Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

Umpolung Cyclization Reaction of *N*-Cinnamoylthioureas in the Presence of DBU

Rei Saito,[a] Naohiro Uemura,[a] Hiroki Ishikawa,[a] Akina Magara,[a] Yasushi Yoshida,[a,b] Takashi Mino,[a,b] Yoshio Kasashima,[c] and Masami Sakamoto*[a,b]

[a]Department of Applied Chemistry and Biotechnology, Graduate School of Engineering, Yayoi-cho, Inage-ku, Chiba 265-8522, Japan
[b]Molecular Chirality Research Center, Yayoi-cho, Inage-ku, Chiba 265-8522, Japan
[c]Education Center, Faculty of Creative Engineering, Chiba Institute of Technology, Shibazono, Narashino, Chiba 275-0023, Japan.

Contents

General.

NMR spectra were recorded in $CDCl_3$ solutions on Bruker 300 and 400 spectrometers for ^{1}H- and ^{13}C-NMR. Chemical shifts are reported in parts per million (ppm) relative to TMS as an internal standard. IR spectra were recorded on a JASCO FT/IR-230 spectrometer. High-resolution mass spectra (HRMS) were performed on an Orbitrap ThermoFisher Exactive ion trap mass spectrometer. X-ray single crystallographic analysis was conducted using a SMART APEX II (Bruker AXS) and APEX II ULTRA (Bruker AXS). Commercially available reagents and solvents were used without further purification.

Single crystal X-Ray crystallographic analysis of 2h (CCDC 1859352)

Colorless prism (0.20 x 0.10 x 0.05 mm^3), monoclinic space group $P2_1/c$, a = 12.8458(5) Å, b = 5.3427(2) Å, c = 24.6144(10) Å, β = 101.767(3) °, V = 1653.82(11) $Å^3$, Z = 4, λ (CuKα) = 1.54178 Å, ρ = 1.303 g/cm^3, μ (CuKα) = 1.776 mm^{-1}, 10898 reflections measured (T = 173 K, 3.514 ° < θ < 68.341 °) , nb of independent data collected: 3012, nb of independent data used for refinement: 2264 in the final least-squares refinement cycles on F^2, the model converged at R_1 = 0.0495, wR_2 = 0.1324 [I > 2s(I)], R_1 = 0.0696, wR_2 = 0.1416 (all data), and GOF = 1.007, H-atom parameters constrained.

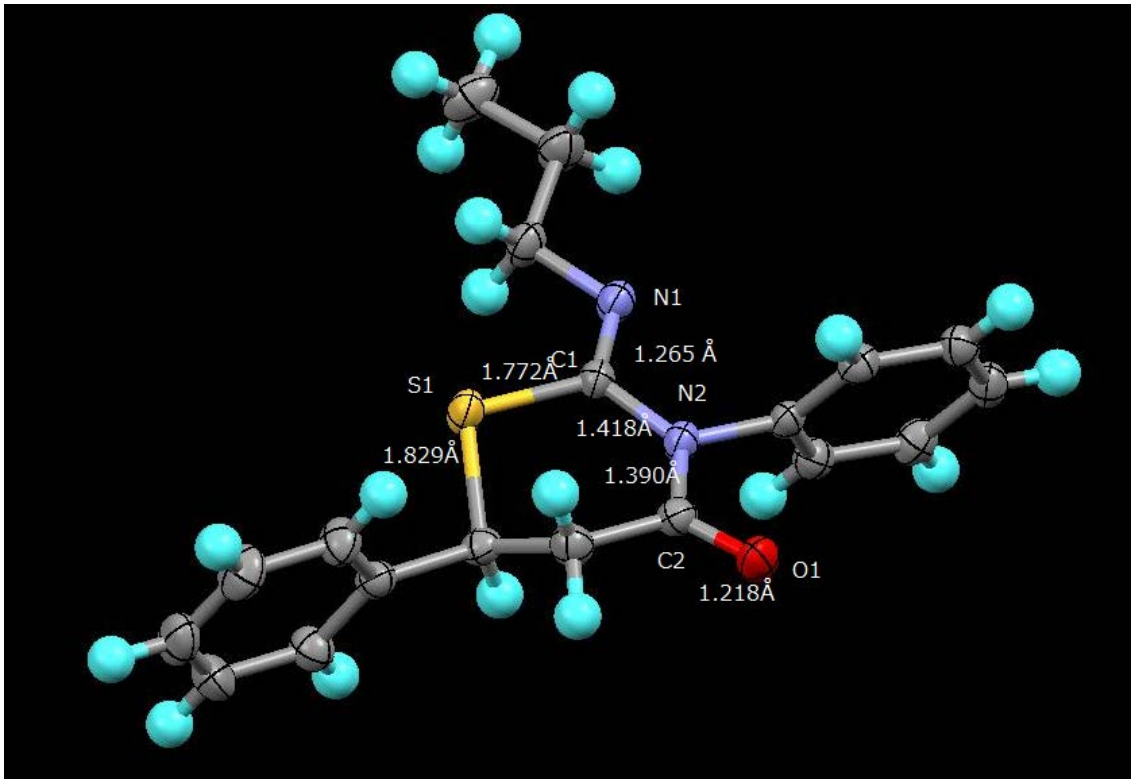


Figure S1. Perspective view of **2h**. Ellipsoids were drawn in 50% probability. Tortional angles: S-C1-N1-C2: 4.09 °, S-C1-N2-C2: 11.13 °, C1-N2-C1-O1: 5.29 °, C2-N1-C1-N1: 11.5 °.

Single crystal X-Ray structure analysis of 2i (CCDC 1859353)

Colorless prism (0.20 x 0.05 x 0.05 mm^3), monoclinic space group $P2_1/c$, a = 13.0104(7) Å, b = 5.4301(3) Å, c = 24.2997(15) Å, β = 101.772(4) °, V = 1680.61(17) $Å^3$, Z = 4, λ (CuKα) = 1.54178 Å, ρ = 1.282 g/cm^3, μ (CuKα) = 1.747 mm^{-1}, 11611 reflections measured (T = 173 K, 3.470 ° < θ < 68.239 °) , nb of independent data collected: 3051, nb of independent data used for refinement: 2600 in the final least-squares refinement cycles on F^2, the model converged at R_1 = 0.0468, wR_2 = 0.1307 [I > 2s(I)], R_1 = 0.0545, wR_2 = 0.1367 (all data), and GOF = 1.029, H-atom parameters constrained.

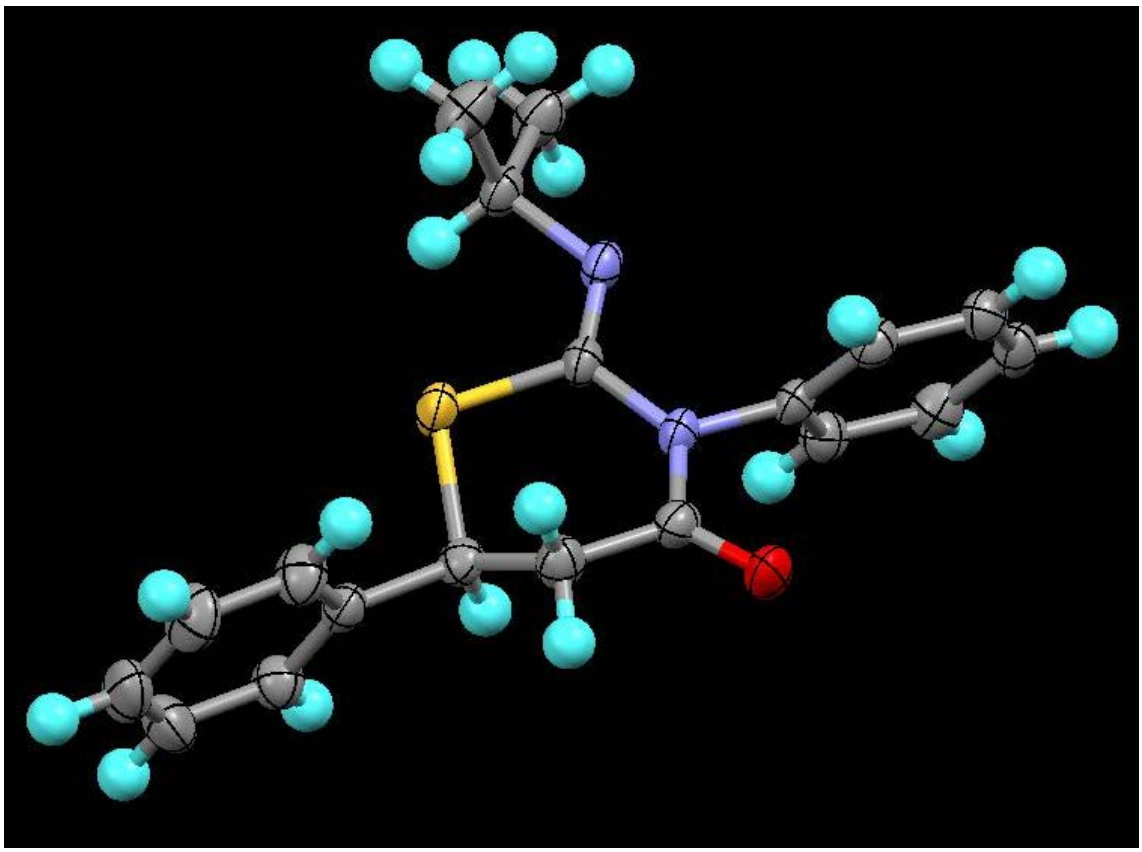


Figure S2. Perspective view of **2i**. Ellipsoids were drawn in 50% probability.

Single crystal X-Ray structure analysis of 2j (CCDC 1859354)

Colorless prism (0.50 x 0.20 x 0.10 mm^3), monoclinic space group $P2_1/c$, a = 13.613(2) Å, b = 5.3251(9) Å, c = 26.026(4) Å, β = 95.958(3) °, V = 1876.4(6) $Å^3$, Z = 4, λ (MoKα) = 0.71073 Å, ρ = 1.318 g/cm^3, μ (MoKα) = 0.188 mm^{-1}, 10165 reflections measured (T = 173 K, 1.504 ° < θ < 27.502 °) , nb of independent data collected: 4244, nb of independent data used for refinement: 2649 in the final least-squares refinement cycles on F^2, the model converged at R_1 = 0.0521, wR_2 = 0.1235 [I > 2s(I)], R_1 = 0.0974, wR_2 = 0.1579 (all data), and GOF = 0.966, H-atom parameters constrained.

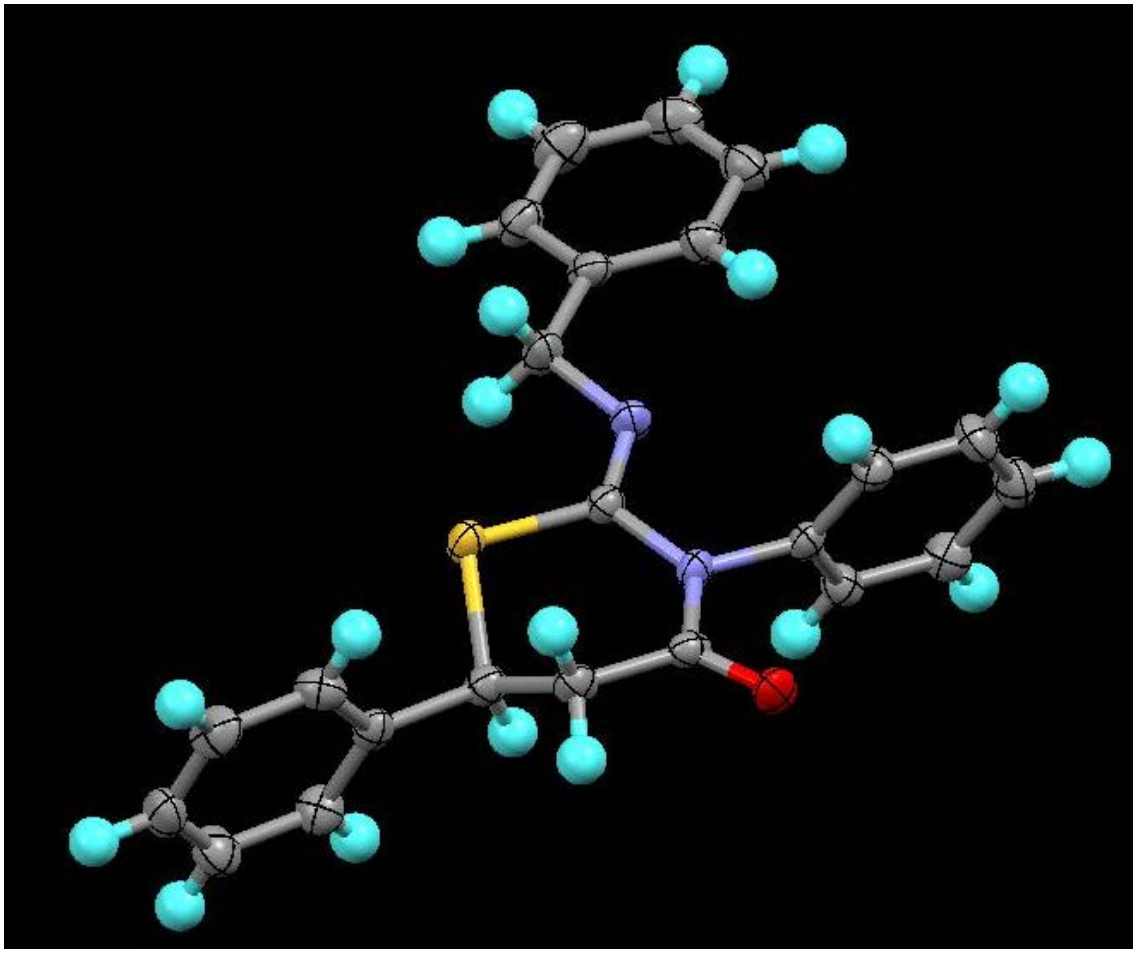


Figure S3. Perspective view of **2j**. Ellipsoids were drawn in 50% probability.

Single crystal X-Ray structure analysis of 3i (CCDC 1859407)

Colorless prism (0.30 x 0.20 x 0.10 mm^3), monoclinic space group $P2_1/c$, a = 12.4130(15) Å, b = 17.816(2) Å, c = 7.9085(10) Å, β = 106.841(2) °, V = 1674.0(4) $Å^3$, Z = 4, λ (MoKα) = 0.71073 Å, ρ = 1.287 g/cm^3, μ (MoKα) = 0.199 mm^{-1}, 9554 reflections measured (T = 173 K, 2.5558 ° < □ < 27.5219 °) , nb of independent data collected: 3838, nb of independent data used for refinement: 2379 in the final least-squares refinement cycles on F^2, the model converged at R_1 = 0.0512, wR_2 = 0.1170 [I > 2s(I)], R_1 = 0.0924, wR_2 = 0.1447 (all data), and GOF = 0.929, H-atom parameters constrained.

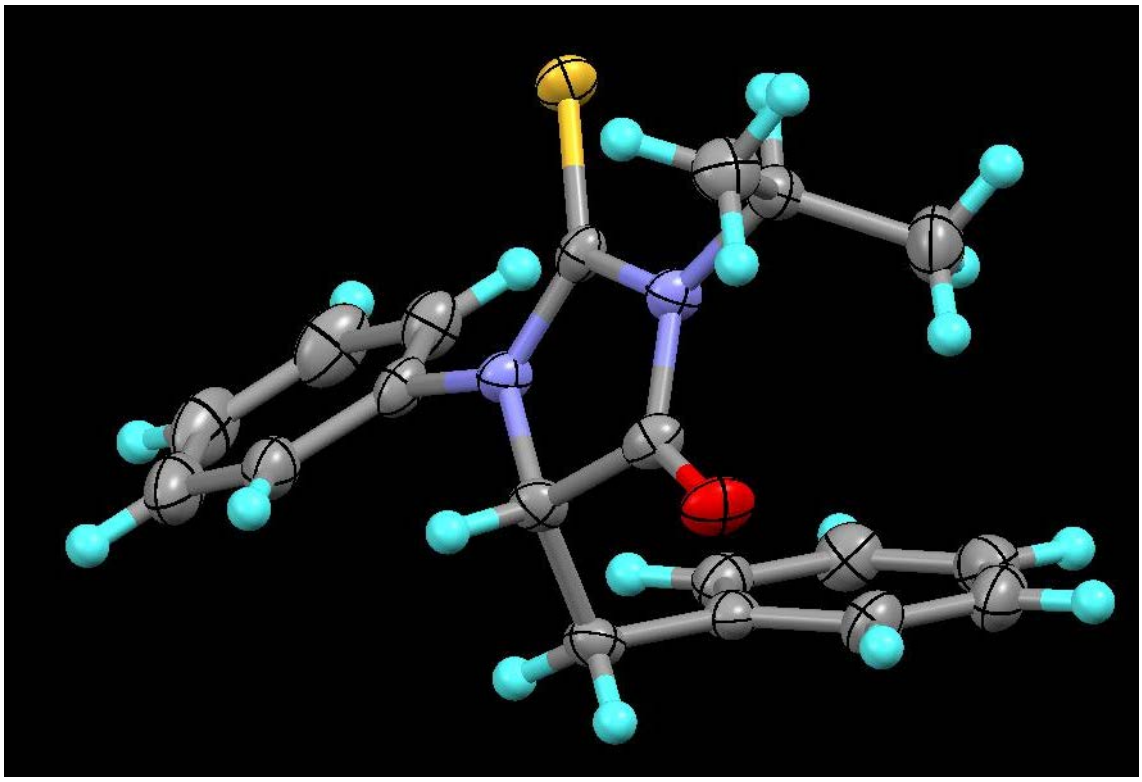


Figure S4. Perspective view of **3i**. Ellipsoids were drawn in 50% probability.

Single crystal X-Ray structure analysis of 3j (CCDC 1859355)

Colorless prism (0.50 x 0.50 x 0.10 mm^3), triclinic space group *P*-1, *a* = 8.887(2) Å, *b* = 9.348(2) Å, *c* = 12.182(3) Å, α = 80.025(3) °, β = 72.125(3) °, γ = 88.273(3) °, *V* = 948.3(4) $Å^3$, *Z* = 2, λ (MoKα) = 0.71073 Å, ρ = 1.304 g/cm^3, μ (MoKα) = 0.186 mm^{-1}, 5472 reflections measured (T = 173 K, 2.2128 ° < θ < 27.5491 °) , nb of independent data collected: 4141, nb of independent data used for refinement: 3585 in the final least-squares refinement cycles on F^2, the model converged at R_1 = 0.0365 wR_2 = 0.0914 [I > 2s(I)], R_1 = 0.0429, wR_2 = 0.0954 (all data), and GOF = 1.065, H-atom parameters constrained.

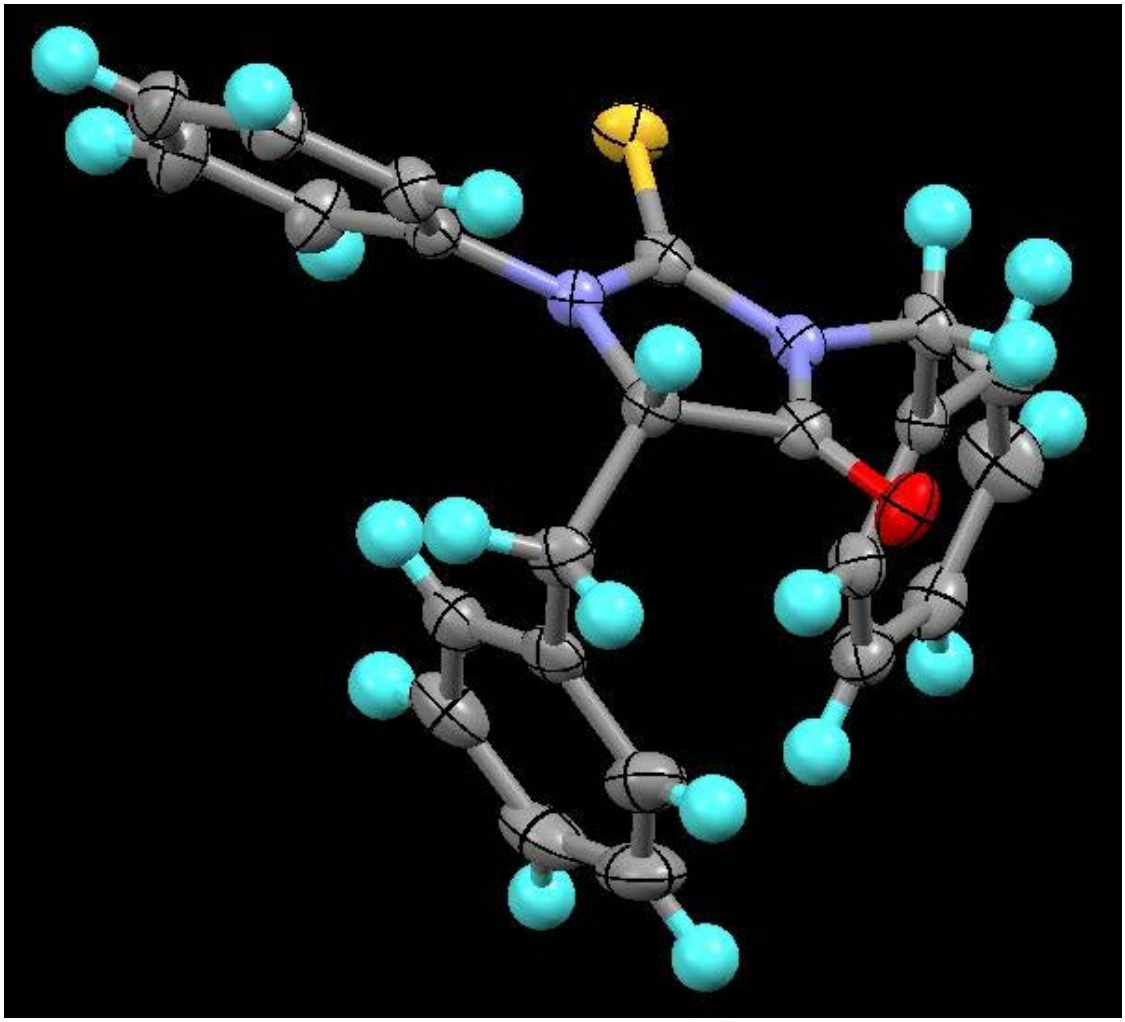


Figure S5. Perspective view of **3j**. Ellipsoids were drawn in 50% probability.

Single crystal X-Ray structure analysis of 4g (CCDC 1859357)

Colorless prism (0.50 x 0.50 x 0.10 mm^3), monoclinic space group *C*2/c, *a* = 34.665(4) Å, *b* = 6.9265(9) Å, *c* = 14.4146(18) Å, β = 113.1370(10) °, *V* = 3182.7(7) $Å^3$, *Z* = 8, λ (MoKα) = 0.71073 Å, ρ = 1.296 g/cm^3, μ (MoKα) = 0.207 mm^{-1}, 17622 reflections measured (T = 173 K, 2.5558 ° < θ < 27.5219 °) , nb of independent data collected: 3651, nb of independent data used for refinement: 3146 in the final least-squares refinement cycles on F^2, the model converged at R_1 = 0.0310, wR_2 = 0.0789 [$I > 2s(I)$], R_1 = 0.0380, wR_2 = 0.0871 (all data), and GOF = 1.042, H-atom parameters constrained.

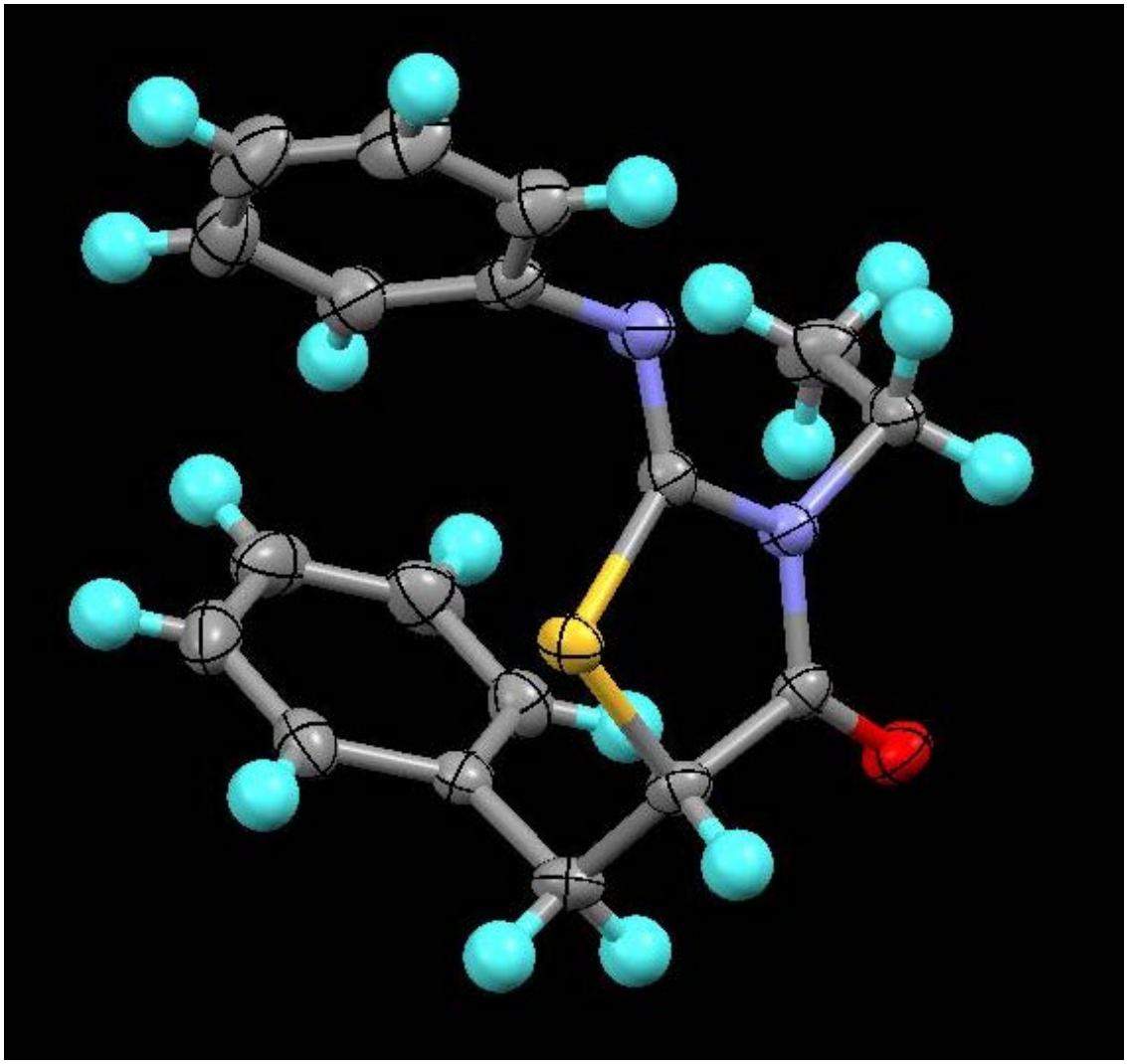


Figure S6. Perspective view of **4g**. Ellipsoids were drawn in 50% probability.

Single crystal X-Ray structure analysis of 5c (CCDC 1859359)

Colorless prism (0.40 x 0.30 x 0.10 mm^3), triclinic space group *P*-1, *a* = 8.7745(14) Å, *b* = 9.4352(16) Å, *c* = 20.409(3) Å, α = 93.504(2) °, β = 97.479(2) °, γ = 90.918(2) °, *V* = 1671.6(5) $Å^3$, *Z* = 4, λ (MoKα) = 0.71073 Å, ρ = 1.218 g/cm^3, μ (MoKα) = 0.200 mm^{-1}, 9602 reflections measured (T = 173 K, 2.1632 ° < θ < 23.5028 °) , nb of independent data collected: 7319, nb of independent data used for refinement: 4764 in the final least-squares refinement cycles on F^2, the model converged at R_1 = 0.0538, wR_2 = 0.1302 [I > 2s(I)], R_1 = 0.0851, wR_2 = 0.1602 (all data), and GOF = 0.999, H-atom parameters constrained.

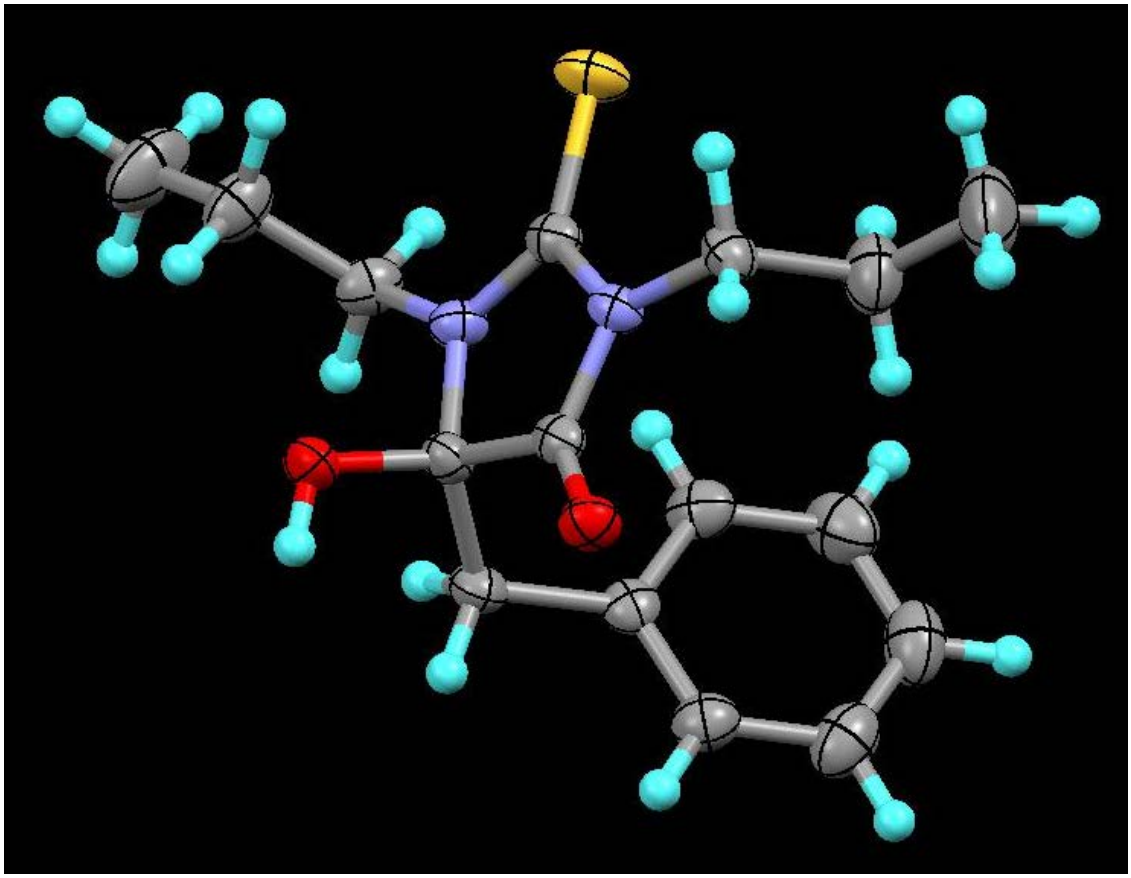
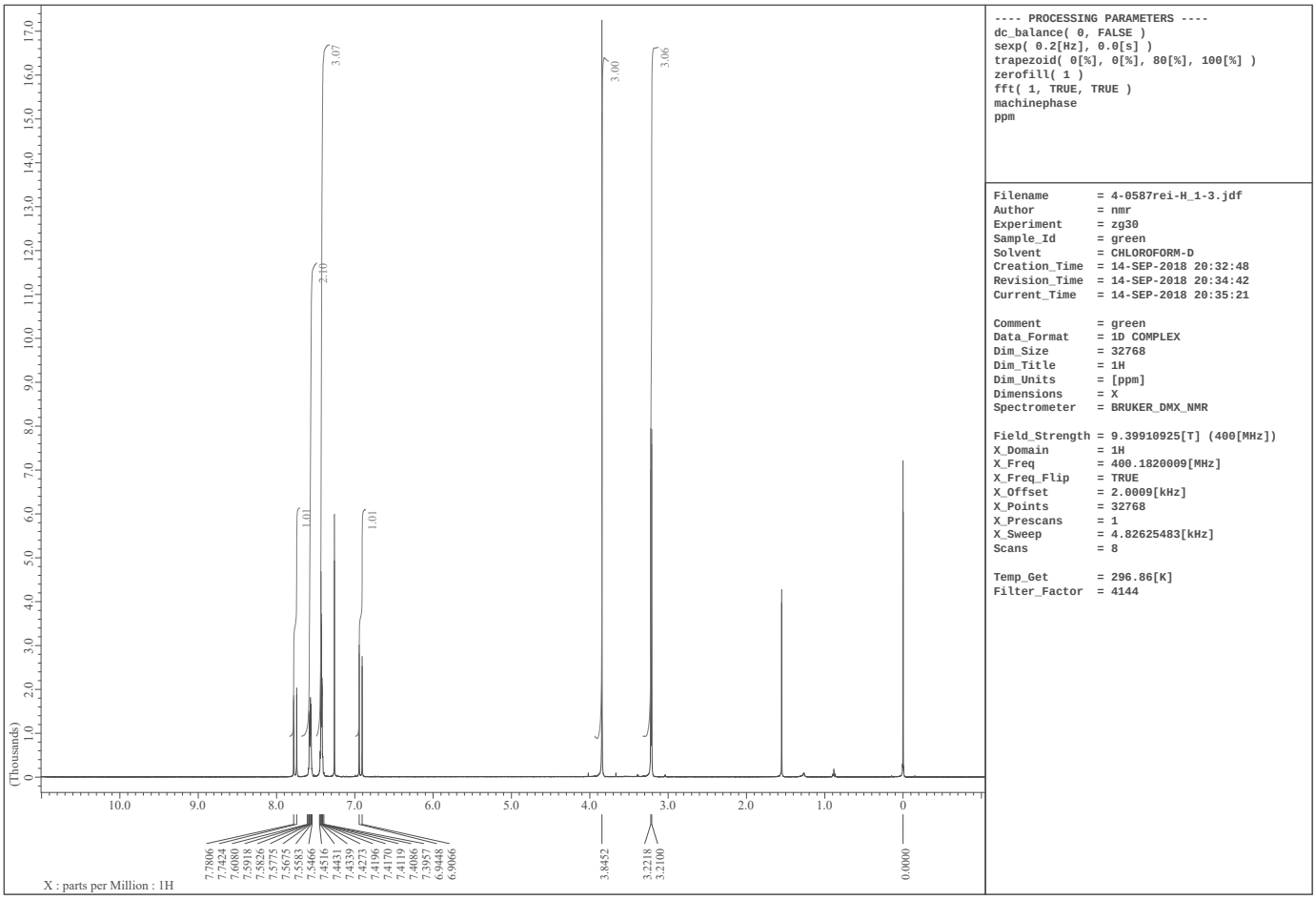


Figure S7. Perspective view of **5c**. Ellipsoids were drawn in 50% probability.

Figure S8. ^{1}H and ^{13}C NMR spectra of **1a**

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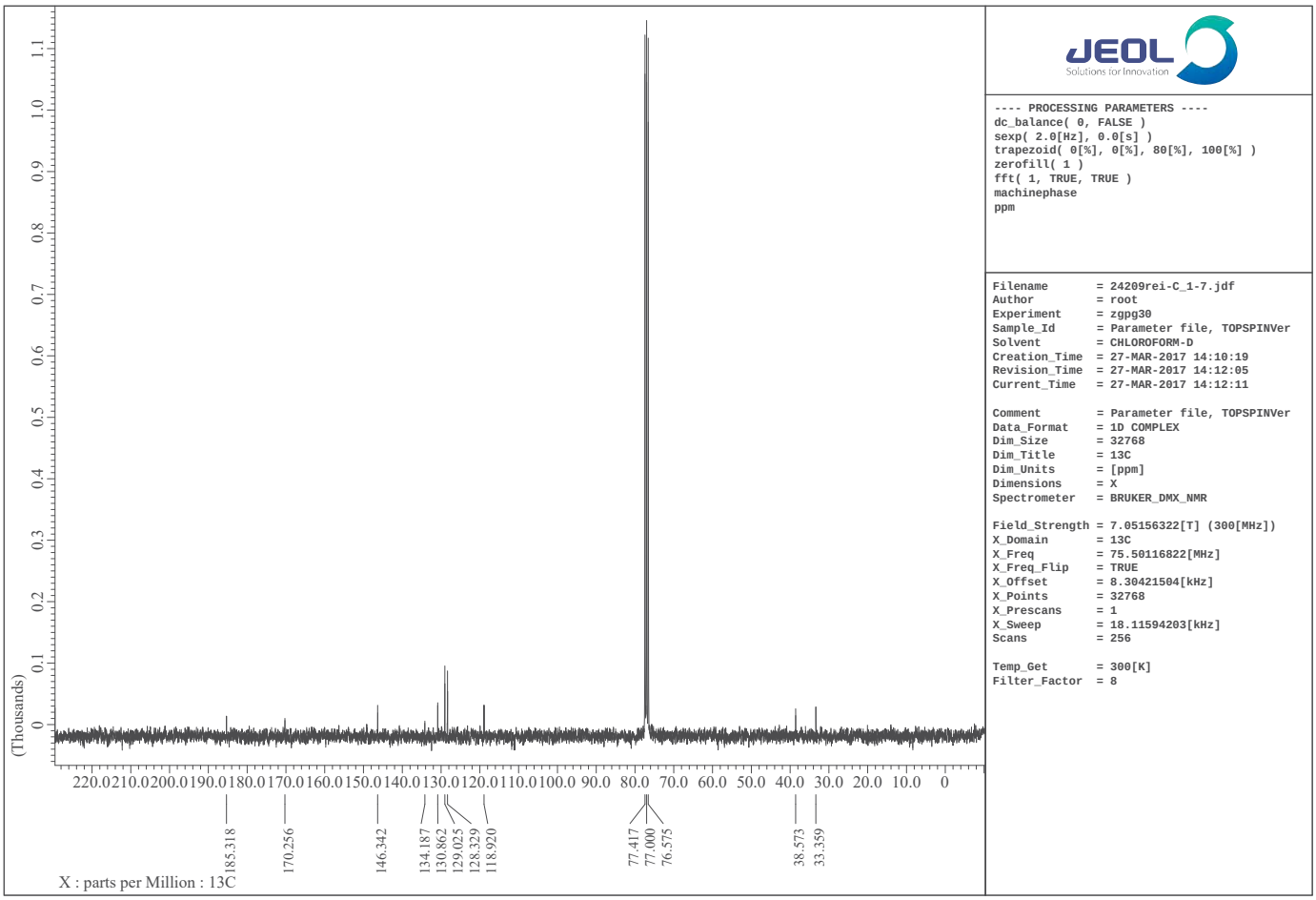


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Dimensions      = X
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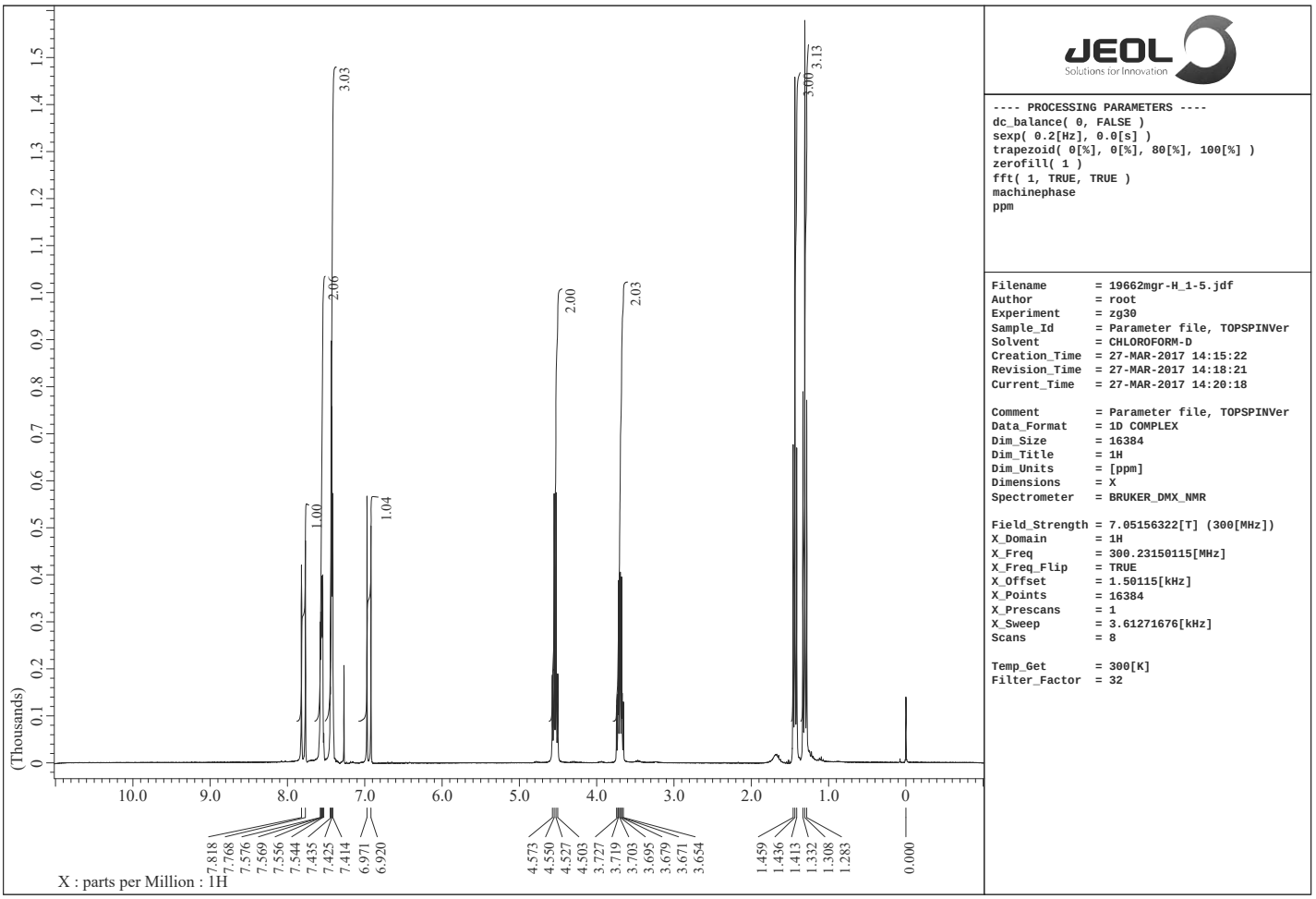
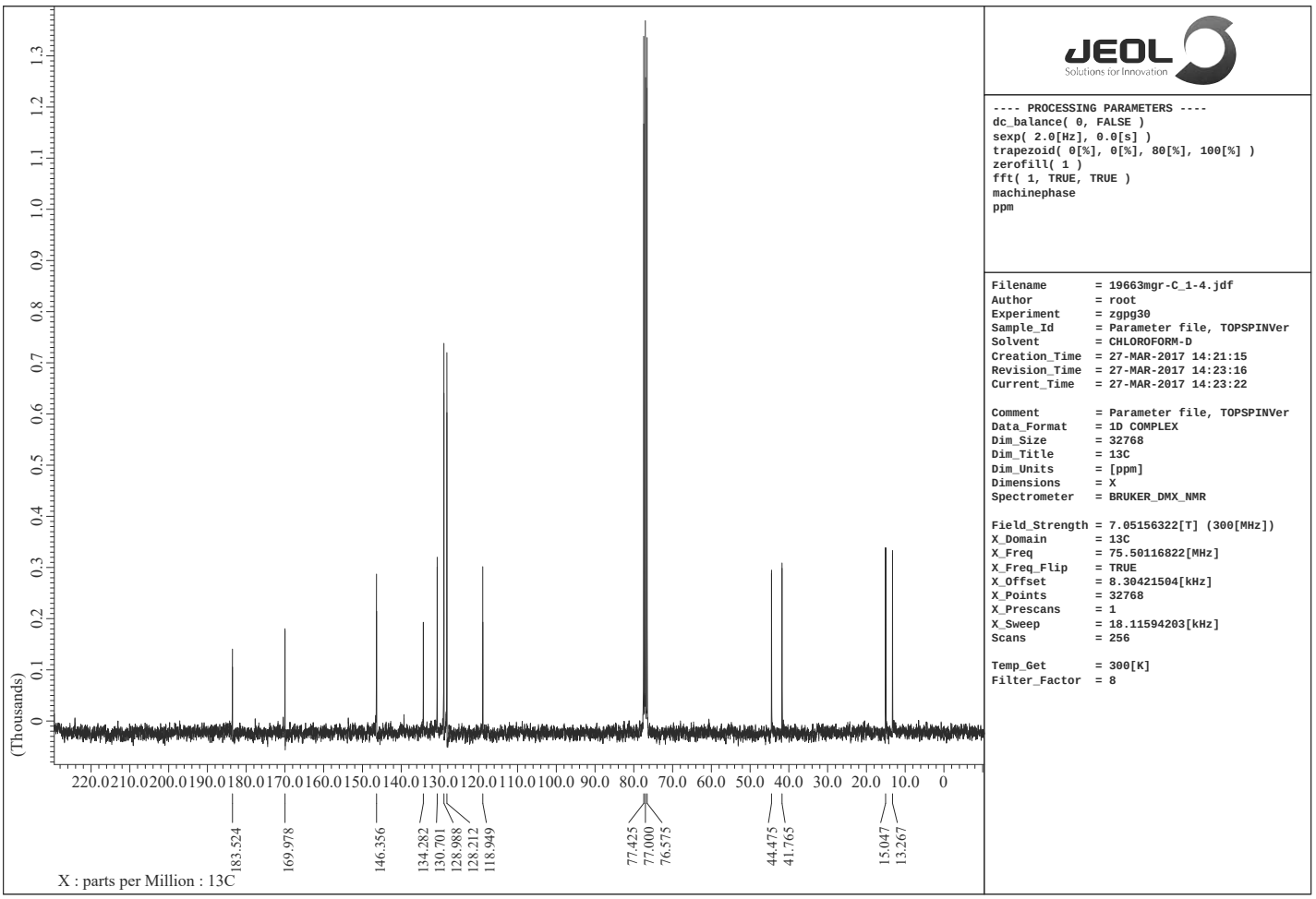
Figure S9. ^{1}H and ^{13}C NMR spectra of **1b**

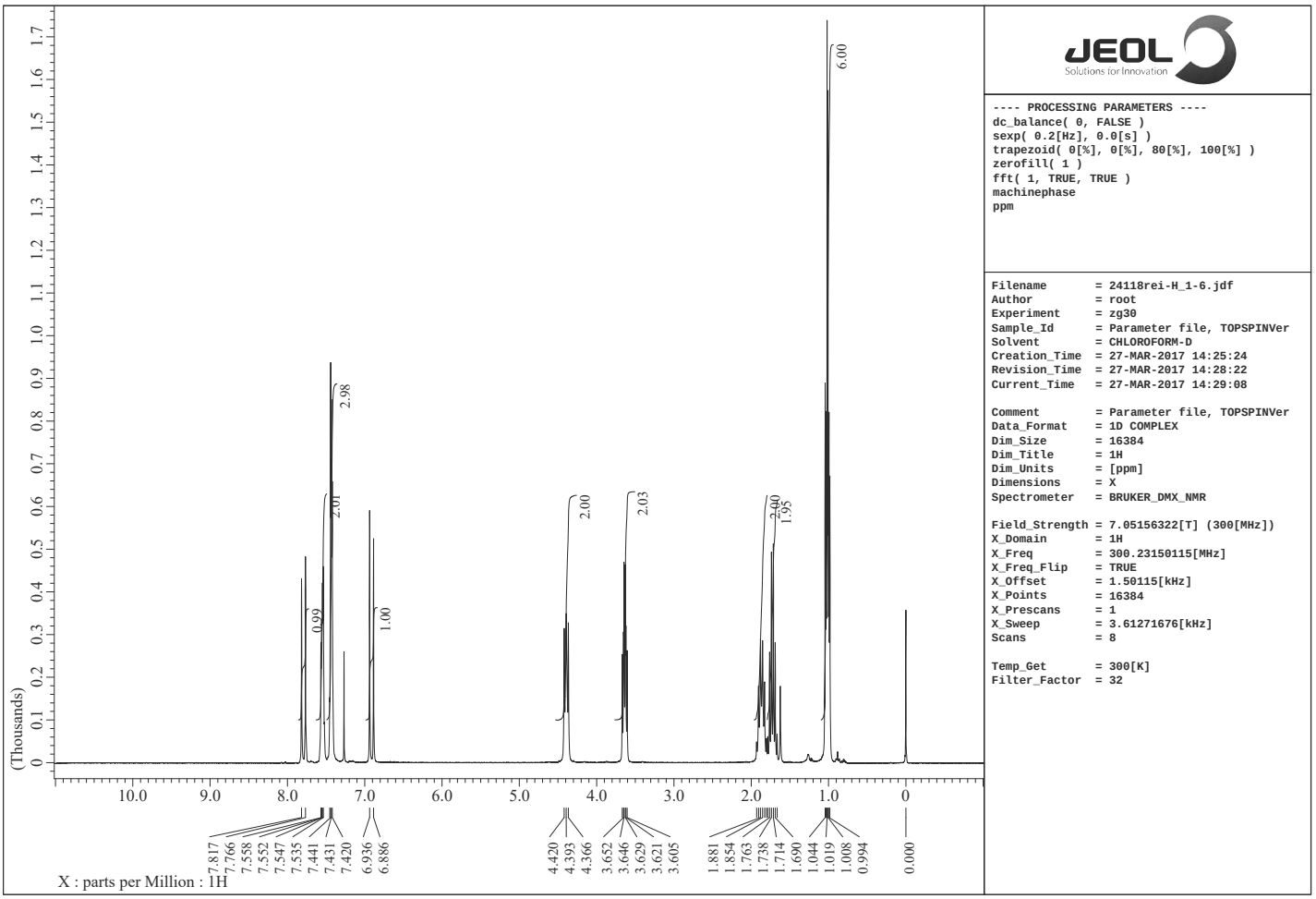


<<S11>>



<<S12>>

Figure S10. ^{1}H and ^{13}C NMR spectra of **1c**



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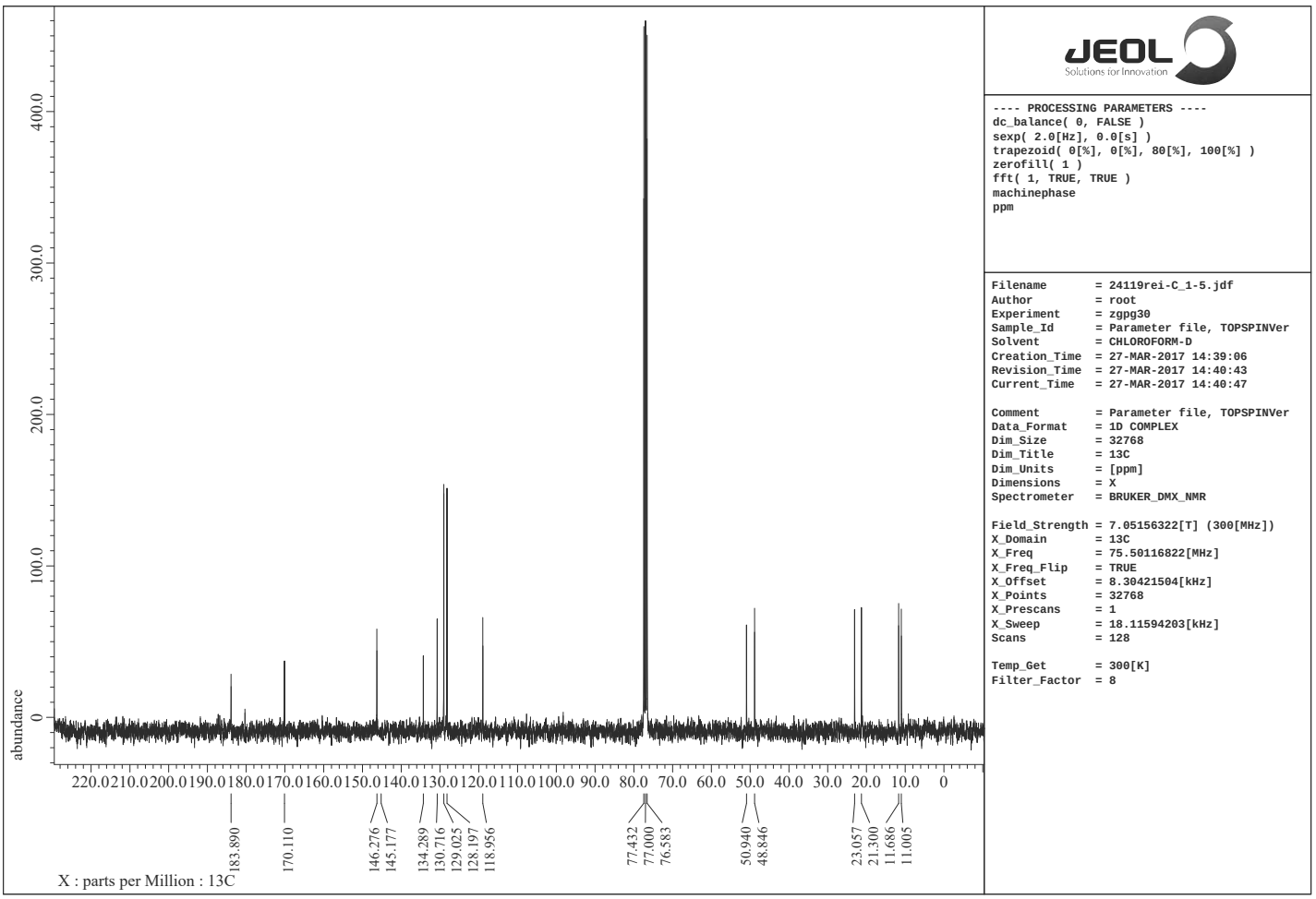
N-Cinnamoyl-N,N'-dipropylthiourea (1c)



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X_Freq_Flip     = TRUE
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Filter_Factor   = 8
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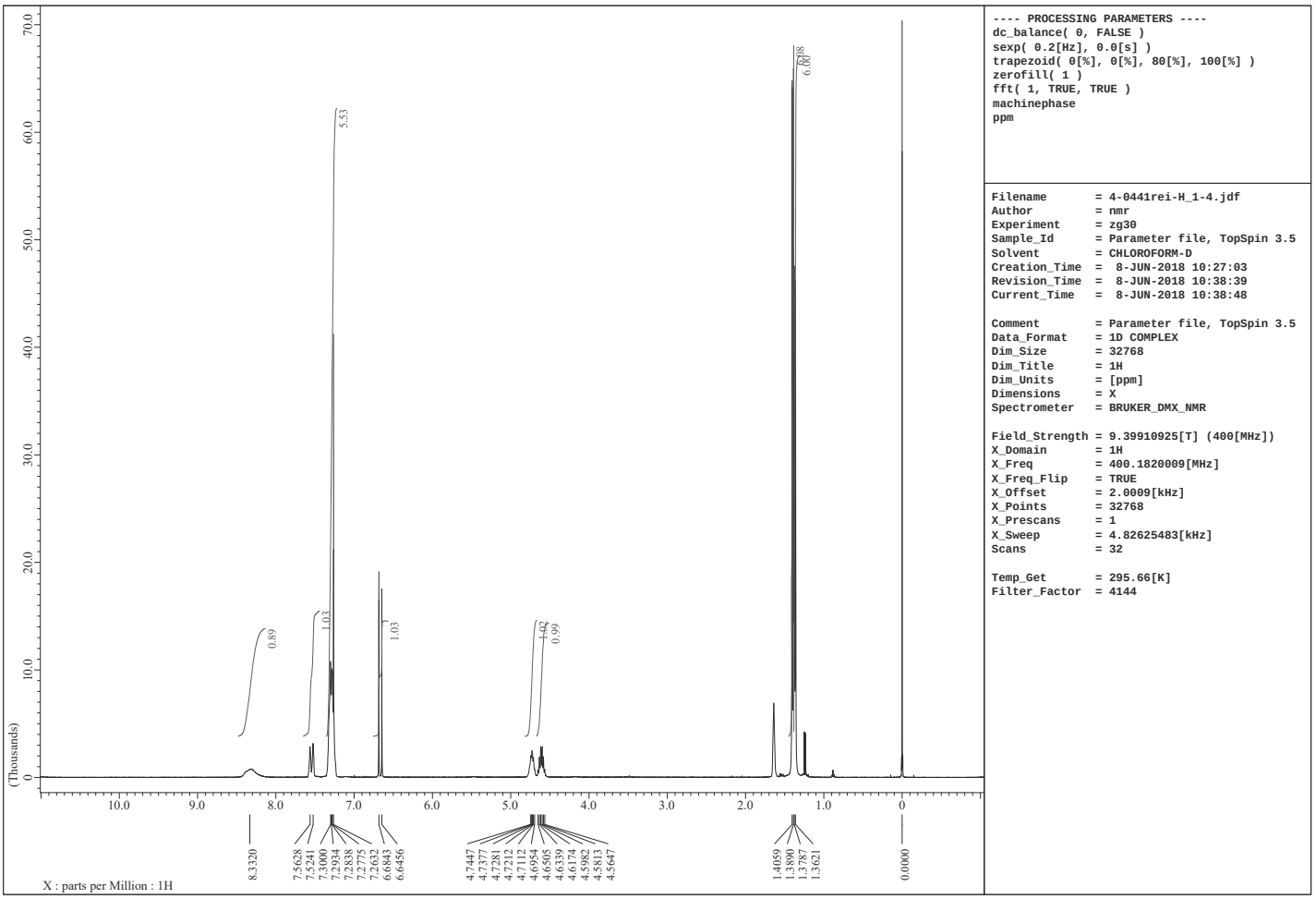
N-Cinnamoyl-N,N'-dipropylthiourea (1c)

Figure S11. ^{1}H and ^{13}C NMR spectra of **1d**

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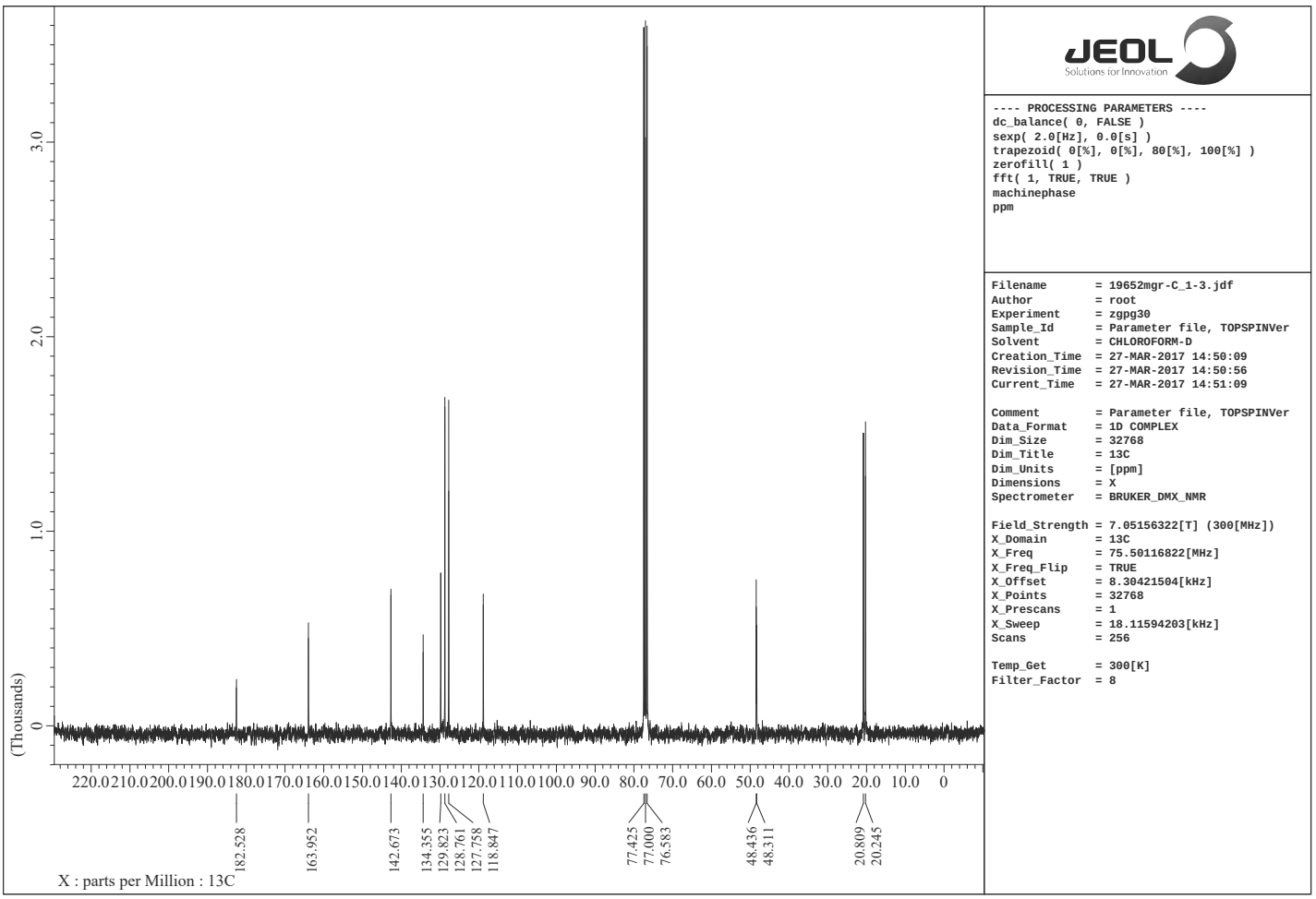
N-Cinnamoyl-N,N'-diisopropylthiourea (1d)

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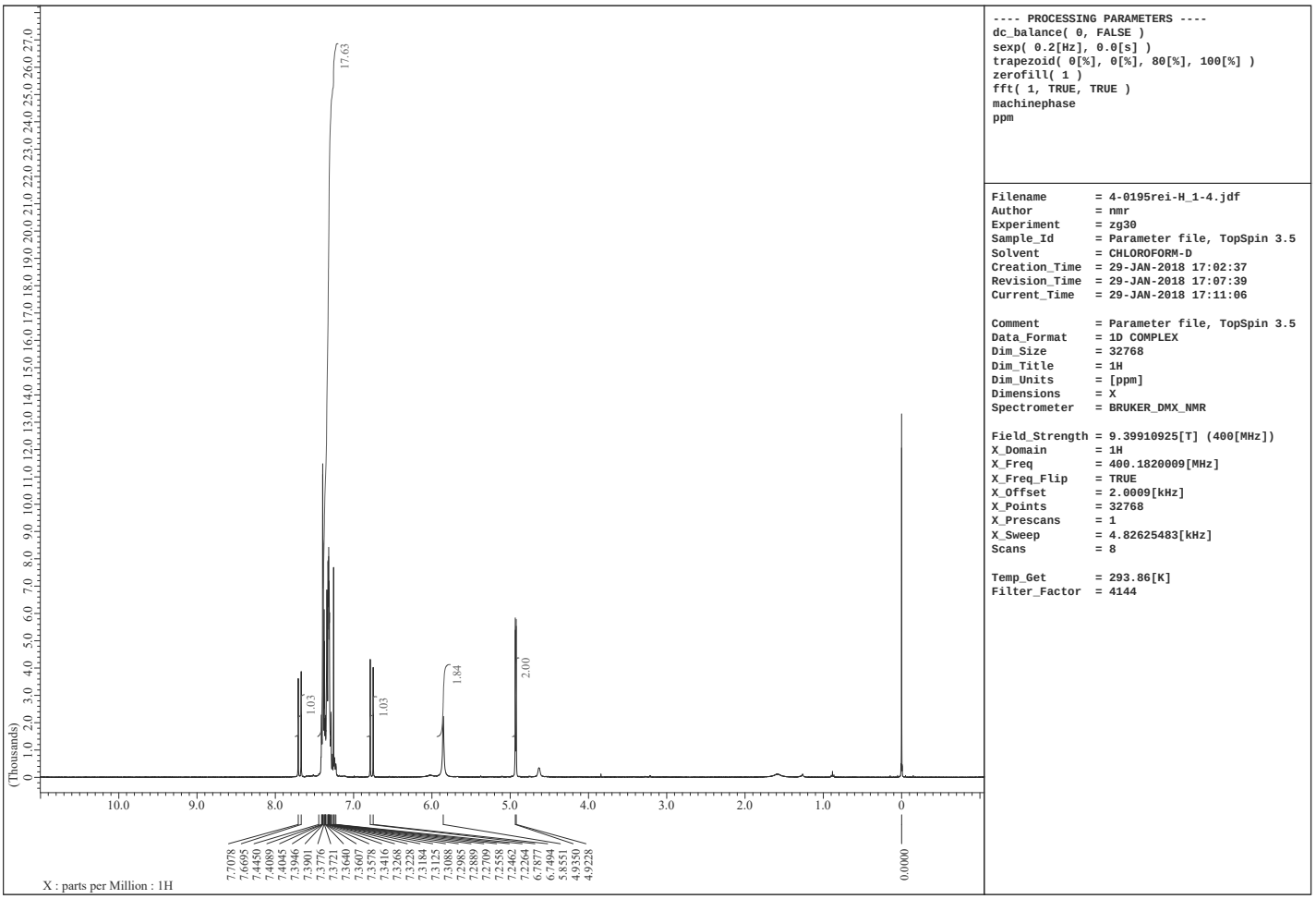
N-Cinnamoyl-N,N'-diisopropylthiourea (1d)

Figure S12. ^{1}H and ^{13}C NMR spectra of **1e**



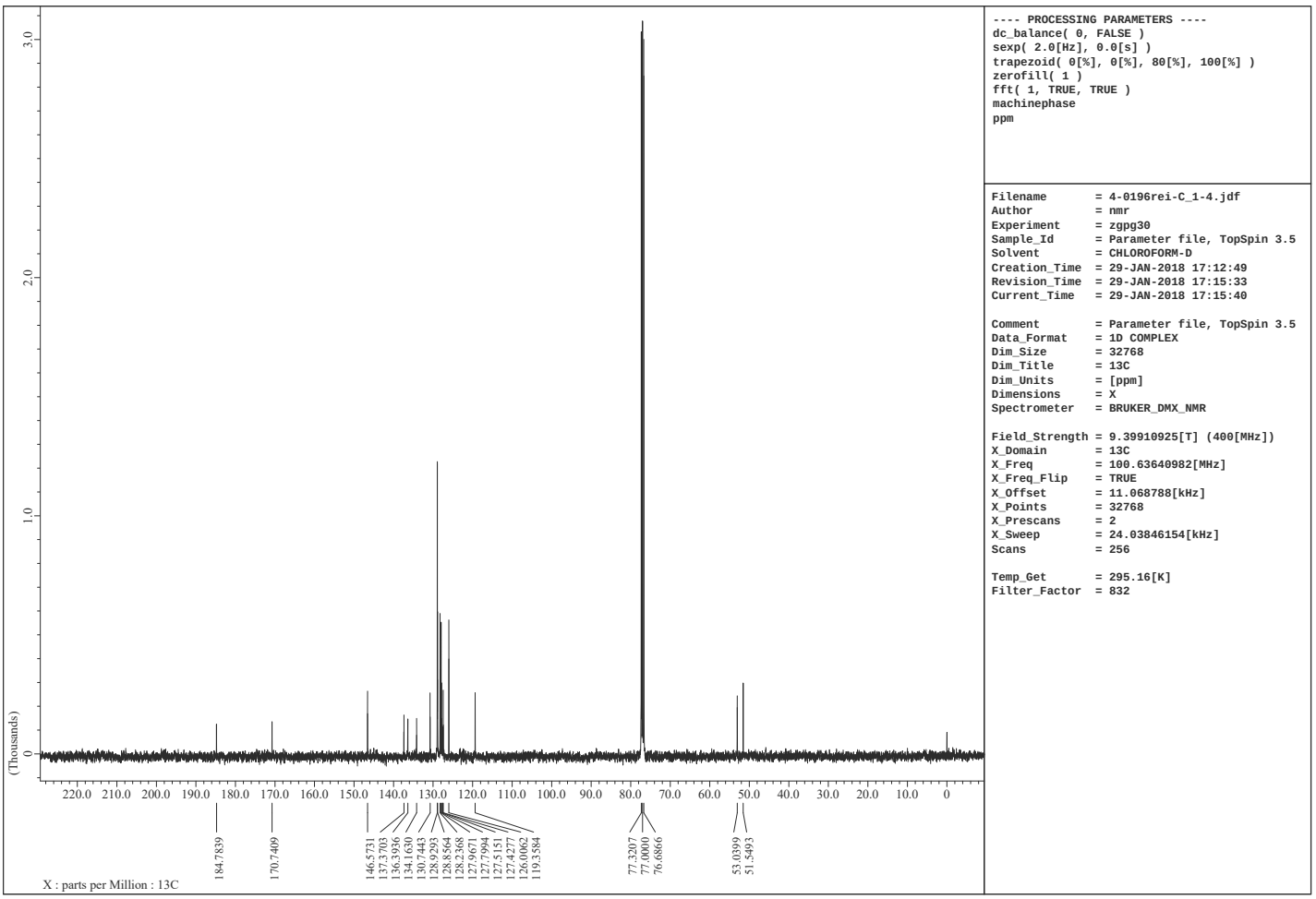
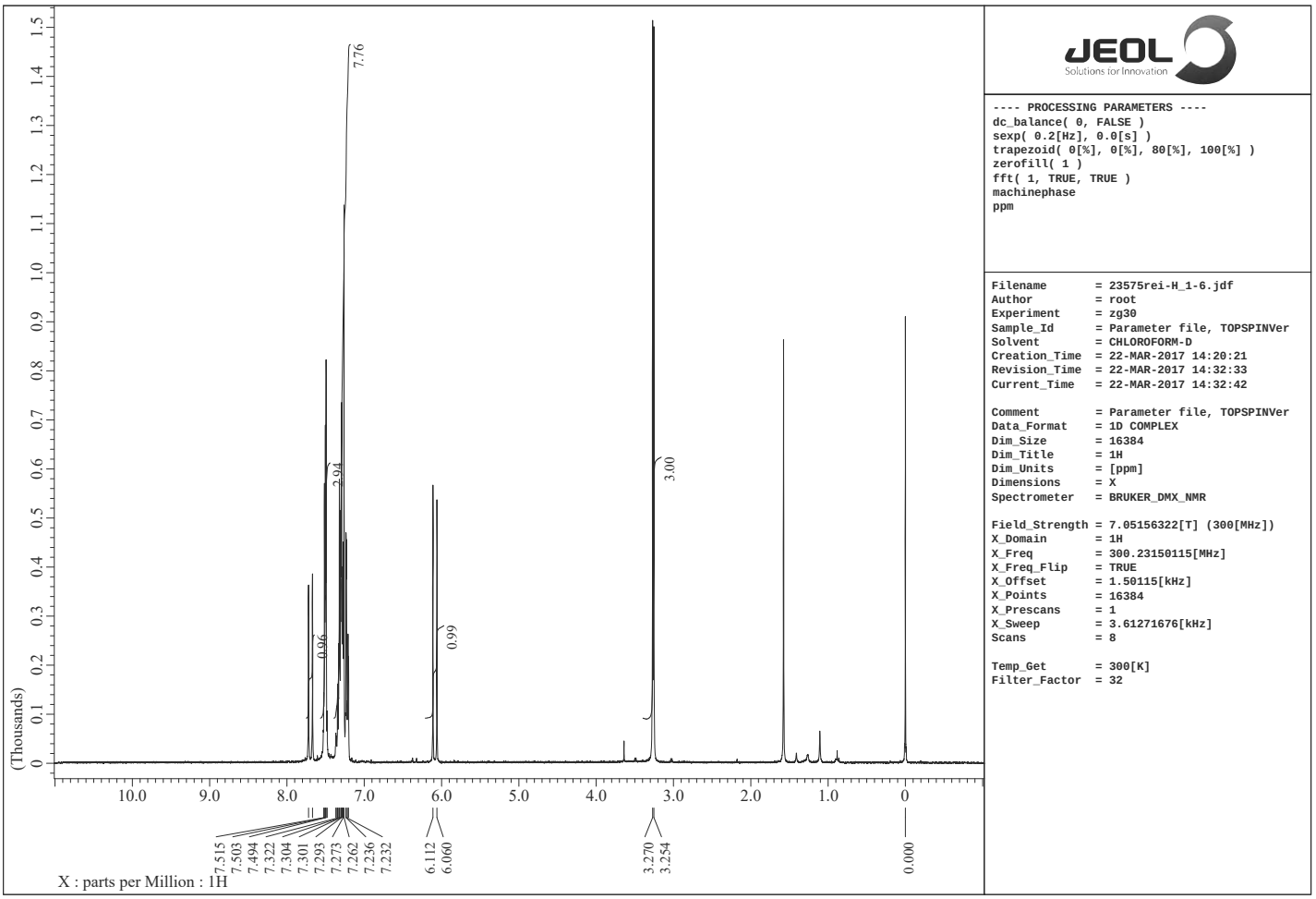


Figure S13. ^{1}H and ^{13}C NMR spectra of **1f**



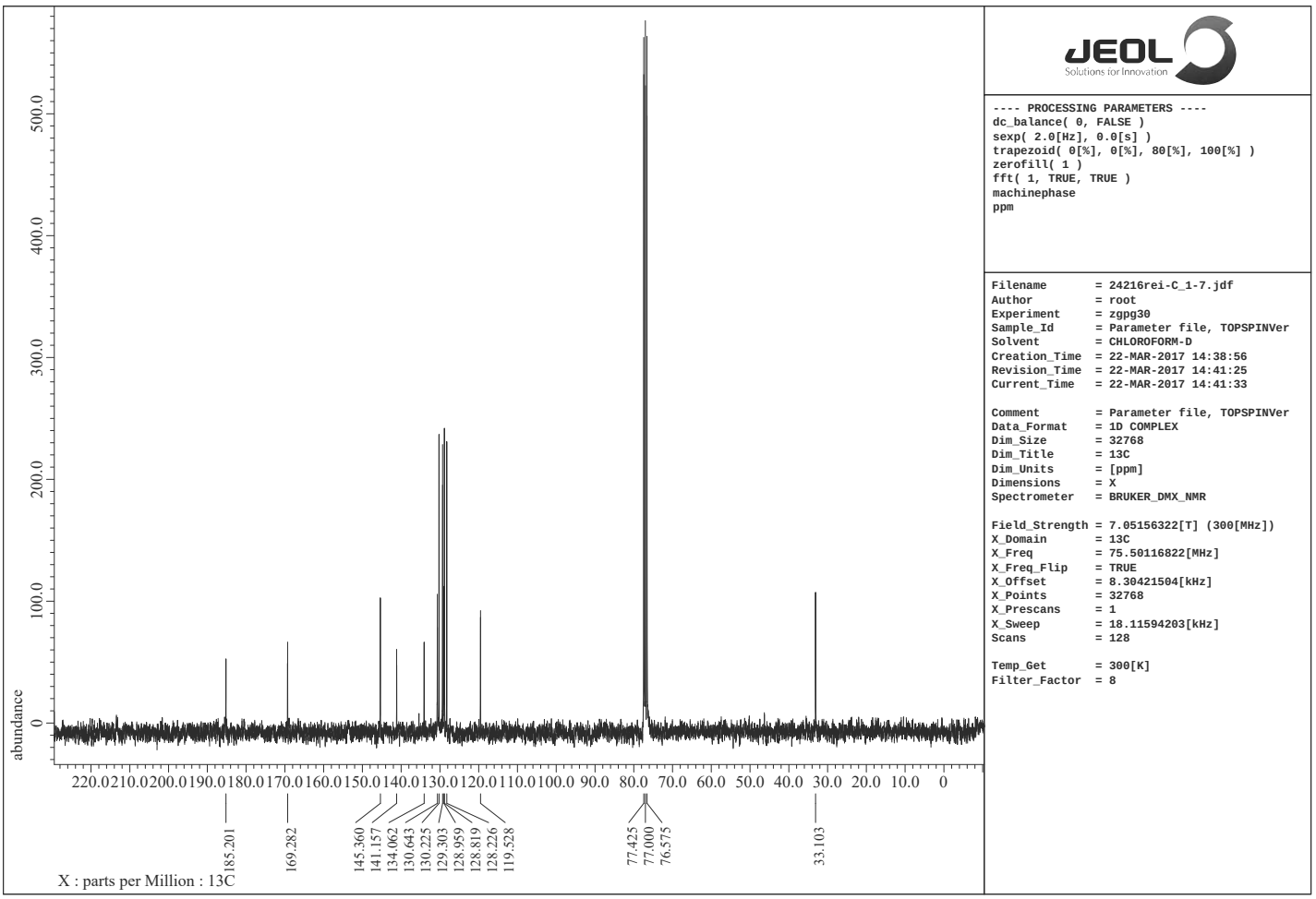
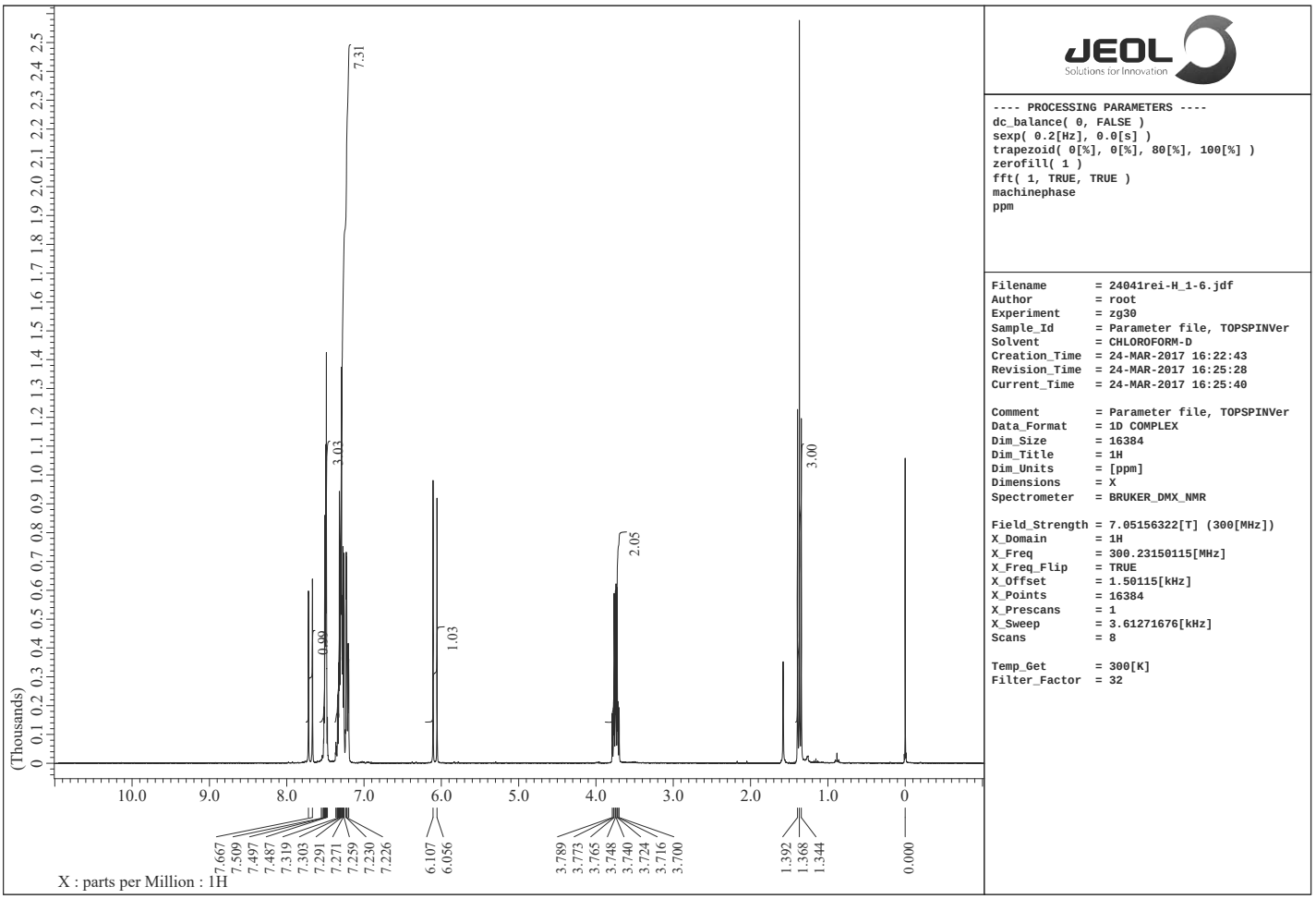


Figure S14. ^{1}H and ^{13}C NMR spectra of **1g**



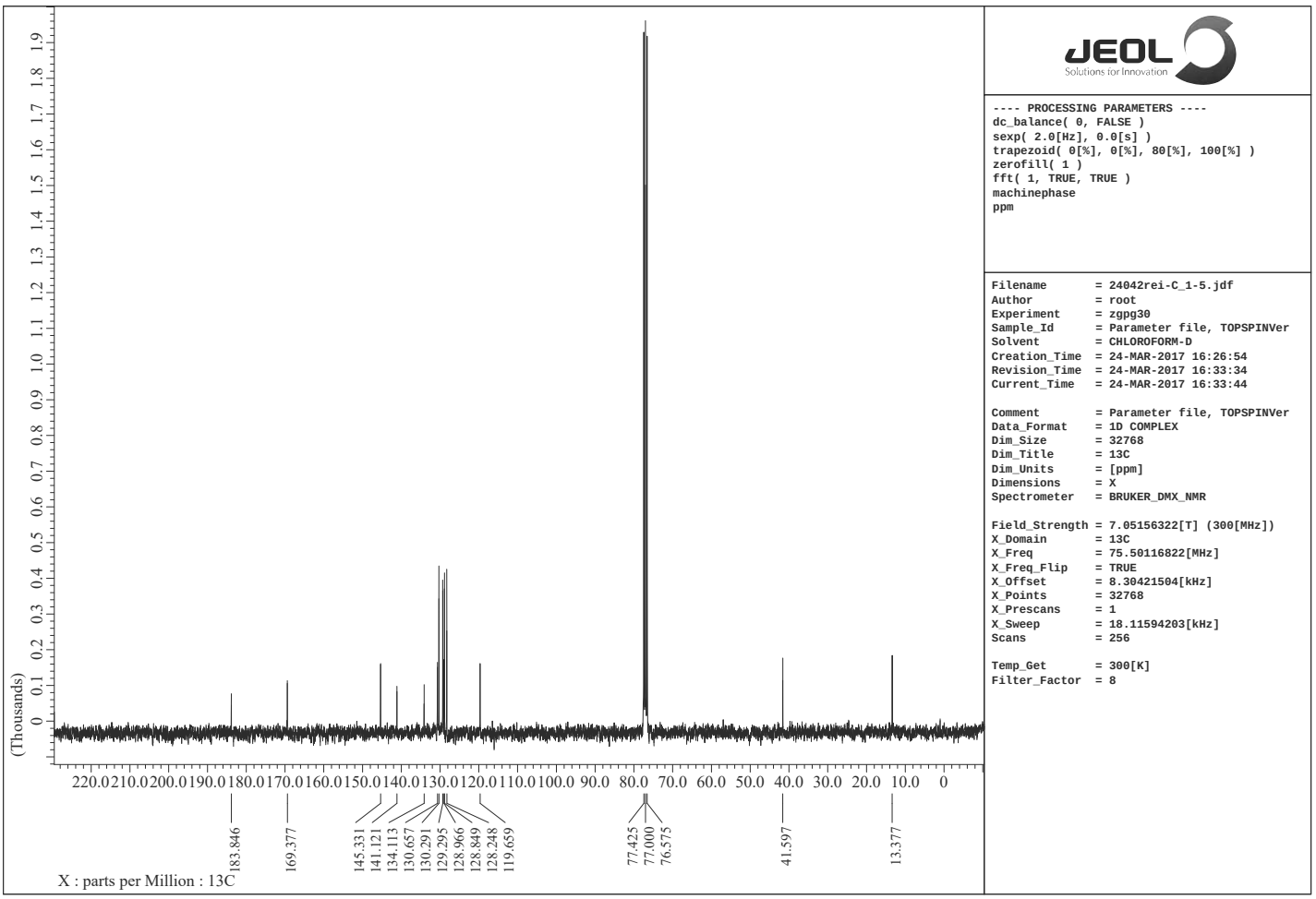
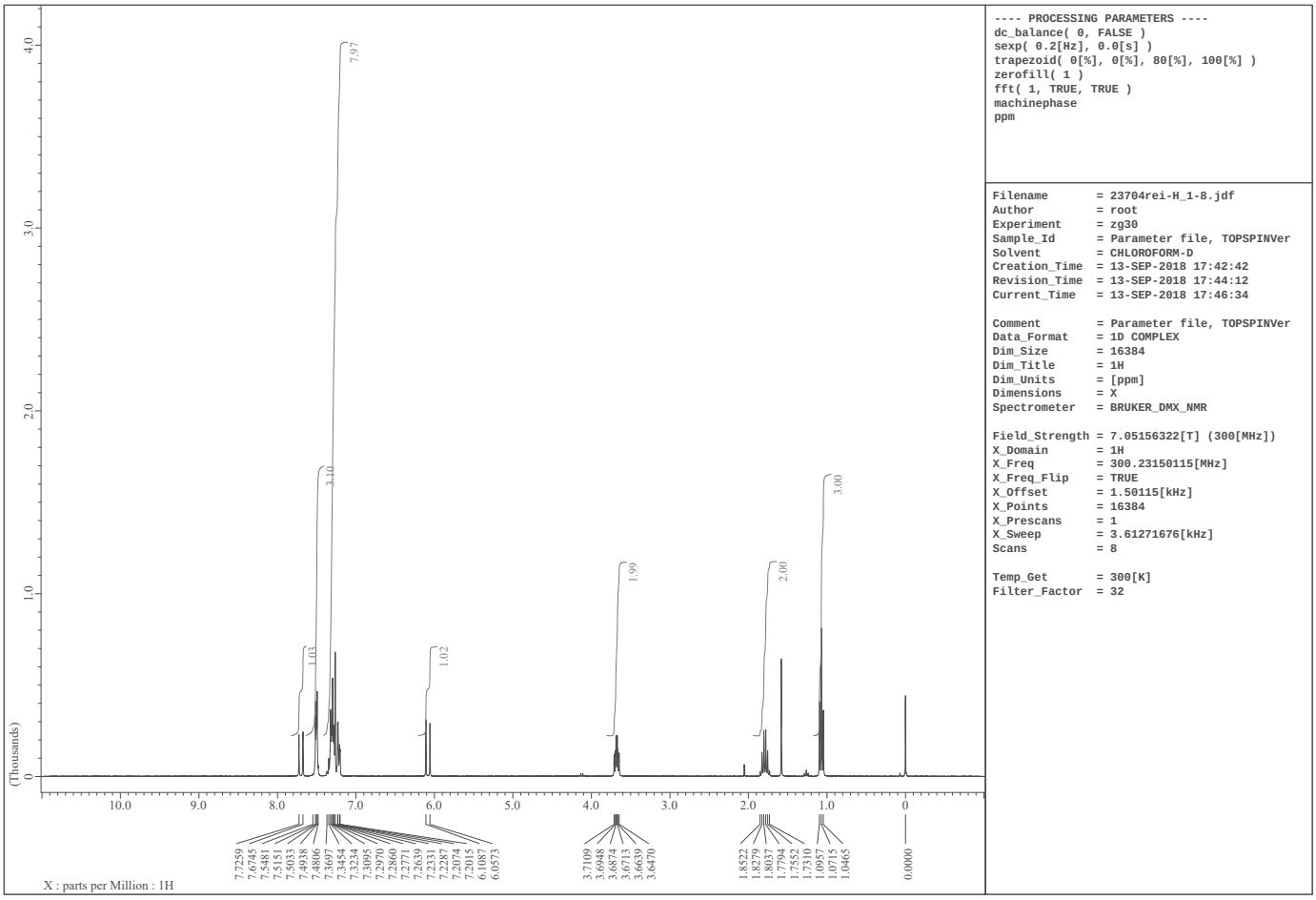
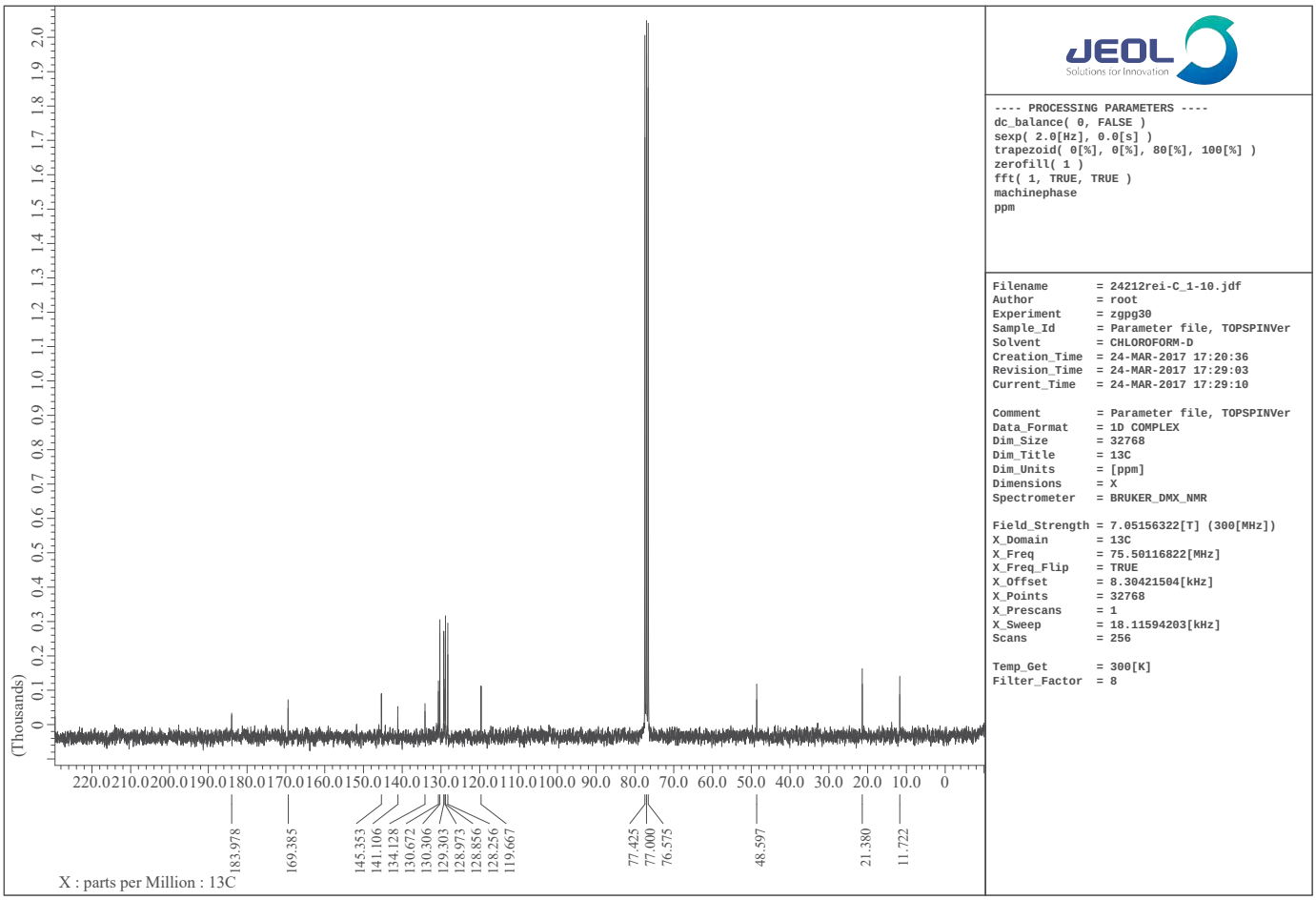


Figure S15. ^{1}H and ^{13}C NMR spectra of **1h**

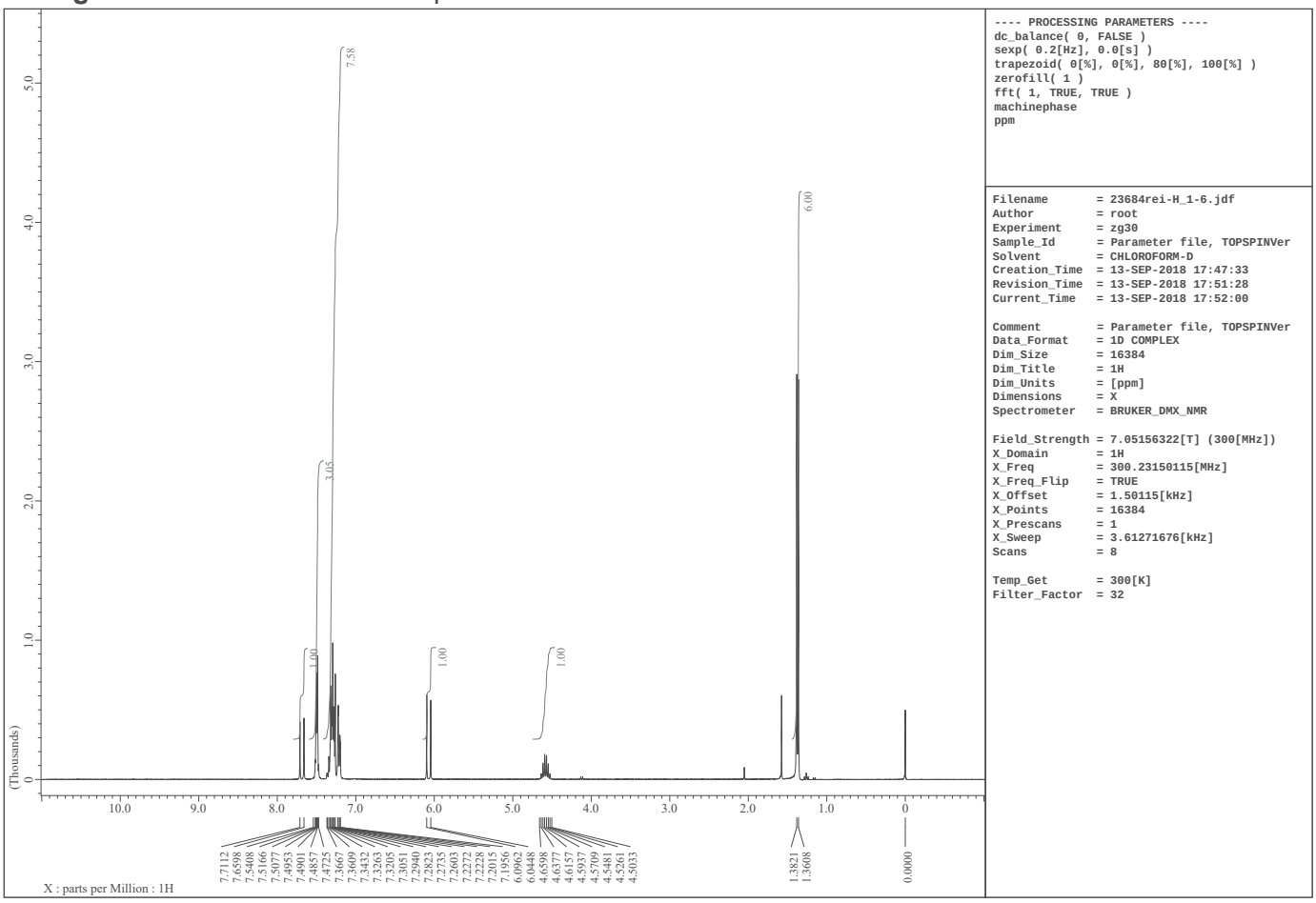



```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Filename        = 23704rei-H_1-8.jdf
Author          = root
Experiment      = zg30
Sample_Id       = Parameter file, TOPSPINVer
Solvent         = CHLOROFORM-D
Creation_Time   = 13-SEP-2018 17:42:42
Revision_Time   = 13-SEP-2018 17:44:12
Current_Time    = 13-SEP-2018 17:46:34

Comment         = Parameter file, TOPSPINVer
Data_Format     = 1D COMPLEX
Dim_Size        = 16384
Dim_Title       = 1H
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = BRUKER_DMX_NMR

Field_Strength = 7.05156322[T] (300[MHz])
X_Domain        = 1H
X_Freq          = 300.23150115[MHz]
X_Freq_Flip     = TRUE
X_Offset        = 1.50115[kHz]
X_Points        = 16384
X_Prescans      = 1
X_Sweep         = 3.61271676[kHz]
Scans           = 8

Temp_Get        = 300[K]
Filter_Factor   = 32
```



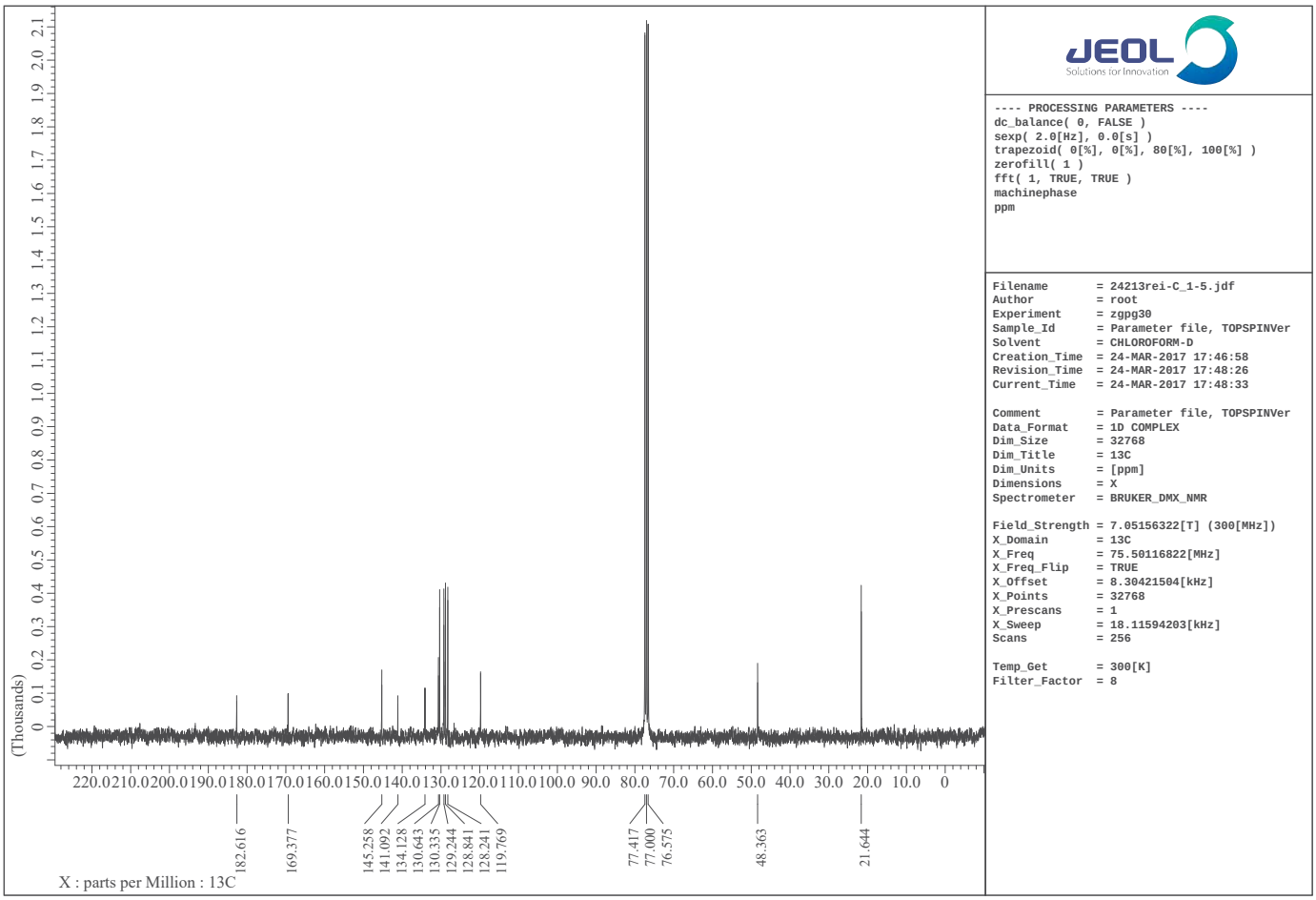

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Filename        = 24212rei-C_1-10.jdf
Author          = root
Experiment      = zgpg30
Sample_Id       = Parameter file, TOPSPINVer
Solvent         = CHLOROFORM-D
Creation_Time   = 24-MAR-2017 17:20:36
Revision_Time   = 24-MAR-2017 17:29:03
Current_Time    = 24-MAR-2017 17:29:10

Comment         = Parameter file, TOPSPINVer
Data_Format     = 1D COMPLEX
Dim_Size        = 32768
Dim_Title       = 13C
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = BRUKER_DMX_NMR

Field_Strength = 7.05156322[T] (300[MHz])
X_Domain        = 13C
X_Freq          = 75.50116822[MHz]
X_Freq_Flip     = TRUE
X_Offset        = 8.30421504[kHz]
X_Points        = 32768
X_Prescans      = 1
X_Sweep         = 18.11594203[kHz]
Scans           = 256

Temp_Get        = 300[K]
Filter_Factor   = 8
```

Figure S16. ^{1}H and ^{13}C NMR spectra of **1i**




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

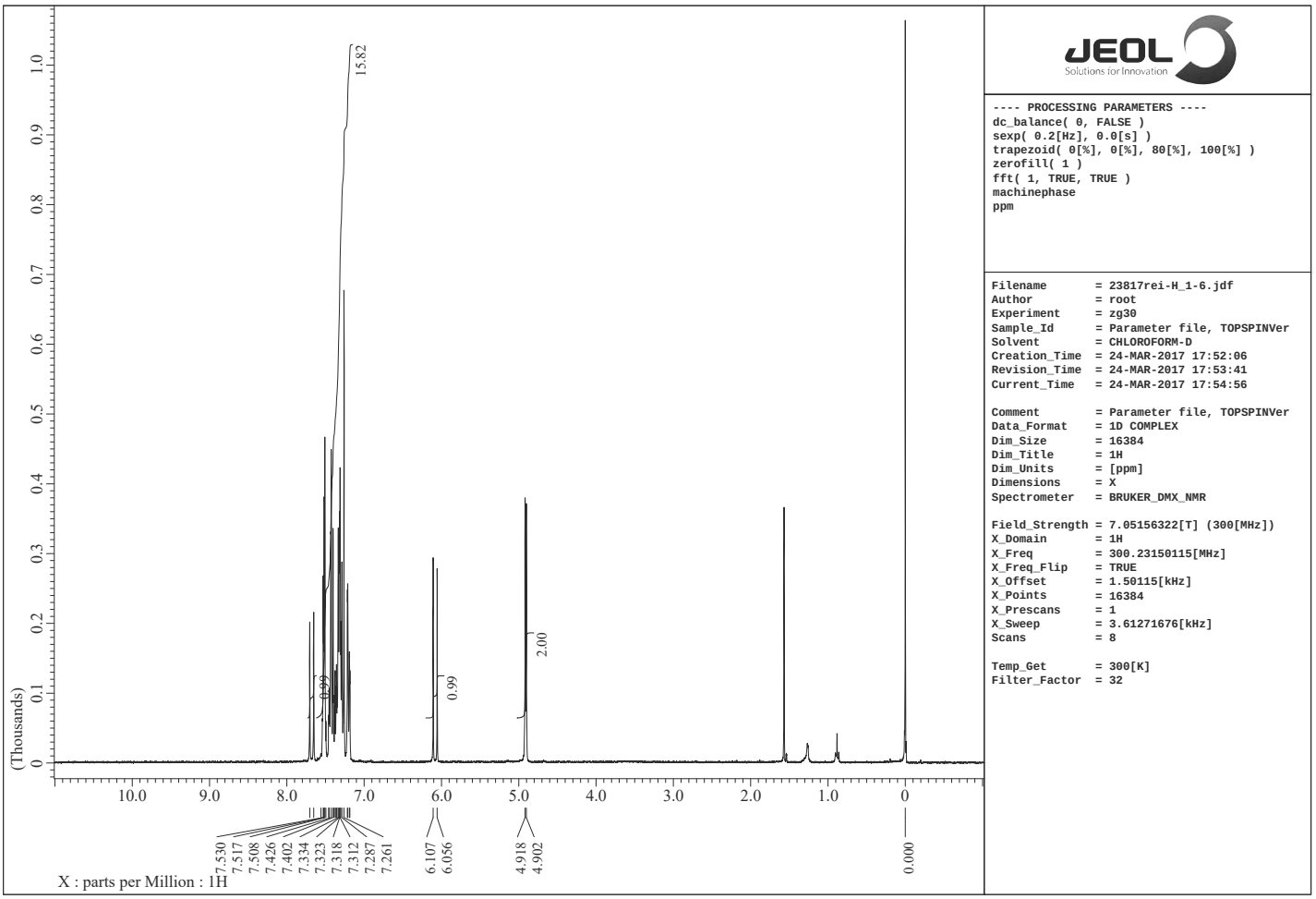
```
Filename        = 23684rei-H_1-6.jdf
Author          = root
Experiment      = zg30
Sample_Id       = Parameter file, TOPSPINVer
Solvent         = CHLOROFORM-D
Creation_Time   = 13-SEP-2018 17:47:33
Revision_Time   = 13-SEP-2018 17:51:28
Current_Time    = 13-SEP-2018 17:52:00

Comment         = Parameter file, TOPSPINVer
Data_Format     = 1D COMPLEX
Dim_Size        = 16384
Dim_Title       = 1H
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = BRUKER_DMX_NMR

Field_Strength = 7.05156322[T] (300[MHz])
X_Domain        = 1H
X_Freq          = 300.23150115[MHz]
X_Freq_Flip     = TRUE
X_Offset        = 1.50115[kHz]
X_Points        = 16384
X_Prescans      = 1
X_Sweep         = 3.61271676[kHz]
Scans           = 8

Temp_Get        = 300[K]
Filter_Factor   = 32
```




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

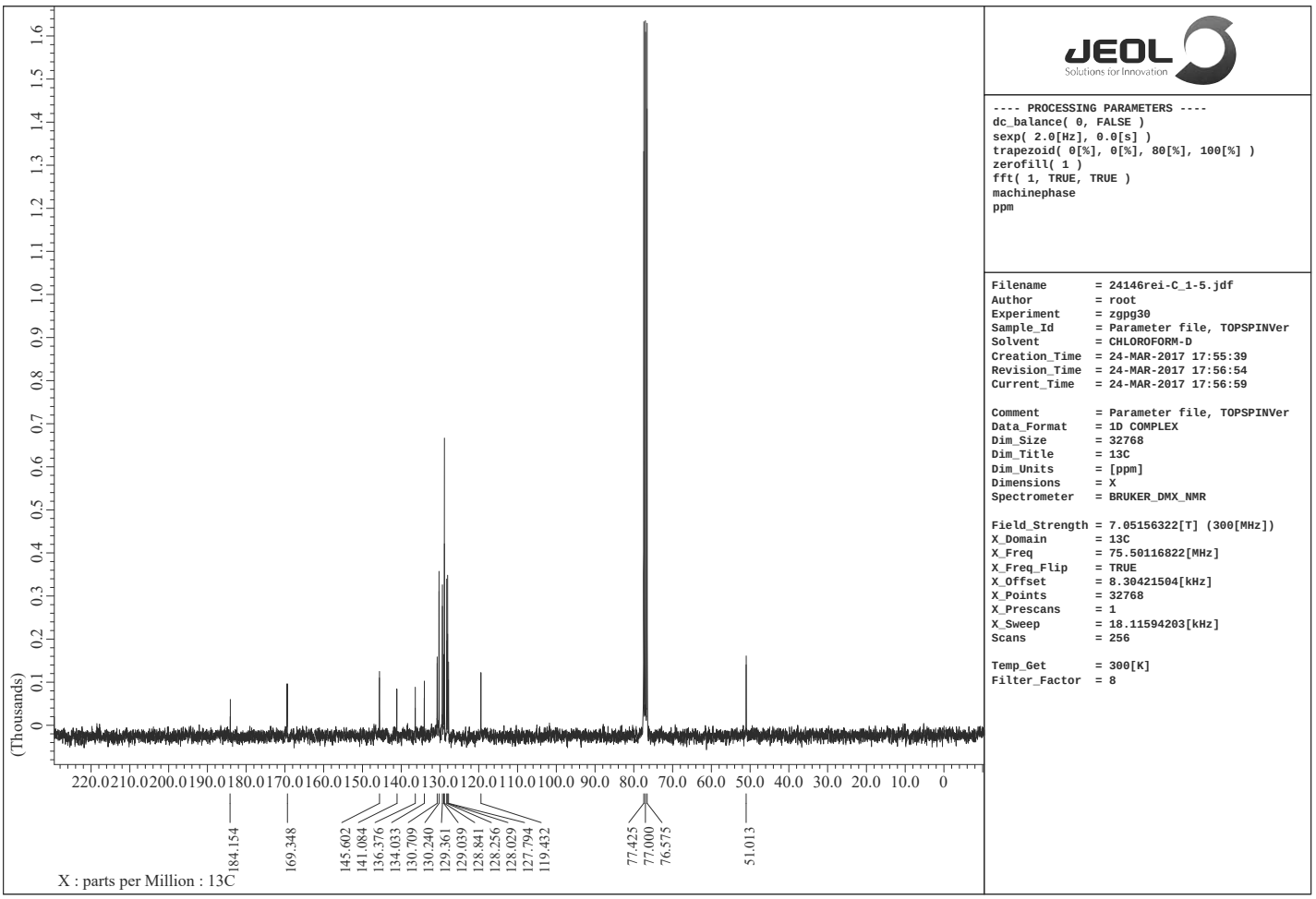
```
Filename        = 24213rei-C_1-5.jdf
Author          = root
Experiment      = zgpg30
Sample_Id       = Parameter file, TOPSPINVer
Solvent         = CHLOROFORM-D
Creation_Time   = 24-MAR-2017 17:46:58
Revision_Time   = 24-MAR-2017 17:48:26
Current_Time    = 24-MAR-2017 17:48:33

Comment         = Parameter file, TOPSPINVer
Data_Format     = 1D COMPLEX
Dim_Size        = 32768
Dim_Title       = 13C
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = BRUKER_DMX_NMR

Field_Strength = 7.05156322[T] (300[MHz])
X_Domain        = 13C
X_Freq          = 75.50116822[MHz]
X_Freq_Flip     = TRUE
X_Offset        = 8.30421504[kHz]
X_Points        = 32768
X_Prescans      = 1
X_Sweep         = 18.11594203[kHz]
Scans           = 256

Temp_Get        = 300[K]
Filter_Factor   = 8
```

Figure S17. ^{1}H and ^{13}C NMR spectra of **1j**




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Filename       = 23817rei-H_1-6.jdf
Author         = root
Experiment     = zg30
Sample_Id      = Parameter file, TOPSPINVer
Solvent        = CHLOROFORM-D
Creation_Time  = 24-MAR-2017 17:52:06
Revision_Time  = 24-MAR-2017 17:53:41
Current_Time   = 24-MAR-2017 17:54:56

Comment        = Parameter file, TOPSPINVer
Data_Format    = 1D COMPLEX
Dim_Size       = 16384
Dim_Title      = 1H
Dim_Units      = [ppm]
Dimensions     = X
Spectrometer   = BRUKER_DMX_NMR

Field_Strength = 7.05156322[T] (300[MHz])
X_Domain       = 1H
X_Freq         = 300.23150115[MHz]
X_Freq_Flip    = TRUE
X_Offset       = 1.50115[kHz]
X_Points       = 16384
X_Prescans     = 1
X_Sweep        = 3.61271676[kHz]
Scans          = 8

Temp_Get       = 300[K]
Filter_Factor  = 32
```

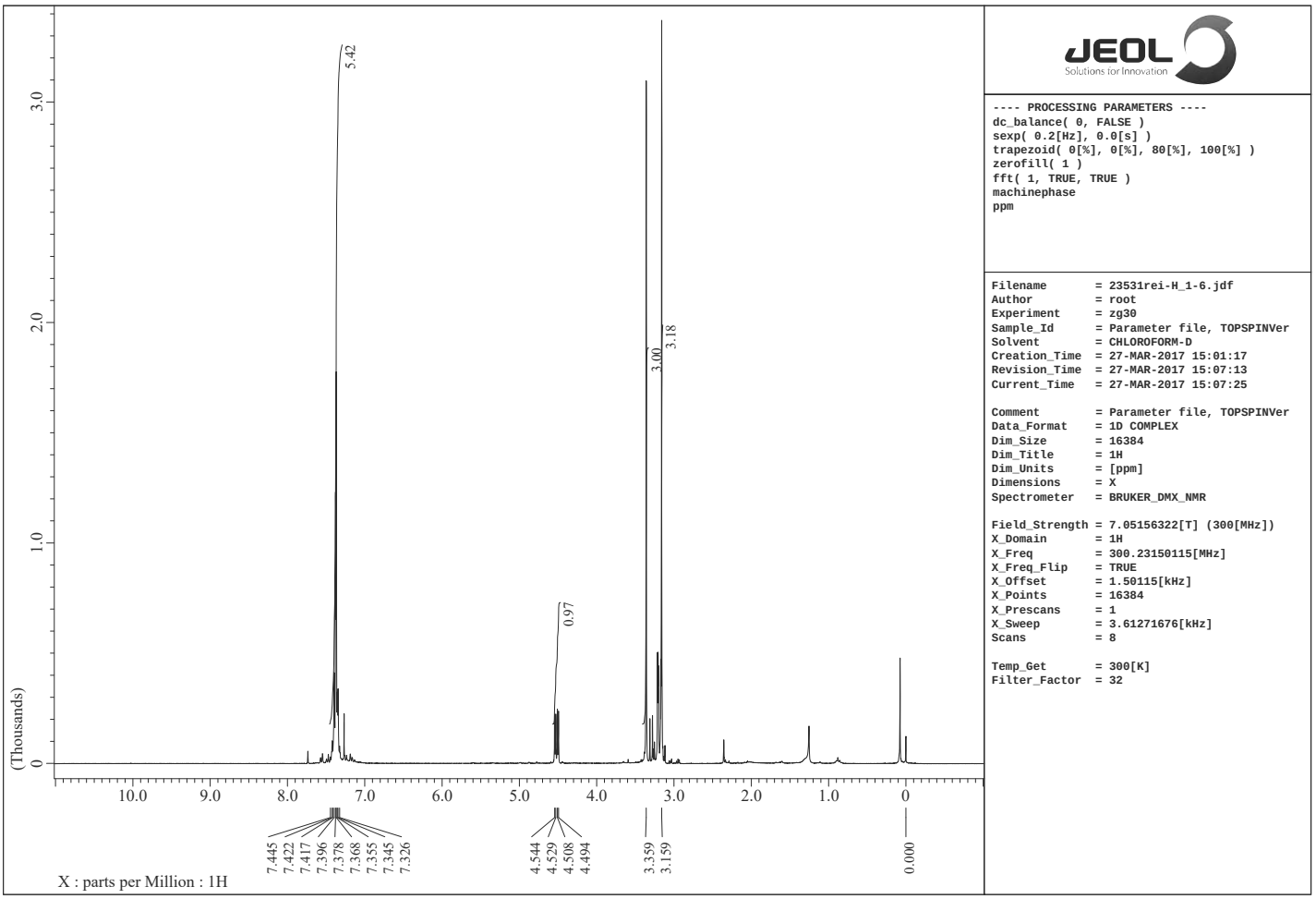
N-Cinnamoyl-N-phenyl-N'-benzylthiourea (1j)



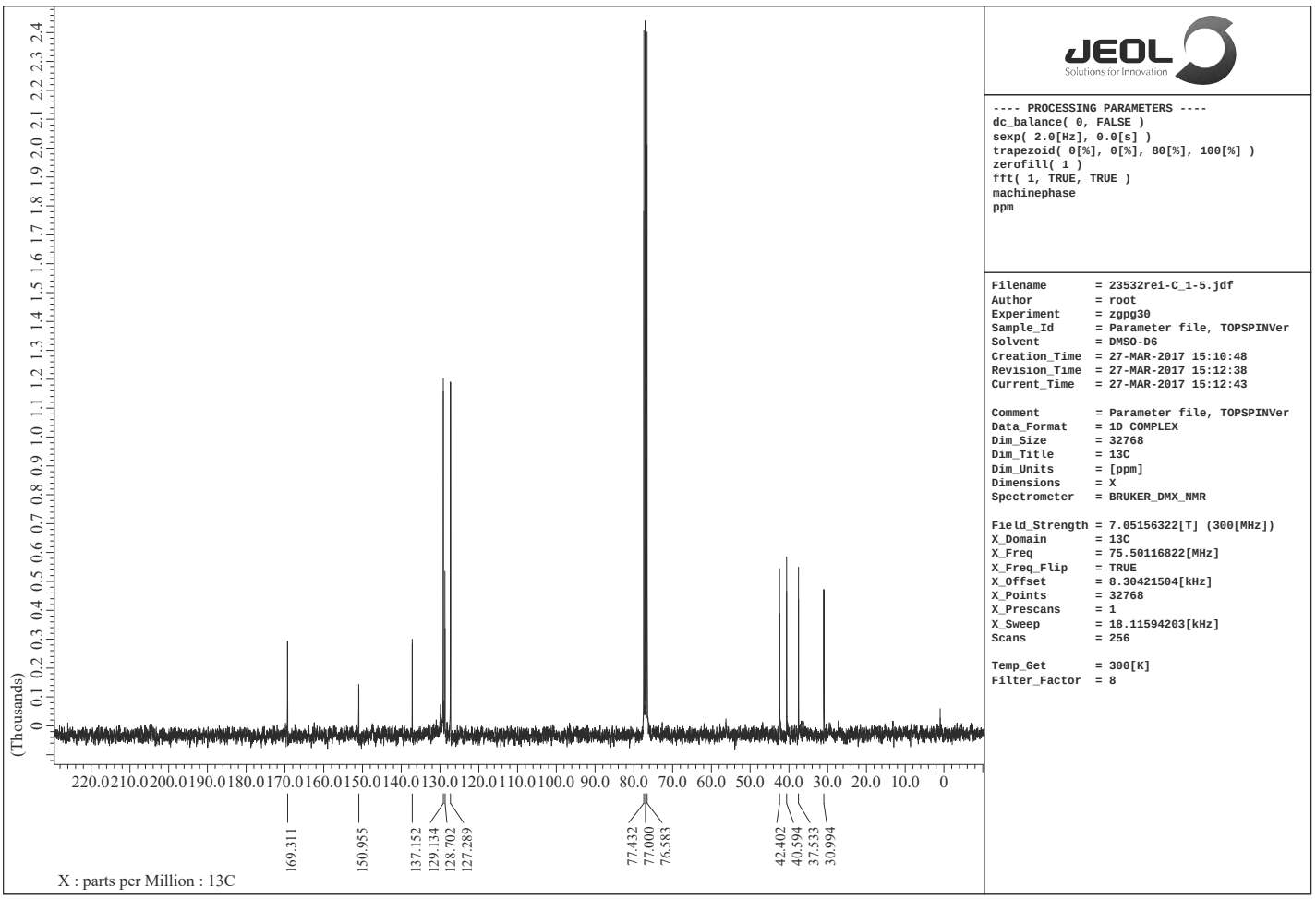

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Filename       = 24146rei-C_1-5.jdf
Author         = root
Experiment     = zgpg30
Sample_Id      = Parameter file, TOPSPINVer
Solvent        = CHLOROFORM-D
Creation_Time  = 24-MAR-2017 17:55:39
Revision_Time  = 24-MAR-2017 17:56:54
Current_Time   = 24-MAR-2017 17:56:59

Comment        = Parameter file, TOPSPINVer
Data_Format    = 1D COMPLEX
Dim_Size       = 32768
Dim_Title      = 13C
Dim_Units      = [ppm]
Dimensions     = X
Spectrometer   = BRUKER_DMX_NMR

Field_Strength = 7.05156322[T] (300[MHz])
X_Domain       = 13C
X_Freq         = 75.50116822[MHz]
X_Freq_Flip    = TRUE
X_Offset       = 8.30421504[kHz]
X_Points       = 32768
X_Prescans     = 1
X_Sweep        = 18.11594203[kHz]
Scans          = 256

Temp_Get       = 300[K]
Filter_Factor  = 8
```

N-Cinnamoyl-N-phenyl-N'-benzylthiourea (1j)

Figure S18. ^{1}H and ^{13}C NMR spectra of **2a**

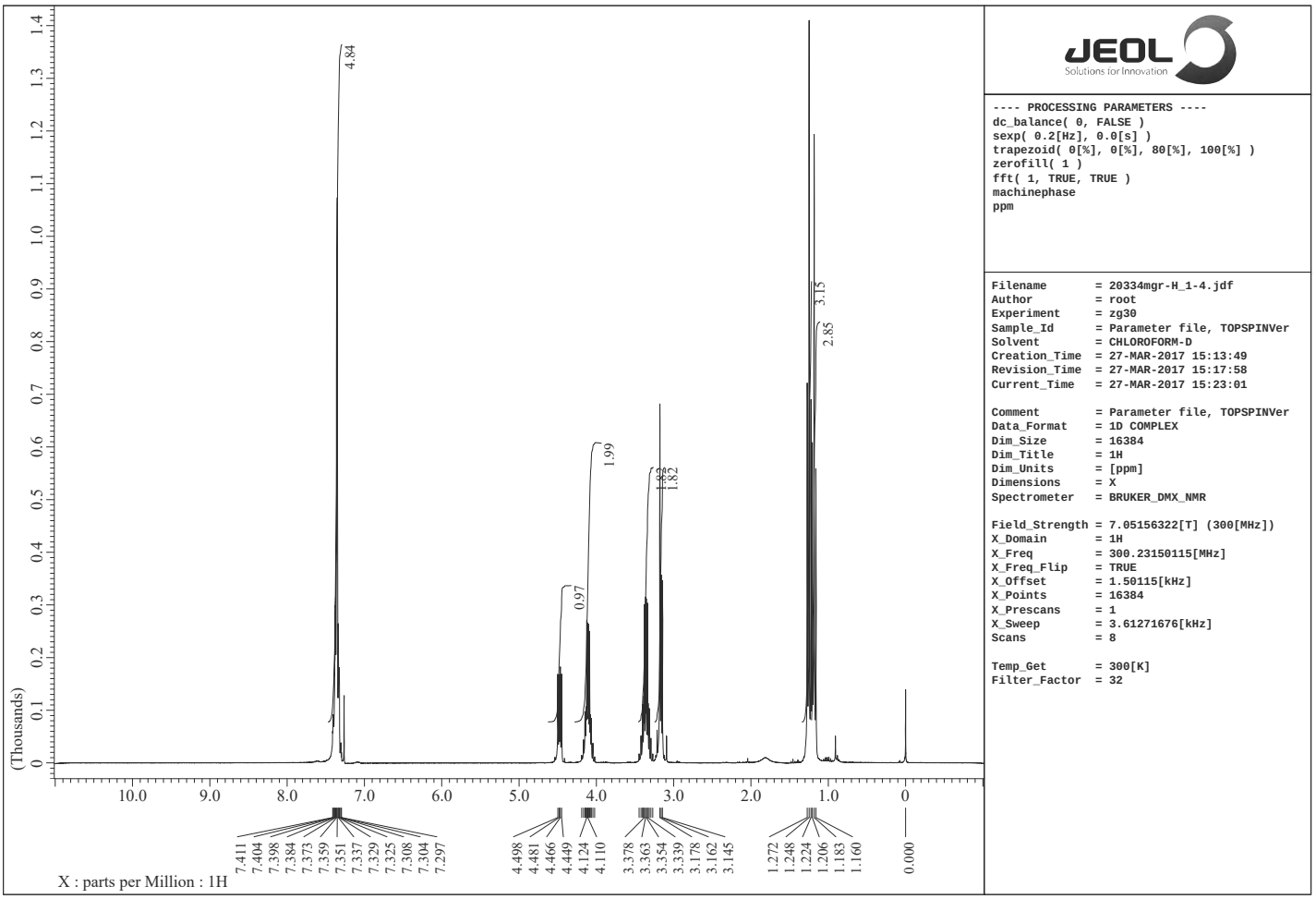



```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Filename       = 23531rei-H_1-6.jdf
Author         = root
Experiment     = zg30
Sample_Id      = Parameter file, TOPSPINVer
Solvent        = CHLOROFORM-D
Creation_Time  = 27-MAR-2017 15:01:17
Revision_Time  = 27-MAR-2017 15:07:13
Current_Time   = 27-MAR-2017 15:07:25

Comment        = Parameter file, TOPSPINVer
Data_Format    = 1D COMPLEX
Dim_Size       = 16384
Dim_Title      = 1H
Dim_Units      = [ppm]
Dimensions     = X
Spectrometer   = BRUKER_DMX_NMR

Field_Strength = 7.05156322[T] (300[MHz])
X_Domain       = 1H
X_Freq         = 300.23150115[MHz]
X_Freq_Flip    = TRUE
X_Offset       = 1.50115[kHz]
X_Points       = 16384
X_Prescans     = 1
X_Sweep        = 3.61271676[kHz]
Scans          = 8

Temp_Get       = 300[K]
Filter_Factor  = 32
```




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Filename       = 23532rei-C_1-5.jdf
Author         = root
Experiment     = zgpg30
Sample_Id      = Parameter file, TOPSPINVer
Solvent        = DMSO-D6
Creation_Time  = 27-MAR-2017 15:10:48
Revision_Time  = 27-MAR-2017 15:12:38
Current_Time   = 27-MAR-2017 15:12:43

Comment        = Parameter file, TOPSPINVer
Data_Format    = 1D COMPLEX
Dim_Size       = 32768
Dim_Title      = 13C
Dim_Units      = [ppm]
Dimensions     = X
Spectrometer   = BRUKER_DMX_NMR

Field_Strength = 7.05156322[T] (300[MHz])
X_Domain       = 13C
X_Freq         = 75.50116822[MHz]
X_Freq_Flip    = TRUE
X_Offset       = 8.30421504[kHz]
X_Points       = 32768
X_Prescans     = 1
X_Sweep        = 18.11594203[kHz]
Scans          = 256

Temp_Get       = 300[K]
Filter_Factor  = 8
```

Figure S19. ^{1}H and ^{13}C NMR spectra of **2b**



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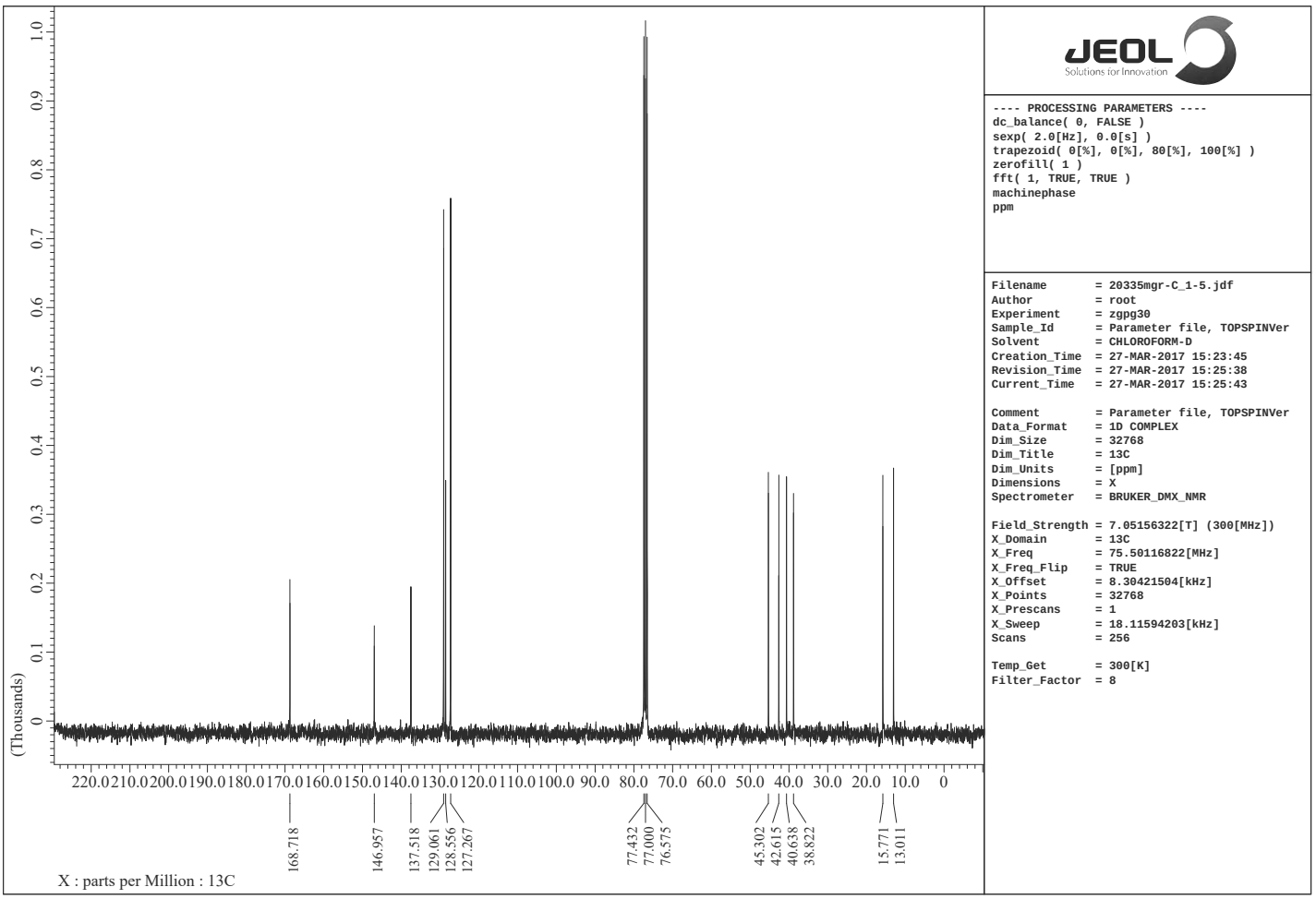
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename        = 20334mgr-H_1-4.jdf
Author          = root
Experiment      = zg30
Sample_Id       = Parameter file, TOPSPINVer
Solvent         = CHLOROFORM-D
Creation_Time   = 27-MAR-2017 15:13:49
Revision_Time   = 27-MAR-2017 15:17:58
Current_Time    = 27-MAR-2017 15:23:01

Comment         = Parameter file, TOPSPINVer
Data_Format     = 1D COMPLEX
Dim_Size        = 16384
Dim_Title       = 1H
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = BRUKER_DMX_NMR

Field_Strength = 7.05156322[T] (300[MHz])
X_Domain        = 1H
X_Freq          = 300.23150115[MHz]
X_Freq_Flip     = TRUE
X_Offset        = 1.50115[kHz]
X_Points        = 16384
X_Prescans      = 1
X_Sweep         = 3.61271676[kHz]
Scans           = 8

Temp_Get        = 300[K]
Filter_Factor   = 32
```



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```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

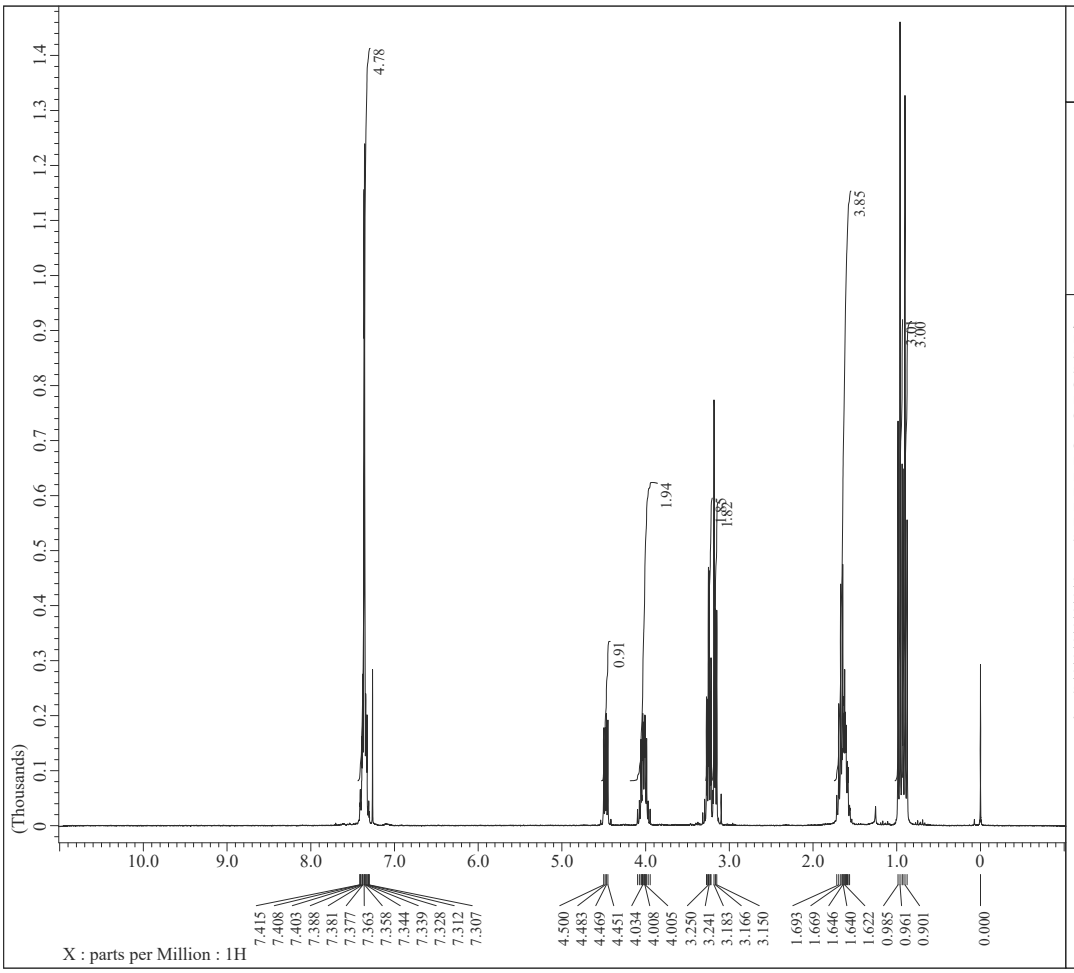
```
Filename        = 20335mgr-C_1-5.jdf
Author          = root
Experiment      = zgpg30
Sample_Id       = Parameter file, TOPSPINVer
Solvent         = CHLOROFORM-D
Creation_Time   = 27-MAR-2017 15:23:45
Revision_Time   = 27-MAR-2017 15:25:38
Current_Time    = 27-MAR-2017 15:25:43

Comment         = Parameter file, TOPSPINVer
Data_Format     = 1D COMPLEX
Dim_Size        = 32768
Dim_Title       = 13C
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = BRUKER_DMX_NMR

Field_Strength = 7.05156322[T] (300[MHz])
X_Domain        = 13C
X_Freq          = 75.50116822[MHz]
X_Freq_Flip     = TRUE
X_Offset        = 8.30421504[kHz]
X_Points        = 32768
X_Prescans      = 1
X_Sweep         = 18.11594203[kHz]
Scans           = 256

Temp_Get        = 300[K]
Filter_Factor   = 8
```

Figure S20. ^{1}H and ^{13}C NMR spectra of **2c**



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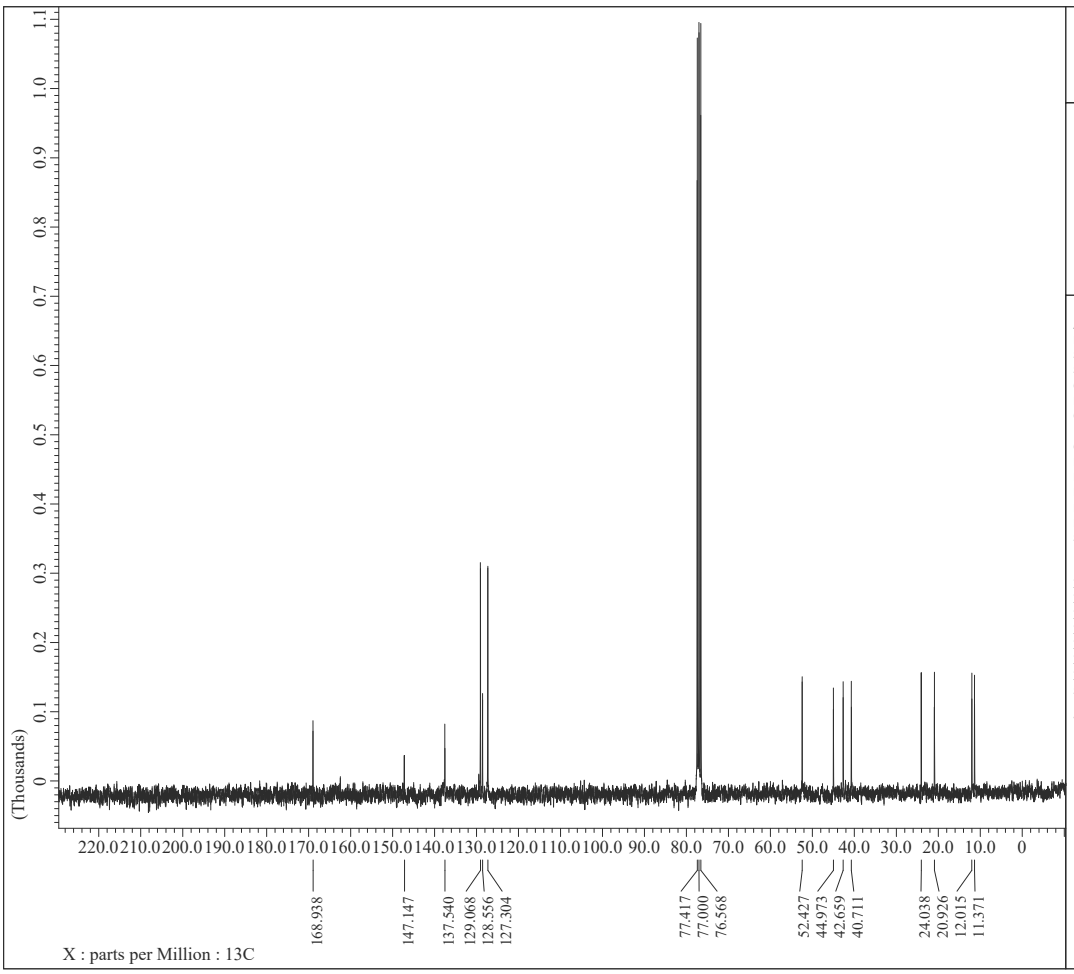
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename        = 24227rei-H_1-4.jdf
Author          = root
Experiment      = zg30
Sample_Id       = Parameter file, TOPSPINVer
Solvent         = CHLOROFORM-D
Creation_Time   = 31-MAR-2017 17:16:45
Revision_Time   = 31-MAR-2017 17:21:59
Current_Time    = 31-MAR-2017 17:22:03

Comment         = Parameter file, TOPSPINVer
Data_Format     = 1D COMPLEX
Dim_Size        = 16384
Dim_Title       = 1H
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = BRUKER_DMX_NMR

Field_Strength = 7.05156322[T] (300[MHz])
X_Domain        = 1H
X_Freq          = 300.23150115[MHz]
X_Freq_Flip     = TRUE
X_Offset        = 1.50115[kHz]
X_Points        = 16384
X_Prescans      = 1
X_Sweep         = 3.61271676[kHz]
Scans           = 8

Temp_Get        = 300[K]
Filter_Factor   = 32
```



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```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

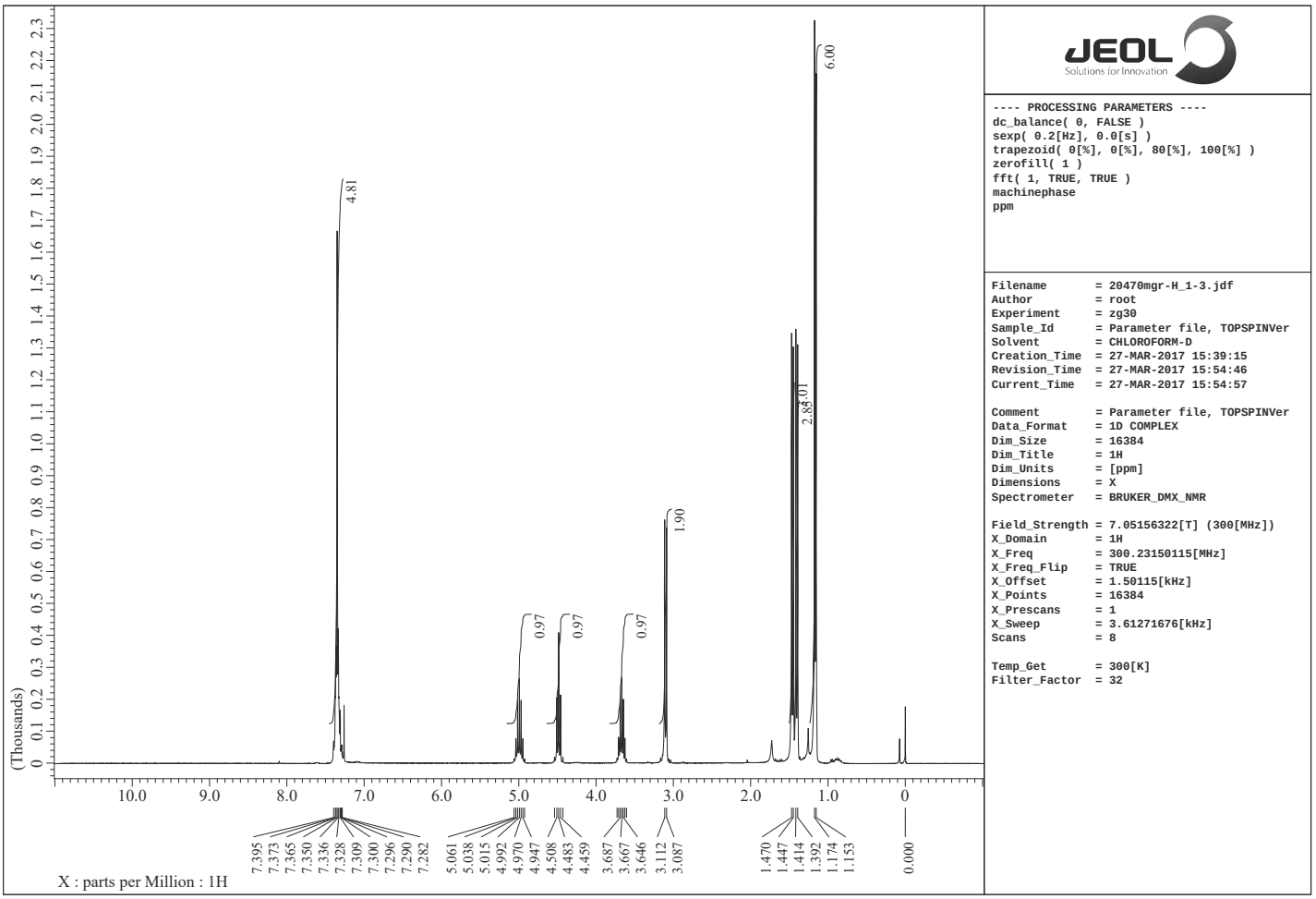
```
Filename        = 24228rei-C_1-4.jdf
Author          = root
Experiment      = zgpg30
Sample_Id       = Parameter file, TOPSPINVer
Solvent         = CHLOROFORM-D
Creation_Time   = 31-MAR-2017 17:31:53
Revision_Time   = 31-MAR-2017 17:33:46
Current_Time    = 31-MAR-2017 17:33:49

Comment         = Parameter file, TOPSPINVer
Data_Format     = 1D COMPLEX
Dim_Size        = 32768
Dim_Title       = 13C
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = BRUKER_DMX_NMR

Field_Strength = 7.05156322[T] (300[MHz])
X_Domain        = 13C
X_Freq          = 75.50116822[MHz]
X_Freq_Flip     = TRUE
X_Offset        = 8.30421504[kHz]
X_Points        = 32768
X_Prescans      = 1
X_Sweep         = 18.11594203[kHz]
Scans           = 256

Temp_Get        = 300[K]
Filter_Factor   = 8
```

Figure S21. ^{1}H and ^{13}C NMR spectra of **2d**



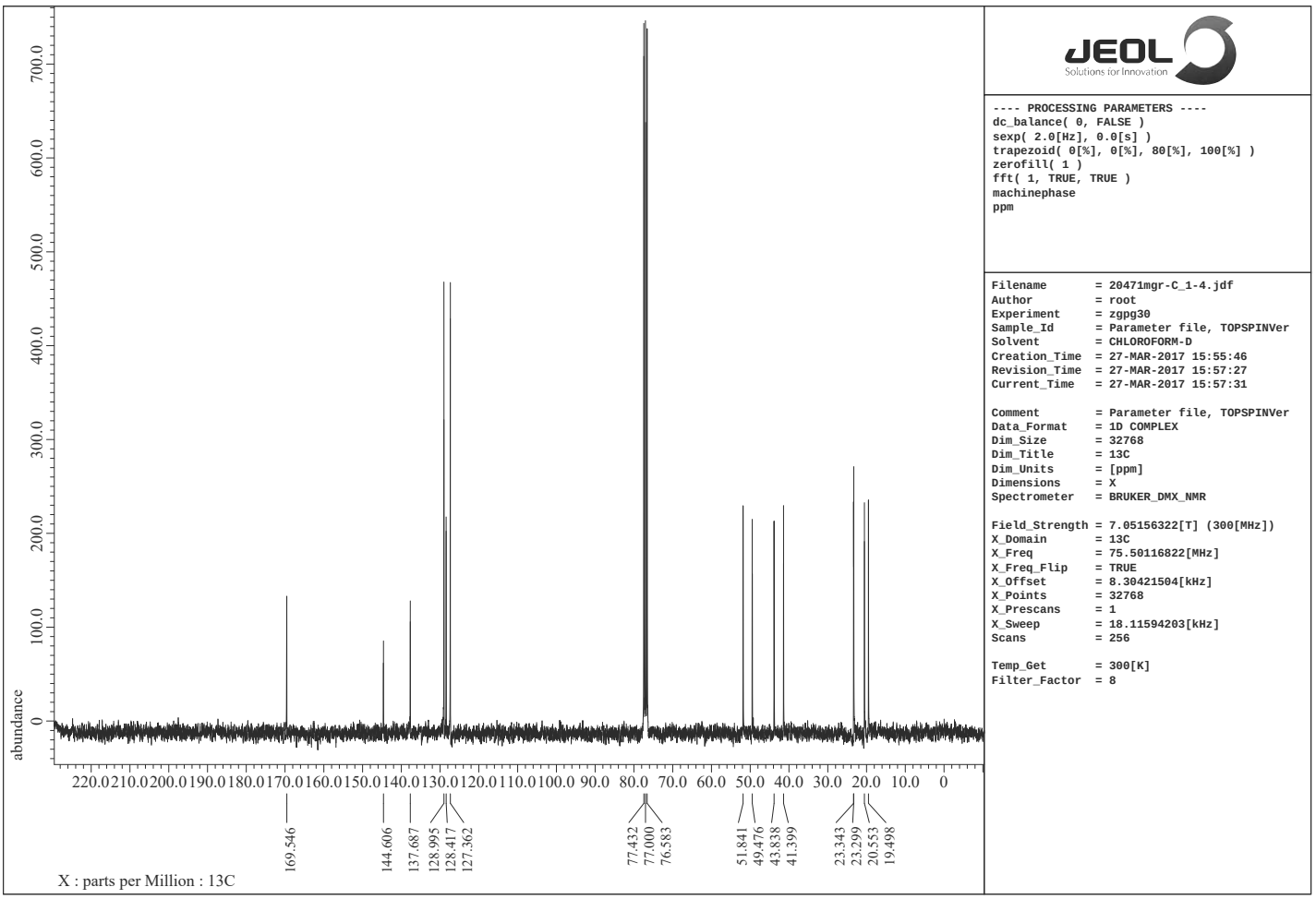
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm

Filename = 20470mgr-H_1-3.jdf
Author = root
Experiment = zg30
Sample_Id = Parameter file, TOPSPINVer
Solvent = CHLOROFORM-D
Creation_Time = 27-MAR-2017 15:39:15
Revision_Time = 27-MAR-2017 15:54:46
Current_Time = 27-MAR-2017 15:54:57

Comment = Parameter file, TOPSPINVer
Data_Format = 1D COMPLEX
Dim_Size = 16384
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Spectrometer = BRUKER_DMX_NMR

Field_Strength = 7.05156322[T] (300[MHz])
X_Domain = 1H
X_Freq = 300.23150115[MHz]
X_Freq_Flip = TRUE
X_Offset = 1.50115[kHz]
X_Points = 16384
X_Prescans = 1
X_Sweep = 3.61271676[kHz]
Scans = 8

Temp_Get = 300[K]
Filter_Factor = 32



---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm

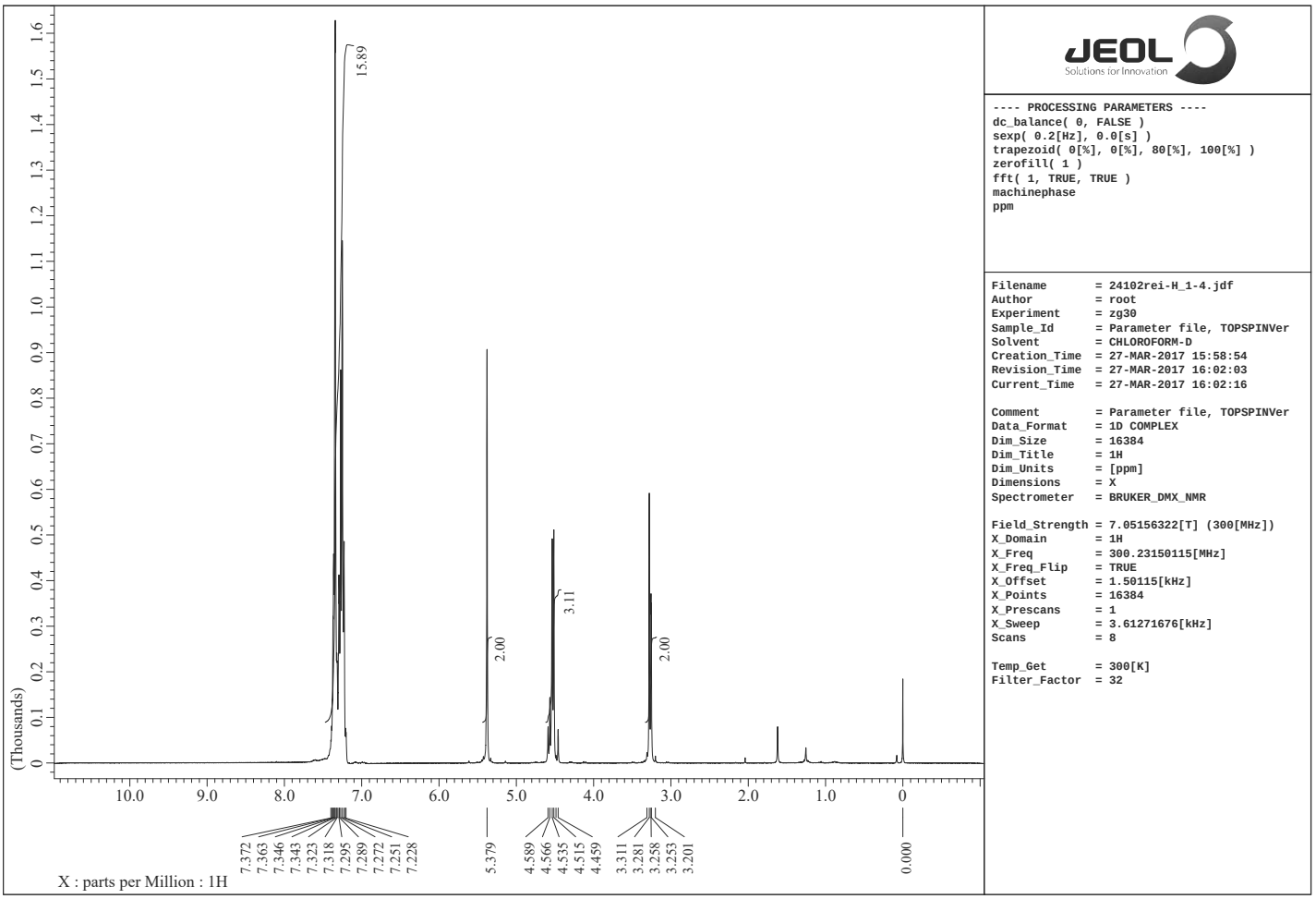
Filename = 20471mgr-C_1-4.jdf
Author = root
Experiment = zgpg30
Sample_Id = Parameter file, TOPSPINVer
Solvent = CHLOROFORM-D
Creation_Time = 27-MAR-2017 15:55:46
Revision_Time = 27-MAR-2017 15:57:27
Current_Time = 27-MAR-2017 15:57:31

Comment = Parameter file, TOPSPINVer
Data_Format = 1D COMPLEX
Dim_Size = 32768
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Spectrometer = BRUKER_DMX_NMR

Field_Strength = 7.05156322[T] (300[MHz])
X_Domain = 13C
X_Freq = 75.50116822[MHz]
X_Freq_Flip = TRUE
X_Offset = 8.30421504[kHz]
X_Points = 32768
X_Prescans = 1
X_Sweep = 18.11594203[kHz]
Scans = 256

Temp_Get = 300[K]
Filter_Factor = 8

Figure S22. ^{1}H and ^{13}C NMR spectra of **2e**



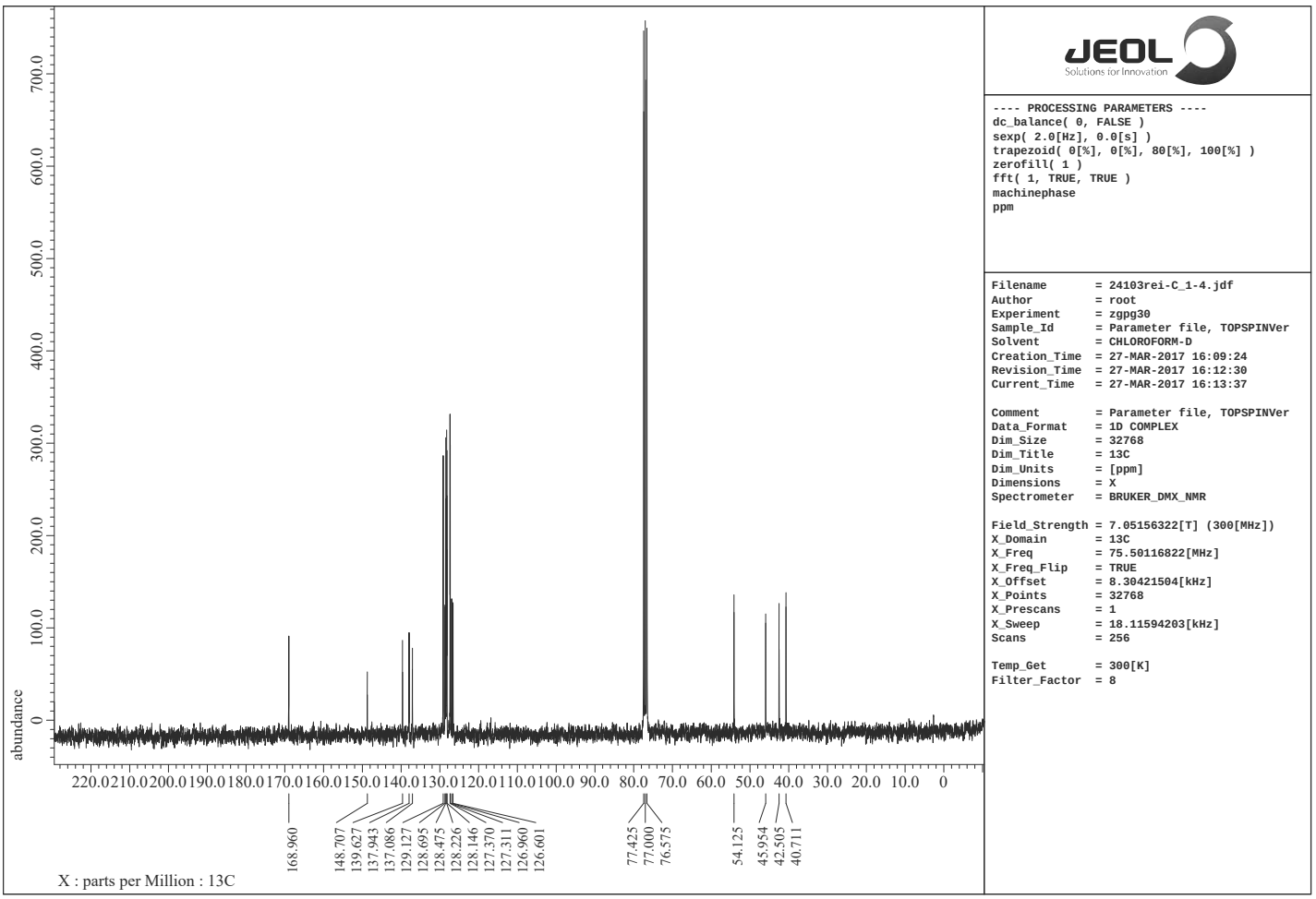
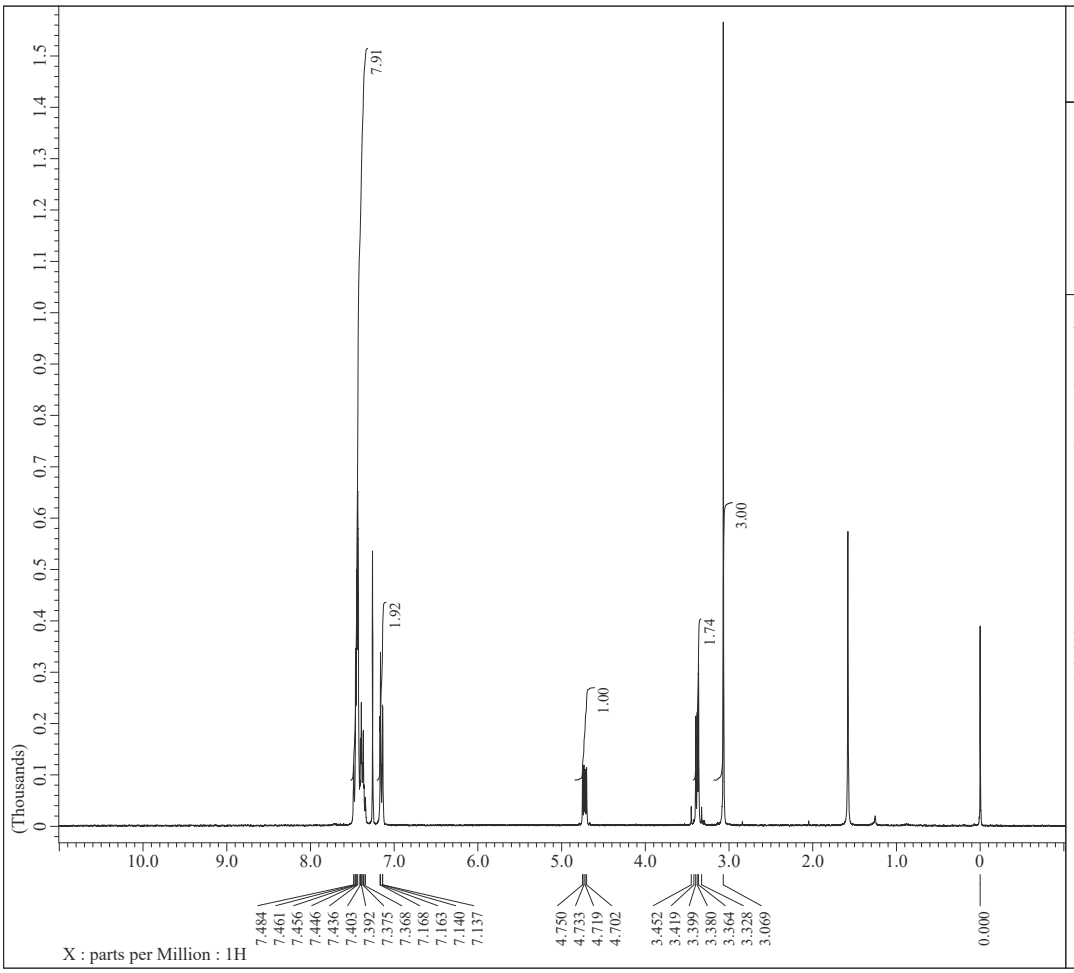


Figure S23. ^{1}H and ^{13}C NMR spectra of **2f**



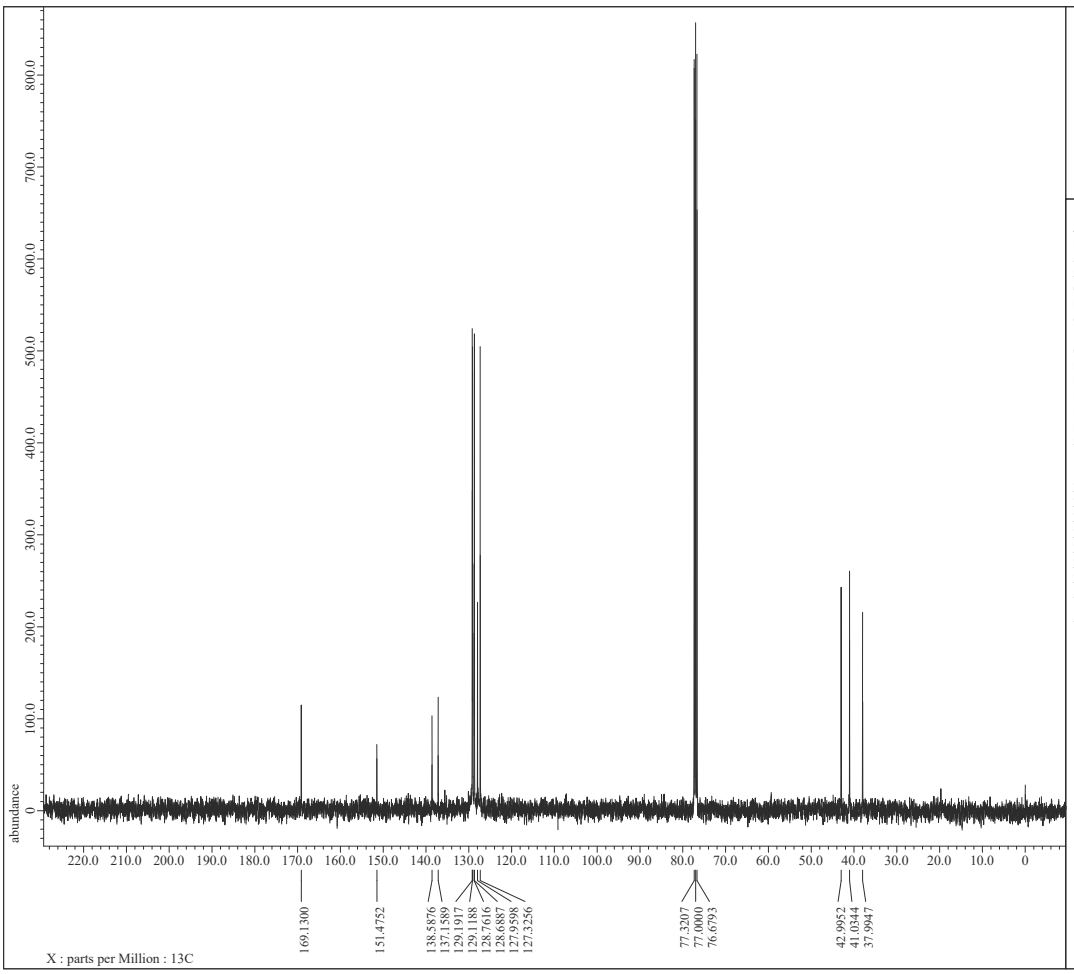

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename        = 22200rei-H_1-5.jdf
Author          = root
Experiment      = zg30
Sample_Id       = Parameter file, TOPSPINVer
Solvent         = CHLOROFORM-D
Creation_Time   = 27-MAR-2017 16:17:12
Revision_Time   = 27-MAR-2017 16:20:35
Current_Time    = 27-MAR-2017 16:20:47

Comment         = Parameter file, TOPSPINVer
Data_Format     = 1D COMPLEX
Dim_Size        = 16384
Dim_Title       = 1H
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = BRUKER_DMX_NMR

Field_Strength = 7.05156322[T] (300[MHz])
X_Domain        = 1H
X_Freq          = 300.23150115[MHz]
X_Freq_Flip     = TRUE
X_Offset        = 1.50115[kHz]
X_Points        = 16384
X_Prescans      = 1
X_Sweep         = 3.61271676[kHz]
Scans           = 8

Temp_Get        = 300[K]
Filter_Factor   = 32
```




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

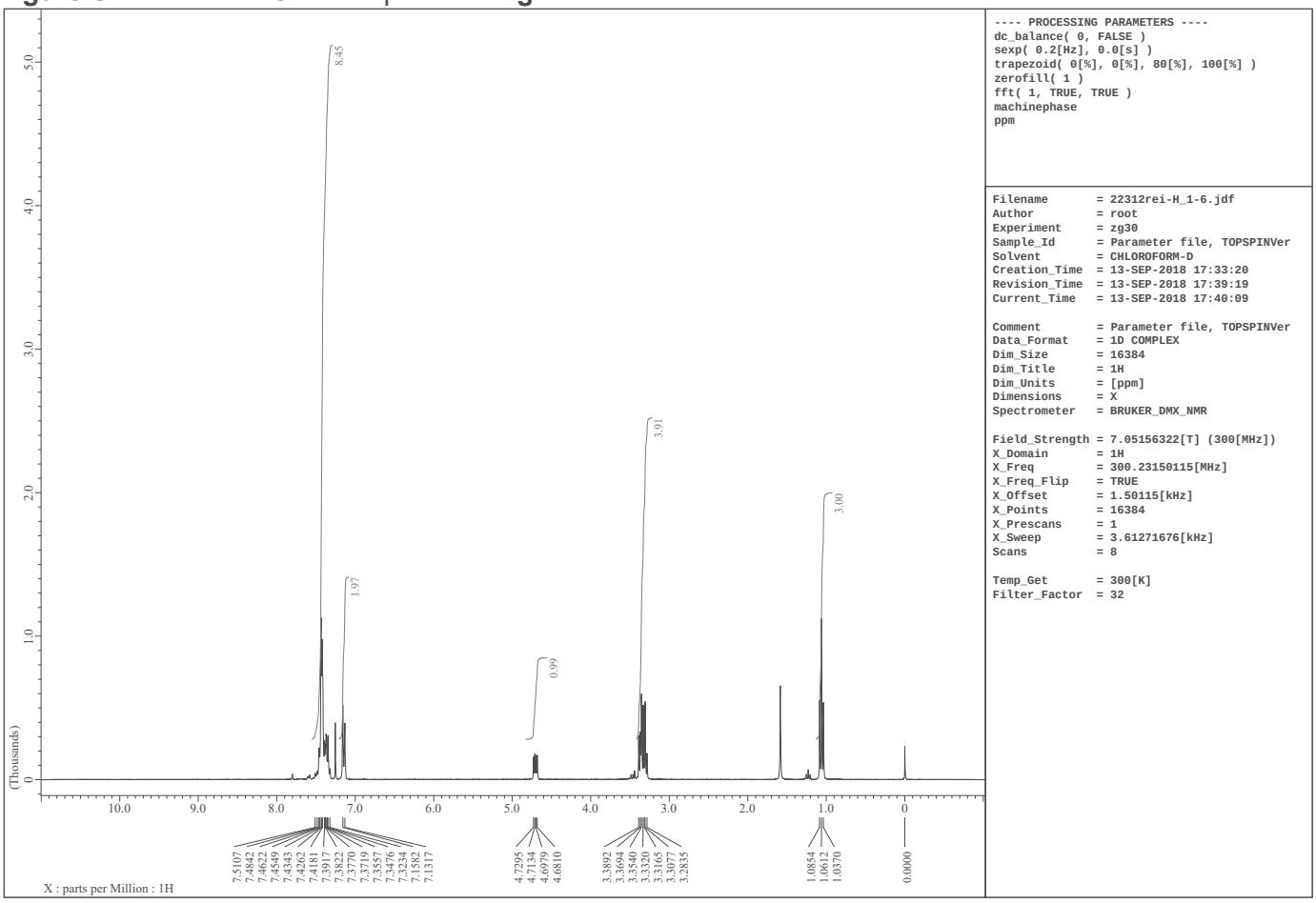
```
Filename        = 4-0404rei-C_2-4.jdf
Author          = nmr
Experiment      = zgpg30
Sample_Id       = Parameter file, TopSpin 3.5
Solvent         = CHLOROFORM-D
Creation_Time   =  2-MAY-2018 14:03:33
Revision_Time   =  2-MAY-2018 14:04:52
Current_Time    =  2-MAY-2018 14:04:58

Comment         = Parameter file, TopSpin 3.5
Data_Format     = 1D COMPLEX
Dim_Size        = 32768
Dim_Title       = 13C
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = BRUKER_DMX_NMR

Field_Strength = 9.39910925[T] (400[MHz])
X_Domain        = 13C
X_Freq          = 100.63640982[MHz]
X_Freq_Flip     = TRUE
X_Offset        = 11.068788[kHz]
X_Points        = 32768
X_Prescans      = 2
X_Sweep         = 24.03846154[kHz]
Scans           = 70

Temp_Get        = 296.56[K]
Filter_Factor   = 832
```

Figure S24. ^{1}H and ^{13}C NMR spectra of **2g**



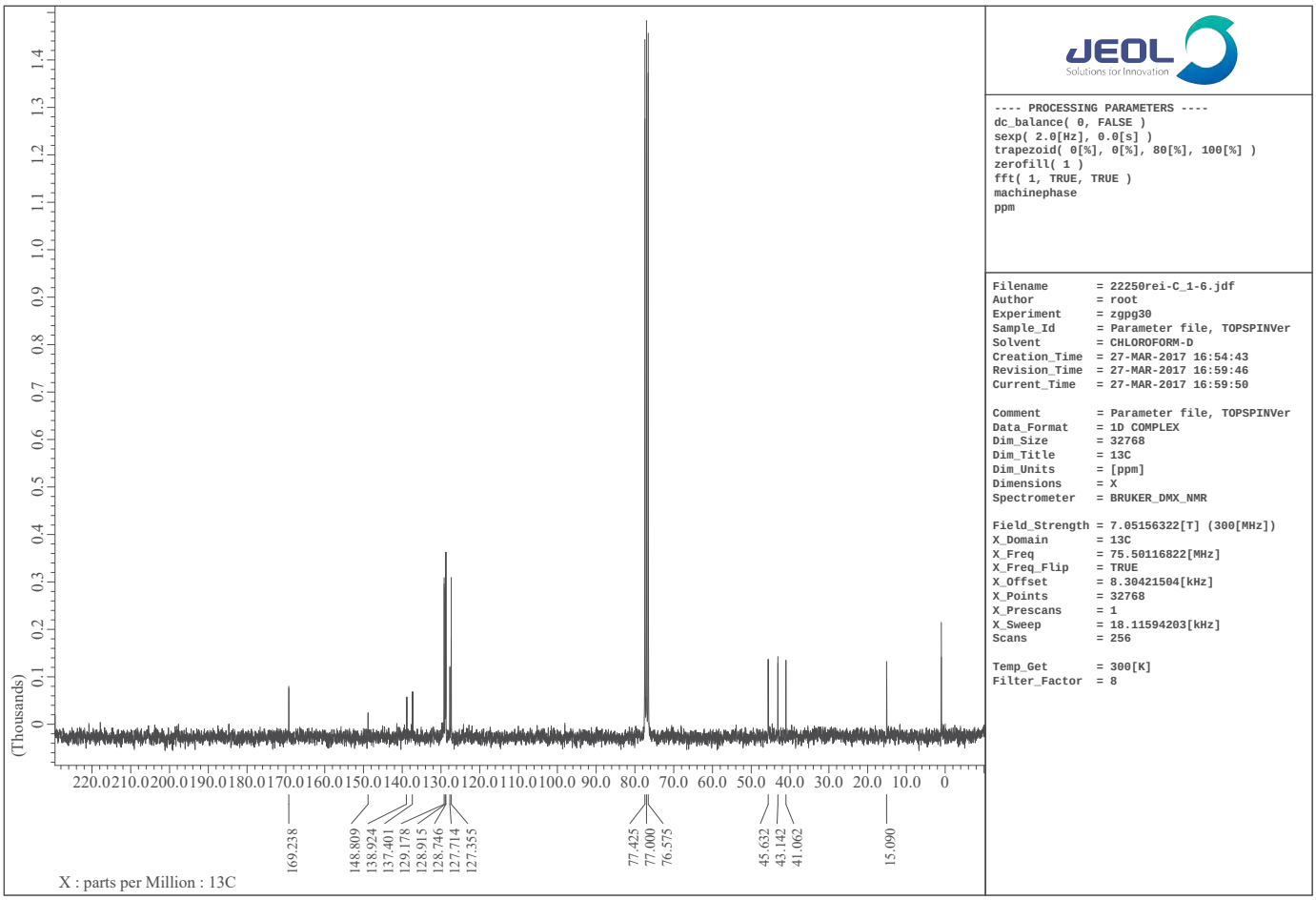
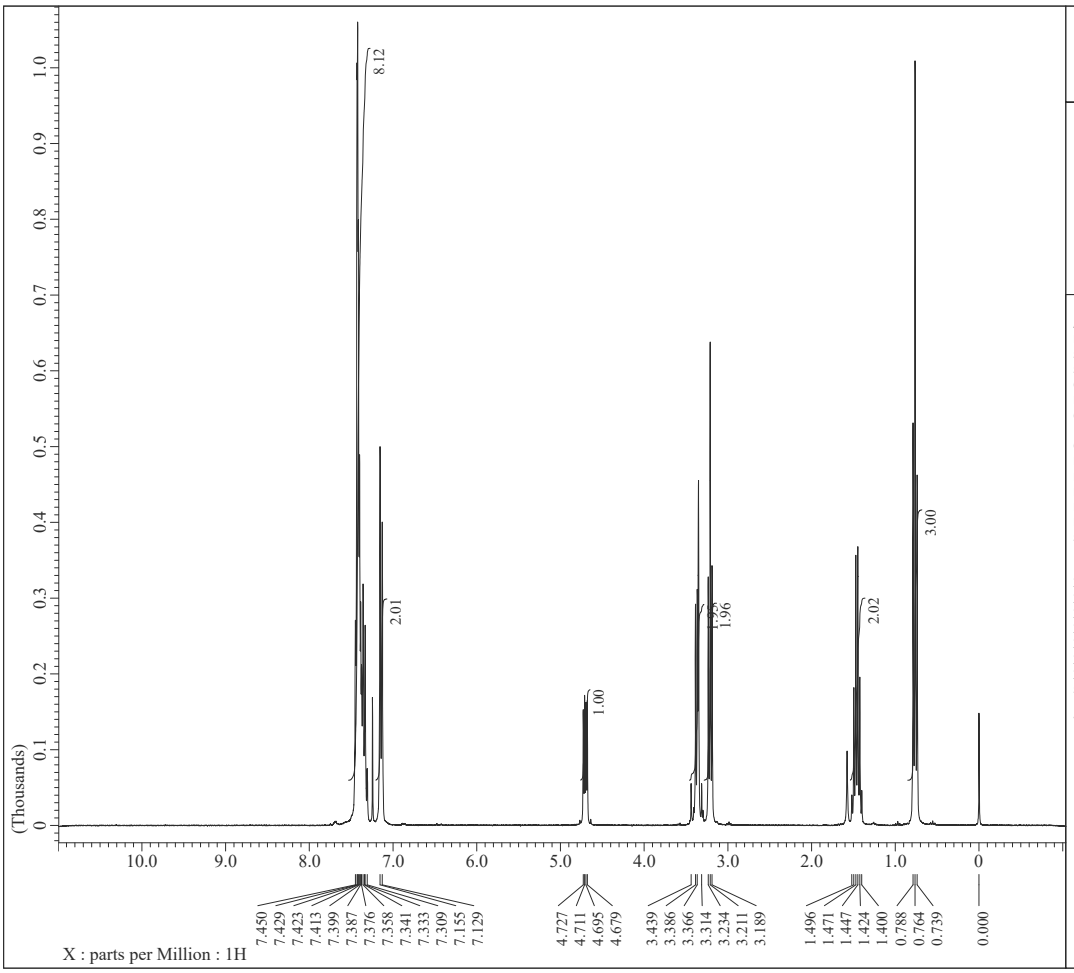


Figure S25. ^{1}H and ^{13}C NMR spectra of **2h**



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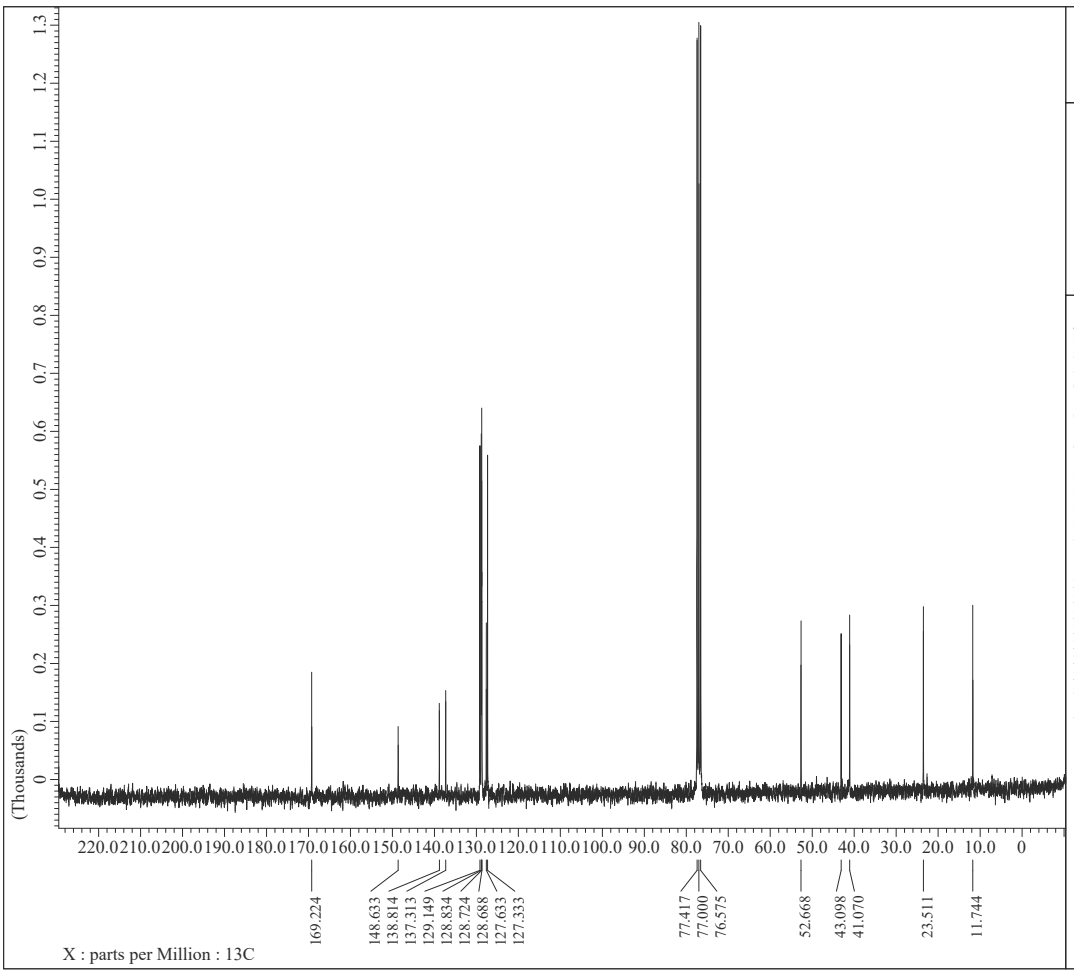
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename        = 22364rei-H_1-5.jdf
Author          = root
Experiment      = zg30
Sample_Id       = Parameter file, TOPSPINVer
Solvent         = CHLOROFORM-D
Creation_Time   = 27-MAR-2017 17:02:25
Revision_Time   = 27-MAR-2017 17:14:07
Current_Time    = 27-MAR-2017 17:18:00

Comment         = Parameter file, TOPSPINVer
Data_Format     = 1D COMPLEX
Dim_Size        = 16384
Dim_Title       = 1H
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = BRUKER_DMX_NMR

Field_Strength = 7.05156322[T] (300[MHz])
X_Domain        = 1H
X_Freq          = 300.23150115[MHz]
X_Freq_Flip     = TRUE
X_Offset        = 1.50115[kHz]
X_Points        = 16384
X_Prescans      = 1
X_Sweep         = 3.61271676[kHz]
Scans           = 8

Temp_Get        = 292.16[K]
Filter_Factor   = 32
```



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```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

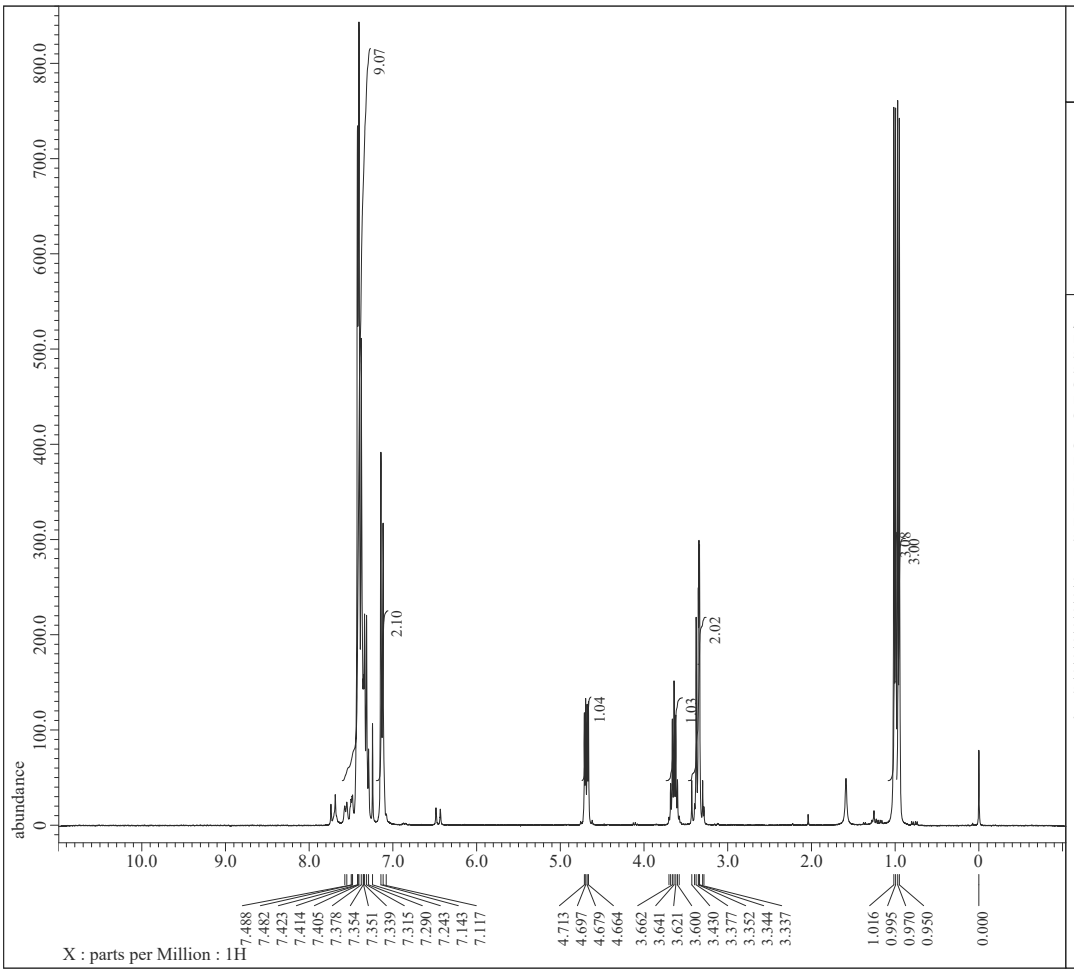
```
Filename        = 22365rei-C_1-5.jdf
Author          = root
Experiment      = zgpg30
Sample_Id       = Parameter file, TOPSPINVer
Solvent         = CHLOROFORM-D
Creation_Time   = 27-MAR-2017 17:19:00
Revision_Time   = 27-MAR-2017 17:20:34
Current_Time    = 27-MAR-2017 17:20:38

Comment         = Parameter file, TOPSPINVer
Data_Format     = 1D COMPLEX
Dim_Size        = 32768
Dim_Title       = 13C
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = BRUKER_DMX_NMR

Field_Strength = 7.05156322[T] (300[MHz])
X_Domain        = 13C
X_Freq          = 75.50116822[MHz]
X_Freq_Flip     = TRUE
X_Offset        = 8.30421504[kHz]
X_Points        = 32768
X_Prescans      = 1
X_Sweep         = 18.11594203[kHz]
Scans           = 256

Temp_Get        = 293.16[K]
Filter_Factor   = 8
```

Figure S26. ^{1}H and ^{13}C NMR spectra of **2i**



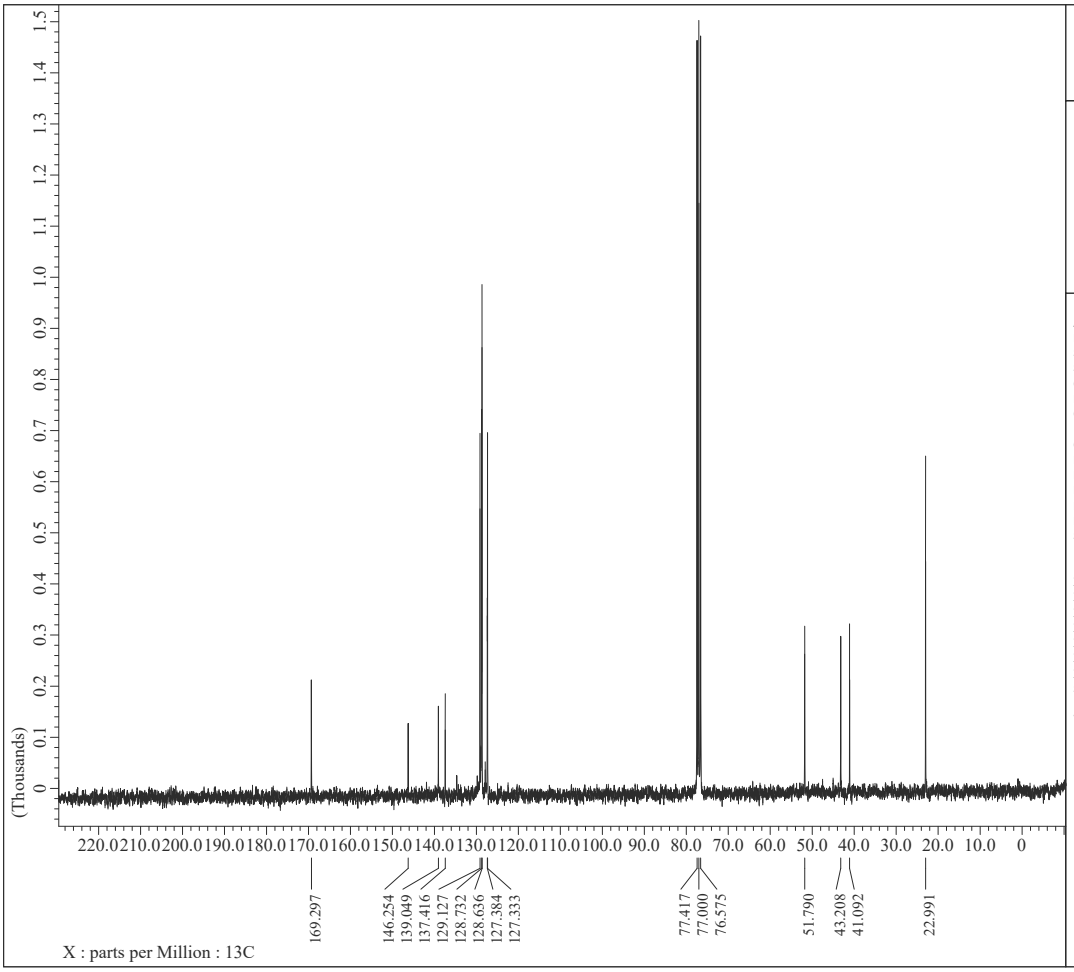

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename        = 22292rei-H_1-6.jdf
Author          = root
Experiment      = zg30
Sample_Id       = Parameter file, TOPSPINVer
Solvent         = CHLOROFORM-D
Creation_Time   = 27-MAR-2017 17:39:18
Revision_Time   = 27-MAR-2017 17:42:13
Current_Time    = 27-MAR-2017 17:42:33

Comment         = Parameter file, TOPSPINVer
Data_Format     = 1D COMPLEX
Dim_Size        = 16384
Dim_Title       = 1H
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = BRUKER_DMX_NMR

Field_Strength = 7.05156322[T] (300[MHz])
X_Domain        = 1H
X_Freq          = 300.23150115[MHz]
X_Freq_Flip     = TRUE
X_Offset        = 1.50115[kHz]
X_Points        = 16384
X_Prescans      = 1
X_Sweep         = 3.61271676[kHz]
Scans           = 8

Temp_Get        = 300[K]
Filter_Factor   = 32
```




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

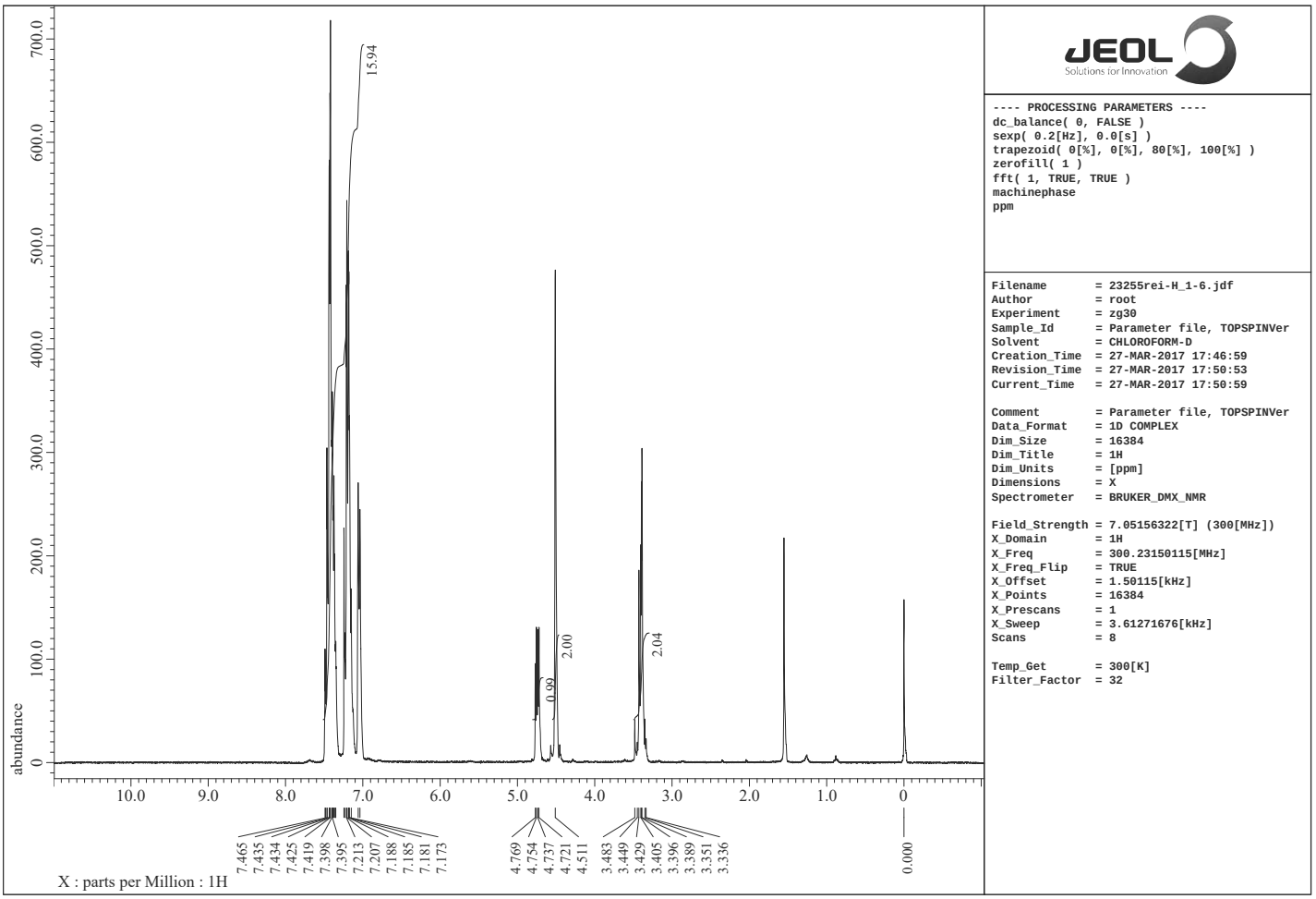
```
Filename        = 22293rei-C_1-5.jdf
Author          = root
Experiment      = zgpg30
Sample_Id       = Parameter file, TOPSPINVer
Solvent         = CHLOROFORM-D
Creation_Time   = 27-MAR-2017 17:21:44
Revision_Time   = 27-MAR-2017 17:24:20
Current_Time    = 27-MAR-2017 17:24:24

Comment         = Parameter file, TOPSPINVer
Data_Format     = 1D COMPLEX
Dim_Size        = 32768
Dim_Title       = 13C
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = BRUKER_DMX_NMR

Field_Strength = 7.05156322[T] (300[MHz])
X_Domain        = 13C
X_Freq          = 75.50116822[MHz]
X_Freq_Flip     = TRUE
X_Offset        = 8.30421504[kHz]
X_Points        = 32768
X_Prescans      = 1
X_Sweep         = 18.11594203[kHz]
Scans           = 256

Temp_Get        = 300[K]
Filter_Factor   = 8
```

Figure S27. ^{1}H and ^{13}C NMR spectra of **2j**



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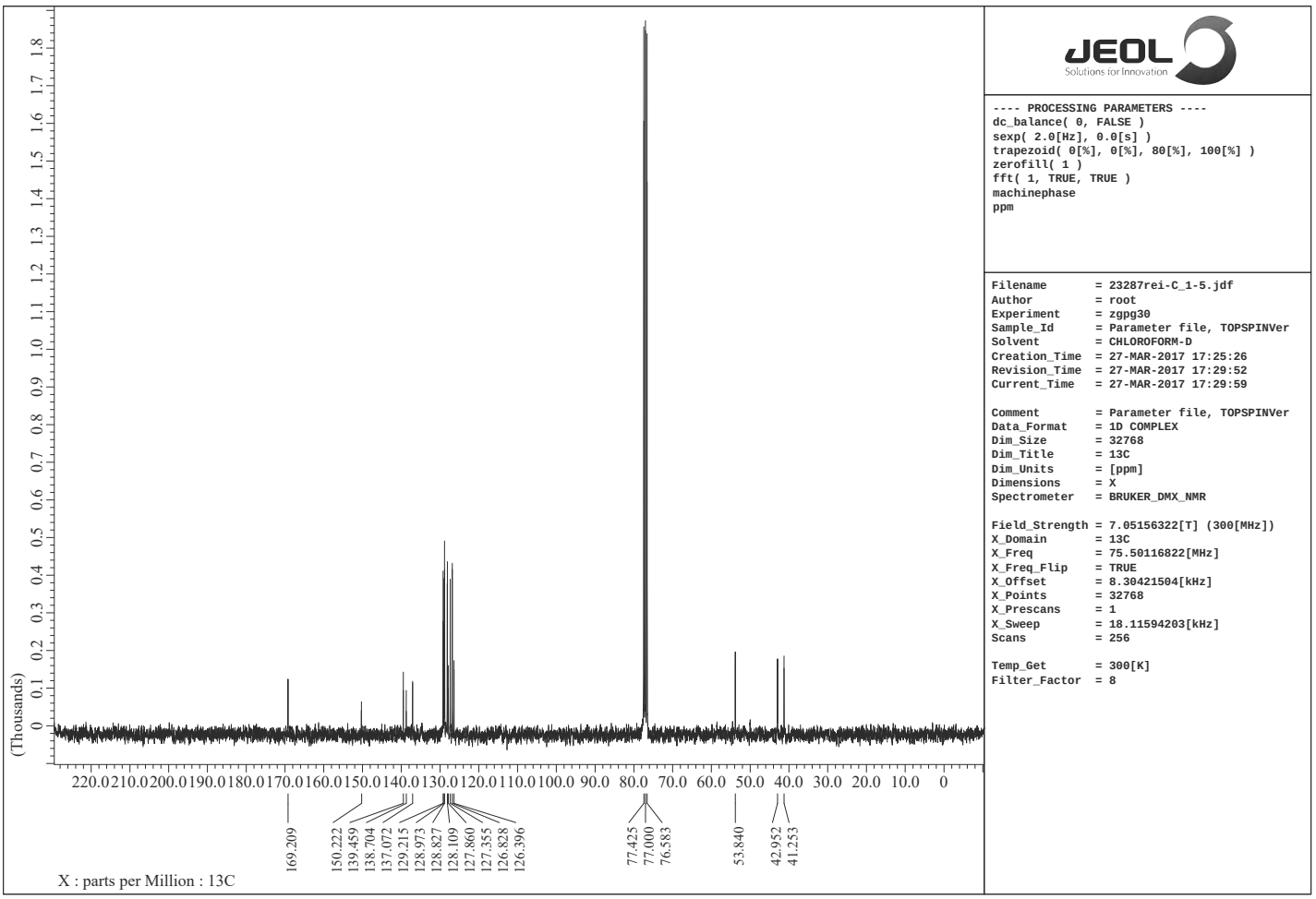
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename        = 23255rei-H_1-6.jdf
Author          = root
Experiment      = zg30
Sample_Id       = Parameter file, TOPSPINVer
Solvent         = CHLOROFORM-D
Creation_Time   = 27-MAR-2017 17:46:59
Revision_Time   = 27-MAR-2017 17:50:53
Current_Time    = 27-MAR-2017 17:50:59

Comment         = Parameter file, TOPSPINVer
Data_Format     = 1D COMPLEX
Dim_Size        = 16384
Dim_Title       = 1H
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = BRUKER_DMX_NMR

Field_Strength = 7.05156322[T] (300[MHz])
X_Domain        = 1H
X_Freq          = 300.23150115[MHz]
X_Freq_Flip     = TRUE
X_Offset        = 1.50115[kHz]
X_Points        = 16384
X_Prescans      = 1
X_Sweep         = 3.61271676[kHz]
Scans           = 8

Temp_Get        = 300[K]
Filter_Factor   = 32
```



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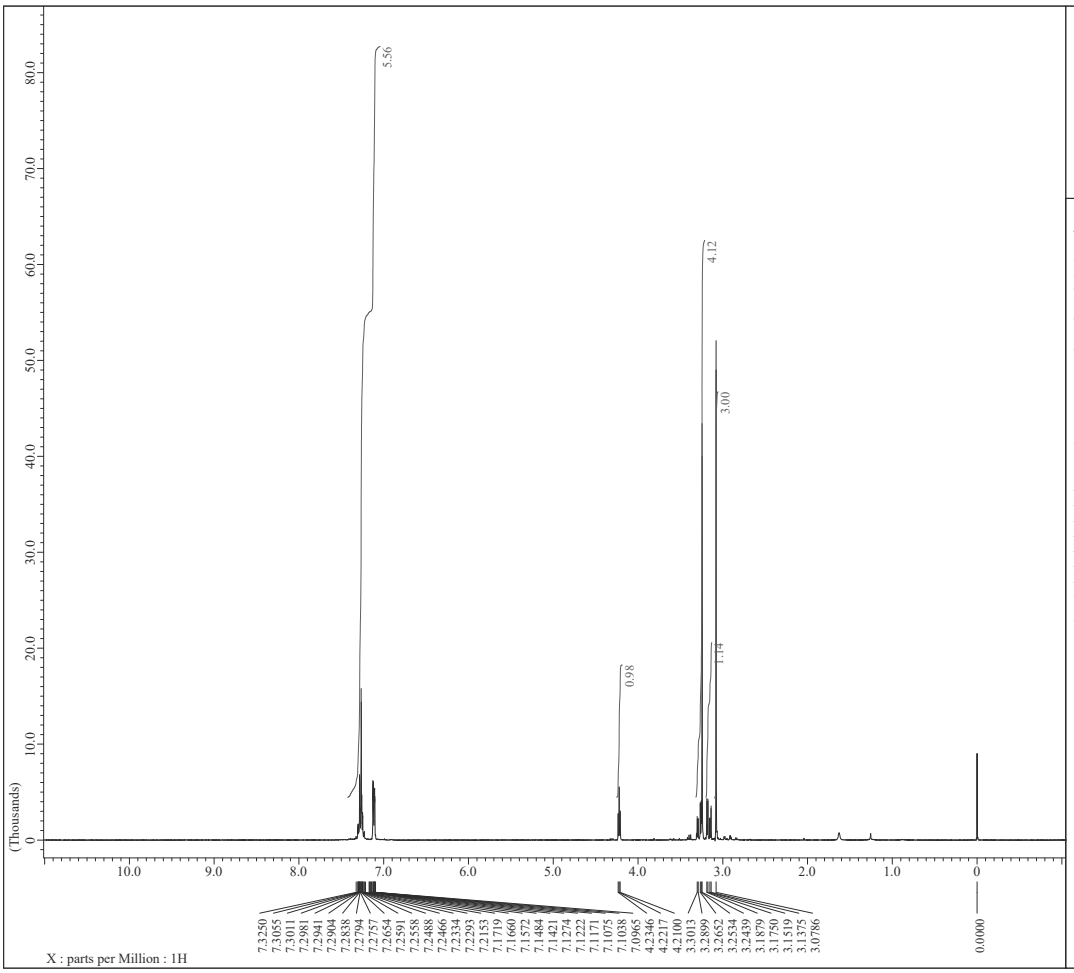
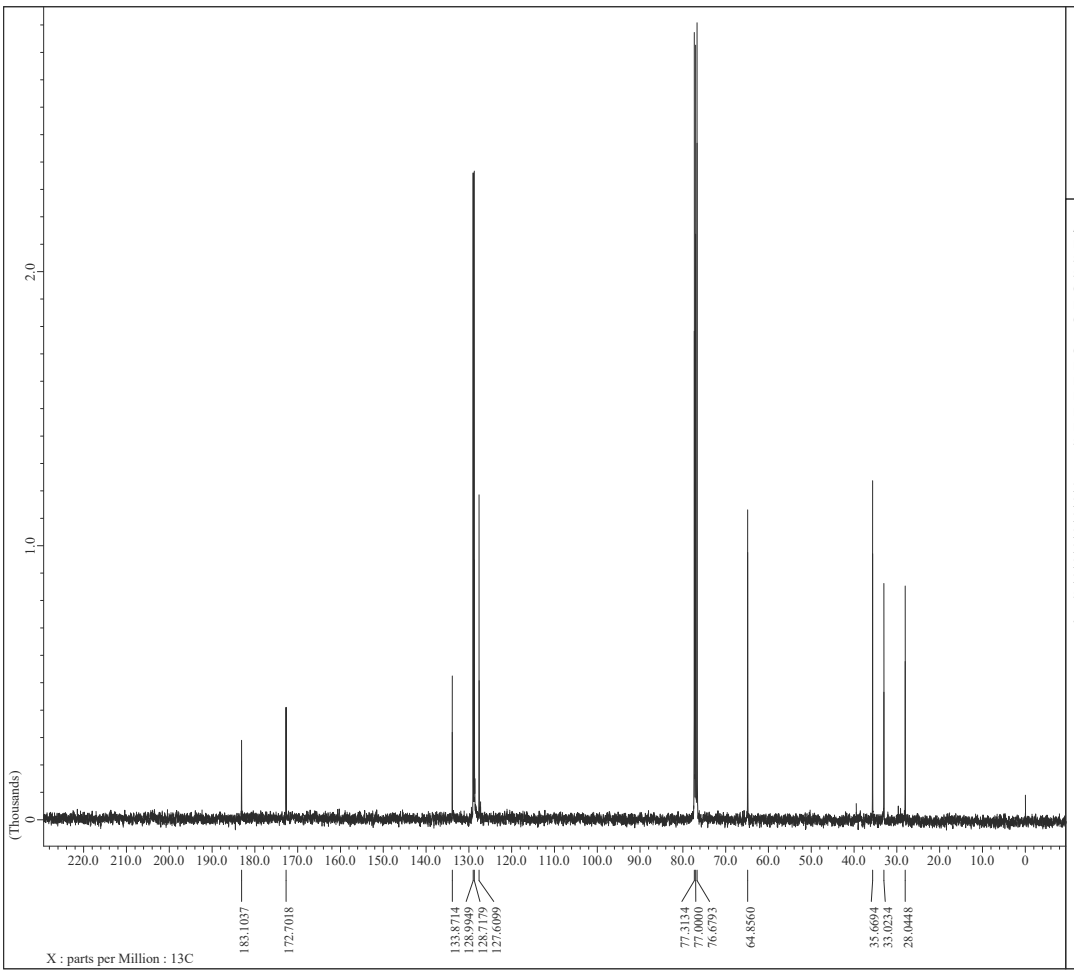
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename        = 23287rei-C_1-5.jdf
Author          = root
Experiment      = zgpg30
Sample_Id       = Parameter file, TOPSPINVer
Solvent         = CHLOROFORM-D
Creation_Time   = 27-MAR-2017 17:25:26
Revision_Time   = 27-MAR-2017 17:29:52
Current_Time    = 27-MAR-2017 17:29:59

Comment         = Parameter file, TOPSPINVer
Data_Format     = 1D COMPLEX
Dim_Size        = 32768
Dim_Title       = 13C
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = BRUKER_DMX_NMR

Field_Strength = 7.05156322[T] (300[MHz])
X_Domain        = 13C
X_Freq          = 75.50116822[MHz]
X_Freq_Flip     = TRUE
X_Offset        = 8.30421504[kHz]
X_Points        = 32768
X_Prescans      = 1
X_Sweep         = 18.11594203[kHz]
Scans           = 256

Temp_Get        = 300[K]
Filter_Factor   = 8
```

Figure S28. ^{1}H and ^{13}C NMR spectra of **3a**

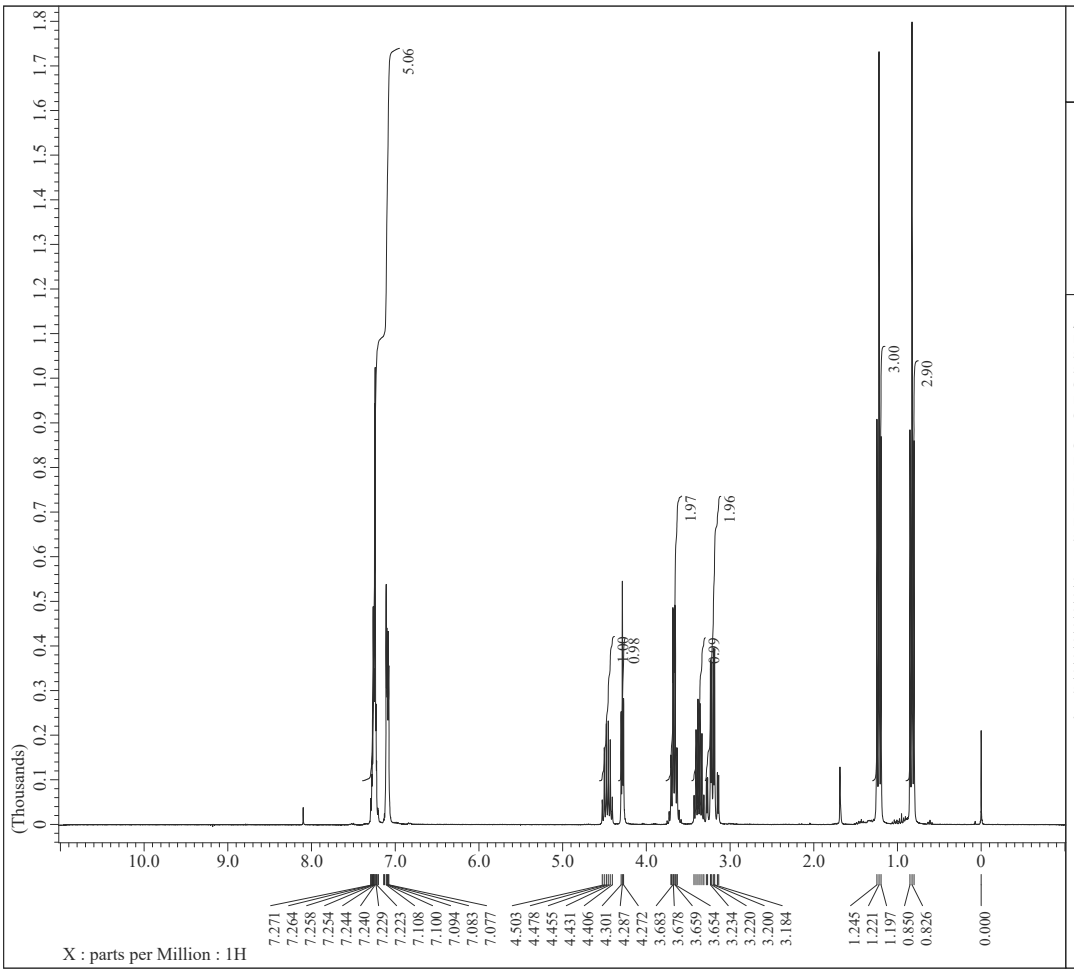



```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Filename        = 4-0391rei-H_2-4.jdf
Author          = nmr
Experiment      = zg30
Sample_Id       = Parameter file, TopSpin 3.5
Solvent         = CHLOROFORM-D
Creation_Time   = 17-APR-2018 18:07:56
Revision_Time   = 17-APR-2018 18:13:21
Current_Time    = 17-APR-2018 18:13:28

Comment         = Parameter file, TopSpin 3.5
Data_Format     = 1D COMPLEX
Dim_Size        = 32768
Dim_Title       = 1H
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = BRUKER_DMX_NMR

Field_Strength = 9.39910925[T] (400[MHz])
X_Domain        = 1H
X_Freq          = 400.1820009[MHz]
X_Freq_Flip     = TRUE
X_Offset        = 2.0009[kHz]
X_Points        = 32768
X_Prescans      = 1
X_Sweep         = 4.82625483[kHz]
Scans           = 8

Temp_Get        = 296.76[K]
Filter_Factor   = 4144
```



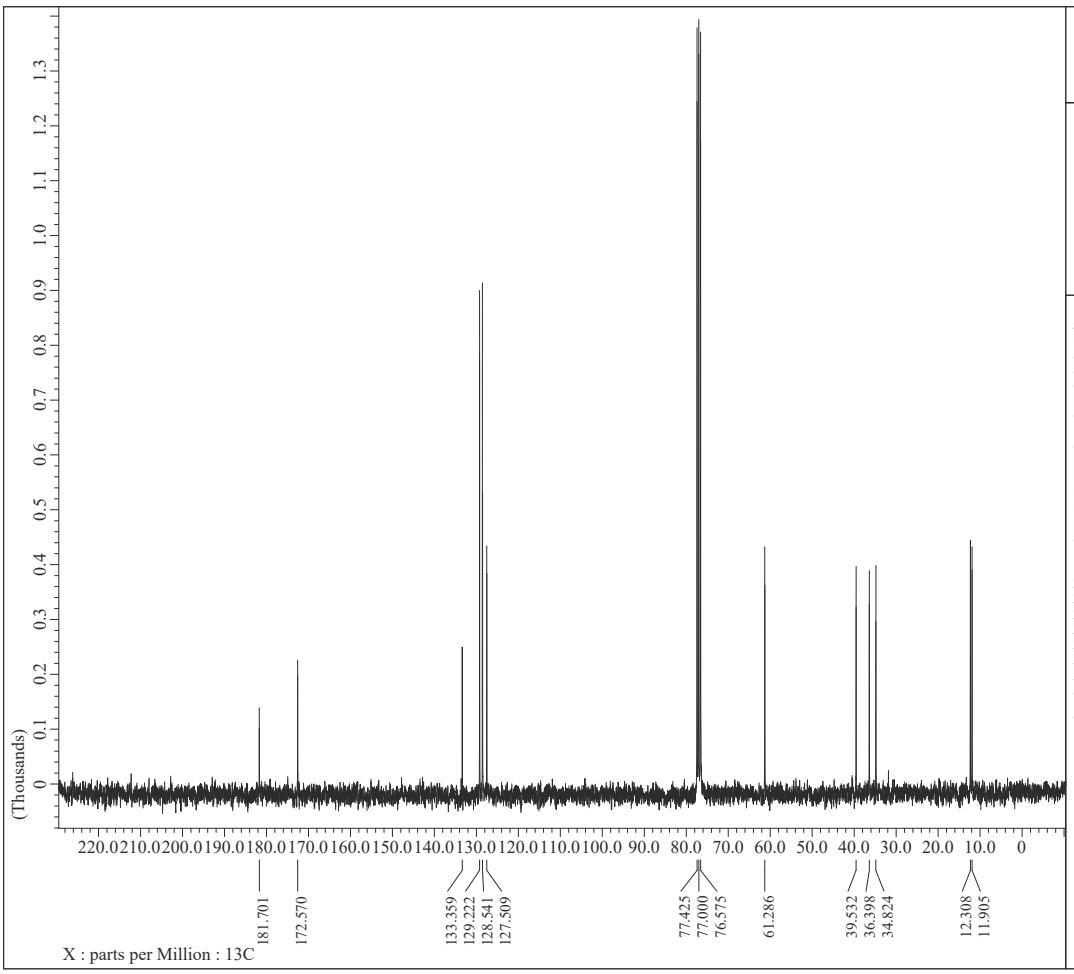

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Filename        = 4-0390rei-C_1-4.jdf
Author          = nmr
Experiment      = zgpg30
Sample_Id       = Parameter file, TopSpin 3.5
Solvent         = CHLOROFORM-D
Creation_Time   = 17-APR-2018 18:05:28
Revision_Time   = 17-APR-2018 18:07:04
Current_Time    = 17-APR-2018 18:07:13

Comment         = Parameter file, TopSpin 3.5
Data_Format     = 1D COMPLEX
Dim_Size        = 32768
Dim_Title       = 13C
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = BRUKER_DMX_NMR

Field_Strength = 9.39910925[T] (400[MHz])
X_Domain        = 13C
X_Freq          = 100.63640982[MHz]
X_Freq_Flip     = TRUE
X_Offset        = 11.068788[kHz]
X_Points        = 32768
X_Prescans      = 2
X_Sweep         = 24.03846154[kHz]
Scans           = 256

Temp_Get        = 297.56[K]
Filter_Factor   = 832
```

Figure S29. ^{1}H and ^{13}C NMR spectra of **3b**




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

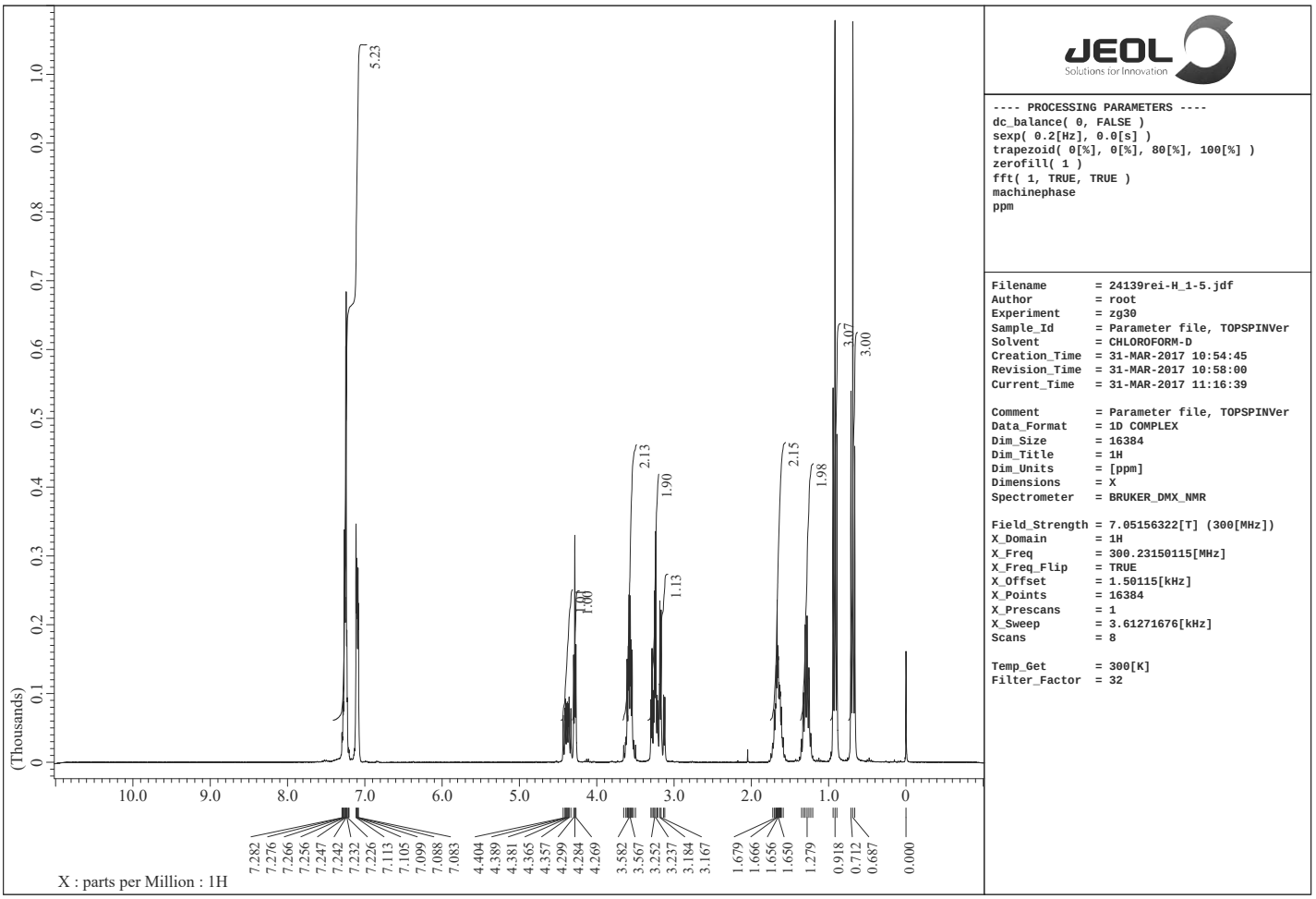
```
Filename        = 24159rei-H_1-6.jdf
Author          = root
Experiment      = zg30
Sample_Id       = Parameter file, TOPSPINVer
Solvent         = CHLOROFORM-D
Creation_Time   = 31-MAR-2017 10:40:10
Revision_Time   = 31-MAR-2017 10:43:18
Current_Time    = 31-MAR-2017 10:48:33

Comment         = Parameter file, TOPSPINVer
Data_Format     = 1D COMPLEX
Dim_Size        = 16384
Dim_Title       = 1H
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = BRUKER_DMX_NMR

Field_Strength = 7.05156322[T] (300[MHz])
X_Domain        = 1H
X_Freq          = 300.23150115[MHz]
X_Freq_Flip     = TRUE
X_Offset        = 1.50115[kHz]
X_Points        = 16384
X_Prescans      = 1
X_Sweep         = 3.61271676[kHz]
Scans           = 8

Temp_Get        = 300[K]
Filter_Factor   = 32
```




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename        = 24160rei-C_1-5.jdf
Author          = root
Experiment      = zgpg30
Sample_Id       = Parameter file, TOPSPINVer
Solvent         = CHLOROFORM-D
Creation_Time   = 31-MAR-2017 10:49:38
Revision_Time   = 31-MAR-2017 10:50:39
Current_Time    = 31-MAR-2017 10:50:44

Comment         = Parameter file, TOPSPINVer
Data_Format     = 1D COMPLEX
Dim_Size        = 32768
Dim_Title       = 13C
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = BRUKER_DMX_NMR

Field_Strength = 7.05156322[T] (300[MHz])
X_Domain        = 13C
X_Freq          = 75.50116822[MHz]
X_Freq_Flip     = TRUE
X_Offset        = 8.30421504[kHz]
X_Points        = 32768
X_Prescans      = 1
X_Sweep         = 18.11594203[kHz]
Scans           = 128

Temp_Get        = 300[K]
Filter_Factor   = 8
```

Figure S30. ^{1}H and ^{13}C NMR spectra of **3c**



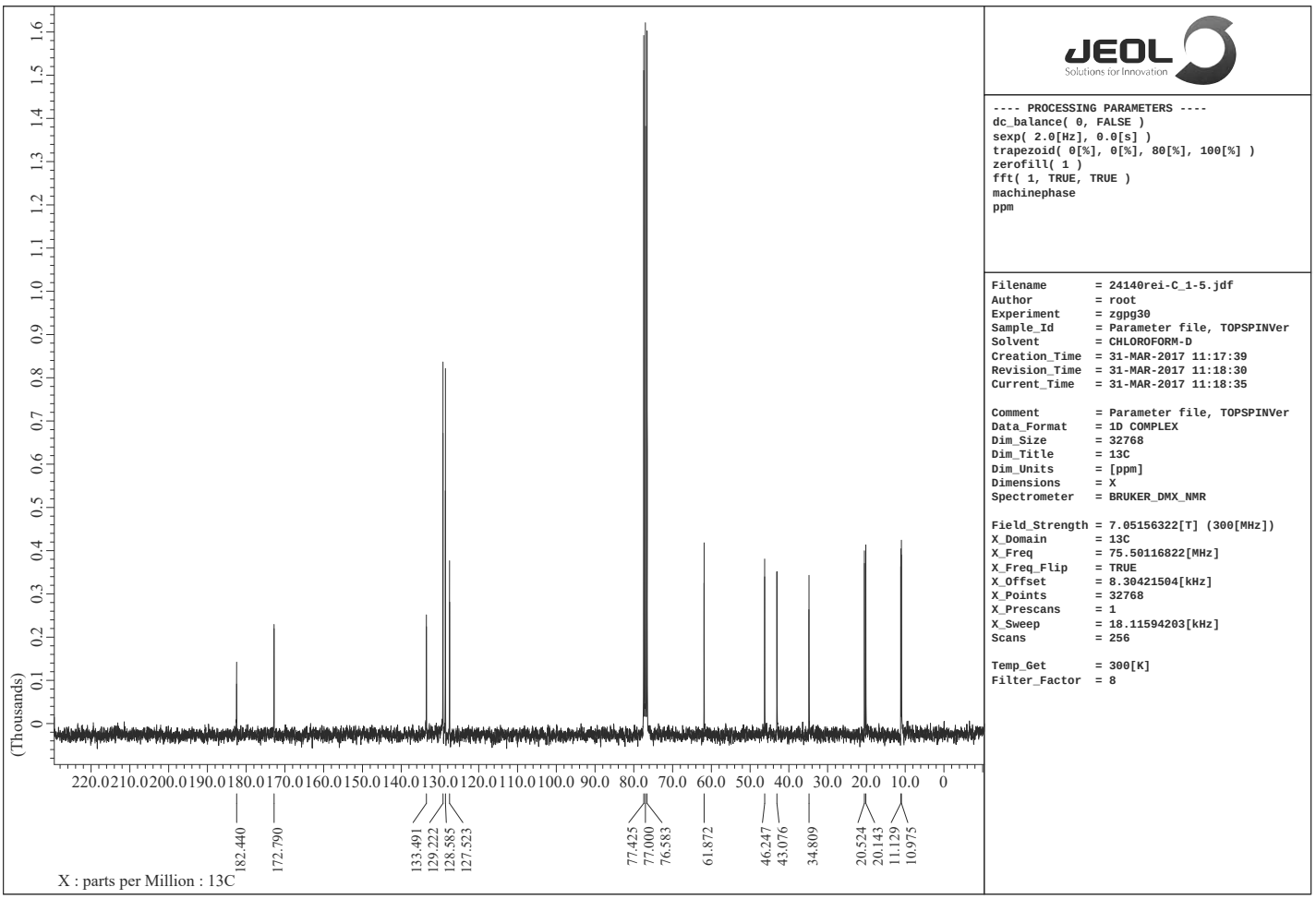
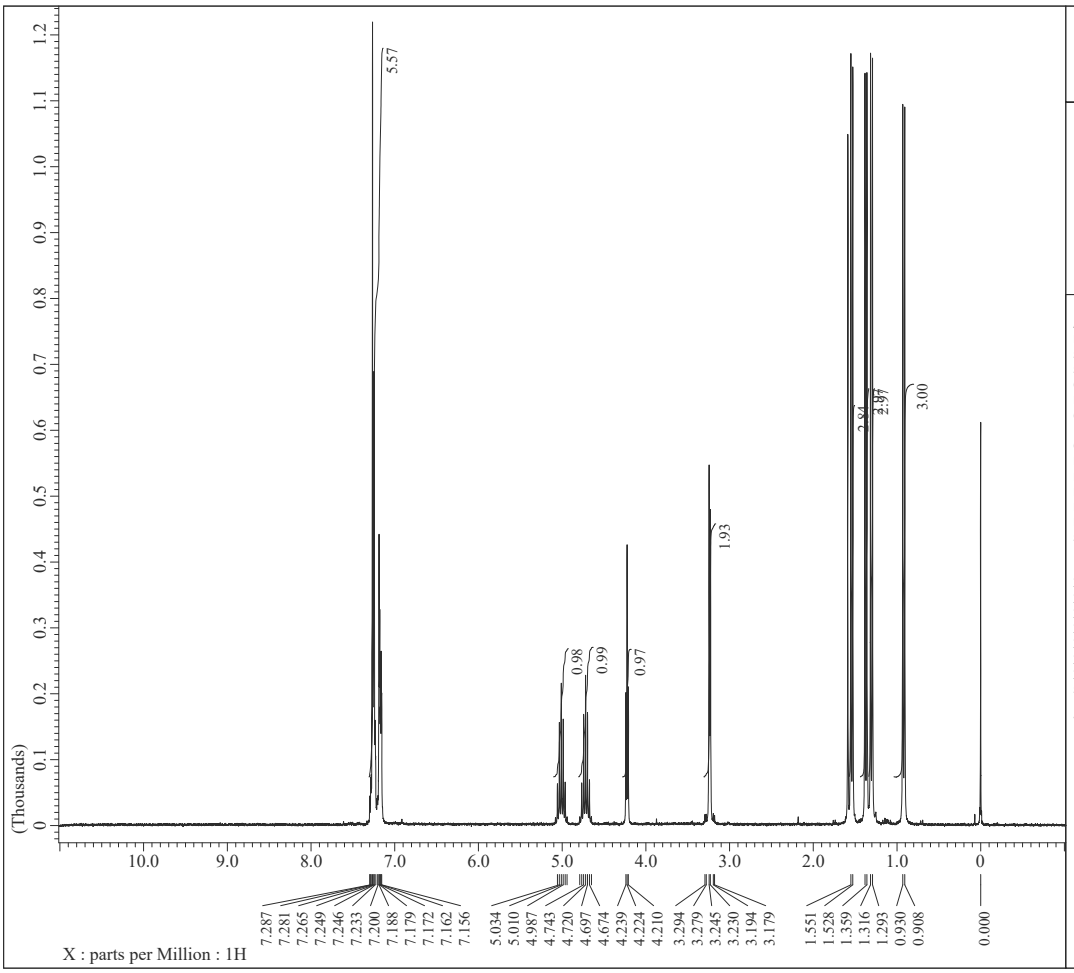
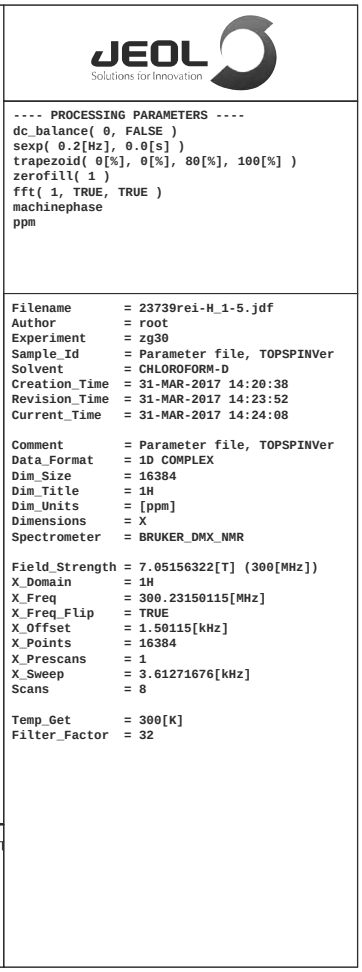
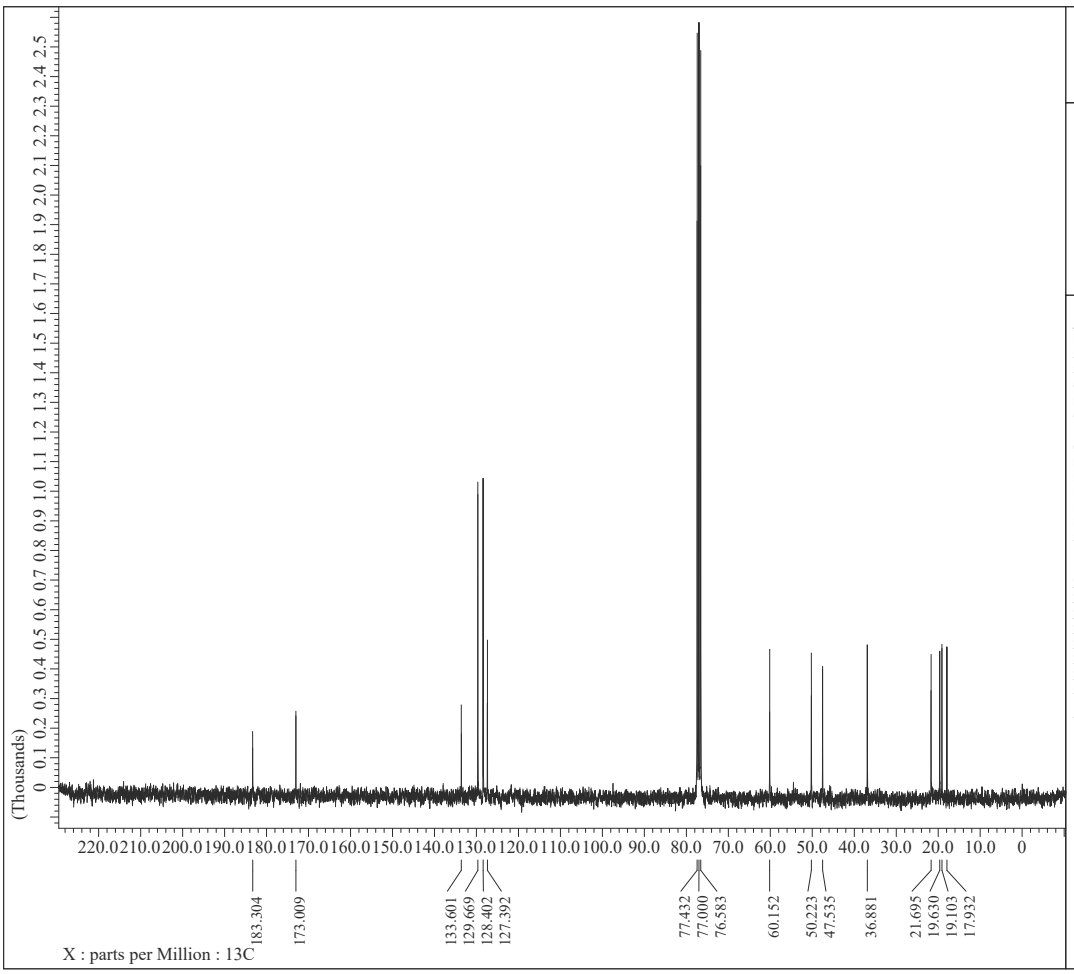


Figure S31. ^{1}H and ^{13}C NMR spectra of **3d**







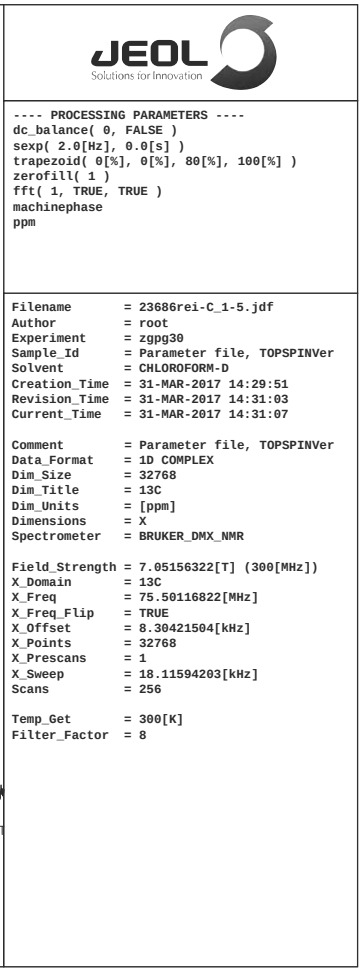
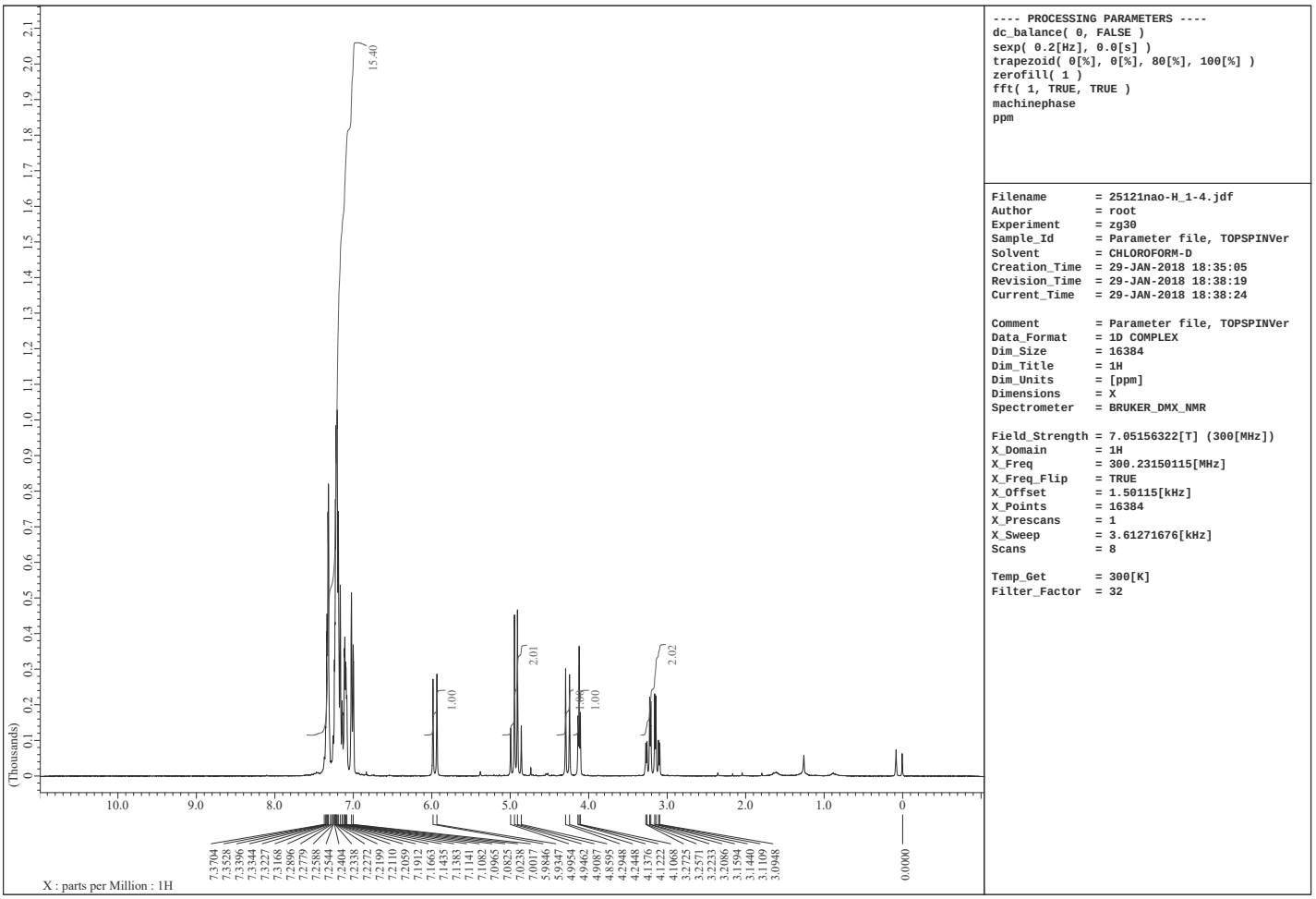
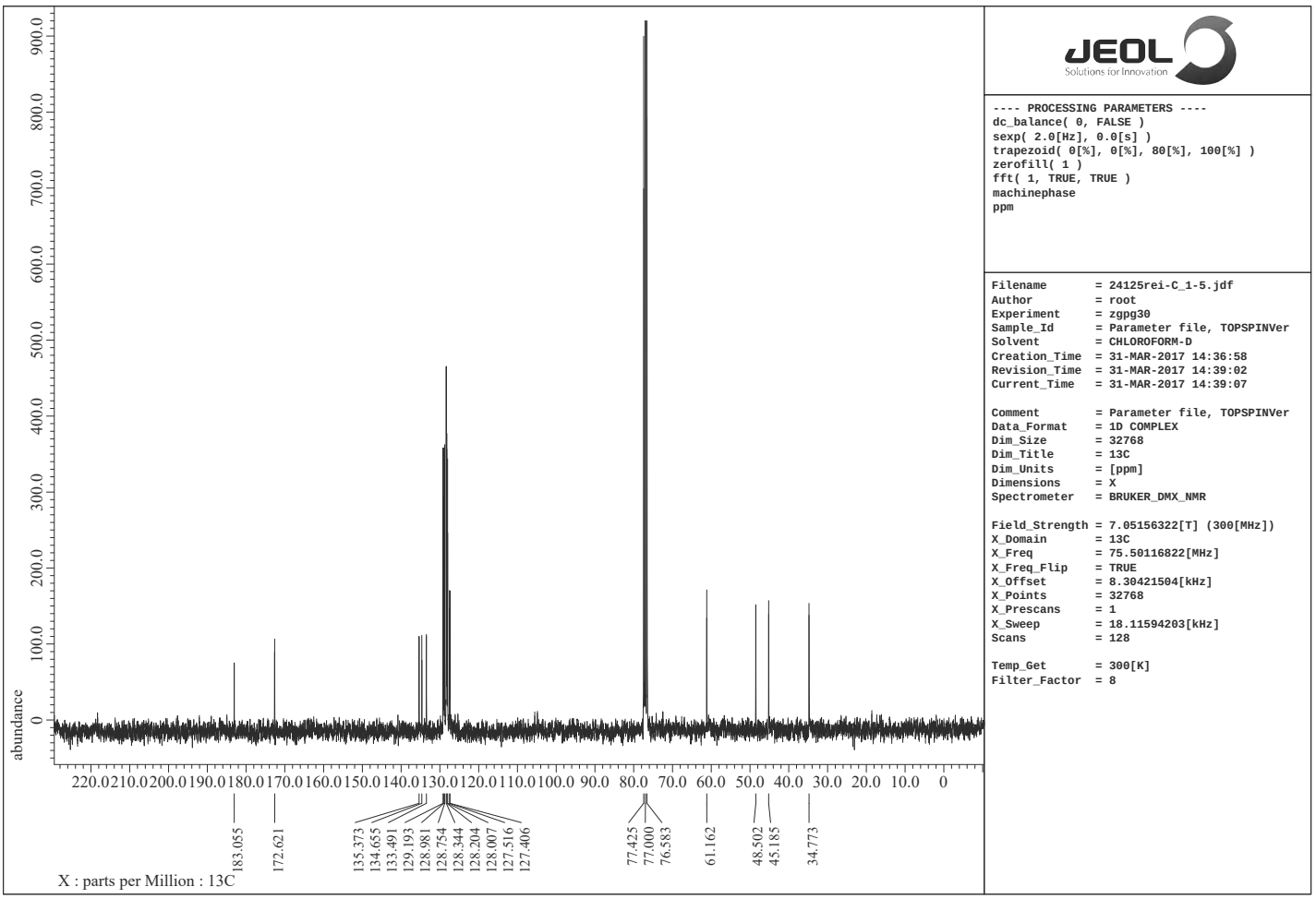


Figure S32. ^{1}H and ^{13}C NMR spectra of **3e**




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Filename        = 25121nao-H_1-4.jdf
Author          = root
Experiment      = zg30
Sample_Id       = Parameter file, TOPSPINVer
Solvent         = CHLOROFORM-D
Creation_Time   = 29-JAN-2018 18:35:05
Revision_Time   = 29-JAN-2018 18:38:19
Current_Time    = 29-JAN-2018 18:38:24

Comment         = Parameter file, TOPSPINVer
Data_Format     = 1D COMPLEX
Dim_Size        = 16384
Dim_Title       = 1H
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = BRUKER_DMX_NMR

Field_Strength = 7.05156322[T] (300[MHz])
X_Domain        = 1H
X_Freq          = 300.23150115[MHz]
X_Freq_Flip     = TRUE
X_Offset        = 1.50115[kHz]
X_Points        = 16384
X_Prescans      = 1
X_Sweep         = 3.61271676[kHz]
Scans           = 8

Temp_Get        = 300[K]
Filter_Factor   = 32
```



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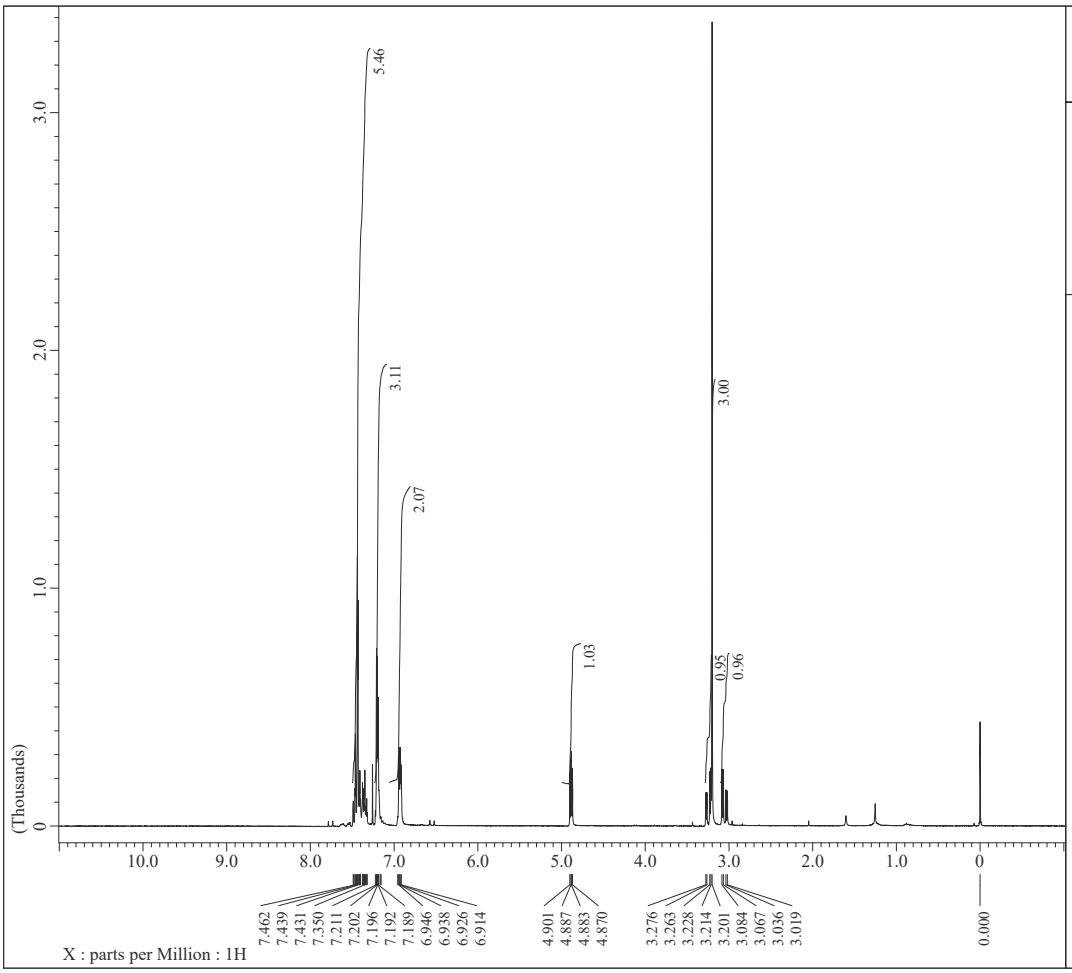
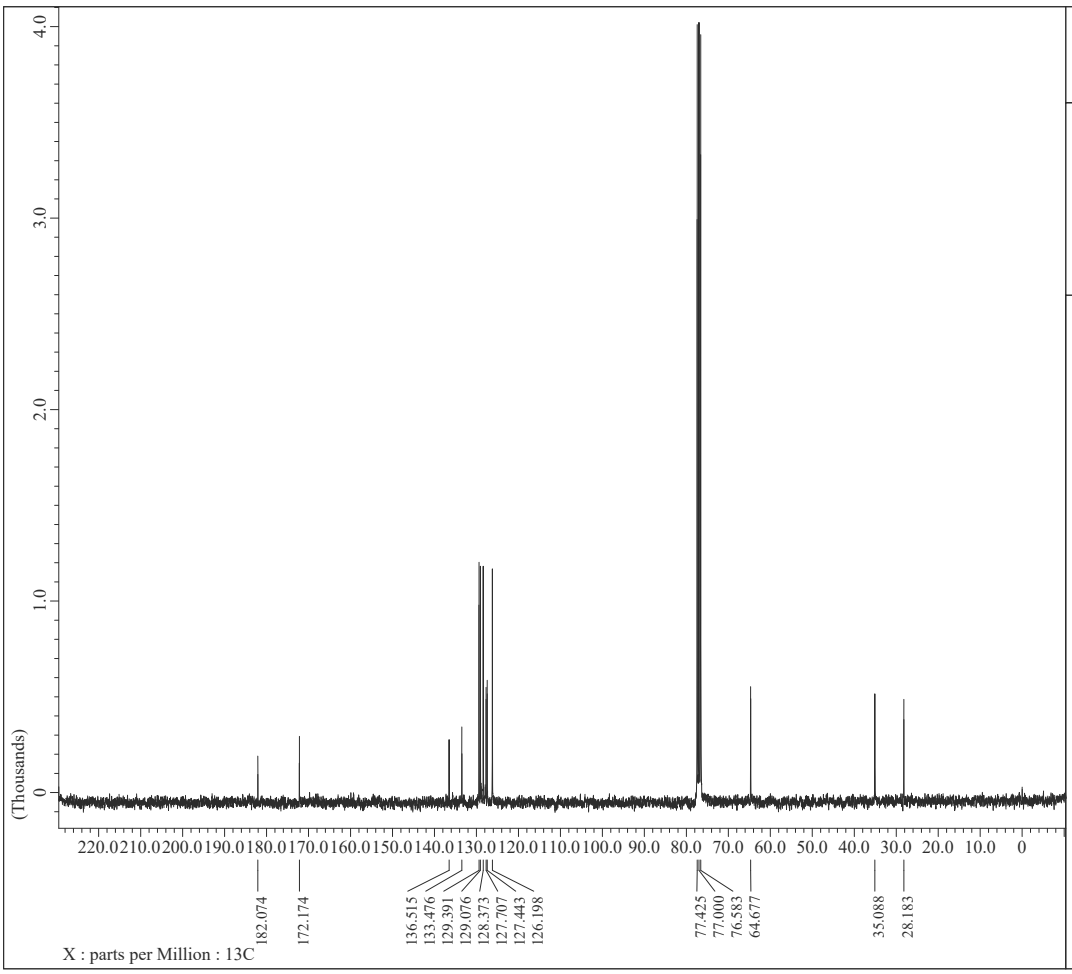
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Filename        = 24125rei-C_1-5.jdf
Author          = root
Experiment      = zgpg30
Sample_Id       = Parameter file, TOPSPINVer
Solvent         = CHLOROFORM-D
Creation_Time   = 31-MAR-2017 14:36:58
Revision_Time   = 31-MAR-2017 14:39:02
Current_Time    = 31-MAR-2017 14:39:07

Comment         = Parameter file, TOPSPINVer
Data_Format     = 1D COMPLEX
Dim_Size        = 32768
Dim_Title       = 13C
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = BRUKER_DMX_NMR

Field_Strength = 7.05156322[T] (300[MHz])
X_Domain        = 13C
X_Freq          = 75.50116822[MHz]
X_Freq_Flip     = TRUE
X_Offset        = 8.30421504[kHz]
X_Points        = 32768
X_Prescans      = 1
X_Sweep         = 18.11594203[kHz]
Scans           = 128

Temp_Get        = 300[K]
Filter_Factor   = 8
```

Figure S33. ^{1}H and ^{13}C NMR spectra of **3f**




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

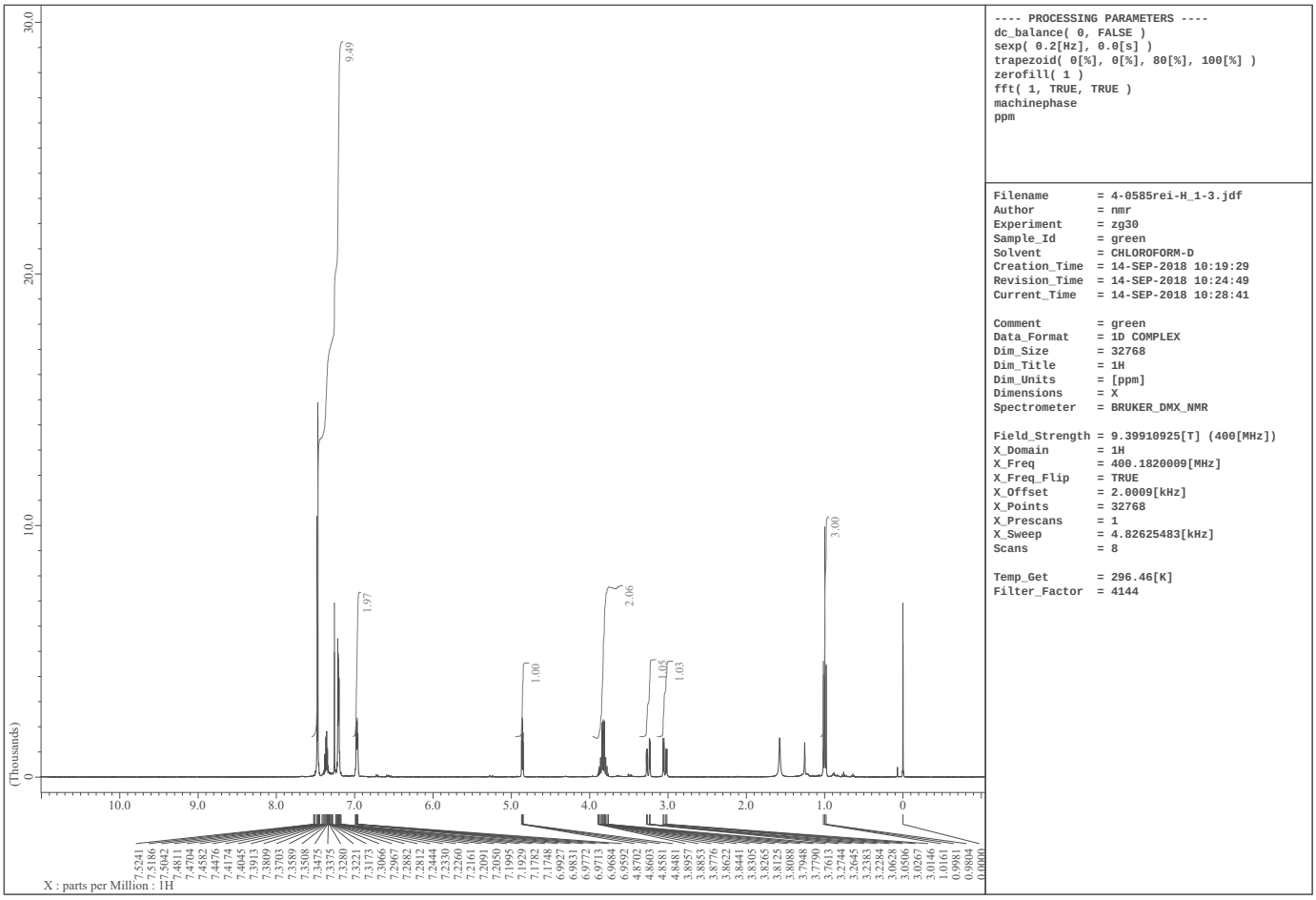
```
Filename        = 23832rei-H_1-6.jdf
Author          = root
Experiment      = zg30
Sample_Id       = Parameter file, TOPSPINVer
Solvent         = CHLOROFORM-D
Creation_Time   = 31-MAR-2017 14:45:25
Revision_Time   = 31-MAR-2017 14:48:35
Current_Time    = 31-MAR-2017 14:48:41

Comment         = Parameter file, TOPSPINVer
Data_Format     = 1D COMPLEX
Dim_Size        = 16384
Dim_Title       = 1H
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = BRUKER_DMX_NMR

Field_Strength = 7.05156322[T] (300[MHz])
X_Domain        = 1H
X_Freq          = 300.23150115[MHz]
X_Freq_Flip     = TRUE
X_Offset        = 1.50115[kHz]
X_Points        = 16384
X_Prescans      = 1
X_Sweep         = 3.61271676[kHz]
Scans           = 8

Temp_Get        = 300[K]
Filter_Factor   = 32
```



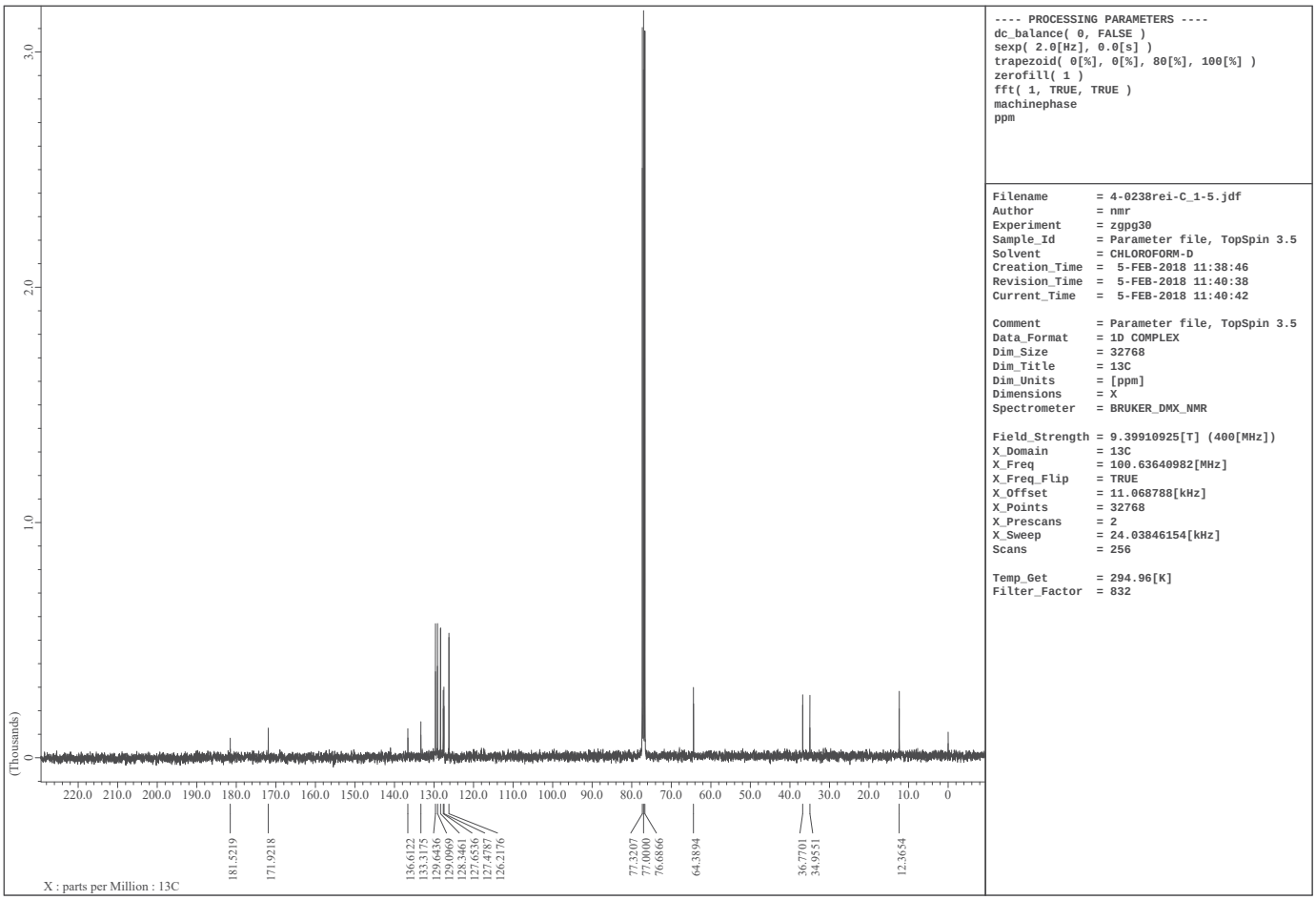

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename        = 23835rei-C_1-5.jdf
Author          = root
Experiment      = zgpg30
Sample_Id       = Parameter file, TOPSPINVer
Solvent         = CHLOROFORM-D
Creation_Time   = 31-MAR-2017 14:49:32
Revision_Time   = 31-MAR-2017 14:50:35
Current_Time    = 31-MAR-2017 14:50:39

Comment         = Parameter file, TOPSPINVer
Data_Format     = 1D COMPLEX
Dim_Size        = 32768
Dim_Title       = 13C
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = BRUKER_DMX_NMR

Field_Strength = 7.05156322[T] (300[MHz])
X_Domain        = 13C
X_Freq          = 75.50116822[MHz]
X_Freq_Flip     = TRUE
X_Offset        = 8.30421504[kHz]
X_Points        = 32768
X_Prescans      = 1
X_Sweep         = 18.11594203[kHz]
Scans           = 512

Temp_Get        = 300[K]
Filter_Factor   = 8
```

Figure S34. ^{1}H and ^{13}C NMR spectra of **3g**

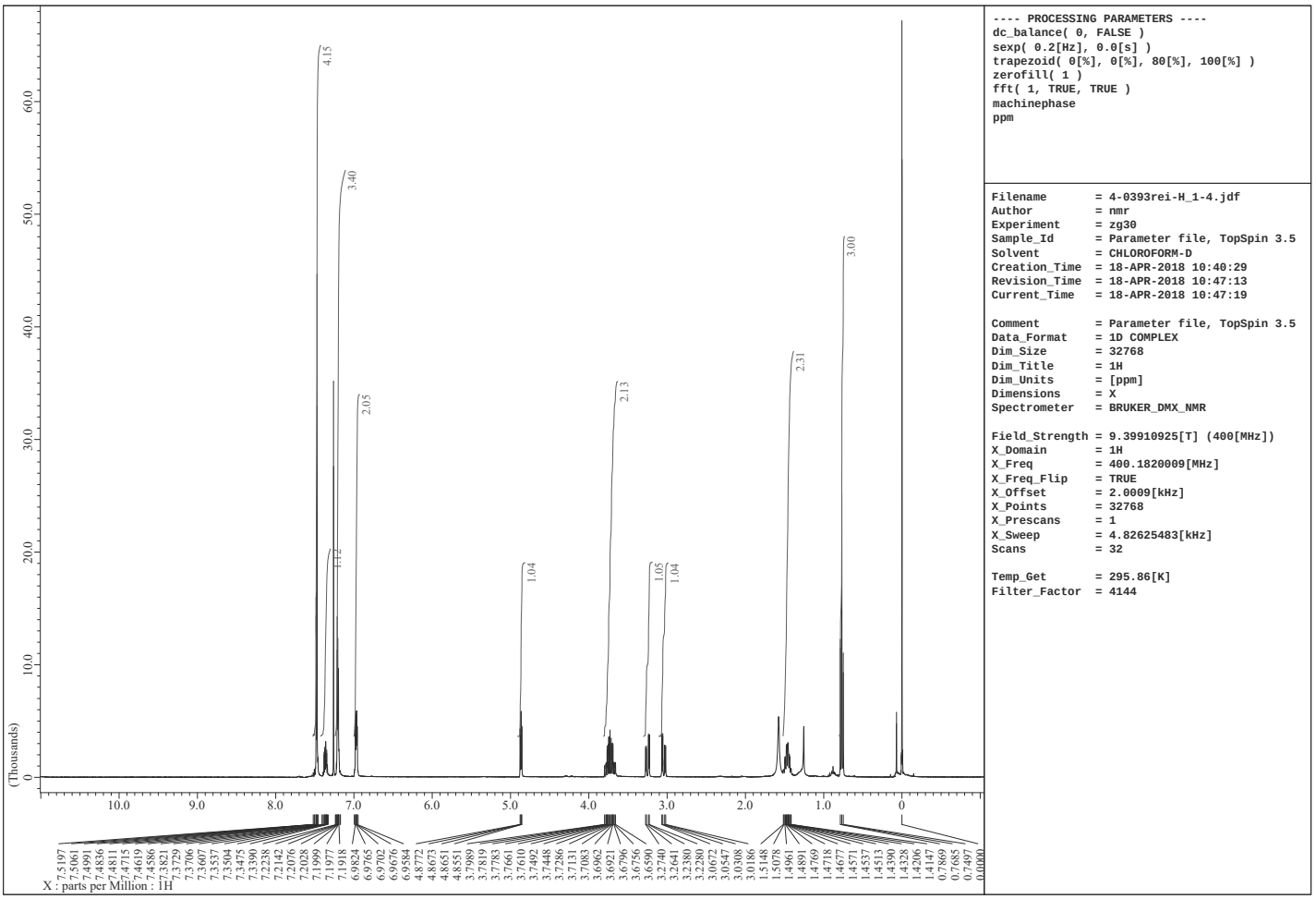



```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Filename        = 4-0585rei-H_1-3.jdf
Author          = nmr
Experiment      = zg30
Sample_Id       = green
Solvent         = CHLOROFORM-D
Creation_Time   = 14-SEP-2018 10:19:29
Revision_Time   = 14-SEP-2018 10:24:49
Current_Time    = 14-SEP-2018 10:28:41

Comment         = green
Data_Format     = 1D COMPLEX
Dim_Size        = 32768
Dim_Title       = 1H
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = BRUKER_DMX_NMR

Field_Strength = 9.39910925[T] (400[MHz])
X_Domain        = 1H
X_Freq          = 400.1820009[MHz]
X_Freq_Flip     = TRUE
X_Offset        = 2.0009[kHz]
X_Points        = 32768
X_Prescans      = 1
X_Sweep         = 4.82625483[kHz]
Scans           = 8

Temp_Get        = 296.46[K]
Filter_Factor   = 4144
```

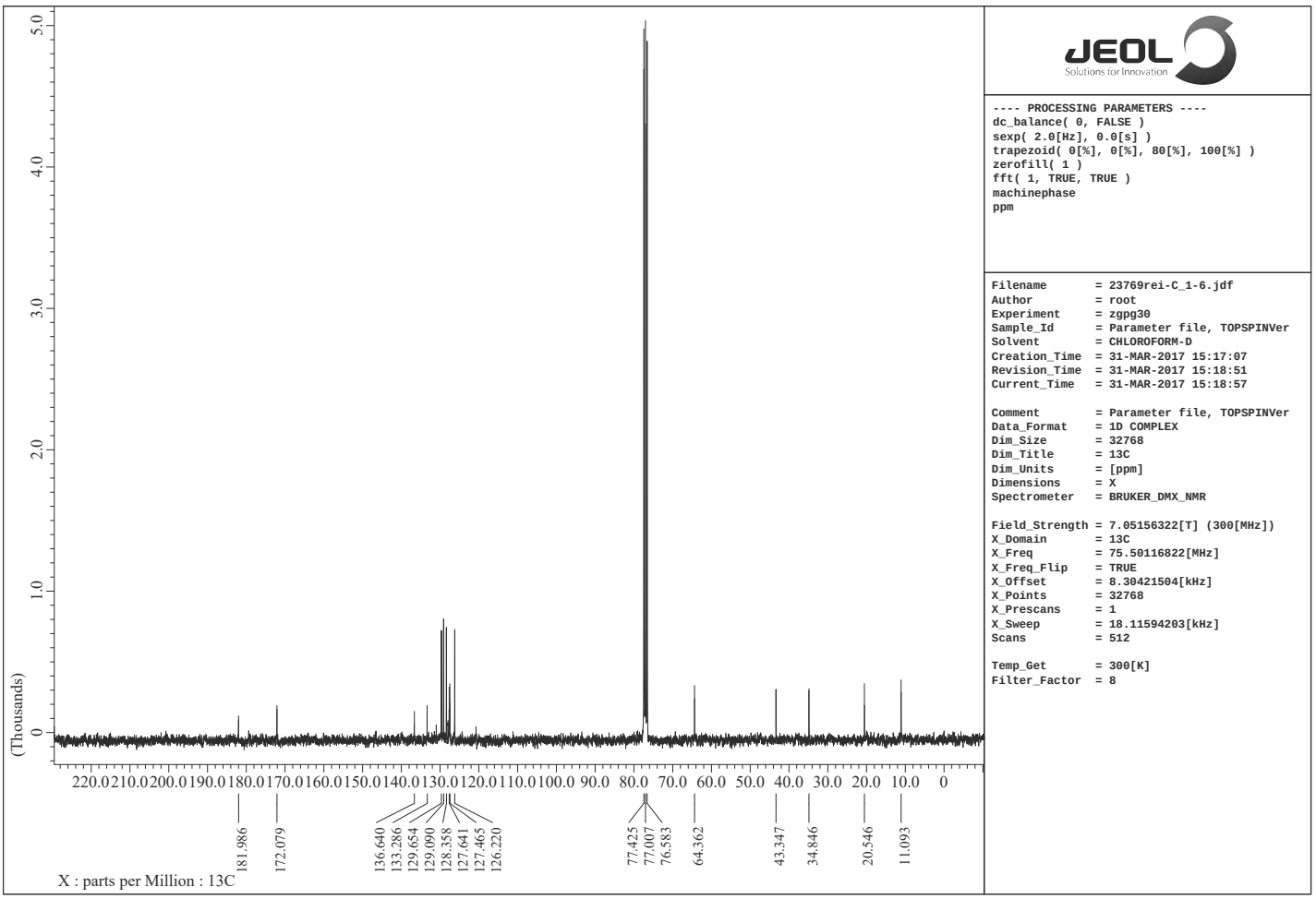



```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Filename        = 4-0238rei-C_1-5.jdf
Author          = nmr
Experiment      = zgpg30
Sample_Id       = Parameter file, TopSpin 3.5
Solvent         = CHLOROFORM-D
Creation_Time   =  5-FEB-2018 11:38:46
Revision_Time   =  5-FEB-2018 11:40:38
Current_Time    =  5-FEB-2018 11:40:42

Comment         = Parameter file, TopSpin 3.5
Data_Format     = 1D COMPLEX
Dim_Size        = 32768
Dim_Title       = 13C
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = BRUKER_DMX_NMR

Field_Strength = 9.39910925[T] (400[MHz])
X_Domain        = 13C
X_Freq          = 100.63640982[MHz]
X_Freq_Flip     = TRUE
X_Offset        = 11.068788[kHz]
X_Points        = 32768
X_Prescans      = 2
X_Sweep         = 24.03846154[kHz]
Scans           = 256

Temp_Get        = 294.96[K]
Filter_Factor   = 832
```

Figure S35. ^{1}H and ^{13}C NMR spectra of **3h**

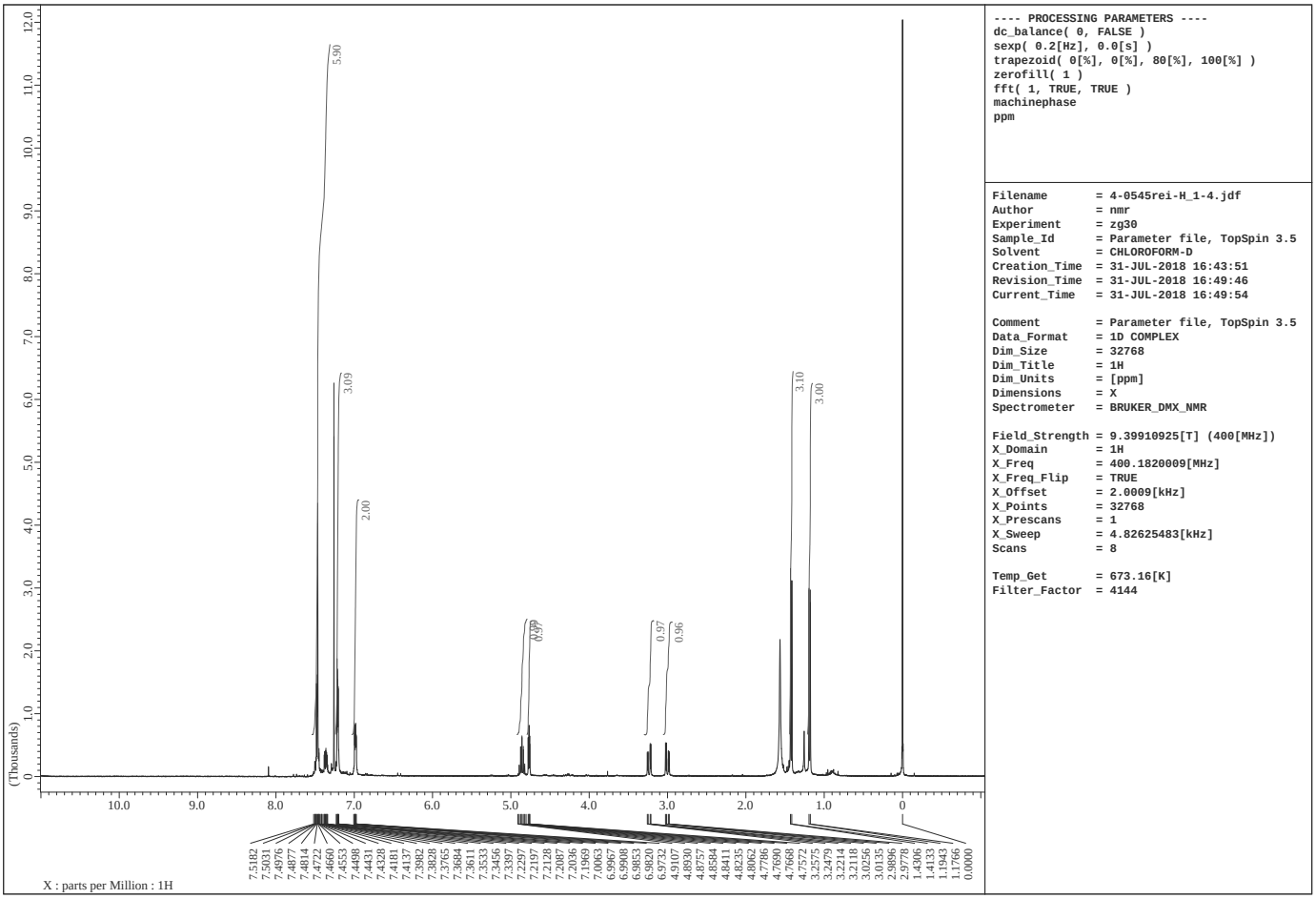



```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Filename        = 4-0393rei-H_1-4.jdf
Author          = nmr
Experiment      = zg30
Sample_Id       = Parameter file, TopSpin 3.5
Solvent         = CHLOROFORM-D
Creation_Time   = 18-APR-2018 10:40:29
Revision_Time   = 18-APR-2018 10:47:13
Current_Time    = 18-APR-2018 10:47:19

Comment         = Parameter file, TopSpin 3.5
Data_Format     = 1D COMPLEX
Dim_Size        = 32768
Dim_Title       = 1H
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = BRUKER_DMX_NMR

Field_Strength = 9.39910925[T] (400[MHz])
X_Domain        = 1H
X_Freq          = 400.1820009[MHz]
X_Freq_Flip     = TRUE
X_Offset        = 2.0009[kHz]
X_Points        = 32768
X_Prescans      = 1
X_Sweep         = 4.82625483[kHz]
Scans           = 32

Temp_Get        = 295.86[K]
Filter_Factor   = 4144
```

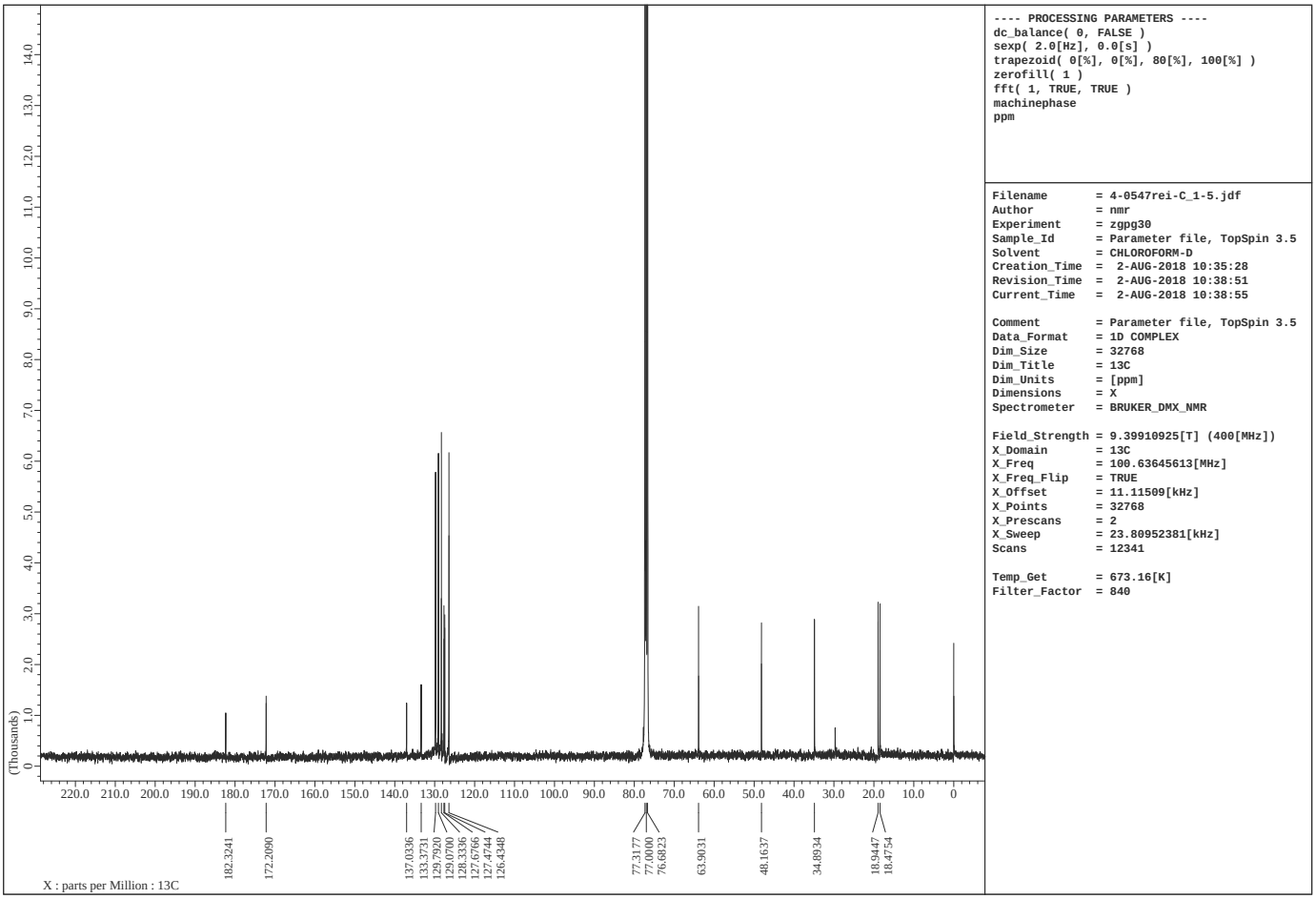



```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Filename        = 23769rei-C_1-6.jdf
Author          = root
Experiment      = zgpg30
Sample_Id       = Parameter file, TOPSPINVer
Solvent         = CHLOROFORM-D
Creation_Time   = 31-MAR-2017 15:17:07
Revision_Time   = 31-MAR-2017 15:18:51
Current_Time    = 31-MAR-2017 15:18:57

Comment         = Parameter file, TOPSPINVer
Data_Format     = 1D COMPLEX
Dim_Size        = 32768
Dim_Title       = 13C
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = BRUKER_DMX_NMR

Field_Strength = 7.05156322[T] (300[MHz])
X_Domain        = 13C
X_Freq          = 75.50116822[MHz]
X_Freq_Flip     = TRUE
X_Offset        = 8.30421504[kHz]
X_Points        = 32768
X_Prescans      = 1
X_Sweep         = 18.11594203[kHz]
Scans           = 512

Temp_Get        = 300[K]
Filter_Factor   = 8
```

Figure S36. ^{1}H and ^{13}C NMR spectra of **3i**

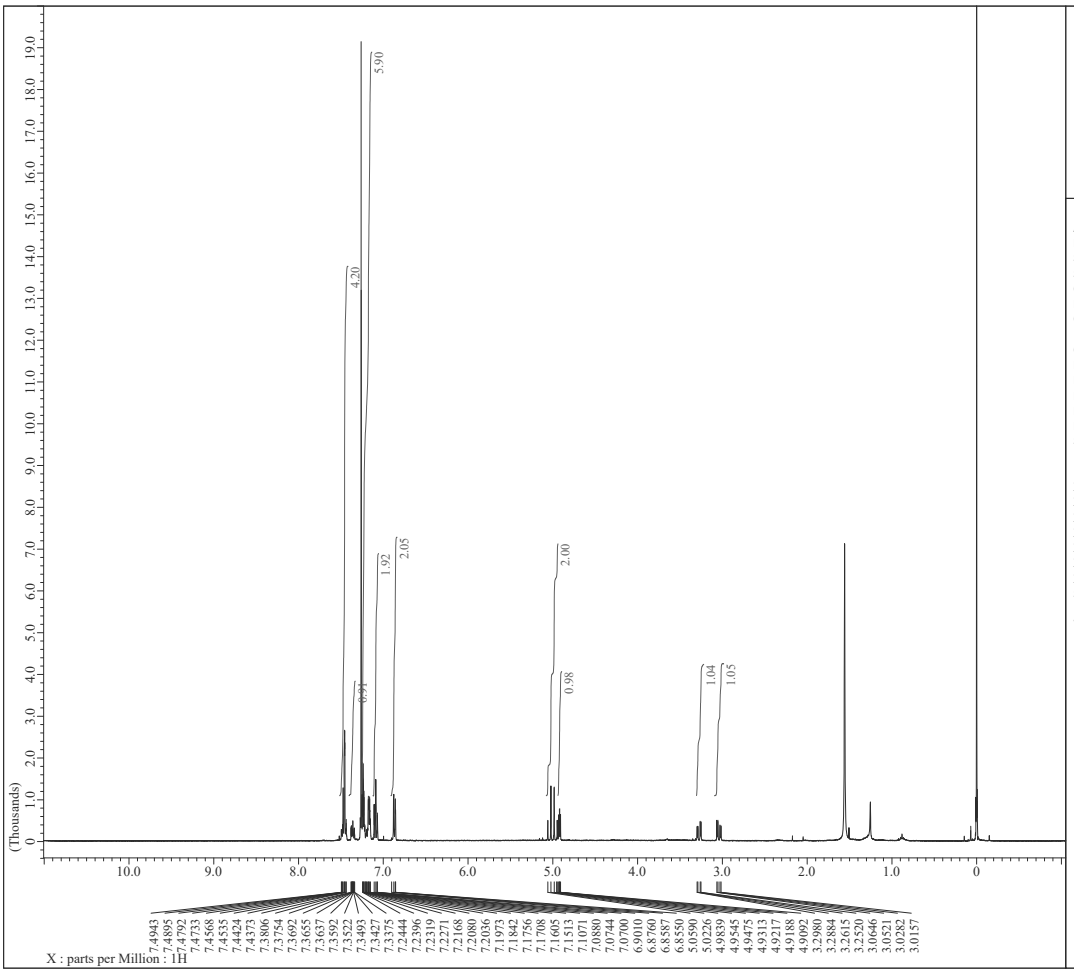



```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Filename       = 4-0545rei-H_1-4.jdf
Author         = nmr
Experiment     = zg30
Sample_Id      = Parameter file, TopSpin 3.5
Solvent        = CHLOROFORM-D
Creation_Time  = 31-JUL-2018 16:43:51
Revision_Time  = 31-JUL-2018 16:49:46
Current_Time   = 31-JUL-2018 16:49:54

Comment        = Parameter file, TopSpin 3.5
Data_Format    = 1D COMPLEX
Dim_Size       = 32768
Dim_Title      = 1H
Dim_Units      = [ppm]
Dimensions     = X
Spectrometer   = BRUKER_DMX_NMR

Field_Strength = 9.39910925[T] (400[MHz])
X_Domain       = 1H
X_Freq         = 400.1820009[MHz]
X_Freq_Flip    = TRUE
X_Offset       = 2.0009[kHz]
X_Points       = 32768
X_Prescans     = 1
X_Sweep        = 4.82625483[kHz]
Scans          = 8

Temp_Get       = 673.16[K]
Filter_Factor  = 4144
```

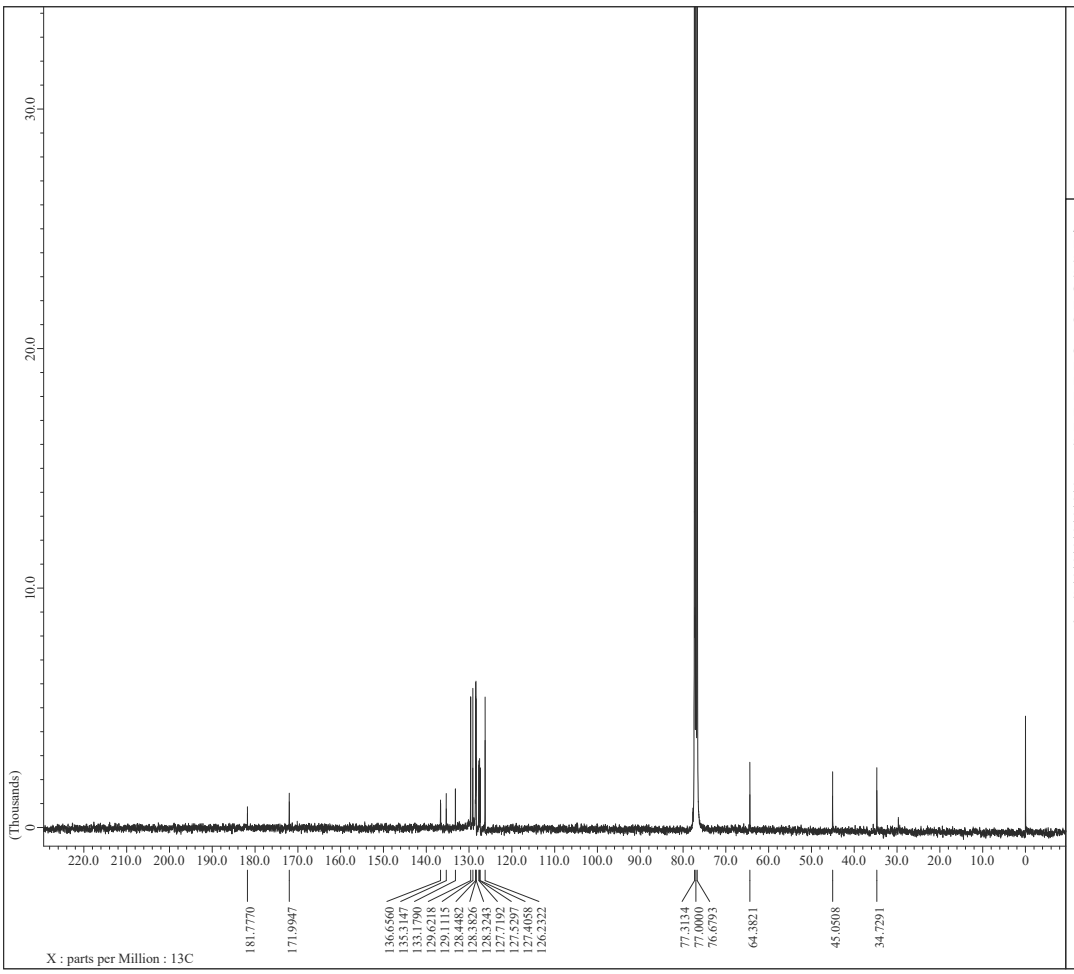



```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Filename       = 4-0547rei-C_1-5.jdf
Author         = nmr
Experiment     = zgpg30
Sample_Id      = Parameter file, TopSpin 3.5
Solvent        = CHLOROFORM-D
Creation_Time  =  2-AUG-2018 10:35:28
Revision_Time  =  2-AUG-2018 10:38:51
Current_Time   =  2-AUG-2018 10:38:55

Comment        = Parameter file, TopSpin 3.5
Data_Format    = 1D COMPLEX
Dim_Size       = 32768
Dim_Title      = 13C
Dim_Units      = [ppm]
Dimensions     = X
Spectrometer   = BRUKER_DMX_NMR

Field_Strength = 9.39910925[T] (400[MHz])
X_Domain       = 13C
X_Freq         = 100.63645613[MHz]
X_Freq_Flip    = TRUE
X_Offset       = 11.11509[kHz]
X_Points       = 32768
X_Prescans     = 2
X_Sweep        = 23.80952381[kHz]
Scans          = 12341

Temp_Get       = 673.16[K]
Filter_Factor  = 840
```

Figure S37. ^{1}H and ^{13}C NMR spectra of **3j**

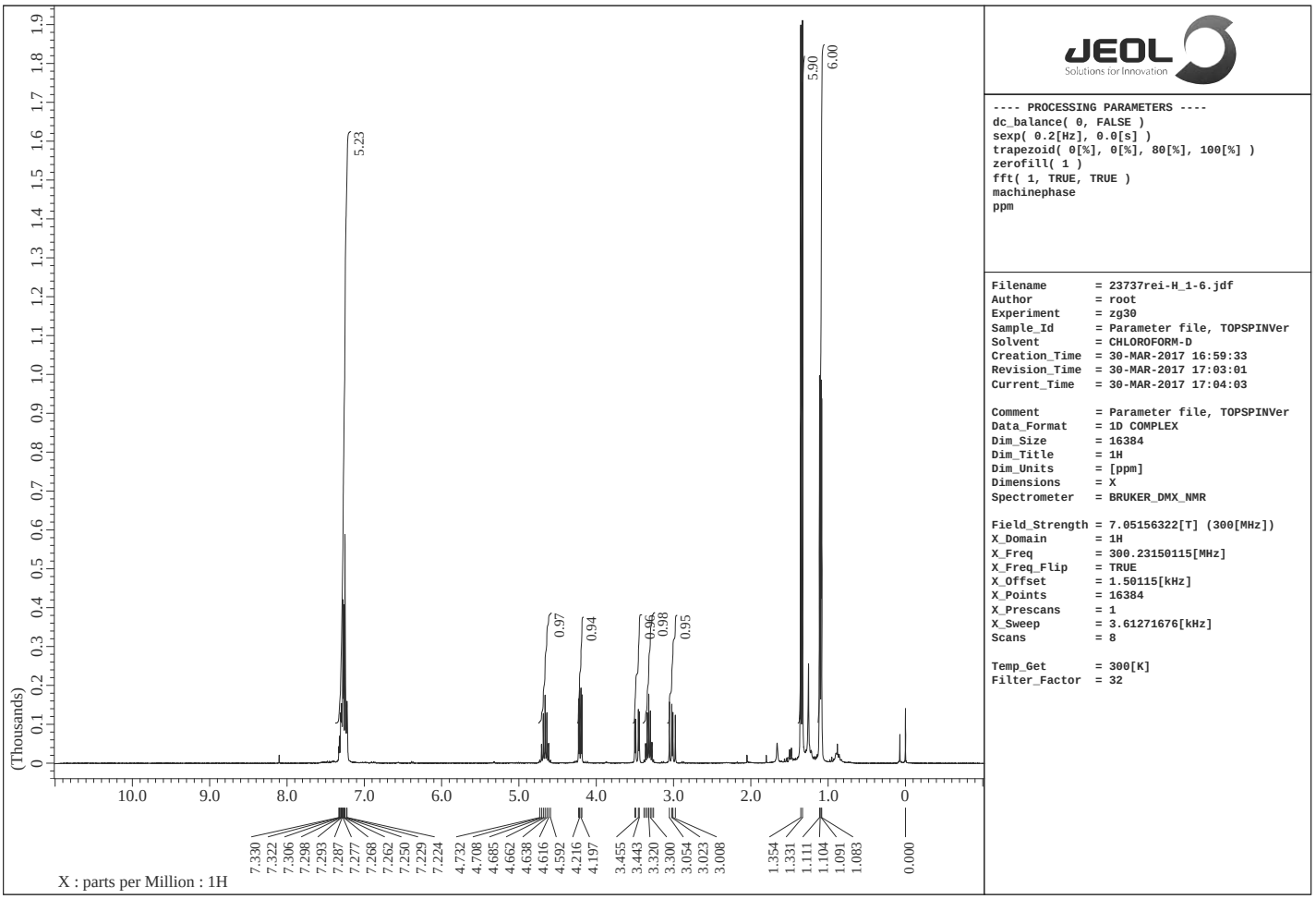



```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Filename        = 4-0392rei-H_1-7.jdf
Author          = nmr
Experiment      = zg30
Sample_Id       = Parameter file, TopSpin 3.5
Solvent         = CHLOROFORM-D
Creation_Time   =  2-MAY-2018 14:05:59
Revision_Time   =  2-MAY-2018 14:11:26
Current_Time    =  2-MAY-2018 14:11:31

Comment         = Parameter file, TopSpin 3.5
Data_Format     = 1D COMPLEX
Dim_Size        = 32768
Dim_Title       = 1H
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = BRUKER_DMX_NMR

Field_Strength = 9.39910925[T] (400[MHz])
X_Domain        = 1H
X_Freq          = 400.1820009[MHz]
X_Freq_Flip     = TRUE
X_Offset        = 2.0009[kHz]
X_Points        = 32768
X_Prescans      = 1
X_Sweep         = 4.82625483[kHz]
Scans           = 16

Temp_Get        = 296.36[K]
Filter_Factor   = 4144
```



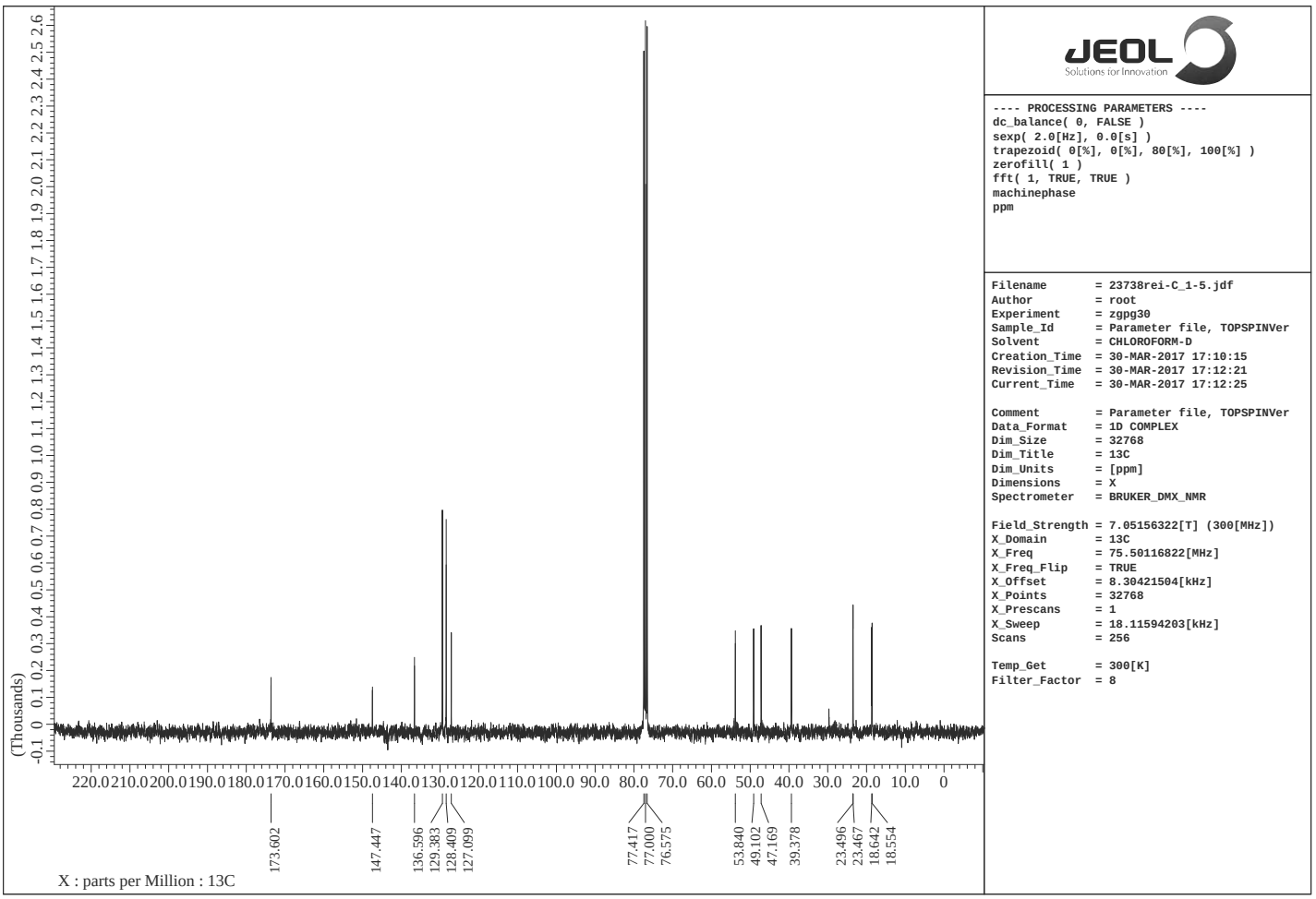

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Filename        = 4-0392rei-C_1-4.jdf
Author          = nmr
Experiment      = zgpg30
Sample_Id       = Parameter file, TopSpin 3.5
Solvent         = CHLOROFORM-D
Creation_Time   = 18-APR-2018 10:03:12
Revision_Time   = 18-APR-2018 10:08:34
Current_Time    = 18-APR-2018 10:08:42

Comment         = Parameter file, TopSpin 3.5
Data_Format     = 1D COMPLEX
Dim_Size        = 32768
Dim_Title       = 13C
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = BRUKER_DMX_NMR

Field_Strength = 9.39910925[T] (400[MHz])
X_Domain        = 13C
X_Freq          = 100.63640982[MHz]
X_Freq_Flip     = TRUE
X_Offset        = 11.068788[kHz]
X_Points        = 32768
X_Prescans      = 2
X_Sweep         = 24.03846154[kHz]
Scans           = 14773

Temp_Get        = 297.16[K]
Filter_Factor   = 832
```

Figure S38. ^{1}H and ^{13}C NMR spectra of **4d**




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

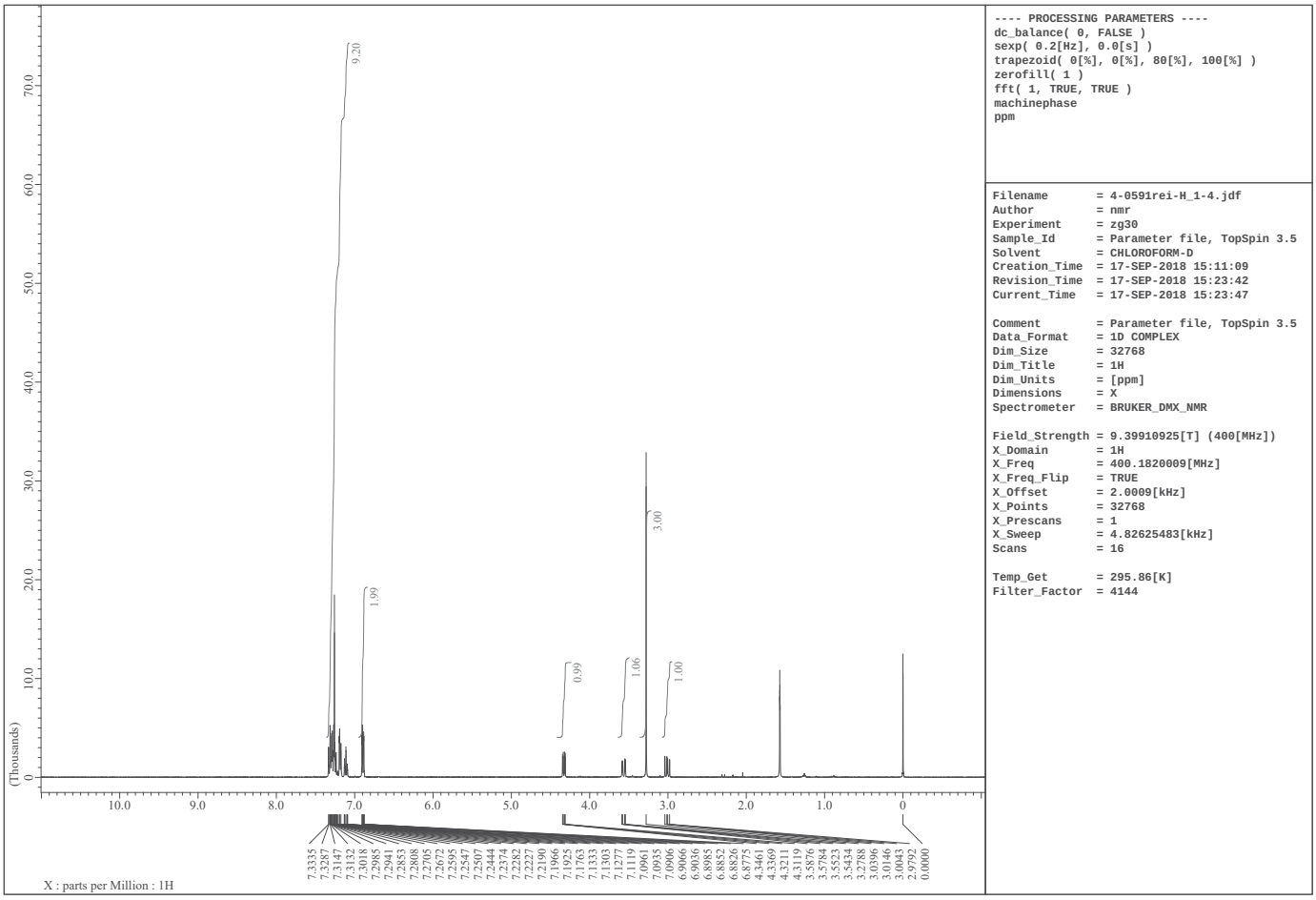
```
Filename        = 23737rei-H_1-6.jdf
Author          = root
Experiment      = zg30
Sample_Id       = Parameter file, TOPSPINVer
Solvent         = CHLOROFORM-D
Creation_Time   = 30-MAR-2017 16:59:33
Revision_Time   = 30-MAR-2017 17:03:01
Current_Time    = 30-MAR-2017 17:04:03

Comment         = Parameter file, TOPSPINVer
Data_Format     = 1D COMPLEX
Dim_Size        = 16384
Dim_Title       = 1H
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = BRUKER_DMX_NMR

Field_Strength = 7.05156322[T] (300[MHz])
X_Domain        = 1H
X_Freq          = 300.23150115[MHz]
X_Freq_Flip     = TRUE
X_Offset        = 1.50115[kHz]
X_Points        = 16384
X_Prescans      = 1
X_Sweep         = 3.61271676[kHz]
Scans           = 8

Temp_Get        = 300[K]
Filter_Factor   = 32
```



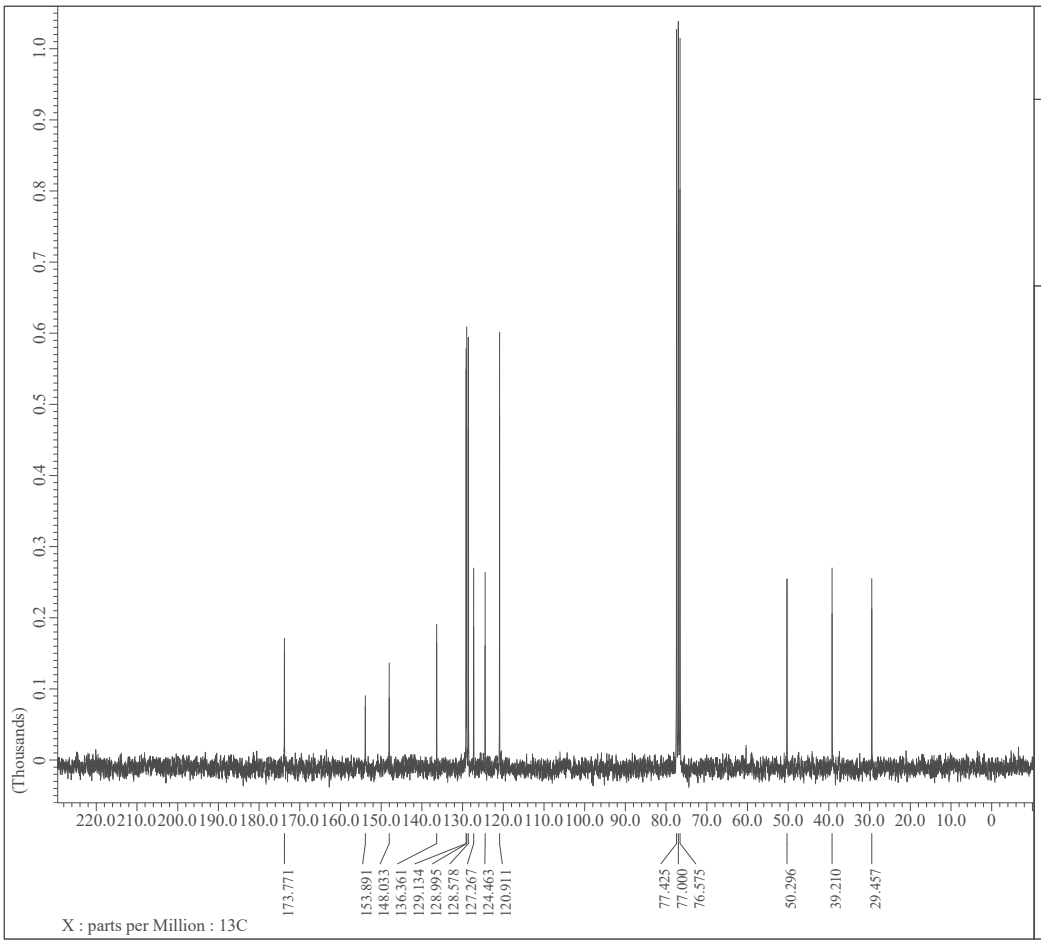

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename        = 23738rei-C_1-5.jdf
Author          = root
Experiment      = zgpg30
Sample_Id       = Parameter file, TOPSPINVer
Solvent         = CHLOROFORM-D
Creation_Time   = 30-MAR-2017 17:10:15
Revision_Time   = 30-MAR-2017 17:12:21
Current_Time    = 30-MAR-2017 17:12:25

Comment         = Parameter file, TOPSPINVer
Data_Format     = 1D COMPLEX
Dim_Size        = 32768
Dim_Title       = 13C
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = BRUKER_DMX_NMR

Field_Strength = 7.05156322[T] (300[MHz])
X_Domain        = 13C
X_Freq          = 75.50116822[MHz]
X_Freq_Flip     = TRUE
X_Offset        = 8.30421504[kHz]
X_Points        = 32768
X_Prescans      = 1
X_Sweep         = 18.11594203[kHz]
Scans           = 256

Temp_Get        = 300[K]
Filter_Factor   = 8
```

Figure S39. ^{1}H and ^{13}C NMR spectra of **4f**

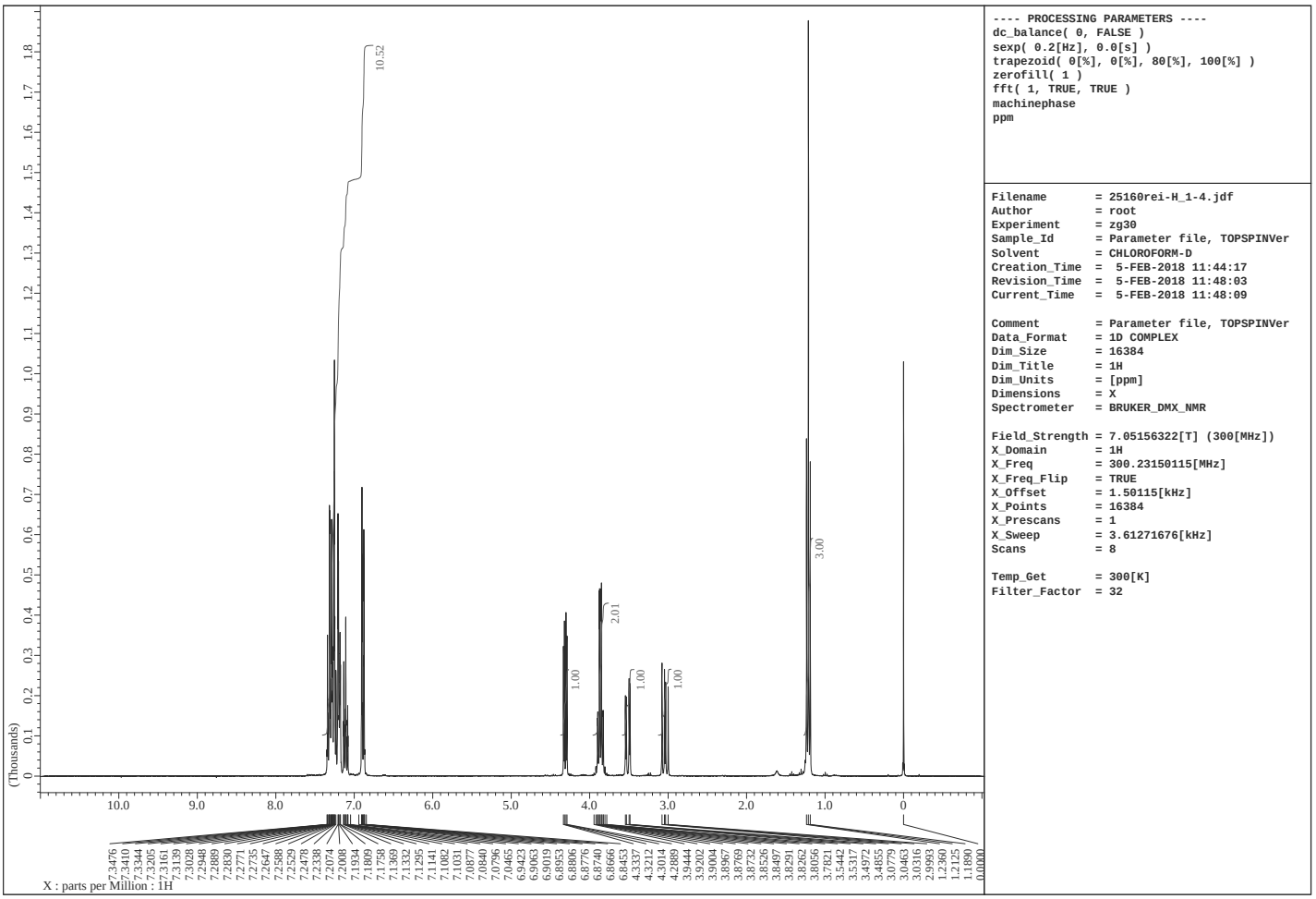



```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Filename        = 4-0591rei-H_1-4.jdf
Author          = nmr
Experiment      = zg30
Sample_Id       = Parameter file, TopSpin 3.5
Solvent         = CHLOROFORM-D
Creation_Time   = 17-SEP-2018 15:11:09
Revision_Time   = 17-SEP-2018 15:23:42
Current_Time    = 17-SEP-2018 15:23:47

Comment         = Parameter file, TopSpin 3.5
Data_Format     = 1D COMPLEX
Dim_Size        = 32768
Dim_Title       = 1H
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = BRUKER_DMX_NMR

Field_Strength = 9.39910925[T] (400[MHz])
X_Domain        = 1H
X_Freq          = 400.1820009[MHz]
X_Freq_Flip     = TRUE
X_Offset        = 2.0009[kHz]
X_Points        = 32768
X_Prescans      = 1
X_Sweep         = 4.82625483[kHz]
Scans           = 16

Temp_Get        = 295.86[K]
Filter_Factor   = 4144
```



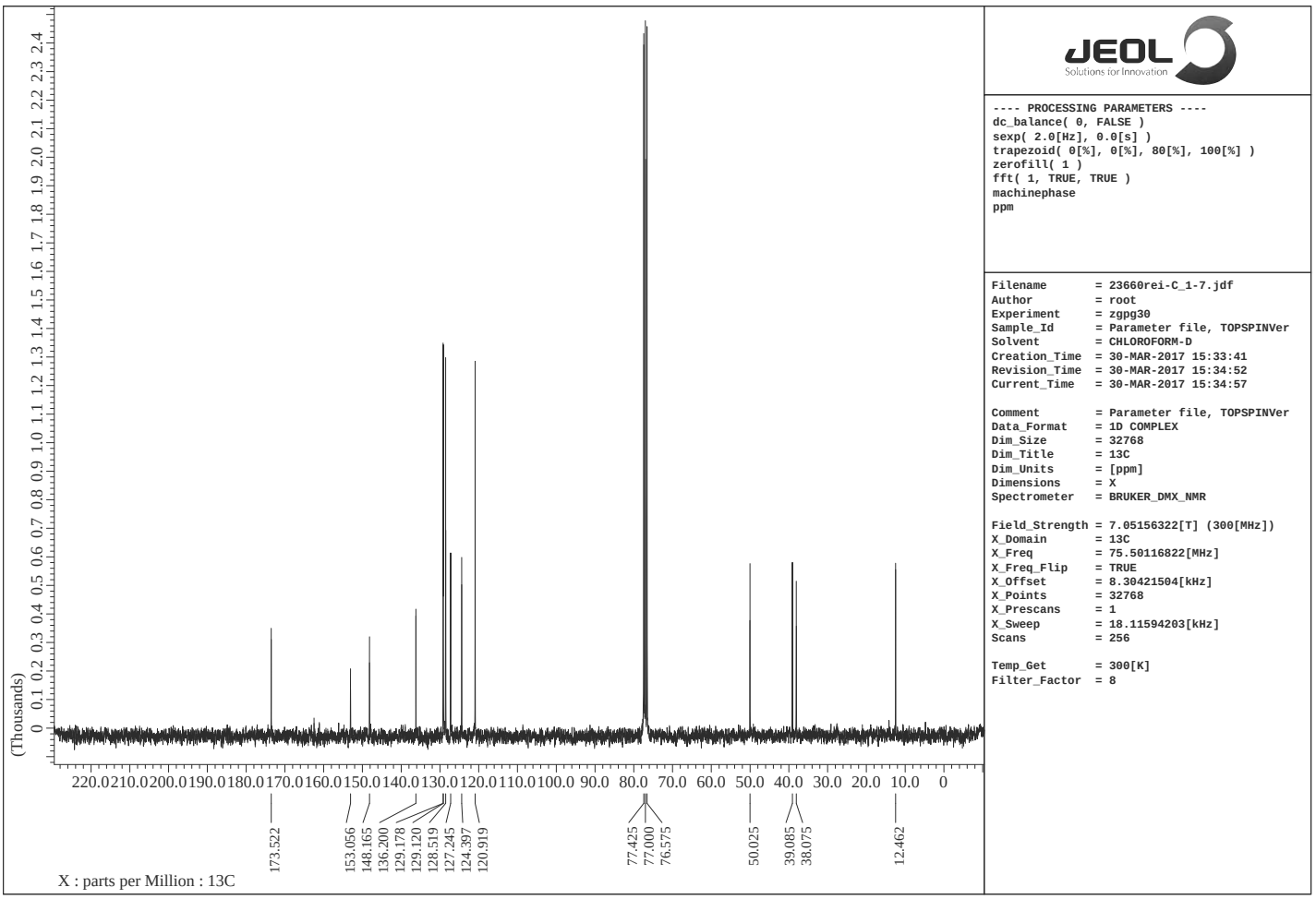

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Filename        = 23830rei-C_1-5.jdf
Author          = root
Experiment      = zgpg30
Sample_Id       = Parameter file, TOPSPINVer
Solvent         = CHLOROFORM-D
Creation_Time   = 30-MAR-2017 15:14:57
Revision_Time   = 30-MAR-2017 15:16:52
Current_Time    = 30-MAR-2017 15:16:57

Comment         = Parameter file, TOPSPINVer
Data_Format     = 1D COMPLEX
Dim_Size        = 32768
Dim_Title       = 13C
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = BRUKER_DMX_NMR

Field_Strength = 7.05156322[T] (300[MHz])
X_Domain        = 13C
X_Freq          = 75.50116822[MHz]
X_Freq_Flip     = TRUE
X_Offset        = 8.30421504[kHz]
X_Points        = 32768
X_Prescans      = 1
X_Sweep         = 18.11594203[kHz]
Scans           = 128

Temp_Get        = 300[K]
Filter_Factor   = 8
```

Figure S40. ^{1}H and ^{13}C NMR spectra of **4g**




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

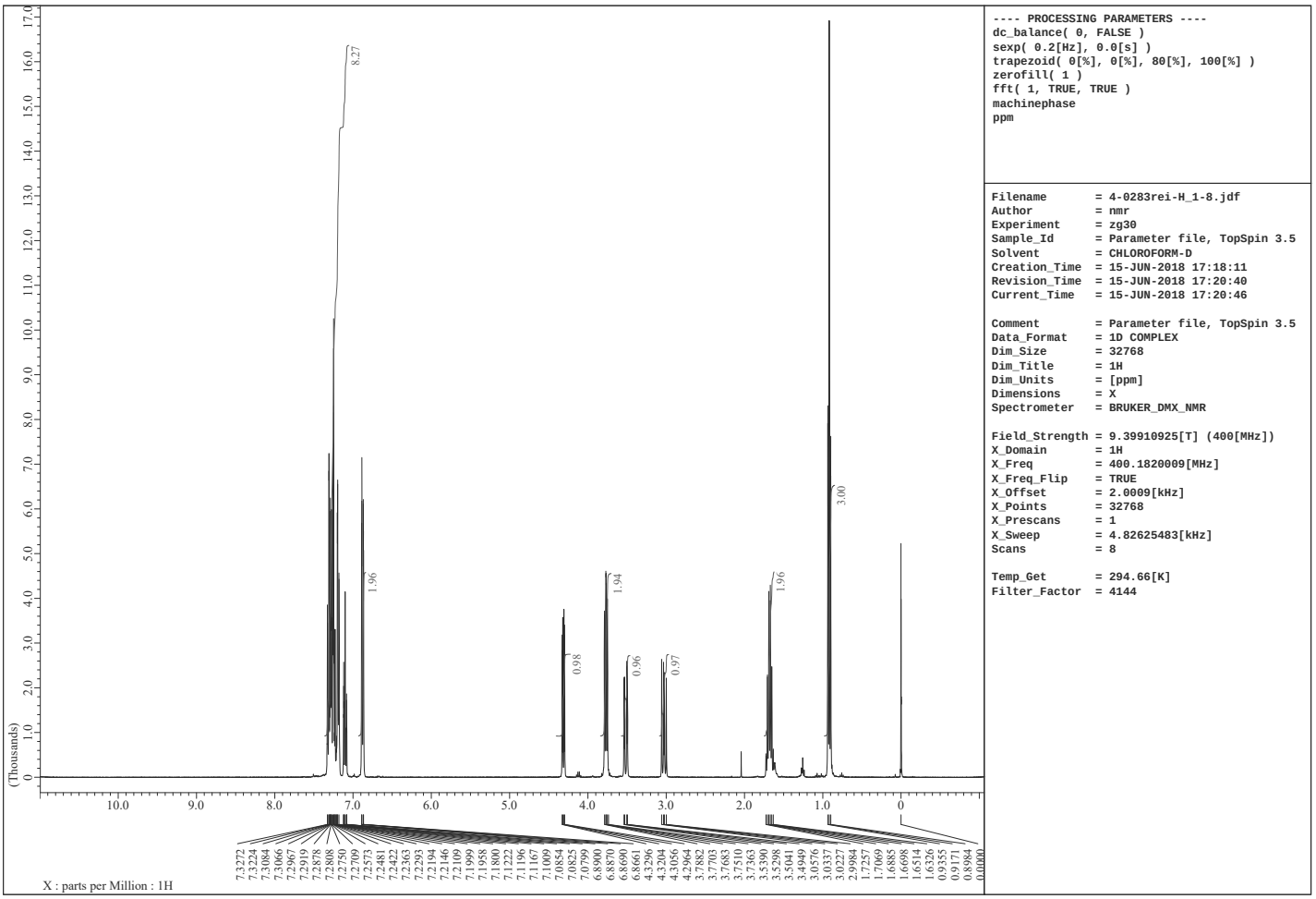
```
Filename        = 25160rei-H_1-4.jdf
Author          = root
Experiment      = zg30
Sample_Id       = Parameter file, TOPSPINVer
Solvent         = CHLOROFORM-D
Creation_Time   =  5-FEB-2018 11:44:17
Revision_Time   =  5-FEB-2018 11:48:03
Current_Time    =  5-FEB-2018 11:48:09

Comment         = Parameter file, TOPSPINVer
Data_Format     = 1D COMPLEX
Dim_Size        = 16384
Dim_Title       = 1H
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = BRUKER_DMX_NMR

Field_Strength = 7.05156322[T] (300[MHz])
X_Domain        = 1H
X_Freq          = 300.23150115[MHz]
X_Freq_Flip     = TRUE
X_Offset        = 1.50115[kHz]
X_Points        = 16384
X_Prescans      = 1
X_Sweep         = 3.61271676[kHz]
Scans           = 8

Temp_Get        = 300[K]
Filter_Factor   = 32
```



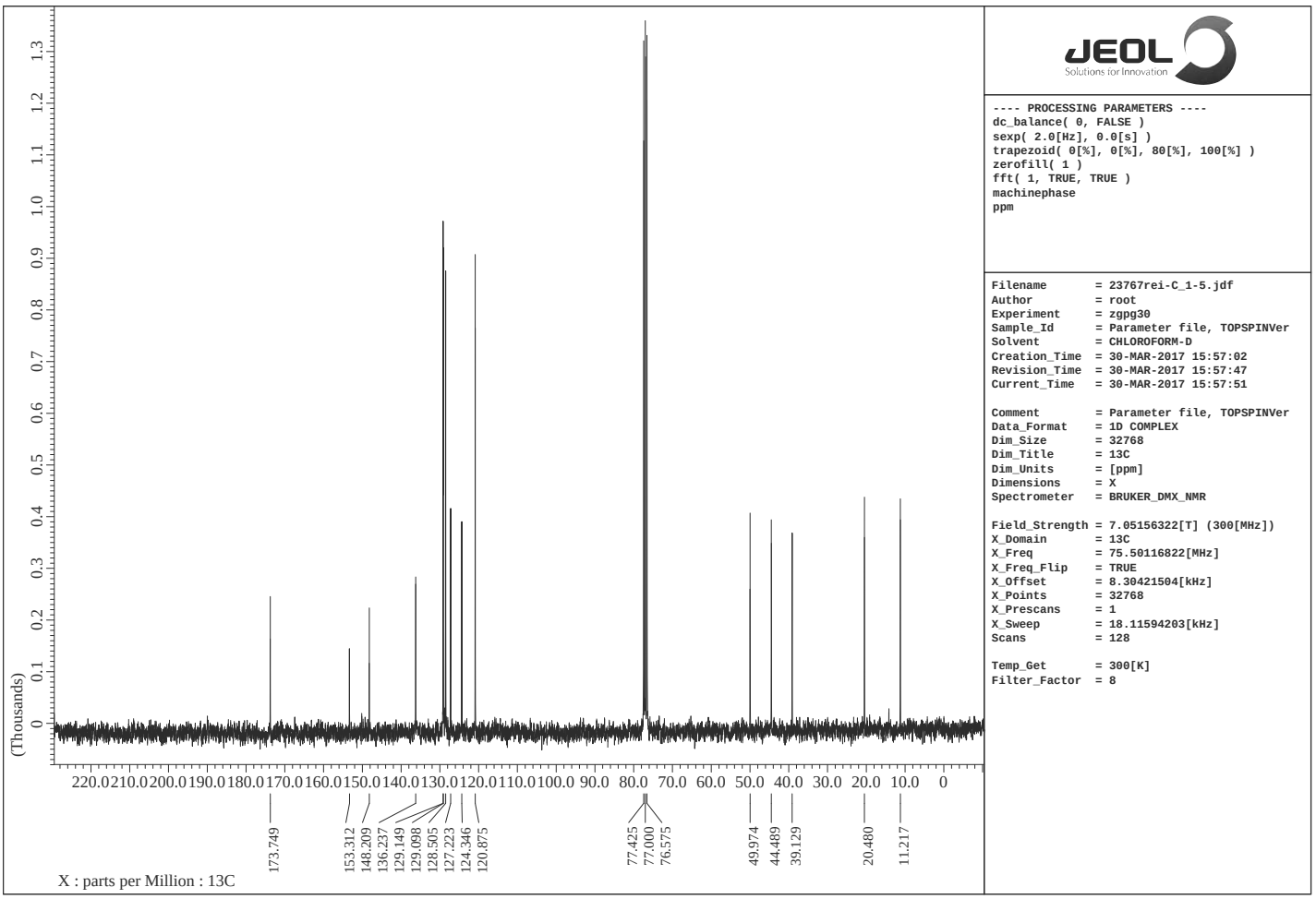

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename        = 23660rei-C_1-7.jdf
Author          = root
Experiment      = zgpg30
Sample_Id       = Parameter file, TOPSPINVer
Solvent         = CHLOROFORM-D
Creation_Time   = 30-MAR-2017 15:33:41
Revision_Time   = 30-MAR-2017 15:34:52
Current_Time    = 30-MAR-2017 15:34:57

Comment         = Parameter file, TOPSPINVer
Data_Format     = 1D COMPLEX
Dim_Size        = 32768
Dim_Title       = 13C
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = BRUKER_DMX_NMR

Field_Strength = 7.05156322[T] (300[MHz])
X_Domain        = 13C
X_Freq          = 75.50116822[MHz]
X_Freq_Flip     = TRUE
X_Offset        = 8.30421504[kHz]
X_Points        = 32768
X_Prescans      = 1
X_Sweep         = 18.11594203[kHz]
Scans           = 256

Temp_Get        = 300[K]
Filter_Factor   = 8
```

Figure S41. ^{1}H and ^{13}C NMR spectra of **4h**

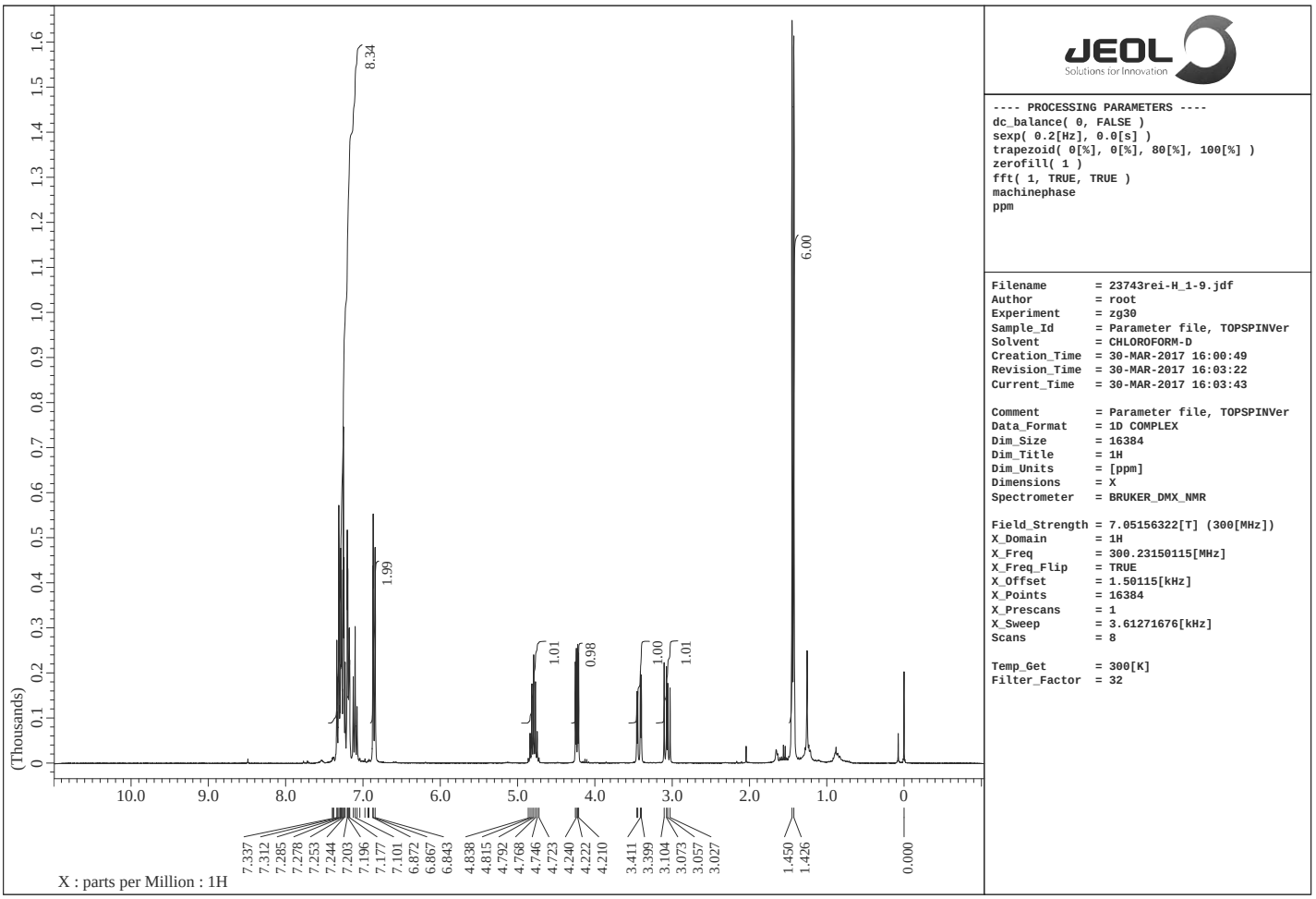



```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Filename        = 4-0283rei-H_1-8.jdf
Author          = nmr
Experiment      = zg30
Sample_Id       = Parameter file, TopSpin 3.5
Solvent         = CHLOROFORM-D
Creation_Time   = 15-JUN-2018 17:18:11
Revision_Time   = 15-JUN-2018 17:20:40
Current_Time    = 15-JUN-2018 17:20:46

Comment         = Parameter file, TopSpin 3.5
Data_Format     = 1D COMPLEX
Dim_Size        = 32768
Dim_Title       = 1H
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = BRUKER_DMX_NMR

Field_Strength = 9.39910925[T] (400[MHz])
X_Domain        = 1H
X_Freq          = 400.1820009[MHz]
X_Freq_Flip     = TRUE
X_Offset        = 2.0009[kHz]
X_Points        = 32768
X_Prescans      = 1
X_Sweep         = 4.82625483[kHz]
Scans           = 8

Temp_Get        = 294.66[K]
Filter_Factor   = 4144
```




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Filename        = 23767rei-C_1-5.jdf
Author          = root
Experiment      = zgpg30
Sample_Id       = Parameter file, TOPSPINVer
Solvent         = CHLOROFORM-D
Creation_Time   = 30-MAR-2017 15:57:02
Revision_Time   = 30-MAR-2017 15:57:47
Current_Time    = 30-MAR-2017 15:57:51

Comment         = Parameter file, TOPSPINVer
Data_Format     = 1D COMPLEX
Dim_Size        = 32768
Dim_Title       = 13C
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = BRUKER_DMX_NMR

Field_Strength = 7.05156322[T] (300[MHz])
X_Domain        = 13C
X_Freq          = 75.50116822[MHz]
X_Freq_Flip     = TRUE
X_Offset        = 8.30421504[kHz]
X_Points        = 32768
X_Prescans      = 1
X_Sweep         = 18.11594203[kHz]
Scans           = 128

Temp_Get        = 300[K]
Filter_Factor   = 8
```

Figure S42. ^{1}H and ^{13}C NMR spectra of **4i**



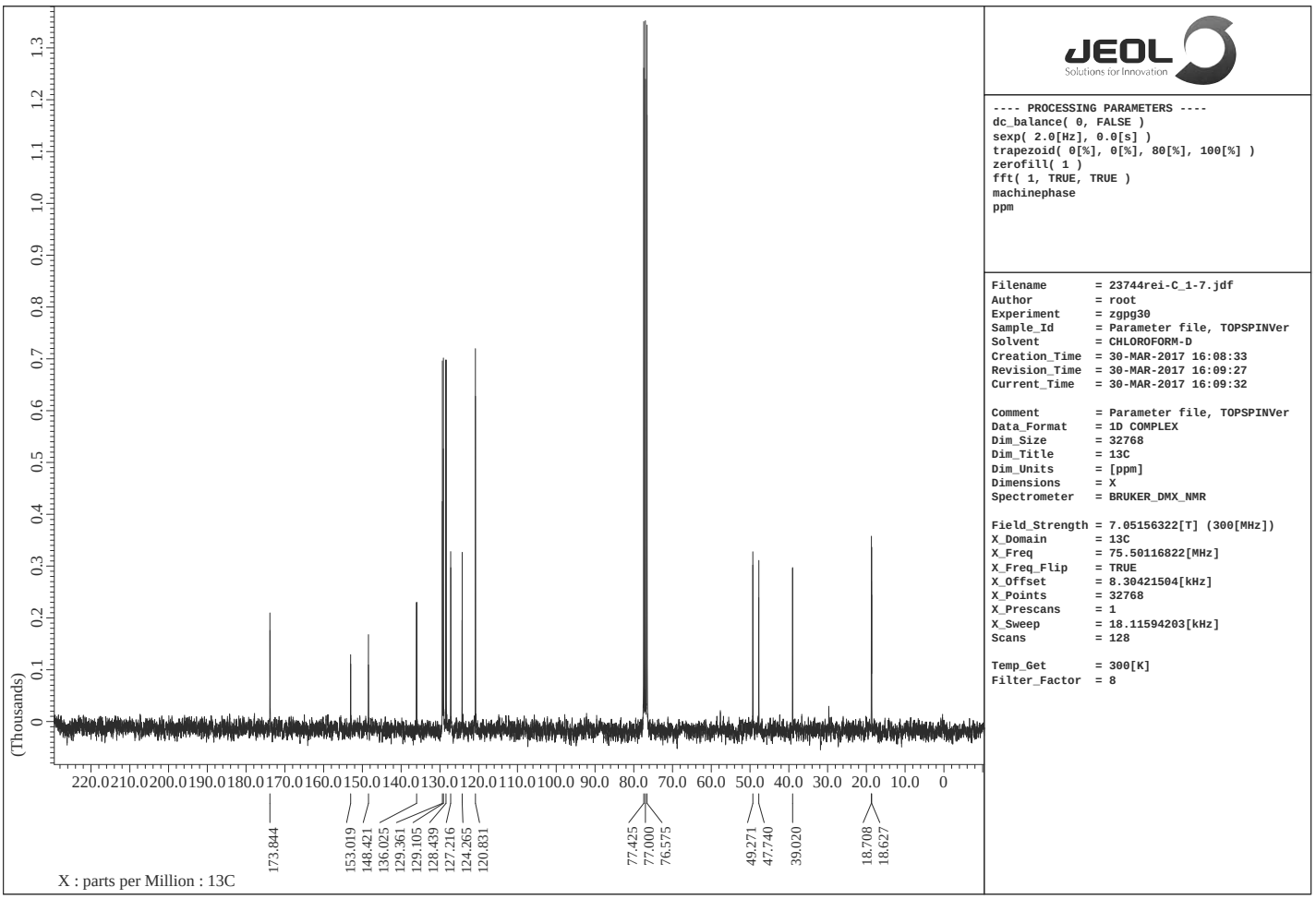
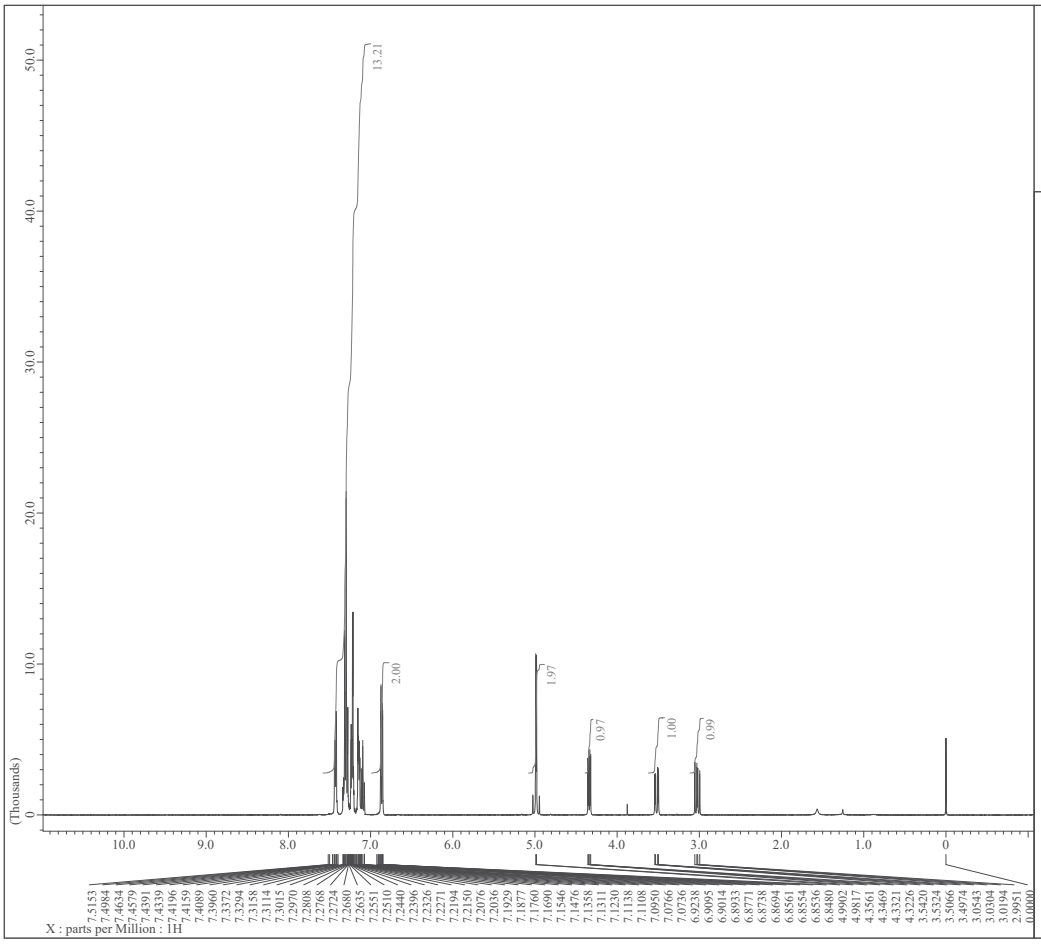
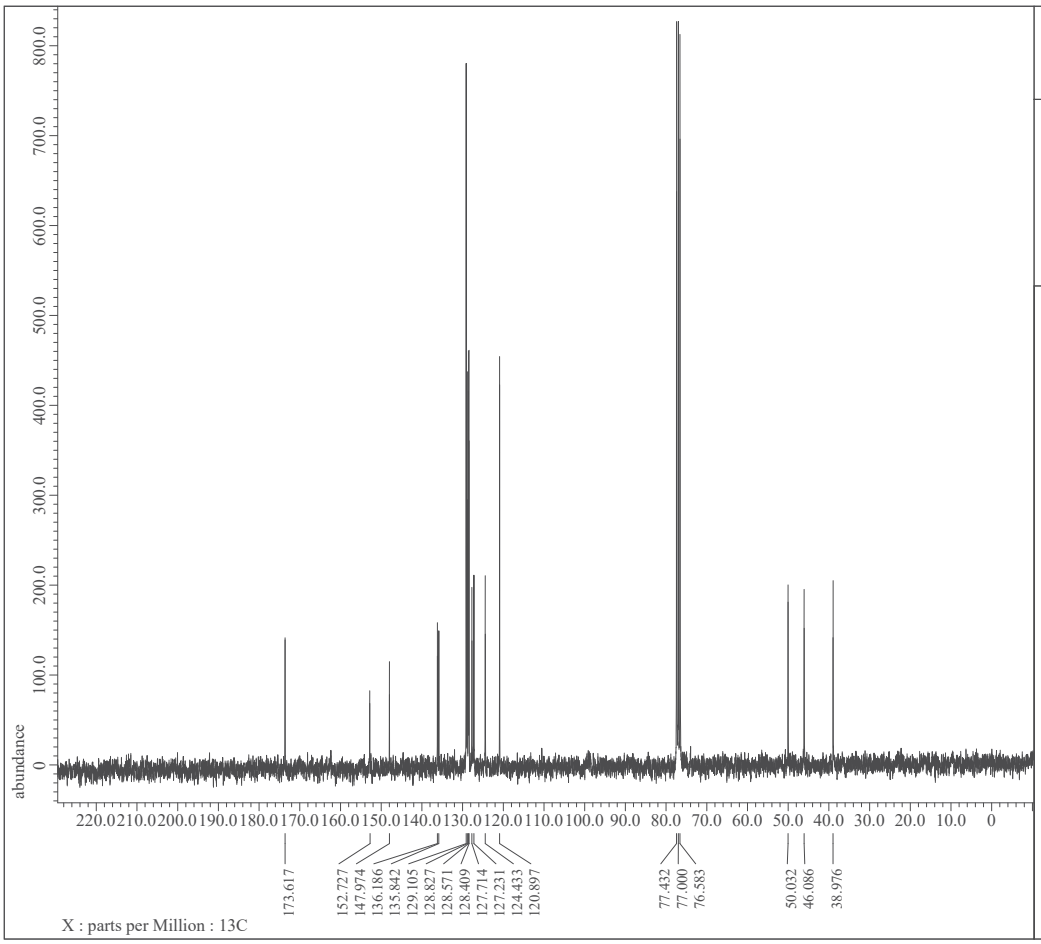


Figure S43. ^{1}H and ^{13}C NMR spectra of **4j**




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

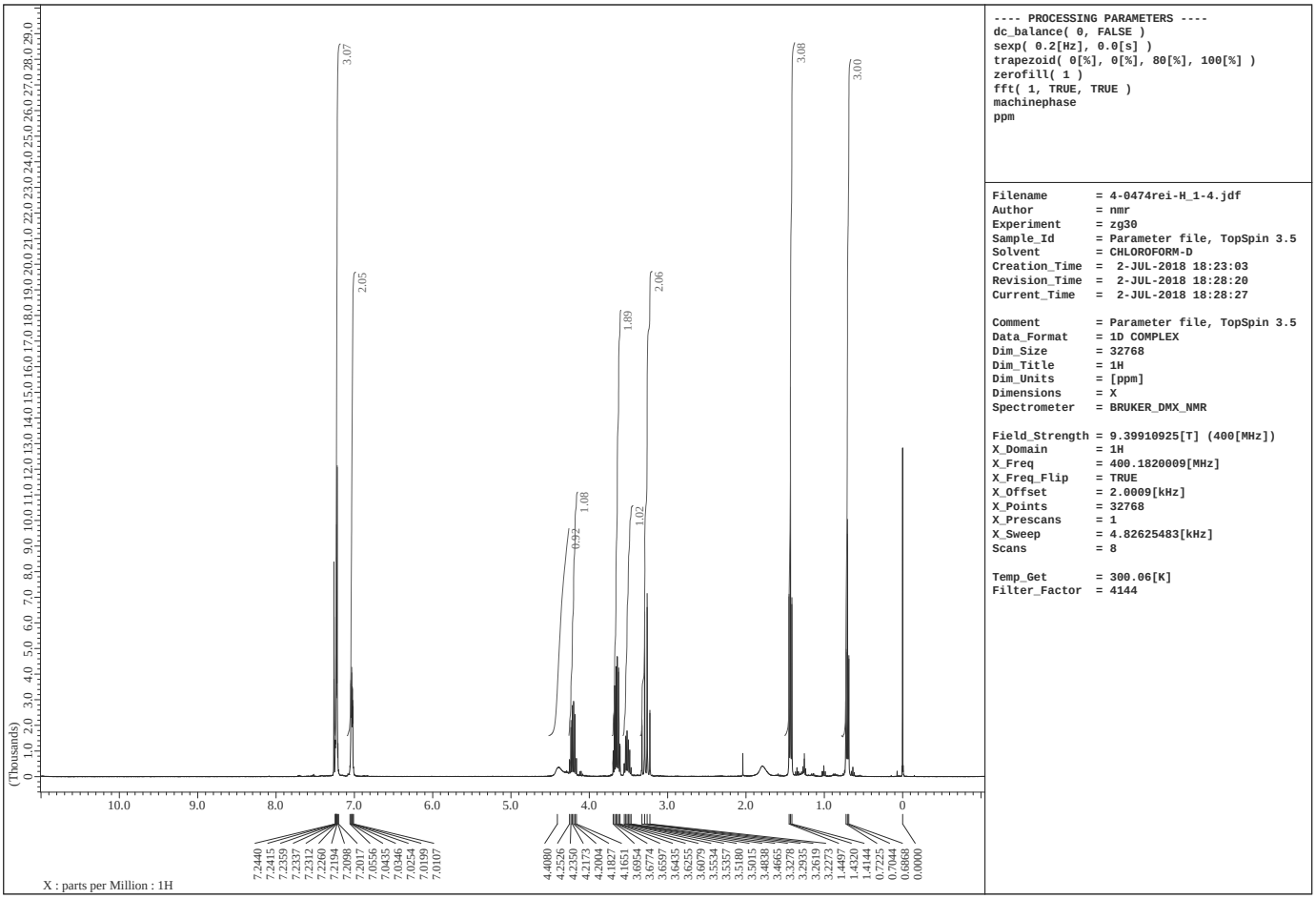
```
Filename        = 4-0589rei-H_1-3.jdf
Author          = nmr
Experiment      = zg30
Sample_Id       = green
Solvent         = CHLOROFORM-D
Creation_Time   = 14-SEP-2018 20:37:18
Revision_Time   = 14-SEP-2018 20:42:07
Current_Time    = 14-SEP-2018 20:42:32

Comment         = green
Data_Format     = 1D COMPLEX
Dim_Size        = 32768
Dim_Title       = 1H
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = BRUKER_DMX_NMR

Field_Strength = 9.39910925[T] (400[MHz])
X_Domain        = 1H
X_Freq          = 400.1820009[MHz]
X_Freq_Flip     = TRUE
X_Offset        = 2.0009[kHz]
X_Points        = 32768
X_Prescans      = 1
X_Sweep         = 4.82625483[kHz]
Scans           = 8

Temp_Get        = 296.76[K]
Filter_Factor   = 4144
```



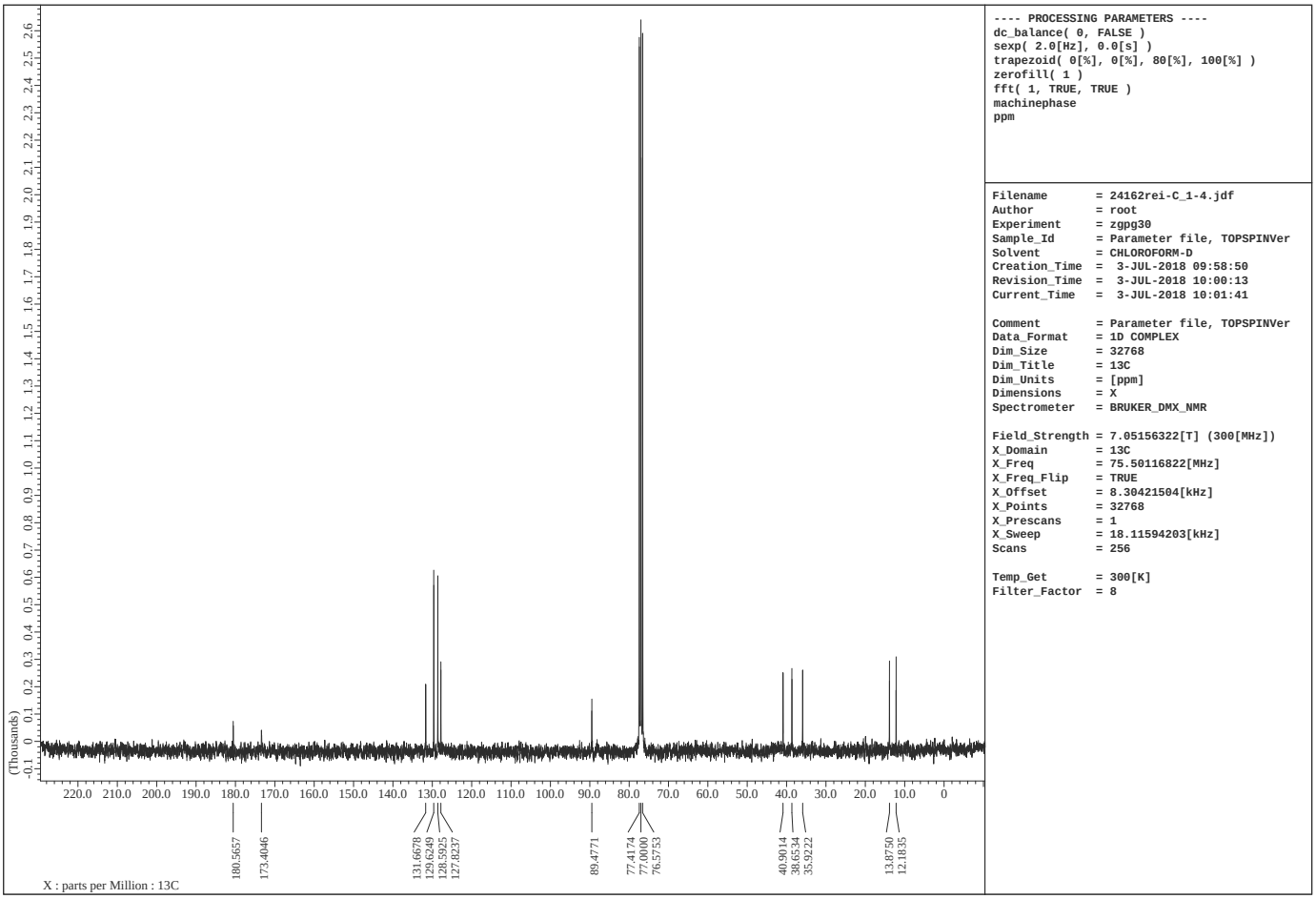

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename        = 24203rei-C_1-5.jdf
Author          = root
Experiment      = zgpg30
Sample_Id       = Parameter file, TOPSPINVer
Solvent         = CHLOROFORM-D
Creation_Time   = 30-MAR-2017 16:52:27
Revision_Time   = 30-MAR-2017 16:54:49
Current_Time    = 30-MAR-2017 16:54:53

Comment         = Parameter file, TOPSPINVer
Data_Format     = 1D COMPLEX
Dim_Size        = 32768
Dim_Title       = 13C
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = BRUKER_DMX_NMR

Field_Strength = 7.05156322[T] (300[MHz])
X_Domain        = 13C
X_Freq          = 75.50116822[MHz]
X_Freq_Flip     = TRUE
X_Offset        = 8.30421504[kHz]
X_Points        = 32768
X_Prescans      = 1
X_Sweep         = 18.11594203[kHz]
Scans           = 128

Temp_Get        = 300[K]
Filter_Factor   = 8
```

Figure S44. ^{1}H and ^{13}C NMR spectra of **5b**

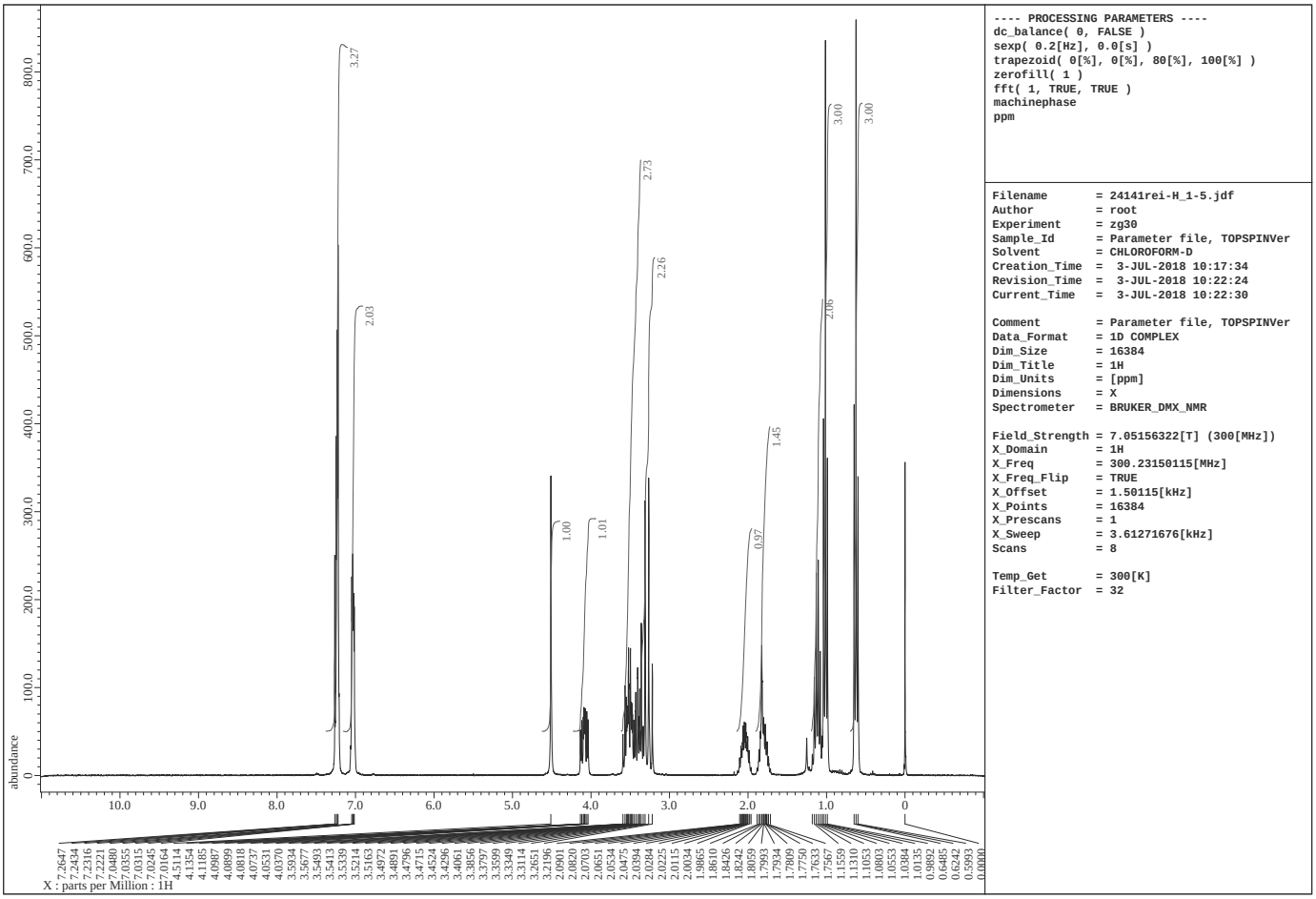



```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Filename        = 4-0474rei-H_1-4.jdf
Author          = nmr
Experiment      = zg30
Sample_Id       = Parameter file, TopSpin 3.5
Solvent         = CHLOROFORM-D
Creation_Time   =  2-JUL-2018 18:23:03
Revision_Time   =  2-JUL-2018 18:28:20
Current_Time    =  2-JUL-2018 18:28:27

Comment         = Parameter file, TopSpin 3.5
Data_Format     = 1D COMPLEX
Dim_Size        = 32768
Dim_Title       = 1H
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = BRUKER_DMX_NMR

Field_Strength = 9.39910925[T] (400[MHz])
X_Domain        = 1H
X_Freq          = 400.1820009[MHz]
X_Freq_Flip     = TRUE
X_Offset        = 2.0009[kHz]
X_Points        = 32768
X_Prescans      = 1
X_Sweep         = 4.82625483[kHz]
Scans           = 8

Temp_Get        = 300.06[K]
Filter_Factor   = 4144
```

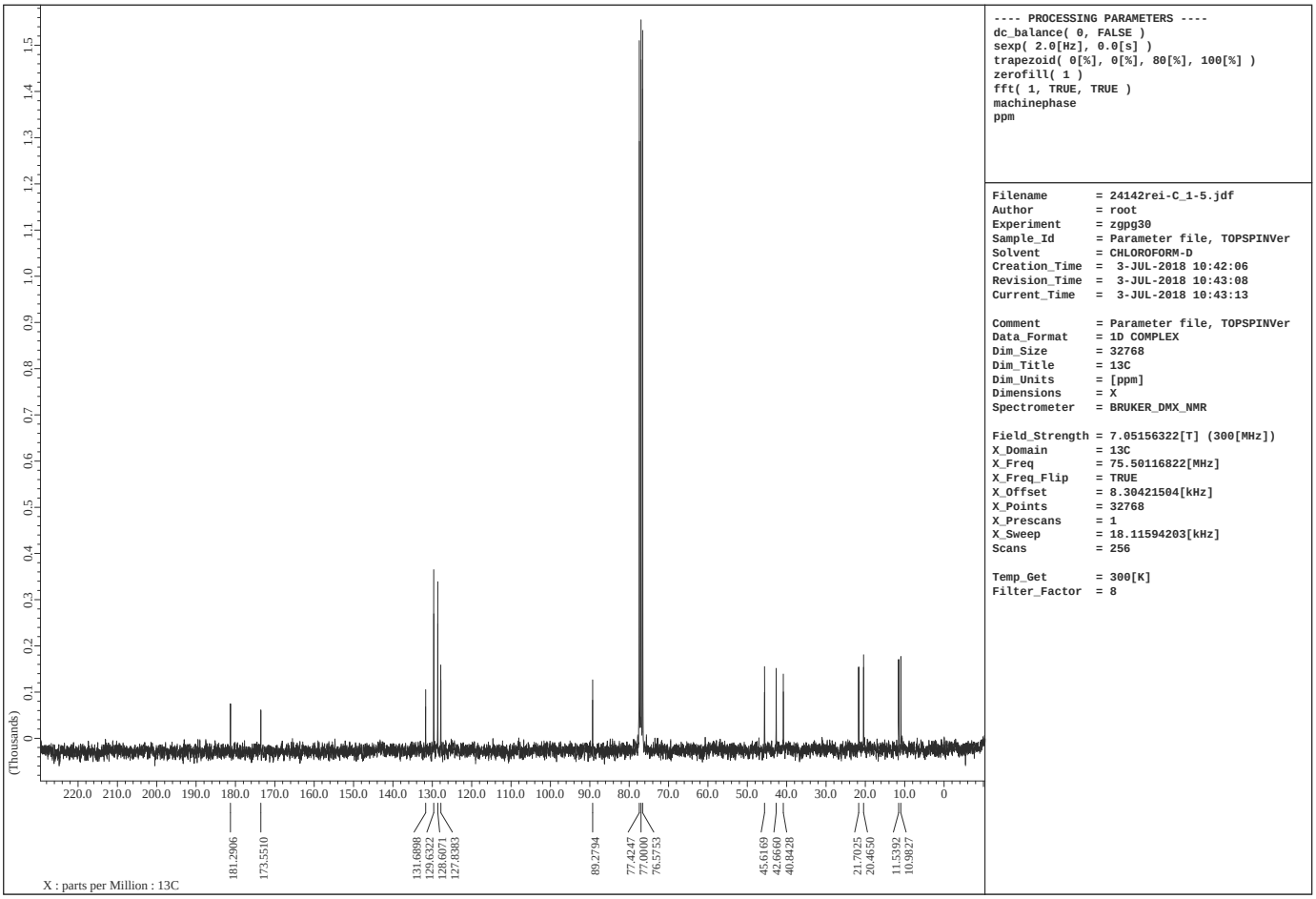



```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Filename        = 24162rei-C_1-4.jdf
Author          = root
Experiment      = zgpg30
Sample_Id       = Parameter file, TOPSPINVer
Solvent         = CHLOROFORM-D
Creation_Time   =  3-JUL-2018 09:58:50
Revision_Time   =  3-JUL-2018 10:00:13
Current_Time    =  3-JUL-2018 10:01:41

Comment         = Parameter file, TOPSPINVer
Data_Format     = 1D COMPLEX
Dim_Size        = 32768
Dim_Title       = 13C
Dim_Units       = [ppm]
Dimensions      = X
Spectrometer    = BRUKER_DMX_NMR

Field_Strength = 7.05156322[T] (300[MHz])
X_Domain        = 13C
X_Freq          = 75.50116822[MHz]
X_Freq_Flip     = TRUE
X_Offset        = 8.30421504[kHz]
X_Points        = 32768
X_Prescans      = 1
X_Sweep         = 18.11594203[kHz]
Scans           = 256

Temp_Get        = 300[K]
Filter_Factor   = 8
```

Figure S45. ^{1}H and ^{13}C NMR spectra of **5c**




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Filename       = 24141rei-H_1-5.jdf
Author         = root
Experiment     = zg30
Sample_Id      = Parameter file, TOPSPINVer
Solvent        = CHLOROFORM-D
Creation_Time  =  3-JUL-2018 10:17:34
Revision_Time  =  3-JUL-2018 10:22:24
Current_Time   =  3-JUL-2018 10:22:30

Comment        = Parameter file, TOPSPINVer
Data_Format    = 1D COMPLEX
Dim_Size       = 16384
Dim_Title      = 1H
Dim_Units      = [ppm]
Dimensions     = X
Spectrometer   = BRUKER_DMX_NMR

Field_Strength = 7.05156322[T] (300[MHz])
X_Domain       = 1H
X_Freq         = 300.23150115[MHz]
X_Freq_Flip    = TRUE
X_Offset       = 1.50115[kHz]
X_Points       = 16384
X_Prescans     = 1
X_Sweep        = 3.61271676[kHz]
Scans          = 8

Temp_Get       = 300[K]
Filter_Factor  = 32
```




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Filename       = 24142rei-C_1-5.jdf
Author         = root
Experiment     = zgpg30
Sample_Id      = Parameter file, TOPSPINVer
Solvent        = CHLOROFORM-D
Creation_Time  =  3-JUL-2018 10:42:06
Revision_Time  =  3-JUL-2018 10:43:08
Current_Time   =  3-JUL-2018 10:43:13

Comment        = Parameter file, TOPSPINVer
Data_Format    = 1D COMPLEX
Dim_Size       = 32768
Dim_Title      = 13C
Dim_Units      = [ppm]
Dimensions     = X
Spectrometer   = BRUKER_DMX_NMR

Field_Strength = 7.05156322[T] (300[MHz])
X_Domain       = 13C
X_Freq         = 75.50116822[MHz]
X_Freq_Flip    = TRUE
X_Offset       = 8.30421504[kHz]
X_Points       = 32768
X_Prescans     = 1
X_Sweep        = 18.11594203[kHz]
Scans          = 256

Temp_Get       = 300[K]
Filter_Factor  = 8
```