

# Supporting Information

## One-pot Synthesis of Symmetrical Bis-sulfonyl 2,6-Diarylpyridines via BiCl<sub>3</sub>-Catalyzed and K<sub>2</sub>S<sub>2</sub>O<sub>8</sub>-Mediated Domino Annulation of $\beta$ -Ketosulfones and *N,N*-Dimethylacetamide

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# Compound 4a (<sup>1</sup>H-NMR spectral data)

YCM1319

Pulse Sequence: s2pu1

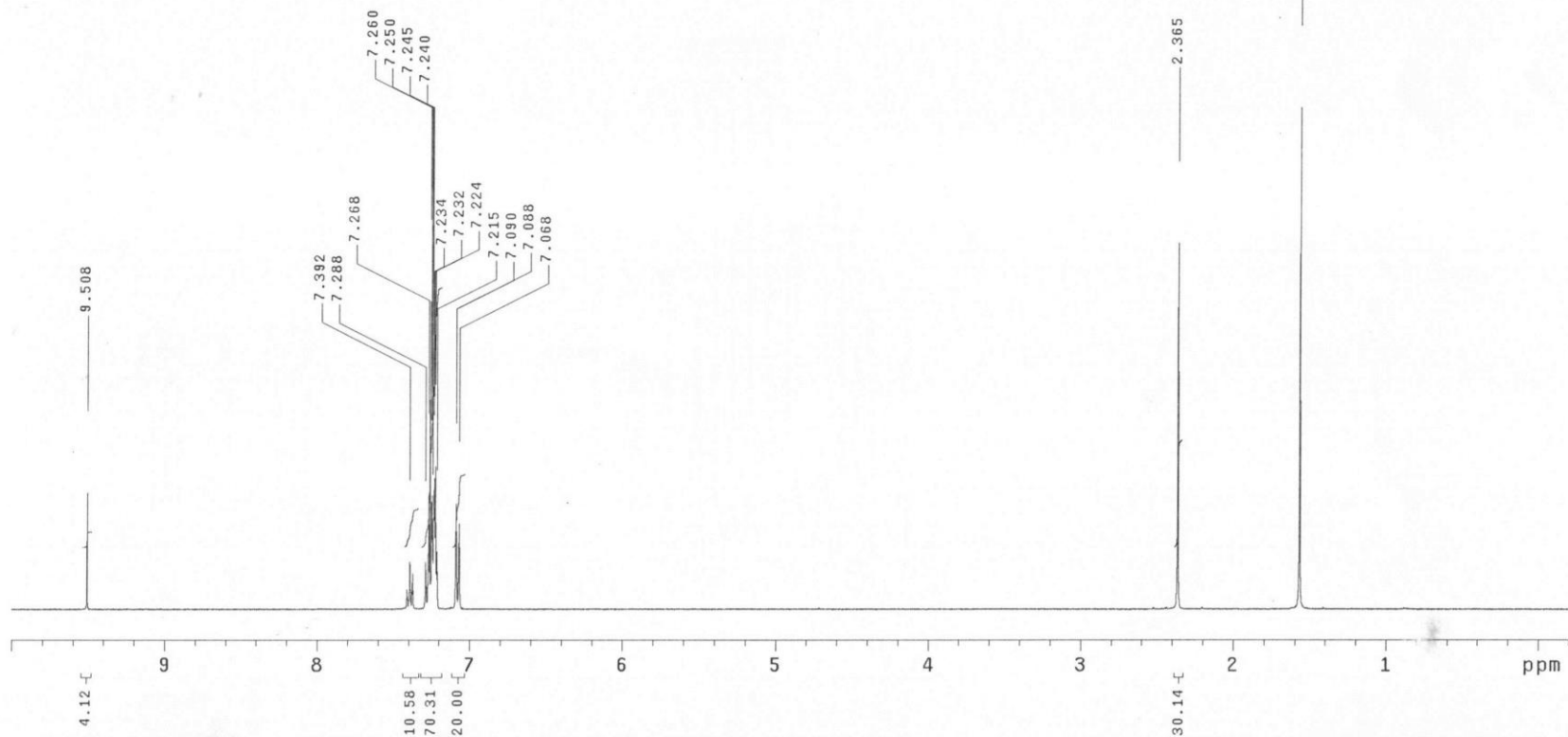
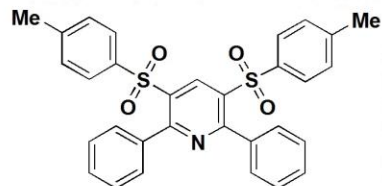
UNITYplus-400 "unity400"

Date: Sep 19 2022

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 32 repetitions



# Compound 4a (<sup>13</sup>C-NMR spectral data)

YCM1319

Pulse Sequence: s2pu1

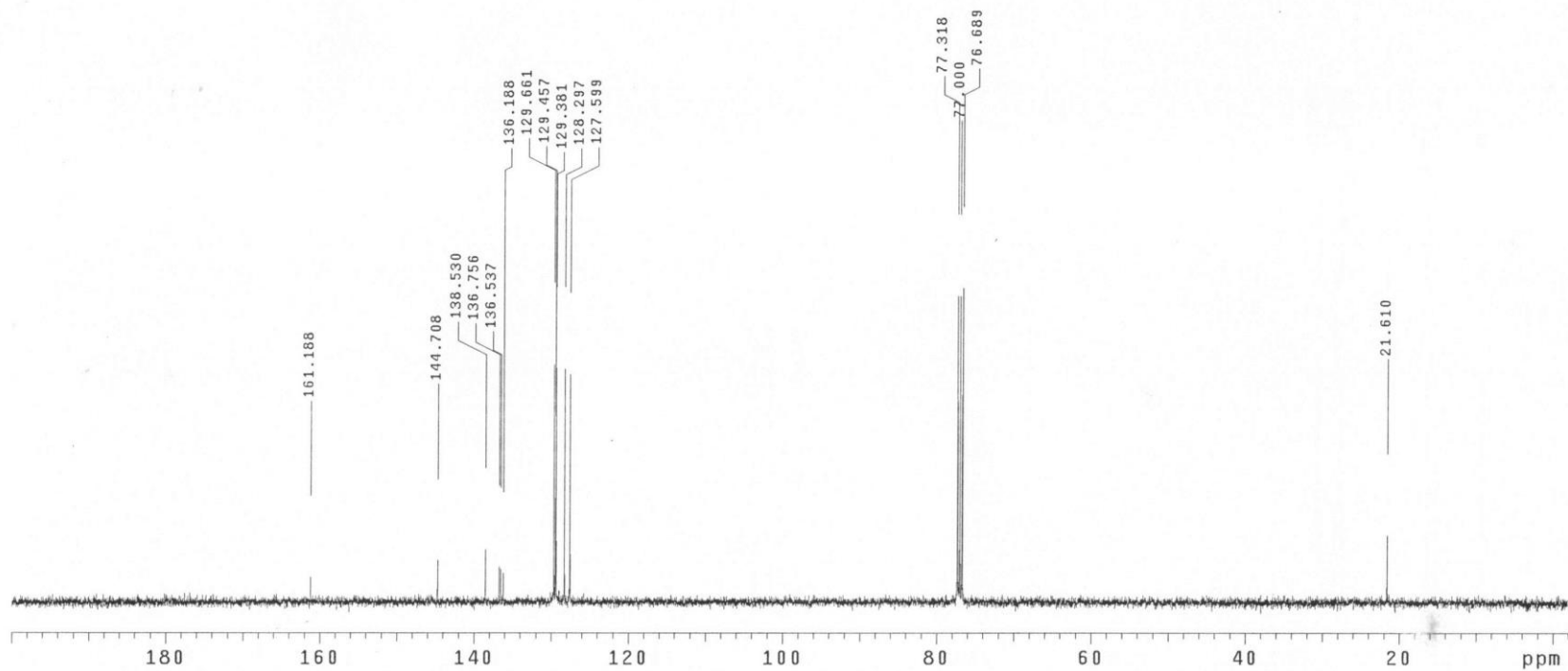
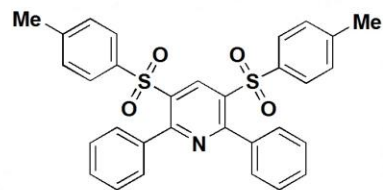
UNITYplus-400 "unity400"

Date: Sep 19 2022

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 6448 repetitions



# Compound 4b (<sup>1</sup>H-NMR spectral data)

YCM927

Pulse Sequence: s2pu1

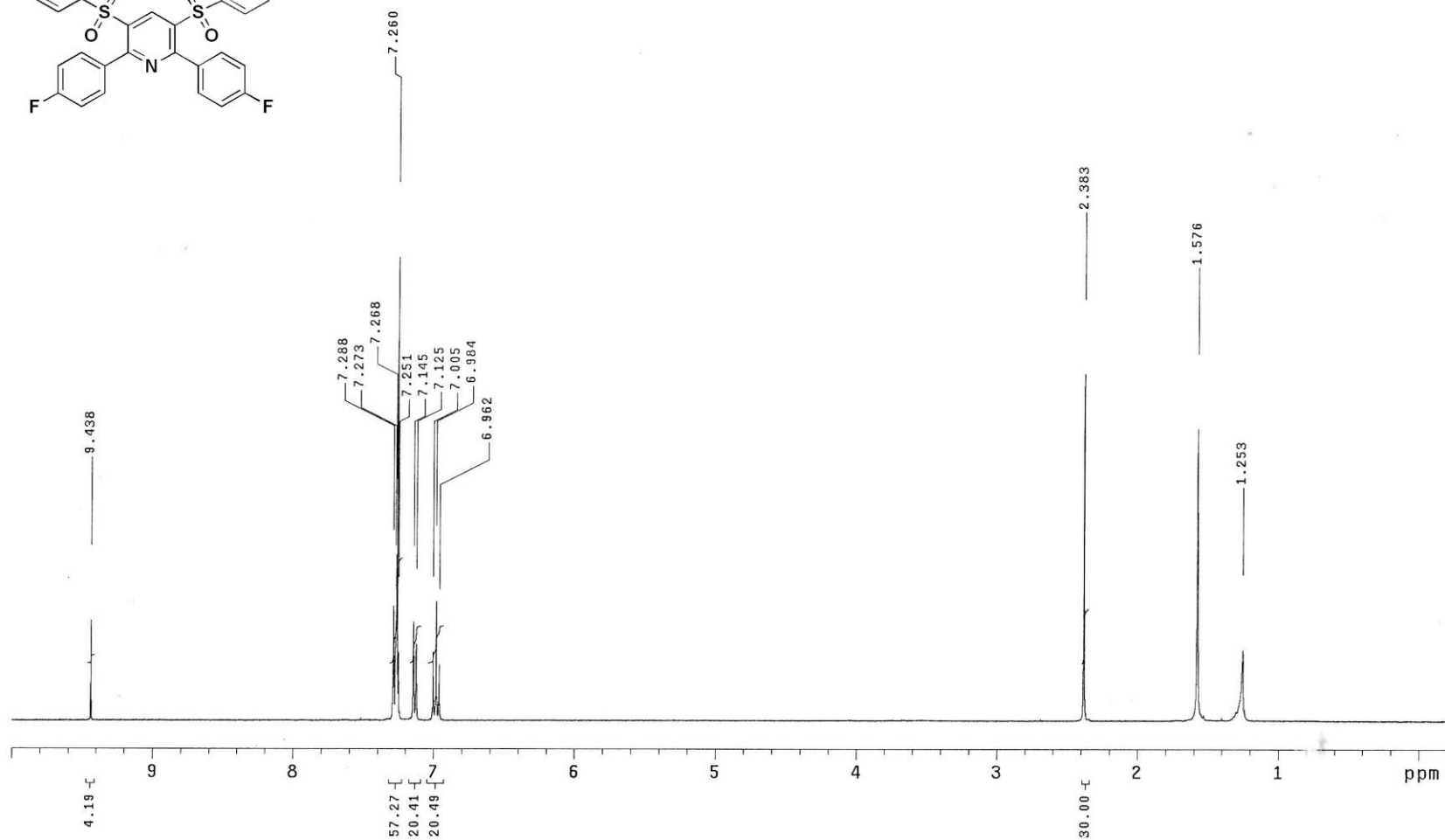
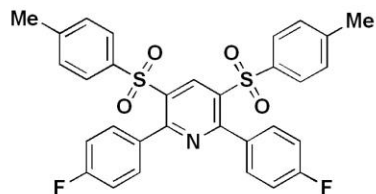
UNITYplus-400 "unity400"

Date: Sep 29 2022

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 76 repetitions



# Compound 4b (<sup>13</sup>C-NMR spectral data)

YCM927

Pulse Sequence: s2pu1

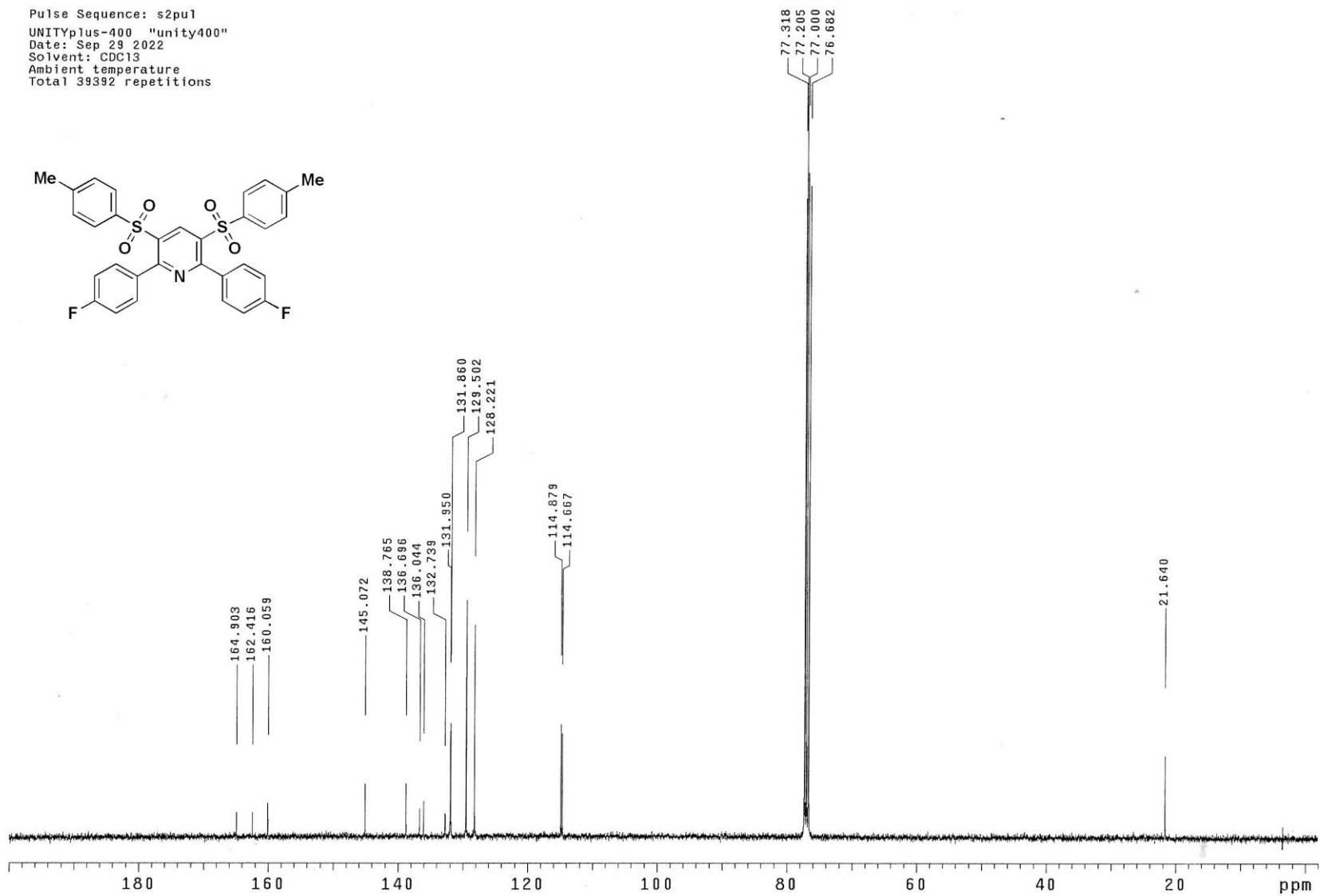
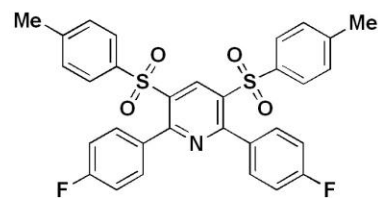
UNITYplus-400 "unity400"

Date: Sep 29 2022

Solvent: CDCl<sub>3</sub>

Ambient temperature

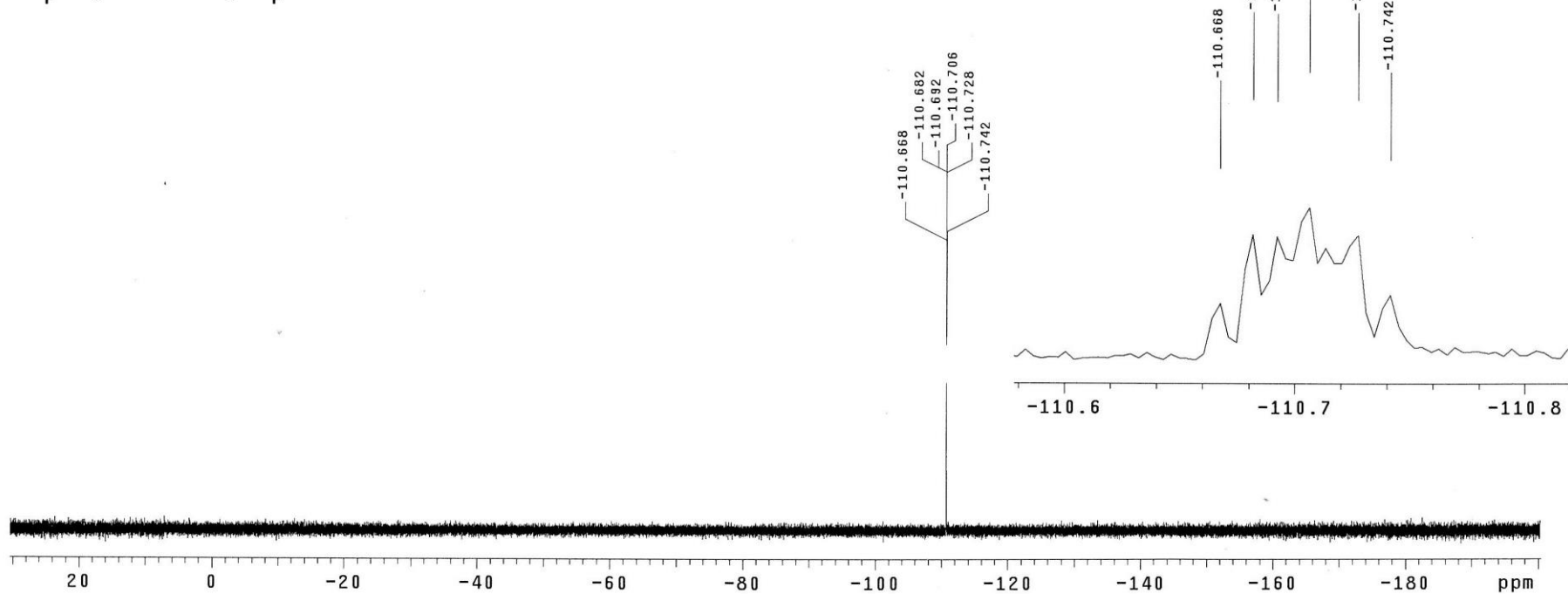
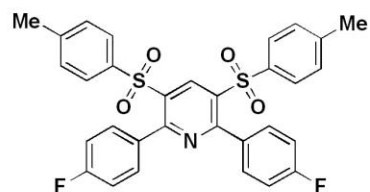
Total 39392 repetitions



# Compound 4b (<sup>19</sup>F-NMR spectral data)

4b

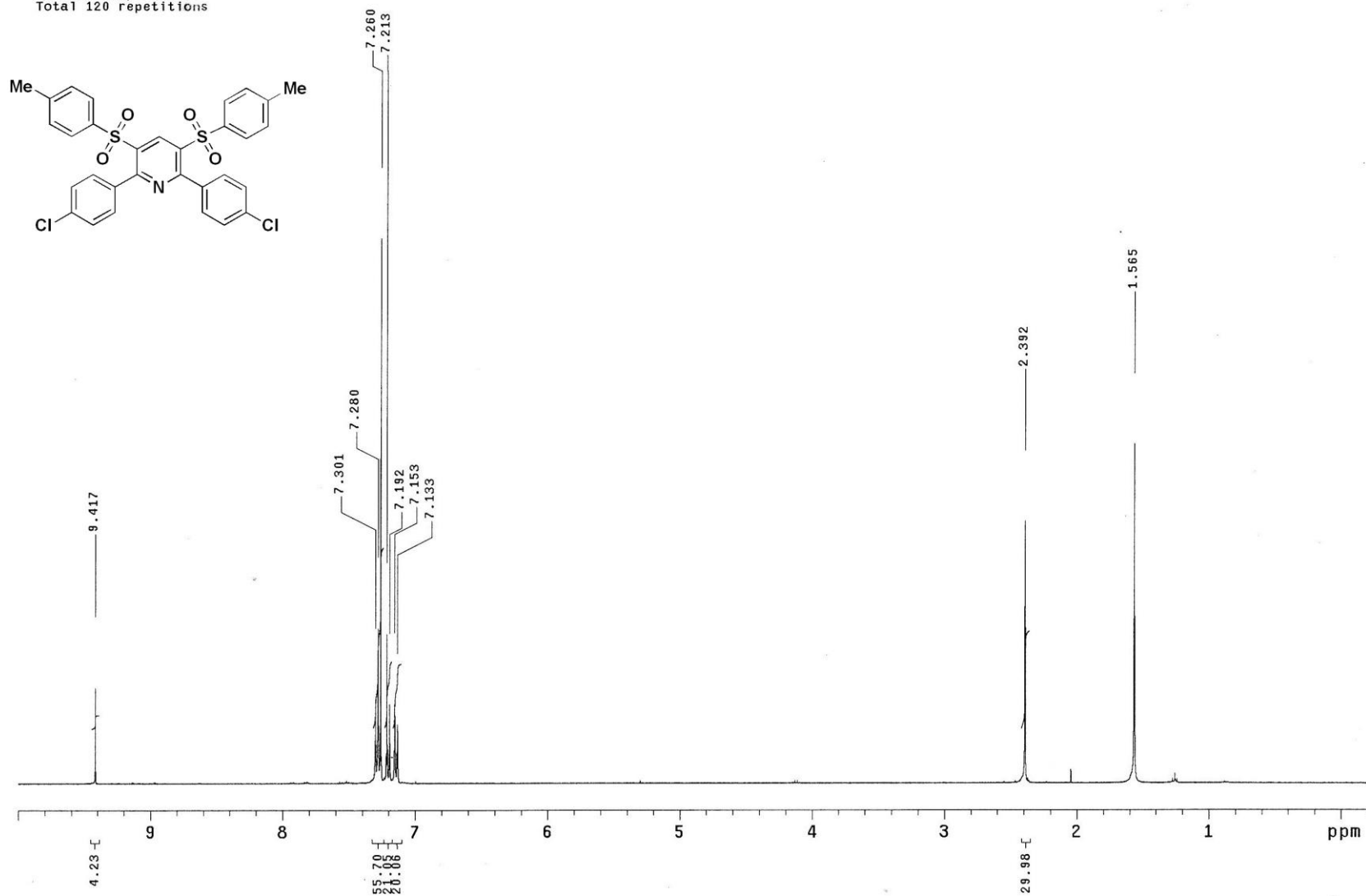
Pulse Sequence: s2pu1  
Mercury-400BB "MerPlus400"  
Date: Aug 5 2024  
Solvent: cdcl3  
Ambient temperature  
Total 96 repetitions



# Compound 4c (<sup>1</sup>H-NMR spectral data)

YCM3239

Pulse Sequence: s2pu1  
 UNITYplus-400 "unity400"  
 Date: Feb 7 2023  
 Solvent: CDCl<sub>3</sub>  
 Ambient temperature  
 Total 120 repetitions



# Compound 4c (<sup>13</sup>C-NMR spectral data)

YCM3239

Pulse Sequence: s2pu1

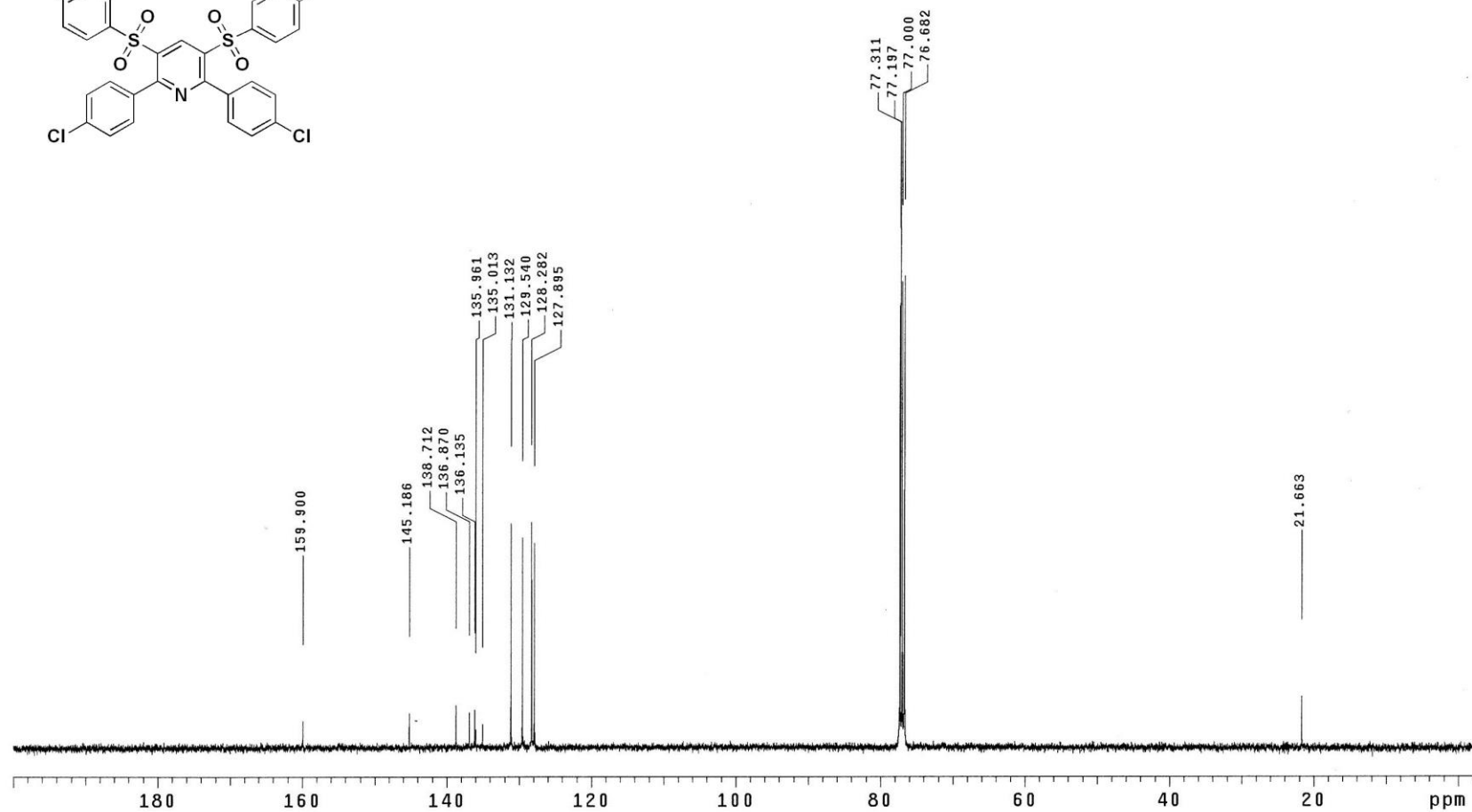
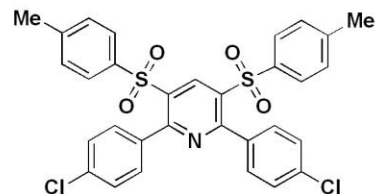
UNITYplus-400 "unity400"

Date: Feb 7 2023

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 32160 repetitions





# Compound 4d (<sup>1</sup>H-NMR spectral data)

YCM1006

Pulse Sequence: s2pu1

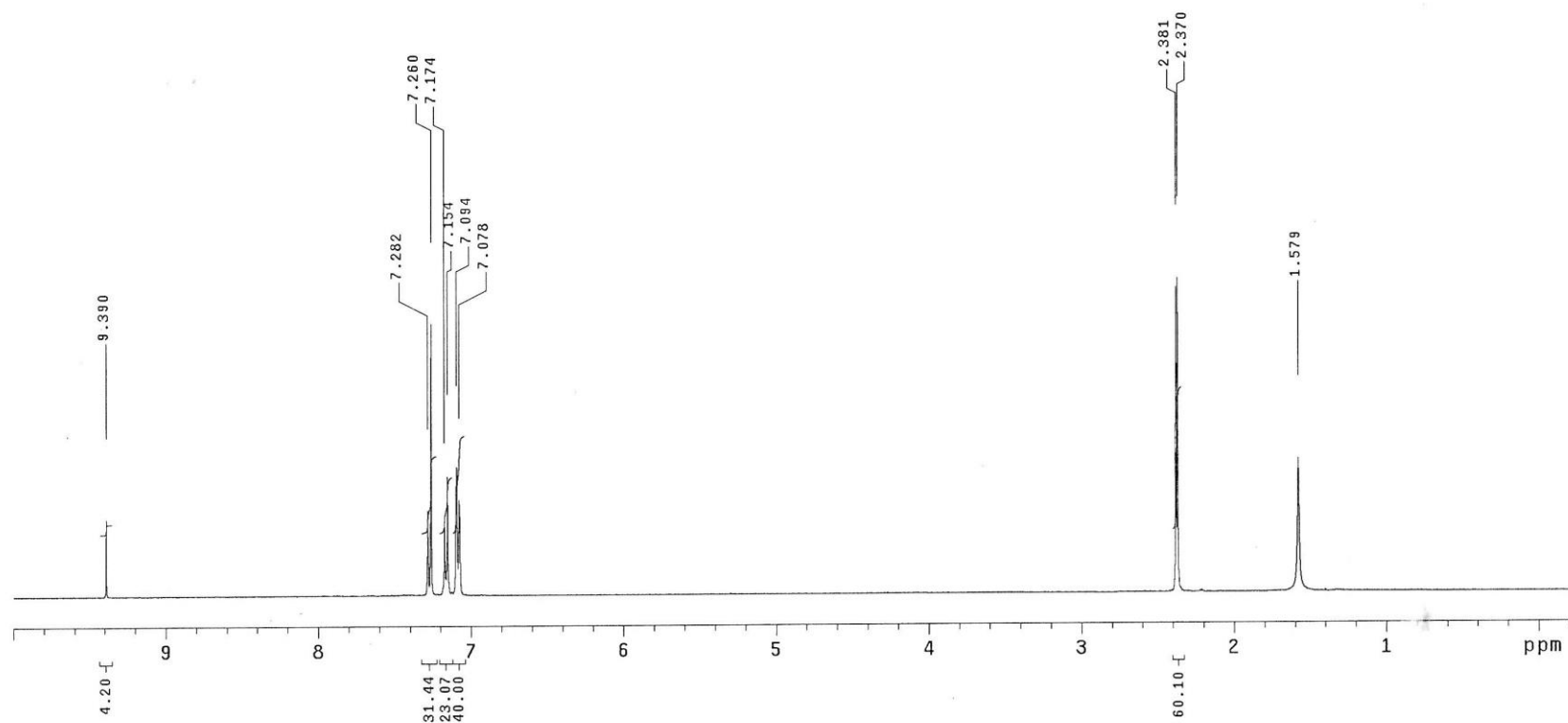
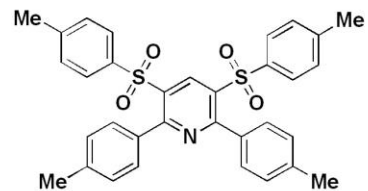
UNITYplus-400 "unity400"

Date: Oct 6 2022

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 32 repetitions



# Compound 4d (<sup>13</sup>C-NMR spectral data)

YCM1006

Pulse Sequence: s2pu1

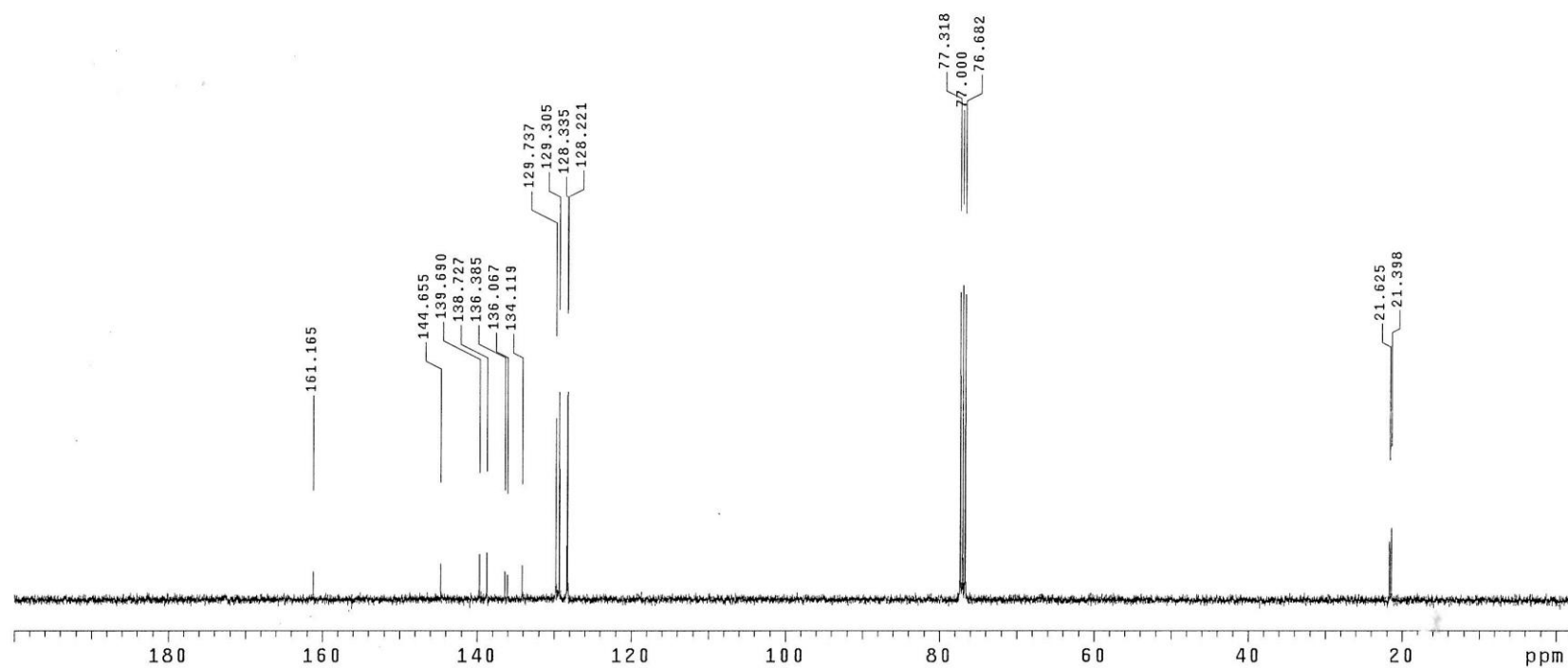
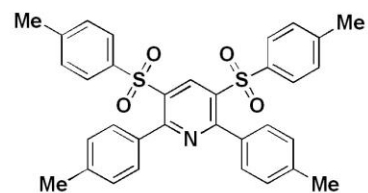
UNITYplus-400 "unity400"

Date: Oct 6 2022

Solvent: CDCl<sub>3</sub>

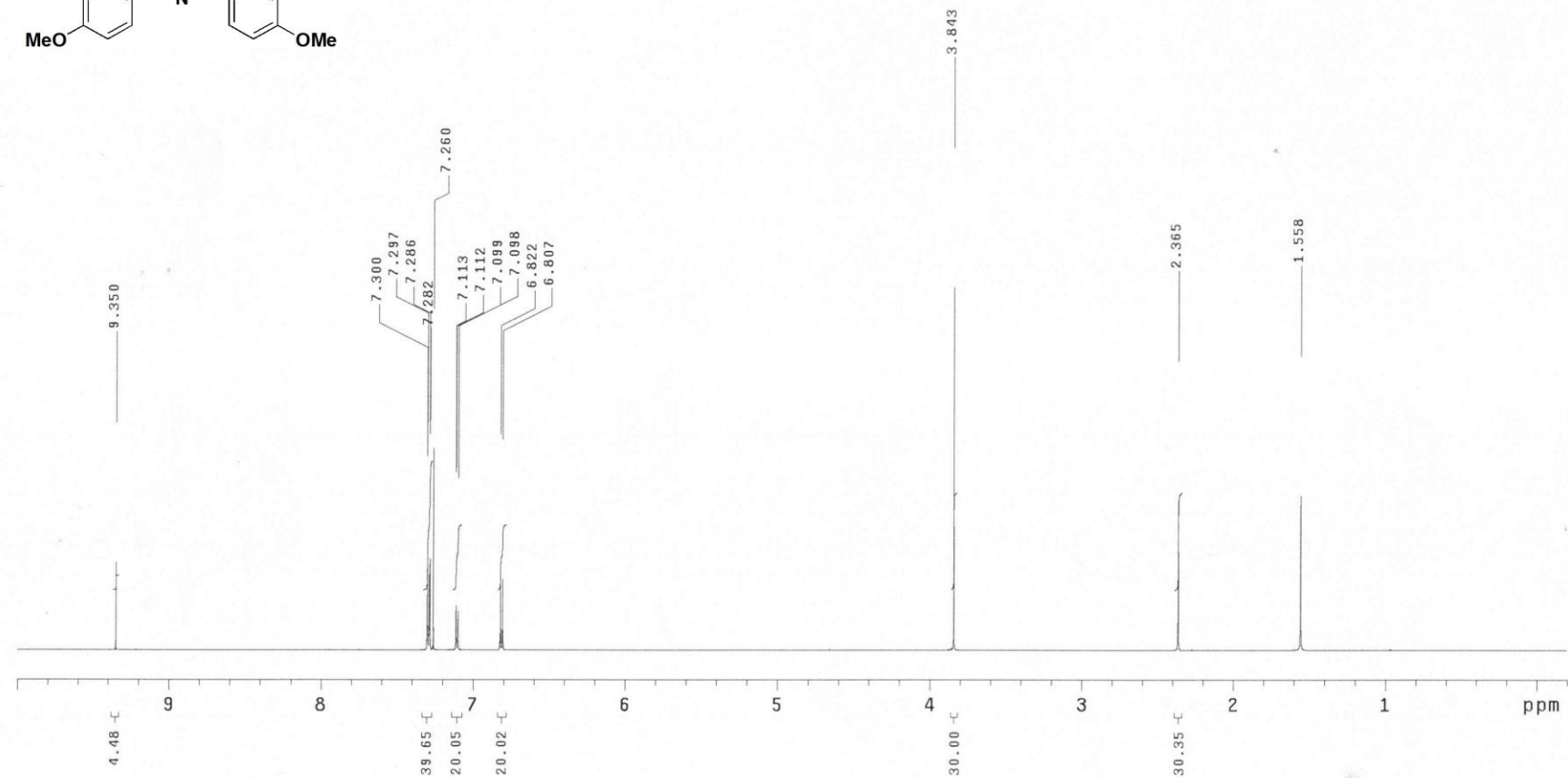
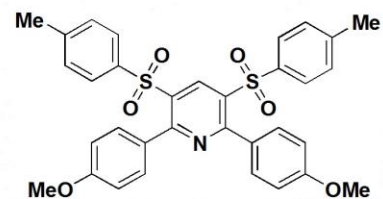
Ambient temperature

Total 7056 repetitions



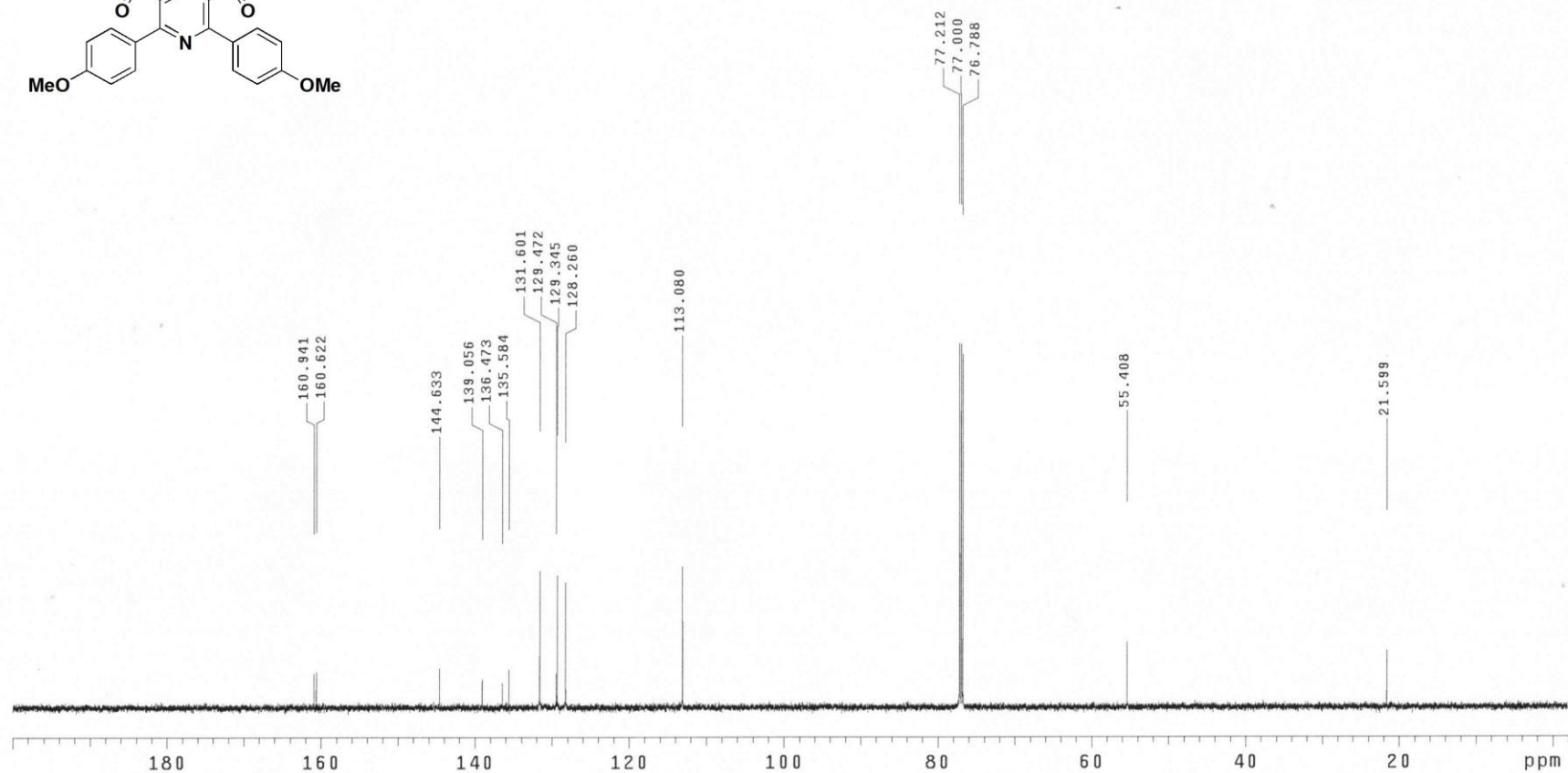
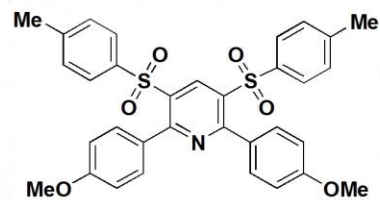
# Compound 4e (<sup>1</sup>H-NMR spectral data)

Pulse Sequence: s2pu1  
UNITYplus-600 "KMU600.kmu.edu.tw"  
Date: Sep 22 2022  
Solvent: cdc13  
Temp. 28.0 C / 301.1 K  
Total 32 repetitions



# Compound 4e (<sup>13</sup>C-NMR spectral data)

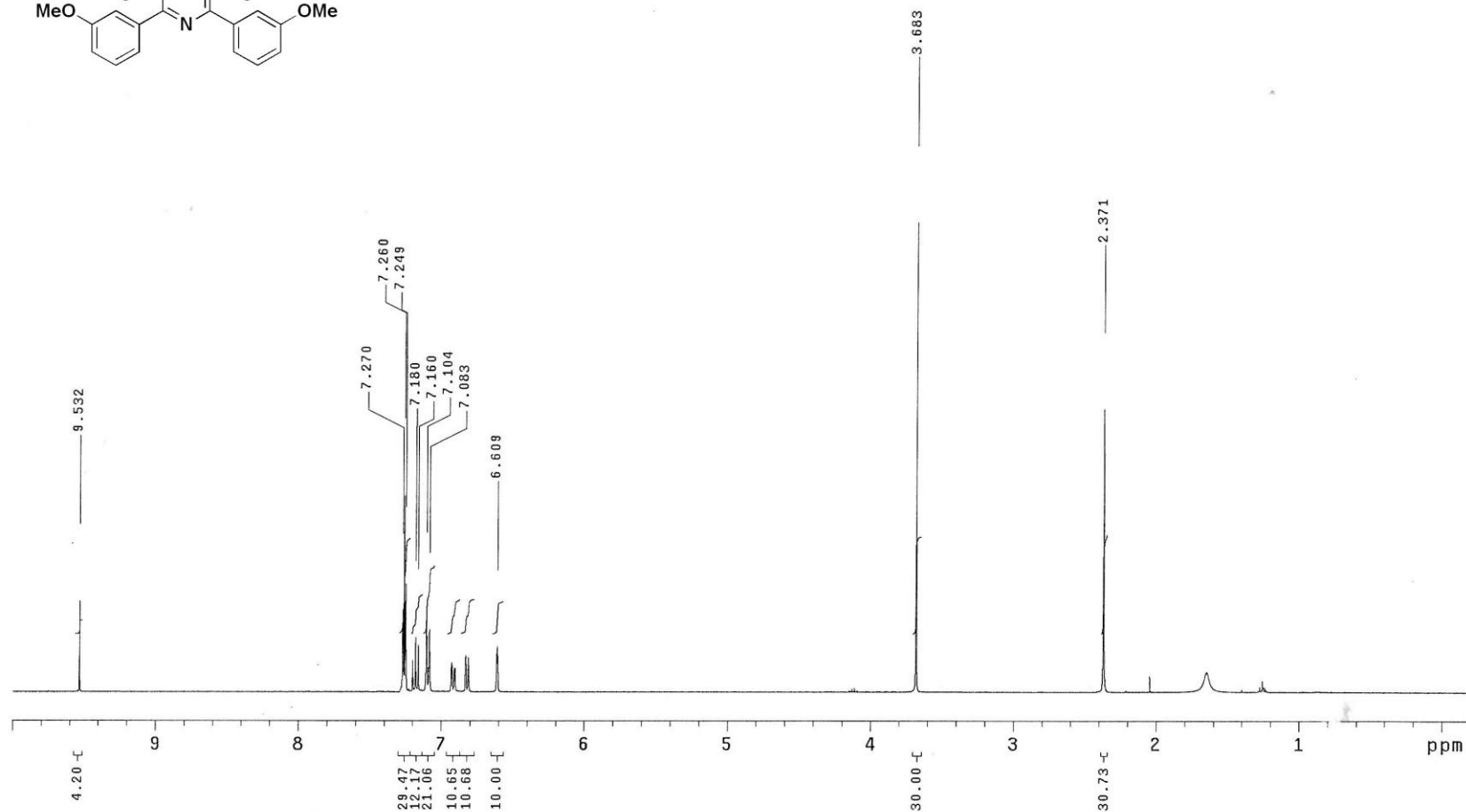
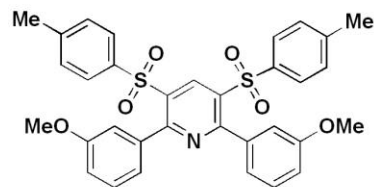
Pulse Sequence: s2pu1  
 UNITYplus-600 "KMU600.kmu.edu.tw"  
 Date: Sep 22 2022  
 Solvent: cdcl3  
 Temp. 28.0 C / 301.1 K  
 Total 544 repetitions



# Compound 4f (<sup>1</sup>H-NMR spectral data)

YCM1005

Pulse Sequence: s2pu1  
 UNITYplus-400 "unity400"  
 Date: Oct 5 2022  
 Solvent: CDCl<sub>3</sub>  
 Ambient temperature  
 Total 32 repetitions



# Compound 4f (<sup>13</sup>C-NMR spectral data)

YCM1005

Pulse Sequence: s2pu1

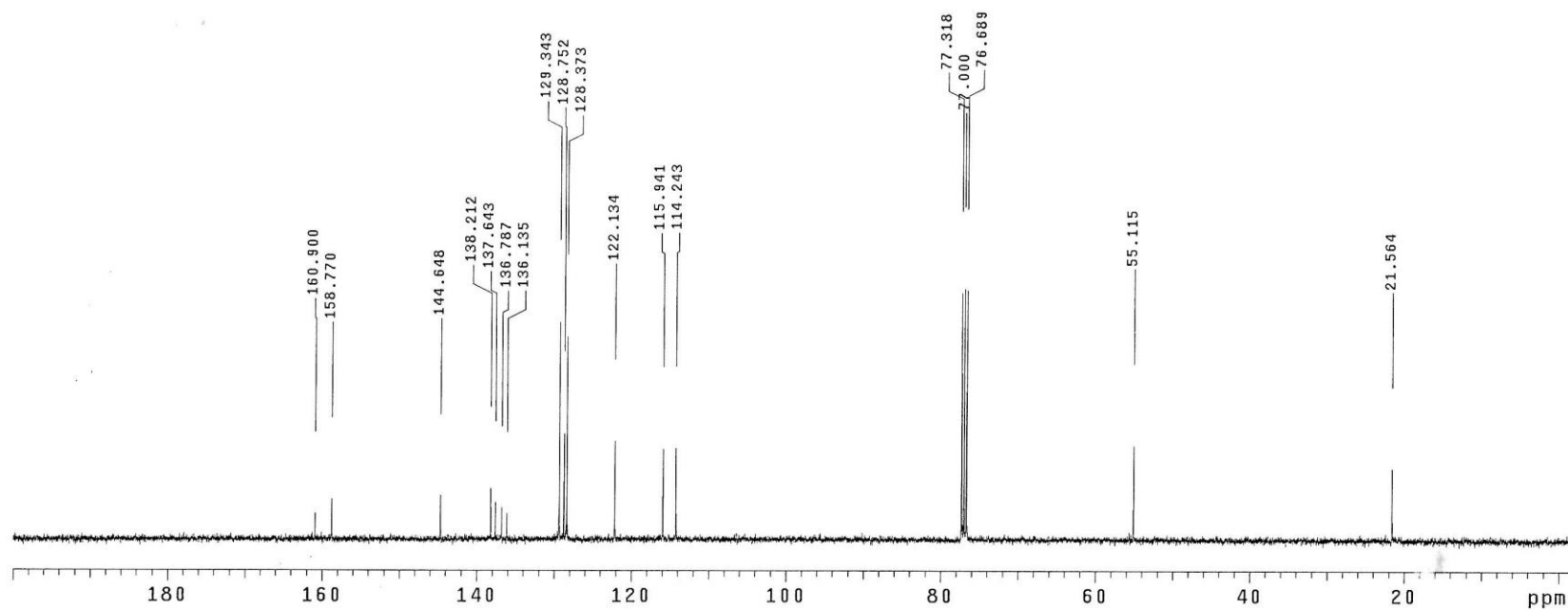
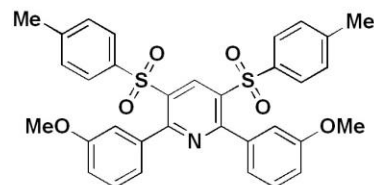
UNITYplus-400 "unity400"

Date: Oct 5 2022

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 7200 repetitions



# Compound 4g (<sup>1</sup>H-NMR spectral data)

YCM2327

Pulse Sequence: s2pu1

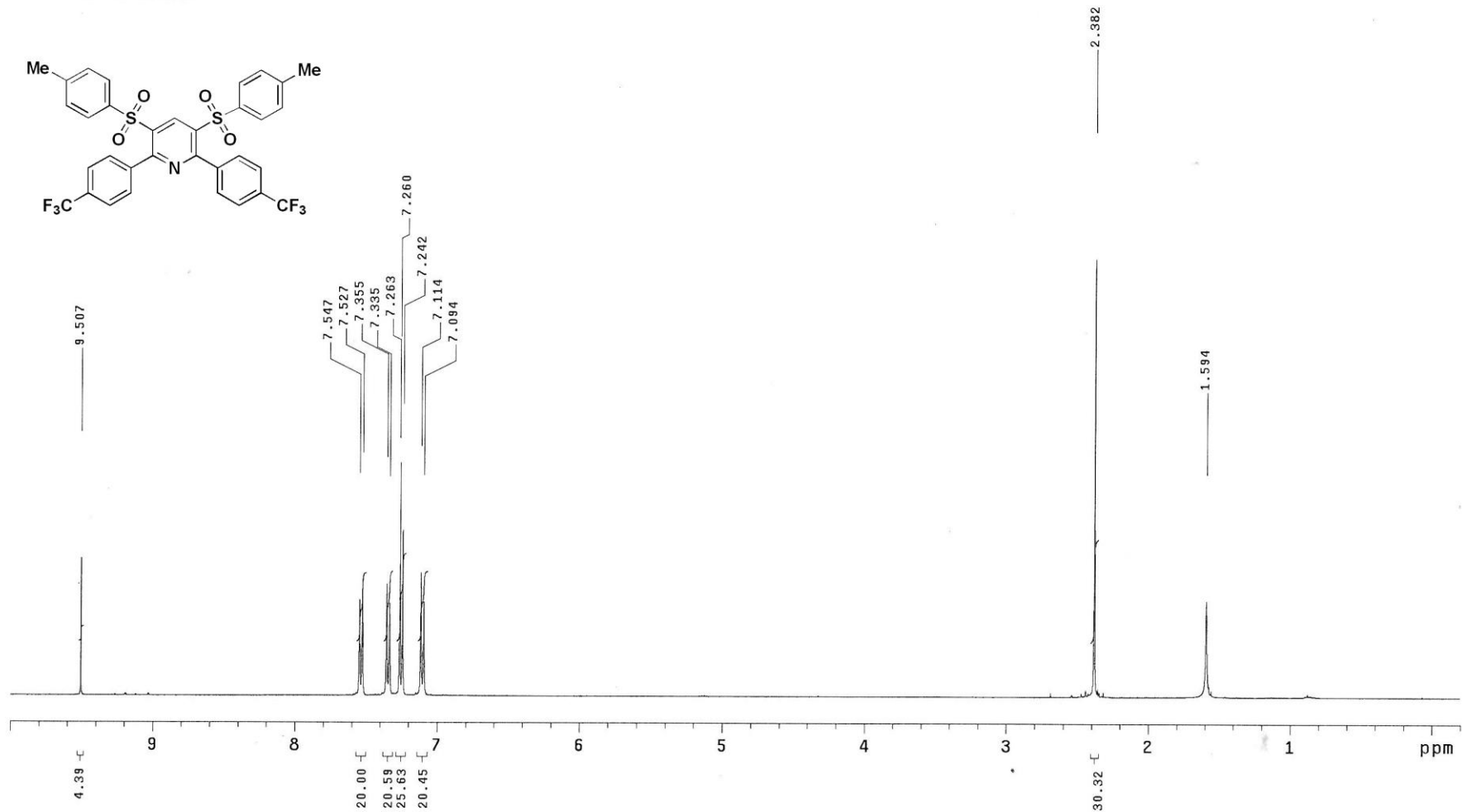
Mercury-400BB "MerPlus400"

Date: Jan 9 2023

Solvent: cdcl3

Ambient temperature

Total 32 repetitions



# Compound 4g (<sup>13</sup>C-NMR spectral data)

YCM2327

Pulse Sequence: s2pu1

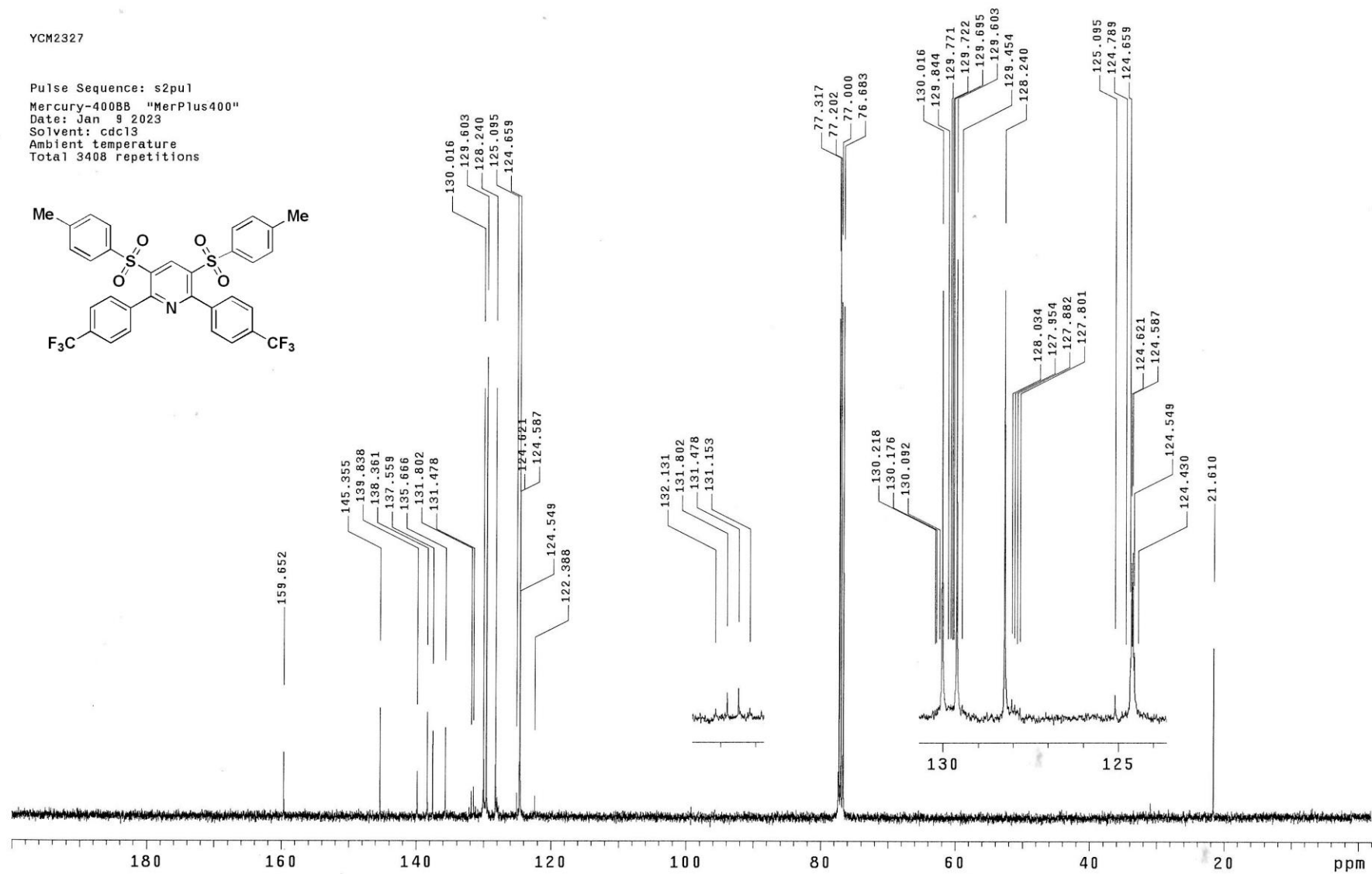
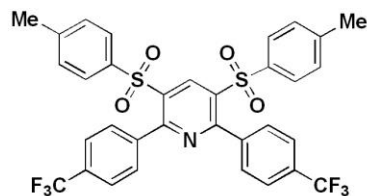
Mercury-400BB "MerPlus400"

Date: Jan 9 2023

Solvent: cdc13

Ambient temperature

Total 3408 repetitions

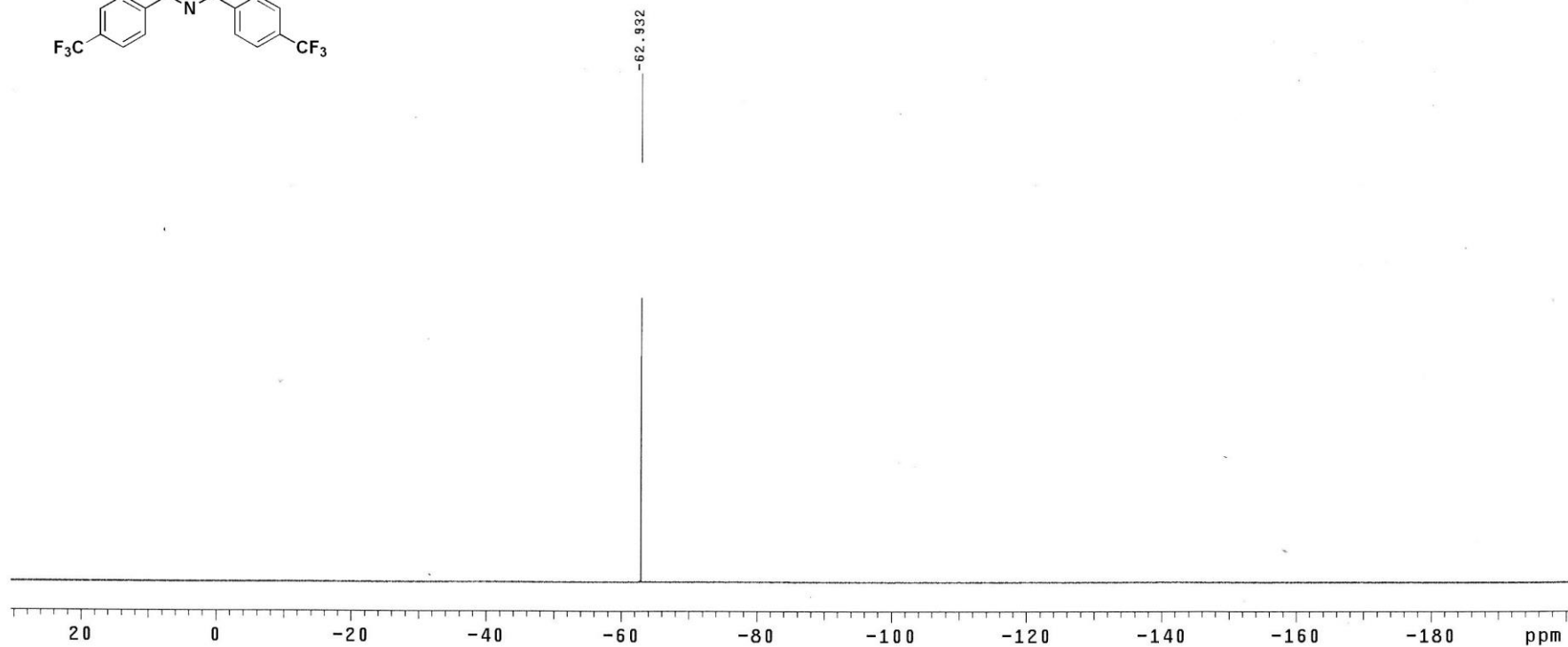
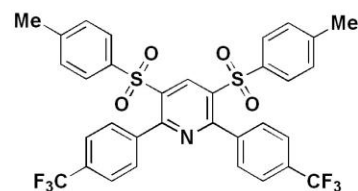




# Compound 4g (<sup>19</sup>F-NMR spectral data)

4g

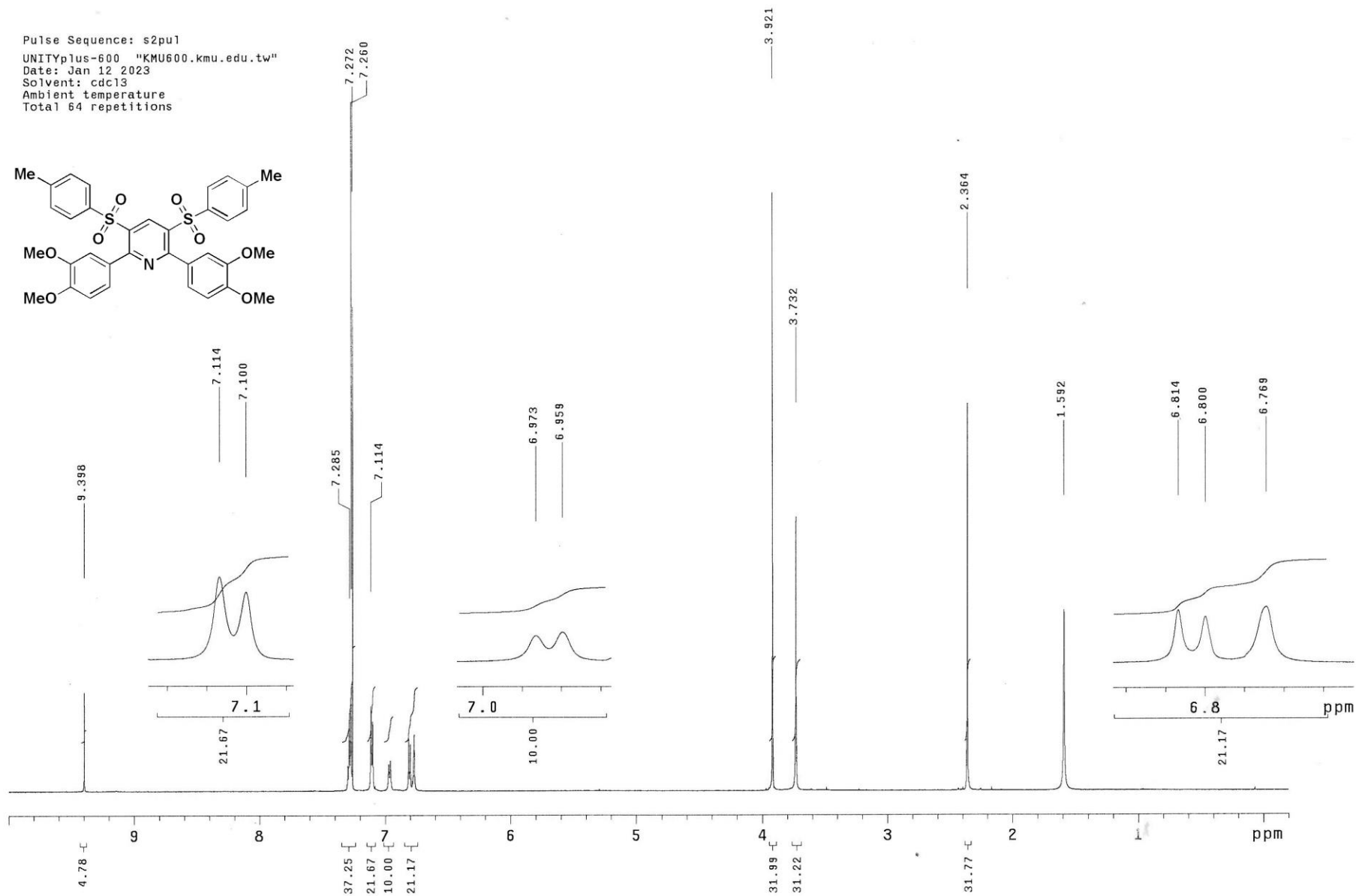
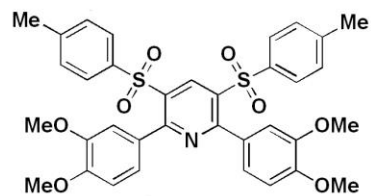
Pulse Sequence: s2pu1,  
Mercury-400BB "MerPlus400"  
Date: Aug 5 2024  
Solvent: cdcl3  
Ambient temperature  
Total 64 repetitions



# Compound 4h (<sup>1</sup>H-NMR spectral data)

YCM9196

Pulse Sequence: s2pu1  
 UNITYplus-600 "KMU600.kmu.edu.tw"  
 Date: Jan 12 2023  
 Solvent: cdc13  
 Ambient temperature  
 Total 64 repetitions



# Compound 4h (<sup>13</sup>C-NMR spectral data)

YCM9196

Pulse Sequence: s2pu1

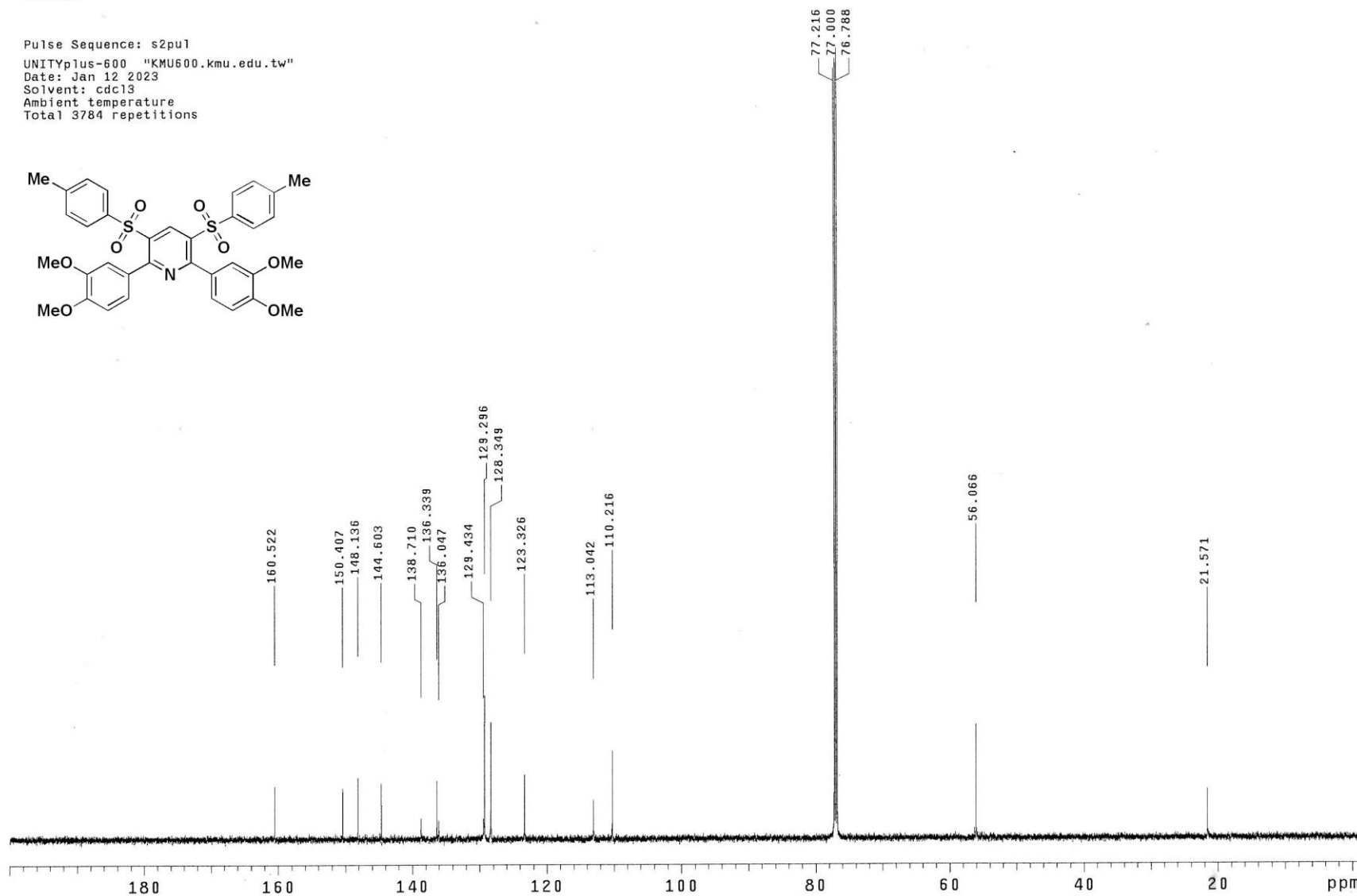
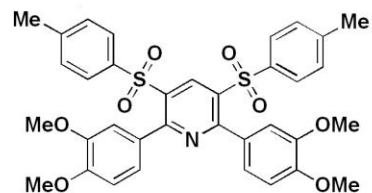
UNITYplus-600 "KMU600.kmu.edu.tw"

Date: Jan 12 2023

Solvent: cdc13

Ambient temperature

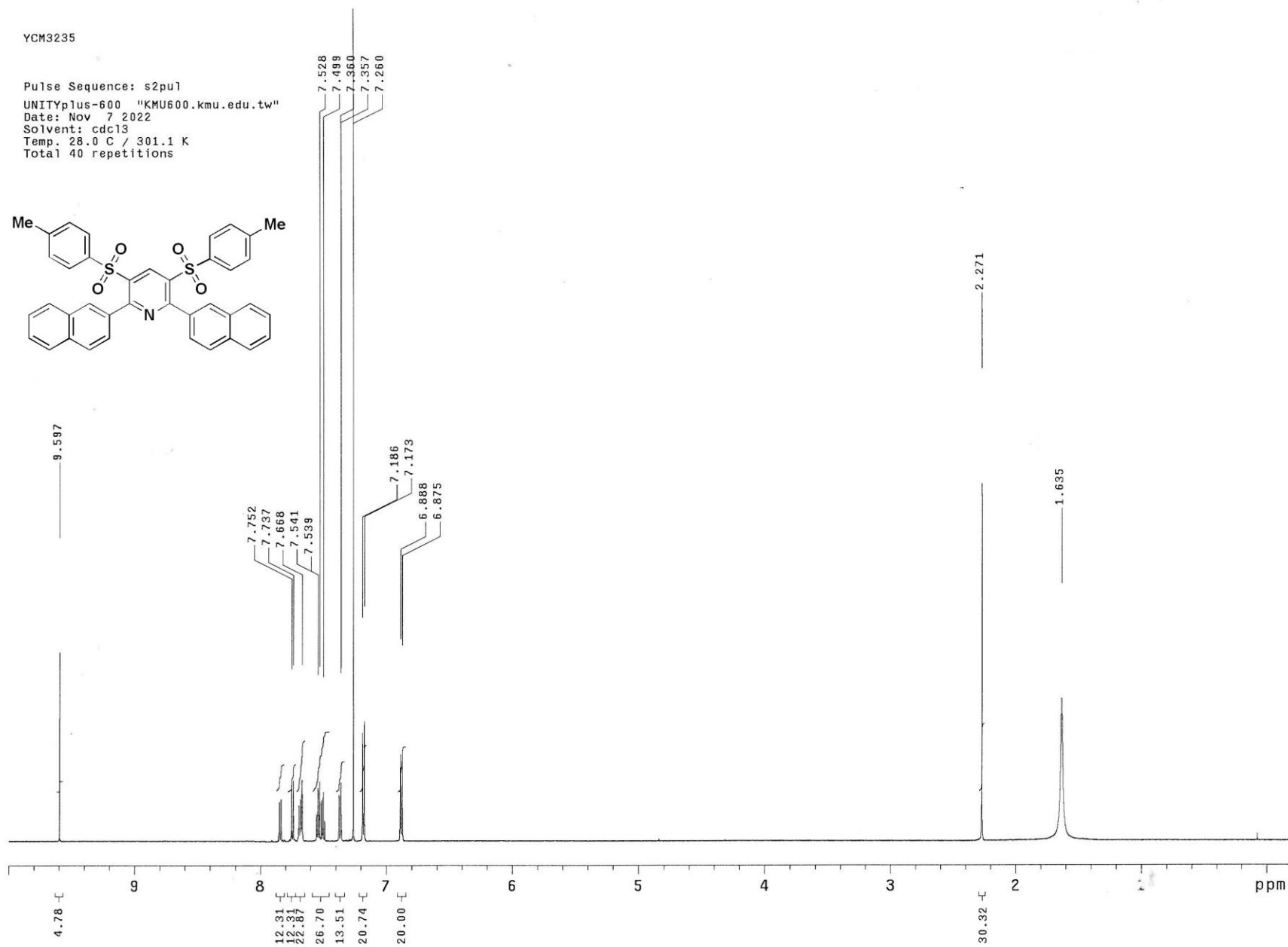
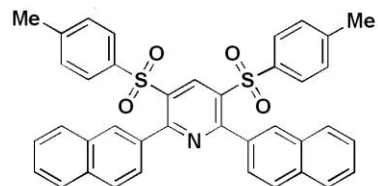
Total 3784 repetitions



# Compound 4i (<sup>1</sup>H-NMR spectral data)

YCM3235

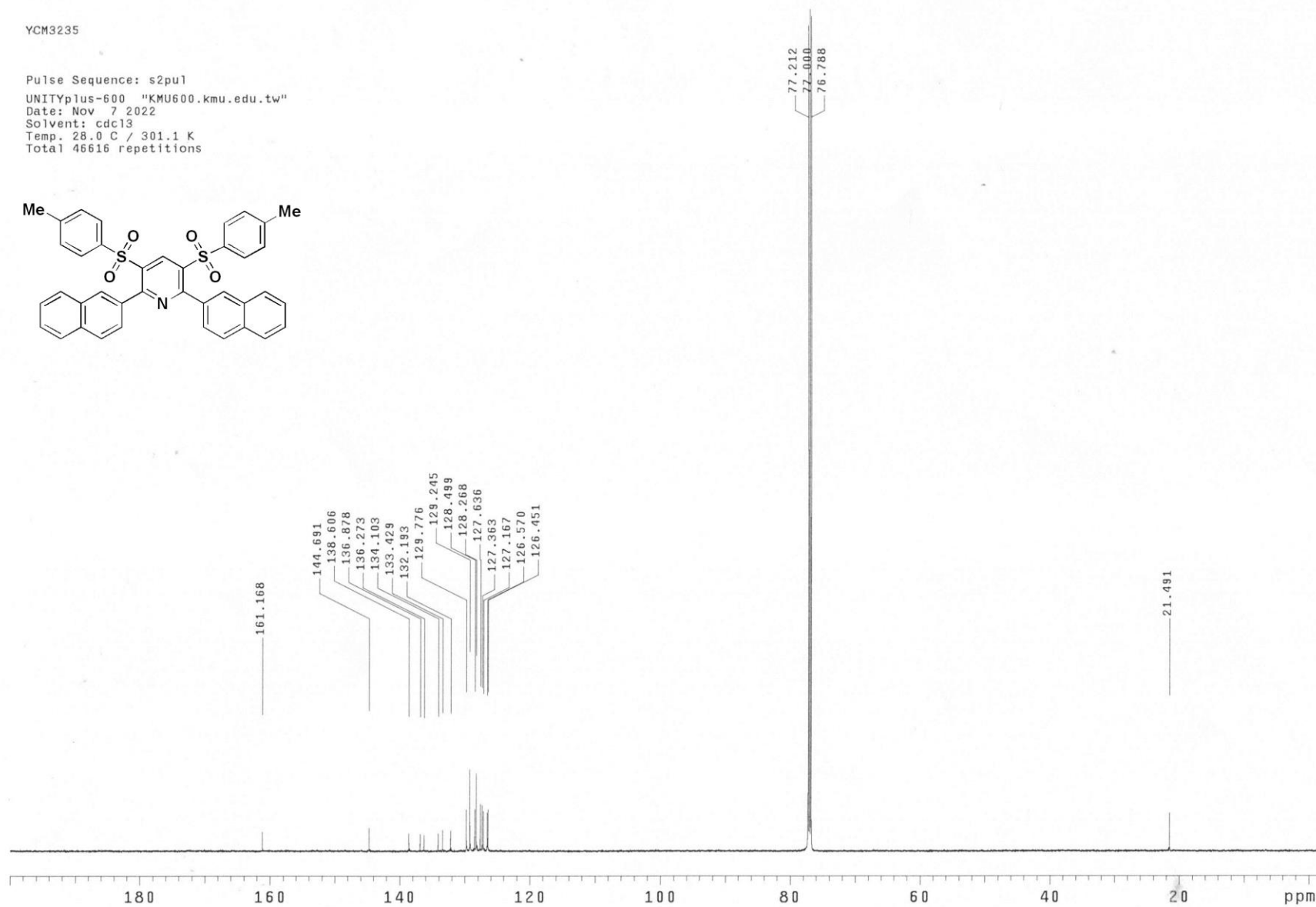
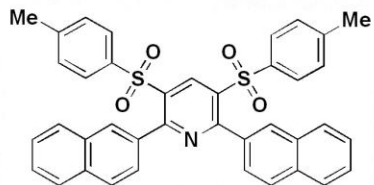
Pulse Sequence: s2pu1  
 UNITYplus-600 "KMU600.kmu.edu.tw"  
 Date: Nov 7 2022  
 Solvent: cdc13  
 Temp. 28.0 C / 301.1 K  
 Total 40 repetitions



# Compound 4i (<sup>13</sup>C-NMR spectral data)

YCM3235

Pulse Sequence: s2pu1  
UNITYplus-600 "KMU600.kmu.edu.tw"  
Date: Nov 7 2022  
Solvent: cdc13  
Temp. 28.0 C / 301.1 K  
Total 46616 repetitions



# Compound 4j (<sup>1</sup>H-NMR spectral data)

YCM1625

Pulse Sequence: s2pu1

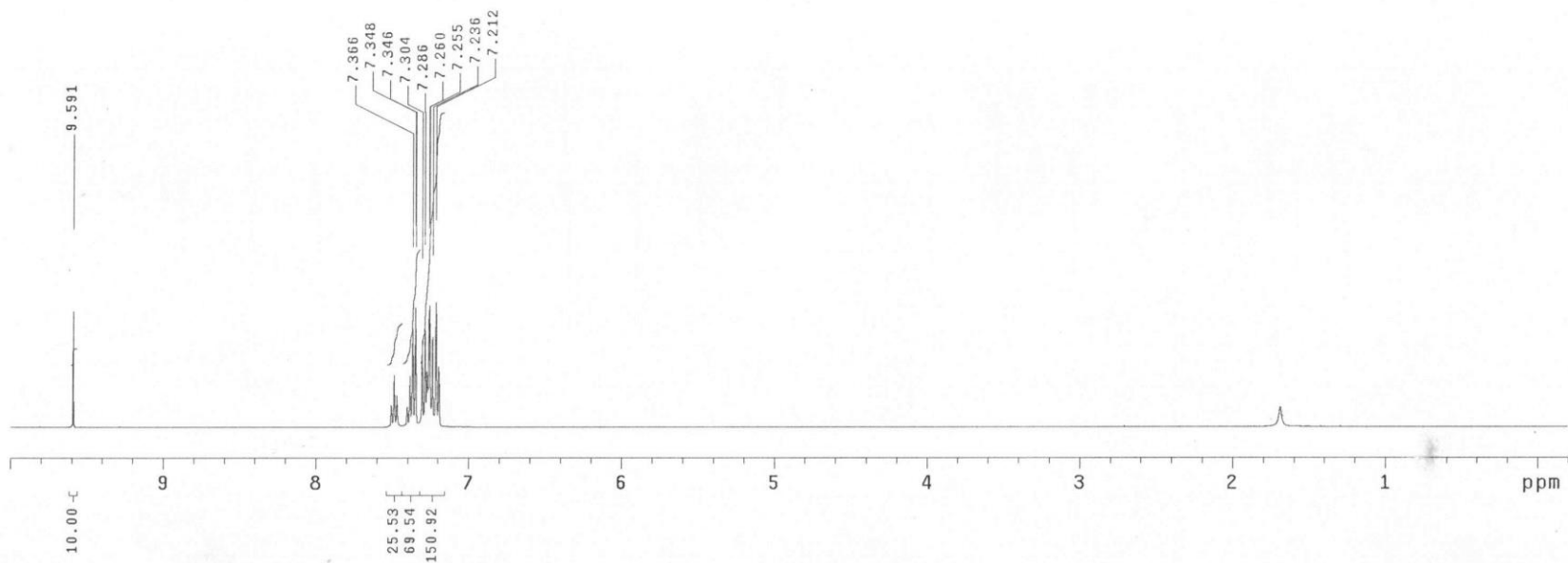
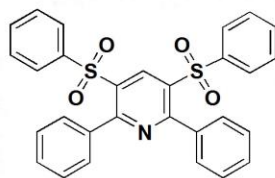
UNITYplus-400 "unity400"

Date: Sep 15 2022

Solvent: CDCl<sub>3</sub>

Ambient temperature

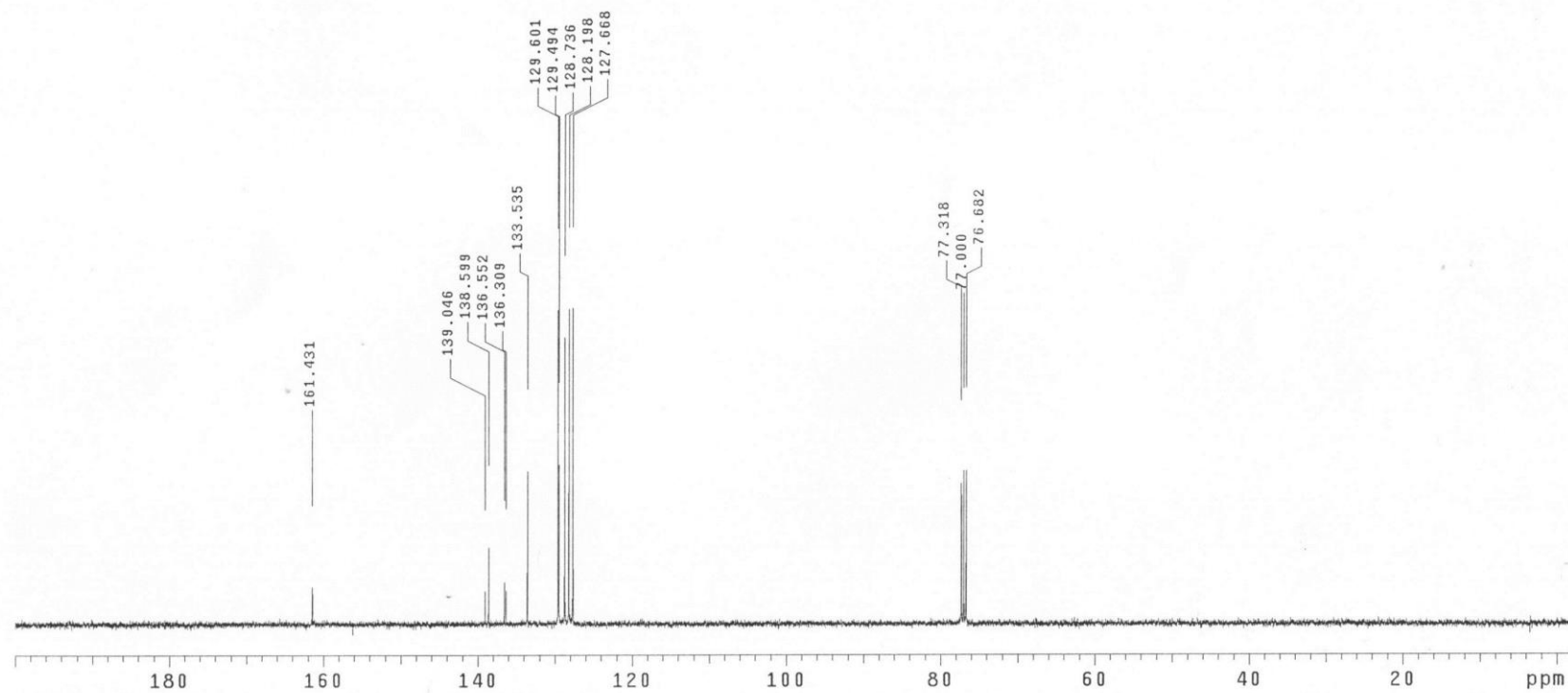
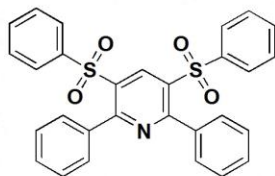
Total 32 repetitions



# Compound 4j (<sup>13</sup>C-NMR spectral data)

YCM1625

Pulse Sequence: s2pu1  
UNITYplus-400 "unity400"  
Date: Sep 15 2022  
Solvent: CDCl<sub>3</sub>  
Ambient temperature  
Total 2016 repetitions



# Compound 4k (<sup>1</sup>H-NMR spectral data)

YCM5670

Pulse Sequence: s2pu1

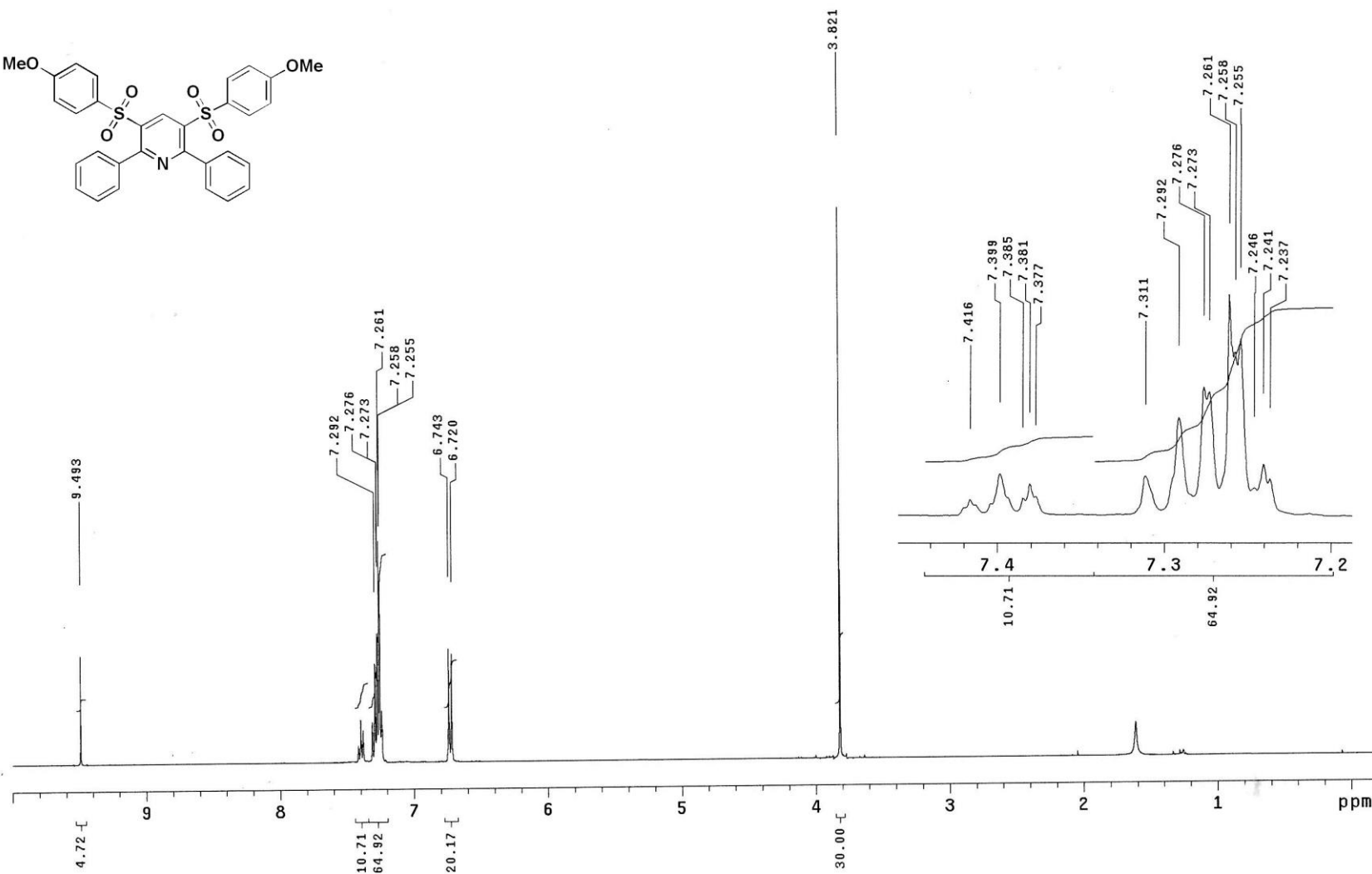
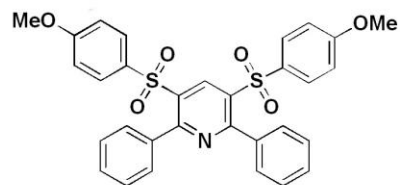
UNITYplus-400 "unity400"

Date: Nov 7 2022

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 32 repetitions





# Compound 4k (<sup>13</sup>C-NMR spectral data)

YCM5670

Pulse Sequence: s2pu1

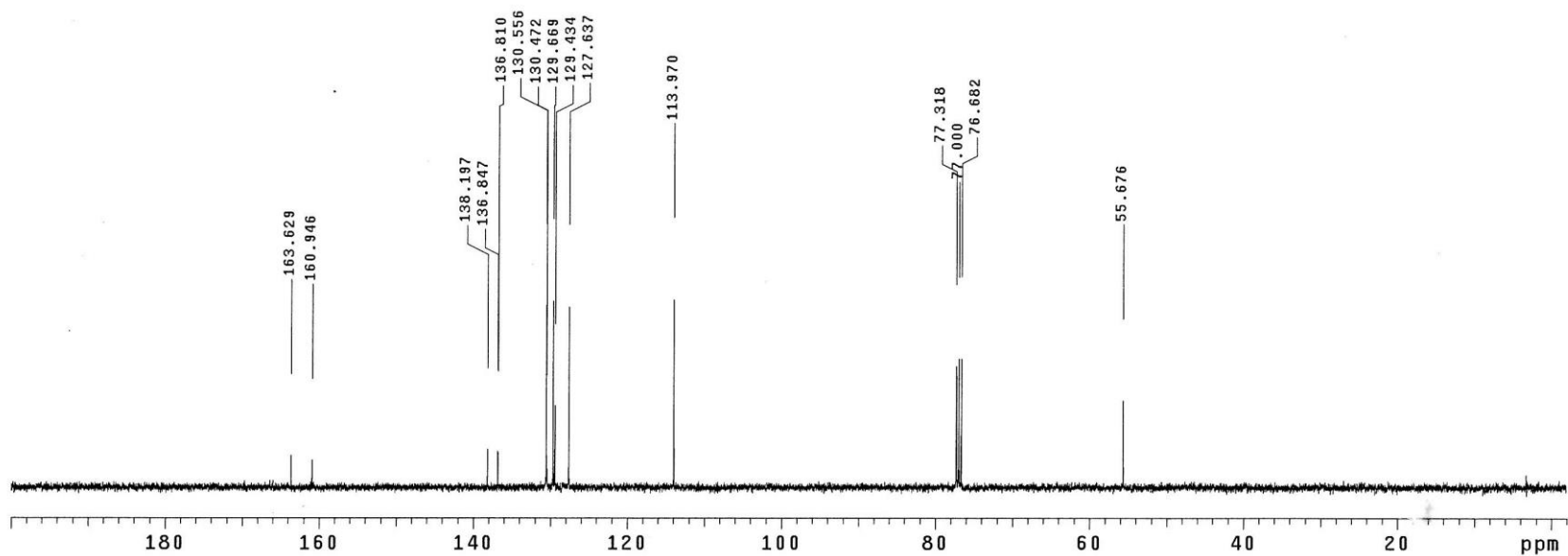
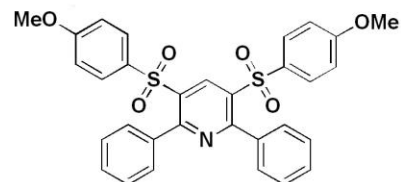
UNITYplus-400 "unity400"

Date: Nov 7 2022

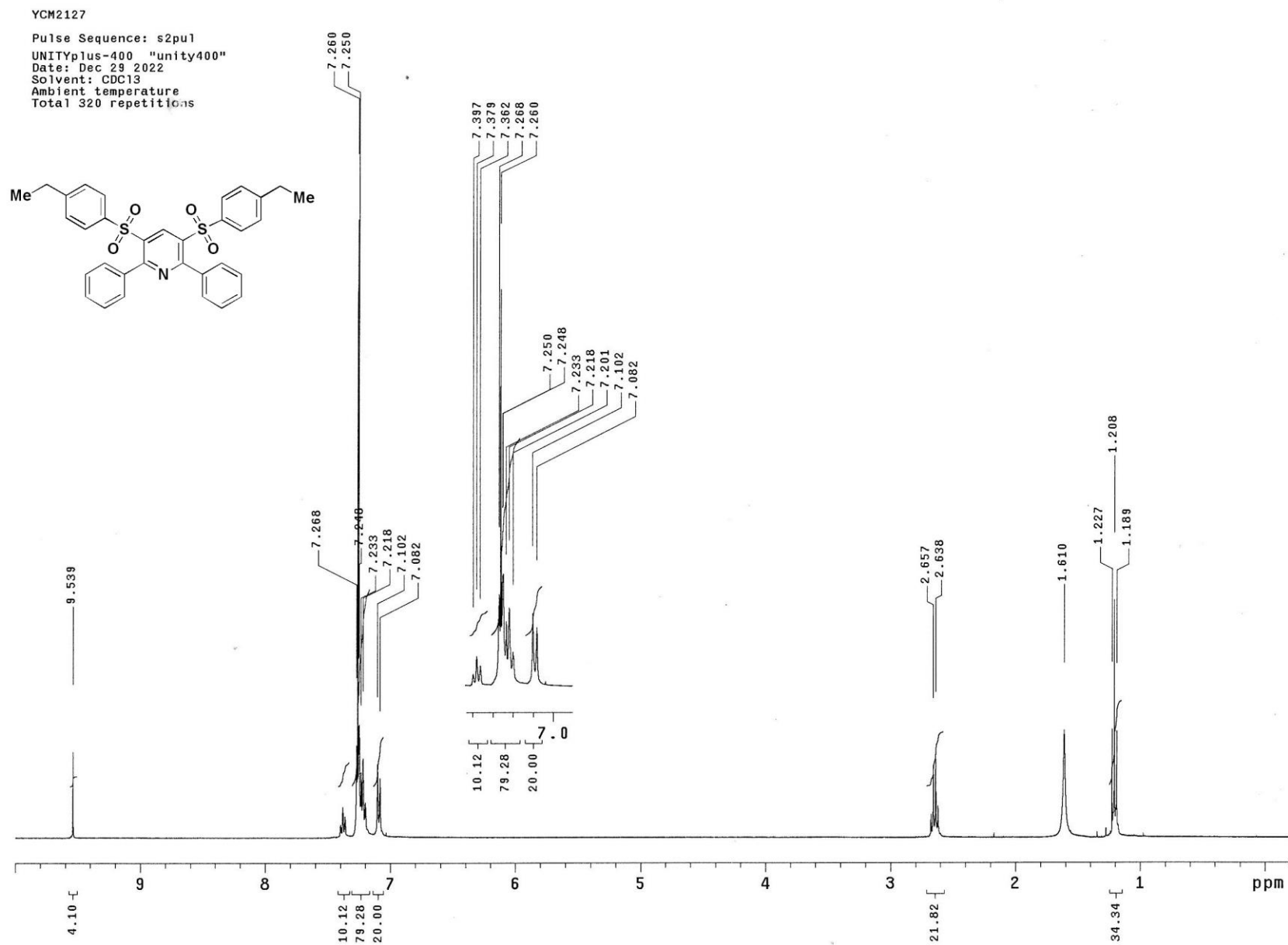
Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 1072 repetitions



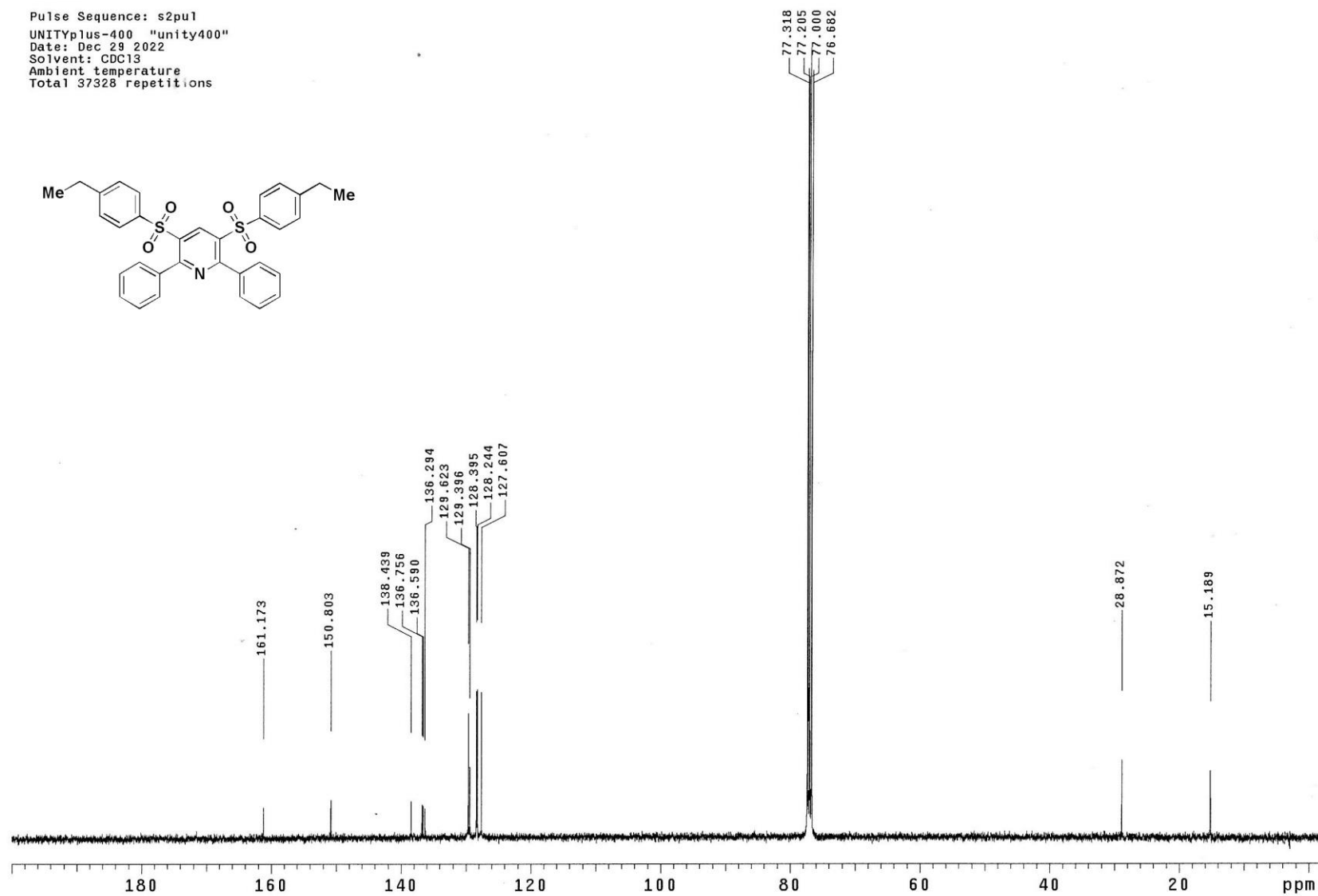
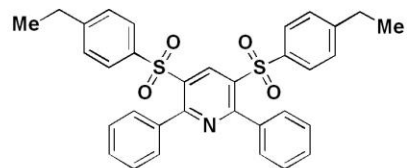
# Compound 4I (<sup>1</sup>H-NMR spectral data)



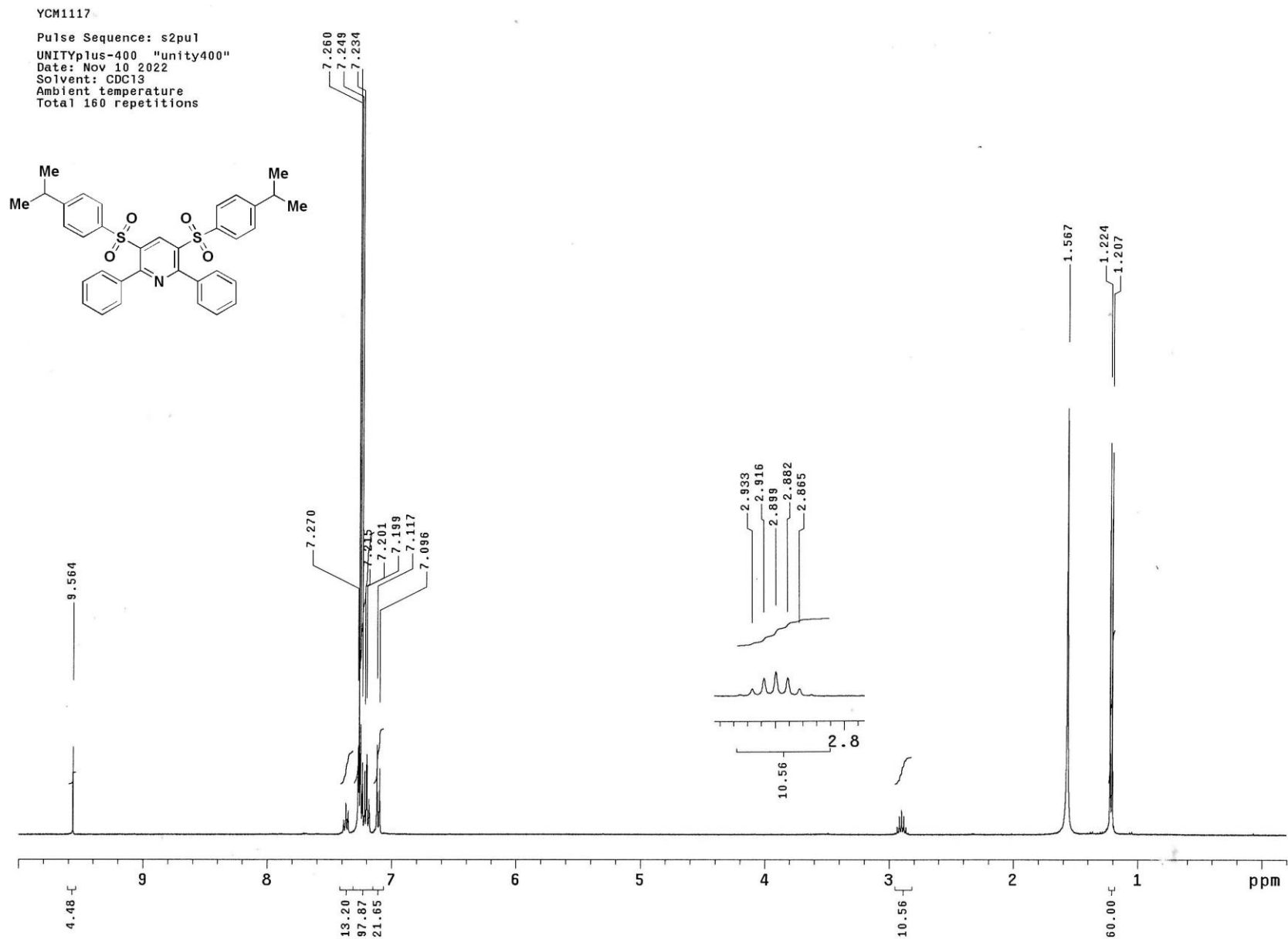
# Compound 4I (<sup>13</sup>C-NMR spectral data)

YCM2127

Pulse Sequence: s2pu1  
UNITYplus-400 "unity400"  
Date: Dec 29 2022  
Solvent: CDCl<sub>3</sub>  
Ambient temperature  
Total 37328 repetitions



# Compound 4m (<sup>1</sup>H-NMR spectral data)



# Compound 4m (<sup>13</sup>C-NMR spectral data)

YCM1117

Pulse Sequence: s2pu1

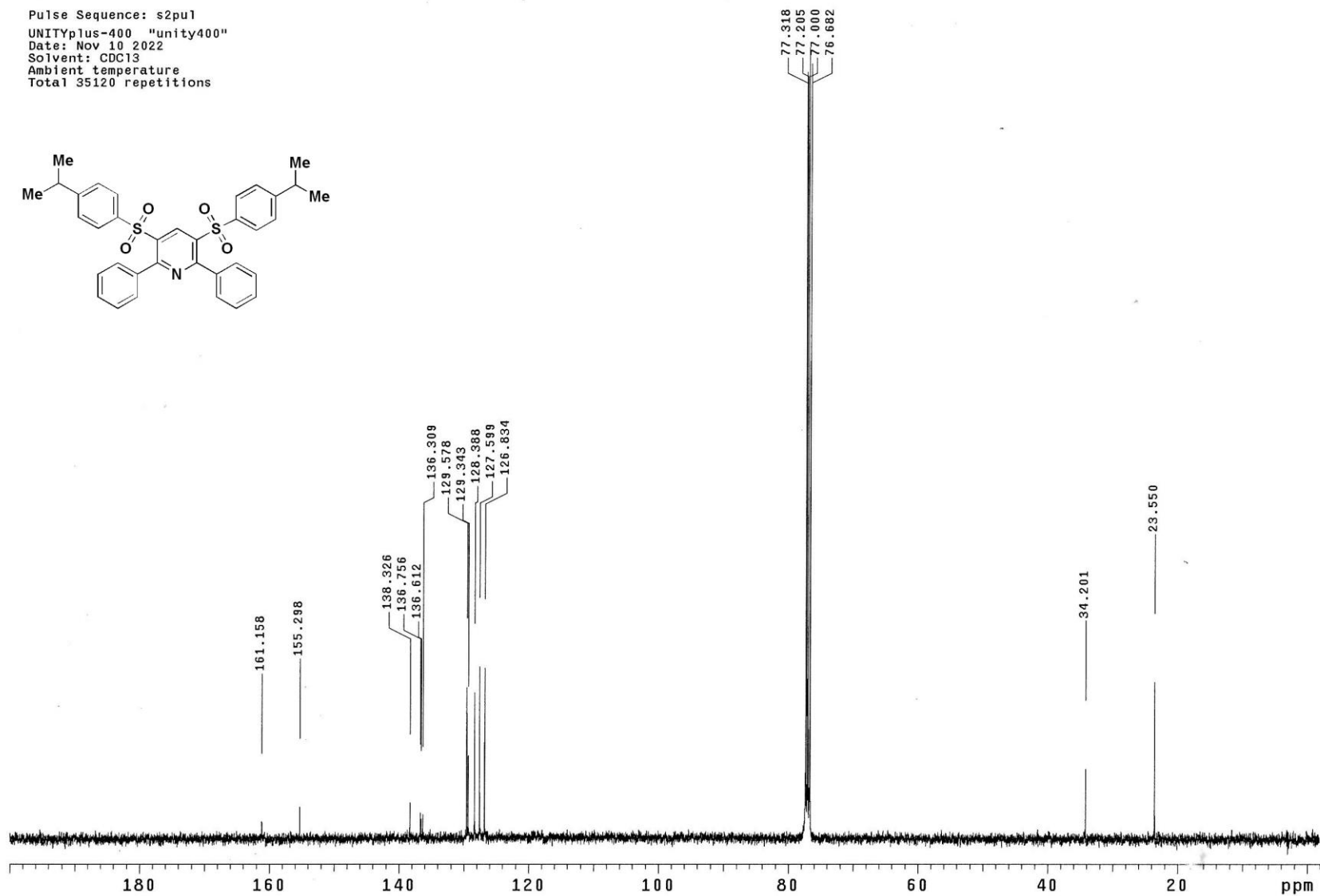
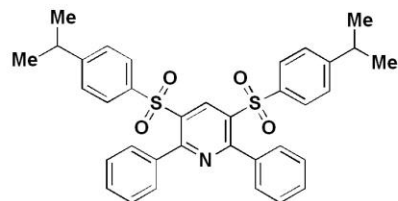
UNITYplus-400 "unity400"

Date: Nov 10 2022

Solvent: CDCl<sub>3</sub>

Ambient temperature

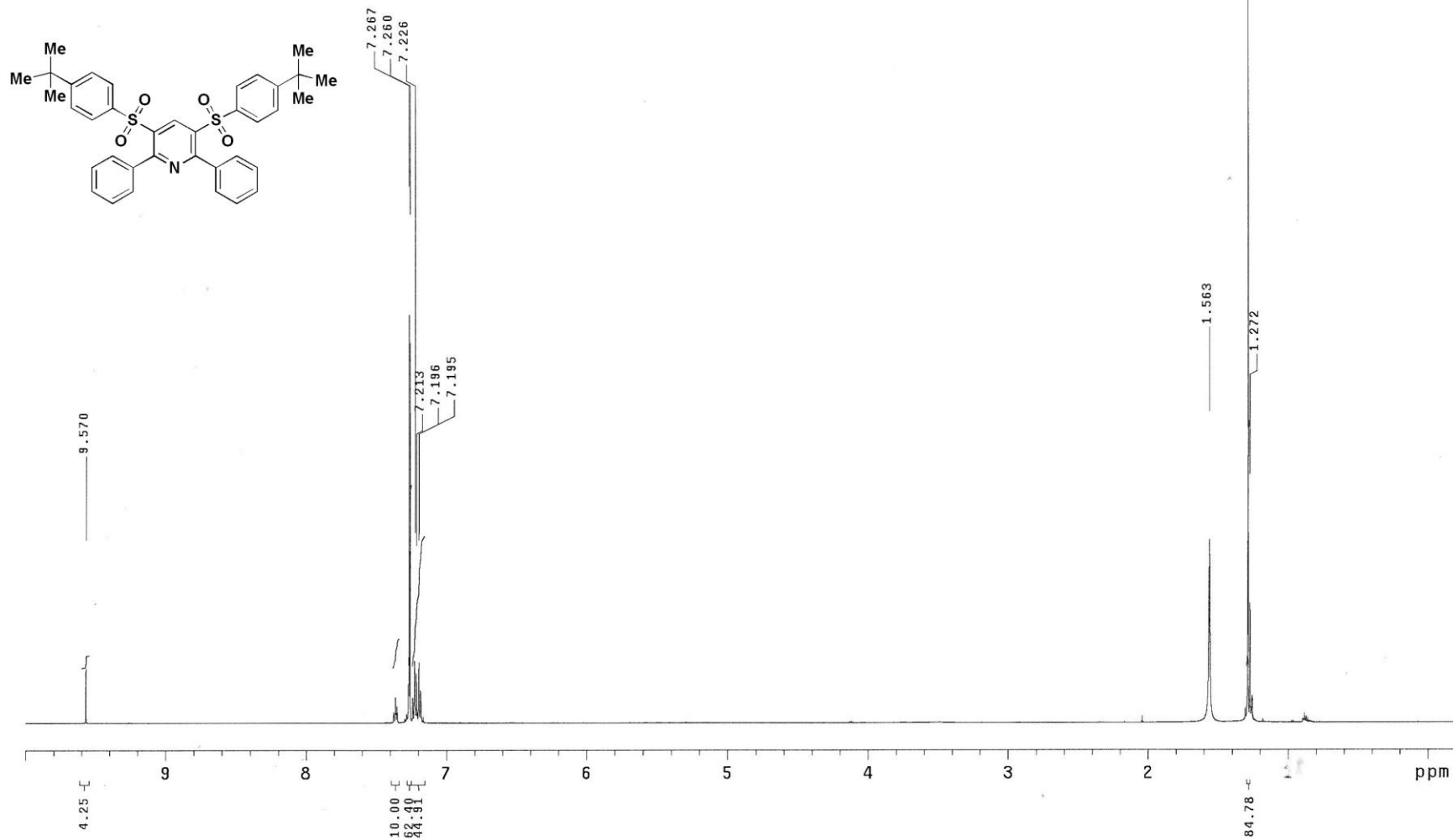
Total 35120 repetitions



# Compound 4n (<sup>1</sup>H-NMR spectral data)

YCM1430

Pulse Sequence: s2pu1  
 UNITYplus-600 "KMU600.kmu.edu.tw"  
 Date: Nov 17 2022  
 Solvent: cdc13  
 Temp. 28.0 C / 301.1 K  
 Total 128 repetitions



# Compound 4n (<sup>13</sup>C-NMR spectral data)

YCM1430

Pulse Sequence: s2pu1

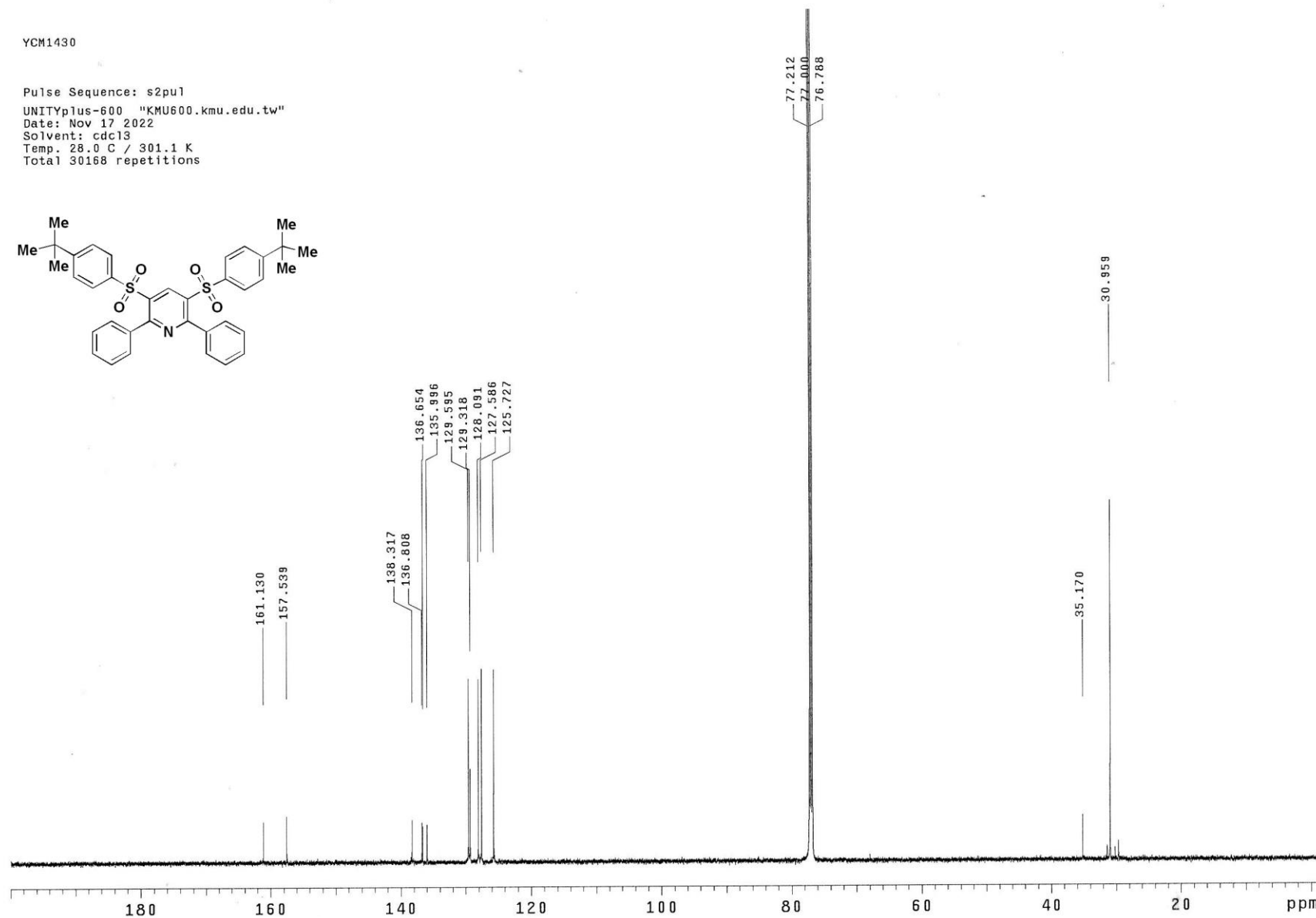
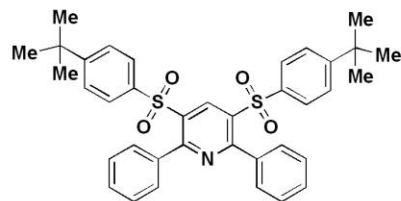
UNITYplus-600 "KMU600.kmu.edu.tw"

Date: Nov 17 2022

Solvent: cdc13

Temp. 28.0 C / 301.1 K

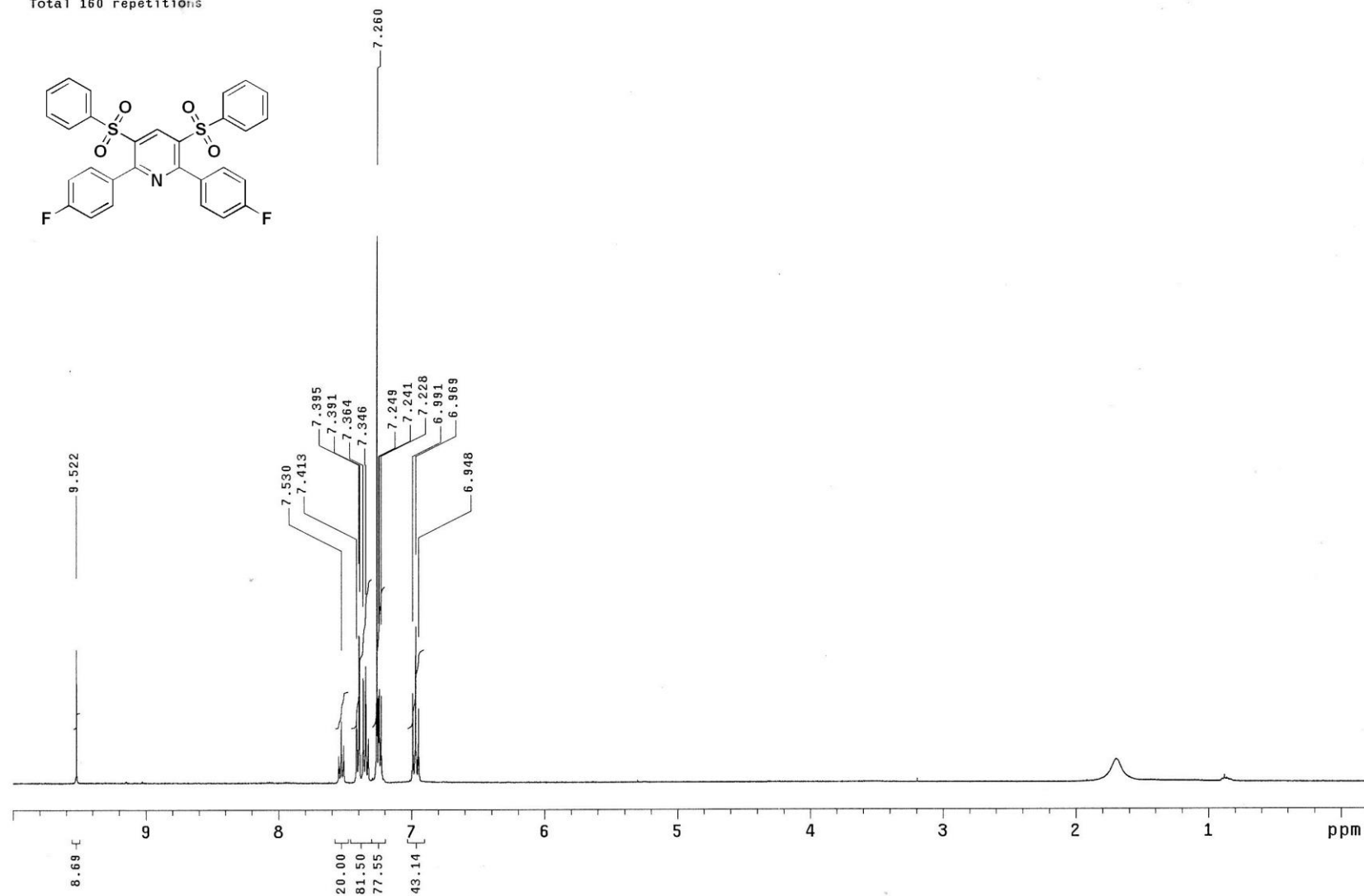
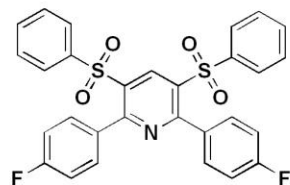
Total 30168 repetitions



# Compound 4o (<sup>1</sup>H-NMR spectral data)

YCM4250

Pulse Sequence: s2pu1  
 UNITYplus-400 "unity400"  
 Date: Feb 1 2023  
 Solvent: CDCl<sub>3</sub>  
 Ambient temperature  
 Total 160 repetitions

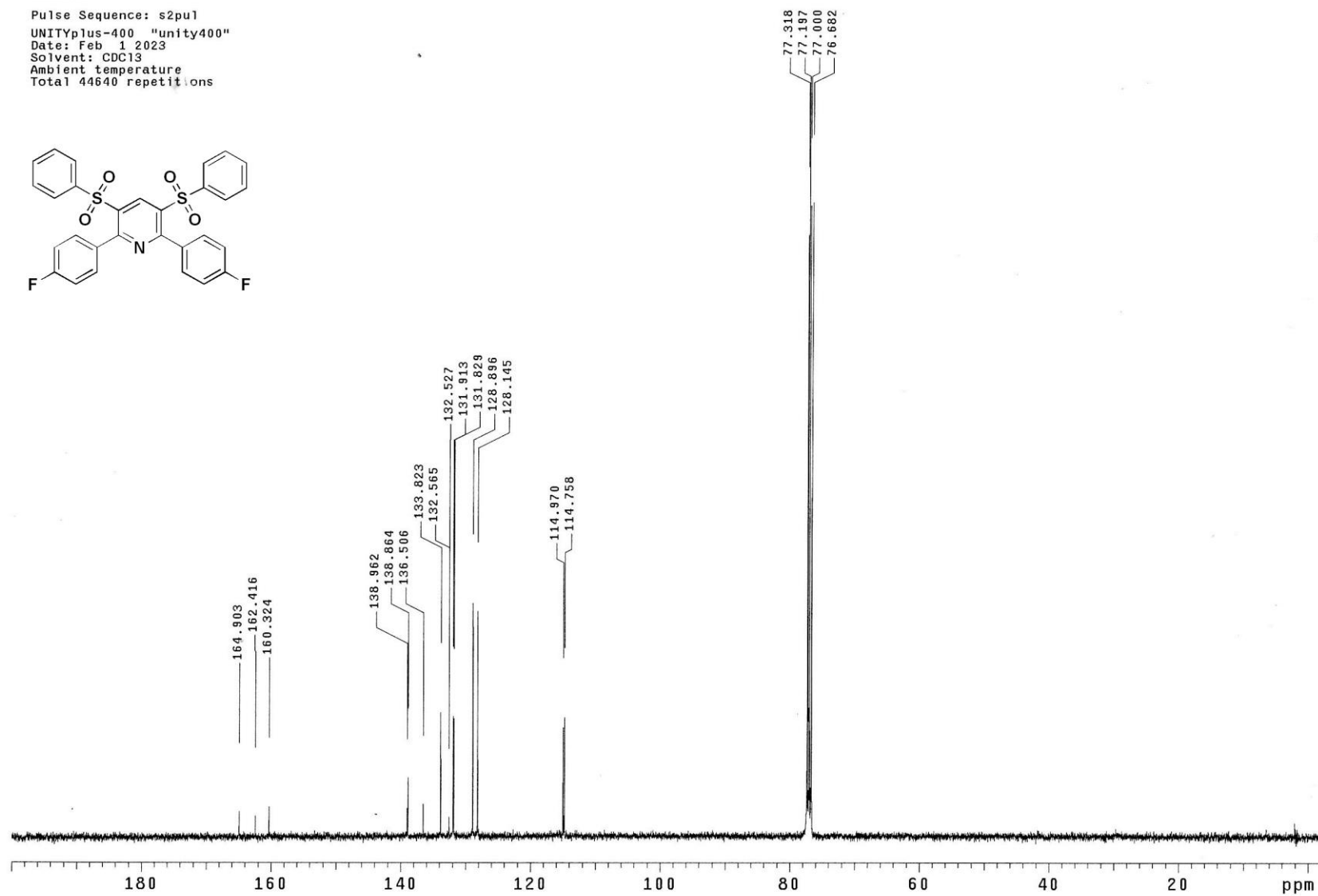
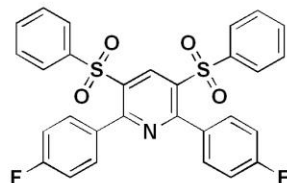




# Compound 4o (<sup>13</sup>C-NMR spectral data)

YCM4250

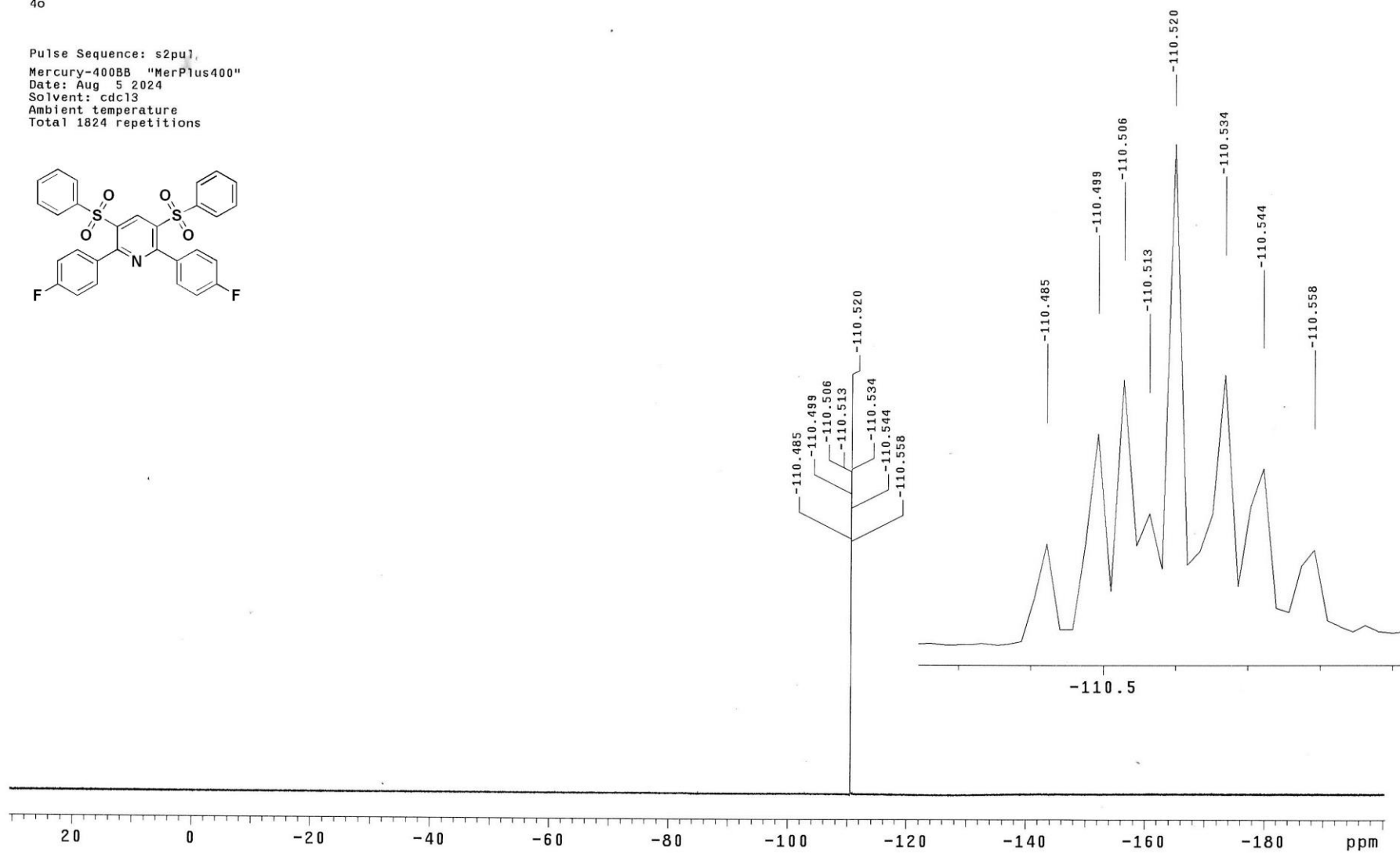
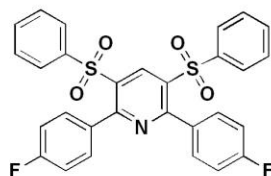
Pulse Sequence: s2pu1  
UNITYplus-400 "unity400"  
Date: Feb 1 2023  
Solvent: CDCl<sub>3</sub>  
Ambient temperature  
Total 44640 repetitions



# Compound 4o (<sup>19</sup>F-NMR spectral data)

4o

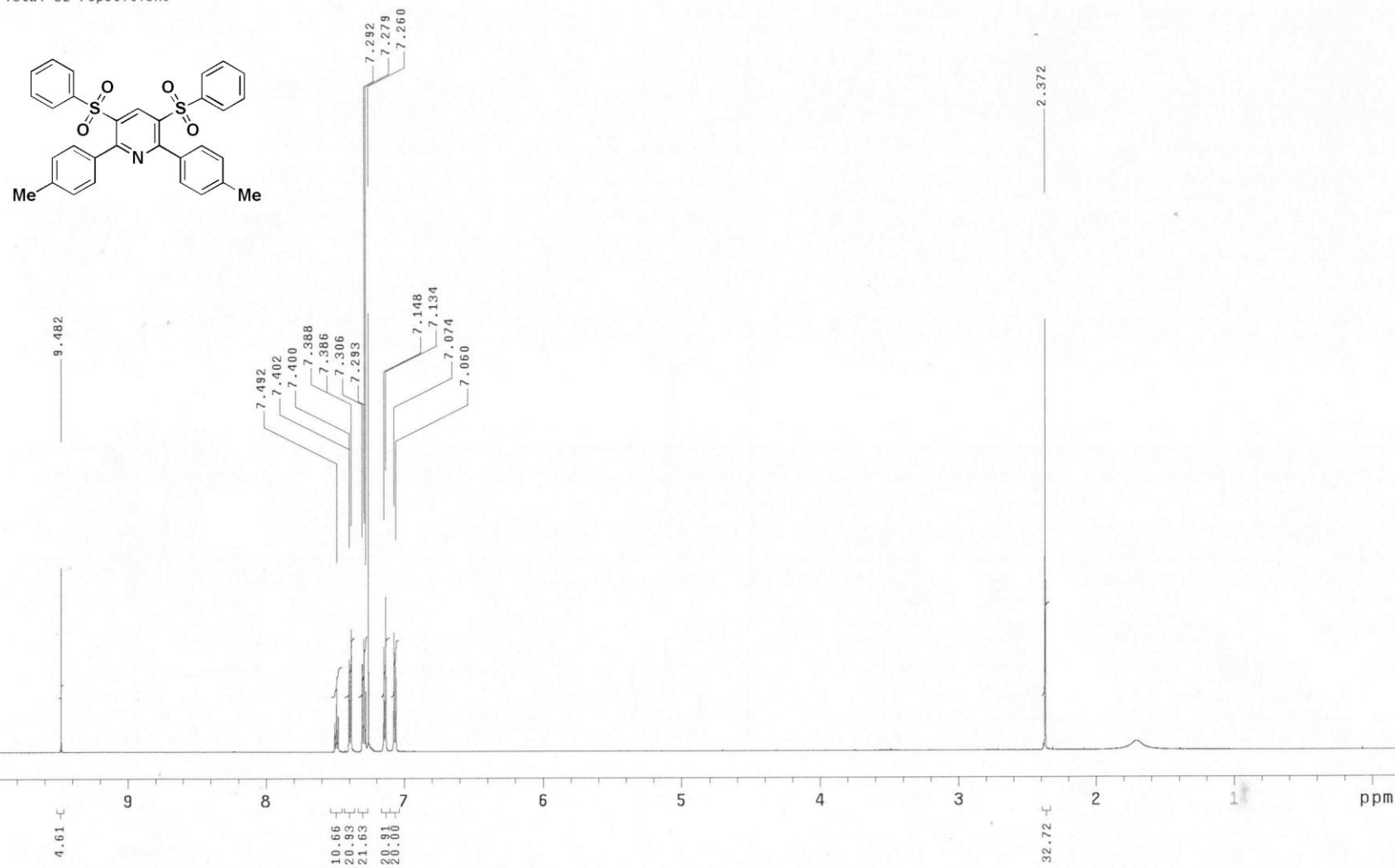
Pulse Sequence: s2pu1  
Mercury-400BB "MerPlus400"  
Date: Aug 5 2024  
Solvent: cdc13  
Ambient temperature  
Total 1824 repetitions



# Compound 4p (<sup>1</sup>H-NMR spectral data)

YCM2327

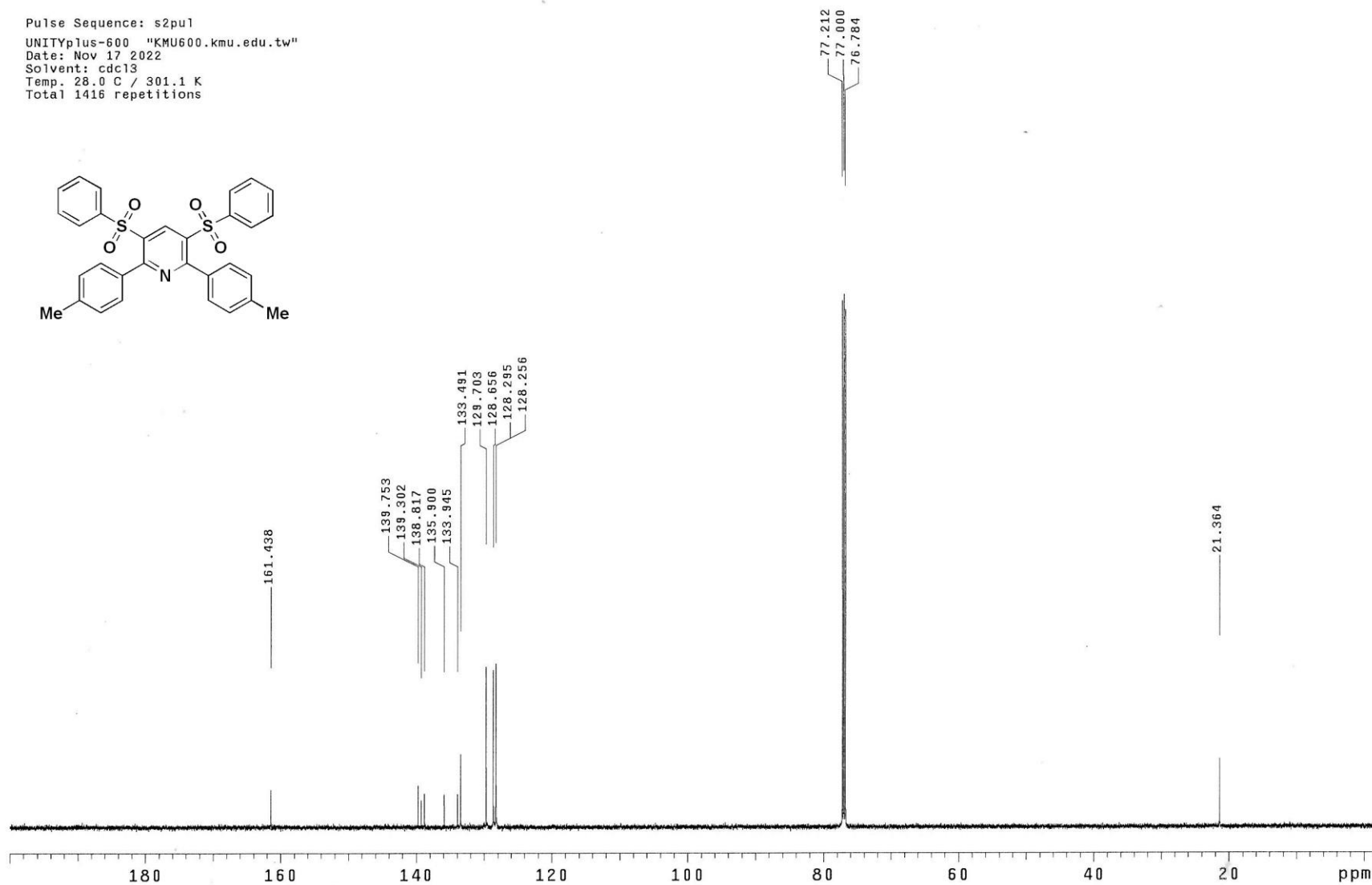
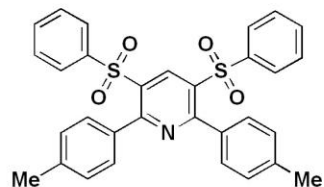
Pulse Sequence: s2pu1  
 UNITYplus-600 "KMU600.kmu.edu.tw"  
 Date: Nov 17 2022  
 Solvent: cdc13  
 Temp. 28.0 C / 301.1 K  
 Total 32 repetitions



# Compound 4p (<sup>13</sup>C-NMR spectral data)

YCM2327

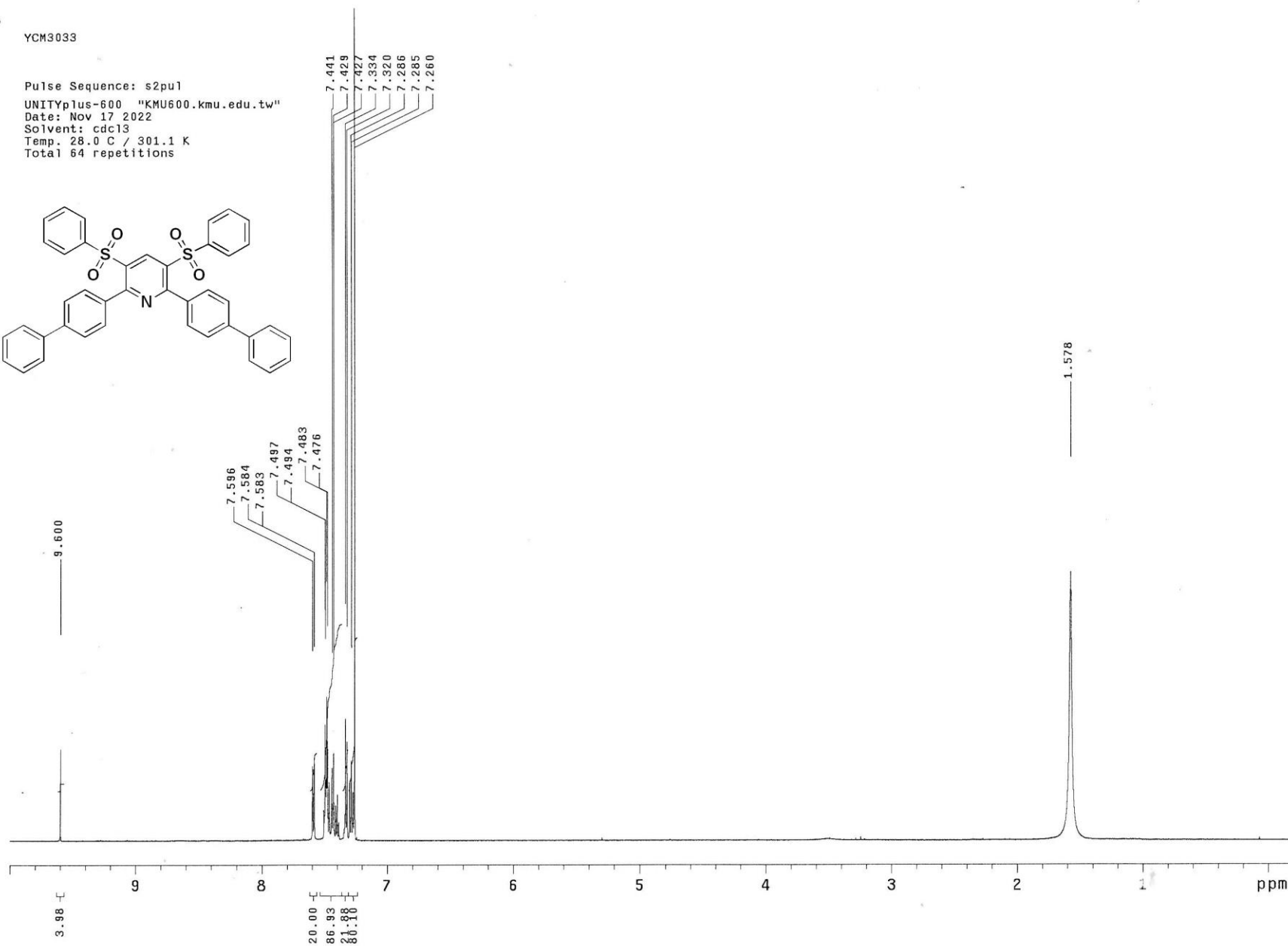
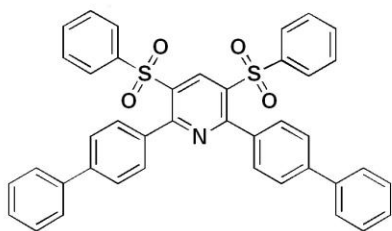
Pulse Sequence: s2pu1  
UNITYplus-600 "KMU600.kmu.edu.tw"  
Date: Nov 17 2022  
Solvent: cdc13  
Temp. 28.0 C / 301.1 K  
Total 1416 repetitions



# Compound 4q (<sup>1</sup>H-NMR spectral data)

YCM3033

Pulse Sequence: s2pu1  
 UNITYplus-600 "KMU600.kmu.edu.tw"  
 Date: Nov 17 2022  
 Solvent: cdc13  
 Temp. 28.0 C / 301.1 K  
 Total 64 repetitions



# Compound 4q (<sup>13</sup>C-NMR spectral data)

YCM3033

Pulse Sequence: s2pu1

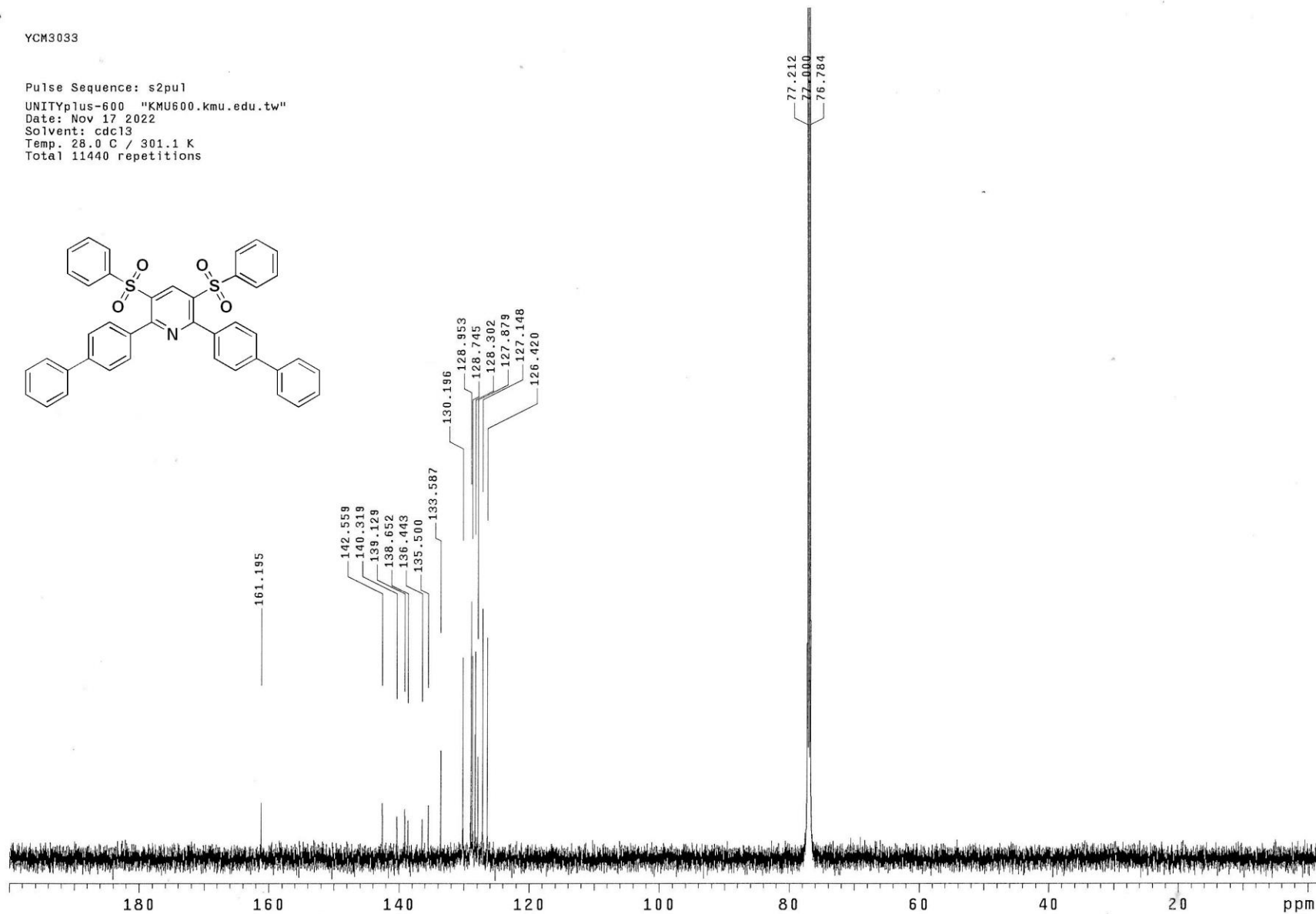
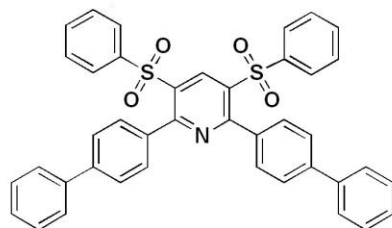
UNITYplus-600 "KMU600.kmu.edu.tw"

Date: Nov 17 2022

Solvent: cdc13

Temp. 28.0 C / 301.1 K

Total 11440 repetitions



# Compound 4r (<sup>1</sup>H-NMR spectral data)

YCM5962

Pulse Sequence: s2pu1

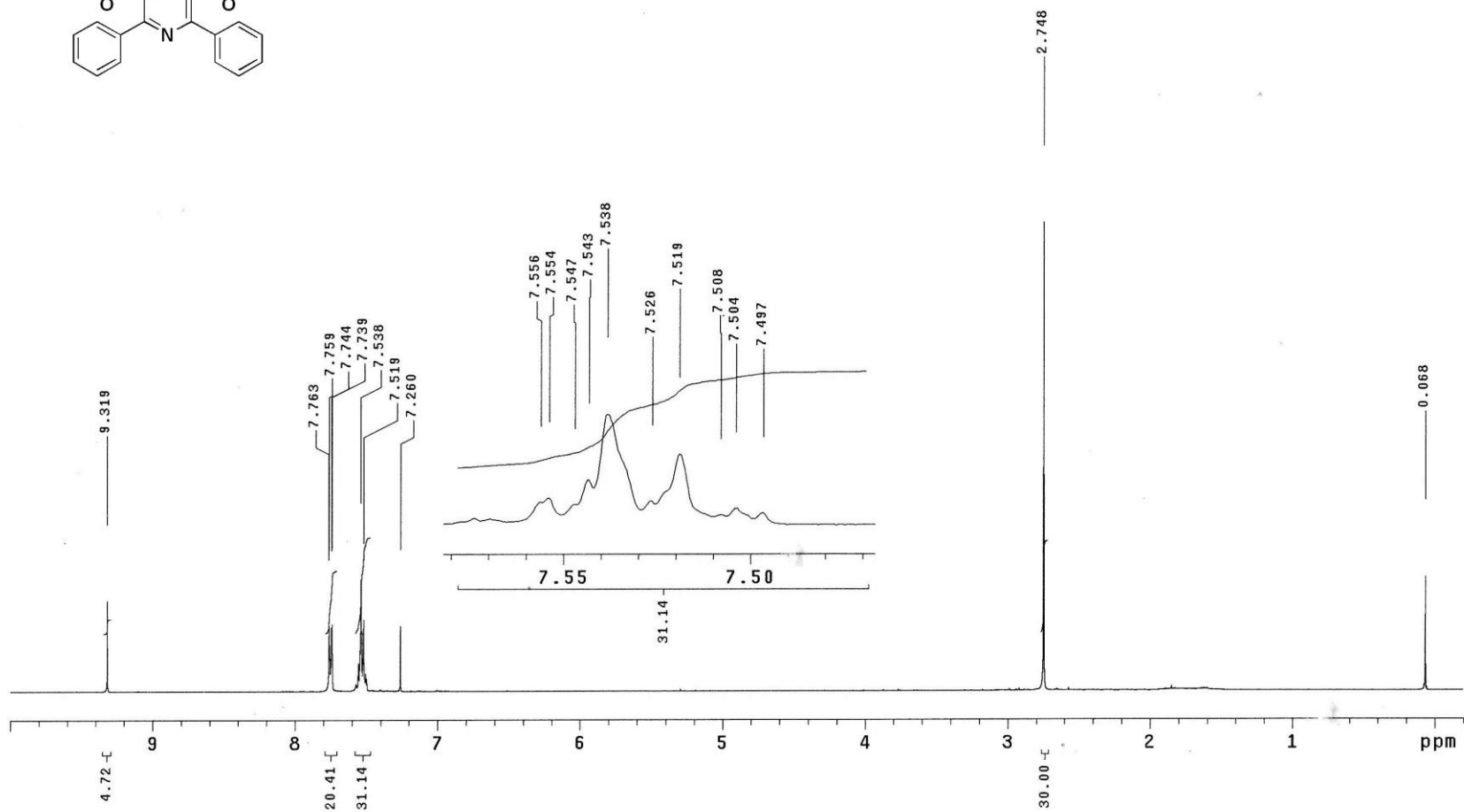
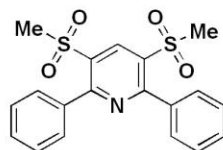
UNITYplus-400 "unity400"

Date: Nov 29 2022

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 32 repetitions



# Compound 4r (<sup>13</sup>C-NMR spectral data)

YCM5962

Pulse Sequence: s2pu1

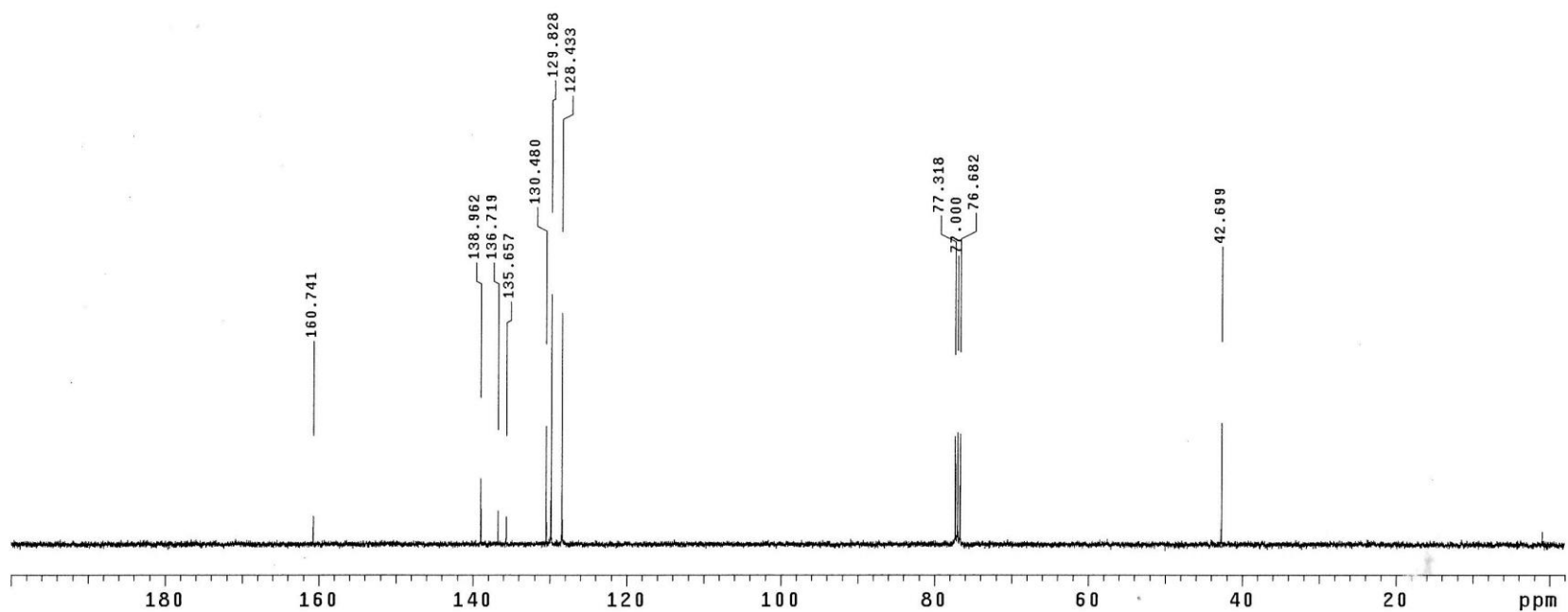
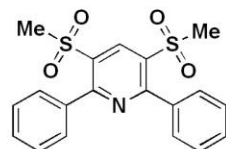
UNITYplus-400 "unity400"

Date: Nov 29 2022

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 2080 repetitions





# Compound 4s (<sup>1</sup>H-NMR spectral data)

YCM2143

Pulse Sequence: s2pu1

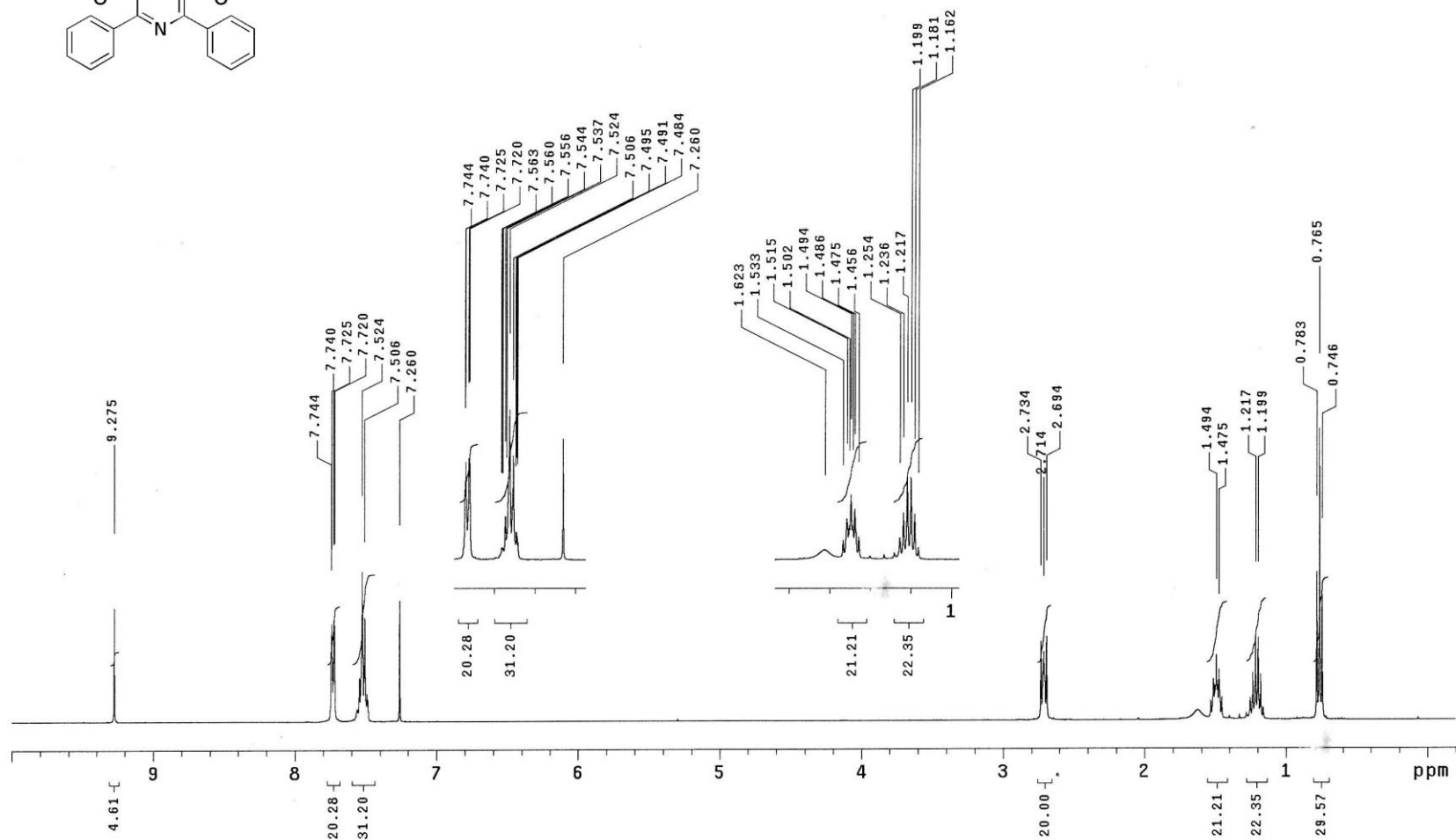
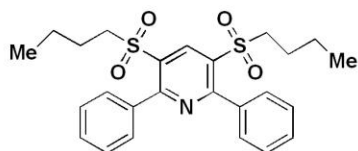
UNITYplus-400 "unity400"

Date: Dec 22 2022

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 32 repetitions



# Compound 4s (<sup>13</sup>C-NMR spectral data)

YCM2143

Pulse Sequence: s2pu1

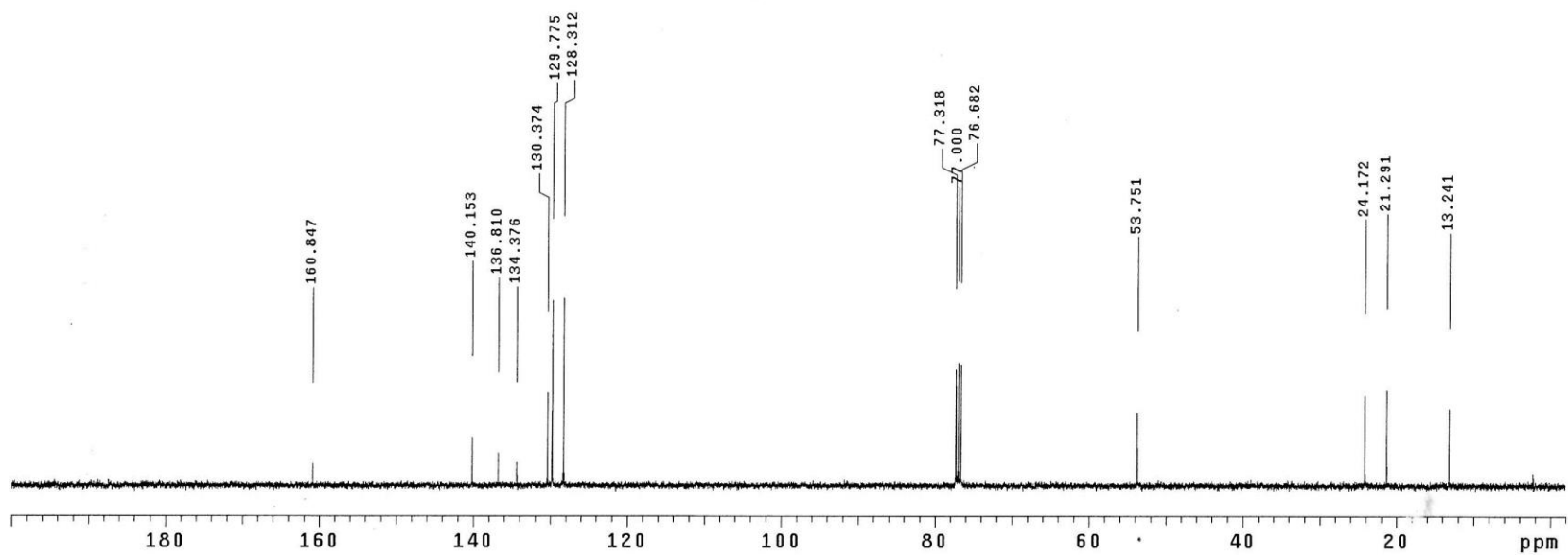
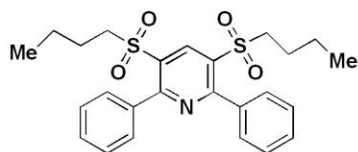
UNITYplus-400 "unity400"

Date: Dec 22 2022

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 1872 repetitions



# Compound 5 (<sup>1</sup>H-NMR spectral data)

YCM5282

Pulse Sequence: s2pu1

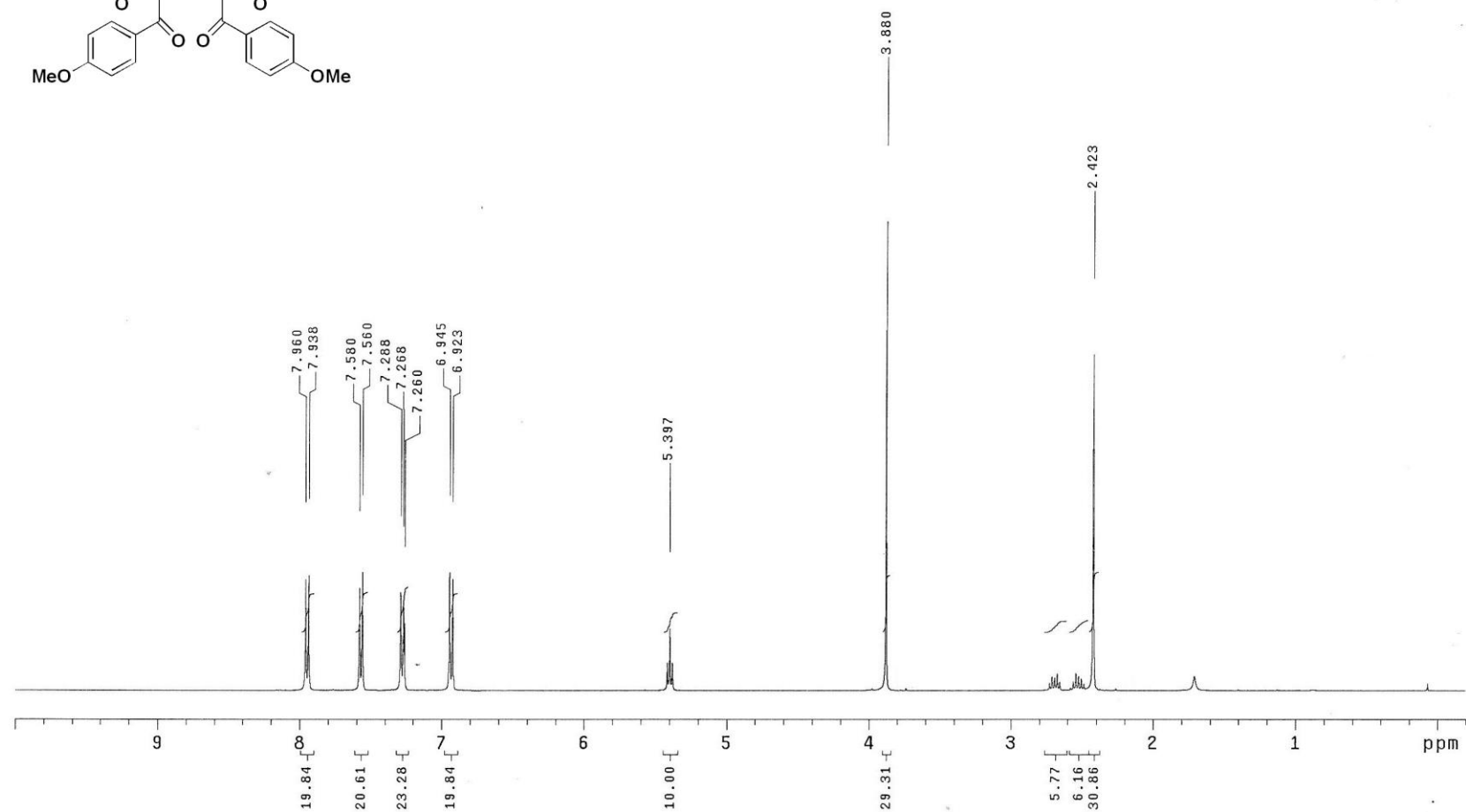
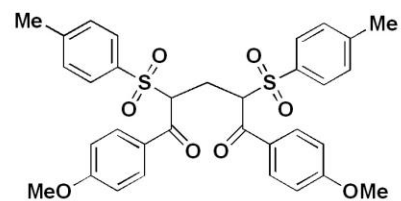
UNITYplus-400 "unity400"

Date: Sep 30 2024

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 32 repetition



# Compound 5 (<sup>13</sup>C-NMR spectral data)

YCM5282

Pulse Sequence: s2pu1

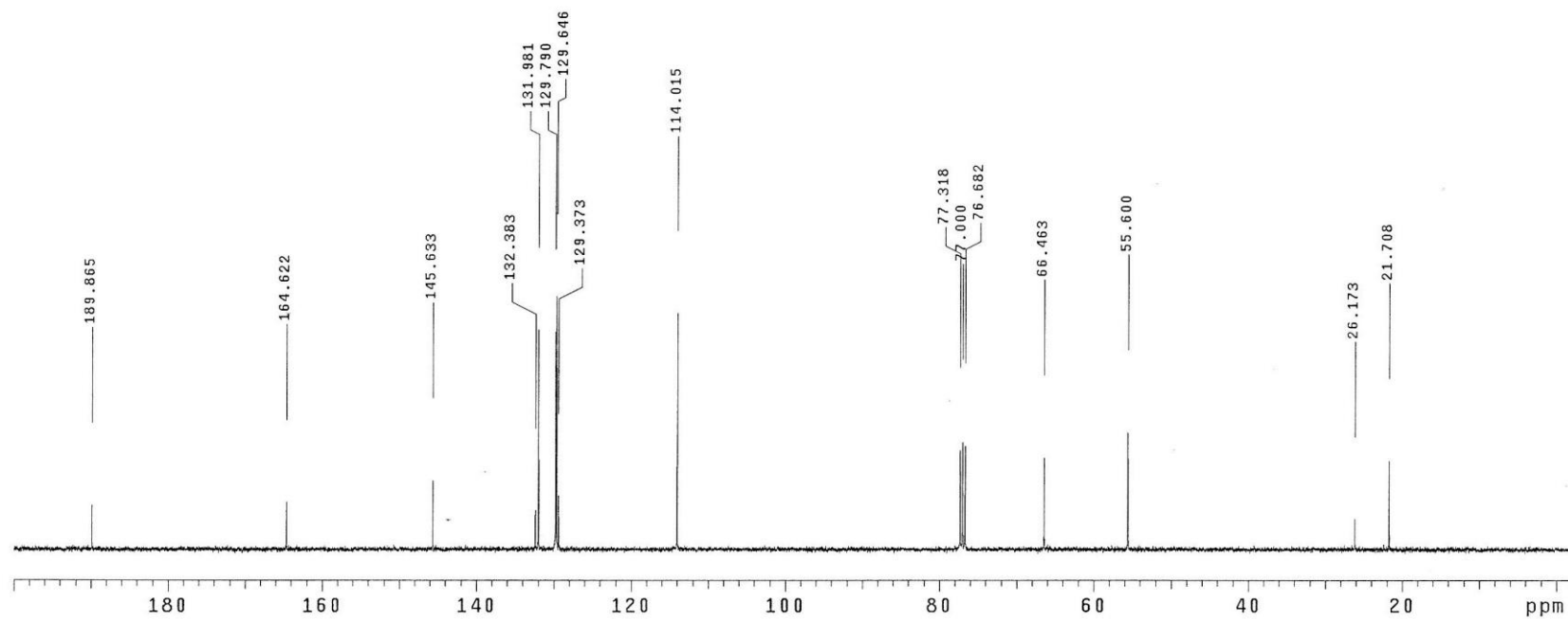
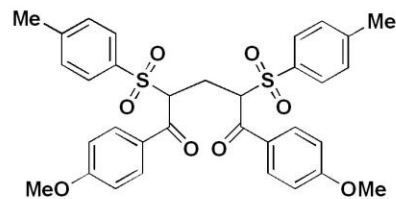
UNITYplus-400 "unity400"

Date: Sep 30 2024

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 2048 repetitions



# Compound 6a (<sup>1</sup>H-NMR spectral data)

HAN0Ph14

Pulse Sequence: s2pu1

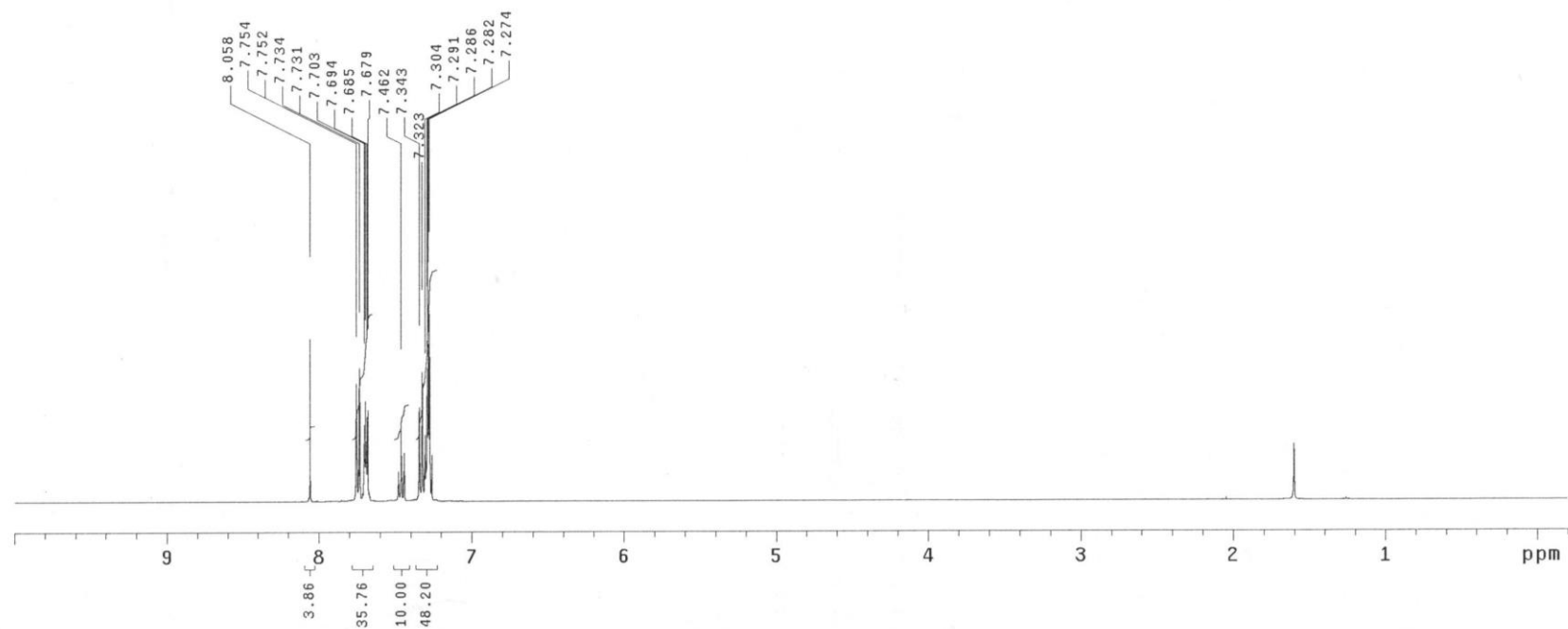
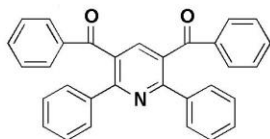
UNITYplus-400 "unity400"

Date: Oct 22 2018

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 32 repetitions



# Compound 6a (<sup>13</sup>C-NMR spectral data)

HANOPh14

Pulse Sequence: s2pu1

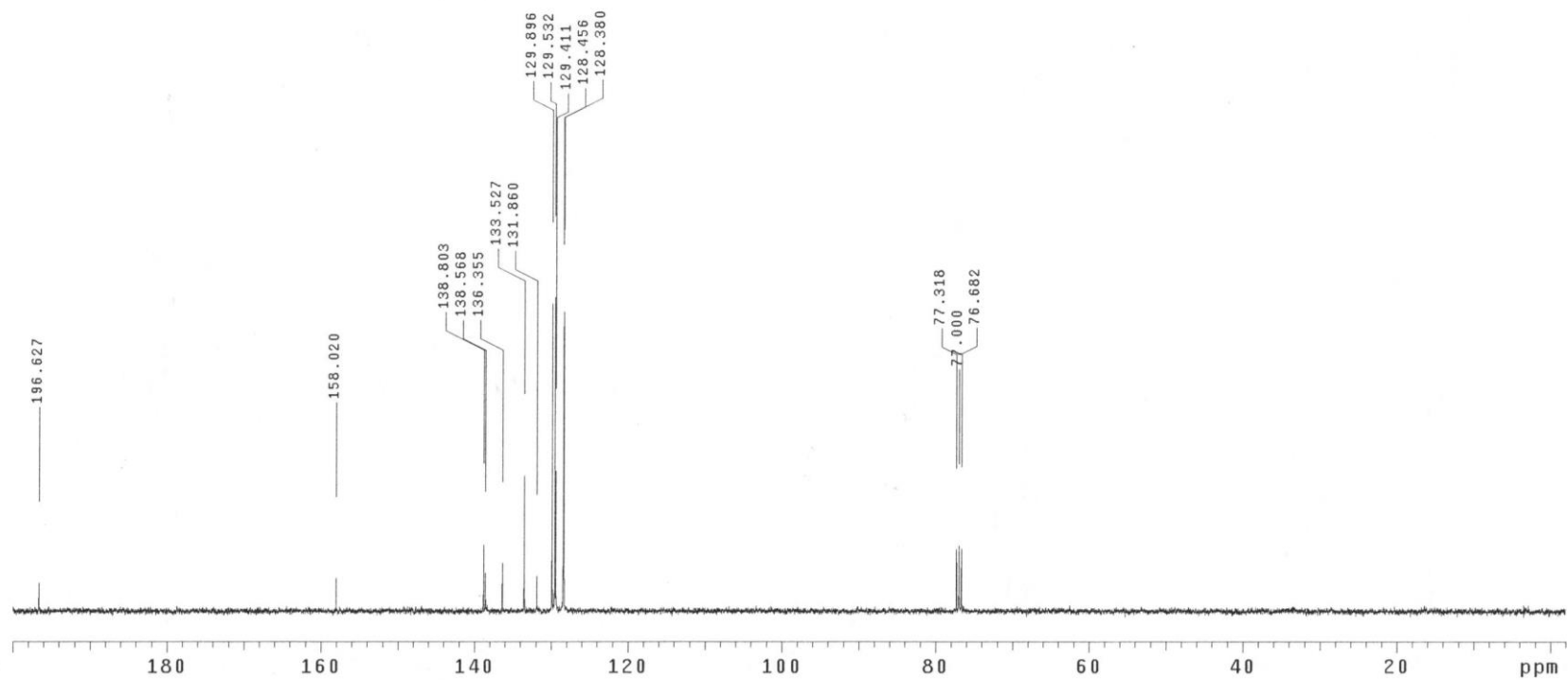
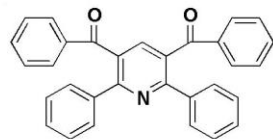
UNITYplus-400 "unity400"

Date: Oct 22 2018

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 400 repetitions



# Compound 8a (<sup>1</sup>H-NMR spectral data)

YCM2329

Pulse Sequence: s2pu1

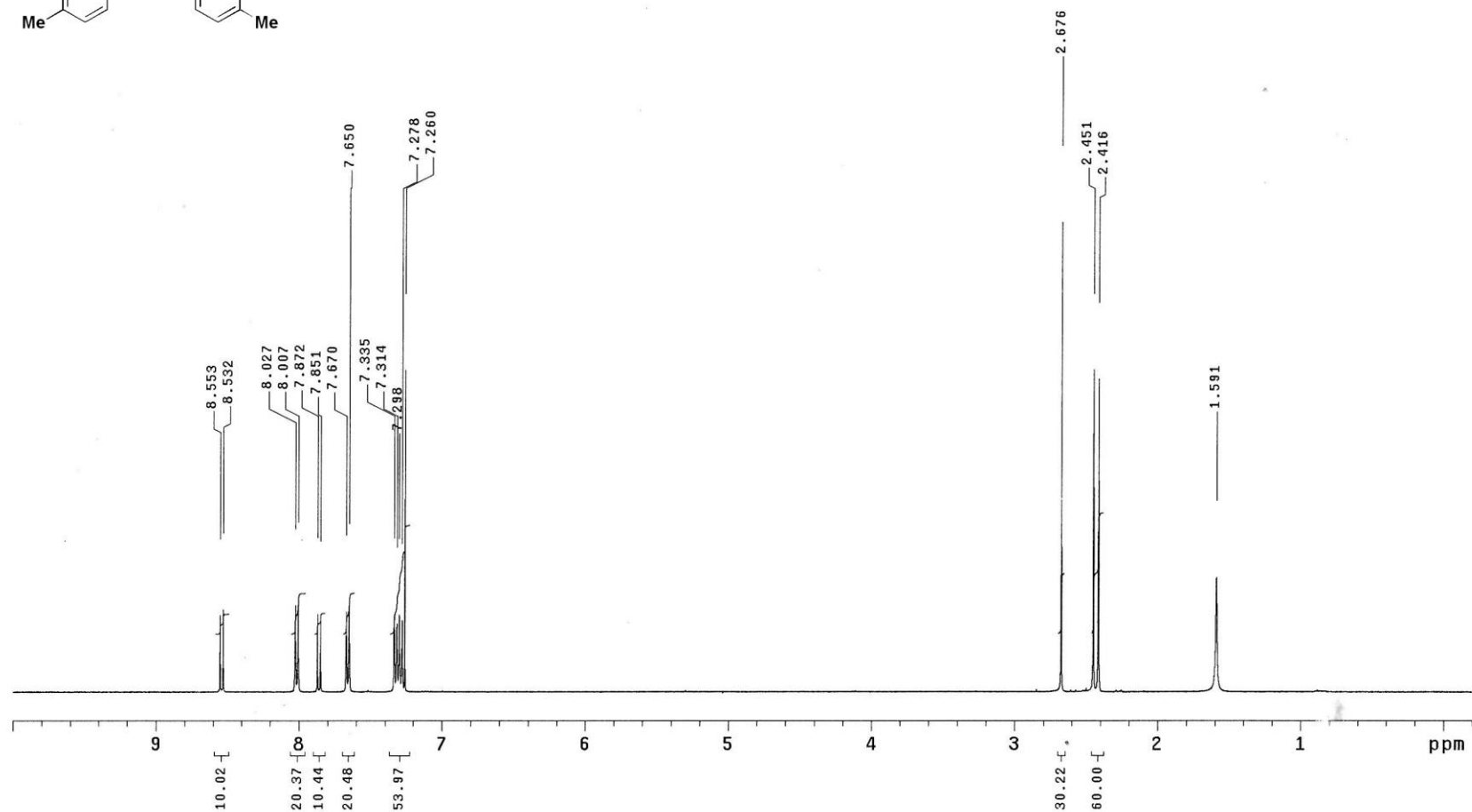
UNITYplus-400 "unity400"

Date: Dec 19 2022

Solvent: CDCl<sub>3</sub>

Ambient temperature

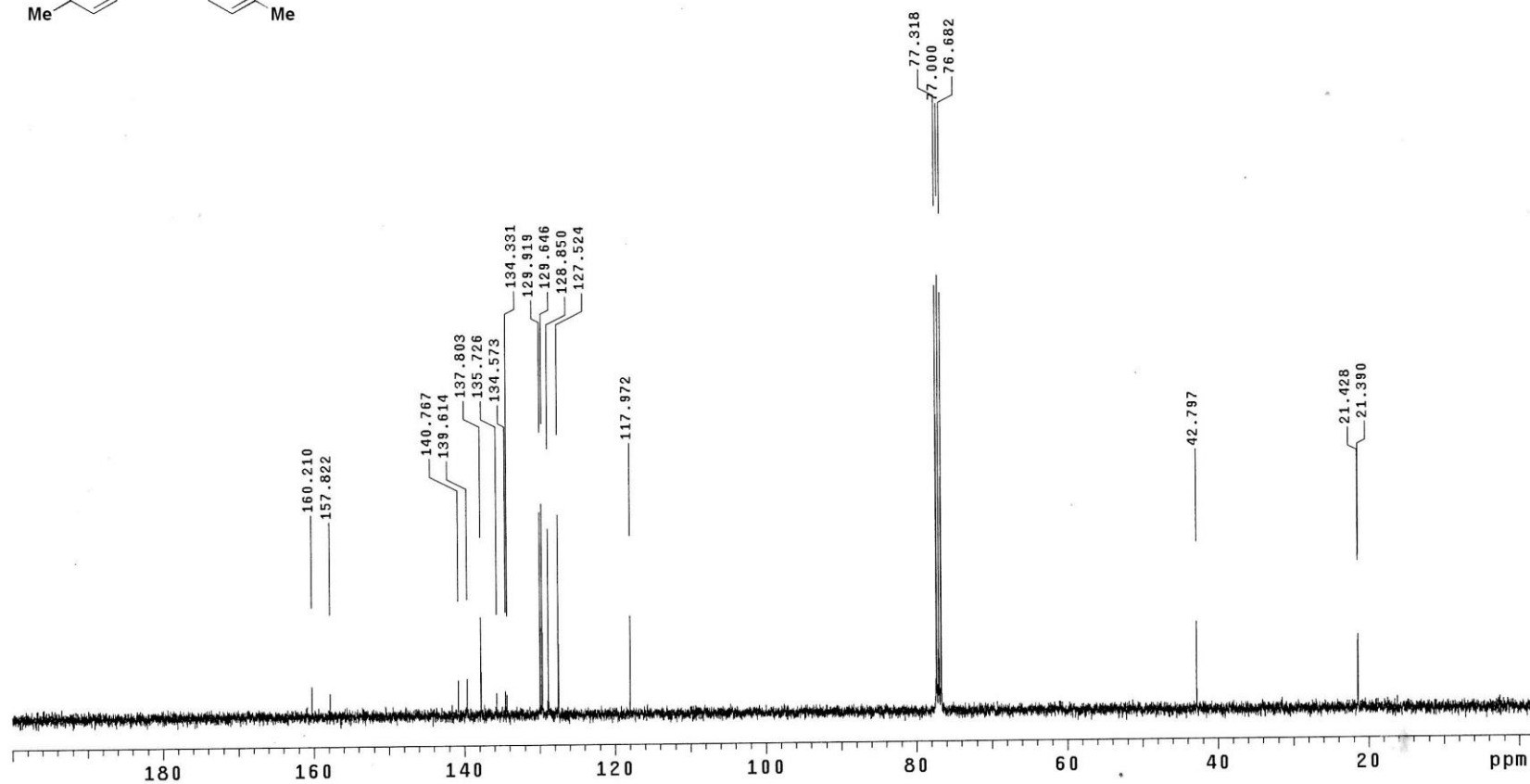
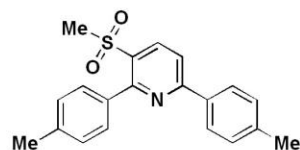
Total 32 repetitions



# Compound 8a (<sup>13</sup>C-NMR spectral data)

YCM2329

Pulse Sequence: s2pu1  
UNITYplus-400 "unity400"  
Date: Dec 19 2022  
Solvent: CDCl<sub>3</sub>  
Ambient temperature  
Total 5888 repetitions

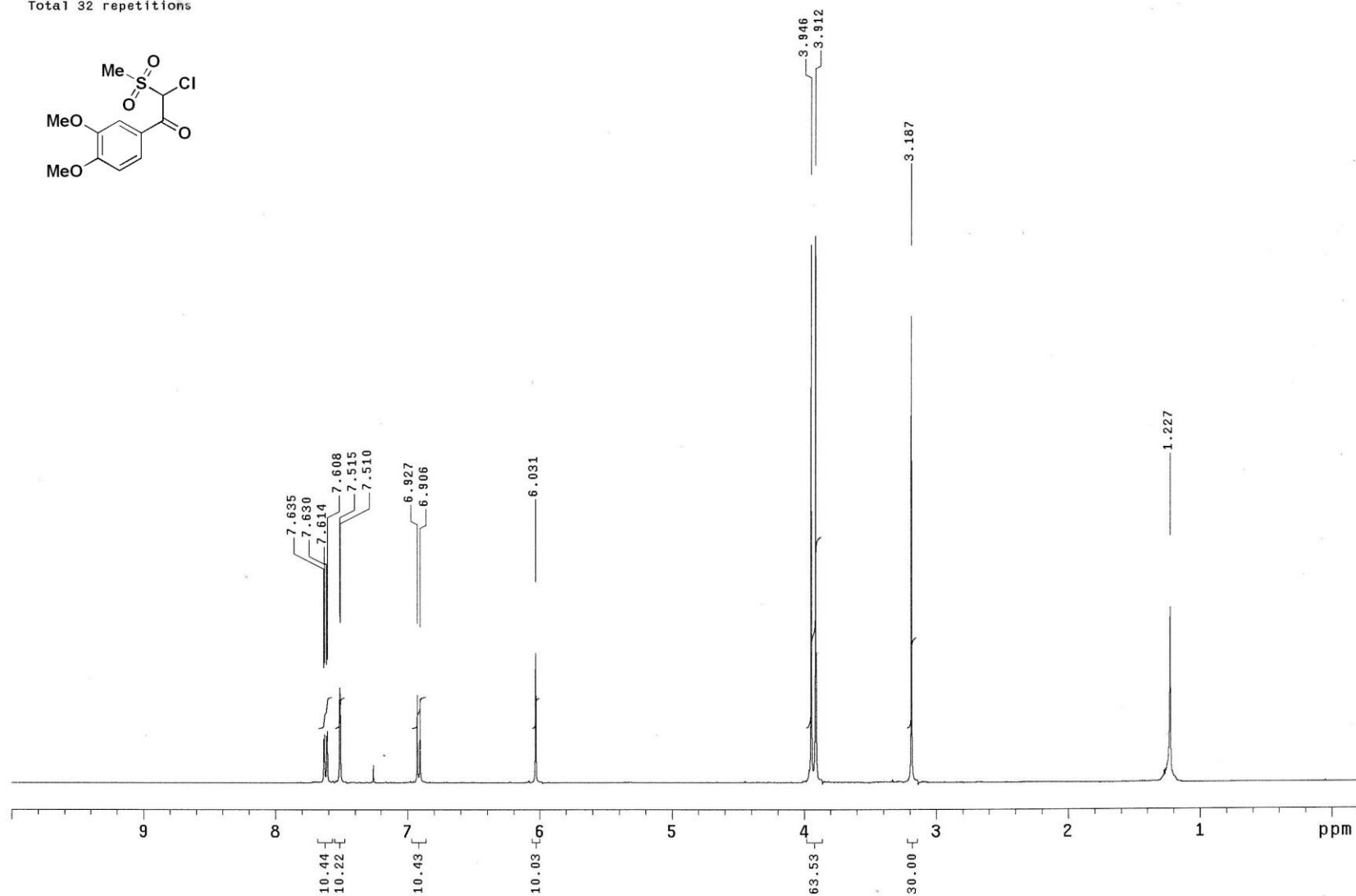
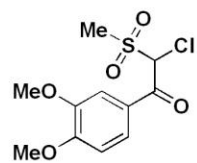




# Compound 9 (<sup>1</sup>H-NMR spectral data)

YC5160

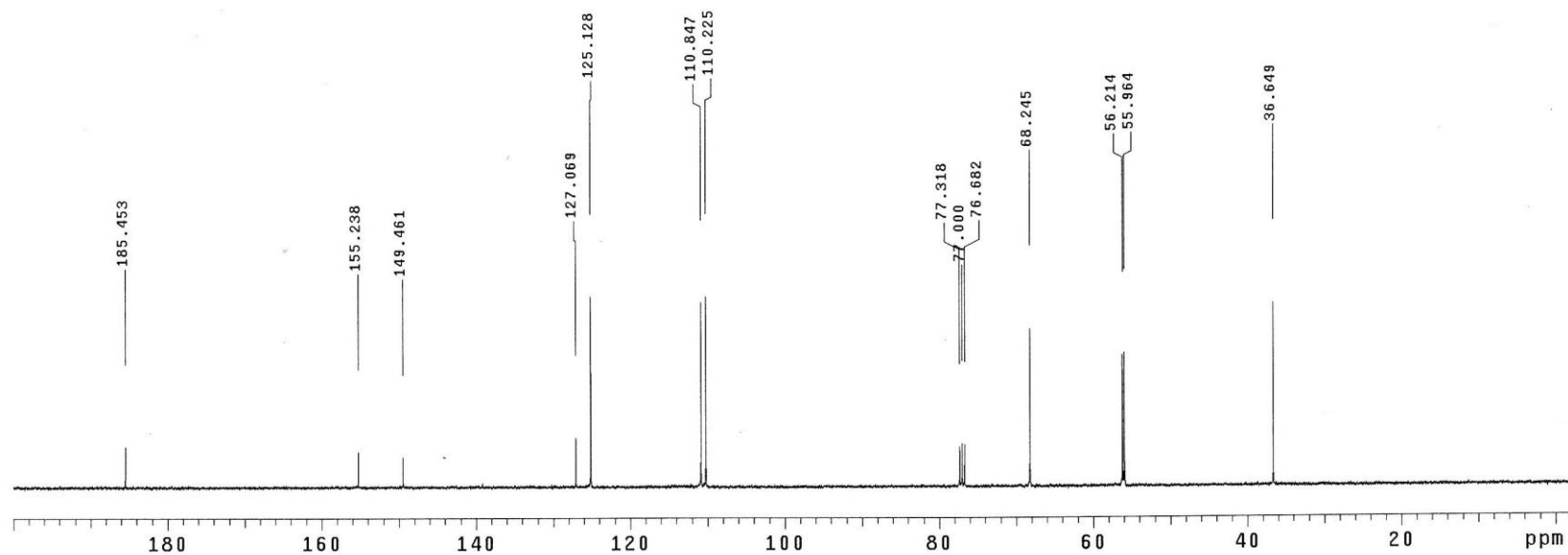
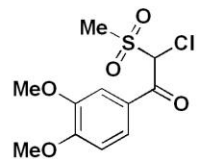
Pulse Sequence: s2pu1  
 UNITYplus-400 "unity400"  
 Date: Jul 26 2023  
 Solvent: CDCl<sub>3</sub>  
 Ambient temperature  
 Total 32 repetitions



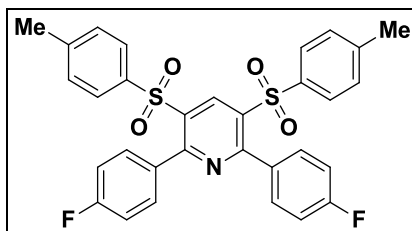
# Compound 9 (<sup>13</sup>C-NMR spectral data)

YC5160

Pulse Sequence: s2pu1  
UNITYplus-400 "unity400"  
Date: Jul 26 2023  
Solvent: CDCl<sub>3</sub>  
Ambient temperature  
Total 1232 repetitions

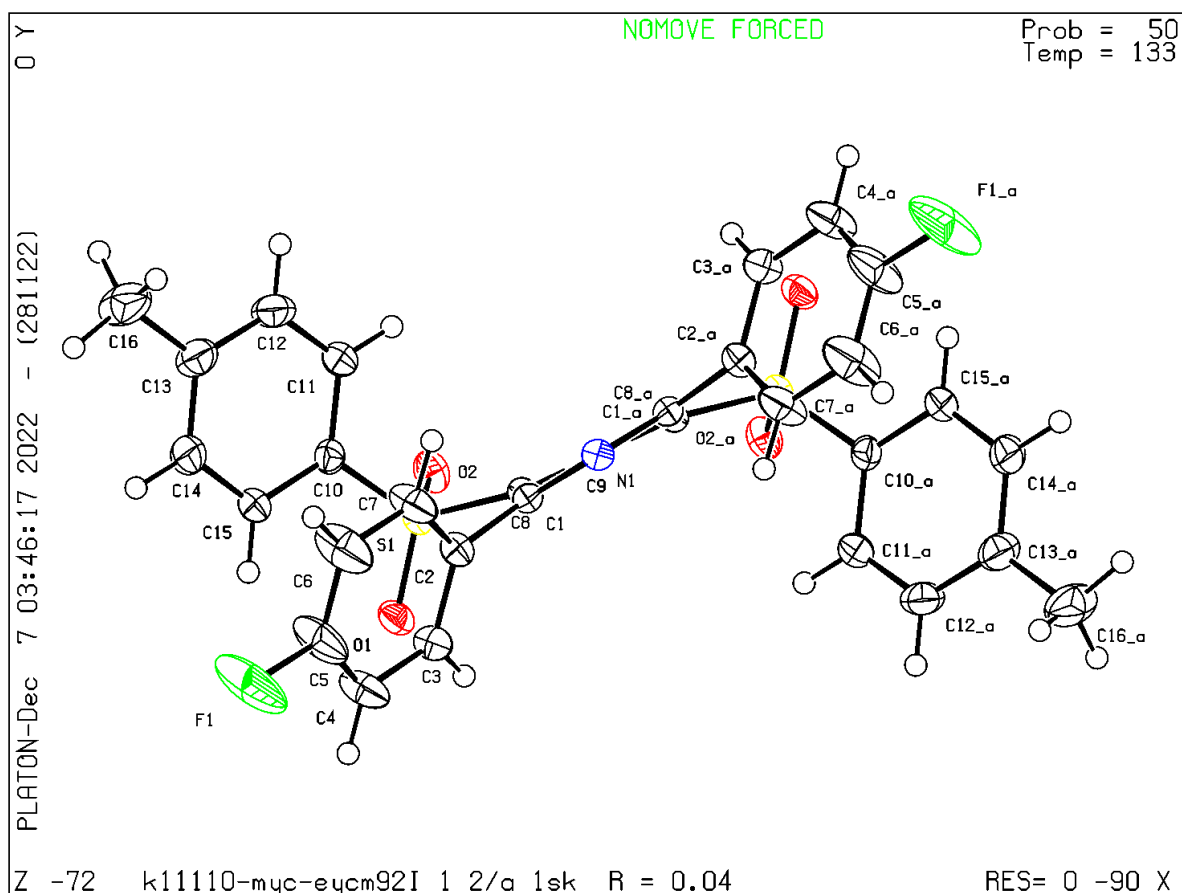


## X-ray crystal data of compound 4b



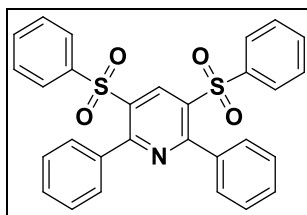
**Sample preparation** : A solution of compound **4b** (30 mg) in CH<sub>2</sub>Cl<sub>2</sub> (10 mL) was placed in a tube (10 mL). EtOAc (2 mL) was added slowly to the vial with a dropper. The vial was closed with little cotton and kept at room temperature for 2 days. Then, colorless prisms were observed.

**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.



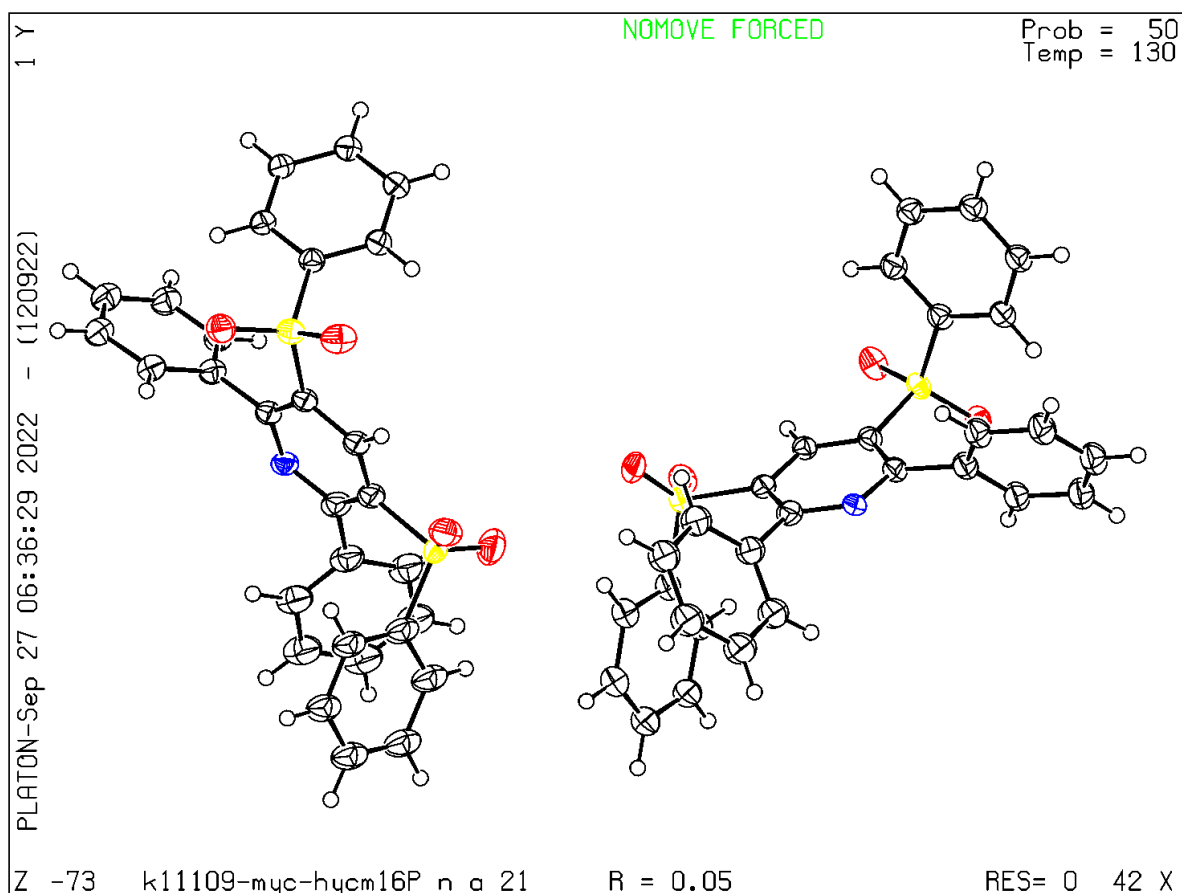
Empirical formula	C <sub>31</sub> H <sub>23</sub> F <sub>2</sub> NO <sub>4</sub> S <sub>2</sub>
Formula weight	575.62
Temperature/K	133(2)
Crystal system	monoclinic
Space group	I2/a
a/Å	12.1425(3)
b/Å	13.6754(3)
c/Å	18.9825(4)
$\alpha$ /°	90
$\beta$ /°	105.144(2)
$\gamma$ /°	90
Volume/Å <sup>3</sup>	3042.65(12)
Z	4
$\rho_{\text{calc}}$ /cm <sup>3</sup>	1.257
$\mu$ /mm <sup>-1</sup>	0.222
F(000)	1192.0
Crystal size/mm <sup>3</sup>	0.15 × 0.15 × 0.1
Radiation	Mo K $\alpha$ ( $\lambda$ = 0.71073)
2 $\Theta$ range for data collection/°	3.716 to 49.996
Index ranges	-14 ≤ h ≤ 14, -16 ≤ k ≤ 16, -22 ≤ l ≤ 22
Reflections collected	19630
Independent reflections	2685 [ $R_{\text{int}}$ = 0.0308, $R_{\text{sigma}}$ = 0.0197]
Data/restraints/parameters	2685/18/183
Goodness-of-fit on F <sup>2</sup>	1.058
Final R indexes [ $I \geq 2\sigma(I)$ ]	$R_1$ = 0.0363, $wR_2$ = 0.0959
Final R indexes [all data]	$R_1$ = 0.0390, $wR_2$ = 0.0976
Largest diff. peak/hole / e Å <sup>-3</sup>	0.53/-0.46

## X-ray crystal data of compound 4j



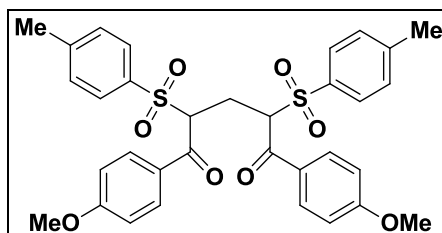
**Sample preparation** : A solution of compound **4j** (30 mg) in CH<sub>2</sub>Cl<sub>2</sub> (10 mL) was placed in a tube (10 mL). EtOAc (2 mL) was added slowly to the vial with a dropper. The vial was closed with little cotton and kept at room temperature for 2 days. Then, colorless prisms were observed.

**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.



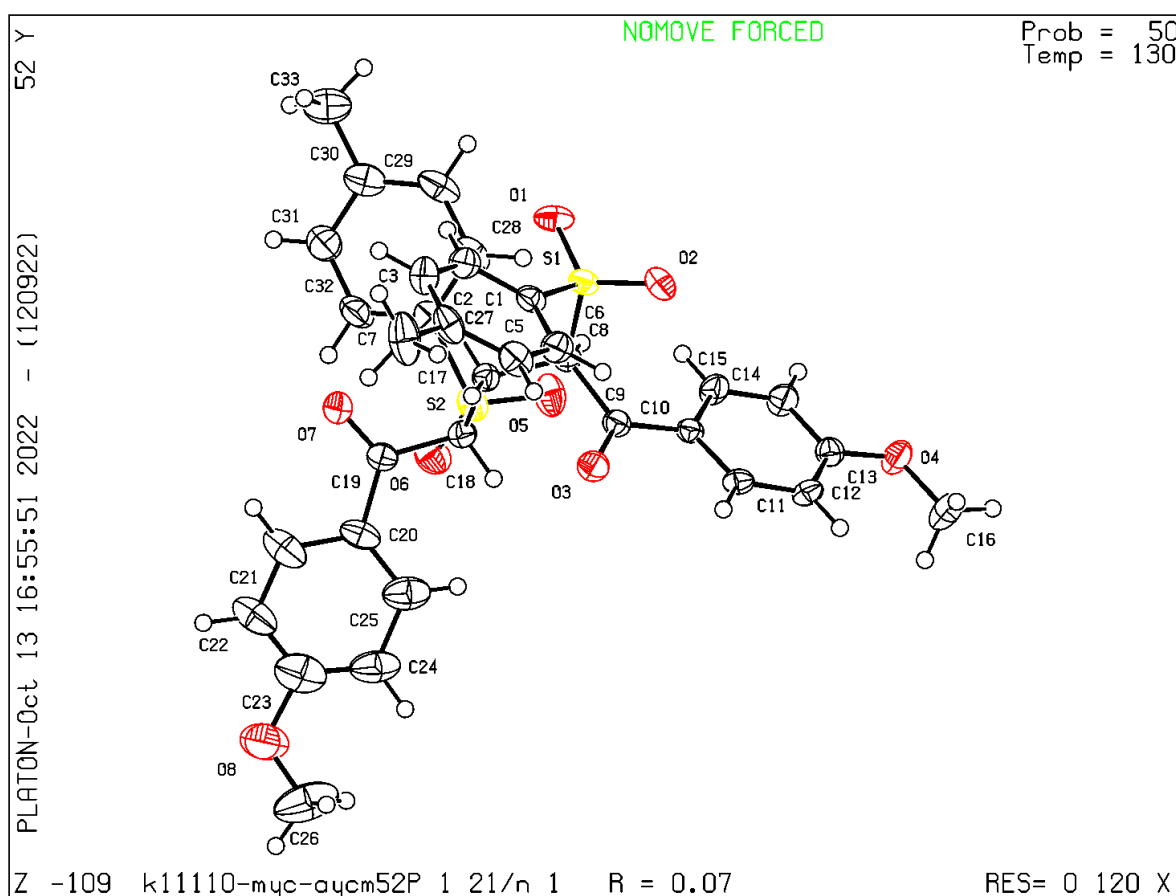
Temperature/K	130(2)
Crystal system	orthorhombic
Space group	Pna2 <sub>1</sub>
a/Å	16.1179(3)
b/Å	12.2499(2)
c/Å	26.8761(5)
$\alpha/^\circ$	90
$\beta/^\circ$	90
$\gamma/^\circ$	90
Volume/Å <sup>3</sup>	5306.49(16)
Z	4
$\rho_{\text{calc}}/\text{cm}^3$	1.281
$\mu/\text{mm}^{-1}$	0.235
F(000)	2128.0
Crystal size/mm <sup>3</sup>	0.4 × 0.2 × 0.2
Radiation	MoK $\alpha$ ( $\lambda$ = 0.71073)
2 $\theta$ range for data collection/ $^\circ$	3.654 to 49.998
Index ranges	-19 ≤ h ≤ 15, -14 ≤ k ≤ 12, -31 ≤ l ≤ 31
Reflections collected	36279
Independent reflections	8765 [ $R_{\text{int}}$ = 0.0266, $R_{\text{sigma}}$ = 0.0280]
Data/restraints/parameters	8765/361/649
Goodness-of-fit on F <sup>2</sup>	1.060
Final R indexes [ $I \geq 2\sigma(I)$ ]	$R_1$ = 0.0501, $wR_2$ = 0.1213
Final R indexes [all data]	$R_1$ = 0.0550, $wR_2$ = 0.1244
Largest diff. peak/hole / e Å <sup>-3</sup>	0.47/-0.60
Flack parameter	0.070(19)

## X-ray crystal data of compound 5



**Sample preparation** : A solution of compound **5** (30 mg) in CH<sub>2</sub>Cl<sub>2</sub> (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 <sub>33</sub> H <sub>32</sub> O <sub>8</sub> S <sub>2</sub>
Formula weight	620.70
Temperature/K	130(2)
Crystal system	monoclinic
Space group	P2 <sub>1</sub> /n
a/Å	12.3904(6)
b/Å	21.7691(7)
c/Å	12.4795(6)
α/°	90
β/°	117.735(6)
γ/°	90
Volume/Å <sup>3</sup>	2979.3(3)
Z	4
ρ <sub>calc</sub> /g/cm <sup>3</sup>	1.384
μ/mm <sup>-1</sup>	0.231
F(000)	1304.0
Crystal size/mm <sup>3</sup>	0.4 × 0.4 × 0.3
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.742 to 49.994
Index ranges	-14 ≤ h ≤ 14, -25 ≤ k ≤ 25, -14 ≤ l ≤ 14
Reflections collected	59375
Independent reflections	5233 [R <sub>int</sub> = 0.0810, R <sub>sigma</sub> = 0.0350]
Data/restraints/parameters	5233/84/392
Goodness-of-fit on F <sup>2</sup>	1.026
Final R indexes [I ≥ 2σ (I)]	R <sub>1</sub> = 0.0717, wR <sub>2</sub> = 0.1723
Final R indexes [all data]	R <sub>1</sub> = 0.0830, wR <sub>2</sub> = 0.1793
Largest diff. peak/hole / e Å <sup>-3</sup>	1.48/-0.65