Supplementary Information (SI) for Organic & Biomolecular Chemistry.
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# Supporting Information

# Construction of Diaryl Oxacyclic Sulfones via $Bi(OTf)_3$-catalyzed Intramolecular Cyclocondensation of 1,3-Diaroylsulfones

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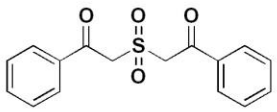
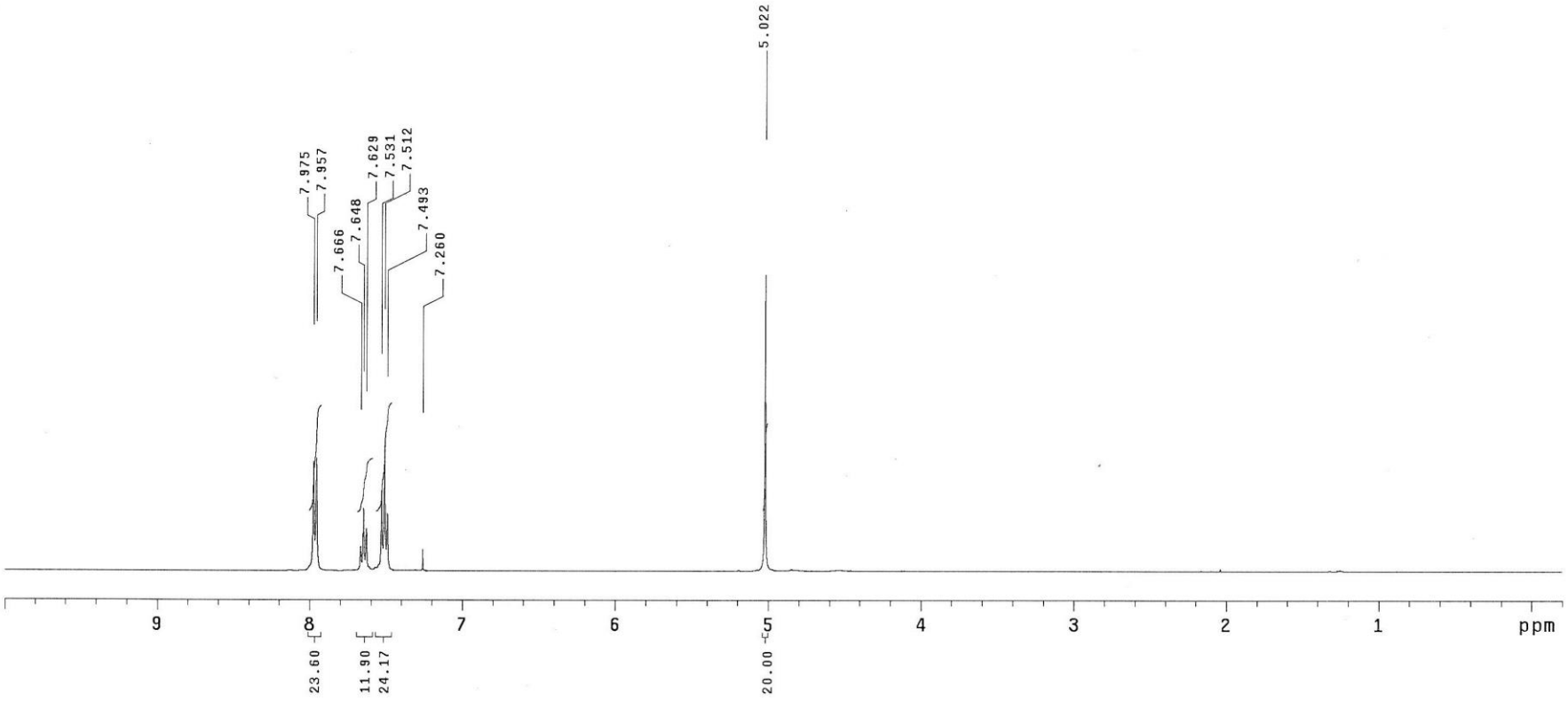
# Compound 4a ($^1$H-NMR spectral data)

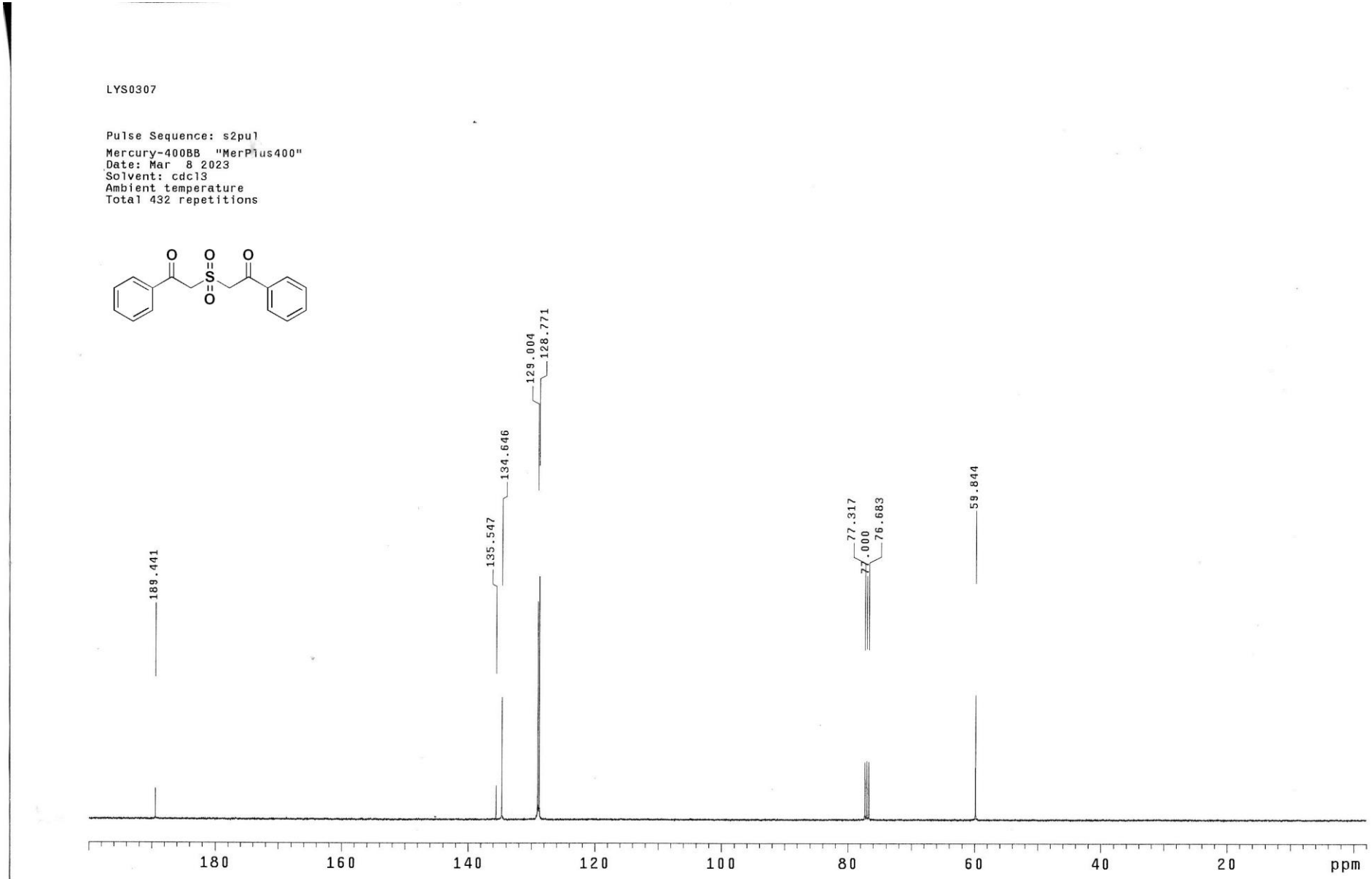
LYS0307

Pulse Sequence: s2pul
Mercury-400BB "MerPlus400"
Date: Mar 8 2023
Solvent: cdcl3
Ambient temperature
Total 32 repetitions

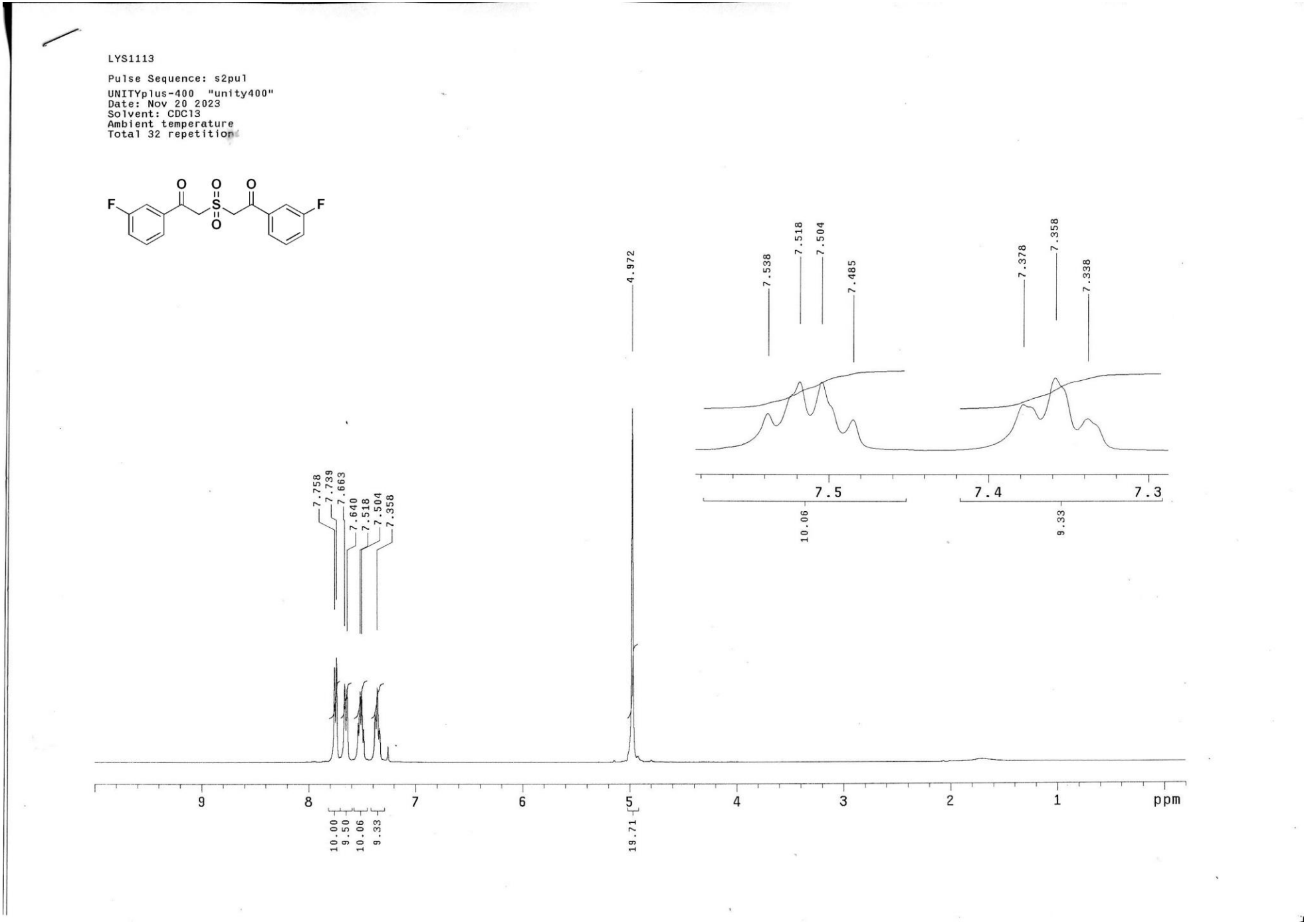




# Compound 4a ($^{13}$C-NMR spectral data)



# Compound 4b ($^1$H-NMR spectral data)

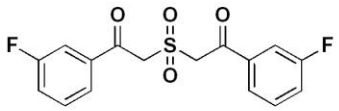


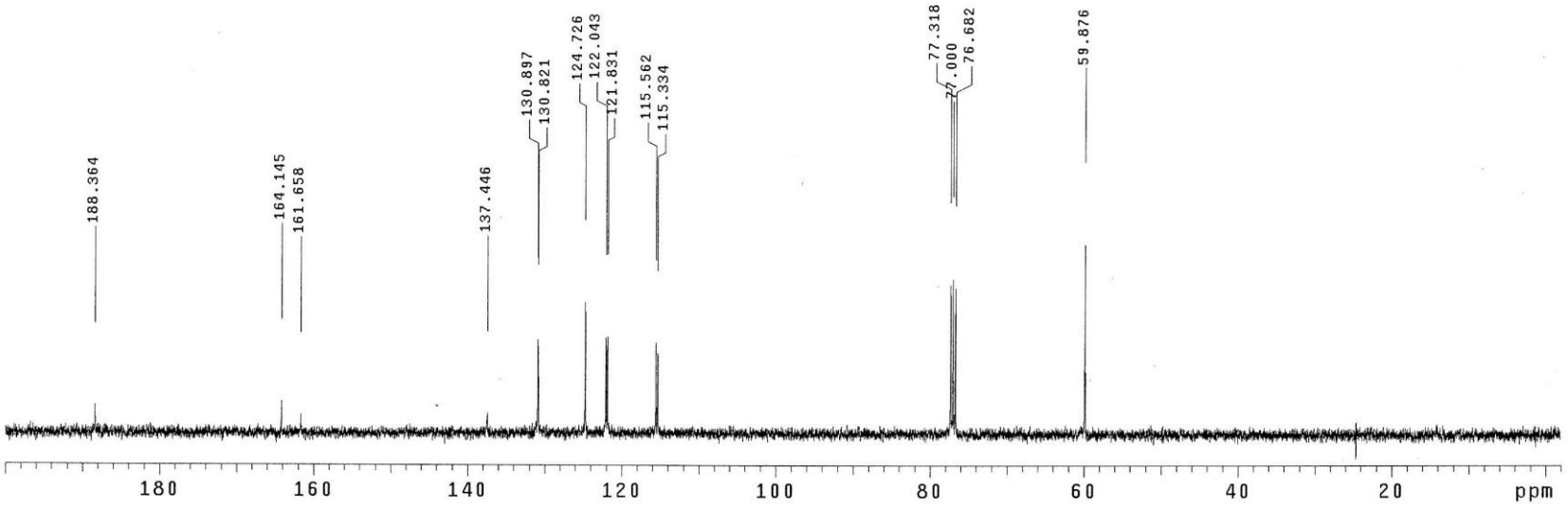
# Compound 4b ($^{13}$C-NMR spectral data)

LYS1113

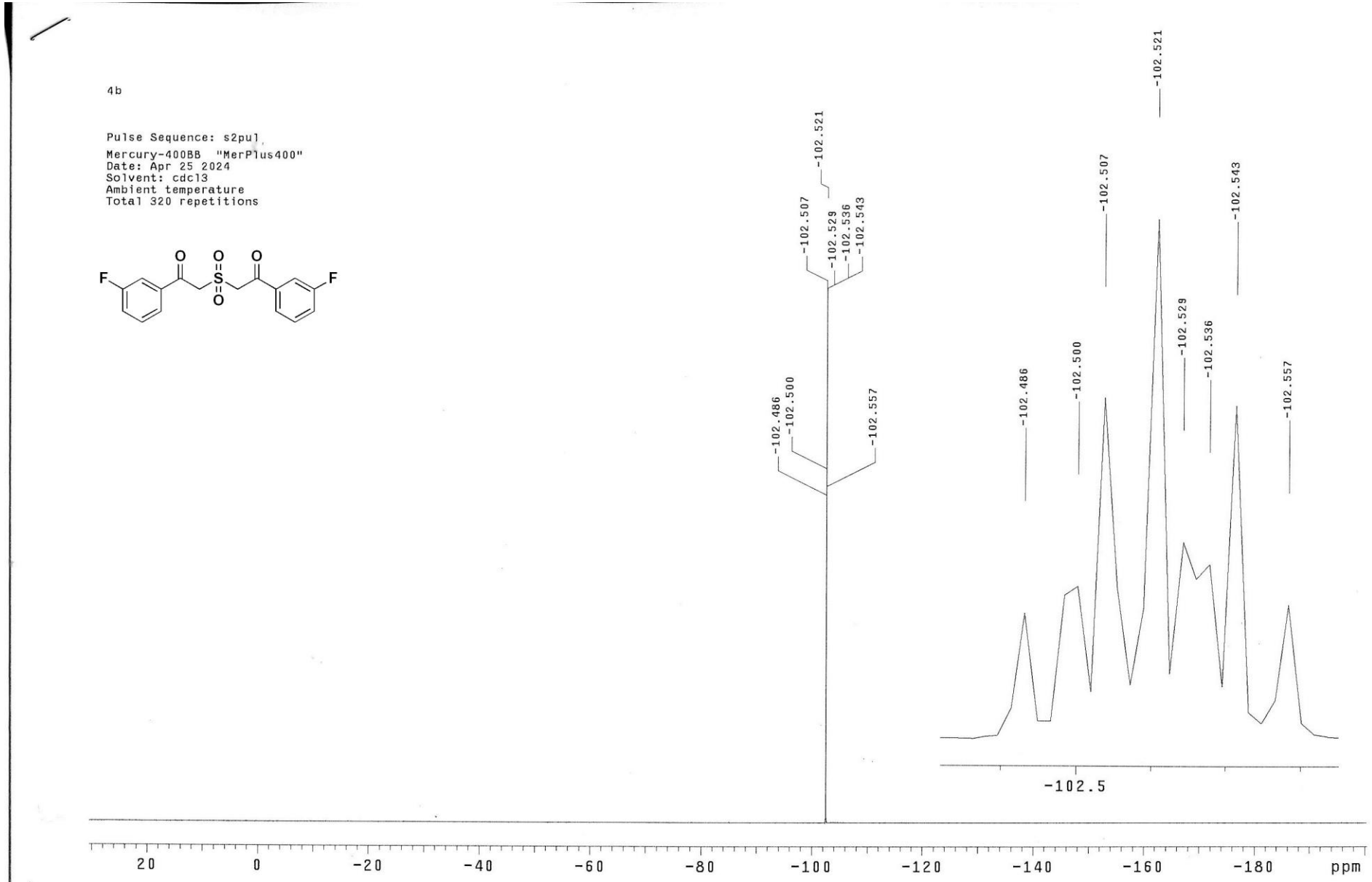
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Nov 20 2023
Solvent: CDCl3
Ambient temperature
Total 4208 repetitions



# Compound 4b ($^{19}$F-NMR spectral data)

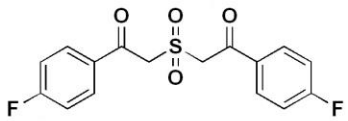


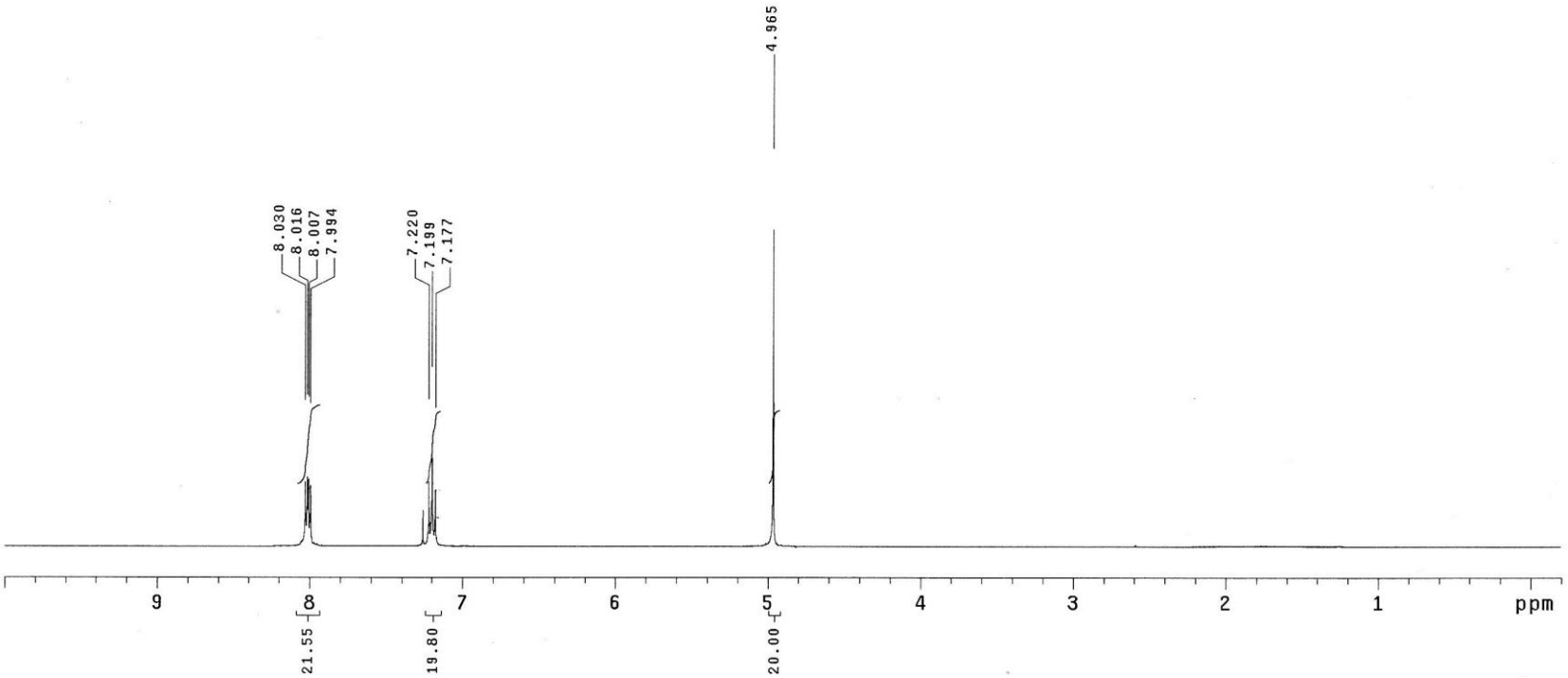
# Compound 4c ($^1$H-NMR spectral data)

LYS0314

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Mar 14 2023
Solvent: CDCl3
Ambient temperature
Total 32 repetitions



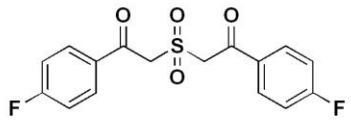



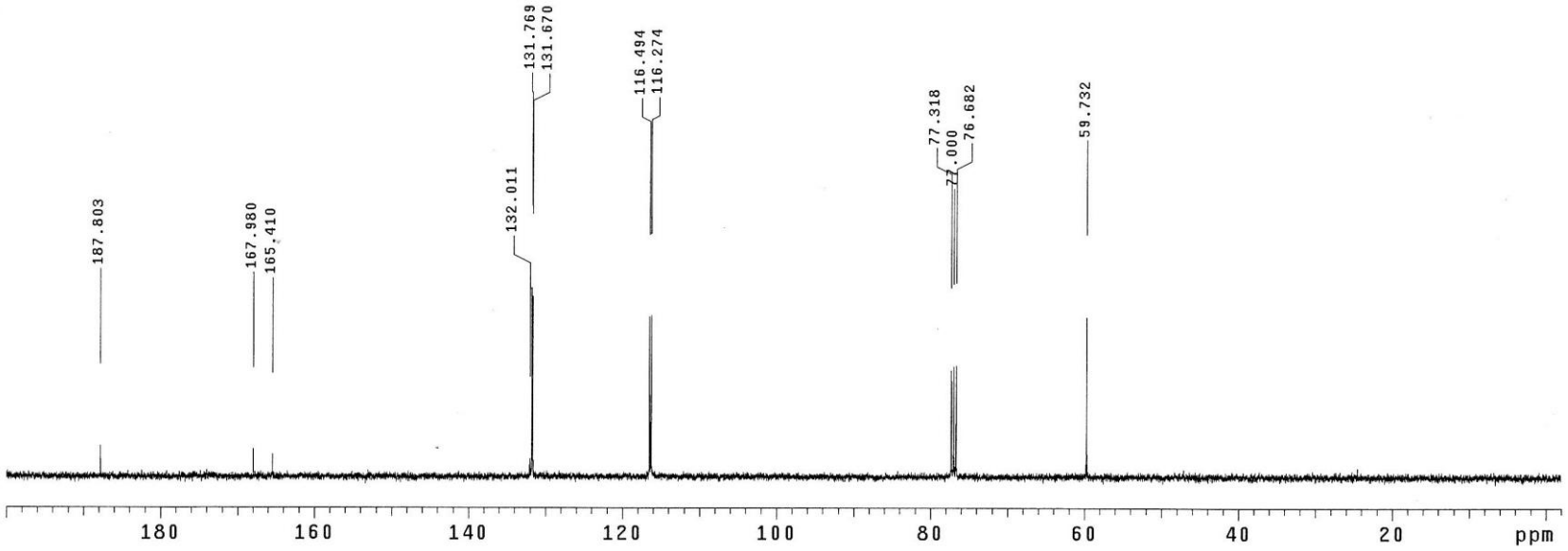
# Compound 4c ($^{13}$C-NMR spectral data)

LYS0314

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Mar 14 2023
Solvent: CDCl3
Ambient temperature
Total 2320 repetitions



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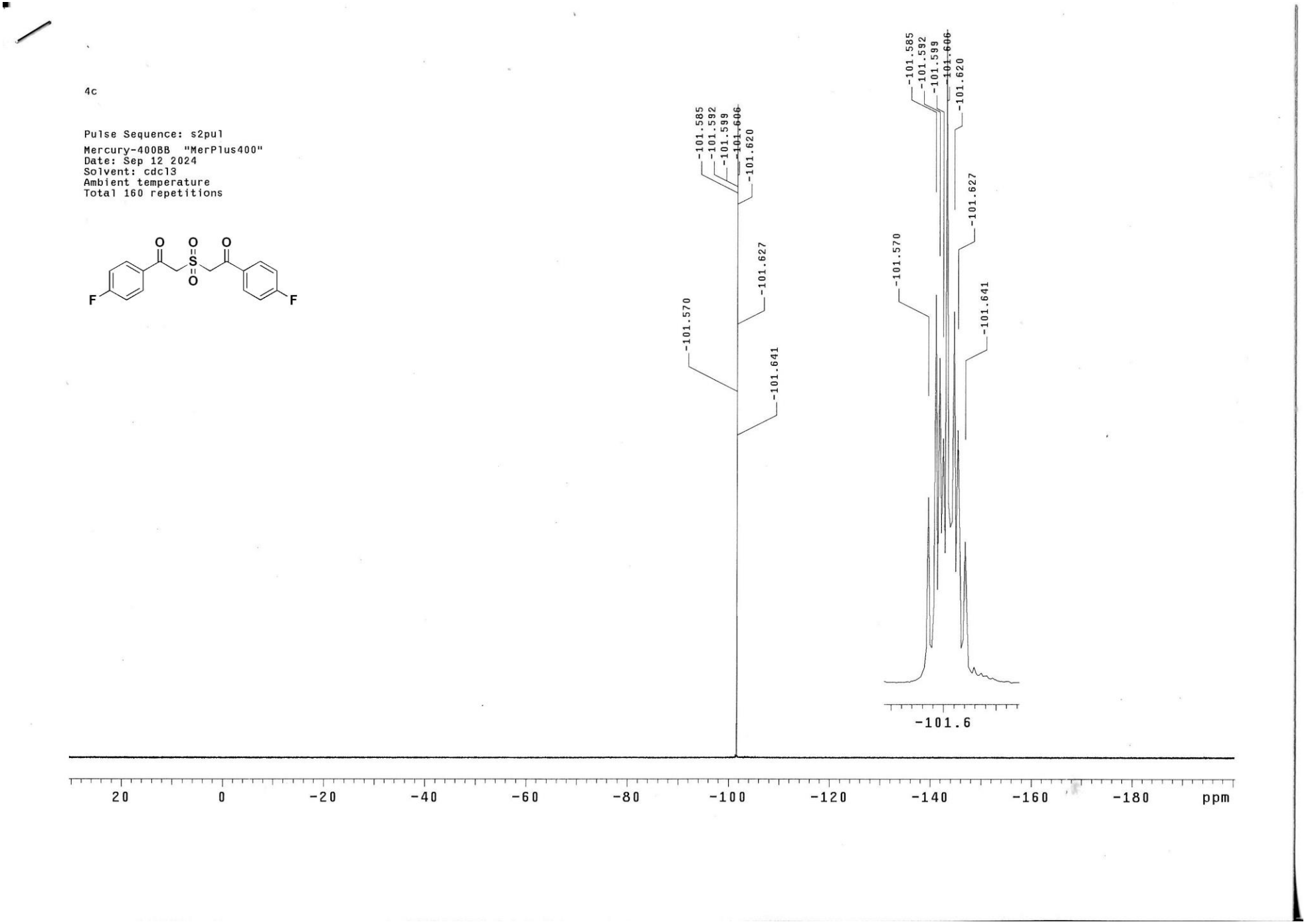
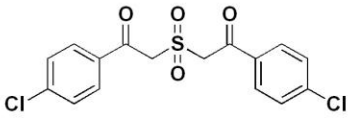


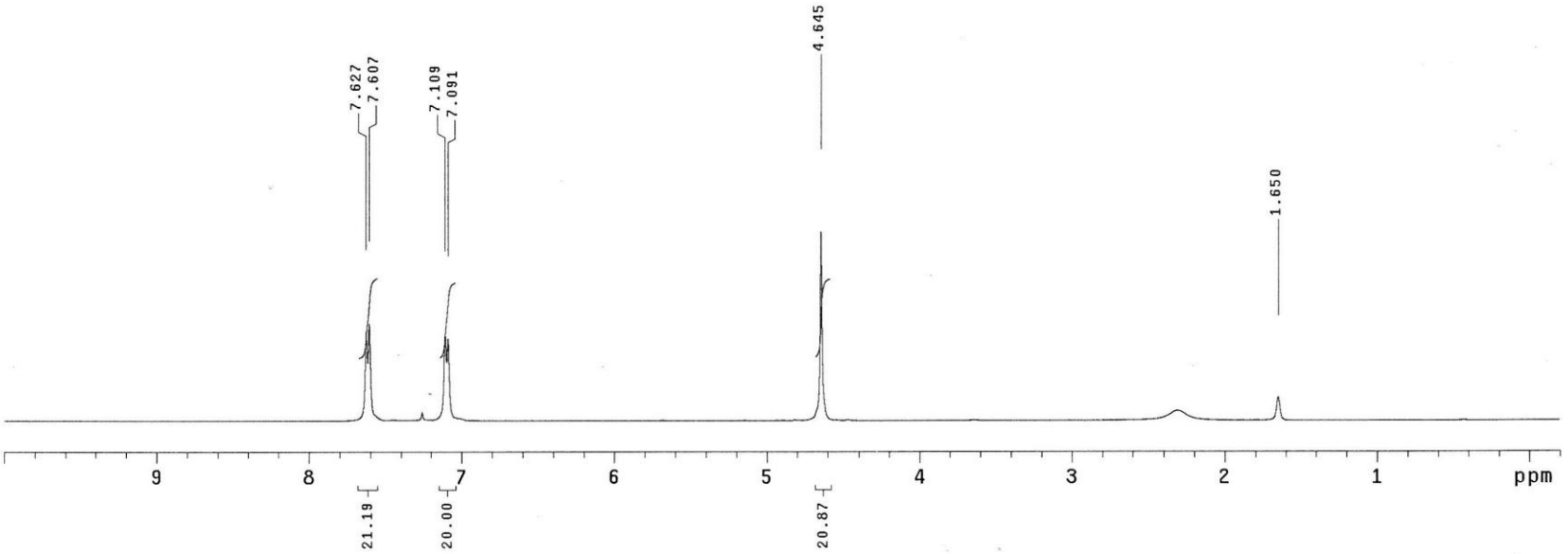
# Compound 4d ($^1$H-NMR spectral data)

LYS0426

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Apr 27 2023
Solvent: CDCl3
Ambient temperature
Total 16 repetitions



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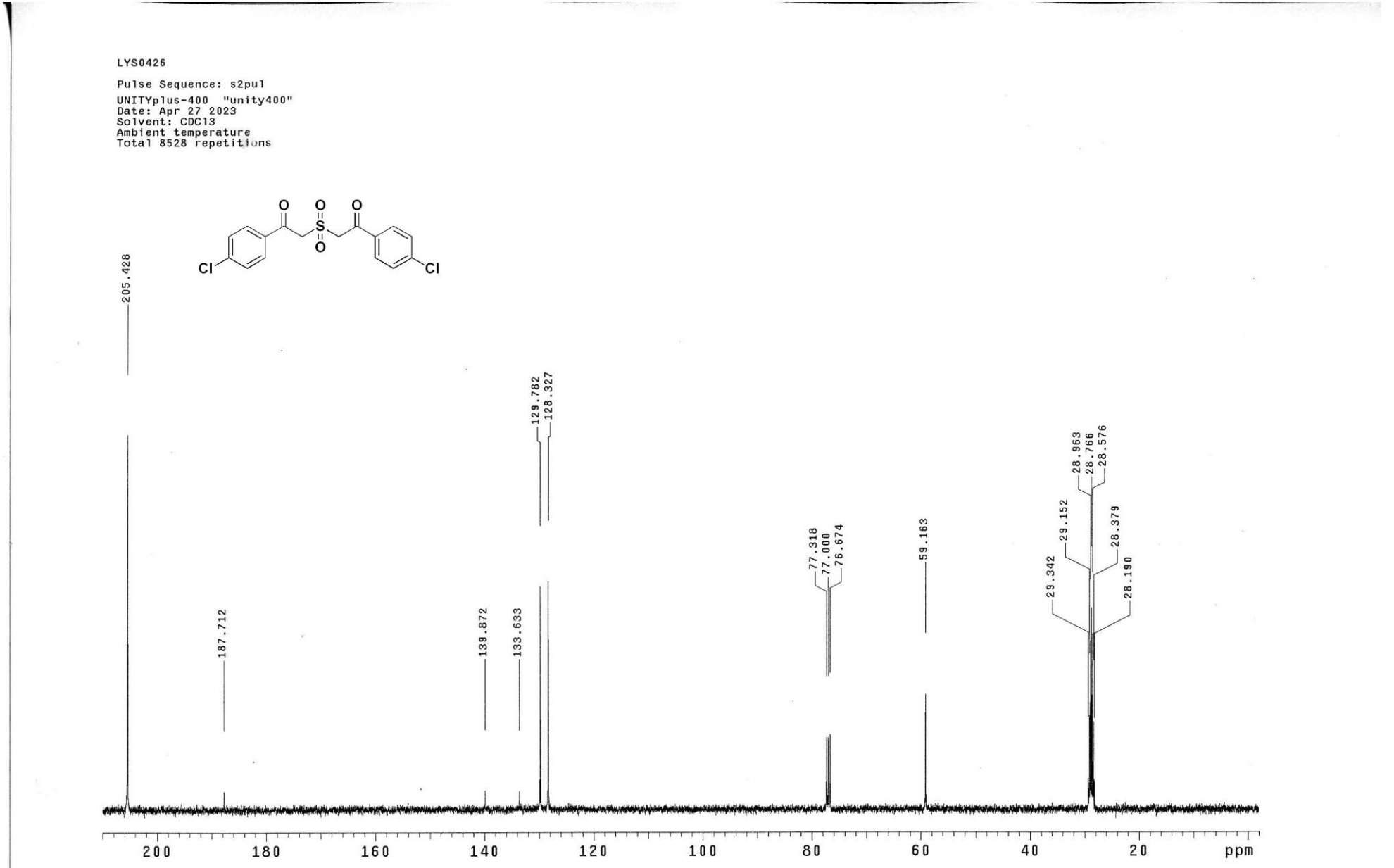
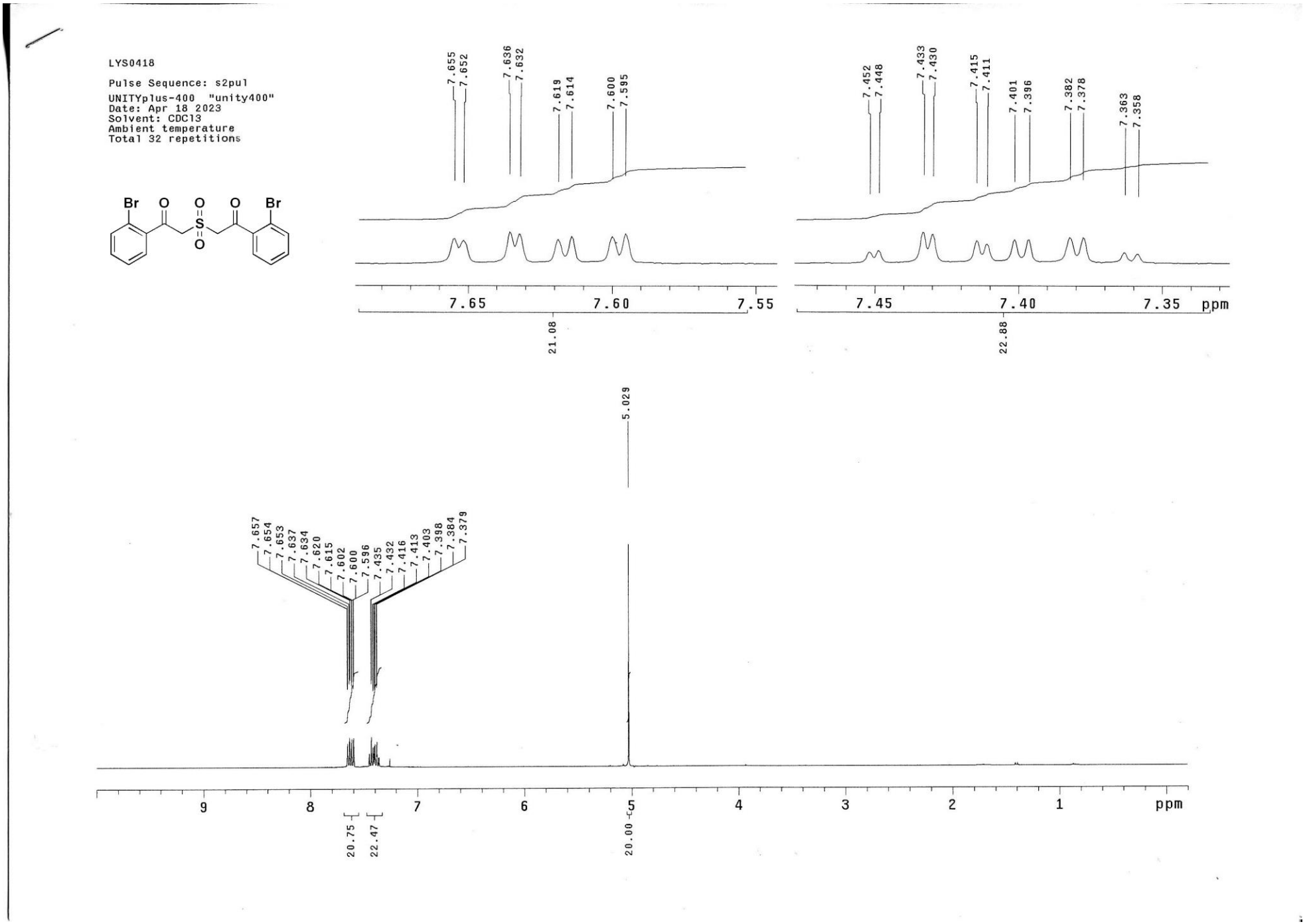


# Compound 4e ($^1$H-NMR spectral data)

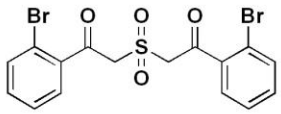


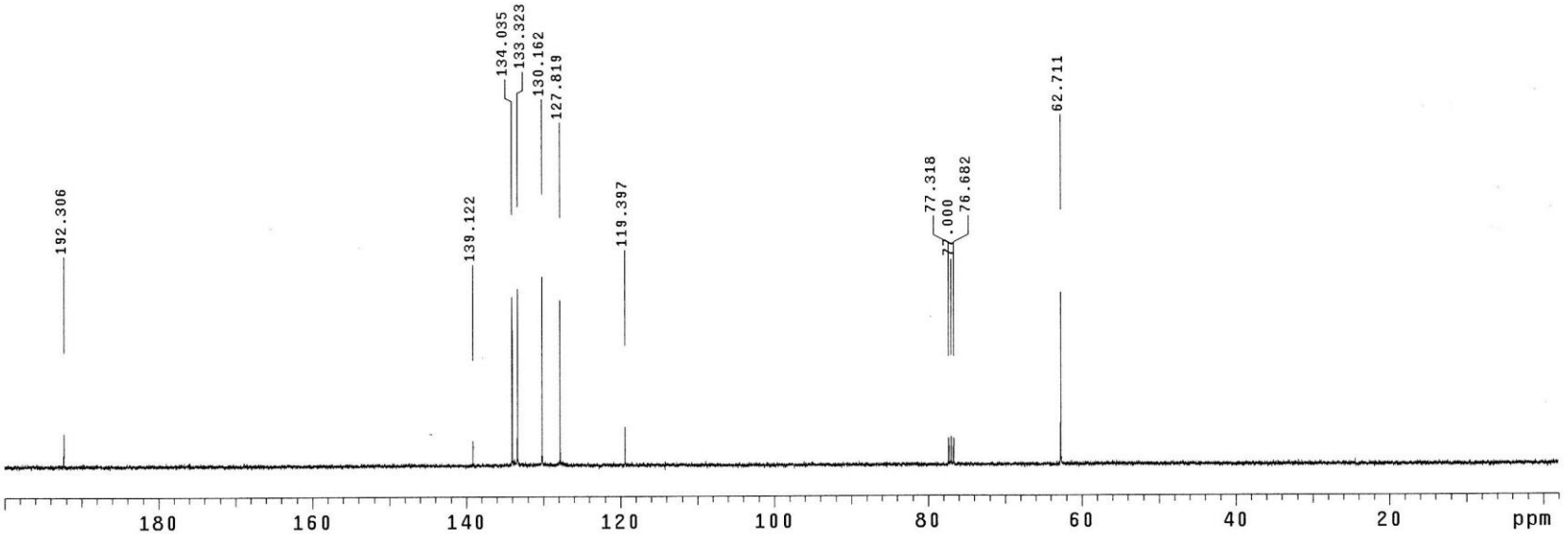
# Compound 4e ($^{13}$C-NMR spectral data)

LYS0418

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Apr 18 2023
Solvent: CDCl3
Ambient temperature
Total 272 repetitions



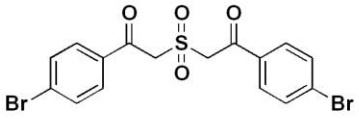



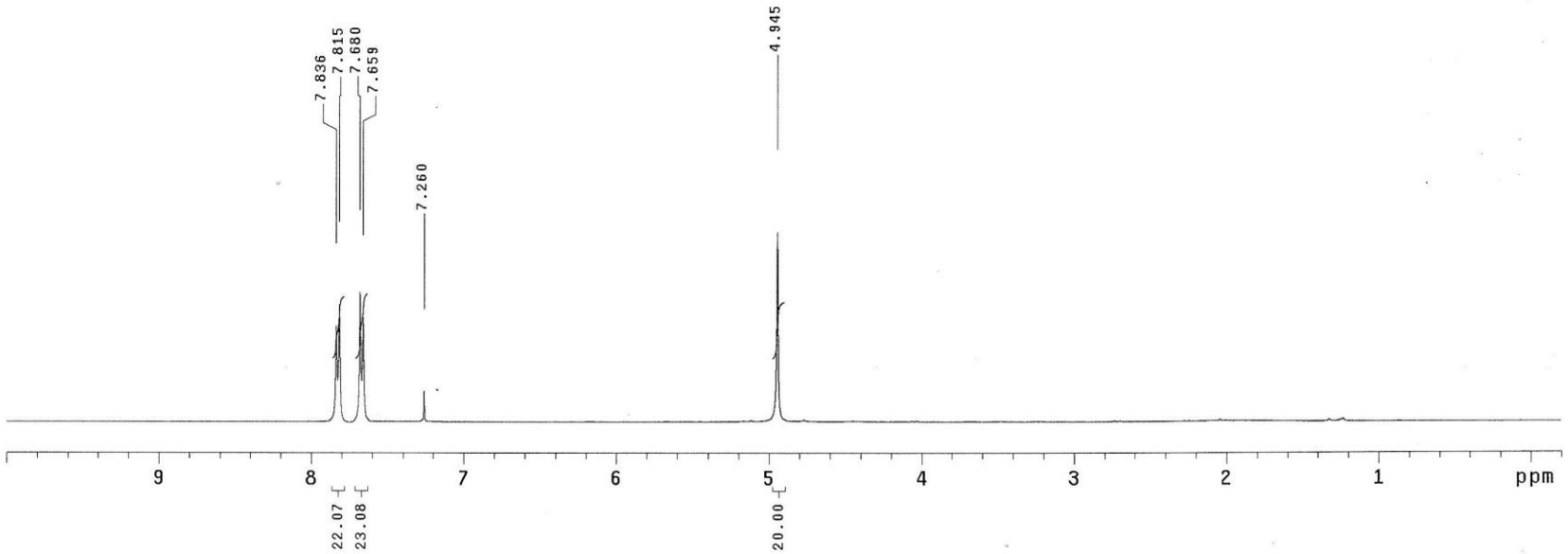
# Compound 4f ($^1$H-NMR spectral data)

LYS1030

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Oct 30 2023
Solvent: CDCl3
Ambient temperature
Total 32 repetitions



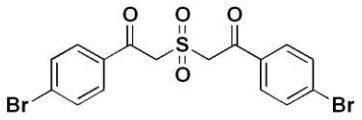



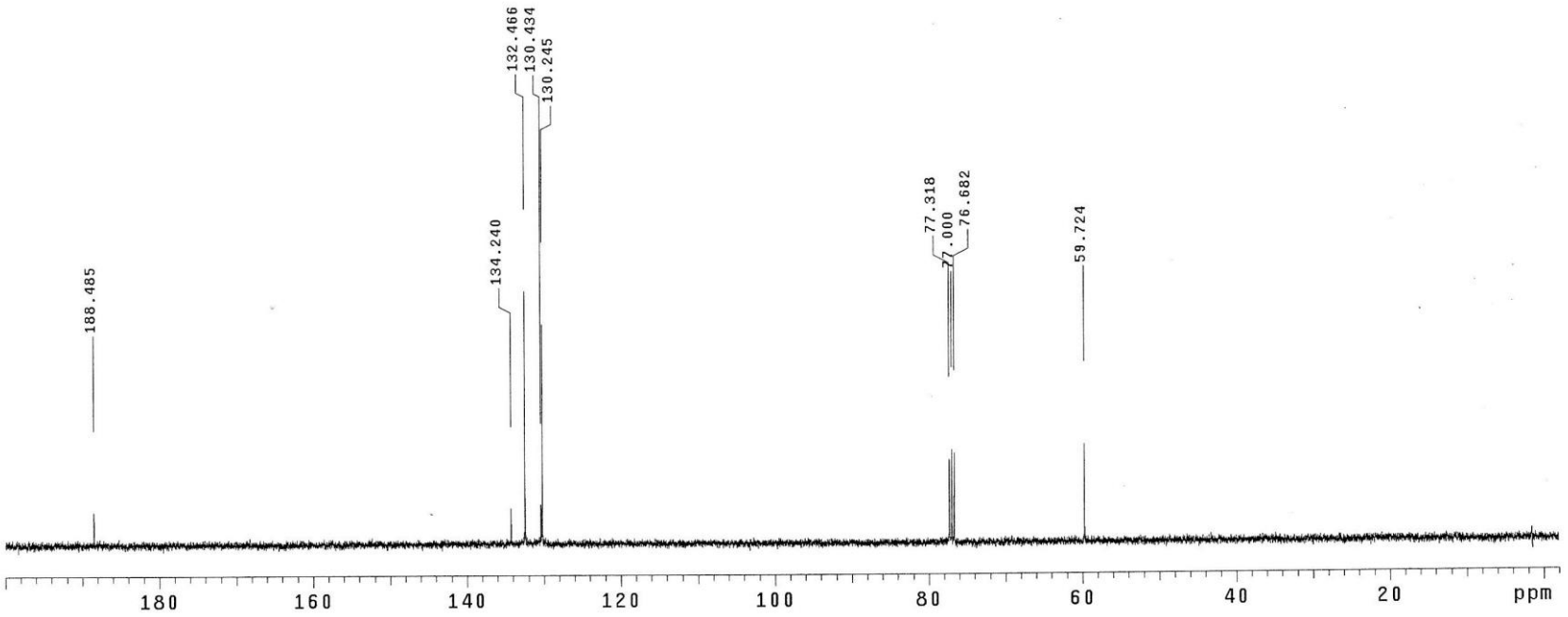
# Compound 4f ($^{13}$C-NMR spectral data)

LYS1030

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Oct 30 2023
Solvent: CDCl3
Ambient temperature
Total 1072 repetitions



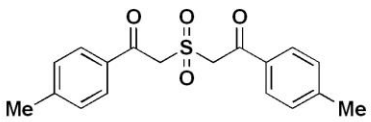



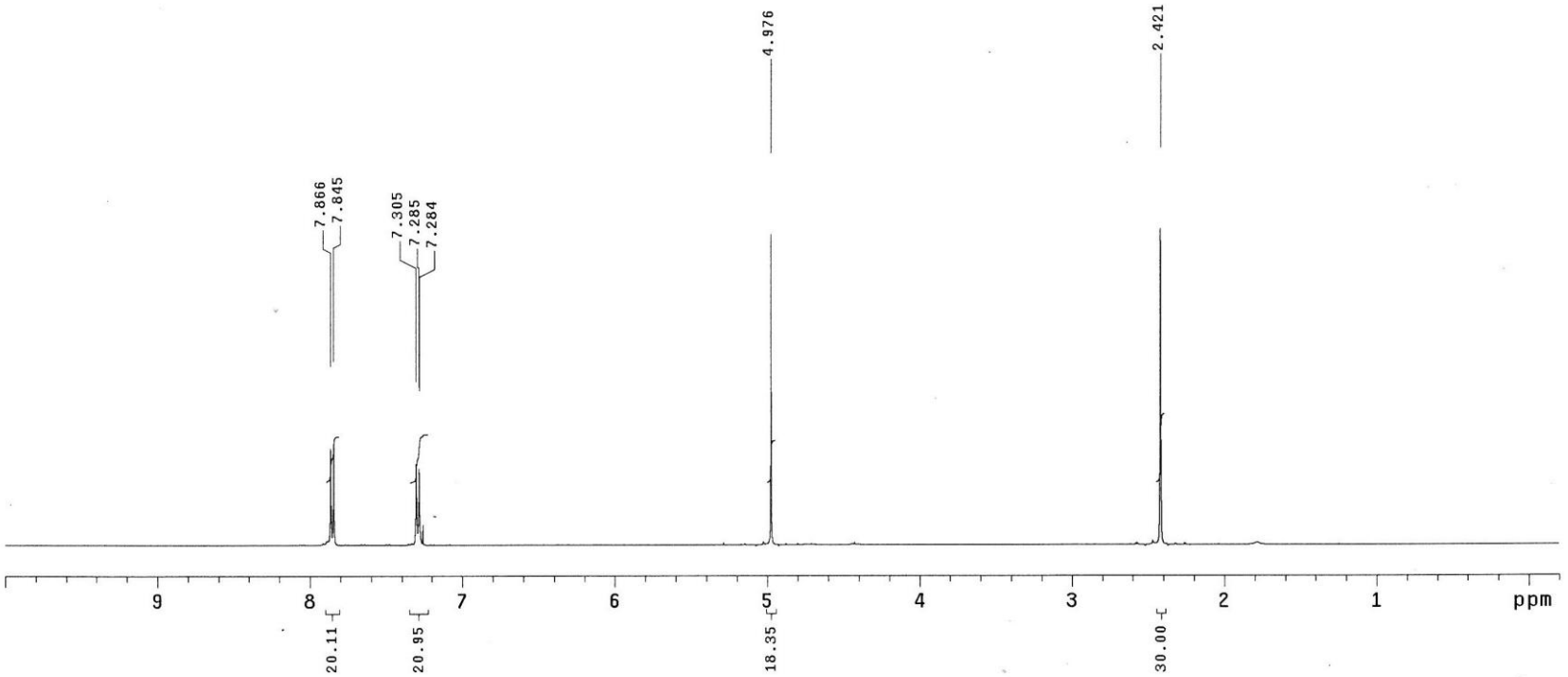
# Compound 4g ($^1$H-NMR spectral data)

LYS0315

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Mar 15 2023
Solvent: CDCl3
Ambient temperature
Total 32 repetitions



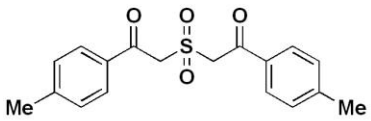



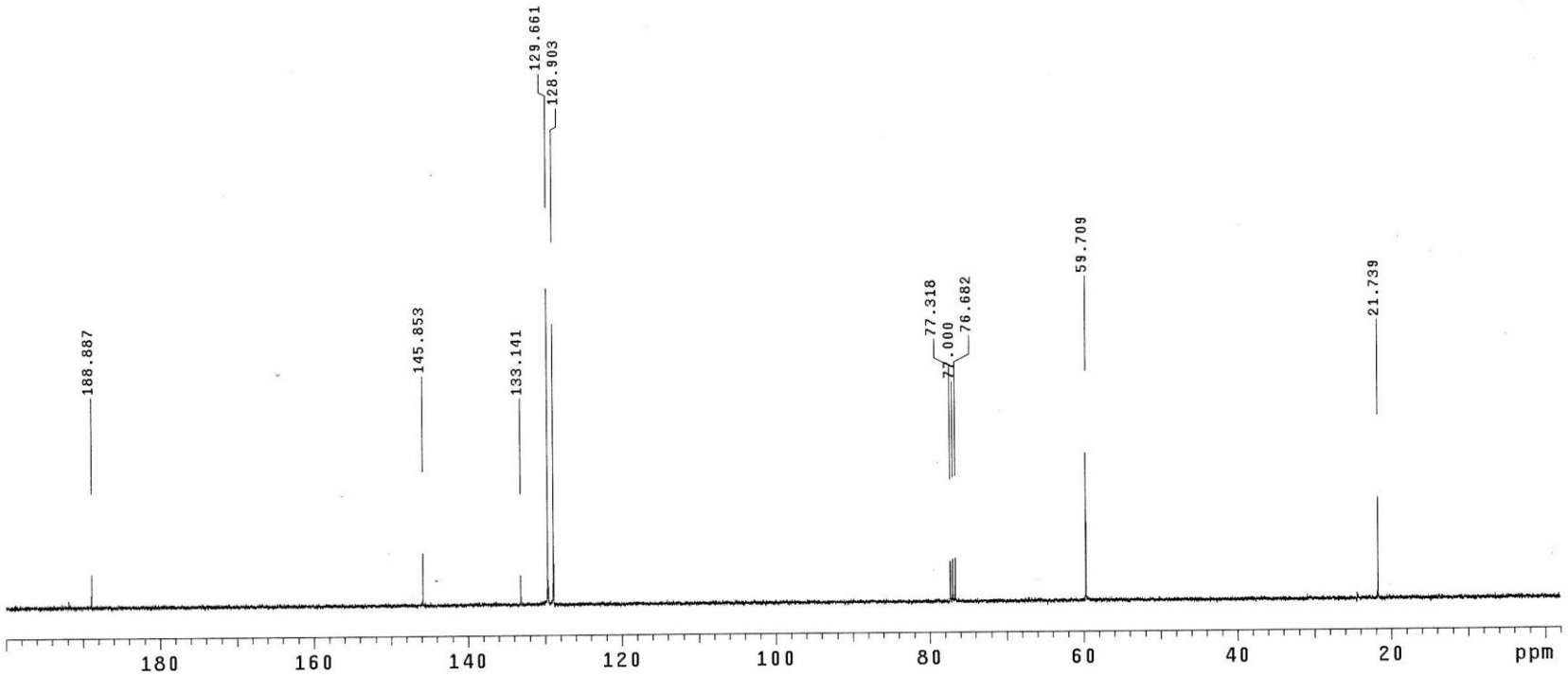
# Compound 4g ($^{13}$C-NMR spectral data)

LYS0315

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Mar 15 2023
Solvent: CDCl3
Ambient temperature
Total 352 repetitions



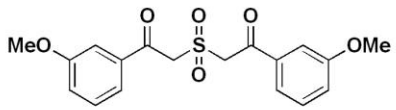



# Compound 4h ($^1$H-NMR spectral data)

LYS0319

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Mar 20 2023
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

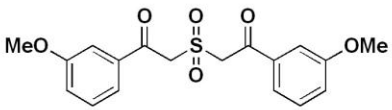


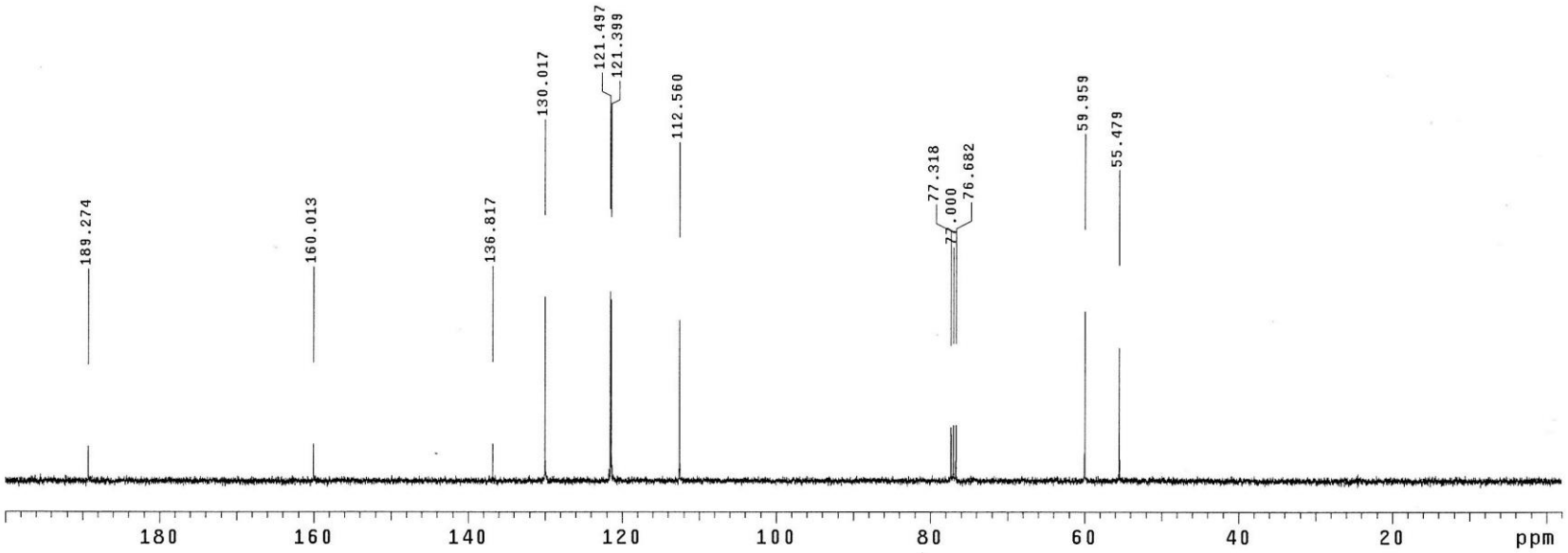
# Compound 4h ($^{13}$C-NMR spectral data)

LYS0319

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Mar 20 2023
Solvent: CDCl3
Ambient temperature
Total 336 repetitions



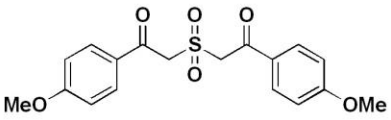



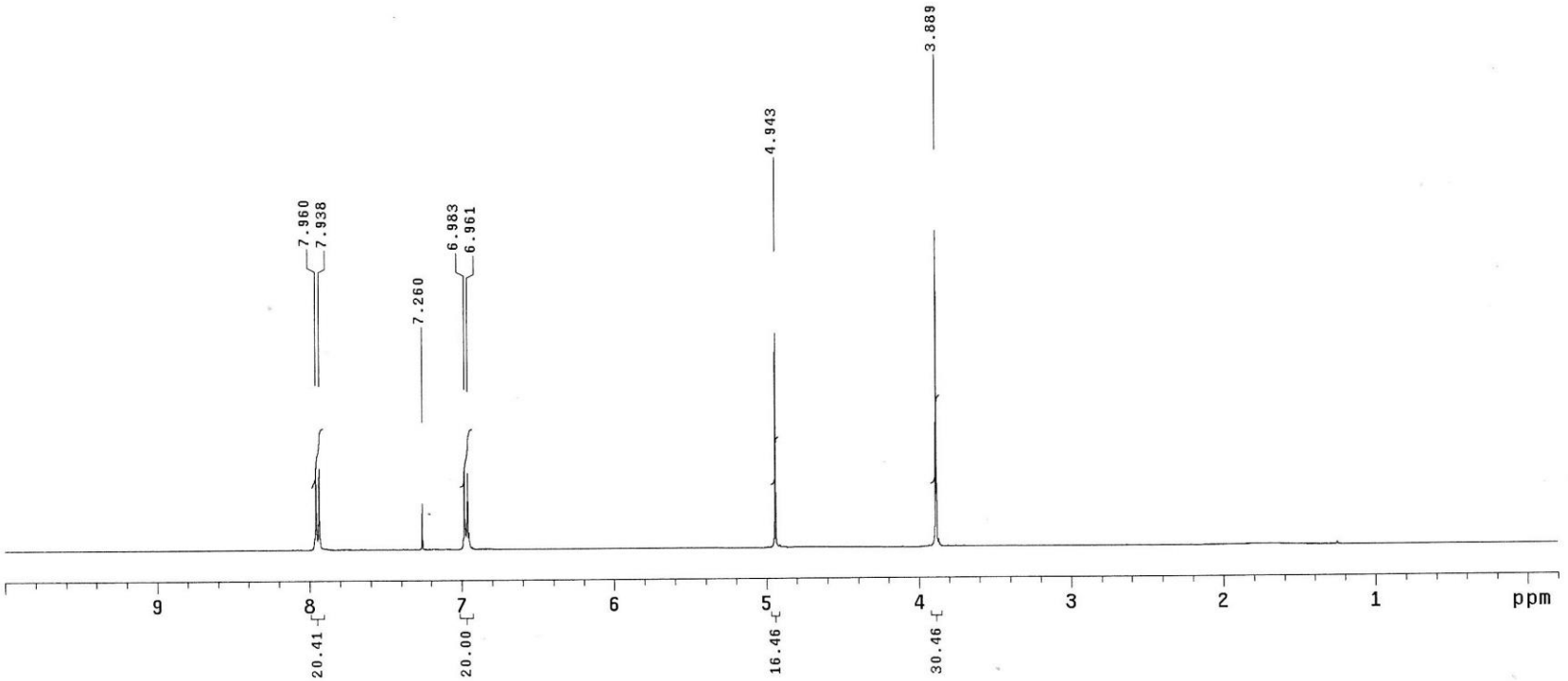
# Compound 4i ($^1$H-NMR spectral data)

LYS0317

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Mar 16 2023
Solvent: CDCl3
Ambient temperature
Total 32 repetitions



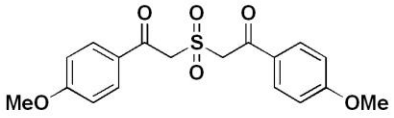



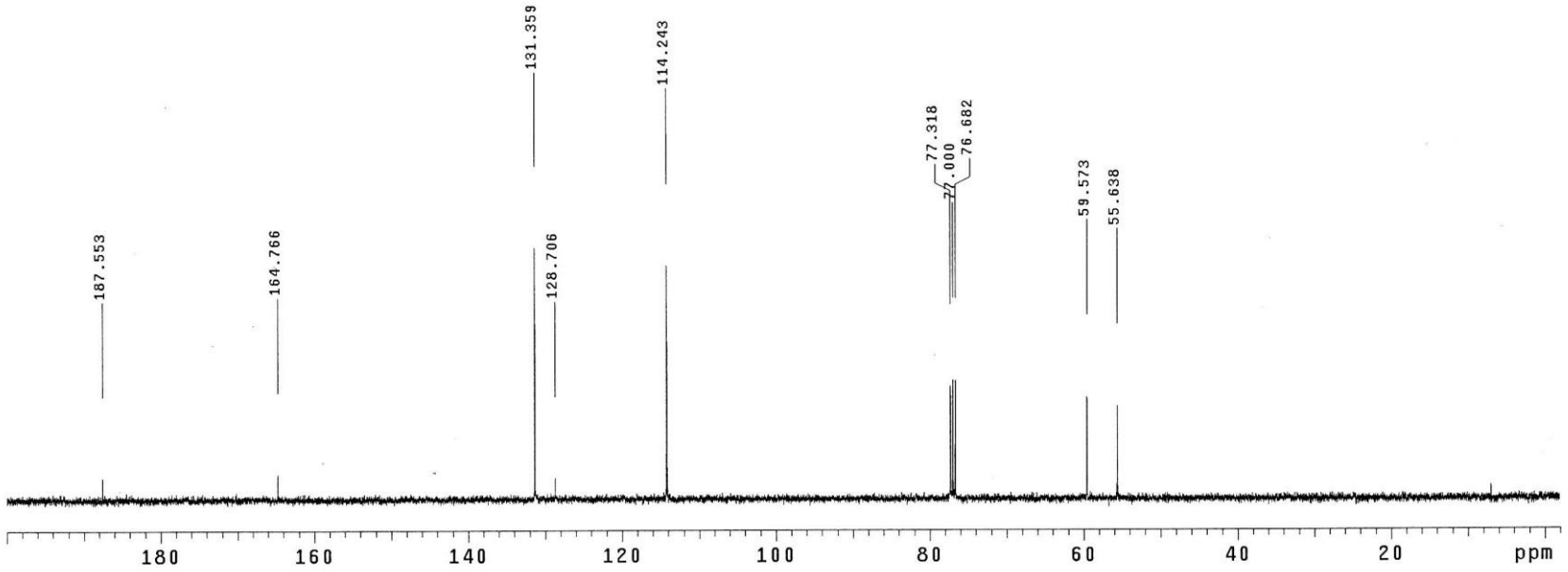
# Compound 4i ($^{13}$C-NMR spectral data)

LYS0317

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Mar 16 2023
Solvent: CDCl3
Ambient temperature
Total 1600 repetitions

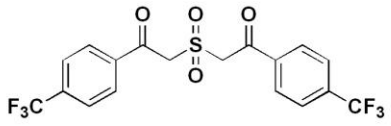


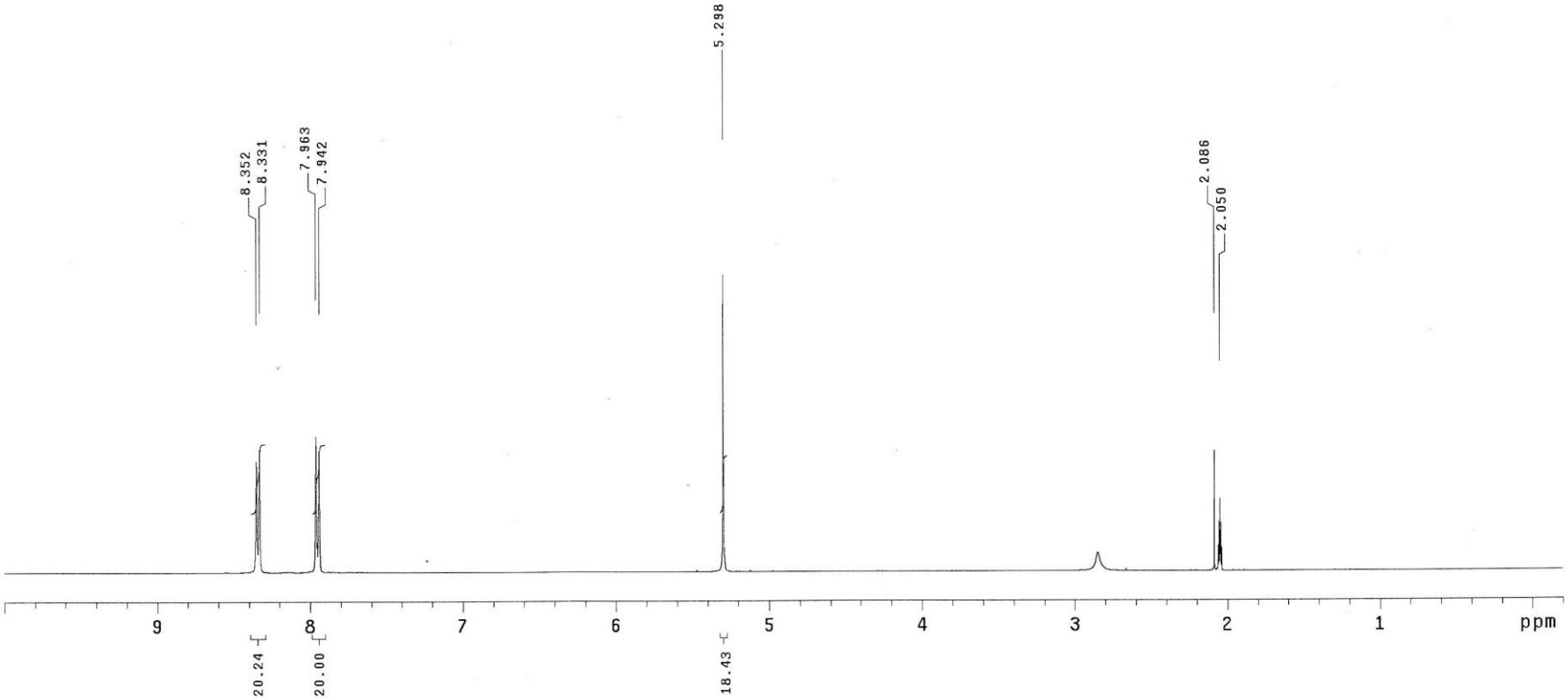



# Compound 4j ($^1$H-NMR spectral data)

LYS0321

Pulse Sequence: s2pul
Mercury-400BB "MerPlus400"
Date: Mar 22 2023
Solvent: acetone
Ambient temperature
Total 32 repetitions



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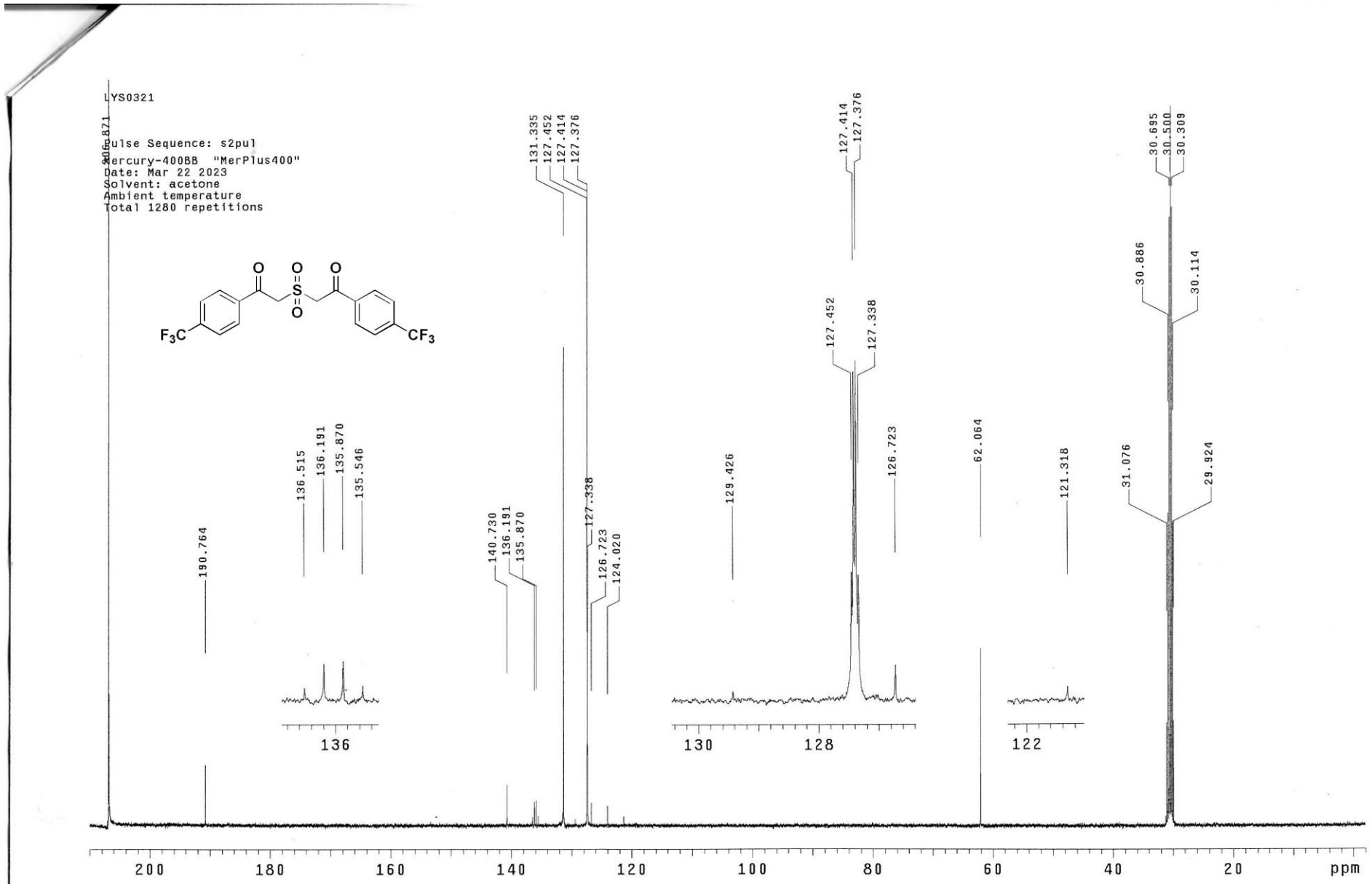

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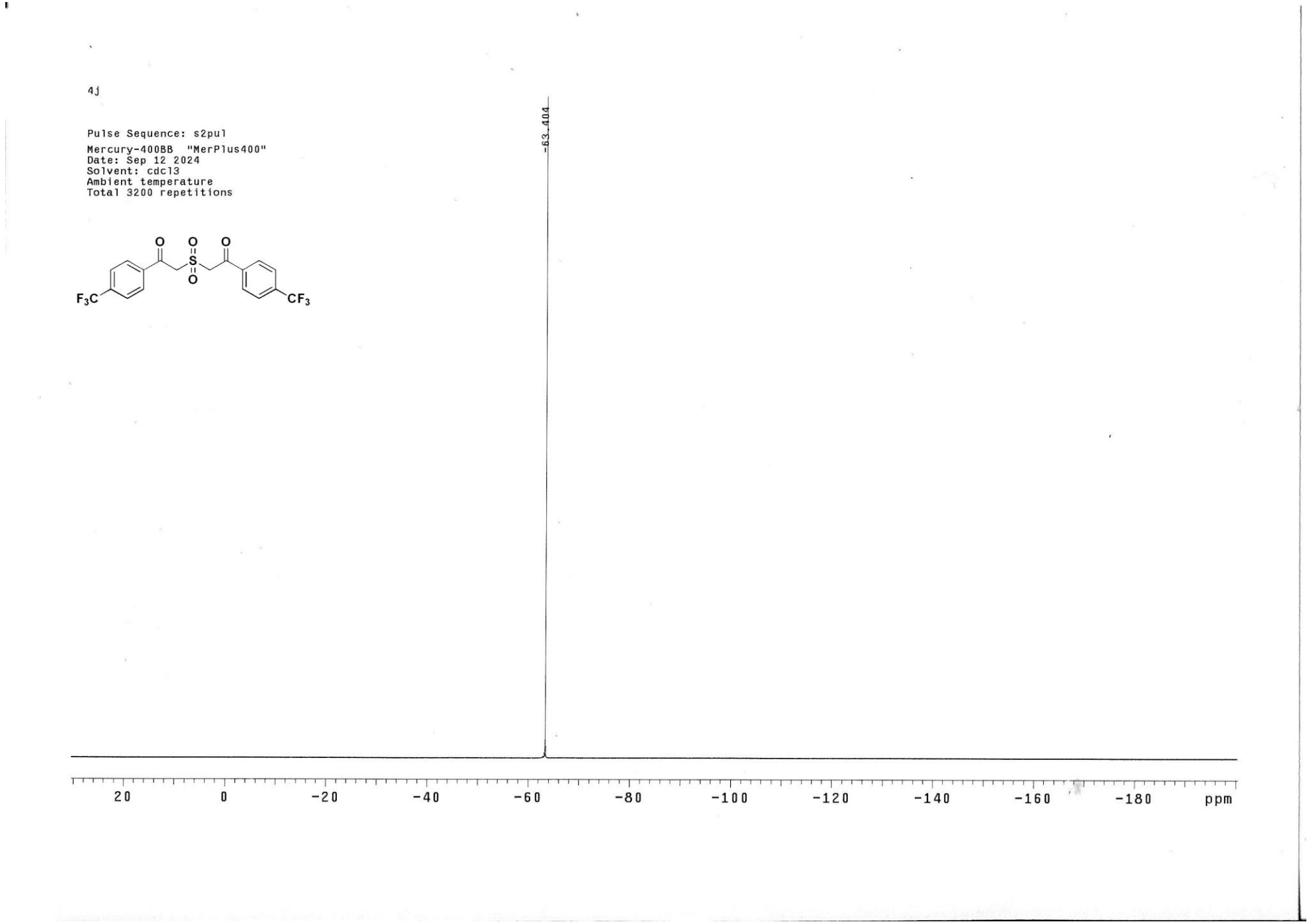

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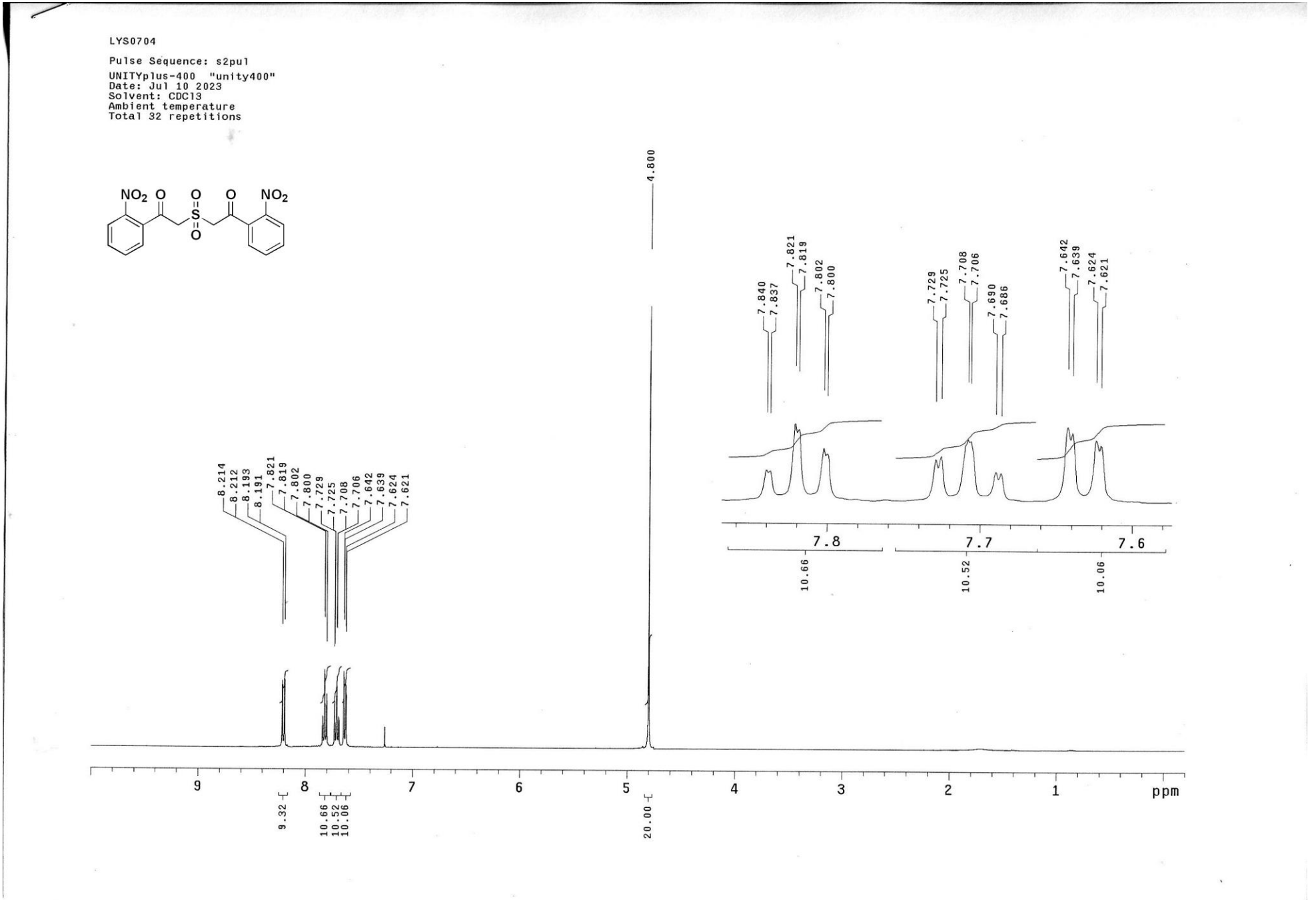
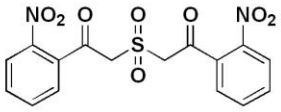


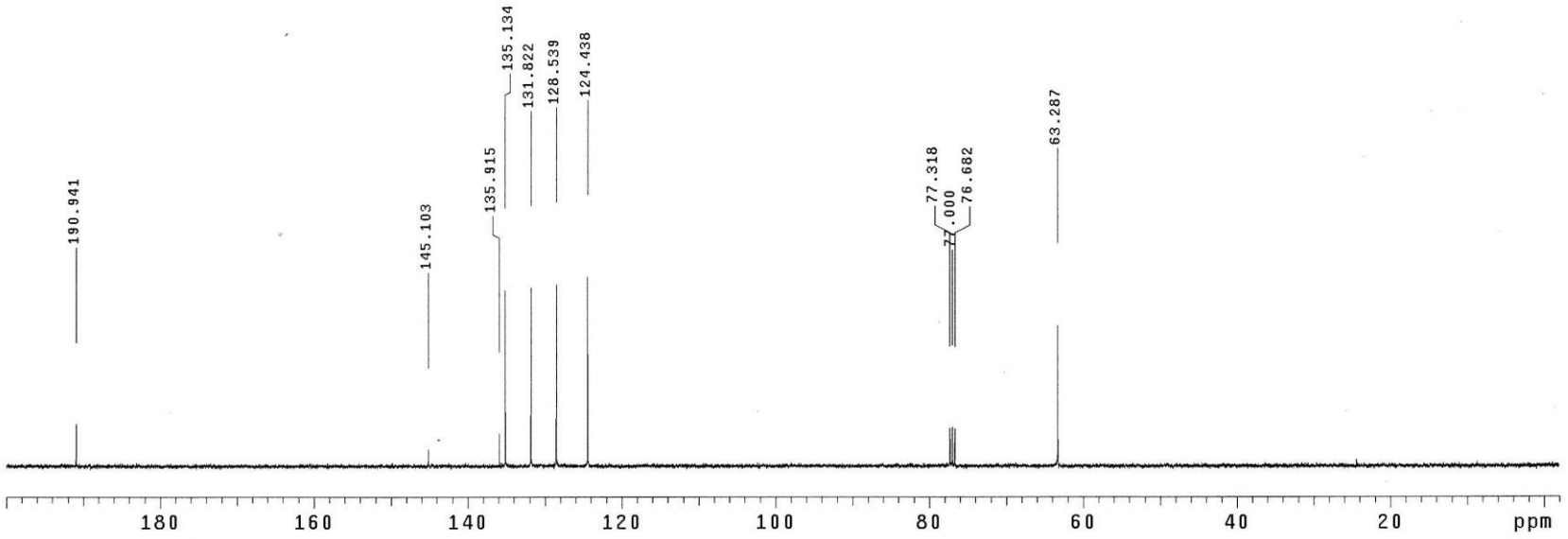
# Compound 4k ($^{13}$C-NMR spectral data)

LYS0704

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jul 10 2023
Solvent: CDCl3
Ambient temperature
Total 720 repetitions



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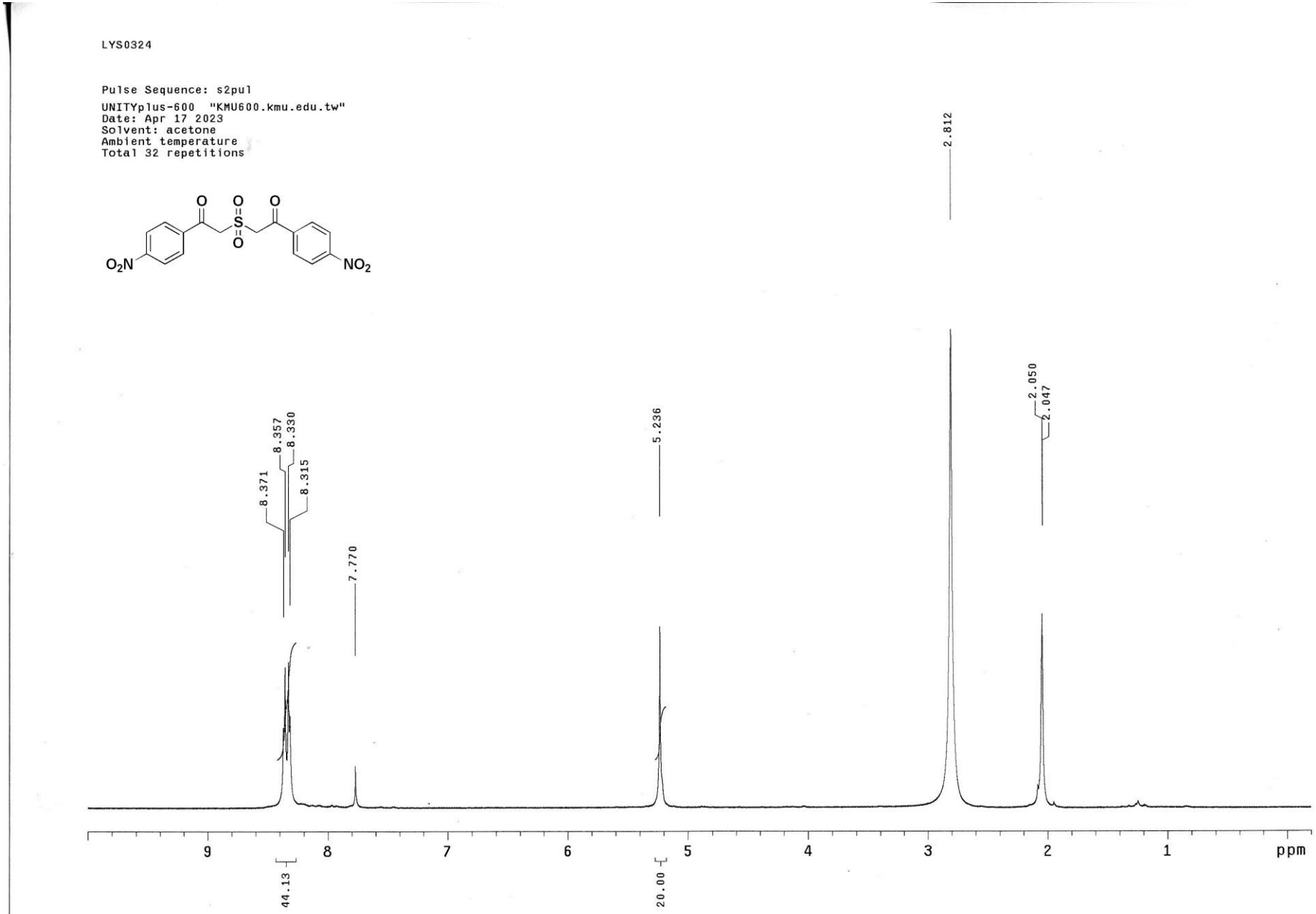
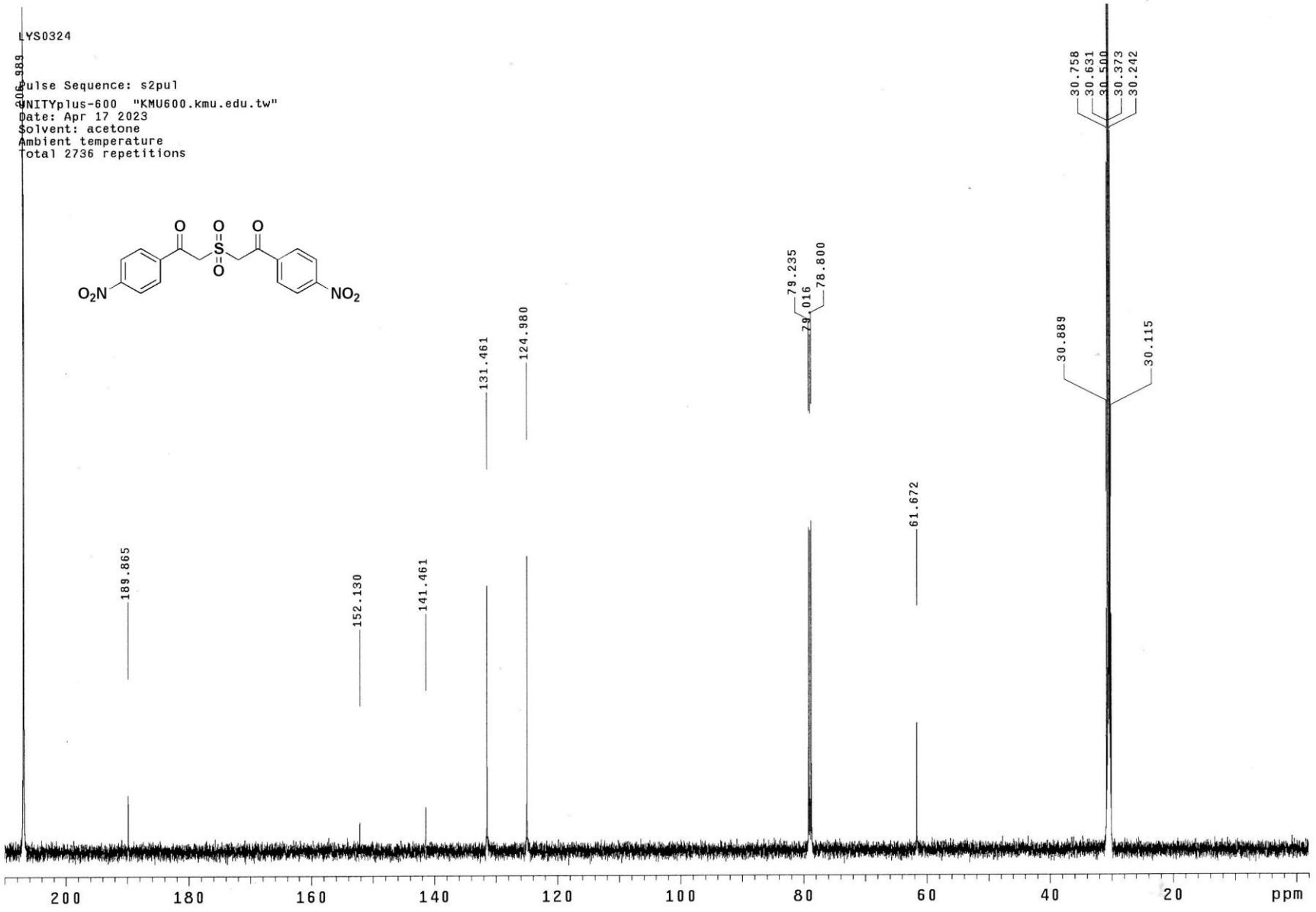


# Compound 4l ($^{13}$C-NMR spectral data)



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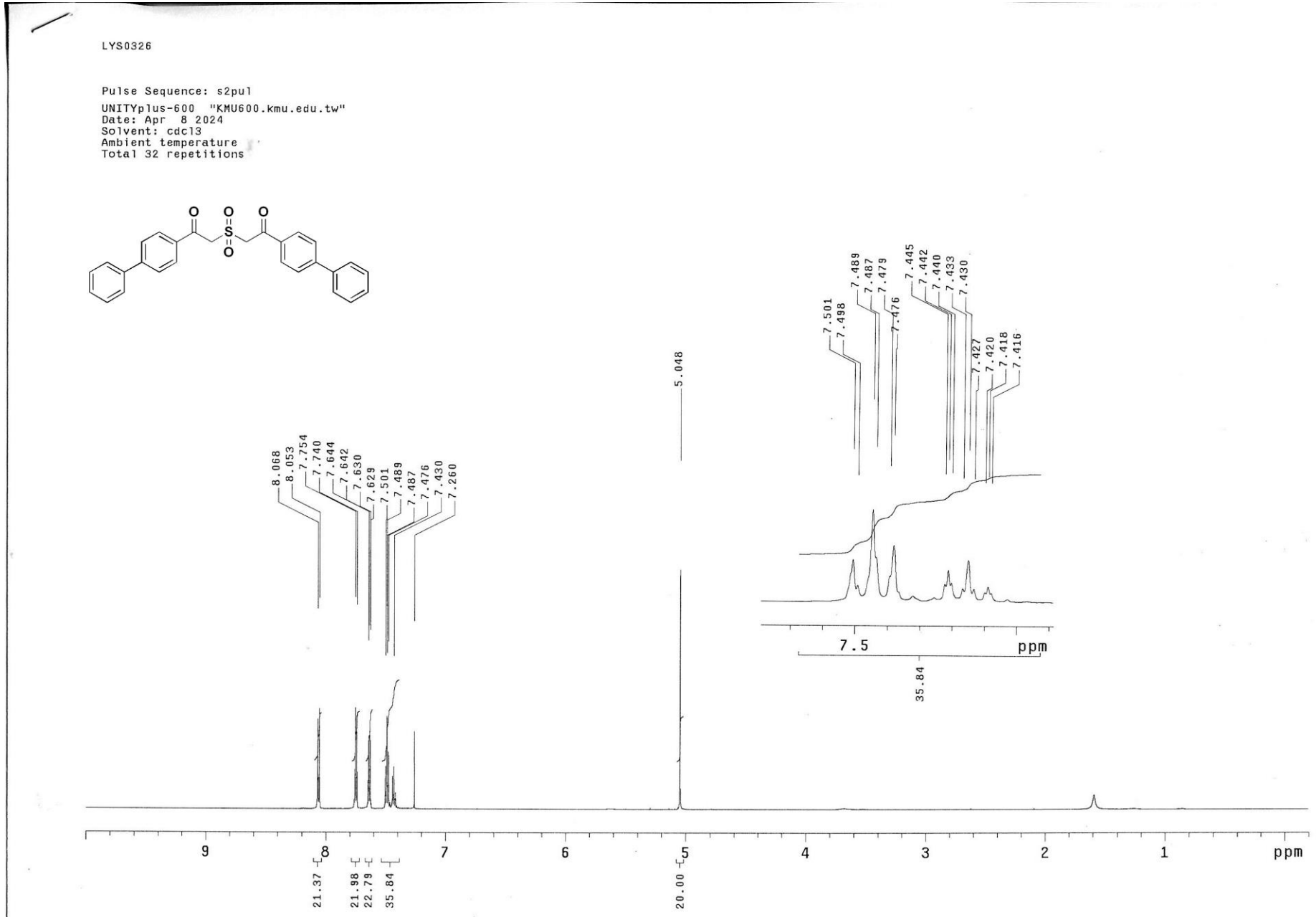

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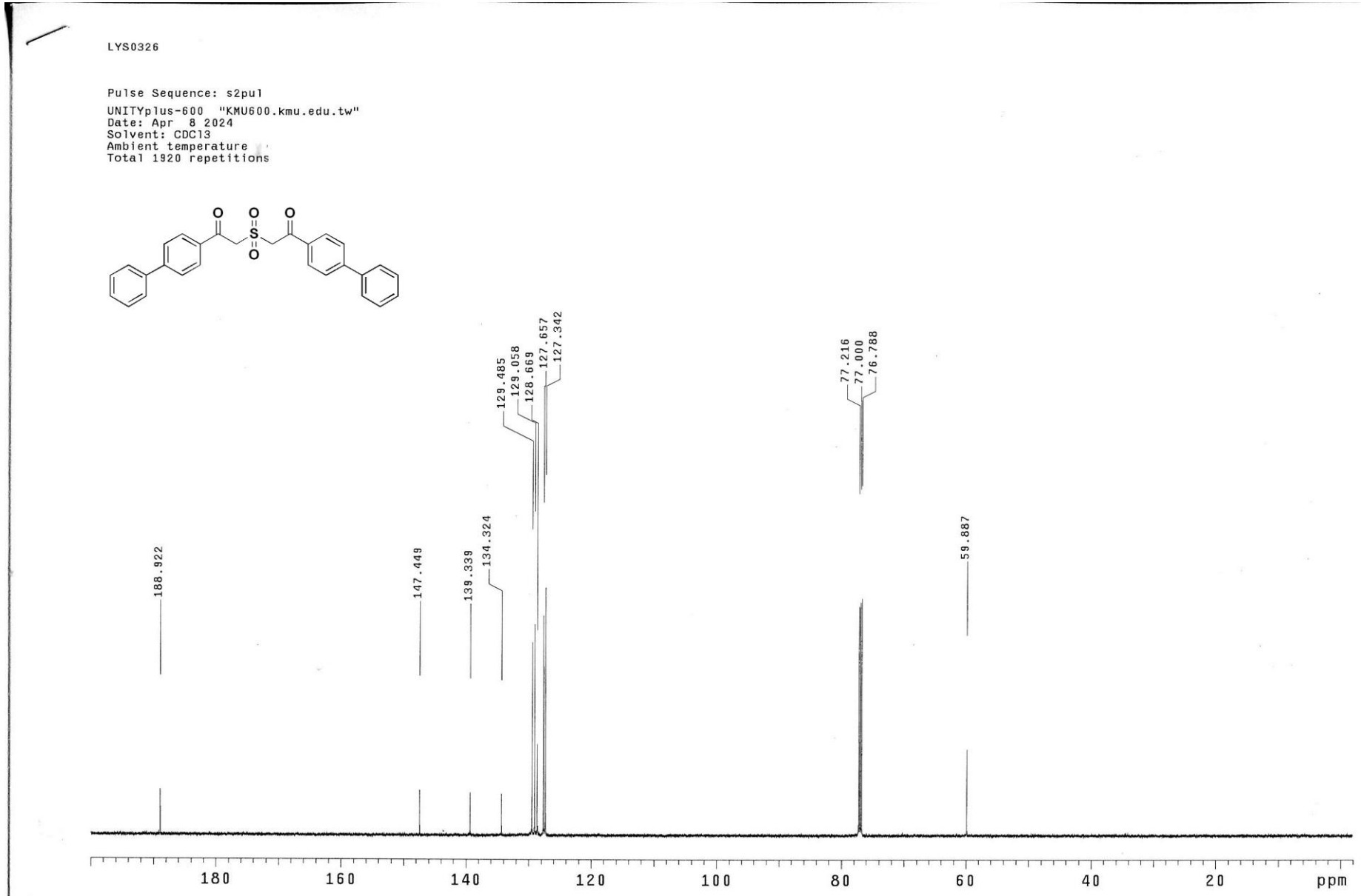
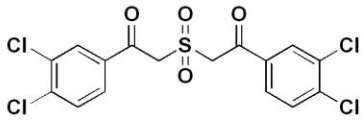


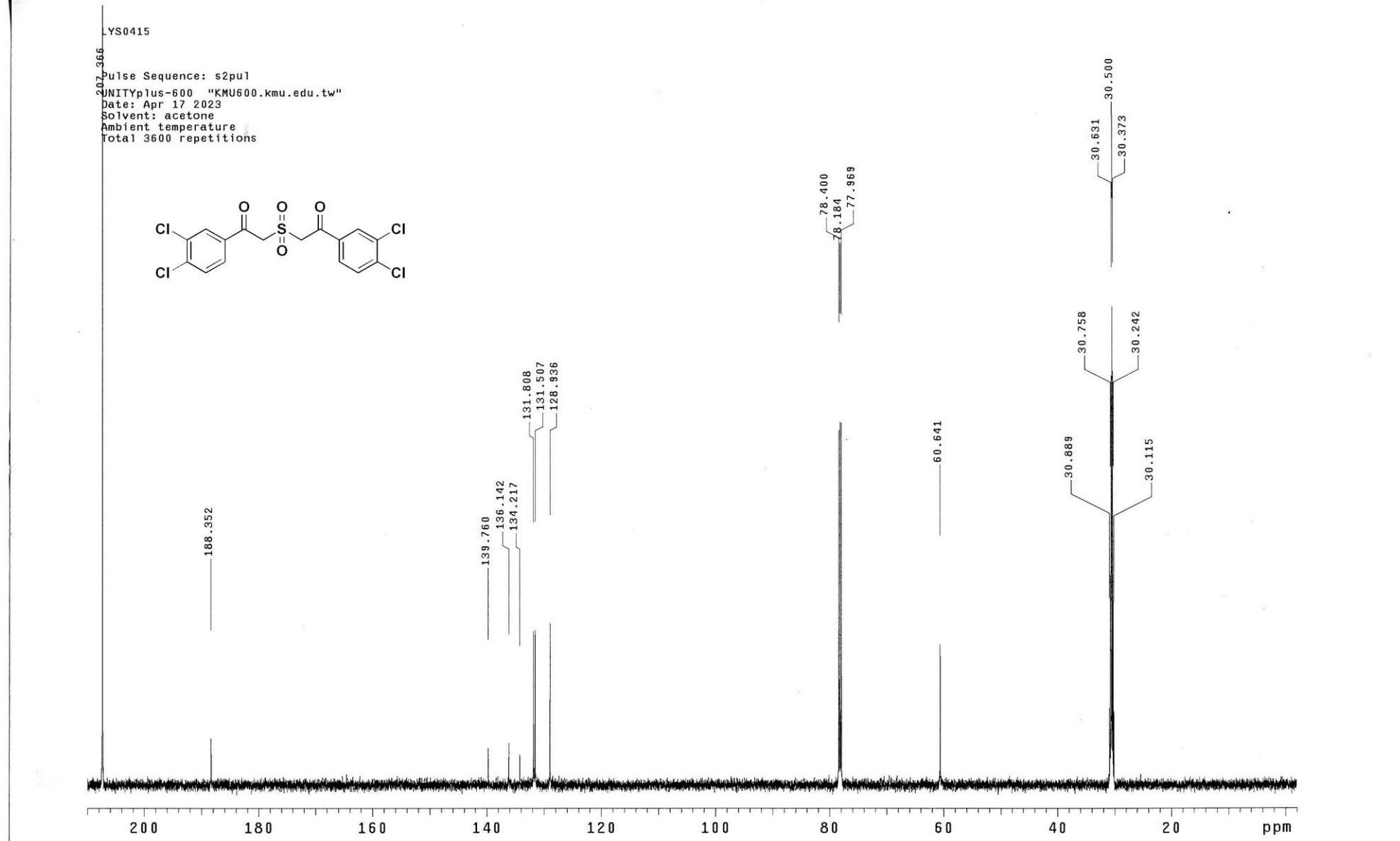
# Compound 4n ($^1$H-NMR spectral data)

LYS0415

Pulse Sequence: s2pul
UNITYplus-600 "KMU600.kmu.edu.tw"
Date: Apr 17 2023
Solvent: acetone
Ambient temperature
Total 60 repetitions



# Compound 4n ($^{13}$C-NMR spectral data)

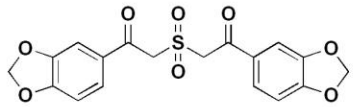


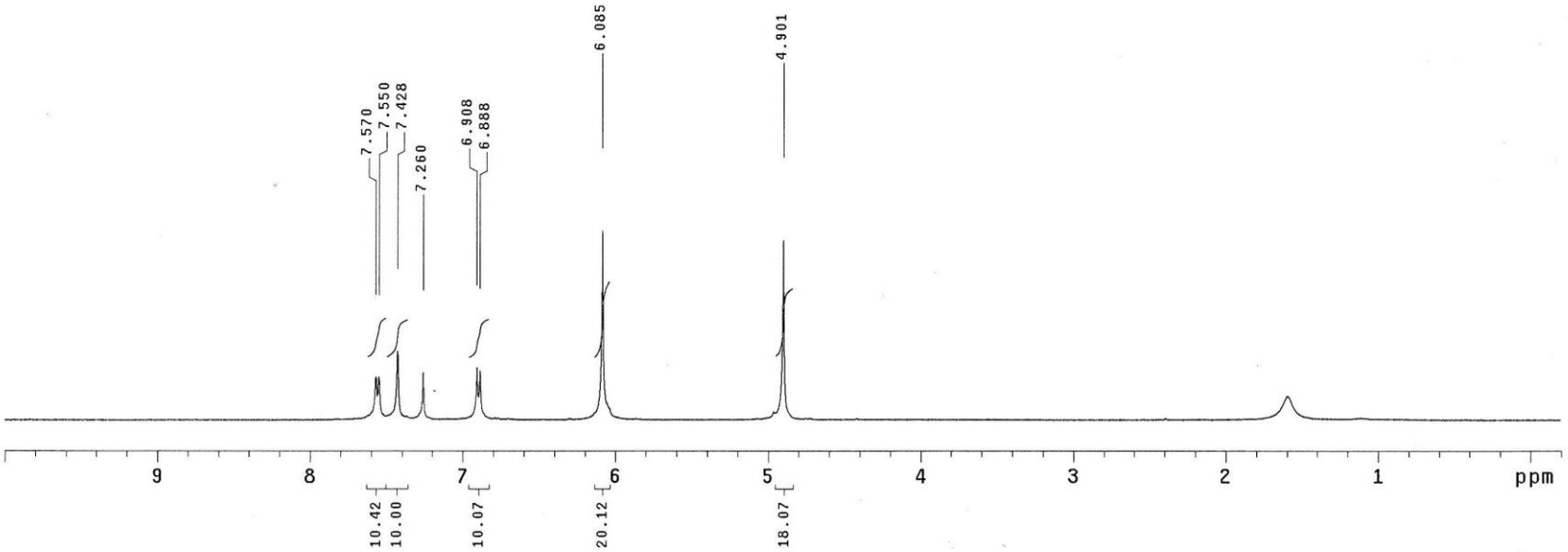
# Compound 4o ($^1$H-NMR spectral data)

LYS0426

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 4 2023
Solvent: CDCl3
Ambient temperature
Total 64 repetitions



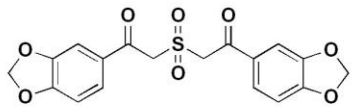


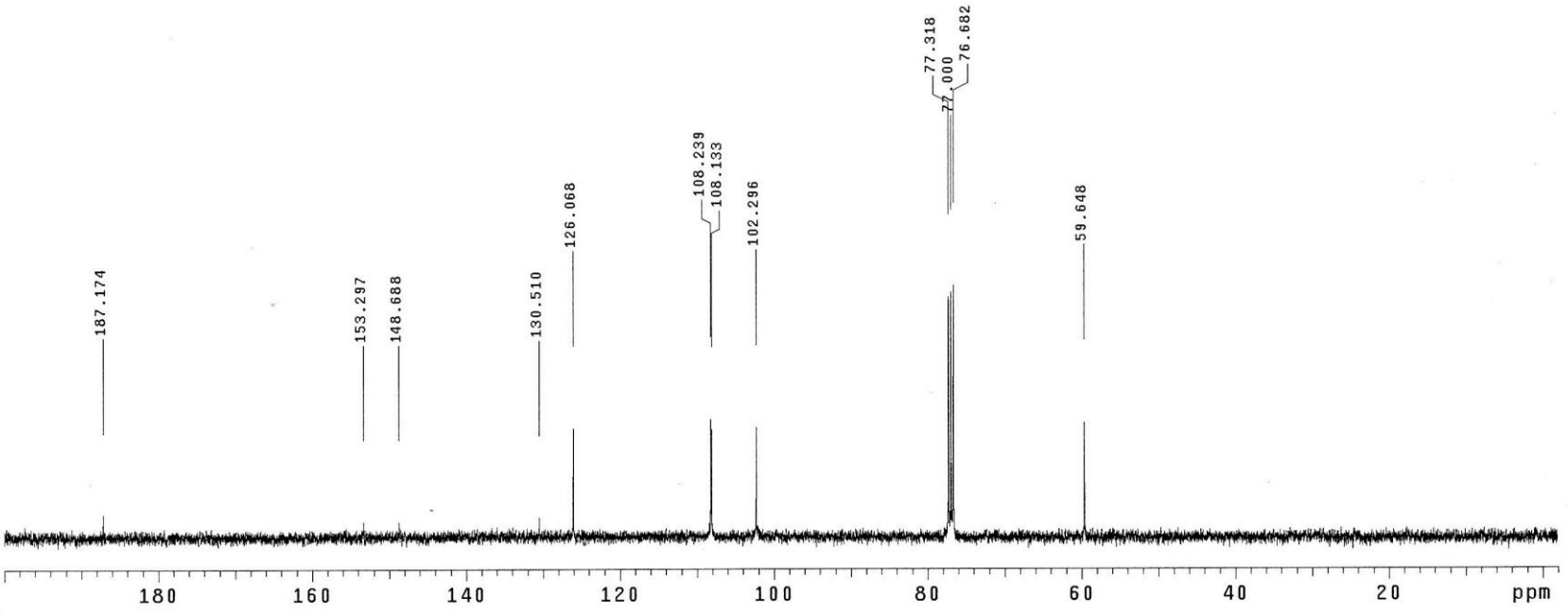
# Compound 4o ($^{13}$C-NMR spectral data)

LYS0426

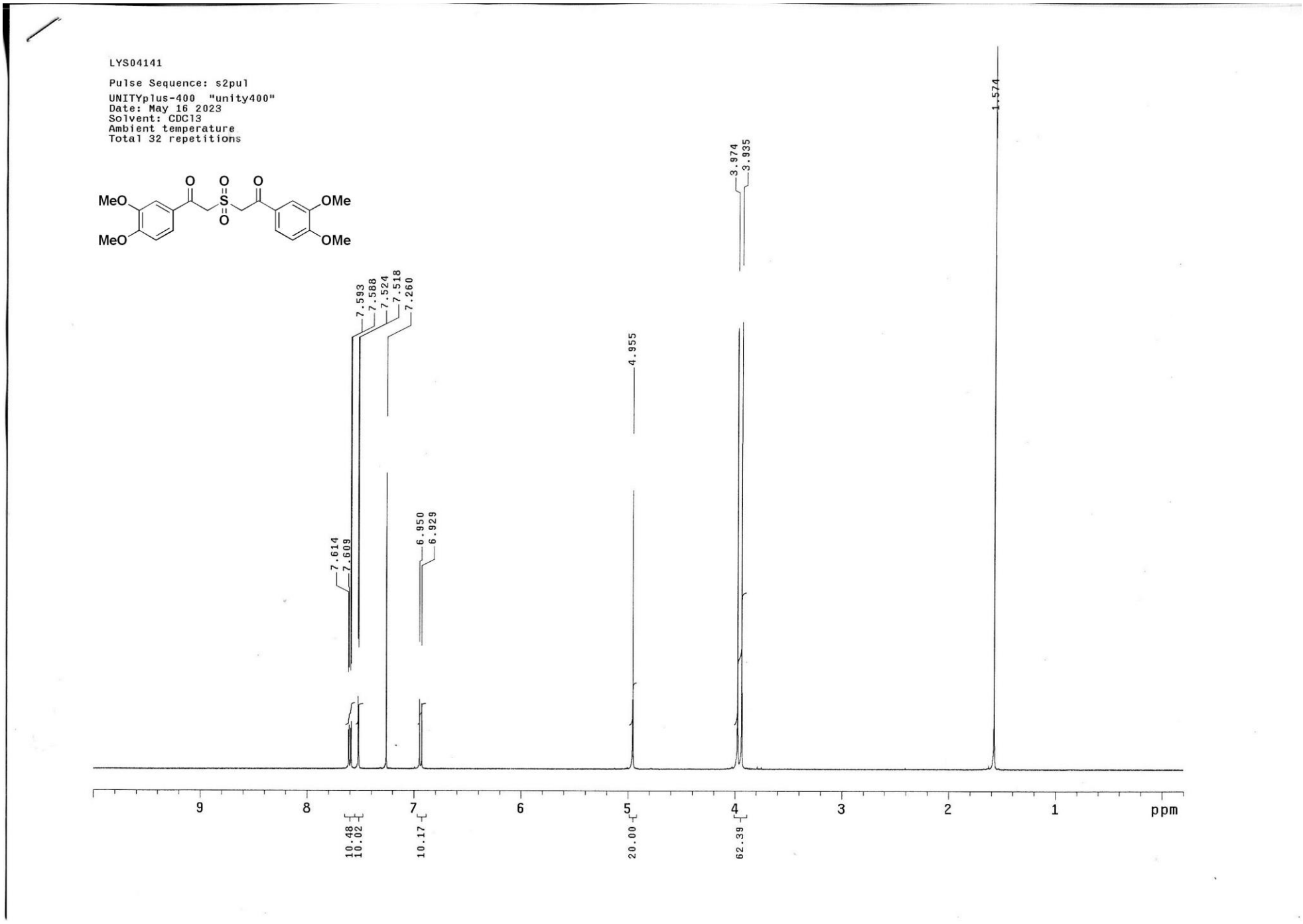
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 4 2023
Solvent: CDCl3
Ambient temperature
Total 9792 repetitions





# Compound 4p ($^1$H-NMR spectral data)

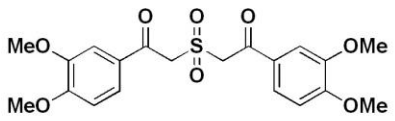


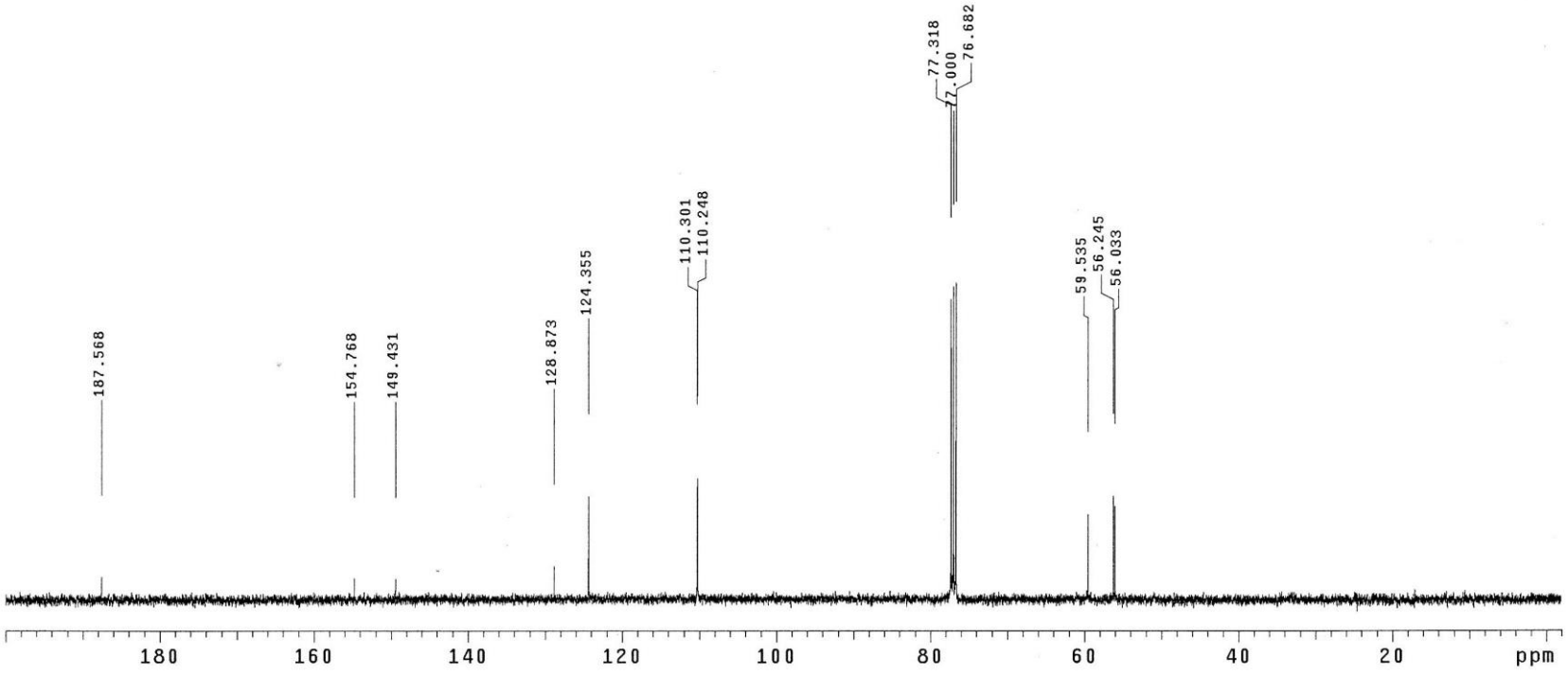
# Compound 4p ($^{13}$C-NMR spectral data)

LYS04141

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 16 2023
Solvent: CDCl3
Ambient temperature
Total 8432 repetitions



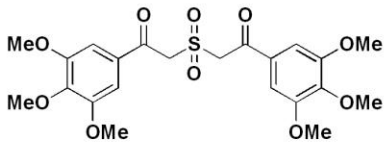



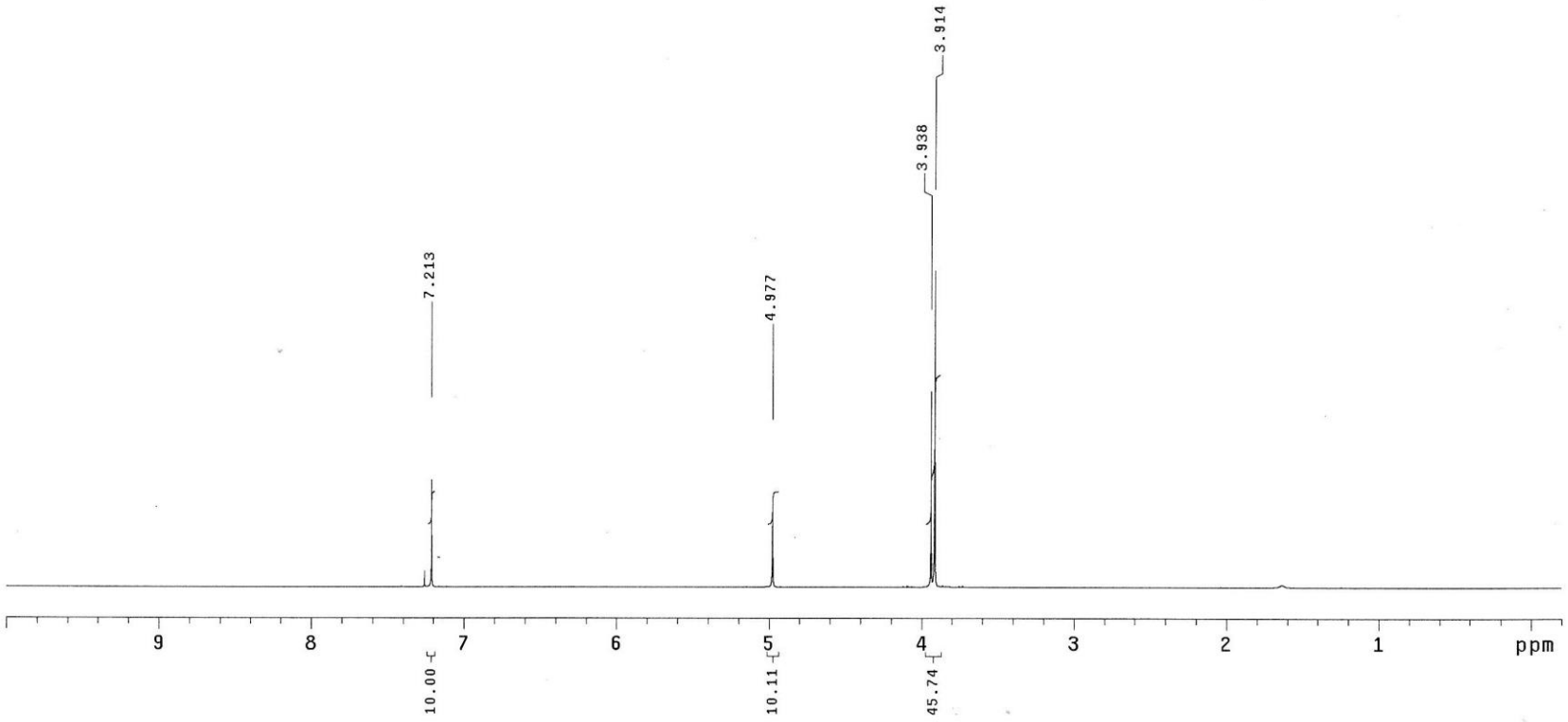
# Compound 4q ($^1$H-NMR spectral data)

LYS0501

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 2 2023
Solvent: CDCl3
Ambient temperature
Total 32 repetitions



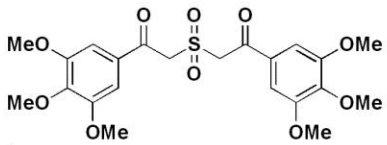



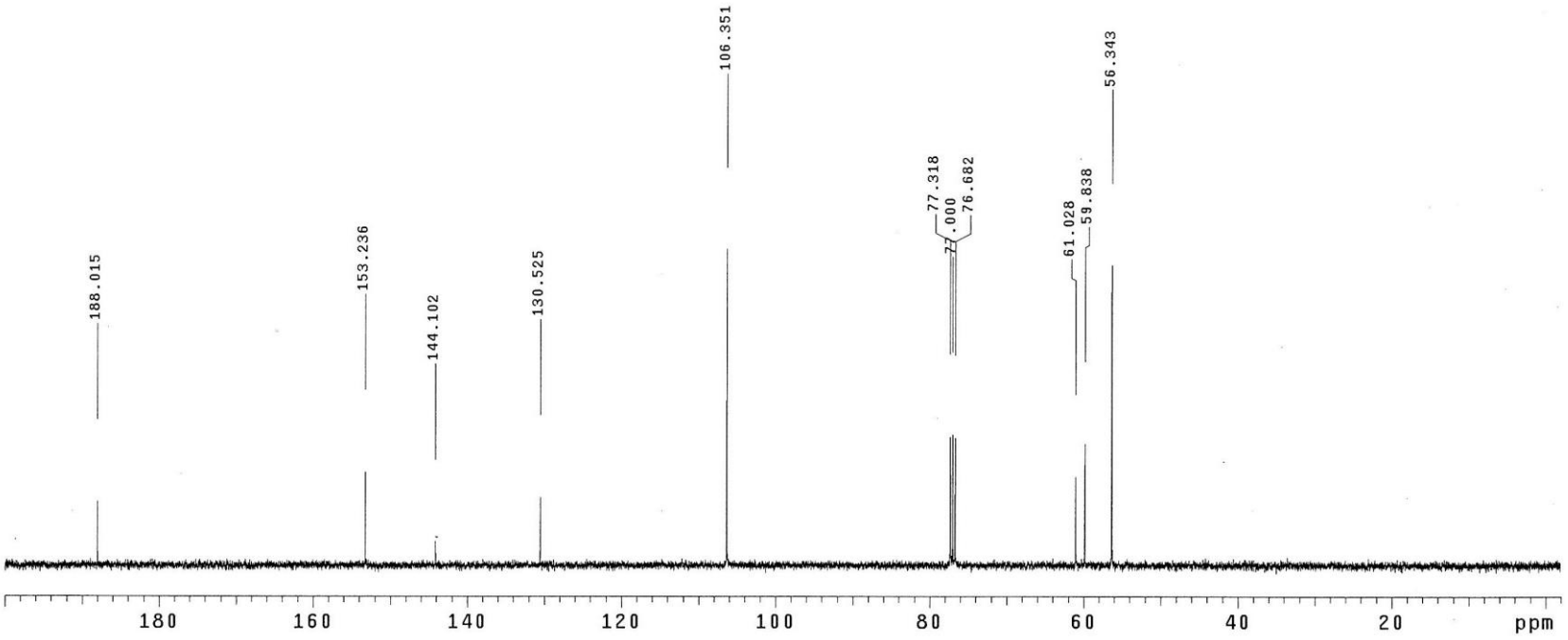
# Compound 4q ($^{13}$C-NMR spectral data)

LYS0501

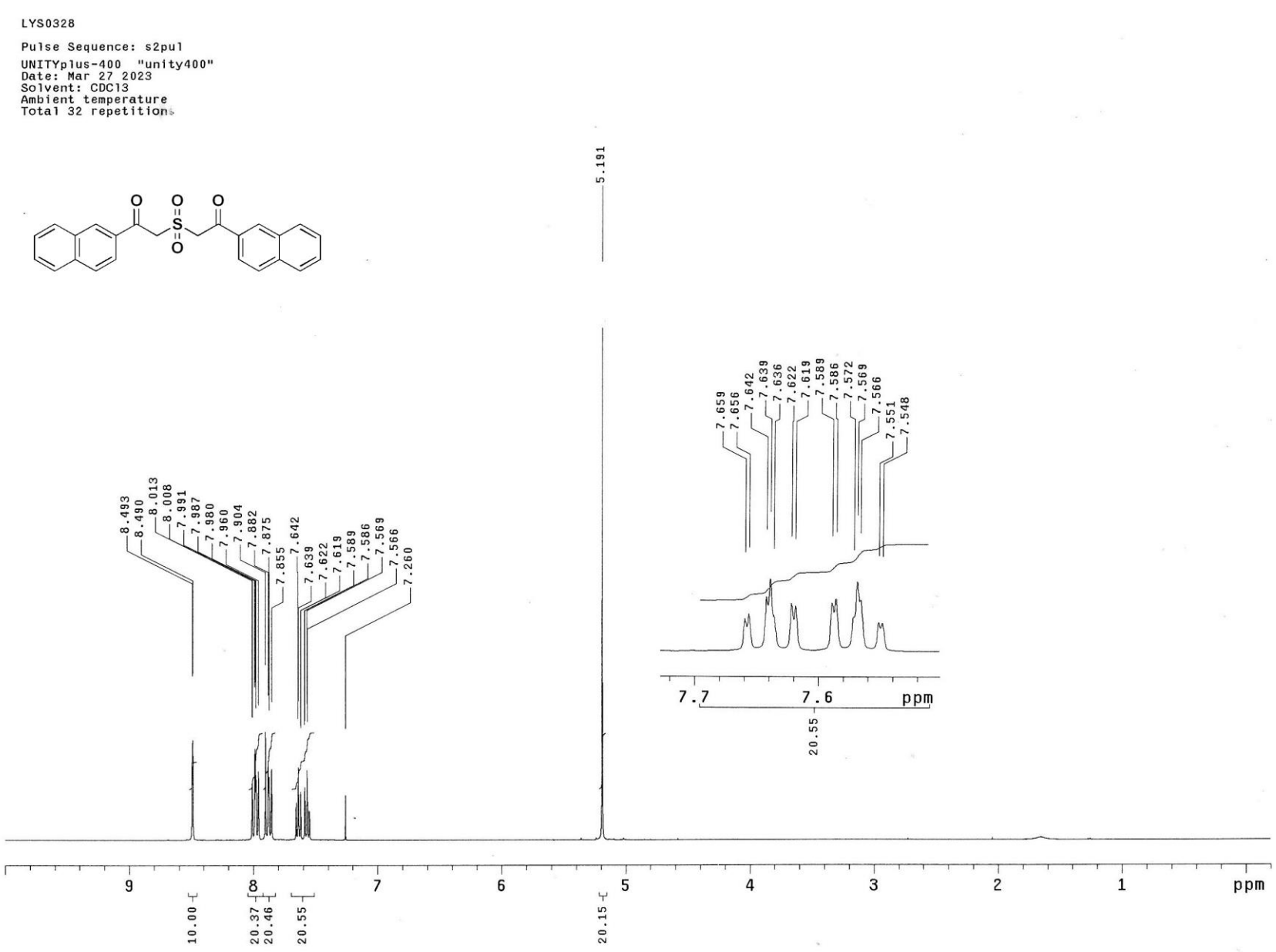
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 2 2023
Solvent: CDCl3
Ambient temperature
Total 1184 repetitions



# Compound 4r ($^1$H-NMR spectral data)

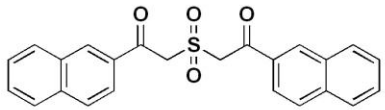


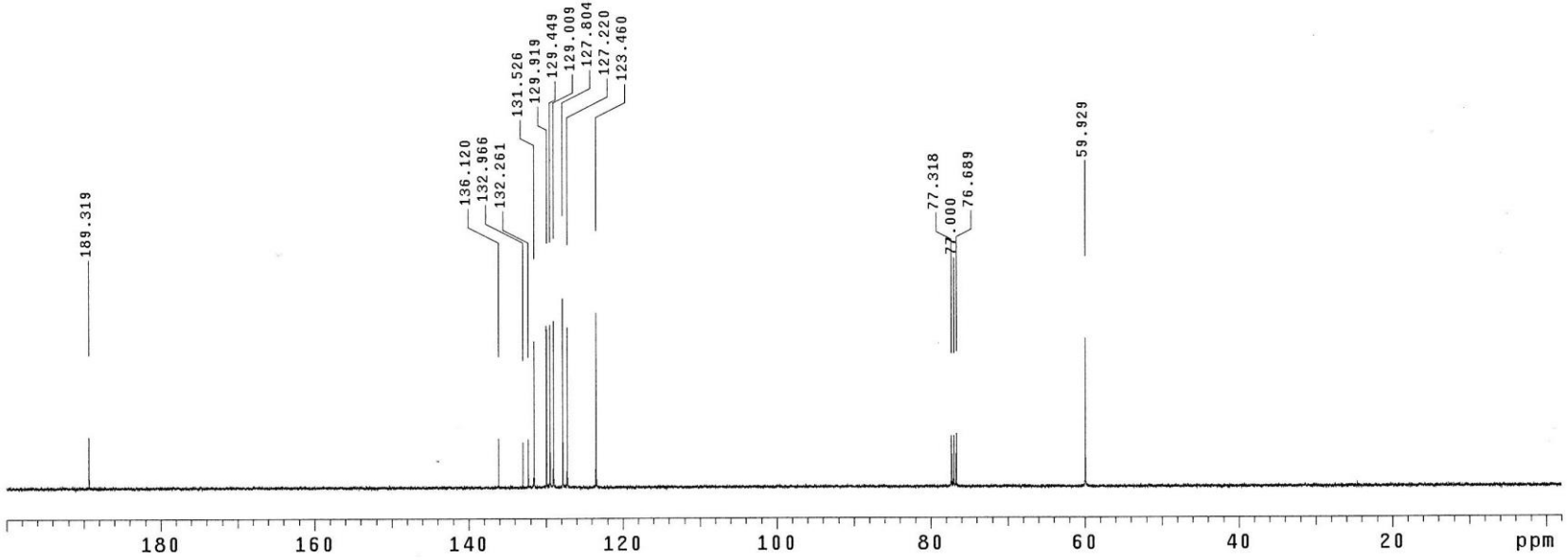
# Compound 4r ($^{13}$C-NMR spectral data)

LYS0328

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Mar 27 2023
Solvent: CDCl3
Ambient temperature
Total 1696 repetitions

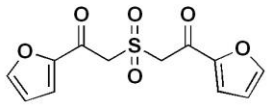




# Compound 4s ($^1$H-NMR spectral data)

LYS0508

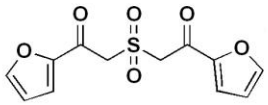
Pulse Sequence: s2pul
UNITYplus-600 "KMU600.kmu.edu.tw"
Date: May 9 2023
Solvent: cdcl3
Ambient temperature
Total 32 repetitions

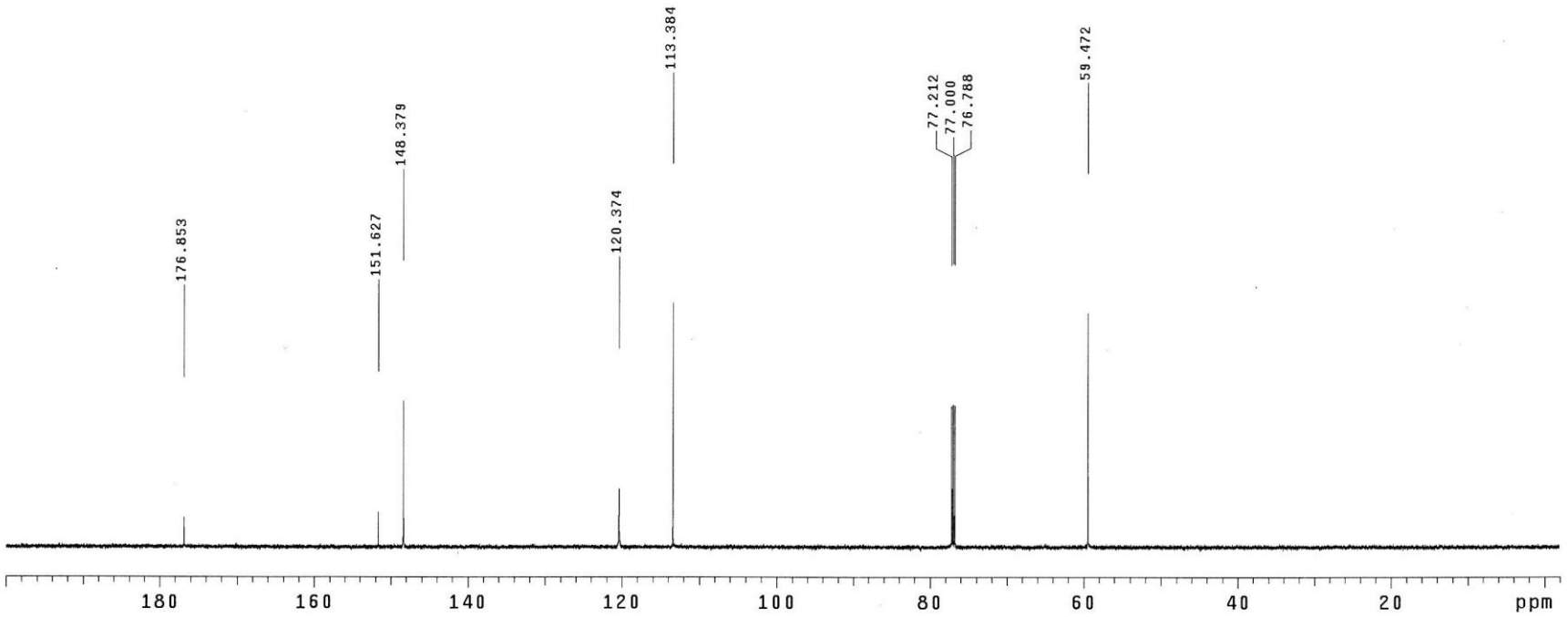


# Compound 4s ($^{13}$C-NMR spectral data)

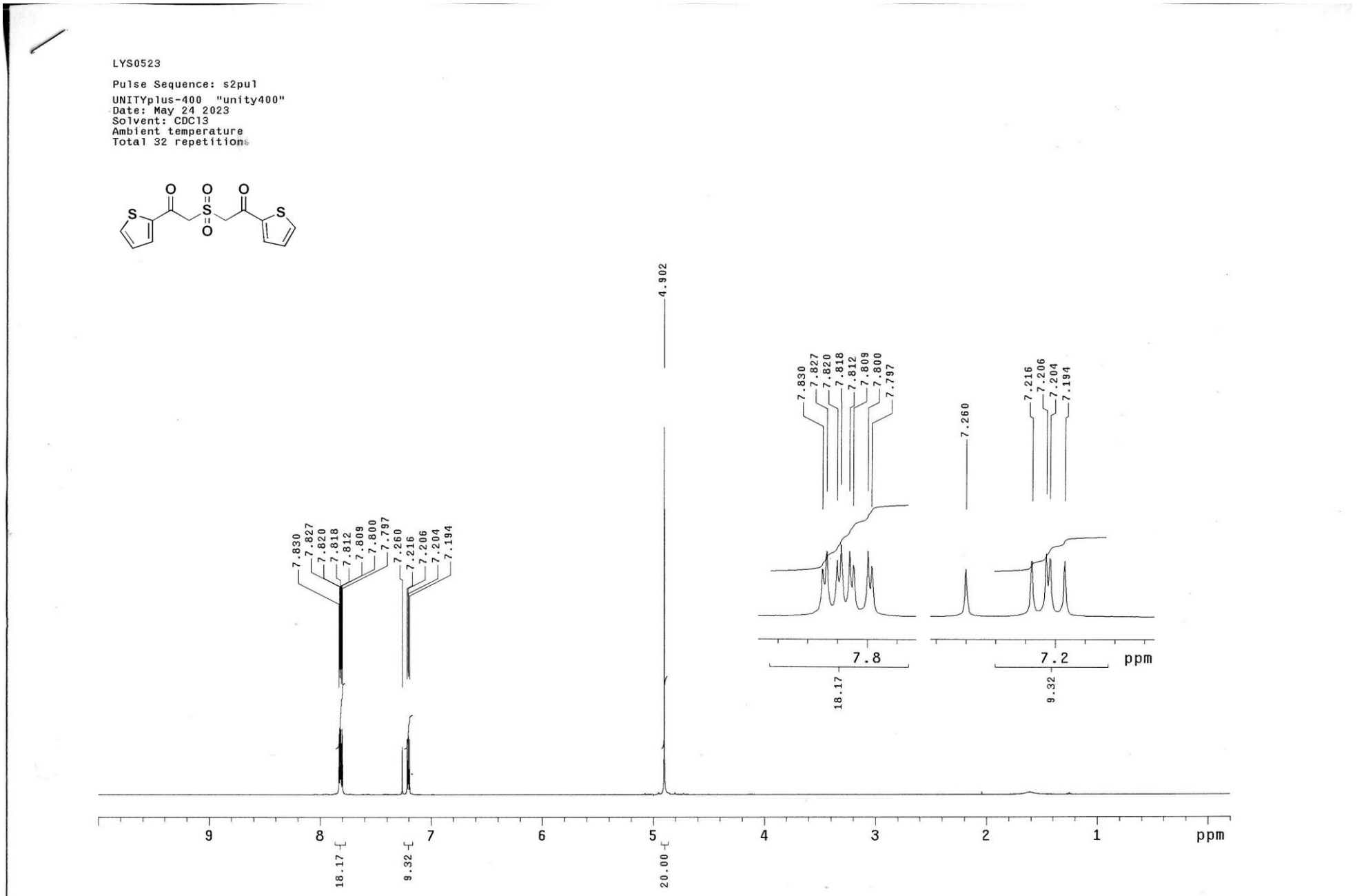
LYS0508

Pulse Sequence: s2pul
UNITYplus-600 "KMU600.kmu.edu.tw"
Date: May 9 2023
Solvent: cdcl3
Ambient temperature
Total 400 repetitions





# Compound 4t ($^1$H-NMR spectral data)

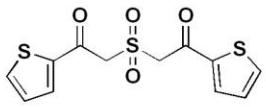


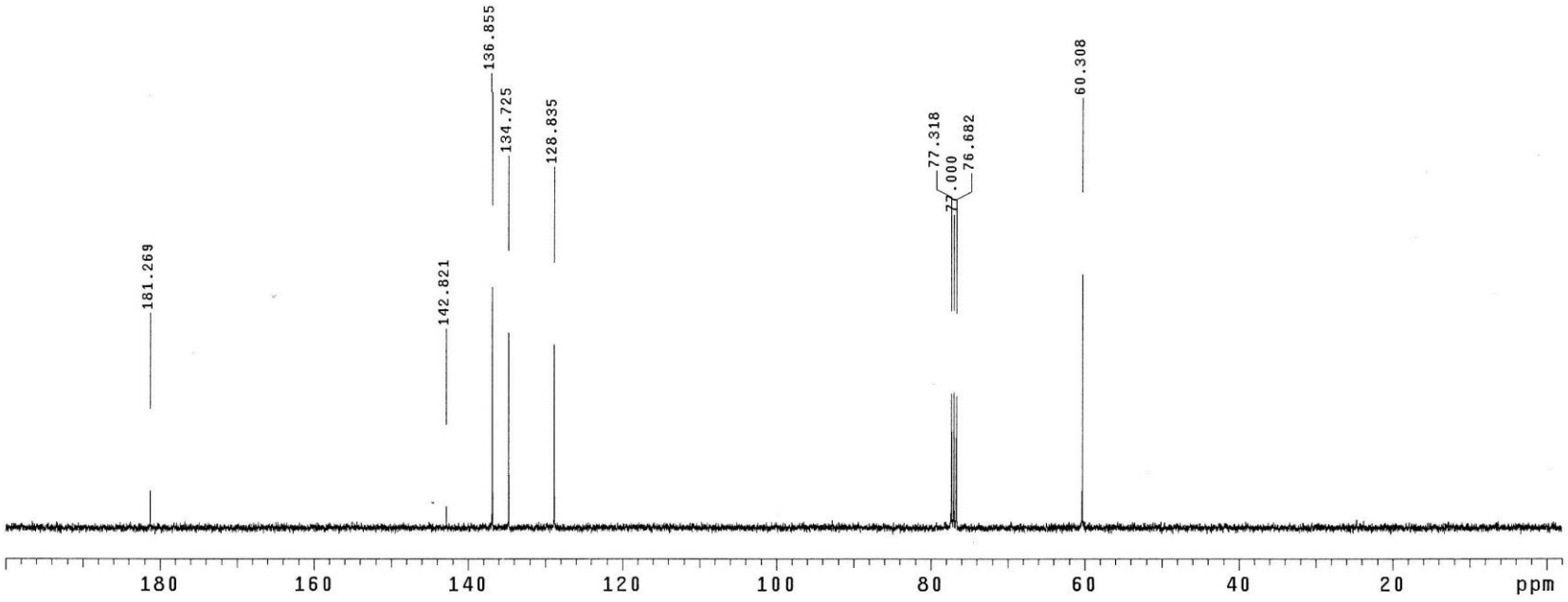
# Compound 4t ($^{13}$C-NMR spectral data)

LYS0523

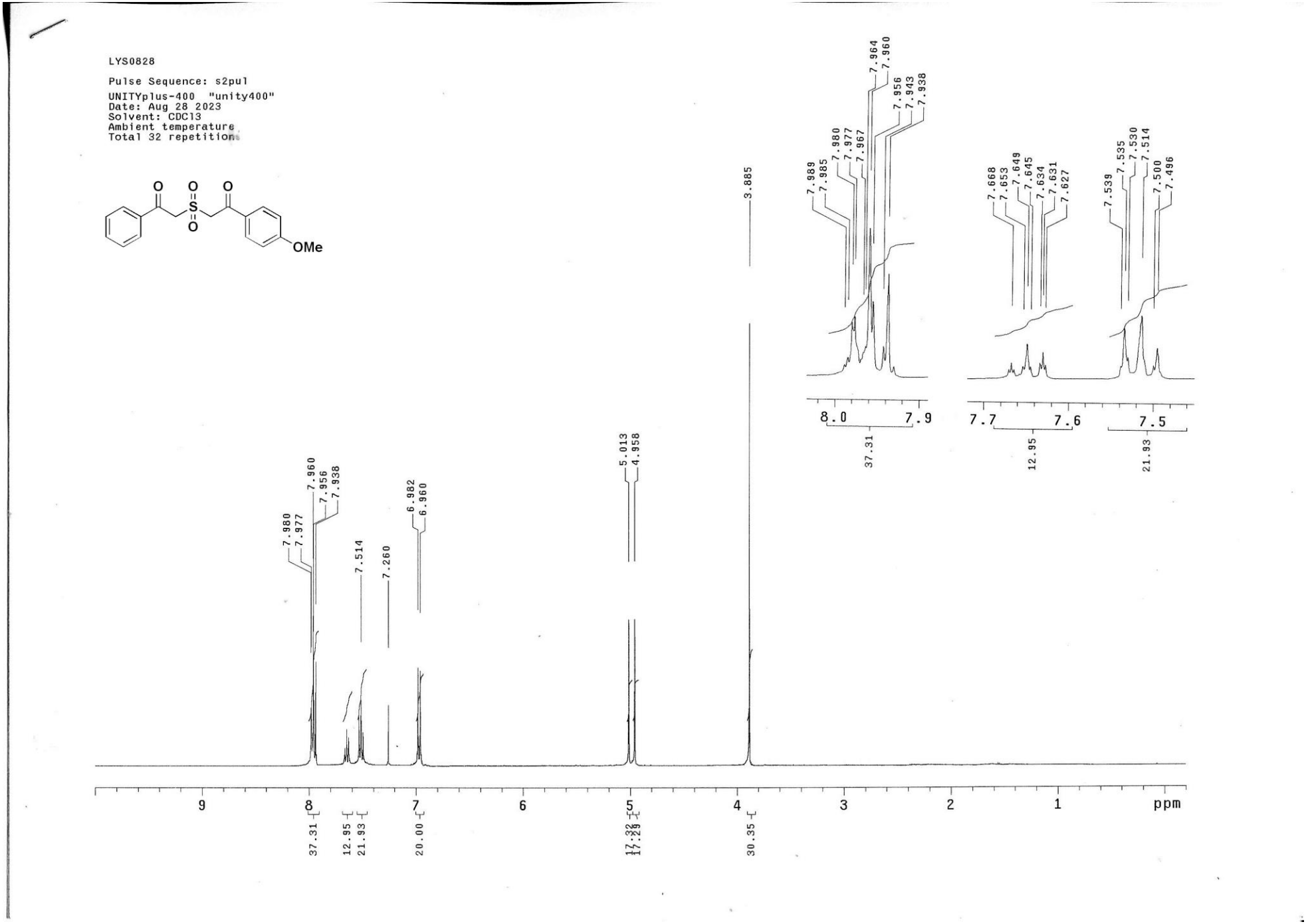
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 24 2023
Solvent: CDCl3
Ambient temperature
Total 3088 repetitions





# Compound 4u ($^1$H-NMR spectral data)

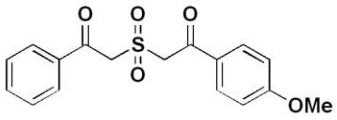


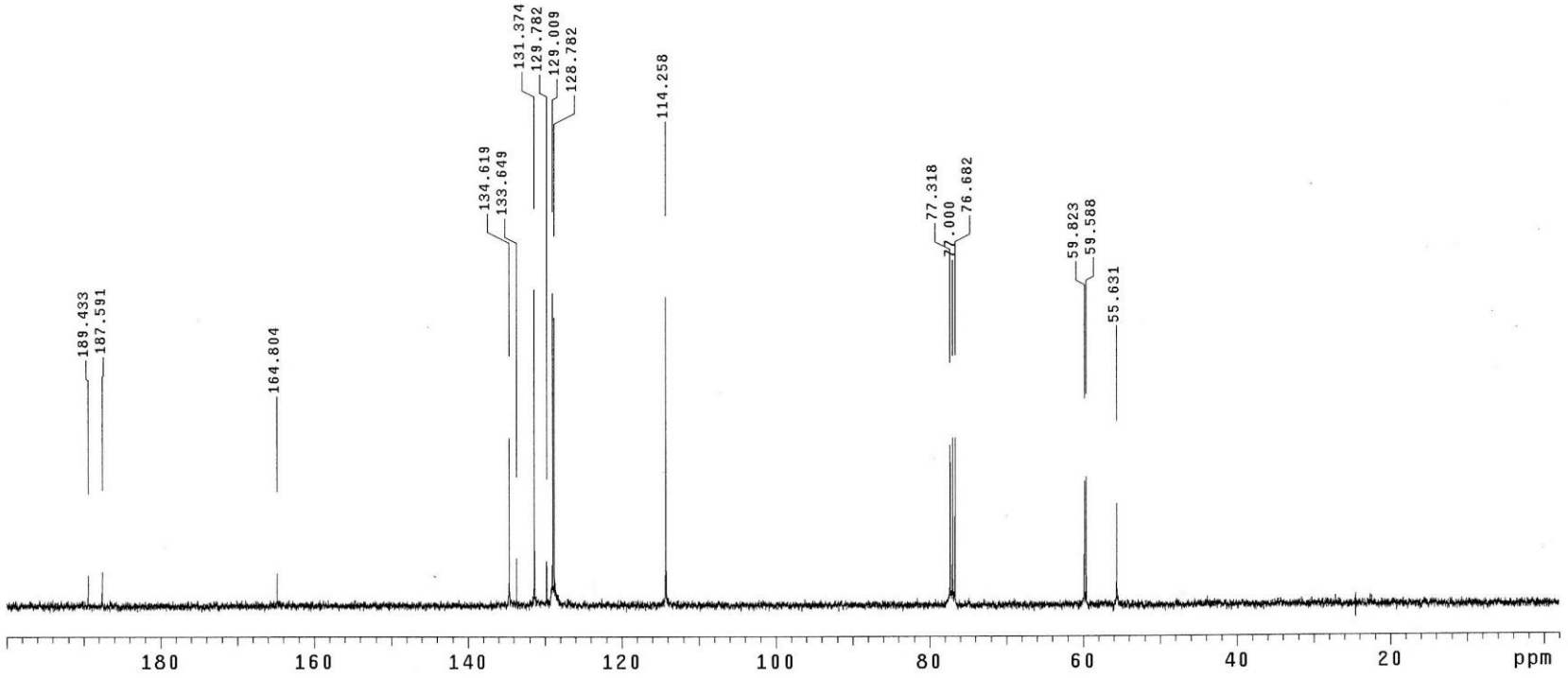
# Compound 4u ($^{13}$C-NMR spectral data)

LYS0828

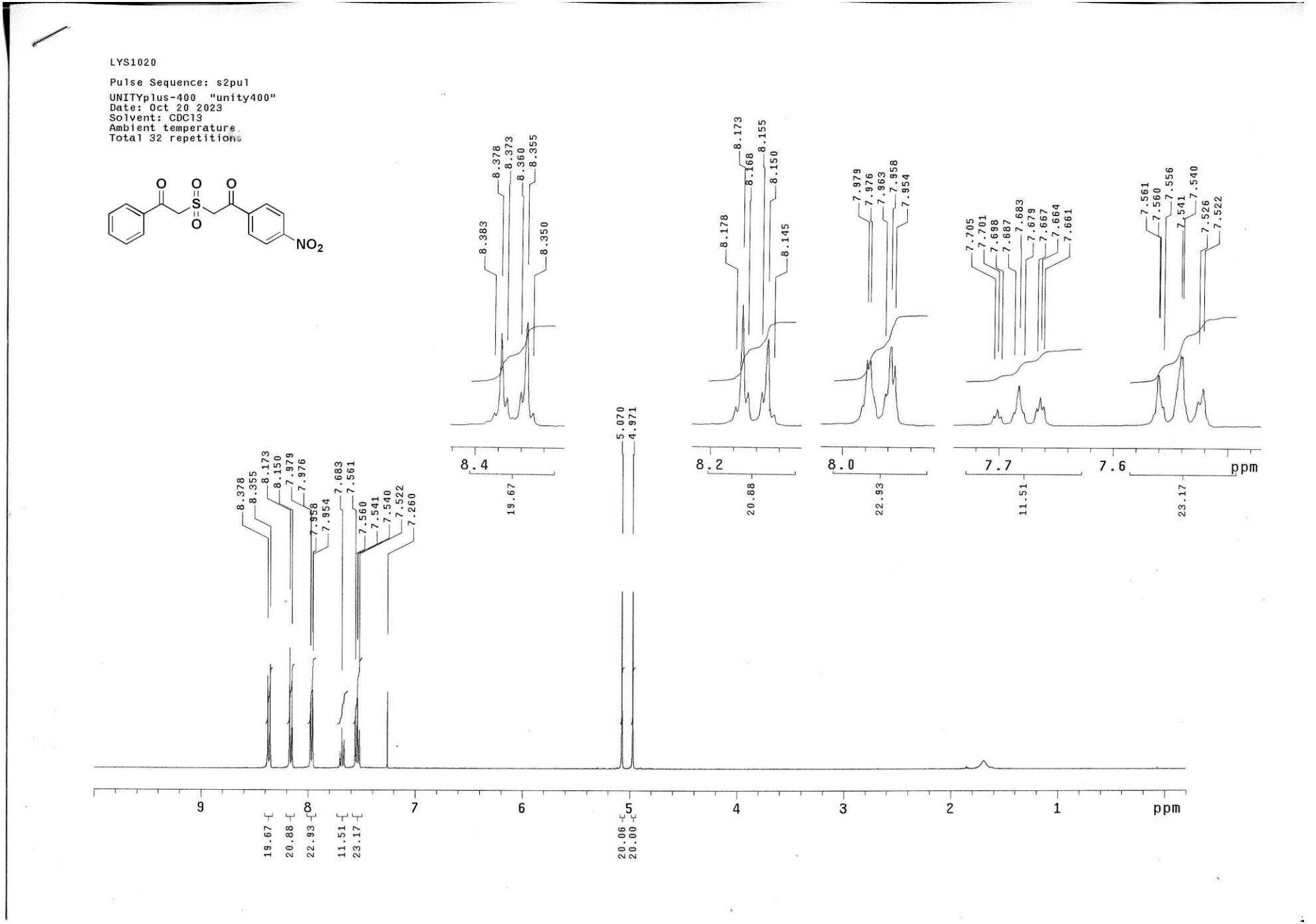
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Aug 28 2023
Solvent: CDCl3
Ambient temperature
Total 3680 repetitions



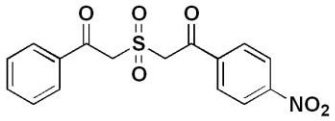
# Compound 4v ($^1$H-NMR spectral data)

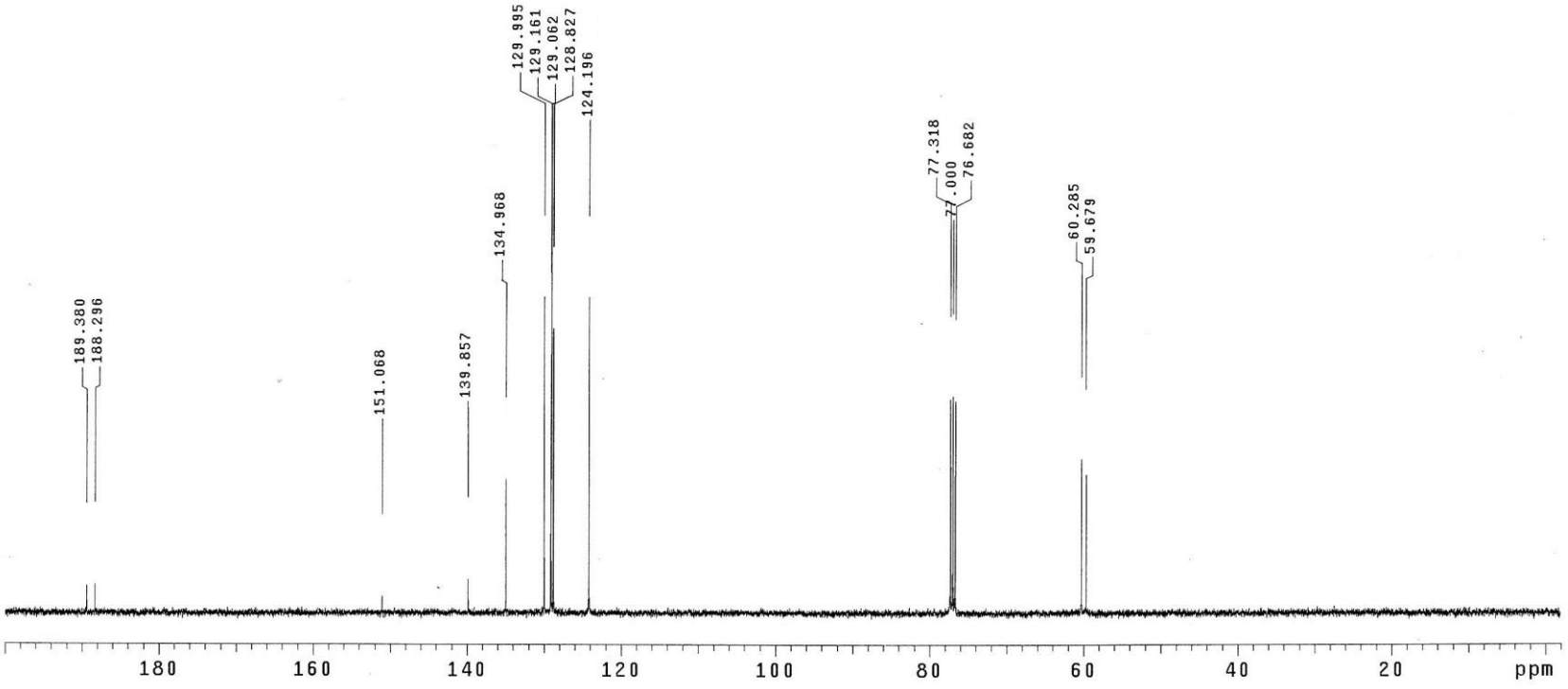


# Compound 4v ($^{13}$C-NMR spectral data)

LYS1020

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Oct 20 2023
Solvent: CDCl3
Ambient temperature
Total 6256 repetitions



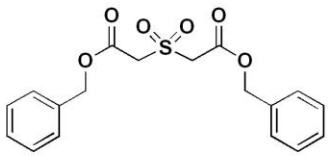



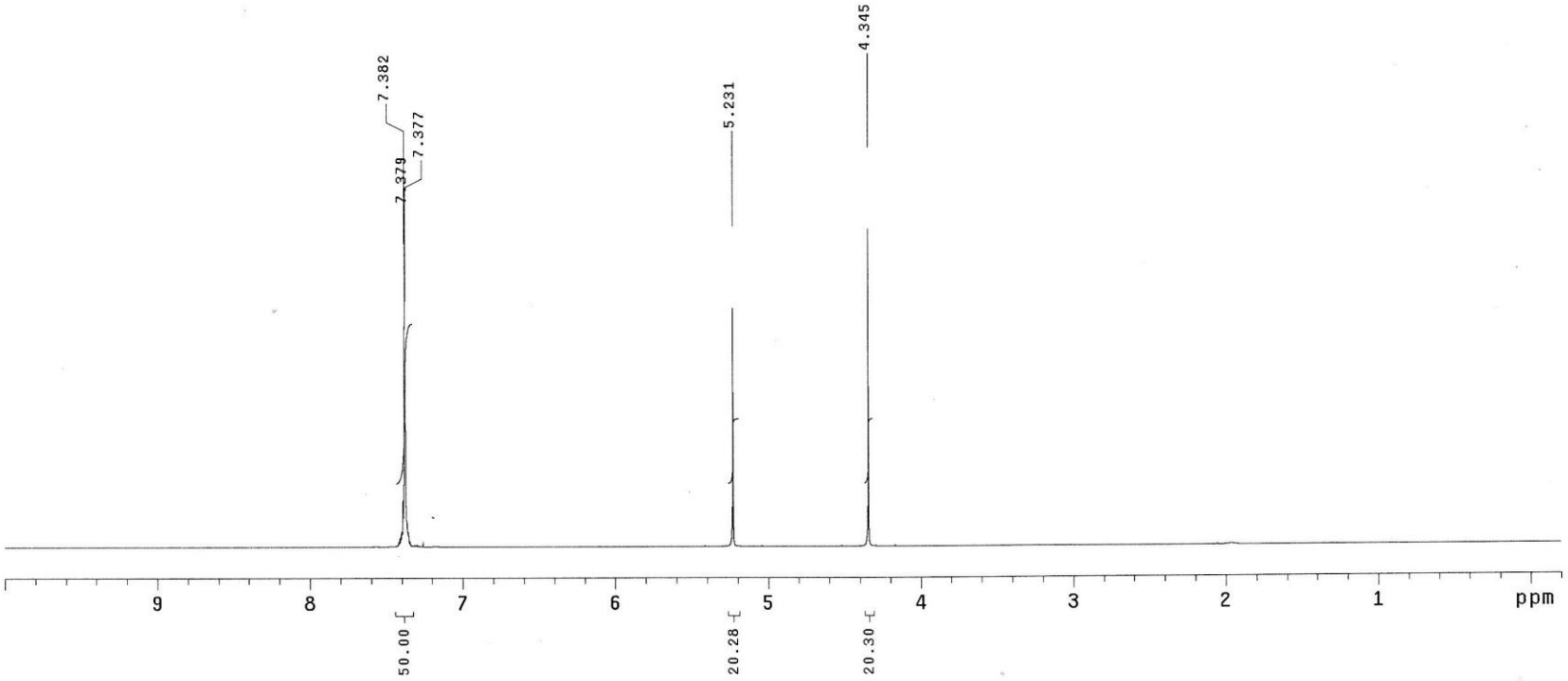
# Compound 4w ($^1$H-NMR spectral data)

YCBT0901

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Sep 1 2023
Solvent: CDCl3
Ambient temperature
Total 32 repetitions



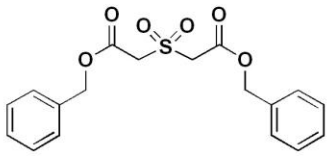


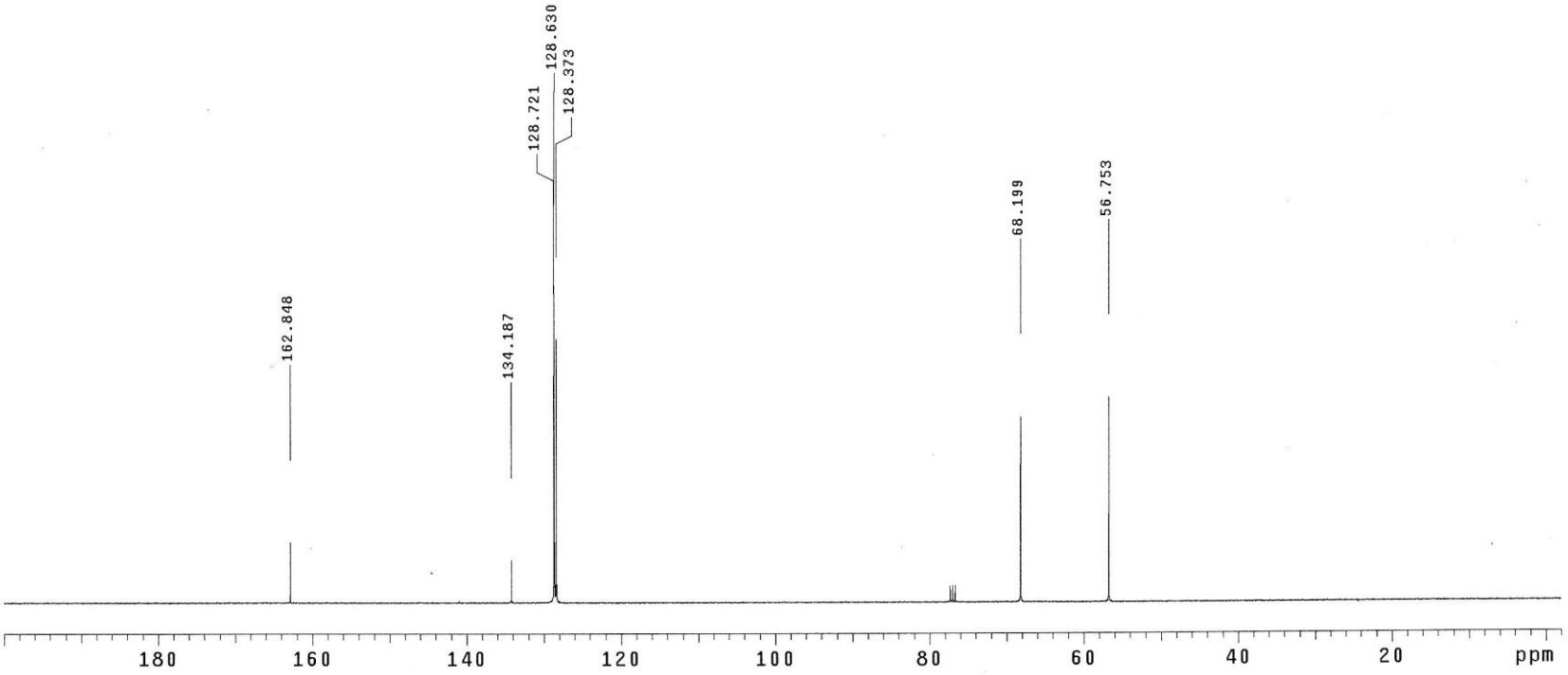
# Compound 4w ($^{13}$C-NMR spectral data)

YCBT0901

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Sep 1 2023
Solvent: CDCl3
Ambient temperature
Total 3712 repetitions

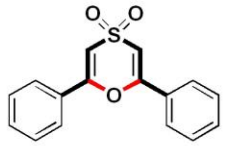


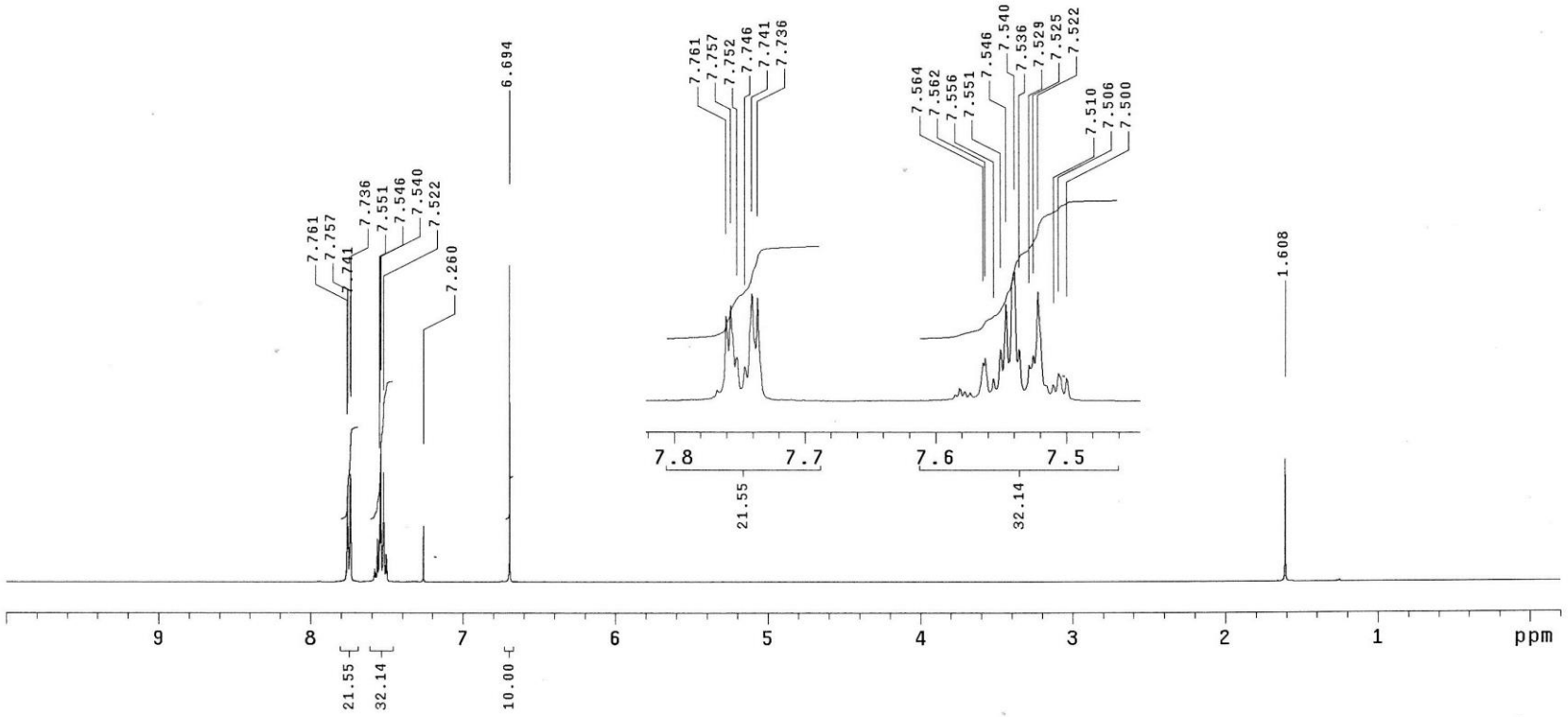


# Compound 6a ($^1$H-NMR spectral data)

YN0704

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Jul 5 2023
Solvent: CDCl3
Ambient temperature
Total 32 repetitions



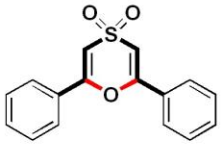


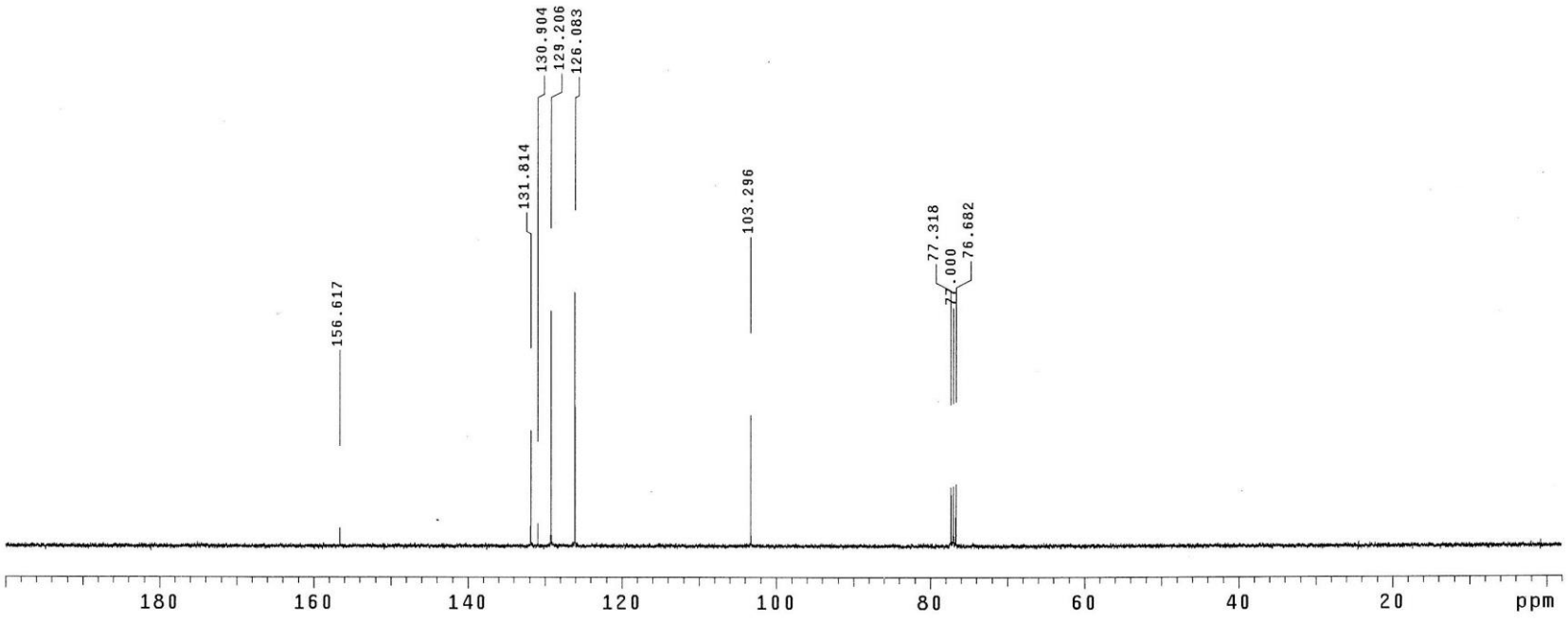
# Compound 6a ($^{13}$C-NMR spectral data)

YN0704

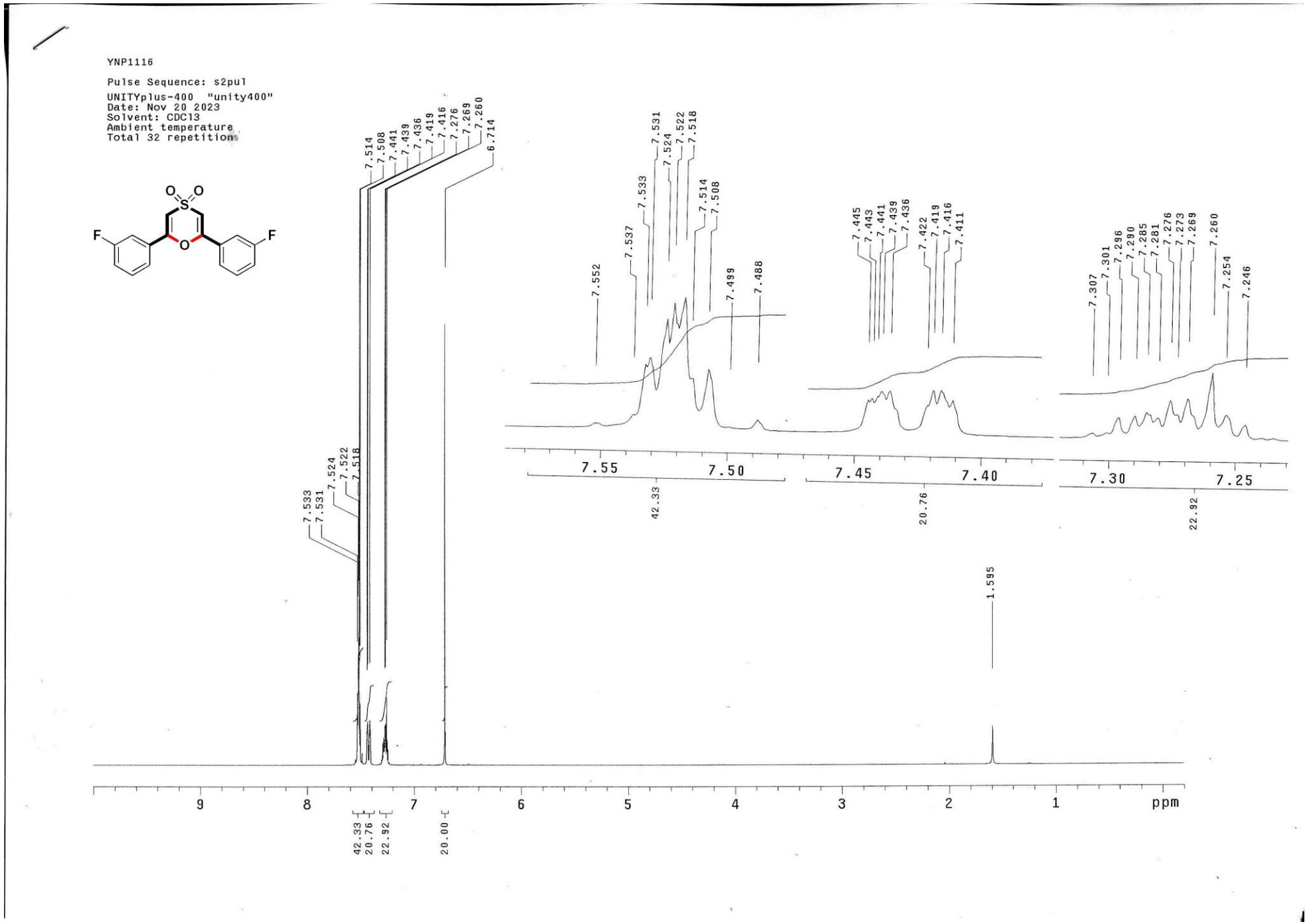
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jul 5 2023
Solvent: CDCl3
Ambient temperature
Total 1104 repetitions



# Compound 6b ($^1$H-NMR spectral data)

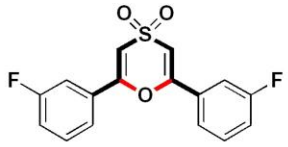


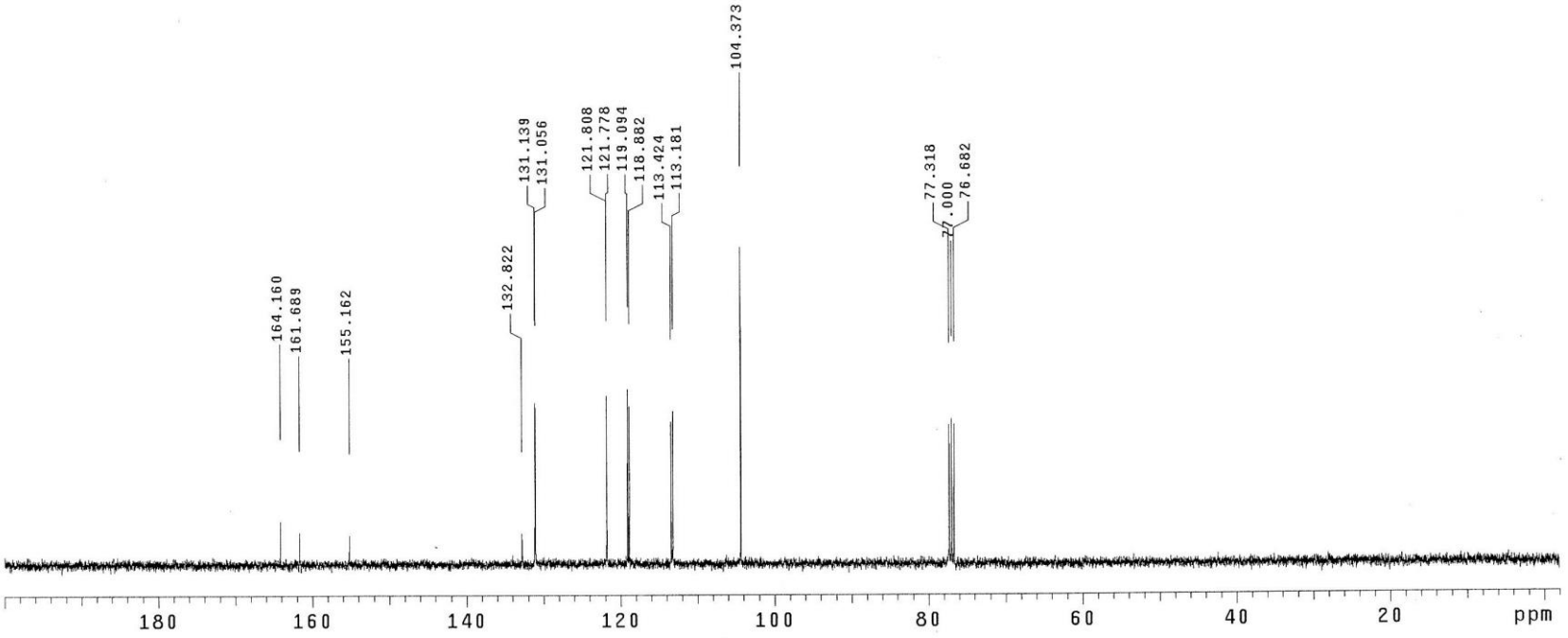
# Compound 6b ($^{13}$C-NMR spectral data)

YNP1116

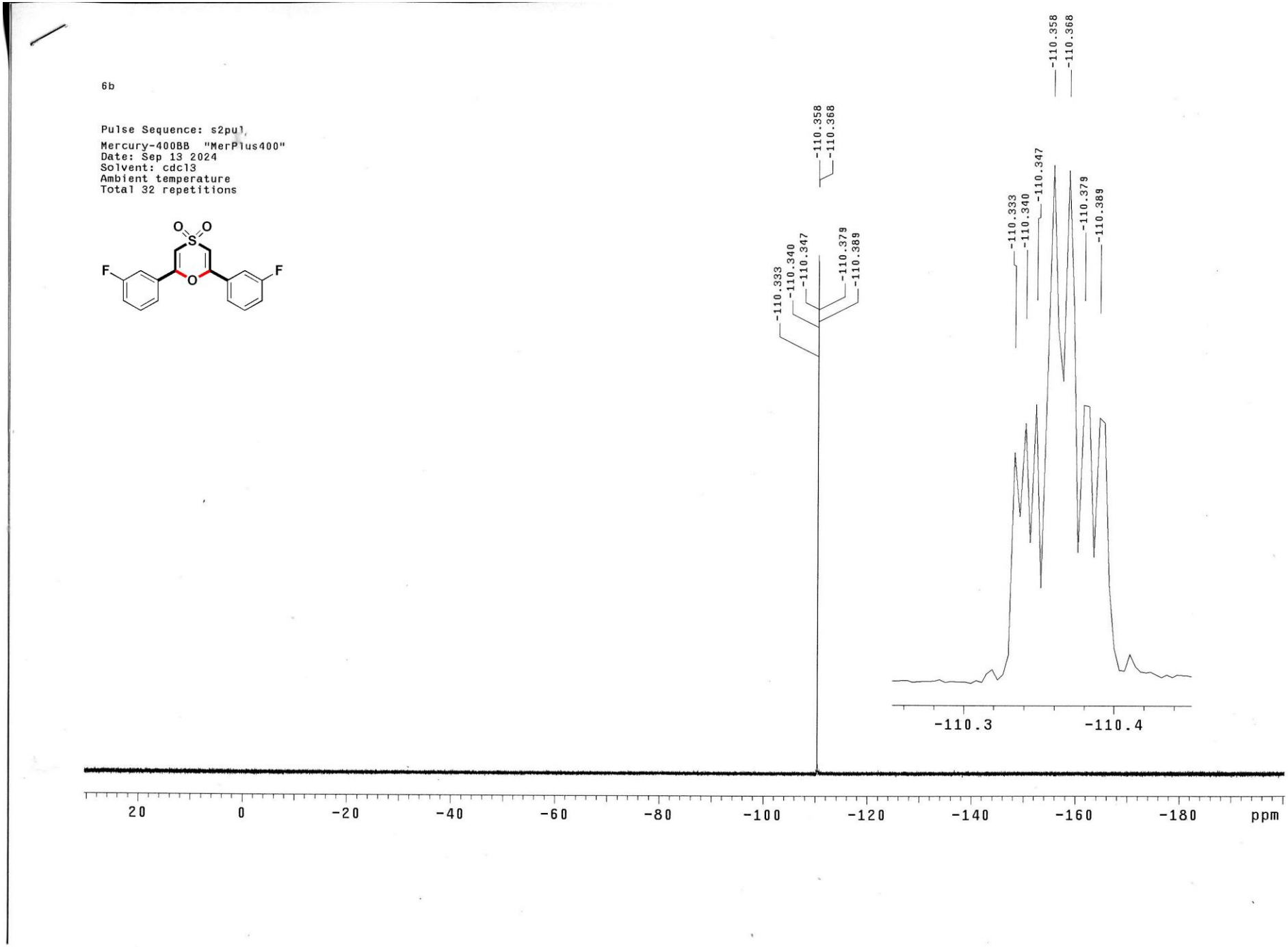
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Nov 20 2023
Solvent: CDCl3
Ambient temperature
Total 1600 repetitions

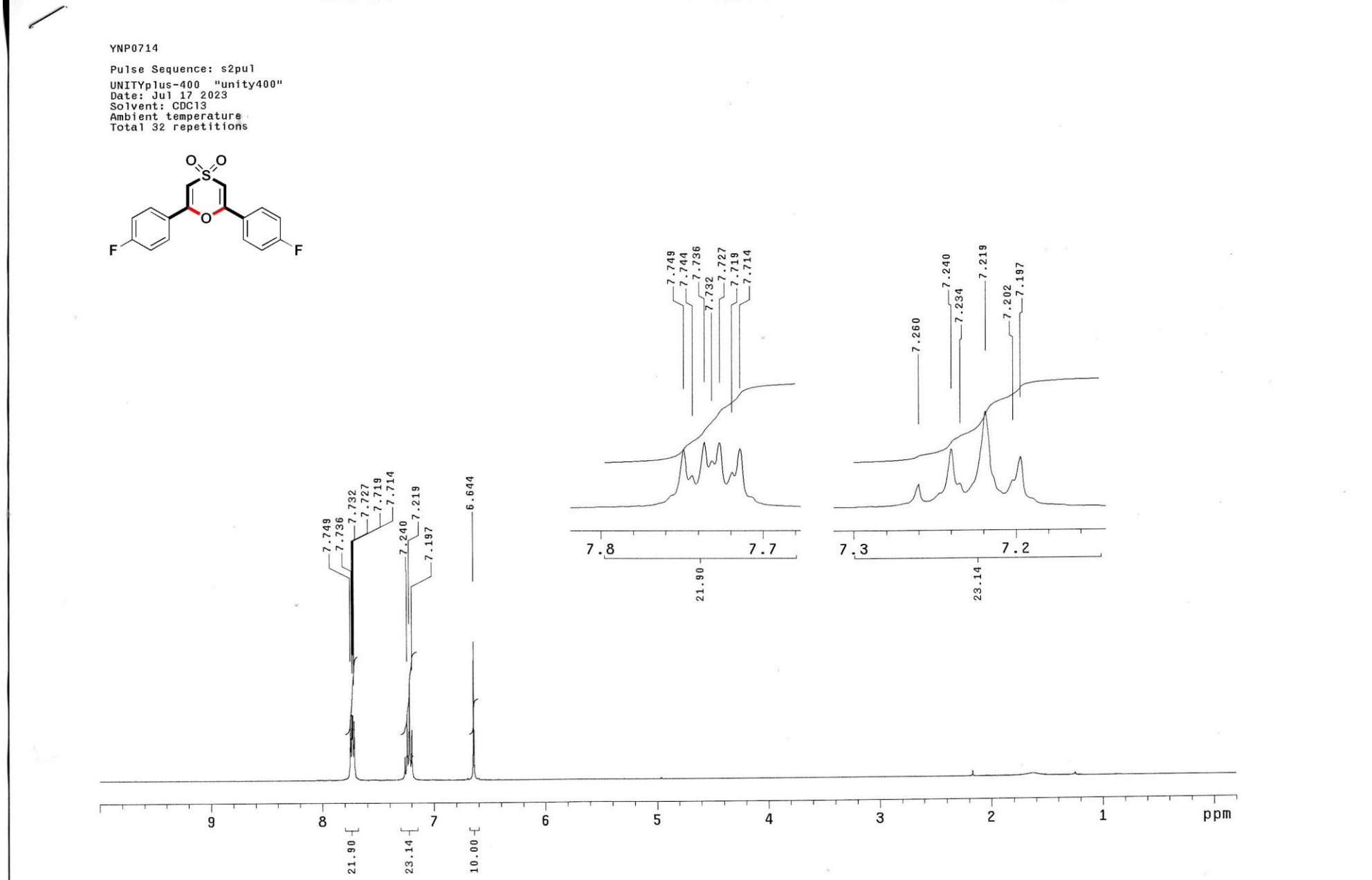


# Compound 6b ($^{19}$F-NMR spectral data)



# Compound 6c ($^1$H-NMR spectral data)

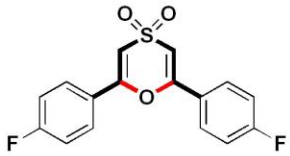


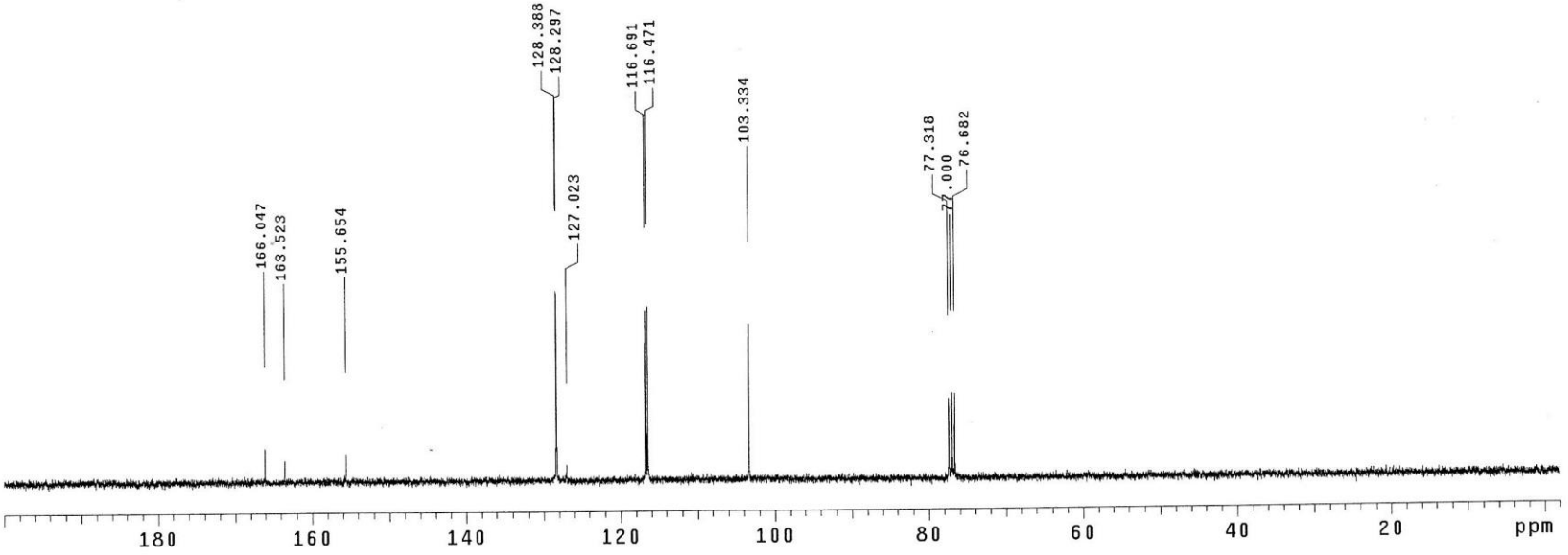
# Compound 6c ($^{13}$C-NMR spectral data)

YNP0714

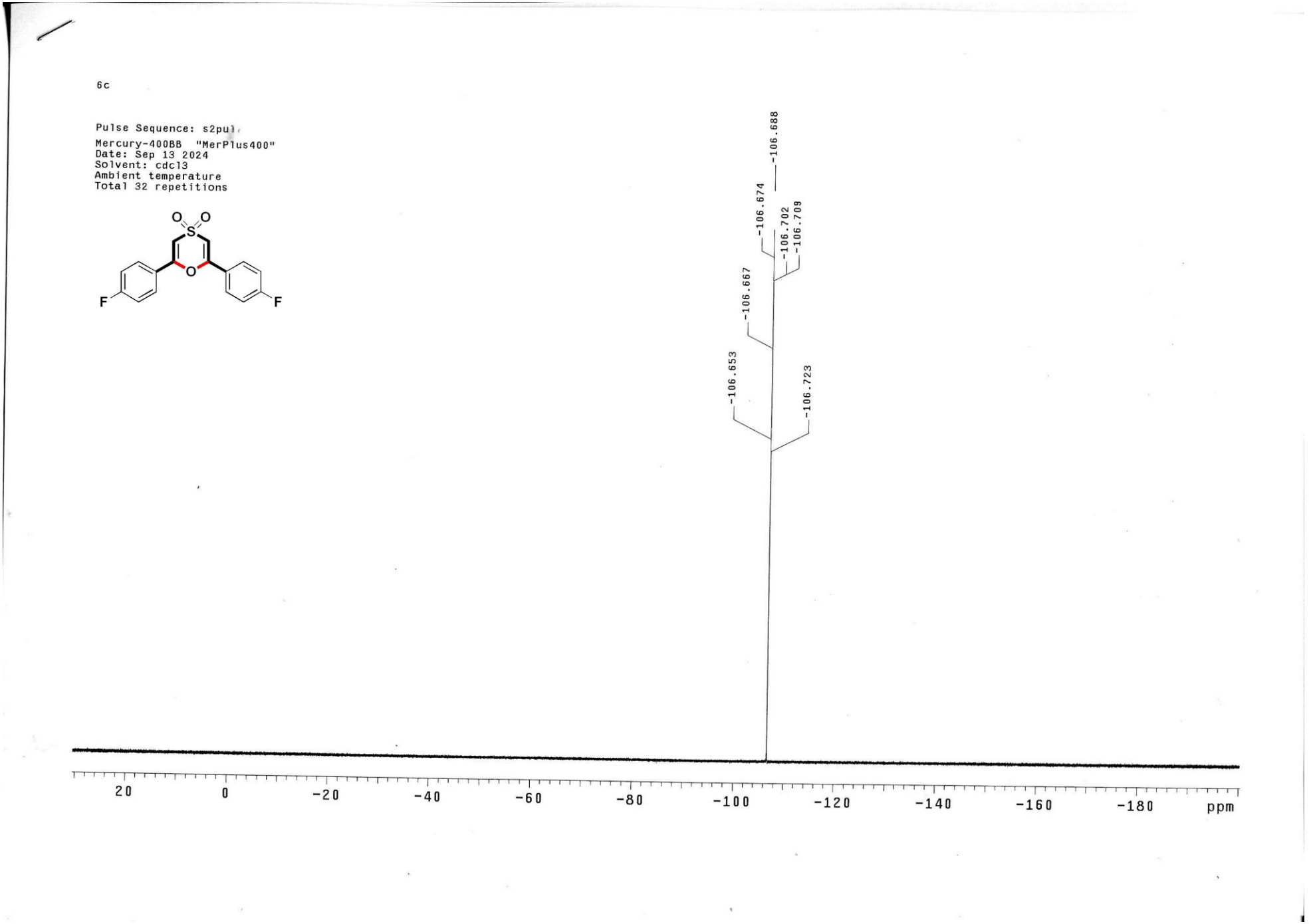
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jul 17 2023
Solvent: CDCl3
Ambient temperature
Total 2624 repetitions



# Compound 6c ($^{19}$F-NMR spectral data)

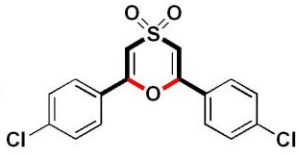


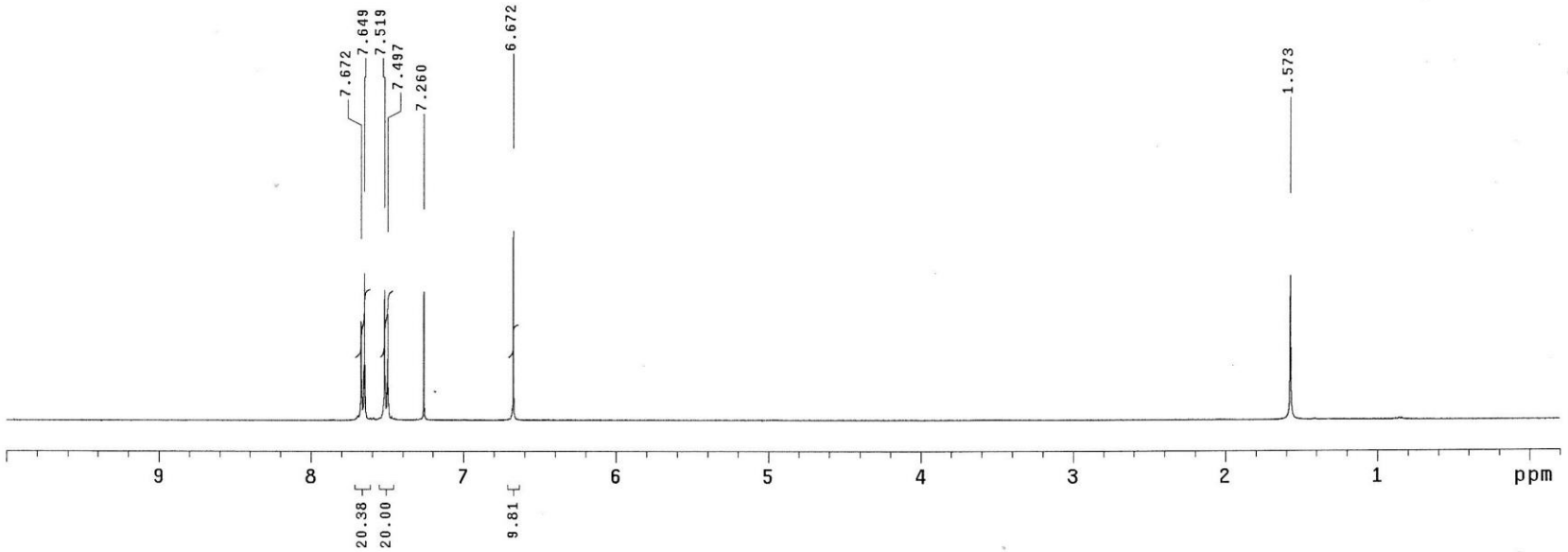
# Compound 6d ($^1$H-NMR spectral data)

LYZ0719

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jul 20 2023
Solvent: CDCl3
Ambient temperature
Total 32 repetitions



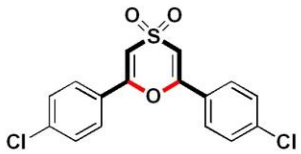



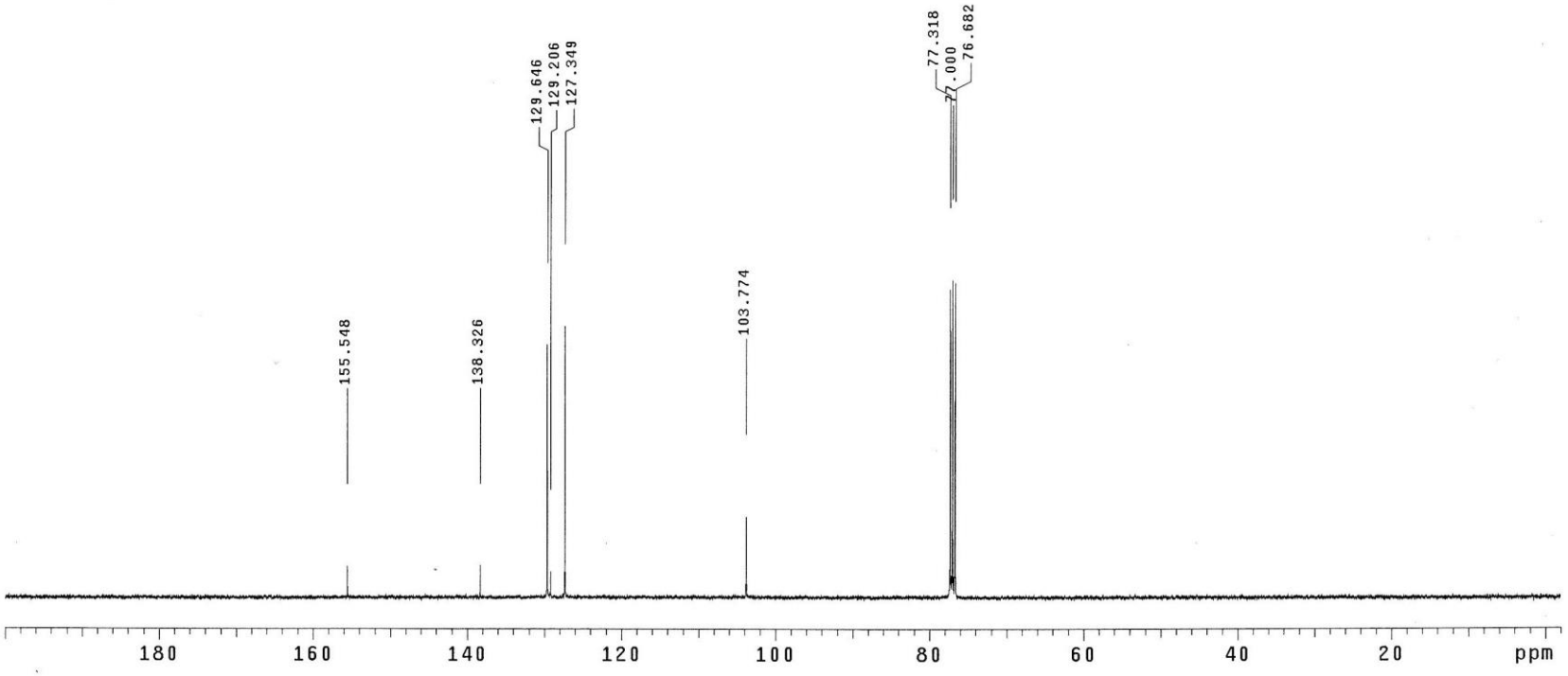
# Compound 6d ($^{13}$C-NMR spectral data)

LYZ0719

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jul 20 2023
Solvent: CDCl3
Ambient temperature
Total 32000 repetitions

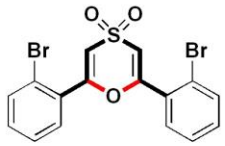


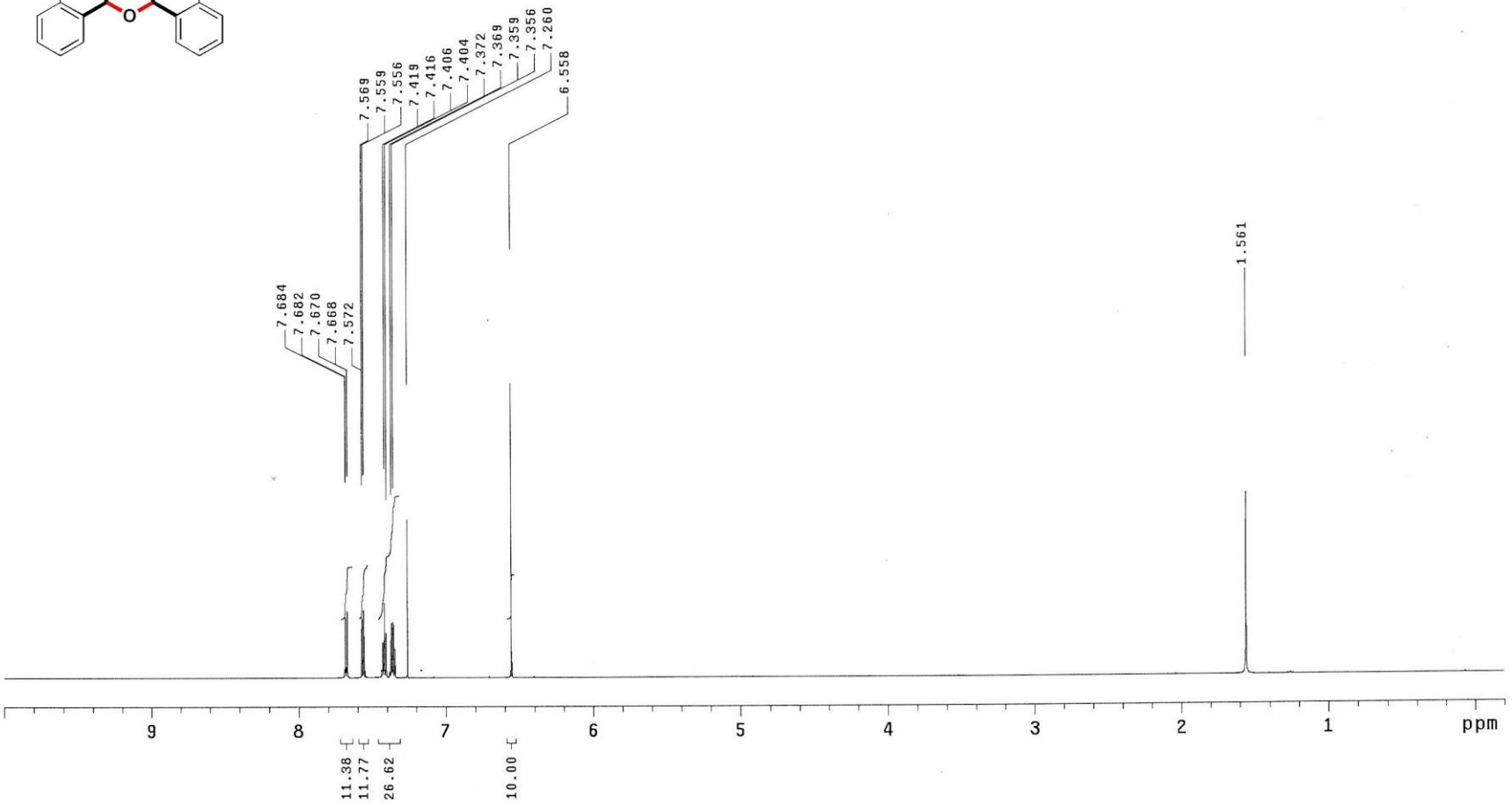



# Compound 6e ($^1$H-NMR spectral data)

YNP1020

Pulse Sequence: s2pul
UNITYplus-600 "KMU600.kmu.edu.tw"
Date: Oct 23 2023
Solvent: cdcl3
Ambient temperature
Total 32 repetitions



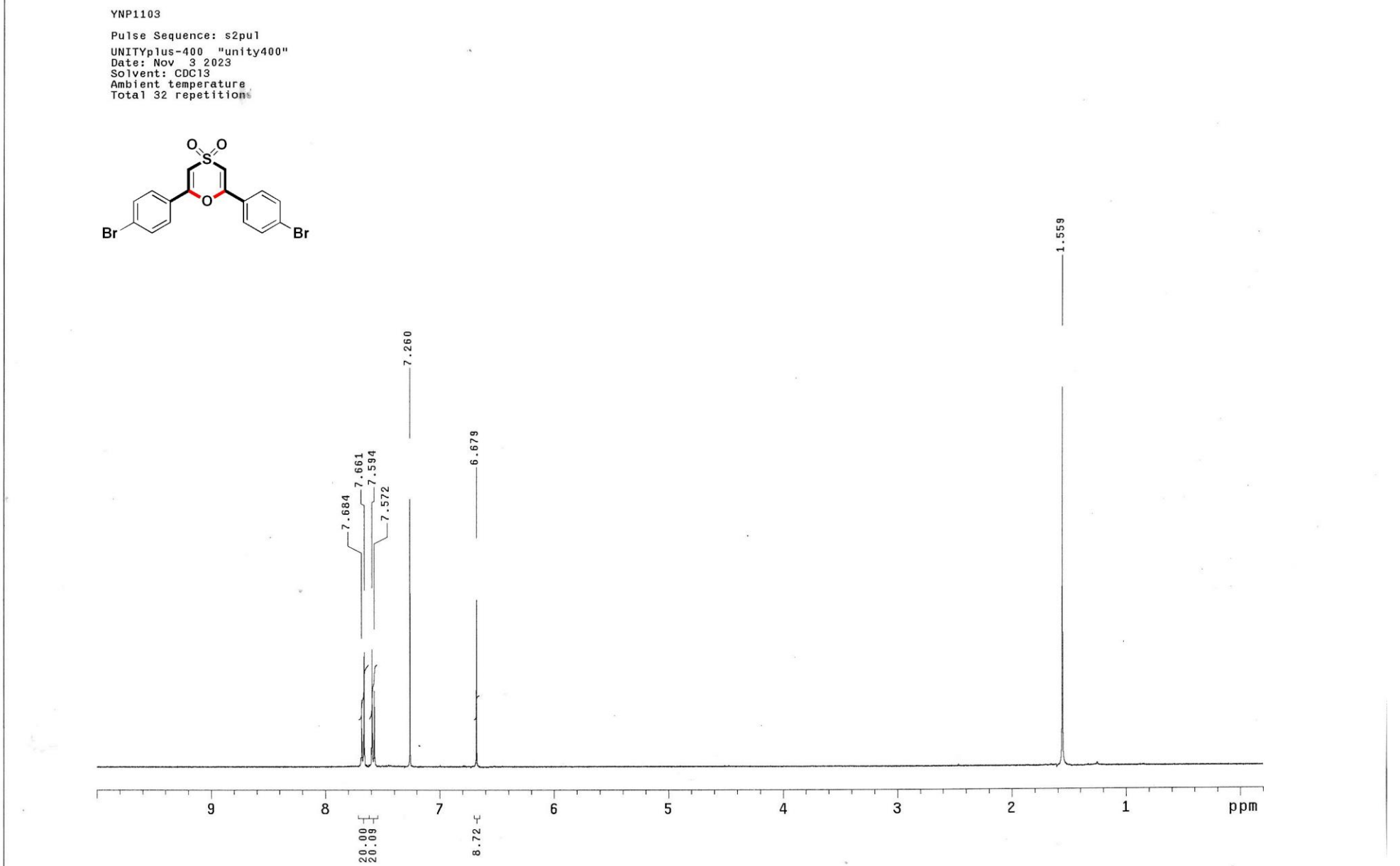



# Compound 6e ($^{13}$C-NMR spectral data)

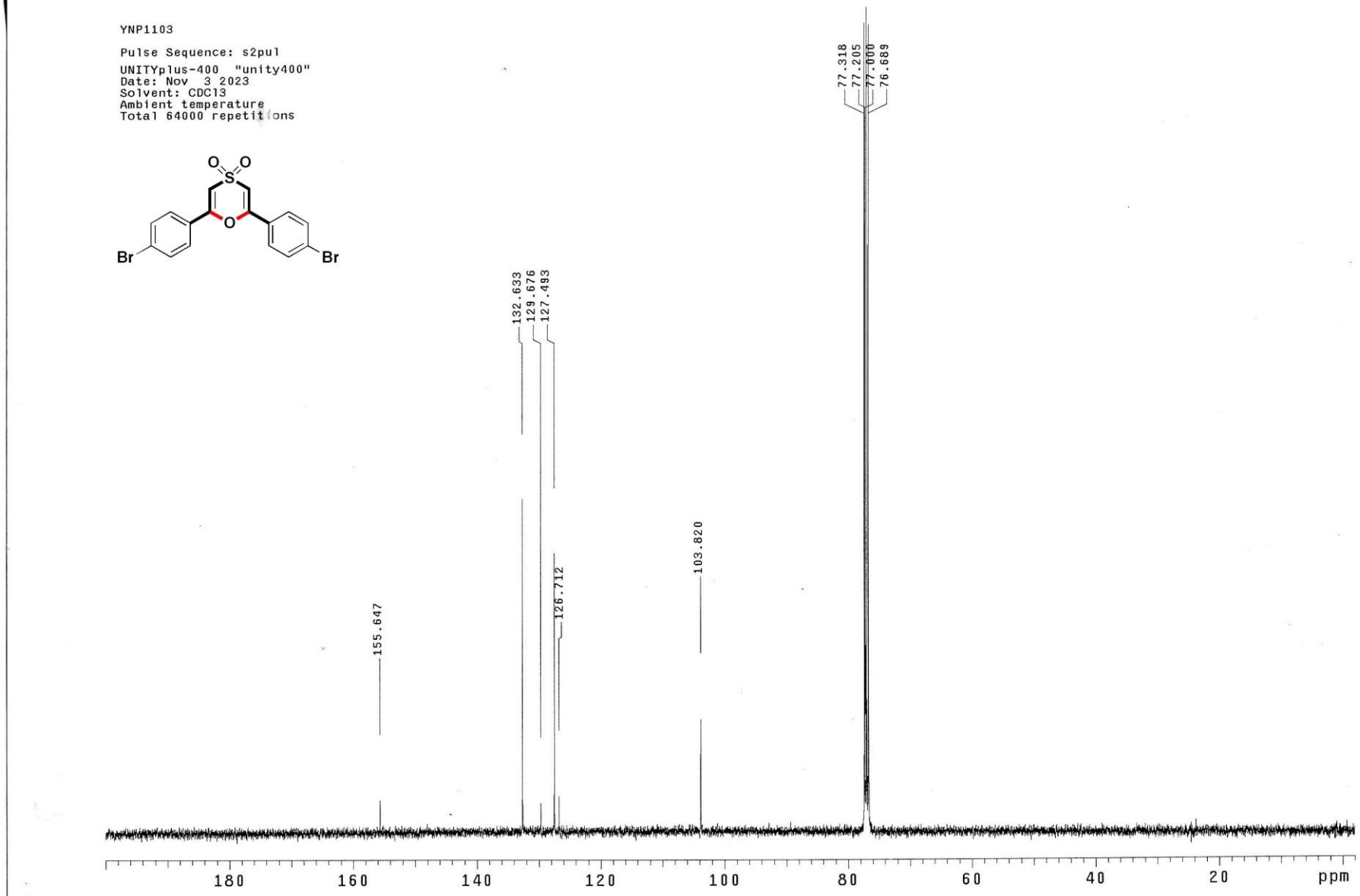
YNP1020

Pulse Sequence: s2pul
UNITYplus-600 "KMU600.kmu.edu.tw"
Date: Oct 23 2023
Solvent: cdcl3
Ambient temperature
Total 1792 repetitions

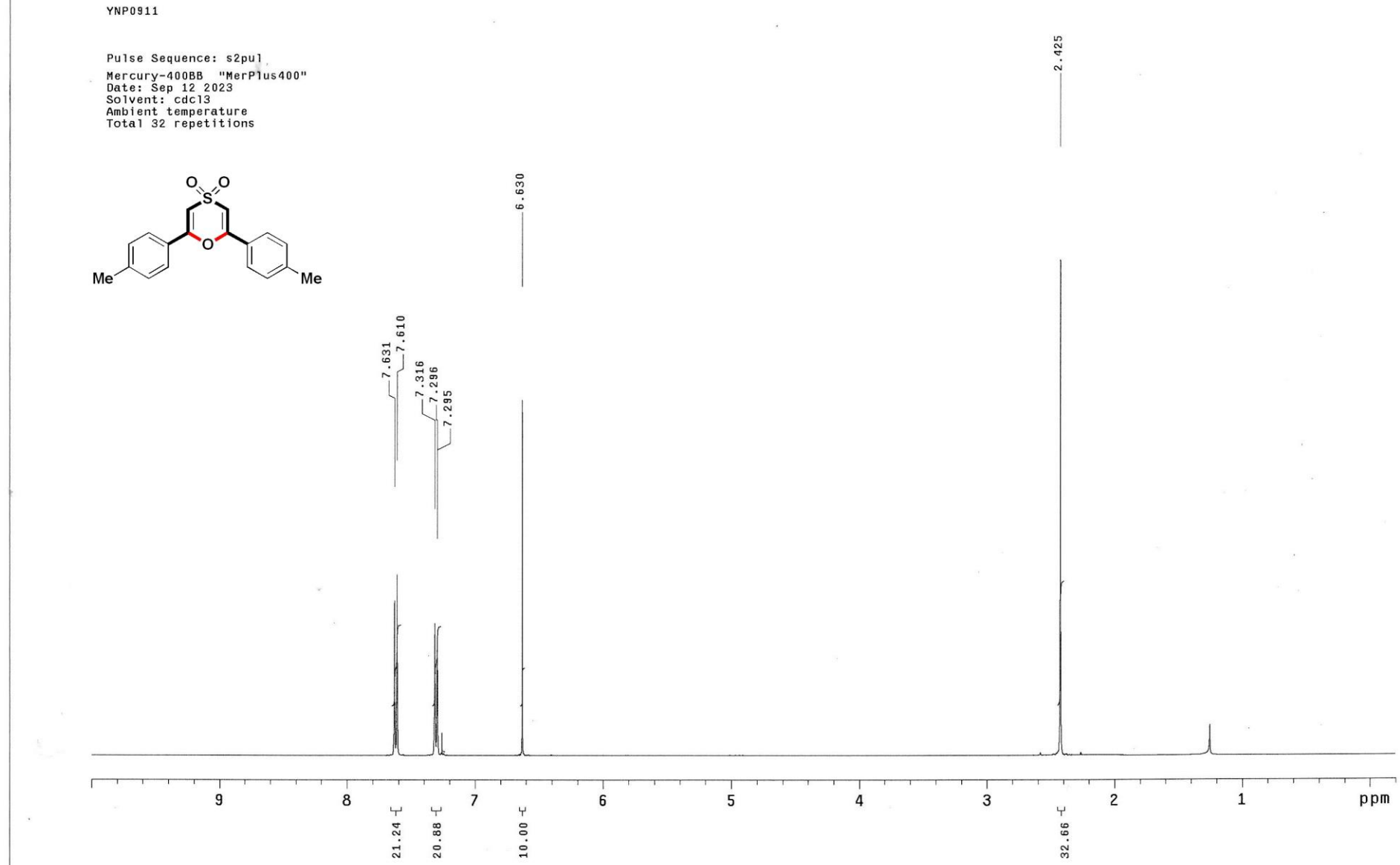
# Compound 6f ($^1$H-NMR spectral data)



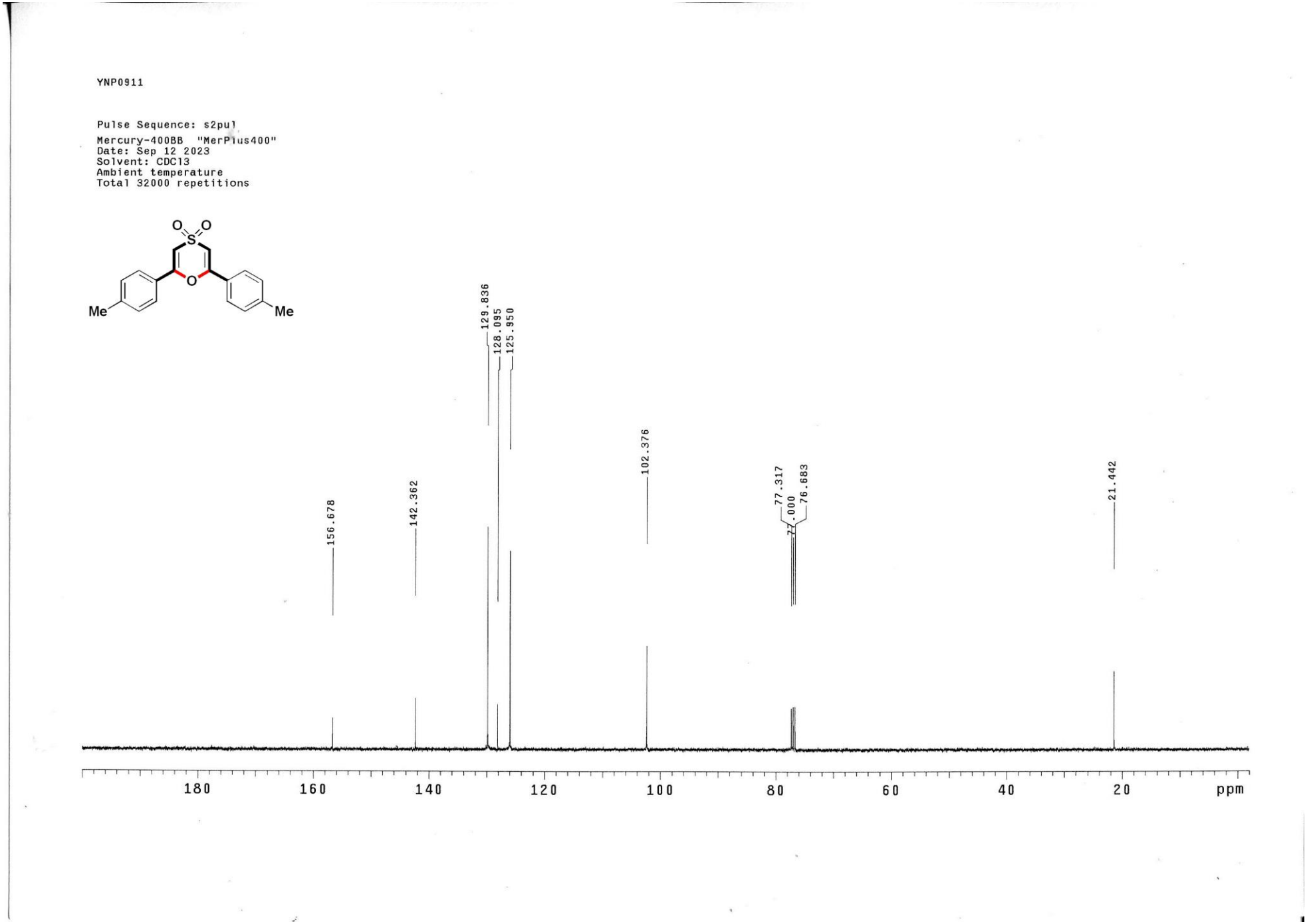
# Compound 6f ($^{13}$C-NMR spectral data)



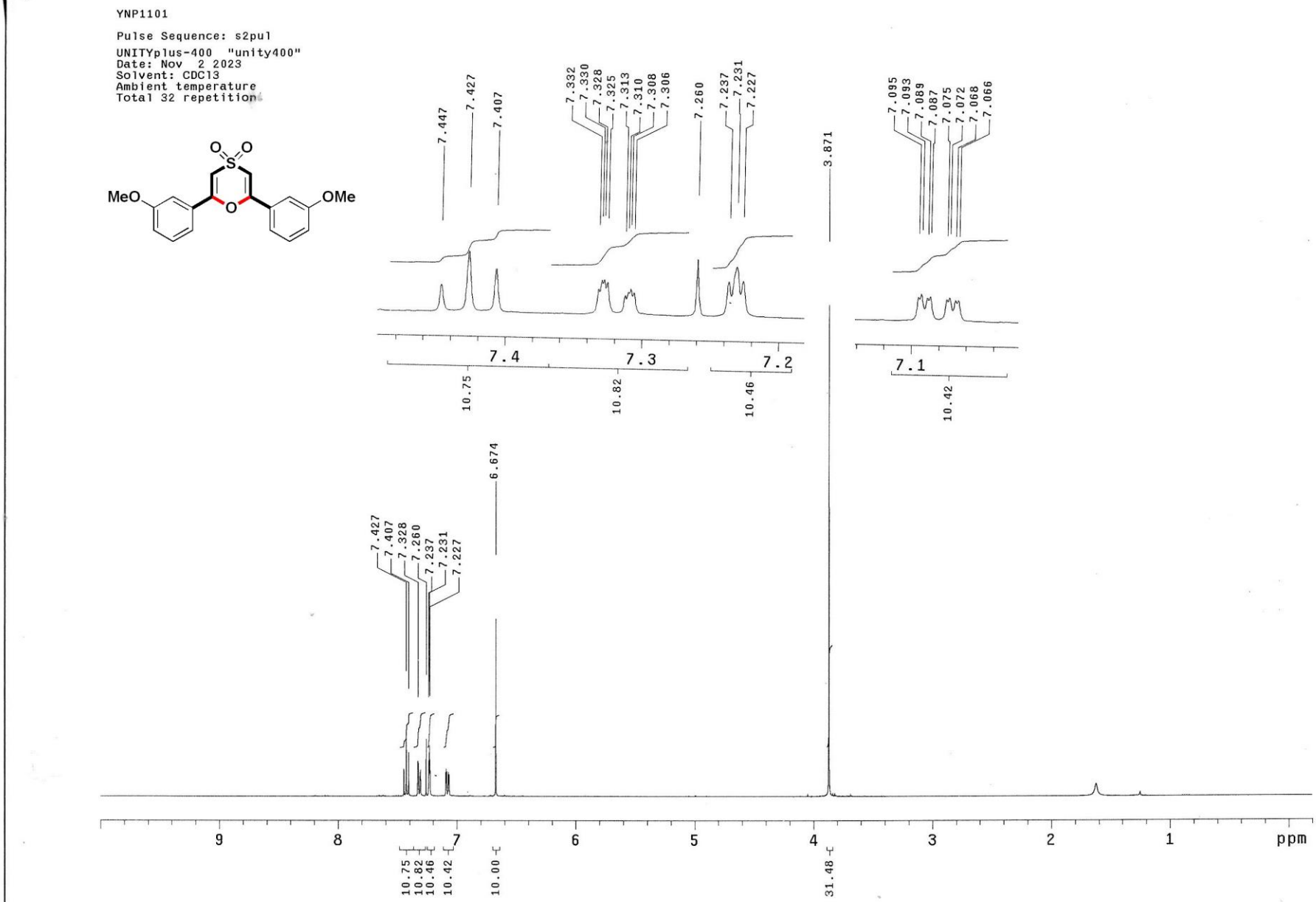
# Compound 6g ($^1$H-NMR spectral data)



# Compound 6g ($^{13}$C-NMR spectral data)



# Compound 6h ($^1$H-NMR spectral data)

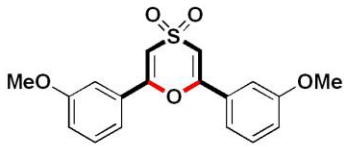


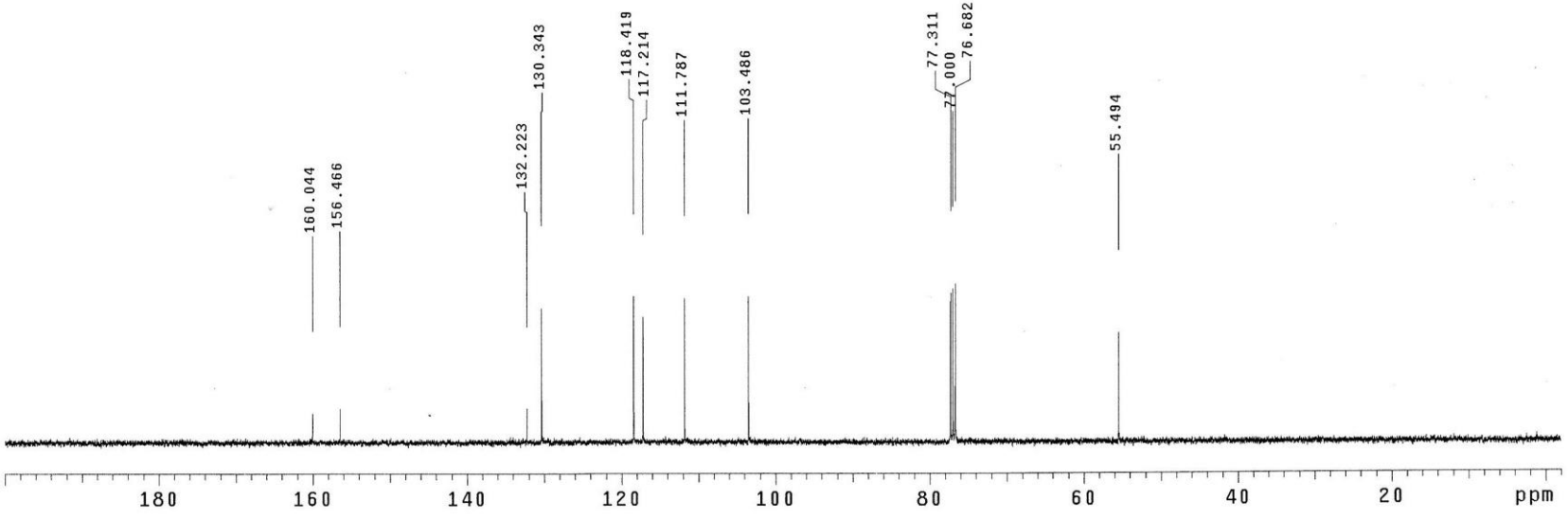
# Compound 6h ($^{13}$C-NMR spectral data)

YNP1101

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Nov 2 2023
Solvent: CDCl3
Ambient temperature
Total 4128 repetitions



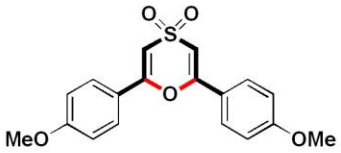



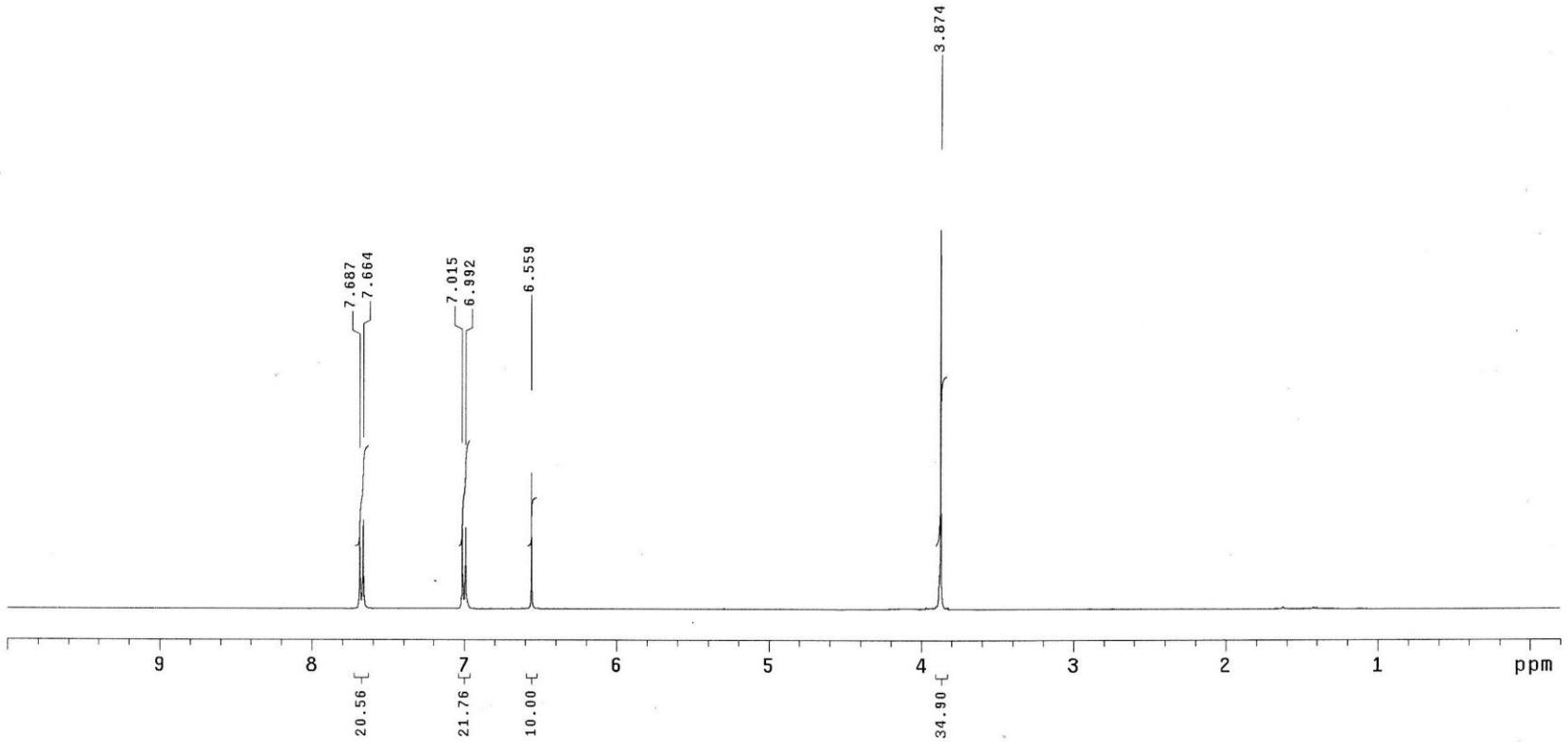
# Compound 6i ($^1$H-NMR spectral data)

YNP0913

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Sep 13 2023
Solvent: CDCl3
Ambient temperature
Total 32 repetitions



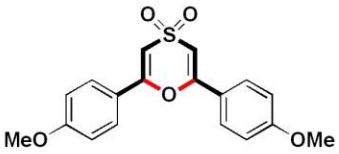



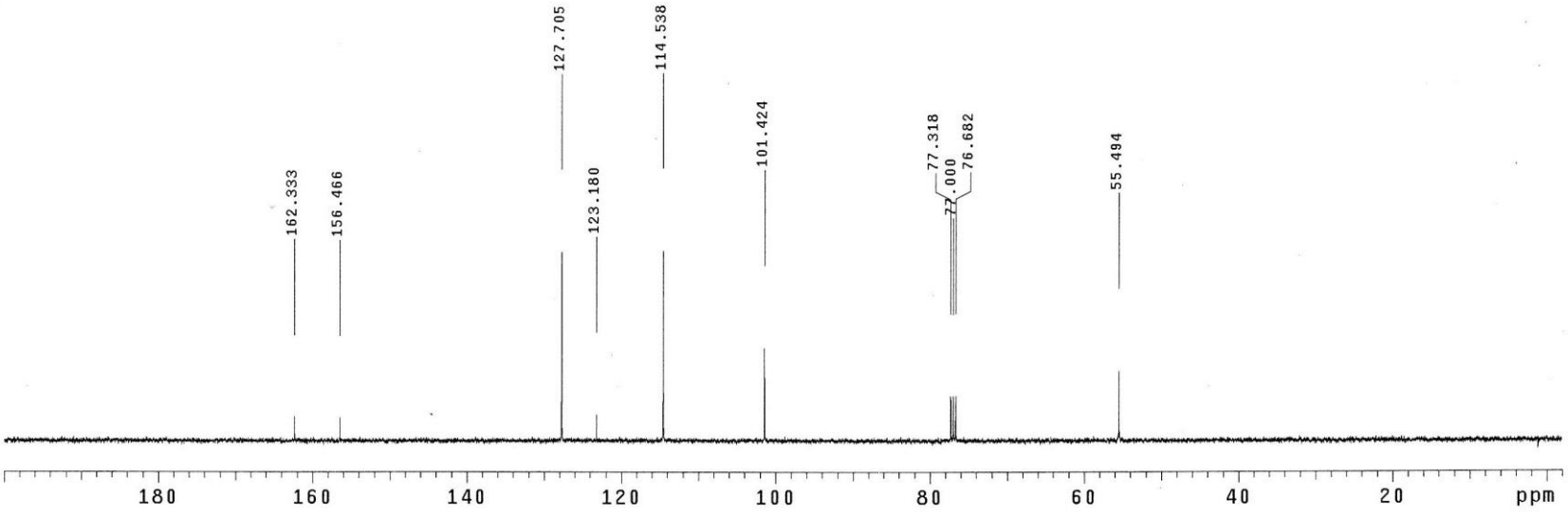
# Compound 6i ($^{13}$C-NMR spectral data)

YNP0913

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Sep 13 2023
Solvent: CDCl3
Ambient temperature
Total 640 repetitions



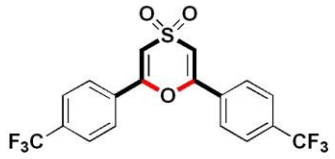



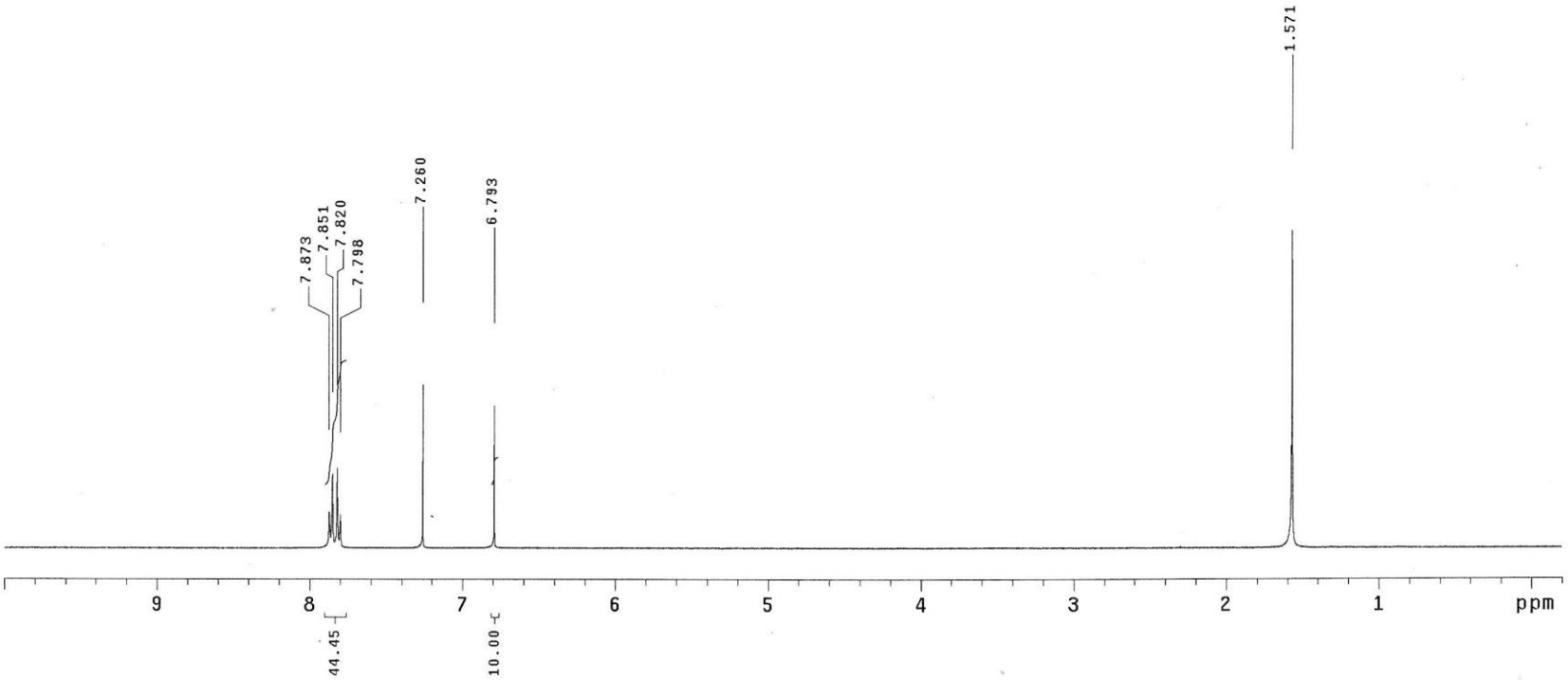
# Compound 6j ($^1$H-NMR spectral data)

YNP0921

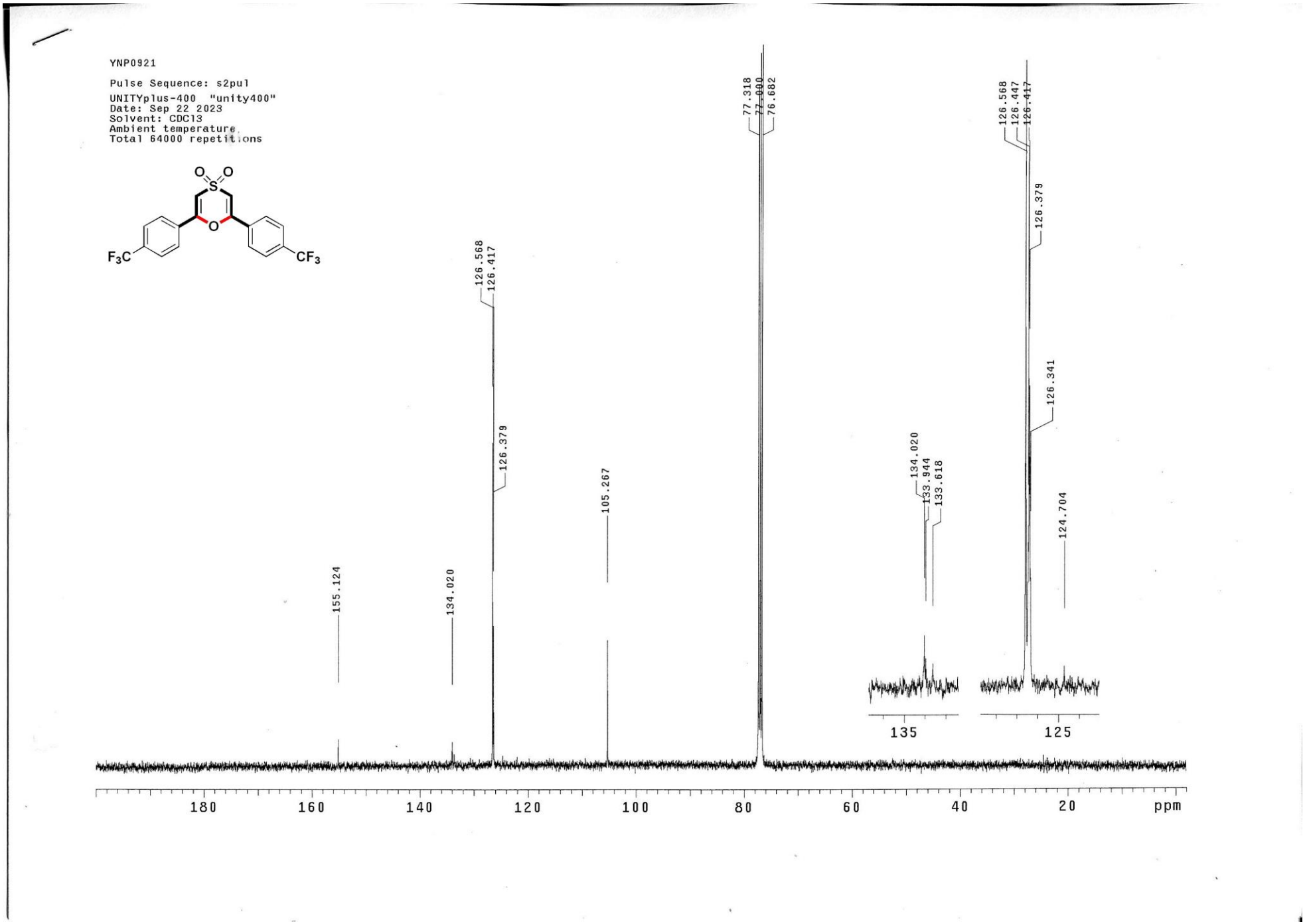
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Sep 22 2023
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

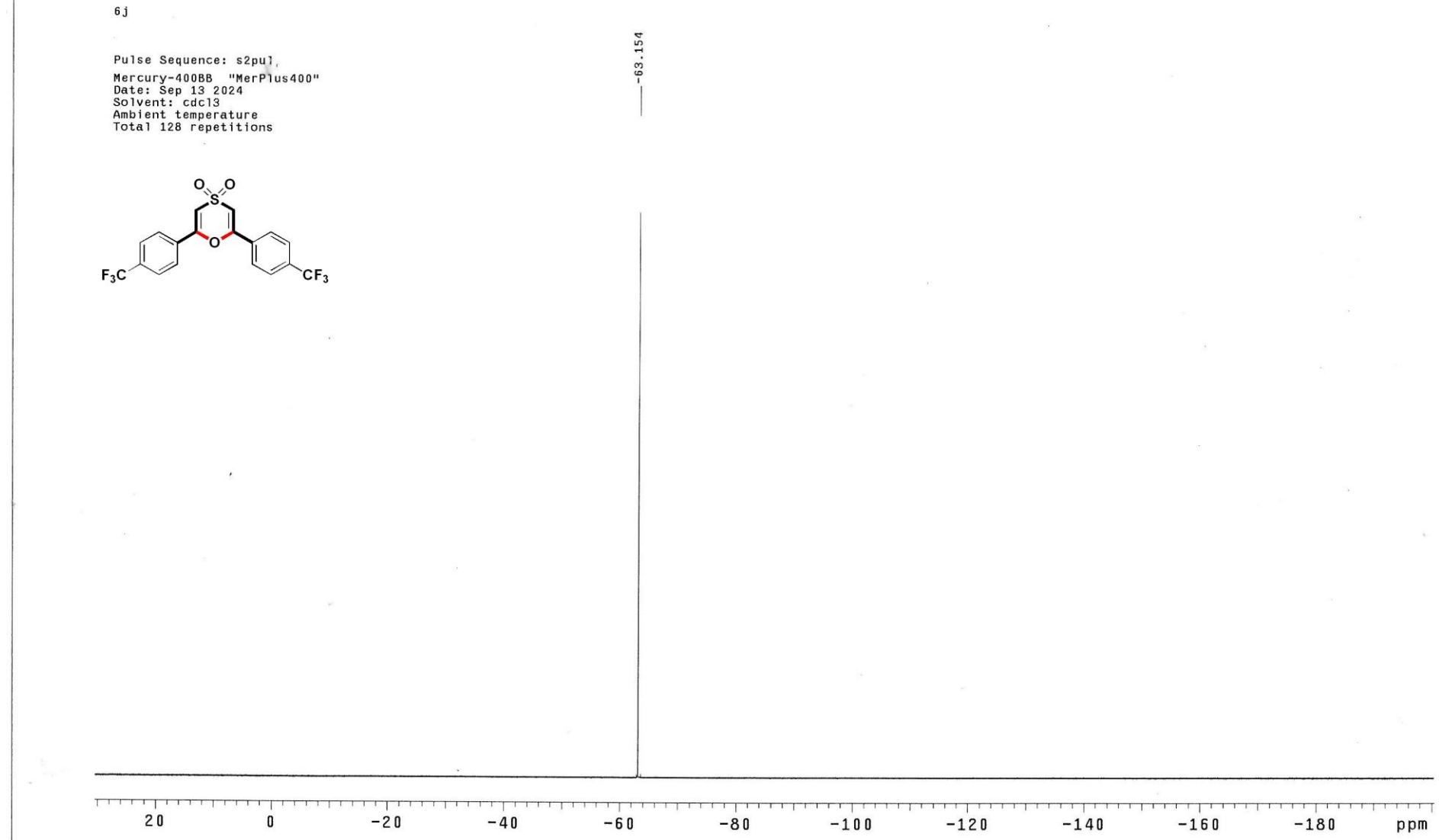


# Compound 6j ($^{13}$C-NMR spectral data)



# Compound 6j ($^{19}$F-NMR spectral data)

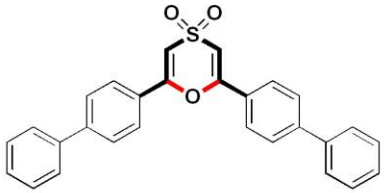


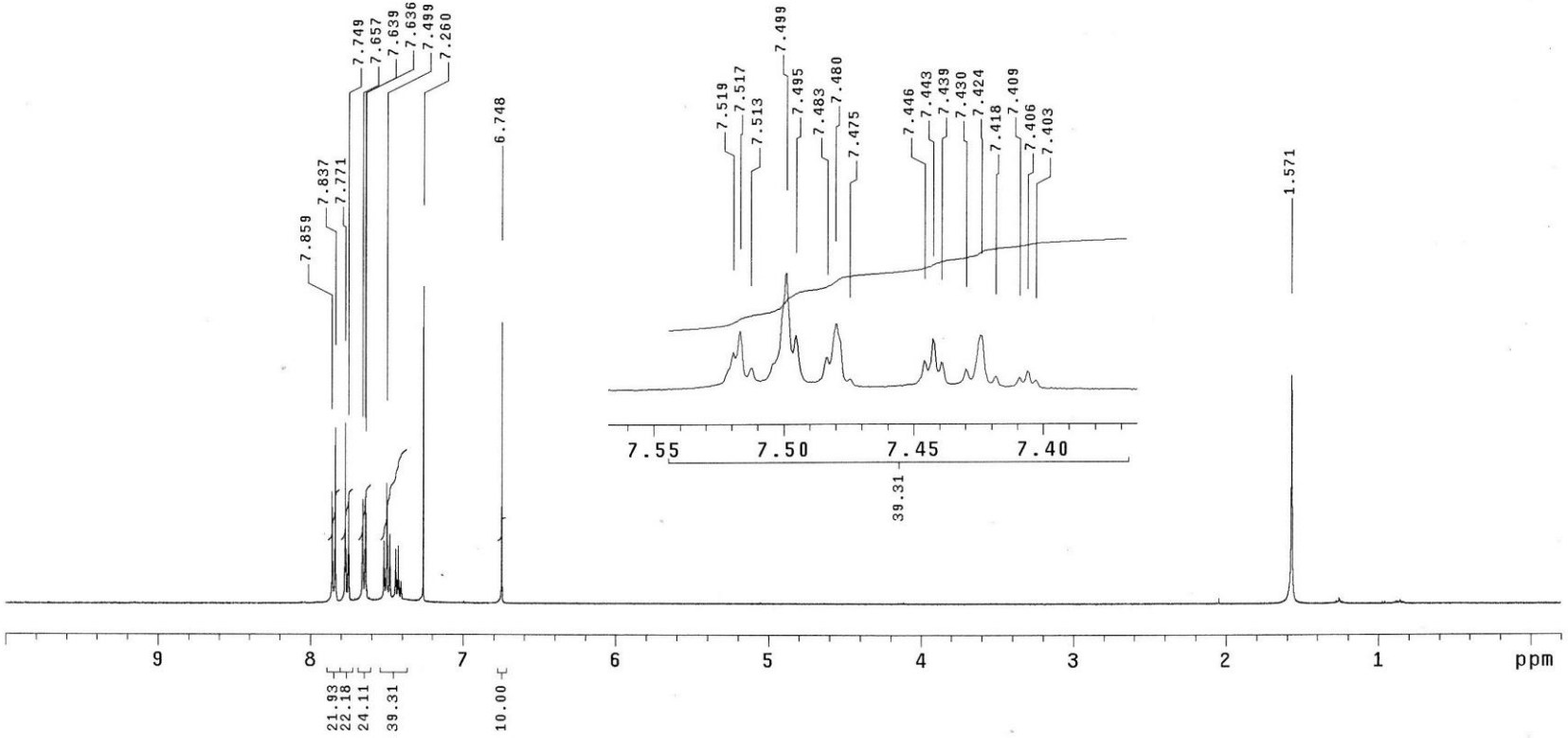
# Compound 6m ($^1$H-NMR spectral data)

YNP0801

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Aug 9 2023
Solvent: CDCl3
Ambient temperature
Total 32 repetitions



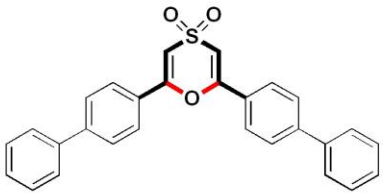


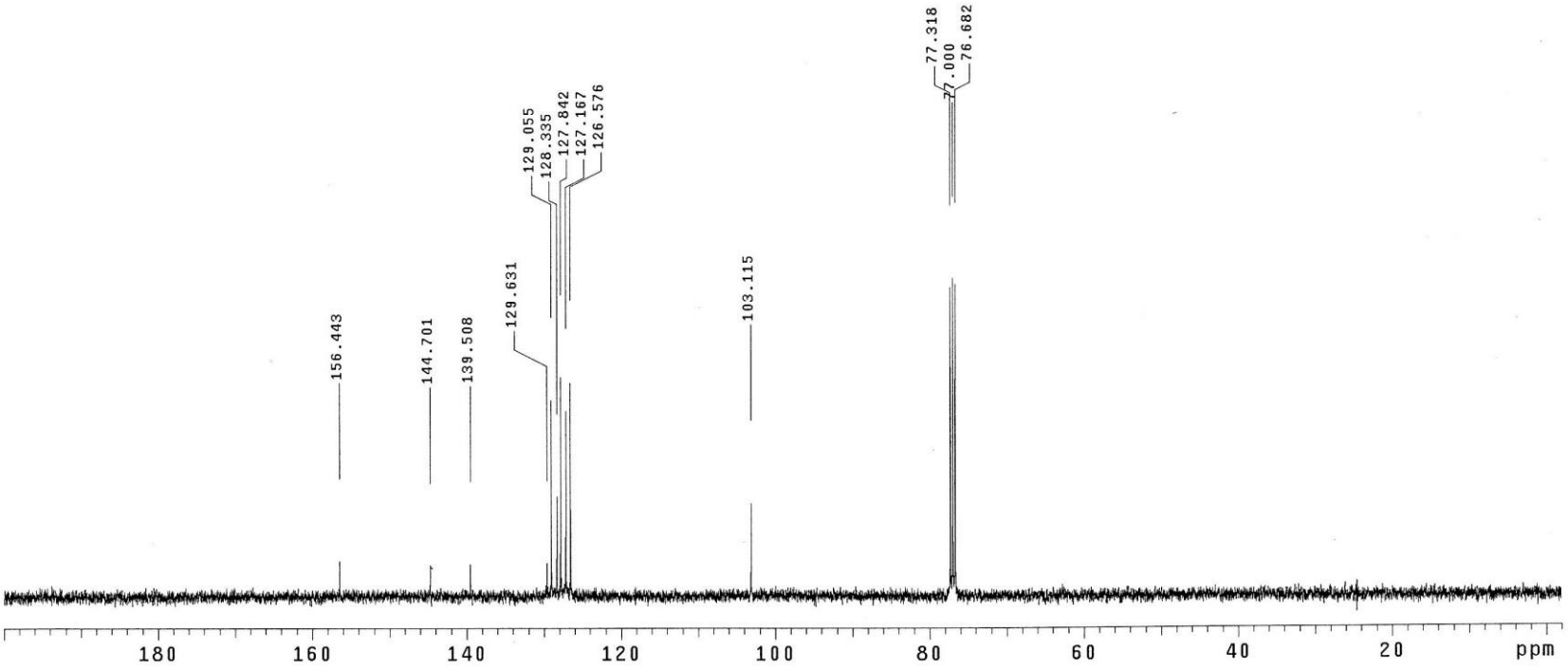
# Compound 6m ($^{13}$C-NMR spectral data)

YNP0801

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Aug 9 2023
Solvent: CDCl3
Ambient temperature
Total 5552 repetitions

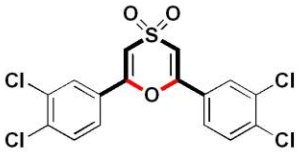


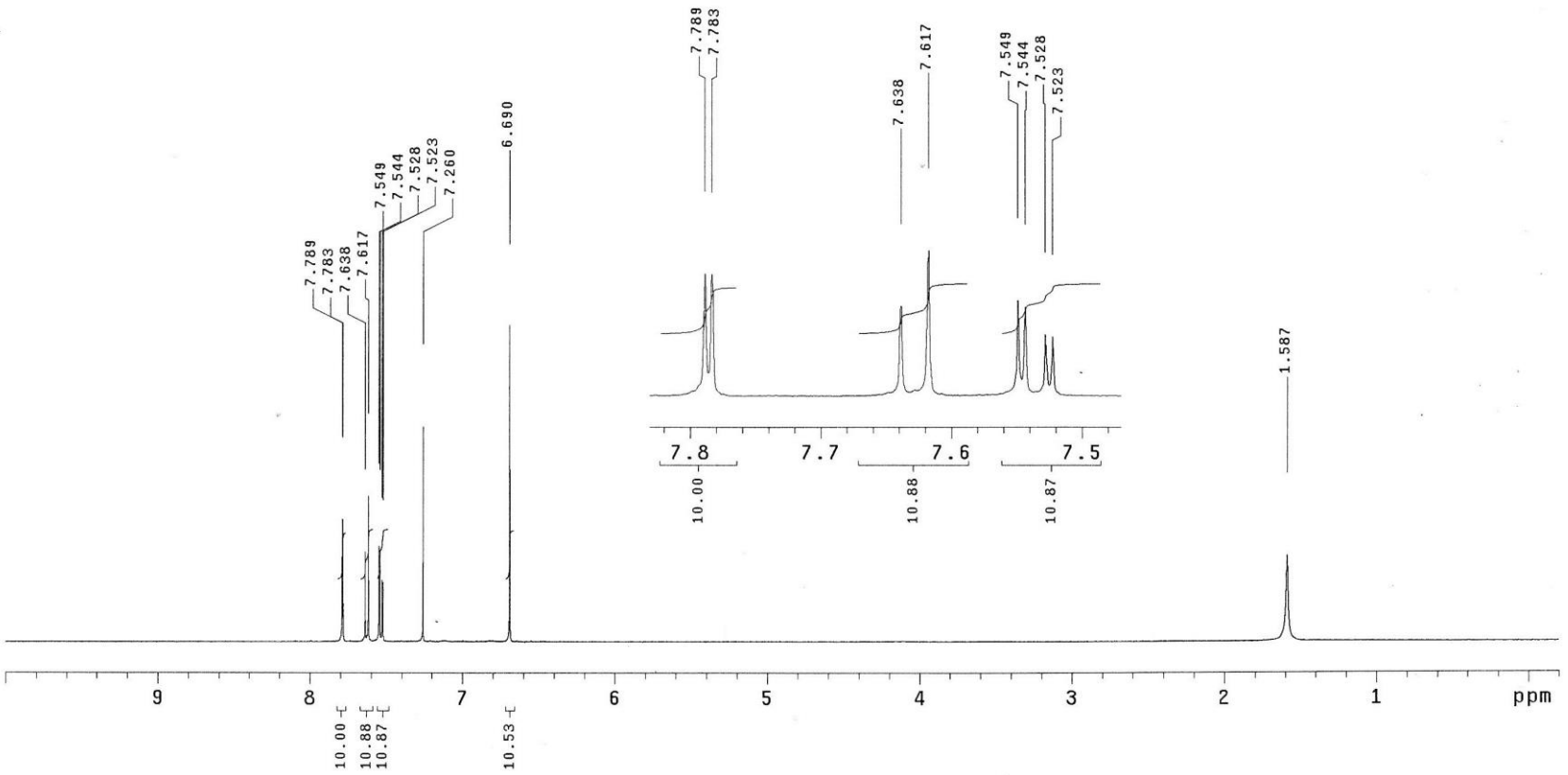


# Compound 6n ($^1$H-NMR spectral data)

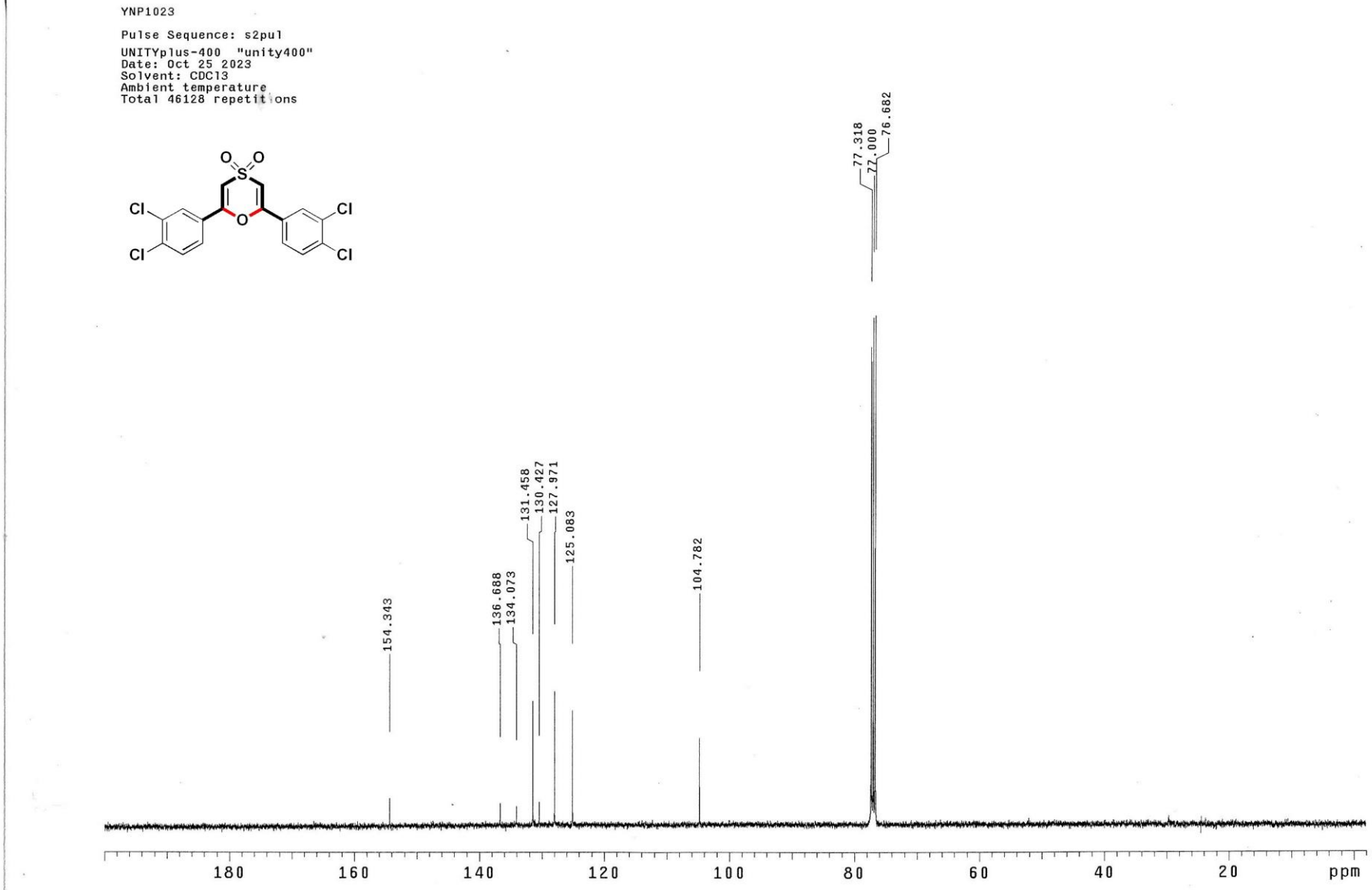
YNP1023

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Oct 25 2023
Solvent: CDCl3
Ambient temperature
Total 64 repetitions



# Compound 6n ($^{13}$C-NMR spectral data)

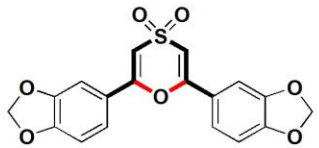


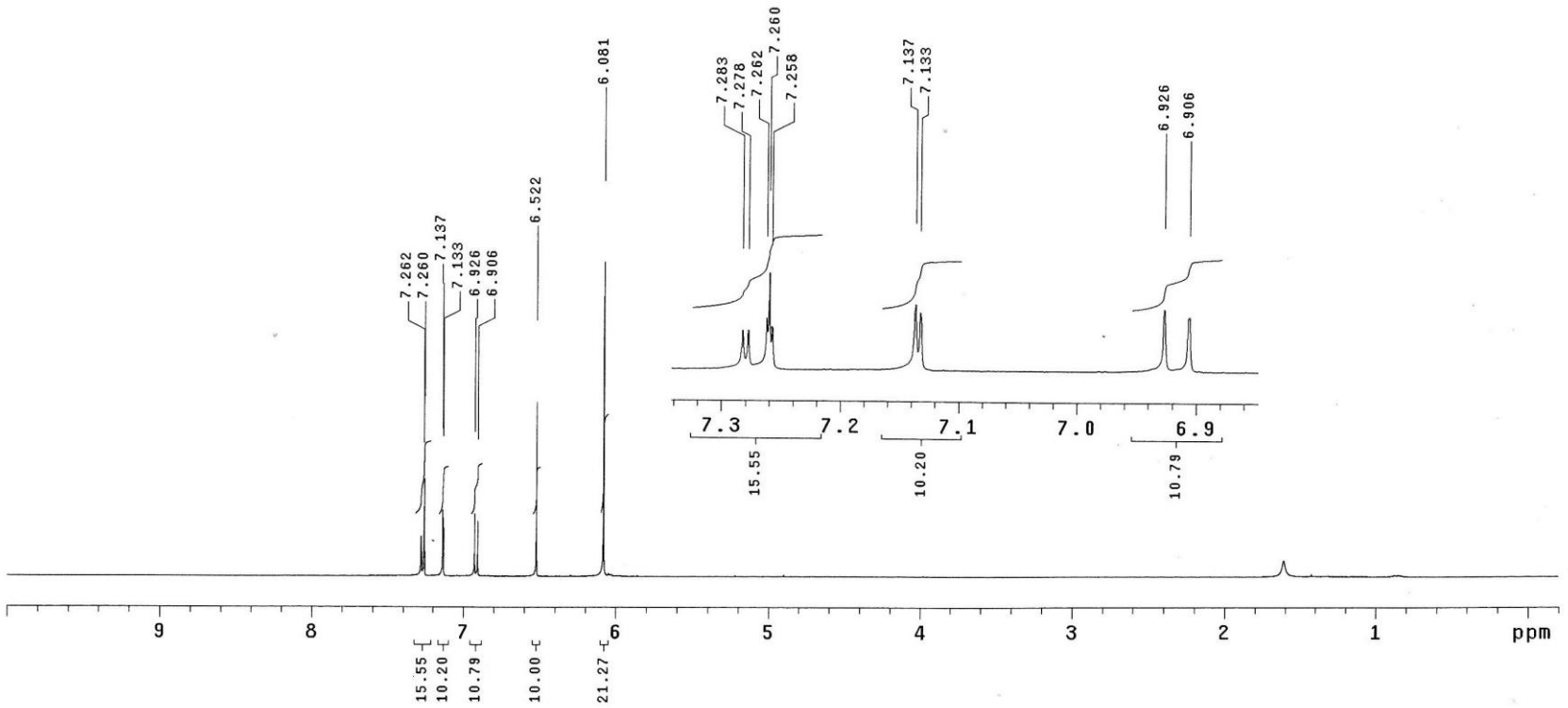
# Compound 6o ($^1$H-NMR spectral data)

YNP222

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Feb 23 2024
Solvent: CDCl3
Ambient temperature
Total 32 repetitions



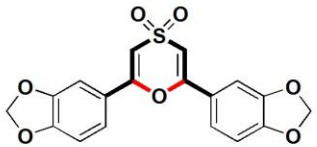


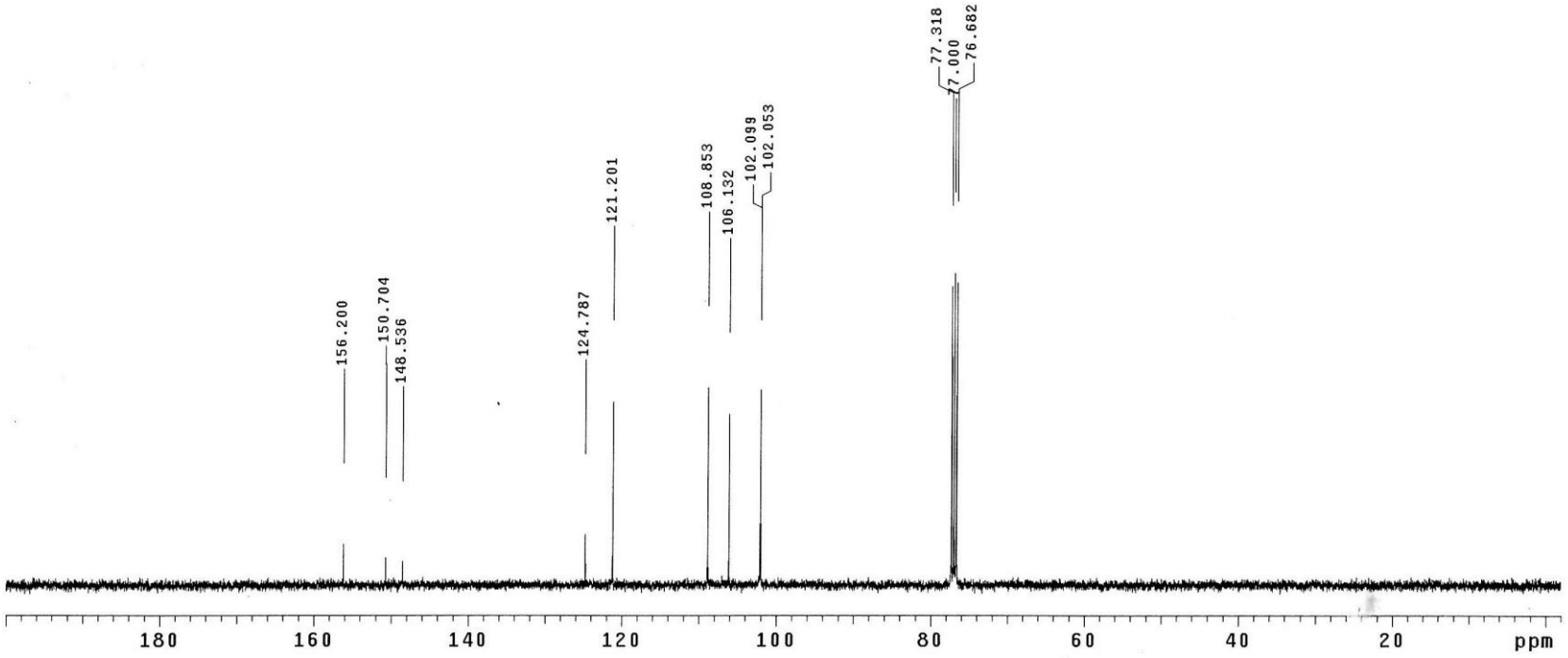
# Compound 6o ($^{13}$C-NMR spectral data)

YNP222

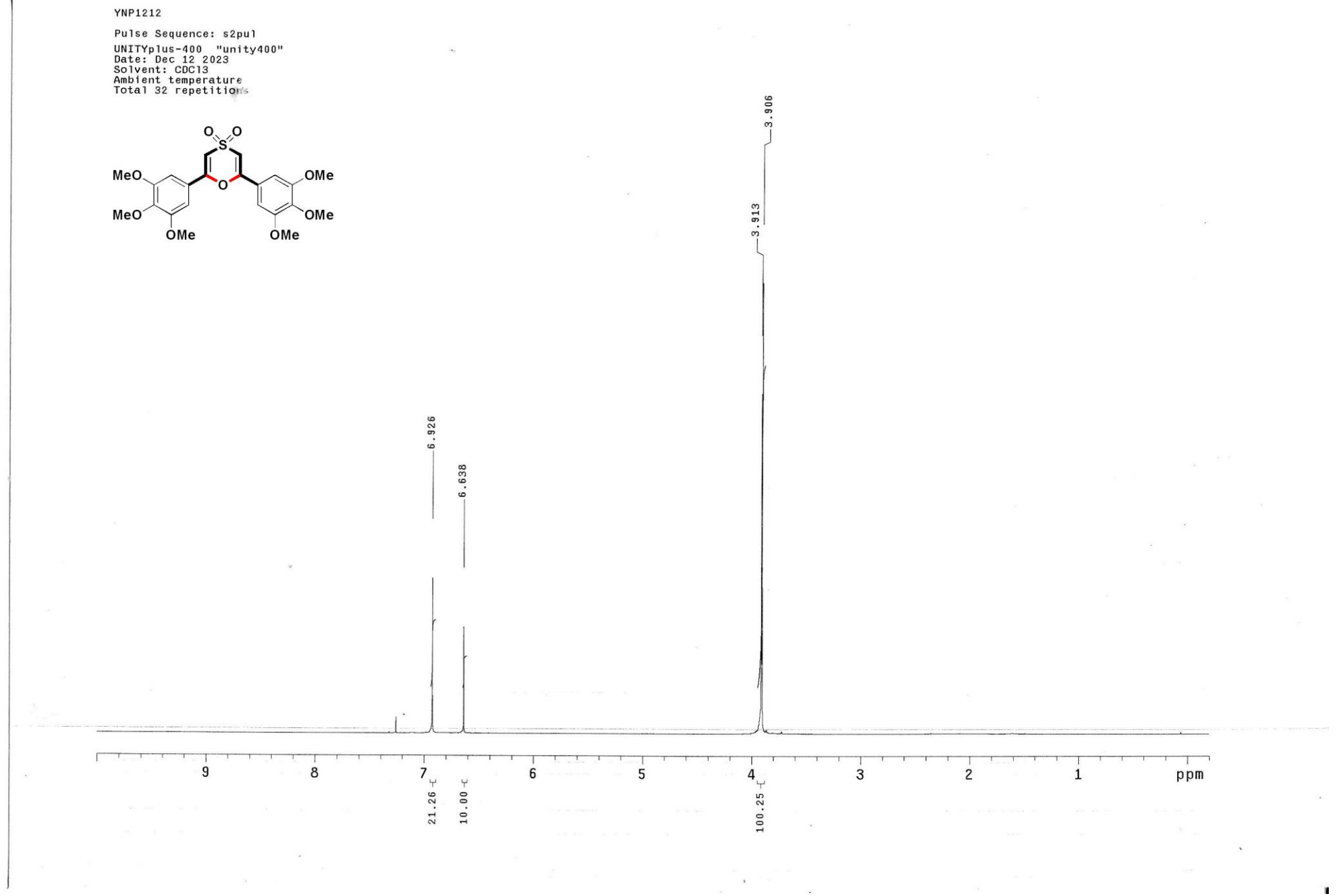
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Feb 23 2024
Solvent: CDCl3
Ambient temperature
Total 6688 repetitions





# Compound 6q ($^1$H-NMR spectral data)

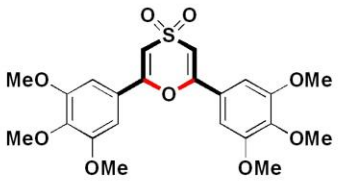


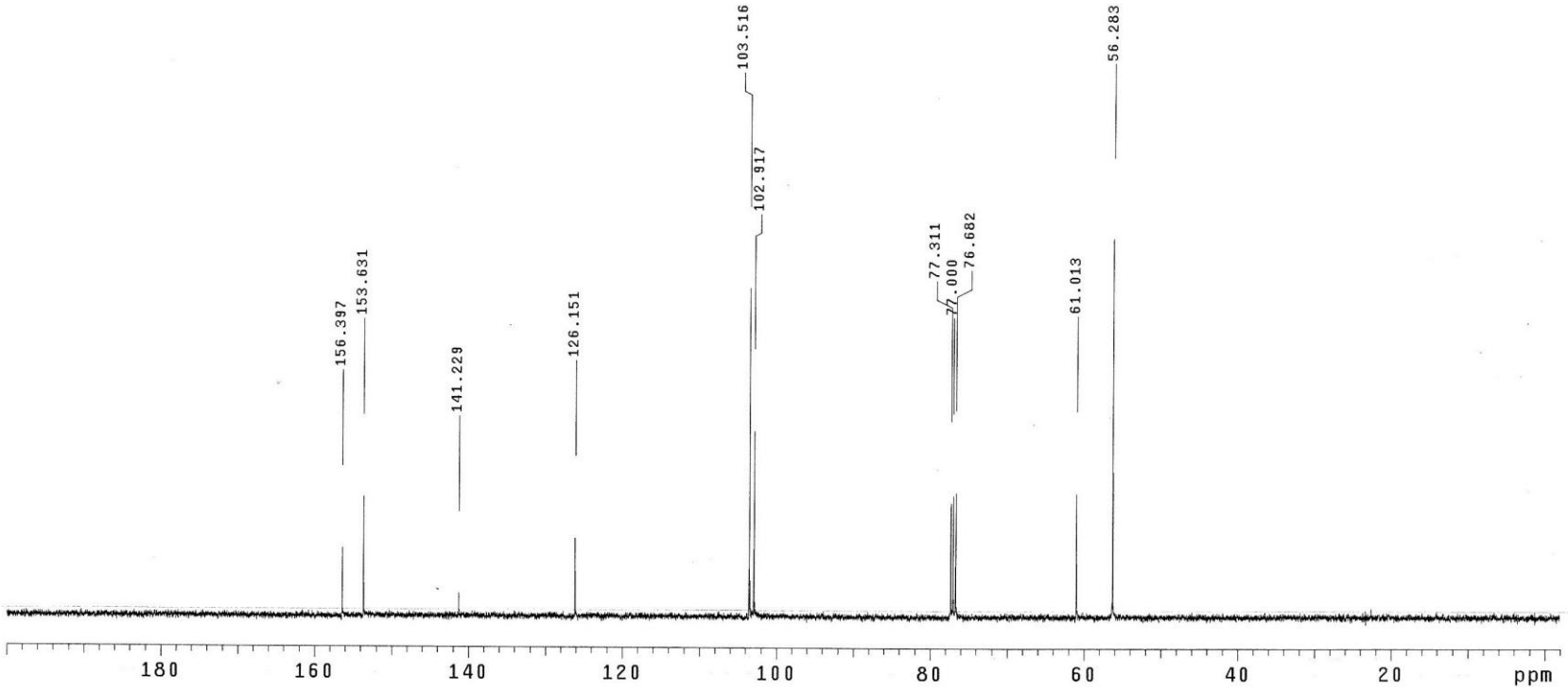
# Compound 6q ($^{13}$C-NMR spectral data)

YNP1212

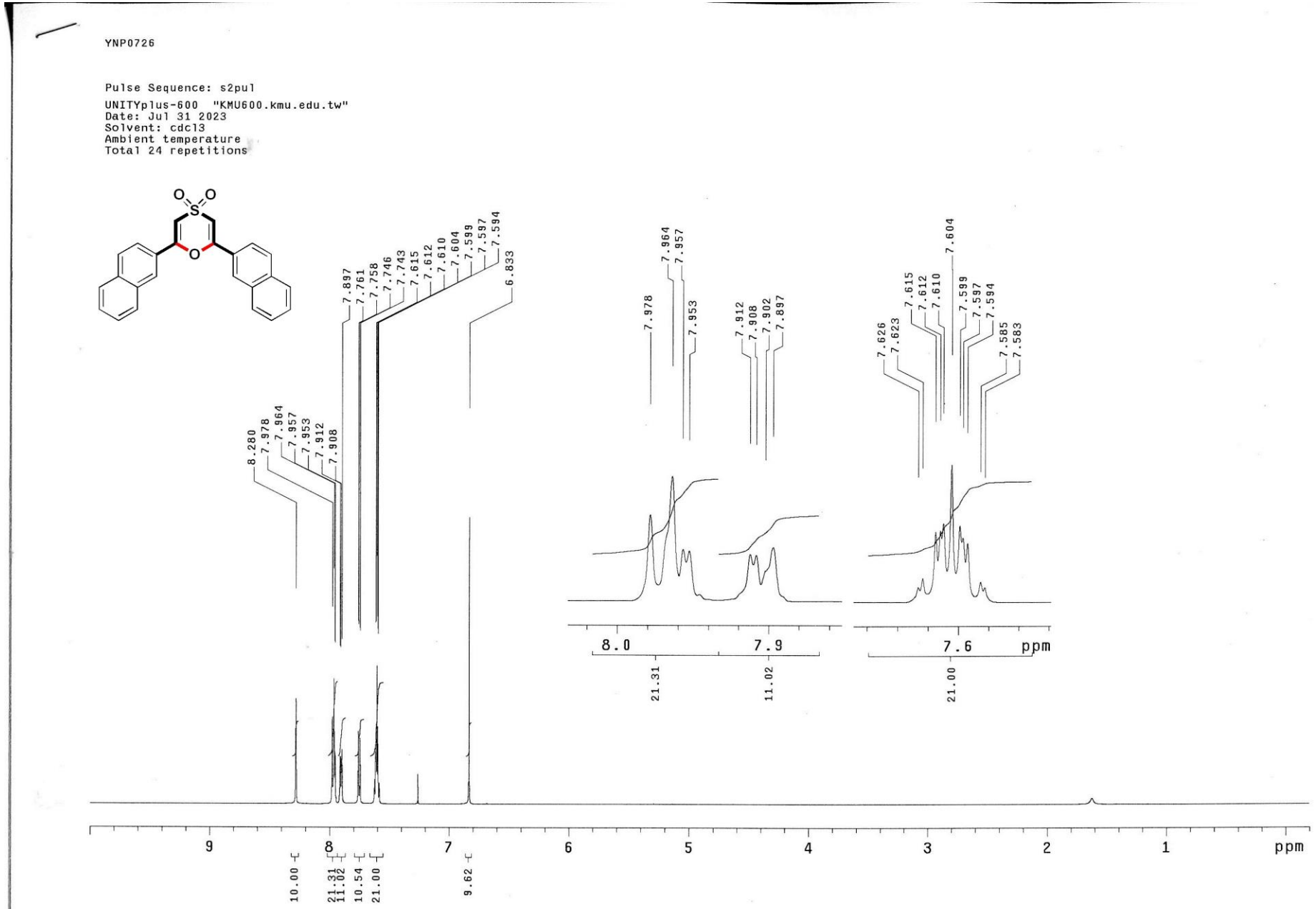
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Dec 12 2023
Solvent: CDCl3
Ambient temperature
Total 2368 repetitions



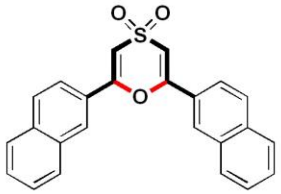
# Compound 6r ($^1$H-NMR spectral data)

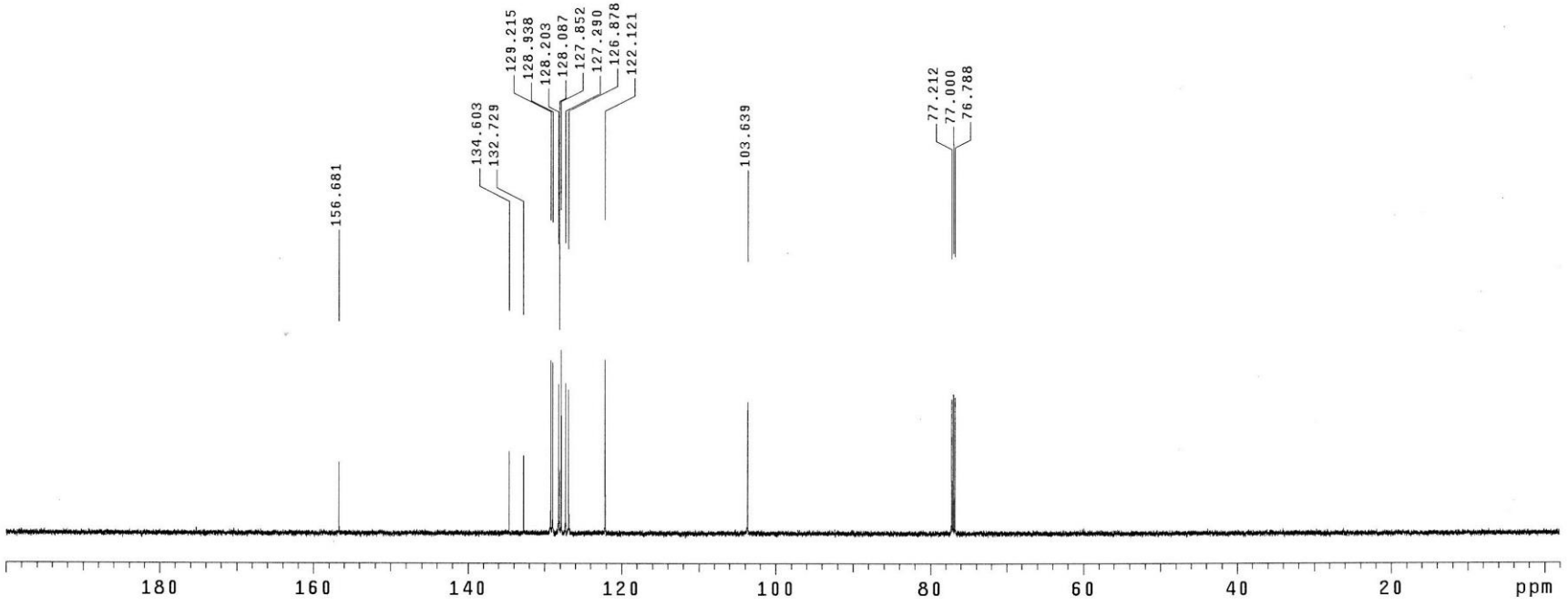


# Compound 6r ($^{13}$C-NMR spectral data)

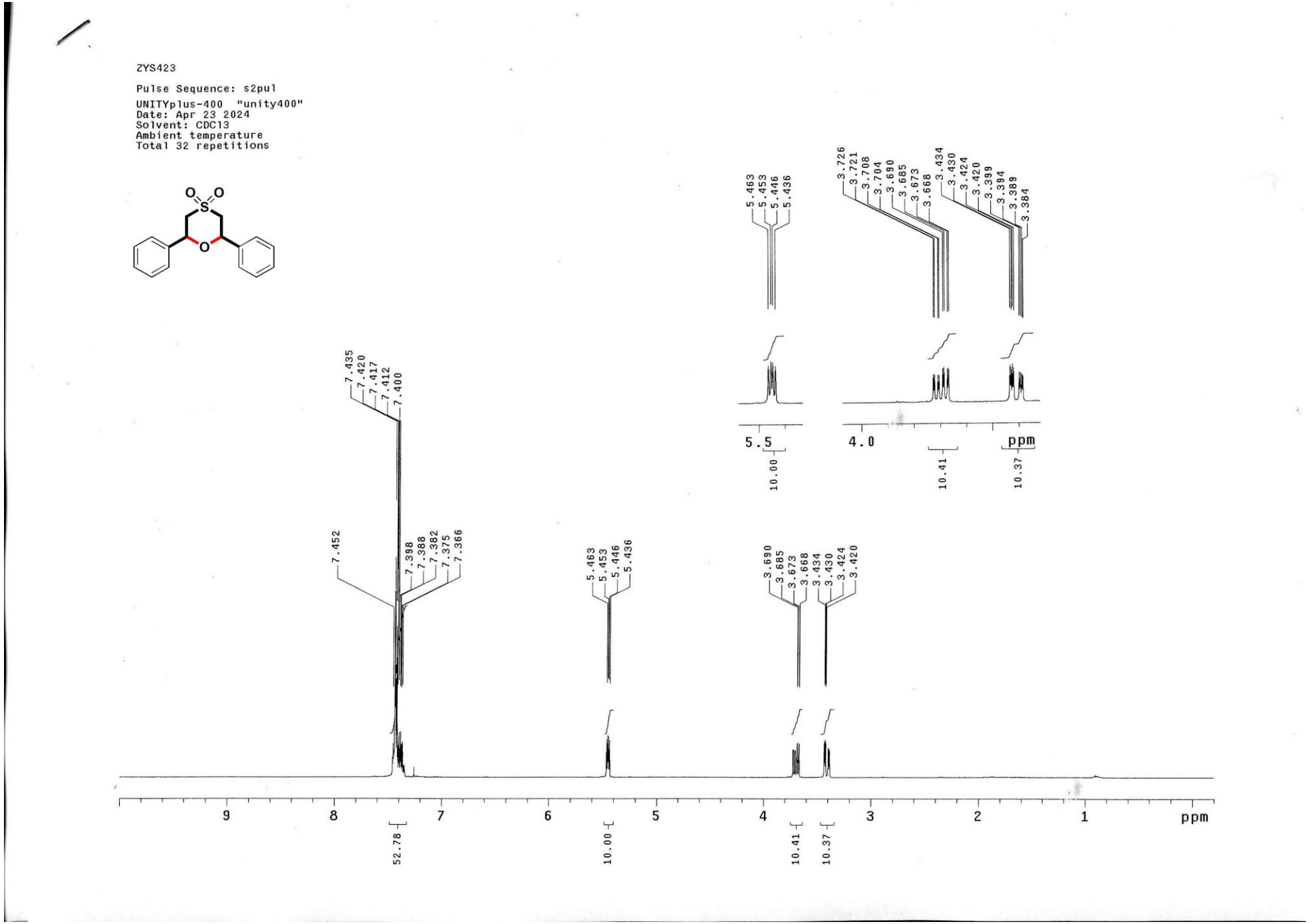
YNP0726

Pulse Sequence: s2pul
UNITYplus-600 "KMU600.kmu.edu.tw"
Date: Jul 31 2023
Solvent: cdcl3
Ambient temperature
Total 80 repetitions





# Compound 8a ($^1$H-NMR spectral data)

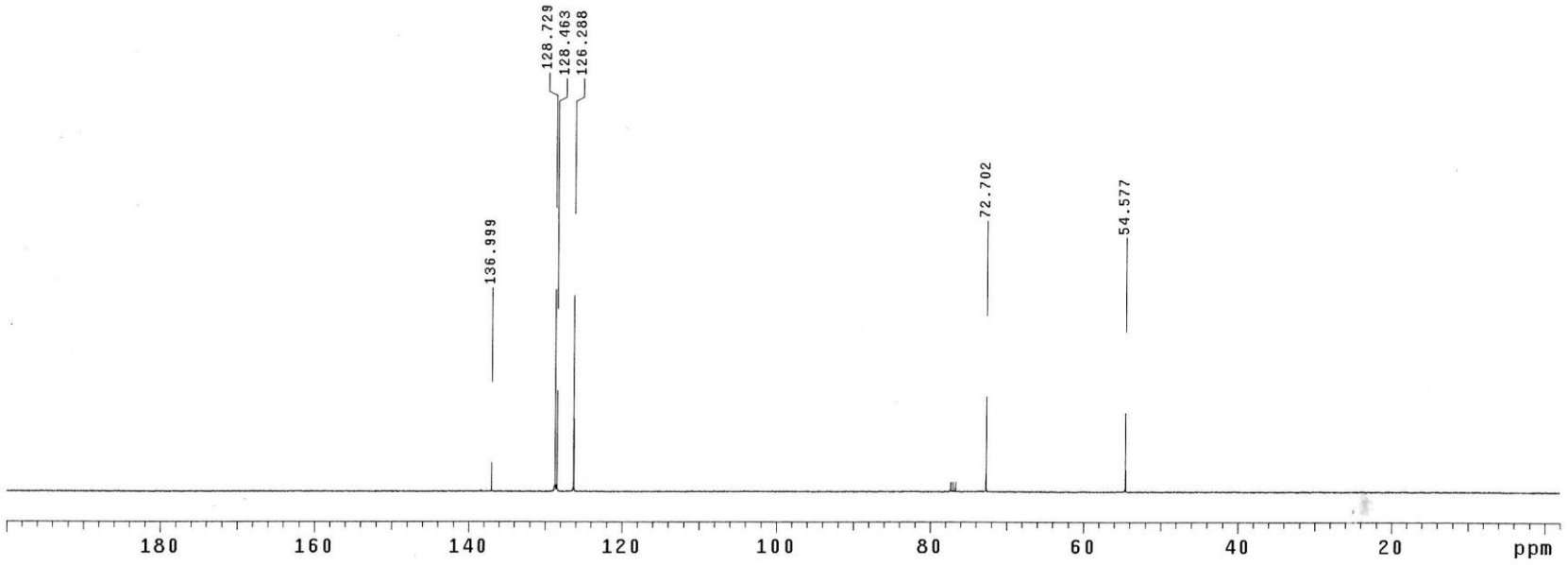


# Compound 8a ($^{13}$C-NMR spectral data)

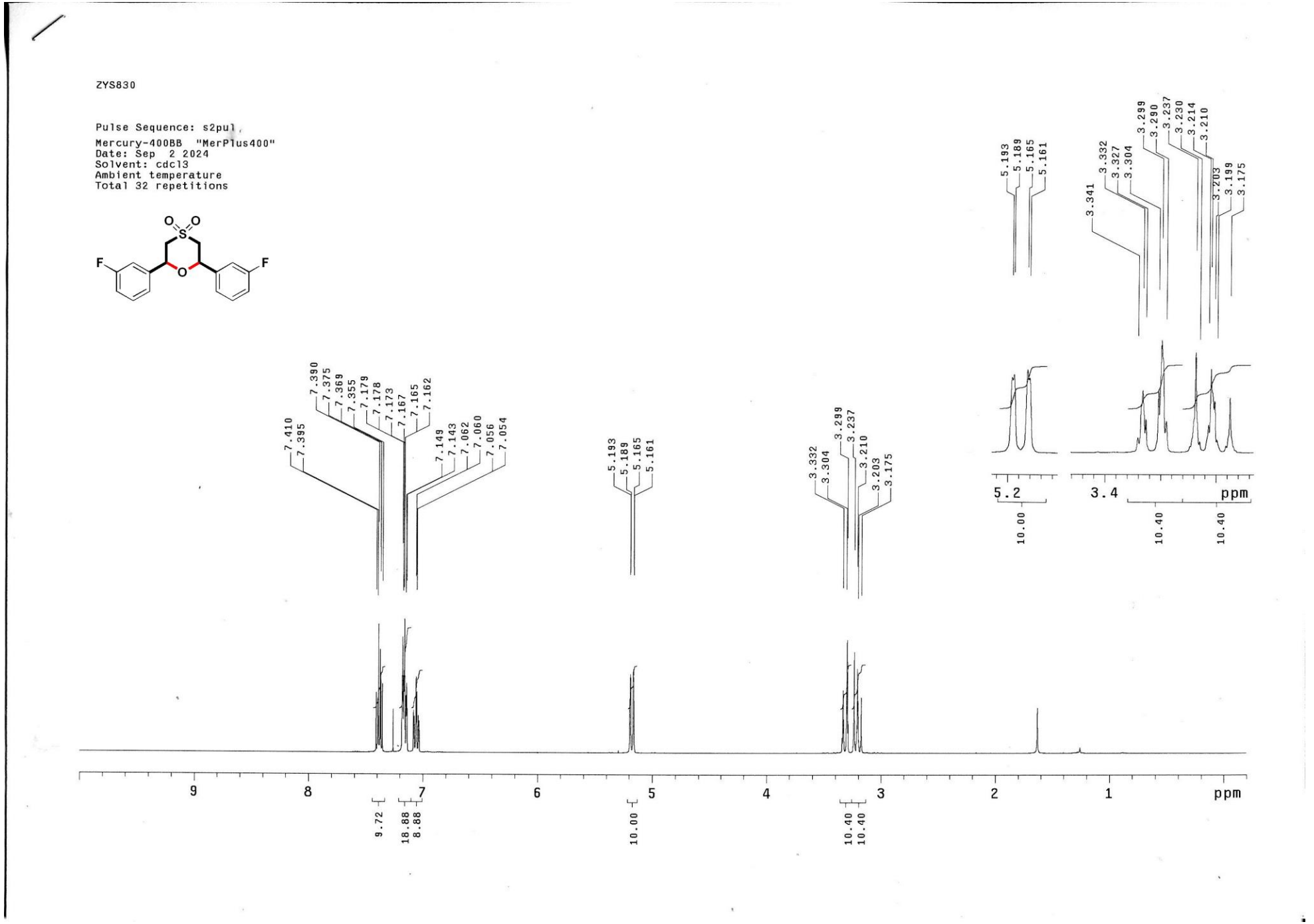
ZYS423

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Apr 23 2024
Solvent: CDCl3
Ambient temperature
Total 720 repetitions

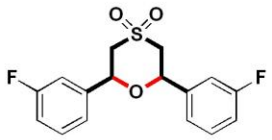
# Compound 8b ($^1$H-NMR spectral data)

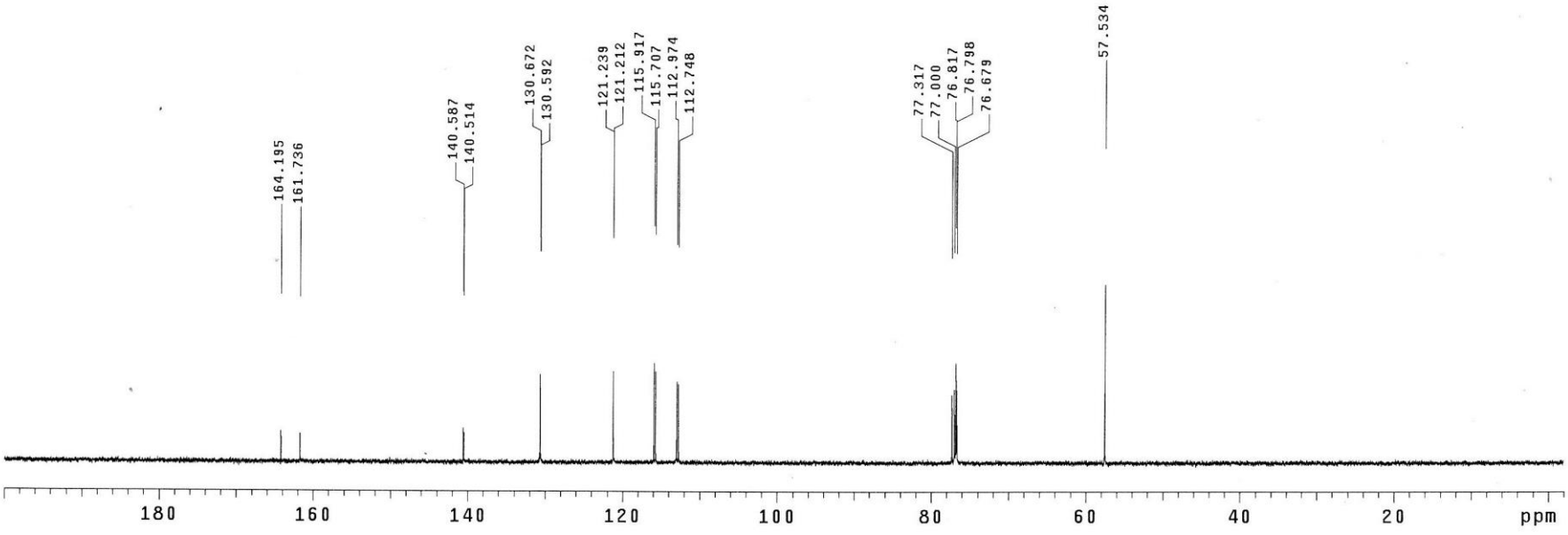


# Compound 8b ($^{13}$C-NMR spectral data)

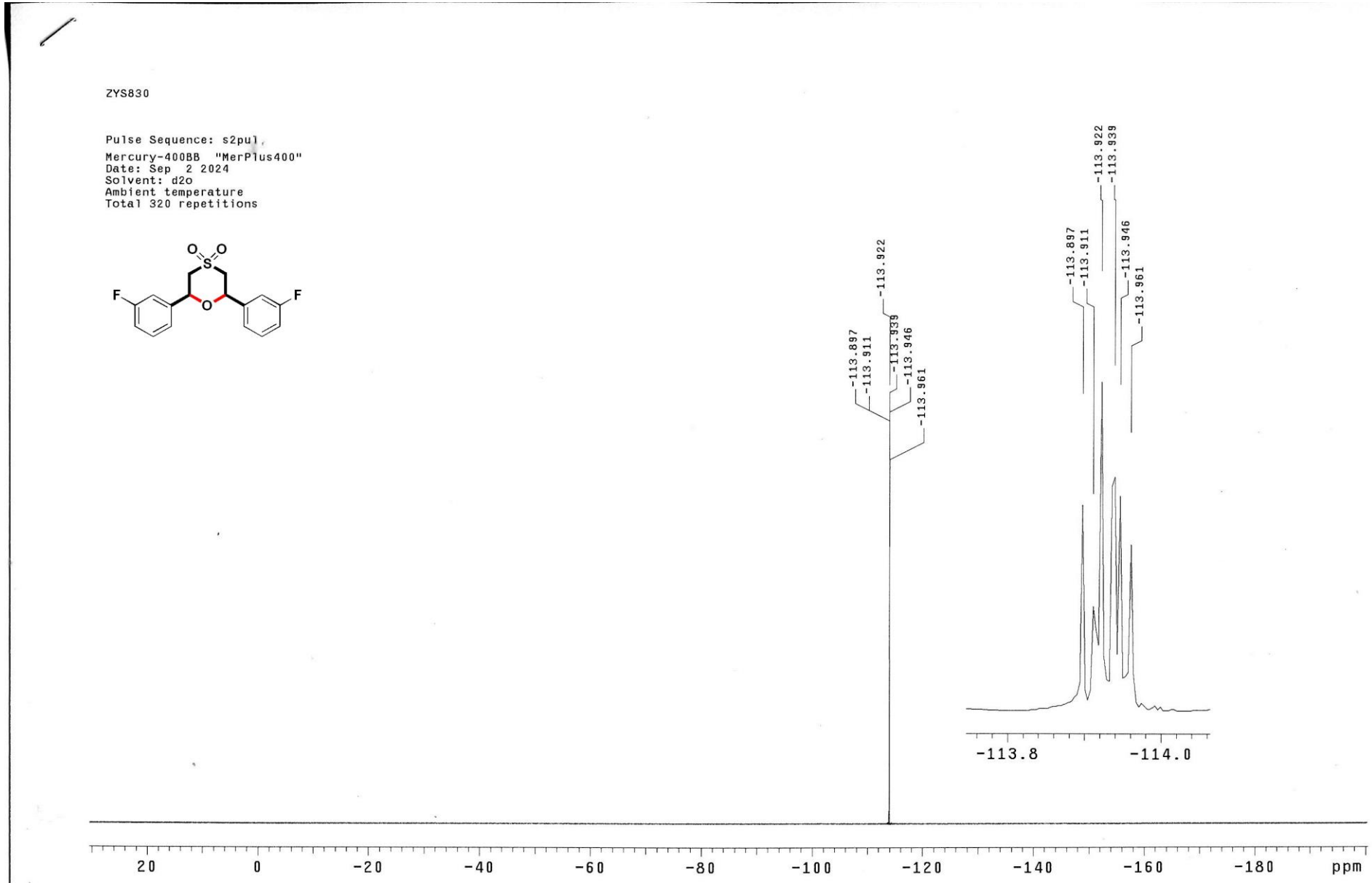
ZYS830

Pulse Sequence: s2pul
Mercury-400BB "MerPlus400"
Date: Sep 2 2024
Solvent: cdcl3
Ambient temperature
Total 160 repetitions

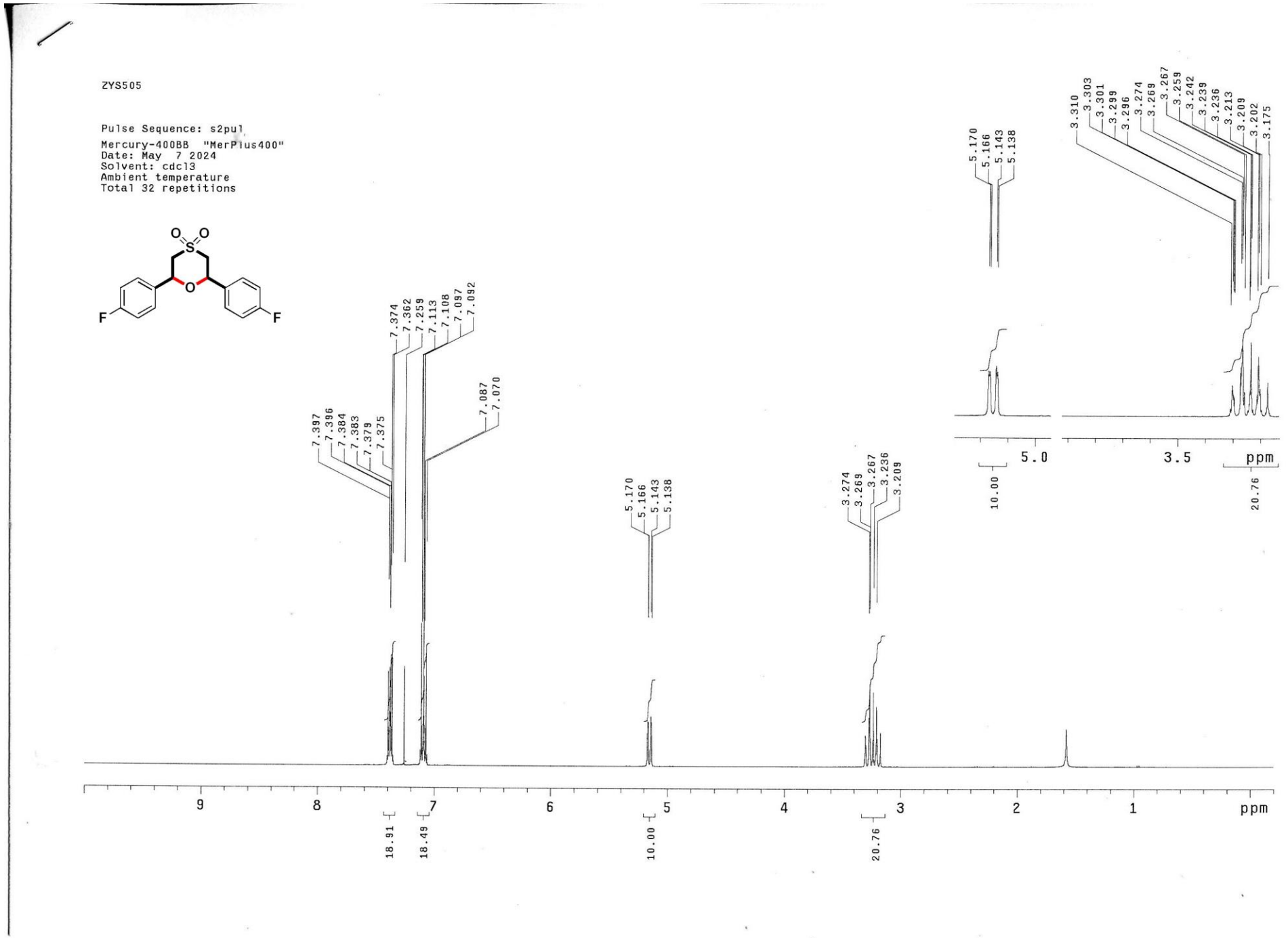


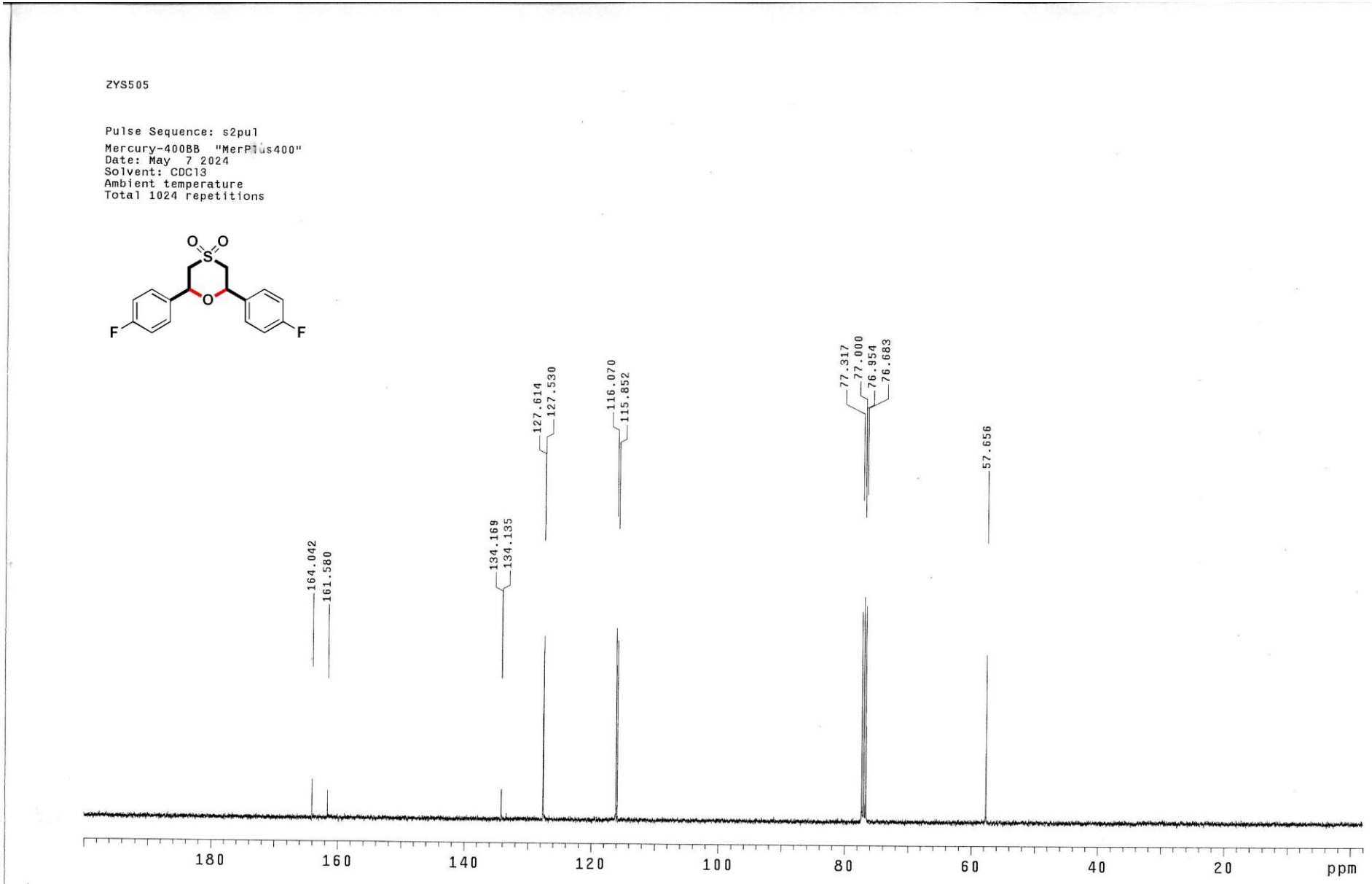
# Compound 8b ($^{19}$F-NMR spectral data)



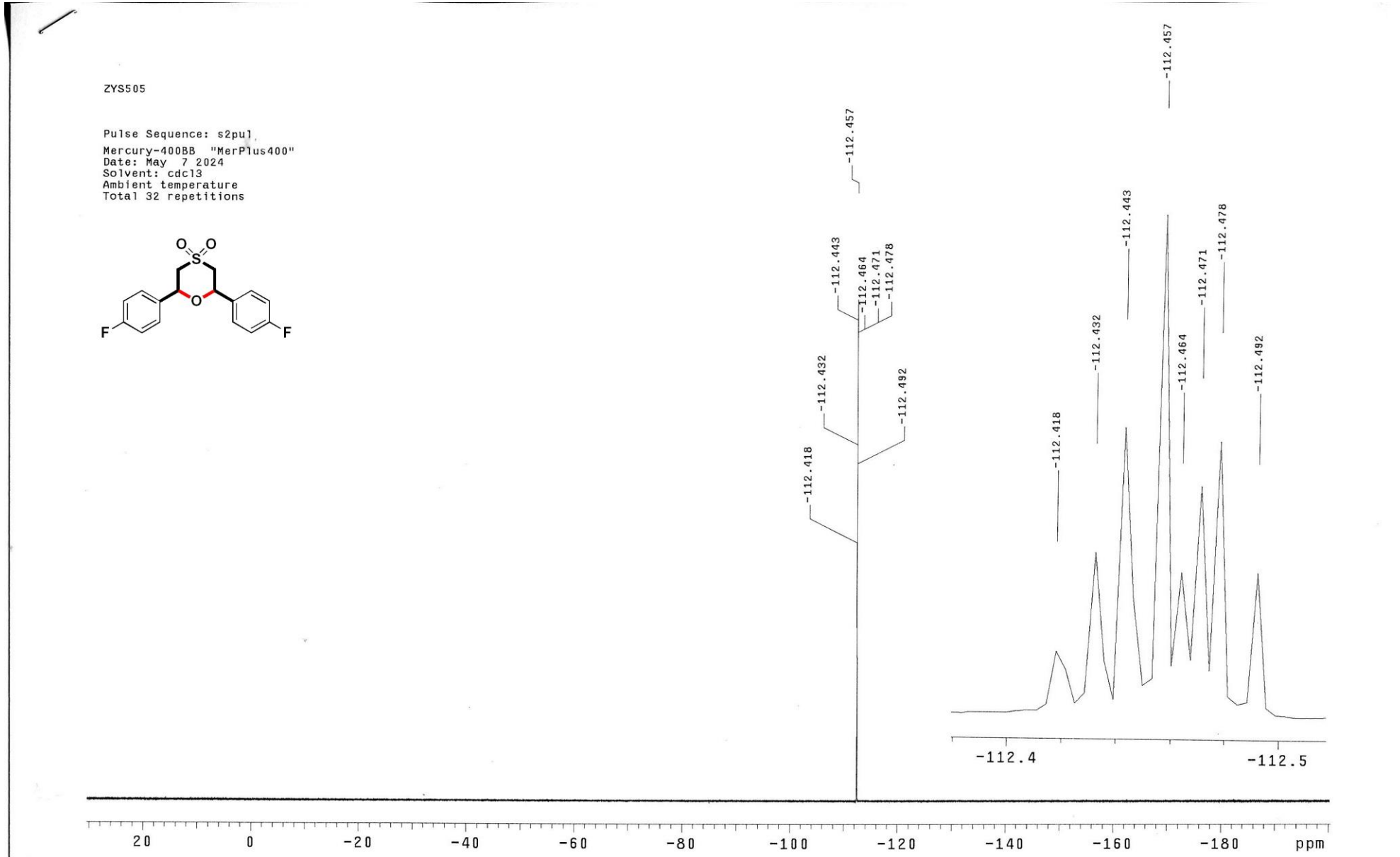
# Compound 8c ($^1$H-NMR spectral data)



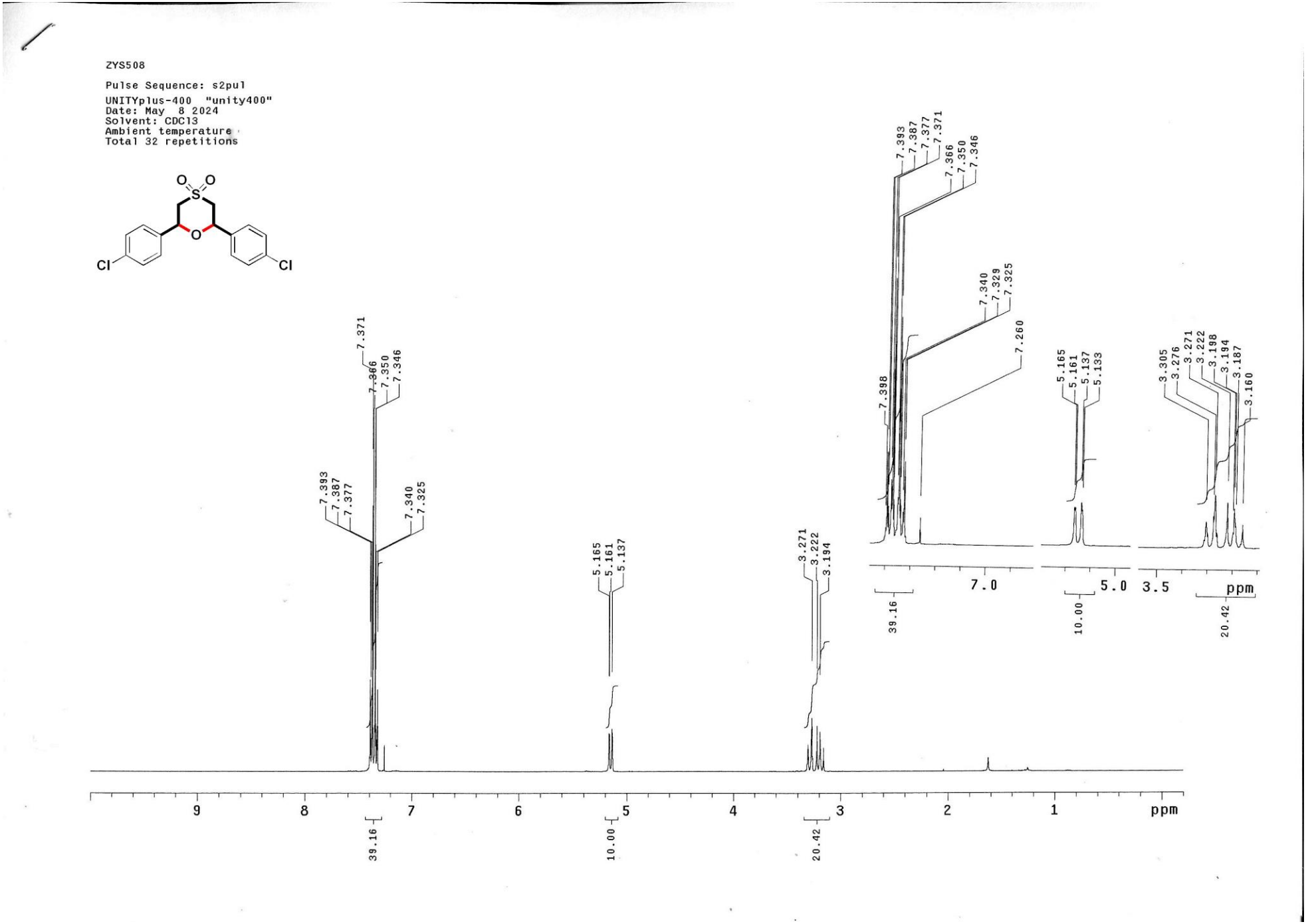
# Compound 8c ($^{13}$C-NMR spectral data)



# Compound 8c ($^{19}$F-NMR spectral data)



# Compound 8d ($^1$H-NMR spectral data)

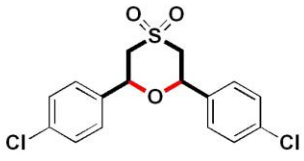


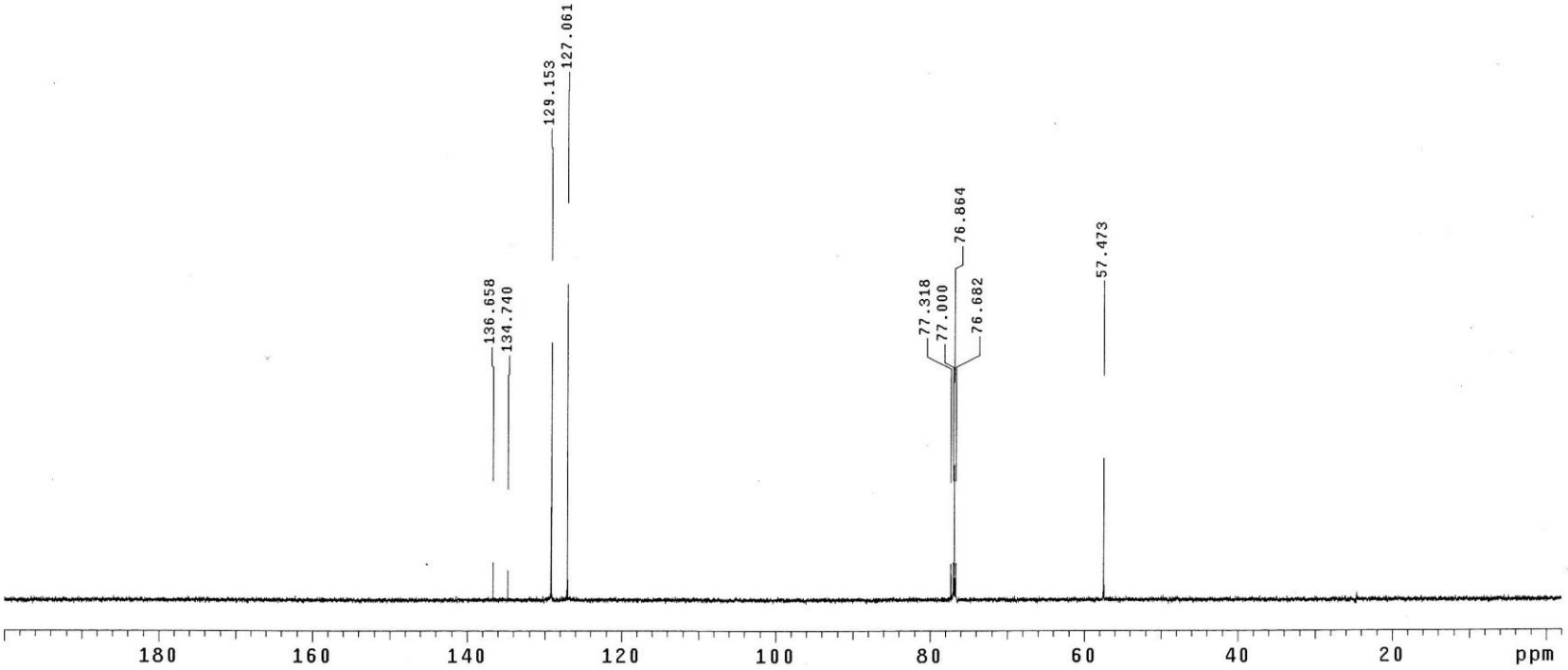
# Compound 8d ($^{13}$C-NMR spectral data)

ZYS508

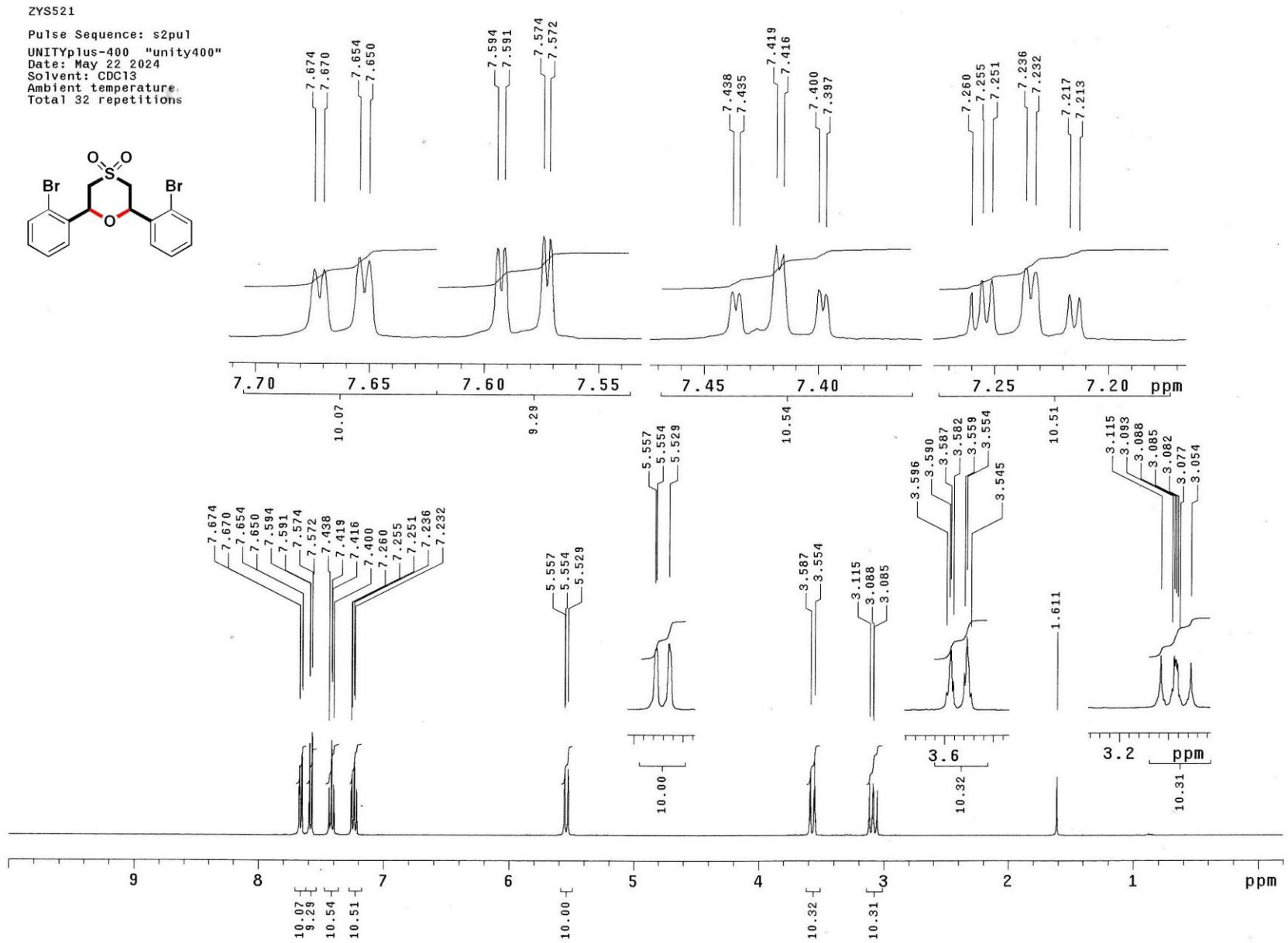
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 8 2024
Solvent: CDCl3
Ambient temperature
Total 432 repetitions



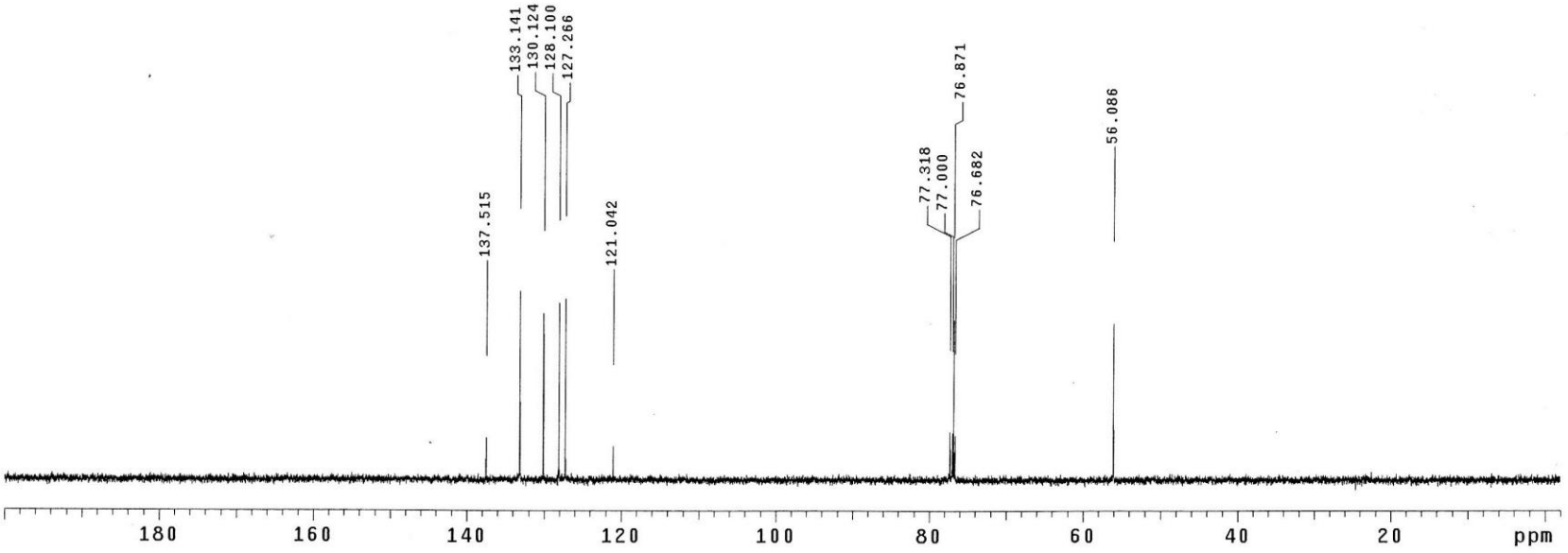
# Compound 8e ($^1$H-NMR spectral data)



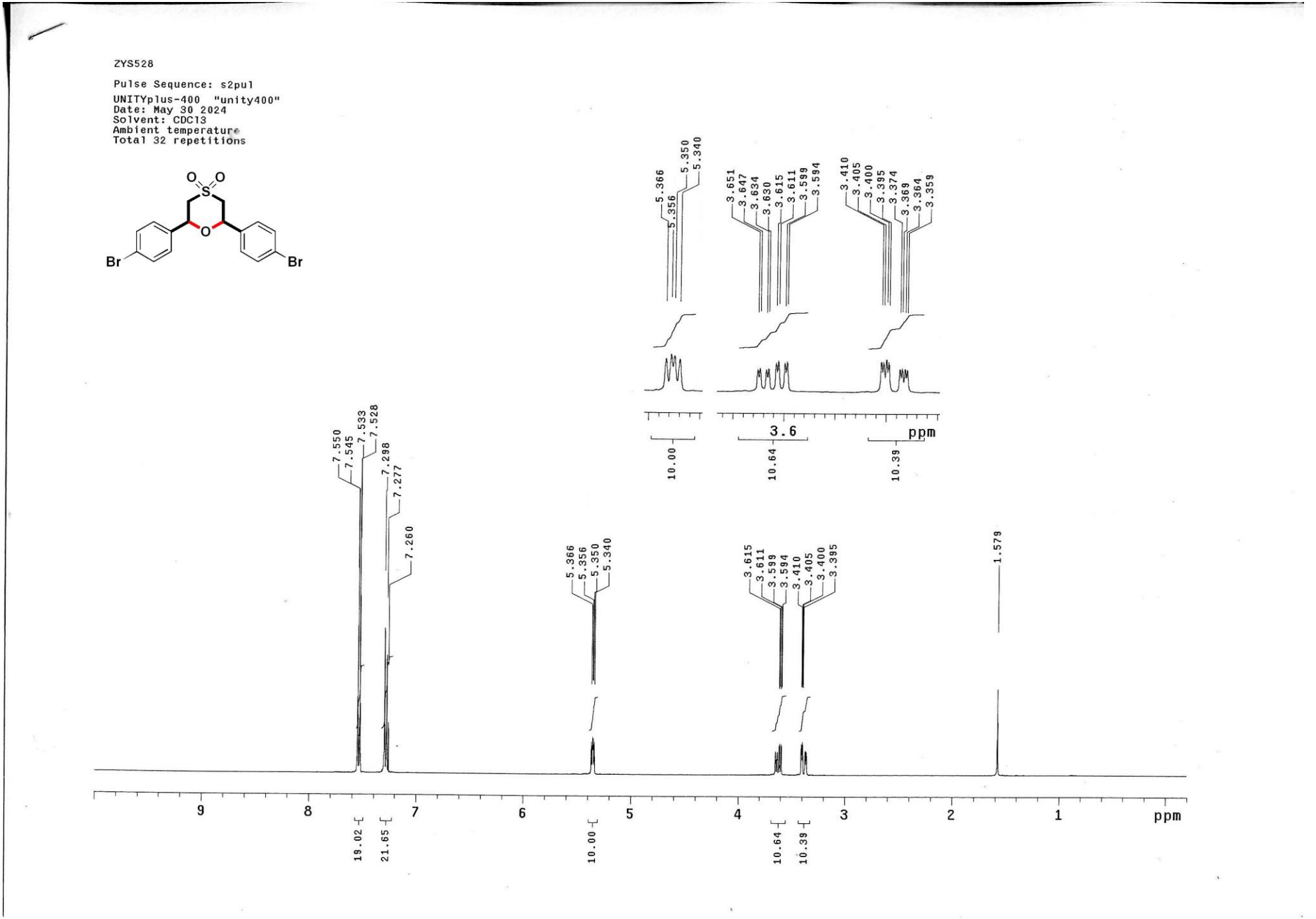
# Compound 8e ($^{13}$C-NMR spectral data)

ZYS521

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: May 22 2024
Solvent: CDCl3
Ambient temperature
Total 256 repetitions

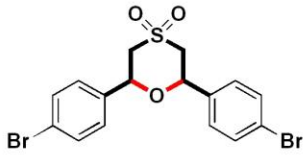
# Compound 8f ($^1$H-NMR spectral data)

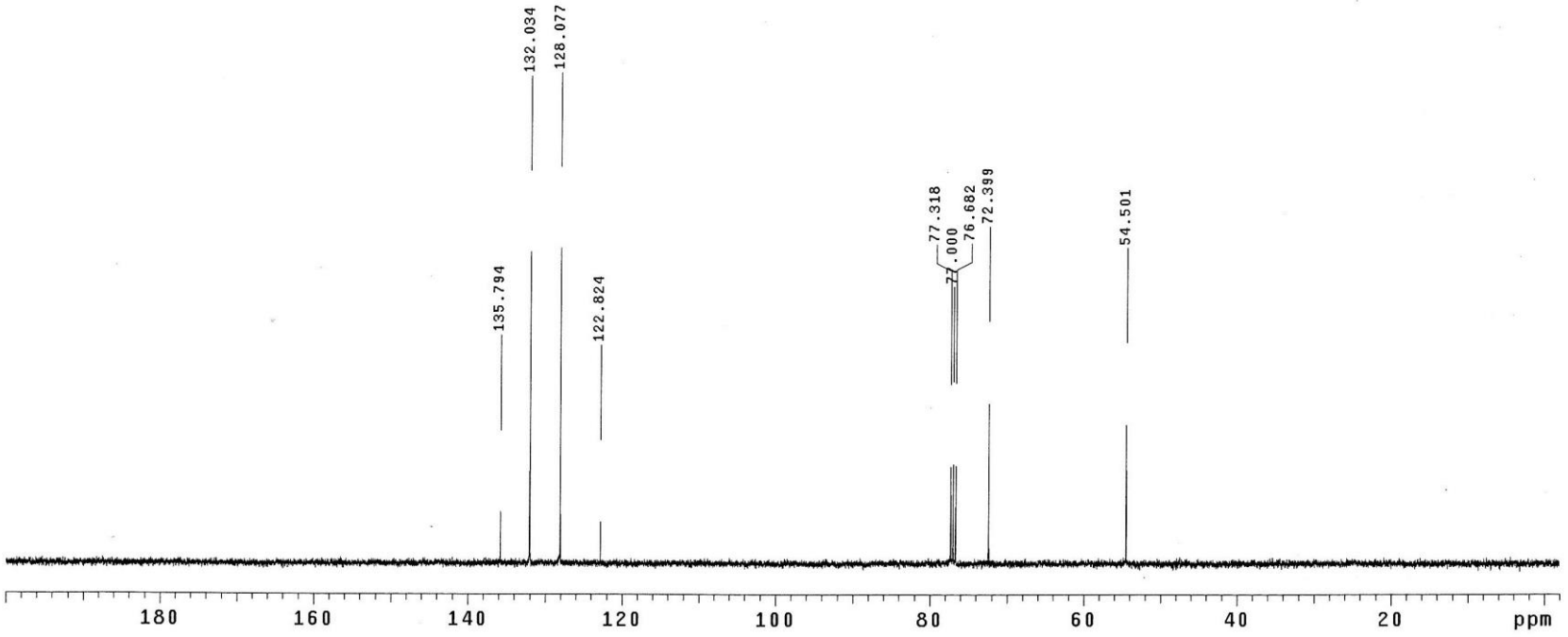


# Compound 8f ($^{13}$C-NMR spectral data)

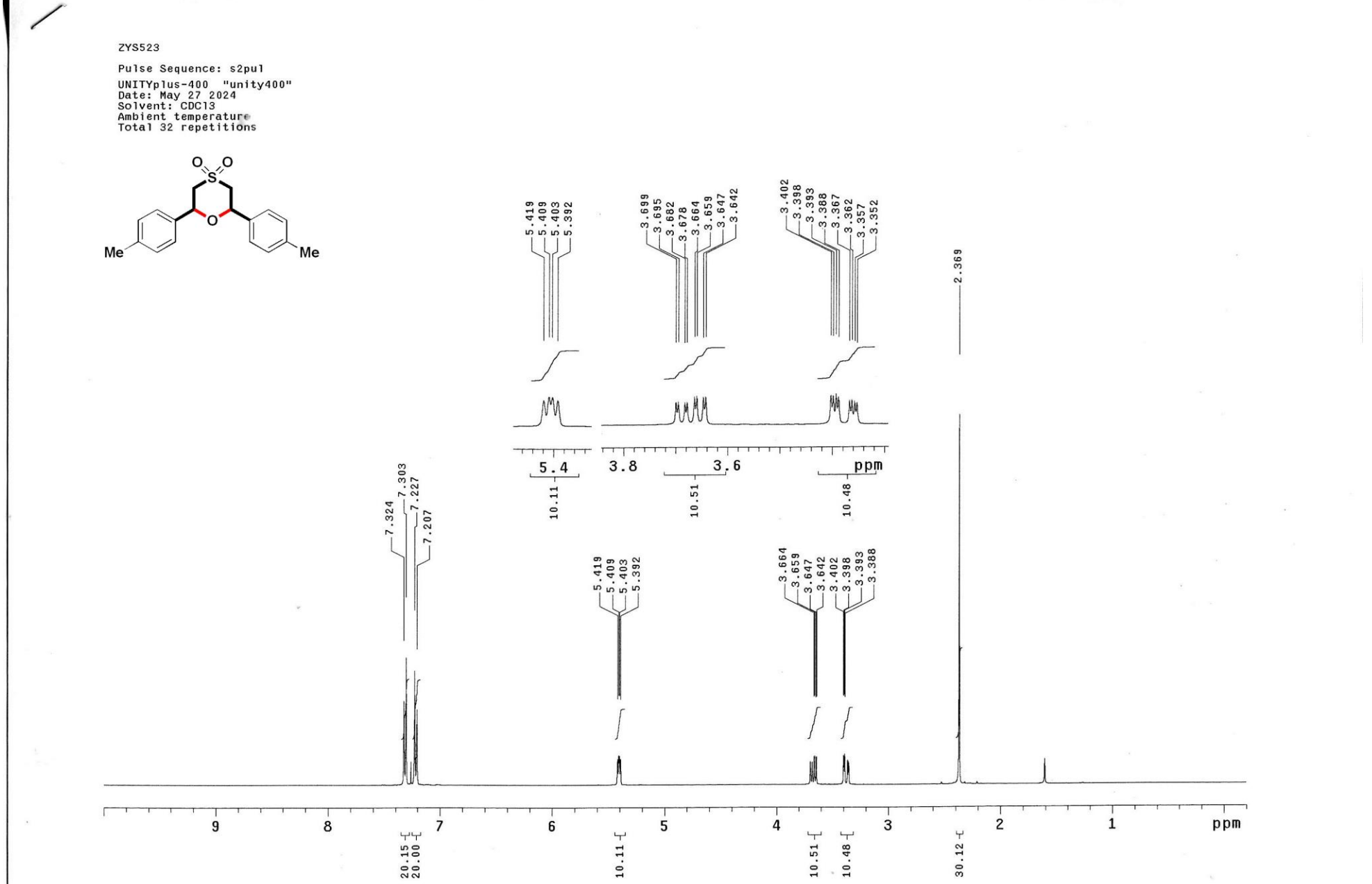
ZYS528

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: May 30 2024
Solvent: CDCl3
Ambient temperature
Total 1200 repetitions



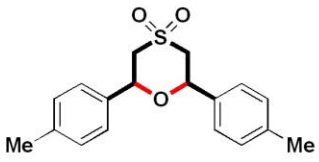
# Compound 8g ($^1$H-NMR spectral data)

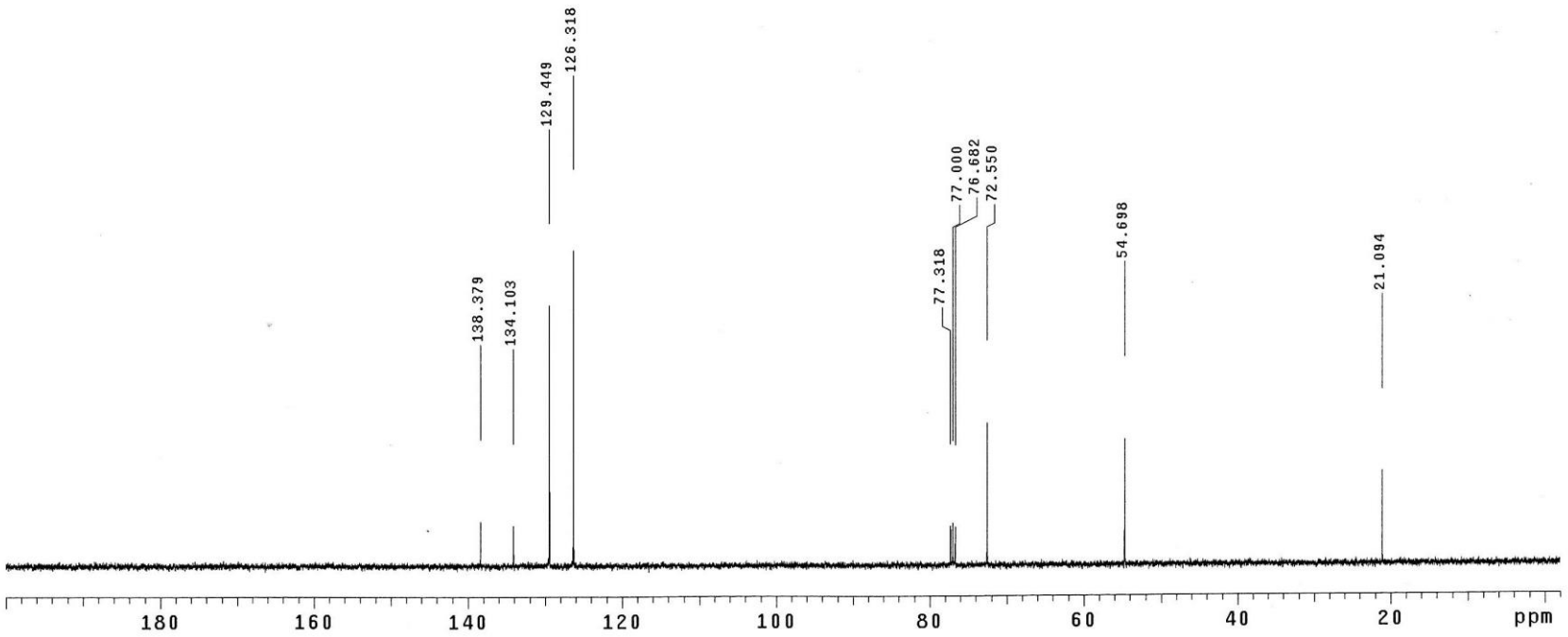


# Compound 8g ($^{13}$C-NMR spectral data)

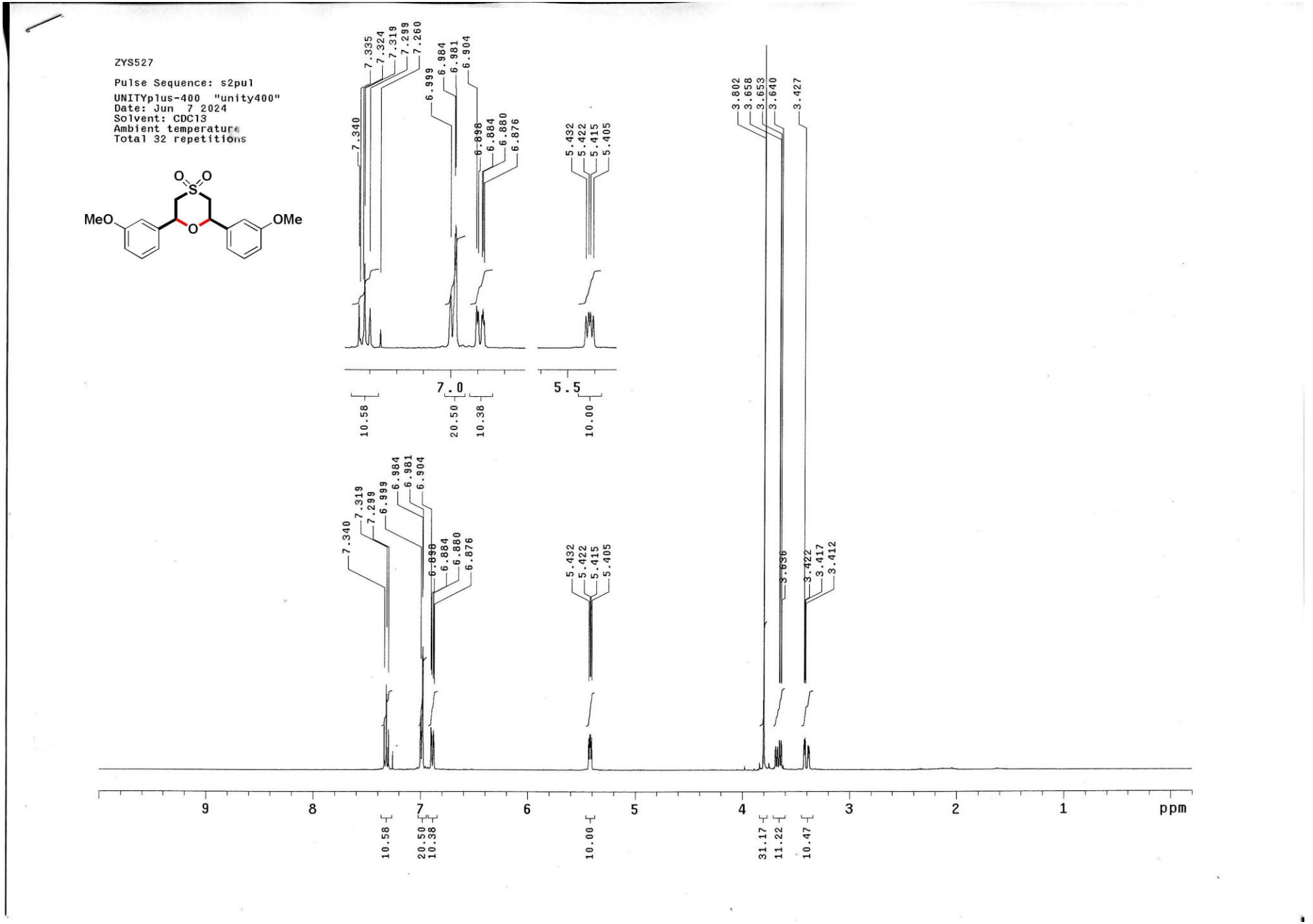
ZYS523

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: May 27 2024
Solvent: CDCl3
Ambient temperature
Total 240 repetitions



# Compound 8h ($^1$H-NMR spectral data)

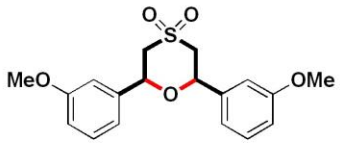


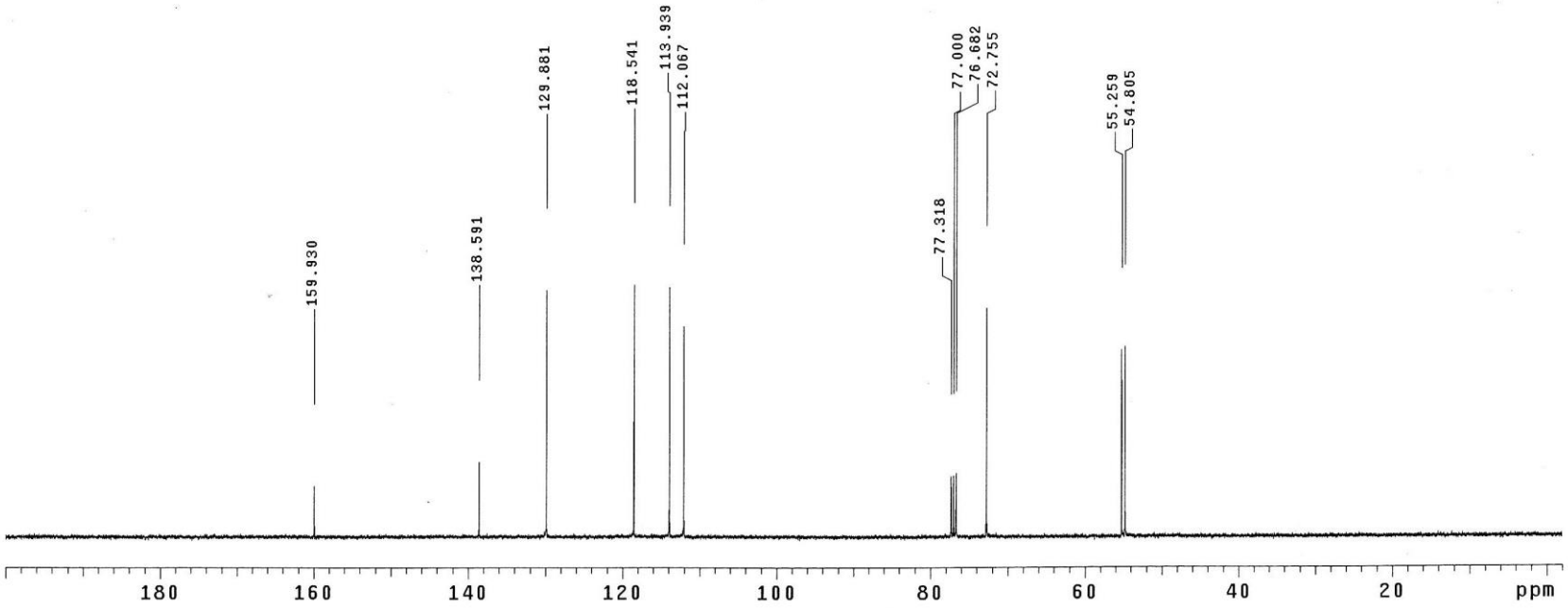
# Compound 8h ($^{13}$C-NMR spectral data)

ZYS527

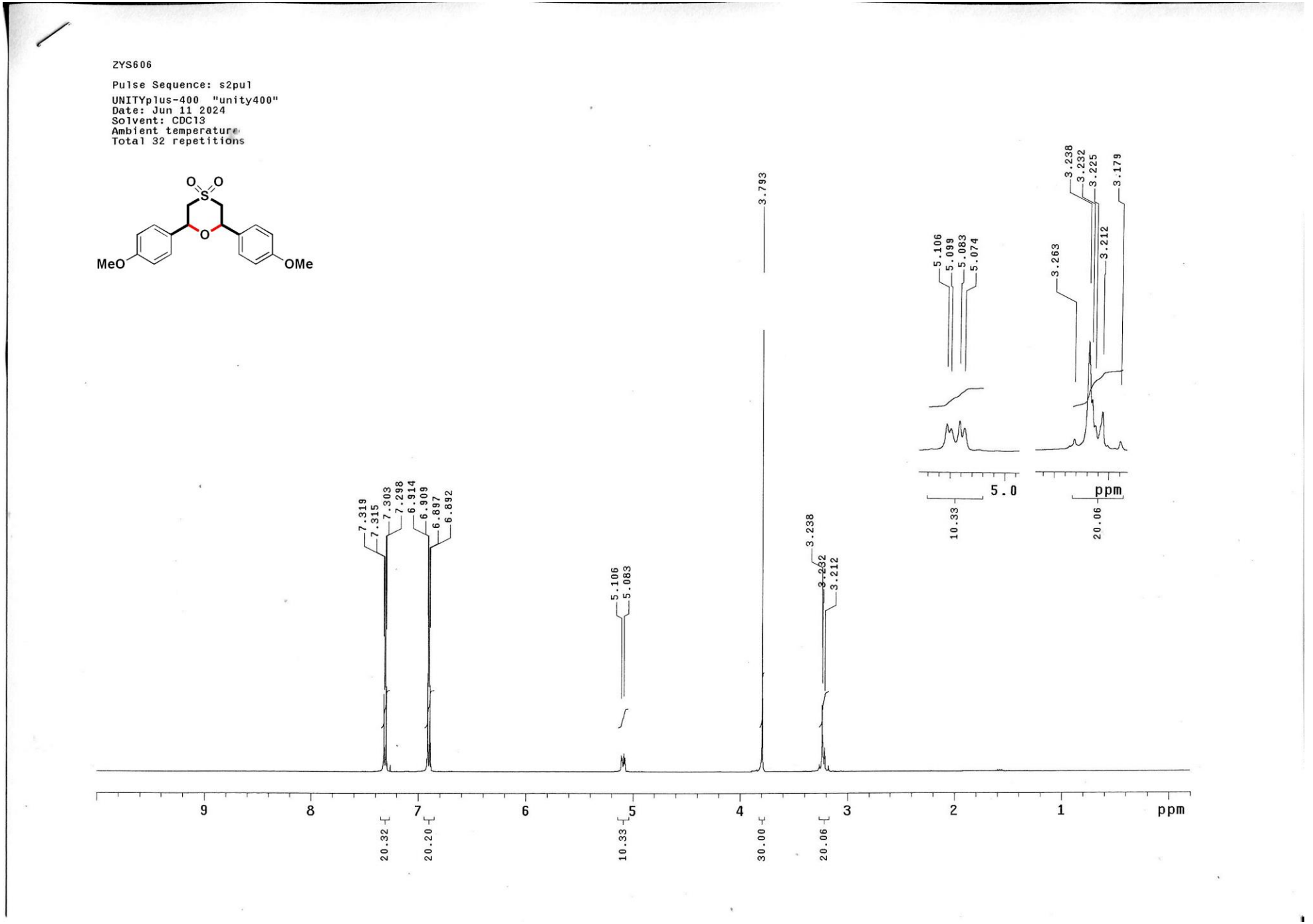
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jun 7 2024
Solvent: CDCl3
Ambient temperature
Total 1600 repetitions



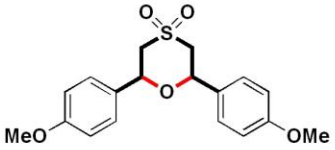
# Compound 8i ($^1$H-NMR spectral data)

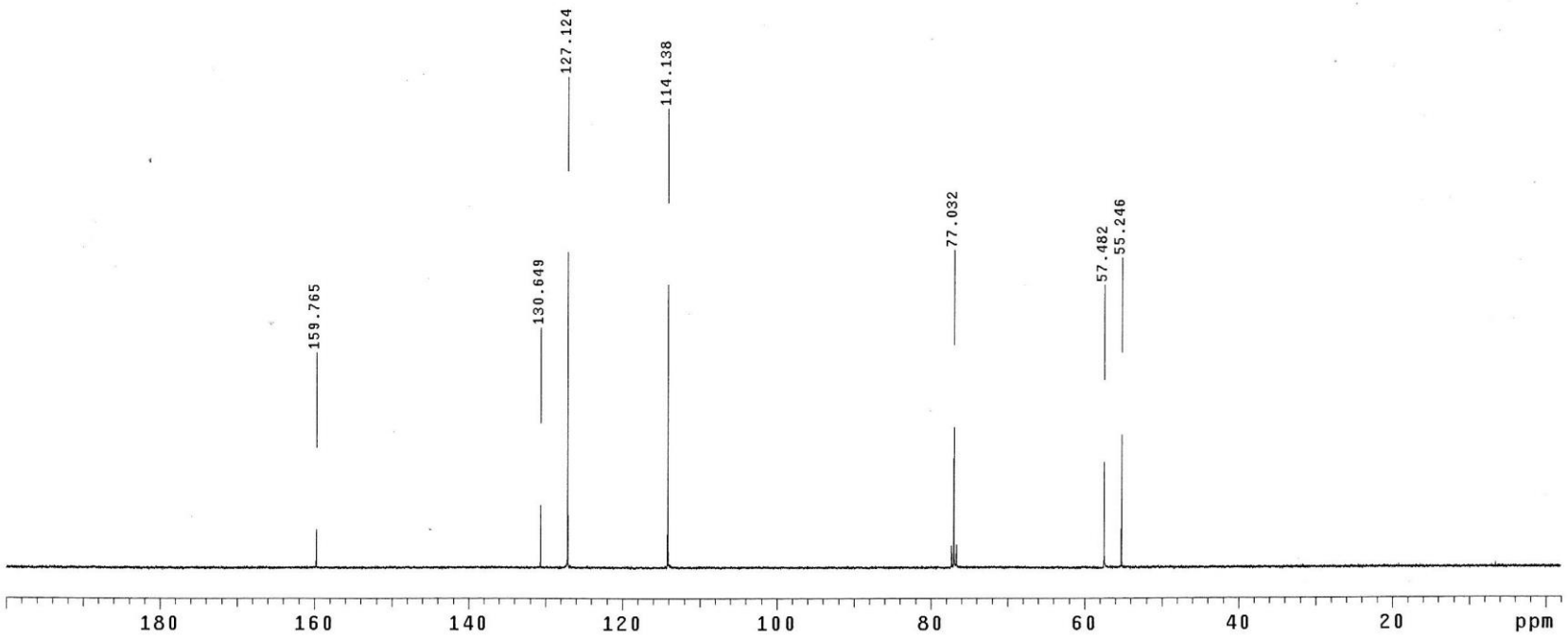


# Compound 8i ($^{13}$C-NMR spectral data)

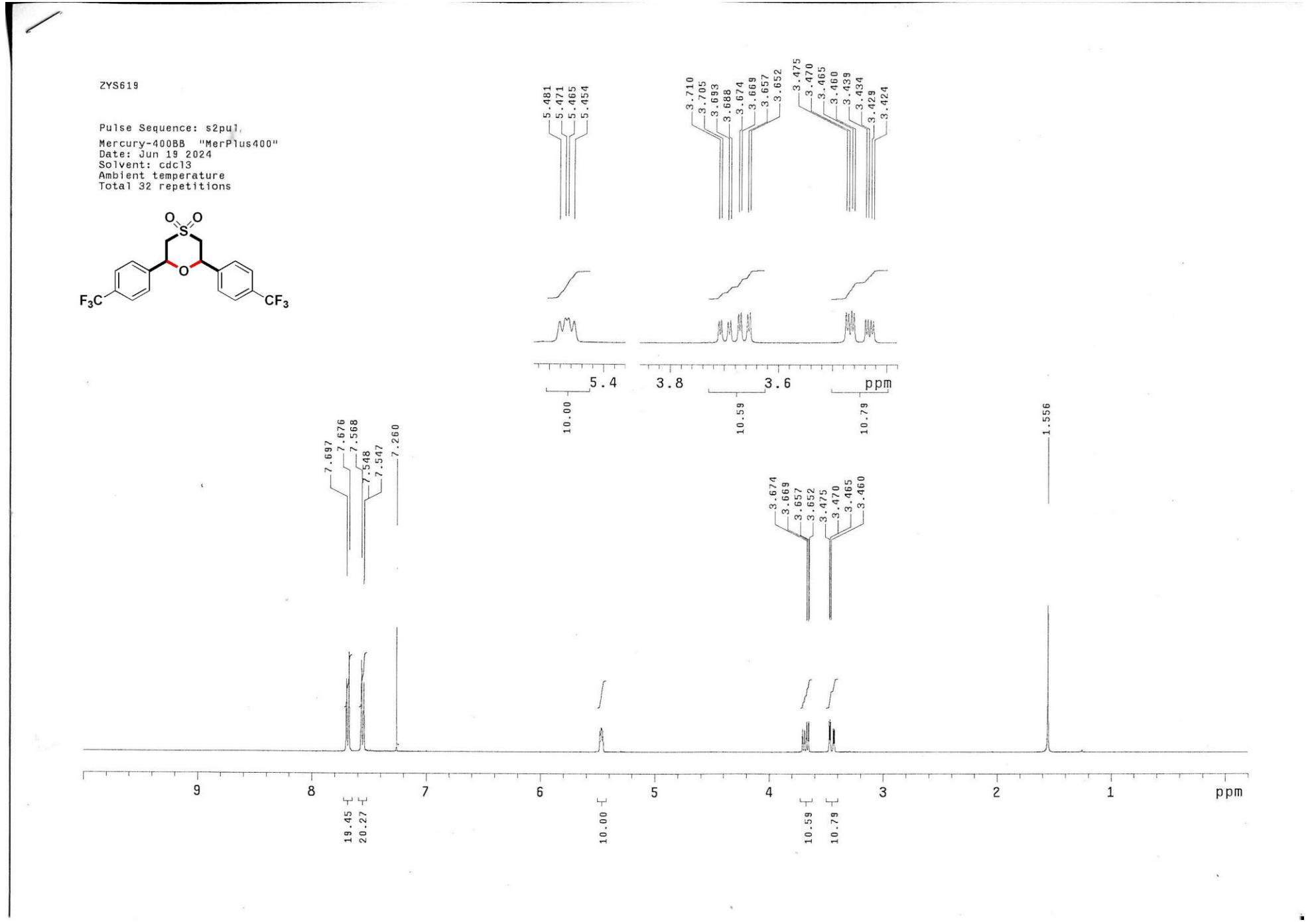
ZYS606

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Jun 11 2024
Solvent: CDCl3
Ambient temperature
Total 512 repetitions

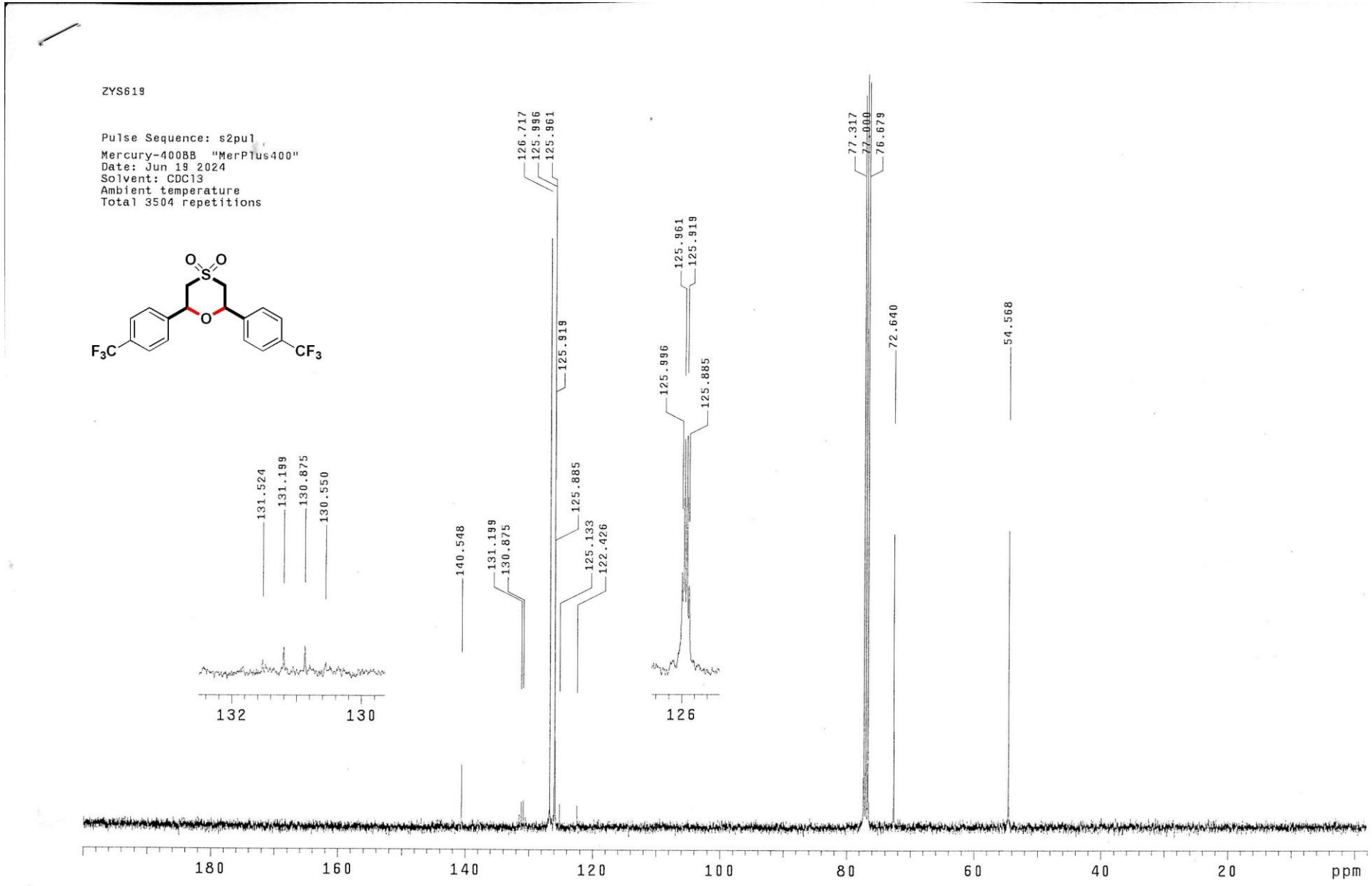


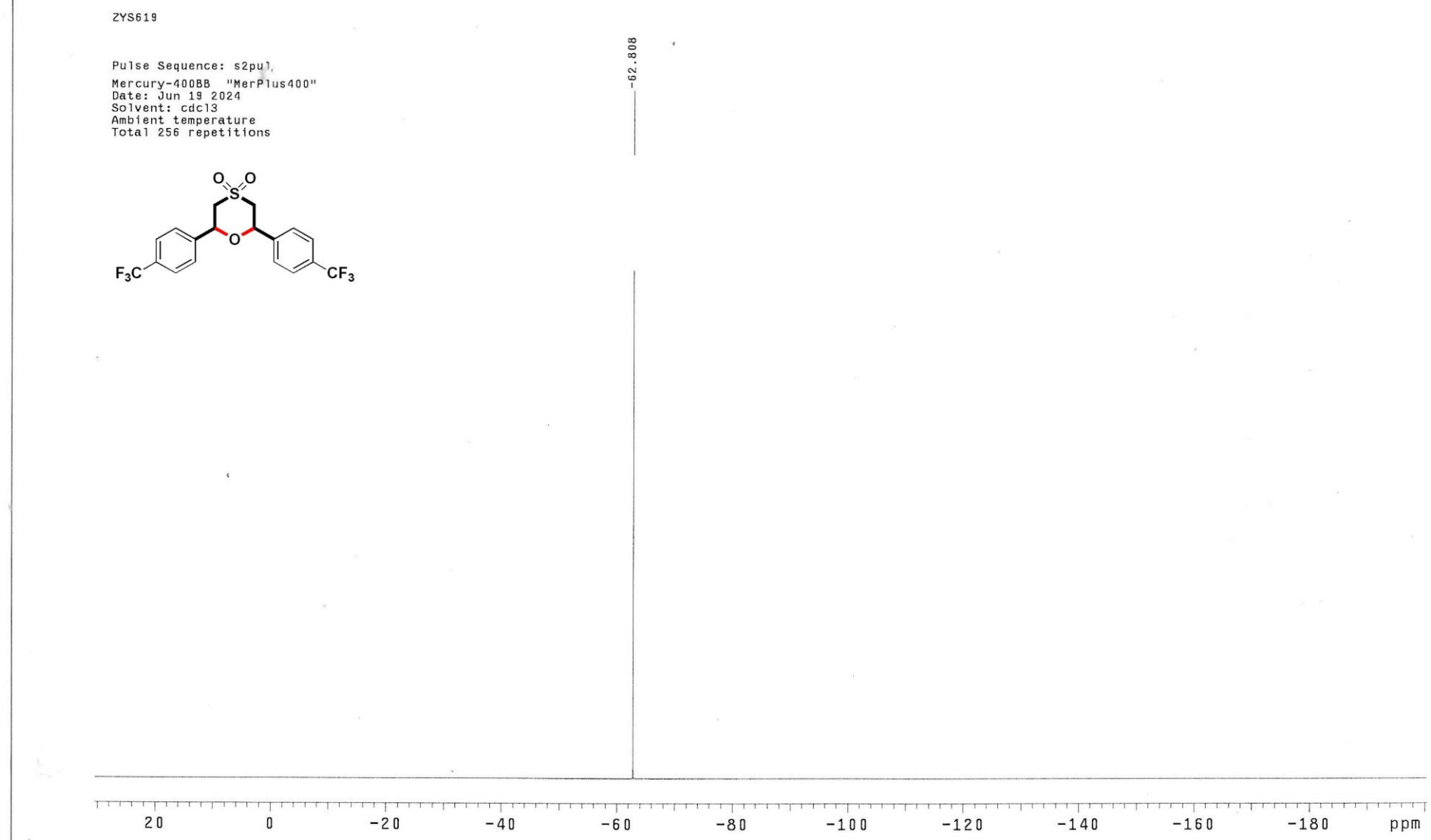
# Compound 8j ($^1$H-NMR spectral data)



# Compound 8j ($^{13}$C-NMR spectral data)



# Compound 8j ($^{19}$F-NMR spectral data)

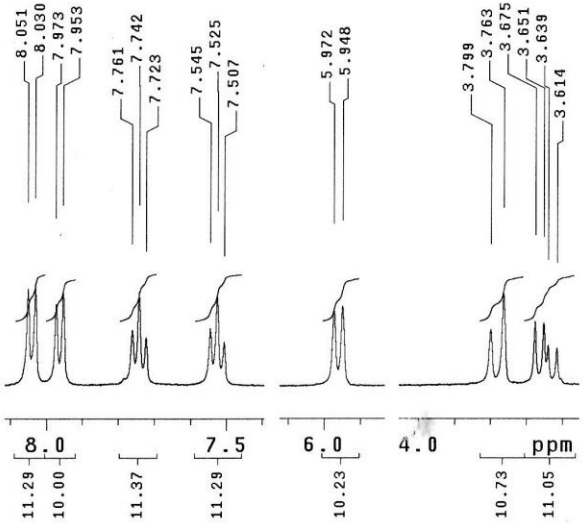


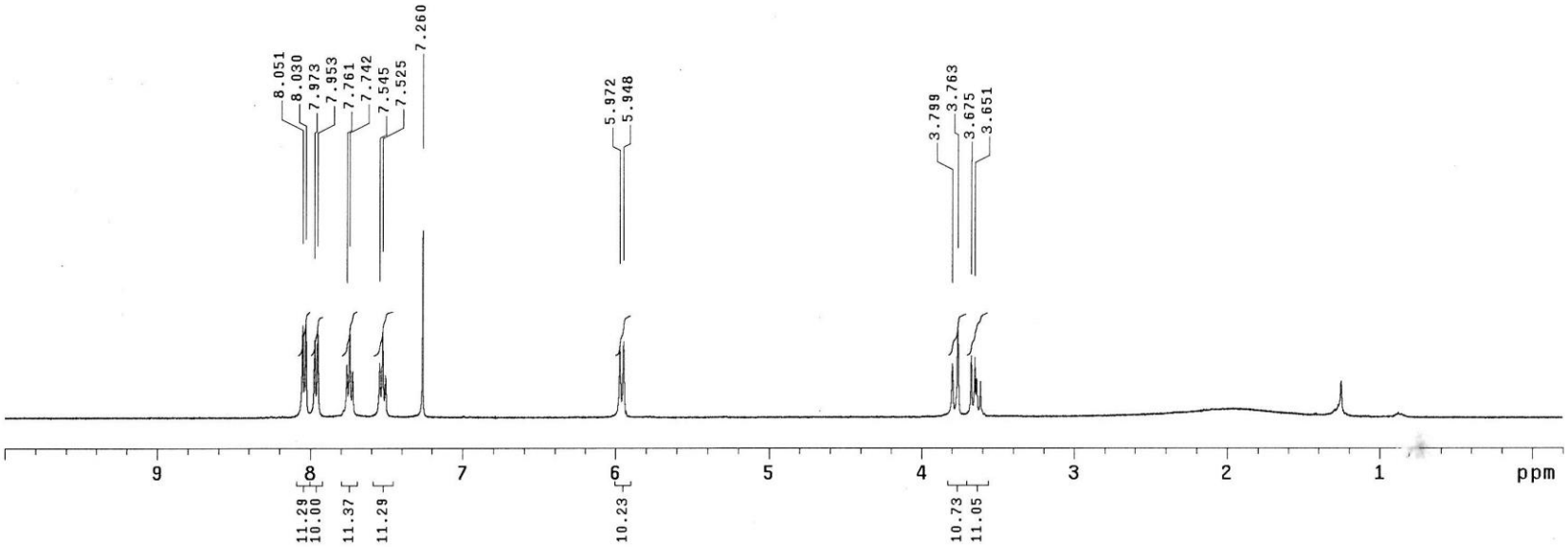
# Compound 8k ($^1$H-NMR spectral data)

ZYS910

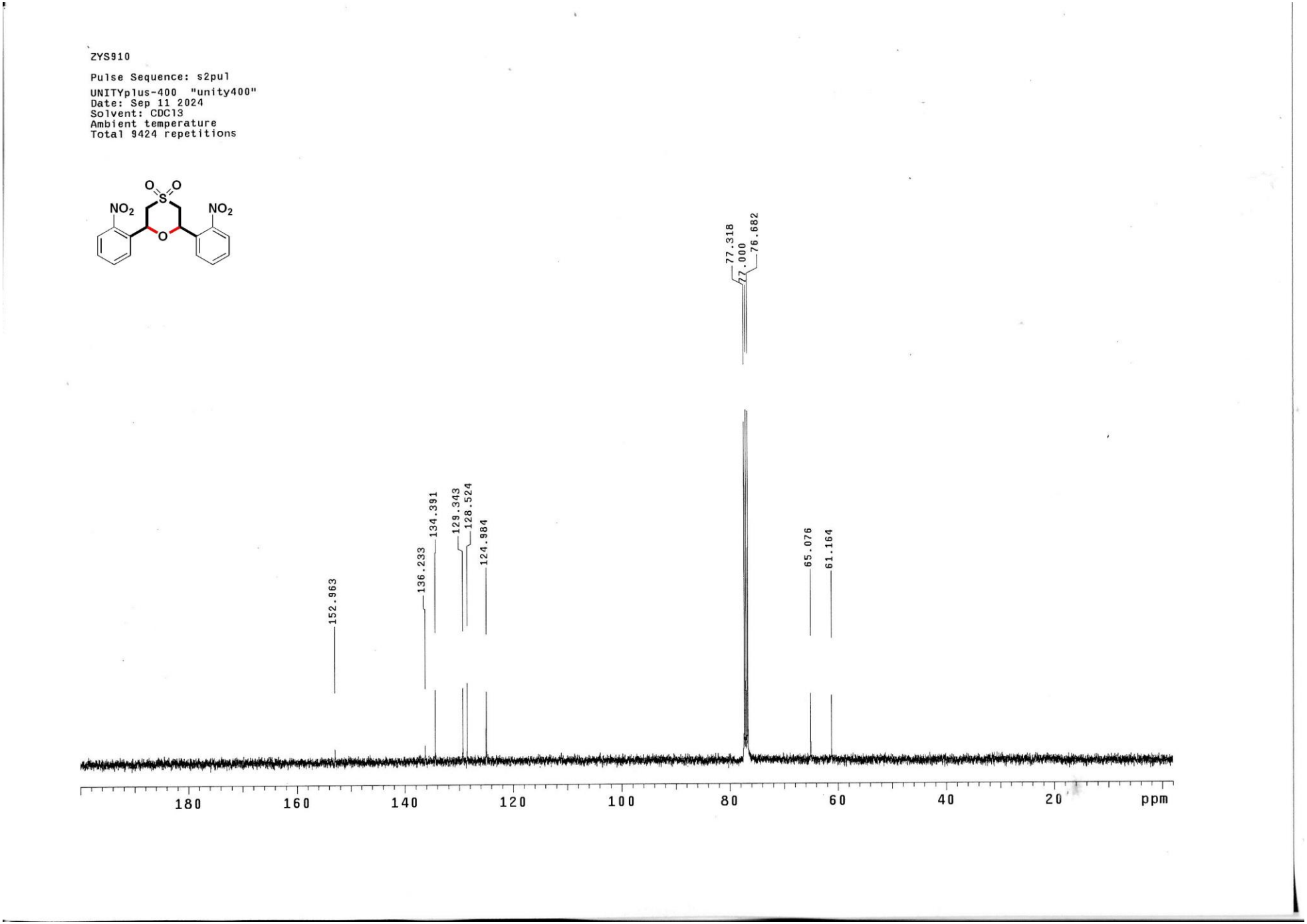
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Sep 11 2024
Solvent: CDCl3
Ambient temperature
Total 64 repetitions

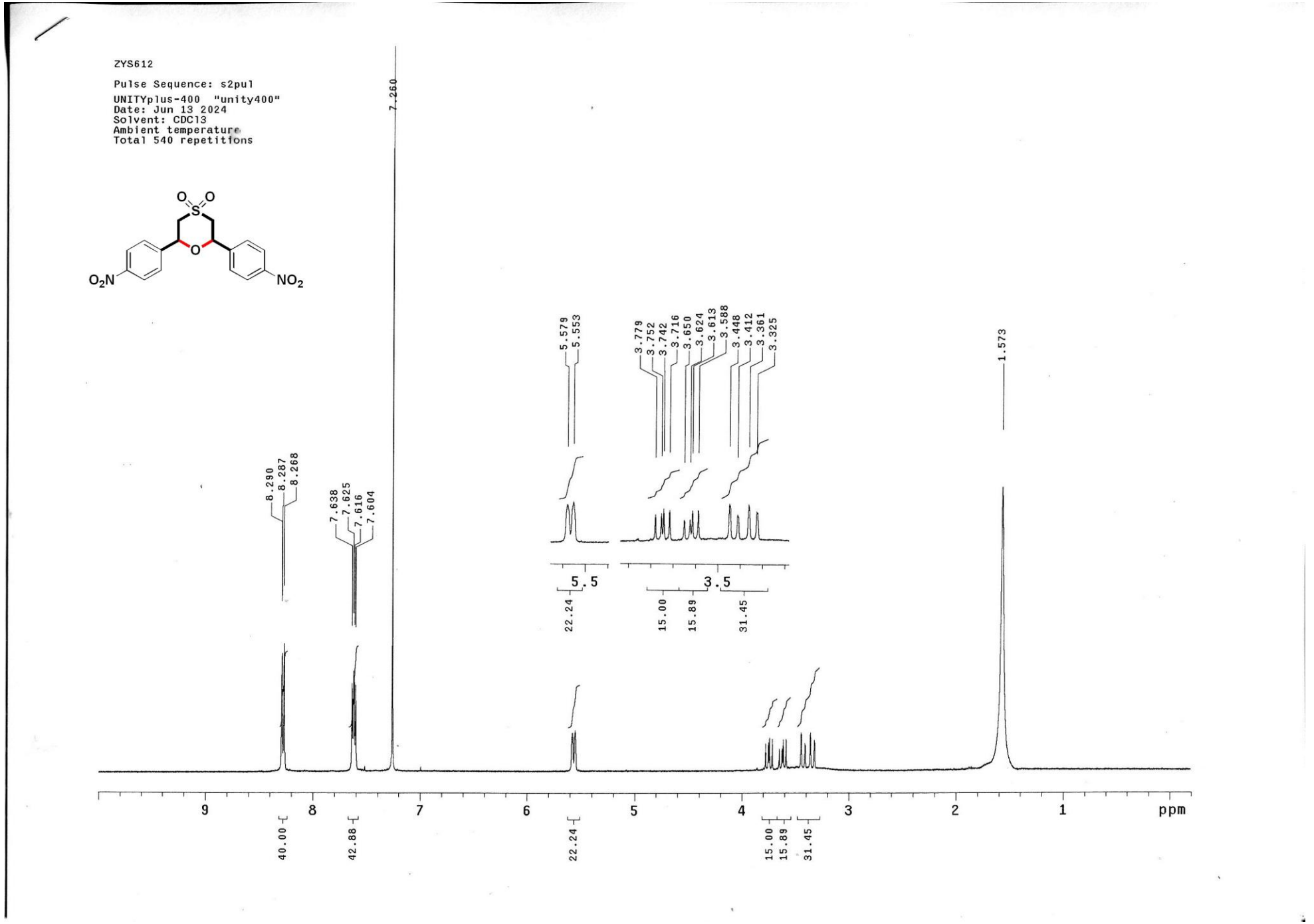



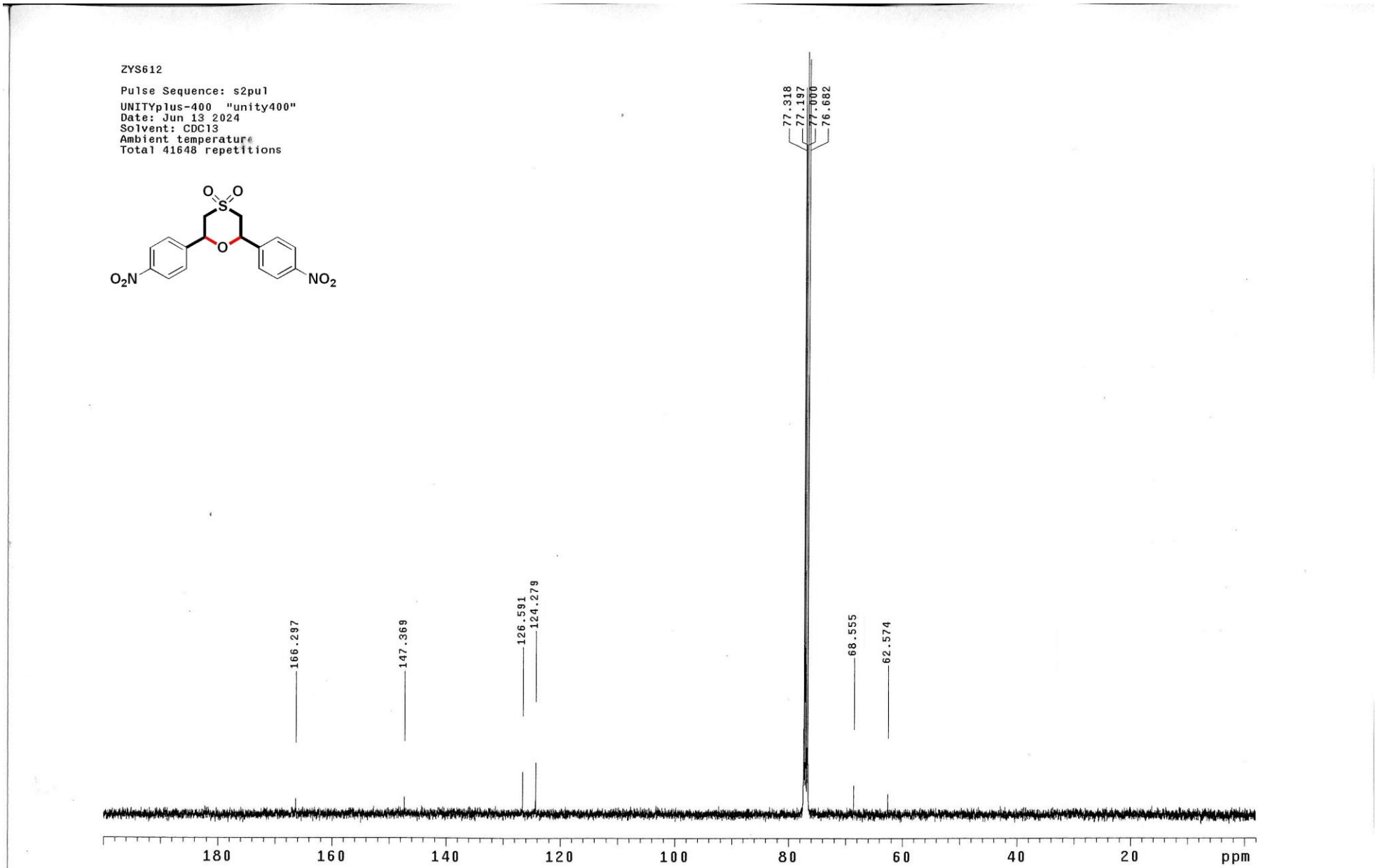
# Compound 8k ($^{13}$C-NMR spectral data)



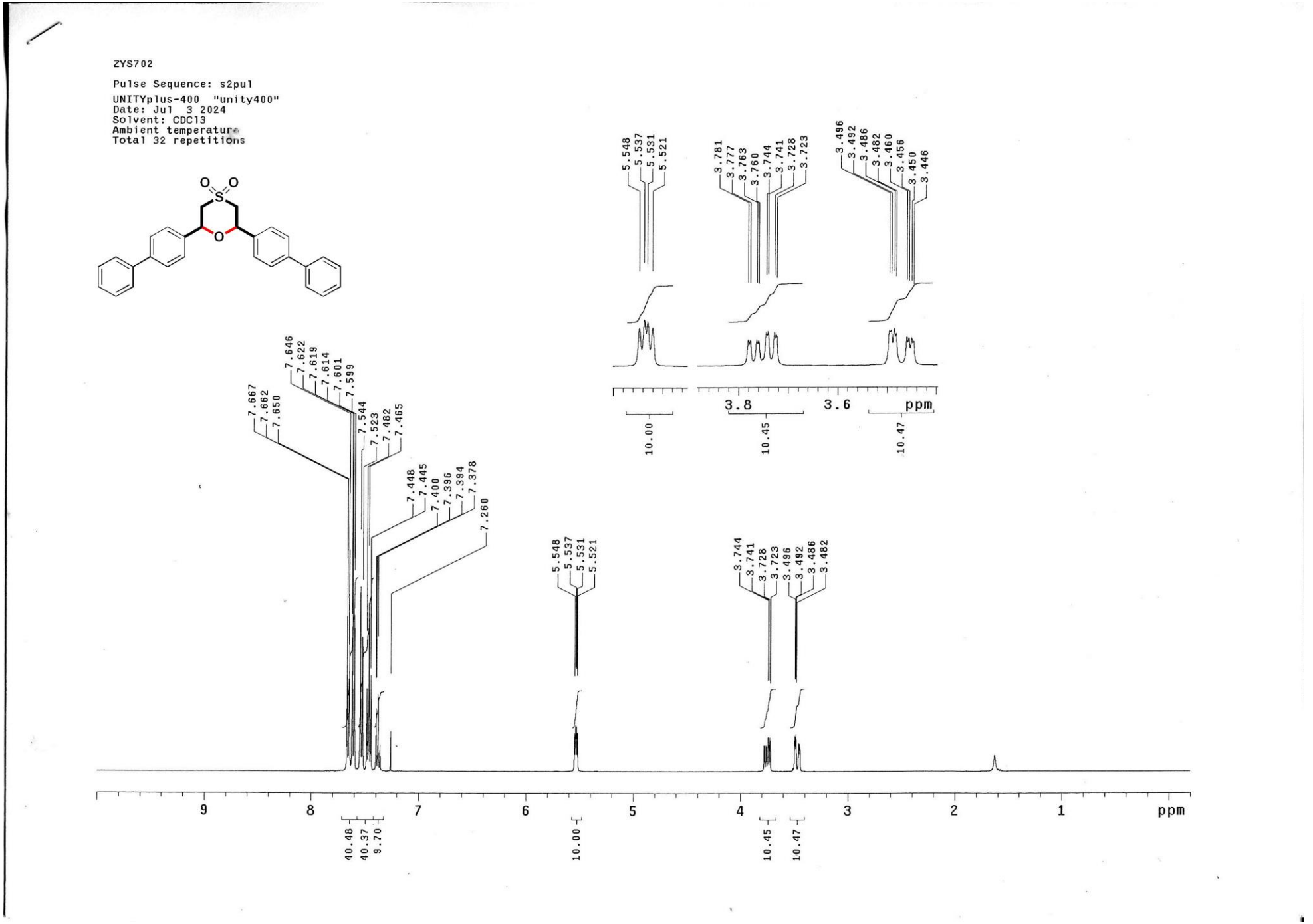
# Compound 8l ($^1$H-NMR spectral data)



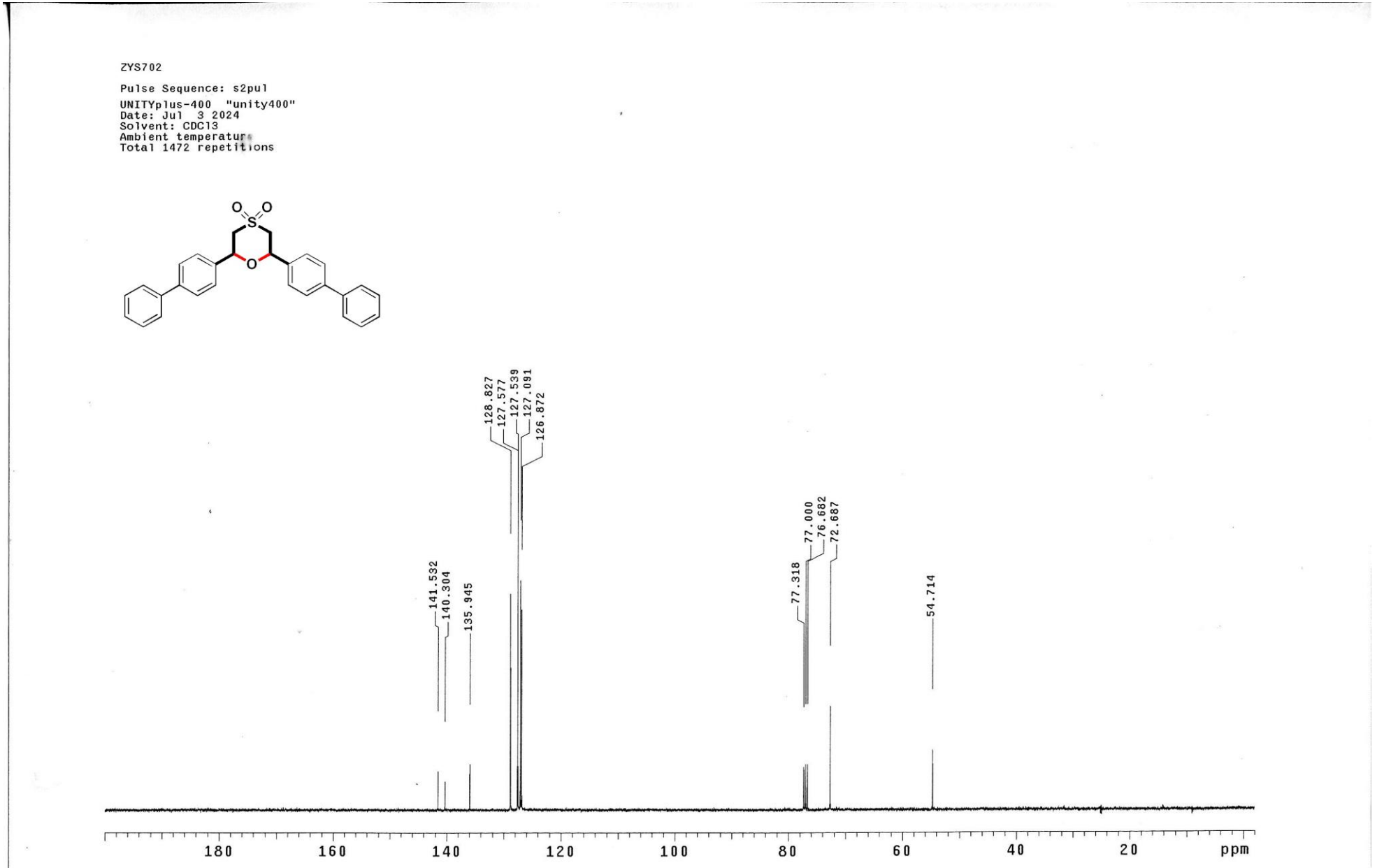
# Compound 8l ($^{13}$C-NMR spectral data)



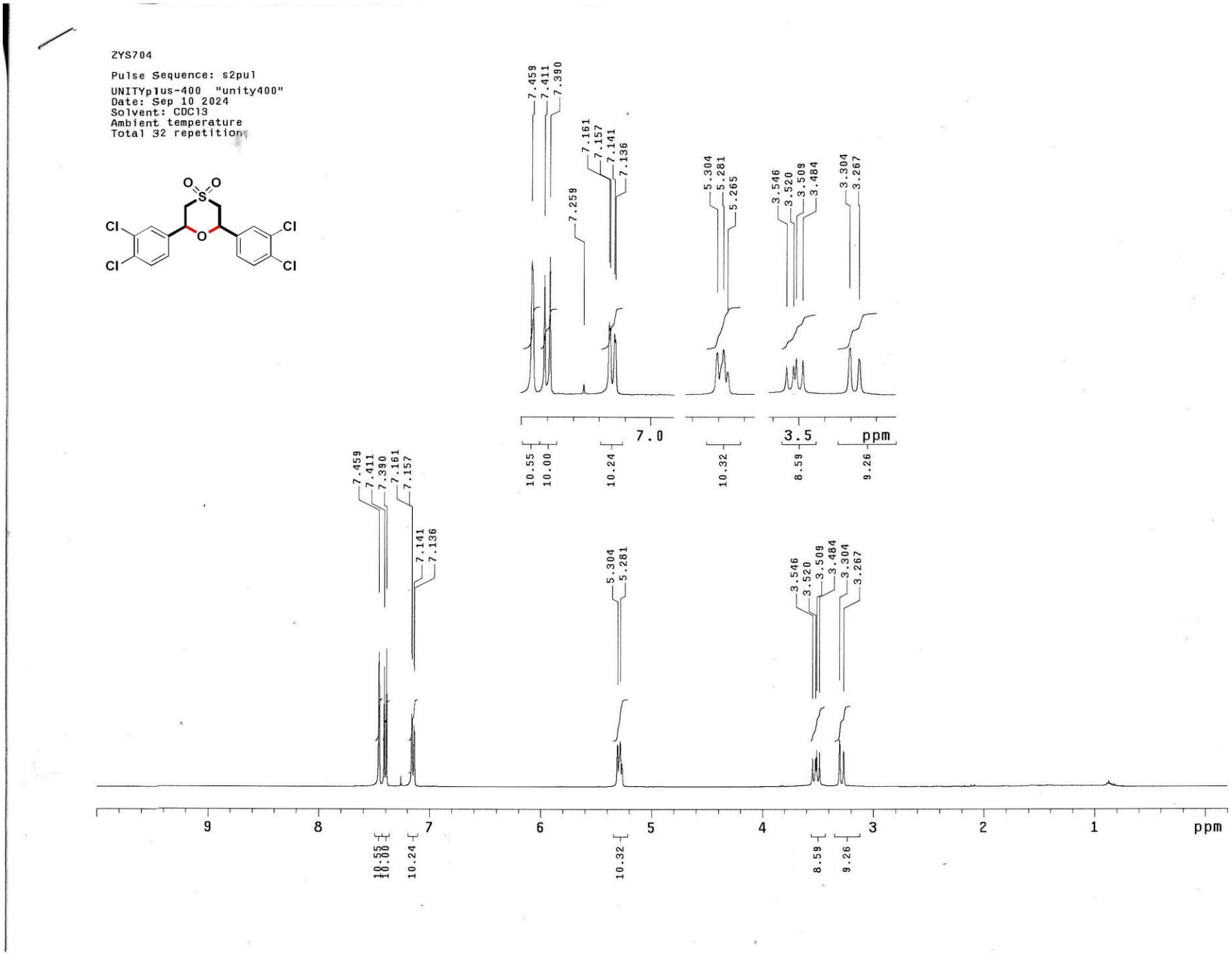
# Compound 8m ($^1$H-NMR spectral data)



# Compound 8m ($^{13}$C-NMR spectral data)



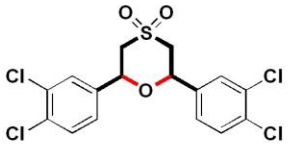
# Compound 8n ($^1$H-NMR spectral data)

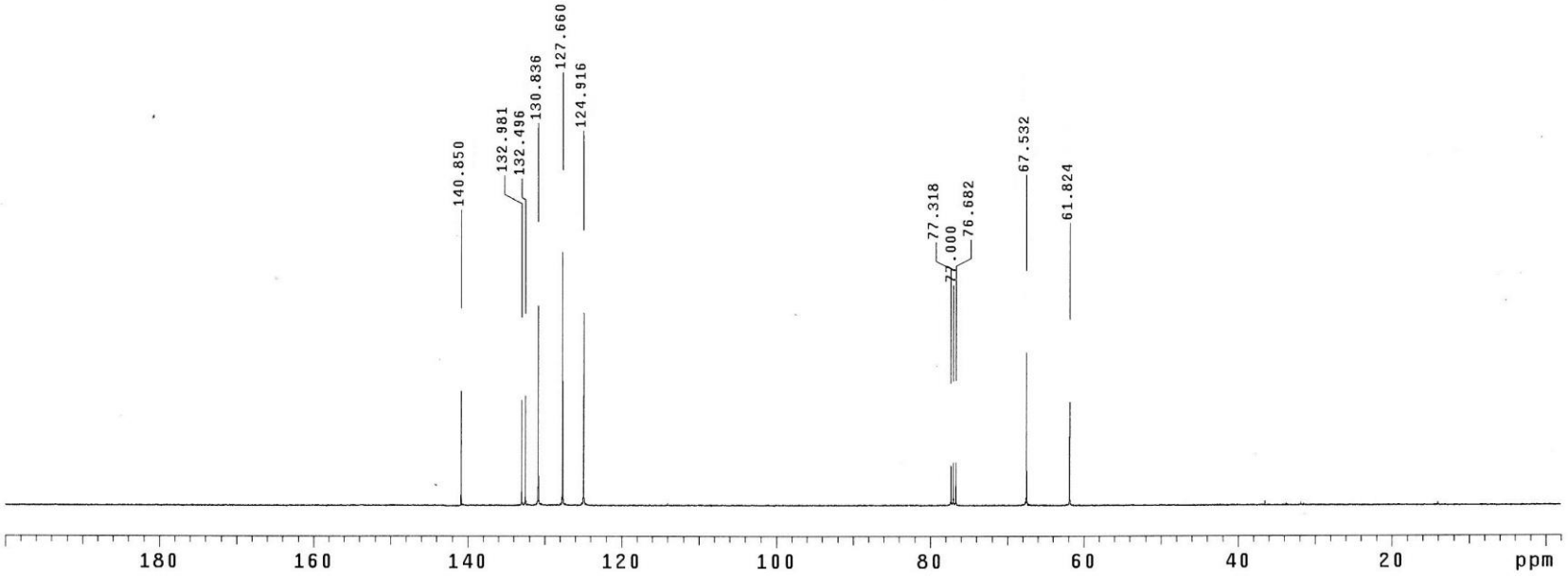


# Compound 8n ($^{13}$C-NMR spectral data)

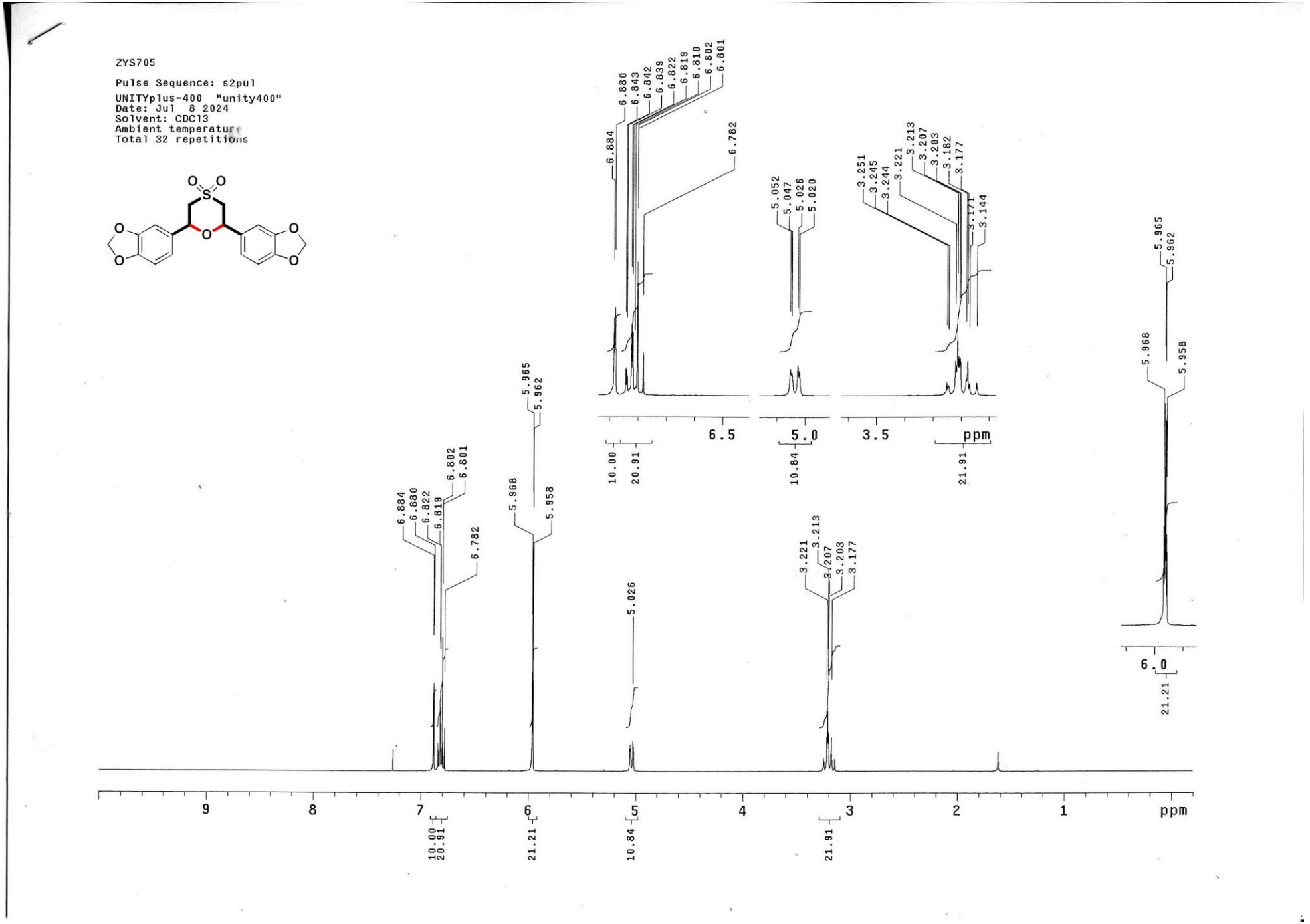
ZYS704

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Sep 10 2024
Solvent: CDCl3
Ambient temperature
Total 64000 repetitions



# Compound 8o ($^1$H-NMR spectral data)

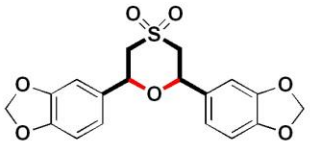


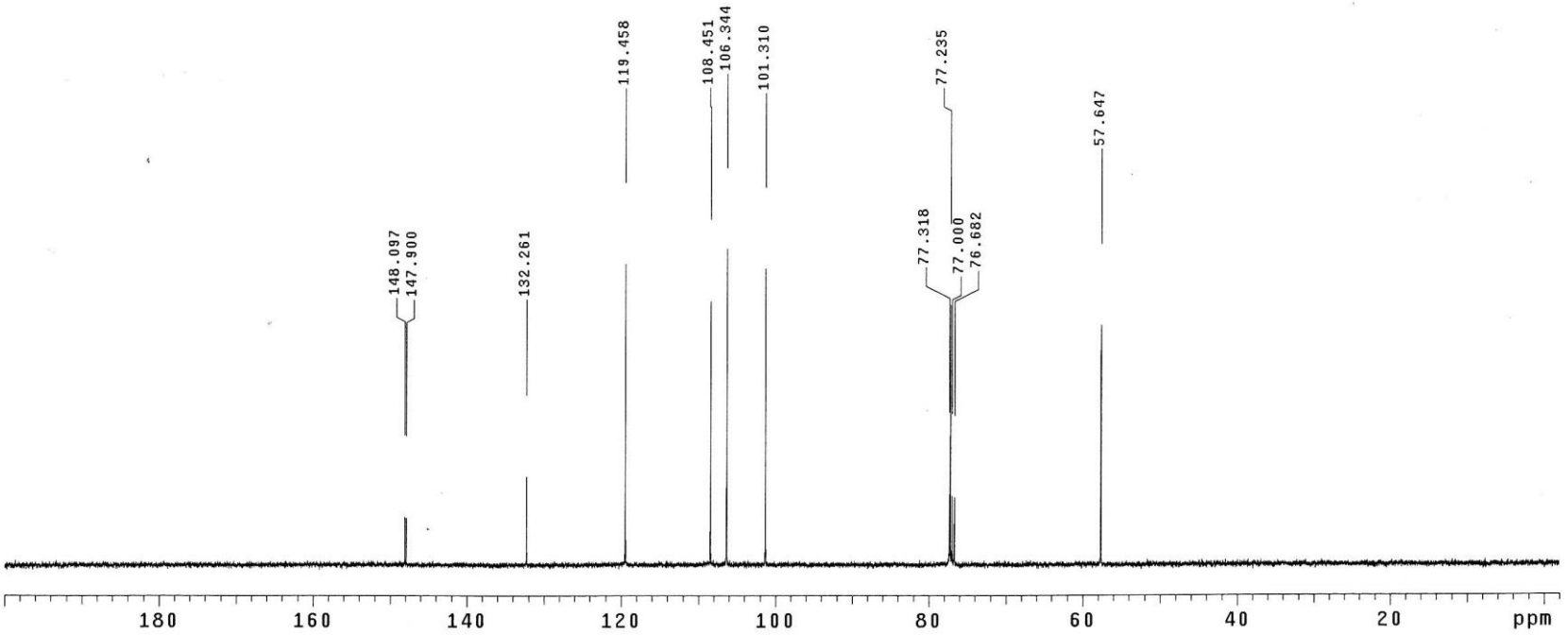
# Compound 8o ($^{13}$C-NMR spectral data)

ZYS705

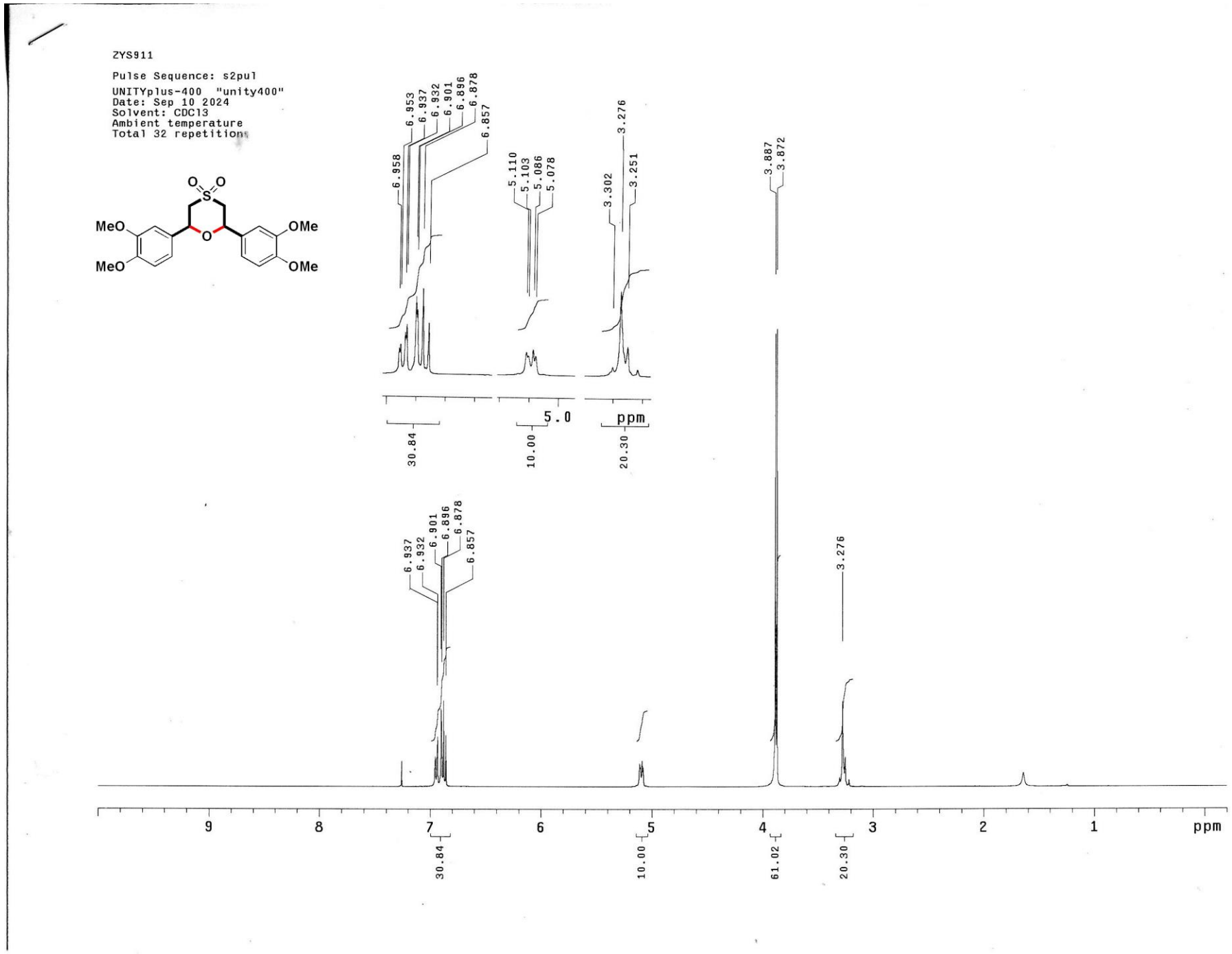
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jul 8 2024
Solvent: CDCl3
Ambient temperature
Total 1376 repetitions





# Compound 8p ($^1$H-NMR spectral data)

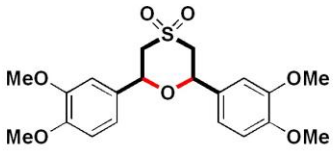


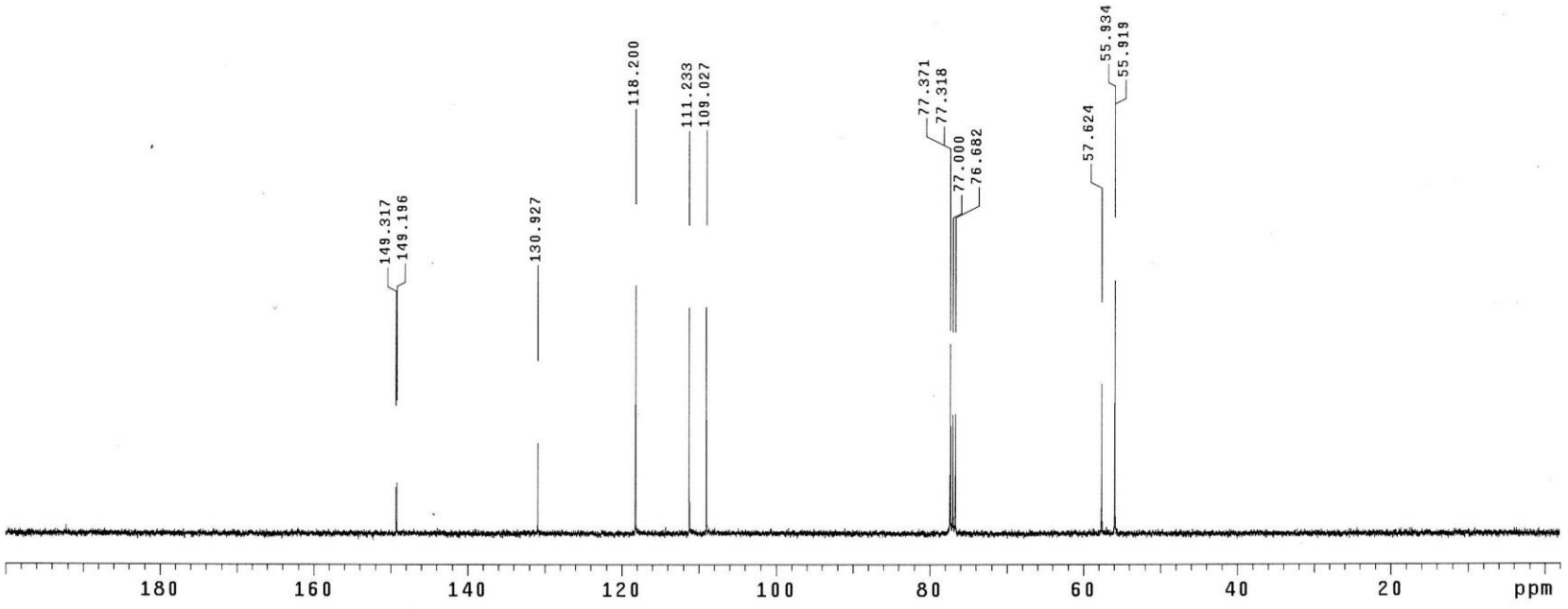
# Compound 8p ($^{13}$C-NMR spectral data)

ZYS911

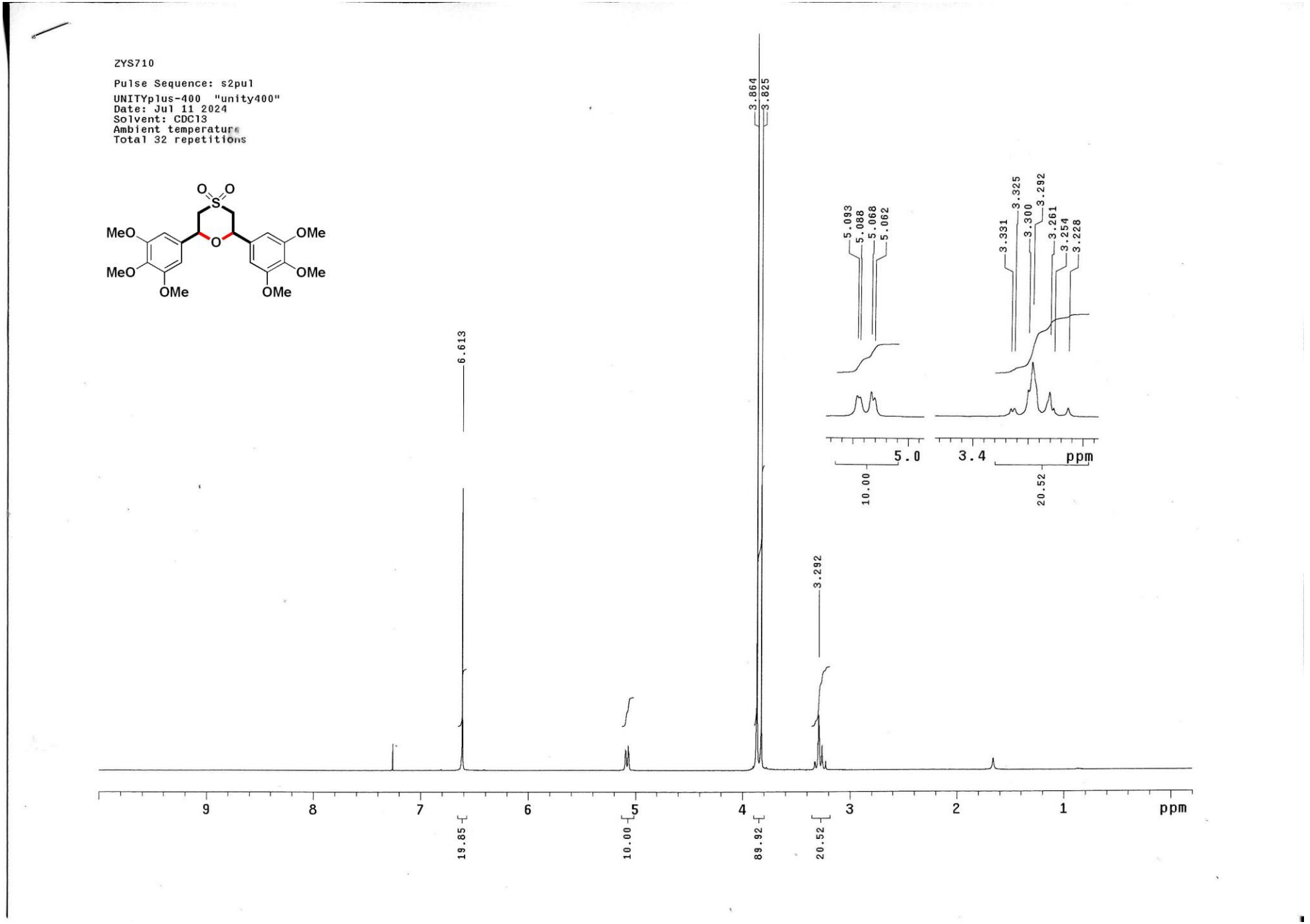
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Sep 10 2024
Solvent: CDCl3
Ambient temperature
Total 1312 repetitions



# Compound 8q ($^1$H-NMR spectral data)

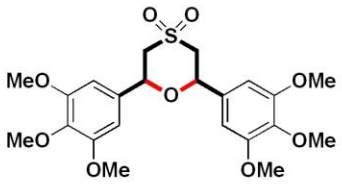


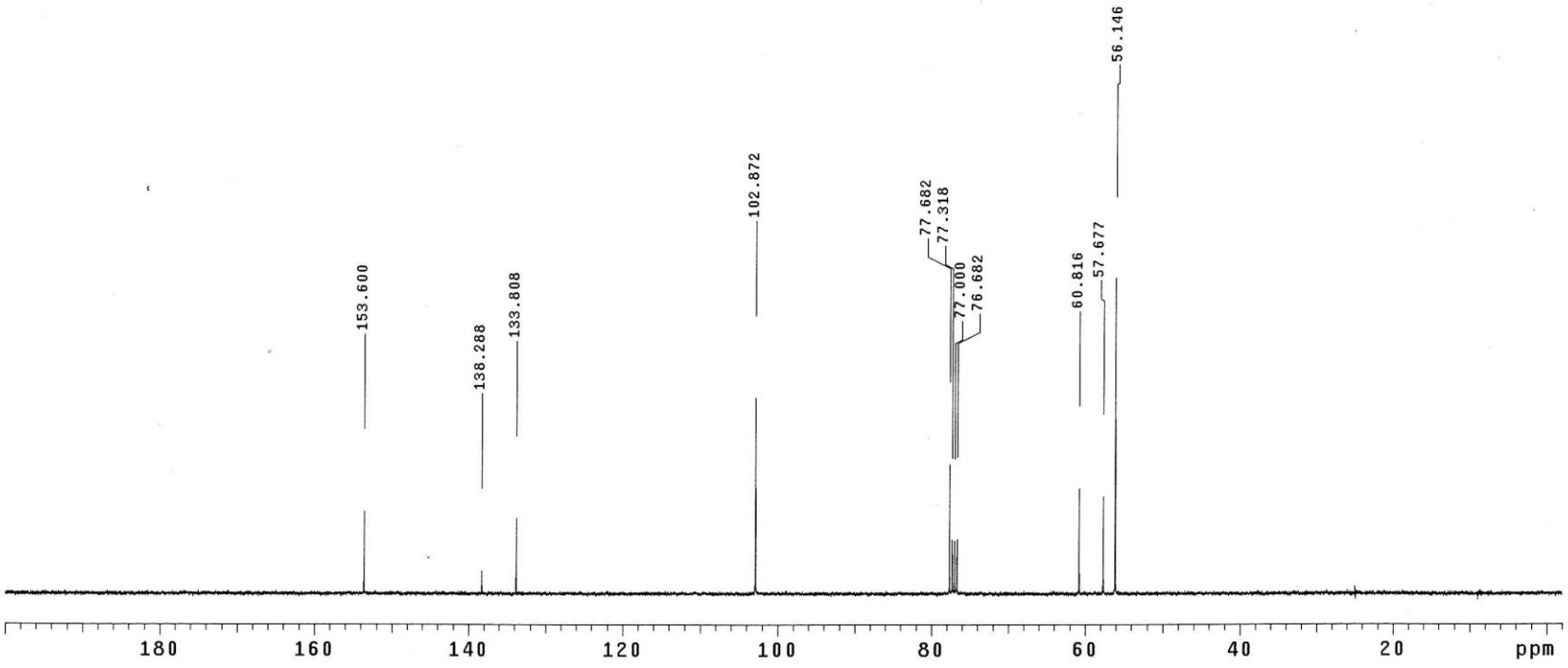
# Compound 8q ($^{13}$C-NMR spectral data)

ZYS710

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jul 11 2024
Solvent: CDCl3
Ambient temperature
Total 2384 repetitions



# Compound 8r ($^1$H-NMR spectral data)

ZYS719

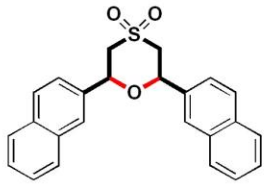
Sample Name:

Data Collected on:
agilentnmr-vnmrs600
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 29 2024



# Compound 8r ($^{13}$C-NMR spectral data)

ZYS719

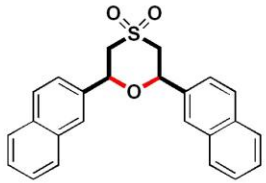
Sample Name:

Data Collected on:
agilentnmr-vnmrs600
Archive directory:

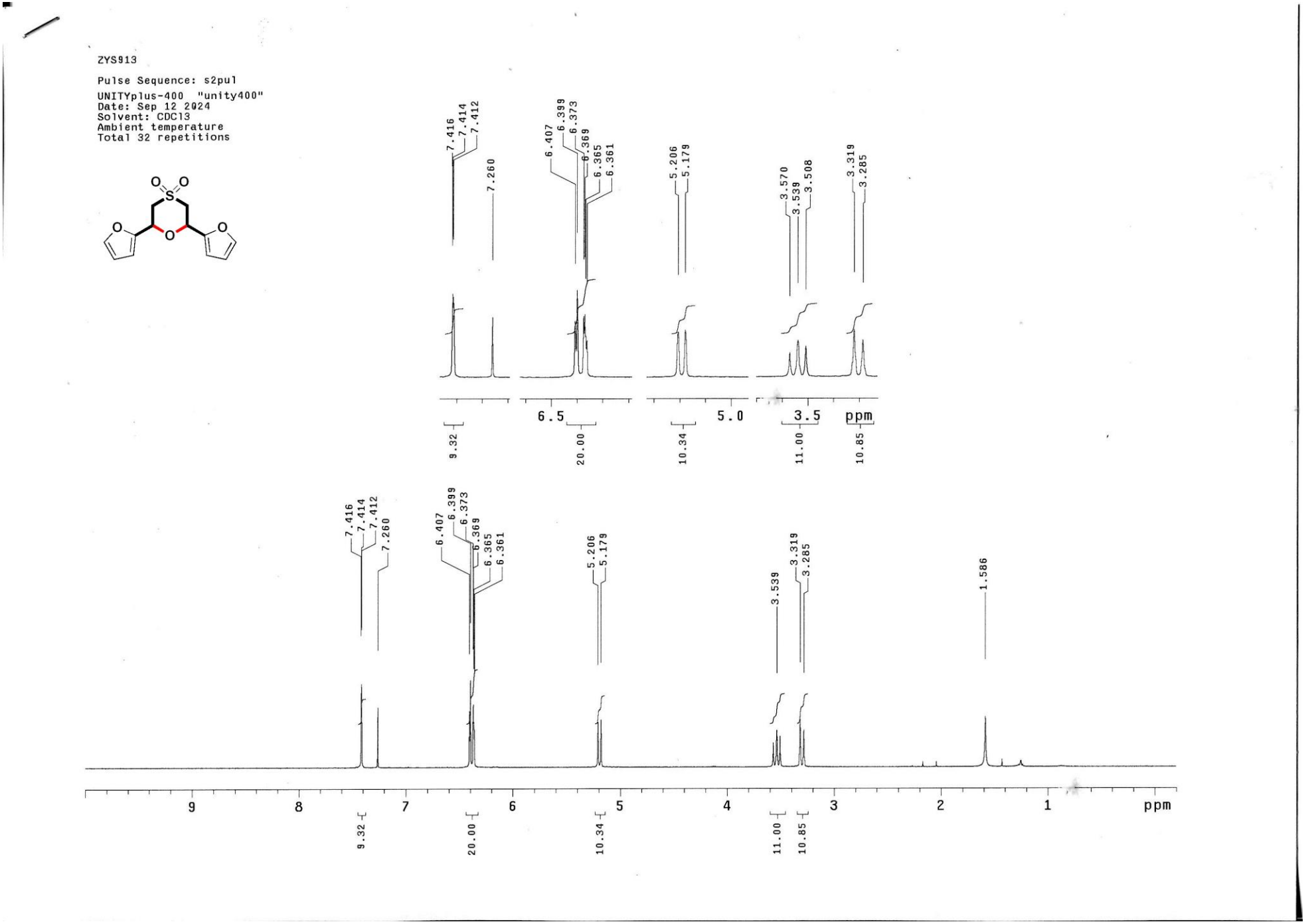
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: CDCl3
Data collected on: Jul 29 2024



# Compound 8s ($^1$H-NMR spectral data)

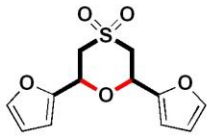


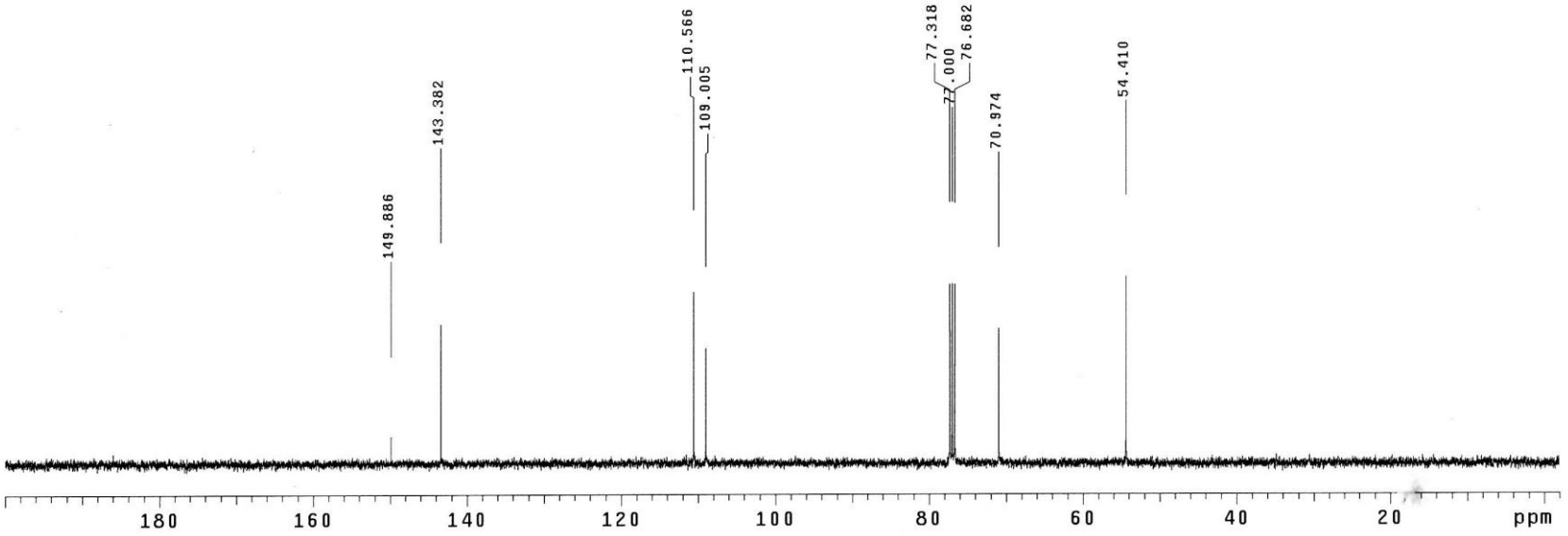
# Compound 8s ($^{13}$C-NMR spectral data)

ZYS913

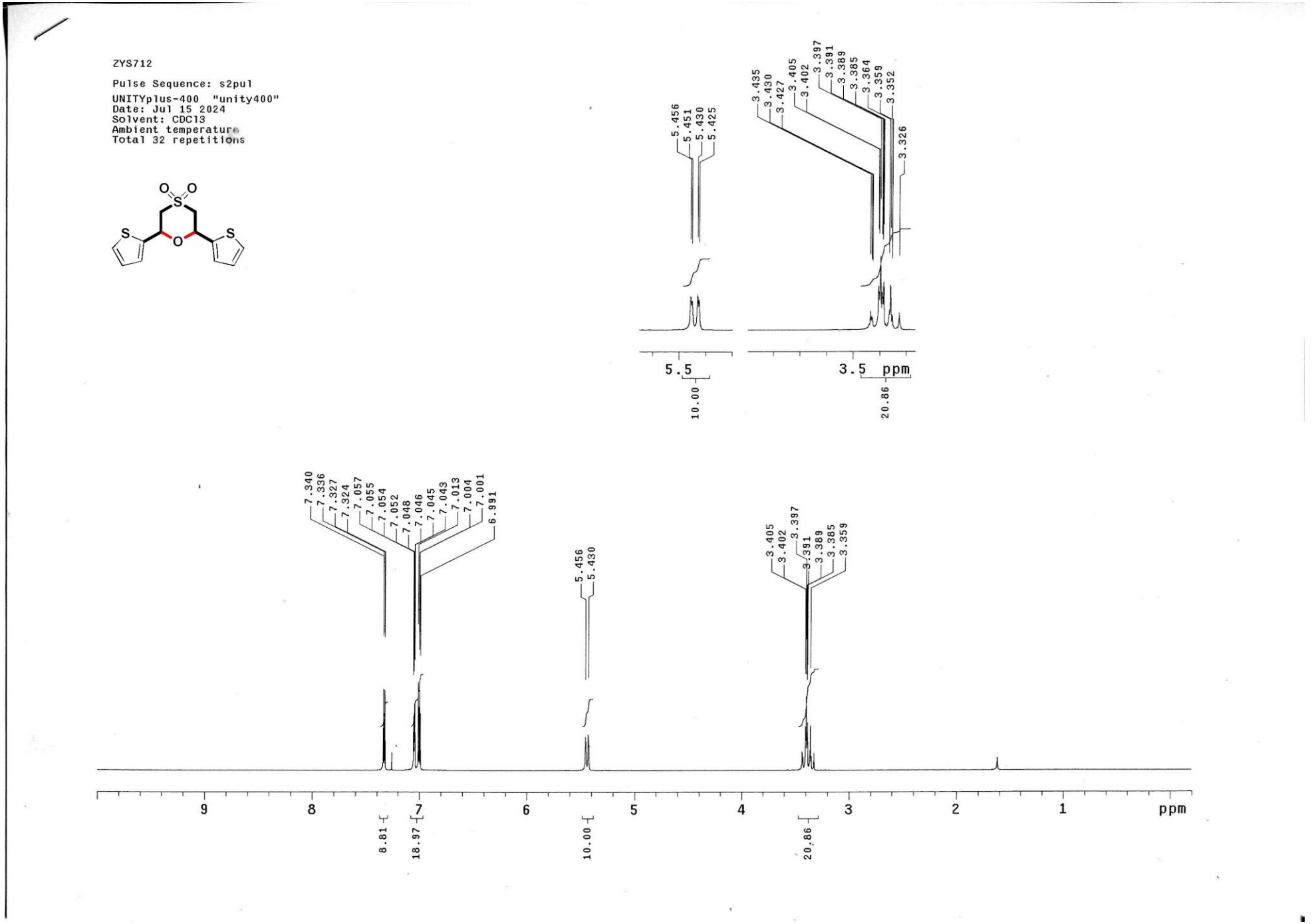
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Sep 12 2024
Solvent: CDCl3
Ambient temperature
Total 1504 repetitions





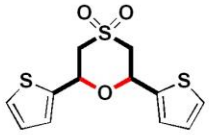
# Compound 8t ($^1$H-NMR spectral data)

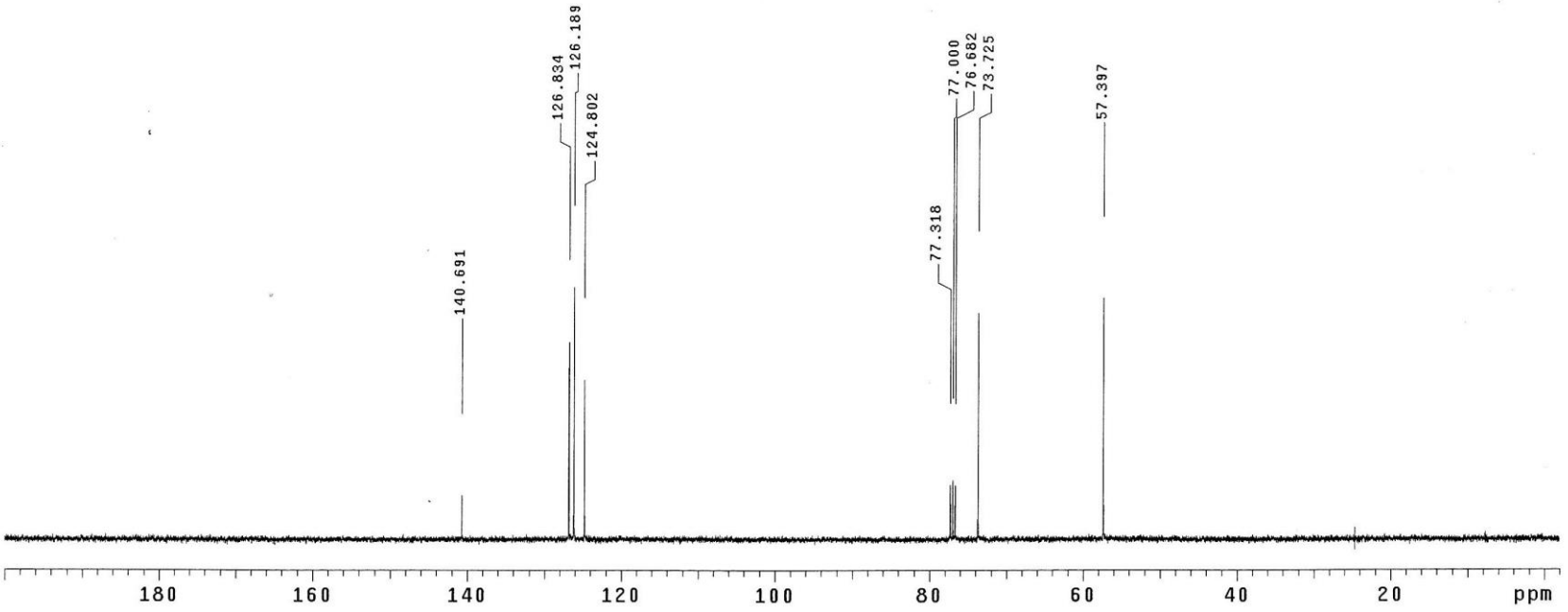


# Compound 8t ($^{13}$C-NMR spectral data)

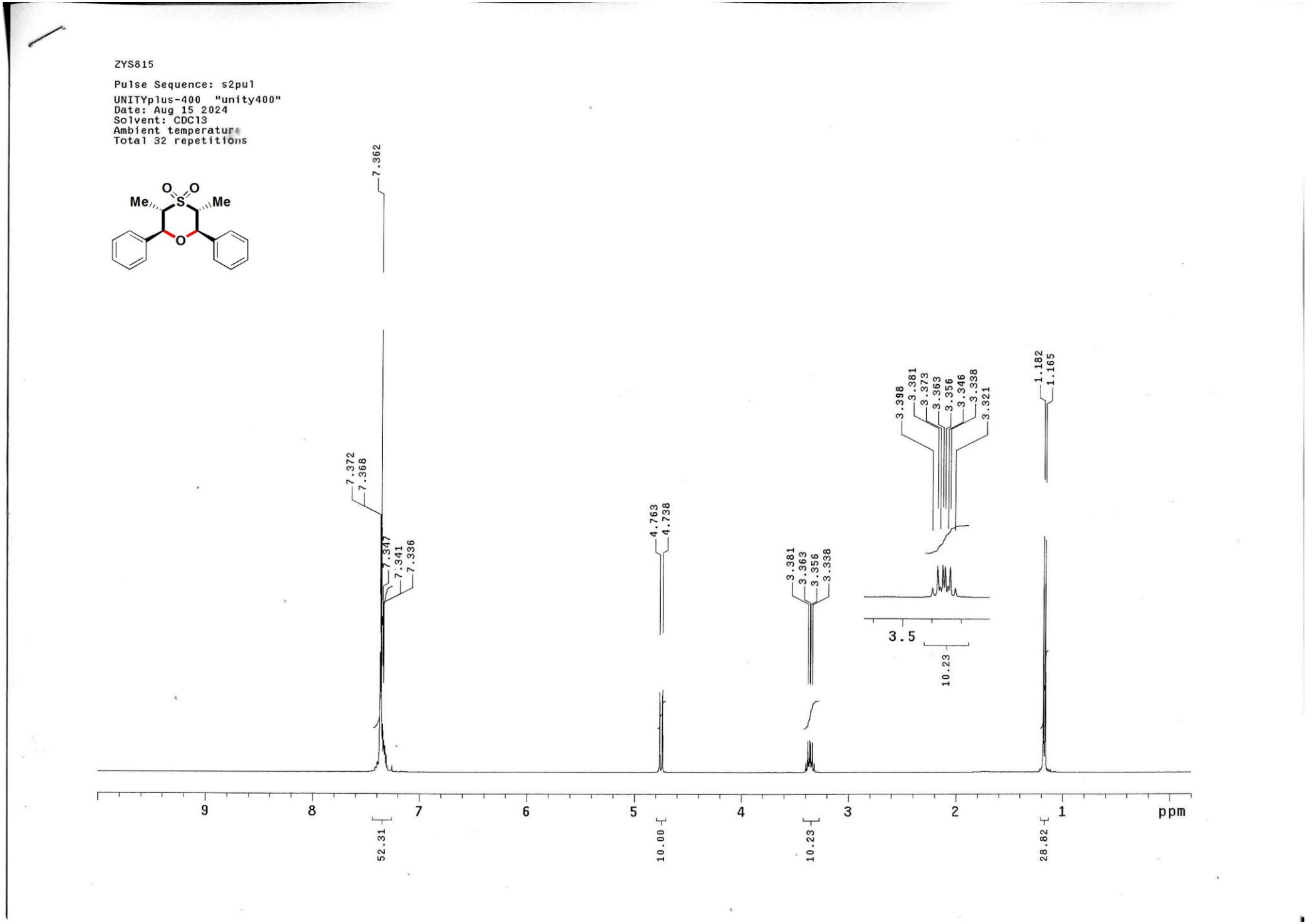
ZYS712

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Jul 15 2024
Solvent: CDCl3
Ambient temperature
Total 544 repetitions



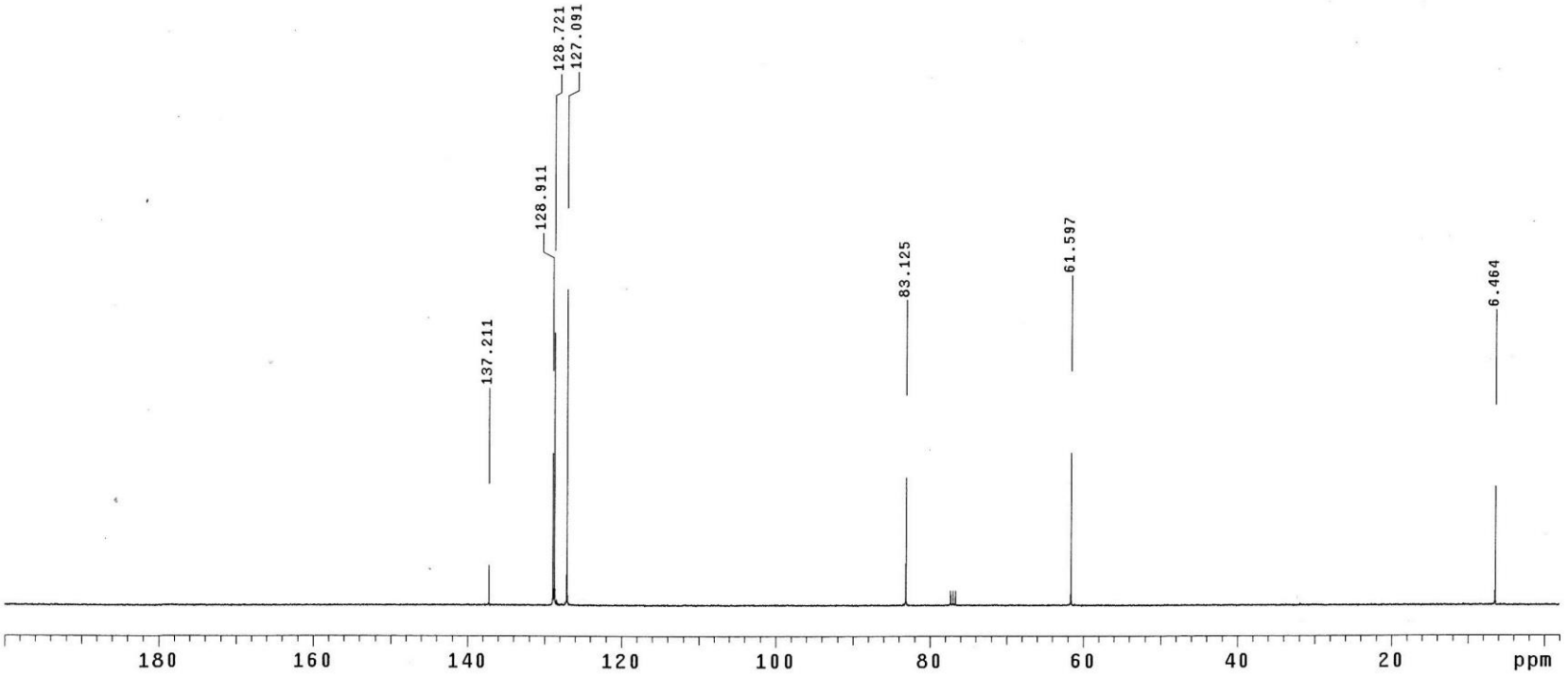
# Compound 8u ($^1$H-NMR spectral data)



# Compound 8u ($^{13}$C-NMR spectral data)

ZYS815

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Aug 15 2024
Solvent: CDCl3
Ambient temperature
Total 720 repetitions

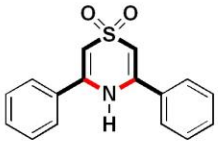



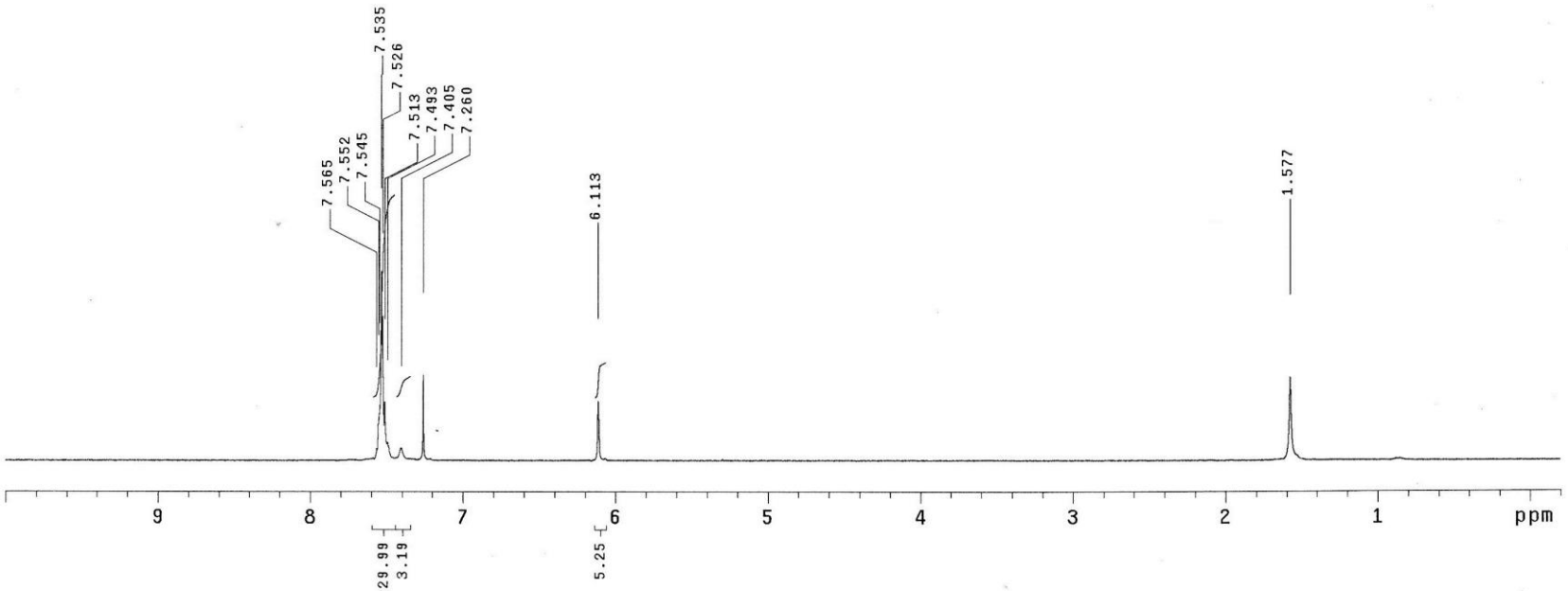
# Compound 9 ($^1$H-NMR spectral data)

YNN9296

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Aug 7 2023
Solvent: CDCl3
Ambient temperature
Total 32 repetitions



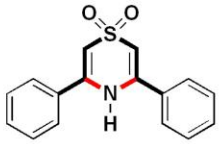



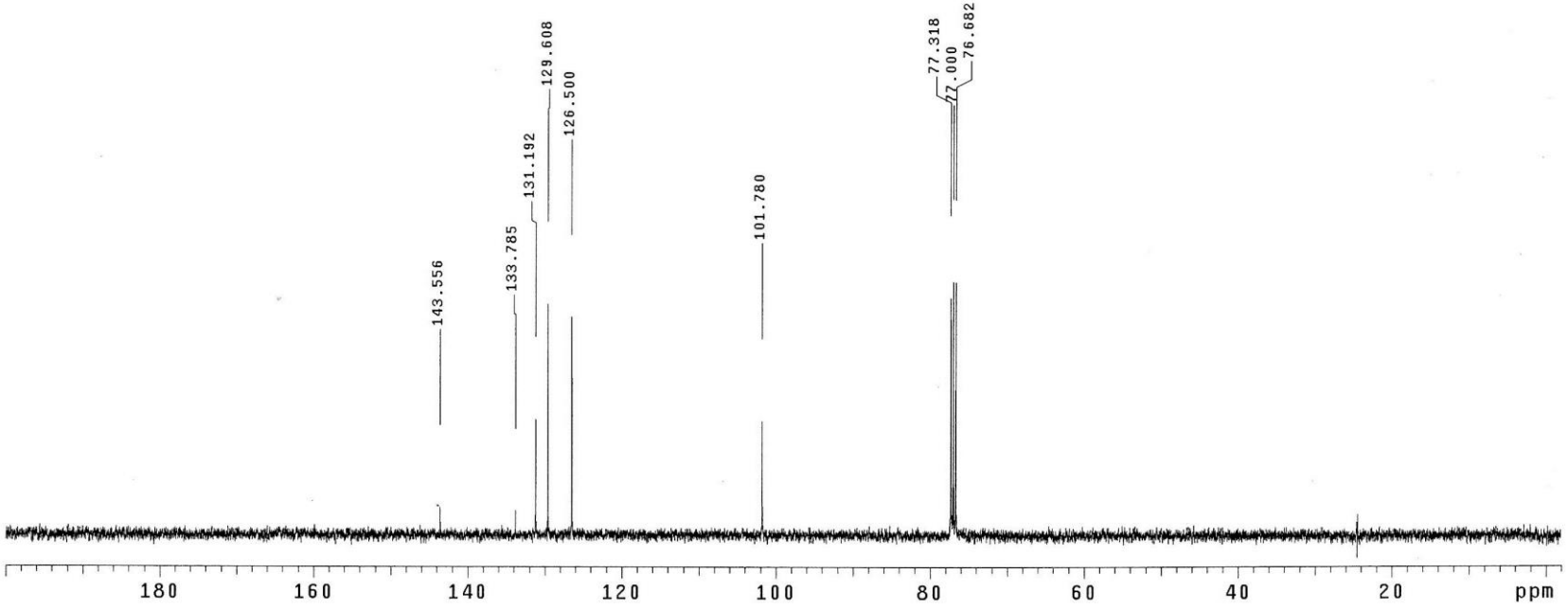
# Compound 9 ($^{13}$C-NMR spectral data)

YNN9296

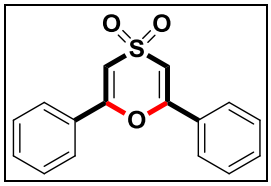
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Aug 7 2023
Solvent: CDCl3
Ambient temperature
Total 4800 repetitions



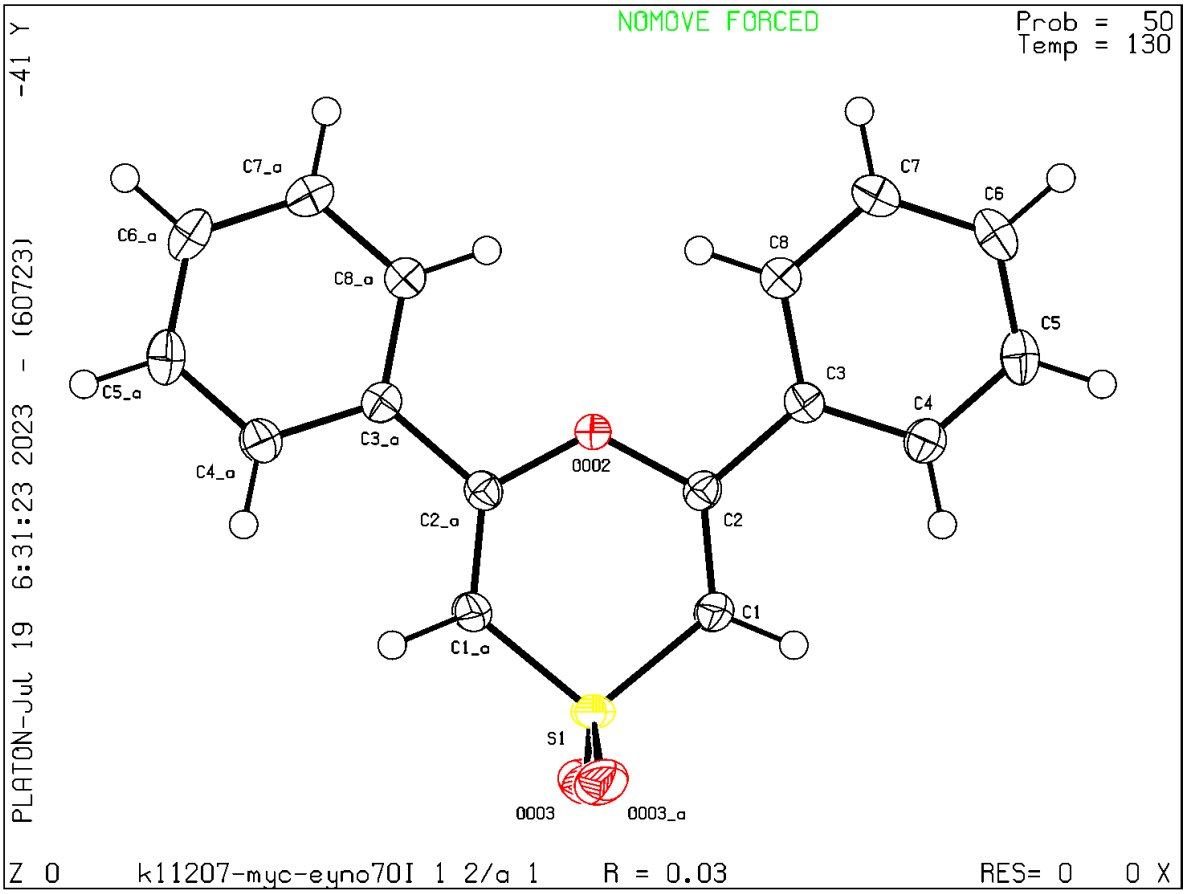



# X-ray crystal data of compound 6a



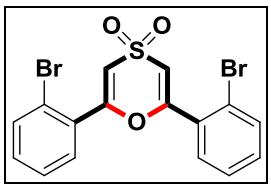

**Sample preparation** : A solution of compound **6a** (10 mg) in $CH_2Cl_2$ (10 mL) was placed in a tube (10 mL). EtOAc (2 mL) was added slowly to the vial with a dropper. The vial was closed with little cotton and kept at room temperature for 2 days. Then, colorless prisms were observed.

**Crystal measurement** : X-ray crystal structures were determined with a Bruker Enraf-Nonius single-crystal diffractometer (CAD4, Kappa CCD). Thermal ellipsoids are drawn at 50% probability level.



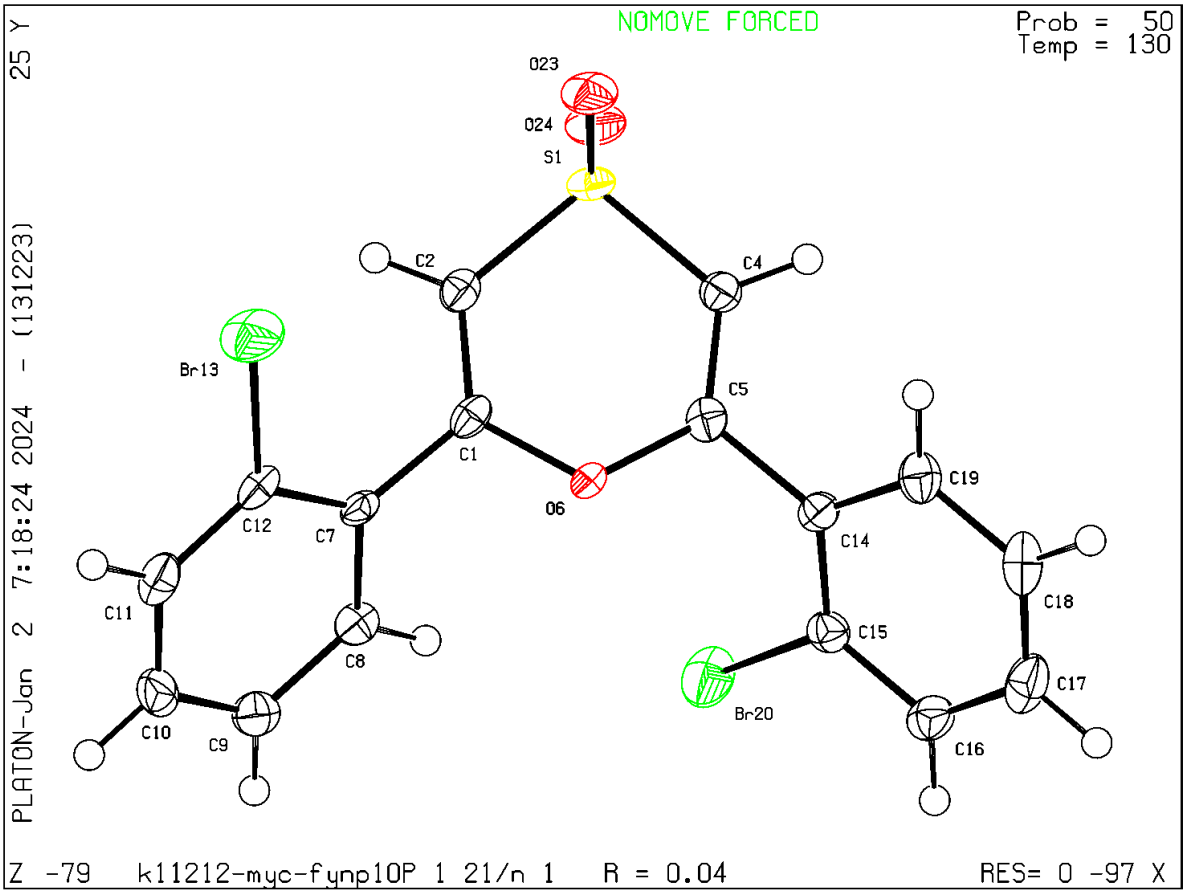
| | |
|---|---|
| Temperature/K | 130(2) |
| Crystal system | monoclinic |
| Space group | I2/a |
| a/Å | 10.1345(3) |
| b/Å | 8.3361(3) |
| c/Å | 15.3383(4) |
| α/° | 90 |
| β/° | 93.540(3) |
| γ/° | 90 |
| Volume/Å $^3$ | 1293.34(7) |
| Z | 8 |
| $\rho_{calc}$g/cm$^3$ | 1.460 |
| μ/mm$^{-1}$ | 0.254 |
| F(000) | 592.0 |
| Crystal size/mm$^3$ | 0.5 × 0.4 × 0.4 |
| Radiation | Mo Kα (λ = 0.71073) |
| 2Θ range for data collection/° | 5.322 to 54.284 |
| Index ranges | -12 ≤ h ≤ 12, -10 ≤ k ≤ 10, -19 ≤ l ≤ 19 |
| Reflections collected | 15060 |
| Independent reflections | 1377 [$R_{int}$ = 0.0486, $R_{sigma}$ = 0.0224] |
| Data/restraints/parameters | 1377/0/92 |
| Goodness-of-fit on F$^2$ | 1.061 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0338, w$R_2$ = 0.0882 |
| Final R indexes [all data] | $R_1$ = 0.0361, w$R_2$ = 0.0897 |
| Largest diff. peak/hole / e Å $^{-3}$ | 0.20/-0.40 |

# X-ray crystal data of compound 6e



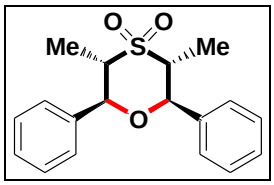

**Sample preparation** : A solution of compound **6e** (10 mg) in $CH_2Cl_2$ (10 mL) was placed in a tube (10 mL). EtOAc (2 mL) was added slowly to the vial with a dropper. The vial was closed with little cotton and kept at room temperature for 2 days. Then, colorless prisms were observed.

**Crystal measurement** : X-ray crystal structures were determined with a Bruker Enraf-Nonius single-crystal diffractometer (CAD4, Kappa CCD). Thermal ellipsoids are drawn at 50% probability level.



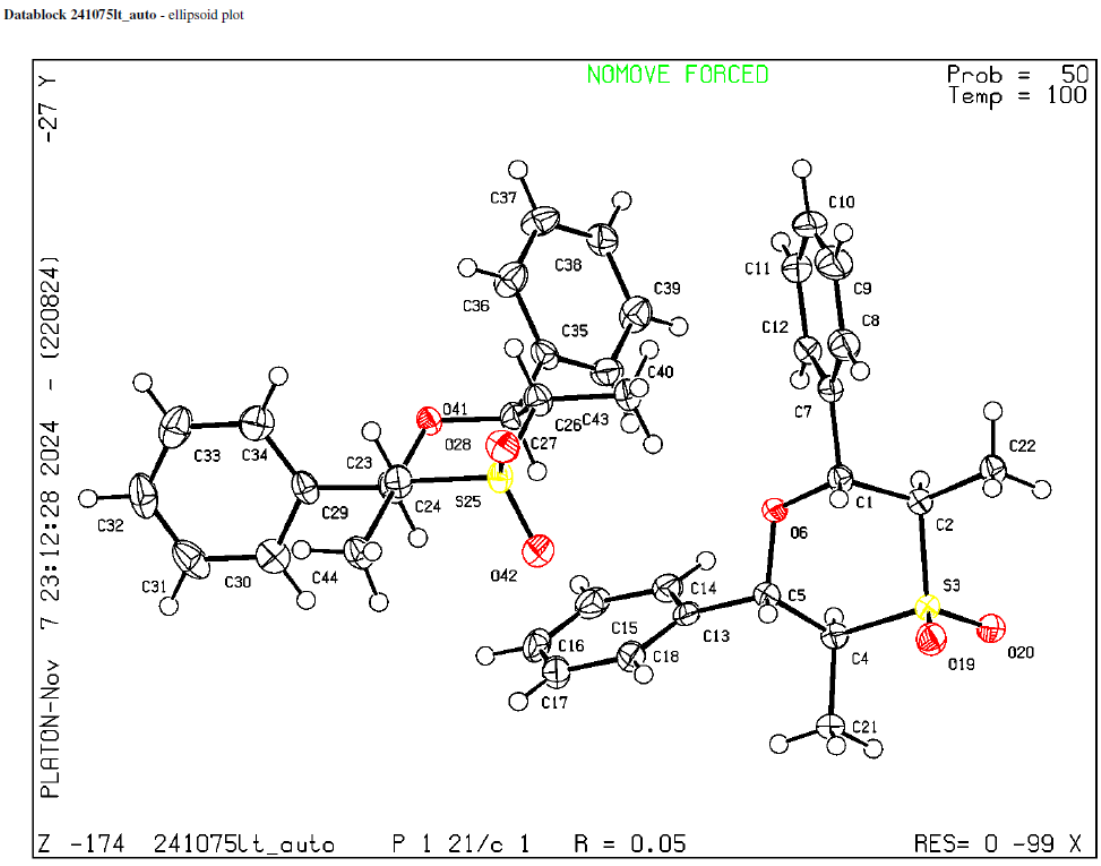
| | |
|---|---|
| Empirical formula | $C_{16}H_{10}Br_2O_3S$ |
| Formula weight | 442.12 |
| Temperature/K | 130(2) |
| Crystal system | monoclinic |
| Space group | $P2_1/n$ |
| a/Å | 8.4471(3) |
| b/Å | 10.9120(4) |
| c/Å | 17.0111(6) |
| α/° | 90 |
| β/° | 101.652(4) |
| γ/° | 90 |
| Volume/Å $^3$ | 1535.68(10) |
| Z | 4 |
| $\rho_{calc}$g/cm$^3$ | 1.912 |
| μ/mm$^{-1}$ | 5.423 |
| F(000) | 864.0 |
| Crystal size/mm$^3$ | 0.4 × 0.4 × 0.2 |
| Radiation | Mo Kα (λ = 0.71073) |
| 2Θ range for data collection/° | 4.462 to 54.25 |
| Index ranges | $-10 \leq h \leq 10$, $-13 \leq k \leq 13$, $-21 \leq l \leq 21$ |
| Reflections collected | 17704 |
| Independent reflections | 3230 [$R_{int}$ = 0.0467, $R_{sigma}$ = 0.0419] |
| Data/restraints/parameters | 3230/0/199 |
| Goodness-of-fit on $F^2$ | 1.079 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0432, $wR_2$ = 0.0940 |
| Final R indexes [all data] | $R_1$ = 0.0601, $wR_2$ = 0.0994 |
| Largest diff. peak/hole / e Å $^{-3}$ | 1.60/-0.66 |

# X-ray crystal data of compound 8u



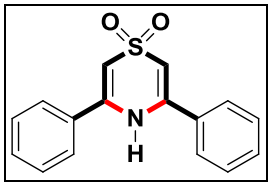

**Sample preparation** : A solution of compound **8u** (10 mg) in $CH_2Cl_2$ (10 mL) was placed in a tube (10 mL). EtOAc (2 mL) was added slowly to the vial with a dropper. The vial was closed with little cotton and kept at room temperature for 2 days. Then, colorless prisms were observed.

**Crystal measurement** : X-ray crystal structures were determined with a Bruker Enraf-Nonius single-crystal diffractometer (CAD4, Kappa CCD). Thermal ellipsoids are drawn at 50% probability level.



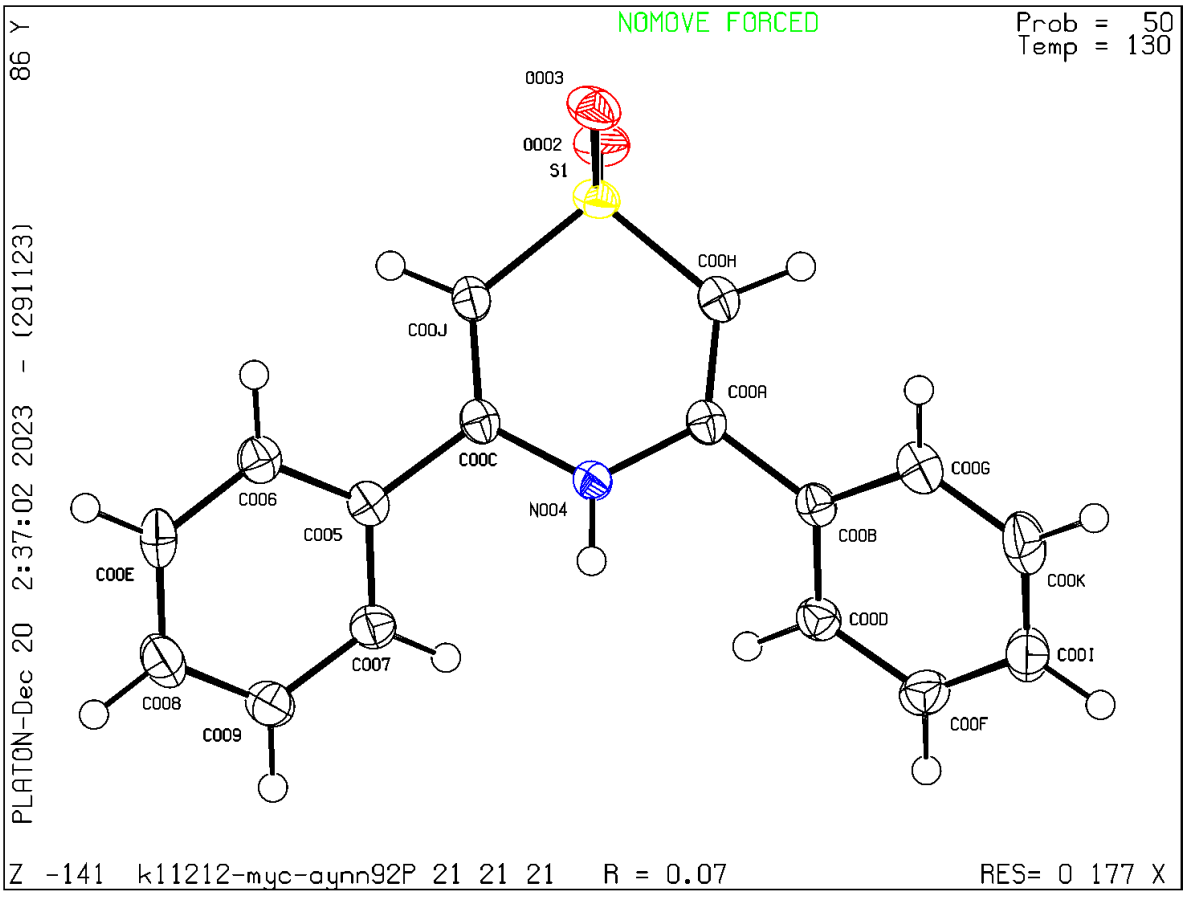
| | |
|---|---|
| Empirical formula | $C_{18}H_{20}O_3S$ |
| Formula weight | 316.40 |
| Temperature/K | 100.00(10) |
| Crystal system | monoclinic |
| Space group | $P2_1/c$ |
| a/Å | 10.49110(10) |
| b/Å | 17.9817(2) |
| c/Å | 17.8130(2) |
| α/° | 90 |
| β/° | 102.3990(10) |
| γ/° | 90 |
| Volume/Å $^3$ | 3282.01(6) |
| Z | 8 |
| $\rho_{calc}$g/cm$^3$ | 1.281 |
| μ/mm$^{-1}$ | 1.831 |
| F(000) | 1344.0 |
| Crystal size/mm$^3$ | 0.09 × 0.07 × 0.06 |
| Radiation | Cu Kα (λ = 1.54184) |
| 2Θ range for data collection/° | 7.07 to 146.2 |
| Index ranges | $-12 \leq h \leq 12$, $-22 \leq k \leq 20$, $-21 \leq l \leq 21$ |
| Reflections collected | 22177 |
| Independent reflections | 6354 [$R_{int}$ = 0.0336, $R_{sigma}$ = 0.0342] |
| Data/restraints/parameters | 6354/0/401 |
| Goodness-of-fit on $F^2$ | 1.049 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0475, $wR_2$ = 0.1201 |
| Final R indexes [all data] | $R_1$ = 0.0548, $wR_2$ = 0.1248 |
| Largest diff. peak/hole / e Å $^{-3}$ | 0.78/-0.59 |

# X-ray crystal data of compound 9




**Sample preparation** : A solution of compound **9** (10 mg) in $CH_2Cl_2$ (10 mL) was placed in a tube (10 mL). EtOAc (2 mL) was added slowly to the vial with a dropper. The vial was closed with little cotton and kept at room temperature for 2 days. Then, colorless prisms were observed.

**Crystal measurement** : X-ray crystal structures were determined with a Bruker Enraf-Nonius single-crystal diffractometer (CAD4, Kappa CCD). Thermal ellipsoids are drawn at 50% probability level.



| | |
|---|---|
| Empirical formula | $C_{16}H_{13}NO_2S$ |
| Formula weight | 283.33 |
| Temperature/K | 130(2) |
| Crystal system | orthorhombic |
| Space group | $P2_12_12_1$ |
| a/Å | 7.3209(4) |
| b/Å | 11.0345(5) |
| c/Å | 16.7334(9) |
| α/° | 90 |
| β/° | 90 |
| γ/° | 90 |
| Volume/Å $^3$ | 1351.77(12) |
| Z | 4 |
| $\rho_{calc}$g/cm$^3$ | 1.392 |
| μ/mm$^{-1}$ | 0.239 |
| F(000) | 592.0 |
| Crystal size/mm$^3$ | 0.2 × 0.2 × 0.1 |
| Radiation | Mo Kα (λ = 0.71073) |
| 2Θ range for data collection/° | 4.868 to 54.188 |
| Index ranges | $-9 \leq h \leq 6$, $-13 \leq k \leq 14$, $-20 \leq l \leq 20$ |
| Reflections collected | 8961 |
| Independent reflections | 2701 [$R_{int}$ = 0.0599, $R_{sigma}$ = 0.0974] |
| Data/restraints/parameters | 2701/96/181 |
| Goodness-of-fit on $F^2$ | 1.133 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0731, $wR_2$ = 0.1183 |
| Final R indexes [all data] | $R_1$ = 0.1090, $wR_2$ = 0.1271 |
| Largest diff. peak/hole / e Å $^{-3}$ | 0.42/-0.49 |
| Flack parameter | 0.01(5) |