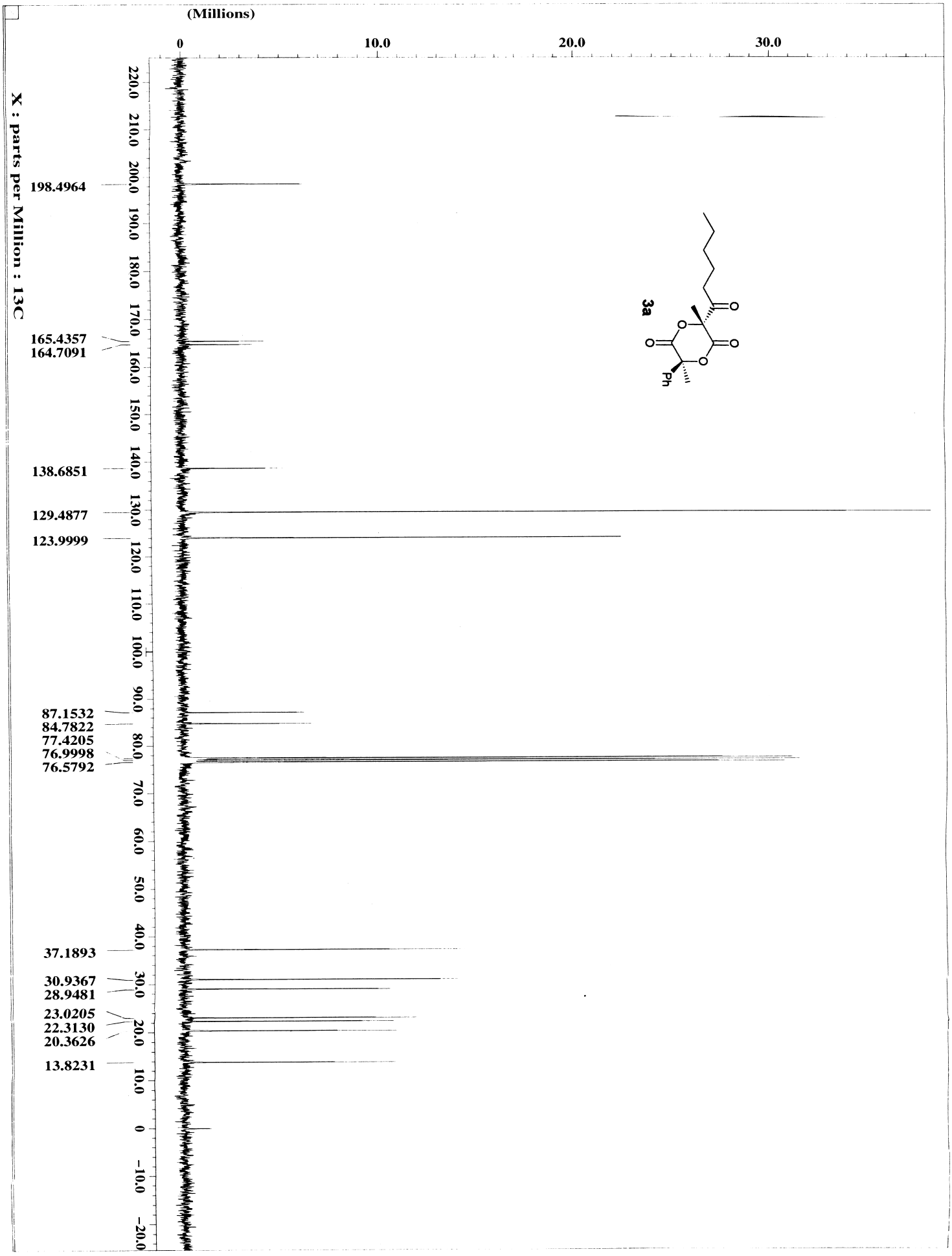
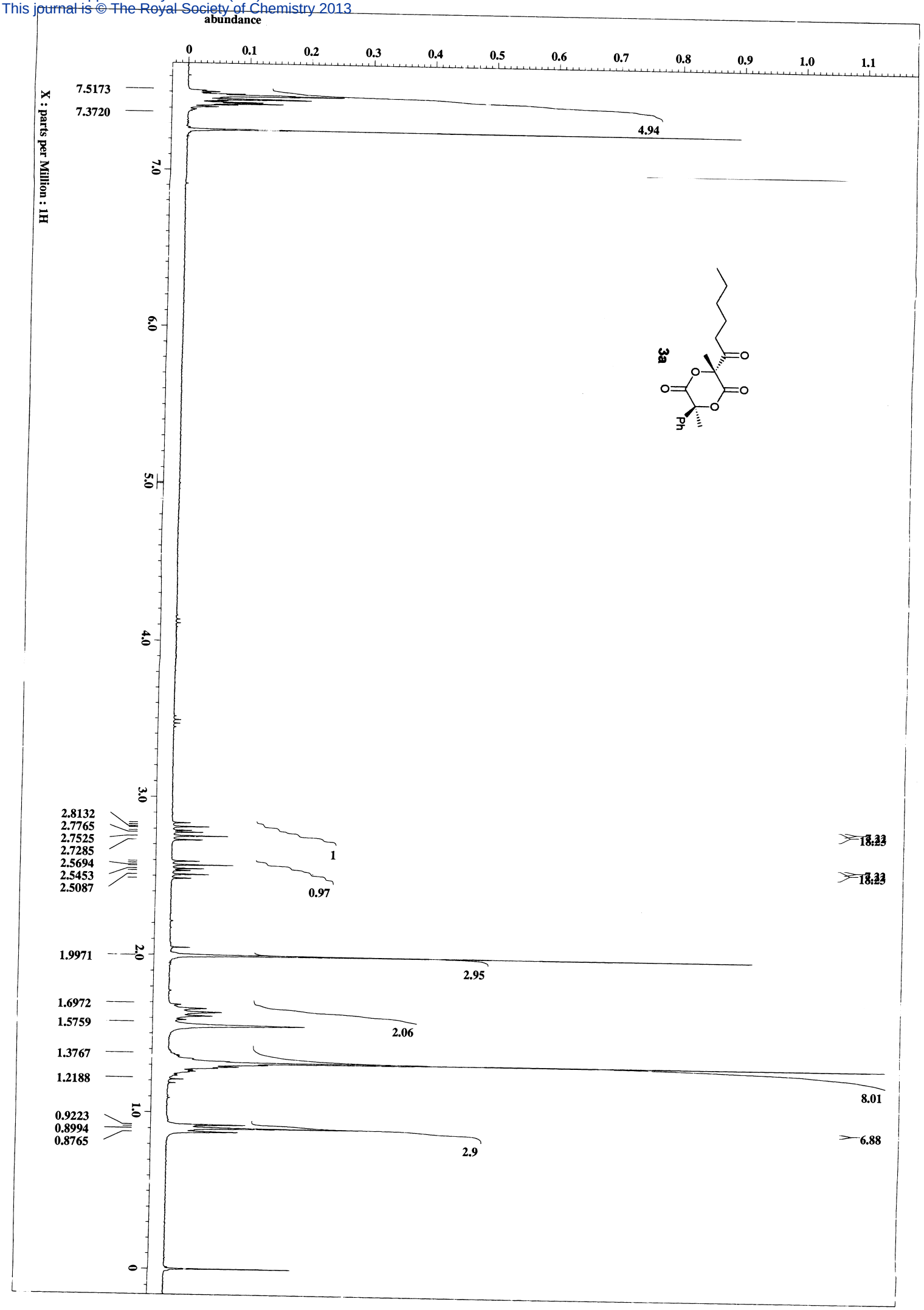
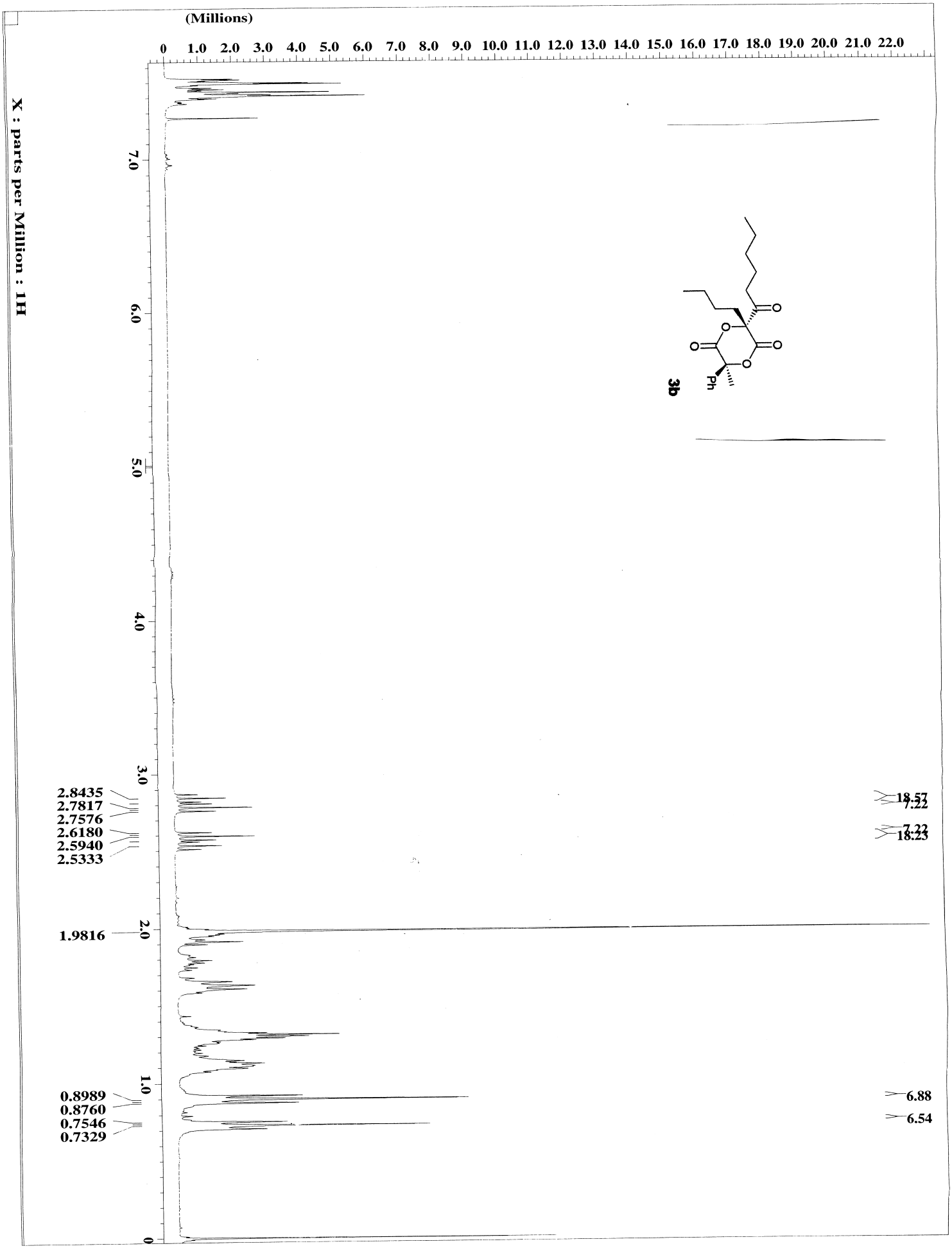
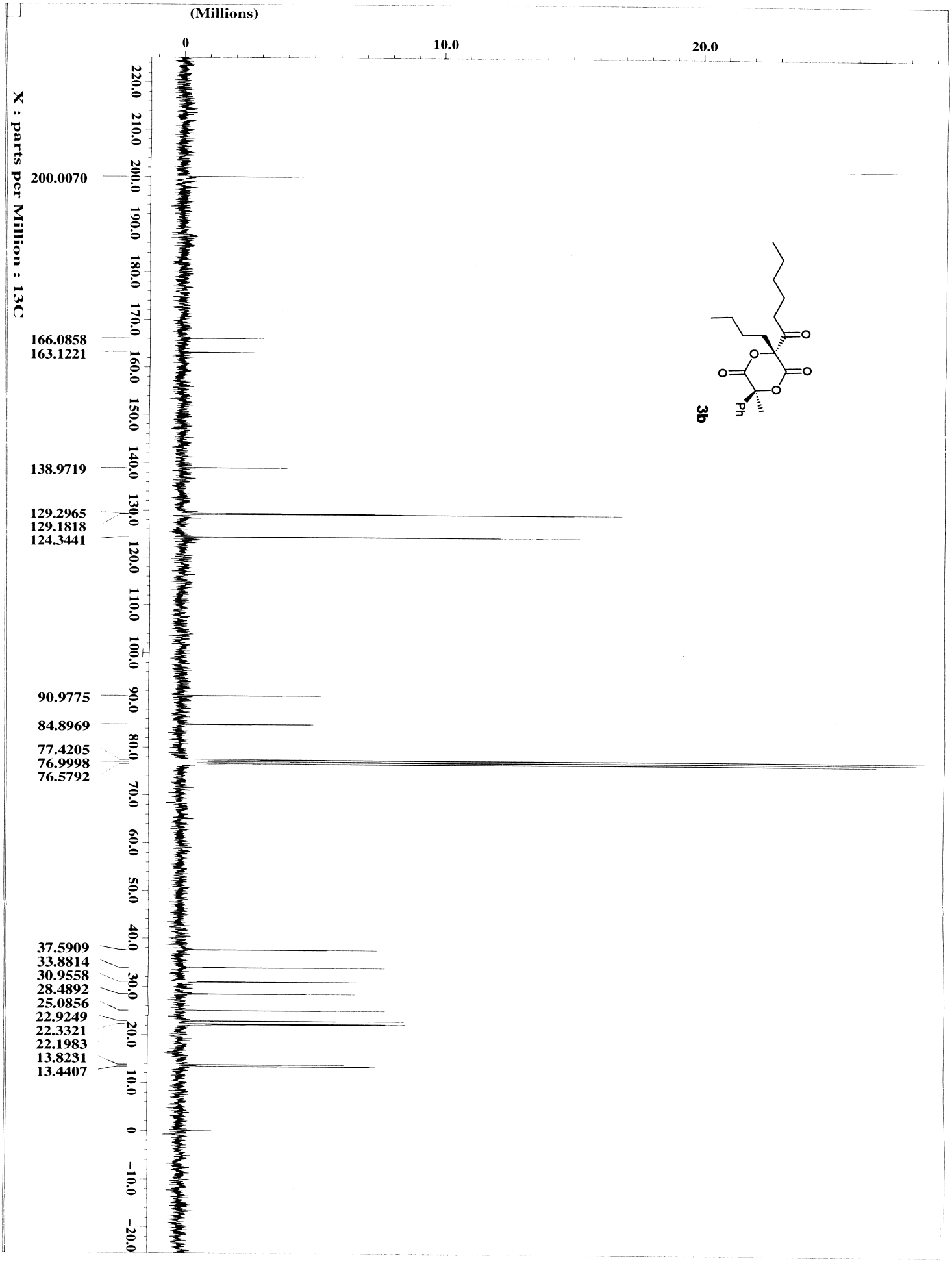
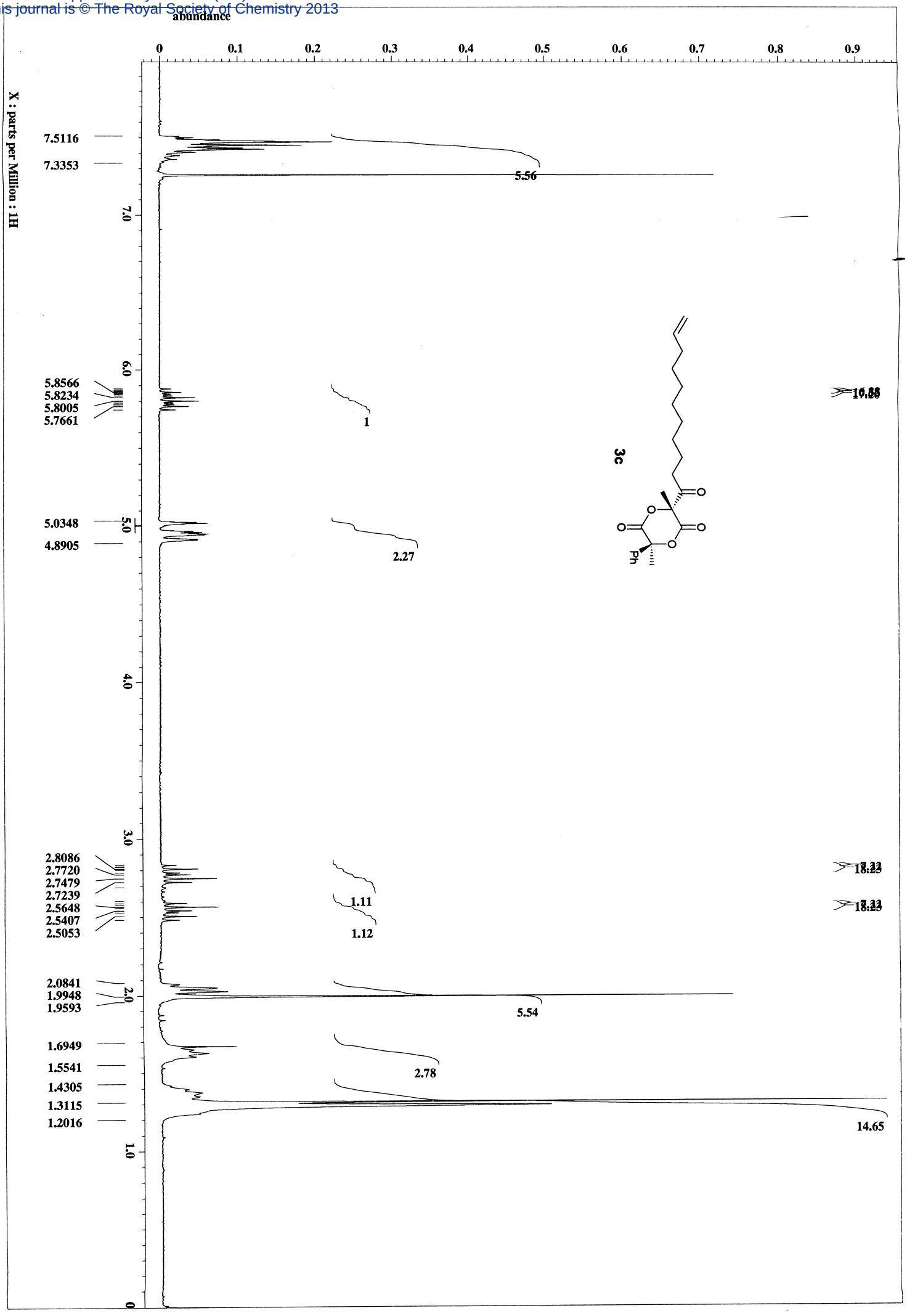
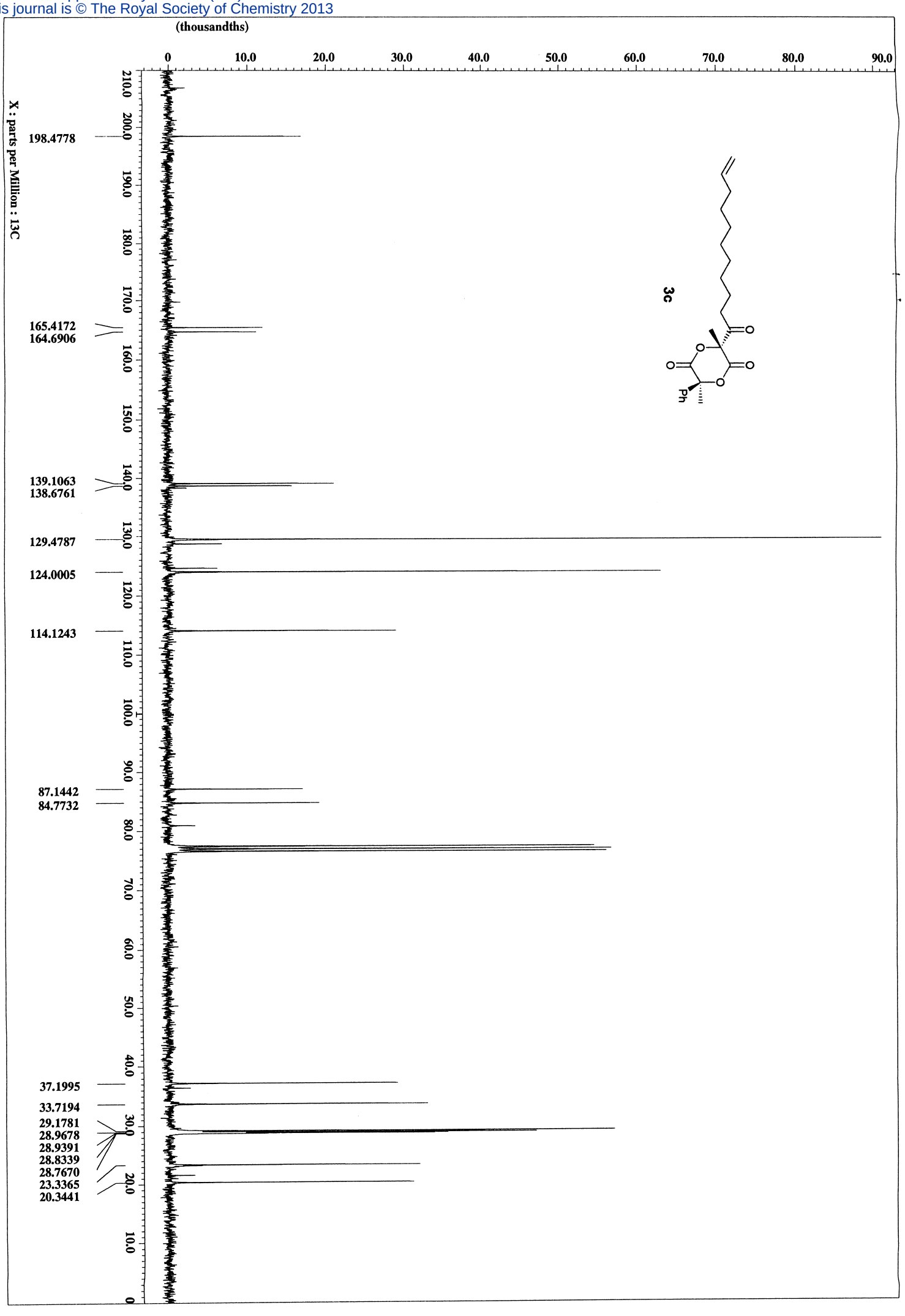


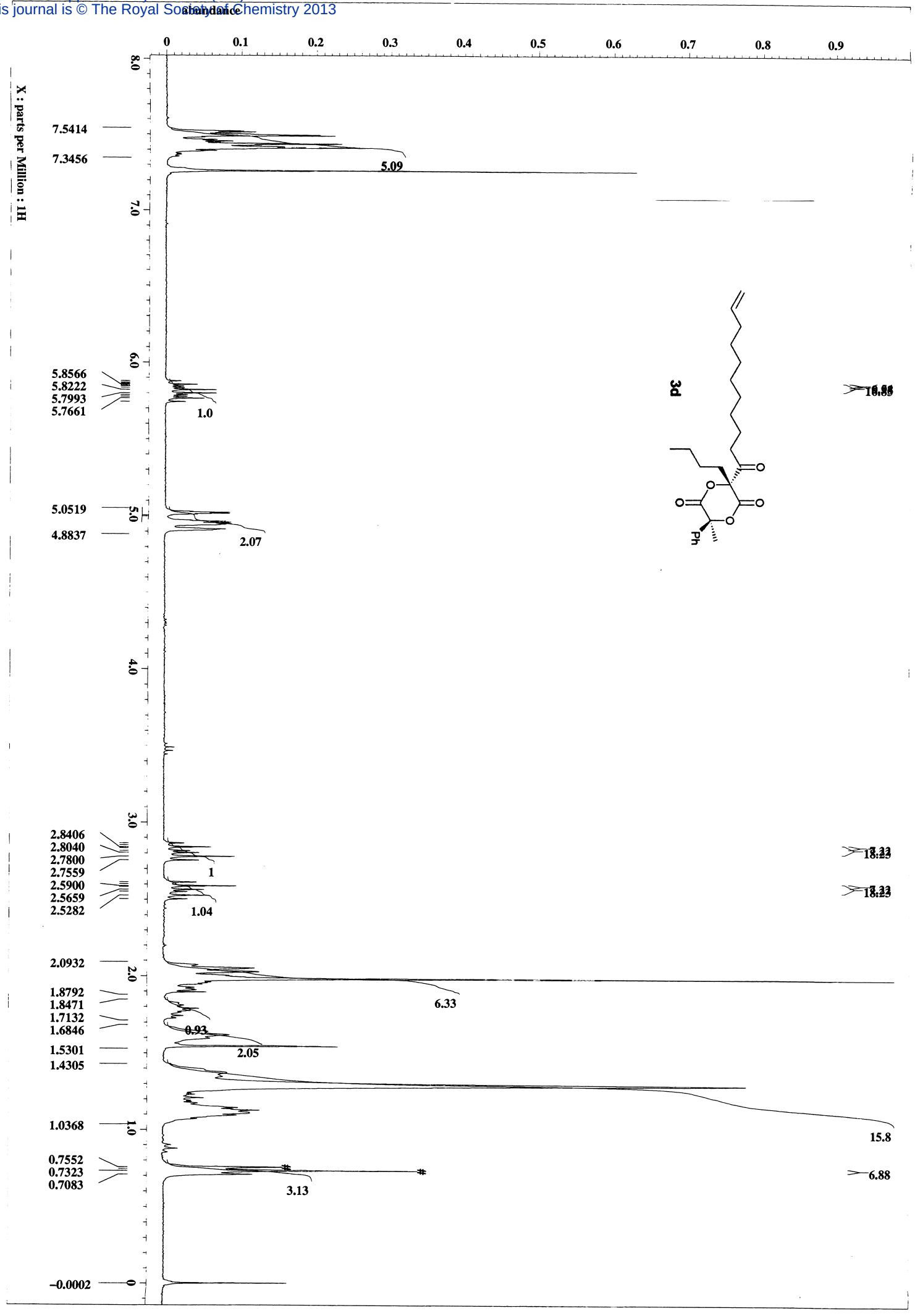

abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
X : parts per Million : 1H
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.5173
7.3720
4.94
3a
Ph
2.8132
2.7765
2.7525
2.7285
2.5694
2.5453
2.5087
1
0.97
1.9971
2.95
1.6972
1.5759
2.06
1.3767
1.2188
8.01
0.9223
0.8994
0.8765
2.9
6.88

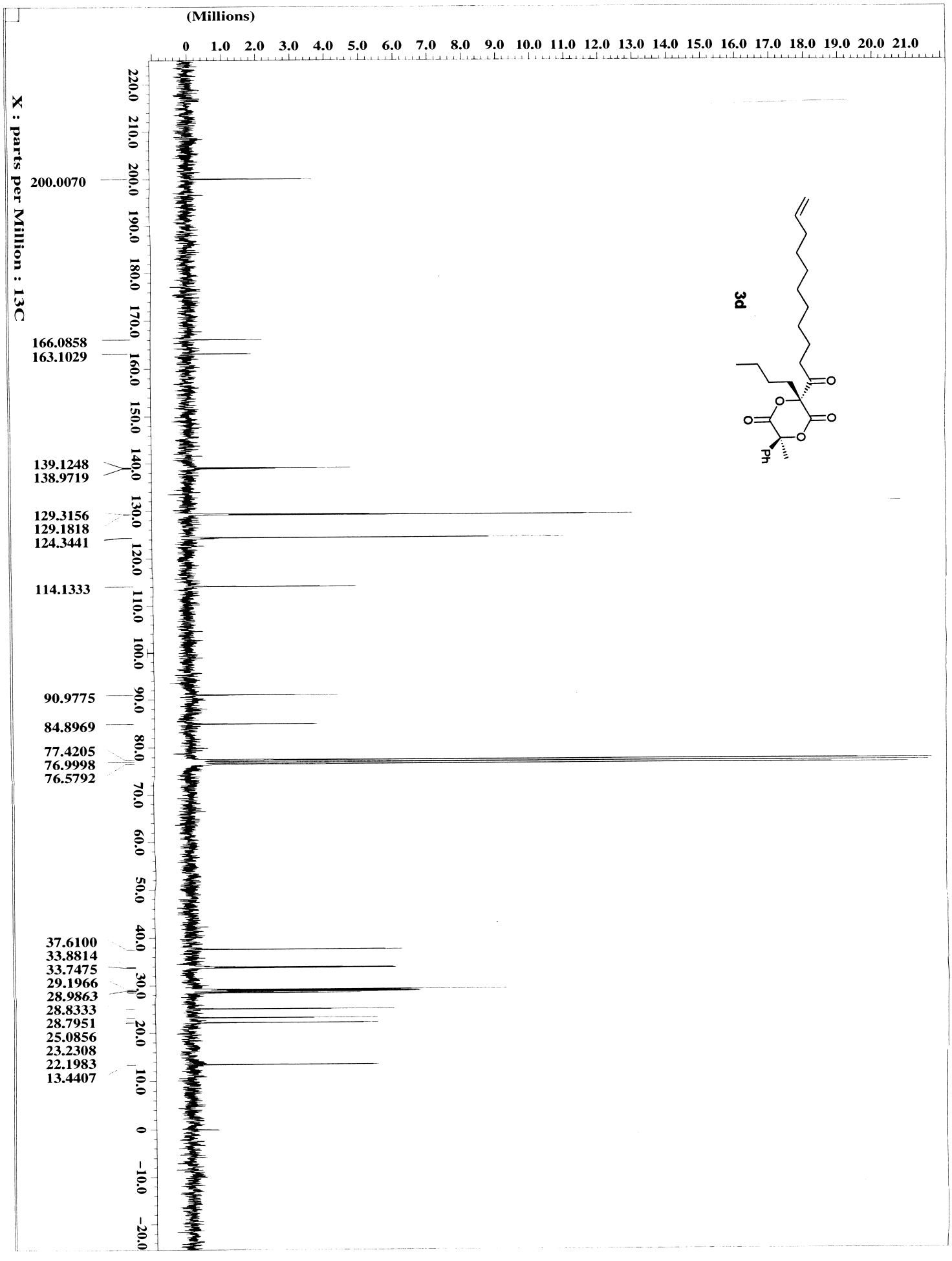


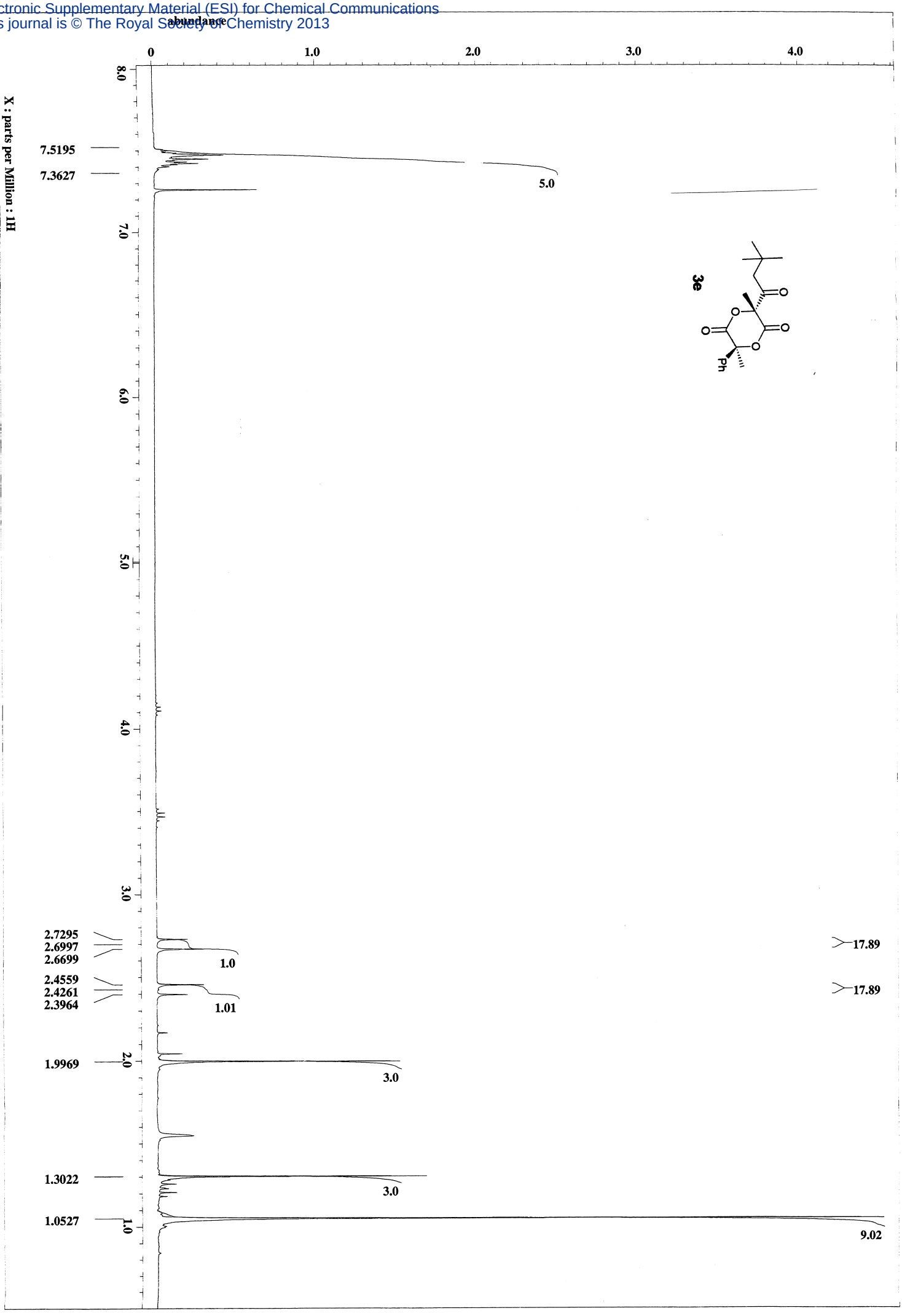


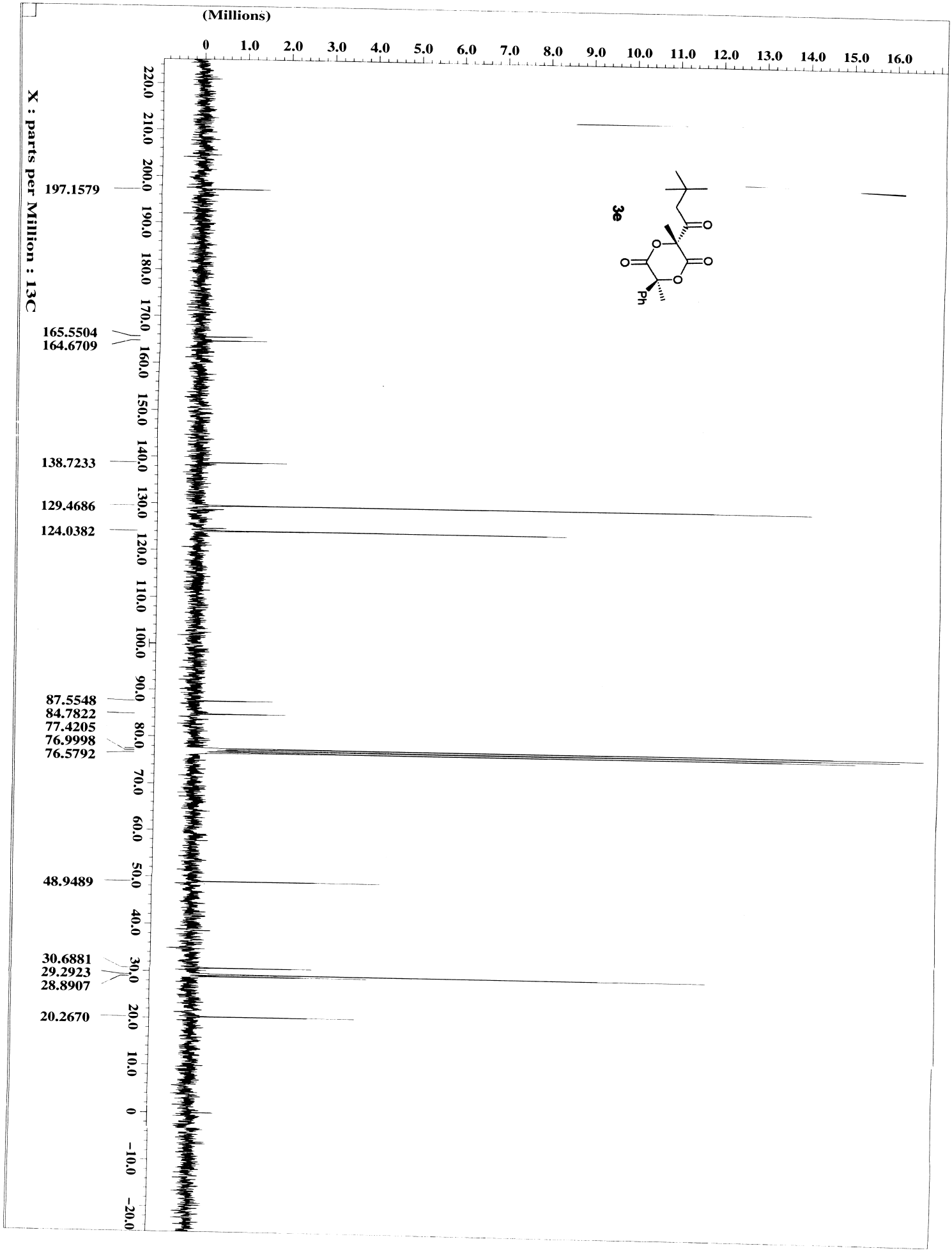


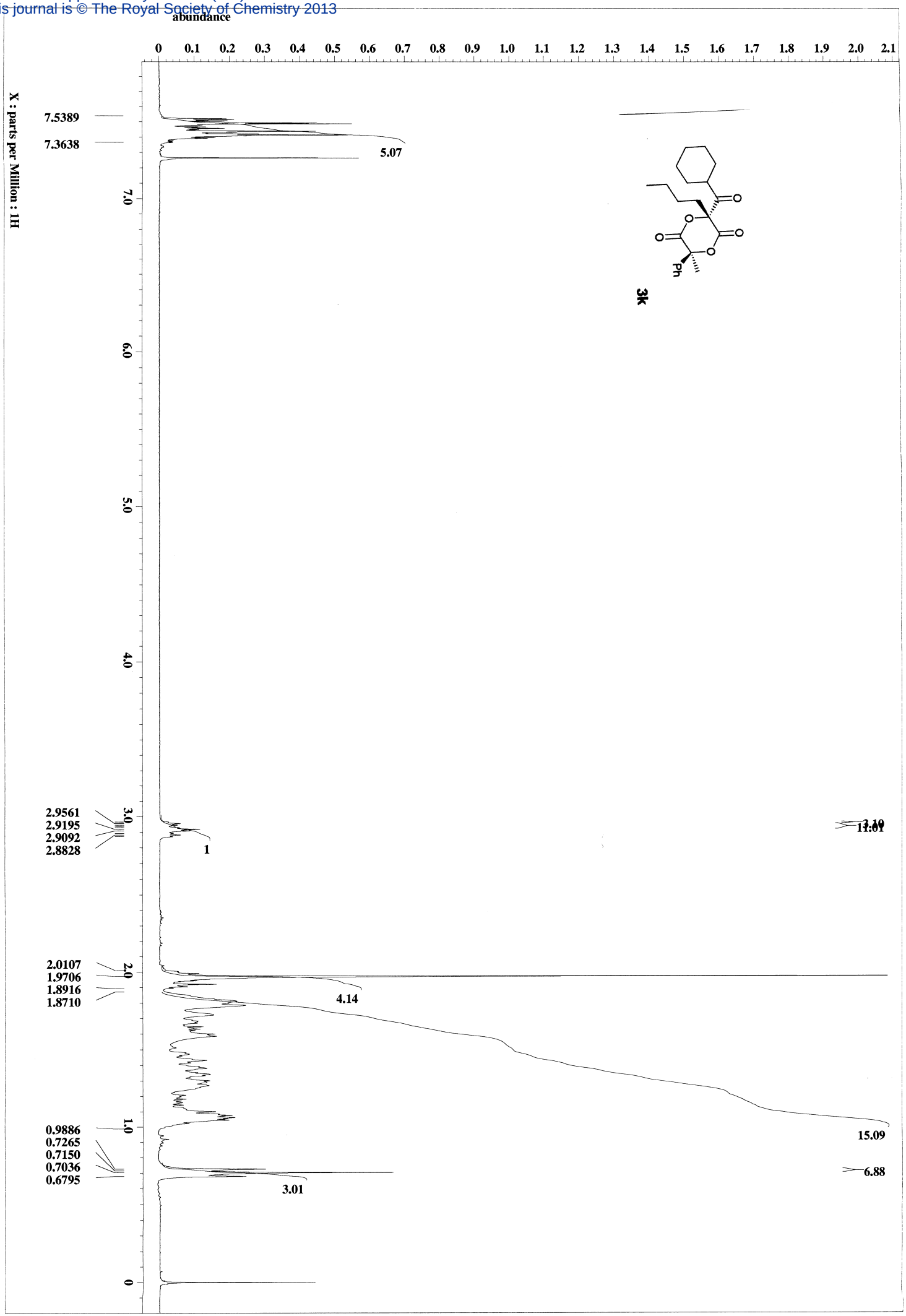


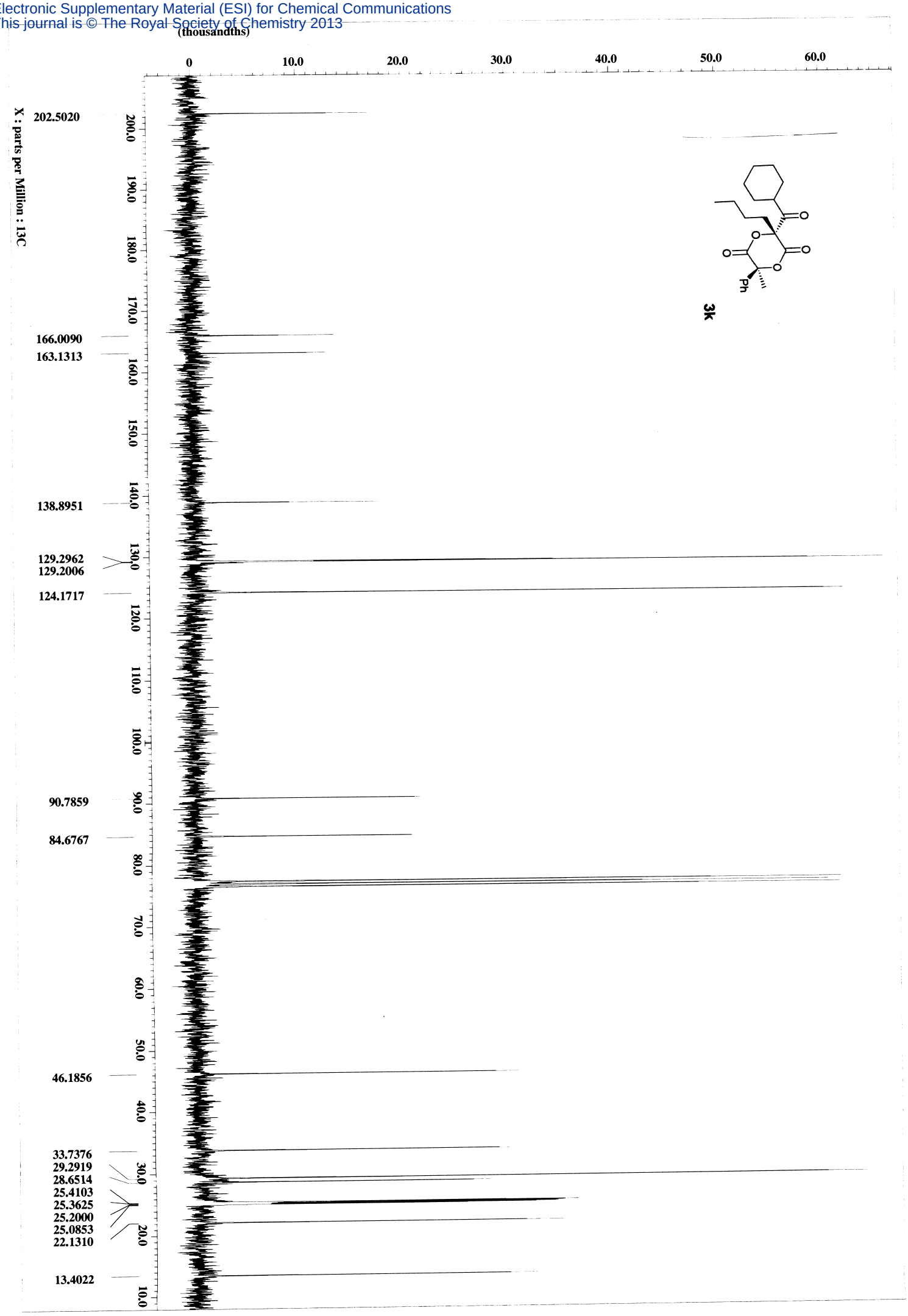


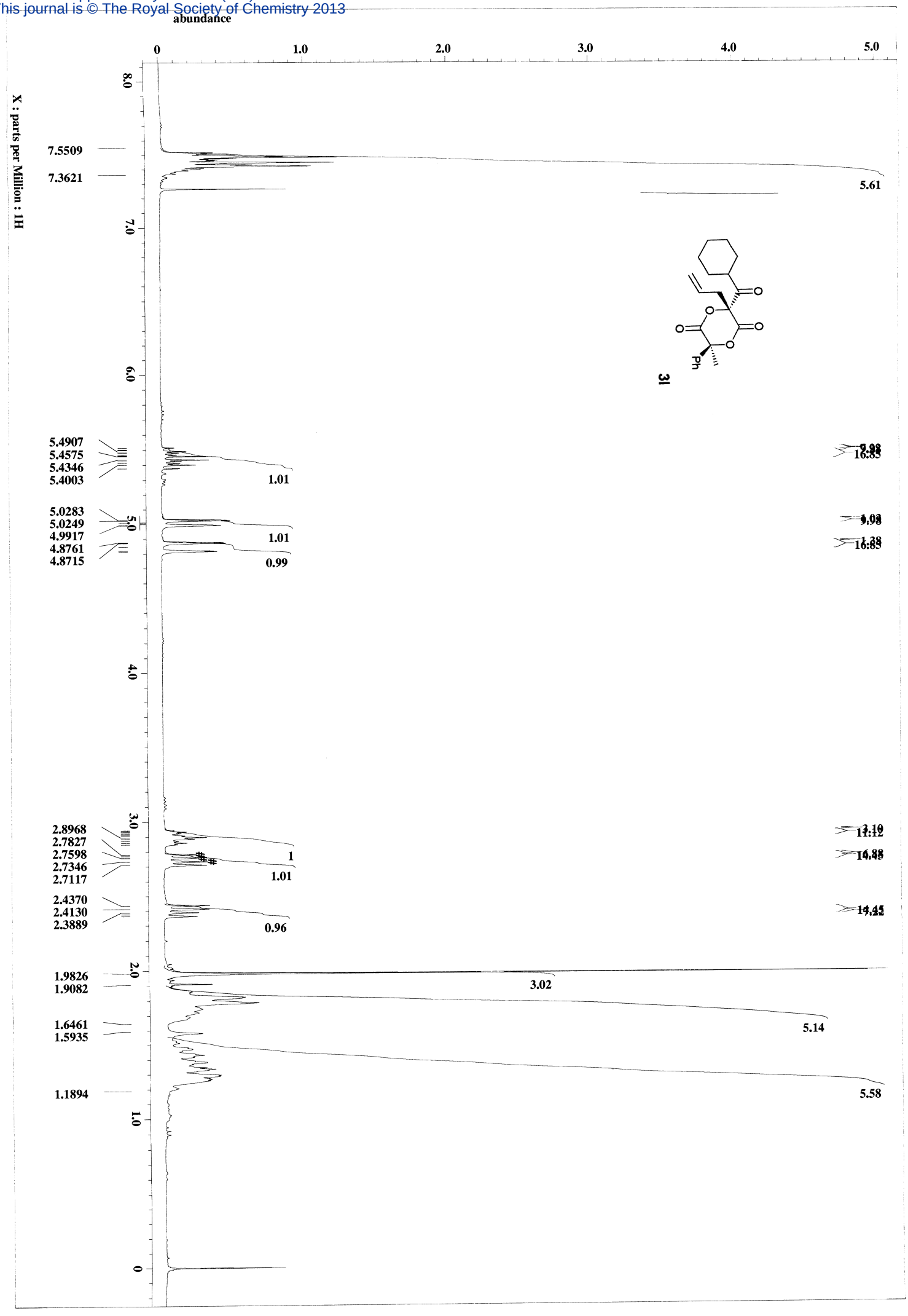


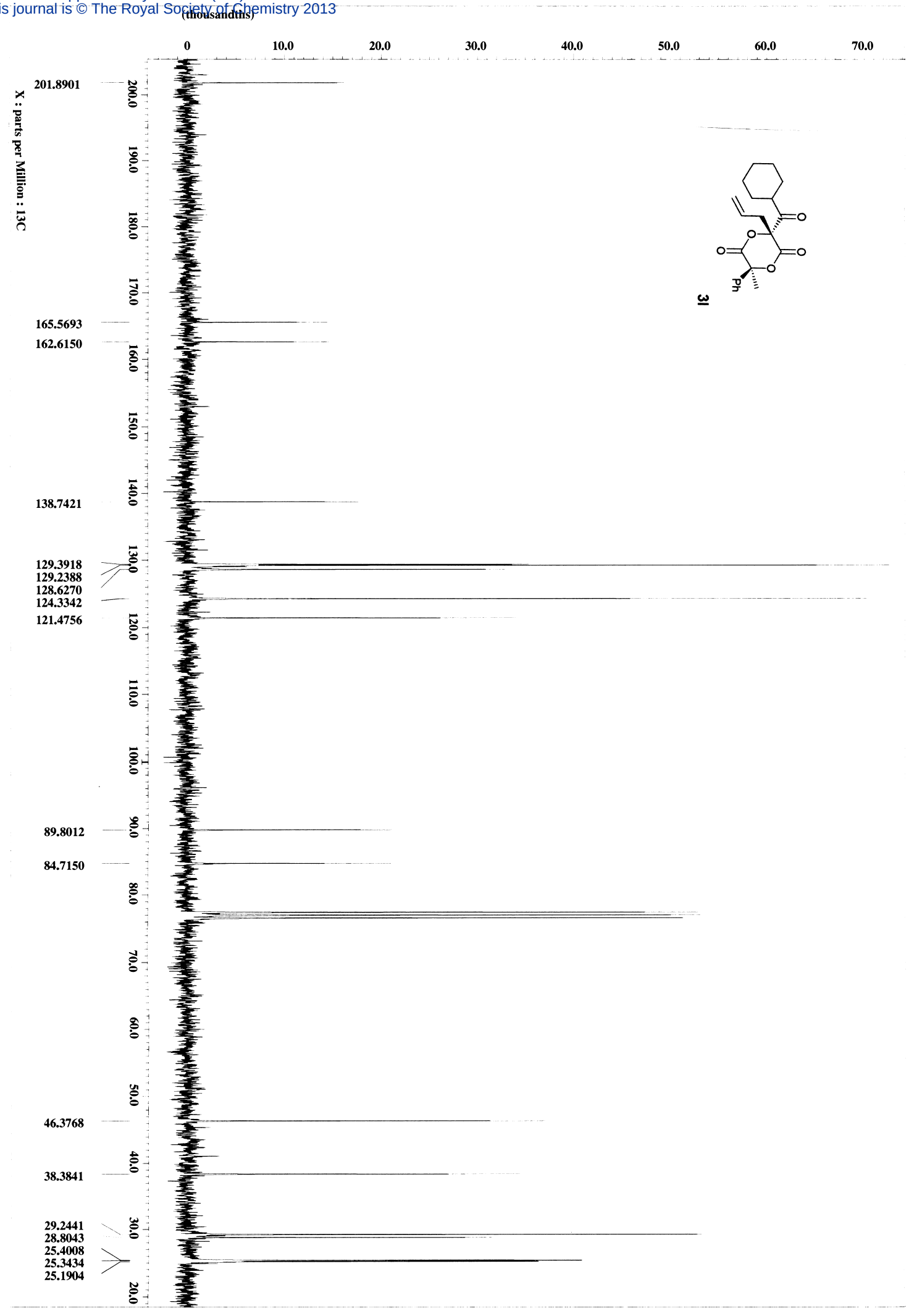


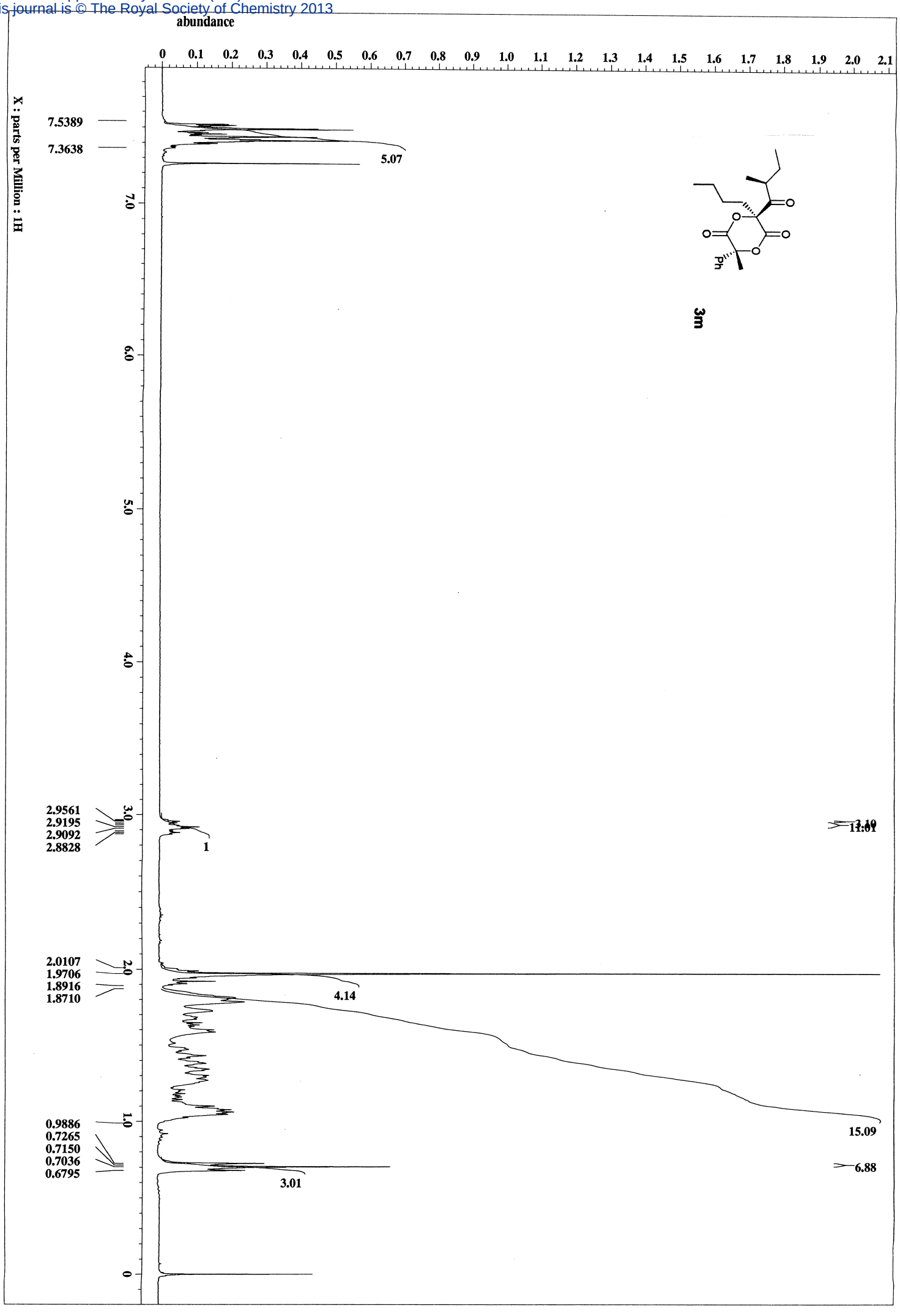


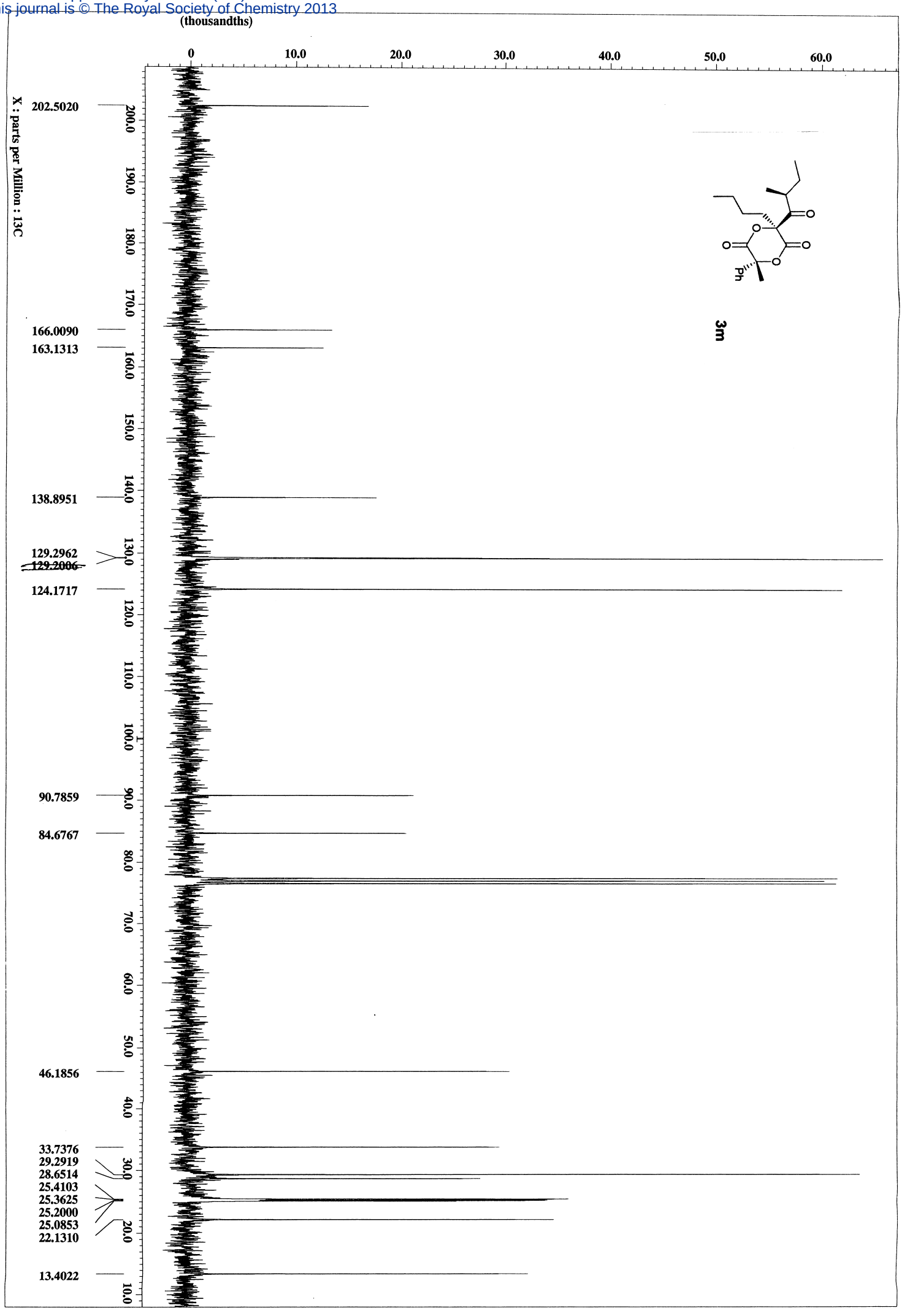


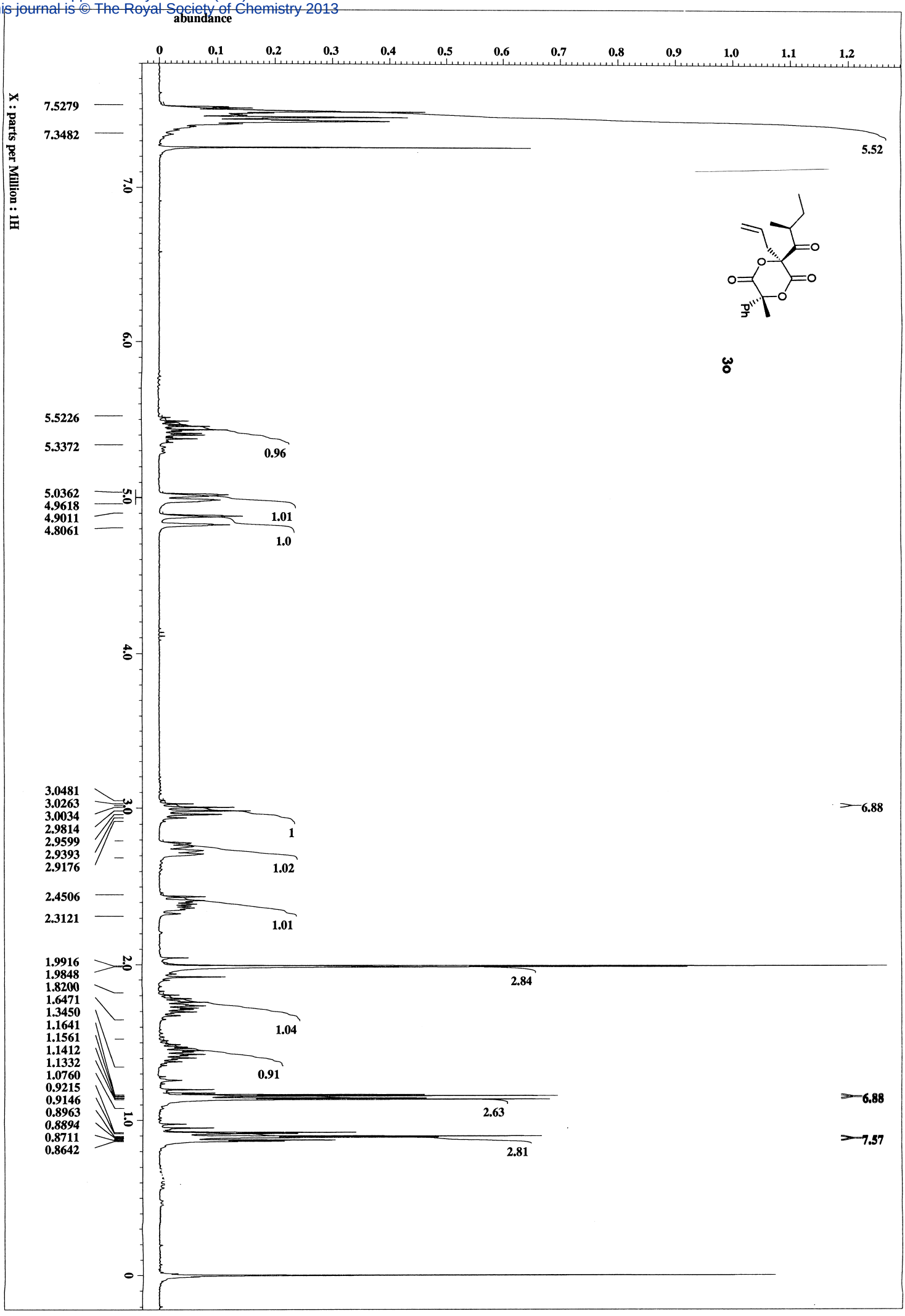


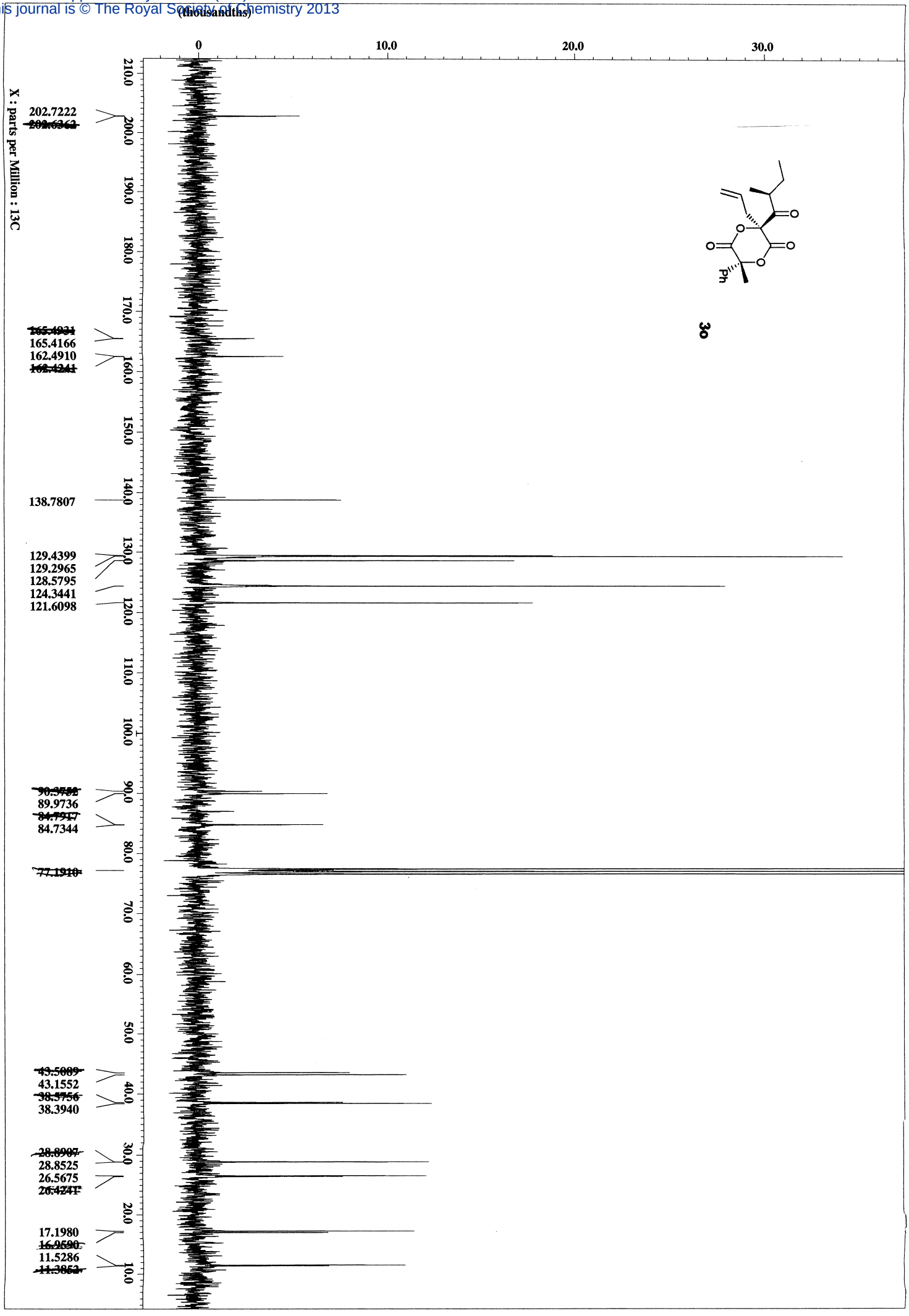


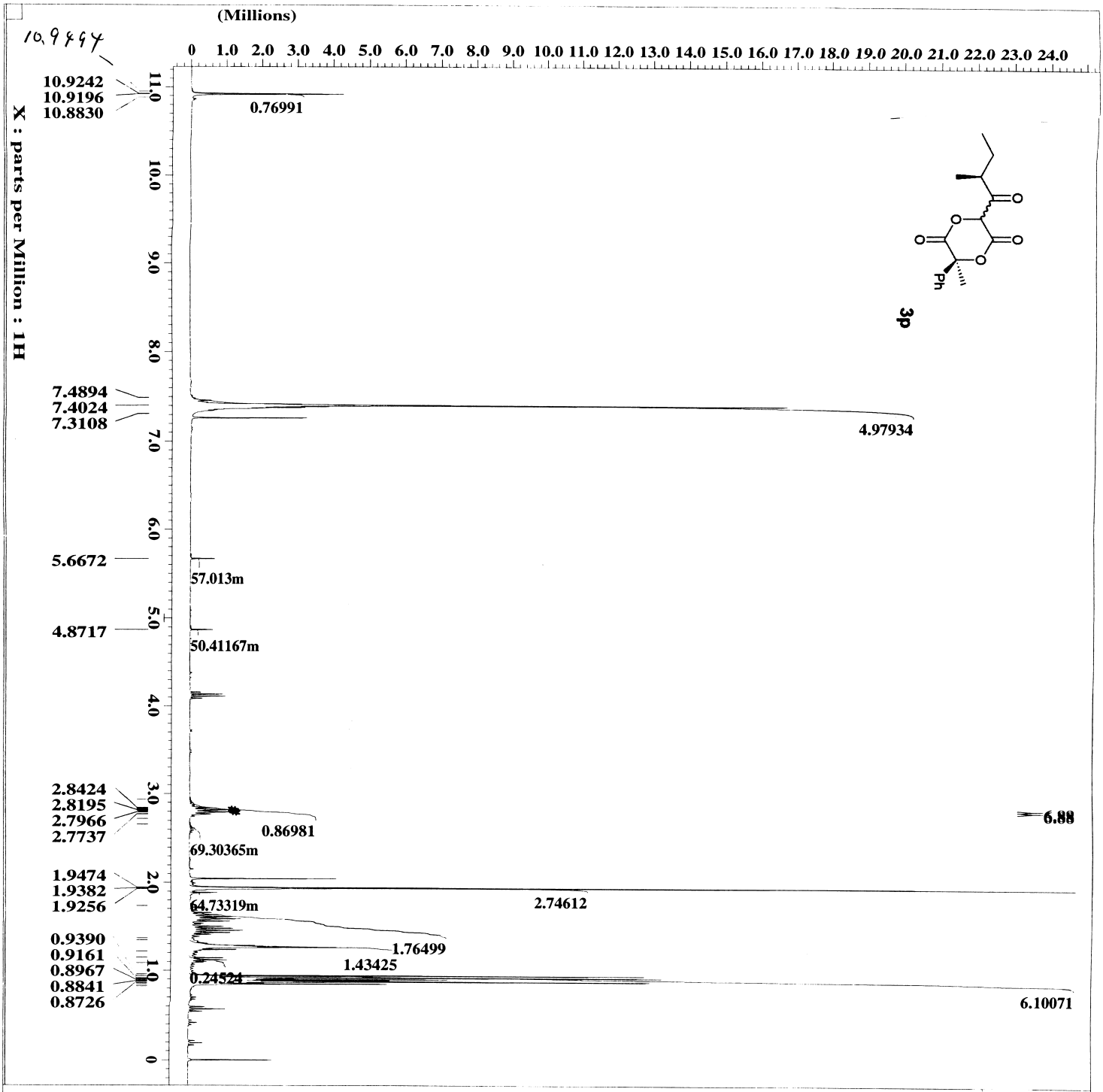




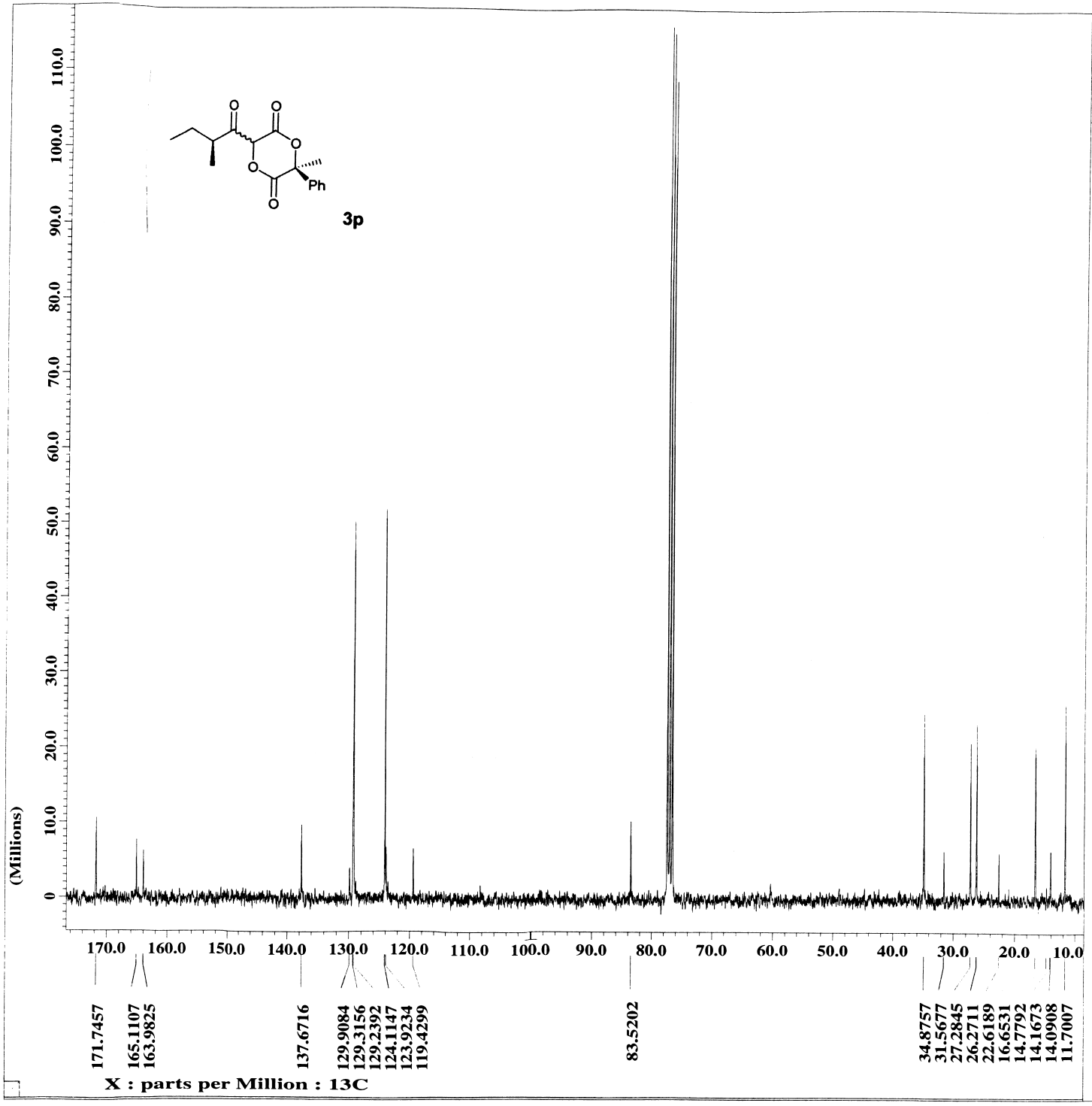






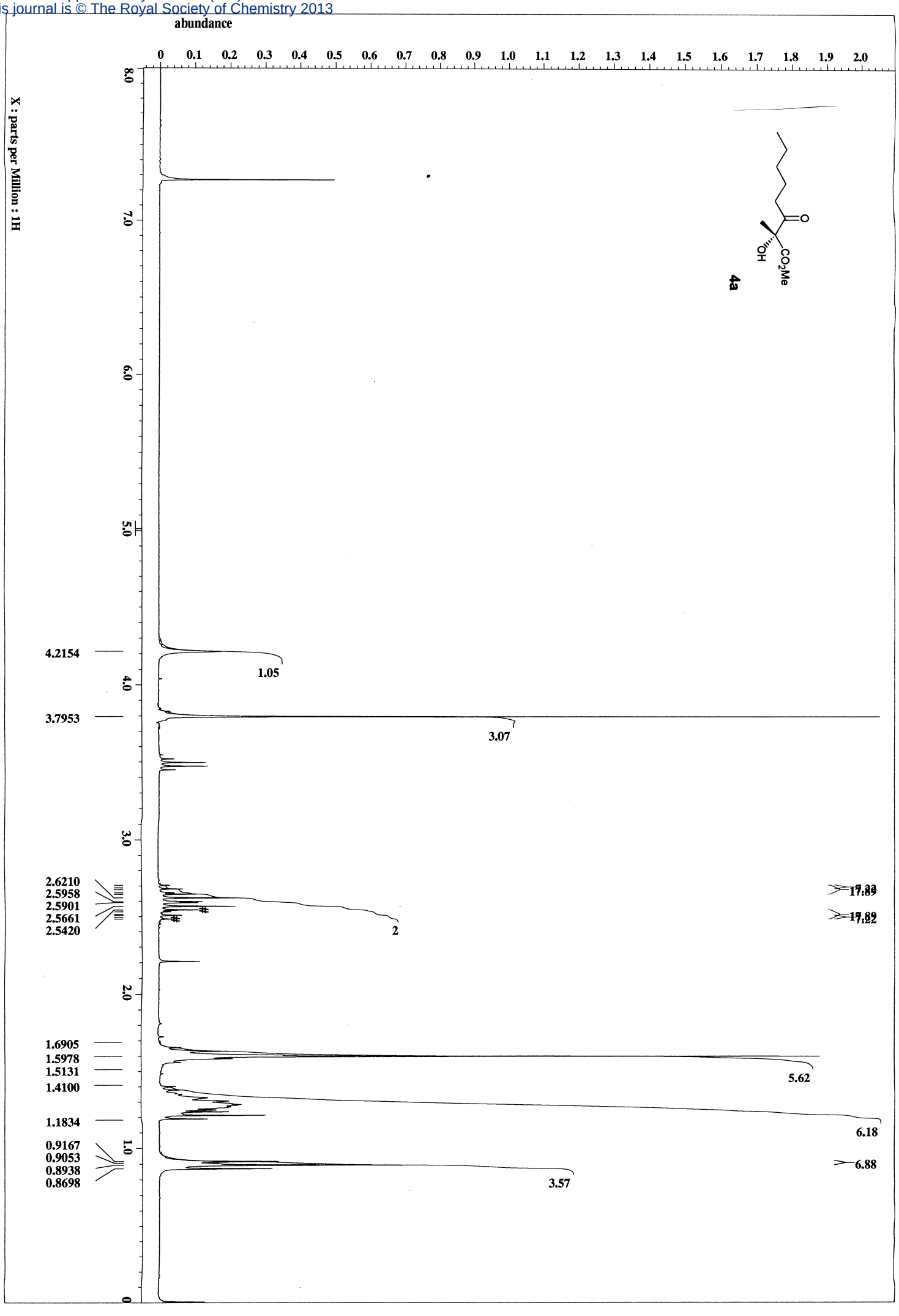


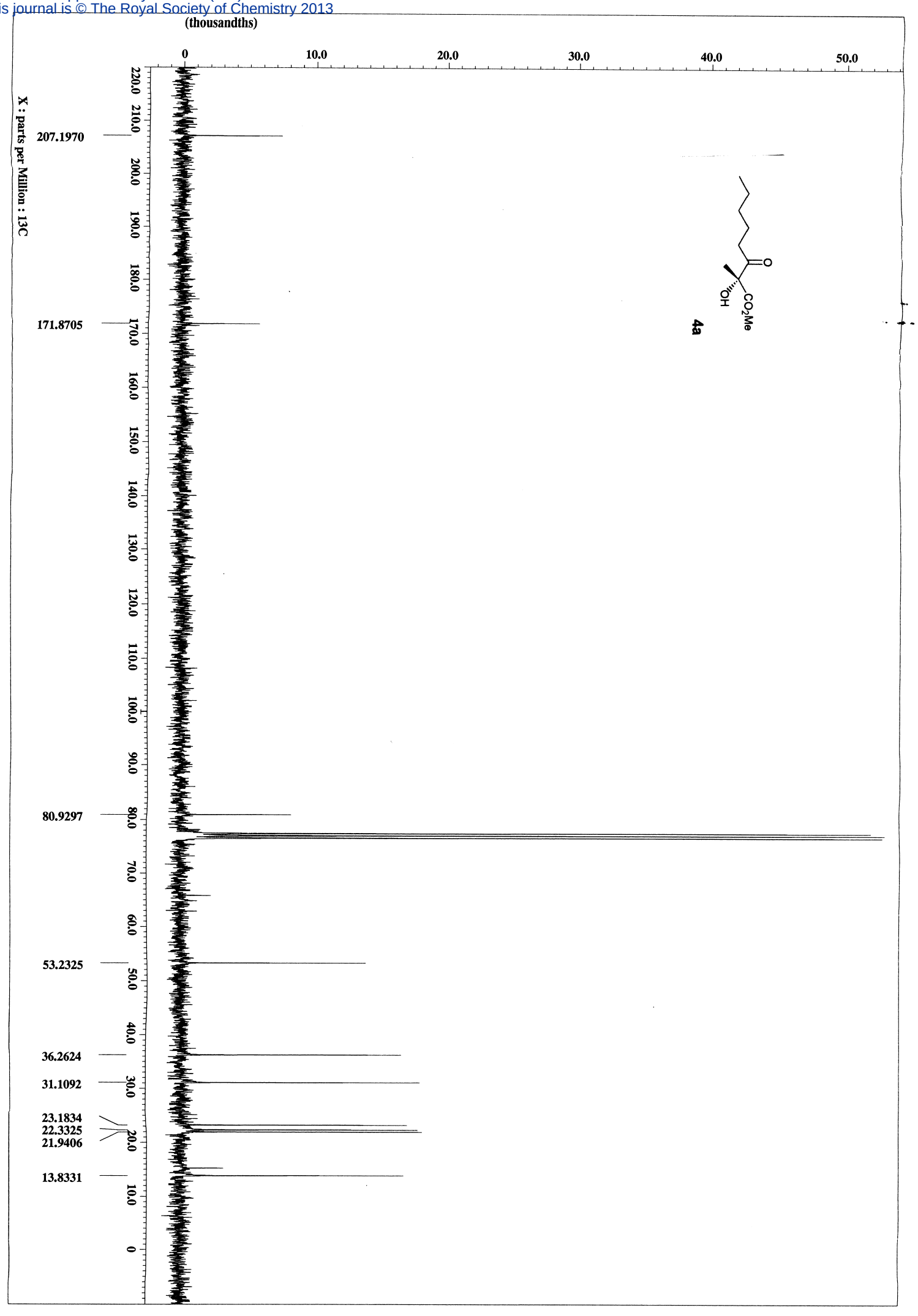

```
---- ACQUISITION PARAMETERS ----
Derived from: single_pulse.1327
File Name                     = single_pulse.1329
Author                        =
Sample ID                     = S#825616
Content                       = single_pulse
Creation Date                 = 30-NOV-2005 22:59:01
Revision Date                 = 30-NOV-2005 23:14:15
Spec Site                     = ECA300 (2 JMT30-2)

Spec Type                     = DELTA2_NMR
Data Format                   = 1D COMPLEX
Dimensions                    = X
Dim Title                     = 1H
Dim Size                      = 13107
Dim Units                     = [ppm]
Experiment                    = single_pulse.ex2
Probe_id                      = 2692
Temp_get                      = 24.7[dC]
Spin_get                      = 16[Hz]
Solvent                       = CHLOROFORM-D
Recvr_gain                    = 42
Scans                         = 8
X_prescans                    = 0
Digital_filter                = TRUE
Filter_factor                 = 8
X_points                      = 16384
X_domain                      = 1H
X_offset                      = 5[ppm]
X_freq                        = 300.52965592[MHz]
X_sweep                       = 5.63570784[kHz]
X_acq_time                    = 2.90717696[s]
X_resolution                  = 0.34397631[Hz]
Relaxation_delay              = 5[s]
Repetition_time               = 7.90717696[s]
X_angle                       = 45[deg]
X_90_width                    = 10.6[us]
X_pulse                       = 5.3[us]
X_atn                         = 5.8[dB]
Dante_presat                  = FALSE
Irr_mode                      = off
Irr_domain                    = 1H
Irr_freq                      = 300.52965592[MHz]
Irr_offset                    = 5[ppm]
Irr_pwidth                    = 0.153[ms]
Dead_time                     = 0[us]
Delay                         = 0[us]
Tri_mode                      = off
Tri_domain                    = 1H
Tri_freq                      = 300.52965592[MHz]
Tri_offset                    = 5[ppm]
Tri_pwidth                    = 1[us]
Obs_pwidth                    = 1[us]
Qui_pwidth                    = 1[us]
Qua_pwidth                    = 1[us]
Sex_pwidth                    = 1[us]
Sep_pwidth                    = 1[us]
Oct_pwidth                    = 1[us]
Non_pwidth                    = 1[us]
Dec_pwidth                    = 1[us]
```

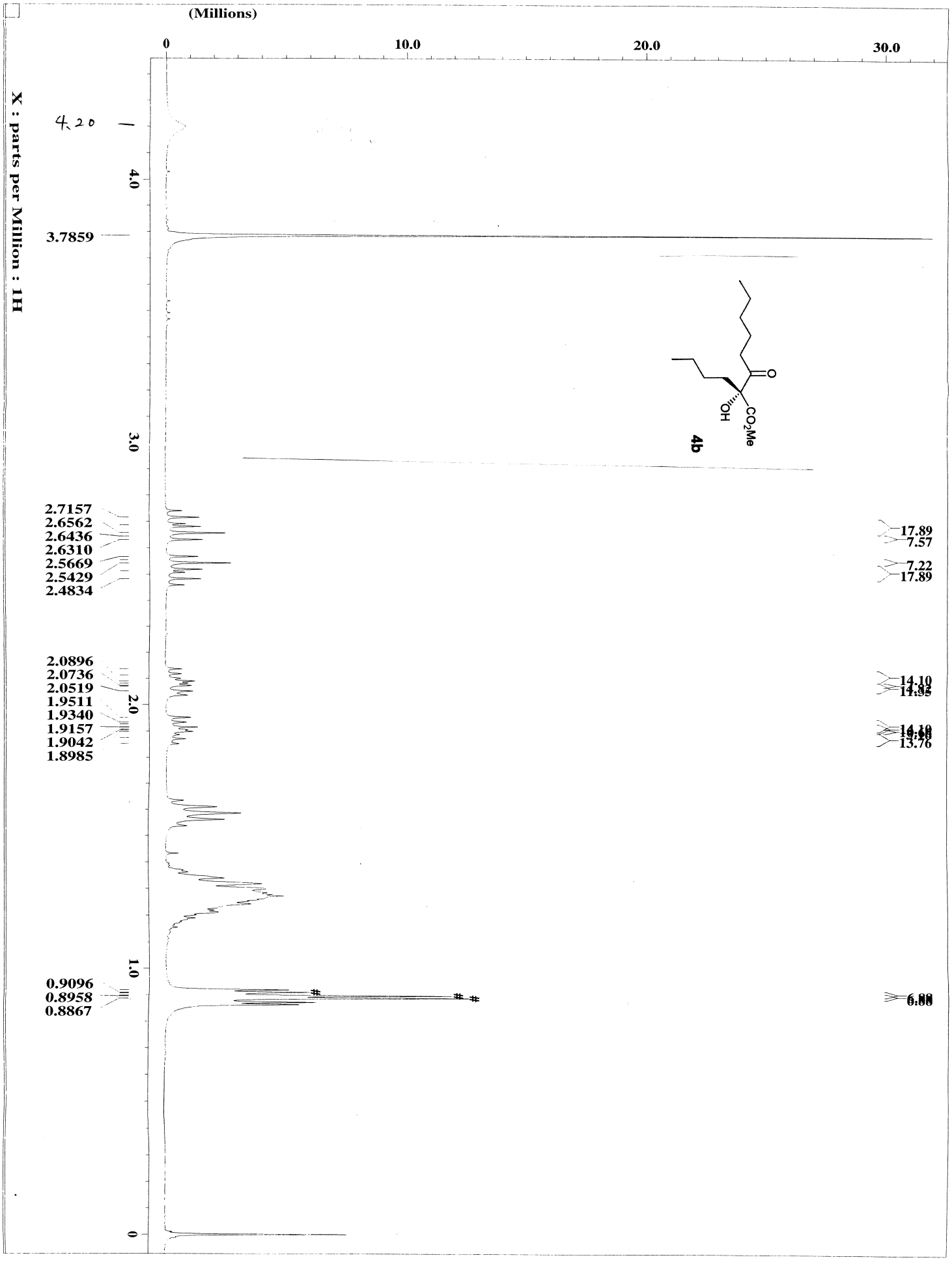


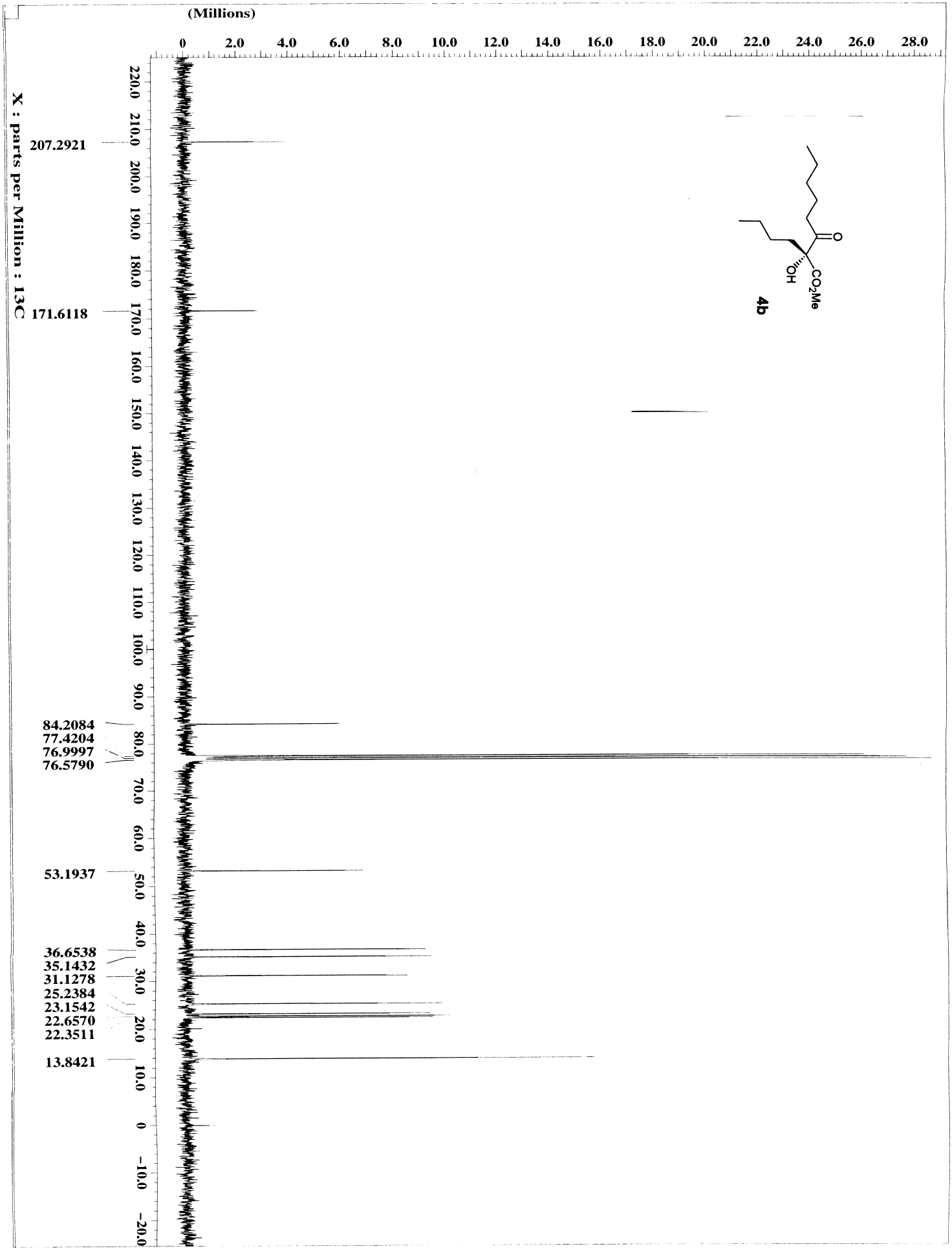
JEOL

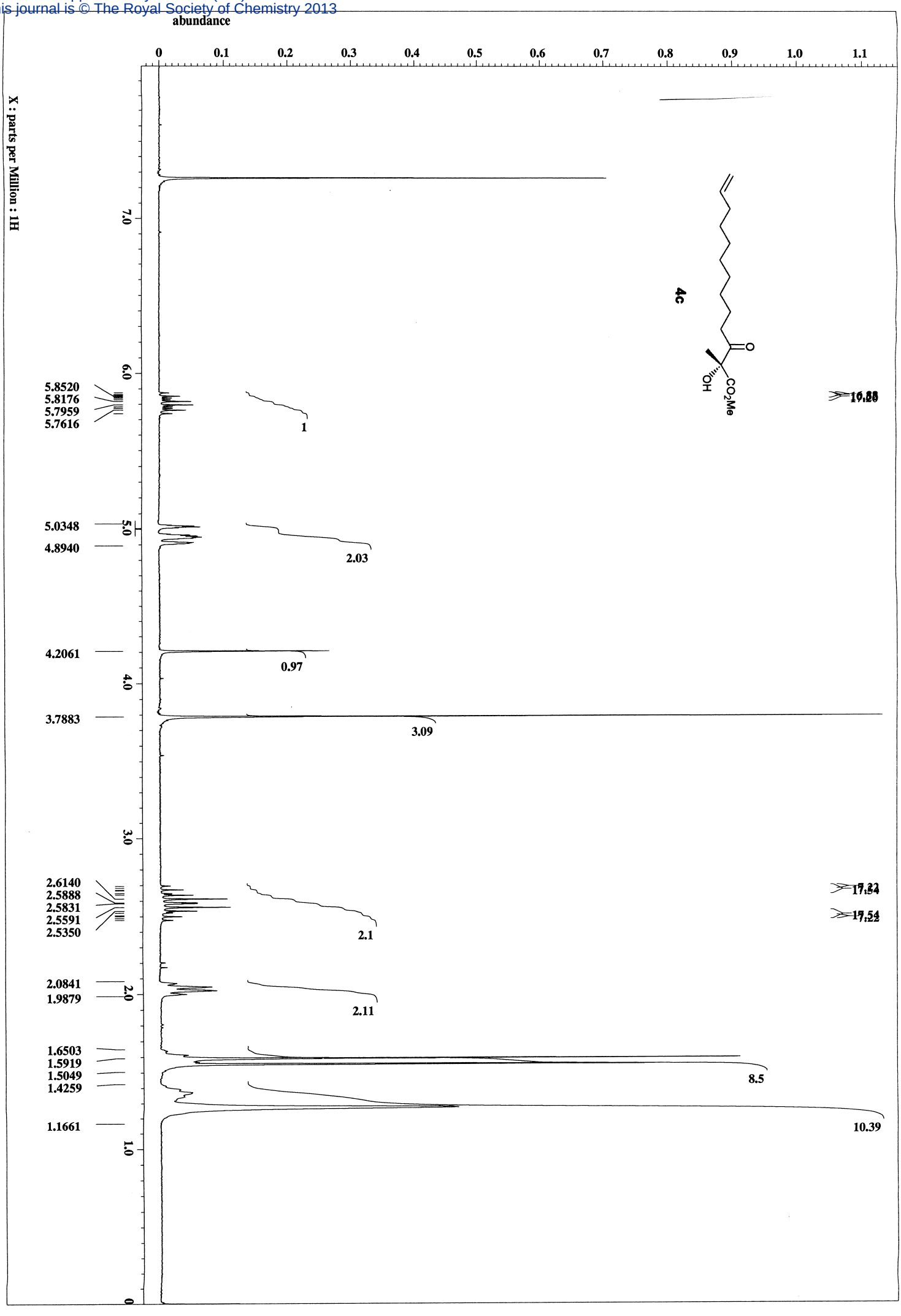
```
---- ACQUISITION PARAMETERS ----
Derived from: single_pulse_dec_copy.23
File Name          = single_pulse_dec_copy.
Author             =
Sample ID          = S#826804
Content            = single pulse decoupled
Creation Date      = 30-NOV-2005 23:29:43

Revision Date      = 30-NOV-2005 23:30:56
Spec Site          = ECA300 (2 JMT30-2)

Spec Type          = DELTA2_NMR
Data Format        = 1D COMPLEX
Dimensions         = X
Dim Title          = 13C
Dim Size           = 13107
Dim Units          = [ppm]
Experiment         = single_pulse_dec
Probe_id           = 2692
Temp_get           = 24.8[dC]
Spin_get           = 14[Hz]
Solvent            = CHLOROFORM-D
Recvr_gain         = 60
Scans              = 591
X_prescans         = 4
Digital_filter     = TRUE
Filter_factor      = 8
X_points           = 16384
X_domain           = 13C
X_offset           = 100[ppm]
X_freq             = 75.56823426[MHz]
X_sweep            = 23.67424242[kHz]
X_acq_time         = 0.69206016[s]
X_resolution       = 1.44496109[Hz]
Relaxation_delay   = 2[s]
Repetition_time    = 2.69206016[s]
X_angle            = 30[deg]
X_90_width         = 9.6[us]
X_pulse            = 3.2[us]
X_atn              = 8.6[dB]
Noe_time           = 2[s]
Decoupling         = TRUE
Irr_domain         = 1H
Irr_freq           = 300.52965592[MHz]
Irr_offset         = 5[ppm]
Irr_pwidth         = 0.153[ms]
Irr_atn_noe        = 28.8[dB]
Irr_atn_dec        = 28.8[dB]
Irr_noise          = WALTZ
Dead_time          = 0[us]
Delay              = 0[us]
Tri_pwidth         = 1[us]
Obs_pwidth         = 1[us]
Qui_pwidth         = 1[us]
Qua_pwidth         = 1[us]
Sex_pwidth         = 1[us]
Sep_pwidth         = 1[us]
Oct_pwidth         = 1[us]
Non_pwidth         = 1[us]
Dec_pwidth         = 1[us]
```

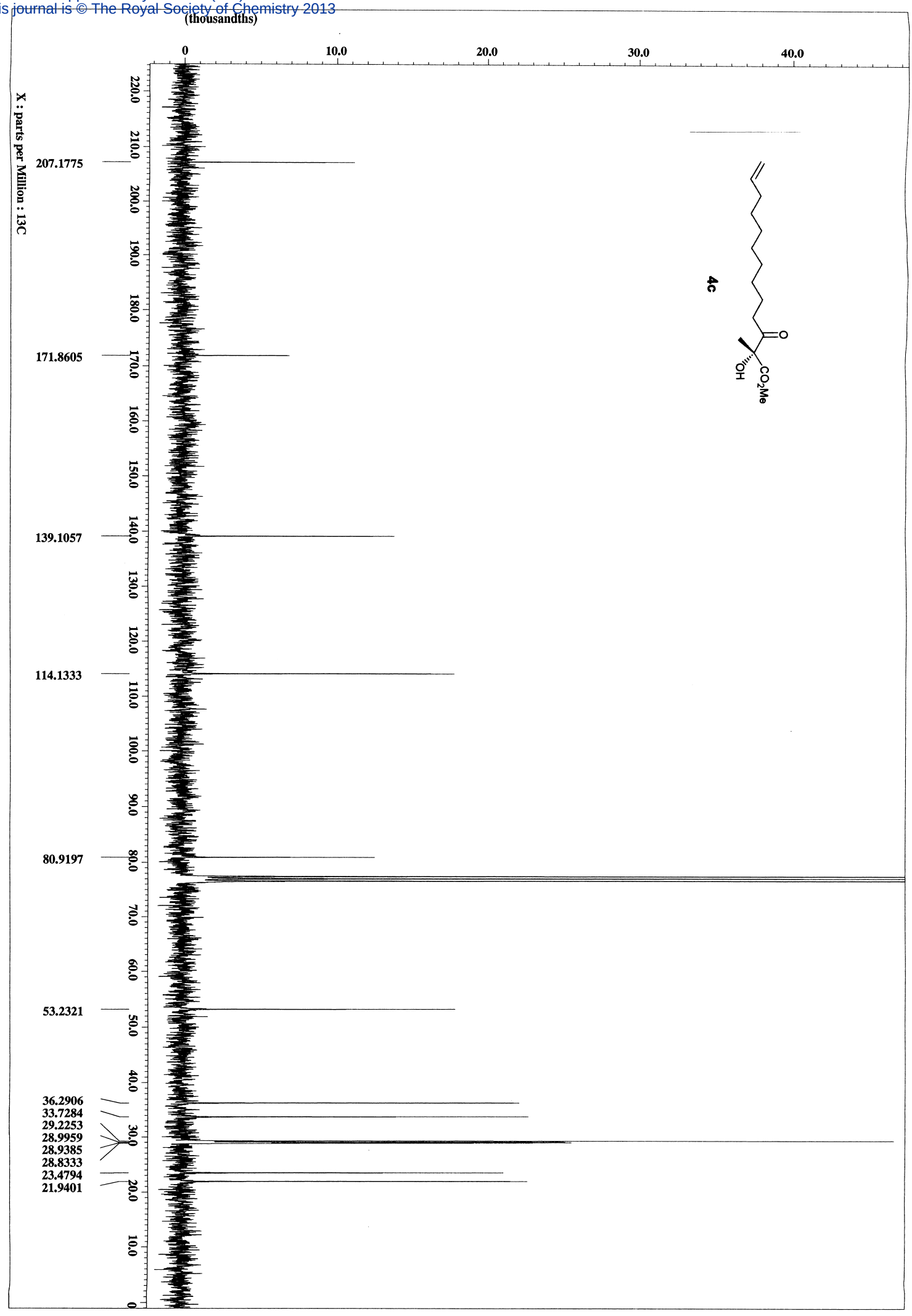


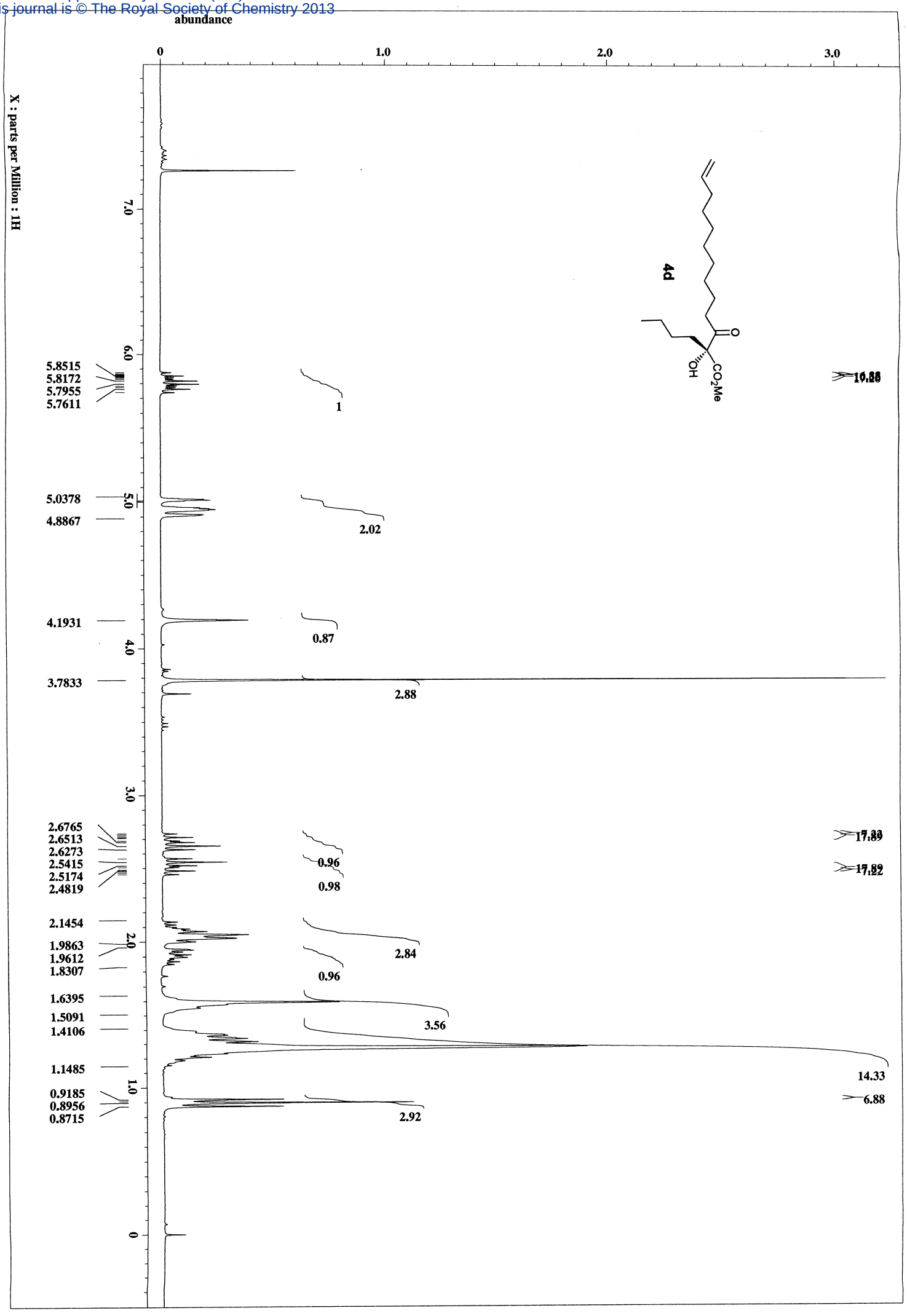


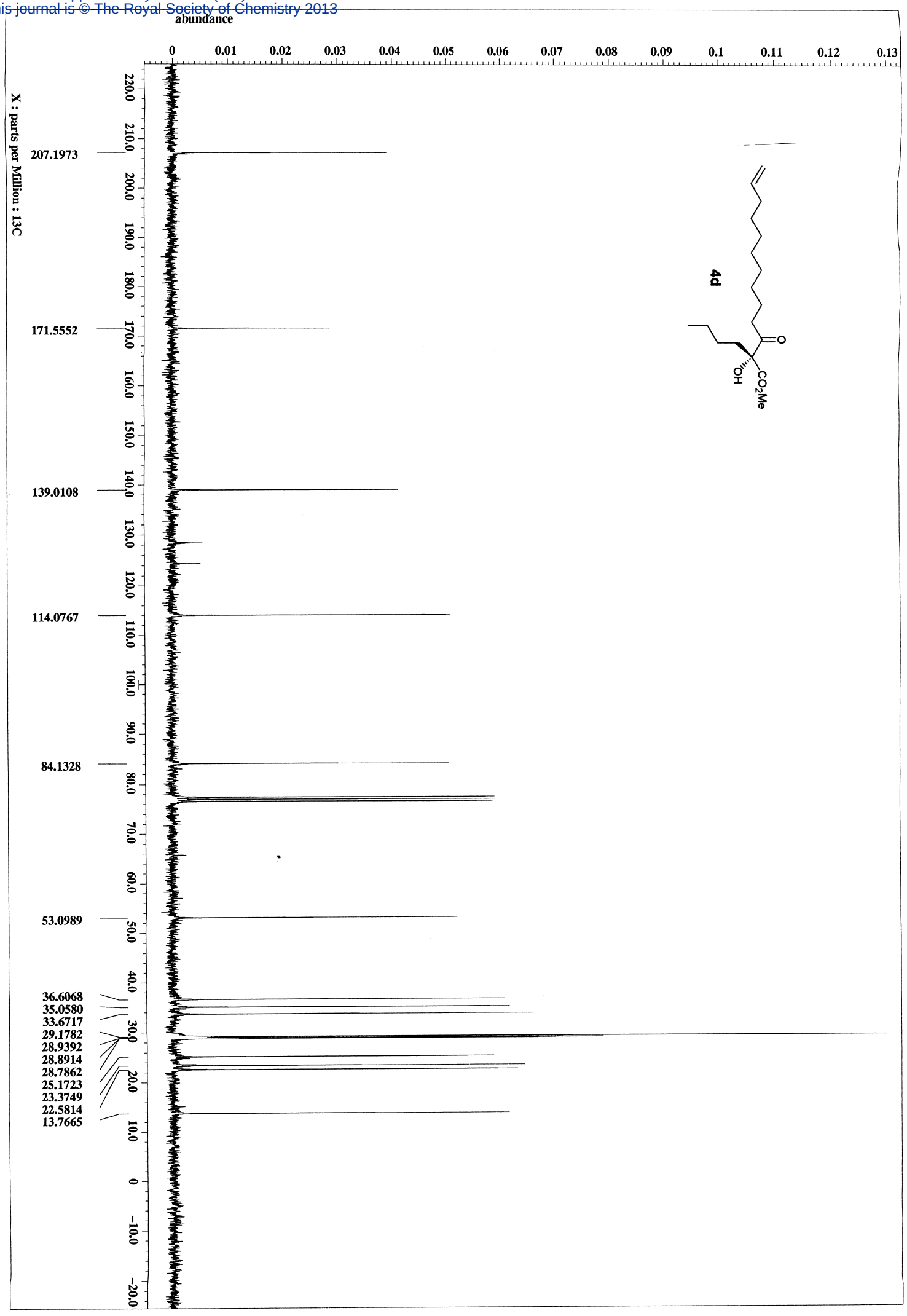


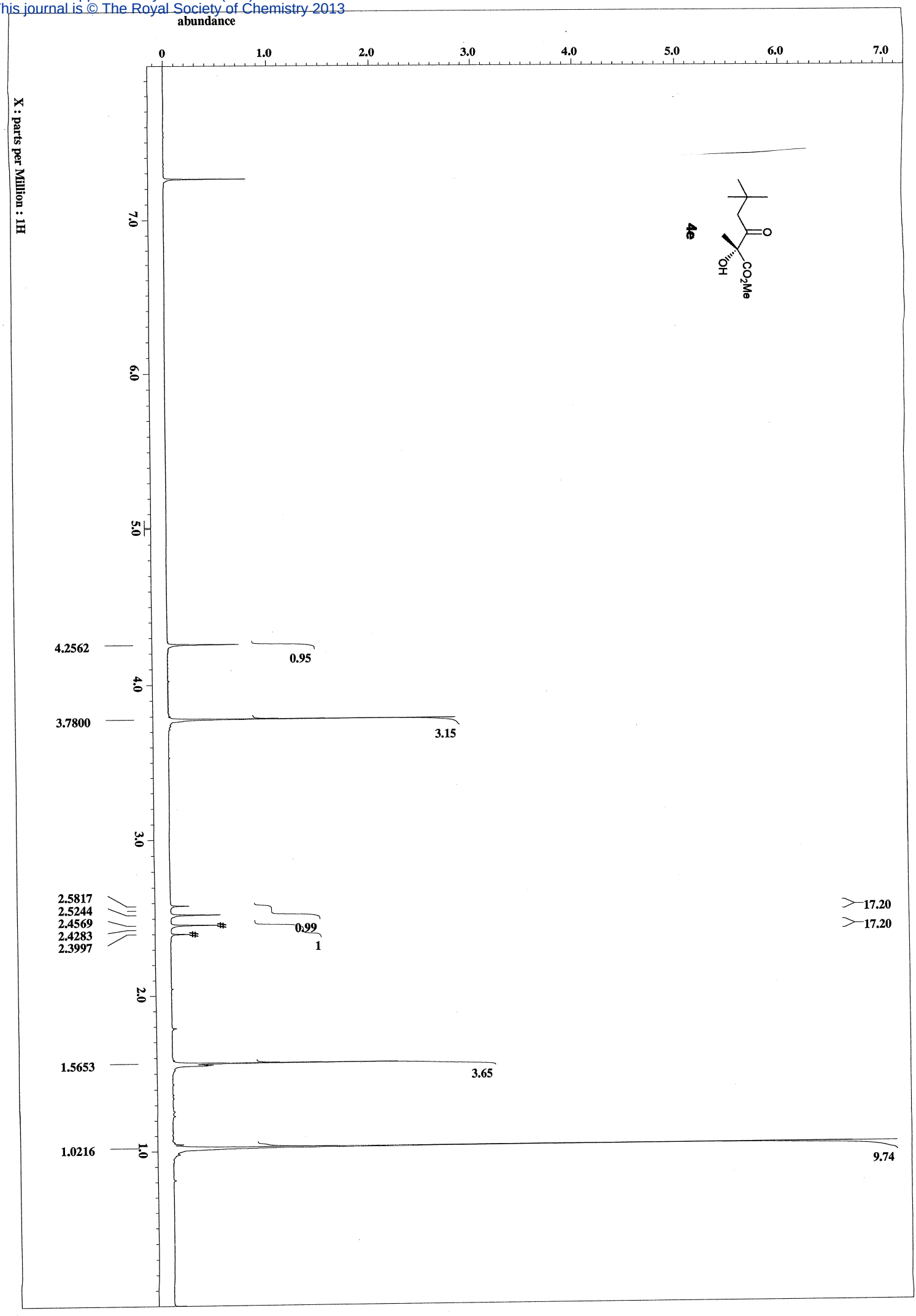


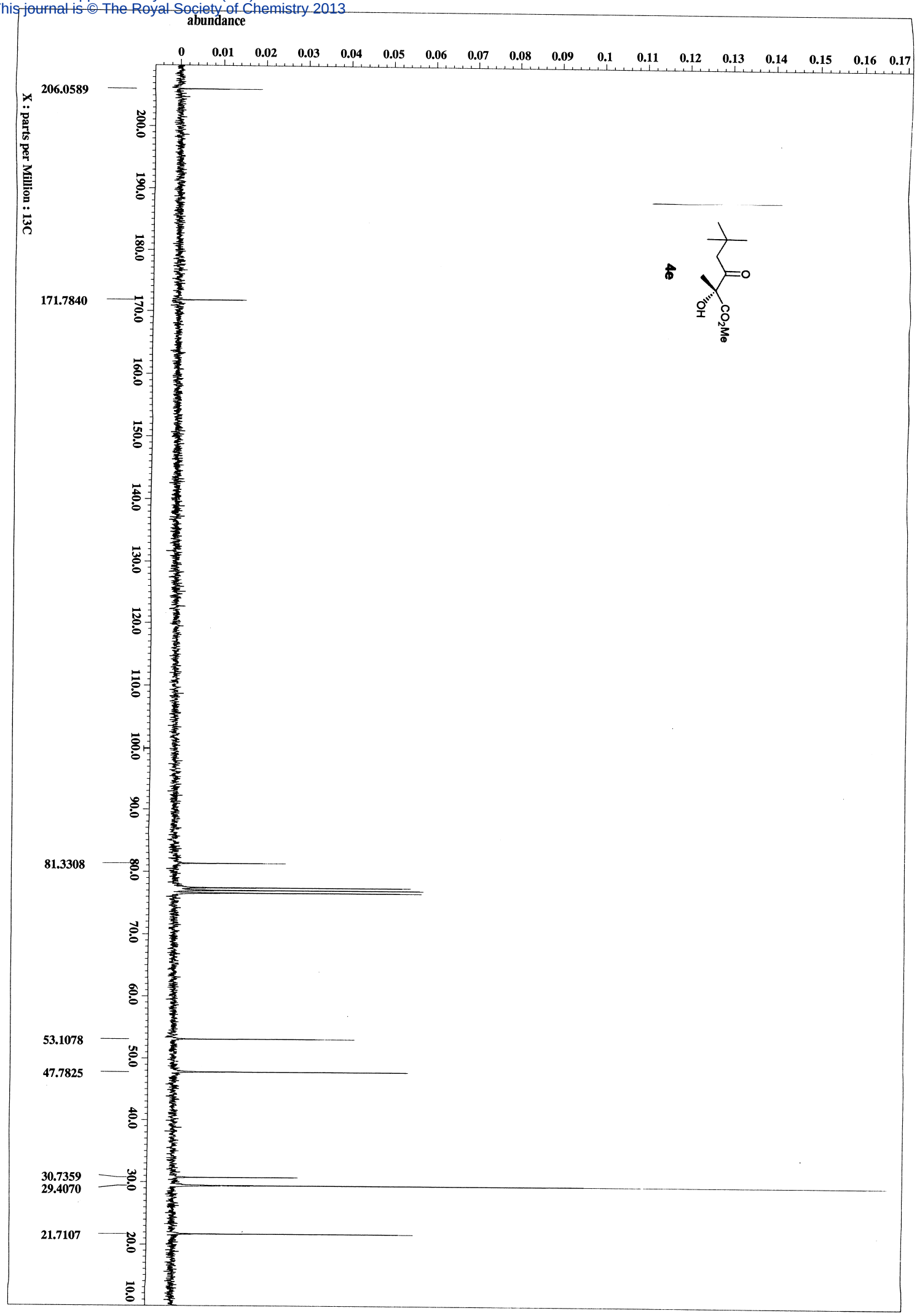


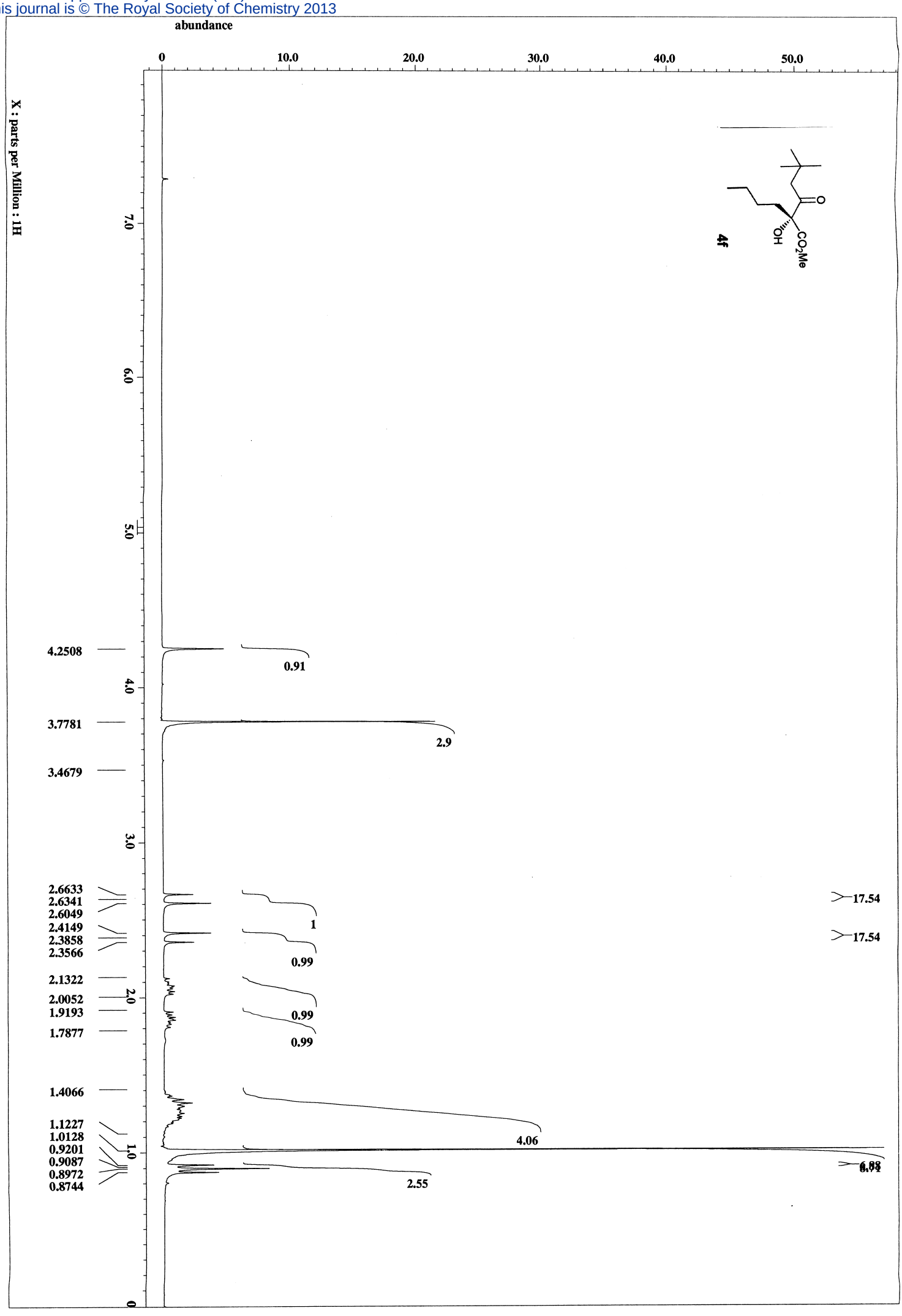


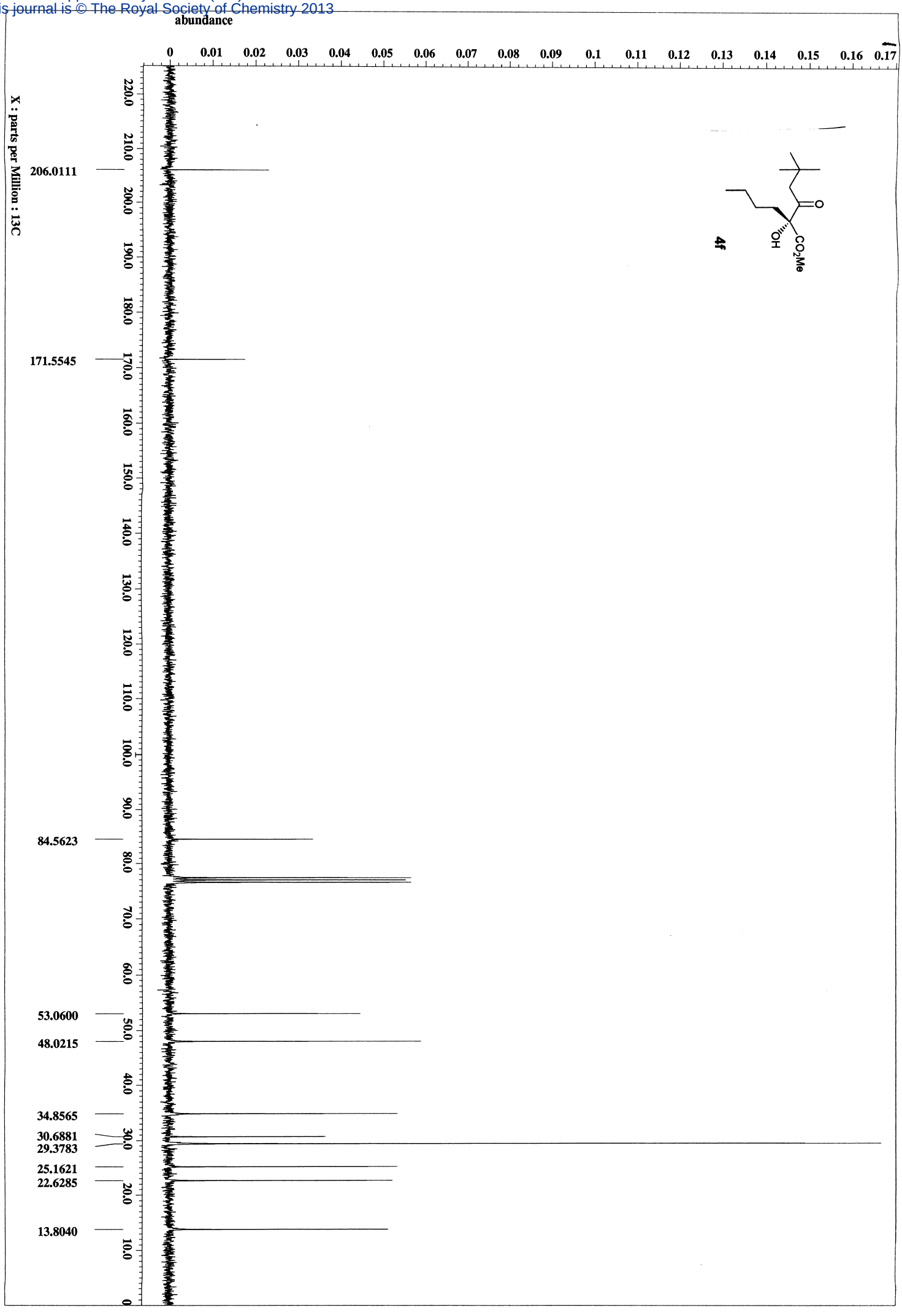


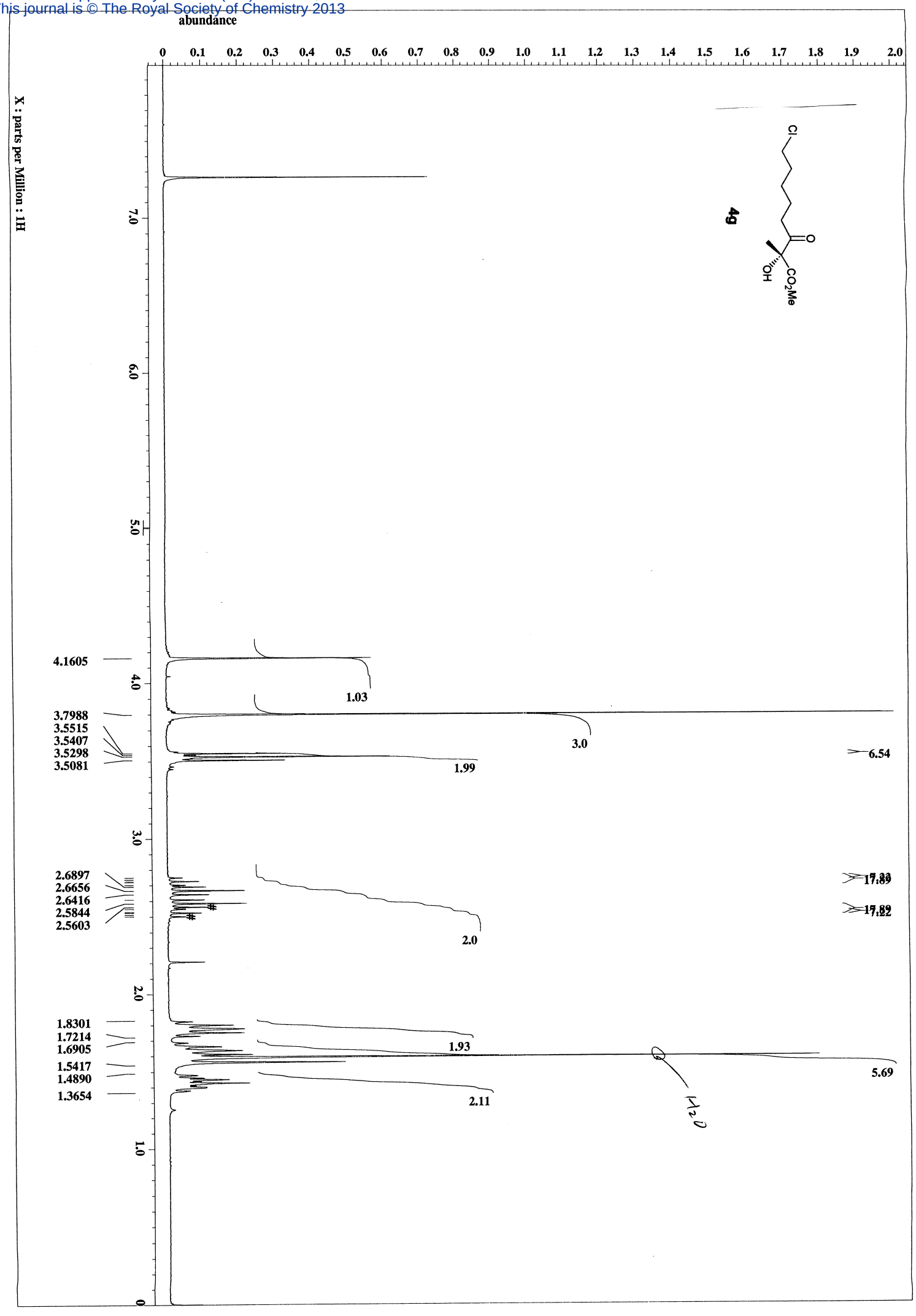


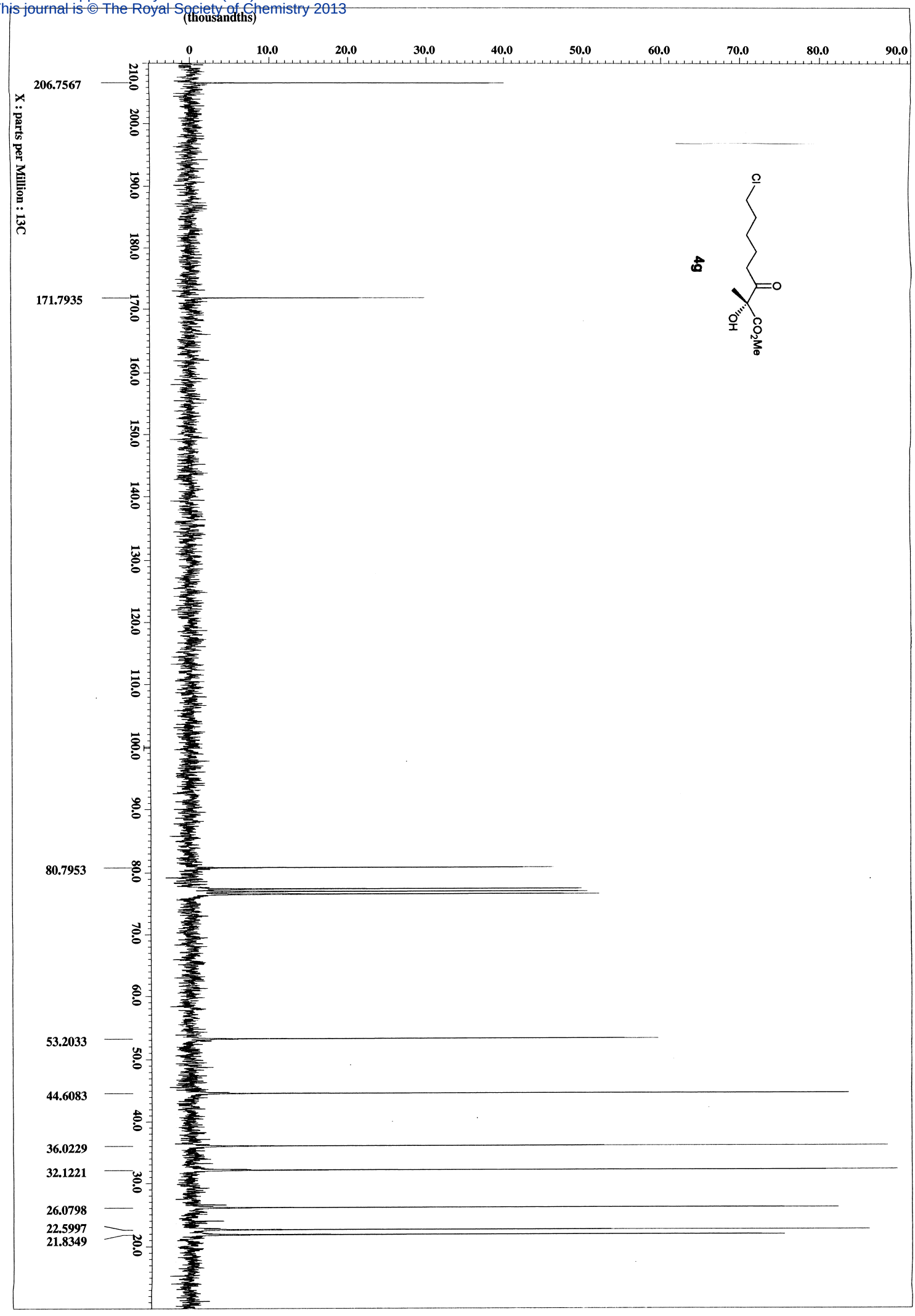


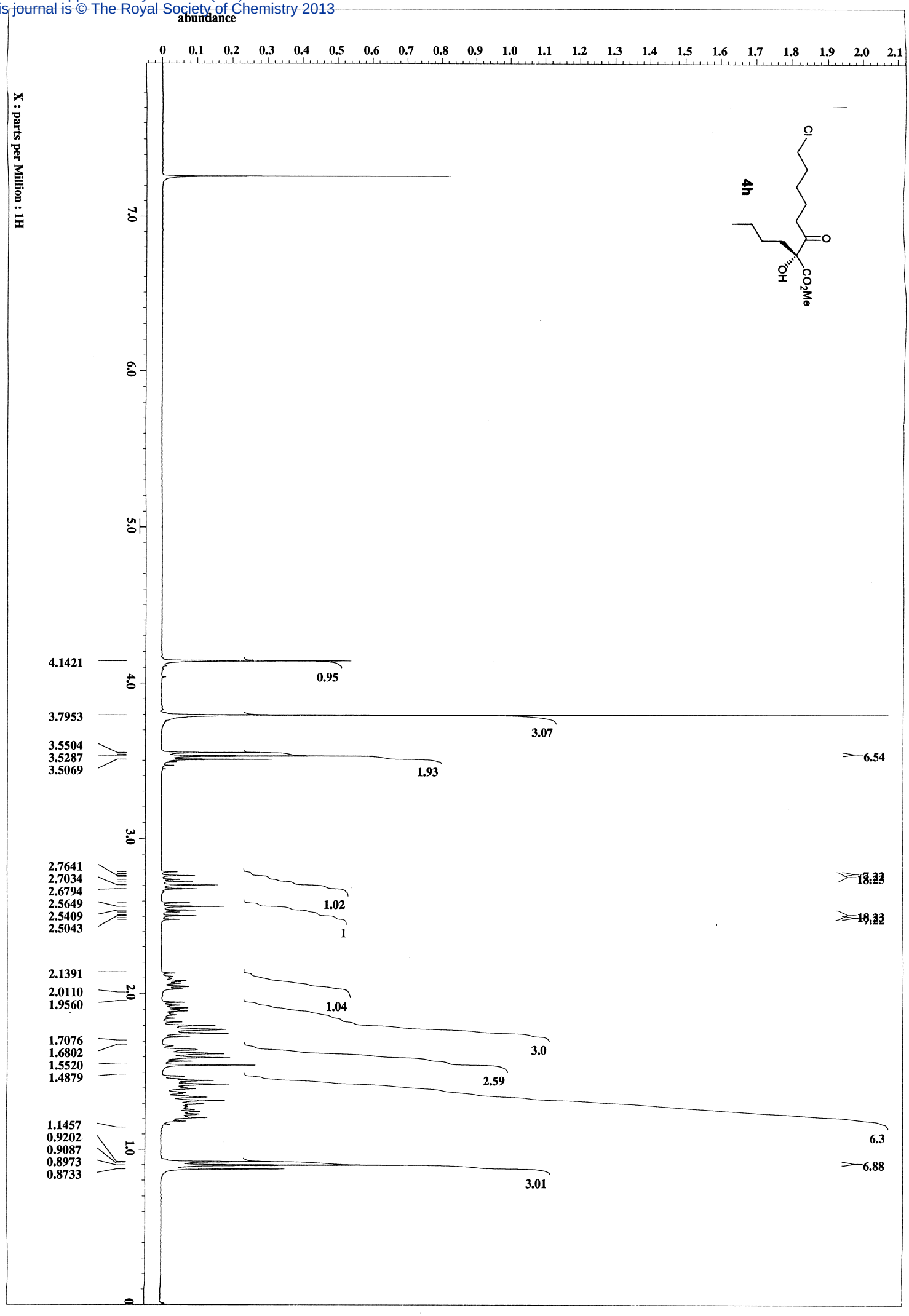


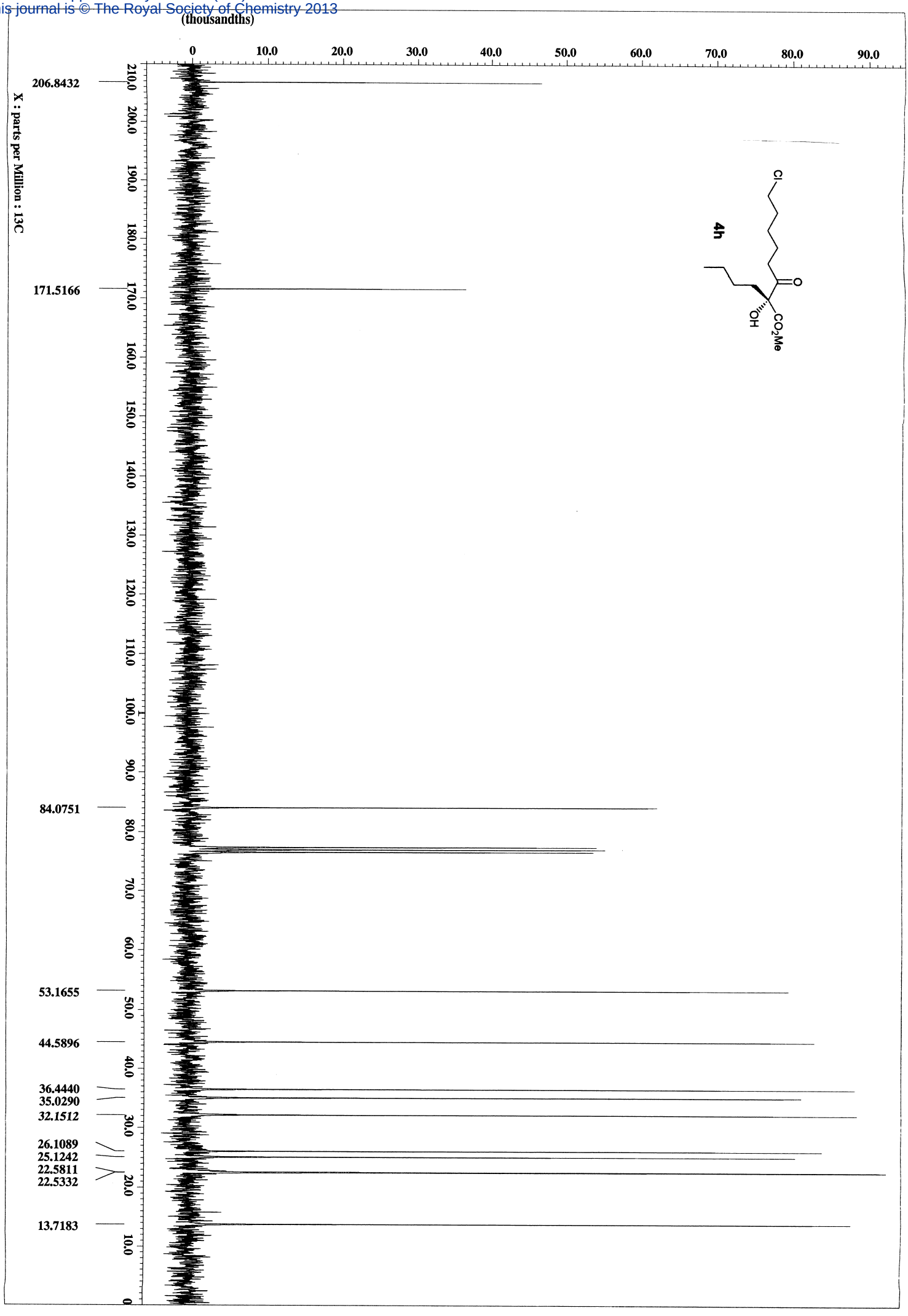


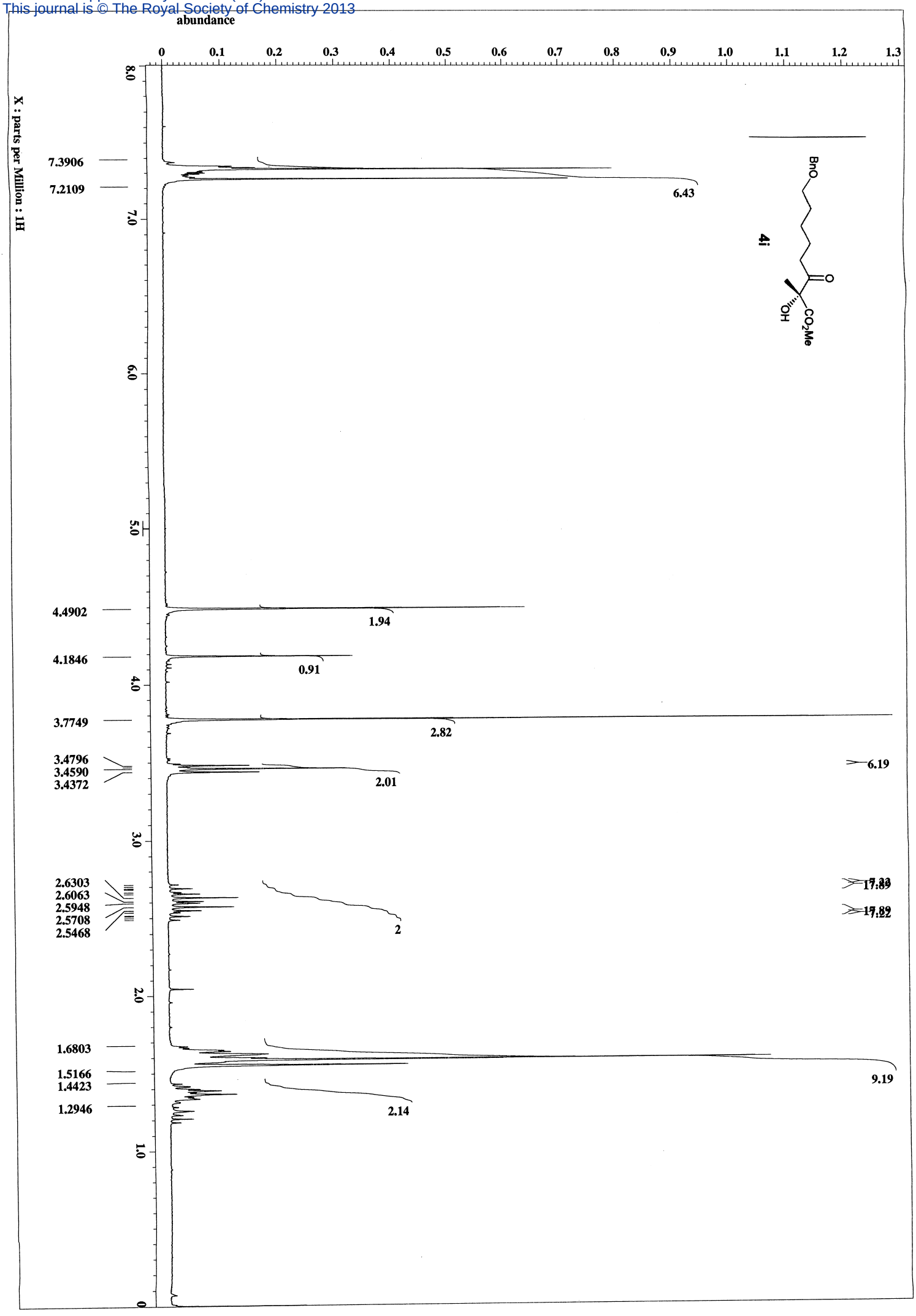


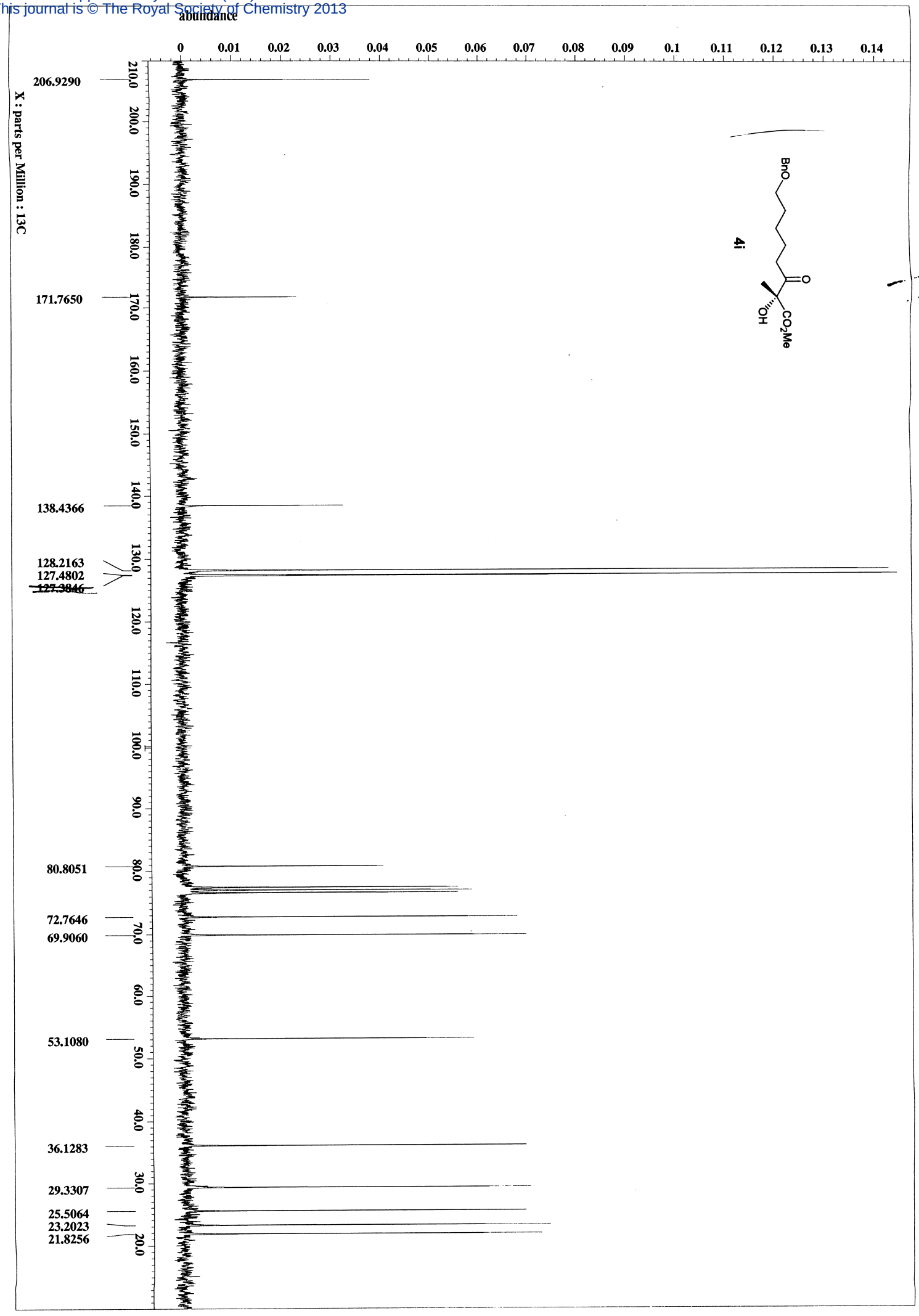


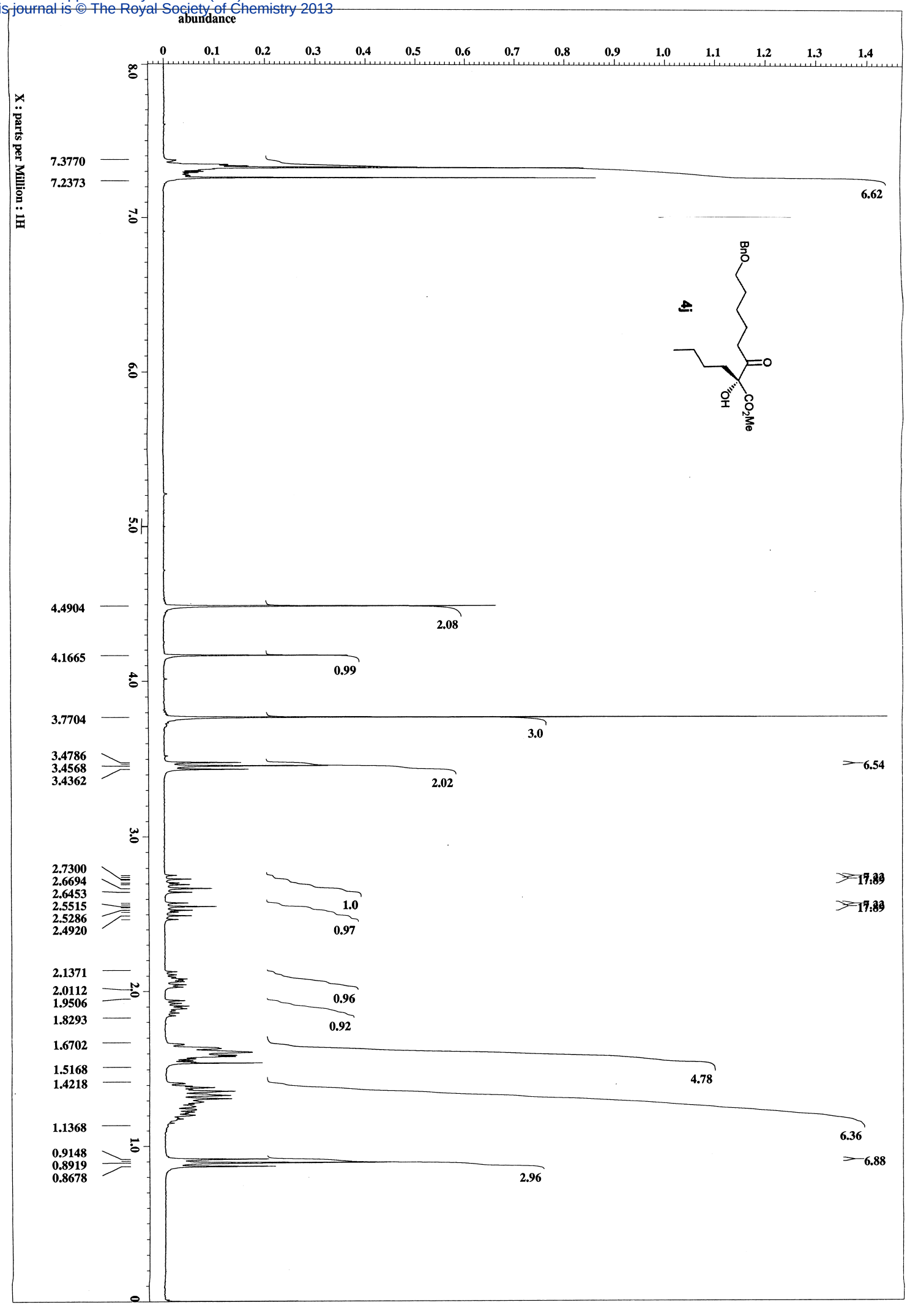


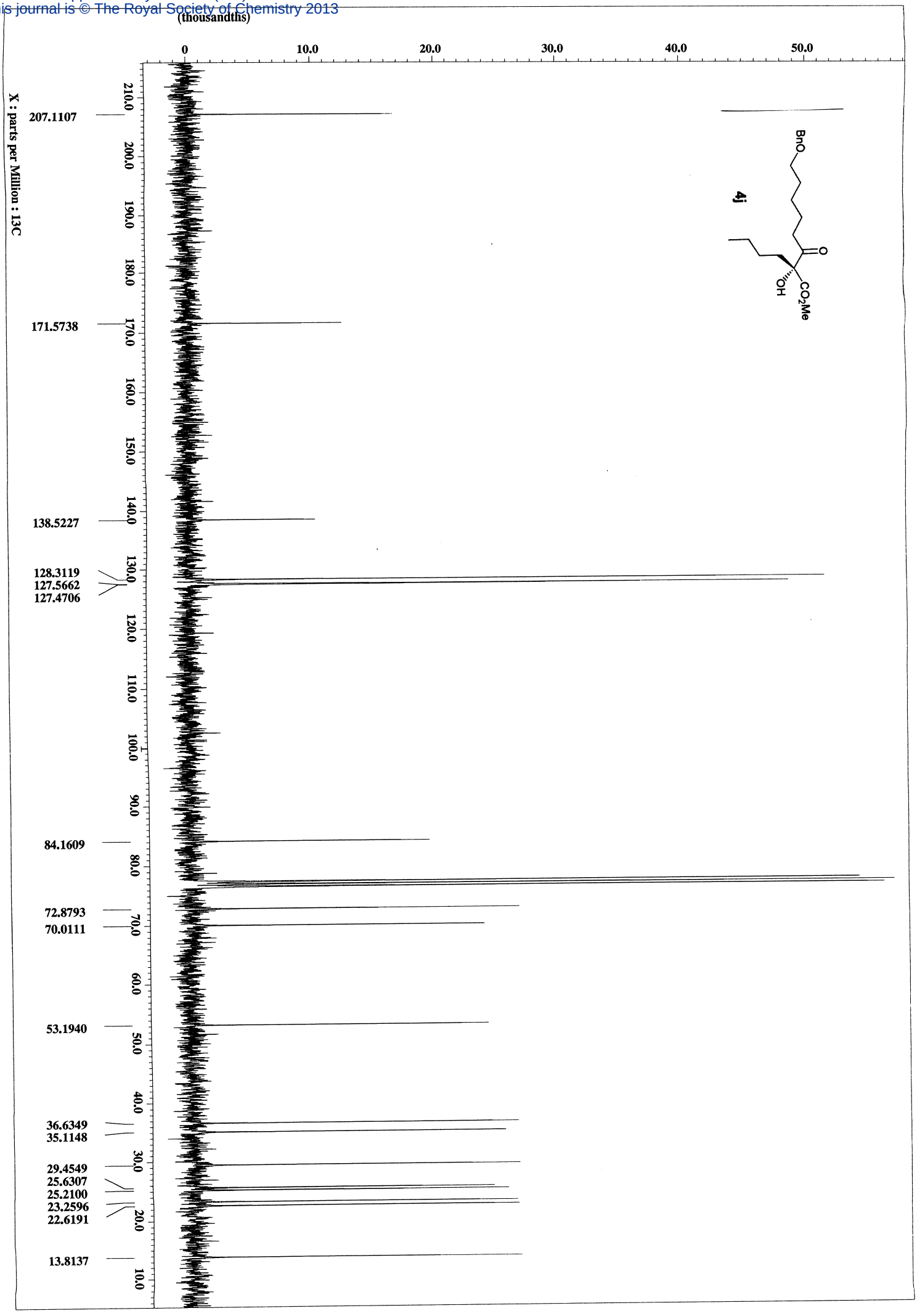


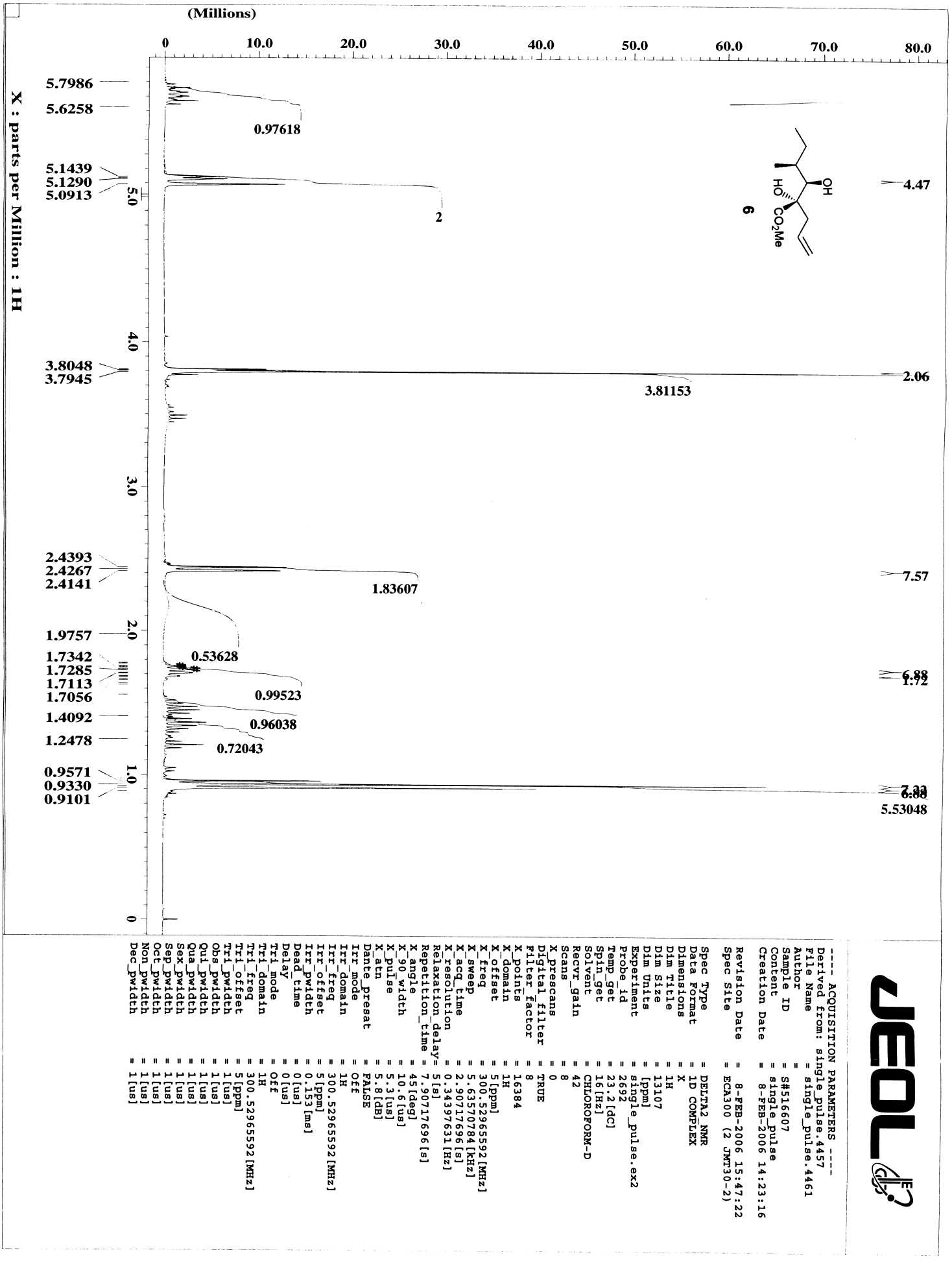


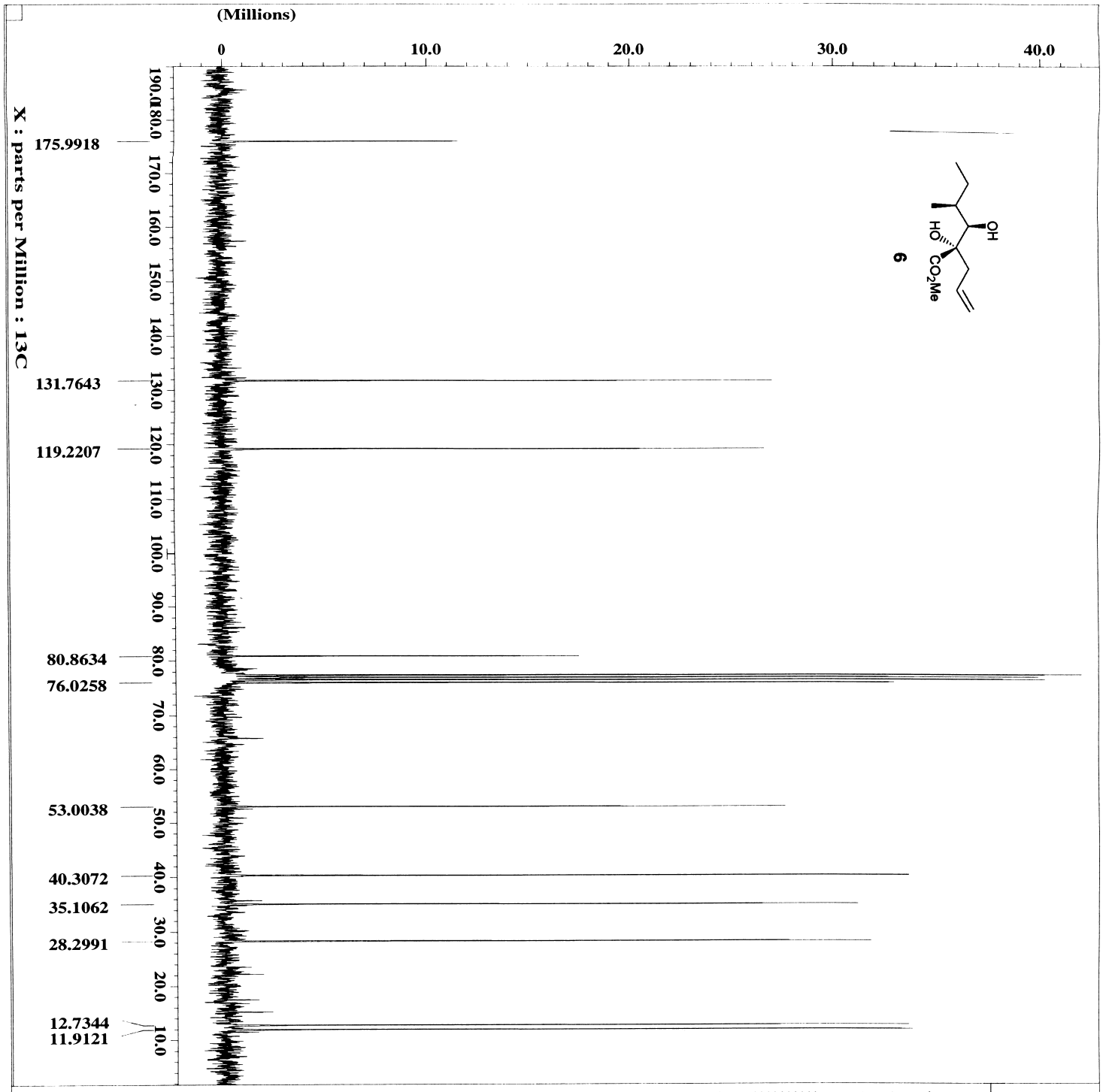




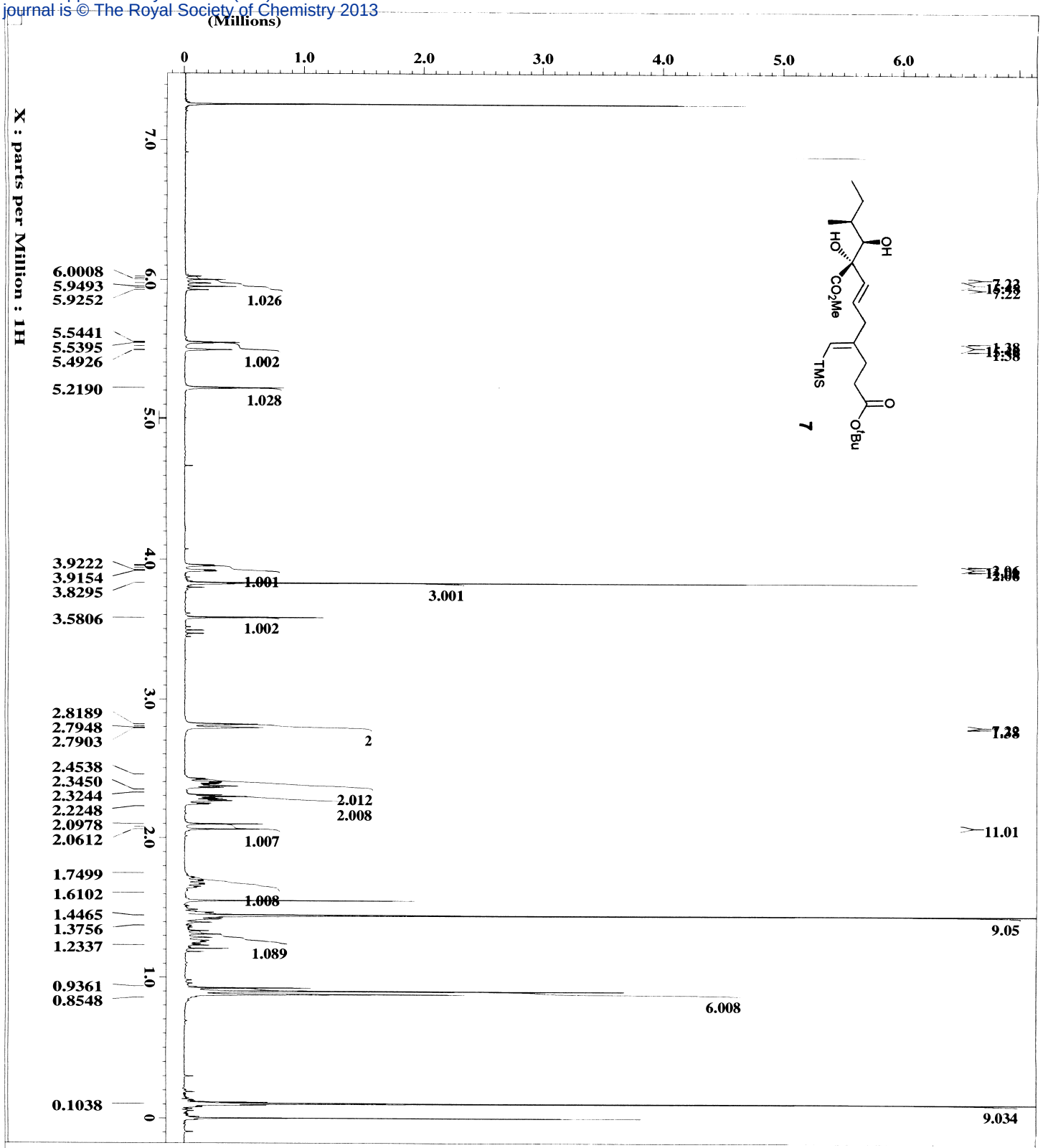




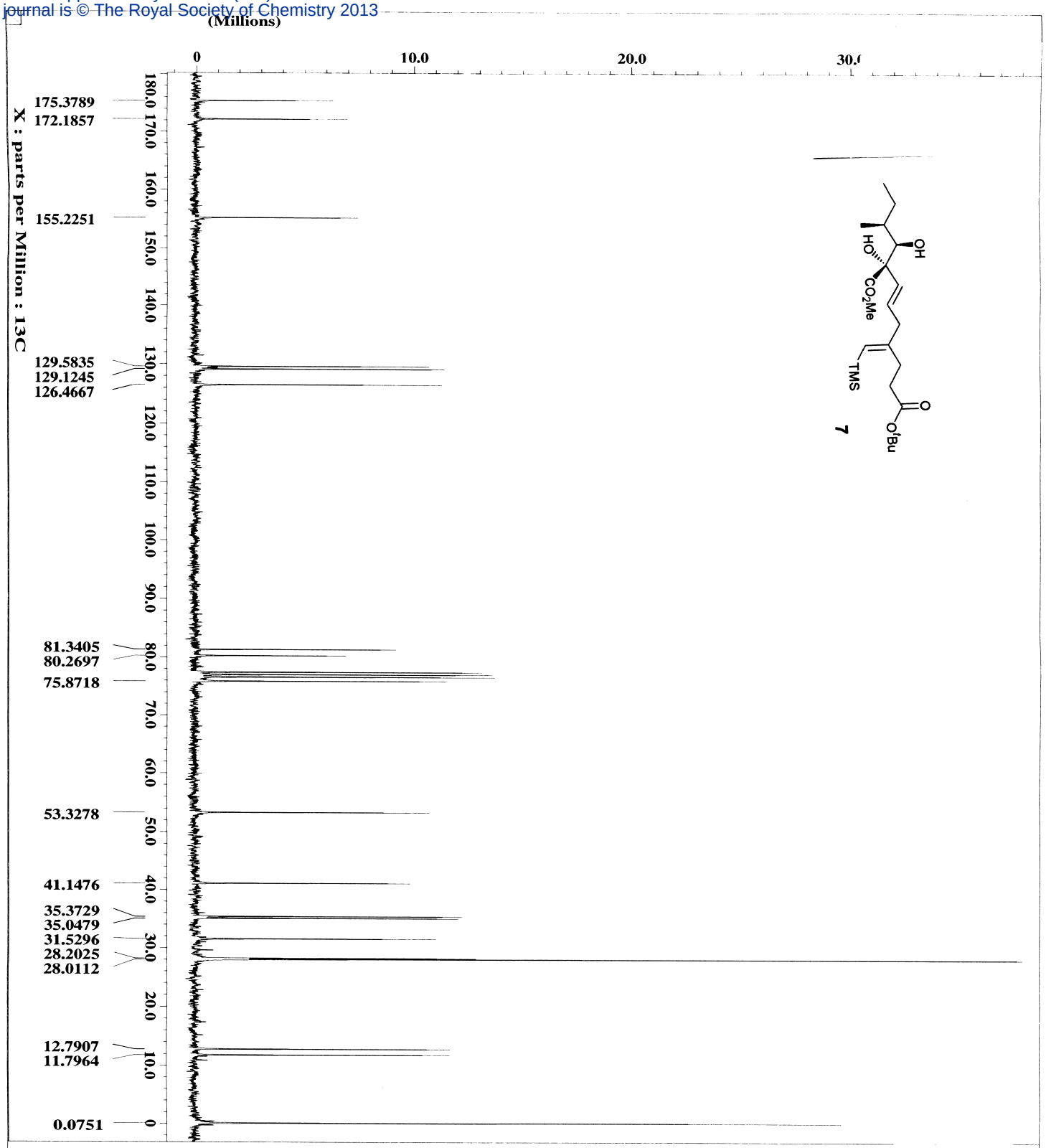




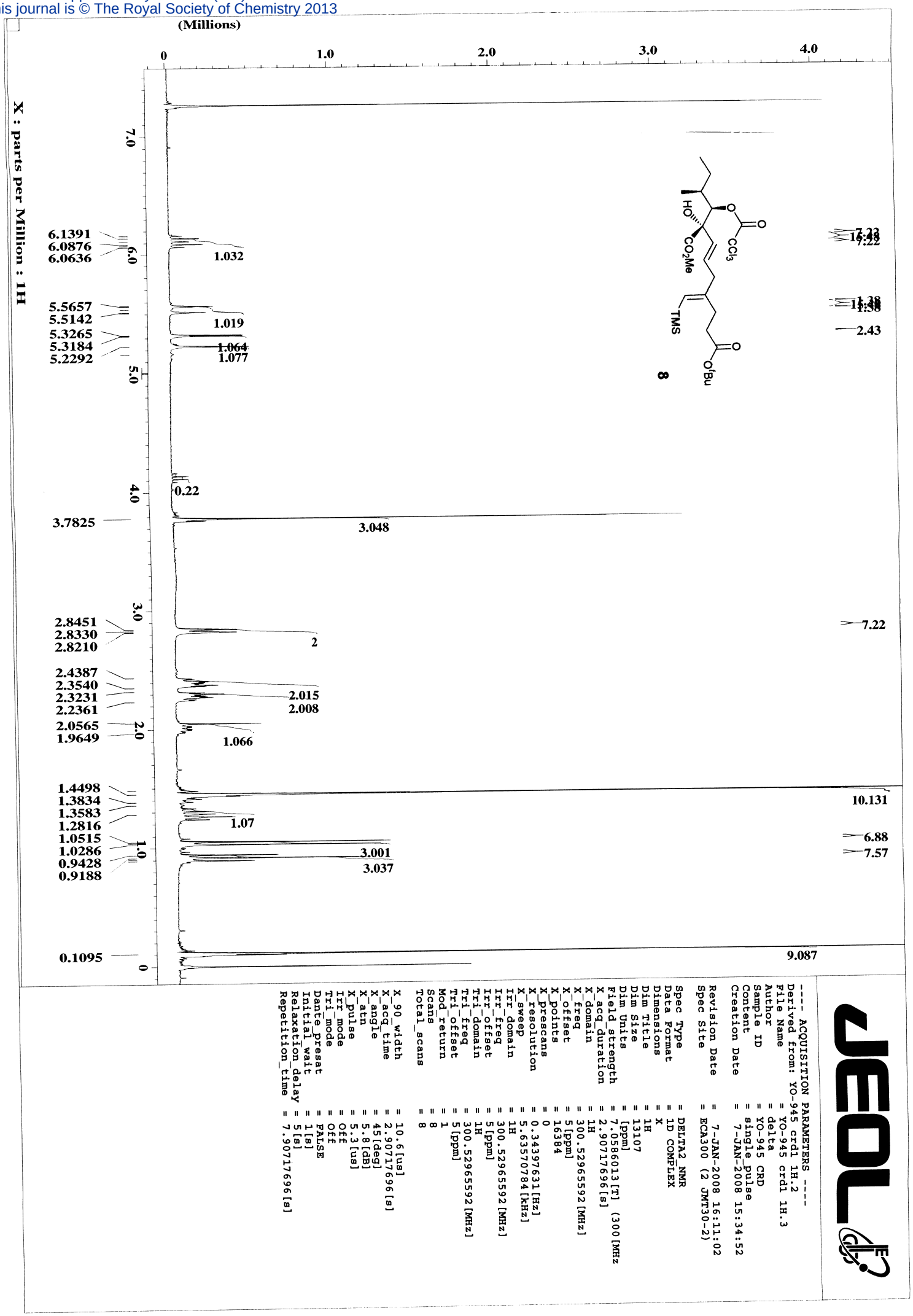

```
---- ACQUISITION PARAMETERS ----
Derived from: single_pulse_dec_copy.66
File Name                     = single_pulse_dec_copy.
Author                        =
Sample ID                     = S#517608
Content                       = single pulse decoupled
Creation Date                 = 8-FEB-2006 14:40:06
Revision Date                 = 8-FEB-2006 15:53:43
Spec Site                     = ECA300 (2 JMT30-2)

Spec Type                     = DELTA2_NMR
Data Format                   = 1D COMPLEX
Dimensions                    = X
Dim Title                     = 13C
Dim Size                      = 13107
Dim Units                     = [ppm]
Experiment                    = single_pulse_dec
Probe_id                      = 2692
Temp_get                      = 23.7[dC]
Spin_get                      = 13[Hz]
Solvent                       = CHLOROFORM-D
Recvr_gain                    = 60
Scans                         = 289
X_prescans                    = 4
Digital_filter                = TRUE
Filter_factor                 = 8
X_points                      = 16384
X_domain                      = 13C
X_offset                      = 100[ppm]
X_freq                        = 75.56823426[MHz]
X_sweep                       = 23.67424242[kHz]
X_acq_time                    = 0.69206016[s]
X_resolution                  = 1.44496109[Hz]
Relaxation_delay              = 2[s]
Repetition_time               = 2.69206016[s]
X_angle                       = 30[deg]
X_90_width                    = 9.6[us]
X_pulse                       = 3.2[us]
X_atn                         = 8.6[dB]
Noe_time                      = 2[s]
Decoupling                    = TRUE
Irr_domain                    = 1H
Irr_freq                      = 300.52965592[MHz]
Irr_offset                    = 5[ppm]
Irr_pwidth                    = 0.153[ms]
Irr_atn_noe                   = 28.8[dB]
Irr_atn_dec                   = 28.8[dB]
Irr_noise                     = WALTZ
Dead_time                     = 0[us]
Delay                         = 0[us]
Tri_pwidth                    = 1[us]
Obs_pwidth                    = 1[us]
Qui_pwidth                    = 1[us]
Qua_pwidth                    = 1[us]
Sex_pwidth                    = 1[us]
Sep_pwidth                    = 1[us]
Oct_pwidth                    = 1[us]
Non_pwidth                    = 1[us]
Dec_pwidth                    = 1[us]
```




```
---- ACQUISITION PARAMETERS ----
Derived from: single_pulse.7366
File Name                = single_pulse.7370
Author                   = delta
Sample ID                = YO-866
Content                  = single_pulse
Creation Date            = 26-OCT-2007 16:20:10

Revision Date            = 26-OCT-2007 16:30:06
Spec Site                = ECA300 (2 JMT30-2)

Spec Type                = DELTA2_NMR
Data Format              = 1D COMPLEX
Dimensions               = X
Dim Title                = 1H
Dim Size                 = 13107
Dim Units                = [ppm]
Field_strength           = 7.0586013[T] (300[MHz
X_acq_duration           = 2.90717696[s]
X_domain                 = 1H
X_freq                   = 300.52965592[MHz]
X_offset                 = 5[ppm]
X_points                 = 16384
X_prescans               = 0
X_resolution             = 0.34397631[Hz]
X_sweep                  = 5.63570784[kHz]
Irr_domain               = 1H
Irr_freq                 = 300.52965592[MHz]
Irr_offset               = 5[ppm]
Tri_domain               = 1H
Tri_freq                 = 300.52965592[MHz]
Tri_offset               = 5[ppm]
Mod_return               = 1
Scans                    = 8
Total_scans              = 8

X_90_width               = 10.6[us]
X_acq_time               = 2.90717696[s]
X_angle                  = 45[deg]
X_atn                    = 5.8[dB]
X_pulse                  = 5.3[us]
Irr_mode                 = Off
Tri_mode                 = Off
Dante_presat             = FALSE
Initial_wait             = 1[s]
Relaxation_delay         = 5[s]
Repetition_time          = 7.90717696[s]
```




```
---- ACQUISITION PARAMETERS ----
File Name                 = single_pulse_dec.318
Author                    = delta
Sample ID                 = YO-866
Content                   = single pulse decouple
Creation Date             = 26-OCT-2007 16:40:03

Revision Date             = 26-OCT-2007 16:34:40
Spec Site                 = ECA300 (2 JMT30-2)

Spec Type                 = DELTA2_NMR
Data Format               = 1D COMPLEX
Dimensions                = X
Dim Title                 = 13C
Dim Size                  = 13107
Dim Units                 = [ppm]
Field_strength            = 7.05860013[T] (300[MHz
X_acq_duration            = 0.69206016[s]
X_domain                  = 13C
X_freq                    = 75.56823426[MHz]
X_offset                  = 100[ppm]
X_points                  = 16384
X_prescans                = 4
X_resolution              = 1.44496109[Hz]
X_sweep                   = 23.67424242[kHz]
Irr_domain                = 1H
Irr_freq                  = 300.52965592[MHz]
Irr_offset                = 5[ppm]
Mod_return                = 1
Scans                     = 361
Total_scans               = 361

X_90_width                = 9.4[us]
X_acq_time                = 0.69206016[s]
X_angle                   = 30[deg]
X_atn                     = 8.6[dB]
X_pulse                   = 3.13333333[us]
Irr_atn_dec               = 29.7[dB]
Irr_atn_noe               = 29.7[dB]
Irr_noise                 = WALTZ
Decoupling                = TRUE
Initial_wait              = 1[s]
Noe                       = TRUE
Noe_time                  = 2[s]
Relaxation_delay          = 2[s]
Repetition_time           = 2.69206016[s]
```




```
---- ACQUISITION PARAMETERS ----
Derived from: YO-945 crd1 1H.2
File Name                 = YO-945 crd1 1H.3
Author                    = delta
Sample ID                 = YO-945 CRD
Content                   = single_pulse
Creation Date             =  7-JAN-2008 15:34:52
Revision Date             =  7-JAN-2008 16:11:02
Spec Site                 = ECA300 (2 JMT30-2)

Spec Type                 = DELTA2_NMR
Data Format               = 1D COMPLEX
Dimensions                = X
Dim Title                 = 1H
Dim Size                  = 13107
Dim Units                 = [ppm]
Field_strength            = 7.0586013[T] (300[MHz
X_acq_duration            = 2.90717696[s]
X_domain                  = 1H
X_freq                    = 300.52965592[MHz]
X_offset                  = 5[ppm]
X_points                  = 16384
X_prescans                = 0
X_resolution              = 0.34397631[Hz]
X_sweep                   = 5.63570784[kHz]
Irr_domain                = 1H
Irr_freq                  = 300.52965592[MHz]
Irr_offset                = 5[ppm]
Tri_domain                = 1H
Tri_freq                  = 300.52965592[MHz]
Tri_offset                = 5[ppm]
Mod_return                = 1
Scans                     = 8
Total_scans               = 8

X_90_width                = 10.6[us]
X_acq_time                = 2.90717696[s]
X_angle                   = 45[deg]
X_atn                     = 5.8[dB]
X_pulse                   = 5.3[us]
Irr_mode                  = Off
Tri_mode                  = Off
Dante_presat              = FALSE
Initial_wait              = 1[s]
Relaxation_delay          = 5[s]
Repetition_time           = 7.90717696[s]
```

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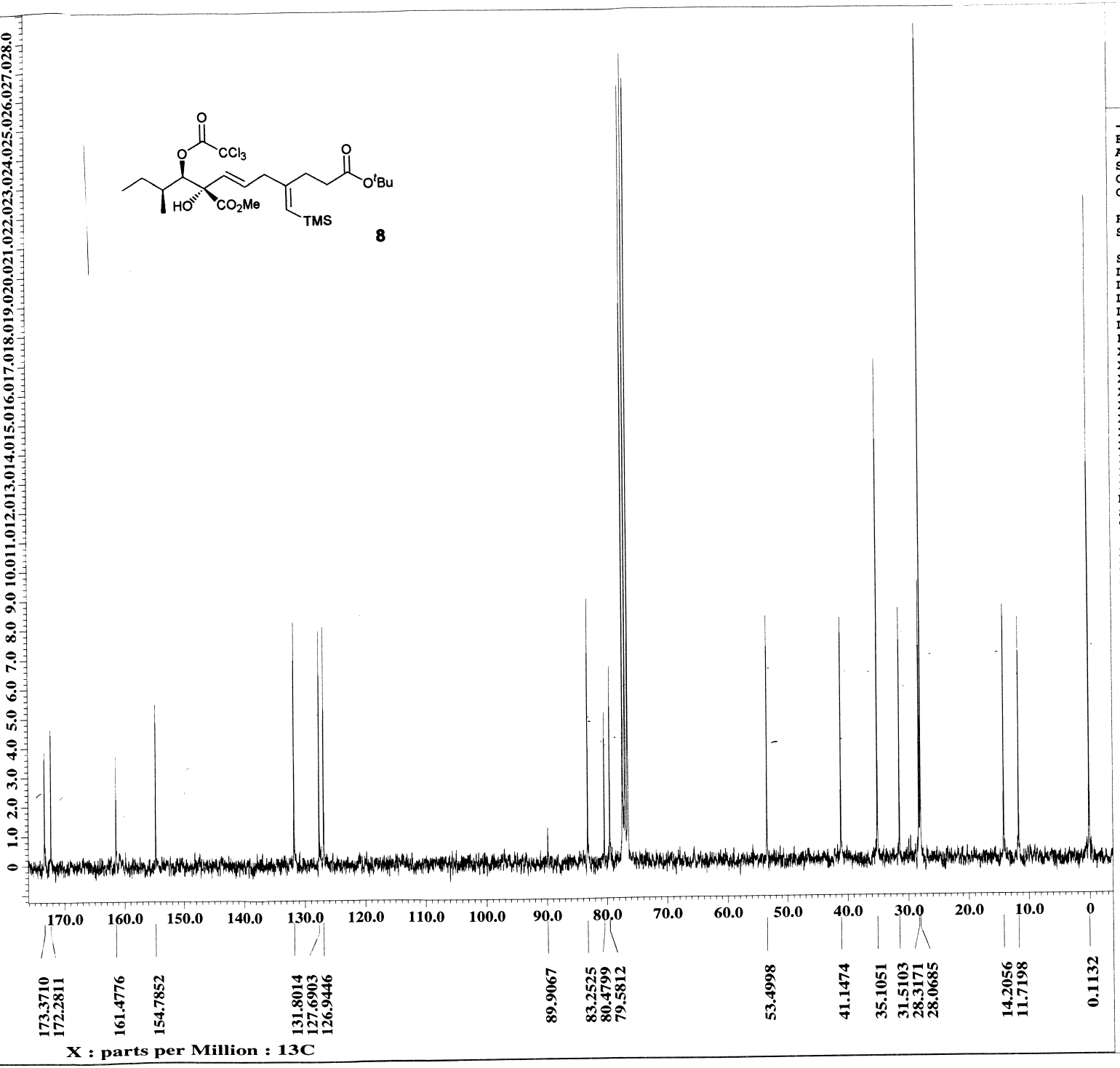


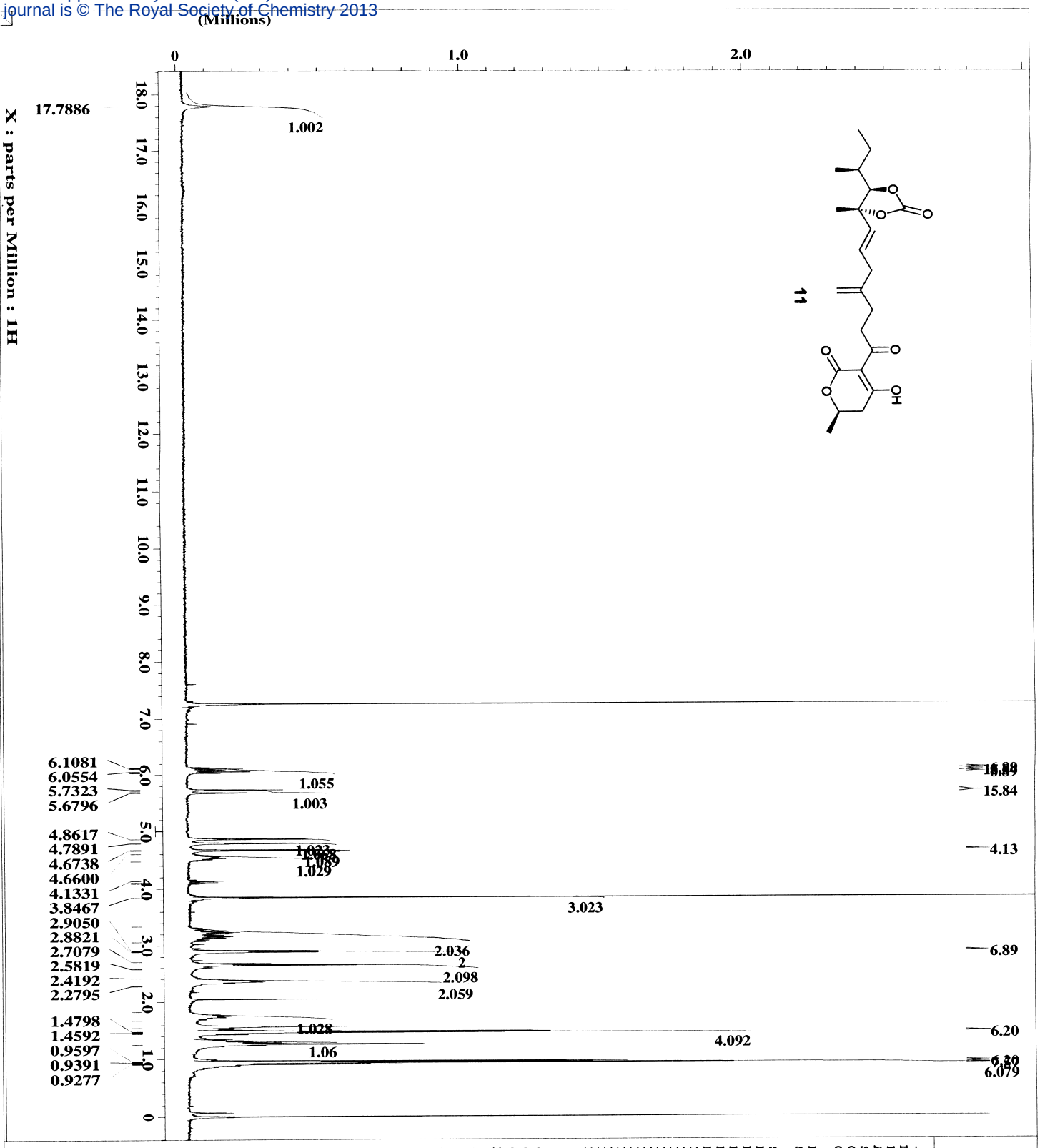
JEOL

```
---- ACQUISITION PARAMETERS ----
File Name          = single_pulse_dec.111
Author             = delta
Sample ID          = YO-945
Content            = single pulse decouple
Creation Date      =  7-JAN-2008 16:31:52

Revision Date      =  7-JAN-2008 16:26:21
Spec Site          = ECA300 (2 JMT30-2)

Spec Type          = DELTA2_NMR
Data Format        = 1D COMPLEX
Dimensions         = X
Dim Title          = 13C
Dim Size           = 13107
Dim Units          = [ppm]
Field_strength     = 7.0586013[T]  (300[MHz
X_acq_duration     = 0.69206016[s]
X_domain           = 13C
X_freq             = 75.56823426[MHz]
X_offset           = 100[ppm]
X_points           = 16384
X_prescans         = 4
X_resolution       = 1.44496109[Hz]
X_sweep            = 23.67424242[kHz]
Irr_domain         = 1H
Irr_freq           = 300.52965592[MHz]
Irr_offset         = 5[ppm]
Mod_return         = 1
Scans              = 648
Total_scans        = 648

X_90_width         = 9.4[us]
X_acq_time         = 0.69206016[s]
X_angle            = 30[deg]
X_atn              = 8.6[dB]
X_pulse            = 3.13333333[us]
Irr_atn_dec        = 29.7[dB]
Irr_atn_noe        = 29.7[dB]
Irr_noise          = WALTZ
Decoupling         = TRUE
Initial_wait       = 1[s]
Noe                = TRUE
Noe_time           = 2[s]
Relaxation_delay   = 2[s]
Repetition_time    = 2.69206016[s]
```




```
---- ACQUISITION PARAMETERS ----
Derived from: single_pulse.2914
File Name                 = single_pulse.2918
Author                    = delta
Sample ID                 = YO-956
Content                   = single_pulse
Creation Date             = 19-JAN-2008 10:47:06
Revision Date             = 19-JAN-2008 10:54:29
Spec Site                 = ECA300 (2 JMT30-2)

Spec Type                 = DELTA2_NMR
Data Format               = 1D COMPLEX
Dimensions                = X
Dim Title                 = 1H
Dim Size                  = 13107
Dim Units                 = [ppm]
Field_strength            = 7.0586013[T] (300[MHz
X_acq_duration            = 1.4522776[s]
X_domain                  = 1H
X_freq                    = 300.52965592[MHz]
X_offset                  = 5[ppm]
X_points                  = 16384
X_prescans                = 0
X_resolution              = 0.68857351[Hz]
X_sweep                   = 11.28158845[kHz]
Irr_domain                = 1H
Irr_freq                  = 300.52965592[MHz]
Irr_offset                = 5[ppm]
Tri_domain                = 1H
Tri_freq                  = 300.52965592[MHz]
Tri_offset                = 5[ppm]
Mod_return                = 1
Scans                     = 8
Total_scans               = 8

X_90_width                = 11.6[us]
X_acq_time                = 1.4522776[s]
X_angle                   = 45[deg]
X_atn                     = 5.8[dB]
X_pulse                   = 5.8[us]
Irr_mode                  = Off
Tri_mode                  = Off
Dante_presat              = FALSE
Initial_wait              = 1[s]
Relaxation_delay          = 5[s]
Repetition_time           = 6.4522776[s]
```

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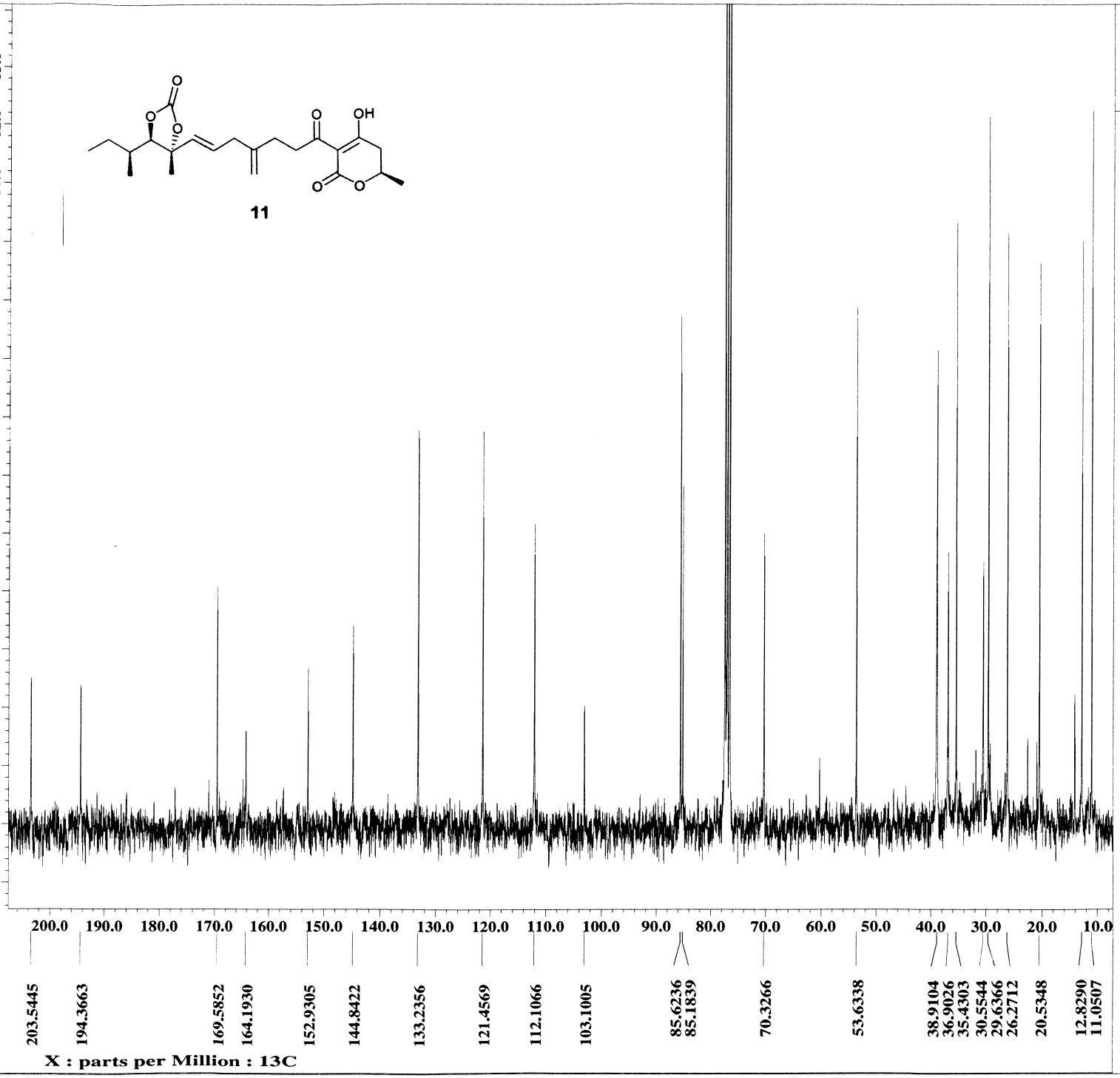


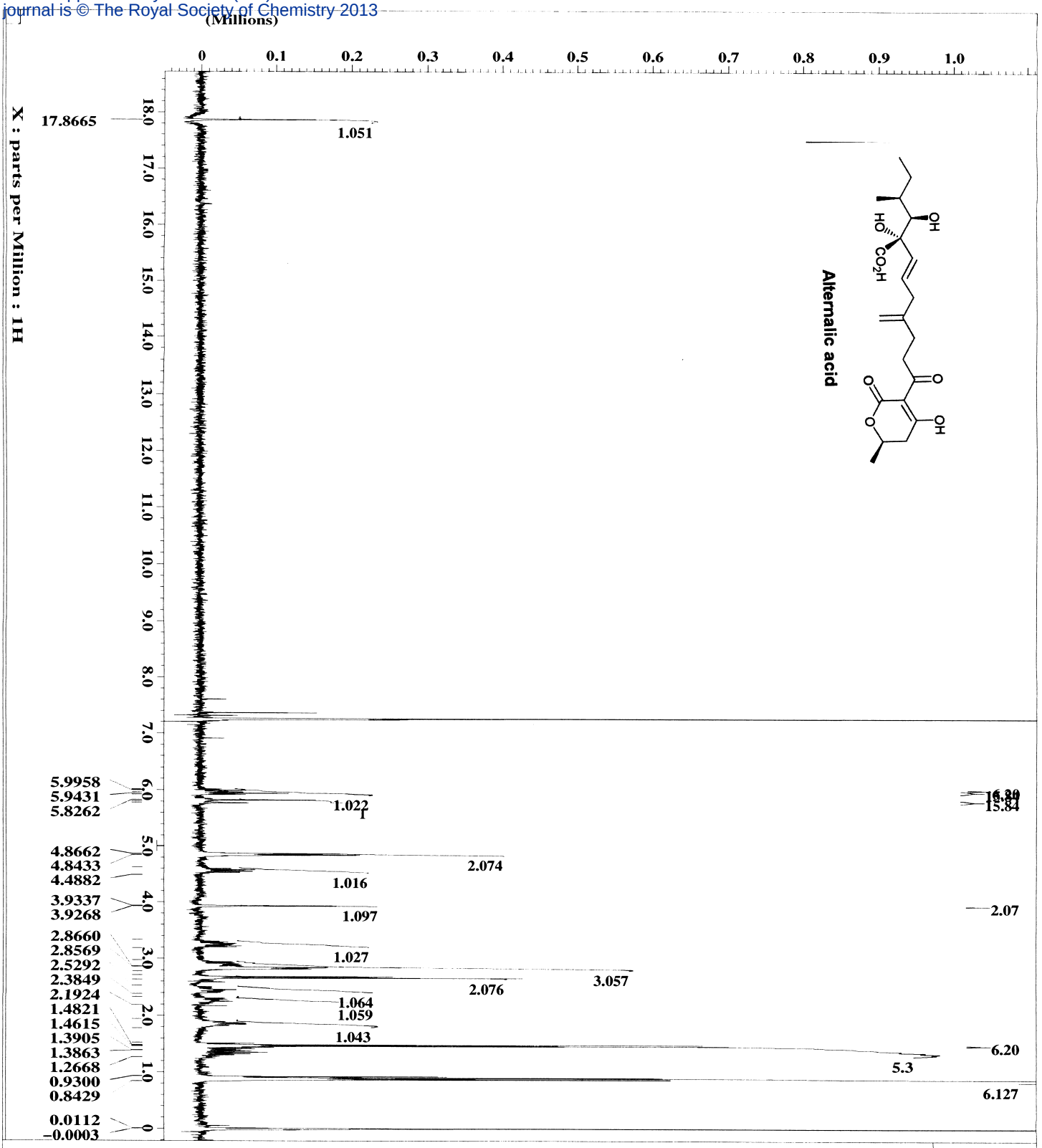
JEOL

```
---- ACQUISITION PARAMETERS ----
File Name          = single_pulse_dec.172
Author             = delta
Sample ID          = YO-956
Content            = single pulse decouple
Creation Date      = 19-JAN-2008 21:52:25

Revision Date      = 19-JAN-2008 21:47:33
Spec Site          = ECA300 (2 JMT30-2)

Spec Type          = DELTA2_NMR
Data Format        = 1D COMPLEX
Dimensions         = X
Dim Title          = 13C
Dim Size           = 13107
Dim Units          = [ppm]
Field_strength     = 7.0586013[T] (300[MHz
X_acq_duration     = 0.69206016[s]
X_domain           = 13C
X_freq             = 75.56823426[MHz]
X_offset           = 100[ppm]
X_points           = 16384
X_prescans         = 4
X_resolution       = 1.44496109[Hz]
X_sweep            = 23.67424242[kHz]
Irr_domain         = 1H
Irr_freq           = 300.52965592[MHz]
Irr_offset         = 5[ppm]
Mod_return         = 1
Scans              = 921
Total_scans        = 921

X_90_width         = 9.4[us]
X_acq_time         = 0.69206016[s]
X_angle            = 30[deg]
X_atn              = 8.6[dB]
X_pulse            = 3.13333333[us]
Irr_atn_dec        = 28.2[dB]
Irr_atn_noe        = 28.2[dB]
Irr_noise          = WALTZ
Decoupling         = TRUE
Initial_wait       = 1[s]
Noe                = TRUE
Noe_time           = 2[s]
Relaxation_delay   = 2[s]
Repetition_time    = 2.69206016[s]
```

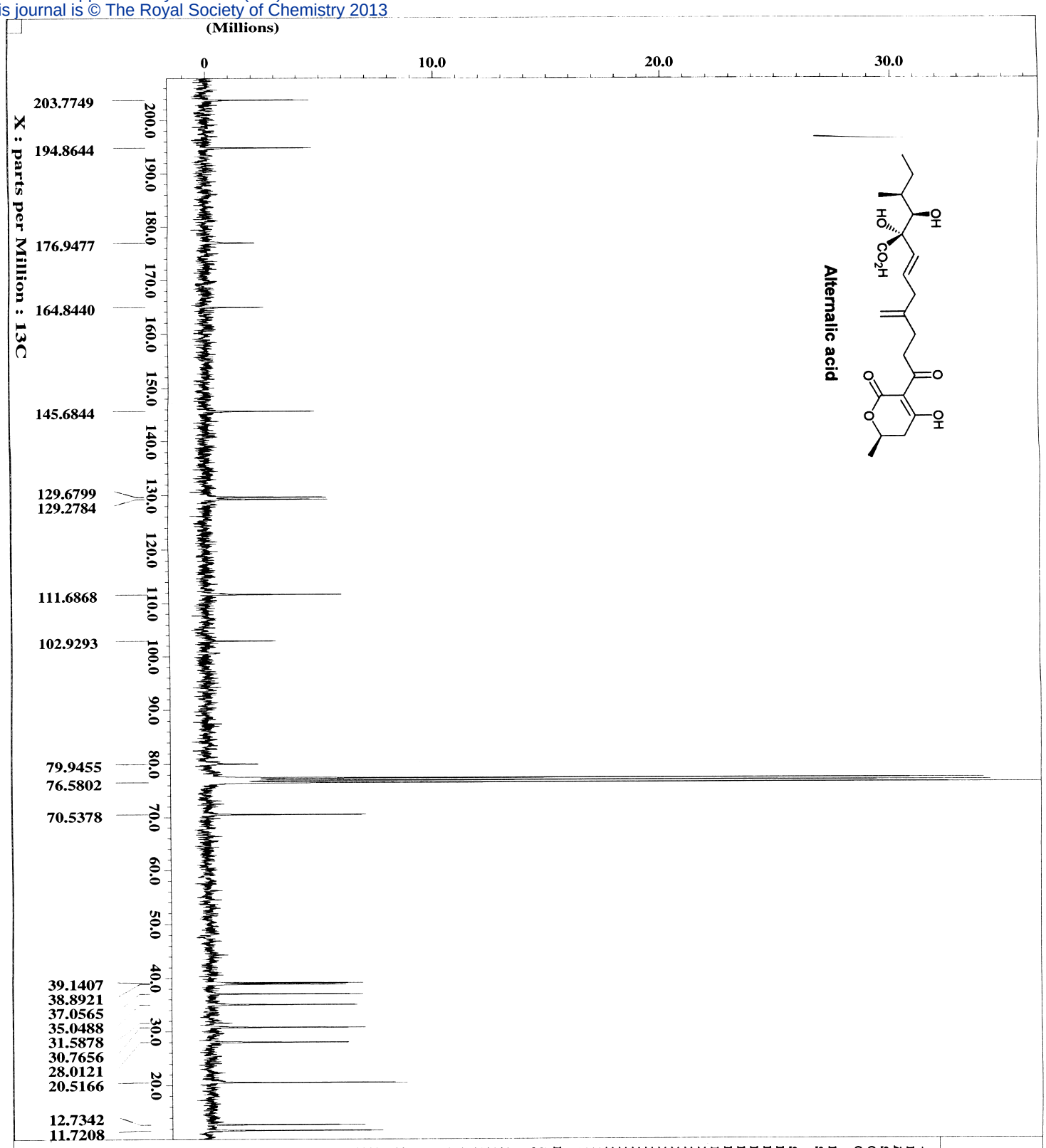



```
---- ACQUISITION PARAMETERS ----
Derived from: single_pulse.3086
File Name                     = single_pulse.3413
Author                        = delta
Sample ID                     = YO-962 recrystall
Content                       = single_pulse
Creation Date                 = 22-JAN-2008 20:19:39

Revision Date                 = 29-JAN-2008 21:07:33
Spec Site                     = ECA300 (2 JMT30-2)

Spec Type                     = DELTA2_NMR
Data Format                   = 1D REAL
Dimensions                    = X
Dim Title                     = 1H
Dim Size                      = 13107
Dim Units                     = [ppm]
Field_strength                = 7.0586013[T] (300[MHz
X_acq_duration                = 1.45227776[s]
X_domain                      = 1H
X_freq                        = 300.52965592[MHz]
X_offset                      = 5[ppm]
X_points                      = 16384
X_prescans                    = 0
X_resolution                  = 0.68857351[Hz]
X_sweep                       = 11.28158845[kHz]
Irr_domain                    = 1H
Irr_freq                      = 300.52965592[MHz]
Irr_offset                    = 5[ppm]
Tri_domain                    = 1H
Tri_freq                      = 300.52965592[MHz]
Tri_offset                    = 5[ppm]
Mod_return                    = 1
Scans                         = 8
Total_scans                   = 8

X_90_width                    = 11.6[us]
X_acq_time                    = 1.45227776[s]
X_angle                       = 45[deg]
X_atn                         = 5.8[dB]
X_pulse                       = 5.8[us]
Irr_mode                      = Off
Tri_mode                      = Off
Dante_presat                  = FALSE
Initial_wait                  = 1[s]
Relaxation_delay              = 5[s]
Repetition_time               = 6.45227776[s]
```




```
---- ACQUISITION PARAMETERS ----
File Name                 = single_pulse_dec.219
Author                    = delta
Sample ID                 = Alternaric acid
Content                   = single pulse decouple
Creation Date             = 12-FEB-2008 17:17:30

Revision Date             = 12-FEB-2008 17:12:32
Spec Site                 = ECA300 (2 JM730-2)

Spec Type                 = DELTA2_NMR
Data Format               = 1D COMPLEX
Dimensions                = X
Dim Title                 = 13C
Dim Size                  = 13107
Dim Units                 = [ppm]
Field_strength            = 7.0586013[T] (300[MHz
X_acq_duration            = 0.69206016[s]
X_domain                  = 13C
X_freq                    = 75.56823426[MHz]
X_offset                  = 100[ppm]
X_points                  = 16384
X_prescans                = 4
X_resolution              = 1.44496109[Hz]
X_sweep                   = 23.67424242[kHz]
Irr_domain                = 1H
Irr_freq                  = 300.52965592[MHz]
Irr_offset                = 5[ppm]
Mod_return                = 1
Scans                     = 1024
Total_scans               = 1024

X_90_width                = 9.4[us]
X_acq_time                = 0.69206016[s]
X_angle                   = 30[deg]
X_atn                     = 8.6[dB]
X_pulse                   = 3.13333333[us]
Irr_atn_dec               = 29.7[dB]
Irr_atn_noe               = 29.7[dB]
Irr_noise                 = WALTZ
Decoupling                = TRUE
Initial_wait              = 1[s]
Noe                       = TRUE
Noe_time                  = 2[s]
Relaxation_delay          = 2[s]
Repetition_time           = 2.69206016[s]
```