Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

SUPPORTING INFORMATION

Mechanistic study of the selective hydrogenation of carboxylic acid derivatives over supported rhenium catalysts

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Supplementary results

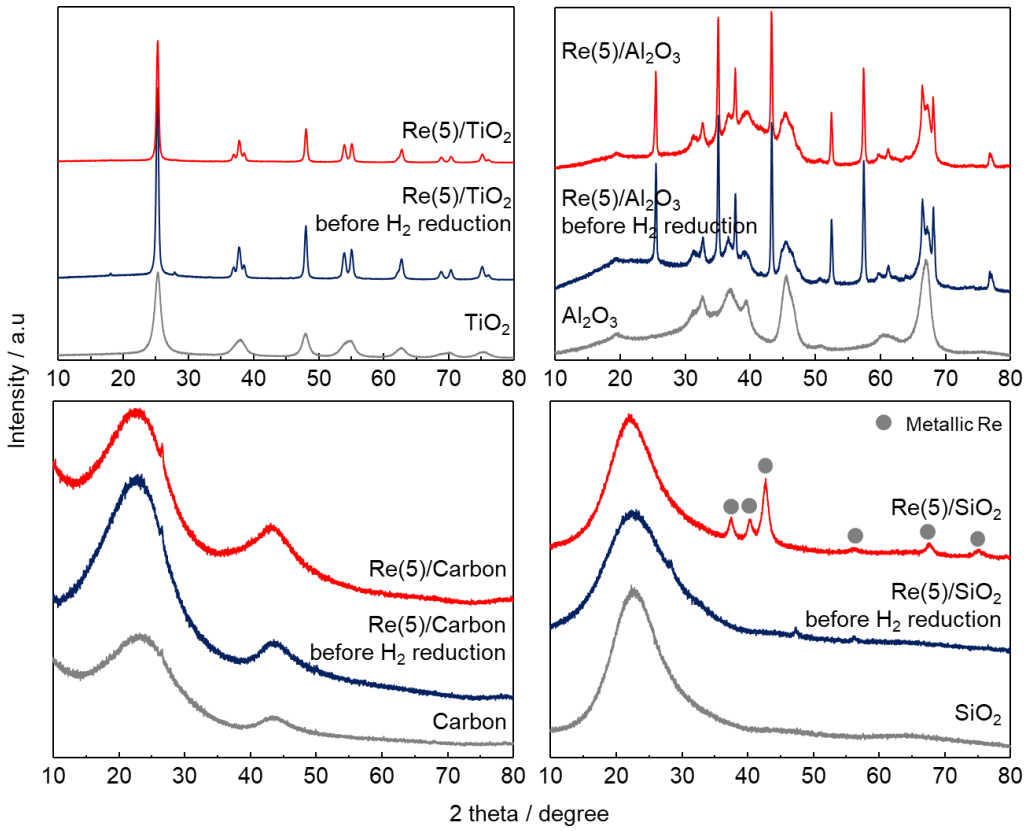


Figure S1. *Ex situ* XRD patterns of $Re(5)/TiO_2$, $Re(5)/SiO_2$, $Re(5)/Al_2O_3$, and Re/Carbon. The samples were reduced at T = 500 °C under H_2 flow before the XRD measurements.

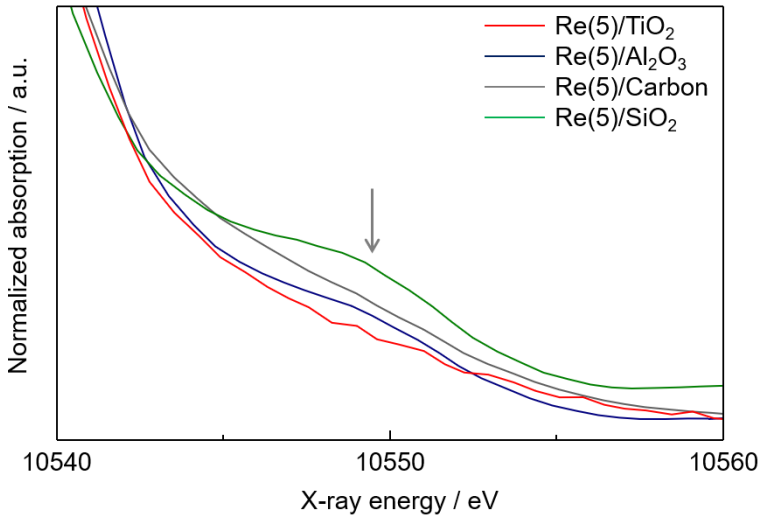


Figure S2. Zoomed *in situ* Re L_3-edge XANES spectra of $Re(5)/TiO_2$, $Re(5)/Al_2O_3$, Re(5)/Carbon, and $Re(5)/SiO_2$. XANES spectra were measured at 500 °C under the flow of 5% H_2/He (100 mL min^{-1}).

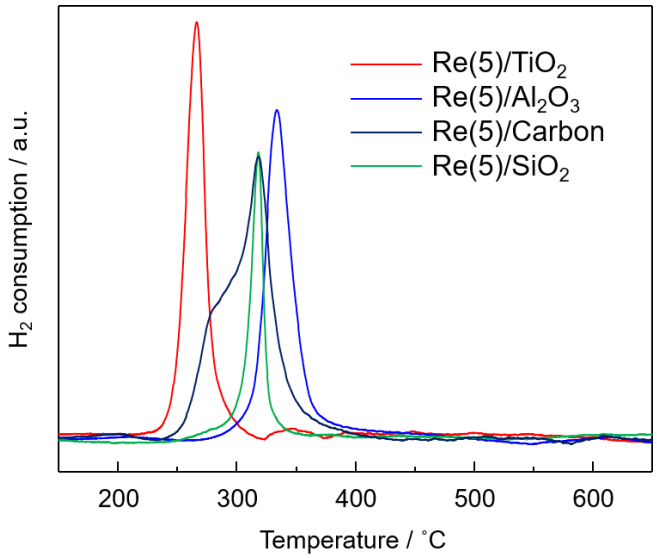


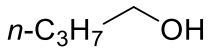
Figure S3. H_2-TPR profile of Re(5)/TiO_2, Re(5)/SiO_2, and Re(5)/Al_2O_3 after the calcination at 500 °C in air and of Re(5)/Carbon after the drying in air. The sample was heated with a temperature ramp-rate of 10 °C min^{-1} in a flow of 5% H_2/Ar (20 cm^3 min^{-1}).

Product Separation and NMR analysis

After the catalytic reaction, product mixtures were subjected to column chromatography on silica gel 60 (spherical, 63-210 μm, Kanto Chemical Co. Ltd.; eluent: hexane/ethyl acetate = 90/10, v/v), and subsequently analyzed by GC and GCMS. ^{1}H and ^{13}C NMR analysis was carried out for those isolated products. ^{1}H and ^{13}C NMR spectra were recorded at ambient temperature on a JEOL-ECX 600 spectrometer (^{1}H: 600.17 MHz, ^{13}C: 150.92 MHz), using tetramethylsilane as the internal standard.

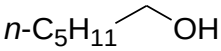
^{1}H and ^{13}C NMR spectra for the desired products were assigned according to the corresponding literature values. Abbreviations used in the NMR experiments: s, singlet; d, doublet; dd, doublet of doublets; t, triplet; q, quartet; m, multiplet; br, broad. GC-MS spectra were recorded on a SHIMADZU QP2010.

Butan-1-ol:[1]



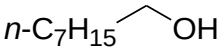
^{1}H NMR (600.17 MHz, $CDCl_3$, TMS): δ 3.63 (S, 2H), 1.77 (br s, 1H), 1.58-1.52 (m, 2H), 1.42-1.33 (m, 2H), 0.92 (t, *J* = 6.87 Hz, 3H); ^{13}C NMR (150.92 MHz, $CDCl_3$) δ 62.59, 32.784, 18.42, 13.79; GC-MS m/e 74.10.

Hexan-1-ol:[2]



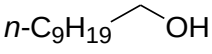
^{1}H NMR (600.17 MHz, $CDCl_3$, TMS): δ 3.61 (t, *J* = 6.18 Hz, 2H), 2.09 (br s, 1H), 1.57-1.54 (m, 2H), 1.32-1.30 (m, 6H), 0.89 (t, *J* = 6.87 Hz, 3H); ^{13}C NMR (150.92 MHz, $CDCl_3$) δ 62.83, 32.64, 31.58, 25.37, 22.56, 13.94; GC-MS m/e 102.15.

Octan-1-ol:[2]



^{1}H NMR (600.17 MHz, $CDCl_3$, TMS): δ 3.61 (t, *J* = 6.54 Hz, 2H), 2.20 (br s, 1H), 1.56-1.53 (m, 2H), 1.33-1.28 (m, 10H), 0.88 (t, *J* = 6.83 Hz, 3H); ^{13}C NMR (150.92 MHz, $CDCl_3$) δ 62.82, 32.68, 31.77, 29.35, 29.23, 25.70, 22.59, 14.00; GC-MS m/e 130.14.

Decan-1-ol:[2]



^{1}H NMR (600.17 MHz, $CDCl_3$, TMS): δ 3.61 (t, *J* = 6.54 Hz, 2H), 2.18 (br s, 1H), 1.56-1.54 (m, 2H), 1.31-1.26 (m, 14H), 0.88 (t, *J* = 6.87 Hz, 3H); ^{13}C NMR (150.92 MHz, $CDCl_3$) δ 62.82, 32.69, 31.84, 29.58, 29.51, 29.40, 29.27, 25.70, 22.61, 14.02; GC-MS m/e 158.18.

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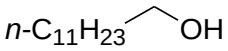
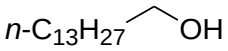


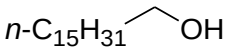
^{1}H NMR (600.17 MHz, $CDCl_3$, TMS): δ 3.63 (t, *J* = 6.54 Hz, 2H), 1.58-1.54 (m, 2H), 1.45 (br s, 1H), 1.35-1.25 (m, 18H), 0.88 (t, *J* = 6.87 Hz, 3H); ^{13}C NMR (150.92 MHz, $CDCl_3$) δ 63.03, 32.77, 31.89, 29.64, 29.61, 29.59, 29.58, 29.42, 29.32, 25.72, 22.66, 14.09; GC-MS m/e 186.20.

Tetradecan-1-ol:[2]



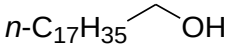
^{1}H NMR (600.17 MHz, $CDCl_3$, TMS): δ 3.63 (t, *J* = 6.87 Hz, 2H), 1.57-1.55 (m, 2H), 1.45 (br s, 1H), 1.37-1.25 (m, 22H), 0.88 (t, *J* = 6.87 Hz, 3H), ; ^{13}C NMR (150.92 MHz, $CDCl_3$) δ 63.06, 32.79, 31.90, 29.65 (C×2), 29.60 (C×2), 29.42 (C×2), 29.35 (C×2), 25.72, 22.68, 14.10; GC-MS m/e 214.25.

Hexadecan-1-ol:[2]



^{1}H NMR (600.17 MHz, $CDCl_3$, TMS): δ 3.63 (t, *J* = 6.87 Hz, 2H), 1.57-1.52 (m, 2H), 1.35-1.25 (m, 27H), 0.88 (t, *J* = 6.87 Hz, 3H), ; ^{13}C NMR (150.92 MHz, $CDCl_3$) δ 63.03, 32.79, 31.91, 29.68 (C×2), 29.65 (C×2), 29.60 (C×2), 29.42 (C×2), 29.35 (C×2), 25.72, 22.68, 14.11; GC-MS m/e 242.28.

Octadecan-1-ol:[2]



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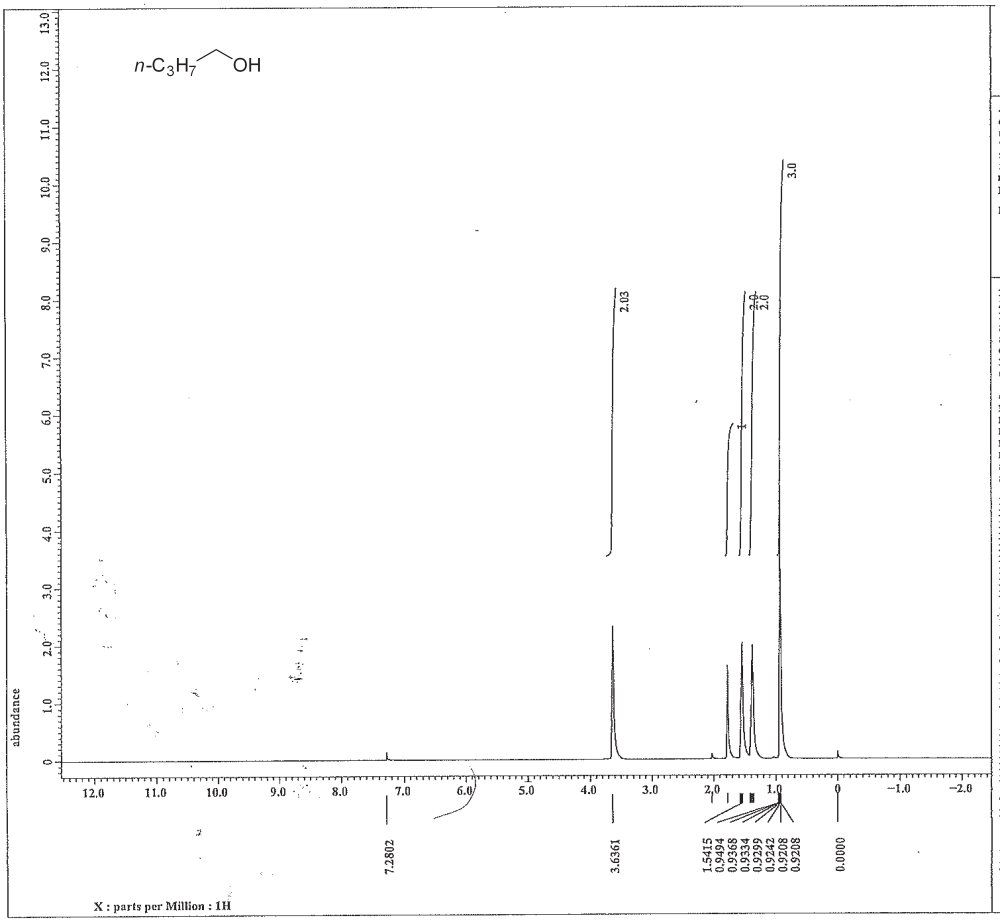
References

1 S. R. Wann, P. T. Thorsen and M. M. Kreevoy, *J. Org. Chem.*, 1981, **46**, 2579–2581.

2 T. Toyao, S. M. A. H. Siddiki, Y. Morita, T. Kamachi, A. S. Touchy, W. Onodera, K. Kon, S. Furukawa, H. Ariga, K. Asakura, K. Yoshizawa and K. Shimizu, *Chem. - A Eur. J.* 2017, **23**, 14848–14859.

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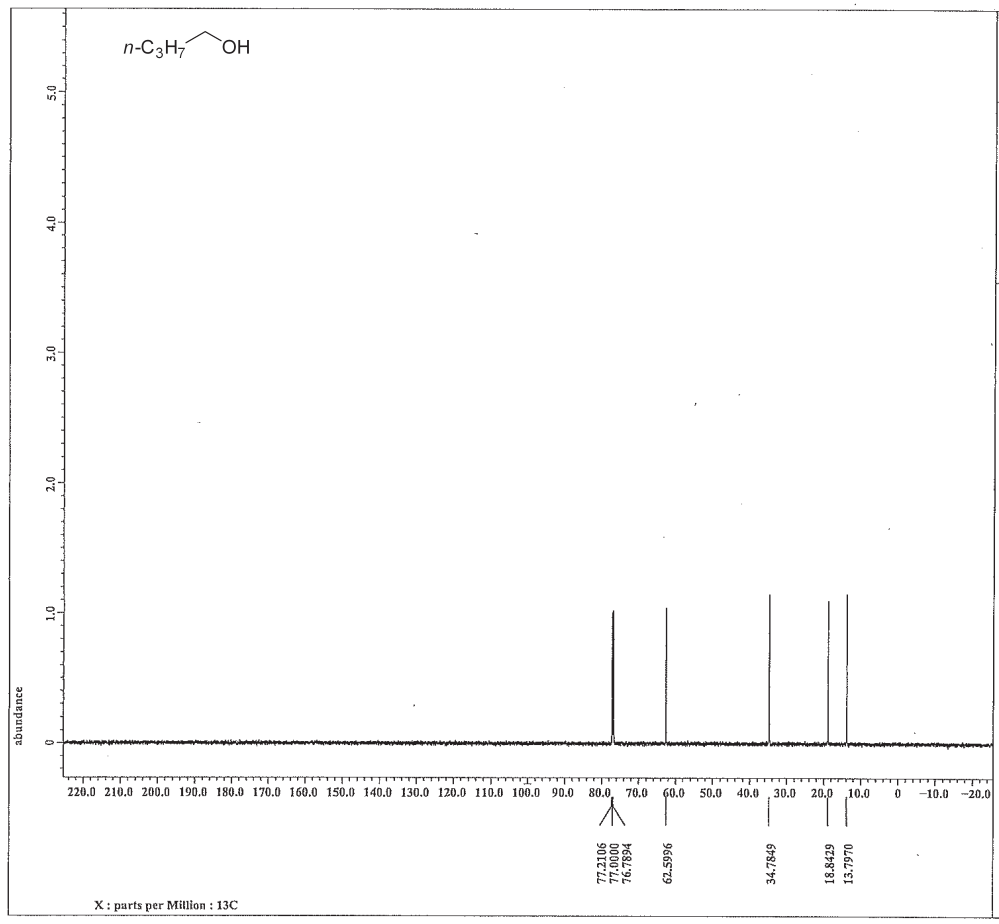


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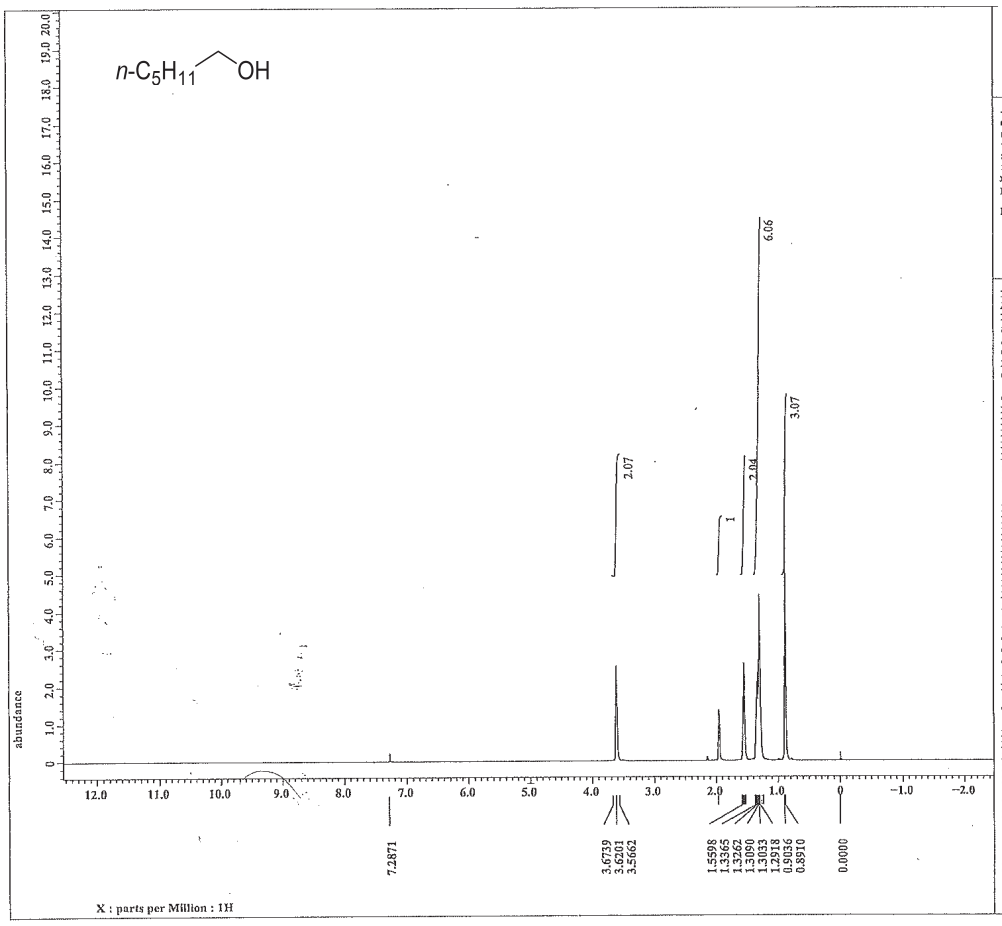


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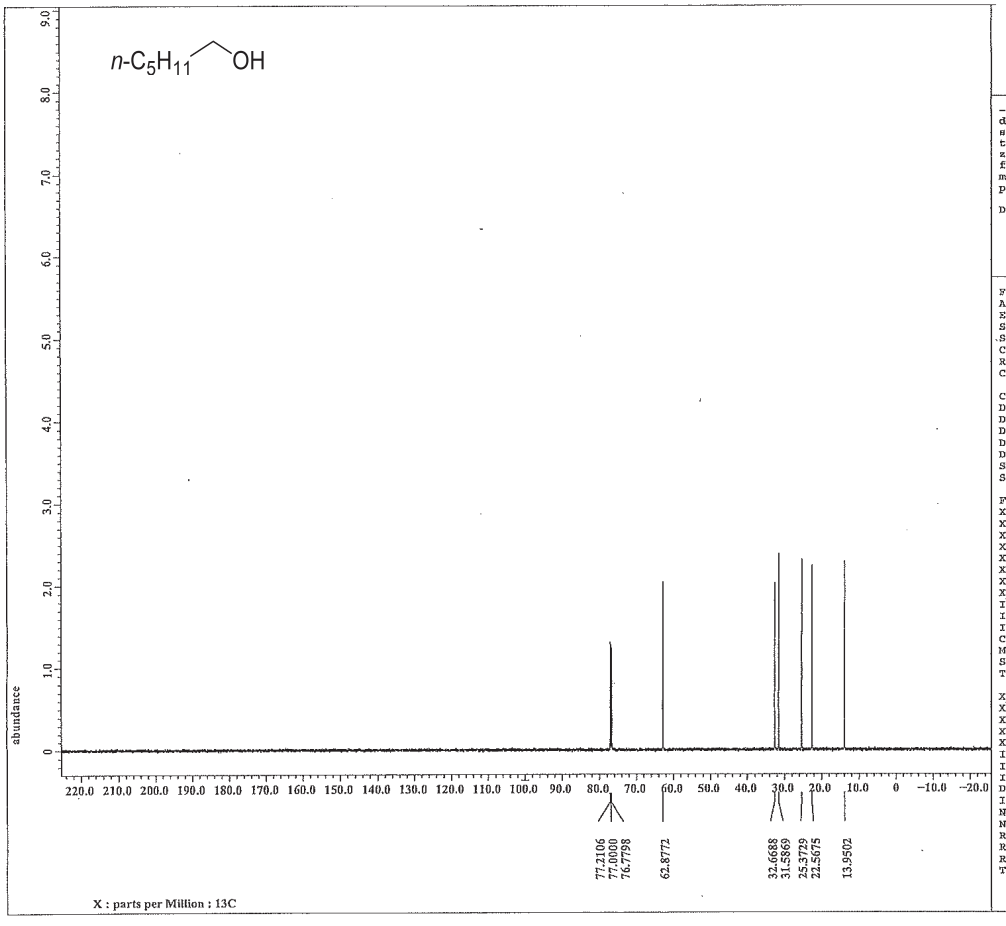


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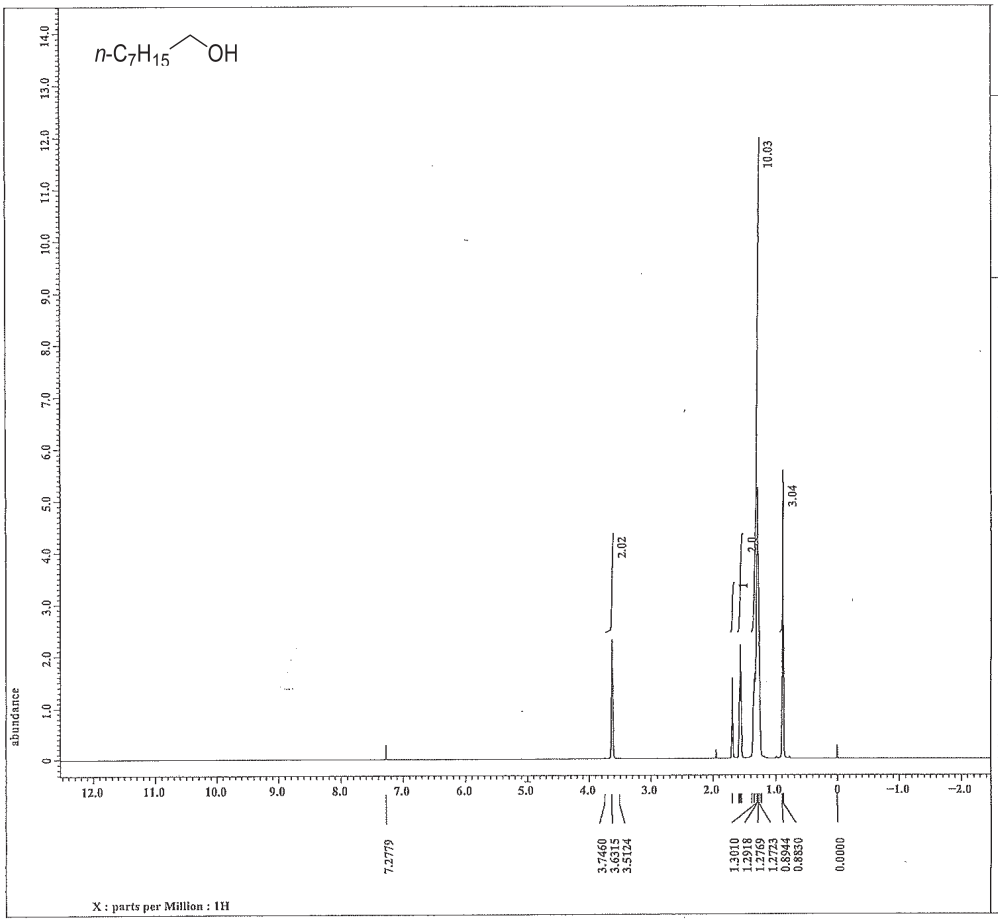


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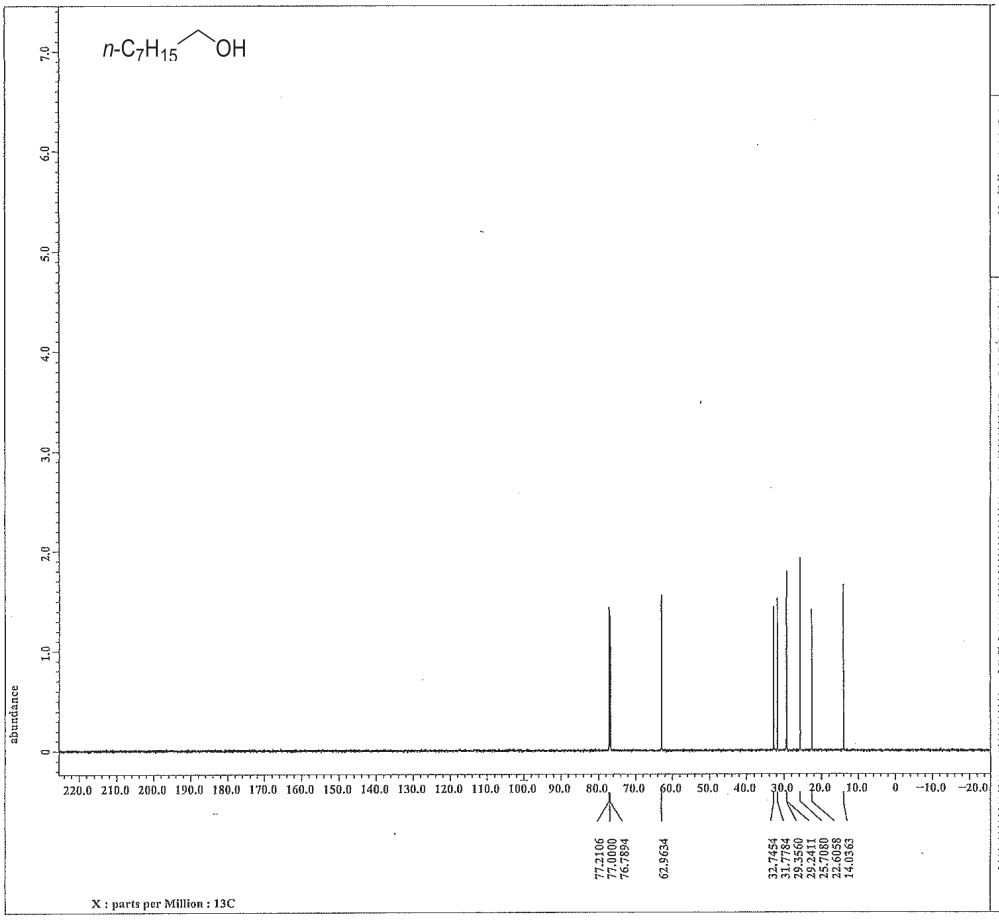


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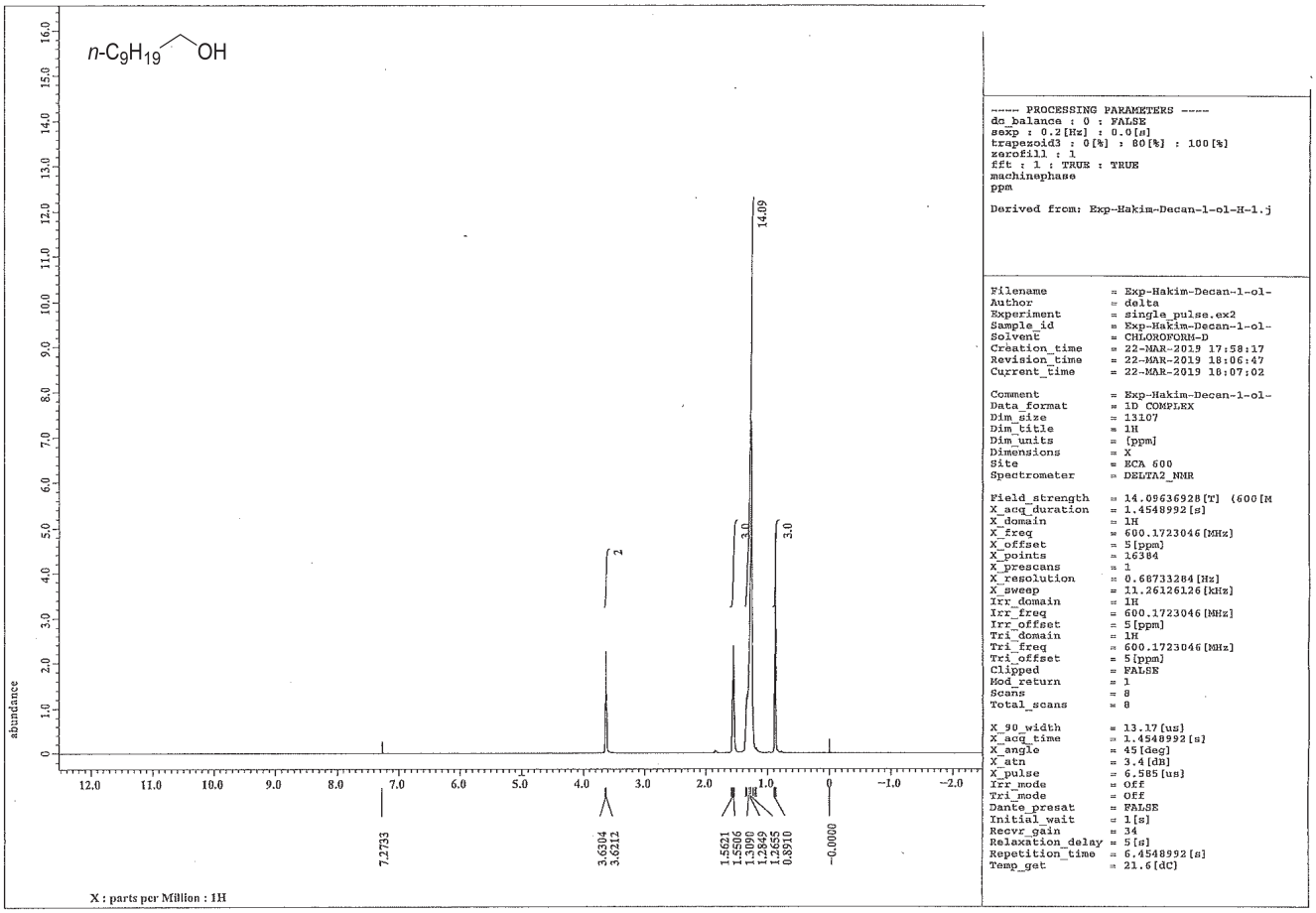
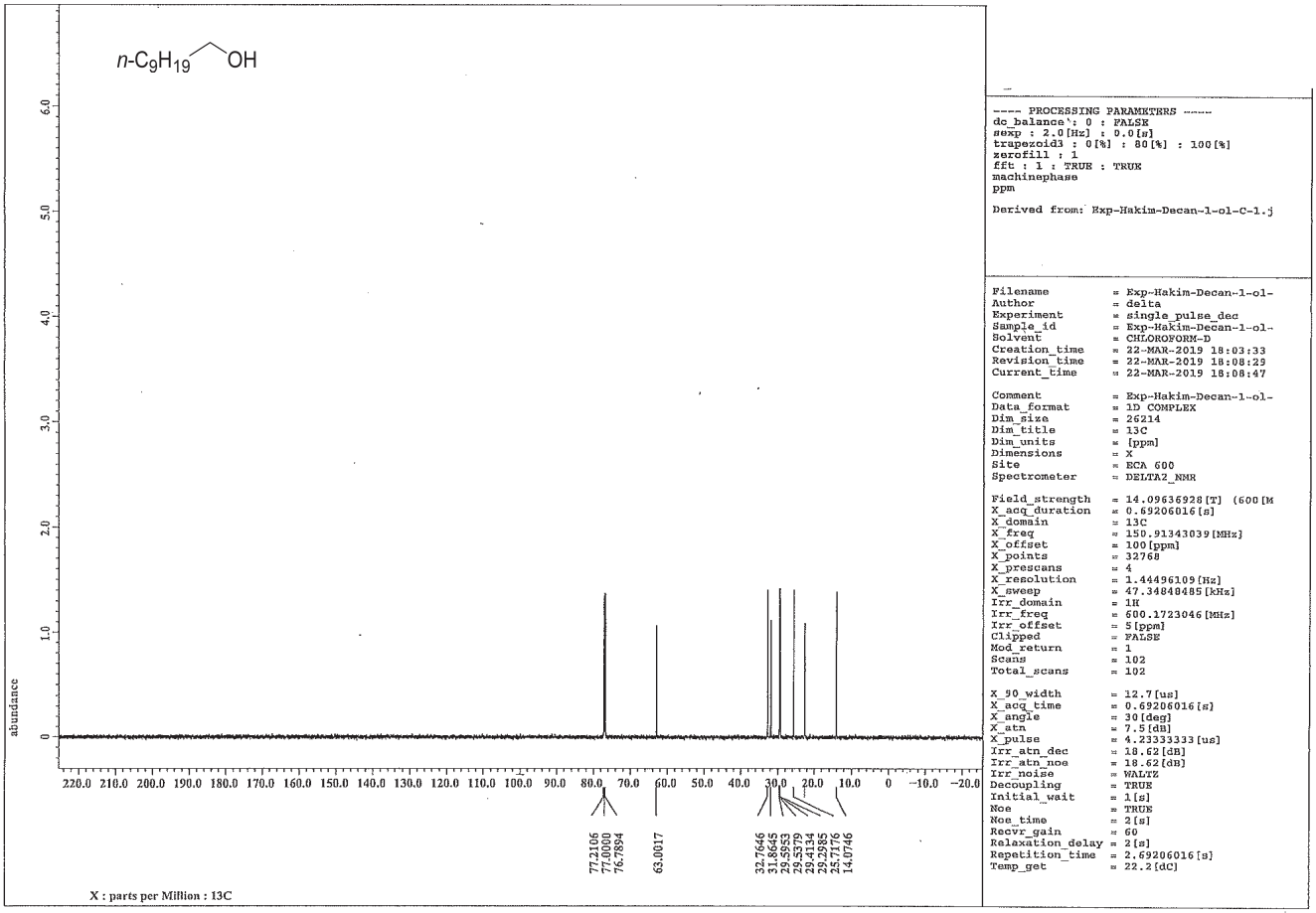
Current_time	= 22-MAR-2019 18:01:37
Comment	= Exp-Hakim-Octan-1-ol-
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 600
Spectrometer	= DELTA2_NMR
Field_strength	= 14.09636928[T] (600[M
X_acq_duration	= 0.69206016[s]
X_domain	= 13C
X_freq	= 150.91343039[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.44496109[Hz]
X_sweep	= 47.34848485[kHz]
Irr_domain	= 1H
Irr_freq	= 600.1723046[MHz]
Irr_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 232.0
Total_scans	= 232.0
X_90_width	= 12.7[us]
X_acq_time	= 0.69206016[s]
X_angle	= 30[deg]
X_atn	= 7.5[dB]
X_pulse	= 4.23333333[us]
Irr_atn_dec	= 18.62[dB]
Irr_atn_noe	= 18.62[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	= 2.69206016[s]
Temp_get	= 22.1[dC]




```
----- PROCESSING PARAMETERS -----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: Exp-Hakim-Decan-1-ol-H-1.j
```

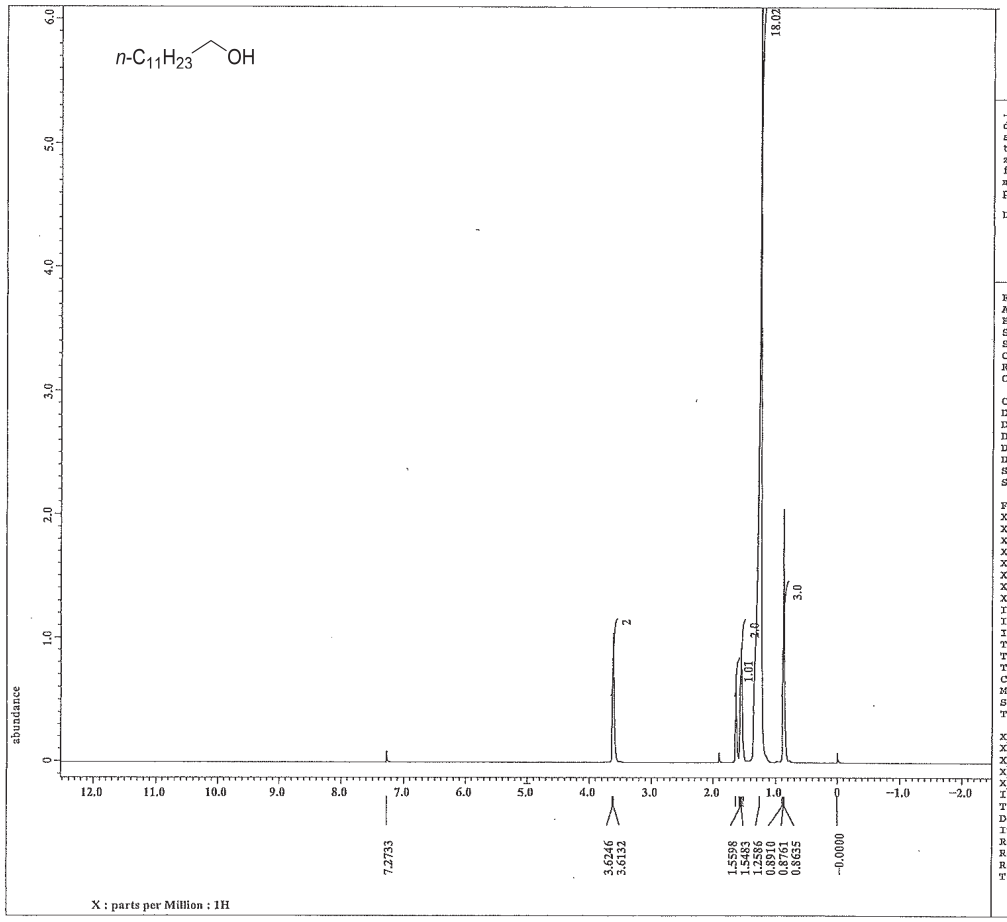
Filename	= Exp-Hakim-Decan-1-ol-
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= Exp-Hakim-Decan-1-ol-
Solvent	= CHLOROFORM-D
Creation_time	= 22-MAR-2019 17:58:17
Revision_time	= 22-MAR-2019 18:06:47
Current_time	= 22-MAR-2019 18:07:02
Comment	= Exp-Hakim-Decan-1-ol-
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 600
Spectrometer	= DELTA2_NMR
Field_strength	= 14.09636928[T] (600[M
X_acq_duration	= 1.4548992[s]
X_domain	= 1H
X_freq	= 600.1723046[MHz]
X_offset	= 5[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.68733284[Hz]
X_sweep	= 11.26126126[kHz]
Irr_domain	= 1H
Irr_freq	= 600.1723046[MHz]
Irr_offset	= 5[ppm]
Tri_domain	= 1H
Tri_freq	= 600.1723046[MHz]
Tri_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 8
Total_scans	= 8
X_90_width	= 13.17[us]
X_acq_time	= 1.4548992[s]
X_angle	= 45[deg]
X_atn	= 3.4[dB]
X_pulse	= 6.585[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 34
Relaxation_delay	= 5[s]
Repetition_time	= 6.4548992[s]
Temp_get	= 21.6[dC]




```
---- PROCESSING PARAMETERS -----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: Exp-Hakim-Decan-1-ol-C-1.j
```

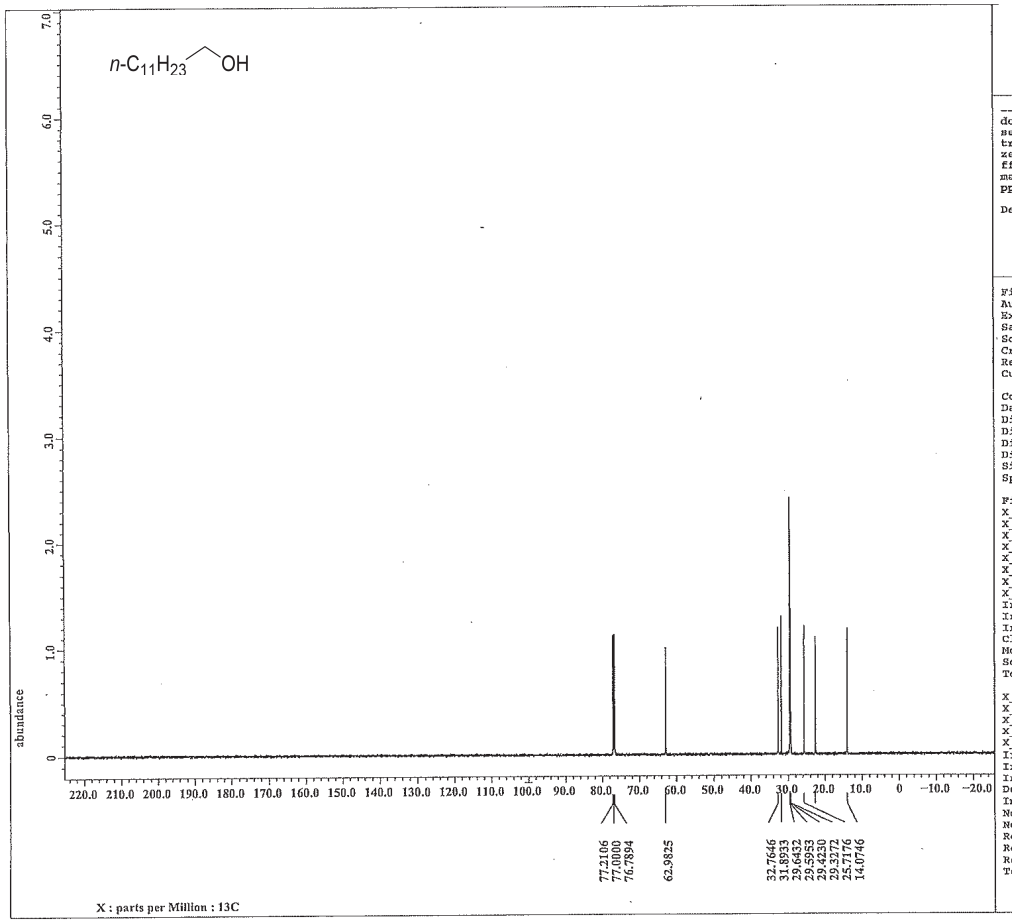
Filename	= Exp-Hakim-Decan-1-ol-
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= Exp-Hakim-Decan-1-ol-
Solvent	= CHLOROFORM-D
Creation_time	= 22-MAR-2019 18:03:33
Revision_time	= 22-MAR-2019 18:08:29
Current_time	= 22-MAR-2019 18:08:47
Comment	= Exp-Hakim-Decan-1-ol-
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 600
Spectrometer	= DELTA2_NMR
Field_strength	= 14.09636928[T] (600[M
X_acq_duration	= 0.69206016[s]
X_domain	= 13C
X_freq	= 150.91343039[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.44496109[Hz]
X_sweep	= 47.34840485[kHz]
Irr_domain	= 1H
Irr_freq	= 600.1723046[MHz]
Irr_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 102
Total_scans	= 102
X_90_width	= 12.7[us]
X_acq_time	= 0.69206016[s]
X_angle	= 30[deg]
X_atn	= 7.5[dB]
X_pulse	= 4.23333333[us]
Irr_atn_dec	= 18.62[dB]
Irr_atn_noe	= 18.62[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	= 2.69206016[s]
Temp_get	= 22.2[dC]




```
----- PROCESSING PARAMETERS -----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: Exp-Hakim-Dodecanol-H-1.jd
```

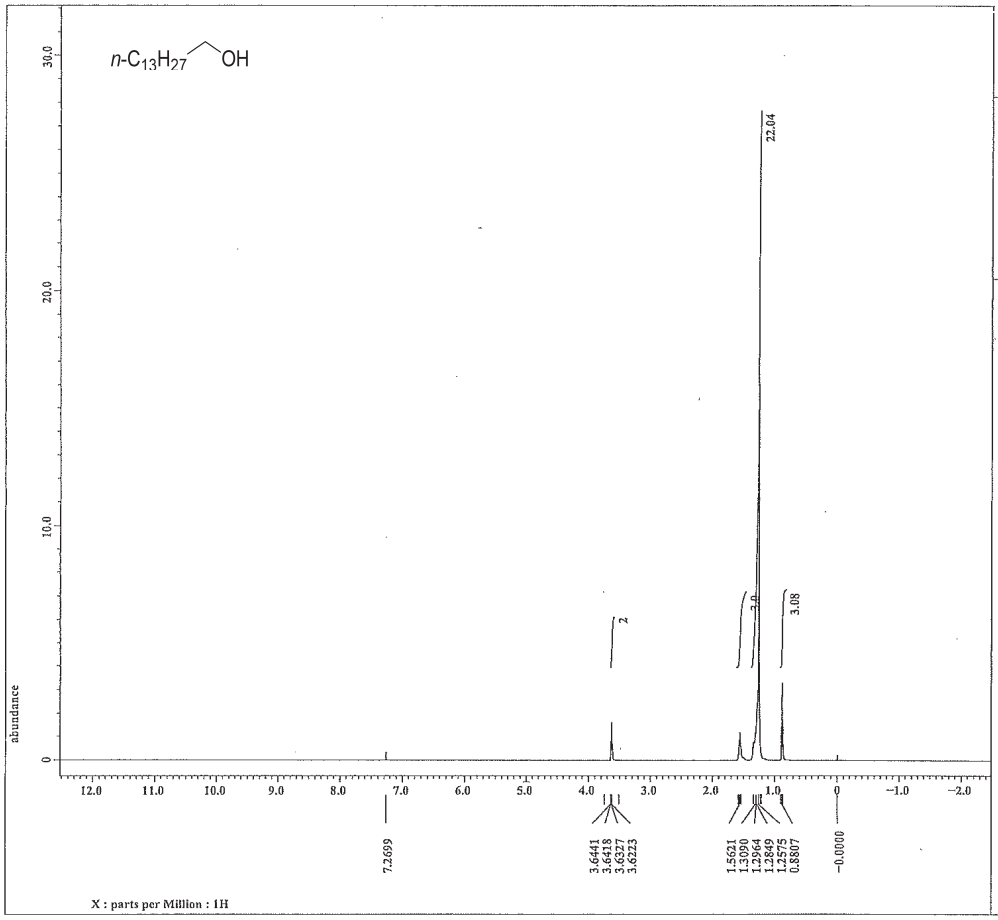
Filename	= Exp-Hakim-Dodecanol-H
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= Exp-Hakim-Dodecanol-H
Solvent	= CHLOROFORM-D
Creation_time	= 29-MAR-2019 11:10:50
Revision_time	= 29-MAR-2019 11:21:07
Current_time	= 29-MAR-2019 11:21:36
Comment	= Exp-Hakim-Dodecanol-H
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 600
Spectrometer	= DELTA2_NMR
Field_strength	= 14.09636928[T] (600[M
X_acq_duration	= 1.4548992[s]
X_domain	= 1H
X_freq	= 600.1723046[MHz]
X_offset	= 5[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.68733284[Hz]
X_sweep	= 11.26126126[kHz]
Irr_domain	= 1H
Irr_freq	= 600.1723046[MHz]
Irr_offset	= 5[ppm]
Tri_domain	= 1H
Tri_freq	= 600.1723046[MHz]
Tri_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 8
Total_scans	= 8
X_90_width	= 13.17[us]
X_acq_time	= 1.4548992[s]
X_angle	= 45[deg]
X_atn	= 3.4[dB]
X_pulse	= 6.585[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 30
Relaxation_delay	= 5[s]
Repetition_time	= 6.4548992[s]
Temp_get	= 21.5[dC]




```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: Exp-Hakim-Dodecanol-C-1.jd
```

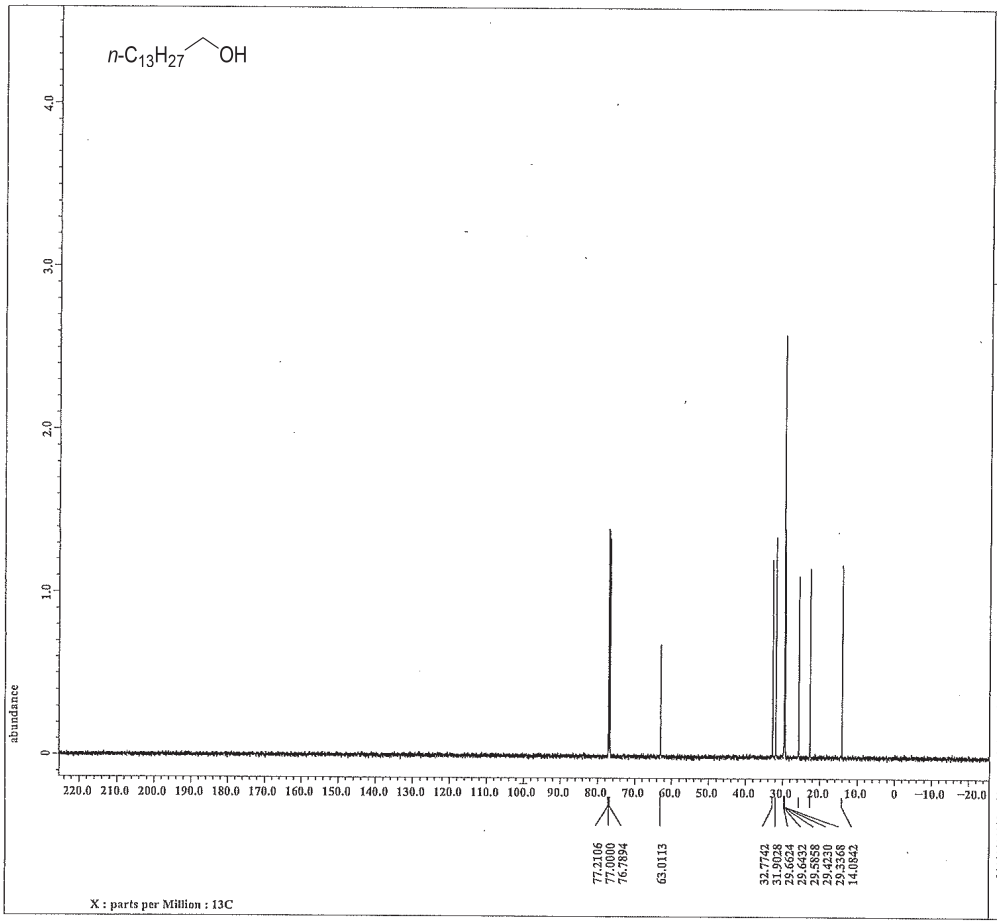
Filename	= Exp-Hakim-Dodecanol-C
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= Exp-Hakim-Dodecanol-C
Solvent	= CHLOROFORM-D
Creation_time	= 29-MAR-2019 11:25:53
Revision_time	= 29-MAR-2019 11:33:15
Current_time	= 29-MAR-2019 11:33:48
Comment	= Exp-Hakim-Dodecanol-C
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 600
Spectrometer	= DELTA2_NMR
Field_strength	= 14.09636928[T] (600[M
X_acq_duration	= 0.69206016[s]
X_domain	= 13C
X_freq	= 150.91343039[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.44496109[Hz]
X_sweep	= 47.34848485[kHz]
Irr_domain	= 1H
Irr_freq	= 600.1723046[MHz]
Irr_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 320
Total_scans	= 320
X_90_width	= 12.7[us]
X_acq_time	= 0.69206016[s]
X_angle	= 30[deg]
X_atn	= 7.5[dB]
X_pulse	= 4.23333333[us]
Irr_atn_dec	= 18.62[dB]
Irr_atn_noe	= 18.62[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	= 2.69206016[s]
Temp_get	= 22.2[dC]




```
----- PROCESSING PARAMETERS -----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: Exp-Hakim-Tetradecanol-H-1
```

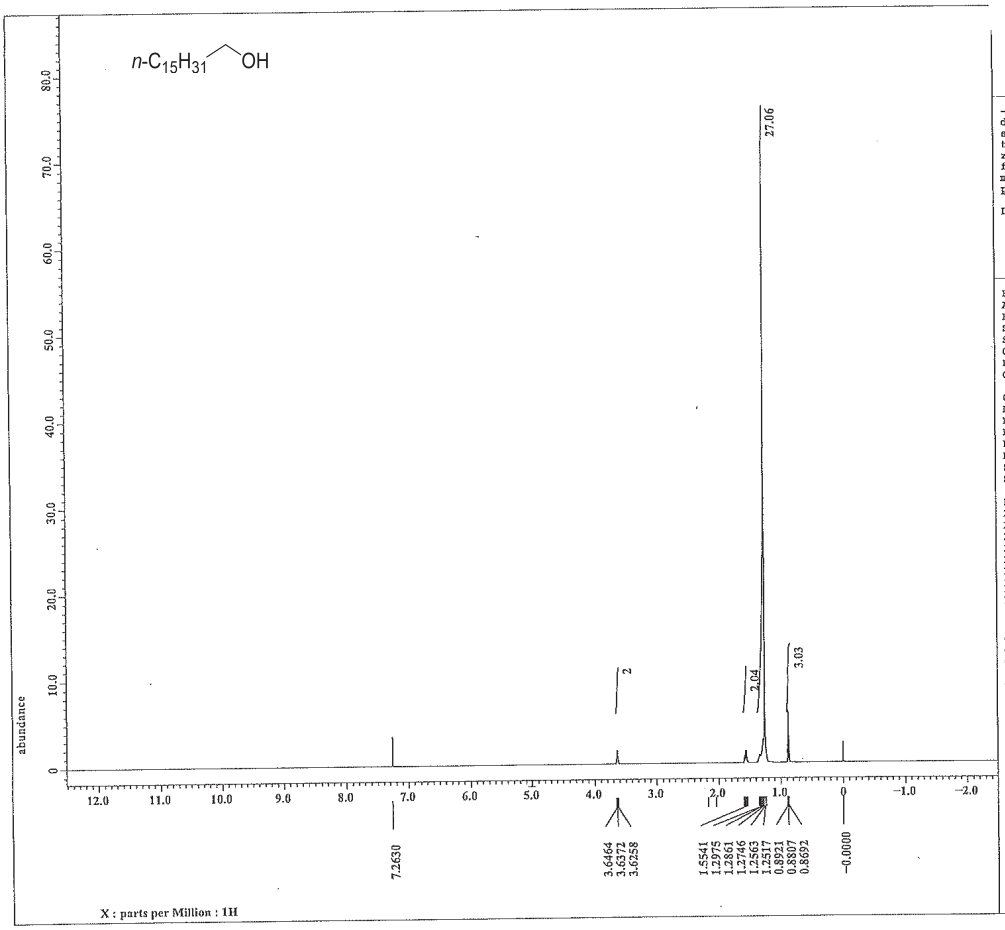
Filename	= Exp-Hakim-Tetradecano
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= Exp-Hakim-Tetradecano
Solvent	= CHLOROFORM-D
Creation_time	= 29-MAR-2019 11:32:46
Revision_time	= 29-MAR-2019 11:53:45
Current_time	= 29-MAR-2019 11:54:26
Comment	= Exp-Hakim-Tetradecano
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 600
Spectrometer	= DELTA2_NMR
Field_strength	= 14.09636928[T] (600[M
X_acq_duration	= 1.4548992[s]
X_domain	= 1H
X_freq	= 600.1723046[MHz]
X_offset	= 5[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.68733284[Hz]
X_sweep	= 11.26126126[kHz]
Irr_domain	= 1H
Irr_freq	= 600.1723046[MHz]
Irr_offset	= 5[ppm]
Tri_domain	= 1H
Tri_freq	= 600.1723046[MHz]
Tri_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 8
Total_scans	= 8
X_90_width	= 13.17[us]
X_acq_time	= 1.4548992[s]
X_angle	= 45[deg]
X_atn	= 3.4[dB]
X_pulse	= 6.585[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 30
Relaxation_delay	= 5[s]
Repetition_time	= 6.4548992[s]
Temp_get	= 21.6[dC]




```
----- PROCESSING PARAMETERS -----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: Exp-Hakim-Tetradecanol-C-1
```

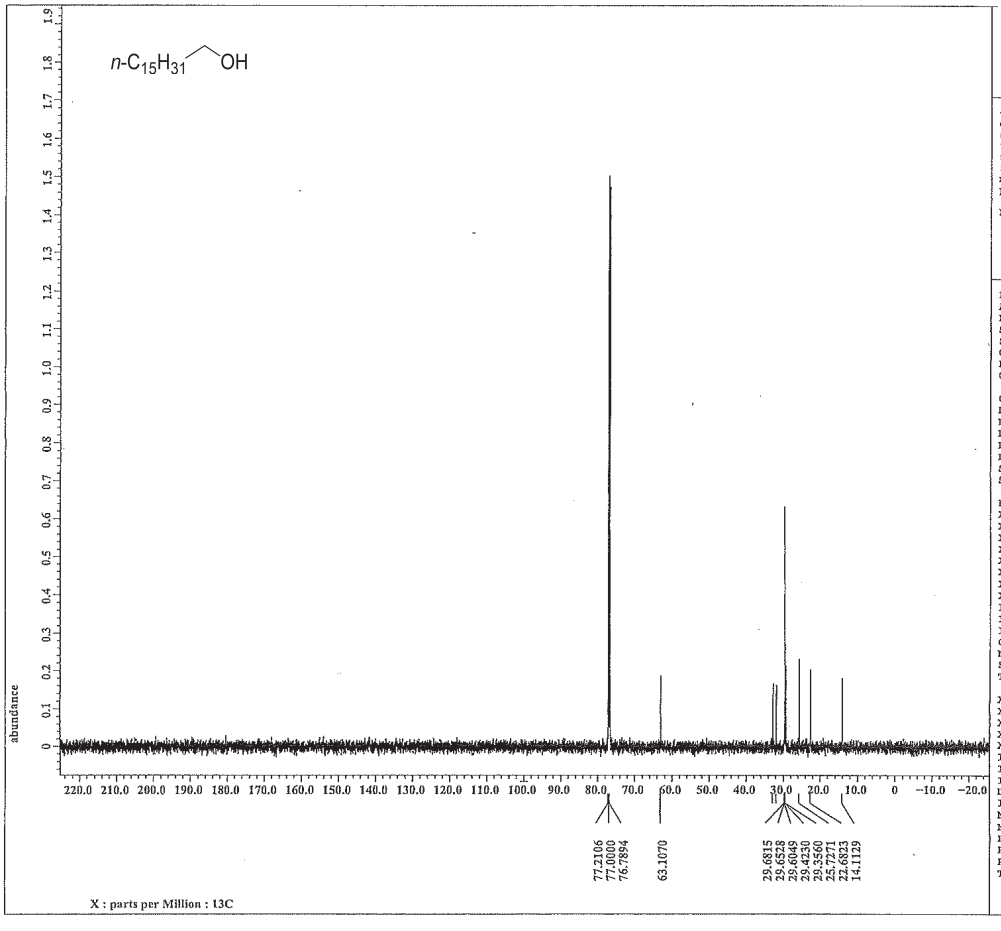
Filename	= Exp-Hakim-Tetradecano
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= Exp-Hakim-Tetradecano
Solvent	= CHLOROFORM-D
Creation_time	= 29-MAR-2019 11:42:11
Revision_time	= 29-MAR-2019 11:49:01
Current_time	= 29-MAR-2019 11:49:28
Comment	= Exp-Hakim-Tetradecano
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 600
Spectrometer	= DELTA2_NMR
Field_strength	= 14.09636928[T] (600[M
X_acq_duration	= 0.69206016[s]
X_domain	= 13C
X_freq	= 150.91343039[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.44496109[Hz]
X_sweep	= 47.34848485[kHz]
Irr_domain	= 1H
Irr_freq	= 600.1723046[MHz]
Irr_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 194
Total_scans	= 194
X_90_width	= 12.7[us]
X_acq_time	= 0.69206016[s]
X_angle	= 30[deg]
X_atn	= 7.5[dB]
X_pulse	= 4.23333333[us]
Irr_atn_dec	= 18.62[dB]
Irr_atn_noe	= 18.62[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	= 2.69206016[s]
Temp_get	= 22.1[dC]




```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: Exp-Hakim-Hexaadecanol-H-1
```

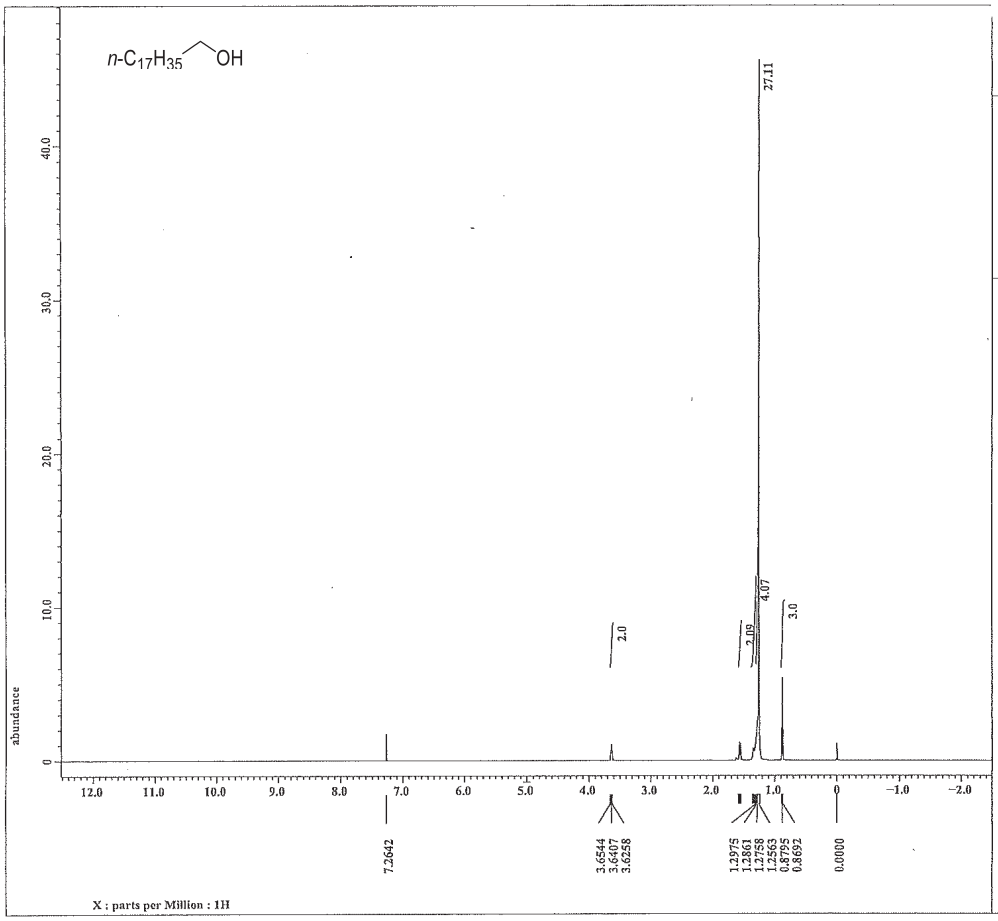
Filename	= Exp-Hakim-Hexaadecano
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= Exp-Hakim-Hexaadecano
Solvent	= CHLOROFORM-D
Creation_time	= 29-MAR-2019 11:49:01
Revision_time	= 29-MAR-2019 11:57:57
Current_time	= 29-MAR-2019 11:58:15
Comment	= Exp-Hakim-Hexaadecano
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 600
Spectrometer	= DELTA2_NMR
Field_strength	= 14.09636928[T] (600[M
X_acq_duration	= 1.4548992[s]
X_domain	= 1H
X_freq	= 600.1723046[MHz]
X_offset	= 5[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.68733284[Hz]
X_sweep	= 11.26126126[kHz]
Irr_domain	= 1H
Irr_freq	= 600.1723046[MHz]
Irr_offset	= 5[ppm]
Tri_domain	= 1H
Tri_freq	= 600.1723046[MHz]
Tri_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 8
Total_scans	= 8
X_90_width	= 13.17[us]
X_acq_time	= 1.4548992[s]
X_angle	= 45[deg]
X_atn	= 3.4[dB]
X_pulse	= 6.585[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 46
Relaxation_delay	= 5[s]
Repetition_time	= 6.4548992[s]
Temp_get	= 21.6[dC]




```
------ PROCESSING PARAMETERS ------
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: Exp-Hakim-Hexaadecanol-C-1
```

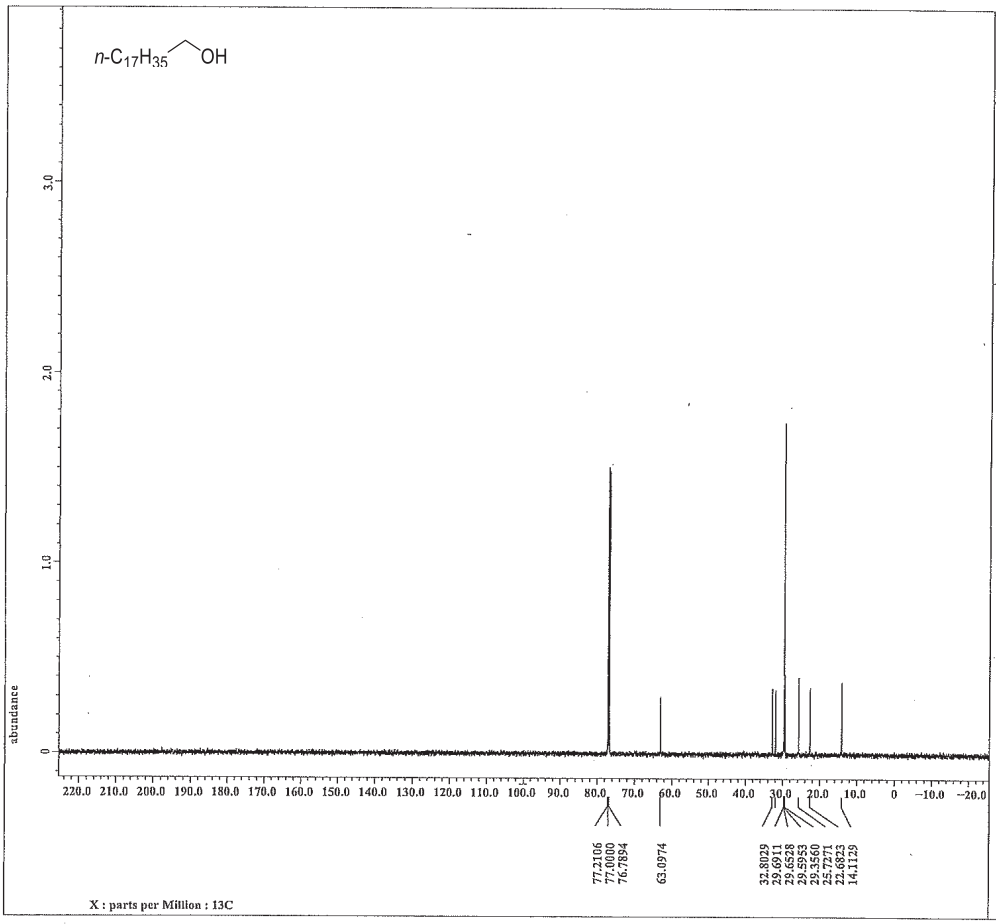
Filename	= Exp-Hakim-Hexaadecano
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= Exp-Hakim-Hexaadecano
Solvent	= CHLOROFORM-D
Creation_time	= 29-MAR-2019 11:54:55
Revision_time	= 29-MAR-2019 12:02:31
Current_time	= 29-MAR-2019 12:02:57
Comment	= Exp-Hakim-Hexaadecano
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 600
Spectrometer	= DELTA2_NMR
Field_strength	= 14.09636928[T] (600[M
X_acq_duration	= 0.69206016[s]
X_domain	= 13C
X_freq	= 150.91343039[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.44496109[Hz]
X_sweep	= 47.34848485[kHz]
Irr_domain	= 1H
Irr_freq	= 600.1723046[MHz]
Irr_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 115.0
Total_scans	= 115.0
X_90_width	= 12.7[us]
X_acq_time	= 0.69206016[s]
X_angle	= 30[deg]
X_atn	= 7.5[dB]
X_pulse	= 4.23333333[us]
Irr_atn_dec	= 18.62[dB]
Irr_atn_noe	= 18.62[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	= 2.69206016[s]
Temp_get	= 22.1[dC]




```
------ PROCESSING PARAMETERS ------
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: Exp-Hakim-Octadecanol-H-1.
```

Filename	= Exp-Hakim-Octadecanol
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= Exp-Hakim-Octadecanol
Solvent	= CHLOROFORM-D
Creation_time	= 29-MAR-2019 12:01:45
Revision_time	= 29-MAR-2019 12:15:26
Current_time	= 29-MAR-2019 12:15:41
Comment	= Exp-Hakim-Octadecanol
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 600
Spectrometer	= DELTA2_NMR
Field_strength	= 14.09636928[T] (600[M
X_acq_duration	= 1.4548992[s]
X_domain	= 1H
X_freq	= 600.1723046[MHz]
X_offset	= 5[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.68733284[Hz]
X_sweep	= 11.26126126[kHz]
Irr_domain	= 1H
Irr_freq	= 600.1723046[MHz]
Irr_offset	= 5[ppm]
Tri_domain	= 1H
Tri_freq	= 600.1723046[MHz]
Tri_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 8
Total_scans	= 8
X_90_width	= 13.17[us]
X_acq_time	= 1.4548992[s]
X_angle	= 45[deg]
X_atn	= 3.4[dB]
X_pulse	= 6.585[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 40
Relaxation_delay	= 5[s]
Repetition_time	= 6.4548992[s]
Temp_get	= 21.4[dC]




```
------ PROCESSING PARAMETERS ------
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: Exp-Hakim-Octadecanol-C-1.
```

Filename	= Exp-Hakim-Octadecanol
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= Exp-Hakim-Octadecanol
Solvent	= CHLOROFORM-D
Creation_time	= 29-MAR-2019 12:12:00
Revision_time	= 29-MAR-2019 12:16:56
Current_time	= 29-MAR-2019 12:17:29
Comment	= Exp-Hakim-Octadecanol
Data_format	= 1D COMPLEX
Dim_size	= 262144
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 600
Spectrometer	= DELTA2_NMR
Field_strength	= 14.09636928[T] (600[M
X_acq_duration	= 0.69206016[s]
X_domain	= 13C
X_freq	= 150.91343039[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 1.44496109[Hz]
X_sweep	= 47.34848485[kHz]
Irr_domain	= 1H
Irr_freq	= 600.1723046[MHz]
Irr_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 213
Total_scans	= 213
X_90_width	= 12.7[us]
X_acq_time	= 0.69206016[s]
X_angle	= 30[deg]
X_atn	= 7.5[dB]
X_pulse	= 4.23333333[us]
Irr_atn_dec	= 18.62[dB]
Irr_atn_noe	= 18.62[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	= 2.69206016[s]
Temp_get	= 22.1[dC]