

## **Supporting Information**

# **Pd-catalyzed Threefold Arylations of Mono, Di and Tetra-bromoquinones using Triarylbismuth Reagents**

Maddali L. N. Rao,\* Somnath Giri

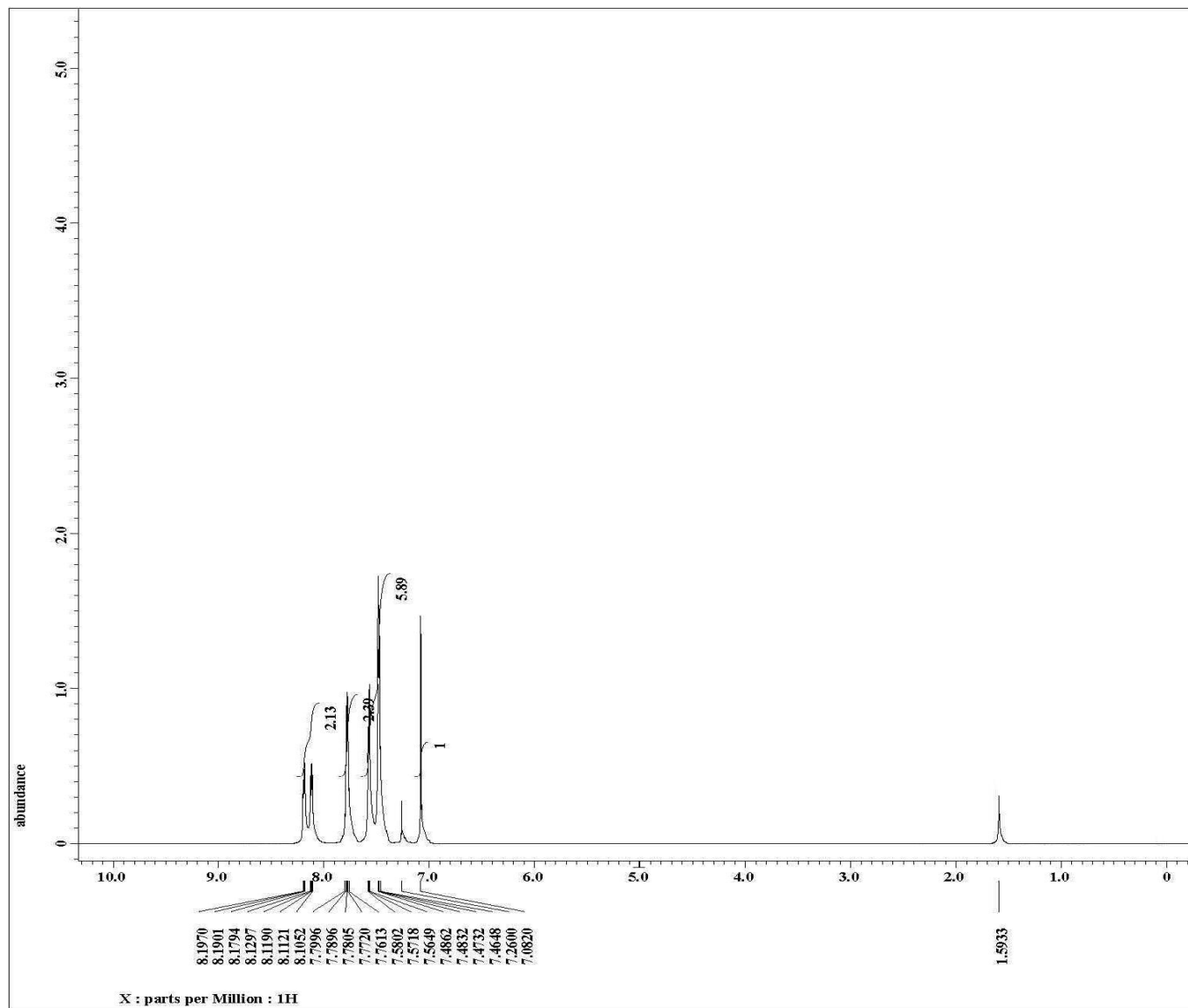
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**Contents**

*<sup>1</sup>H NMR, <sup>13</sup>C NMR & HRMS Spectra of compounds (2.1- 7.8).....S2-S179*





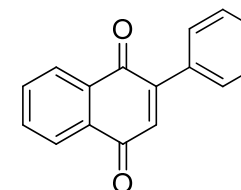
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Author       = N.Ahmed
Experiment    = single pulse.ex2
Sample id    = S#431159
Solvent      = CHLOROFORM-D
Creation time = 16-OCT-2009 11:30:17
Revision time = 16-MAY-2012 15:50:44
Current time  = 16-MAY-2012 15:52:49

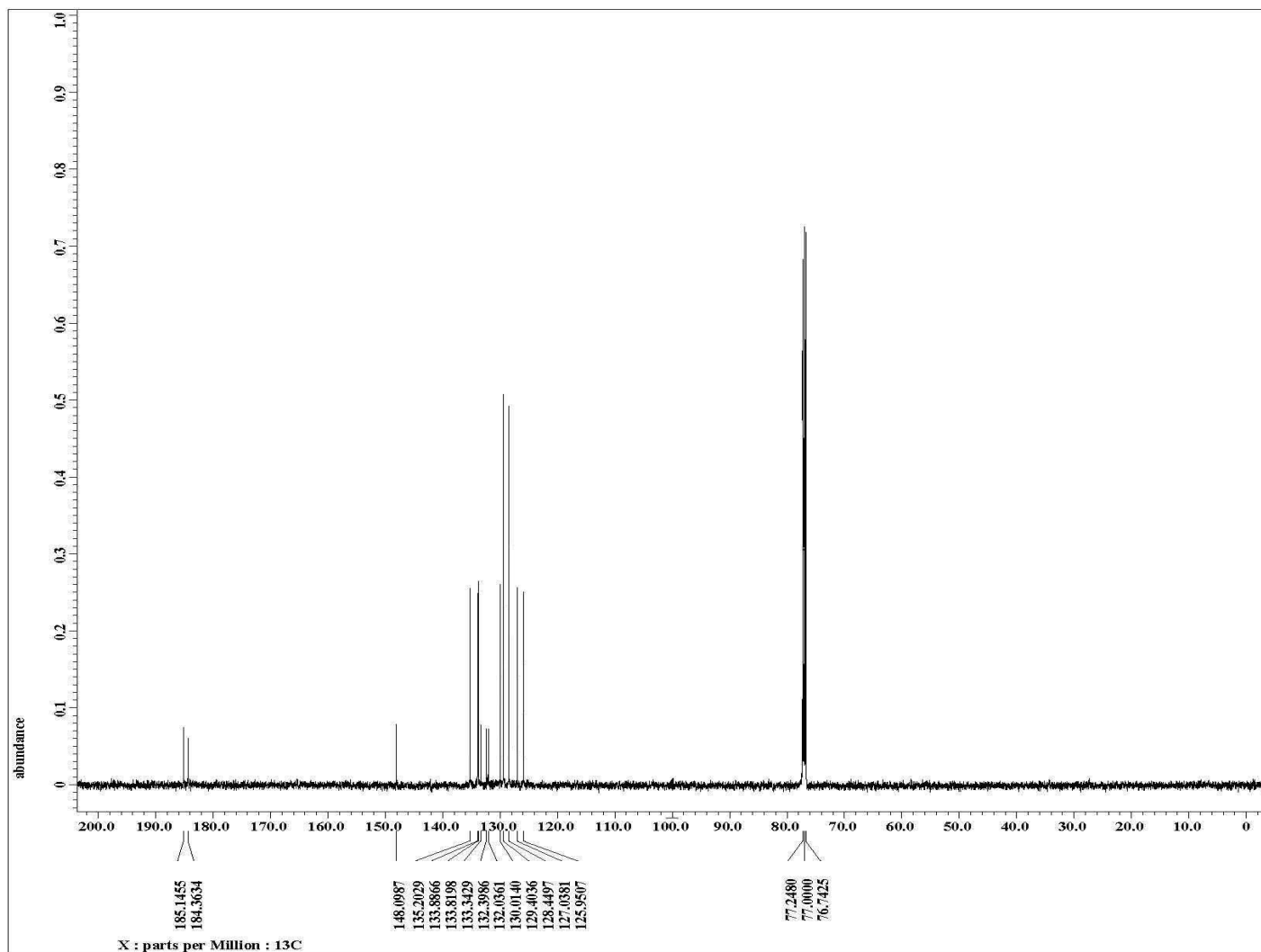
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Irr_freq       = 500.15991521 [MHz]
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Tri_domain     = 1H
Tri_freq       = 500.15991521 [MHz]
Tri_offset     = 5.0 [ppm]
Clipped        = FALSE
Mod return     = 1
Scans          = 16
Total_scans    = 16

X_90_width     = 13.25 [us]
X_acq_time      = 2.61619712 [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      = 46
Relaxation delay = 2 [s]
Repetition_time = 4.61619712 [s]
Temp_get        = 19.5 [dC]
    
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<sup>1</sup>H NMR spectrum of 2-phenyl-1,4-naphthoquinone (**2.1**)



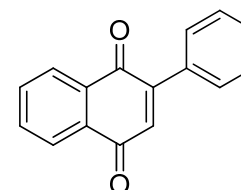
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Author       = N.Ahmed
Experiment   = single_pulse_dec
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Solvent      = CHLOROFORM-D
Creation time = 16-OCT-2009 12:03:32
Revision time = 2-JUL-2011 20:44:42
Current Time  = 2-JUL-2011 20:45:14

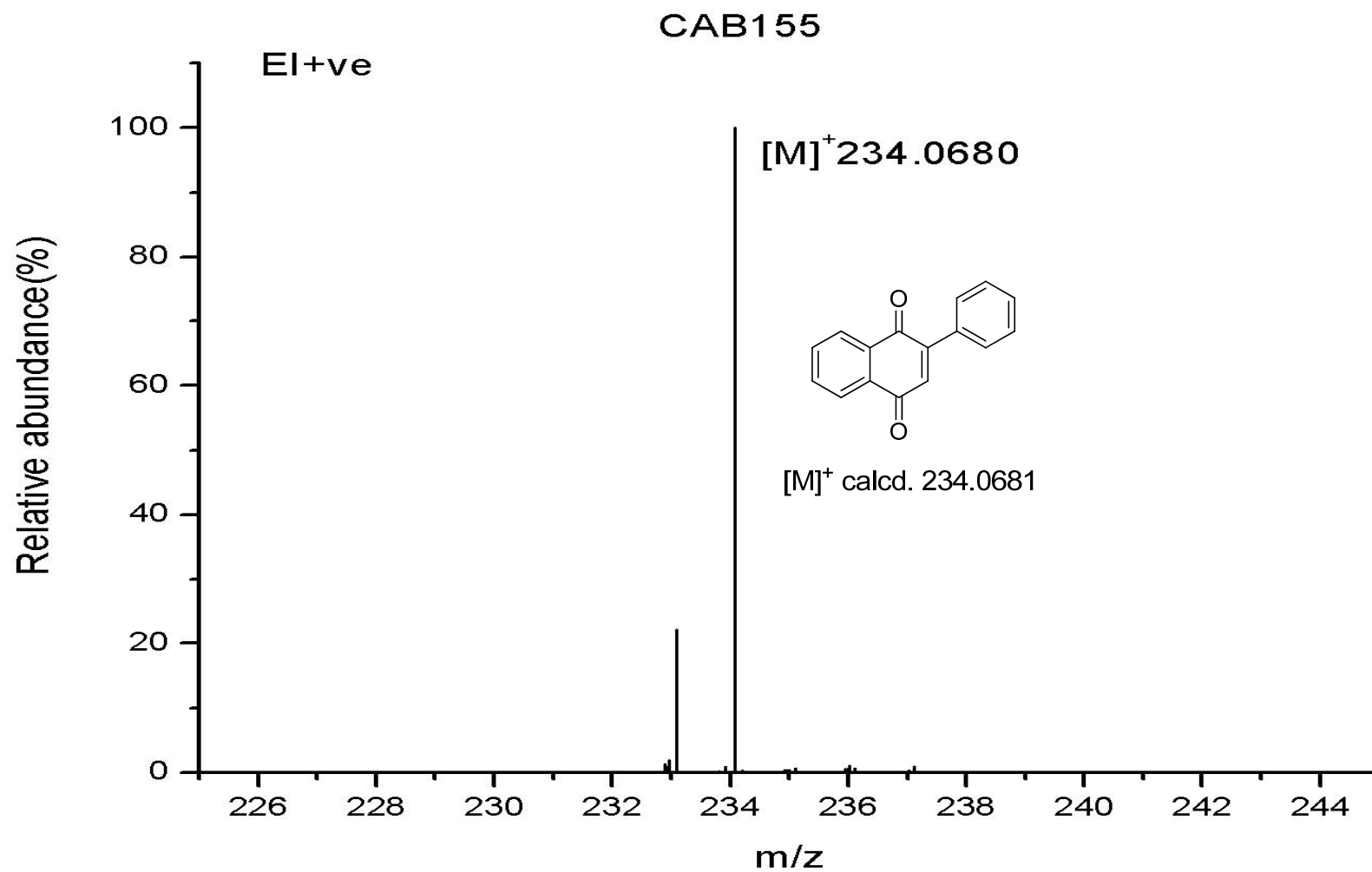
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Spectrometer  = DELTA2 NMR

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X_domain       = 13C
X_freq         = 125.76529768 [MHz]
X_offset       = 100 [ppm]
X_points       = 32768
X_prescans     = 4
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X_sweep        = 39.3081761 [kHz]
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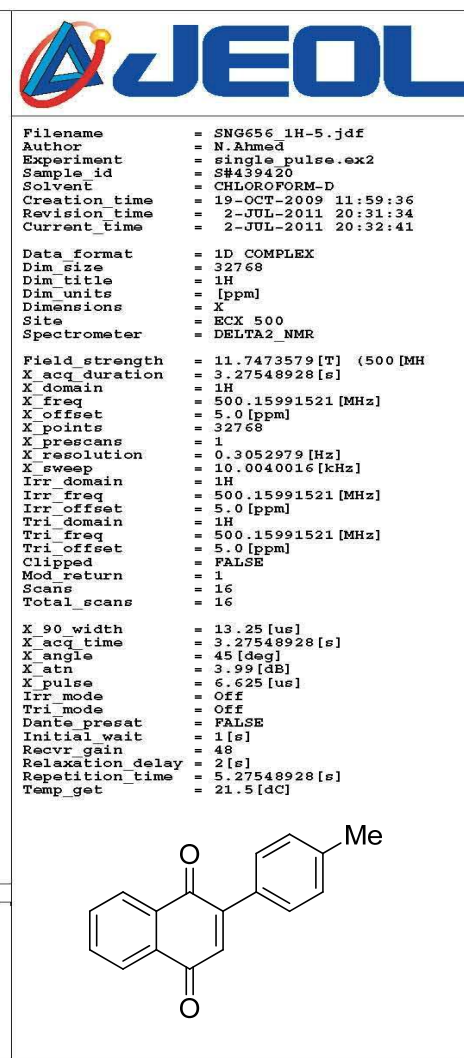
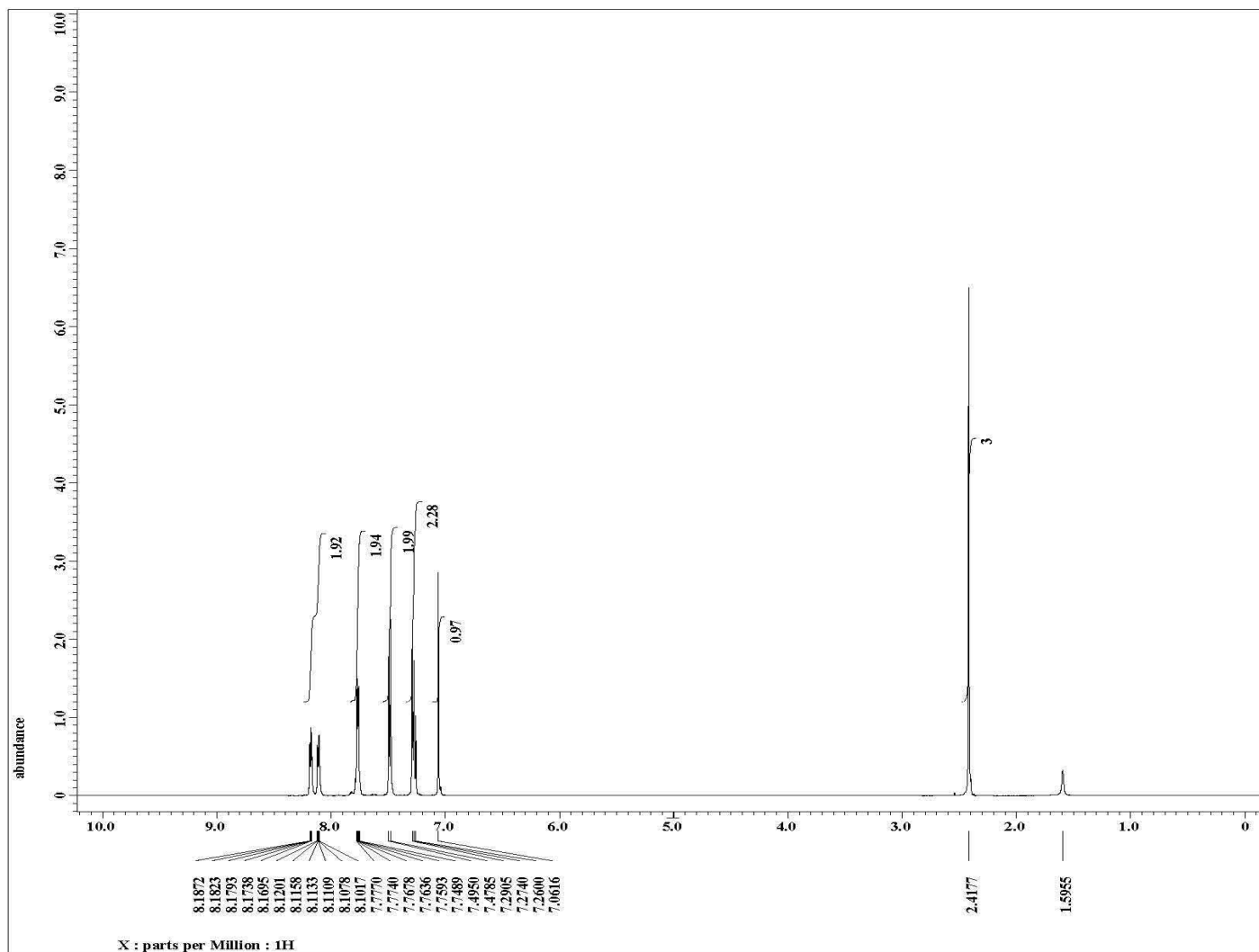
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X_angle        = 30 [deg]
X_atn          = 7.1 [dB]
X_pulse        = 3.20666667 [us]
Irr_atn_dec    = 19.5 [dB]
Irr_atn_noe    = 21.5 [dB]
Irr_noise      = WALTZ
Decoupling     = TRUE
Initial_wait   = 1 [s]
Noe            = TRUE
Noe_time       = 1 [s]
Recvr_gain     = 60
Relaxation_delay = 1 [s]
Repetition_time = 1.83361792 [s]
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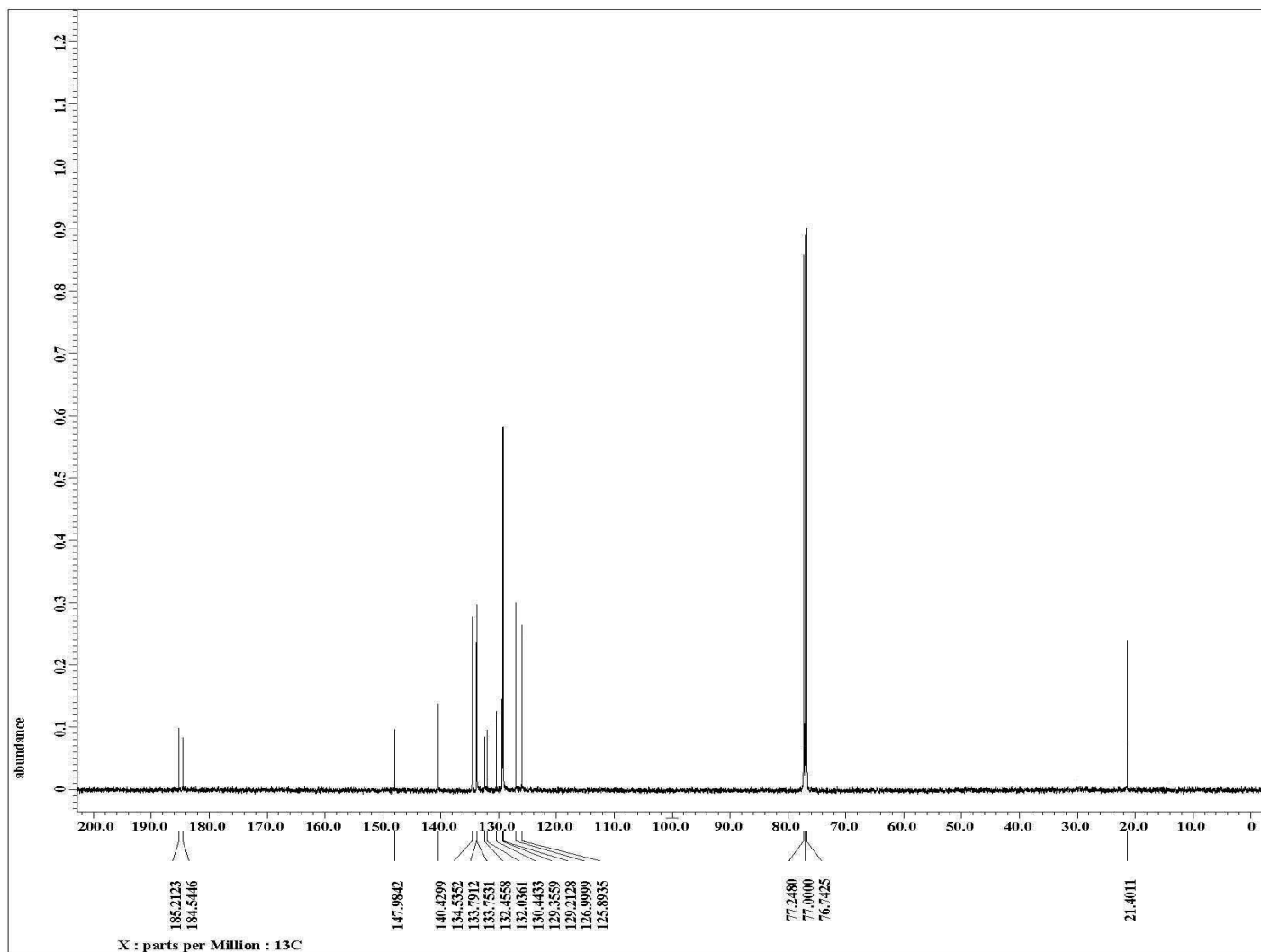
$^{13}\text{C}$  NMR spectrum of 2-phenyl-1,4-naphthoquinone (2.1)



HRMS spectrum of 2-phenyl-1,4-naphthoquinone (**2.1**)



<sup>1</sup>H NMR spectrum of 2-*p*-tolyl-1,4-naphthoquinone (2.2)



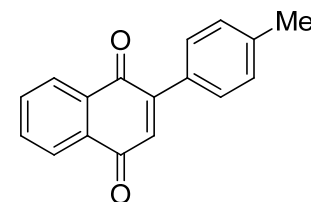
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Author       = N.Ahmed
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Solvent      = CHLOROFORM-D
Creation time = 19-OCT-2009 20:05:55
Revision time = 2-JUL-2011 20:35:38
Current Time  = 2-JUL-2011 20:36:27

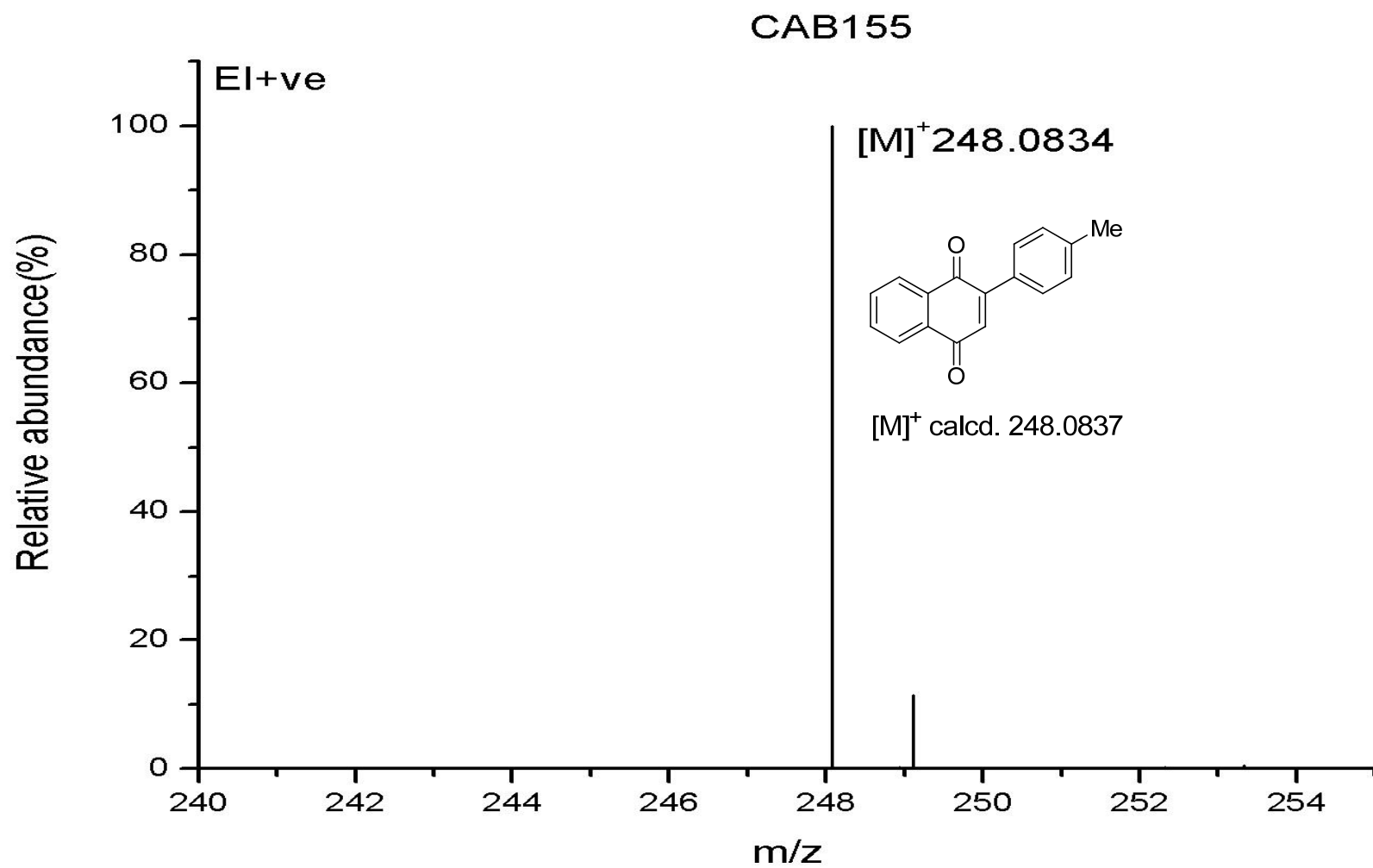
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Dim units     = [ppm]
Dimensions    = X
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Spectrometer  = DELTA2 NMR

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X_domain       = 13C
X_freq         = 125.76529768 [MHz]
X_offset       = 100 [ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.19959034 [Hz]
X_sweep        = 39.3081761 [kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521 [MHz]
Irr_offset     = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 2000
Total_scans    = 2000

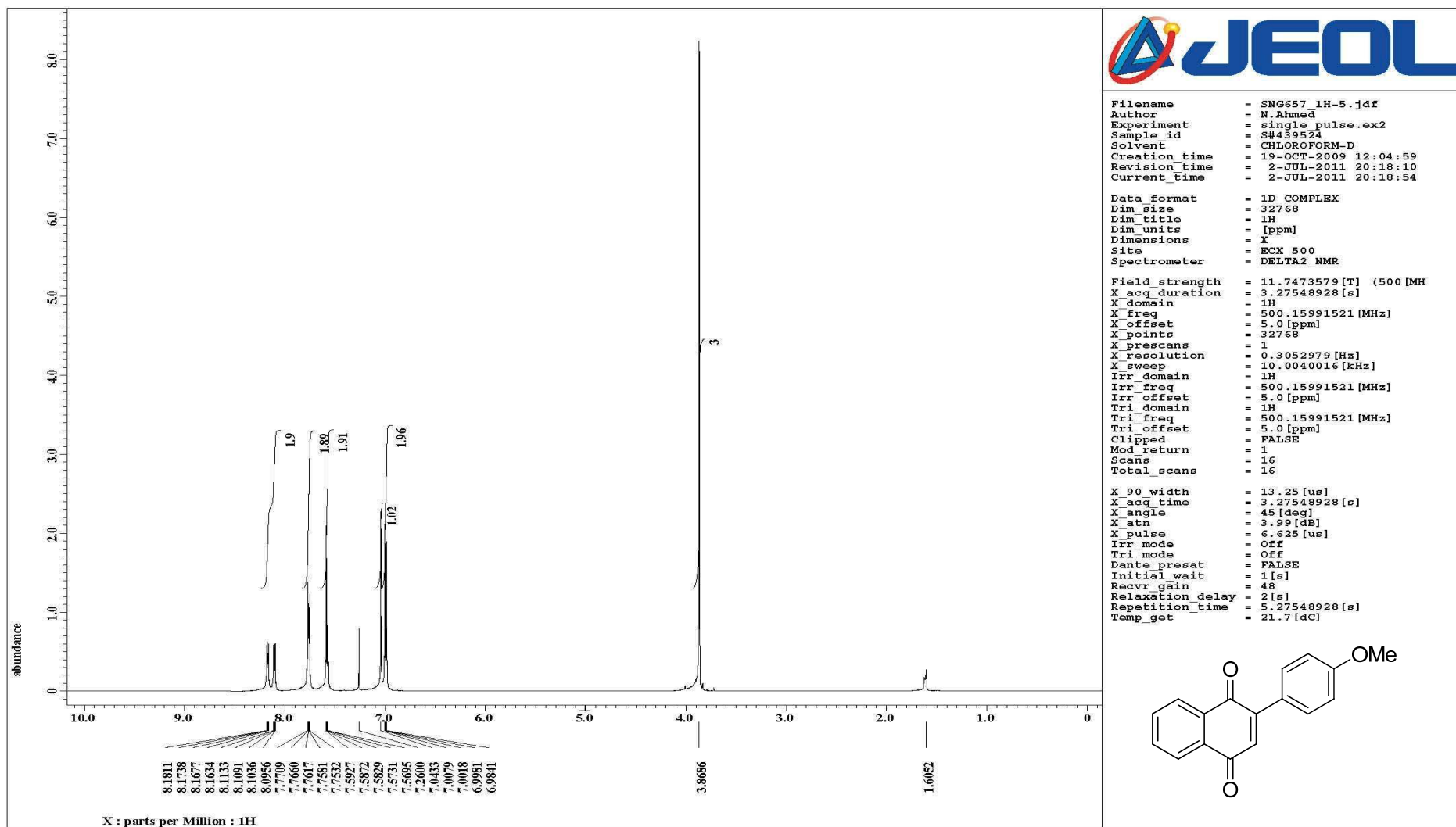
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X_acq_time     = 0.83361792 [s]
X_angle        = 30 [deg]
X_atn          = 7.1 [dB]
X_pulse        = 3.20666667 [us]
Irr_atn_dec    = 19.5 [dB]
Irr_atn_noe    = 21.5 [dB]
Irr_noise      = WALTZ
Decoupling     = TRUE
Initial_wait   = 1 [s]
Noe            = TRUE
Noe_time       = 1.19 [s]
Recvr_gain     = 60
Relaxation_delay = 1.19 [s]
Repetition_time = 2.02361792 [s]
Temp_get       = 17.1 [dC]
    
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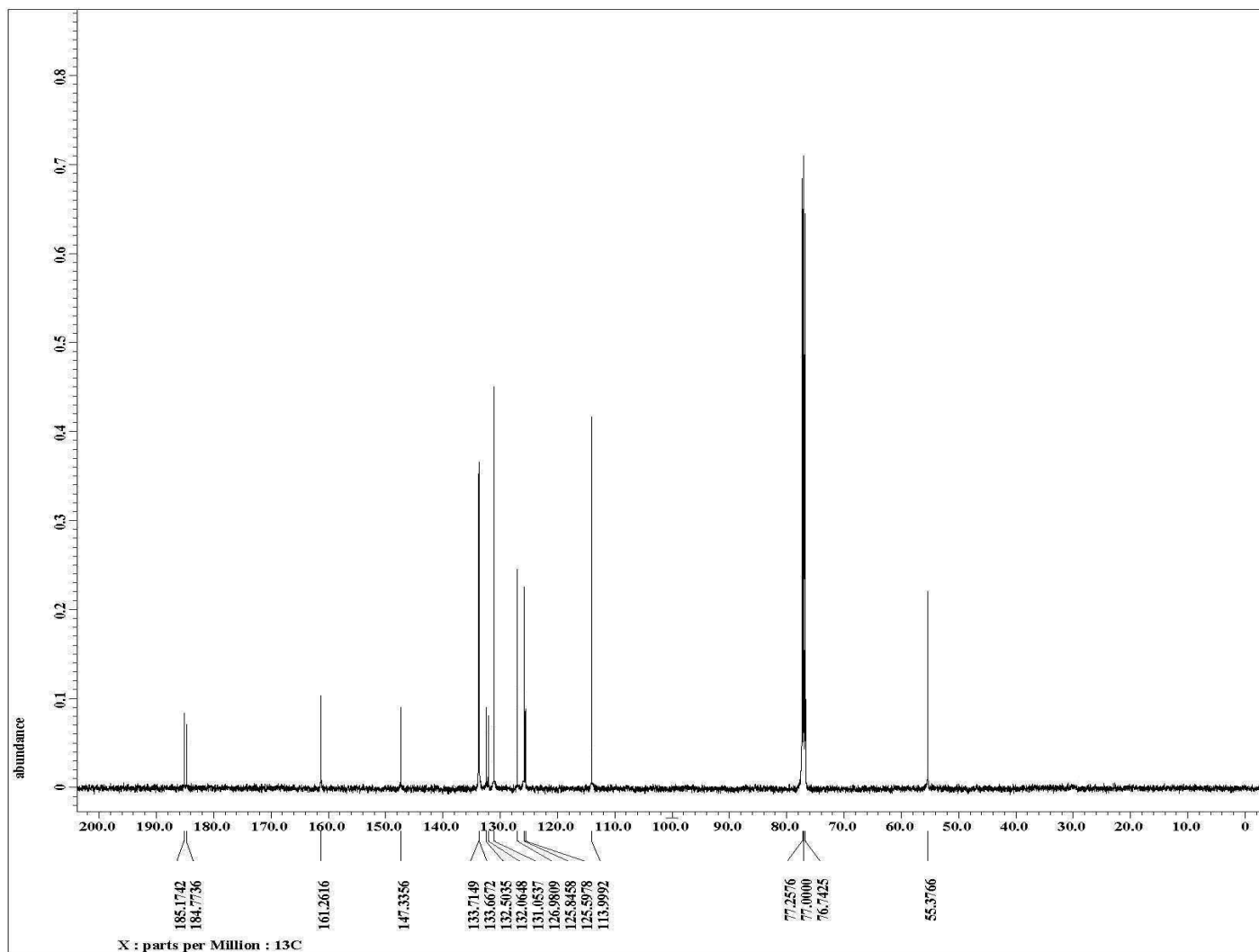
$^{13}\text{C}$  NMR spectrum of 2-*p*-tolyl-1,4-naphthoquinone (2.2)



HRMS spectrum of 2-*p*-tolyl-1,4-naphthoquinone (**2.2**)



<sup>1</sup>H NMR spectrum of 2-(4-methoxyphenyl)-1,4-naphthoquinone (2.3)



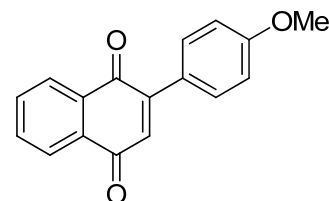
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Author       = N.Ahmed
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Solvent      = CHLOROFORM-D
Creation time = 19-OCT-2009 21:17:40
Revision time = 2-JUL-2011 20:22:27
Current Time  = 2-JUL-2011 20:23:31

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Dim units     = [ppm]
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Spectrometer  = DELTA2 NMR

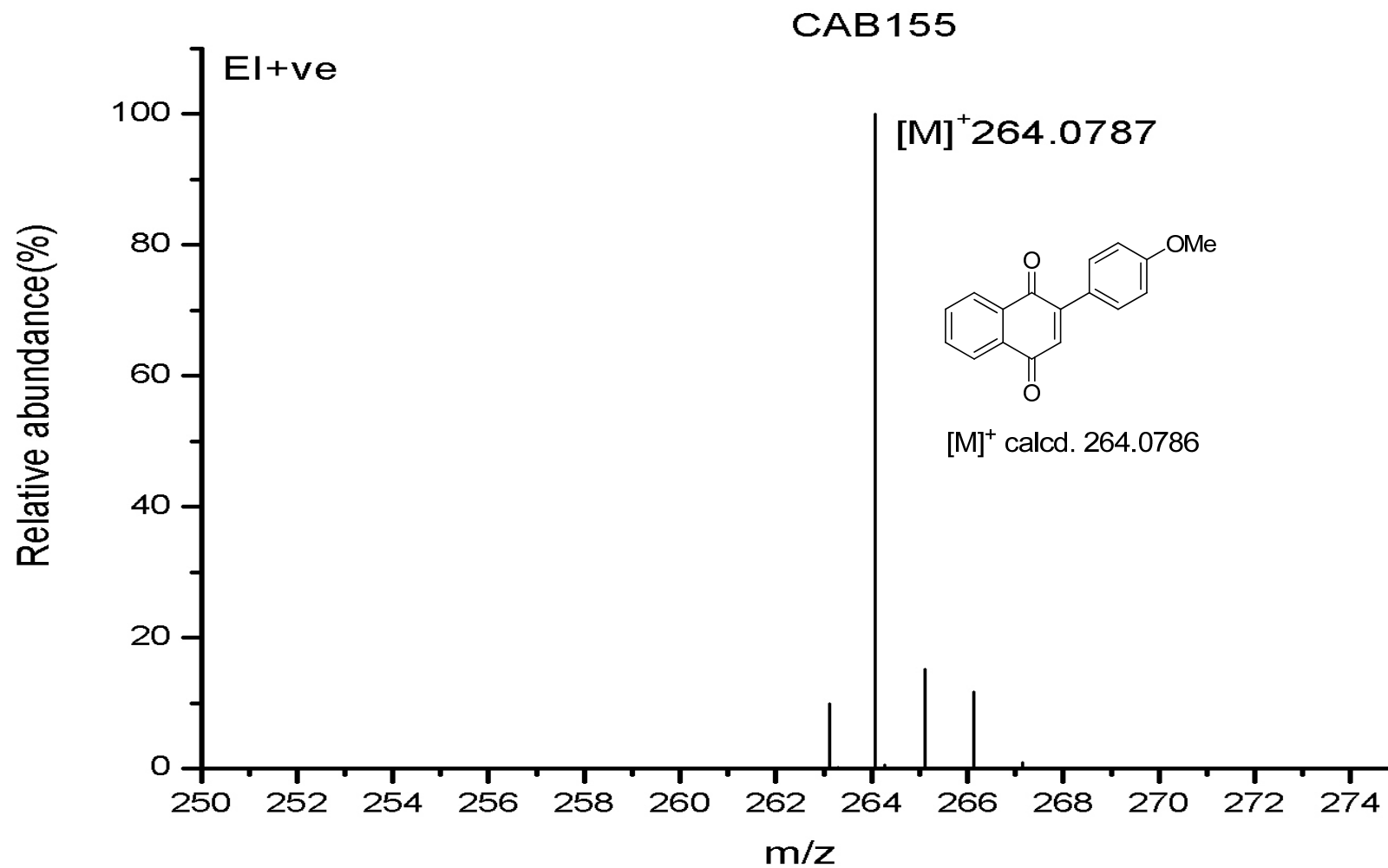
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X_domain       = 13C
X_freq         = 125.76529768 [MHz]
X_offset       = 100 [ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.19959034 [Hz]
X_sweep        = 39.3081761 [kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521 [MHz]
Irr_offset     = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 2000
Total_scans    = 2000

X_90_width    = 9.62 [us]
X_acq_time     = 0.83361792 [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       = 1.19 [s]
Recvr_gain     = 60
Relaxation_delay = 1.19 [s]
Repetition_time = 2.02361792 [s]
Temp_get       = 17.2 [dC]
    
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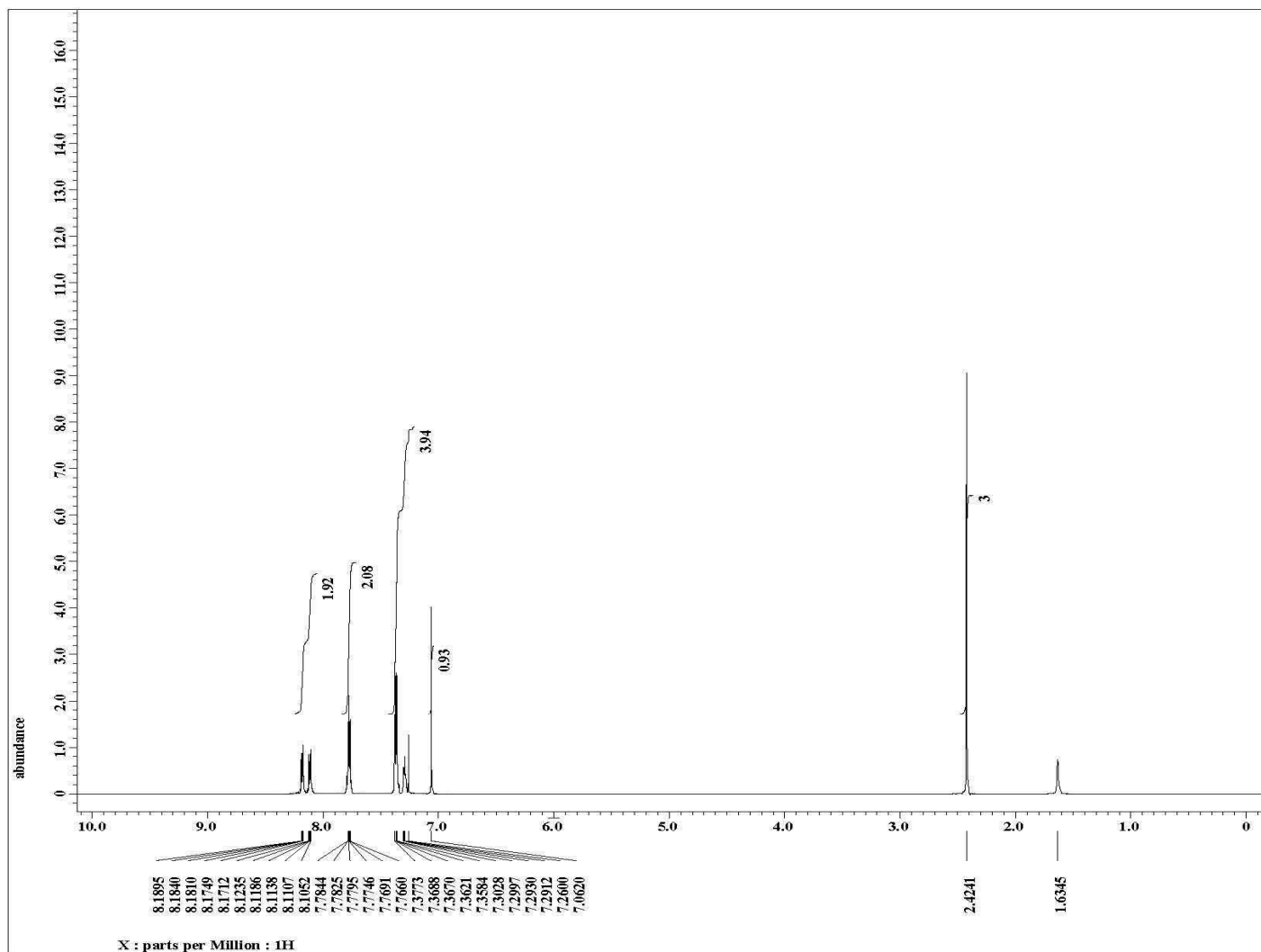


$^{13}\text{C}$  NMR spectrum of 2-(4-methoxyphenyl)-1,4-naphthoquinone (2.3)





HRMS spectrum of 2-(4-methoxyphenyl)-1,4-naphthoquinone (**2.3**)



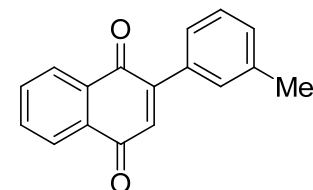
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Author       = N.Ahmed
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Solvent      = CHLOROFORM-D
Creation time = 7-OCT-2010 11:16:12
Revision time = 2-JUL-2011 23:13:17
Current time  = 2-JUL-2011 23:13:59

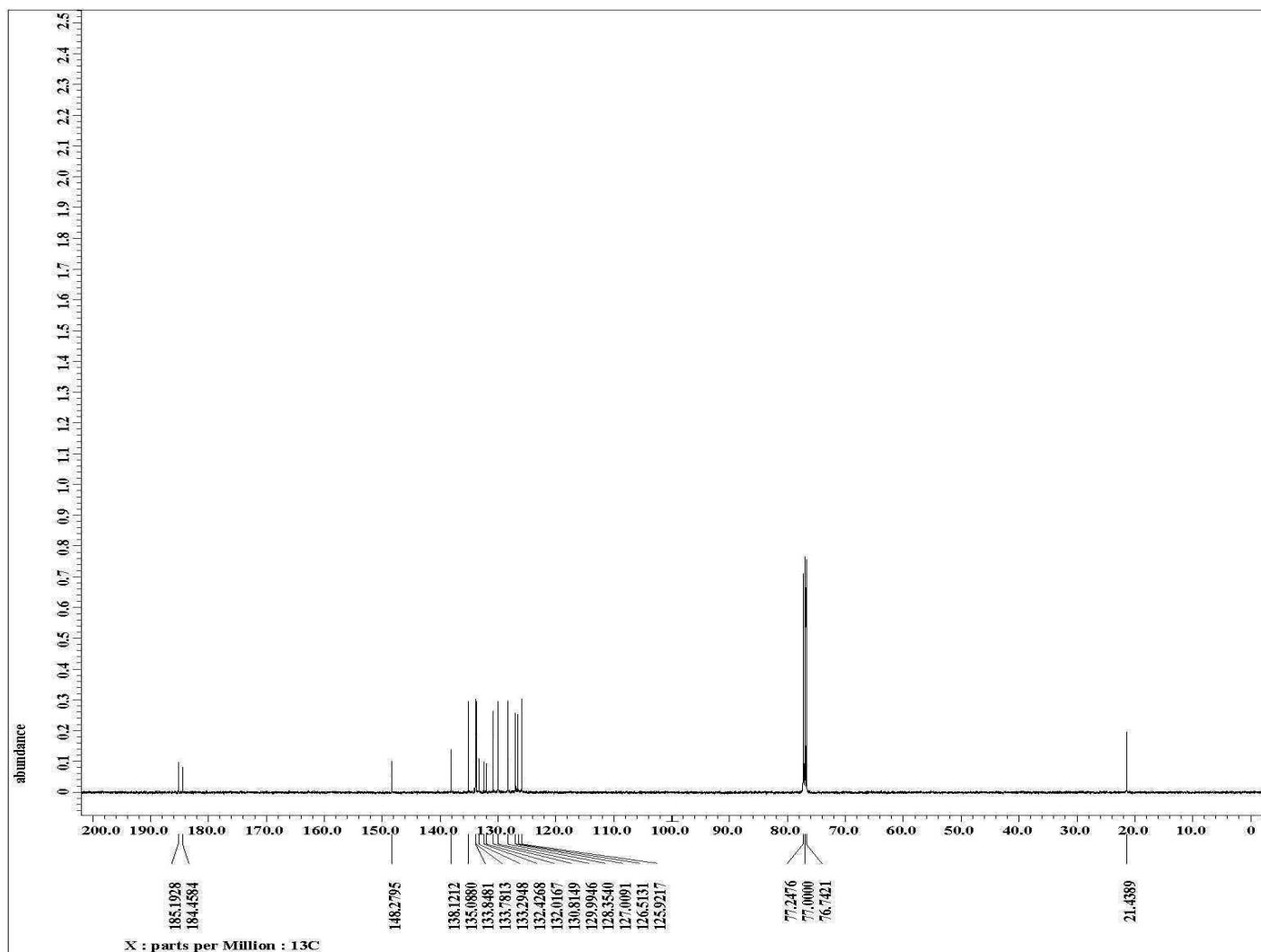
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Site          = ECX 500
Spectrometer  = DELTA2 NMR

Field strength = 11.7473579 [T] (500 [MH
X_acq_duration = 3.27155712 [s]
X_domain       = 1H
X_freq         = 500.15991521 [MHz]
X_offset       = 6 [ppm]
X_points       = 32768
X_prescans     = 1
X_resolution   = 0.30566485 [Hz]
X_sweep        = 10.01602564 [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      = 3.27155712 [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      = 46
Relaxation_delay = 1 [s]
Repetition_time = 4.27155712 [s]
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<sup>1</sup>H NMR spectrum of 2-*m*-tolyl-1,4-naphthoquinone (2.4)



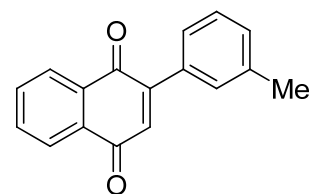
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Experiment    = single_pulse_dec
Sample id    = S4563807
Solvent      = CHLOROFORM-D
Creation time = 7-OCT-2010 19:38:00
Revision time = 22-AUG-2011 11:03:57
Current time  = 22-AUG-2011 11:04:50

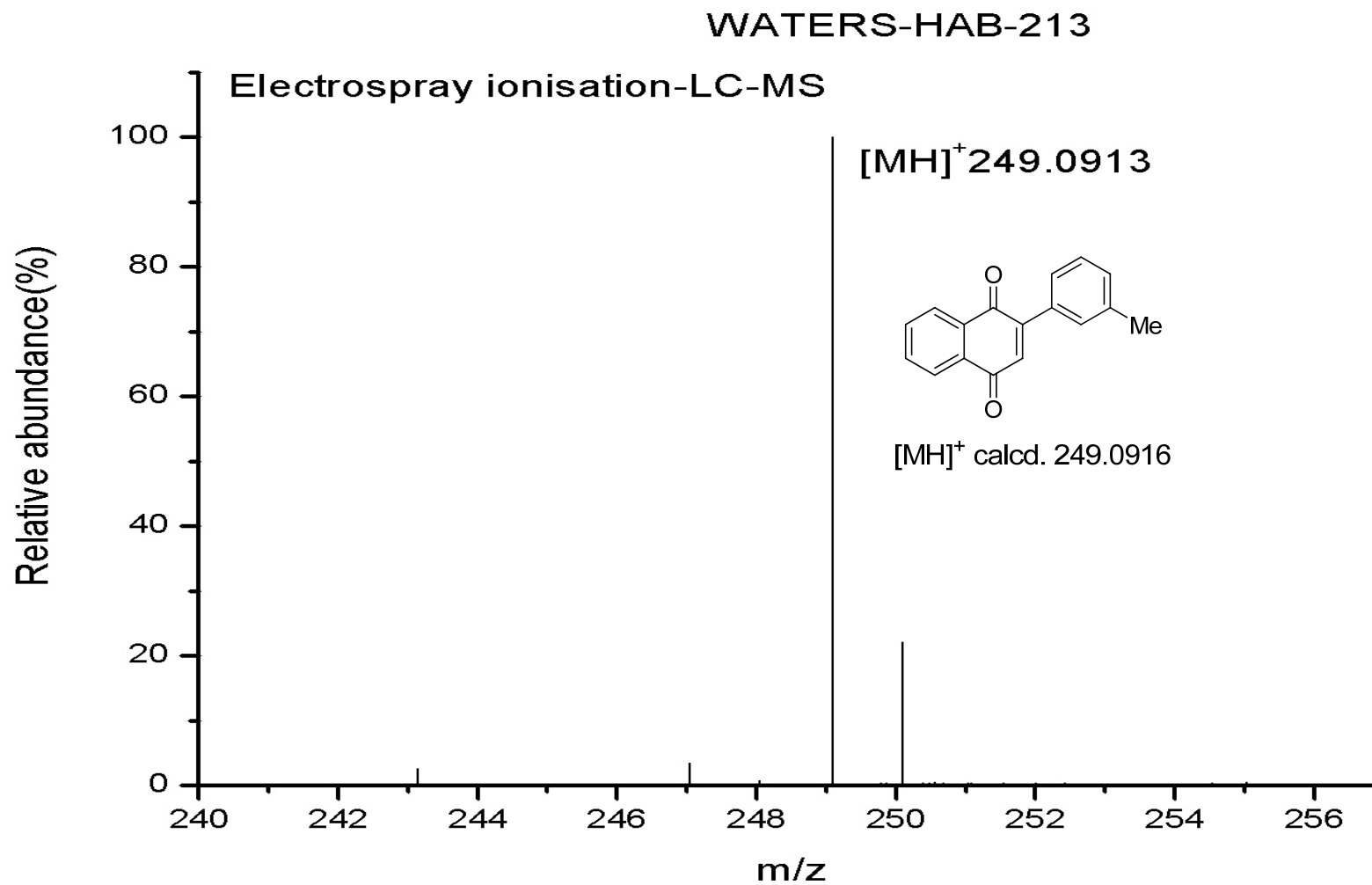
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Dim units     = [ppm]
Dimensions    = X
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Spectrometer  = DELTA2_NMR

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X_domain       = 13C
X_freq         = 125.76529768 [MHz]
X_offset       = 100 [ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.19959034 [Hz]
X_sweep        = 39.3081761 [kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521 [MHz]
Irr_offset     = 5.0 [ppm]
Clipped        = FALSE
Mod return     = 1
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Total_scans    = 2000

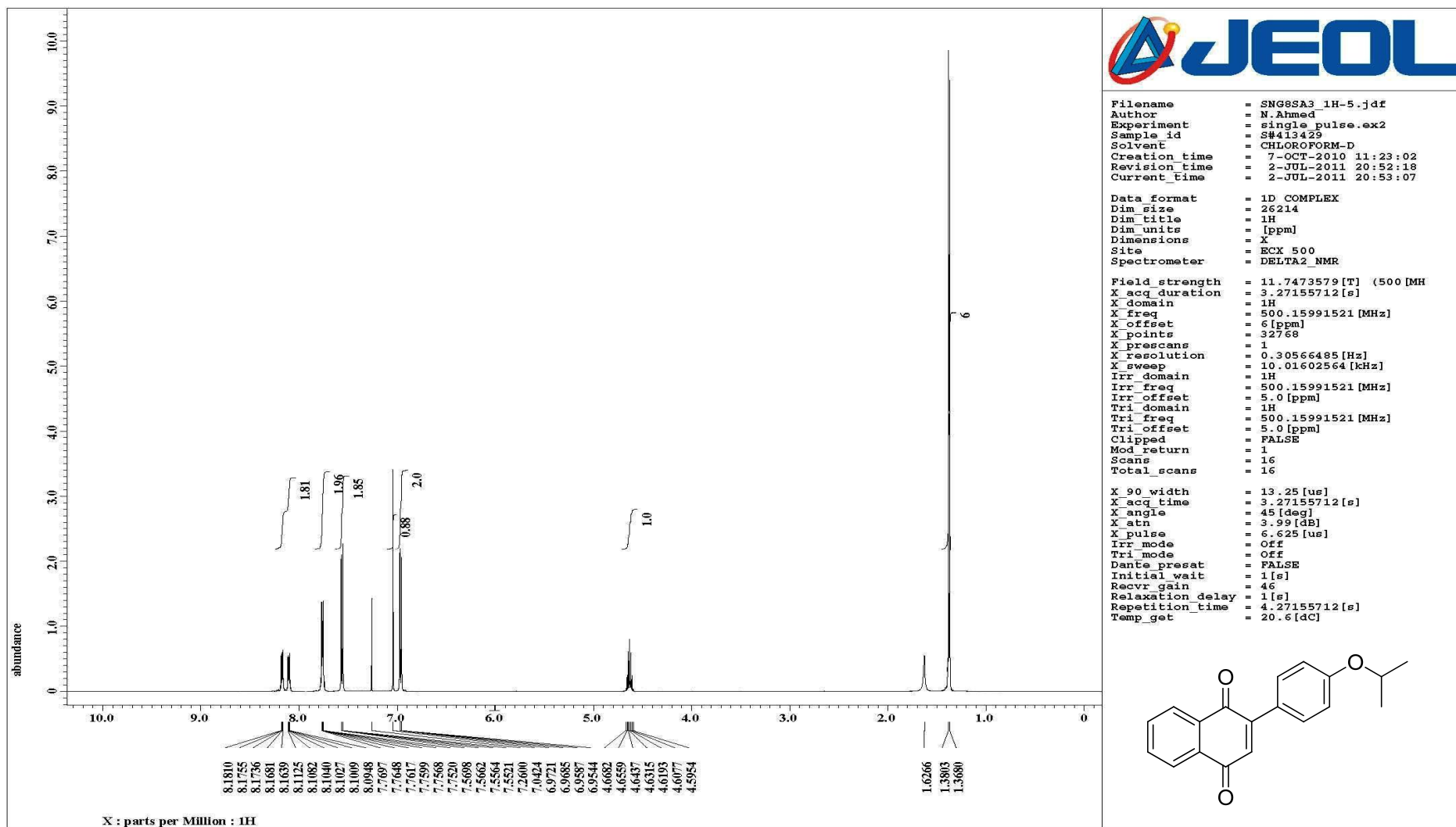
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X_acq_time     = 0.83361792 [s]
X_angle        = 30 [deg]
X_atn          = 7.1 [dB]
X_pulse        = 3.20666667 [us]
Irr_atn_dec    = 19.5 [dB]
Irr_atn_noe    = 21.5 [dB]
Irr_noise      = WALTZ
Decoupling     = TRUE
Initial wait   = 1 [s]
Noe            = TRUE
Noe_time       = 1 [s]
Recvr_gain     = 60
Relaxation_delay = 1 [s]
Repetition_time = 1.83361792 [s]
Temp_get       = 18.6 [dC]
    
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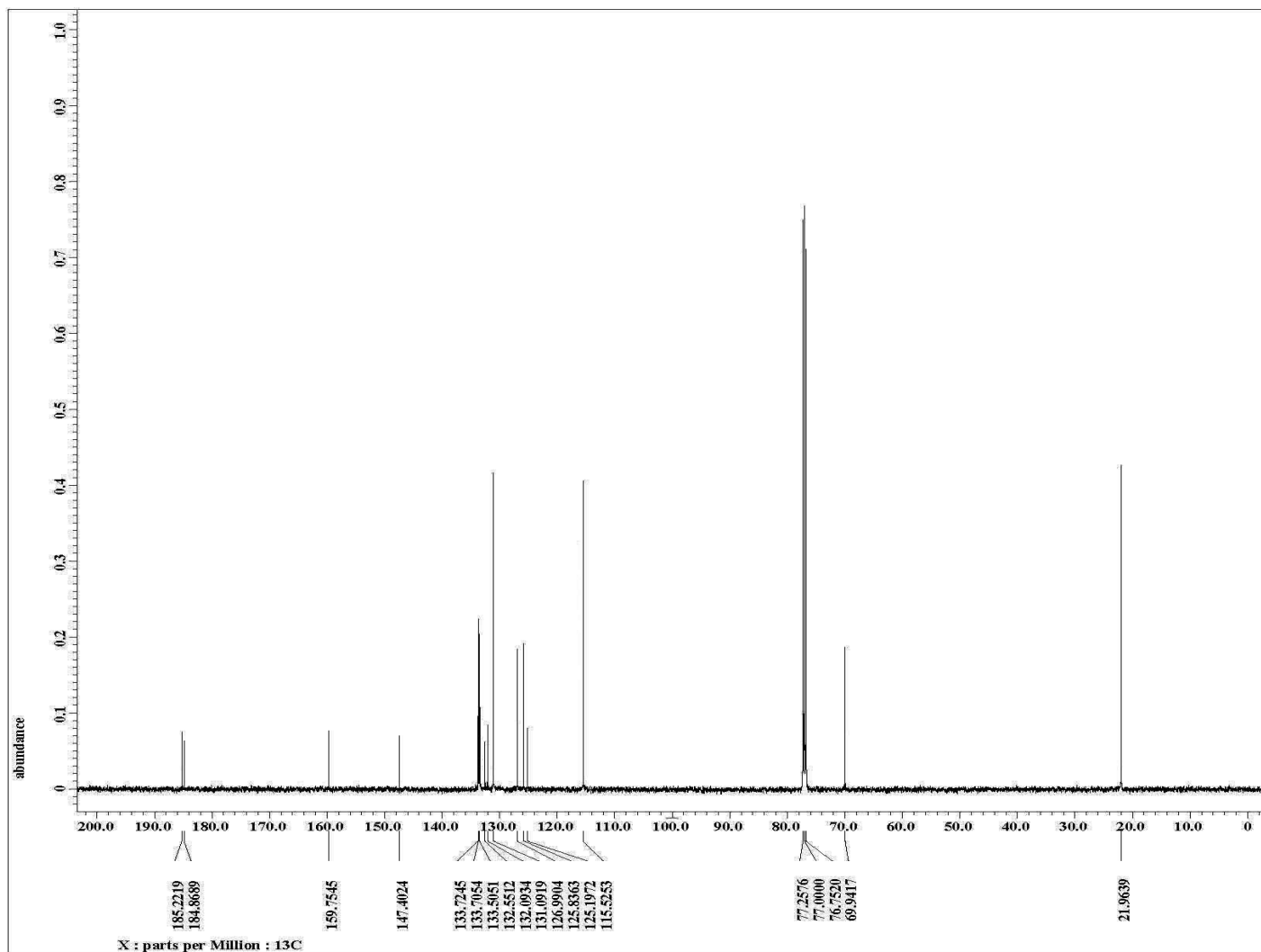
$^{13}\text{C}$  spectrum of 2-*m*-tolyl-1,4-naphthoquinone (2.4)



HRMS spectrum of 2-*m*-tolyl-1,4-naphthoquinone (**2.4**)



<sup>1</sup>H NMR spectrum of 2-(4-isopropoxyphenyl)-1,4-naphthoquinone (2.5)



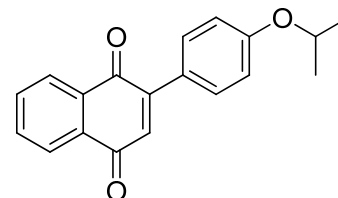
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Experiment   = single_pulse_dec
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Solvent      = CHLOROFORM-D
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Revision time = 2-JUL-2011 20:55:39
Current Time  = 2-JUL-2011 20:56:12

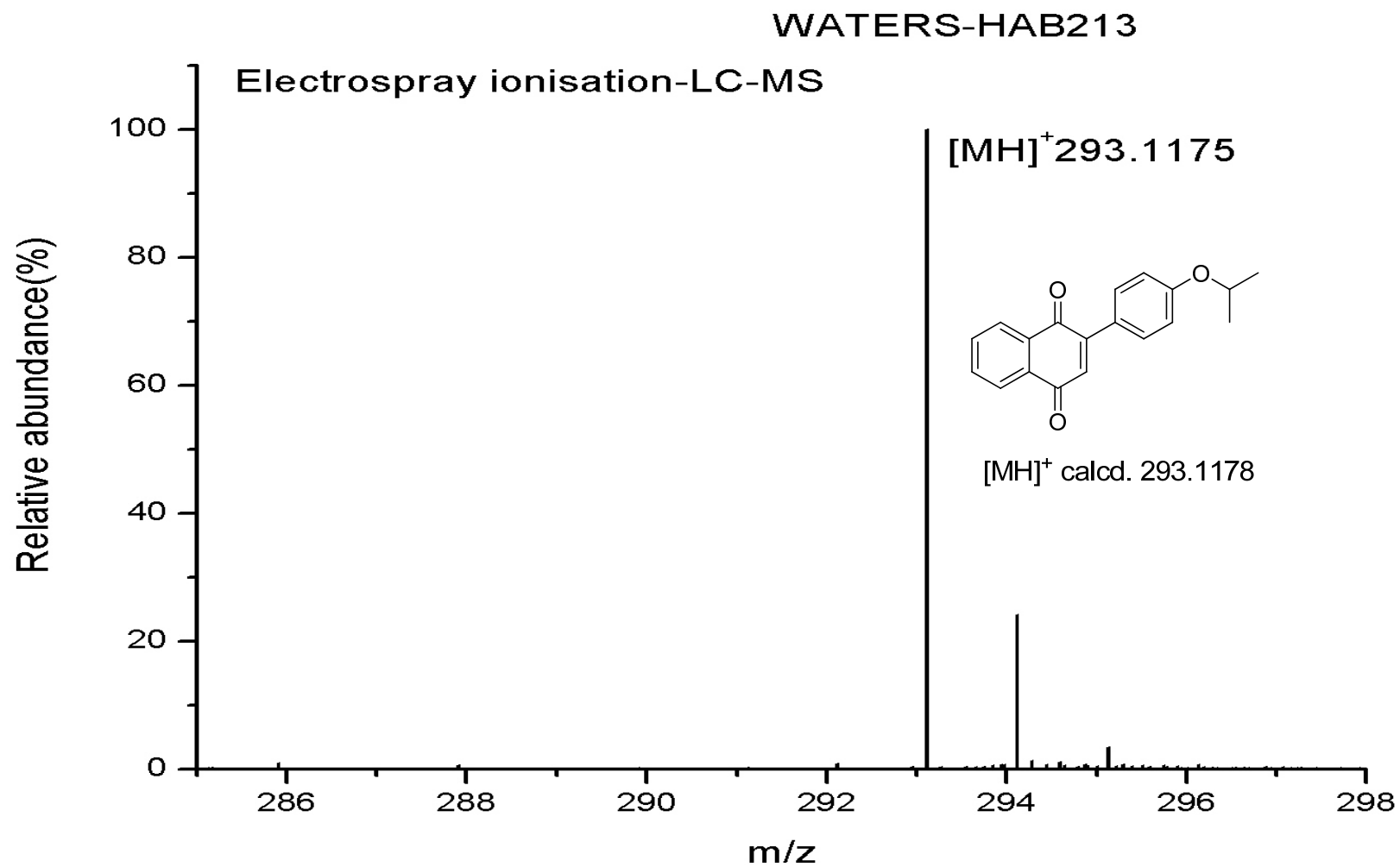
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Dim title     = 13C
Dim units     = [ppm]
Dimensions    = X
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Spectrometer  = DELTA2 NMR

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X_acq_duration = 0.83361792 [s]
X_domain       = 13C
X_freq         = 125.76529768 [MHz]
X_offset       = 100 [ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.19959034 [Hz]
X_sweep        = 39.3081761 [kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521 [MHz]
Irr_offset     = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 2000
Total_scans    = 2000

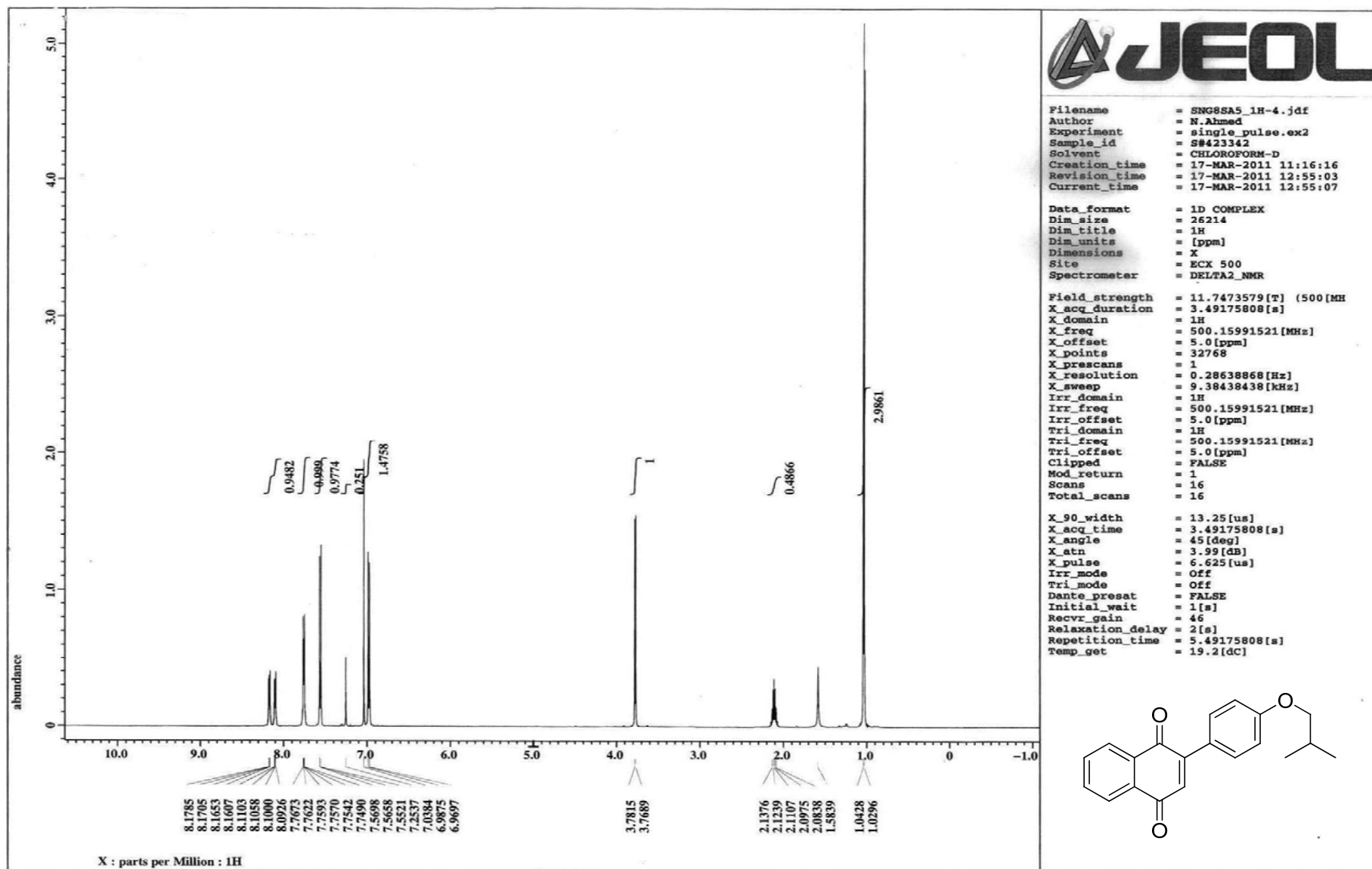
X_90_width     = 9.62 [us]
X_acq_time      = 0.83361792 [s]
X_angle         = 30 [deg]
X_atn           = 7.1 [dB]
X_pulse         = 3.20666667 [us]
Irr_atn_dec     = 19.5 [dB]
Irr_atn_noe     = 21.5 [dB]
Irr_noise       = WALTZ
Decoupling      = TRUE
Initial_wait    = 1 [s]
Noe             = TRUE
Noe_time        = 1 [s]
Recvr_gain      = 60
Relaxation_delay = 1 [s]
Repetition_time = 1.83361792 [s]
Temp_get        = 18.3 [dC]
    
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$^{13}\text{C}$  NMR spectrum of 2-(4-isopropoxyphenyl)-1,4-naphthoquinone (2.5)

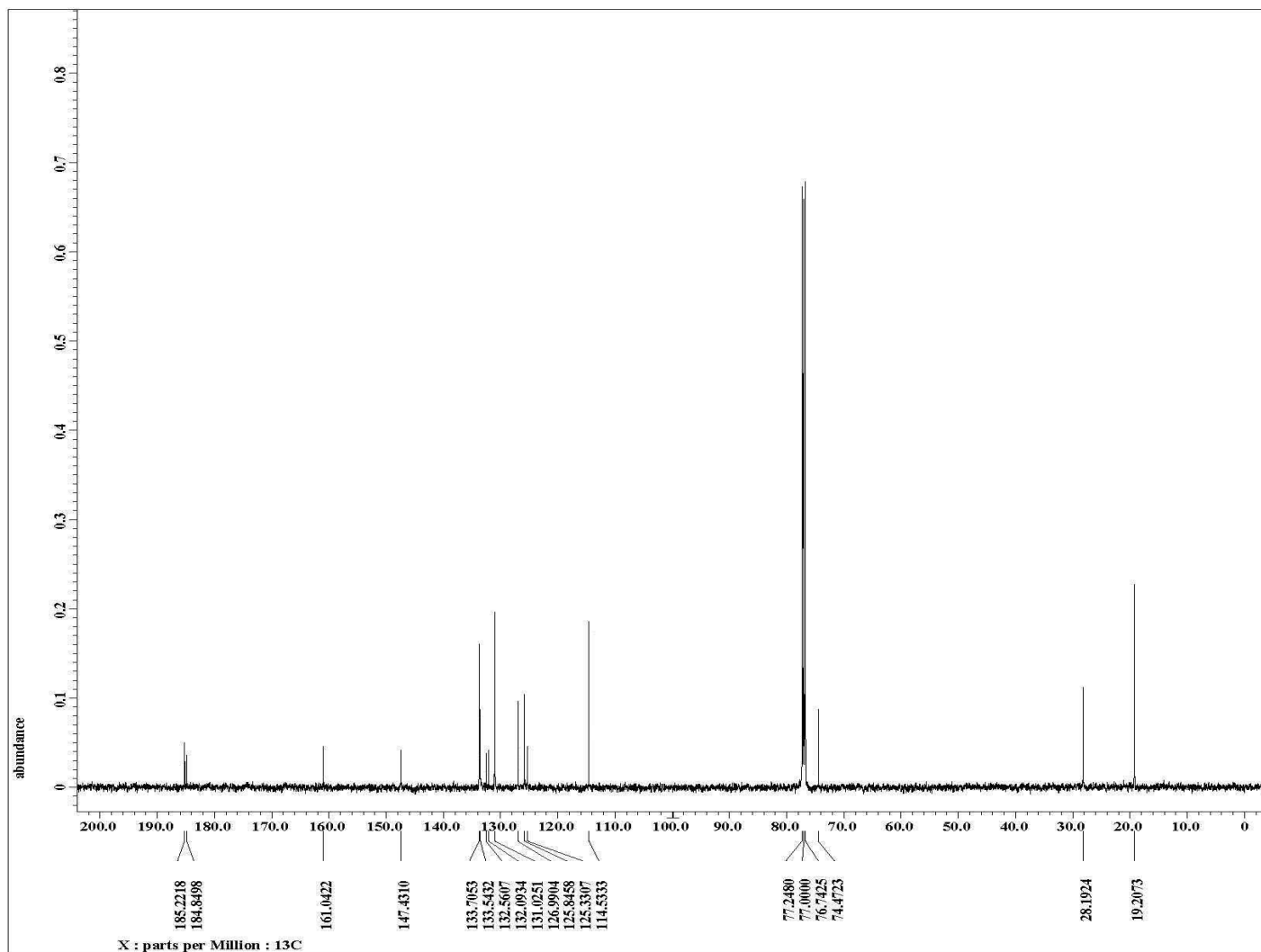


HRMS spectrum of 2-(4-isopropoxyphenyl)-1,4-naphthoquinone (**2.5**)



$^1\text{H}$  NMR spectrum of 2-(4-isopropoxyphenyl)-1,4-naphthoquinone (2.6)





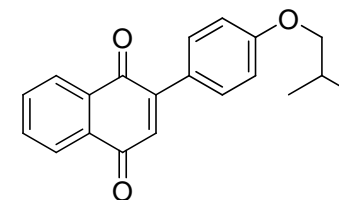
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Filename      = SNG8SA5 CARBON-3.jdf
Author       = N.Ahmed
Experiment   = single_pulse_dec
Sample_id    = S#726302
Solvent      = CHLOROFORM-D
Creation time = 17-MAR-2011 19:53:33
Revision time = 17-MAR-2011 20:52:34
Current Time  = 2-JUL-2011 22:51:12

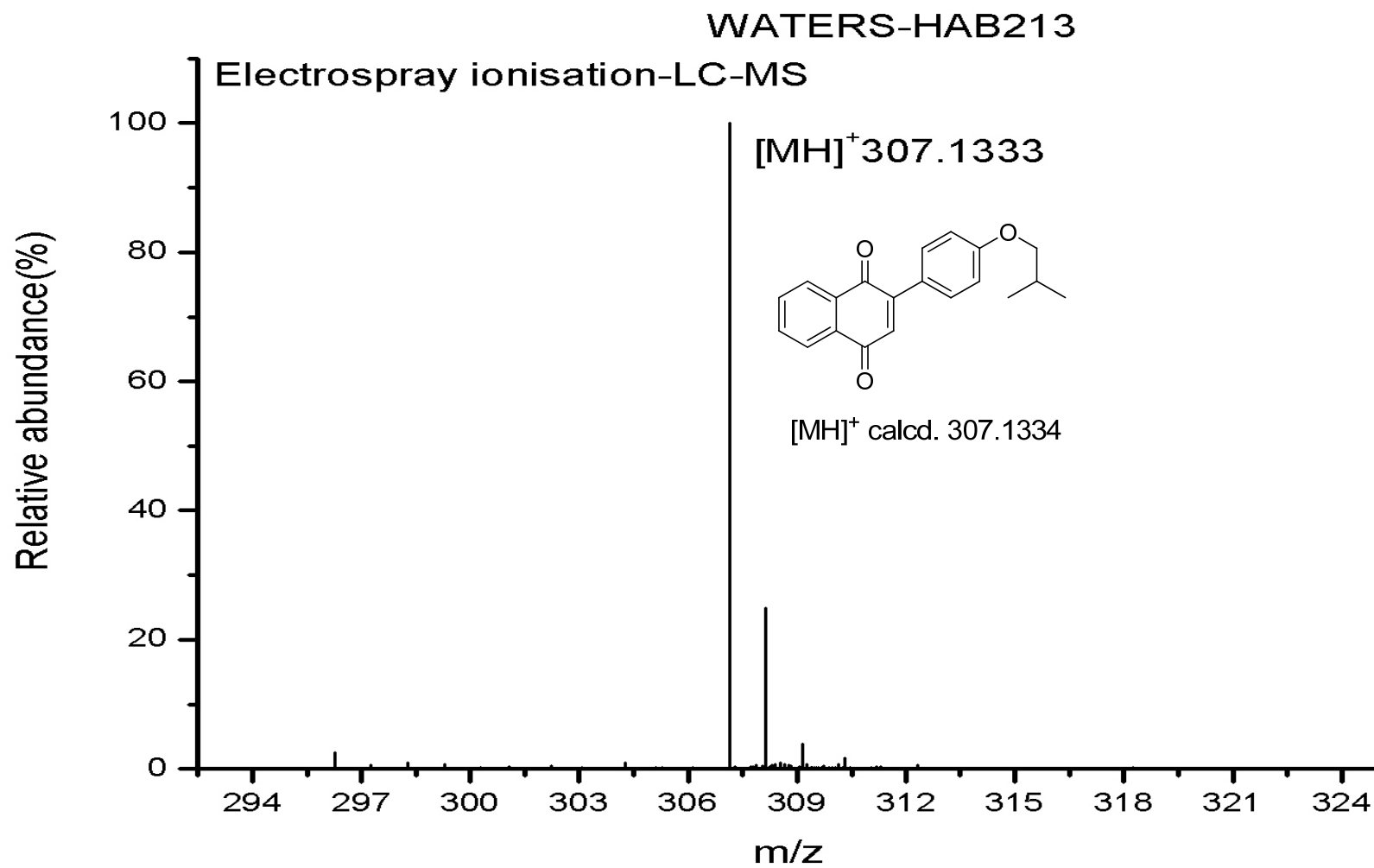
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Dim units     = [ppm]
Dimensions    = X
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Spectrometer  = DELTA2 NMR

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X_acq_duration = 0.83361792 [s]
X_domain       = 13C
X_freq         = 125.76529768 [MHz]
X_offset       = 100 [ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.19959034 [Hz]
X_sweep        = 39.3081761 [kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521 [MHz]
Irr_offset     = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 1024
Total_scans    = 1024

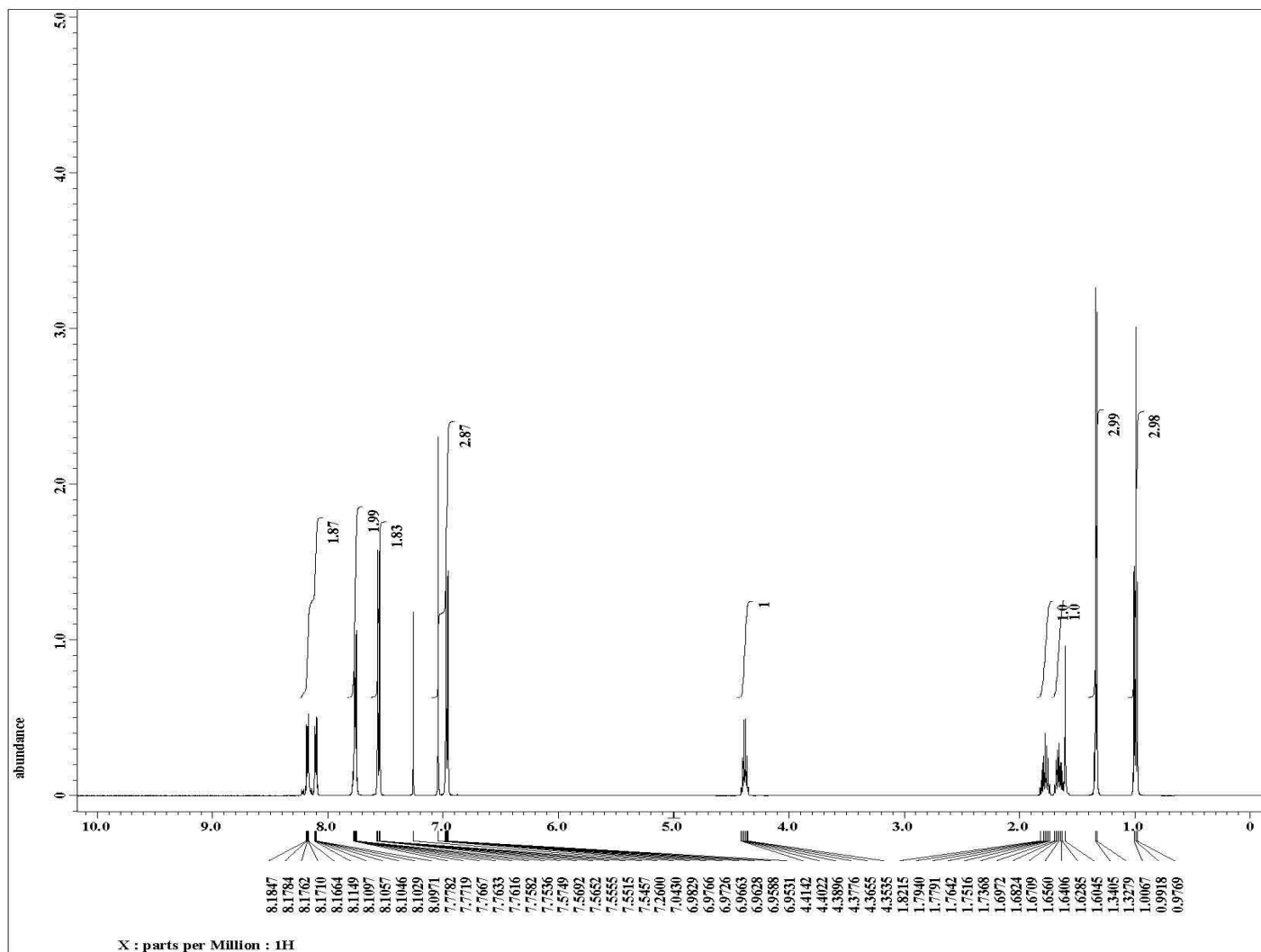
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X_acq_time     = 0.83361792 [s]
X_angle        = 30 [deg]
X_atn          = 7.1 [dB]
X_pulse        = 3.20666667 [us]
Irr_atn_dec    = 21.5 [dB]
Irr_atn_noe    = 21.5 [dB]
Irr_noise      = WALTZ
Decoupling     = TRUE
Initial_wait   = 1 [s]
Noe            = TRUE
Noe_time       = 1 [s]
Recvr_gain     = 60
Relaxation_delay = 1 [s]
Repetition_time = 1.83361792 [s]
Temp_get       = 18.3 [dC]
    
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$^{13}\text{C}$  NMR spectrum of 2-(4-isopropoxyphenyl)-1,4-naphthoquinone (2.6)



HRMS spectrum of 2-(4-isopropoxyphenyl)-1,4-naphthoquinone (**2.6**)

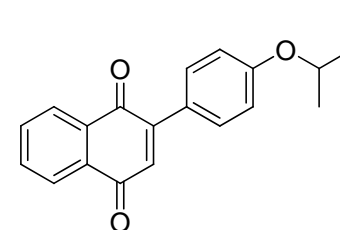


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 Sample\_id = S#423651  
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 Revision time = 2-JUL-2011 23:03:48  
 Current time = 2-JUL-2011 23:04:26

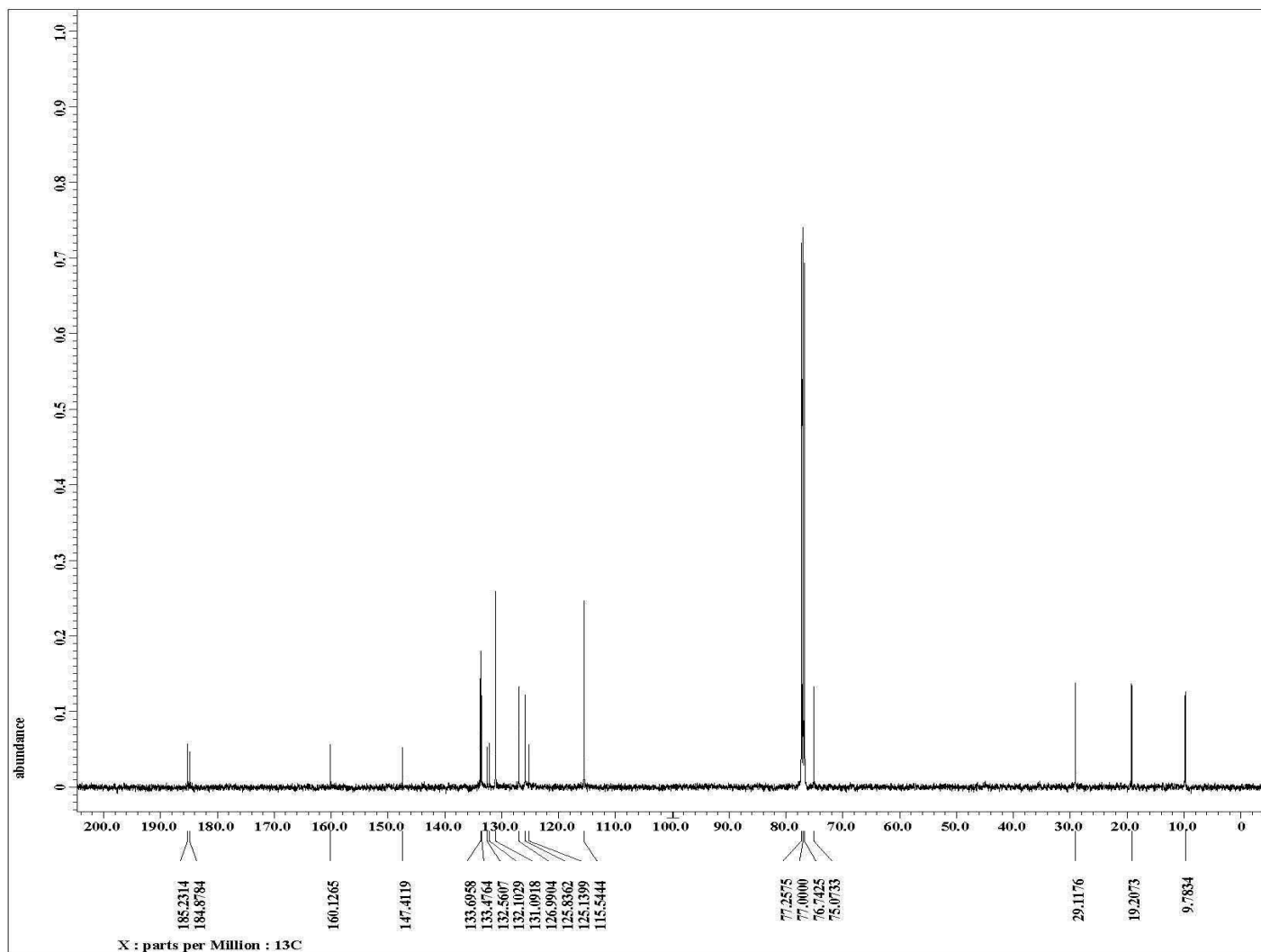
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 Dim\_title = 1H  
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 Site = ECX 500  
 Spectrometer = DELTA2 NMR

Field strength = 11.7473579 [T] (500 [MH  
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 X\_freq = 500.15991521 [MHz]  
 X\_offset = 5.0 [ppm]  
 X\_points = 32768  
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 X\_sweep = 9.38438438 [kHz]  
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 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 = 44  
 Relaxation\_delay = 2 [s]  
 Repetition\_time = 5.49175808 [s]  
 Temp\_get = 19.2 [dC]



$^1\text{H}$  NMR spectrum of 2-(4-sec-butoxyphenyl)-1,4-naphthoquinone (2.7)



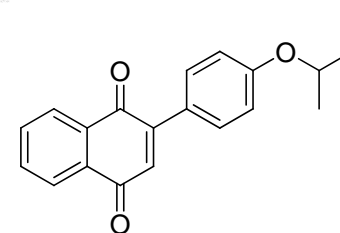
```

Filename      = SNG8SA7 CARBON-3.jdf
Author       = N.Ahmed
Experiment   = single_pulse_dec
Sample_id    = S#776239
Solvent      = CHLOROFORM-D
Creation time = 17-MAR-2011 21:17:24
Revision time = 17-MAR-2011 22:16:26
Current Time  = 2-JUL-2011 23:05:58

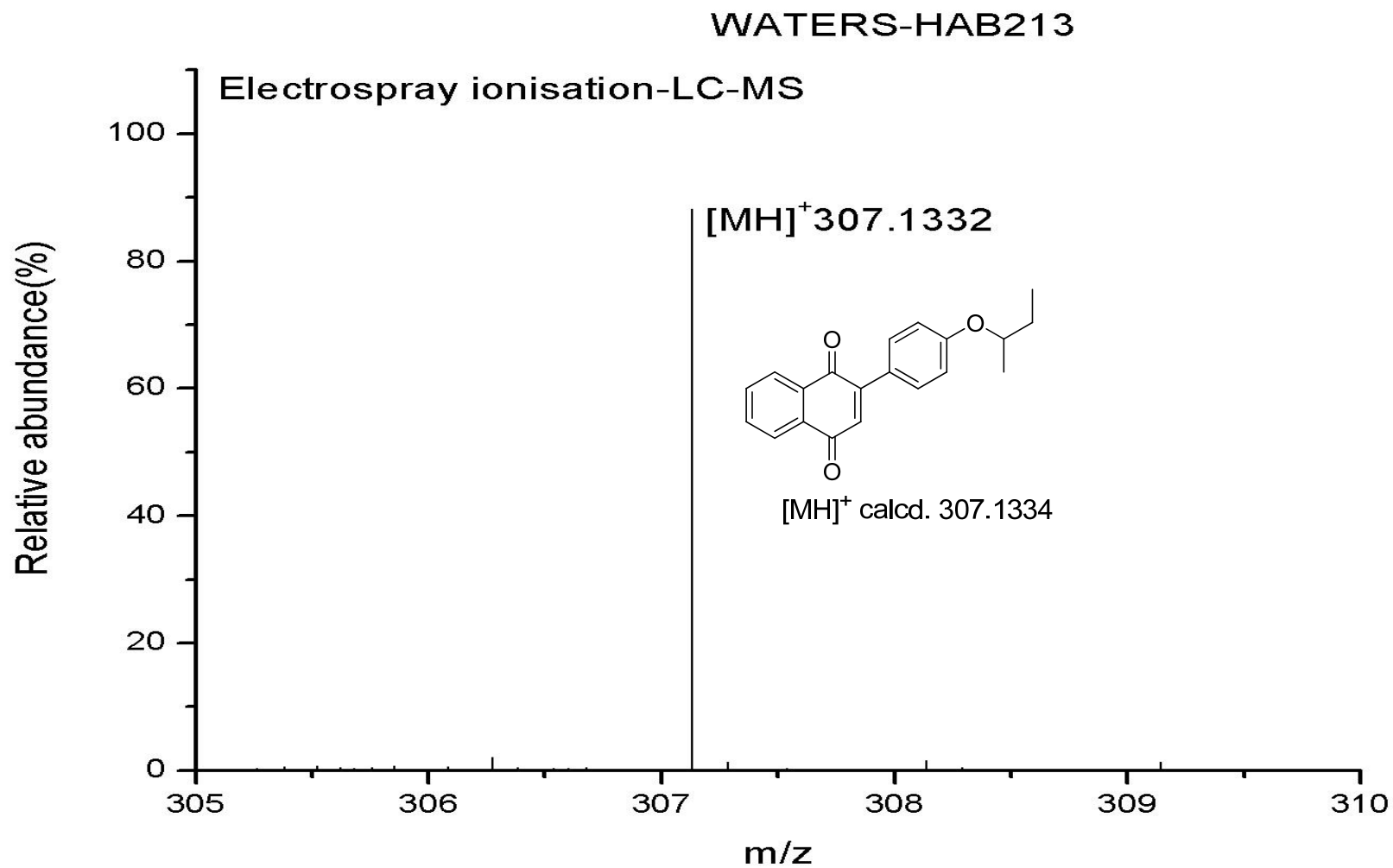
Data format   = 1D COMPLEX
Dim size      = 26214
Dim title     = 13C
Dim units     = [ppm]
Dimensions    = X
Site          = ECX 500
Spectrometer  = DELTA2 NMR

Field strength = 11.7473579 [T] (500 [MH]
X_acq_duration = 0.83361792 [s]
X_domain       = 13C
X_freq         = 125.76529768 [MHz]
X_offset       = 100 [ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.19959034 [Hz]
X_sweep        = 39.3081761 [kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521 [MHz]
Irr_offset     = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 1024
Total_scans    = 1024

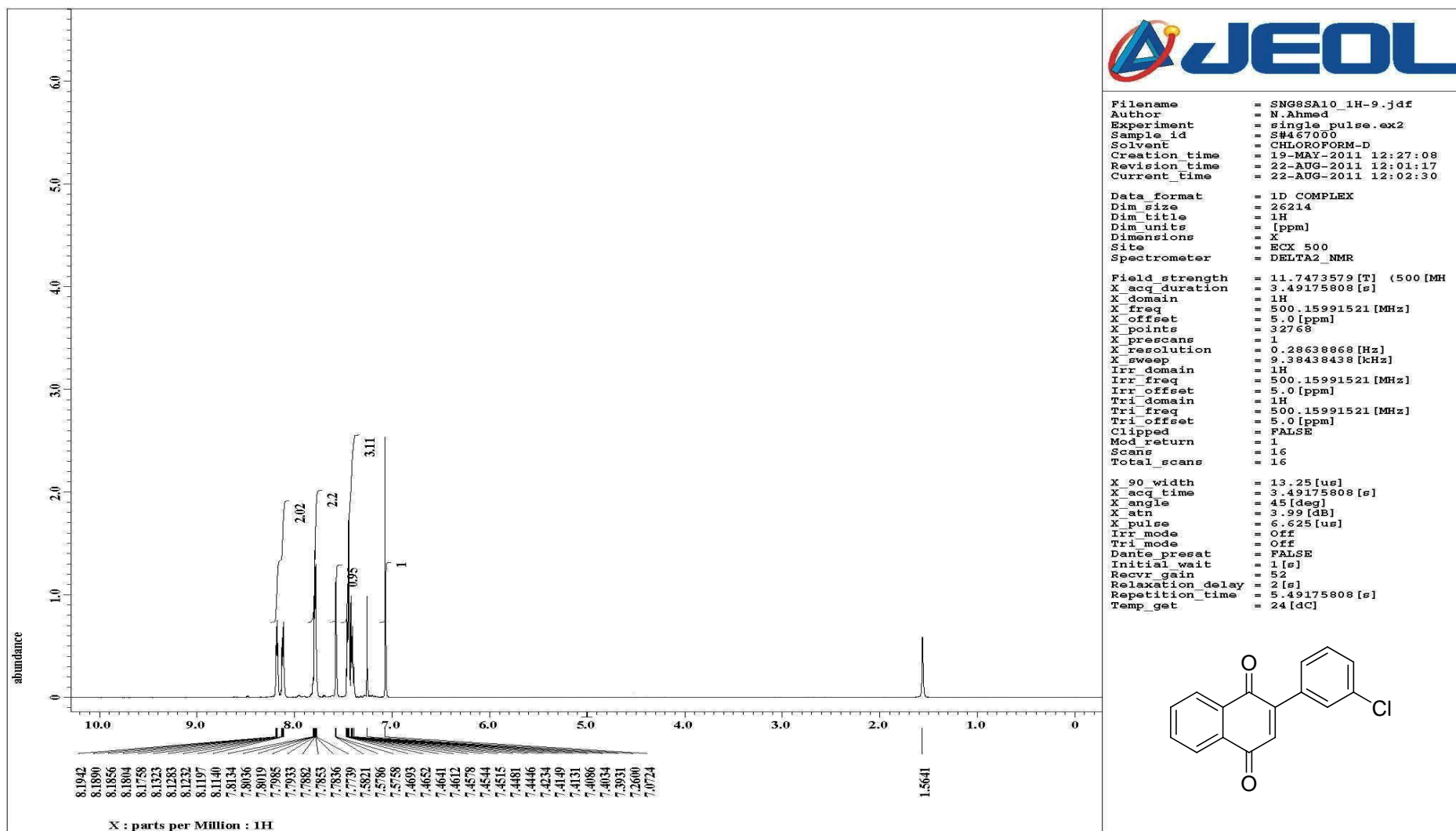
X_90_width     = 9.62 [us]
X_acq_time     = 0.83361792 [s]
X_angle        = 30 [deg]
X_atn          = 7.1 [dB]
X_pulse        = 3.20666667 [us]
Irr_atn_dec    = 21.5 [dB]
Irr_atn_noe    = 21.5 [dB]
Irr_noise      = WALTZ
Decoupling     = TRUE
Initial_wait   = 1 [s]
Noe            = TRUE
Noe_time       = 1 [s]
Recvr_gain     = 60
Relaxation_delay = 1 [s]
Repetition_time = 1.83361792 [s]
Temp_get       = 18 [dC]
    
```



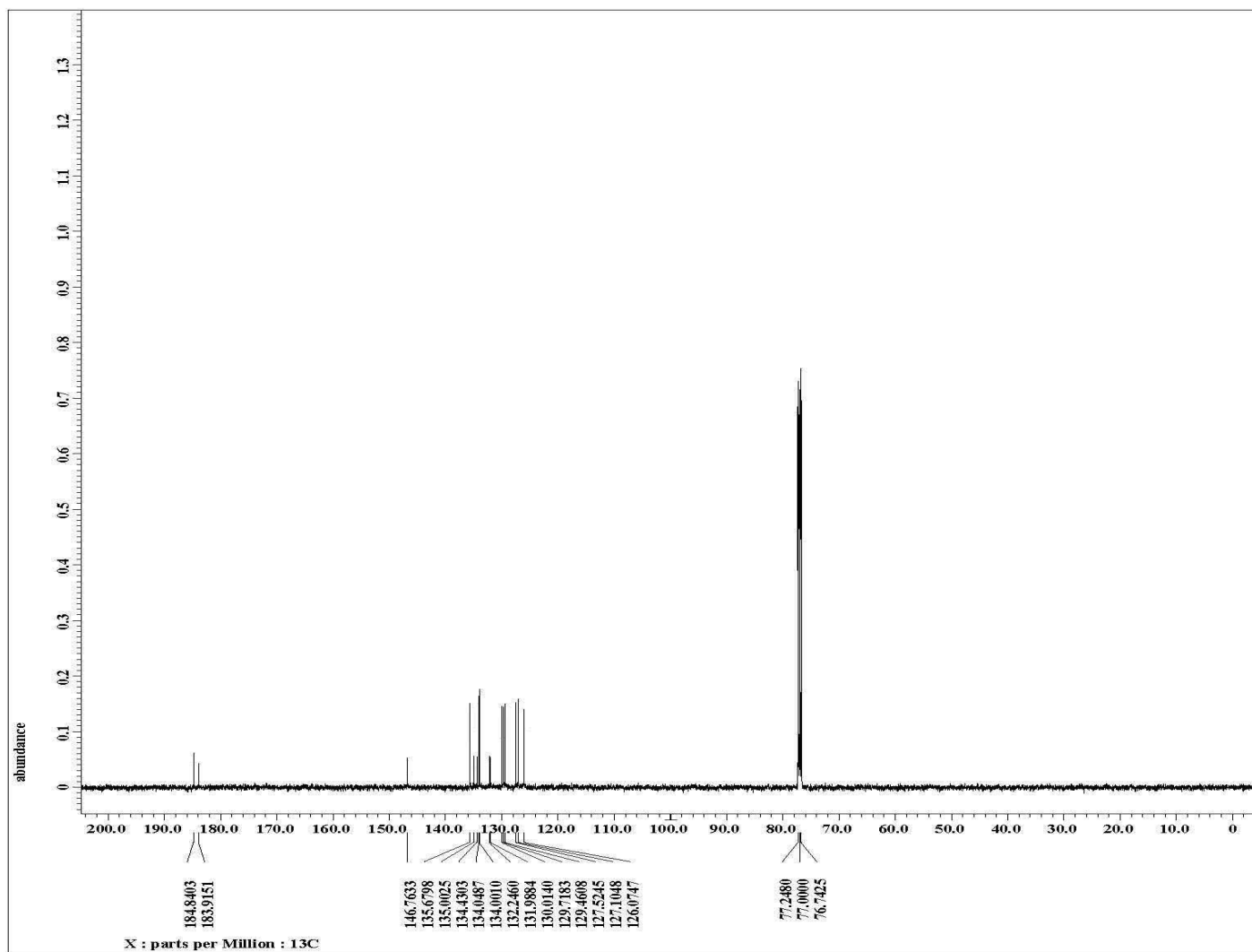
<sup>13</sup>C spectrum of 2-(4-sec-butoxyphenyl)-1,4-naphthoquinone (2.7)



HRMS spectrum of 2-(4-sec-butoxyphenyl)-1,4-naphthoquinone (**2.7**)



<sup>1</sup>H NMR spectrum of 2-(3-chlorophenyl)-1,4-naphthoquinone (2.8)



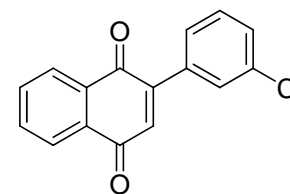
```

Filename      = SNG8SA10_13C-4.jdf
Author       = N.Ahmed
Experiment   = single_pulse_dec
Sample id    = S4591911
Solvent      = CHLOROFORM-D
Creation time = 19-MAY-2011 17:49:52
Revision time = 22-AUG-2011 12:09:25
Current time  = 22-AUG-2011 12:10:37

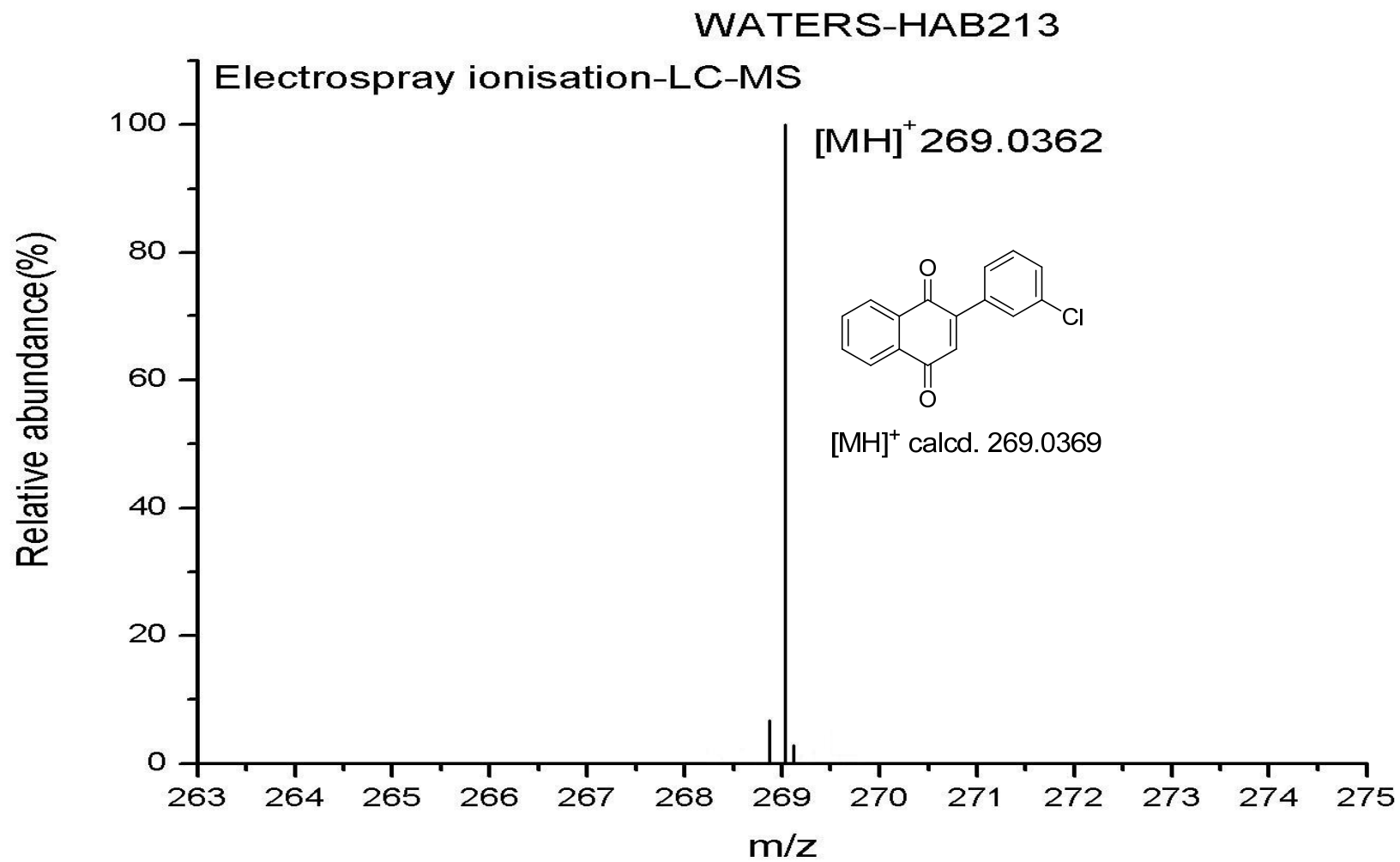
Data format   = 1D COMPLEX
Dim size      = 26214
Dim title     = 13C
Dim units     = [ppm]
Dimensions    = X
Site          = ECU 500
Spectrometer  = DELTA2_NMR

Field strength = 11.7473579 [T] (500 [MH
X_acq_duration = 0.83361792 [s]
X_domain       = 13C
X_freq         = 125.76529768 [MHz]
X_offset       = 100 [ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.19959034 [Hz]
X_sweep        = 39.3081761 [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     = 0.83361792 [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 = 1.83361792 [s]
Temp_get       = 24 [dC]
    
```

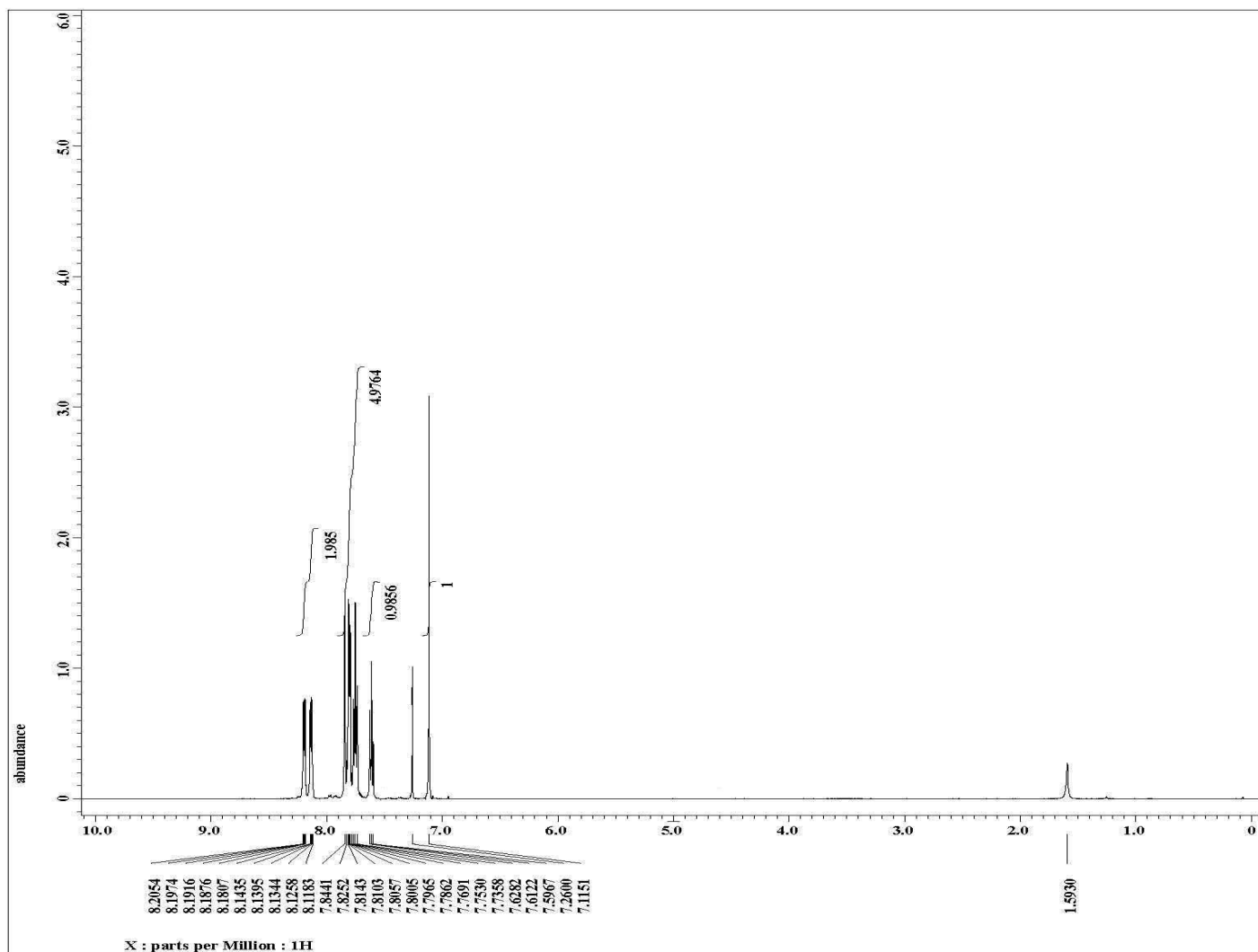


$^{13}\text{C}$  NMR spectrum of 2-(3-chlorophenyl)-1,4-naphthoquinone (**2.8**)



HRMS spectrum of 2-(3-chlorophenyl)-1,4-naphthoquinone (**2.8**)





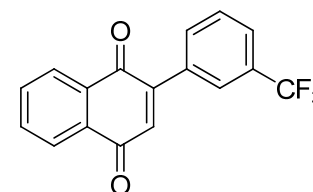
```

Filename      = SNG8SA13_1H-5.jdf
Author       = N.Ahmed
Experiment   = single_pulse.ex2
Sample id    = S4390194
Solvent      = CHLOROFORM-D
Creation time = 18-MAY-2011 10:02:48
Revision time = 20-AUG-2011 19:20:09
Current time  = 20-AUG-2011 19:21:22

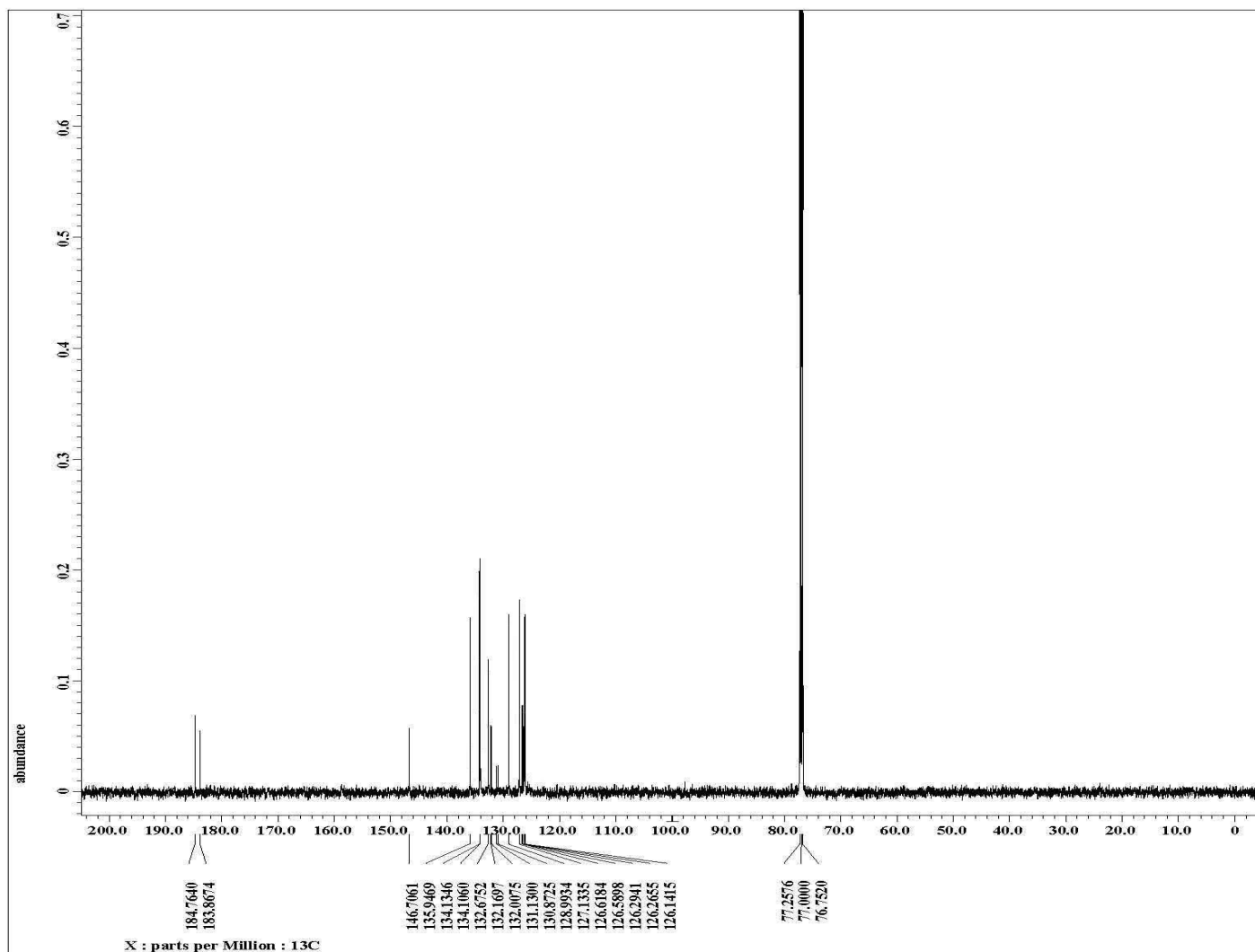
Data format   = 1D COMPLEX
Dim size      = 26214
Dim title     = 1H
Dim units     = [ppm]
Dimensions    = X
Site          = ECX 500
Spectrometer  = DELTA2_NMR

Field strength = 11.7473579 [T] (500 [MH
X_acq_duration = 3.49175808 [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      = 50
Relaxation_delay = 2 [s]
Repetition_time = 5.49175808 [s]
Temp_get        = 23 [dC]
    
```



$^1\text{H}$  NMR spectrum of 2-(3-(trifluoromethyl)phenyl)-1,4-naphthoquinone (2.9)



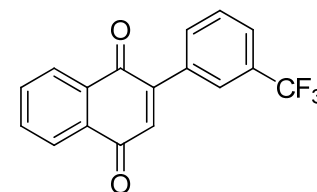
```

Filename      = SNG8SA13_13C-3.jdf
Author       = N. Ahmed
Experiment   = single_pulse_dec
Sample_id    = S#587762
Solvent      = CHLOROFORM-D
Creation_time = 18-MAY-2011 21:48:58
Revision_time = 26-SEP-2011 16:40:55
Current_time  = 26-SEP-2011 16:43:45

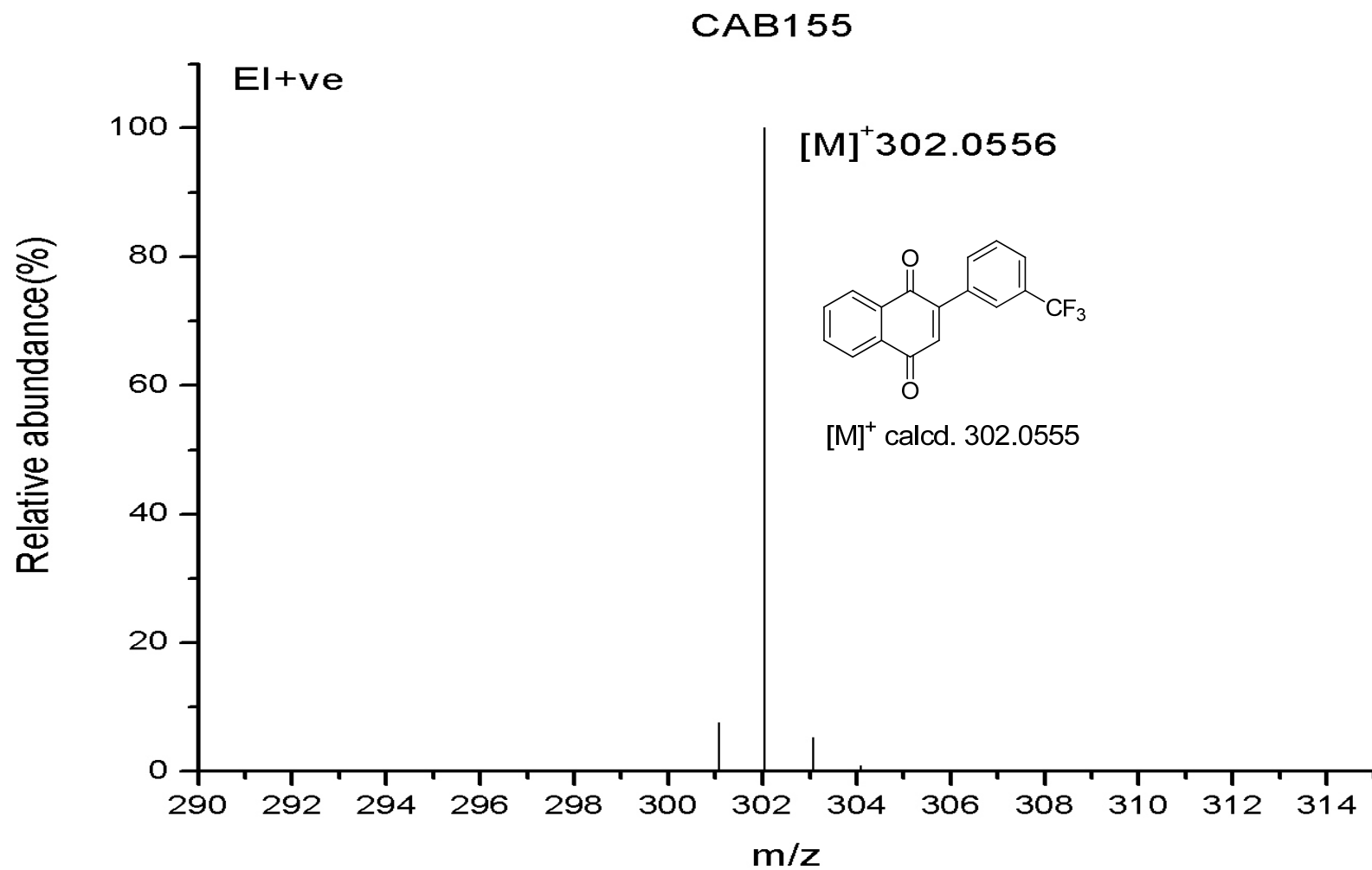
Data_format   = 1D COMPLEX
Dim_size      = 26214
Dim_title     = 13C
Dim_units     = [ppm]
Dimensions    = X
Site          = ECX 500
Spectrometer  = DELTA2_NMR

Field_strength = 11.7473579 [T] (500 [MH]
X_acq_duration = 0.83361792 [s]
X_domain      = 13C
X_freq        = 125.76529768 [MHz]
X_offset      = 100 [ppm]
X_points      = 32768
X_prescans     = 4
X_resolution   = 1.19959034 [Hz]
X_sweep       = 39.3081761 [kHz]
Irr_domain    = 1H
Irr_freq      = 500.15991521 [MHz]
Irr_offset    = 5.0 [ppm]
Clipped       = FALSE
Mod_return    = 1
Scans         = 1000
Total_scans   = 1000

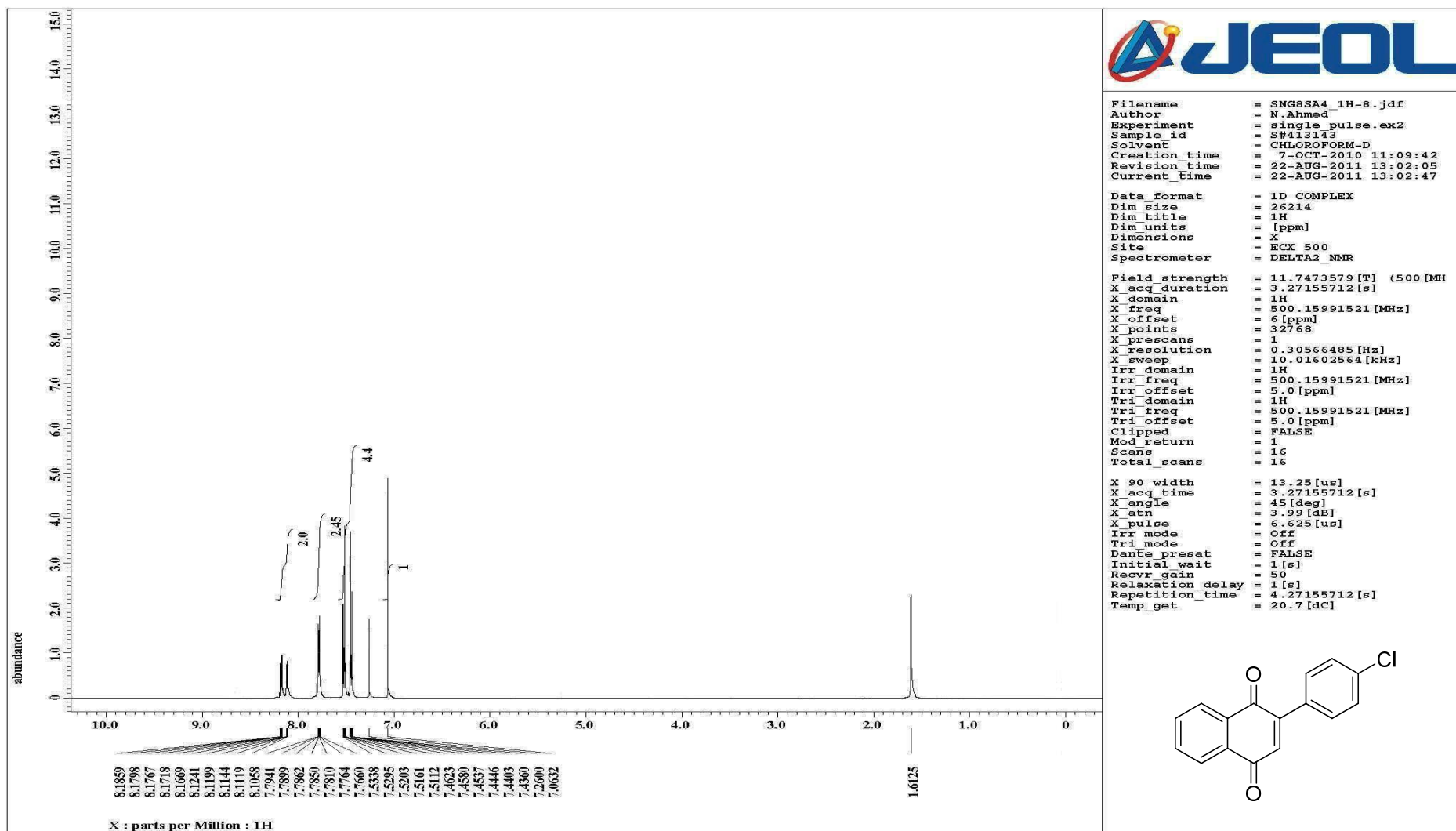
X_90_width    = 9.62 [us]
X_acq_time    = 0.83361792 [s]
X_angle       = 30 [deg]
X_atn         = 7.1 [dB]
X_pulse       = 3.20666667 [us]
Irr_atn_dec   = 19.5 [dB]
Irr_atn_noe   = 21.5 [dB]
Irr_noise     = WALTZ
Decoupling    = TRUE
Initial_wait  = 1 [s]
Noe           = TRUE
Noe_time      = 1 [s]
Recvr_gain    = 60
Relaxation_delay = 1 [s]
Repetition_time = 1.83361792 [s]
Temp_get      = 23 [dC]
    
```



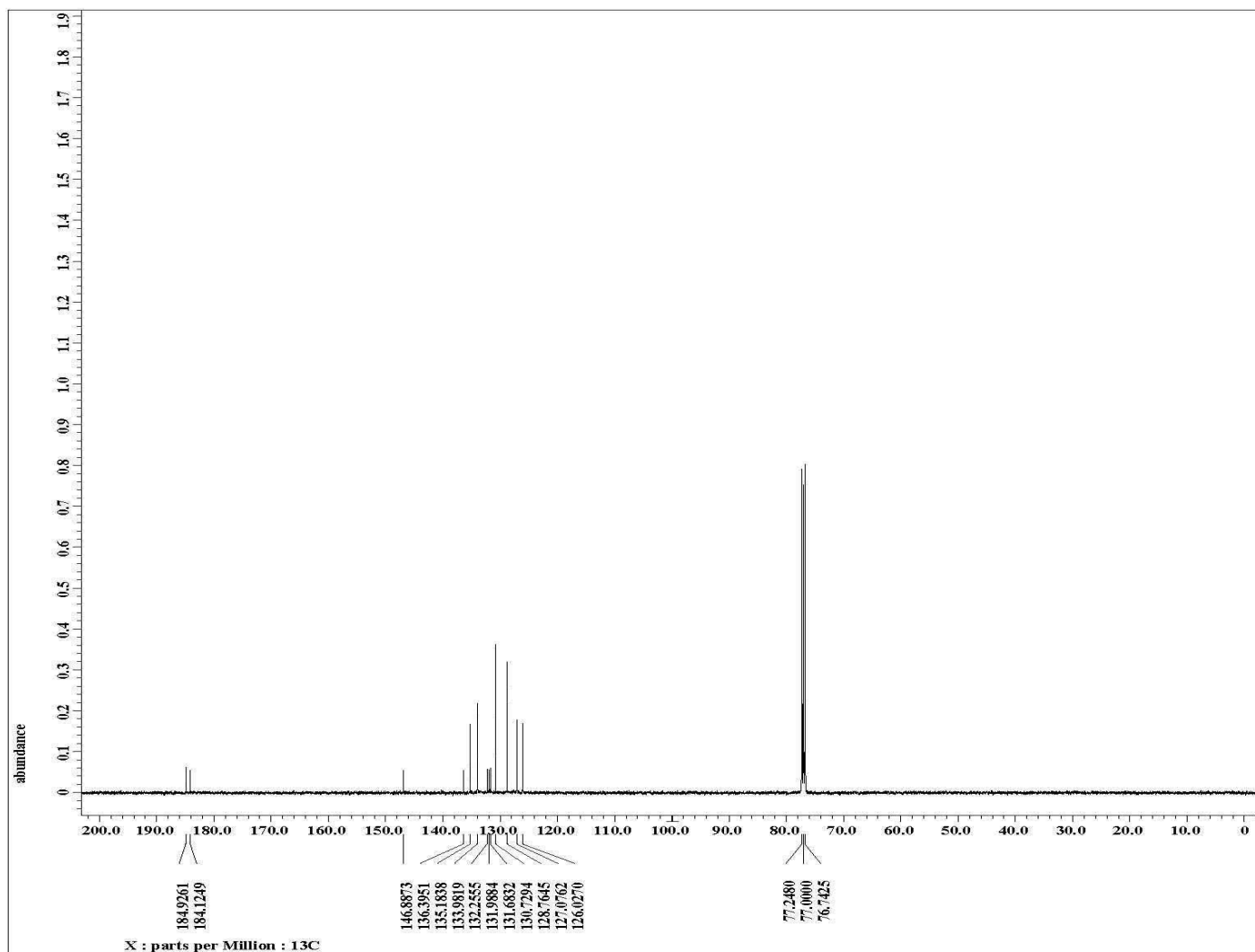
$^{13}\text{C}$  spectrum of 2-(3-(trifluoromethyl)phenyl)-1,4-naphthoquinone (**2.9**)



HRMS spectrum of 2-(3-(trifluoromethyl)phenyl)-1,4-naphthoquinone (**2.9**)



<sup>1</sup>H NMR spectrum of 2-(4-chlorophenyl)-1,4-naphthoquinone (2.10)



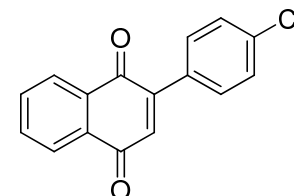
```

Filename      = SNG8SA4_13C-4.jdf
Author       = N.Ahmed
Experiment   = single_pulse_dec
Sample id    = S4563721
Solvent      = CHLOROFORM-D
Creation time = 7-OCT-2010 18:31:21
Revision time = 22-AUG-2011 15:08:34
Current time  = 22-AUG-2011 15:09:18

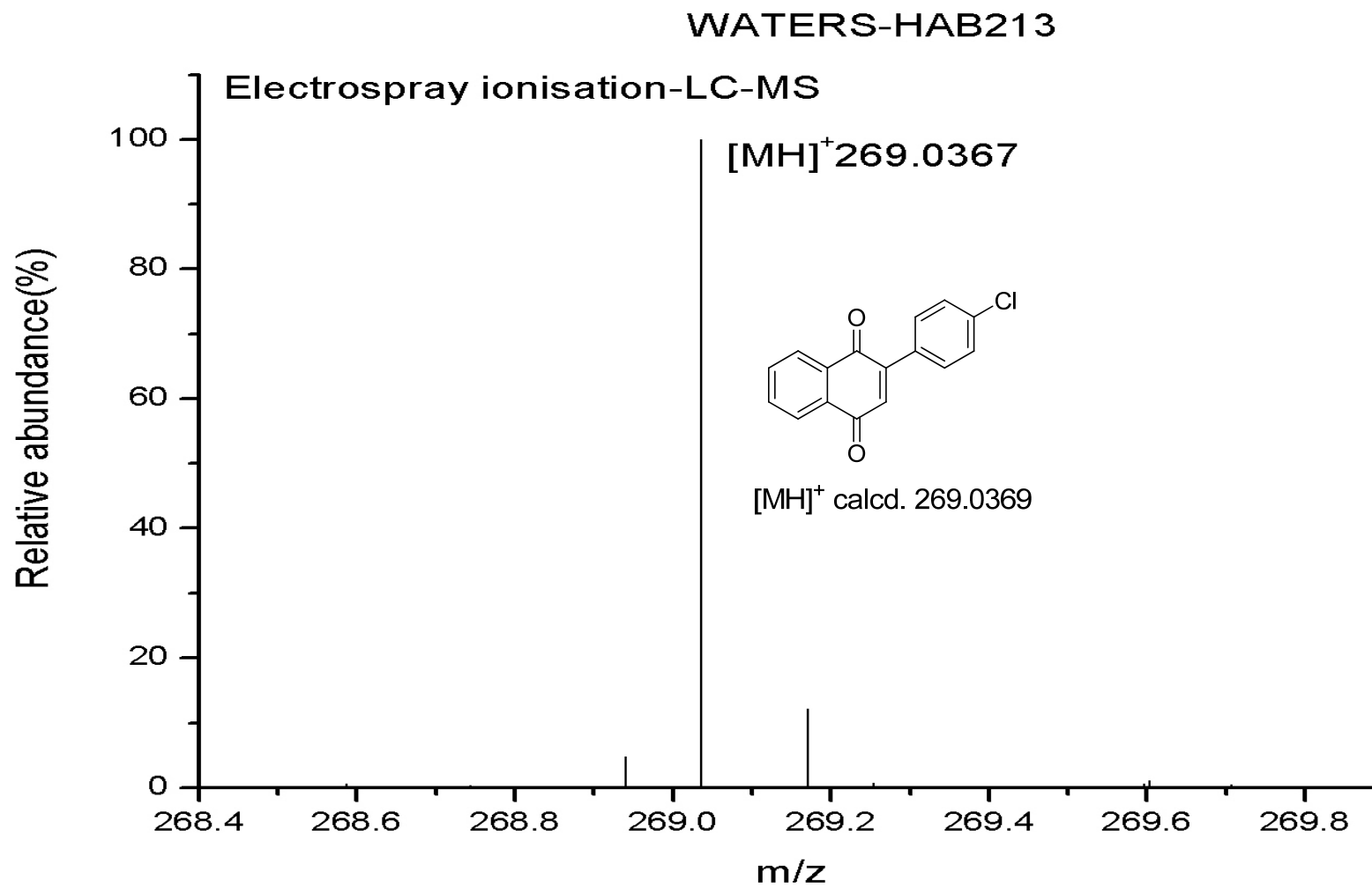
Data format   = 1D COMPLEX
Dim size      = 26214
Dim title     = 13C
Dim units     = [ppm]
Dimensions    = X
Site          = ECX 500
Spectrometer  = DELTA2_NMR

Field strength = 11.7473579 [T] (500 [MH
X_acq_duration = 0.83361792 [s]
X_domain       = 13C
X_freq         = 125.76529768 [MHz]
X_offset       = 100 [ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.19959034 [Hz]
X_sweep        = 39.3081761 [kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521 [MHz]
Irr_offset     = 5.0 [ppm]
Clipped        = FALSE
Mod return     = 1
Scans          = 2000
Total_scans    = 2000

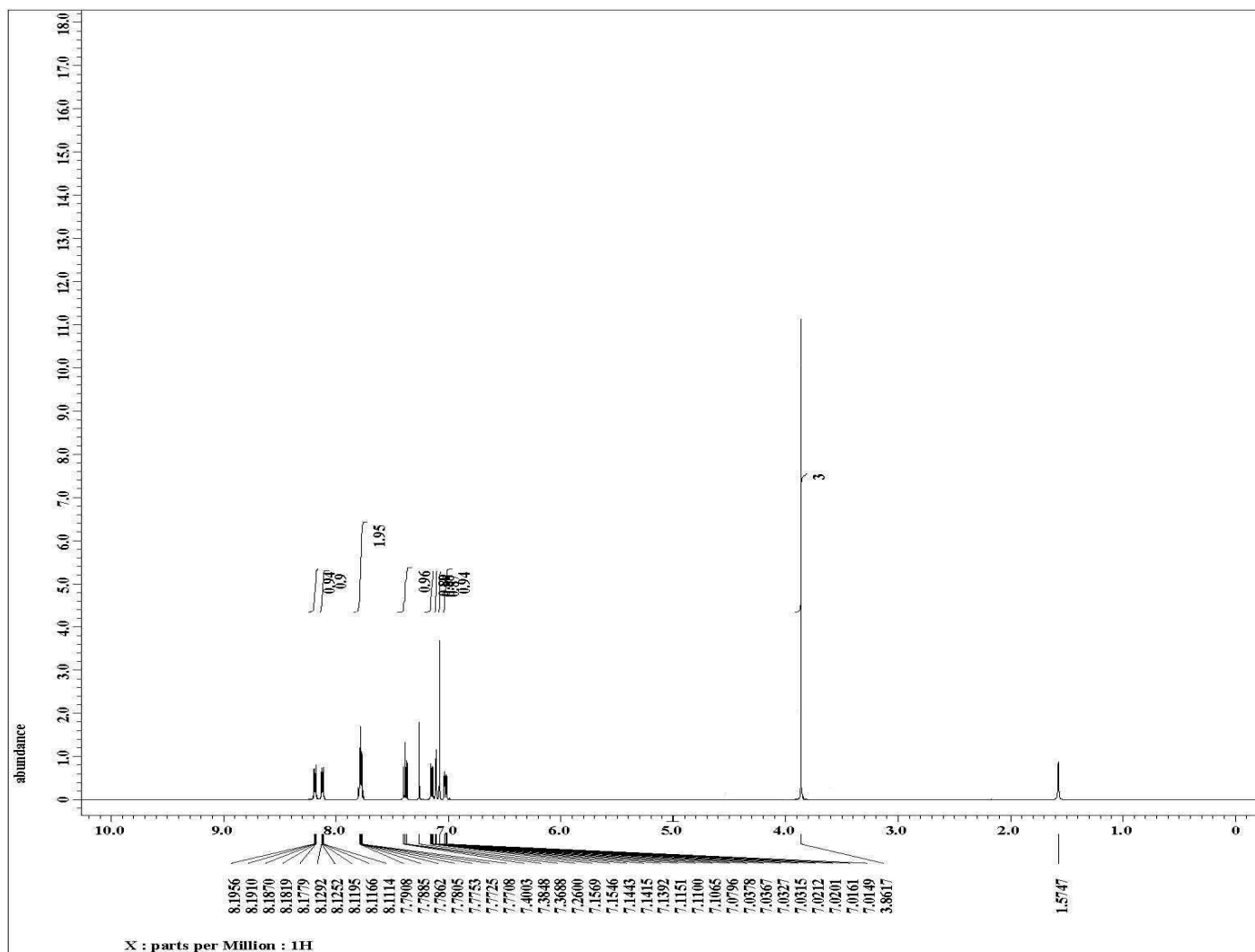
X_90_width     = 9.62 [us]
X_acq_time     = 0.83361792 [s]
X_angle        = 30 [deg]
X_atn          = 7.1 [dB]
X_pulse        = 3.20666667 [us]
Irr_atn_dec    = 19.5 [dB]
Irr_atn_noe    = 21.5 [dB]
Irr_noise      = WALTZ
Decoupling     = TRUE
Initial wait   = 1 [s]
Noe            = TRUE
Noe_time       = 1 [s]
Recvr_gain     = 60
Relaxation_delay = 1 [s]
Repetition_time = 1.83361792 [s]
Temp_get       = 19 [dC]
    
```



$^{13}\text{C}$  spectrum of 2-(4-chlorophenyl)-1,4-naphthoquinone (2.10)



HRMS spectrum of 2-(4-chlorophenyl)-1,4-naphthoquinone (**2.10**)



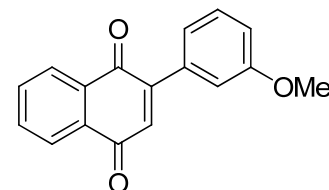
```

Filename      = SNG8SA26_1H-6.jdf
Author       = N. Ahmed
Experiment   = single_pulse.ex2
Sample id    = SM400462
Solvent      = CHLOROFORM-D
Creation time = 20-MAY-2011 11:04:11
Revision time = 22-AUG-2011 12:38:32
Current time  = 22-AUG-2011 12:39:36

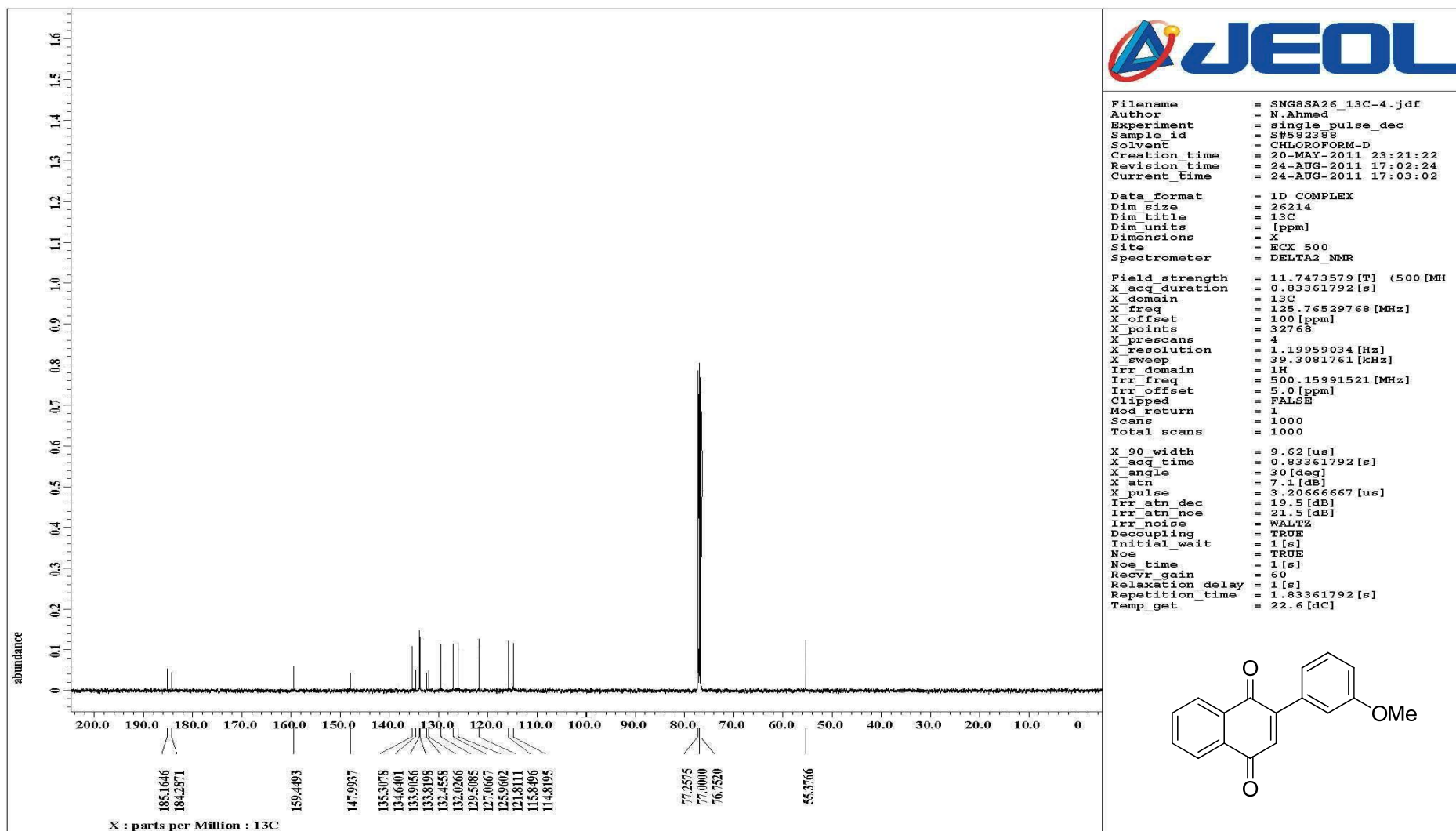
Data format   = 1D COMPLEX
Dim size      = 26214
Dim title     = 1H
Dim units     = [ppm]
Dimensions    = X
Site          = ECX 500
Spectrometer  = DELTA2_NMR

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     = 50
Relaxation_delay = 2 [s]
Repetition_time = 5.49175808 [s]
Temp_get       = 23.1 [dC]
    
```

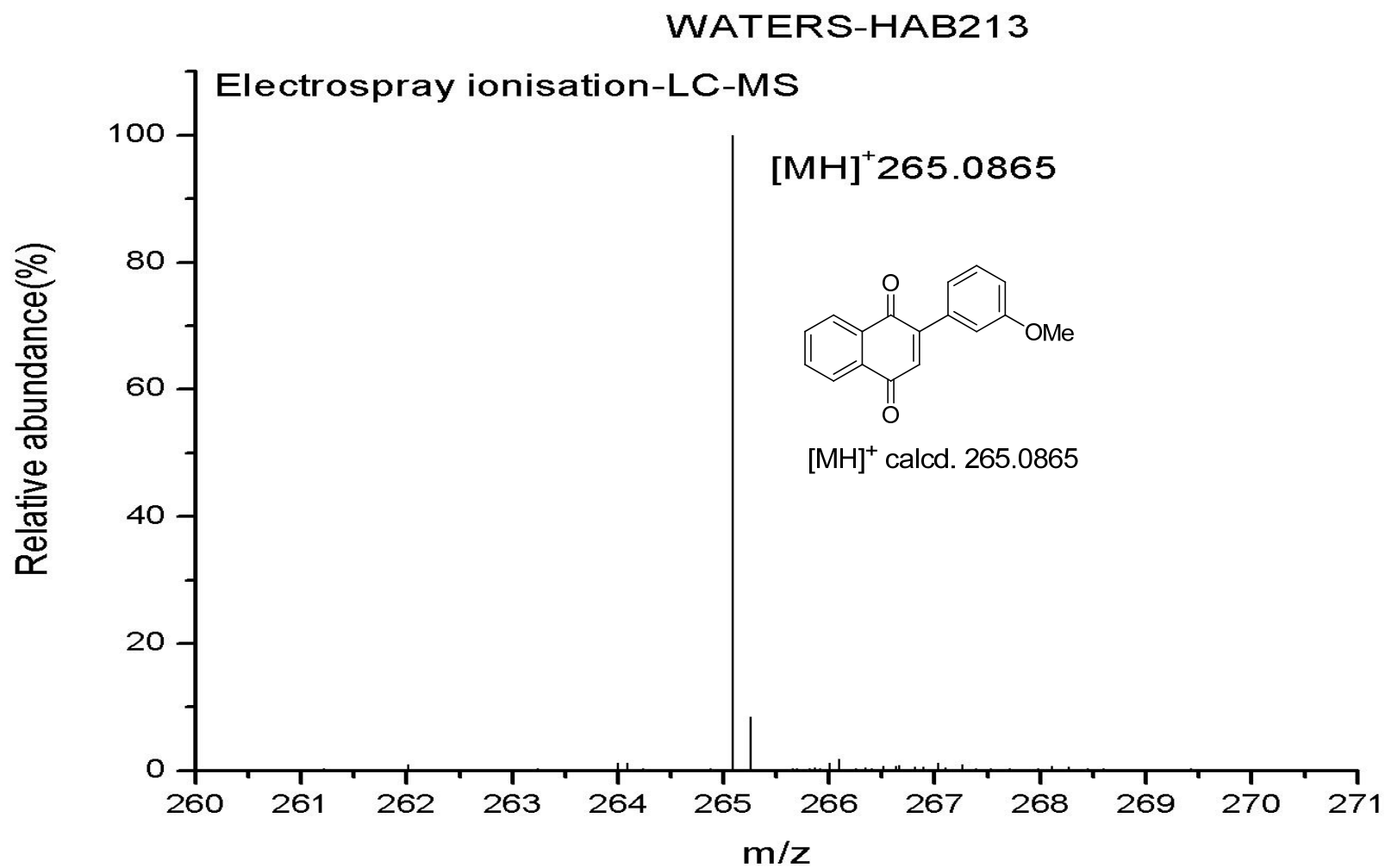


$^1\text{H}$  NMR spectrum of 2-(3-methoxyphenyl)-1,4-naphthoquinone (2.11)

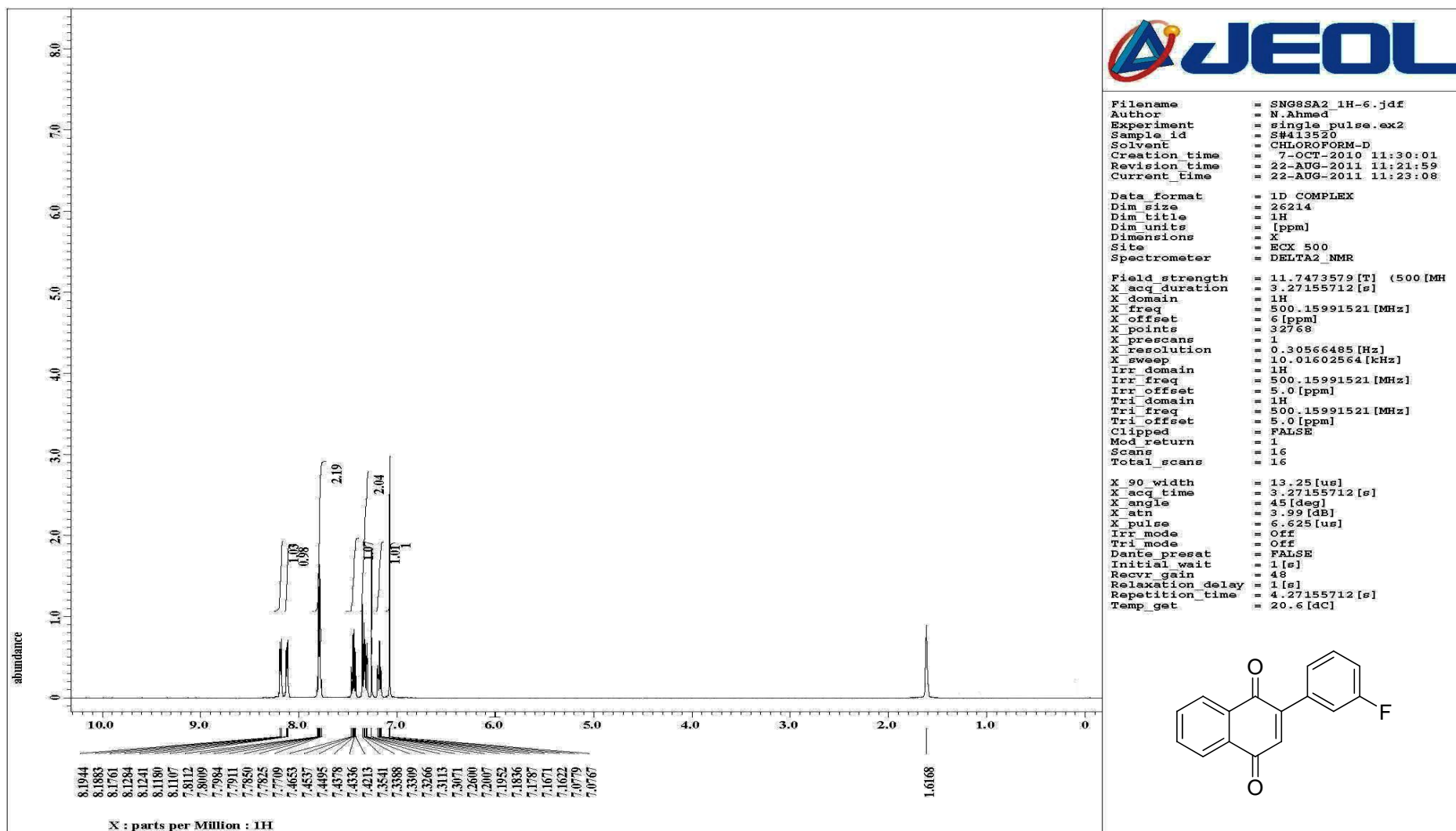


$^{13}\text{C}$  spectrum of 2-(3-methoxyphenyl)-1,4-naphthoquinone (2.11)

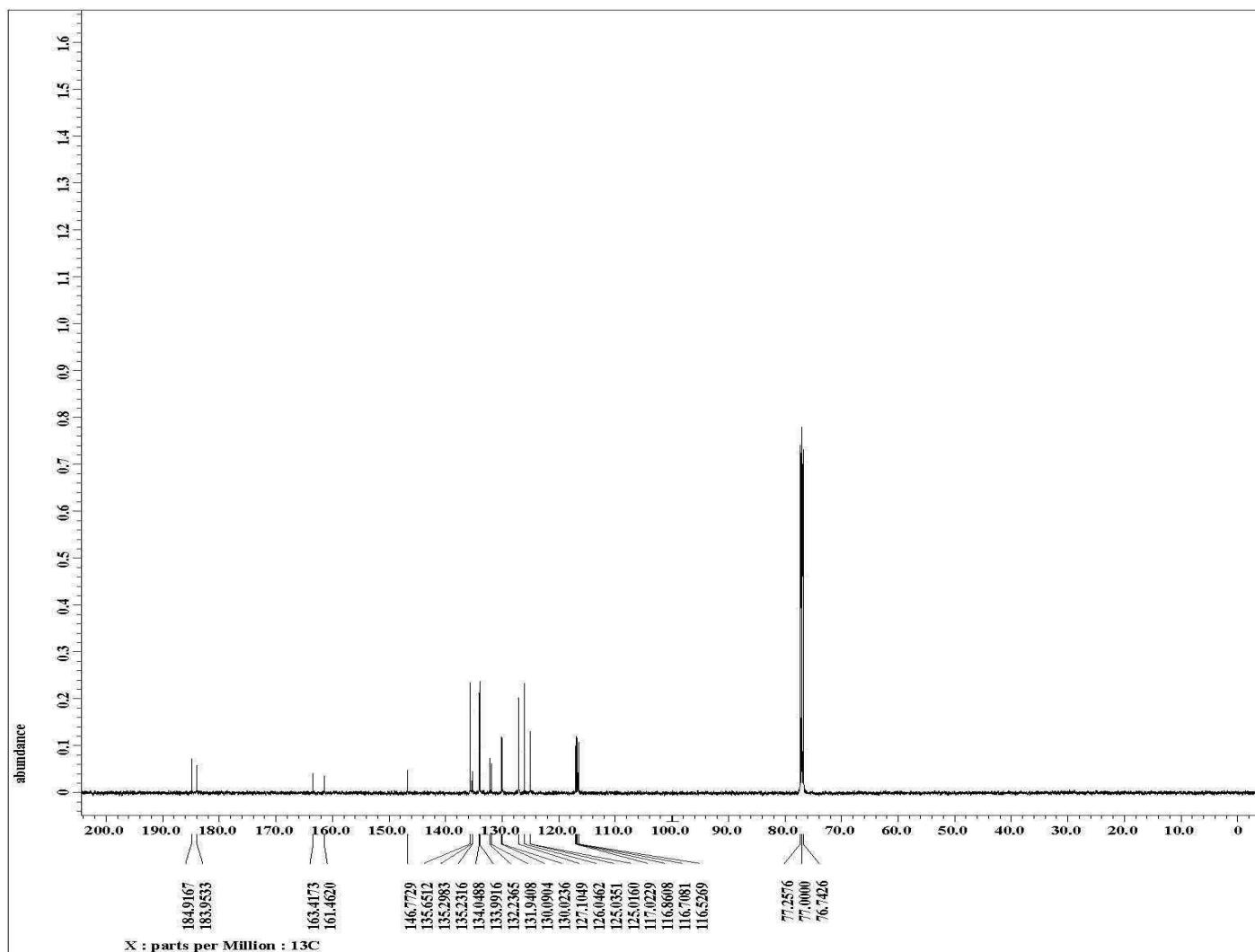




HRMS spectrum of 2-(3-methoxyphenyl)-1,4-naphthoquinone (**2.11**)



$^1\text{H}$  NMR spectrum of 2-(3-fluorophenyl)-1,4-naphthoquinone (2.12)



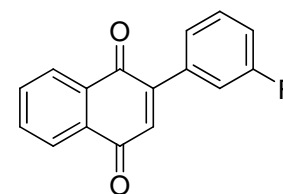
```

Filename      = SNG8SA2_13C-17.jdf
Author       = N.Ahmed
Experiment   = single_pulse_dec
Sample id    = S4564015
Solvent      = CHLOROFORM-D
Creation time = 7-OCT-2010 21:51:47
Revision time = 22-AUG-2011 11:39:21
Current time  = 22-AUG-2011 11:44:18

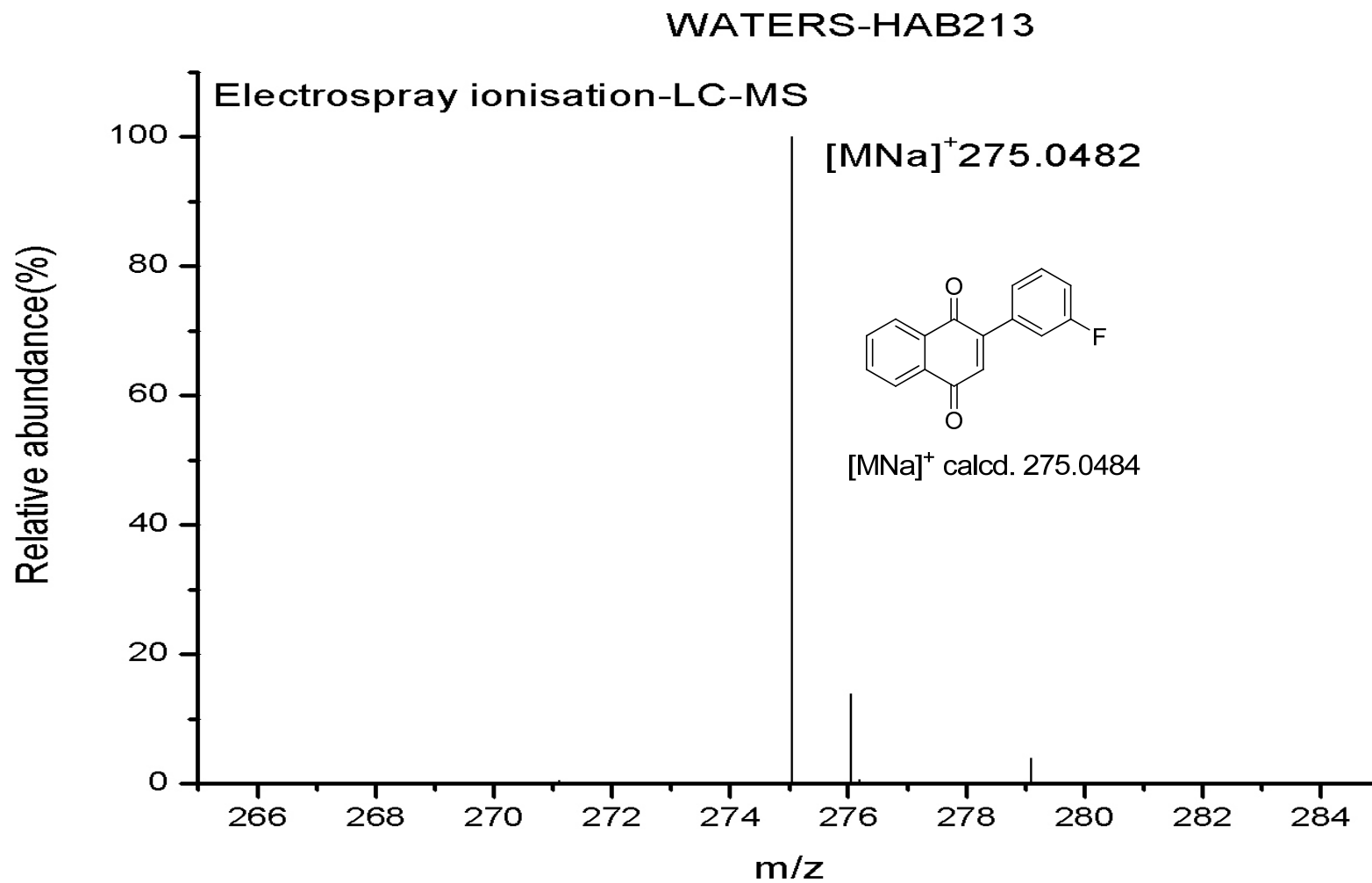
Data format   = 1D COMPLEX
Dim size      = 26214
Dim title     = 13C
Dim units     = [ppm]
Dimensions    = X
Site          = ECX 500
Spectrometer  = DELTA2_NMR

Field strength = 11.7473579 [T] (500 [MH
X_acq_duration = 0.83361792 [s]
X_domain       = 13C
X_freq         = 125.76529768 [MHz]
X_offset       = 100 [ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.19959034 [Hz]
X_sweep        = 39.3081761 [kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521 [MHz]
Irr_offset     = 5.0 [ppm]
Clipped        = FALSE
Mod return     = 1
Scans          = 2000
Total_scans    = 2000

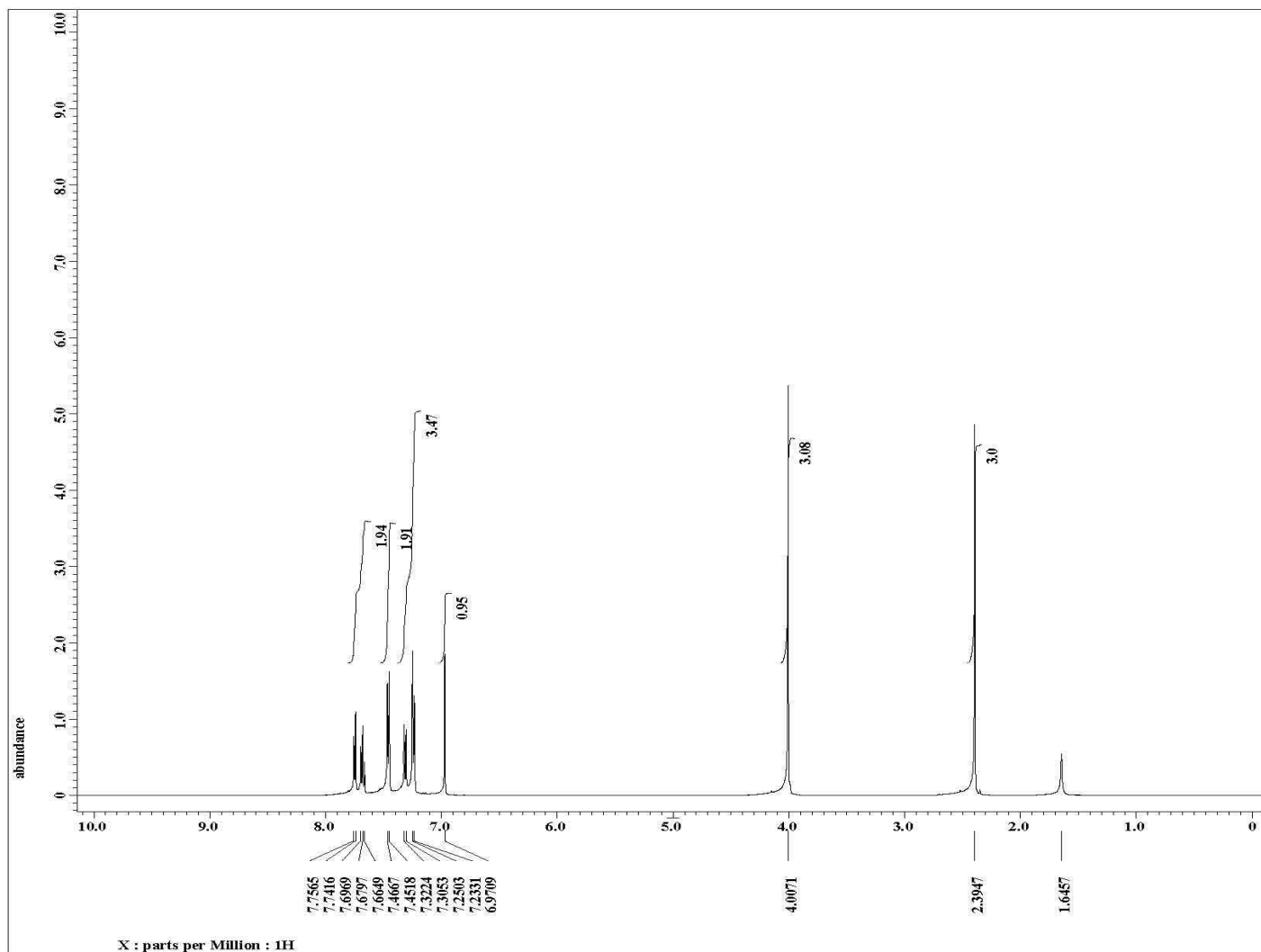
X_90_width     = 9.62 [us]
X_acq_time     = 0.83361792 [s]
X_angle        = 30 [deg]
X_atn          = 7.1 [dB]
X_pulse        = 3.20666667 [us]
Irr_atn_dec    = 19.5 [dB]
Irr_atn_noe    = 21.5 [dB]
Irr_noise      = WALTZ
Decoupling     = TRUE
Initial wait   = 1 [s]
Noe            = TRUE
Noe_time       = 1 [s]
Recvr_gain     = 60
Relaxation_delay = 1 [s]
Repetition_time = 1.83361792 [s]
Temp_get       = 18.2 [dC]
    
```



$^{13}\text{C}$  NMR spectrum of 2-(3-fluorophenyl)-1,4-naphthoquinone (**2.12**)



HRMS spectrum of 2-(3-fluorophenyl)-1,4-naphthoquinone (**2.12**)



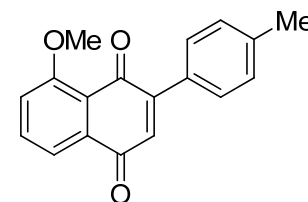
```

Filename      = SNG6211 1H-6.jdf
Author       = N.Ahmed
Experiment    = single_pulse.ex2
Sample_id    = S#456389
Solvent      = CHLOROFORM-D
Creation time = 1-APR-2010 12:18:43
Revision time = 2-JUL-2011 19:52:09
Current Time  = 2-JUL-2011 19:52:30

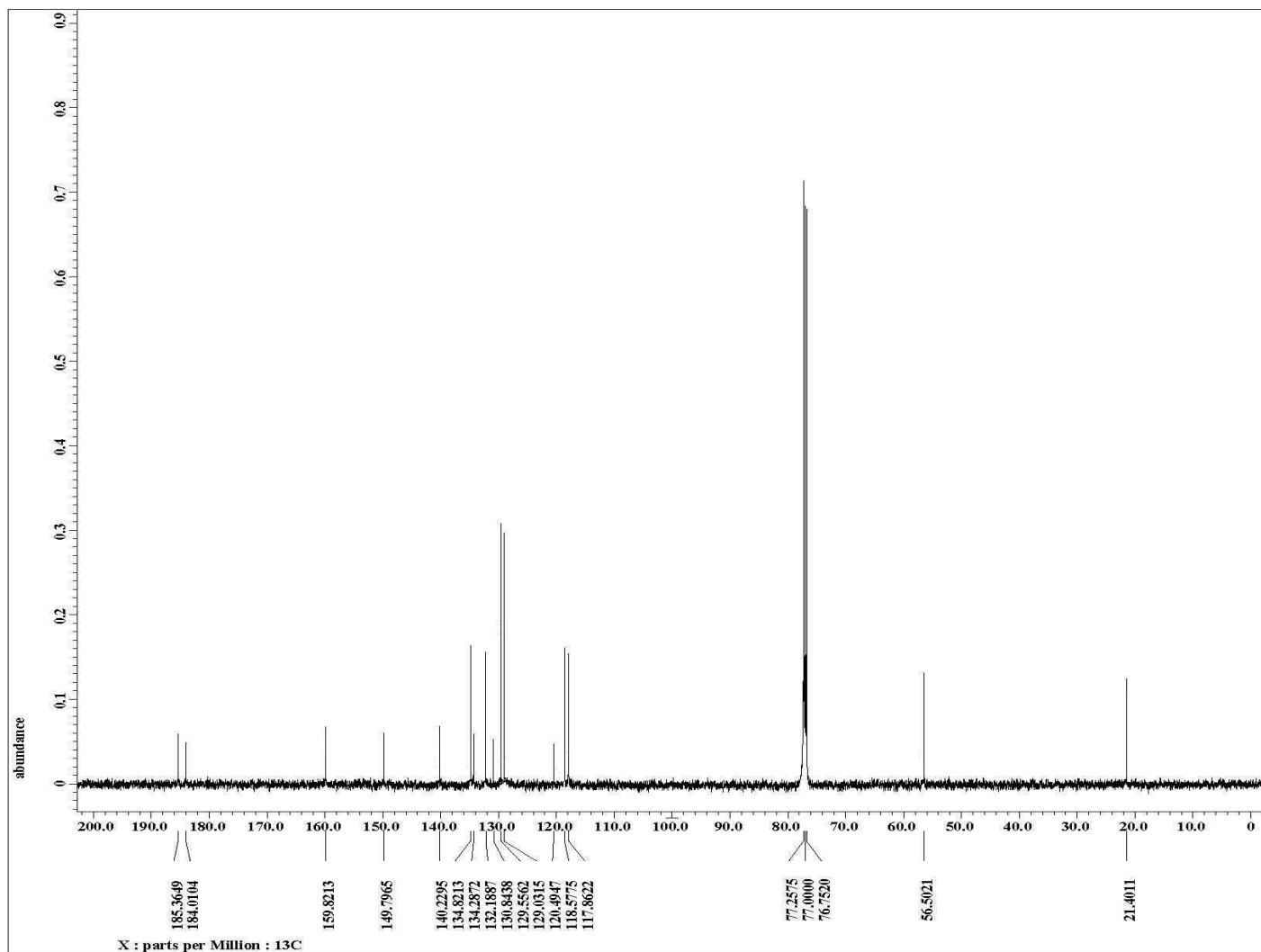
Data format   = 1D COMPLEX
Dim size      = 26214
Dim title     = 1H
Dim units     = [ppm]
Dimensions    = X
Site          = ECX 500
Spectrometer  = DELTA2 NMR

Field strength = 11.7473579 [T] (500 [MH
X_acq_duration = 1.74587904 [s]
X_domain       = 1H
X_freq         = 500.15991521 [MHz]
X_offset       = 5.0 [ppm]
X_points       = 32768
X_prescans     = 1
X_resolution   = 0.57277737 [Hz]
X_sweep        = 18.76876877 [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     = 9.25 [us]
X_acq_time      = 1.74587904 [s]
X_angle         = 45 [deg]
X_atn          = 3.99 [dB]
X_pulse         = 4.625 [us]
Irr_mode        = Off
Tri_mode        = Off
Dante_presat    = FALSE
Initial_wait    = 1 [s]
Recvr_gain      = 48
Relaxation_delay = 2 [s]
Repetition_time = 3.74587904 [s]
Temp_get        = 22.1 [dC]
    
```



$^1\text{H}$  NMR spectrum of 8-methoxy-2-*p*-tolyl-1,4-naphthoquinone (**3.1**)



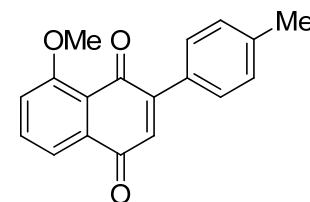
```

Filename      = SNG62111_13C-3.jdf
Author       = N.Ahmed
Experiment   = single_pulse_dec
Sample_id    = S#604448
Solvent      = CHLOROFORM-D
Creation time = 5-APR-2010 22:42:47
Revision time = 2-JUL-2011 19:54:57
Current time  = 2-JUL-2011 19:55:48

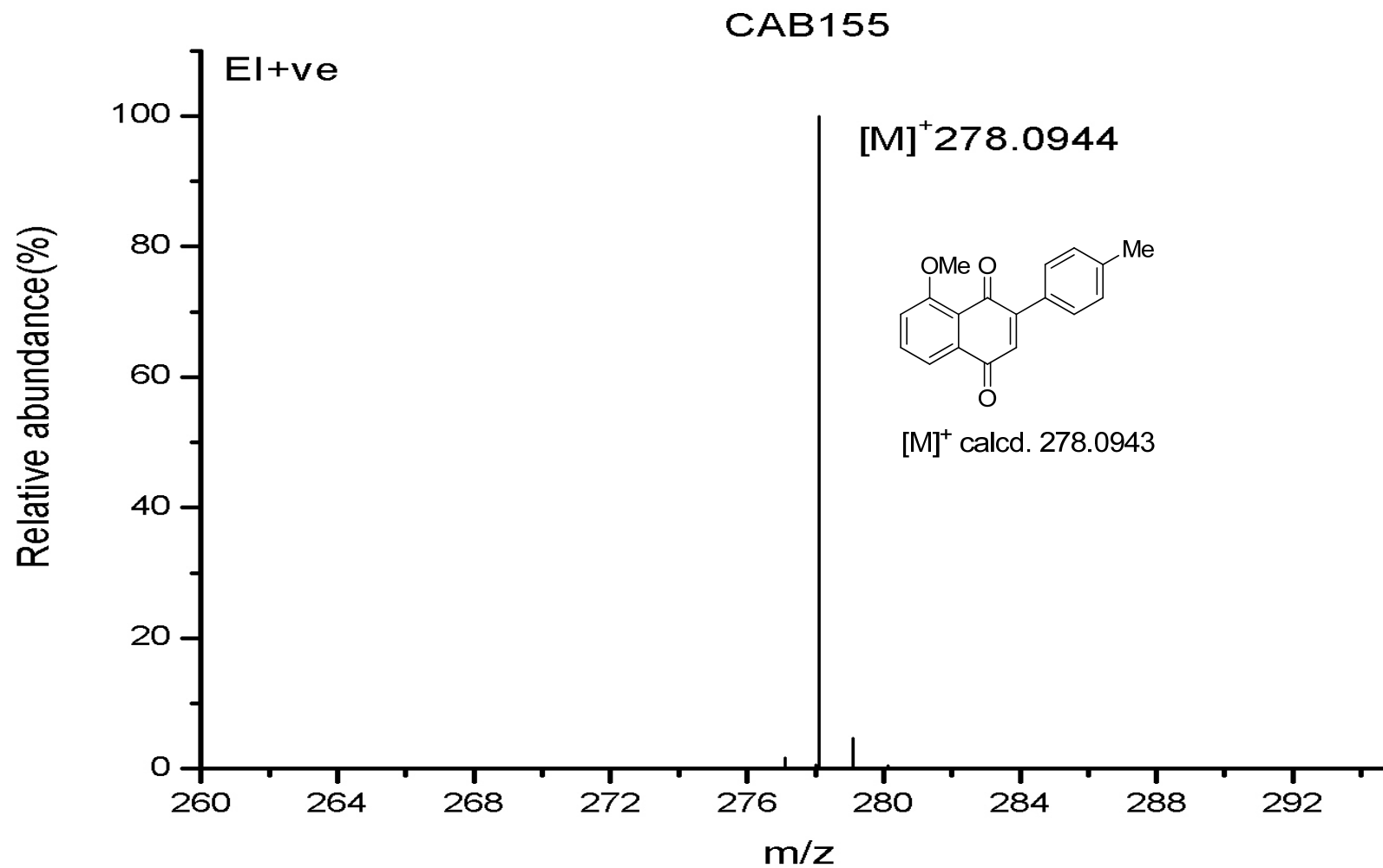
Data format   = 1D_COMPLEX
Dim_size      = 26214
Dim_title     = 13C
Dim_units     = [ppm]
Dimensions    = X
Site          = ECX 500
Spectrometer  = DELTA2 NMR

Field strength = 11.7473579 [T] (500 [MH]
X_acq_duration = 0.83361792 [s]
X_domain      = 13C
X_freq        = 125.76529768 [MHz]
X_offset      = 100 [ppm]
X_points      = 32768
X_prescans    = 4
X_resolution  = 1.19959034 [Hz]
X_sweep       = 39.3081761 [kHz]
Irr_domain    = 1H
Irr_freq      = 500.15991521 [MHz]
Irr_offset    = 5.0 [ppm]
Clipped       = FALSE
Mod_return    = 1
Scans         = 1000
Total_scans   = 1000

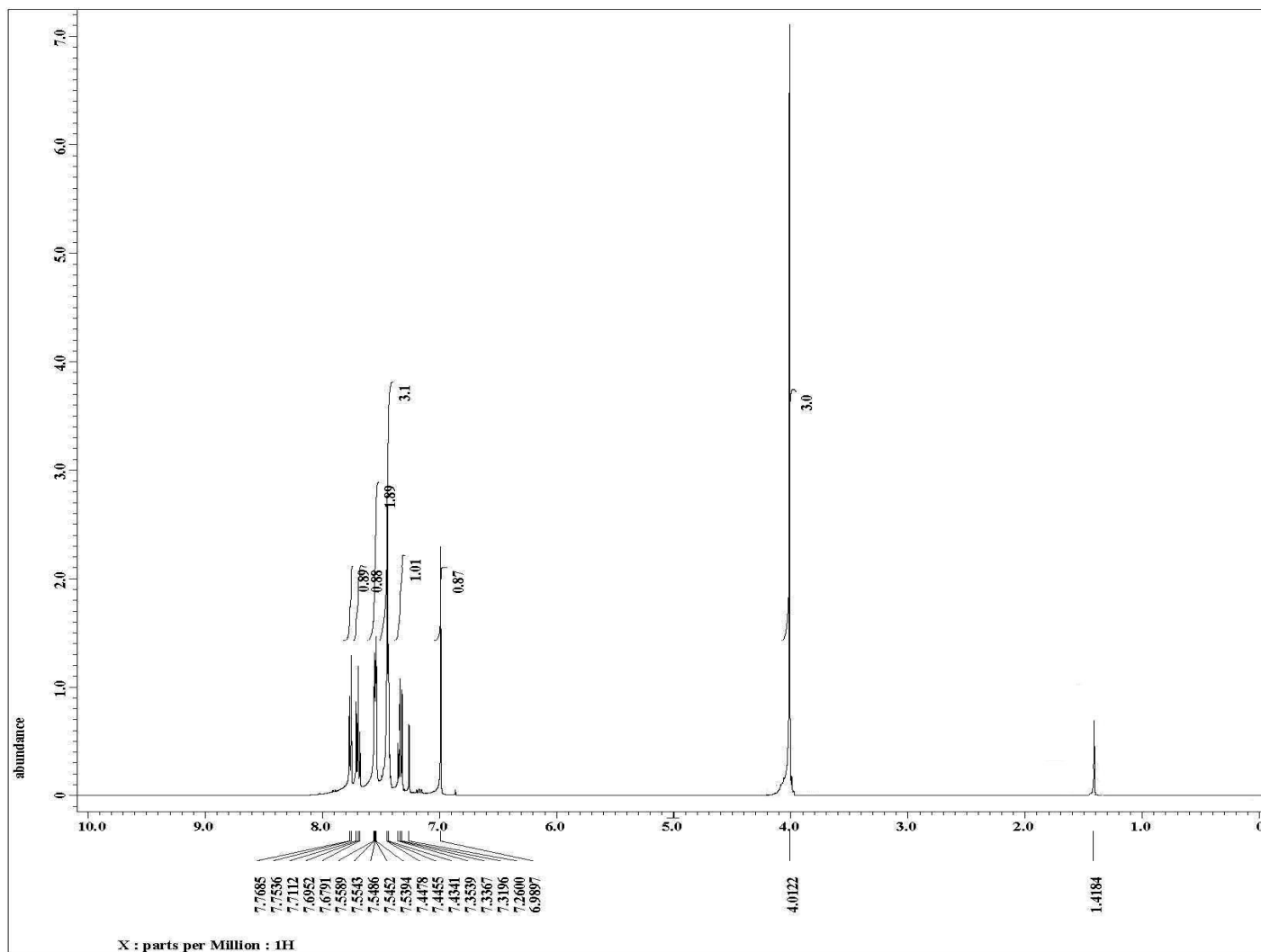
X_90_width    = 9.62 [us]
X_acq_time     = 0.83361792 [s]
X_angle       = 30 [deg]
X_atn         = 7.1 [dB]
X_pulse       = 3.20666667 [us]
Irr_atn_dec   = 19.5 [dB]
Irr_atn_noe   = 21.5 [dB]
Irr_noise     = WALTZ
Decoupling    = TRUE
Initial_wait  = 1 [s]
Noe           = TRUE
Noe_time      = 1 [s]
Recvr_gain    = 60
Relaxation_delay = 1 [s]
Repetition_time = 1.83361792 [s]
Temp_get      = 15.9 [dC]
    
```



$^{13}\text{C}$  NMR spectrum of 8-methoxy-2-*p*-tolyl-1,4-naphthoquinone (**3.1**)



HRMS spectrum of 8-methoxy-2-*p*-tolyl-1,4-naphthoquinone (**3.1**)



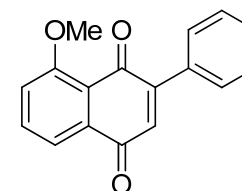
```

Filename      = SNG6210_1H-7.jdf
Author       = N.Ahmed
Experiment   = single_pulse.ex2
Sample_id    = S#456210
Solvent      = CHLOROFORM-D
Creation time = 1-APR-2010 12:12:07
Revision time = 2-JUL-2011 19:59:22
Current Time  = 2-JUL-2011 20:00:12

Data format   = 1D COMPLEX
Dim size      = 26214
Dim title     = 1H
Dim units     = [ppm]
Dimensions    = X
Site          = ECX 500
Spectrometer  = DELTA2 NMR

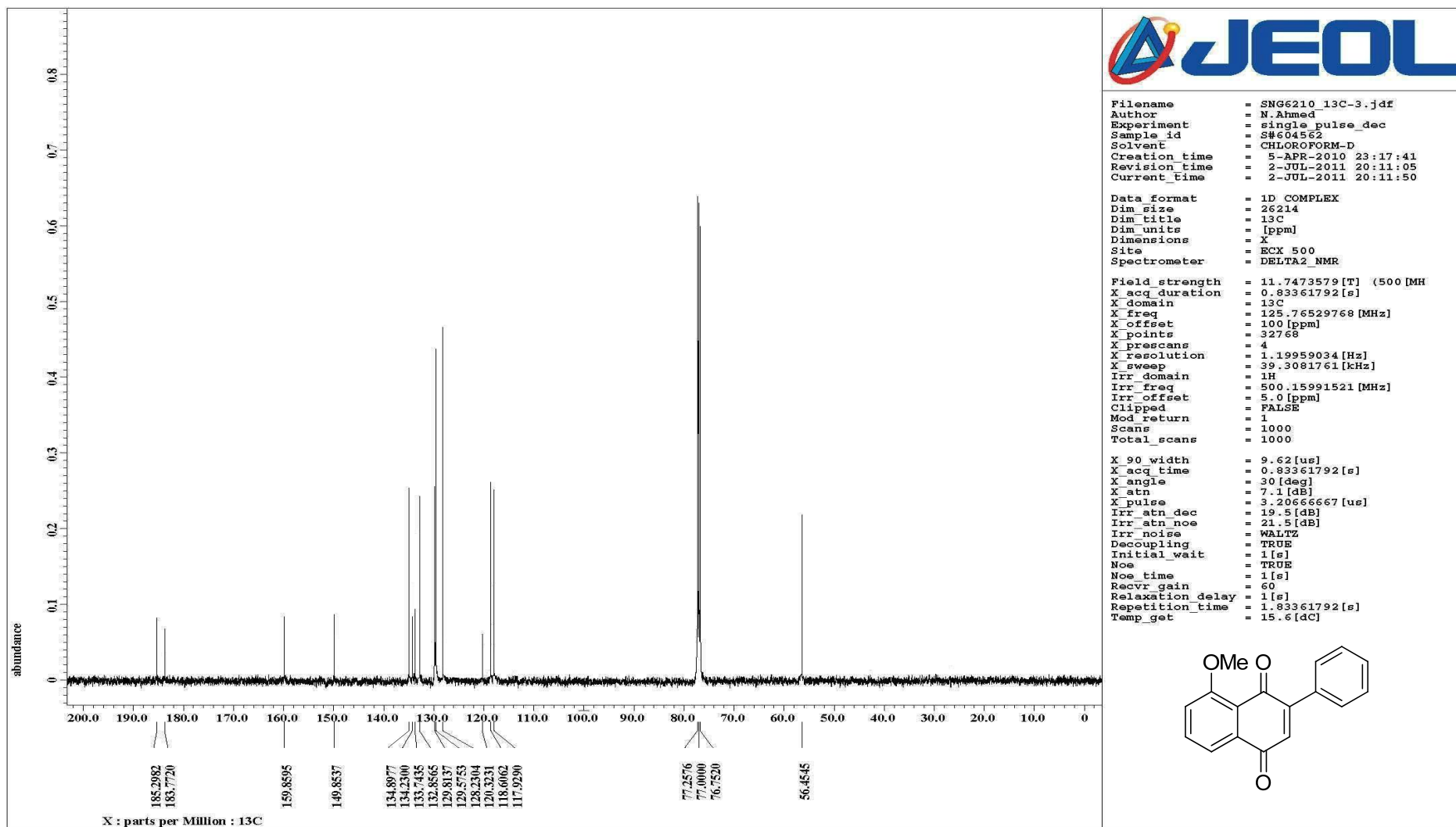
Field strength = 11.7473579 [T] (500 [MH
X_acq_duration = 1.74587904 [s]
X_domain       = 1H
X_freq         = 500.15991521 [MHz]
X_offset       = 5.0 [ppm]
X_points       = 32768
X_prescans     = 1
X_resolution   = 0.57277737 [Hz]
X_sweep        = 18.76876877 [kHz]
Irr_domain     = 1H
Irr_freq       = 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     = 9.25 [us]
X_acq_time     = 1.74587904 [s]
X_angle        = 45 [deg]
X_atn          = 3.99 [dB]
X_pulse        = 4.625 [us]
Irr_mode       = Off
Tri_mode       = Off
Dante_presat   = FALSE
Initial_wait   = 1 [s]
Recvr_gain     = 48
Relaxation_delay = 2 [s]
Repetition_time = 3.74587904 [s]
Temp_get       = 22.1 [dC]
    
```

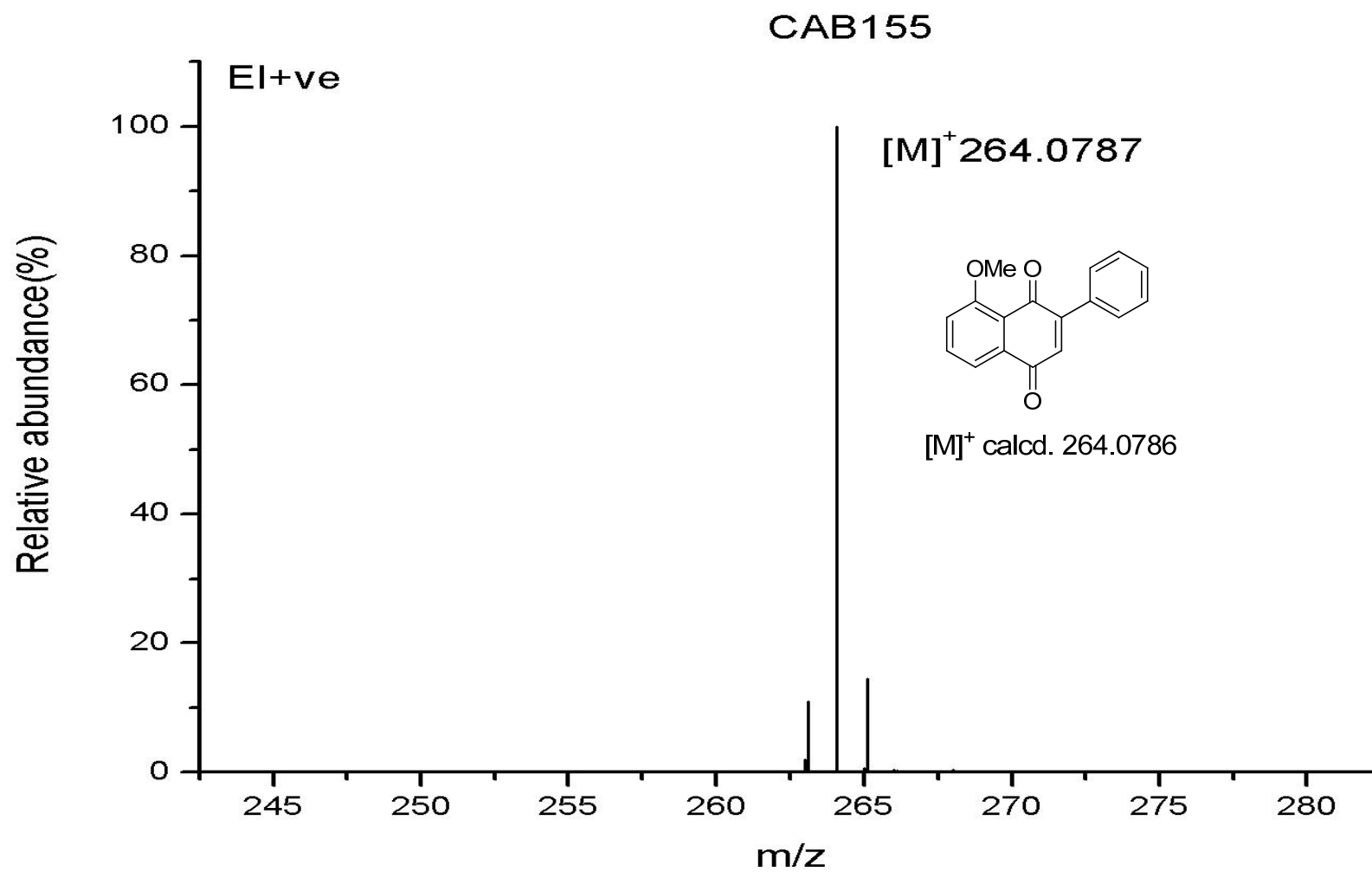


$^1\text{H}$  NMR spectrum of 8-methoxy-2-phenyl-1,4-naphthoquinone (3.2)

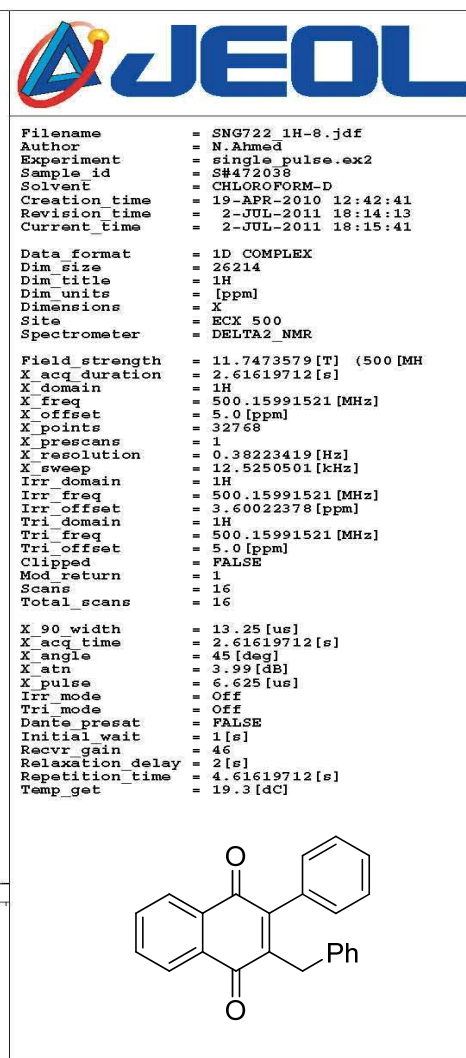
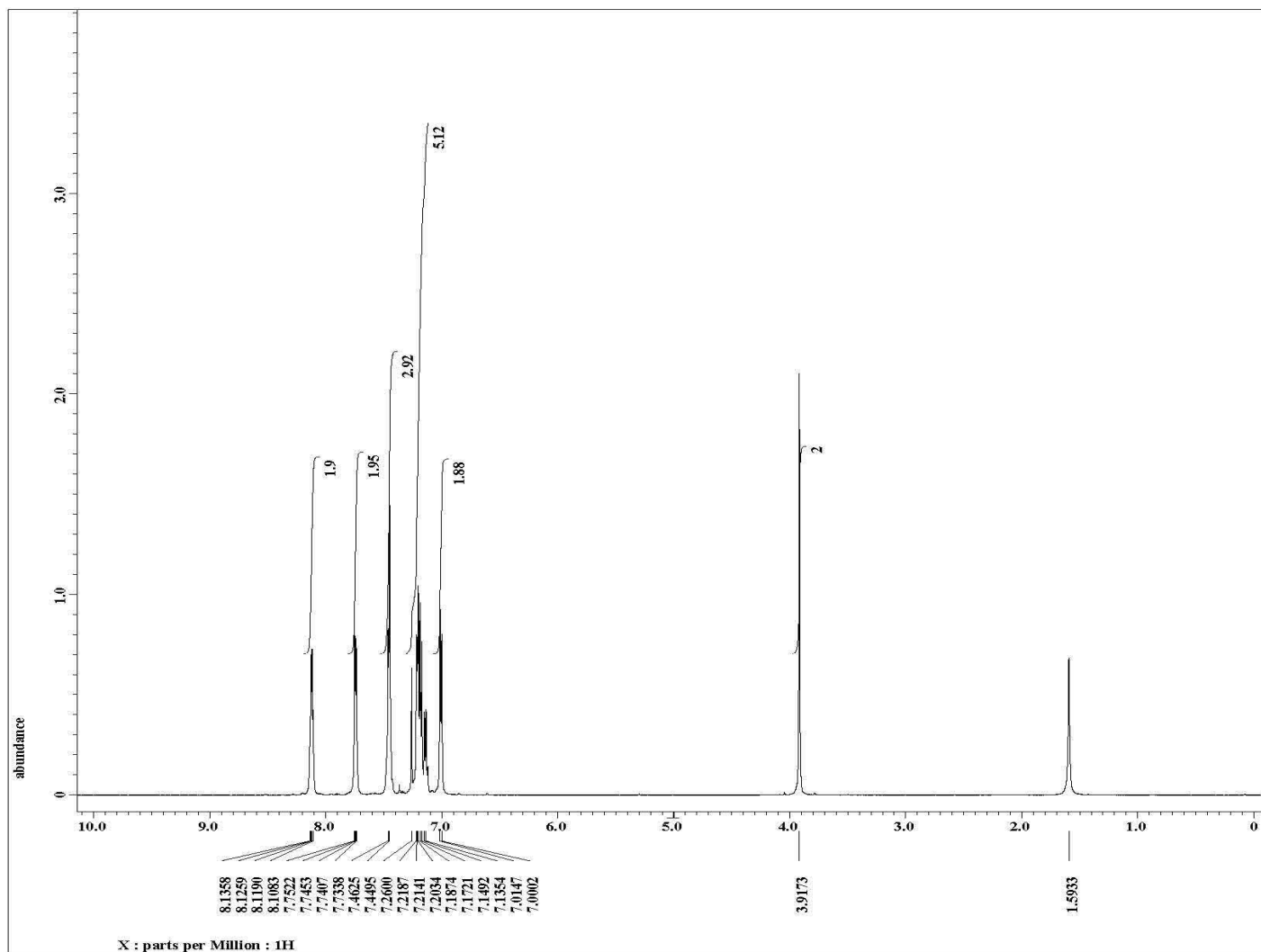




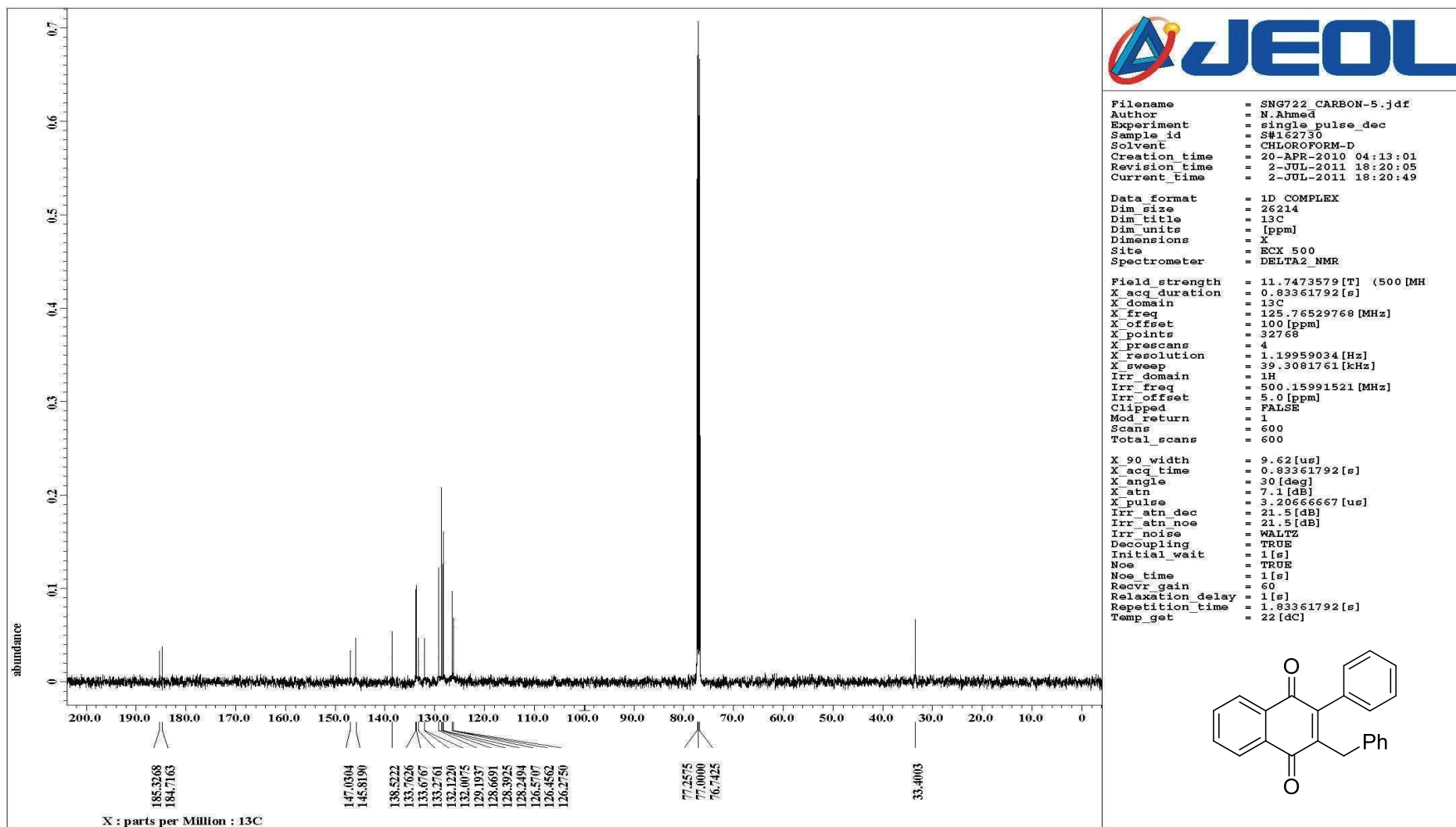
<sup>13</sup>C NMR spectrum of 8-methoxy-2-phenyl-1,4-naphthoquinone (3.2)



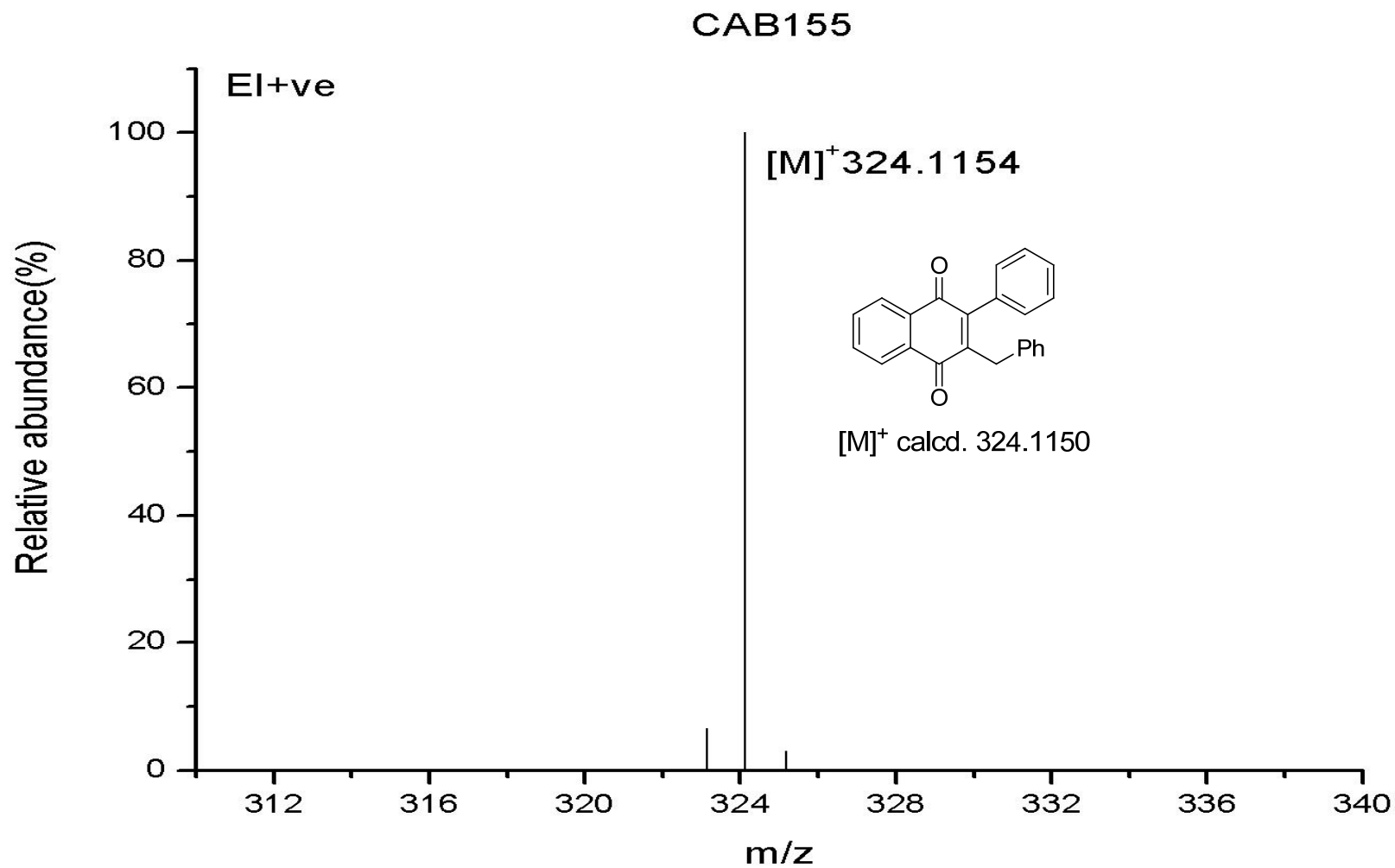
HRMS spectrum of 8-methoxy-2-phenyl-1,4-naphthoquinone (**3.2**)



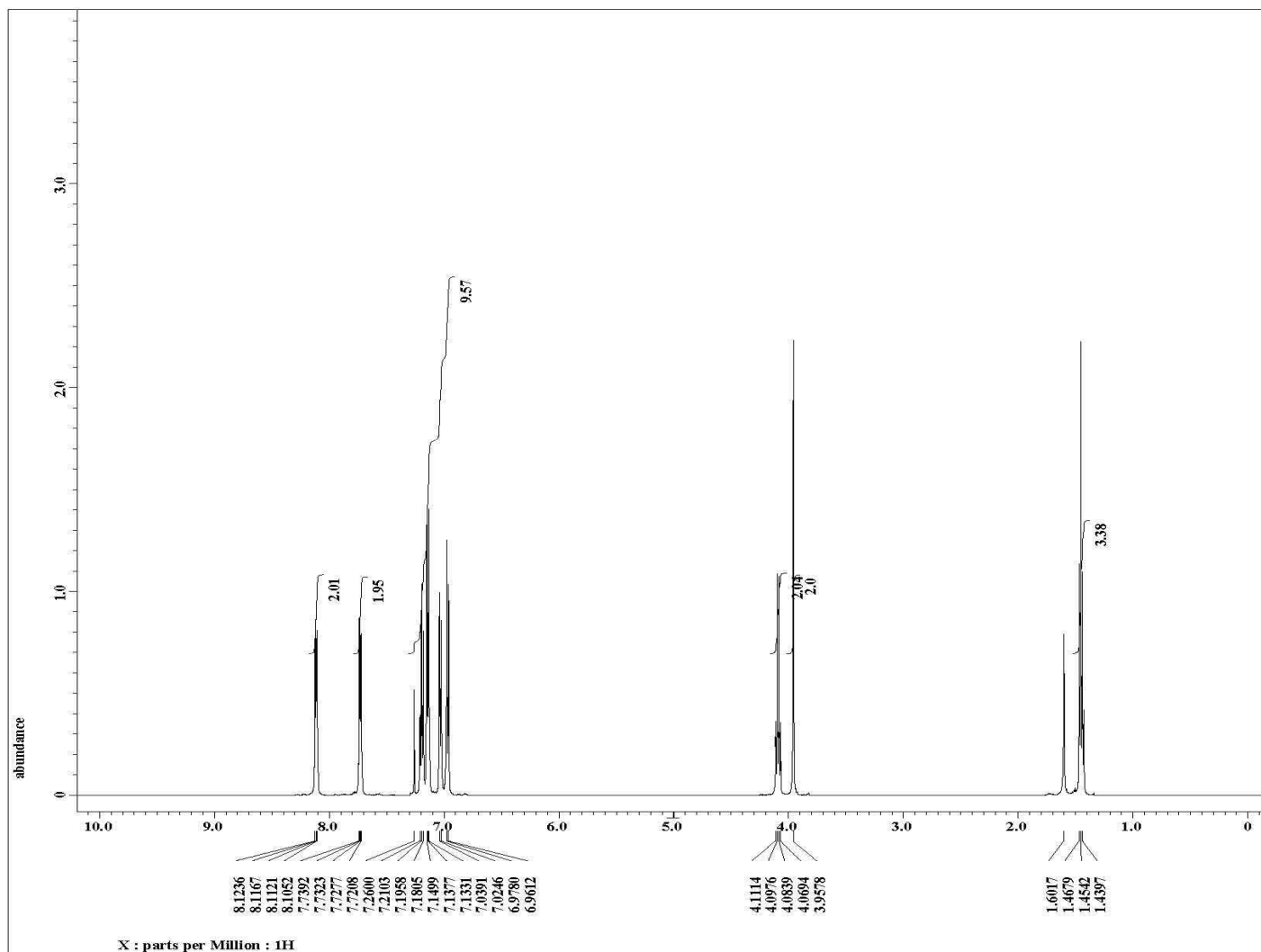
<sup>1</sup>H NMR spectrum of 2-benzyl-3-phenyl-1,4-naphthoquinone (**3.3**)



<sup>13</sup>C NMR spectrum of 2-benzyl-3-phenyl-1,4-naphthoquinone (3.3)



HRMS spectrum of 2-benzyl-3-phenyl-1,4-naphthoquinone (**3.3**)



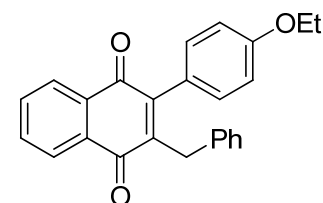
```

Filename      = SNG725 1H-4.jdf
Author       = N.Ahmed
Experiment   = single_pulse.ex2
Sample_id    = S#472638
Solvent      = CHLOROFORM-D
Creation time = 19-APR-2010 13:04:21
Revision time = 2-JUL-2011 18:28:12
Current time  = 2-JUL-2011 18:28:57

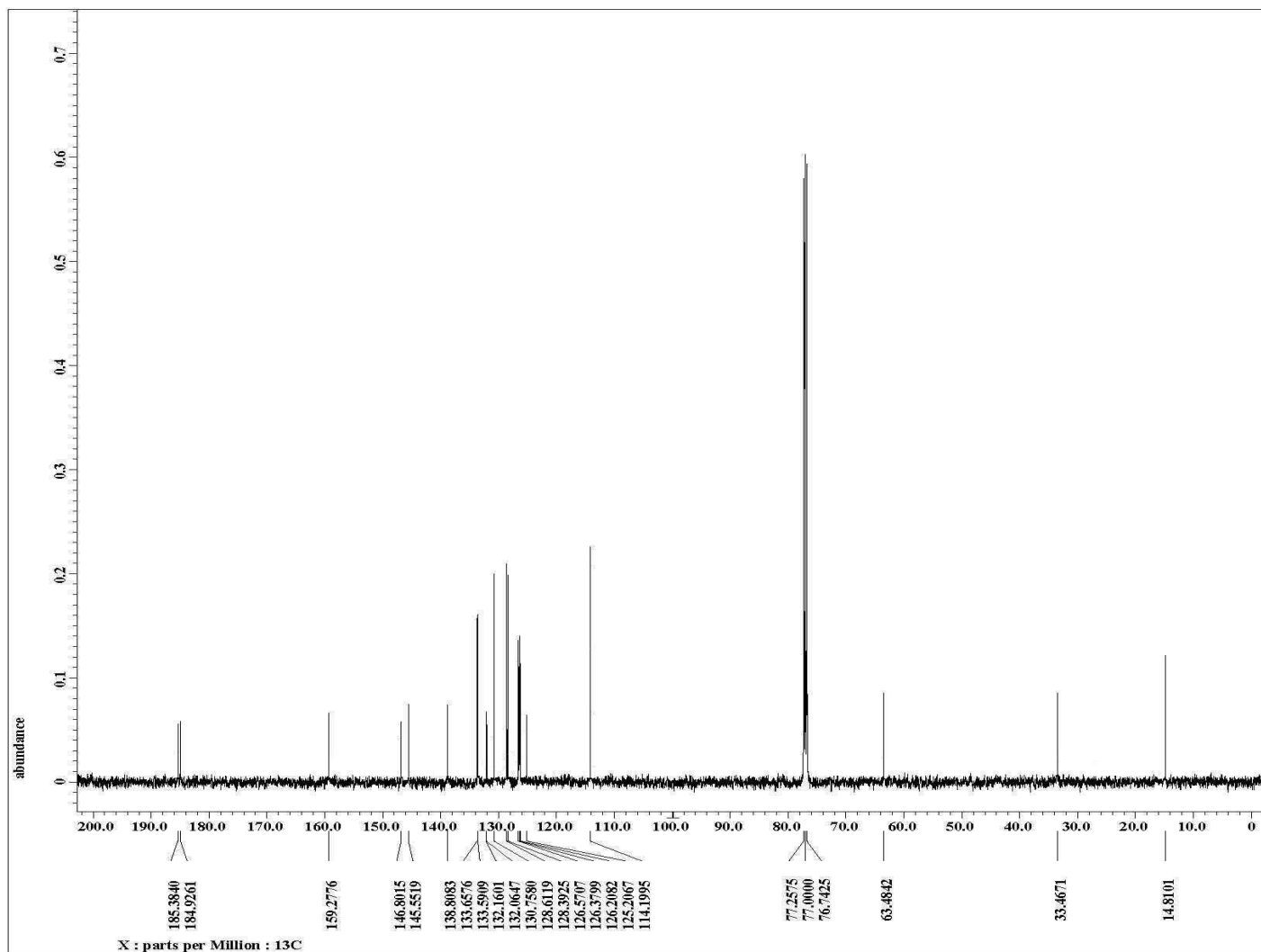
Data format   = 1D COMPLEX
Dim_size      = 26214
Dim_title     = 1H
Dim_units     = [ppm]
Dimensions    = X
Site          = ECX 500
Spectrometer  = DELTA2 NMR

Field strength = 11.7473579 [T] (500 [MH
X_acq_duration = 2.61619712 [s]
X_domain       = 1H
X_freq         = 500.15991521 [MHz]
X_offset       = 5.0 [ppm]
X_points       = 32768
X_prescans     = 1
X_resolution   = 0.38223419 [Hz]
X_sweep        = 12.5250501 [kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521 [MHz]
Irr_offset     = 3.60022378 [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     = 2.61619712 [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     = 40
Relaxation_delay = 2 [s]
Repetition_time = 4.61619712 [s]
Temp_get       = 18.9 [dC]
    
```



$^1\text{H}$  NMR spectrum of 2-benzyl-3-(4-ethoxyphenyl)-1,4-naphthoquinone (**3.4**)



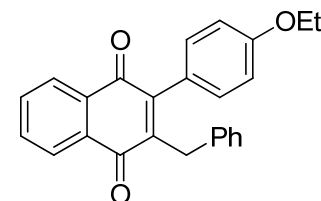
```

Filename      = SNG725 CARBON-3.jdf
Author       = N.Ahmed
Experiment   = single_pulse_dec
Sample_id    = S#204333
Solvent      = CHLOROFORM-D
Creation time = 20-APR-2010 05:21:13
Revision time = 20-APR-2010 06:03:04
Current Time  = 2-JUL-2011 18:31:51

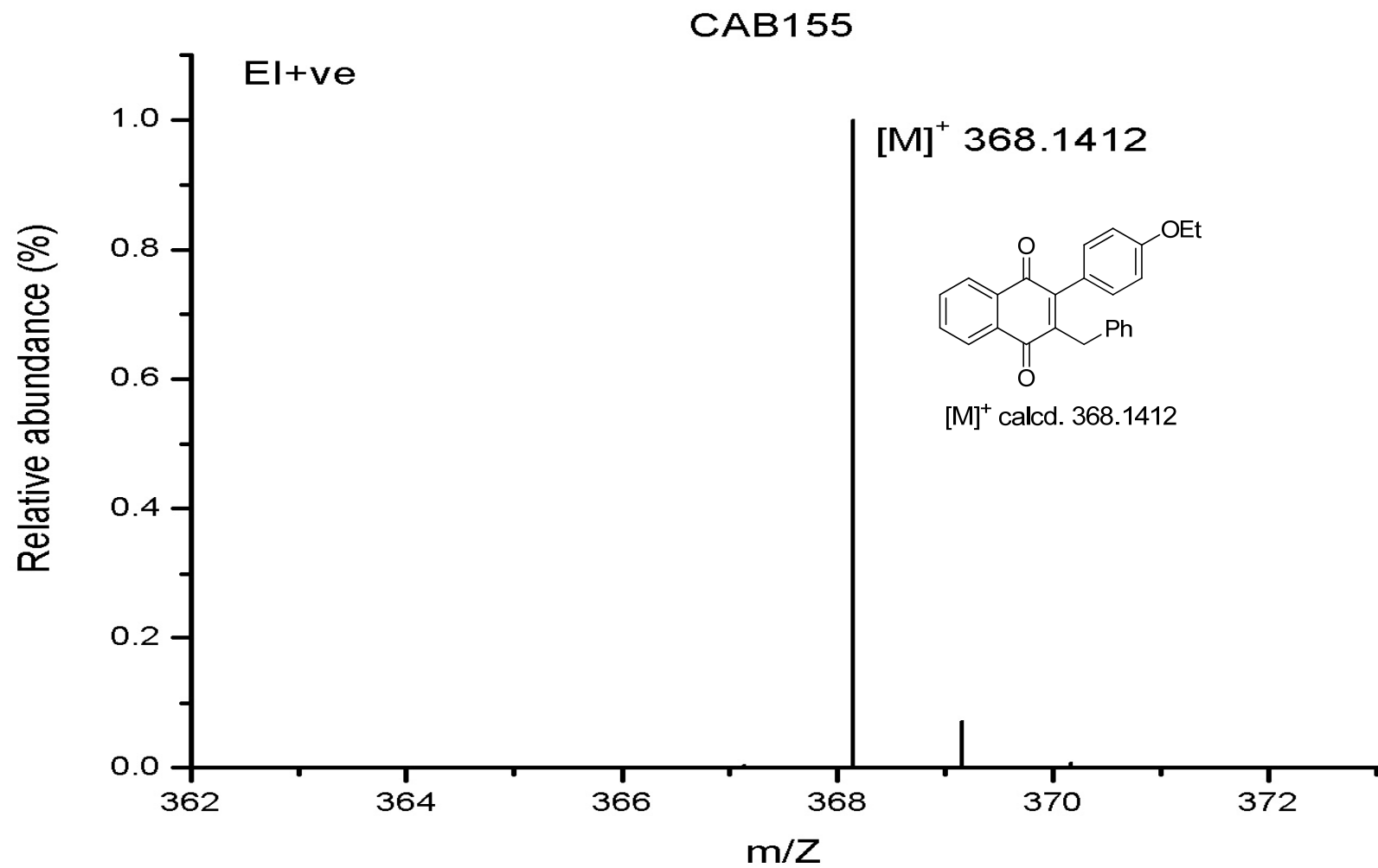
Data format   = 1D COMPLEX
Dim size      = 26214
Dim title     = 13C
Dim units     = [ppm]
Dimensions    = X
Site          = ECX 500
Spectrometer  = DELTA2 NMR

Field strength = 11.7473579 [T] (500 [MH
X_acq_duration = 0.83361792 [s]
X_domain       = 13C
X_freq         = 125.76529768 [MHz]
X_offset       = 100 [ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.19959034 [Hz]
X_sweep        = 39.3081761 [kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521 [MHz]
Irr_offset     = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 600
Total_scans    = 600

X_90_width    = 9.62 [us]
X_acq_time     = 0.83361792 [s]
X_angle        = 30 [deg]
X_atn          = 7.1 [dB]
X_pulse        = 3.20666667 [us]
Irr_atn_dec    = 21.5 [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 = 1.83361792 [s]
Temp_get       = 21.9 [dC]
    
```

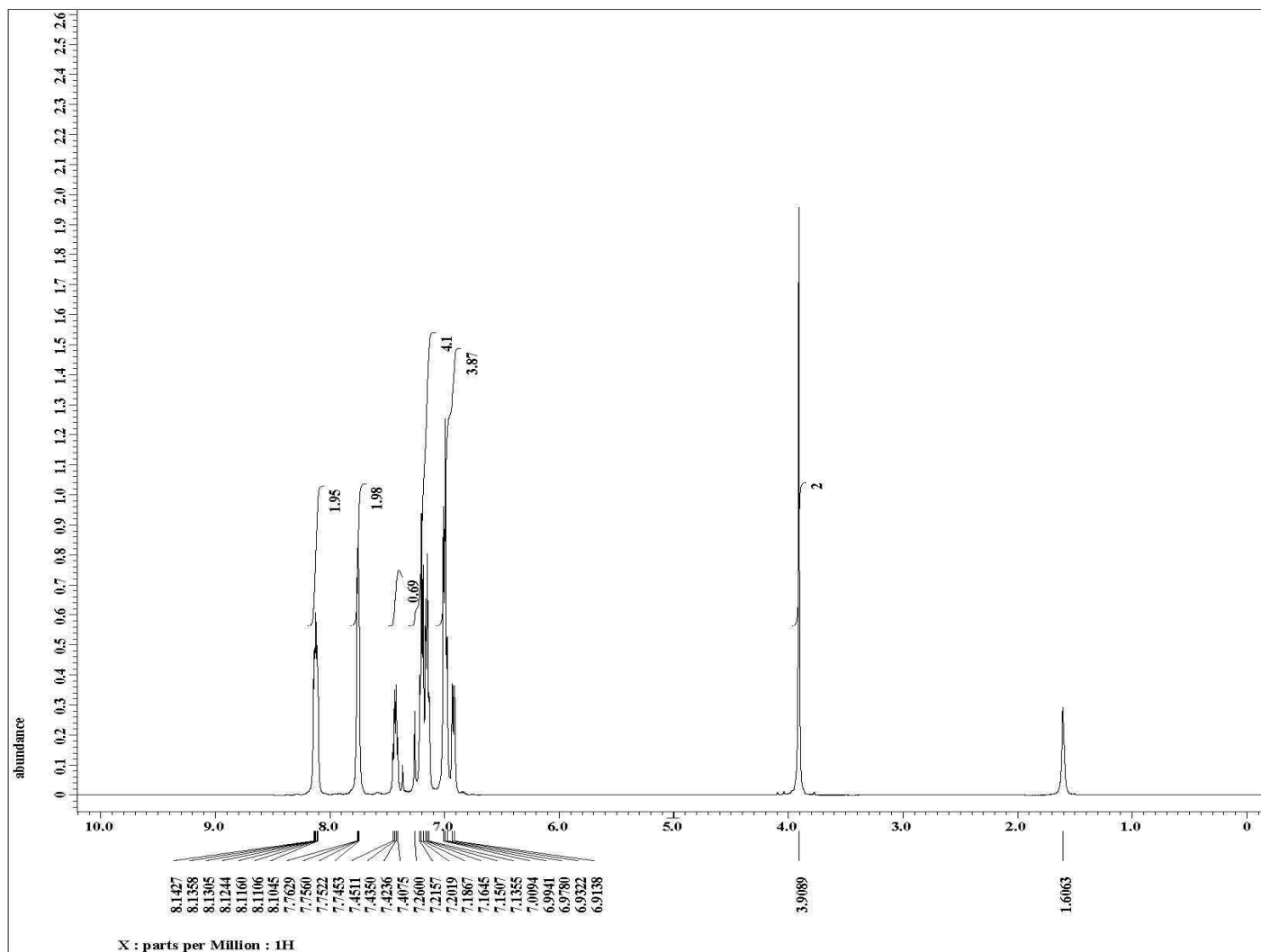


$^{13}\text{C}$  NMR spectrum of 2-benzyl-3-(4-ethoxyphenyl)-1,4-naphthoquinone (**3.4**)



HRMS spectrum of 2-benzyl-3-(4-ethoxyphenyl)-1,4-naphthoquinone (**3.4**)



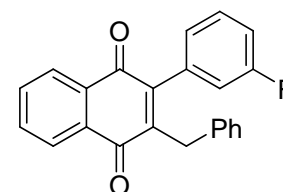


Filename = SNG726 1H-6.jdf  
Author = N.Ahmed  
Experiment = single\_pulse.ex2  
Sample\_id = S#472472  
Solvent = CHLOROFORM-D  
Creation time = 19-APR-2010 12:57:18  
Revision time = 2-JUL-2011 19:01:27  
Current time = 2-JUL-2011 19:01:59

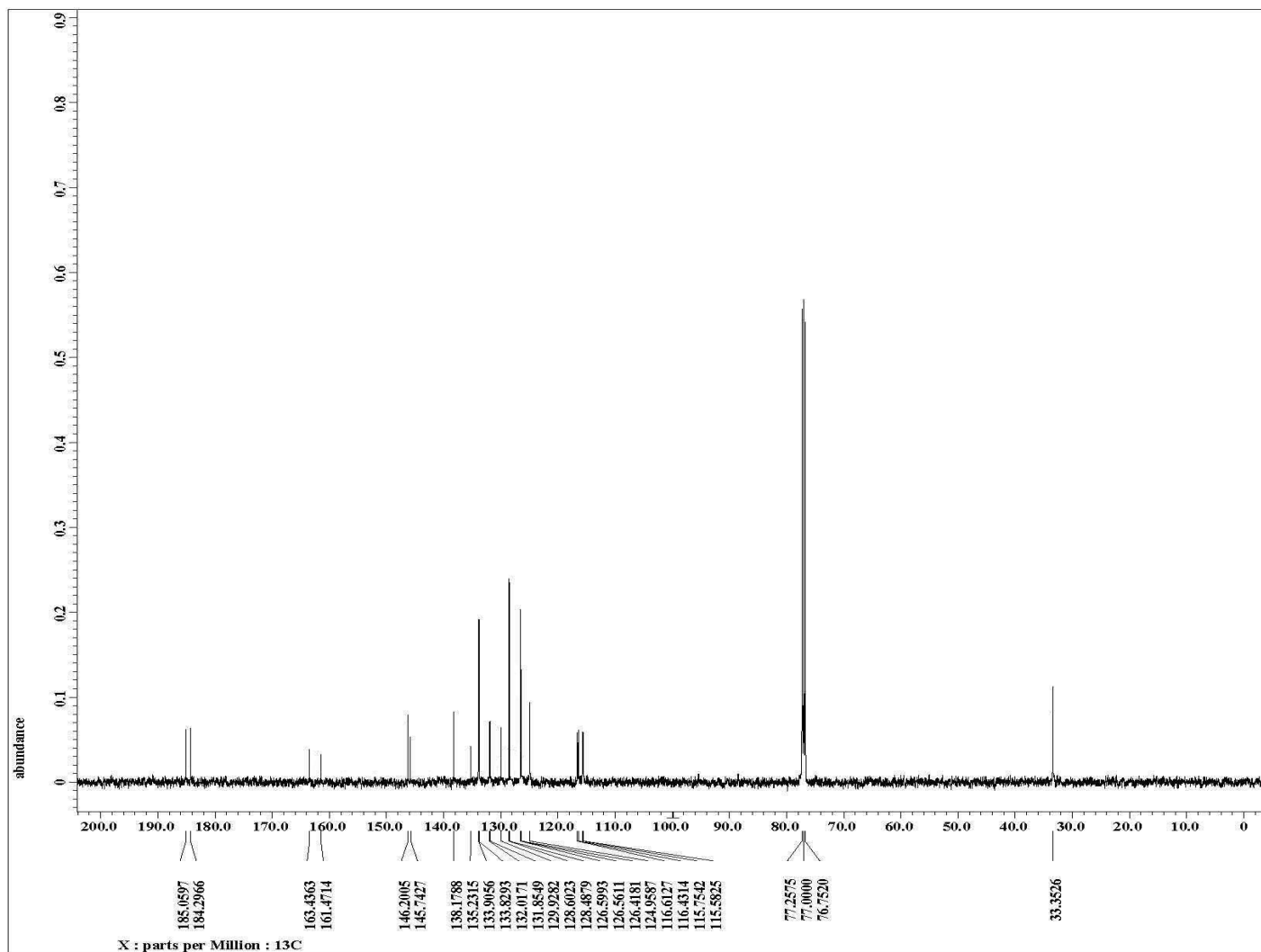
Data format = 1D COMPLEX  
Dim size = 26214  
Dim title = 1H  
Dim units = [ppm]  
Dimensions = X  
Site = ECX 500  
Spectrometer = DELTA2 NMR

Field strength = 11.7473579 [T] (500 [MH  
X\_acq\_duration = 2.61619712 [s]  
X\_domain = 1H  
X\_freq = 500.15991521 [MHz]  
X\_offset = 5.0 [ppm]  
X\_points = 32768  
X\_prescans = 1  
X\_resolution = 0.38223419 [Hz]  
X\_sweep = 12.5250501 [kHz]  
Irr\_domain = 1H  
Irr\_freq = 500.15991521 [MHz]  
Irr\_offset = 3.60022378 [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 = 2.61619712 [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 = 42  
Relaxation\_delay = 2 [s]  
Repetition\_time = 4.61619712 [s]  
Temp\_get = 19 [dC]



<sup>1</sup>H NMR spectrum of 2-benzyl-3-(3-fluorophenyl)-1,4-naphthoquinone (3.5)



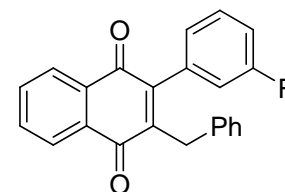
```

Filename      = SNG726 CARBON-3.jdf
Author       = N.Ahmed
Experiment   = single_pulse_dec
Sample id    = S#190576
Solvent      = CHLOROFORM-D
Creation time = 20-APR-2010 04:58:42
Revision time = 20-APR-2010 05:40:34
Current time  = 2-JUL-2011 19:04:45

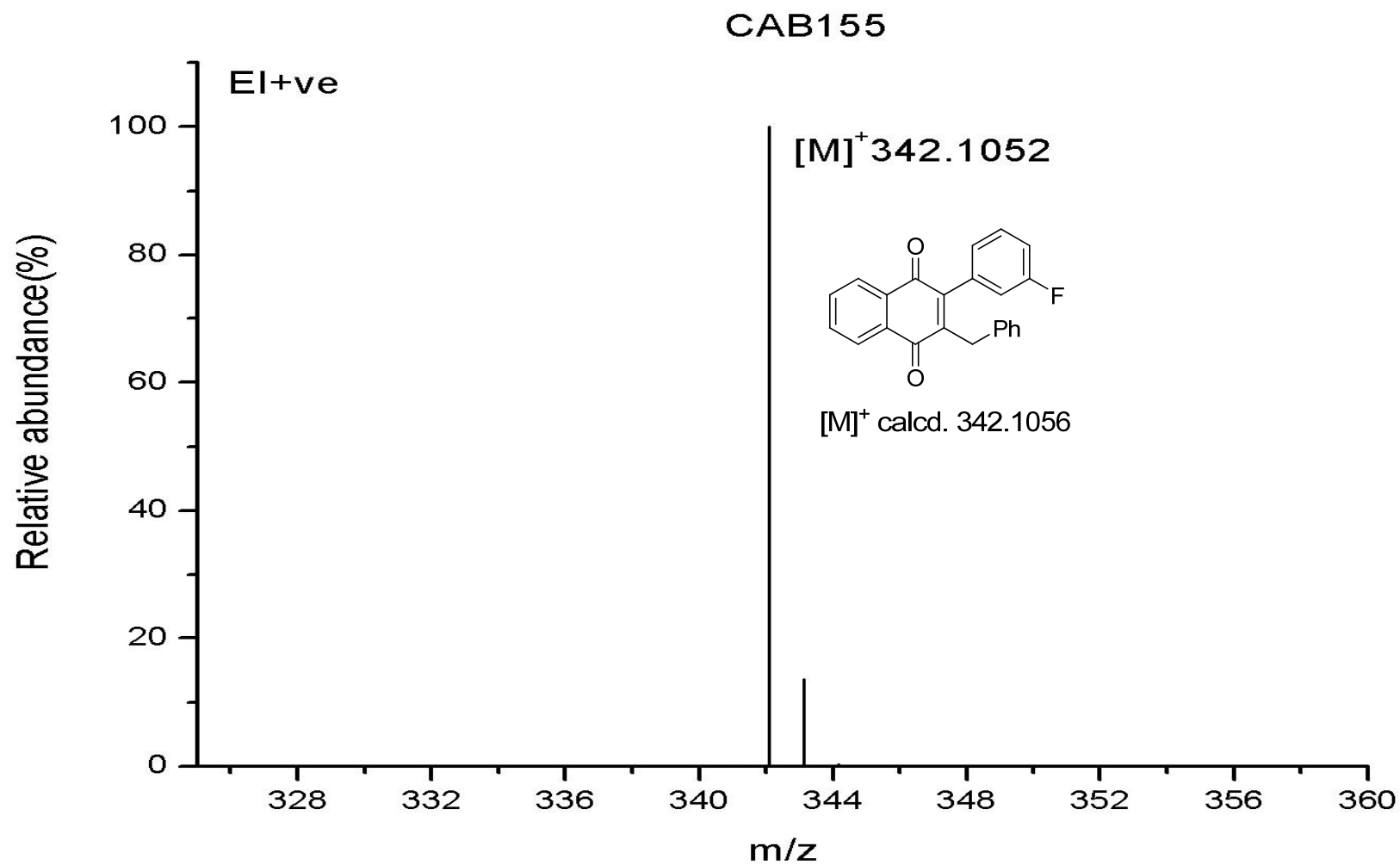
Data format   = 1D COMPLEX
Dim size      = 26214
Dim title     = 13C
Dim units     = [ppm]
Dimensions    = X
Site          = ECX 500
Spectrometer  = DELTA2 NMR

Field strength = 11.7473579 [T] (500 [MH]
X_acq_duration = 0.83361792 [s]
X_domain       = 13C
X_freq         = 125.76529768 [MHz]
X_offset       = 100 [ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.19959034 [Hz]
X_sweep        = 39.3081761 [kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521 [MHz]
Irr_offset     = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 600
Total_scans    = 600

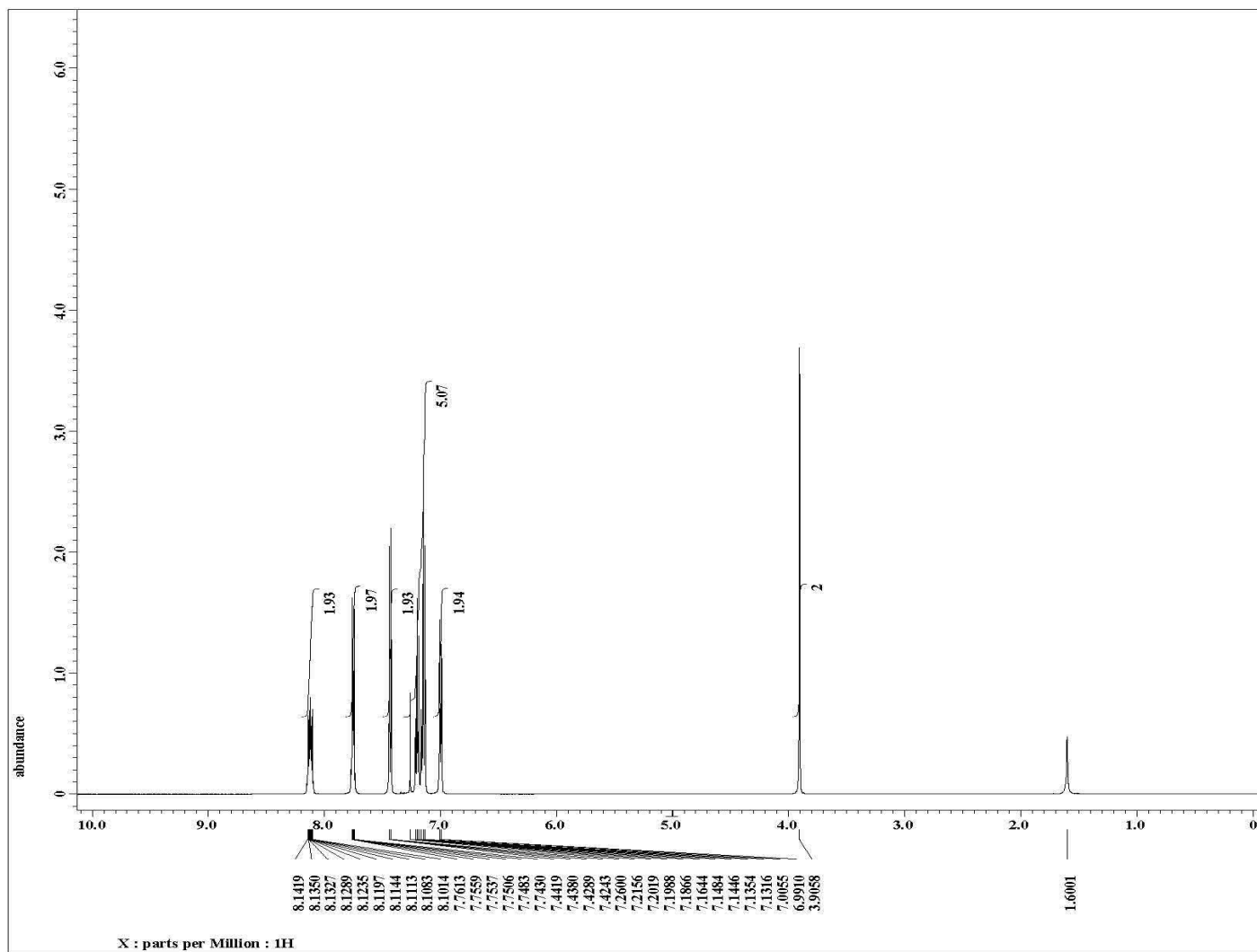
X_90_width     = 9.62 [us]
X_acq_time     = 0.83361792 [s]
X_angle        = 30 [deg]
X_atn          = 7.1 [dB]
X_pulse        = 3.20666667 [us]
Irr_atn_dec    = 21.5 [dB]
Irr_atn_noe    = 21.5 [dB]
Irr_noise      = WALTZ
Decoupling     = TRUE
Initial_wait   = 1 [s]
Noe            = TRUE
Noe_time       = 1 [s]
Recvr_gain     = 60
Relaxation_delay = 1 [s]
Repetition_time = 1.83361792 [s]
Temp_get       = 21.9 [dC]
    
```



$^{13}\text{C}$  NMR spectrum of 2-benzyl-3-(3-fluorophenyl)-1,4-naphthoquinone (**3.5**)



HRMS spectrum of 2-benzyl-3-(3-fluorophenyl)-1,4-naphthoquinone (**3.5**)



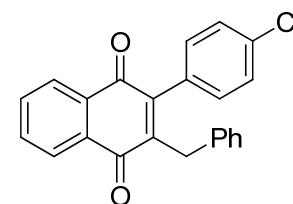
```

Filename      = SNG731 1H-6.jdf
Author       = N.Ahmed
Experiment   = single_pulse.ex2
Sample_id    = S#472879
Solvent      = CHLOROFORM-D
Creation time = 19-APR-2010 13:11:23
Revision time = 2-JUL-2011 18:41:25
Current time  = 2-JUL-2011 18:41:59

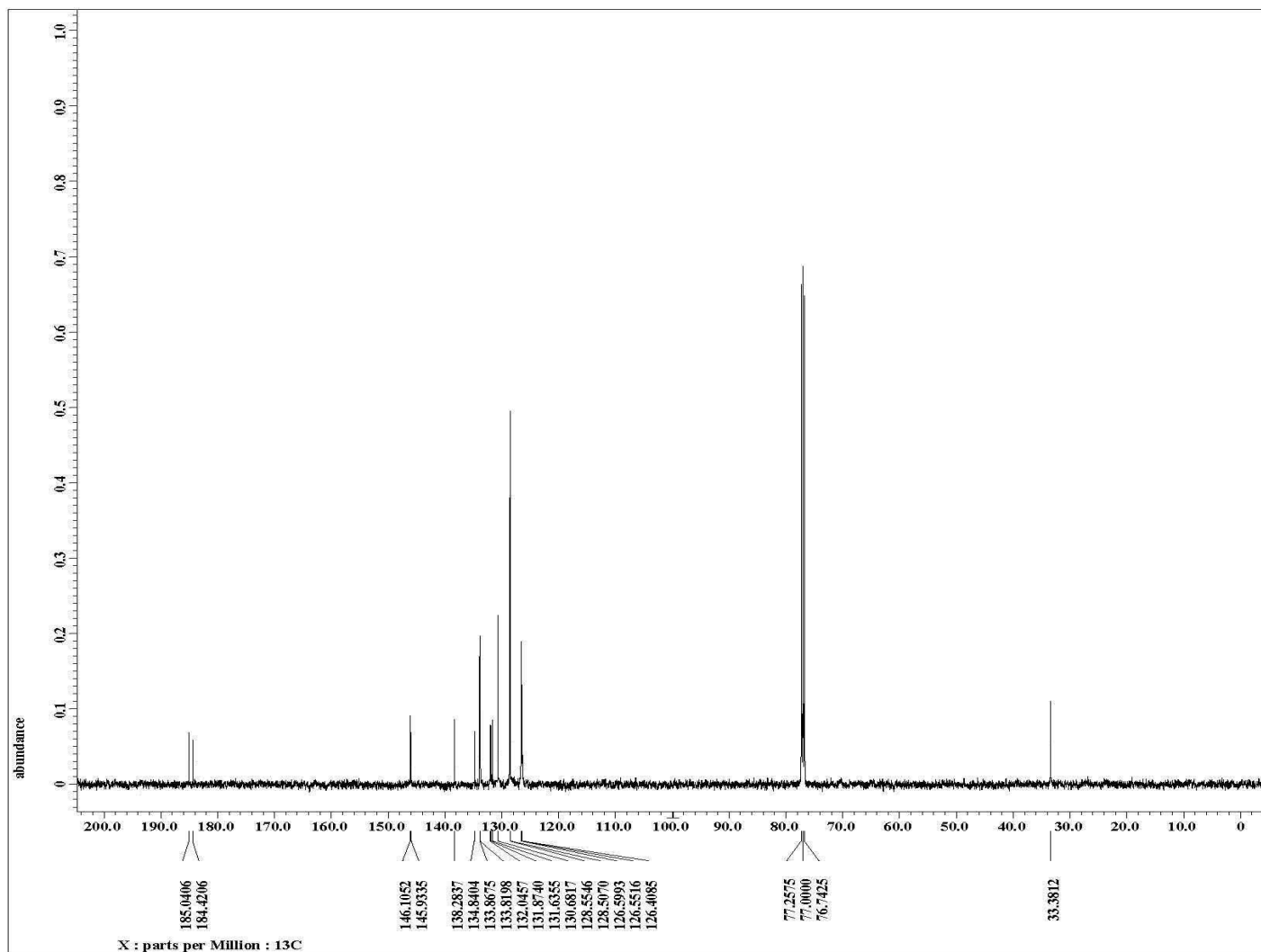
Data format   = 1D COMPLEX
Dim_size      = 26214
Dim_title     = 1H
Dim_units     = [ppm]
Dimensions    = X
Site          = ECX 500
Spectrometer  = DELTA2 NMR

Field strength = 11.7473579 [T] (500 [MH
X_acq_duration = 2.61619712 [s]
X_domain       = 1H
X_freq         = 500.15991521 [MHz]
X_offset       = 5.0 [ppm]
X_points       = 32768
X_prescans     = 1
X_resolution   = 0.38223419 [Hz]
X_sweep        = 12.5250501 [kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521 [MHz]
Irr_offset     = 3.60022378 [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    = 2.61619712 [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    = 42
Relaxation_delay = 2 [s]
Repetition_time = 4.61619712 [s]
Temp_get      = 18.8 [dC]
    
```



$^1\text{H}$  NMR spectrum of 2-benzyl-3-(4-chlorophenyl)-1,4-naphthoquinone (**3.6**)



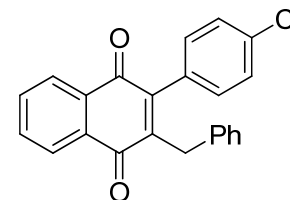
```

Filename      = SNG731 CARBON-3.jdf
Author       = N.Ahmed
Experiment   = single_pulse_dec
Sample_id    = S#217833
Solvent      = CHLOROFORM-D
Creation time = 20-APR-2010 05:43:38
Revision time = 20-APR-2010 06:25:28
Current Time  = 2-JUL-2011 18:46:36

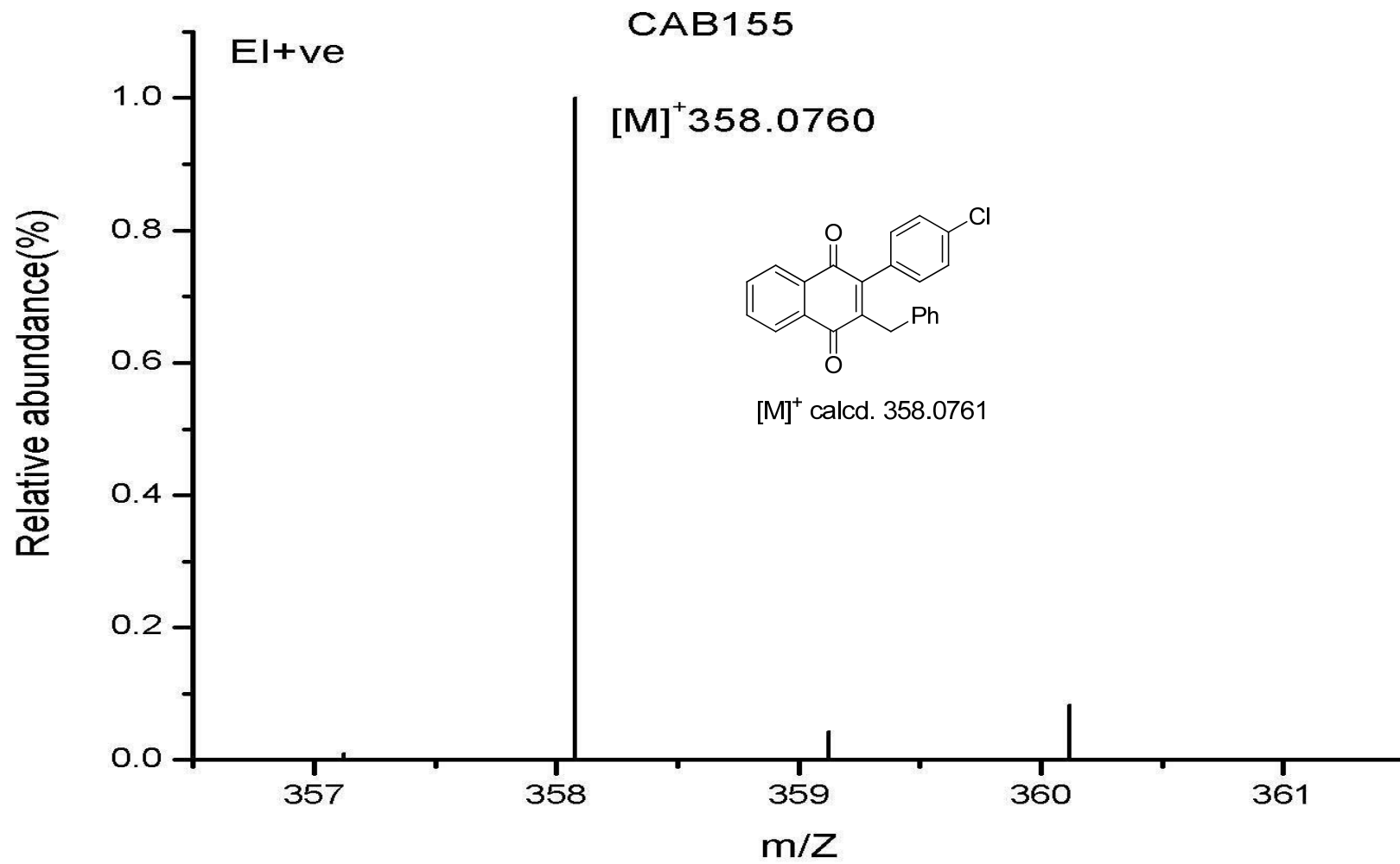
Data format   = 1D COMPLEX
Dim size      = 26214
Dim title     = 13C
Dim units     = [ppm]
Dimensions    = X
Site          = ECX 500
Spectrometer  = DELTA2 NMR

Field strength = 11.7473579 [T] (500 [MH]
X_acq_duration = 0.83361792 [s]
X_domain       = 13C
X_freq         = 125.76529768 [MHz]
X_offset       = 100 [ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.19959034 [Hz]
X_sweep        = 39.3081761 [kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521 [MHz]
Irr_offset     = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 600
Total_scans    = 600

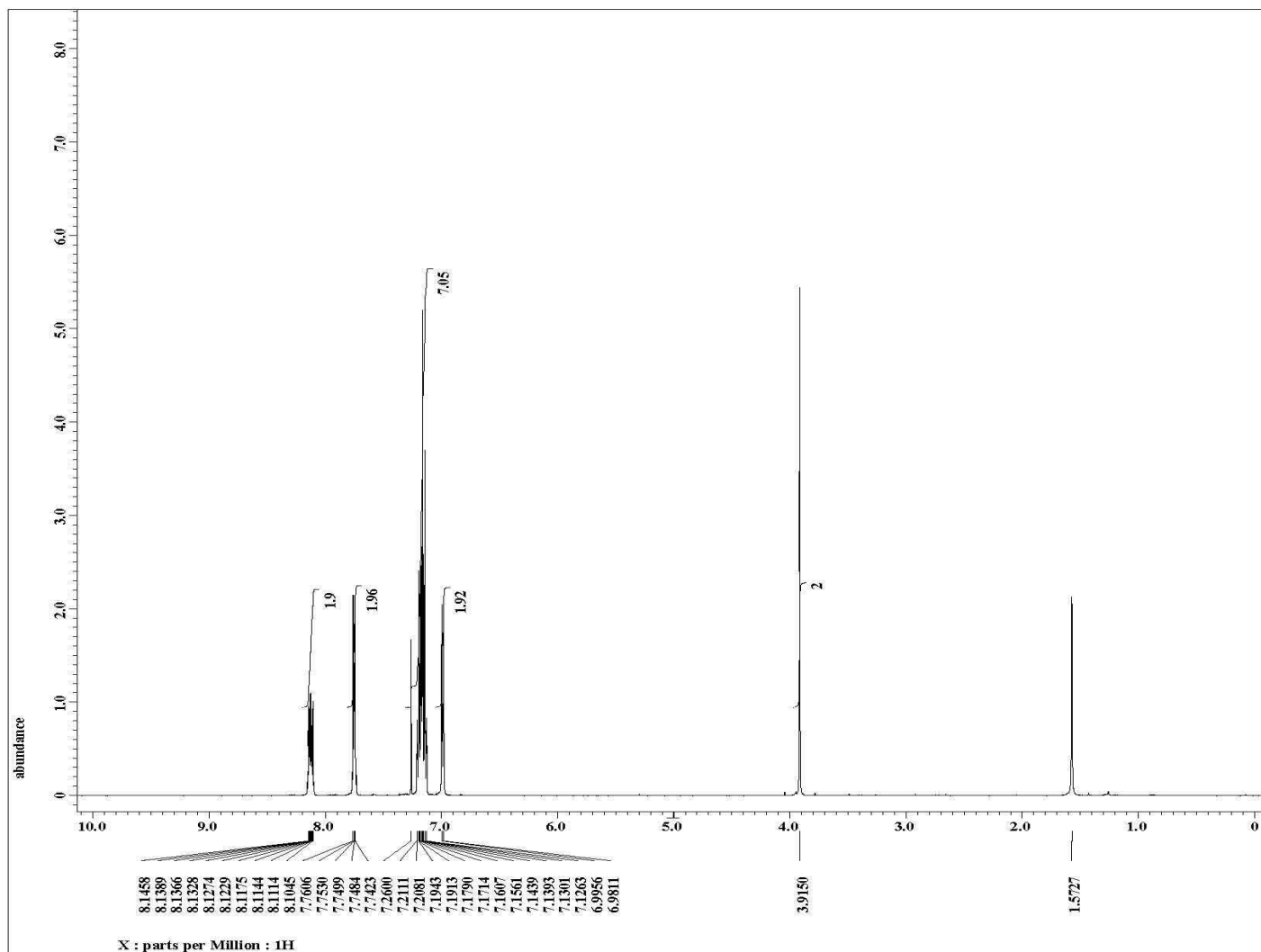
X_90_width     = 9.62 [us]
X_acq_time     = 0.83361792 [s]
X_angle        = 30 [deg]
X_atn          = 7.1 [dB]
X_pulse        = 3.20666667 [us]
Irr_atn_dec    = 21.5 [dB]
Irr_atn_noe    = 21.5 [dB]
Irr_noise      = WALTZ
Decoupling     = TRUE
Initial_wait   = 1 [s]
Noe            = TRUE
Noe_time       = 1 [s]
Recvr_gain     = 60
Relaxation_delay = 1 [s]
Repetition_time = 1.83361792 [s]
Temp_get       = 21.9 [dC]
    
```



$^{13}\text{C}$  NMR spectrum of 2-benzyl-3-(4-chlorophenyl)-1,4-naphthoquinone (**3.6**)



HRMS spectrum of 2-benzyl-3-(4-chlorophenyl)-1,4-naphthoquinone (**3.6**)

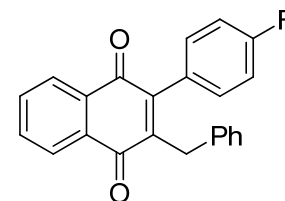


Filename = SNG732 1H-5.jdf  
Author = N.Ahmed  
Experiment = single\_pulse.ex2  
Sample\_id = S#447612  
Solvent = CHLOROFORM-D  
Creation time = 20-APR-2010 12:16:37  
Revision time = 2-JUL-2011 18:49:41  
Current time = 2-JUL-2011 18:50:15

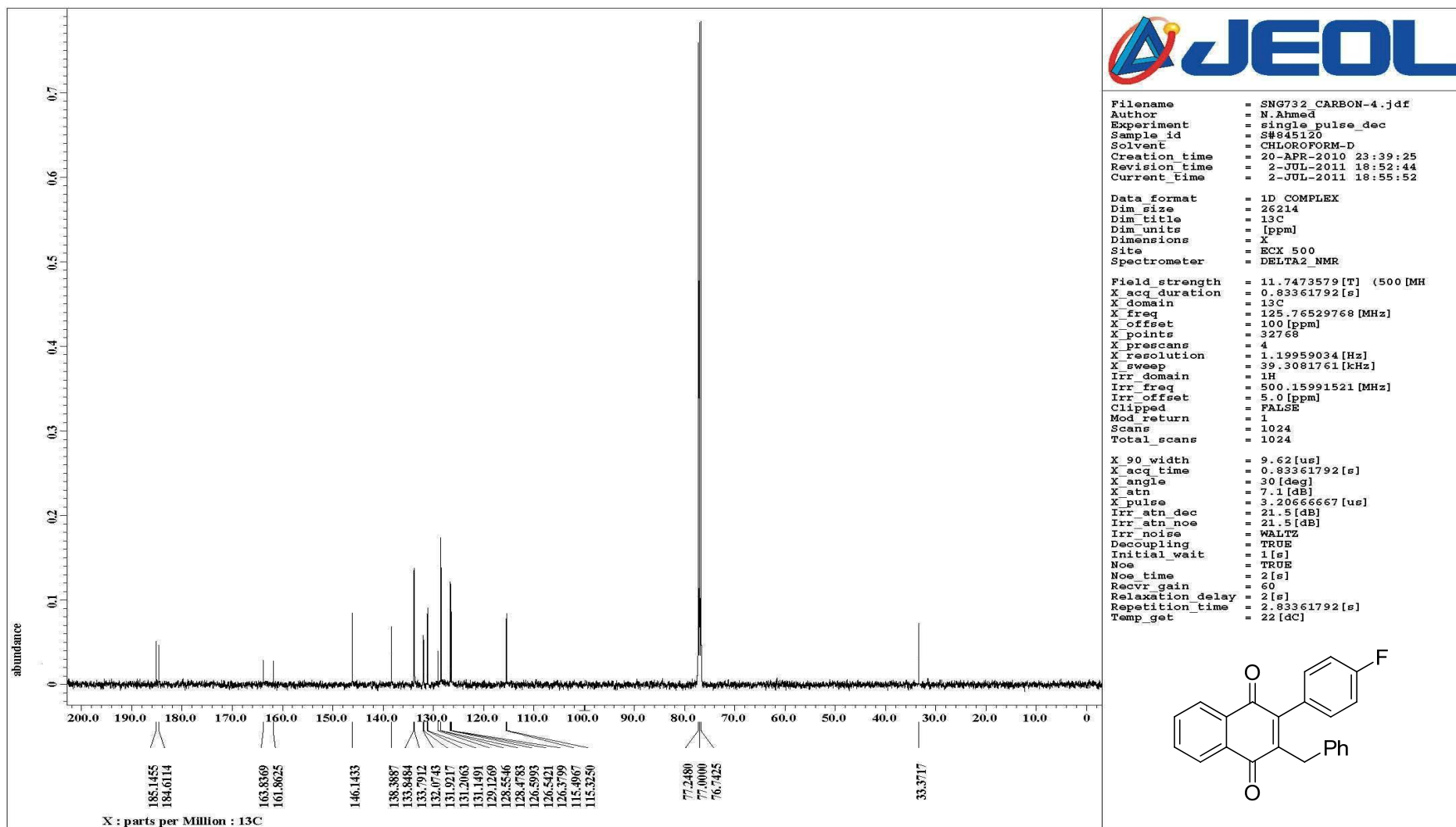
Data format = 1D COMPLEX  
Dim size = 26214  
Dim title = 1H  
Dim units = [ppm]  
Dimensions = X  
Site = ECX 500  
Spectrometer = DELTA2 NMR

Field strength = 11.7473579 [T] (500 [MH  
X\_acq\_duration = 2.61619712 [s]  
X\_domain = 1H  
X\_freq = 500.15991521 [MHz]  
X\_offset = 5.0 [ppm]  
X\_points = 32768  
X\_prescans = 1  
X\_resolution = 0.38223419 [Hz]  
X\_sweep = 12.5250501 [kHz]  
Irr\_domain = 1H  
Irr\_freq = 500.15991521 [MHz]  
Irr\_offset = 4.99886942 [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 = 2.61619712 [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 = 50  
Relaxation\_delay = 2 [s]  
Repetition\_time = 4.61619712 [s]  
Temp\_get = 23.5 [dC]

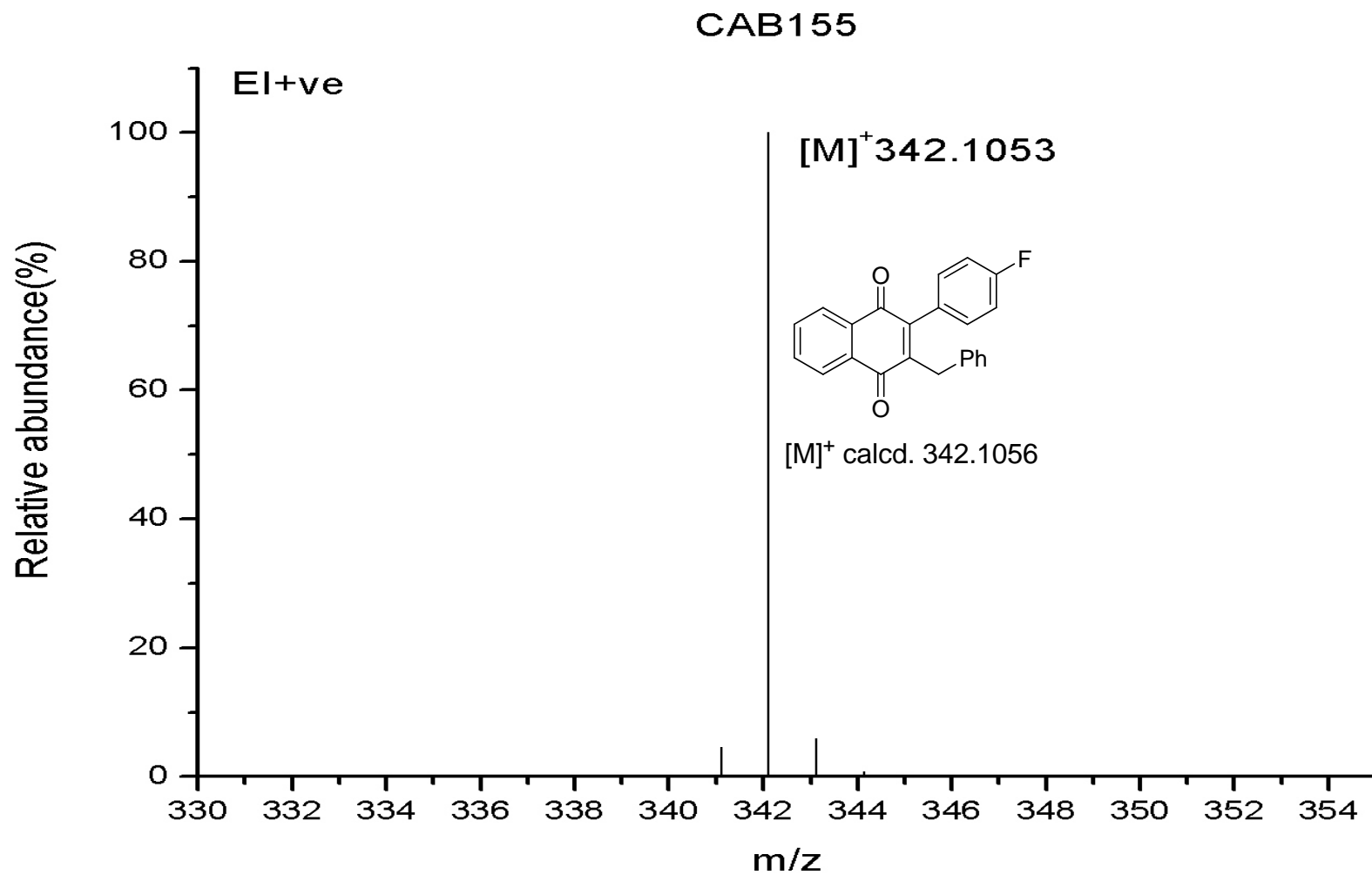


<sup>1</sup>H NMR spectrum of 2-benzyl-3-(4-fluorophenyl)-1,4-naphthoquinone (3.7)

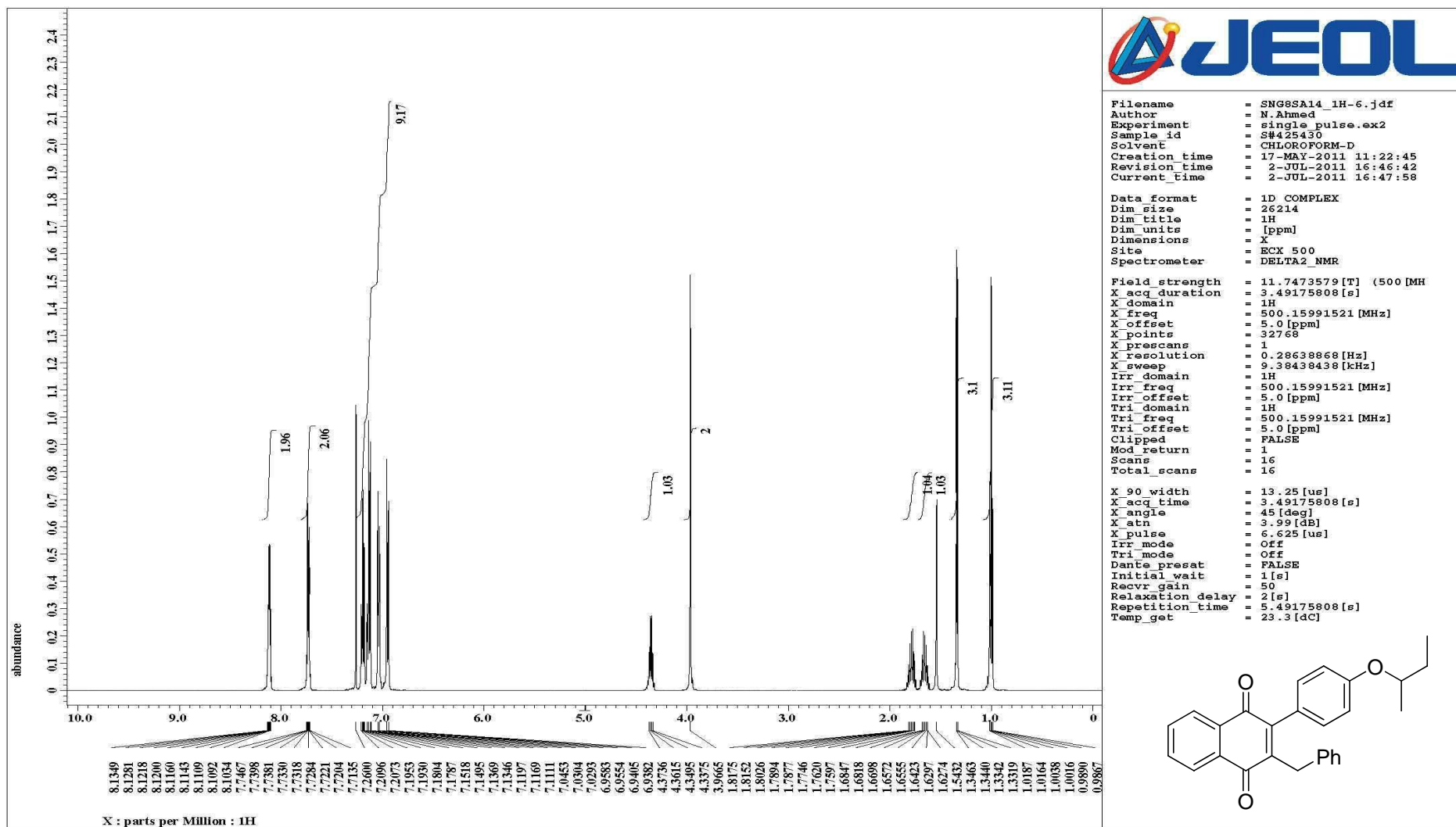


$^{13}\text{C}$  NMR spectrum of 2-benzyl-3-(4-fluorophenyl)-1,4-naphthoquinone (**3.7**)

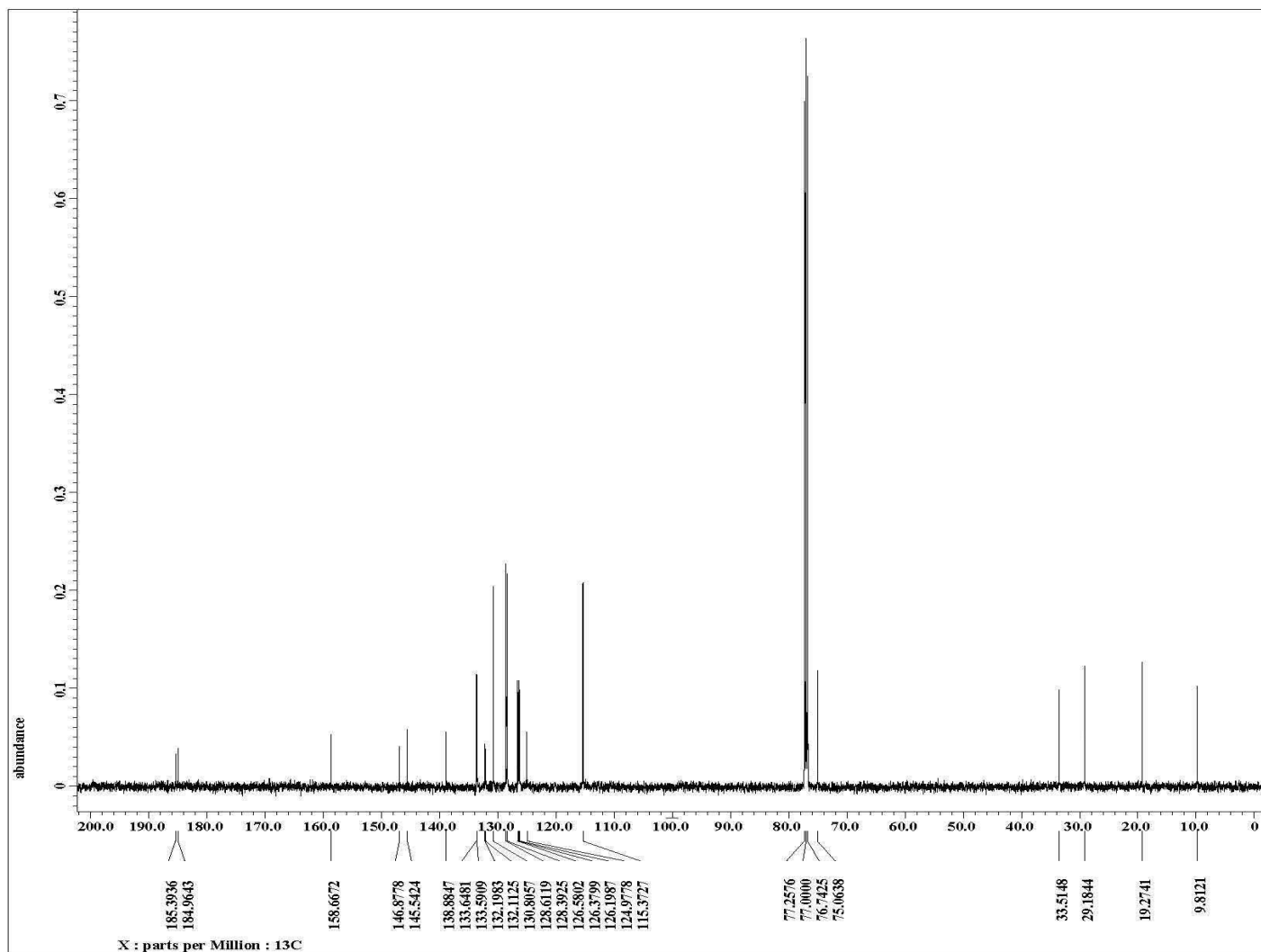




HRMS spectrum of 2-benzyl-3-(4-fluorophenyl)-1,4-naphthoquinone (**3.7**)



<sup>1</sup>H NMR spectrum of 2-benzyl-3-(4-sec-butoxyphenyl)-1,4-naphthoquinone (**3.8**)



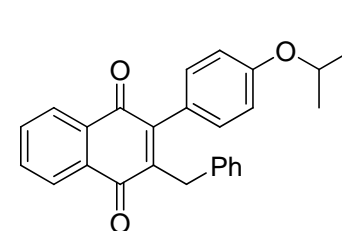
```

Filename      = SNG8SA14_13C-3.jdf
Author       = N.Ahmed
Experiment   = single_pulse_dec
Sample_id    = S#585588
Solvent      = CHLOROFORM-D
Creation time = 18-MAY-2011 20:36:08
Revision time = 2-JUL-2011 16:51:03
Current time  = 2-JUL-2011 16:53:09

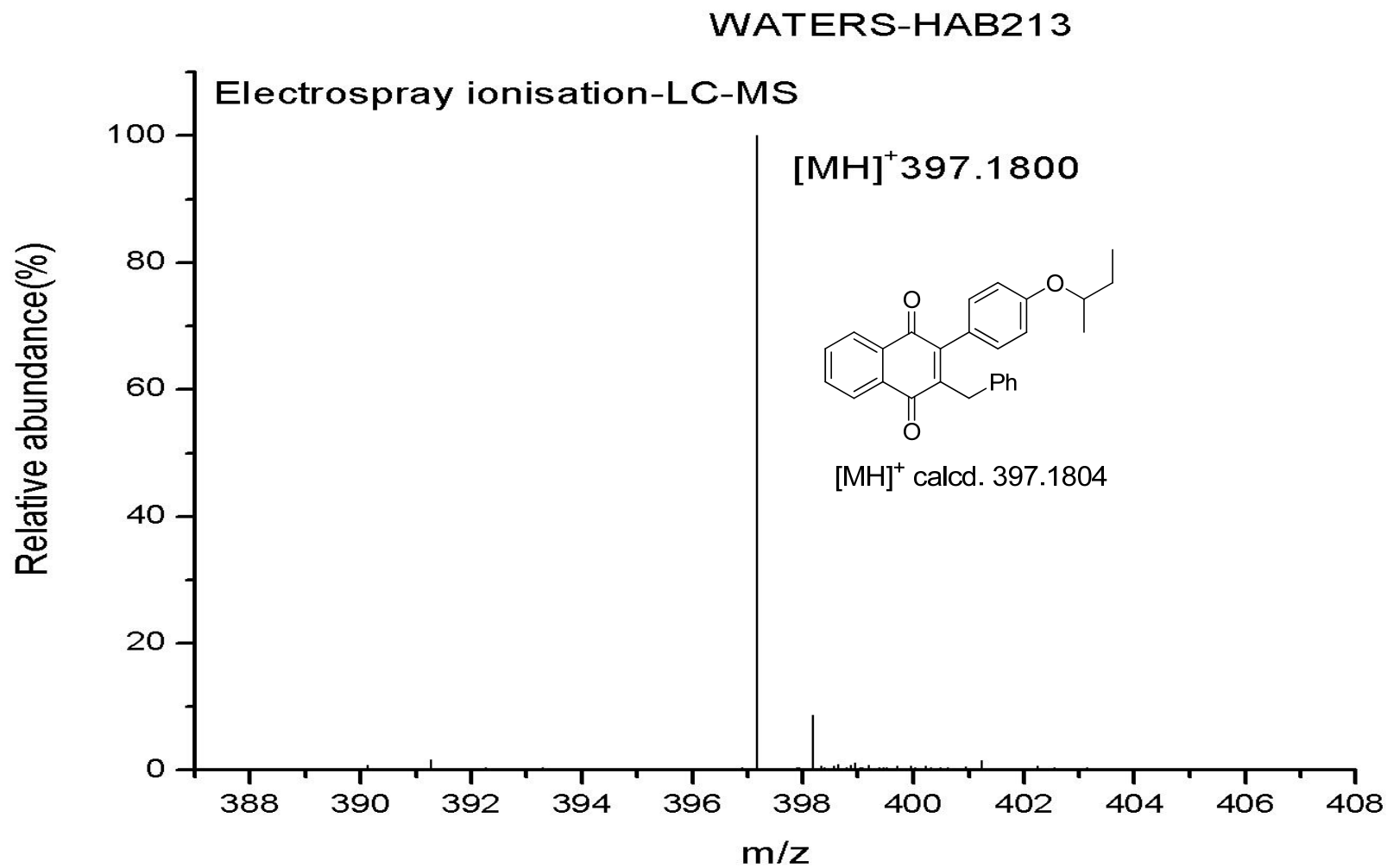
Data format   = 1D COMPLEX
Dim_size      = 26214
Dim_title     = 13C
Dim_units     = [ppm]
Dimensions    = X
Site          = ECX 500
Spectrometer  = DELTA2 NMR

Field strength = 11.7473579 [T] (500 [MH]
X_acq_duration = 0.83361792 [s]
X_domain       = 13C
X_freq         = 125.76529768 [MHz]
X_offset       = 100 [ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.19959034 [Hz]
X_sweep        = 39.3081761 [kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521 [MHz]
Irr_offset     = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 1000
Total_scans    = 1000

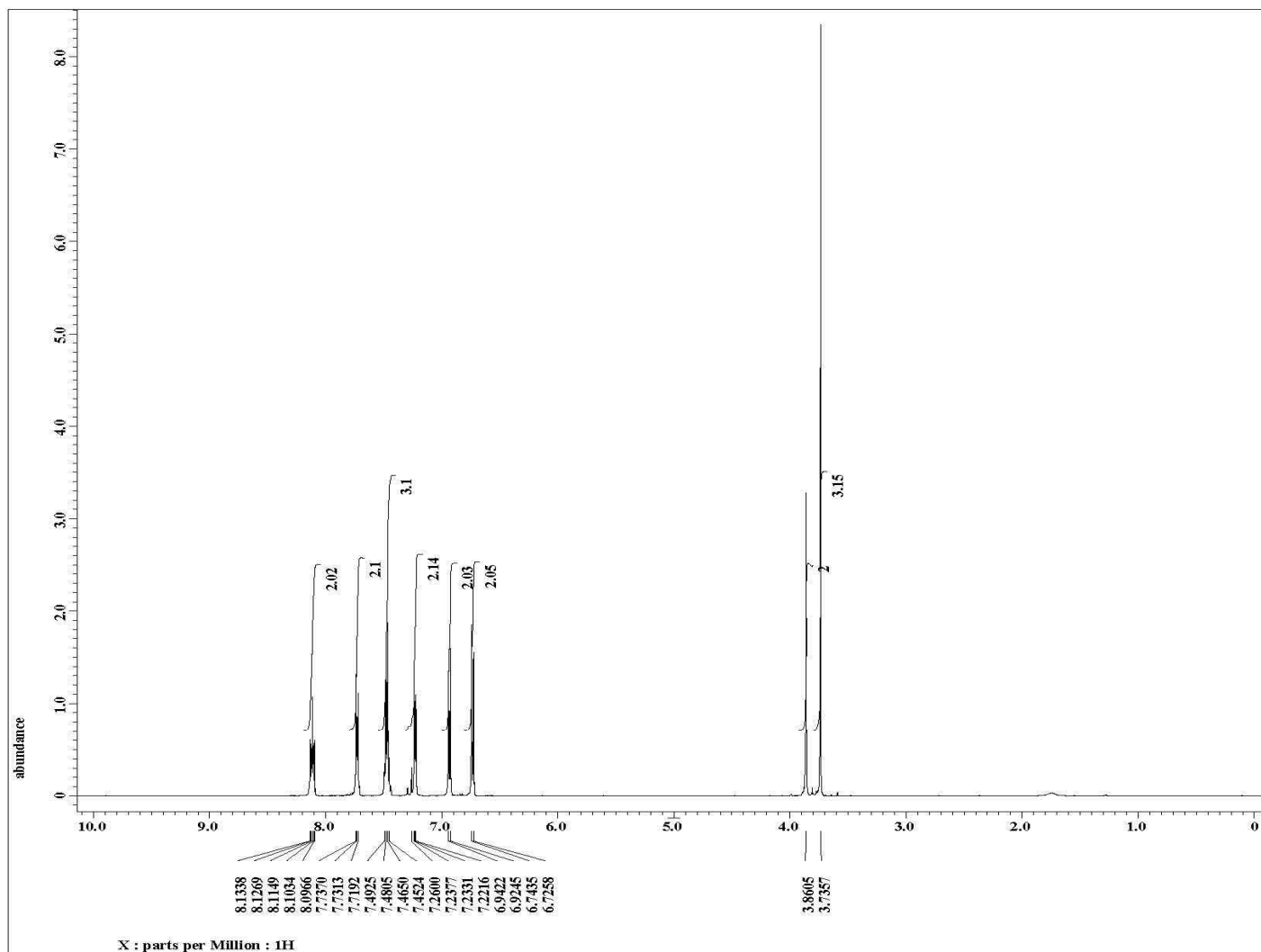
X_90_width     = 9.62 [us]
X_acq_time     = 0.83361792 [s]
X_angle        = 30 [deg]
X_atn          = 7.1 [dB]
X_pulse        = 3.20666667 [us]
Irr_atn_dec    = 19.5 [dB]
Irr_atn_noe    = 21.5 [dB]
Irr_noise      = WALTZ
Decoupling     = TRUE
Initial_wait   = 1 [s]
Noe            = TRUE
Noe_time       = 1 [s]
Recvr_gain     = 60
Relaxation_delay = 1 [s]
Repetition_time = 1.83361792 [s]
Temp_get       = 23.5 [dC]
    
```



$^{13}\text{C}$  NMR spectrum of 2-benzyl-3-(4-sec-butoxyphenyl)-1,4-naphthoquinone (**3.8**)



HRMS spectrum of 2-benzyl-3-(4-sec-butoxyphenyl)-1,4-naphthoquinone (**3.8**)



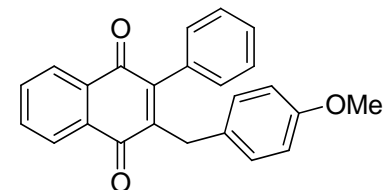
```

Filename      = SNG8SA17_1H-5.jdf
Author       = N.Ahmed
Experiment   = single_pulse.ex2
Sample_id    = S#425126
Solvent      = CHLOROFORM-D
Creation time = 17-MAY-2011 11:11:22
Revision time = 2-JUL-2011 19:23:10
Current Time  = 2-JUL-2011 19:23:37

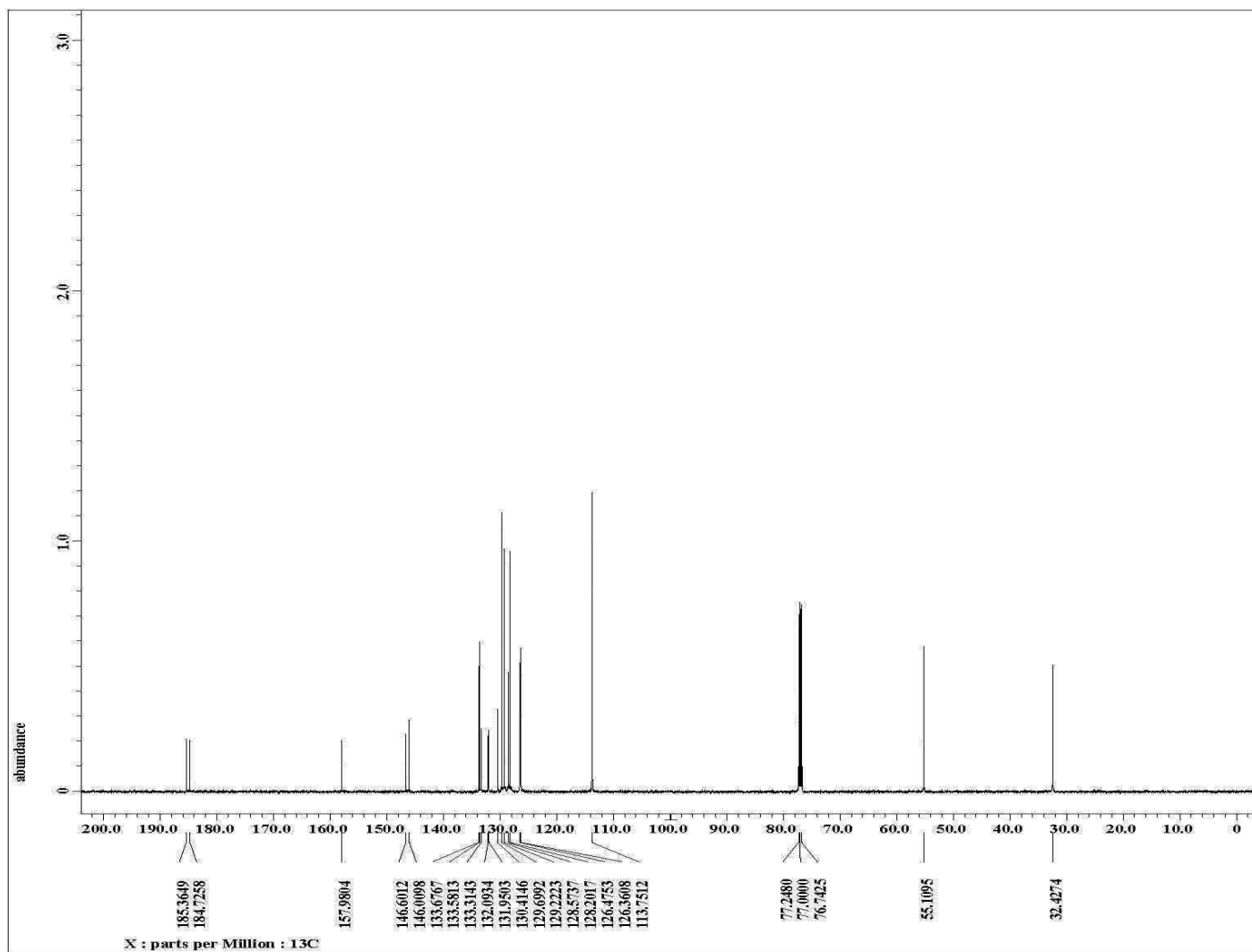
Data format   = 1D COMPLEX
Dim size      = 26214
Dim title     = 1H
Dim units     = [ppm]
Dimensions    = X
Site          = ECX 500
Spectrometer  = DELTA2 NMR

Field strength = 11.7473579 [T] (500 [MH
X_acq_duration = 3.49175808 [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      = 36
Relaxation_delay = 2 [s]
Repetition_time = 5.49175808 [s]
Temp_get        = 22.9 [dC]
    
```



$^1\text{H}$  NMR spectrum of 2-(4-methoxybenzyl)-3-phenyl-1,4-naphthoquinone (**3.9**)



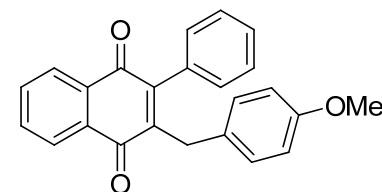
```

Filename      = SNG8SA17_13C-4.jdf
Author       = N. Ahmed
Experiment   = single_pulse_dec
Sample id    = S458524
Solvent      = CHLOROFORM-D
Creation time = 18-MAY-2011 19:23:18
Revision time = 22-AUG-2011 16:16:08
Current time  = 22-AUG-2011 16:17:33

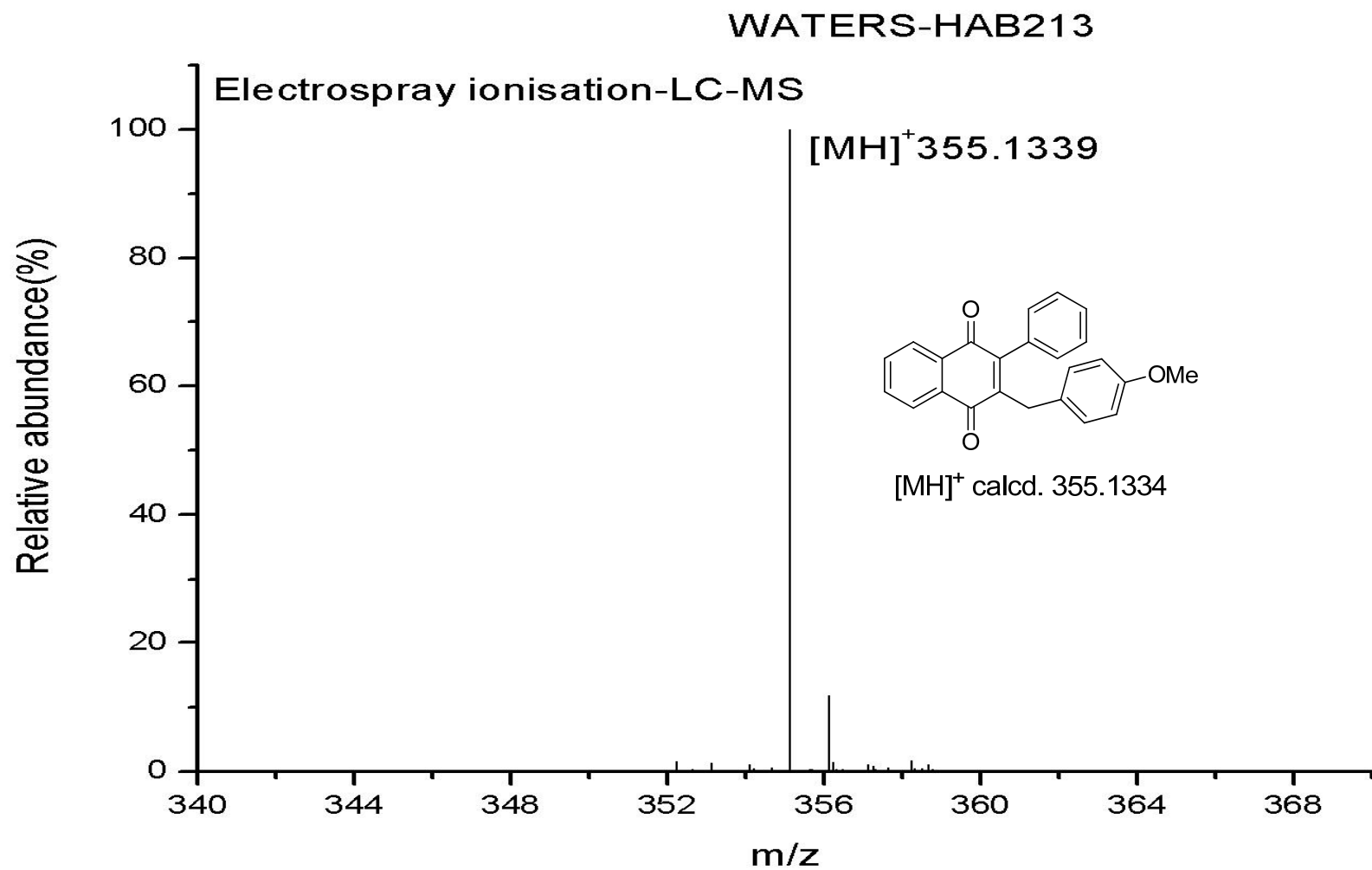
Data format   = 1D COMPLEX
Dim size      = 26214
Dim title     = 13C
Dim units     = [ppm]
Dimensions    = X
Site          = ECU 500
Spectrometer  = DELTA2_NMR

Field strength = 11.7473579 [T] (500 [MH
X_acq_duration = 0.83361792 [s]
X_domain       = 13C
X_freq         = 125.76529768 [MHz]
X_offset       = 100 [ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.19959034 [Hz]
X_sweep        = 39.3081761 [kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521 [MHz]
Irr_offset     = 5.0 [ppm]
Clipped        = FALSE
Mod return     = 1
Scans          = 1000
Total_scans    = 1000

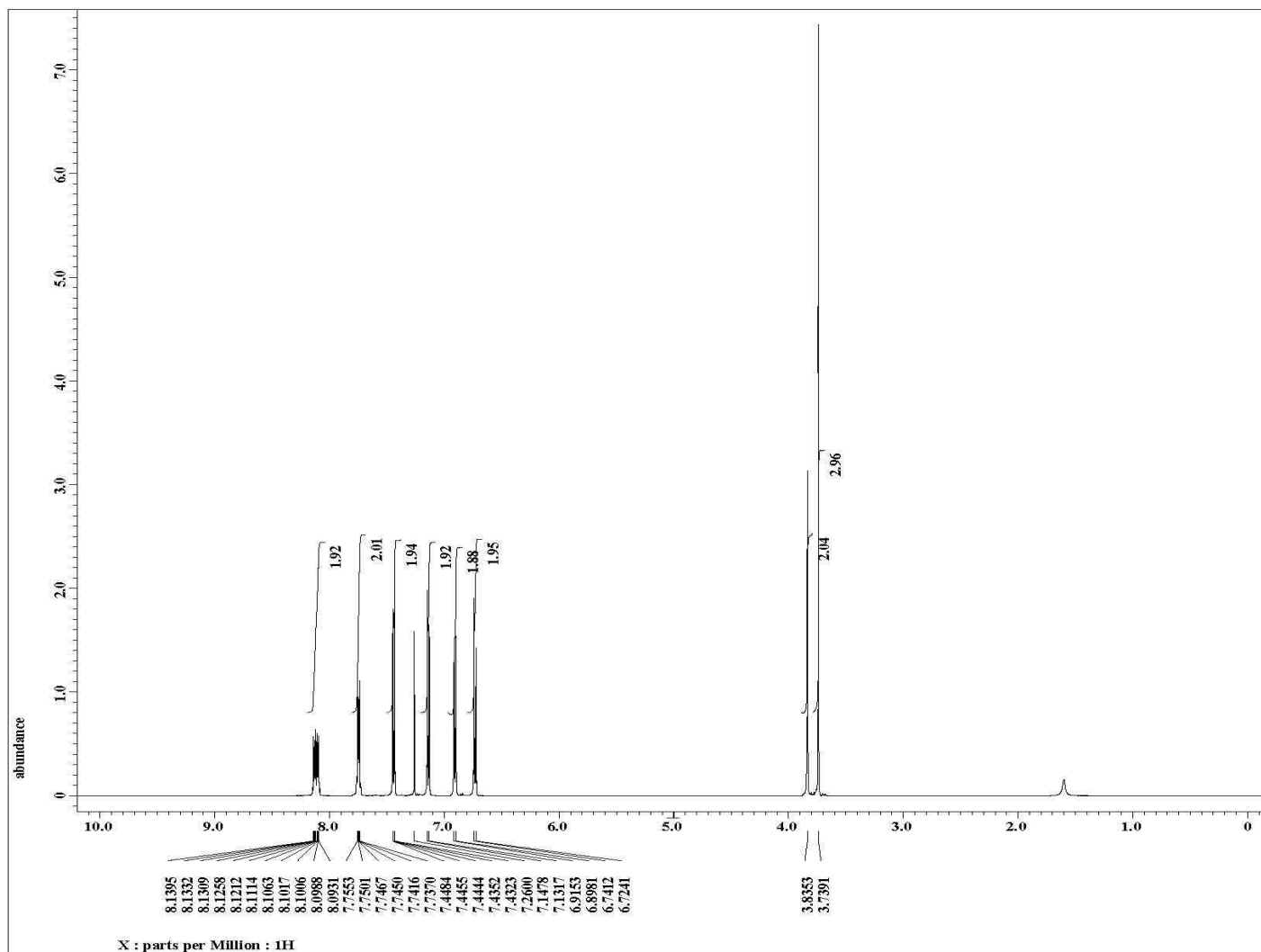
X_90_width     = 9.62 [us]
X_acq_time     = 0.83361792 [s]
X_angle        = 30 [deg]
X_atn          = 7.1 [dB]
X_pulse        = 3.20666667 [us]
Irr_atn_dec    = 19.5 [dB]
Irr_atn_noe    = 21.5 [dB]
Irr_noise      = WALTZ
Decoupling     = TRUE
Initial wait   = 1 [s]
Noe            = TRUE
Noe_time       = 1 [s]
Recvr_gain     = 60
Relaxation_delay = 1 [s]
Repetition_time = 1.83361792 [s]
Temp_get       = 23.9 [dC]
    
```



$^{13}\text{C}$  NMR spectrum of 2-(4-methoxybenzyl)-3-phenyl-1,4-naphthoquinone (**3.9**)



HRMS spectrum of 2-(4-methoxybenzyl)-3-phenyl-1,4-naphthoquinone (**3.9**)

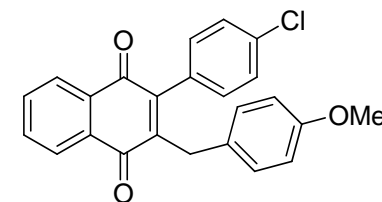


Filename = SNG8SA19\_1H-5.jdf  
Author = N. Ahmed  
Experiment = single\_pulse.ex2  
Sample\_id = S#380447  
Solvent = CHLOROFORM-D  
Creation time = 18-MAY-2011 10:17:34  
Revision time = 2-JUL-2011 19:33:21  
Current time = 2-JUL-2011 19:34:19

Data format = 1D COMPLEX  
Dim size = 26214  
Dim title = 1H  
Dim units = [ppm]  
Dimensions = X  
Site = ECX 500  
Spectrometer = DELTA2 NMR

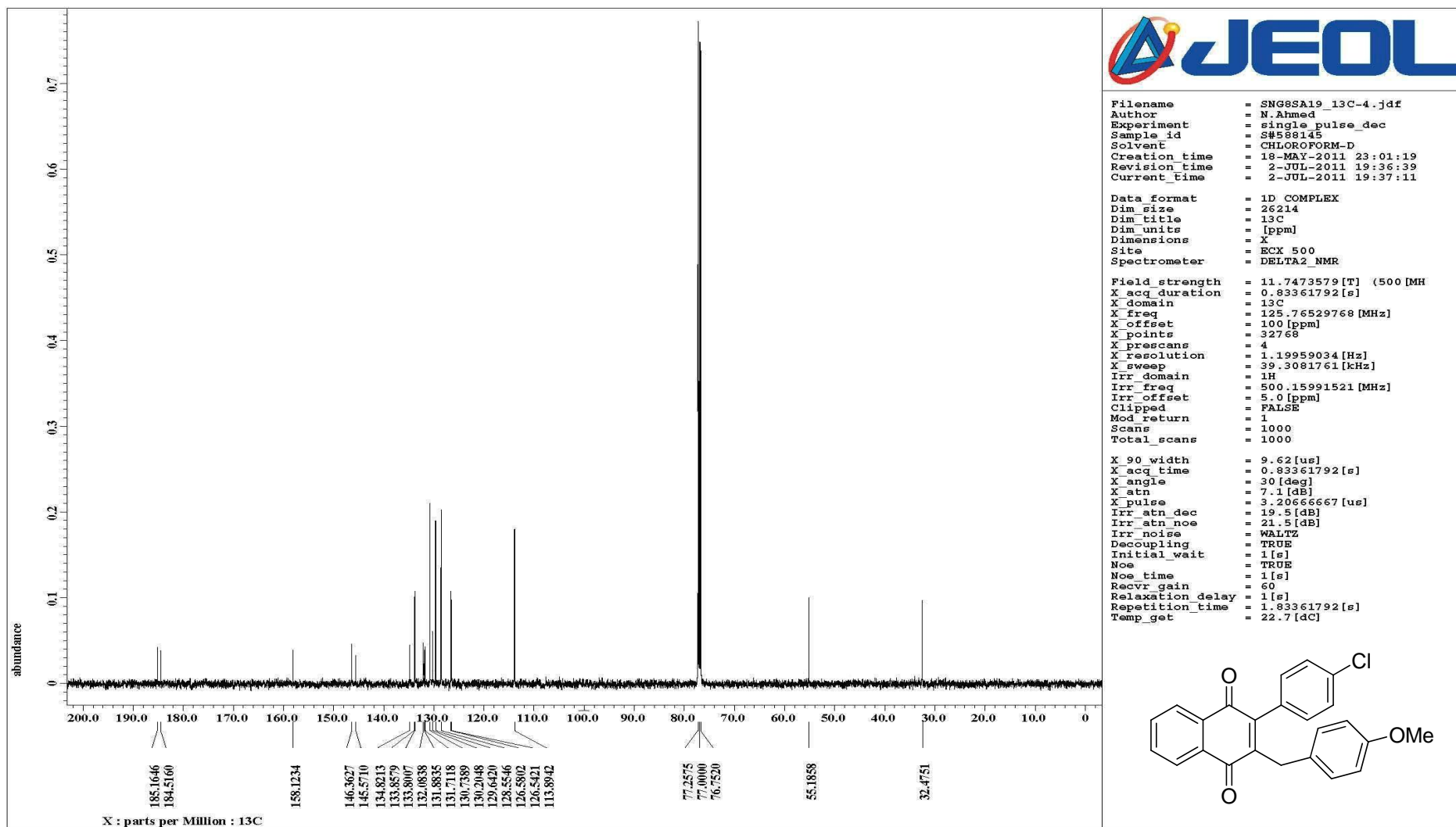
Field strength = 11.7473579 [T] (500 [MH  
X\_acq\_duration = 3.49175808 [s]  
X\_domain = 1H  
X\_freq = 500.15991521 [MHz]  
X\_offset = 5.0 [ppm]  
X\_points = 32768  
X\_prescans = 1  
X\_resolution = 0.28638868 [Hz]  
X\_sweep = 9.38438438 [kHz]  
Irr\_domain = 1H  
Irr\_freq = 500.15991521 [MHz]  
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\_presat = FALSE  
Initial\_wait = 1 [s]  
Recvr\_gain = 50  
Relaxation\_delay = 2 [s]  
Repetition\_time = 5.49175808 [s]  
Temp\_get = 23.1 [dC]

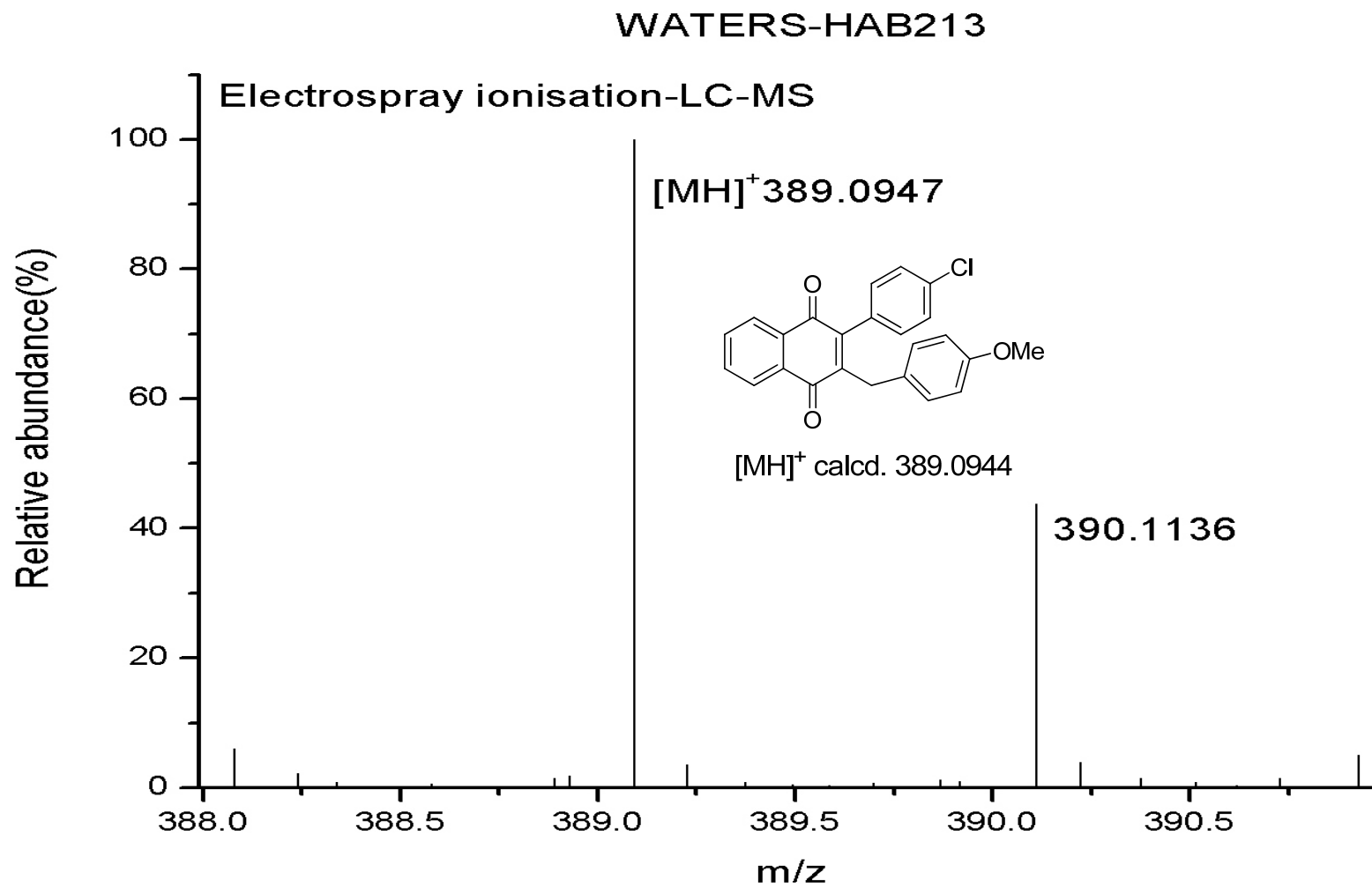


<sup>1</sup>H NMR spectrum of 2-(4-chlorophenyl)-3-(4-methoxybenzyl)-1,4-naphthoquinone (**3.10**)

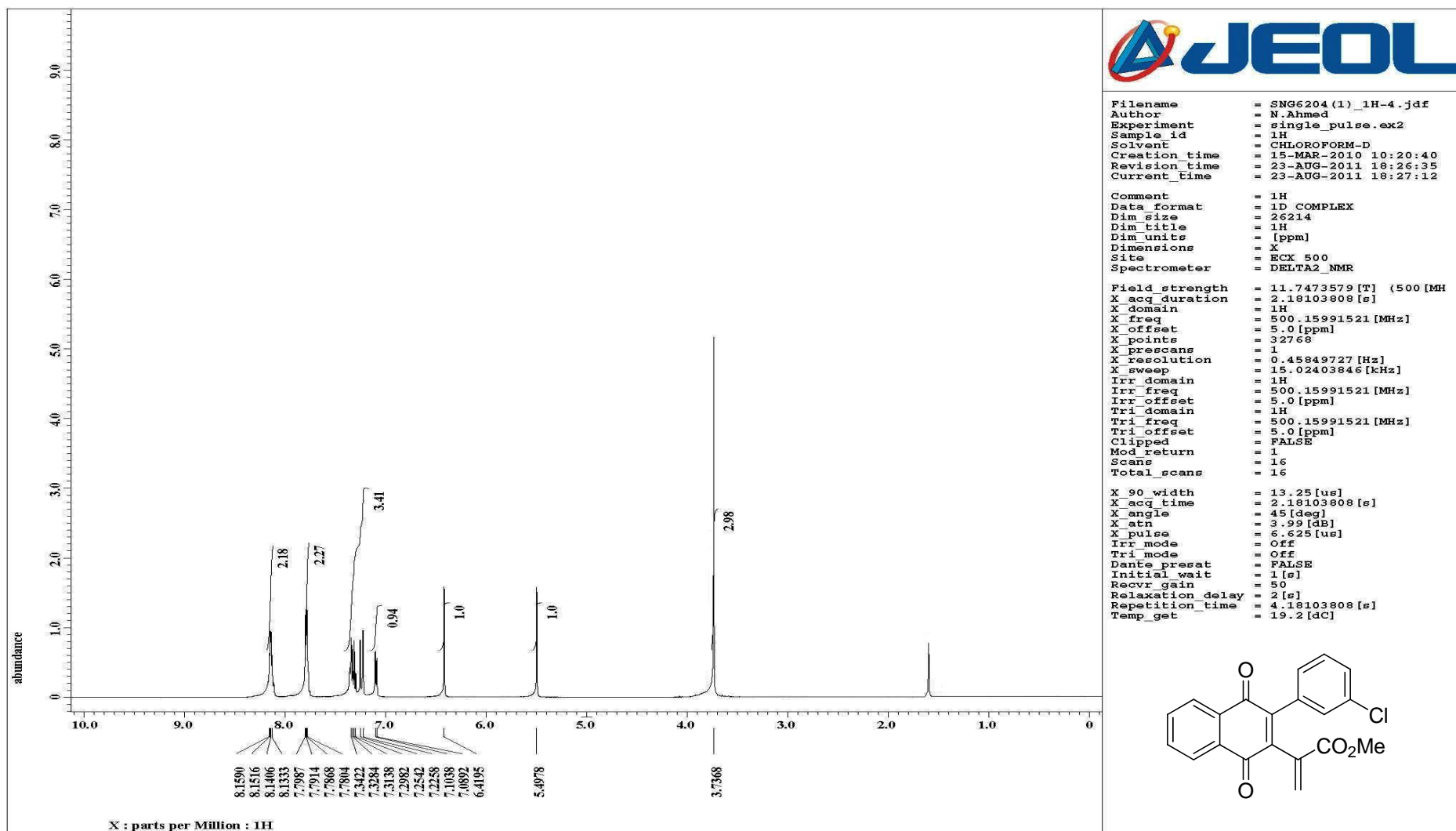




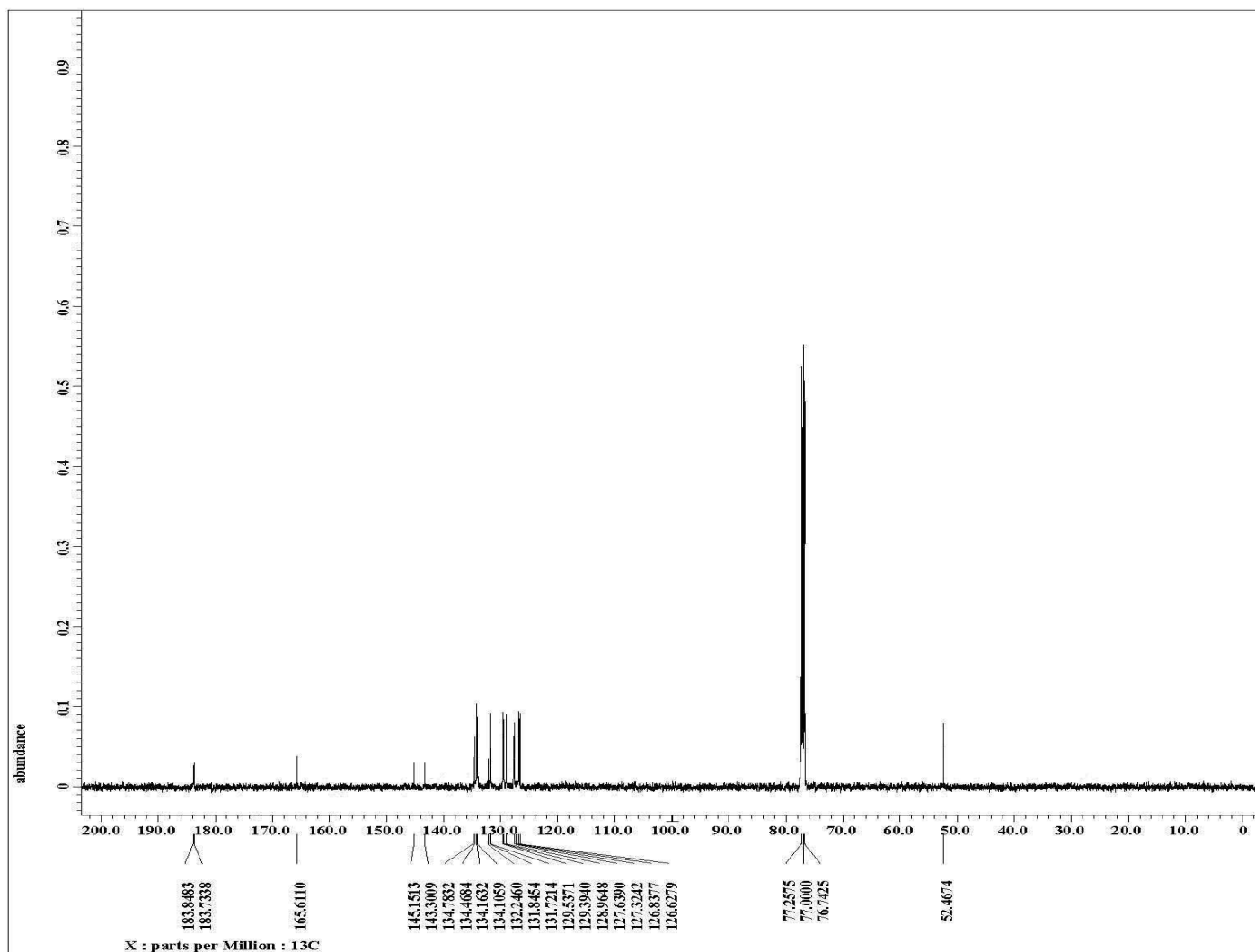
<sup>13</sup>C NMR spectrum of 2-(4-chlorophenyl)-3-(4-methoxybenzyl)-1,4-naphthoquinone (**3.10**)



HRMS spectrum of 2-(4-chlorophenyl)-3-(4-methoxybenzyl)-1,4-naphthoquinone (**3.10**)



<sup>1</sup>H NMR spectrum of methyl 2-(3-(3-chlorophenyl)-1,4-dioxo-1,4-dihydronaphthalen-2-yl)acrylate (**3.11**)



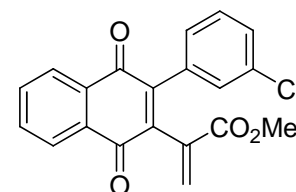
```

Filename      = SNG6204_1H-6.jdf
Author       = N.Ahmed
Experiment   = single_pulse_dec
Sample id    = S4490112
Solvent      = CHLOROFORM-D
Creation time = 15-MAR-2010 13:31:08
Revision time = 23-AUG-2011 18:52:12
Current time  = 23-AUG-2011 18:53:13

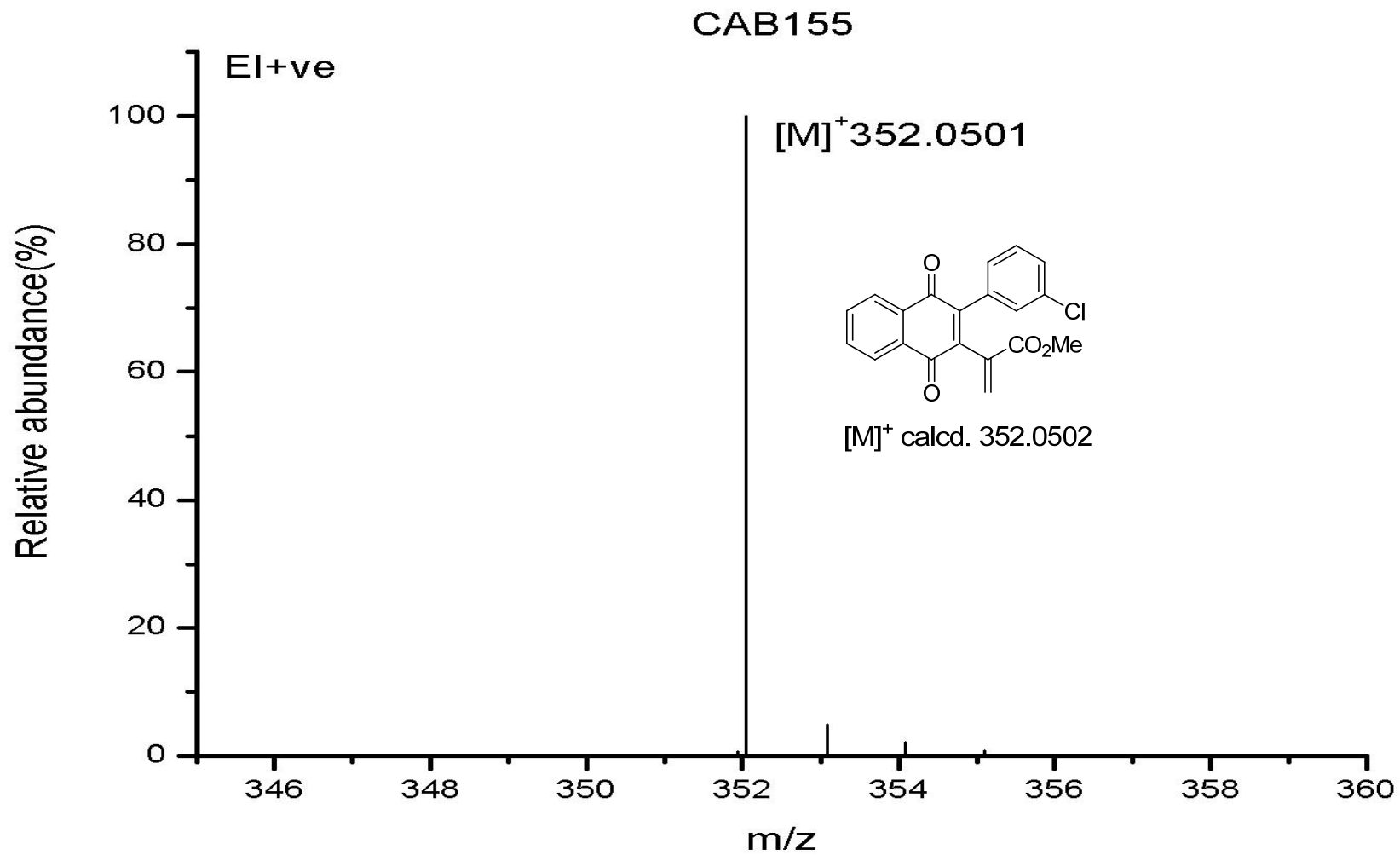
Data format   = 1D COMPLEX
Dim size      = 26214
Dim title     = 13C
Dim units     = [ppm]
Dimensions    = X
Site          = ECU 500
Spectrometer  = DELTA2_NMR

Field strength = 11.7473579 [T] (500 [MH
X_acq_duration = 0.83361792 [s]
X_domain       = 13C
X_freq         = 125.76529768 [MHz]
X_offset       = 100 [ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.19959034 [Hz]
X_sweep        = 39.3081761 [kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521 [MHz]
Irr_offset     = 5.0 [ppm]
Clipped        = FALSE
Mod return     = 1
Scans          = 1000
Total_scans    = 1000

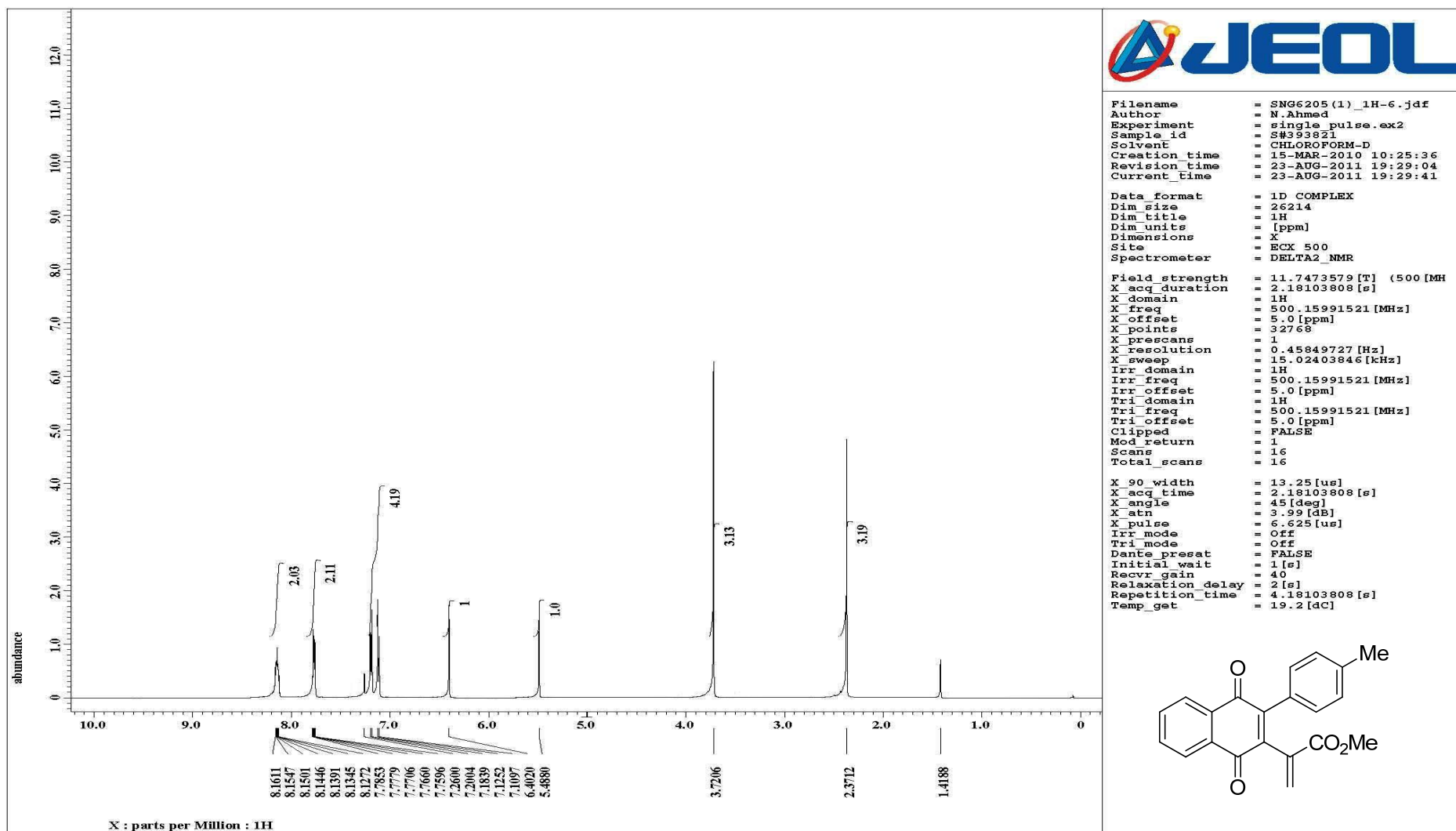
X_90_width     = 9.62 [us]
X_acq_time     = 0.83361792 [s]
X_angle        = 30 [deg]
X_atn          = 7.1 [dB]
X_pulse        = 3.20666667 [us]
Irr_atn_dec    = 19.5 [dB]
Irr_atn_noe    = 21.5 [dB]
Irr_noise      = WALTZ
Decoupling     = TRUE
Initial wait   = 1 [s]
Noe            = TRUE
Noe_time       = 1 [s]
Recvr_gain     = 60
Relaxation_delay = 1 [s]
Repetition_time = 1.83361792 [s]
Temp_get       = 20 [dC]
    
```



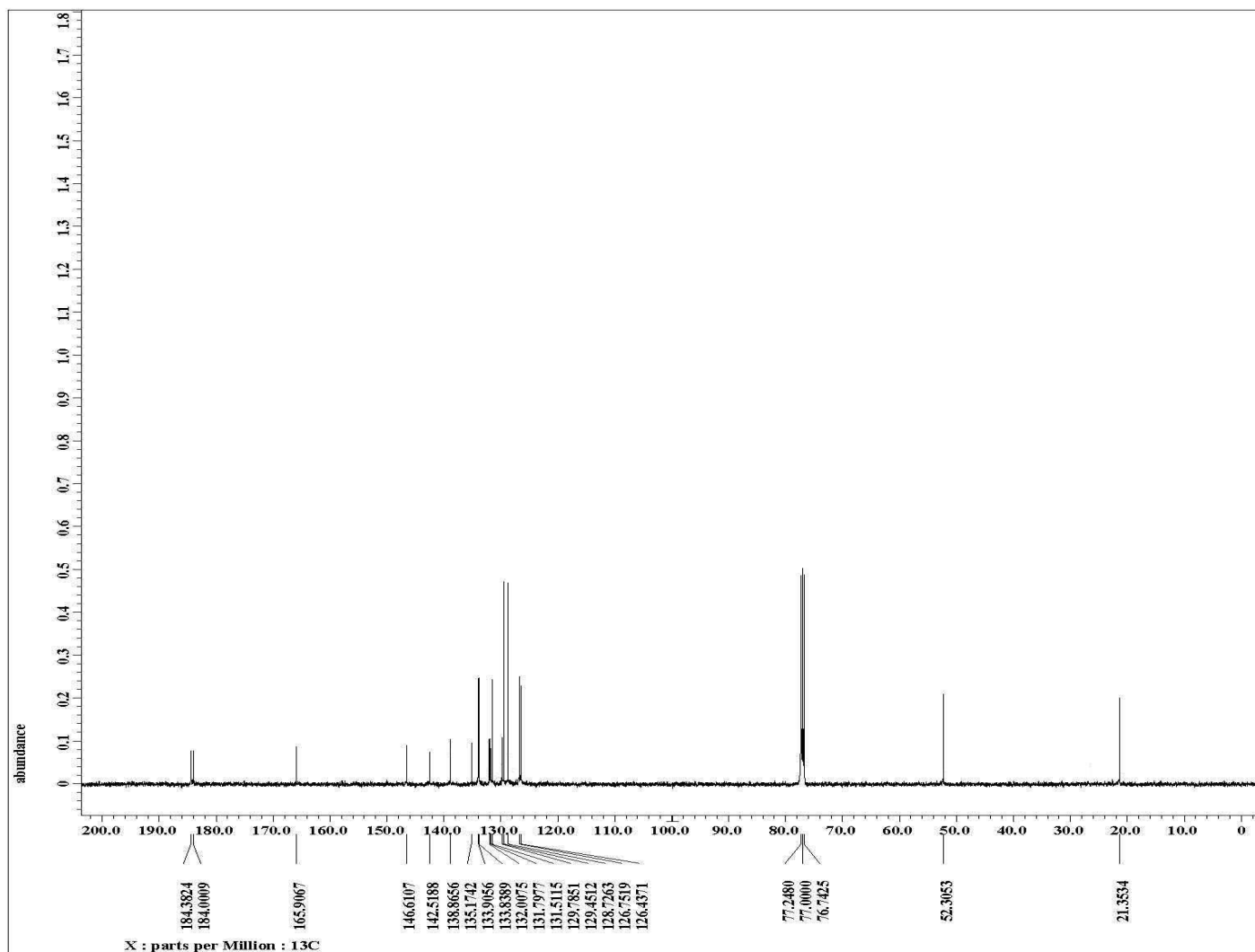
$^{13}\text{C}$  NMR spectrum of methyl 2-(3-(3-chlorophenyl)-1,4-dioxo-1,4-dihydronaphthalen-2-yl)acrylate (**3.11**)



HRMS spectrum of methyl 2-(3-(3-chlorophenyl)-1,4-dioxo-1,4-dihydronaphthalen-2-yl)acrylate (**3.11**)



<sup>1</sup>H NMR spectrum of methyl 2-(1,4-dioxo-3-*p*-tolyl)-1,4-dihydronaphthalen-2-yl)acrylate (**3.12**)



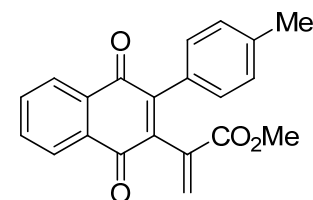
```

Filename      = SNG6205_1H-5.jdf
Author       = N.Ahmed
Experiment    = single_pulse_dec
Sample_id    = S4469482
Solvent      = CHLOROFORM-D
Creation time = 15-MAR-2010 12:56:14
Revision time = 23-AUG-2011 19:42:51
Current time  = 23-AUG-2011 19:43:37

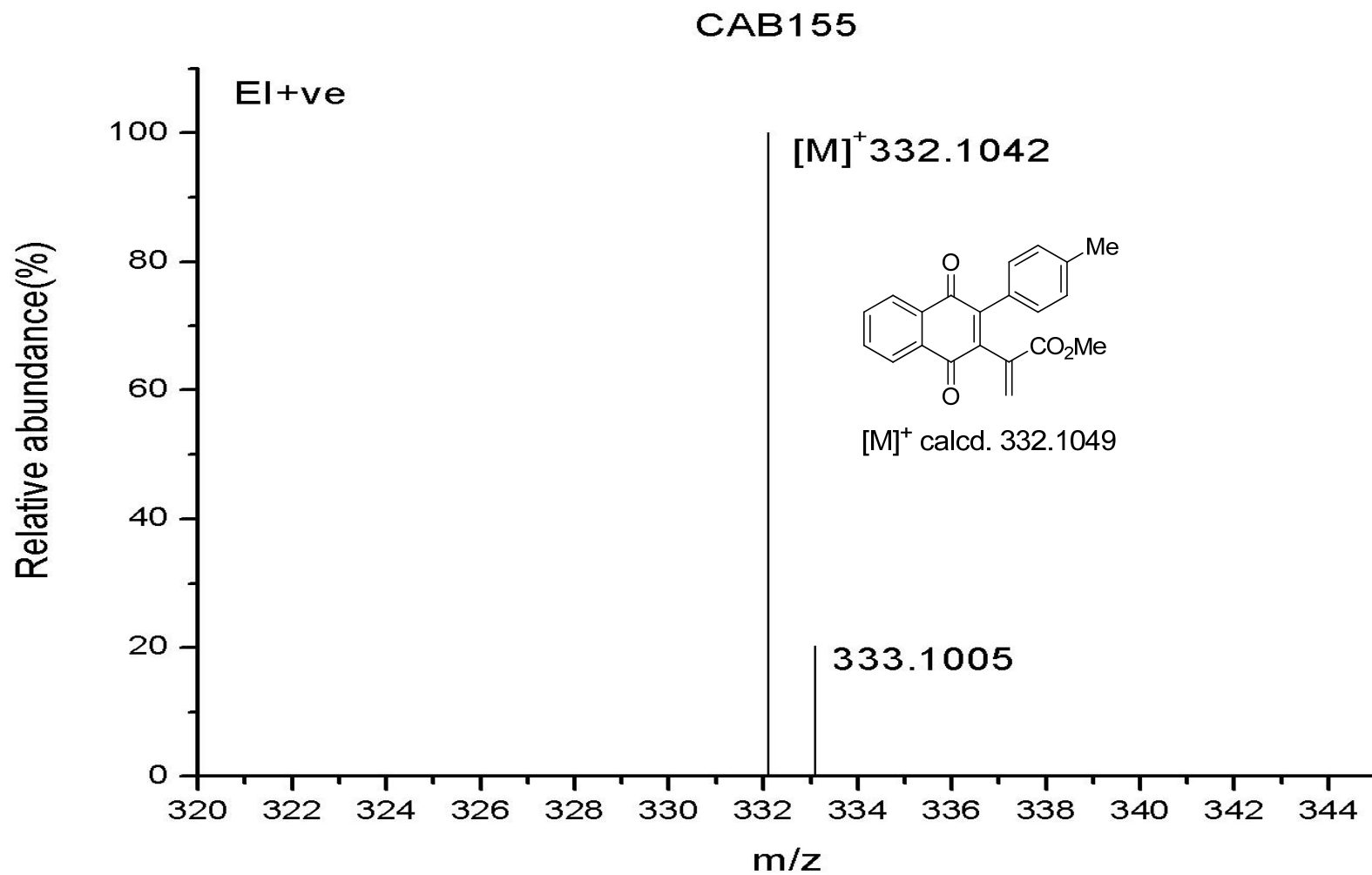
Data format   = 1D COMPLEX
Dim size      = 26214
Dim title     = 13C
Dim units     = [ppm]
Dimensions    = X
Site          = ECU 500
Spectrometer  = DELTA2_NMR

Field strength = 11.7473579 [T] (500 [MH
X_acq_duration = 0.83361792 [s]
X_domain      = 13C
X_freq        = 125.76529768 [MHz]
X_offset      = 100 [ppm]
X_points      = 32768
X_prescans    = 4
X_resolution  = 1.19959034 [Hz]
X_sweep       = 39.3081761 [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    = 0.83361792 [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 = 1.83361792 [s]
Temp_get      = 20 [dC]
    
```

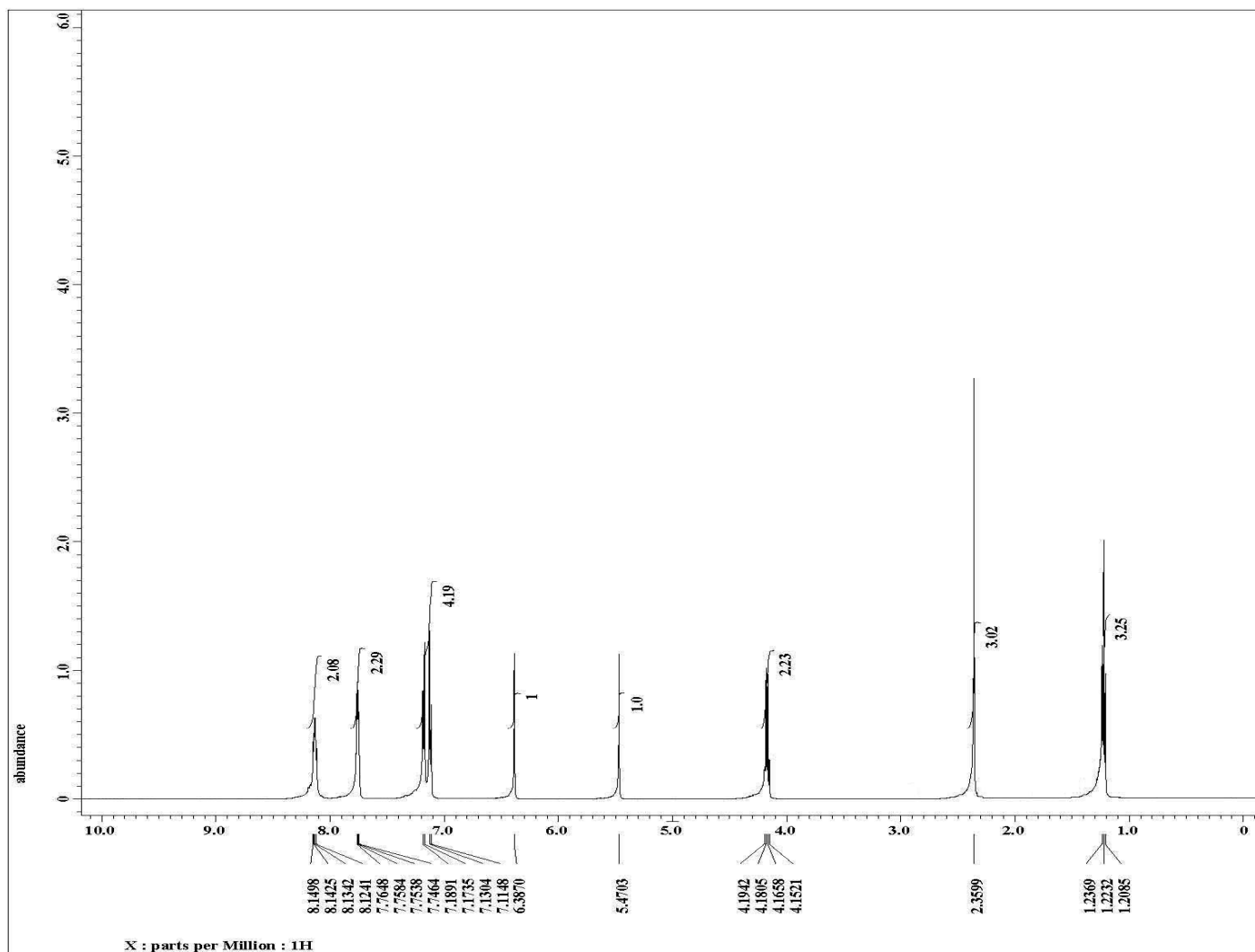


$^{13}\text{C}$  NMR spectrum of methyl 2-(1,4-dioxo-3-*p*-tolyl)-1,4-dihydronaphthalen-2-yl)acrylate (**3.12**)



HRMS spectrum of methyl 2-(1,4-dioxo-3-*p*-tolyl)-1,4-dihydronaphthalen-2-yl)acrylate (**3.12**)





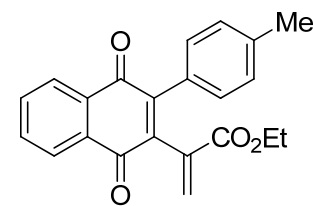
```

Filename      = SNG6201_1H-4.jdf
Author       = N. Ahmed
Experiment   = single_pulse.ex2
Sample id    = S4409258
Solvent      = CHLOROFORM-D
Creation time = 12-MAR-2010 10:55:34
Revision time = 23-AUG-2011 23:03:32
Current time  = 23-AUG-2011 23:04:22

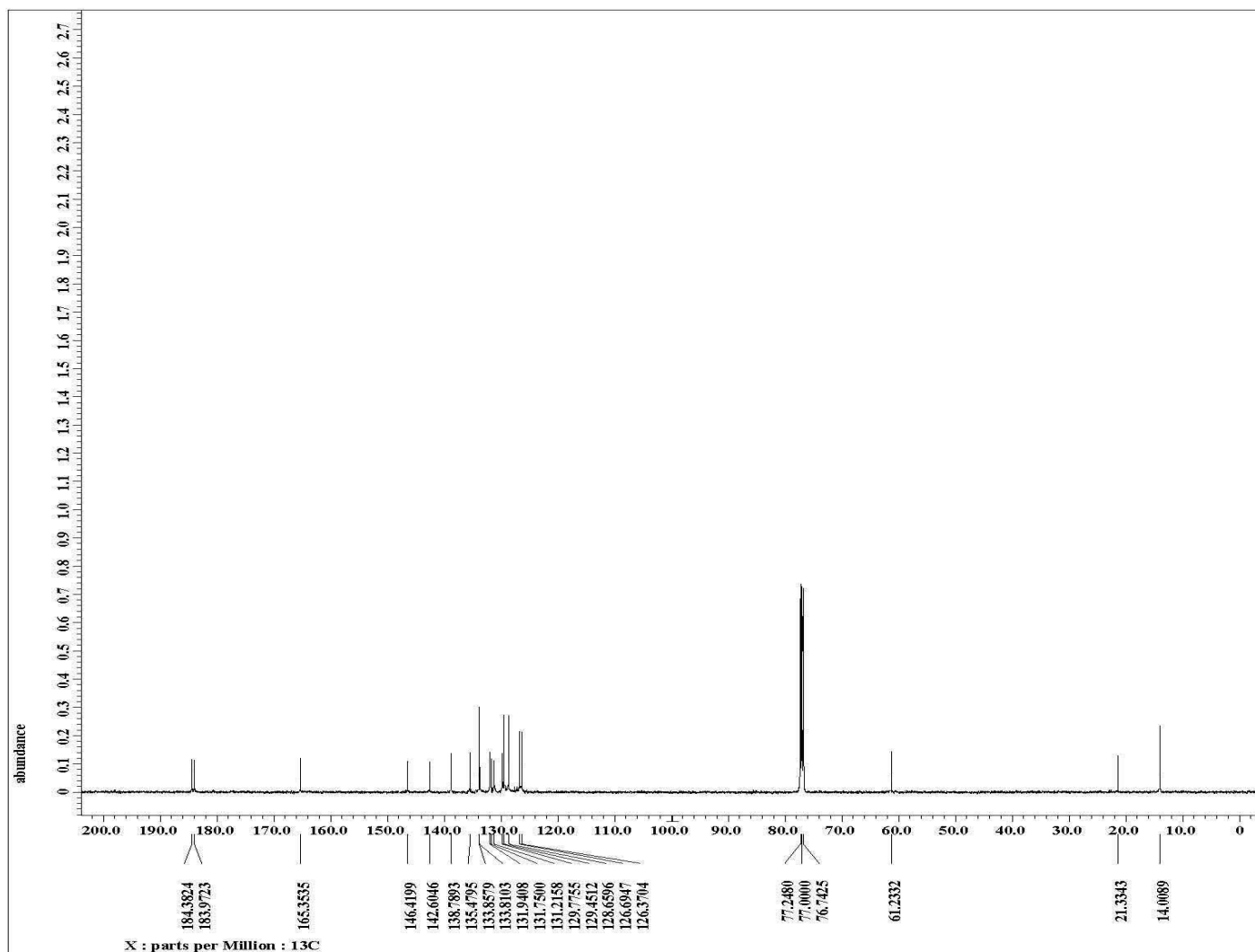
Data format   = 1D COMPLEX
Dim size      = 26214
Dim title     = 1H
Dim units     = [ppm]
Dimensions    = X
Site          = ECU 500
Spectrometer  = DELTA2_NMR

Field strength = 11.7473579 [T] (500 [MH
X_acq_duration = 2.18103808 [s]
X_domain       = 1H
X_freq         = 500.15991521 [MHz]
X_offset       = 5.0 [ppm]
X_points       = 32768
X_prescans     = 1
X_resolution   = 0.45849727 [Hz]
X_sweep        = 15.02403846 [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     = 2.18103808 [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     = 36
Relaxation_delay = 2 [s]
Repetition_time = 4.18103808 [s]
Temp_get       = 19.3 [dC]
    
```



$^1\text{H}$  NMR spectrum of ethyl 2-(1,4-dioxo-3-p-tolyl)-1,4-dihydronaphthalen-2-yl)acrylate (**3.13**)



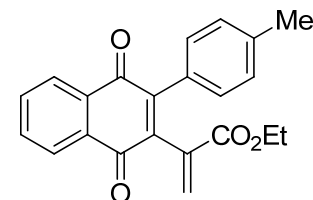
```

Filename      = SNG6201 CARBON-3.jdf
Author       = N.Ahmed
Experiment   = single_pulse_dec
Sample id    = S4308545
Solvent      = CHLOROFORM-D
Creation time = 13-MAR-2010 08:47:20
Revision time = 13-MAR-2010 09:26:58
Current time  = 23-AUG-2011 23:19:26

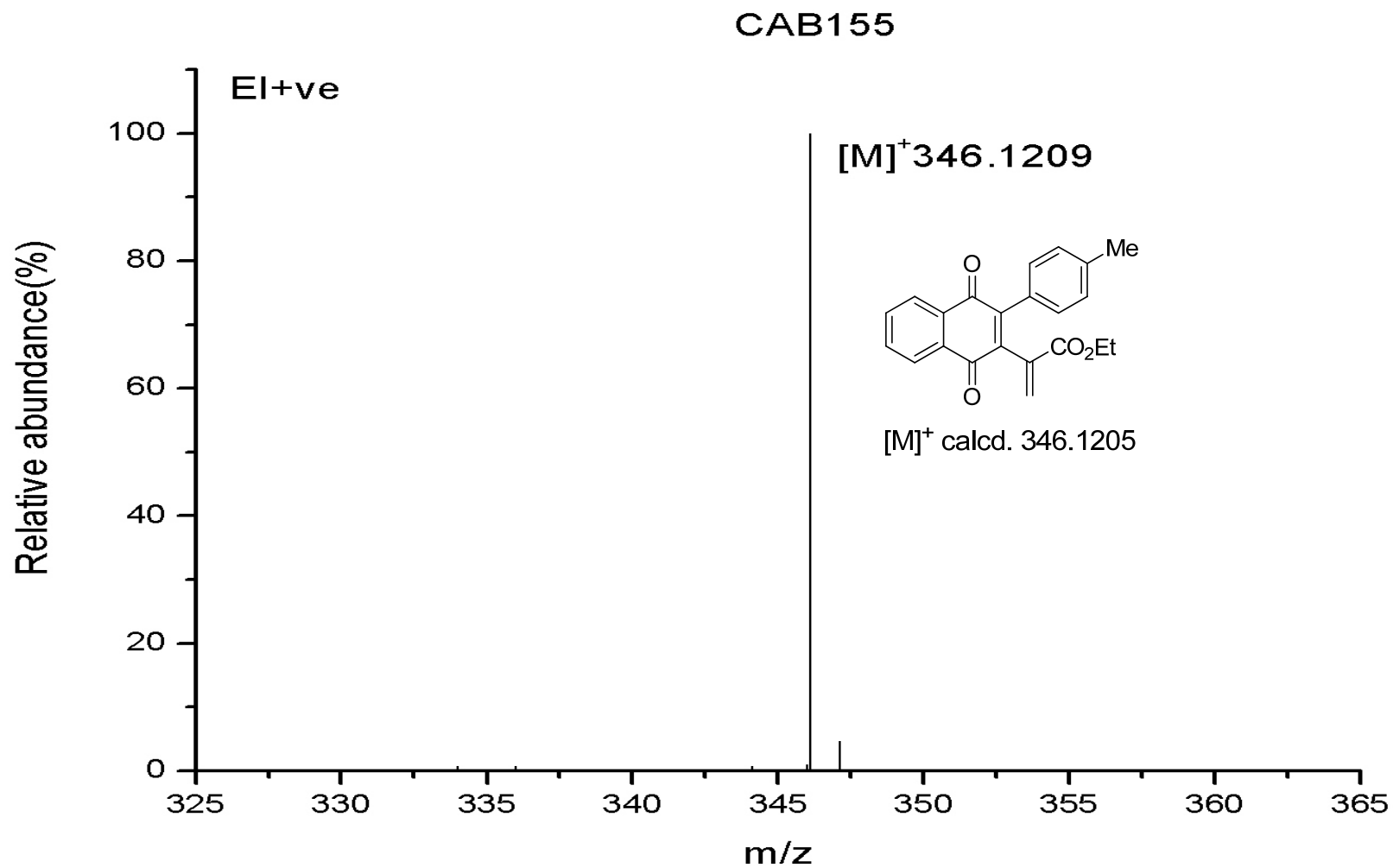
Data format   = 1D COMPLEX
Dim size      = 26214
Dim title     = 13C
Dim units     = [ppm]
Dimensions    = X
Site          = ECU 500
Spectrometer  = DELTA2_NMR

Field strength = 11.7473579 [T] (500 [MH
X_acq_duration = 0.83361792 [s]
X_domain       = 13C
X_freq         = 125.76529768 [MHz]
X_offset       = 100 [ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.19959034 [Hz]
X_sweep        = 39.3081761 [kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521 [MHz]
Irr_offset     = 5.0 [ppm]
Clipped        = FALSE
Mod return     = 1
Scans          = 1024
Total_scans    = 1024

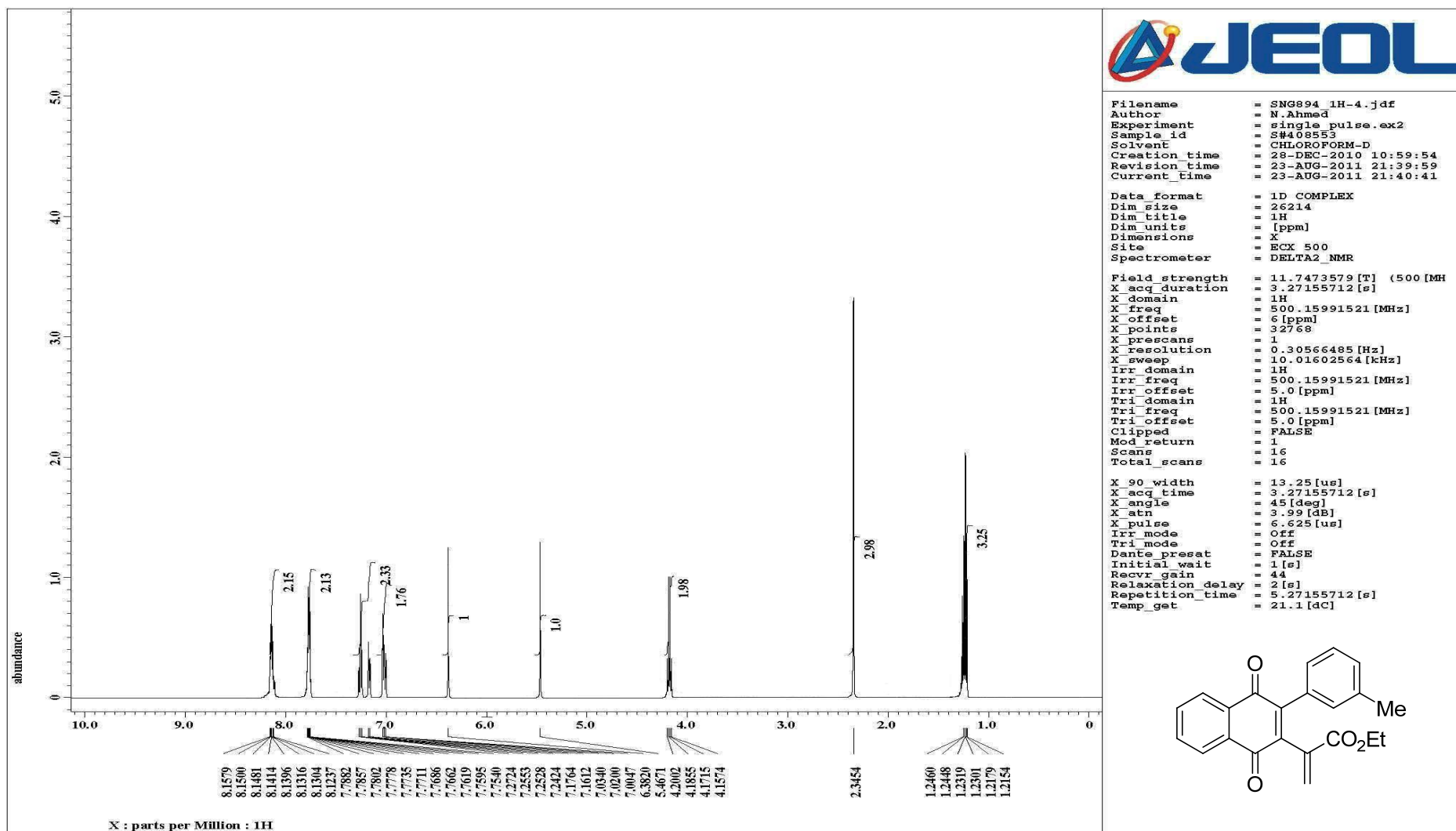
X_90_width     = 9.62 [us]
X_acq_time     = 0.83361792 [s]
X_angle        = 30 [deg]
X_atn          = 7.1 [dB]
X_pulse        = 3.20666667 [us]
Irr_atn_dec    = 21.5 [dB]
Irr_atn_noe    = 21.5 [dB]
Irr_noise      = WALTZ
Decoupling     = TRUE
Initial wait   = 1 [s]
Noe            = TRUE
Noe_time       = 2 [s]
Recvr_gain     = 60
Relaxation_delay = 2 [s]
Repetition_time = 2.83361792 [s]
Temp_get       = 15.4 [dC]
    
```



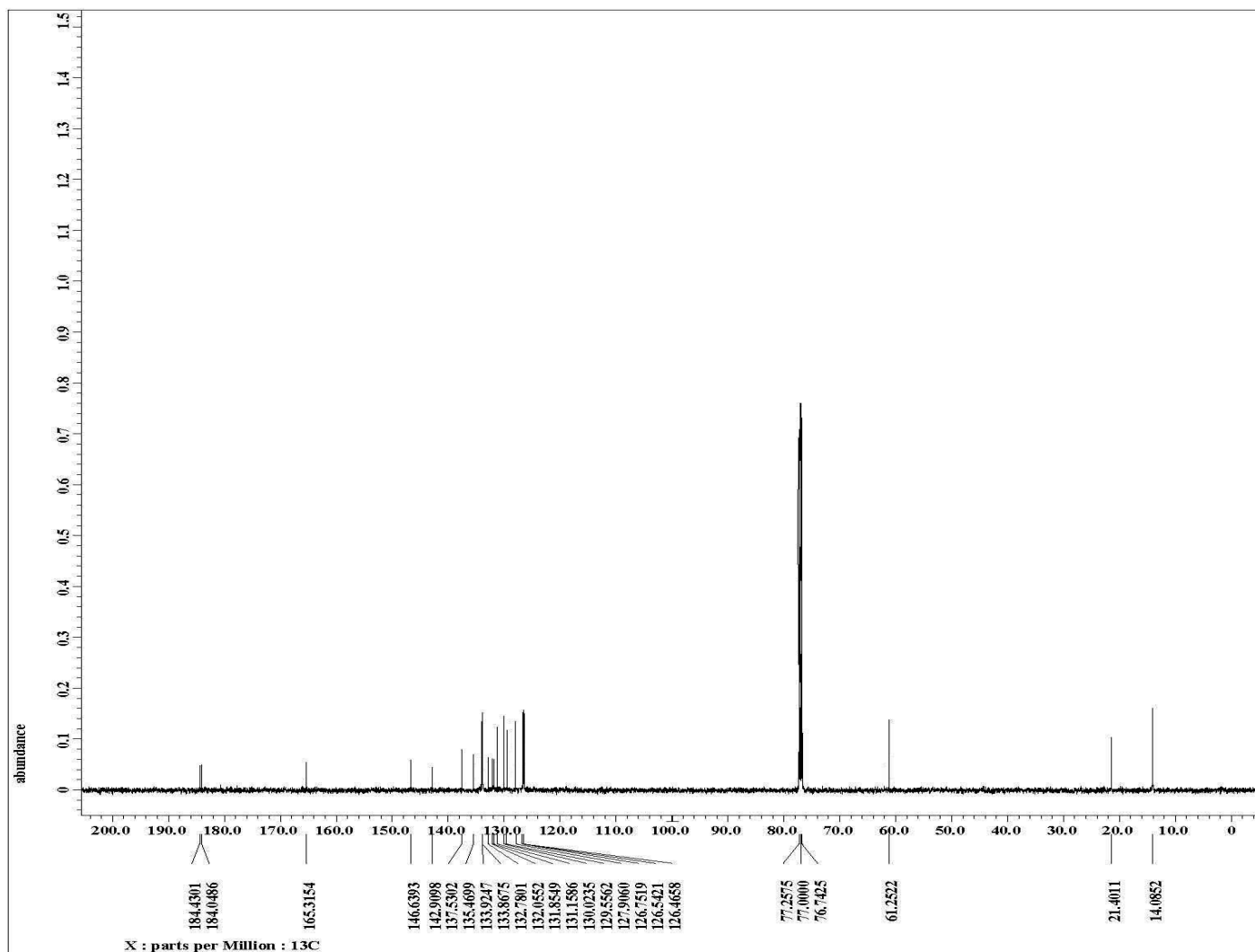
$^{13}\text{C}$  NMR spectrum of ethyl 2-(1,4-dioxo-3-p-tolyl)-1,4-dihydronaphthalen-2-yl)acrylate (**3.13**)



HRMS spectrum of ethyl 2-(1,4-dioxo-3-*p*-tolyl)-1,4-dihydronaphthalen-2-yl)acrylate (**3.13**)



<sup>1</sup>H NMR spectrum of ethyl 2-(1,4-dioxo-3-*m*-tolyl-1,4-dihydronaphthalen-2-yl)acrylate (**3.14**)



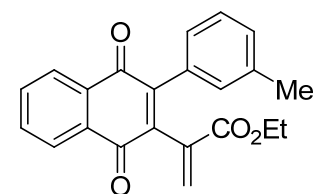
```

Filename      = SNG894_13C-4.jdf
Author       = N.Ahmed
Experiment   = single_pulse_dec
Sample id    = SM492010
Solvent      = CHLOROFORM-D
Creation time = 28-DEC-2010 14:32:09
Revision time = 23-AUG-2011 22:35:45
Current time  = 23-AUG-2011 22:36:45

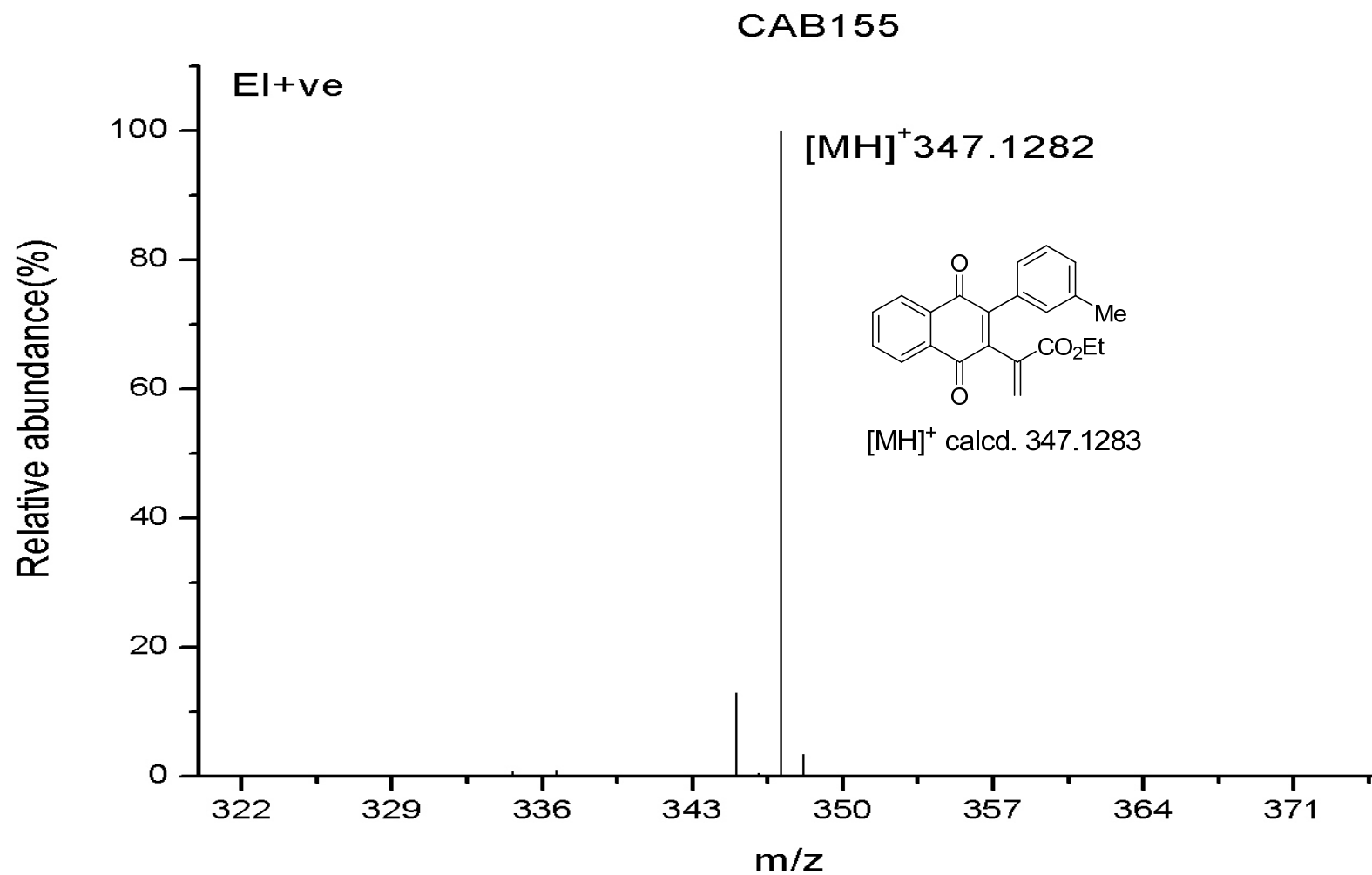
Data format   = 1D COMPLEX
Dim size      = 26214
Dim title     = 13C
Dim units     = [ppm]
Dimensions    = X
Site          = ECK 500
Spectrometer  = DELTA2_NMR

Field strength = 11.7473579 [T] (500 [MH
X_acq_duration = 0.83361792 [s]
X_domain       = 13C
X_freq         = 125.76529768 [MHz]
X_offset       = 100 [ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.19959034 [Hz]
X_sweep        = 39.3081761 [kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521 [MHz]
Irr_offset     = 5.0 [ppm]
Clipped        = FALSE
Mod return     = 1
Scans          = 1000
Total_scans    = 1000

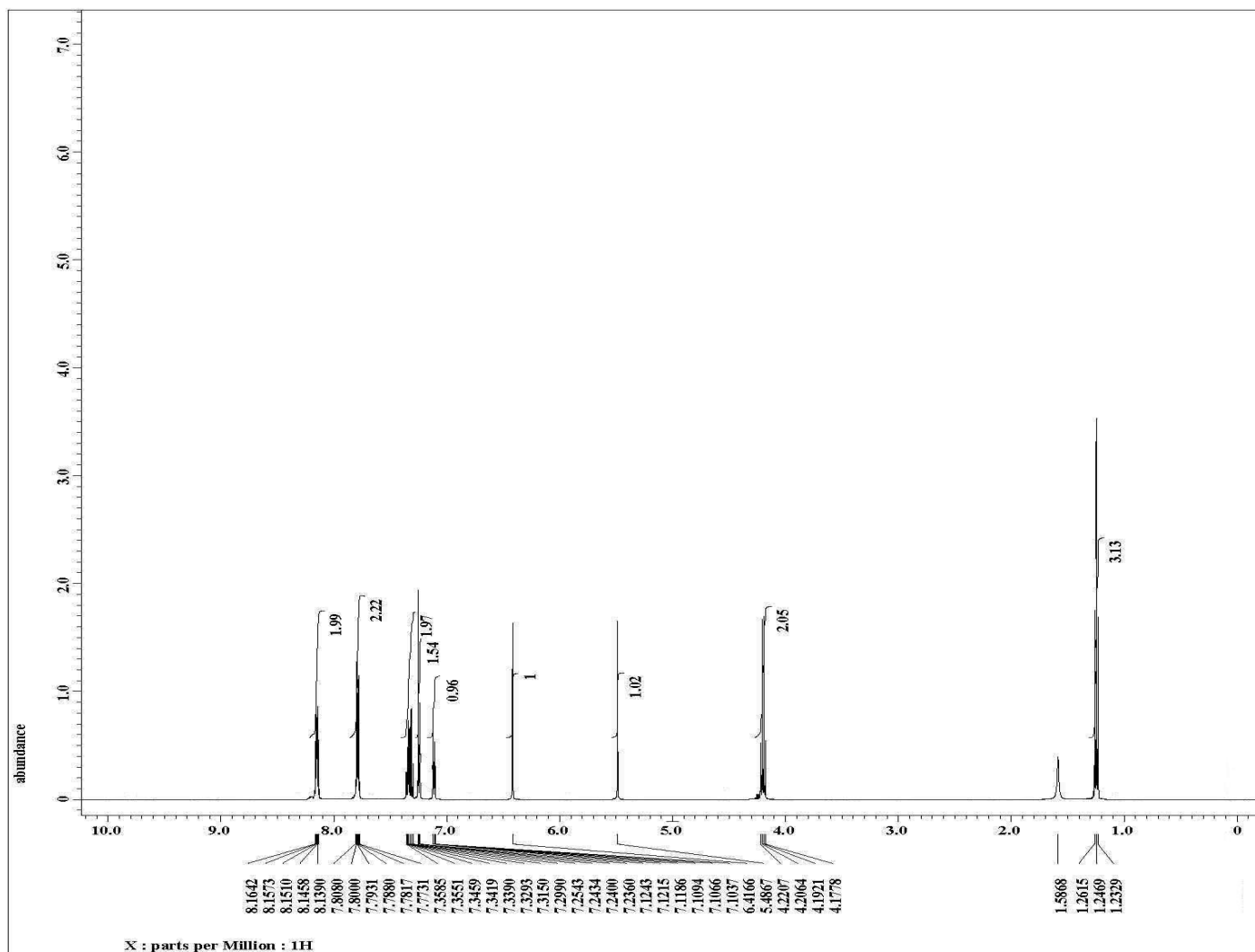
X_90_width     = 9.62 [us]
X_acq_time     = 0.83361792 [s]
X_angle        = 30 [deg]
X_atn          = 7.1 [dB]
X_pulse        = 3.20666667 [us]
Irr_atn_dec    = 19.5 [dB]
Irr_atn_noe    = 21.5 [dB]
Irr_noise      = WALTZ
Decoupling     = TRUE
Initial wait   = 1 [s]
Noe            = TRUE
Noe_time       = 1 [s]
Recvr_gain     = 60
Relaxation_delay = 1 [s]
Repetition_time = 1.83361792 [s]
Temp_get       = 23.9 [dC]
    
```



$^{13}\text{C}$  NMR spectrum of ethyl 2-(1,4-dioxo-3-*m*-tolyl-1,4-dihydronaphthalen-2-yl)acrylate (**3.14**)



HRMS spectra of ethyl 2-(1,4-dioxo-3-*m*-tolyl-1,4-dihydronaphthalen-2-yl)acrylate (**3.14**)



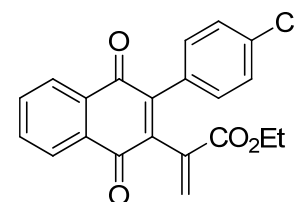
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Filename      = SNG8SA8_1H-4.jdf
Author       = N. Ahmed
Experiment   = single_pulse.ex2
Sample id    = SM423494
Solvent      = CHLOROFORM-D
Creation time = 17-MAR-2011 11:23:41
Revision time = 24-AUG-2011 10:11:16
Current time  = 24-AUG-2011 10:12:18

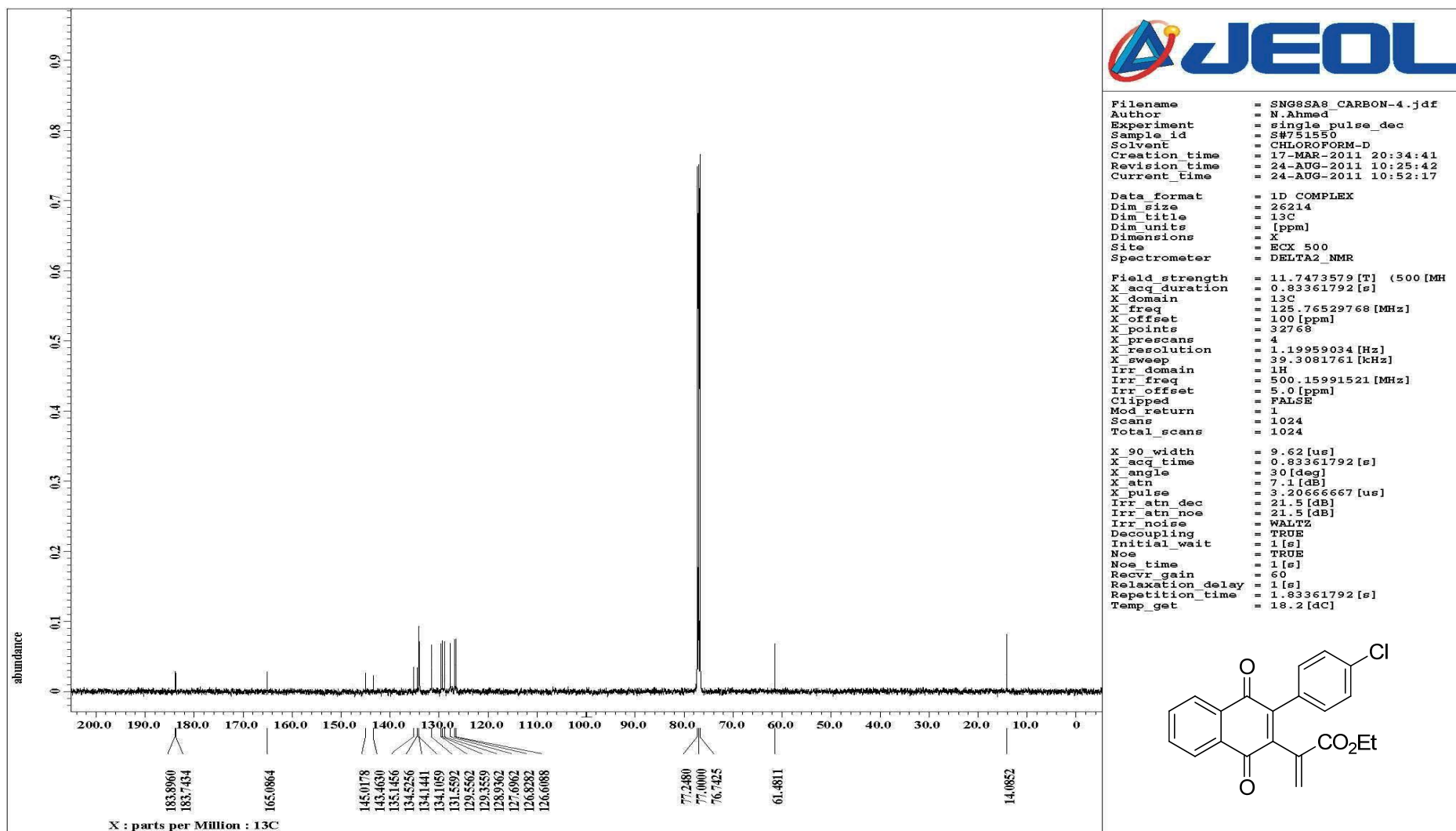
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Dim title     = 1H
Dim units     = [ppm]
Dimensions    = X
Site          = ECU 500
Spectrometer  = DELTA2_NMR

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     = 48
Relaxation_delay = 2 [s]
Repetition_time = 5.49175808 [s]
Temp_get       = 19.2 [dC]
    
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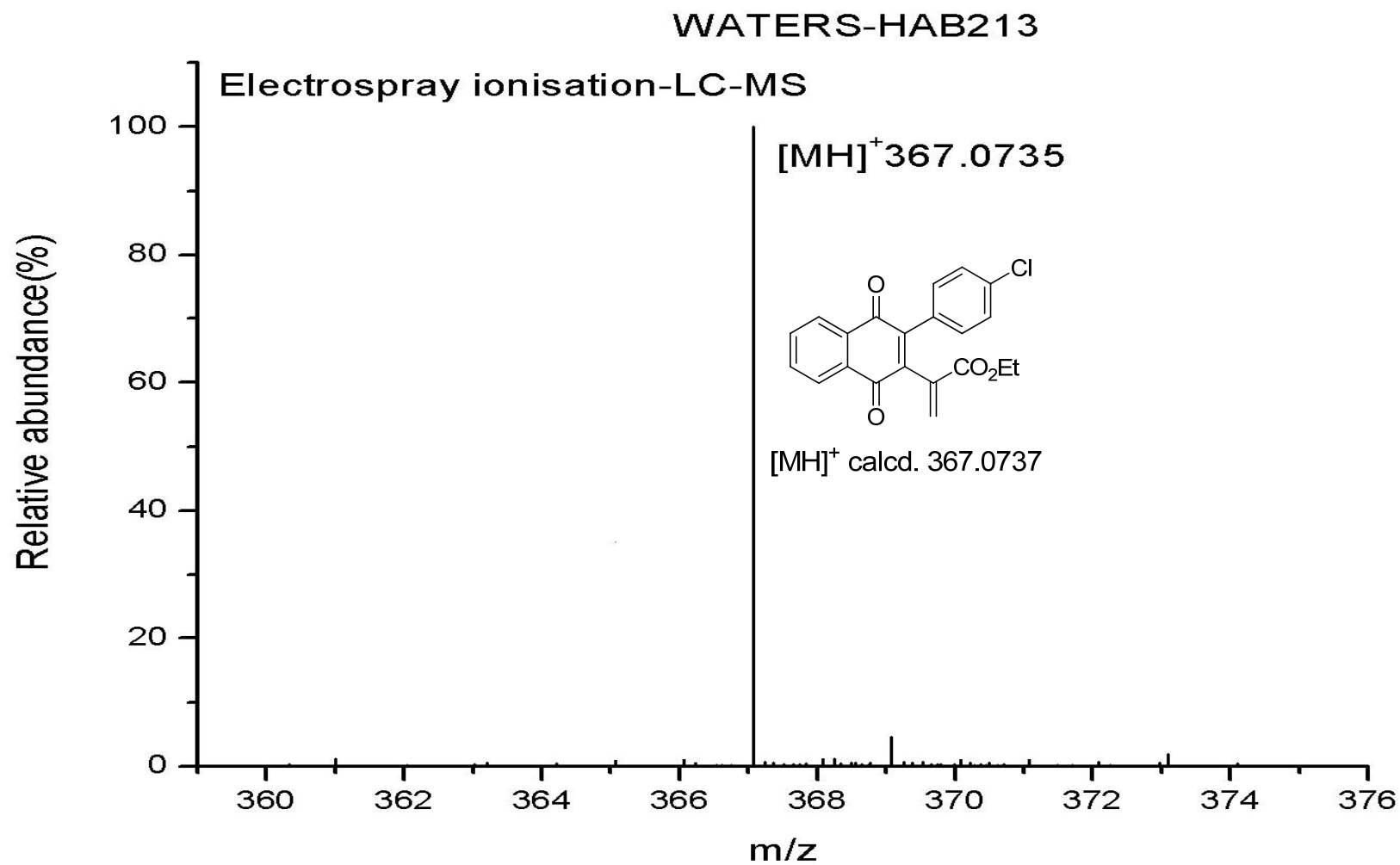


<sup>1</sup>H NMR spectrum of ethyl 2-(3-(4-chlorophenyl)-1,4-dioxo-1,4-dihydronaphthalen-2-yl)acrylate (3.15)

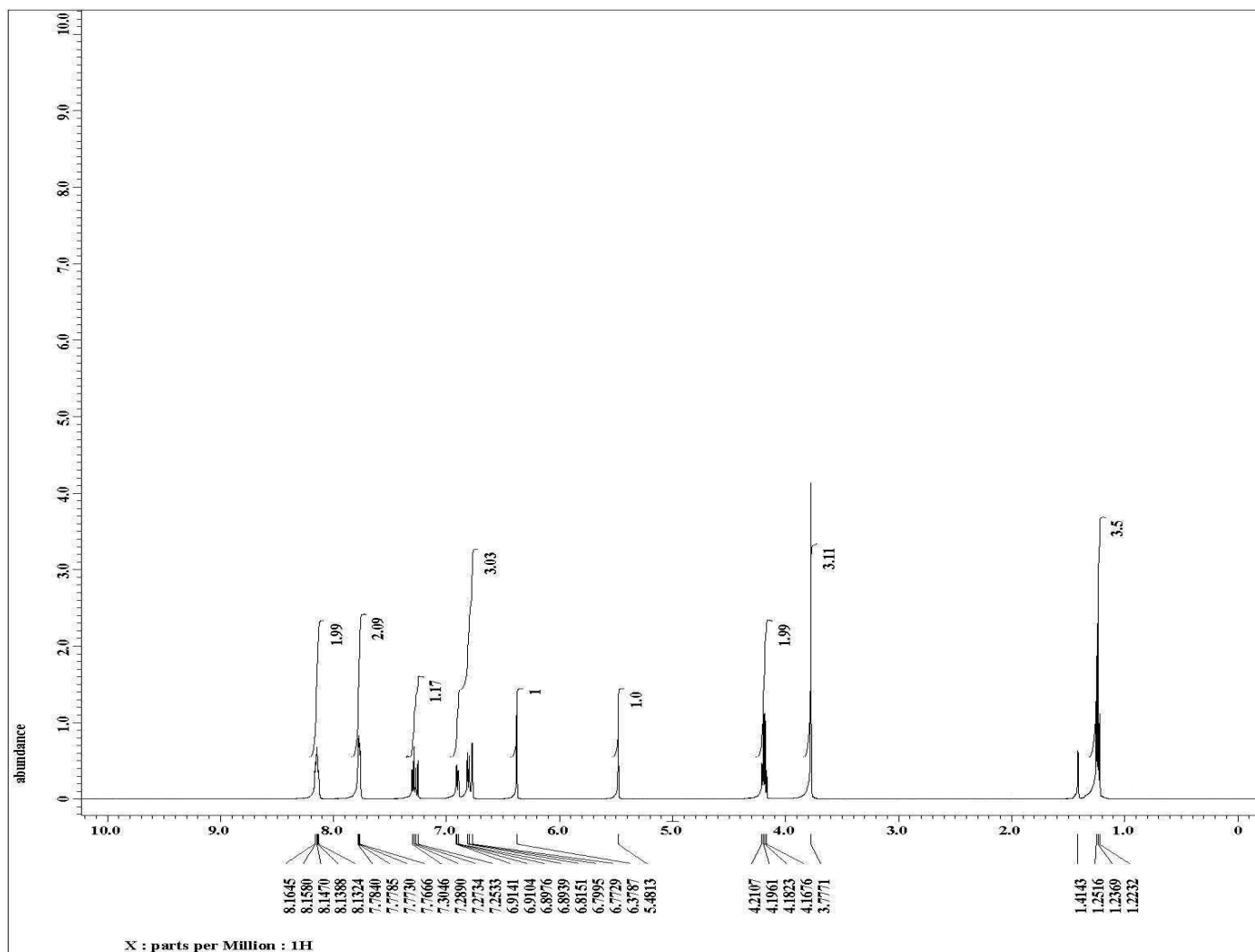


<sup>13</sup>C NMR spectrum of ethyl 2-(3-(4-chlorophenyl)-1,4-dioxo-1,4-dihydronaphthalen-2-yl)acrylate (**3.15**)





HRMS spectrum of ethyl 2-(3-(4-chlorophenyl)-1,4-dioxo-1,4-dihydronaphthalen-2-yl)acrylate (**3.15**)



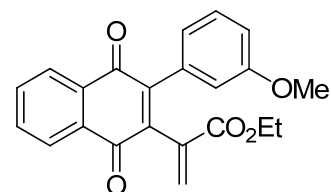
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Author       = N. Ahmed
Experiment   = single_pulse.ex2
Sample id    = S8408746
Solvent      = CHLOROFORM-D
Creation time = 12-MAR-2010 10:48:41
Revision time = 24-AUG-2011 09:54:12
Current time  = 24-AUG-2011 09:54:27

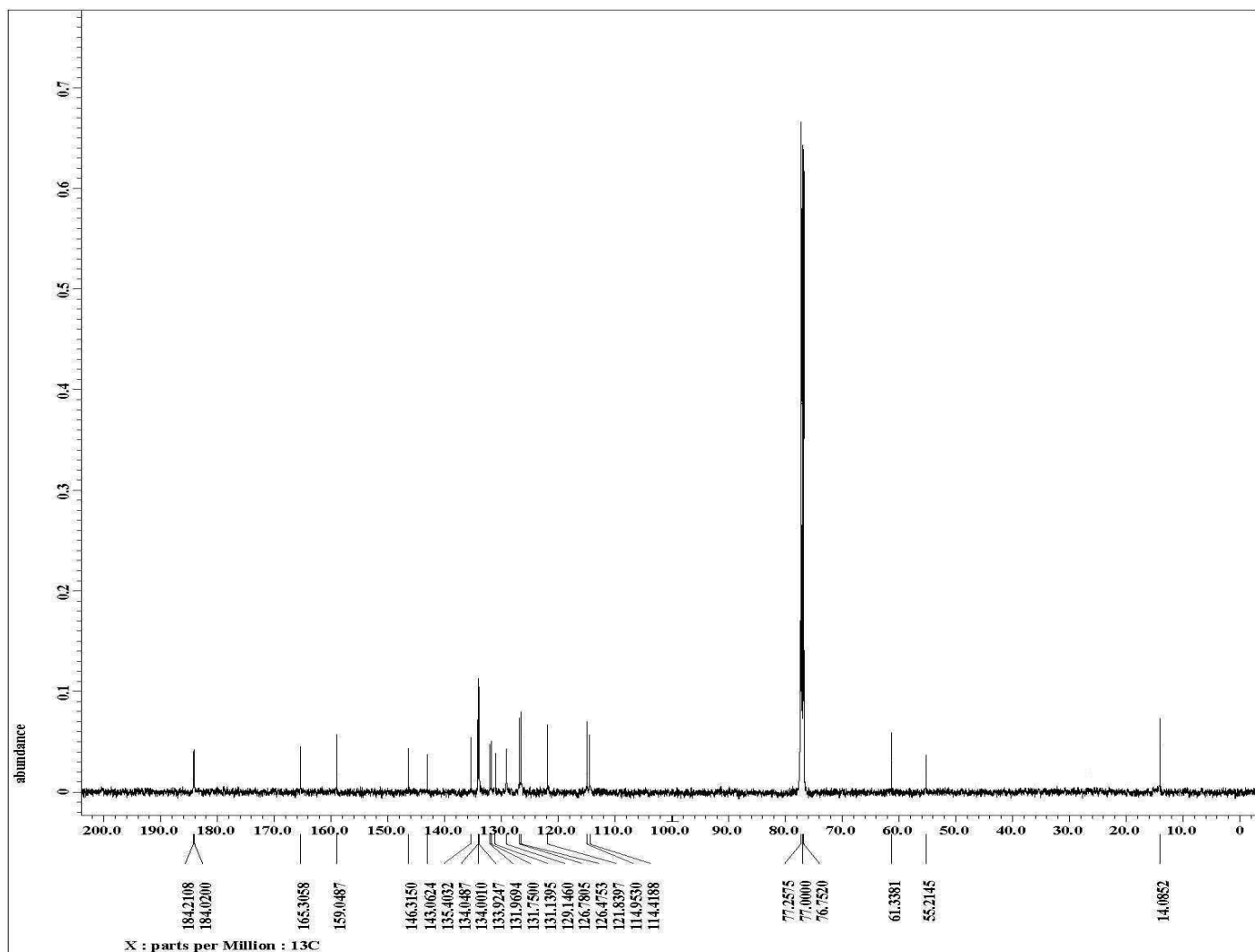
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Dimensions    = X
Site          = ECU 500
Spectrometer  = DELTA2_NMR

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X_domain       = 1H
X_freq         = 500.15991521 [MHz]
X_offset       = 5.0 [ppm]
X_points       = 32768
X_prescans     = 1
X_resolution   = 0.45849727 [Hz]
X_sweep        = 15.02403846 [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      = 2.18103808 [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 = 2 [s]
Repetition_time = 4.18103808 [s]
Temp_get        = 19.6 [dC]
    
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<sup>1</sup>H NMR spectrum of ethyl 2-(3-(3-methoxyphenyl)-1,4-dioxo-1,4-dihydronaphthalen-2-yl)acrylate (**3.16**)



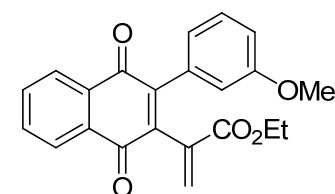
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Author       = N.Ahmed
Experiment   = single_pulse_dec
Sample id    = S4277043
Solvent      = CHLOROFORM-D
Creation time = 13-MAR-2010 07:54:36
Revision time = 24-AUG-2011 10:00:48
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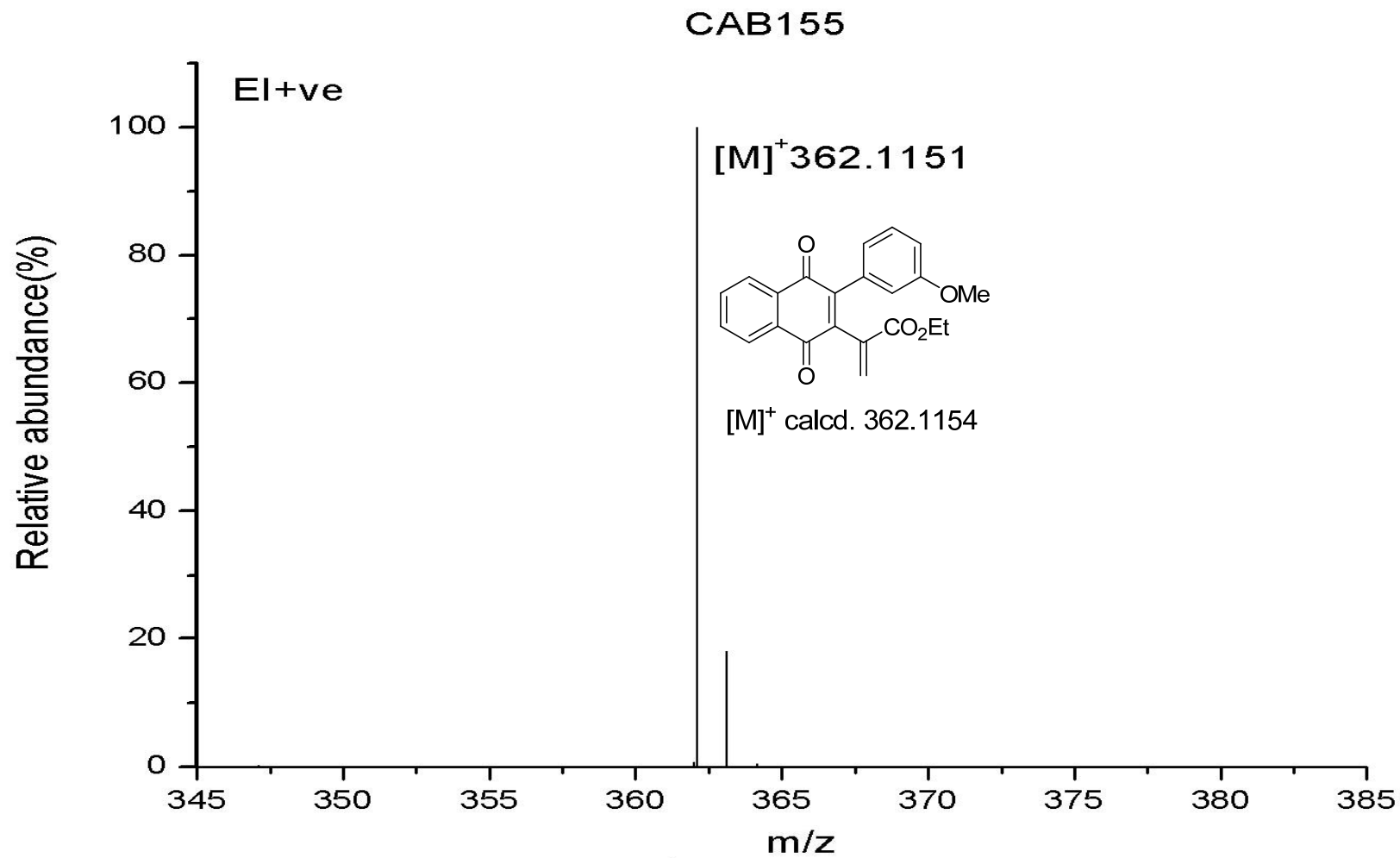
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Dim units     = [ppm]
Dimensions    = X
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Spectrometer  = DELTA2_NMR

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X_domain       = 13C
X_freq         = 125.76529768 [MHz]
X_offset       = 100 [ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.19959034 [Hz]
X_sweep        = 39.3081761 [kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521 [MHz]
Irr_offset     = 5.0 [ppm]
Clipped        = FALSE
Mod return     = 1
Scans          = 1024
Total_scans    = 1024

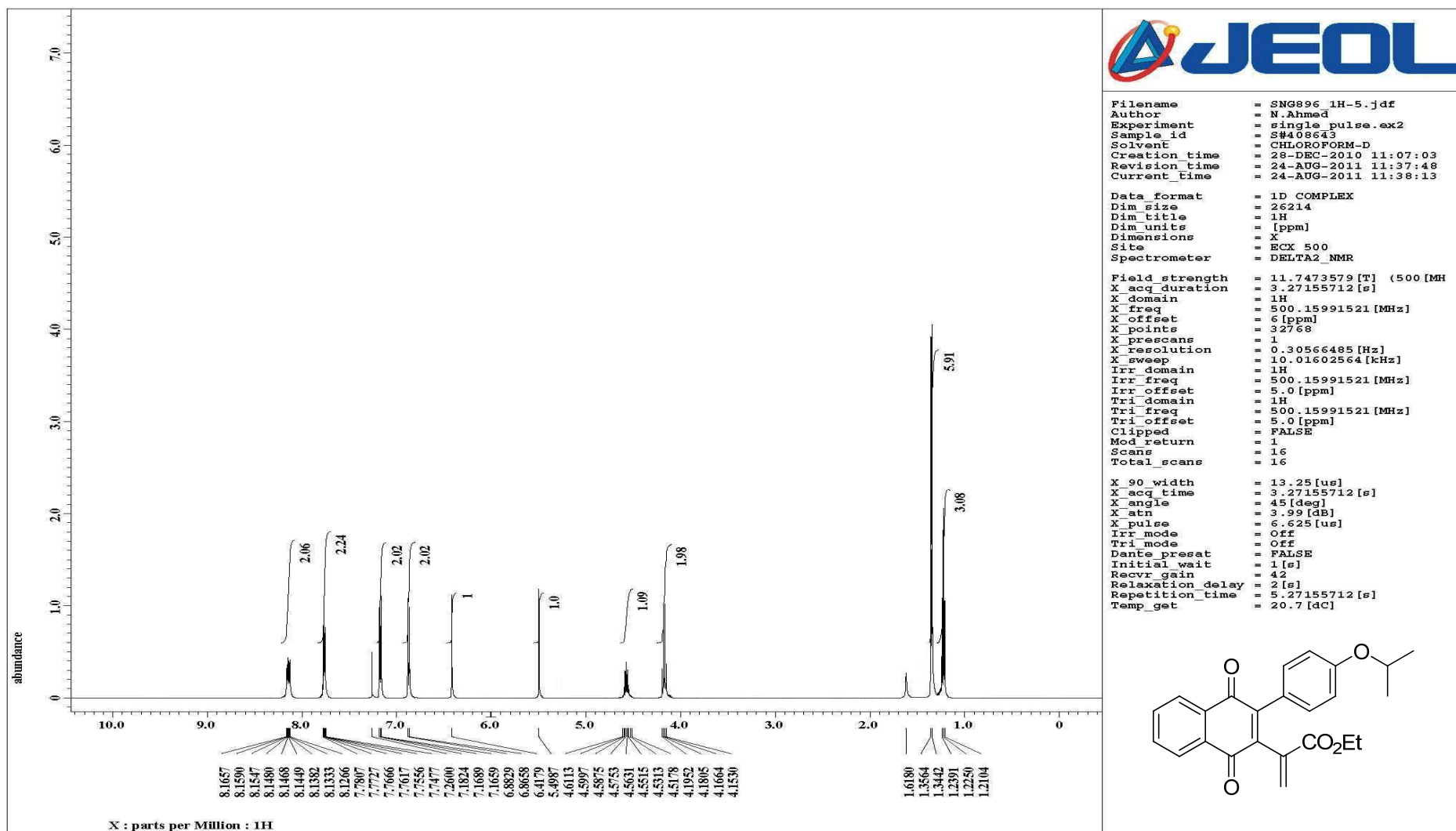
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X_atn          = 7.1 [dB]
X_pulse        = 3.20666667 [us]
Irr_atn_dec    = 21.5 [dB]
Irr_atn_noe    = 21.5 [dB]
Irr_noise      = WALTZ
Decoupling     = TRUE
Initial wait   = 1 [s]
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Noe_time       = 2 [s]
Recvr_gain     = 60
Relaxation_delay = 2 [s]
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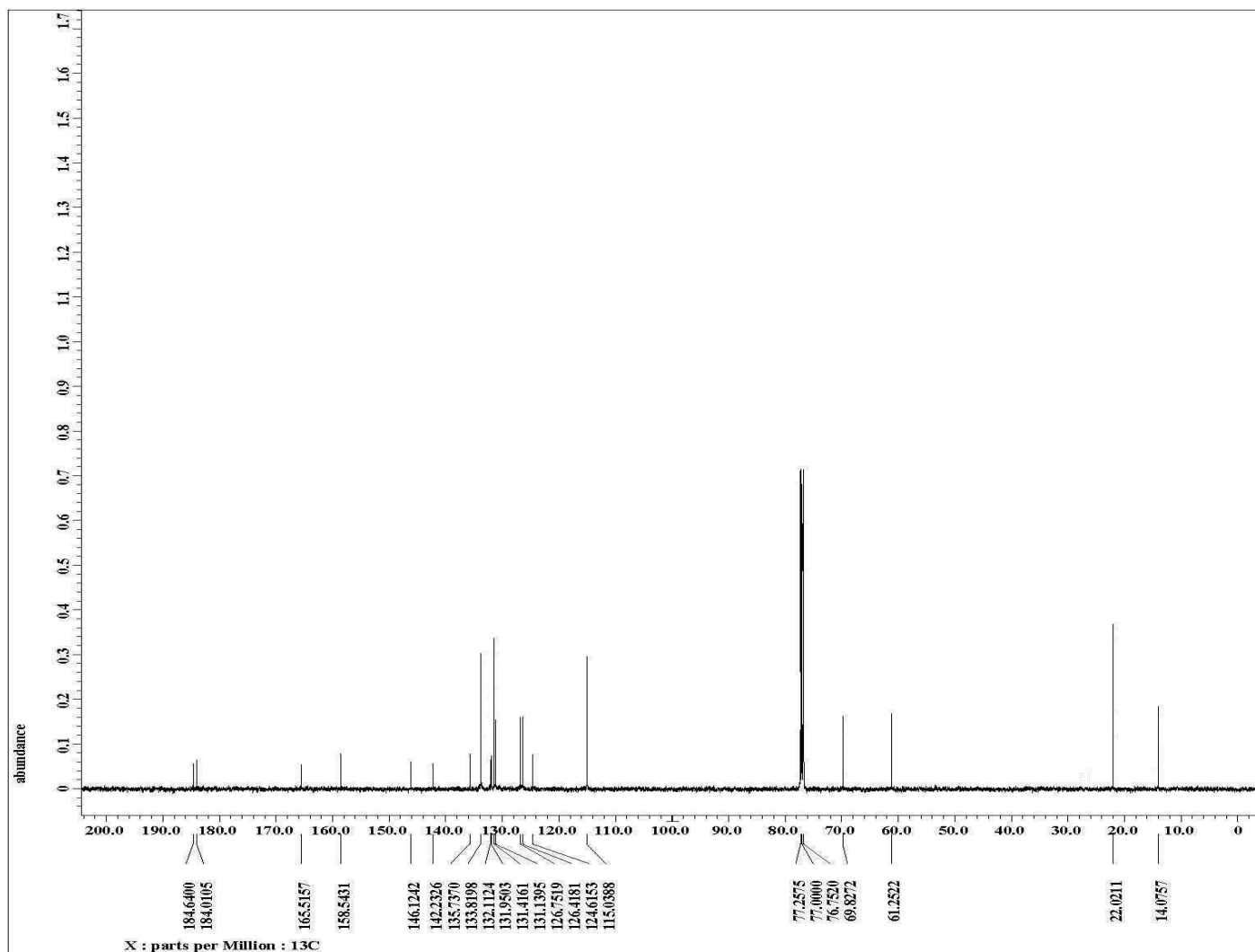
$^{13}\text{C}$  NMR spectrum of ethyl 2-(3-(3-methoxyphenyl)-1,4-dioxo-1,4-dihydronaphthalen-2-yl)acrylate (**3.16**)



HRMS spectrum of ethyl 2-(3-(3-methoxyphenyl)-1,4-dioxo-1,4-dihydronaphthalen-2-yl)acrylate (**3.16**)



<sup>1</sup>H NMR spectrum of ethyl 2-(3-(4-isopropoxyphenyl)-1,4-dioxo-1,4-dihydronaphthalen-2-yl)acrylate (**3.17**)



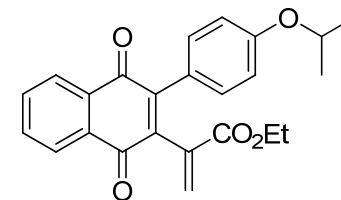
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Author       = N. Ahmed
Experiment   = single_pulse_dec
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Solvent      = CHLOROFORM-D
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Revision time = 24-AUG-2011 11:54:15
Current time  = 24-AUG-2011 11:54:53

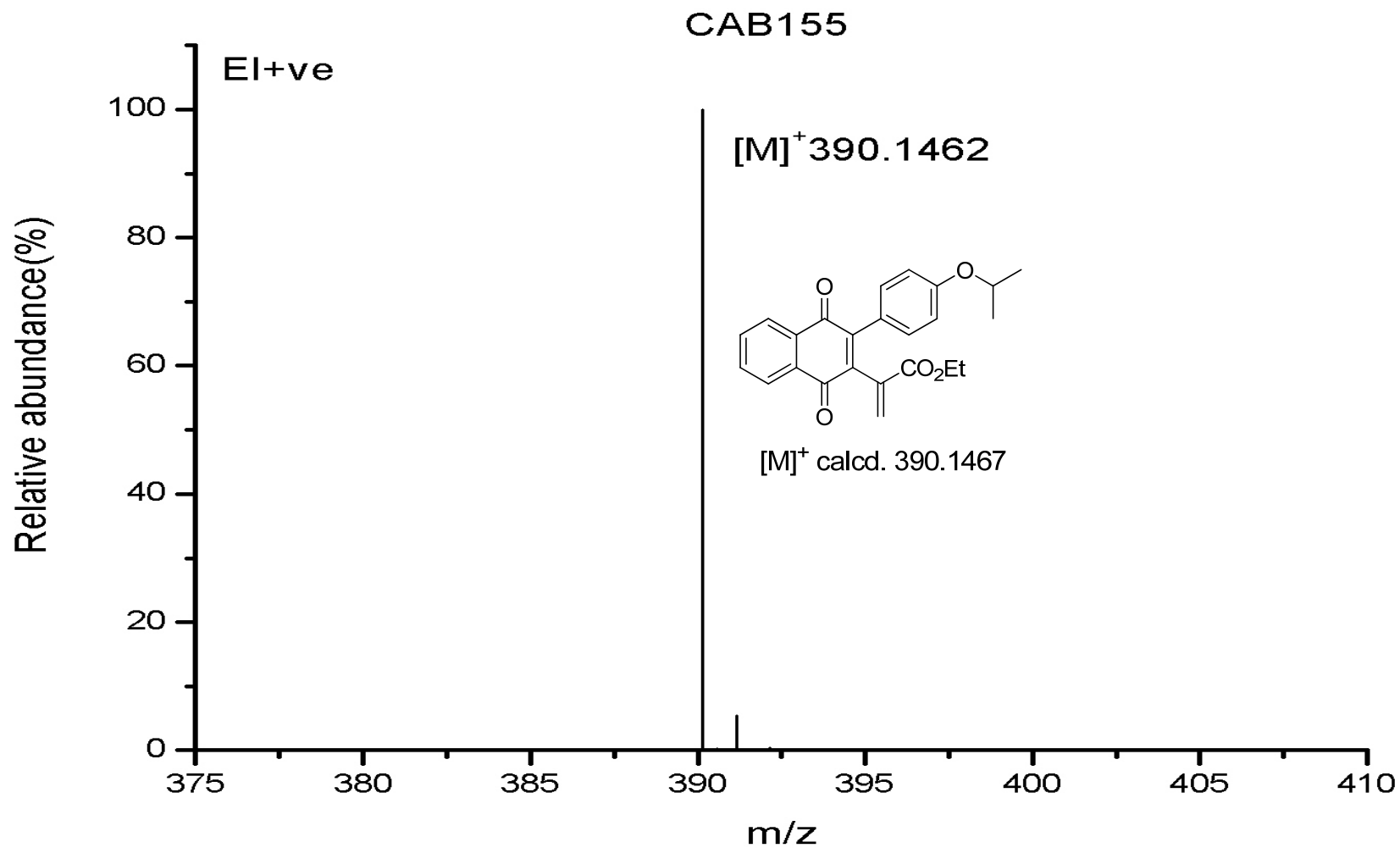
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Spectrometer  = DELTA2_NMR

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X_acq_duration = 0.83361792 [s]
X_domain      = 13C
X_freq        = 125.76529768 [MHz]
X_offset      = 100 [ppm]
X_points      = 32768
X_prescans    = 4
X_resolution  = 1.19959034 [Hz]
X_sweep       = 39.3081761 [kHz]
Irr_domain    = 1H
Irr_freq      = 500.15991521 [MHz]
Irr_offset    = 5.0 [ppm]
Clipped       = FALSE
Mod return    = 1
Scans         = 1000
Total_scans   = 1000

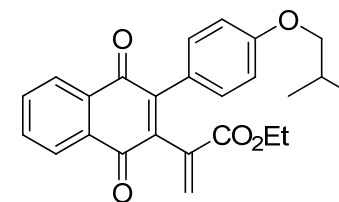
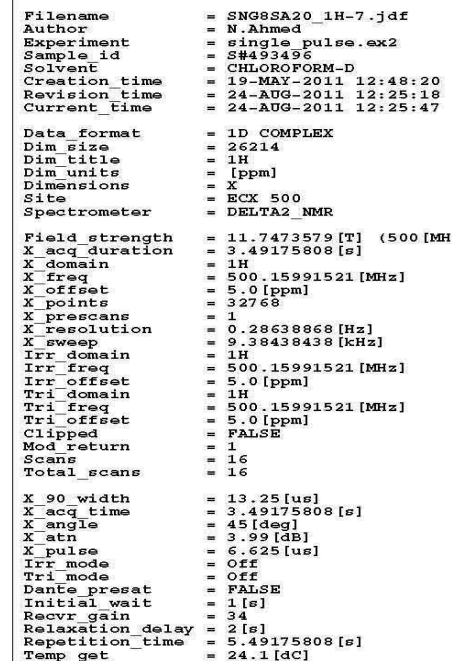
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X_atn         = 7.1 [dB]
X_pulse       = 3.20666667 [us]
Irr_atn_dec   = 19.5 [dB]
Irr_atn_noe   = 21.5 [dB]
Irr_noise     = WALTZ
Decoupling    = TRUE
Initial wait  = 1 [s]
Noe           = TRUE
Noe_time      = 1 [s]
Recvr_gain    = 60
Relaxation_delay = 1 [s]
Repetition_time = 1.83361792 [s]
Temp_get      = 24.8 [dC]
    
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<sup>13</sup>C NMR spectrum of ethyl 2-(3-(4-isopropoxyphenyl)-1,4-dioxo-1,4-dihydronaphthalen-2-yl)acrylate (**3.17**)

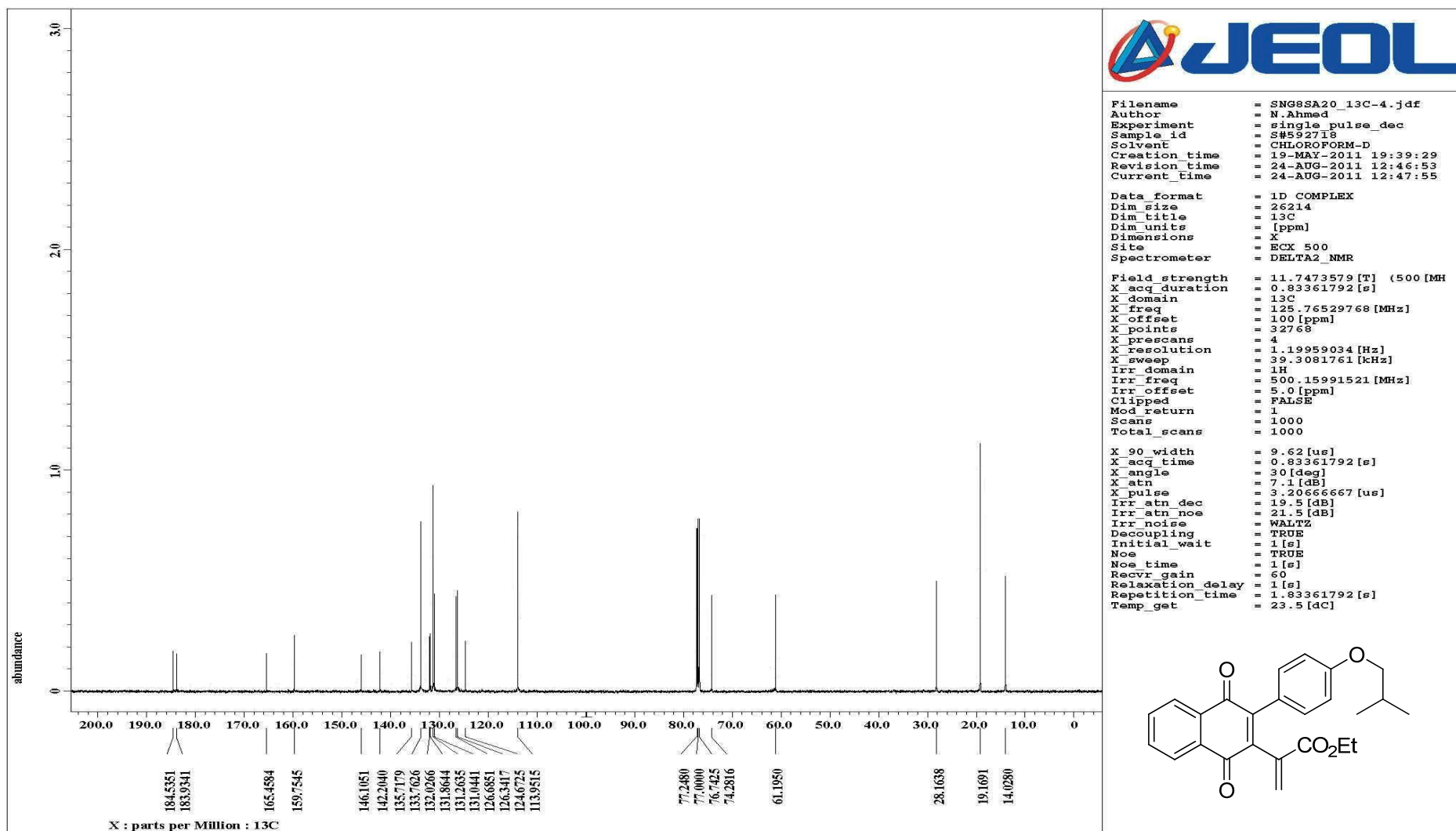


HRMS spectrum of ethyl 2-(3-(4-isopropoxyphenyl)-1,4-dioxo-1,4-dihydronaphthalen-2-yl)acrylate (**3.17**)

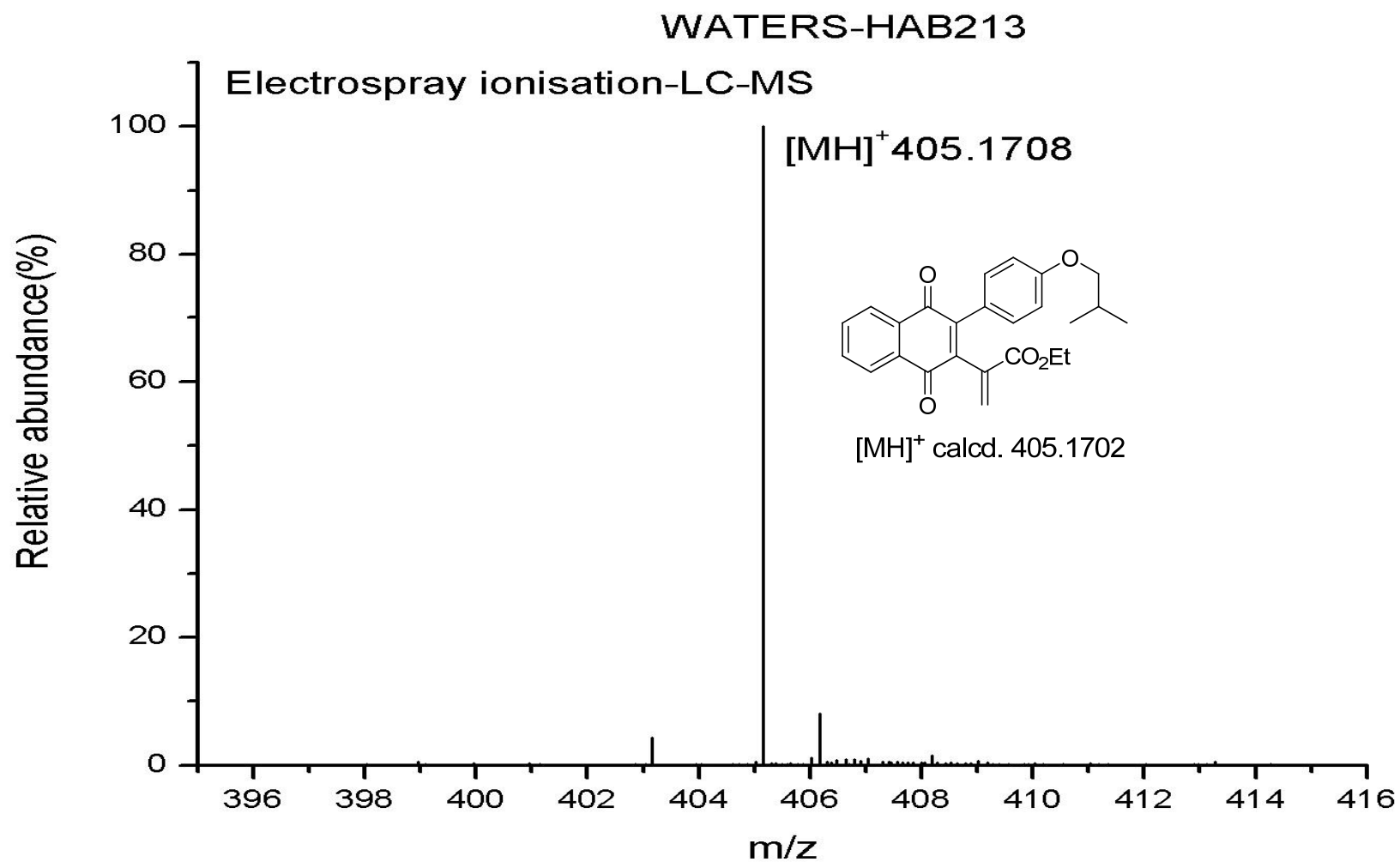


**S90**

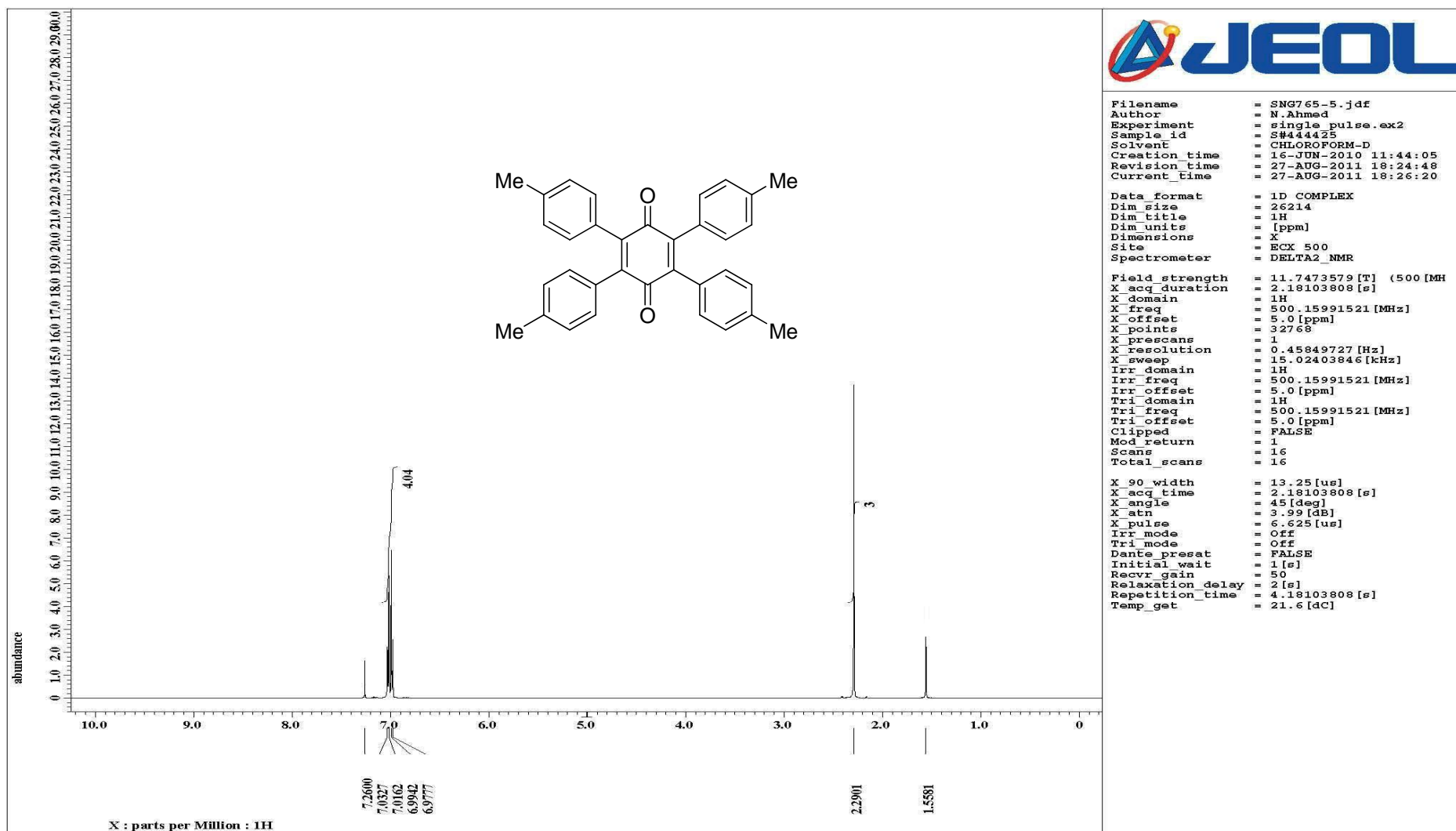




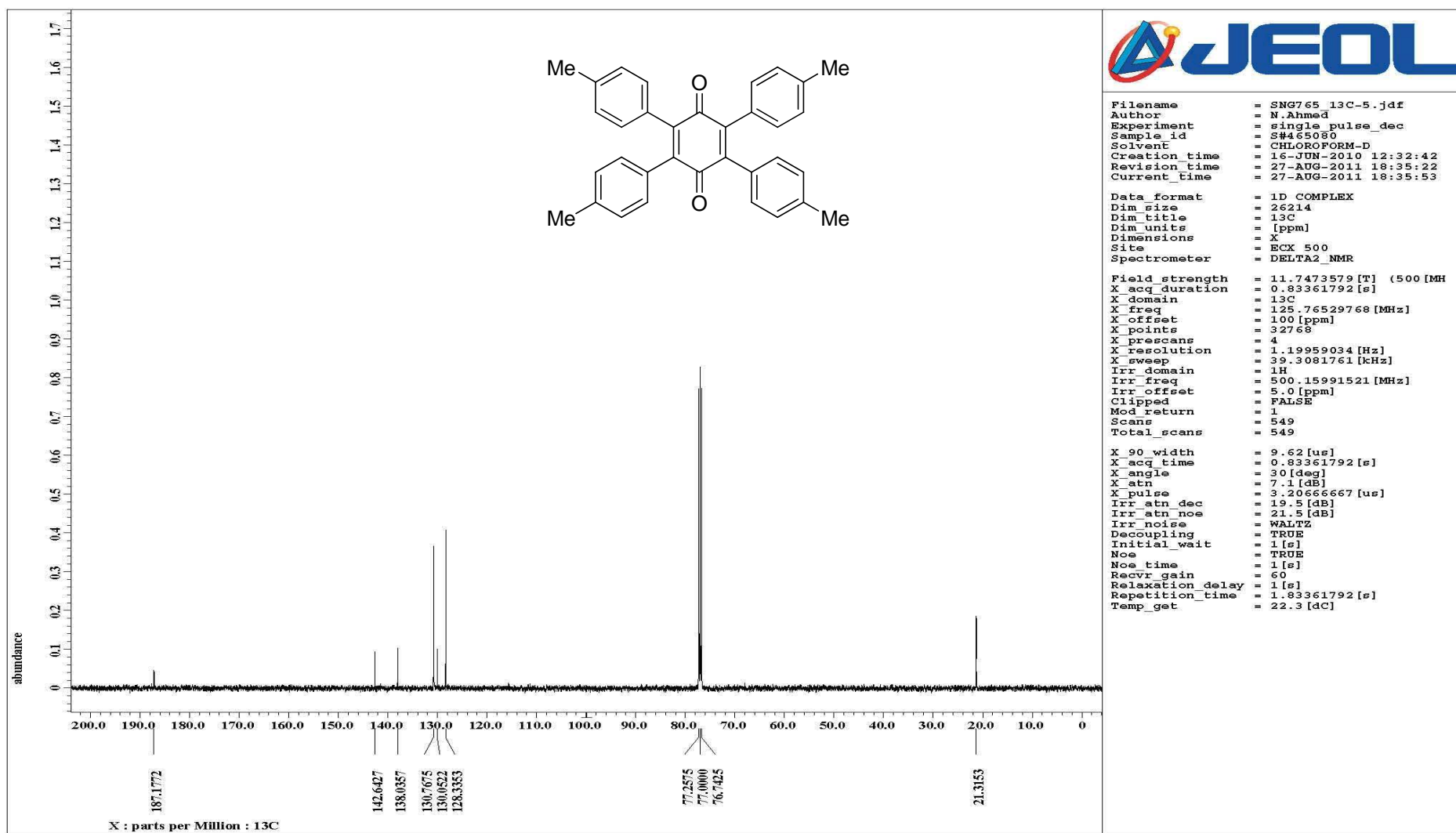
$^{13}\text{C}$  NMR spectrum of ethyl 2-(3-(4-isobutoxyphenyl)-1,4-dioxo-1,4-dihydronaphthalen-2-yl)acrylate (**3.18**)



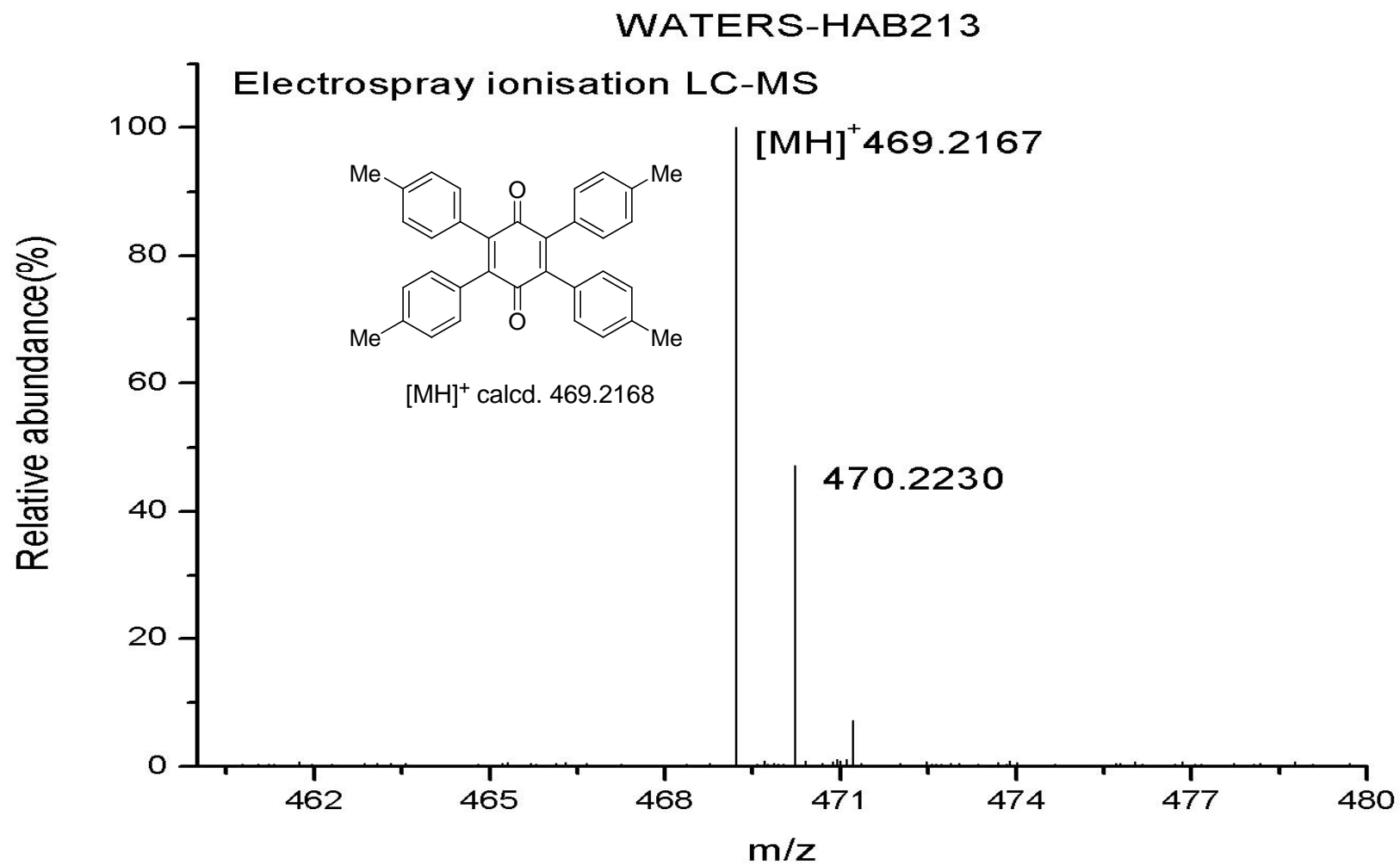
HRMS spectrum of ethyl 2-(3-(4-isobutoxyphenyl)-1,4-dioxo-1,4-dihydronaphthalen-2-yl)acrylate (**3.18**)



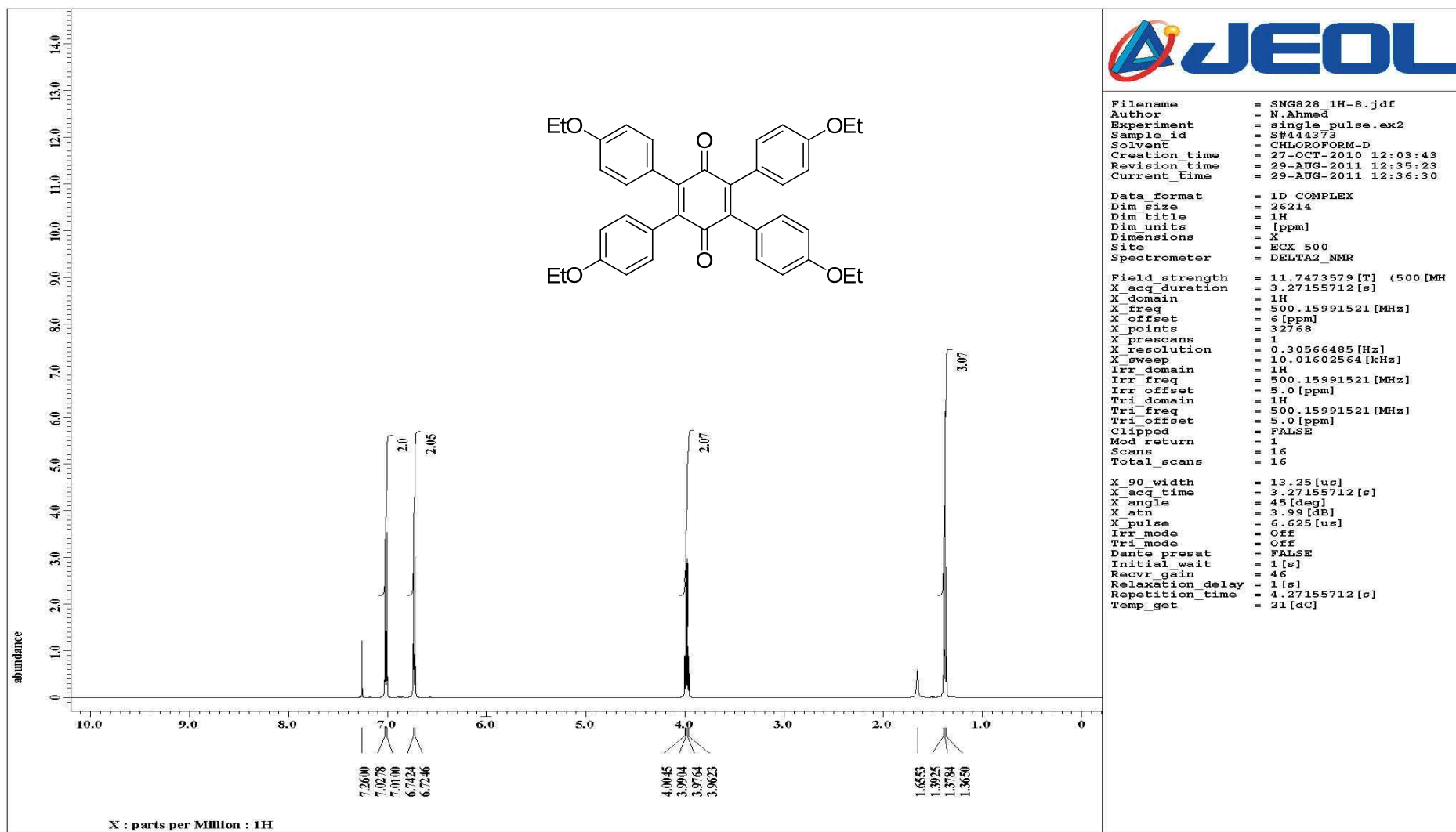
<sup>1</sup>H NMR spectrum of 2,3,5,6-tetra-4-tolylcyclohexa-2,5-diene-1,4-dione (5.1)



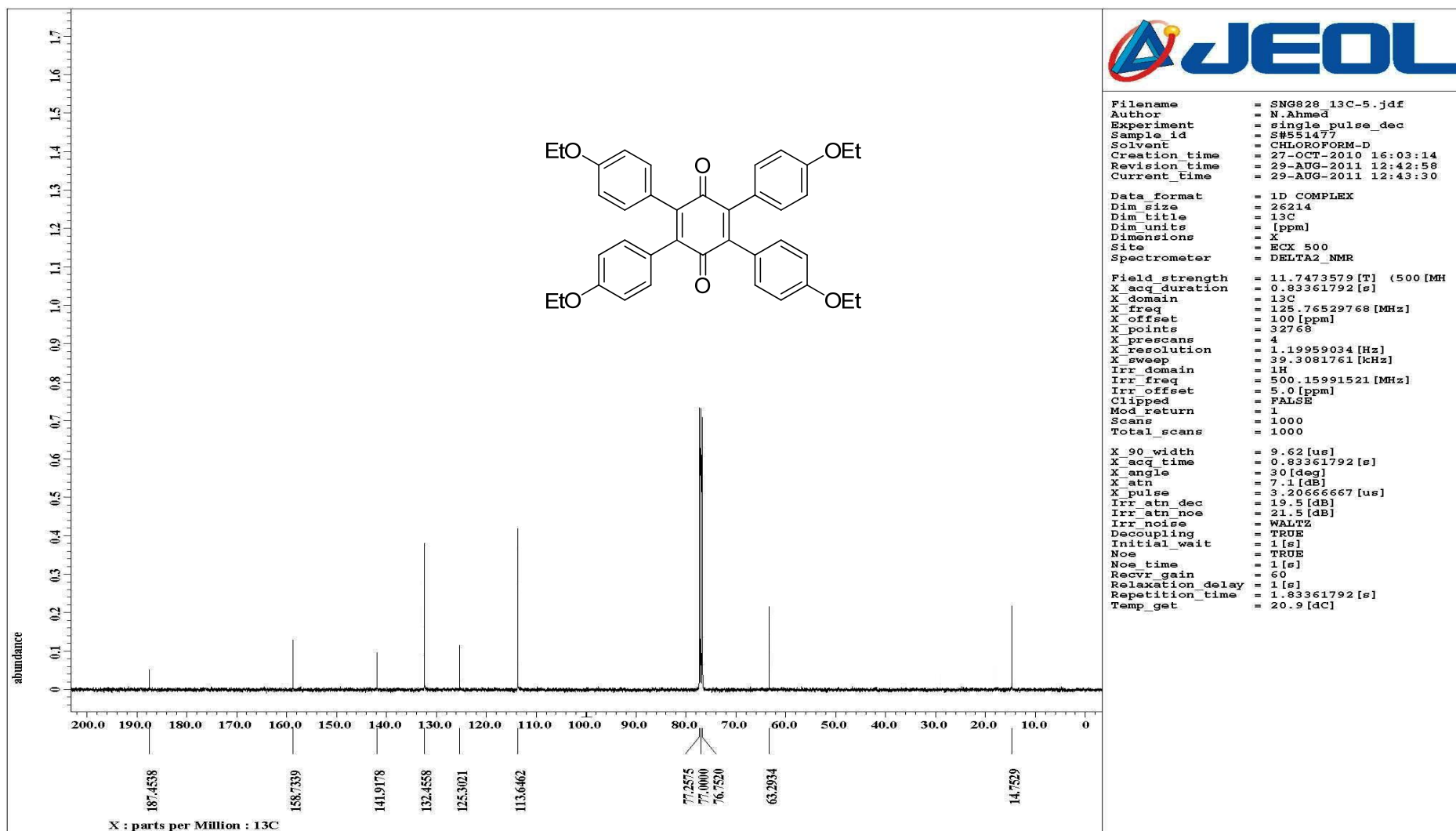
<sup>13</sup>C NMR spectrum of 2,3,5,6-tetra-4-tolylcyclohexa-2,5-diene-1,4-dione (5.1)



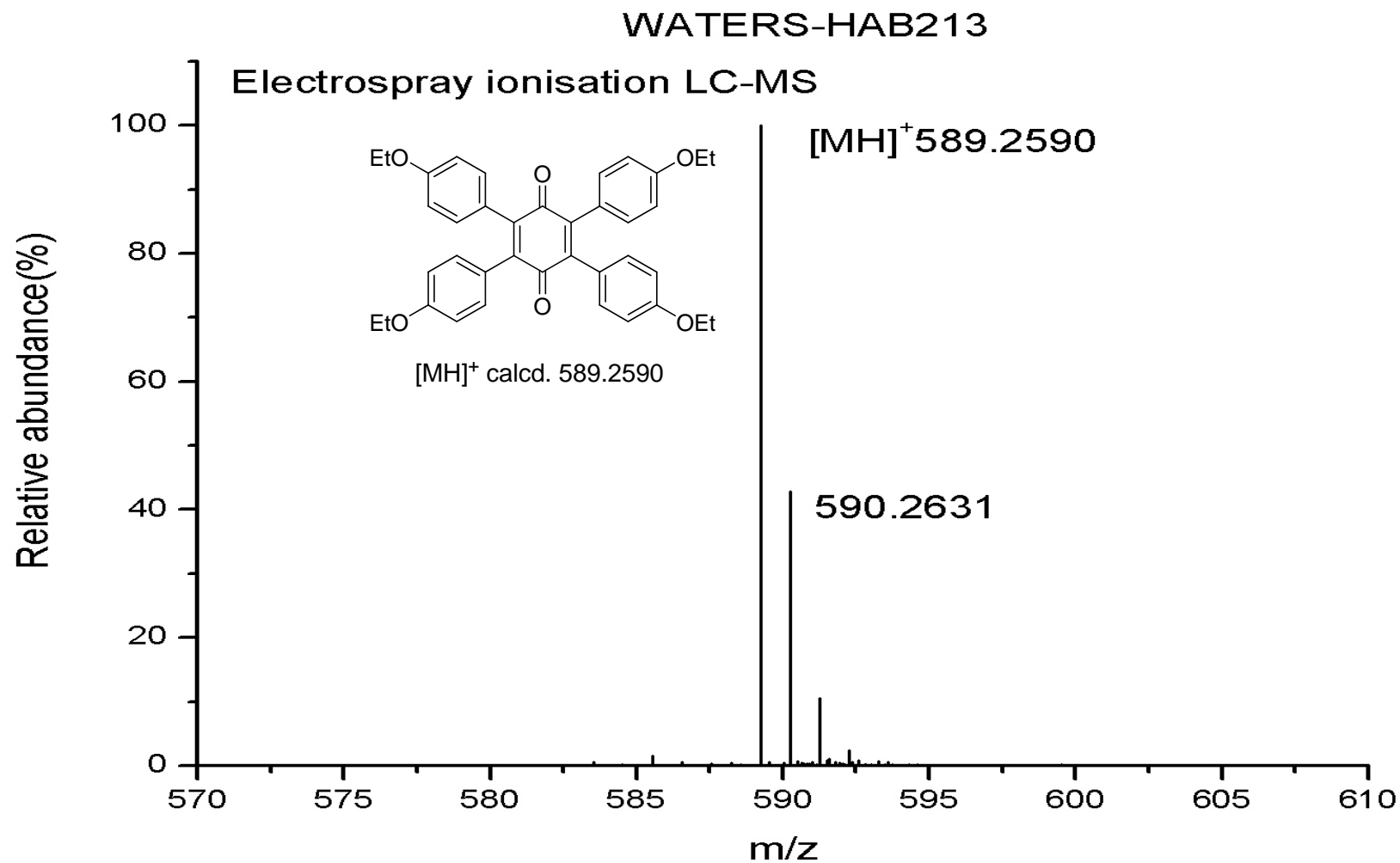
HRMS spectrum of 2,3,5,6-tetra(4-tolyl)cyclohexa-2,5-diene-1,4-dione (**5.1**)



<sup>1</sup>H NMR spectrum of 2,3,5,6-tetrakis(4-ethoxyphenyl)cyclohexa-2,5-diene-1,4-dione (5.2)

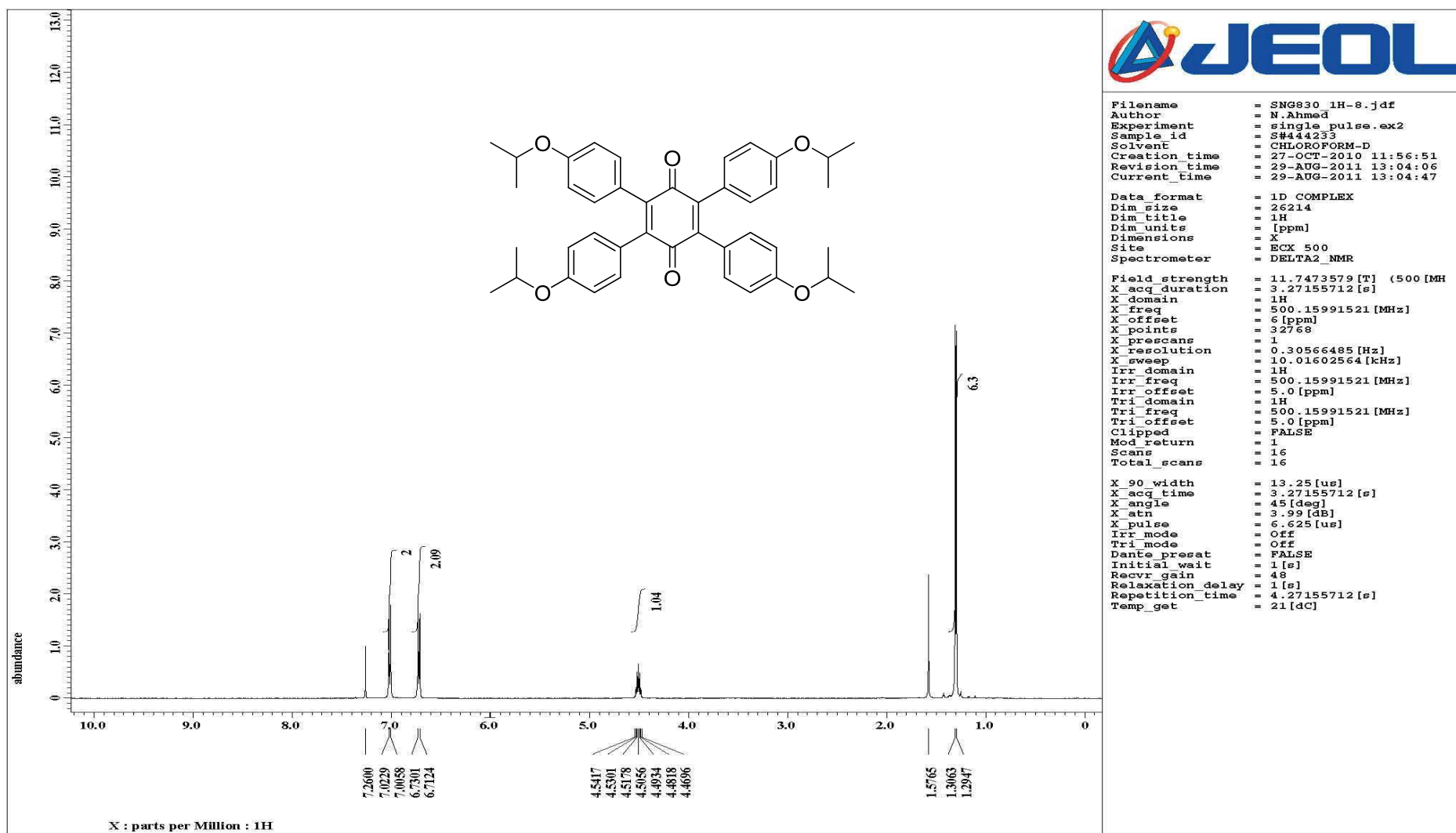


<sup>13</sup>C NMR spectrum of 2,3,5,6-tetrakis(4-ethoxyphenyl)cyclohexa-2,5-diene-1,4-dione (5.2)

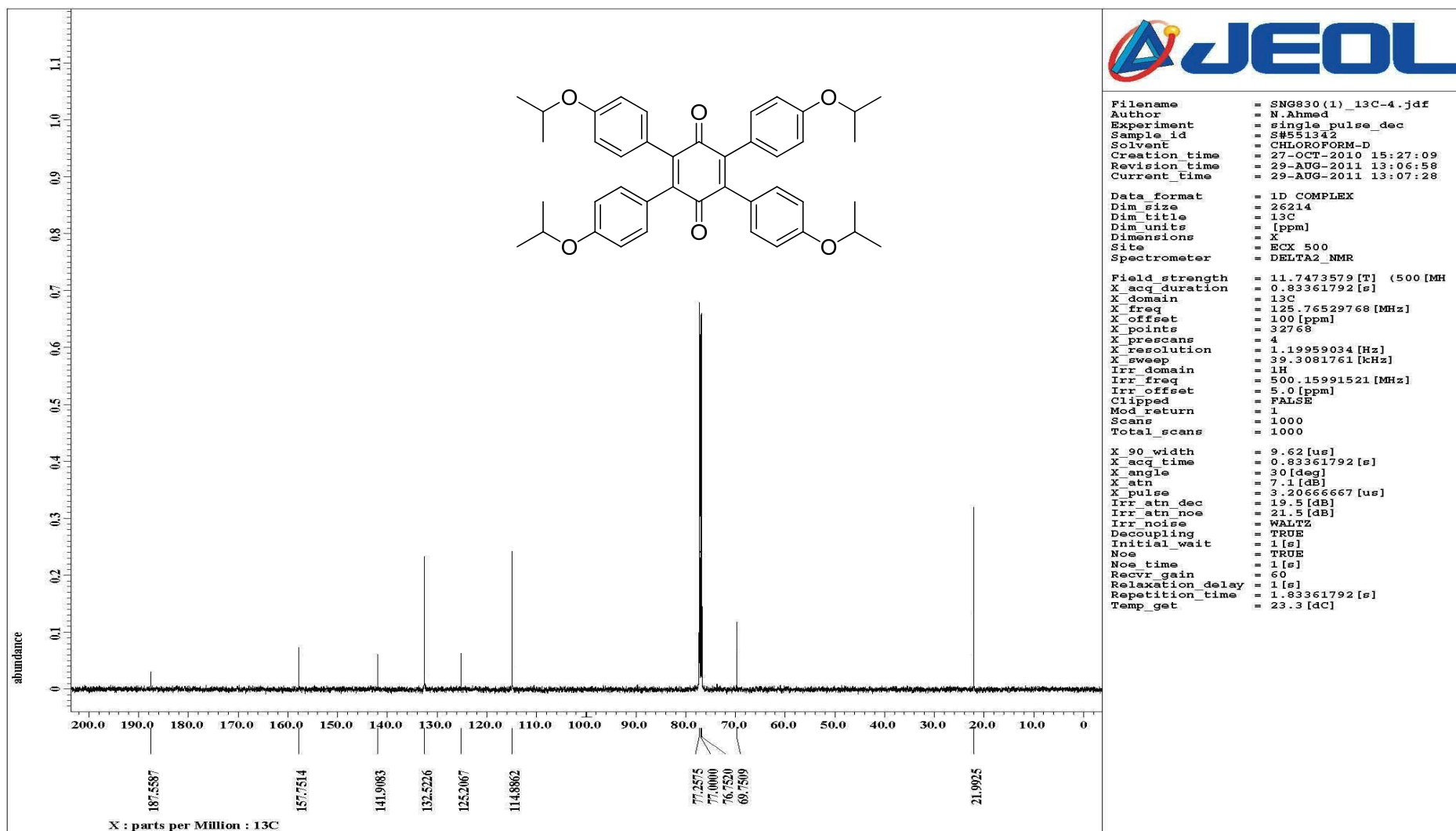


HRMS spectrum of 2,3,5,6-tetrakis(4-ethoxyphenyl)cyclohexa-2,5-diene-1,4-dione (**5.2**)

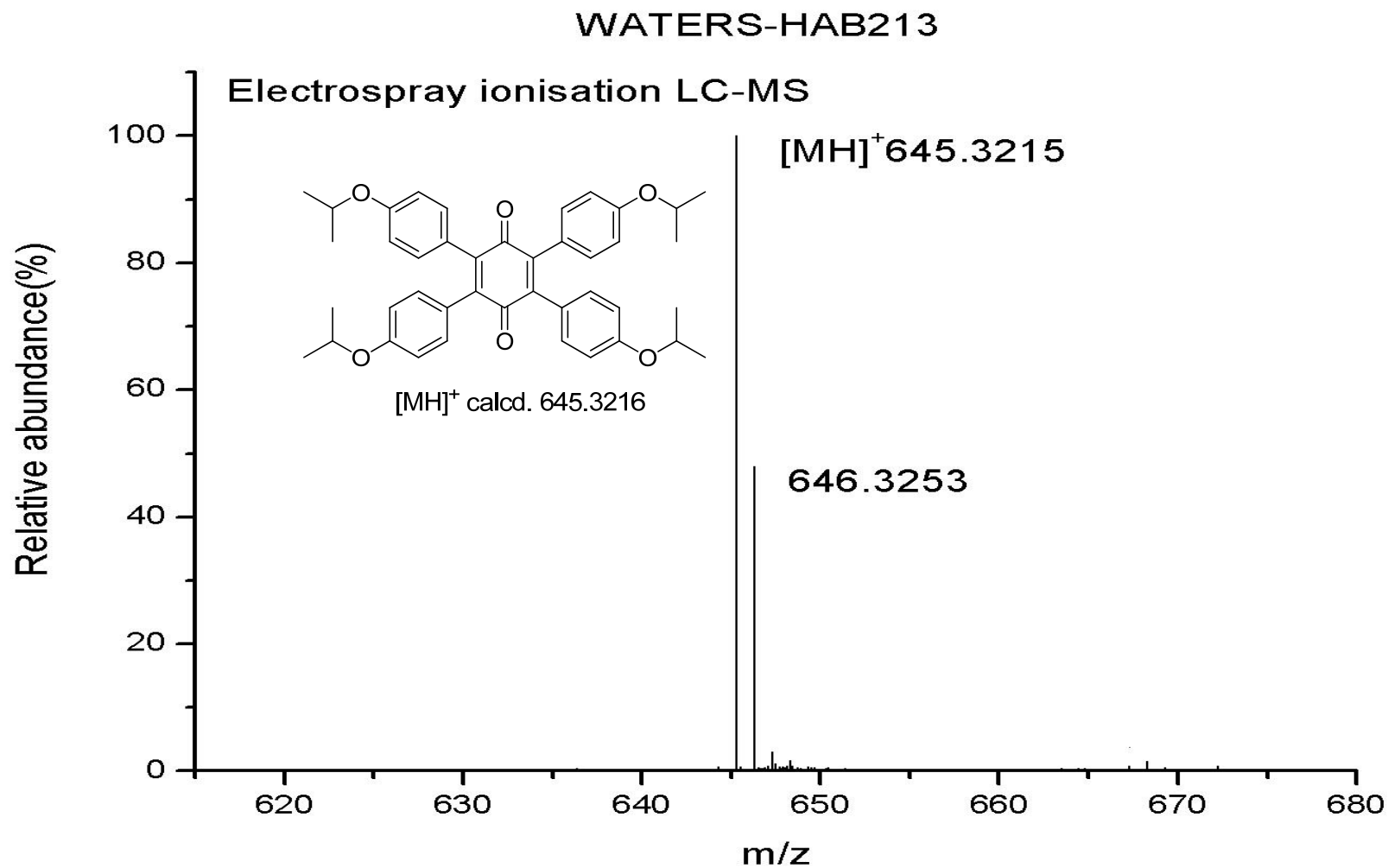




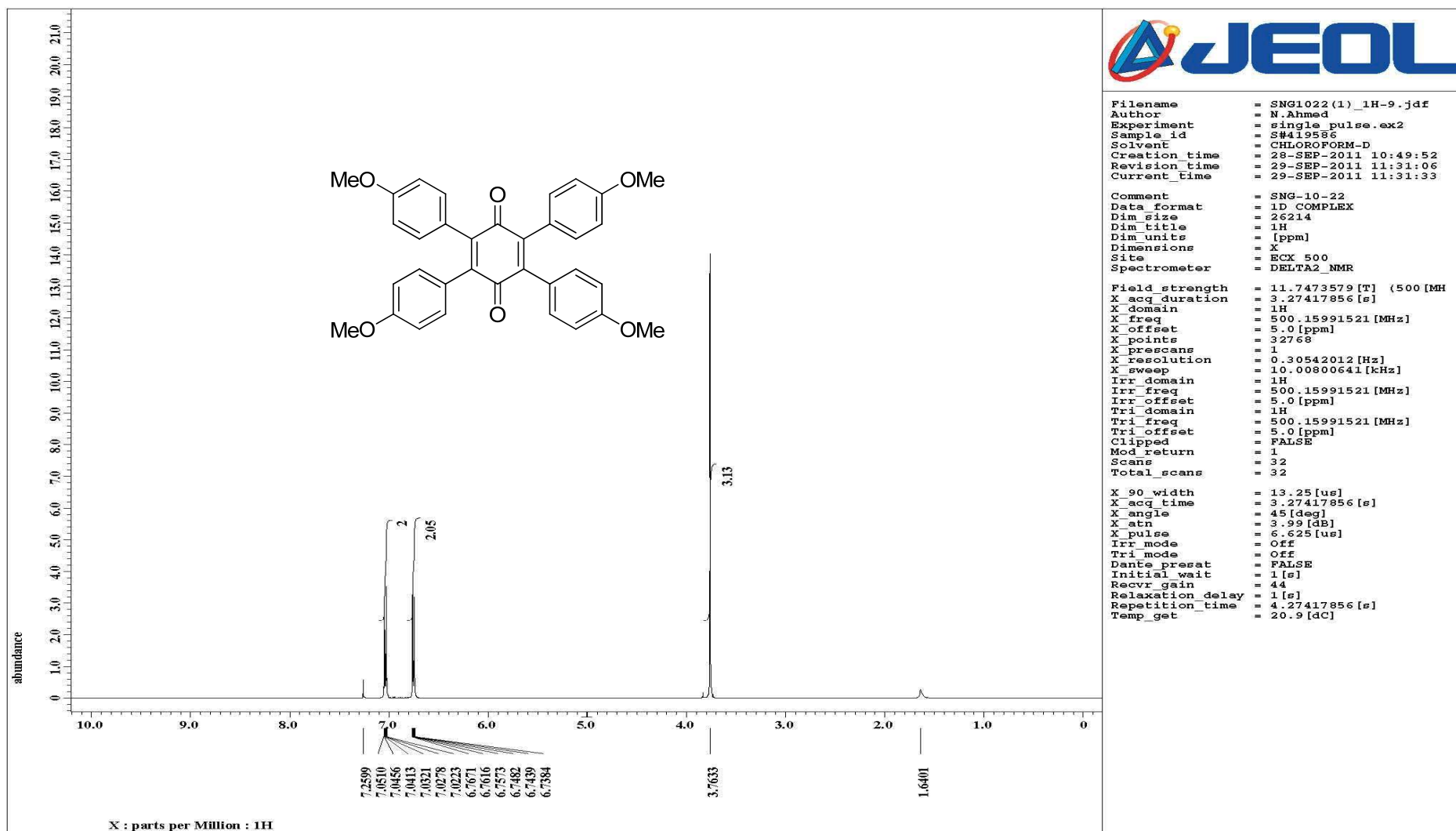
<sup>1</sup>H NMR spectrum of 2,3,5,6-tetrakis(4-isopropoxyphenyl)cyclohexa-2,5-diene-1,4-dione (5.3)



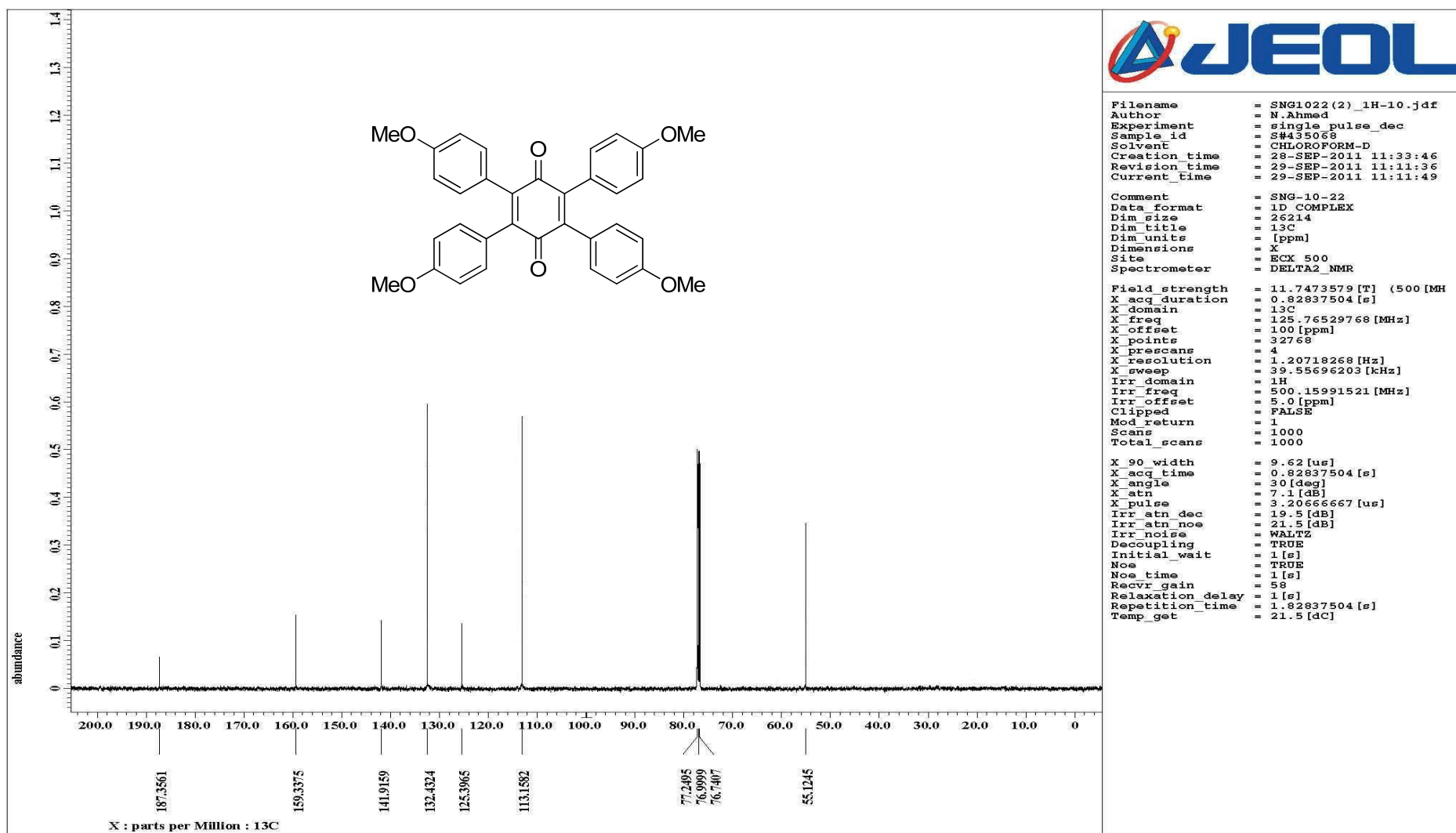
<sup>13</sup>C NMR spectrum of 2,3,5,6-tetrakis(4-isopropoxyphenyl)cyclohexa-2,5-diene-1,4-dione (5.3)



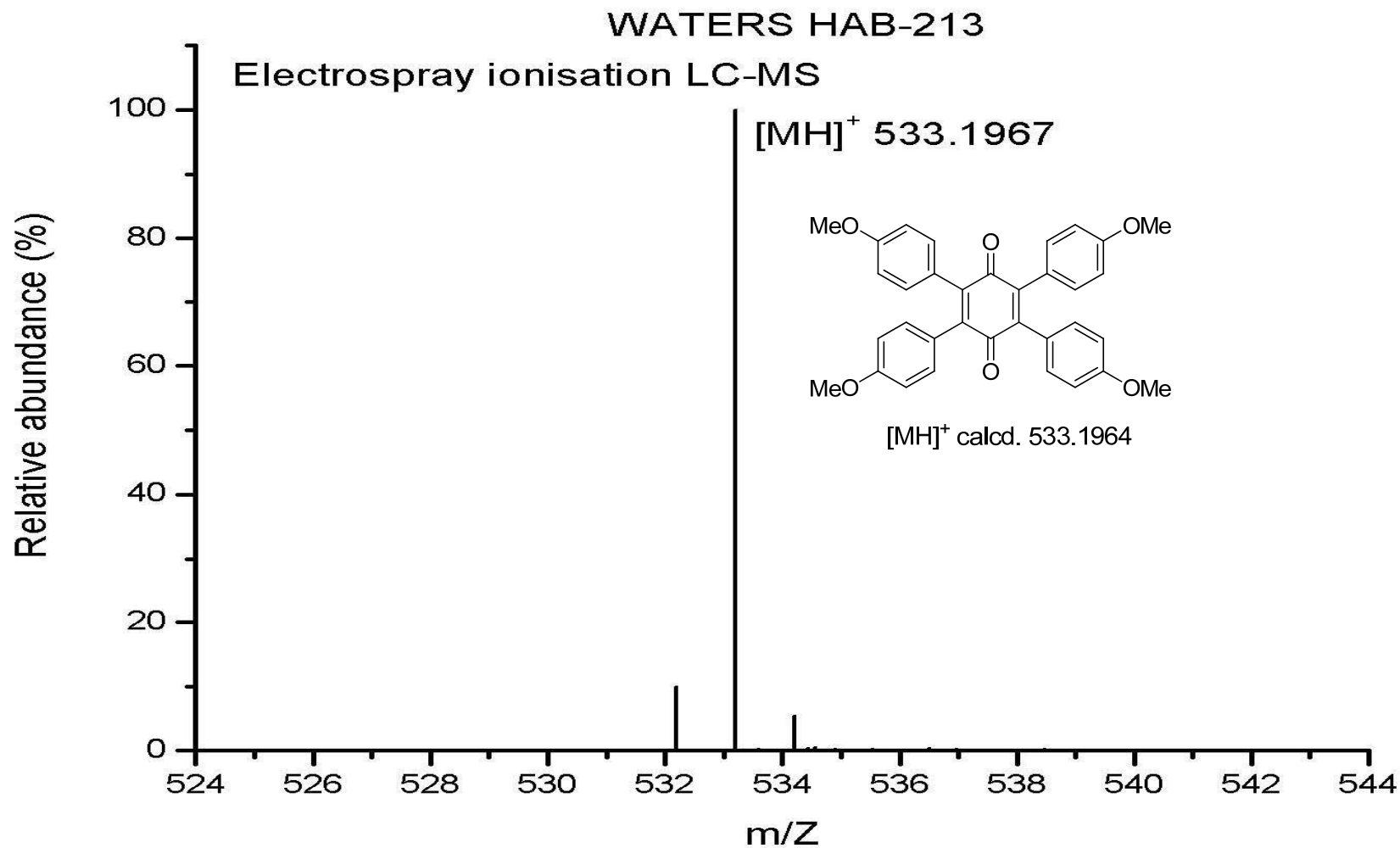
HRMS spectrum of 2,3,5,6-tetrakis(4-isopropoxyphenyl)cyclohexa-2,5-diene-1,4-dione (**5.3**)



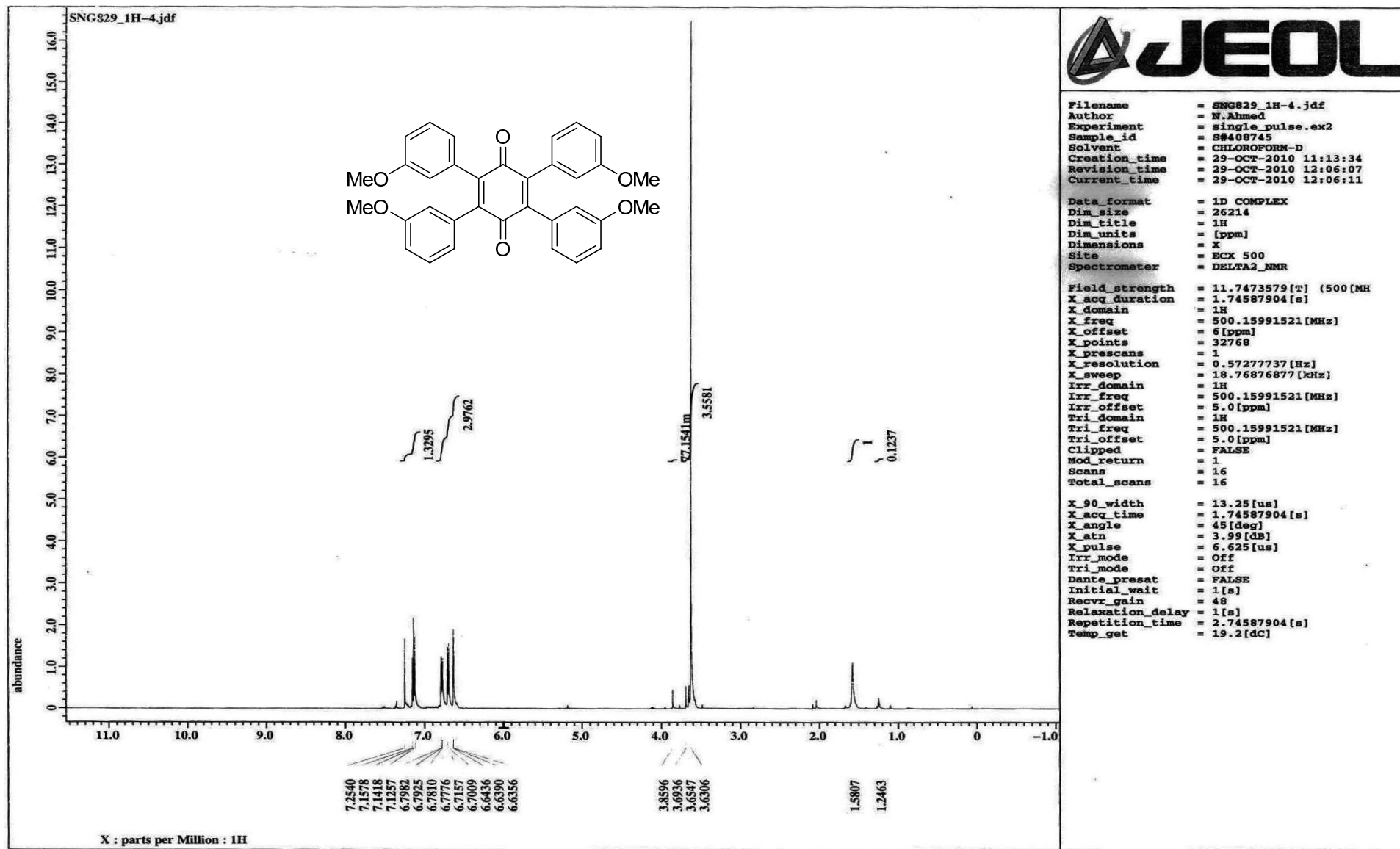
<sup>1</sup>H NMR spectrum of 2,3,5,6-tetrakis(4-methoxyphenyl)cyclohexa-2,5-diene-1,4-dione (5.4)



<sup>13</sup>C NMR spectrum of 2,3,5,6-tetrakis(4-methoxyphenyl)cyclohexa-2,5-diene-1,4-dione (5.4)

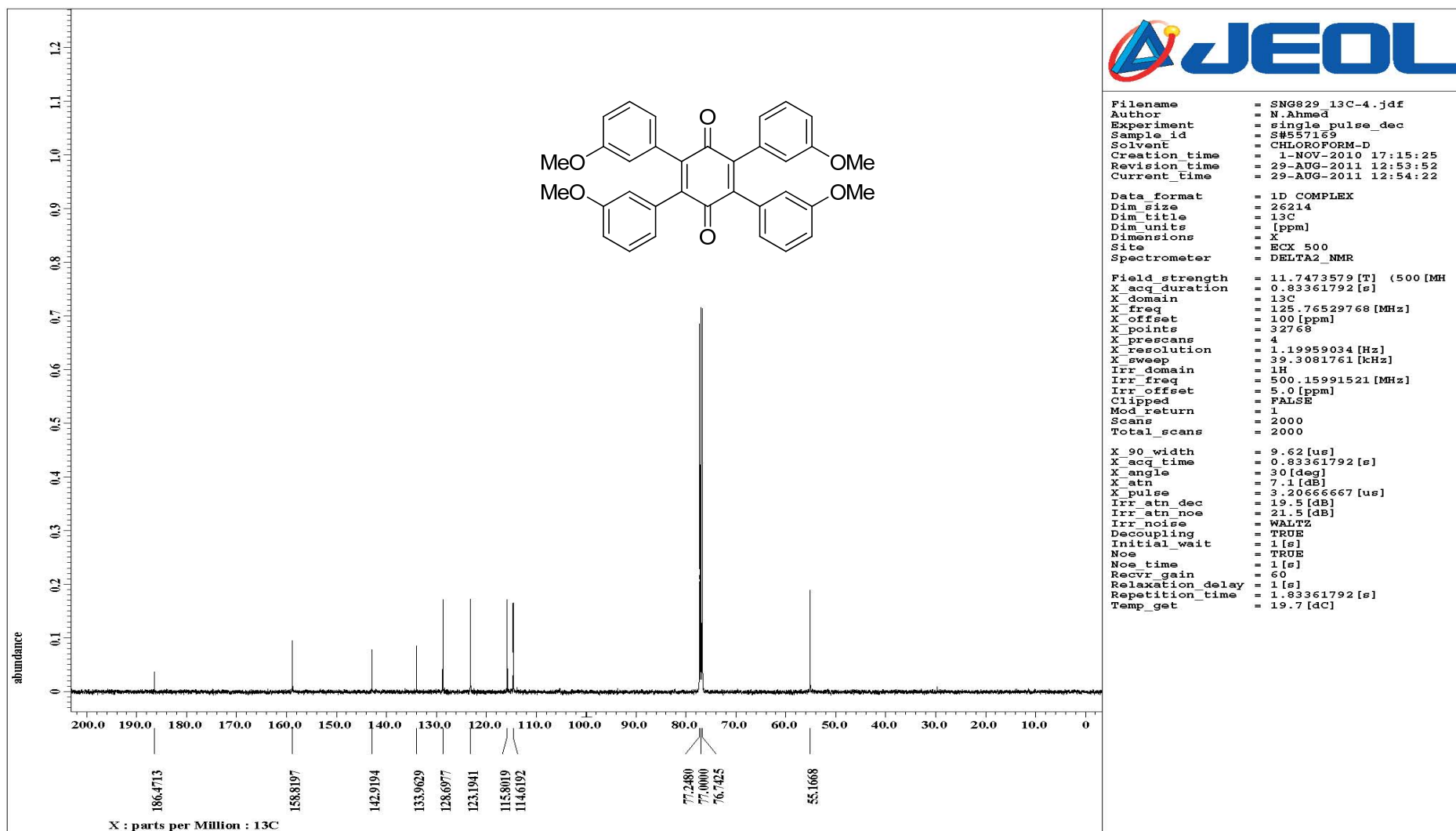


HRMS spectrum of 2,3,5,6-tetrakis(4-methoxyphenyl)cyclohexa-2,5-diene-1,4-dione (**5.4**)



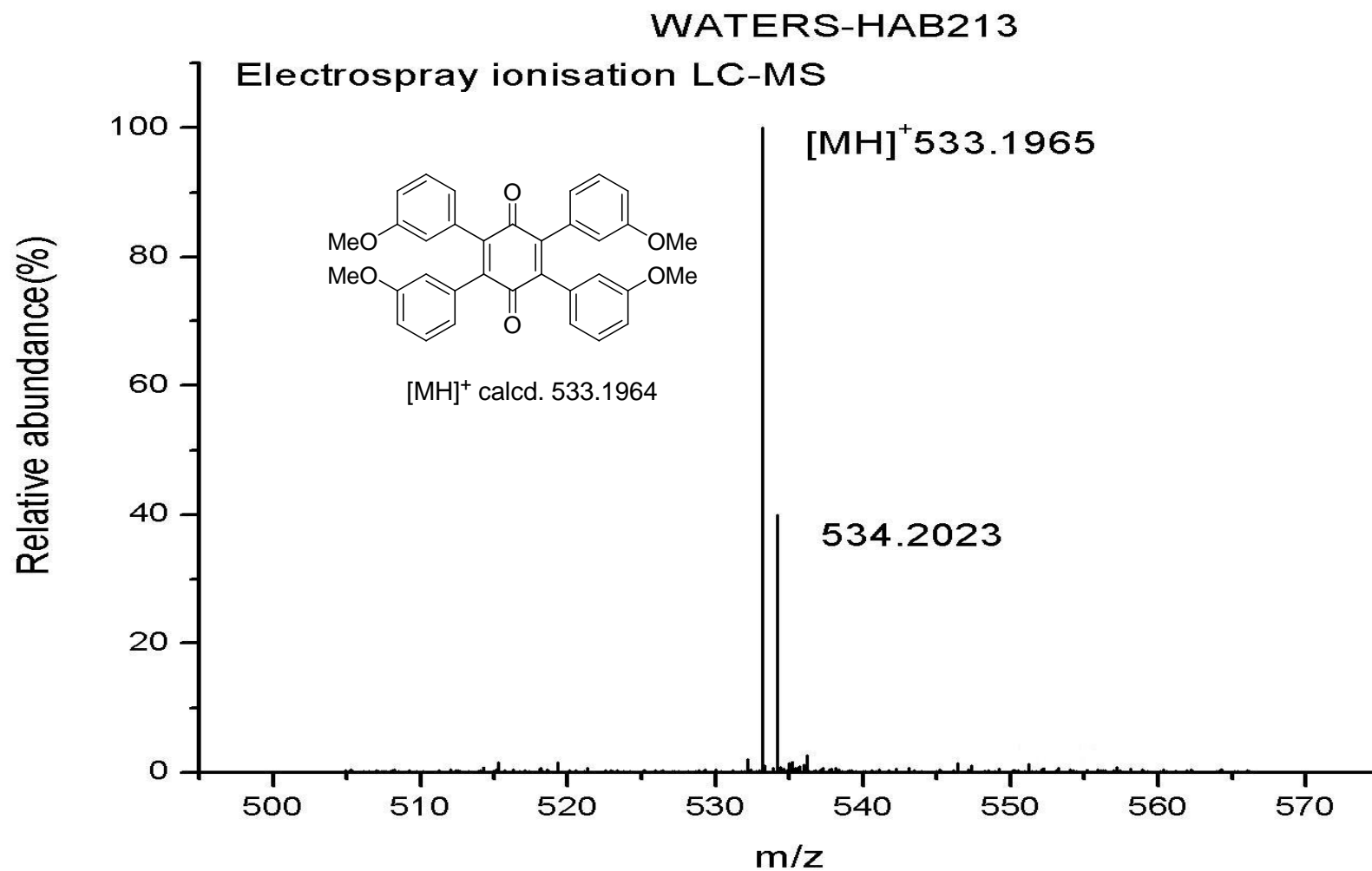
<sup>1</sup>H NMR spectrum of 2,3,5,6-tetrakis(3-methoxyphenyl)cyclohexa-2,5-diene-1,4-dione (5.5)



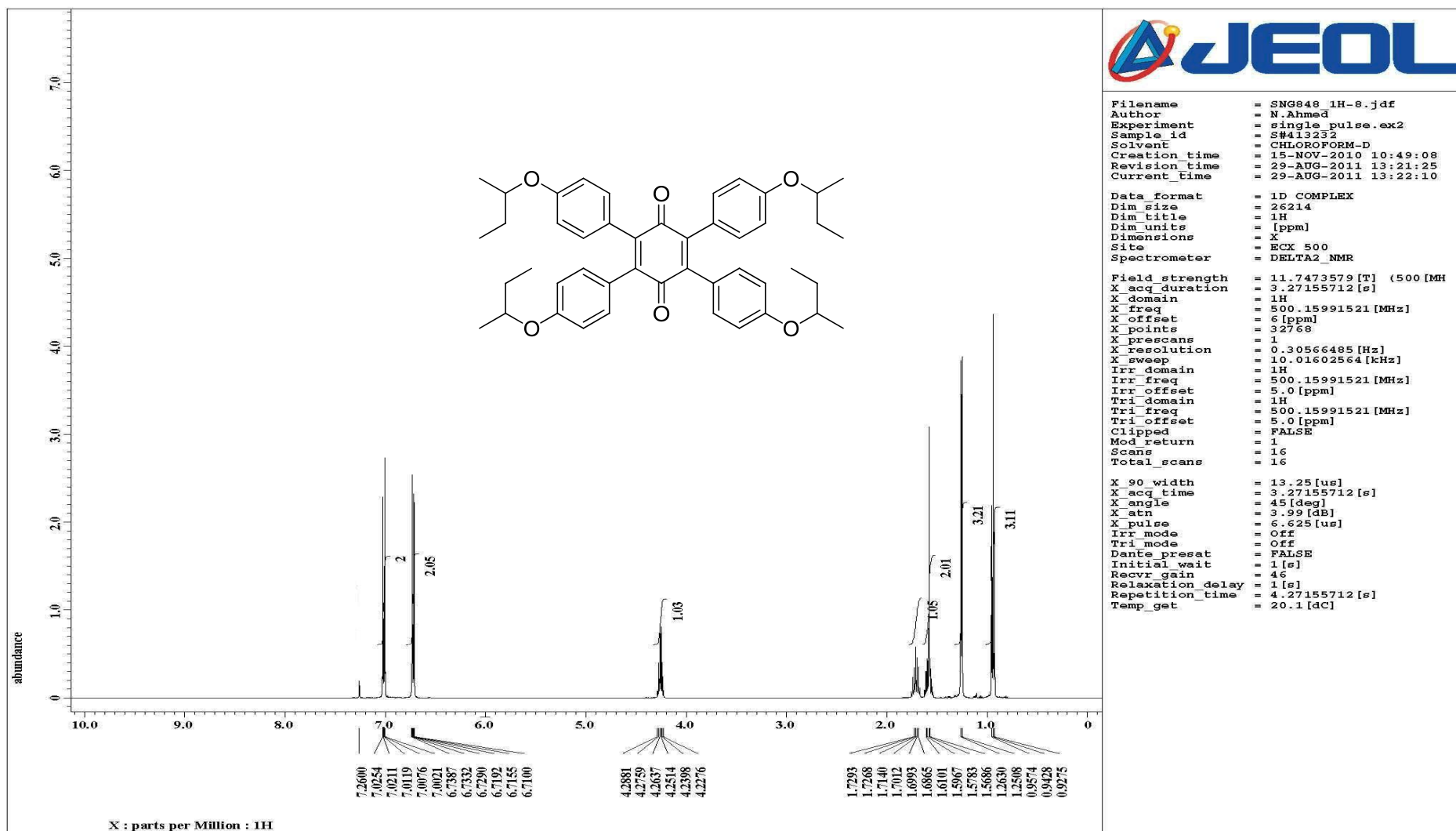


<sup>13</sup>C NMR spectrum of 2,3,5,6-tetrakis(3-methoxyphenyl)cyclohexa-2,5-diene-1,4-dione (5.5)

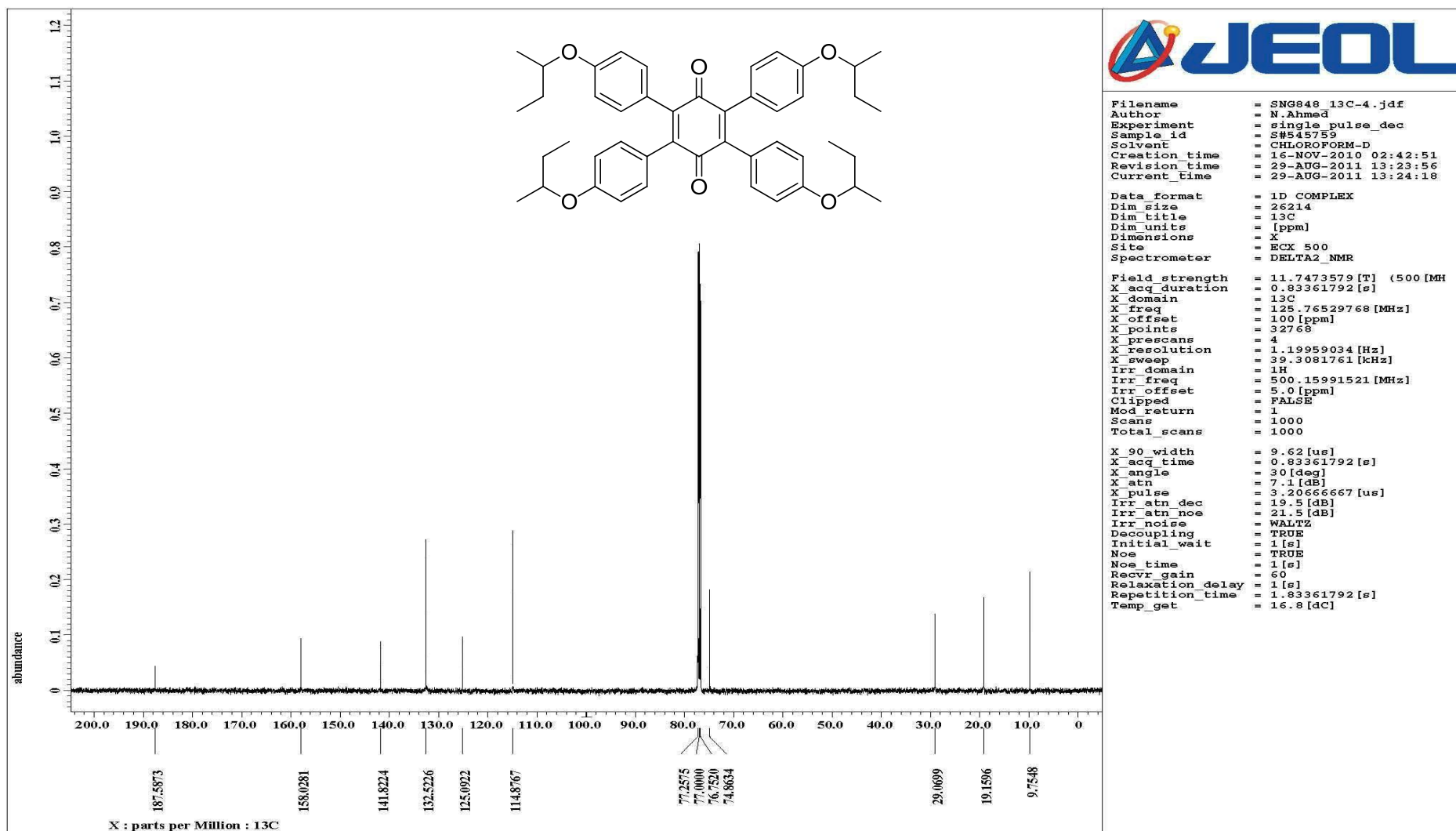




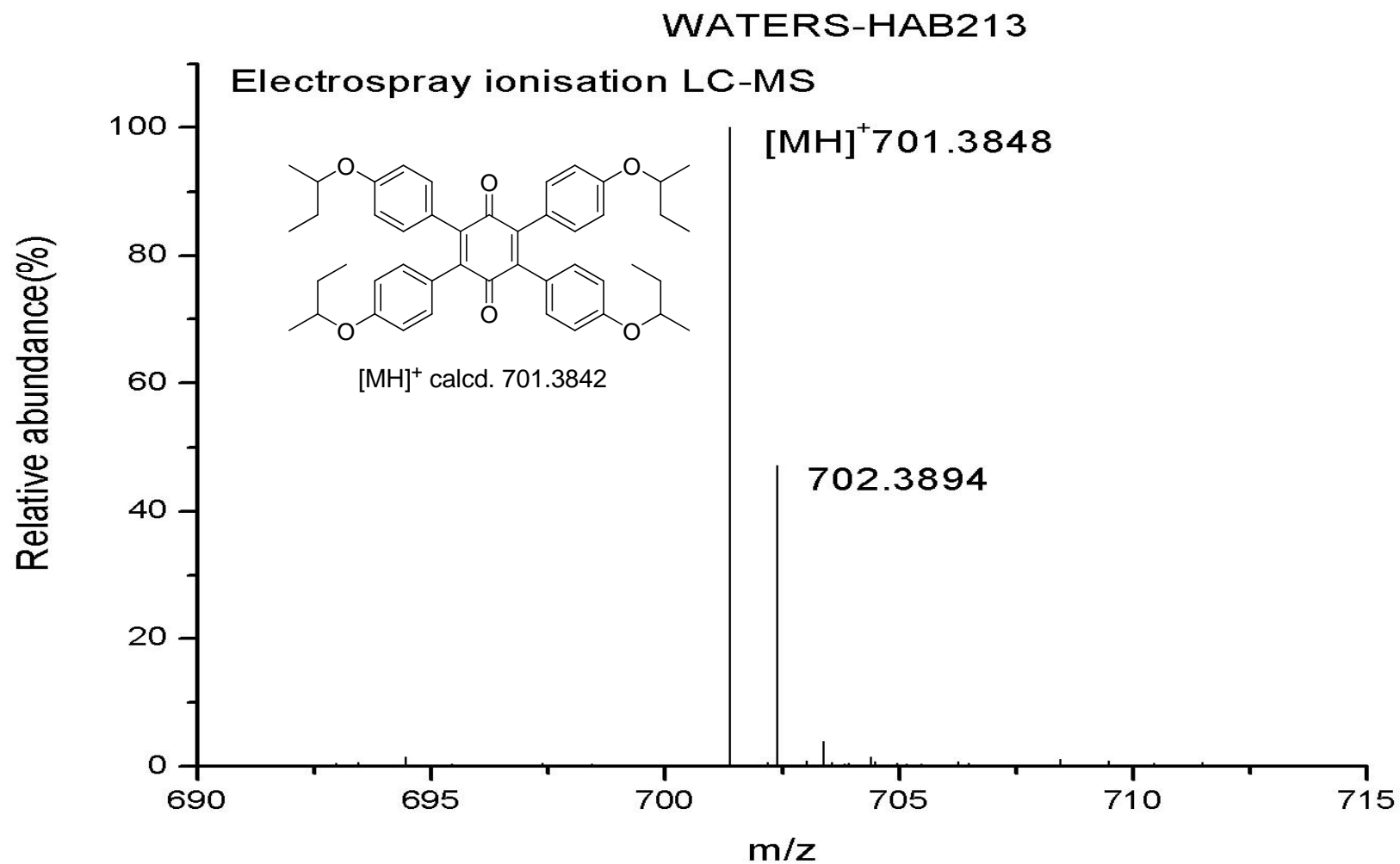
HRMS spectrum of 2,3,5,6-tetrakis(3-methoxyphenyl)cyclohexa-2,5-diene-1,4-dione (**5.5**)



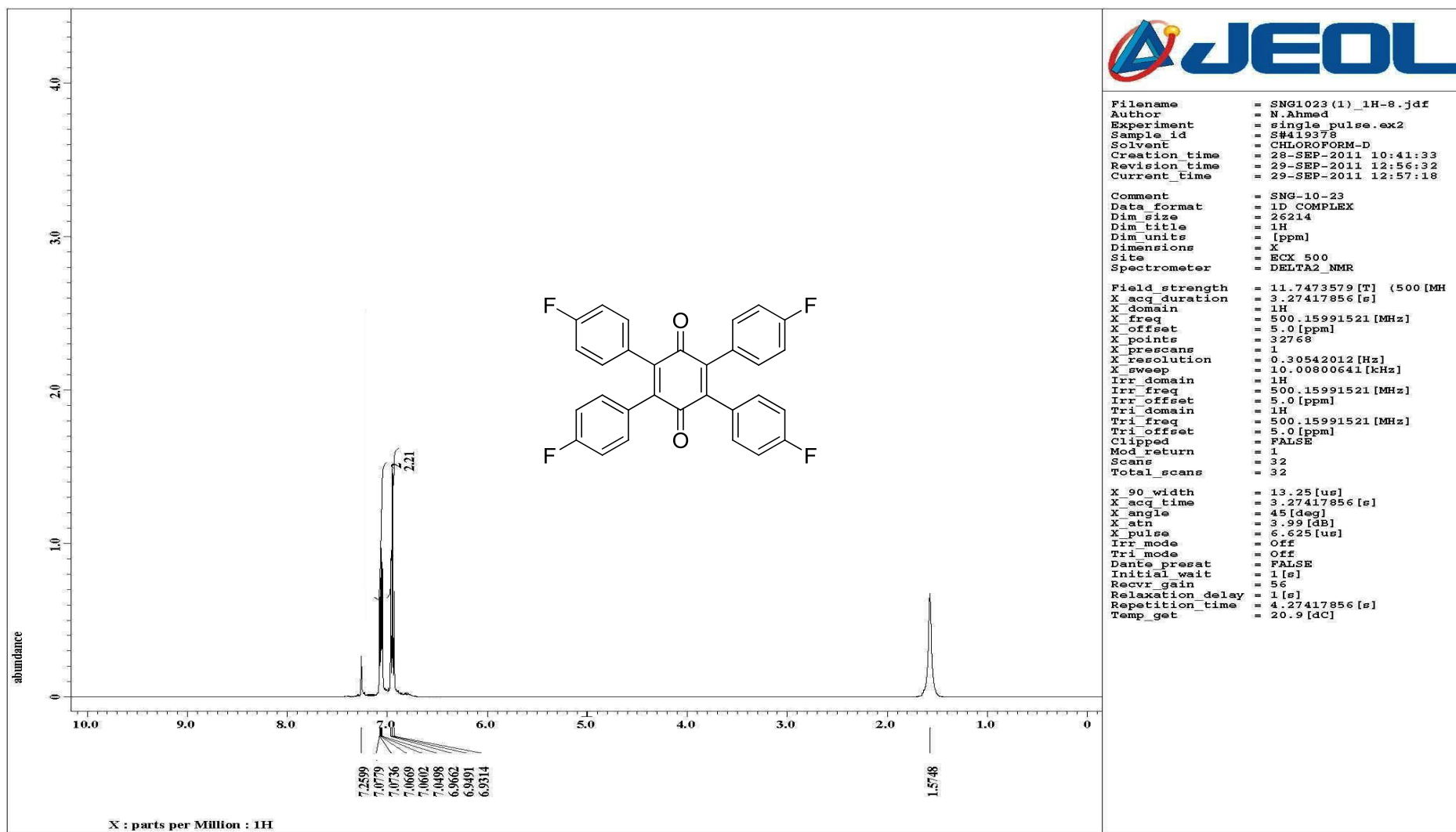
<sup>1</sup>H NMR spectrum of 2,3,5,6-tetrakis(4-sec-butoxyphenyl)cyclohexa-2,5-diene-1,4-dione (5.6)



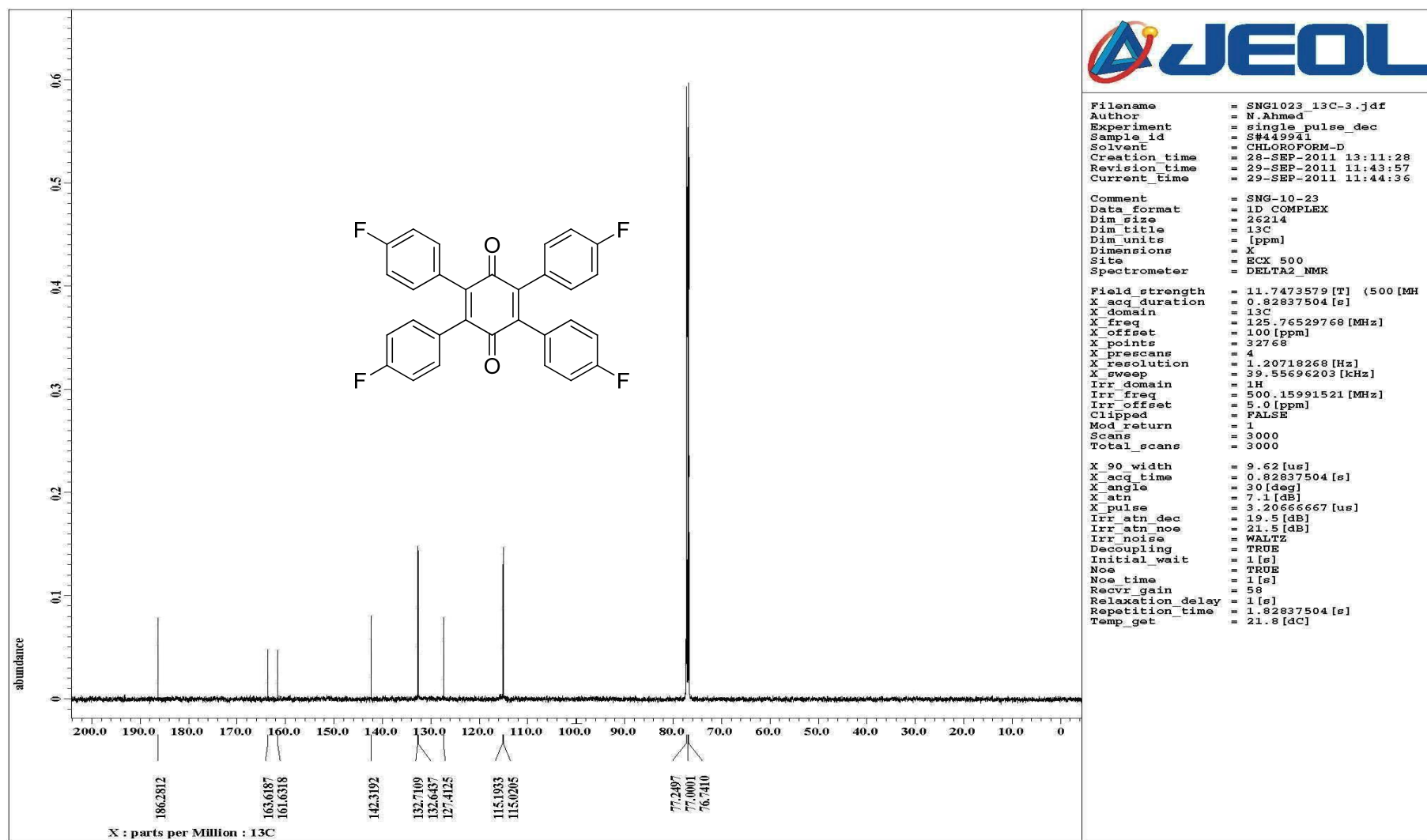
<sup>13</sup>C NMR spectrum of 2,3,5,6-tetrakis(4-*sec*-butoxyphenyl)cyclohexa-2,5-diene-1,4-dione (5.6)



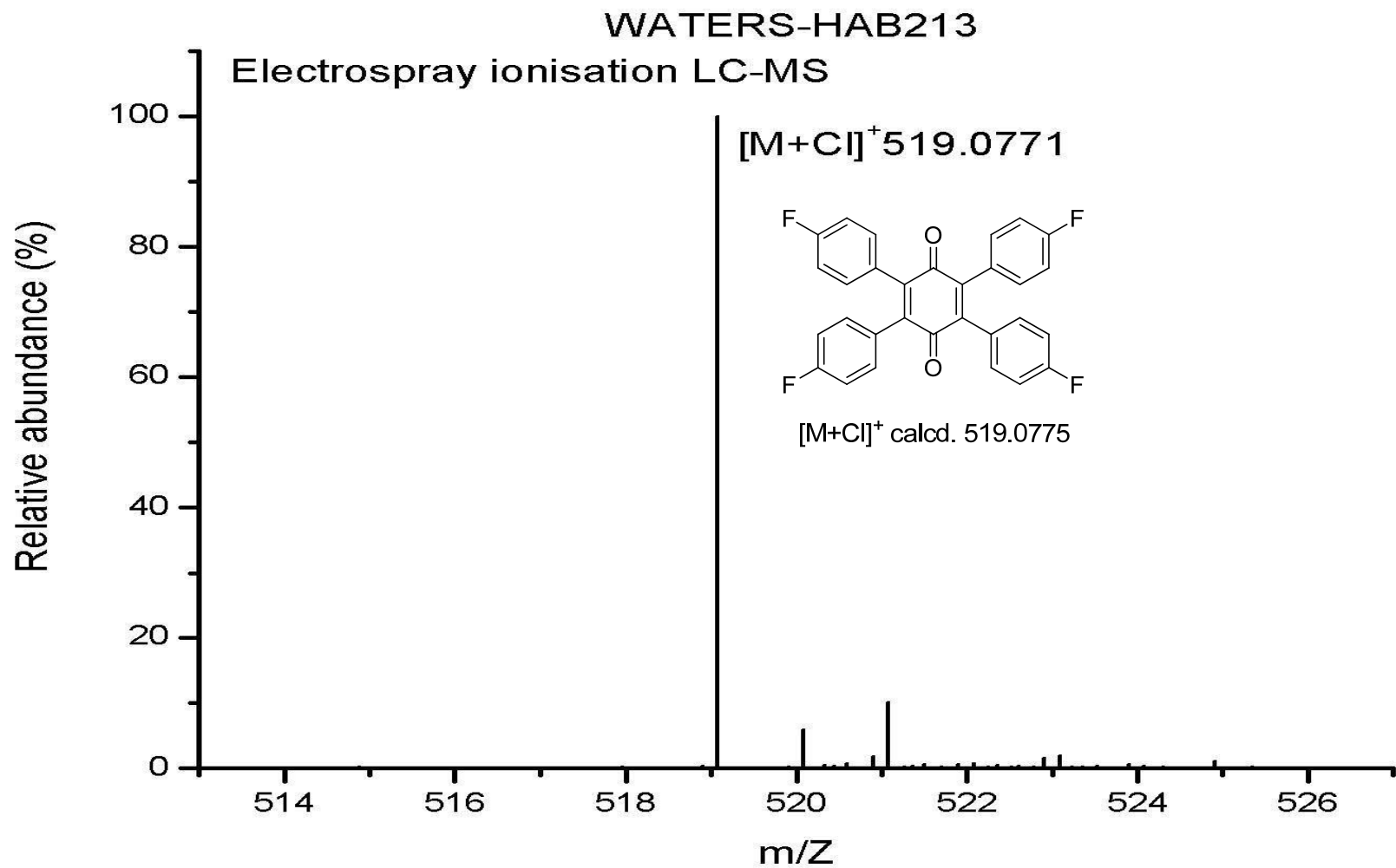
HRMS spectrum of 2,3,5,6-tetrakis(4-*sec*-butoxyphenyl)cyclohexa-2,5-diene-1,4-dione (**5.6**)



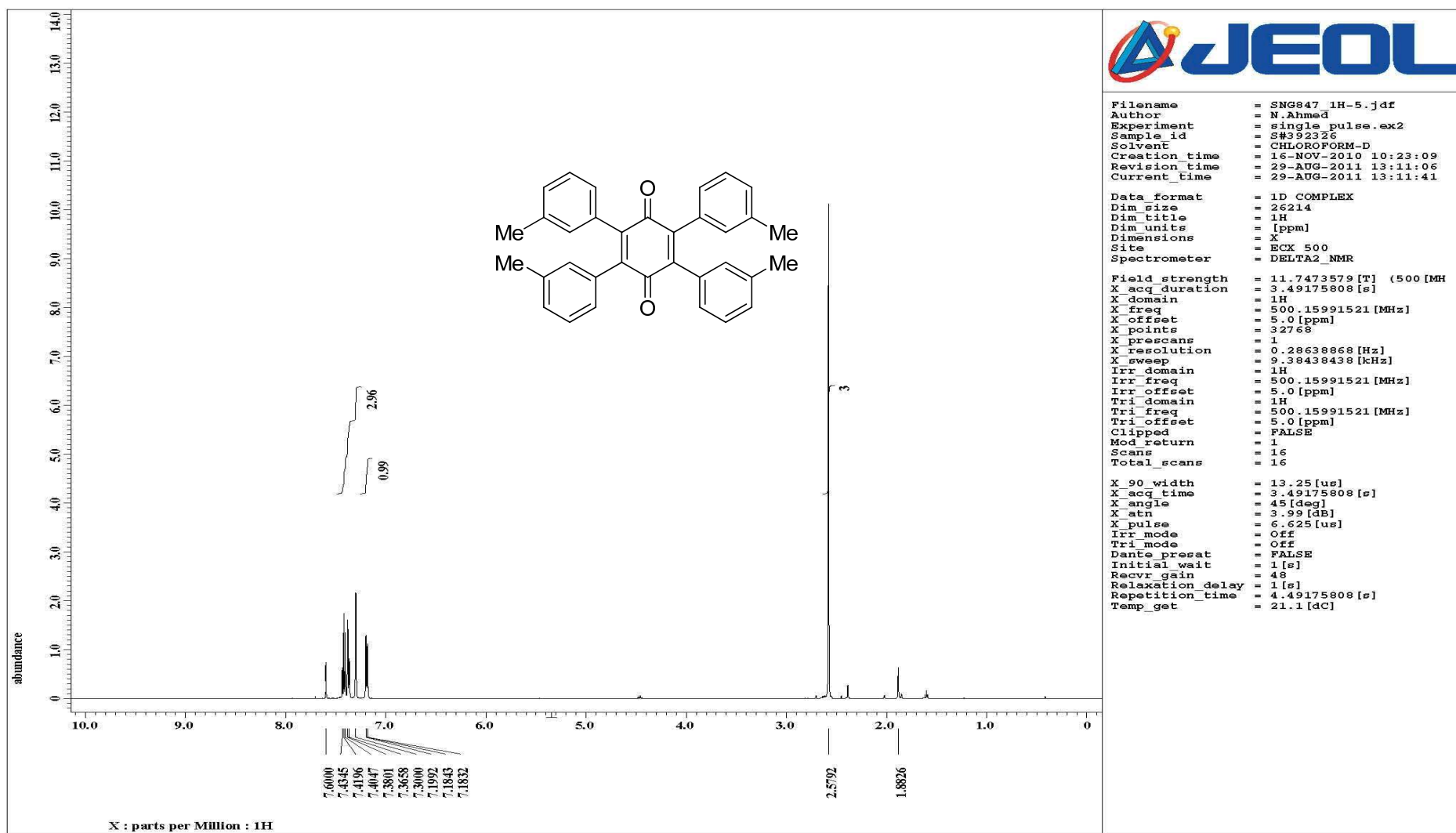
<sup>1</sup>H NMR spectrum of 2,3,5,6-tetrakis(4-fluorophenyl)cyclohexa-2,5-diene-1,4-dione (5.7)



<sup>13</sup>C NMR spectrum of 2,3,5,6-tetrakis(4-fluorophenyl)cyclohexa-2,5-diene-1,4-dione (5.7)

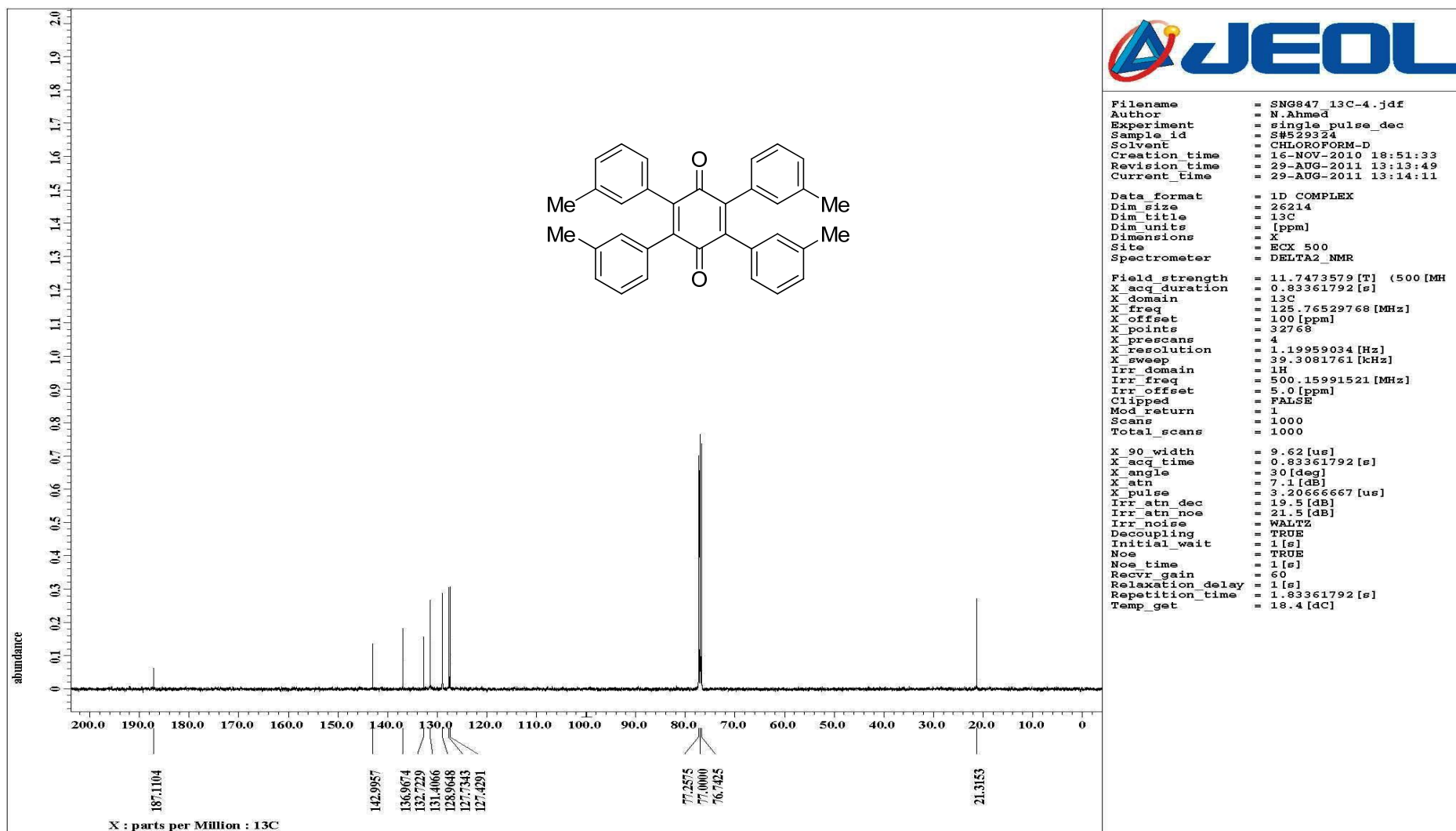


HRMS spectrum of 2,3,5,6-tetrakis(4-fluorophenyl)cyclohexa-2,5-diene-1,4-dione (**5.7**)

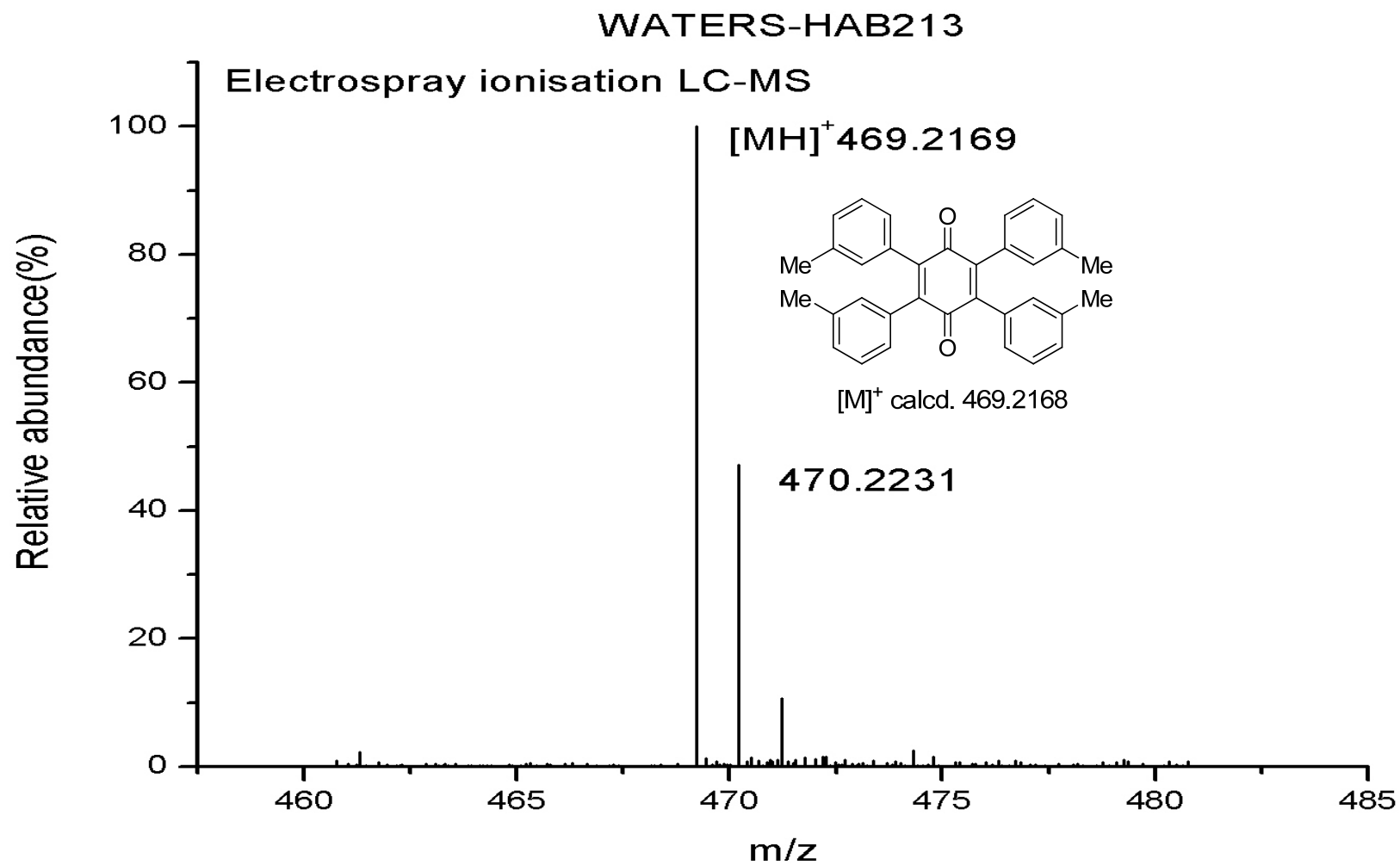


<sup>1</sup>H NMR spectrum of 2,3,5,6-tetra 3-tolylcyclohexa-2,5-diene-1,4-dione (**5.8**)

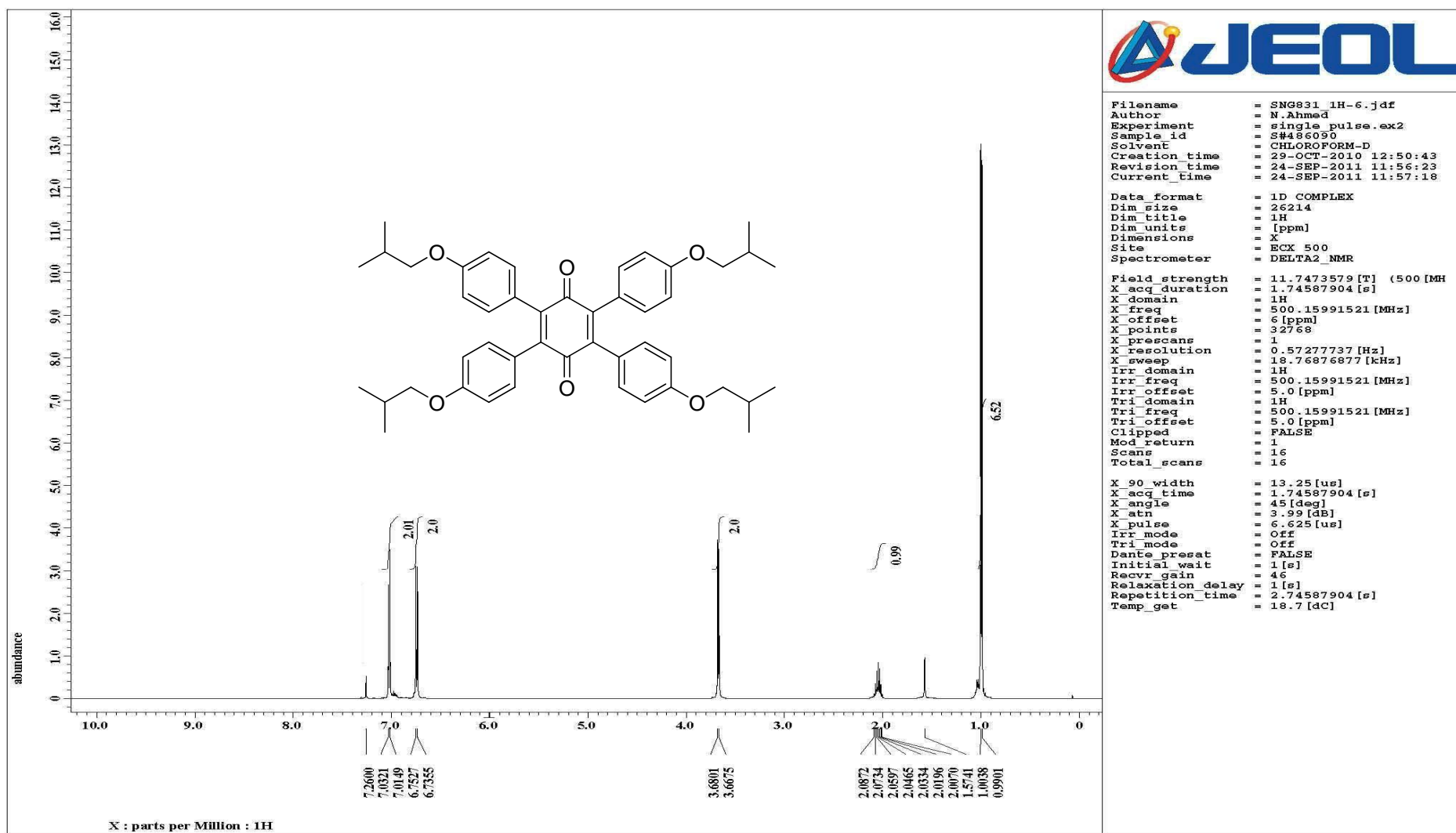




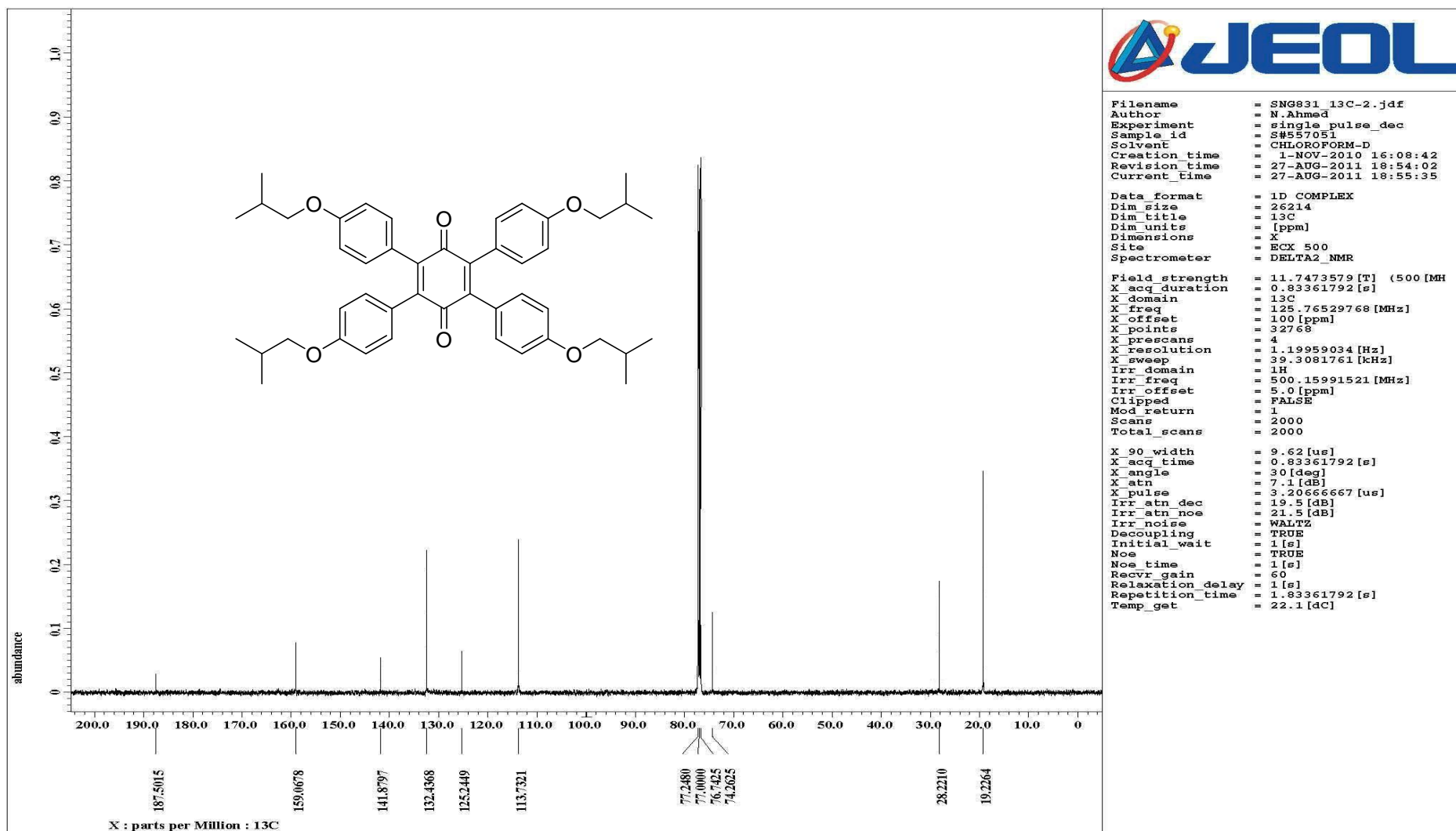
<sup>13</sup>C NMR spectrum of 2,3,5,6-tetra 3-tolylcyclohexa-2,5-diene-1,4-dione (5.8)



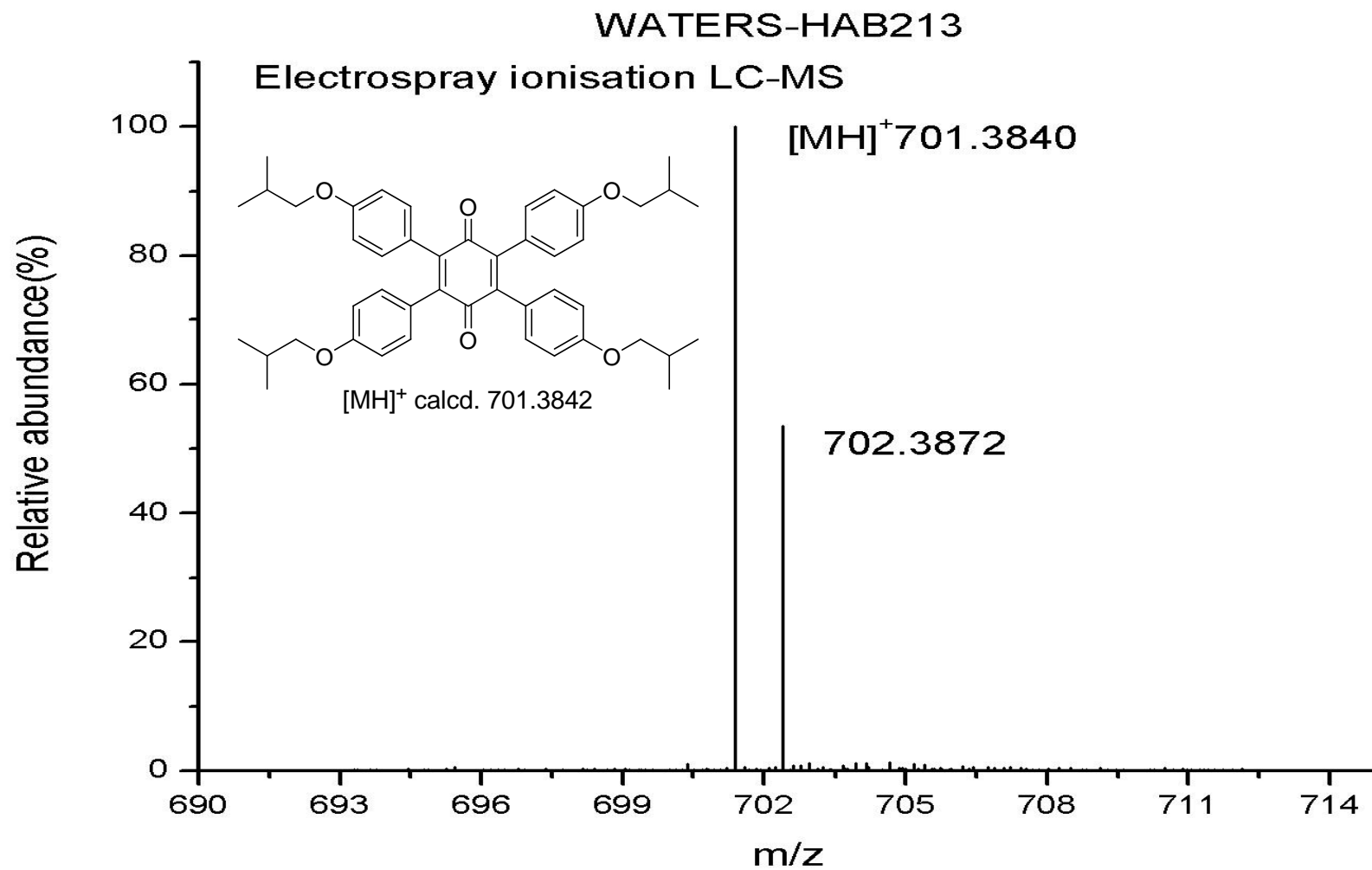
HRMS spectrum of 2,3,5,6-tetra 3-tolylcyclohexa-2,5-diene-1,4-dione (**5.8**)



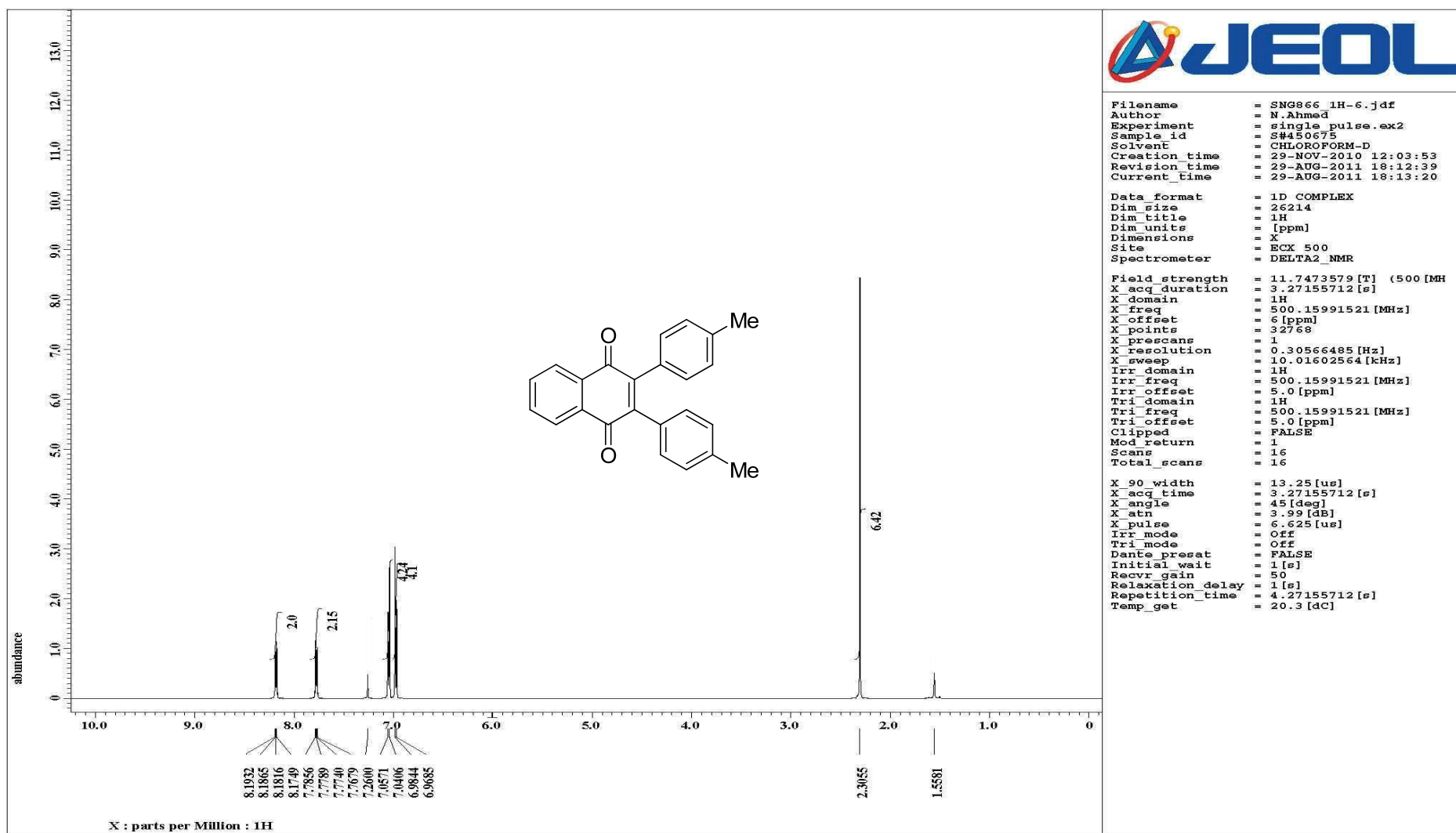
<sup>1</sup>H NMR spectrum of 2,3,5,6-tetrakis(4-isobutoxyphenyl)cyclohexa-2,5-diene-1,4-dione (5.9)



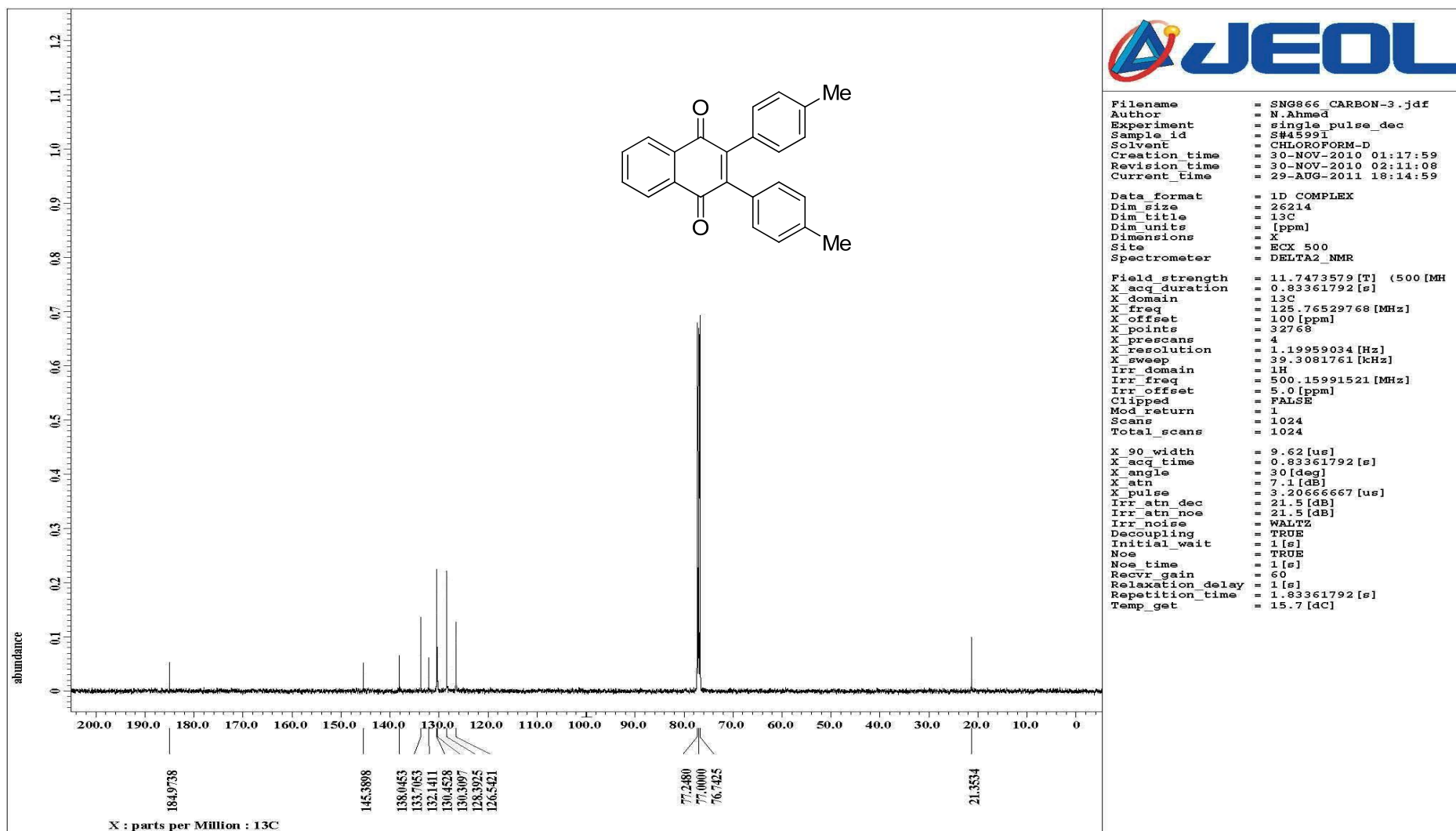
<sup>13</sup>C NMR spectrum of 2,3,5,6-tetrakis(4-isobutoxyphenyl)cyclohexa-2,5-diene-1,4-dione (5.9)



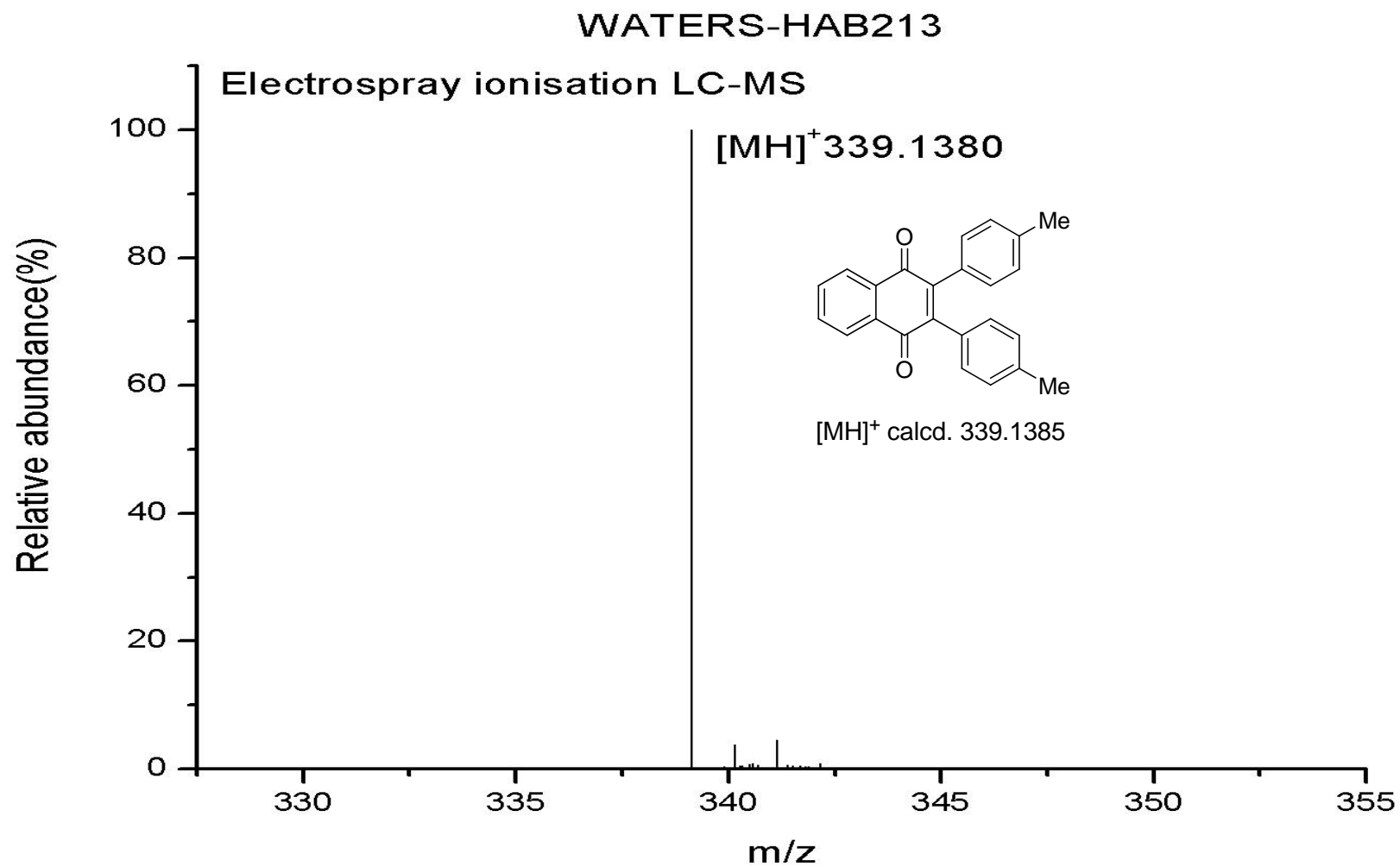
HRMS spectrum of 2,3,5,6-tetrakis(4-isobutoxyphenyl)cyclohexa-2,5-diene-1,4-dione (**5.9**)



<sup>1</sup>H NMR spectrum of 2,3-di-4-tolyl-1,4-naphthoquinone (6.1)

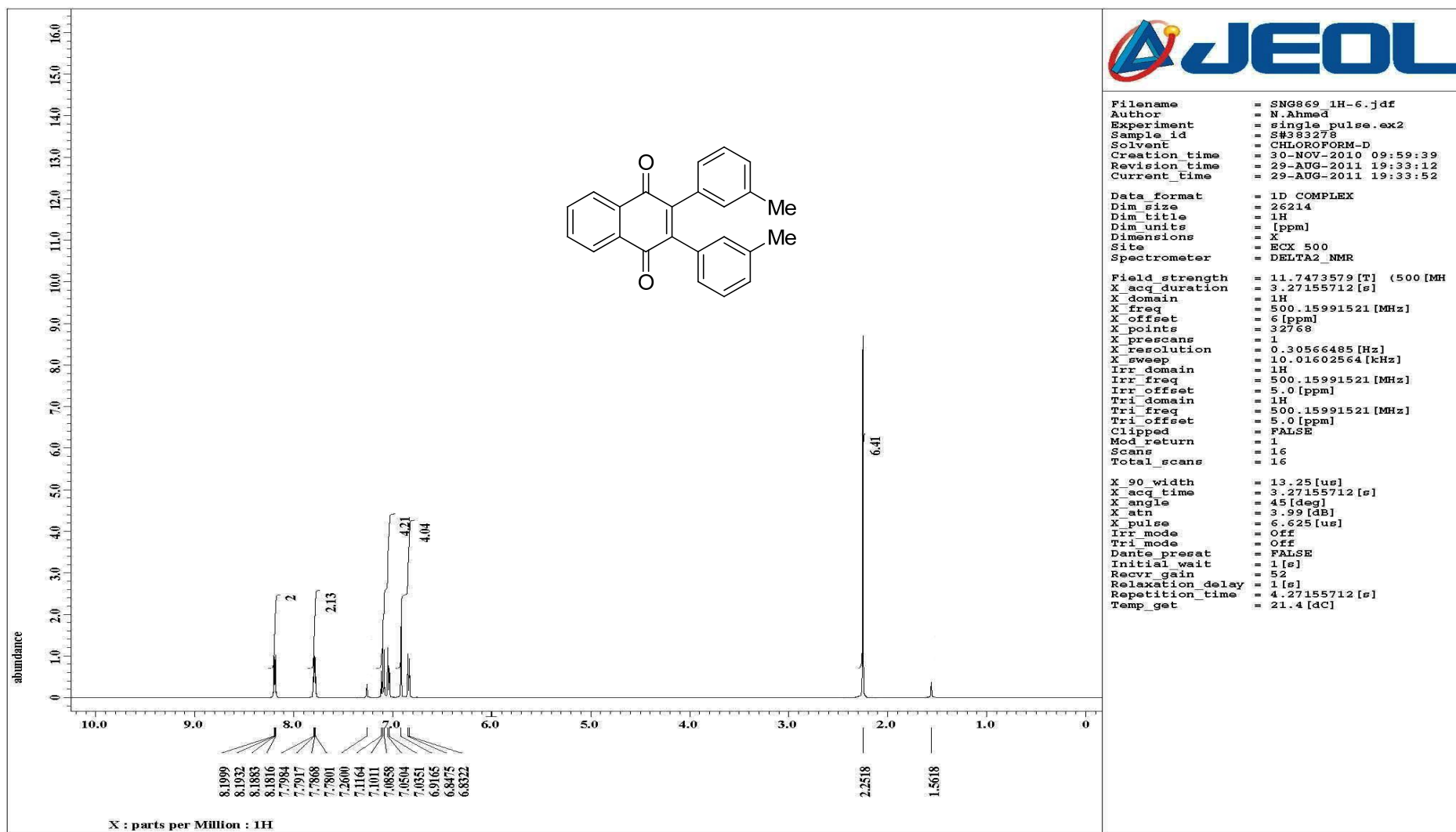


<sup>13</sup>C NMR spectrum of 2,3-di-4-tolyl-1,4-naphthoquinone (6.1)

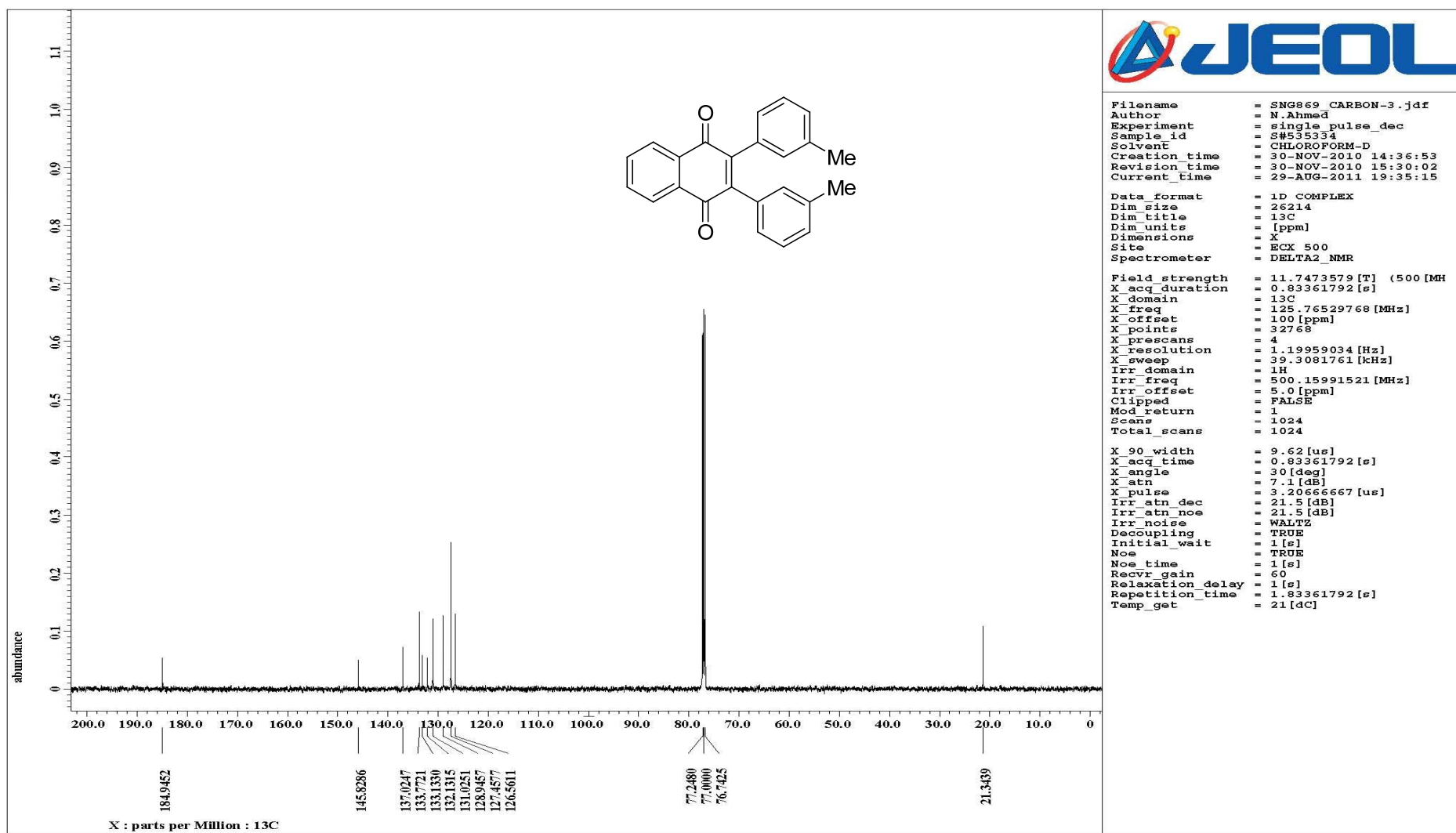


HRMS spectrum of 2,3-di-4-tolyl-1,4-naphthoquinone (**6.1**)

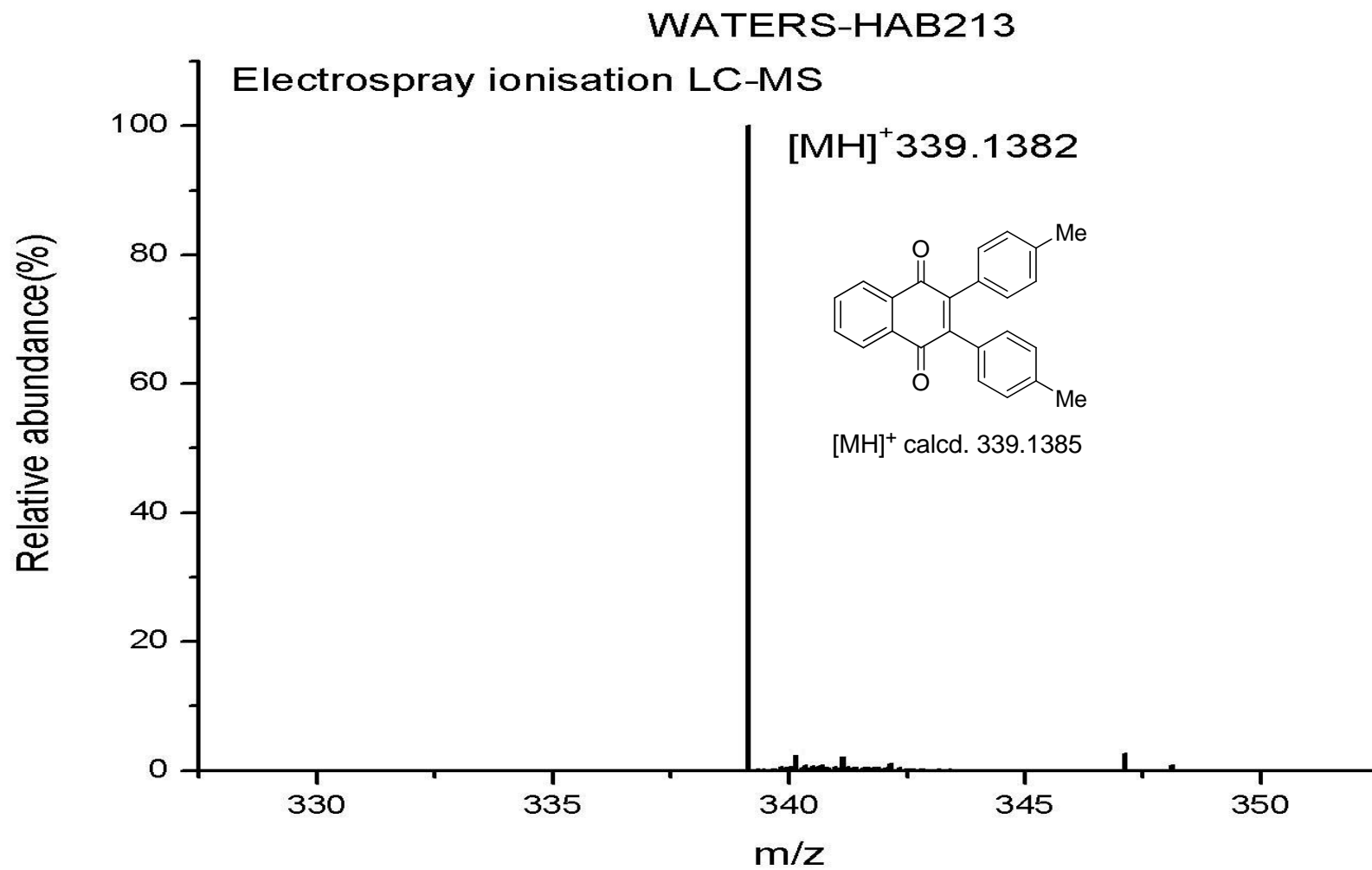




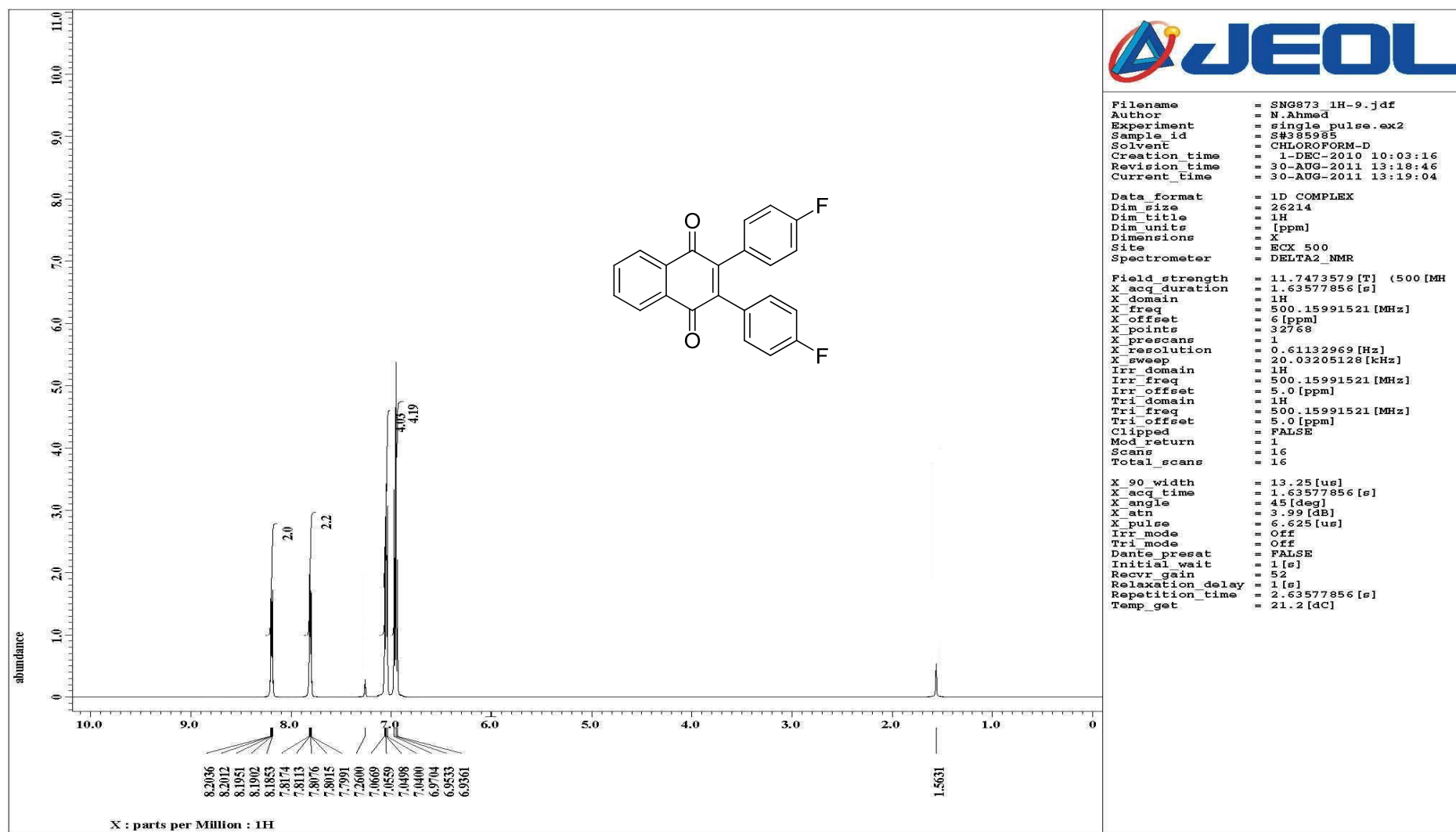
<sup>1</sup>H NMR spectrum of 2,3-di-3-tolyl-1,4-naphthoquinone (6.2)



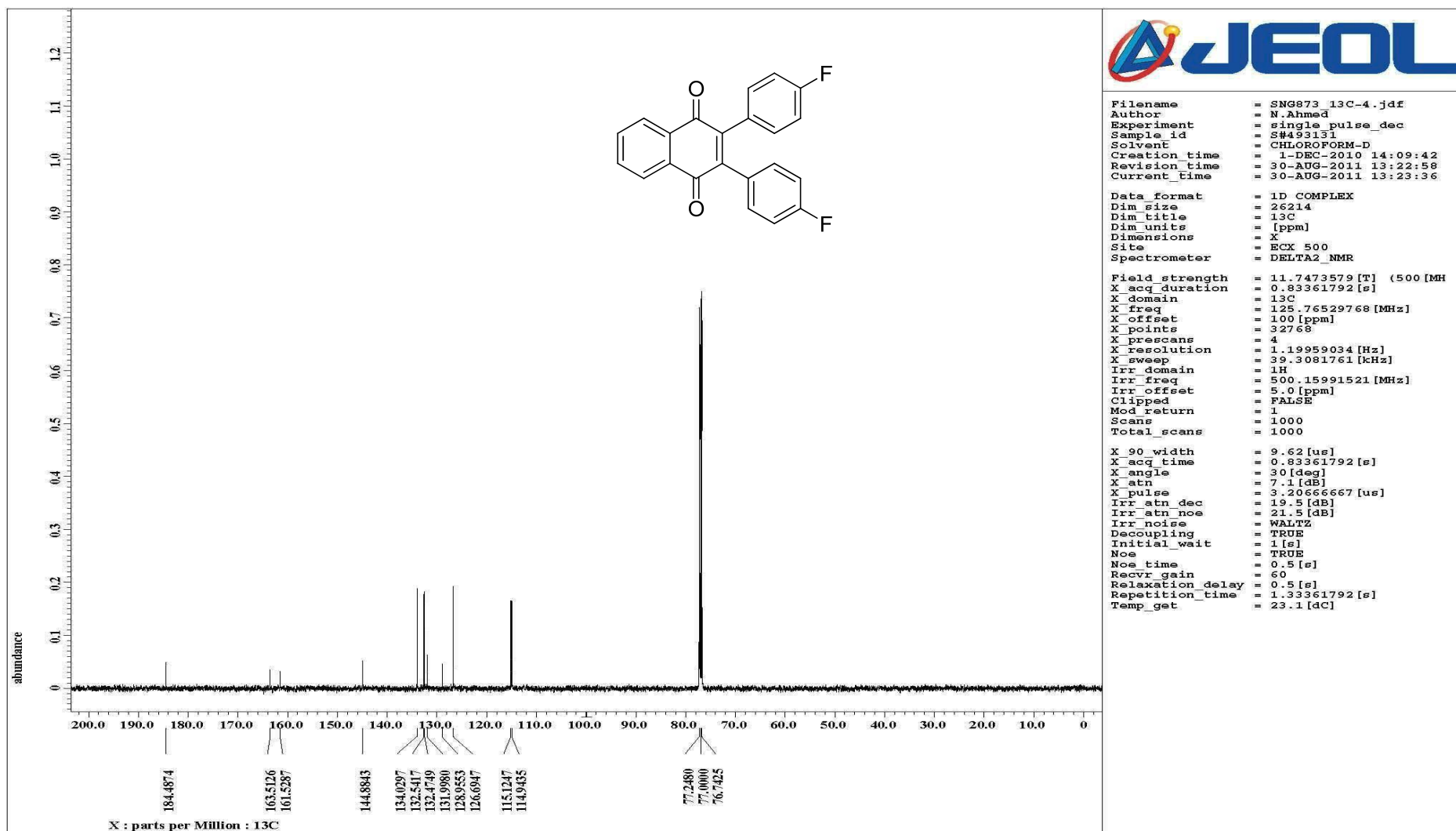
<sup>13</sup>C NMR spectrum of 2,3-di-3-tolyl-1,4-naphthoquinone (6.2)



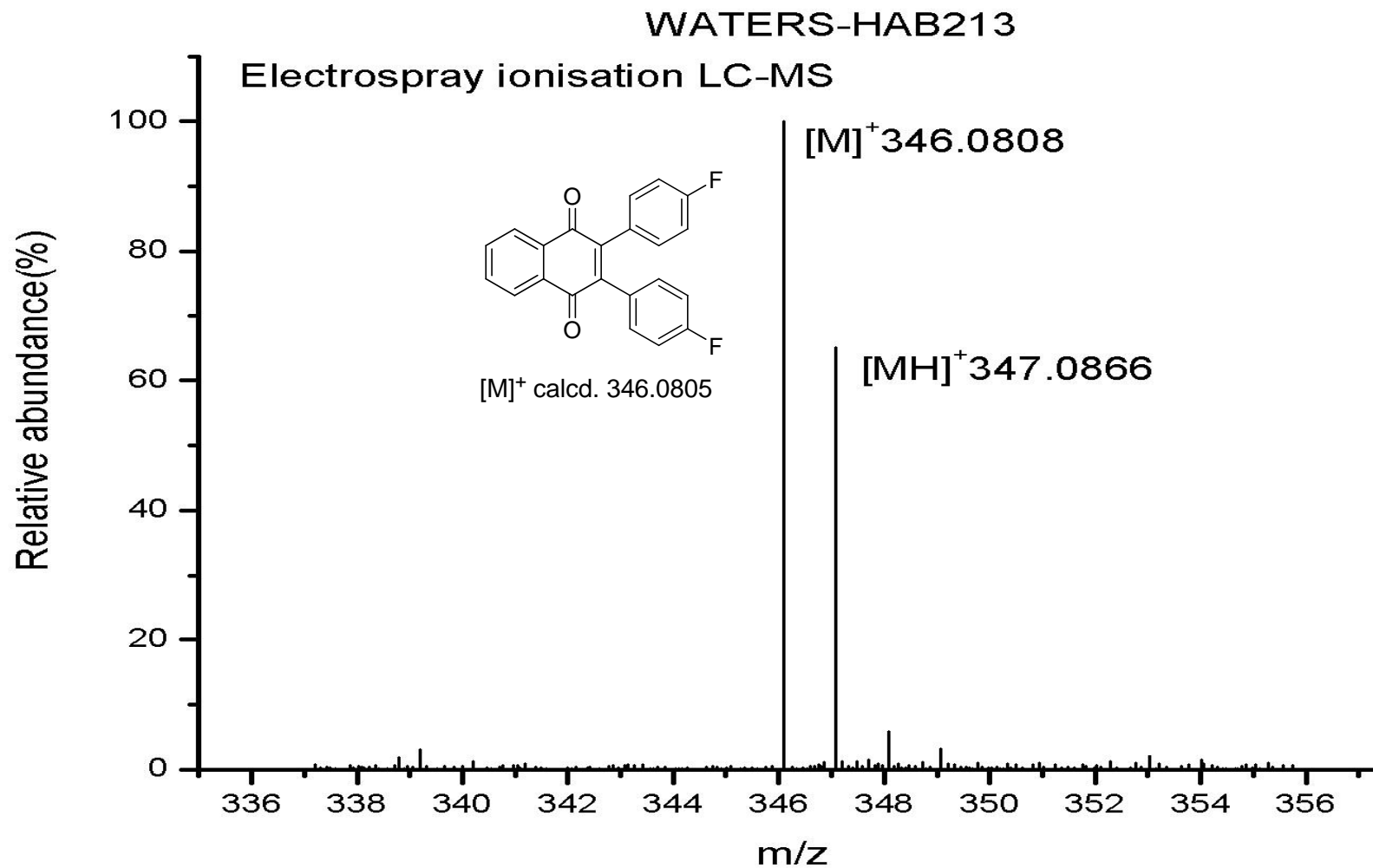
HRMS spectrum of 2,3-di-3-tolyl-1,4-naphthoquinone (**6.2**)



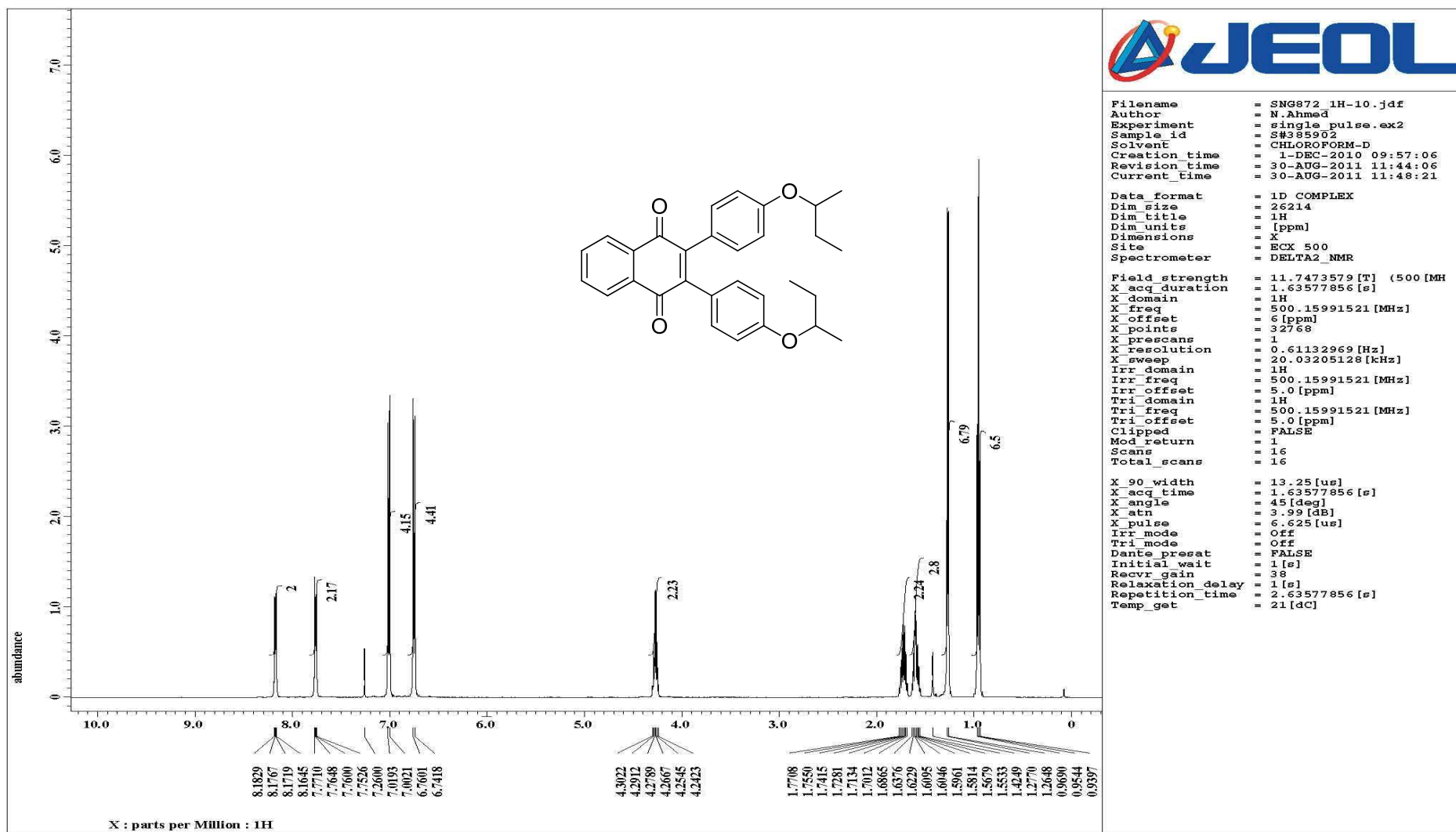
<sup>1</sup>H NMR spectrum of 2,3-bis(4-fluorophenyl)-1,4-naphthoquinone (6.3)



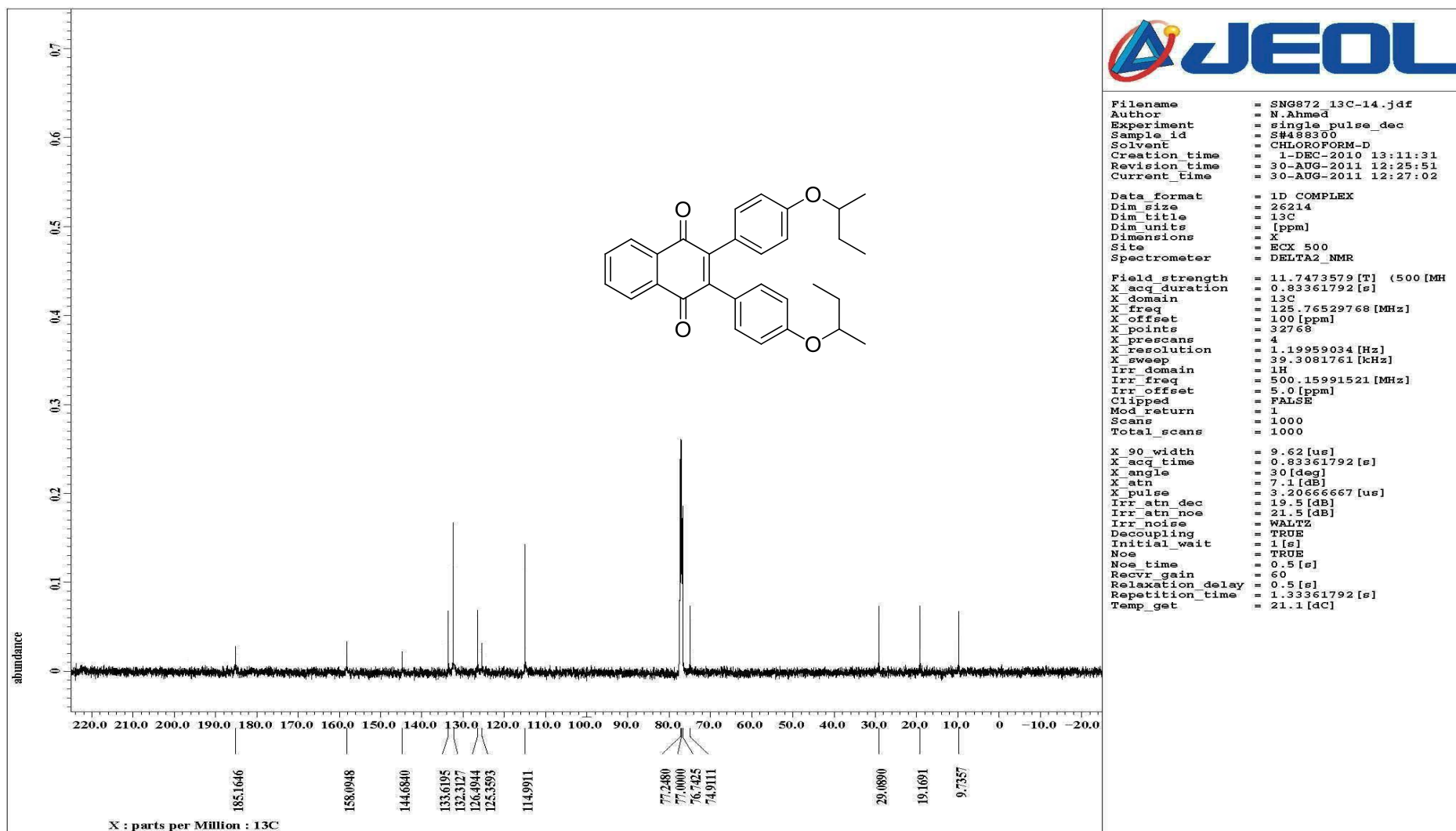
<sup>13</sup>C NMR spectrum of 2,3-bis(4-fluorophenyl)-1,4-naphthoquinone (6.3)



HRMS spectrum of 2,3-bis(4-fluorophenyl)-1,4-naphthoquinone (**6.3**)

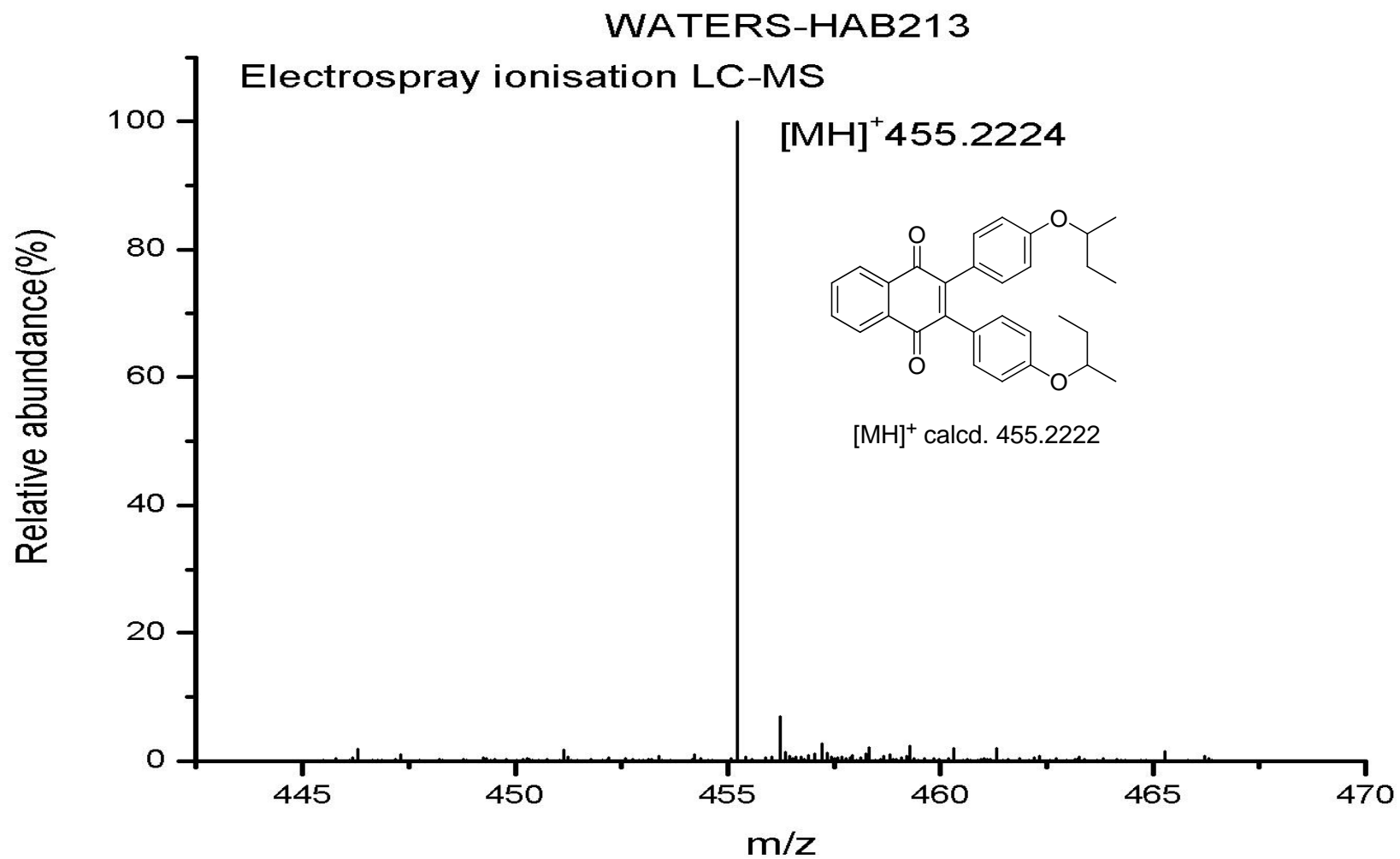


<sup>1</sup>H NMR spectrum of 2,3-bis(4-sec-butoxyphenyl)-1,4-naphthoquinone (6.4)

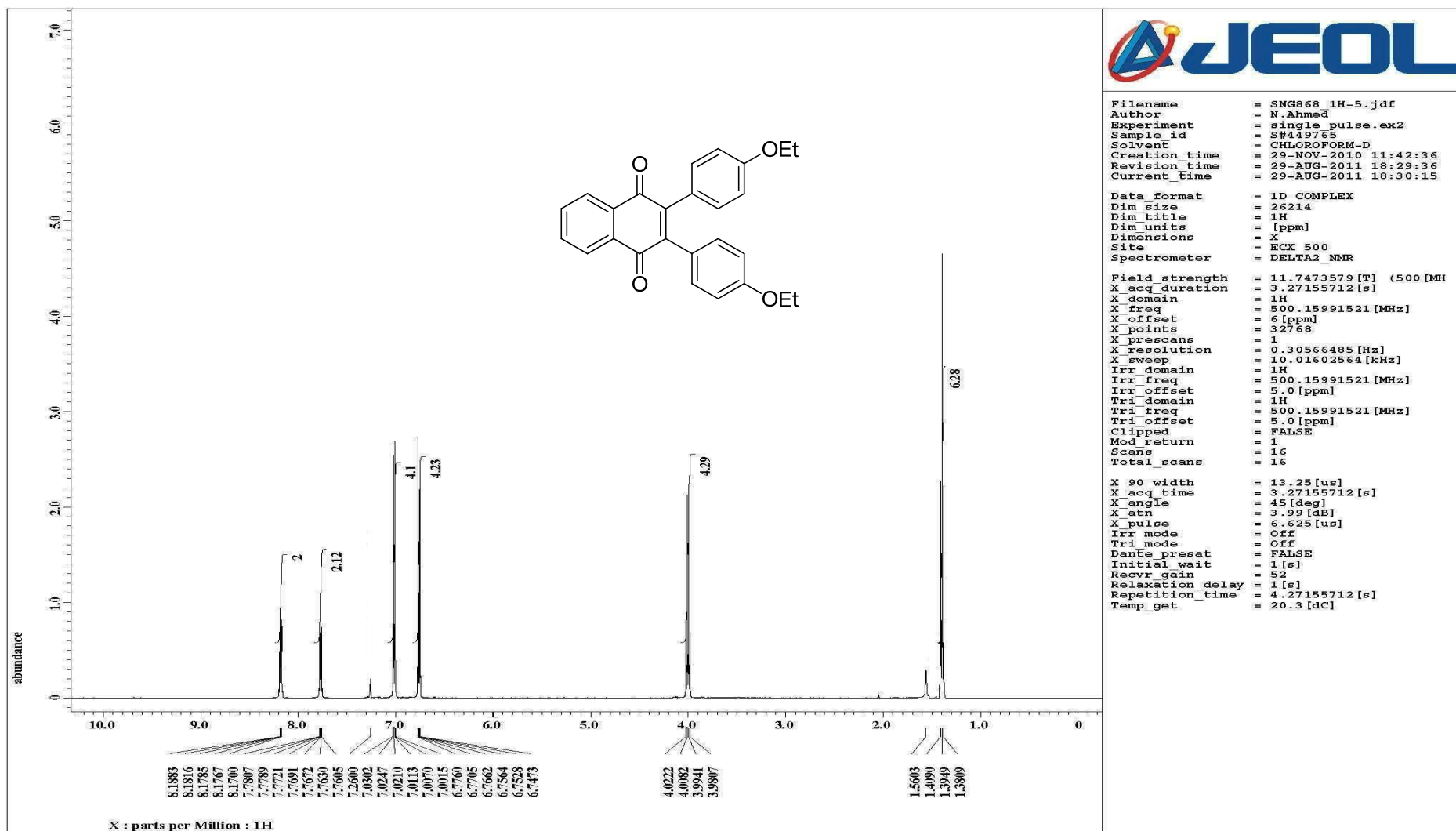


<sup>13</sup>C NMR spectrum of 2,3-bis(4-sec-butoxyphenyl)-1,4-naphthoquinone (6.4)

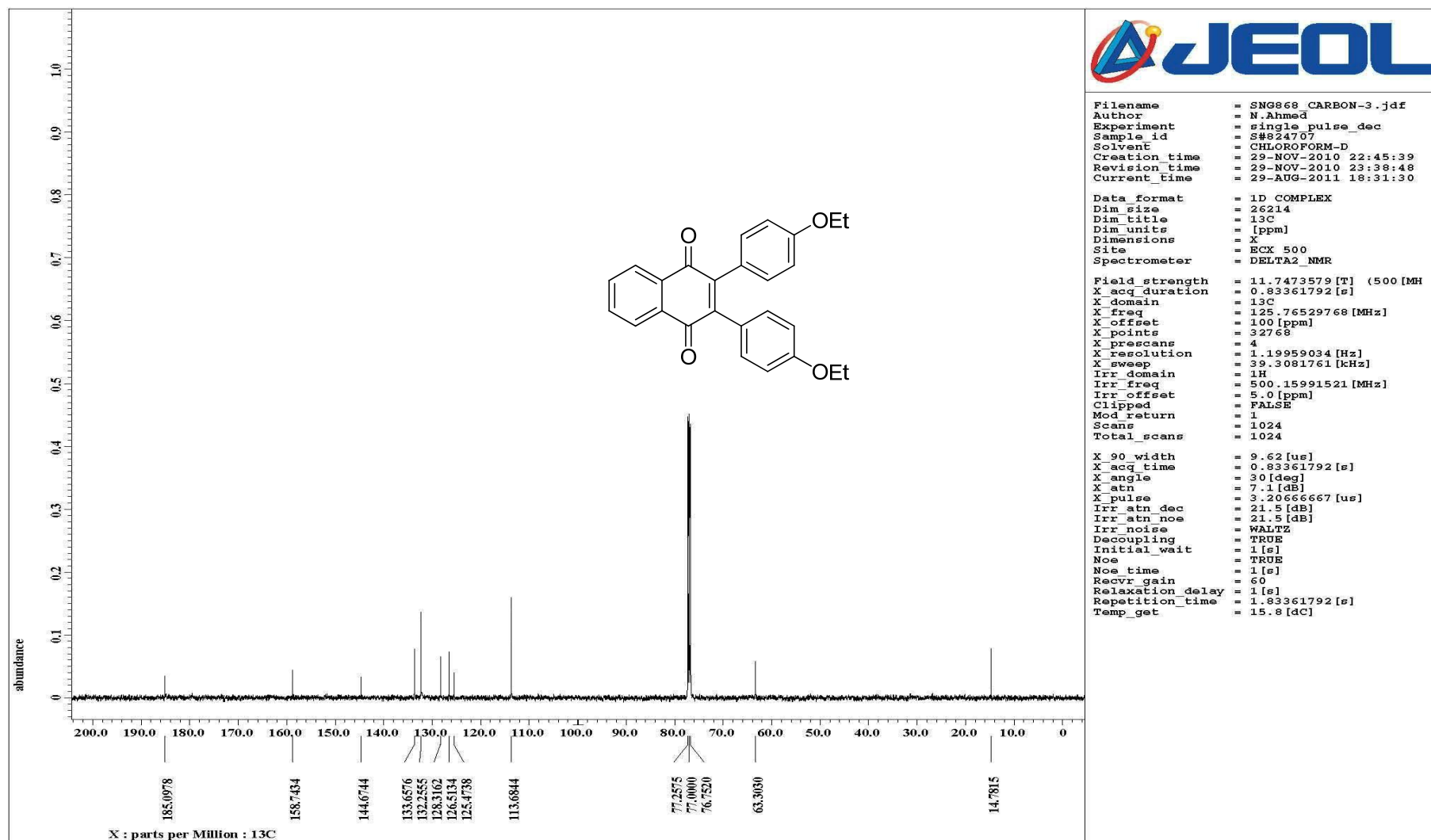




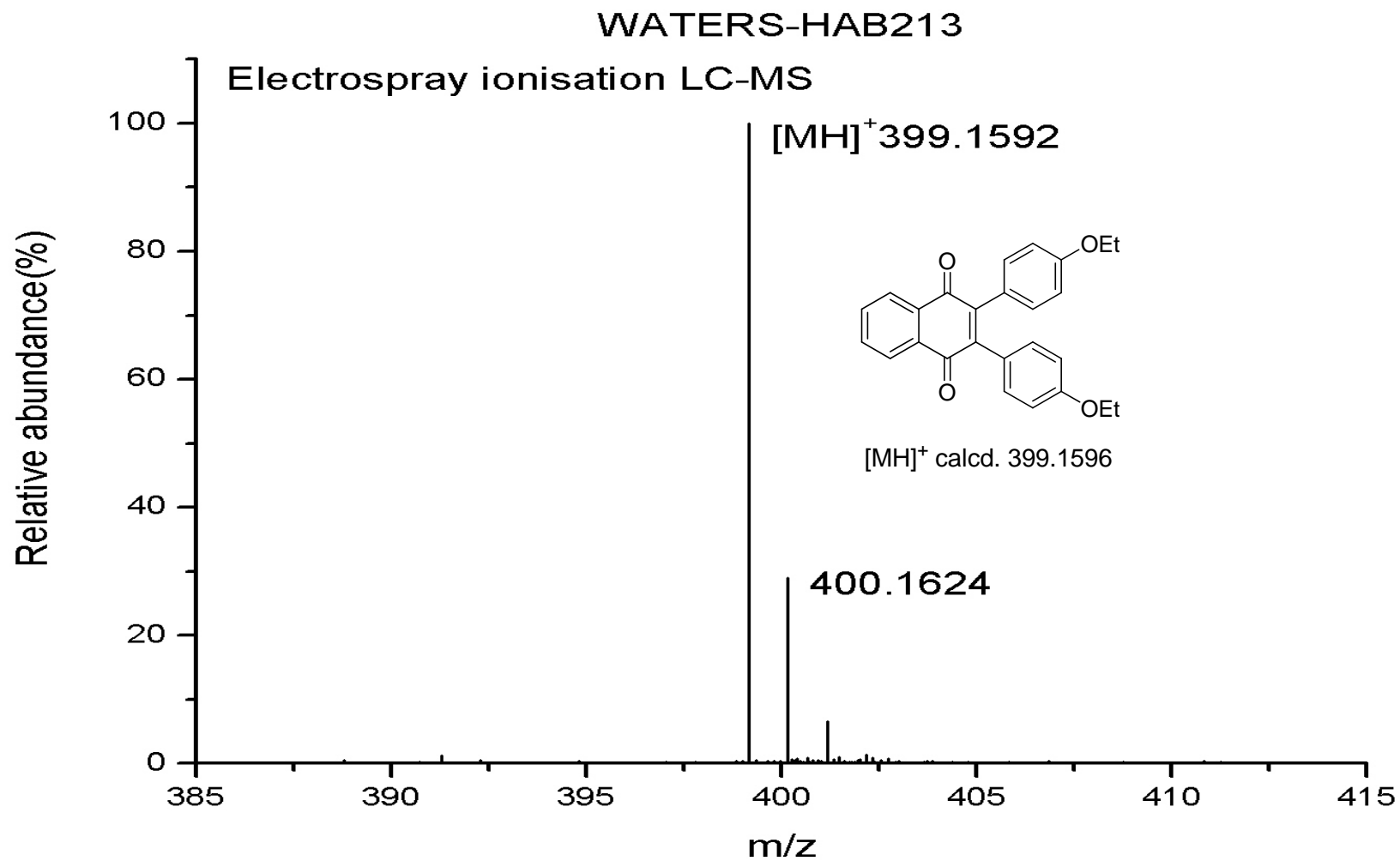
HRMS spectrum of 2,3-bis(4-sec-butoxyphenyl)-1,4-naphthoquinone (**6.4**)



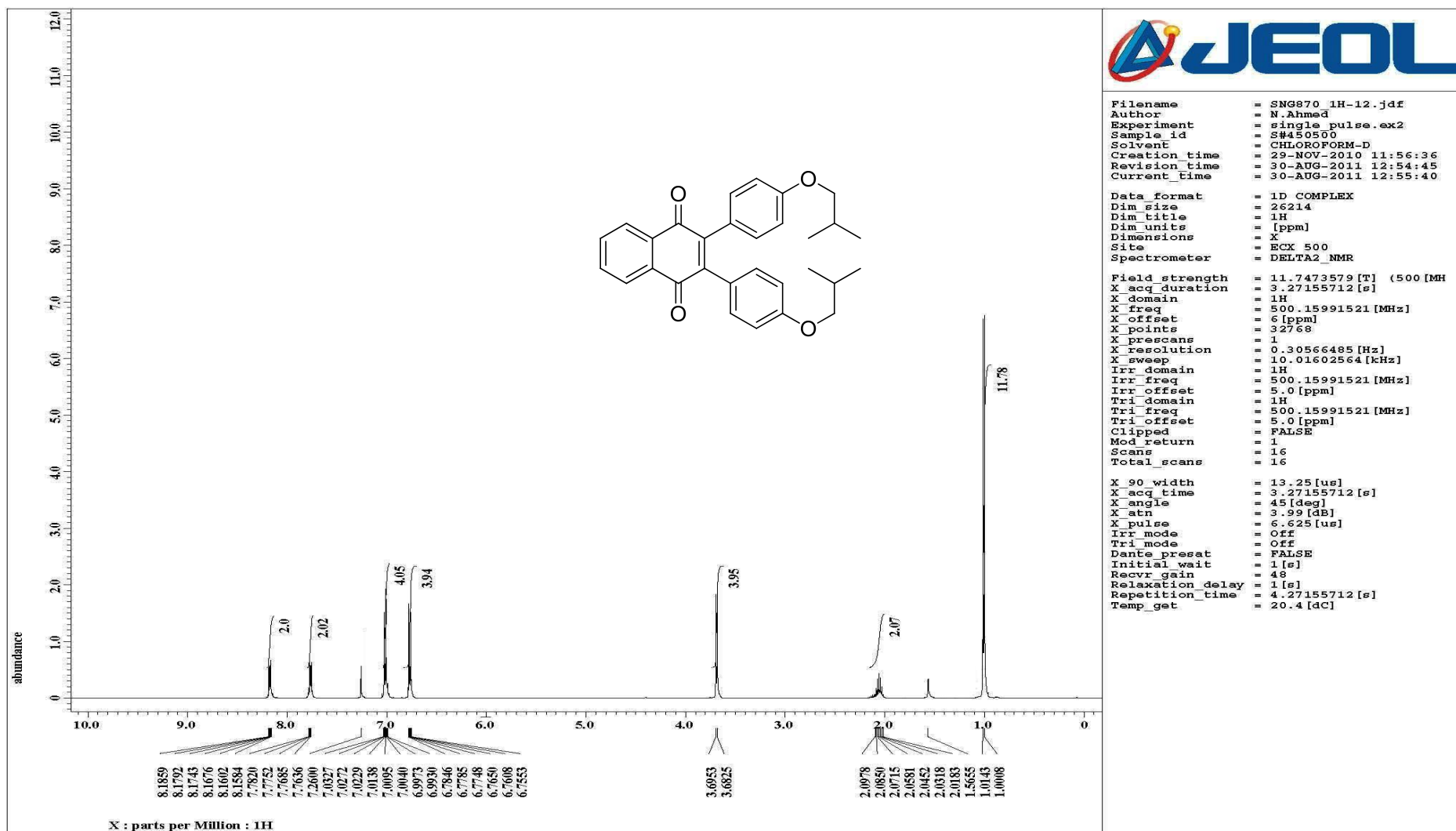
<sup>1</sup>H NMR spectrum of 2,3-bis(4-ethoxyphenyl)-1,4-naphthoquinone (6.5)



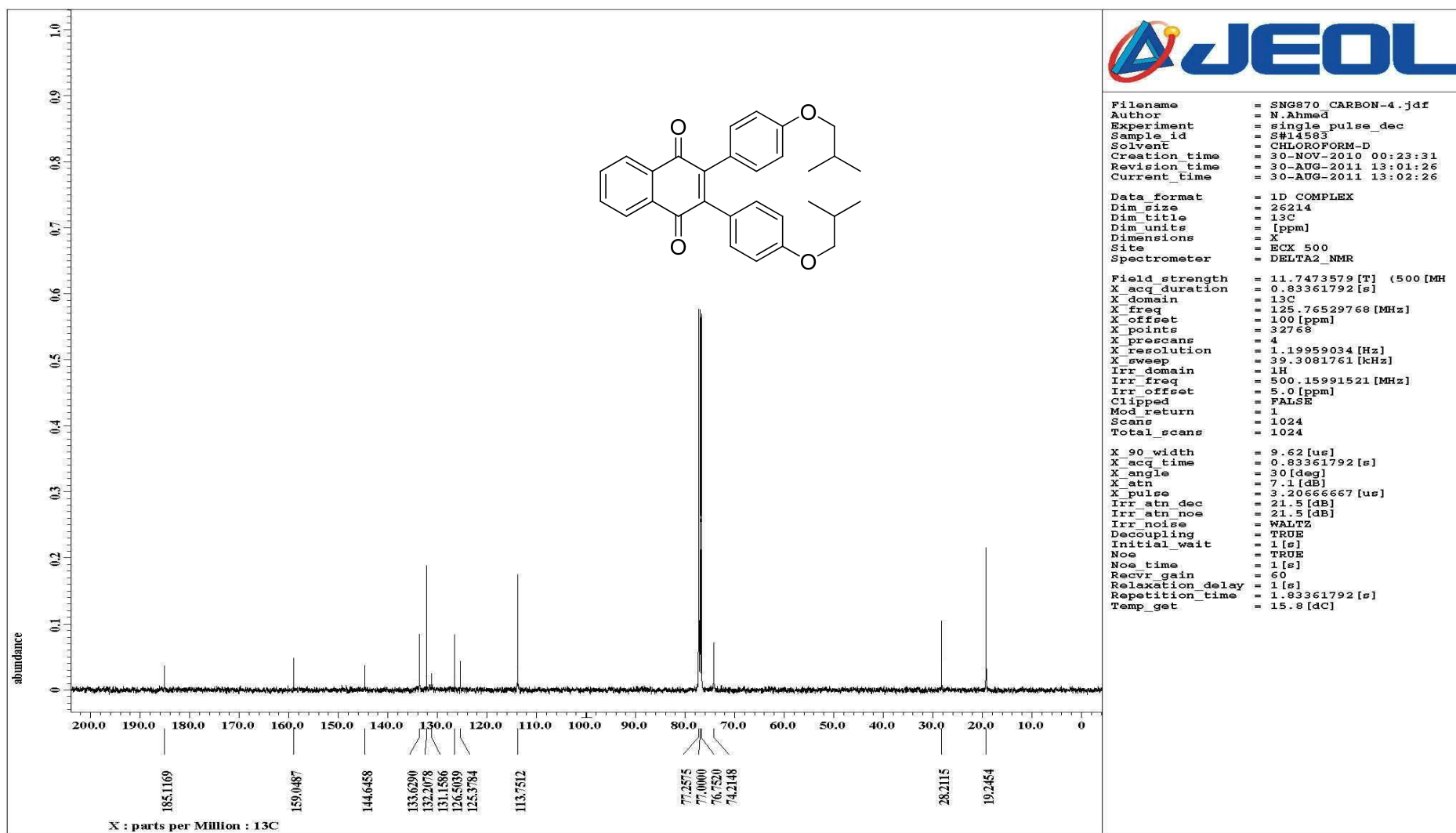
<sup>13</sup>C NMR spectrum of 2,3-bis(4-ethoxyphenyl)-1,4-naphthoquinone (6.5)



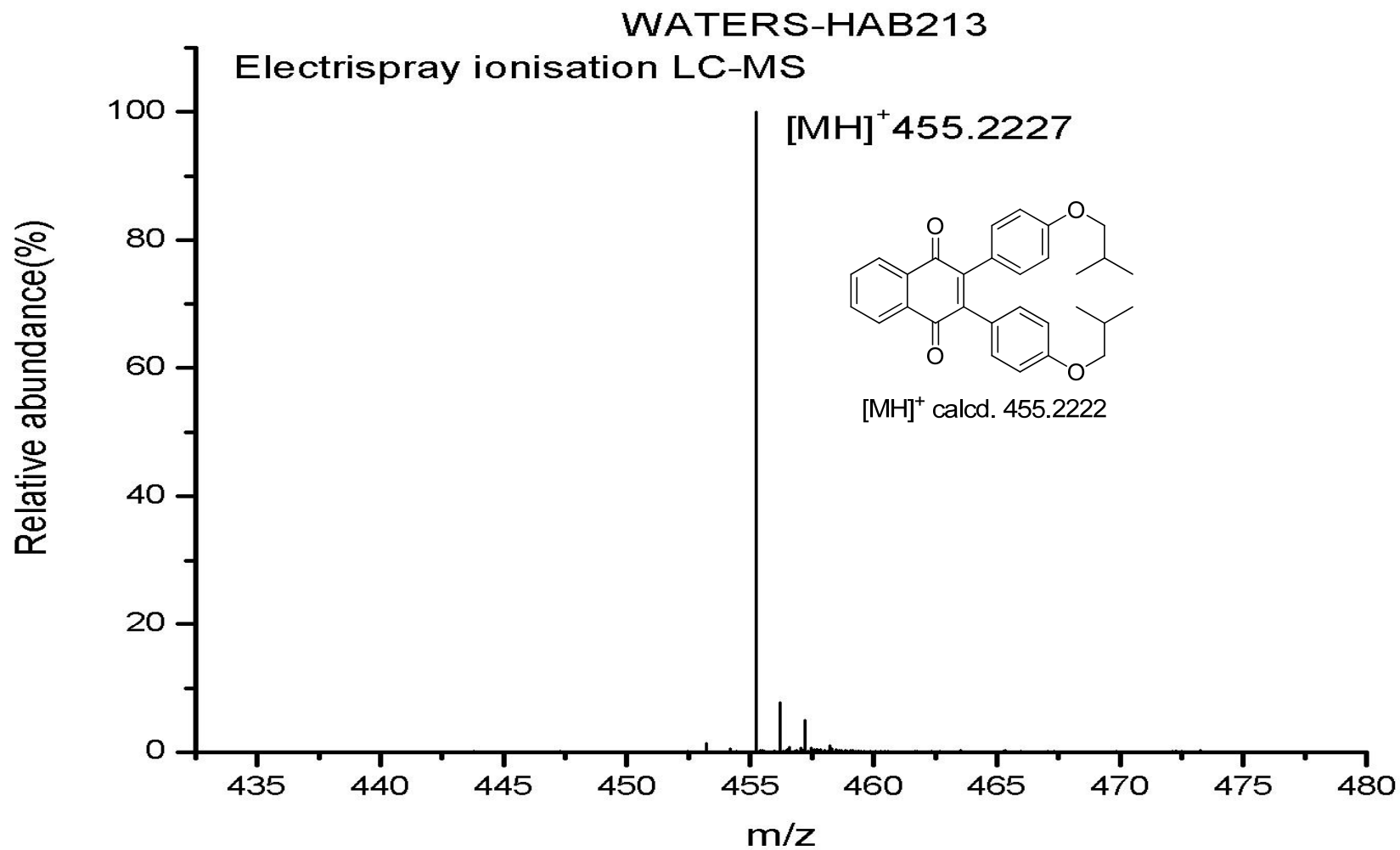
HRMS spectrum of 2,3-bis(4-ethoxyphenyl)-1,4-naphthoquinone (**6.5**)



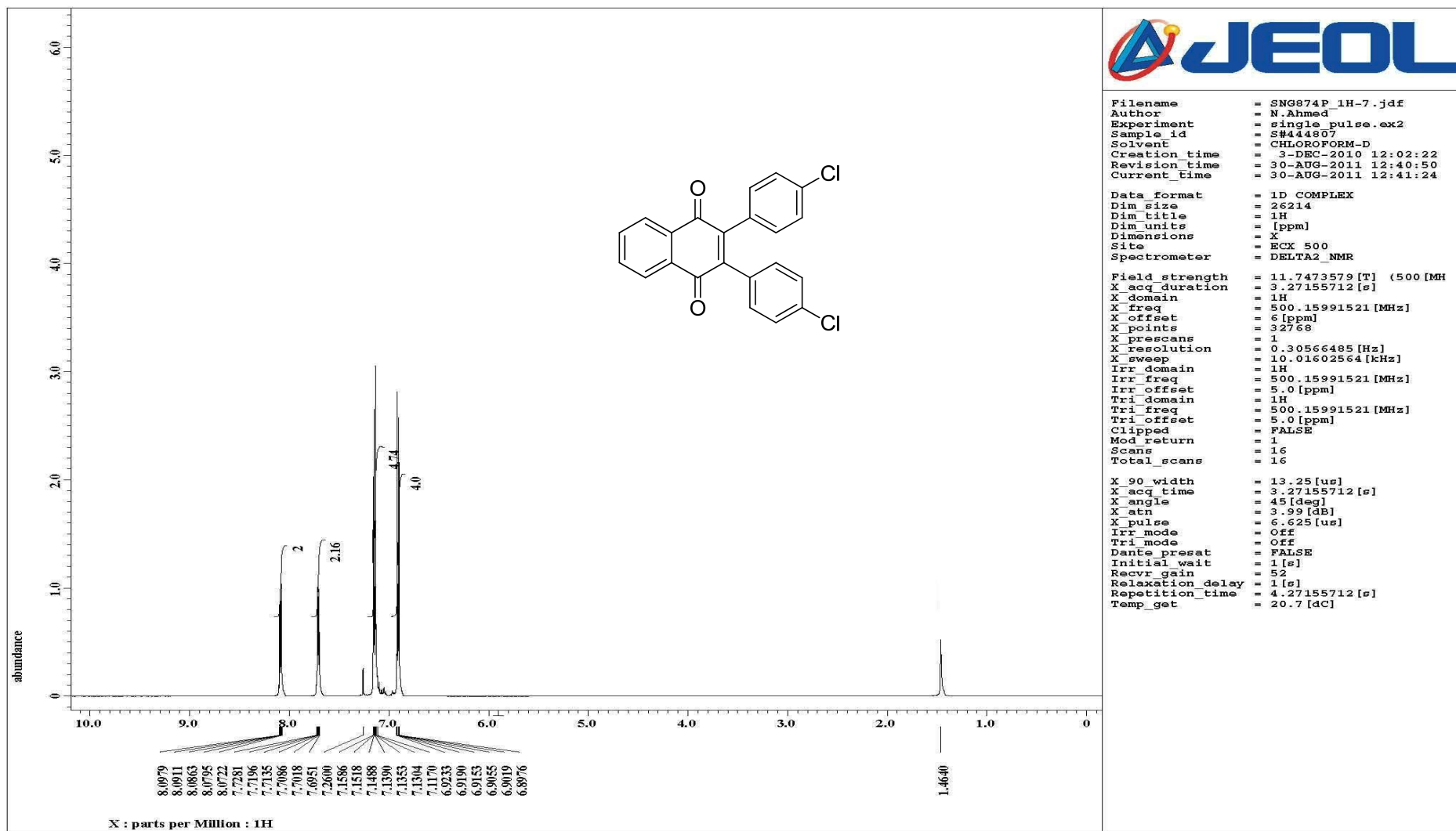
<sup>1</sup>H NMR spectrum of 2,3-bis(4-isobutoxyphenyl)-1,4-naphthoquinone (6.6)



<sup>13</sup>C NMR spectrum of 2,3-bis(4-isobutoxyphenyl)-1,4-naphthoquinone (6.6)

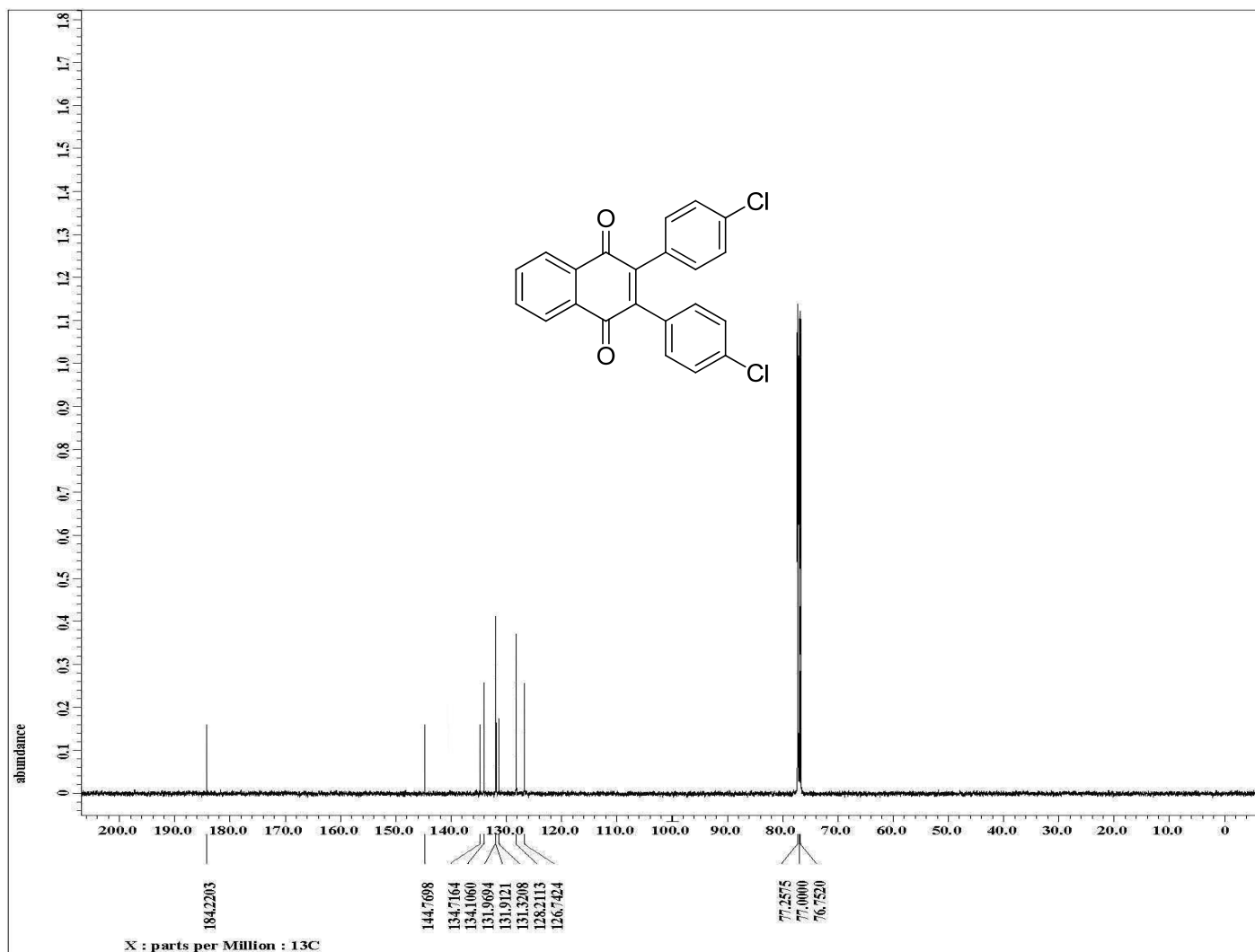


HRMS spectrum of 2,3-bis(4-isobutoxyphenyl)-1,4-naphthoquinone (**6.6**)



<sup>1</sup>H NMR spectrum of 2,3-bis(4-chlorophenyl)-1,4-naphthoquinone (6.7)





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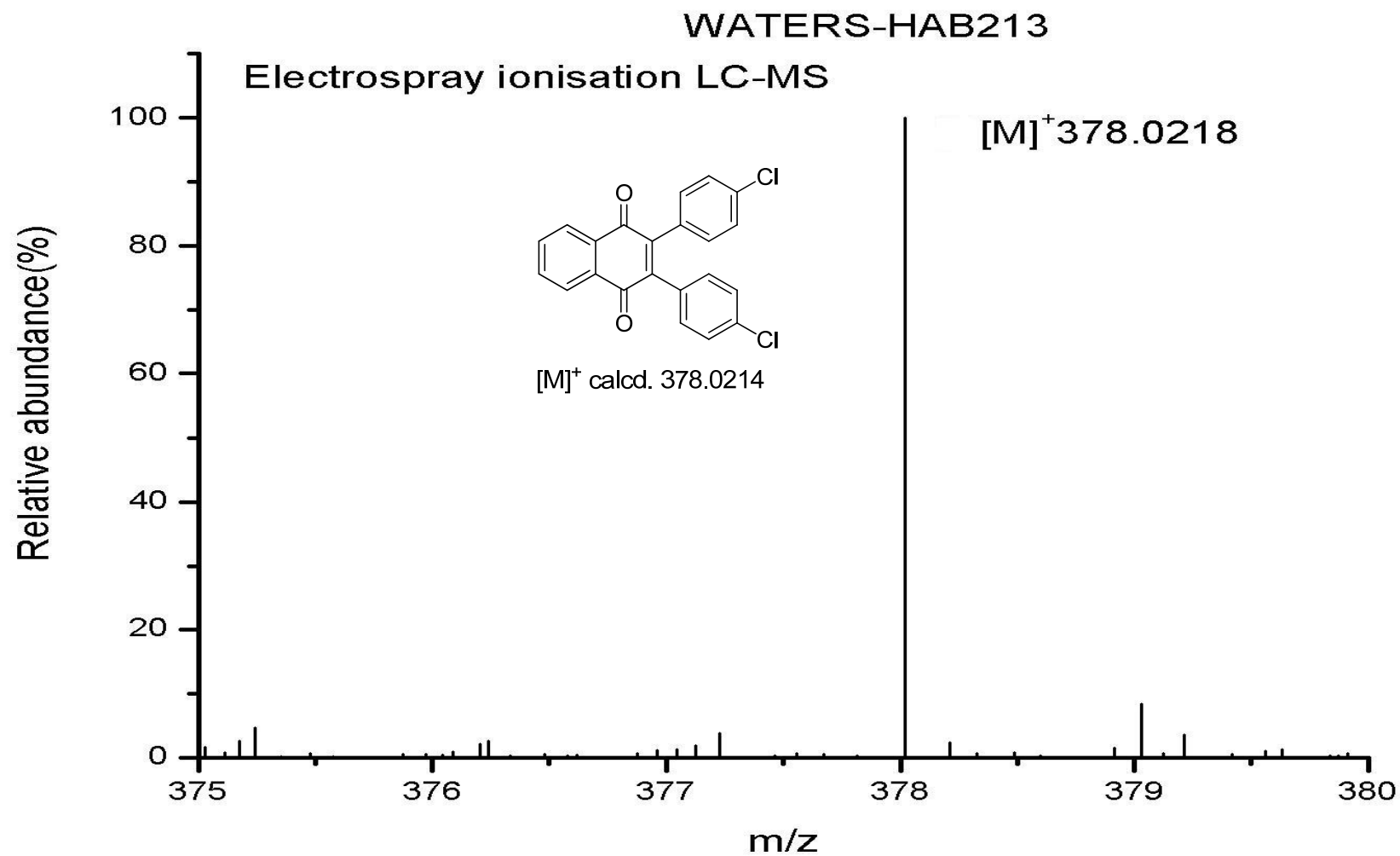
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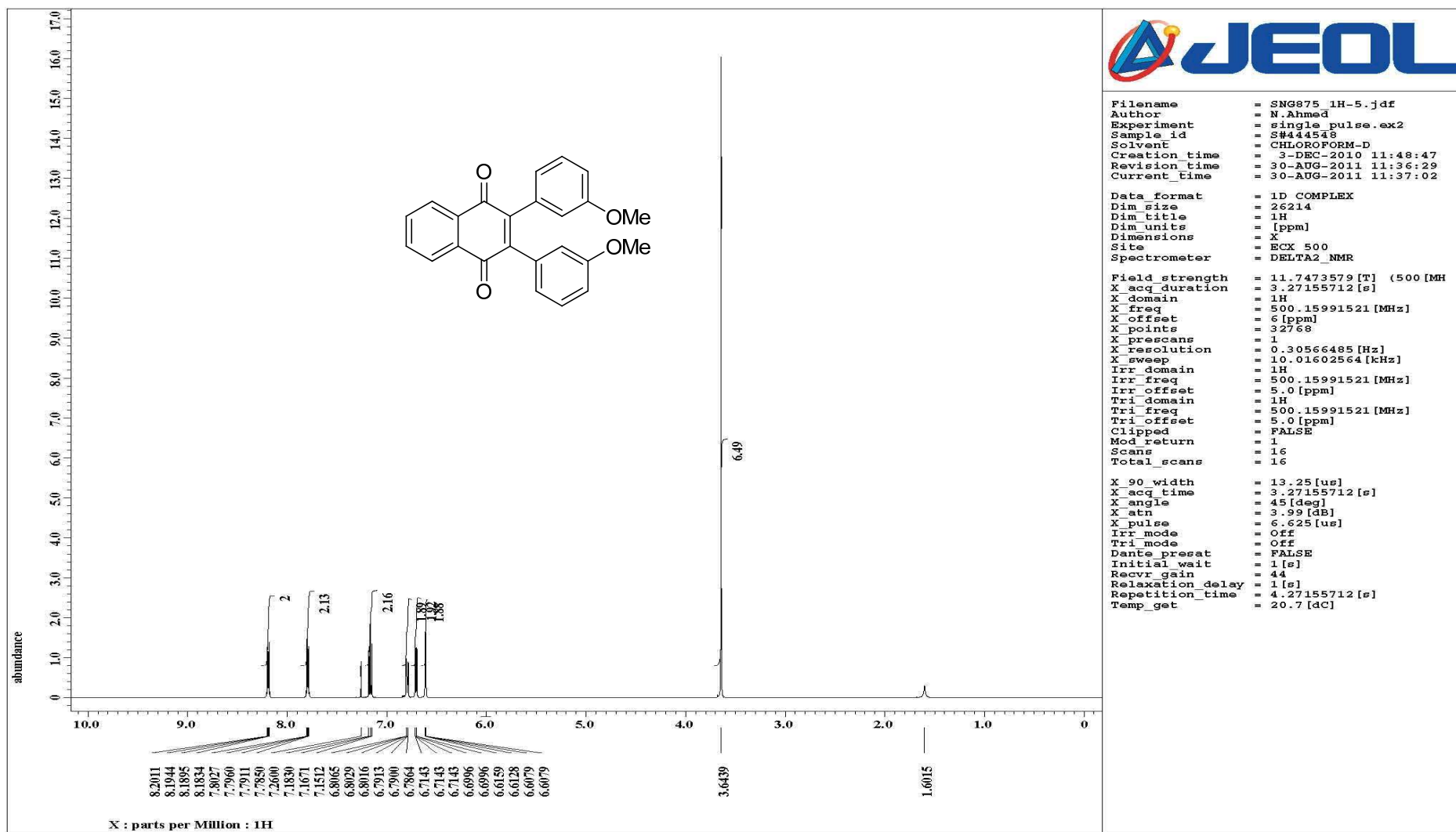
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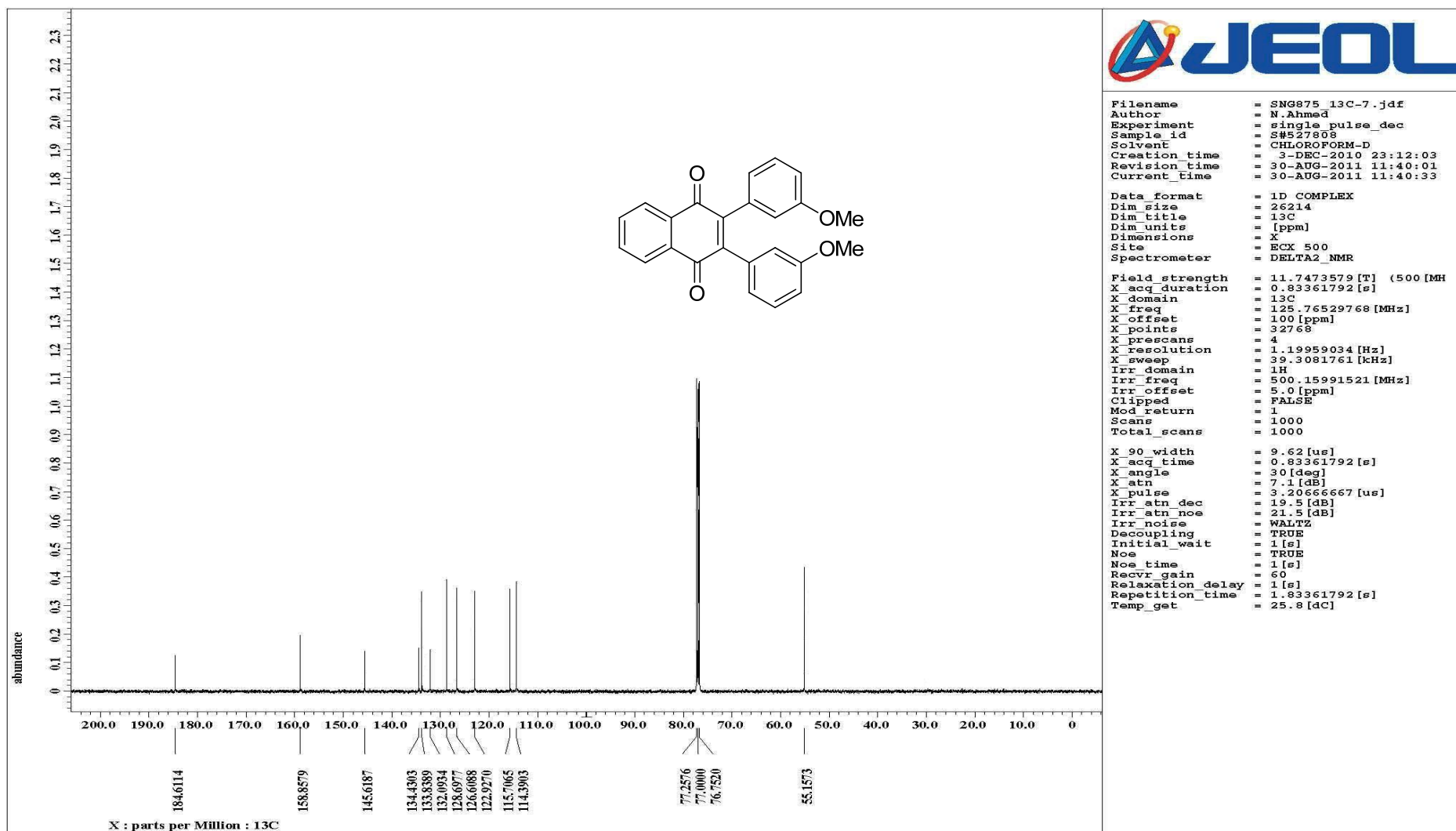
<sup>13</sup>C NMR spectrum of 2,3-bis(4-chlorophenyl)-1,4-naphthoquinone (6.7)



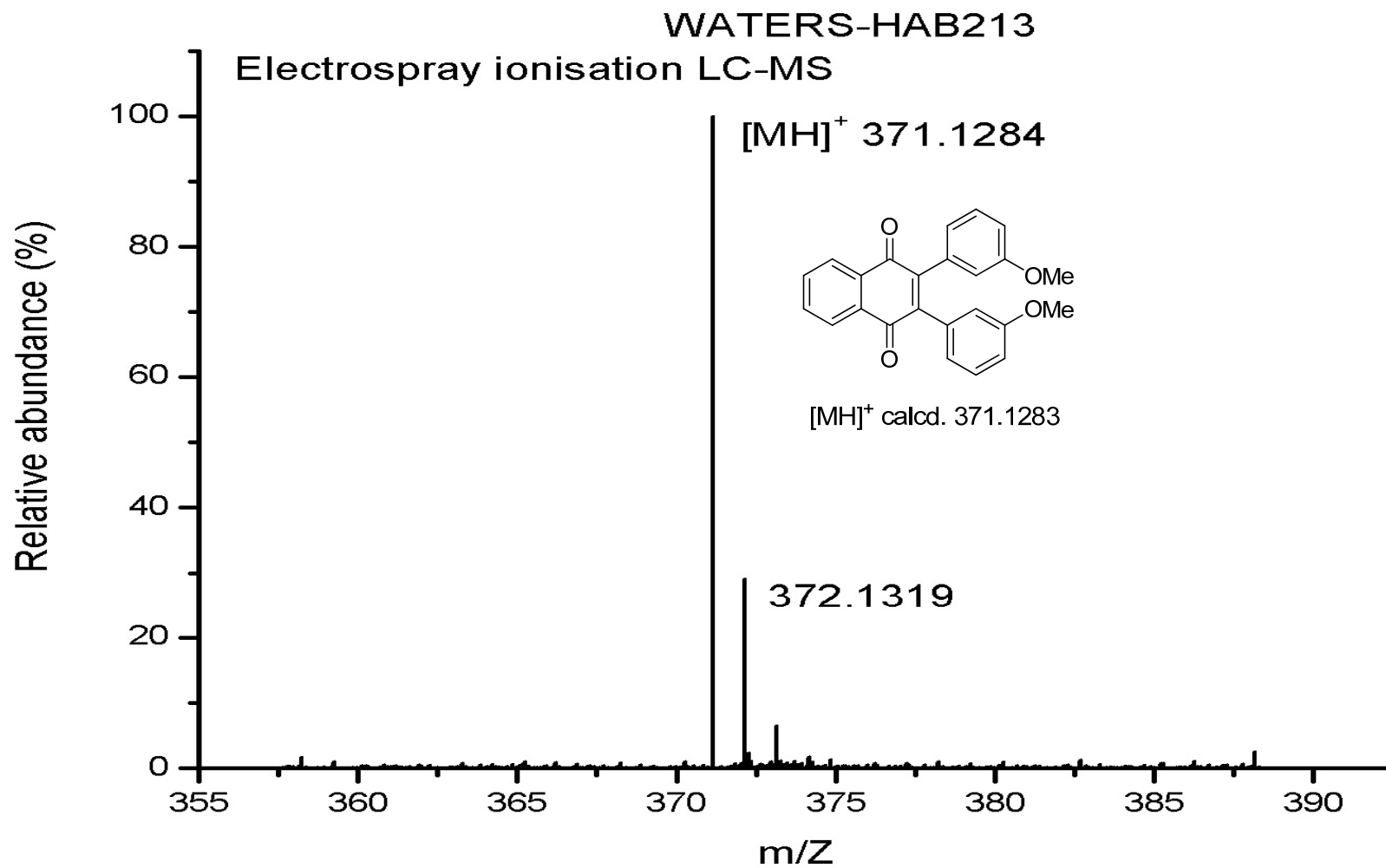
HRMS spectrum of 2,3-bis(4-chlorophenyl)-1,4-naphthoquinone (6.7)



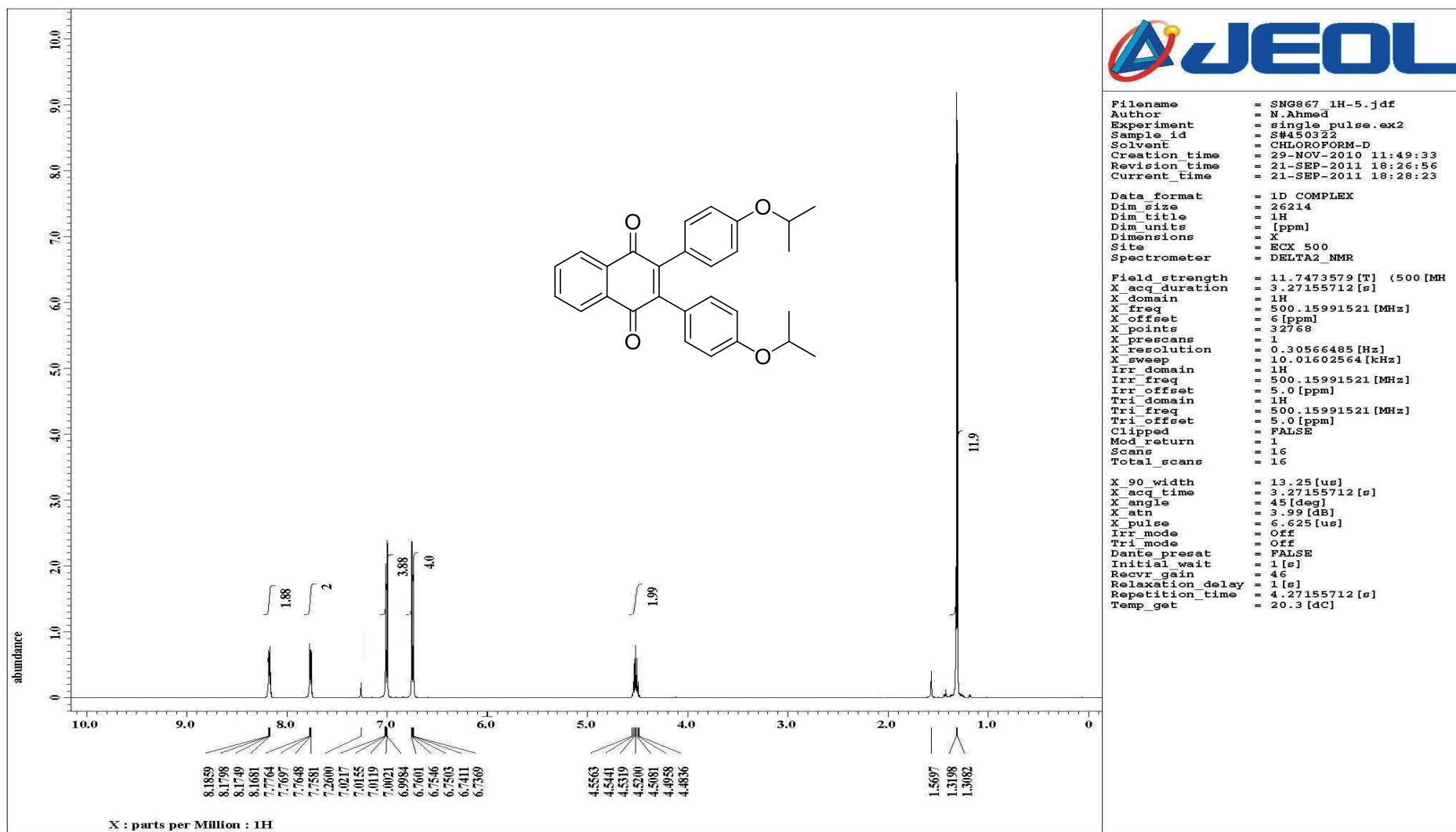
<sup>1</sup>H NMR spectrum of 2,3-bis(3-methoxyphenyl)-1,4-naphthoquinone (6.8)



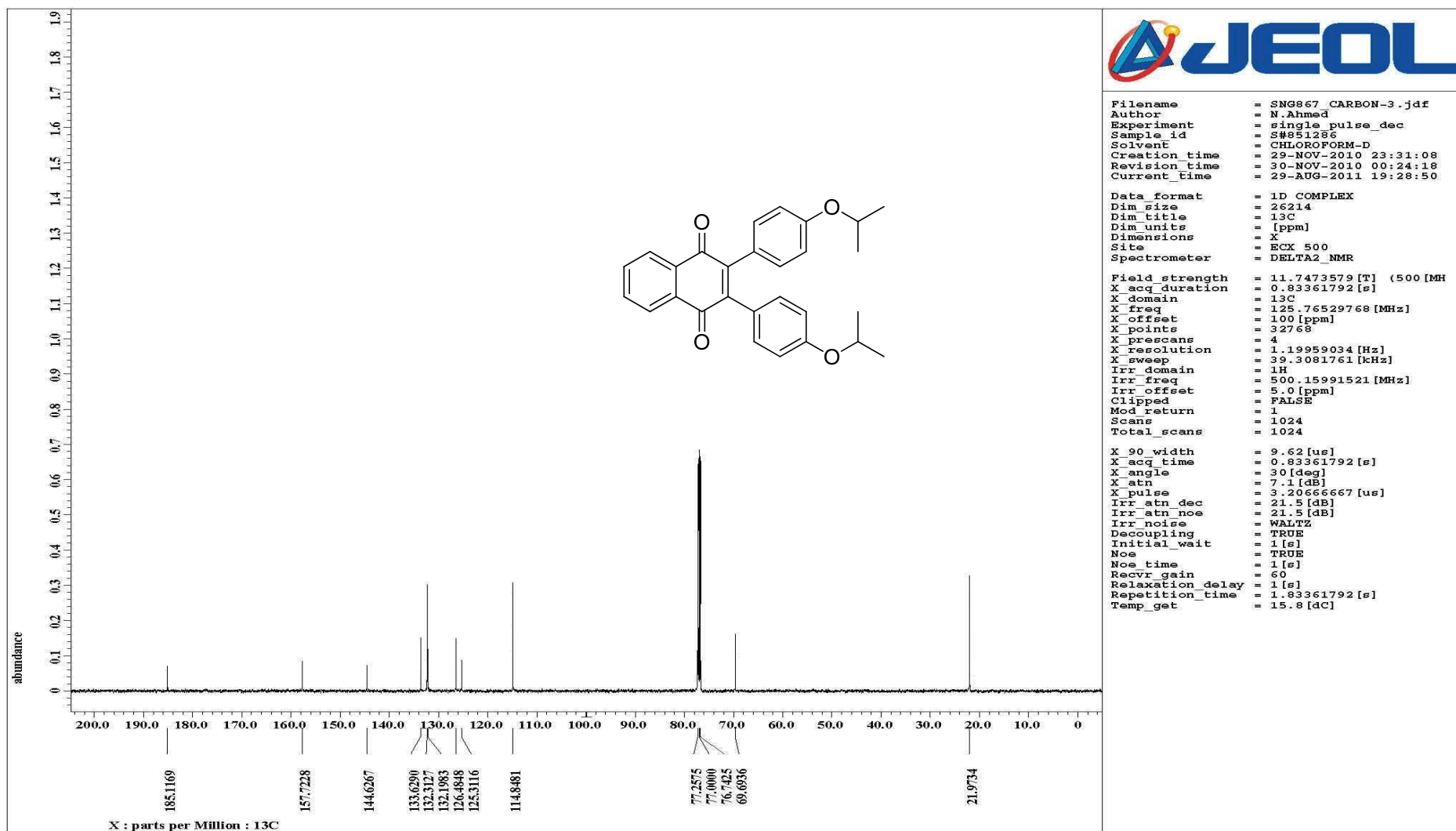
<sup>13</sup>C NMR spectrum of 2,3-bis(3-methoxyphenyl)-1,4-naphthoquinone (6.8)



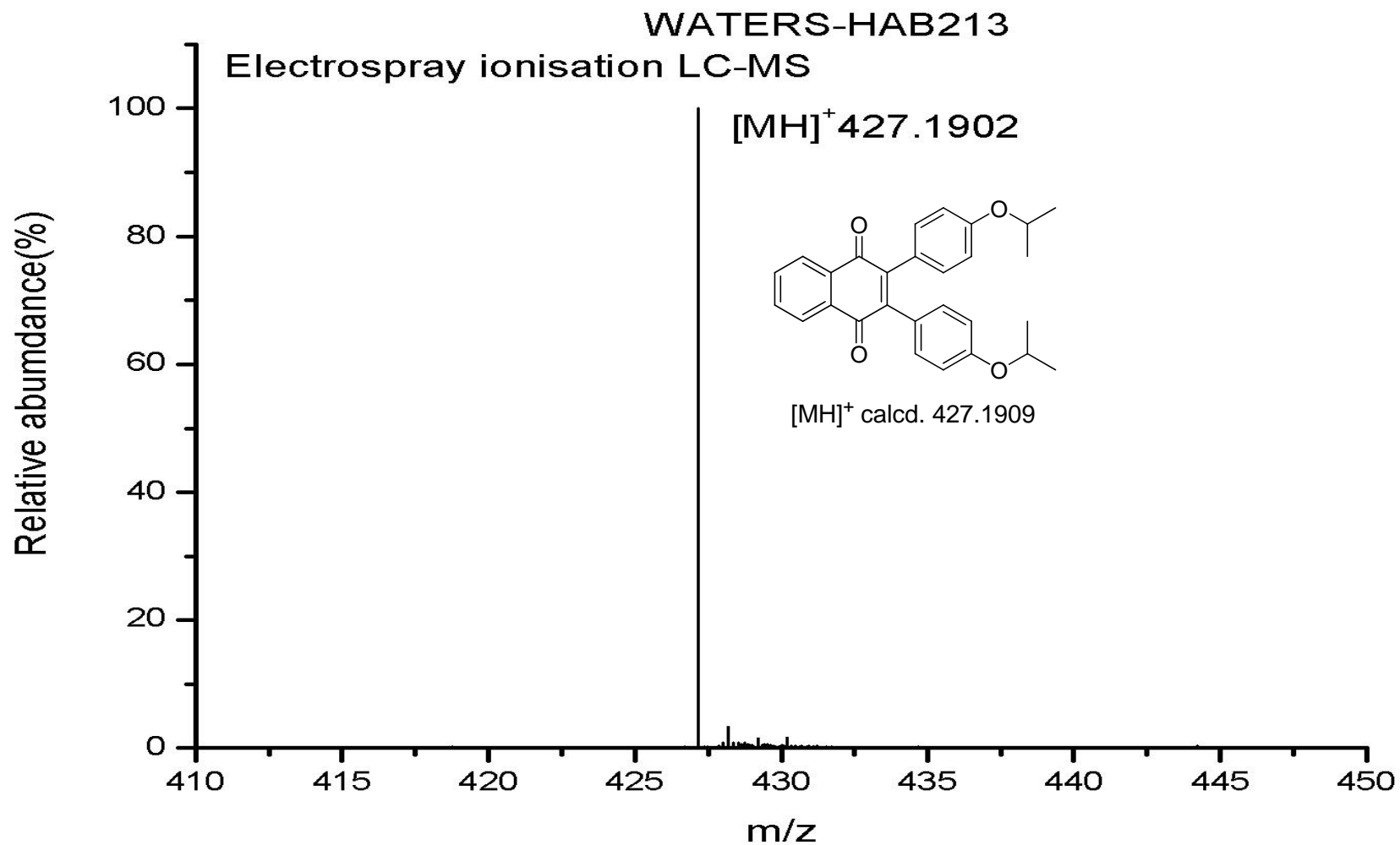
HRMS spectrum of 2,3-bis(3-methoxyphenyl)-1,4-naphthoquinone (**6.8**)



<sup>1</sup>H NMR spectrum of 2,3-bis(4-isopropoxyphenyl)-1,4-naphthoquinone (6.9)

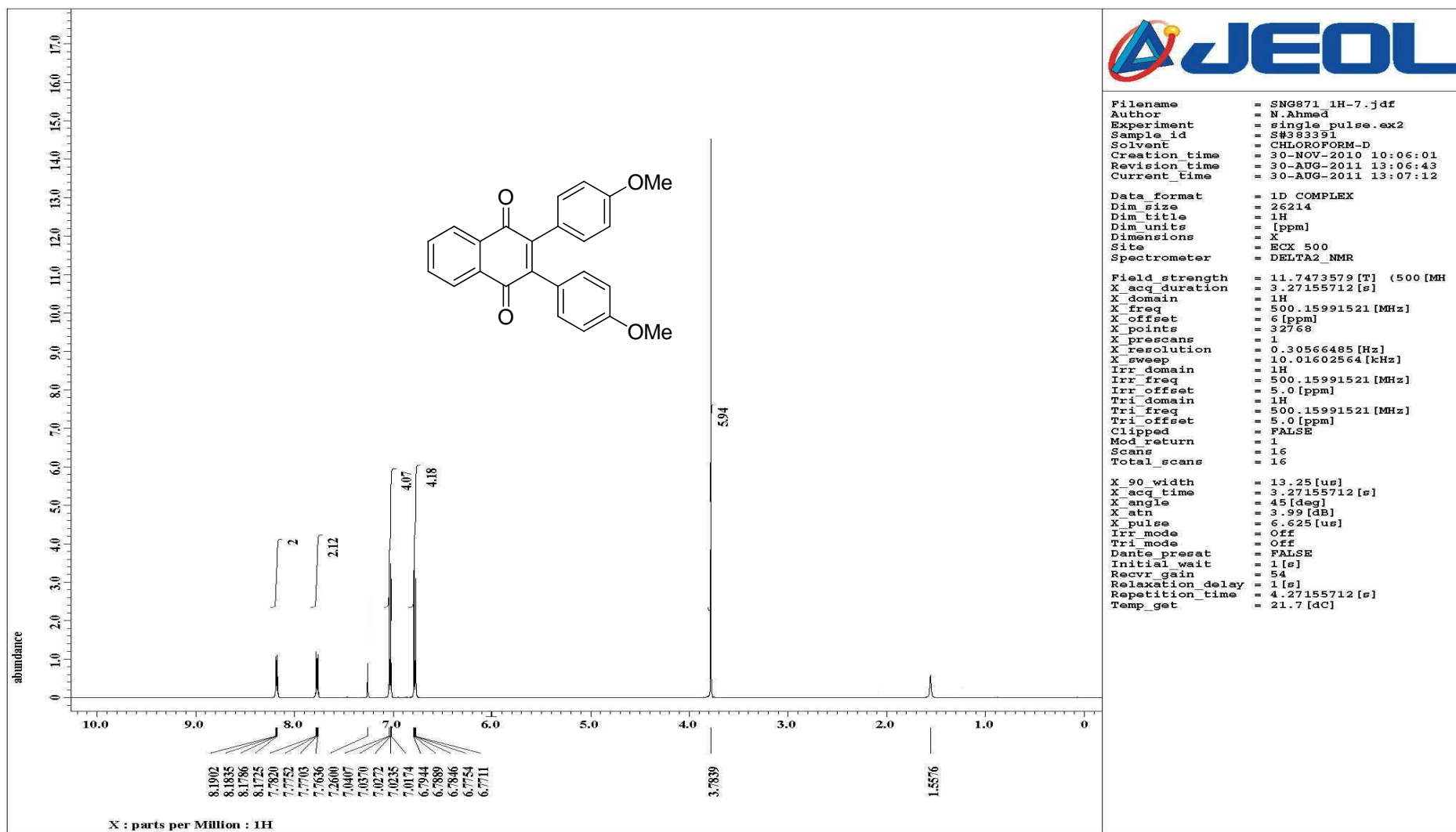


$^{13}\text{C}$  NMR spectrum of 2,3-bis(4-isopropoxyphenyl)-1,4-naphthoquinone (**6.9**)

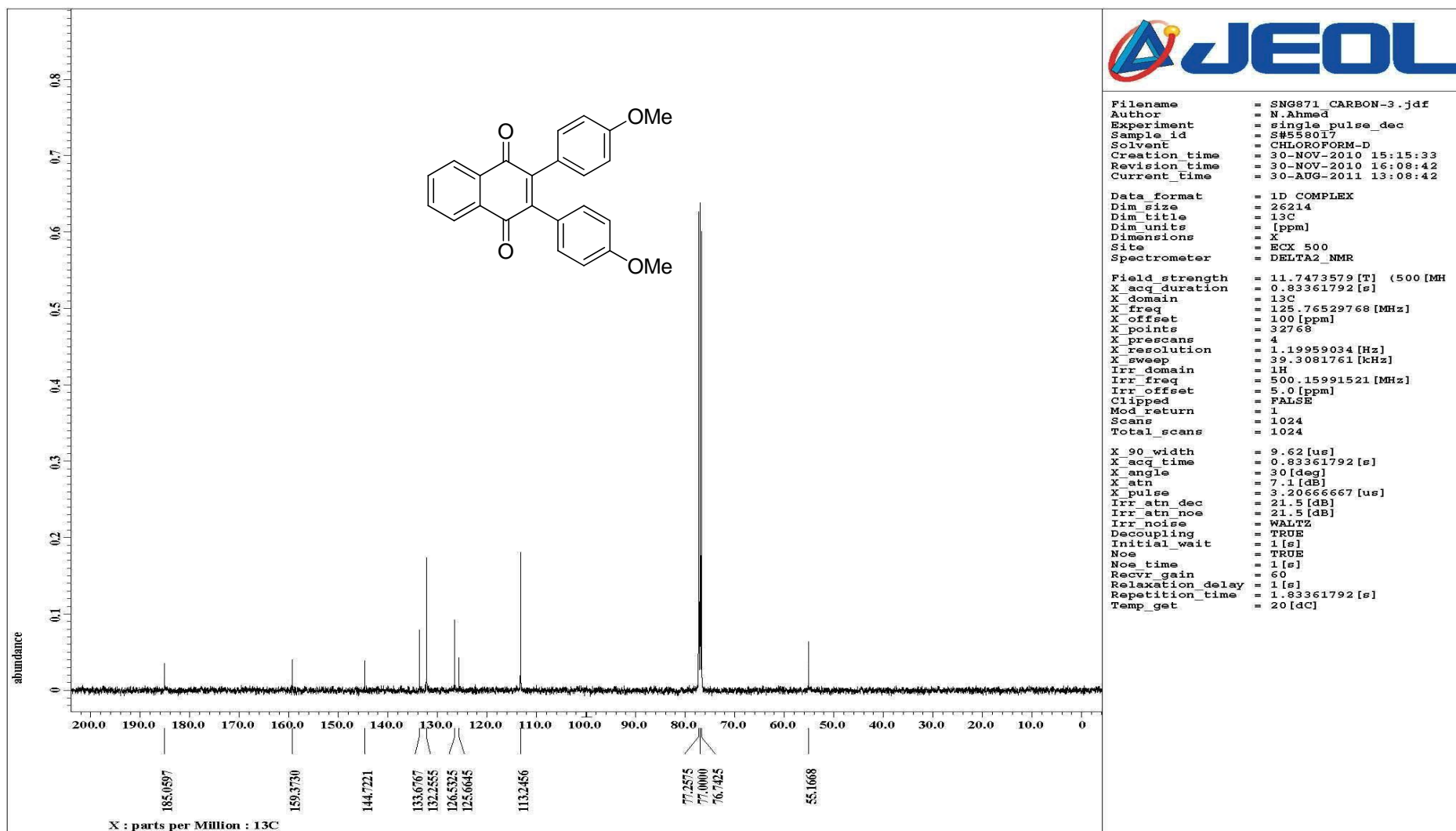


HRMS spectrum of 2,3-bis(4-isopropoxyphenyl)-1,4-naphthoquinone (**6.9**)

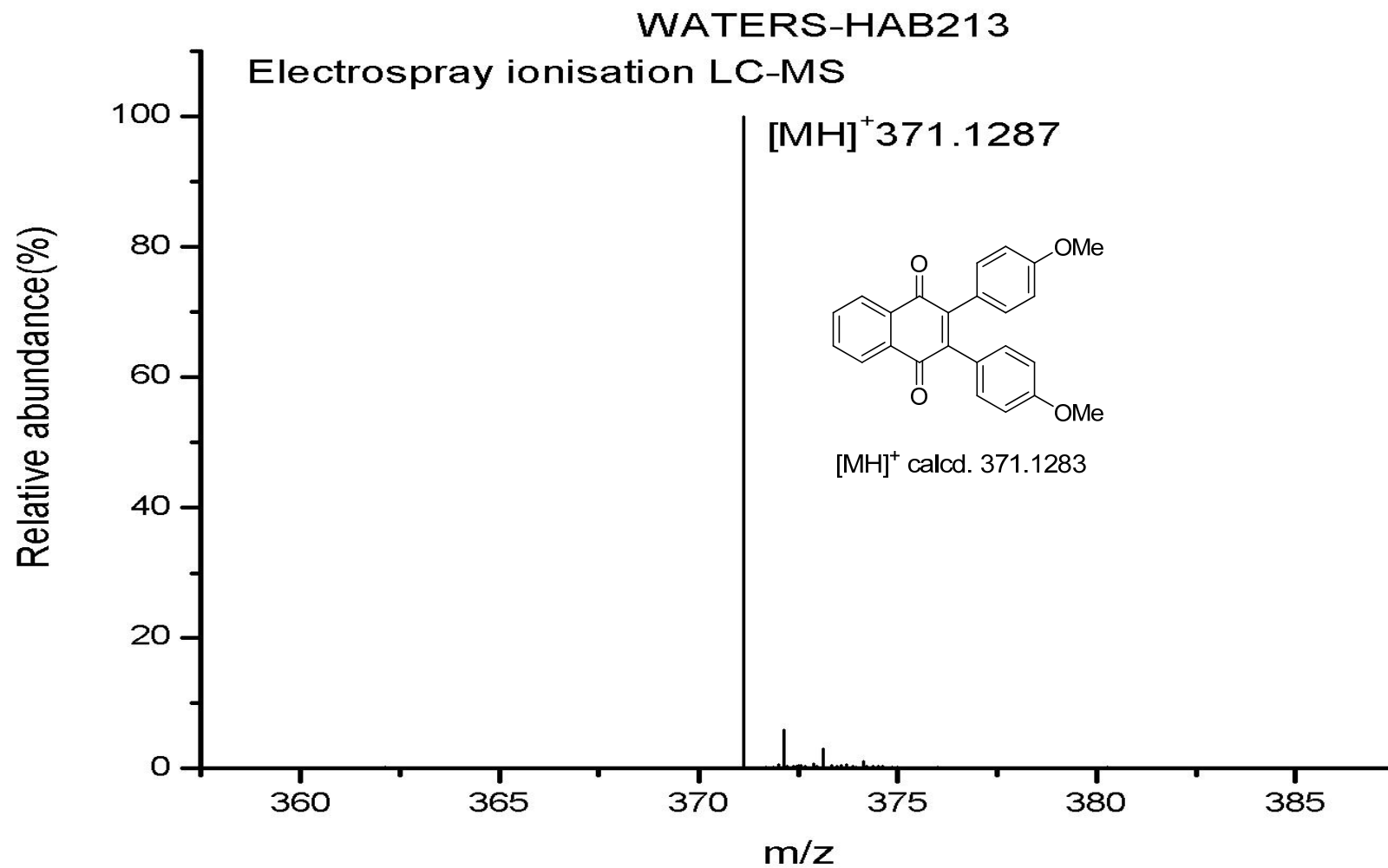




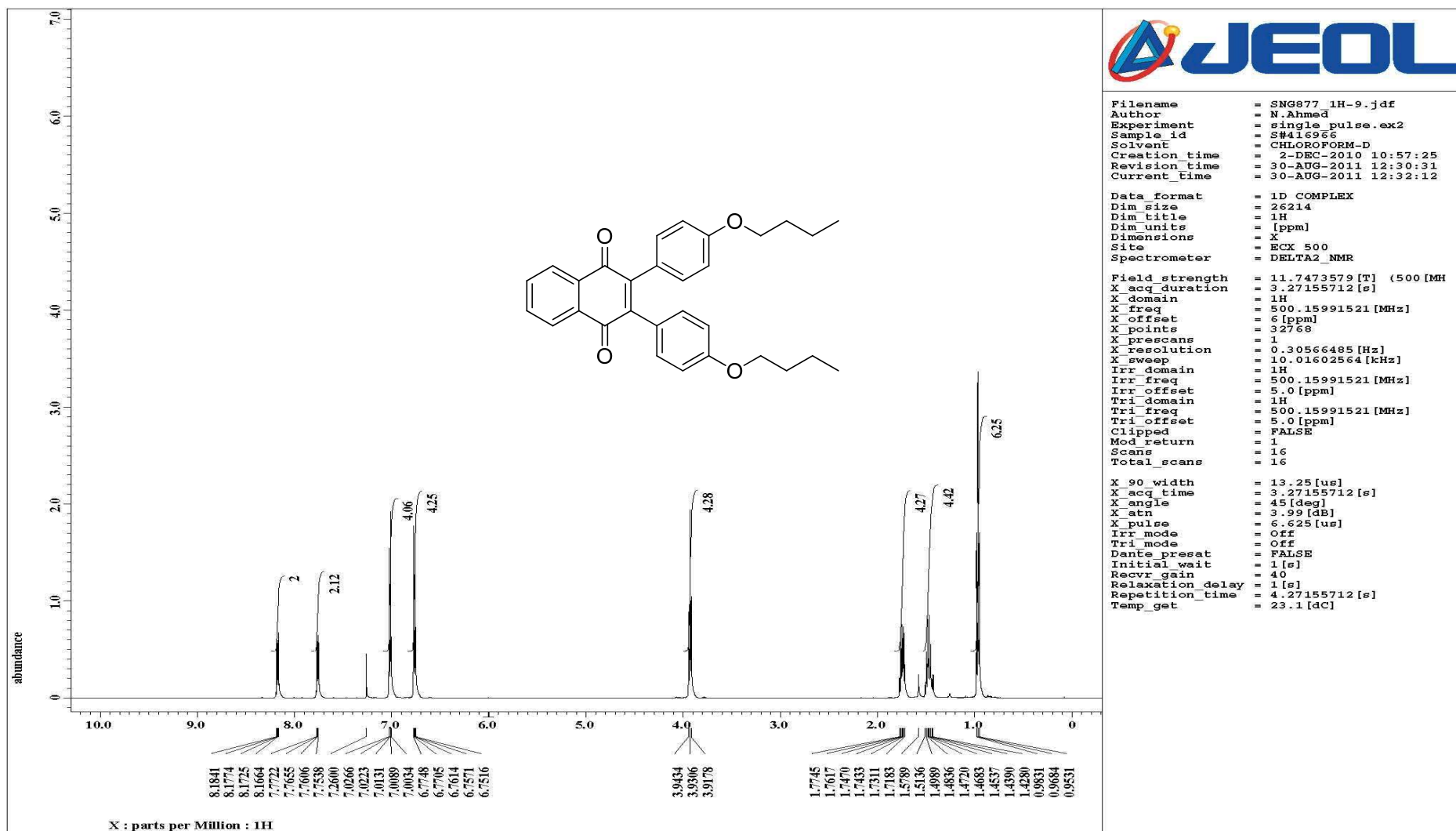
<sup>1</sup>H NMR spectrum of 2,3-bis(4-methoxyphenyl)-1,4-naphthoquinone (6.10)



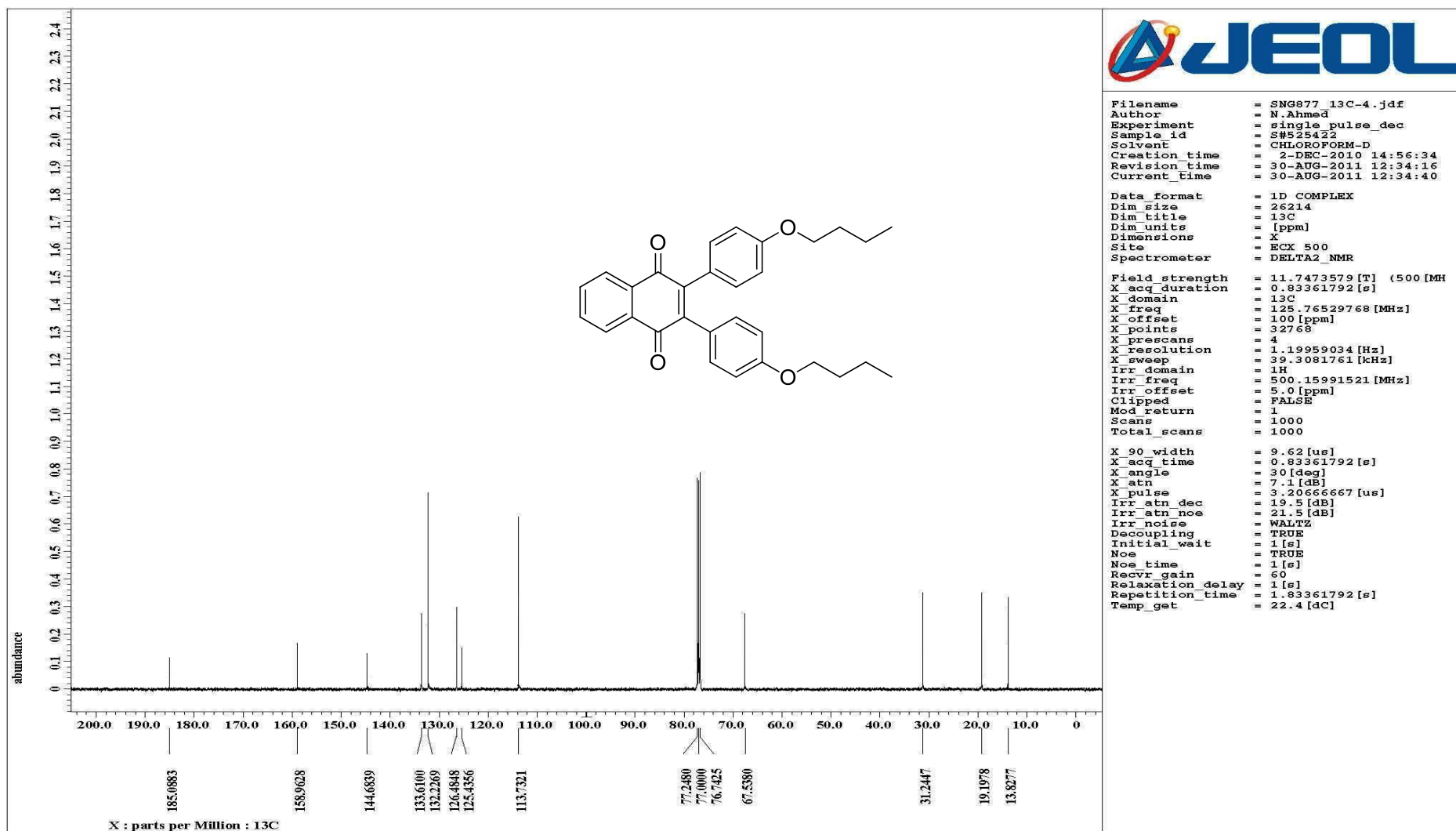
<sup>13</sup>C NMR spectrum of 2,3-bis(4-methoxyphenyl)-1,4-naphthoquinone (6.10)



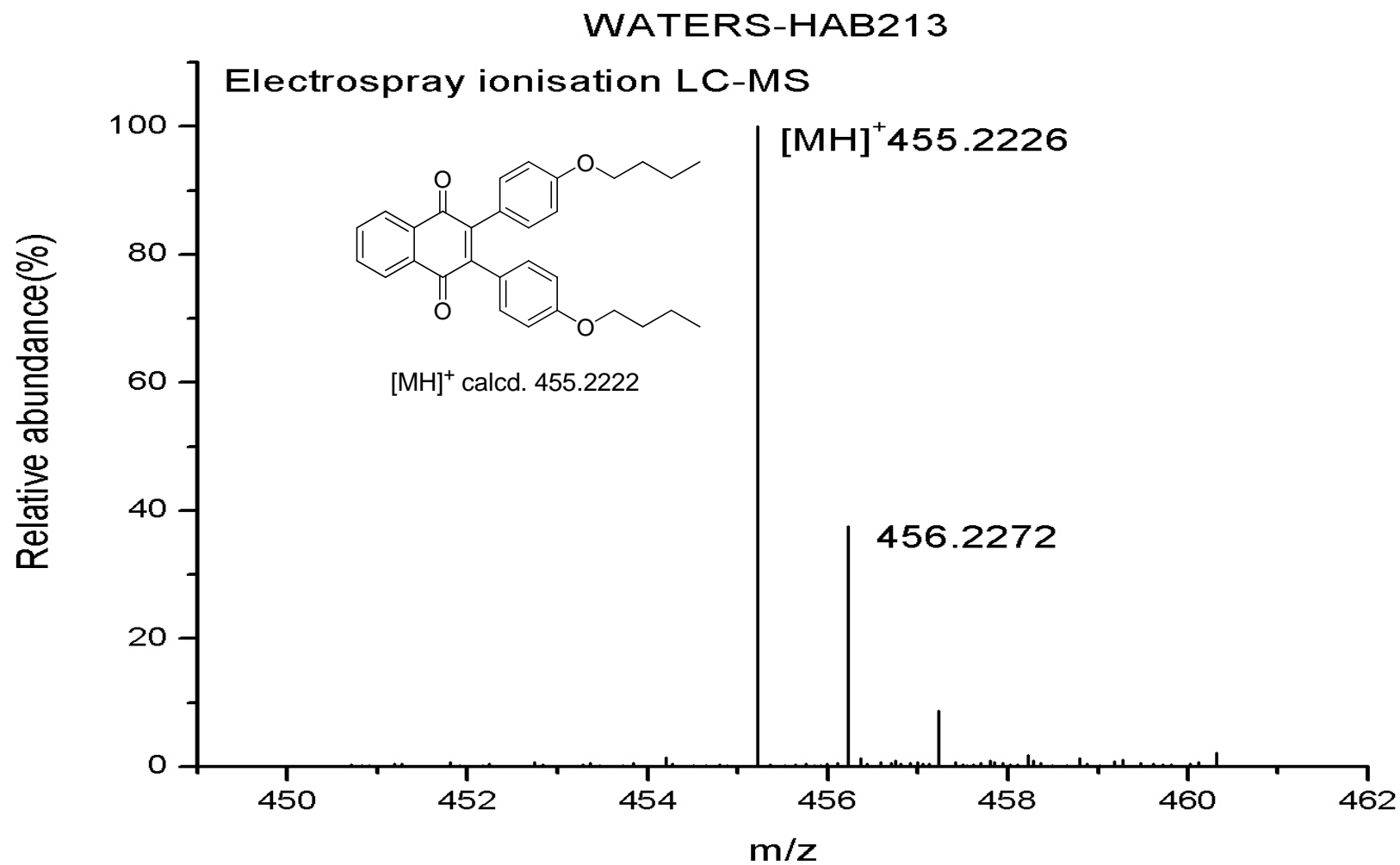
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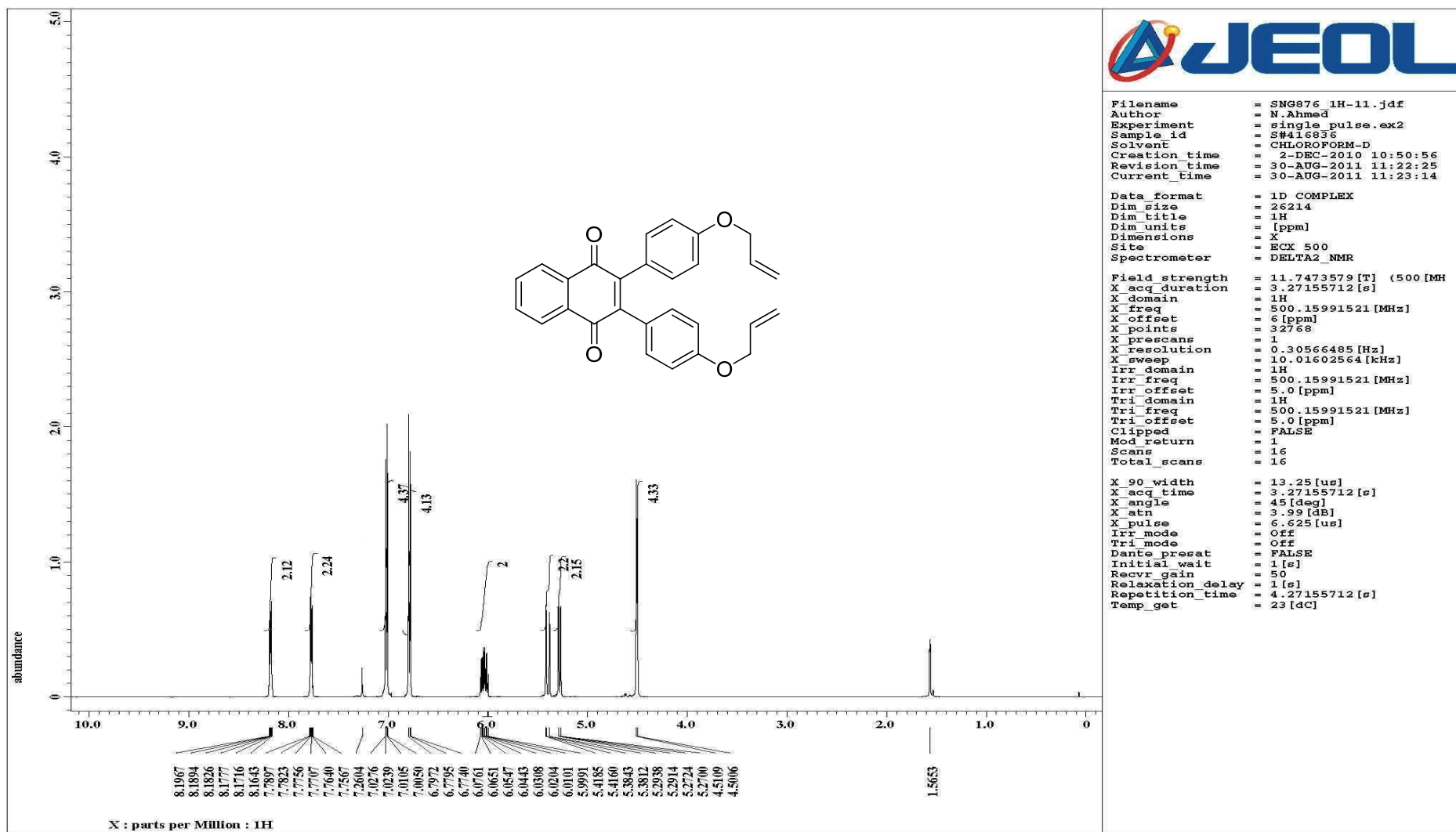
<sup>1</sup>H NMR spectrum of 2,3-bis(4-butoxyphenyl)-1,4-naphthoquinone (6.11)



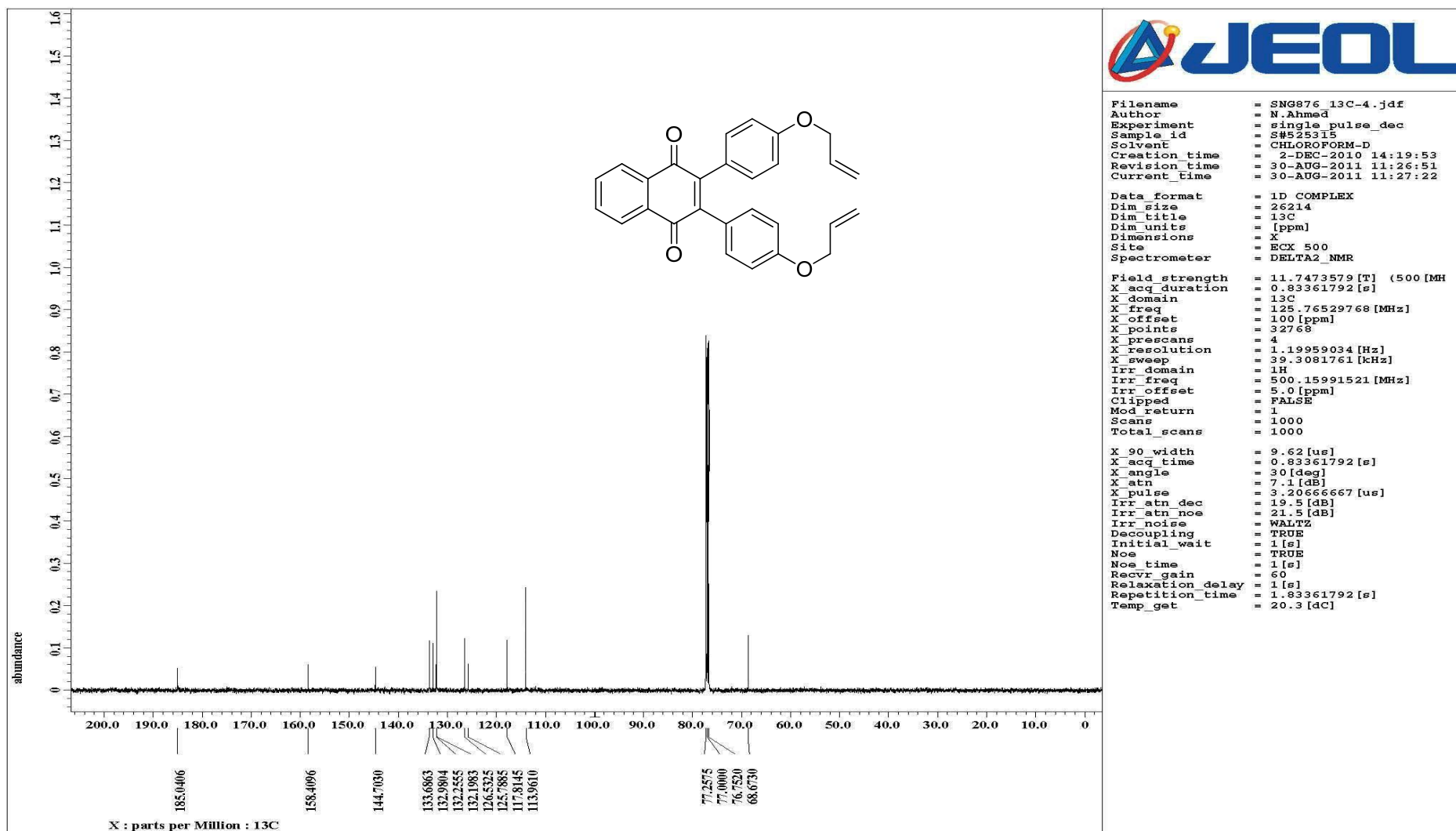
<sup>13</sup>C NMR spectrum of 2,3-bis(4-butoxyphenyl)-1,4-naphthoquinone (6.11)



HRMS spectrum of 2,3-bis(4-butoxyphenyl)-1,4-naphthoquinone (**6.11**)

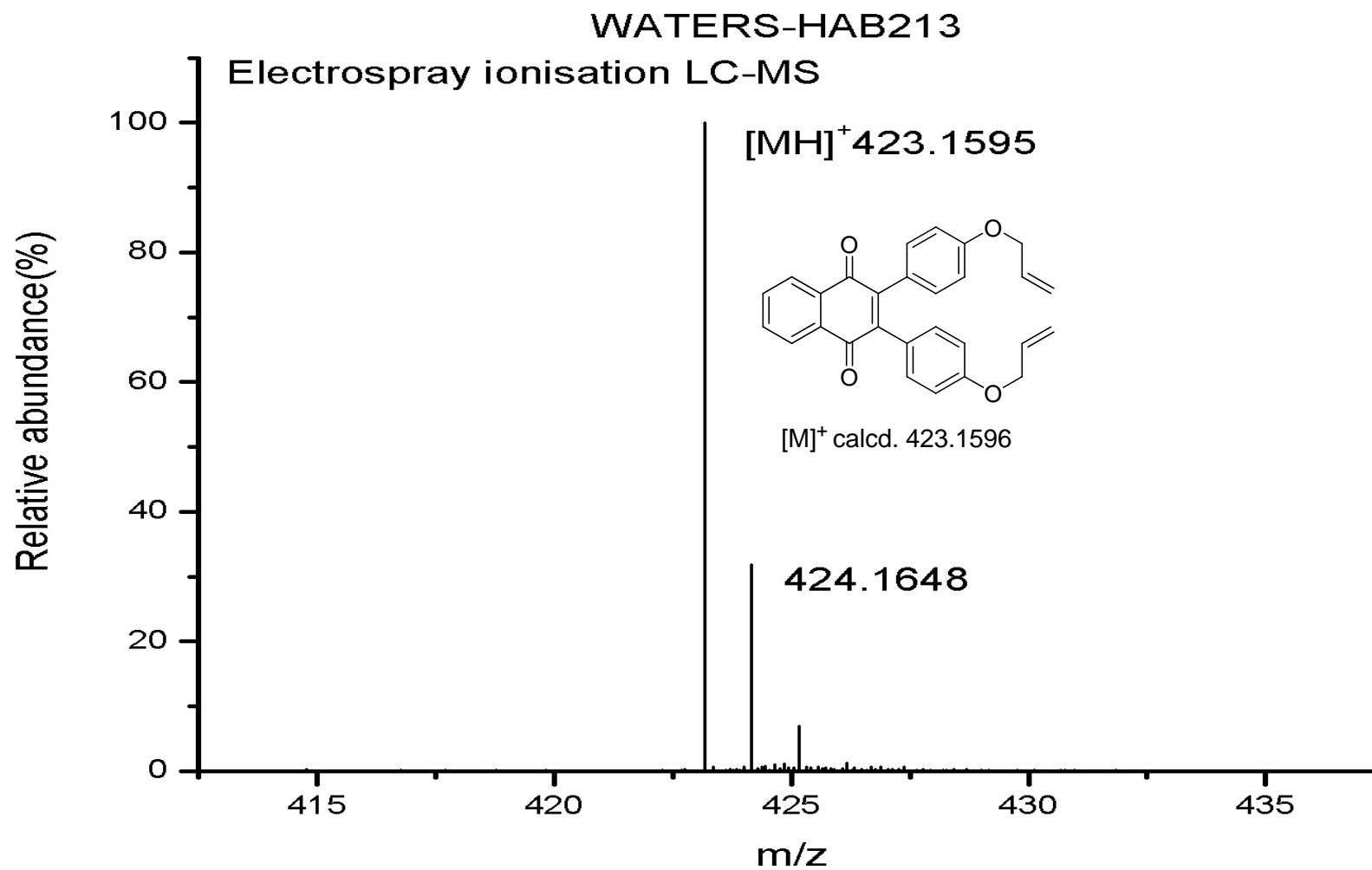


<sup>1</sup>H NMR spectrum of 2,3-bis(4-(allyloxy)phenyl)-1,4-naphthoquinone (6.12)

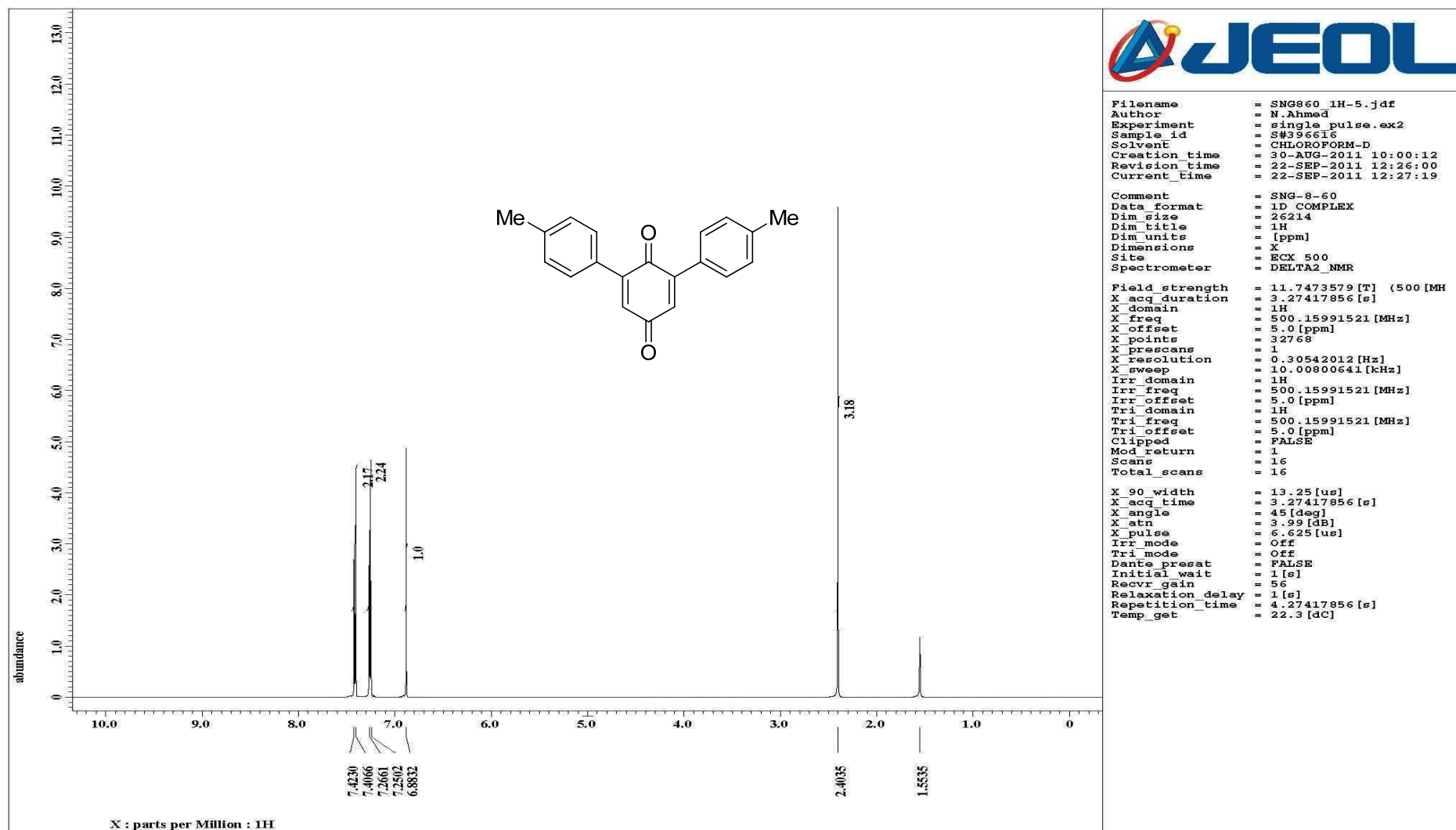


<sup>13</sup>C NMR spectrum of 2,3-bis(4-(allyloxy)phenyl)-1,4-naphthoquinone (6.12)

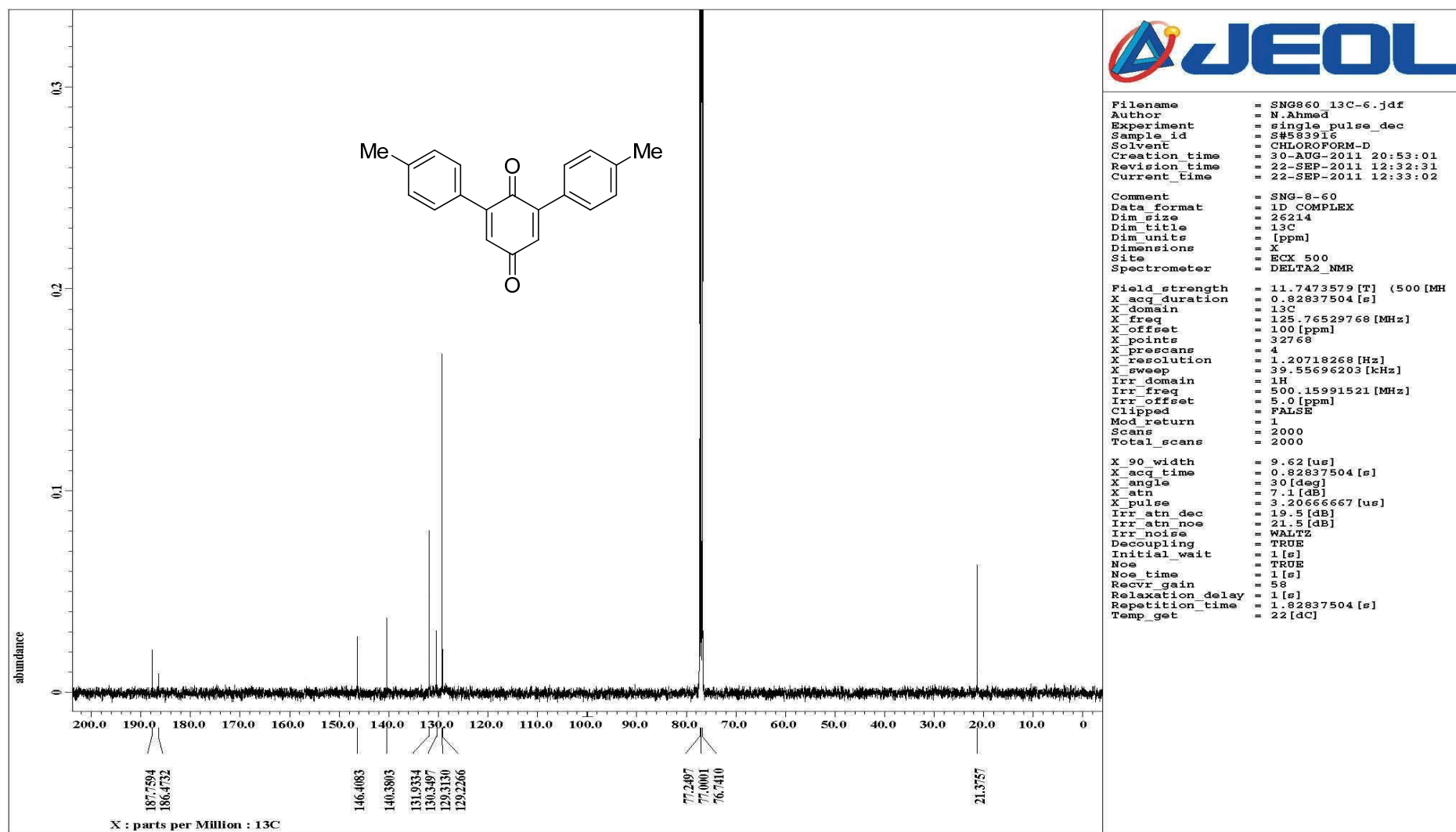




HRMS spectrum of 2,3-bis(4-(allyloxy)phenyl)-1,4-naphthoquinone (**6.12**)

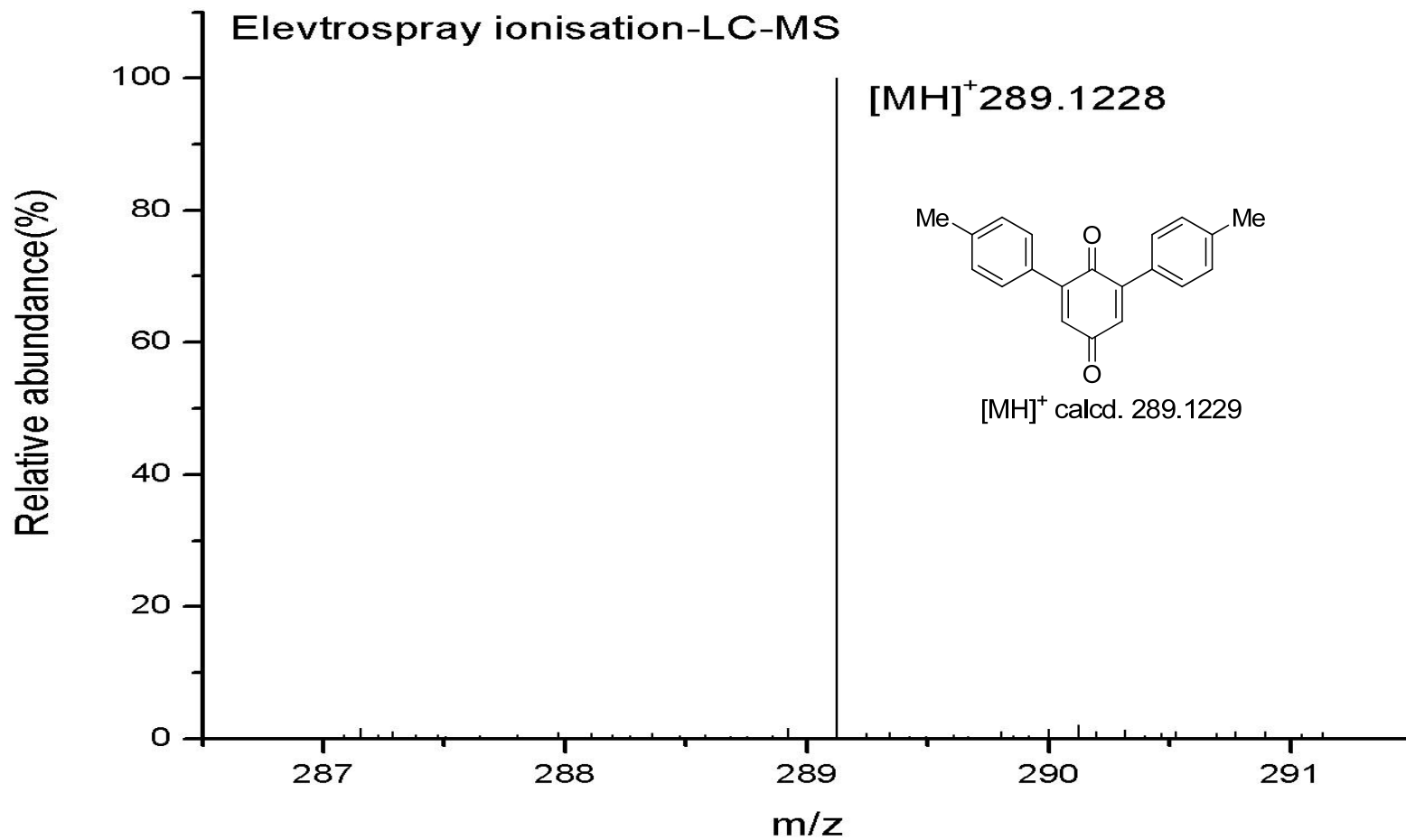


<sup>1</sup>H NMR spectrum of 2,6-di-(4-methylphenyl)-1,4-benzoquinone (7.1)

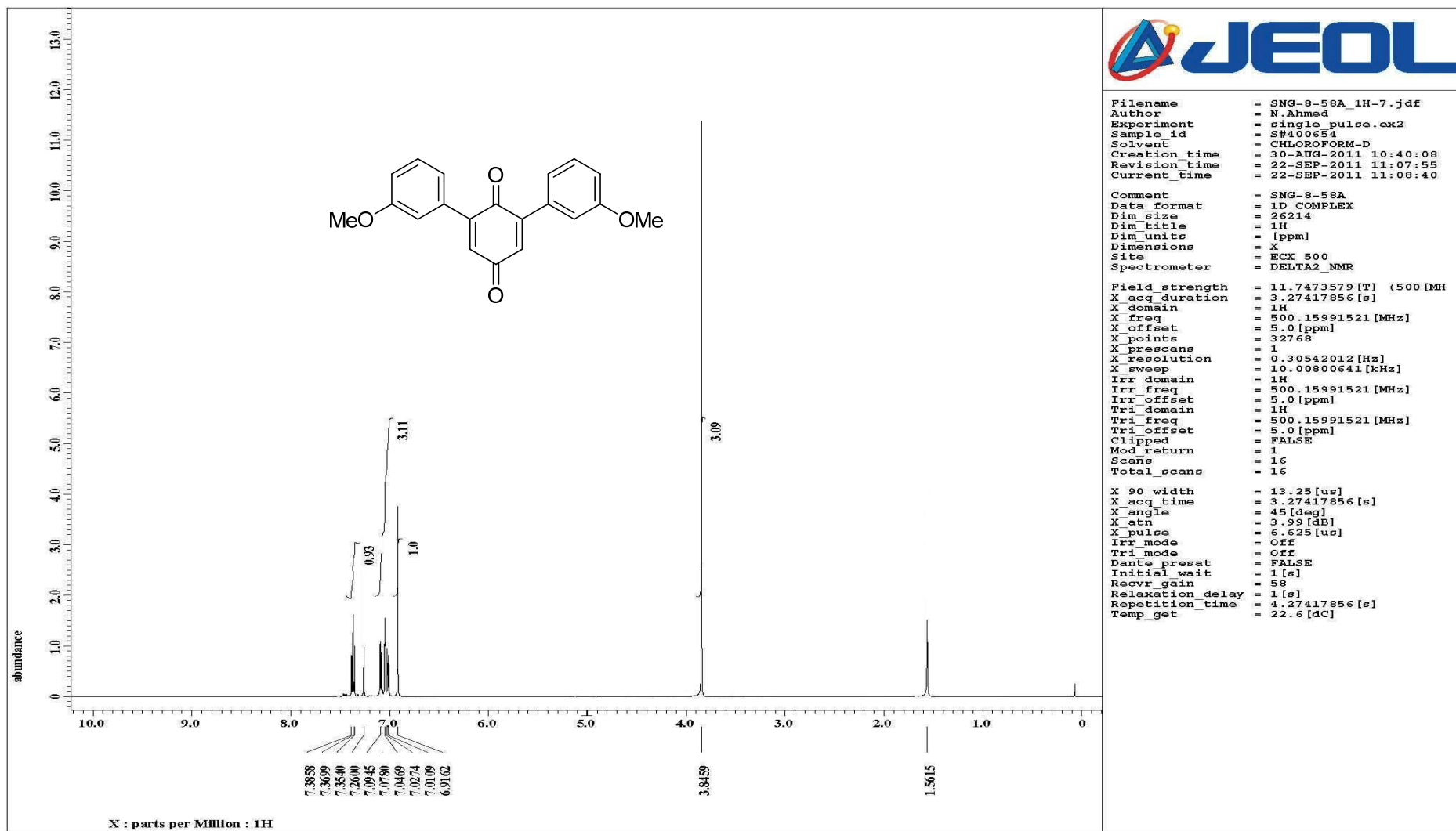


<sup>13</sup>C NMR spectrum of 2,6-di-(4-methylphenyl)-1,4-benzoquinone (7.1)

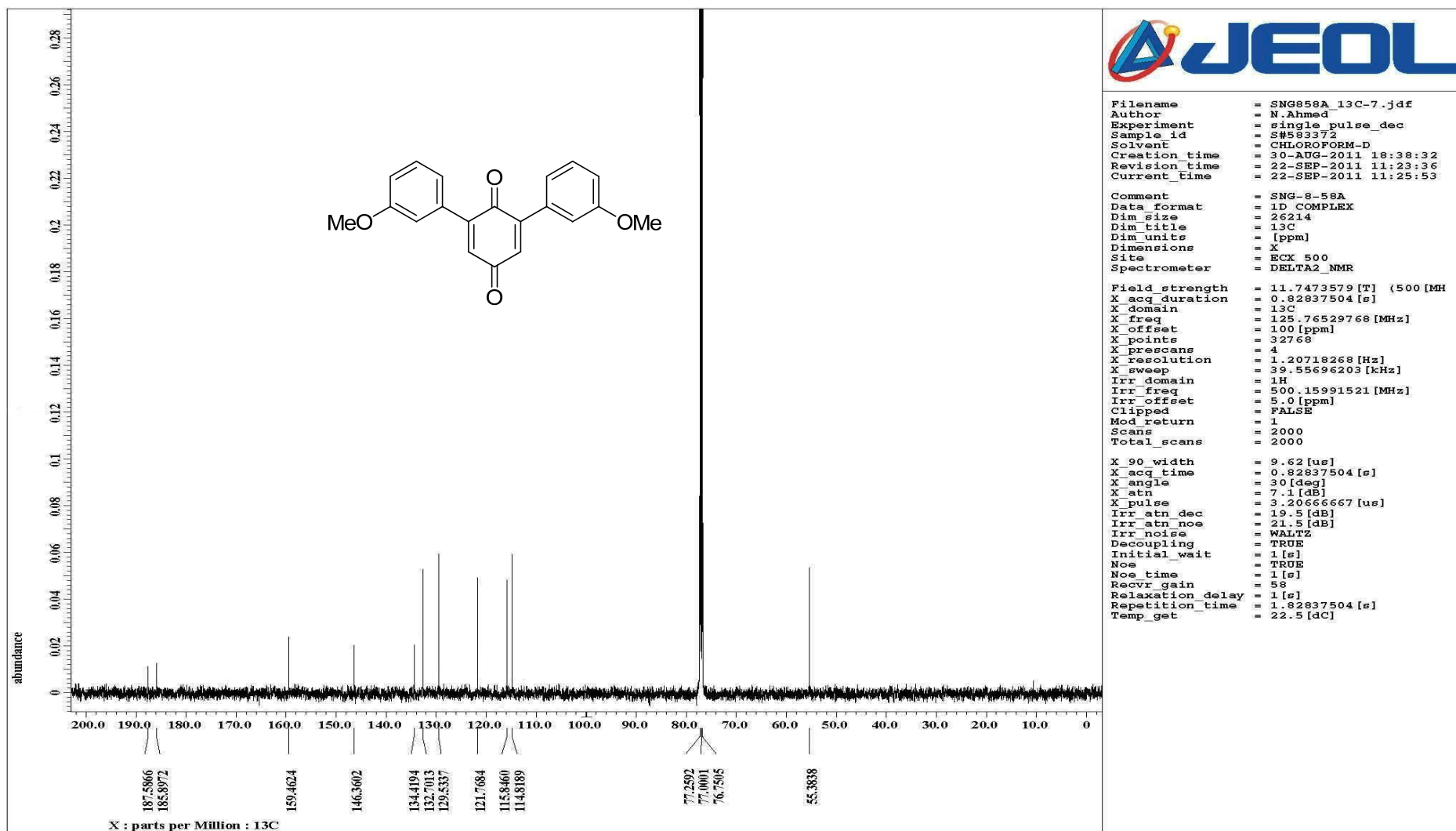
WATERS-HAB213



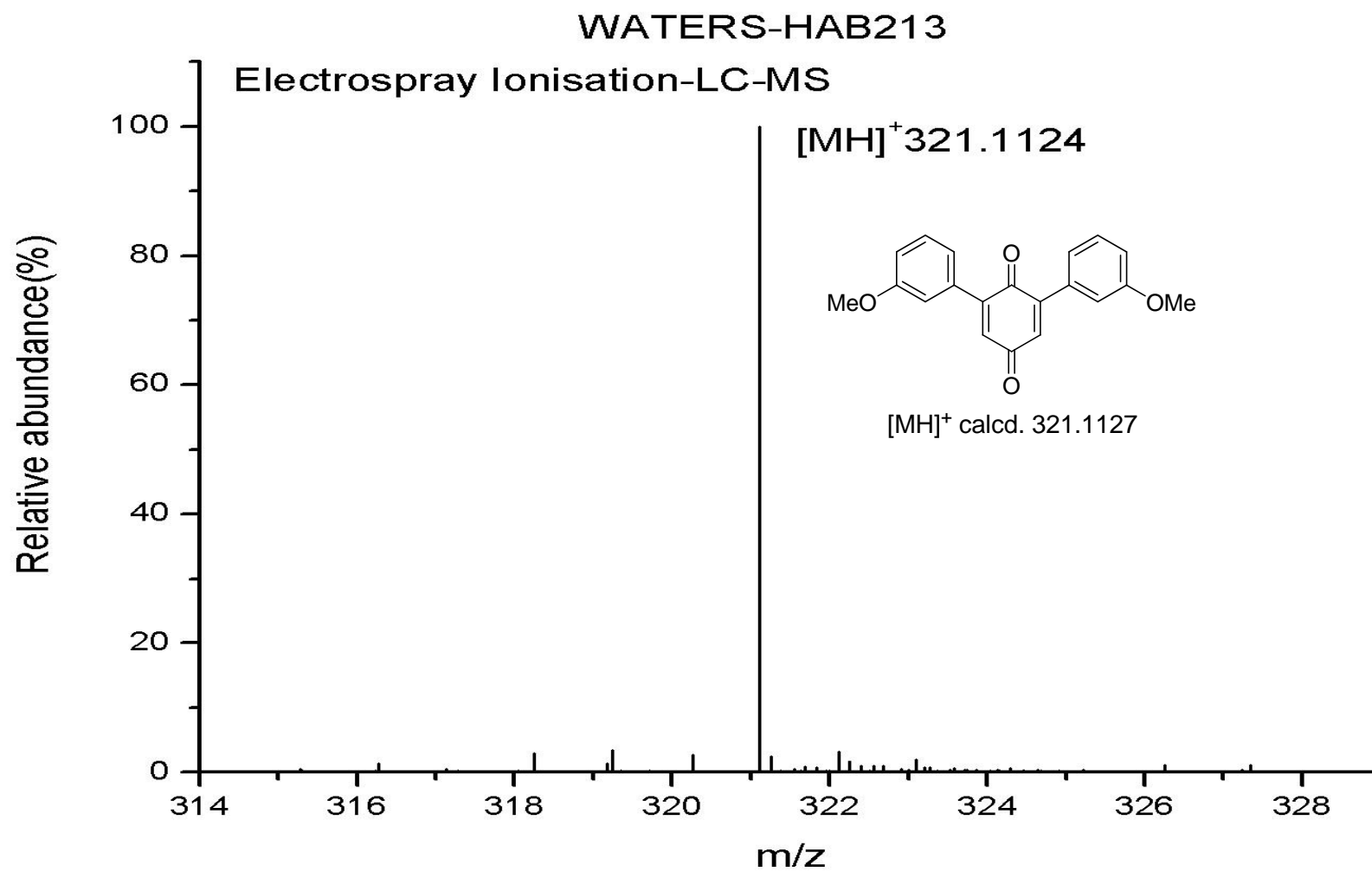
HRMS spectrum of 2,6-di-(4-methylphenyl)-1,4-benzoquinone (**7.1**)



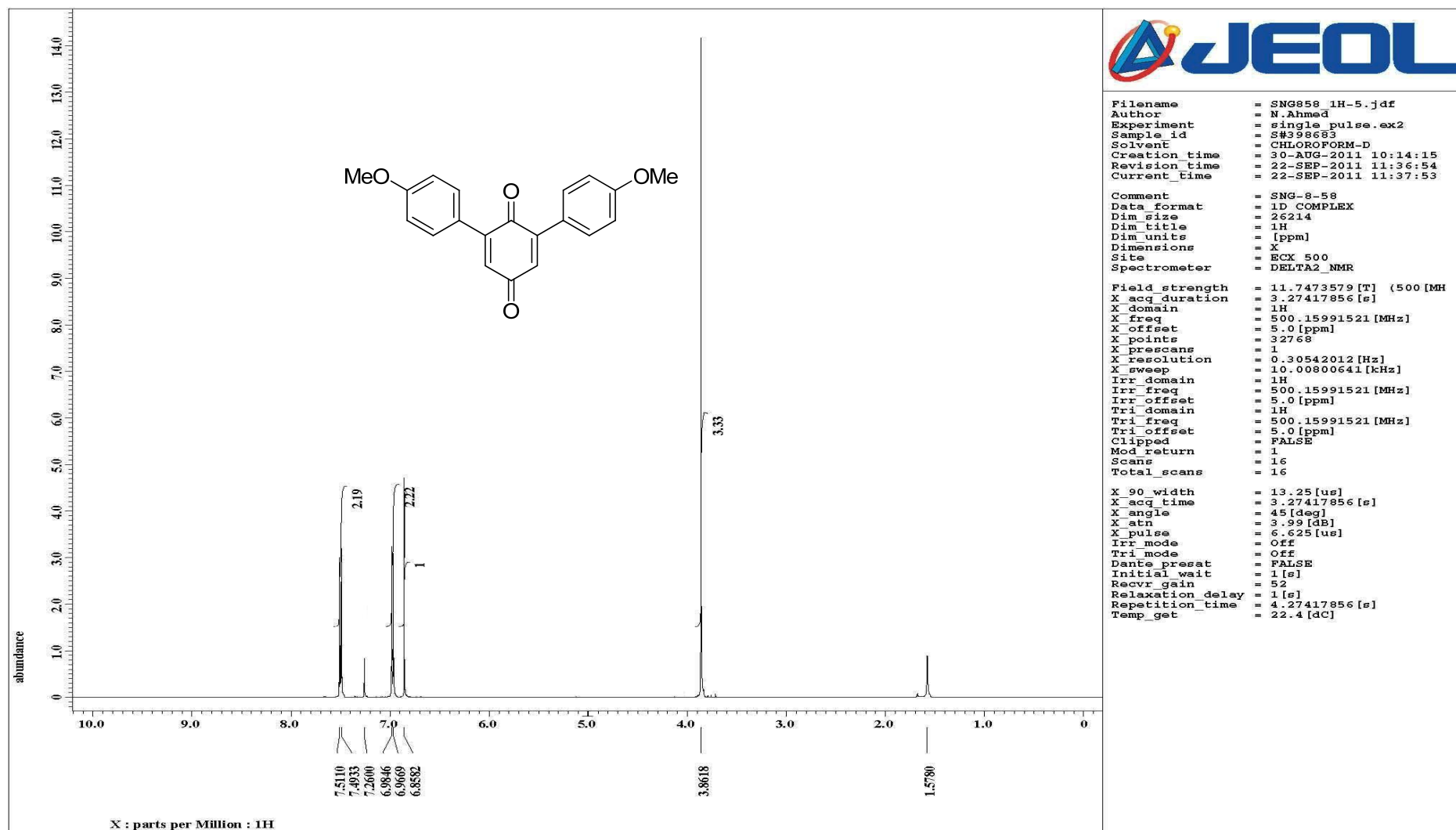
<sup>1</sup>H NMR spectrum of 2,6-bis(3-methoxyphenyl)-1,4-benzoquinone (7.2)



$^{13}\text{C}$  NMR spectrum of 2,6-bis(3-methoxyphenyl)-1,4-benzoquinone (7.2)

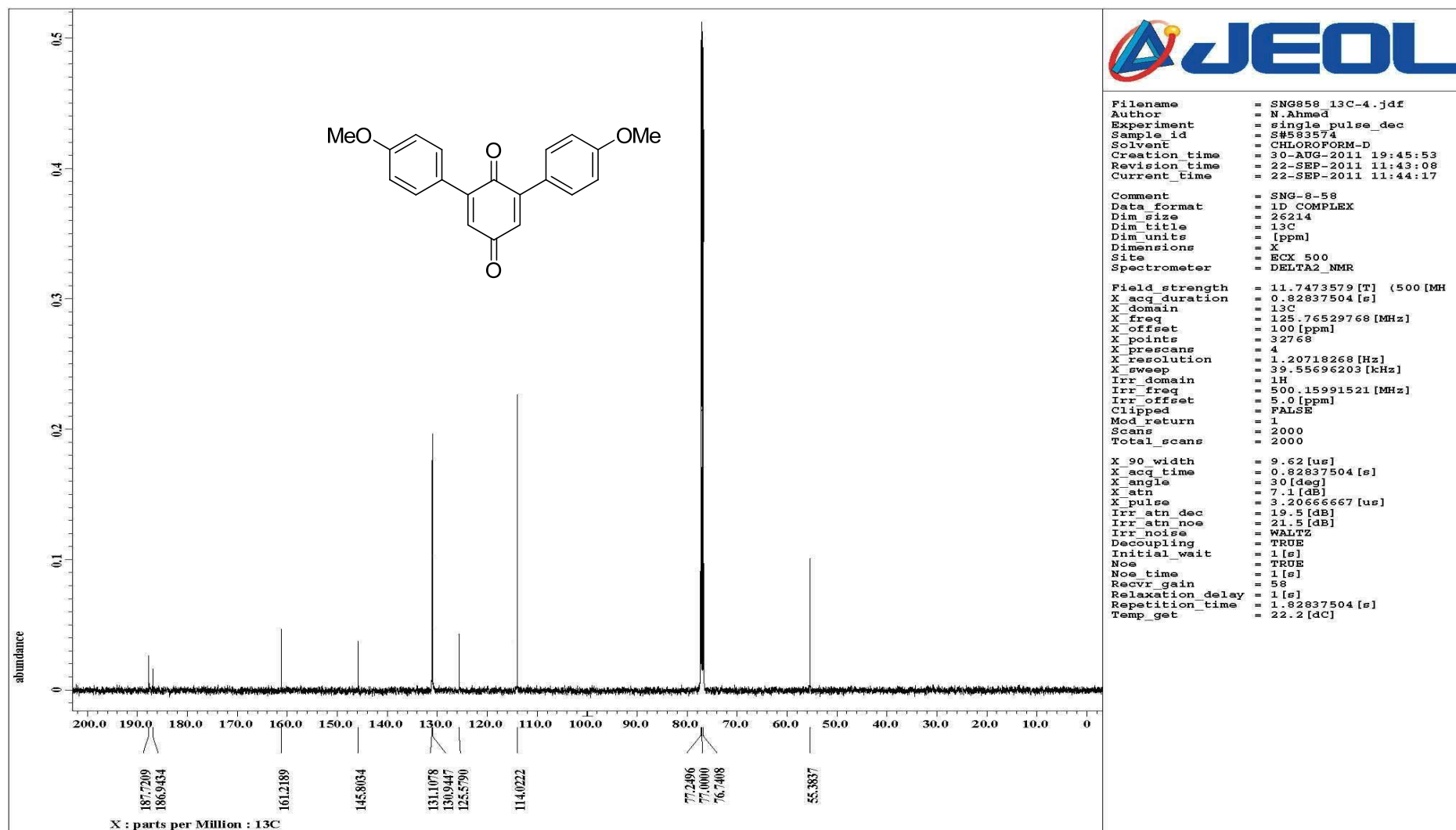


HRMS spectrum of 2,6-bis(3-methoxyphenyl)-1,4-benzoquinone (**7.2**)

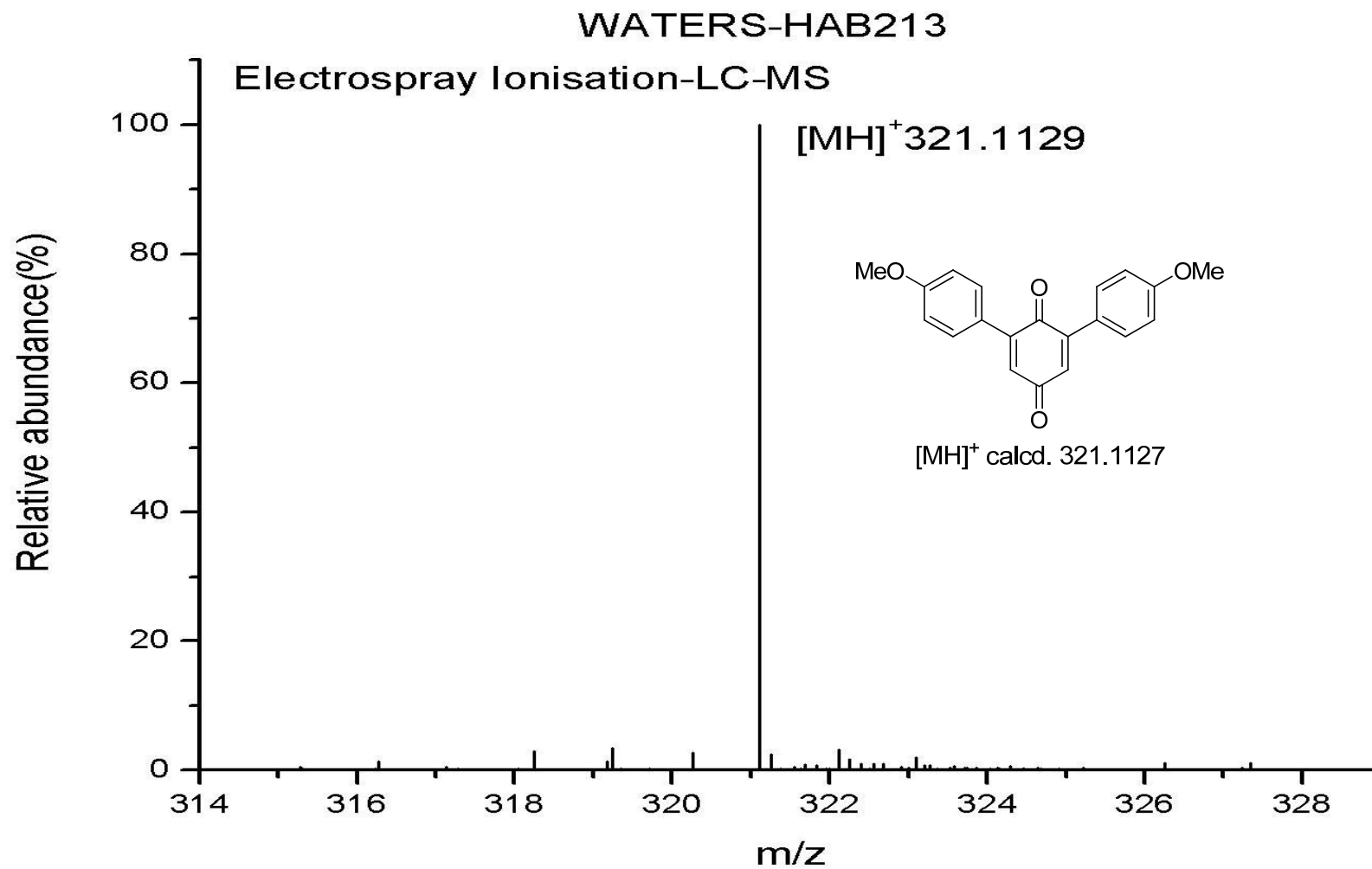


<sup>1</sup>H NMR spectrum of 2,6-bis(4-methoxyphenyl)-1,4-benzoquinone (7.3)

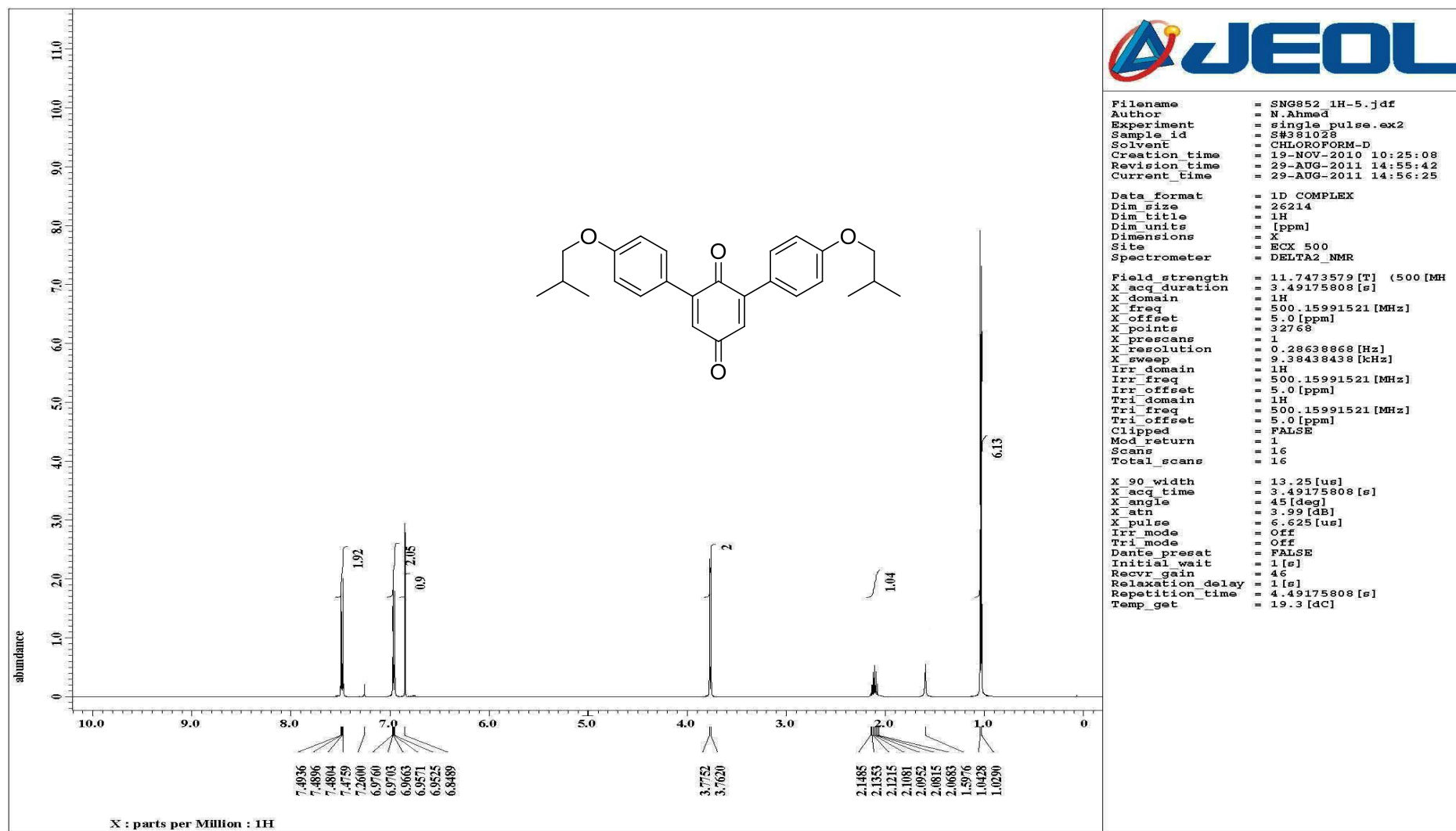




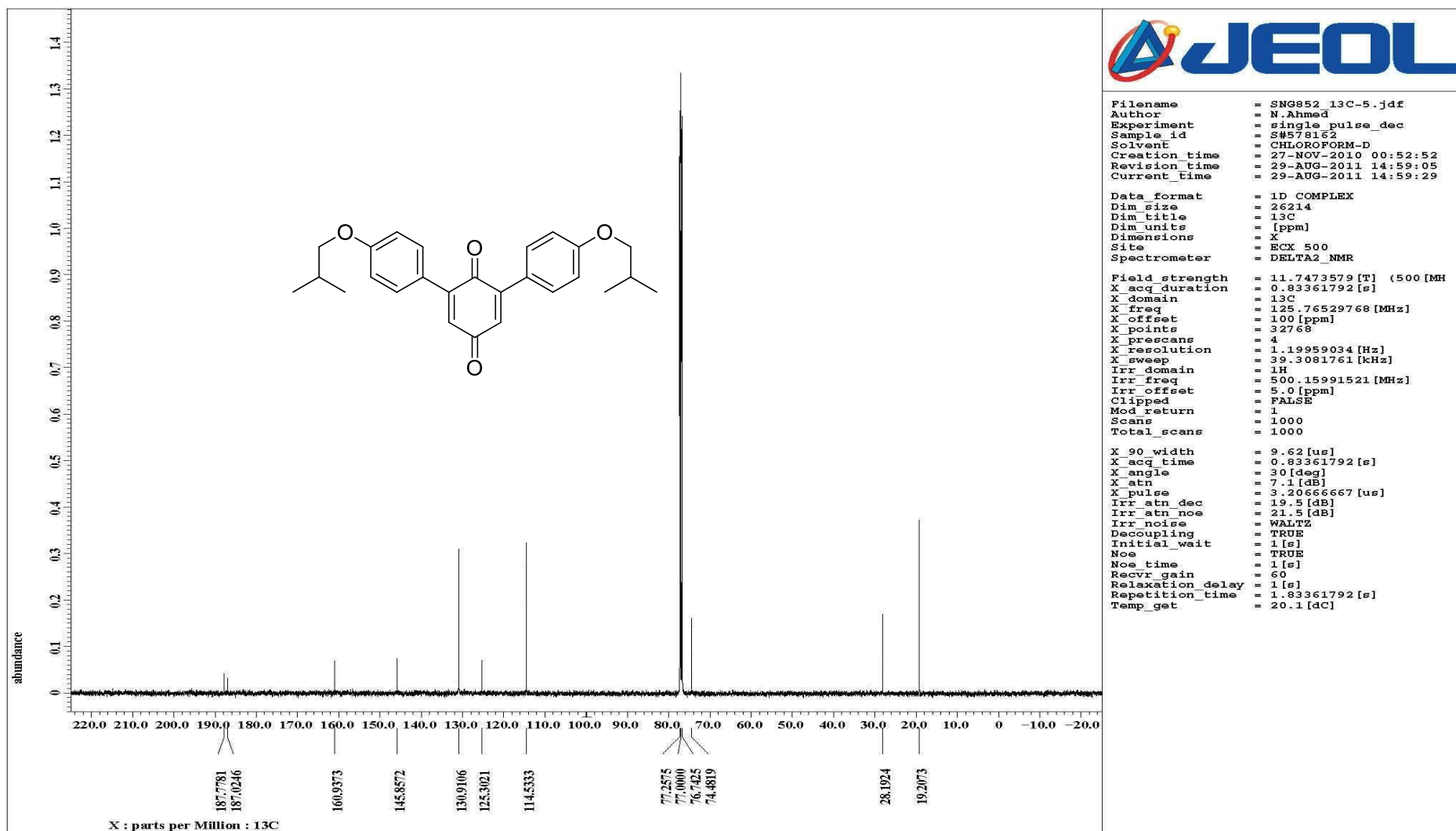
<sup>13</sup>C NMR spectrum of 2,6-bis(4-methoxyphenyl)-1,4-benzoquinone (7.3)



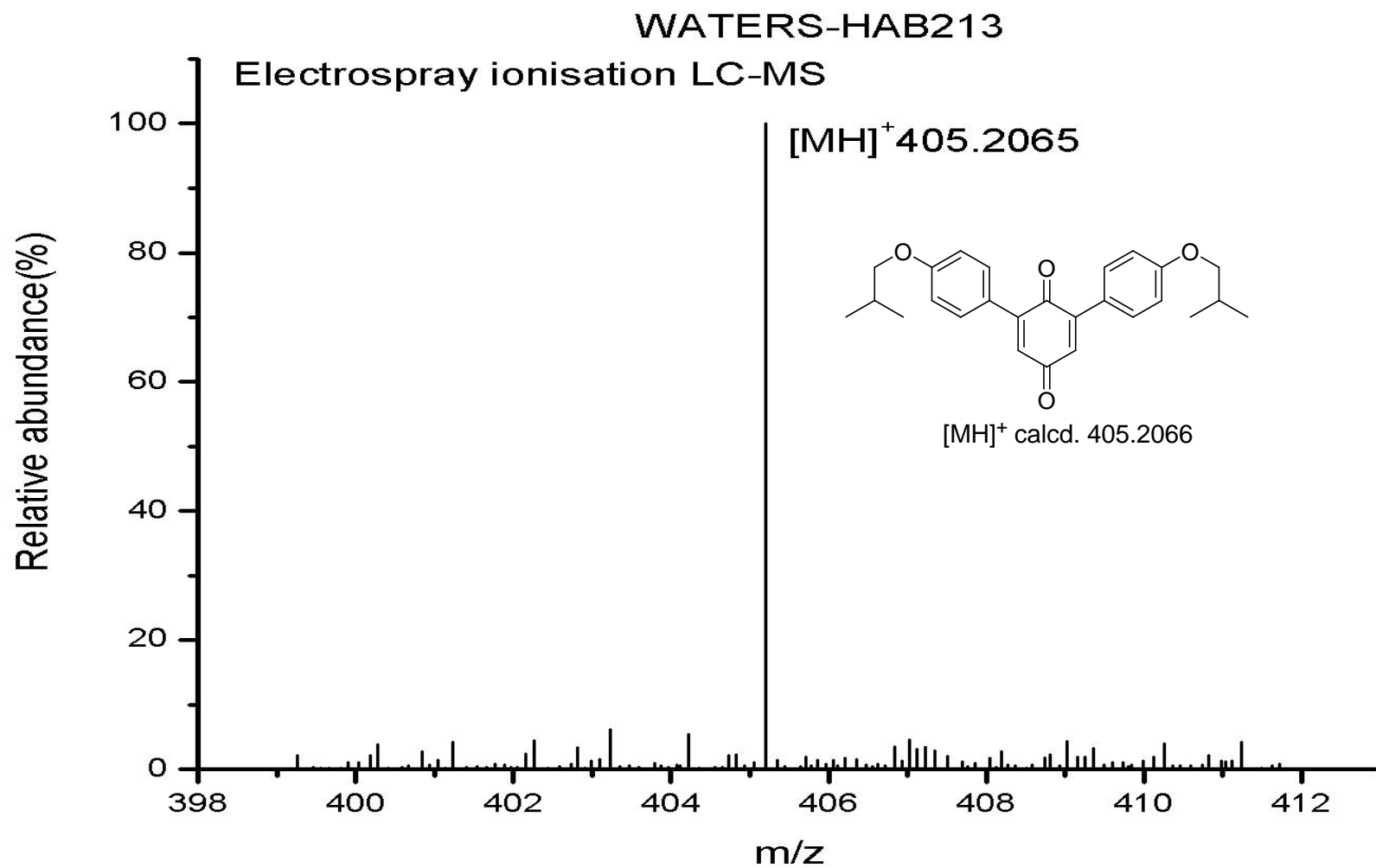
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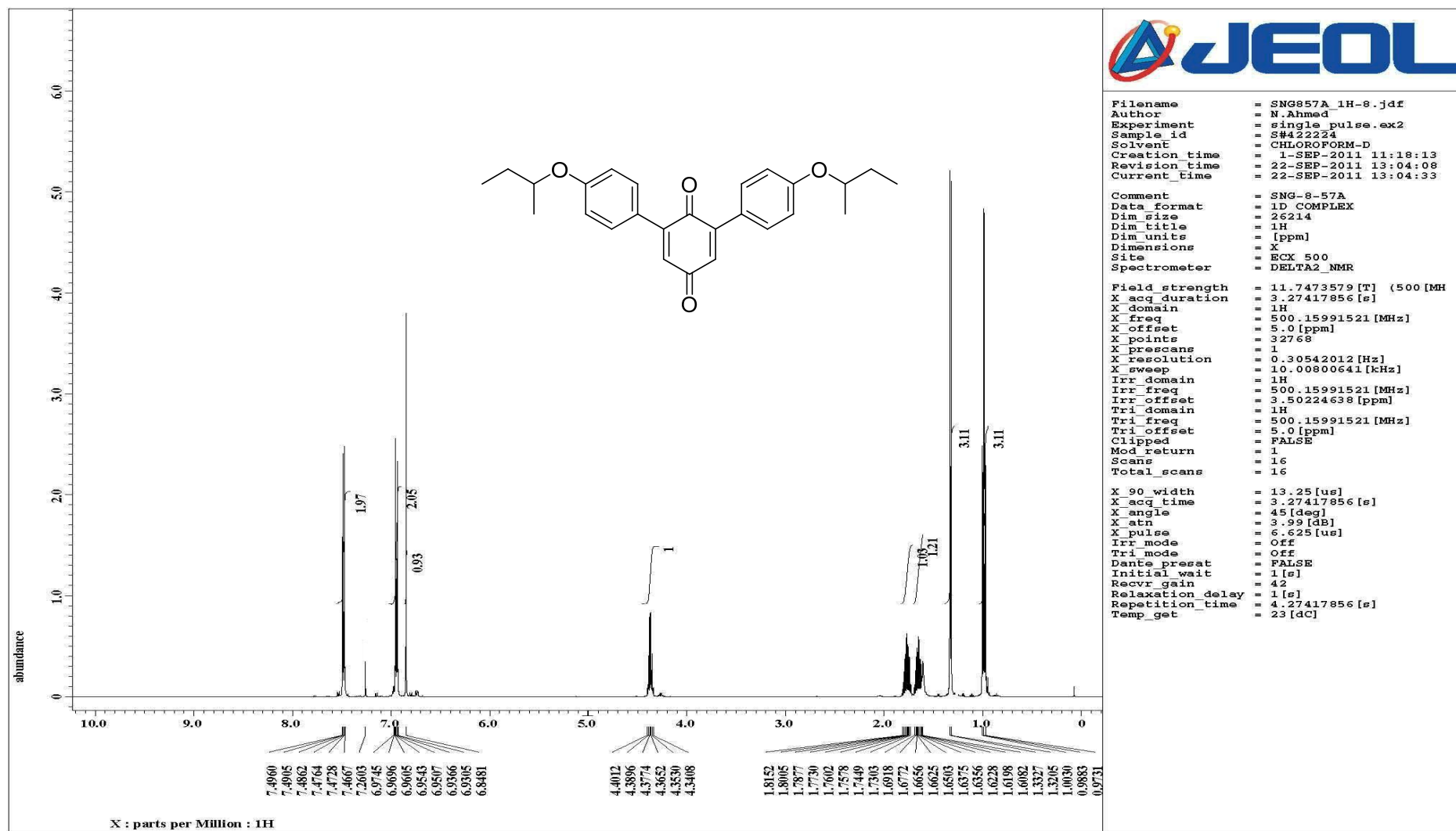
<sup>1</sup>H NMR spectrum of 2,6-bis(4-isobutoxyphenyl)-1,4-benzoquinone (7.4)



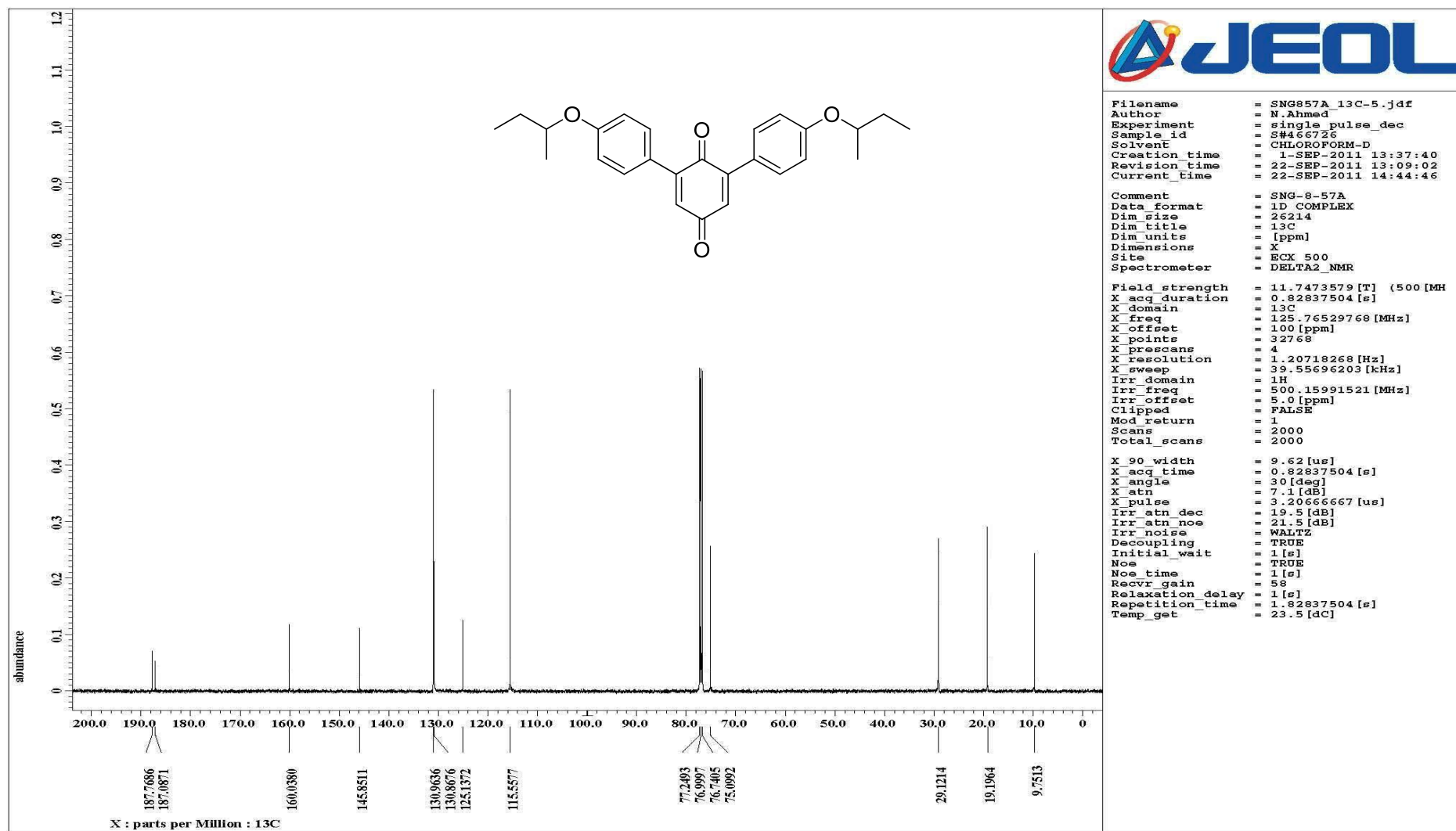
<sup>13</sup>C NMR spectrum of 2,6-bis(4-isobutoxyphenyl)-1,4-benzoquinone (7.4)



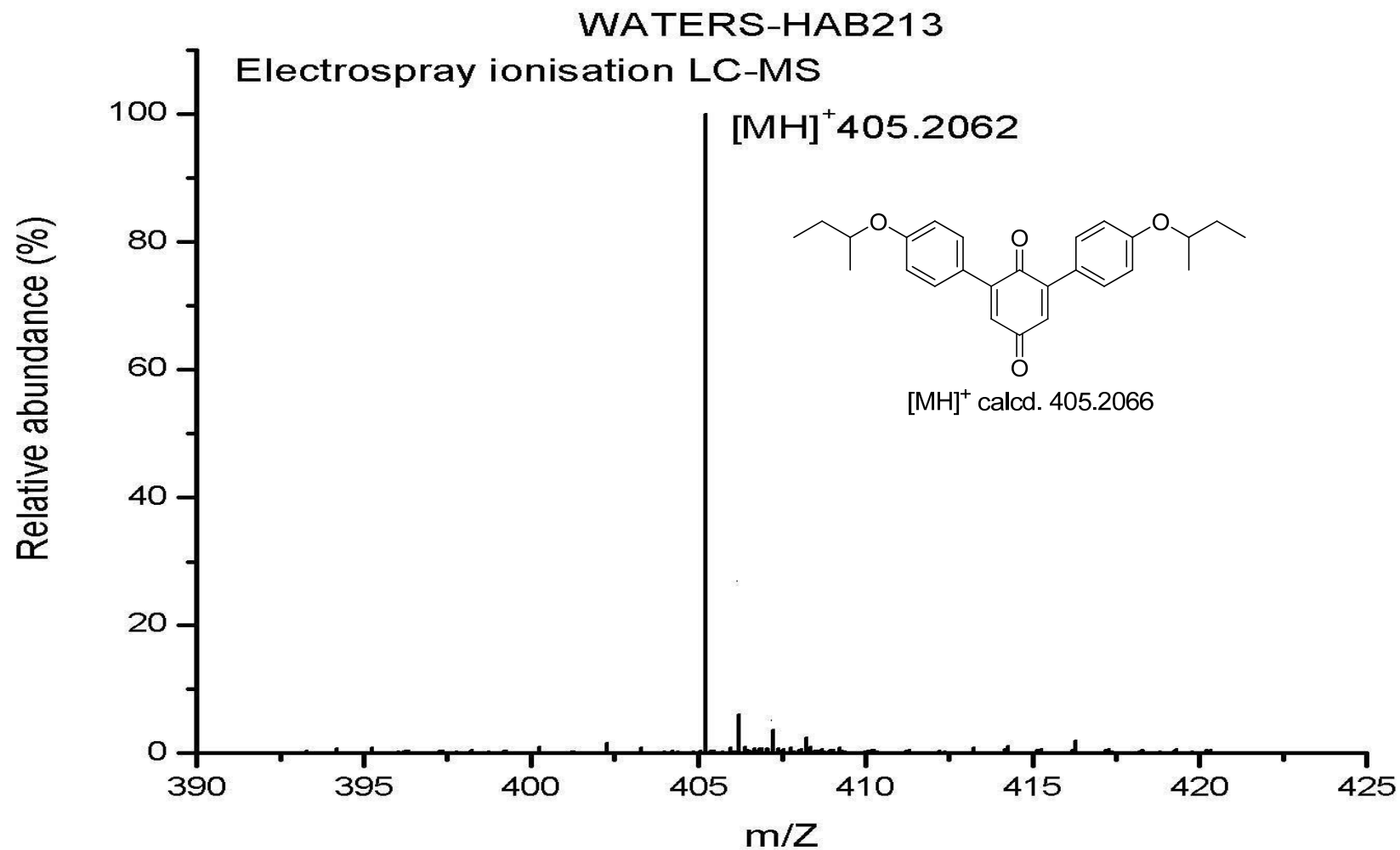
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<sup>1</sup>H NMR spectrum of 2,6-bis(4-sec-butoxyphenyl)-1,4-benzoquinone (7.5)

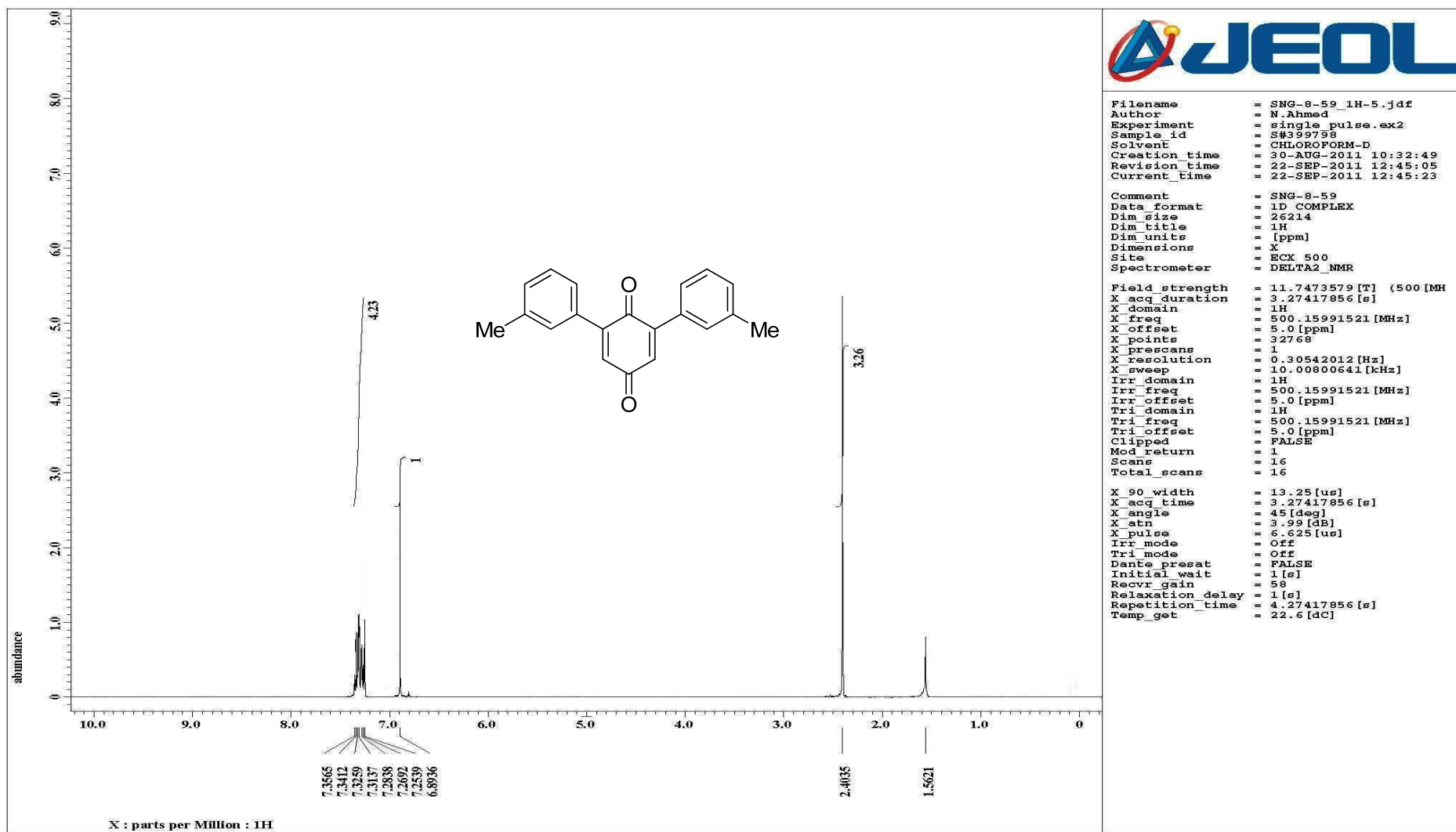


<sup>13</sup>C NMR spectrum of 2,6-bis(4-sec-butoxyphenyl)-1,4-benzoquinone (7.5)

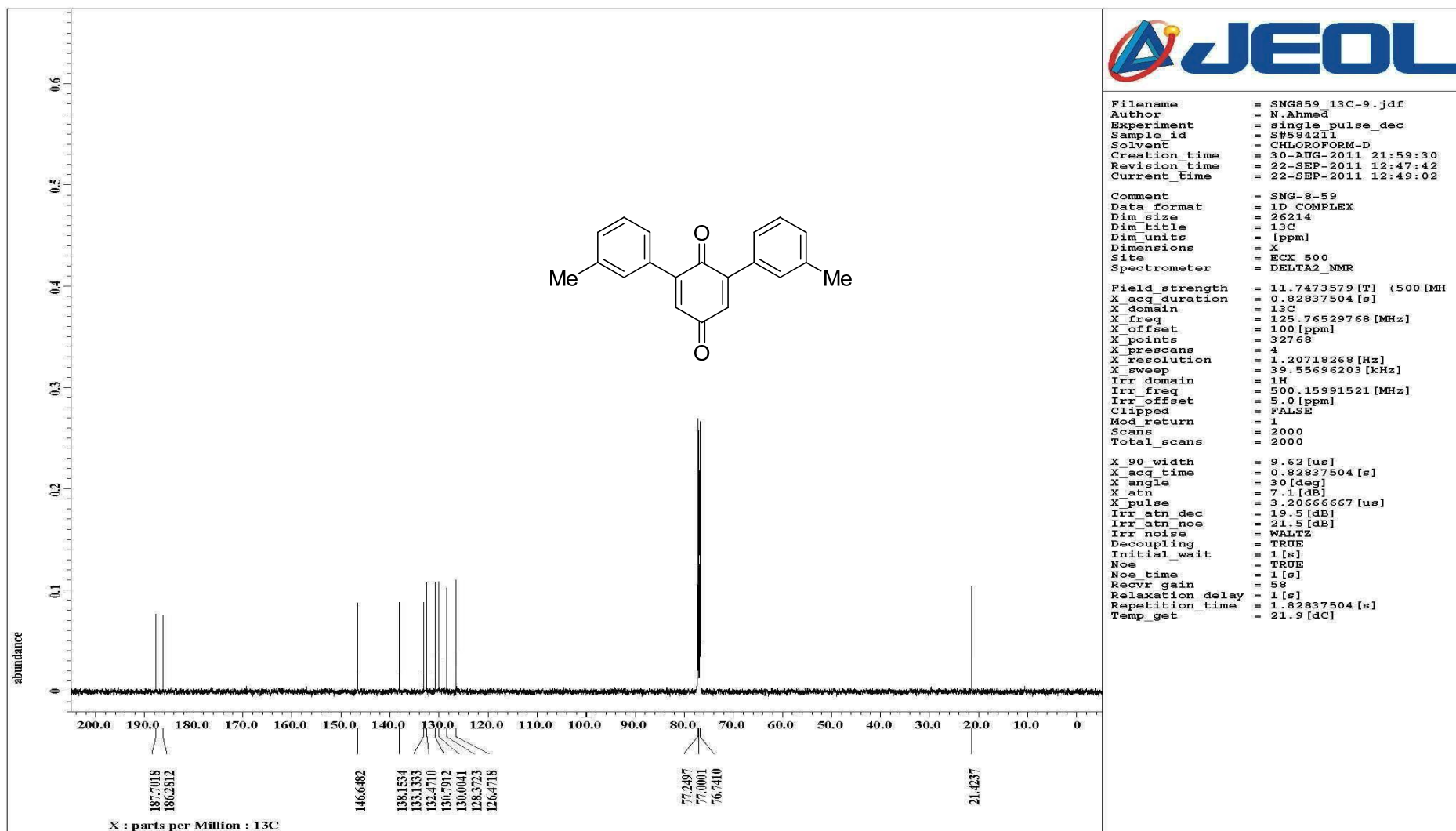


HRMS spectrum of 2,6-bis(4-sec-butoxyphenyl)-1,4-benzoquinone (**7.5**)

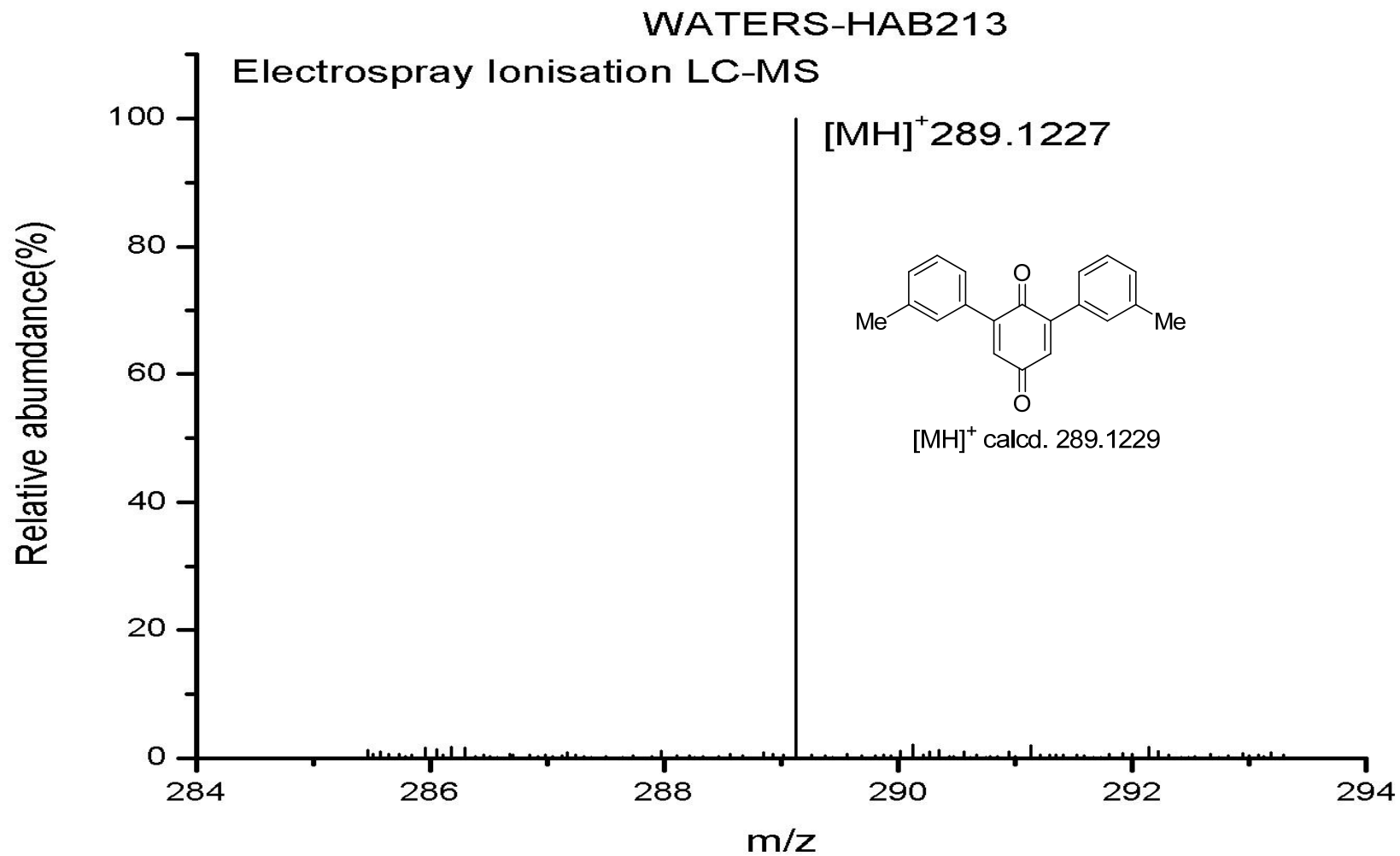




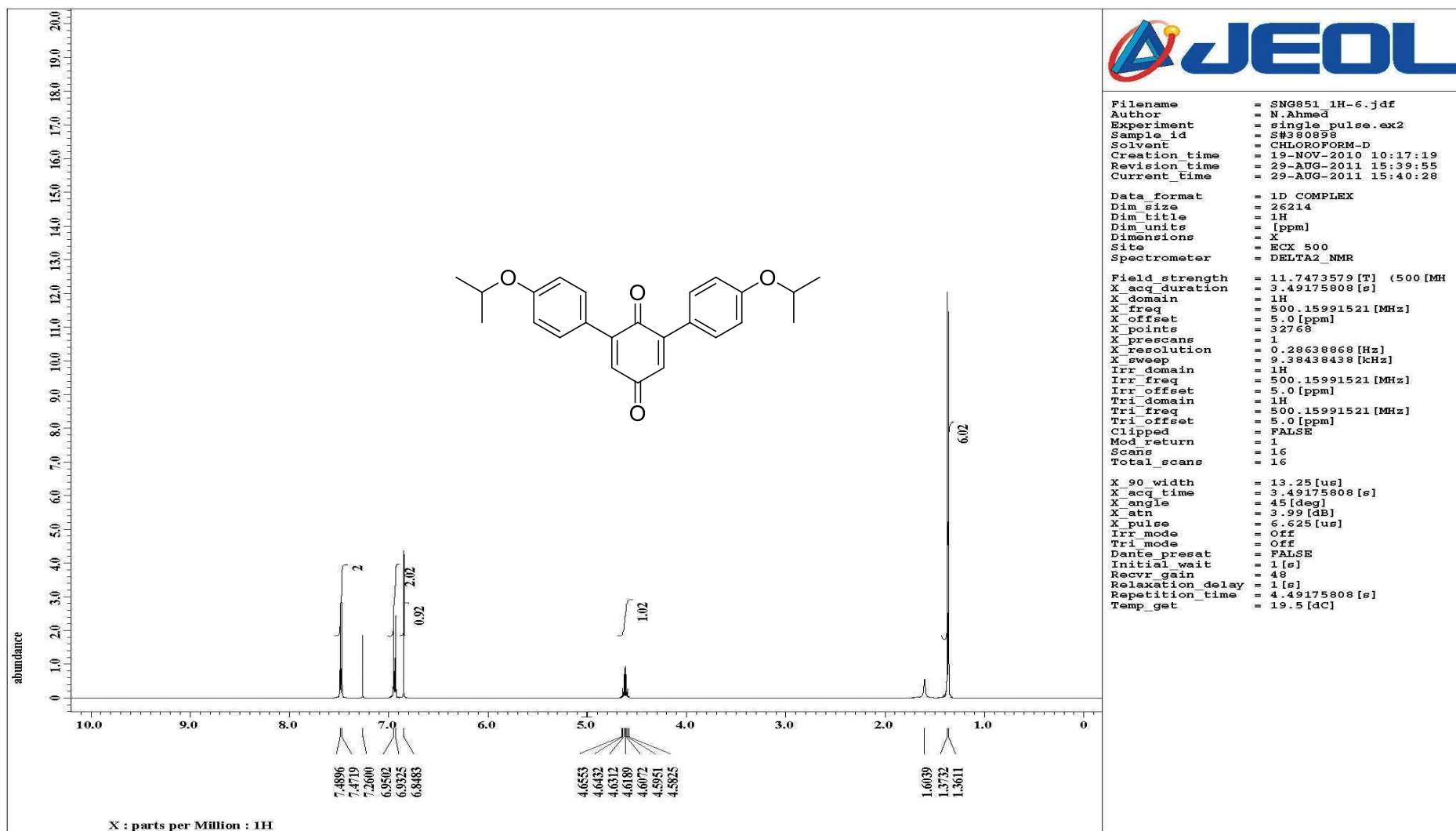
<sup>1</sup>H NMR spectrum of 2,6-di-(3-methylphenyl)-1,4-benzoquinone (7.6)



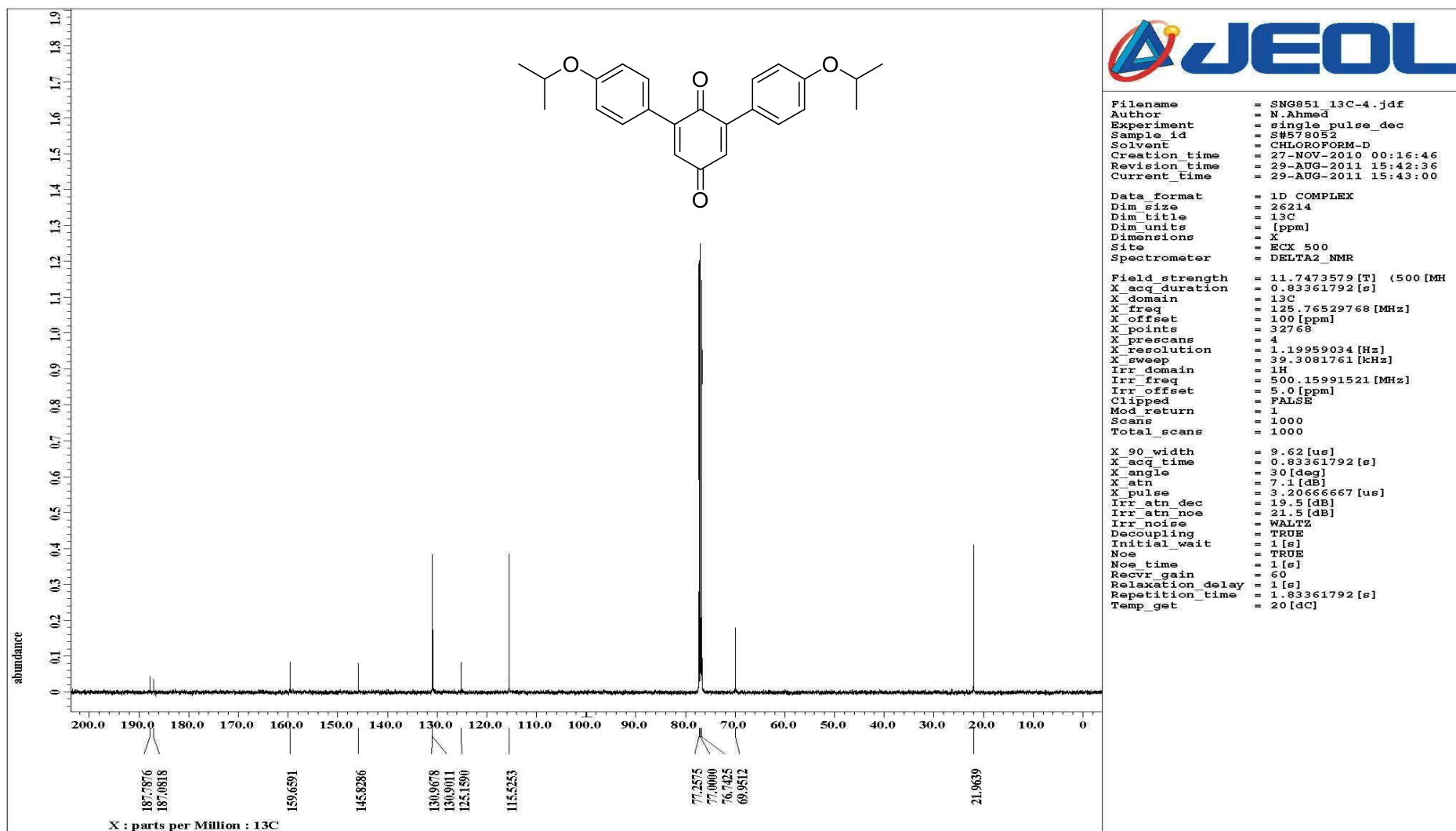
<sup>13</sup>C NMR spectrum of 2,6-di-(3-methylphenyl)-1,4-benzoquinone (7.6)



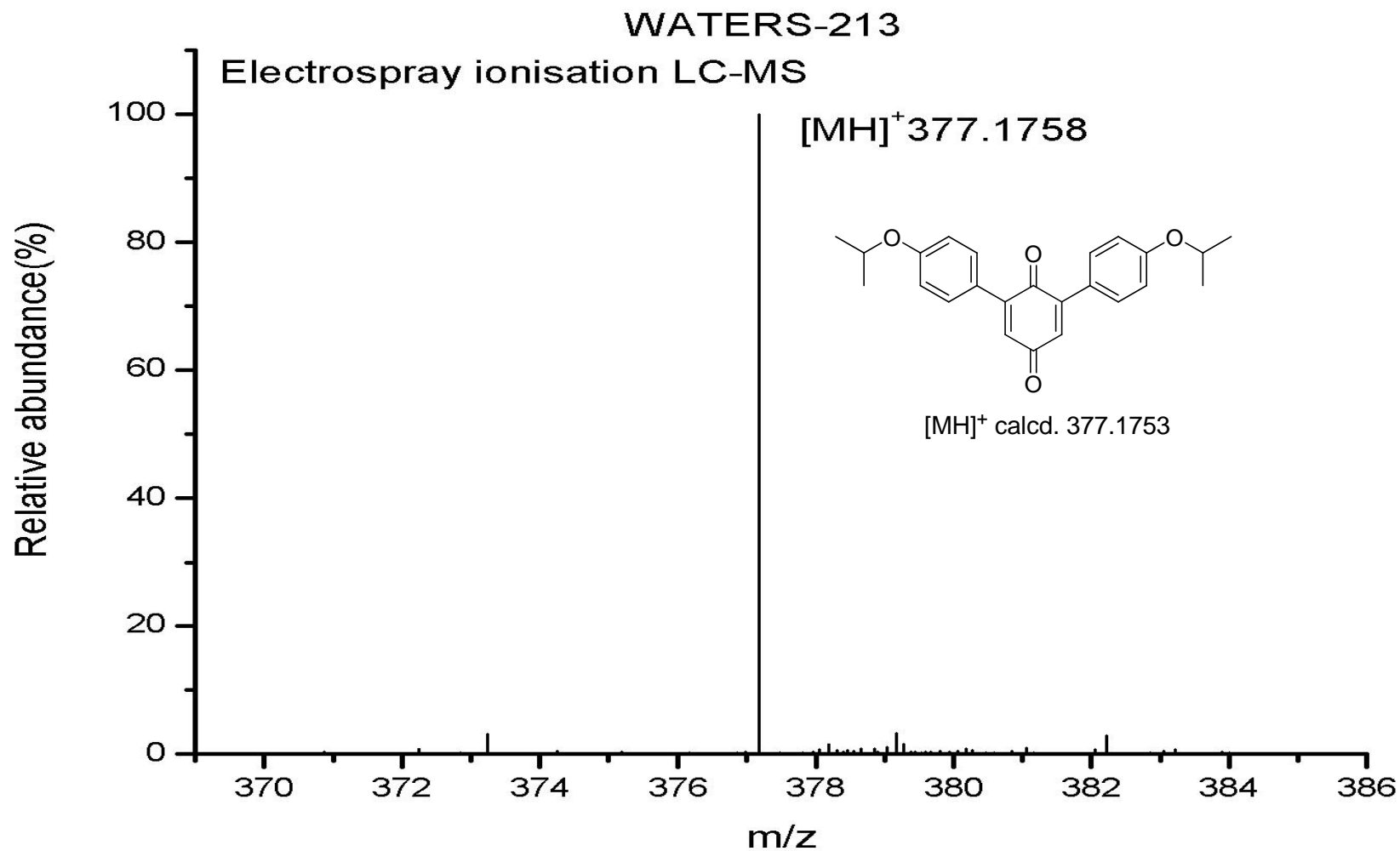
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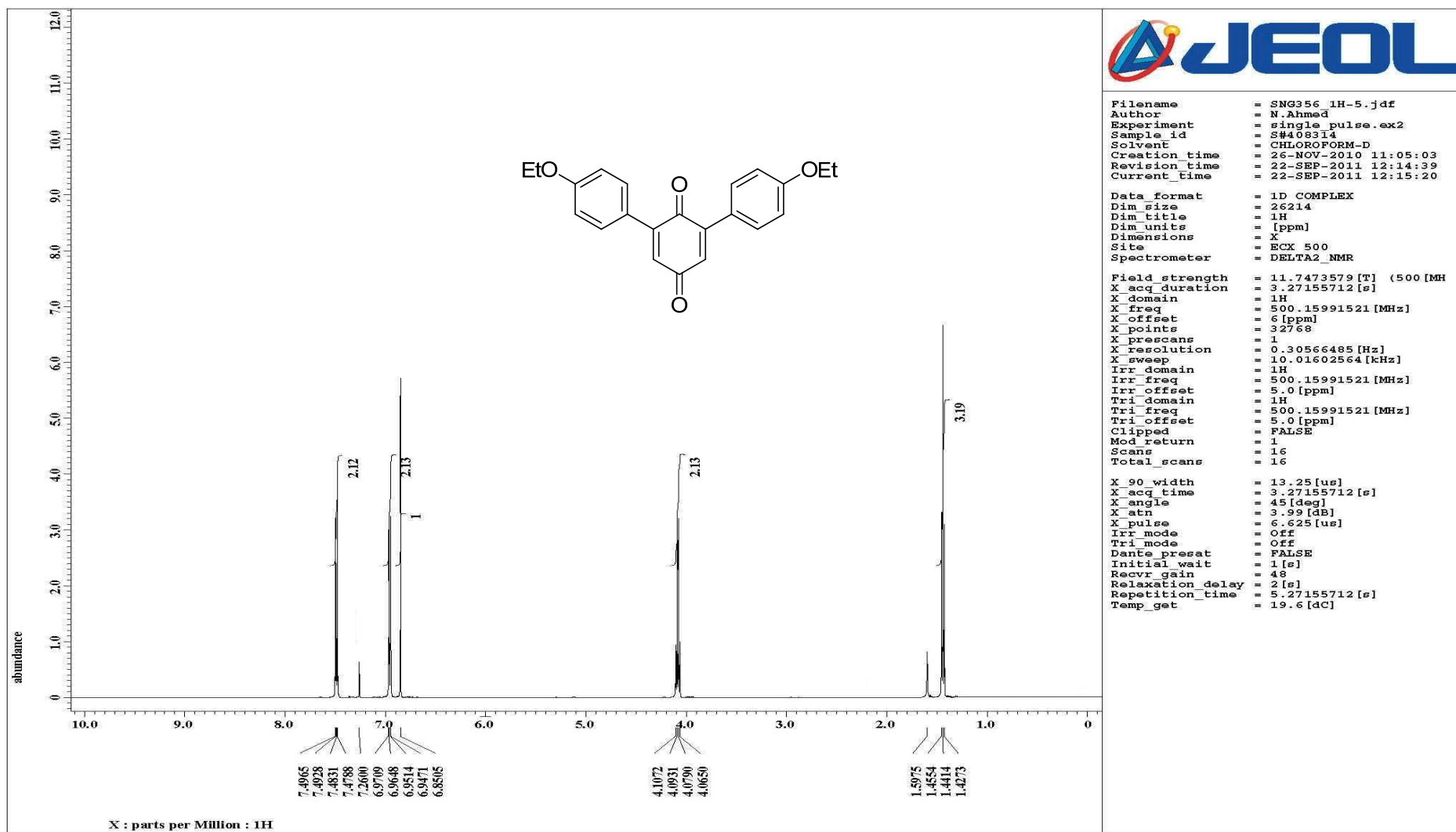
<sup>1</sup>H spectrum of 2,6-bis(4-isopropoxyphenyl)-1,4-benzoquinone (7.7)



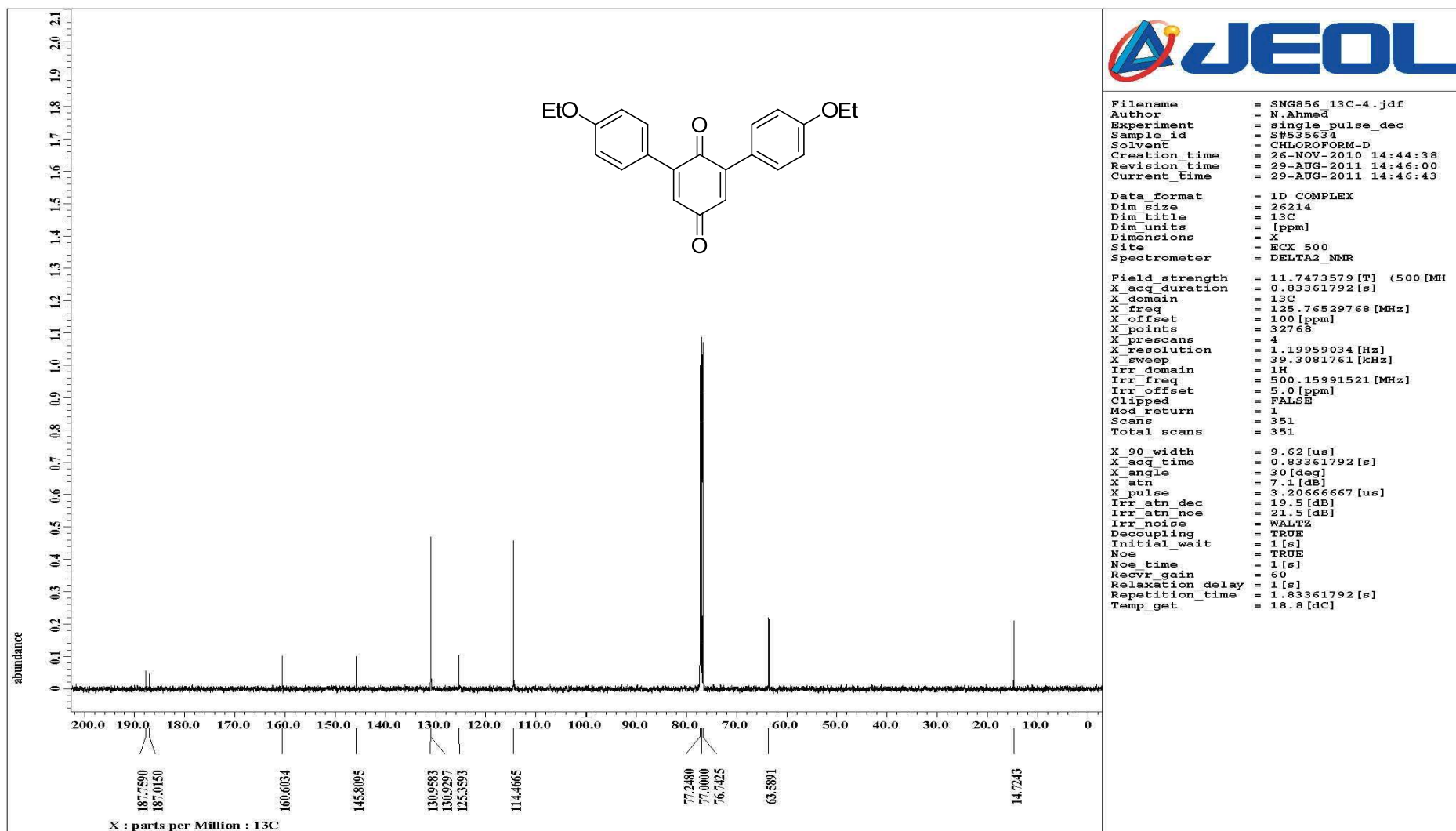
<sup>13</sup>C NMR spectrum of 2,6-bis(4-isopropoxyphenyl)-1,4-benzoquinone (7.7)



HRMS spectrum of 2,6-bis(4-isopropoxyphenyl)-1,4-benzoquinone (**7.7**)

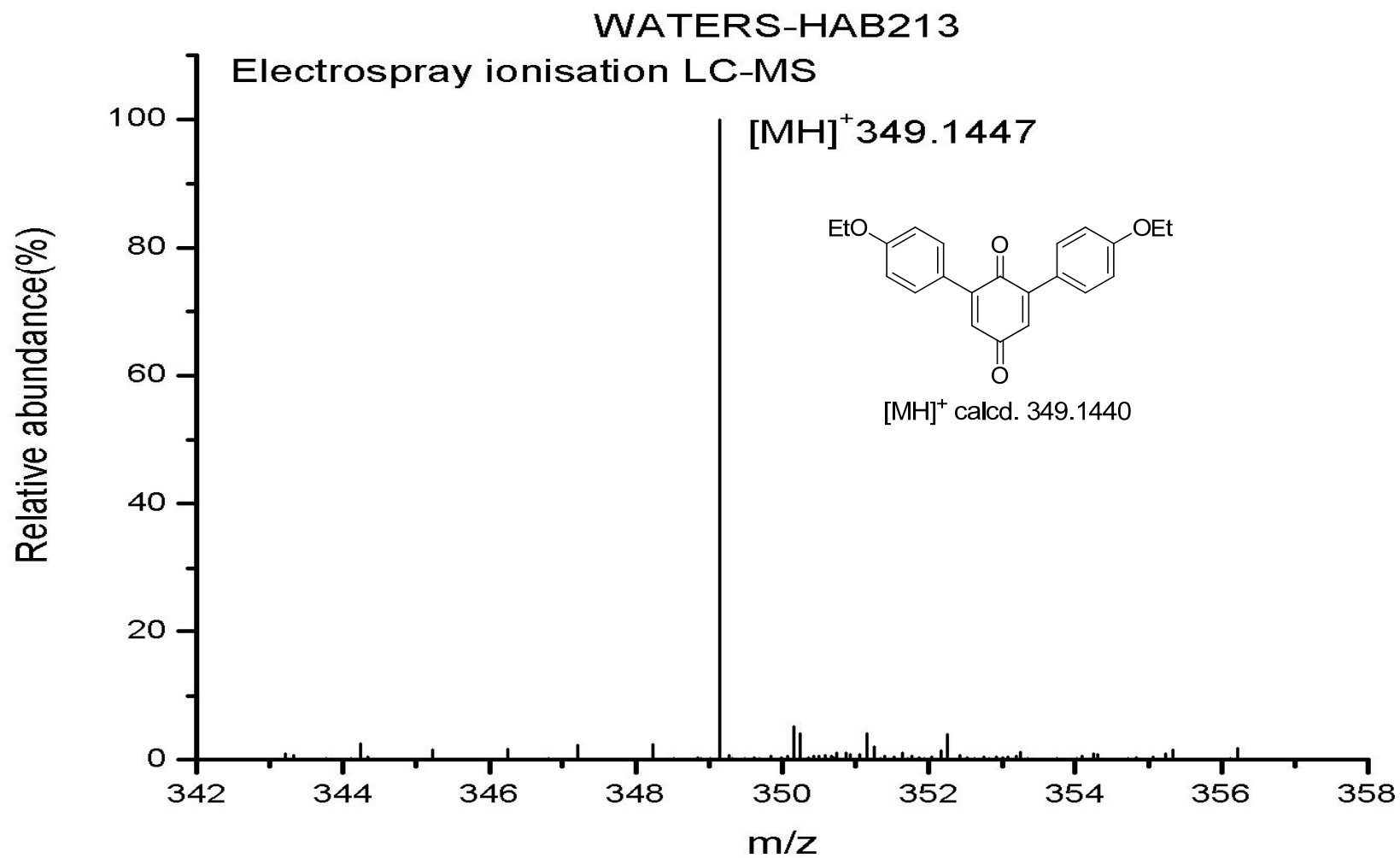


<sup>1</sup>H NMR spectrum of 2,6-bis(4-ethoxyphenyl)-1,4-benzoquinone (7.8)



<sup>13</sup>C NMR spectrum of 2,6-bis(4-ethoxyphenyl)-1,4-benzoquinone (7.8)





HRMS spectrum of 2,6-bis(4-ethoxyphenyl)-1,4-benzoquinone (**7.8**)