Supplementary Information (SI) for CrystEngComm.

*Supplementary Information*

# Construction of sterically bent π-conjugated arylene by implanting into bulky NHC Cu(I) coordination polymers in crystalline media

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## Contents

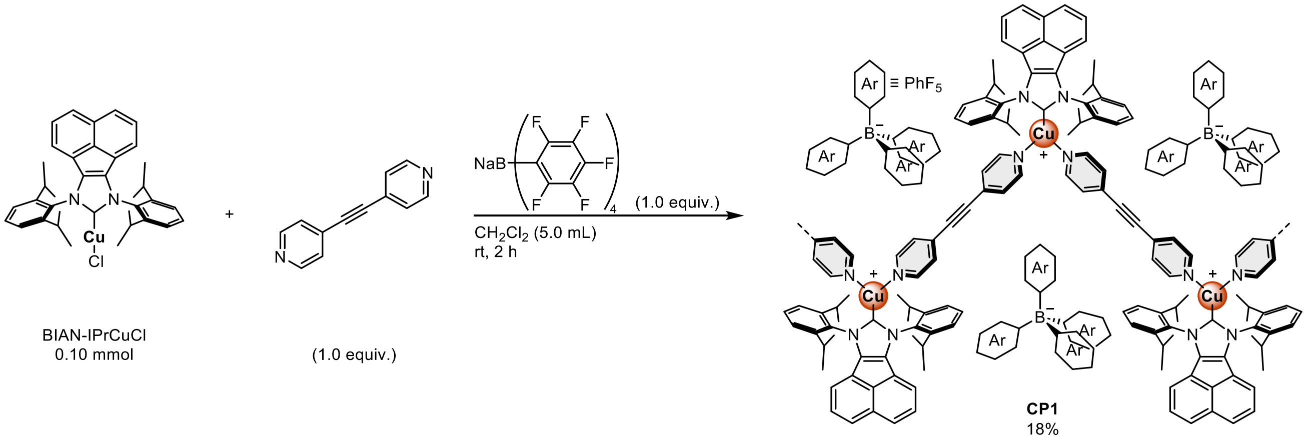
## 1. General

All commercially available reagents and solvents are reagent grade and were used without further purification unless otherwise noted. Solvents for the synthesis were purchased from commercial suppliers and dried over molecular sieves (4 Å). NMR spectra were recorded on a JEOL JNM-ECX400P, JNM-ECS400 ($^1$H: 400 MHz; $^{13}$C: 100 MHz) using acetone-$d_6$ or tetramethylsilane and $CDCl_3$ as internal standards, respectively. Elemental analyses and low- and high-resolution mass spectra were recorded at the Global Facility Center at Hokkaido University.

## 2. Synthesis

The compound BIAN-IPrCuCl (BIAN: bis(imino)acenaphthene, IPrCuCl: chloro[1,3-bis(2,6-diisopropylp-henyl)imidazol-2-ylidene]Cu(I)),[1] 1,2-bis(4-pyridyl)acetylene,[2] sodium tetrakis(pentafluorophenyl)borate,[3] and sodium tetrakis[3,5-bis(trifluoromethyl)phenyl]borate[3] were prepared according to the previously reported literatures.

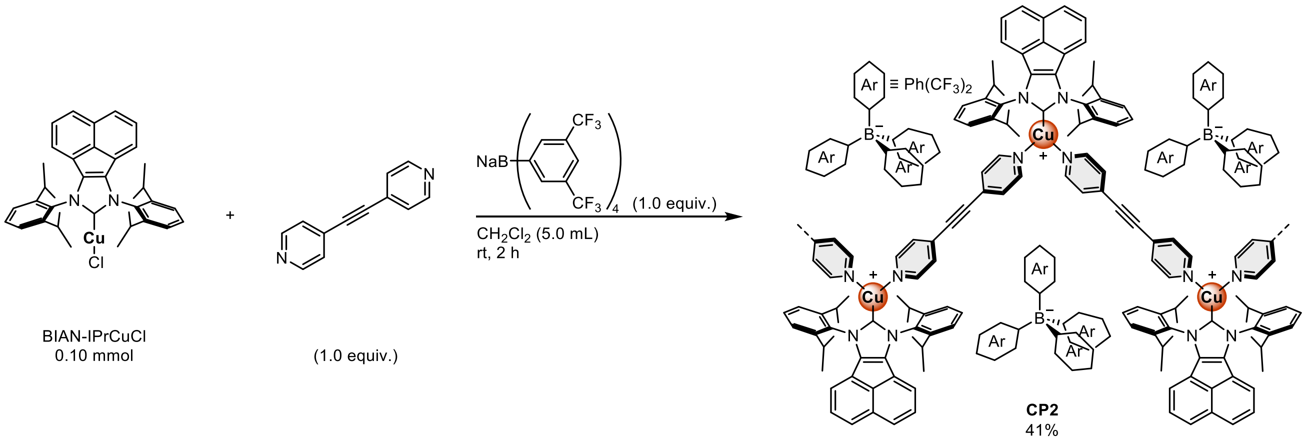
### 2.1. Synthesis of NHC Cu(I) coordination polymer 1



The cationic NHC Cu(I) coordination polymer CP**1** was synthesized according to the modified literature procedure.[4] To an oven-dried 20 mL two-neck round-bottom flask was added 1,2-bis(4-pyridyl)acetylene (18.0 mg, 0.10 mmol, 1.0 equiv.) and BIAN-IPrCuCl (BIAN: bis(imino)acenaphthene, IPrCuCl: chloro[1,3-bis(2,6-diisopropylphenyl)imidazol-2-yliden-e]Cu(I)) (61.2 mg, 0.10 mmol, 1.0 equiv.). The flask was connected to a vacuum/nitrogen manifold through a rubber tube. It was evacuated and then backfilled with nitrogen. This process was repeated three times. $CH_2Cl_2$ (5.0 mL) was then added to the flask under nitrogen atmosphere. The reagents contained $CH_2Cl_2$ solution were added sodium tetrakis(pentafluorophenyl)borate ($NaB(PhF_5)_4$, 70.2 mg, 0.10 mmol, 1.0 equiv.), and the reaction was performed under room temperature for 2 h. The suspended $CH_2Cl_2$ solution was followed by separating the liquid organic layer using centrifuge. The organic layers were collected, and the solvent was removed *in vacuo*. Further purification by reprecipitation using $CH_2Cl_2$/Hex and subsequent vacuum drying gave light-yellowish powder of **1** (25.6 mg, 0.018 mmol, 18%). The obtained powder was well soluble in chloroform, thus, Acetone-$d_6$ was used for dissolving the crystal for measurements of the $^1$H and $^{13}$C NMR spectra in solution phase. $^1$H NMR (400 MHz, Acetone-$d_6$, δ): 8.67 (dd, $J$ = 1.6 Hz, $J$ = 4.0 Hz, 4H), 7.99 (d, $J$ = 8.4 Hz, 2H), 7.70 (t, $J$ = 7.8 Hz, 2H), 7.62-7.55 (m, 6H), 7.53 (dd, $J$ = 1.6 Hz, $J$ = 4.4 Hz, 4H), 7.14

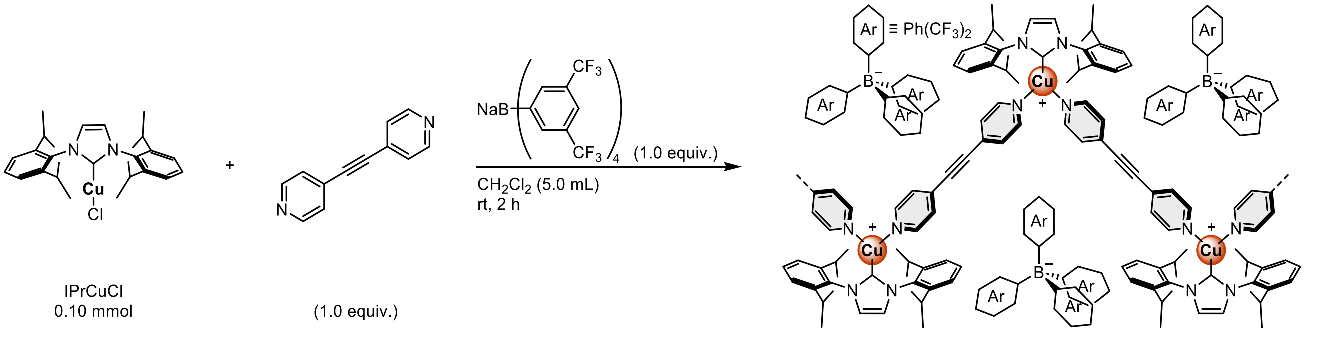
(d, *J* = 6.8 Hz, 2H), 2.94 (septet, *J* = 6.9 Hz, 4H), 1.37 (d, *J* = 6.8 Hz, 12H), 1.16 (d, *J* = 6.8 Hz, 12H). $^{13}$C NMR (100 MHz, Acetone-$d_6$, d): 151.0 (*C*H), 150.3–147.9 (*C*), 146.6 (*C*), 139.6 (*C*), 140.4–135.7 (*C*), 134.2 (*C*), 132.7 (*C*), 131.8 (*C*H), 131.5 (*C*), 131.0 (*C*), 130.7 (*C*), 129.6 (*C*H), 129.5–129.4 (*C*), 129.0 (*C*H), 126.9 (*C*), 126.4 (*C*H), 125.9 (*C*), 125.5 (*C*H), 122.1 (*C*H), 91.1 (*C*), 29.7 (*C*H), 25.1 (*C*H$_3$), 23.8 (*C*H$_3$). HRMS (ESI) m/z: [M]$^+$ calcd. for $C_{49}H_{48}N_4Cu$, 755.31695; found, 755.31705; calcd. for $C_{24}{}^{10}BF_{20}$, 677.98155; found, 677.98246. Elemental analysis: calcd. for $C_{73}H_{48}BCuF_{20}N_4$: C, 61.08; H, 3.37; N, 3.90; found: C, 57.53; H, 2.77; N, 3.47. The analytically pure light-yellowish single crystal **1** was prepared by recrystallization using $CH_2Cl_2$/EtOH.

## 2.2. Synthesis of NHC Cu(I) coordination polymer 2



The cationic NHC Cu(I) coordination polymer CP**2** was synthesized according to the modified literature procedure.[4] To an oven-dried 20 mL two-neck round-bottom flask was added 1,2-bis(4-pyridyl)acetylene (18.0 mg, 0.10 mmol, 1.0 equiv.) and BIAN-IPrCuCl (BIAN: bis(imino)acenaphthene, IPrCuCl: chloro[1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene]Cu(I)) (61.2 mg, 0.10 mmol, 1.0 equiv.). The flask was connected to a vacuum/nitrogen manifold through a rubber tube. It was evacuated and then backfilled with nitrogen. This process was repeated three times. $CH_2Cl_2$ (5.0 mL) was then added to the flask under nitrogen atmosphere. The reagents contained $CH_2Cl_2$ solution was added sodium tetrakis[3,5-bis(trifluoromethyl)phenyl]borate ($NaB(Ph(CF_3)_2)_4$, 88.6 mg, 0.10 mmol, 1.0 equiv.), and the reaction was performed under room temperature for 2 h. The suspended $CH_2Cl_2$ solution was followed by separating the liquid organic layer using centrifuge. The organic layers were collected, and the solvent was removed *in vacuo*. Further purification by reprecipitation using $CH_2Cl_2$/Hex and subsequent vacuum drying gave light-yellowish powder of **2** (67.0 mg, 0.041 mmol, 41%). The $CDCl_3$ was used for dissolving the crystal for measurements of the $^1$H and $^{13}$C NMR spectra in solution phase. $^1$H NMR (400 MHz, $CDCl_3$, δ): 7.88 (d, *J* = 8.4 Hz, 2H), 7.54 (s, 4H), 7.69 (s, 8H), 7.52–7.43 (m, 10H), 7.20 (d, *J* = 6.0 Hz, 4H), 7.12 (d, *J* = 7.2 Hz, 2H), 2.83 (septet, *J* = 6.9 Hz, 4H), 1.14 (dd, *J* = 6.8 Hz, *J* = 6.8 Hz, 24H). $^{13}$C NMR (100 MHz, $CDCl_3$, d): 161.8 (q, *J* = 49.8 Hz, *C*), 148.8 (*C*H), 146.3 (*C*), 139.1 (*C*), 134.9 (*C*H), 134.4 (*C*), 131.8 (*C*), 131.0 (*C*H), 130.9 (*C*), 130.1 (*C*), 129.5–128.1 (*C*), 128.9 (*C*H), 128.1 (*C*H), 127.1 (*C*H), 126.0 (*C*), 125.1 (*C*H), 123.3 (*C*), 121.4 (*C*H), 120.6 (*C*), 117.5 (*C*H), 91.6 (*C*), 29.0 (*C*H), 24.5 (*C*H$_3$), 23.6 (*C*H$_3$). HRMS (ESI) m/z: [M]$^+$ calcd. for $C_{49}H_{48}N_4Cu$, 755.31695; found, 755.31622; calcd. for $C_{32}H_{12}{}^{10}BF_{24}$, 862.06906; found, 862.07011. Elemental analysis: calcd. for $C_{81}H_{60}BCuF_{24}N_4$: C, 60.07; H, 3.73; N, 3.46; found: C, 59.45; H, 3.59; N, 3.31. The analytically pure light-yellowish single crystal **2** was prepared by recrystallization using $CH_2Cl_2$/EtOH.

### 2.3. Synthesis of NHC Cu(I) coordination polymer 3



**CP3**
95%

The cationic NHC Cu(I) coordination polymer CP**3** was synthesized according to the modified literature procedure.[4] To an oven-dried 20 mL two-neck round-bottom flask was added 1,2-bis(4-pyridyl)acetylene (18.0 mg, 0.10 mmol, 1.0 equiv.) and chloro[1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene]Cu(I) (IPrCuCl, 48.8 mg, 0.10 mmol, 1.0 equiv.). The flask was connected to a vacuum/nitrogen manifold through a rubber tube. It was evacuated and then backfilled with nitrogen. This process was repeated three times. $CH_2Cl_2$ (5.0 mL) was then added to the flask under nitrogen atmosphere. The reagents contained $CH_2Cl_2$ solution was added sodium tetrakis[3,5-bis(trifluoromethyl)phenyl]borate ($NaB(Ph(CF_3)_2)_4$, 88.6 mg, 0.10 mmol, 1.0 equiv.), and the reaction was performed under room temperature for 2 h. The suspended $CH_2Cl_2$ solution was followed by separating the liquid organic layer using centrifuge. The organic layers were collected, and the solvent was removed *in vacuo*. Further purification by reprecipitation using $CH_2Cl_2$/Hex and subsequent vacuum drying gave light-yellowish powder of **3** (141.4 mg, 0.095 mmol, 95%). The $CDCl_3$ was used for dissolving the crystal for measurements of the $^1H$ and $^{13}C$ NMR spectra in solution phase. $^1H$ NMR (400 MHz, $CDCl_3$, δ): 7.66 (s, 8H), 7.52 (t, *J* = 7.8 Hz, 2H) 7.44 (broad, 6H), 7.32 (d, *J* = 8.0 Hz, 4H), 7.27 (s, 2H), 7.10 (d, *J* = 5.6 Hz, 4H), 2.54 (septet, *J* = 6.9 Hz, 4H), 1.23 (d, *J* = 6.8 Hz, 12H), 1.08 (d, *J* = 6.8 Hz, 12H). $^{13}C$ NMR (100 MHz, $CDCl_3$, d): 161.9 (q, *J* = 49.9 Hz, *C*), 148.6 (*C*H), 146.2 (*C*), 134.9 (*C*H), 132.1 (*C*), 130.8 (*C*H), 129.0 (dq, *J* = 11.5 Hz, *J* = 62.9 Hz, *C*), 127.3 (*C*H), 126.0 (*C*), 124.7 (*C*H), 123.6 (*C*H), 123.3 (*C*), 120.6 (*C*), 117.6 (*C*H), 91.7 (*C*), 28.8 (*C*H), 24.5 (*C*$H_3$), 23.7 (*C*$H_3$). HRMS (ESI) m/z: $[M]^+$ calcd. for $C_{39}H_{44}N_4Cu$, 631.28565; found, 631.28512; calcd. for $C_{32}H_{12}{}^{10}BF_{24}$, 862.06906; found, 862.07009. Elemental analysis: calcd. for $C_{71}H_{56}BCuF_{24}N_4$: C, 57.02; H, 3.77; N, 3.75; found: C, 57.10; H, 3.83; N, 3.50. The analytically pure light-yellowish single crystal **3** was prepared by recrystallization using $CH_2Cl_2$/EtOH.

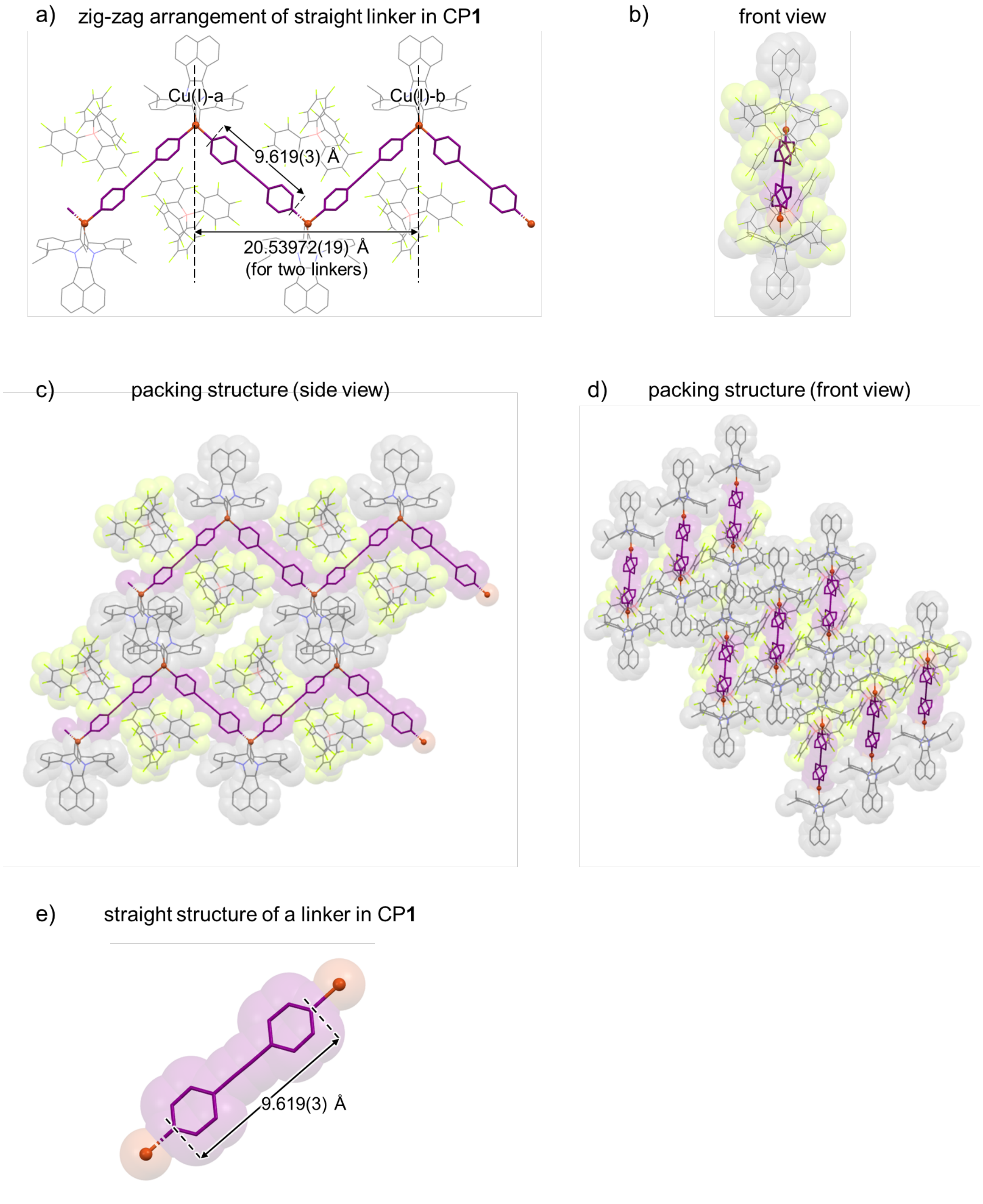
## 3. Data for Single-Crystal X-Ray Structural Analyses

Single-crystal X-ray structural analyses were carried out on a Rigaku XtaLAB Synergy diffractometer using graphite monochromated Mo-$K_\alpha$ radiation. The structure was solved by direct methods and expanded using Fourier techniques. Non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined using the riding model. All calculations were performed using the Olex2 crystallographic software package except for refinement, which was performed using SHELXL-2013.[5]

**Table S1**. Summary of X-ray crystallographic data of the crystal **1**, **2**, and **3**.

| compound | Crystal **1** | Crystal **2** | Crystal **3** |
|---|---|---|---|
| CCDC Number | 2435084 | 2435085 | 2435086 |
| Empirical Formula | $C_{73}H_{48}BCuF_{20}N_4$ | $C_{81}H_{60}BCuF_{24}N_4$ | $C_{71}H_{56}BCuF_{24}N_4$ |
| Formula Weight | 1435.50 | 1619.68 | 1495.54 |
| Crystal System | triclinic | monoclinic | monoclinic |
| Crystal Size / mm | 0.10 × 0.10 × 0.01 | 0.20 × 0.10 × 0.10 | 0.20 × 0.20 × 0.10 |
| $a$ / Å | 11.41140(10) | 13.43416(5) | 12.27189(4) |
| $b$ / Å | 16.17480(10) | 19.85881(7) | 15.93292(4) |
| $c$ / Å | 19.6865(2) | 28.77729(10) | 36.59908(11) |
| $\alpha$ / ° | 113.2060(10) | 90 | 90 |
| $\beta$ / ° | 90.6480(10) | 93.4025(3) | 98.9216(3) |
| $\gamma$ / ° | 94.6670(10) | 90 | 90 |
| $V$ / Å$^3$ | 3324.88(5) | 7663.85(5) | 7069.53(3) |
| Space Group | $P$-1 | $P2_1$/c | $P2_1$/c |
| $Z$ value | 2 | 4 | 4 |
| $D_{\mathrm{calc}}$ / g cm$^{-3}$ | 1.434 | 1.404 | 1.405 |
| Temperature / K | 153 | 153 | 153 |
| $2\theta$max / ° | 152.542 | 153.150 | 152.634 |
| $\mu$(Cu $K_\alpha$) / mm$^{-1}$ | 1.369 | 1.330 | 1.390 |
| No. of Reflections | Total: 123929<br>Unique: 13389<br>Rint = 0.0382 | Total: 145062<br>Unique: 15890<br>Rint = 0.0307 | Total: 255188<br>Unique: 14384<br>Rint = 0.0415 |
| $R_1$[a] | 0.0400 | 0.0788 | 0.0546 |
| $wR_2$[b] | 0.1039 | 0.2149 | 0.1442 |
| GOF[c] | 1.047 | 1.070 | 1.050 |
| Max./Mini. peak $I$[d] / Å$^3$ | 0.75 e$^-$/-0.50 e$^-$ | 1.78 e$^-$/-0.84 e$^-$ | 0.88 e$^-$/-0.65 e$^-$ |
| Flack Parameter | - | - | - |

[a]: All data. [b]: All reflections. [c]: Goodness of Fit Indicator. [d]: in Final Diff. Map.


a) zig-zag arrangement of straight linker in CP**1**

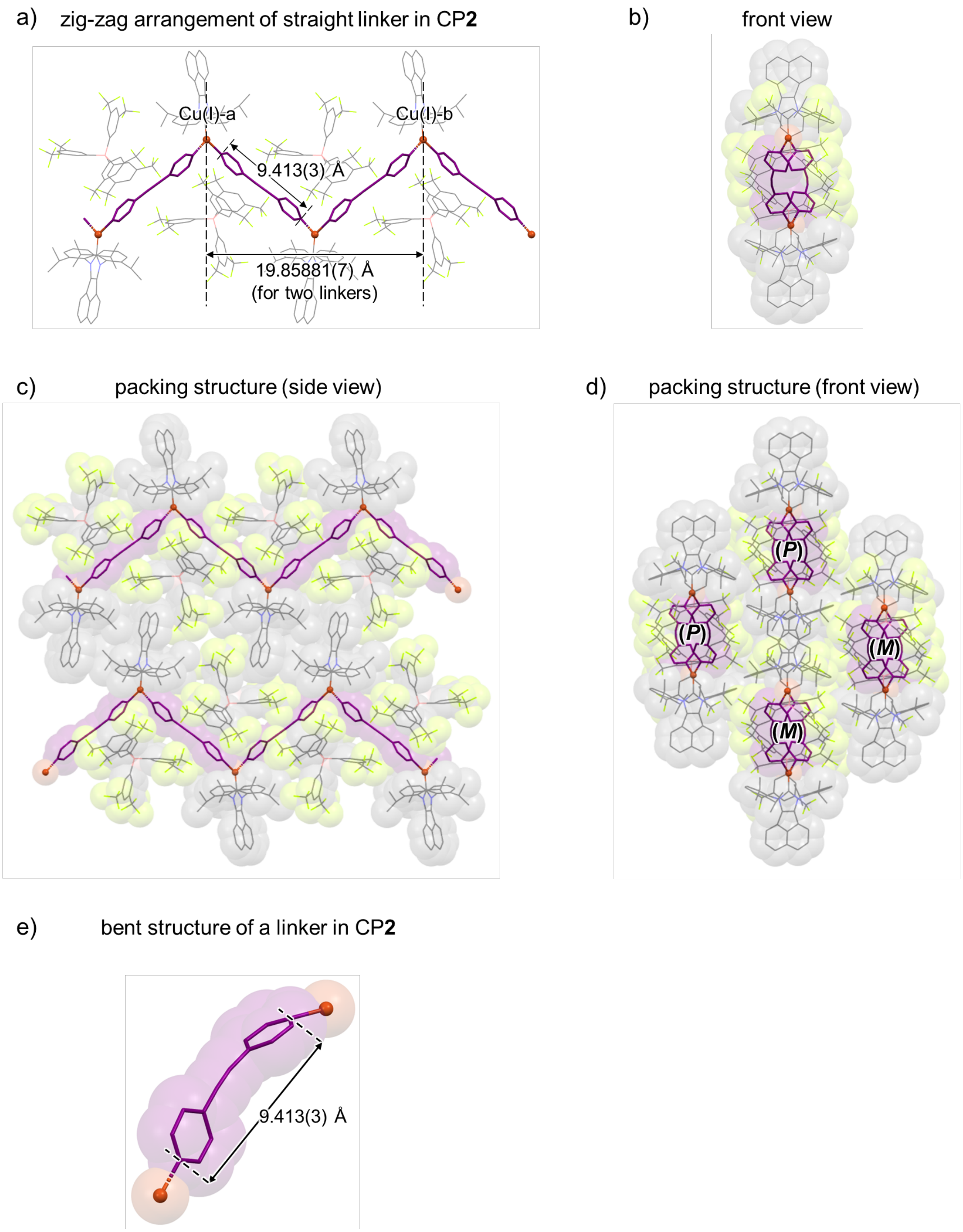
b) front view

c) packing structure (side view)

d) packing structure (front view)

e) straight structure of a linker in CP**1**

**Figure S1.** Molecular packing structure of crystal **1** at 153 K. H atoms are omitted for clarity. a) 1D zig-zag structure and b) the view from chain axis. c) Inter-chain packing structure and d) the view from chain axis. e) Illustration of the straight structure of a linker in chain.



a) zig-zag arrangement of straight linker in CP**2**

b) front view

c) packing structure (side view)

d) packing structure (front view)

e) bent structure of a linker in CP**2**

**Figure S2.** Molecular packing structure of crystal **2** at 153 K. H atoms are omitted for clarity. a) 1D helical structure and b) the view from helical axis. c) Inter-columnar packing structure and d) the view from helical axis. e) Illustration of the bent structure of a linker in column.

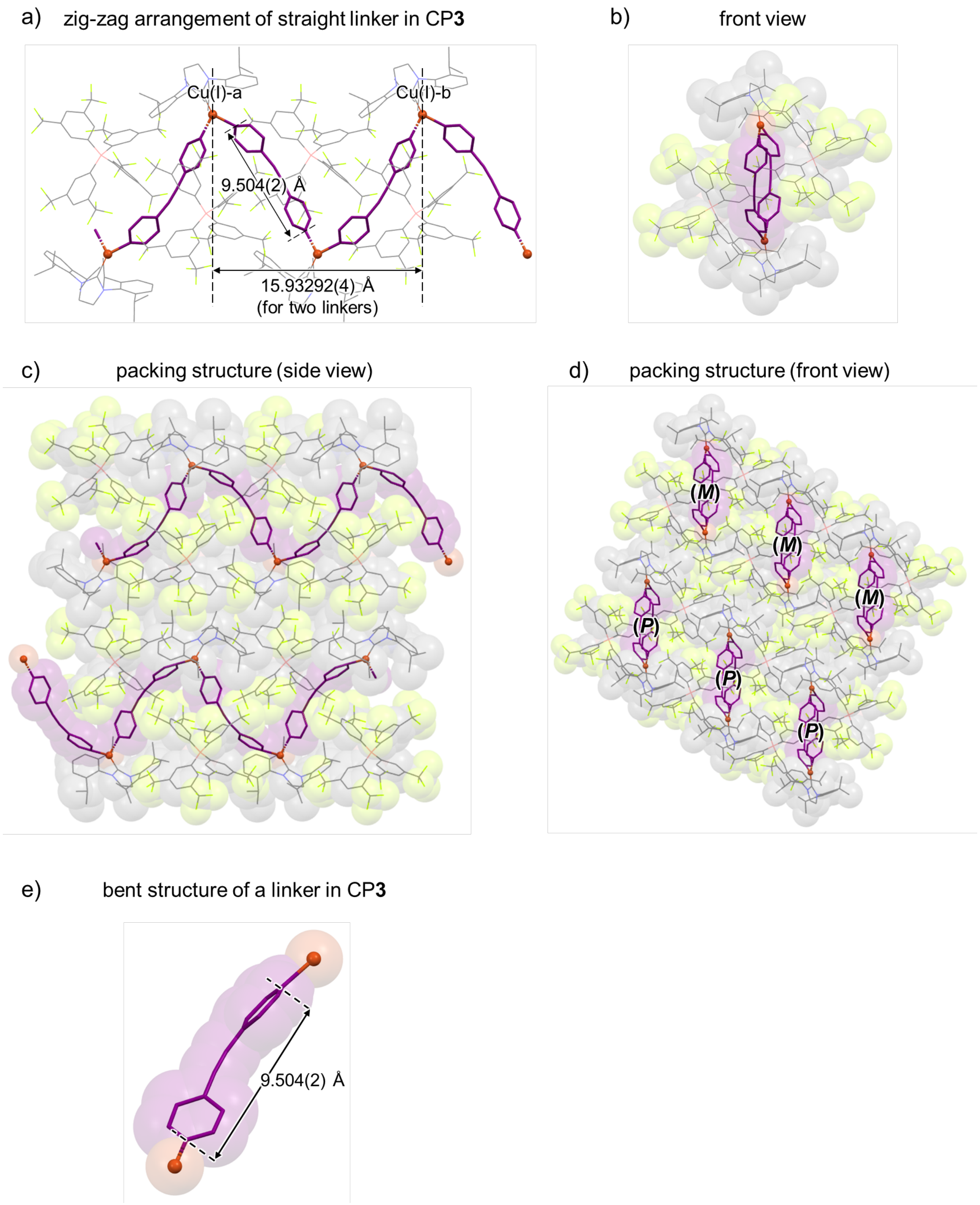


**Figure S3.** Molecular packing structure of crystal **3** at 153 K. H atoms are omitted for clarity. a) 1D helical structure and b) the view from helical axis. c) Inter-columnar packing structure and d) the view from helical axis. e) Illustration of the bent structure of a linker in column.

## 4. References

1. Q. Cao, J. L. Howard, E. Wheatley, D. L. Browne, *Angew. Chem.*, **2018**, *130*, 11509–11513.; I. I. Ishfaq, N. V. Tzouras, W. Janssens, T. Scattolin, L. Bourda, S. Bhandary, K. Van Hecke, S. P. Nolan, C. S. J. Cazin, *Chem. Eur. J.*, **2022**, *28*, e202201224.
2. Y. Li, Z. Su, H. Hao, J. Zhuang, *Chem. Commun.*, **2020**, *56*, 7669–7672.
3. D. Röth, J. Stirn, D. W. Stephan, L. Greb, *J. Am. Chem. Soc.,* **2021**, *143*, 15845–15851.
4. M. Jin, R. Ando, M. J. Jellen, M. A. Garcia-Garibay, H. Ito, *J. Am. Chem. Soc.*, **2021**, *143*, 1144–1153.
5. Sheldrick, G. M. SHELXL-2013, Program for the Refinement of Crystal Structures; University of Göttingen, Göttingen, Germany, 2013.

## 5. NMR Spectra

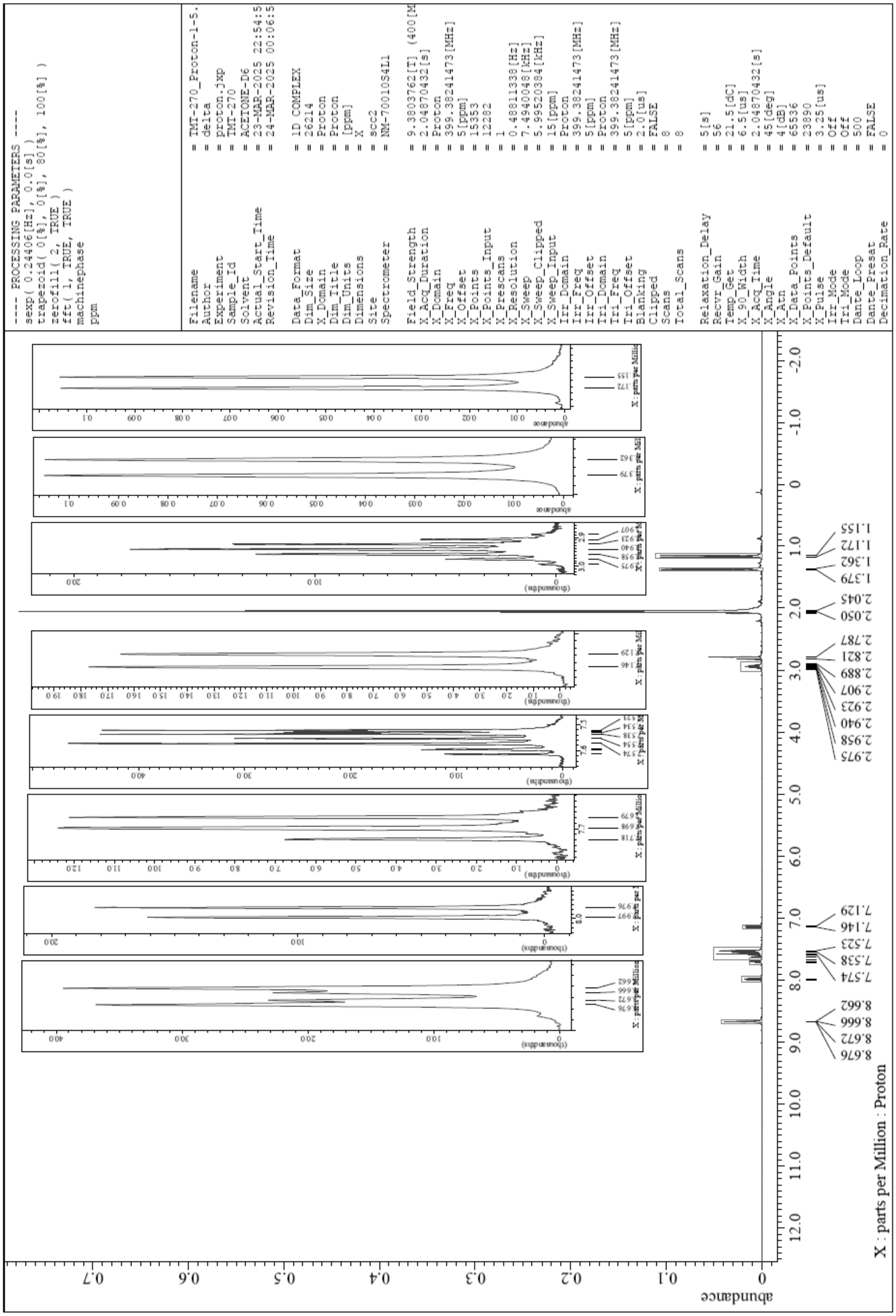


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**Figure S4**. $^1$H NMR spectrum (400 MHz, Acetone-$d_6$) of **1**.

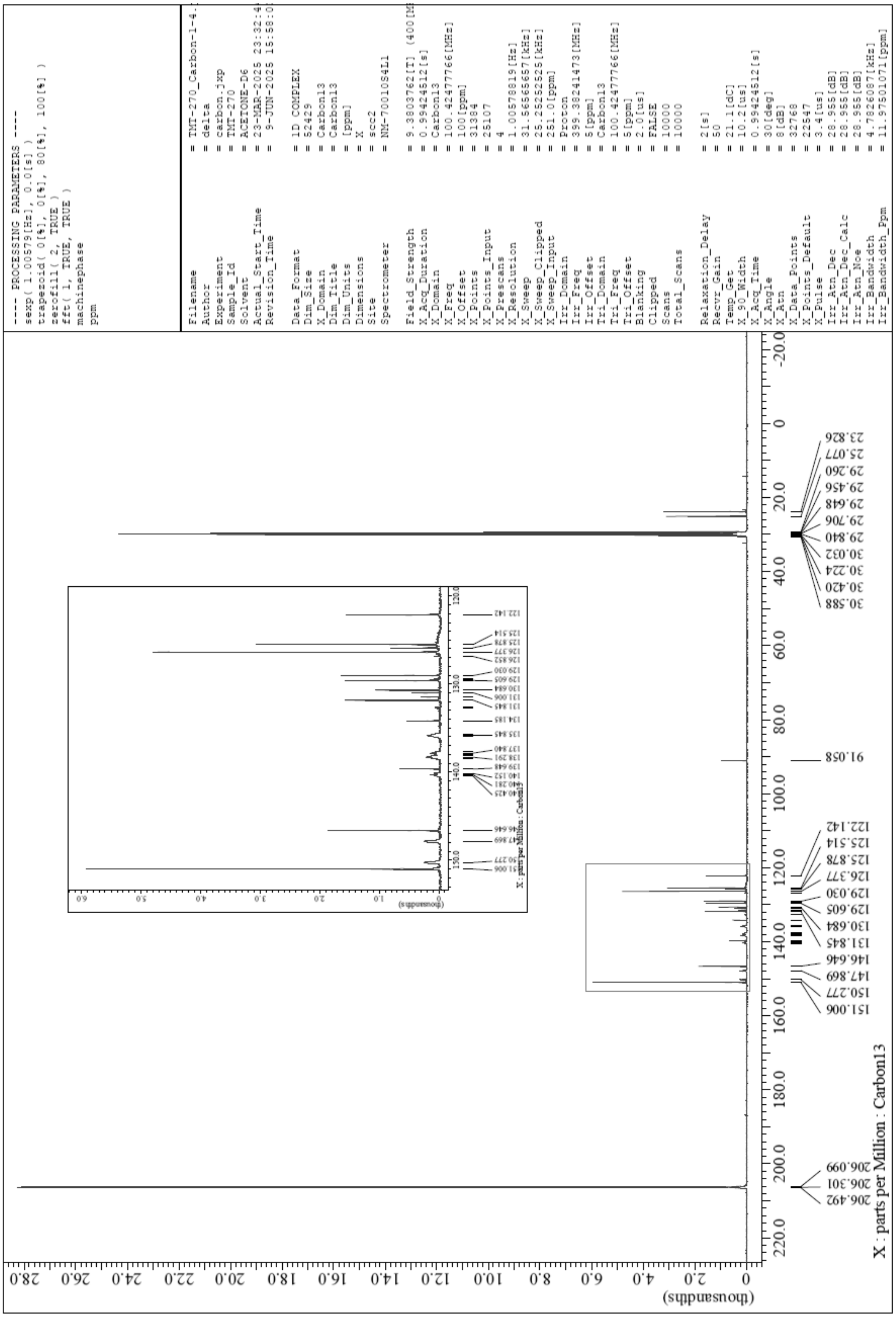

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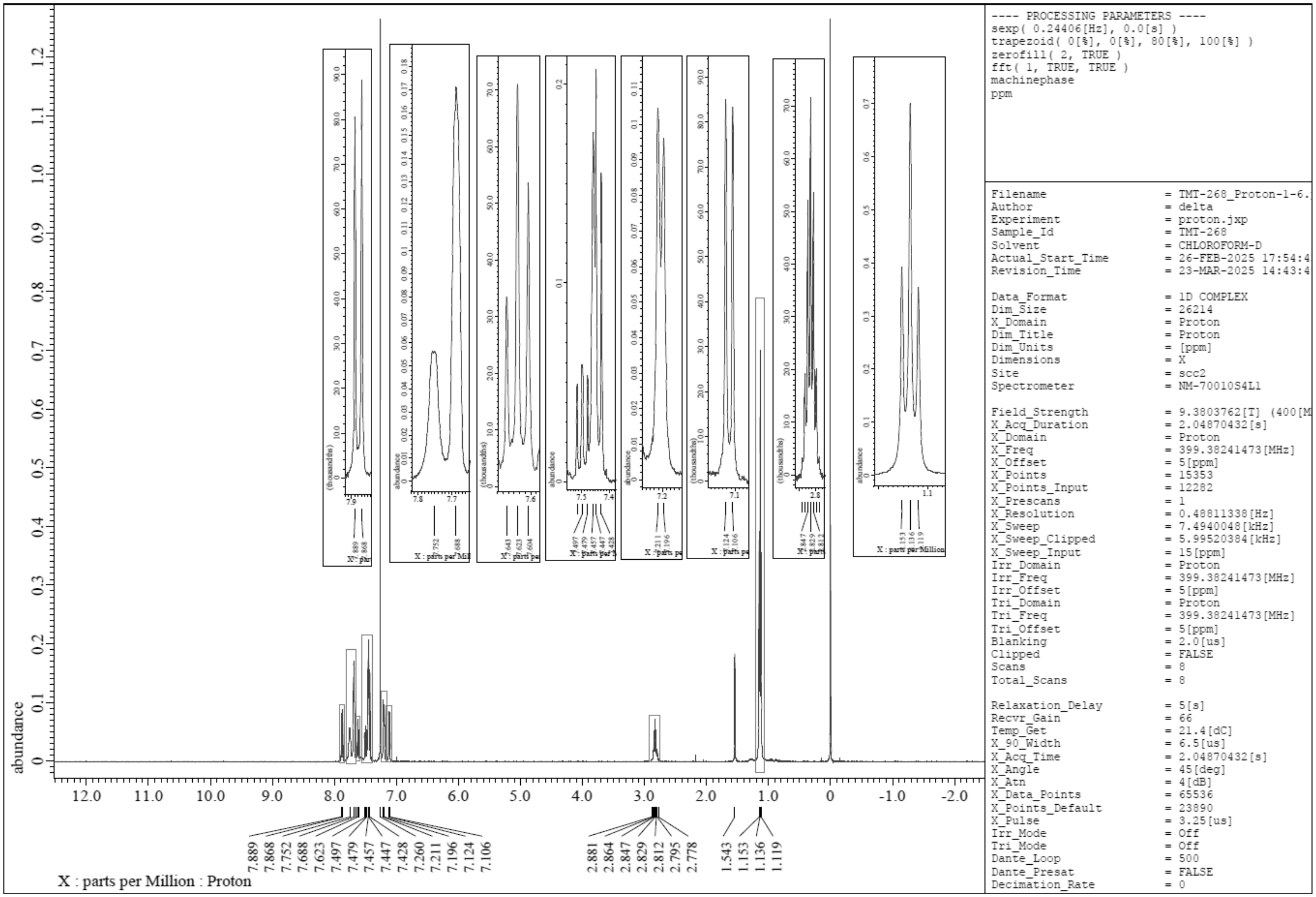
**Figure S5**. $^{13}$C NMR spectrum (100 MHz, Acetone-$d_6$) of **1**.



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Spectrometer              = NM-70010S4L1

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Total_Scans               = 8

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Tri_Mode                  = Off
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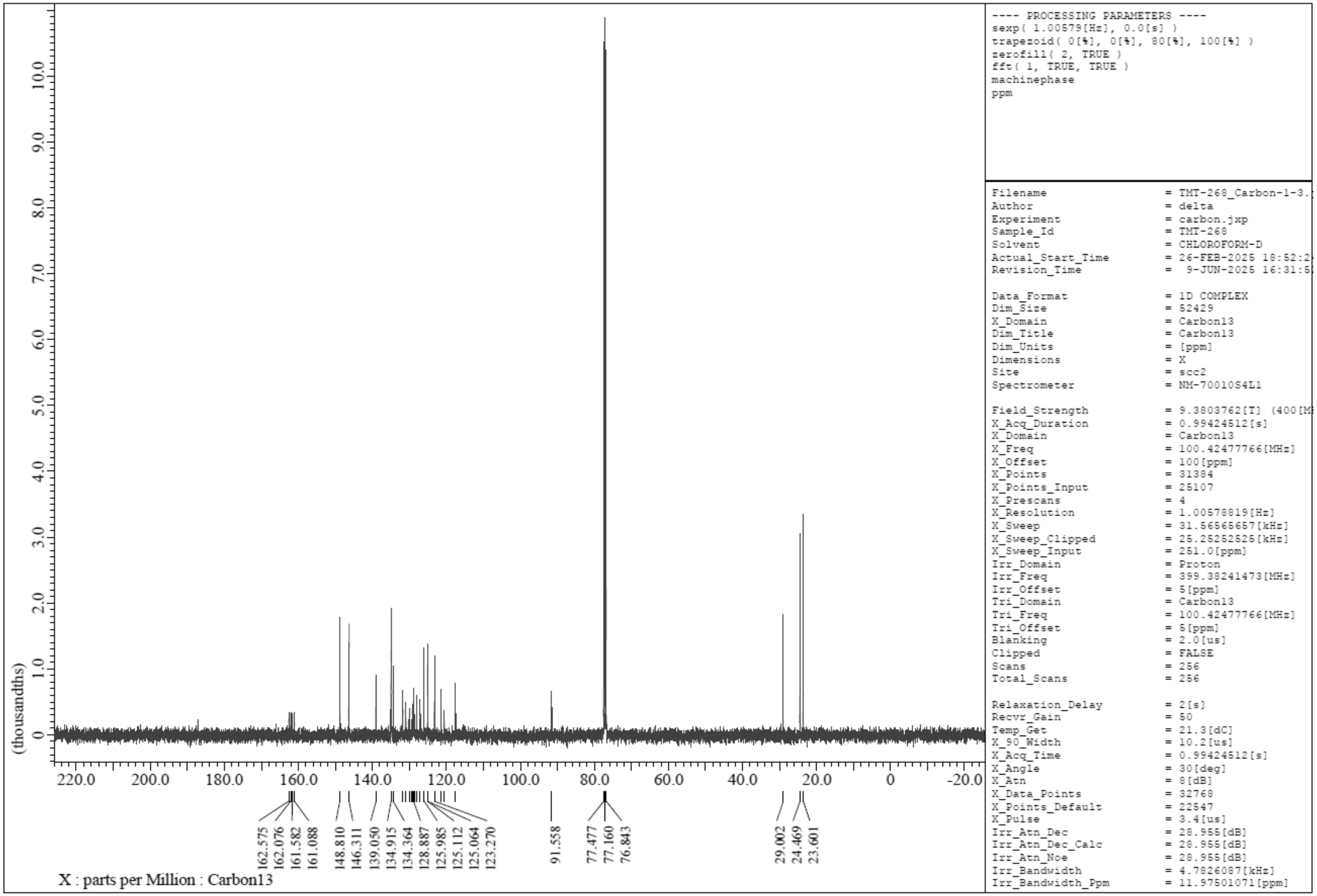
Decimation_Rate           = 0
```

**Figure S6**. ${}^1$H NMR spectrum (400 MHz, $CDCl_3$) of **2**.



```
---- PROCESSING PARAMETERS ----
sexp( 1.00579[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 2, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

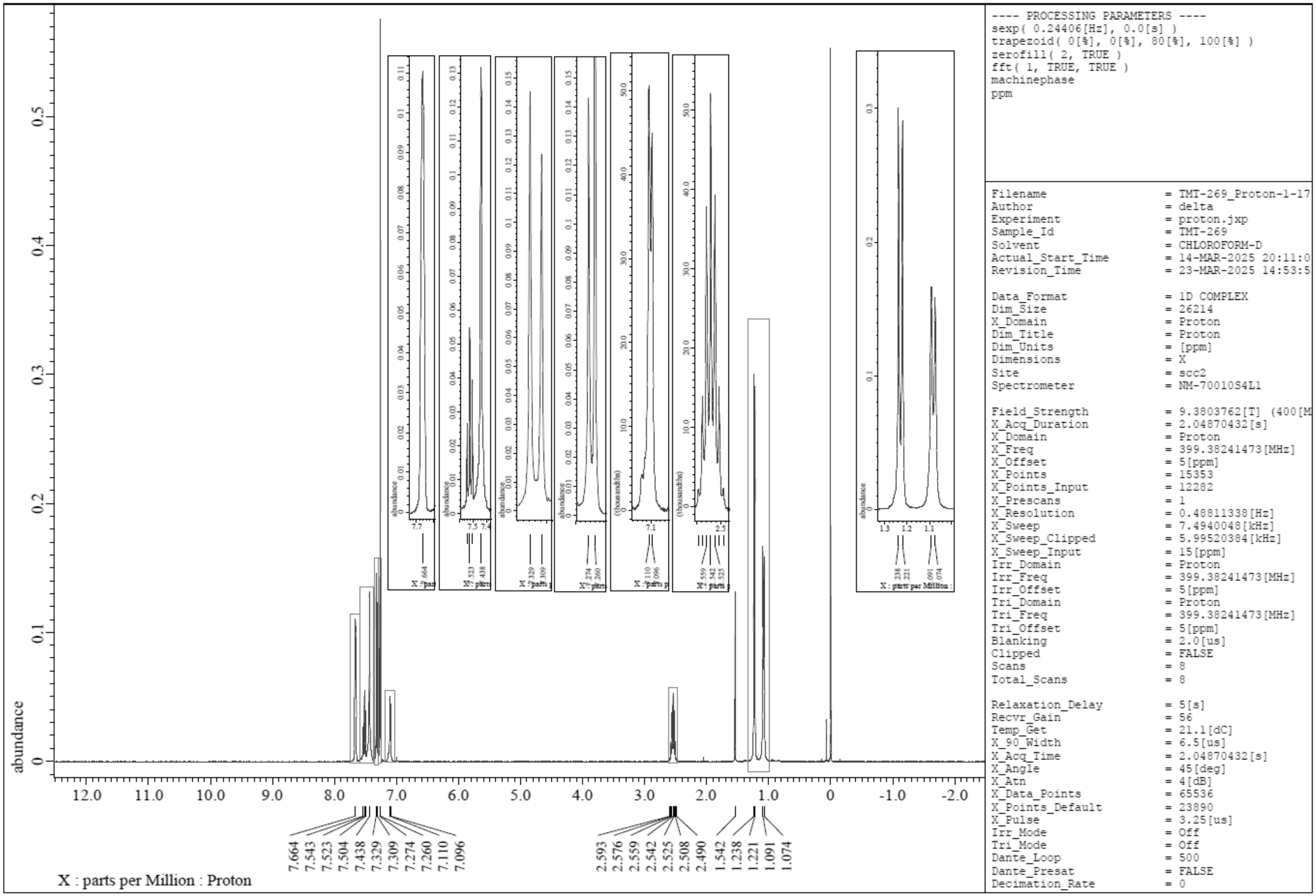
Filename                  = TMT-268_Carbon-1-3.
Author                    = delta
Experiment                = carbon.jxp
Sample_Id                 = TMT-268
Solvent                   = CHLOROFORM-D
Actual_Start_Time         = 26-FEB-2025 18:52:2
Revision_Time             =  9-JUN-2025 16:31:5

Data_Format               = 1D COMPLEX
Dim_Size                  = 52429
X_Domain                  = Carbon13
Dim_Title                 = Carbon13
Dim_Units                 = [ppm]
Dimensions                = X
Site                      = scc2
Spectrometer              = NM-70010S4L1

Field_Strength            = 9.3803762[T] (400[M
X_Acq_Duration            = 0.99424512[s]
X_Domain                  = Carbon13
X_Freq                    = 100.42477766[MHz]
X_Offset                  = 100[ppm]
X_Points                  = 31384
X_Points_Input            = 25107
X_Prescans                = 4
X_Resolution              = 1.00578819[Hz]
X_Sweep                   = 31.56565657[kHz]
X_Sweep_Clipped           = 25.25252525[kHz]
X_Sweep_Input             = 251.0[ppm]
Irr_Domain                = Proton
Irr_Freq                  = 399.38241473[MHz]
Irr_Offset                = 5[ppm]
Tri_Domain                = Carbon13
Tri_Freq                  = 100.42477766[MHz]
Tri_Offset                = 5[ppm]
Blanking                  = 2.0[us]
Clipped                   = FALSE
Scans                     = 256
Total_Scans               = 256

Relaxation_Delay          = 2[s]
Recvr_Gain                = 50
Temp_Get                  = 21.3[dC]
X_90_Width                = 10.2[us]
X_Acq_Time                = 0.99424512[s]
X_Angle                   = 30[deg]
X_Atn                     = 8[dB]
X_Data_Points             = 32768
X_Points_Default          = 22547
X_Pulse                   = 3.4[us]
Irr_Atn_Dec               = 28.955[dB]
Irr_Atn_Dec_Calc          = 28.955[dB]
Irr_Atn_Noe               = 28.955[dB]
Irr_Bandwidth             = 4.7826087[kHz]
Irr_Bandwidth_Ppm         = 11.97501071[ppm]
```

**Figure S7**. $^{13}$C NMR spectrum (100 MHz, $CDCl_3$) of **2**.



```
---- PROCESSING PARAMETERS ----
sexp( 0.24406[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 2, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

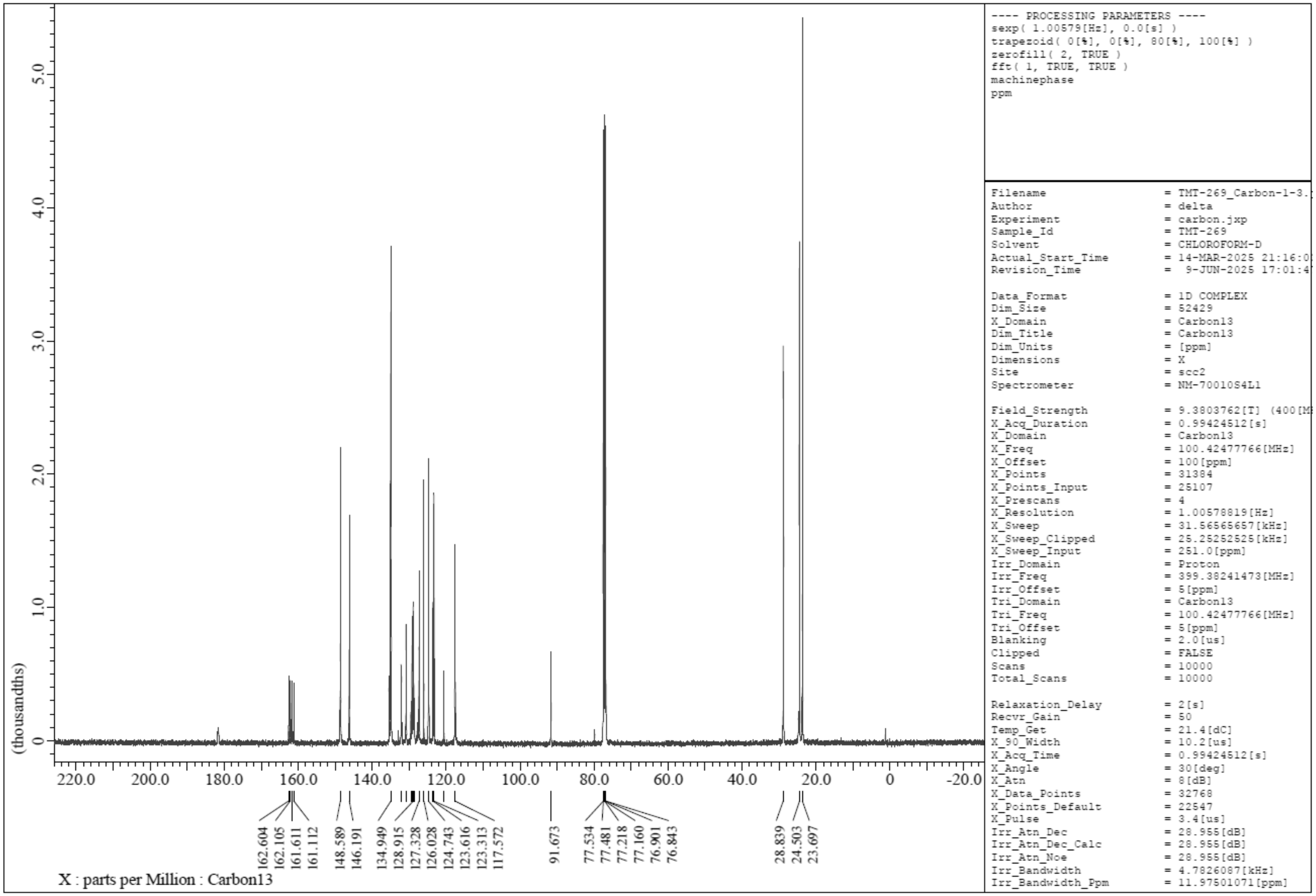
Filename              = TMT-269_Proton-1-17
Author                = delta
Experiment            = proton.jxp
Sample_Id             = TMT-269
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 14-MAR-2025 20:11:0
Revision_Time         = 23-MAR-2025 14:53:5

Data_Format           = 1D COMPLEX
Dim_Size              = 26214
X_Domain              = Proton
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Site                  = scc2
Spectrometer          = NM-70010S4L1

Field_Strength        = 9.3803762[T] (400[M
X_Acq_Duration        = 2.04870432[s]
X_Domain              = Proton
X_Freq                = 399.38241473[MHz]
X_Offset              = 5[ppm]
X_Points              = 15353
X_Points_Input        = 12282
X_Prescans            = 1
X_Resolution          = 0.48811338[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
X_Sweep_Input         = 15[ppm]
Irr_Domain            = Proton
Irr_Freq              = 399.38241473[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.38241473[MHz]
Tri_Offset            = 5[ppm]
Blanking              = 2.0[us]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 56
Temp_Get              = 21.1[dC]
X_90_Width            = 6.5[us]
X_Acq_Time            = 2.04870432[s]
X_Angle               = 45[deg]
X_Atn                 = 4[dB]
X_Data_Points         = 65536
X_Points_Default      = 23890
X_Pulse               = 3.25[us]
Irr_Mode              = Off
Tri_Mode              = Off
Dante_Loop            = 500
Dante_Presat          = FALSE
Decimation_Rate       = 0
```

**Figure S8**. $^1$H NMR spectrum (400 MHz, $CDCl_3$) of **3**.



```
---- PROCESSING PARAMETERS ----
sexp( 1.00579[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 2, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename                 = TMT-269_Carbon-1-3.
Author                   = delta
Experiment               = carbon.jxp
Sample_Id                = TMT-269
Solvent                  = CHLOROFORM-D
Actual_Start_Time        = 14-MAR-2025 21:16:0
Revision_Time            =  9-JUN-2025 17:01:4

Data_Format              = 1D COMPLEX
Dim_Size                 = 52429
X_Domain                 = Carbon13
Dim_Title                = Carbon13
Dim_Units                = [ppm]
Dimensions               = X
Site                     = scc2
Spectrometer             = NM-70010S4L1

Field_Strength           = 9.3803762[T] (400[M
X_Acq_Duration           = 0.99424512[s]
X_Domain                 = Carbon13
X_Freq                   = 100.42477766[MHz]
X_Offset                 = 100[ppm]
X_Points                 = 31384
X_Points_Input           = 25107
X_Prescans               = 4
X_Resolution             = 1.00578819[Hz]
X_Sweep                  = 31.56565657[kHz]
X_Sweep_Clipped          = 25.25252525[kHz]
X_Sweep_Input            = 251.0[ppm]
Irr_Domain               = Proton
Irr_Freq                 = 399.38241473[MHz]
Irr_Offset               = 5[ppm]
Tri_Domain               = Carbon13
Tri_Freq                 = 100.42477766[MHz]
Tri_Offset               = 5[ppm]
Blanking                 = 2.0[us]
Clipped                  = FALSE
Scans                    = 10000
Total_Scans              = 10000

Relaxation_Delay         = 2[s]
Recvr_Gain               = 50
Temp_Get                 = 21.4[dC]
X_90_Width               = 10.2[us]
X_Acq_Time               = 0.99424512[s]
X_Angle                  = 30[deg]
X_Atn                    = 8[dB]
X_Data_Points            = 32768
X_Points_Default         = 22547
X_Pulse                  = 3.4[us]
Irr_Atn_Dec              = 28.955[dB]
Irr_Atn_Dec_Calc         = 28.955[dB]
Irr_Atn_Noe              = 28.955[dB]
Irr_Bandwidth            = 4.7826087[kHz]
Irr_Bandwidth_Ppm        = 11.97501071[ppm]
```

**Figure S9**. ${}^{13}C$ NMR spectrum (100 MHz, $CDCl_3$) of **3**.