Electronic Supplementary Information

The temperature-controllable photomechanical behavior of α-isocyanostilbene derivative

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Contents

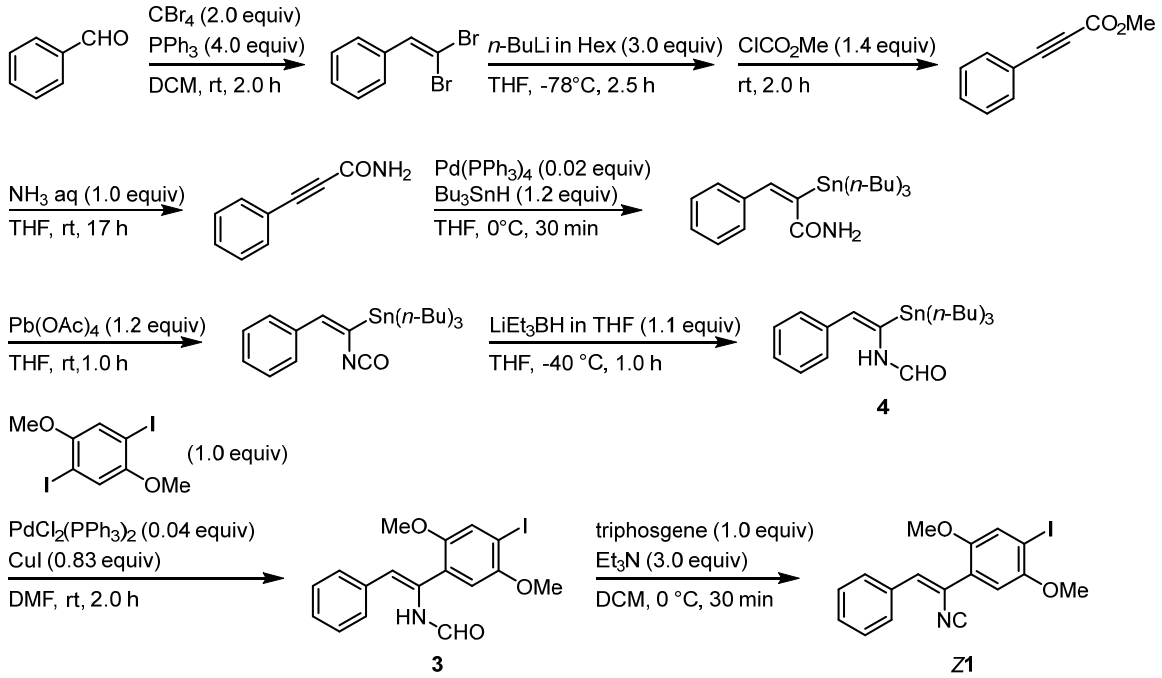
1. General

All commercially available reagents and solvents are of reagent grade and were used without further purification unless otherwise noted. Solvents for the synthesis were purchased from commercial suppliers, degassed by three freeze-pump-thaw cycles and further dried over molecular sieves (4 Å). Purification by column chromatography was performed with a silica gel 60N (spherical, neutral, 40–100 μm mesh, Kanto chemicals, Japan). NMR spectra were recorded on a JEOL ECA-600 spectrometer (^{1}H: 600 MHz; ^{13}C: 151 MHz) using tetramethylsilane and $CDCl_3$ as internal standards, respectively. UV-vis absorption spectra were recorded on a JASCO V-750 spectrometer. The absorption spectra of the solid samples were recorded on a JASCO V-750 spectrophotometer equipped with JASCO ISV-922 integrating sphere. Emission spectra were recorded on a JASCO FP-8600 spectrometer. Luminescence microscopic spectra were recorded on a Photonic Hamamatsu PMA-12 Multichannel Analyzer (C14631-01). A cooling/heating stage on JHC 10002L was used for temperature changes of solid samples. High resolution mass spectra were recorded on a Thermo Scientific Exactive at the Center for analytical instrumentation at Chiba University. Photographs were obtained using Olympus BX53, SZX10, or Leica M205c microscopes with Sony α7S, Olympus DP74, or Leica Flexacam C3 digital cameras, respectively. Differential scanning calorimetry (DSC) measurements were recorded on a Shimadzu DSC60 instrument using Al_2O_3 as a reference material. SEM images were recorded on a JEOL JCM-7000 instrument.

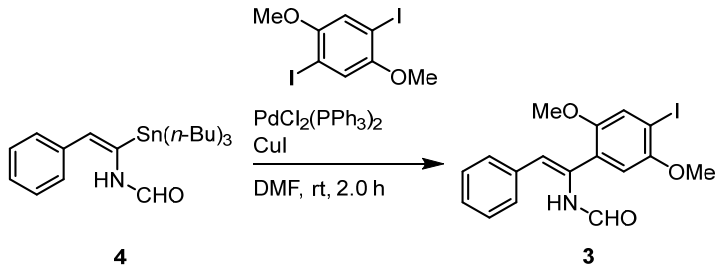
Single crystal X-ray diffraction analyses: A suitable crystal was mounted with Paratone oil on a MiTeGen MicroMounts and transferred to the Four-circle Kappa Geometry Goniometer of a RIGAKU XtaLAB Synergy-S or R/Si system with 1.2 kW PhotonJet-S microfocus rotating anode using graphite monochromated Cu-Kα radiation and HyPix-6000HE detector. Cell parameters were determined and refined, and raw frame data were integrated using CrysAlis^{Pro} (Rigaku Oxford Diffraction). The structures were solved by dual-space methods with (SHELXT)[S1] and refined by full-matrix least-squares techniques against F^2 (SHELXL-2018/3)[S2] by using Olex2 software package.[S3] The intensities were corrected for Lorentz and polarization effects. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were placed using AFIX instructions.

2. Synthesis

Synthesis of *Z***1** was performed according to the scheme below. Because the synthesis of **4** was reported previously, [S5] its preparation is not described below.



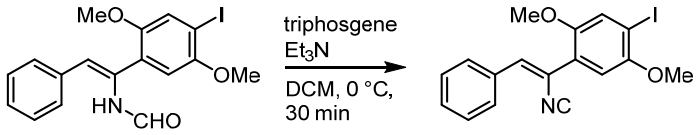
Synthesis of ***3***



An oven-dried two-neck flask was connected to a vacuum/nitrogen manifold through a rubber tube. It was evacuated and then backfilled with nitrogen. This cycle was repeated three times. To this flask, 1,4-diiodo-2,5-dimethoxybenzene (390 mg, 1.0 mmol), bis(triphenylphosphine)palladium(II) (28.1 mg, 4.0×10^{-2} mmol), copper(I) iodide (158 mg, 0.83 mmol) were added and dissolved in *N*,*N*-dimethylformamide (DMF) (4.2 mL). Then, **4**[S5] (436 mg, 1.0 mmol) was added and stirred at room temperature for 2.0 h. After the reaction completion was monitored by TLC analysis, the reaction was quenched by the addition of ca. 20 mL of ethyl acetate. The solution was extracted with ethyl acetate, and then washed with H_2O. The combined organic layers were dried over $MgSO_4$ and then evaporated in vacuo. The residue was purified by column chromatography on silica gel (ethyl acetate/*n*-hexane = 1:2) and obtained **3** as a yellow oil (287 mg, 0.7 mmol, 70%).

^{1}H NMR (600 MHz, $CDCl_3$, δ): 3.80 (s, 3H), 3.89 (s, 3H), 5.87 (s, 1H), 6.88 (s, 1H), 7.27–7.30 (m, 1H), 7.33 (s, 1H), 7.37–7.42 (m, 4H), 7.55, 7.56 (s, 1H, two sets of *H*N signals of amide rotamers), 8.06, 8.08 (s, 1H, two sets of C*H*O signals of amide rotamers). ^{13}C NMR (151 MHz, $CDCl_3$, δ): 56.4 (*C*H_3), 57.2 (*C*H_3), 87.3 (*C*), 113.5 (*C*H), 115.2 (*CH*), 122.4 (*C*H), 123.4 (*CH*), 125.7 (*C*), 127.6 (*C*H), 128.6 (*C*H), 129.2 (*C*H), 132.9 (*C*), 134.7 (*C*), 151.2 (*C*), 153.0 (*C*), 158.8 (*C*), 163.0 (*CH*). MS-ESI (*m*/*z*): $[M+H]^+$ called for $C_{17}H_{17}O_3NI$, 410.0248; found, 410.0240.

Synthesis of Z1



3 *Z***1**

An oven-dried two-neck flask was connected to a vacuum/nitrogen manifold through a rubber tube. It was evacuated and then backfilled with nitrogen. This cycle was repeated three times. To this flask, **3** (49.1 mg, 0.12 mmol), triethyamine (18.3 mg, 0.18 mmol) were added and dissolved in dichloromethane (3.0 mL). Then, triphosgene (17.8 mg, 6.0×10^{-2} mmol) was added and stirred at 0 °C for 30 min. After the reaction completion was monitored by TLC analysis, the reaction was quenched by the addition of ca. 20 mL of H_2O. The solution was extracted with dichloromethane and then washed with H_2O. The combined organic layers were dried over $MgSO_4$ and then evaporated in vacuo. The residue was purified by column chromatography on silica gel (dichloromethane/*n*-hexane = 2:1) and obtained *Z***1** as a yellow solid (24.3 mg, 6.2×10^{-2} mmol, 52%).

^{1}H NMR (600 MHz, $CDCl_3$, δ): 3.87 (s, 3H), 3.90 (s, 3H), 7.01 (s, 1H), 7.13 (s, 1H), 7.38–7.40 (m, 2H), 7.45 (t, J = 7.2 Hz, 2H), 7.77 (d, J = 7.8 Hz, 2H). ^{13}C NMR (151 MHz, $CDCl_3$, δ): 56.7 (*C*H_3), 57.2 (*C*H_3), 87.1 (*C*), 111.5 (*C*H), 119.5 (*C*), 123.4 (*C*H), 124.1 (*C*), 128.8 (*C*H), 129.5 (*C*H), 129.6 (*C*H), 132.2 (*C*H), 133.5 (*C*), 151.4 (*C*), 152.8 (*C*), 168.6 (*C*). MS-ESI (*m*/*z*): $[M+Na]^+$ calcd for $C_{17}H_{14}O_2NINa$, 413.9961; found, 413.9962.

3. Photophysical properties

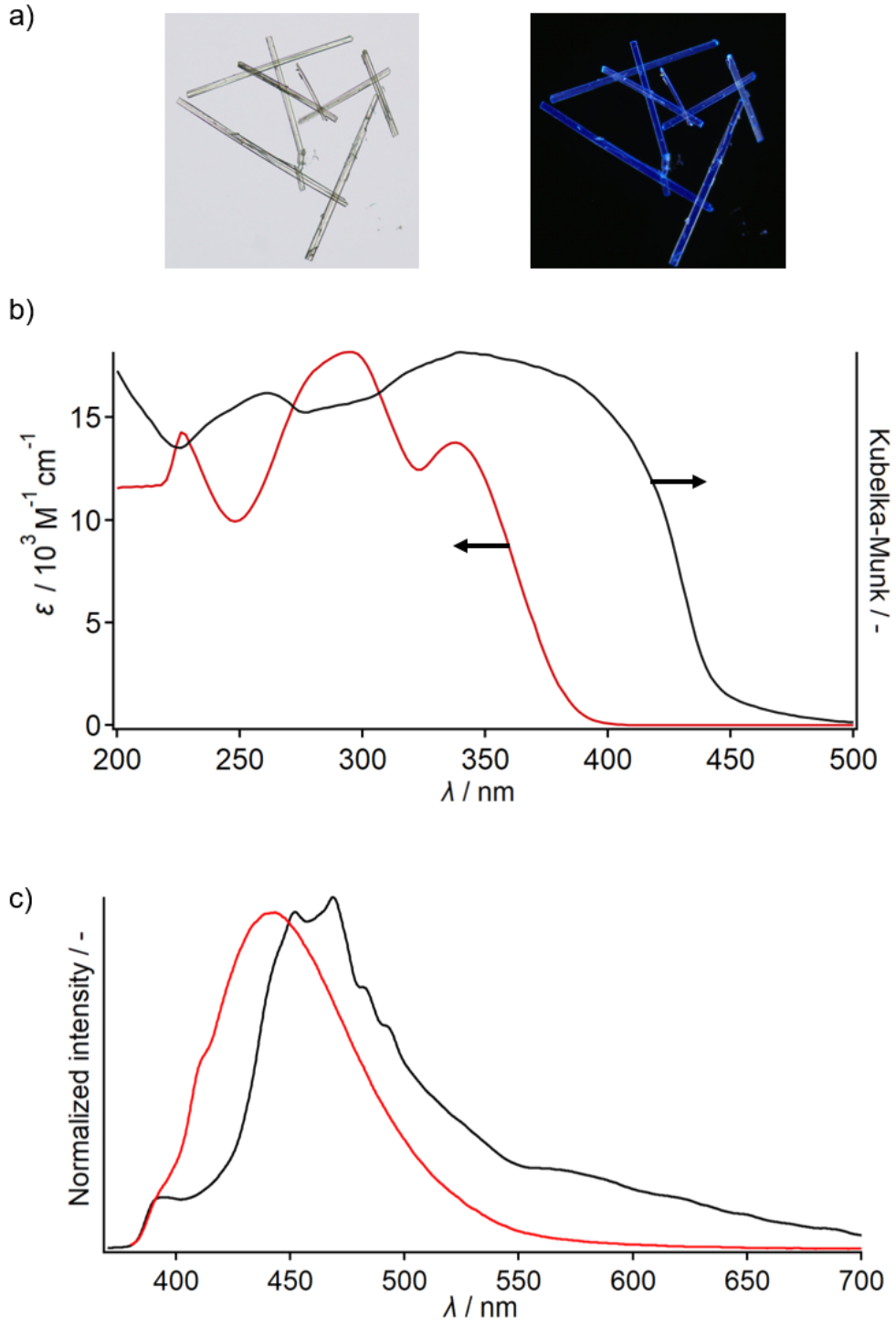


Fig. S1 a) Photographs of the crystals of *Z***1** taken under room light (left) and UV light (right). b) UV/vis absorption spectra of *Z***1** in CH_2Cl_2 (c = 10 µM, red line) and in the solid state (black line). c) Emission spectra of *Z***1** in CH_2Cl_2 (c = 10 µM, red line, λ_{ex} = 365 nm) and in the solid state (black line, λ_{ex} = 330 nm).

4. Photomechanical behaviors and their temperature dependence

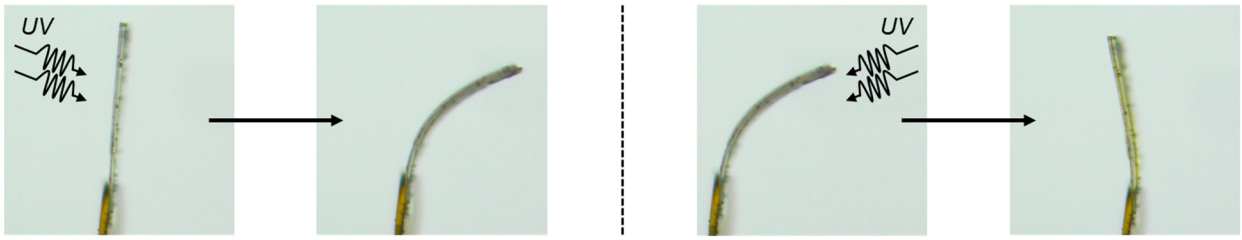


Fig. S2 Photographs of the crystals of *Z***1** upon photoirradiation by UV light.

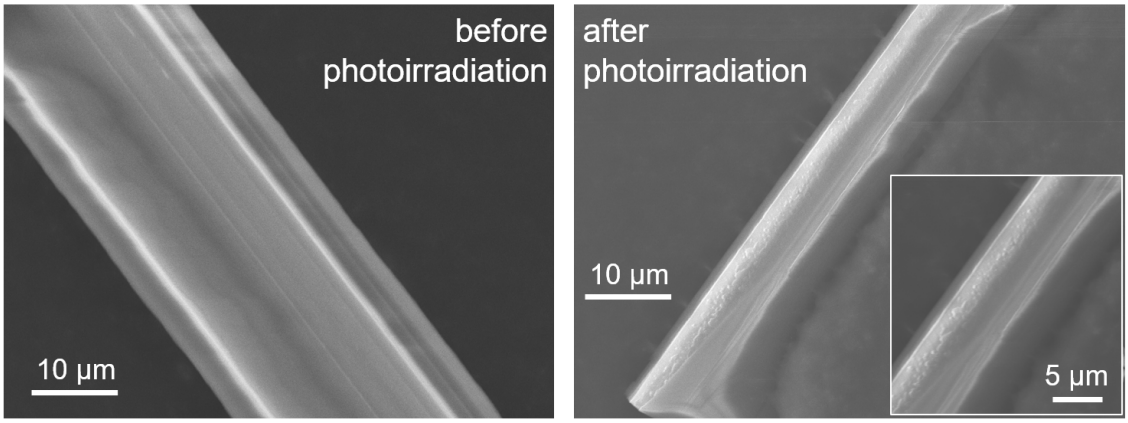


Fig. S3 Changes in SEM images of *Z***1** photoirradiation-induced bending at room temperature by UV light.

Note: Although the surface of the as-grown *Z***1** crystal before irradiation is smooth, that after photoirradiation and bending exhibits multiple small rough features, indicating a clear decrease in surface smoothness. We attribute the increased surface roughness to the formation of photogenerated species (**2** and/or *E***1**) within the ordered crystal lattice of *Z***1**.

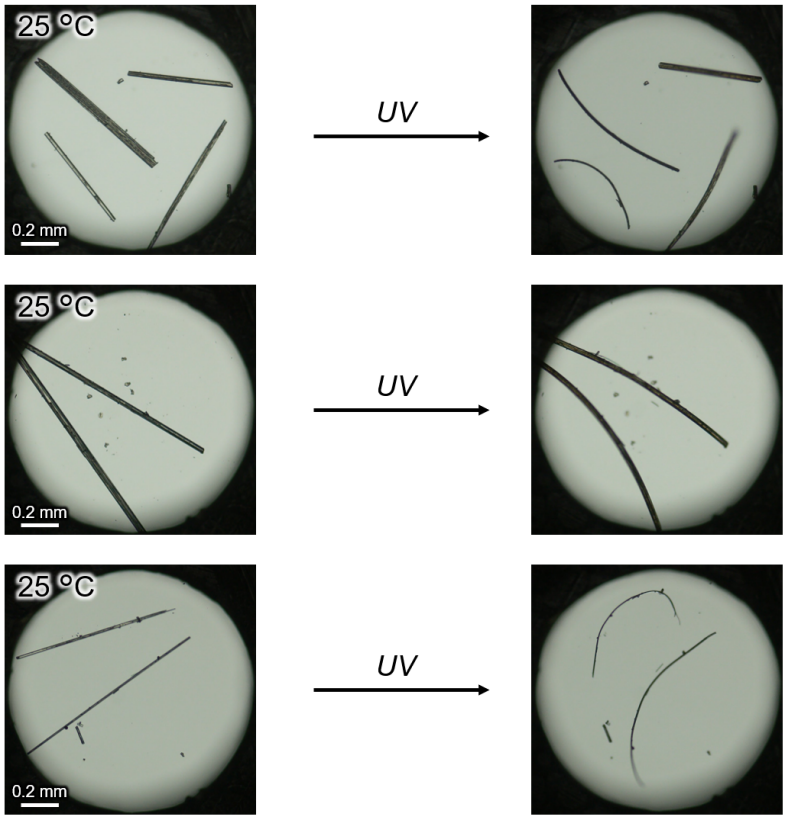


Fig. S4 Photographs of the crystals of *Z***1** upon photoirradiation by UV light.

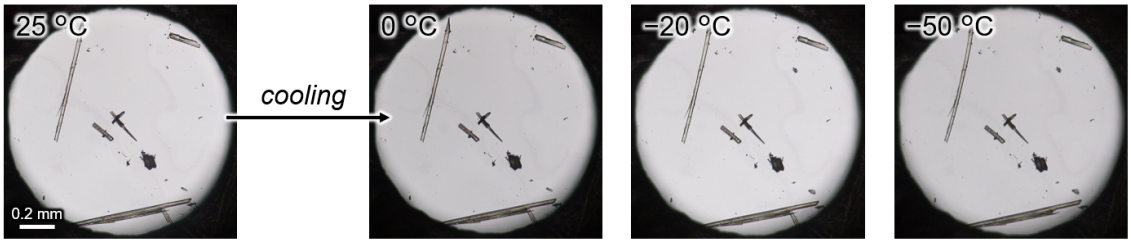


Fig. S5 Photographs of the crystals of *Z***1** taken under room light upon cooling from 25 to −50 °C.
Note: No shape change occurred without UV light.

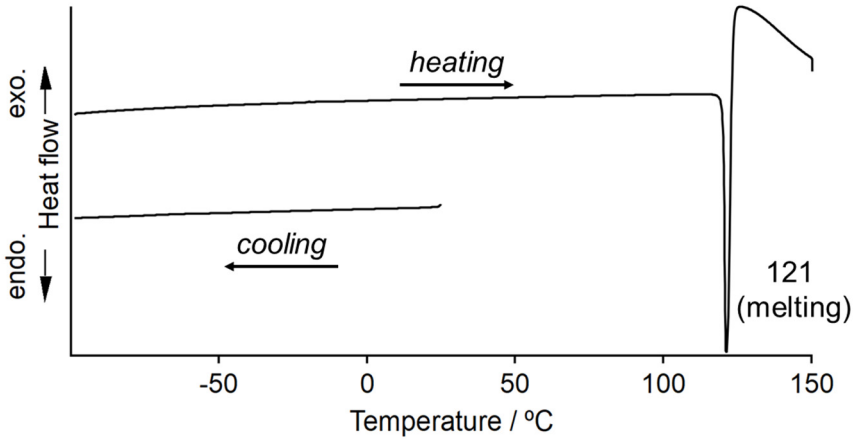


Fig. S6 DSC traces of *Z***1** at the heating/cooling rate of 5.0 °C/min.

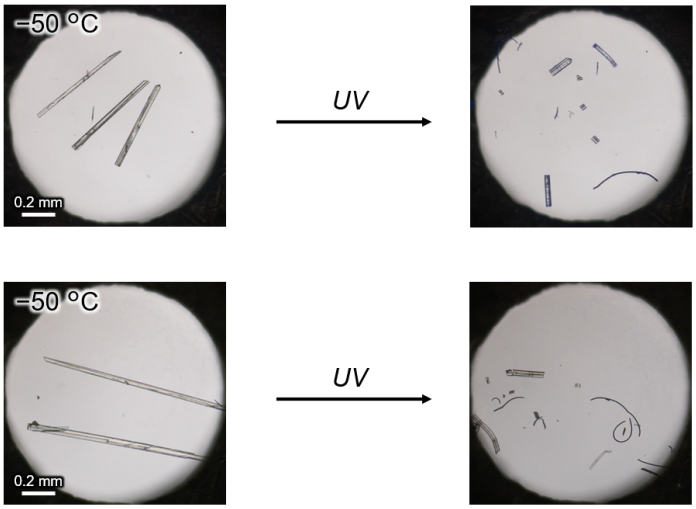


Fig. S7 Photographs of the crystals of *Z***1** upon photoirradiation at −50 °C (UV light).
Note: All the crystals of *Z***1** were split.

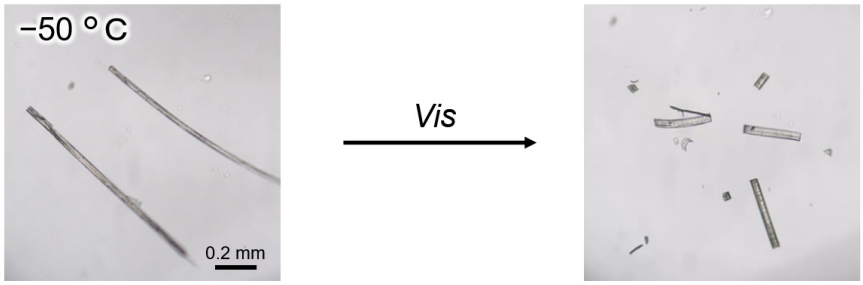


Fig. S8 Photographs of the crystals of *Z***1** upon visible-light irradiation by at −50 °C.
Note: All the crystals of *Z***1** were split, as observed under UV-light irradiation.

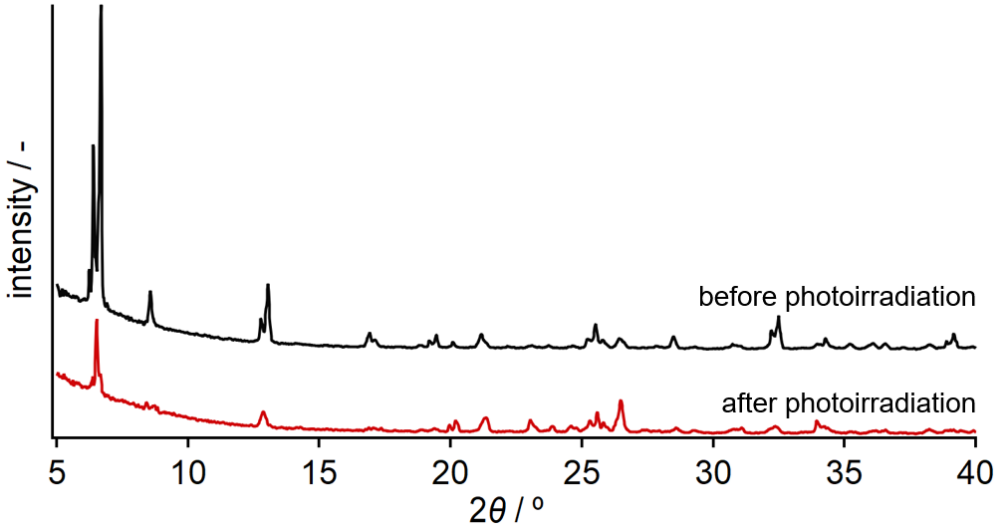


Fig. S9 Changes in PXRD patterns of *Z***1** before and after photoirradiation by UV light at −50 °C for 60 min.

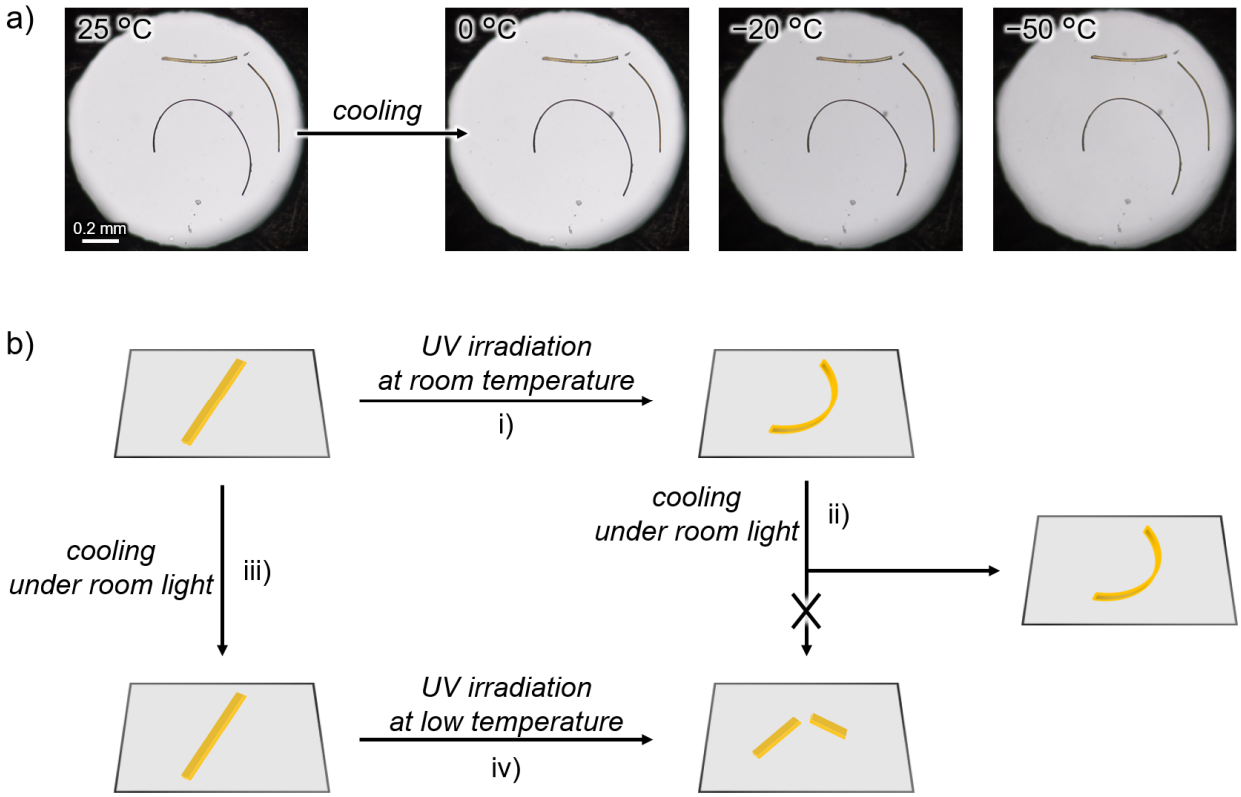


Fig. S10 a) Photographs of the bent crystals, which were obtained by UV light illumination of *Z***1** at 25 °C (i in Fig. S10b), upon cooling under room light (ii in Fig. S10b), in which no shape change occurred. b) Schematic representation of the experiments in Fig. S10a (i and ii) and in Fig. 2c (iii and iv).

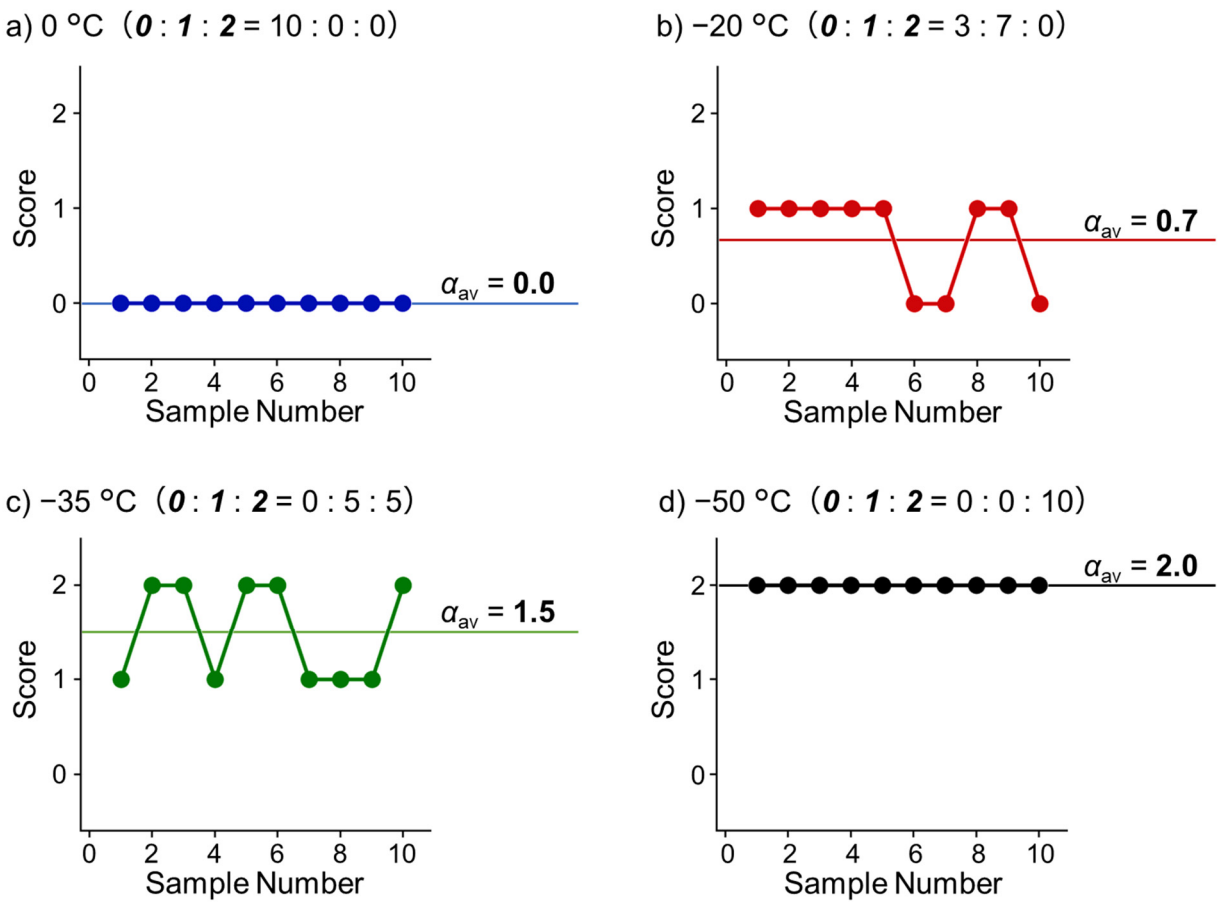


Fig. S11 Plots of the score by using ten individual crystals of *Z***1** at various temperatures.

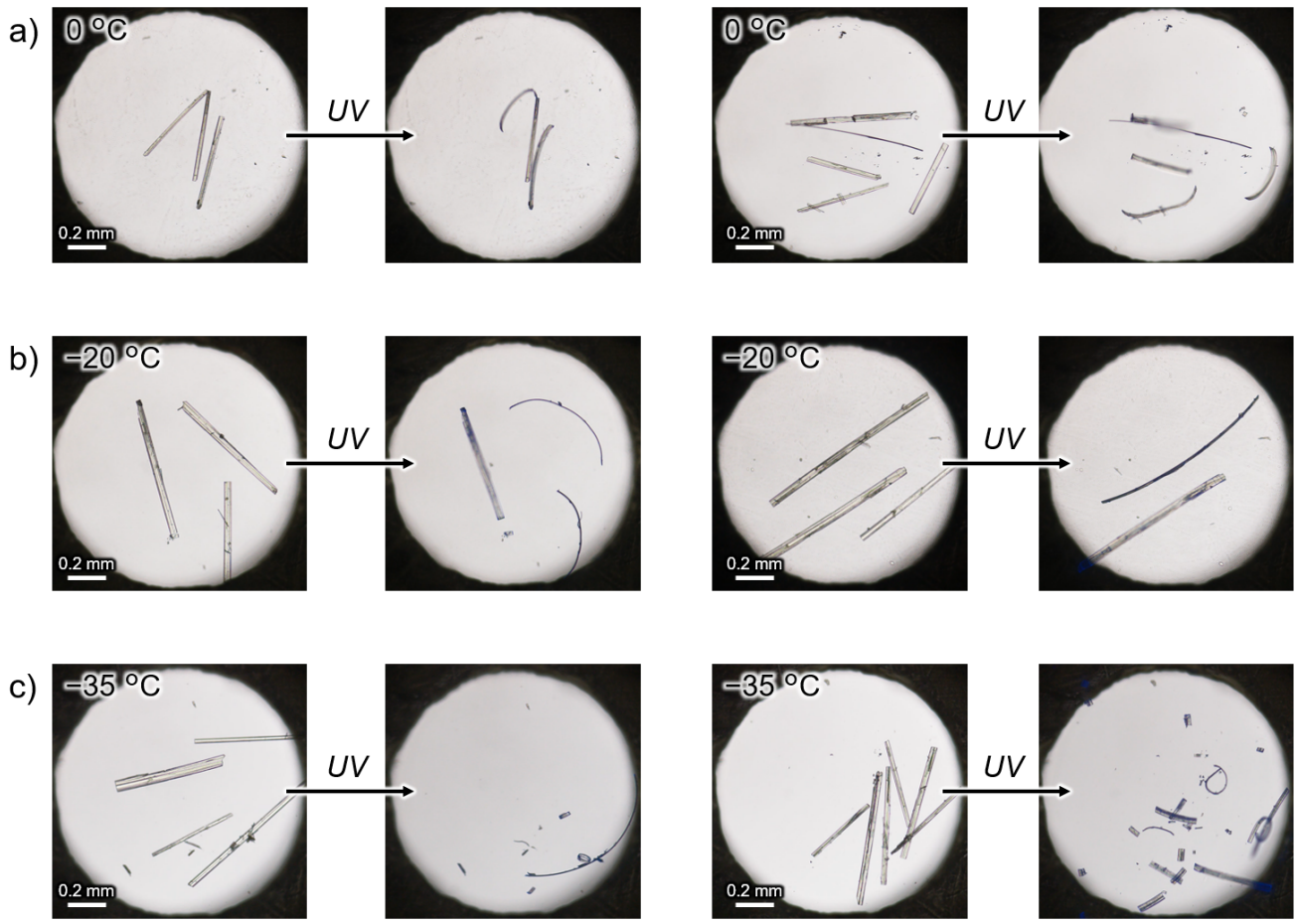


Fig. S12 Photographs of the crystals of *Z***1** upon photoirradiation at various temperatures.

5. Analyses of photochemical reactions

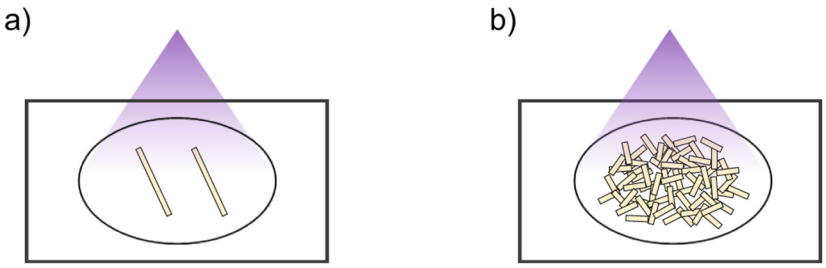


Fig. S13 Schematic representations of sample amounts of *Z***1** for a) observing the photomechanical effect and b) NMR measurements of the photoirradiated samples.

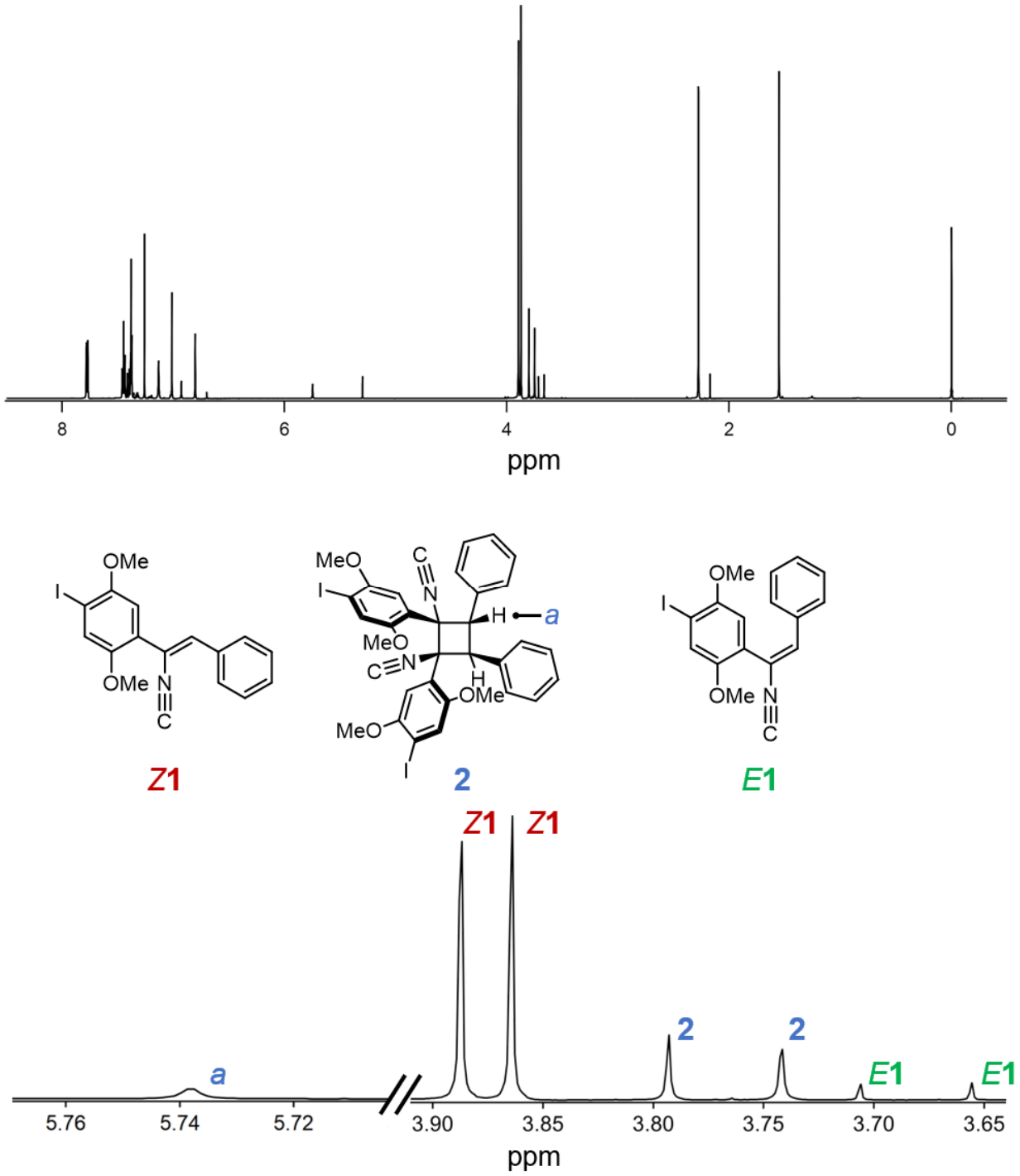


Fig. S14 Entire (above) and selected (bottom) regions of ^{1}H NMR spectrum of the samples, obtained by photoirradiation of *Z***1** for 60 min at −50 °C, in $CDCl_3$.

Note: Based on the previous works,[6,7] the observed signals of δ = 3.75, 3.81, and 5.75 ppm can be ascribed to **2**[6] and those of δ = 3.66 and 3.71 ppm can be ascribed to *E***1**.[7]

6. Crystal structure analyses

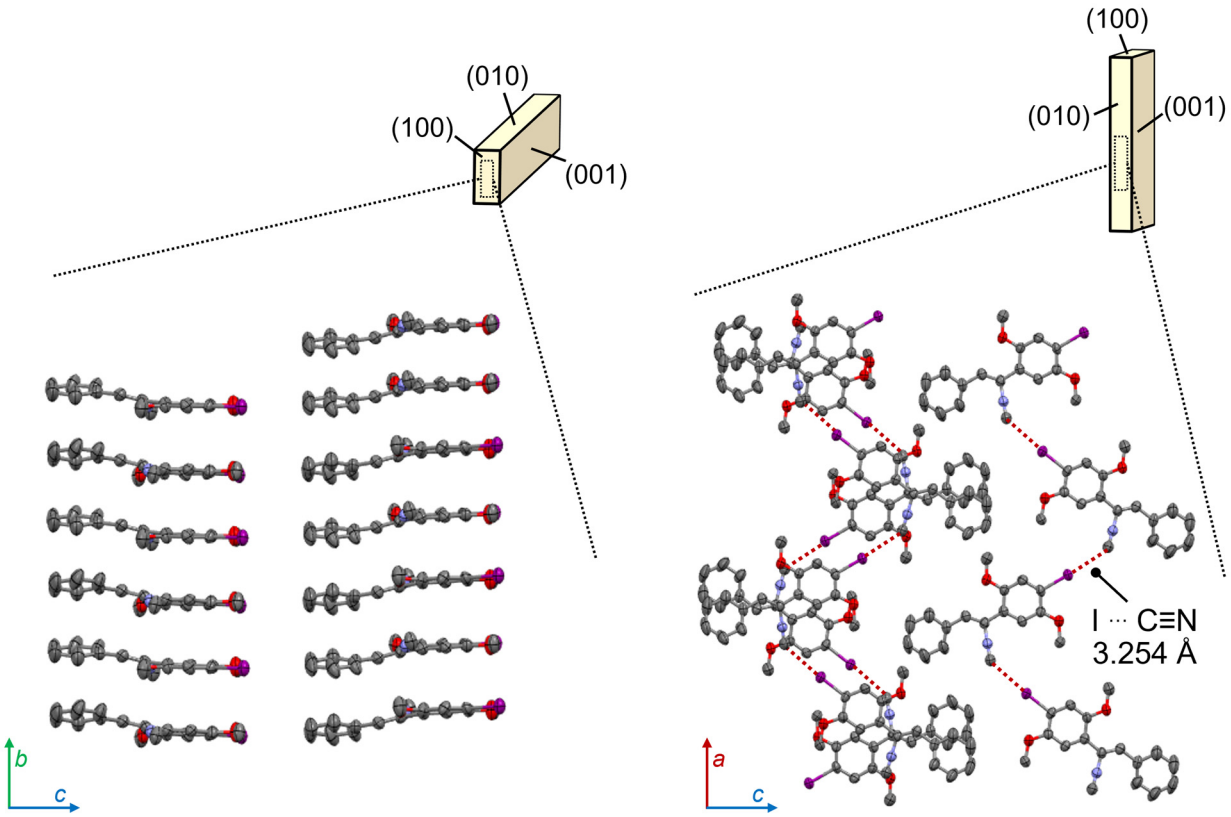


Fig. S15 Single-crystal structure of *Z***1** at 25 °C.

Table S1. Summary of X-ray crystallographic data.

compound	***Z*1** (25 °C)	***Z*1** (0 °C)	***Z*1** (−20 °C)
CCDC Number	2525256	2525257	2525258
Empirical Formula	$C_{17}H_{14}INO_2$	$C_{17}H_{14}INO_2$	$C_{17}H_{14}INO_2$
Formula Weight	391.19	391.19	391.19
Crystal System	orthorhombic	orthorhombic	orthorhombic
Crystal Size / mm	0.41 × 0.03 × 0.02	0.41 × 0.03 × 0.02	0.41 × 0.03 × 0.02
a / Å	16.1022(4)	16.0841(4)	16.0875(5)
b / Å	7.1059(2)	7.0891(2)	7.0639(3)
c / Å	27.7748(7)	27.7472(5)	27.7232(9)
α / °	90	90	90
β / °	90	90	90
γ / °	90	90	90
V / Å^3	3178.01(16)	3163.79(13)	3150.48(19)
Space Group	*Pbca*	*Pbca*	*Pbca*
Z / *Z*' values	8 / 1	8 / 1	8 / 1
D_{calc} / g cm^{-3}	1.635	1.643	1.649
Temperature / K	298.03(18)	273.00(10)	253.00(10)
$2\theta_{max}$ / °	136.428	136.482	136.428
μ(Cu K$_\alpha$) / mm^{-1}	15.864	15.935	16.002
No. of Reflections	Total: 10521	Total: 9790	Total: 9808
	Unique: 2895	Unique: 2893	Unique: 2864
	R_{int} = 0.0807	R_{int} = 0.0667	R_{int} = 0.0703
R_1[a]	0.0668	0.0651	0.0635
wR_2[b]	0.1789	0.2083	0.1749
GOF[c]	1.073	1.083	1.100
Max./Mini. peak *I*[d] / Å^3	1.80/−1.15	2.29/−0.98	1.91/−0.97

compound	***Z*1** (−50 °C)	***Z*1** (−100 °C)	**2**
CCDC Number	2525259	2525260	2525261
Empirical Formula	$C_{17}H_{14}INO_2$	$C_{17}H_{14}INO_2$	$C_{34}H_{28}I_2N_2O_4$
Formula Weight	391.19	391.19	782.38
Crystal System	orthorhombic	orthorhombic	monoclinic
Crystal Size / mm	0.41 × 0.03 × 0.02	0.41 × 0.03 × 0.02	0.28 × 0.16 × 0.03
a / Å	16.1063(6)	16.0629(5)	11.2144(3)
b / Å	7.0543(5)	7.0075(2)	14.0636(3)
c / Å	27.6933(10)	27.6441(9)	19.9281(5)
α / °	90	90	90
β / °	90	90	97.398(2)
γ / °	90	90	90
V / Å^3	3146.5(3)	3111.65(17)	3116.79(13)
Space Group	*Pbca*	*Pbca*	$P2_1/n$
Z / *Z*' values	8 / 1	8 / 1	4 / 1
D_{calc} / g cm^{-3}	1.652	1.670	1.667
Temperature / K	223.00(10)	173.02(10)	173.00(10)
$2\theta_{max}$ / °	154.812	136.46	136.472
μ(Cu K$_\alpha$) / mm^{-1}	16.023	16.202	16.175
No. of Reflections	Total: 10257	Total: 10322	Total: 20616
	Unique: 3118	Unique: 2834	Unique: 5683
	R_{int} = 0.0843	R_{int} = 0.0692	R_{int} = 0.0769
R_1[a]	0.0805	0.0560	0.0545
wR_2[b]	0.2185	0.1591	0.1549
GOF[c]	1.082	1.052	1.011
Max./Mini. peak *I*[d] / Å^3	2.26/−0.87	1.79/−1.45	2.06/−1.42

[a]:$I > 2.00\sigma(I)$. [b]:All reflections. [c]:Goodness of Fit Indicator. [d]:in Final Diff. Map.

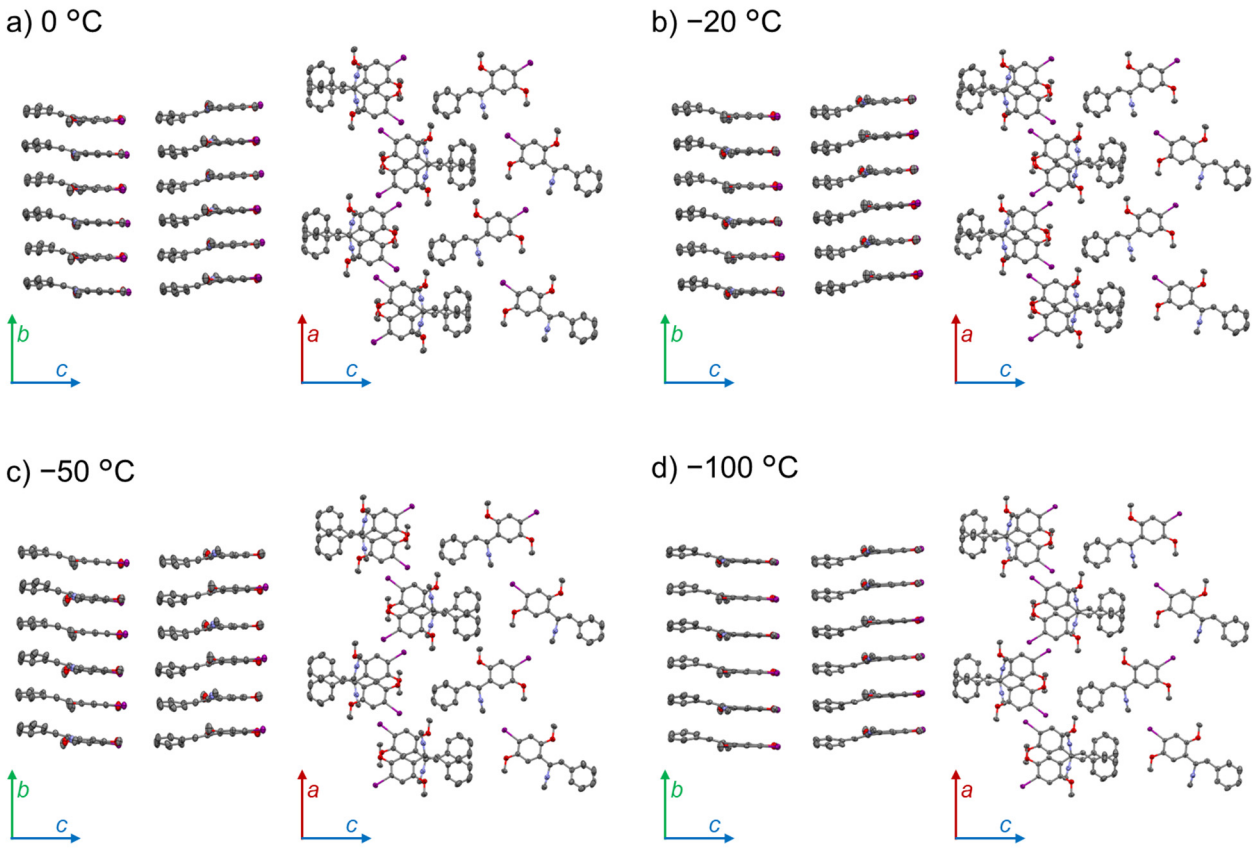


Fig. S16 Single-crystal structure of *Z***1** at various temperatures.

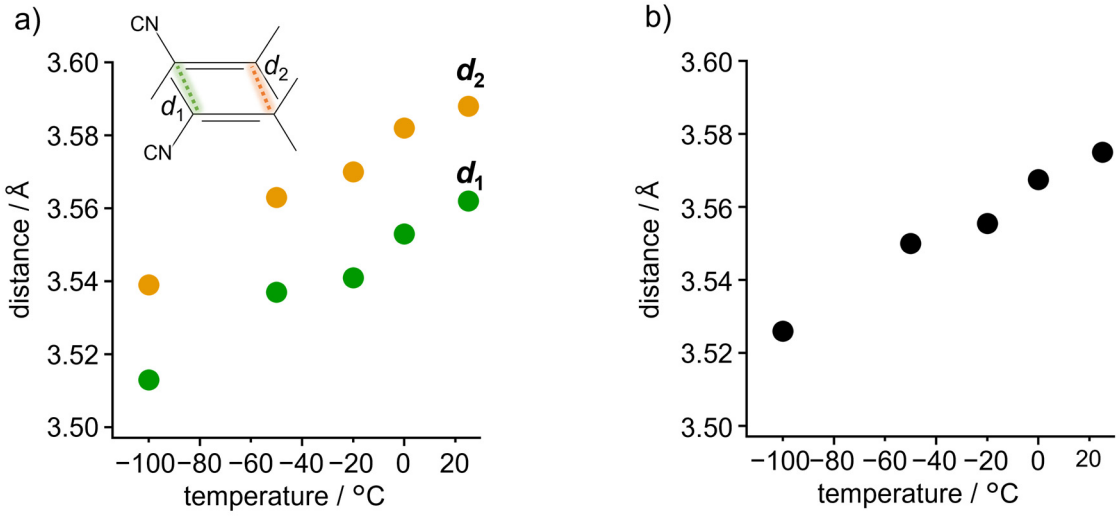


Fig. S17 a) Plots of two intercarbon distances (d_1 and d_2) within the neighboring molecules of *Z***1** versus temperature. b) Plots of the average of d_1 and d_2 versus temperature.

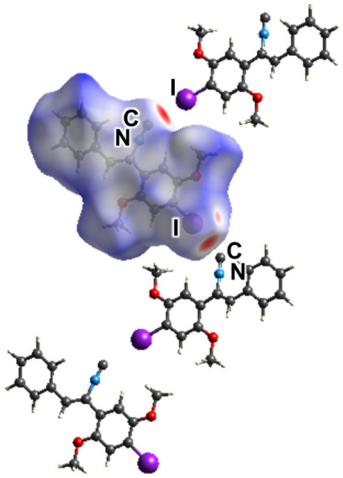


Fig. S18 Hirshfeld surfaces of *Z***1** mapped using d_{norm}.

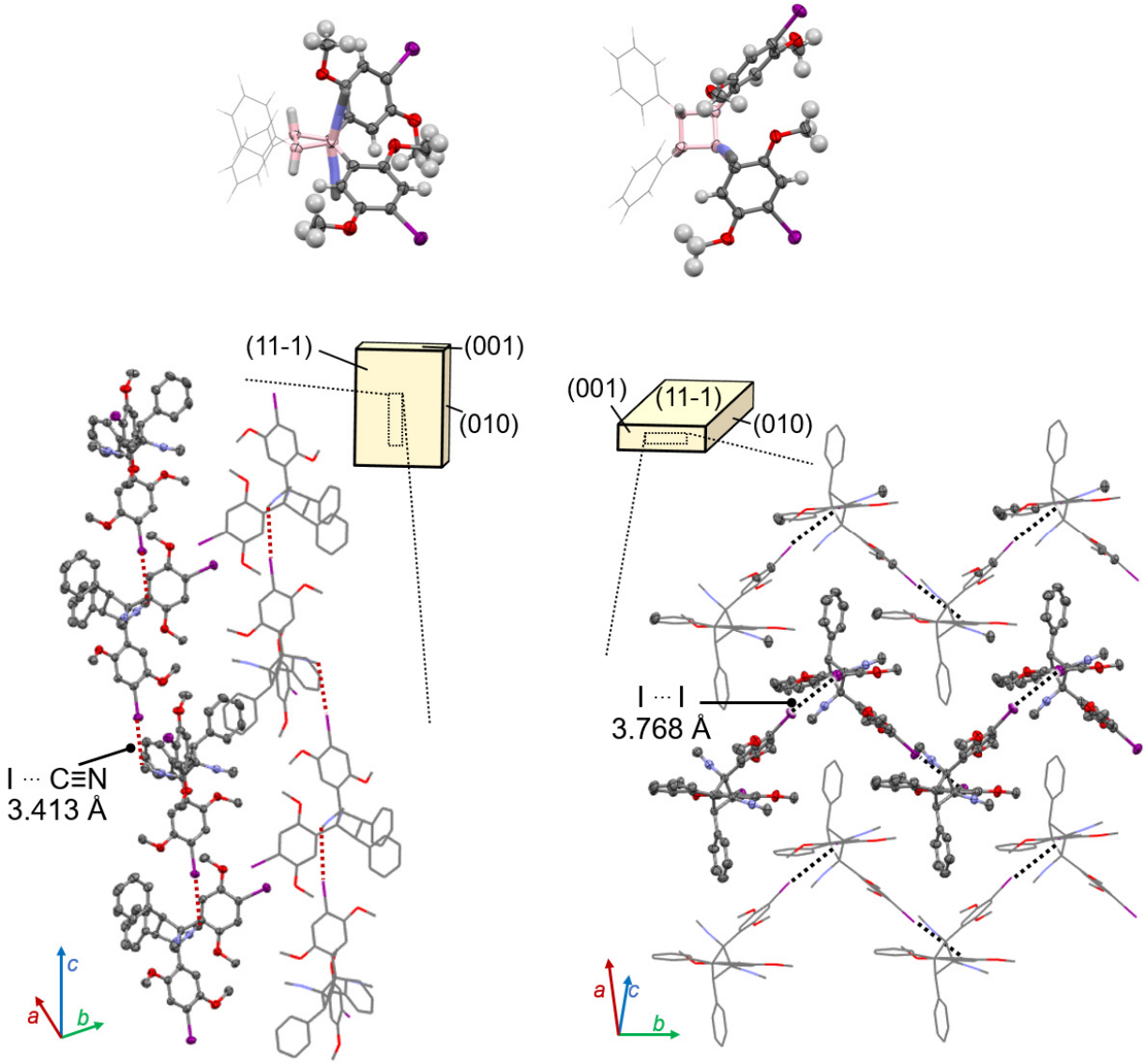


Fig. S19 Single-crystal structure of **2**.

7. References

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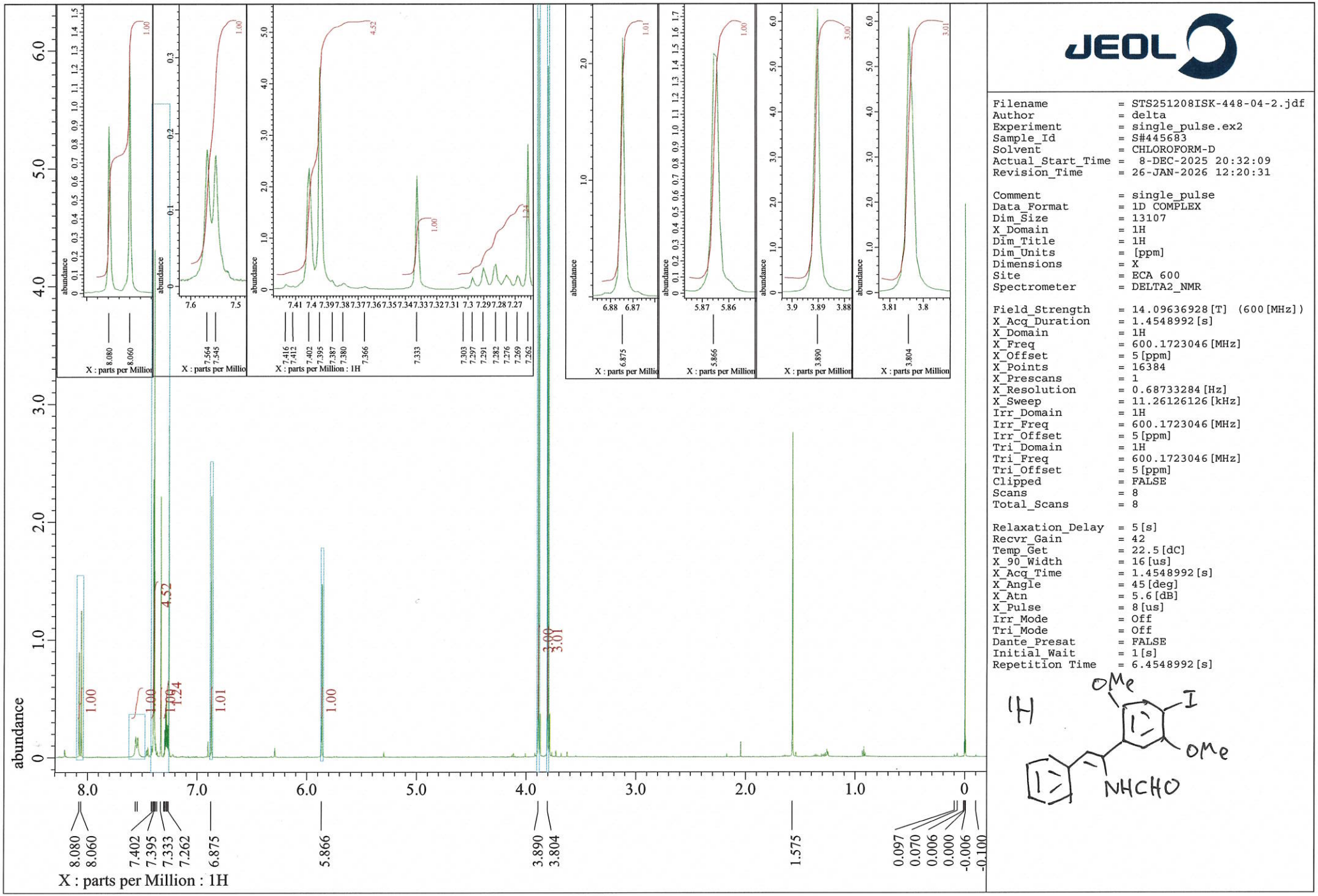
[S6] a) J. Qi, L. Lan, Q. Chen, L. Li, P. Naumov and H. Zhang, *Angew*. *Chem*. *Int*. *Ed*., **2025**, *64*, e202417409; b) J. Lin, S. Tang, L. Li, L. Fang, Q. Zeng, G. Sun, S. Wu, P. Naumov and J. Gong, *J*. *Am*. *Chem*. *Soc*., **2025**, *147*, 11346–11358; c) J. Lin, J. Zhou, L. Li, I. Tahir, S. Wu, P. Naumov and J. Gong, *Chem*. *Mater*., **2024**, *36*, 8338–8348.

[S7] a) A. F. Palermo, B. S. Y. Chiu, P. Patel and S. A. L. Rousseaux, *J*. *Am*. *Chem*. *Soc*., **2023**, *145*, 24981–24989; b) J. W. Chung, S. J. Yoon, B. K. An and S. Y. Park, *J*. *Phys*. *Chem*. *C*, **2013**, *117*, 11285–11291.



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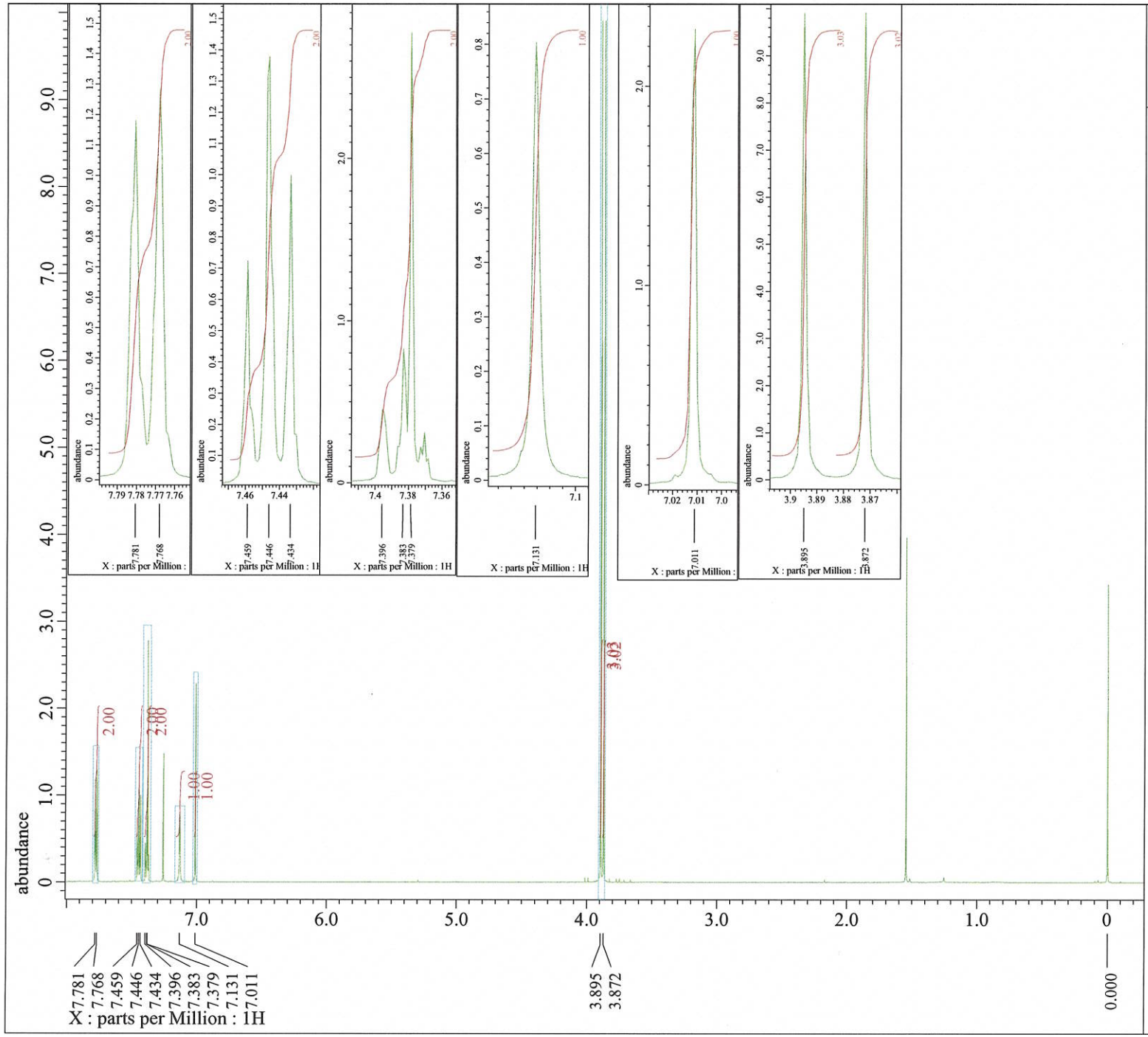
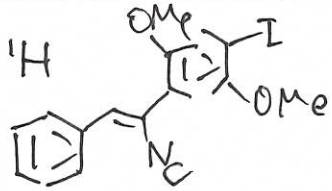
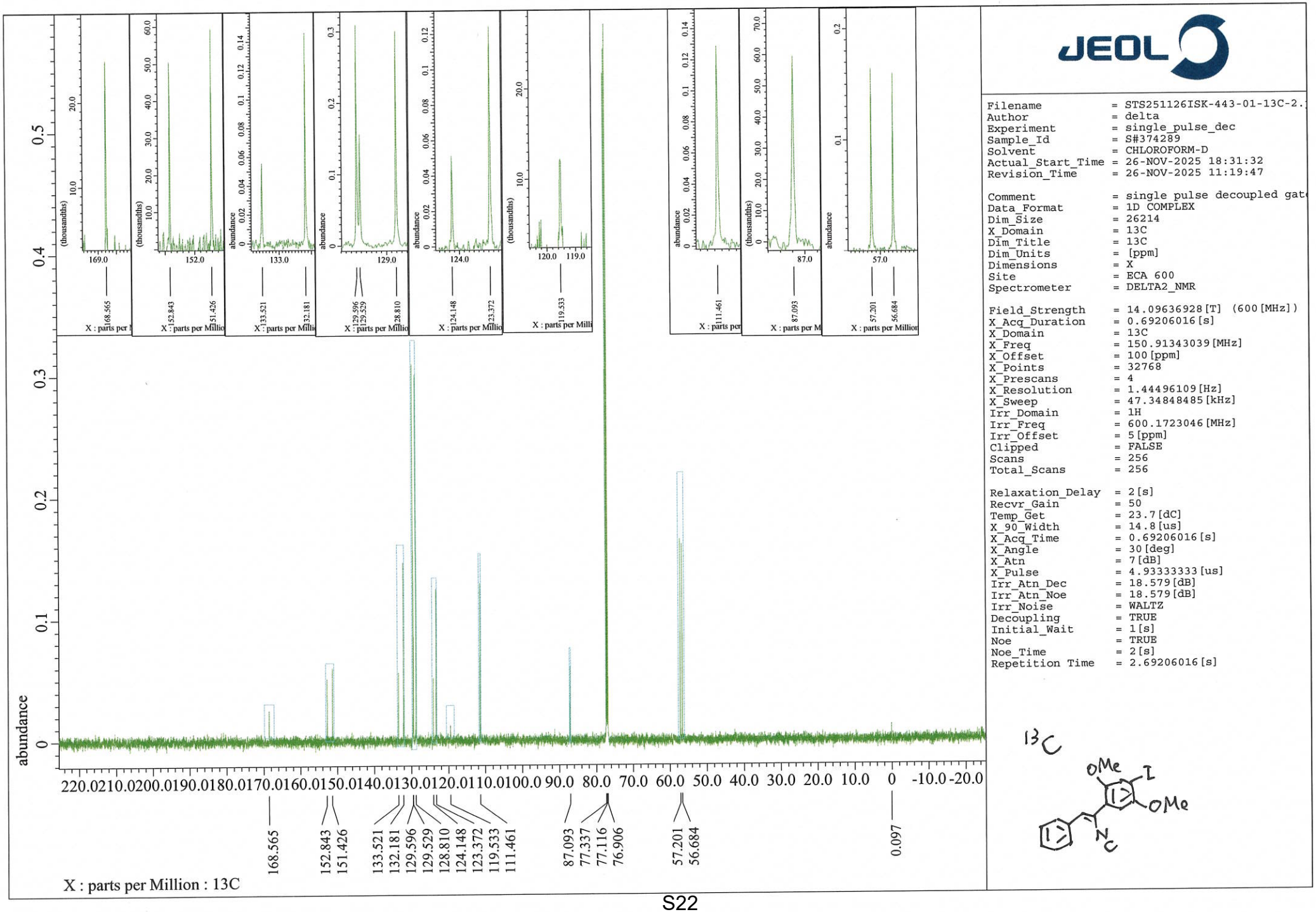
Dim_Title	= 1H
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECA 600
Spectrometer	= DELTA2_NMR
Field_Strength	= 14.09636928[T] (600[MHz])
X_Acq_Duration	= 1.4548992[s]
X_Domain	= 1H
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.68733284[Hz]
X_Sweep	= 11.26126126[kHz]
Irr_Domain	= 1H
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= 1H
Tri_Freq	= 600.1723046[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 42
Temp_Get	= 22.5[dC]
X_90_Width	= 16[us]
X_Acq_Time	= 1.4548992[s]
X_Angle	= 45[deg]
X_Atn	= 5.6[dB]
X_Pulse	= 8[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition Time	= 6.4548992[s]

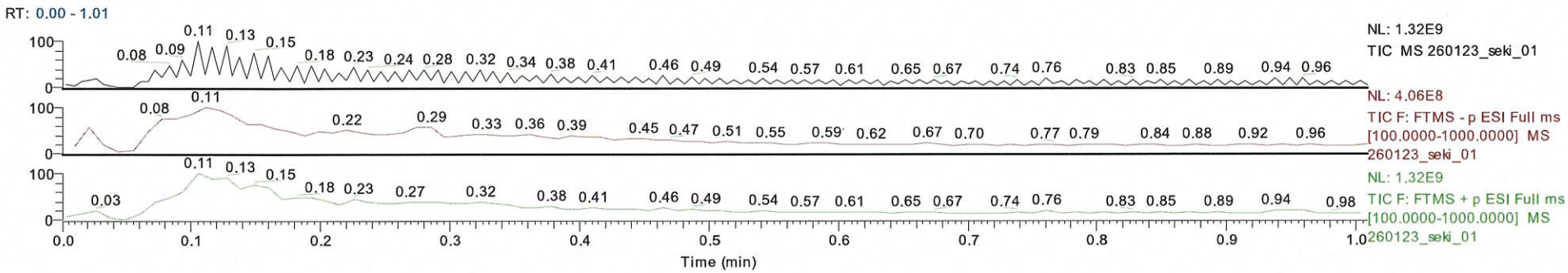

JEOL
Filename = STS251208ISK-452-01-13C-2.
Author = delta
Experiment = single_pulse_dec
Sample_Id = S#526278
Solvent = CHLOROFORM-D
Actual_Start_Time = 8-DEC-2025 22:44:02
Revision_Time = 8-DEC-2025 16:02:30
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = 13C
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECA 600
Spectrometer = DELTA2_NMR
Field_Strength = 14.09636928[T] (600[MHz])
X_Acq_Duration = 0.69206016[s]
X_Domain = 13C
X_Freq = 150.91343039[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.44496109[Hz]
X_Sweep = 47.34848485[kHz]
Irr_Domain = 1H
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 24.3[dC]
X_90_Width = 14.8[us]
X_Acq_Time = 0.69206016[s]
X_Angle = 30[deg]
X_Atn = 7[dB]
X_Pulse = 4.93333333[us]
Irr_Atn_Dec = 18.579[dB]
Irr_Atn_Noe = 18.579[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition Time = 2.69206016[s]
13C
OMe
I
OMe
NHCHO
abundance
X : parts per Million : 13C
163.002
158.827
153.035
151.196
134.728
132.947
129.232
128.571
127.642
125.727
122.357
115.243
113.462
87.304
77.346
77.135
76.925
57.230
56.387

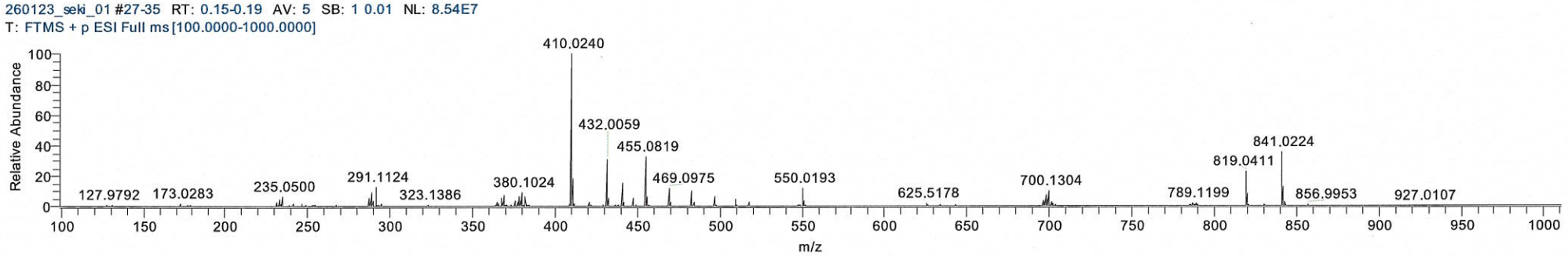


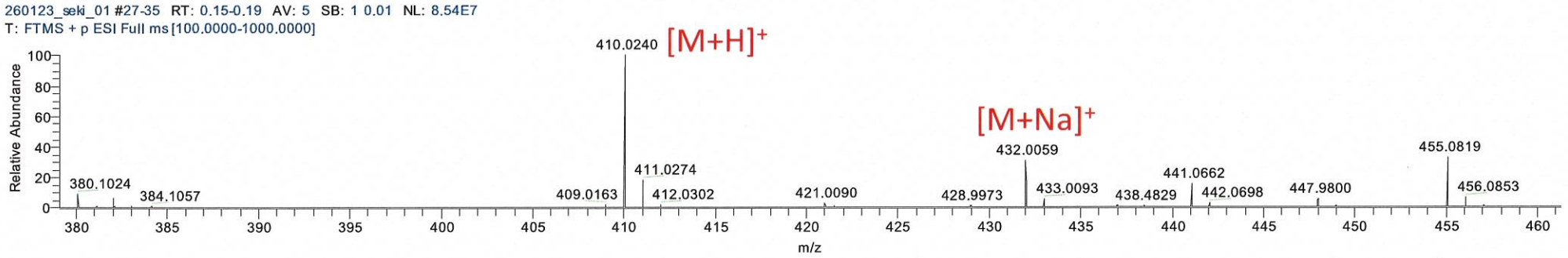
Filename	= STS250918ISK-402-01-2.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_Id	= S#575772
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 19-SEP-2025 00:12:24
Revision_Time	= 26-NOV-2025 12:01:13
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= 1H
Dim_Title	= 1H
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECA 600
Spectrometer	= DELTA2_NMR
Field_Strength	= 14.09636928[T] (600[MHz])
X_Acq_Duration	= 1.4548992[s]
X_Domain	= 1H
X_Freq	= 600.1723046[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.68733284[Hz]
X_Sweep	= 11.26126126[kHz]
Irr_Domain	= 1H
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= 1H
Tri_Freq	= 600.1723046[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 42
Temp_Get	= 24.5[dC]
X_90_Width	= 16[us]
X_Acq_Time	= 1.4548992[s]
X_Angle	= 45[deg]
X_Atn	= 5.6[dB]
X_Pulse	= 8[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition Time	= 6.4548992[s]

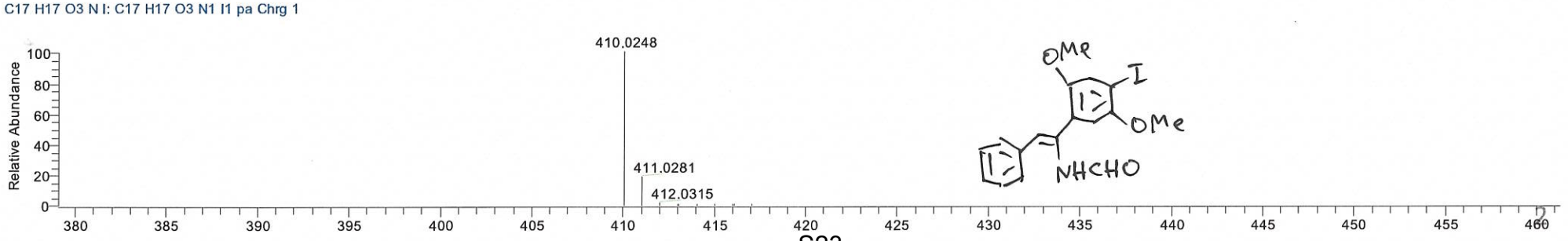


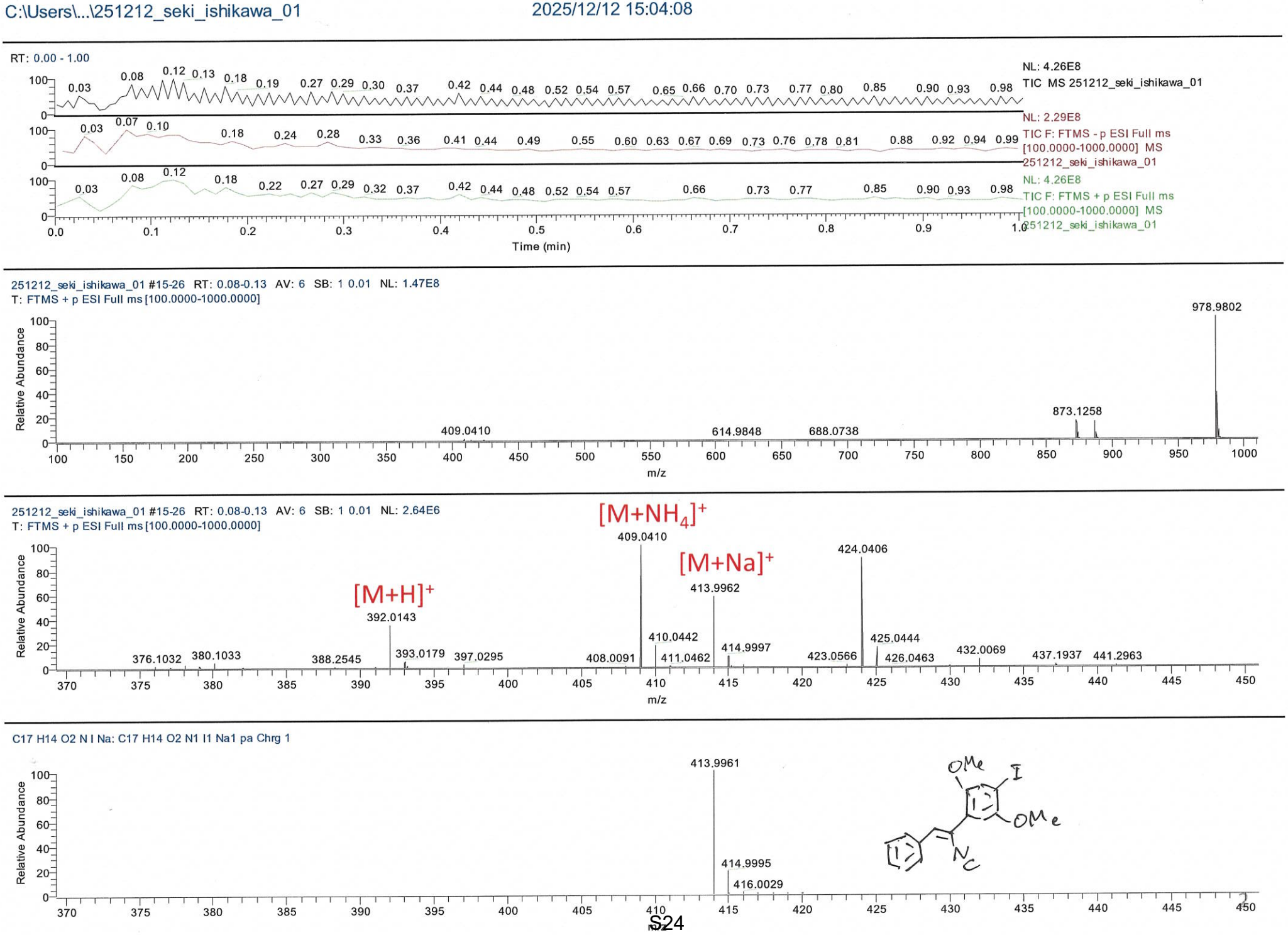

JEOL
Filename = STS251126ISK-443-01-13C-2.
Author = delta
Experiment = single_pulse_dec
Sample_Id = S#374289
Solvent = CHLOROFORM-D
Actual_Start_Time = 26-NOV-2025 18:31:32
Revision_Time = 26-NOV-2025 11:19:47
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = 13C
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECA 600
Spectrometer = DELTA2_NMR
Field_Strength = 14.09636928[T] (600[MHz])
X_Acq_Duration = 0.69206016[s]
X_Domain = 13C
X_Freq = 150.91343039[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.44496109[Hz]
X_Sweep = 47.34848485[kHz]
Irr_Domain = 1H
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 23.7[dC]
X_90_Width = 14.8[us]
X_Acq_Time = 0.69206016[s]
X_Angle = 30[deg]
X_Atn = 7[dB]
X_Pulse = 4.93333333[us]
Irr_Atn_Dec = 18.579[dB]
Irr_Atn_Noe = 18.579[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition Time = 2.69206016[s]
13C
OMe
I
OMe
NC
abundance
X : parts per Million : 13C
168.565
152.843
151.426
133.521
132.181
129.596
129.529
128.810
124.148
123.372
119.533
111.461
87.093
77.337
77.116
76.906
57.201
56.684
0.097


RT: 0.00 - 1.01
NL: 1.32E9
TIC MS 260123_seki_01
NL: 4.06E8
TIC F: FTMS - p ESI Full ms [100.0000-1000.0000] MS 260123_seki_01
NL: 1.32E9
TIC F: FTMS + p ESI Full ms [100.0000-1000.0000] MS 260123_seki_01
Time (min)


260123_seki_01 #27-35 RT: 0.15-0.19 AV: 5 SB: 1 0.01 NL: 8.54E7
T: FTMS + p ESI Full ms [100.0000-1000.0000]
Relative Abundance
m/z


260123_seki_01 #27-35 RT: 0.15-0.19 AV: 5 SB: 1 0.01 NL: 8.54E7
T: FTMS + p ESI Full ms [100.0000-1000.0000]
[M+H]+
[M+Na]+
Relative Abundance
m/z


C17 H17 O3 N I: C17 H17 O3 N1 I1 pa Chrg 1
Relative Abundance
OMe
I
OMe
NHCHO


C:\Users\...\251212_seki_ishikawa_01
2025/12/12 15:04:08
RT: 0.00 - 1.00
NL: 4.26E8
TIC MS 251212_seki_ishikawa_01
NL: 2.29E8
TIC F: FTMS - p ESI Full ms [100.0000-1000.0000] MS 251212_seki_ishikawa_01
NL: 4.26E8
TIC F: FTMS + p ESI Full ms [100.0000-1000.0000] MS 251212_seki_ishikawa_01
Time (min)
251212_seki_ishikawa_01 #15-26 RT: 0.08-0.13 AV: 6 SB: 1 0.01 NL: 1.47E8
T: FTMS + p ESI Full ms [100.0000-1000.0000]
978.9802
873.1258
409.0410
614.9848
688.0738
Relative Abundance
m/z
251212_seki_ishikawa_01 #15-26 RT: 0.08-0.13 AV: 6 SB: 1 0.01 NL: 2.64E6
T: FTMS + p ESI Full ms [100.0000-1000.0000]
[M+NH4]+
[M+Na]+
[M+H]+
409.0410
424.0406
413.9962
392.0143
410.0442
414.9997
425.0444
376.1032
380.1033
388.2545
393.0179
397.0295
408.0091
411.0462
423.0566
426.0463
432.0069
437.1937
441.2963
Relative Abundance
m/z
C17 H14 O2 N I Na: C17 H14 O2 N1 I1 Na1 pa Chrg 1
413.9961
414.9995
416.0029
OMe
I
OMe
N
C
Relative Abundance
m/z