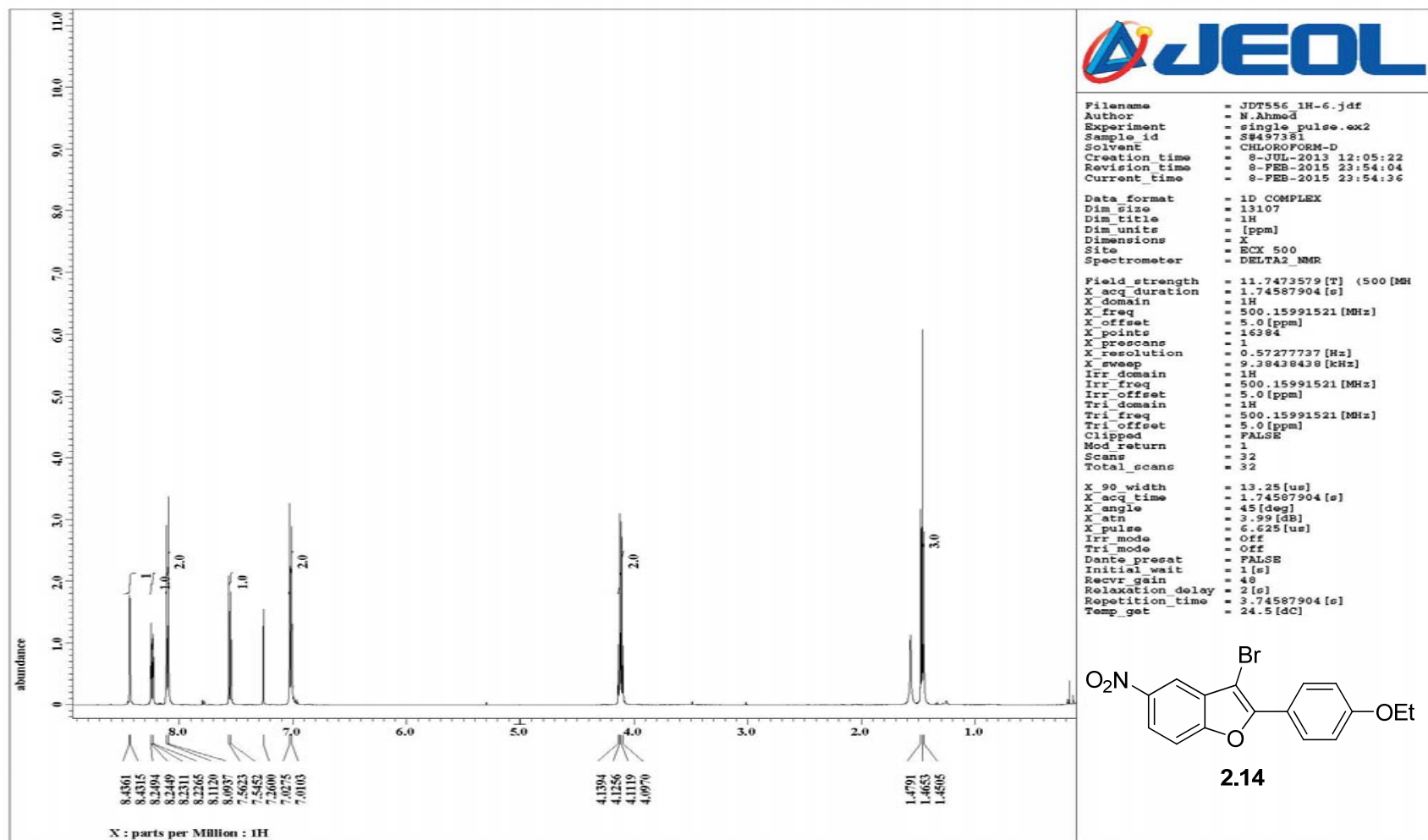
125 MHz ^{13}C NMR spectrum of compound **2.12**



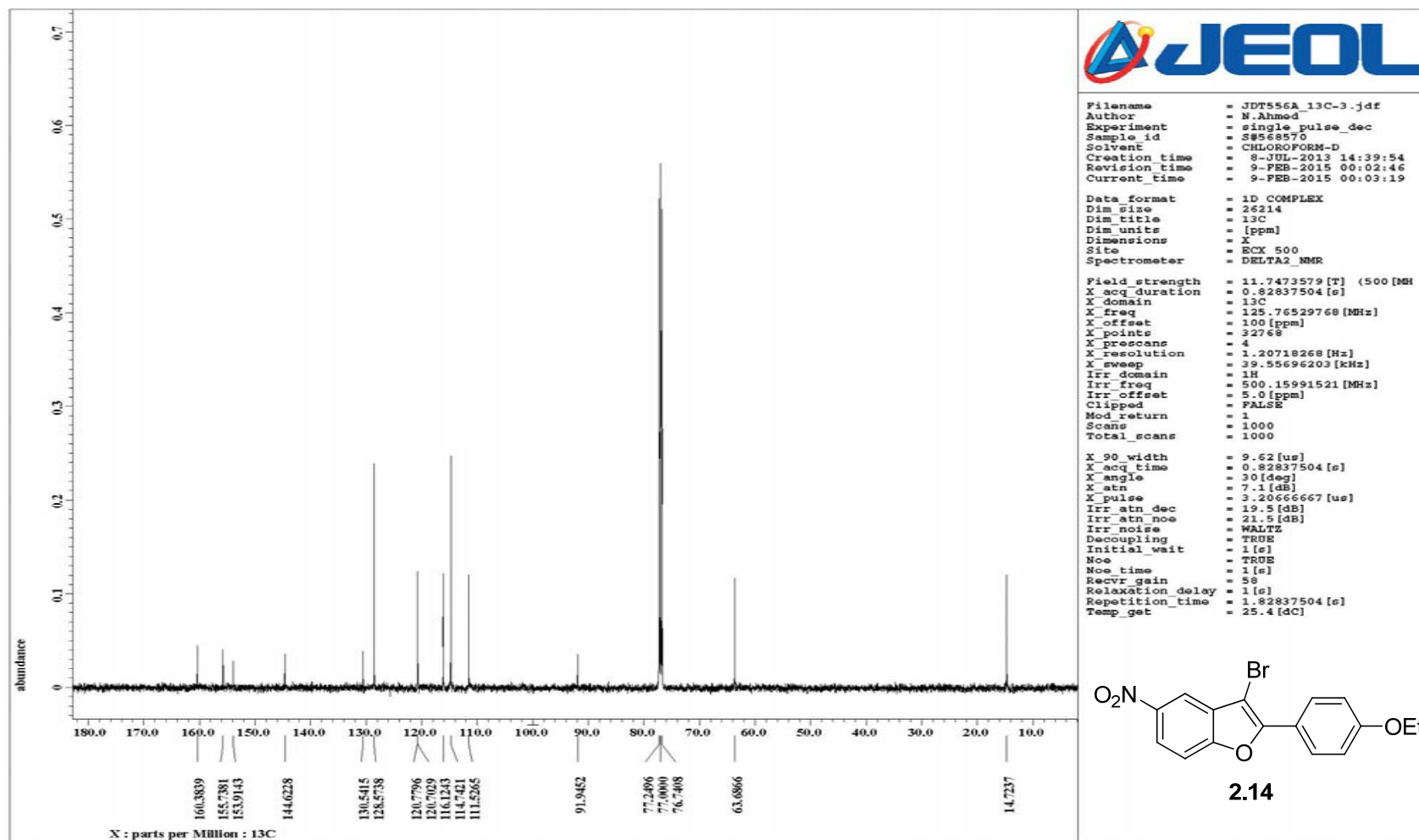
500 MHz ^1H NMR spectrum of compound **2.13**



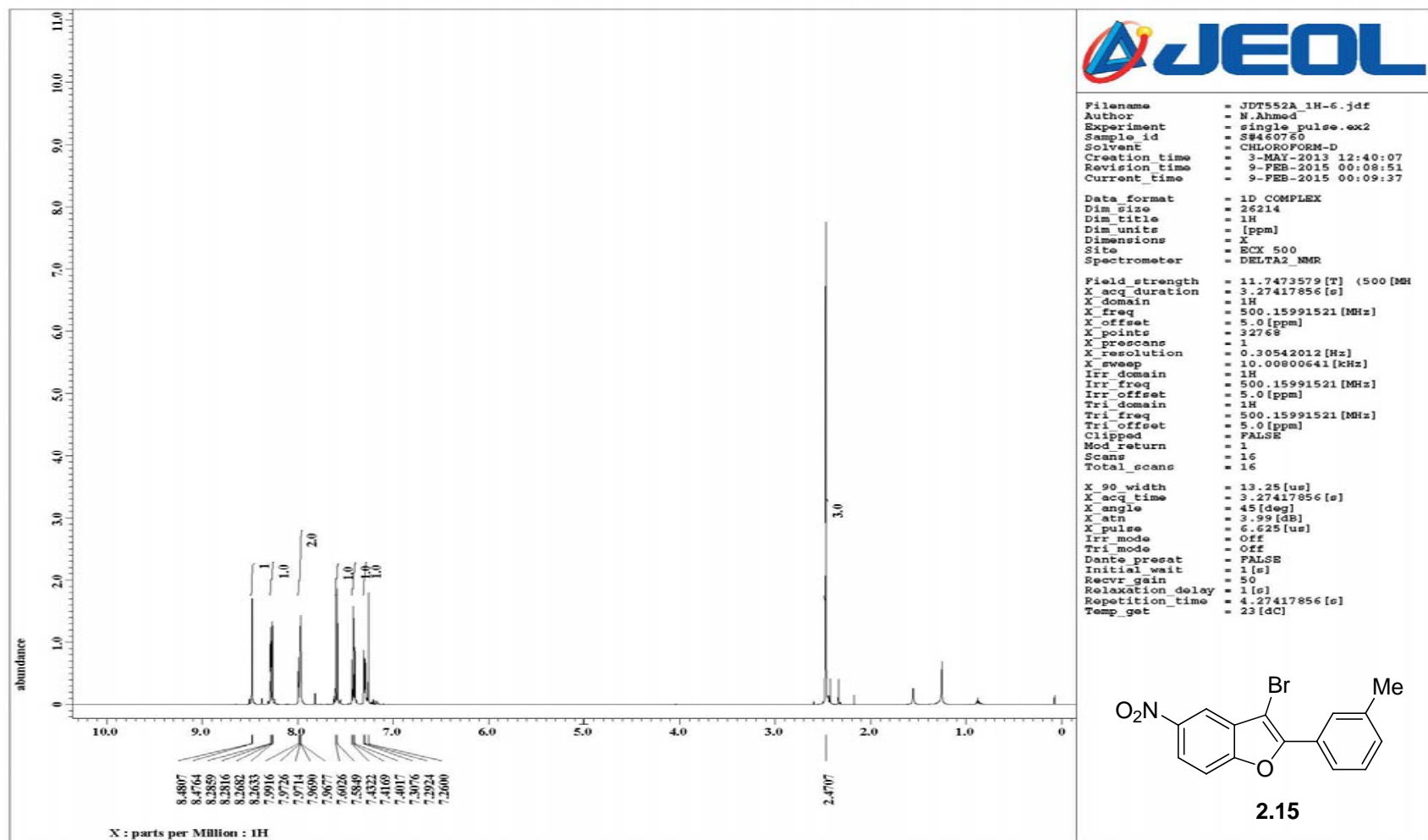
125 MHz ^{13}C NMR spectrum of compound **2.13**



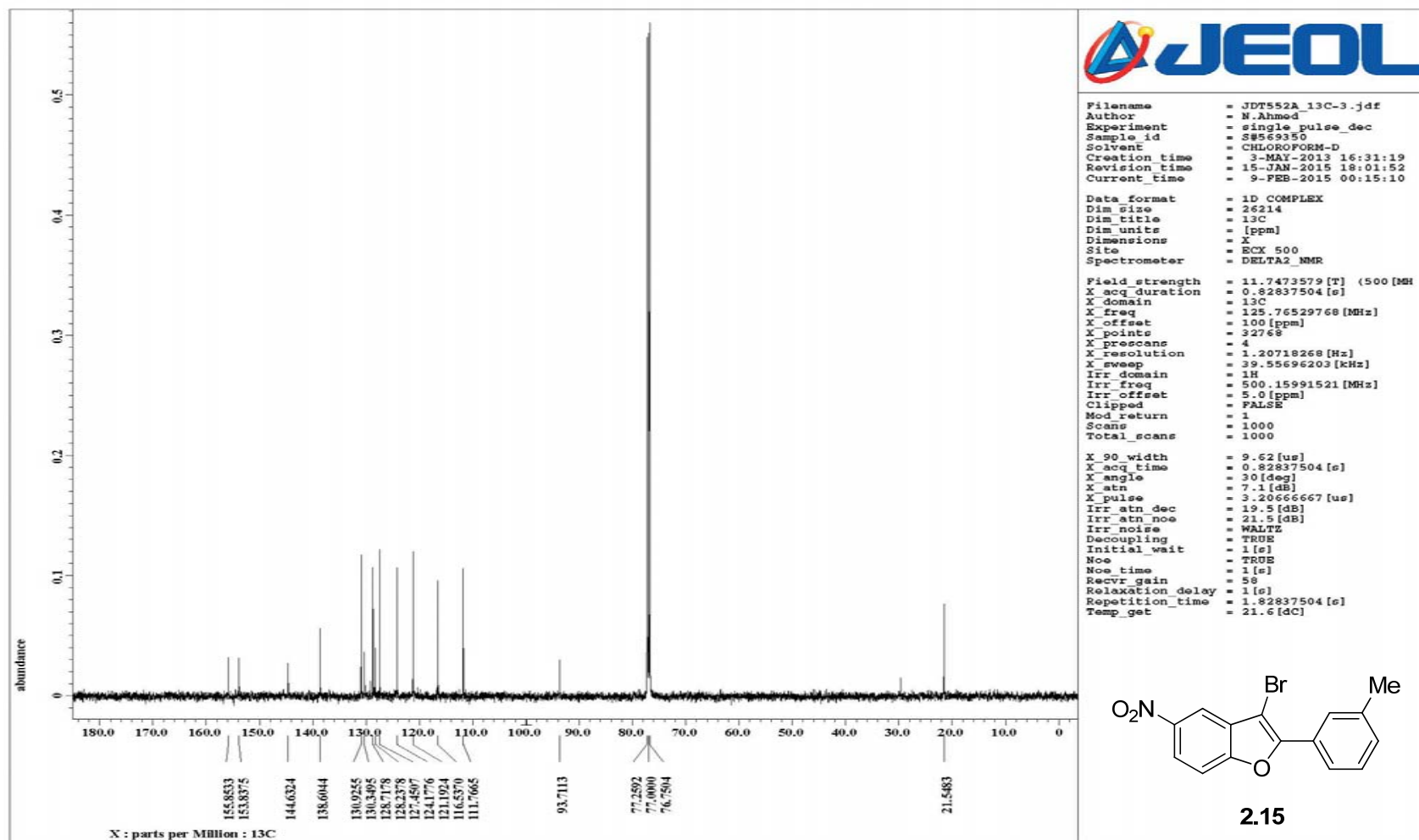
500 MHz ^1H NMR spectrum of compound **2.14**



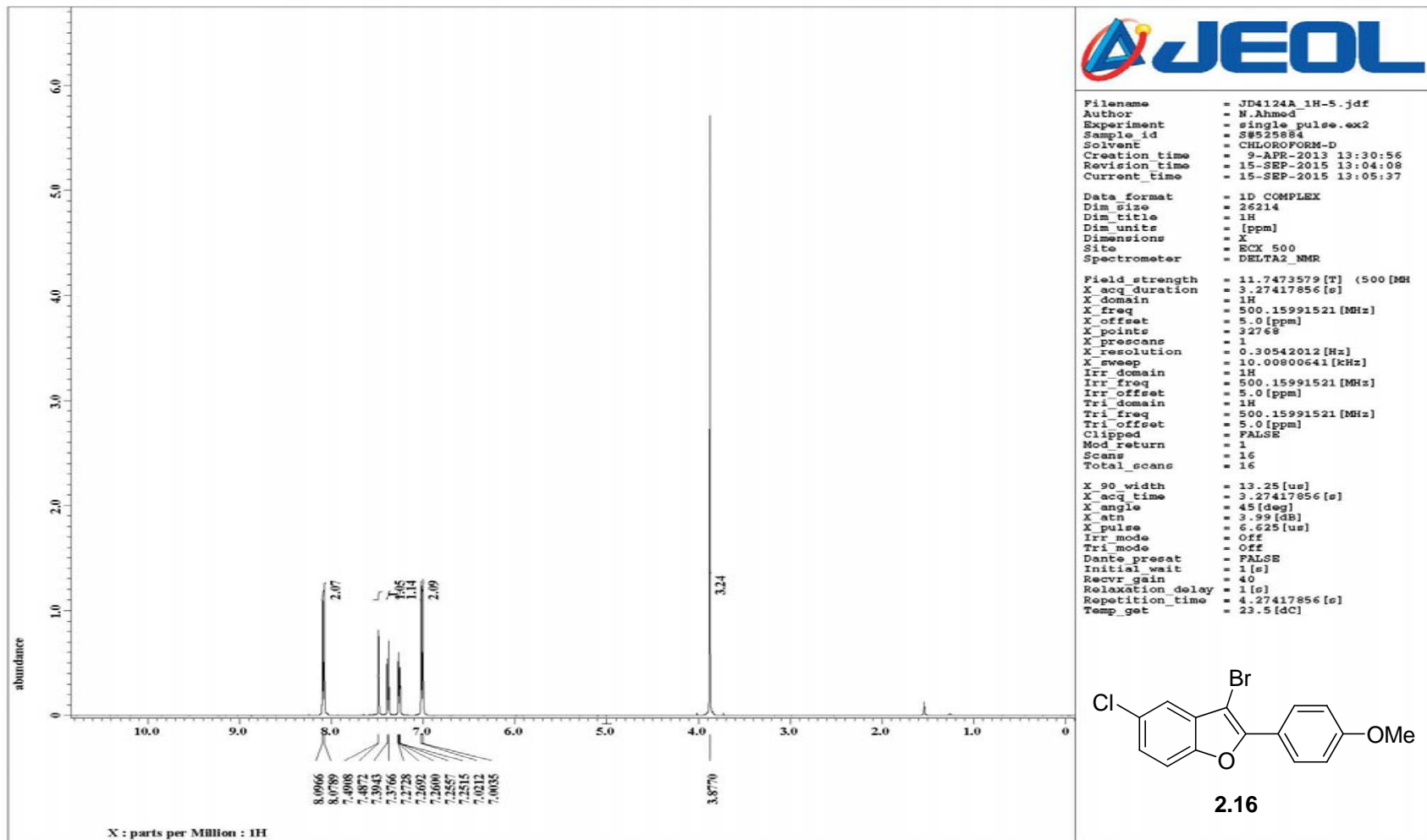
125 MHz ^{13}C NMR spectrum of compound **2.14**



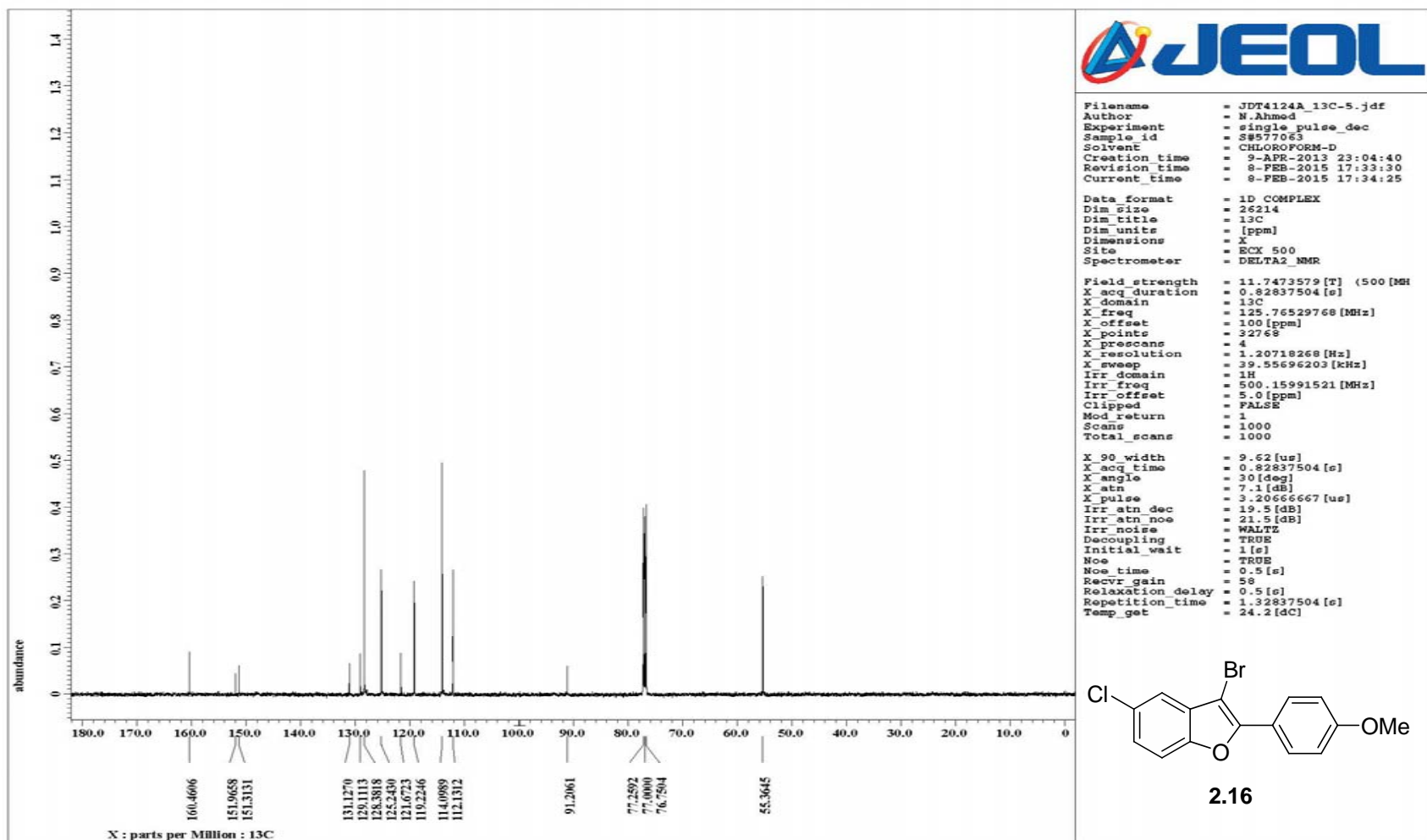
500 MHz ¹H NMR spectrum of compound **2.15**



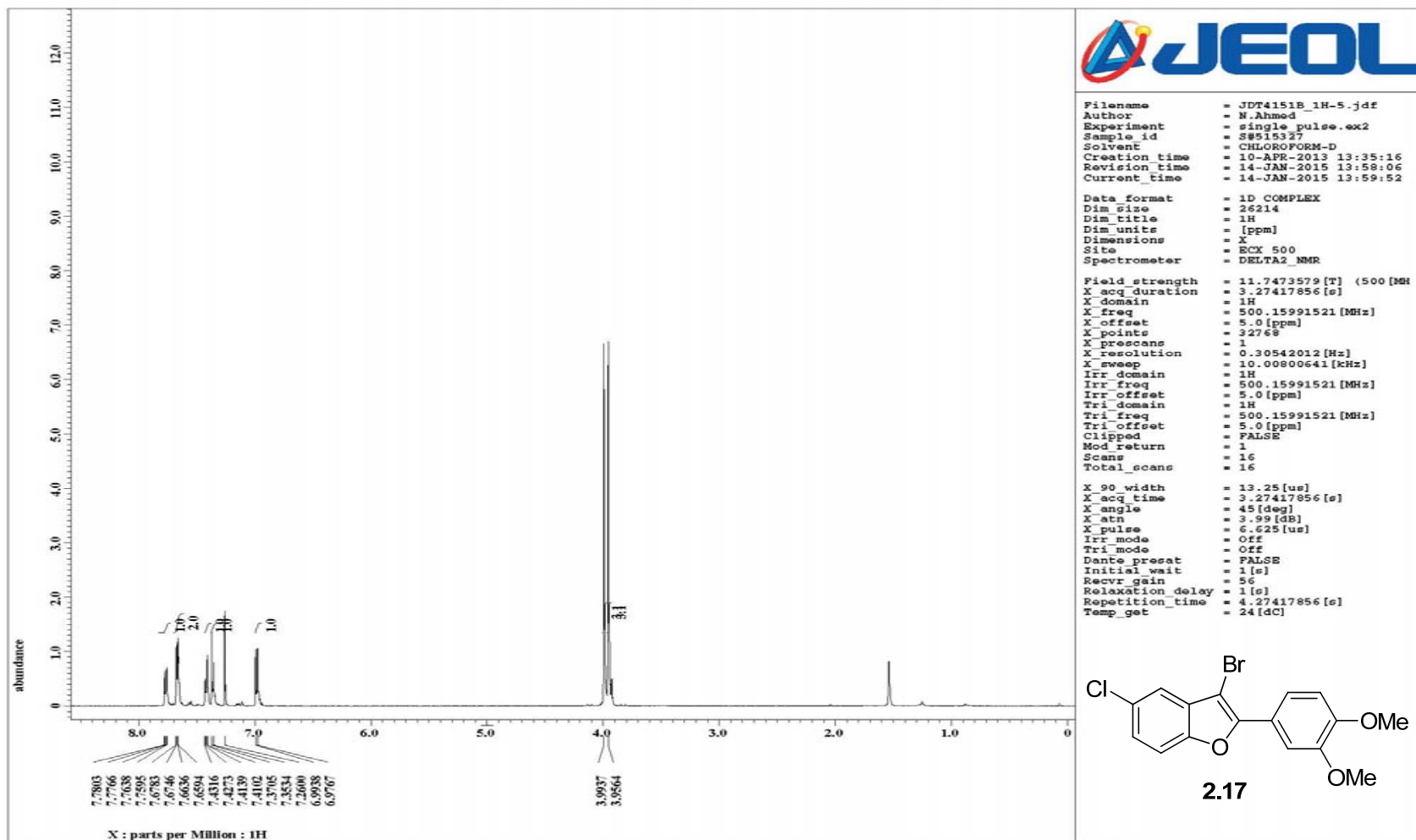
125 MHz ^{13}C NMR spectrum of compound **2.15**



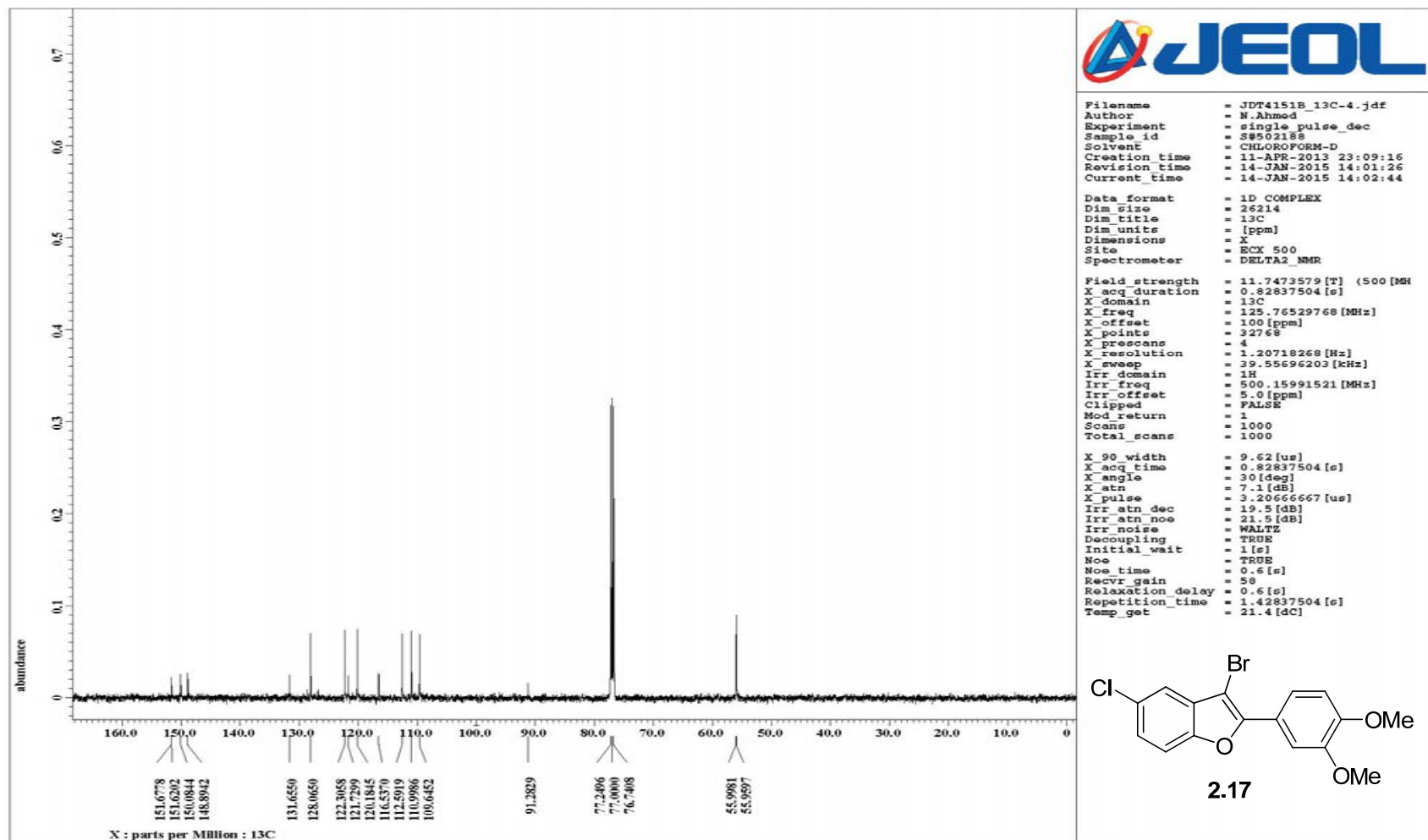
500 MHz ^1H NMR spectrum of compound **2.16**



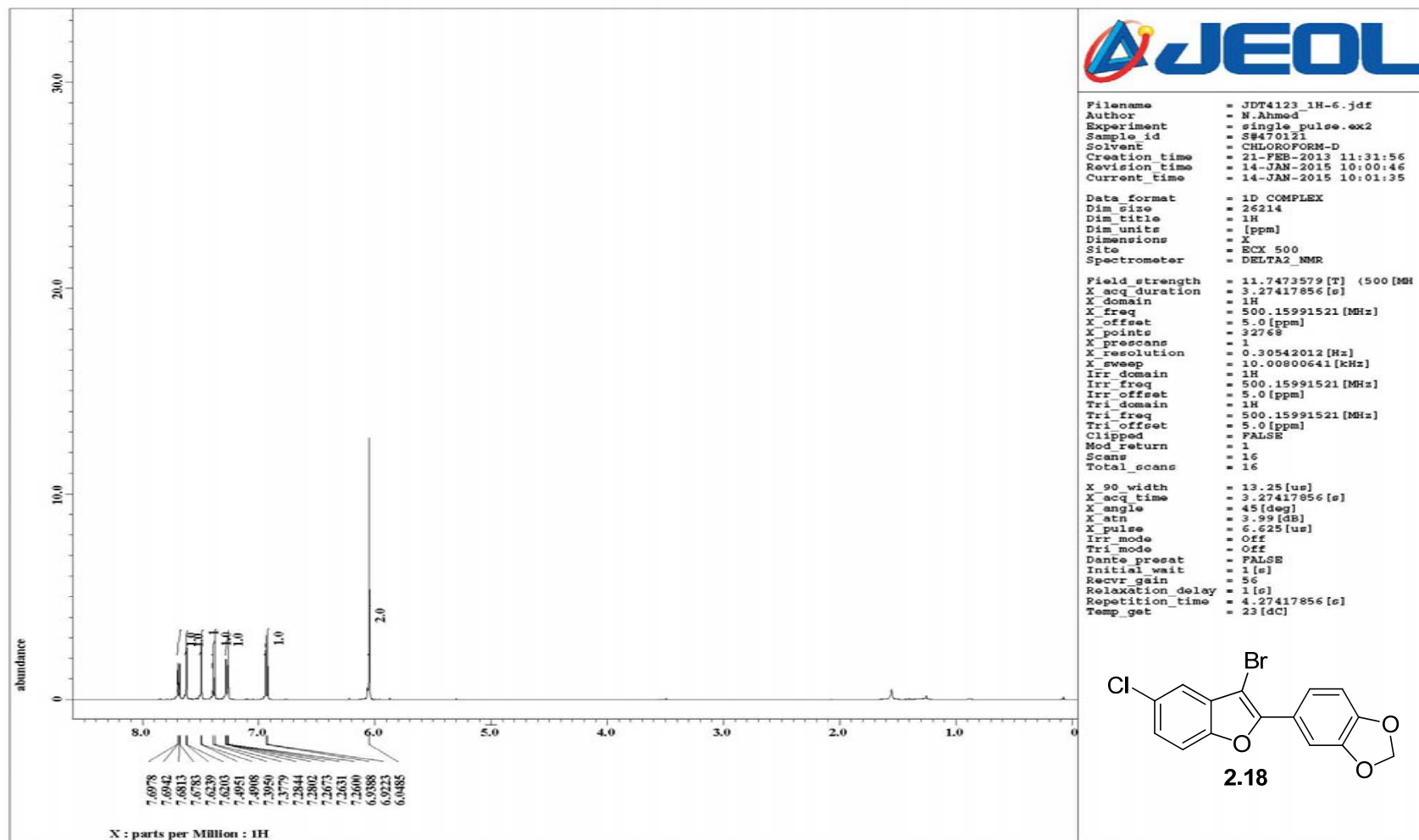
125 MHz ^{13}C NMR spectrum of compound **2.16**



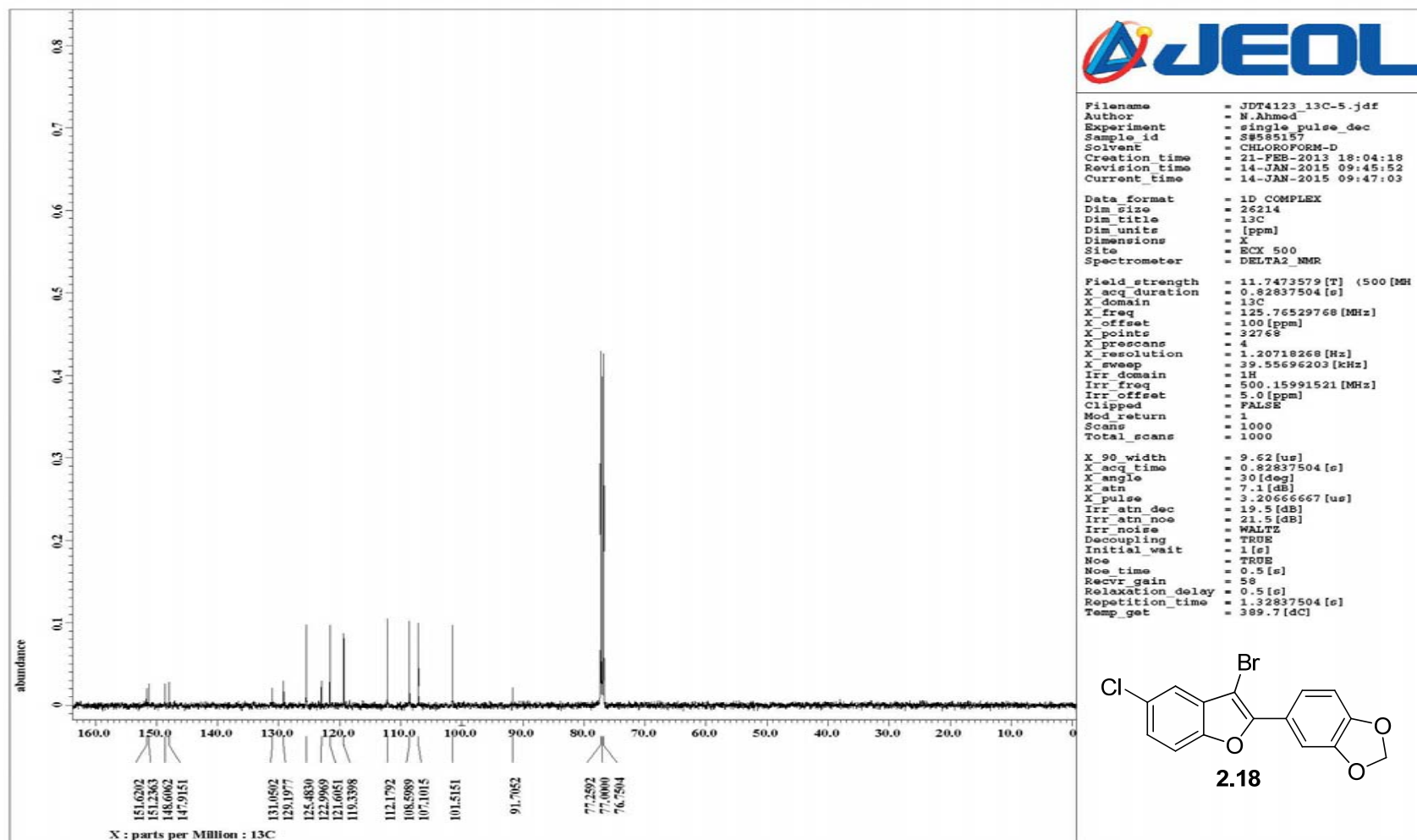
500 MHz ^1H NMR spectrum of compound **2.17**



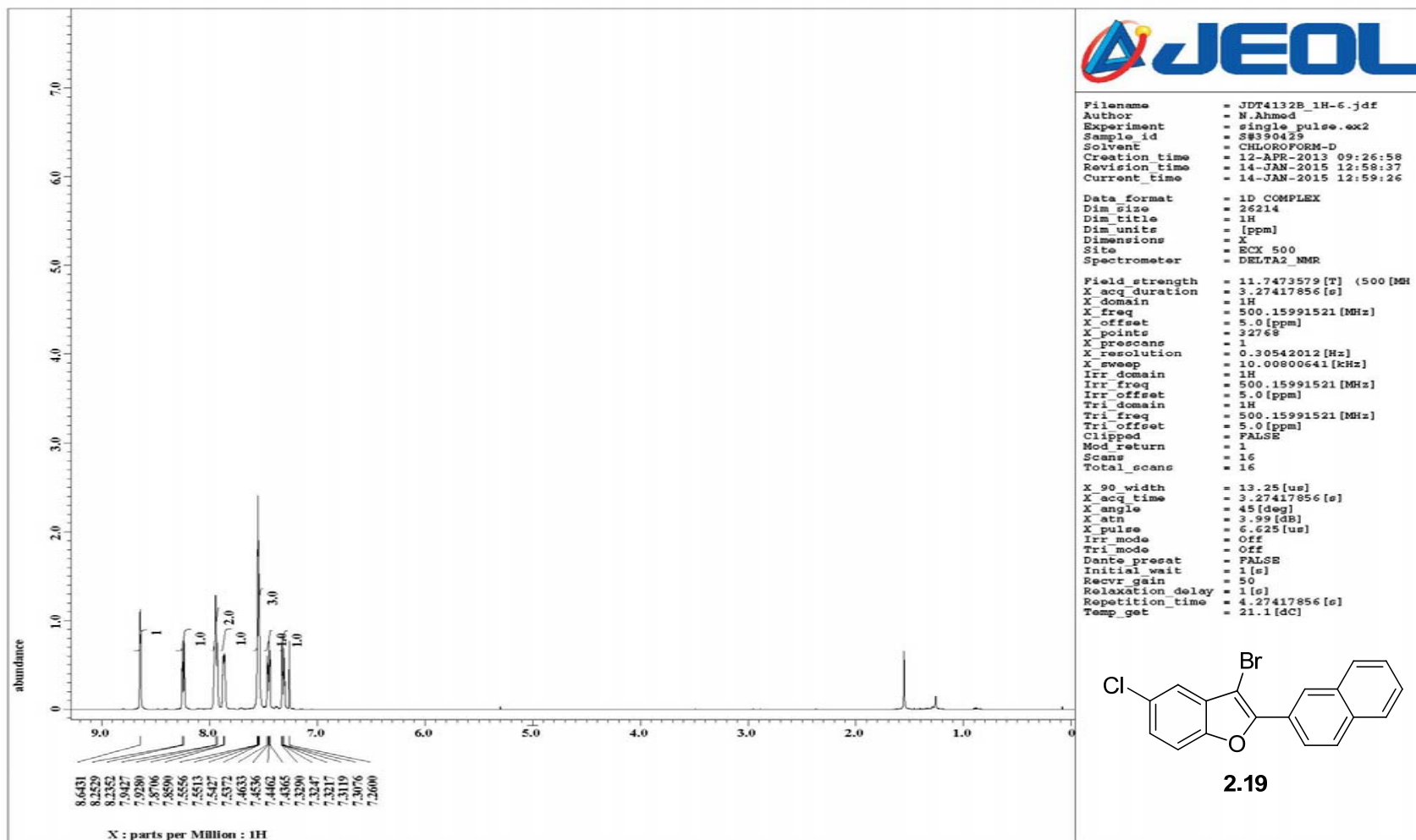
125 MHz ^{13}C NMR spectrum of compound **2.17**



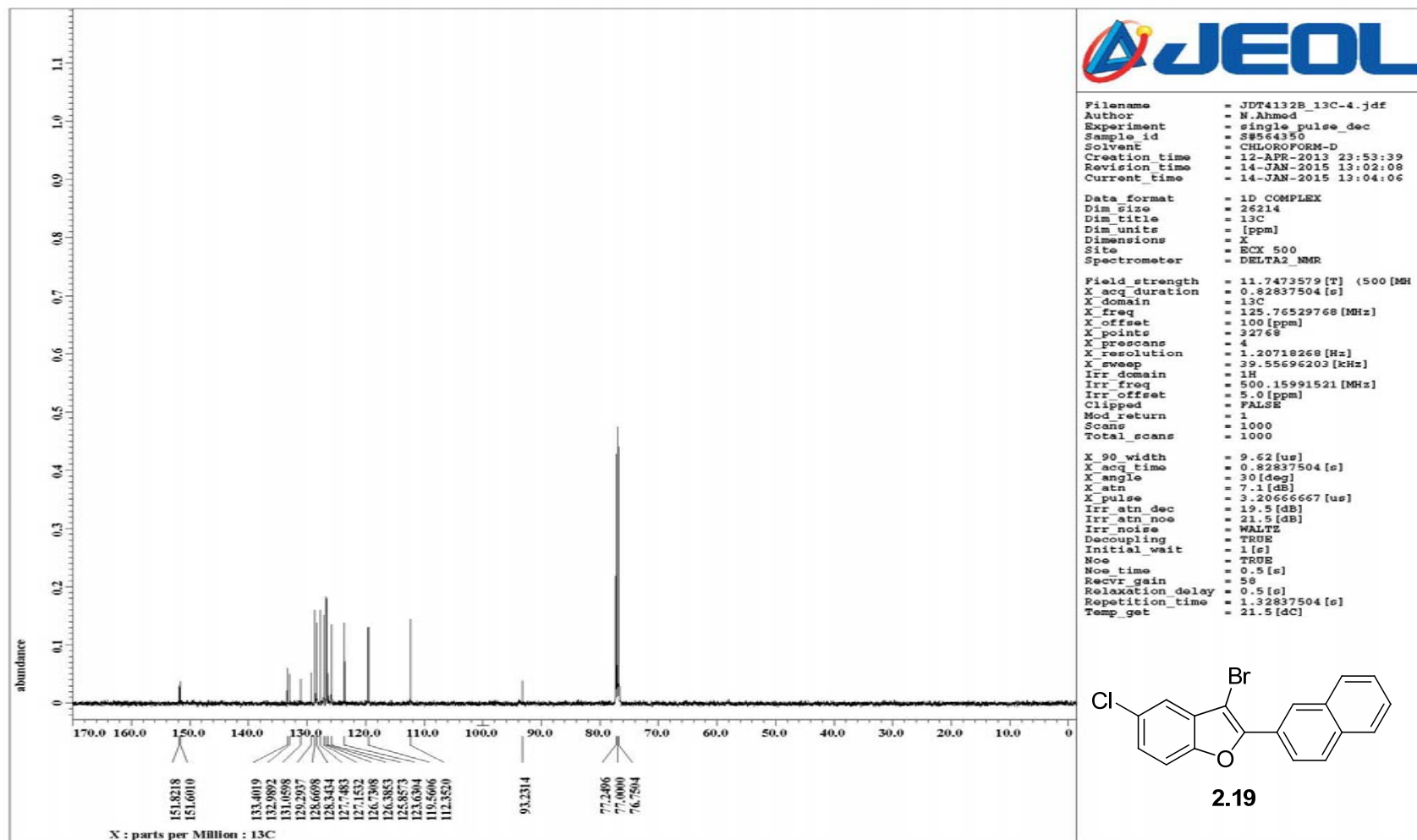
500 MHz ^1H NMR spectrum of compound **2.18**



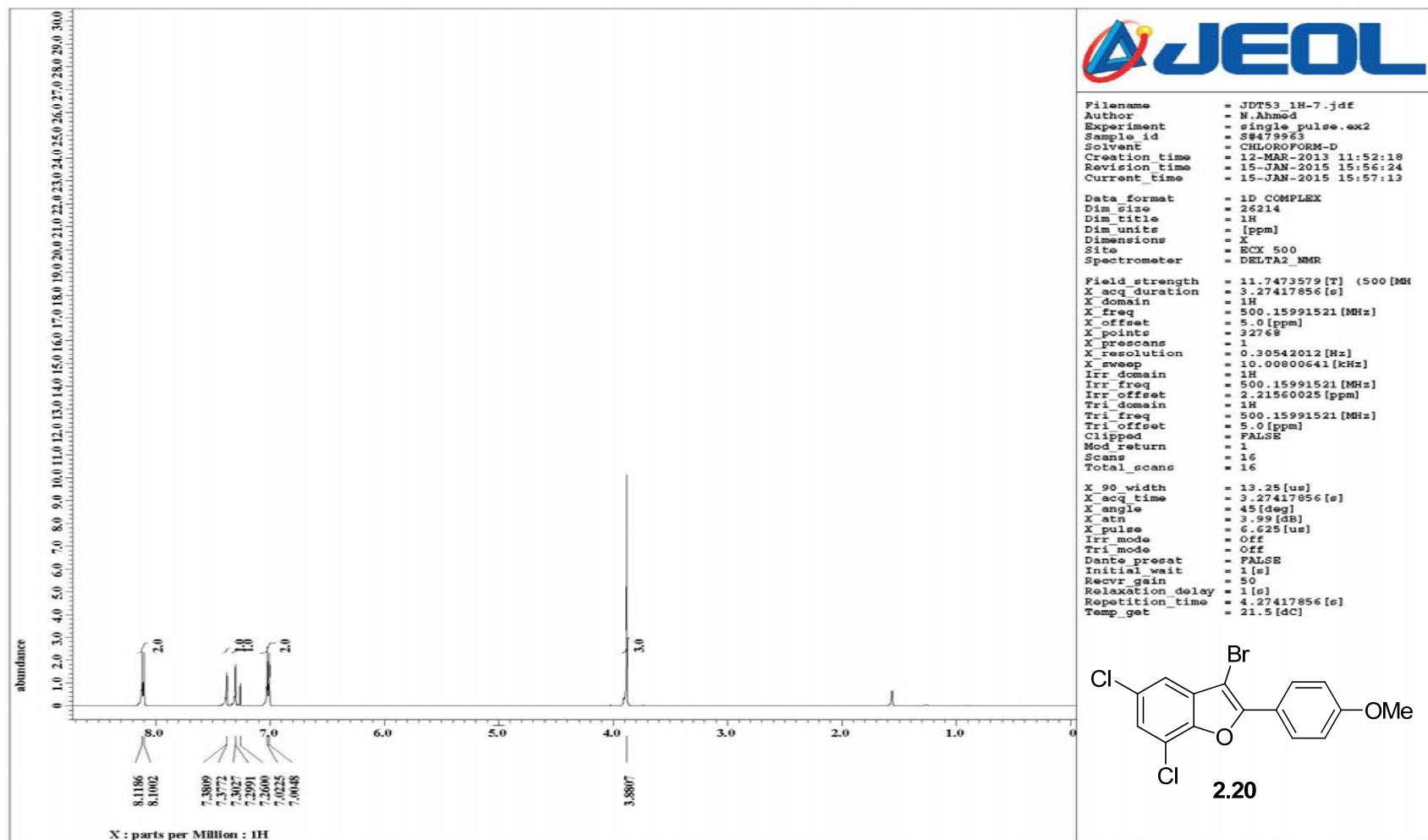
125 MHz ^{13}C NMR spectrum of compound **2.18**



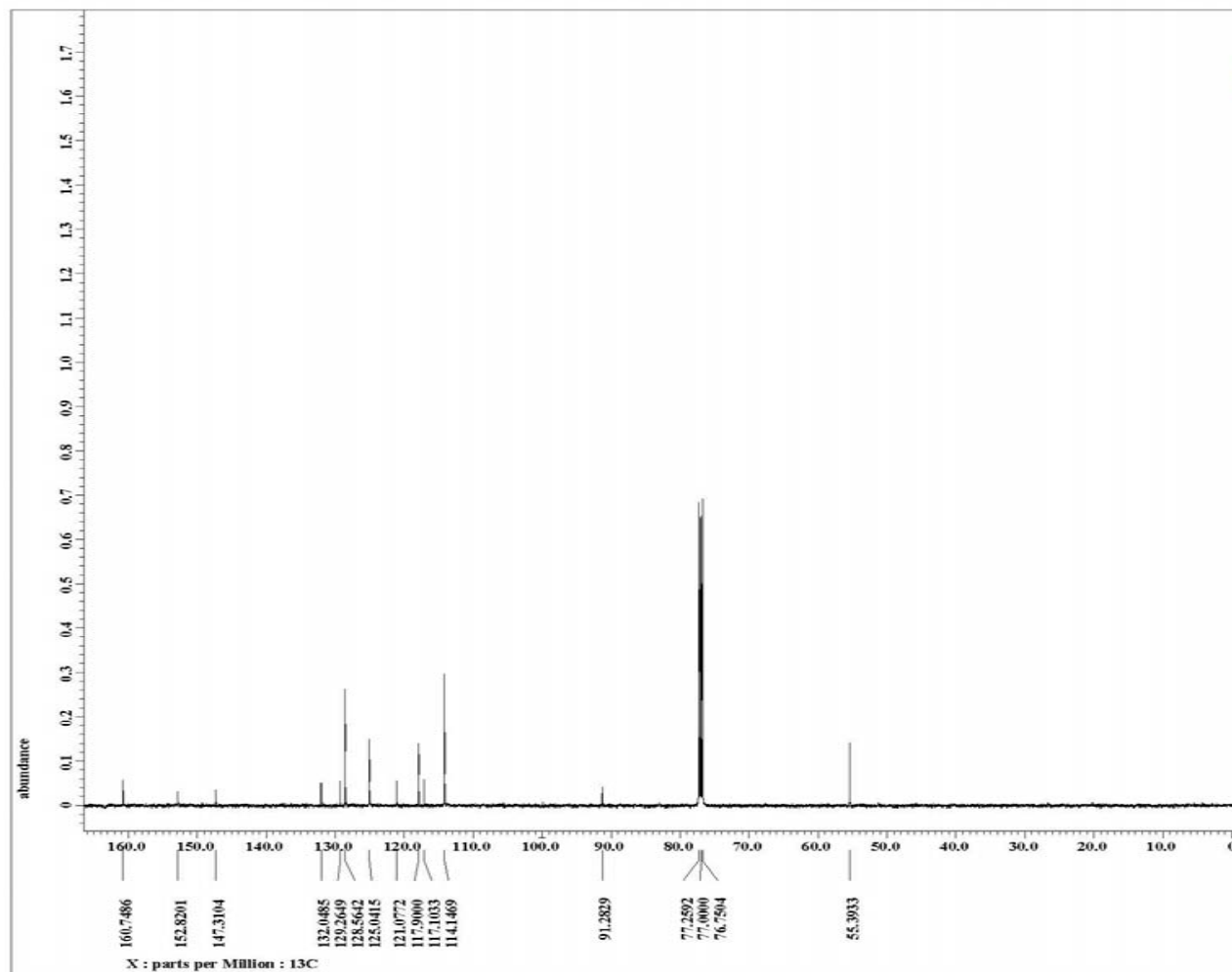
500 MHz ^1H NMR spectrum of compound **2.19**



125 MHz ^{13}C NMR spectrum of compound **2.19**



500 MHz ^1H NMR spectrum of compound **2.20**



```

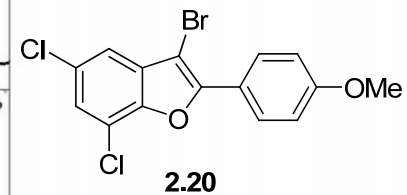
Filename      = JDT53_13C-3.jdr
Author       = M.Ahmed
Experiment   = single pulse_dec
Sample id    = S#577406
Solvent      = CHLOROFORM-D
Creation time = 12-MAR-2013 16:11:35
Revision time = 15-JAN-2015 15:59:59
Current time  = 15-JAN-2015 16:01:06

Data format  = 1D COMPLEX
Dim Size     = 26214
Dim title    = 13C
Dim units    = [ppm]
Dimensions   = X
Site         = ECX 500
Spectrometer = DELTA2_NMR

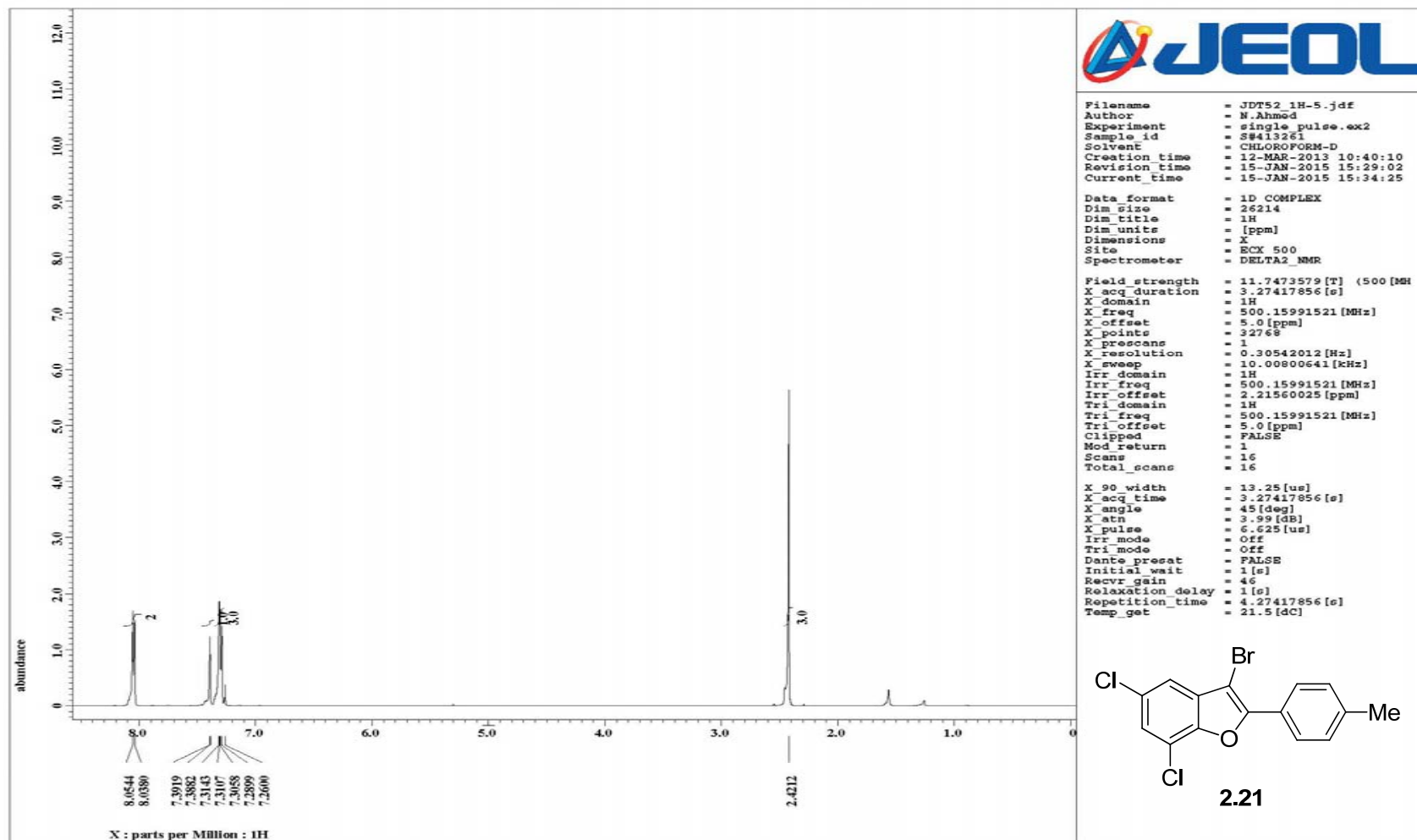
Field strength = 11.7473579 [T] (500 [MH]
X_acq duration = 0.82837504 [s]
X_domain      = 13C
X_freq        = 125.76529768 [MHz]
X_offset      = 100 [ppm]
X_points      = 32768
X_prescans    = 4
X_resolution  = 1.20718268 [Hz]
X_sweep       = 39.55696203 [kHz]
Irr_domain    = 1H
Irr_freq      = 500.15991521 [MHz]
Irr_offset    = 5.0 [ppm]
Clipped       = FALSE
Mod_return    = 1
Scans         = 1000
Total_scans   = 1000

X_90_width   = 9.62 [us]
X_acq time    = 0.82837504 [s]
X_angle      = 30 [deg]
X_atn        = 7.1 [dB]
X_pulse      = 3.20666667 [us]
Irr_atn_dec  = 19.5 [dB]
Irr_atn_noe  = 21.5 [dB]
Irr_noise    = WALTZ
Decoupling    = TRUE
Initial wait  = 1 [s]
Noe          = TRUE
Noe time     = 1 [s]
Recvr gain   = 60
Relaxation delay = 1 [s]
Repetition_time = 1.82837504 [s]
Temp_get     = 22 [dC]

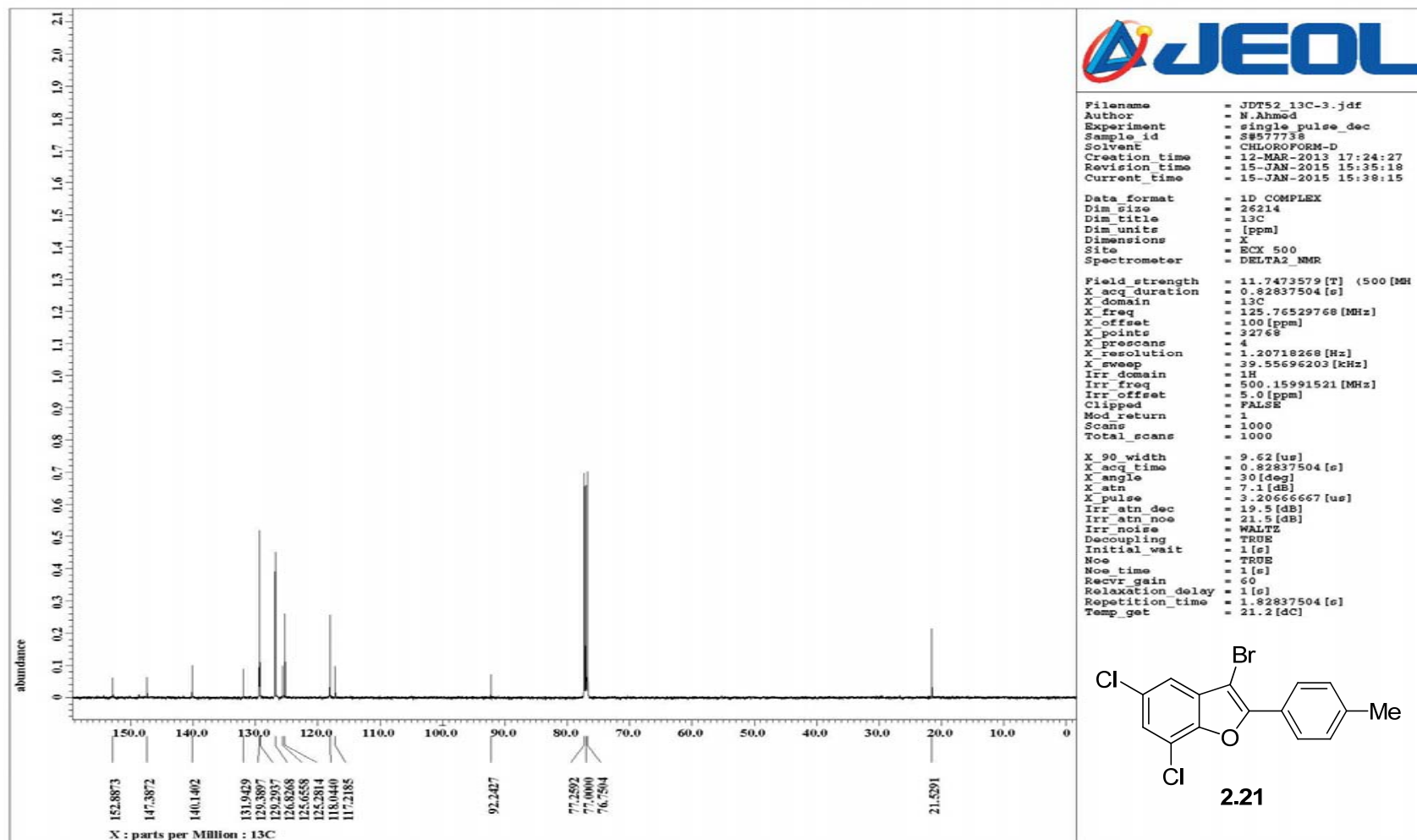
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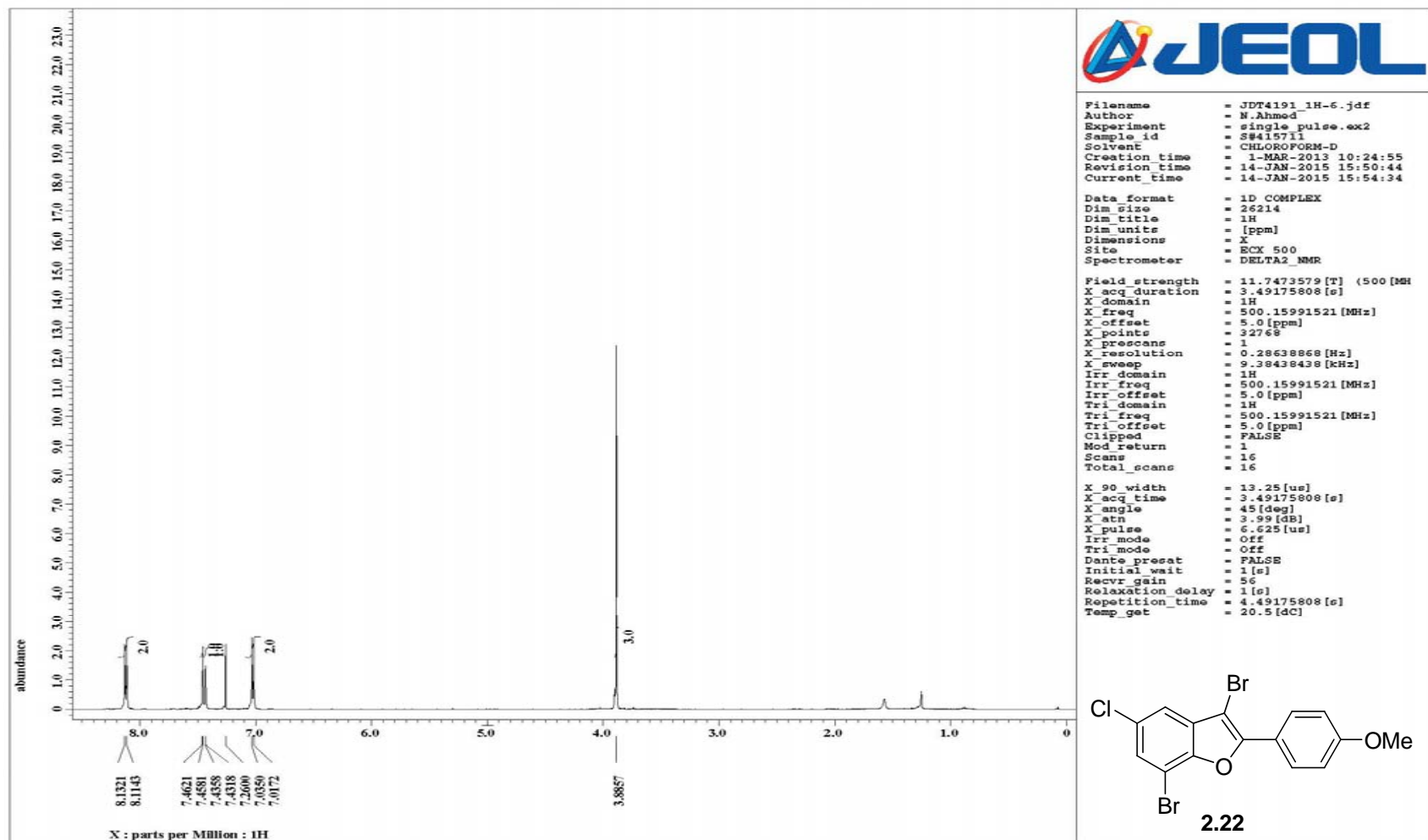
125 MHz ^{13}C NMR spectrum of compound **2.20**



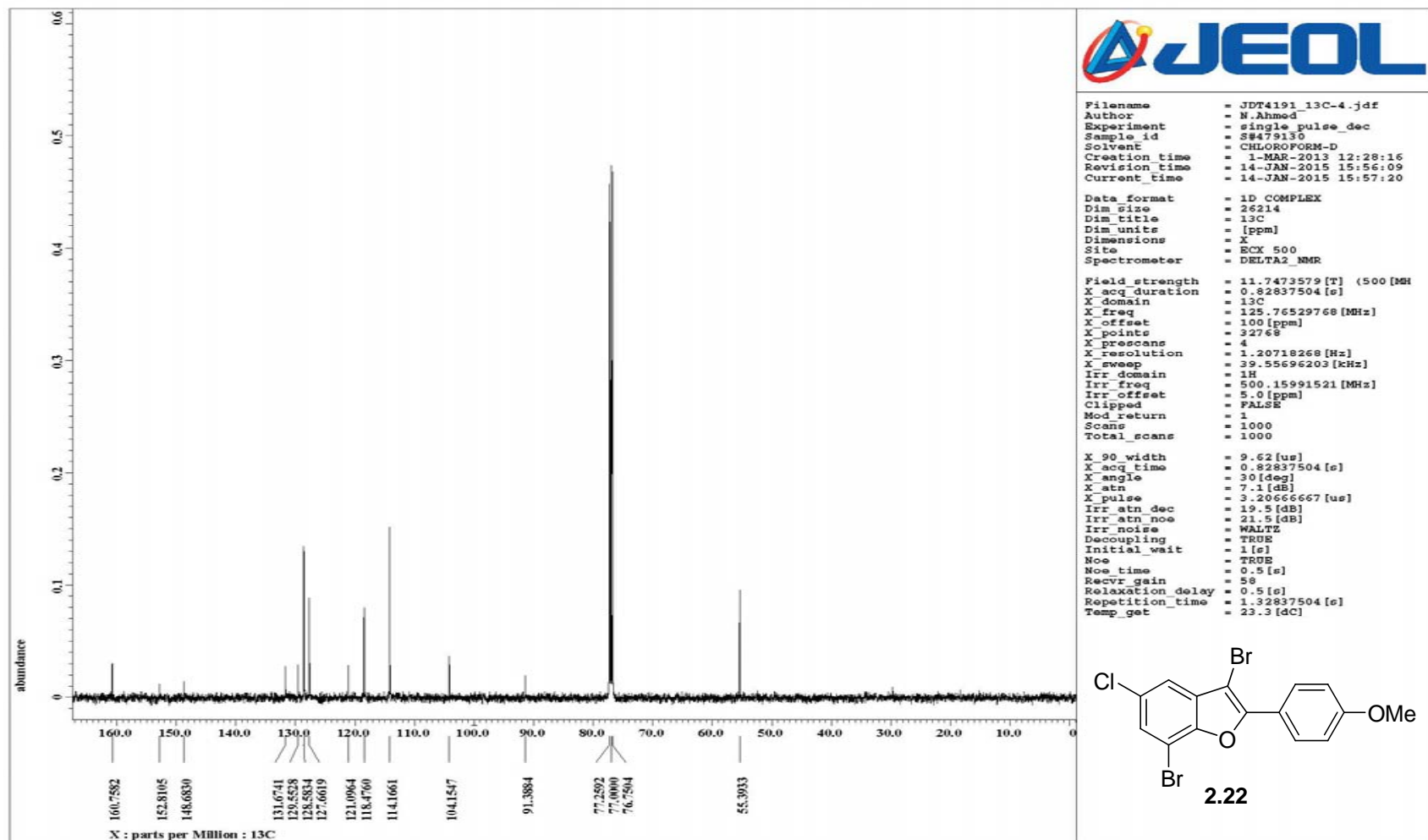
500 MHz ^1H NMR spectrum of compound **2.21**



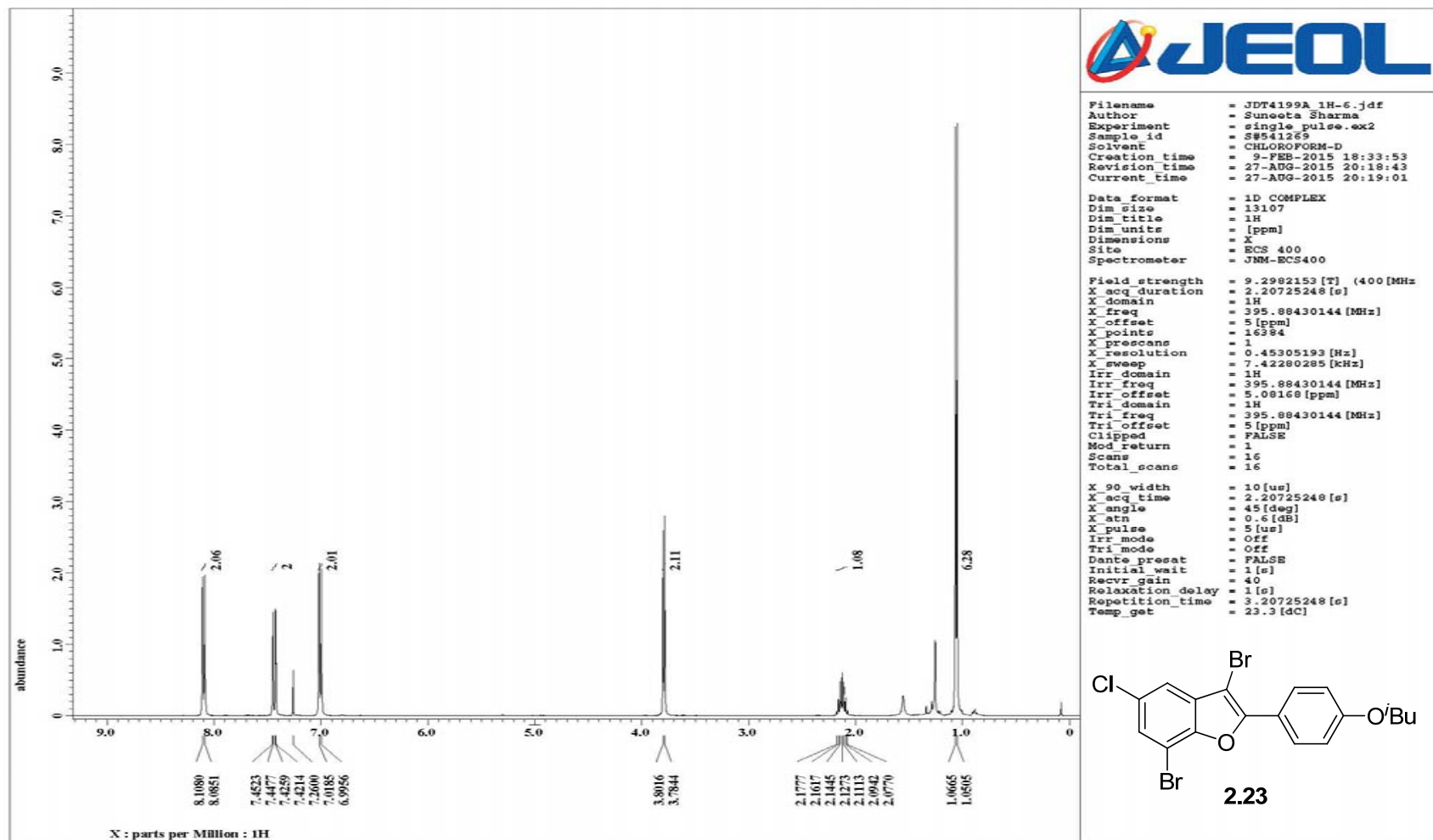
125 MHz ^{13}C NMR spectrum of compound **2.21**



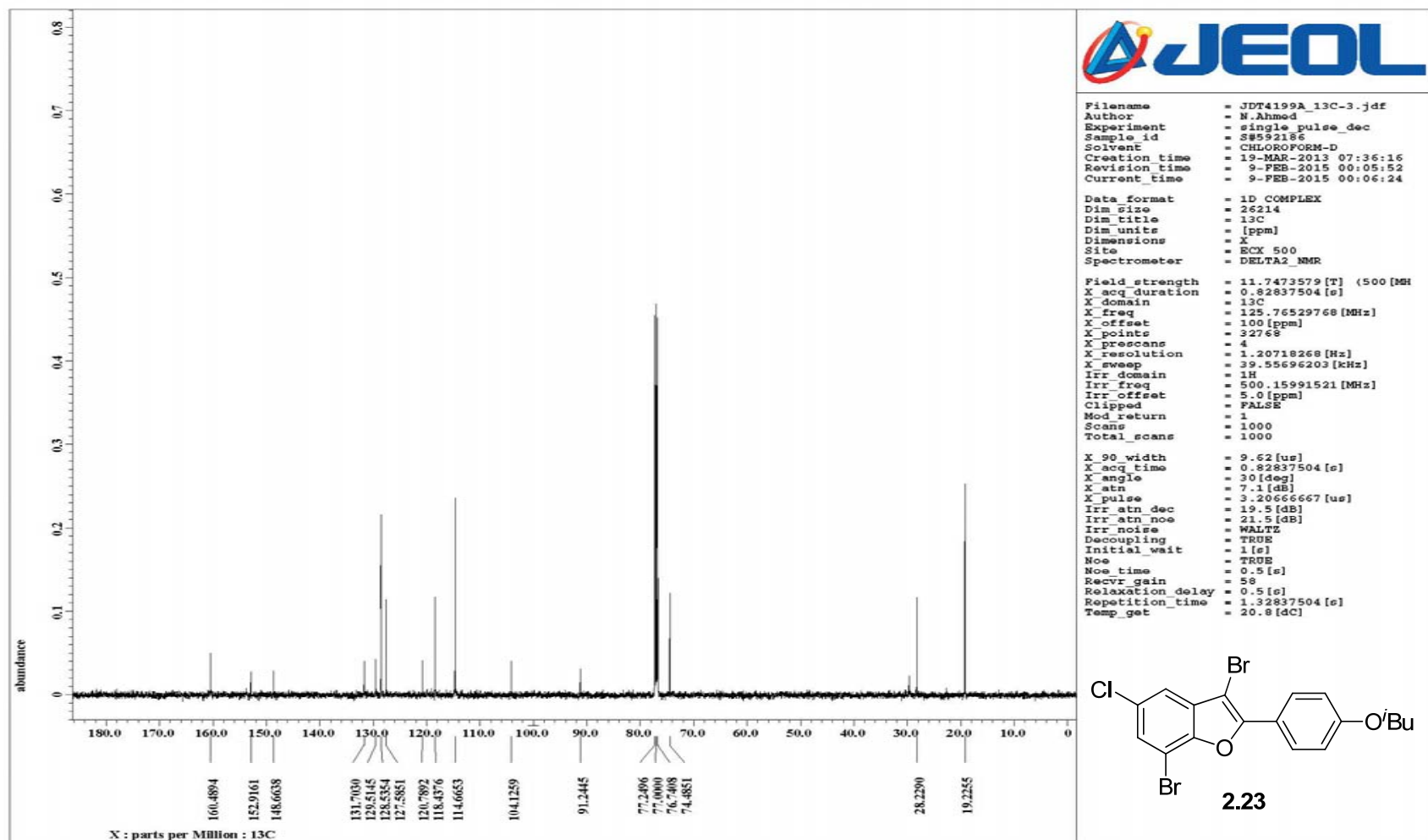
500 MHz ¹H NMR spectrum of compound **2.22**



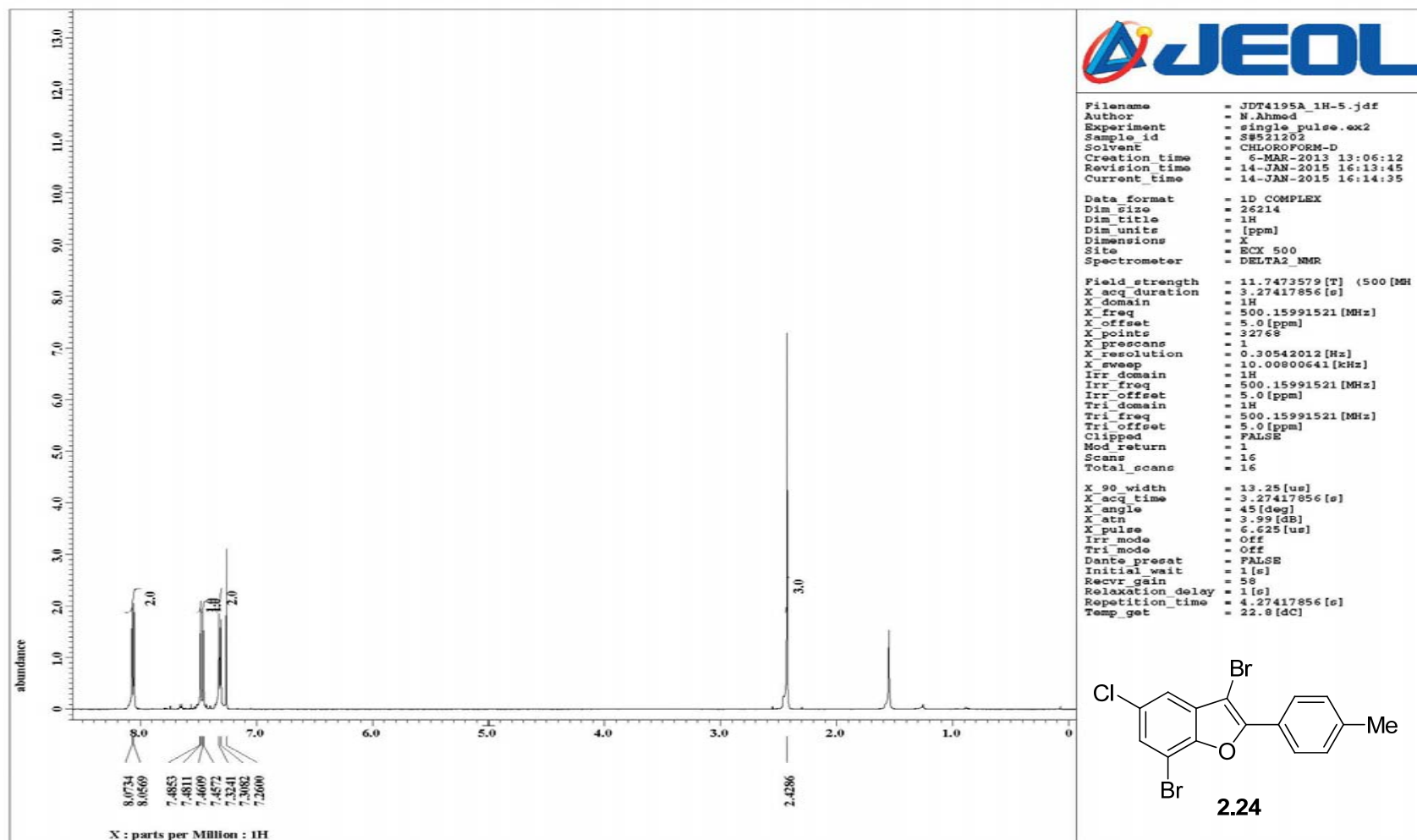
125 MHz ^{13}C NMR spectrum of compound **2.22**



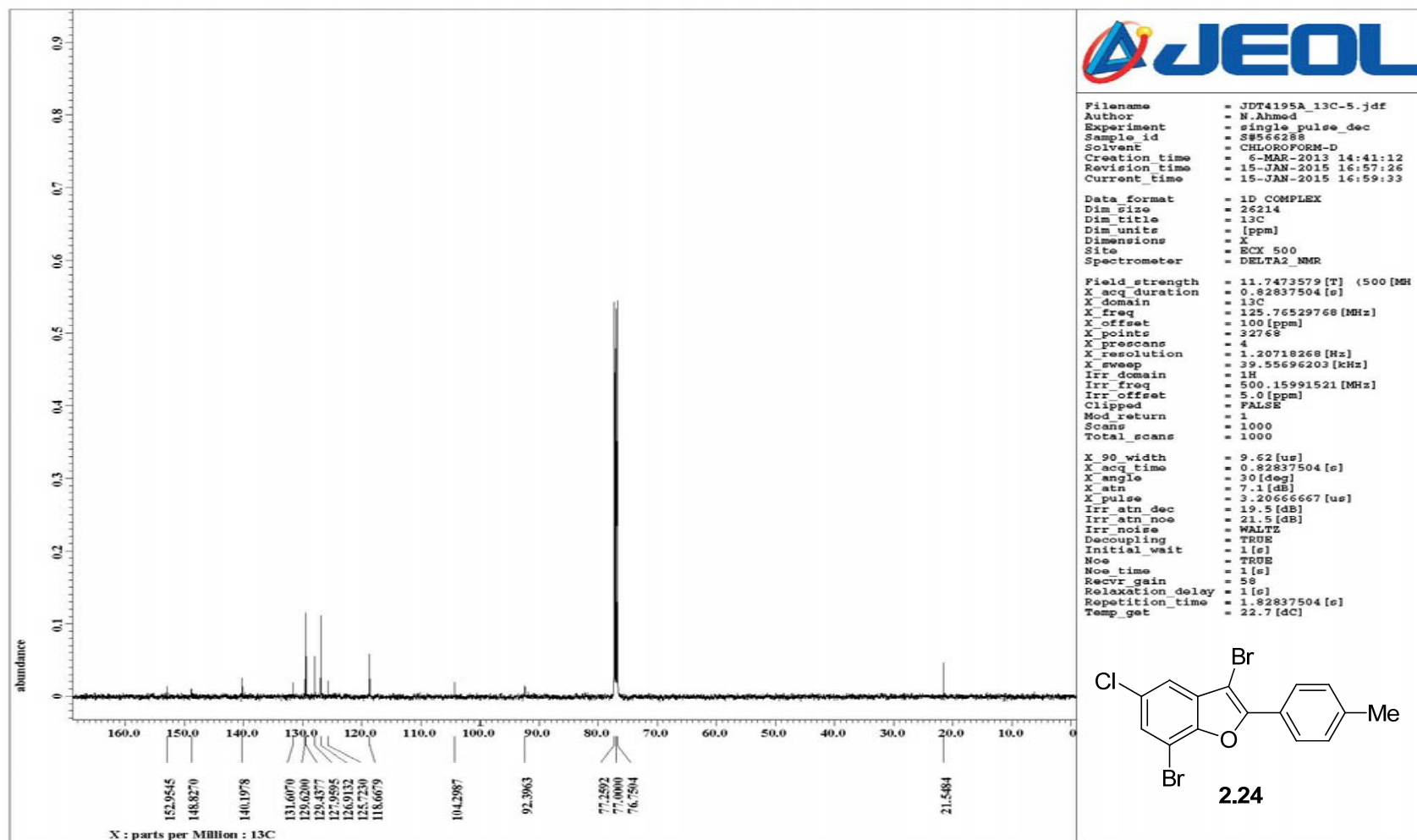
400 MHz ¹H NMR spectrum of compound **2.23**



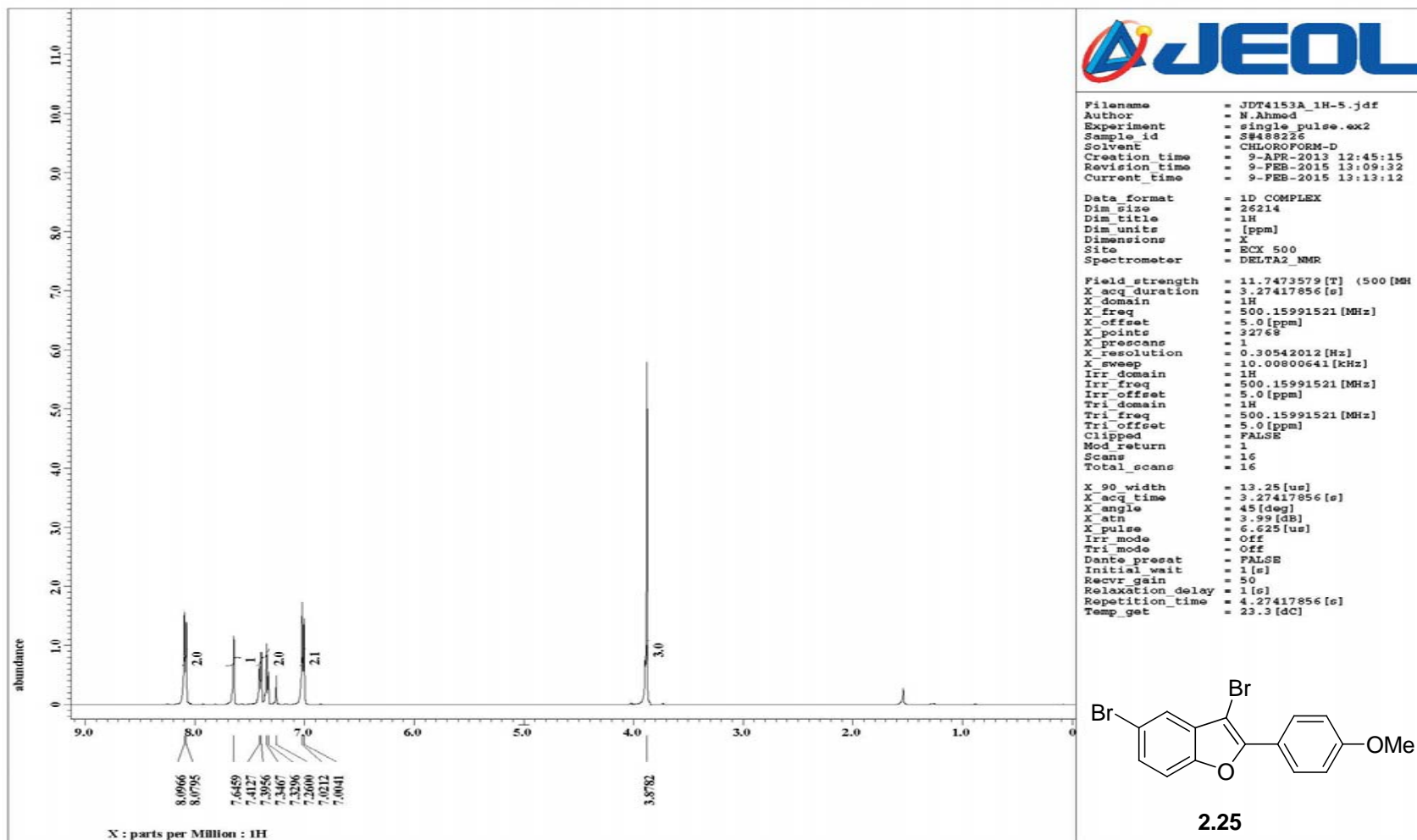
125 MHz ^{13}C NMR spectrum of compound **2.23**



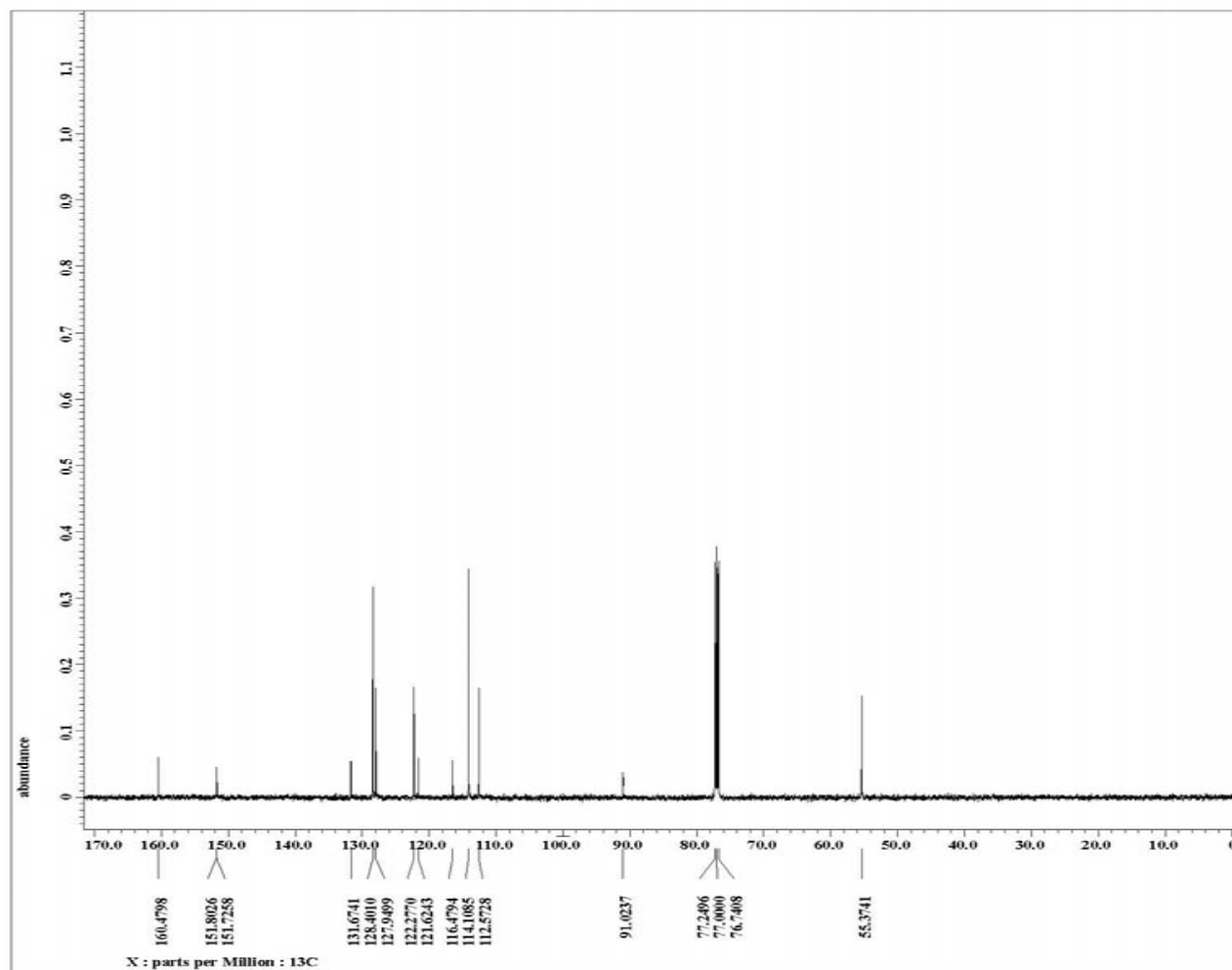
500 MHz ^1H NMR spectrum of compound **2.24**



125 MHz ^{13}C NMR spectrum of compound **2.24**



500 MHz ^1H NMR spectrum of compound **2.25**



```

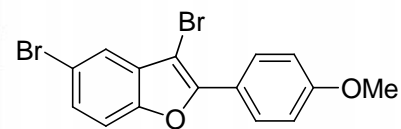
Filename      = JDT4153A_13C-3.jdf
Author       = N.Ahmed
Experiment    = single_pulse_dec
Sample id    = S#576839
Solvent      = CHLOROFORM-D
Creation time = 9-APR-2013 22:36:27
Revision time = 9-FEB-2015 12:46:16
Current time  = 9-FEB-2015 12:46:42

Data format   = 1D COMPLEX
Dim size      = 26214
Dim title     = 13C
Dim units     = [ppm]
Dimensions    = X
Site          = ECX 500
Spectrometer  = DELTA2_NMR

Field strength = 11.7473579 [T] (500 [MH]
X_acq duration = 0.82837504 [s]
X_domain      = 13C
X_freq        = 125.76529768 [MHz]
X_offset      = 100 [ppm]
X_points      = 32768
X_prescans    = 4
X_resolution  = 1.20718268 [Hz]
X_sweep       = 39.55696203 [kHz]
Irr_domain    = 1H
Irr_freq      = 500.15991521 [MHz]
Irr_offset    = 5.0 [ppm]
Clipped       = FALSE
Mod_return    = 1
Scans         = 1000
Total_scans   = 1000

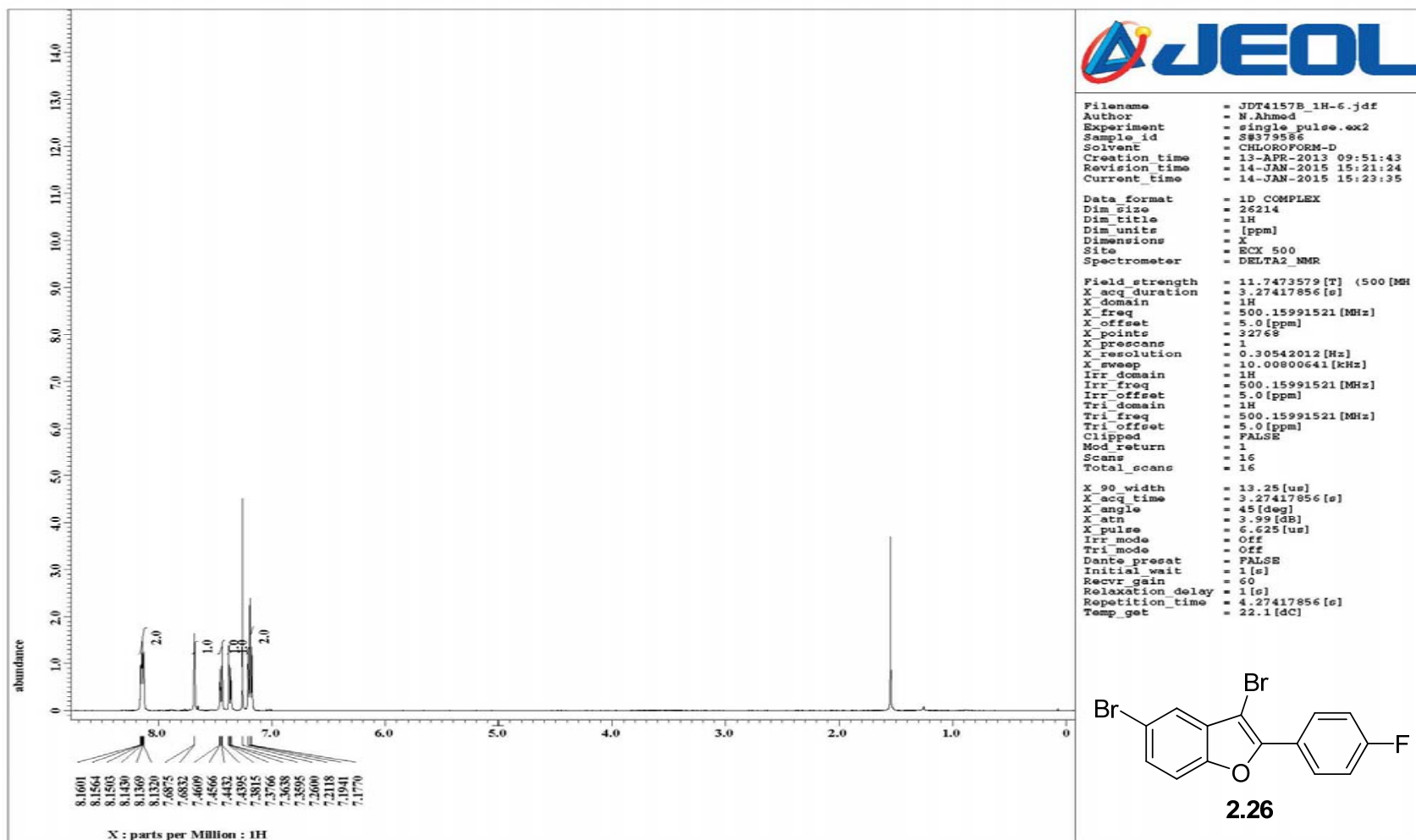
X_90_width   = 9.62 [us]
X_acq time    = 0.82837504 [s]
X_angle       = 30 [deg]
X_atn         = 7.1 [dB]
X_pulse       = 3.20666667 [us]
Irr_atn_dec   = 19.5 [dB]
Irr_atn_noe   = 21.5 [dB]
Irr_noise     = WALTZ
Decoupling    = TRUE
Initial wait  = 1 [s]
Noe           = TRUE
Noe time      = 0.5 [s]
Recvr gain    = 58
Relaxation delay = 0.5 [s]
Repetition_time = 1.32837504 [s]
Temp_get      = 24.2 [dC]

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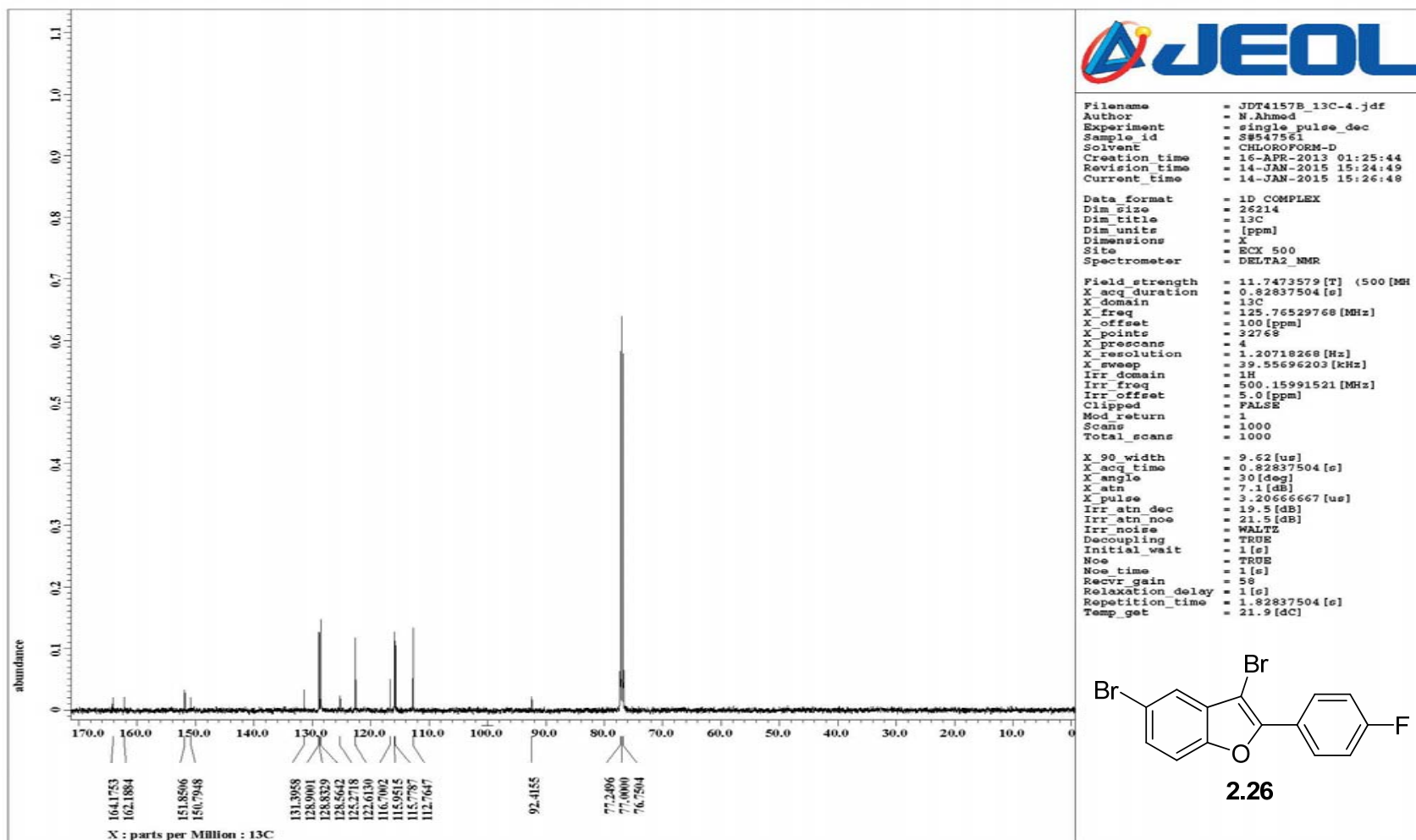


2.25

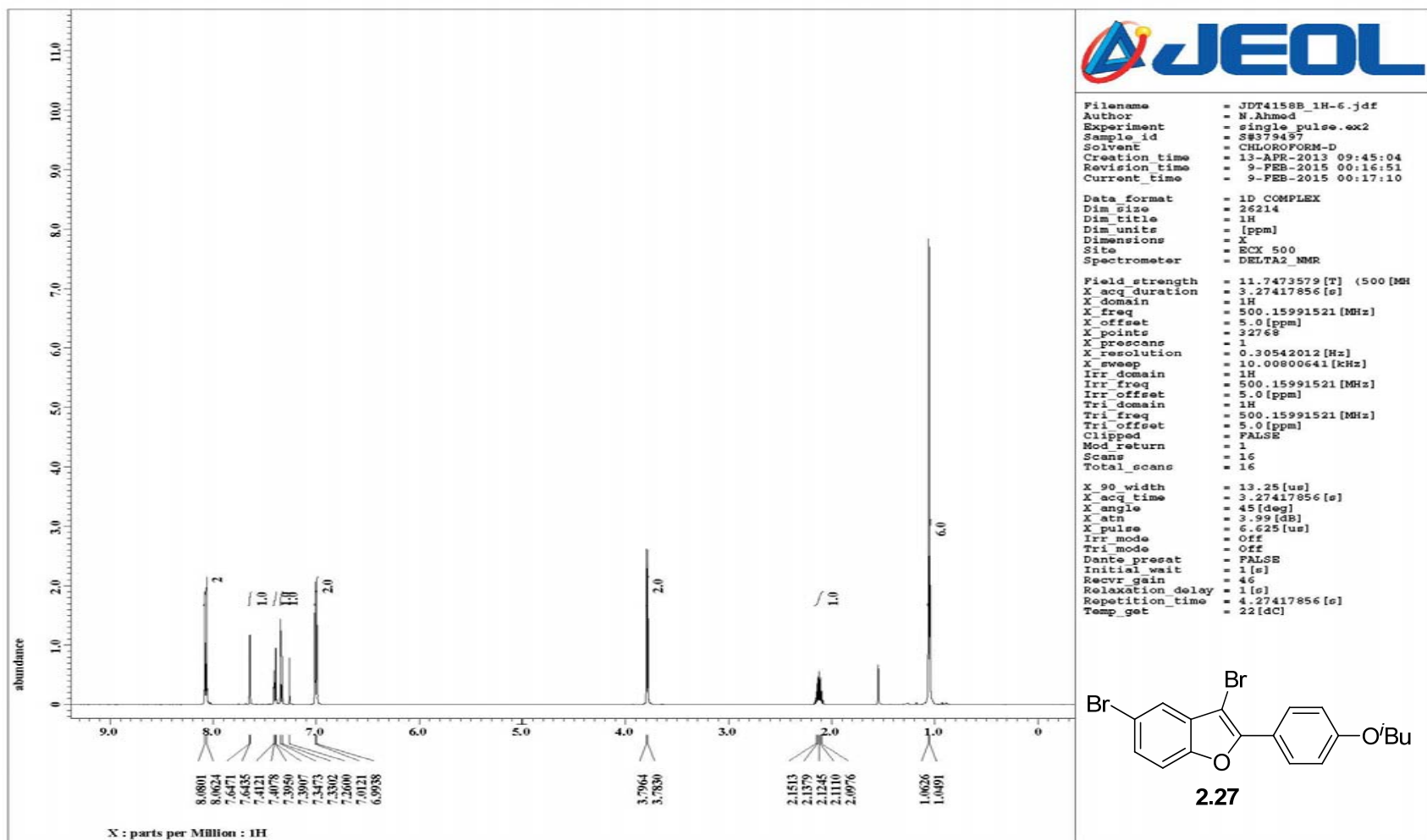
125 MHz ^{13}C NMR spectrum of compound 2.25



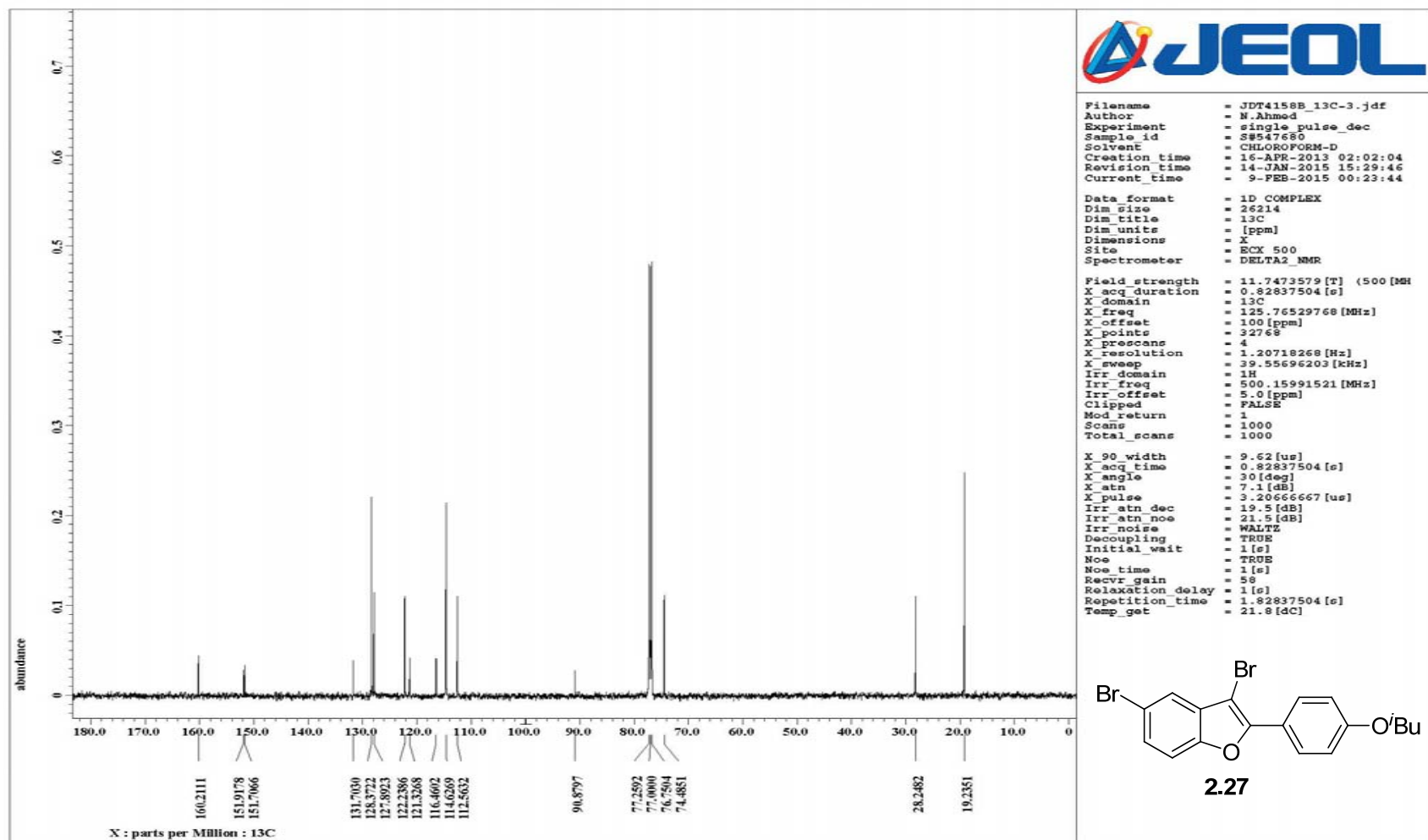
500 MHz ^1H NMR spectrum of compound **2.26**



125 MHz ^{13}C NMR spectrum of compound **2.26**

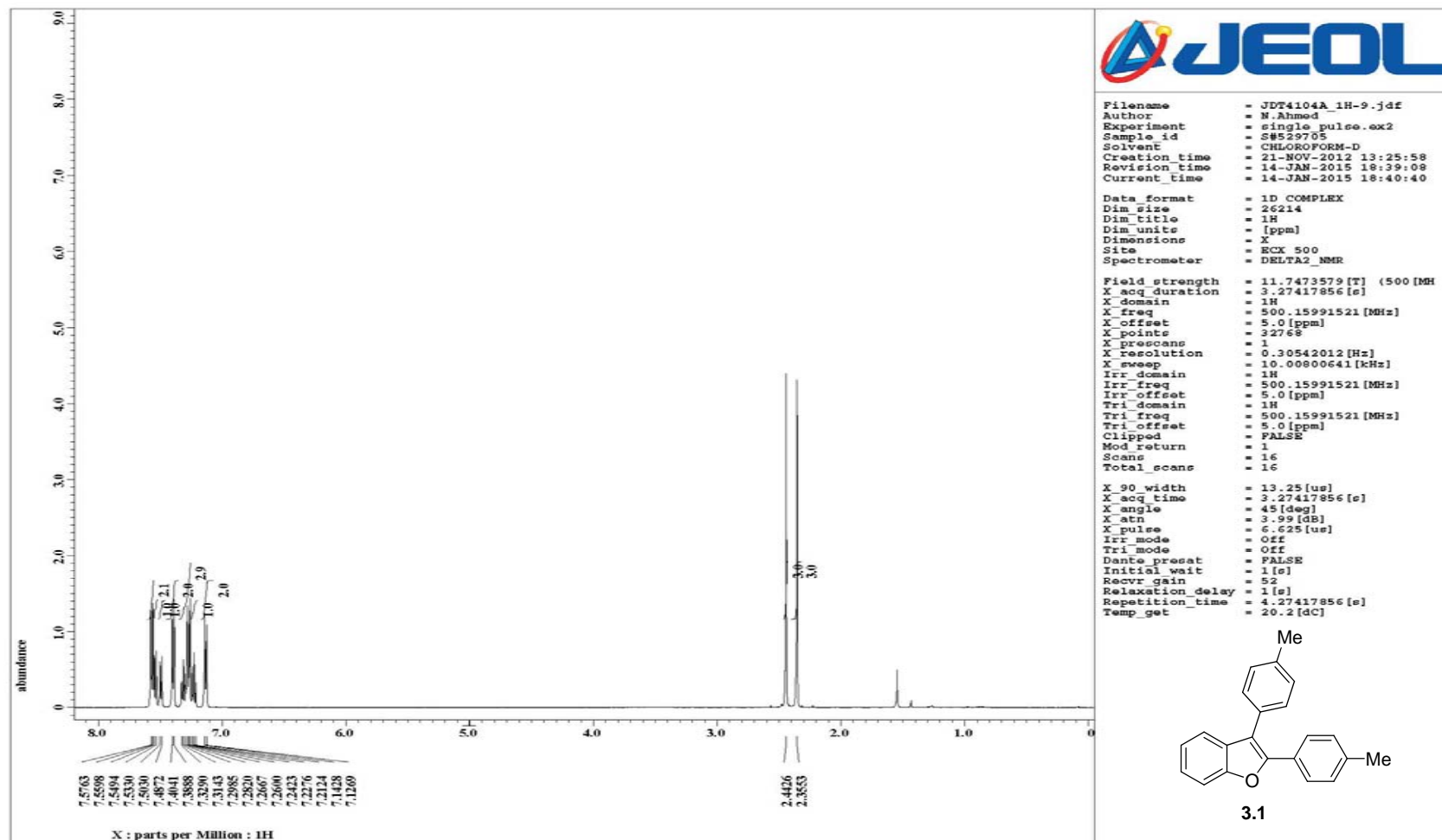


500 MHz ¹H NMR spectrum of compound **2.27**

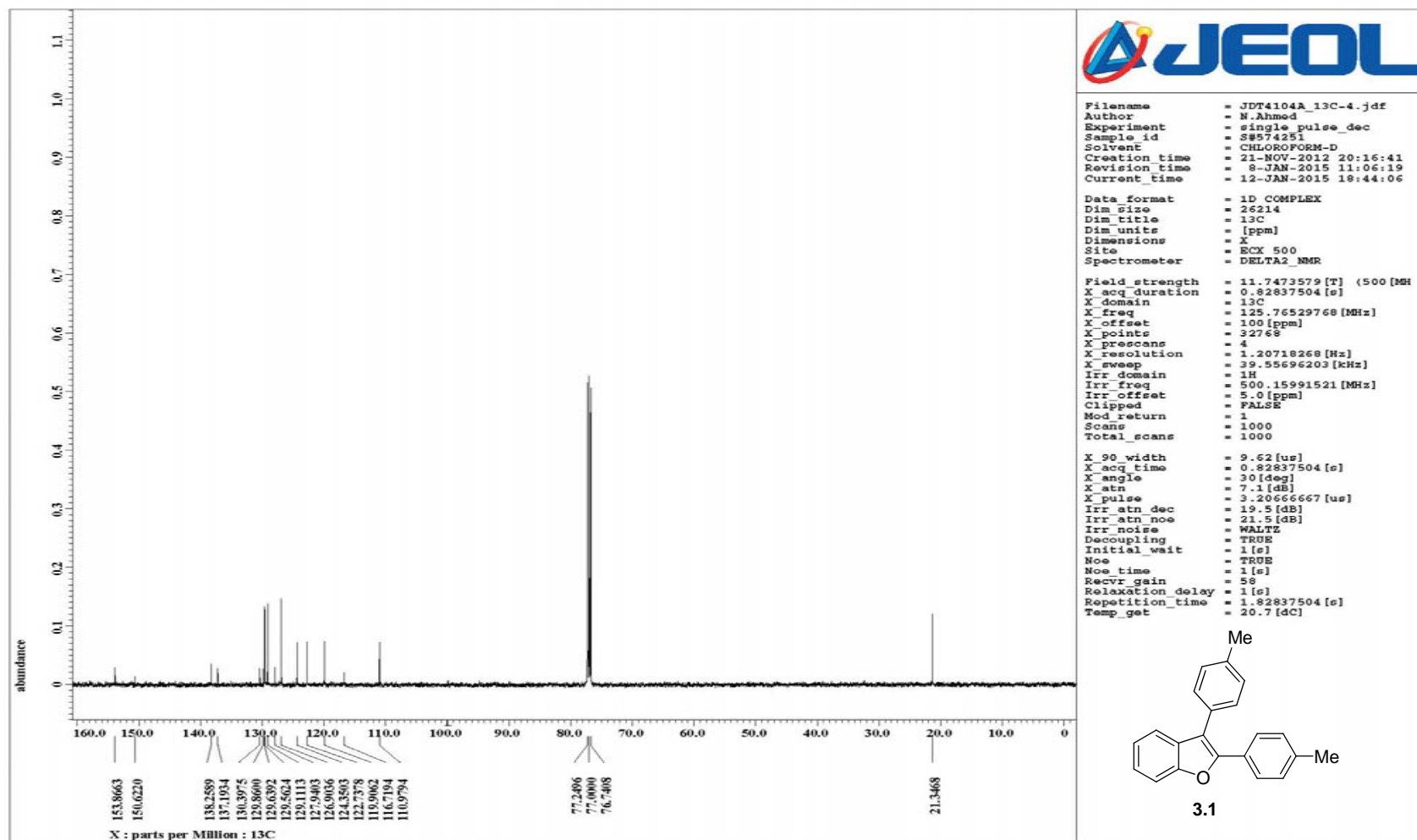


125 MHz ^{13}C NMR spectrum of compound **2.27**

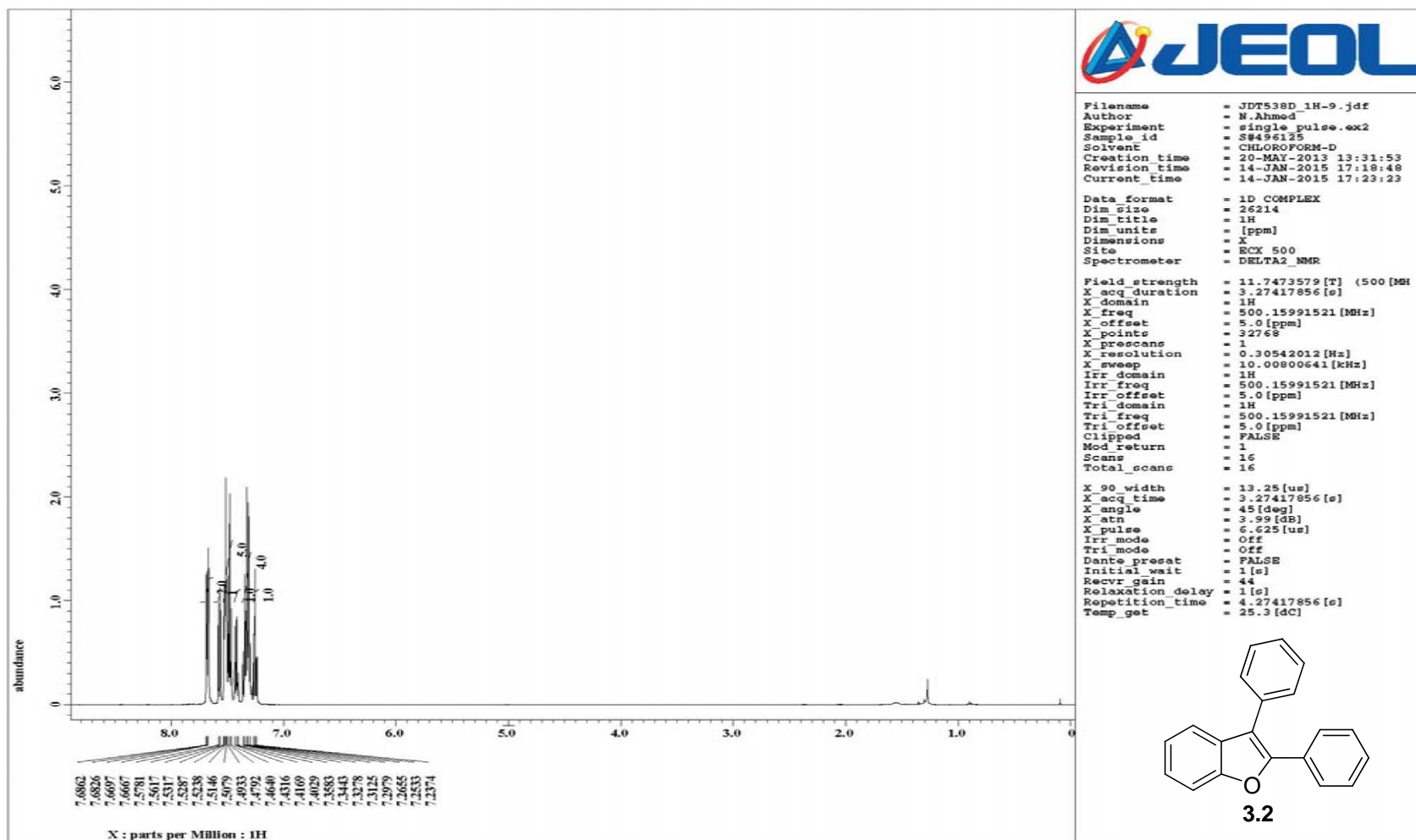
3. ^1H , ^{13}C Spectra of Compounds (3.1-3.7):



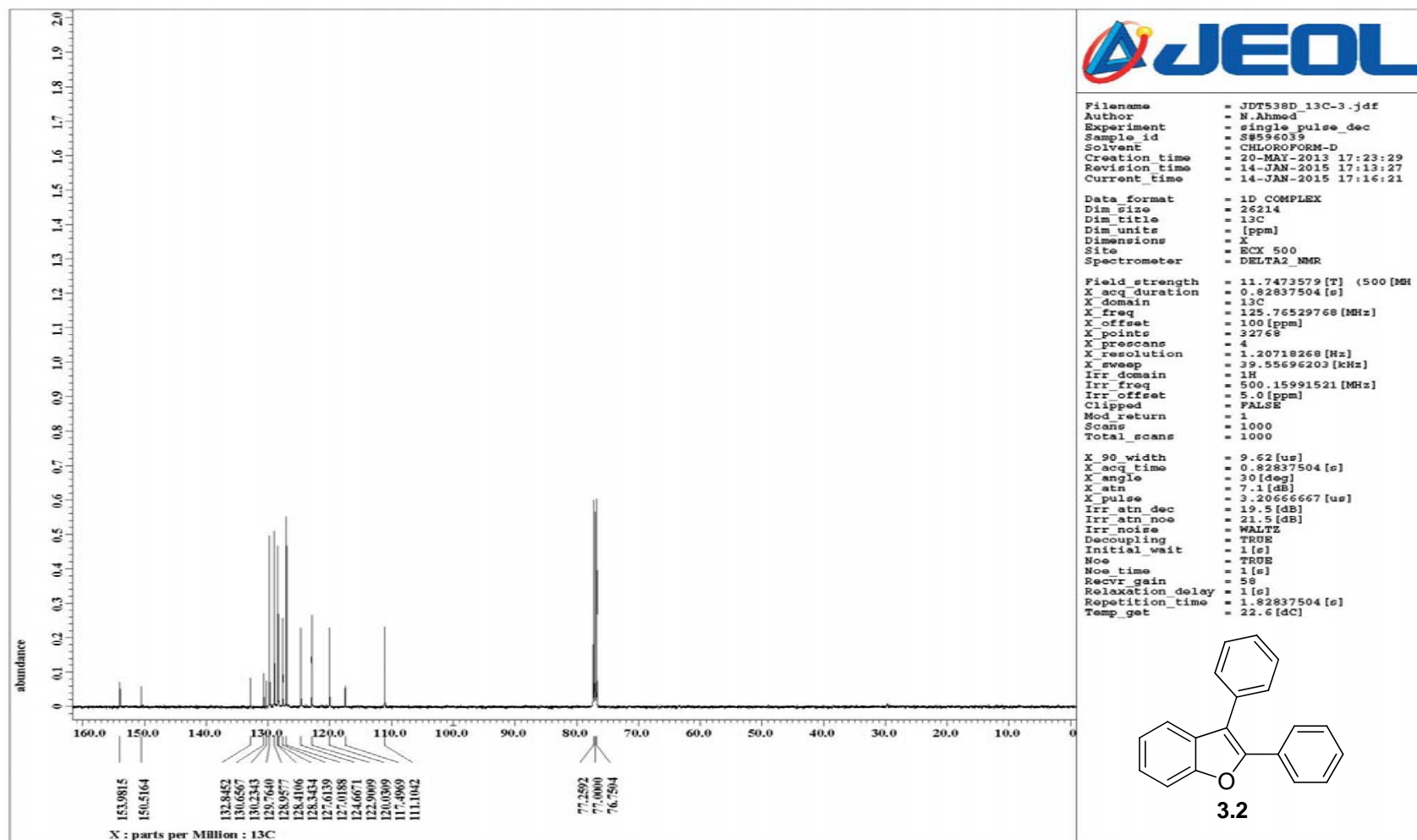
500 MHz ^1H NMR spectrum of compound **3.1**



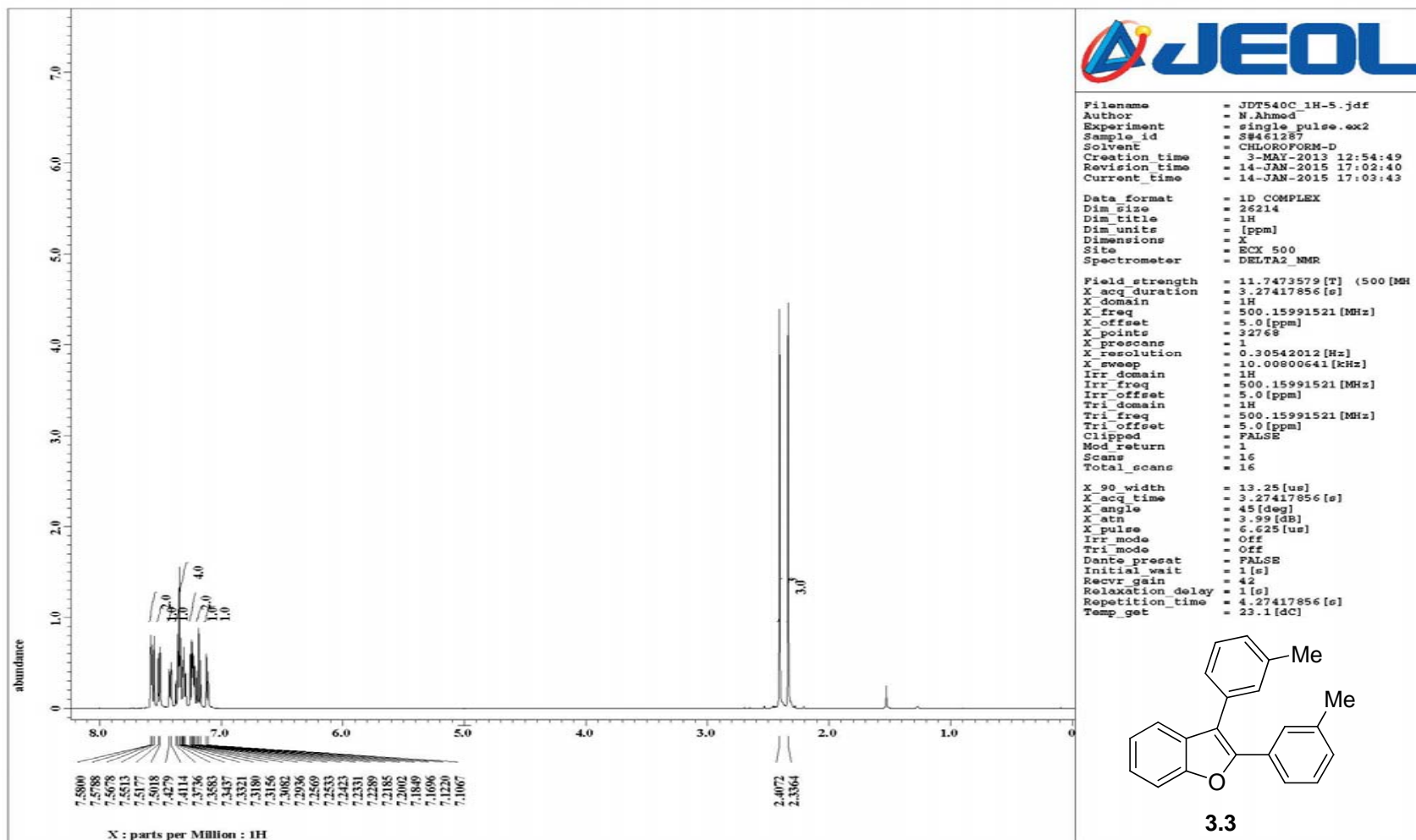
125 MHz ^{13}C NMR spectrum of compound **3.1**



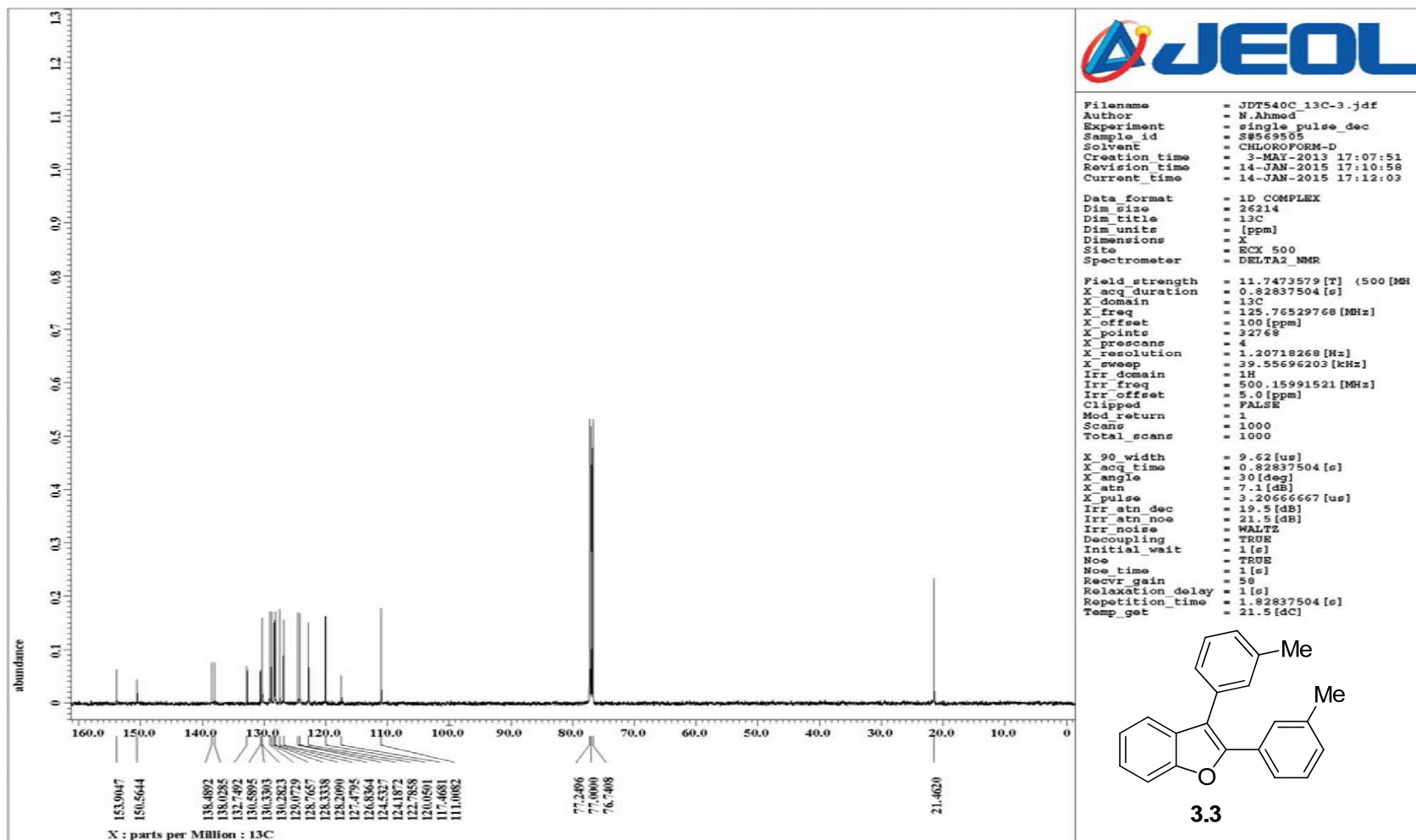
500 MHz ^1H NMR spectrum of compound **3.2**



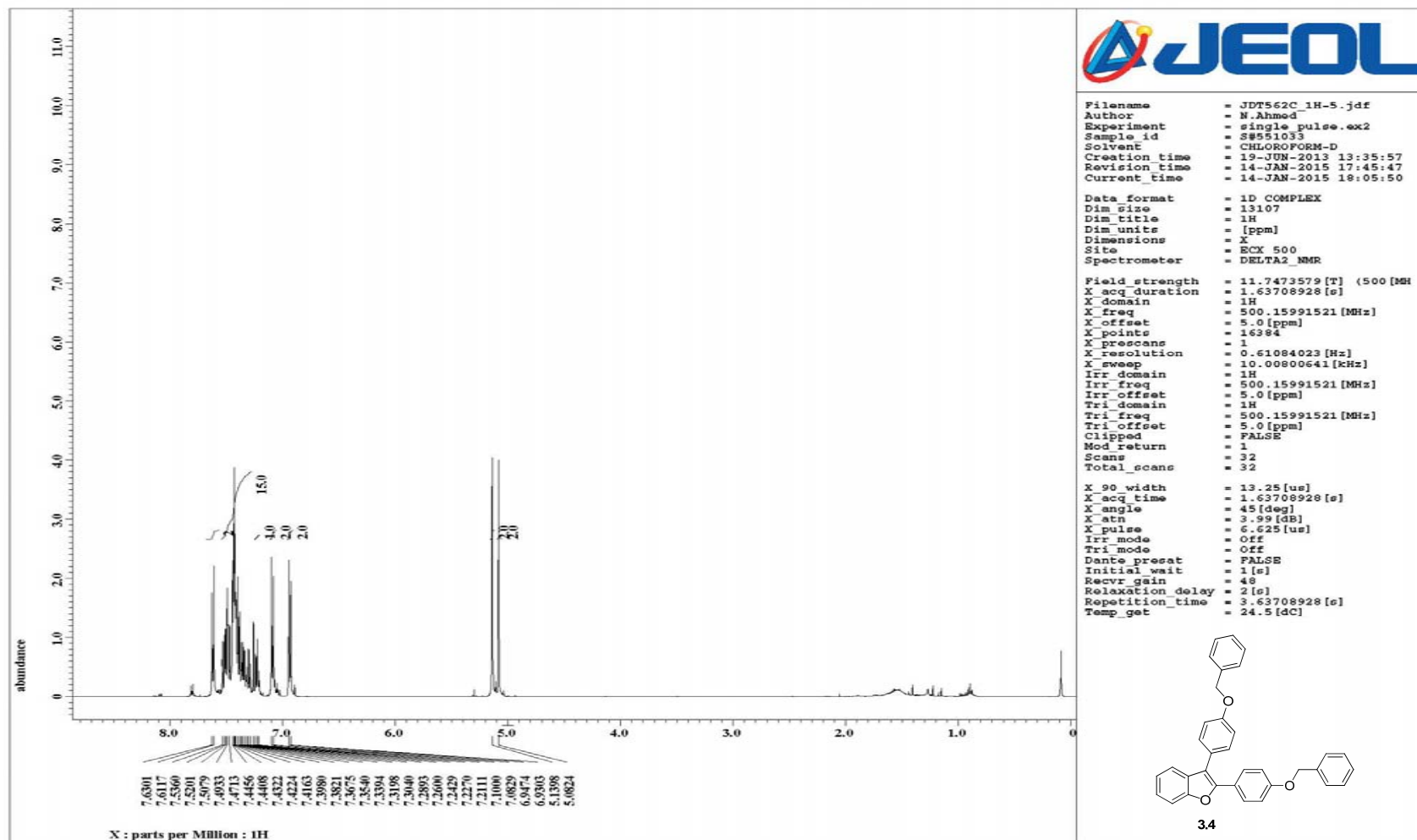
125 MHz ^{13}C NMR spectrum of compound **3.2**



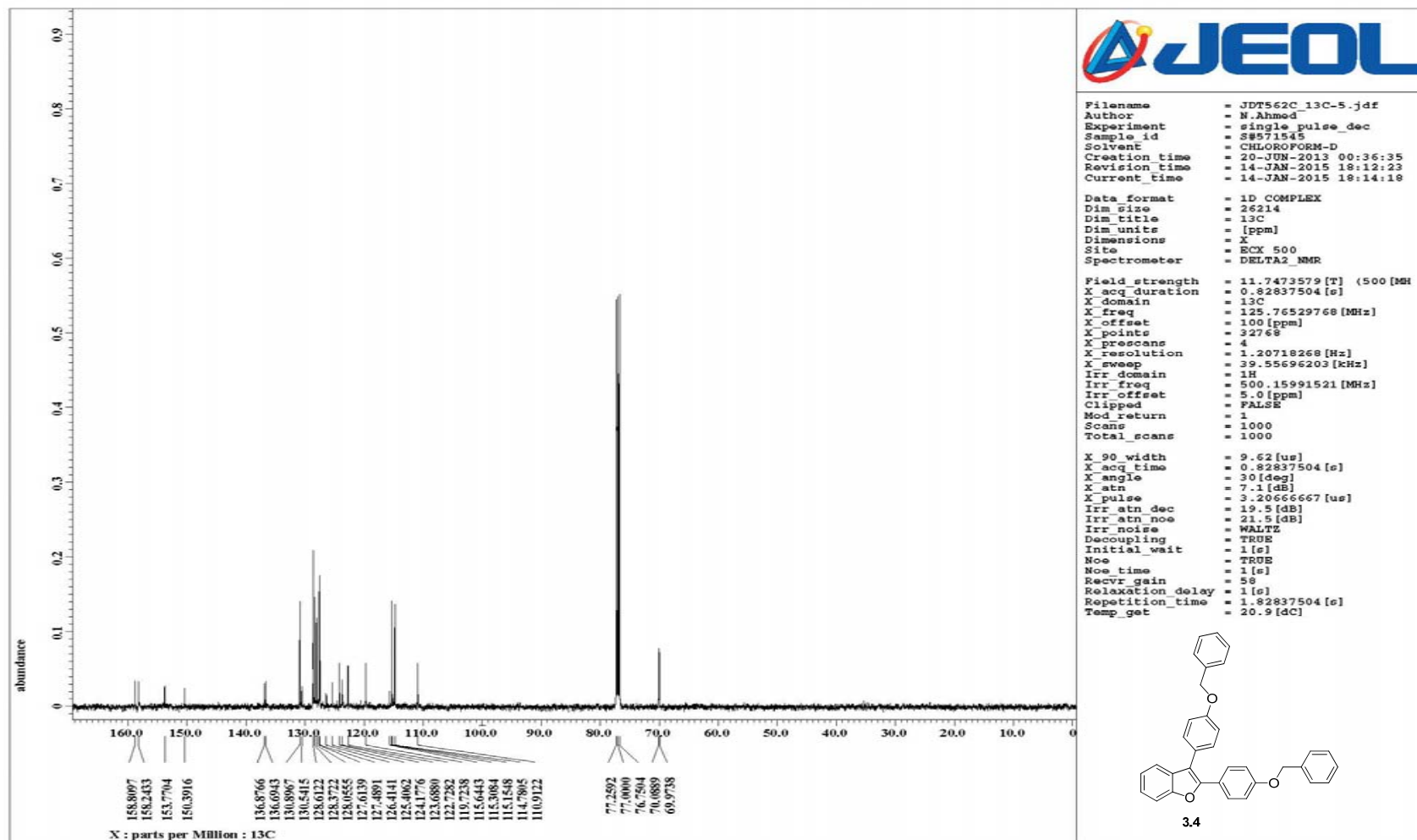
500 MHz ¹H NMR spectrum of compound 3.3



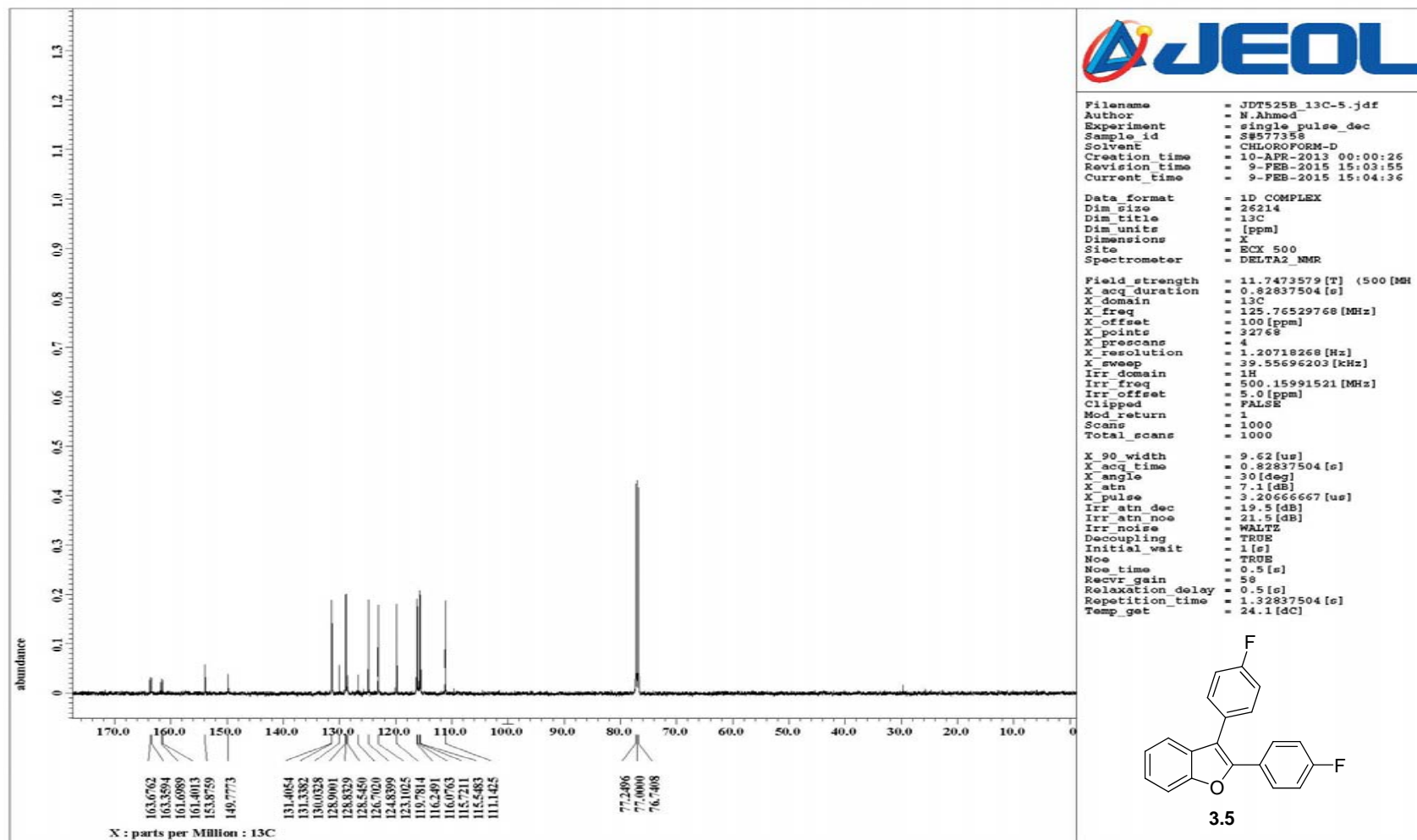
125 MHz ^{13}C NMR spectrum of compound 3.3



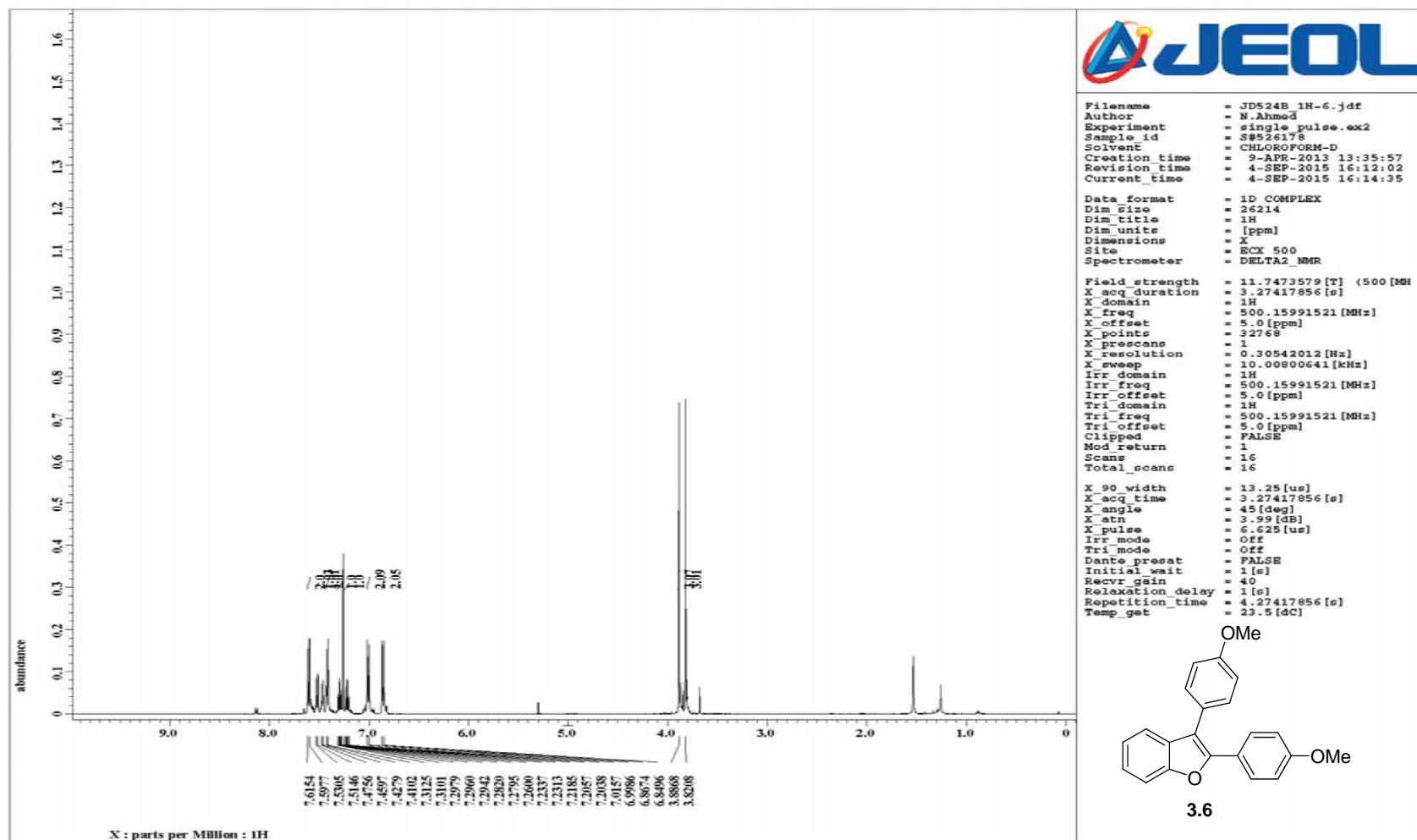
500 MHz ^1H NMR spectrum of compound **3.4**



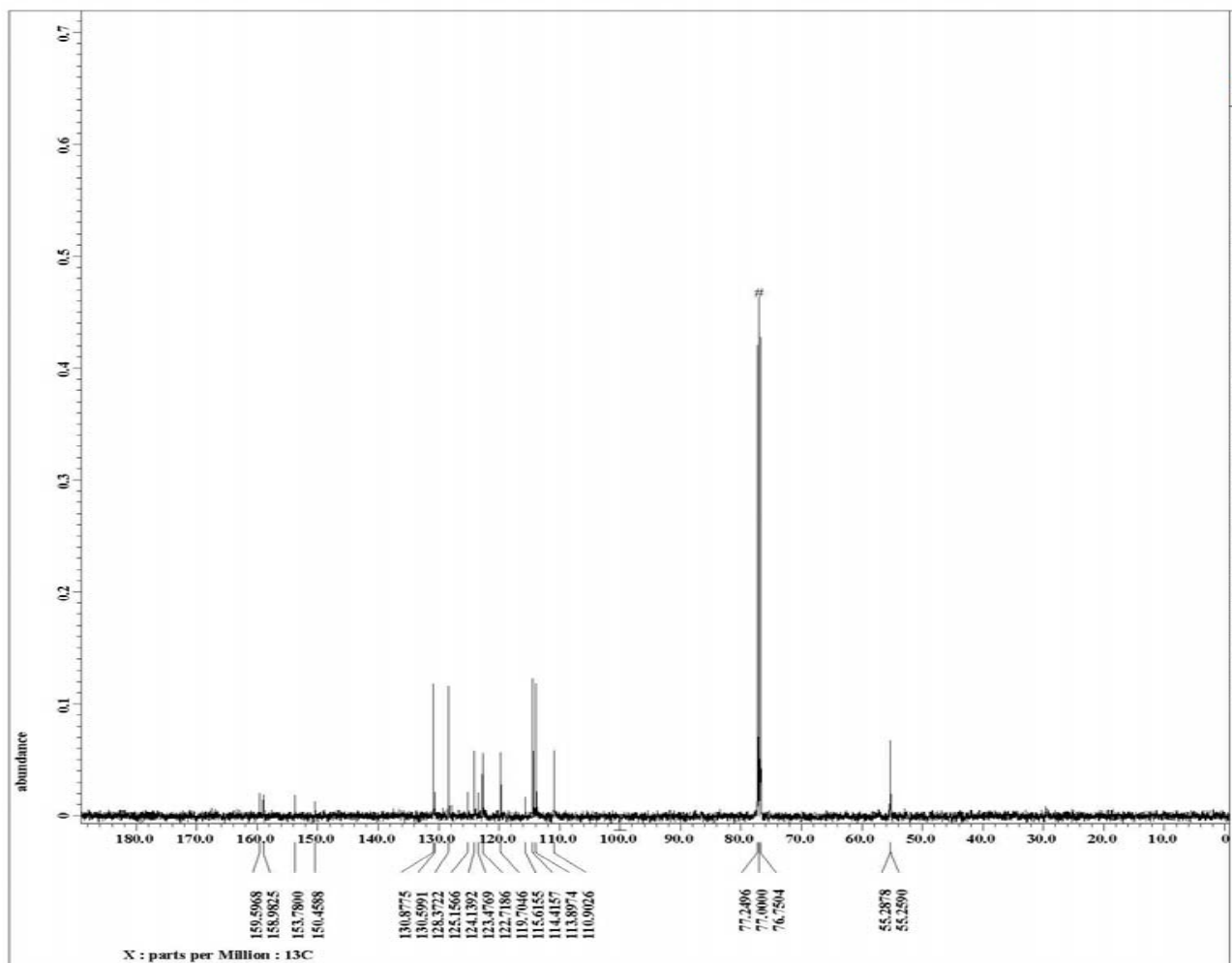
125 MHz ^{13}C NMR spectrum of compound 3.4



125 MHz ^{13}C NMR spectrum of compound **3.5**



500 MHz ¹H NMR spectrum of compound **3.6**



```

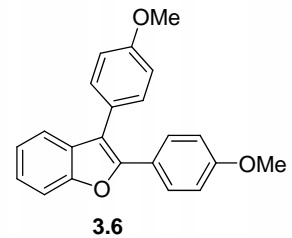
Filename      = JDT524B_13C-5.jdf
Author       = N.Ahmed
Experiment   = single_pulse_dec
Sample id    = S#577254
Solvent      = CHLOROFORM-D
Creation time = 9-APR-2013 23:33:02
Revision time = 4-SEP-2015 10:18:53
Current time  = 4-SEP-2015 10:21:55

Data format  = 1D COMPLEX
Dim Size     = 26214
Dim title    = 13C
Dim units    = [ppm]
Dimensions   = X
Site         = ECY 500
Spectrometer = DELTA2_NMR

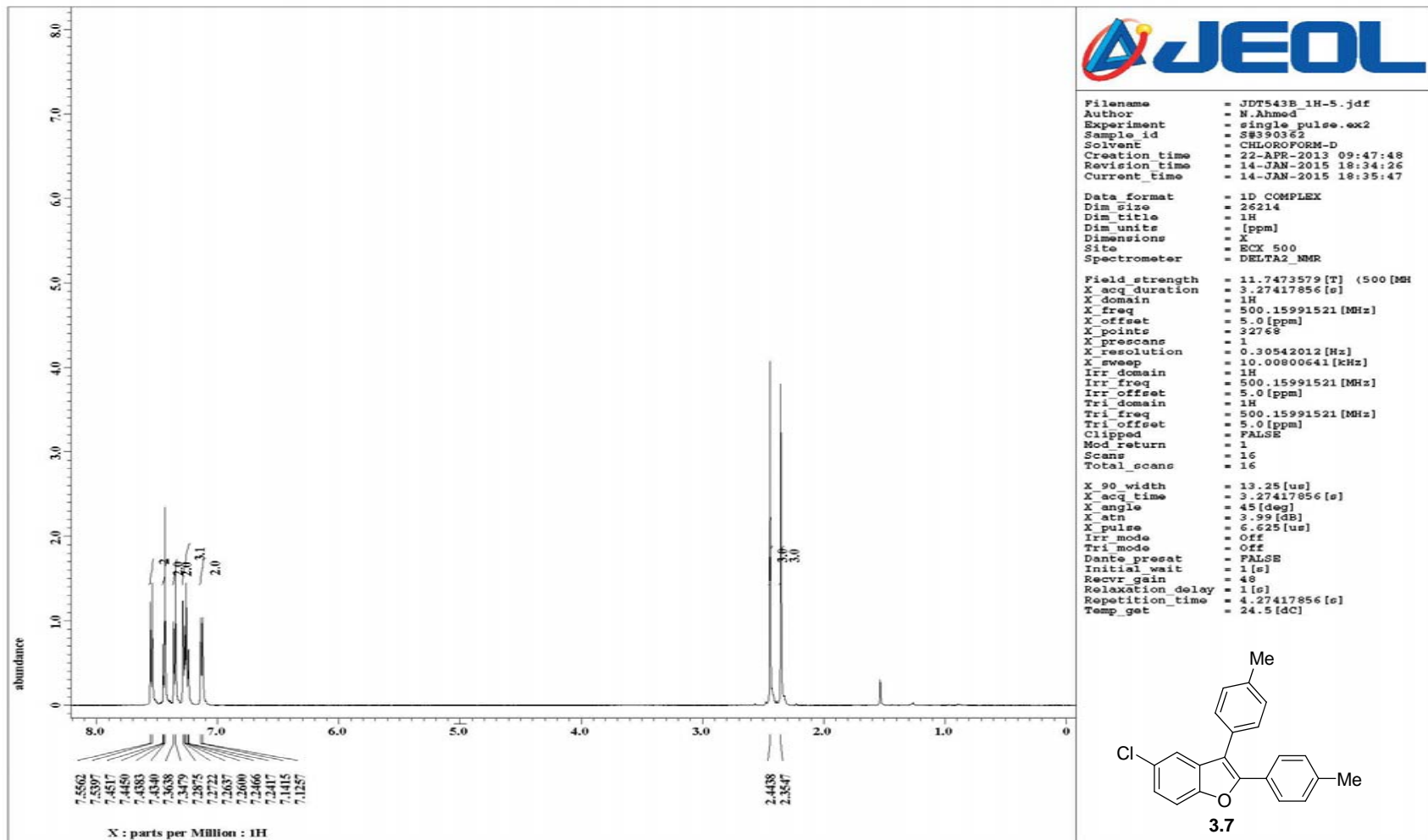
Field strength = 11.7473579 [T] (500 [MH]
X_acq_duration = 0.82837504 [s]
X_domain       = 13C
X_freq         = 125.76529768 [MHz]
X_offset       = 100 [ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.20718268 [Hz]
X_sweep        = 39.55696203 [kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521 [MHz]
Irr_offset     = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 1000
Total_scans    = 1000

X_90_width    = 9.62 [us]
X_acq_time    = 0.82837504 [s]
X_angle       = 30 [deg]
X_atn         = 7.1 [dB]
X_pulse       = 3.20666667 [us]
Irr_atn_dec   = 19.5 [dB]
Irr_atn_noe   = 21.5 [dB]
Irr_noise     = WALTZ
Decoupling    = TRUE
Initial_wait   = 1 [s]
Noe           = TRUE
Noe_time      = 0.5 [s]
Recvr_gain    = 58
Relaxation_delay = 0.5 [s]
Repetition_time = 1.32837504 [s]
Temp_get      = 24.2 [dC]

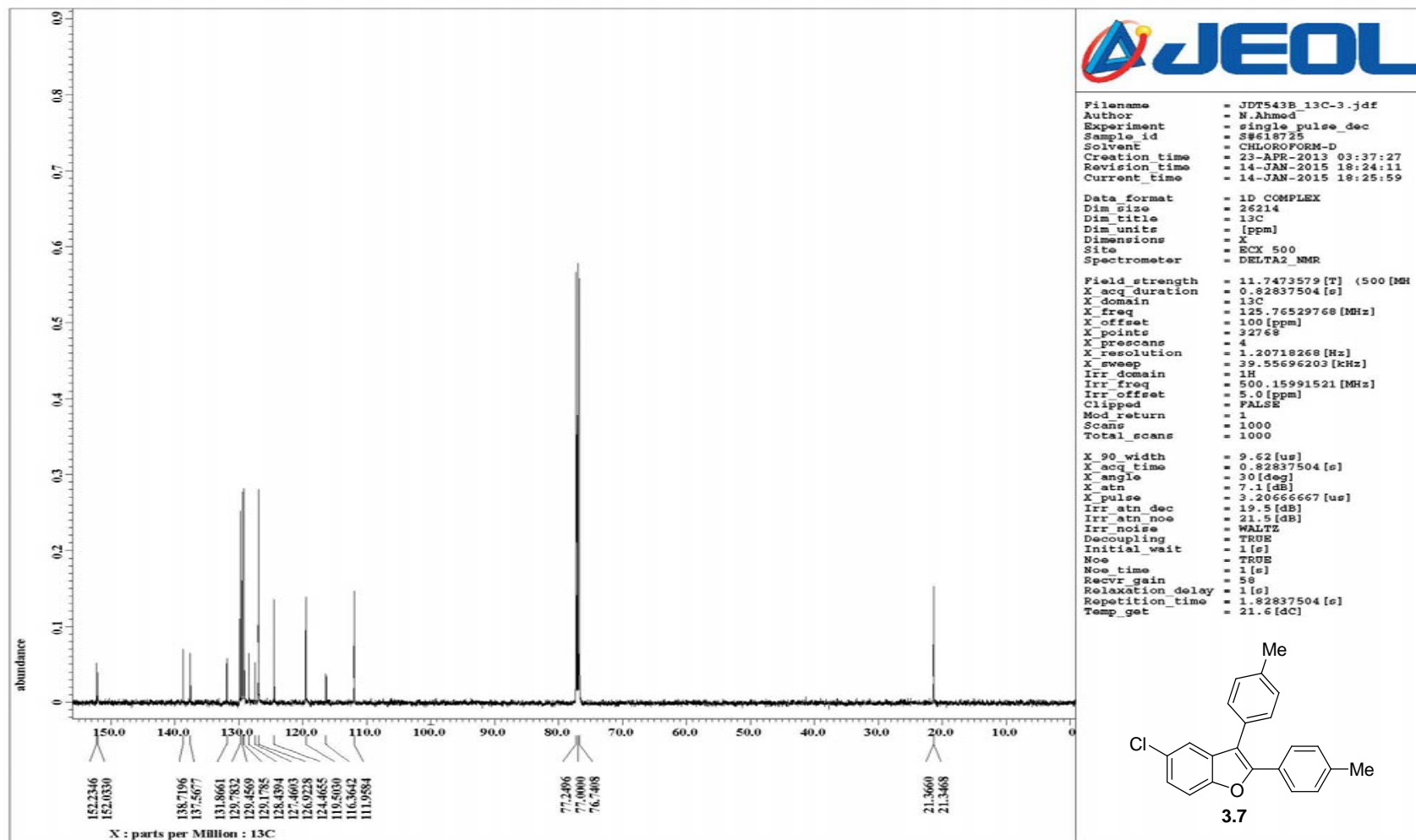
```



125 MHz ¹³C NMR spectrum of compound 3.6

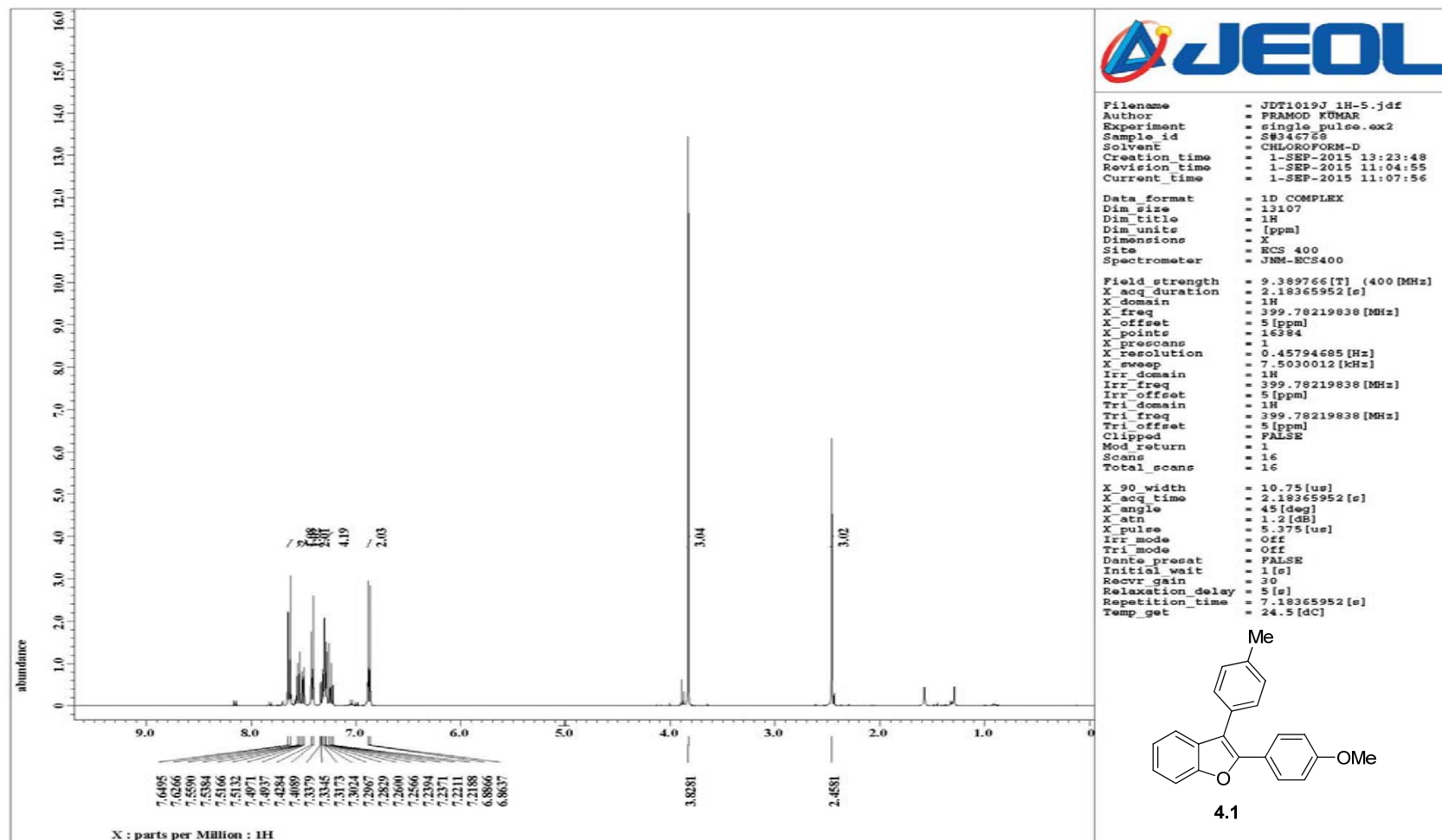


500 MHz ^1H NMR spectrum of compound **3.7**

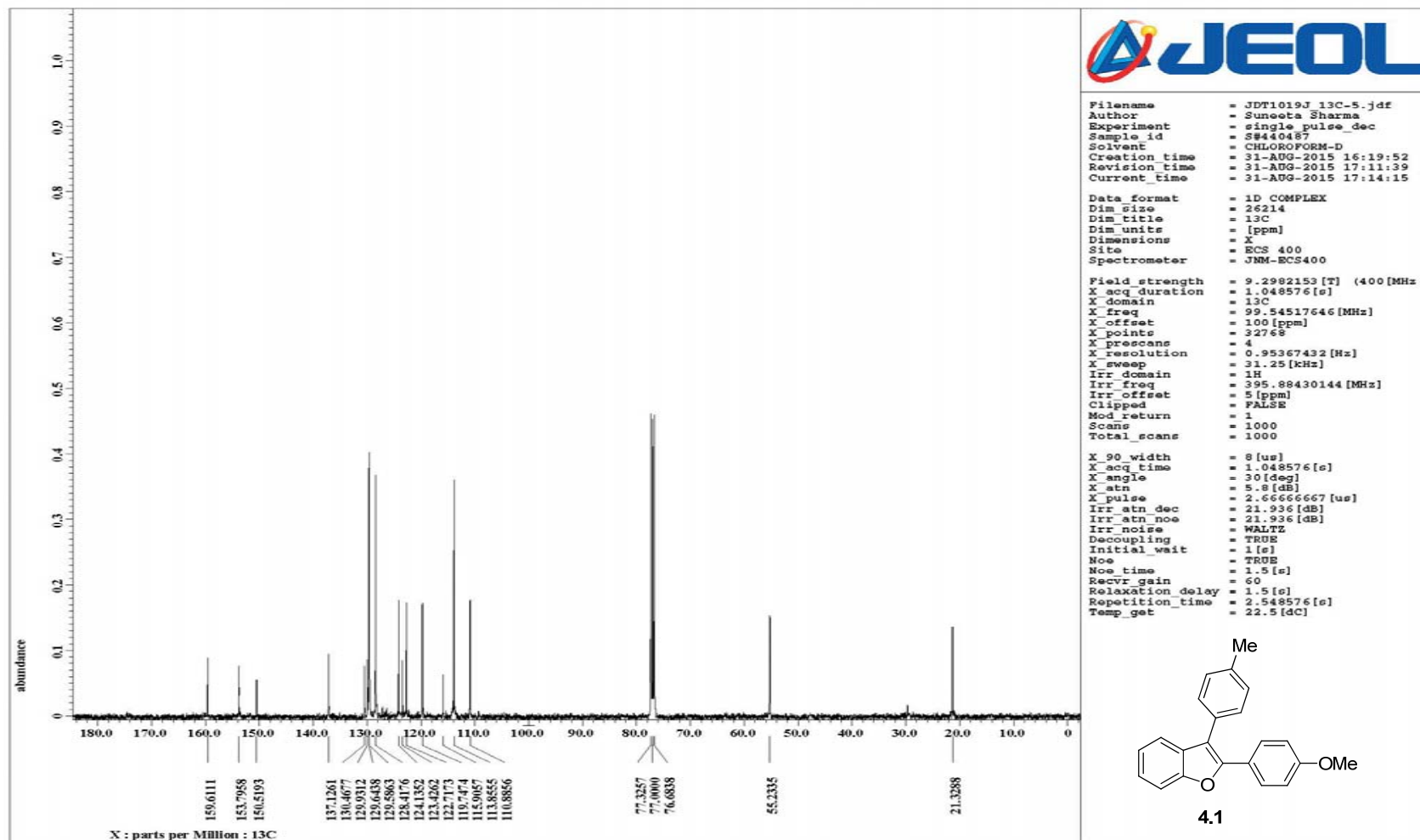


125 MHz ^{13}C NMR spectrum of compound **3.7**

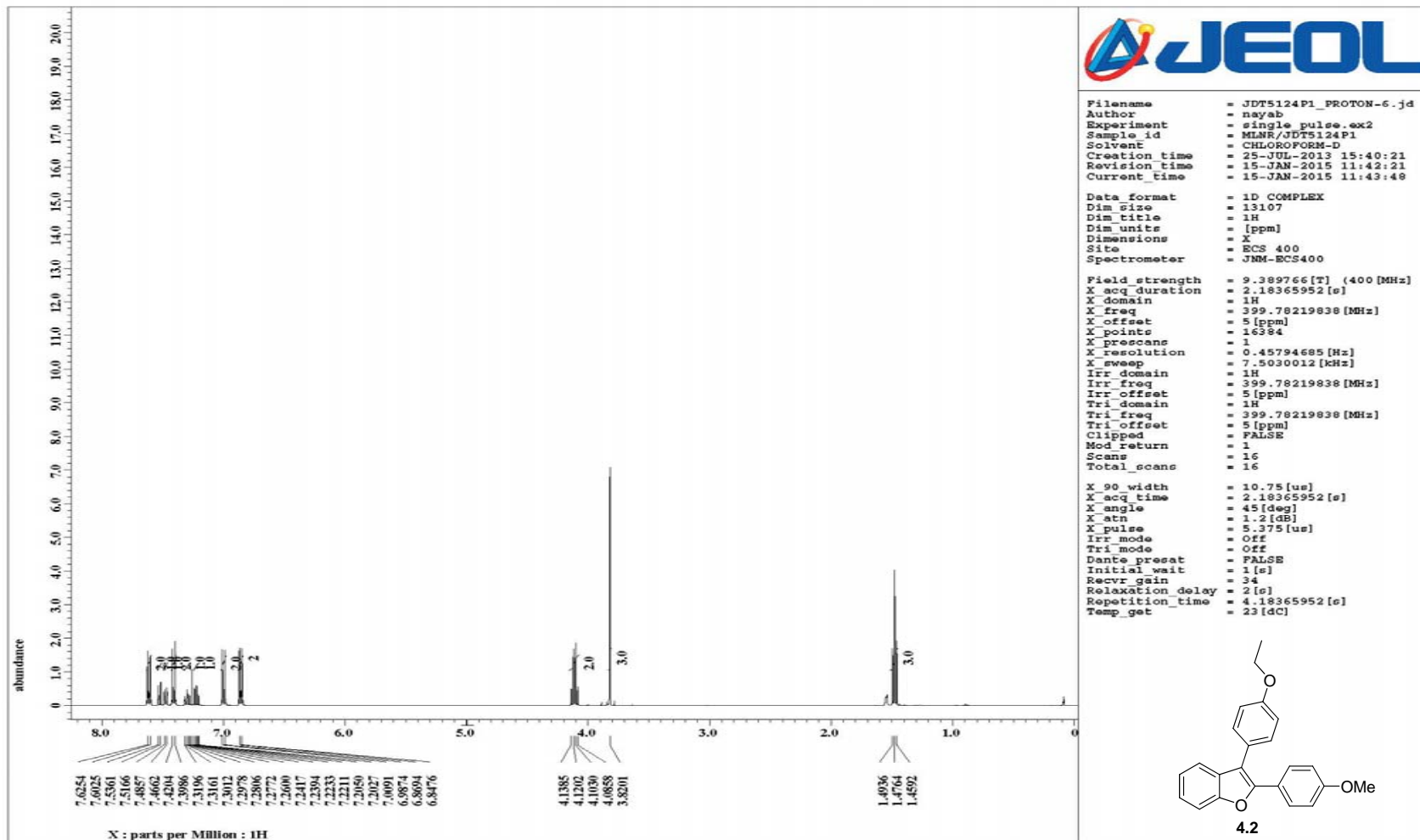
4. ¹H, ¹³C Spectra of Compounds (4.1-4.3):



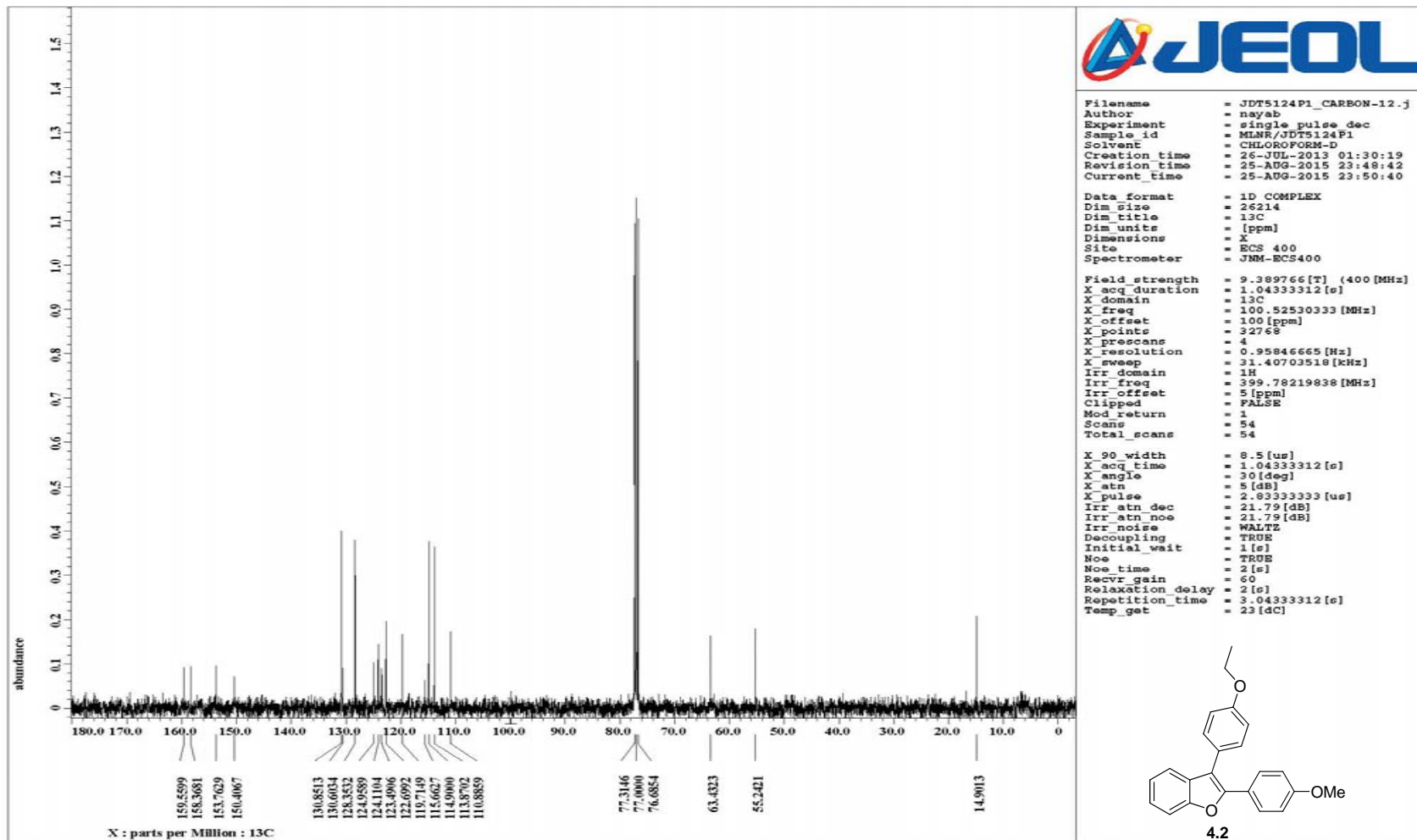
400 MHz ¹H NMR spectrum of compound **4.1**



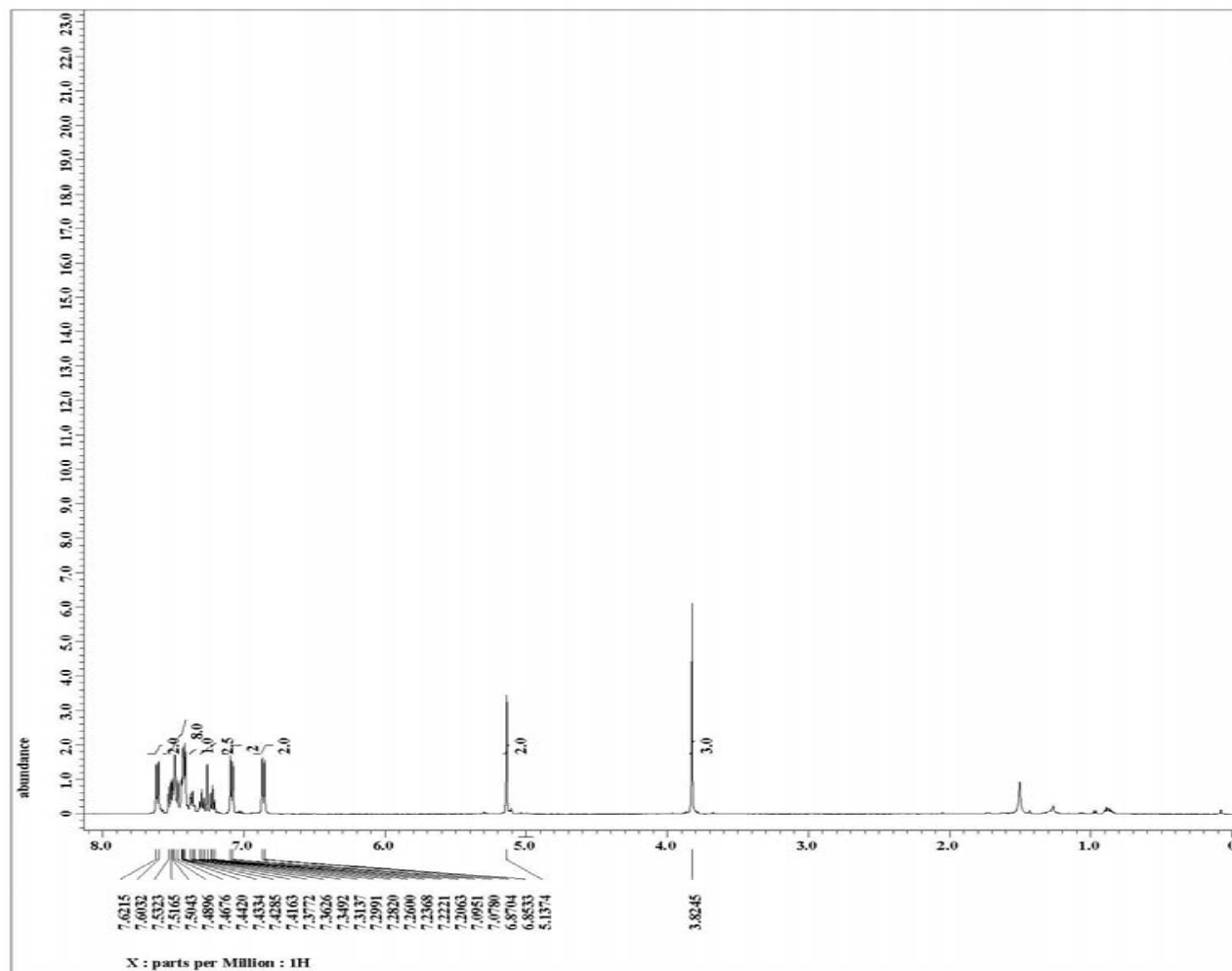
100 MHz ^{13}C NMR spectrum of compound **4.1**



400 MHz ^1H NMR spectrum of compound **4.2**



100 MHz ^{13}C NMR spectrum of compound **4.2**



```

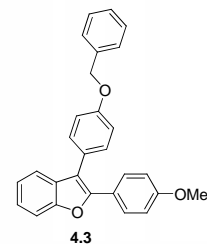
Filename      = JDT5131P_1H-5.jdf
Author       = N.Ahmed
Experiment    = single pulse.ex2
Sample id     = S#412587
Solvent       = CHLOROFORM-D
Creation time = 10-JUL-2013 09:44:00
Revision time = 15-JAN-2015 13:11:15
Current Time  = 15-JAN-2015 13:11:54

Data format   = 1D COMPLEX
Dim Size      = 13107
Dim title     = 1H
Dim units     = [ppm]
Dimensions    = X
Site          = ECK 500
Spectrometer  = DELTA2 NMR

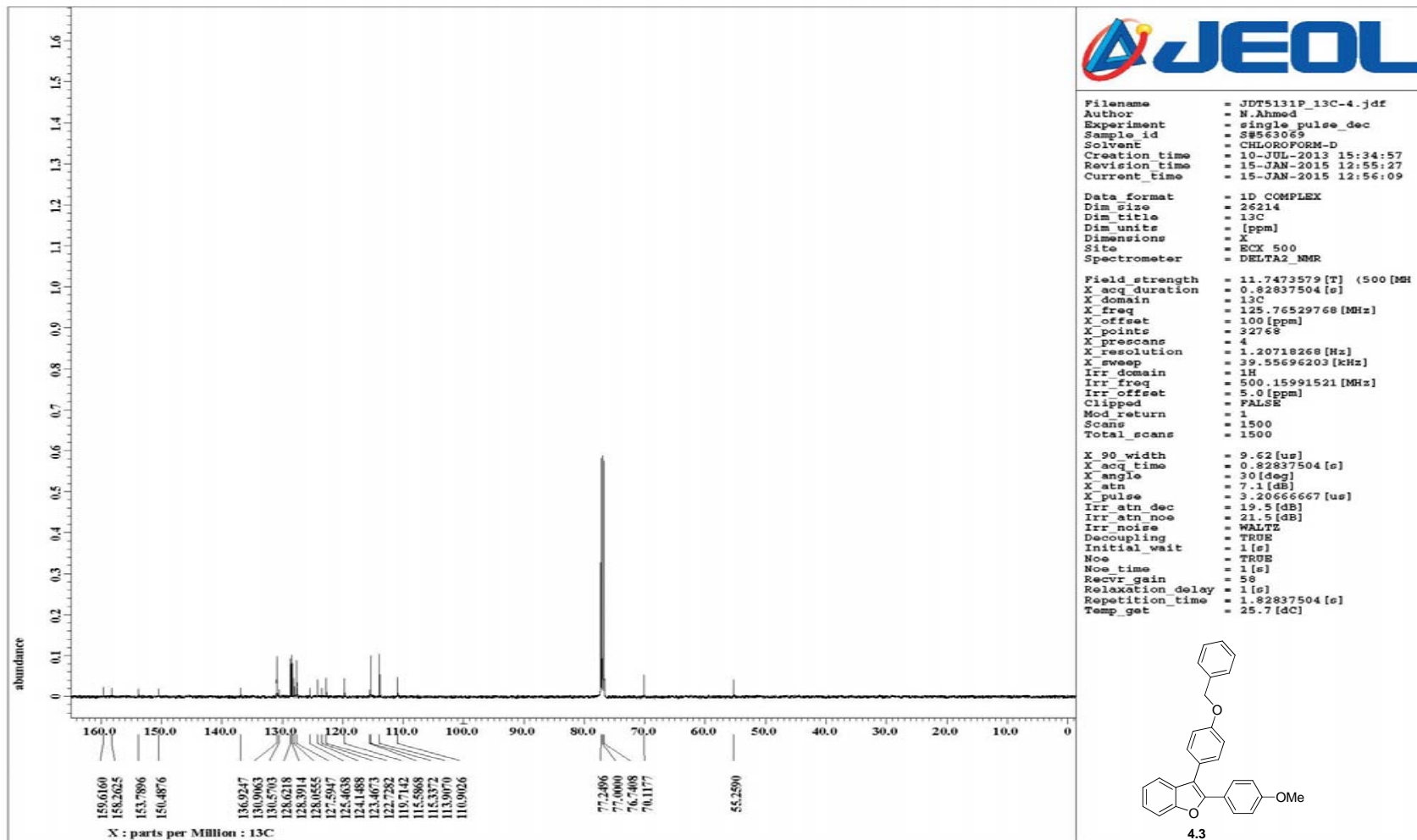
Field strength = 11.7473579 [T] (500 [MH]
X_acq duration = 1.63708928 [s]
X_domain       = 1H
X_freq         = 500.15991521 [MHz]
X_offset       = 5.0 [ppm]
X_points       = 16384
X_prescans     = 1
X_resolution   = 0.61084023 [Hz]
X_sweep        = 10.00800641 [kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521 [MHz]
Irr_offset     = 5.0 [ppm]
Tri_domain     = 1H
Tri_freq       = 500.15991521 [MHz]
Tri_offset     = 5.0 [ppm]
Clipped       = FALSE
Mod Return    = 1
Scans         = 32
Total scans    = 32

X_90 width    = 13.25 [us]
X_acq time    = 1.63708928 [s]
X_angle       = 45 [deg]
X_atn         = 3.99 [dB]
X_pulse       = 6.625 [us]
Irr mode      = Off
Tri mode      = Off
Dante preset  = FALSE
Initial wait  = 1 [s]
Recvr gain    = 52
Relaxation delay = 2 [s]
Repetition time = 3.63708928 [s]
Temp_get      = 24.4 [dC]

```

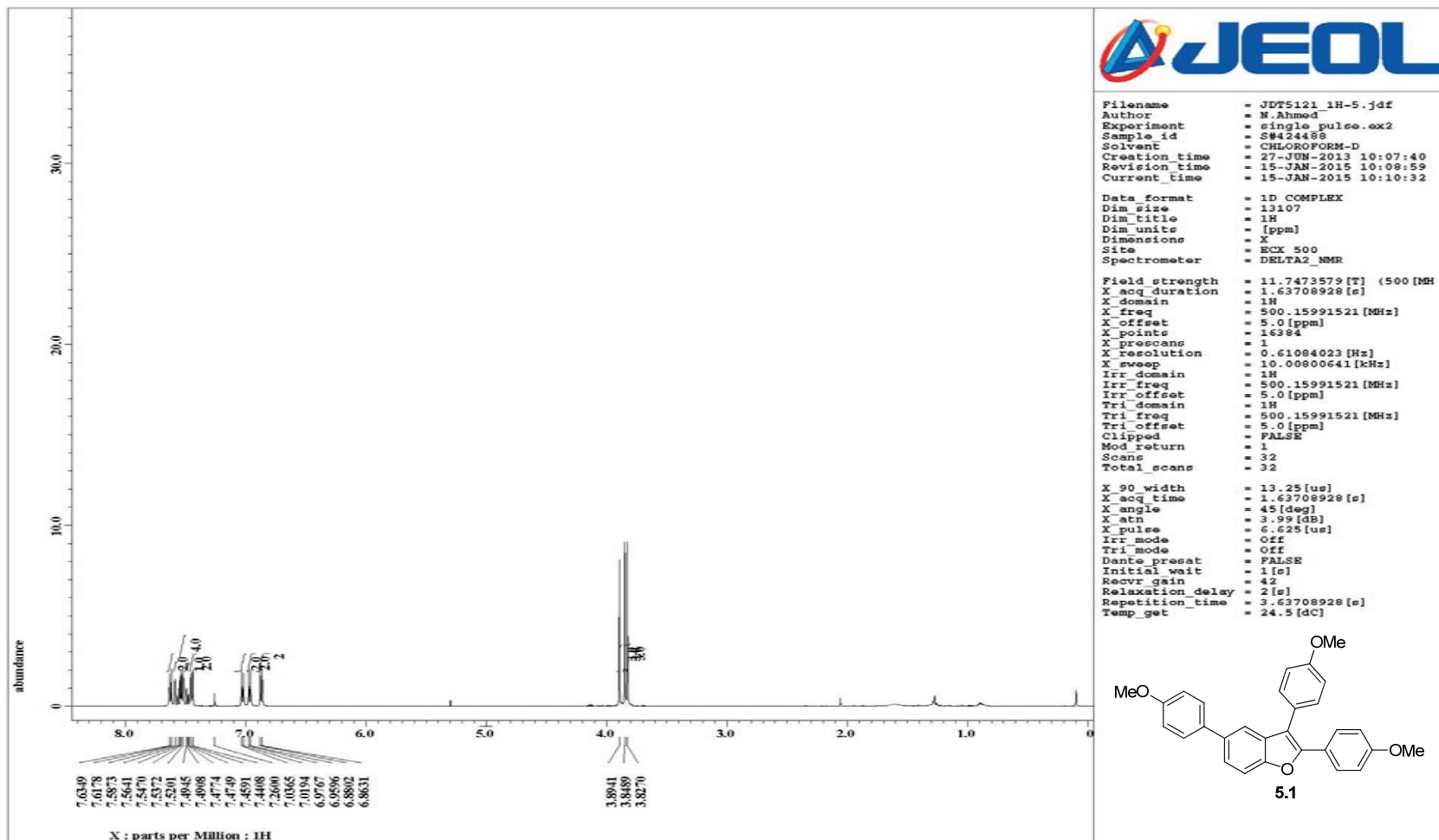


500 MHz ¹H NMR spectrum of compound 4.3

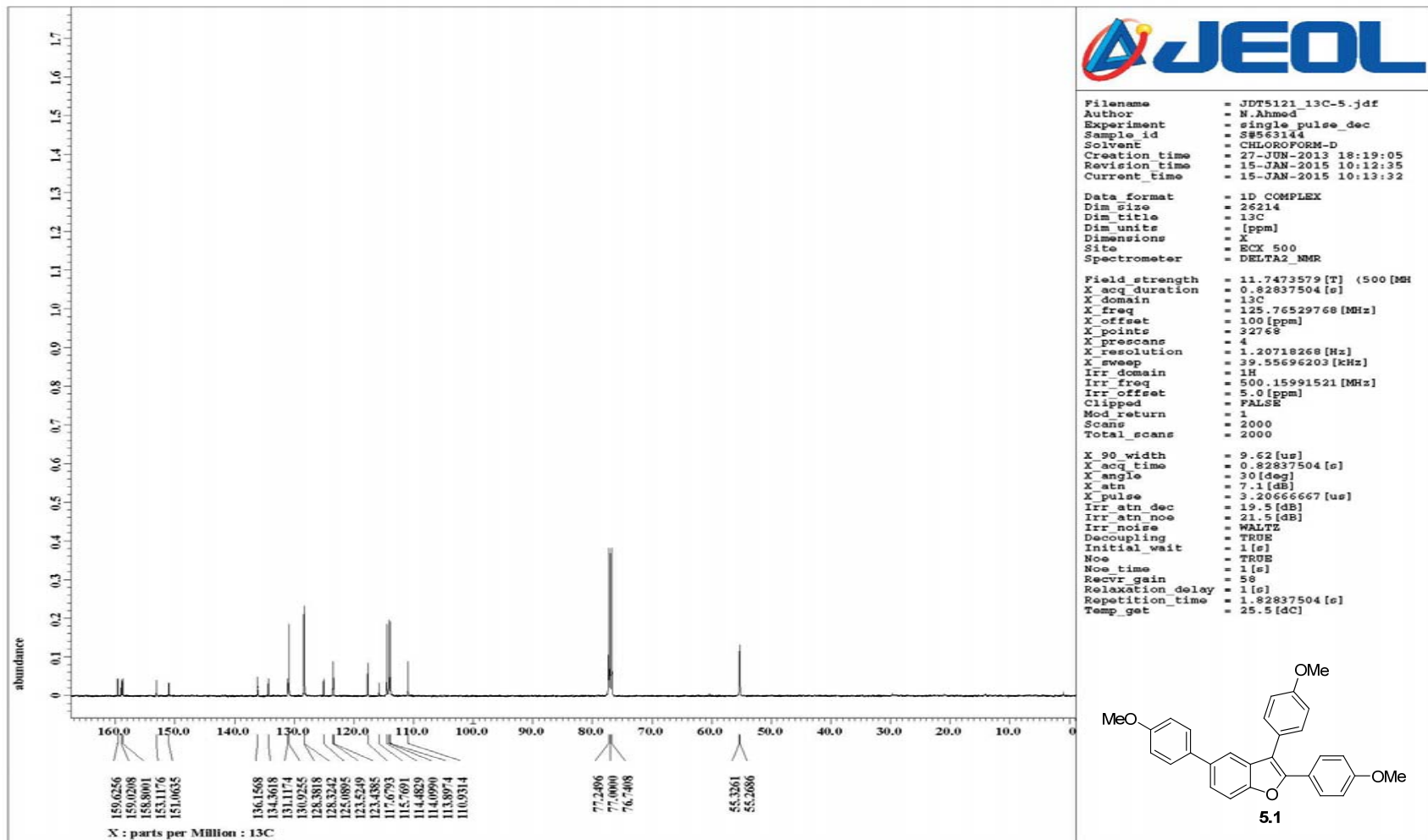


125 MHz ^{13}C NMR spectrum of compound **4.3**

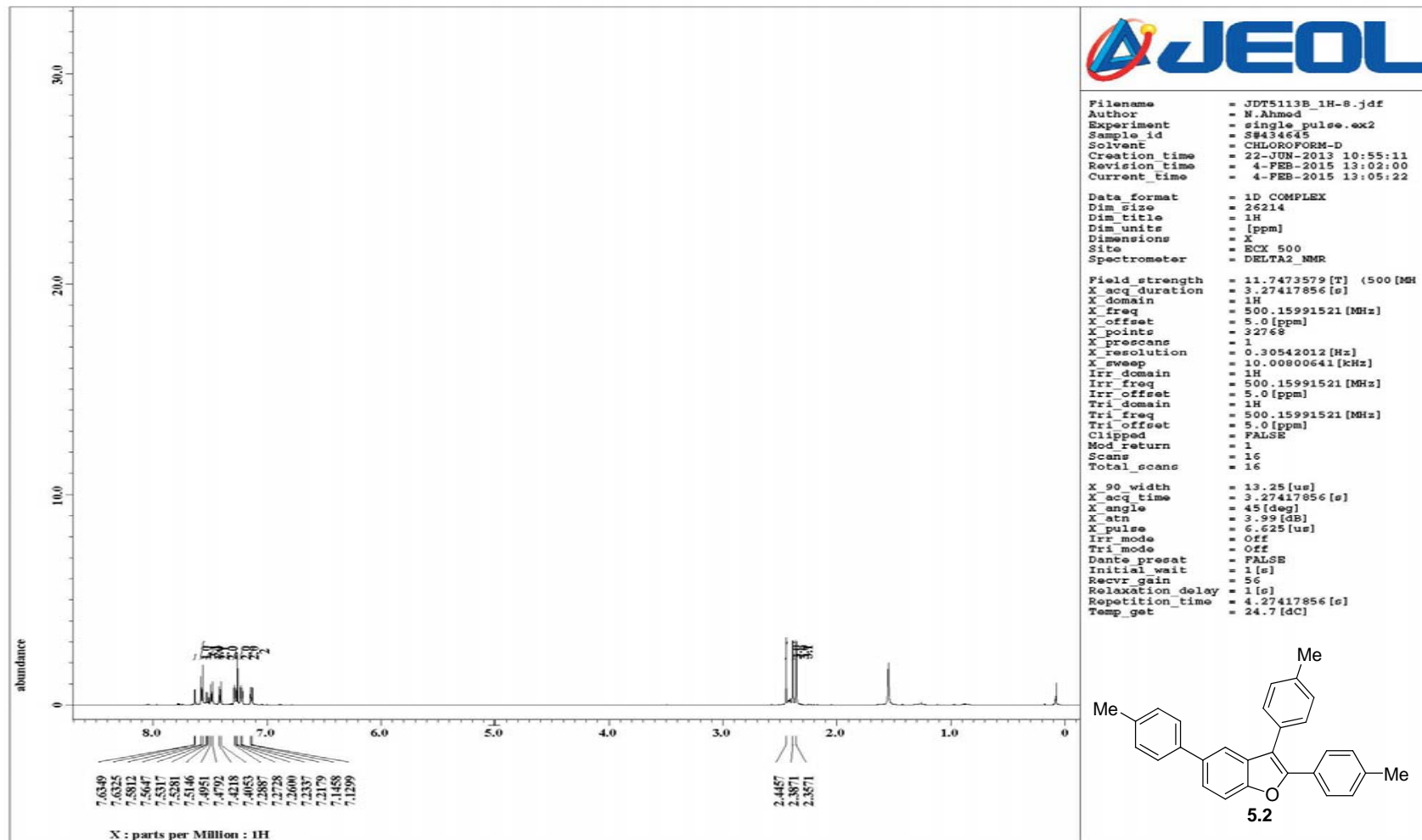
5. ^1H , ^{13}C Spectra of Compounds (5.1-5.4):



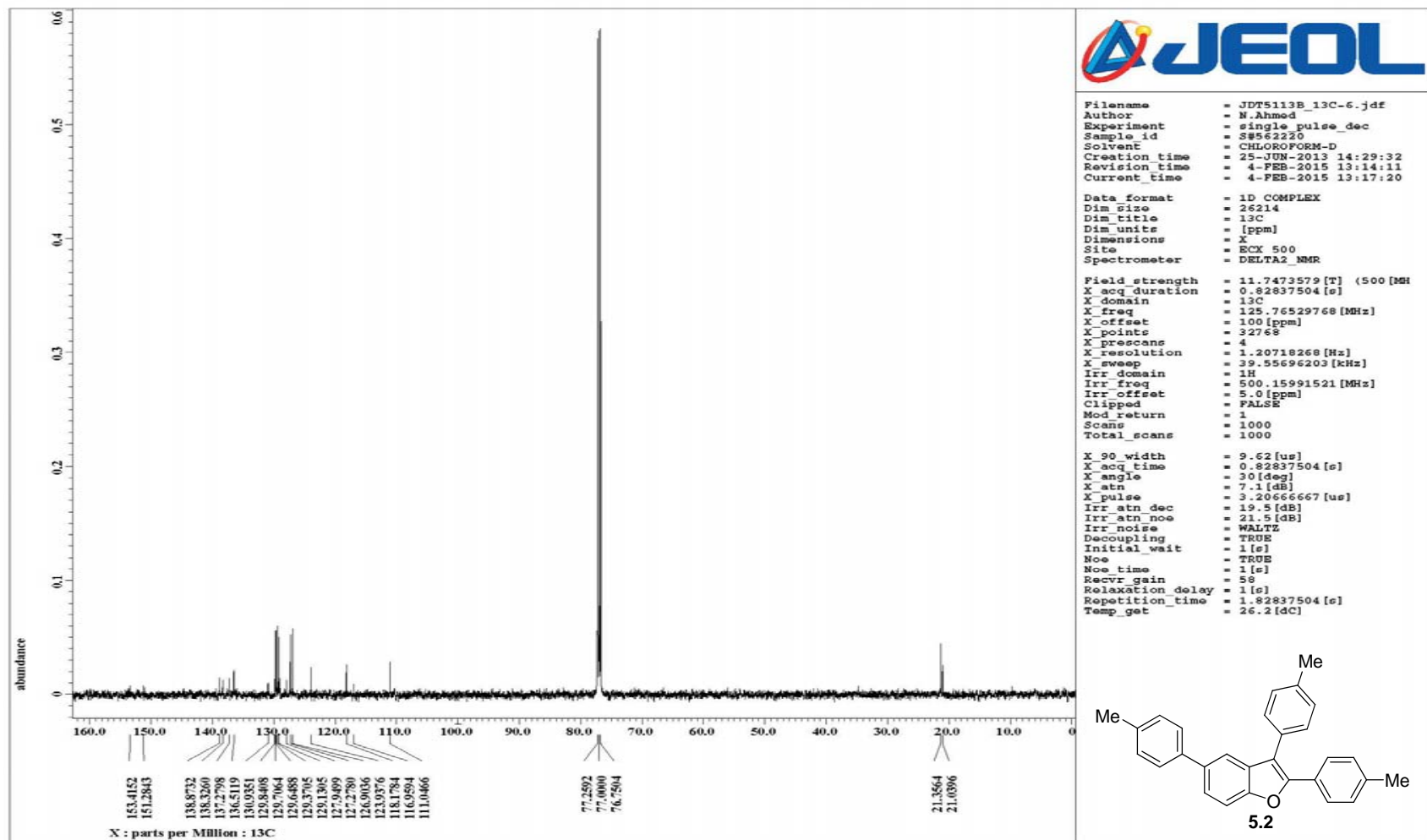
500 MHz ^1H NMR spectrum of compound **5.1**



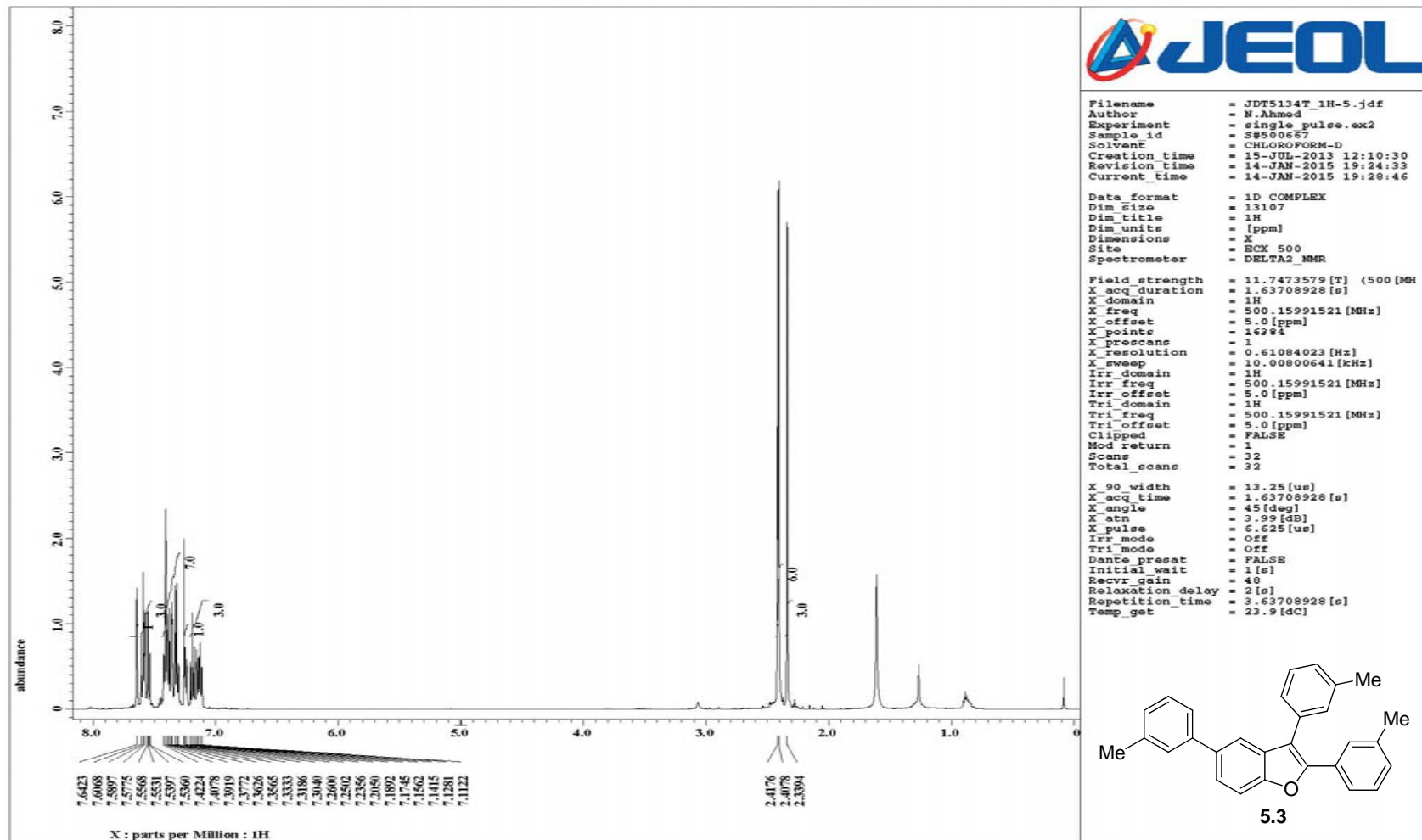
125 MHz ^{13}C NMR spectrum of compound **5.1**



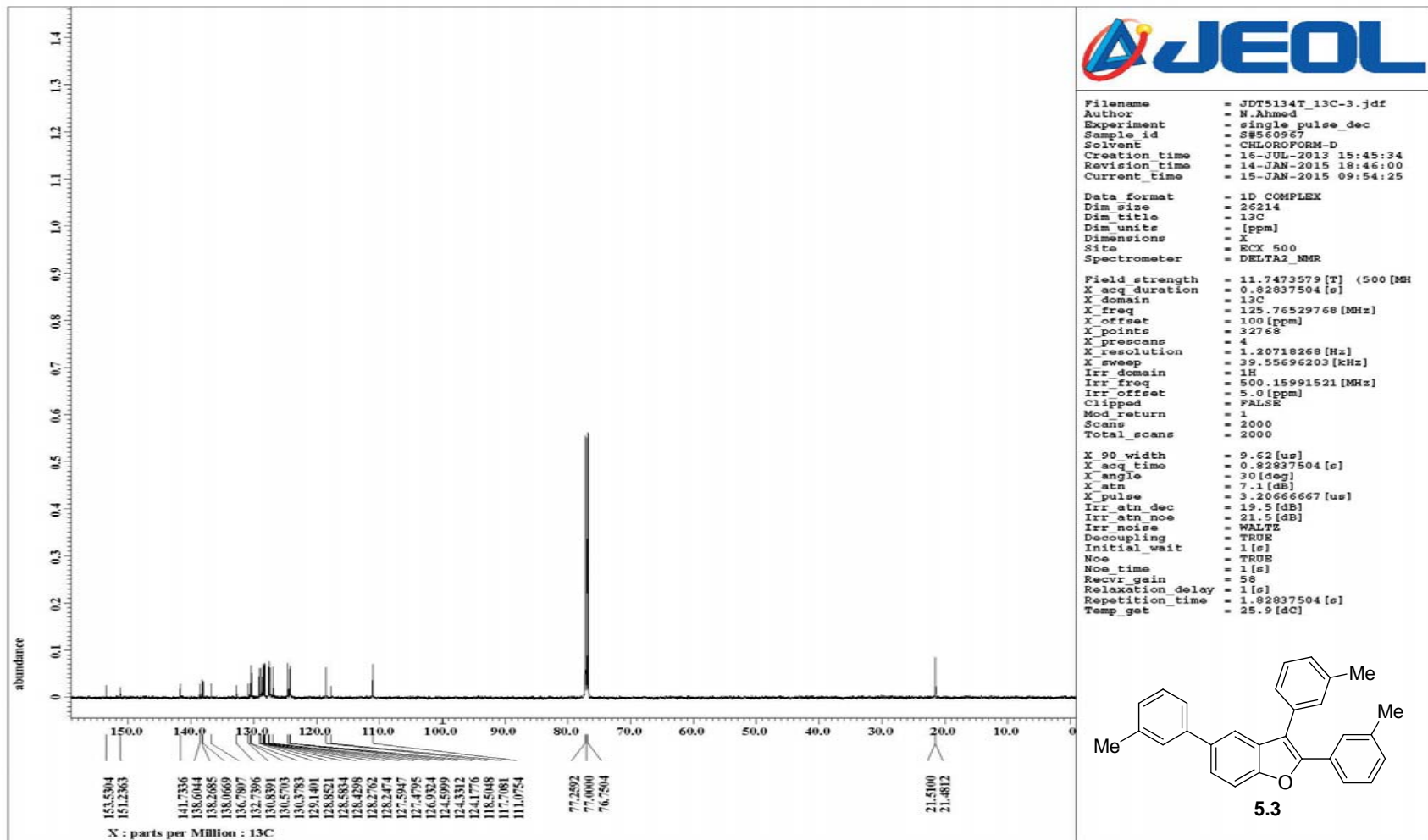
500 MHz ^1H NMR spectrum of compound **5.2**



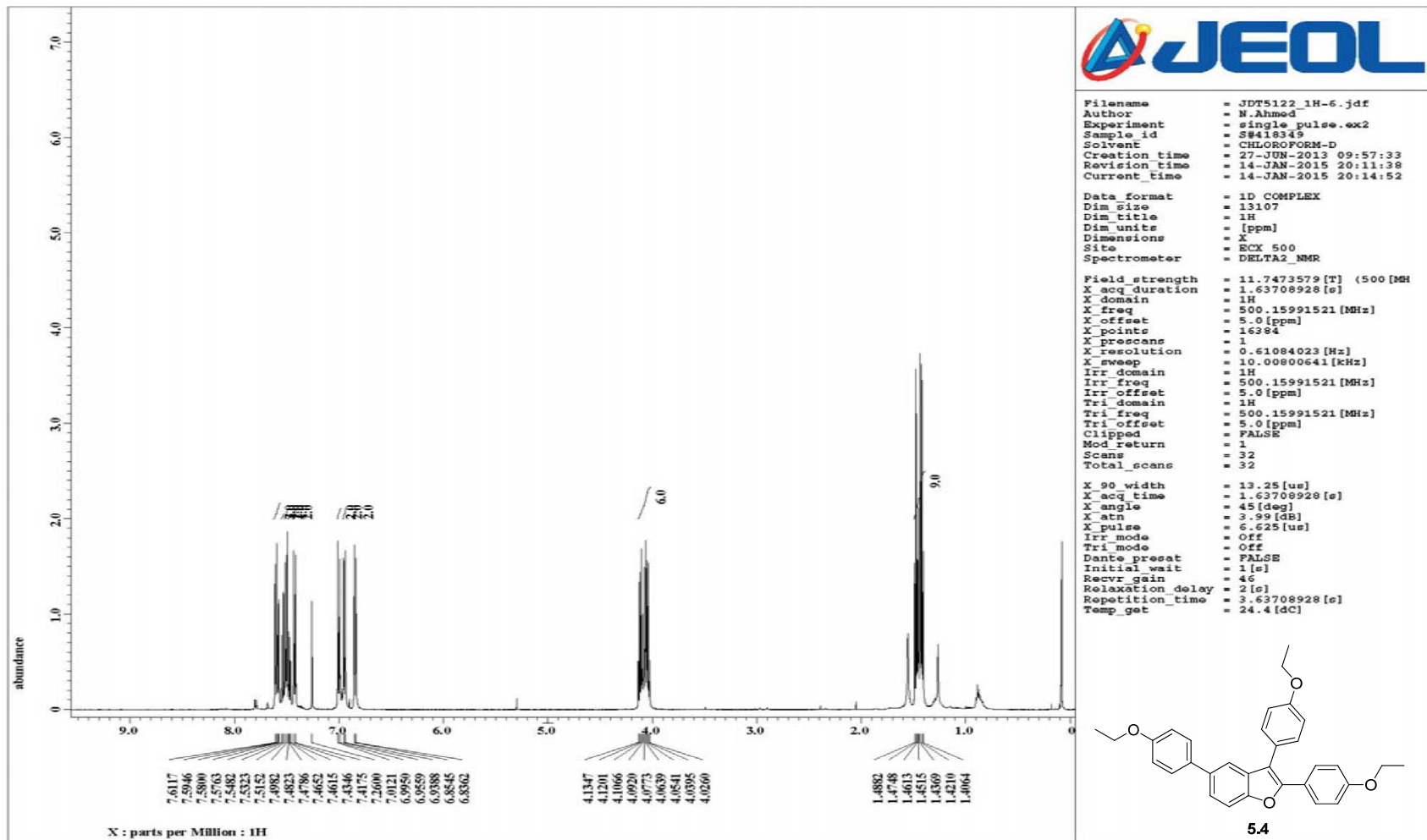
125 MHz ^{13}C NMR spectrum of compound **5.2**



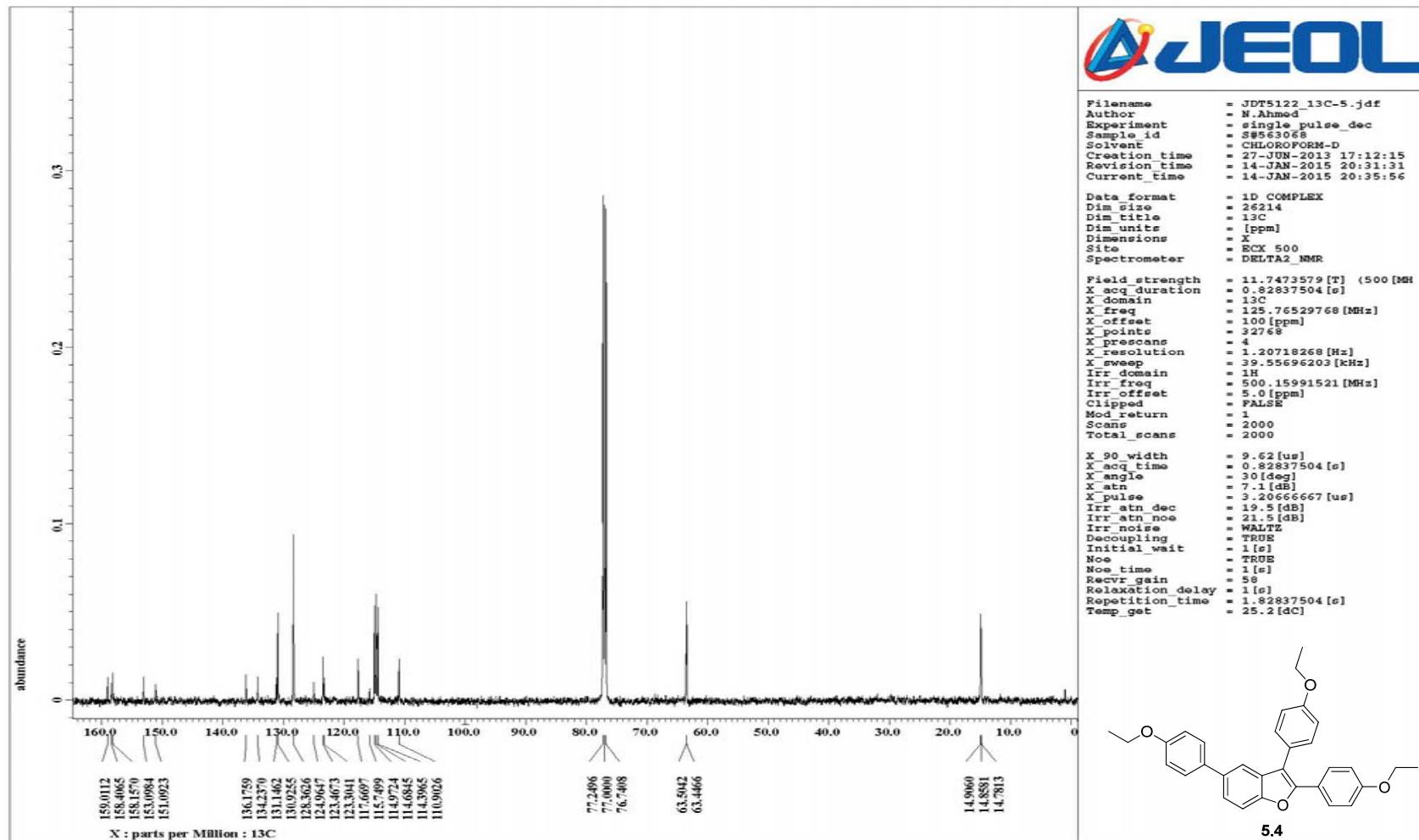
500 MHz ¹H NMR spectrum of compound **5.3**



125 MHz ^{13}C NMR spectrum of compound **5.3**



500 MHz ^1H NMR spectrum of compound 5.4



125 MHz ^{13}C NMR spectrum of compound **5.4**