Supplementary Material

Diastereoselective photochemical radical addition of a cyclic ether to olefins: addition of THF radicals to dialkyl maleates

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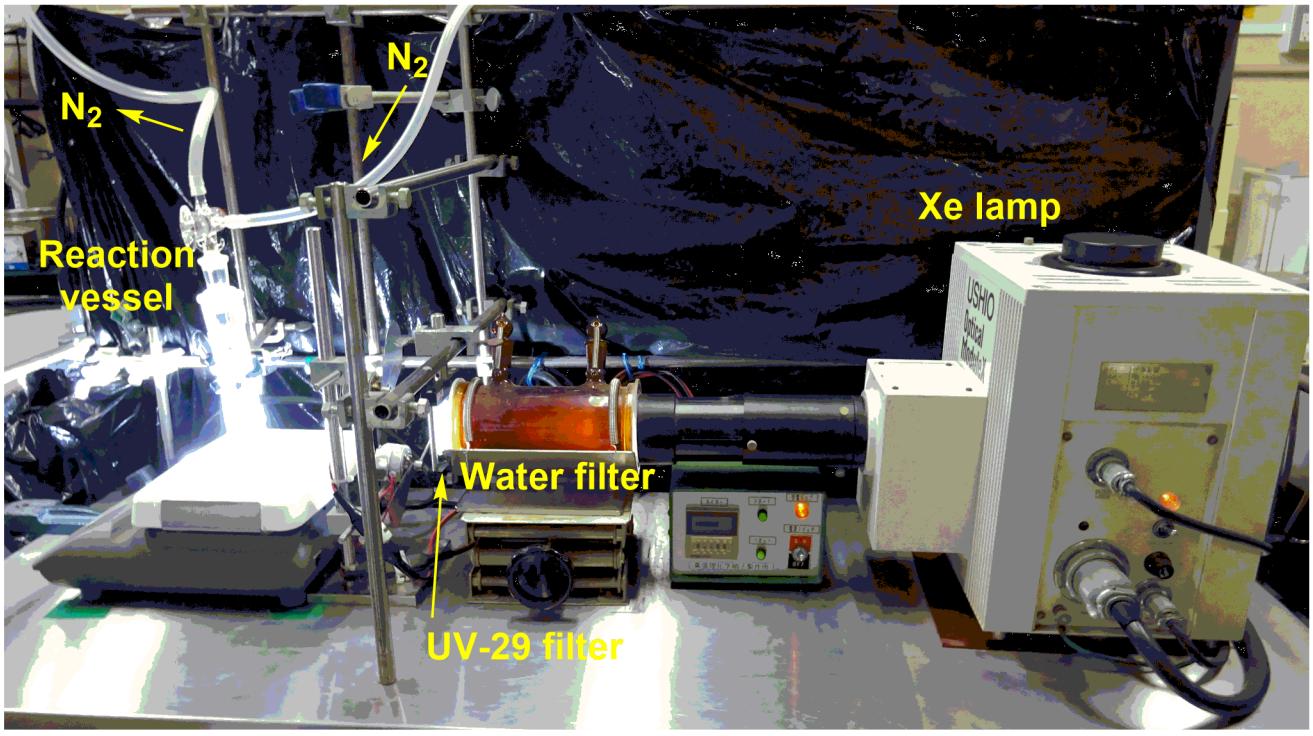
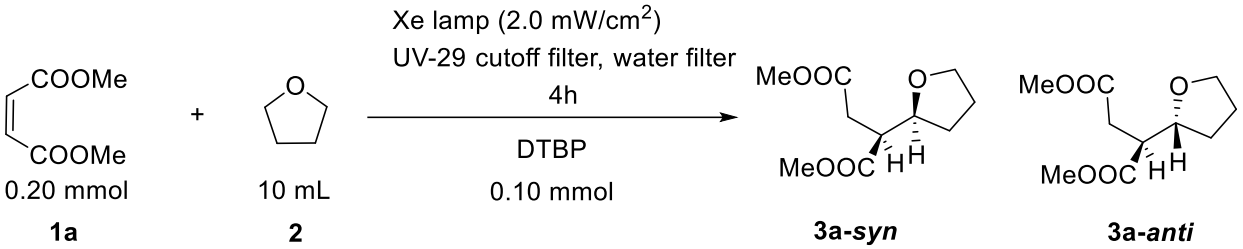
1. Experimental

1.1. Experimental setup



1.2. Experimental details of the reactions in Table 1

1.2.1. Entry 1: 2-(Tetrahydro-2-furanyl)butanedioic acid 1,4-dimethyl ester (**3a-*syn*/*anti***)[S1–S3]



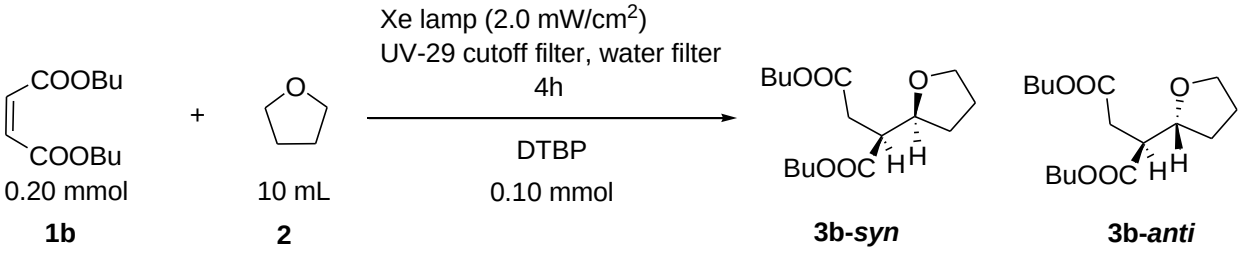
Run 1

Dimethyl maleate (**1a**, 28.87 mg, 0.20 mmol) and DTBP (14.76 mg, 0.10 mmol) in THF (**2**, 10 mL). Yield of **3a**: 100 % (*syn* / *anti* = 61 / 39) (conversion: 100 %) (NMR, $CDCl_3$).

Run 2

Dimethyl maleate (**1a**, 28.79 mg, 0.20 mmol) and DTBP (14.76 mg, 0.10 mmol) in THF (**2**, 10 mL). Yield of **3a**: 95 % (*syn* / *anti* = 60 / 35) (conversion: 100 %) (NMR, $CDCl_3$).

1.2.2. Entry 2: 2-(Tetrahydro-2-furanyl)butanedioic acid 1,4-dibutyl ester (**3b-*syn*/*anti***)



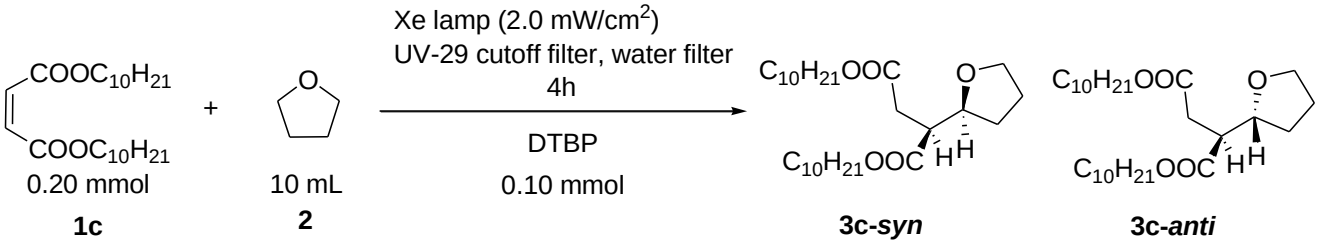
Run 1

Dibutyl maleate (**1b**, 45.52 mg, 0.20 mmol) and DTBP (15.14 mg, 0.10 mmol) in THF (**2**, 10 mL). Yield of **3b**: 100 % (*syn* / *anti* = 64 / 36) (conversion: 100 %) (NMR, $CDCl_3$).

Run 2

Dibutyl maleate (**1b**, 45.61 mg, 0.20 mmol) and DTBP (14.68 mg, 0.10 mmol) in THF (**2**, 10 mL). Yield of **3b**: 100 % (*syn* / *anti* = 65 / 35) (conversion: 100 %) (NMR, $CDCl_3$).

1.2.3. Entry 3: 2-(Tetrahydro-2-furanyl)butanedioic acid 1,4-didecyl ester (**3c-*syn*/*anti***)



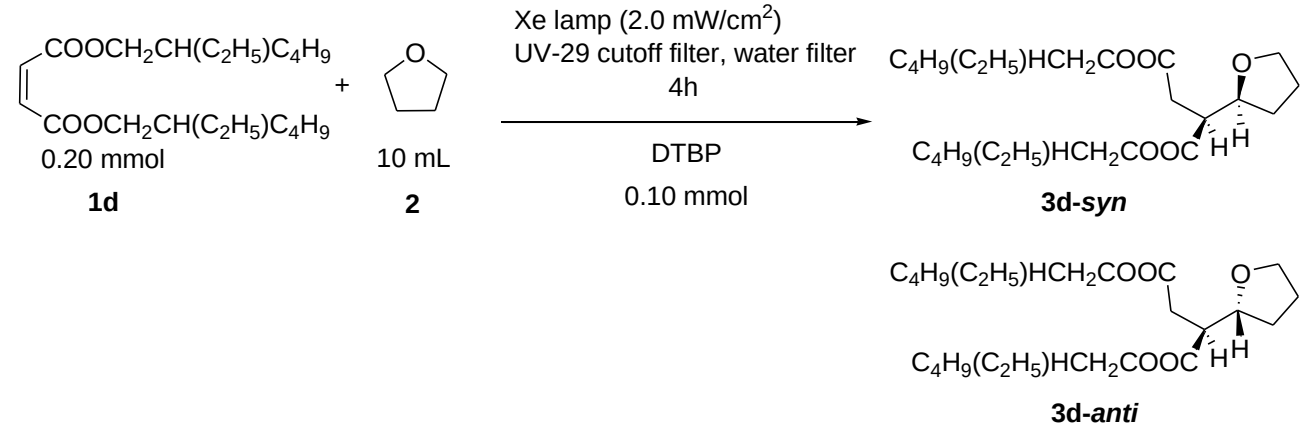
Run 1

Didecyl maleate (**1c**, 79.08 mg, 0.20 mmol) and DTBP (14.86 mg, 0.10 mmol) in THF (**2**, 10 mL). Yield of **3c**: 86 % (*syn* / *anti* = 60 / 26) (conversion: 100 %) (NMR, $CDCl_3$).

Run 2

Didecyl maleate (**1c**, 79.56 mg, 0.20 mmol) and DTBP (14.85 mg, 0.10 mmol) in THF (**2**, 10 mL). Yield of **3c**: 89 % (*syn* / *anti* = 60 / 29) (conversion: 100 %) (NMR, $CDCl_3$).

1.2.4. Entry 4: 2-(Tetrahydro-2-furanyl)butanedioic acid 1,4-bis(2-ethylhexyl) ester (**3d-*syn*/*anti***)



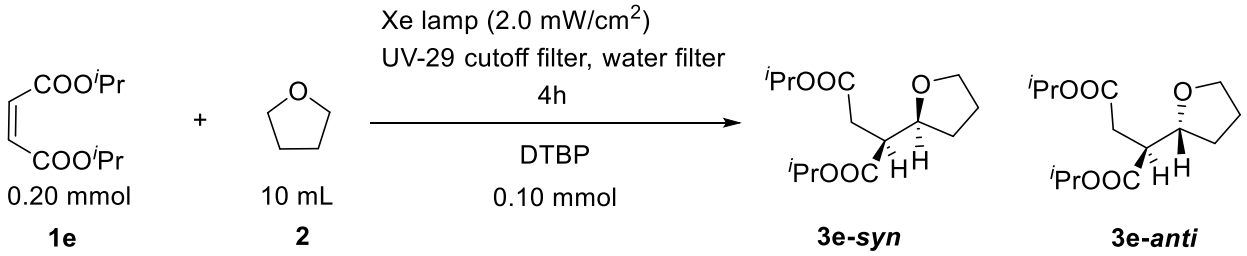
Run 1

Bis (2-ethylhexyl) maleate (**1d**, 68.07 mg, 0.20 mmol) and DTBP (14.79 mg, 0.10 mmol) in THF (**2**, 10 mL). Yield of **3d**: 99 % (*syn* / *anti* = 67 / 32) (conversion: 100 %) (NMR, $CDCl_3$).

Run 2

Bis (2-ethylhexyl) maleate (**1d**, 68.18 mg, 0.20 mmol) and DTBP (14.63 mg, 0.10 mmol) in THF (**2**, 10 mL). Yield of **3d**: 96 % (*syn* / *anti* = 62/ 34) (conversion: 100 %) (NMR, $CDCl_3$).

1.2.5. Entry 5: 2-(Tetrahydro-2-furanyl)butanedioic acid 1,4-diisopropyl ester (**3e-*syn*/*anti***) [S3]



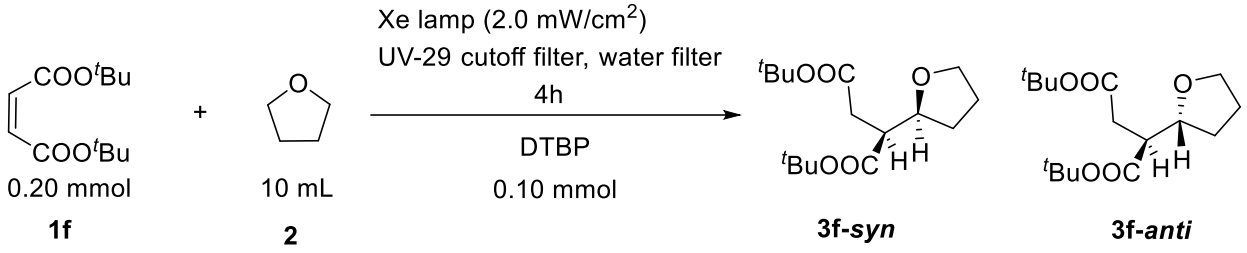
Run 1

Diisopropyl maleate (**1e**, 40.32 mg, 0.20 mmol) and DTBP (14.60 mg, 0.10 mmol) in THF (**2**, 10 mL). Yield of **3e**: 91 % (*syn* / *anti* = 61 / 30) (conversion: 100 %) (NMR, $CDCl_3$).

Run 2

Diisopropyl maleate (**1e**, 68.07 mg, 0.20 mmol) and DTBP (14.79 mg, 0.10 mmol) in THF (**2**, 10 mL). Yield of **3e**: 96 % (*syn* / *anti* = 64 / 32) (conversion: 100 %) (NMR, $CDCl_3$).

1.2.6. Entry 6: 2-(Tetrahydro-2-furanyl)butanedioic acid 1,4- di-*tert*-butyl ester (**3f-*syn*/*anti***)



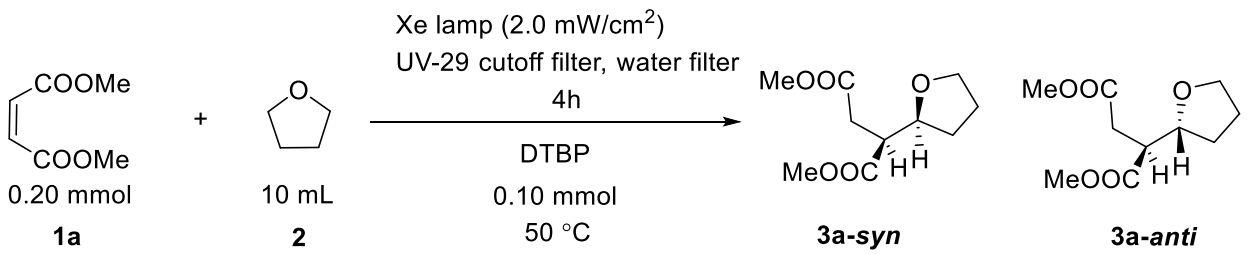
Run 1

Di-*tert*-butyl maleate (**1f**, 45.50 mg, 0.20 mmol) and DTBP (14.51 mg, 0.10 mmol) in THF (**2**, 10 mL). Yield of **3f**: 96 % (*syn* / *anti* = 67 / 29) (conversion: 100 %) (NMR, $CDCl_3$).

Run 2

Di-*tert*-butyl maleate (**1f**, 45.59 mg, 0.20 mmol) and DTBP (14.75 mg, 0.10 mmol) in THF (**2**, 10 mL). Yield of **3f**: 96 % (*syn* / *anti* = 67 / 29) (conversion: 100 %) (NMR, $CDCl_3$).

1.3. Reaction of 1a and 2 at 50 °C (**3a-*cis*-*syn*/*anti***)[S1–S3]



Dimethyl maleate (**1a**, 28.84 mg, 0.20 mmol) and DTBP (14.56 mg, 0.10 mmol) in THF (**2**, 10 mL). Irradiation time: 4h. Irradiation temperature: 50 °C. Yield of **3a**: 100 % (*syn* / *anti* = 61 / 38) (conversion: 100 %) (NMR, $CDCl_3$).

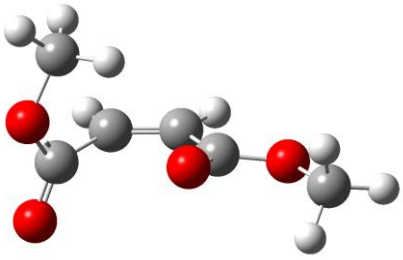
References

S1. Hayakawa, M.; Shimizu, R.; Omori, H.; Shirota, H.; Uchida, K.; Mashimo, H.; Xu, H.; Yamada, R.; Niino, S.; Wakame, Y.; Liu, C.; Aoyama, T.; Ouchi, A., *Tetrahedron*, **2020**, *76*, 131557.

S2. Rohe, S.; Morris, A. O.; McCallum, T.; Barriault, L., *Angew. Chem. Int. Ed.*, **2018**, *57*, 15664–15669.

S3. Papadopoulos, G. N.; Kokotou, M. G.; Spiliopoulou, N.; Nikitas, N. F.; Voutyritsa, E.; Tzaras, D. I.; Kaplaneris. N.; Kokotos, C. G., *ChemSusChem*, **2020**, *13*, 5934–5944.

2. Calculated stable conformers and energies of maleic acid and its dialkyl esters. [S4, S5]



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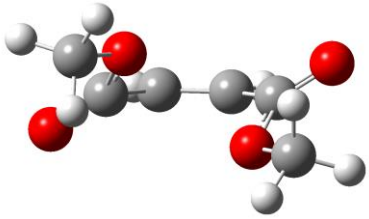

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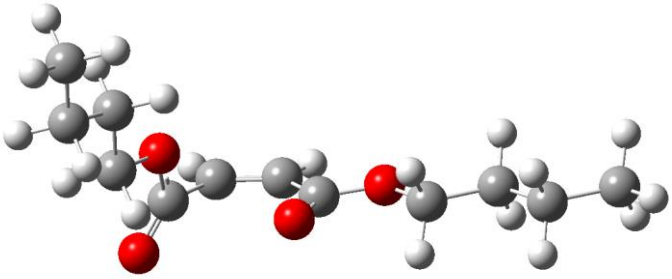

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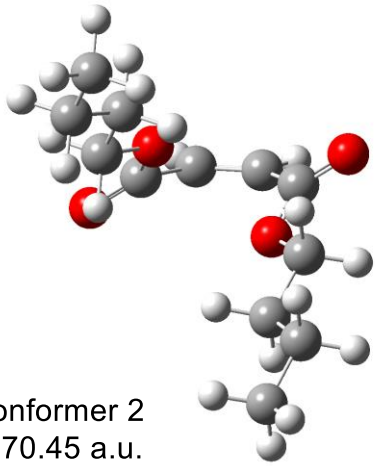

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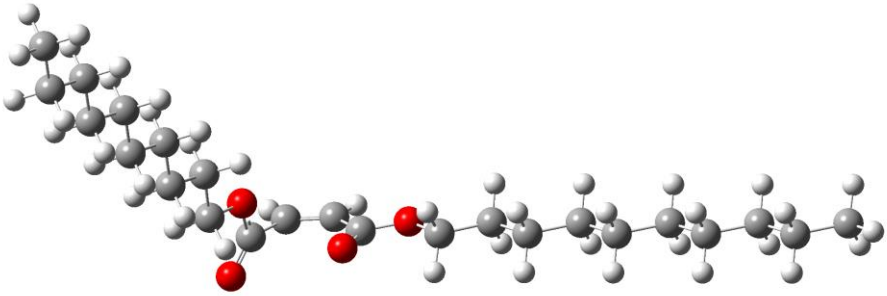

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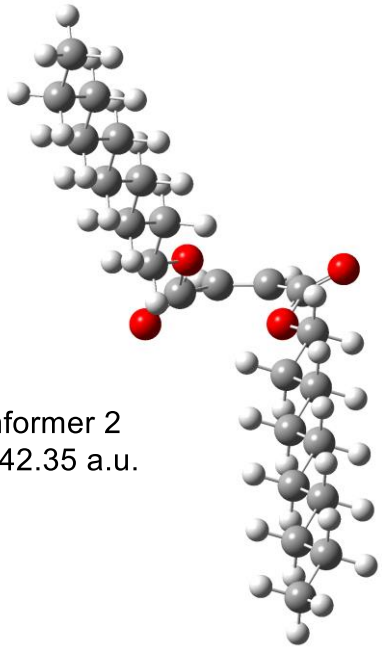

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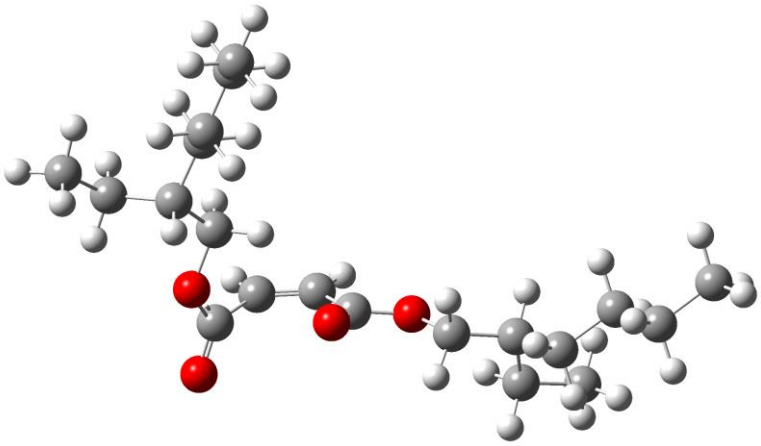

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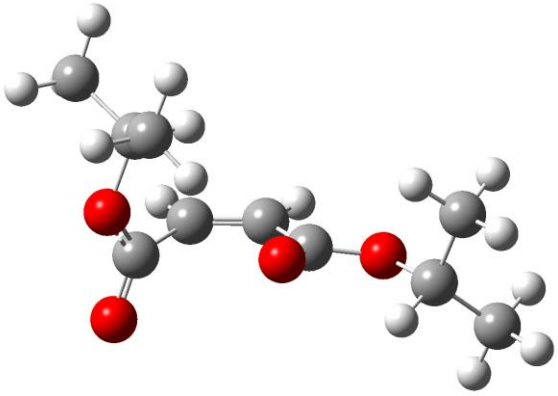

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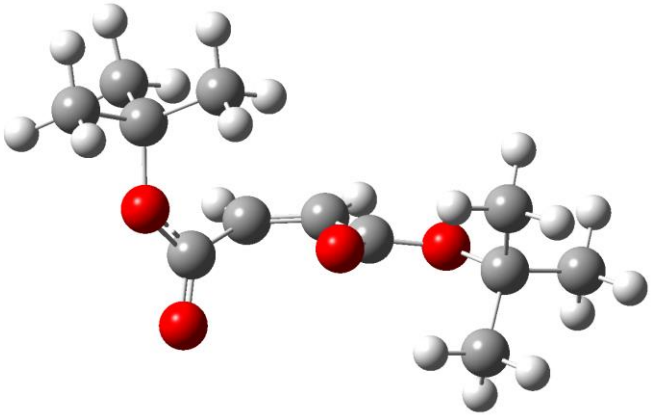

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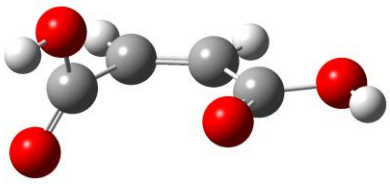

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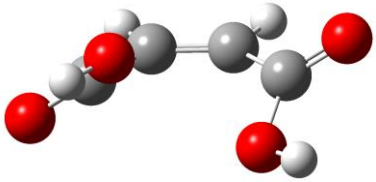

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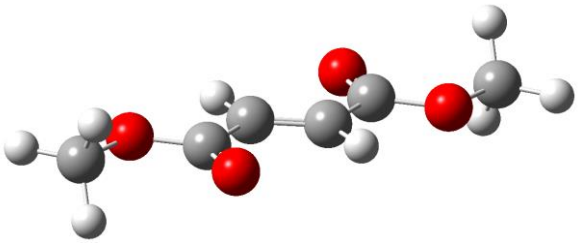

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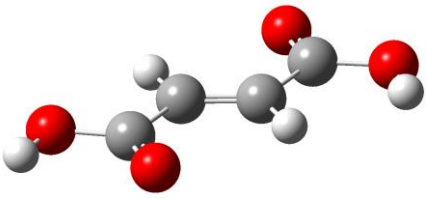

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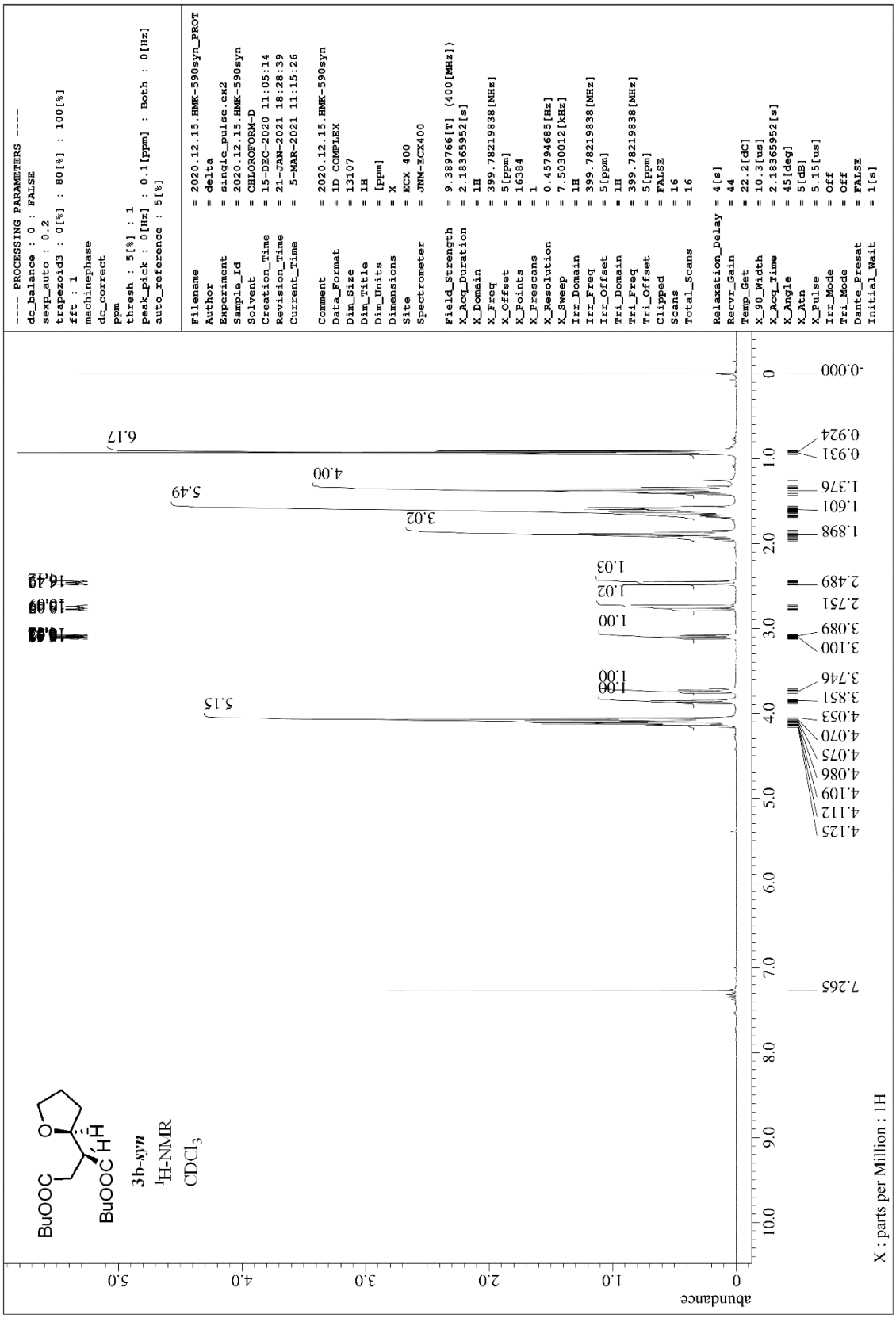
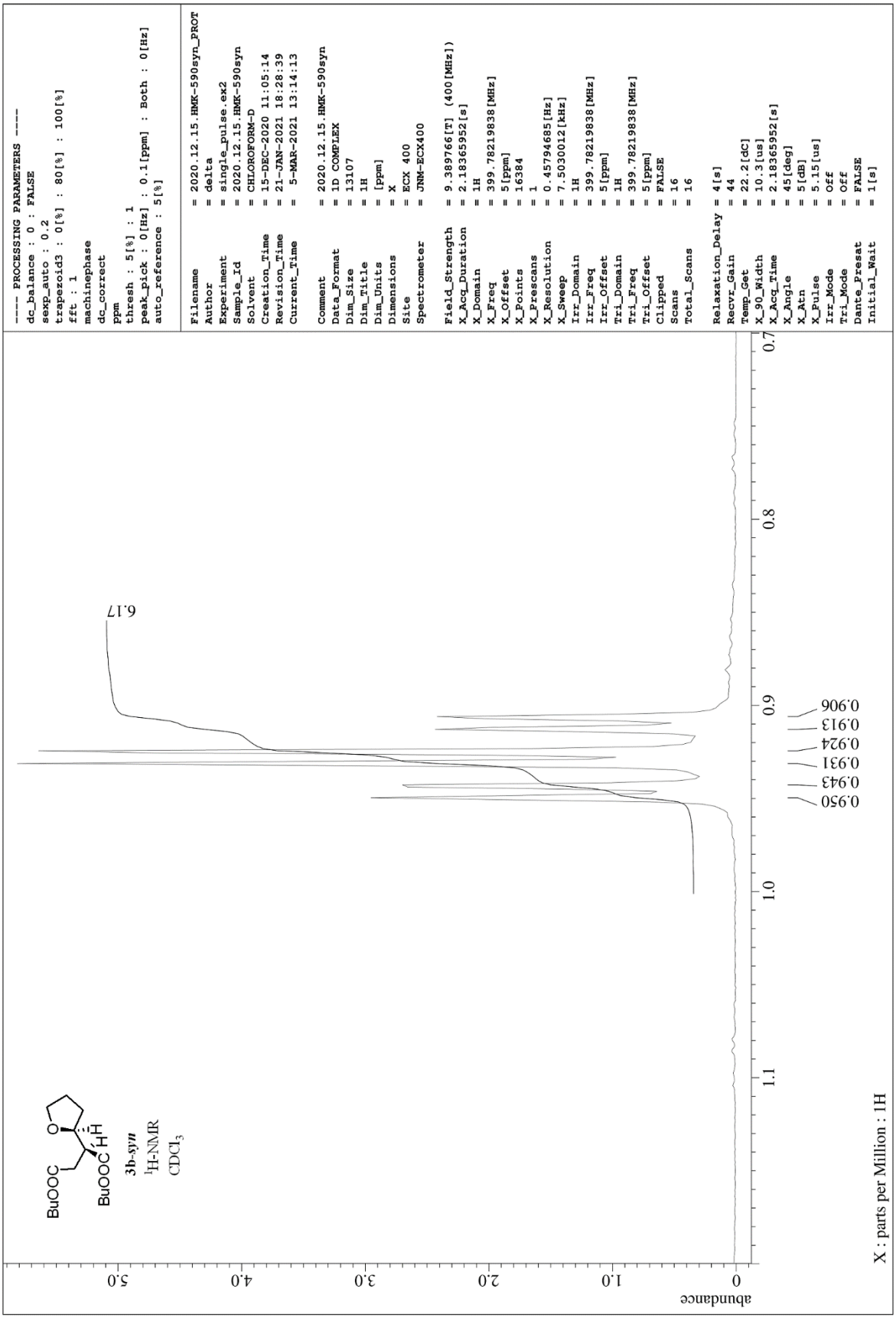
References

S4. Stable conformations were calculated by B3LYP/6-31++G(d,p) using Gaussian 16; Gaussian 16, Revision A.03, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2016.

S5. Graphics were prepared using GausView 6; GaussView, Version 6, Dennington, Roy; Keith, Todd A.; Millam, John M. Semichem Inc., Shawnee Mission, KS, 2016.

3. ^{1}H-NMR and ^{13}C-NMR spectra.

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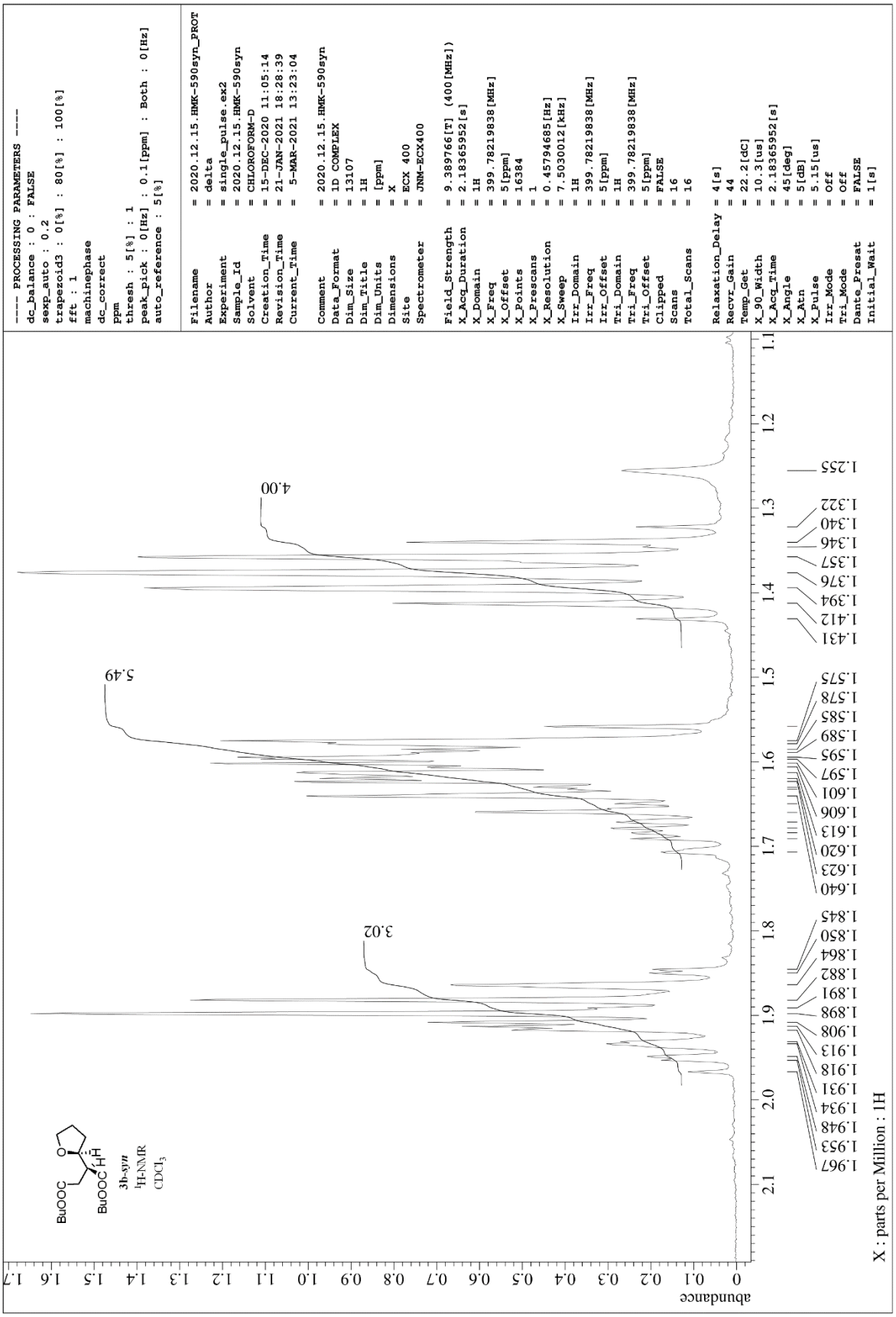
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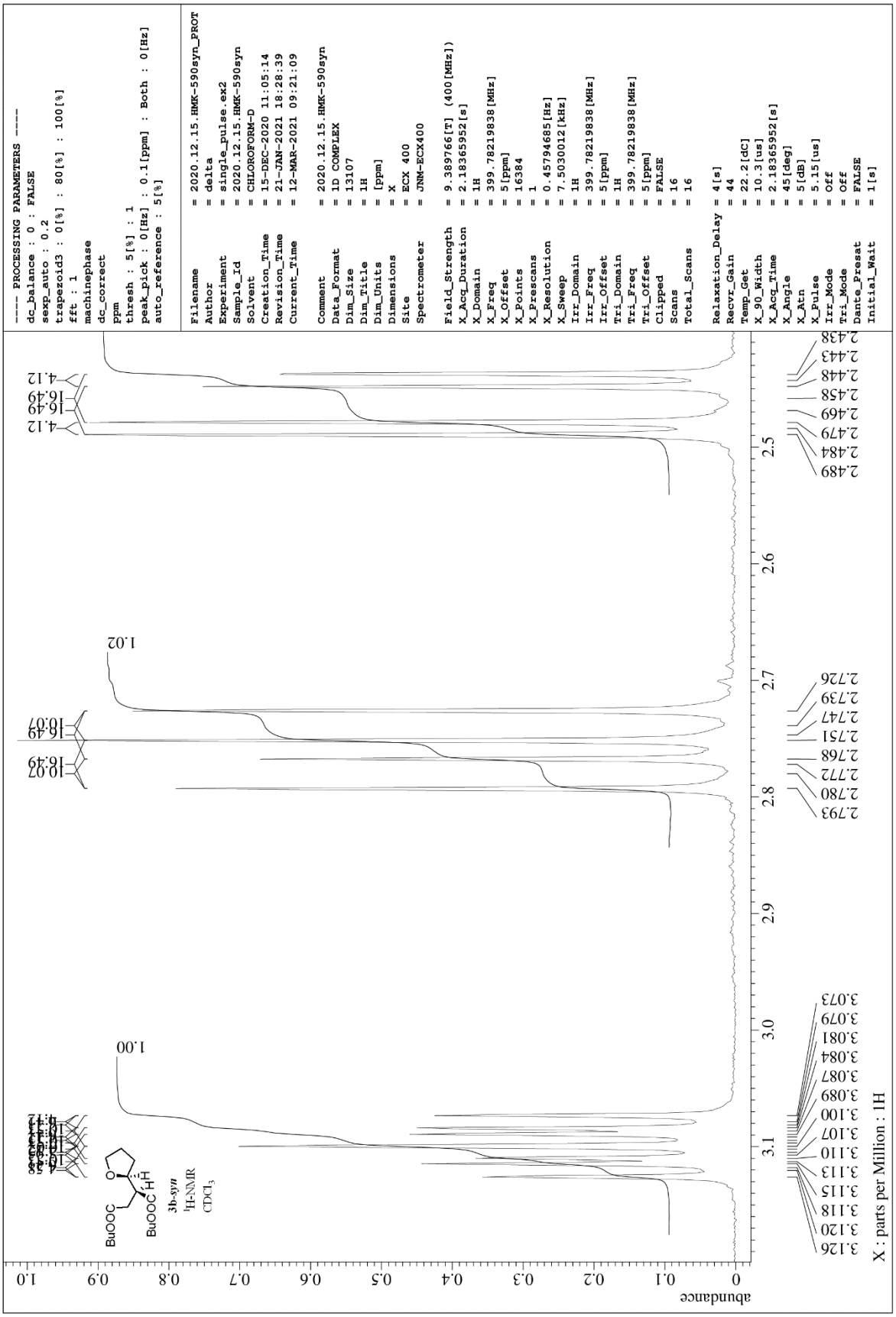
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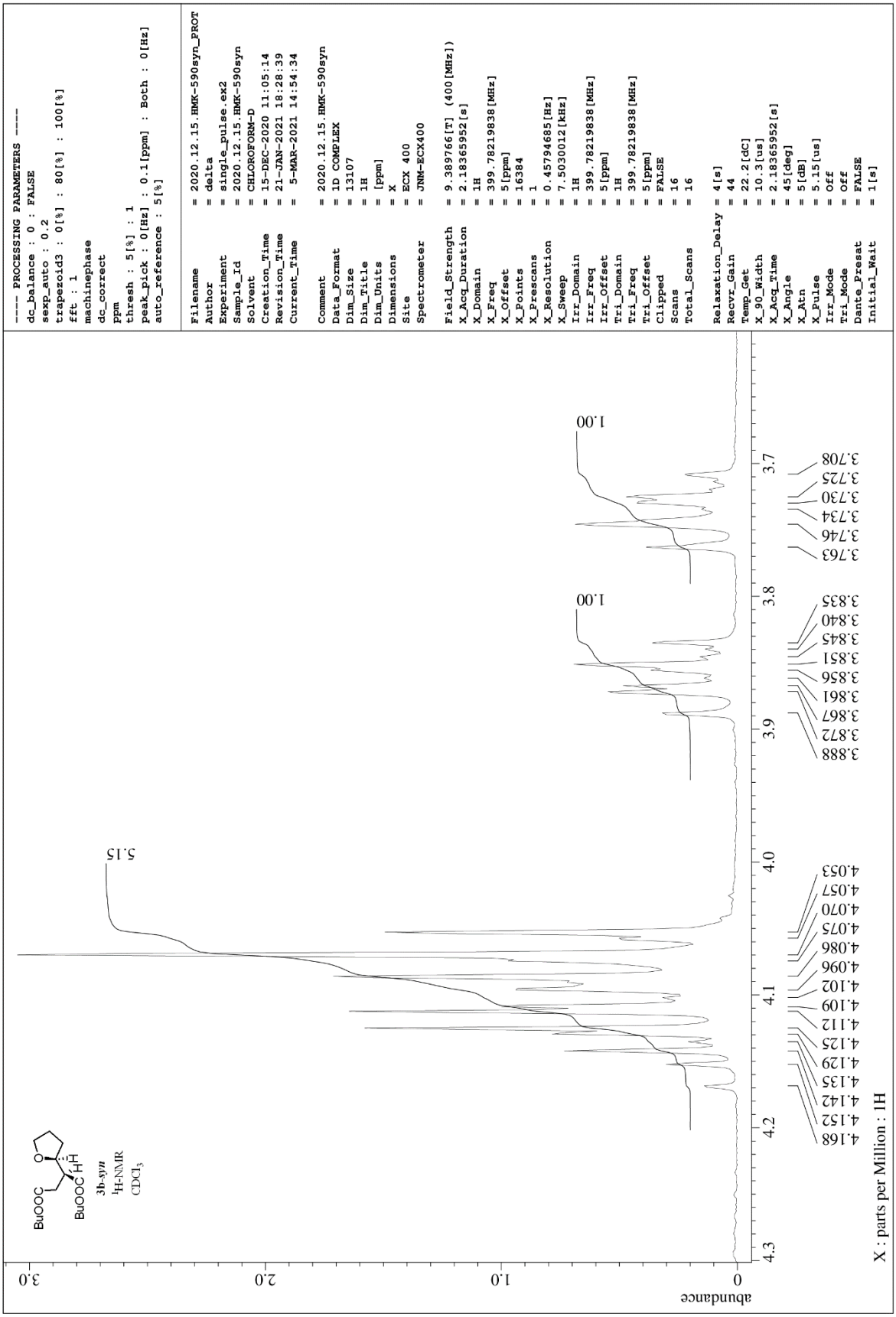
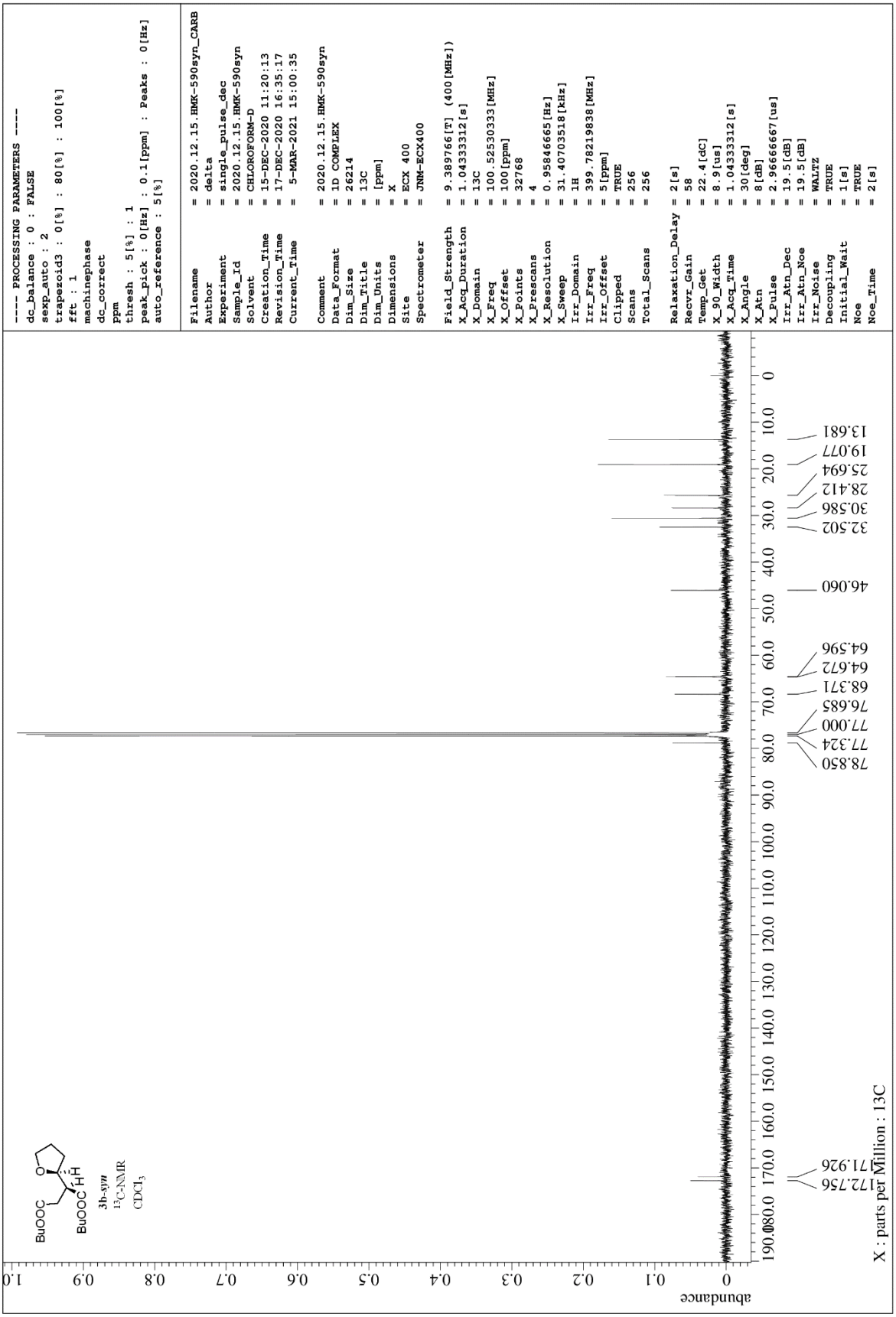
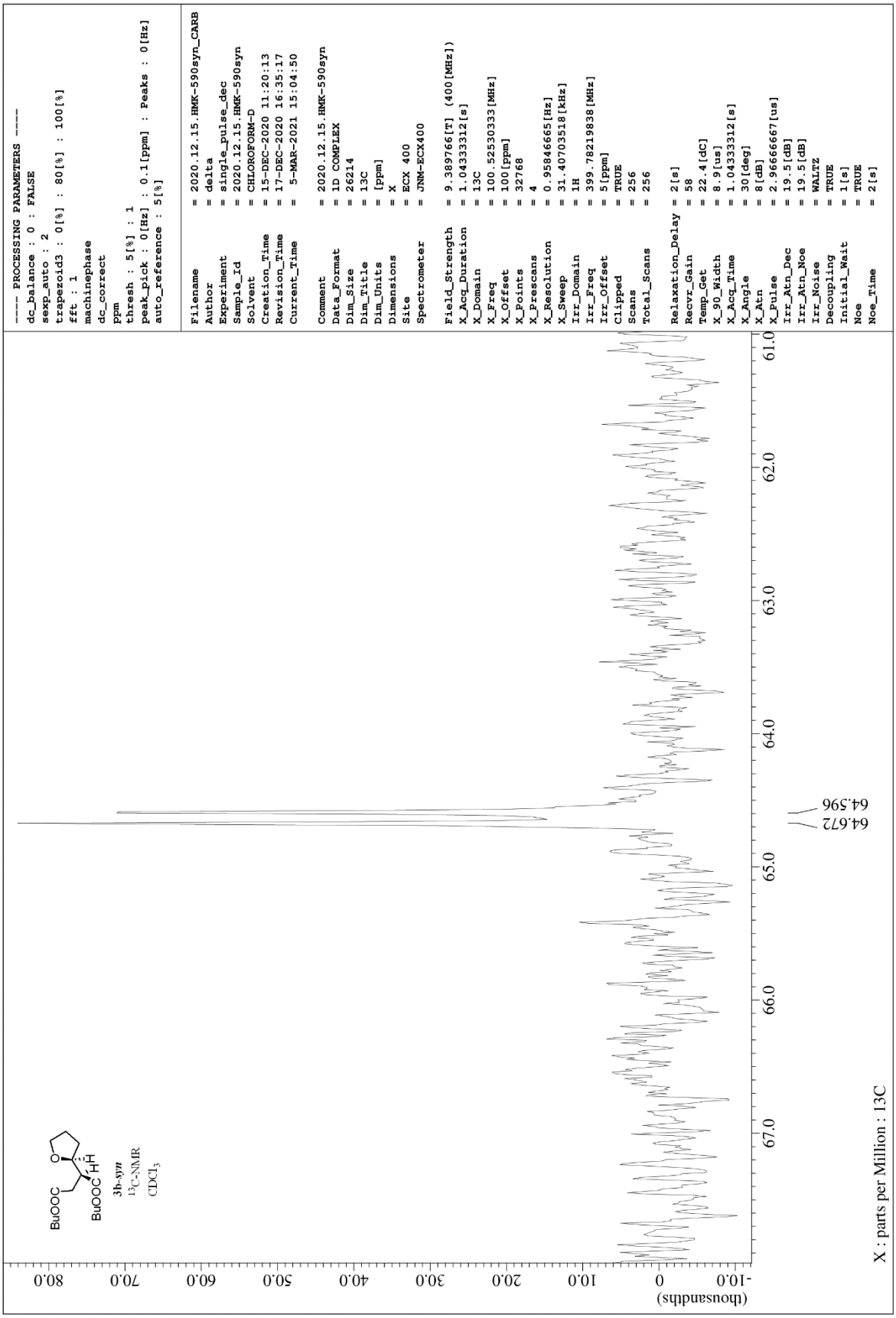
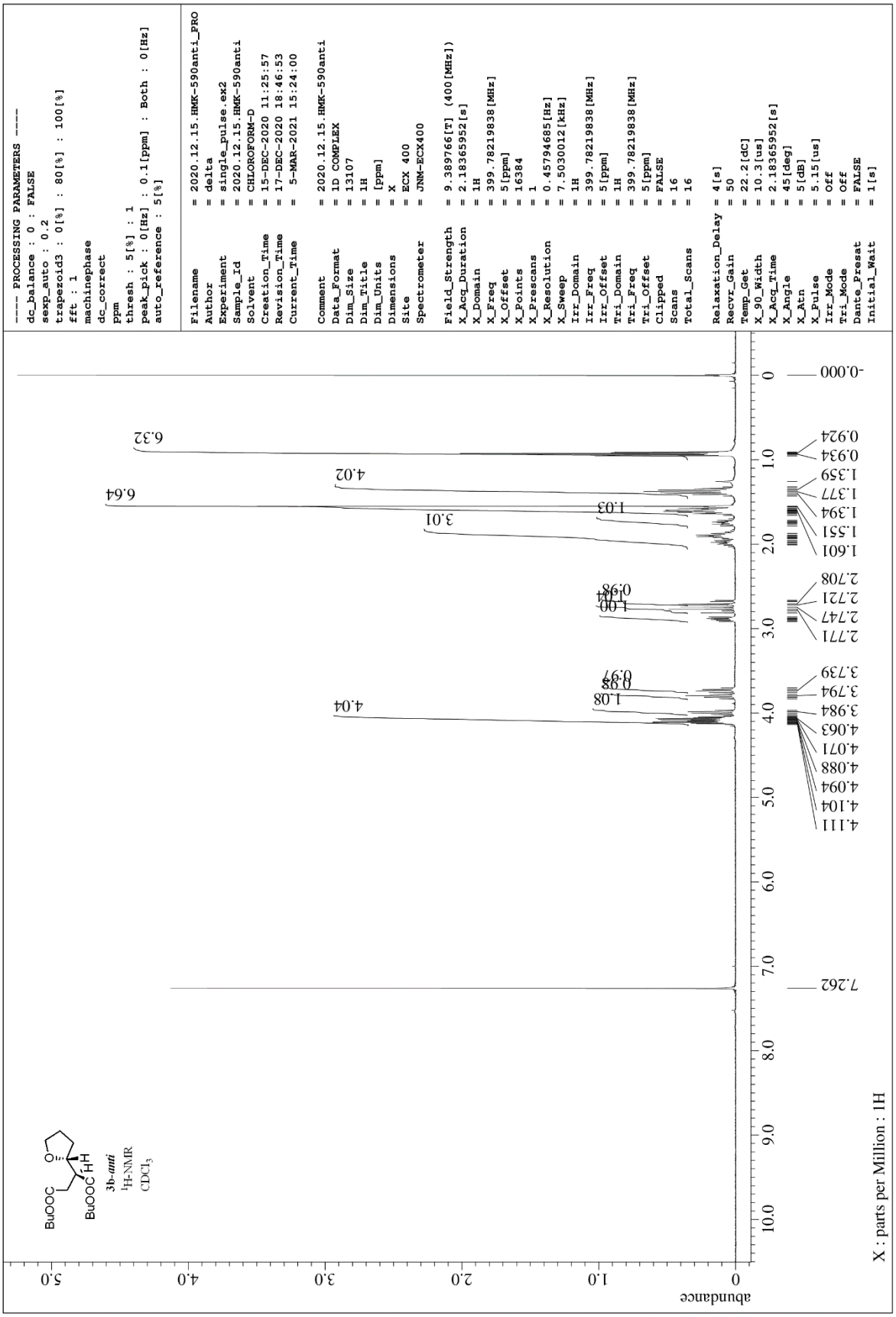
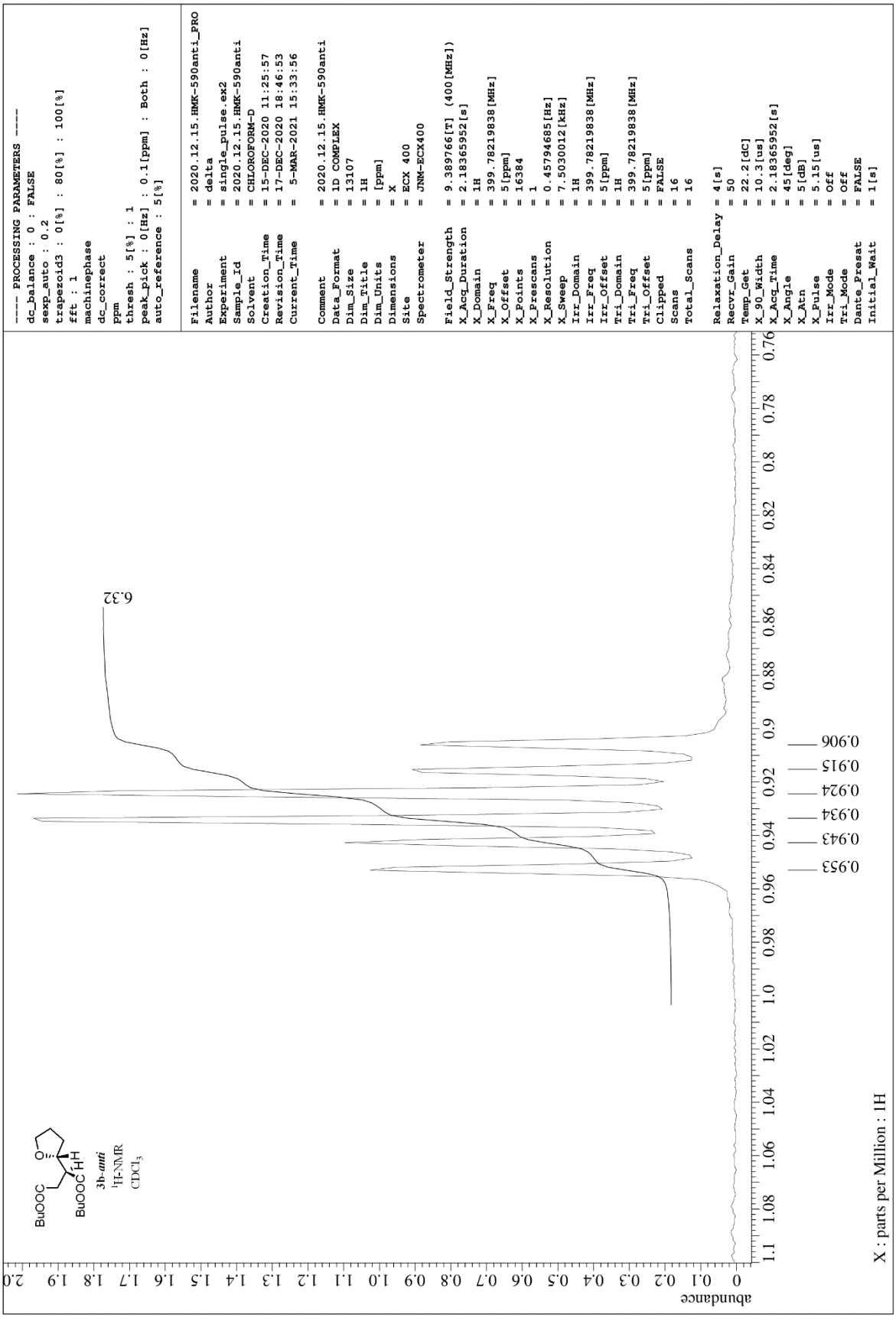
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 5[dB]
X_Pulse = 5.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
4.12
16.49
16.49
4.12
10.07
16.49
16.49
10.07
1.02
1.00
BuOOC
BuOOC
3b-syn
^{1}H-NMR
$CDCl_3$
abundance
X : parts per Million : 1H

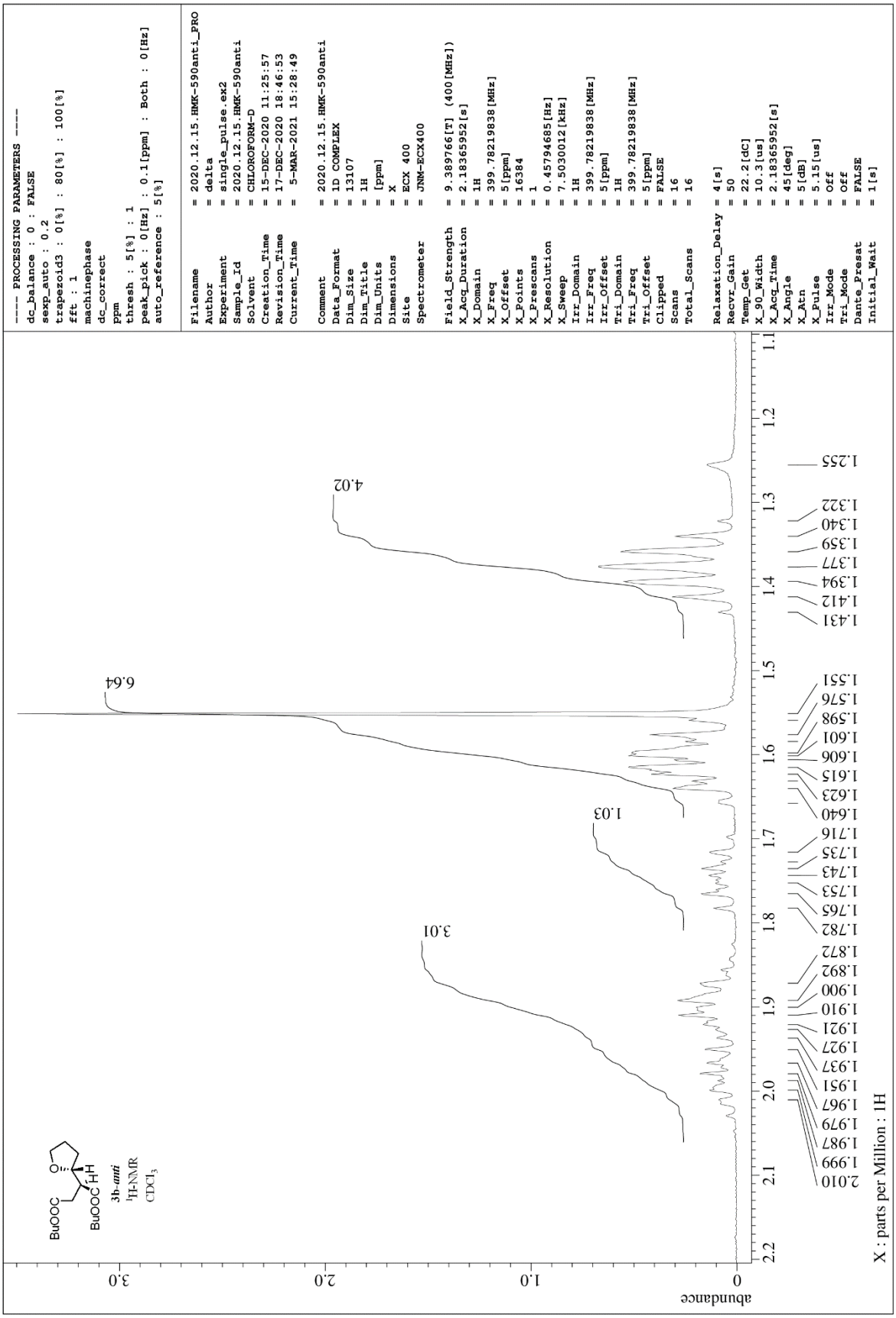

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.15.HMK-590syn_PROT
Author = delta
Experiment = single_pulse_ex2
Sample_Id = 2020.12.15.HMK-590syn
Solvent = CHLOROFORM-D
Creation_Time = 15-DEC-2020 11:05:14
Revision_Time = 21-JAN-2021 18:28:39
Current_Time = 5-MAR-2021 14:54:34
Comment = 2020.12.15.HMK-590syn
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 44
Temp_Get = 22.2[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 5[dB]
X_Pulse = 5.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
BuOOC
BuOOC H
3b-syn
^{1}H-NMR
$CDCl_3$
5.15
1.00
1.00
3.763
3.746
3.734
3.730
3.725
3.708
3.888
3.872
3.867
3.861
3.856
3.851
3.845
3.840
3.835
4.168
4.152
4.142
4.135
4.129
4.125
4.112
4.109
4.102
4.096
4.086
4.075
4.070
4.057
4.053
abundance
X : parts per Million : 1H

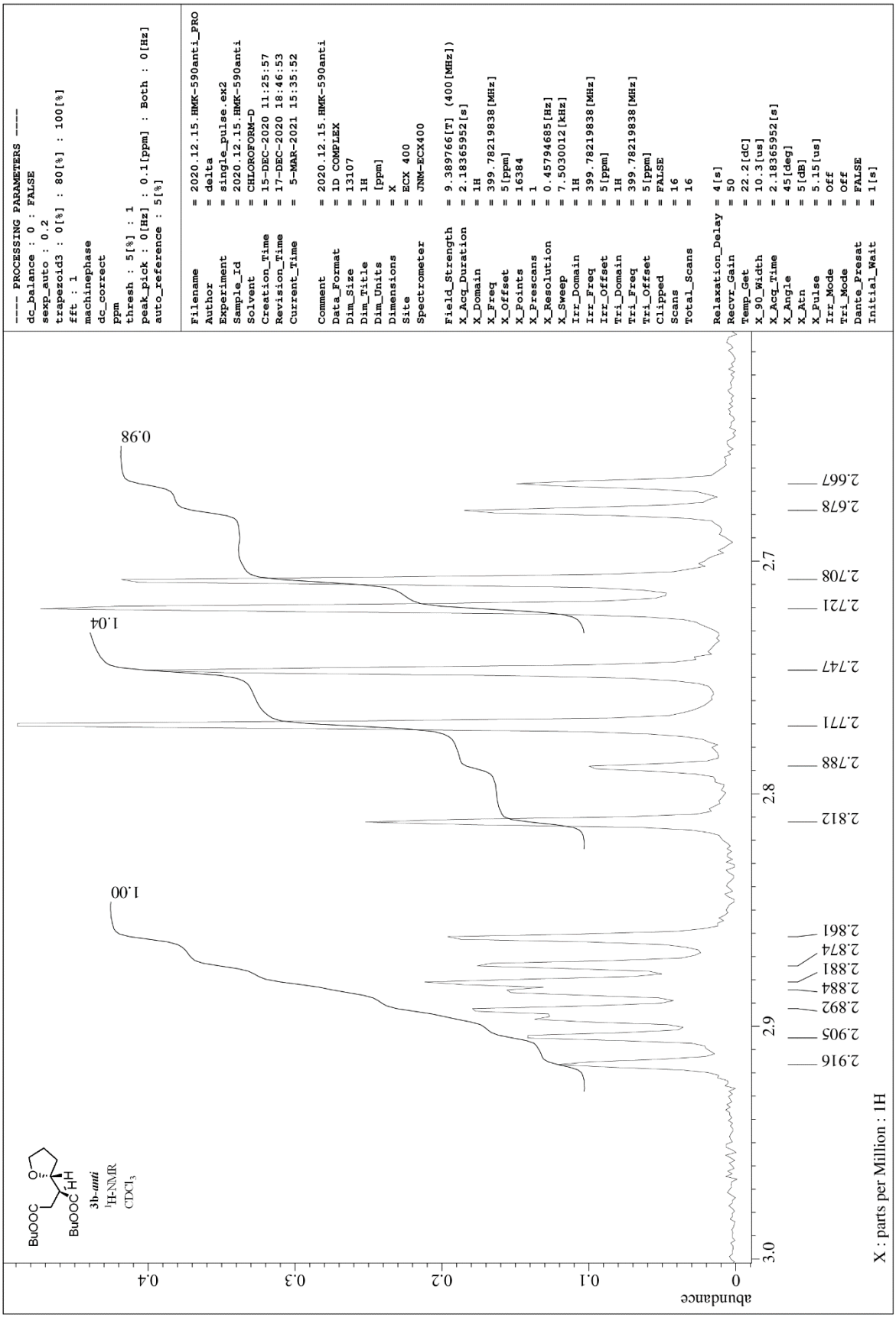

BuOOC
BuOOC
3h-syn
^{13}C-NMR
$CDCl_3$
abundance
X : parts per Million : 13C
172.756
171.926
78.850
77.324
77.000
76.685
68.371
64.672
64.596
46.060
32.502
30.586
28.412
25.694
19.077
13.681
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Peaks : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.15.HMK-590syn_CARB
Author = delta
Experiment = single_pulse_dec
Sample_Id = 2020.12.15.HMK-590syn
Solvent = CHLOROFORM-D
Creation_Time = 15-DEC-2020 11:20:13
Revision_Time = 17-DEC-2020 16:35:17
Current_Time = 5-MAR-2021 15:00:35
Comment = 2020.12.15.HMK-590syn
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.043333312[s]
X_Domain = 13C
X_Freq = 100.525303333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 22.4[dC]
X_90_Width = 8.9[us]
X_Acq_Time = 1.043333312[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 2.96666667[us]
Irr_Atn_Dec = 19.5[dB]
Irr_Atn_Noe = 19.5[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]

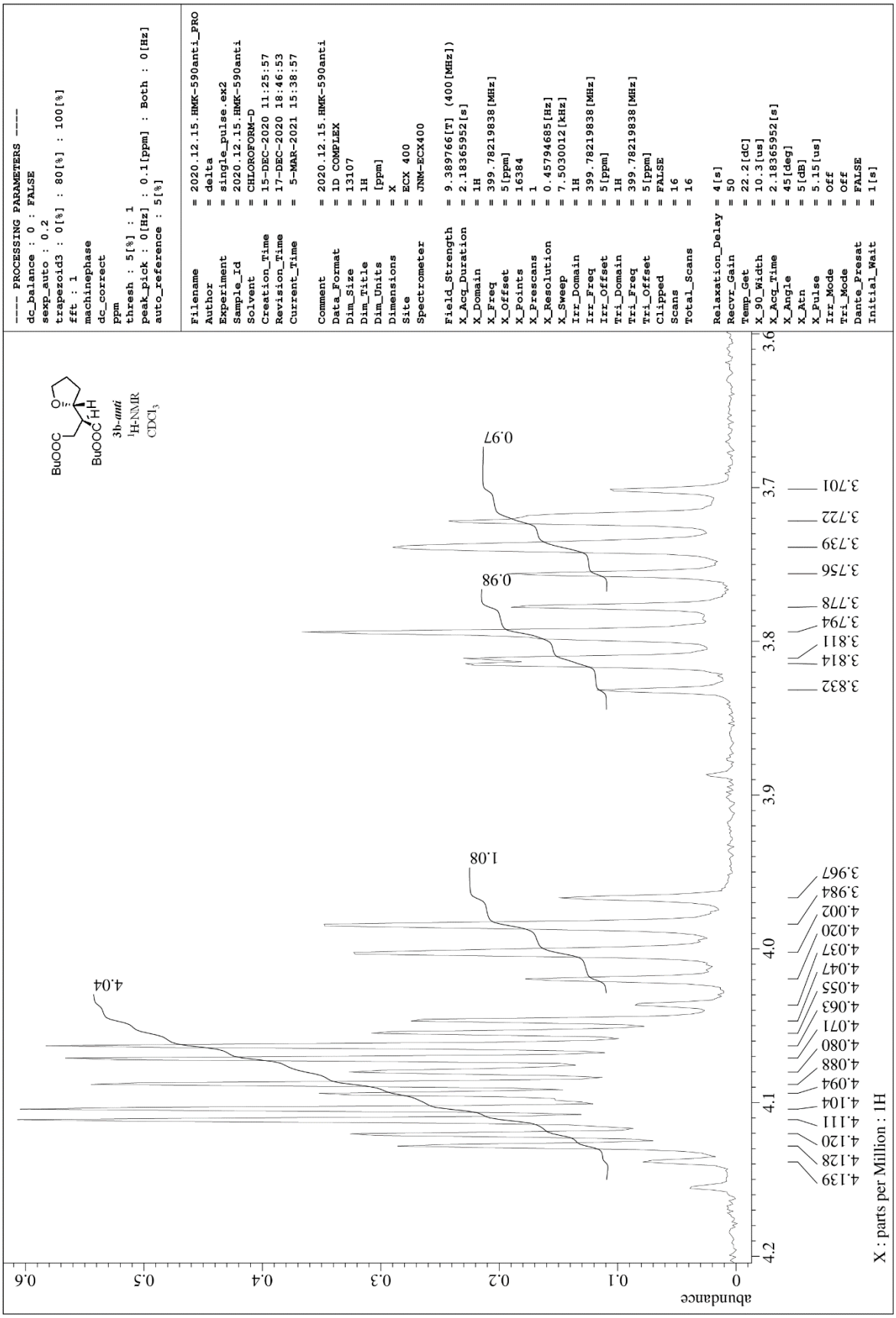

BuOOC
BuOOC
3h-syn
13C-NMR
CDCl3
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
(thousandths)
67.0
66.0
65.0
64.0
63.0
62.0
61.0
64.672
64.596
X : parts per Million : 13C
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Peaks : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.15.HMK-590syn_CARB
Author = delta
Experiment = single_pulse_dec
Sample_Id = 2020.12.15.HMK-590syn
Solvent = CHLOROFORM-D
Creation_Time = 15-DEC-2020 11:20:13
Revision_Time = 17-DEC-2020 16:35:17
Current_Time = 5-MAR-2021 15:04:50
Comment = 2020.12.15.HMK-590syn
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.525303333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 22.4[dC]
X_90_Width = 8.9[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 2.96666667[us]
Irr_Atn_Dec = 19.5[dB]
Irr_Atn_Noe = 19.5[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]

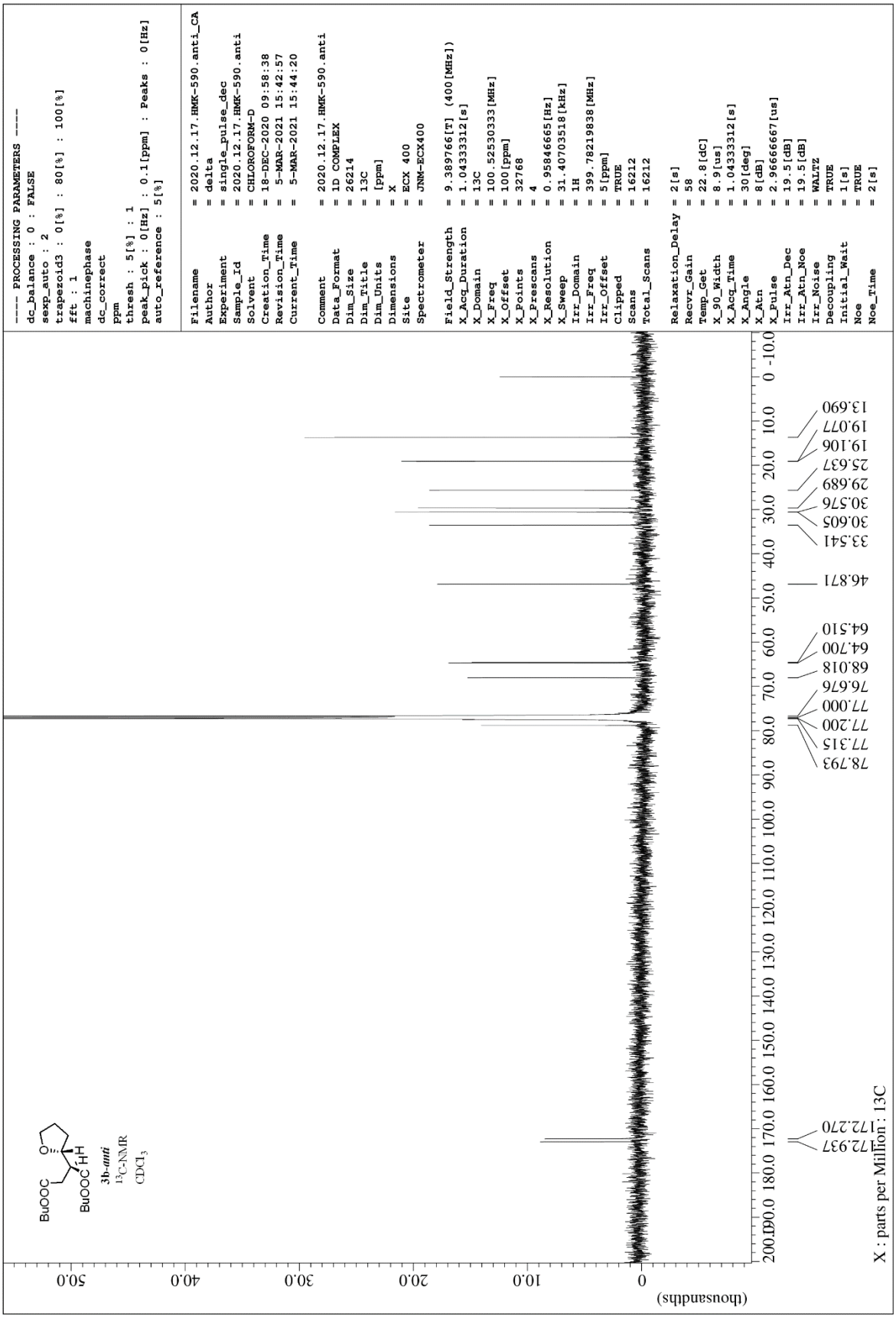

BuOOC
BuOOC H
3b-*anti*
^{1}H-NMR
$CDCl_3$
abundance
X : parts per Million : 1H
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.15.HMK-590anti_PRO
Author = delta
Experiment = single_pulse_ex2
Sample_Id = 2020.12.15.HMK-590anti
Solvent = CHLOROFORM-D
Creation_Time = 15-DEC-2020 11:25:57
Revision_Time = 17-DEC-2020 18:46:53
Current_Time = 5-MAR-2021 15:24:00
Comment = 2020.12.15.HMK-590anti
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 50
Temp_Get = 22.2[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 5[dB]
X_Pulse = 5.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
6.32
6.64
4.02
3.01
1.03
4.04
1.08
1.00
7.262
-0.000
0.924
0.934
1.359
1.377
1.394
1.551
1.601
2.708
2.721
2.747
2.771
3.739
3.794
3.984
4.063
4.071
4.088
4.094
4.104
4.111

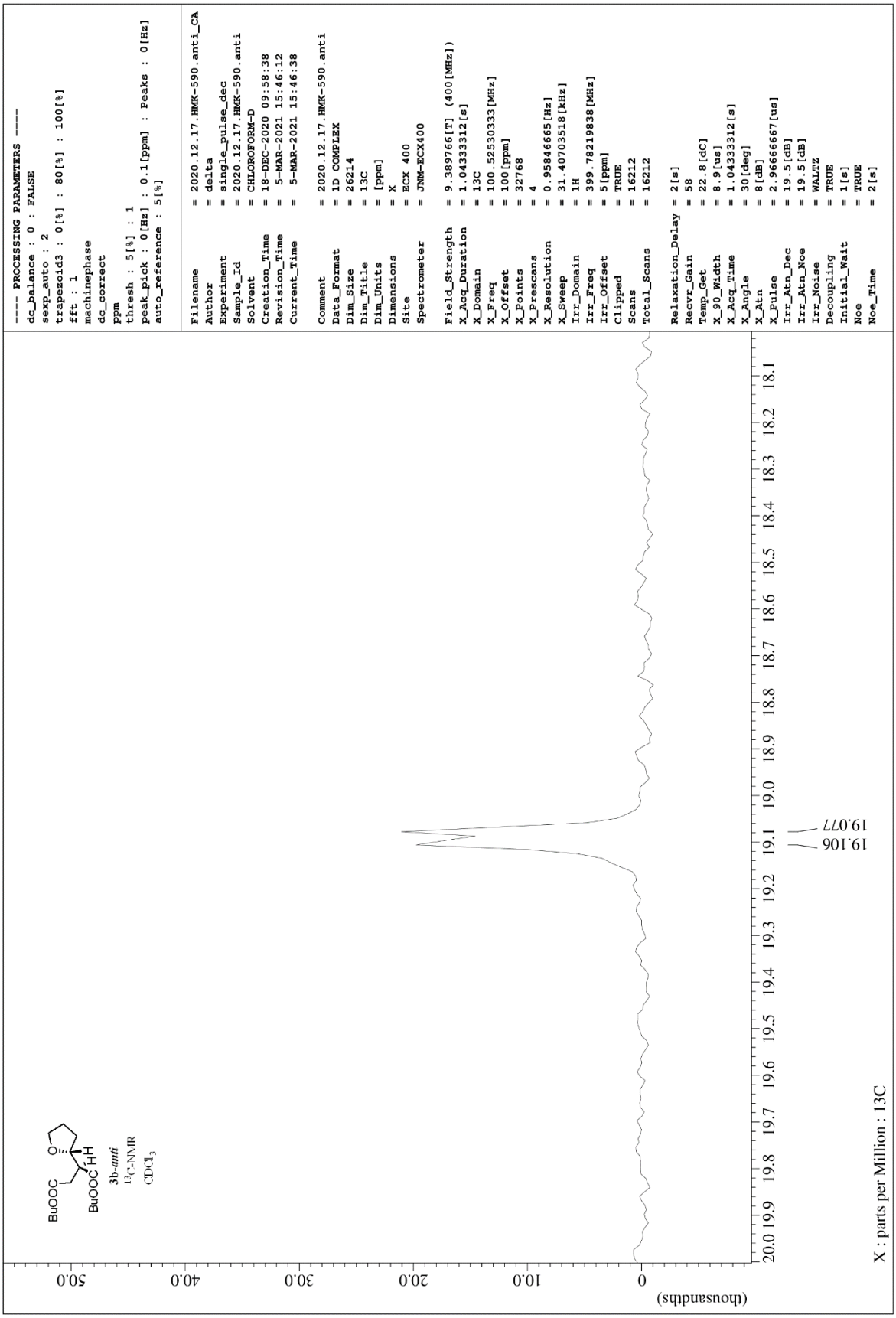

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.15.HMK-590anti_PRO
Author = delta
Experiment = single_pulse_ex2
Sample_Id = 2020.12.15.HMK-590anti
Solvent = CHLOROFORM-D
Creation_Time = 15-DEC-2020 11:25:57
Revision_Time = 17-DEC-2020 18:46:53
Current_Time = 5-MAR-2021 15:33:56
Comment = 2020.12.15.HMK-590anti
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 50
Temp_Get = 22.2[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 5[dB]
X_Pulse = 5.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
BuOOC
BuOOC H
3b-anti
^{1}H-NMR
$CDCl_3$
6.32
0.953
0.943
0.934
0.924
0.915
0.906
abundance
X : parts per Million : 1H

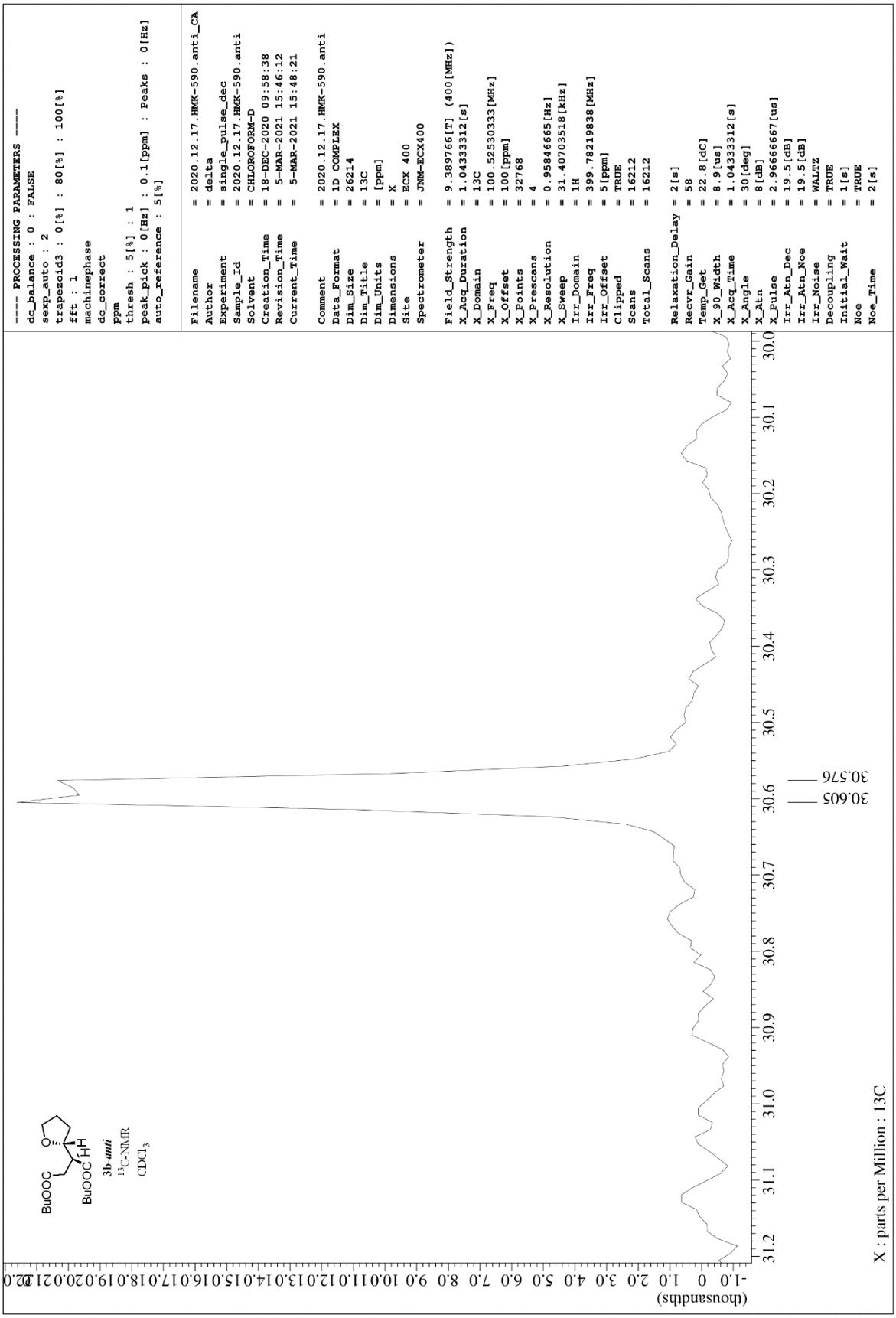

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.15.HMK-590anti_PRO
Author = delta
Experiment = single_pulse_ex2
Sample_Id = 2020.12.15.HMK-590anti
Solvent = CHLOROFORM-D
Creation_Time = 15-DEC-2020 11:25:57
Revision_Time = 17-DEC-2020 18:46:53
Current_Time = 5-MAR-2021 15:28:49
Comment = 2020.12.15.HMK-590anti
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 50
Temp_Get = 22.2[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 5[dB]
X_Pulse = 5.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
BuOOC
BuOOC
H
3b-anti
^{1}H-NMR
$CDCl_3$
6.64
4.02
3.01
1.03
abundance
X : parts per Million : 1H

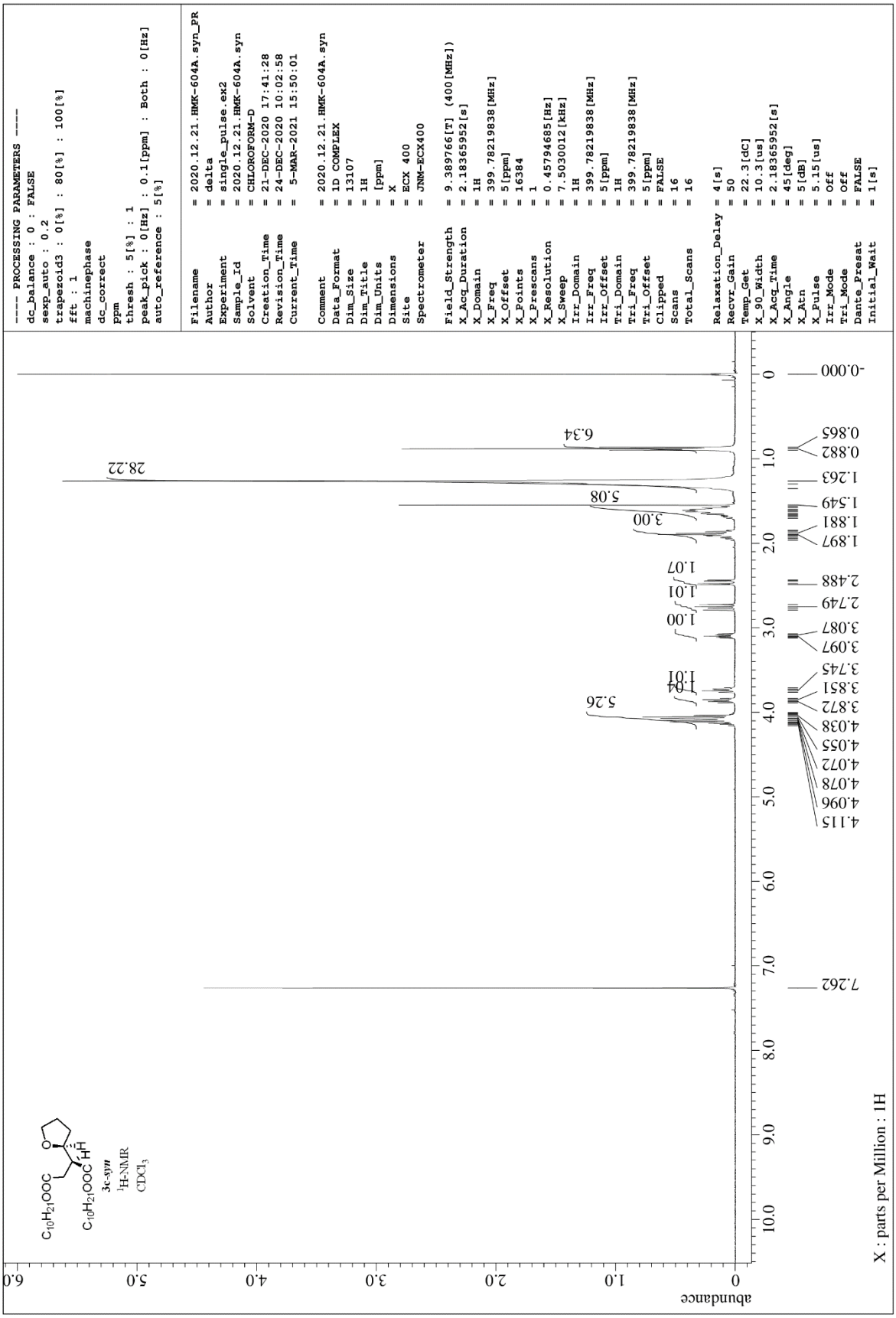

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.15.HMK-590anti_PRO
Author = delta
Experiment = single_pulse_ex2
Sample_Id = 2020.12.15.HMK-590anti
Solvent = CHLOROFORM-D
Creation_Time = 15-DEC-2020 11:25:57
Revision_Time = 17-DEC-2020 18:46:53
Current_Time = 5-MAR-2021 15:35:52
Comment = 2020.12.15.HMK-590anti
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.50300012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 50
Temp_Get = 22.2[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 5[dB]
X_Pulse = 5.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
BuOOC
BuOOC
3b-anti
^{1}H-NMR
$CDCl_3$
abundance
X : parts per Million : 1H
1.00
1.04
0.98
2.916
2.905
2.892
2.884
2.881
2.874
2.861
2.812
2.788
2.771
2.747
2.721
2.708
2.678
2.667

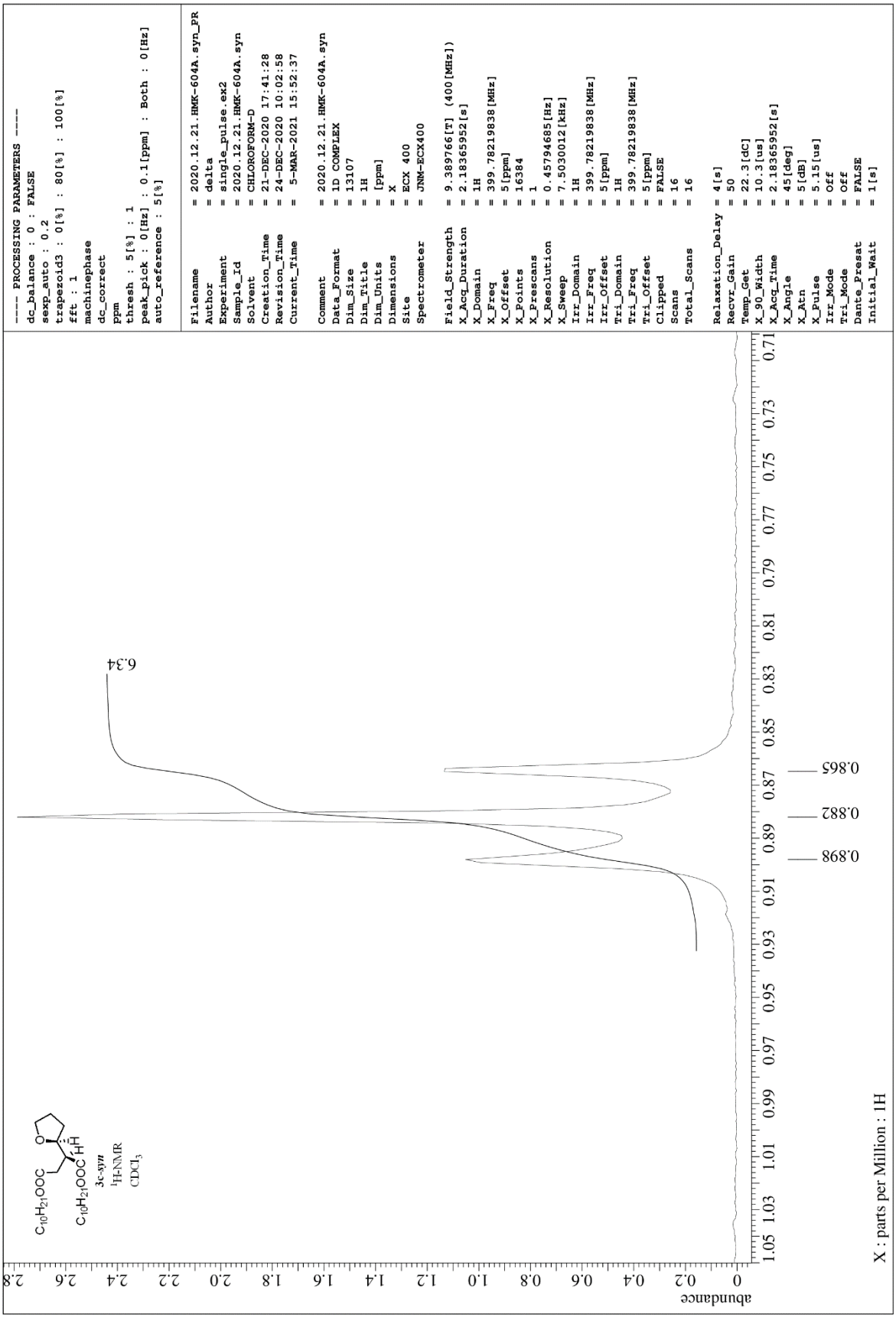

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.15.HMR-590anti_PRO
Author = delta
Experiment = single_pulse_ex2
Sample_Id = 2020.12.15.HMR-590anti
Solvent = CHLOROFORM-D
Creation_Time = 15-DEC-2020 11:25:57
Revision_Time = 17-DEC-2020 18:46:53
Current_Time = 5-MAR-2021 15:38:57
Comment = 2020.12.15.HMR-590anti
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 50
Temp_Get = 22.2[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 5[dB]
X_Pulse = 5.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
BuOOC
BuOOC
3h-anti
^{1}H-NMR
$CDCl_3$
4.04
1.08
0.98
0.97
3.701
3.722
3.739
3.756
3.778
3.794
3.811
3.814
3.832
4.139
4.128
4.120
4.111
4.104
4.094
4.088
4.080
4.071
4.063
4.055
4.047
4.037
4.020
4.002
3.984
3.967
abundance
X : parts per Million : 1H

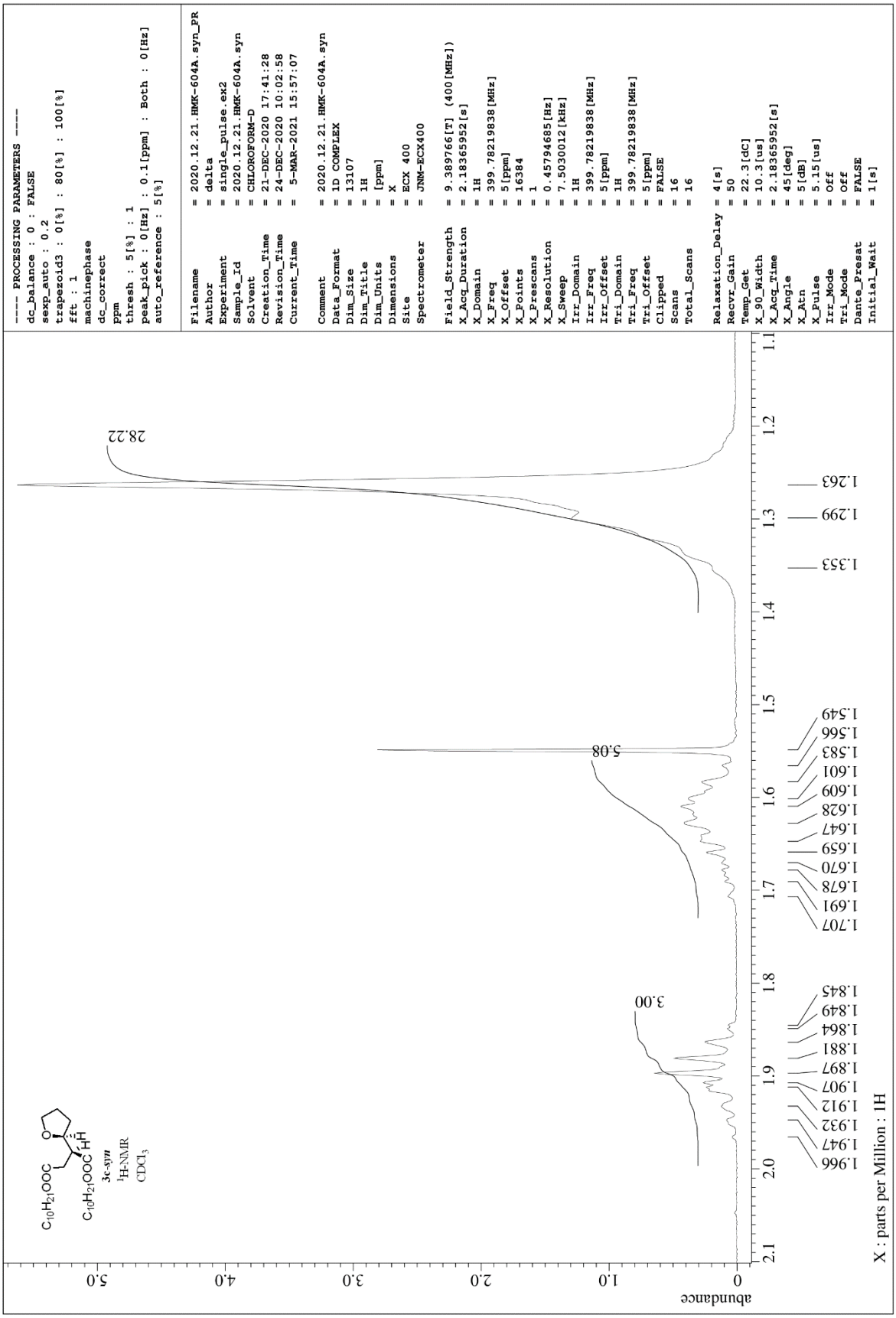

BuOOC
BuOOC H
3b-*anti*
^{13}C-NMR
$CDCl_3$
(thousandths)
X : parts per Million : 13C
172.937
172.270
78.793
77.315
77.200
77.000
76.676
68.018
64.700
64.510
46.871
33.541
30.605
30.576
29.689
25.637
19.106
19.077
13.690
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Peaks : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.17.HMK-590.anti_CA
Author = delta
Experiment = single_pulse_dec
Sample_Id = 2020.12.17.HMK-590.anti
Solvent = CHLOROFORM-D
Creation_Time = 18-DEC-2020 09:58:38
Revision_Time = 5-MAR-2021 15:42:57
Current_Time = 5-MAR-2021 15:44:20
Comment = 2020.12.17.HMK-590.anti
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.525303333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 16212
Total_Scans = 16212
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 22.8[dC]
X_90_Width = 8.9[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 2.96666667[us]
Irr_Atn_Dec = 19.5[dB]
Irr_Atn_Noe = 19.5[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]

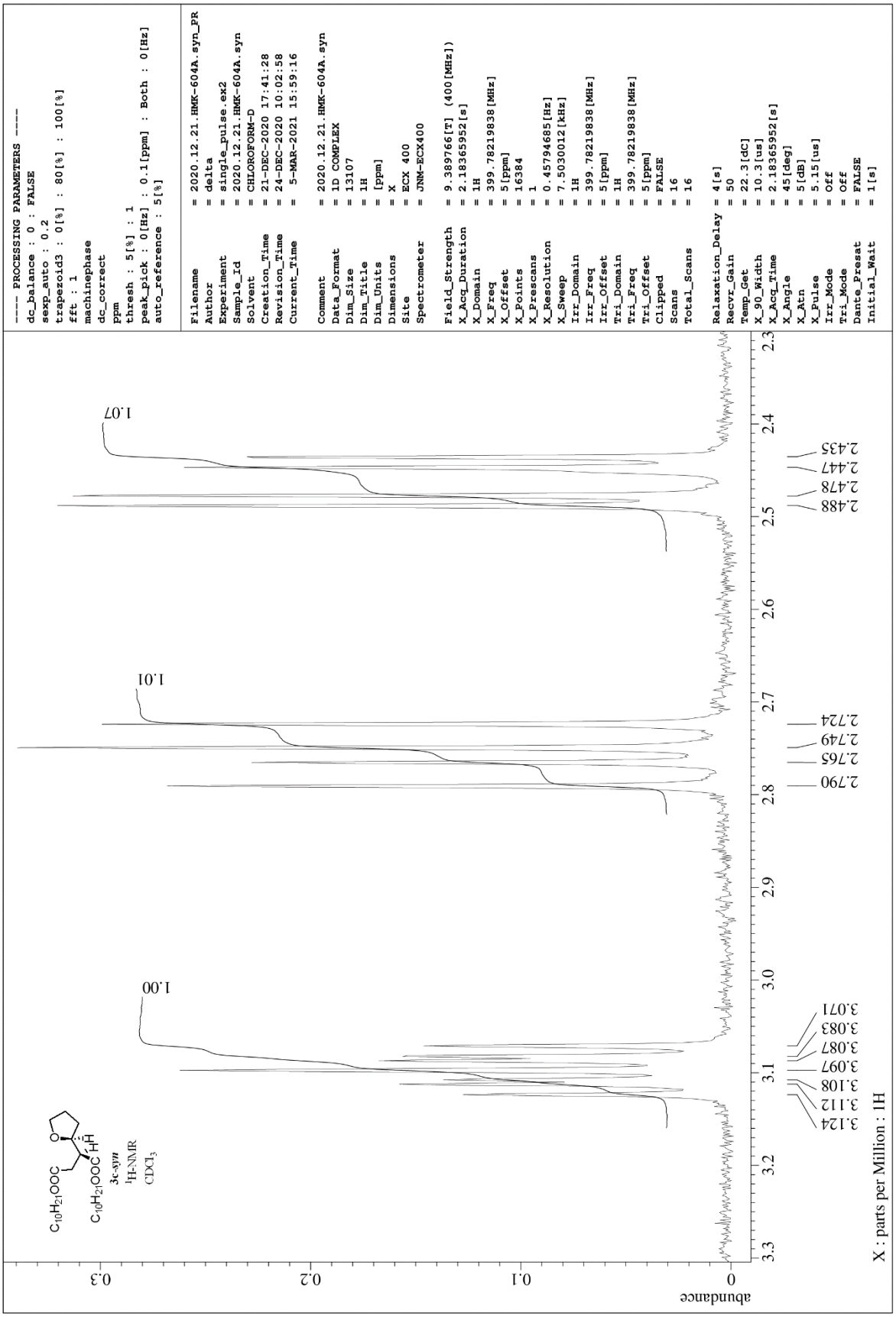

BuOOC
BuOOC
H
3b-anti
13C-NMR
CDCl3
(thousandths)
X : parts per Million : 13C
19.077
19.106
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Peaks : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.17.HMK-590.anti_CA
Author = delta
Experiment = single_pulse_dec
Sample_Id = 2020.12.17.HMK-590.anti
Solvent = CHLOROFORM-D
Creation_Time = 18-DEC-2020 09:58:38
Revision_Time = 5-MAR-2021 15:46:12
Current_Time = 5-MAR-2021 15:46:38
Comment = 2020.12.17.HMK-590.anti
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.525303333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 16212
Total_Scans = 16212
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 22.8[dC]
X_90_Width = 8.9[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 2.96666667[us]
Irr_Atn_Dec = 19.5[dB]
Irr_Atn_Noe = 19.5[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]

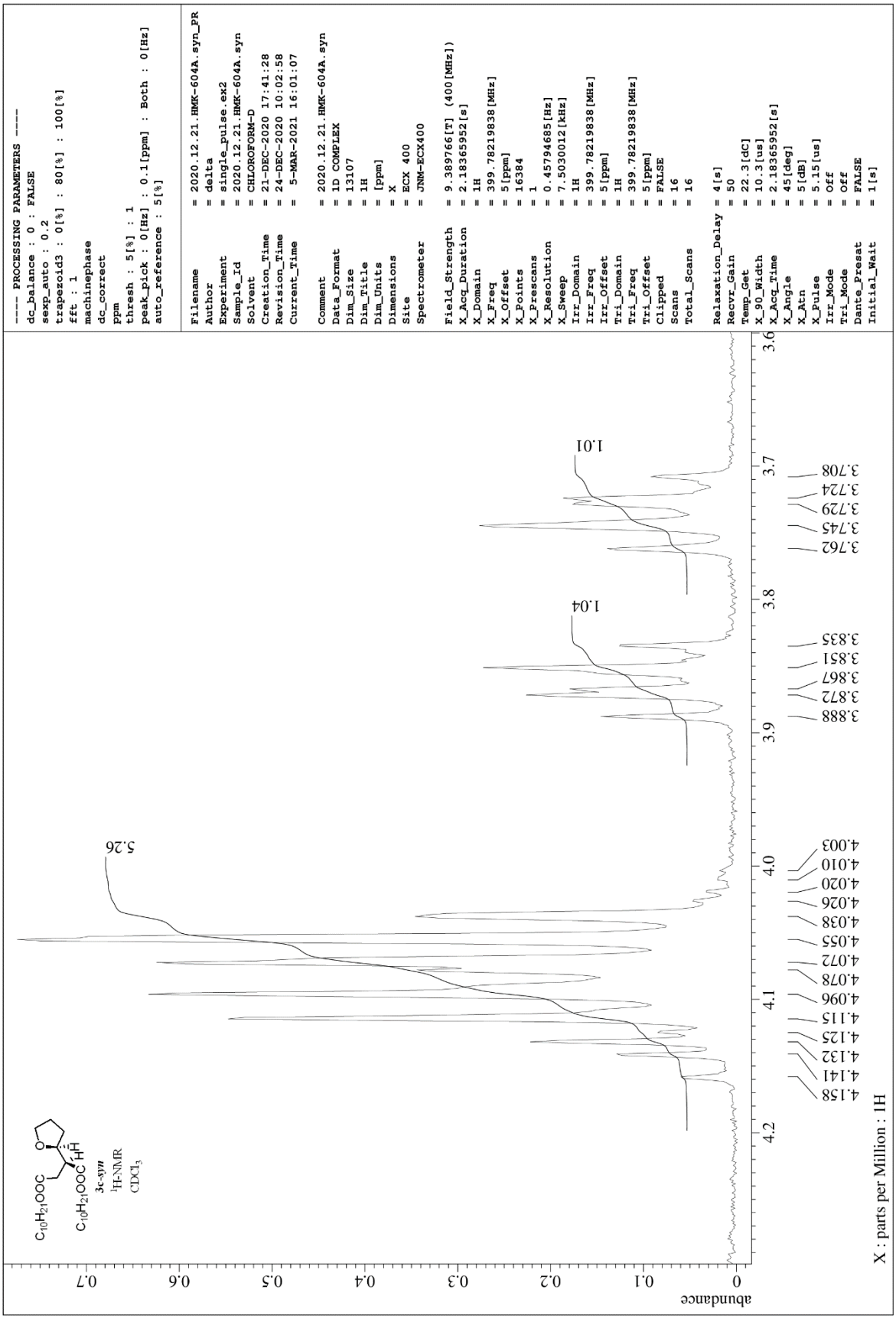

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Peaks : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.17.HMK-590.anti_CA
Author = delta
Experiment = single_pulse_dec
Sample_Id = 2020.12.17.HMK-590.anti
Solvent = CHLOROFORM-D
Creation_Time = 18-DEC-2020 09:58:38
Revision_Time = 5-MAR-2021 15:46:12
Current_Time = 5-MAR-2021 15:48:21
Comment = 2020.12.17.HMK-590.anti
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.525303333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 16212
Total_Scans = 16212
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 22.8[dC]
X_90_Width = 8.9[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 2.96666667[us]
Irr_Atn_Dec = 19.5[dB]
Irr_Atn_Noe = 19.5[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
BuOOC
BuOOC
H
3b-*anti*
^{13}C-NMR
$CDCl_3$
30.605
30.576
(thousandths)
X : parts per Million : 13C

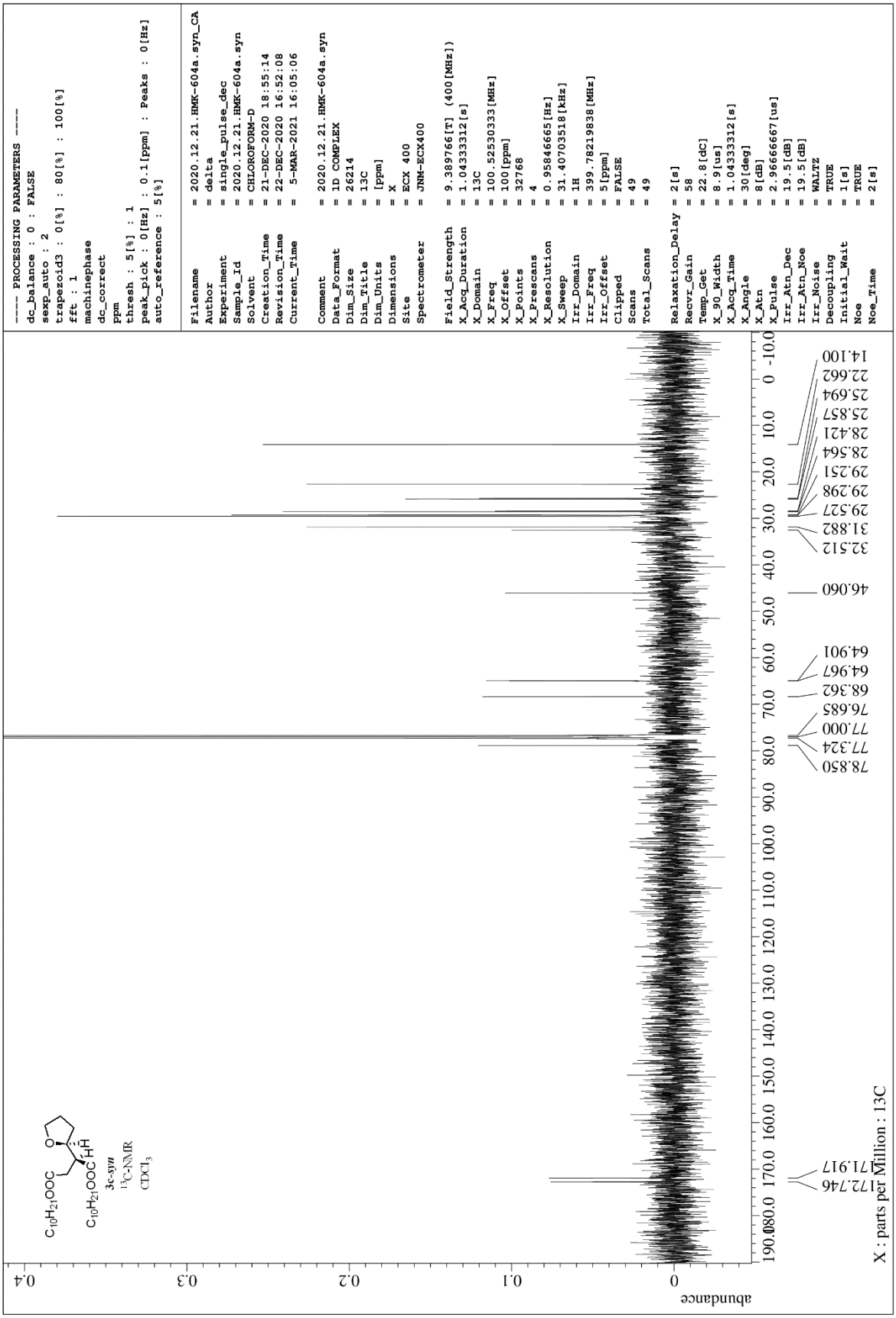

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.21.HMK-604A.syn_PR
Author = delta
Experiment = single_pulse_ex2
Sample_Id = 2020.12.21.HMK-604A.syn
Solvent = CHLOROFORM-D
Creation_Time = 21-DEC-2020 17:41:28
Revision_Time = 24-DEC-2020 10:02:58
Current_Time = 5-MAR-2021 15:50:01
Comment = 2020.12.21.HMK-604A.syn
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 50
Temp_Get = 22.3[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 5[dB]
X_Pulse = 5.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
C10H21OOC
C10H21OOC
3c-syn
1H-NMR
CDCl3
abundance
X : parts per Million : 1H
28.22
6.34
5.08
5.26
3.00
1.07
1.01
1.00
1.01
1.04
7.262
4.115
4.096
4.078
4.072
4.055
4.038
3.872
3.851
3.745
3.097
3.087
2.749
2.488
1.897
1.881
1.549
1.263
0.882
0.865
-0.000

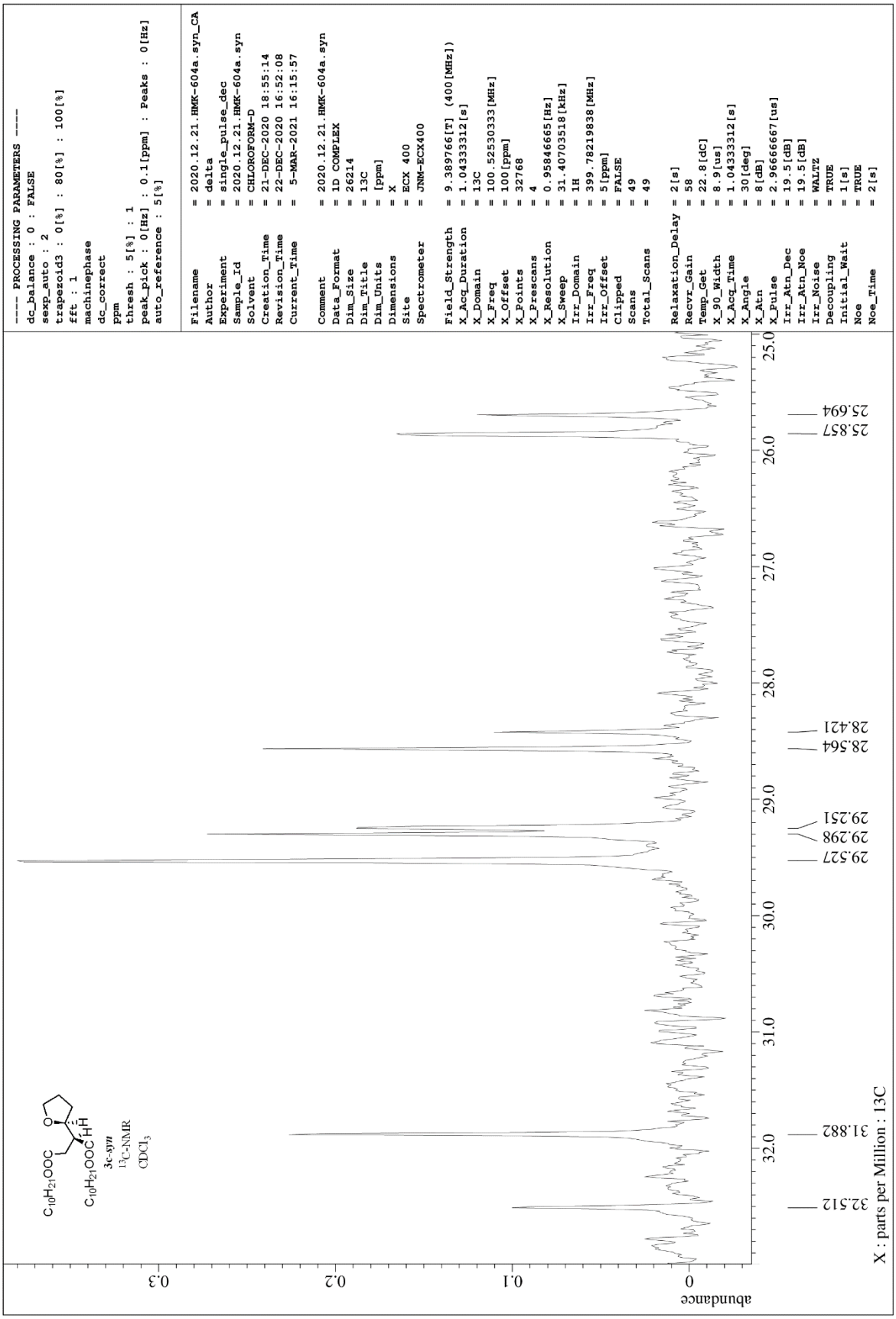

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.21.HMK-604A.syn_PR
Author = delta
Experiment = single_pulse_ex2
Sample_Id = 2020.12.21.HMK-604A.syn
Solvent = CHLOROFORM-D
Creation_Time = 21-DEC-2020 17:41:28
Revision_Time = 24-DEC-2020 10:02:58
Current_Time = 5-MAR-2021 15:52:37
Comment = 2020.12.21.HMK-604A.syn
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 50
Temp_Get = 22.3[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 5[dB]
X_Pulse = 5.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
C10H21OOC
C10H21OOC H
3c-syn
1H-NMR
CDCl3
6.34
0.865
0.882
0.898
abundance
X : parts per Million : 1H

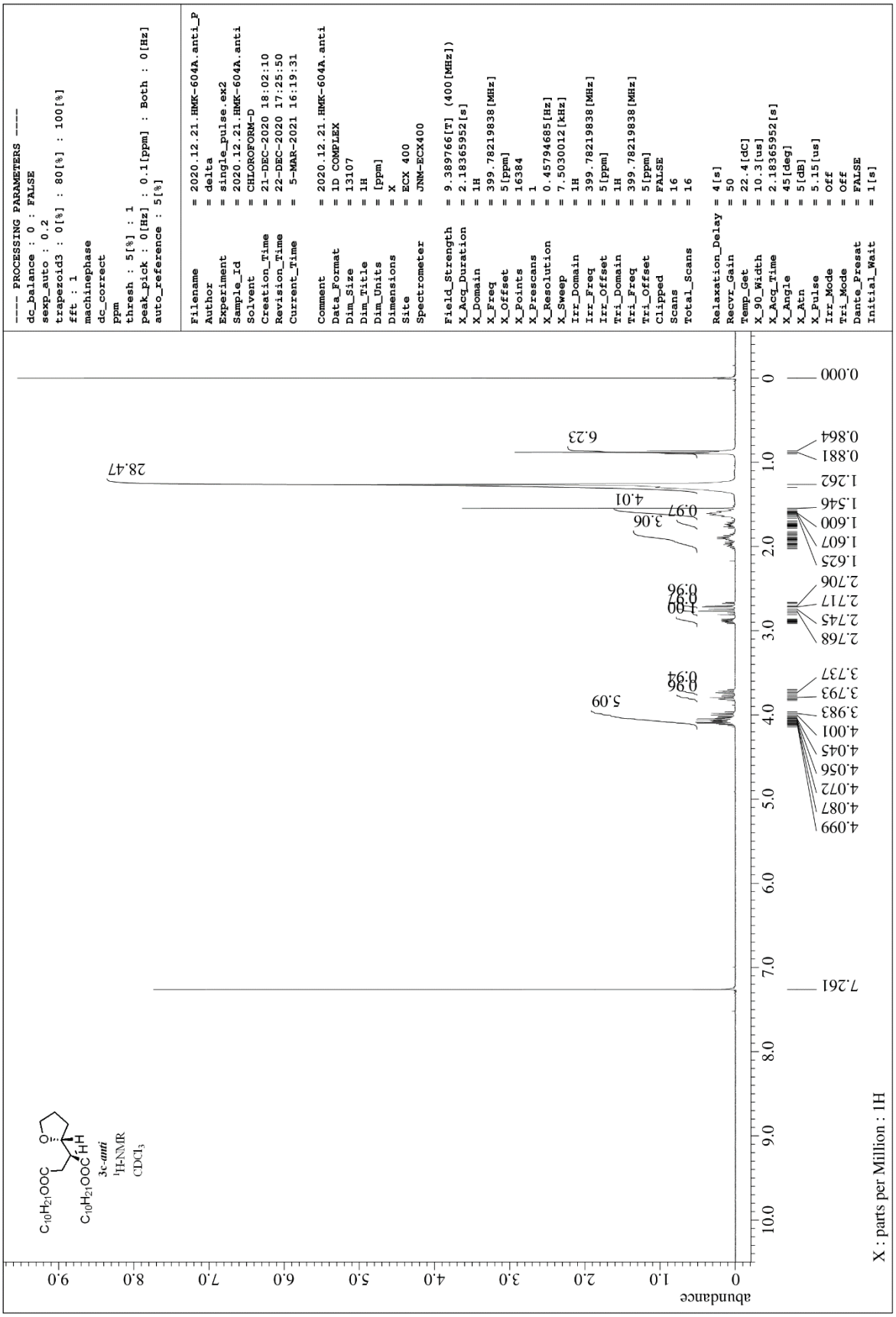

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.21.HMK-604A.syn_PR
Author = delta
Experiment = single_pulse_ex2
Sample_Id = 2020.12.21.HMK-604A.syn
Solvent = CHLOROFORM-D
Creation_Time = 21-DEC-2020 17:41:28
Revision_Time = 24-DEC-2020 10:02:58
Current_Time = 5-MAR-2021 15:57:07
Comment = 2020.12.21.HMK-604A.syn
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 50
Temp_Get = 22.3[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 5[dB]
X_Pulse = 5.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
28.22
5.08
3.00
1.263
1.299
1.353
1.549
1.566
1.583
1.601
1.609
1.628
1.647
1.659
1.670
1.678
1.691
1.707
1.845
1.849
1.864
1.881
1.897
1.907
1.912
1.932
1.947
1.966
abundance
X : parts per Million : 1H

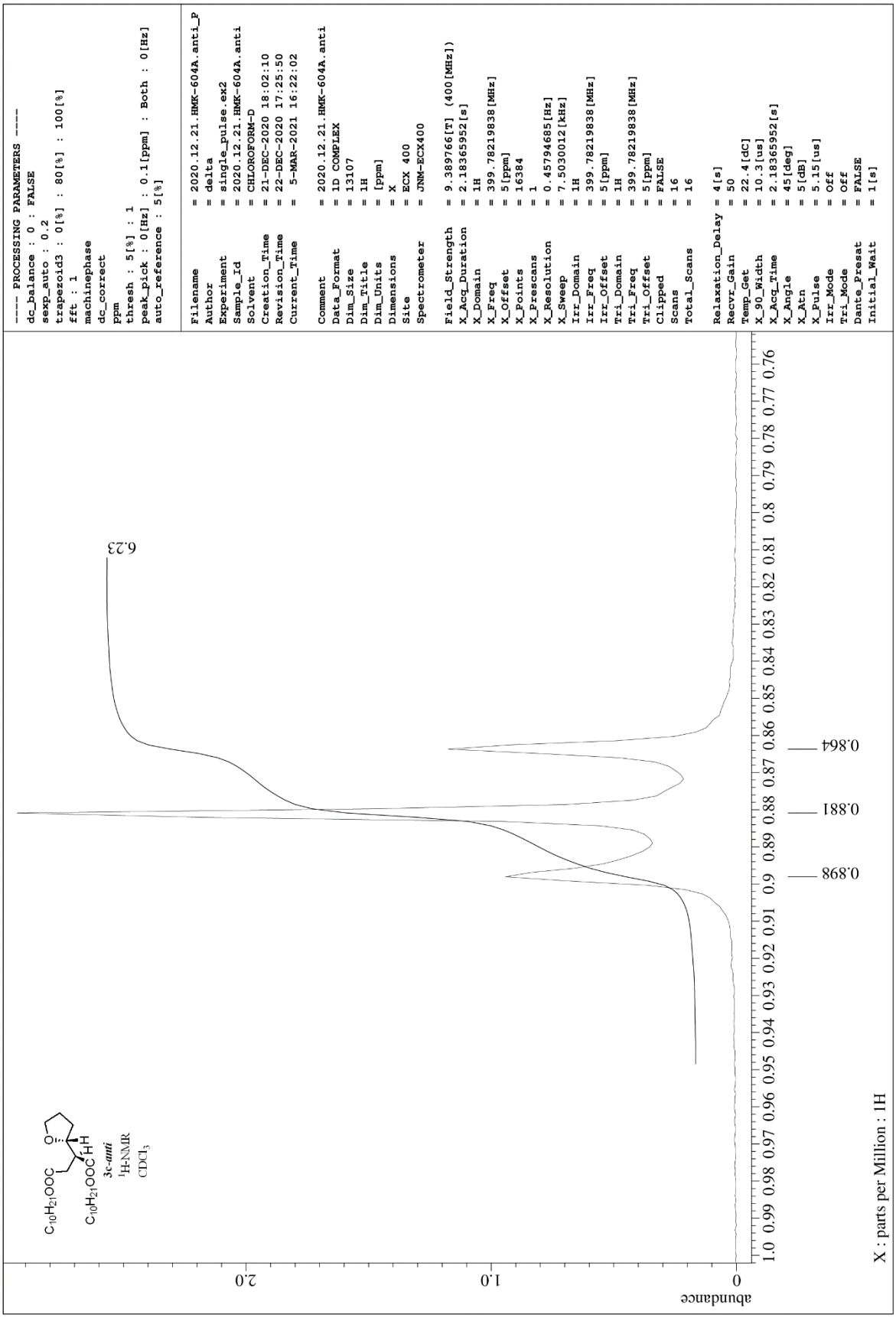

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.21.HMK-604A.syn_PR
Author = delta
Experiment = single_pulse_ex2
Sample_Id = 2020.12.21.HMK-604A.syn
Solvent = CHLOROFORM-D
Creation_Time = 21-DEC-2020 17:41:28
Revision_Time = 24-DEC-2020 10:02:58
Current_Time = 5-MAR-2021 15:59:16
Comment = 2020.12.21.HMK-604A.syn
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 50
Temp_Get = 22.3[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 5[dB]
X_Pulse = 5.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
C10H21OOC
C10H21OOC H
3c-syn
1H-NMR
CDCl3
1.00
1.01
1.07
3.124
3.112
3.108
3.097
3.087
3.083
3.071
2.790
2.765
2.749
2.724
2.488
2.478
2.447
2.435
abundance
X : parts per Million : 1H

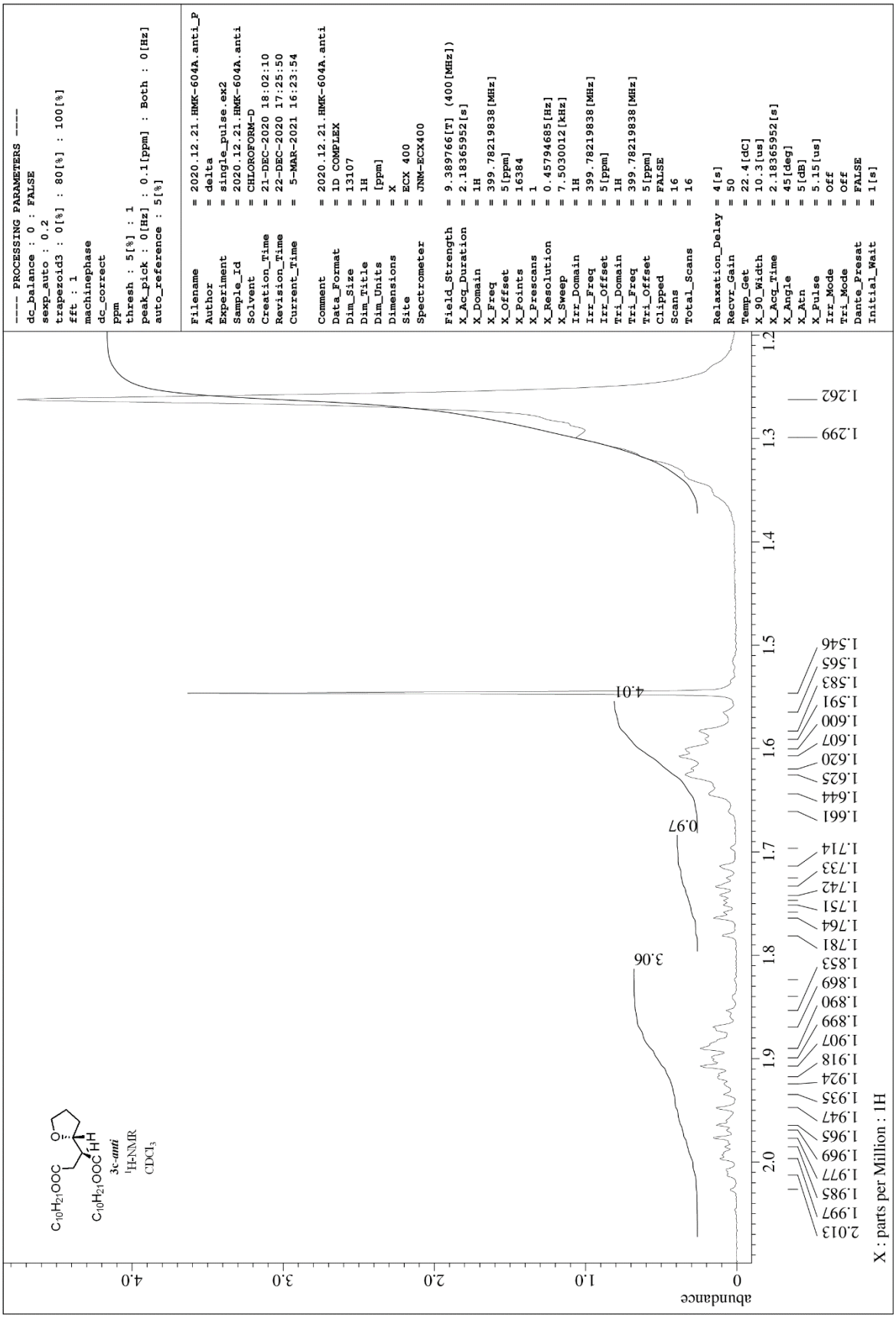

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.21.HMK-604A.syn_PR
Author = delta
Experiment = single_pulse_ex2
Sample_Id = 2020.12.21.HMK-604A.syn
Solvent = CHLOROFORM-D
Creation_Time = 21-DEC-2020 17:41:28
Revision_Time = 24-DEC-2020 10:02:58
Current_Time = 5-MAR-2021 16:01:07
Comment = 2020.12.21.HMK-604A.syn
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 50
Temp_Get = 22.3[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 5[dB]
X_Pulse = 5.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
C10H21OOC
C10H21OOC H
3c-syn
1H-NMR
CDCl3
5.26
1.01
1.04
3.762
3.745
3.729
3.724
3.708
3.888
3.872
3.867
3.851
3.835
4.158
4.141
4.132
4.125
4.115
4.096
4.078
4.072
4.055
4.038
4.026
4.020
4.010
4.003
abundance
X : parts per Million : 1H

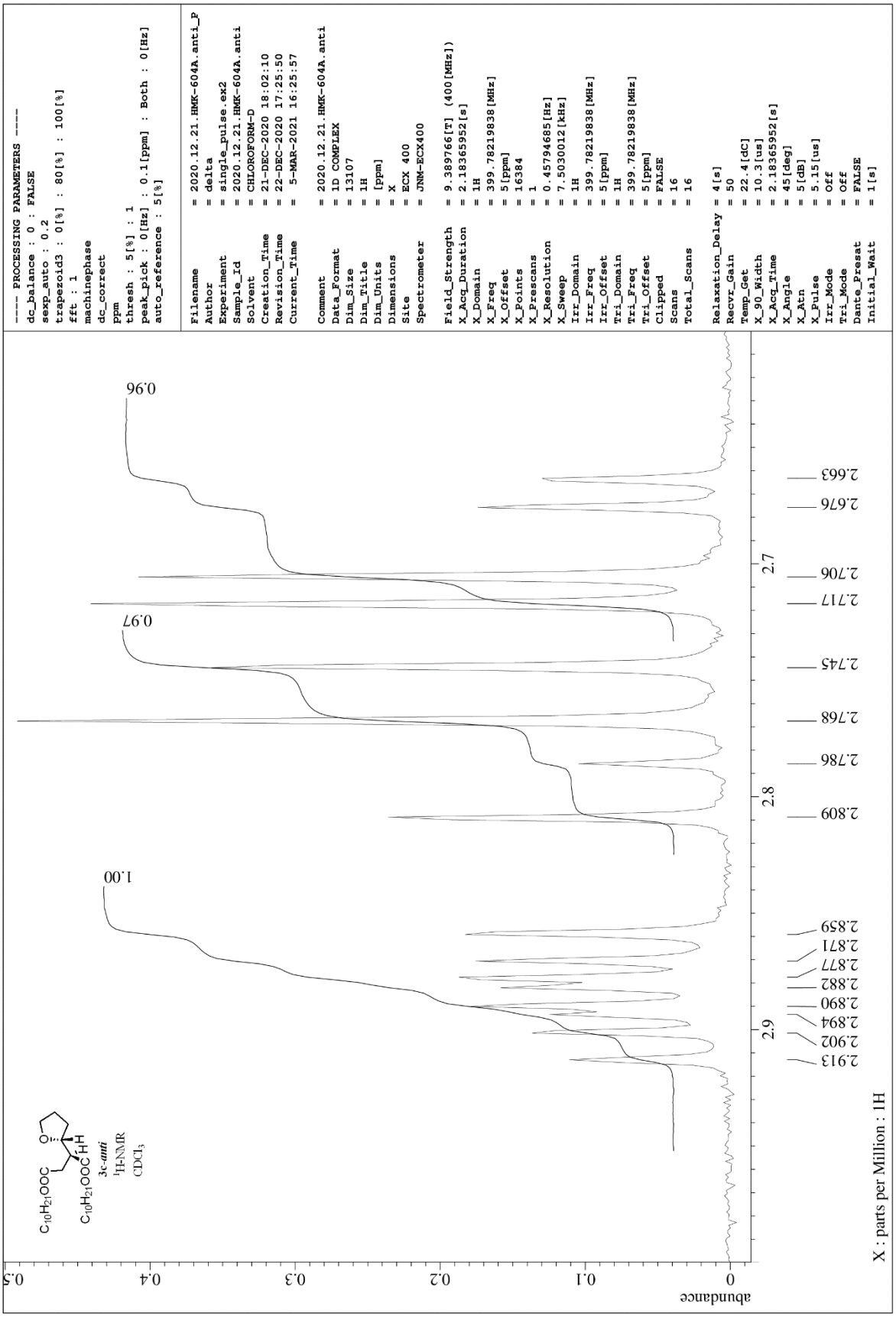

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Peaks : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.21.HMK-604a.syn_CA
Author = delta
Experiment = single_pulse_dec
Sample_Id = 2020.12.21.HMK-604a.syn
Solvent = CHLOROFORM-D
Creation_Time = 21-DEC-2020 18:55:14
Revision_Time = 22-DEC-2020 16:52:08
Current_Time = 5-MAR-2021 16:05:06
Comment = 2020.12.21.HMK-604a.syn
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.525303333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 49
Total_Scans = 49
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 22.8[dC]
X_90_Width = 8.9[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 2.96666667[us]
Irr_Atn_Dec = 19.5[dB]
Irr_Atn_Noe = 19.5[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
C10H21OOC
C10H21OOC H
3c-syn
13C-NMR
CDCl3
abundance
X : parts per Million : 13C
14.100
22.662
25.694
25.857
28.421
28.564
29.251
29.298
29.527
31.882
32.512
46.060
64.901
64.967
68.362
76.685
77.000
77.324
78.850
171.917
172.746

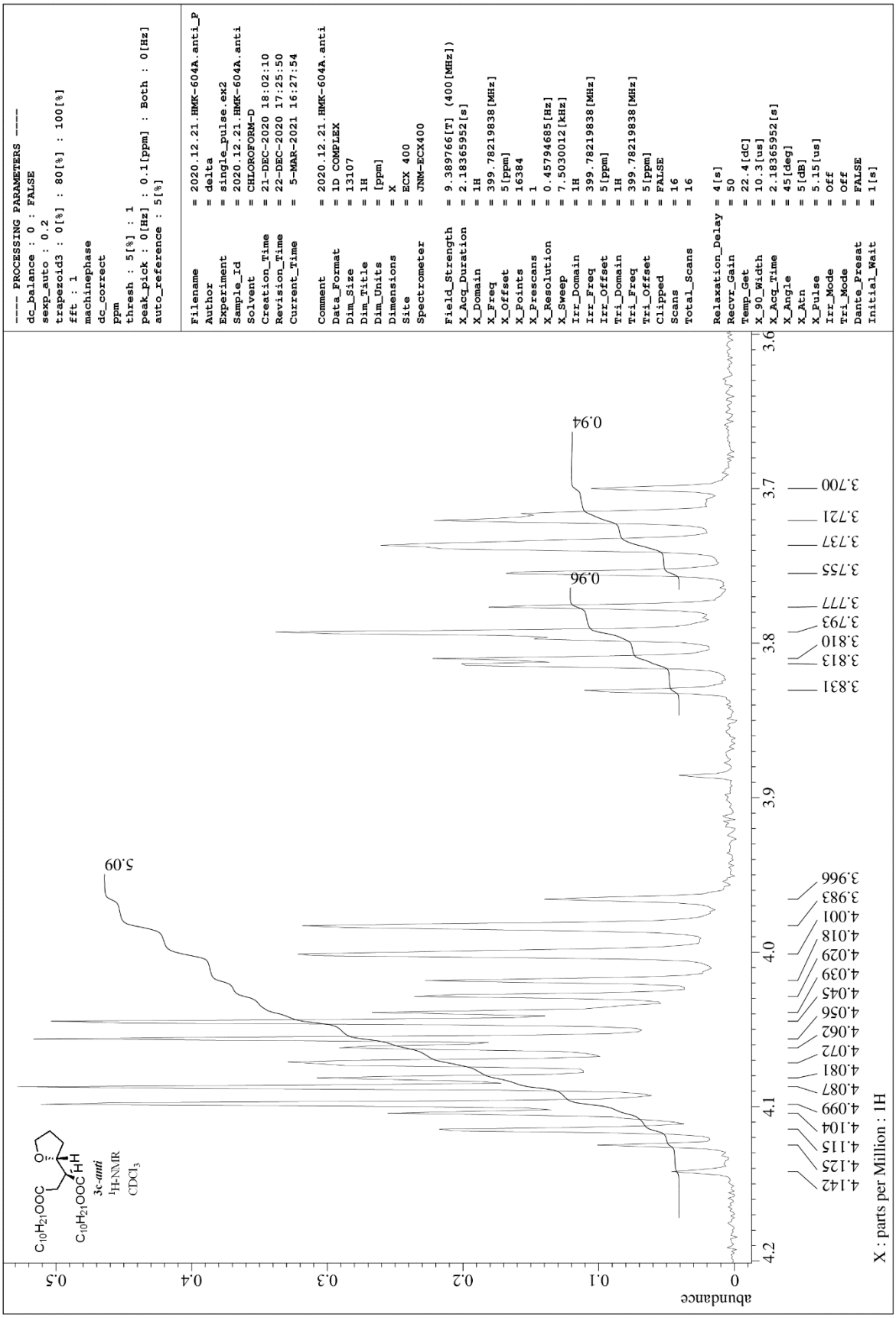

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Peaks : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.21.HMK-604a.syn_CA
Author = delta
Experiment = single_pulse_dec
Sample_Id = 2020.12.21.HMK-604a.syn
Solvent = CHLOROFORM-D
Creation_Time = 21-DEC-2020 18:55:14
Revision_Time = 22-DEC-2020 16:52:08
Current_Time = 5-MAR-2021 16:15:57
Comment = 2020.12.21.HMK-604a.syn
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.525303333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 49
Total_Scans = 49
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 22.8[dC]
X_90_Width = 8.9[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 2.96666667[us]
Irr_Atn_Dec = 19.5[dB]
Irr_Atn_Noe = 19.5[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
C10H21OOC
C10H21OOC
3c-syn
13C-NMR
CDCl3
abundance
0
0.1
0.2
0.3
25.694
25.857
28.421
28.564
29.251
29.298
29.527
31.882
32.512
25.0
26.0
27.0
28.0
29.0
30.0
31.0
32.0
X : parts per Million : 13C

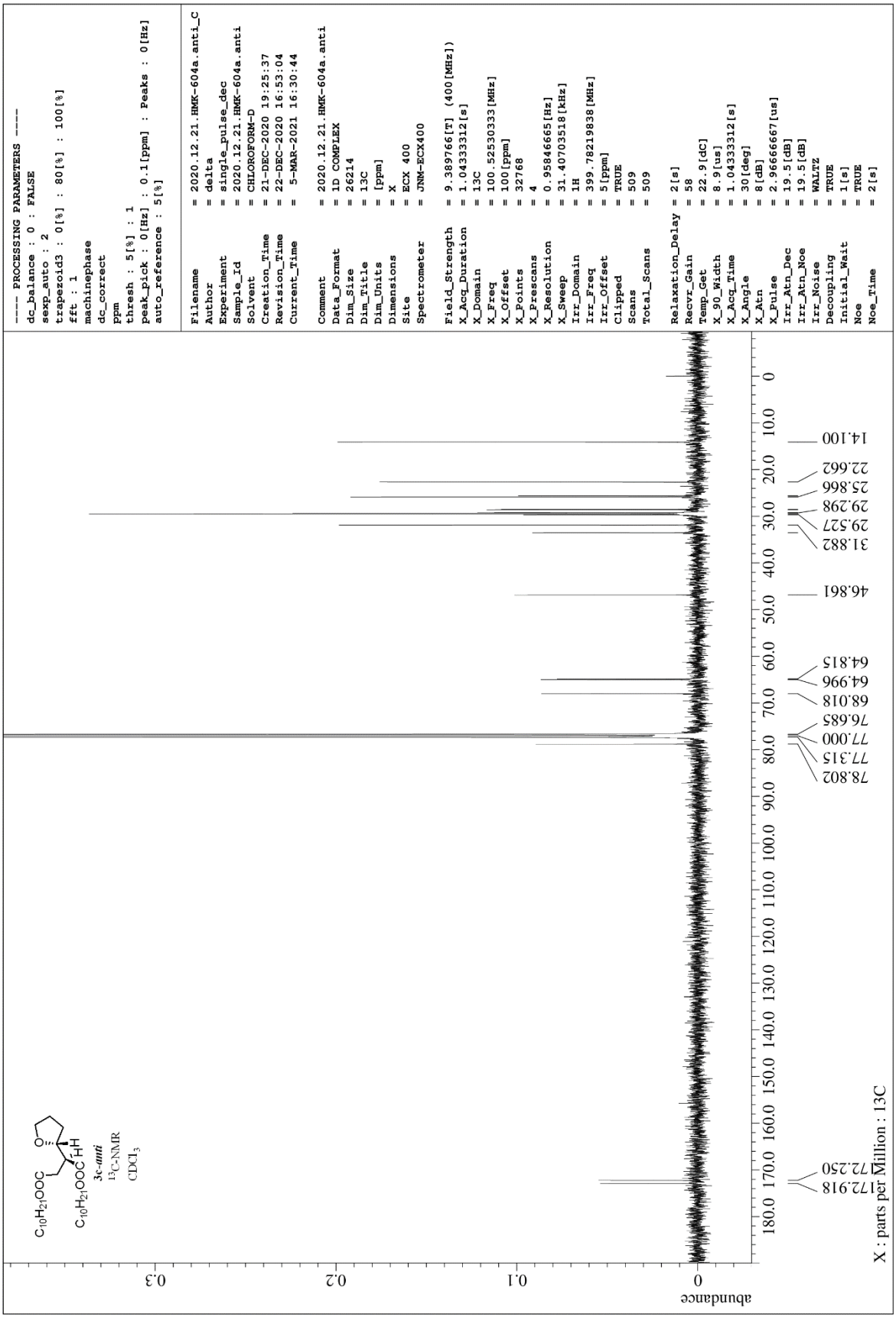

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.21.HMR-604A.anti_P
Author = delta
Experiment = single_pulse_ex2
Sample_Id = 2020.12.21.HMR-604A.anti
Solvent = CHLOROFORM-D
Creation_Time = 21-DEC-2020 18:02:10
Revision_Time = 22-DEC-2020 17:25:50
Current_Time = 5-MAR-2021 16:19:31
Comment = 2020.12.21.HMR-604A.anti
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 50
Temp_Get = 22.4[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 5[dB]
X_Pulse = 5.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
C10H21OOC
C10H21OOC
3c-anti
1H-NMR
CDCl3
abundance
X : parts per Million : 1H
28.47
6.23
5.09
4.01
3.06
1.00
0.97
0.96
0.94
0.89
0.86
0.881
0.864
1.262
1.546
1.600
1.607
1.625
2.706
2.717
2.745
2.768
3.737
3.793
3.983
4.001
4.045
4.056
4.072
4.087
4.099
7.261
0.000

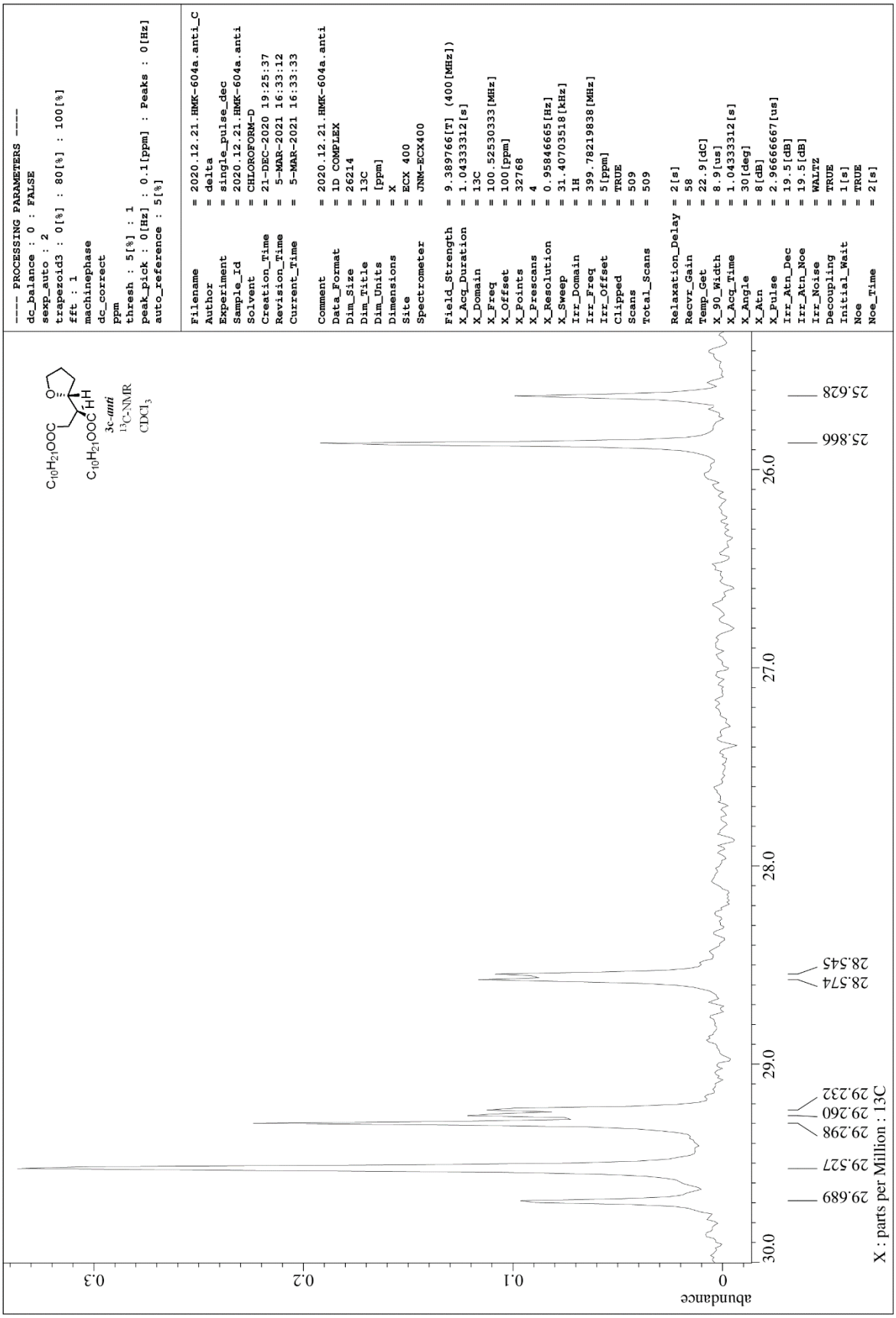

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.21.HMK-604A.anti_P
Author = delta
Experiment = single_pulse_ex2
Sample_Id = 2020.12.21.HMK-604A.anti
Solvent = CHLOROFORM-D
Creation_Time = 21-DEC-2020 18:02:10
Revision_Time = 22-DEC-2020 17:25:50
Current_Time = 5-MAR-2021 16:22:02
Comment = 2020.12.21.HMK-604A.anti
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 50
Temp_Get = 22.4[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 5[dB]
X_Pulse = 5.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
C10H21OOC
C10H21OOC H
3c-anti
1H-NMR
CDCl3
6.23
0.898
0.881
0.864
abundance
2.0
1.0
0
X : parts per Million : 1H
1.0 0.99 0.98 0.97 0.96 0.95 0.94 0.93 0.92 0.91 0.9 0.89 0.88 0.87 0.86 0.85 0.84 0.83 0.82 0.81 0.8 0.79 0.78 0.77 0.76

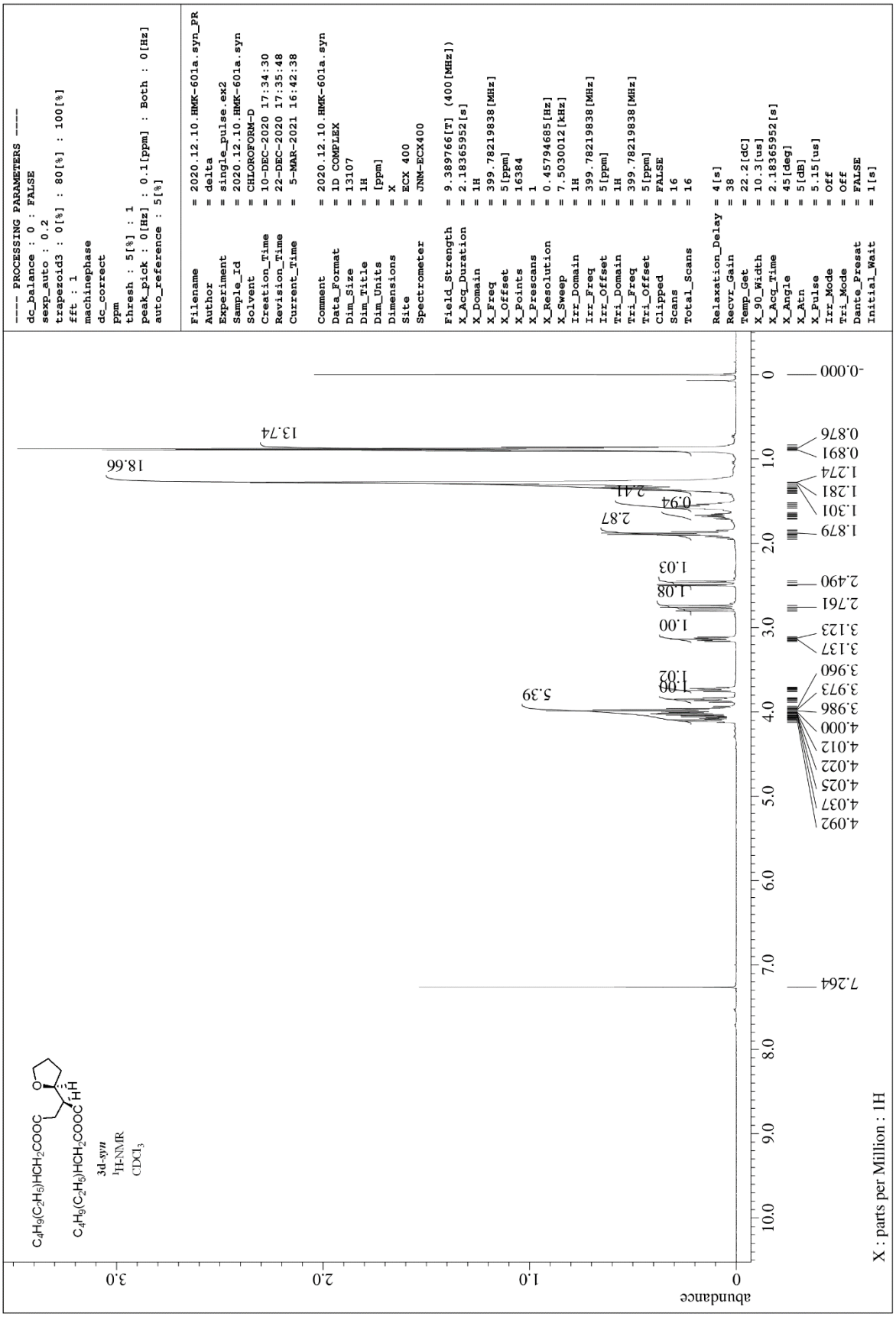

C10H21OOC
C10H21OOC
H
3c-anti
1H-NMR
CDCl3
abundance
X : parts per Million : 1H
4.01
3.06
0.97
1.262
1.299
2.013
1.997
1.985
1.977
1.969
1.965
1.947
1.935
1.924
1.918
1.907
1.899
1.890
1.869
1.853
1.781
1.764
1.751
1.742
1.733
1.714
1.661
1.644
1.625
1.620
1.607
1.600
1.591
1.583
1.565
1.546
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.21.HMR-604A.anti_P
Author = delta
Experiment = single_pulse_ex2
Sample_Id = 2020.12.21.HMR-604A.anti
Solvent = CHLOROFORM-D
Creation_Time = 21-DEC-2020 18:02:10
Revision_Time = 22-DEC-2020 17:25:50
Current_Time = 5-MAR-2021 16:23:54
Comment = 2020.12.21.HMR-604A.anti
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 50
Temp_Get = 22.4[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 5[dB]
X_Pulse = 5.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]

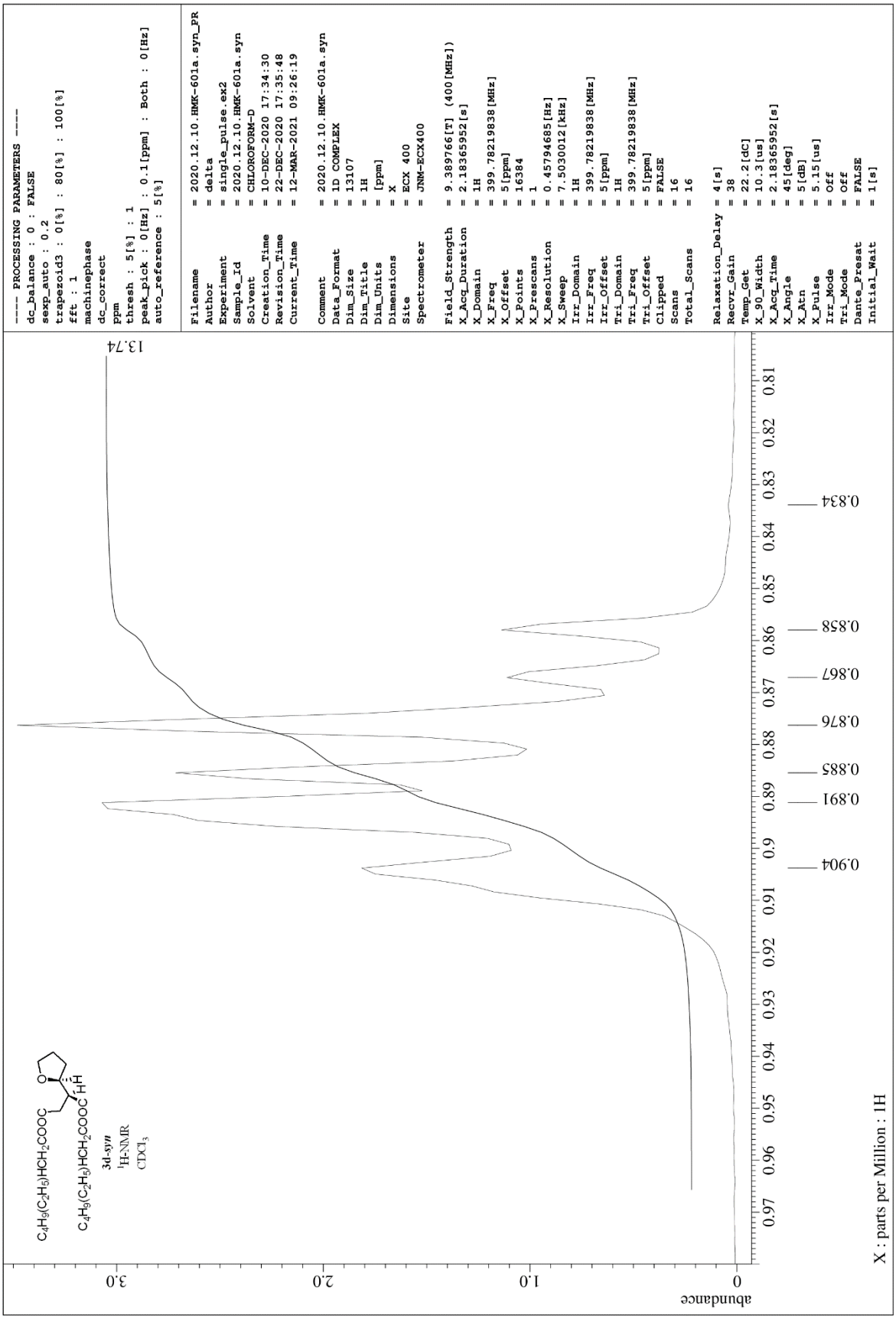

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.21.HMK-604A.anti_P
Author = delta
Experiment = single_pulse_ex2
Sample_Id = 2020.12.21.HMK-604A.anti
Solvent = CHLOROFORM-D
Creation_Time = 21-DEC-2020 18:02:10
Revision_Time = 22-DEC-2020 17:25:50
Current_Time = 5-MAR-2021 16:25:57
Comment = 2020.12.21.HMK-604A.anti
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 50
Temp_Get = 22.4[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 5[dB]
X_Pulse = 5.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
C10H21OOC
C10H21OOC H
3c-anti
1H-NMR
CDCl3
1.00
0.97
0.96
2.913
2.902
2.894
2.890
2.882
2.877
2.871
2.859
2.809
2.786
2.768
2.745
2.717
2.706
2.676
2.663
2.9
2.8
2.7
X : parts per Million : 1H
abundance
0
0.1
0.2
0.3
0.4
0.5

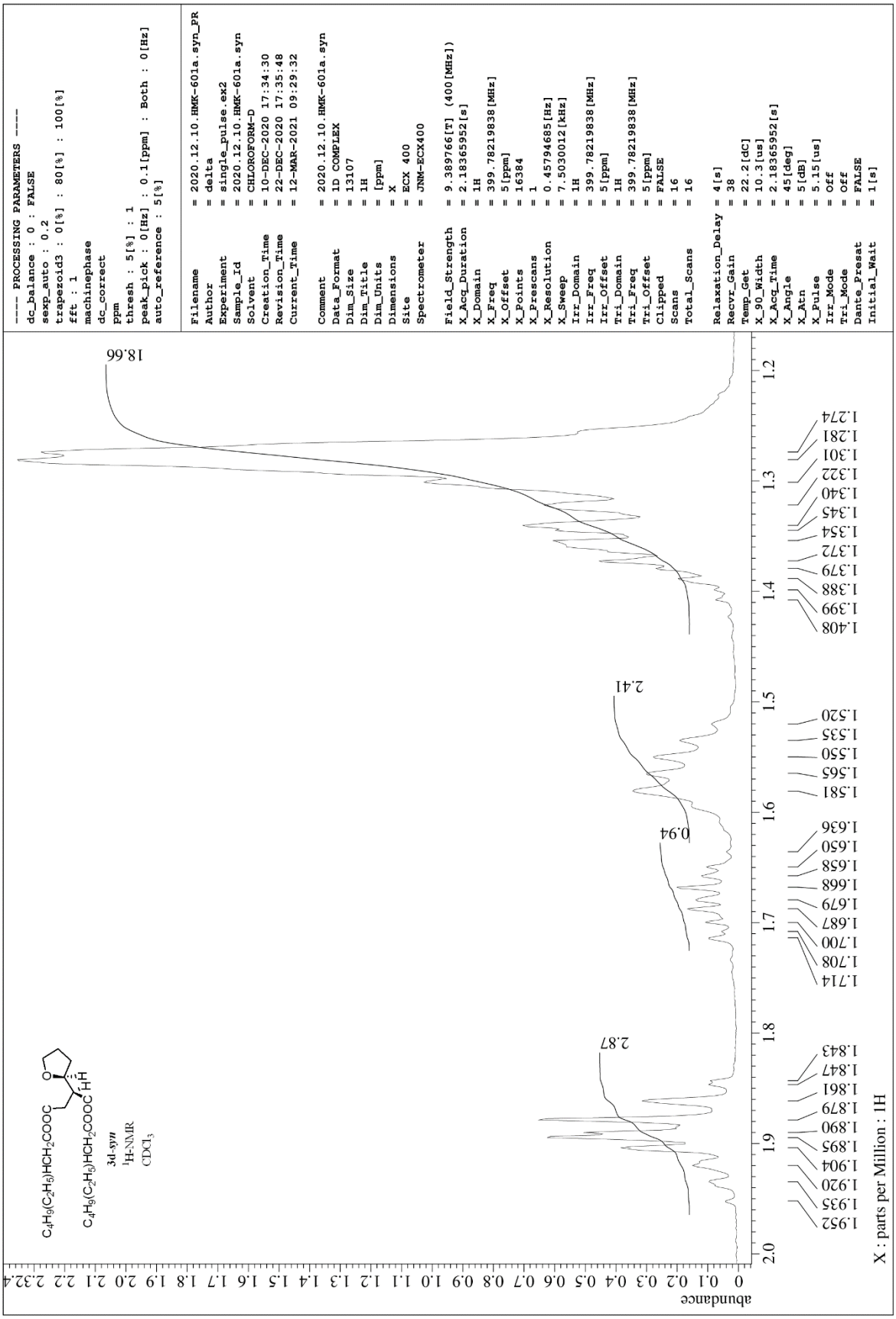

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.21.HMK-604A.anti_P
Author = delta
Experiment = single_pulse_ex2
Sample_Id = 2020.12.21.HMK-604A.anti
Solvent = CHLOROFORM-D
Creation_Time = 21-DEC-2020 18:02:10
Revision_Time = 22-DEC-2020 17:25:50
Current_Time = 5-MAR-2021 16:27:54
Comment = 2020.12.21.HMK-604A.anti
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 50
Temp_Get = 22.4[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 5[dB]
X_Pulse = 5.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
C10H21OOC
C10H21OOC H
3c-anti
1H-NMR
CDCl3
5.09
0.94
0.96
3.700
3.721
3.737
3.755
3.777
3.793
3.810
3.813
3.831
3.966
3.983
4.001
4.018
4.029
4.039
4.045
4.056
4.062
4.072
4.081
4.087
4.099
4.104
4.115
4.125
4.142
abundance
X : parts per Million : 1H

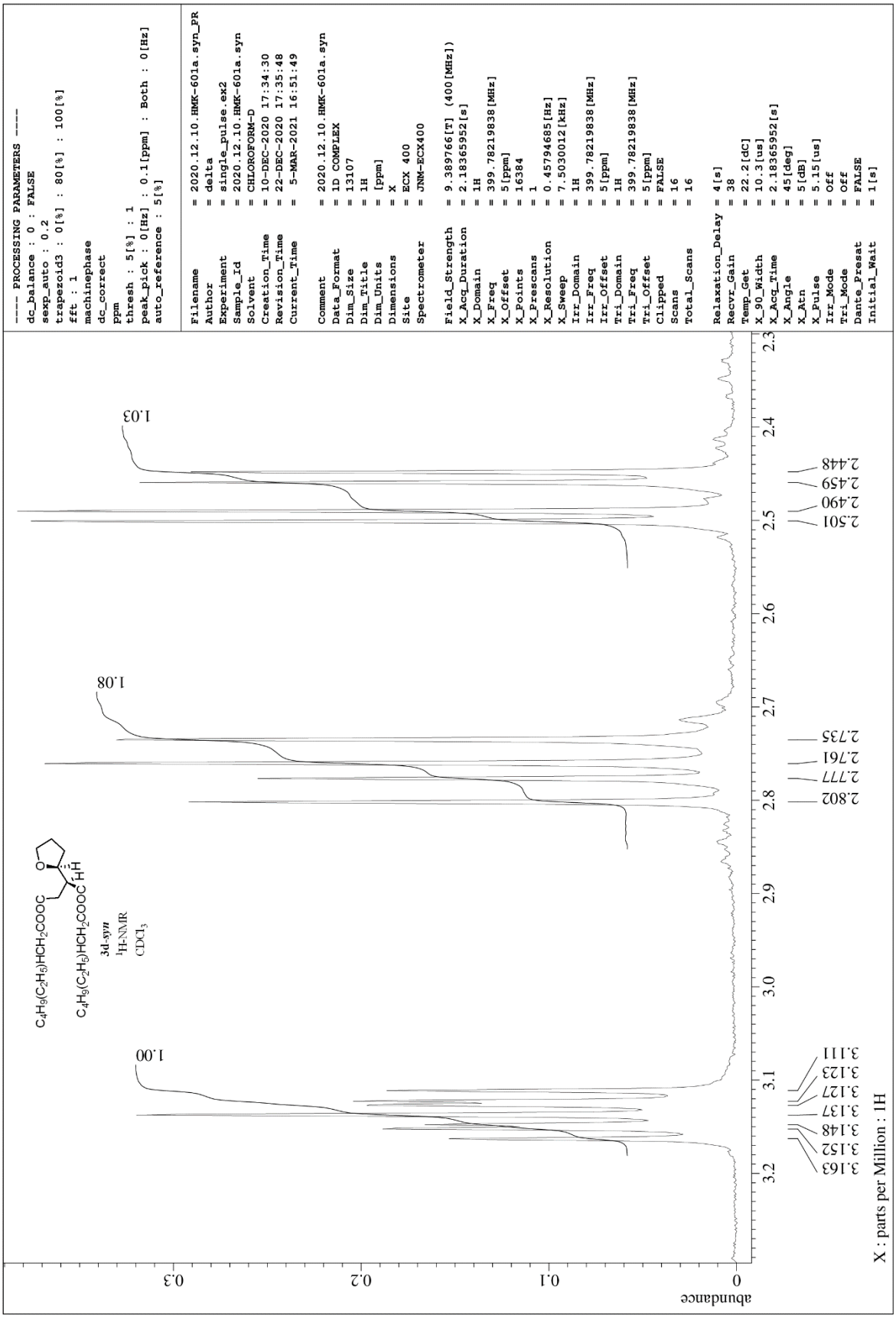

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Peaks : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.21.HMK-604a.anti_C
Author = delta
Experiment = single_pulse_dec
Sample_Id = 2020.12.21.HMK-604a.anti
Solvent = CHLOROFORM-D
Creation_Time = 21-DEC-2020 19:25:37
Revision_Time = 22-DEC-2020 16:53:04
Current_Time = 5-MAR-2021 16:30:44
Comment = 2020.12.21.HMK-604a.anti
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.525303333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 509
Total_Scans = 509
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 22.9[dC]
X_90_Width = 8.9[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 2.96666667[us]
Irr_Atn_Dec = 19.5[dB]
Irr_Atn_Noe = 19.5[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
C10H21OOC
C10H21OOC H
3c-anti
13C-NMR
CDCl3
abundance
0.3
0.2
0.1
0
180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
14.100
22.662
25.866
29.298
29.527
31.882
46.861
64.815
64.996
68.018
76.685
77.000
77.315
78.802
172.250
172.918
X : parts per Million : 13C

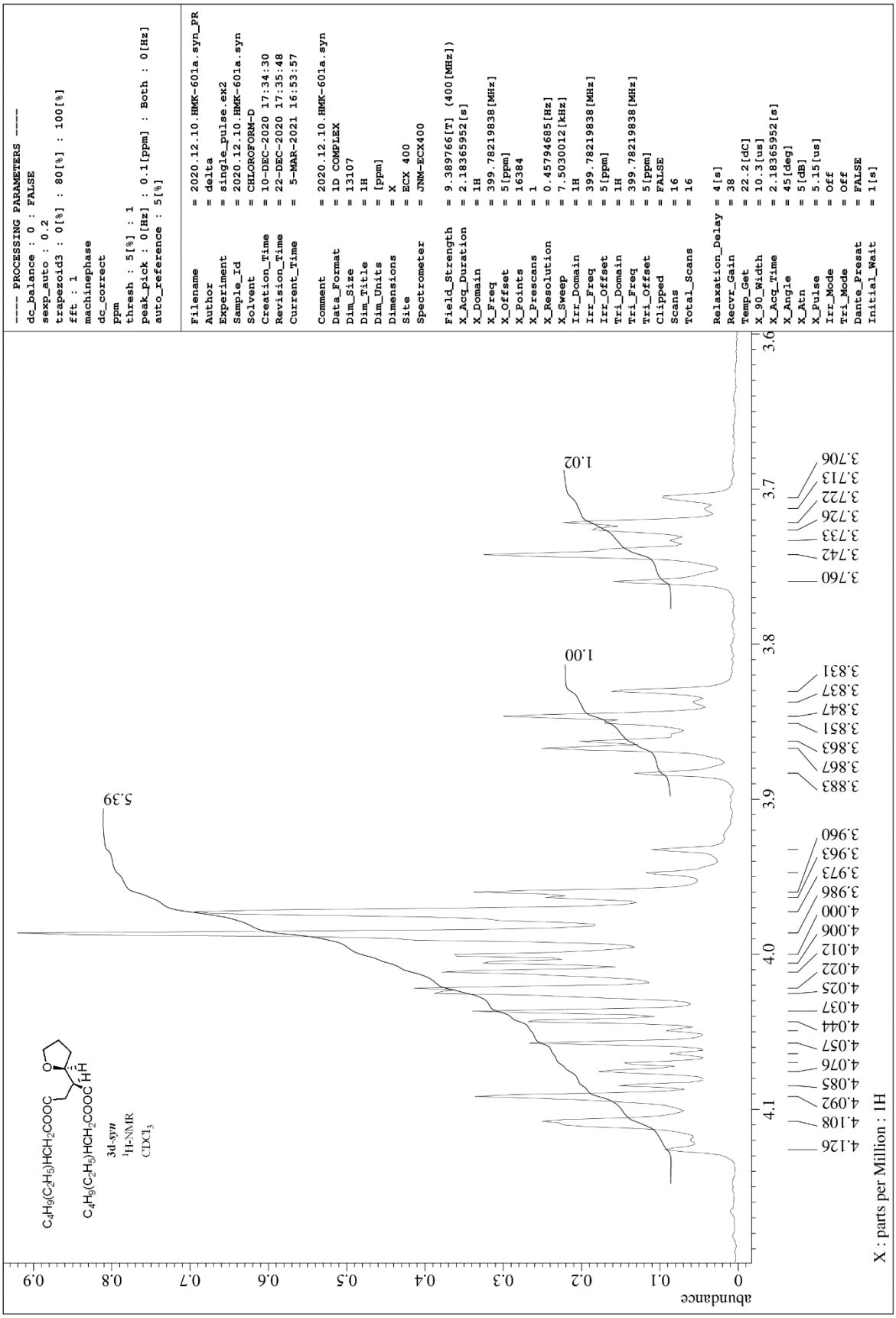

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Peaks : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.21.HMK-604a.anti_C
Author = delta
Experiment = single_pulse_dec
Sample_Id = 2020.12.21.HMK-604a.anti
Solvent = CHLOROFORM-D
Creation_Time = 21-DEC-2020 19:25:37
Revision_Time = 5-MAR-2021 16:33:12
Current_Time = 5-MAR-2021 16:33:33
Comment = 2020.12.21.HMK-604a.anti
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.525303333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 509
Total_Scans = 509
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 22.9[dC]
X_90_Width = 8.9[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 2.96666667[us]
Irr_Atn_Dec = 19.5[dB]
Irr_Atn_Noe = 19.5[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
C10H21OOC
C10H21OOC H
3c-anti
13C-NMR
CDCl3
25.628
25.866
28.545
28.574
29.232
29.260
29.298
29.527
29.689
X : parts per Million : 13C
abundance

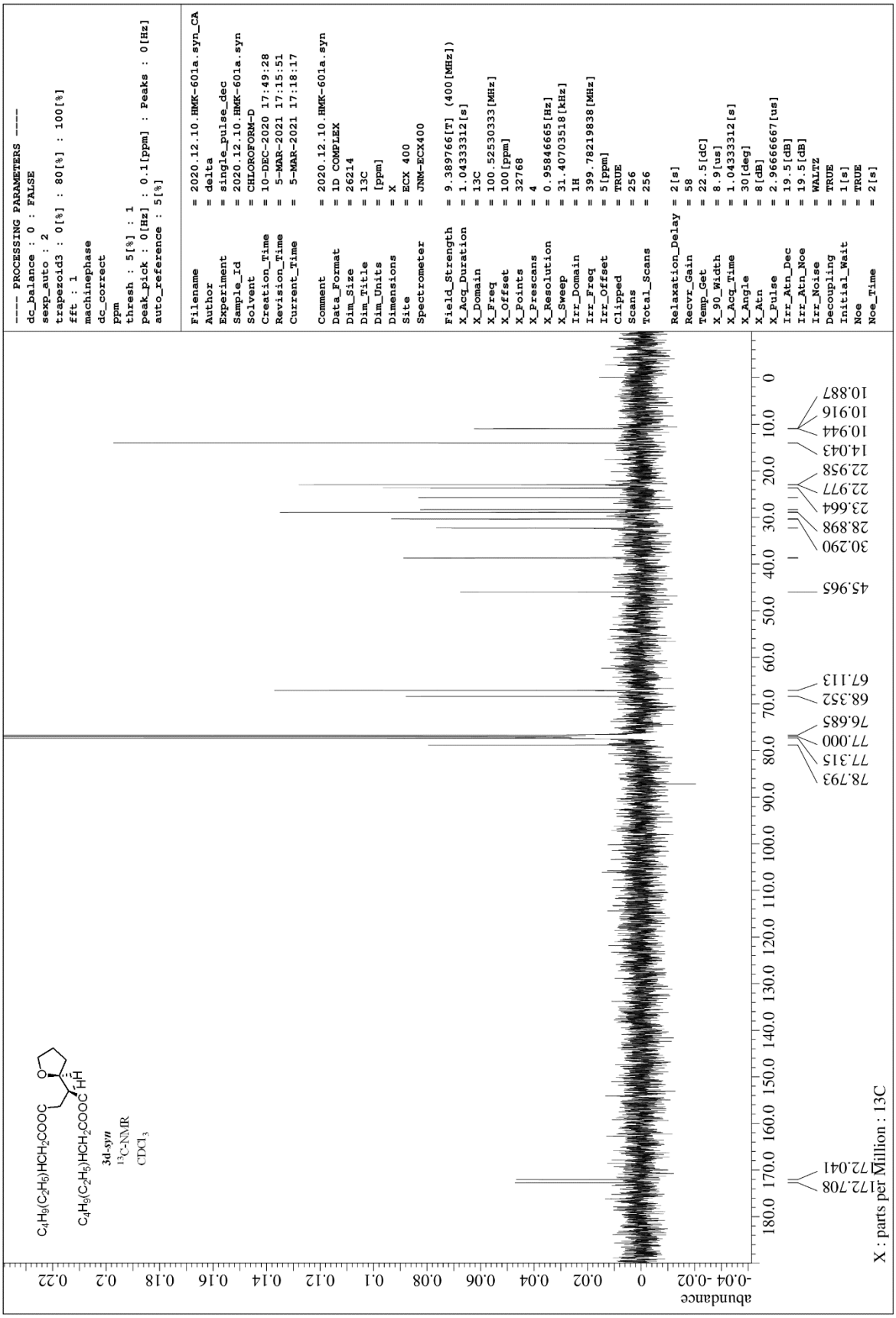

C4H9(C2H5)HCH2COOC
C4H9(C2H5)HCH2COOCHH
3d-syn
1H-NMR
CDCl3
abundance
X : parts per Million : 1H
18.66
13.74
2.41
0.94
2.87
1.03
1.08
1.00
1.02
5.39
7.264
-0.000
0.876
0.891
1.274
1.281
1.301
1.879
2.490
2.761
3.123
3.137
3.960
3.973
3.986
4.000
4.012
4.022
4.025
4.037
4.092

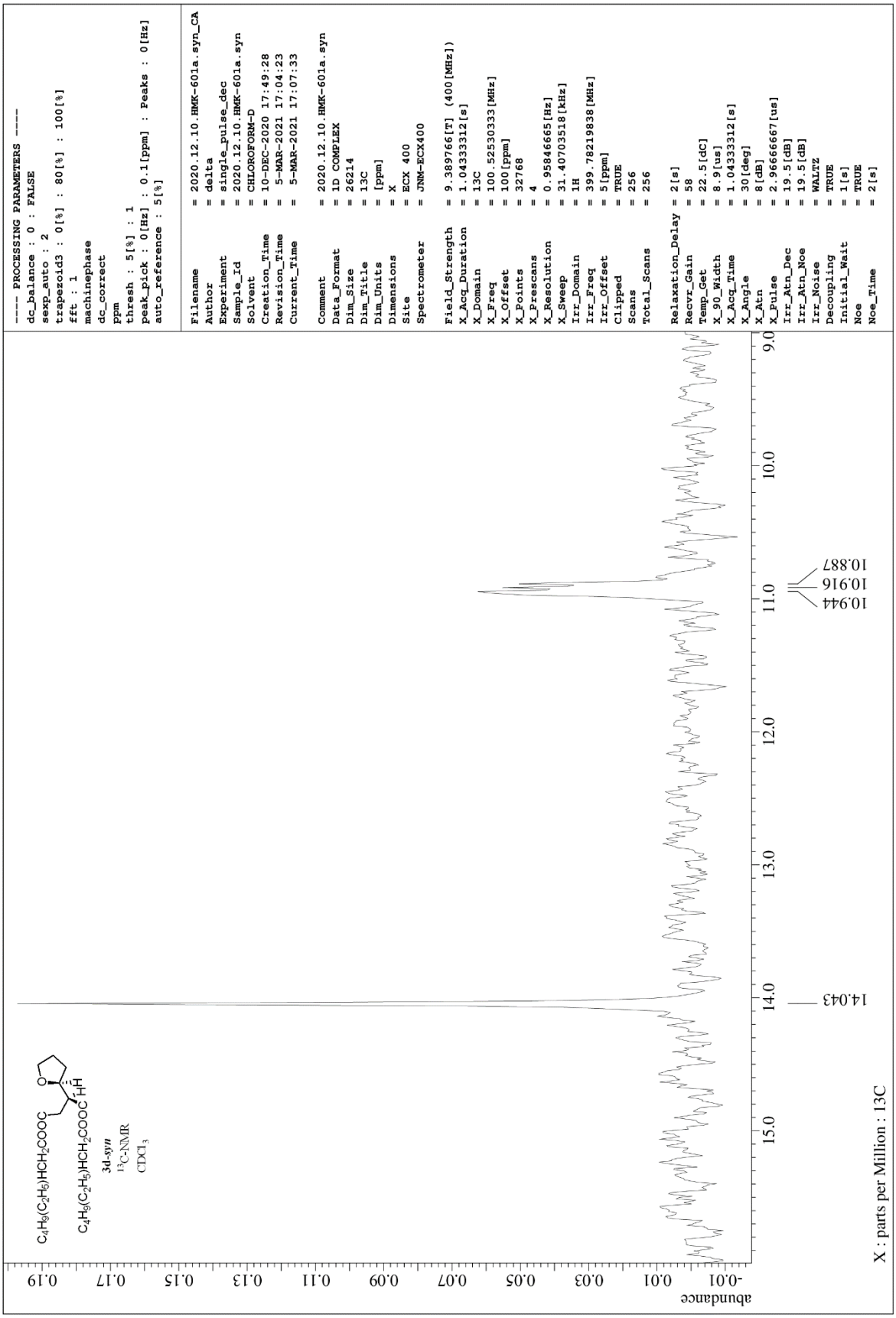

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.10.HMK-601a.syn_PR
Author = delta
Experiment = single_pulse_ex2
Sample_Id = 2020.12.10.HMK-601a.syn
Solvent = CHLOROFORM-D
Creation_Time = 10-DEC-2020 17:34:30
Revision_Time = 22-DEC-2020 17:35:48
Current_Time = 12-MAR-2021 09:26:19
Comment = 2020.12.10.HMK-601a.syn
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 38
Temp_Get = 22.2[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 5[dB]
X_Pulse = 5.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
13.74
3d-syn
^{1}H-NMR
$CDCl_3$
abundance
X : parts per Million : 1H
0.904
0.891
0.885
0.876
0.867
0.858
0.834

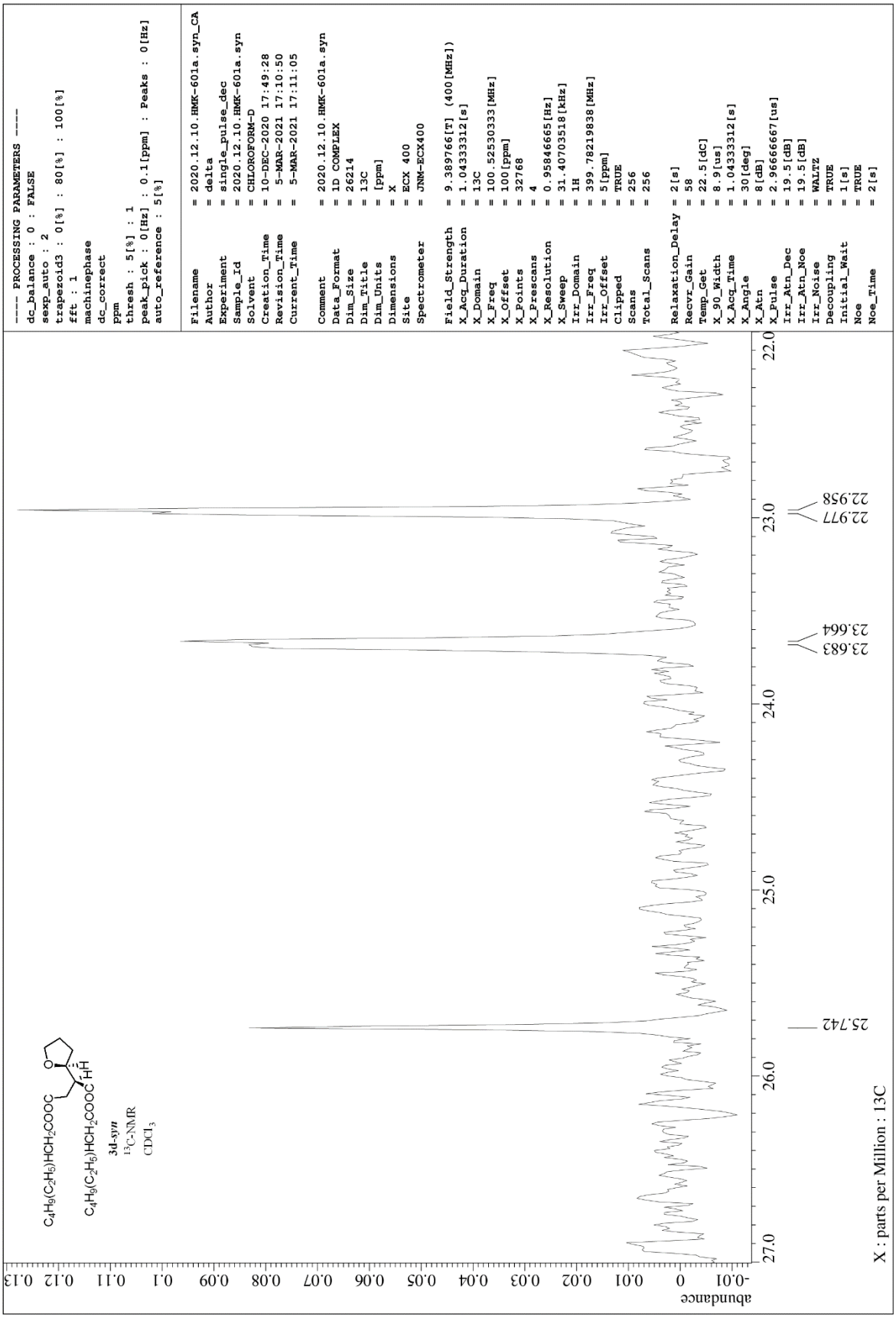

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.10.HMK-601a.syn_PR
Author = delta
Experiment = single_pulse_ex2
Sample_Id = 2020.12.10.HMK-601a.syn
Solvent = CHLOROFORM-D
Creation_Time = 10-DEC-2020 17:34:30
Revision_Time = 22-DEC-2020 17:35:48
Current_Time = 12-MAR-2021 09:29:32
Comment = 2020.12.10.HMK-601a.syn
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 38
Temp_Get = 22.2[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 5[dB]
X_Pulse = 5.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
C4H9(C2H5)HCH2COOC
C4H9(C2H5)HCH2COOC
3d-syn
1H-NMR
CDCl3
18.66
2.87
2.41
0.94
1.952
1.935
1.920
1.904
1.895
1.890
1.879
1.861
1.847
1.843
1.714
1.708
1.700
1.687
1.679
1.668
1.658
1.650
1.636
1.581
1.565
1.550
1.535
1.520
1.408
1.399
1.388
1.379
1.372
1.354
1.345
1.340
1.322
1.301
1.281
1.274
abundance
X : parts per Million : 1H

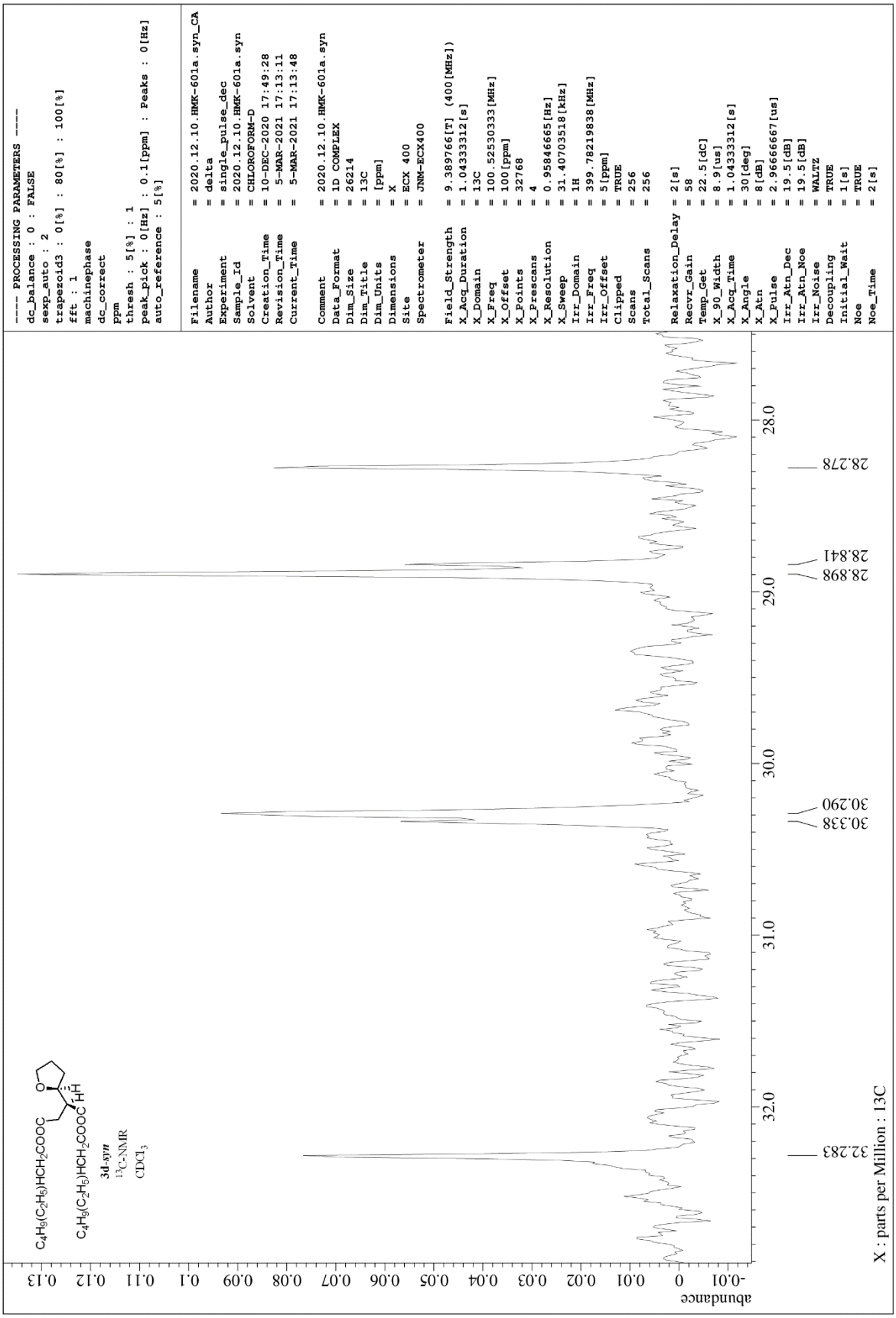

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.10.HMK-601a.syn_PR
Author = delta
Experiment = single_pulse_ex2
Sample_Id = 2020.12.10.HMK-601a.syn
Solvent = CHLOROFORM-D
Creation_Time = 10-DEC-2020 17:34:30
Revision_Time = 22-DEC-2020 17:35:48
Current_Time = 5-MAR-2021 16:51:49
Comment = 2020.12.10.HMK-601a.syn
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 38
Temp_Get = 22.2[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 5[dB]
X_Pulse = 5.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
C4H9(C2H5)HCH2COOC
C4H9(C2H5)HCH2COOC H
3d-syn
1H-NMR
CDCl3
1.00
1.08
1.03
3.163
3.152
3.148
3.137
3.127
3.123
3.111
2.802
2.777
2.761
2.735
2.501
2.490
2.459
2.448
X : parts per Million : 1H
abundance

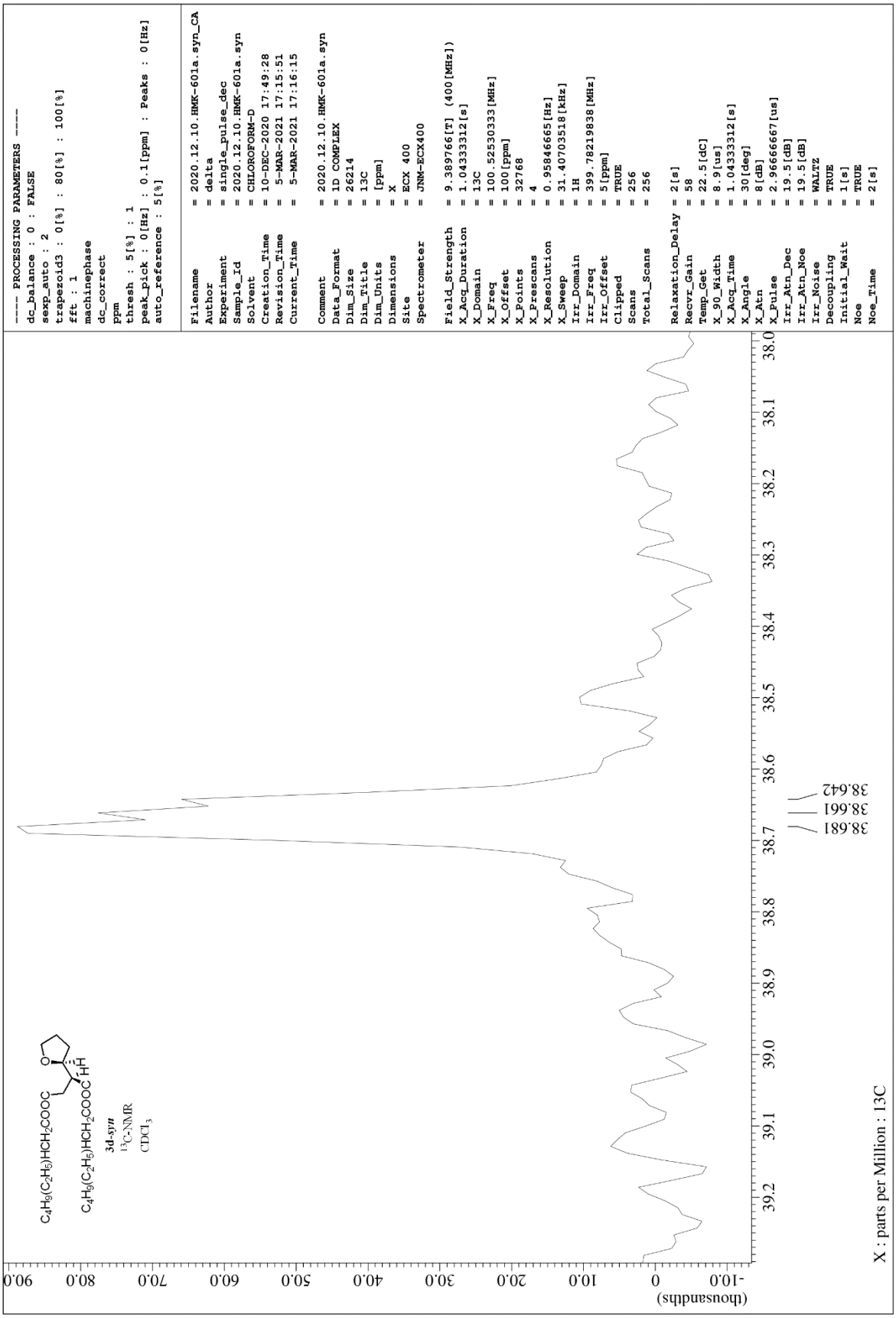

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.10.HMK-601a.syn_PR
Author = delta
Experiment = single_pulse_ex2
Sample_Id = 2020.12.10.HMK-601a.syn
Solvent = CHLOROFORM-D
Creation_Time = 10-DEC-2020 17:34:30
Revision_Time = 22-DEC-2020 17:35:48
Current_Time = 5-MAR-2021 16:53:57
Comment = 2020.12.10.HMK-601a.syn
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 38
Temp_Get = 22.2[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 5[dB]
X_Pulse = 5.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
C4H9(C2H5)HCH2COOC
C4H9(C2H5)HCH2COOC H
3d-syn
1H-NMR
CDCl3
5.39
1.02
1.00
4.126
4.108
4.092
4.085
4.076
4.057
4.044
4.037
4.025
4.022
4.012
4.006
4.000
3.986
3.973
3.963
3.960
3.883
3.867
3.863
3.851
3.847
3.837
3.831
3.760
3.742
3.733
3.726
3.722
3.713
3.706
abundance
X : parts per Million : 1H

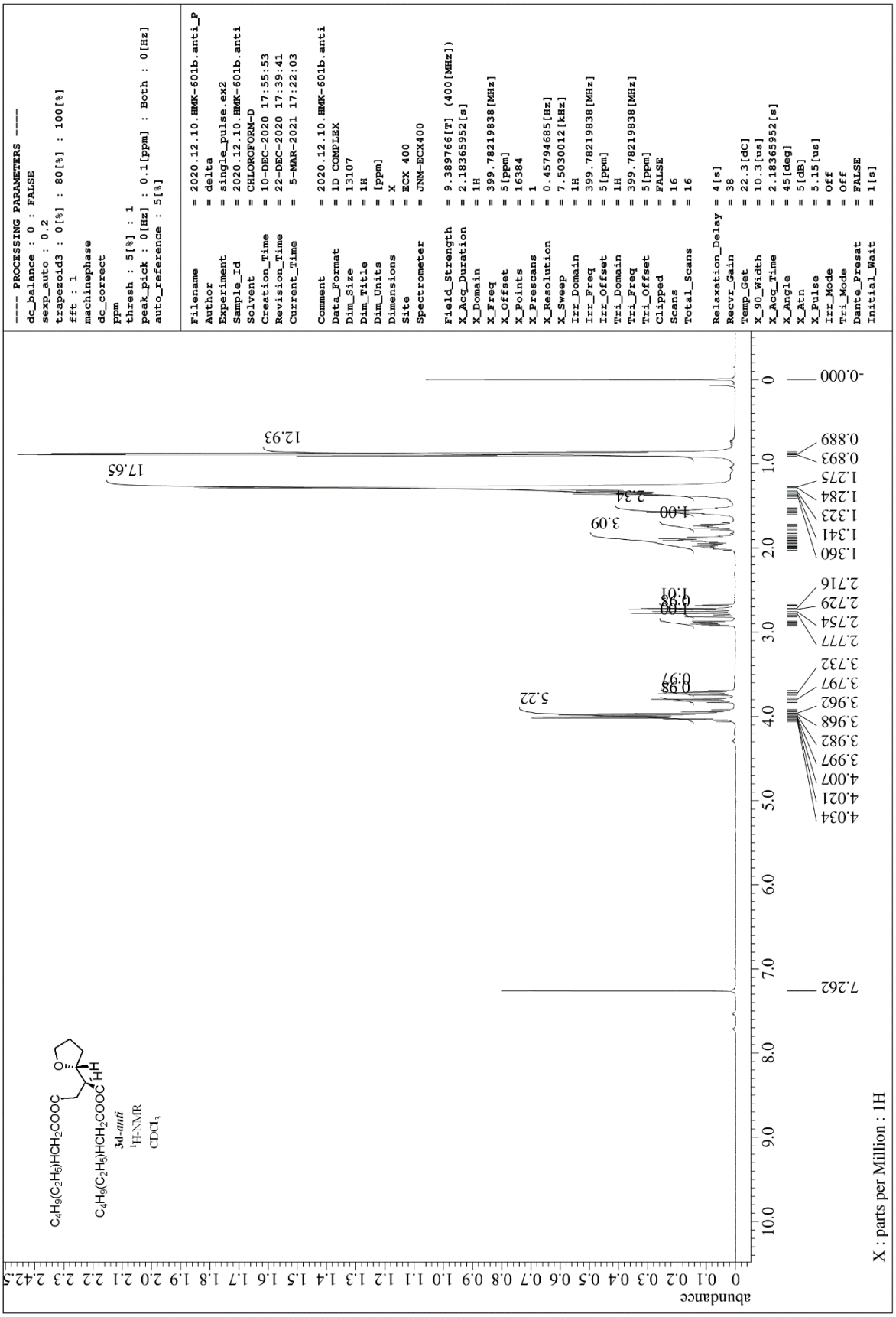

C4H9(C2H5)HCH2COOC
C4H9(C2H5)HCH2COOC
3d-syn
13C-NMR
CDCl3
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Peaks : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.10.HMK-601a.syn_CA
Author = delta
Experiment = single_pulse_dec
Sample_Id = 2020.12.10.HMK-601a.syn
Solvent = CHLOROFORM-D
Creation_Time = 10-DEC-2020 17:49:28
Revision_Time = 5-MAR-2021 17:15:51
Current_Time = 5-MAR-2021 17:18:17
Comment = 2020.12.10.HMK-601a.syn
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.525303333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 22.5[dC]
X_90_Width = 8.9[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 2.96666667[us]
Irr_Atn_Dec = 19.5[dB]
Irr_Atn_Noe = 19.5[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
abundance
X : parts per Million : 13C
172.708
172.041
78.793
77.315
77.000
76.685
68.352
67.113
45.965
30.290
28.898
23.664
22.977
22.958
14.043
10.944
10.916
10.887

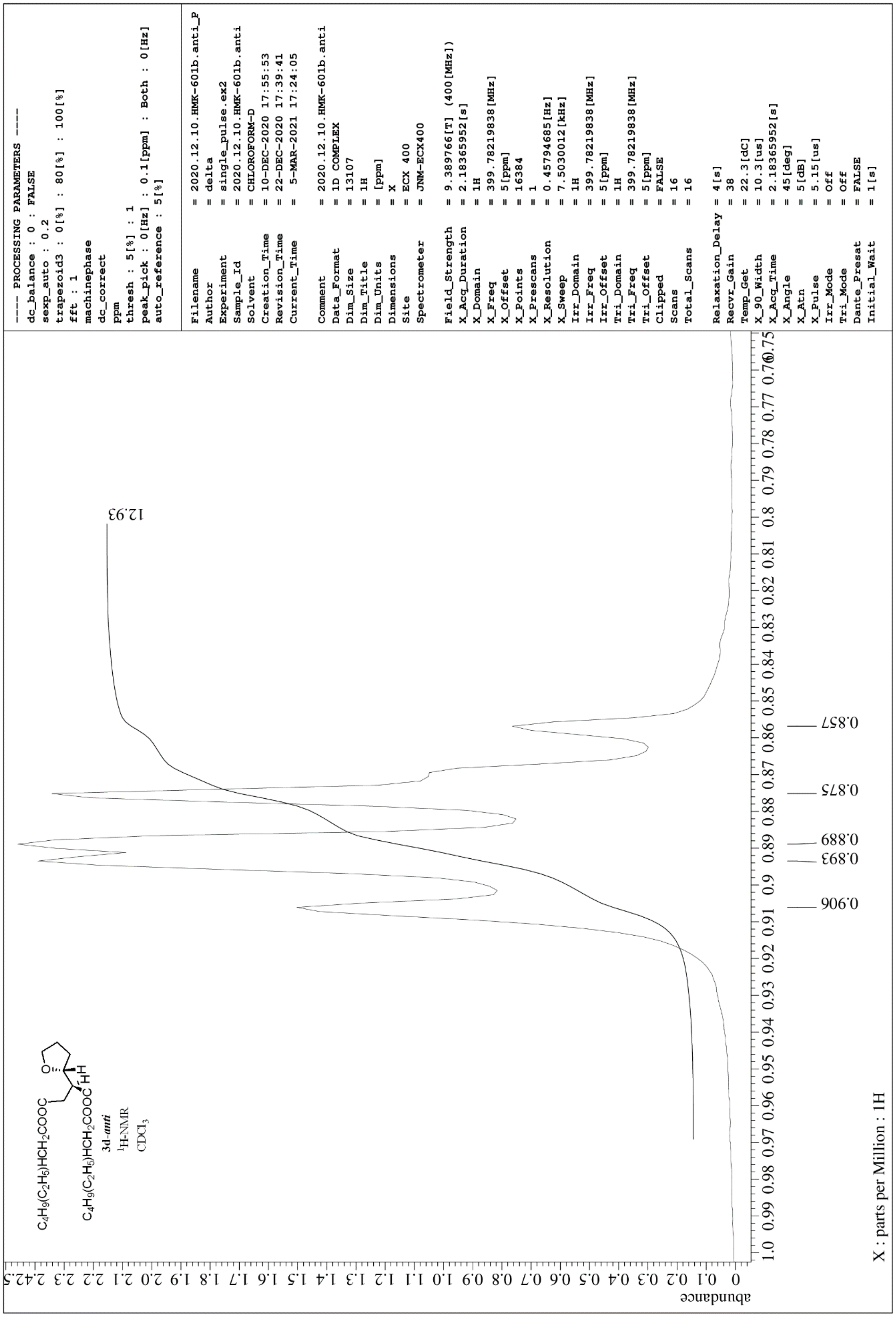

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Peaks : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.10.HMK-601a.syn_CA
Author = delta
Experiment = single_pulse_dec
Sample_Id = 2020.12.10.HMK-601a.syn
Solvent = CHLOROFORM-D
Creation_Time = 10-DEC-2020 17:49:28
Revision_Time = 5-MAR-2021 17:04:23
Current_Time = 5-MAR-2021 17:07:33
Comment = 2020.12.10.HMK-601a.syn
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.525303333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recyc_Gain = 58
Temp_Get = 22.5[dC]
X_90_Width = 8.9[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 2.96666667[us]
Irr_Atn_Dec = 19.5[dB]
Irr_Atn_Noe = 19.5[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
C4H9(C2H5)HCH2COOC
C4H9(C2H5)HCH2COOC
H
3d-syn
13C-NMR
CDCl3
14.043
10.944
10.916
10.887
abundance
X : parts per Million : 13C

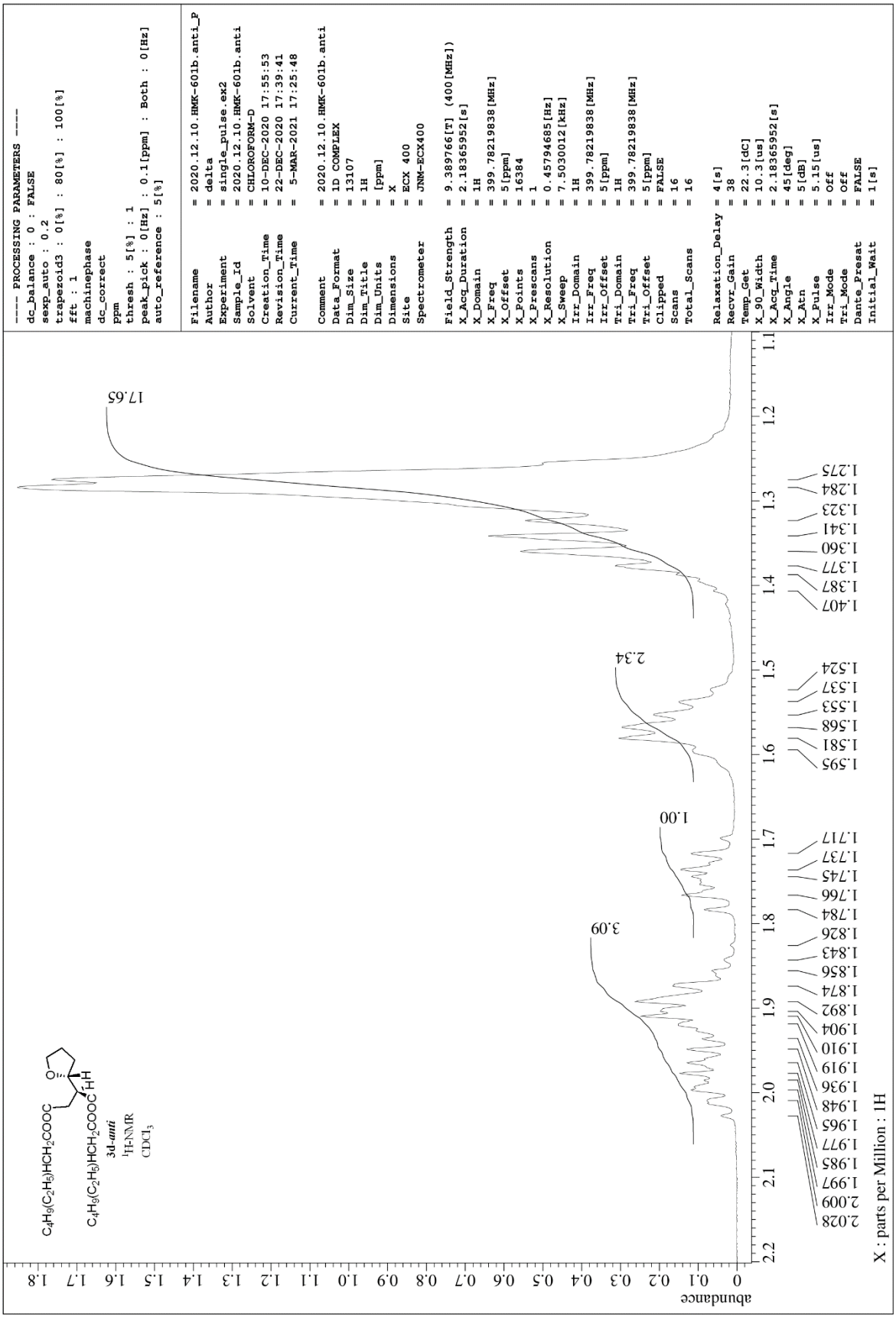

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Peaks : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.10.HMK-601a.syn_CA
Author = delta
Experiment = single_pulse_dec
Sample_Id = 2020.12.10.HMK-601a.syn
Solvent = CHLOROFORM-D
Creation_Time = 10-DEC-2020 17:49:28
Revision_Time = 5-MAR-2021 17:10:50
Current_Time = 5-MAR-2021 17:11:05
Comment = 2020.12.10.HMK-601a.syn
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.525303333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 22.5[dC]
X_90_Width = 8.9[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 2.96666667[us]
Irr_Atn_Dec = 19.5[dB]
Irr_Atn_Noe = 19.5[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
C4H9(C2H5)HCH2COOC
C4H9(C2H5)HCH2COOC
H
3d-syn
13C-NMR
CDCl3
abundance
0.13
0.12
0.11
0.1
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
-0.01
27.0
26.0
25.0
24.0
23.0
22.0
25.742
23.683
23.664
22.977
22.958
X : parts per Million : 13C

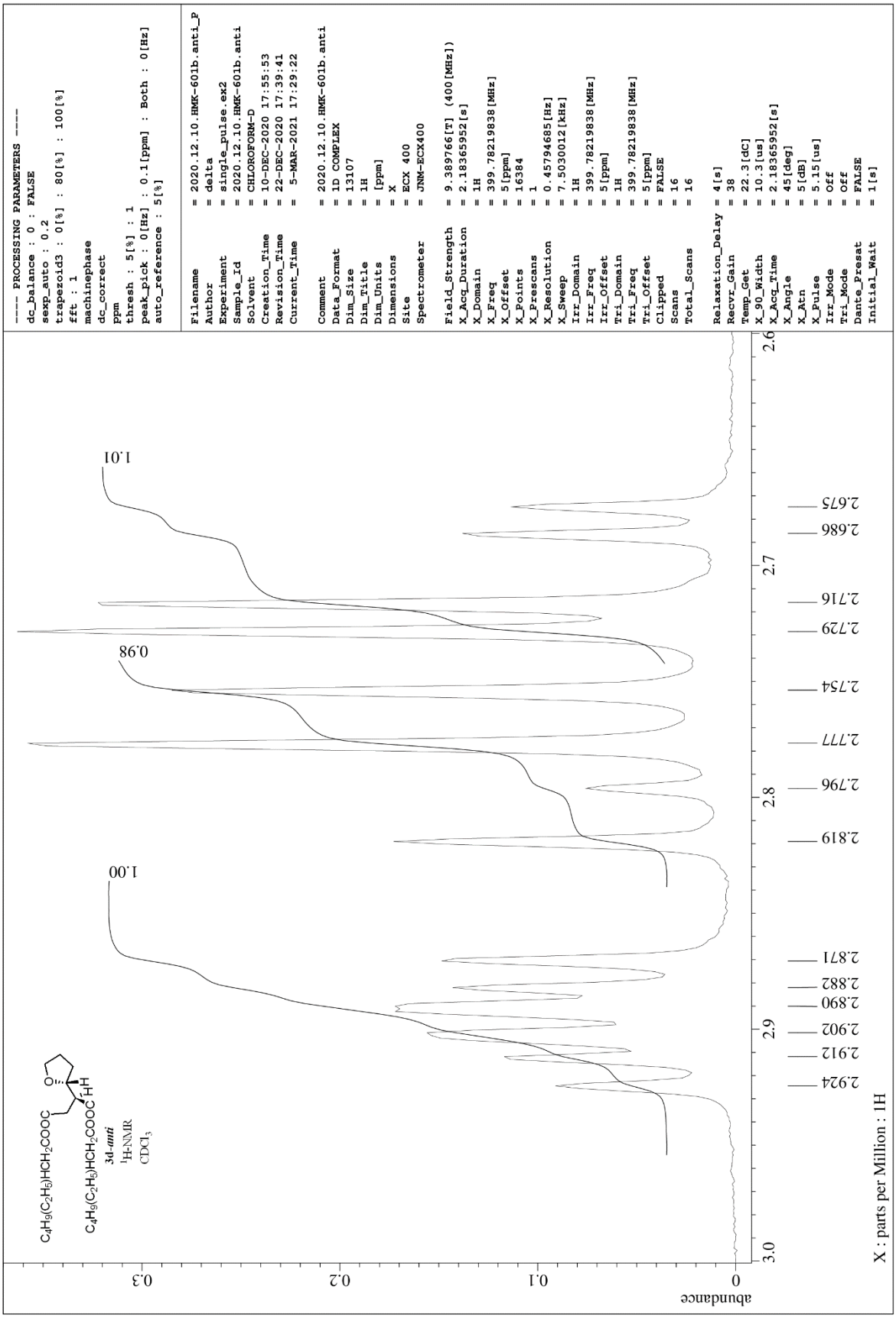

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Peaks : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.10.HMK-601a.syn_CA
Author = delta
Experiment = single_pulse_dec
Sample_Id = 2020.12.10.HMK-601a.syn
Solvent = CHLOROFORM-D
Creation_Time = 10-DEC-2020 17:49:28
Revision_Time = 5-MAR-2021 17:13:11
Current_Time = 5-MAR-2021 17:13:48
Comment = 2020.12.10.HMK-601a.syn
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.525303333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 22.5[dC]
X_90_Width = 8.9[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 2.96666667[us]
Irr_Atn_Dec = 19.5[dB]
Irr_Atn_Noe = 19.5[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
C4H9(C2H5)HCH2COOC
C4H9(C2H5)HCH2COOC
H
3d-syn
13C-NMR
CDCl3
abundance
0.13
0.12
0.11
0.1
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
-0.01
32.0
31.0
30.0
29.0
28.0
32.283
30.338
30.290
28.898
28.841
28.278
X : parts per Million : 13C

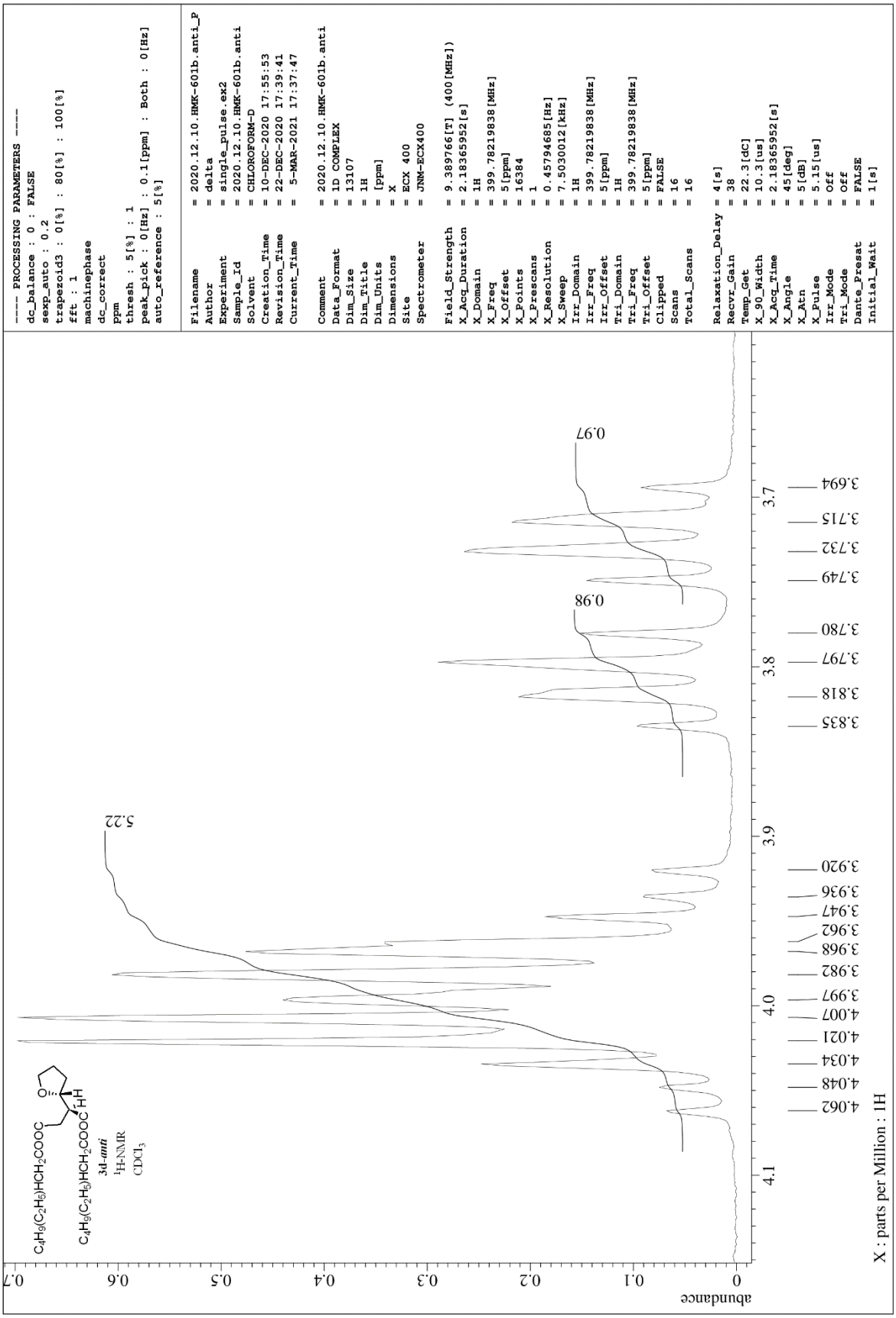

C4H9(C2H5)HCH2COOC
C4H9(C2H5)HCH2COOC
H
3d-syn
13C-NMR
CDCl3
(thousandths)
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
39.2
39.1
39.0
38.9
38.8
38.7
38.6
38.5
38.4
38.3
38.2
38.1
38.0
38.681
38.661
38.642
X : parts per Million : 13C
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Peaks : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.10.HMK-601a.syn_CA
Author = delta
Experiment = single_pulse_dec
Sample_Id = 2020.12.10.HMK-601a.syn
Solvent = CHLOROFORM-D
Creation_Time = 10-DEC-2020 17:49:28
Revision_Time = 5-MAR-2021 17:15:51
Current_Time = 5-MAR-2021 17:16:15
Comment = 2020.12.10.HMK-601a.syn
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.525303333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 22.5[dC]
X_90_Width = 8.9[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 2.96666667[us]
Irr_Atn_Dec = 19.5[dB]
Irr_Atn_Noe = 19.5[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]

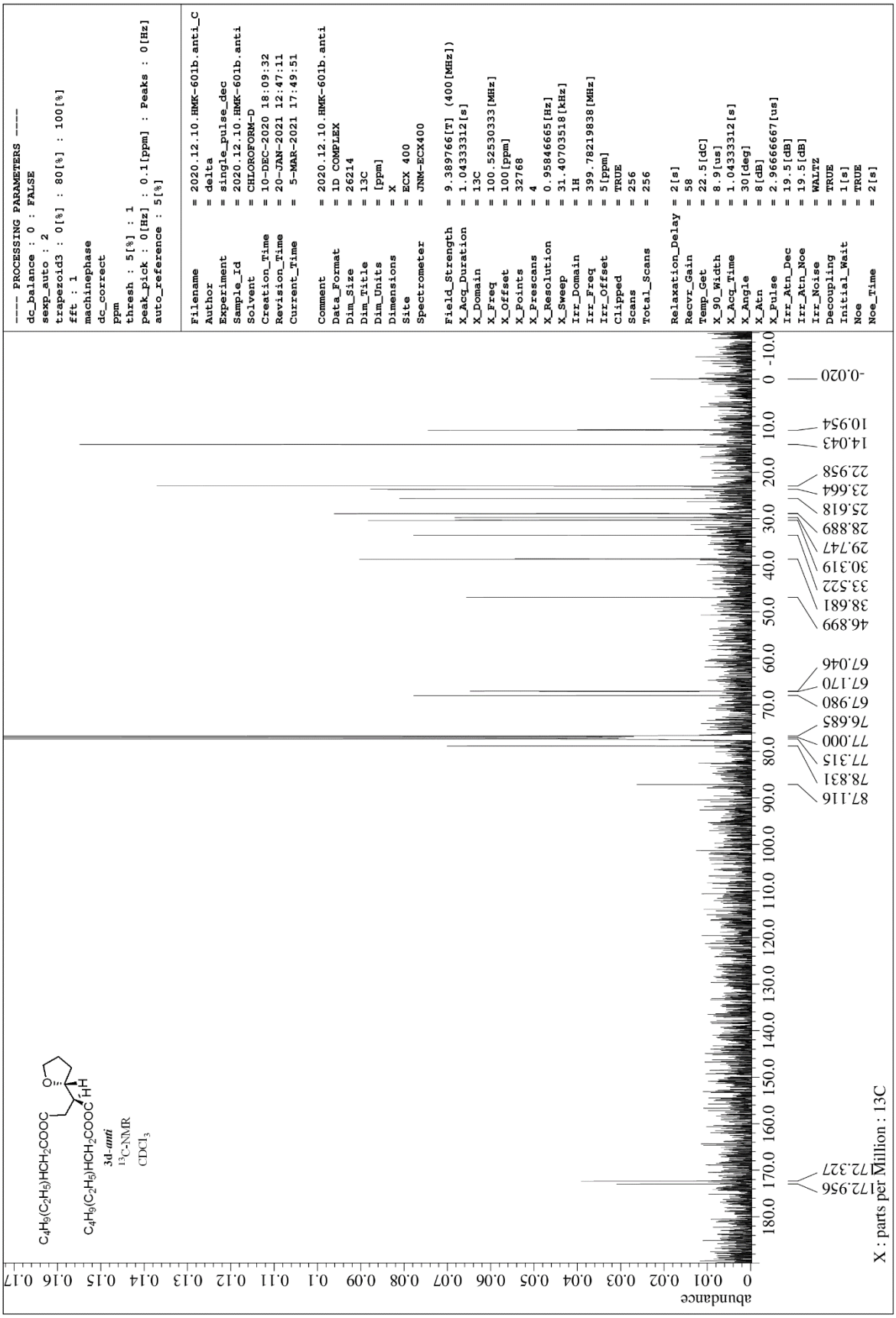

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.10.HMK-601b.anti_P
Author = delta
Experiment = single_pulse_ex2
Sample_Id = 2020.12.10.HMK-601b.anti
Solvent = CHLOROFORM-D
Creation_Time = 10-DEC-2020 17:55:53
Revision_Time = 22-DEC-2020 17:39:41
Current_Time = 5-MAR-2021 17:22:03
Comment = 2020.12.10.HMK-601b.anti
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 38
Temp_Get = 22.3[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 5[dB]
X_Pulse = 5.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
$C_4H_9(C_2H_5)HCH_2COOC$
$C_4H_9(C_2H_5)HCH_2COOC$
3d-anti
^{1}H-NMR
$CDCl_3$
12.93
17.65
2.34
1.00
3.09
1.01
0.98
0.97
5.22
7.262
-0.000
0.889
0.893
1.275
1.284
1.323
1.341
1.360
2.716
2.729
2.754
2.777
3.732
3.797
3.962
3.968
3.982
3.997
4.007
4.021
4.034
abundance
X : parts per Million : 1H

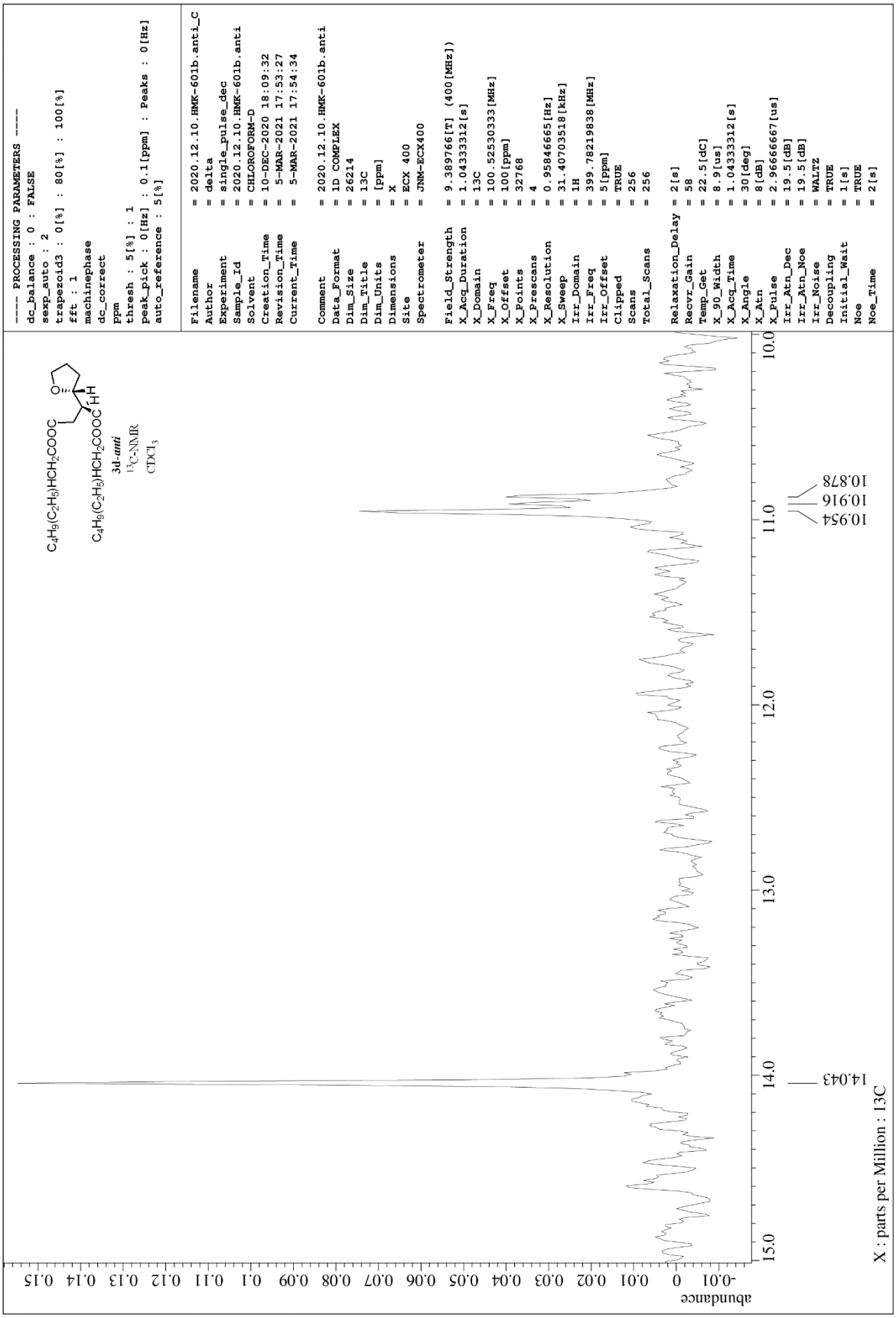

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.10.HMK-601b.anti_P
Author = delta
Experiment = single_pulse.ex2
Sample_Id = 2020.12.10.HMK-601b.anti
Solvent = CHLOROFORM-D
Creation_Time = 10-DEC-2020 17:55:53
Revision_Time = 22-DEC-2020 17:39:41
Current_Time = 5-MAR-2021 17:24:05
Comment = 2020.12.10.HMK-601b.anti
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 38
Temp_Get = 22.3[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 5[dB]
X_Pulse = 5.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
$C_4H_9(C_2H_5)HCH_2COOC$
$C_4H_9(C_2H_5)HCH_2COOC$
3d-*anti*
^{1}H-NMR
$CDCl_3$
12.93
0.857
0.875
0.889
0.893
0.906
X : parts per Million : 1H
abundance

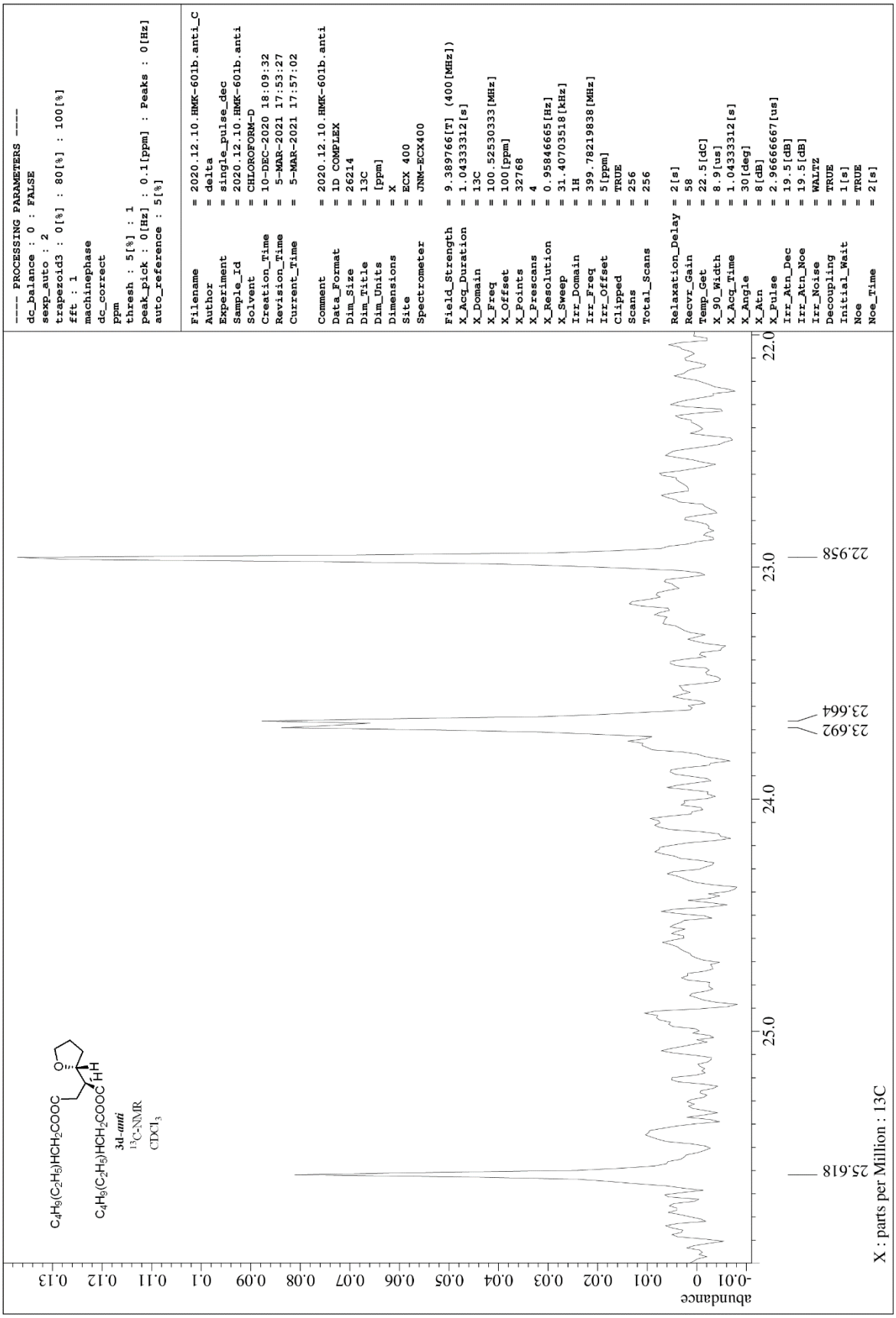

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.10.HMK-601b.anti_P
Author = delta
Experiment = single_pulse_ex2
Sample_Id = 2020.12.10.HMK-601b.anti
Solvent = CHLOROFORM-D
Creation_Time = 10-DEC-2020 17:55:53
Revision_Time = 22-DEC-2020 17:39:41
Current_Time = 5-MAR-2021 17:25:48
Comment = 2020.12.10.HMK-601b.anti
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 38
Temp_Get = 22.3[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 5[dB]
X_Pulse = 5.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
17.65
2.34
1.00
3.09
abundance
X : parts per Million : 1H
$C_4H_9(C_2H_5)HCH_2COOC$
$C_4H_9(C_2H_5)HCH_2COOC$H
3d-*anti*
^{1}H-NMR
$CDCl_3$

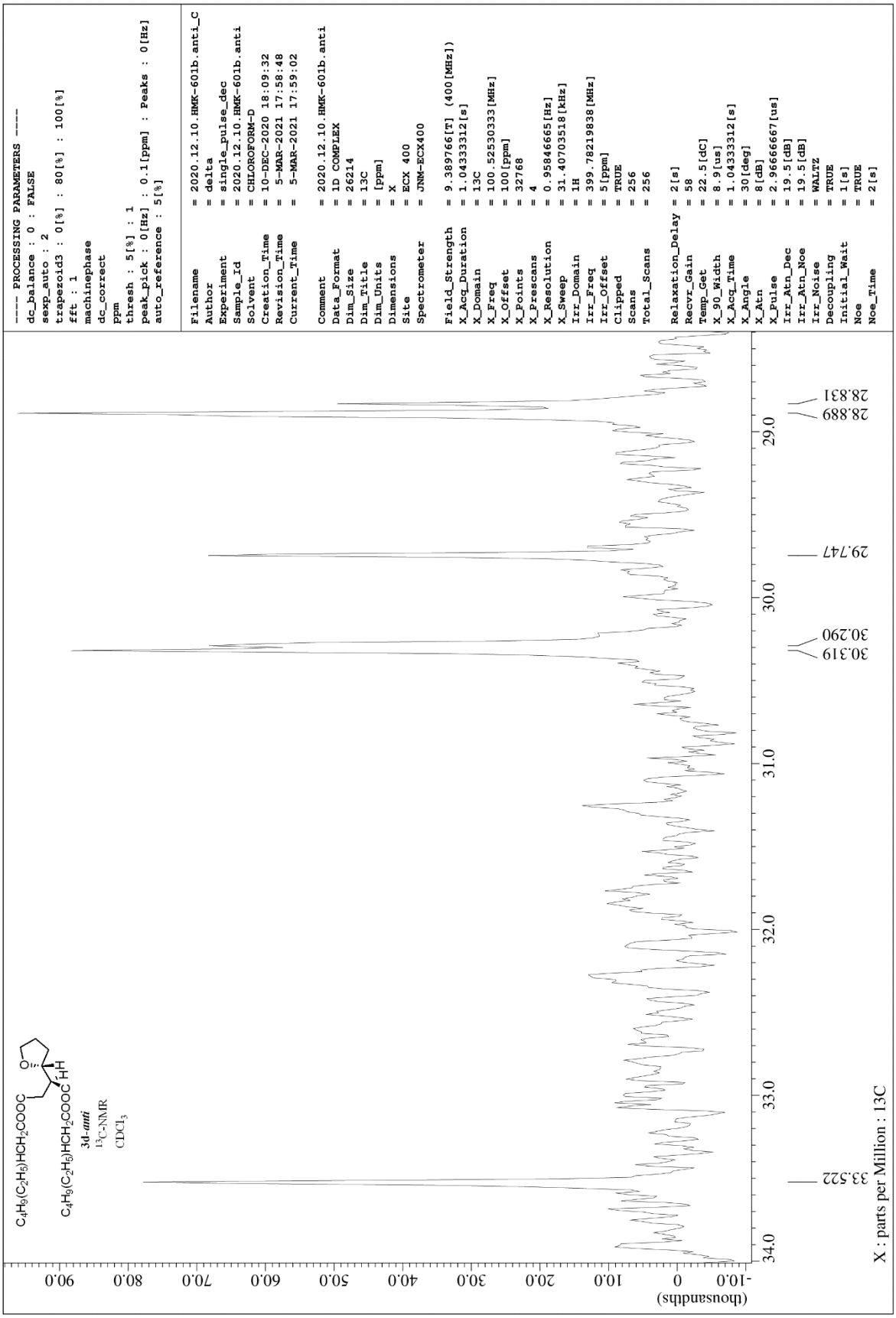

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.10.HMK-601b.anti_P
Author = delta
Experiment = single_pulse_ex2
Sample_Id = 2020.12.10.HMK-601b.anti
Solvent = CHLOROFORM-D
Creation_Time = 10-DEC-2020 17:55:53
Revision_Time = 22-DEC-2020 17:39:41
Current_Time = 5-MAR-2021 17:29:22
Comment = 2020.12.10.HMK-601b.anti
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.50300012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 38
Temp_Get = 22.3[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 5[dB]
X_Pulse = 5.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
C4H9(C2H5)HCH2COOC
C4H9(C2H5)HCH2COOC
3d-anti
1H-NMR
CDCl3
1.01
0.98
1.00
2.924
2.912
2.902
2.890
2.882
2.871
2.819
2.796
2.777
2.754
2.729
2.716
2.686
2.675
abundance
X : parts per Million : 1H

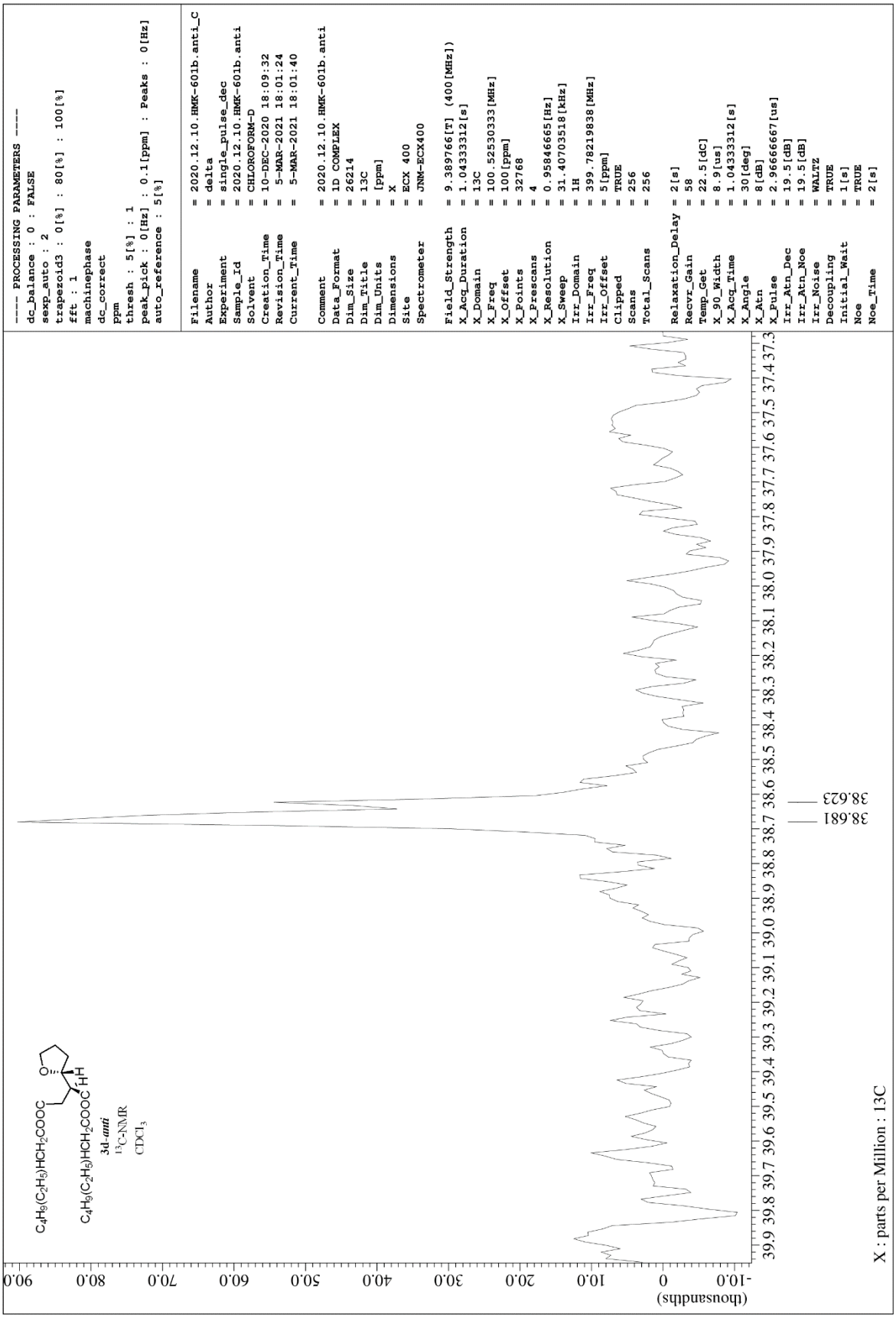

C4H9(C2H5)HCH2COOC
C4H9(C2H5)HCH2COOCH
3d-anti
1H-NMR
CDCl3
5.22
0.97
0.98
4.062
4.048
4.034
4.021
4.007
3.997
3.982
3.968
3.962
3.947
3.936
3.920
3.835
3.818
3.797
3.780
3.749
3.732
3.715
3.694
4.1
4.0
3.9
3.8
3.7
X : parts per Million : 1H
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.10.HMR-601b.anti_P
Author = delta
Experiment = single_pulse_ex2
Sample_Id = 2020.12.10.HMR-601b.anti
Solvent = CHLOROFORM-D
Creation_Time = 10-DEC-2020 17:55:53
Revision_Time = 22-DEC-2020 17:39:41
Current_Time = 5-MAR-2021 17:37:47
Comment = 2020.12.10.HMR-601b.anti
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 38
Temp_Get = 22.3[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 5[dB]
X_Pulse = 5.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]

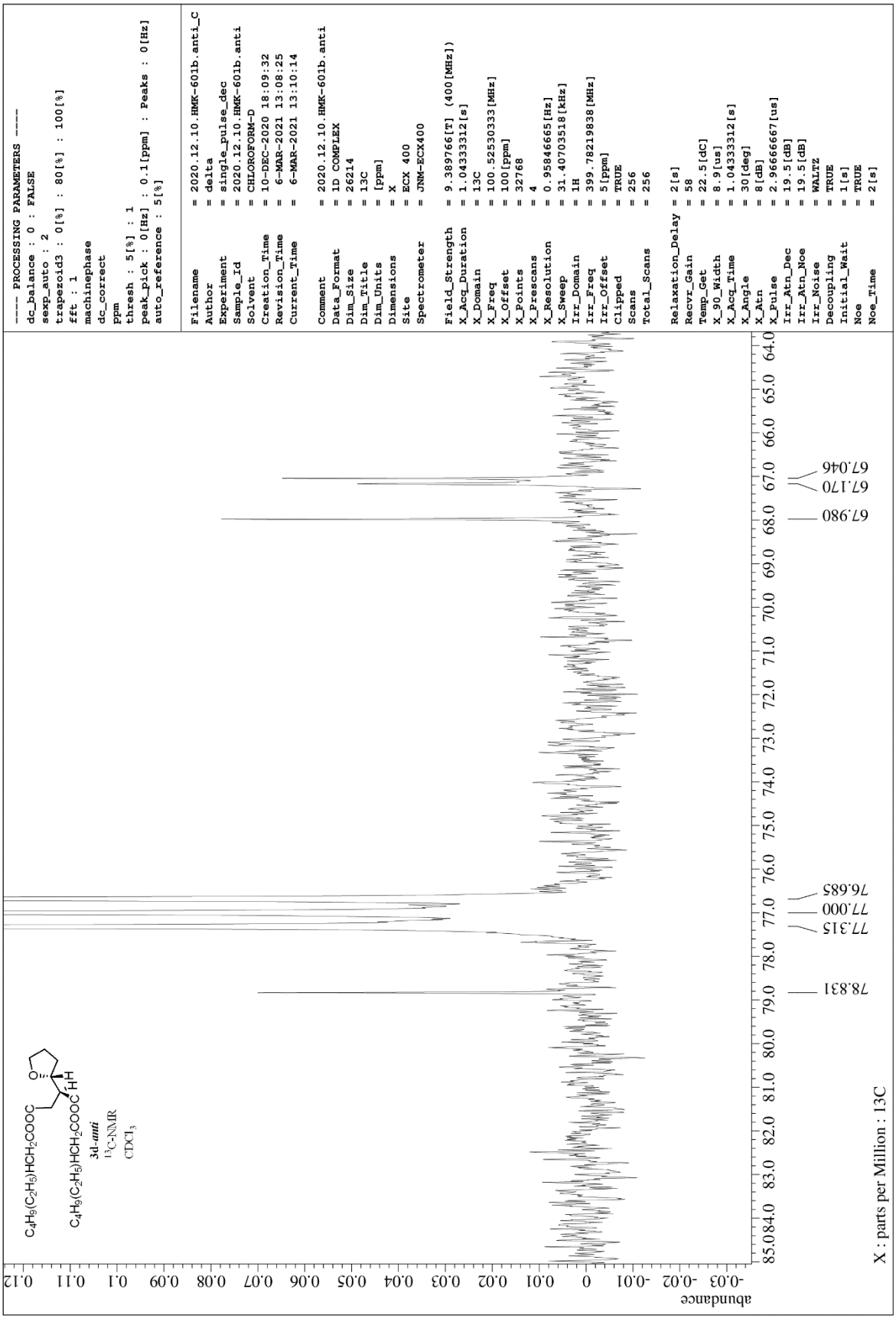

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Peaks : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.10.HMK-601b.anti_C
Author = delta
Experiment = single_pulse_dec
Sample_Id = 2020.12.10.HMK-601b.anti
Solvent = CHLOROFORM-D
Creation_Time = 10-DEC-2020 18:09:32
Revision_Time = 20-JAN-2021 12:47:11
Current_Time = 5-MAR-2021 17:49:51
Comment = 2020.12.10.HMK-601b.anti
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.525303333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 22.5[dC]
X_90_Width = 8.9[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 2.96666667[us]
Irr_Atn_Dec = 19.5[dB]
Irr_Atn_Noe = 19.5[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
C4H9(C2H5)HCH2COOC
C4H9(C2H5)HCH2COOC
H
3d-anti
13C-NMR
CDCl3
abundance
X : parts per Million : 13C
172.956
172.327
87.116
78.831
77.315
77.000
76.685
67.980
67.170
67.046
46.899
38.681
33.522
30.319
29.747
28.889
25.618
23.664
22.958
14.043
10.954
-0.020

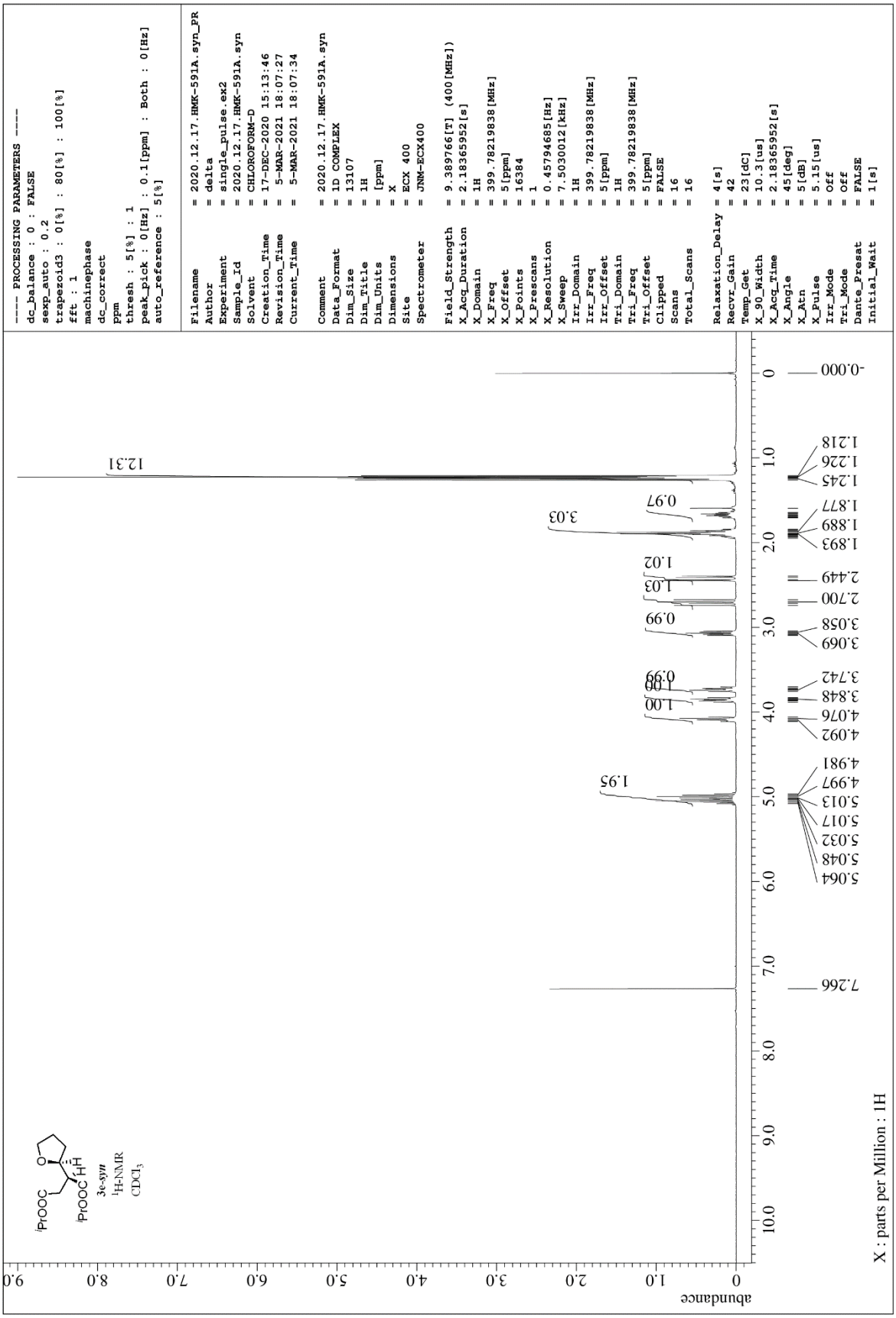

C4H9(C2H5)HCH2COOC
C4H9(C2H5)HCH2COOC
H
3d-anti
13C-NMR
CDCl3
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Peaks : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.10.HMK-601b.anti_C
Author = delta
Experiment = single_pulse_dec
Sample_Id = 2020.12.10.HMK-601b.anti
Solvent = CHLOROFORM-D
Creation_Time = 10-DEC-2020 18:09:32
Revision_Time = 5-MAR-2021 17:53:27
Current_Time = 5-MAR-2021 17:54:34
Comment = 2020.12.10.HMK-601b.anti
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.525303333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 22.5[dC]
X_90_Width = 8.9[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 2.96666667[us]
Irr_Atn_Dec = 19.5[dB]
Irr_Atn_Noe = 19.5[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
abundance
-0.01 0 0.01 0.02 0.03 0.04 0.05 0.06 0.07 0.08 0.09 0.1 0.11 0.12 0.13 0.14 0.15
15.0 14.0 13.0 12.0 11.0 10.0
14.043
10.954
10.916
10.878
X : parts per Million : 13C

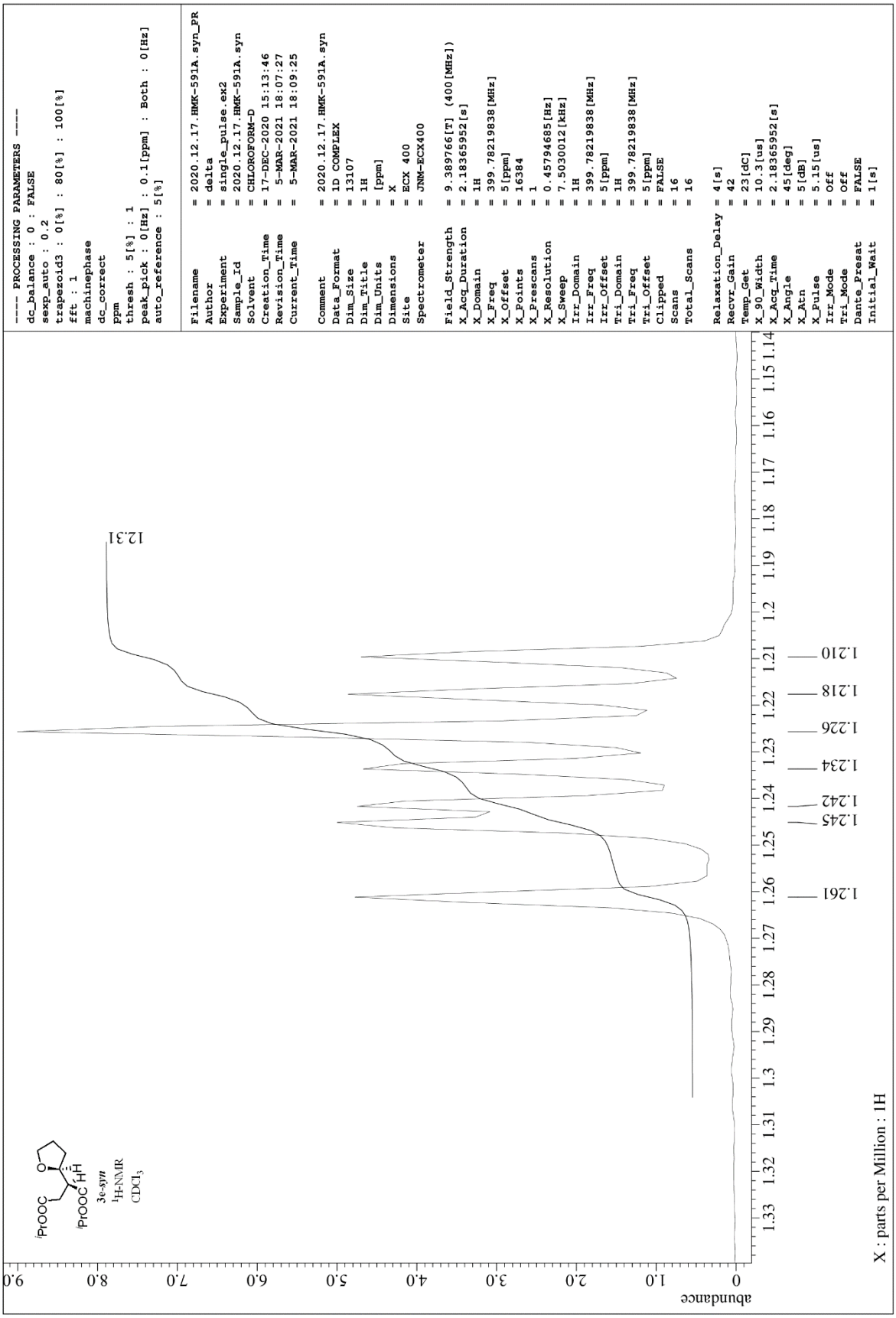

C4H9(C2H5)HCH2COOC
C4H9(C2H5)HCH2COOC
3d-anti
13C-NMR
CDCl3
abundance
0.13
0.12
0.11
0.1
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
-0.01
25.0
24.0
23.0
22.0
25.618
23.692
23.664
22.958
X : parts per Million : 13C
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Peaks : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.10.HMK-601b.anti_C
Author = delta
Experiment = single_pulse_dec
Sample_Id = 2020.12.10.HMK-601b.anti
Solvent = CHLOROFORM-D
Creation_Time = 10-DEC-2020 18:09:32
Revision_Time = 5-MAR-2021 17:53:27
Current_Time = 5-MAR-2021 17:57:02
Comment = 2020.12.10.HMK-601b.anti
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.525303333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 22.5[dC]
X_90_Width = 8.9[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 2.96666667[us]
Irr_Atn_Dec = 19.5[dB]
Irr_Atn_Noe = 19.5[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]

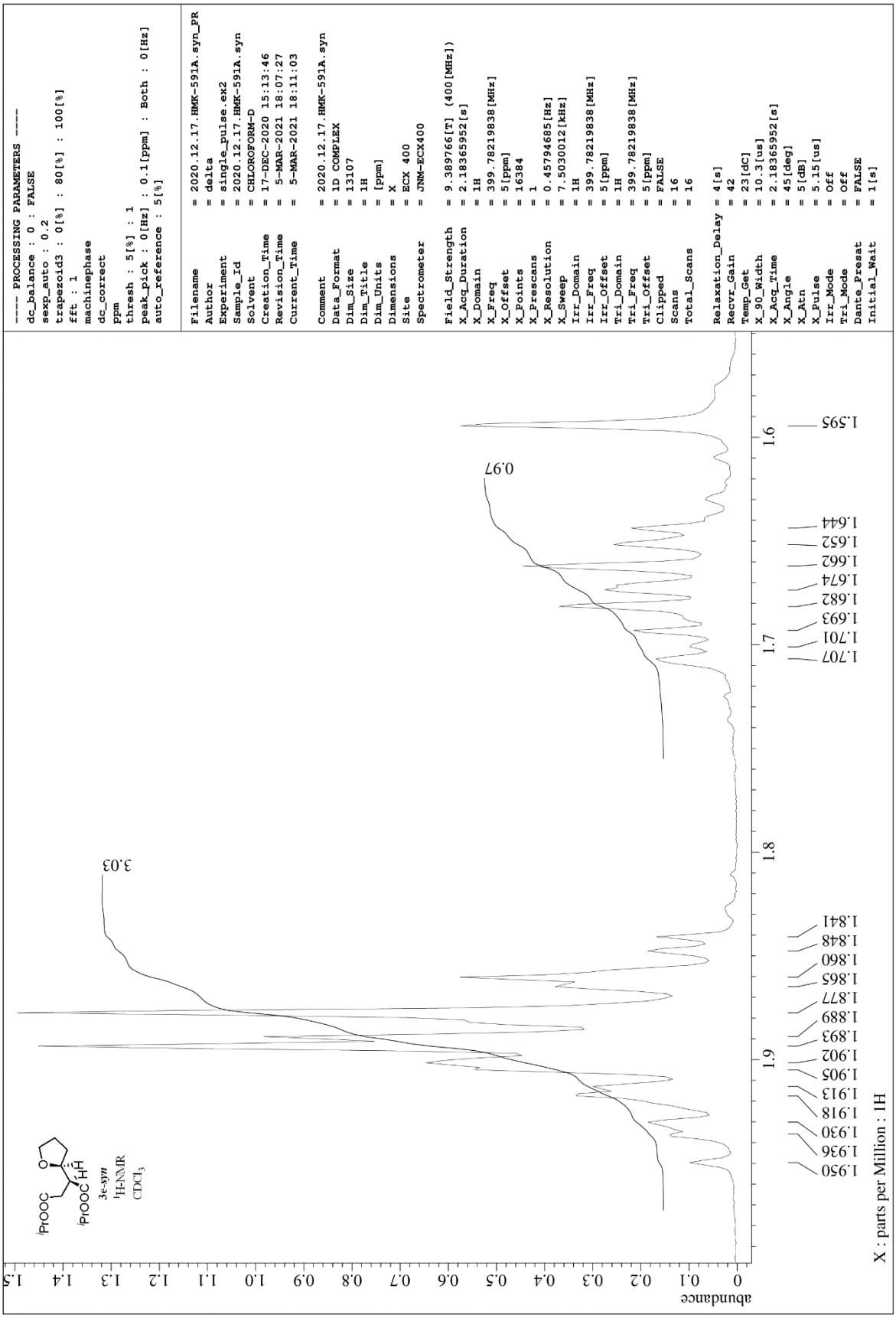

C4H9(C2H5)HCH2COOC
O
H
C4H9(C2H5)HCH2COOC
H
34-anti
13C-NMR
CDCl3
(thousandths)
X : parts per Million : 13C
33.522
30.319
30.290
29.747
28.889
28.831
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Peaks : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.10.HMK-601b.anti_C
Author = delta
Experiment = single_pulse_dec
Sample_Id = 2020.12.10.HMK-601b.anti
Solvent = CHLOROFORM-D
Creation_Time = 10-DEC-2020 18:09:32
Revision_Time = 5-MAR-2021 17:58:48
Current_Time = 5-MAR-2021 17:59:02
Comment = 2020.12.10.HMK-601b.anti
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.525303333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 22.5[dC]
X_90_Width = 8.9[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 2.96666667[us]
Irr_Atn_Dec = 19.5[dB]
Irr_Atn_Noe = 19.5[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]

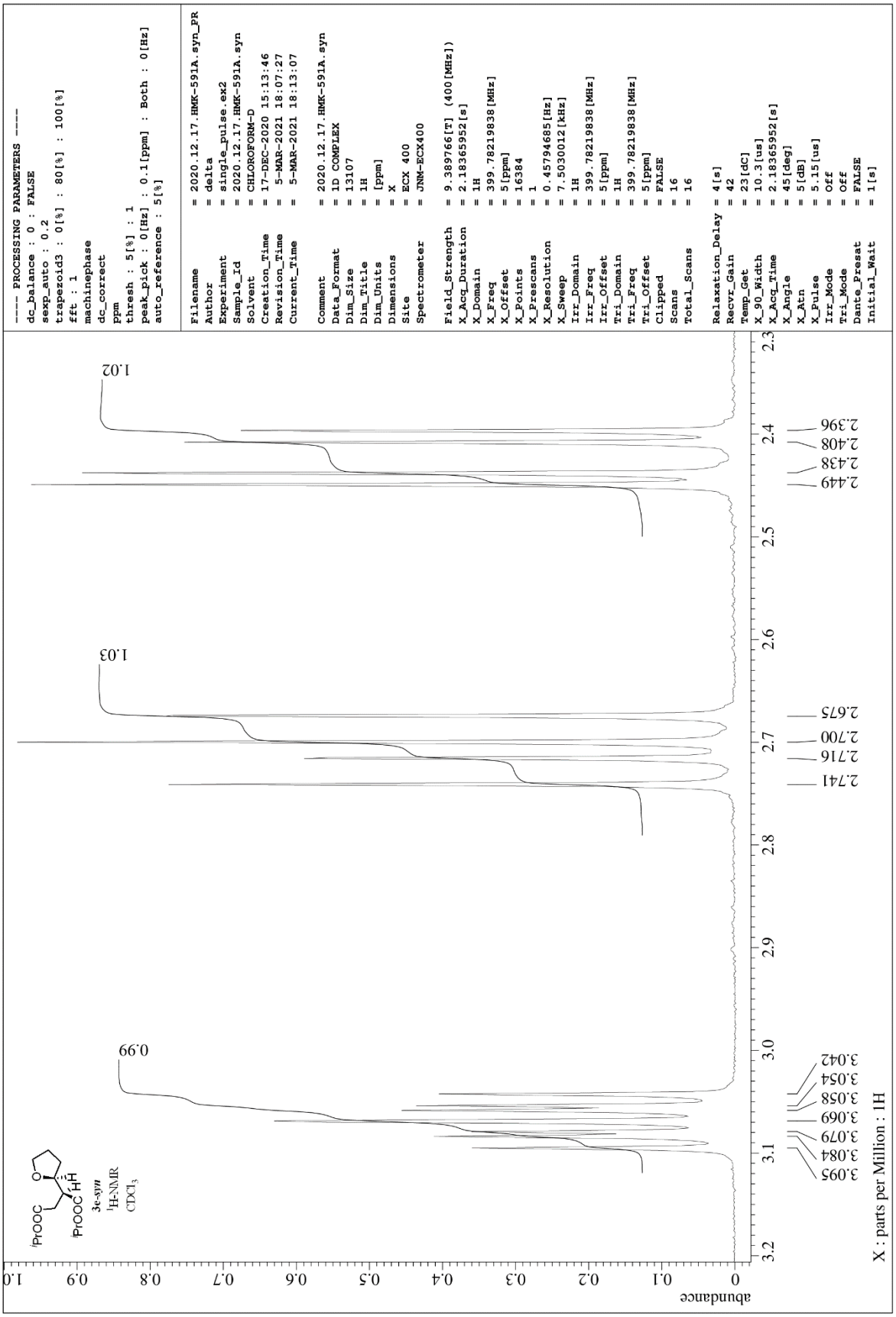

C4H9(C2H5)HCH2COOC
C4H9(C2H5)HCH2COOC
H
3d-anti
13C-NMR
CDCl3
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
(thousandths)
39.9 39.8 39.7 39.6 39.5 39.4 39.3 39.2 39.1 39.0 38.9 38.8 38.7 38.6 38.5 38.4 38.3 38.2 38.1 38.0 37.9 37.8 37.7 37.6 37.5 37.4 37.3
X : parts per Million : 13C
38.681
38.623
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Peaks : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.10.HMK-601b.anti_C
Author = delta
Experiment = single_pulse_dec
Sample_Id = 2020.12.10.HMK-601b.anti
Solvent = CHLOROFORM-D
Creation_Time = 10-DEC-2020 18:09:32
Revision_Time = 5-MAR-2021 18:01:24
Current_Time = 5-MAR-2021 18:01:40
Comment = 2020.12.10.HMK-601b.anti
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.525303333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 22.5[dC]
X_90_Width = 8.9[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 2.96666667[us]
Irr_Atn_Dec = 19.5[dB]
Irr_Atn_Noe = 19.5[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]

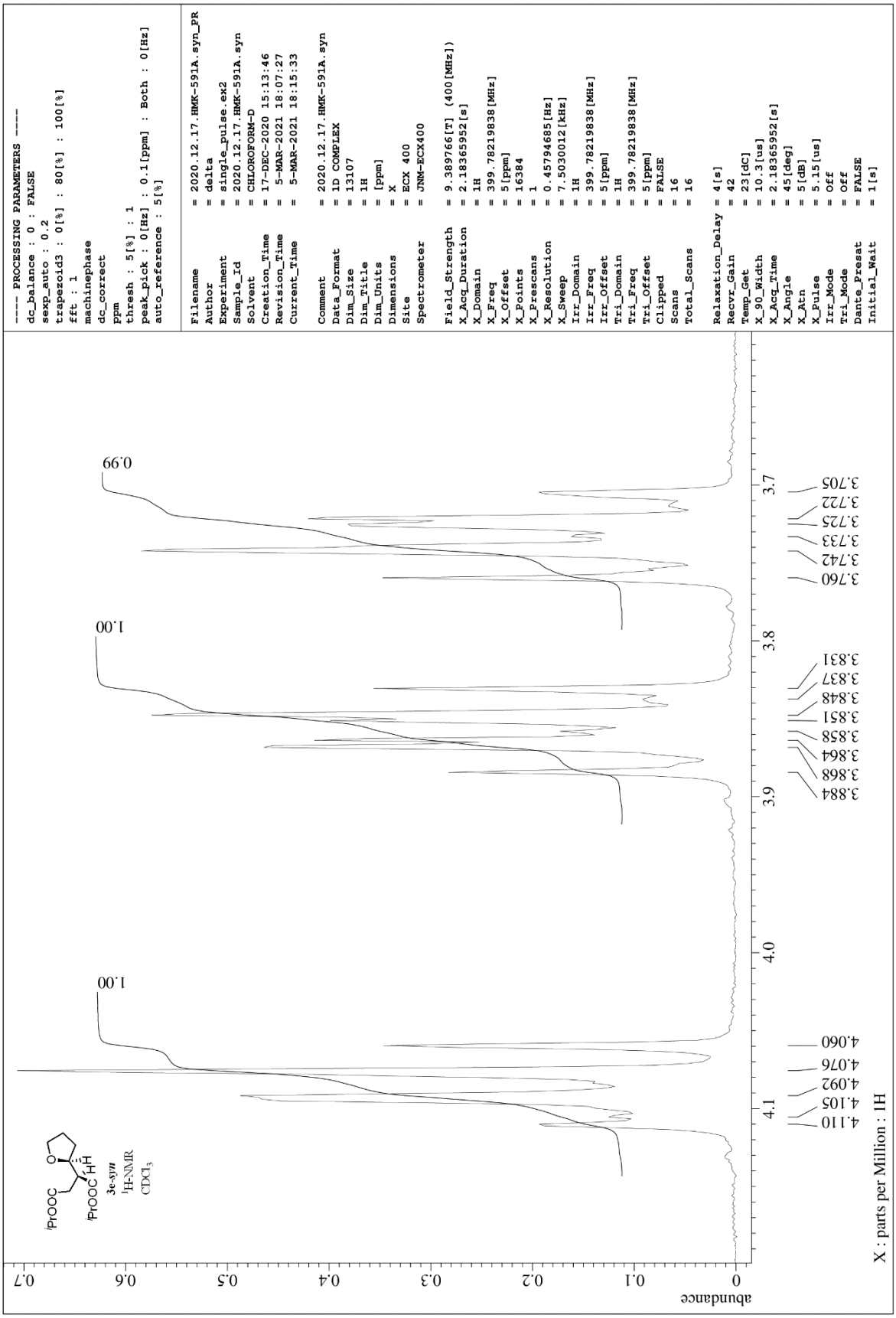

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Peaks : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.10.HMK-601b.anti_C
Author = delta
Experiment = single_pulse_dec
Sample_Id = 2020.12.10.HMK-601b.anti
Solvent = CHLOROFORM-D
Creation_Time = 10-DEC-2020 18:09:32
Revision_Time = 6-MAR-2021 13:08:25
Current_Time = 6-MAR-2021 13:10:14
Comment = 2020.12.10.HMK-601b.anti
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.525303333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 22.5[dC]
X_90_Width = 8.9[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 2.96666667[us]
Irr_Atn_Dec = 19.5[dB]
Irr_Atn_Noe = 19.5[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
C4H9(C2H5)HCH2COOC
C4H9(C2H5)HCH2COOC
3d-anti
13C-NMR
CDCl3
67.046
67.170
67.980
76.685
77.000
77.315
78.831
abundance
X : parts per Million : 13C

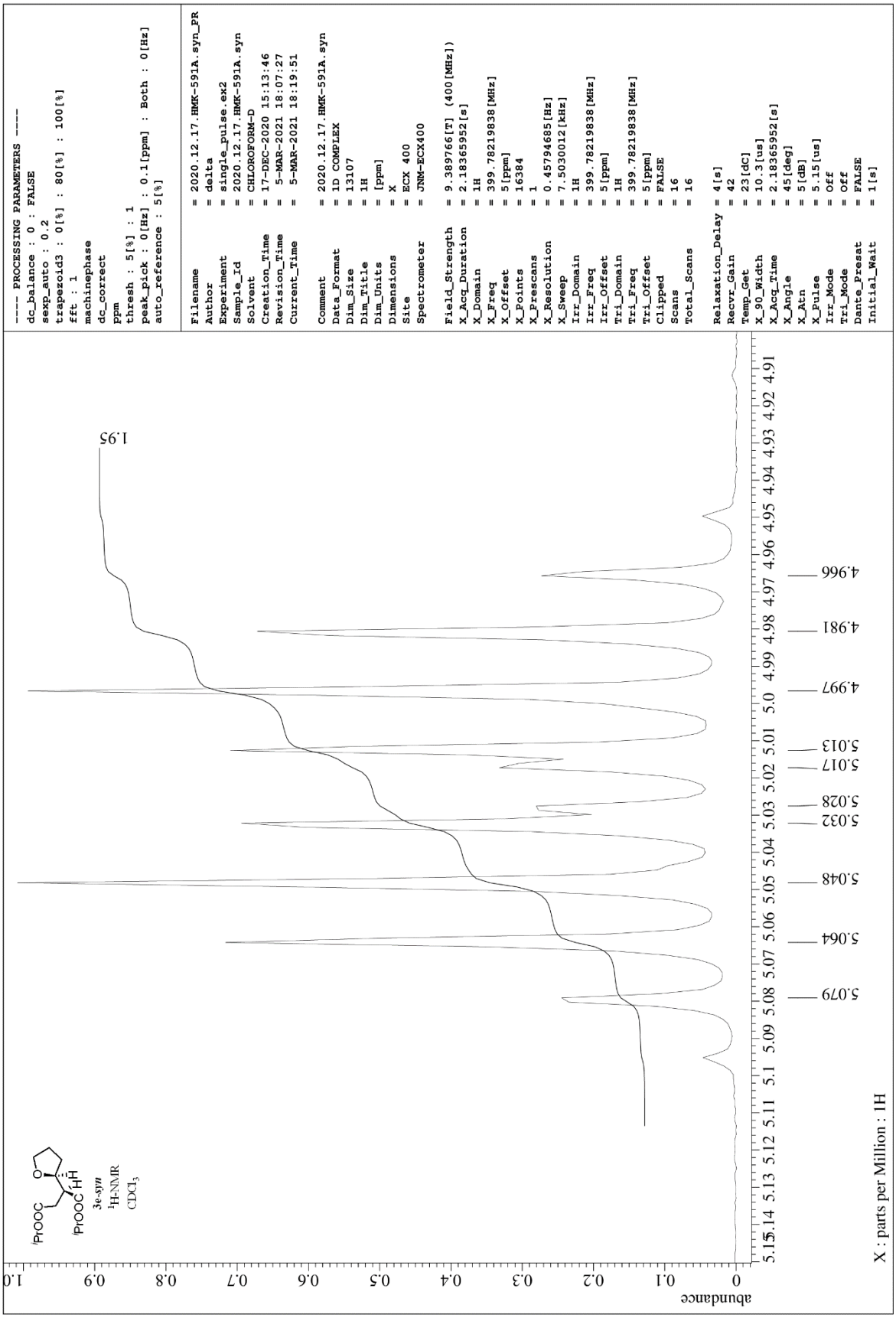

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.17.HMK-591A.syn_PR
Author = delta
Experiment = single_pulse_ex2
Sample_Id = 2020.12.17.HMK-591A.syn
Solvent = CHLOROFORM-D
Creation_Time = 17-DEC-2020 15:13:46
Revision_Time = 5-MAR-2021 18:07:27
Current_Time = 5-MAR-2021 18:07:34
Comment = 2020.12.17.HMK-591A.syn
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 42
Temp_Get = 23[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 5[dB]
X_Pulse = 5.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
iPrOOC
iPrOOC H
3e-syn
1H-NMR
CDCl3
abundance
X : parts per Million : 1H
12.31
3.03
1.95
1.00
1.00
0.99
0.99
1.02
1.03
0.97
7.266
5.064
5.048
5.032
5.017
5.013
4.997
4.981
4.092
4.076
3.848
3.742
3.069
3.058
2.700
2.449
1.893
1.889
1.877
1.245
1.226
1.218
-0.000

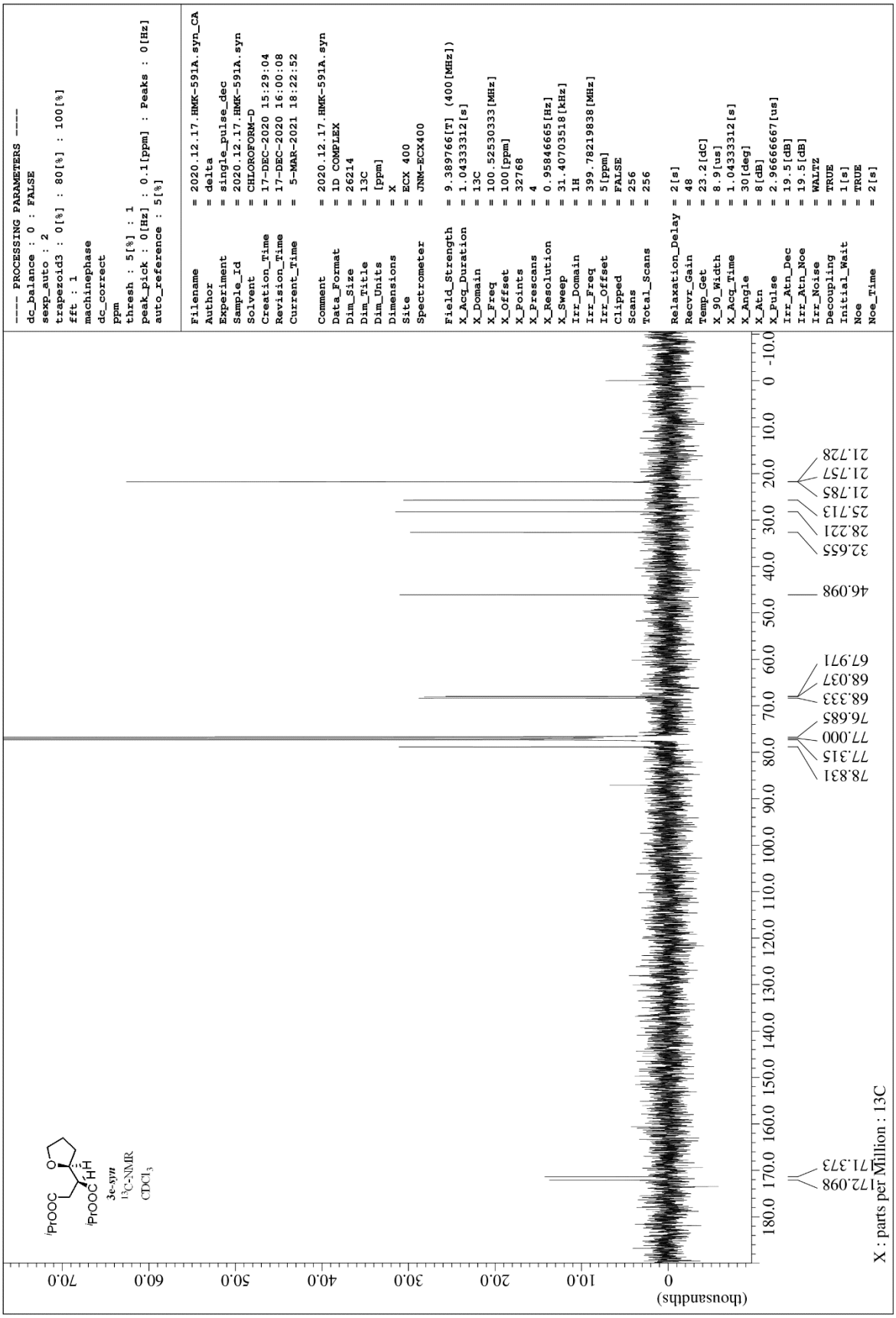

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.17.HMK-591A.syn_PR
Author = delta
Experiment = single_pulse_ex2
Sample_Id = 2020.12.17.HMK-591A.syn
Solvent = CHLOROFORM-D
Creation_Time = 17-DEC-2020 15:13:46
Revision_Time = 5-MAR-2021 18:07:27
Current_Time = 5-MAR-2021 18:09:25
Comment = 2020.12.17.HMK-591A.syn
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 42
Temp_Get = 23[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 5[dB]
X_Pulse = 5.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
12.31
1.261
1.245
1.242
1.234
1.226
1.218
1.210
abundance
X : parts per Million : 1H
3e-syn
^{1}H-NMR
$CDCl_3$

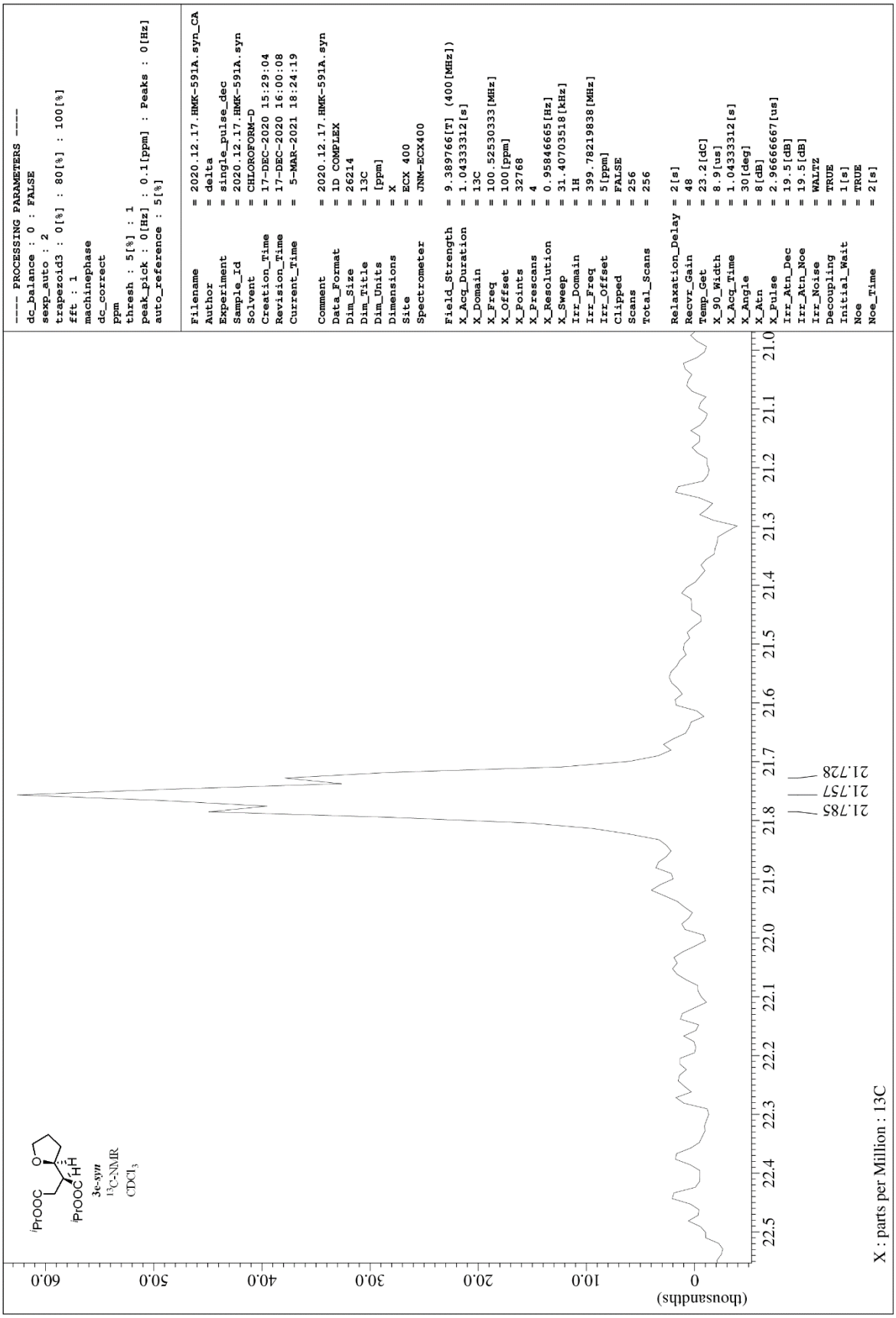

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.17.HMK-591A.syn_PR
Author = delta
Experiment = single_pulse_ex2
Sample_Id = 2020.12.17.HMK-591A.syn
Solvent = CHLOROFORM-D
Creation_Time = 17-DEC-2020 15:13:46
Revision_Time = 5-MAR-2021 18:07:27
Current_Time = 5-MAR-2021 18:11:03
Comment = 2020.12.17.HMK-591A.syn
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 42
Temp_Get = 23[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 5[dB]
X_Pulse = 5.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
abundance
X : parts per Million : 1H
3.03
0.97
1.950
1.936
1.930
1.918
1.913
1.905
1.902
1.893
1.889
1.877
1.865
1.860
1.848
1.841
1.707
1.701
1.693
1.682
1.674
1.662
1.652
1.644
1.595
iPrOOC
iPrOOC
3e-syn
^{1}H-NMR
$CDCl_3$

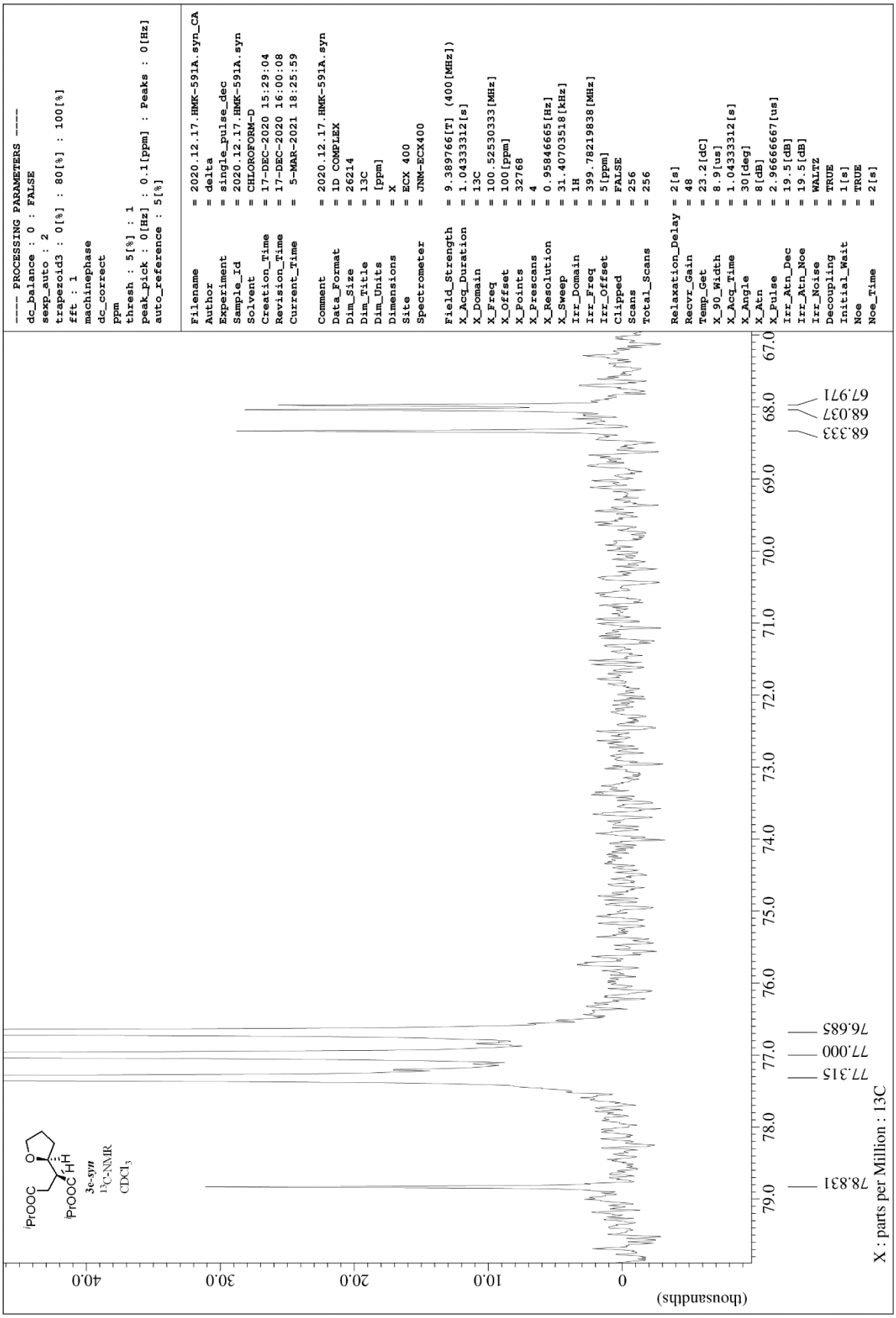

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.17.HMK-591A.syn_PR
Author = delta
Experiment = single_pulse_ex2
Sample_Id = 2020.12.17.HMK-591A.syn
Solvent = CHLOROFORM-D
Creation_Time = 17-DEC-2020 15:13:46
Revision_Time = 5-MAR-2021 18:07:27
Current_Time = 5-MAR-2021 18:13:07
Comment = 2020.12.17.HMK-591A.syn
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 42
Temp_Get = 23[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 5[dB]
X_Pulse = 5.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
iPrOOC
iPrOOC
3e-syn
1H-NMR
CDCl3
0.99
1.03
1.02
abundance
X : parts per Million : 1H
3.095
3.084
3.079
3.069
3.058
3.054
3.042
2.741
2.716
2.700
2.675
2.449
2.438
2.408
2.396

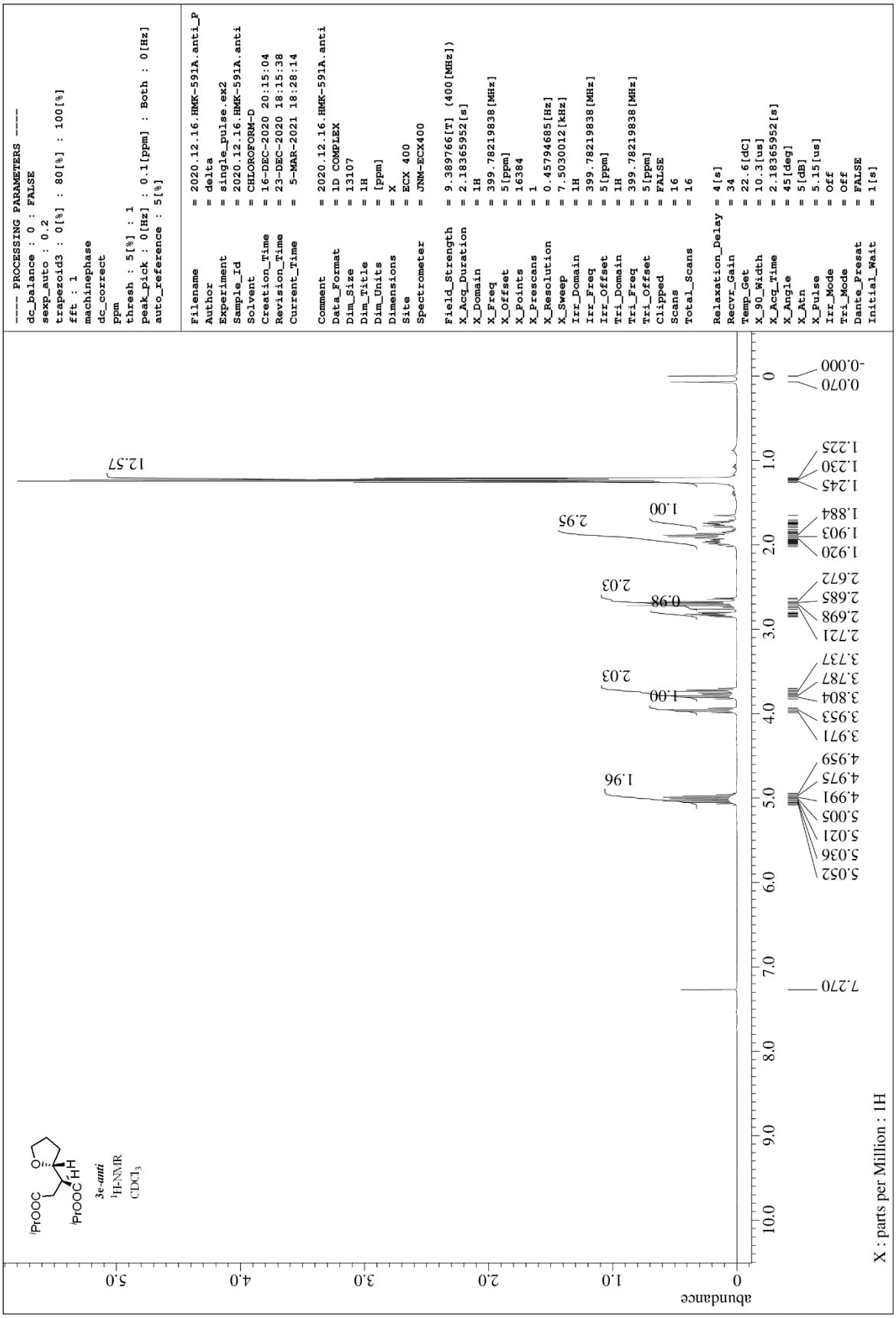

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.17.HMK-591A.syn_PR
Author = delta
Experiment = single_pulse_ex2
Sample_Id = 2020.12.17.HMK-591A.syn
Solvent = CHLOROFORM-D
Creation_Time = 17-DEC-2020 15:13:46
Revision_Time = 5-MAR-2021 18:07:27
Current_Time = 5-MAR-2021 18:15:33
Comment = 2020.12.17.HMK-591A.syn
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 42
Temp_Get = 23[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 5[dB]
X_Pulse = 5.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
iPrOOC
iPrOOC
3e-syn
1H-NMR
CDCl3
0.99
1.00
1.00
4.110
4.105
4.092
4.076
4.060
3.884
3.868
3.864
3.858
3.851
3.848
3.837
3.831
3.760
3.742
3.733
3.725
3.722
3.705
abundance
X : parts per Million : 1H

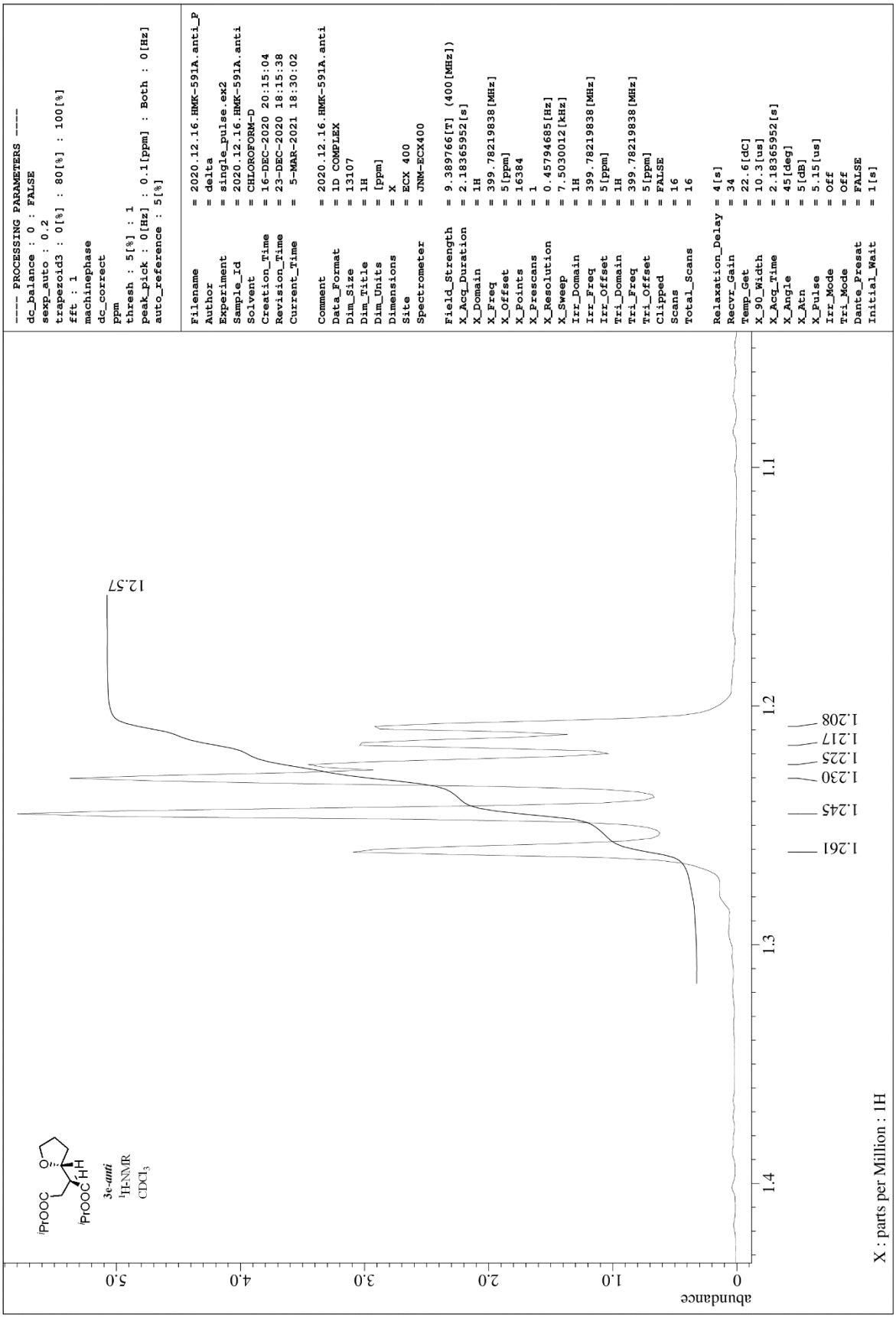

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
exp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.17.HMK-591A.syn_PR
Author = delta
Experiment = single_pulse.ex2
Sample_id = 2020.12.17.HMK-591A.syn
Solvent = CHLOROFORM-D
Creation_Time = 17-DEC-2020 15:13:46
Revision_Time = 5-MAR-2021 18:07:27
Current_Time = 5-MAR-2021 18:19:51
Comment = 2020.12.17.HMK-591A.syn
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.50300012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 42
Temp_Get = 23[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 5[dB]
X_Pulse = 5.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
1.95
4.966
4.981
4.997
5.013
5.017
5.028
5.032
5.048
5.064
5.079
abundance
X : parts per Million : 1H
3e-syn
^{1}H-NMR
$CDCl_3$

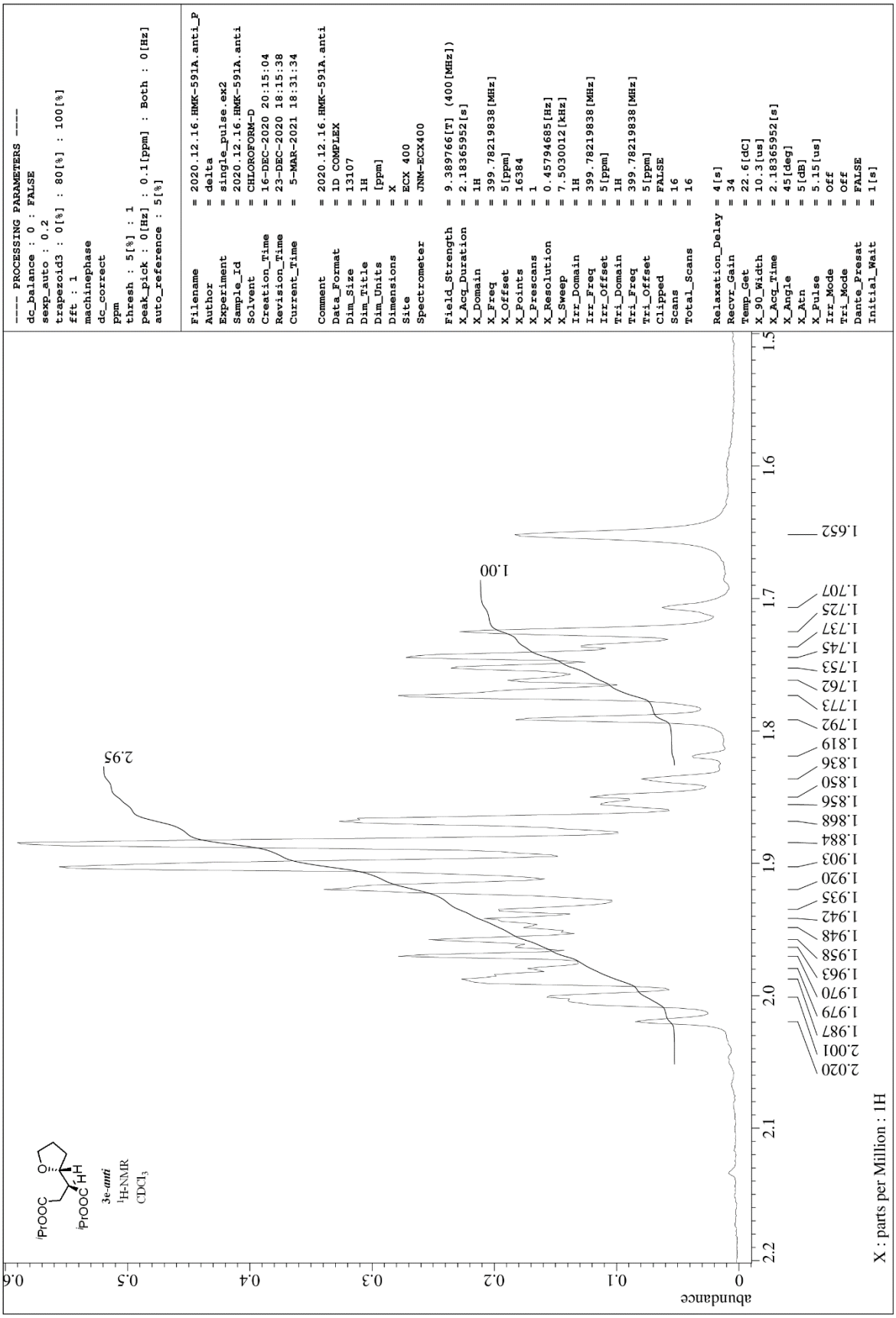

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Peaks : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.17.HMK-591A.syn_CA
Author = delta
Experiment = single_pulse_dec
Sample_Id = 2020.12.17.HMK-591A.syn
Solvent = CHLOROFORM-D
Creation_Time = 17-DEC-2020 15:29:04
Revision_Time = 17-DEC-2020 16:00:08
Current_Time = 5-MAR-2021 18:22:52
Comment = 2020.12.17.HMK-591A.syn
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.525303333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 48
Temp_Get = 23.2[dC]
X_90_Width = 8.9[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 2.96666667[us]
Irr_Atn_Dec = 19.5[dB]
Irr_Atn_Noe = 19.5[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
iPrOOC
iPrOOC
3e-syn
13C-NMR
CDCl3
(thousandths)
X : parts per Million : 13C
172.098
171.373
78.831
77.315
77.000
76.685
68.333
68.037
67.971
46.098
32.655
28.221
25.713
21.785
21.757
21.728

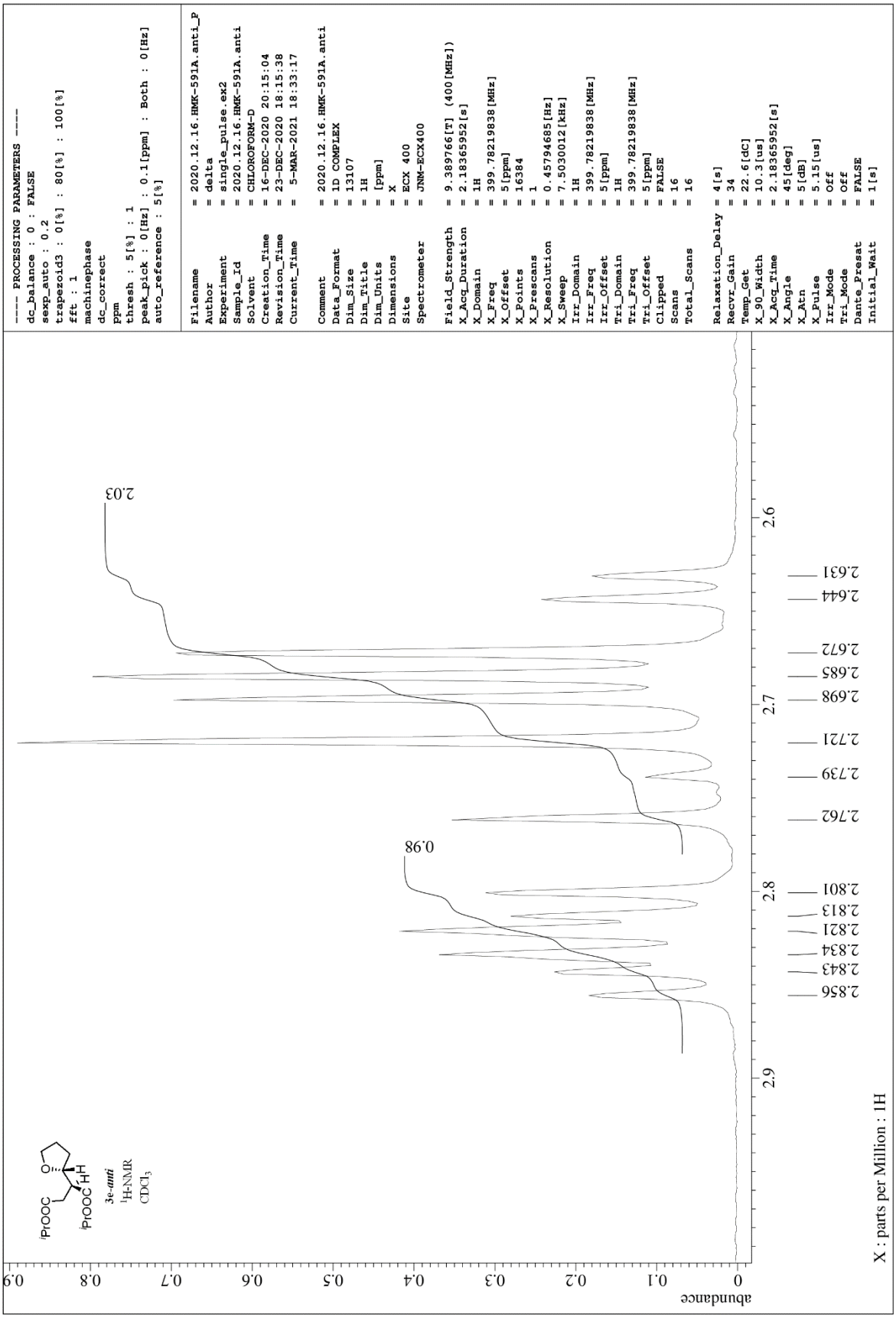

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Peaks : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.17.HMK-591A.syn_CA
Author = delta
Experiment = single_pulse_dec
Sample_Id = 2020.12.17.HMK-591A.syn
Solvent = CHLOROFORM-D
Creation_Time = 17-DEC-2020 15:29:04
Revision_Time = 17-DEC-2020 16:00:08
Current_Time = 5-MAR-2021 18:24:19
Comment = 2020.12.17.HMK-591A.syn
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.525303333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 48
Temp_Get = 23.2[dC]
X_90_Width = 8.9[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 2.96666667[us]
Irr_Atn_Dec = 19.5[dB]
Irr_Atn_Noe = 19.5[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
iPrOOC
iPrOOC
3e-syn
13C-NMR
CDCl3
(thousandths)
60.0
50.0
40.0
30.0
20.0
10.0
0
22.5
22.4
22.3
22.2
22.1
22.0
21.9
21.8
21.7
21.6
21.5
21.4
21.3
21.2
21.1
21.0
21.785
21.757
21.728
X : parts per Million : 13C

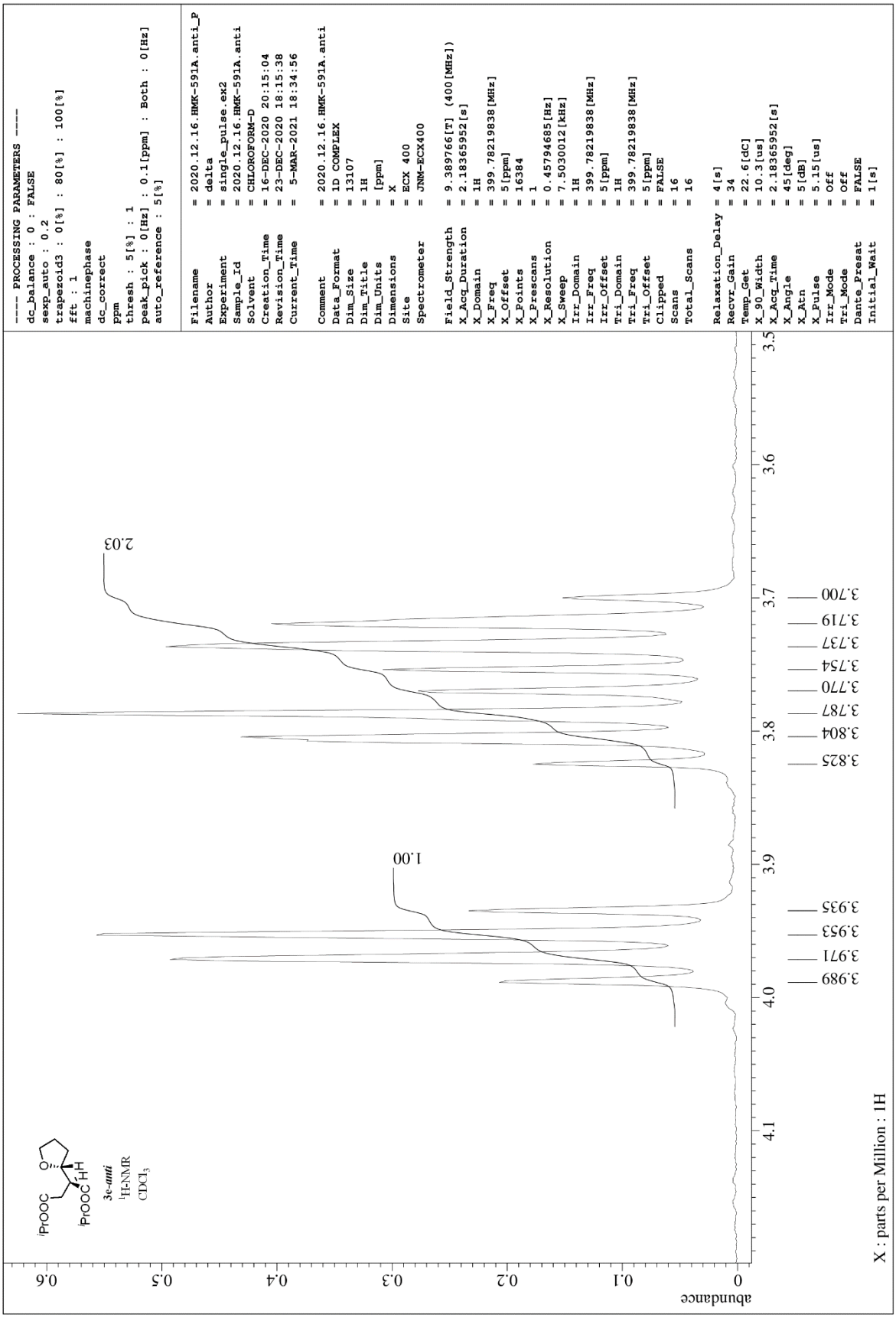

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Peaks : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.17.HMK-591A.syn_CA
Author = delta
Experiment = single_pulse_dec
Sample_Id = 2020.12.17.HMK-591A.syn
Solvent = CHLOROFORM-D
Creation_Time = 17-DEC-2020 15:29:04
Revision_Time = 17-DEC-2020 16:00:08
Current_Time = 5-MAR-2021 18:25:59
Comment = 2020.12.17.HMK-591A.syn
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.525303333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 48
Temp_Get = 23.2[dC]
X_90_Width = 8.9[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 2.96666667[us]
Irr_Atn_Dec = 19.5[dB]
Irr_Atn_Noe = 19.5[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
iPrOOC
iPrOOC H
3e-syn
13C-NMR
CDCl3
(thousandths)
40.0
30.0
20.0
10.0
0
X : parts per Million : 13C
79.0
78.0
77.0
76.0
75.0
74.0
73.0
72.0
71.0
70.0
69.0
68.0
67.0
78.831
77.315
77.000
76.685
68.333
68.037
67.971

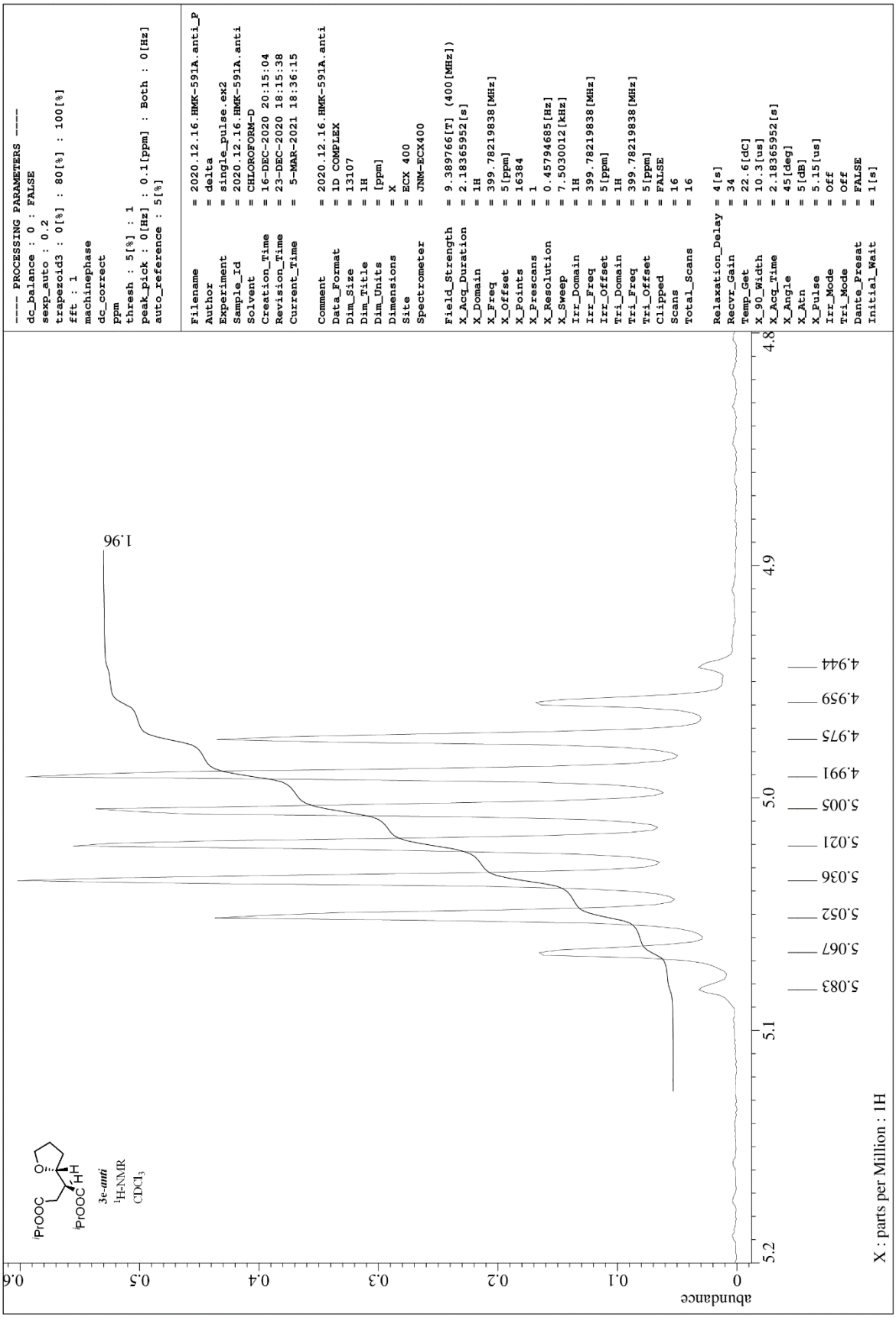

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.16.HMK-591A.anti_P
Author = delta
Experiment = single_pulse_ex2
Sample_Id = 2020.12.16.HMK-591A.anti
Solvent = CHLOROFORM-D
Creation_Time = 16-DEC-2020 20:15:04
Revision_Time = 23-DEC-2020 18:15:38
Current_Time = 5-MAR-2021 18:28:14
Comment = 2020.12.16.HMK-591A.anti
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 34
Temp_Get = 22.6[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 5[dB]
X_Pulse = 5.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
iPrOOC
iPrOOC H
3e-anti
1H-NMR
CDCl3
12.57
2.95
2.03
2.03
1.96
1.00
1.00
0.98
7.270
5.052
5.036
5.021
5.005
4.991
4.975
4.959
3.971
3.953
3.804
3.787
3.737
2.721
2.698
2.685
2.672
1.920
1.903
1.884
1.245
1.230
1.225
0.070
-0.000
abundance
X : parts per Million : 1H

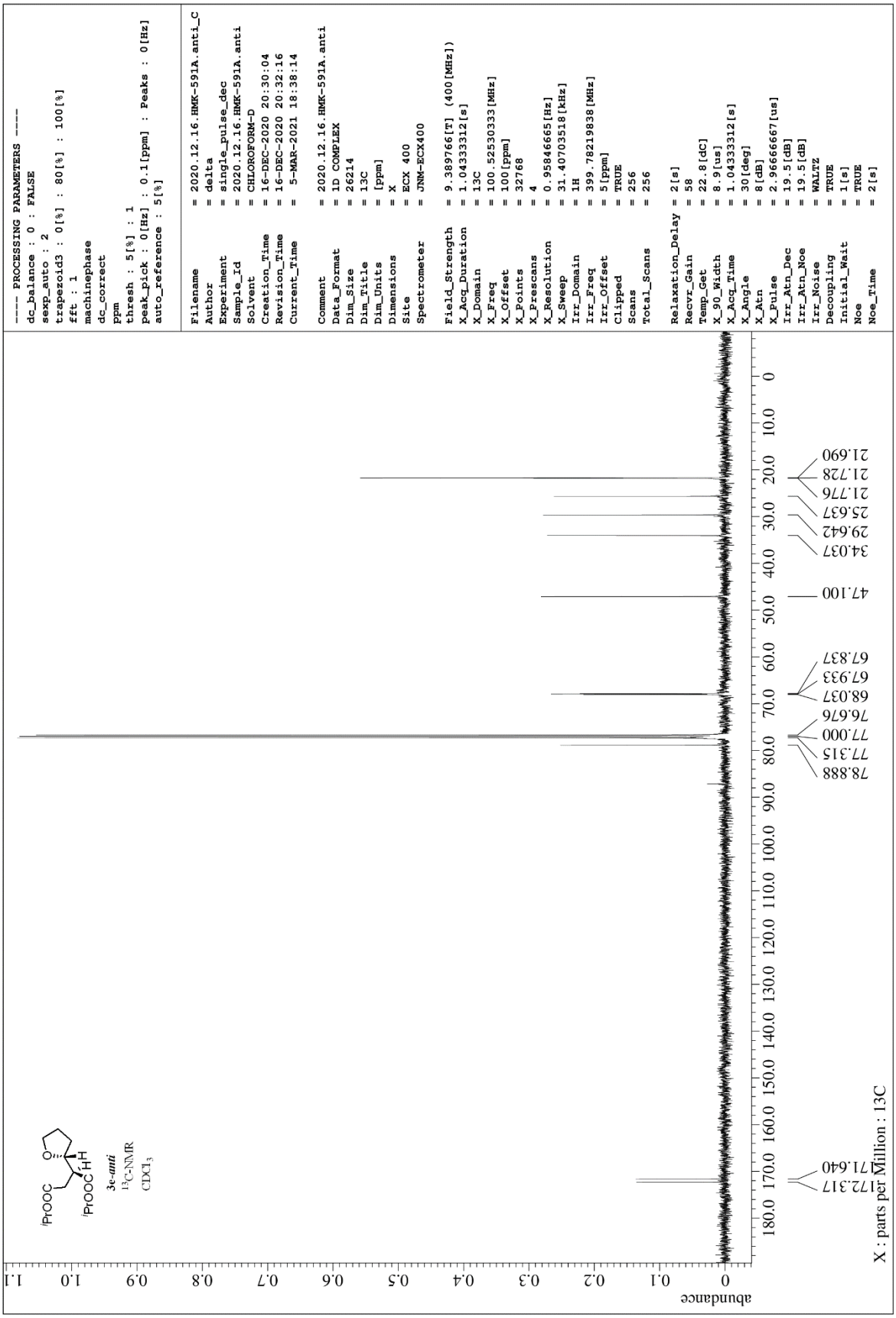

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.16.HMK-591A.anti_P
Author = delta
Experiment = single_pulse_ex2
Sample_Id = 2020.12.16.HMK-591A.anti
Solvent = CHLOROFORM-D
Creation_Time = 16-DEC-2020 20:15:04
Revision_Time = 23-DEC-2020 18:15:38
Current_Time = 5-MAR-2021 18:30:02
Comment = 2020.12.16.HMK-591A.anti
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 34
Temp_Get = 22.6[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 5[dB]
X_Pulse = 5.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
iPrOOC
iPrOOC
3e-anti
1H-NMR
CDCl3
12.57
1.208
1.217
1.225
1.230
1.245
1.261
abundance
X : parts per Million : 1H

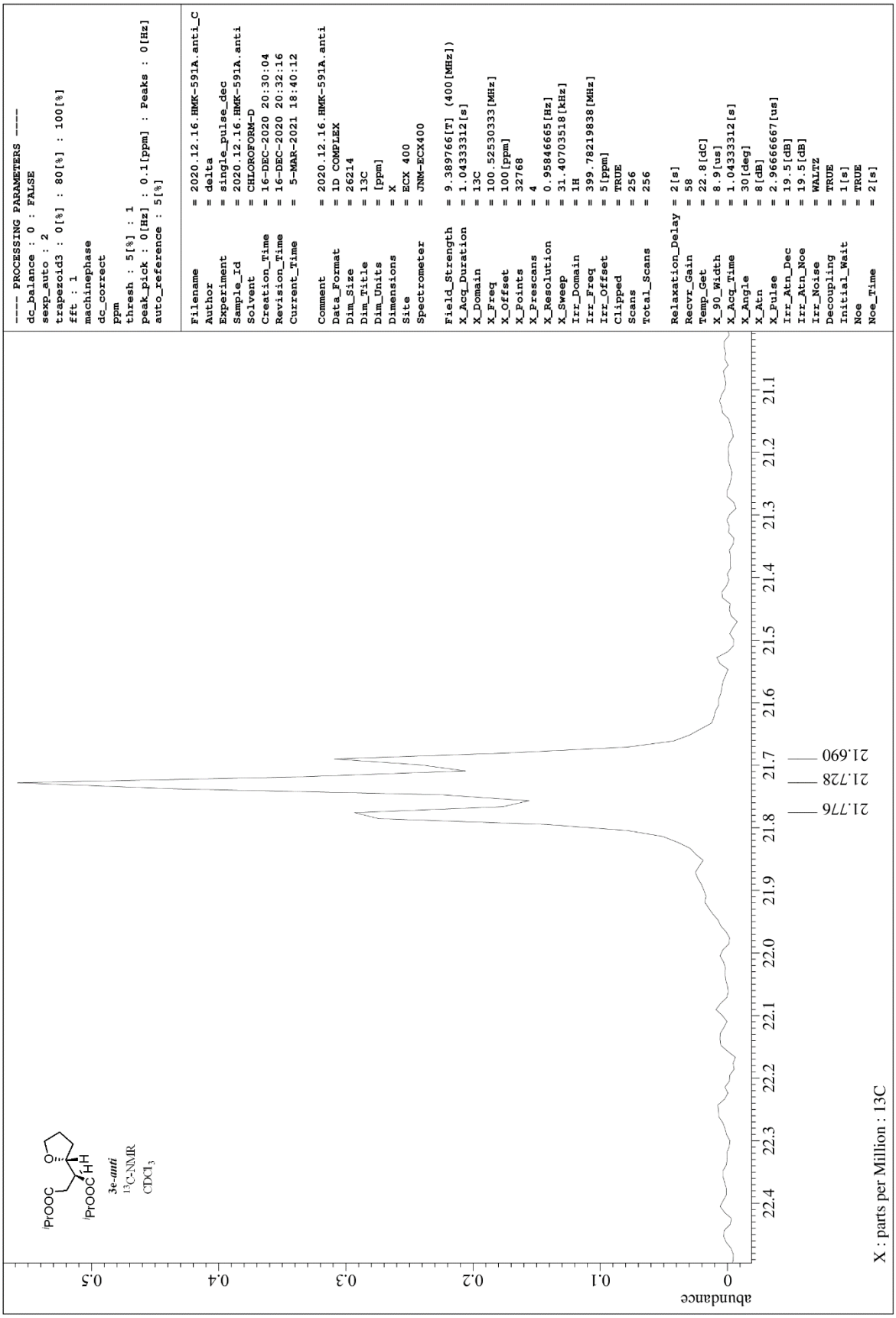

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.16.HMK-591A.anti_P
Author = delta
Experiment = single_pulse_ex2
Sample_Id = 2020.12.16.HMK-591A.anti
Solvent = CHLOROFORM-D
Creation_Time = 16-DEC-2020 20:15:04
Revision_Time = 23-DEC-2020 18:15:38
Current_Time = 5-MAR-2021 18:31:34
Comment = 2020.12.16.HMK-591A.anti
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 34
Temp_Get = 22.6[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 5[dB]
X_Pulse = 5.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
iPrOOC
iPrOOC
H
3e-anti
1H-NMR
CDCl3
abundance
X : parts per Million : 1H
2.95
1.00
1.652
1.707
1.725
1.737
1.745
1.753
1.762
1.773
1.792
1.819
1.836
1.850
1.856
1.868
1.884
1.903
1.920
1.935
1.942
1.948
1.958
1.963
1.970
1.979
1.987
2.001
2.020

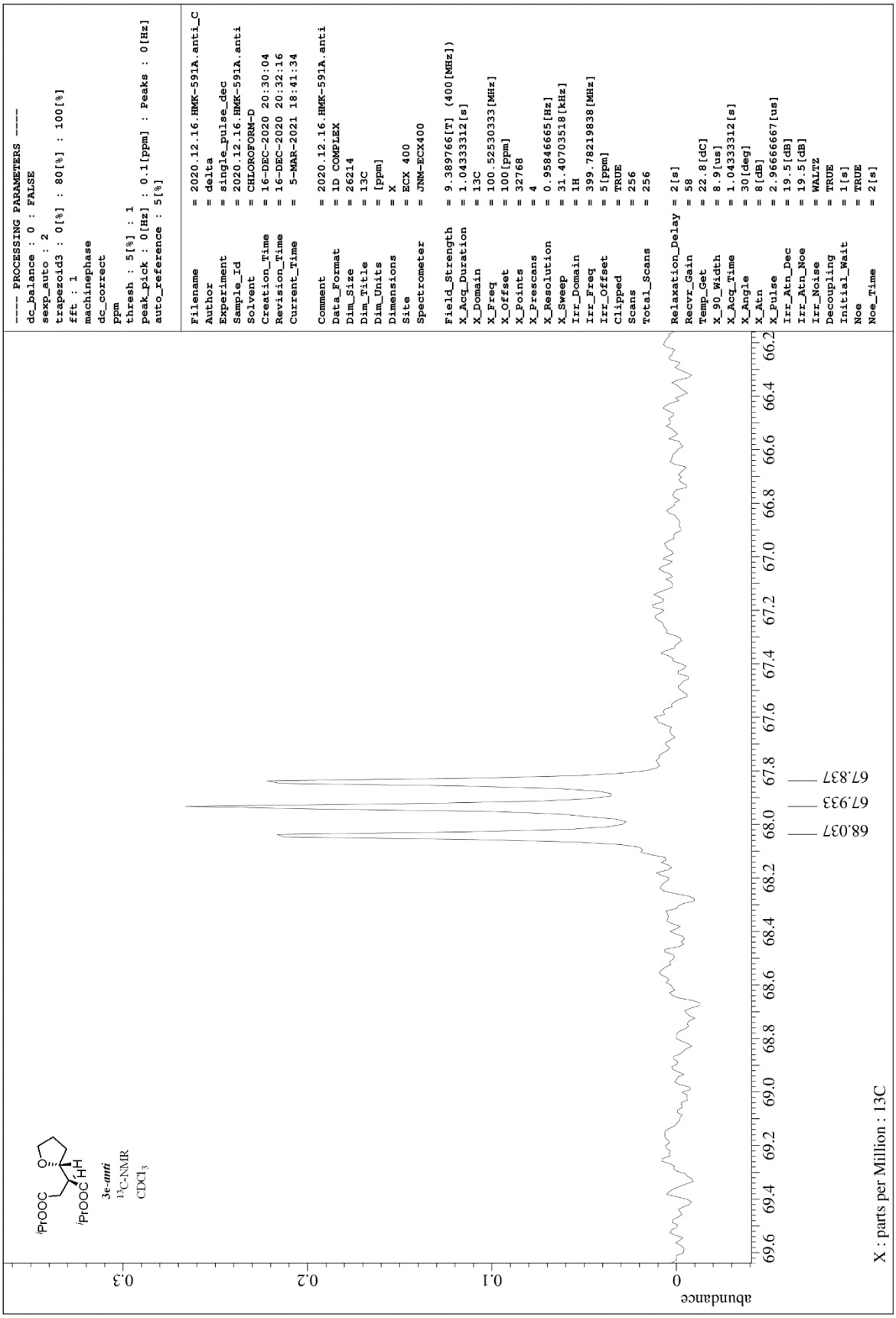

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.16.HMK-591A.anti_P
Author = delta
Experiment = single_pulse_ex2
Sample_Id = 2020.12.16.HMK-591A.anti
Solvent = CHLOROFORM-D
Creation_Time = 16-DEC-2020 20:15:04
Revision_Time = 23-DEC-2020 18:15:38
Current_Time = 5-MAR-2021 18:33:17
Comment = 2020.12.16.HMK-591A.anti
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 34
Temp_Get = 22.6[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 5[dB]
X_Pulse = 5.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
iPrOOC
iPrOOC
H
H
3e-anti
1H-NMR
CDCl3
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
2.03
0.98
2.9
2.8
2.7
2.6
2.856
2.843
2.834
2.821
2.813
2.801
2.762
2.739
2.721
2.698
2.685
2.672
2.644
2.631
X : parts per Million : 1H

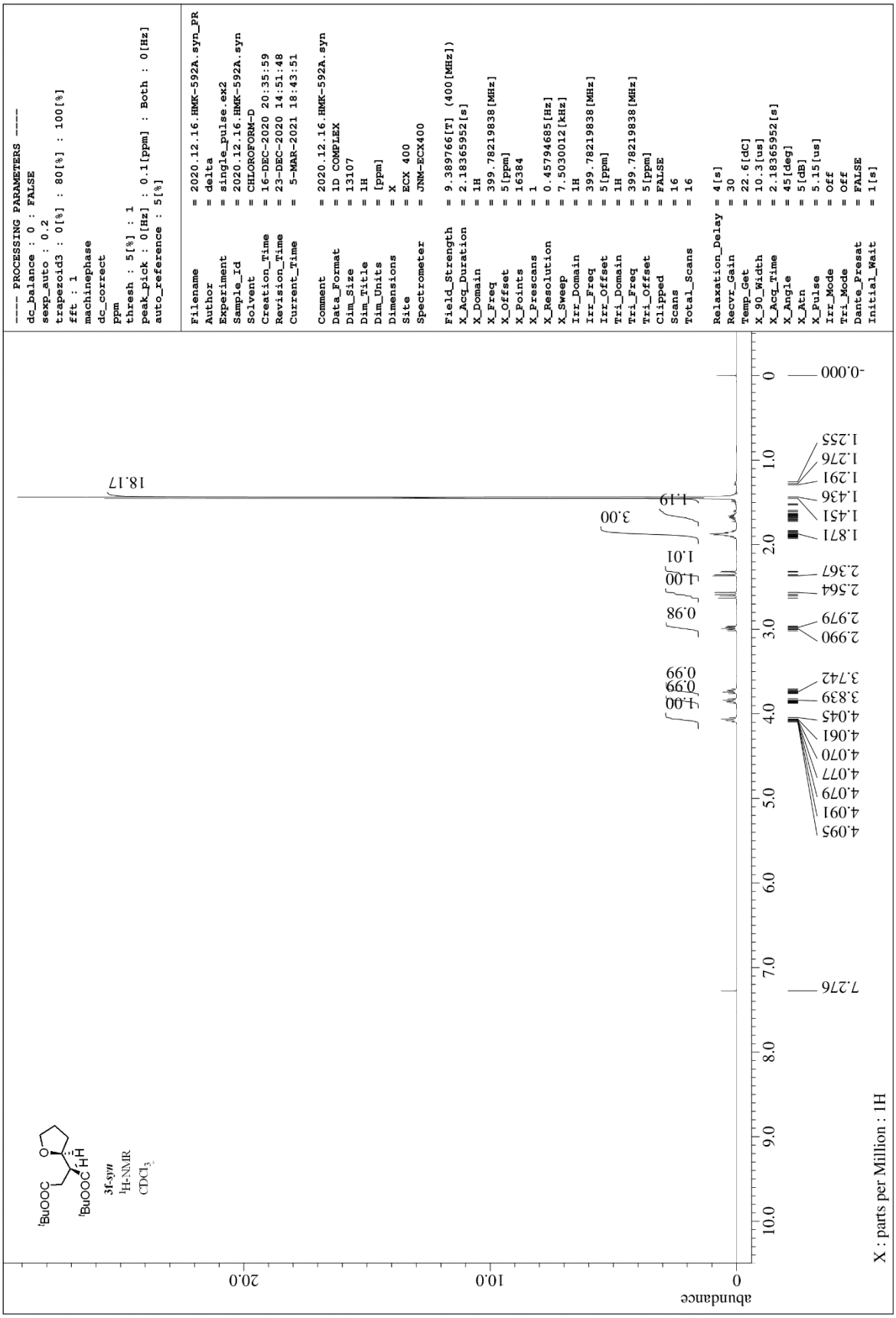

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.16.HMK-591A.anti_P
Author = delta
Experiment = single_pulse_ex2
Sample_Id = 2020.12.16.HMK-591A.anti
Solvent = CHLOROFORM-D
Creation_Time = 16-DEC-2020 20:15:04
Revision_Time = 23-DEC-2020 18:15:38
Current_Time = 5-MAR-2021 18:34:56
Comment = 2020.12.16.HMK-591A.anti
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 34
Temp_Get = 22.6[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 5[dB]
X_Pulse = 5.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
iPrOOC
iPrOOC
H
H
3c-anti
^{1}H-NMR
$CDCl_3$
2.03
1.00
3.989
3.971
3.953
3.935
3.825
3.804
3.787
3.770
3.754
3.737
3.719
3.700
abundance
X : parts per Million : 1H

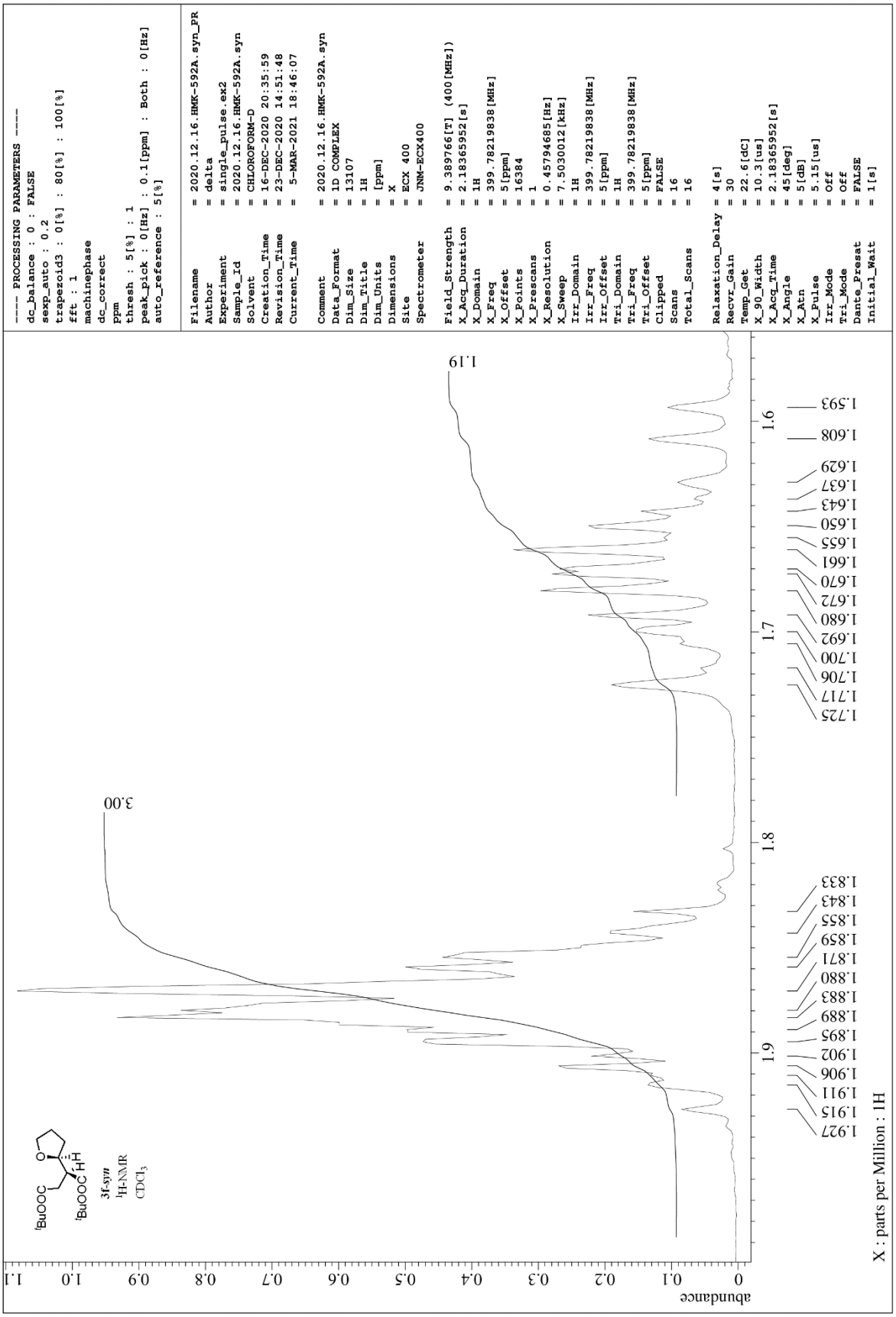

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.16.HMK-591A.anti_P
Author = delta
Experiment = single_pulse_ex2
Sample_Id = 2020.12.16.HMK-591A.anti
Solvent = CHLOROFORM-D
Creation_Time = 16-DEC-2020 20:15:04
Revision_Time = 23-DEC-2020 18:15:38
Current_Time = 5-MAR-2021 18:36:15
Comment = 2020.12.16.HMK-591A.anti
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 34
Temp_Get = 22.6[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 5[dB]
X_Pulse = 5.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
iPrOOC
iPrOOC H H
3e-anti
1H-NMR
CDCl3
1.96
4.944
4.959
4.975
4.991
5.005
5.021
5.036
5.052
5.067
5.083
abundance
X : parts per Million : 1H

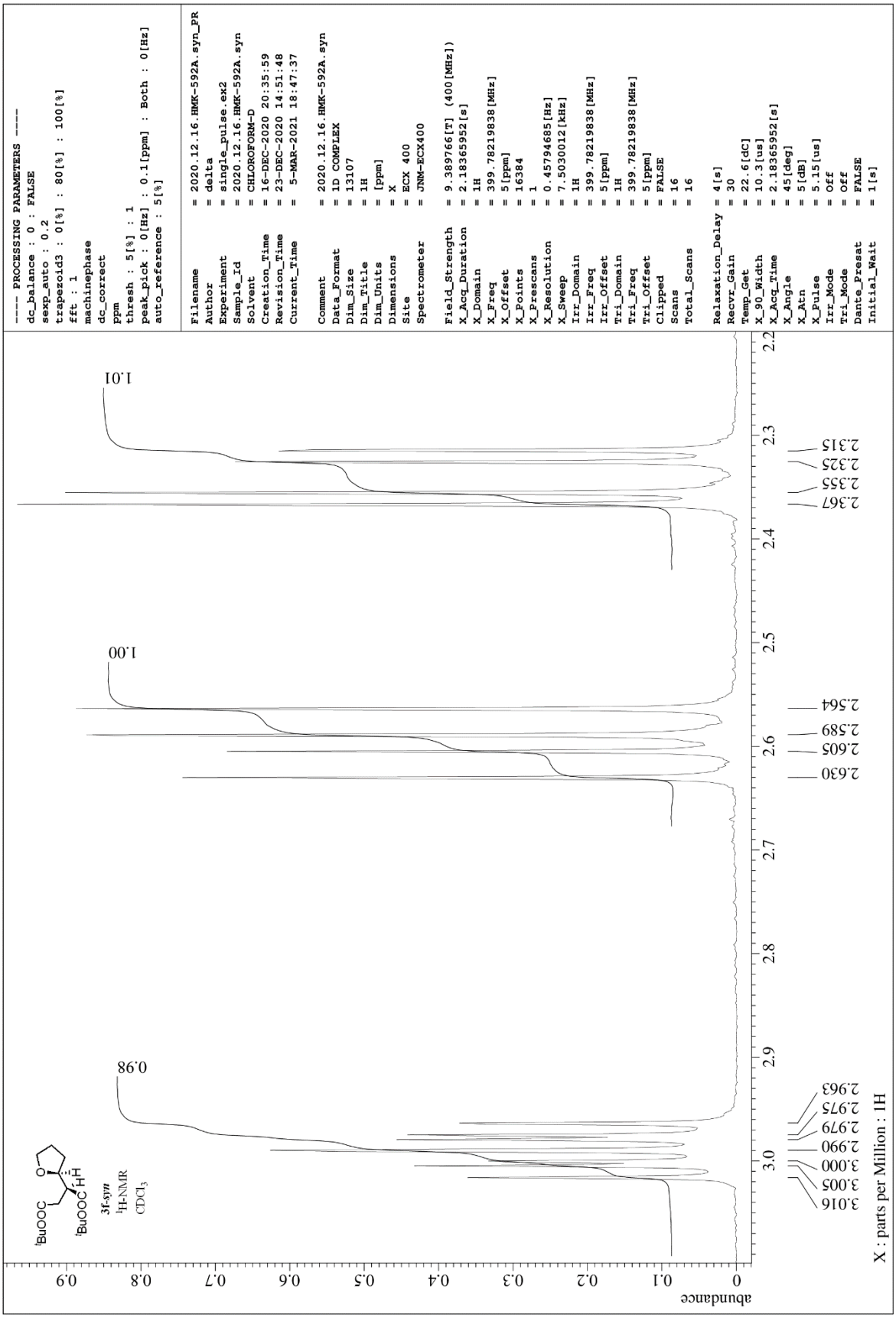

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Peaks : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.16.HMK-591A.anti_C
Author = delta
Experiment = single_pulse_dec
Sample_Id = 2020.12.16.HMK-591A.anti
Solvent = CHLOROFORM-D
Creation_Time = 16-DEC-2020 20:30:04
Revision_Time = 16-DEC-2020 20:32:16
Current_Time = 5-MAR-2021 18:38:14
Comment = 2020.12.16.HMK-591A.anti
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.525303333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 22.8[dC]
X_90_Width = 8.9[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 2.96666667[us]
Irr_Atn_Dec = 19.5[dB]
Irr_Atn_Noe = 19.5[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
iPrOOC
iPrOOC
H
H
3c-anti
13C-NMR
CDCl3
abundance
X : parts per Million : 13C
21.690
21.728
21.776
25.637
29.642
34.037
47.100
67.837
67.933
68.037
76.676
77.000
77.315
78.888
171.640
172.317

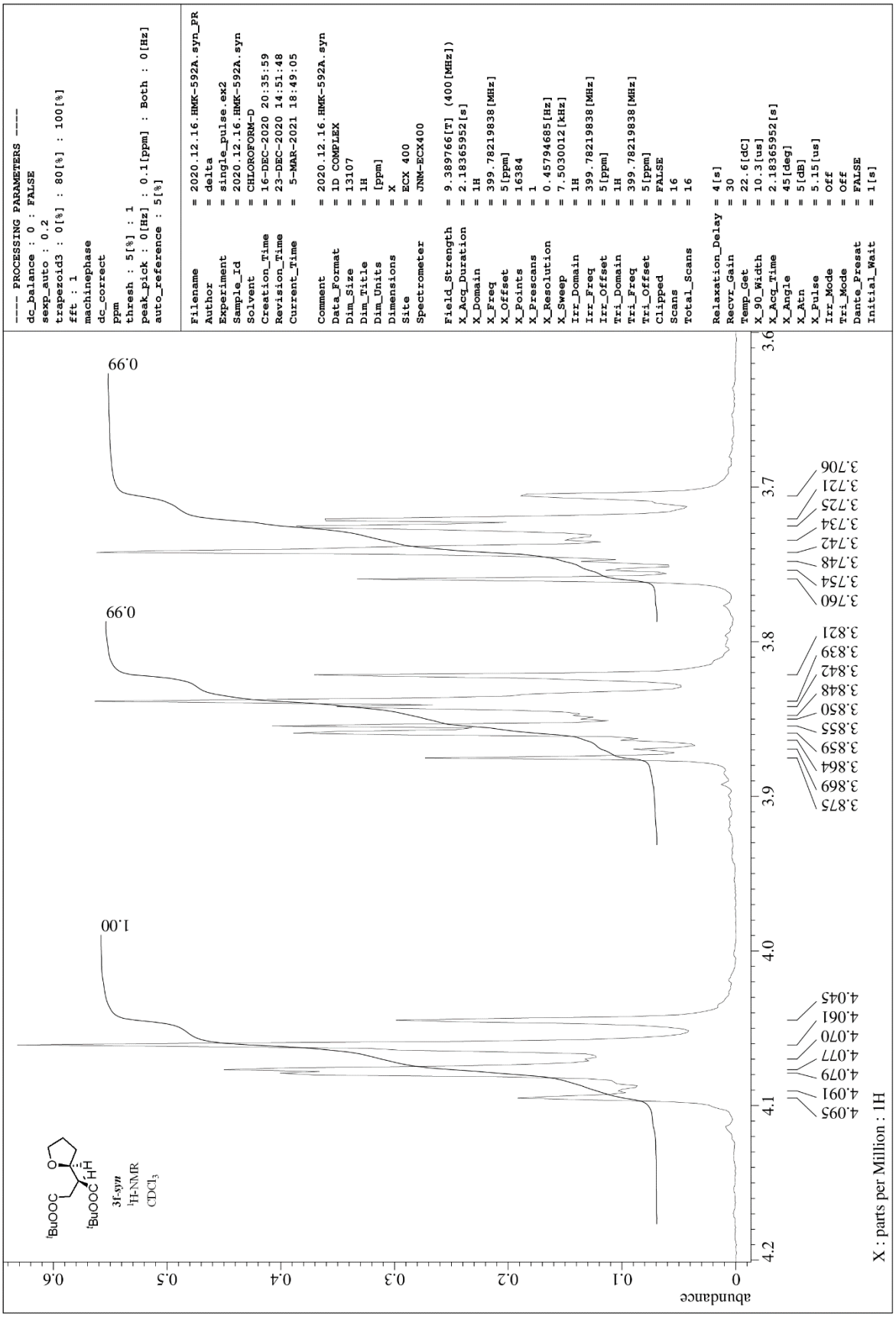

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Peaks : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.16.HMK-591A.anti_C
Author = delta
Experiment = single_pulse_dec
Sample_Id = 2020.12.16.HMK-591A.anti
Solvent = CHLOROFORM-D
Creation_Time = 16-DEC-2020 20:30:04
Revision_Time = 16-DEC-2020 20:32:16
Current_Time = 5-MAR-2021 18:40:12
Comment = 2020.12.16.HMK-591A.anti
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.525303333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 22.8[dC]
X_90_Width = 8.9[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 2.96666667[us]
Irr_Atn_Dec = 19.5[dB]
Irr_Atn_Noe = 19.5[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
iPrOOC
iPrOOC
H
3e-anti
13C-NMR
CDCl3
abundance
0.5
0.4
0.3
0.2
0.1
0
22.4
22.3
22.2
22.1
22.0
21.9
21.8
21.7
21.6
21.5
21.4
21.3
21.2
21.1
21.776
21.728
21.690
X : parts per Million : 13C

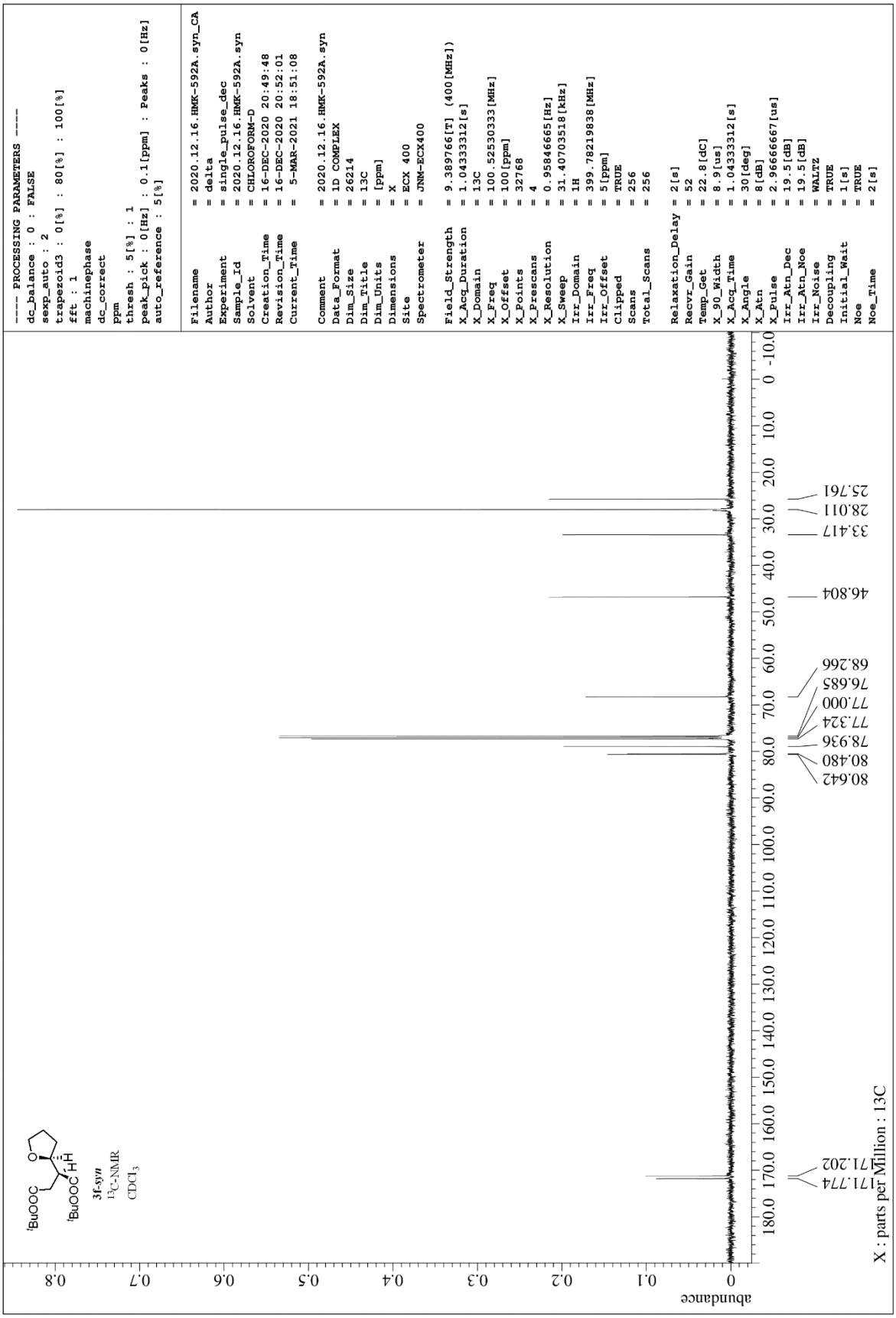

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Peaks : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.16.HMK-591A.anti_C
Author = delta
Experiment = single_pulse_dec
Sample_Id = 2020.12.16.HMK-591A.anti
Solvent = CHLOROFORM-D
Creation_Time = 16-DEC-2020 20:30:04
Revision_Time = 16-DEC-2020 20:32:16
Current_Time = 5-MAR-2021 18:41:34
Comment = 2020.12.16.HMK-591A.anti
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.525303333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 22.8[dC]
X_90_Width = 8.9[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 2.96666667[us]
Irr_Atn_Dec = 19.5[dB]
Irr_Atn_Noe = 19.5[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
iPrOOC
iPrOOC
3e-anti
13C-NMR
CDCl3
abundance
0.3
0.2
0.1
0
69.6
69.4
69.2
69.0
68.8
68.6
68.4
68.2
68.0
67.8
67.6
67.4
67.2
67.0
66.8
66.6
66.4
66.2
68.037
67.933
67.837
X : parts per Million : 13C

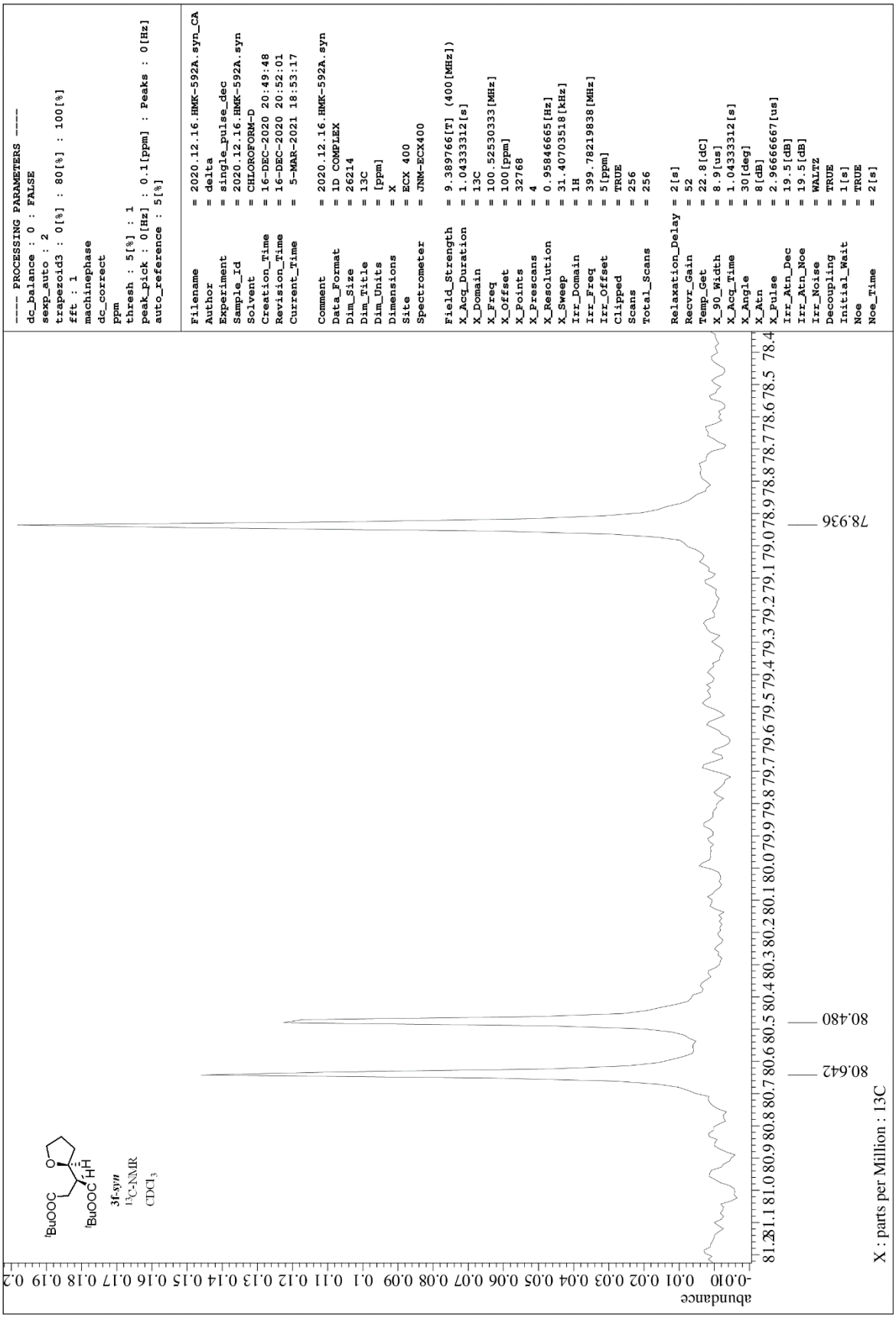

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.16.HMK-592A.syn_PR
Author = delta
Experiment = single_pulse_ex2
Sample_Id = 2020.12.16.HMK-592A.syn
Solvent = CHLOROFORM-D
Creation_Time = 16-DEC-2020 20:35:59
Revision_Time = 23-DEC-2020 14:51:48
Current_Time = 5-MAR-2021 18:43:51
Comment = 2020.12.16.HMK-592A.syn
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 30
Temp_Get = 22.6[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 5[dB]
X_Pulse = 5.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
tBuOOC
tBuOOC
3f-syn
1H-NMR
CDCl3
abundance
X : parts per Million : 1H
18.17
3.00
1.19
1.01
1.00
0.98
1.00
0.99
0.99
7.276
4.095
4.091
4.079
4.077
4.070
4.061
4.045
3.839
3.742
2.990
2.979
2.564
2.367
1.871
1.451
1.436
1.291
1.276
1.255
-0.000

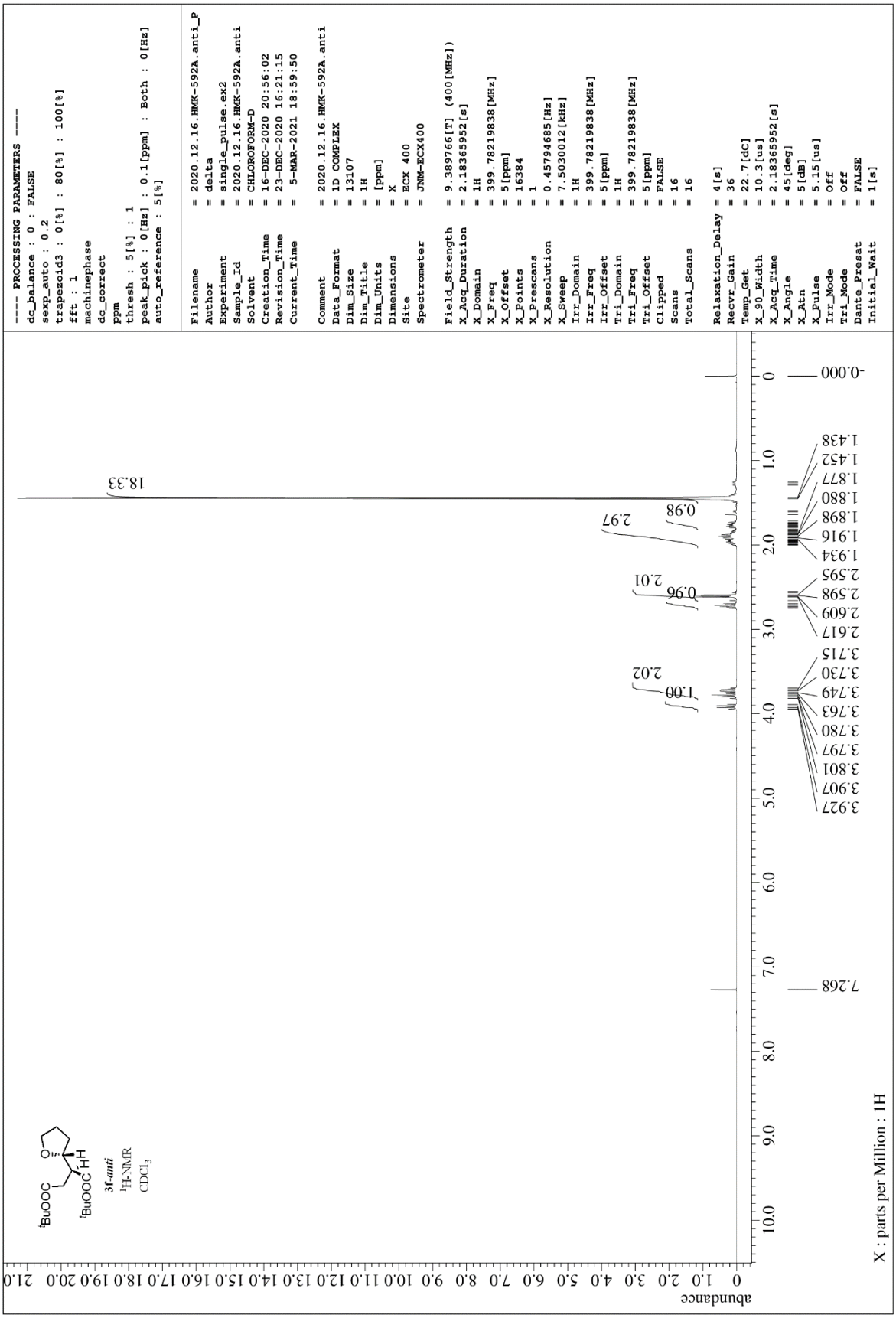

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.16.HMK-592A.syn_PR
Author = delta
Experiment = single_pulse_ex2
Sample_Id = 2020.12.16.HMK-592A.syn
Solvent = CHLOROFORM-D
Creation_Time = 16-DEC-2020 20:35:59
Revision_Time = 23-DEC-2020 14:51:48
Current_Time = 5-MAR-2021 18:46:07
Comment = 2020.12.16.HMK-592A.syn
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 30
Temp_Get = 22.6[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 5[dB]
X_Pulse = 5.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
tBuOOC
tBuOOC
3f-syn
1H-NMR
CDCl3
3.00
1.19
1.927
1.915
1.911
1.906
1.902
1.895
1.889
1.883
1.880
1.871
1.859
1.855
1.843
1.833
1.725
1.717
1.706
1.700
1.692
1.680
1.672
1.670
1.661
1.655
1.650
1.643
1.637
1.629
1.608
1.593
abundance
X : parts per Million : 1H

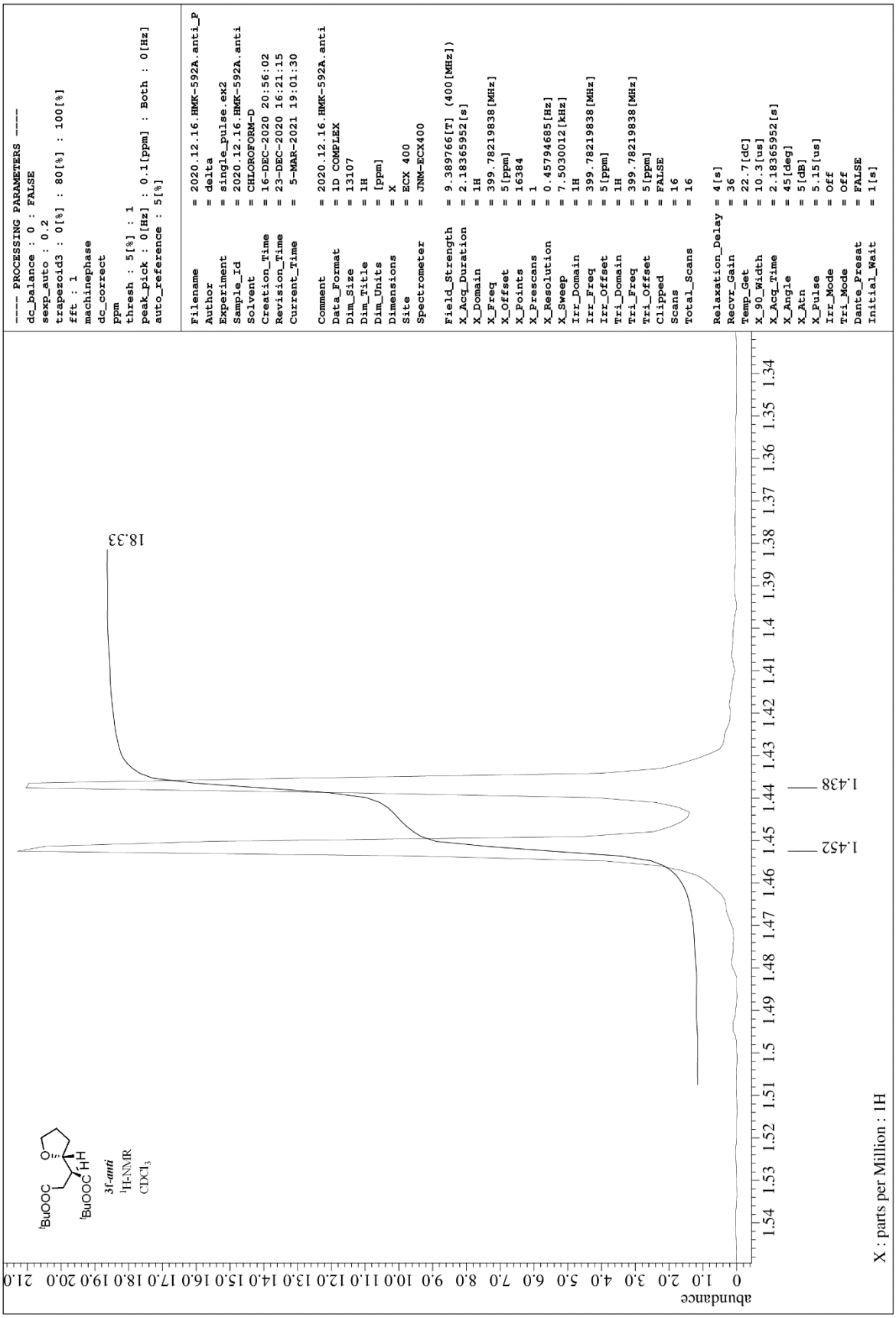

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.16.HMK-592A.syn_PR
Author = delta
Experiment = single_pulse_ex2
Sample_Id = 2020.12.16.HMK-592A.syn
Solvent = CHLOROFORM-D
Creation_Time = 16-DEC-2020 20:35:59
Revision_Time = 23-DEC-2020 14:51:48
Current_Time = 5-MAR-2021 18:47:37
Comment = 2020.12.16.HMK-592A.syn
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 30
Temp_Get = 22.6[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 5[dB]
X_Pulse = 5.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
tBuOOC
tBuOOC H H
3f-syn
1H-NMR
CDCl3
0.98
1.00
1.01
3.016
3.005
3.000
2.990
2.979
2.975
2.963
2.630
2.605
2.589
2.564
2.367
2.355
2.325
2.315
abundance
X : parts per Million : 1H


---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.16.HMK-592A.syn_PR
Author = delta
Experiment = single_pulse_ex2
Sample_Id = 2020.12.16.HMK-592A.syn
Solvent = CHLOROFORM-D
Creation_Time = 16-DEC-2020 20:35:59
Revision_Time = 23-DEC-2020 14:51:48
Current_Time = 5-MAR-2021 18:49:05
Comment = 2020.12.16.HMK-592A.syn
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 30
Temp_Get = 22.6[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 5[dB]
X_Pulse = 5.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
tBuOOC
tBuOOC
3f-syn
1H-NMR
CDCl3
1.00
0.99
0.99
0.99
4.095
4.091
4.079
4.077
4.070
4.061
4.045
3.875
3.869
3.864
3.859
3.855
3.850
3.848
3.842
3.839
3.821
3.760
3.754
3.748
3.742
3.734
3.725
3.721
3.706
abundance
X : parts per Million : 1H

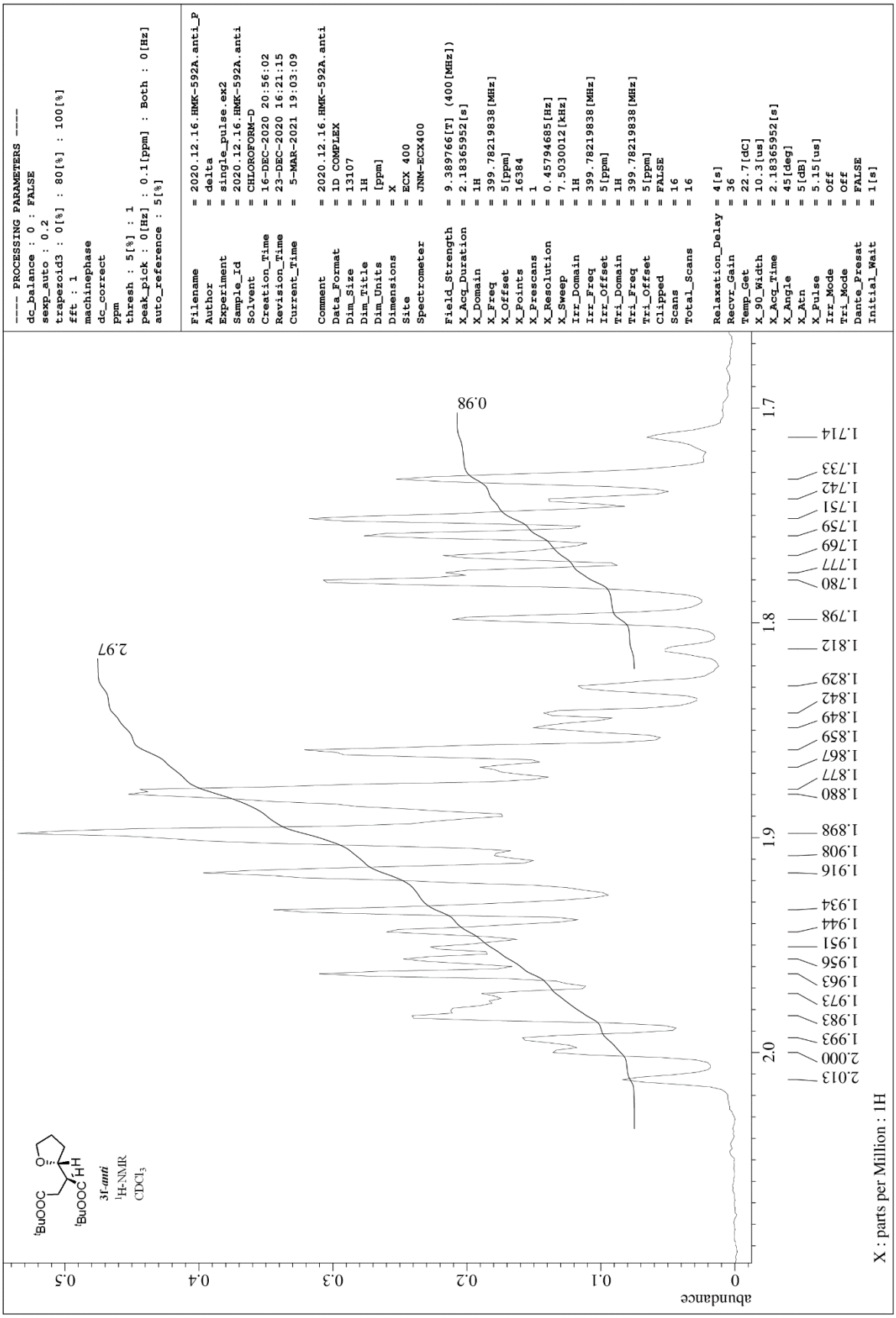

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Peaks : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.16.HMK-592A.syn_CA
Author = delta
Experiment = single_pulse_dec
Sample_Id = 2020.12.16.HMK-592A.syn
Solvent = CHLOROFORM-D
Creation_Time = 16-DEC-2020 20:49:48
Revision_Time = 16-DEC-2020 20:52:01
Current_Time = 5-MAR-2021 18:51:08
Comment = 2020.12.16.HMK-592A.syn
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.525303333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 52
Temp_Get = 22.8[dC]
X_90_Width = 8.9[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 2.96666667[us]
Irr_Atn_Dec = 19.5[dB]
Irr_Atn_Noe = 19.5[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
tBuOOC
tBuOOC
3f-syn
13C-NMR
CDCl3
abundance
X : parts per Million : 13C
171.774
171.202
80.642
80.480
78.936
77.324
77.000
76.685
68.266
46.804
33.417
28.011
25.761

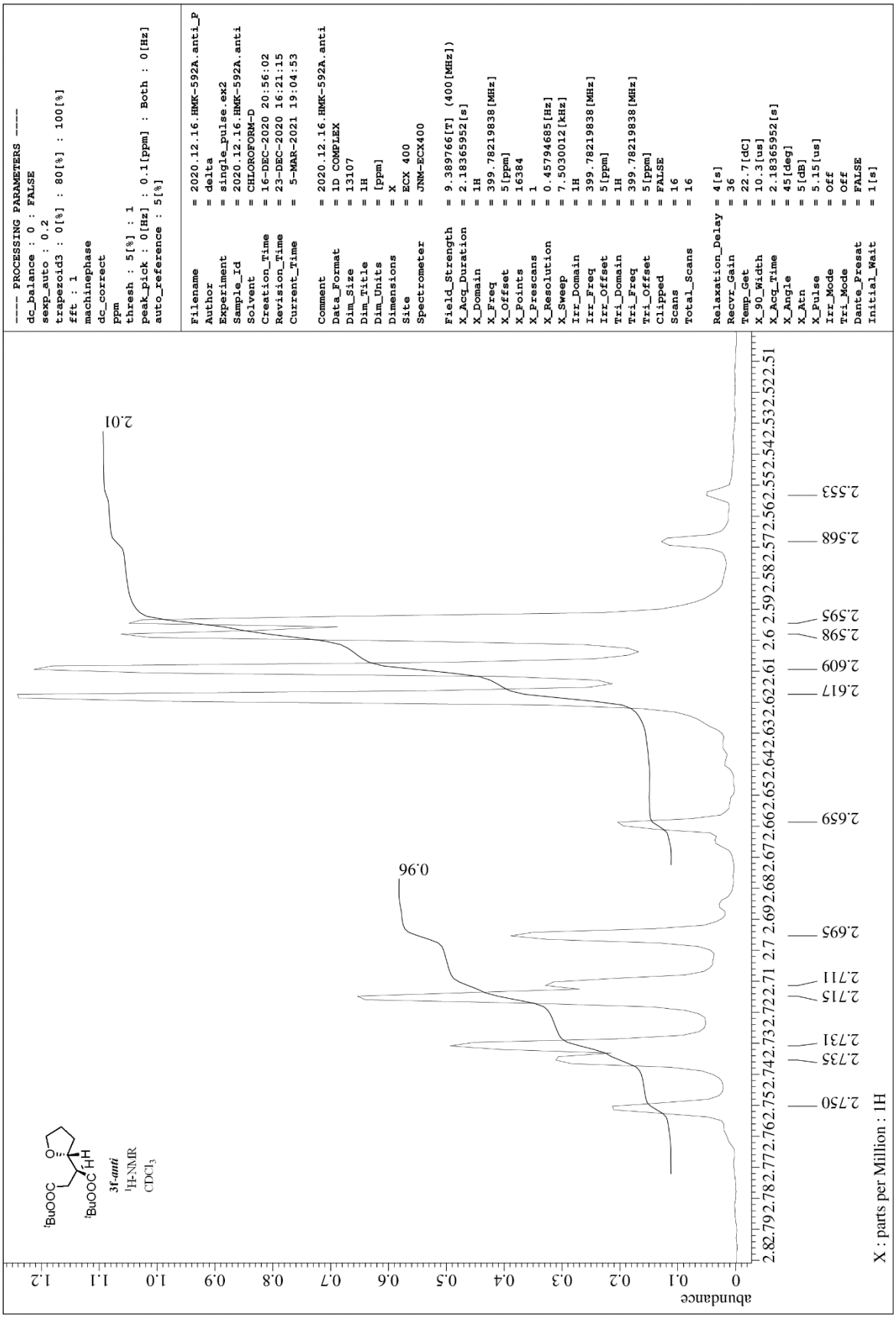

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Peaks : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.16.HMK-592A.syn_CA
Author = delta
Experiment = single_pulse_dec
Sample_Id = 2020.12.16.HMK-592A.syn
Solvent = CHLOROFORM-D
Creation_Time = 16-DEC-2020 20:49:48
Revision_Time = 16-DEC-2020 20:52:01
Current_Time = 5-MAR-2021 18:53:17
Comment = 2020.12.16.HMK-592A.syn
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.525303333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 52
Temp_Get = 22.8[dC]
X_90_Width = 8.9[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 2.96666667[us]
Irr_Atn_Dec = 19.5[dB]
Irr_Atn_Noe = 19.5[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
tBuOOC
tBuOOC
H
3f-syn
13C-NMR
CDCl3
78.936
80.480
80.642
X : parts per Million : 13C
abundance

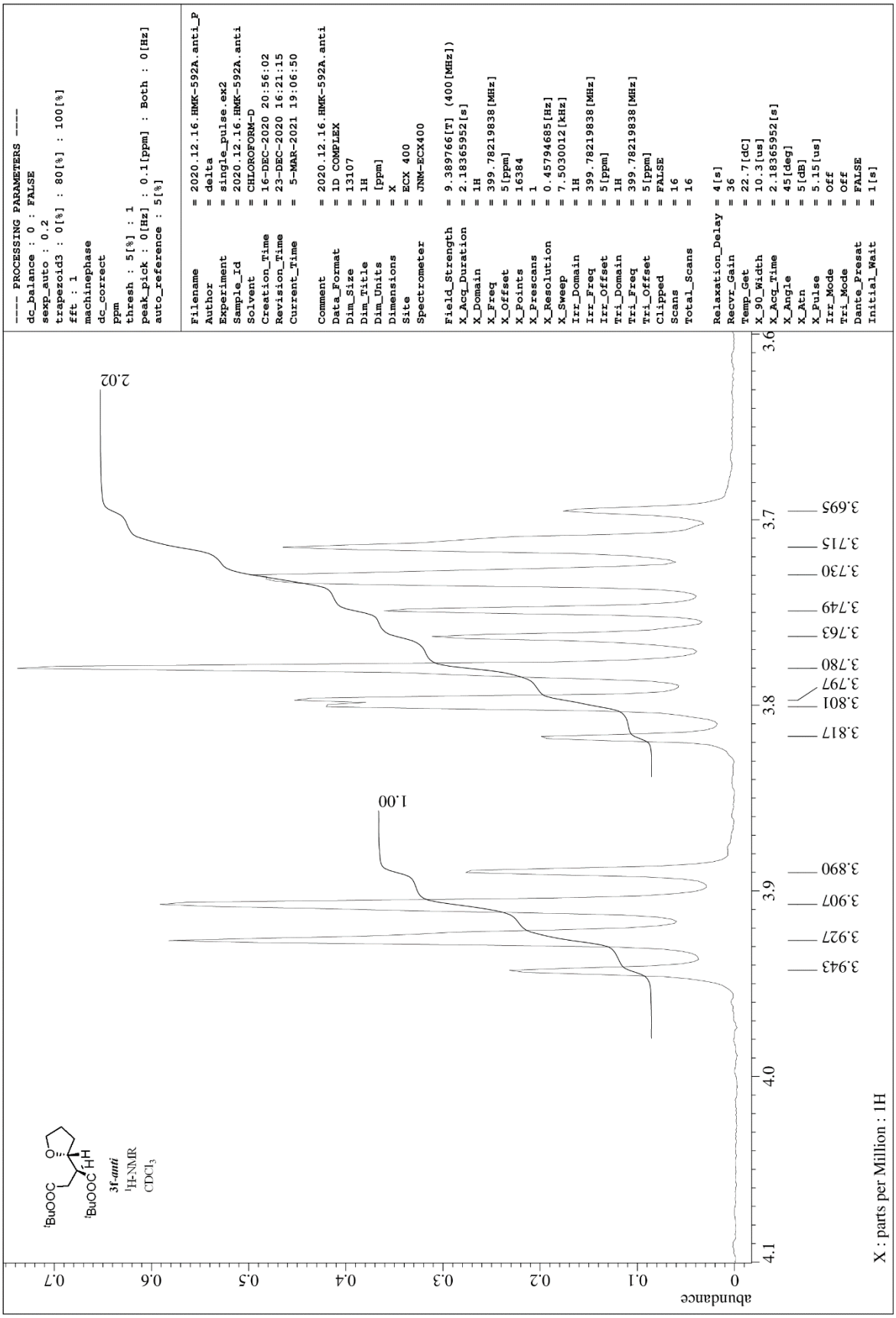

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.16.HMK-592A.anti_P
Author = delta
Experiment = single_pulse_ex2
Sample_Id = 2020.12.16.HMK-592A.anti
Solvent = CHLOROFORM-D
Creation_Time = 16-DEC-2020 20:56:02
Revision_Time = 23-DEC-2020 16:21:15
Current_Time = 5-MAR-2021 18:59:50
Comment = 2020.12.16.HMK-592A.anti
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 36
Temp_Get = 22.7[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 5[dB]
X_Pulse = 5.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
18.33
2.97
0.98
2.01
0.96
2.02
1.00
7.268
3.927
3.907
3.801
3.797
3.780
3.763
3.749
3.730
3.715
2.617
2.609
2.598
2.595
1.934
1.916
1.898
1.880
1.877
1.452
1.438
-0.000
abundance
X : parts per Million : 1H
3S-anti
^{1}H-NMR
$CDCl_3$

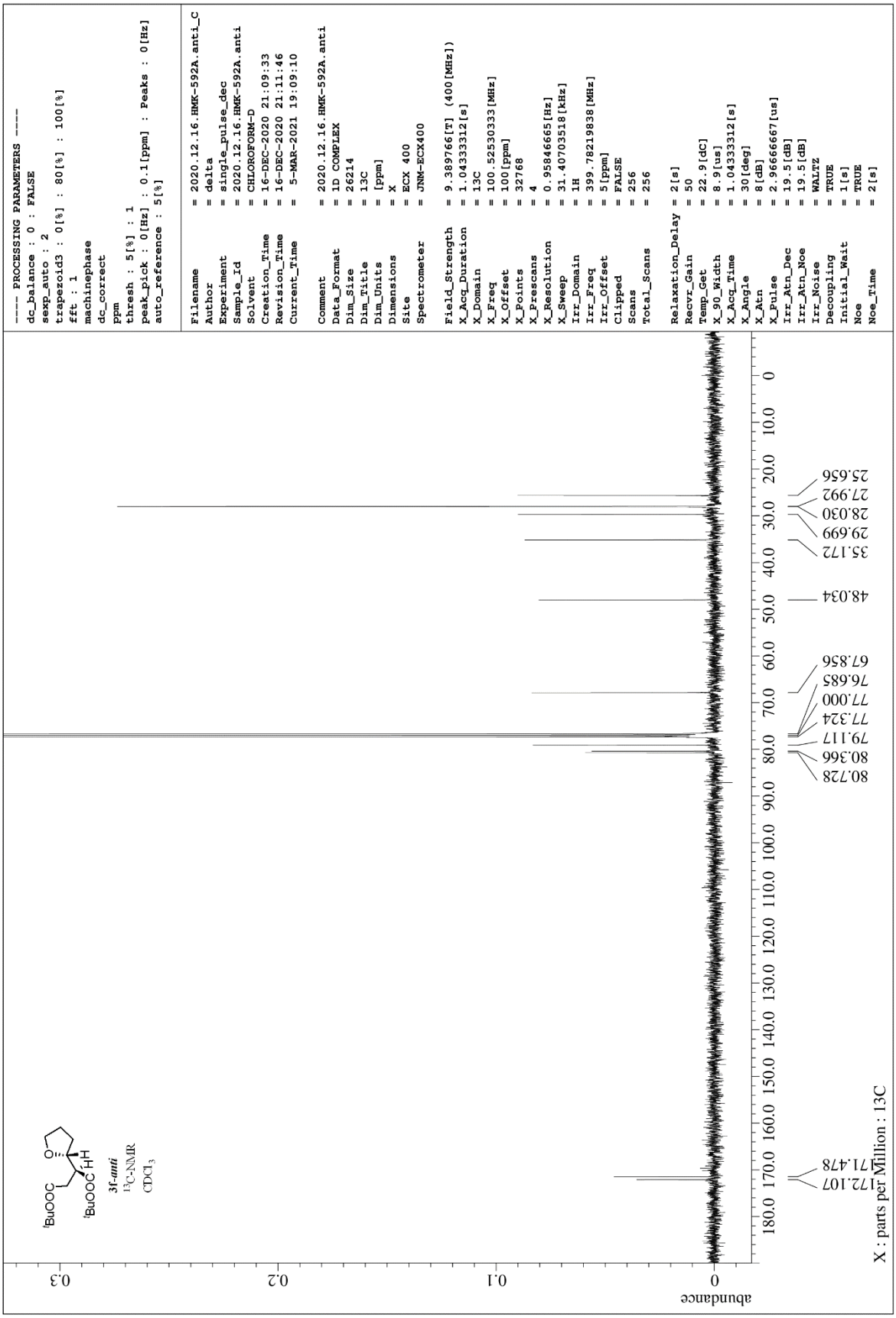


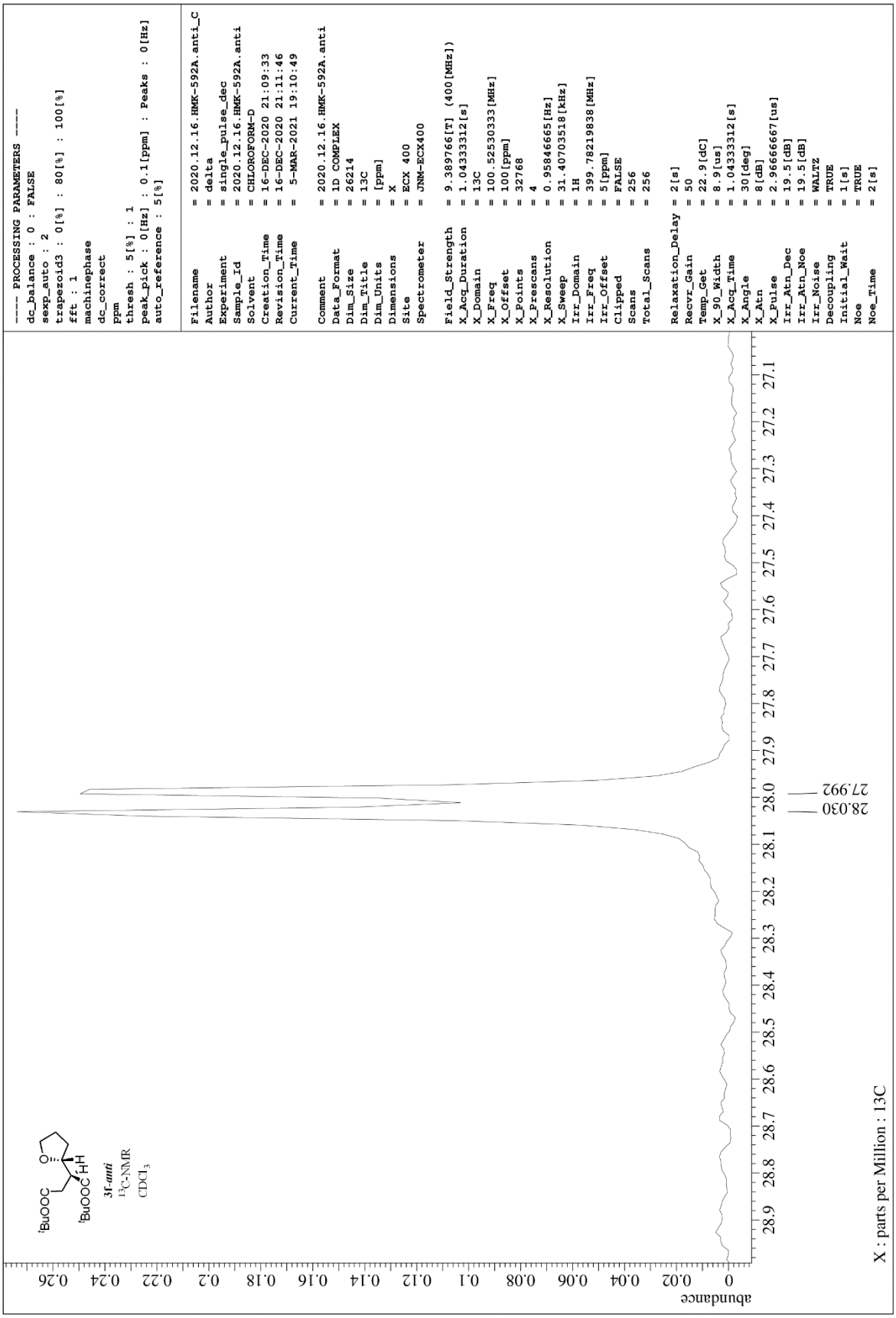

```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]

Filename          = 2020.12.16.HMK-592A.anti_P
Author            = delta
Experiment        = single_pulse_ex2
Sample_Id         = 2020.12.16.HMK-592A.anti
Solvent           = CHLOROFORM-D
Creation_Time     = 16-DEC-2020 20:56:02
Revision_Time     = 23-DEC-2020 16:21:15
Current_Time      =  5-MAR-2021 19:01:30

Comment           = 2020.12.16.HMK-592A.anti
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = 1H
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400
Spectrometer      = JNM-ECX400

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18365952[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45794685[Hz]
X_Sweep           = 7.5030012[kHz]
Irr_Domain        = 1H
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = 1H
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 16
Total_Scans       = 16

Relaxation_Delay  = 4[s]
Recvr_Gain        = 36
Temp_Get          = 22.7[dC]
X_90_Width        = 10.3[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 5[dB]
X_Pulse           = 5.15[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
```

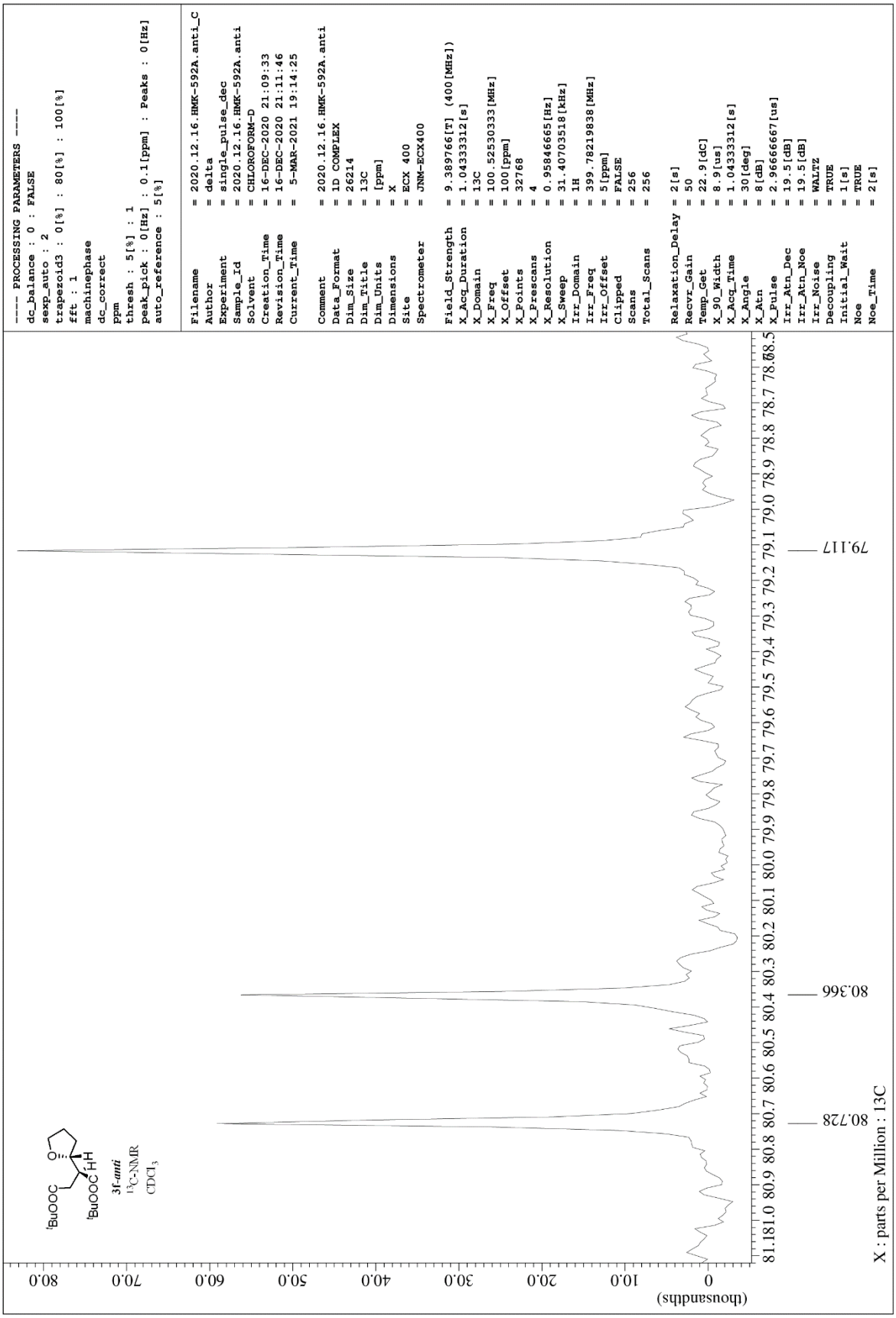

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.16.HMK-592A.anti_P
Author = delta
Experiment = single_pulse_ex2
Sample_Id = 2020.12.16.HMK-592A.anti
Solvent = CHLOROFORM-D
Creation_Time = 16-DEC-2020 20:56:02
Revision_Time = 23-DEC-2020 16:21:15
Current_Time = 5-MAR-2021 19:03:09
Comment = 2020.12.16.HMK-592A.anti
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 36
Temp_Get = 22.7[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 5[dB]
X_Pulse = 5.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
tBuOOC
tBuOOC
H
3f-anti
1H-NMR
CDCl3
2.97
0.98
abundance
X : parts per Million : 1H
2.013
2.000
1.993
1.983
1.973
1.963
1.956
1.951
1.944
1.934
1.916
1.908
1.898
1.880
1.877
1.867
1.859
1.849
1.842
1.829
1.812
1.798
1.780
1.777
1.769
1.759
1.751
1.742
1.733
1.714


---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.16.HMK-592A.anti_P
Author = delta
Experiment = single_pulse_ex2
Sample_Id = 2020.12.16.HMK-592A.anti
Solvent = CHLOROFORM-D
Creation_Time = 16-DEC-2020 20:56:02
Revision_Time = 23-DEC-2020 16:21:15
Current_Time = 5-MAR-2021 19:04:53
Comment = 2020.12.16.HMK-592A.anti
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 36
Temp_Get = 22.7[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 5[dB]
X_Pulse = 5.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
2.01
0.96
2.750
2.735
2.731
2.715
2.711
2.695
2.659
2.617
2.609
2.598
2.595
2.568
2.553
abundance
X : parts per Million : 1H
tBuOOC
tBuOOC H
3f-anti
1H-NMR
CDCl3


---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.16.HMK-592A.anti_P
Author = delta
Experiment = single_pulse_ex2
Sample_Id = 2020.12.16.HMK-592A.anti
Solvent = CHLOROFORM-D
Creation_Time = 16-DEC-2020 20:56:02
Revision_Time = 23-DEC-2020 16:21:15
Current_Time = 5-MAR-2021 19:06:50
Comment = 2020.12.16.HMK-592A.anti
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 36
Temp_Get = 22.7[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 5[dB]
X_Pulse = 5.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
2.02
1.00
3.943
3.927
3.907
3.890
3.817
3.801
3.797
3.780
3.763
3.749
3.730
3.715
3.695
abundance
X : parts per Million : 1H
3f-anti
^{1}H-NMR
$CDCl_3$


3f-anti
^{13}C-NMR
$CDCl_3$
X : parts per Million : 13C
abundance
172.107
171.478
80.728
80.366
79.117
77.324
77.000
76.685
67.856
48.034
35.172
29.699
28.030
27.992
25.656


tBuOOC
tBuOOC
H
3f-anti
13C-NMR
CDCl3
abundance
X : parts per Million : 13C
28.030
27.992
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Peaks : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.16.HMK-592A.anti_C
Author = delta
Experiment = single_pulse_dec
Sample_Id = 2020.12.16.HMK-592A.anti
Solvent = CHLOROFORM-D
Creation_Time = 16-DEC-2020 21:09:33
Revision_Time = 16-DEC-2020 21:11:46
Current_Time = 5-MAR-2021 19:10:49
Comment = 2020.12.16.HMK-592A.anti
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.525303333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 22.9[dC]
X_90_Width = 8.9[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 2.96666667[us]
Irr_Atn_Dec = 19.5[dB]
Irr_Atn_Noe = 19.5[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]


---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Peaks : 0[Hz]
auto_reference : 5[%]
Filename = 2020.12.16.HMK-592A.anti_C
Author = delta
Experiment = single_pulse_dec
Sample_Id = 2020.12.16.HMK-592A.anti
Solvent = CHLOROFORM-D
Creation_Time = 16-DEC-2020 21:09:33
Revision_Time = 16-DEC-2020 21:11:46
Current_Time = 5-MAR-2021 19:14:25
Comment = 2020.12.16.HMK-592A.anti
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.525303333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 22.9[dC]
X_90_Width = 8.9[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 2.96666667[us]
Irr_Atn_Dec = 19.5[dB]
Irr_Atn_Noe = 19.5[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
tBuOOC
tBuOOC
3f-anti
13C-NMR
CDCl3
(thousandths)
X : parts per Million : 13C
79.117
80.366
80.728

