

# Supporting Information

## Tandem C- and O-Alkylative Annulation of $\beta$ -Ketosulfones with 1,2-Bisbromomethyl Arenes. One-pot Construction of Sulfonyl Indanes Dioxadibenzofused Macrocycles

Nai-Chen Hsueh,<sup>a</sup> Kuan-Ting Chen<sup>a</sup> and Meng-Yang Chang<sup>\*a,b,c</sup>

<sup>a</sup>*Department of Medicinal and Applied Chemistry, Kaohsiung Medical University, Kaohsiung 807, Taiwan*

<sup>b</sup>*Department of Medical Research, Kaohsiung Medical University Hospital, Kaohsiung 807, Taiwan*

<sup>c</sup>*NPUST College of Professional Studies, National Pingtung University of Science and Technology,*

*Pingtung 912, Taiwan*

\*Corresponding author, email: [mychang@kmu.edu.tw](mailto:mychang@kmu.edu.tw)

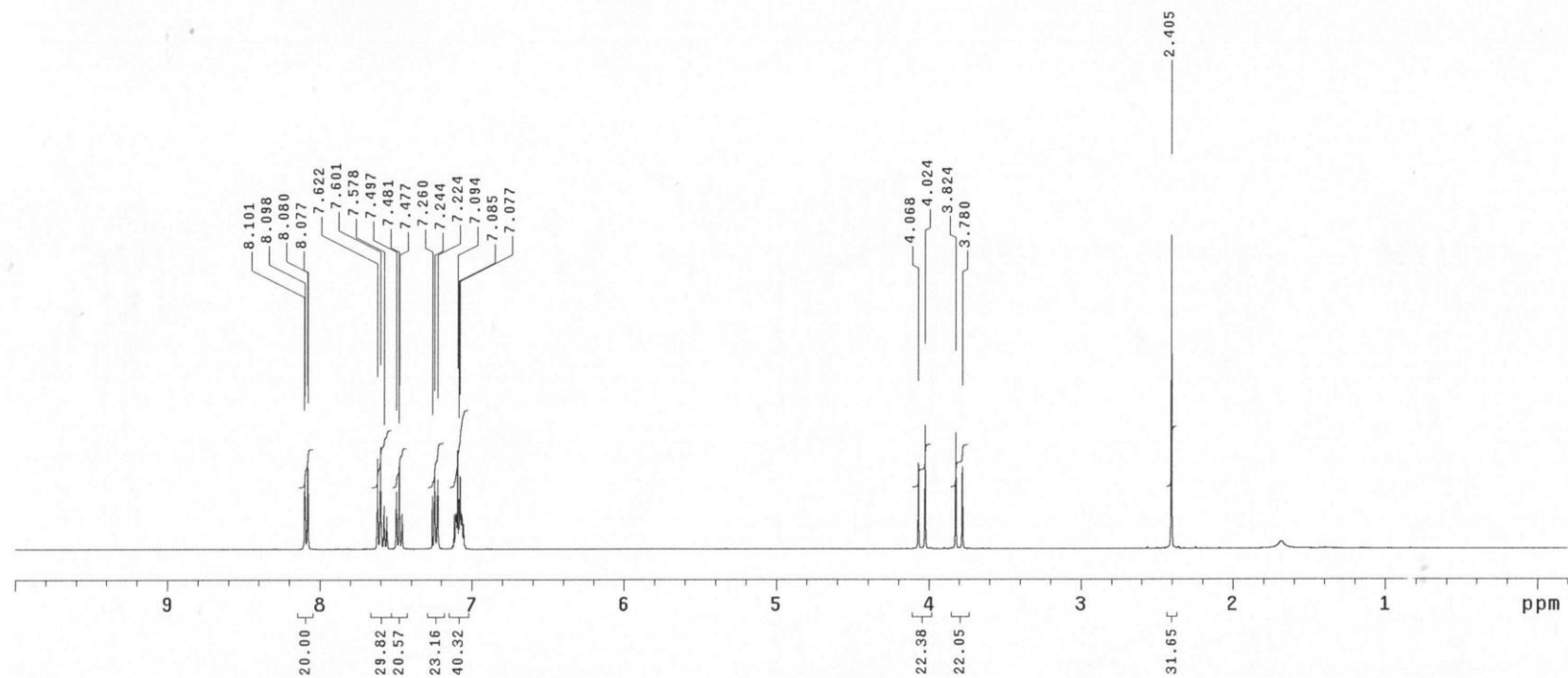
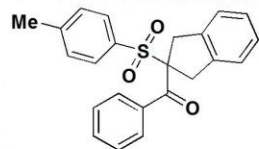
### Table of Contents

1.	<sup>1</sup> H NMR and <sup>13</sup> C NMR spectra copies of <b>7a-7ad</b>	S-2~S-61
2.	<sup>1</sup> H NMR and <sup>13</sup> C NMR spectra copies of <b>8a-8aa, 8m-1, 8ab-1, 8ad</b>	S-62~S-121
3.	<sup>1</sup> H NMR and <sup>13</sup> C NMR spectra copies of <b>12-15</b>	S-122~S-129
4.	X-ray crystal data of <b>7a, 8a, 8c, 8m, 8m-1, 8x-1, 8ab-1, 13, 14</b> and <b>15</b>	S-130~S-149

# Compound 7a (<sup>1</sup>H-NMR spectral data)

KT0421

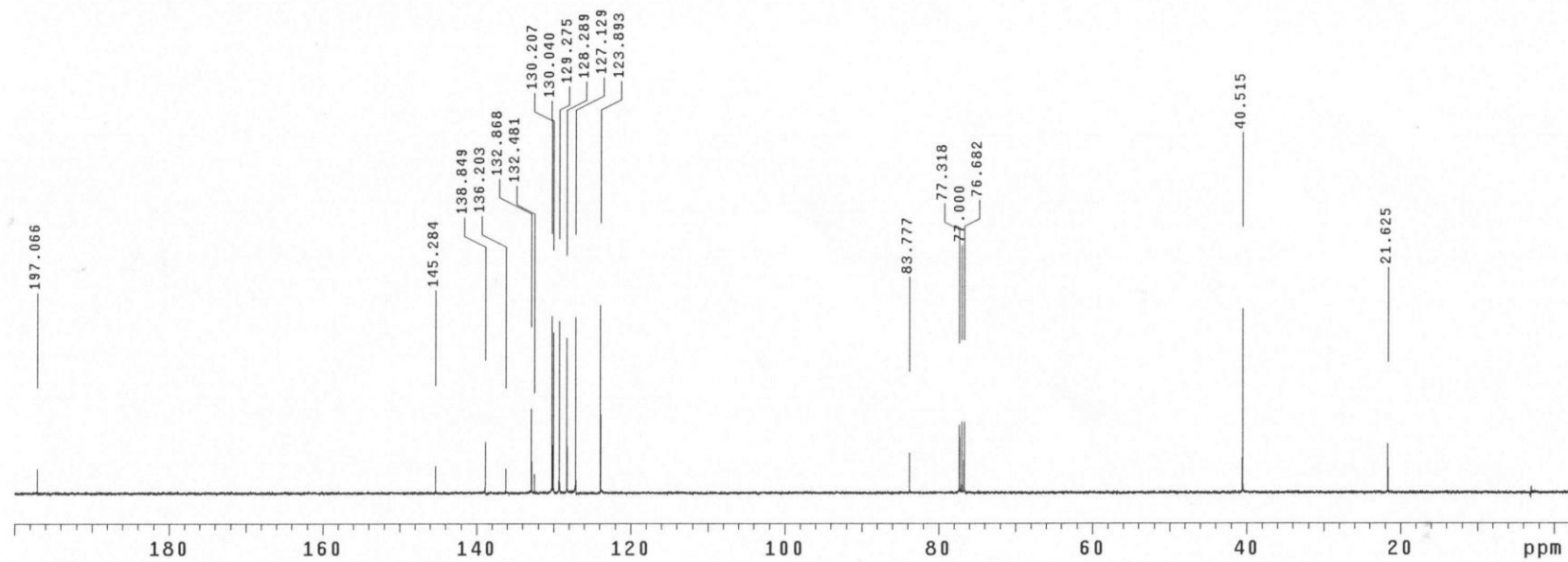
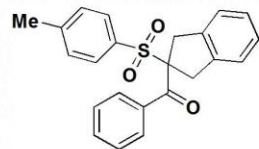
Pulse Sequence: s2pu1  
UNITYplus-400 "unity400"  
Date: Apr 21 2020  
Solvent: CDC13  
Ambient temperature  
Total 32 repetitions



# Compound 7a (<sup>13</sup>C-NMR spectral data)

KT0421

Pulse Sequence: s2pu1  
UNITYplus-400 "unity400"  
Date: Apr 21 2020  
Solvent: CDC13  
Ambient temperature  
Total 2624 repetitions



# Compound 7b (<sup>1</sup>H-NMR spectral data)

NC0624-5

Pulse Sequence: s2pu1

Solvent: CDCl<sub>3</sub>

Ambient temperature

UNITYplus-400 "unity400"

Pulse 38.8 degrees

Acq. time 3.744 sec

Width 6000.6 Hz

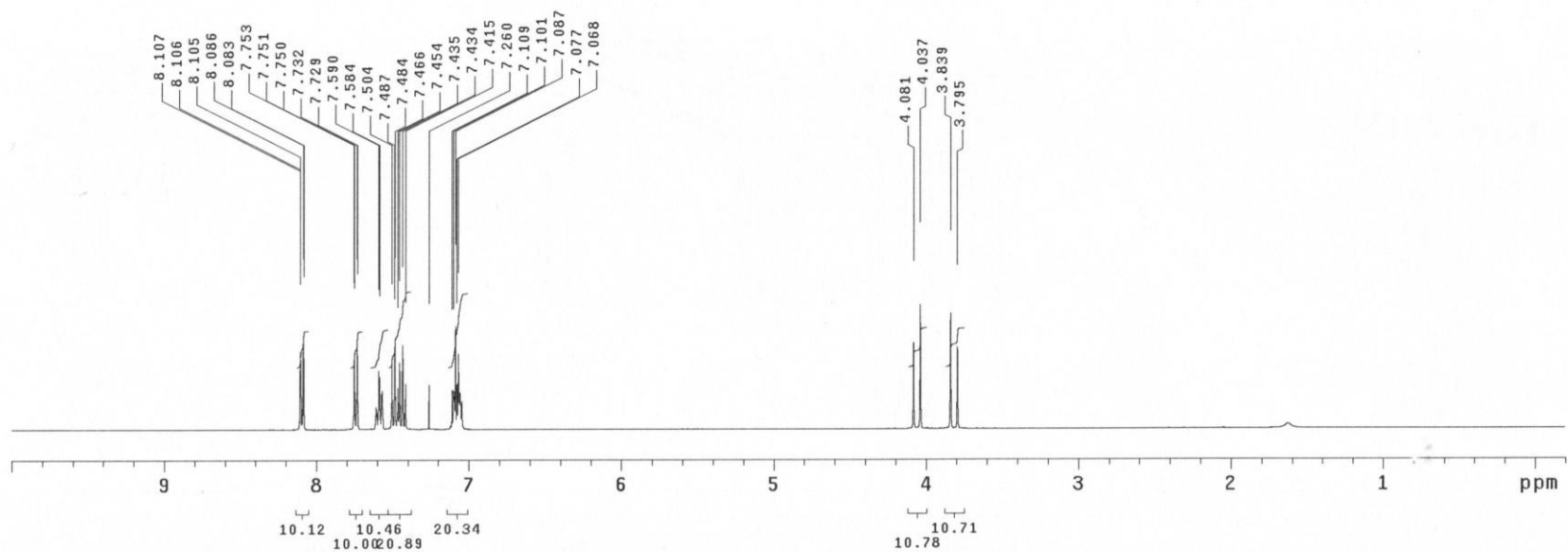
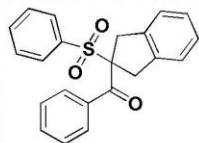
32 repetitions

OBSERVE H1, 400.2743810 MHz

DATA PROCESSING

FT size 65536

Total time 2 min, 0 sec

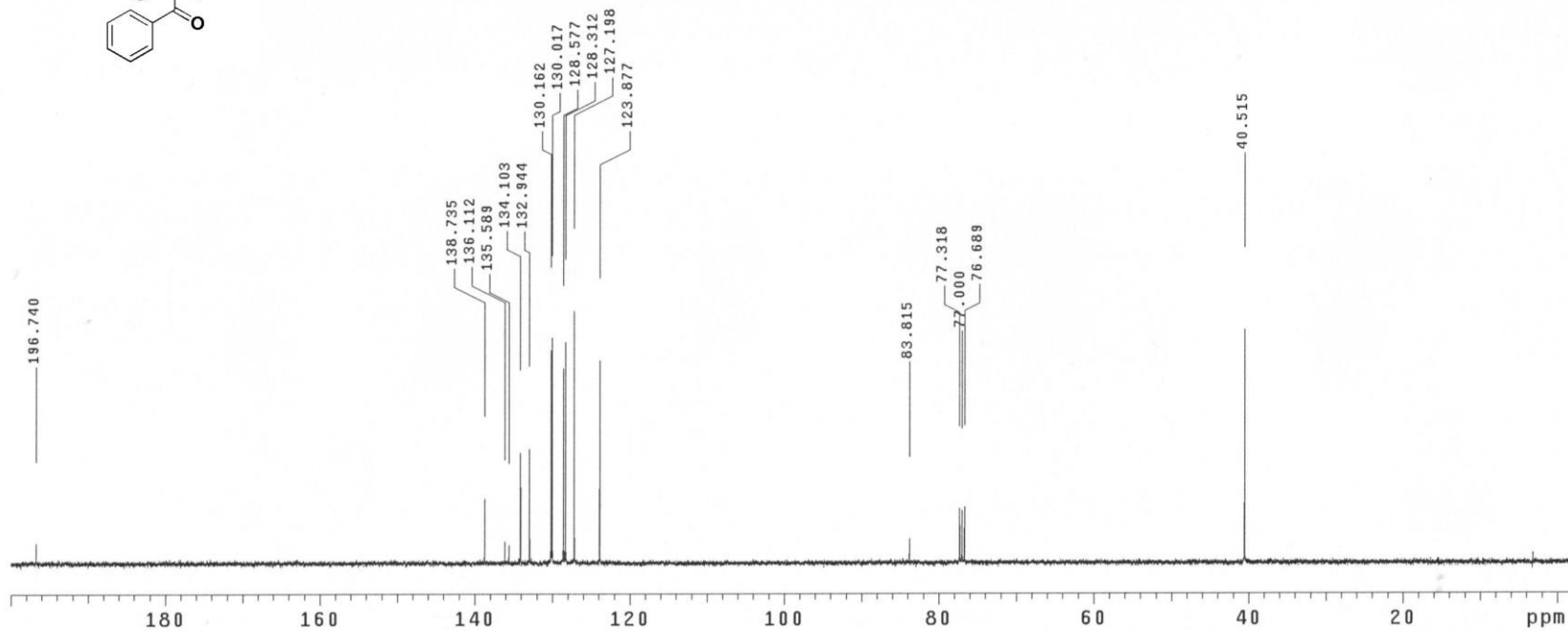
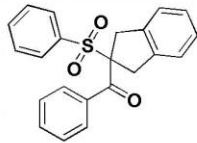


# Compound 7b (<sup>13</sup>C-NMR spectral data)

NC0624-5

Pulse Sequence: s2pu1  
Solvent: CDCl3  
Ambient temperature  
UNITYplus-400 "unity400"

Relax. delay 0.500 sec  
Pulse 65.8 degrees  
Acq. time 1.000 sec  
Width 25000.0 Hz  
512 repetitions  
OBSERVE C13, 100.6490769 MHz  
DECOUPLE H1, 400.2763980 MHz  
Power 43 dB  
on during acquisition  
off during delay  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 1.0 Hz  
FT size 65536  
Total time 6 hr, 42 min, 53 sec



# Compound 7c (<sup>1</sup>H-NMR spectral data)

NC0629-5

Pulse Sequence: s2pu1

Solvent: CDCl<sub>3</sub>

Ambient temperature

UNITYplus-400 "unity400"

Pulse 38.8 degrees

Acq. time 3.744 sec

Width 6000.6 Hz

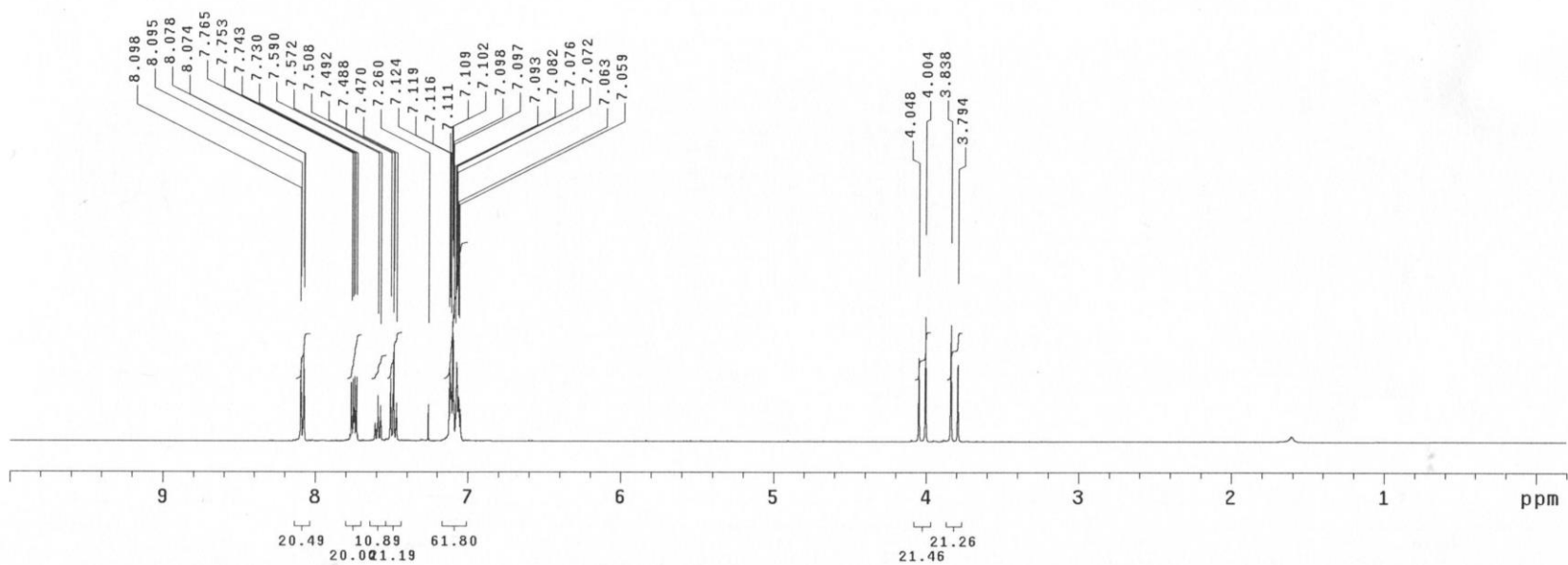
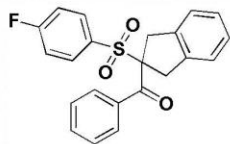
32 repetitions

OBSERVE H1 400.2743814 MHz

DATA PROCESSING

FT size 65536

Total time 2 min, 0 sec



# Compound 7c (<sup>13</sup>C-NMR spectral data)

NC0629-5

Pulse Sequence: s2pu1

Solvent: CDCl<sub>3</sub>

Ambient temperature

UNITYplus-400 "unity400"

Relax. delay 0.500 sec

Pulse 65.8 degrees

Acq. time 1.000 sec

Width 25000.0 Hz

1568 repetitions

OBSERVE C13, 100.6490769 MHz

DECOUPLE H1, 400.2763980 MHz

Power 43 dB

on during acquisition

off during delay

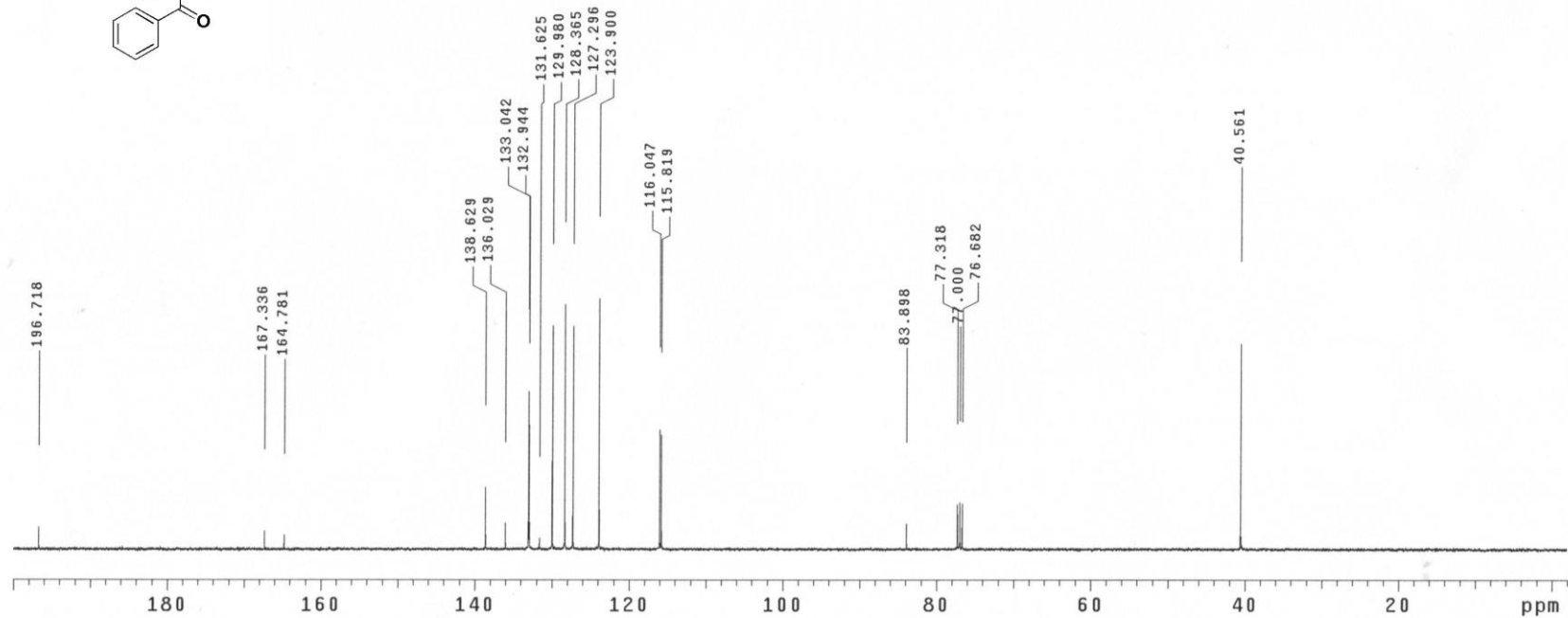
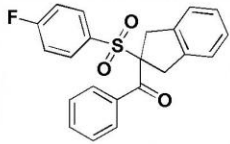
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 13 hr, 25 min, 47 sec



# Compound 7d (<sup>1</sup>H-NMR spectral data)

NC0721-5

Pulse Sequence: s2pu1

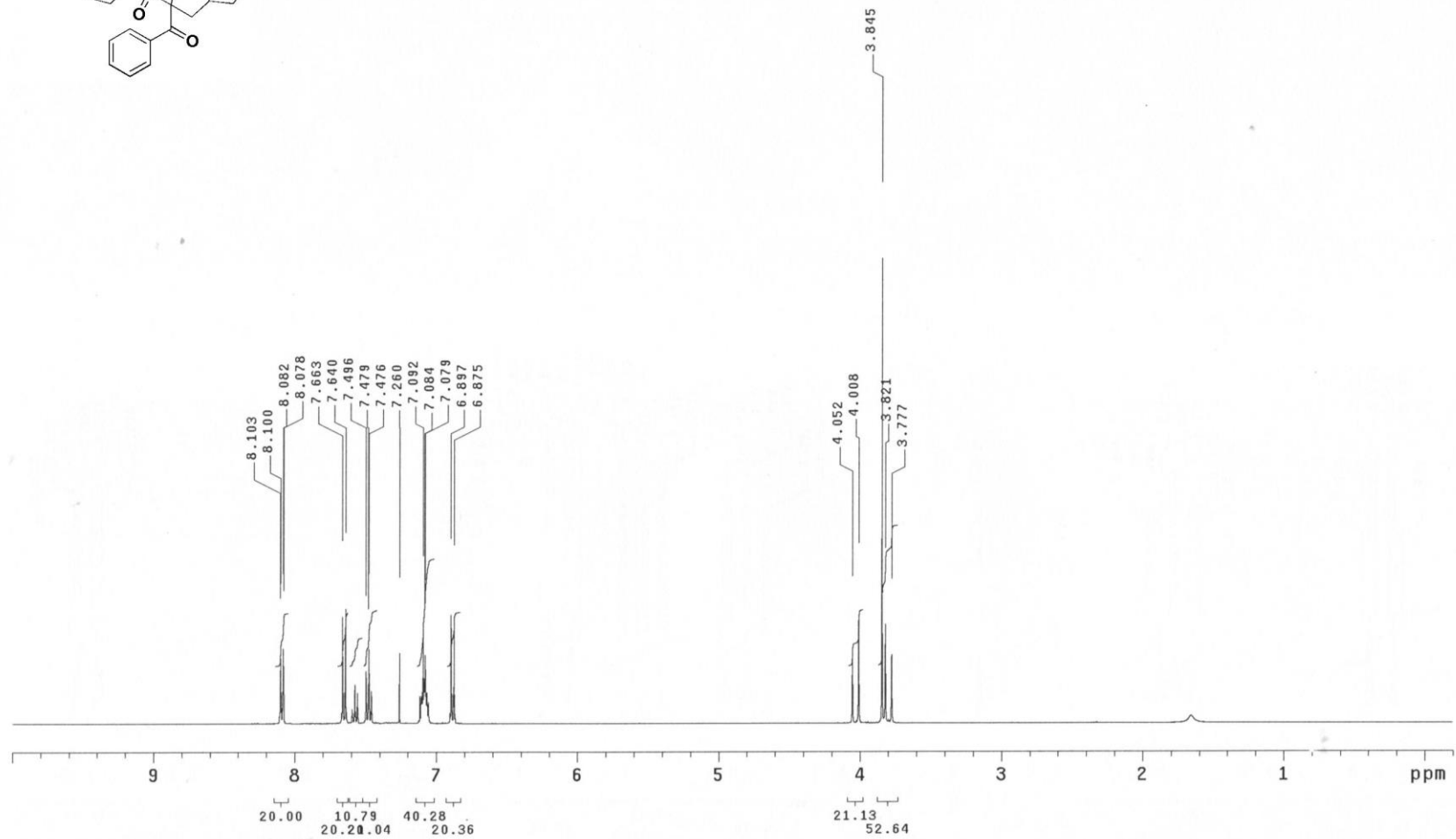
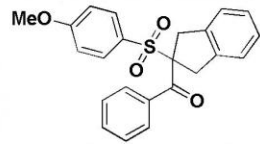
UNITYplus-400 "unity400"

Date: Jul 22 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 32 repetitions





# Compound 7d (<sup>13</sup>C-NMR spectral data)

NC0721-5

Pulse Sequence: s2pu1

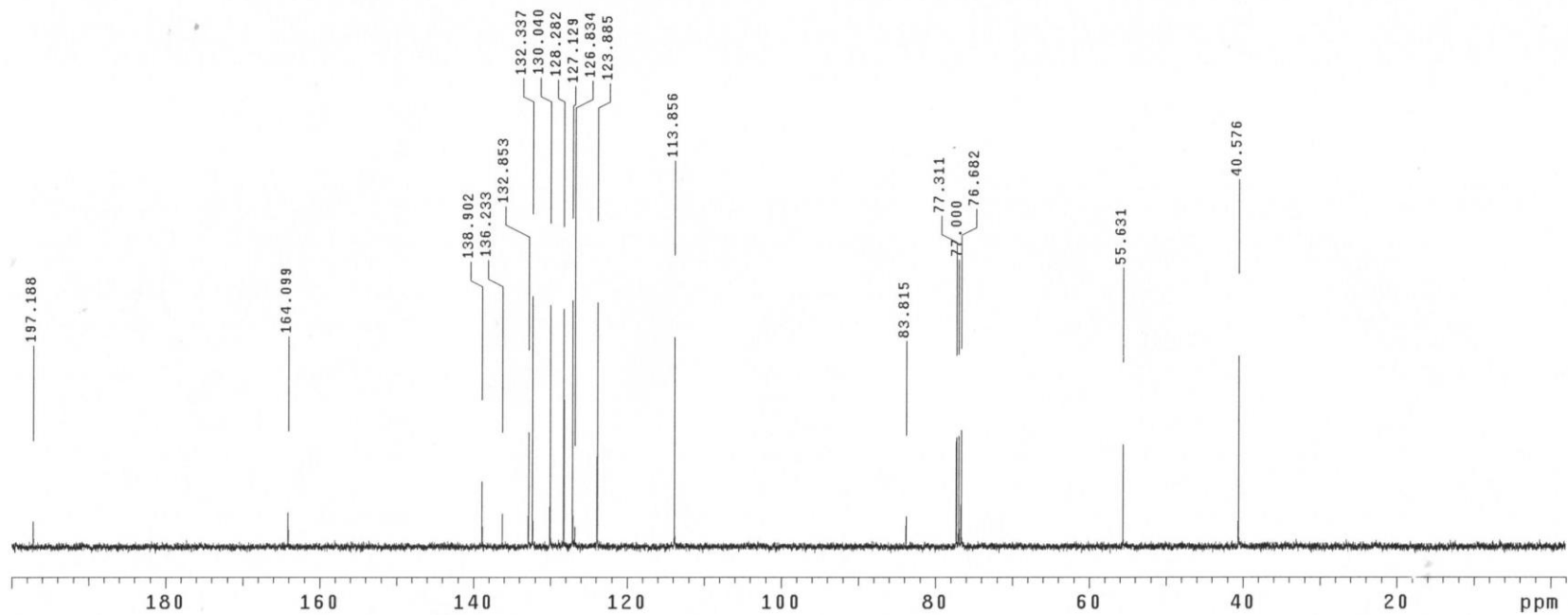
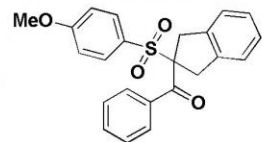
UNITYplus-400 "unity400"

Date: Jul 22 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

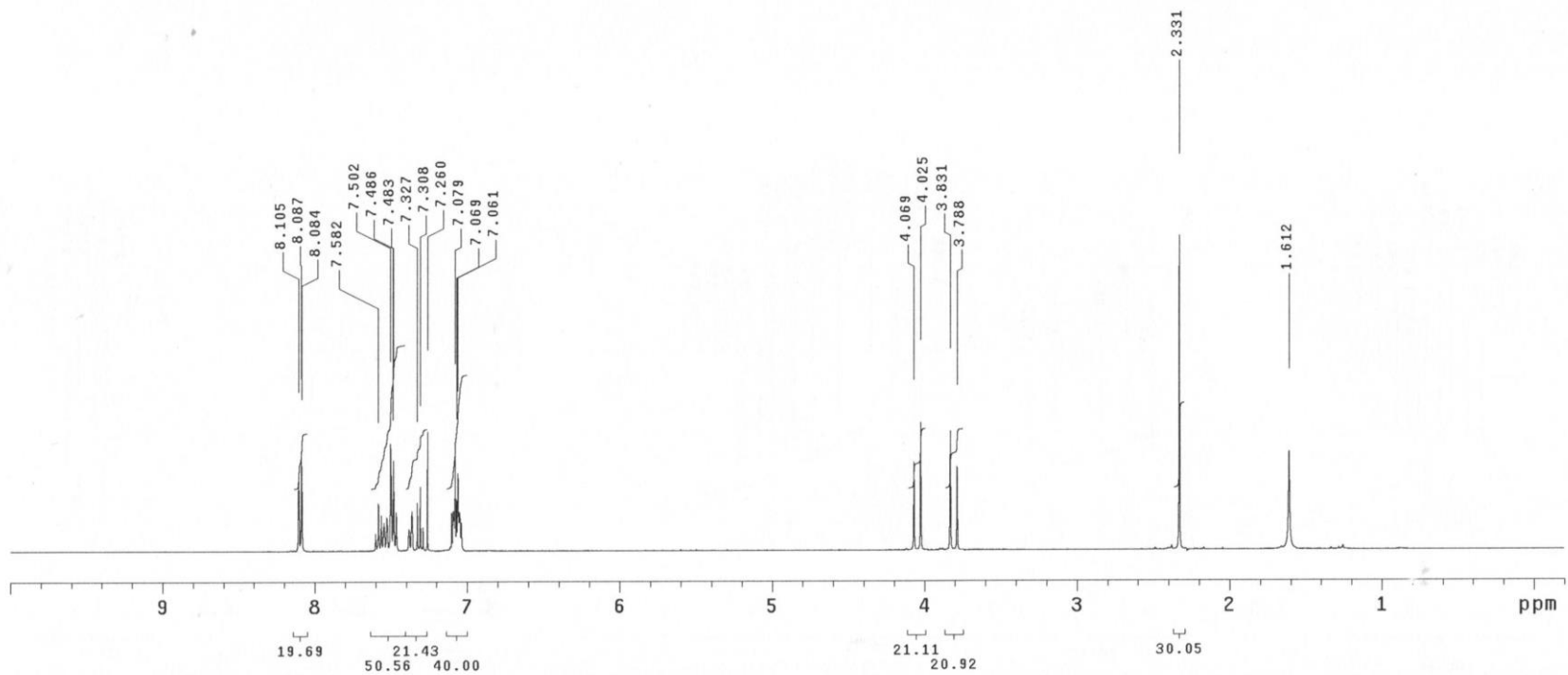
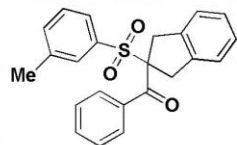
Total 1008 repetitions



# Compound 7e (<sup>1</sup>H-NMR spectral data)

NC0709-5

Pulse Sequence: s2pu1  
UNITYplus-400 "unity400"  
Date: Jul 15 2020  
Solvent: CDCl<sub>3</sub>  
Ambient temperature  
Total 32 repetitions



# Compound 7e (<sup>13</sup>C-NMR spectral data)

NC0709-5

Pulse Sequence: s2pu1

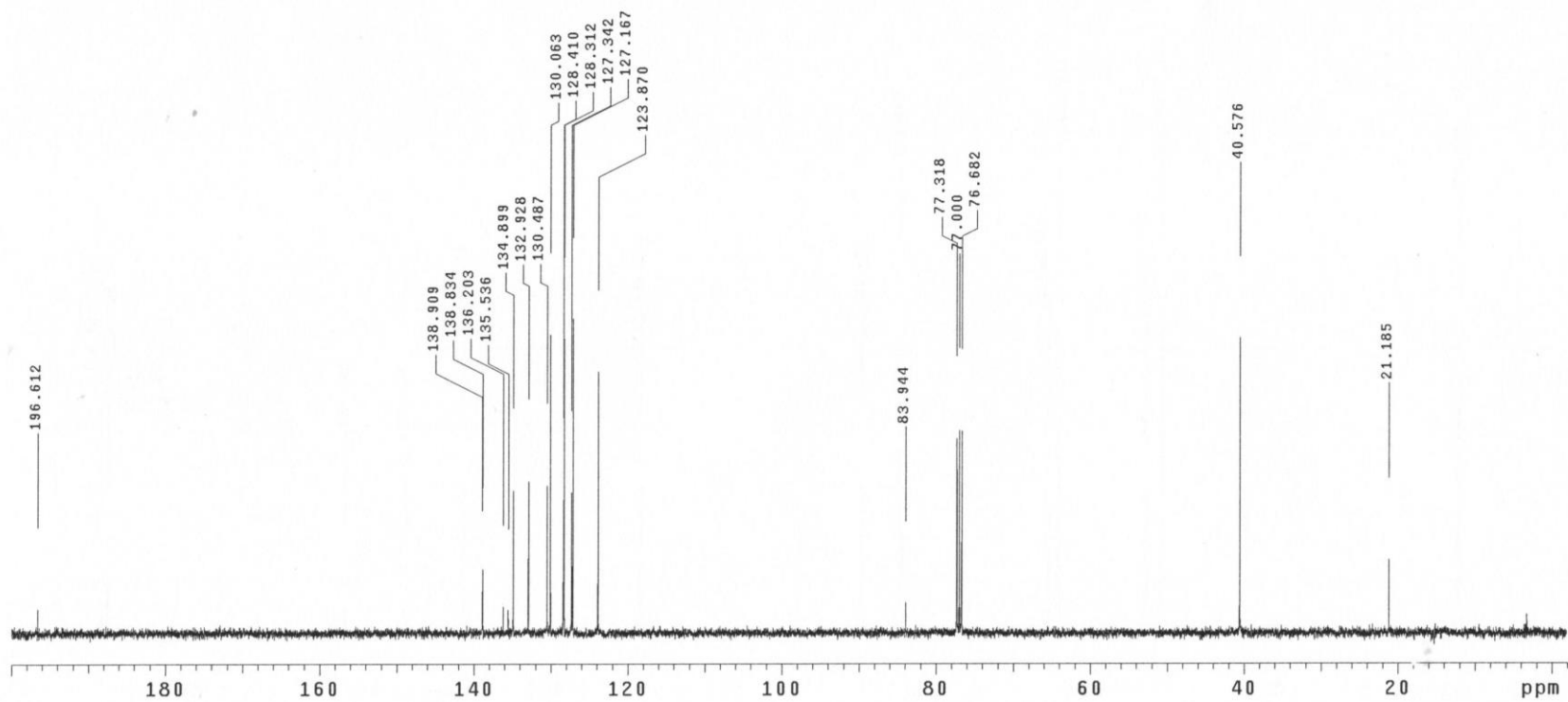
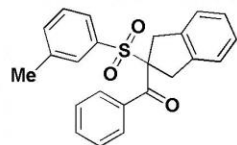
UNITYplus-400 "unity400"

Date: Jul 15 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 3008 repetitions



# Compound 7f (<sup>1</sup>H-NMR spectral data)

NC0702-5

Pulse Sequence: s2pu1

Solvent: CDC13

Ambient temperature

UNITYplus-400 "unity400"

Pulse 38.8 degrees

Acq. time 3.744 sec

Width 6000.6 Hz

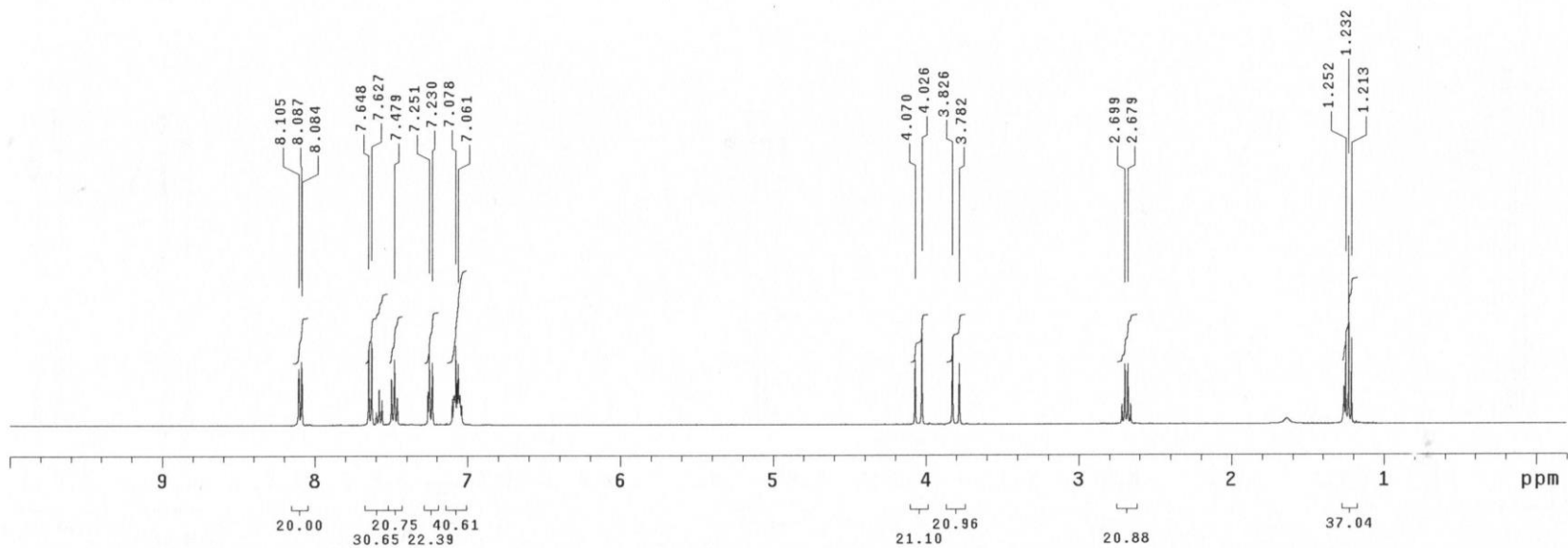
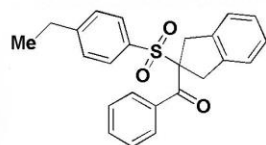
32 repetitions

OBSERVE H1, 400.2743810 MHz

DATA PROCESSING

FT size 65536

Total time 2 min, 0 sec



# Compound 7f (<sup>13</sup>C-NMR spectral data)

NC0702-5

Pulse Sequence: s2pu1

Solvent: CDCl<sub>3</sub>

Ambient temperature

UNITYplus-400 "unity400"

Relax. delay 0.500 sec

Pulse 65.8 degrees

Acq. time 0.800 sec

Width 25000.0 Hz

1600 repetitions

OBSERVE C13, 100.6490776 MHz

DECOUPLE H1, 400.2763980 MHz

Power 43 dB

on during acquisition

off during delay

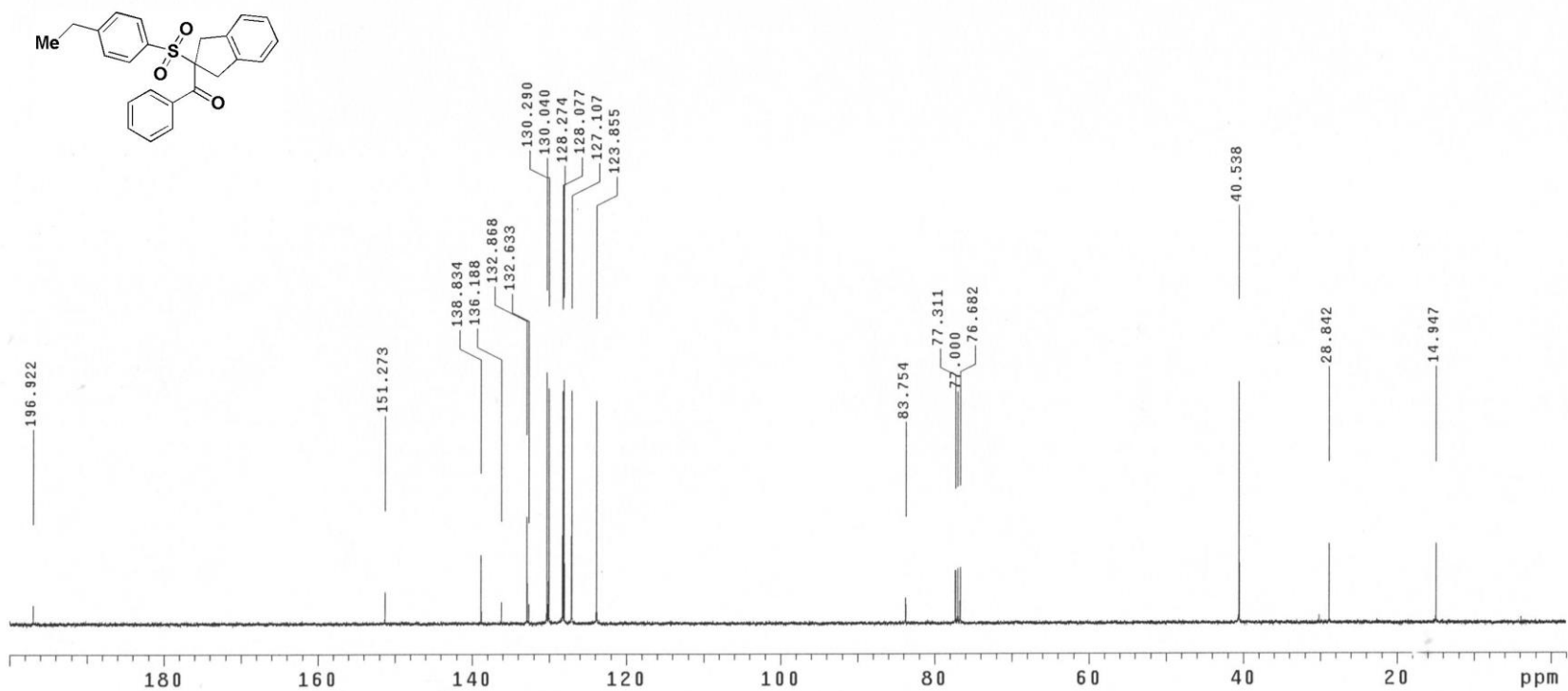
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 11 hr, 39 min, 7 sec



# Compound 7g (<sup>1</sup>H-NMR spectral data)

NC0722-5

Pulse Sequence: s2pu1

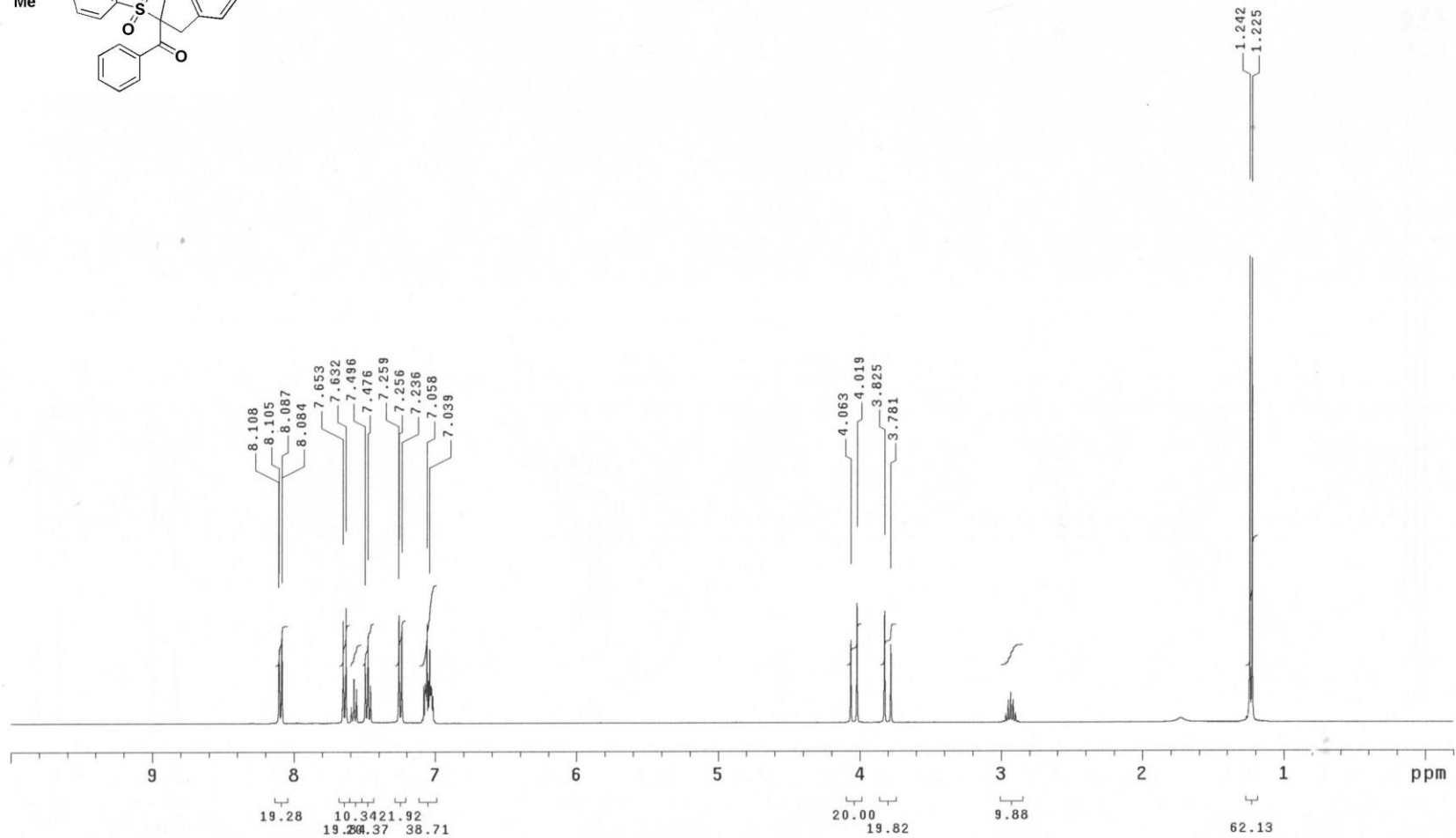
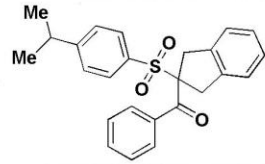
UNITYplus-400 "unity400"

Date: Jul 23 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 32 repetitions



# Compound 7g (<sup>13</sup>C-NMR spectral data)

NC0722-5

Pulse Sequence: s2pu1

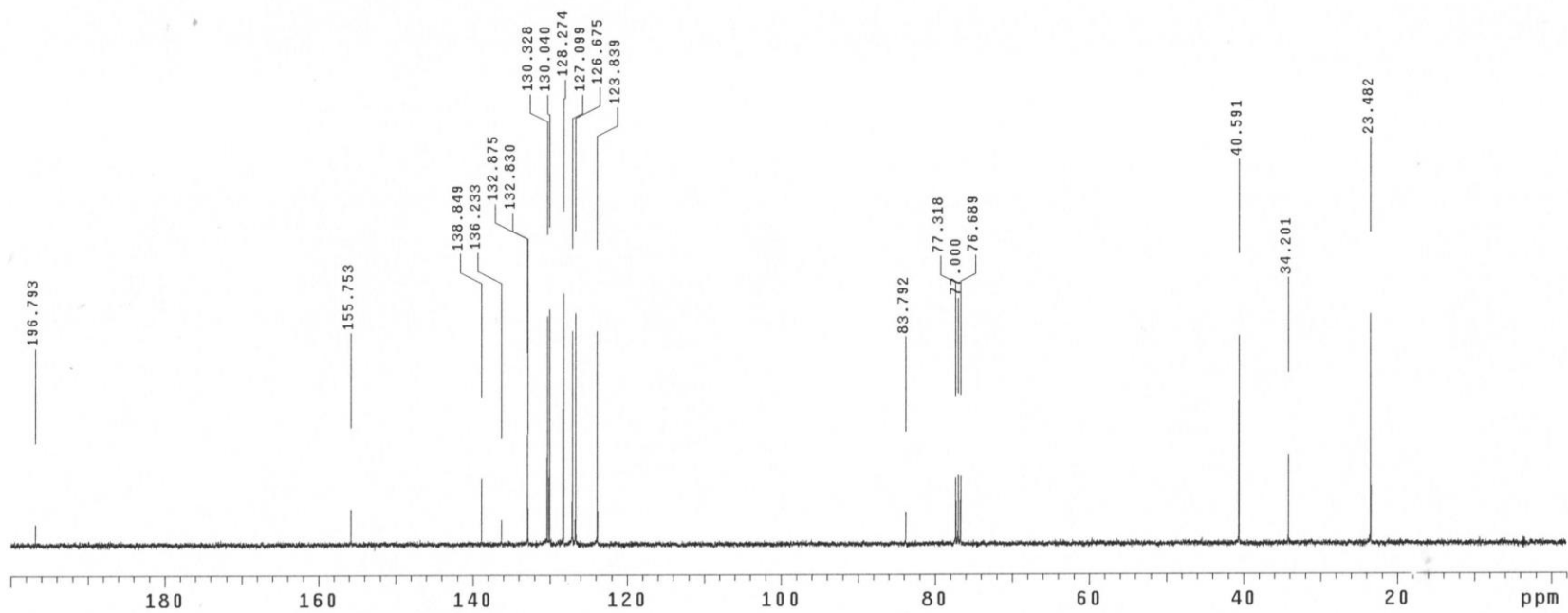
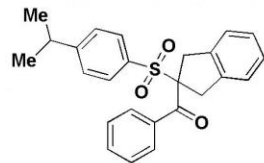
UNITYplus-400 "unity400"

Date: Jul 23 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 640 repetitions



# Compound 7h (<sup>1</sup>H-NMR spectral data)

NC0701-5

Pulse Sequence: s2pu1

Solvent: CDCl<sub>3</sub>

Ambient temperature

UNITYplus-400 "unity400"

Pulse 38.8 degrees

Acq. time 3.744 sec

Width 6000.6 Hz

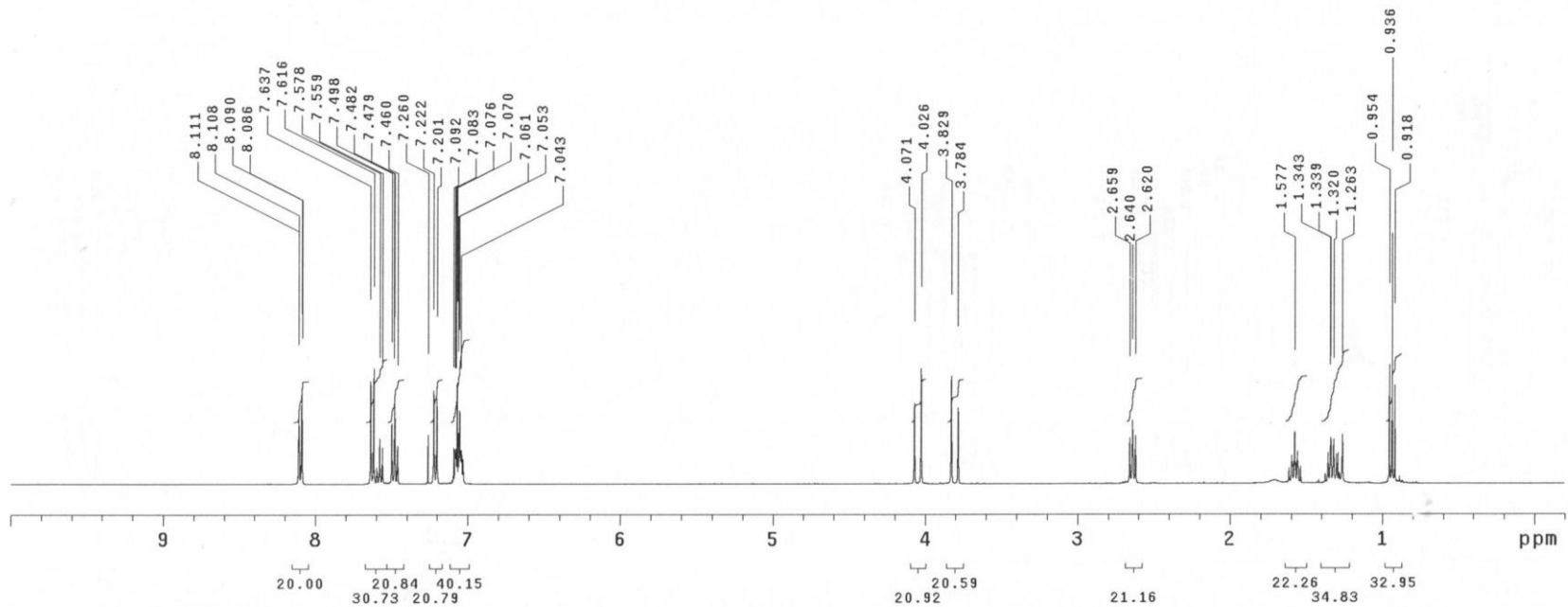
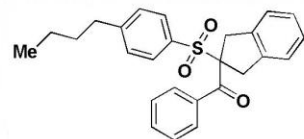
32 repetitions

OBSERVE H1, 400.2743810 MHz

DATA PROCESSING

FT size 65536

Total time 2 min, 0 sec





# Compound 7h (<sup>13</sup>C-NMR spectral data)

NC0701-5

Pulse Sequence: s2pu1

Solvent: CDCl<sub>3</sub>

Ambient temperature

UNITYplus-400 "unity400"

Relax. delay 0.500 sec

Pulse 65.8 degrees

Acq. time 0.800 sec

Width 25000.0 Hz

1760 repetitions

OBSERVE C13, 100.6490776 MHz

DECOUPLE H1, 400.2763980 MHz

Power 43 dB

on during acquisition

off during delay

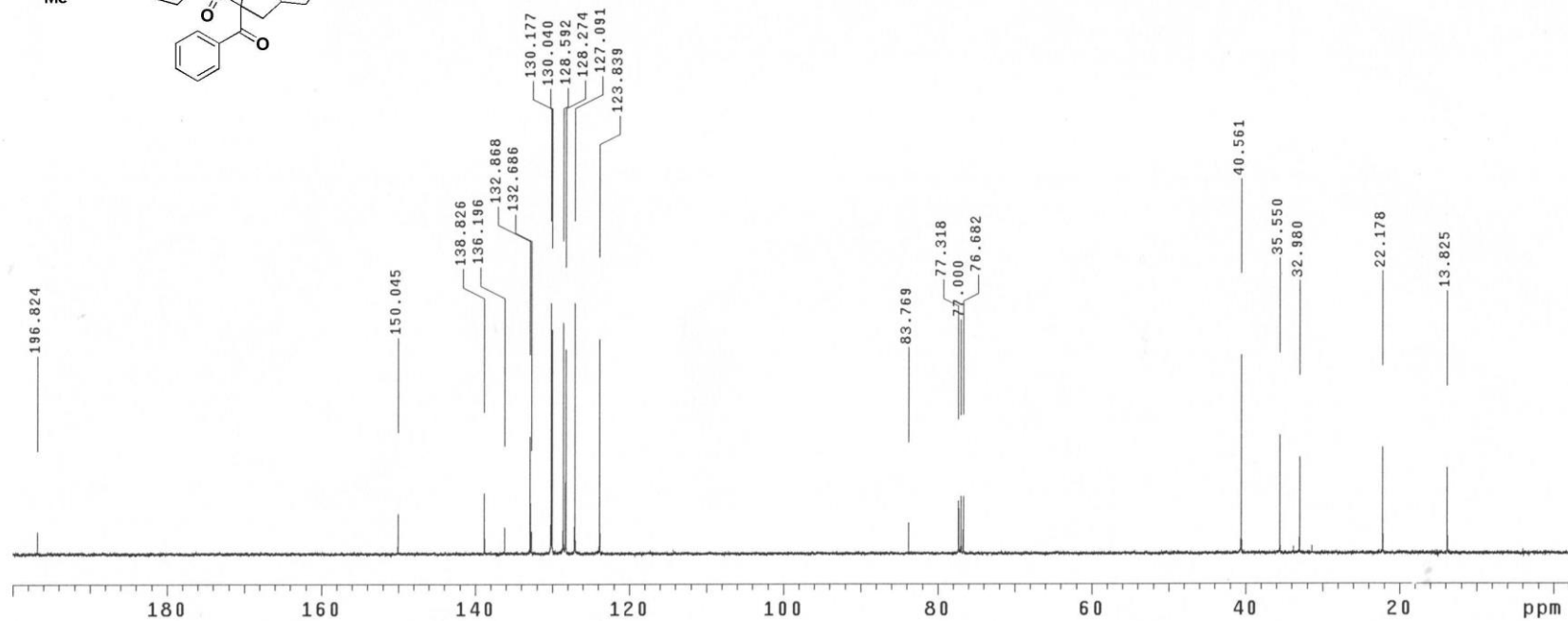
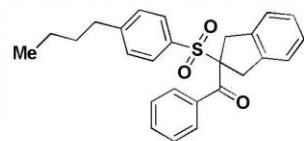
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 11 hr, 39 min, 7 sec



# Compound 7i (<sup>1</sup>H-NMR spectral data)

NC0707-5

Pulse Sequence: s2pu1

Solvent: CDCl<sub>3</sub>

Ambient temperature

UNITYplus-400 "unity400"

Pulse 38.8 degrees

Acq. time 3.744 sec

Width 6000.6 Hz

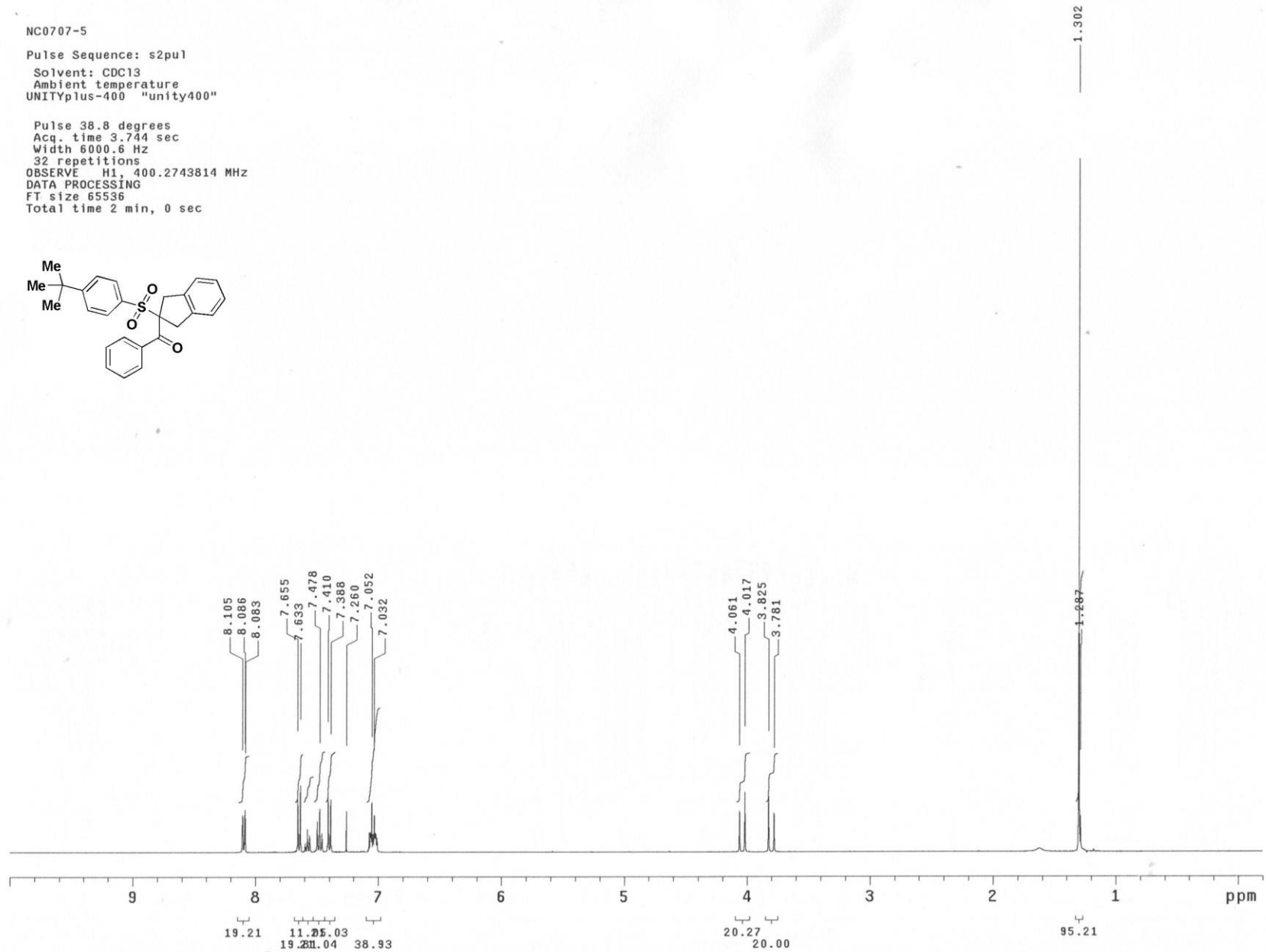
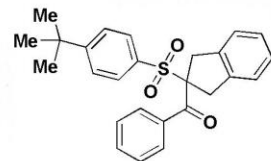
32 repetitions

OBSERVE H1, 400.2743814 MHz

DATA PROCESSING

FT size 65536

Total time 2 min, 0 sec



# Compound 7i (<sup>13</sup>C-NMR spectral data)

NC0707-5

Pulse Sequence: s2pu1

Solvent: CDCl<sub>3</sub>

Ambient temperature

UNITYplus-400 "unity400"

Relax. delay 0.500 sec

Pulse 65.8 degrees

Acq. time 0.800 sec

Width 25000.0 Hz

5312 repetitions

OBSERVE C13, 100.6490746 MHz

DECOUPLE H1, 400.2763980 MHz

Power 43 dB

on during acquisition

off during delay

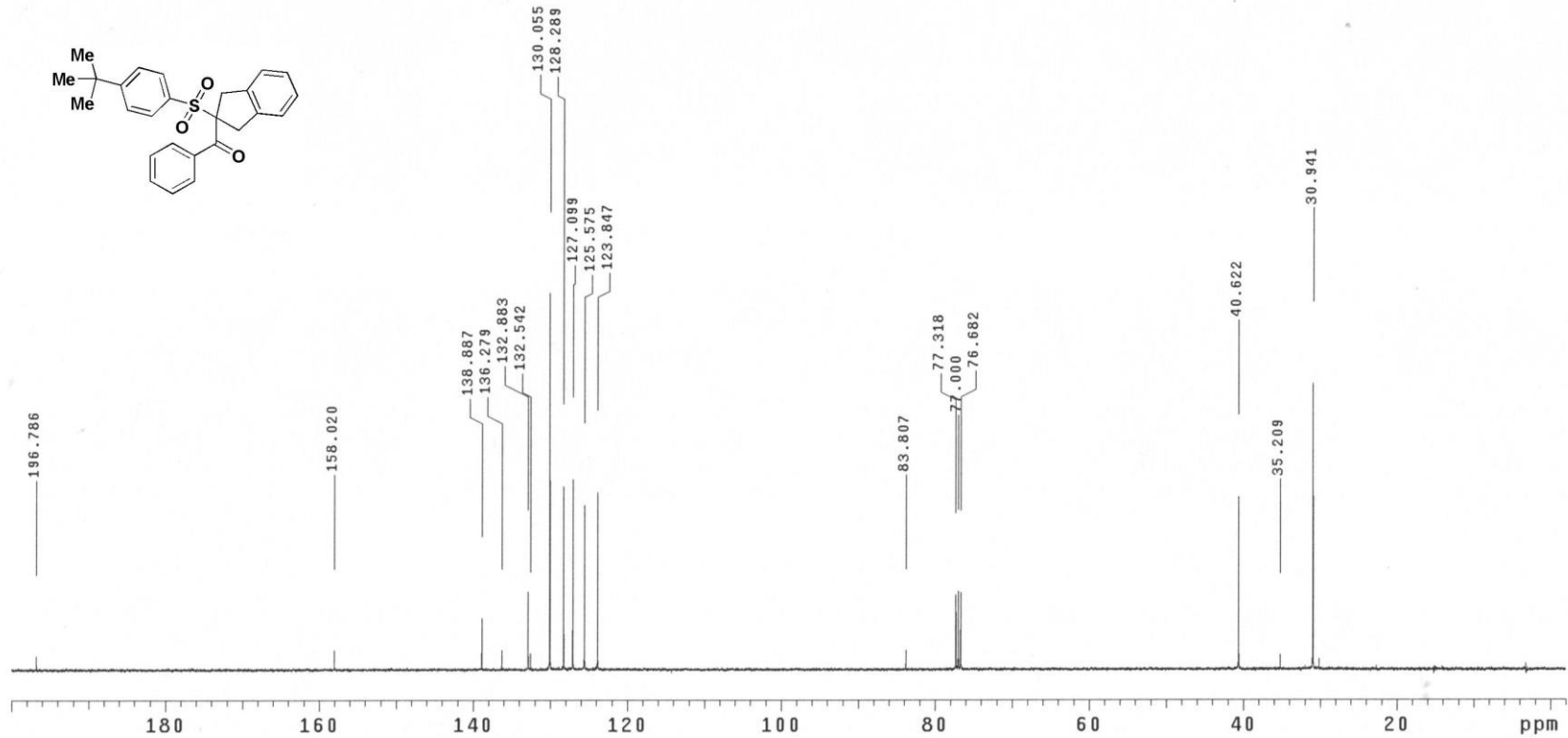
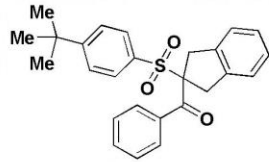
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 11 hr, 39 min, 7 sec



# Compound 7j (<sup>1</sup>H-NMR spectral data)

NC0720-5

Pulse Sequence: s2pu1

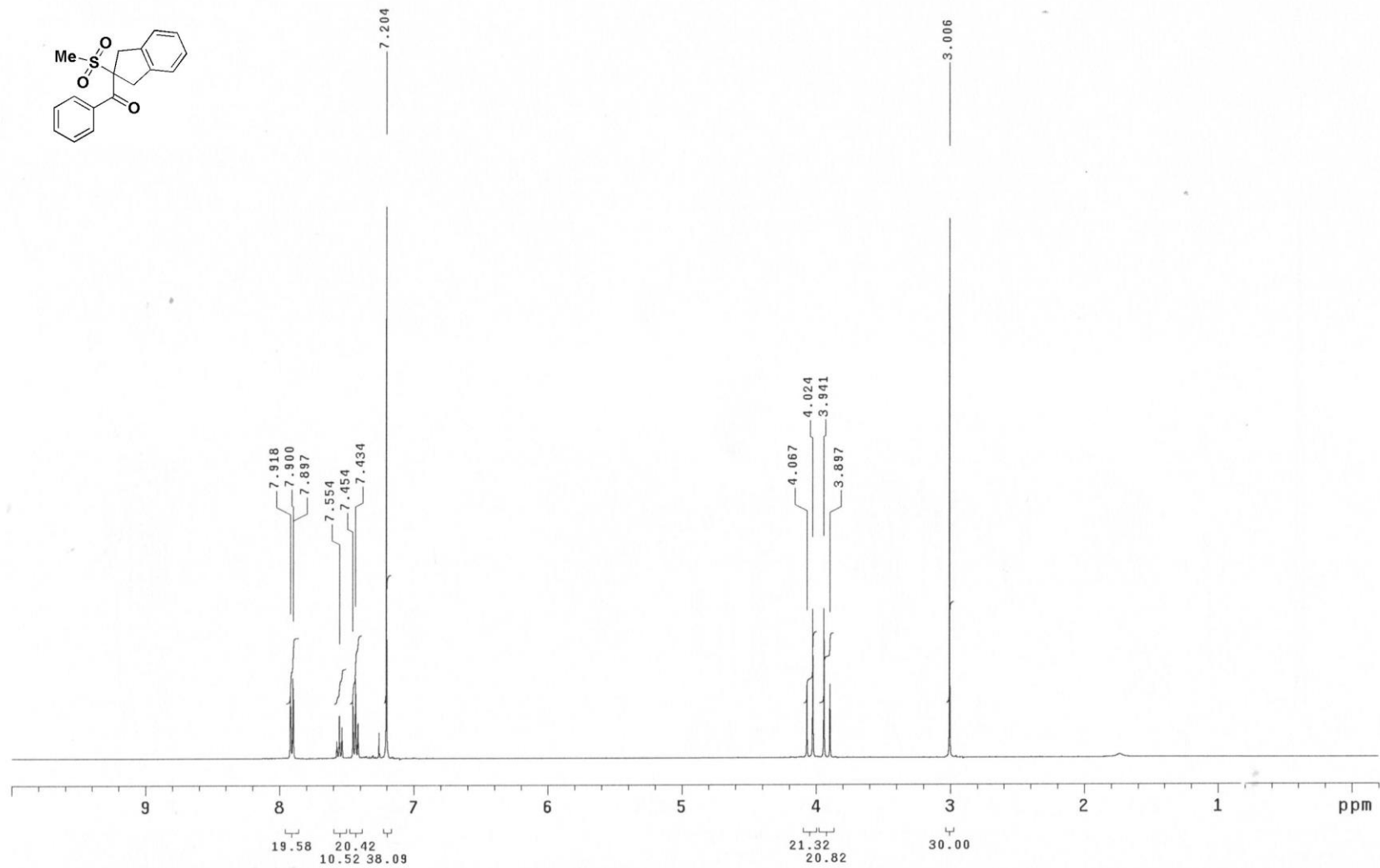
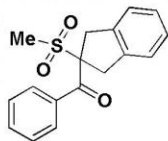
UNITYplus-400 "unity400"

Date: Jul 22 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 32 repetitions



# Compound 7j (<sup>13</sup>C-NMR spectral data)

NC0720-5

Pulse Sequence: s2pu1

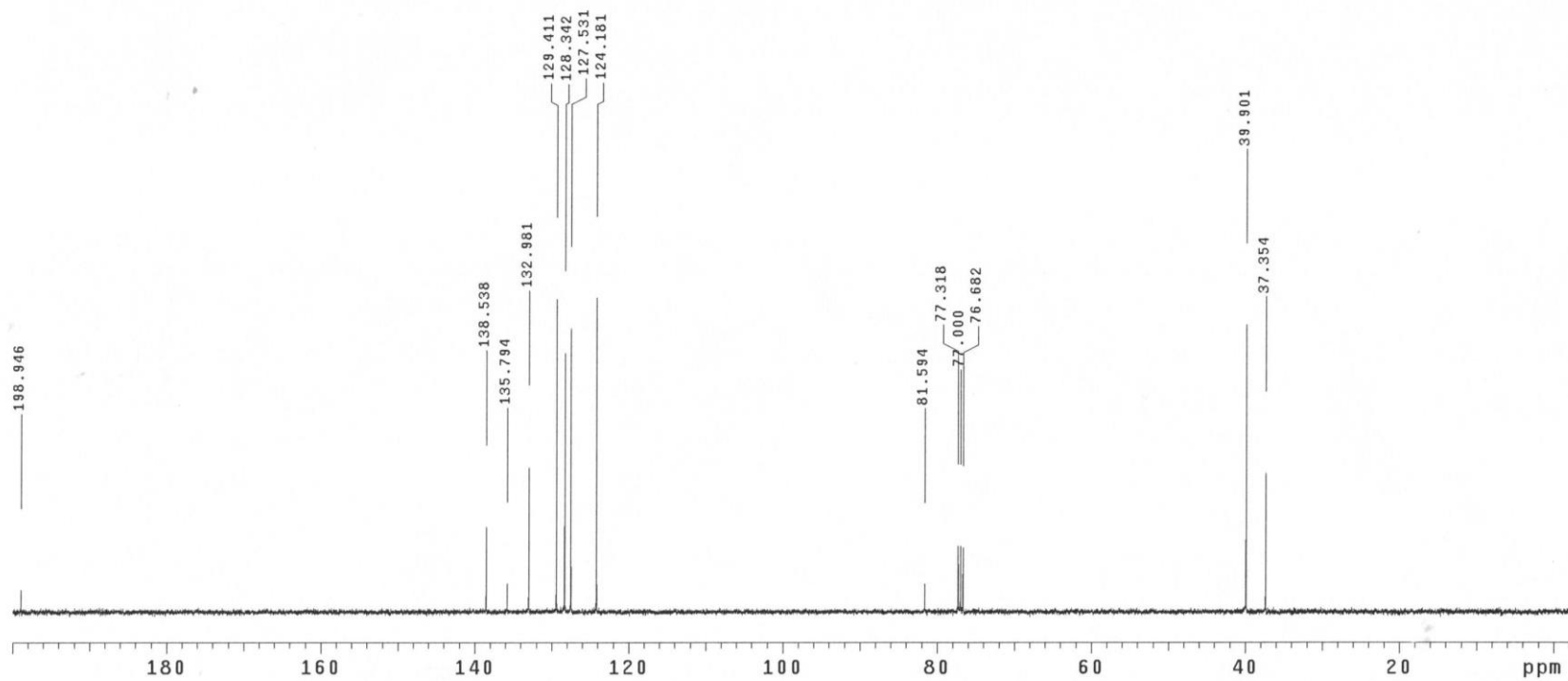
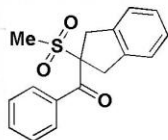
UNITYplus-400 "unity400"

Date: Jul 22 2020

Solvent: CDC13

Ambient temperature

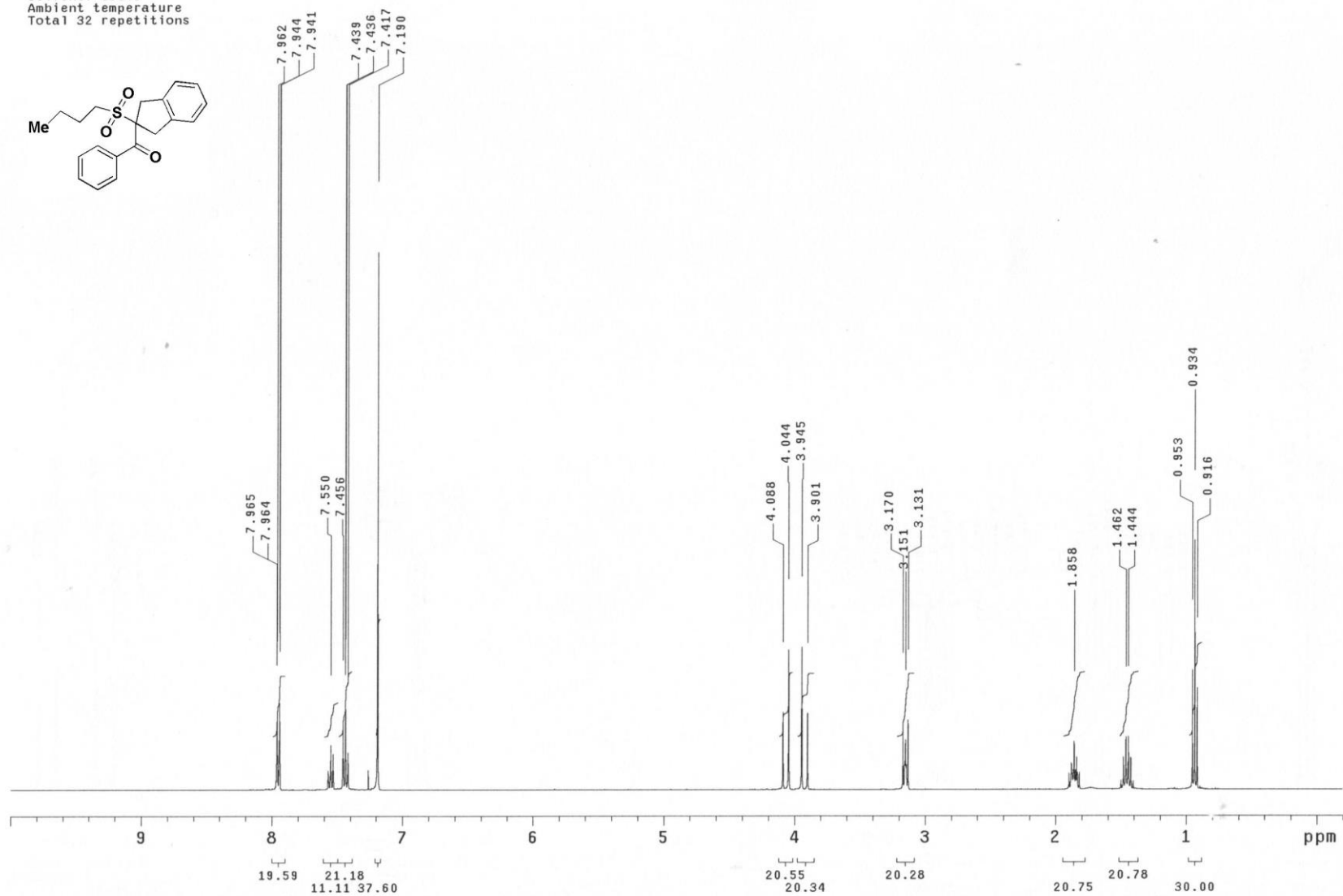
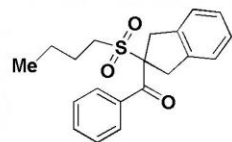
Total 512 repetitions



# Compound 7k (<sup>1</sup>H-NMR spectral data)

NC0713-5

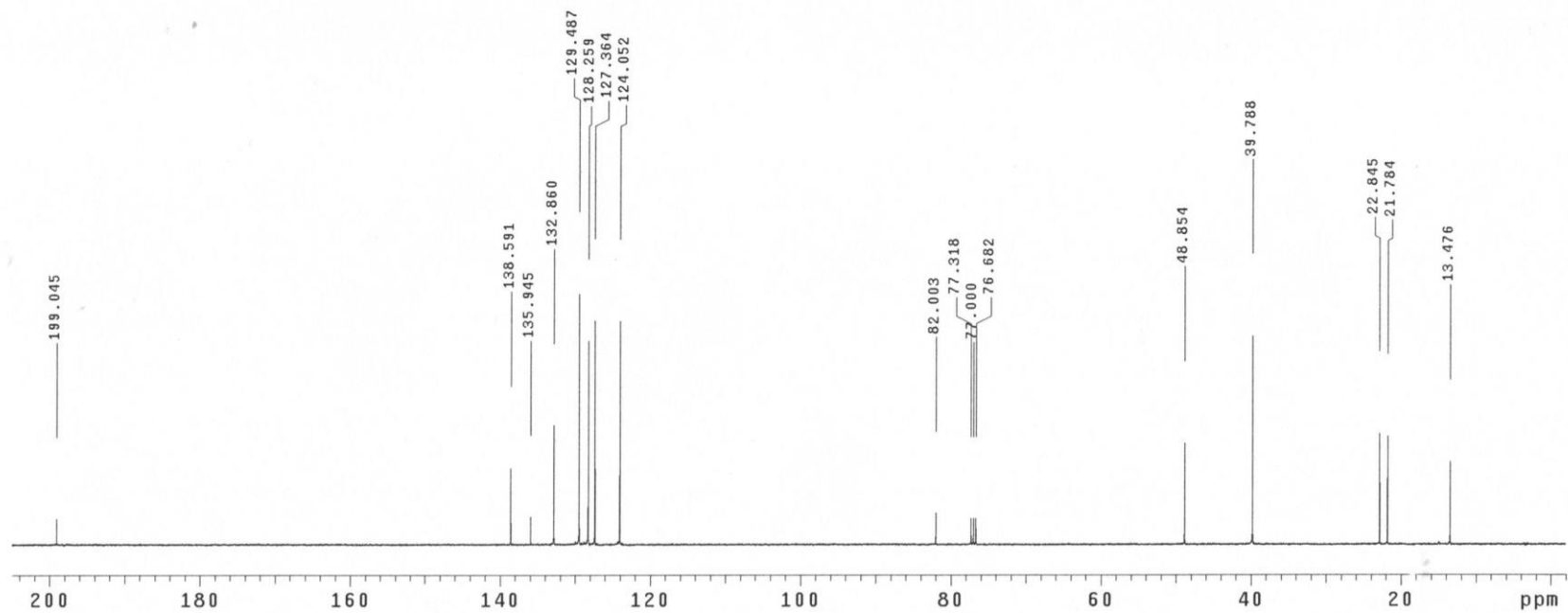
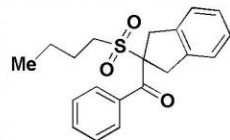
Pulse Sequence: s2pu1  
UNITYplus-400 "unity400"  
Date: Jul 15 2020  
Solvent: CDCl<sub>3</sub>  
Ambient temperature  
Total 32 repetitions



# Compound 7k (<sup>13</sup>C-NMR spectral data)

NC0713-5

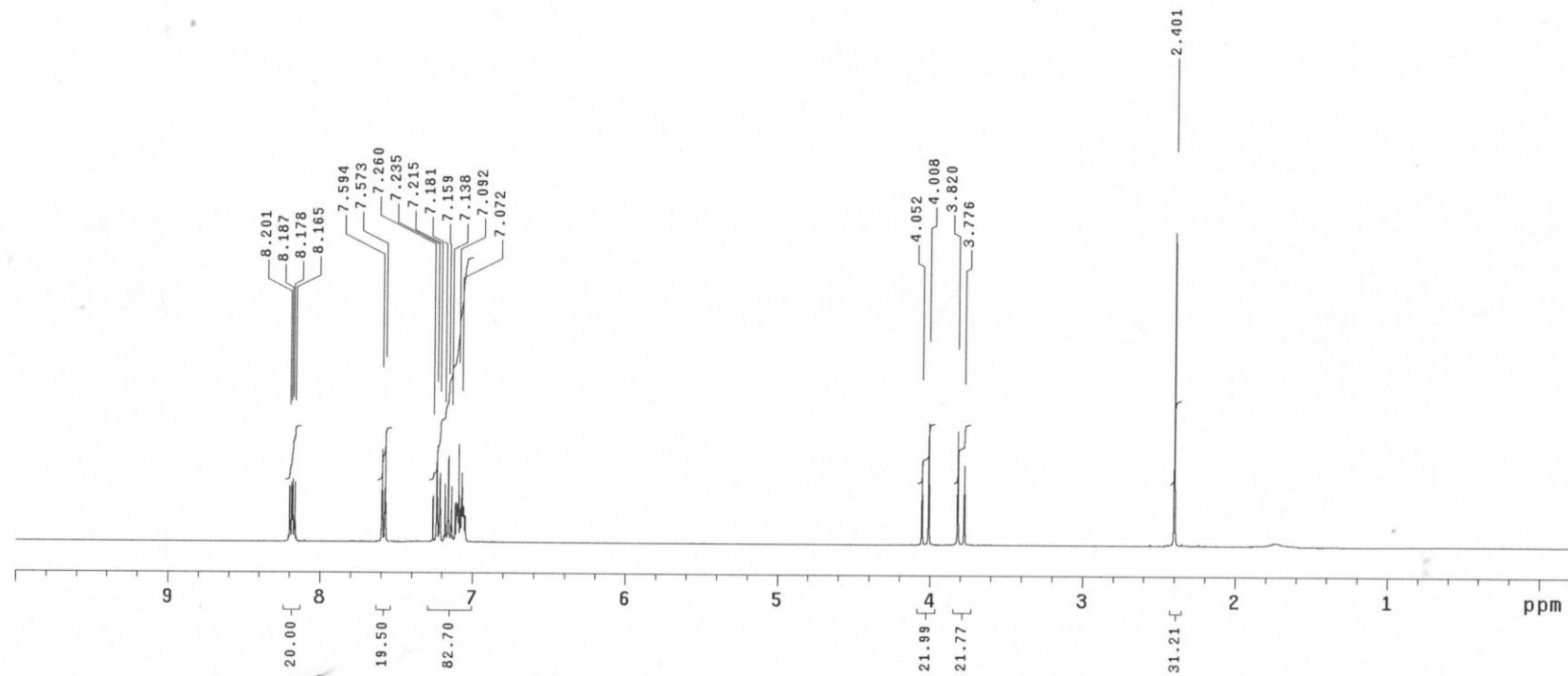
Pulse Sequence: s2pu1  
UNITYplus-400 "unity400"  
Date: Jul 15 2020  
Solvent: CDC13  
Ambient temperature  
Total 32000 repetitions



# Compound 7I (<sup>1</sup>H-NMR spectral data)

KT0609-5

Pulse Sequence: s2pu1  
UNITYplus-400 "unity400"  
Date: Jun 9 2020  
Solvent: CDCl<sub>3</sub>  
Ambient temperature  
Total 32 repetitions

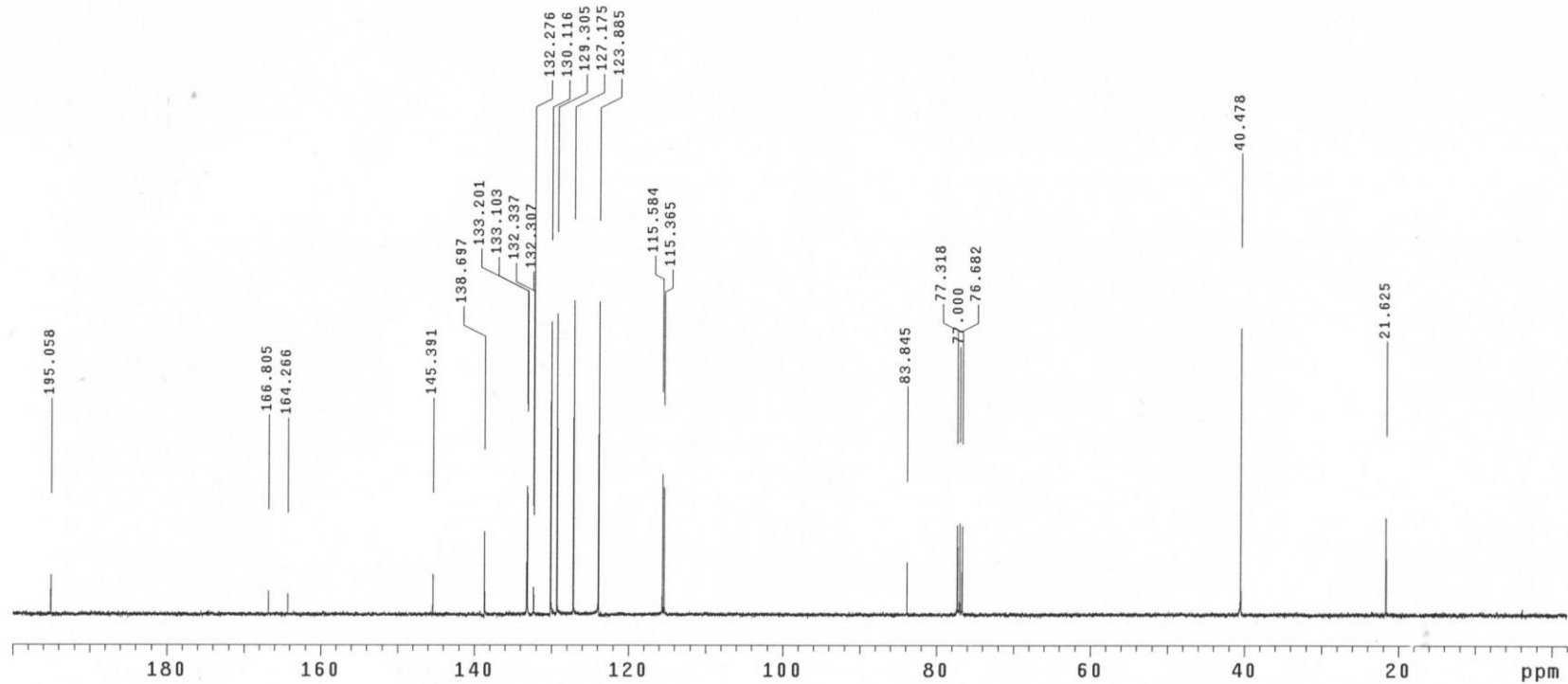
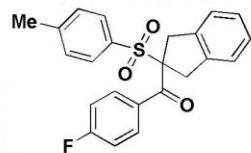




# Compound 7I (<sup>13</sup>C-NMR spectral data)

KT0609-5

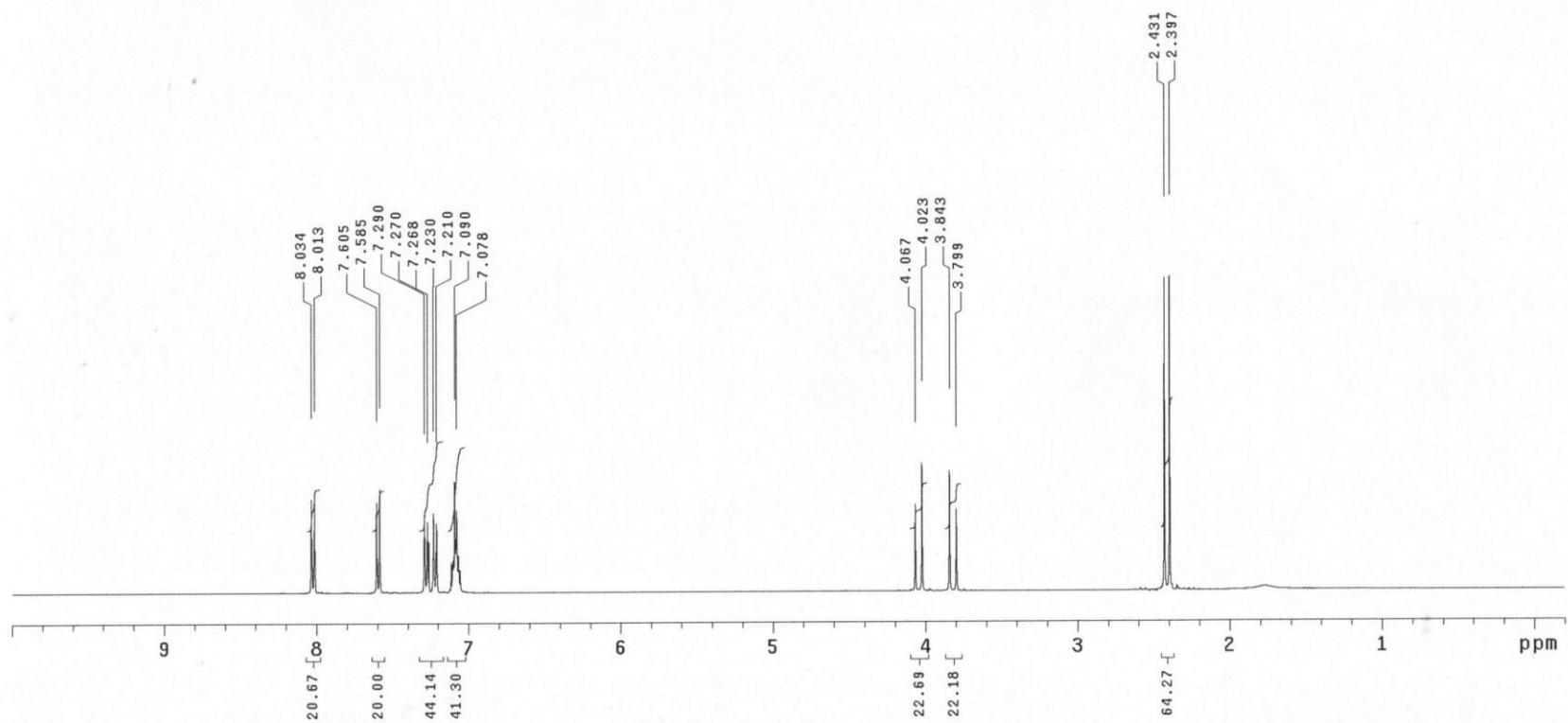
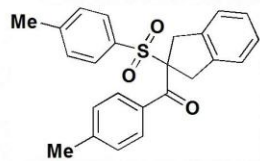
Pulse Sequence: s2pu1  
UNITYplus-400 "unity400"  
Date: Jun 9 2020  
Solvent: CDC13  
Ambient temperature  
Total 3024 repetitions



# Compound 7m (<sup>1</sup>H-NMR spectral data)

KT0512-5

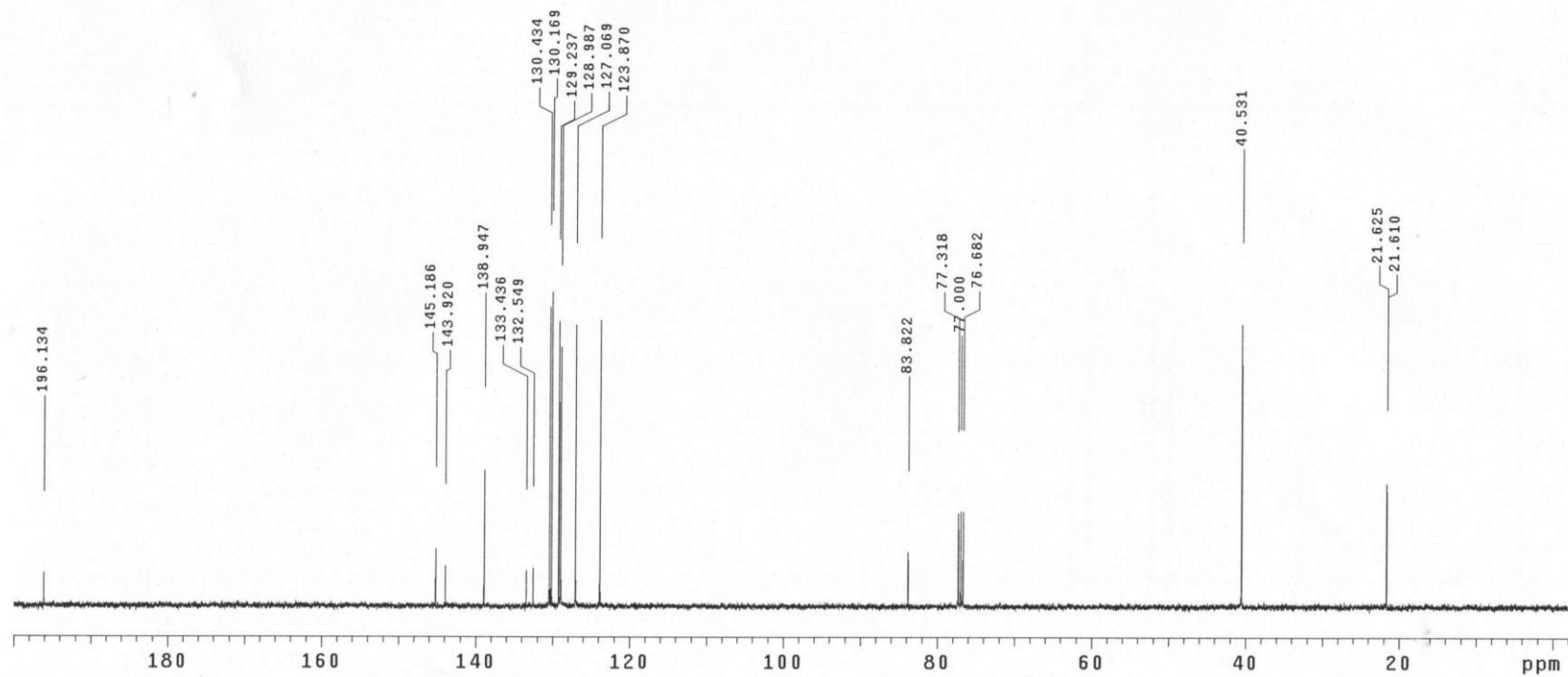
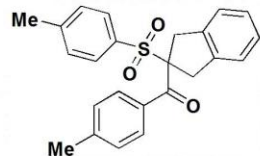
Pulse Sequence: s2pu1  
UNITYplus-400 "unity400"  
Date: May 12 2020  
Solvent: CDCl3  
Ambient temperature  
Total 32 repetitions



# Compound 7m (<sup>13</sup>C-NMR spectral data)

KT0512-5

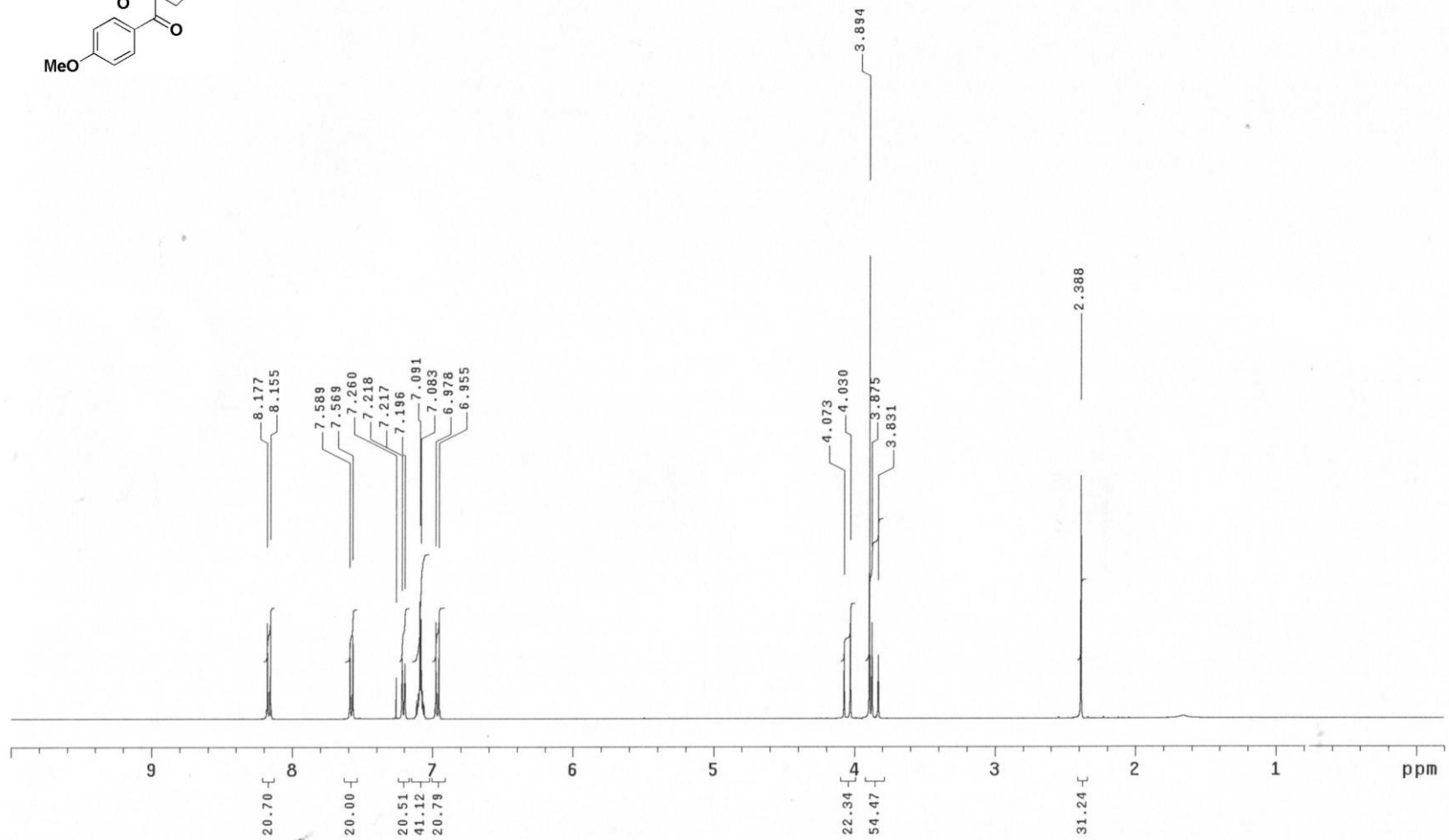
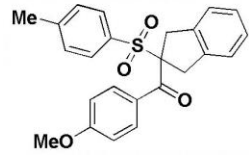
Pulse Sequence: s2pu1  
UNITYplus-400 "unity400"  
Date: May 12 2020  
Solvent: CDCl<sub>3</sub>  
Ambient temperature  
Total 1520 repetitions



# Compound 7n (<sup>1</sup>H-NMR spectral data)

NC0610-5

Pulse Sequence: s2pu1  
UNITYplus-400 "unity400"  
Date: Jun 11 2020  
Solvent: CDCl<sub>3</sub>  
Ambient temperature  
Total 32 repetitions



# Compound 7n (<sup>13</sup>C-NMR spectral data)

NC0610-5

Pulse Sequence: s2pu1

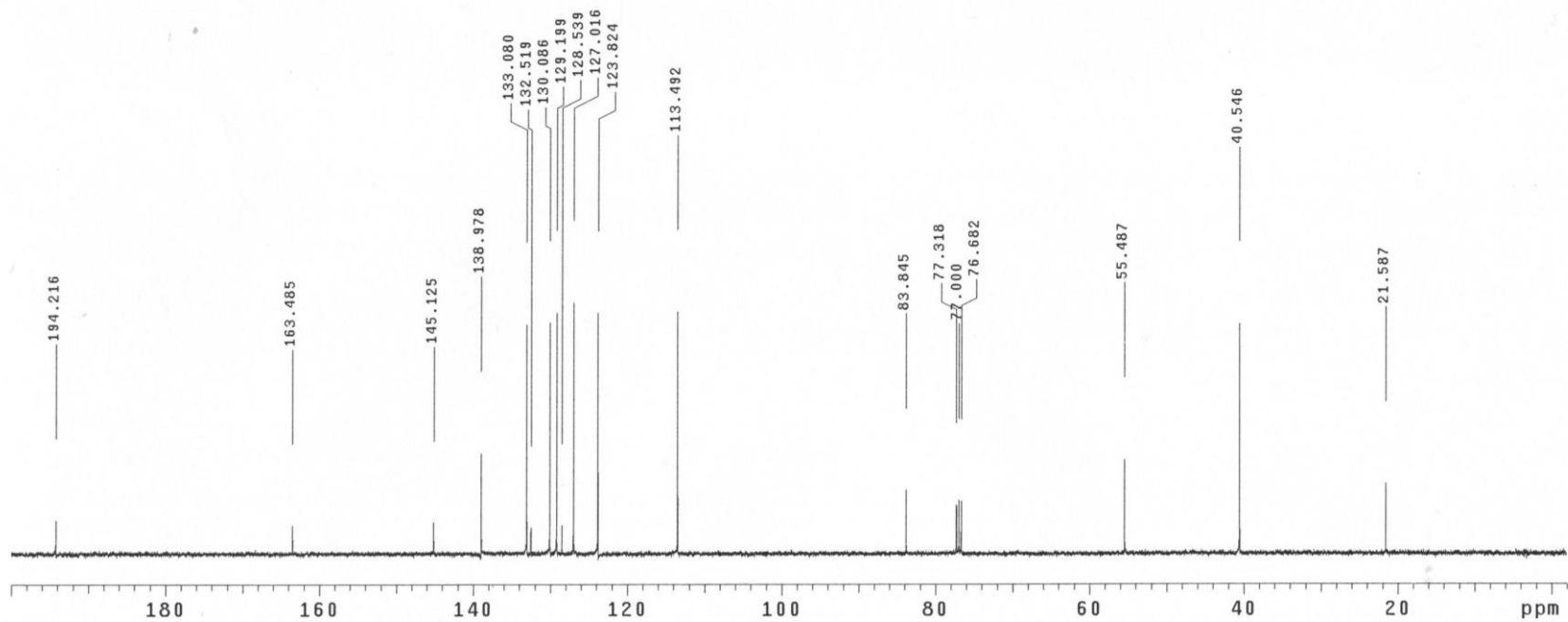
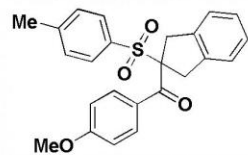
UNITYplus-400 "unity400"

Date: Jun 11 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 720 repetitions



# Compound 7o (<sup>1</sup>H-NMR spectral data)

NC0723-5

Pulse Sequence: s2pu1

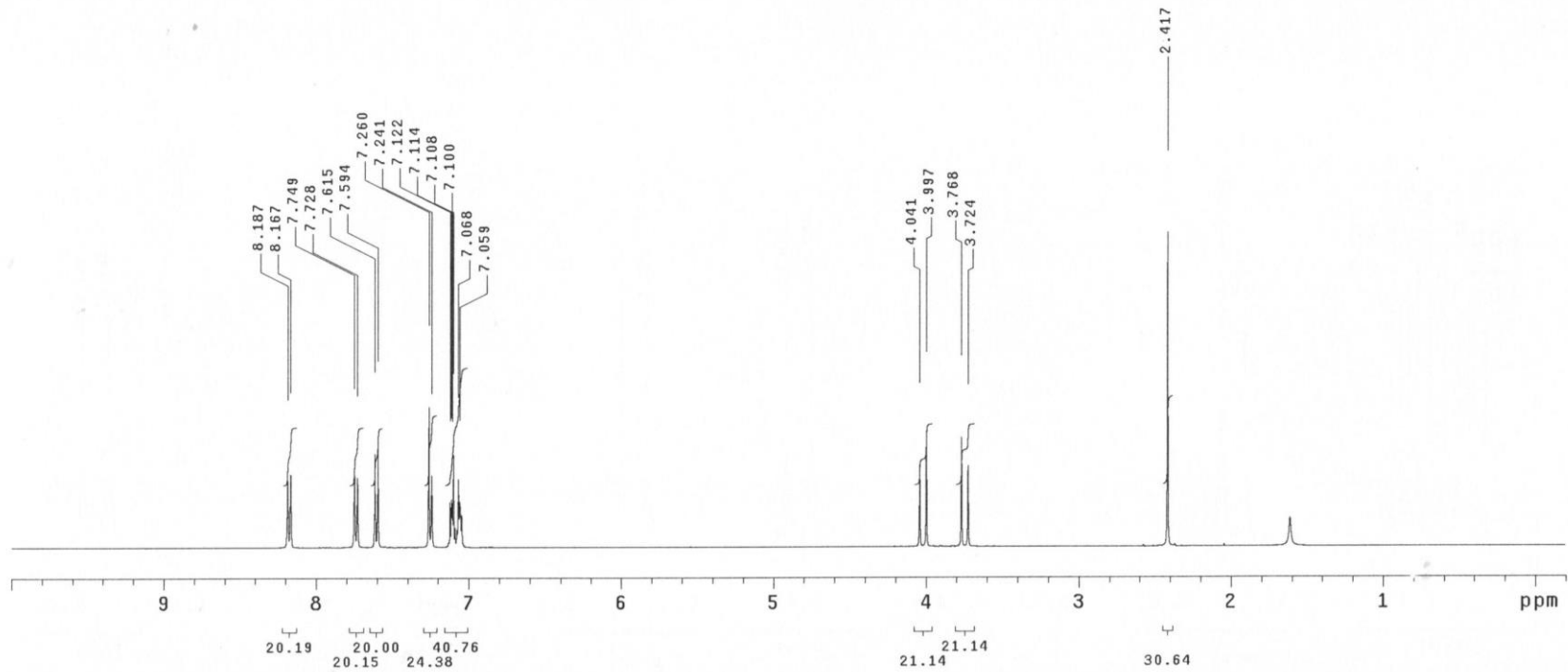
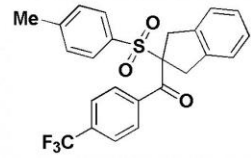
UNITYplus-400 "unity400"

Date: Jul 27 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 32 repetitions



# Compound 7o (<sup>13</sup>C-NMR spectral data)

NC0723-5

Pulse Sequence: s2pu1

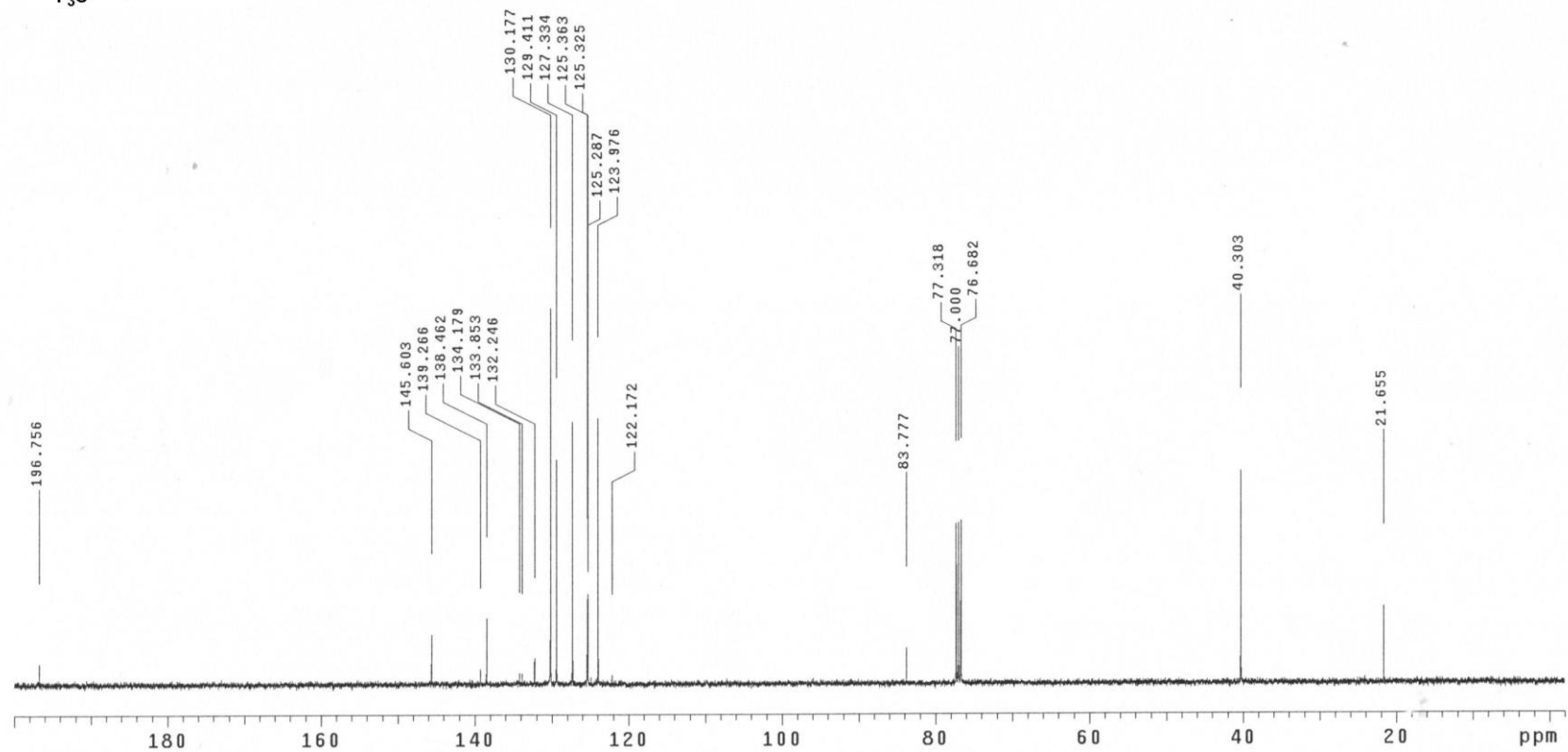
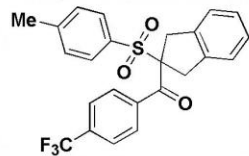
UNITYplus-400 "unity400"

Date: Jul 27 2020

Solvent: CDC13

Ambient temperature

Total 3120 repetitions



# Compound 7p (<sup>1</sup>H-NMR spectral data)

NC0615-5

Pulse Sequence: s2pu1

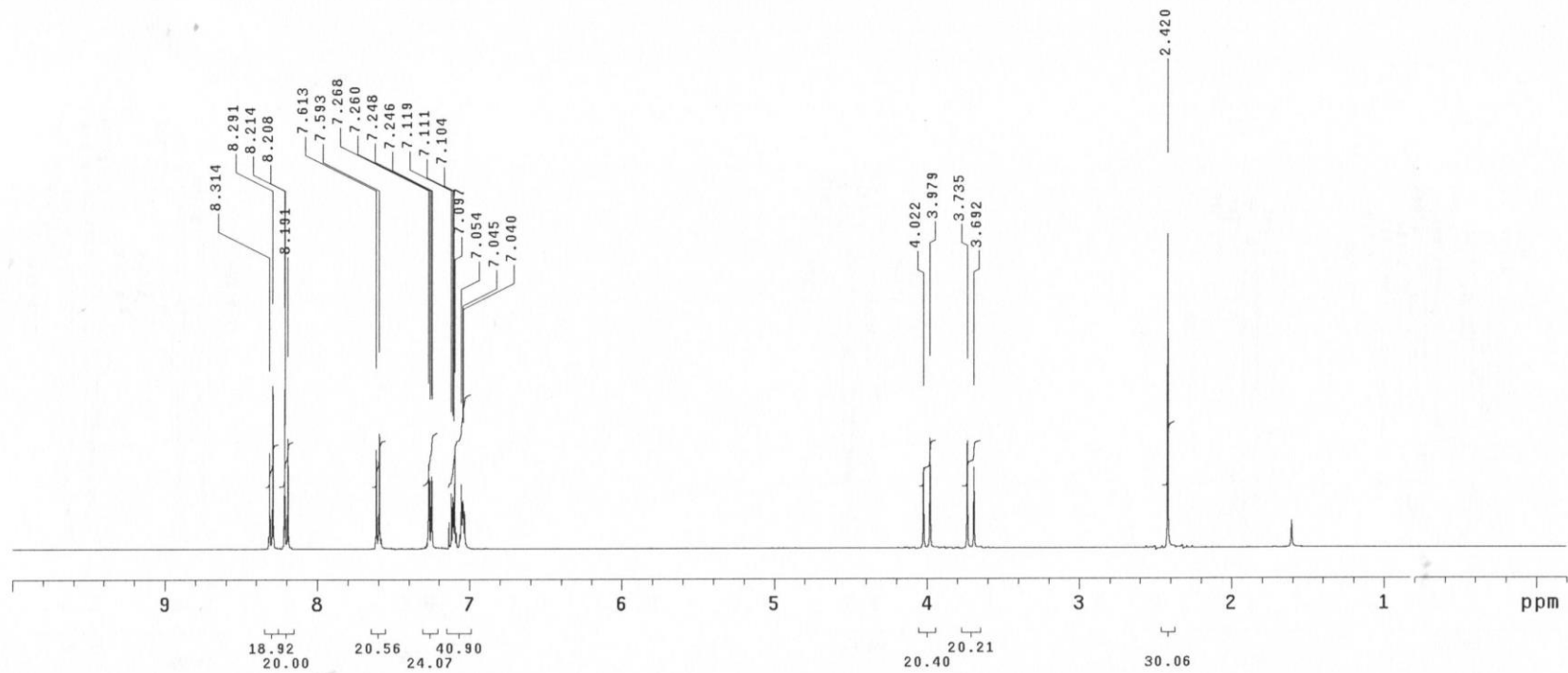
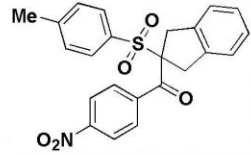
UNITYplus-400 "unity400"

Date: Jul 30 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 32 repetitions





# Compound 7p (<sup>13</sup>C-NMR spectral data)

NC0615-5

Pulse Sequence: s2pu1

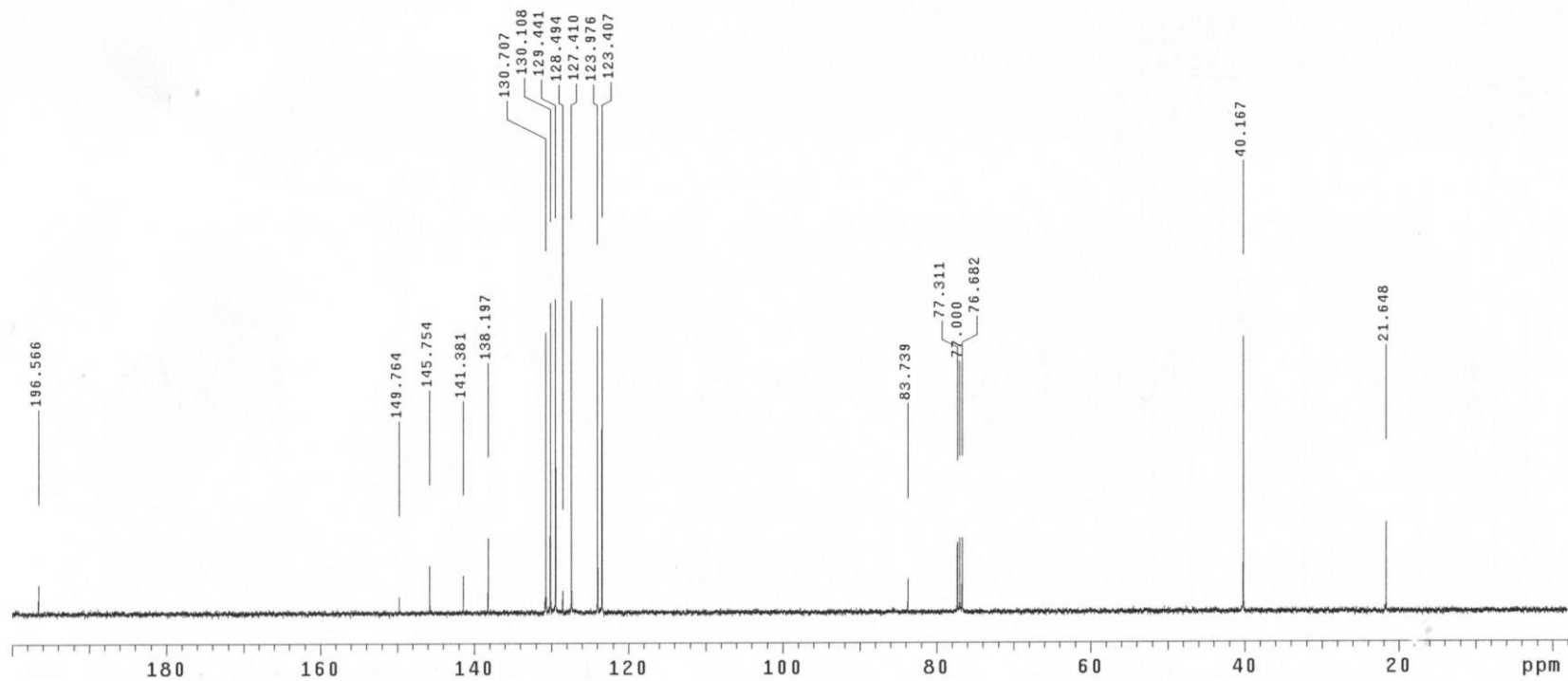
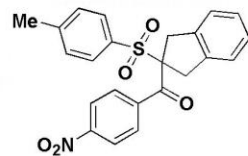
UNITYplus-400 "unity400"

Date: Jul 30 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 1136 repetitions

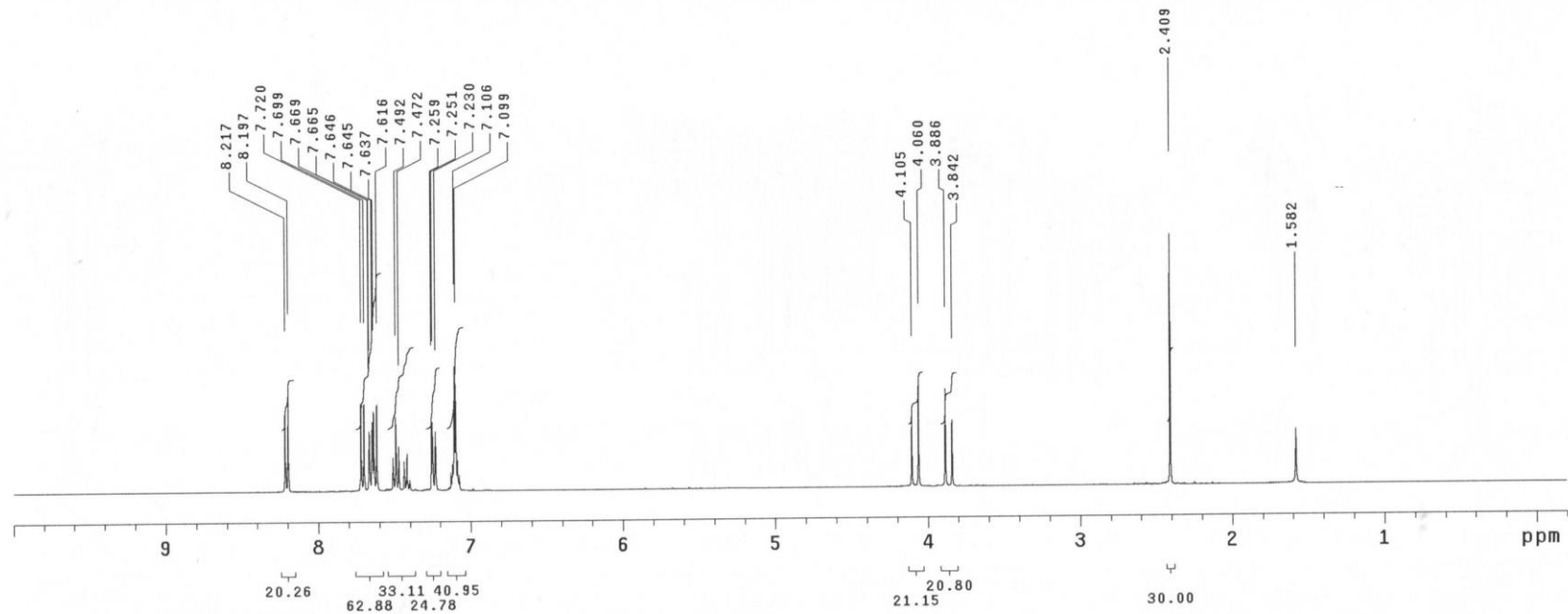
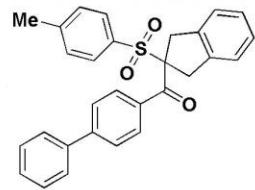


# Compound 7q (<sup>1</sup>H-NMR spectral data)

NC0630-5

Pulse Sequence: s2pu1  
Solvent: CDC13  
Ambient temperature  
UNITYplus-400 "unity400"

Pulse 38.8 degrees  
Acq. time 3.744 sec  
Width 6000.6 Hz  
32 repetitions  
OBSERVE H1, 400.2743817 MHz  
DATA PROCESSING  
FT size 65536  
Total time 2 min, 0 sec

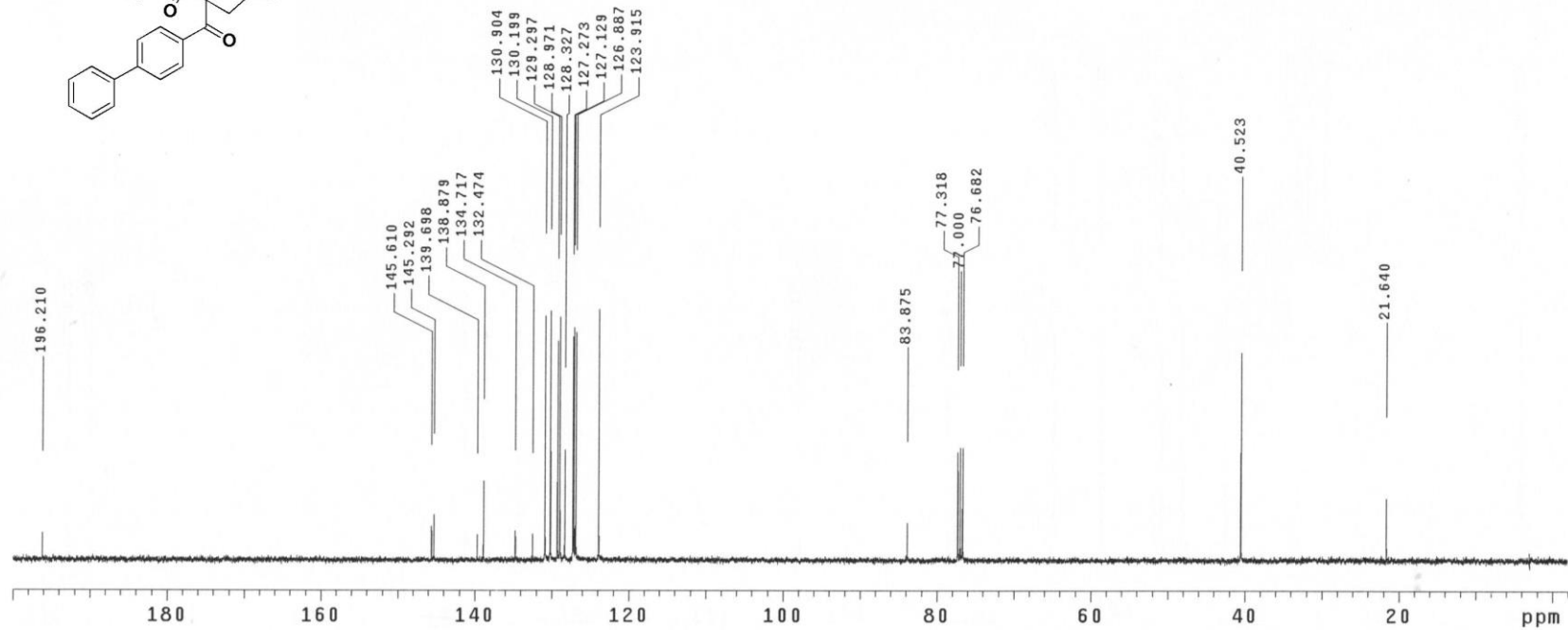
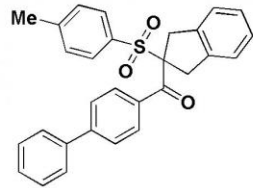


# Compound 7q (<sup>13</sup>C-NMR spectral data)

NC0630-5

Pulse Sequence: s2pu1  
Solvent: CDC13  
Ambient temperature  
UNITYplus-400 "unity400"

Relax. delay 0.500 sec  
Pulse 65.8 degrees  
Acq. time 0.800 sec  
Width 25000.0 Hz  
2480 repetitions  
OBSERVE C13, 100.6490746 MHz  
DECOUPLE H1, 400.2763980 MHz  
Power 43 dB  
on during acquisition  
off during delay  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 1.0 Hz  
FT size 65536  
Total time 11 hr, 39 min, 7 sec



# Compound 7r (<sup>1</sup>H-NMR spectral data)

NC0616-5

Pulse Sequence: s2pu1

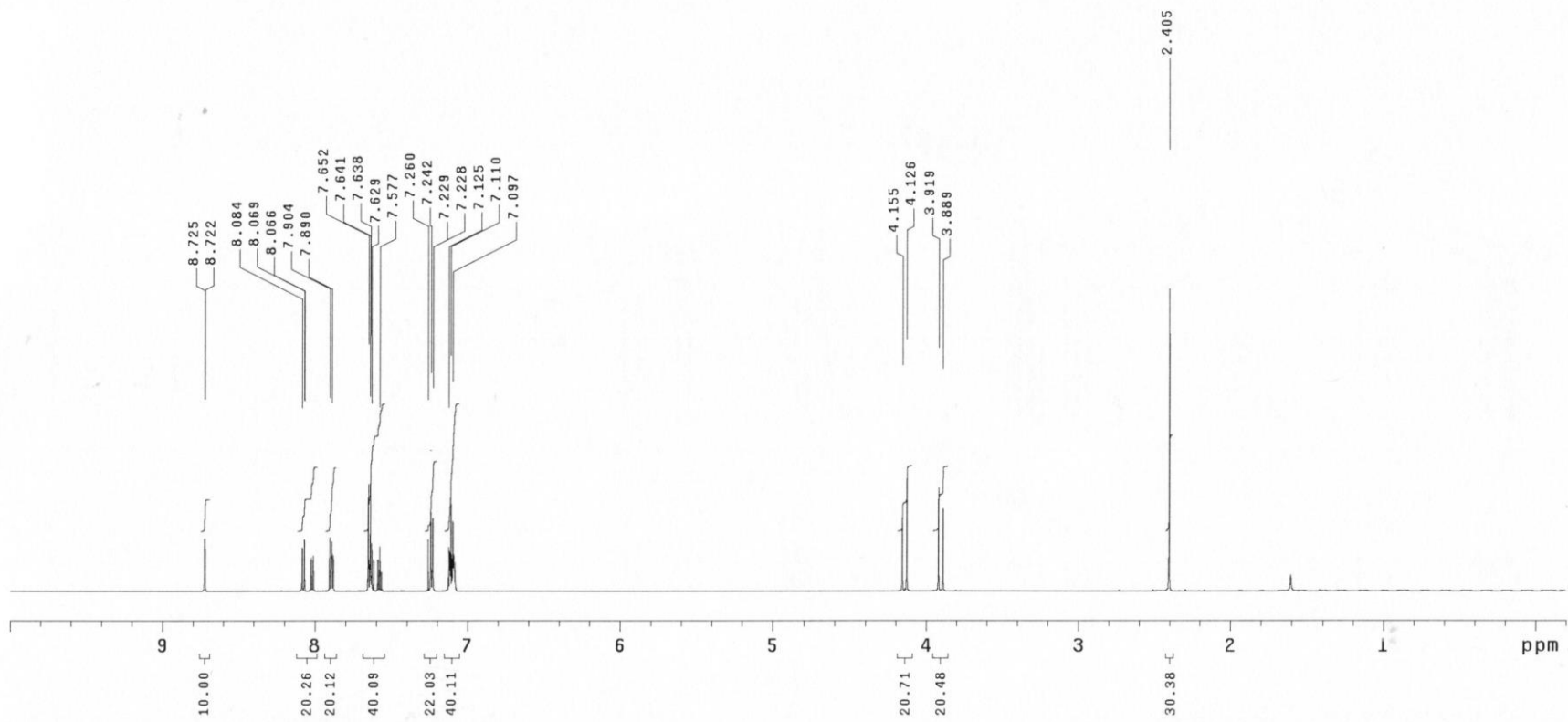
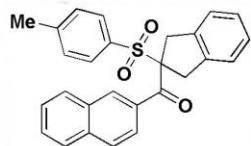
UNITYplus-600 "KMU600.kmu.edu.tw"

Date: Jun 18 2020

Solvent: cdc13

Temp. 28.0 C / 301.1 K

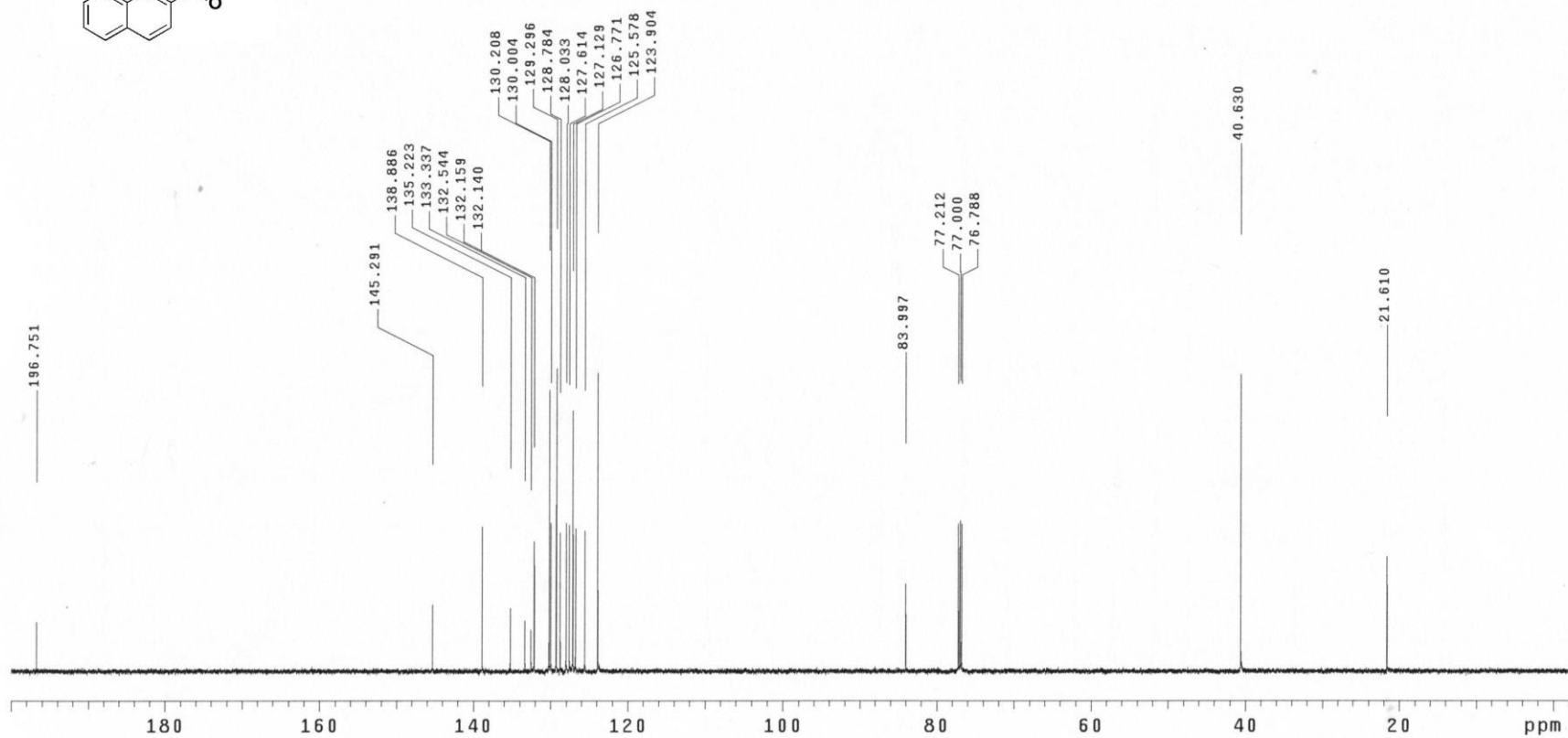
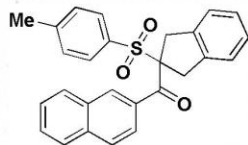
Total 16 repetitions



# Compound 7r (<sup>13</sup>C-NMR spectral data)

NC0616-5

Pulse Sequence: s2pu1  
UNITYplus-600 "KMU600.kmu.edu.tw"  
Date: Jun 18 2020  
Solvent: cdc13  
Temp. 28.0 C / 301.1 K  
Total 128 repetitions



# Compound 7s (<sup>1</sup>H-NMR spectral data)

NC0728-5

Pulse Sequence: s2pu1

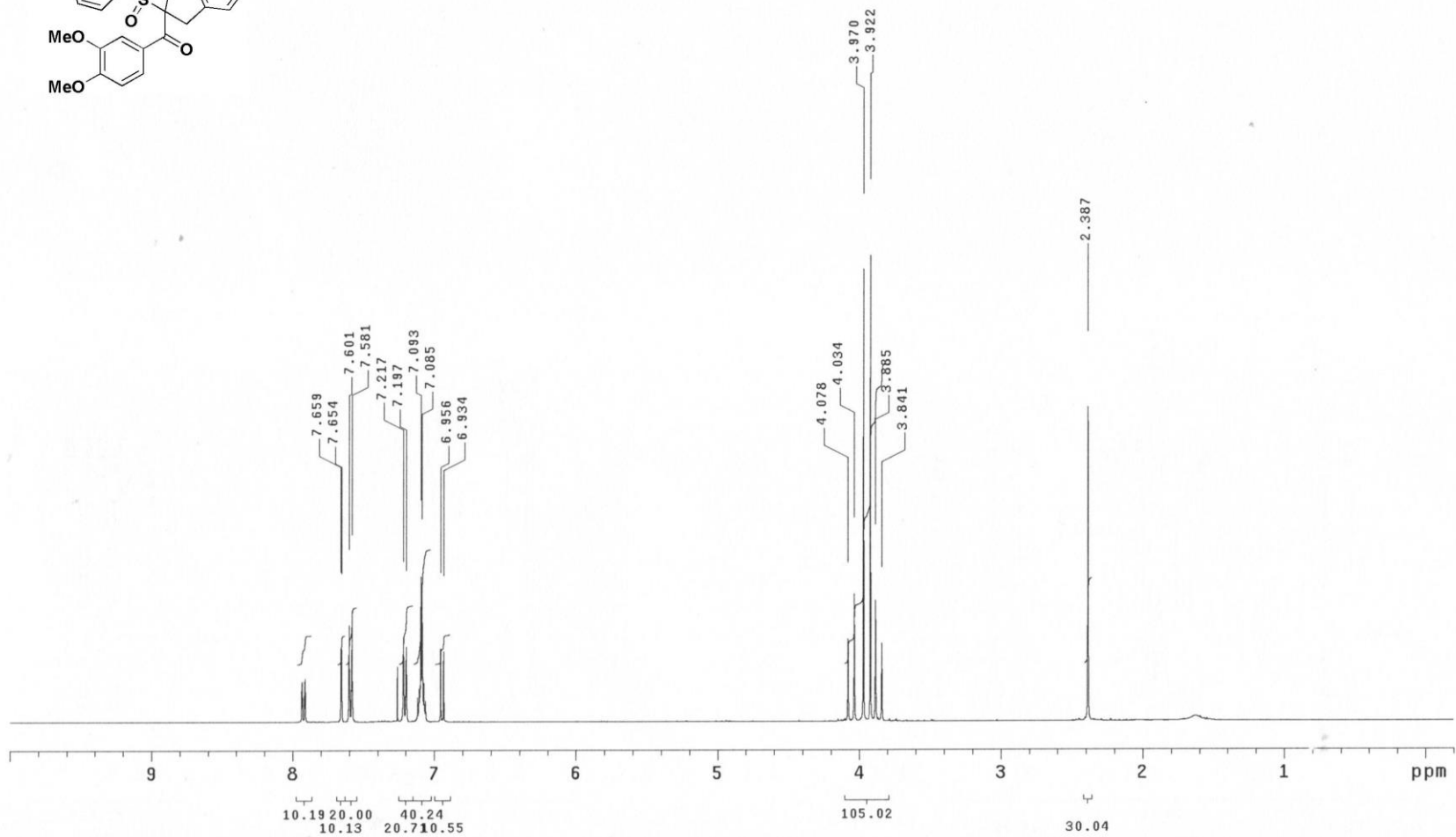
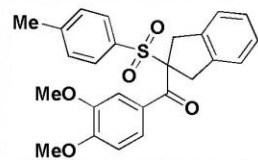
UNITYplus-400 "unity400"

Date: Jul 29 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 32 repetitions



# Compound 7s (<sup>13</sup>C-NMR spectral data)

NC0728-5

Pulse Sequence: s2pu1

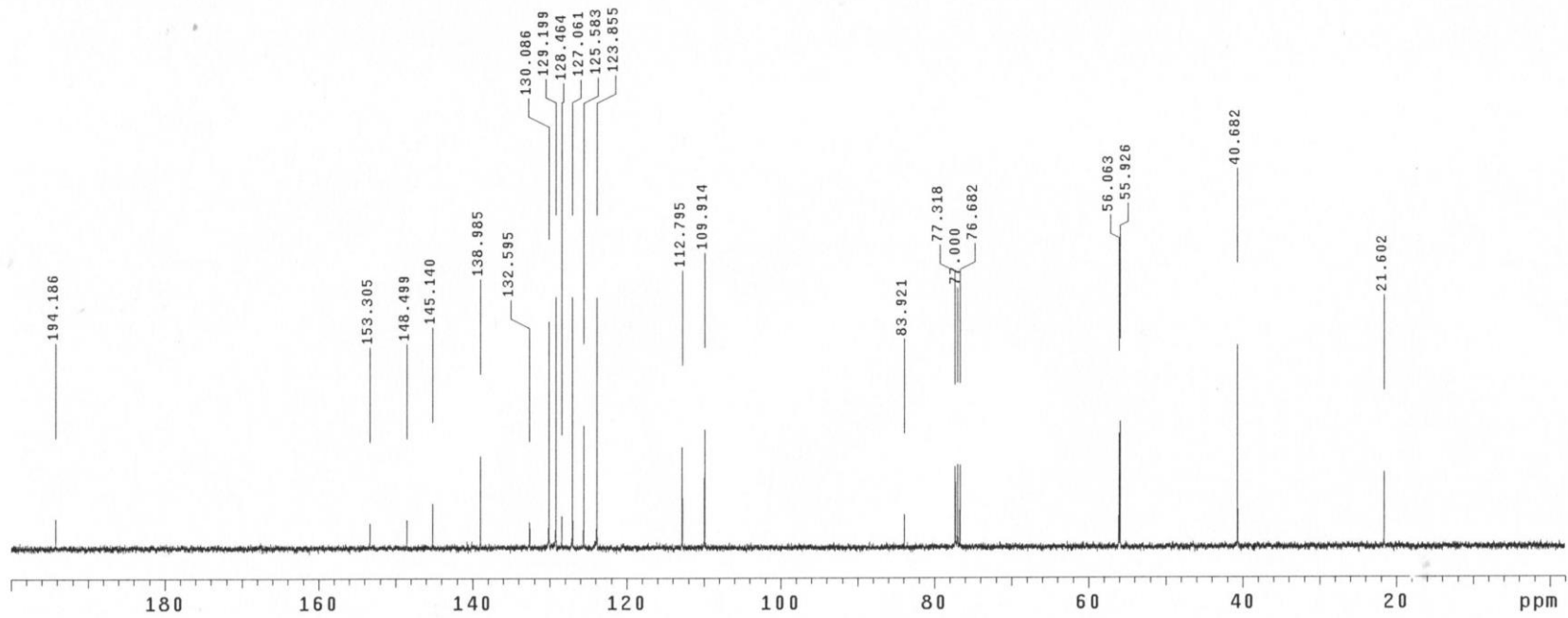
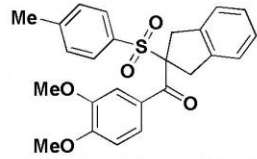
UNITYplus-400 "unity400"

Date: Jul 29 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 848 repetitions



# Compound 7t (<sup>1</sup>H-NMR spectral data)

NC0724-5

Pulse Sequence: s2pu1

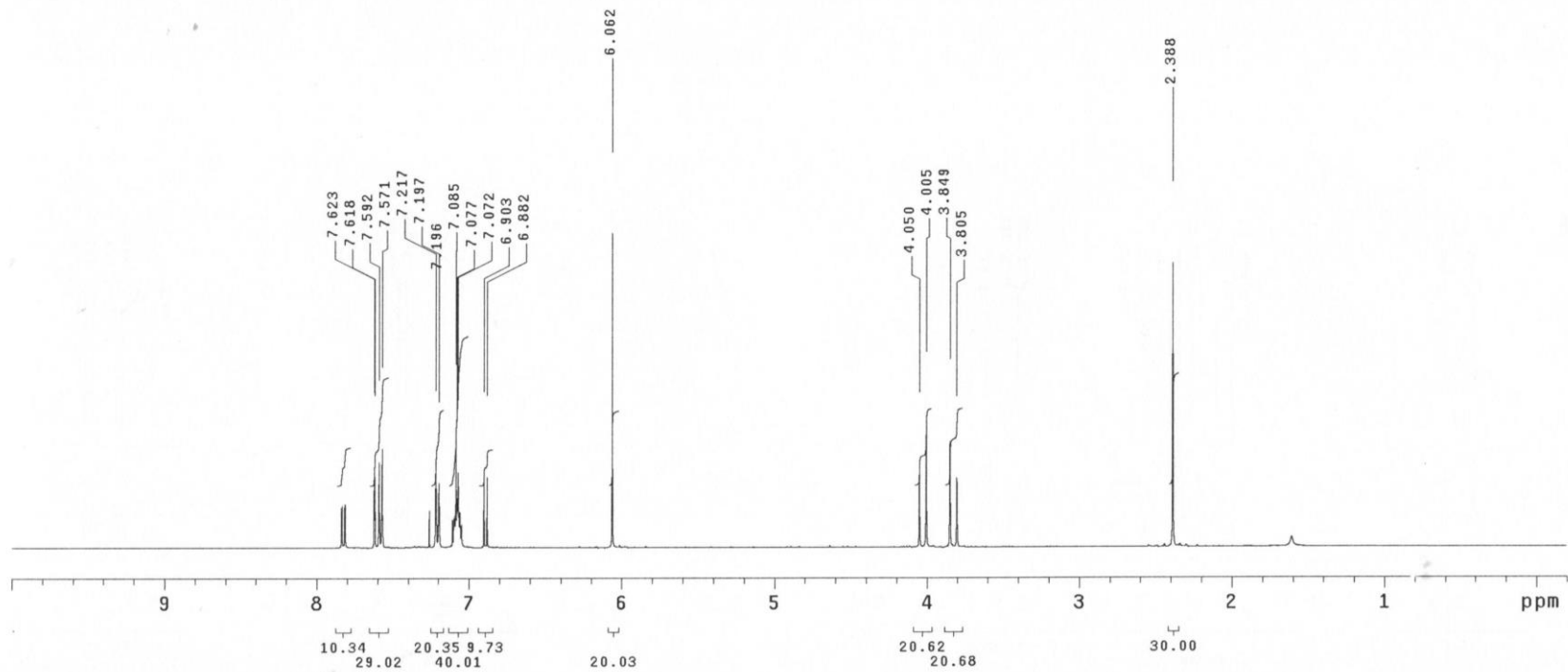
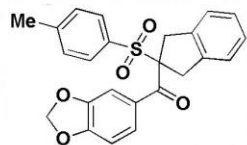
UNITYplus-400 "unity400"

Date: Jul 27 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 32 repetitions





# Compound 7t (<sup>13</sup>C-NMR spectral data)

NC0724-5

Pulse Sequence: s2pu1

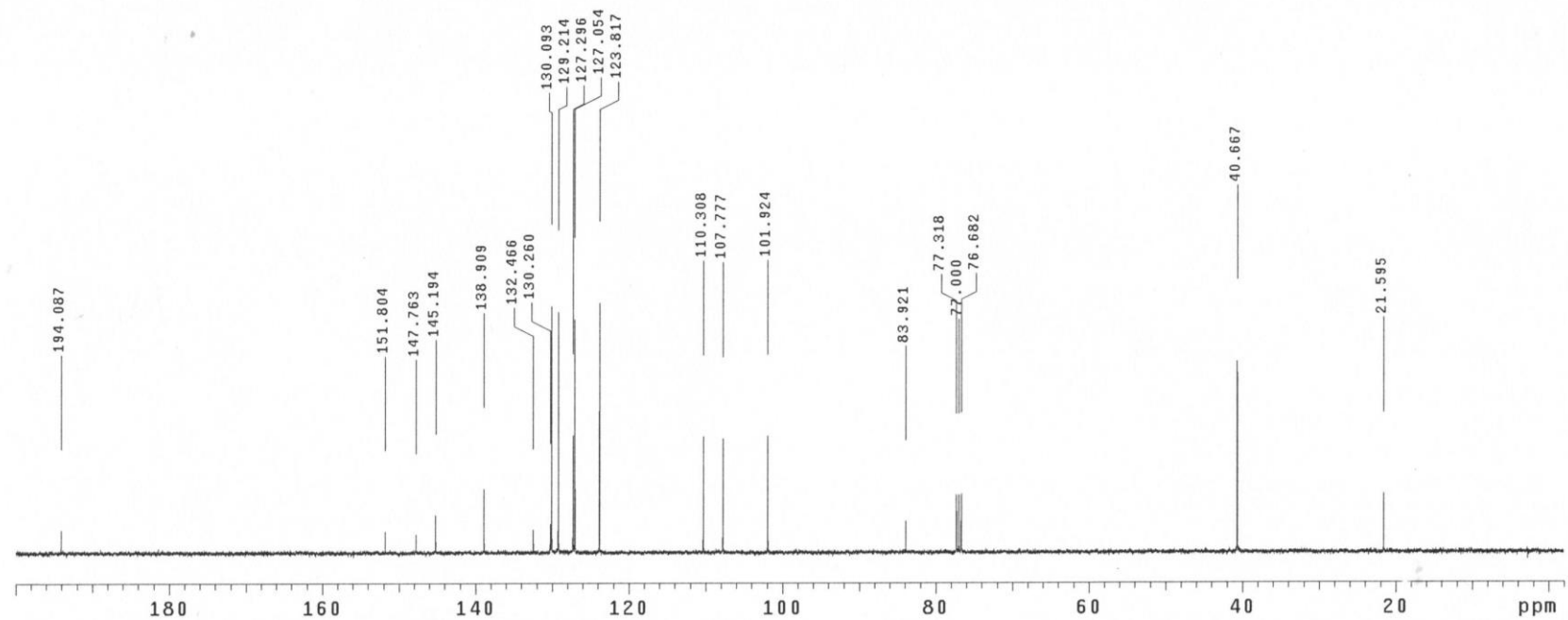
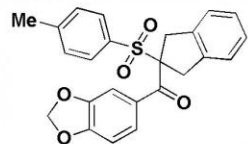
UNITYplus-400 "unity400"

Date: Jul 27 2020

Solvent: CDC13

Ambient temperature

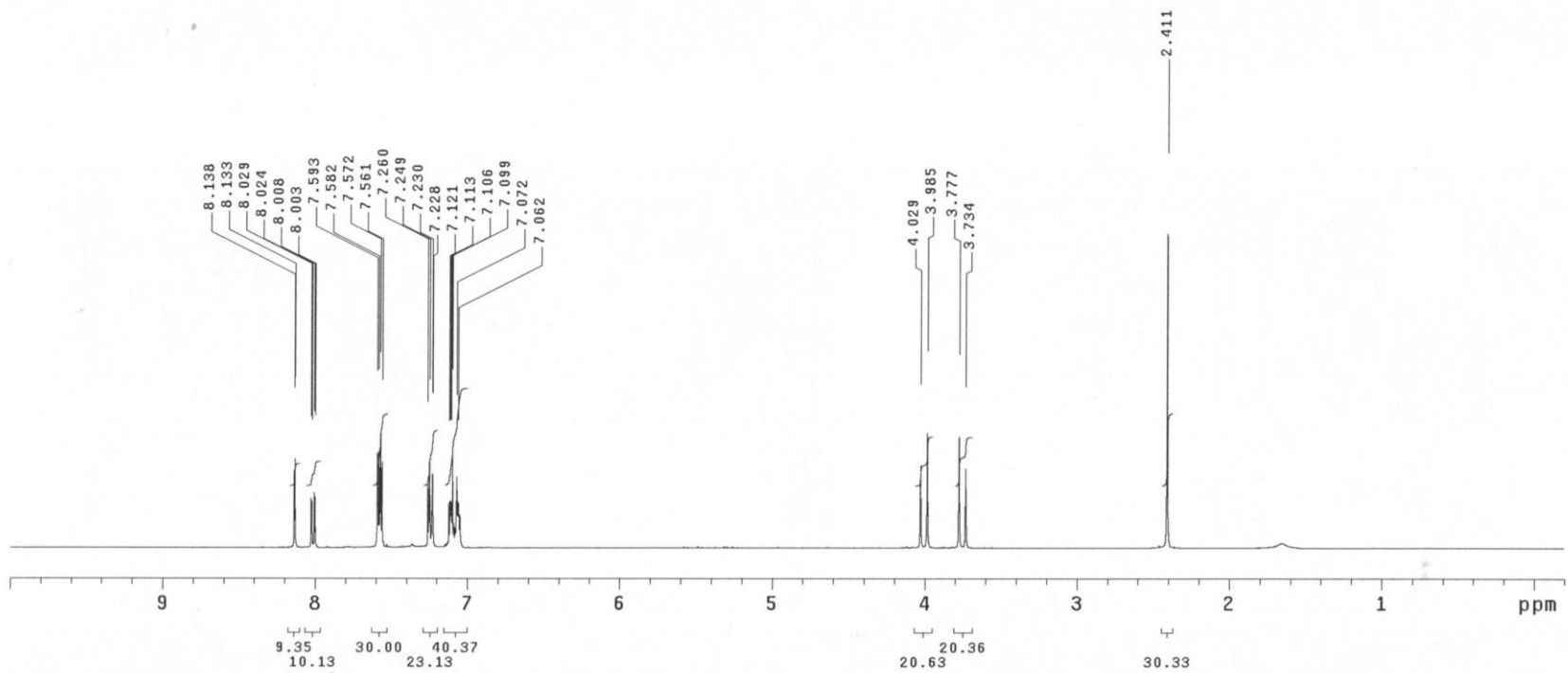
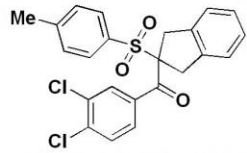
Total 1056 repetitions



# Compound 7u (<sup>1</sup>H-NMR spectral data)

NC0714-5

Pulse Sequence: s2pu1  
UNITYplus-400 "unity400"  
Date: Jul 16 2020  
Solvent: CDCl<sub>3</sub>  
Ambient temperature  
Total 32 repetitions



# Compound 7u (<sup>13</sup>C-NMR spectral data)

NC0714-5

Pulse Sequence: s2pu1

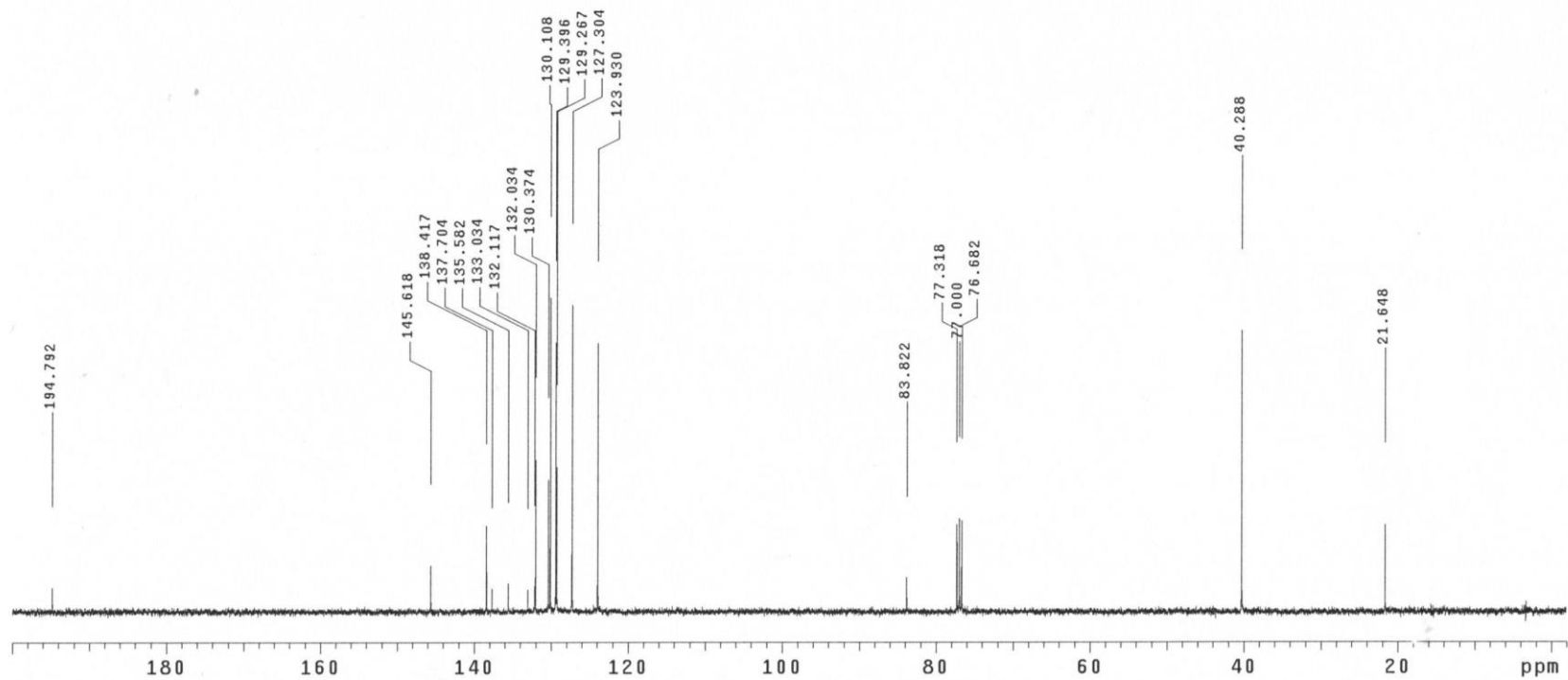
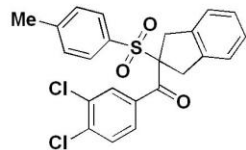
UNITYplus-400 "unity400"

Date: Jul 16 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 1360 repetitions



# Compound 7v (<sup>1</sup>H-NMR spectral data)

NC0730-5

Pulse Sequence: s2pu1

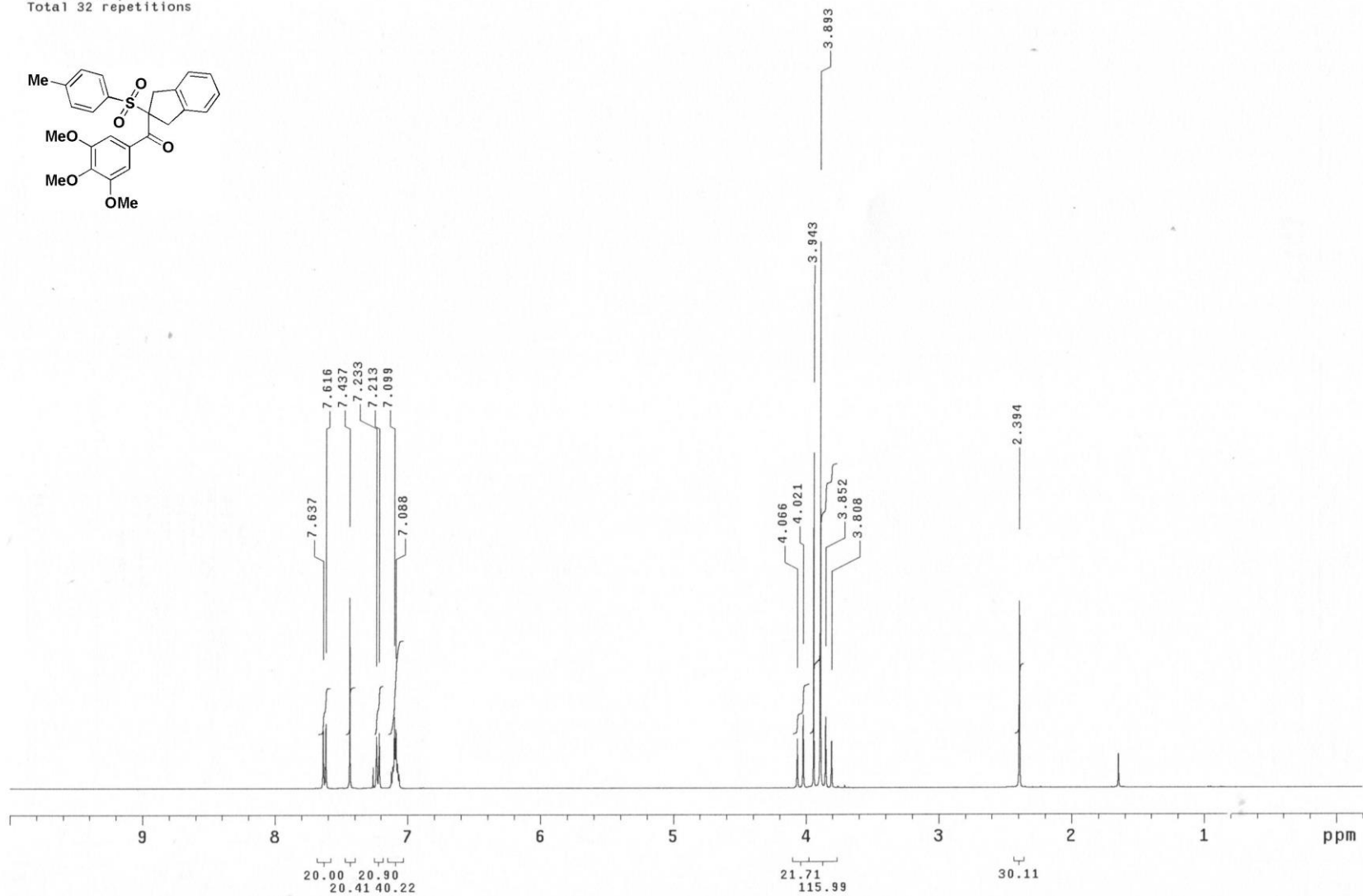
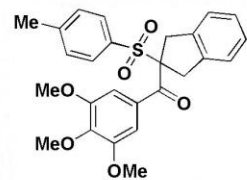
UNITYplus-400 "unity400"

Date: Aug 3 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 32 repetitions



# Compound 7v (<sup>13</sup>C-NMR spectral data)

NC0730-5

Pulse Sequence: s2pu1

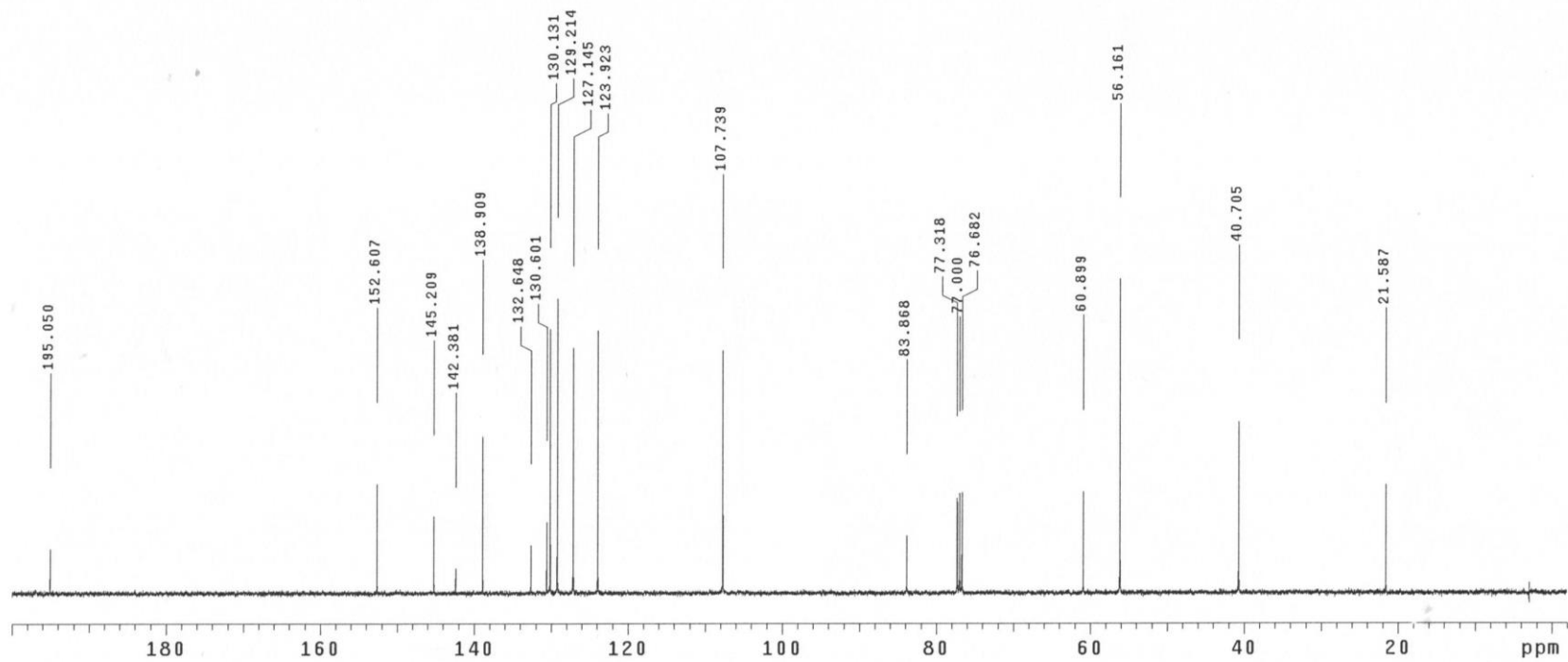
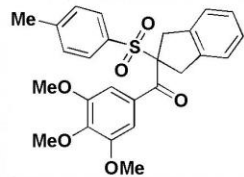
UNITYplus-400 "unity400"

Date: Aug 3 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 1152 repetitions



# Compound 7w (<sup>1</sup>H-NMR spectral data)

NC0804-5

Pulse Sequence: s2pu1

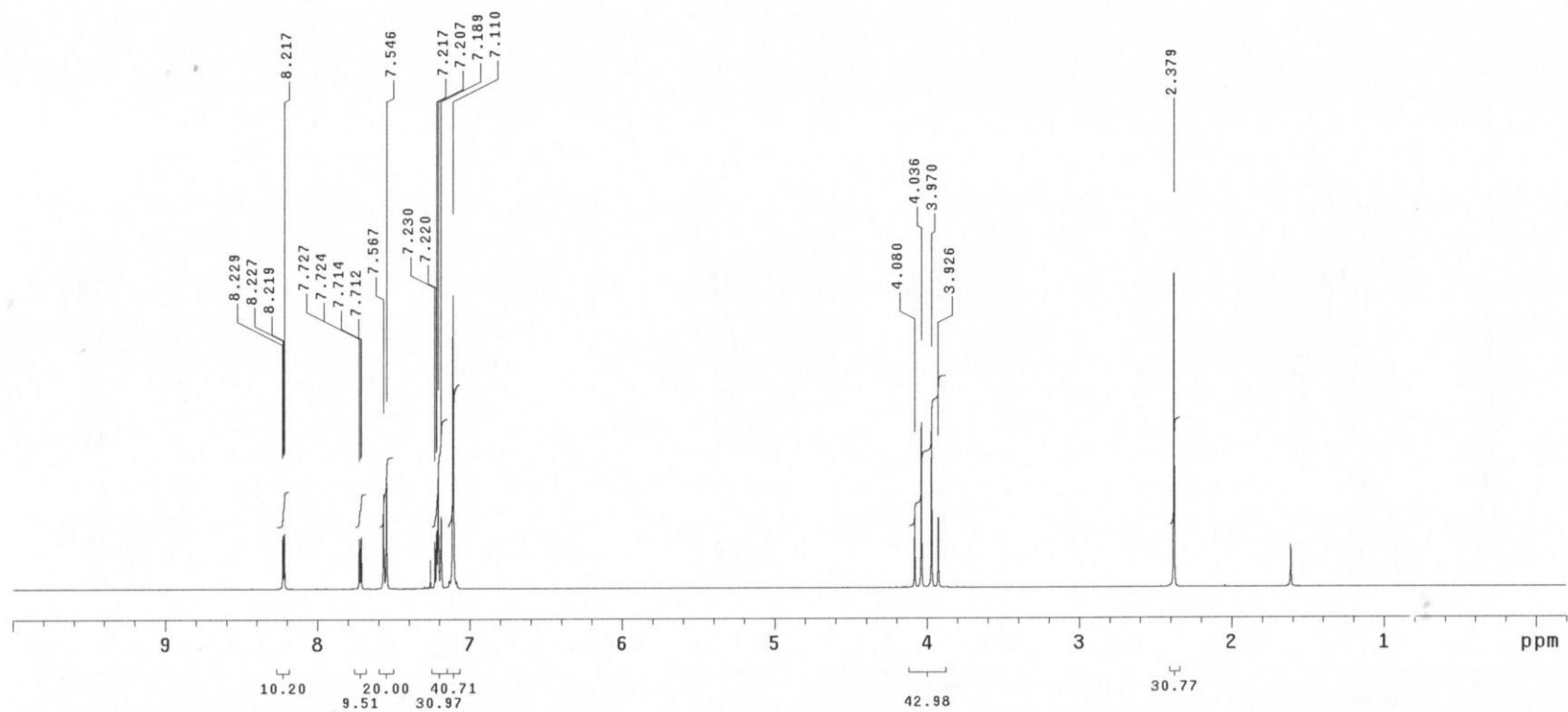
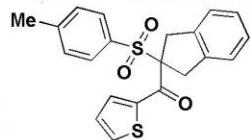
UNITYplus-400 "unity400"

Date: Aug 5 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 32 repetitions



# Compound 7w (<sup>13</sup>C-NMR spectral data)

NC0804-5

Pulse Sequence: s2pu1

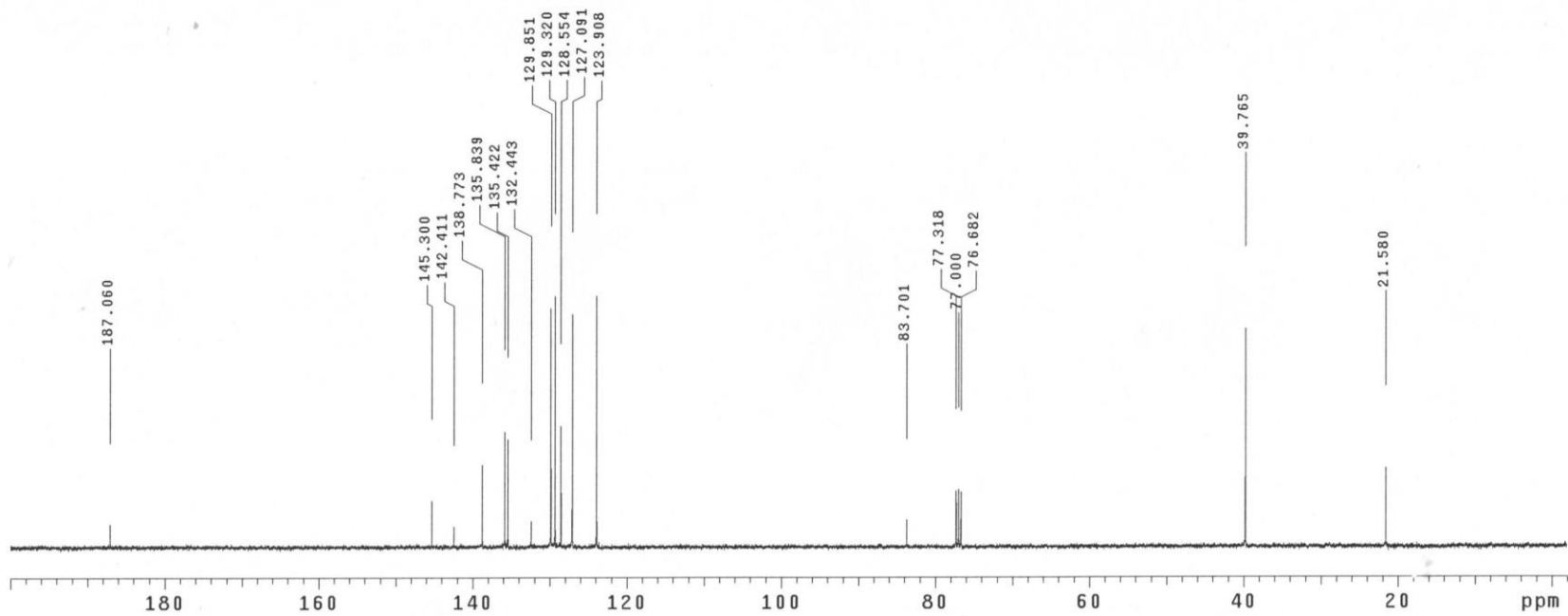
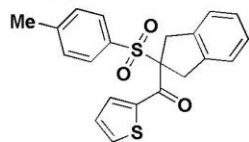
UNITYplus-400 "unity400"

Date: Aug 5 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 672 repetitions



# Compound 7x (<sup>1</sup>H-NMR spectral data)

NC0805-5

Pulse Sequence: s2pu1

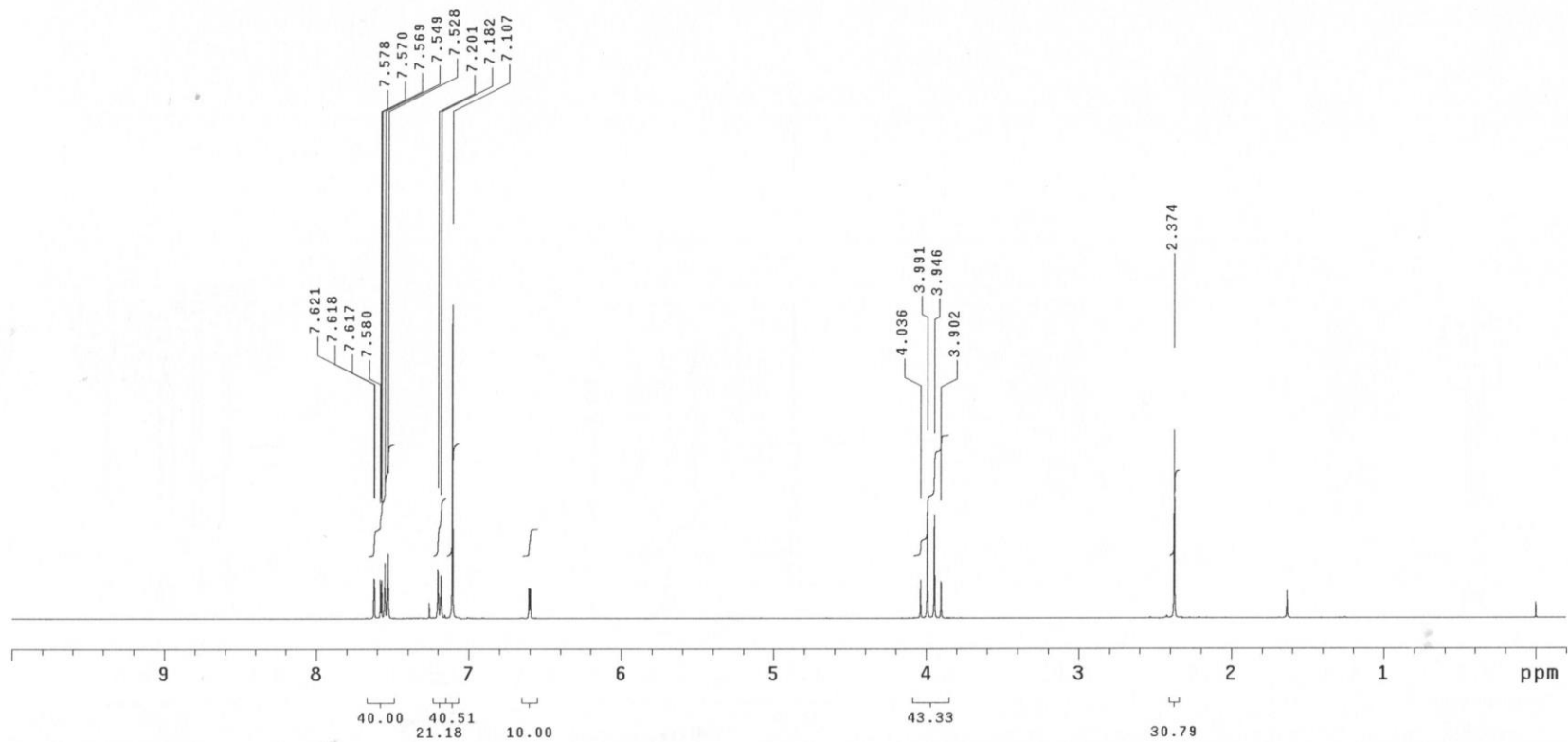
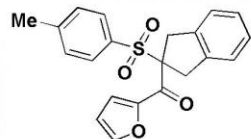
UNITYplus-400 "unity400"

Date: Aug 6 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 32 repetitions





# Compound 7x (<sup>13</sup>C-NMR spectral data)

NC0805-5

Pulse Sequence: s2pu1

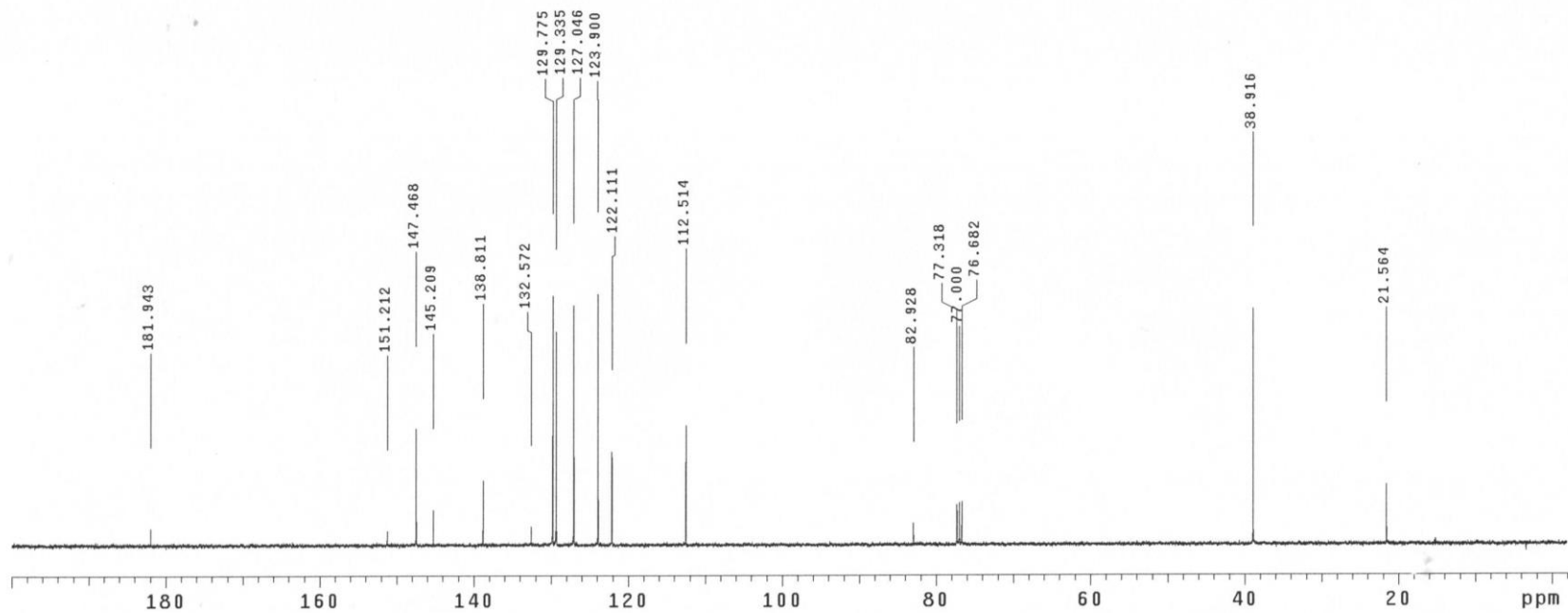
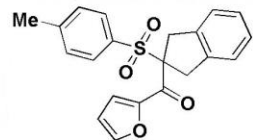
UNITYplus-400 "unity400"

Date: Aug 6 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 720 repetitions



# Compound 7y (<sup>1</sup>H-NMR spectral data)

NC0820-5

Pulse Sequence: s2pu1

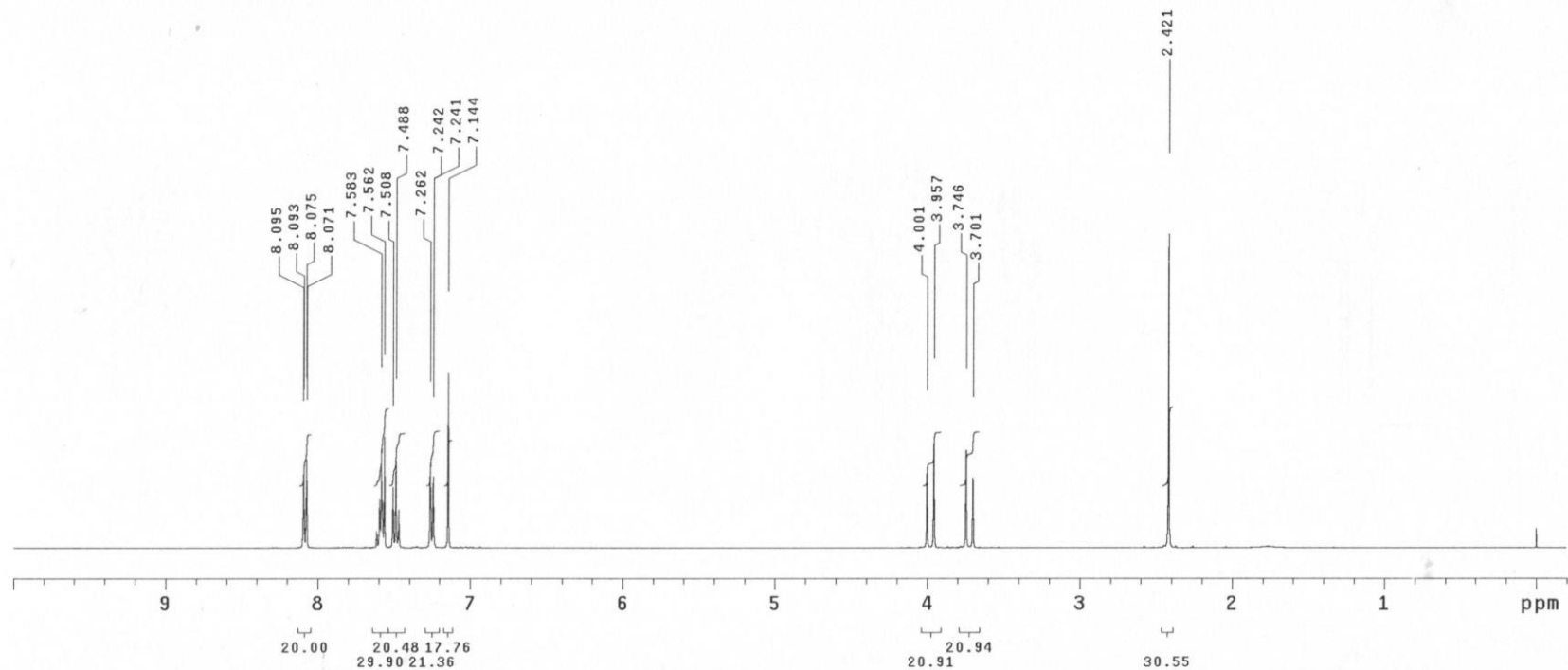
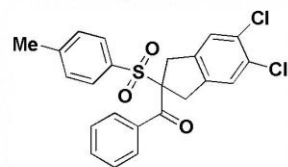
UNITYplus-400 "unity400"

Date: Aug 24 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

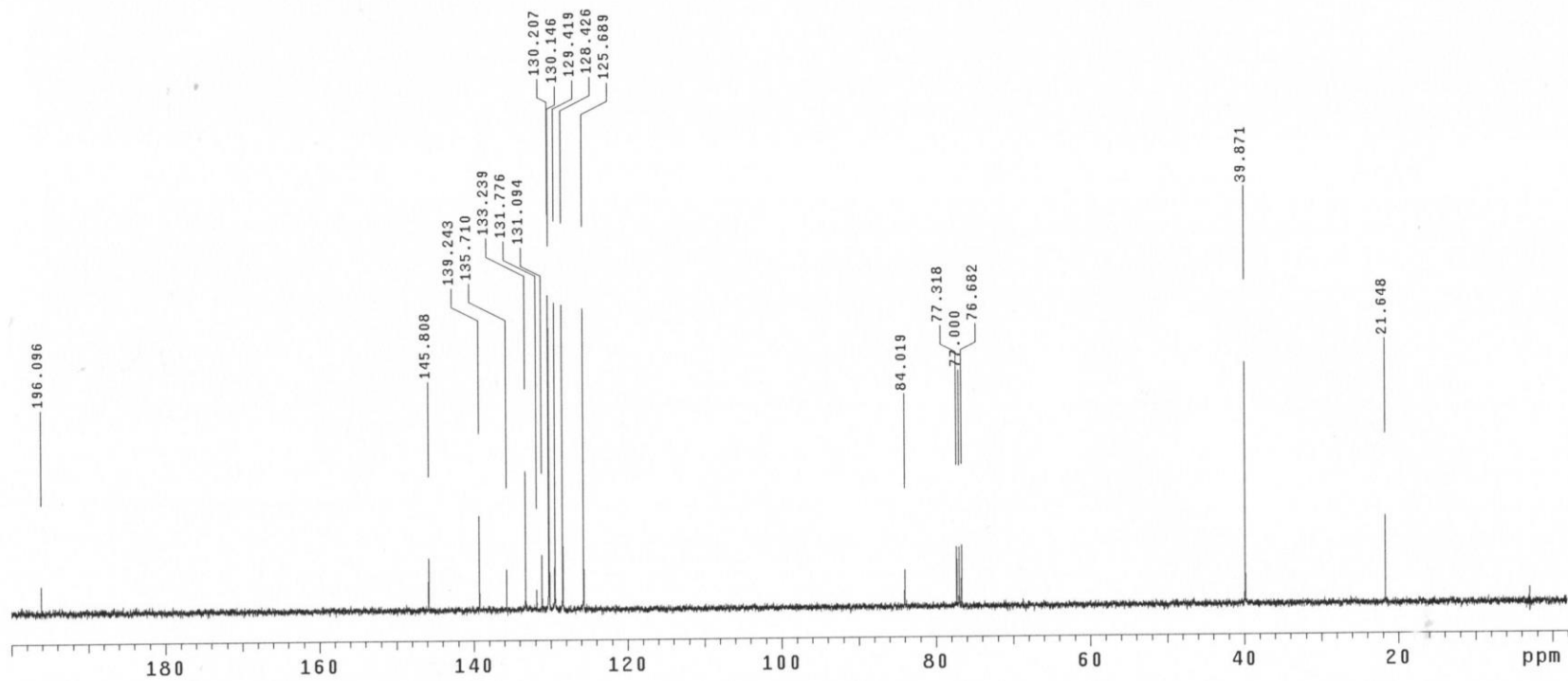
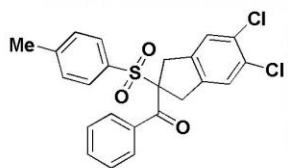
Total 32 repetitions



# Compound 7y (<sup>13</sup>C-NMR spectral data)

NC0820-5

Pulse Sequence: s2pu1  
UNITYplus-400 "unity400"  
Date: Aug 24 2020  
Solvent: CDCl<sub>3</sub>  
Ambient temperature  
Total 400 repetitions



# Compound 7z (<sup>1</sup>H-NMR spectral data)

NC0810-5

Pulse Sequence: s2pu1

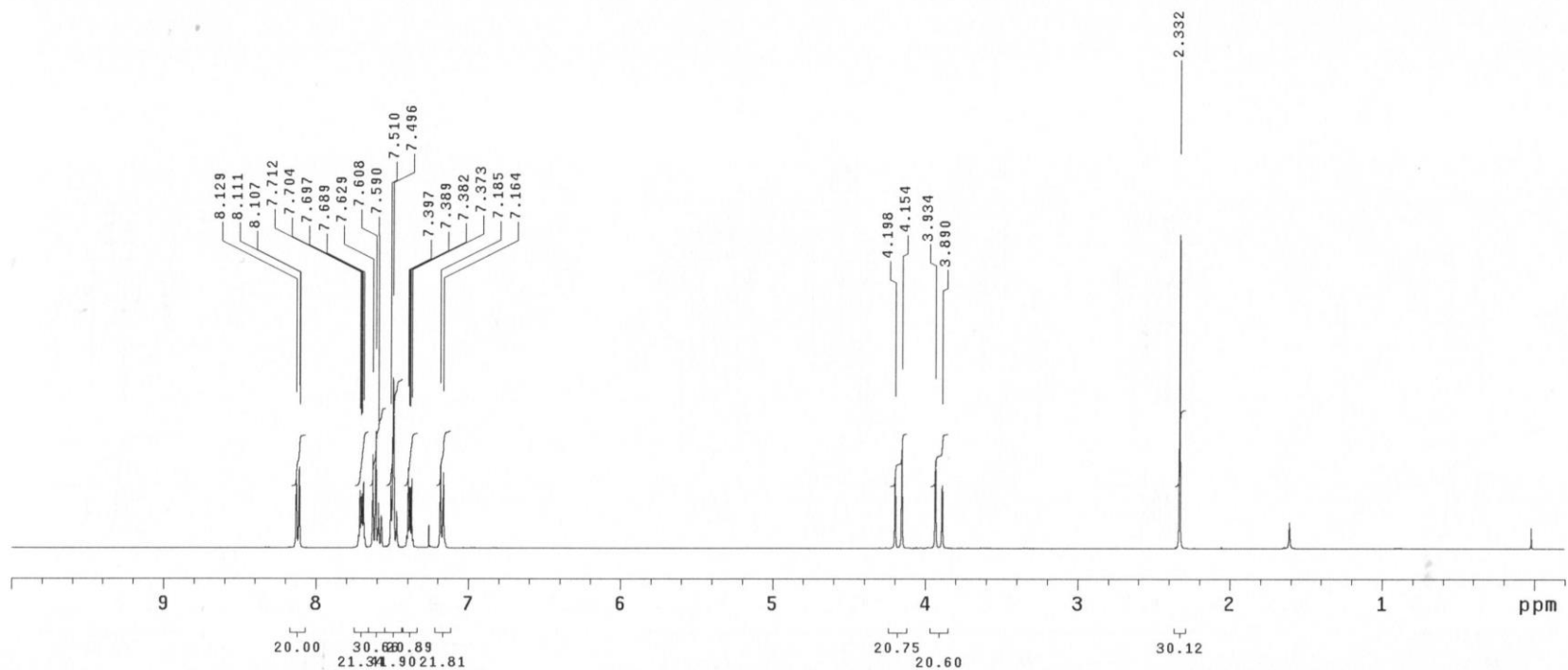
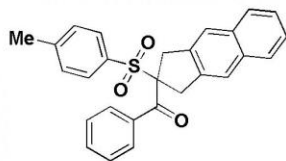
UNITYplus-400 "unity400"

Date: Aug 12 2020

Solvent: CDC13

Ambient temperature

Total 32 repetitions



# Compound 7z (<sup>13</sup>C-NMR spectral data)

NC0810-5

Pulse Sequence: s2pu1

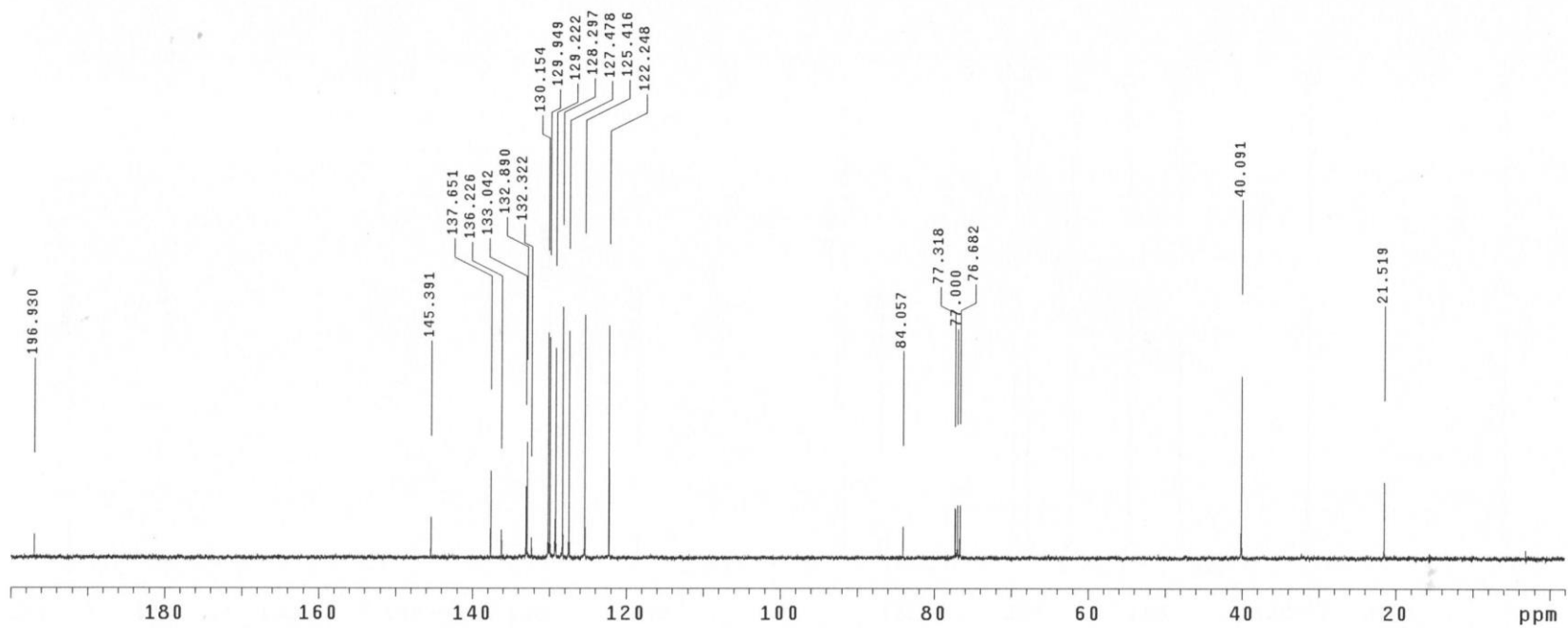
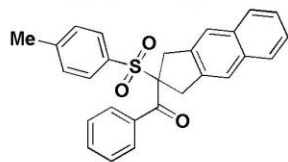
UNITYplus-400 "unity400"

Date: Aug 12 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 672 repetitions



# Compound 7aa (<sup>1</sup>H-NMR spectral data)

NC0821-5

Pulse Sequence: s2pu1

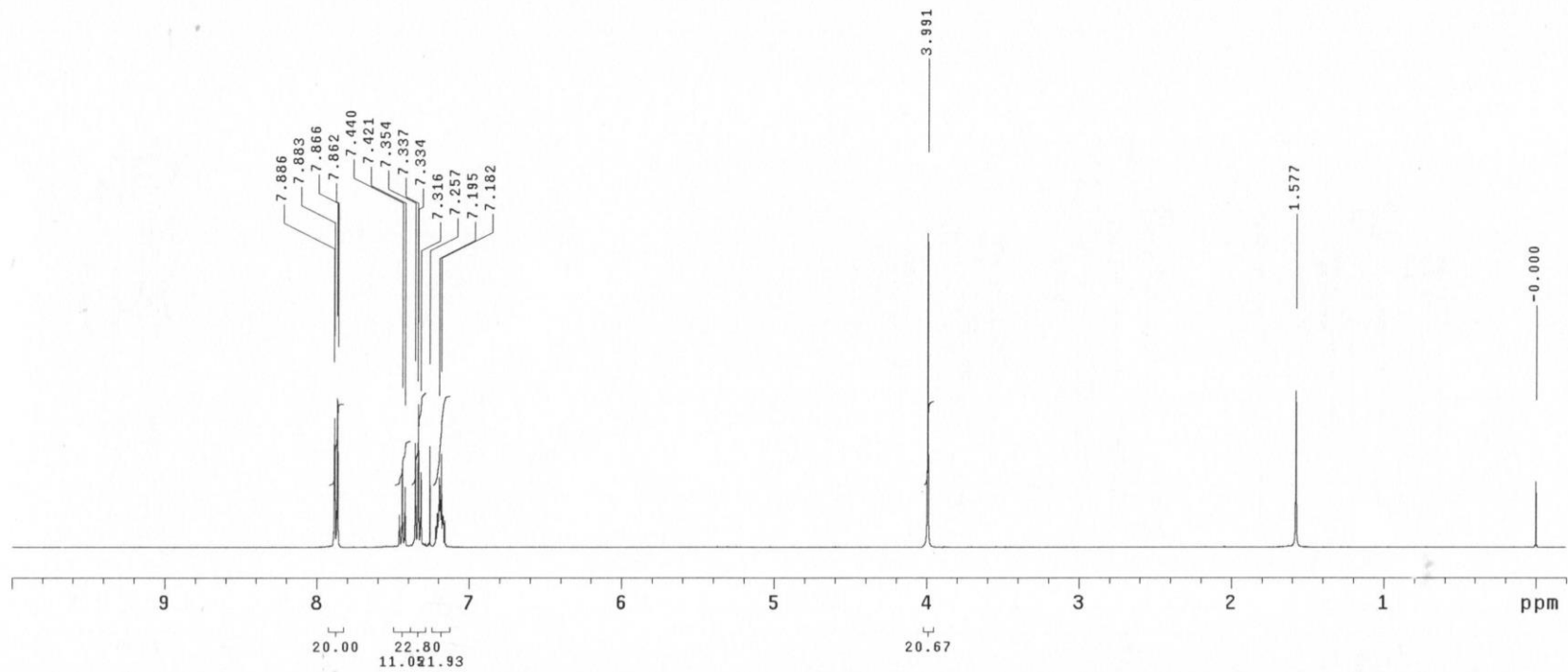
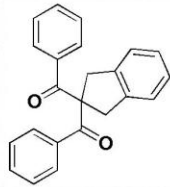
UNITYplus-400 "unity400"

Date: Aug 24 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

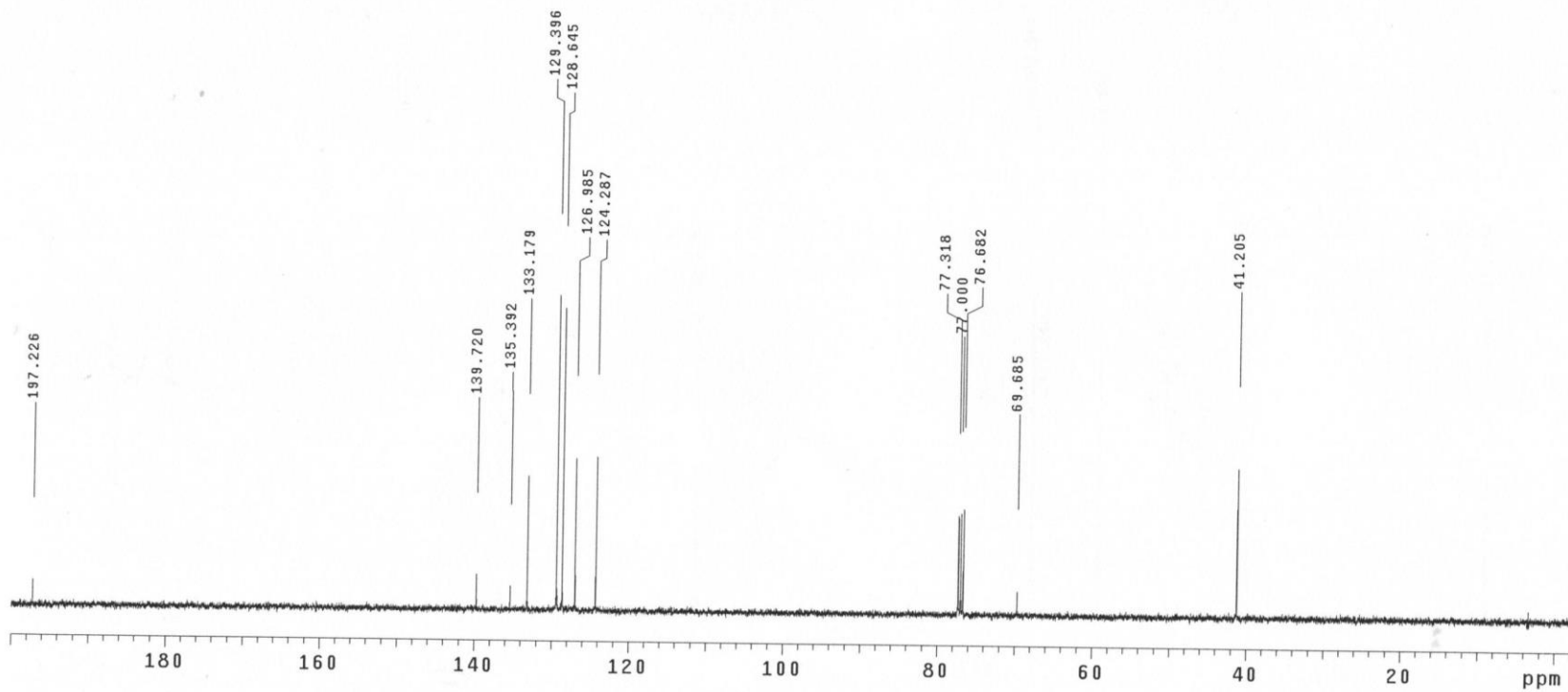
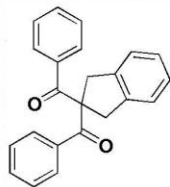
Total 32 repetitions



# Compound 7aa (<sup>13</sup>C-NMR spectral data)

NC0821-5

Pulse Sequence: s2pu1  
UNITYplus-400 "unity400"  
Date: Aug 24 2020  
Solvent: CDCl<sub>3</sub>  
Ambient temperature  
Total 1472 repetitions



# Compound 7ab (<sup>1</sup>H-NMR spectral data)

NC0824-5

Pulse Sequence: s2pu1

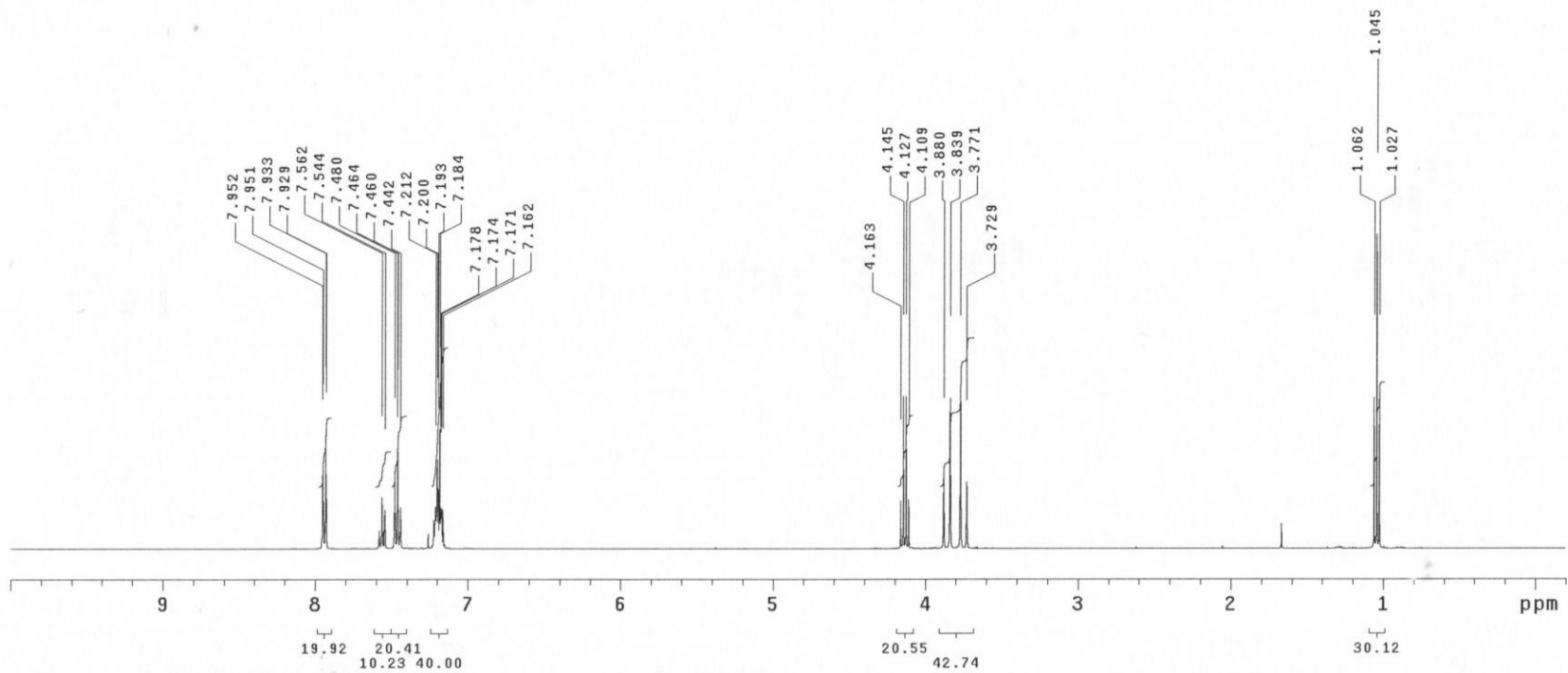
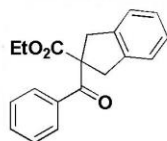
UNITYplus-400 "unity400"

Date: Aug 27 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 32 repetitions





# Compound 7ab (<sup>13</sup>C-NMR spectral data)

NC0824-5

Pulse Sequence: s2pu1

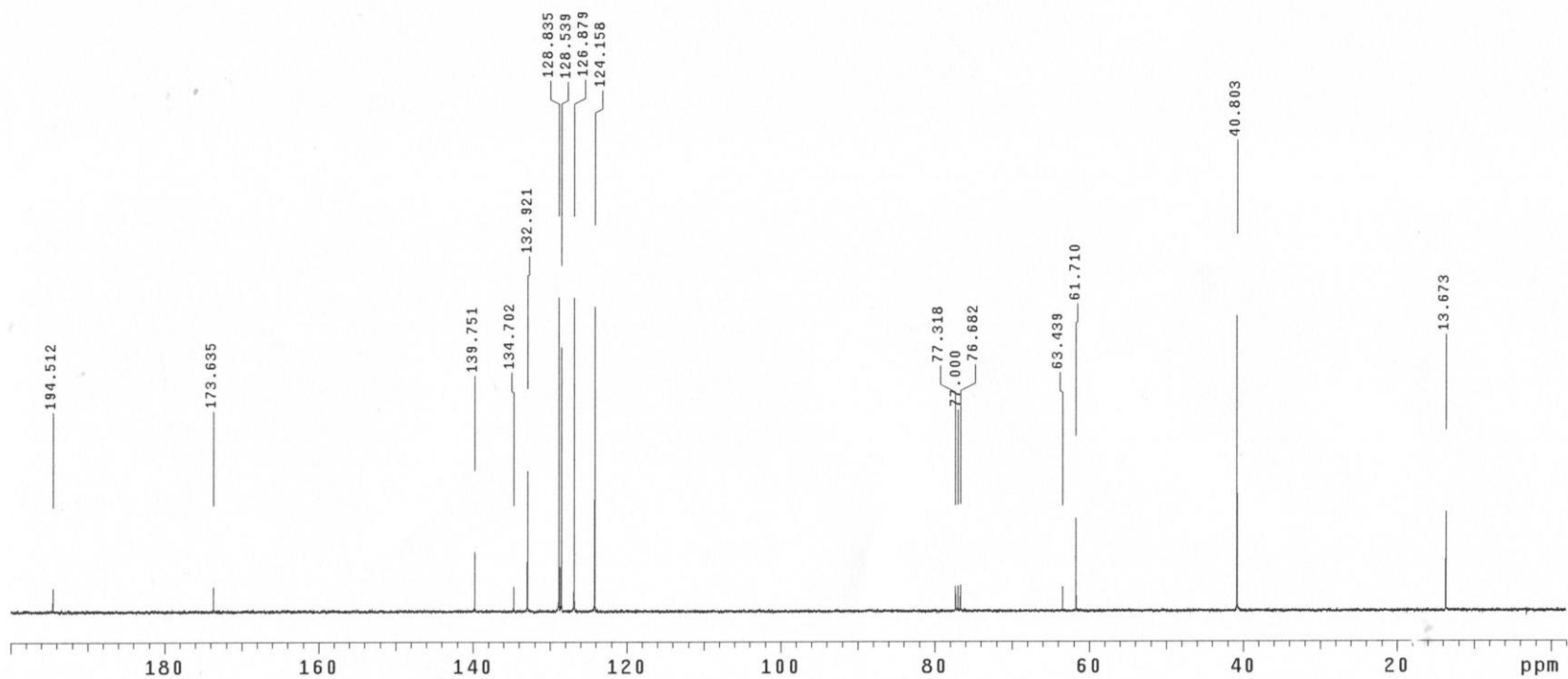
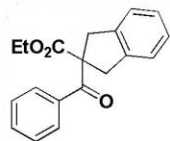
UNITYplus-400 "unity400"

Date: Aug 27 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 400 repetitions



# Compound 7ac (<sup>1</sup>H-NMR spectral data)

NC0831-5

Pulse Sequence: s2pu1

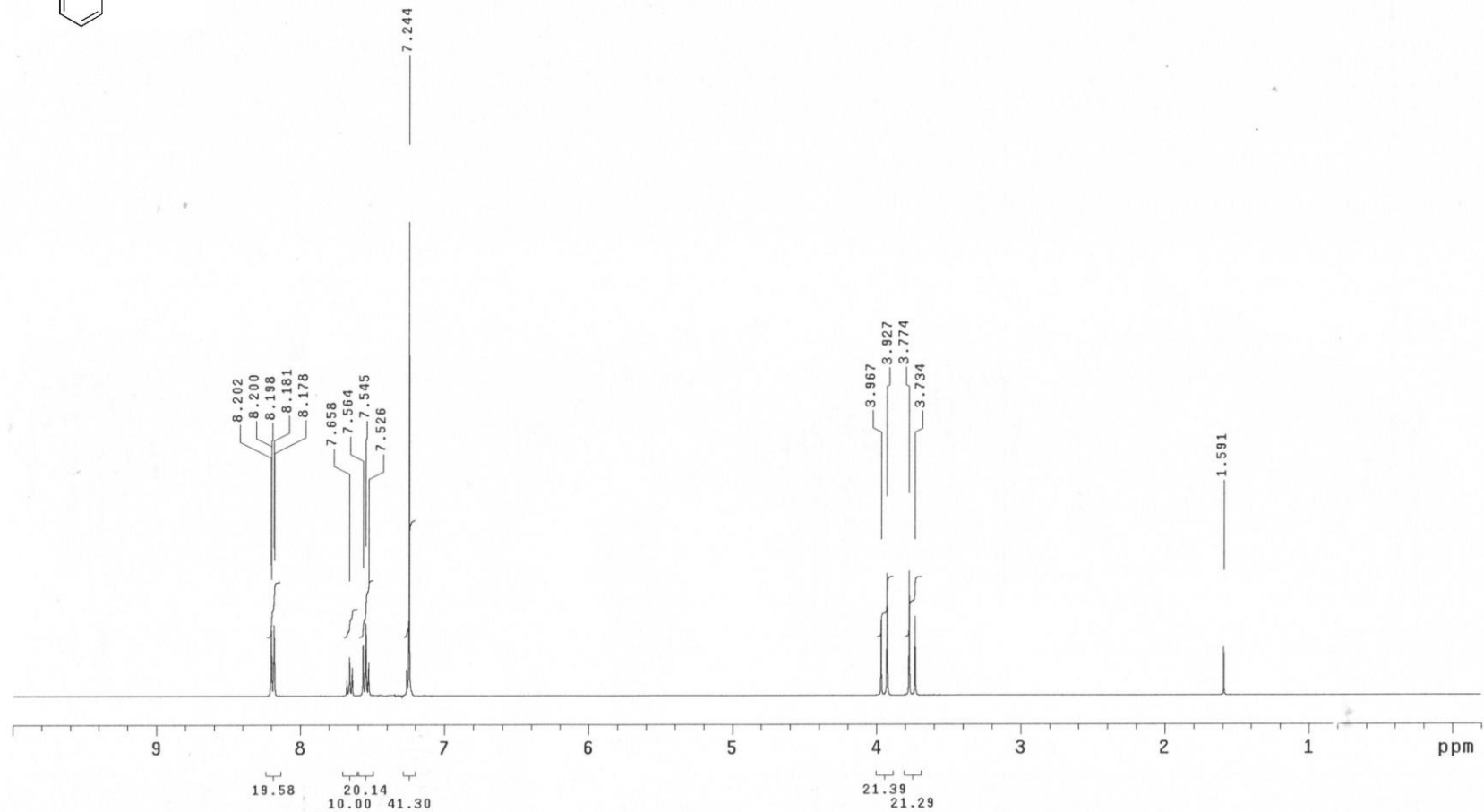
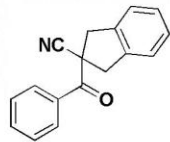
UNITYplus-400 "unity400"

Date: Sep 1 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 32 repetitions



# Compound 7ac (<sup>13</sup>C-NMR spectral data)

NC0831-5

Pulse Sequence: s2pu1

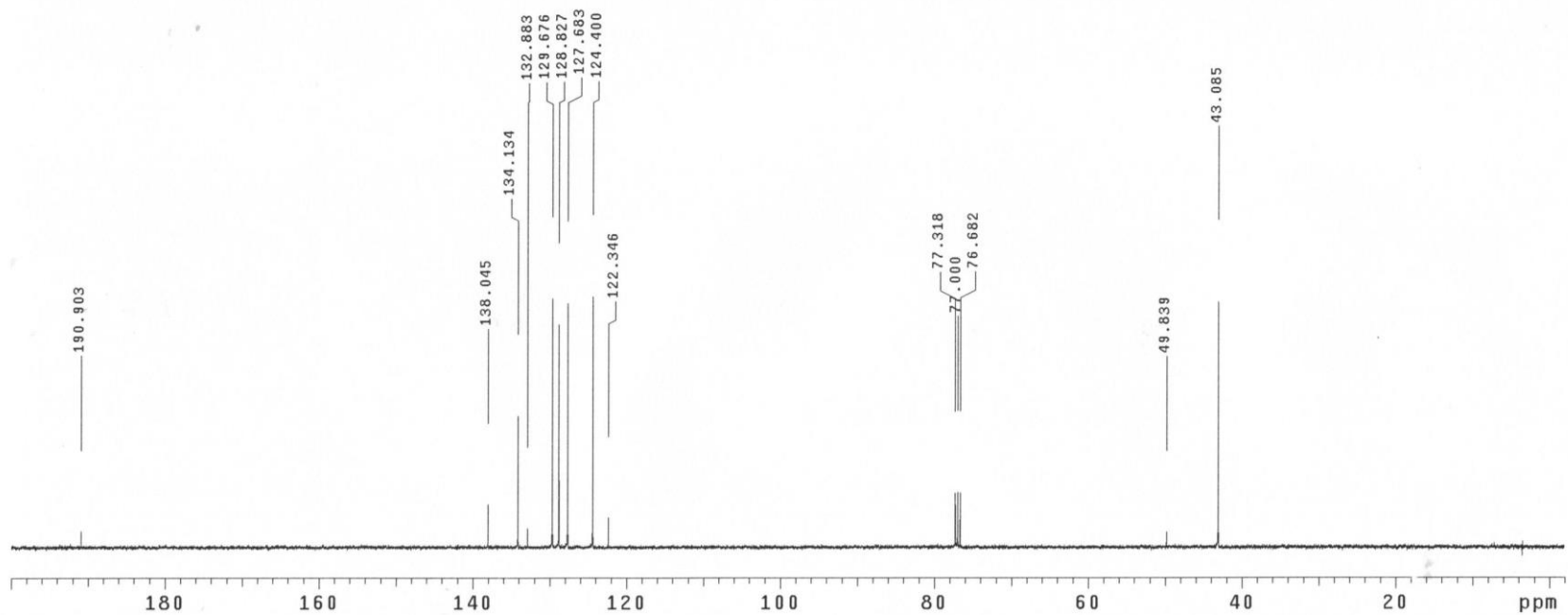
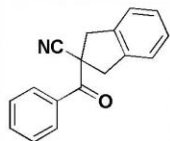
UNITYplus-400 "unity400"

Date: Sep 1 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 816 repetitions



# Compound 7ad (<sup>1</sup>H-NMR spectral data)

NC0903-5

Pulse Sequence: s2pu1

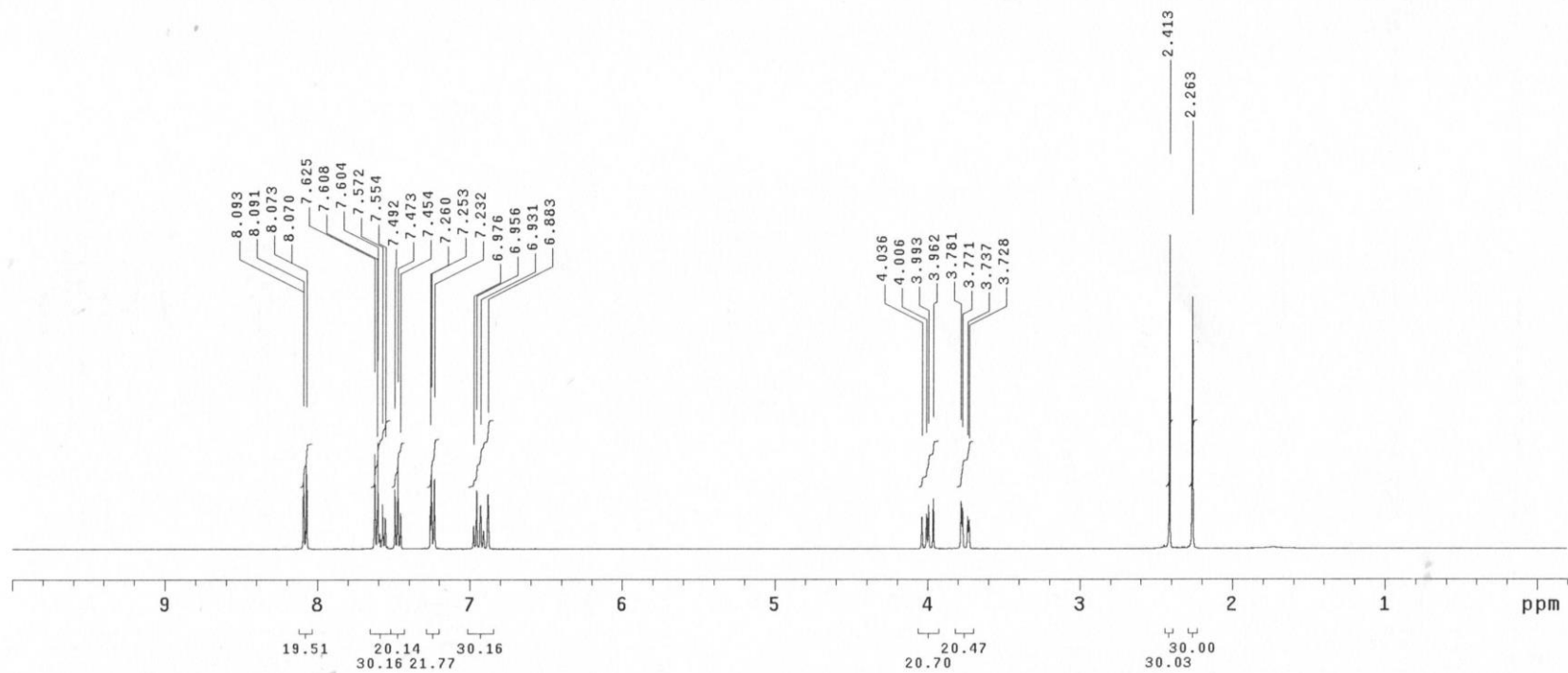
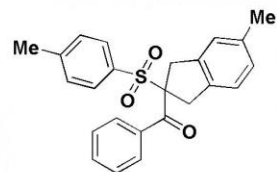
UNITYplus-400 "unity400"

Date: Sep 7 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 32 repetitions



# Compound 7ad (<sup>13</sup>C-NMR spectral data)

NC0903-5

Pulse Sequence: s2pu1

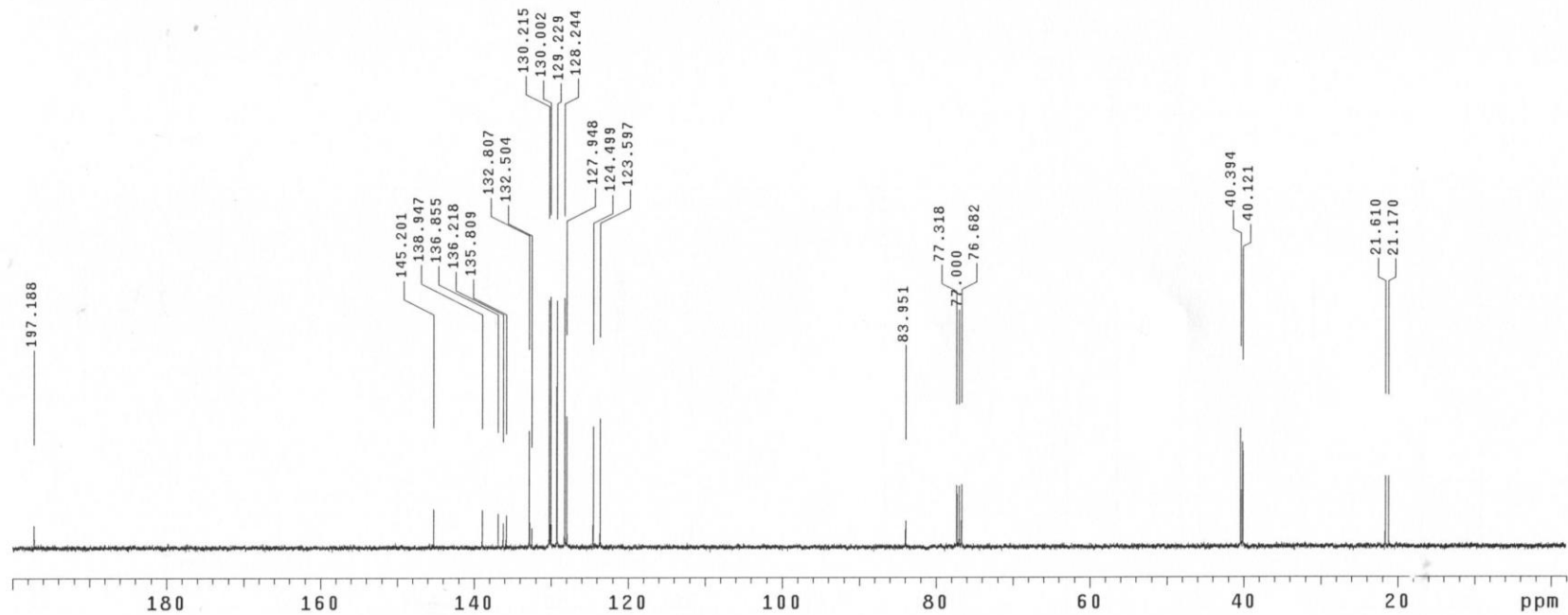
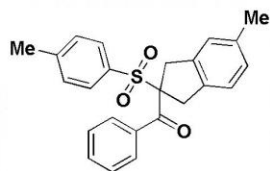
UNITYplus-400 "unity400"

Date: Sep 7 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 832 repetitions



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

KT5557

Pulse Sequence: s2pu1

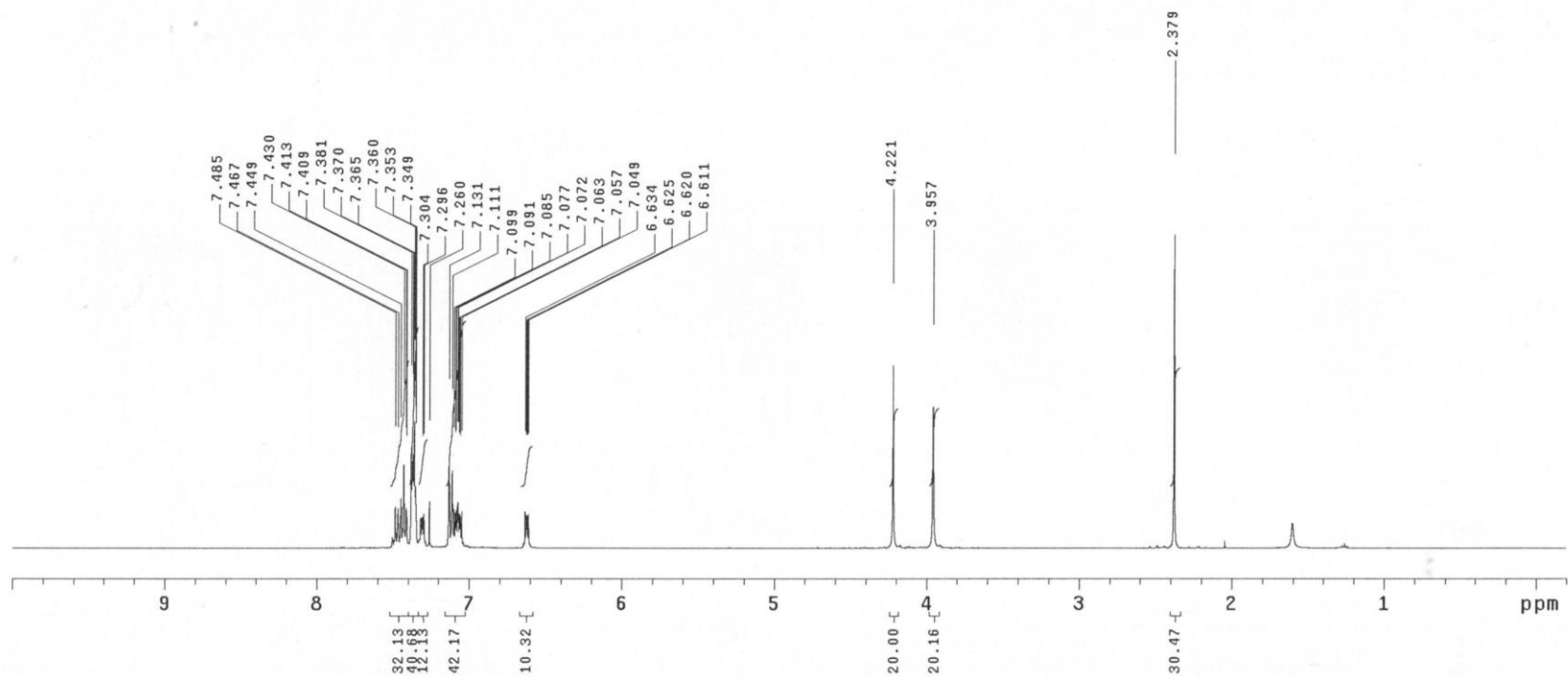
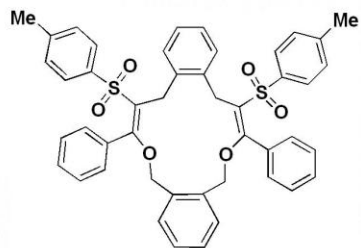
UNITYplus-400 "unity400"

Date: Apr 22 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 32 repetitions



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

KT5557

Pulse Sequence: s2pu1

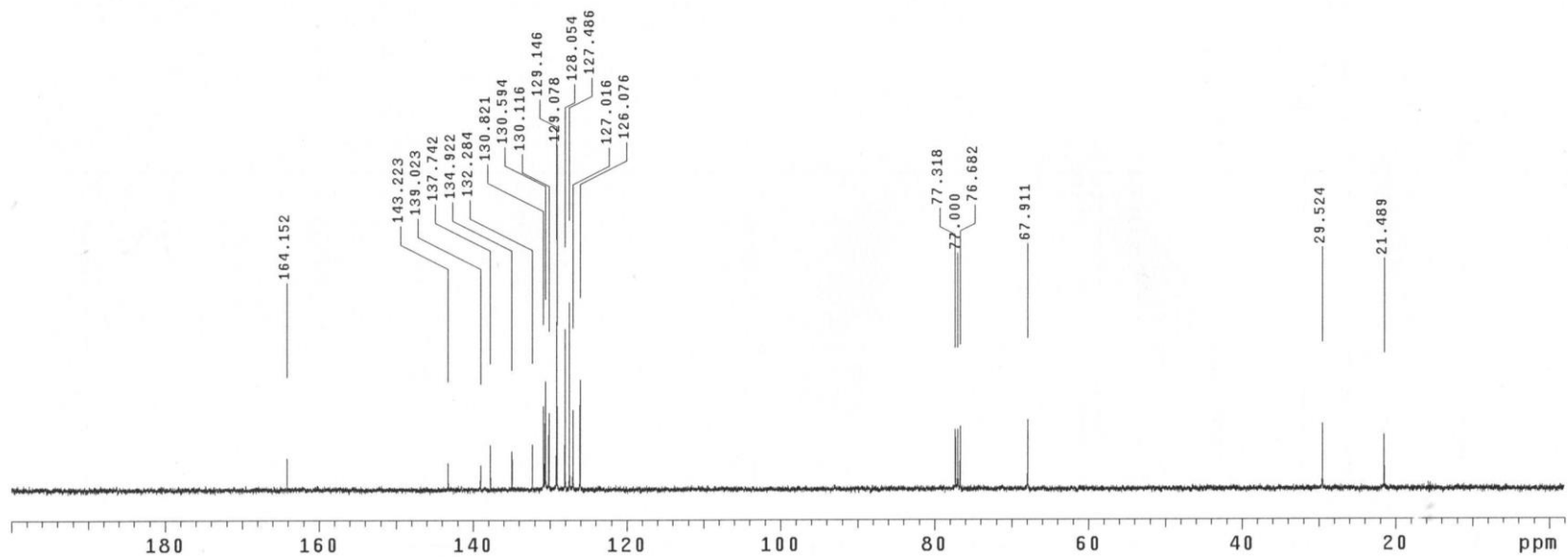
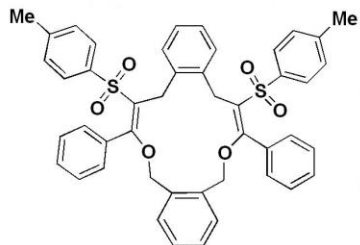
UNITYplus-400 "unity400"

Date: Apr 22 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 640 repetitions



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

NC0624-14

Pulse Sequence: s2pu1

Solvent: CDC13

Ambient temperature

UNITYplus-400 "unity400"

Pulse 38.8 degrees

Acq. time 3.744 sec

Width 6000.6 Hz

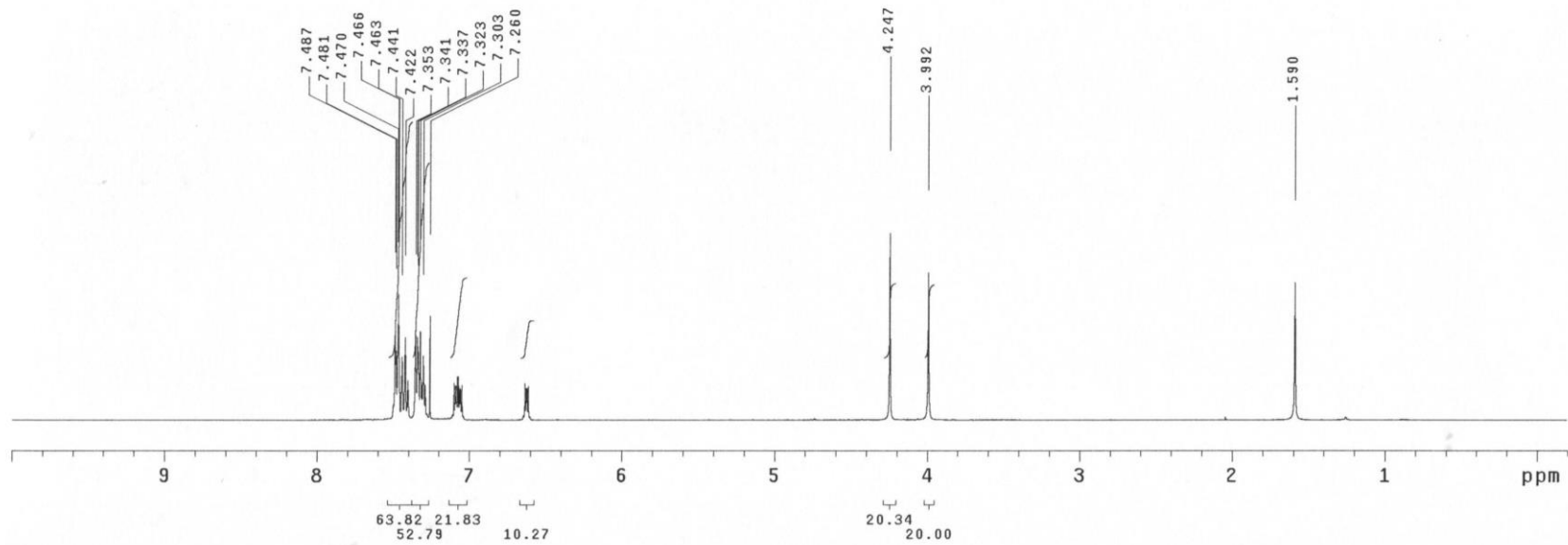
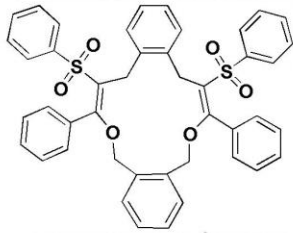
32 repetitions

OBSERVE H1, 400.2743814 MHz

DATA PROCESSING

FT size 65536

Total time 2 min, 0 sec





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

NC0624-14

Pulse Sequence: s2pu1

Solvent: CDC13

Ambient temperature

UNITYplus-400 "unity400"

Relax. delay 0.500 sec

Pulse 65.8 degrees

Acq. time 0.800 sec

Width 25000.0 Hz

3200 repetitions

OBSERVE C13, 100.6490738 MHz

DECOUPLE H1, 400.2763980 MHz

Power 43 dB

on during acquisition

off during delay

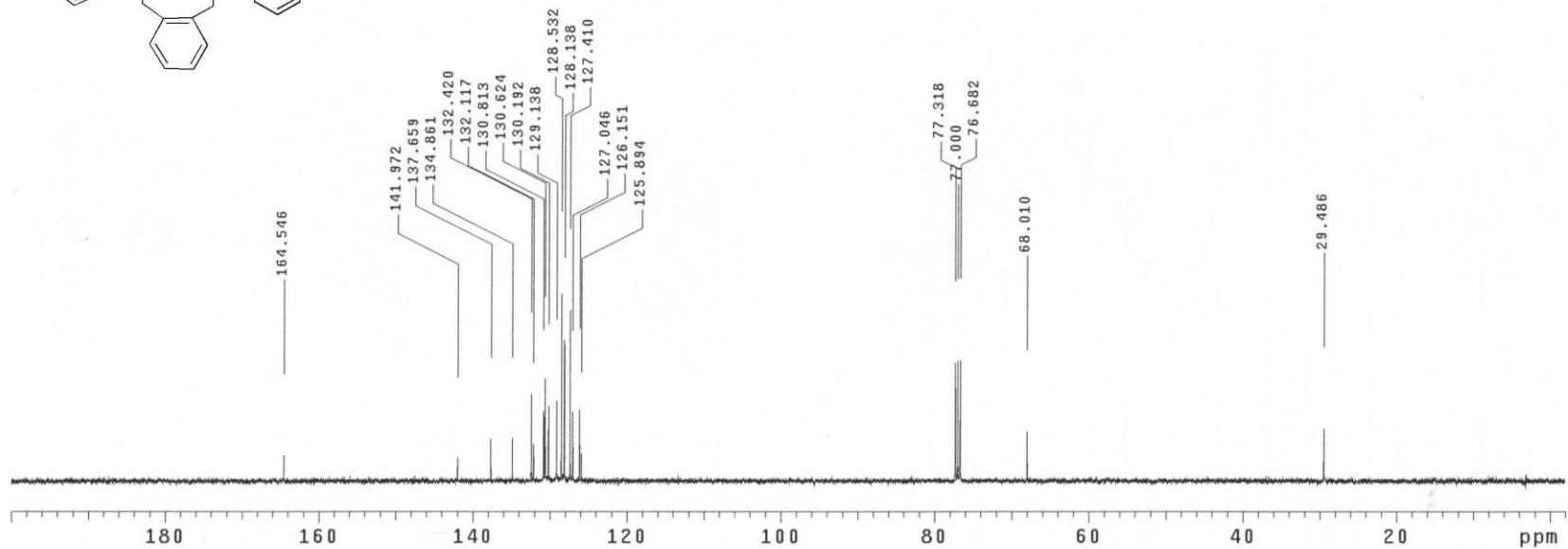
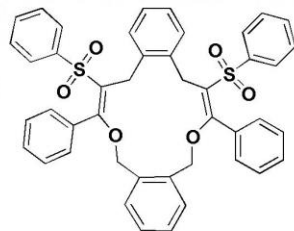
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 11 hr, 39 min, 7 sec

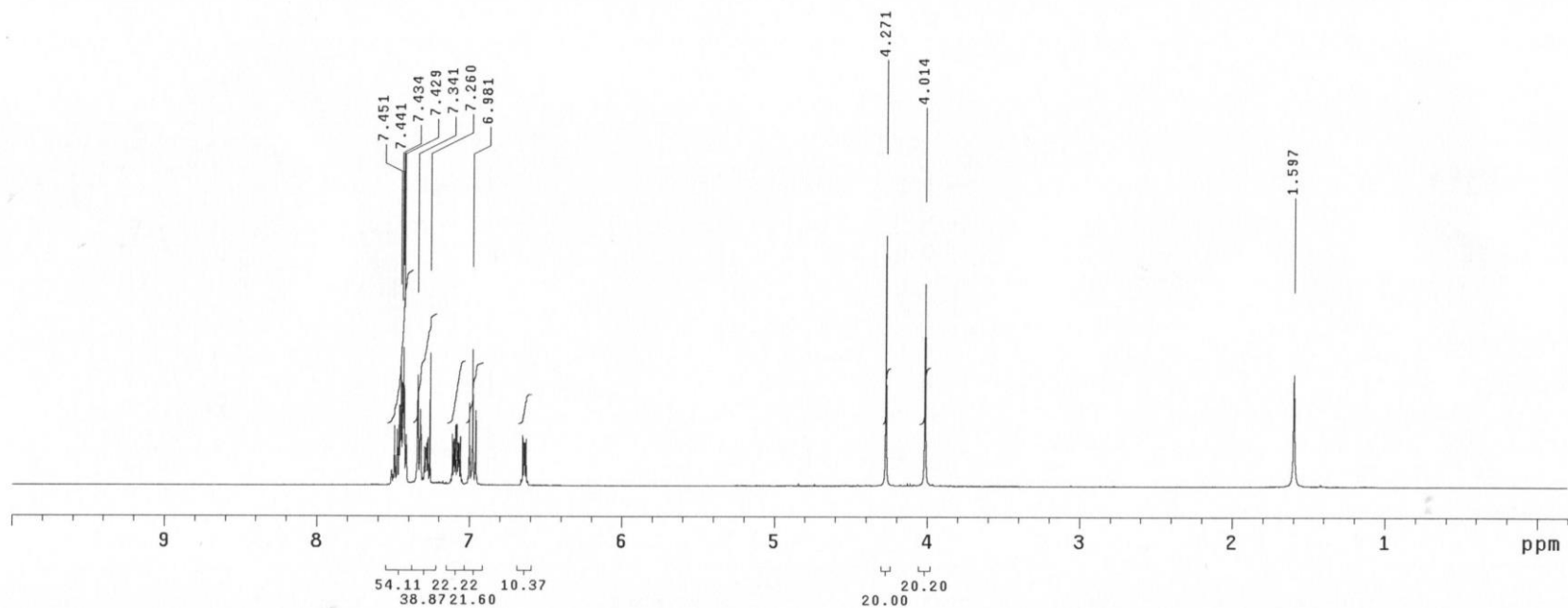
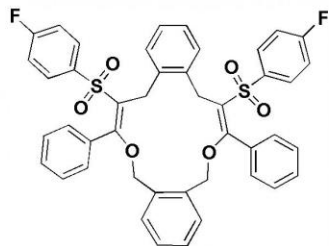


# Compound 8c (<sup>1</sup>H-NMR spectral data)

NC0629-14

Pulse Sequence: s2pu1  
Solvent: CDCl3  
Ambient temperature  
UNITYplus-400 "unity400"

Pulse 38.8 degrees  
Acq. time 3.744 sec  
Width 6000.6 Hz  
64 repetitions  
OBSERVE H1, 400.2743814 MHz  
DATA PROCESSING  
FT size 65536  
Total time 4 min, 0 sec



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

NC0629-14

Pulse Sequence: s2pu1

Solvent: CDCl<sub>3</sub>

Ambient temperature

UNITYplus-400 "unity400"

Relax. delay 0.500 sec

Pulse 65.8 degrees

Acq. time 0.800 sec

Width 25000.0 Hz

2624 repetitions

OBSERVE C13, 100.6490738 MHz

DECOUPLE H1, 400.2763980 MHz

Power 43 dB

on during acquisition

off during delay

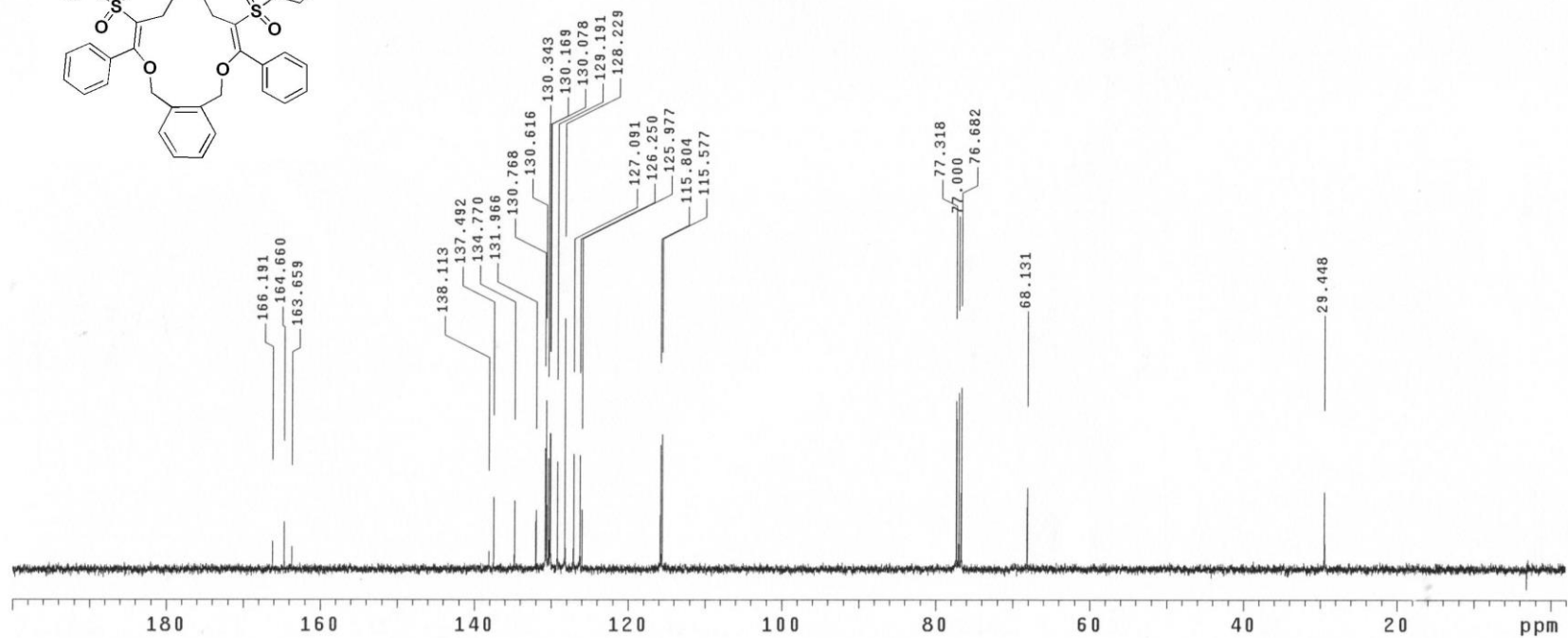
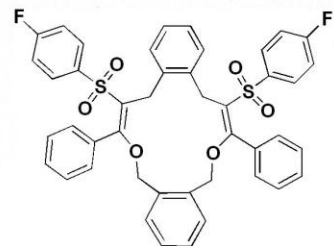
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 11 hr, 39 min, 7 sec



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

NC0721-14

Pulse Sequence: s2pu1

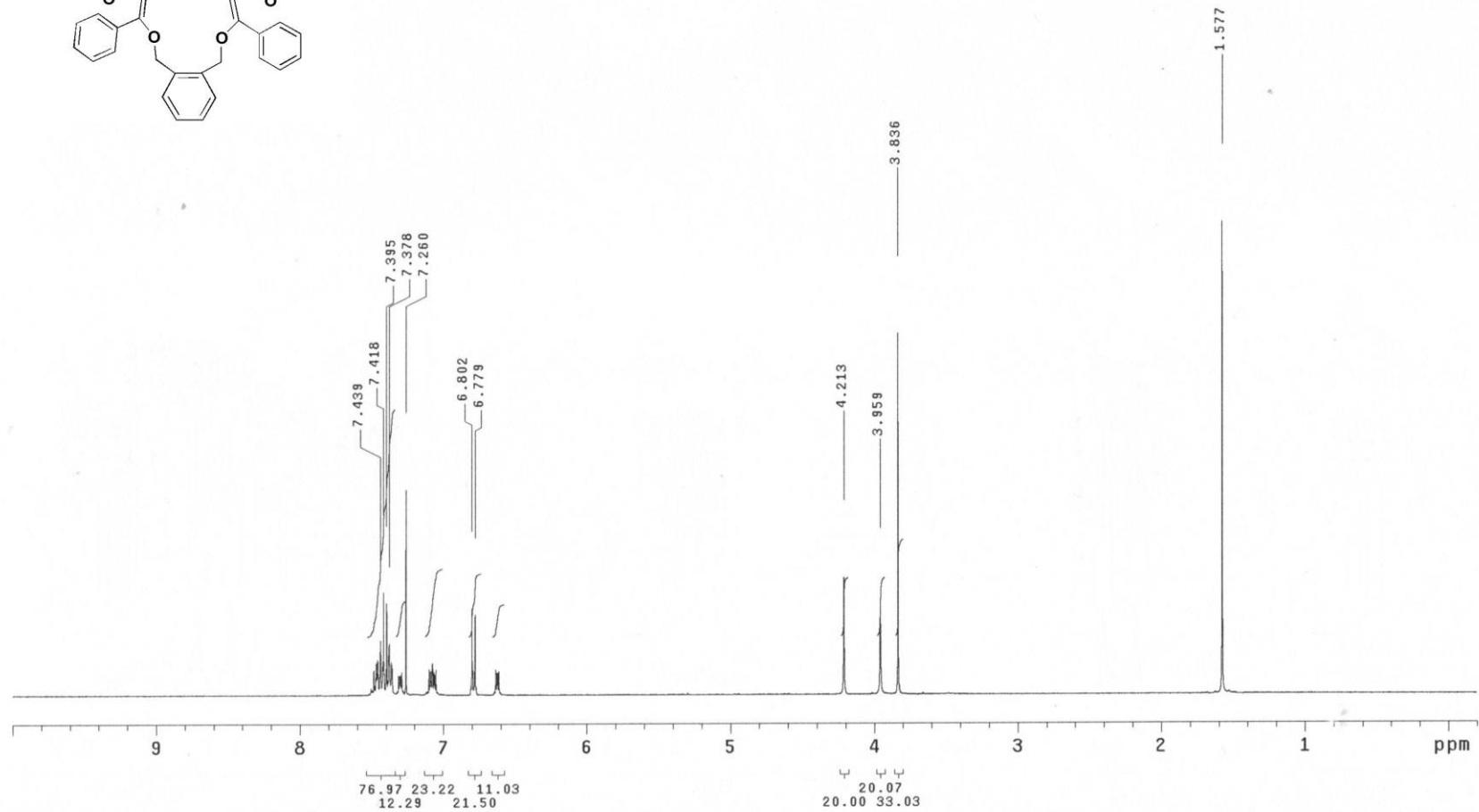
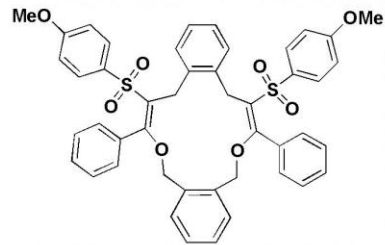
UNITYplus-400 "unity400"

Date: Jul 22 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 32 repetitions



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

NC0721-14

Pulse Sequence: s2pu1

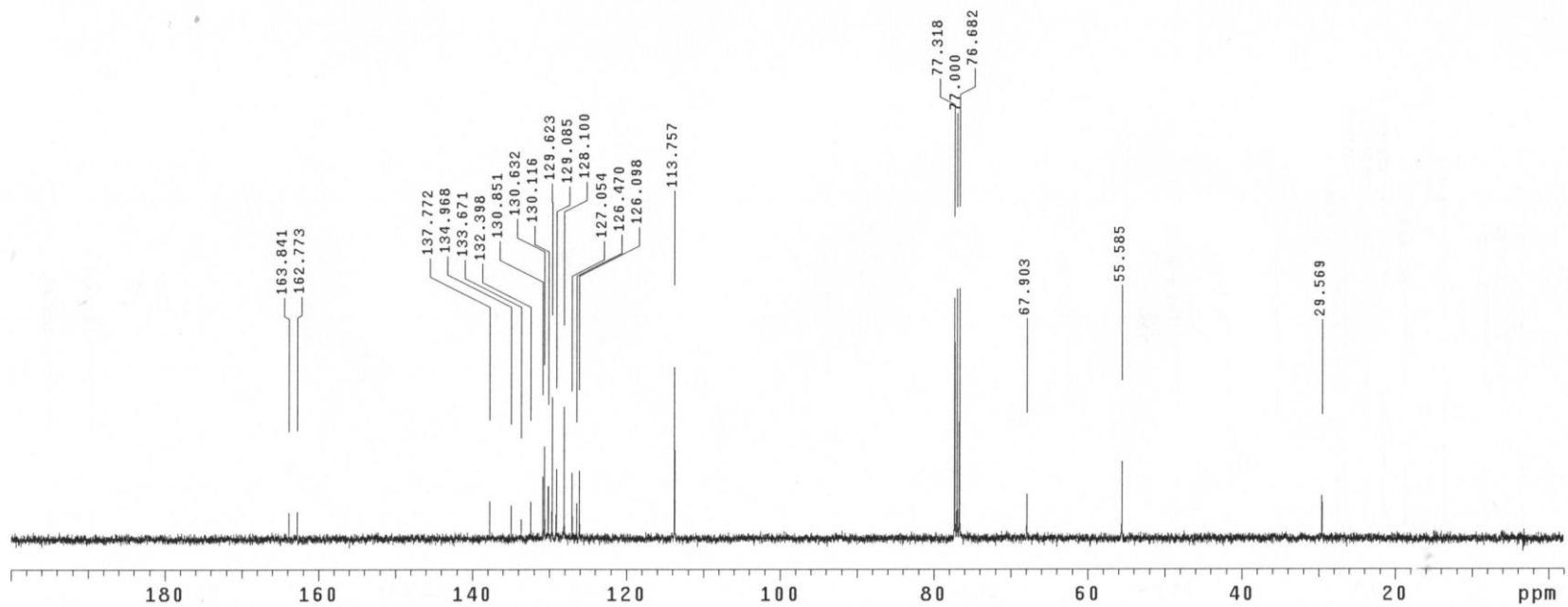
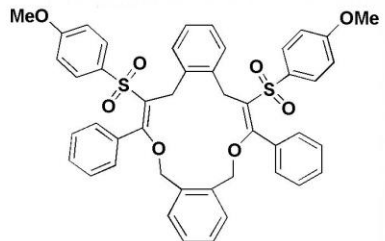
UNITYplus-400 "unity400"

Date: Jul 22 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 4704 repetitions



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

NC0709-14

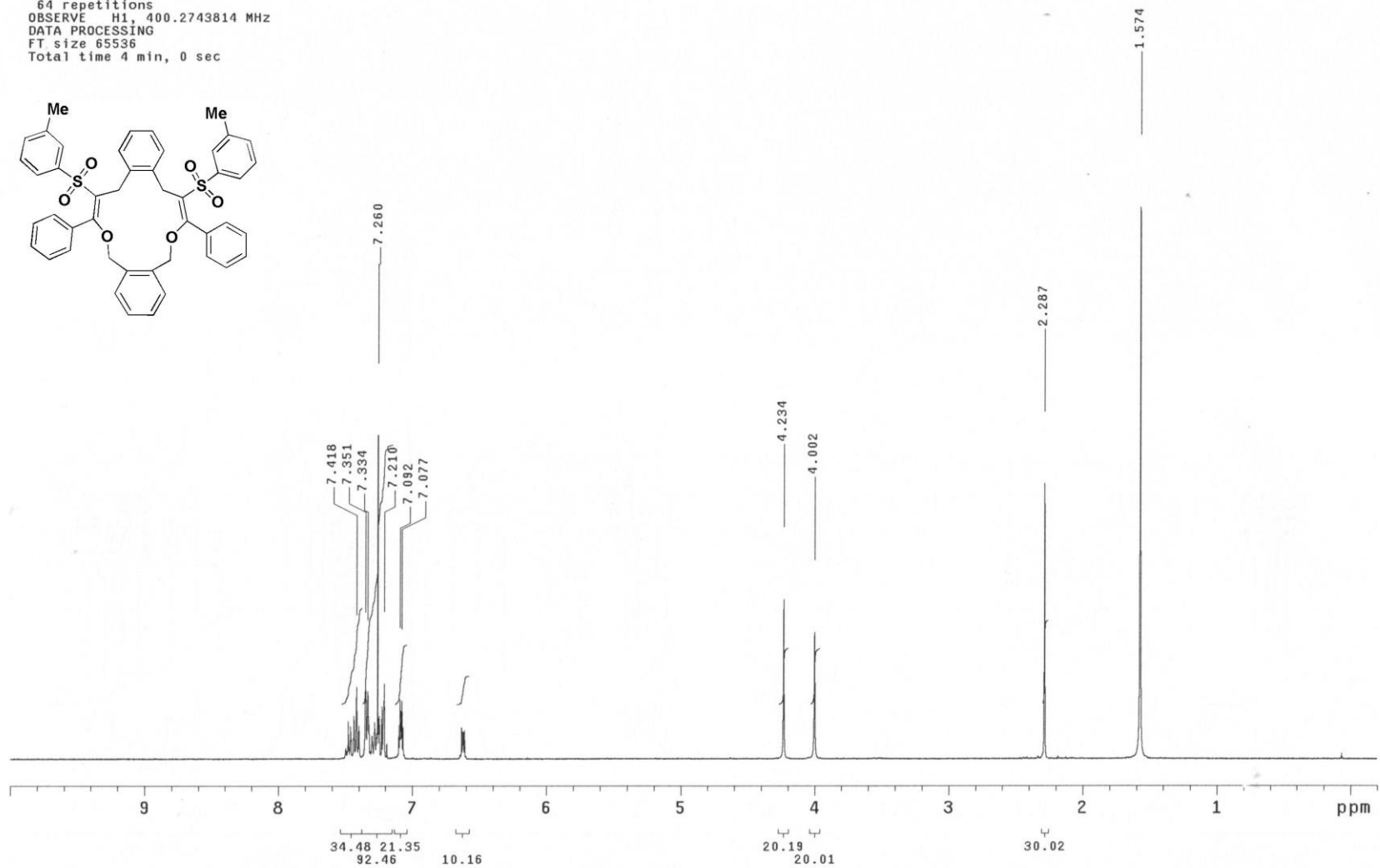
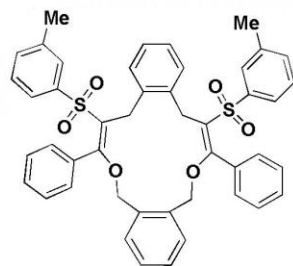
Pulse Sequence: s2pu1

Solvent: CDCl<sub>3</sub>

Ambient temperature

UNITYplus-400 "unity400"

Pulse 38.8 degrees  
Acq. time 3.744 sec  
Width 6000.6 Hz  
64 repetitions  
OBSERVE H1, 400.2743814 MHz  
DATA PROCESSING  
FT size 65536  
Total time 4 min, 0 sec



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

NC0709-14

Pulse Sequence: s2pul

Solvent: CDC13

Ambient temperature

UNITYplus-400 "unity400"

Relax. delay 0.500 sec

Pulse 65.8 degrees

Acq. time 0.800 sec

Width 25000.0 Hz

11376 repetitions

OBSERVE C13, 100.6490731 MHz

DECOUPLE H1, 400.2763980 MHz

Power 43 dB

on during acquisition

off during delay

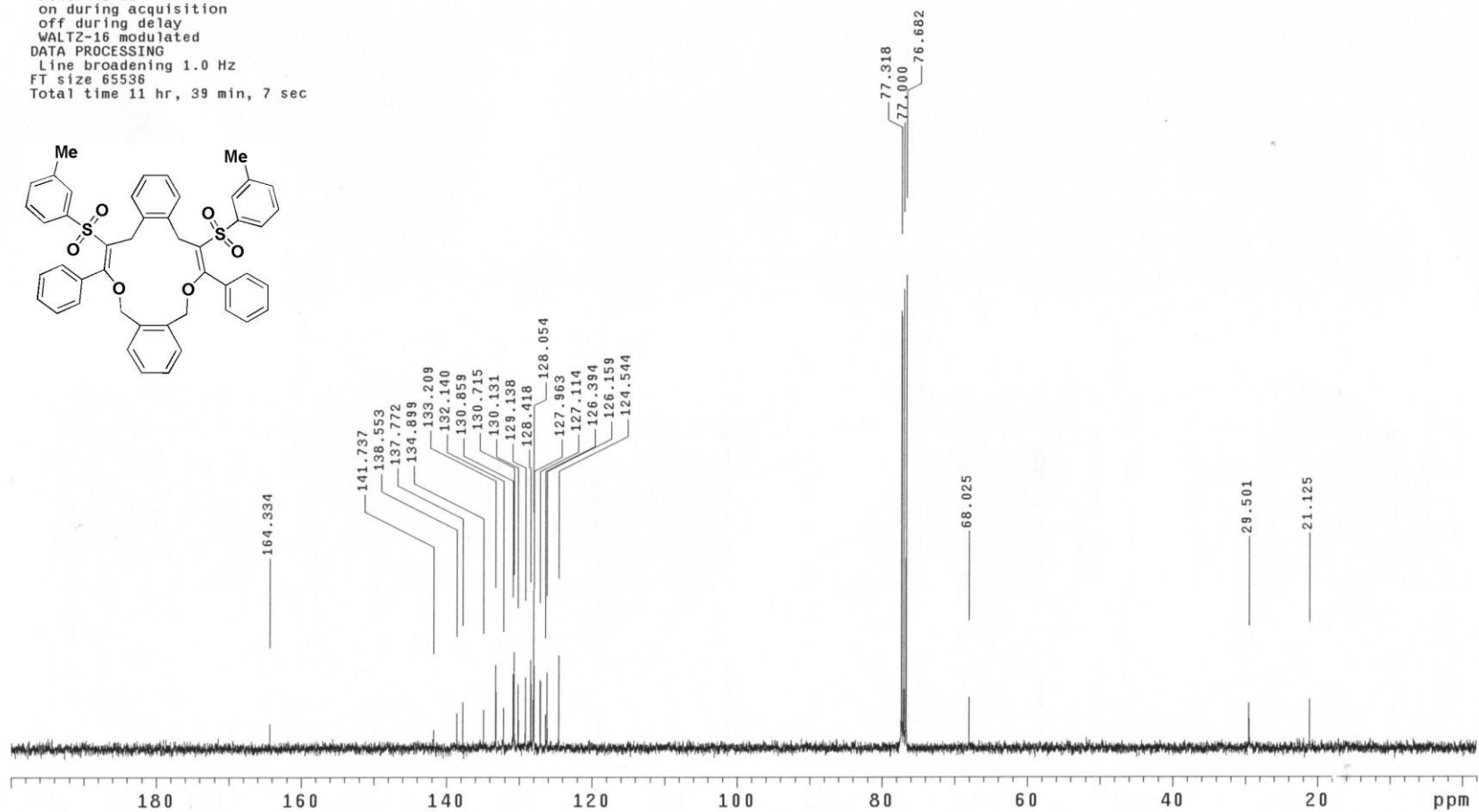
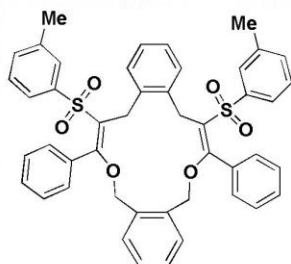
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 11 hr, 39 min, 7 sec



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

NC0702-14

Pulse Sequence: s2pu1

Solvent: CDCl<sub>3</sub>

Ambient temperature

UNITYplus-400 "unity400"

Pulse 38.8 degrees

Acq. time 3.744 sec

Width 6000.6 Hz

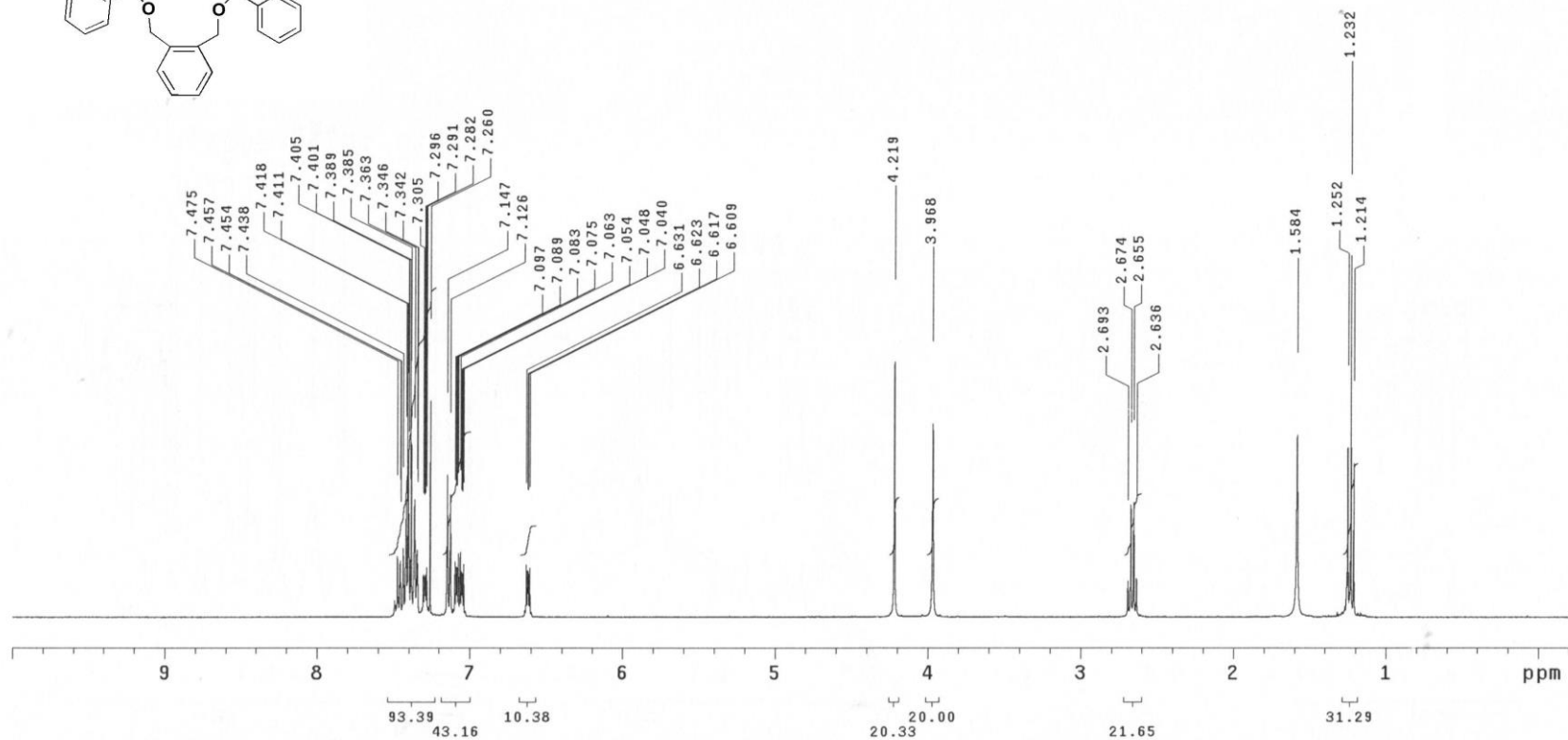
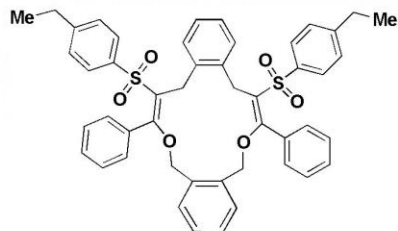
32 repetitions

OBSERVE H1, 400.2743814 MHz

DATA PROCESSING

FT size 65536

Total time 2 min, 0 sec





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

NC0702-14

Pulse Sequence: s2pu1

Solvent: CDCl<sub>3</sub>

Ambient temperature

UNITYplus-400 "unity400"

Relax. delay 0.500 sec

Pulse 65.8 degrees

Acq. time 0.800 sec

Width 25000.0 Hz

2544 repetitions

OBSERVE C13, 100.6490738 MHz

DECOUPLE H1, 400.2763980 MHz

Power 43 dB

on during acquisition

off during delay

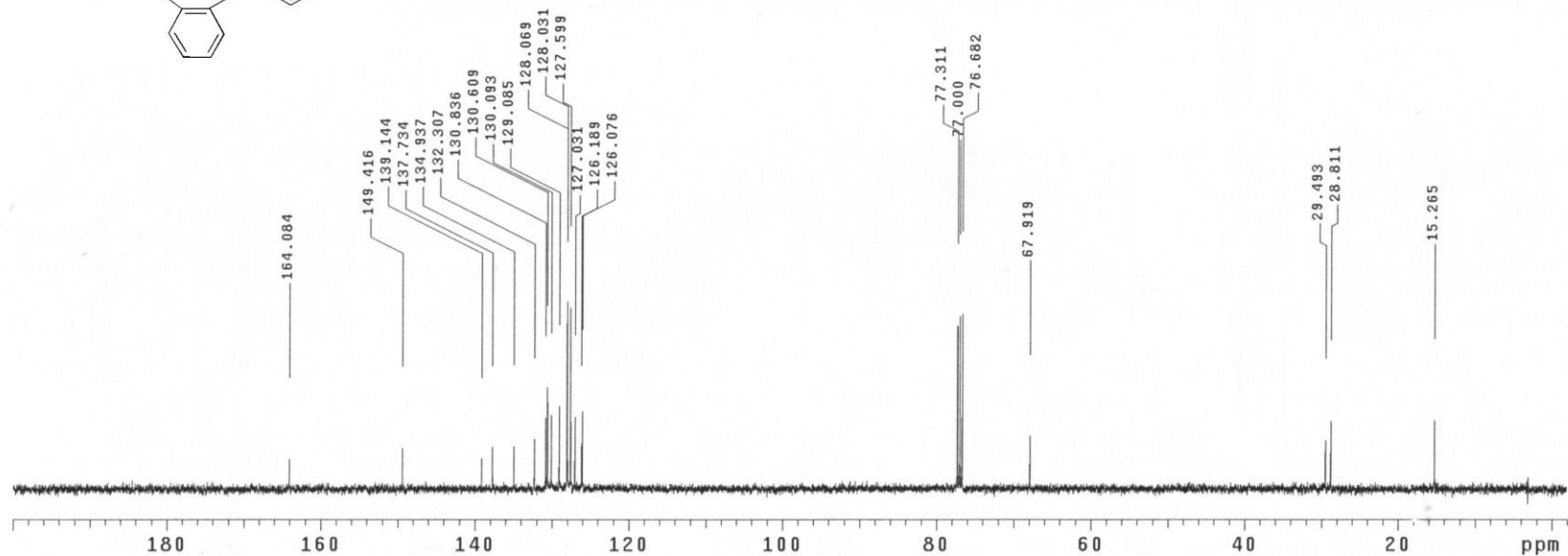
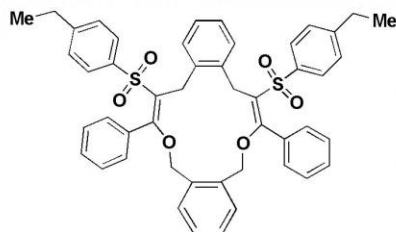
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 23 hr, 18 min, 14 sec



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

NC0722-14

Pulse Sequence: s2pu1

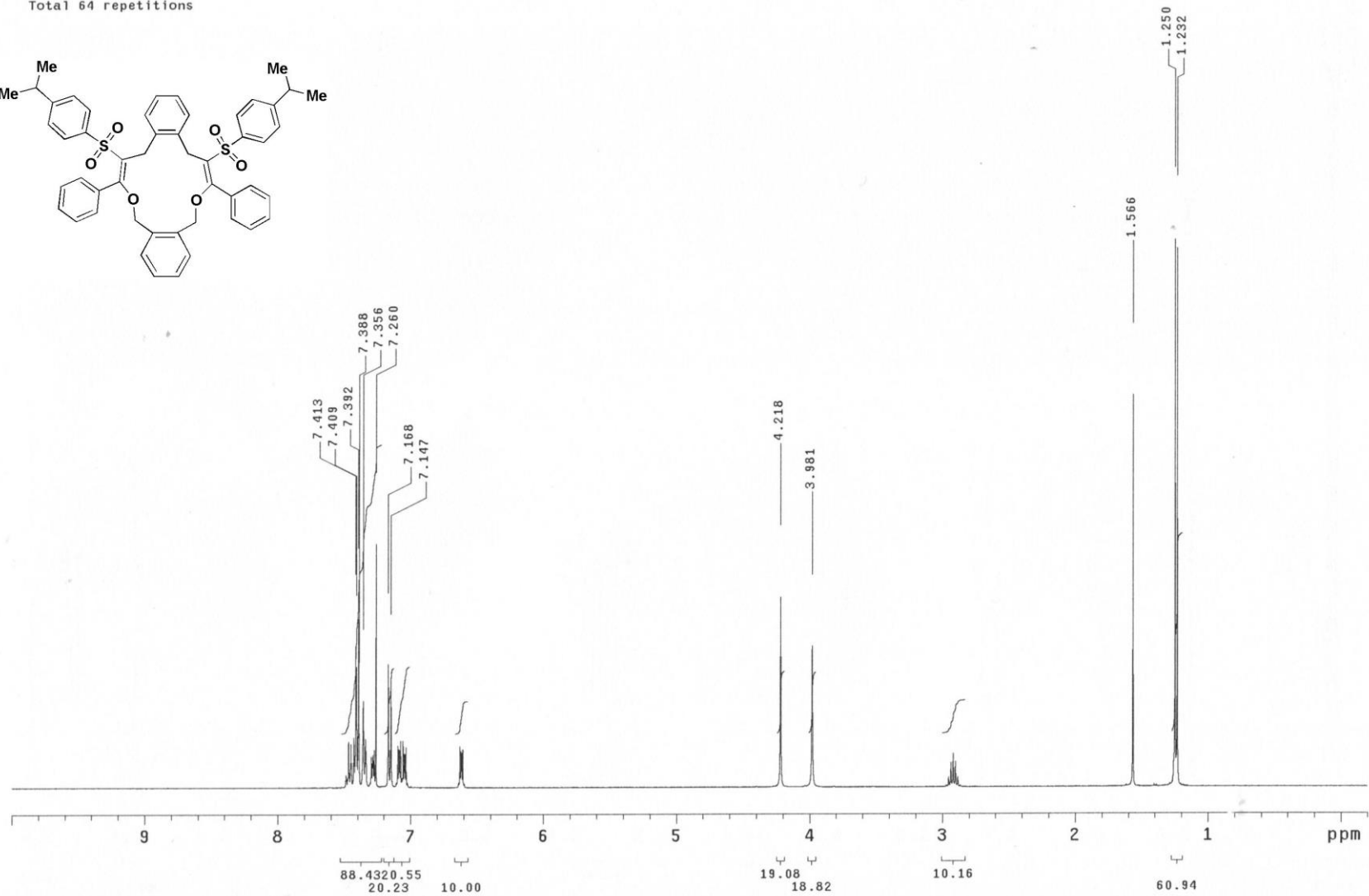
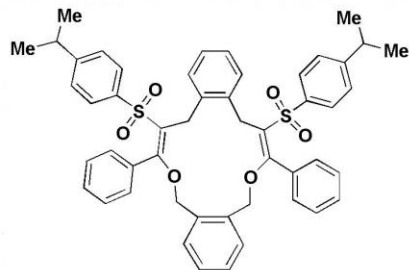
UNITYplus-400 "unity400"

Date: Jul 27 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 64 repetitions



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

NC0722-14

Pulse Sequence: s2pu1

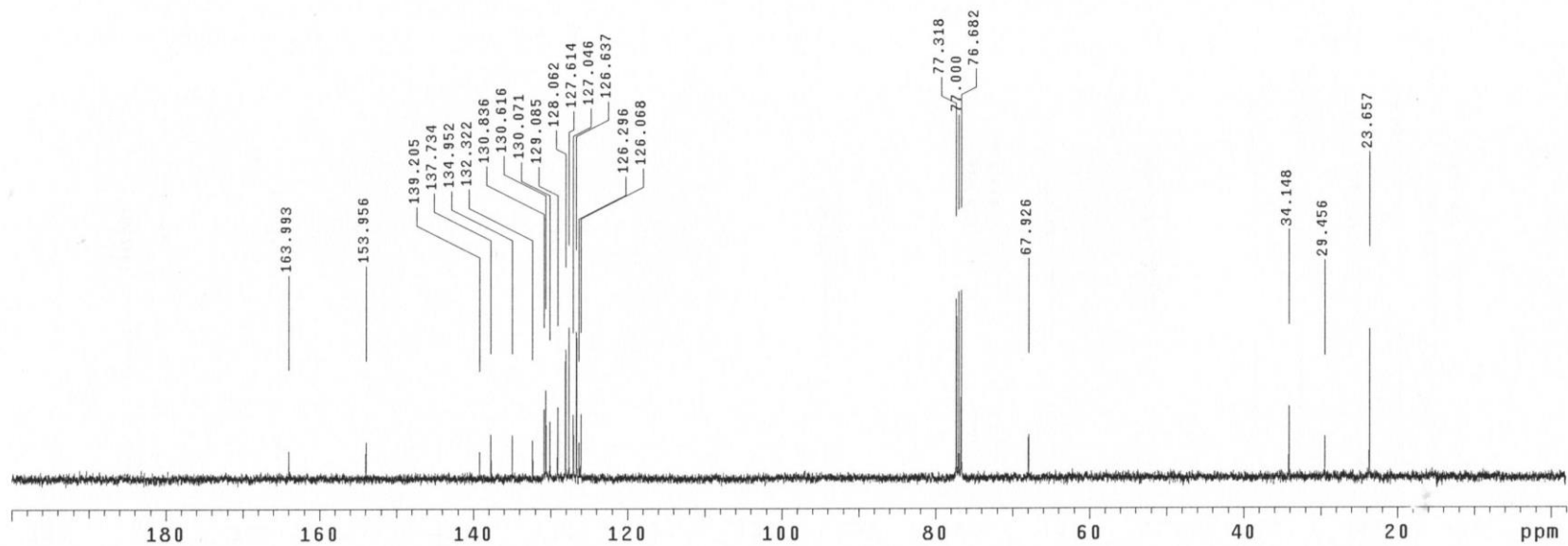
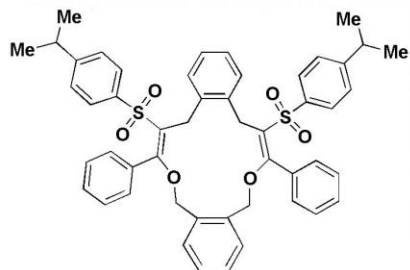
UNITYplus-400 "unity400"

Date: Jul 27 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 2560 repetitions



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

NC0701-14

Pulse Sequence: s2pu1

Solvent: CDCl<sub>3</sub>

Ambient temperature

UNITYplus-400 "unity400"

Pulse 38.8 degrees

Acq. time 3.744 sec

Width 6000.6 Hz

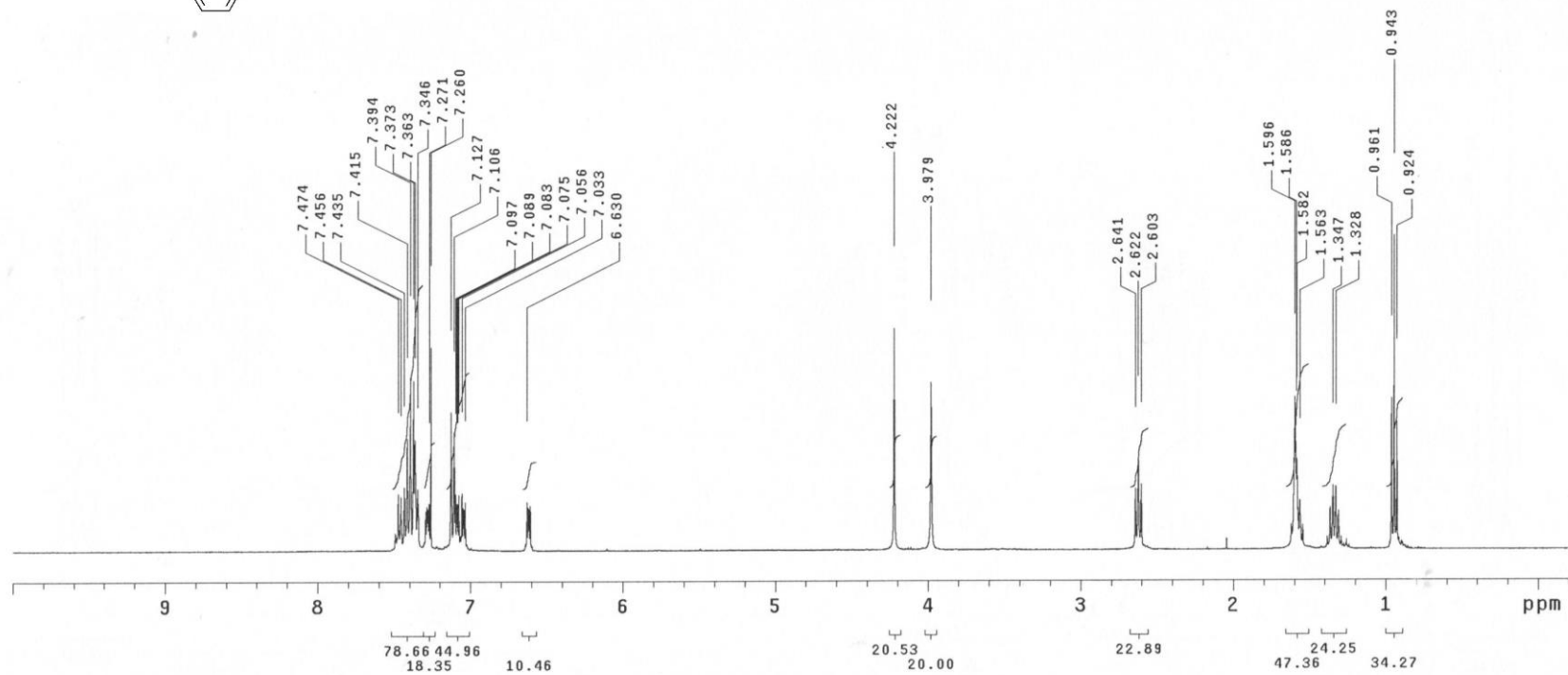
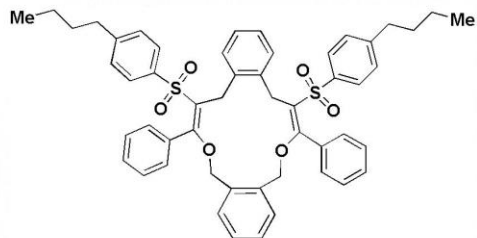
32 repetitions

OBSERVE H1, 400.2743814 MHz

DATA PROCESSING

FT size 65536

Total time 2 min, 0 sec



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

NC0701-14

Pulse Sequence: s2pu1

Solvent: CDCl<sub>3</sub>

Ambient temperature

UNITYplus-400 "unity400"

Relax. delay 0.500 sec

Pulse 65.8 degrees

Acq. time 0.800 sec

Width 25000.0 Hz

1472 repetitions

OBSERVE C13, 100.6490738 MHz

DECOUPLE H1, 400.2763980 MHz

Power 43 dB

on during acquisition

off during delay

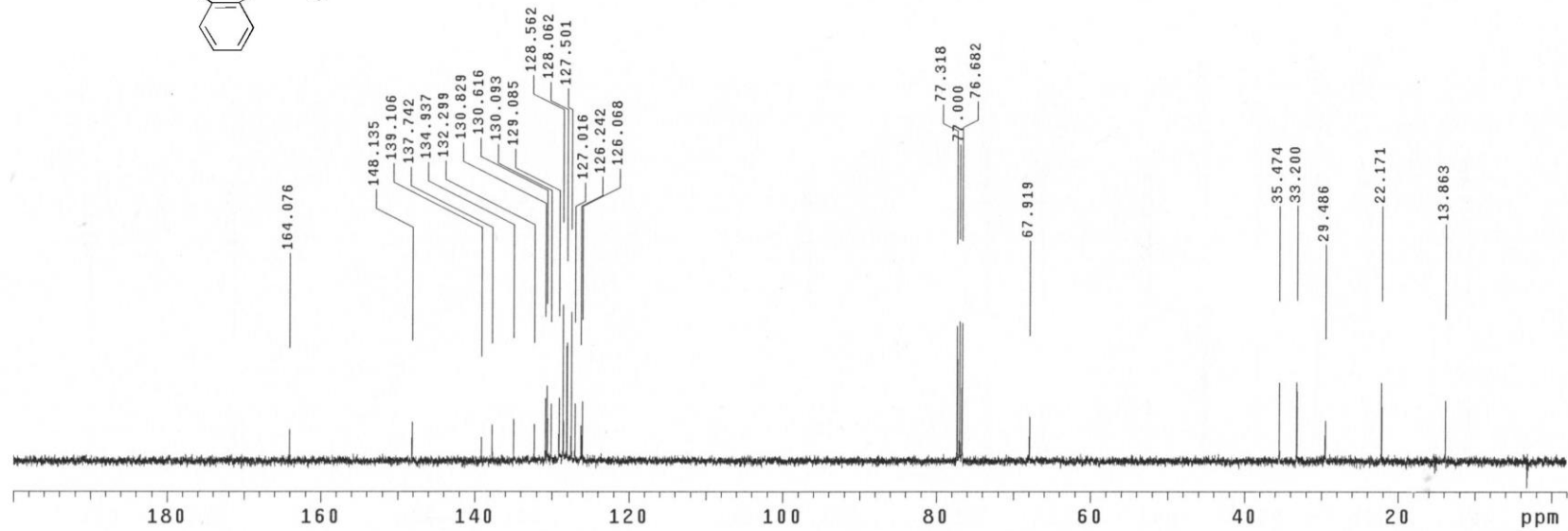
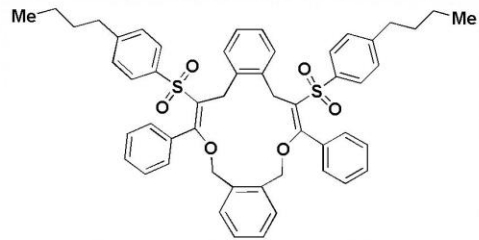
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 11 hr, 39 min, 7 sec



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

NC0707-14

Pulse Sequence: s2pu1

Solvent: CDCl<sub>3</sub>

Ambient temperature

UNITYplus-400 "unity400"

Pulse 38.8 degrees

Acq. time 3.744 sec

Width 6000.6 Hz

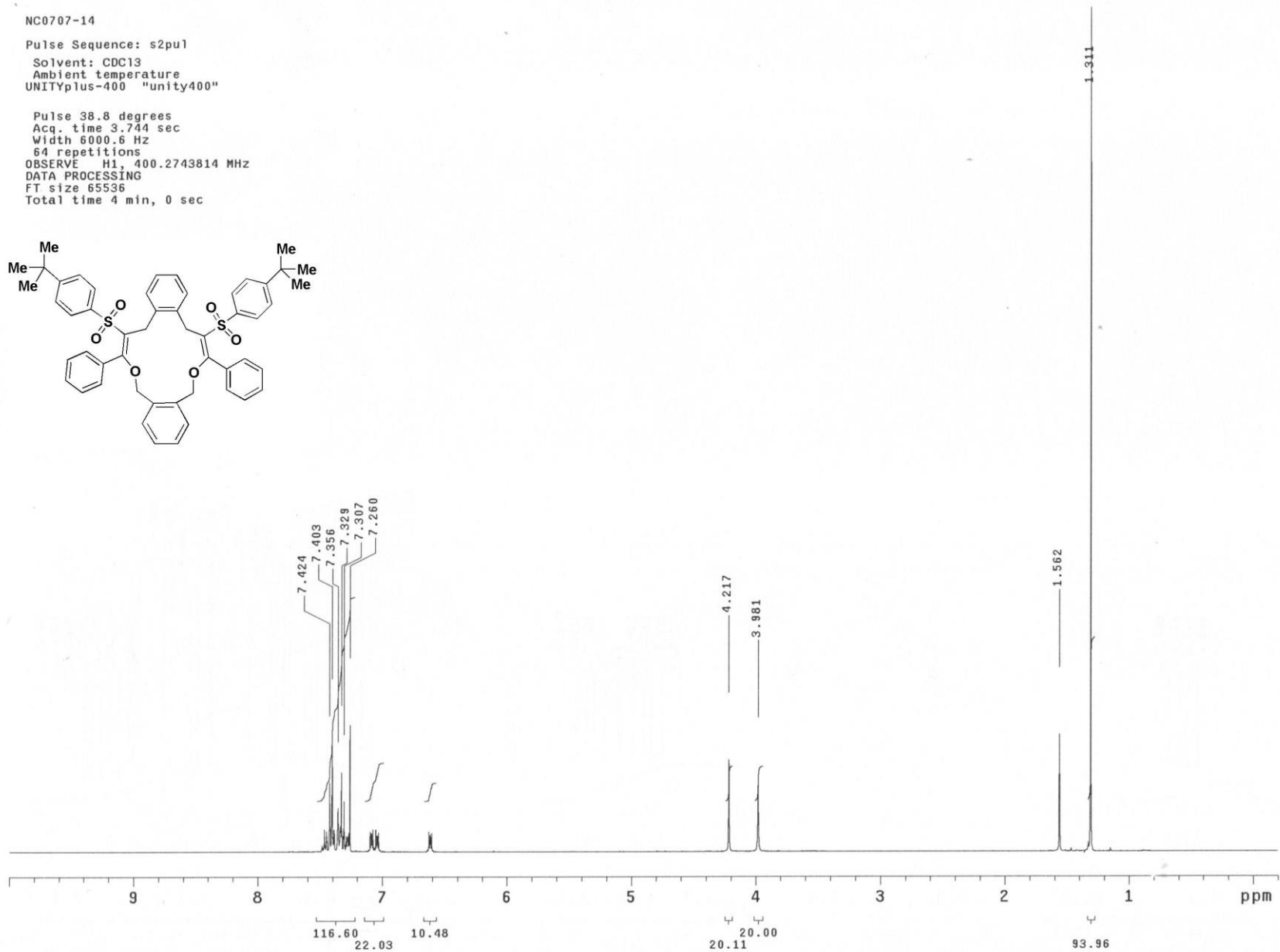
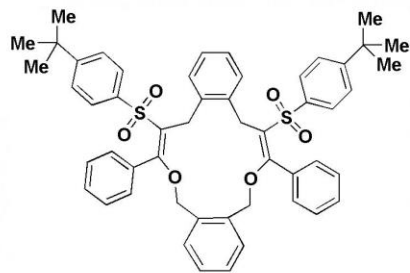
64 repetitions

OBSERVE H1, 400.2743814 MHz

DATA PROCESSING

FT size 65536

Total time 4 min, 0 sec



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

NC0707-14

Pulse Sequence: s2pu1

Solvent: CDCl<sub>3</sub>

Ambient temperature

UNITYplus-400 "unity400"

Relax. delay 0.500 sec

Pulse 65.8 degrees

Acq. time 0.800 sec

Width 25000.0 Hz

5104 repetitions

OBSERVE C13, 100.6490731 MHz

DECOUPLE H1, 400.2763980 MHz

Power 43 dB

on during acquisition

off during delay

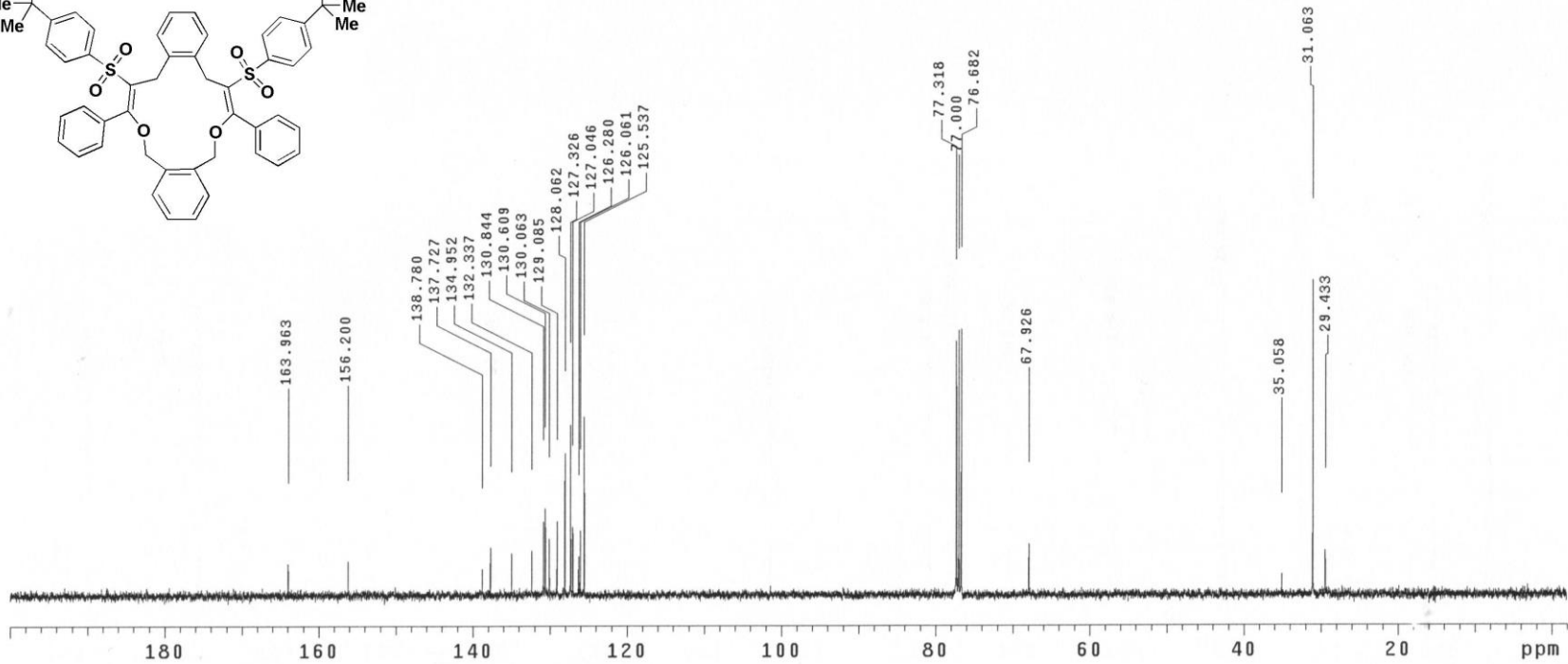
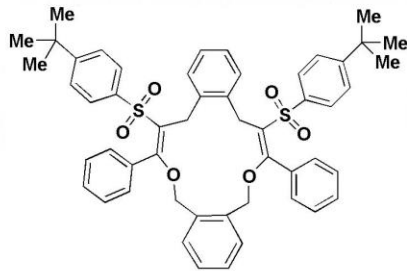
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

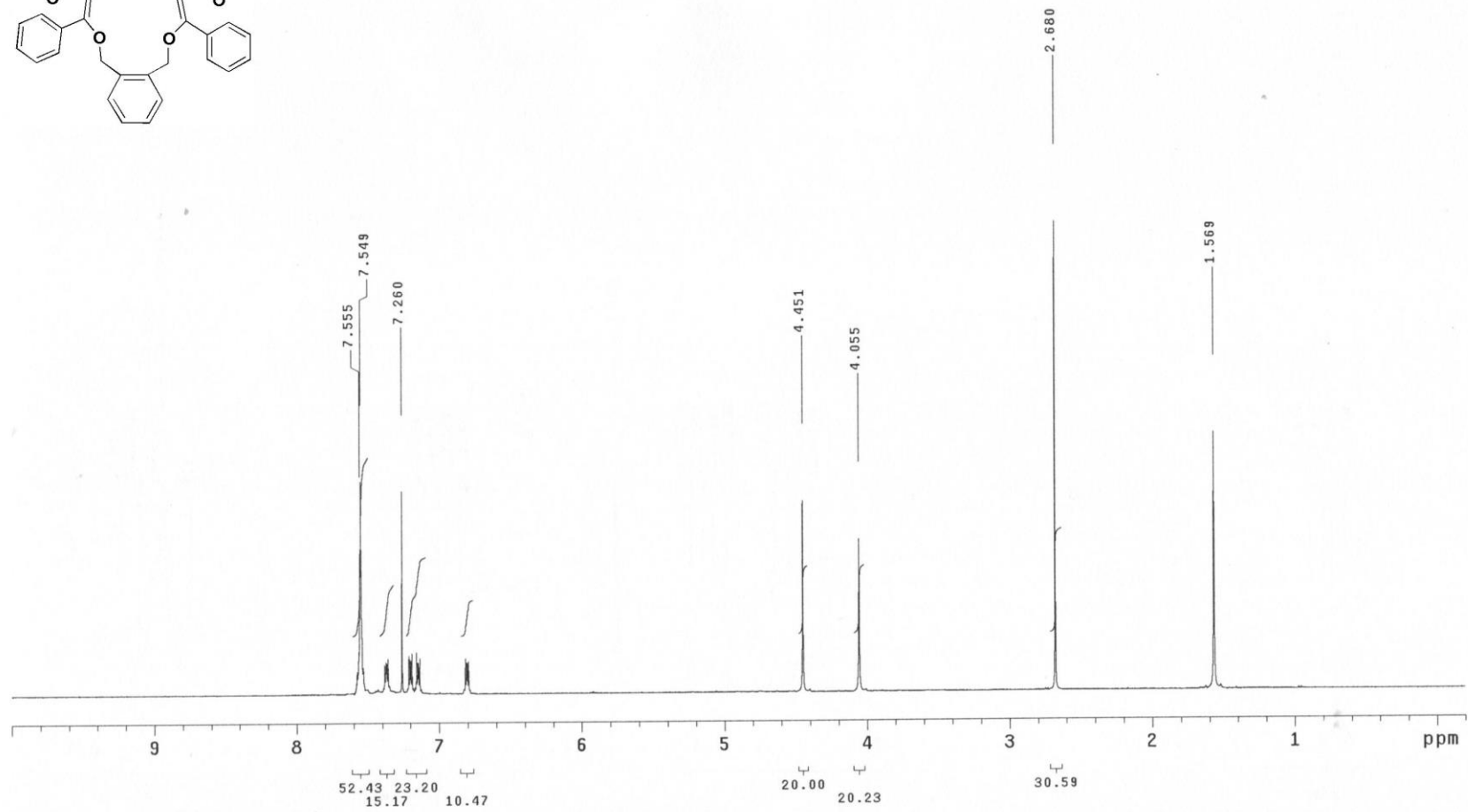
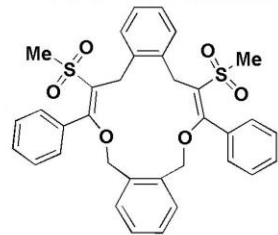
Total time 11 hr, 39 min, 7 sec



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

NC0720-14

Pulse Sequence: s2pu1  
UNITYplus-400 "unity400"  
Date: Aug 5 2020  
Solvent: CDCl<sub>3</sub>  
Ambient temperature  
Total 64 repetitions





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

NC0720-14

Pulse Sequence: s2pu1

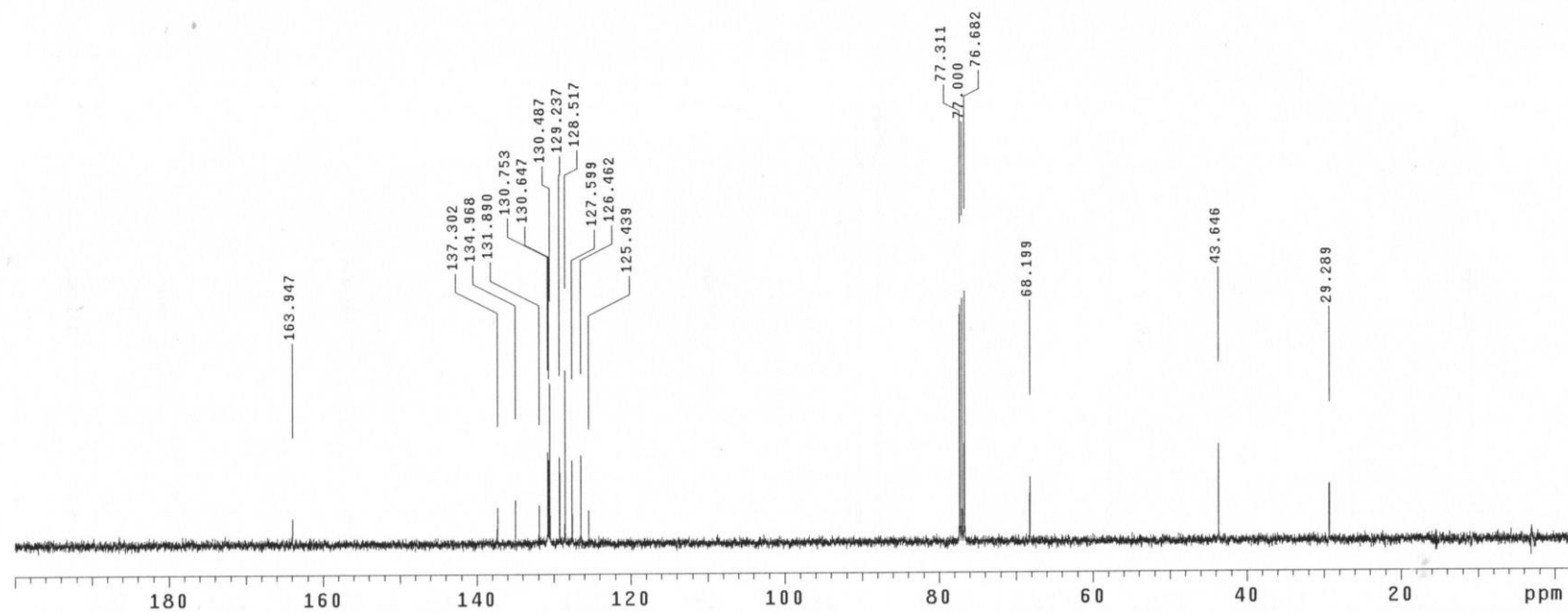
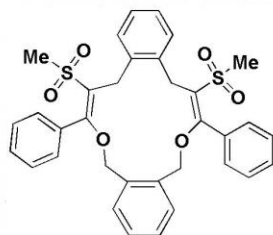
UNITYplus-400 "unity400"

Date: Aug 5 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 4352 repetitions



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

NC0713-14

Pulse Sequence: s2pu1

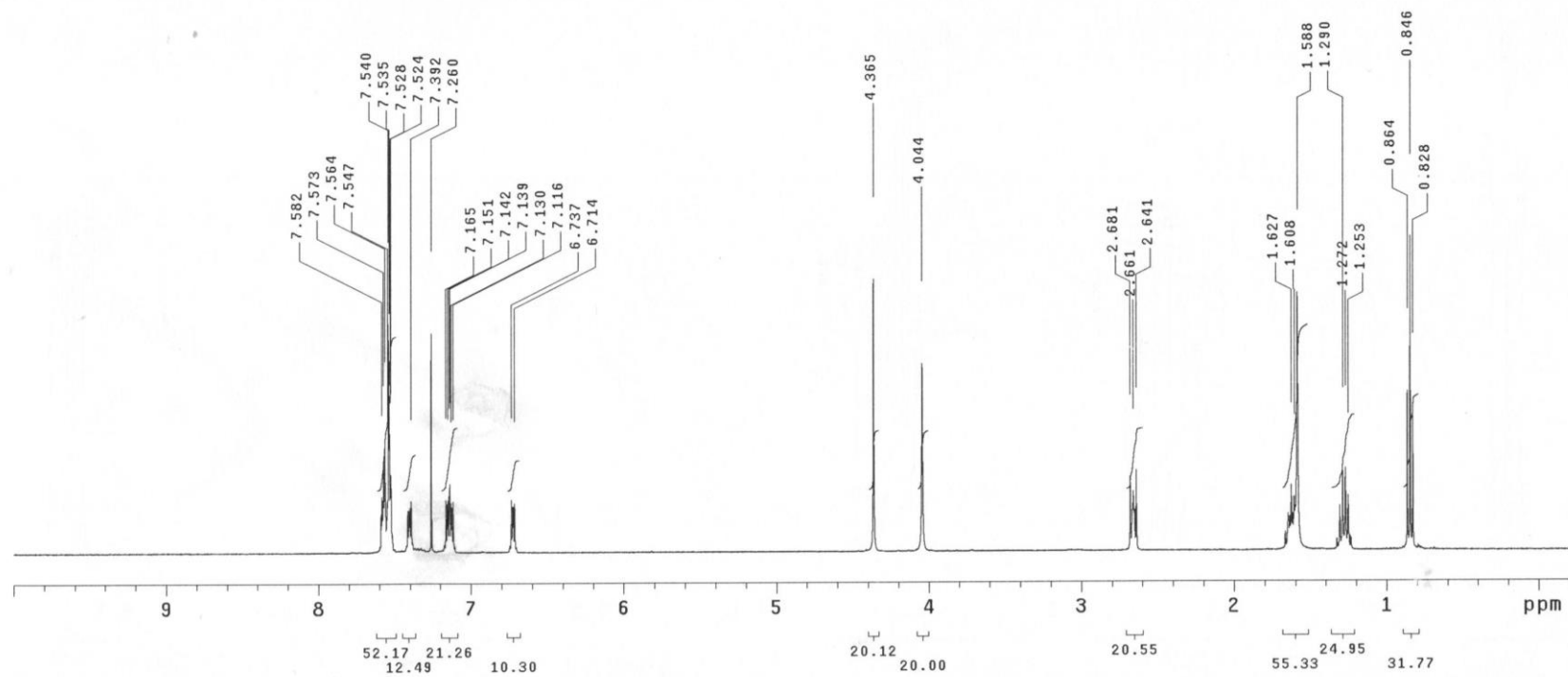
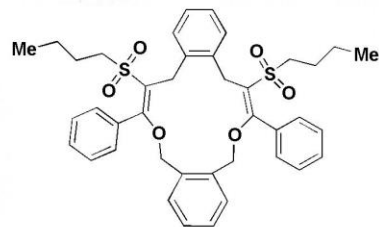
UNITYplus-400 "unity400"

Date: Jul 16 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 32 repetitions



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

NC0713-14

Pulse Sequence: s2pu1

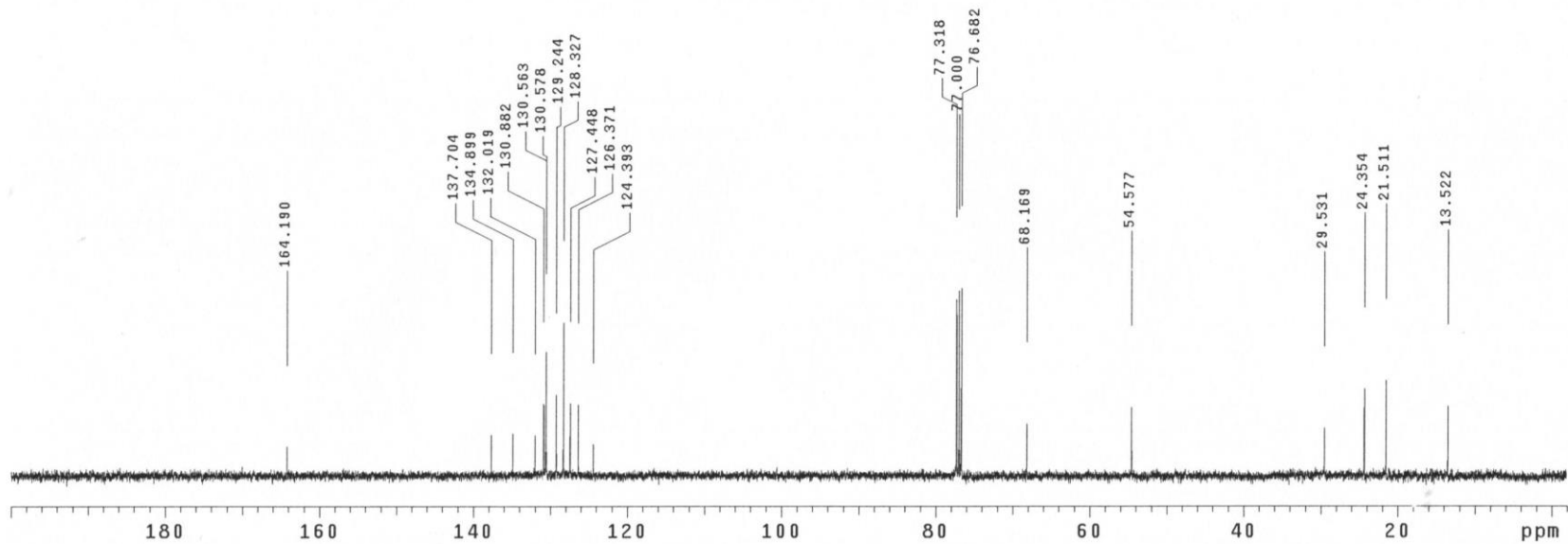
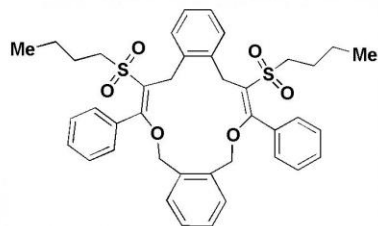
UNITYplus-400 "unity400"

Date: Jul 16 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 2256 repetitions



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

KT0609-14

Pulse Sequence: s2pu1

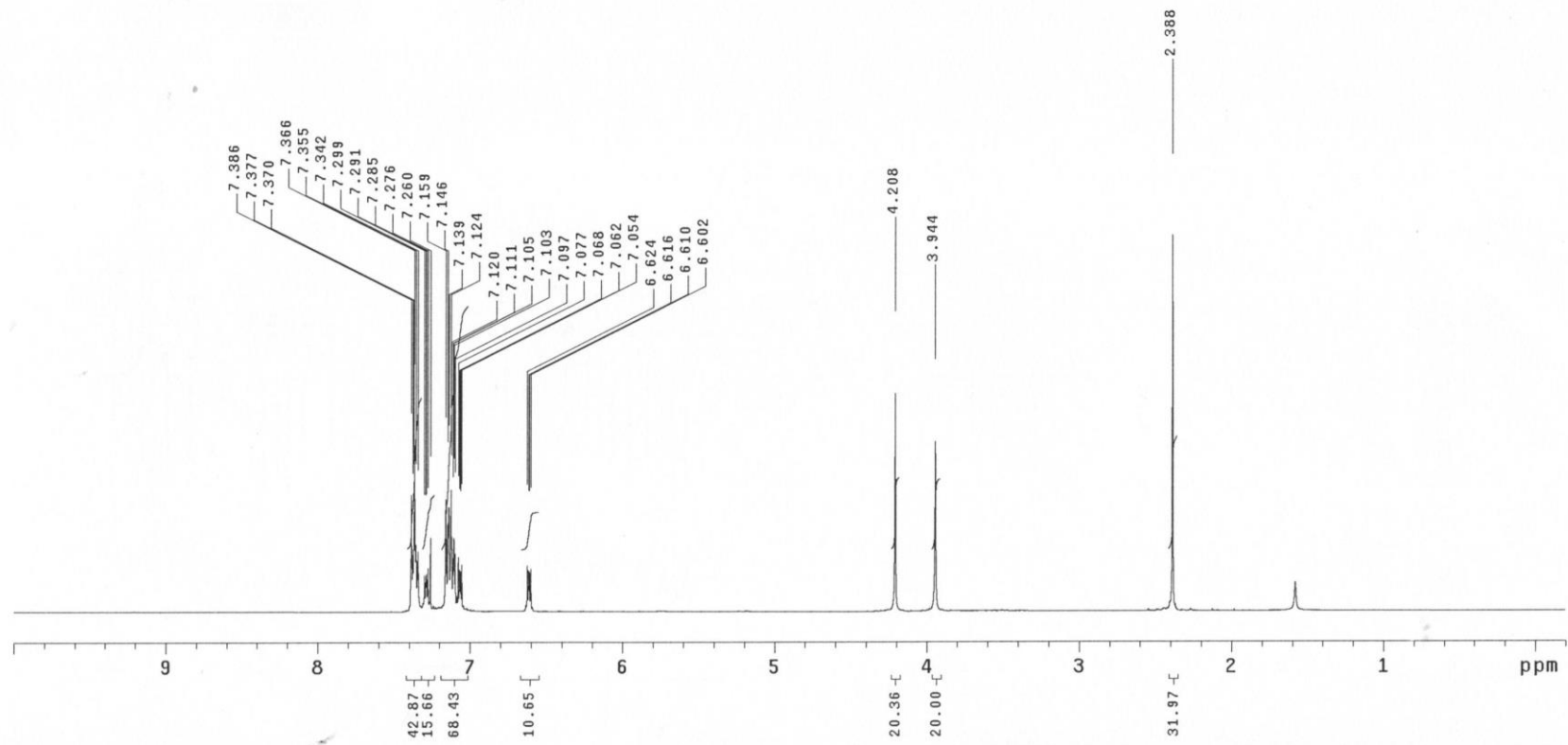
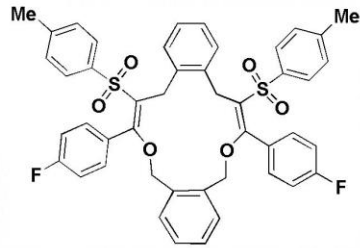
UNITYplus-400 "unity400"

Date: Jun 10 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 32 repetitions



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

KT0609-14

Pulse Sequence: s2pu1

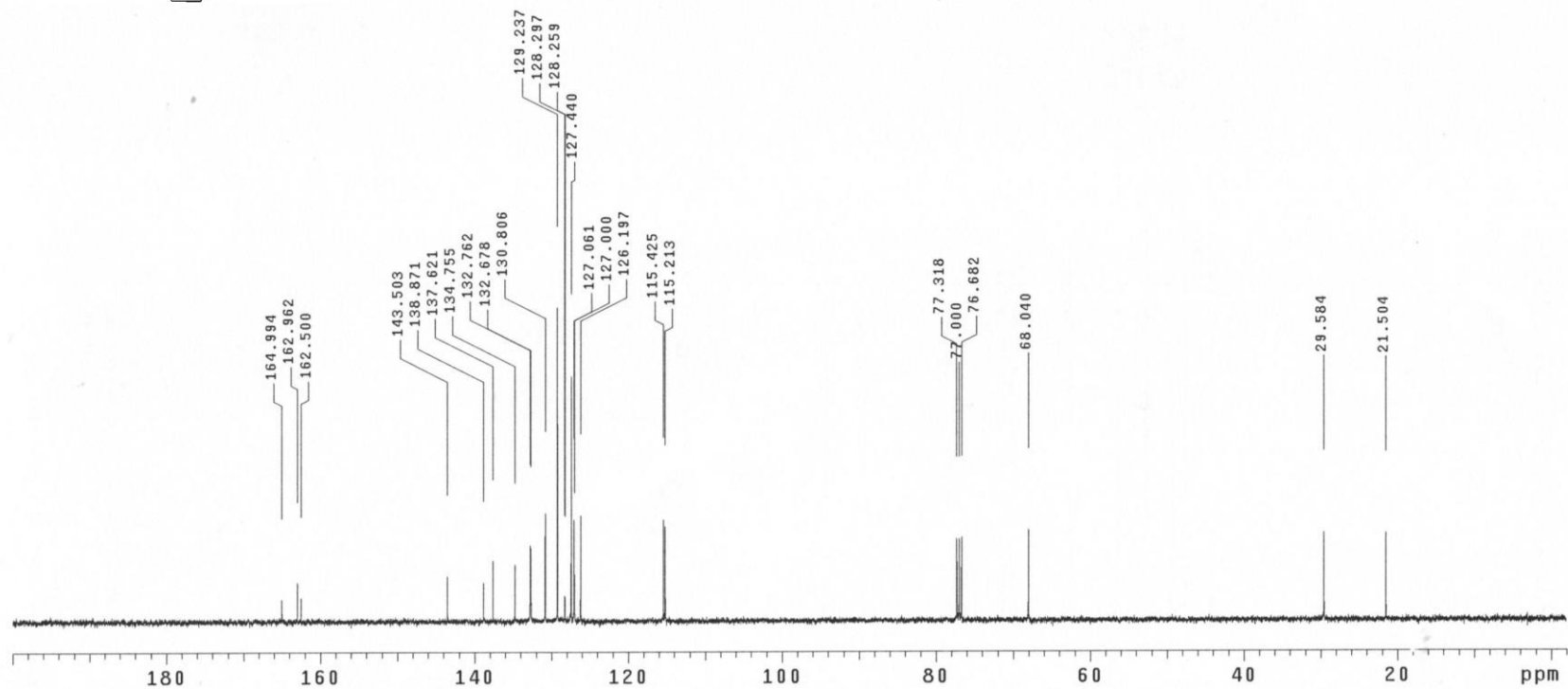
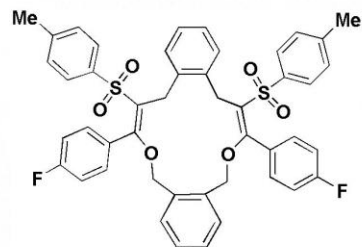
UNITYplus-400 "unity400"

Date: Jun 10 2020

Solvent: CDC13

Ambient temperature

Total 1424 repetitions



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

KT0512-14

Pulse Sequence: s2pu1

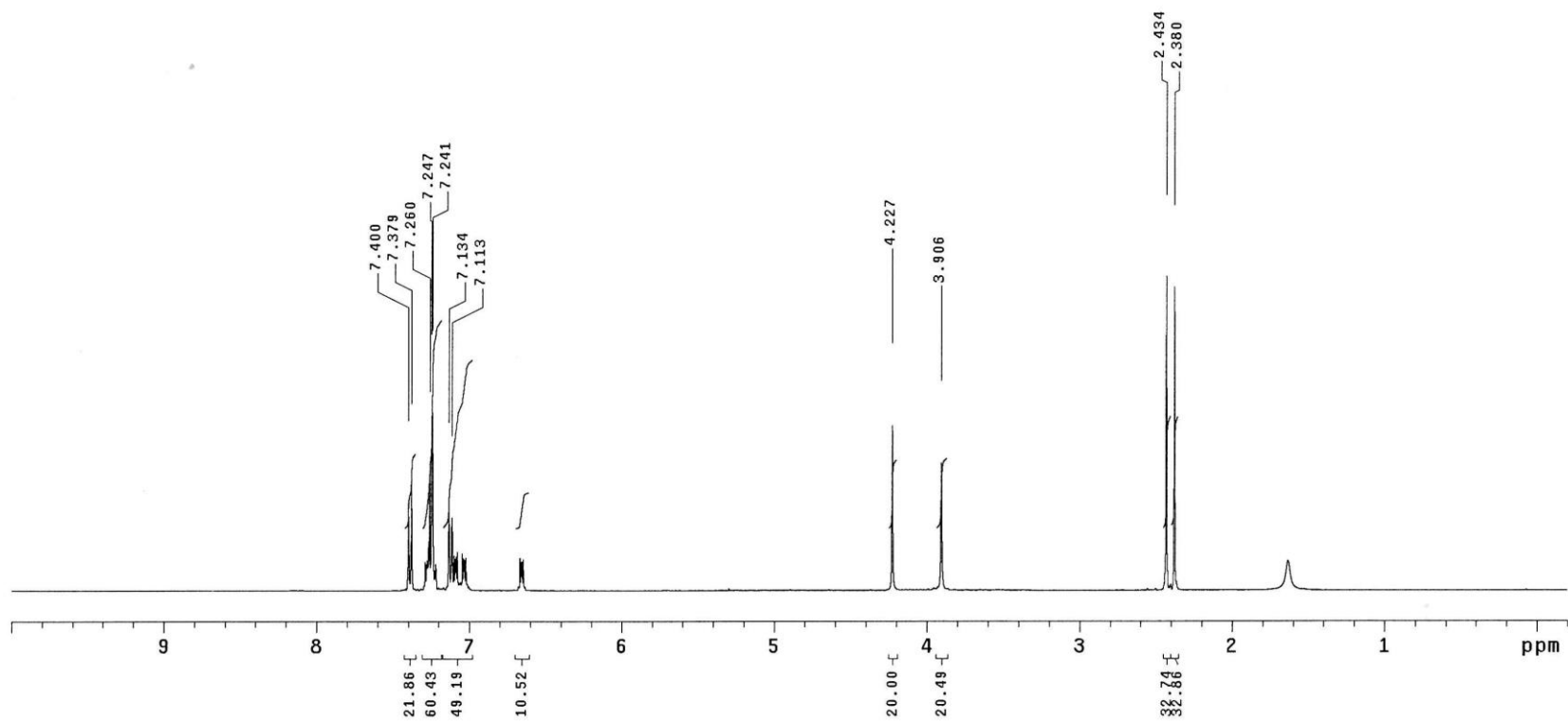
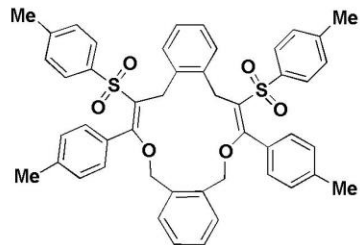
UNITYplus-400 "unity400"

Date: May 28 2020

Solvent: CDC13

Ambient temperature

Total 64 repetitions



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

KT0512-14

Pulse Sequence: s2pu1

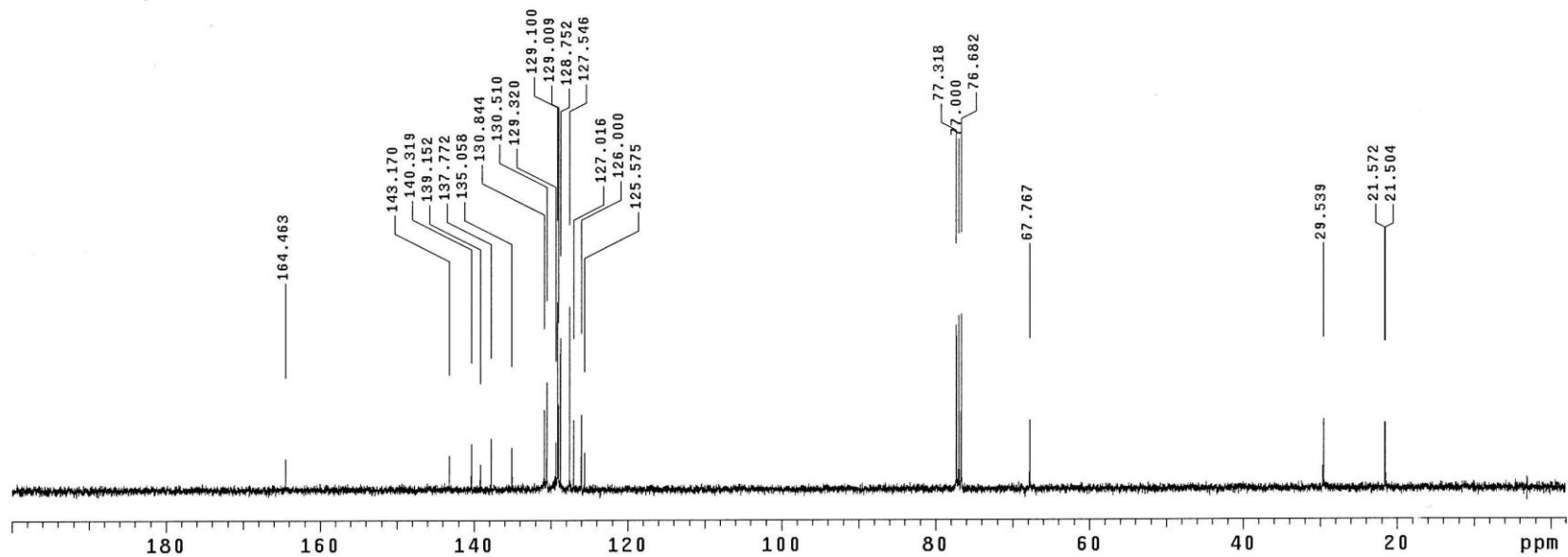
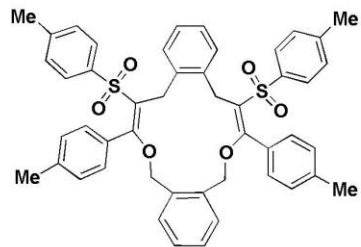
UNITYplus-400 "unity400"

Date: May 28 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 2048 repetitions



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

KTMe56

Pulse Sequence: s2pu1

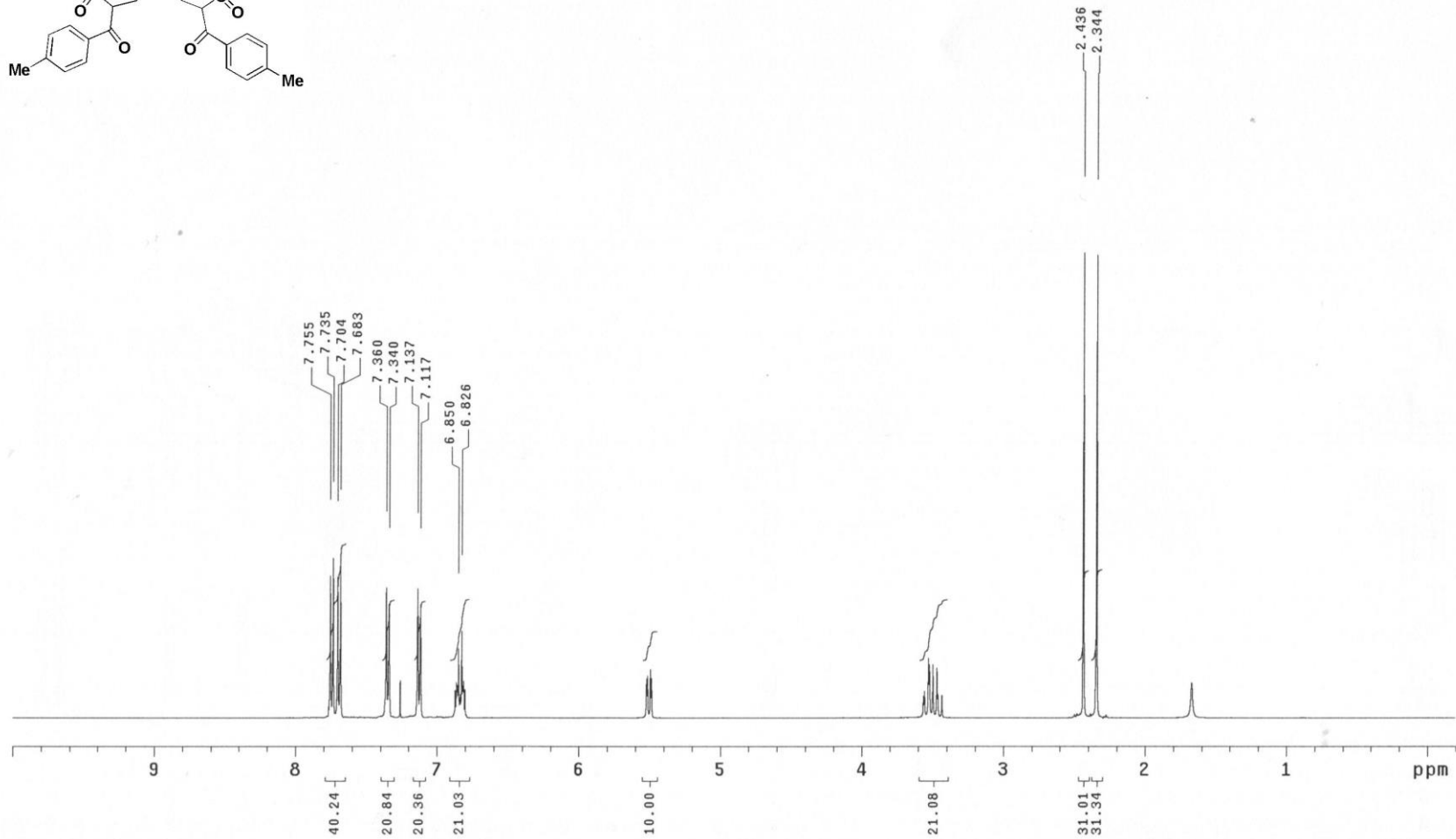
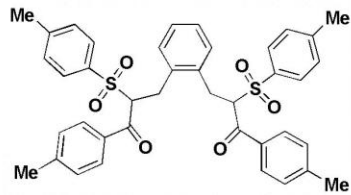
UNITYplus-400 "unity400"

Date: May 25 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 32 repetitions





# Compound 8m-1 (<sup>13</sup>C-NMR spectral data)

KTM56

Pulse Sequence: s2pu1

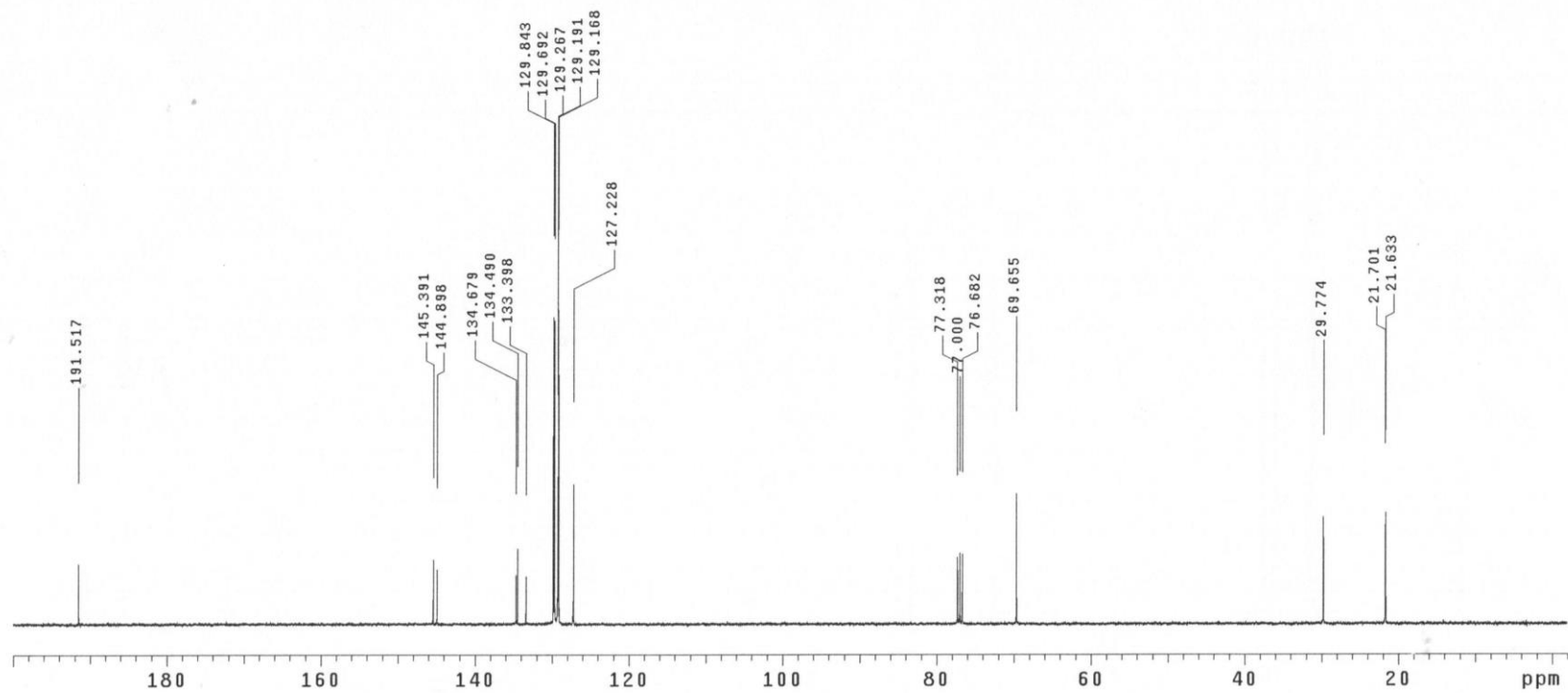
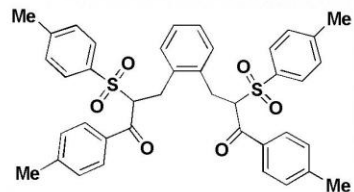
UNITYplus-400 "unity400"

Date: May 25 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 2256 repetitions



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

NC0610-14

Pulse Sequence: s2pu1

Solvent: CDCl<sub>3</sub>

Ambient temperature

UNITYplus-400 "unity400"

Pulse 38.8 degrees

Acq. time 3.744 sec

Width 6000.6 Hz

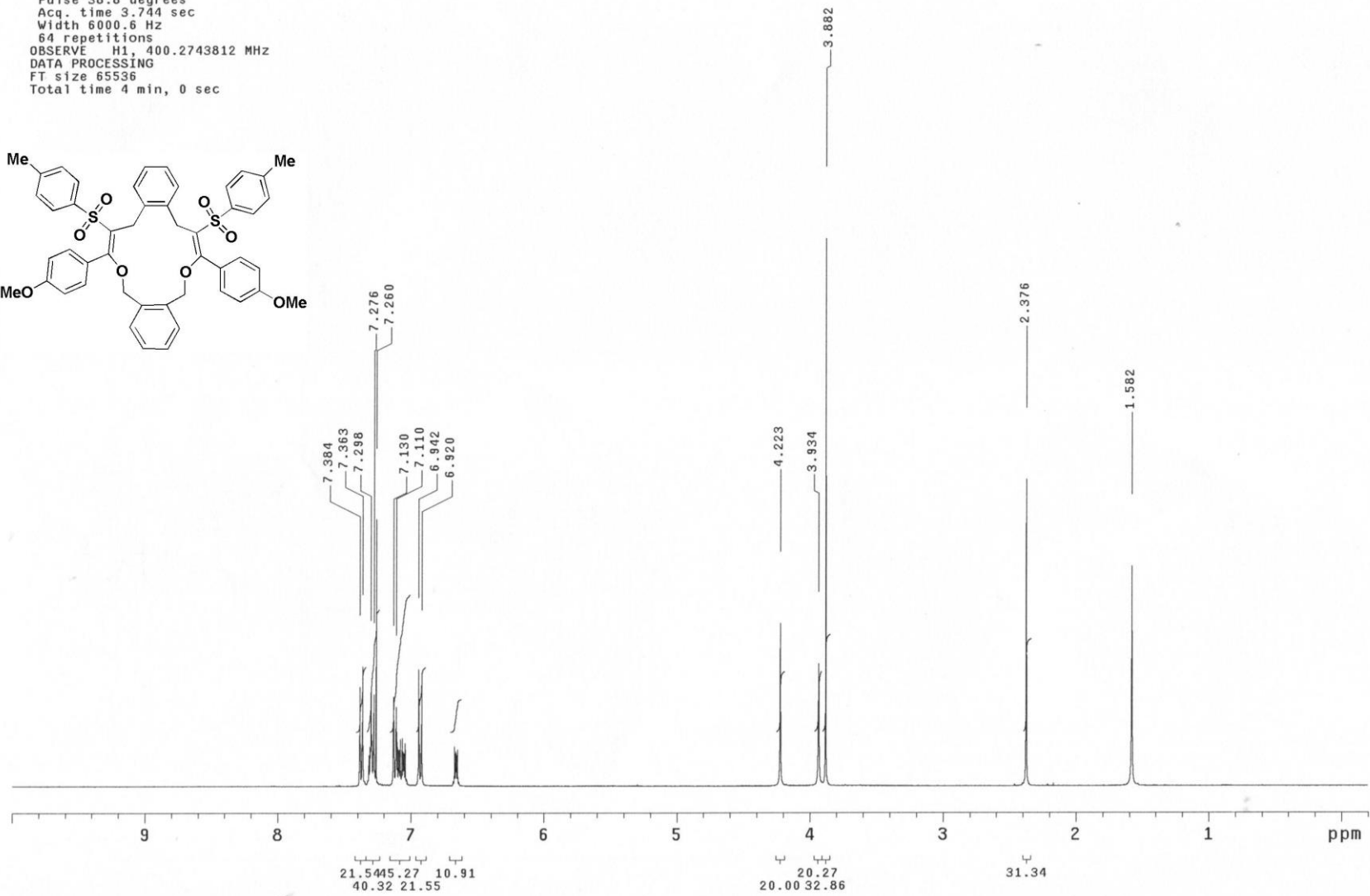
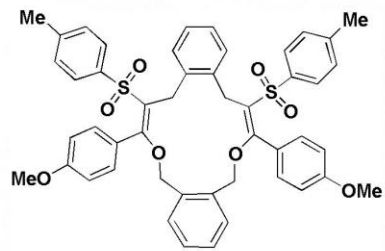
64 repetitions

OBSERVE H1, 400.2743812 MHz

DATA PROCESSING

FT size 65536

Total time 4 min, 0 sec



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

NC0610-14

Pulse Sequence: s2pu1

Solvent: CDCl<sub>3</sub>

Ambient temperature

UNITYplus-400 "unity400"

Relax. delay 0.500 sec

Pulse 65.8 degrees

Acq. time 1.000 sec

Width 25000.0 Hz

7056 repetitions

OBSERVE C13, 100.6490738 MHz

DECOUPLE H1, 400.2763980 MHz

Power 43 dB

on during acquisition

off during delay

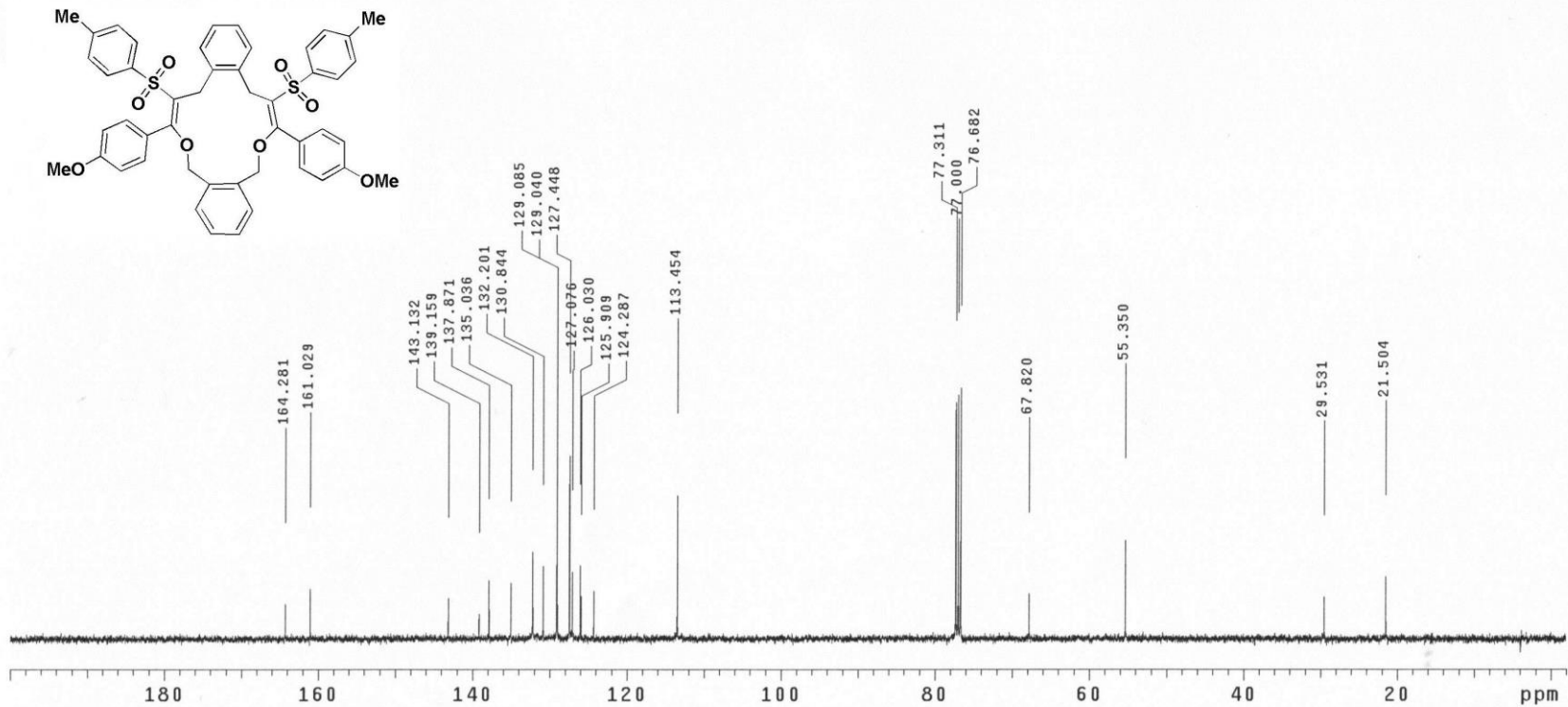
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 13 hr, 25 min, 47 sec



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

NC0723-14

Pulse Sequence: s2pu1

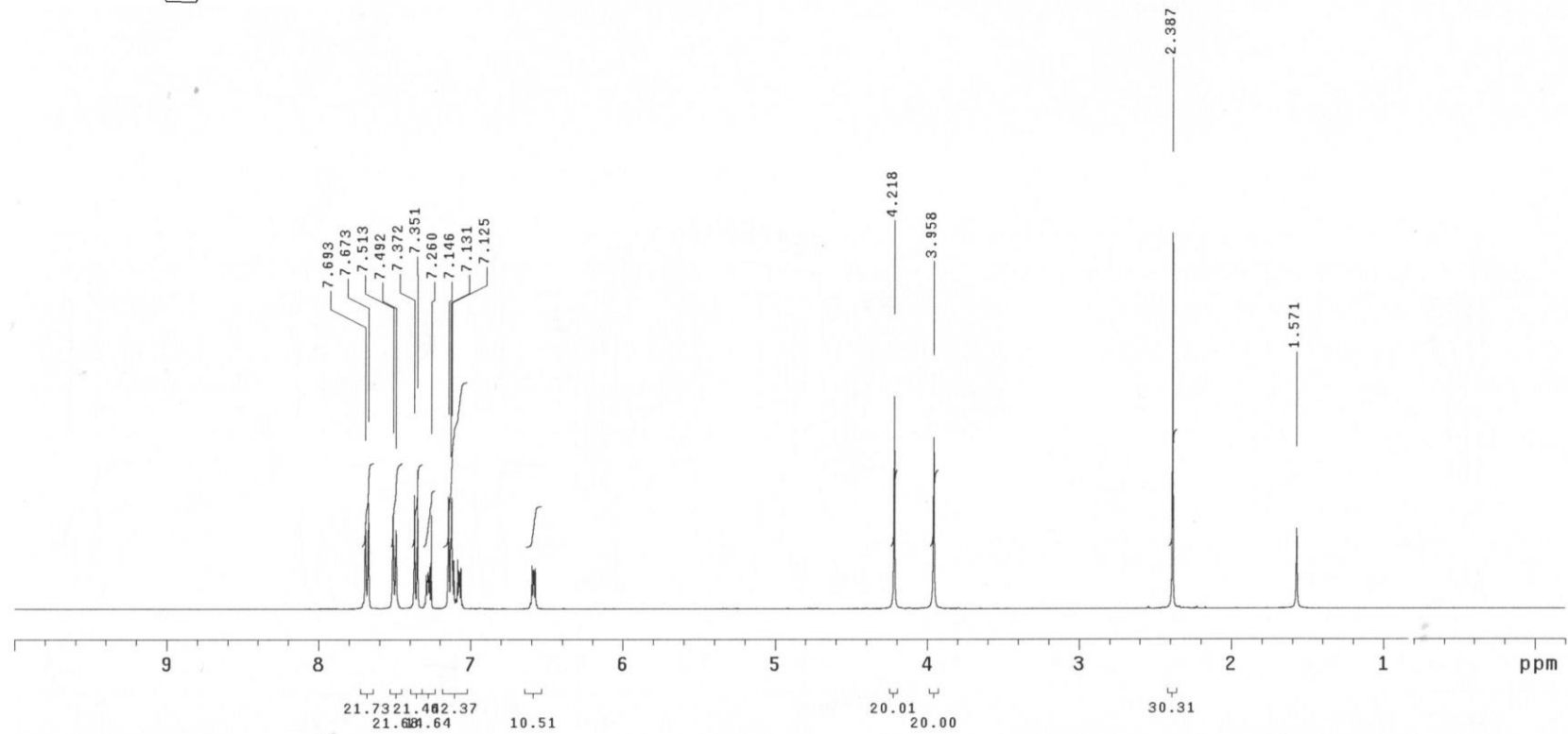
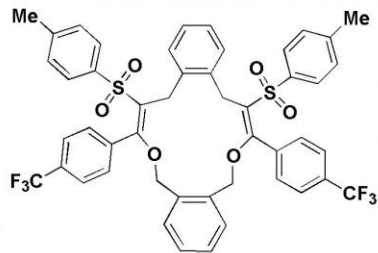
UNITYplus-400 "unity400"

Date: Jul 27 2020

Solvent: CDC13

Ambient temperature

Total 32 repetitions



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

NC0723-14

Pulse Sequence: s2pu1

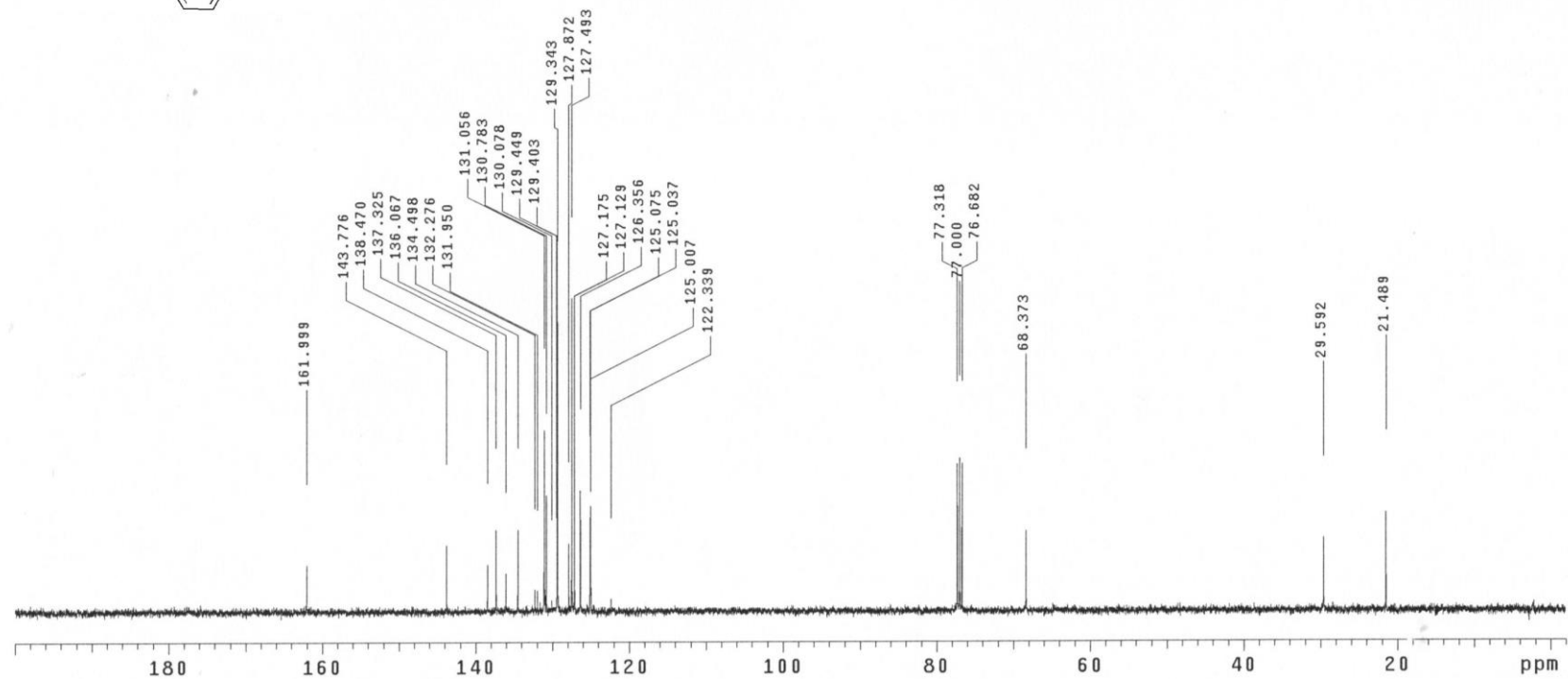
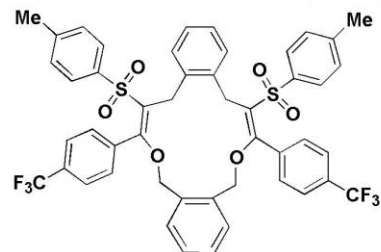
UNITYplus-400 "unity400"

Date: Jul 27 2020

Solvent: CDC13

Ambient temperature

Total 2336 repetitions



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

NC0615-14

Pulse Sequence: s2pu1

Solvent: CDC13

Ambient temperature

UNITYplus-400 "unity400"

Pulse 38.8 degrees

Acq. time 3.744 sec

Width 6000.6 Hz

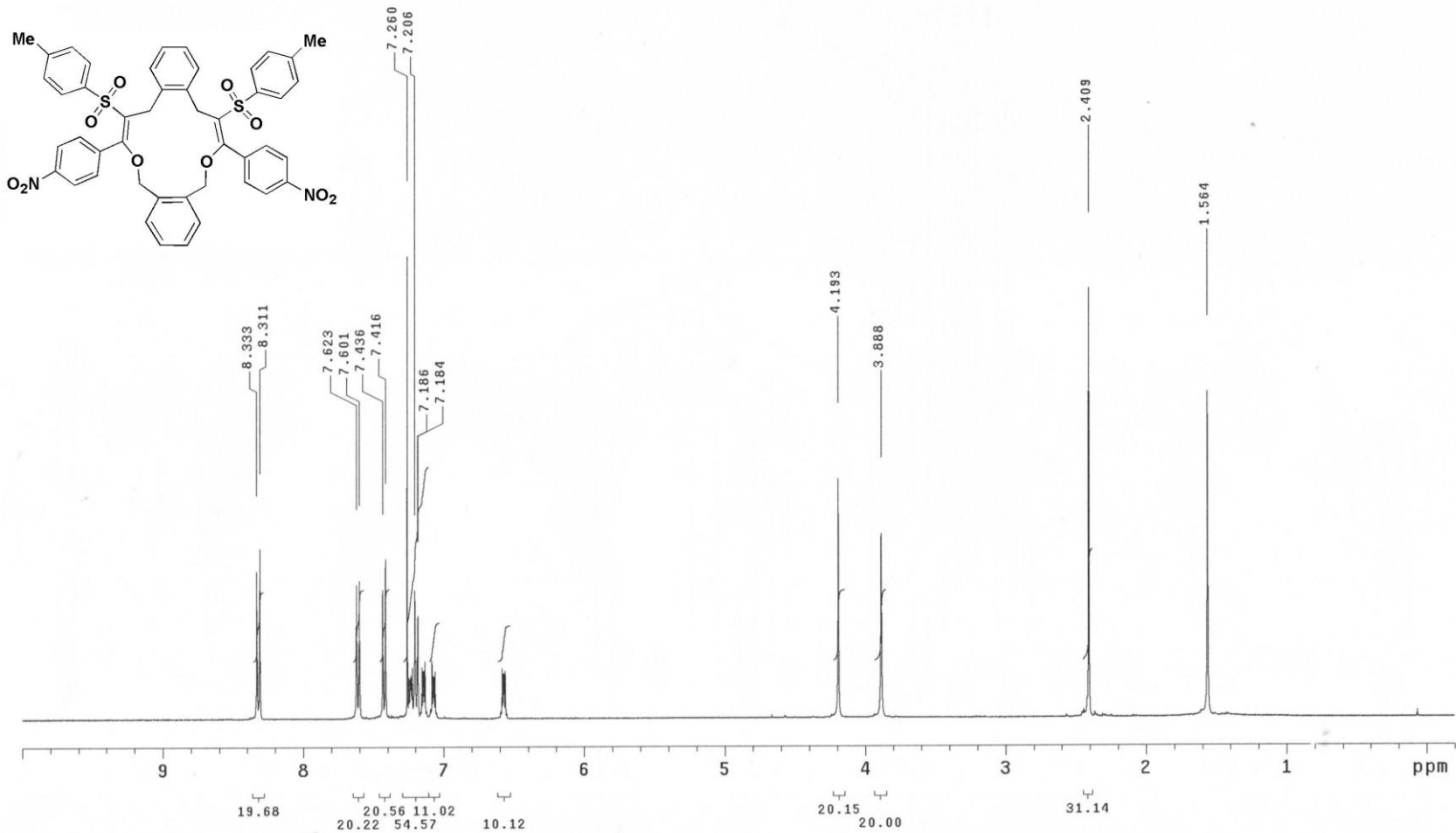
64 repetitions

OBSERVE H1, 400.2743814 MHz

DATA PROCESSING

FT size 65536

Total time 4 min, 0 sec



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

NC0615-14

Pulse Sequence: s2pu1

Solvent: CDC13

Ambient temperature

UNITYplus-400 "unity400"

Relax. delay 0.500 sec

Pulse 65.8 degrees

Acq. time 0.800 sec

Width 25000.0 Hz

7472 repetitions

OBSERVE C13, 100.6490723 MHz

DECOUPLE H1, 400.2763980 MHz

Power 43 dB

on during acquisition

off during delay

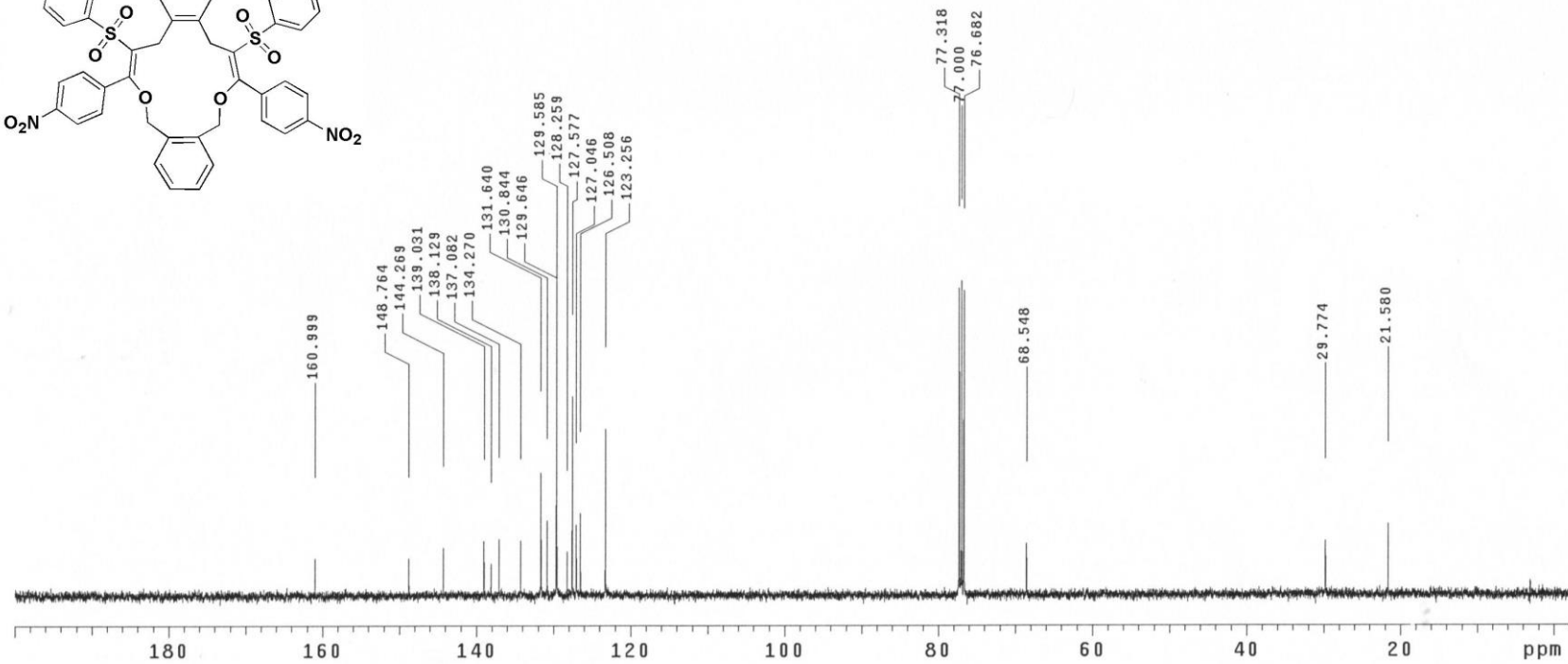
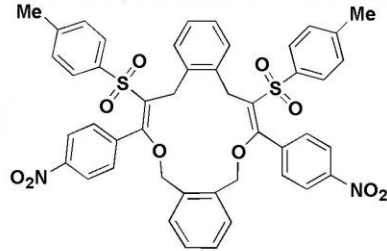
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 11 hr, 39 min, 7 sec



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

NC0630-14

Pulse Sequence: s2pu1

Solvent: CDC13

Ambient temperature

UNITYplus-400 "unity400"

Pulse 38.8 degrees

Acq. time 3.744 sec

Width 6000.6 Hz

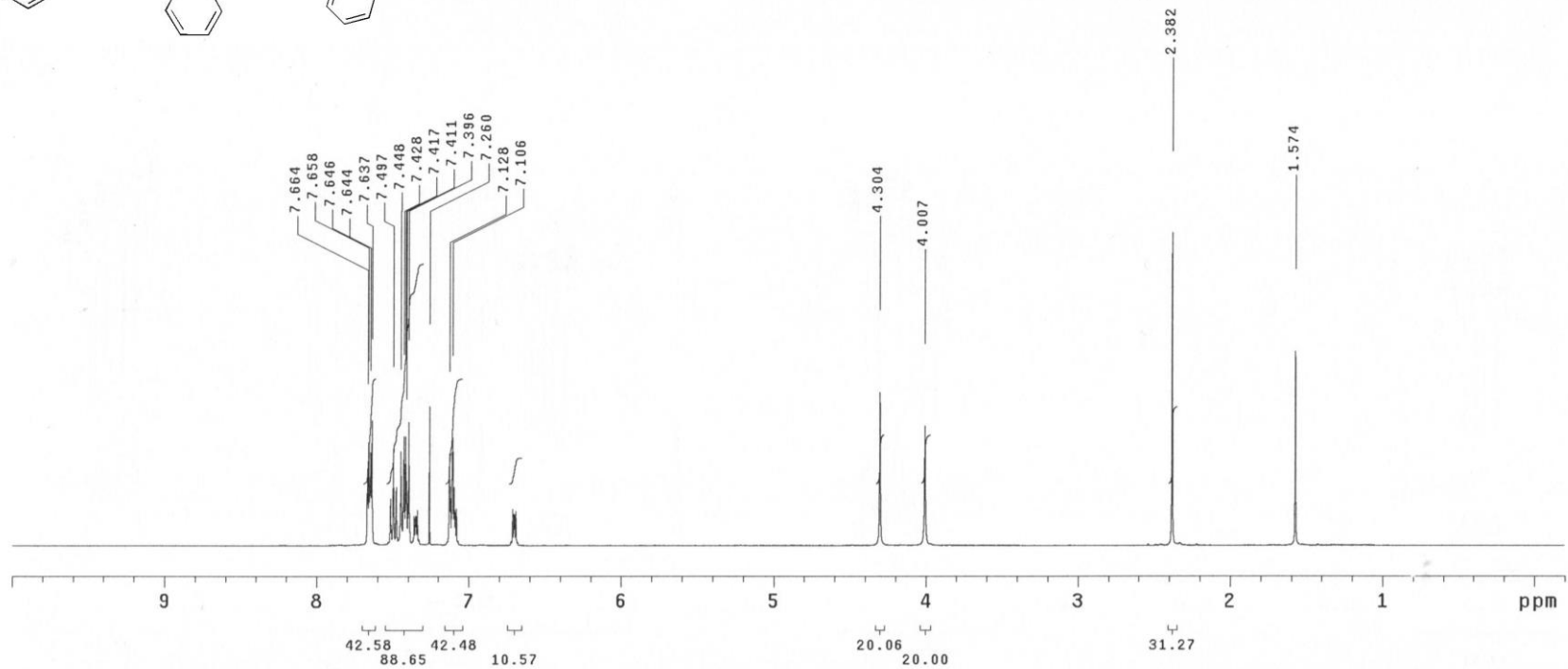
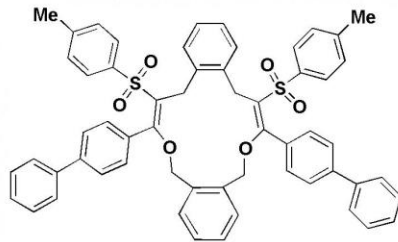
32 repetitions

OBSERVE H1, 400.2743814 MHz

DATA PROCESSING

FT size 65536

Total time 2 min, 0 sec





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

NC0630-14

Pulse Sequence: s2pu1

Solvent: CDCl<sub>3</sub>

Ambient temperature

UNITYplus-400 "unity400"

Relax. delay 0.500 sec

Pulse 65.8 degrees

Acq. time 0.800 sec

Width 25000.0 Hz

3248 repetitions

OBSERVE C13, 100.6490738 MHz

DECOUPLE H1, 400.2763980 MHz

Power 43 dB

on during acquisition

off during delay

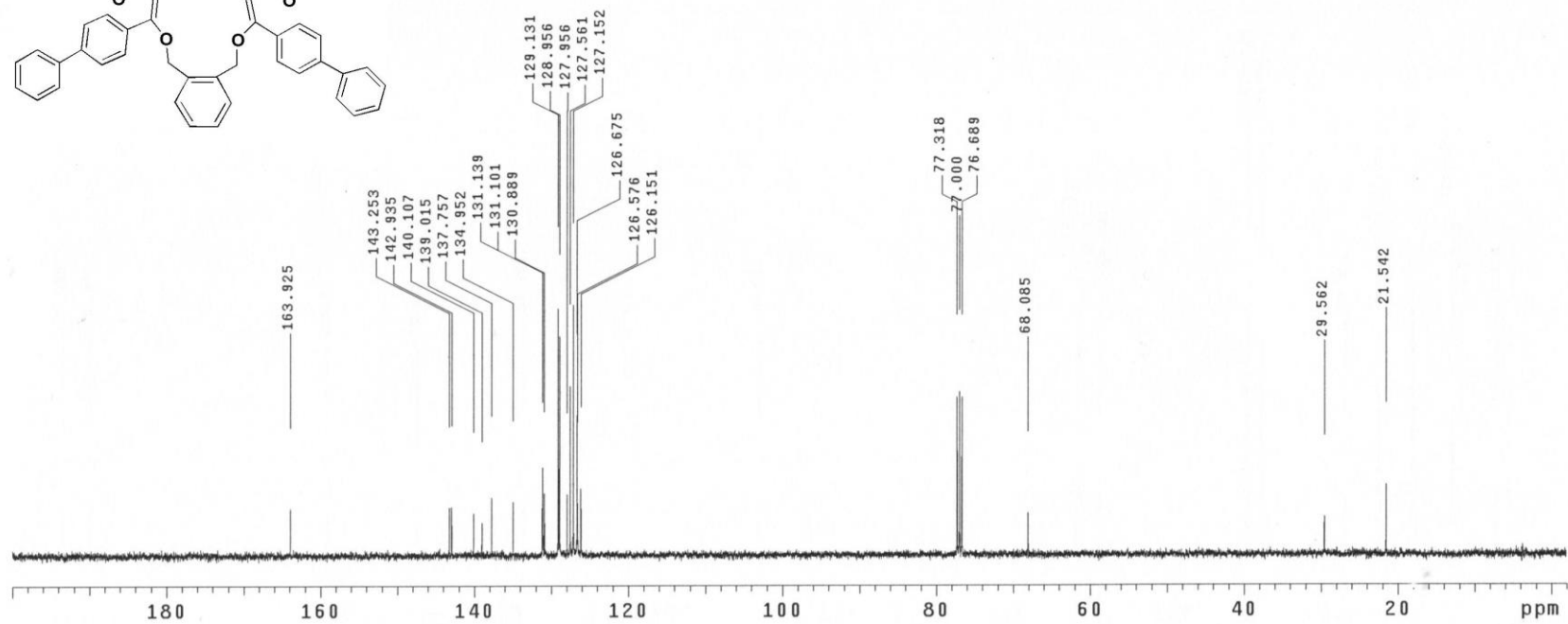
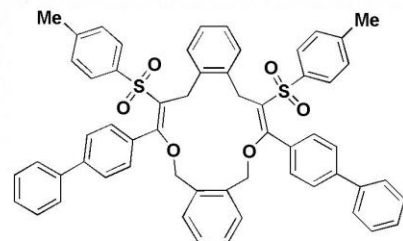
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

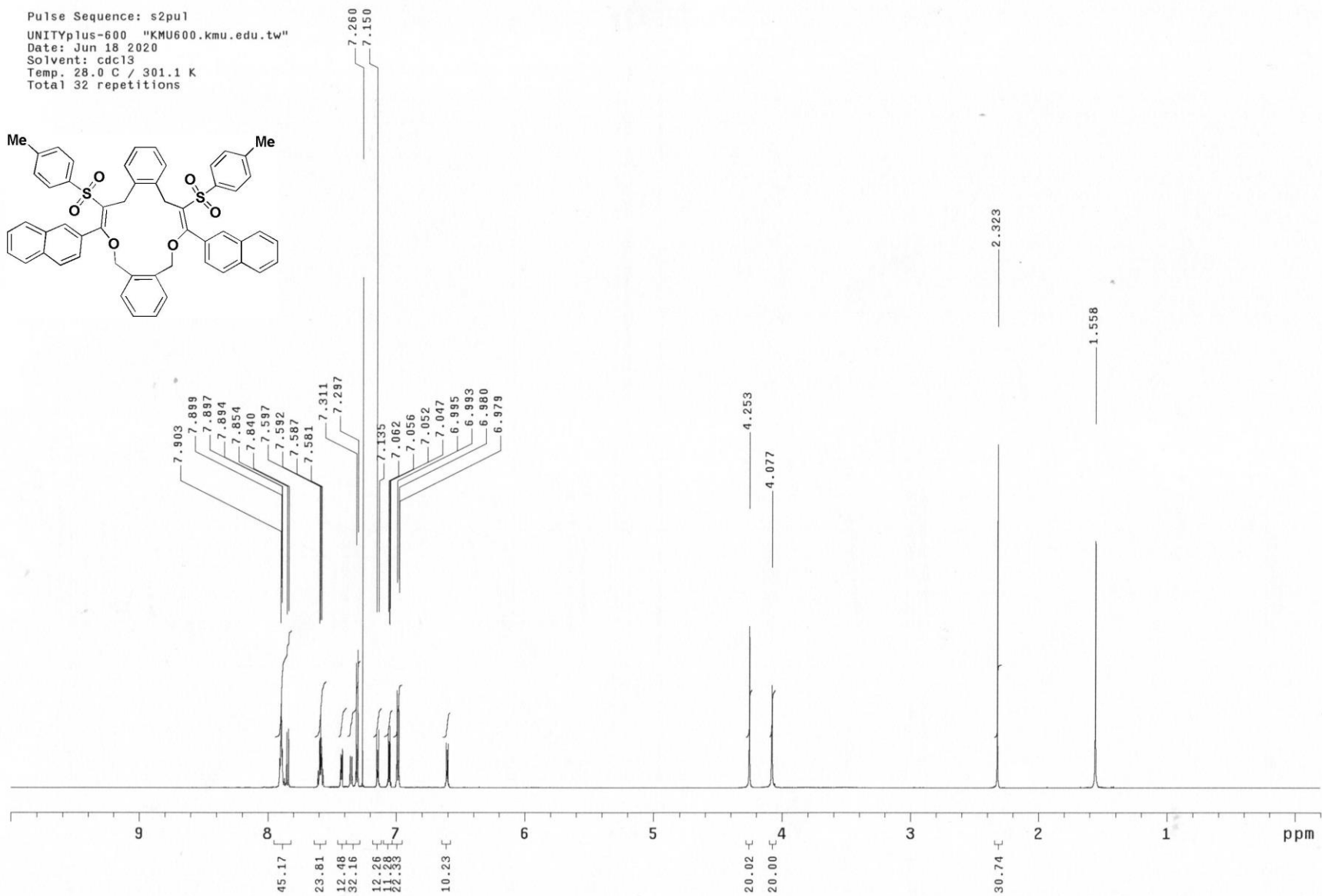
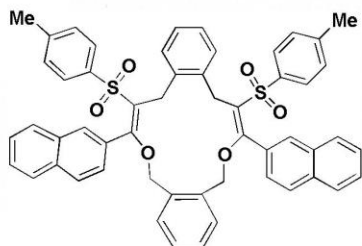
Total time 11 hr, 39 min, 7 sec



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

NC0616-14

Pulse Sequence: s2pu1  
UNITYplus-600 "KMU600.kmu.edu.tw"  
Date: Jun 18 2020  
Solvent: cdc13  
Temp. 28.0 C / 301.1 K  
Total 32 repetitions



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

NC0616-14

Pulse Sequence: s2pu1

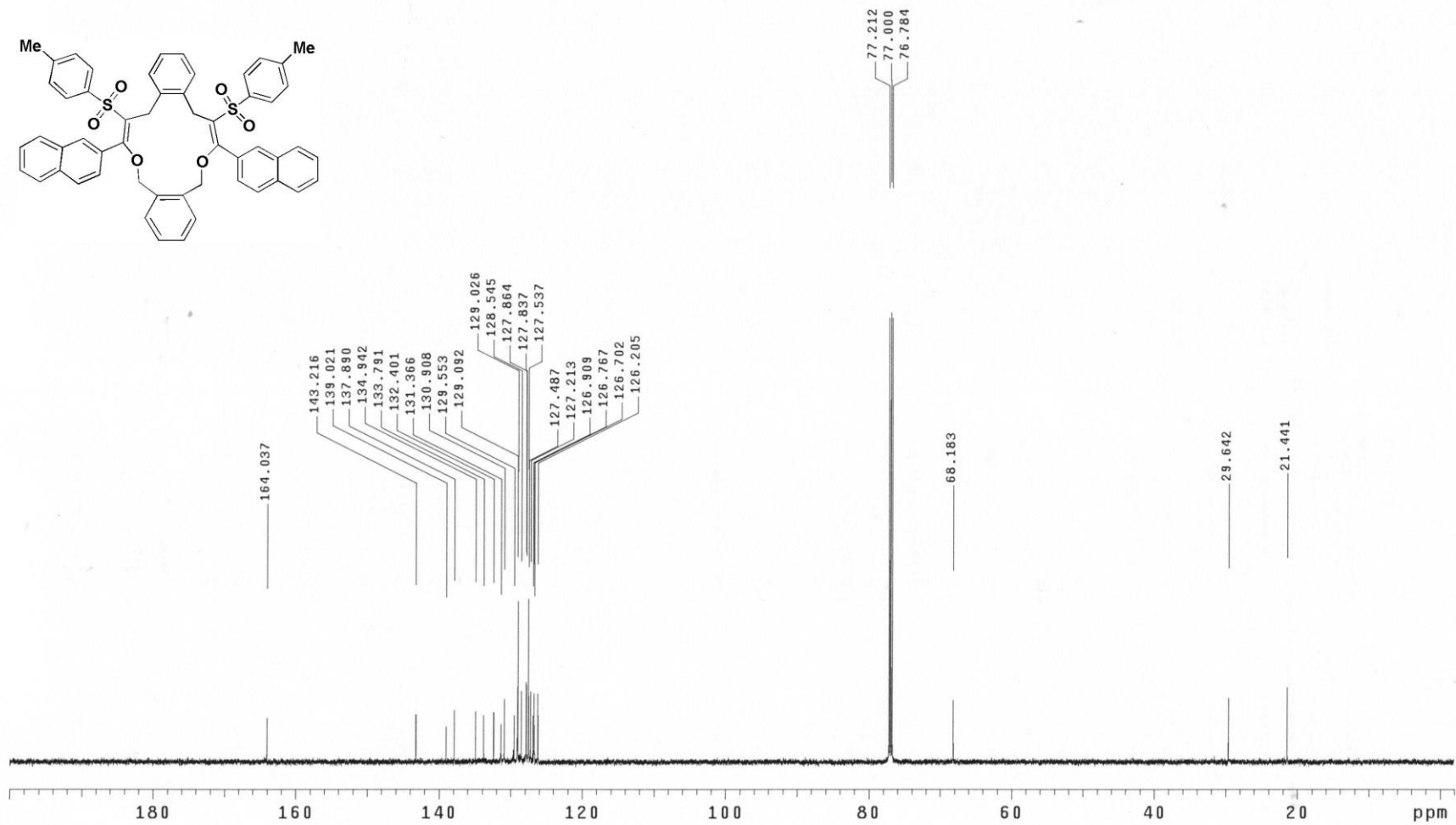
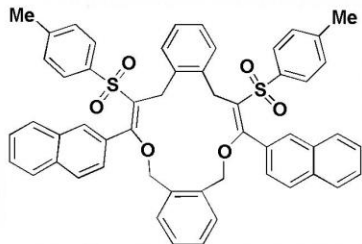
UNITYplus-600 "KMU600.kmu.edu.tw"

Date: Jun 18 2020

Solvent: cdcl3

Temp: 28.0 C / 301.1 K

Total 1640 repetitions



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

NC0728-14

Pulse Sequence: s2pu1

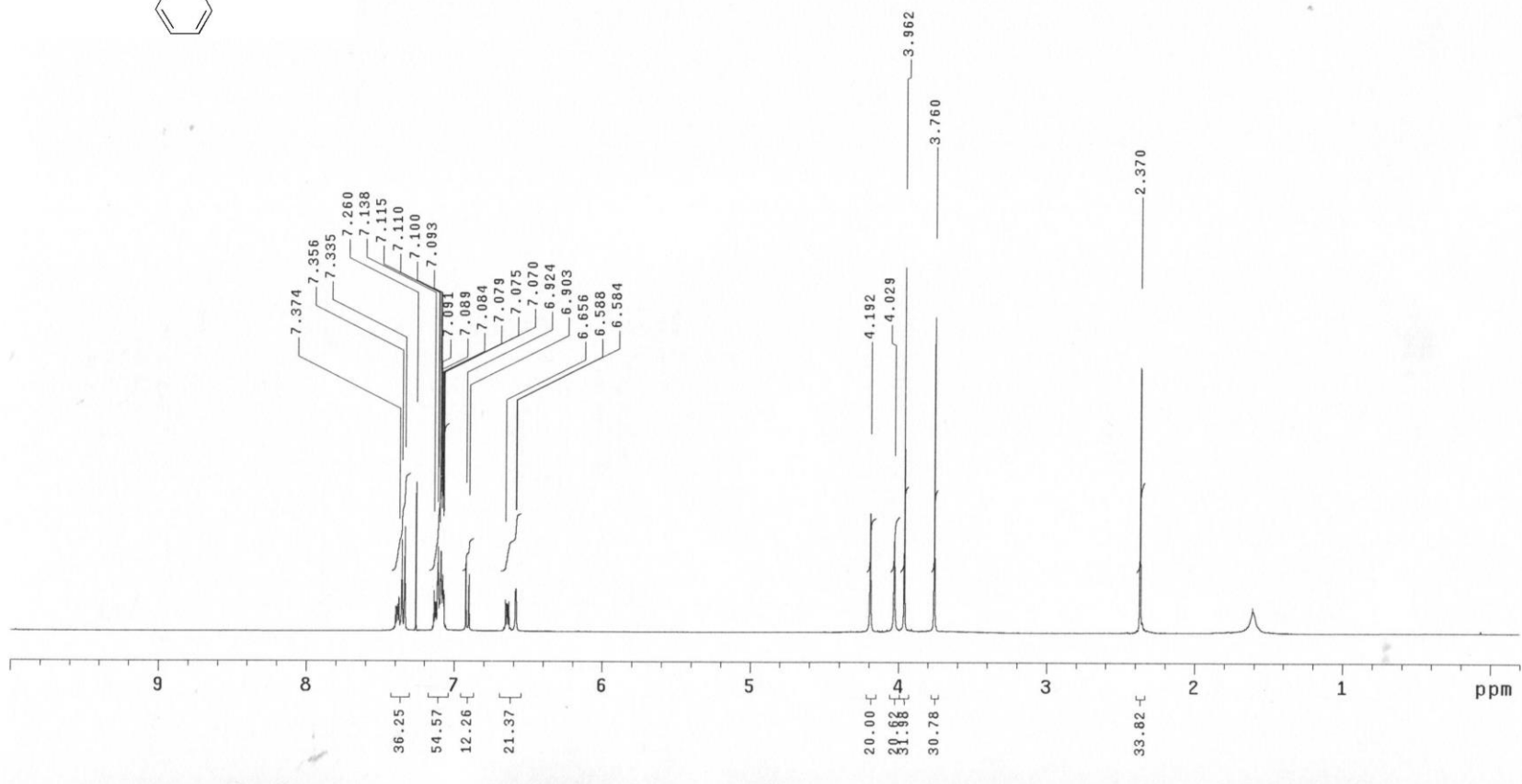
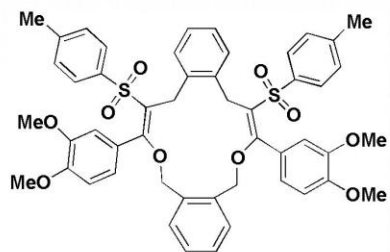
UNITYplus-400 "unity400"

Date: Oct 15 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 32 repetitions



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

NC0728-14

Pulse Sequence: s2pu1

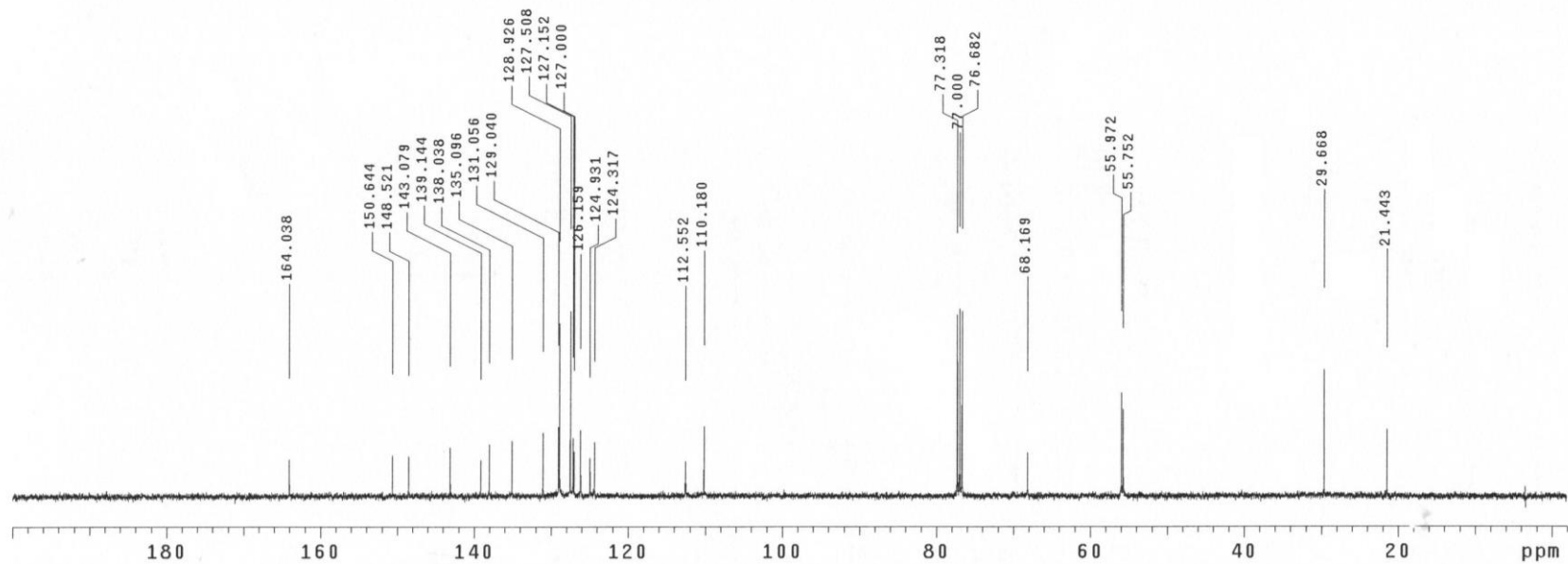
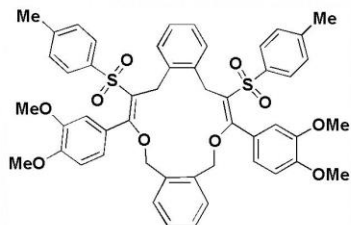
UNITYplus-400 "unity400"

Date: Oct 15 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 5248 repetitions



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

NC0724-14

Pulse Sequence: s2pu1

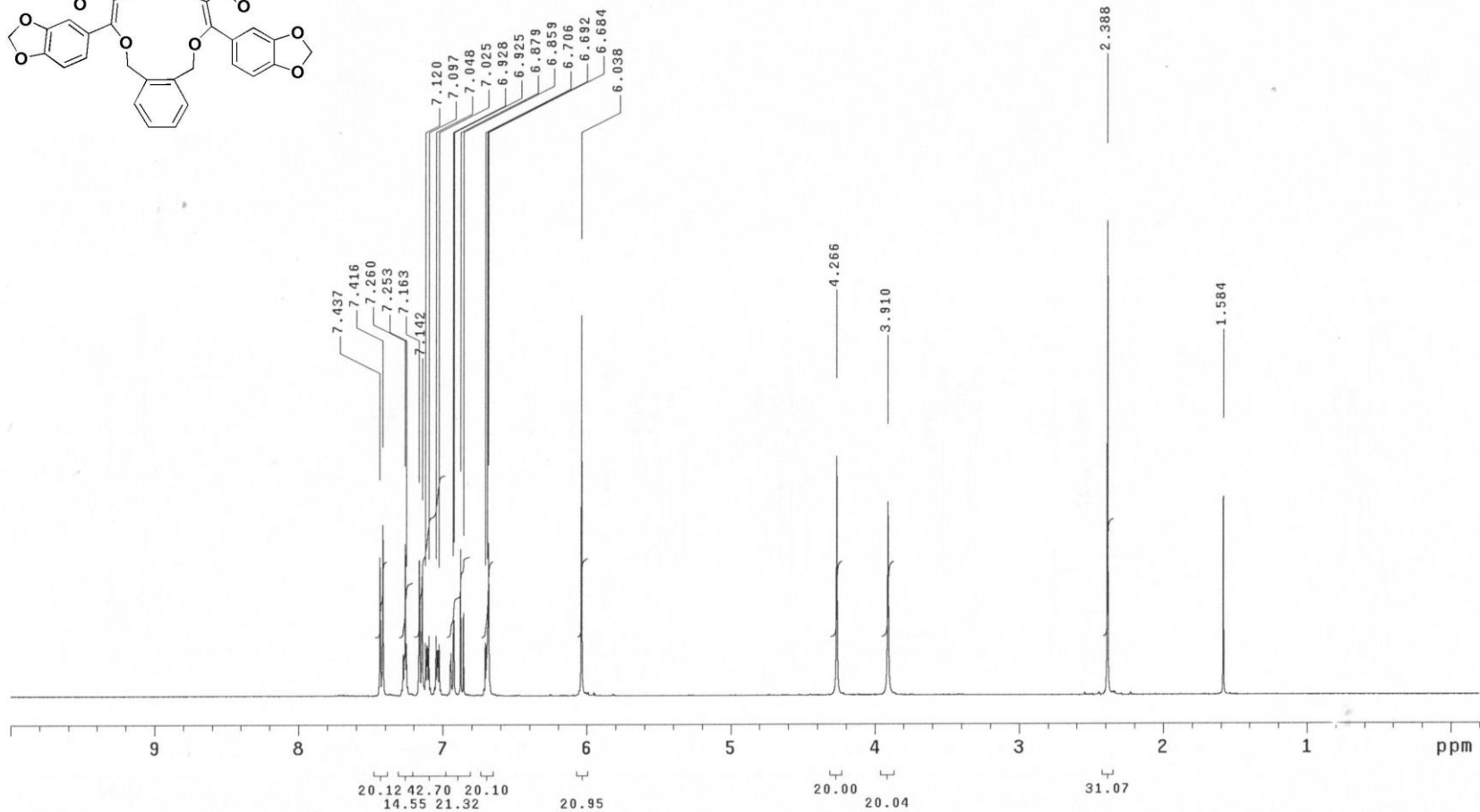
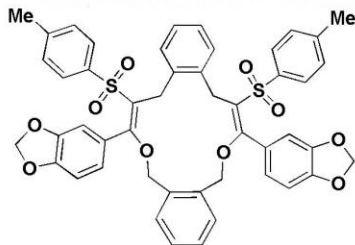
UNITYplus-400 "unity400"

Date: Jul 29 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 32 repetitions



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

NC0724-14

Pulse Sequence: s2pu1

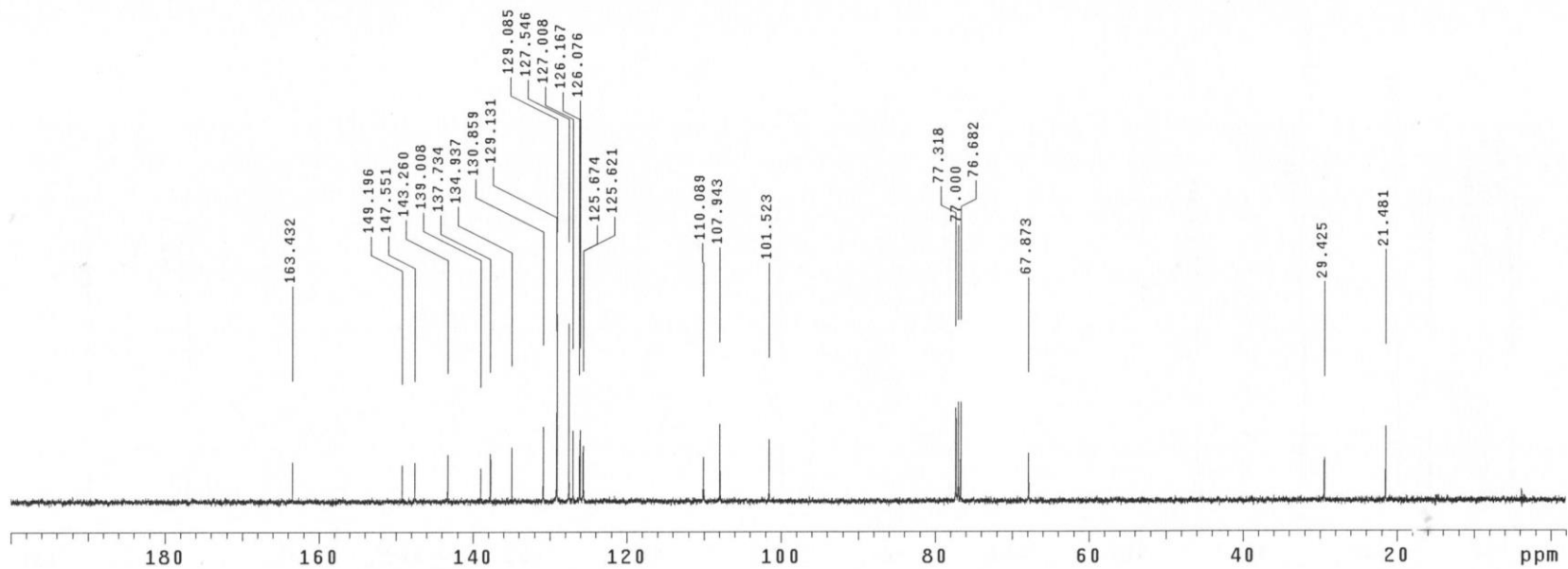
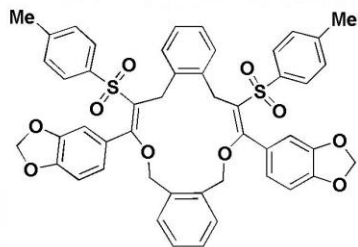
UNITYplus-400 "unity400"

Date: Jul 29 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 1552 repetitions



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

NC0714-14

Pulse Sequence: s2pu1

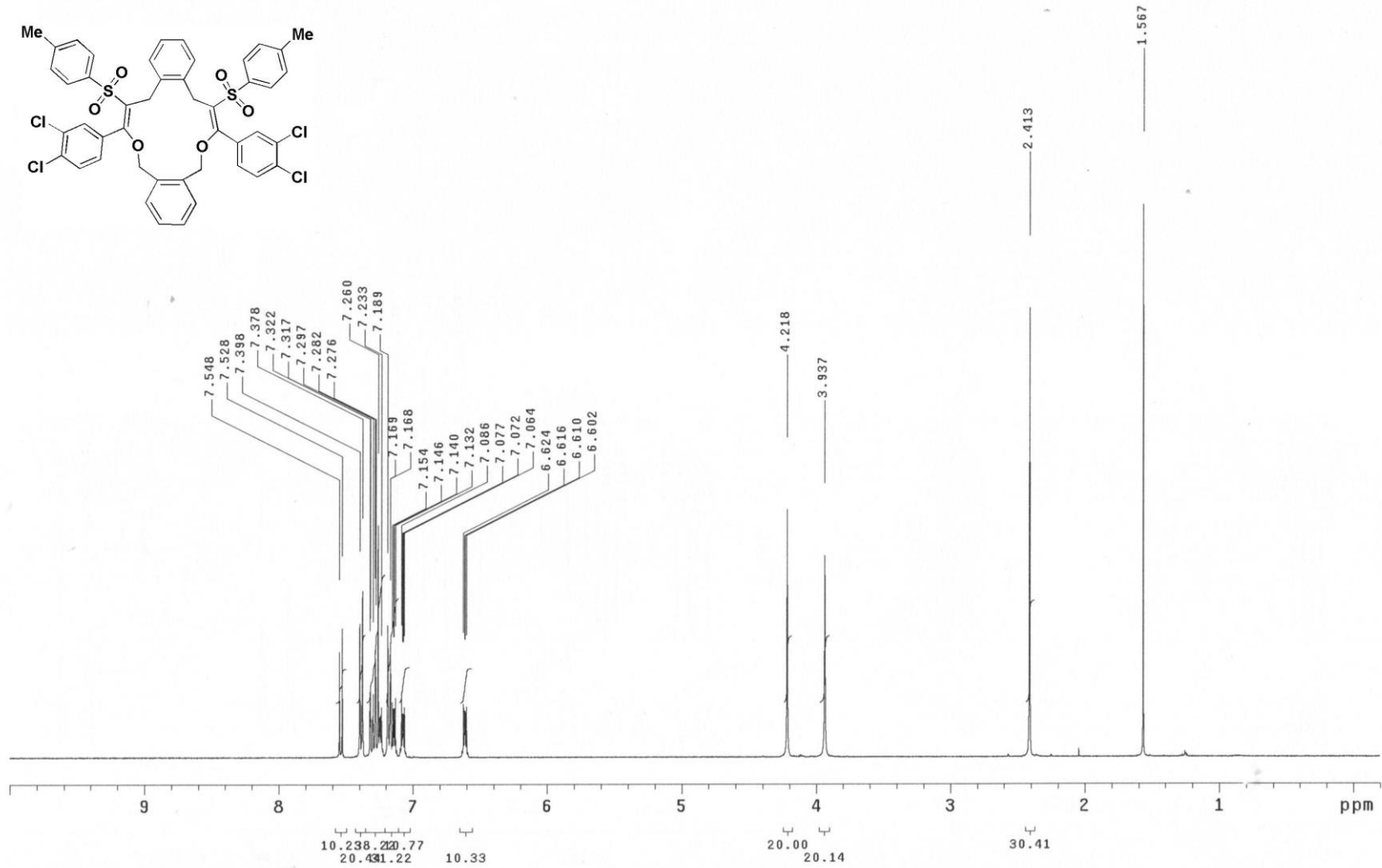
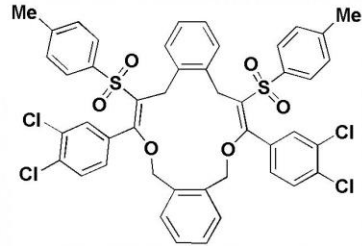
UNITYplus-400 "unity400"

Date: Jul 30 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 32 repetitions





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

NC0714-14

Pulse Sequence: s2pu1

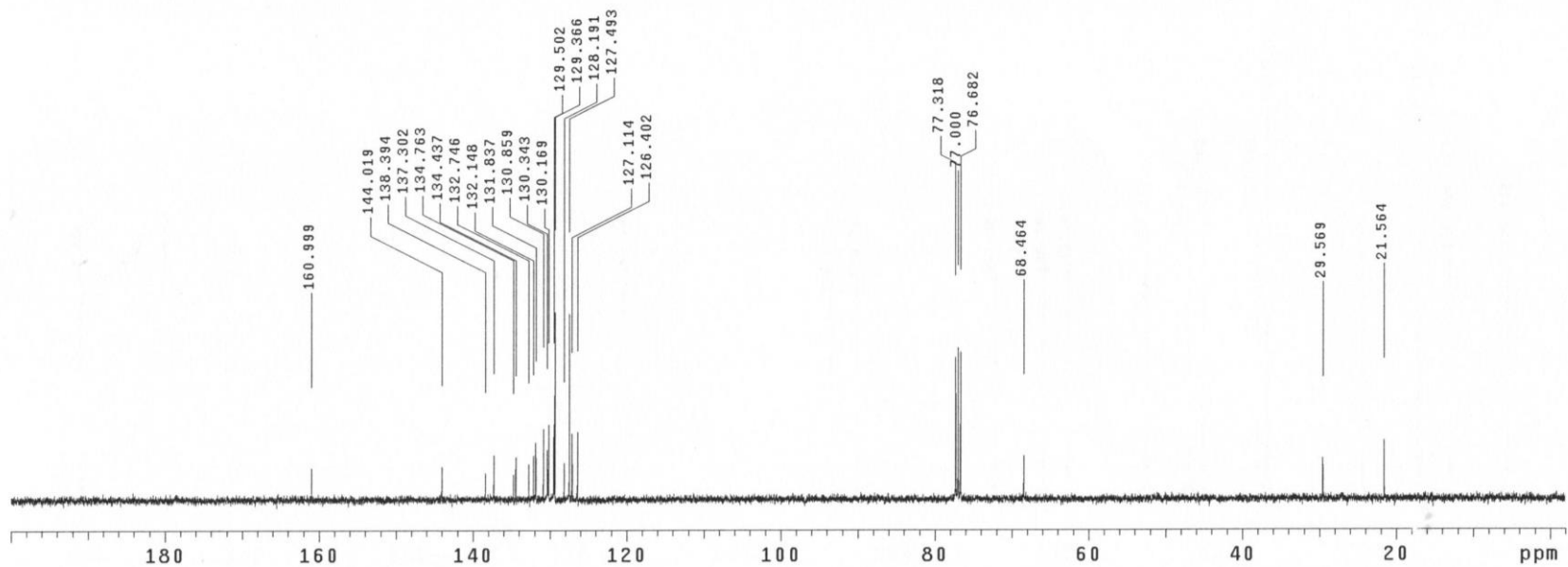
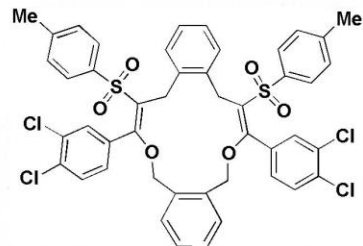
UNITYplus-400 "unity400"

Date: Jul 30 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 3200 repetitions



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

NC0730-14

Pulse Sequence: s2pu1

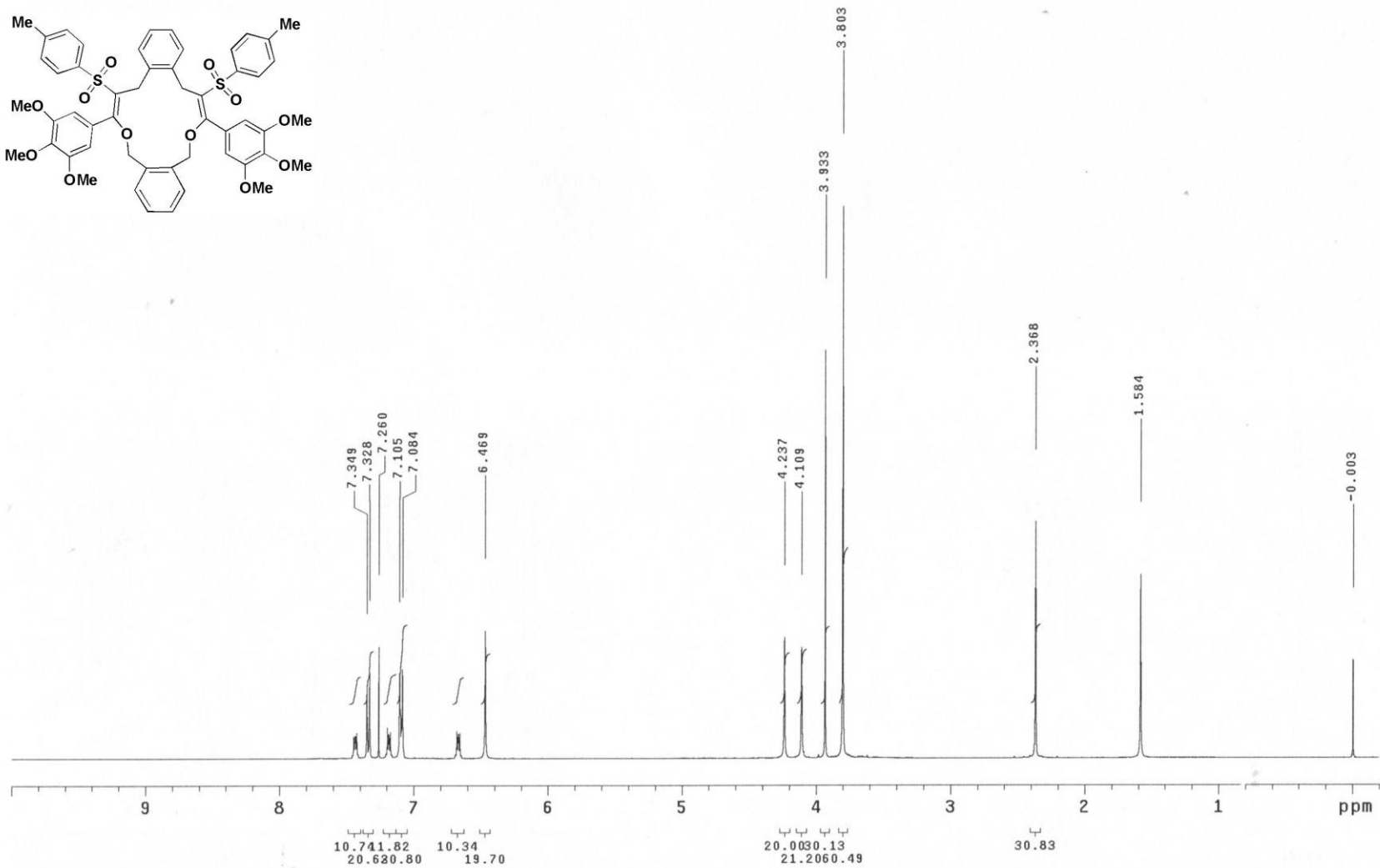
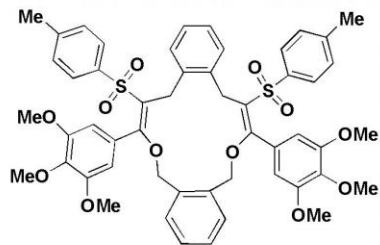
UNITYplus-400 "unity400"

Date: Aug 12 2020

Solvent: CDC13

Ambient temperature

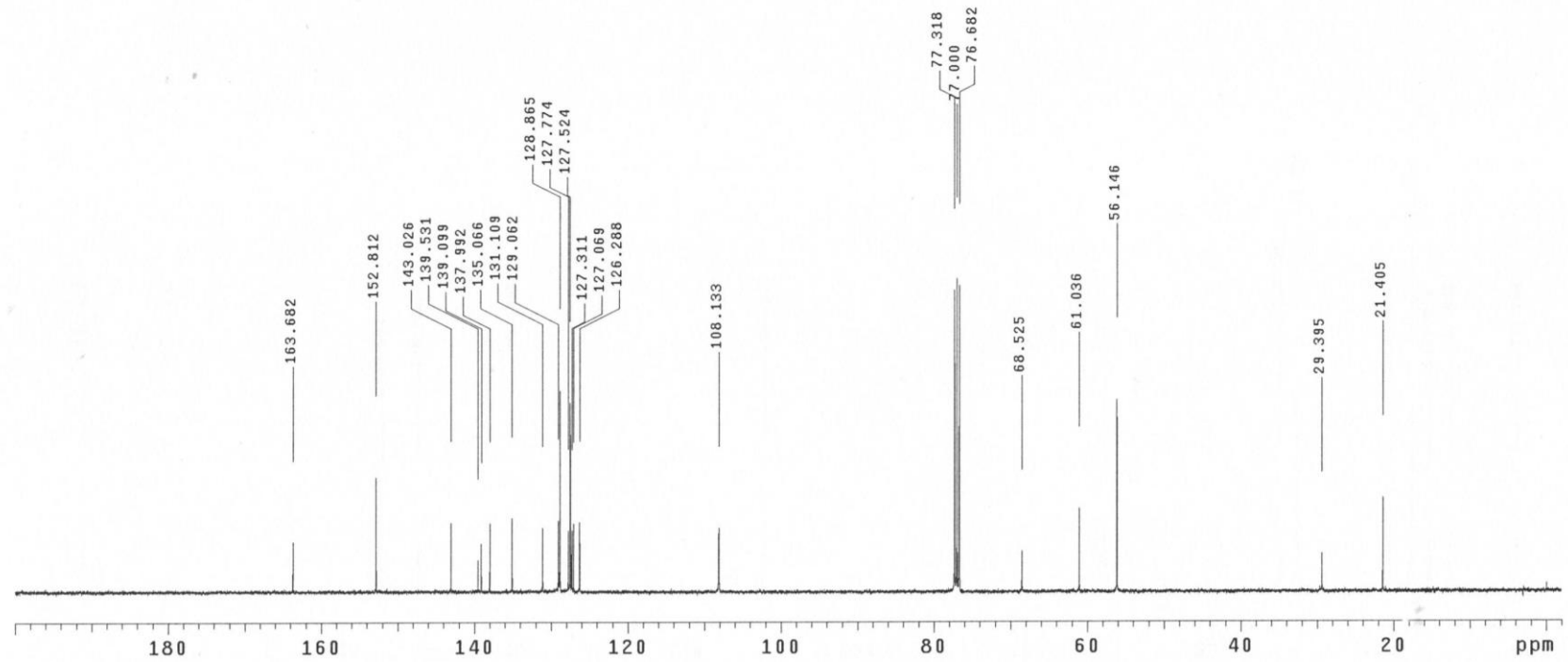
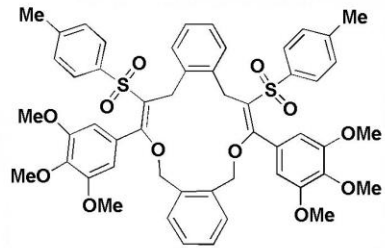
Total 32 repetitions



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

NC0730-14

Pulse Sequence: s2pu1  
UNITYplus-400 "unity400"  
Date: Aug 12 2020  
Solvent: CDC13  
Ambient temperature  
Total 32000 repetitions



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

NC0804-14

Pulse Sequence: s2pu1

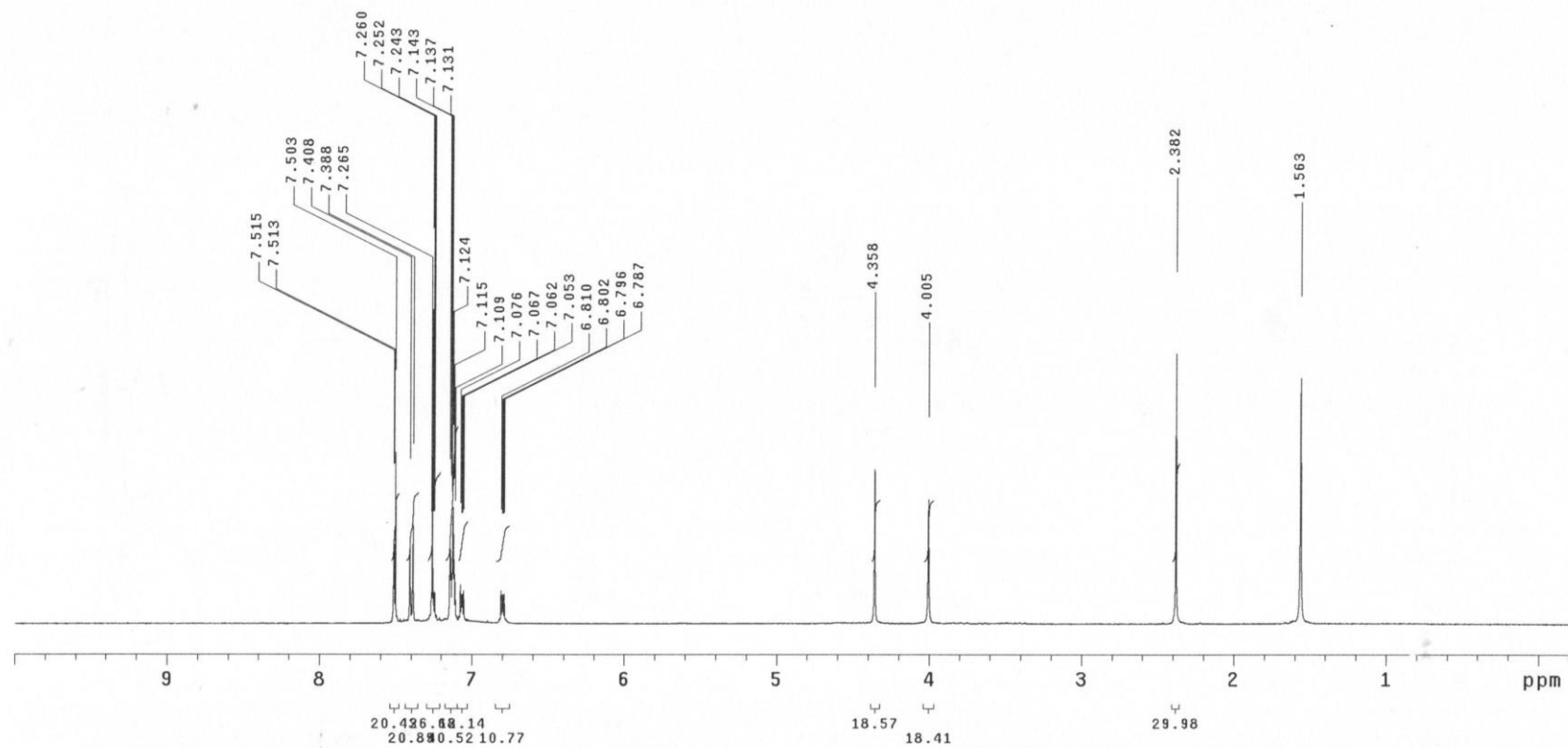
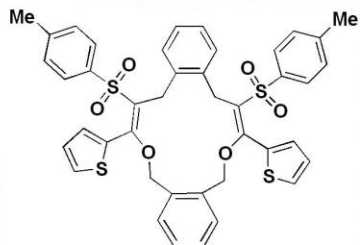
UNITYplus-400 "unity400"

Date: Aug 28 2020

Solvent: CDC13

Ambient temperature

Total 64 repetitions



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

NC0804-14

Pulse Sequence: s2pu1

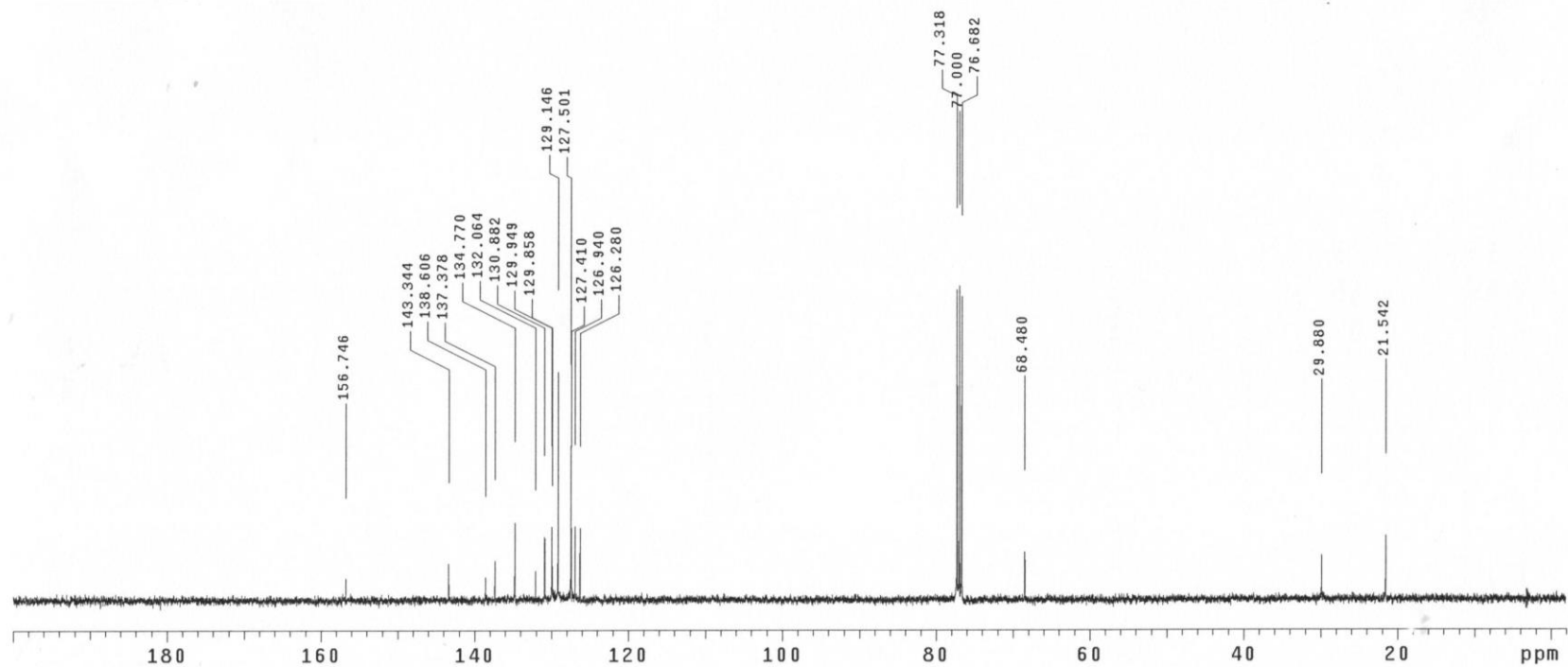
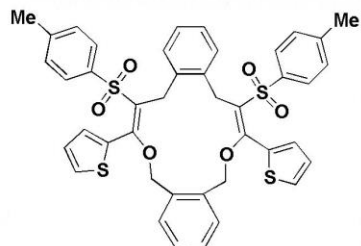
UNITYplus-400 "unity400"

Date: Aug 28 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

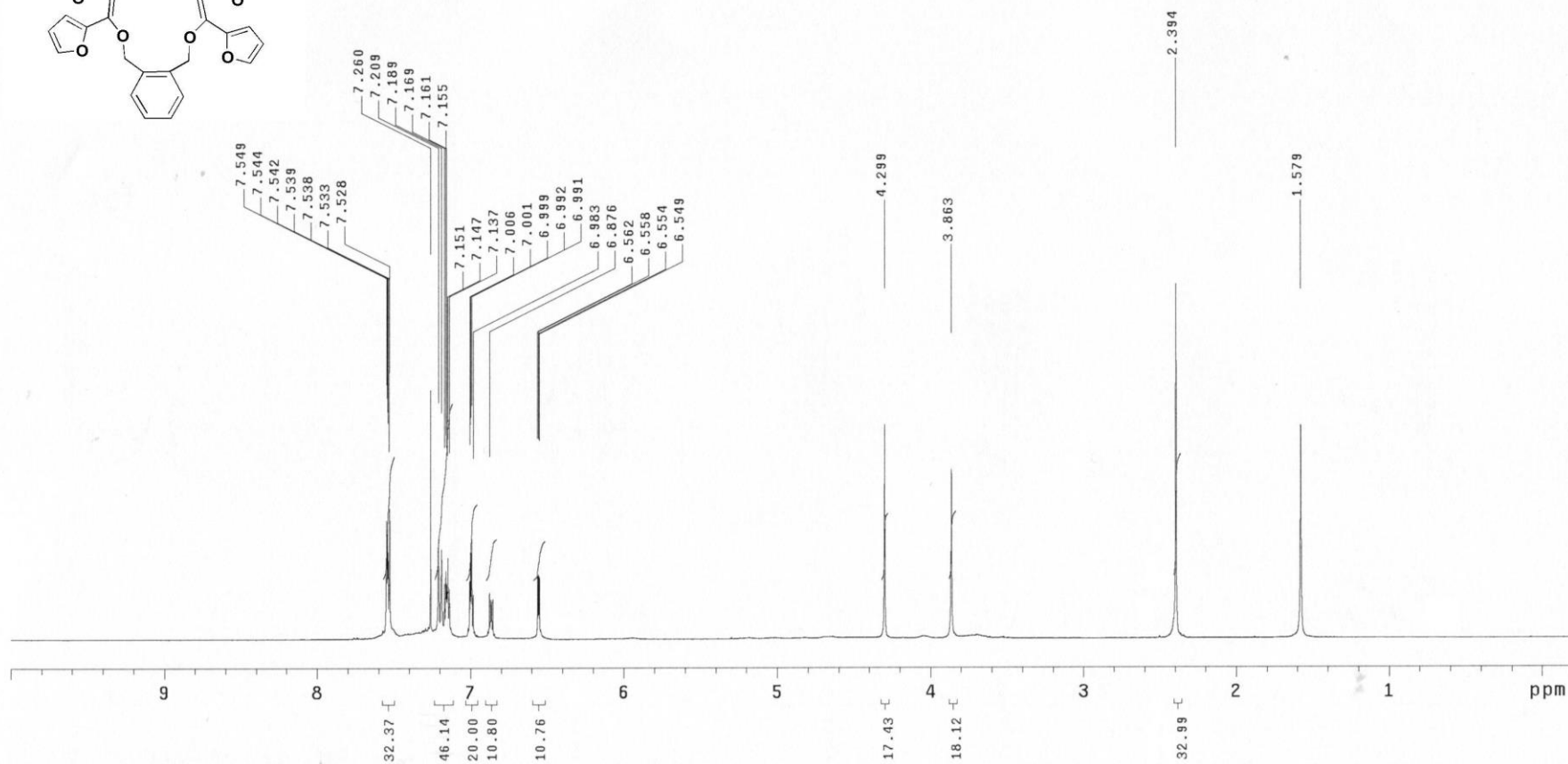
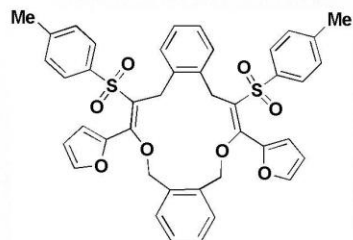
Total 10096 repetitions



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

NC0805-14

Pulse Sequence: s2pu1  
Mercury-400BB "MerPlus400"  
Date: Oct 29 2020  
Solvent: cdc13  
Ambient temperature  
Total 64 repetitions





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

NC0820-14

Pulse Sequence: s2pu1

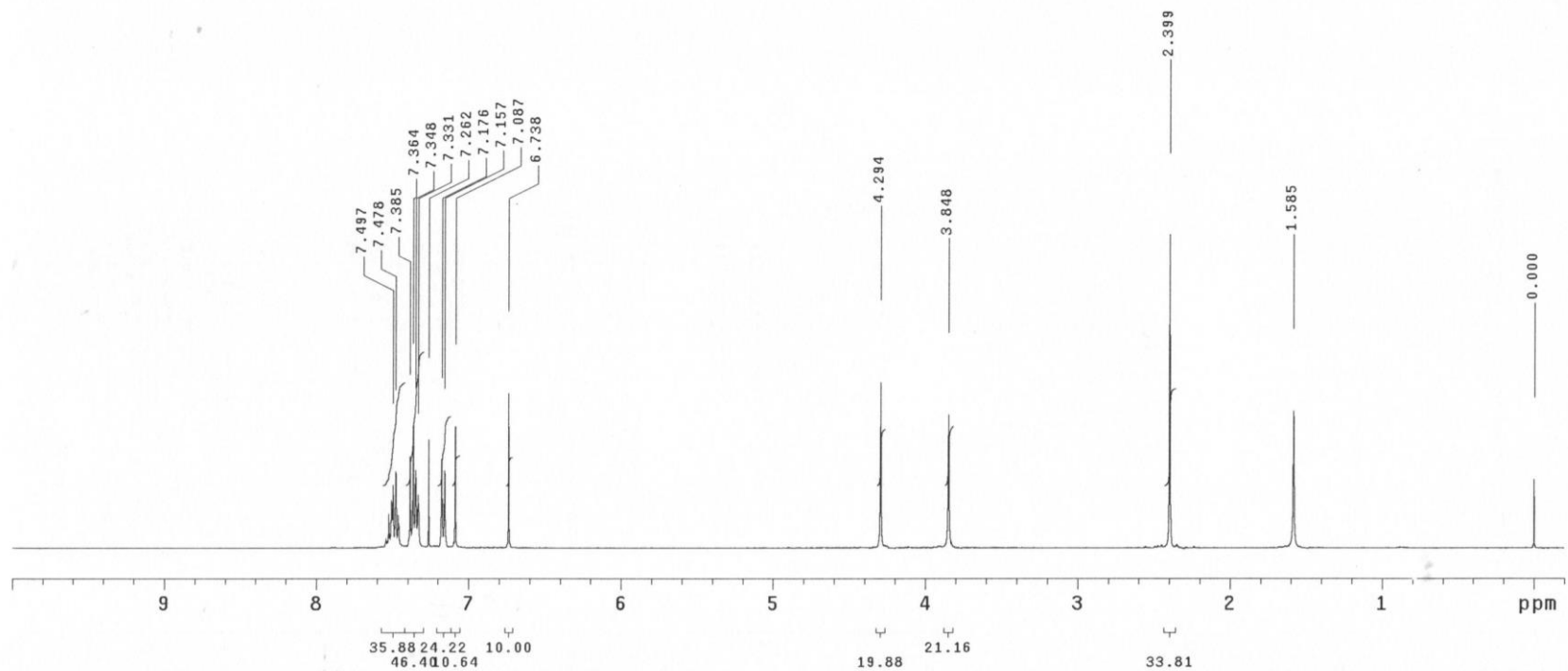
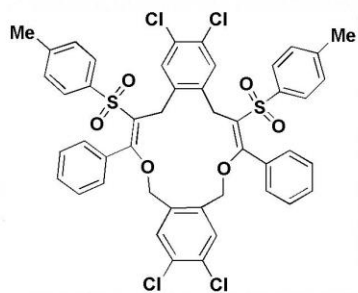
UNITYplus-400 "unity400"

Date: Aug 24 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 32 repetitions





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

NC0820-14

Pulse Sequence: s2pu1

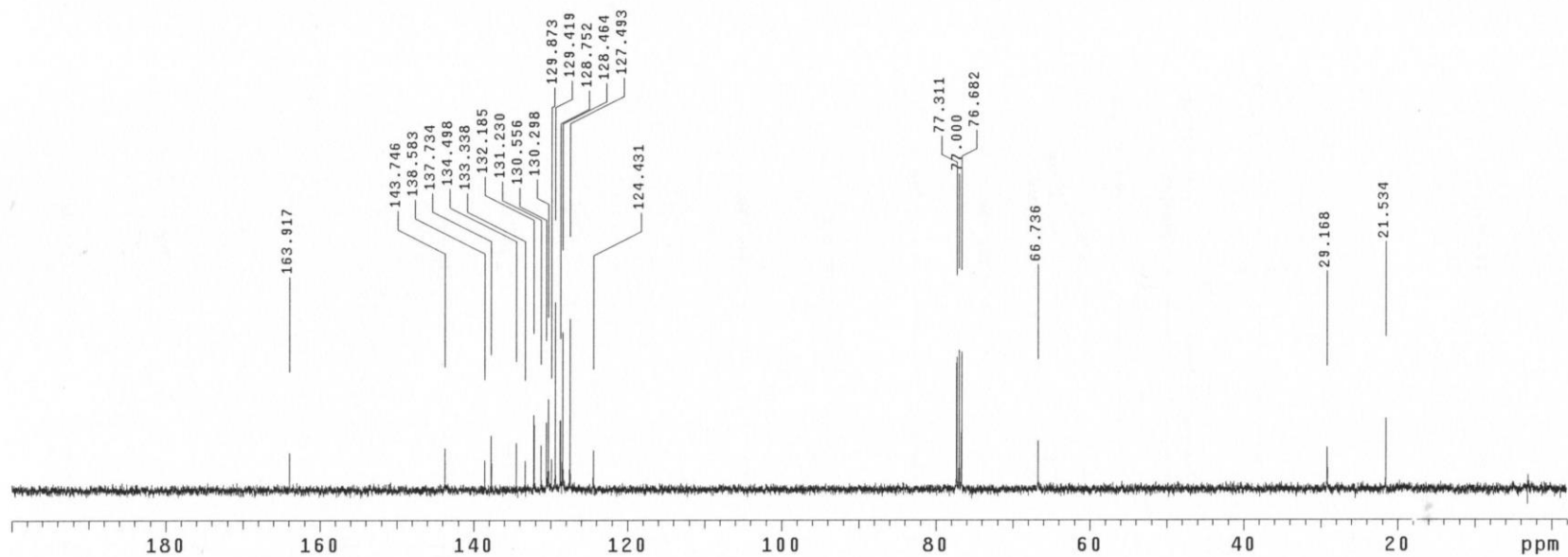
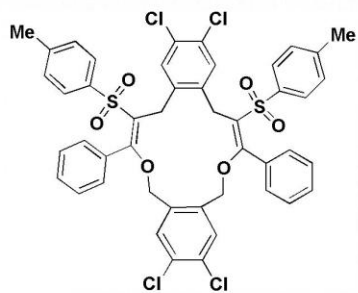
UNITYplus-400 "unity400"

Date: Aug 24 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 1456 repetitions



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

NC0810-14

Pulse Sequence: s2pu1

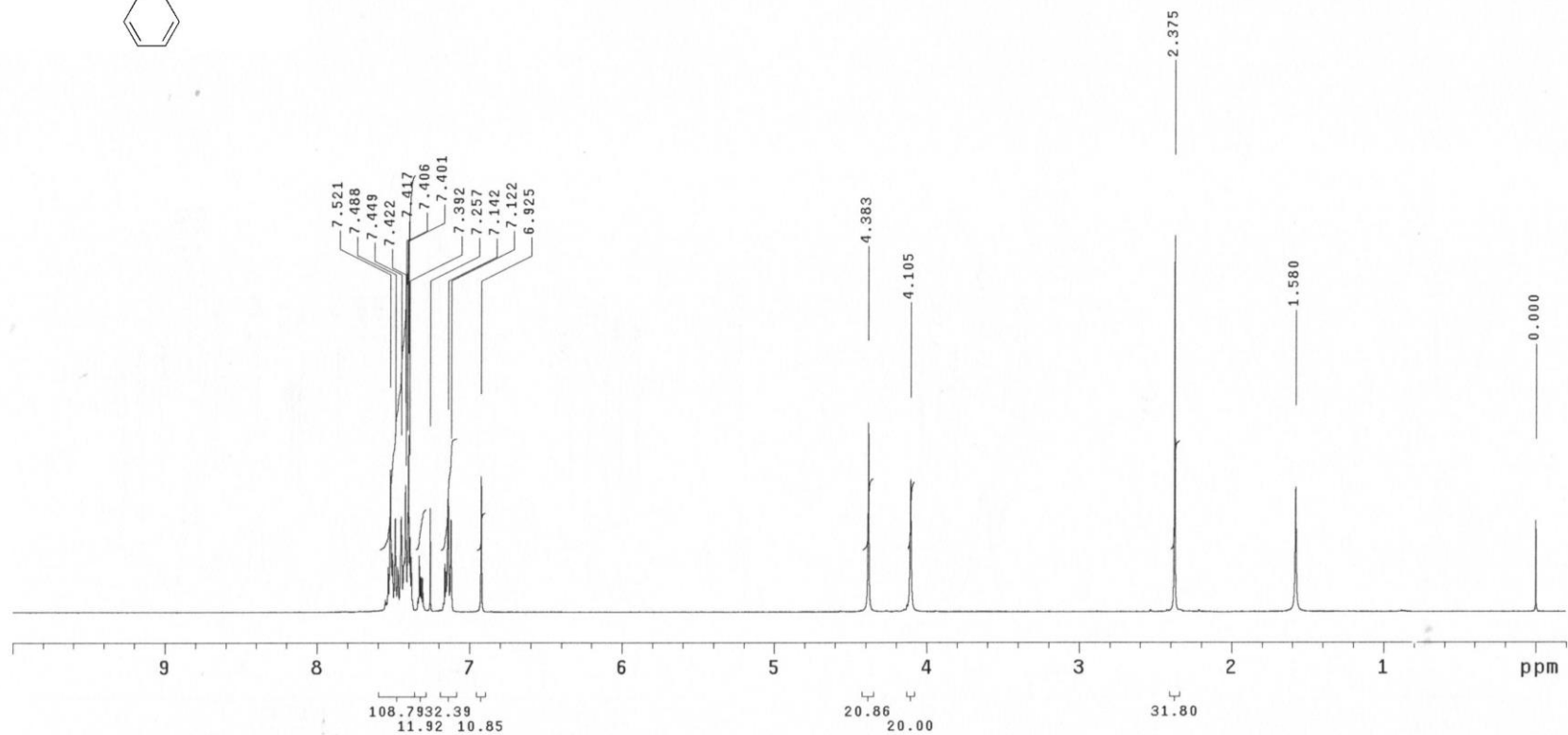
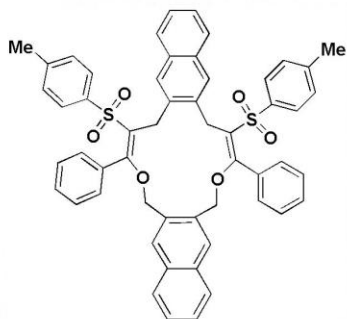
UNITYplus-400 "unity400"

Date: Aug 12 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 32 repetitions





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

NC0821-14

Pulse Sequence: s2pu1

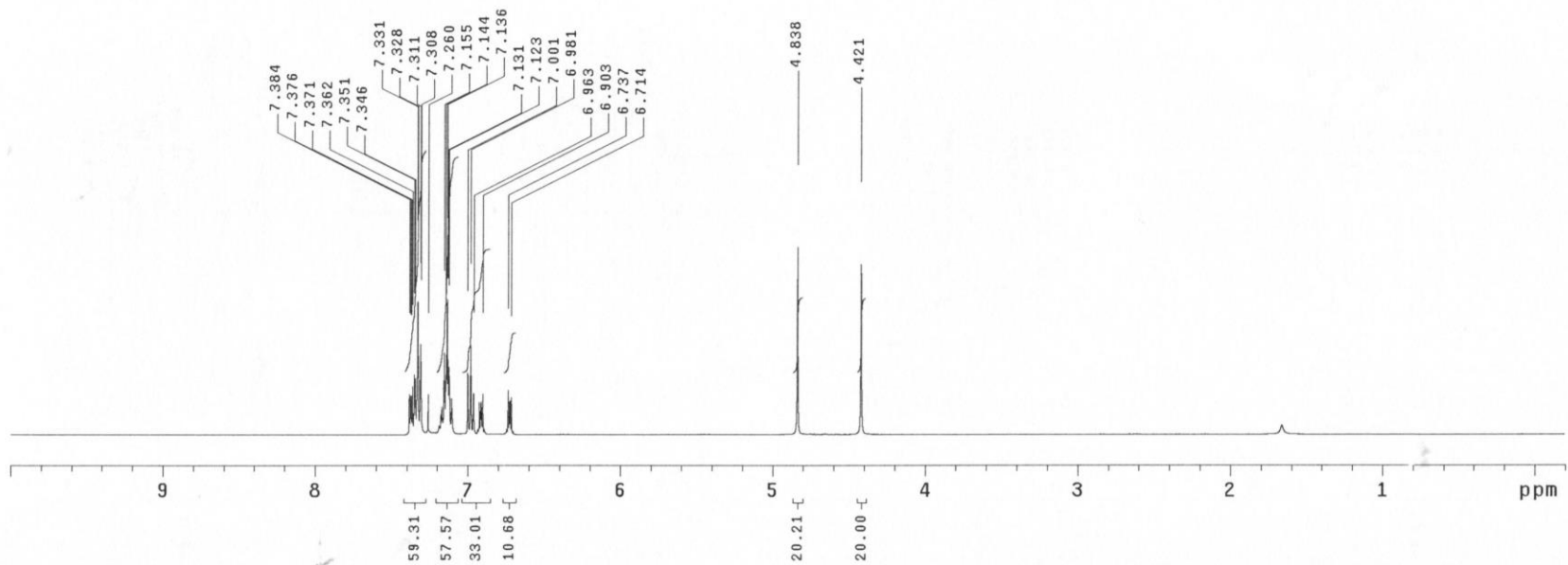
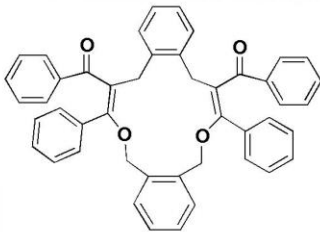
UNITYplus-400 "unity400"

Date: Oct 16 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

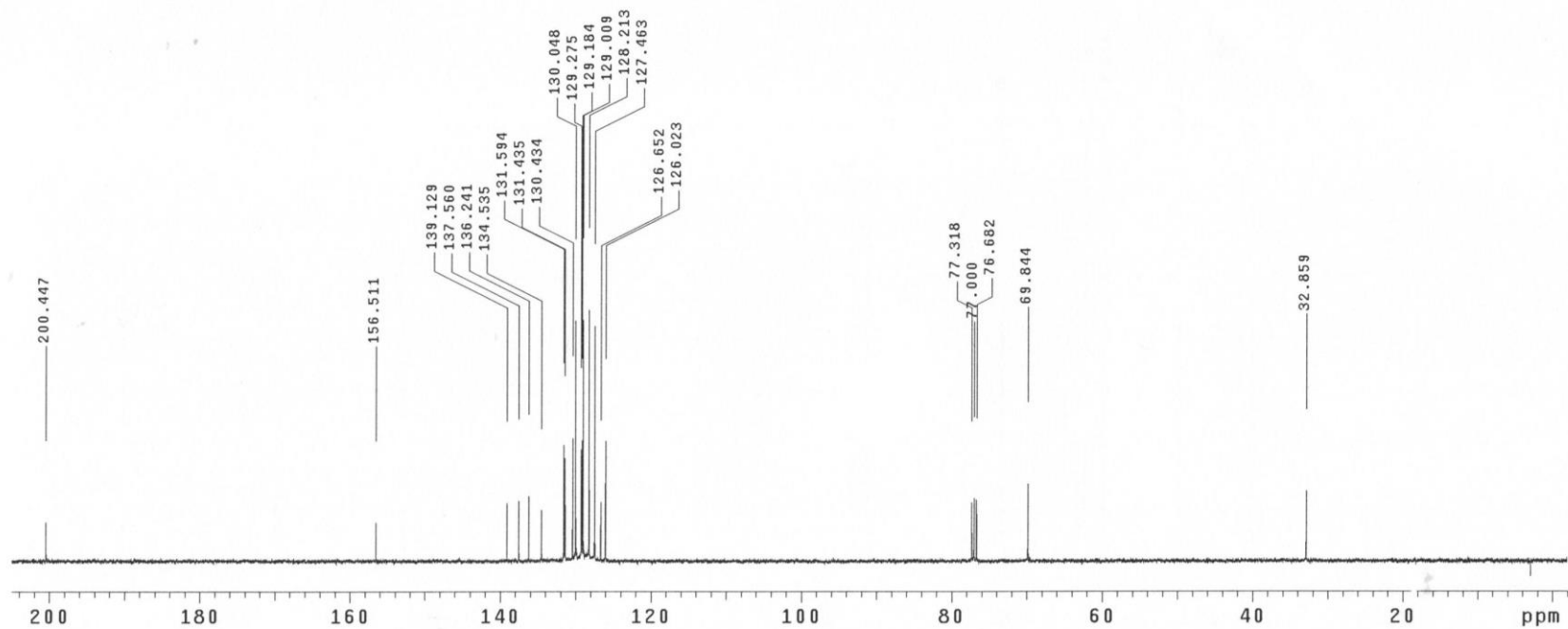
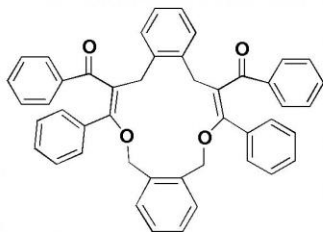
Total 32 repetitions



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

NC0821-14

Pulse Sequence: s2pu1  
UNITYplus-400 "unity400"  
Date: Oct 16 2020  
Solvent: CDCl<sub>3</sub>  
Ambient temperature  
Total 1200 repetitions



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

NC5072

Pulse Sequence: s2pu1

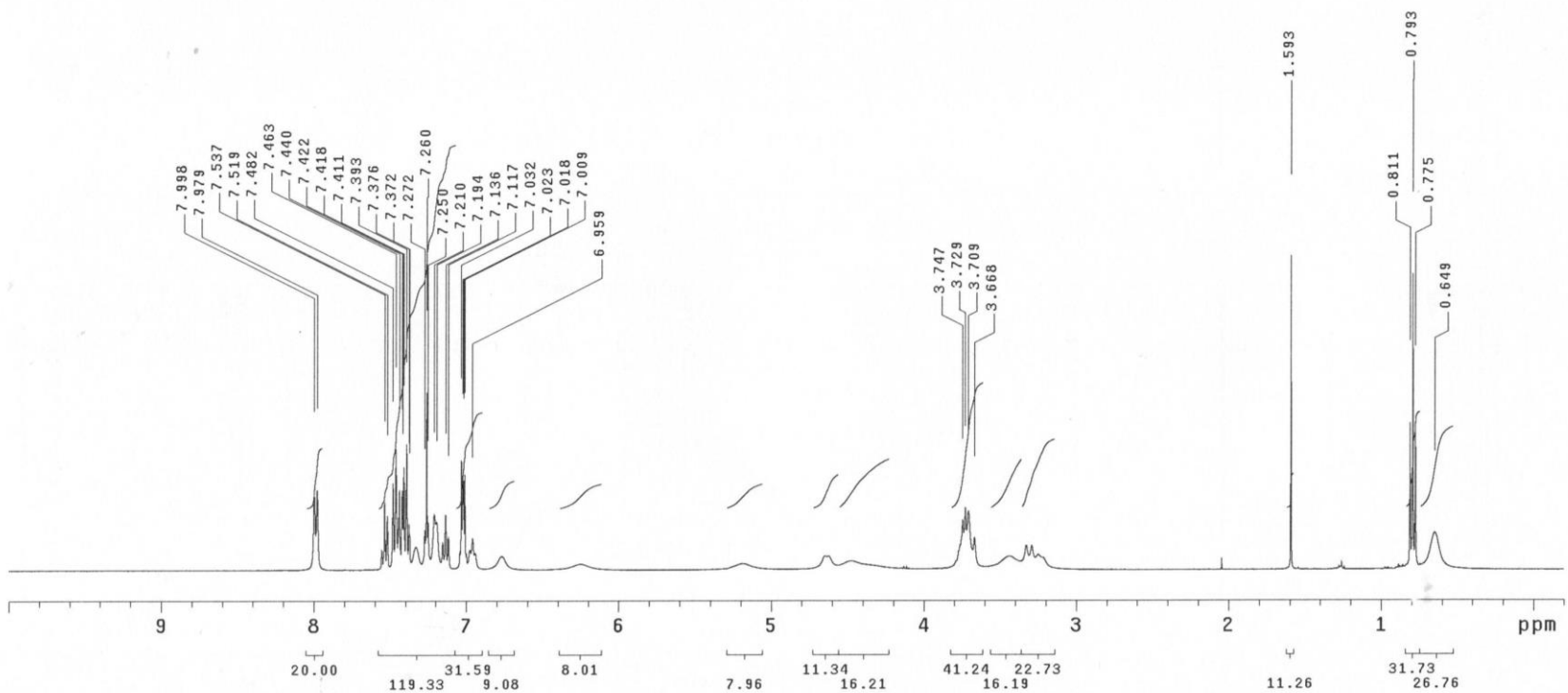
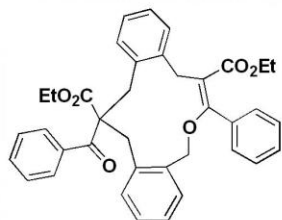
UNITYplus-400 "unity400"

Date: Sep 1 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 32 repetitions





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

NC0903-14

Pulse Sequence: s2pu1

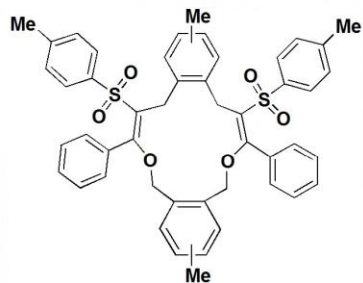
UNITYplus-400 "unity400"

Date: Sep 7 2020

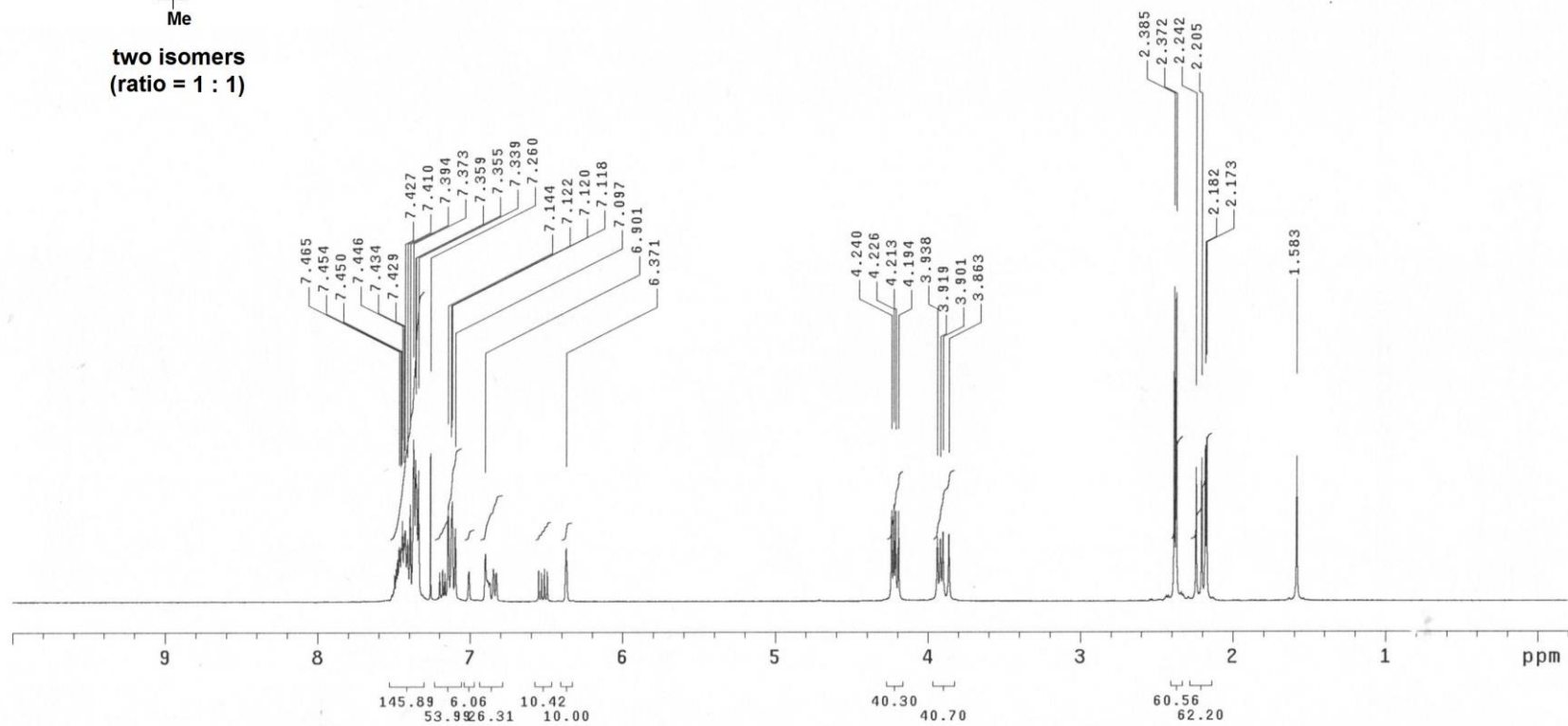
Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 32 repetitions



two isomers  
(ratio = 1 : 1)





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

NC0903-14

Pulse Sequence: s2pu1

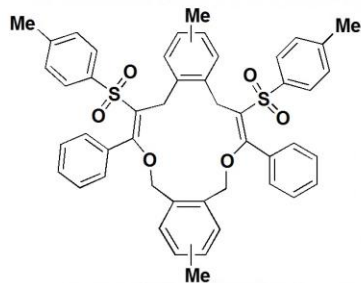
UNITYplus-400 "unity400"

Date: Sep 7 2020

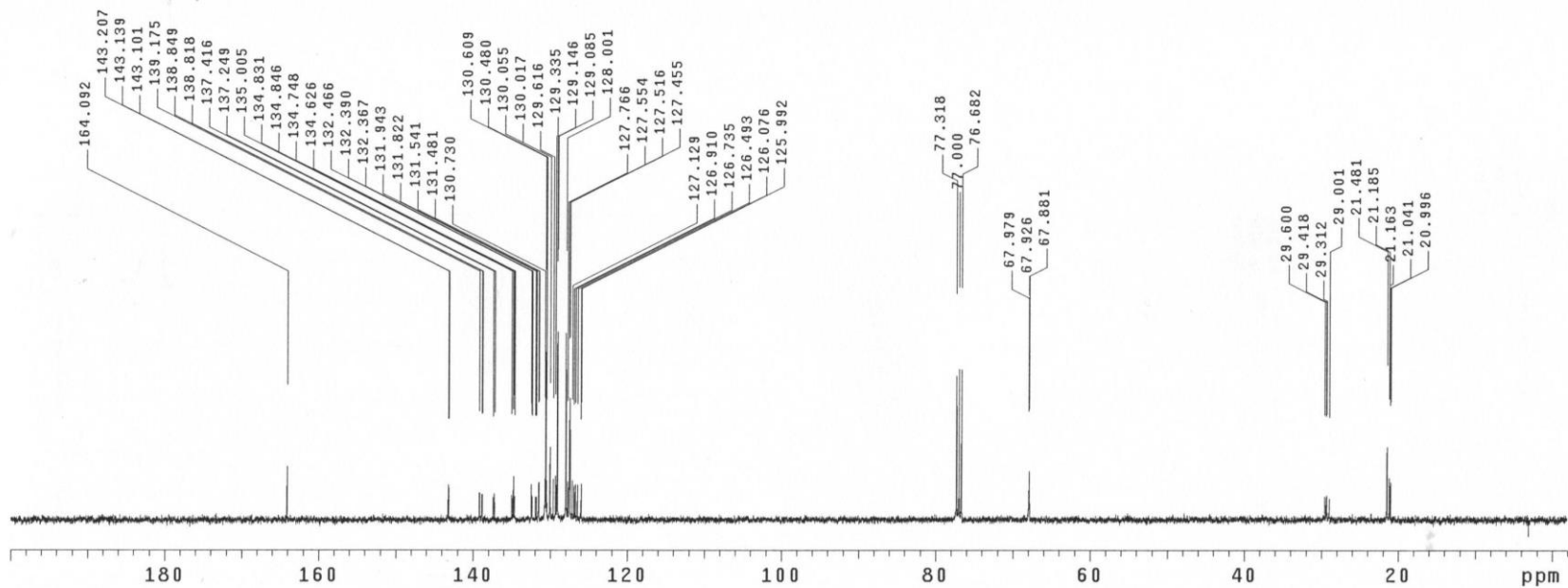
Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 3136 repetitions



two isomers  
(ratio = 1 : 1)



# Compound 12 (<sup>1</sup>H-NMR spectral data)

NC0909-6

Pulse Sequence: s2pu1

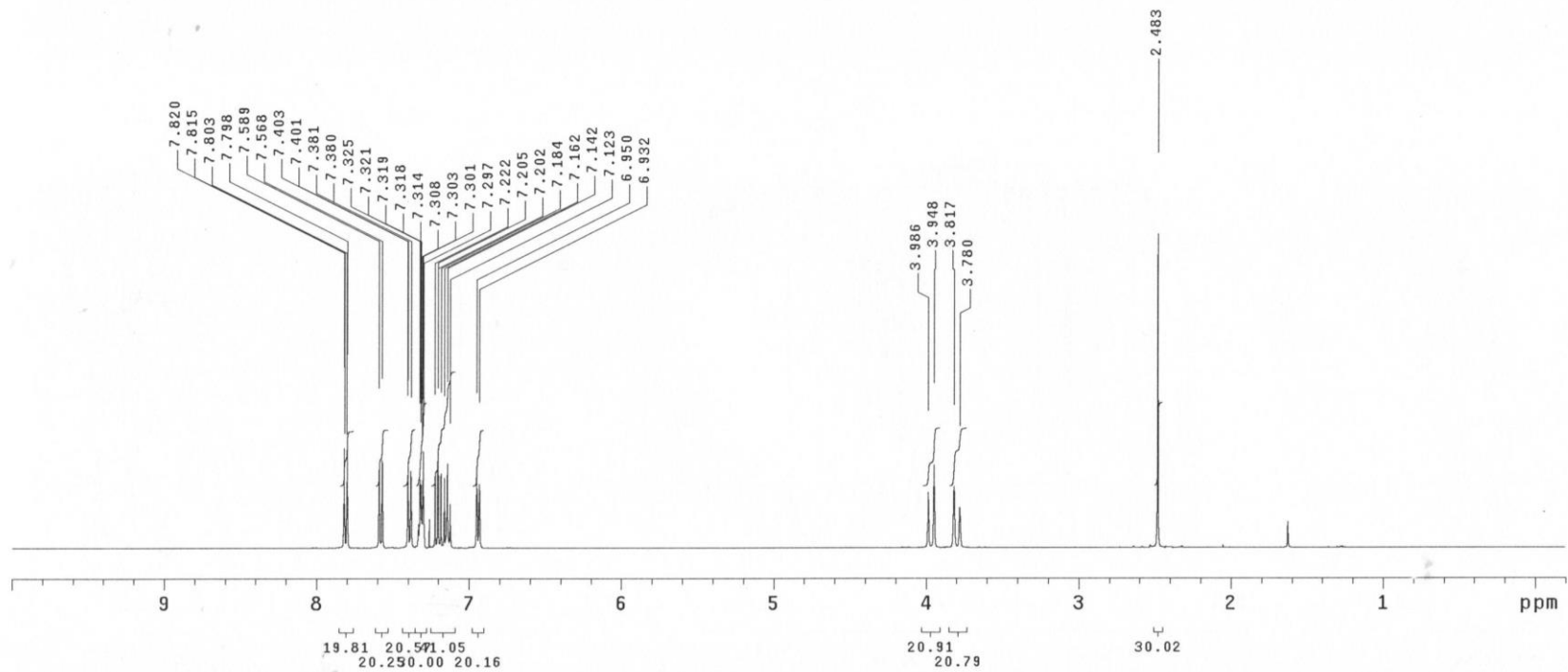
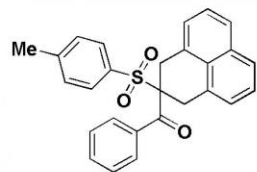
UNITYplus-400 "unity400"

Date: Sep 10 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 32 repetitions



# Compound 12 (<sup>13</sup>C-NMR spectral data)

NC0909-6

Pulse Sequence: s2pu1

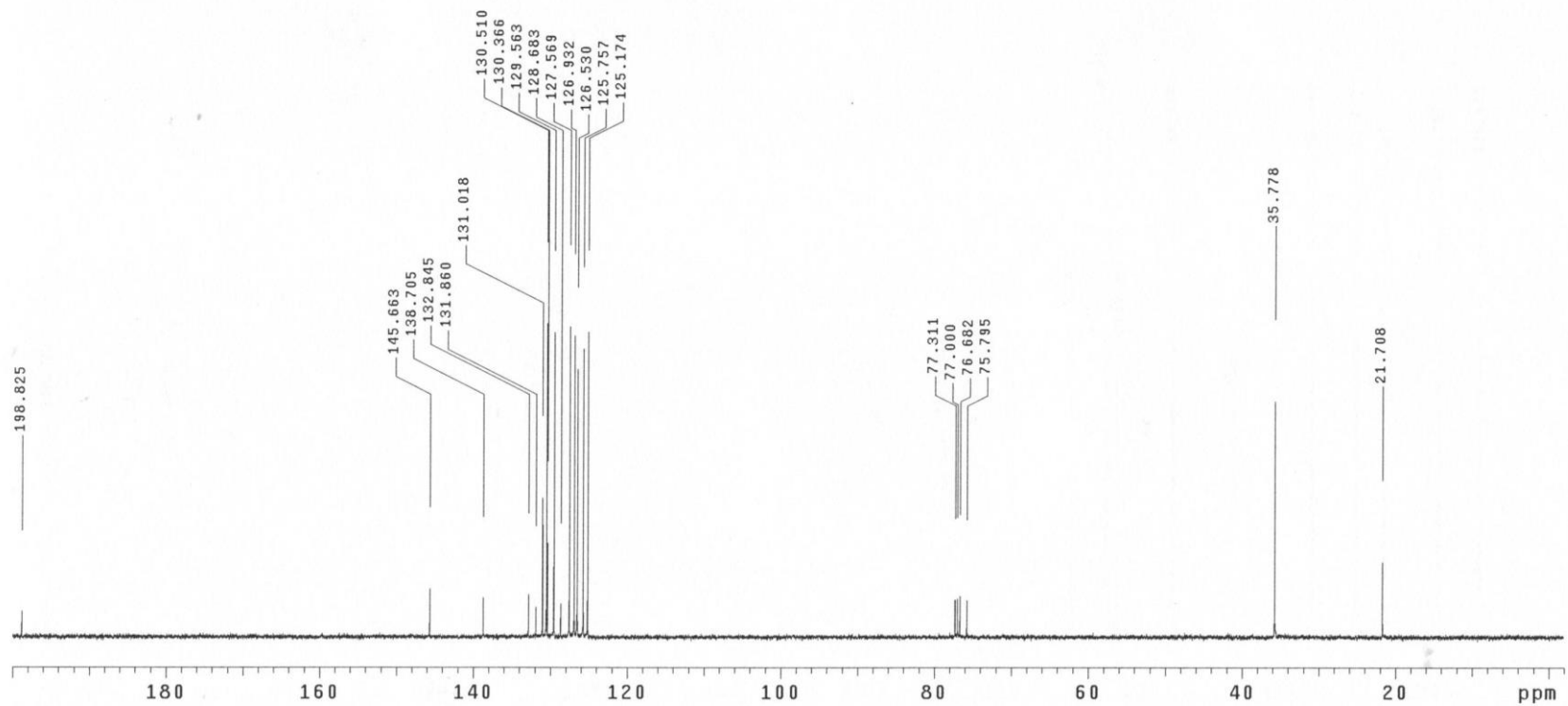
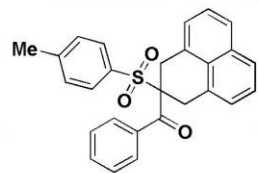
UNITYplus-400 "unity400"

Date: Sep 10 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

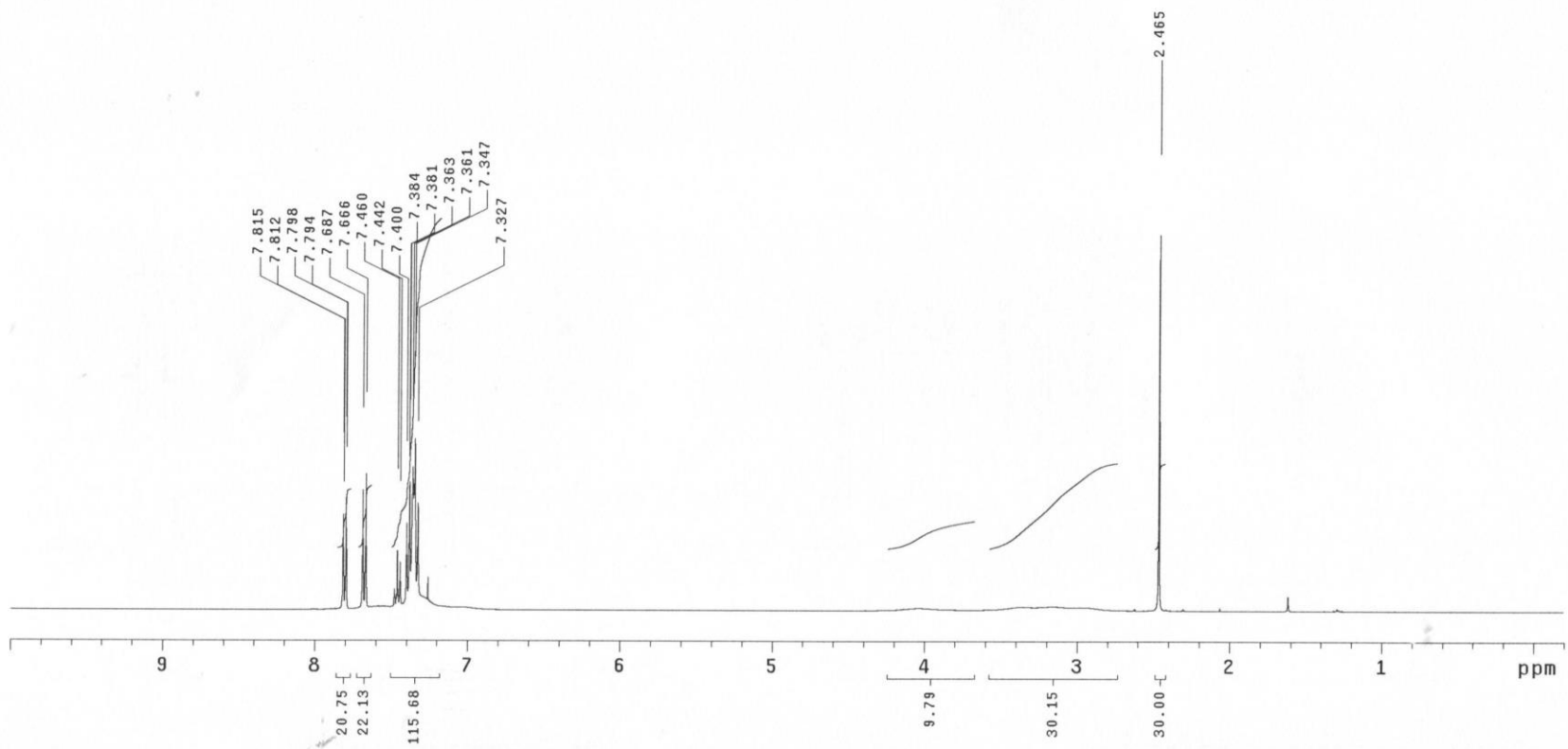
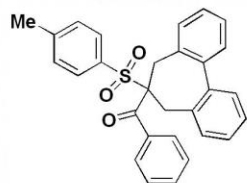
Total 400 repetitions



# Compound 13 (<sup>1</sup>H-NMR spectral data)

NC1015-9

Pulse Sequence: s2pu1  
UNITYplus-400 "unity400"  
Date: Oct 16 2020  
Solvent: CDCl<sub>3</sub>  
Ambient temperature  
Total 32 repetitions



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

NC1015-9

Pulse Sequence: s2pu1

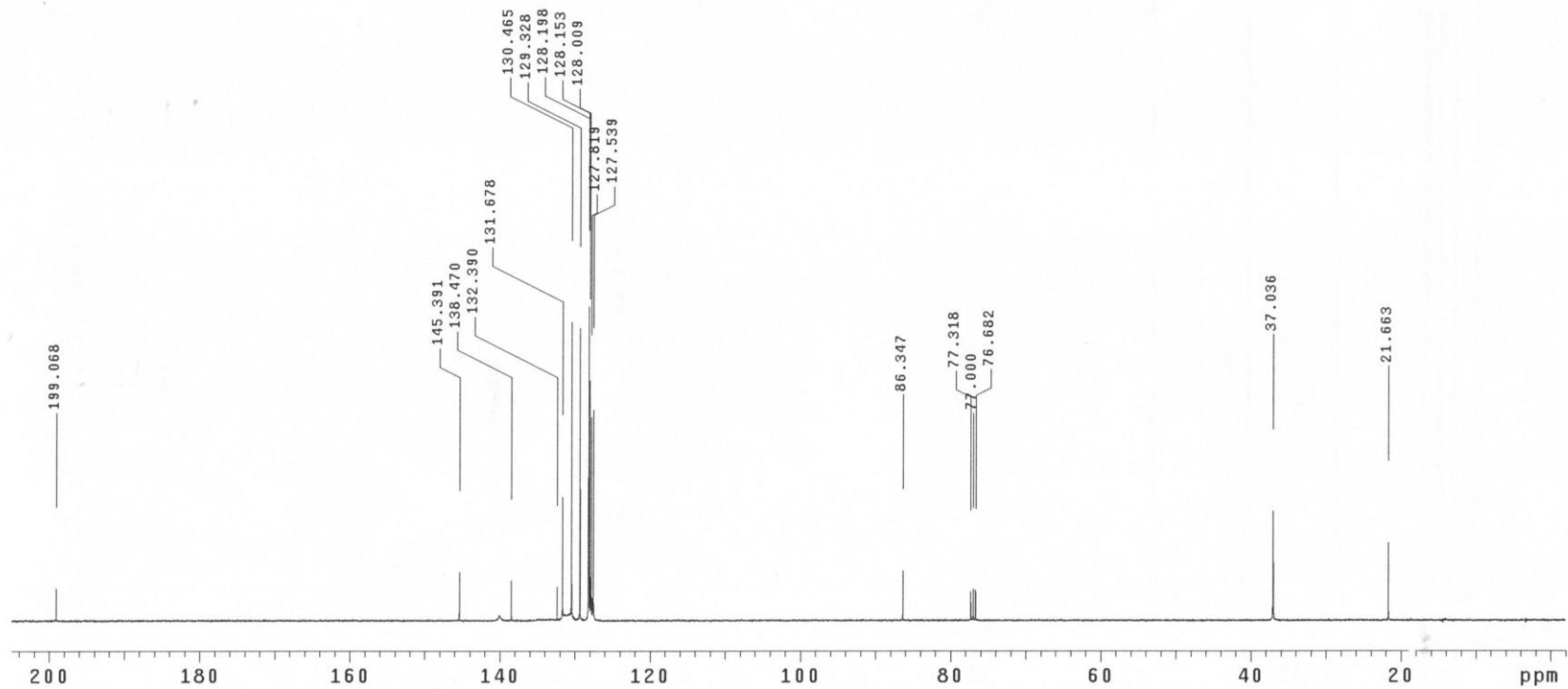
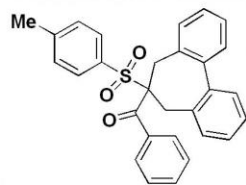
UNITYplus-400 "unity400"

Date: Oct 16 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 2240 repetitions



# Compound 14 (<sup>1</sup>H-NMR spectral data)

NC0907-8

Pulse Sequence: s2pu1

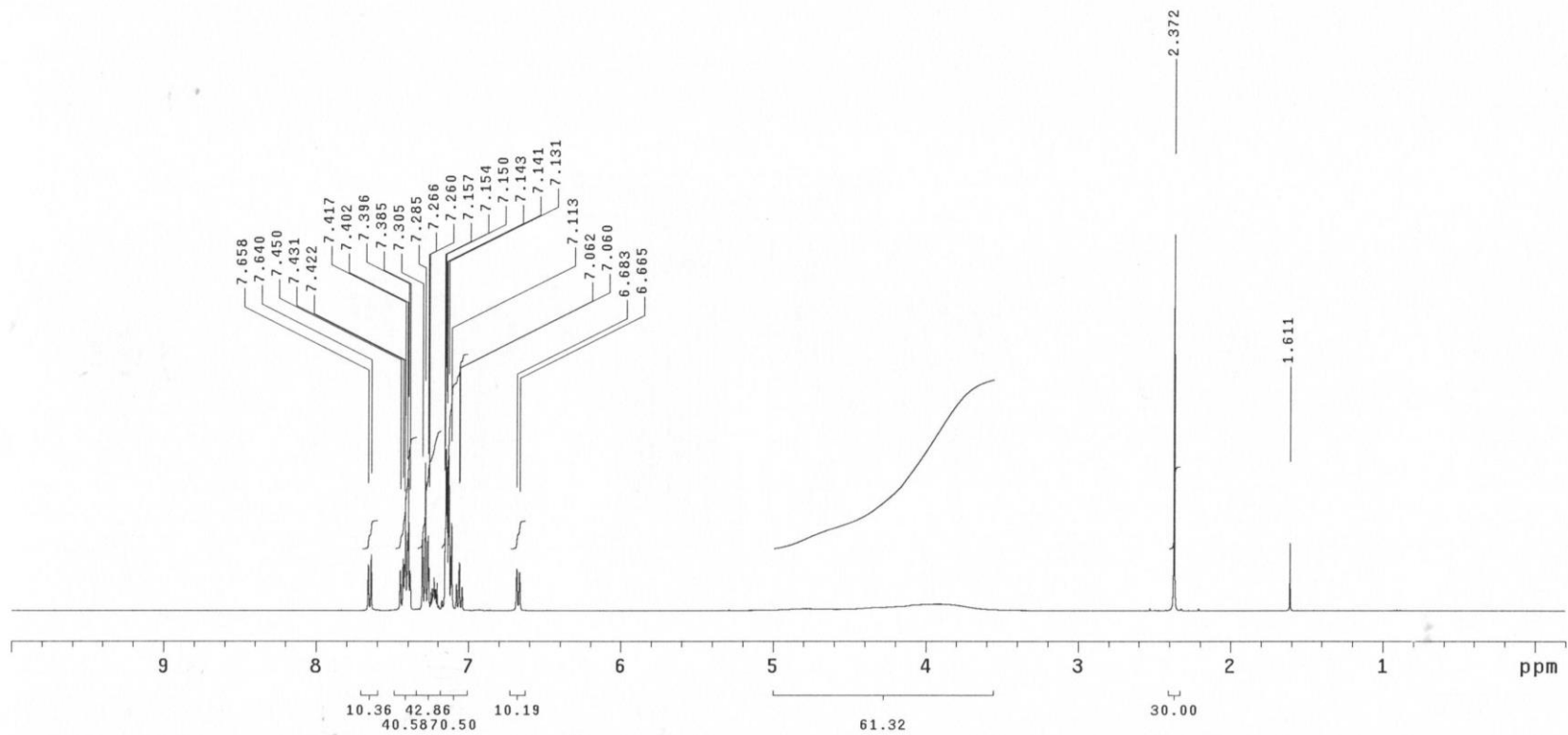
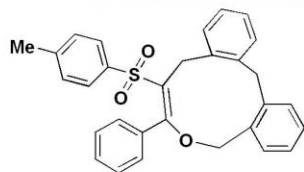
UNITYplus-400 "unity400"

Date: Sep 10 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 32 repetitions



# Compound 14 (<sup>13</sup>C-NMR spectral data)

NC0907-8

Pulse Sequence: s2pu1

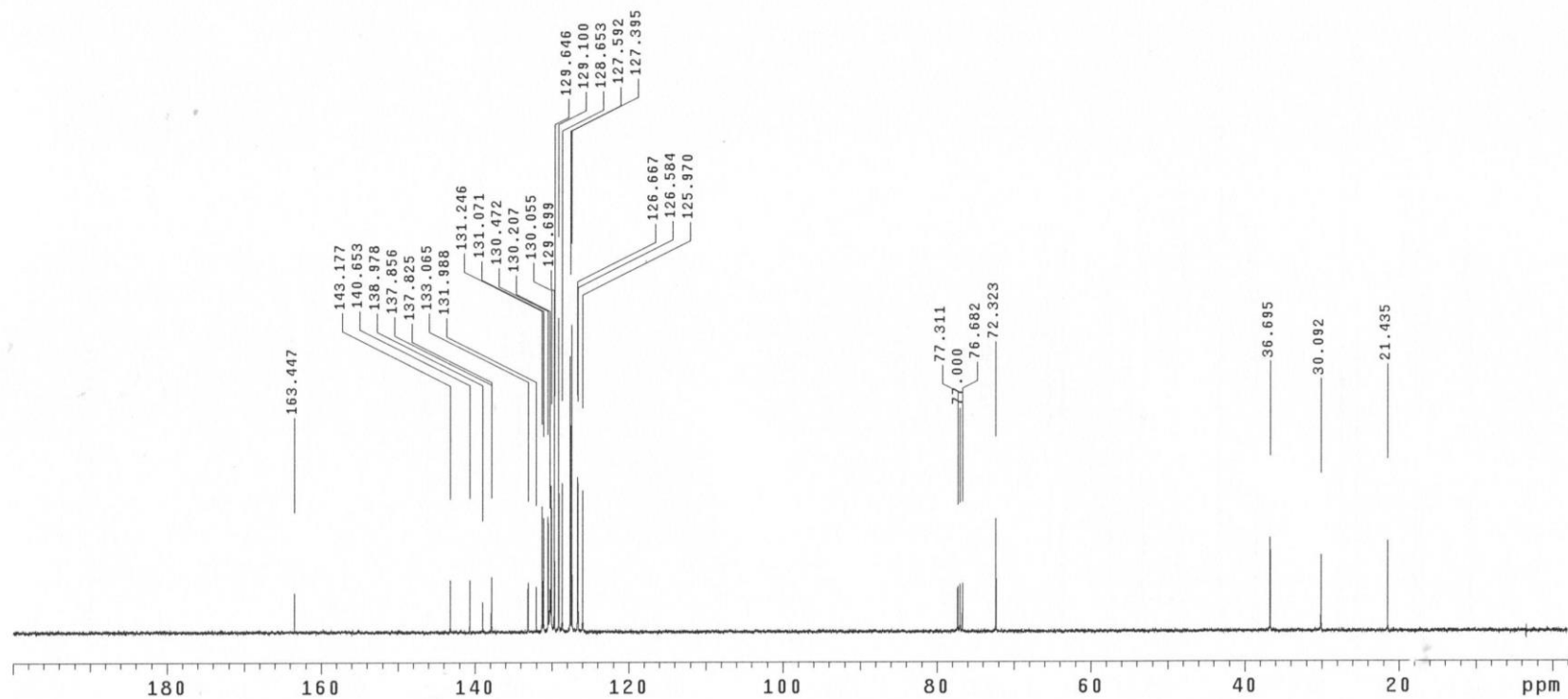
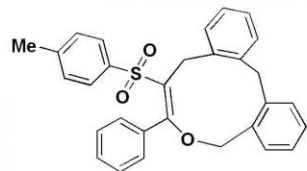
UNITYplus-400 "unity400"

Date: Sep 10 2020

Solvent: CDC13

Ambient temperature

Total 1024 repetitions



# Compound 15 (<sup>1</sup>H-NMR spectral data)

KT04217R

Pulse Sequence: s2pu1

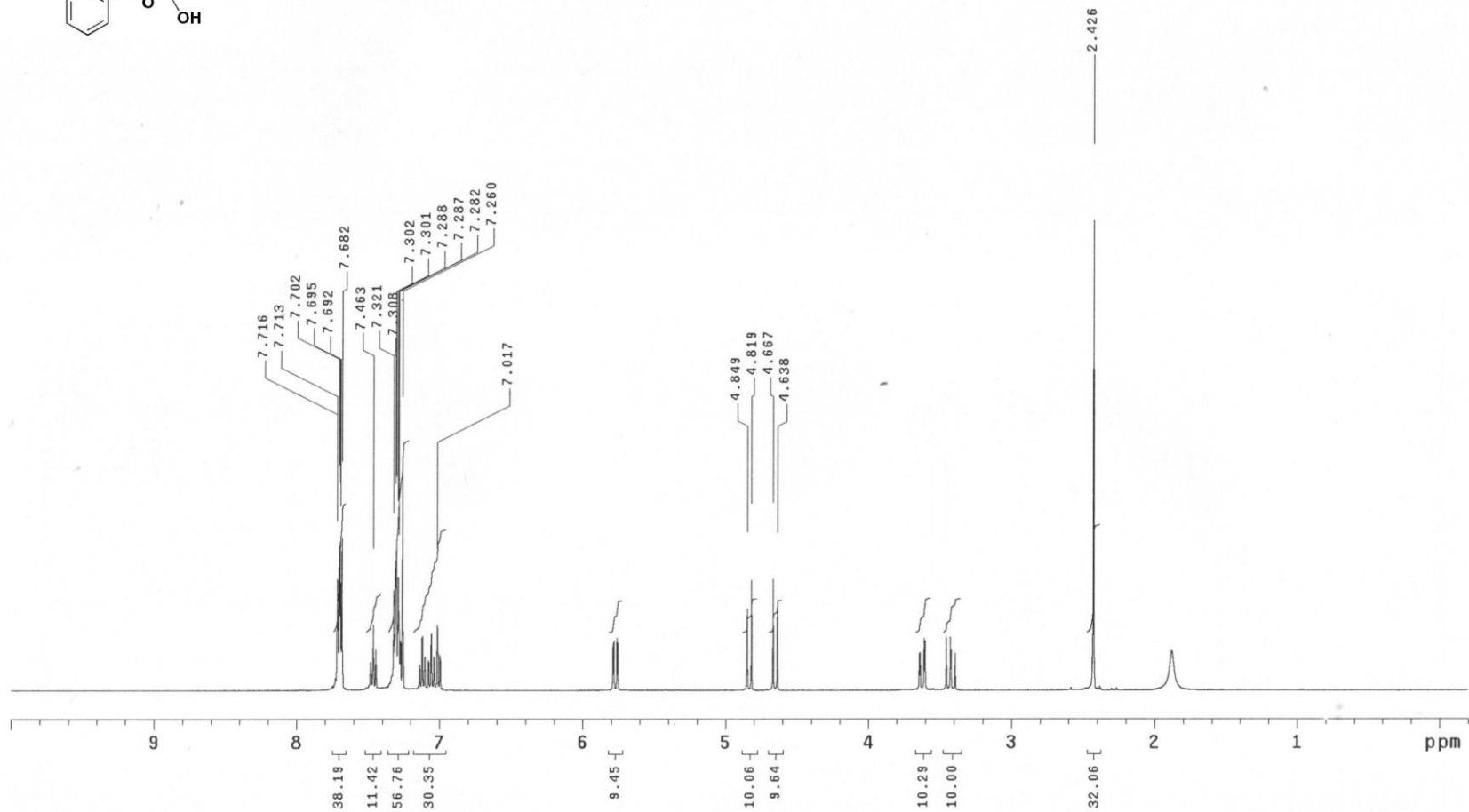
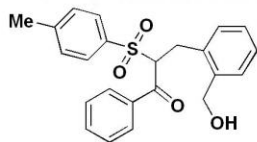
UNITYplus-400 "unity400"

Date: Apr 27 2020

Solvent: CDCl<sub>3</sub>

Ambient temperature

Total 32 repetitions





# Compound 15 (<sup>13</sup>C-NMR spectral data)

KT04217R

Pulse Sequence: s2pu1

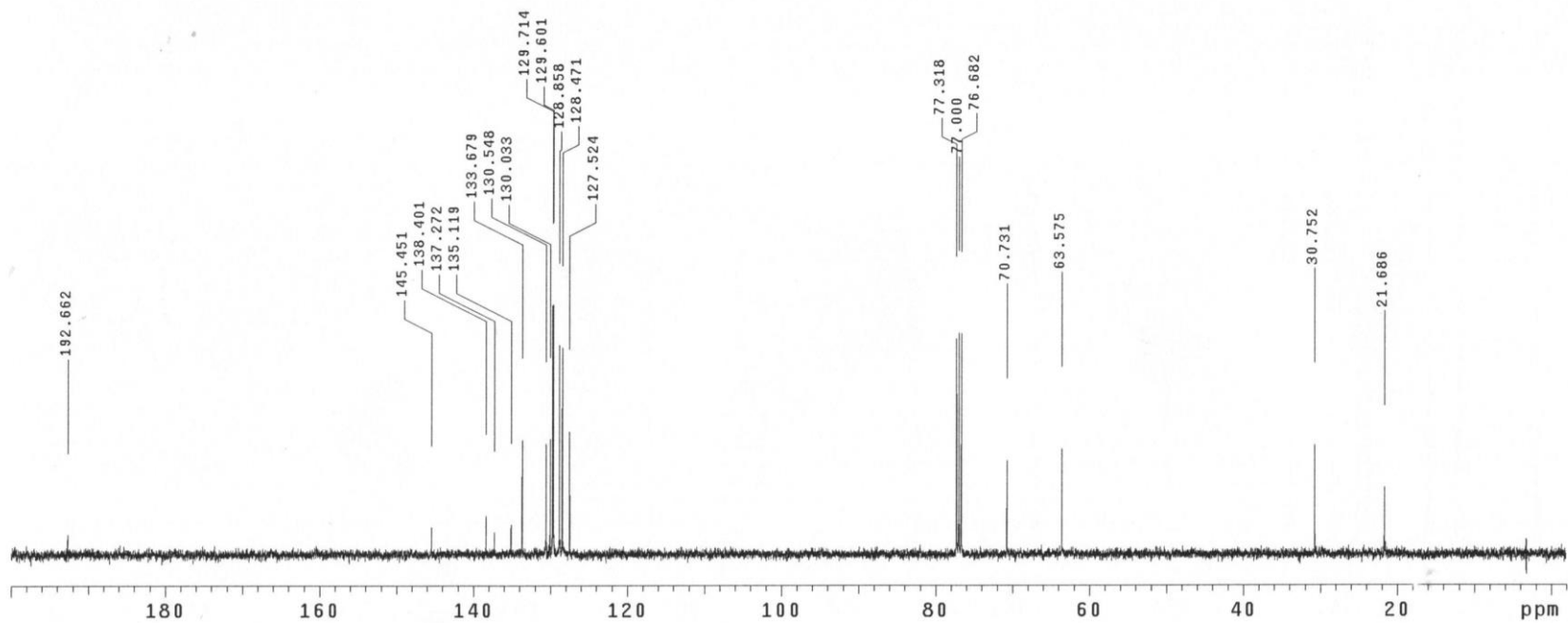
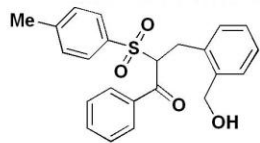
UNITYplus-400 "unity400"

Date: Apr 27 2020

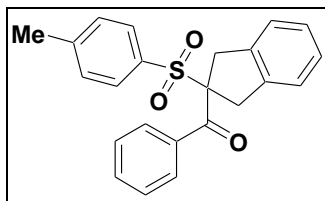
Solvent: CDC13

Ambient temperature

Total 3360 repetitions

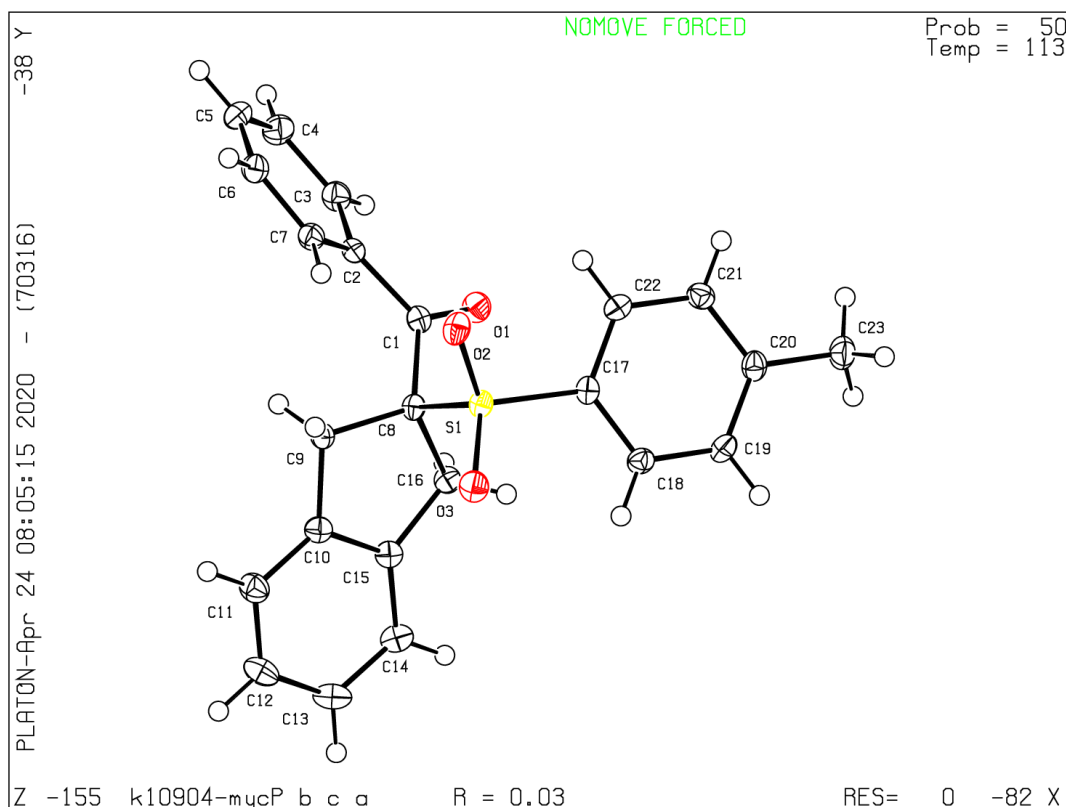


## X-ray crystal data of compound 7a (CCDC 2042099)



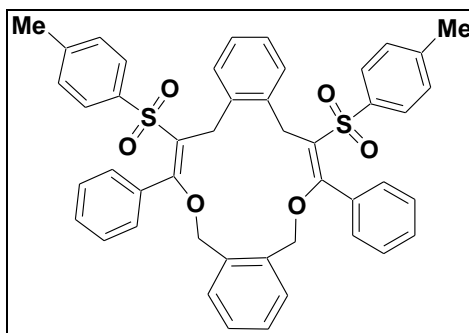
**Sample preparation** : A solution of compound **7a** (30 mg) in CH<sub>2</sub>Cl<sub>2</sub> (10 mL) was placed in a tube (10 mL). EtOAc (2 mL) was added slowly to the vial with a dropper. The vial was closed with little cotton and kept at room temperature for 2 days. Then, colorless prisms were observed.

**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.



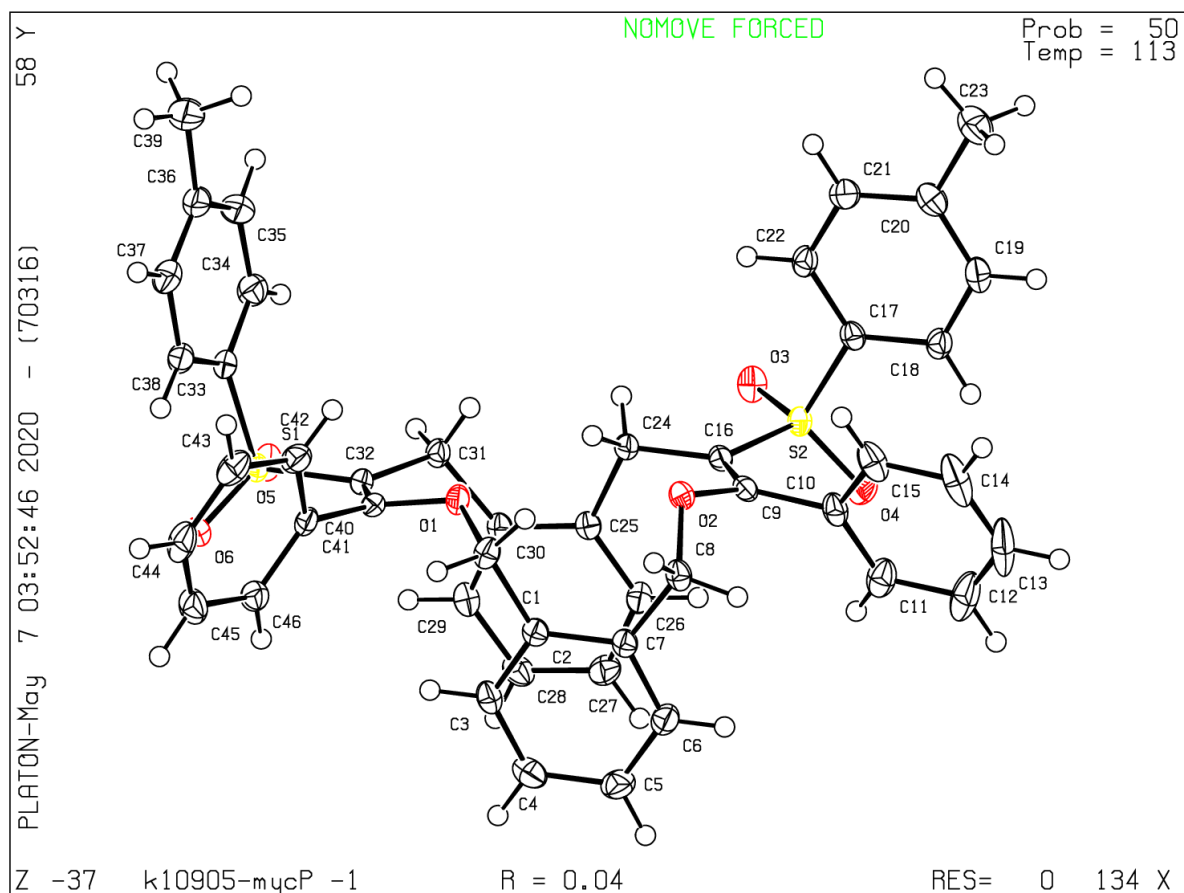
Empirical formula	C <sub>23</sub> H <sub>20</sub> O <sub>3</sub> S
Formula weight	376.45
Temperature/K	113(2)
Crystal system	orthorhombic
Space group	Pbca
a/Å	15.9413(2)
b/Å	11.76610(10)
c/Å	19.6971(2)
α/°	90
β/°	90
γ/°	90
Volume/Å <sup>3</sup>	3694.52(7)
Z	8
ρ <sub>calc</sub> /cm <sup>3</sup>	1.354
μ/mm <sup>-1</sup>	0.196
F(000)	1584.0
Crystal size/mm <sup>3</sup>	0.15 × 0.15 × 0.15
Radiation	Mo Kα (λ = 0.71073)
2θ range for data collection/°	4.136 to 54.116
Index ranges	-20 ≤ h ≤ 19, -14 ≤ k ≤ 13, -24 ≤ l ≤ 25
Reflections collected	73544
Independent reflections	3978 [R <sub>int</sub> = 0.0305, R <sub>sigma</sub> = 0.0132]
Data/restraints/parameters	3978/0/246
Goodness-of-fit on F <sup>2</sup>	1.060
Final R indexes [I ≥ 2σ (I)]	R <sub>1</sub> = 0.0313, wR <sub>2</sub> = 0.0806
Final R indexes [all data]	R <sub>1</sub> = 0.0346, wR <sub>2</sub> = 0.0823
Largest diff. peak/hole / e Å <sup>-3</sup>	0.38/-0.42

## X-ray crystal data of compound 8a (CCDC 2042100)



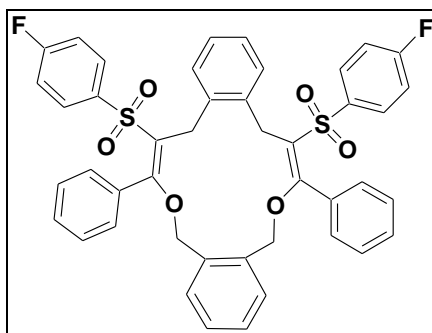
**Sample preparation** : A solution of compound **8a** (30 mg) in CH<sub>2</sub>Cl<sub>2</sub> (10 mL) was placed in a tube (10 mL). EtOAc (2 mL) was added slowly to the vial with a dropper. The vial was closed with little cotton and kept at room temperature for 2 days. Then, colorless prisms were observed.

**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.



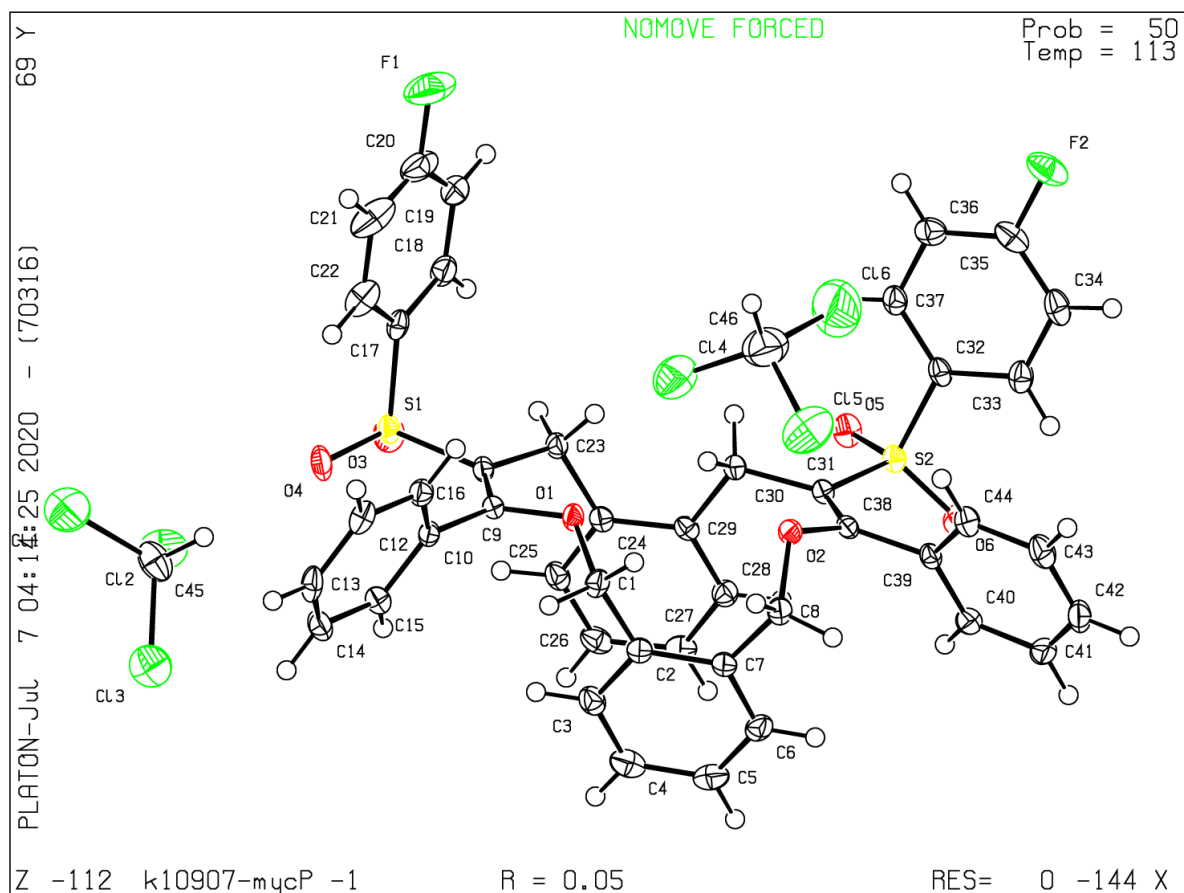
Empirical formula	C <sub>46</sub> H <sub>40</sub> O <sub>6</sub> S <sub>2</sub>
Formula weight	752.90
Temperature/K	113(2)
Crystal system	triclinic
Space group	P-1
a/Å	9.7982(3)
b/Å	13.2829(4)
c/Å	16.3495(4)
α/°	113.228(2)
β/°	99.000(2)
γ/°	97.420(2)
Volume/Å <sup>3</sup>	1888.14(10)
Z	2
ρ <sub>calc</sub> /cm <sup>3</sup>	1.324
μ/mm <sup>-1</sup>	0.192
F(000)	792.0
Crystal size/mm <sup>3</sup>	0.2 × 0.2 × 0.2
Radiation	Mo Kα (λ = 0.71073)
2θ range for data collection/°	4.306 to 54.158
Index ranges	-12 ≤ h ≤ 12, -16 ≤ k ≤ 16, -20 ≤ l ≤ 20
Reflections collected	59934
Independent reflections	7935 [R <sub>int</sub> = 0.0414, R <sub>sigma</sub> = 0.0272]
Data/restraints/parameters	7935/0/490
Goodness-of-fit on F <sup>2</sup>	1.051
Final R indexes [I ≥ 2σ (I)]	R <sub>1</sub> = 0.0367, wR <sub>2</sub> = 0.0968
Final R indexes [all data]	R <sub>1</sub> = 0.0429, wR <sub>2</sub> = 0.1005
Largest diff. peak/hole / e Å <sup>-3</sup>	0.78/-0.41

## X-ray crystal data of compound 8c (CCDC 2042101)



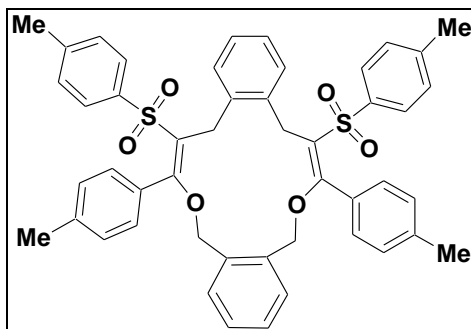
**Sample preparation** : A solution of compound **8c** (30 mg) in CHCl<sub>3</sub> (10 mL) was placed in a tube (10 mL). EtOAc (2 mL) was added slowly to the vial with a dropper. The vial was closed with little cotton and kept at room temperature for 2 days. Then, colorless prisms were observed.

**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.



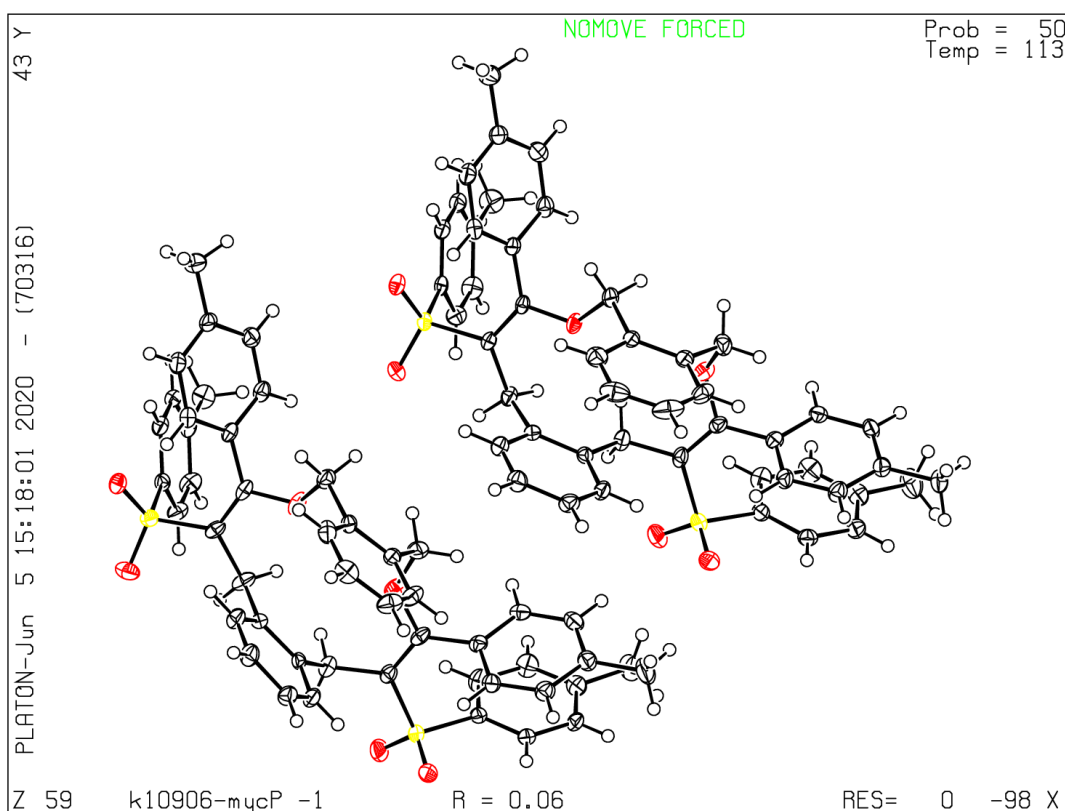
Empirical formula	C <sub>46</sub> H <sub>36</sub> Cl <sub>6</sub> F <sub>2</sub> O <sub>6</sub> S <sub>2</sub>
Formula weight	999.57
Temperature/K	113(2)
Crystal system	triclinic
Space group	P-1
a/Å	10.35170(10)
b/Å	14.6496(2)
c/Å	16.2001(3)
α/°	85.3580(10)
β/°	75.2910(10)
γ/°	69.7540(10)
Volume/Å <sup>3</sup>	2229.33(6)
Z	2
ρ <sub>calc</sub> /cm <sup>3</sup>	1.489
μ/mm <sup>-1</sup>	0.537
F(000)	1024.0
Crystal size/mm <sup>3</sup>	0.25 × 0.2 × 0.2
Radiation	Mo Kα (λ = 0.71073)
2θ range for data collection/°	3.926 to 54.106
Index ranges	-13 ≤ h ≤ 13, -18 ≤ k ≤ 17, -20 ≤ l ≤ 20
Reflections collected	55235
Independent reflections	9369 [R <sub>int</sub> = 0.0284, R <sub>sigma</sub> = 0.0244]
Data/restraints/parameters	9369/0/559
Goodness-of-fit on F <sup>2</sup>	1.053
Final R indexes [I ≥ 2σ (I)]	R <sub>1</sub> = 0.0484, wR <sub>2</sub> = 0.1337
Final R indexes [all data]	R <sub>1</sub> = 0.0525, wR <sub>2</sub> = 0.1374
Largest diff. peak/hole / e Å <sup>-3</sup>	0.83/-1.29

## X-ray crystal data of compound 8m (CCDC 2042102)



**Sample preparation** : A solution of compound **8m** (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.



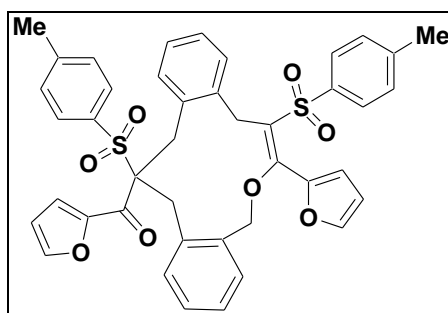


Empirical formula	C <sub>11.29</sub> H <sub>10.35</sub> O <sub>1.41</sub> S <sub>0.47</sub>
Formula weight	183.75
Temperature/K	113(2)
Crystal system	triclinic
Space group	P-1
a/Å	14.1278(3)
b/Å	16.6555(3)
c/Å	17.1139(3)
α/°	85.246(2)
β/°	87.858(2)
γ/°	74.443(2)
Volume/Å <sup>3</sup>	3865.64(13)
Z	17
ρ <sub>calc</sub> /g/cm <sup>3</sup>	1.342
μ/mm <sup>-1</sup>	0.190
F(000)	1648.0
Crystal size/mm <sup>3</sup>	0.3 × 0.3 × 0.3
Radiation	Mo Kα (λ = 0.71073)
2θ range for data collection/°	3.992 to 54.144
Index ranges	-17 ≤ h ≤ 17, -21 ≤ k ≤ 21, -21 ≤ l ≤ 20
Reflections collected	84580
Independent reflections	16148 [R <sub>int</sub> = 0.0484, R <sub>sigma</sub> = 0.0513]
Data/restraints/parameters	16148/0/1017
Goodness-of-fit on F <sup>2</sup>	1.060
Final R indexes [I ≥ 2σ (I)]	R <sub>1</sub> = 0.0579, wR <sub>2</sub> = 0.1527
Final R indexes [all data]	R <sub>1</sub> = 0.0779, wR <sub>2</sub> = 0.1630
Largest diff. peak/hole / e Å <sup>-3</sup>	1.17/-0.62



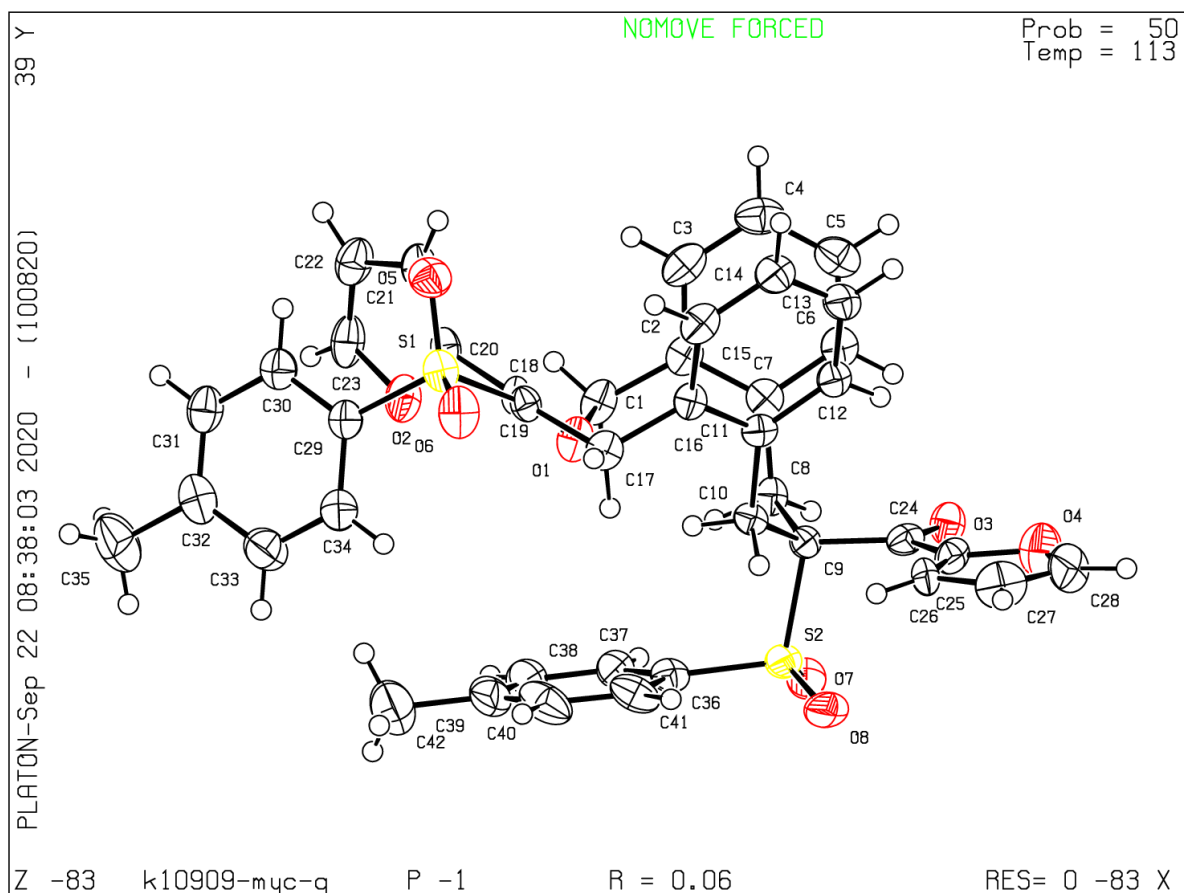
Identification code	K10906-MYC-A
Empirical formula	C <sub>40</sub> H <sub>38</sub> O <sub>6</sub> S <sub>2</sub>
Formula weight	678.82
Temperature/K	113(2)
Crystal system	triclinic
Space group	P-1
a/Å	10.30720(10)
b/Å	14.2750(3)
c/Å	15.3721(4)
α/°	62.701(2)
β/°	86.646(2)
γ/°	73.3530(10)
Volume/Å <sup>3</sup>	1918.57(7)
Z	2
ρ <sub>calc</sub> /cm <sup>3</sup>	1.175
μ/mm <sup>-1</sup>	0.182
F(000)	716.0
Crystal size/mm <sup>3</sup>	0.2 × 0.2 × 0.15
Radiation	Mo Kα (λ = 0.71073)
2θ range for data collection/°	3.308 to 54.01
Index ranges	-12 ≤ h ≤ 13, -18 ≤ k ≤ 17, -19 ≤ l ≤ 19
Reflections collected	43823
Independent reflections	7990 [R <sub>int</sub> = 0.0359, R <sub>sigma</sub> = 0.0327]
Data/restraints/parameters	7990/0/437
Goodness-of-fit on F <sup>2</sup>	1.066
Final R indexes [I ≥ 2σ (I)]	R <sub>1</sub> = 0.0566, wR <sub>2</sub> = 0.1609
Final R indexes [all data]	R <sub>1</sub> = 0.0699, wR <sub>2</sub> = 0.1681
Largest diff. peak/hole / e Å <sup>-3</sup>	0.51/-0.39

## X-ray crystal data of compound 8x-1 (CCDC 2042104)



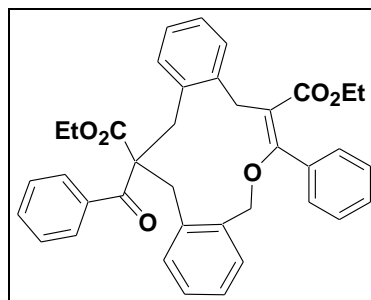
**Sample preparation** : A solution of compound **8x-1** (30 mg) in CH<sub>2</sub>Cl<sub>2</sub> (10 mL) was placed in a tube (10 mL). EtOAc (2 mL) was added slowly to the vial with a dropper. The vial was closed with little cotton and kept at room temperature for 2 days. Then, colorless prisms were 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.



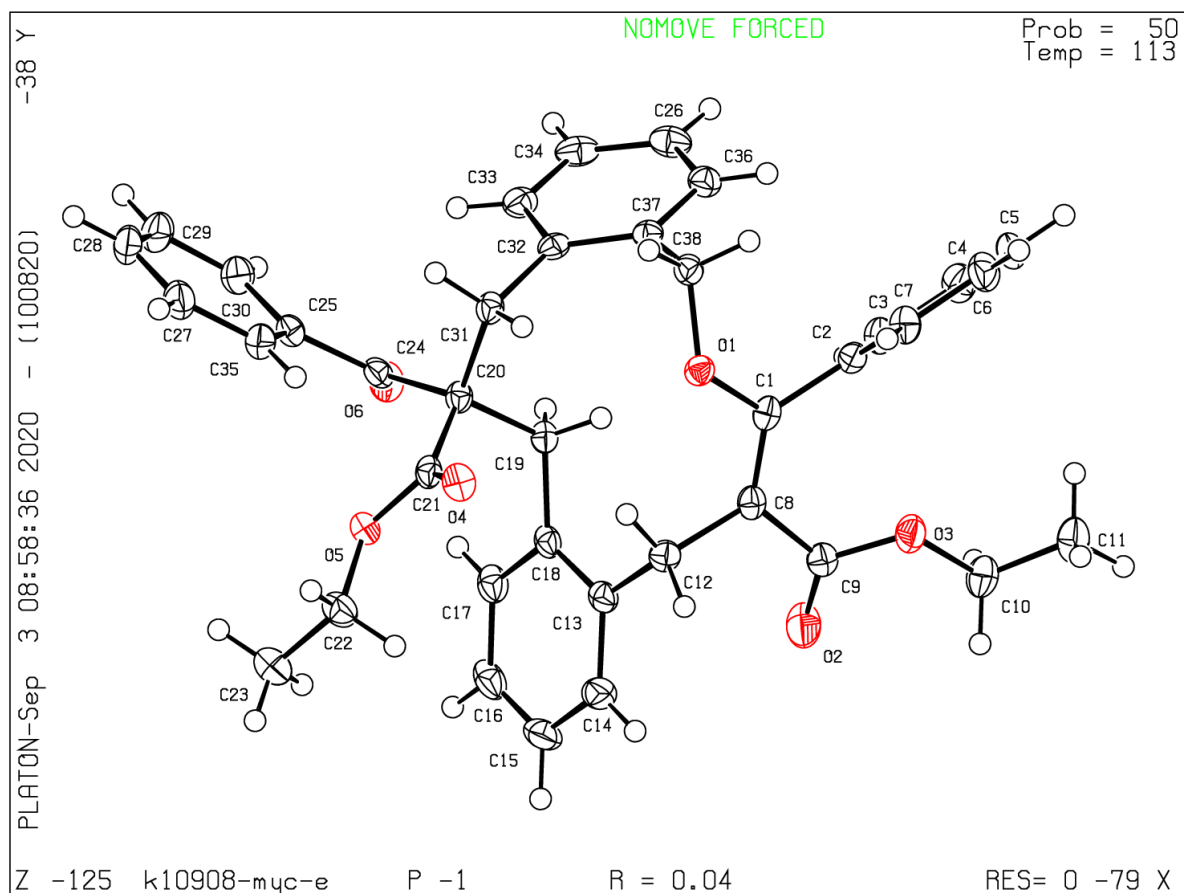
Empirical formula	C42 H36 O8 S2	
Formula weight	732.83	
Temperature	113(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 11.1955(4) Å	$\alpha = 91.424(3)^\circ$ .
	b = 13.5009(6) Å	$\beta = 109.342(4)^\circ$ .
	c = 14.0064(6) Å	$\gamma = 107.452(4)^\circ$ .
Volume	1887.39(15) Å <sup>3</sup>	
Z	2	
Density (calculated)	1.289 Mg/m <sup>3</sup>	
Absorption coefficient	0.194 mm <sup>-1</sup>	
F(000)	768	
Crystal size	0.5 x 0.3 x 0.3 mm <sup>3</sup>	
Theta range for data collection	1.596 to 24.999°.	
Index ranges	-13<=h<=13, -16<=k<=16, -16<=l<=16	
Reflections collected	38013	
Independent reflections	6626 [R(int) = 0.0753]	
Completeness to theta = 24.999°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.75448	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	6626 / 303 / 482	
Goodness-of-fit on F <sup>2</sup>	1.059	
Final R indices [I>2sigma(I)]	R1 = 0.0623, wR2 = 0.1425	
R indices (all data)	R1 = 0.0897, wR2 = 0.1520	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.290 and -0.375 e.Å <sup>-3</sup>	

## X-ray crystal data of compound 8ab-1 (CCDC 2042105)



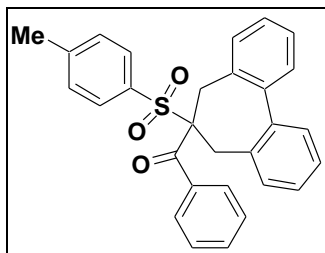
**Sample preparation** : A solution of compound **8ab-1** (30 mg) in CH<sub>2</sub>Cl<sub>2</sub> (10 mL) was placed in a tube (10 mL). EtOAc (2 mL) was added slowly to the vial with a dropper. The vial was closed with little cotton and kept at room temperature for 2 days. Then, colorless prisms were 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.



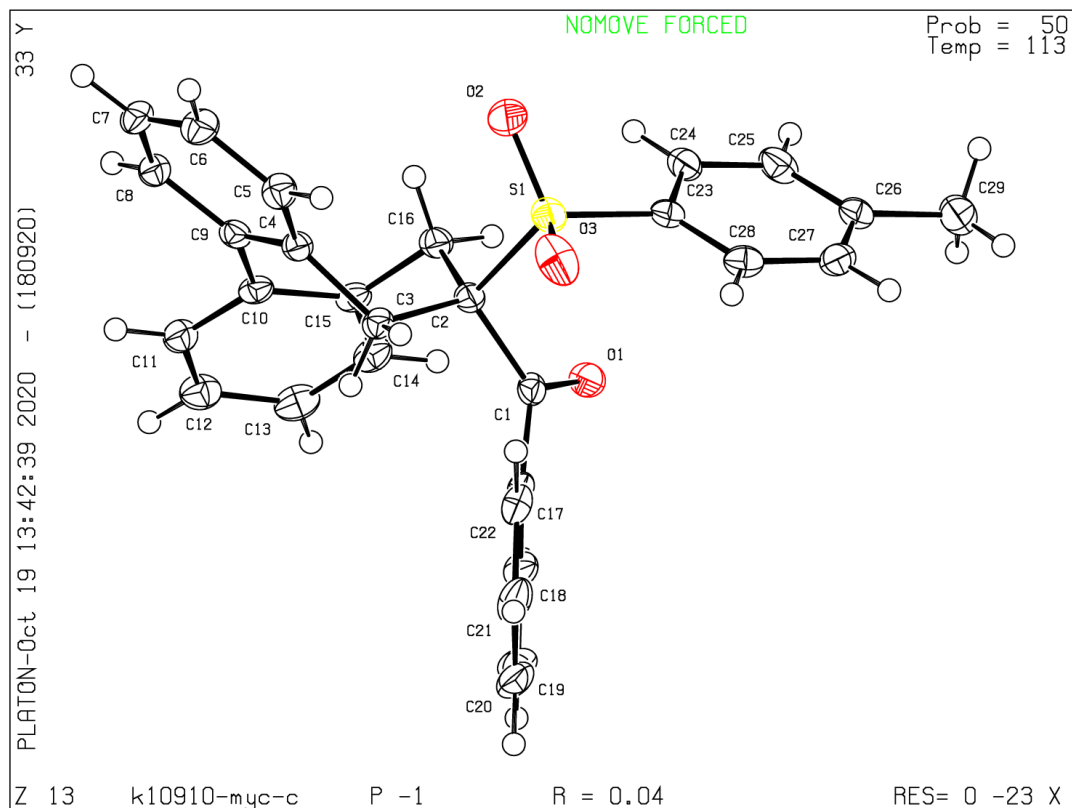
Empirical formula	C38 H36 O6
Formula weight	588.67
Temperature	113(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	$\alpha = 9.1316(2) \text{ \AA}$ $a = 106.306(2)^\circ$ . $\beta = 12.7947(3) \text{ \AA}$ $b = 107.568(2)^\circ$ . $\gamma = 14.4860(4) \text{ \AA}$ $g = 98.437(2)^\circ$ .
Volume	1498.27(7) Å <sup>3</sup>
Z	2
Density (calculated)	1.305 Mg/m <sup>3</sup>
Absorption coefficient	0.087 mm <sup>-1</sup>
F(000)	624
Crystal size	0.5 x 0.3 x 0.3 mm <sup>3</sup>
Theta range for data collection	2.360 to 27.050°.
Index ranges	-11<=h<=11, -16<=k<=16, -18<=l<=18
Reflections collected	37071
Independent reflections	6264 [R(int) = 0.0695]
Completeness to theta = 25.242°	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.83308
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	6264 / 0 / 399
Goodness-of-fit on F <sup>2</sup>	1.116
Final R indices [I>2sigma(I)]	R1 = 0.0413, wR2 = 0.1025
R indices (all data)	R1 = 0.0542, wR2 = 0.1081
Extinction coefficient	n/a
Largest diff. peak and hole	0.285 and -0.245 e.Å <sup>-3</sup>

## X-ray crystal data of compound 13 (CCDC 2042106)



**Sample preparation** : A solution of compound **13** (30 mg) in  $\text{CH}_2\text{Cl}_2$  (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.

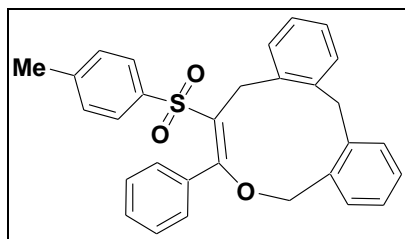
**Crystal measurement** : X-ray crystal structures were determined with a Bruker Enraf-Nonius single-crystal diffractometer (CAD4, Kappa CCD). Thermal ellipsoids are drawn at 50% probability level.





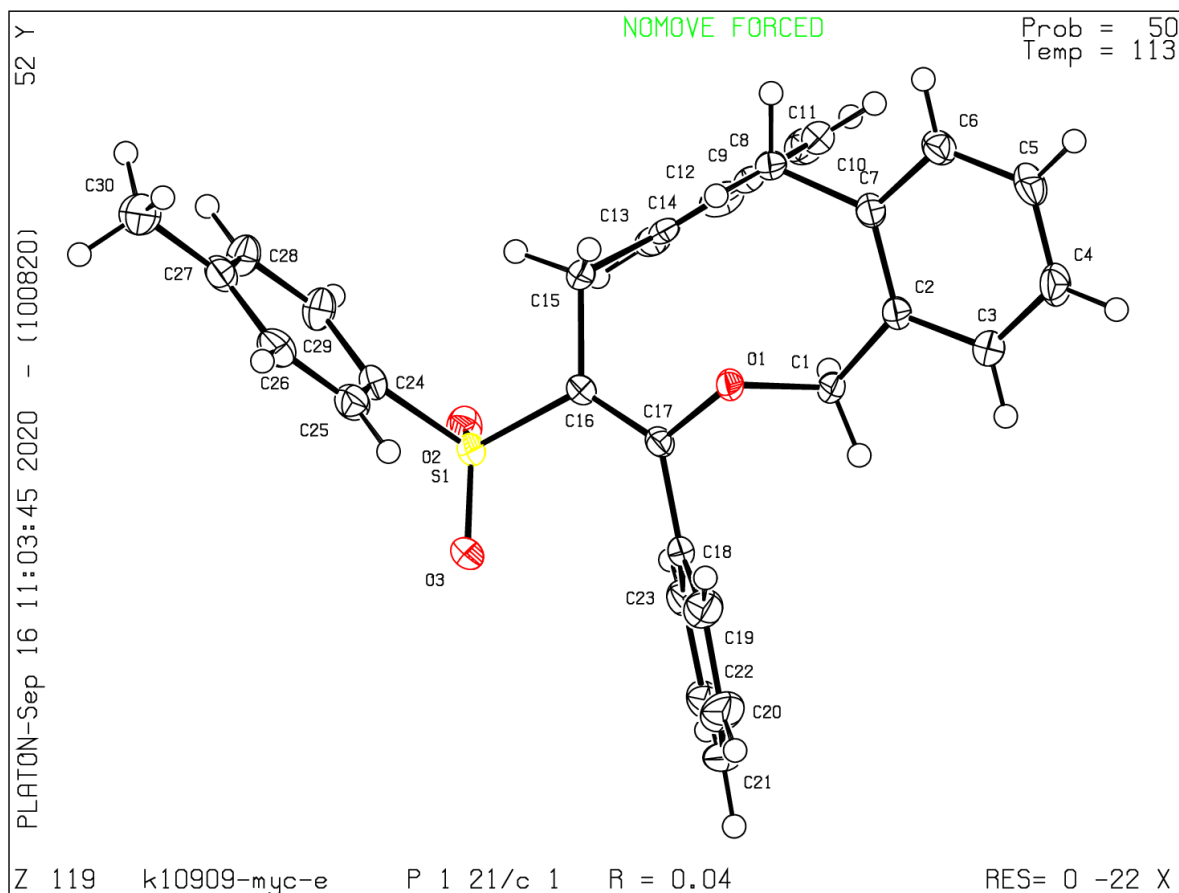
Empirical formula	C <sub>29</sub> H <sub>24</sub> O <sub>3</sub> S
Formula weight	452.54
Temperature/K	113(2)
Crystal system	triclinic
Space group	P-1
a/Å	9.6718(3)
b/Å	10.5127(2)
c/Å	12.8470(3)
α/°	113.403(2)
β/°	103.061(2)
γ/°	99.138(2)
Volume/Å <sup>3</sup>	1121.72(5)
Z	2
ρ <sub>calc</sub> /cm <sup>3</sup>	1.340
μ/mm <sup>-1</sup>	0.174
F(000)	476.0
Crystal size/mm <sup>3</sup>	0.3 × 0.25 × 0.2
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	4.264 to 49.998
Index ranges	-11 ≤ h ≤ 11, -12 ≤ k ≤ 12, -15 ≤ l ≤ 14
Reflections collected	32987
Independent reflections	3958 [R <sub>int</sub> = 0.0599, R <sub>sigma</sub> = 0.0295]
Data/restraints/parameters	3958/0/299
Goodness-of-fit on F <sup>2</sup>	1.056
Final R indexes [I ≥ 2σ (I)]	R <sub>1</sub> = 0.0359, wR <sub>2</sub> = 0.0941
Final R indexes [all data]	R <sub>1</sub> = 0.0398, wR <sub>2</sub> = 0.0970
Largest diff. peak/hole / e Å <sup>-3</sup>	0.26/-0.46

## X-ray crystal data of compound 14 (CCDC 2042107)



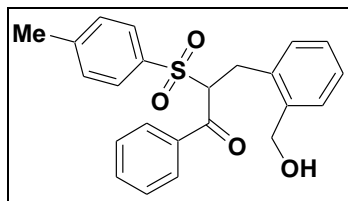
**Sample preparation** : A solution of compound **14** (30 mg) in CH<sub>2</sub>Cl<sub>2</sub> (10 mL) was placed in a tube (10 mL). EtOAc (2 mL) was added slowly to the vial with a dropper. The vial was closed with little cotton and kept at room temperature for 2 days. Then, colorless prisms were observed.

**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.



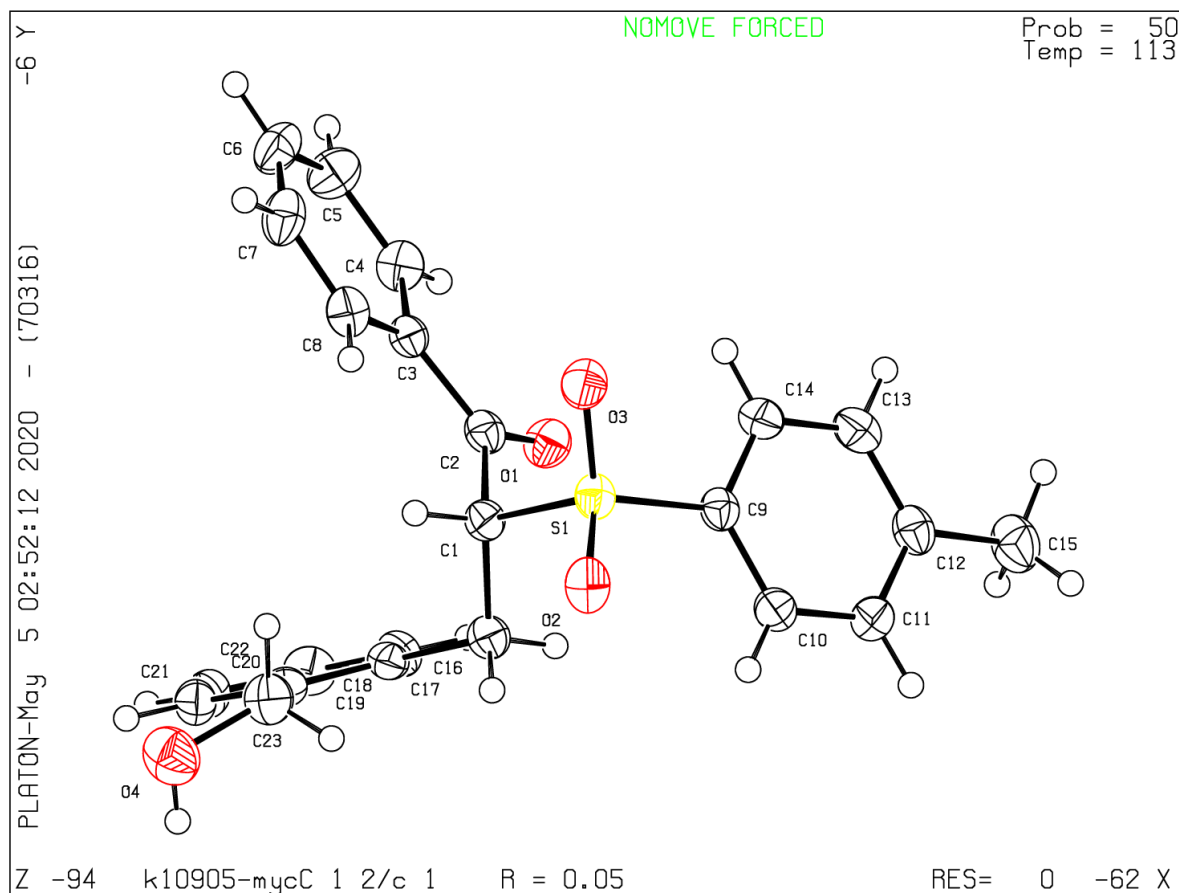
Empirical formula	C <sub>30</sub> H <sub>26</sub> O <sub>3</sub> S
Formula weight	466.57
Temperature/K	113(2)
Crystal system	monoclinic
Space group	P2 <sub>1</sub> /c
a/Å	9.7564(2)
b/Å	14.7638(2)
c/Å	17.1919(3)
α/°	90
β/°	101.0780(10)
γ/°	90
Volume/Å <sup>3</sup>	2430.20(7)
Z	4
ρ <sub>calc</sub> /cm <sup>3</sup>	1.275
μ/mm <sup>-1</sup>	0.163
F(000)	984.0
Crystal size/mm <sup>3</sup>	0.5 × 0.35 × 0.3
Radiation	Mo Kα (λ = 0.71073)
2θ range for data collection/°	4.254 to 54.13
Index ranges	-12 ≤ h ≤ 12, -17 ≤ k ≤ 18, -21 ≤ l ≤ 19
Reflections collected	52824
Independent reflections	5196 [R <sub>int</sub> = 0.0624, R <sub>sigma</sub> = 0.0289]
Data/restraints/parameters	5196/0/308
Goodness-of-fit on F <sup>2</sup>	1.077
Final R indexes [I ≥ 2σ (I)]	R <sub>1</sub> = 0.0357, wR <sub>2</sub> = 0.0919
Final R indexes [all data]	R <sub>1</sub> = 0.0415, wR <sub>2</sub> = 0.0952
Largest diff. peak/hole / e Å <sup>-3</sup>	0.33/-0.44

## X-ray crystal data of compound 15 (CCDC 2042108)



**Sample preparation** : A solution of compound **15** (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>23</sub> H <sub>22</sub> O <sub>4</sub> S
Formula weight	394.46
Temperature/K	113(2)
Crystal system	monoclinic
Space group	C2/c
a/Å	16.1182(3)
b/Å	11.9825(2)
c/Å	20.4080(4)
α/°	90
β/°	105.952(2)
γ/°	90
Volume/Å <sup>3</sup>	3789.75(13)
Z	8
ρ <sub>calc</sub> /cm <sup>3</sup>	1.383
μ/mm <sup>-1</sup>	0.198
F(000)	1664.0
Crystal size/mm <sup>3</sup>	0.2 × 0.15 × 0.15
Radiation	Mo Kα (λ = 0.71073)
2θ range for data collection/°	4.152 to 54.114
Index ranges	-20 ≤ h ≤ 20, -15 ≤ k ≤ 15, -25 ≤ l ≤ 25
Reflections collected	21960
Independent reflections	3978 [R <sub>int</sub> = 0.0246, R <sub>sigma</sub> = 0.0188]
Data/restraints/parameters	3978/0/255
Goodness-of-fit on F <sup>2</sup>	1.103
Final R indexes [I ≥ 2σ (I)]	R <sub>1</sub> = 0.0456, wR <sub>2</sub> = 0.1285
Final R indexes [all data]	R <sub>1</sub> = 0.0502, wR <sub>2</sub> = 0.1315
Largest diff. peak/hole / e Å <sup>-3</sup>	0.50/-0.43