

Supporting Information

Synthesis of Sulfonyl 2-Aryl-5-methylenetetrahydropyrans

Meng-Yang Chang^{*a,b,c} and Kuan-Ting Chen^a

^aDepartment of Medicinal and Applied Chemistry, Kaohsiung Medical University, Kaohsiung 807, Taiwan ^bDepartment of Medical Research, Kaohsiung Medical University Hospital, Kaohsiung 807, Taiwan ^cNPUST College of Professional Studies, National Pingtung University of Science and Technology, Pingtung 912, Taiwan.

*Corresponding author, email: mychang@kmu.edu.tw

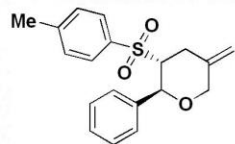
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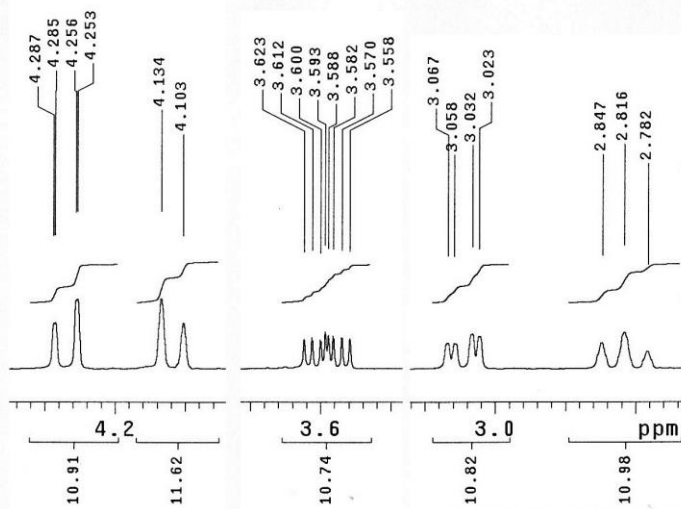
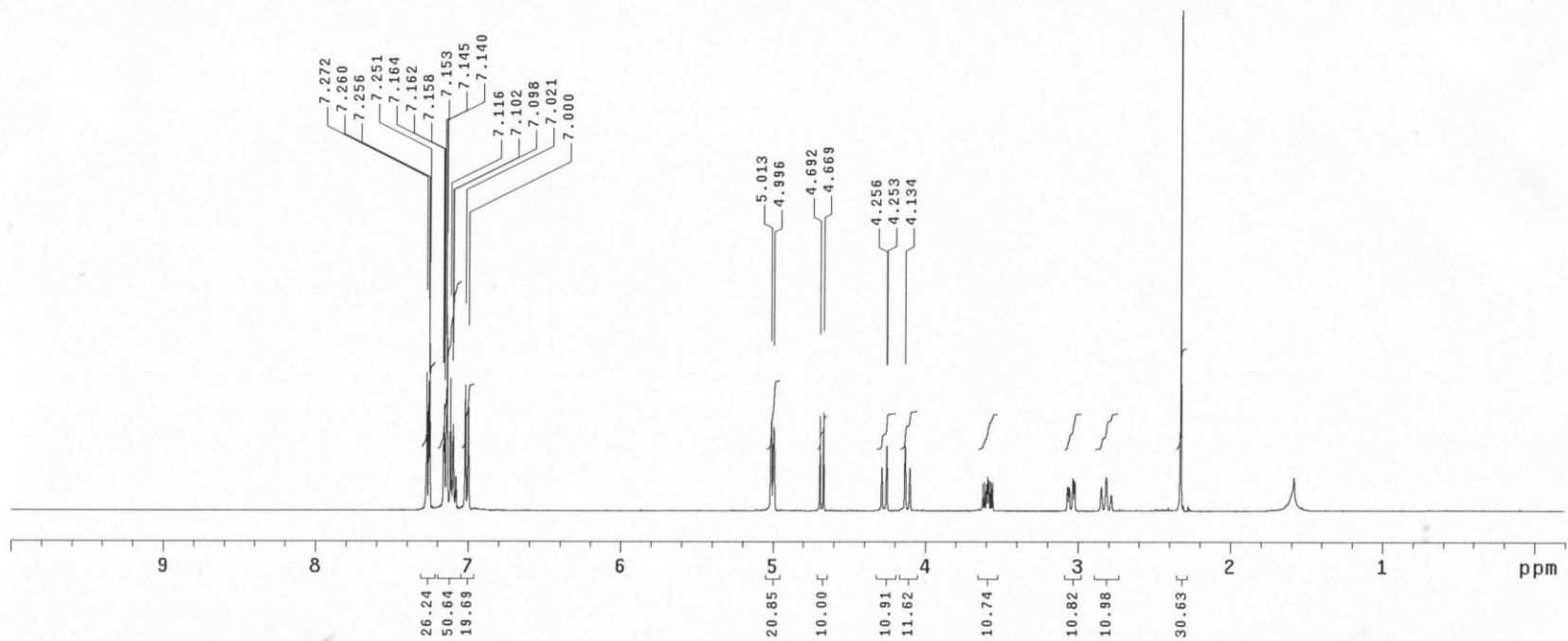
Compound 5a (¹H-NMR spectral data)

KT0501NB

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Jun 2 2020
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetitions



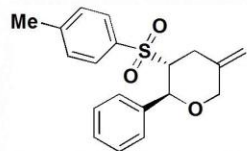
(¹H NMR, 400 MHz, CDCl₃)



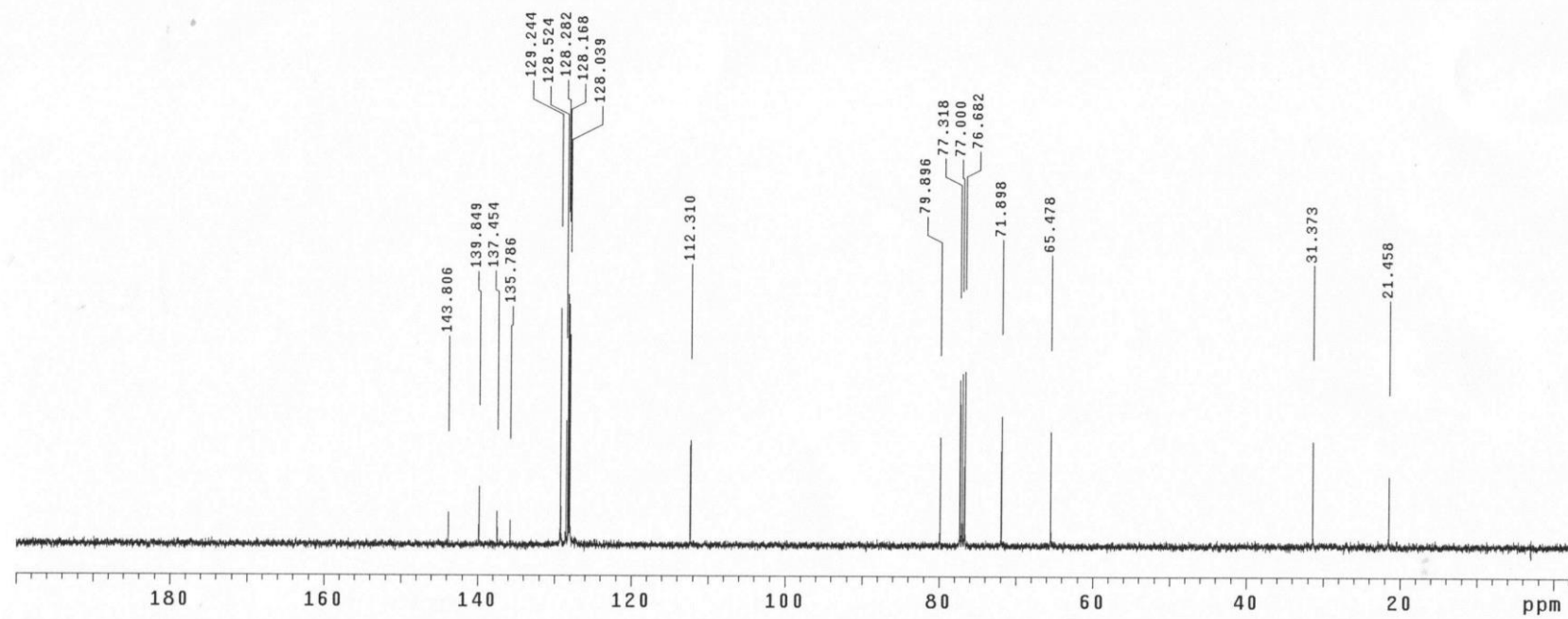
Compound 5a (¹³C-NMR spectral data)

KT0501NB

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Jun 2 2020
Solvent: CDCl₃
Ambient temperature
Total 2224 repetitions



(¹³C NMR, 100 MHz, CDCl₃)



Compound 5b (¹H-NMR spectral data)

KT0514NB

Pulse Sequence: s2pu1

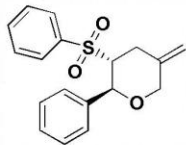
UNITYplus-600 "KMU600.kmu.edu.tw"

Date: Jun 18 2020

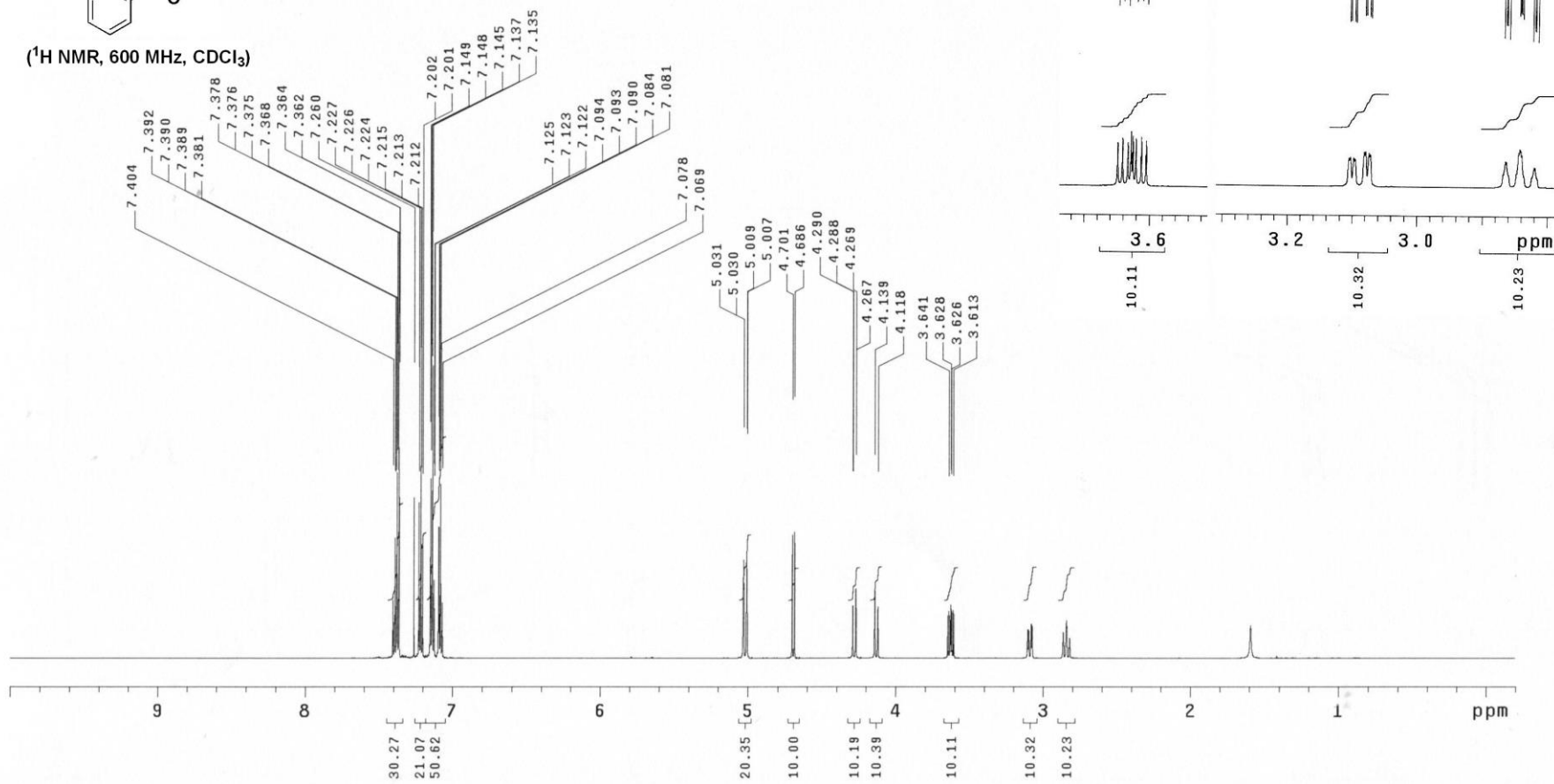
Solvent: cdc13

Temp: 28.0 C / 301.1 K

Total 32 repetitions



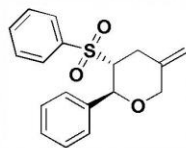
(¹H NMR, 600 MHz, CDCl₃)



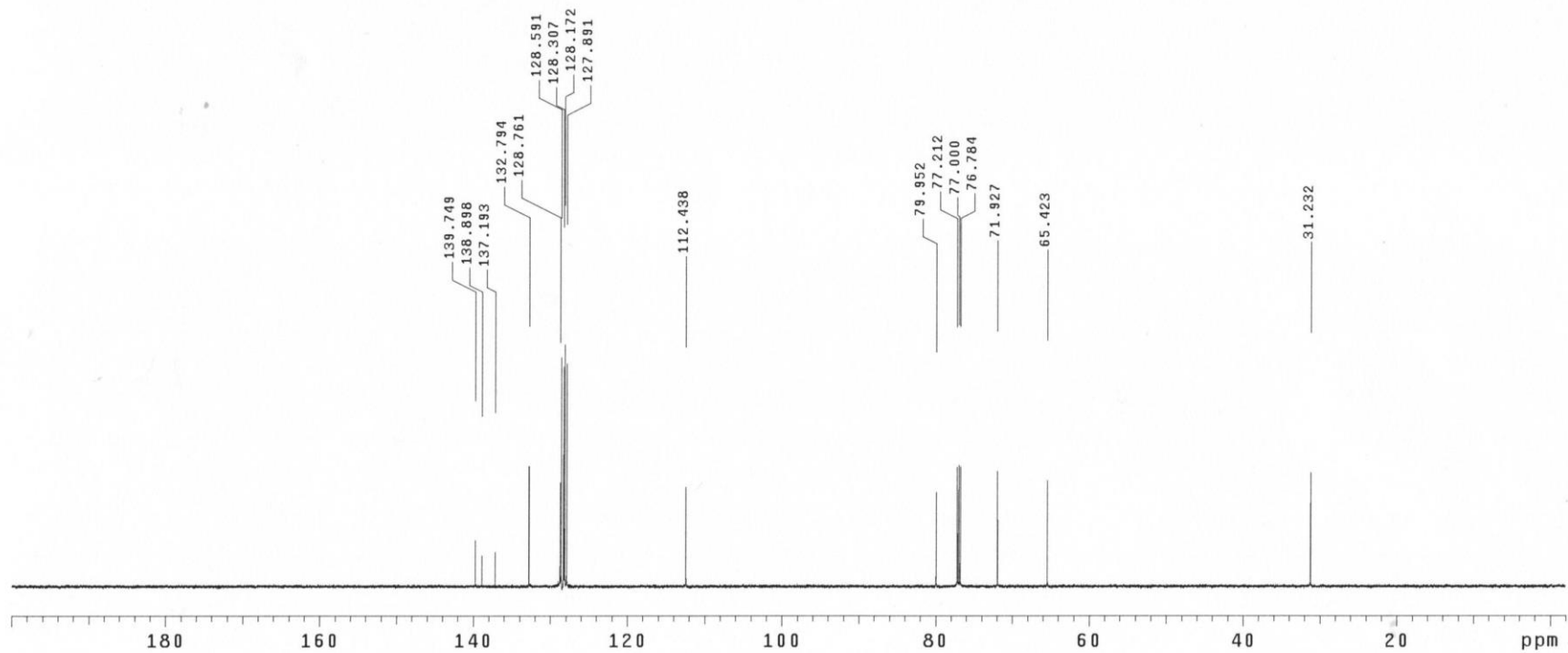
Compound 5b (¹³C-NMR spectral data)

KT0514NB

Pulse Sequence: s2pu1
UNITYplus-600 "KMU600.kmu.edu.tw"
Date: Jun 18 2020
Solvent: cdcl3
Temp: 28.0 C / 301.1 K
Total 360 repetitions



(¹³C NMR, 125 MHz, CDCl₃)



Compound 5c (¹H-NMR spectral data)

KT0515NB

Pulse Sequence: s2pu1

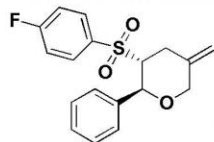
UNITYplus-400 "unity400"

Date: Jul 22 2020

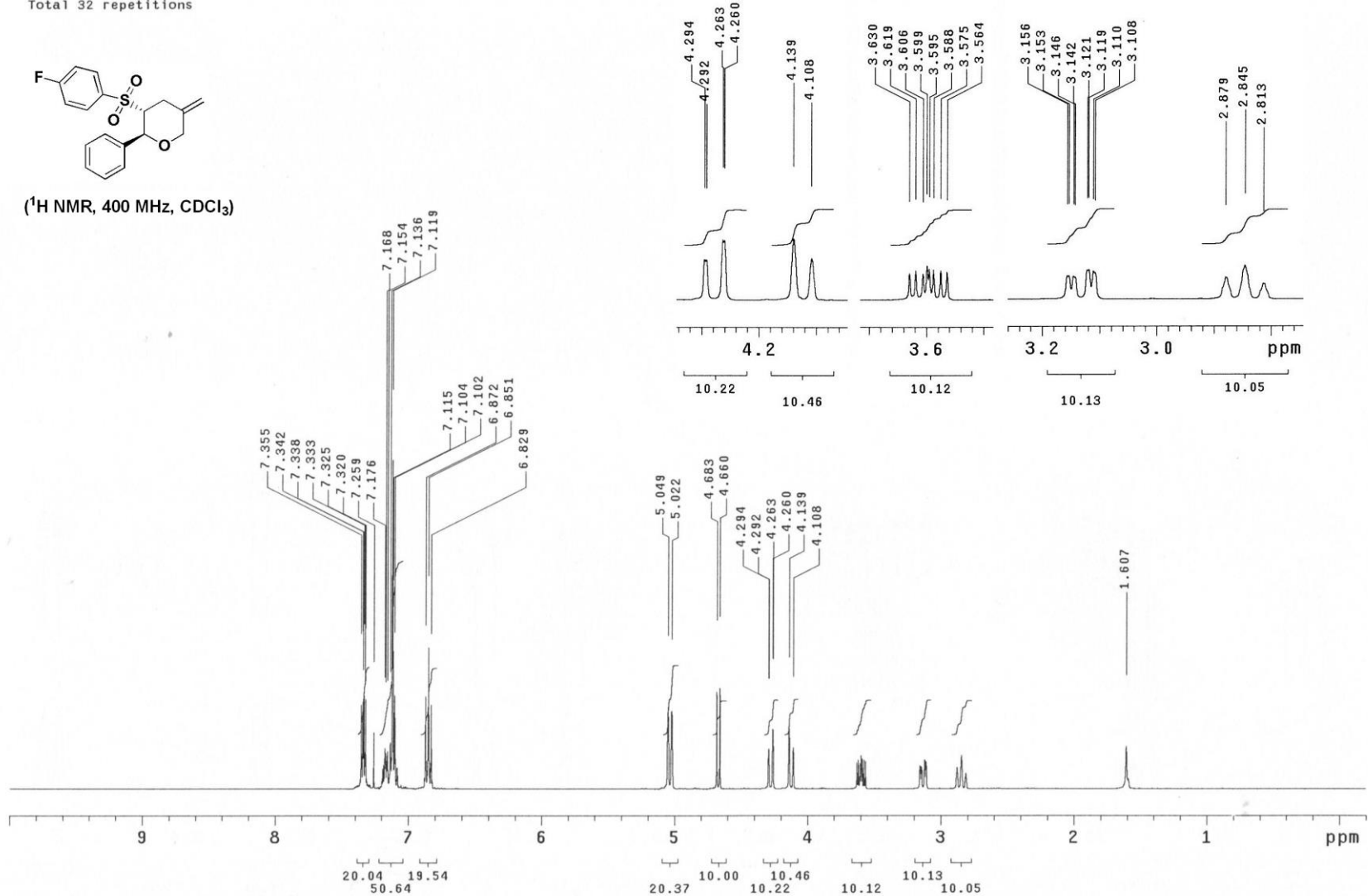
Solvent: CDCl₃

Ambient temperature

Total 32 repetitions



(¹H NMR, 400 MHz, CDCl₃)



Compound 5c (¹³C-NMR spectral data)

KT0515NB

Pulse Sequence: s2pu1

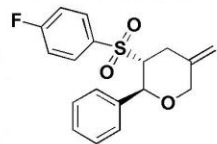
UNITYplus-400 "unity400"

Date: Jul 22 2020

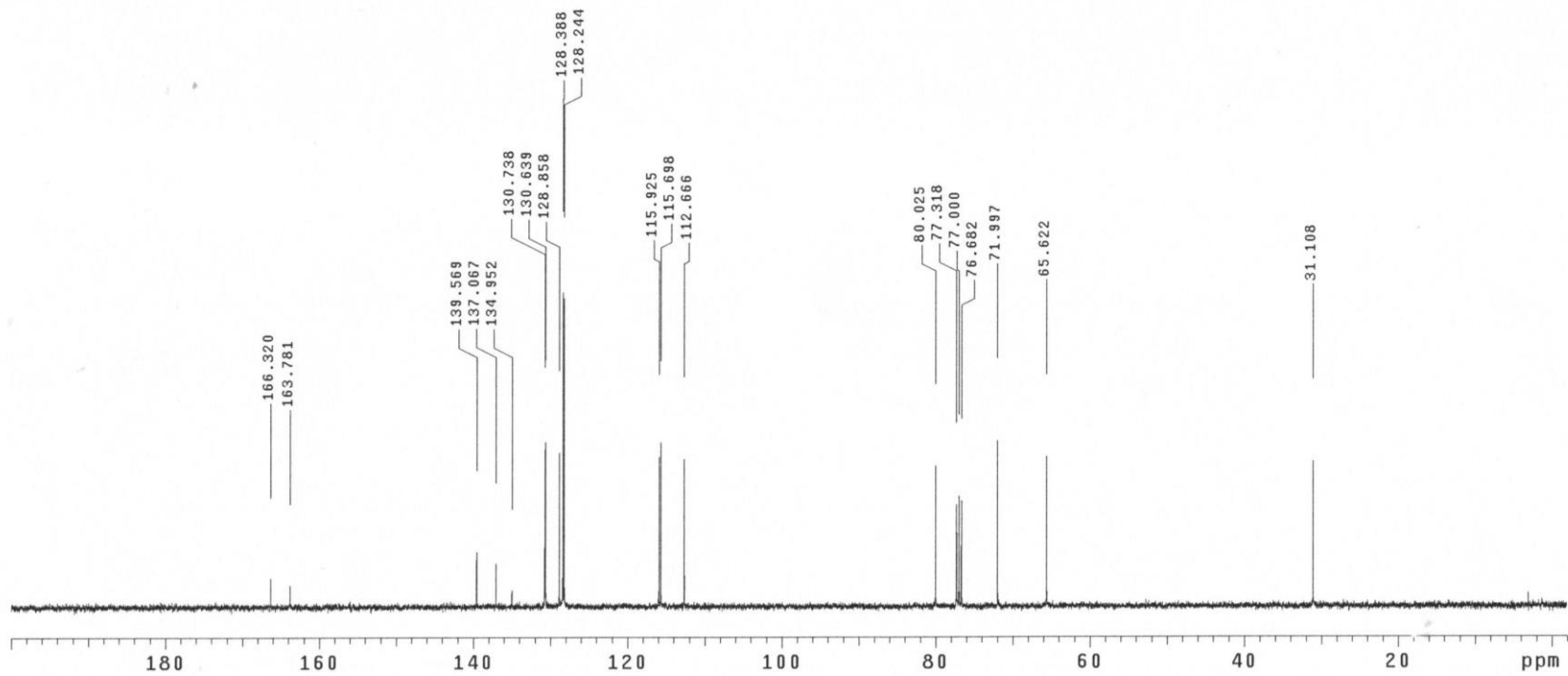
Solvent: CDCl₃

Ambient temperature

Total 1040 repetitions



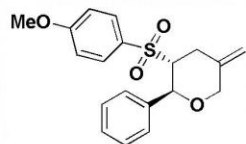
(¹³C NMR, 100 MHz, CDCl₃)



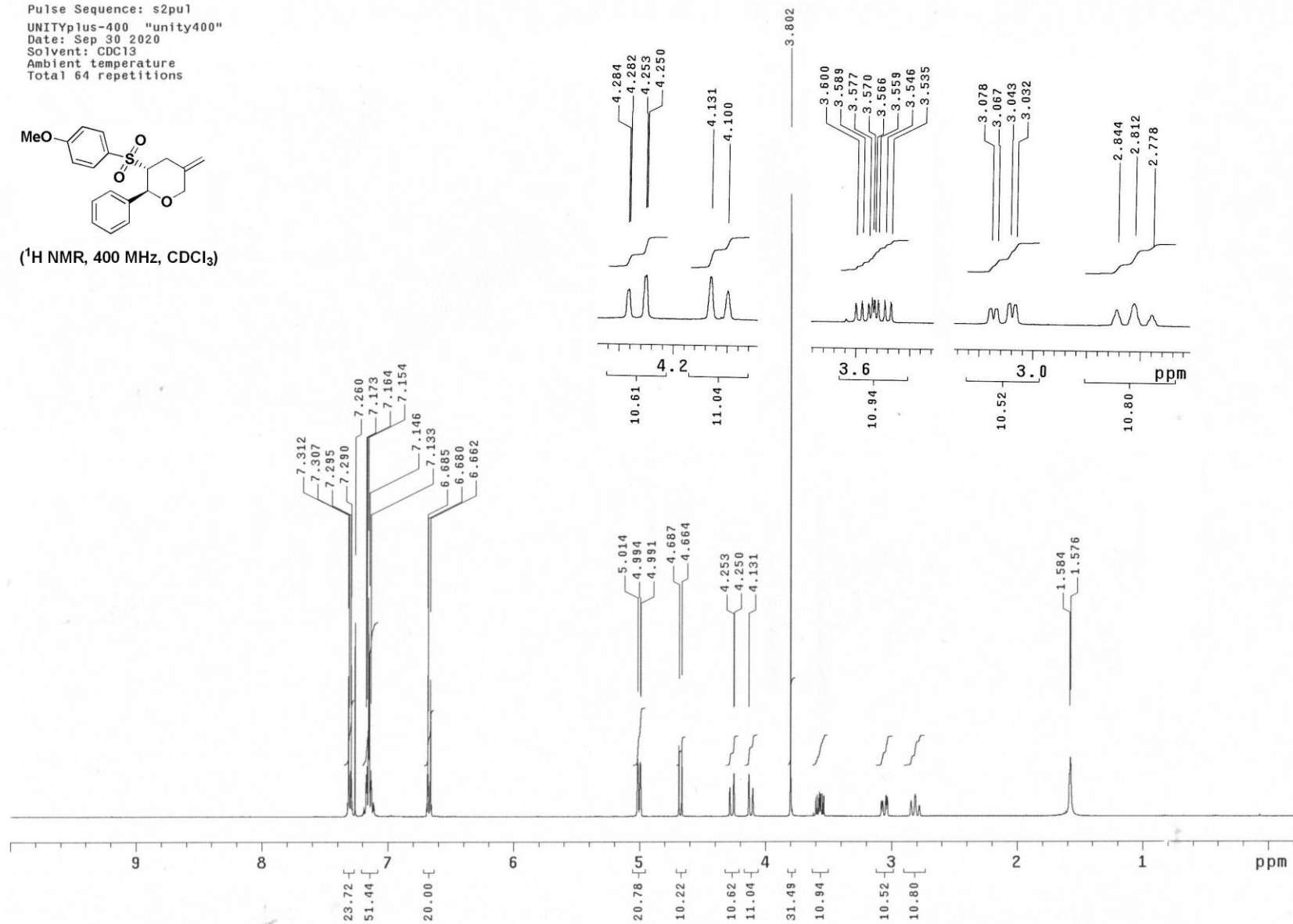
Compound 5d (¹H-NMR spectral data)

KT0806NB

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Sep 30 2020
 Solvent: CDCl₃
 Ambient temperature
 Total 64 repetitions



(¹H NMR, 400 MHz, CDCl₃)



Compound 5d (¹³C-NMR spectral data)

KT0806NB

Pulse Sequence: s2pu1

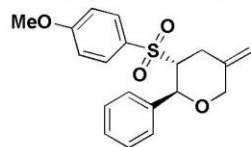
UNITYplus-400 "unity400"

Date: Sep 30 2020

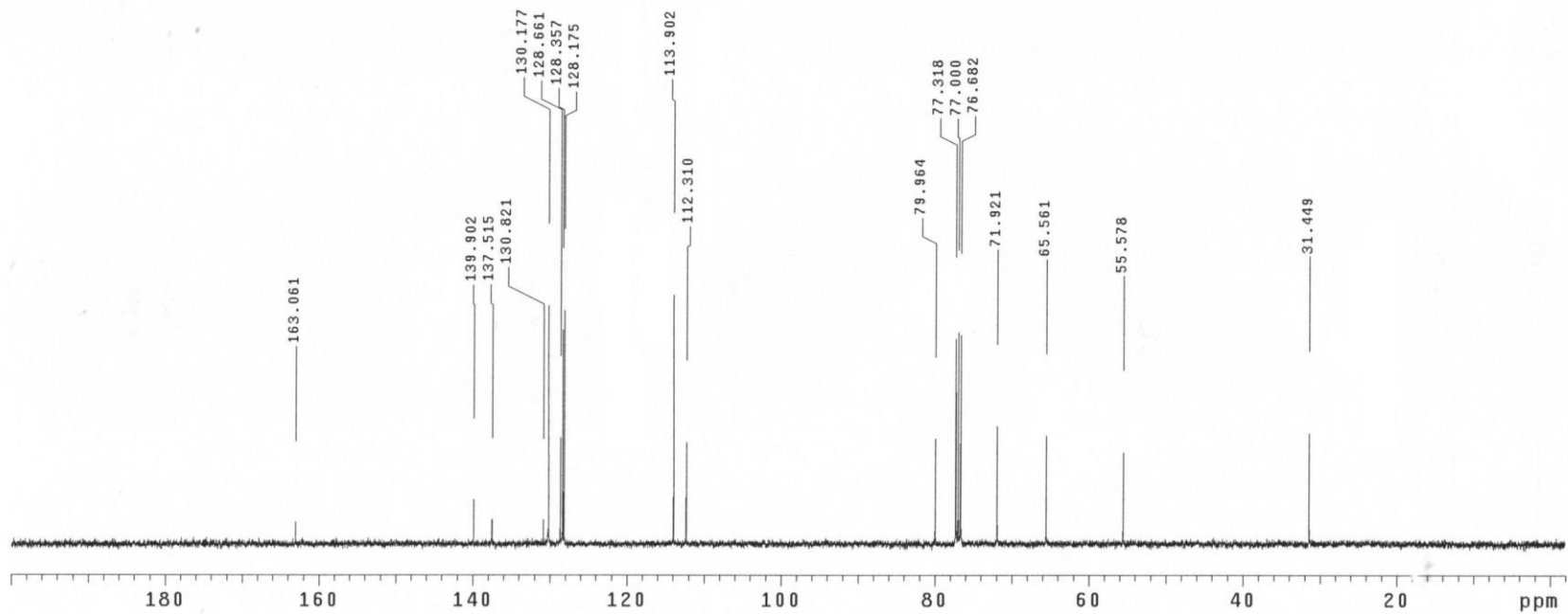
Solvent: CDCl₃

Ambient temperature

Total 5584 repetitions



(¹³C NMR, 100 MHz, CDCl₃)



Compound 5e (¹H-NMR spectral data)

KT0619NB

Pulse Sequence: s2pu1

Solvent: CDC13

Ambient temperature

UNITYplus-400 "unity400"

Pulse 38.8 degrees

Acq. time 3.744 sec

Width 6000.6 Hz

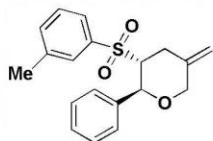
32 repetitions

OBSERVE H1, 400.2743814 MHz

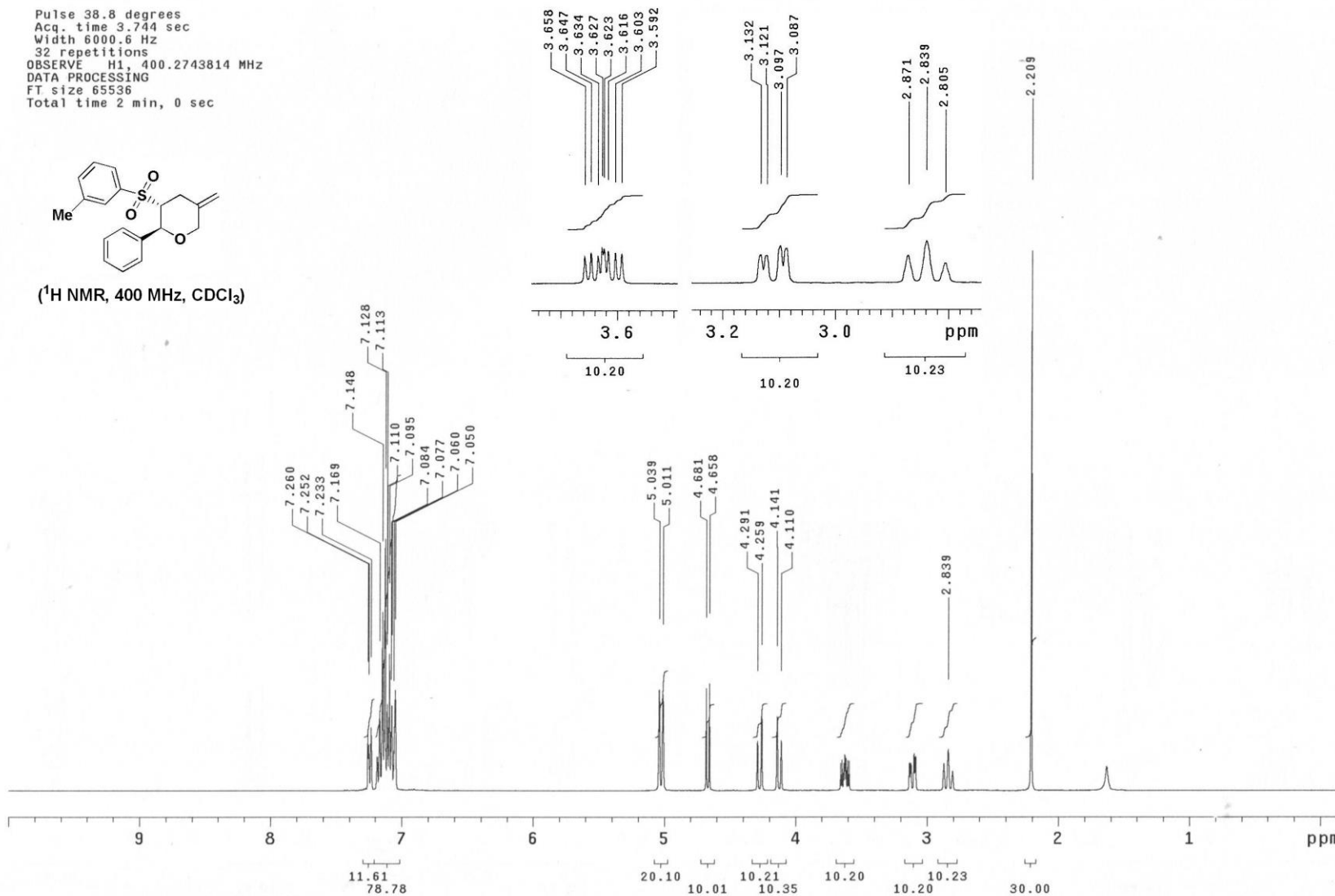
DATA PROCESSING

FT size 65536

Total time 2 min, 0 sec



(¹H NMR, 400 MHz, CDCl₃)



Compound 5e (¹³C-NMR spectral data)

KT0619NB

Pulse Sequence: s2pu1

Solvent: CDCl₃

Ambient temperature

UNITYplus-400 "unity400"

Relax. delay 0.500 sec

Pulse 65.8 degrees

Acq. time 0.800 sec

Width 25000.0 Hz

1216 repetitions

OBSERVE C13, 100.6490769 MHz

DECOUPLE H1, 400.2763980 MHz

Power 43 dB

on during acquisition

off during delay

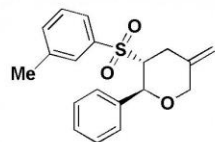
WALTZ-16 modulated

DATA PROCESSING

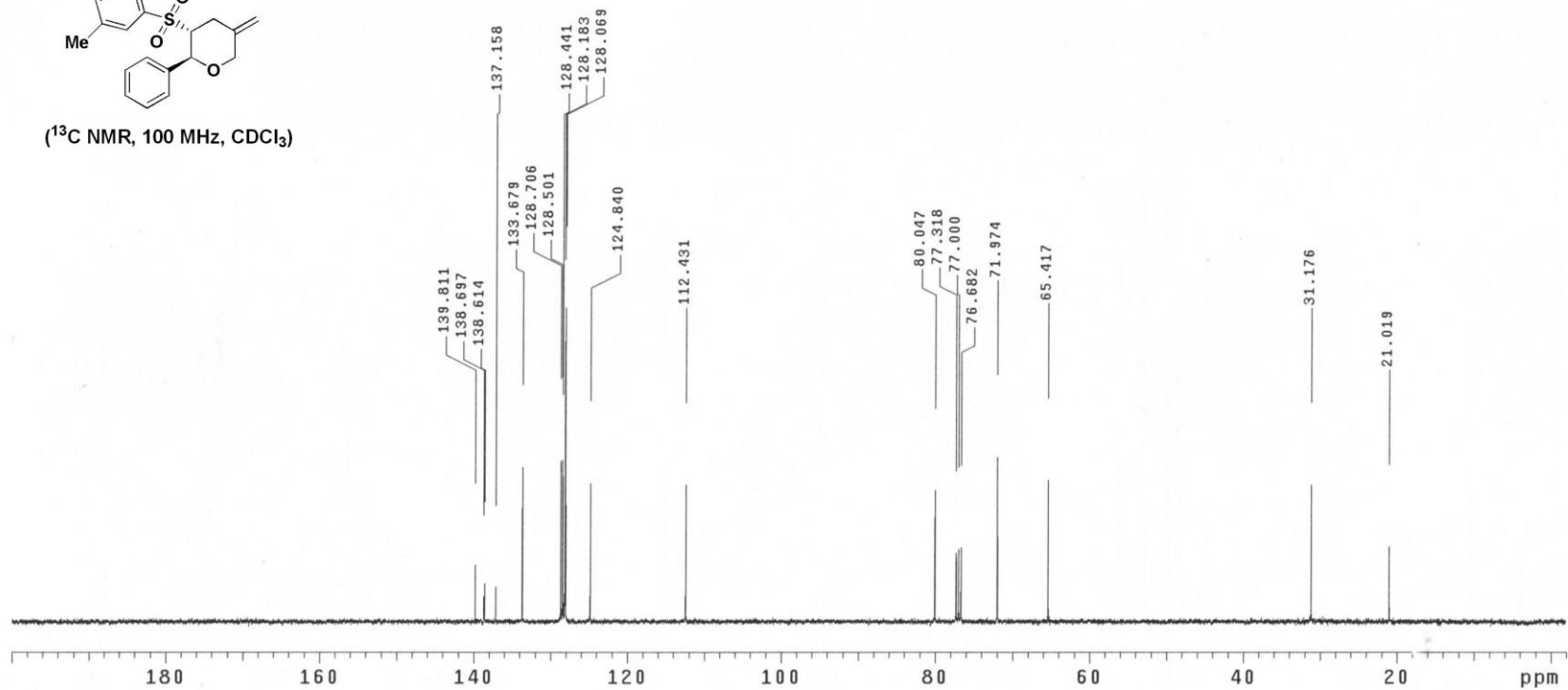
Line broadening 1.0 Hz

FT size 65536

Total time 11 hr, 39 min, 7 sec



(¹³C NMR, 100 MHz, CDCl₃)



Compound 5f (¹H-NMR spectral data)

KT0527NB

Pulse Sequence: s2pu1

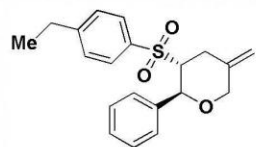
UNITYplus-400 "unity400"

Date: Jun 12 2020

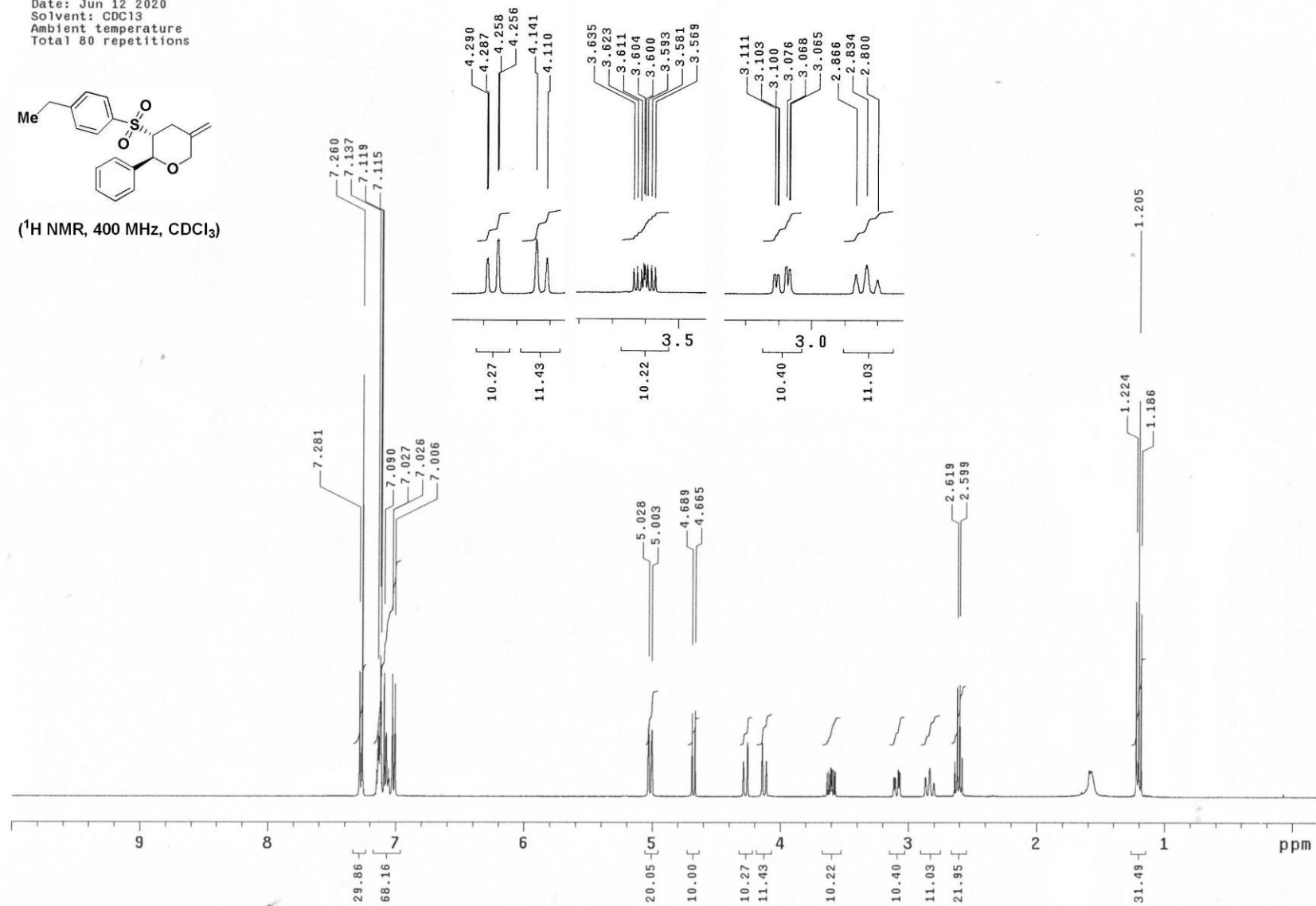
Solvent: CDC13

Ambient temperature

Total 80 repetitions



(¹H NMR, 400 MHz, CDCl₃)



Compound 5f (¹³C-NMR spectral data)

KT0527NB

Pulse Sequence: s2pu1

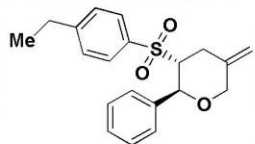
UNITYplus-400 "unity400"

Date: Jun 12 2020

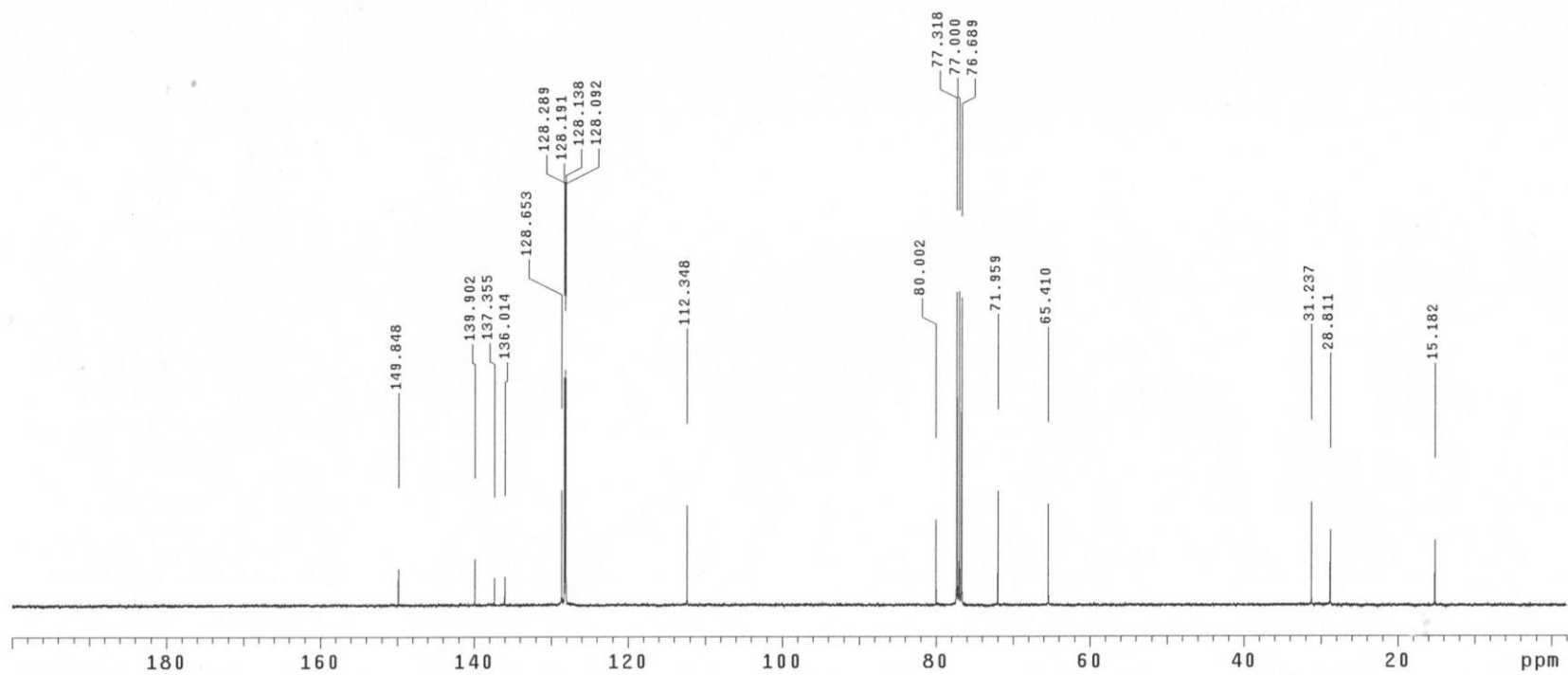
Solvent: CDCl₃

Ambient temperature

Total 32000 repetitions



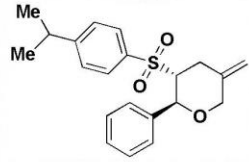
(¹³C NMR, 100 MHz, CDCl₃)



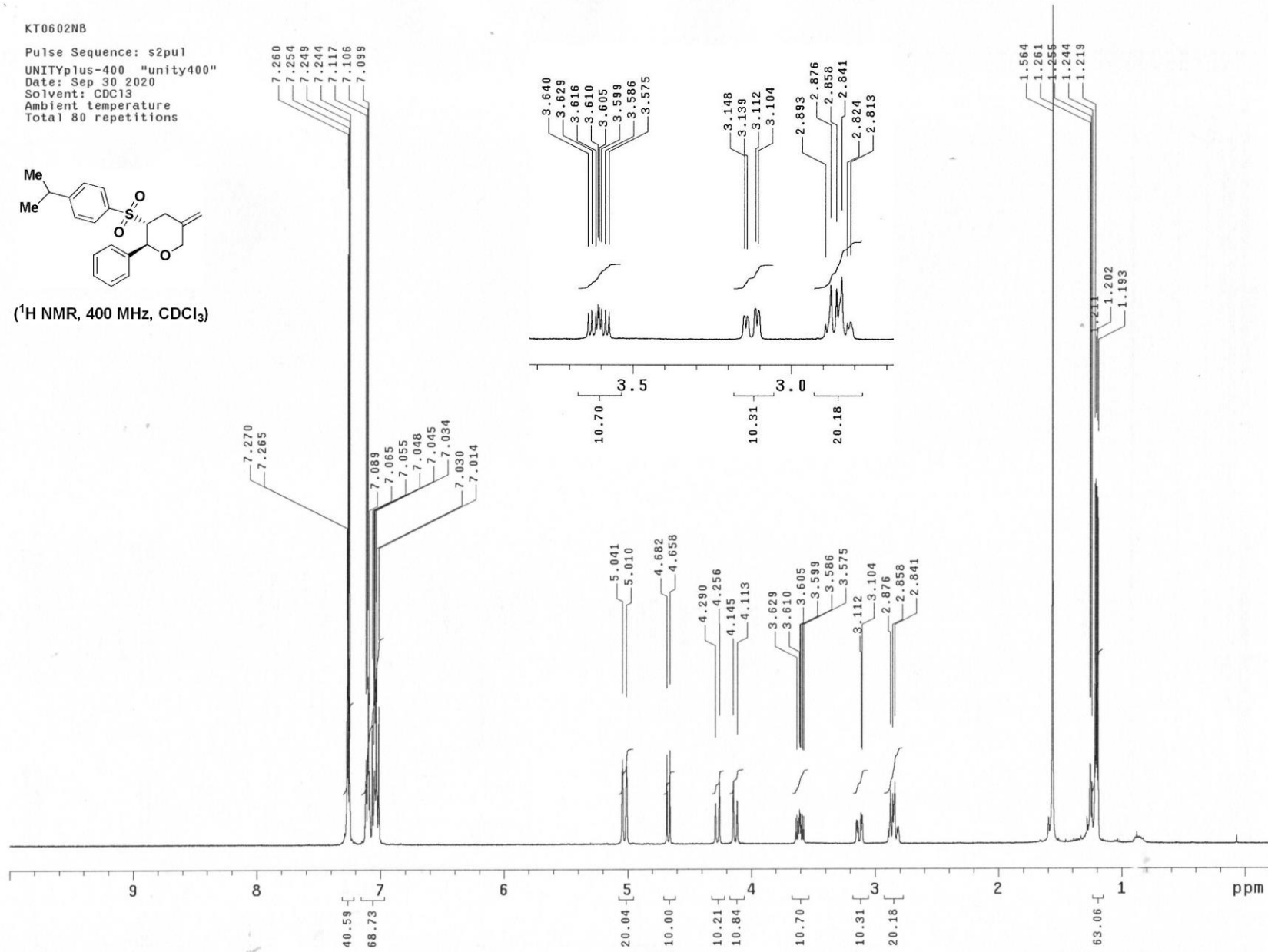
Compound 5g (¹H-NMR spectral data)

KT0602NB

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Sep 30 2020
 Solvent: CDCl₃
 Ambient temperature
 Total 80 repetitions



(¹H NMR, 400 MHz, CDCl₃)



Compound 5g (¹³C-NMR spectral data)

KT0602NB

Pulse Sequence: s2pu1

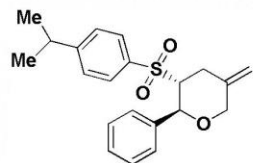
UNITYplus-400 "unity400"

Date: Sep 30 2020

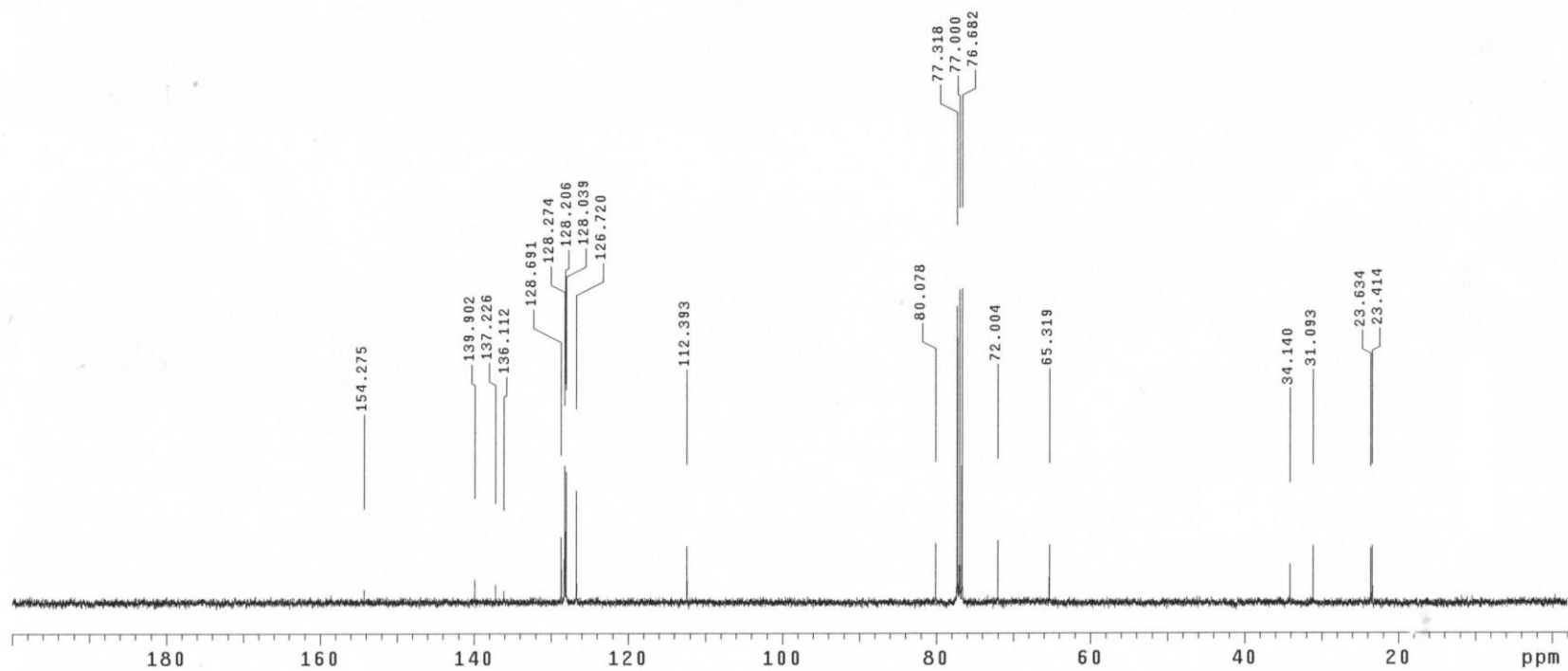
Solvent: CDCl₃

Ambient temperature

Total 9616 repetitions



(¹³C NMR, 100 MHz, CDCl₃)



Compound 5h (¹H-NMR spectral data)

KT0522NB

Pulse Sequence: s2pu1

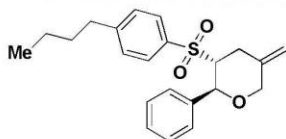
UNITYplus-400 "unity400"

Date: Jun 5 2020

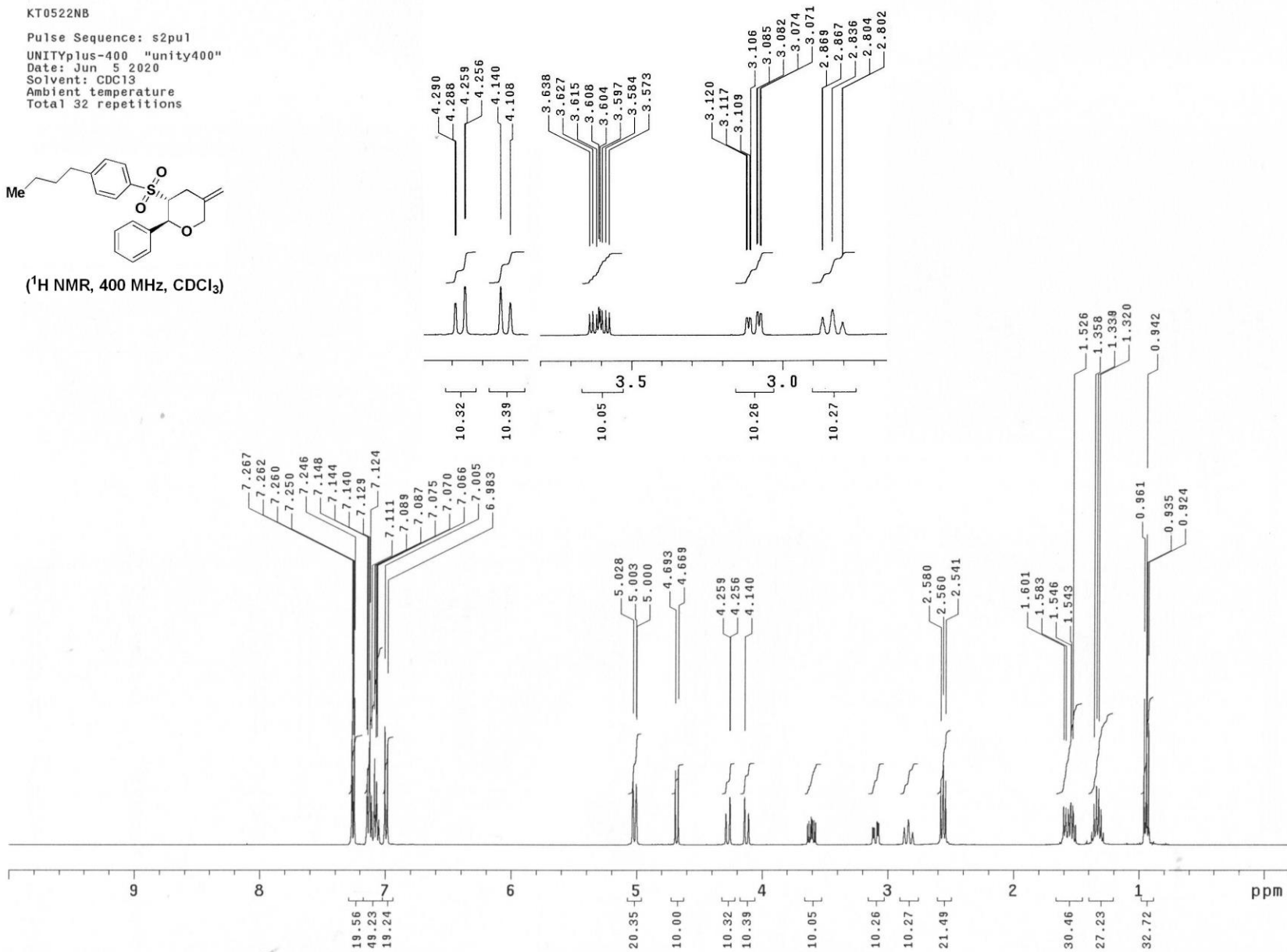
Solvent: CDCl₃

Ambient temperature

Total 32 repetitions



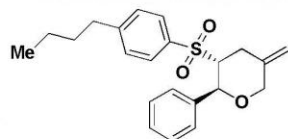
(¹H NMR, 400 MHz, CDCl₃)



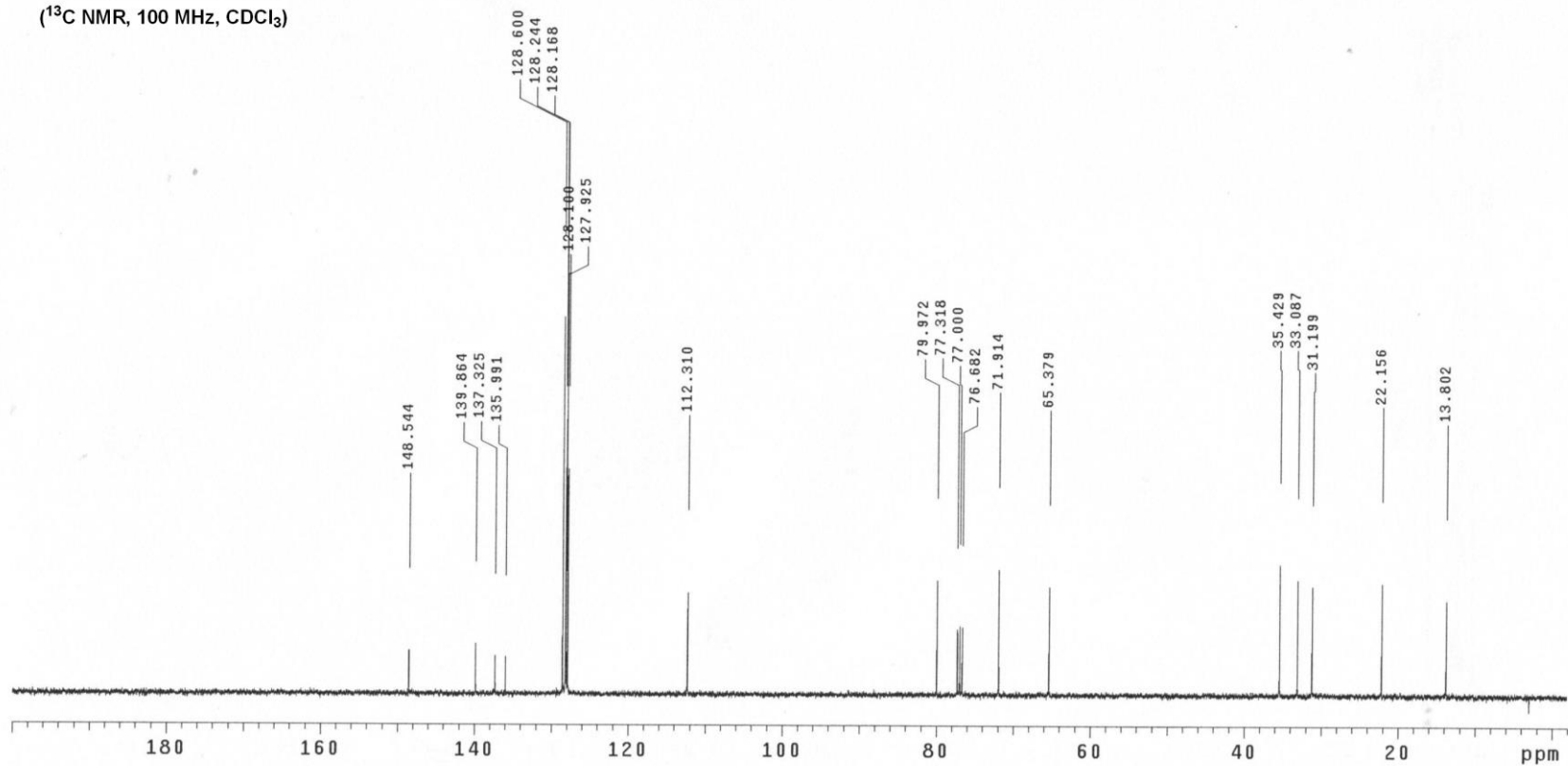
Compound 5h (¹³C-NMR spectral data)

KT0522NB

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Jun 5 2020
Solvent: CDC13
Ambient temperature
Total 640 repetitions



(¹³C NMR, 100 MHz, CDCl₃)



Compound 5i (¹H-NMR spectral data)

KT0702NB

Pulse Sequence: s2pu1

Solvent: CDCl₃

Ambient temperature

UNITYplus-400 "unity400"

Pulse 38.8 degrees

Acq. time 3.744 sec

Width 6000.6 Hz

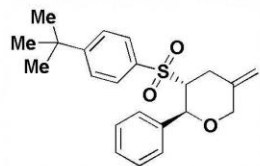
64 repetitions

OBSERVE H1 400.2743814 MHz

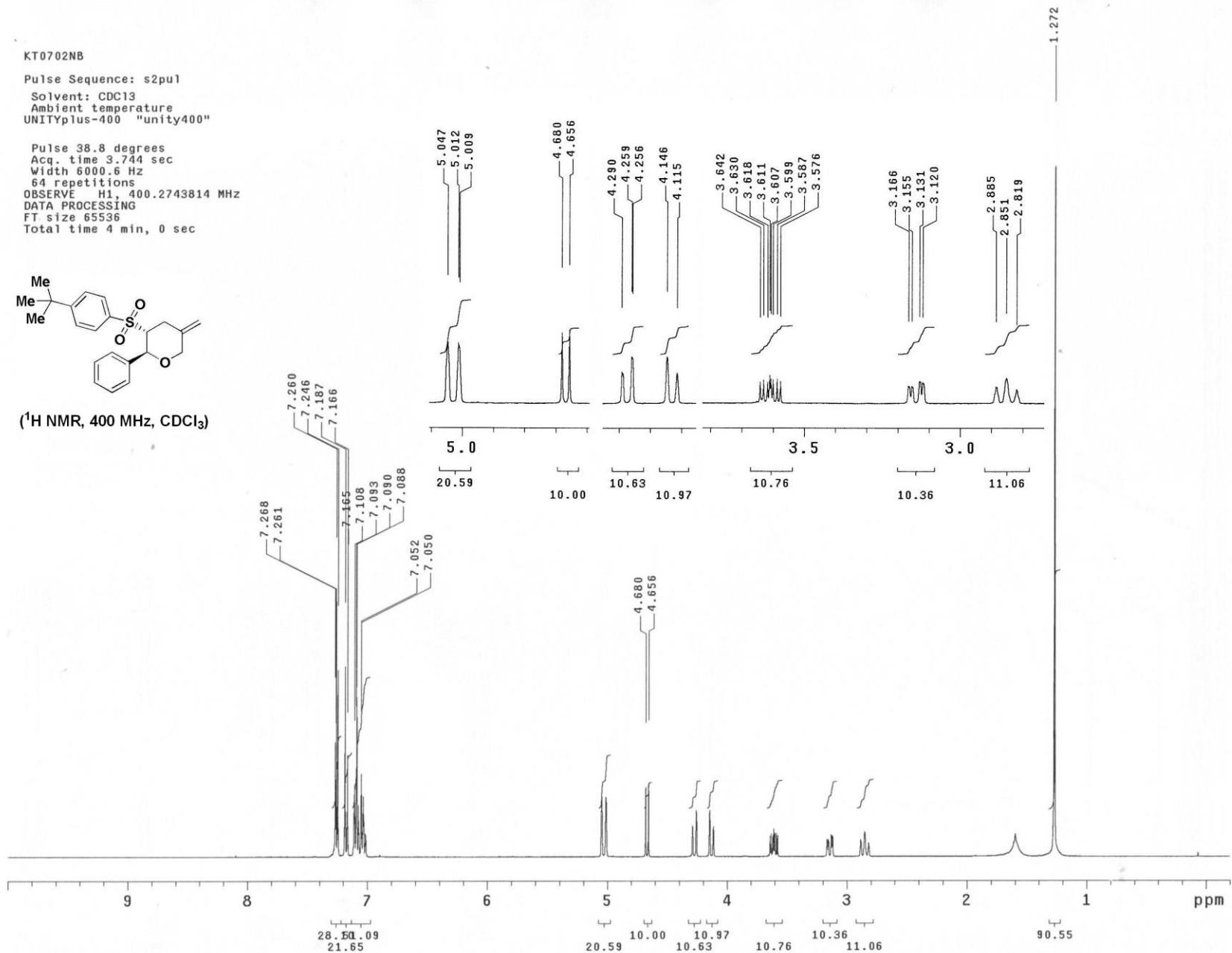
DATA PROCESSING

FT size 65536

Total time 4 min, 0 sec



(¹H NMR, 400 MHz, CDCl₃)



Compound 5i (¹³C-NMR spectral data)

KT0702NB

Pulse Sequence: s2pu1

Solvent: CDCl₃

Ambient temperature

UNITYplus-400 "unity400"

Relax. delay 0.500 sec

Pulse 65.8 degrees

Acq. time 0.800 sec

Width 25000.0 Hz

4432 repetitions

OBSERVE C13, 100.6490731 MHz

DECOUPLE H1, 400.2763980 MHz

Power 43 dB

on during acquisition

off during delay

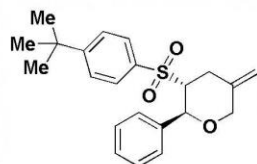
WALTZ-16 modulated

DATA PROCESSING

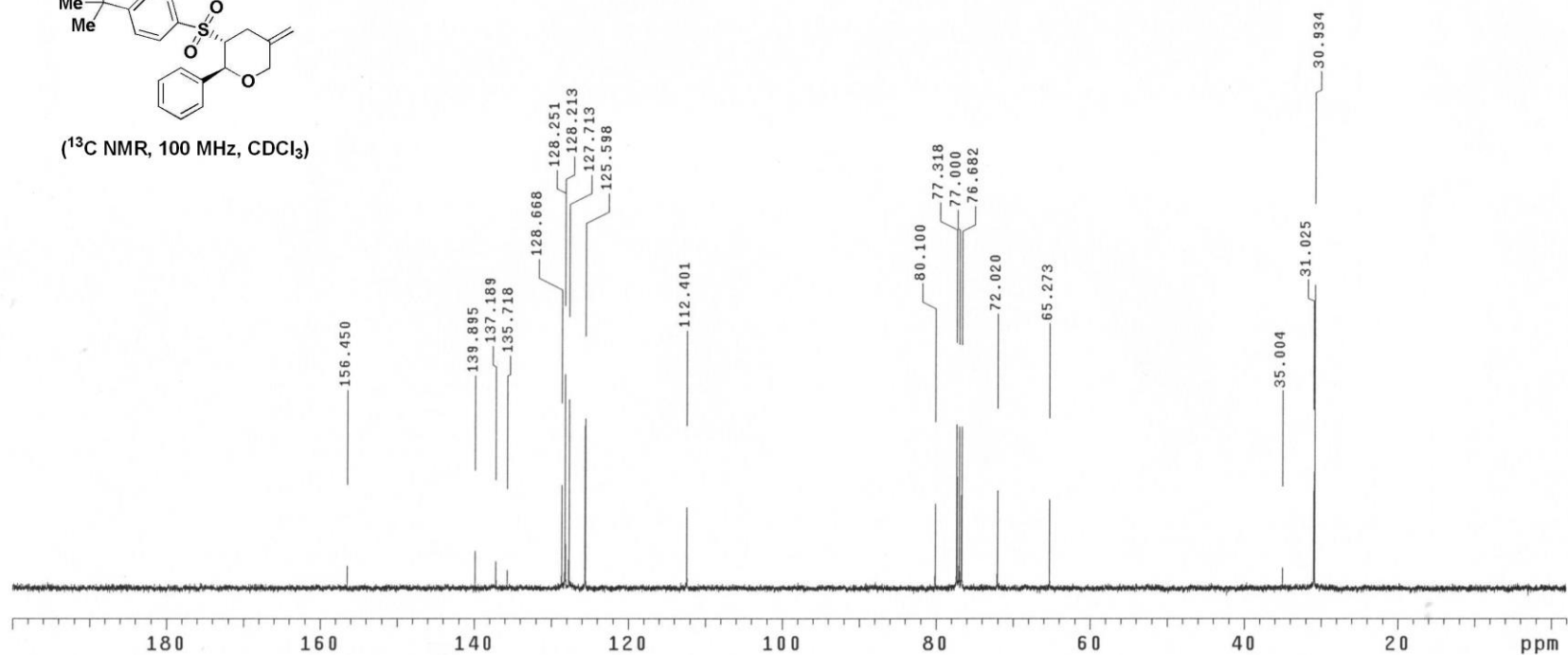
Line broadening 1.0 Hz

FT size 65536

Total time 11 hr, 39 min, 7 sec



(¹³C NMR, 100 MHz, CDCl₃)



Compound 5j (¹H-NMR spectral data)

KT0609NB

Pulse Sequence: s2pu1

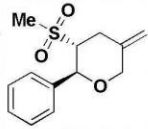
Mercury-400BB "MerPlus400"

Date: Sep 22 2020

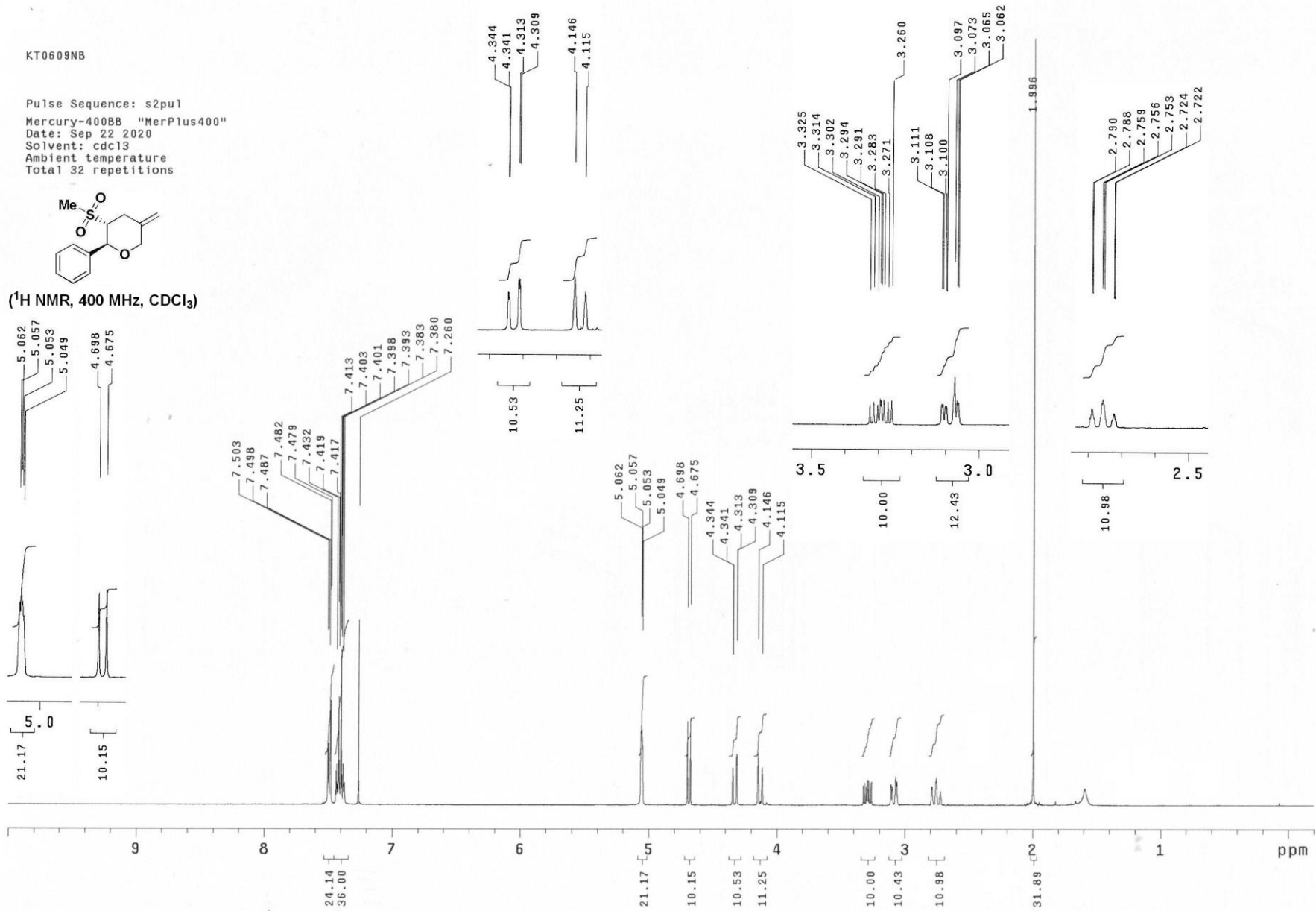
Solvent: cdc13

Ambient temperature

Total 32 repetitions



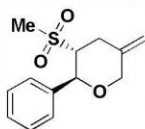
(¹H NMR, 400 MHz, CDCl₃)



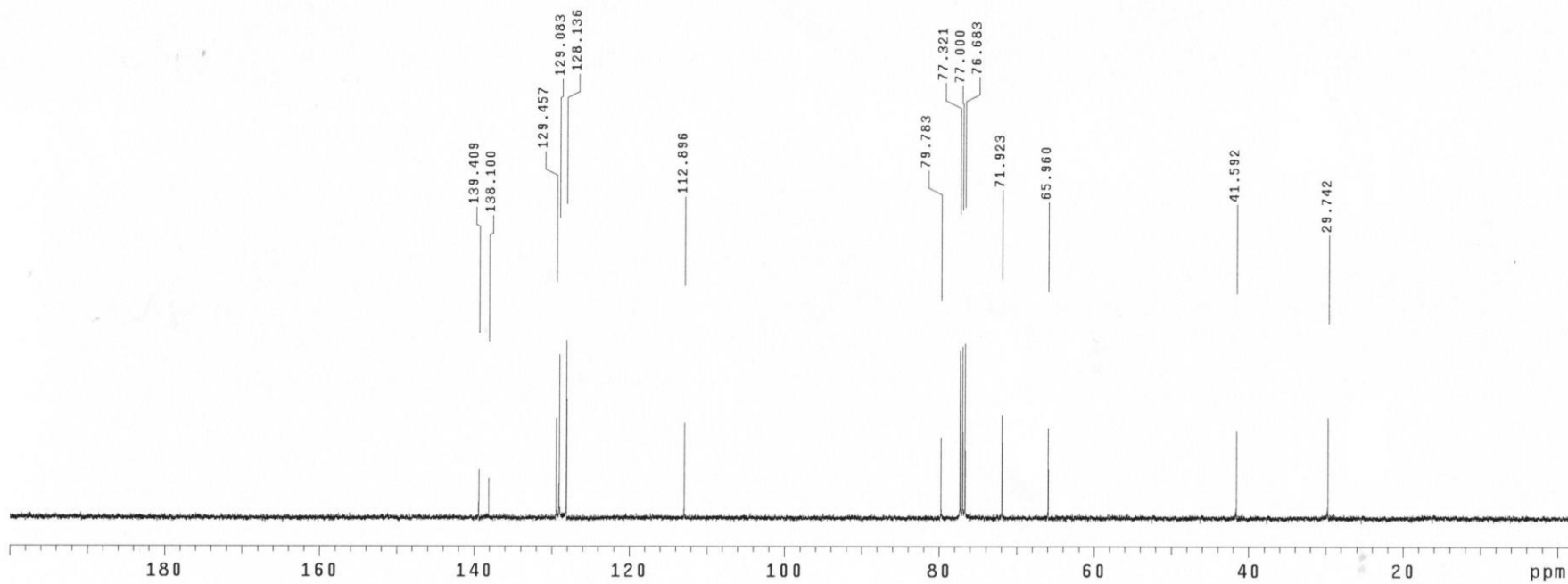
Compound 5j (¹³C-NMR spectral data)

KT0609NB

Pulse Sequence: s2pu1
Mercury-400BB "MerPlus400"
Date: Sep 22 2020
Solvent: cdcl3
Ambient temperature
Total 720 repetitions



(¹³C NMR, 100 MHz, CDCl₃)



Compound 5k (¹H-NMR spectral data)

KT0622NB

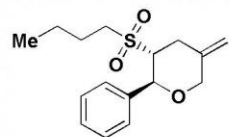
Pulse Sequence: s2pu1

Solvent: CDCl₃

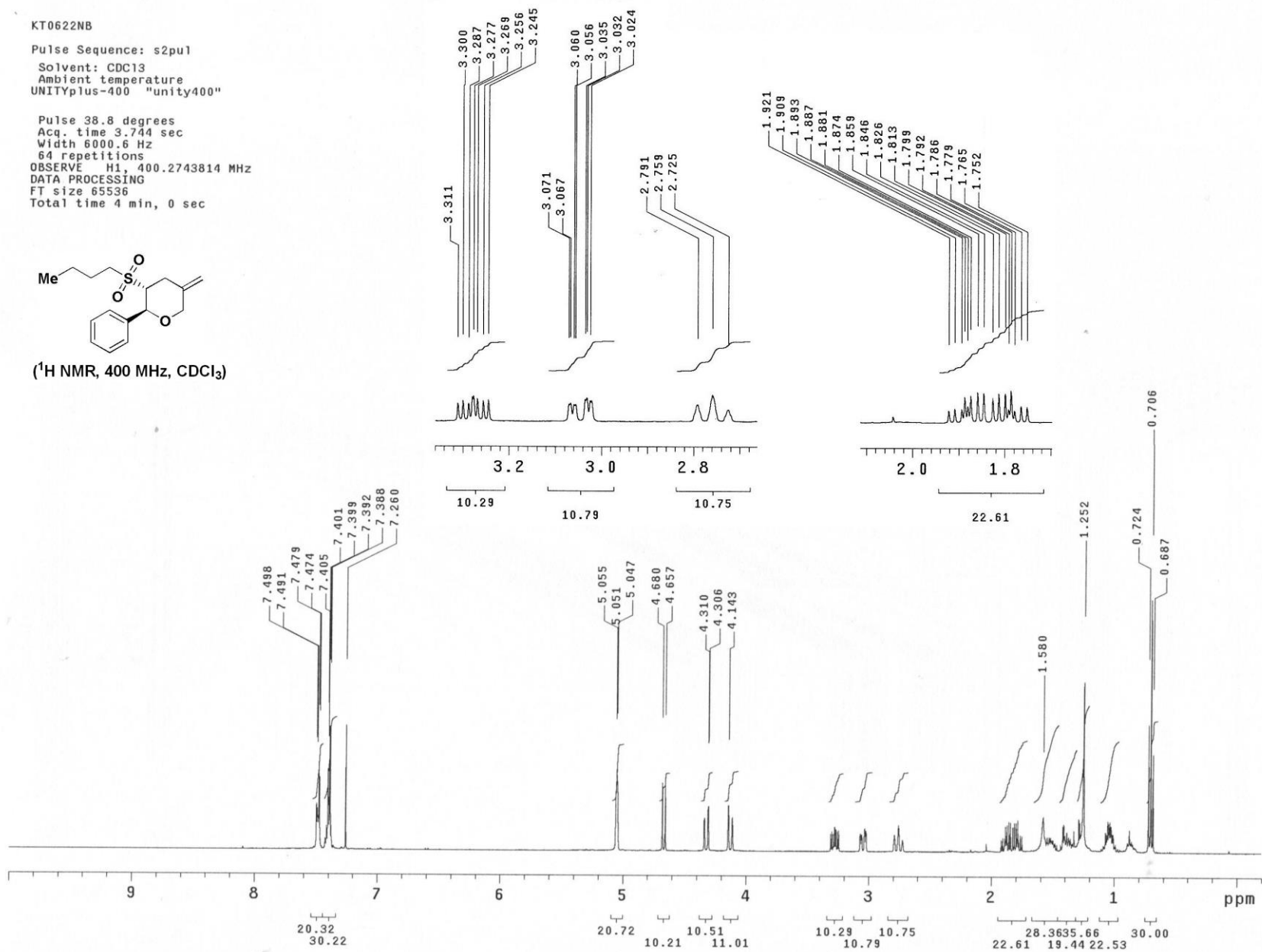
Ambient temperature

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



(¹H NMR, 400 MHz, CDCl₃)



Compound 5k (¹³C-NMR spectral data)

KT0622NB

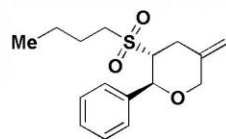
Pulse Sequence: s2pu1

Solvent: CDCl₃

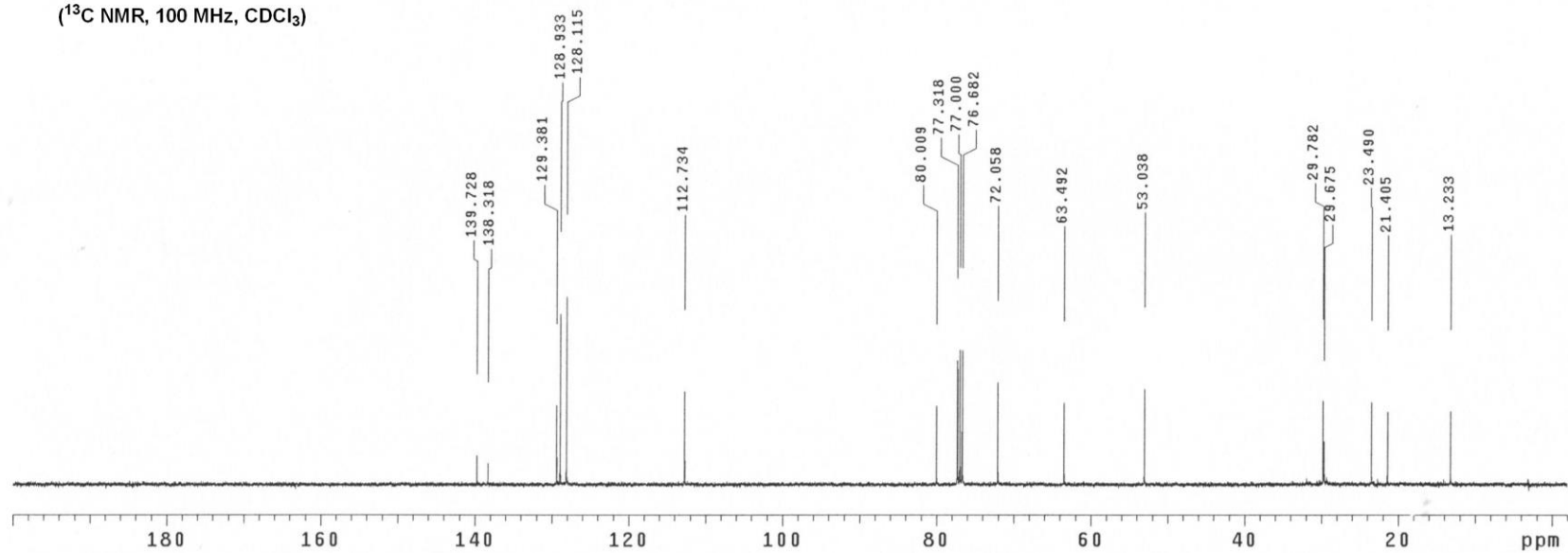
Ambient temperature

UNITYplus-400 "unity400"

Relax. delay 0.500 sec
Pulse 65.8 degrees
Acq. time 0.800 sec
Width 25000.0 Hz
7232 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



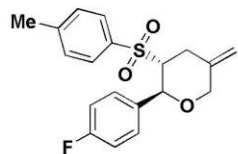
(¹³C NMR, 100 MHz, CDCl₃)



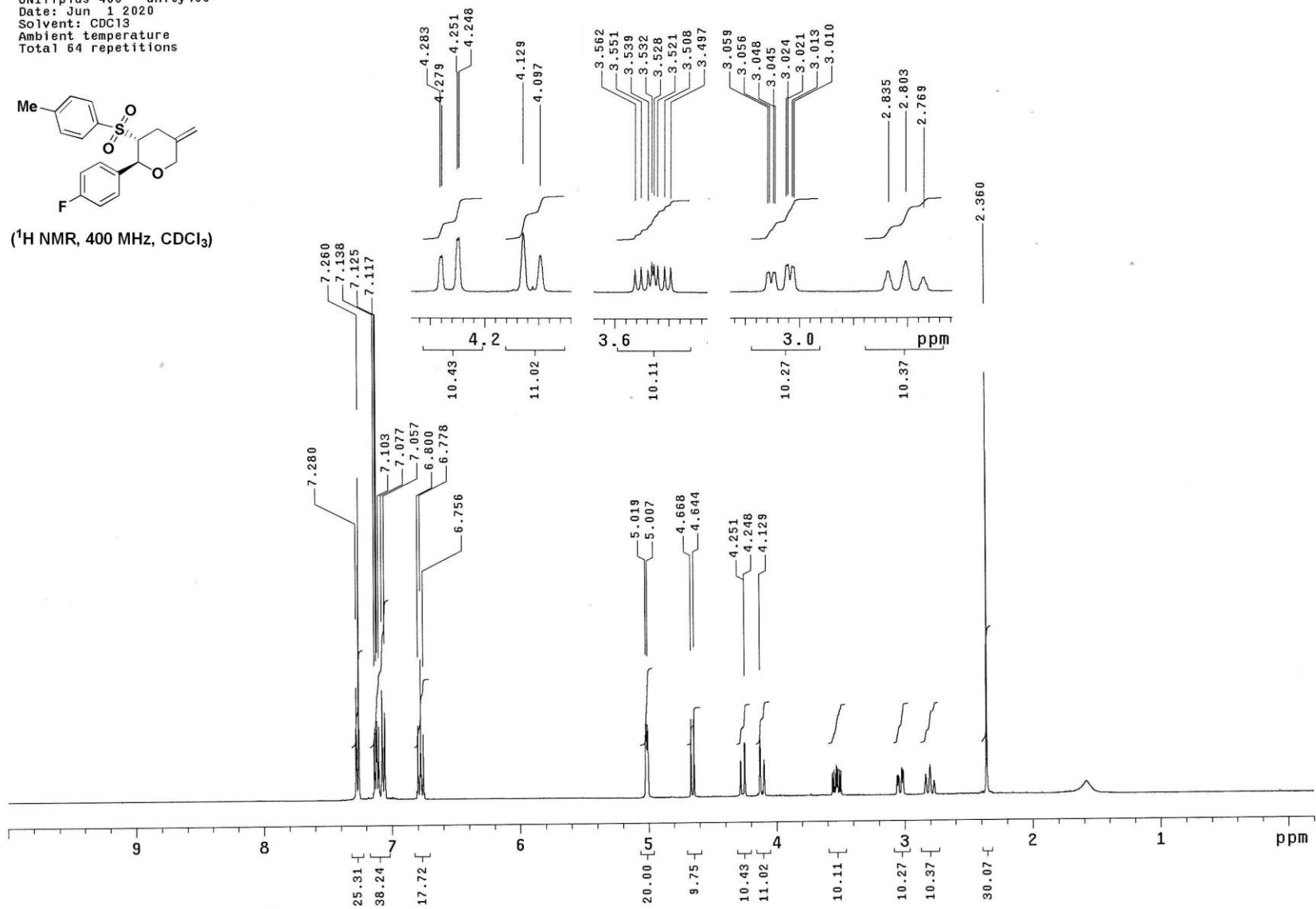
Compound 5I (¹H-NMR spectral data)

KT0506NB

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Jun 1 2020
 Solvent: CDCl₃
 Ambient temperature
 Total 64 repetitions



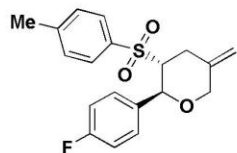
(¹H NMR, 400 MHz, CDCl₃)



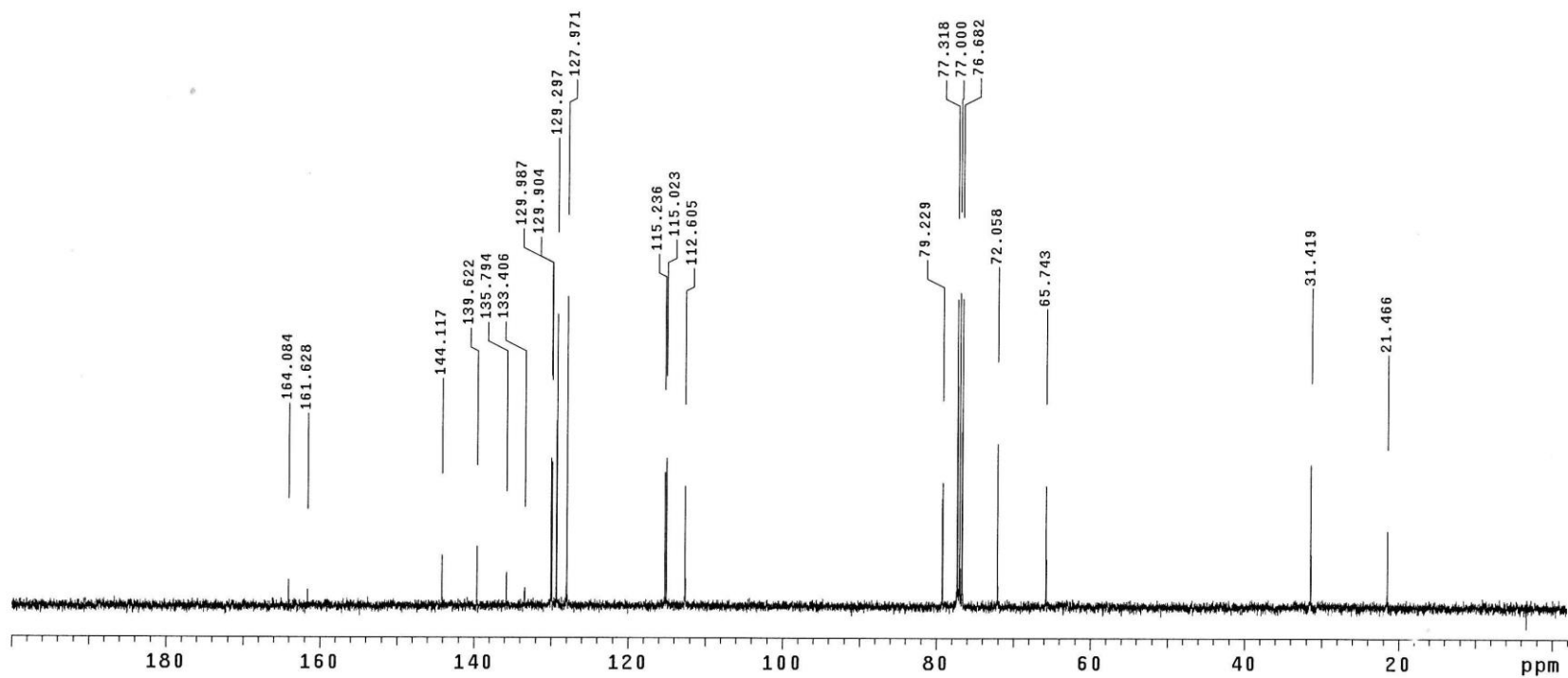
Compound 5I (¹³C-NMR spectral data)

KT0506NB

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Jun 1 2020
Solvent: CDCl₃
Ambient temperature
Total 7040 repetitions



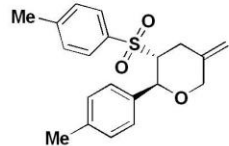
(¹³C NMR, 100 MHz, CDCl₃)



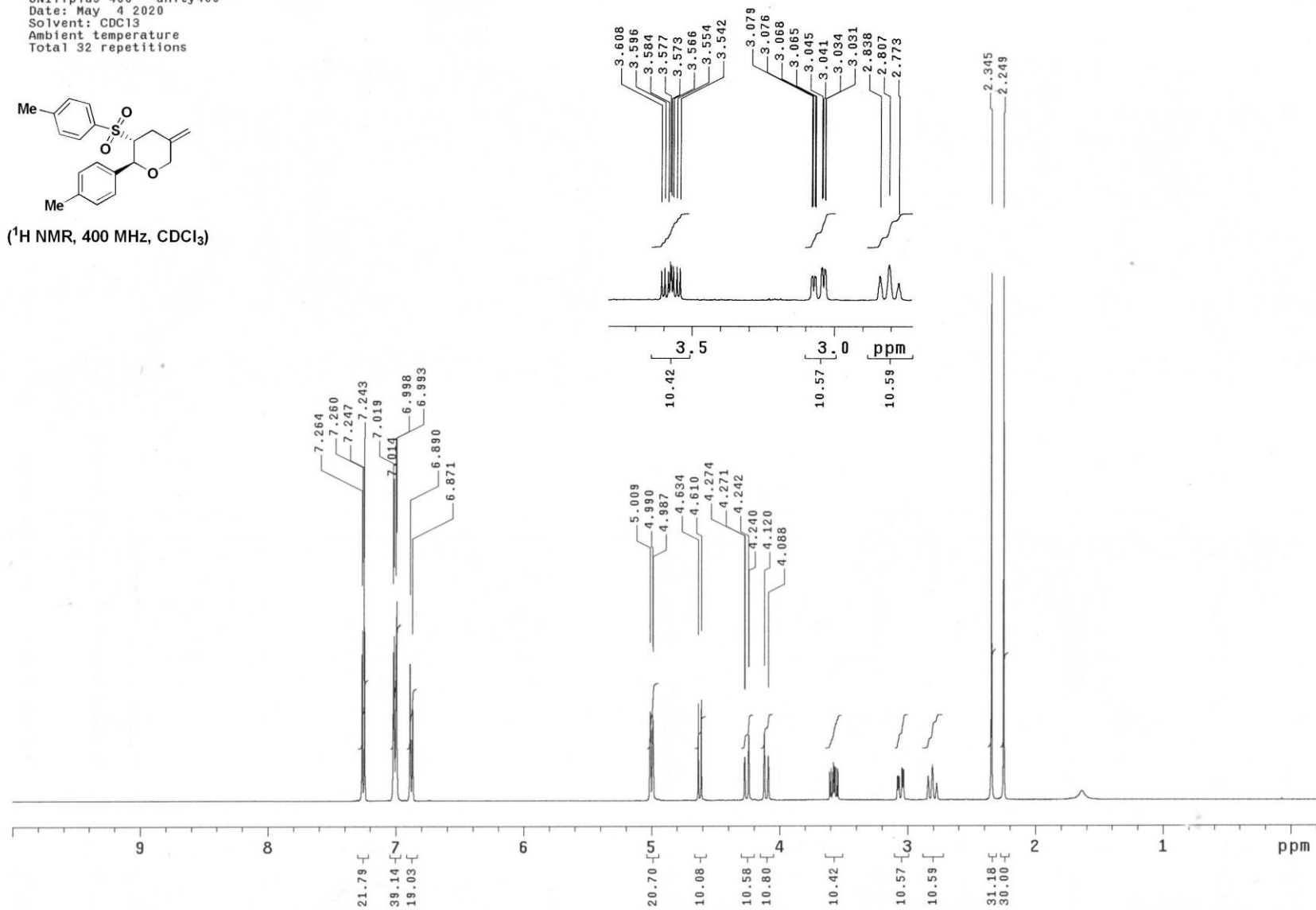
Compound 5m (¹H-NMR spectral data)

KTup37

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: May 4 2020
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetitions



(¹H NMR, 400 MHz, CDCl₃)



Compound 5m (¹³C-NMR spectral data)

KTup37

Pulse Sequence: s2pu1

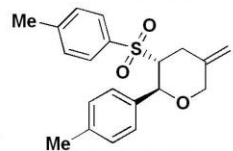
UNITYplus-400 "unity400"

Date: May 4 2020

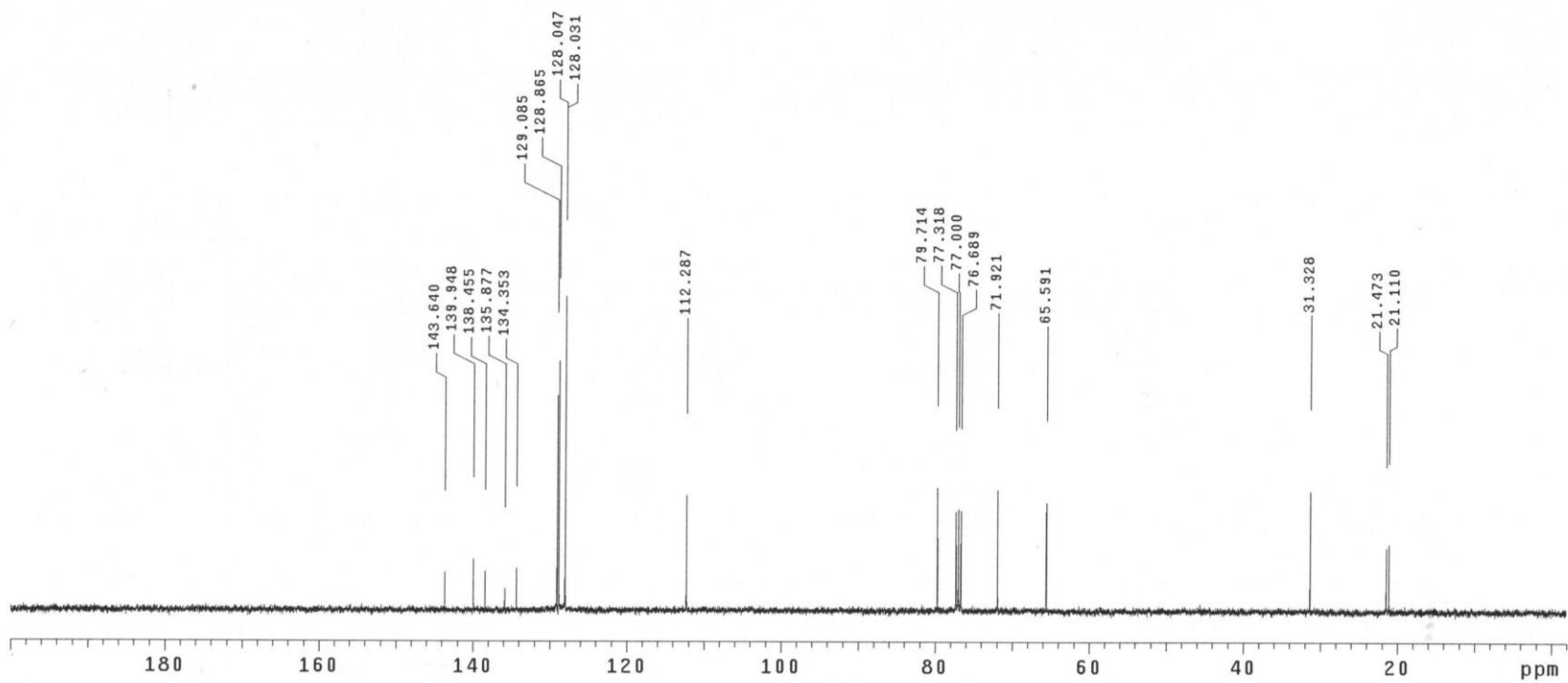
Solvent: CDCl₃

Ambient temperature

Total 1328 repetitions



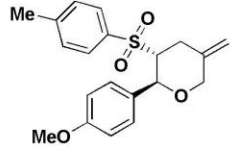
(¹³C NMR, 100 MHz, CDCl₃)



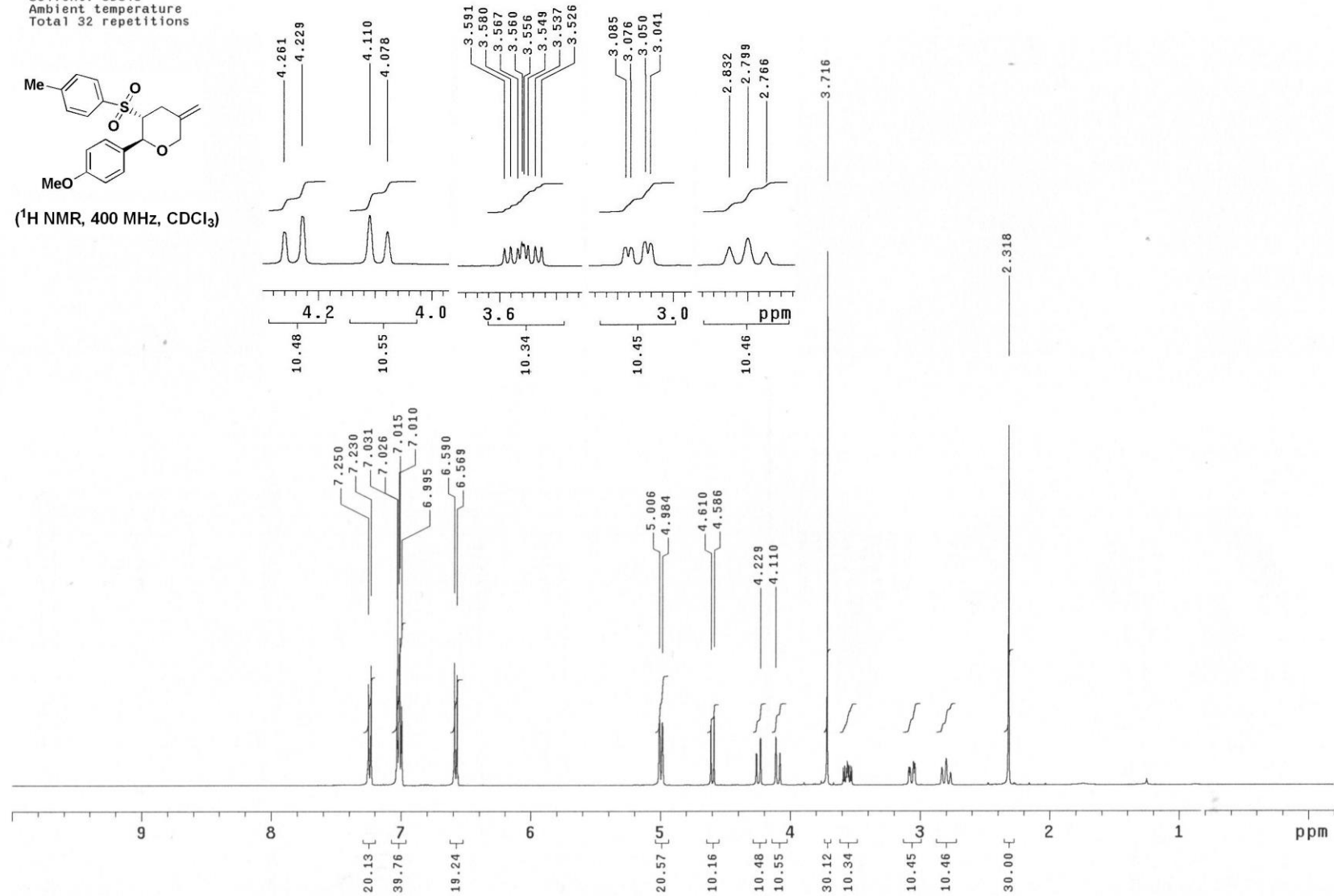
Compound 5n (¹H-NMR spectral data)

KT0424NB

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: May 8 2020
Solvent: CDCl₃
Ambient temperature
Total 32 repetitions



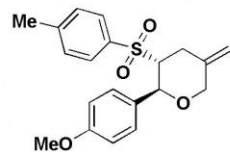
(¹H NMR, 400 MHz, CDCl₃)



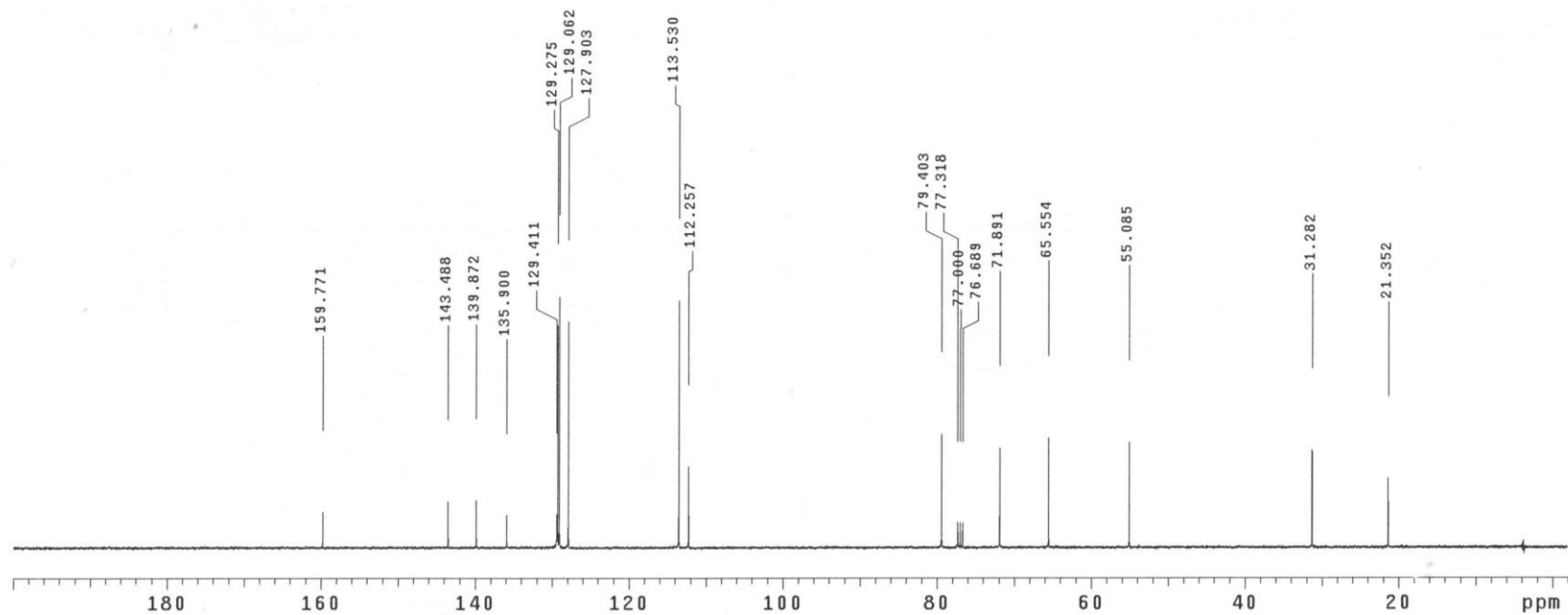
Compound 5n (¹³C-NMR spectral data)

KT0424NB

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: May 8 2020
Solvent: CDCl₃
Ambient temperature
Total 320 repetitions



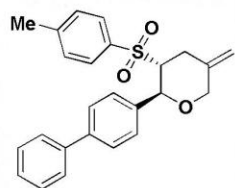
(¹³C NMR, 100 MHz, CDCl₃)



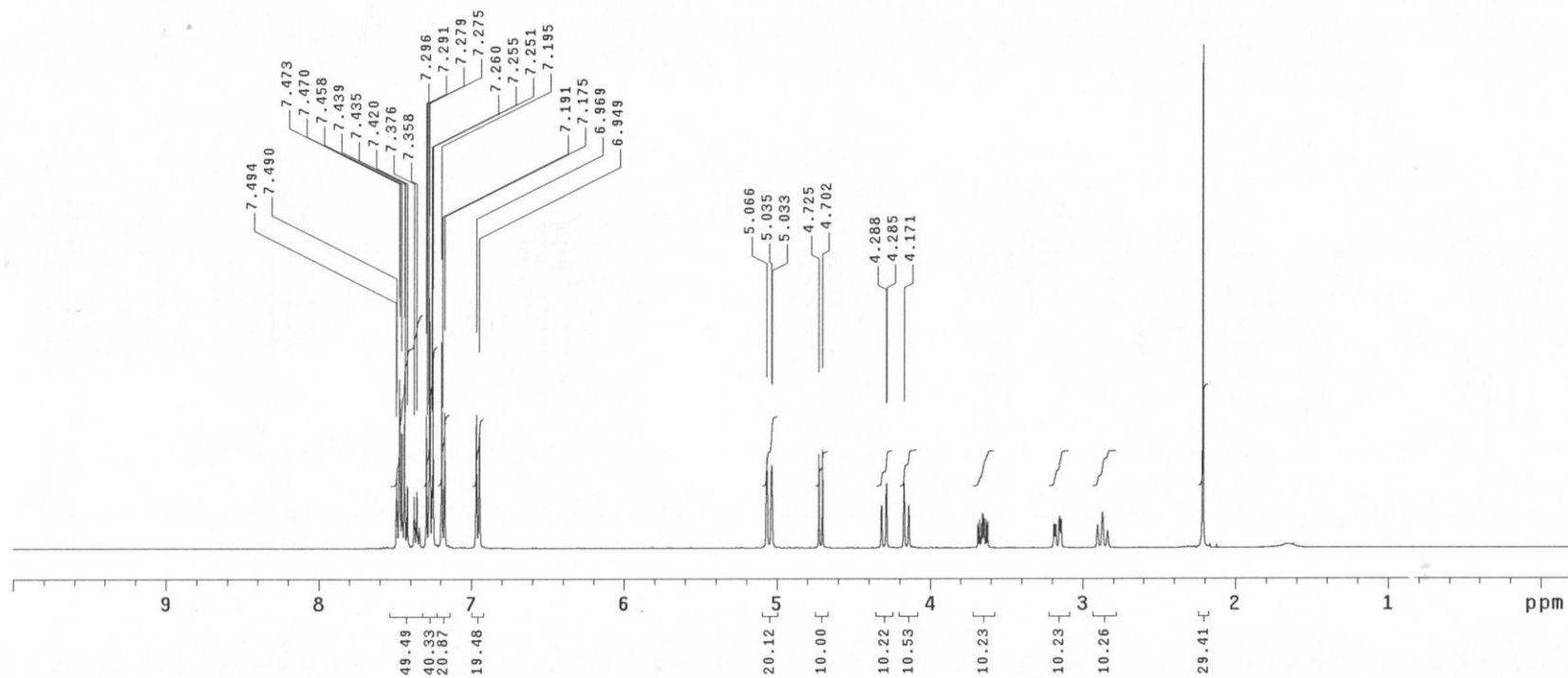
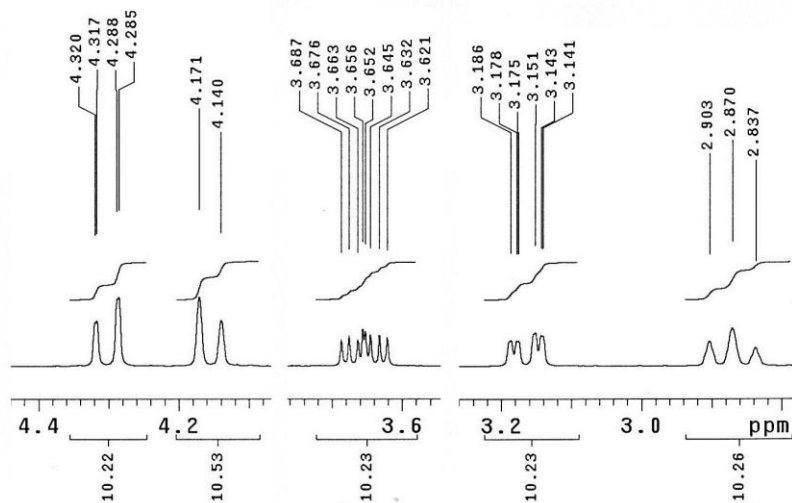
Compound 5q (¹H-NMR spectral data)

KT0505NB

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: May 18 2020
 Solvent: CDC13
 Ambient temperature
 Total 32 repetitions



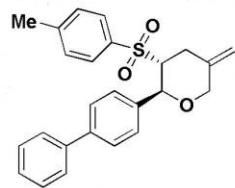
(¹H NMR, 400 MHz, CDCl₃)



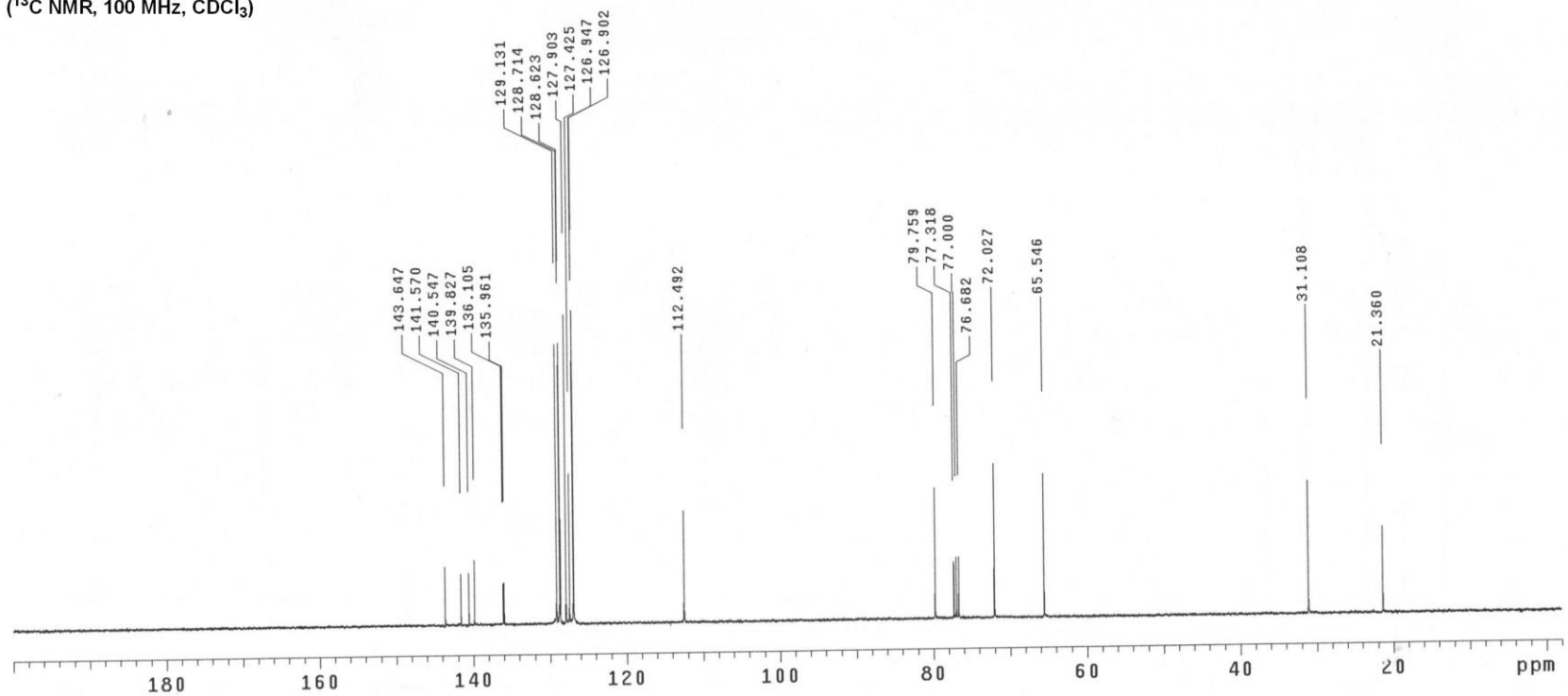
Compound 5q (¹³C-NMR spectral data)

KT0505NB

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: May 18 2020
Solvent: CDCl₃
Ambient temperature
Total 64000 repetitions



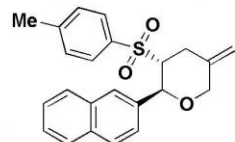
(¹³C NMR, 100 MHz, CDCl₃)



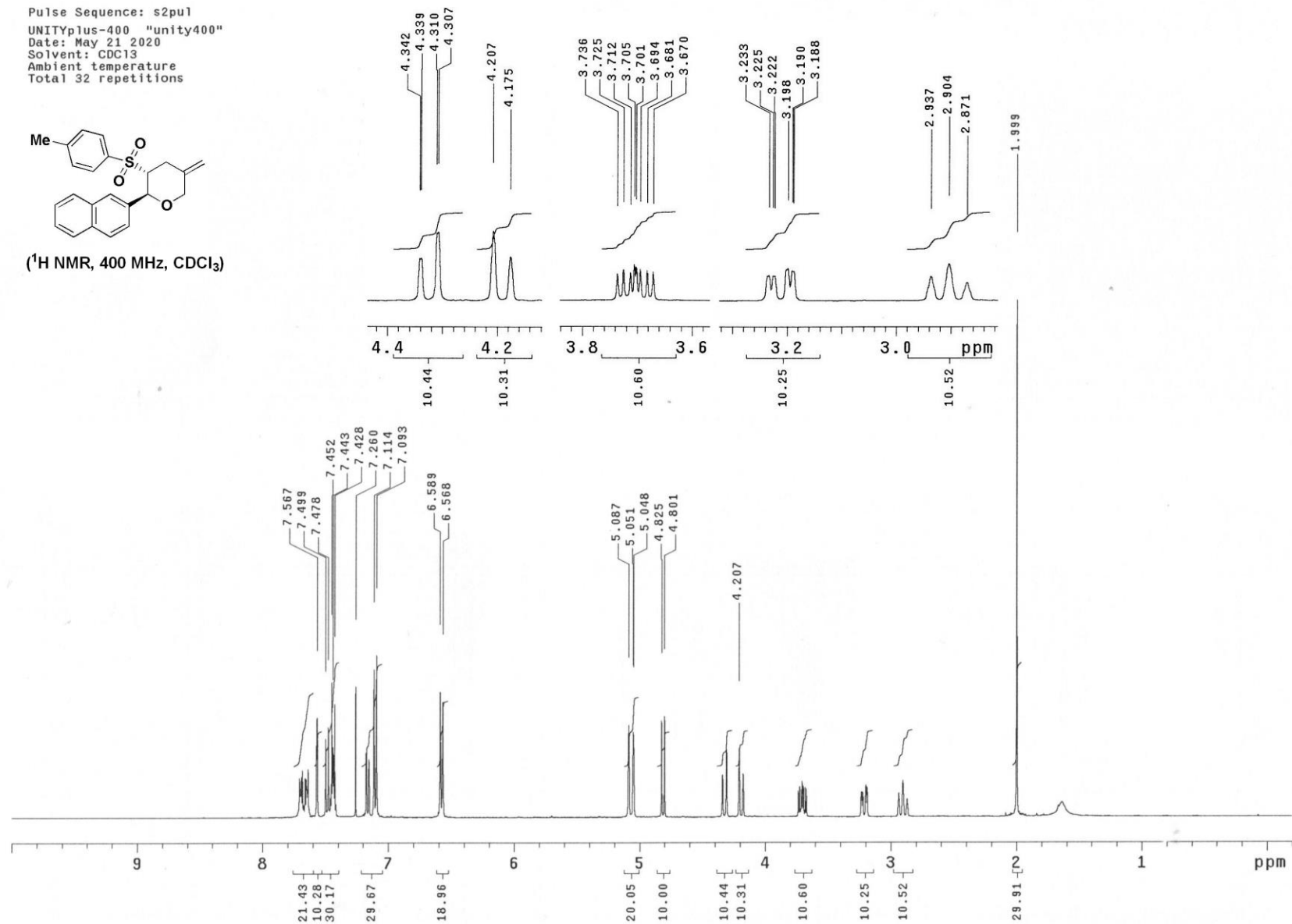
Compound 5r (¹H-NMR spectral data)

KT0513NB

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: May 21 2020
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetitions



(¹H NMR, 400 MHz, CDCl₃)



Compound 5r (¹³C-NMR spectral data)

KT0513NB

Pulse Sequence: s2pu1

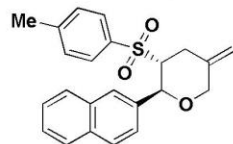
UNITYplus-400 "unity400"

Date: May 21 2020

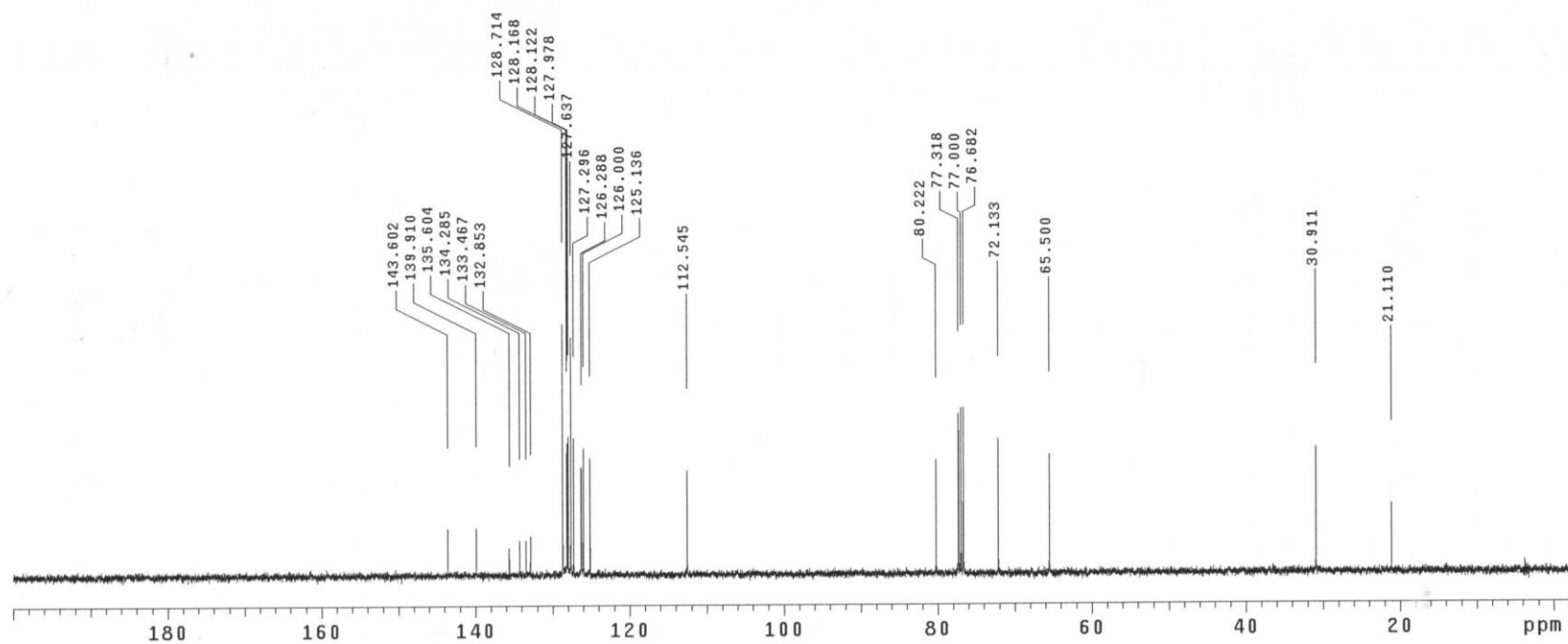
Solvent: CDCl₃

Ambient temperature

Total 2320 repetitions



(¹³C NMR, 100 MHz, CDCl₃)



Compound 5s (¹H-NMR spectral data)

KT0715NB

Pulse Sequence: s2pu1

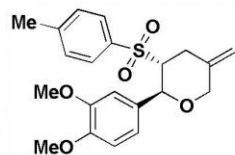
UNITYplus-400 "unity400"

Date: Aug 27 2020

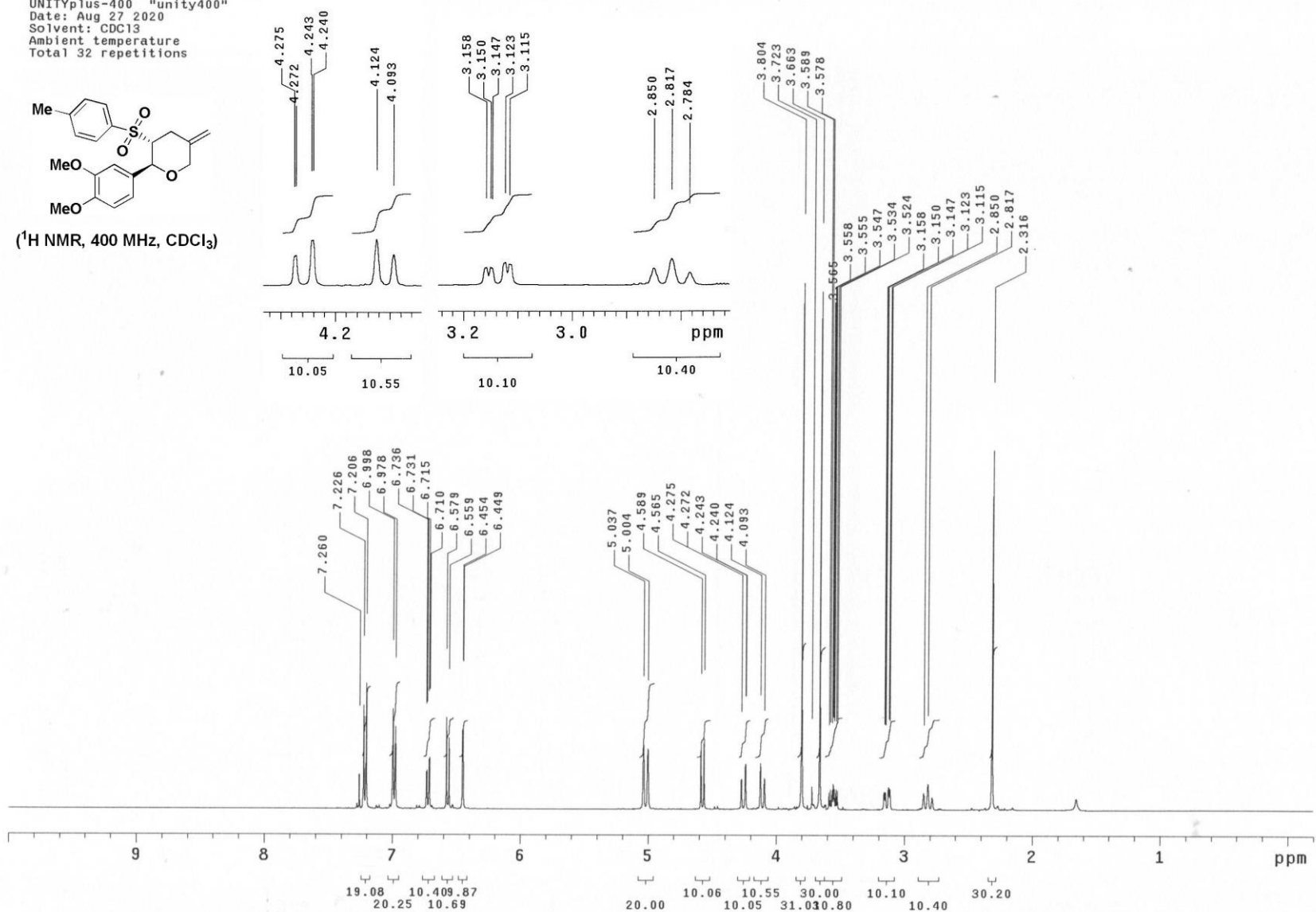
Solvent: CDCl₃

Ambient temperature

Total 32 repetitions



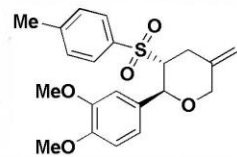
(¹H NMR, 400 MHz, CDCl₃)



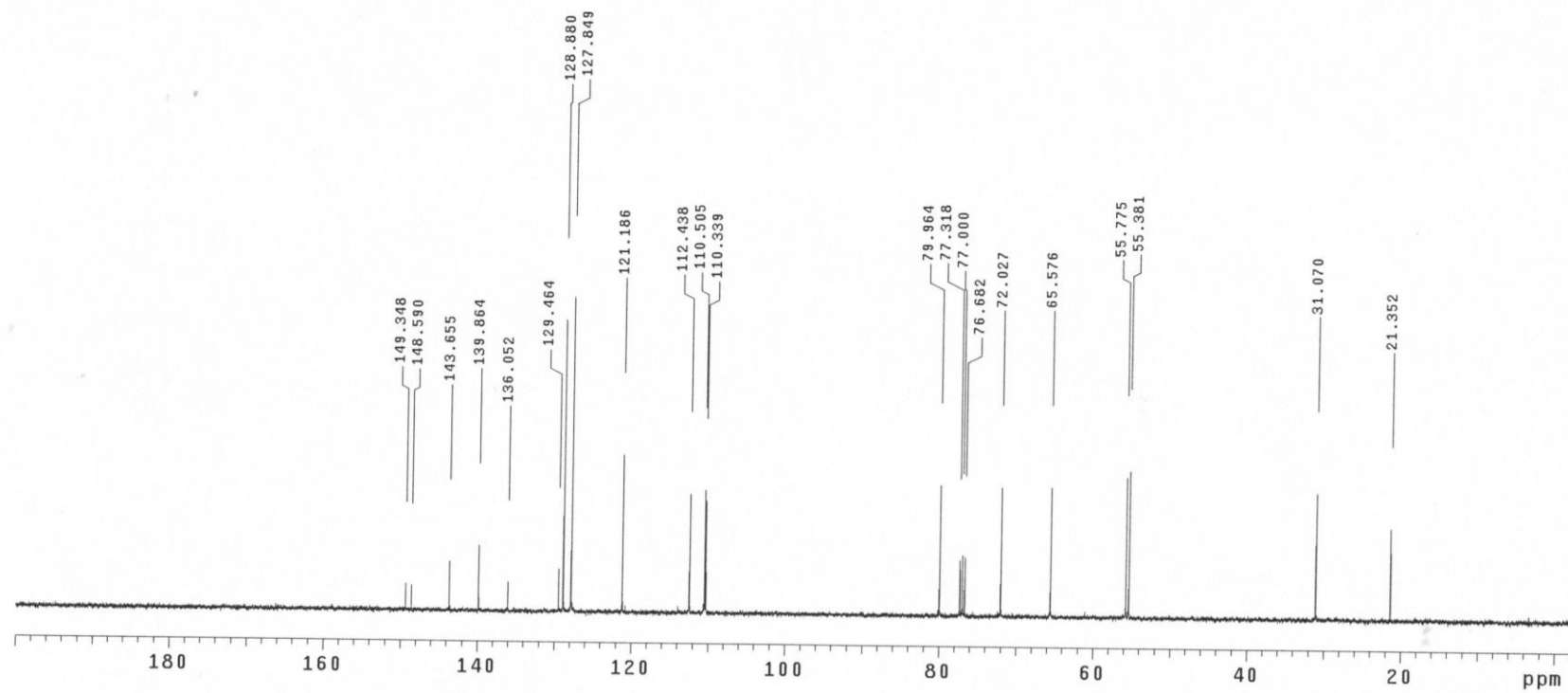
Compound 5s (¹³C-NMR spectral data)

KT0715NB

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Aug 27 2020
Solvent: CDCl₃
Ambient temperature
Total 912 repetitions



(¹³C NMR, 100 MHz, CDCl₃)



Compound 5t (¹H-NMR spectral data)

KT0713NB

Pulse Sequence: s2pu1

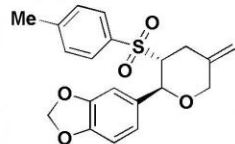
UNITYplus-400 "unity400"

Date: Jul 29 2020

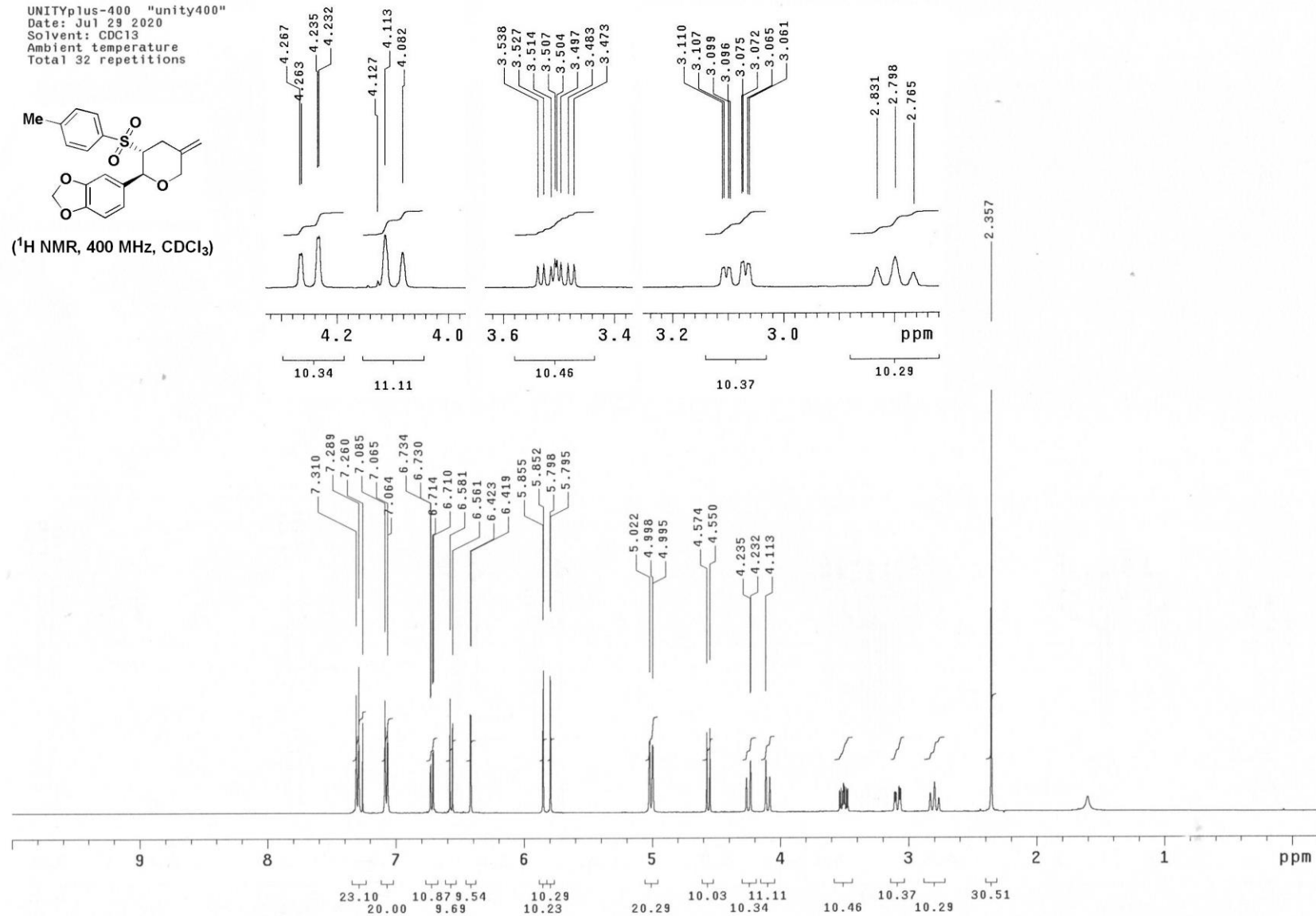
Solvent: CDCl₃

Ambient temperature

Total 32 repetitions



(¹H NMR, 400 MHz, CDCl₃)



Compound 5t (¹³C-NMR spectral data)

KT0713NB

Pulse Sequence: s2pu1

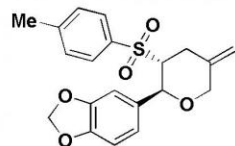
UNITYplus-400 "unity400"

Date: Jul 29 2020

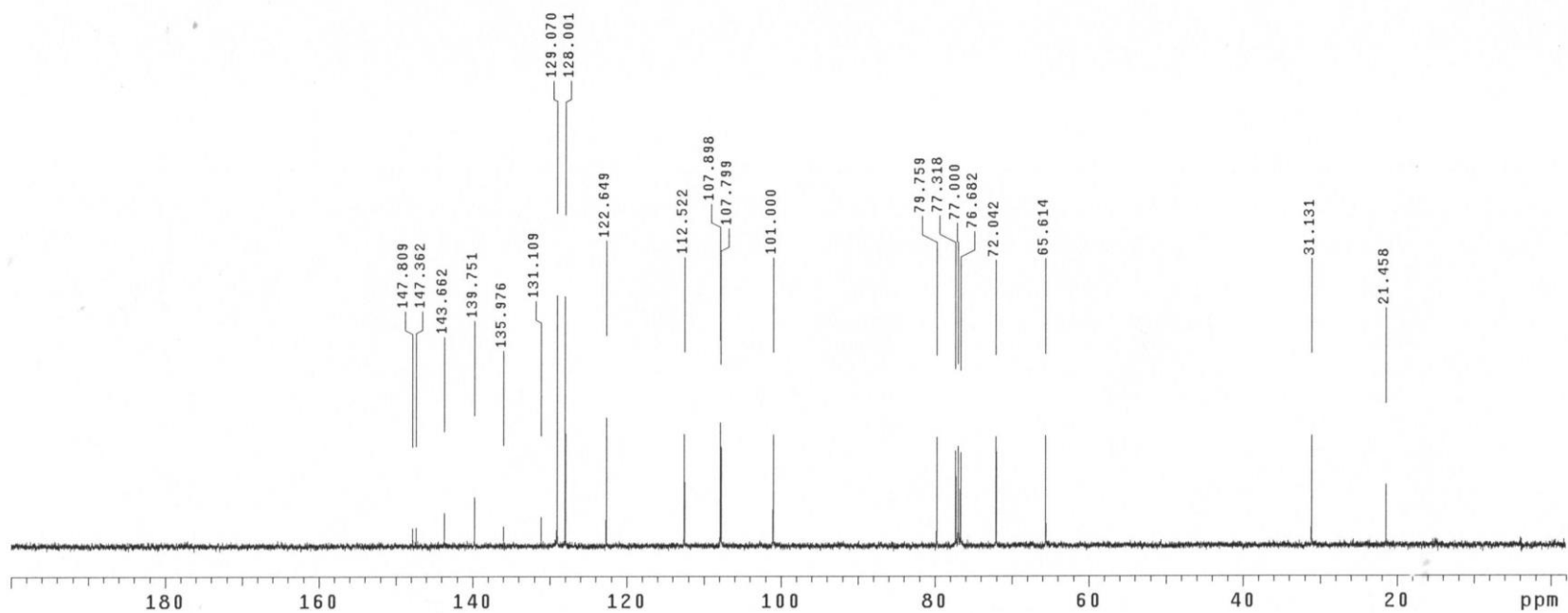
Solvent: CDCl₃

Ambient temperature

Total 1376 repetitions



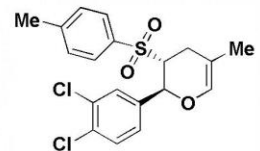
(¹³C NMR, 100 MHz, CDCl₃)



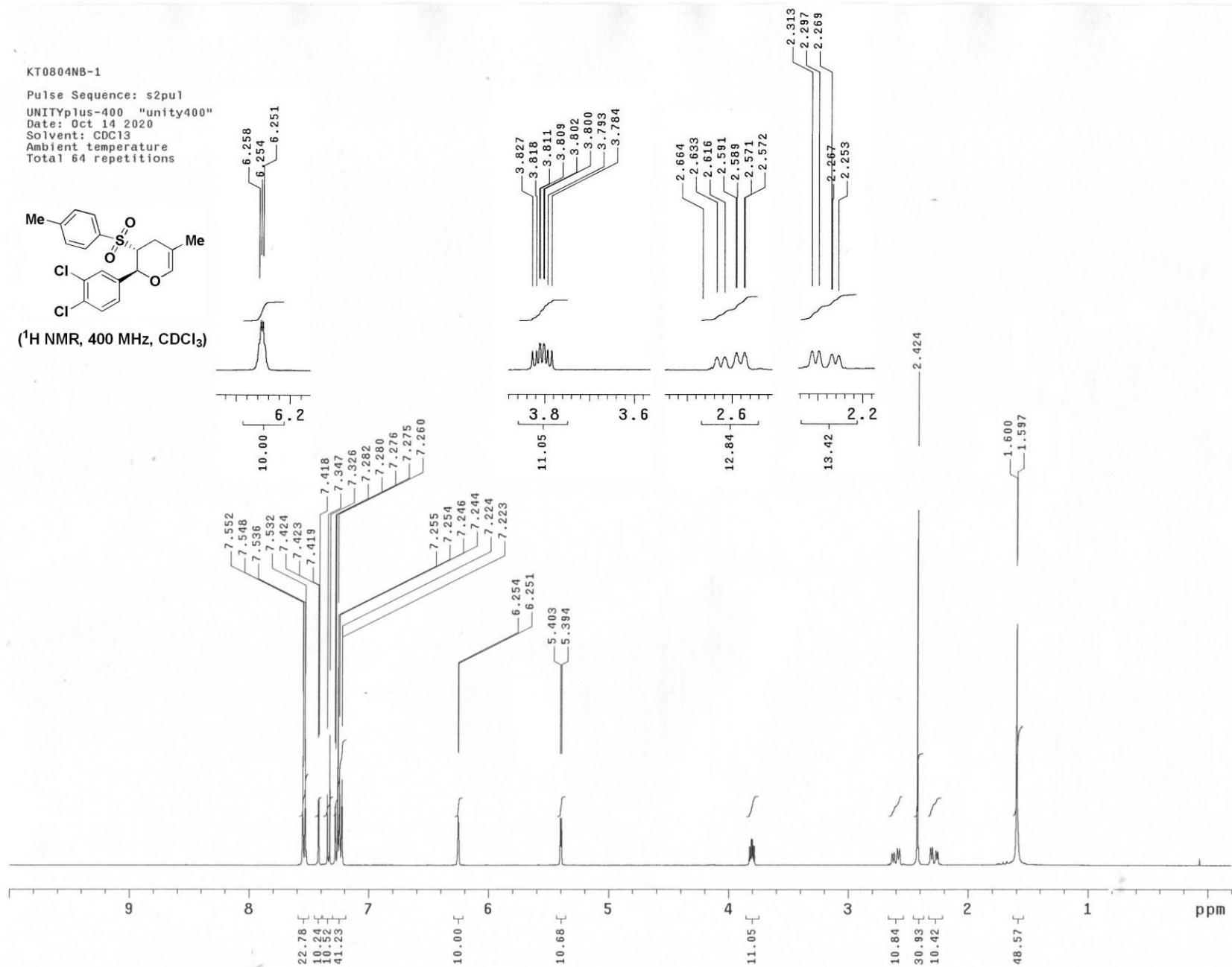
Compound 5u-1 (¹H-NMR spectral data)

KT0804NB-1

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Oct 14 2020
 Solvent: CDCl₃
 Ambient temperature
 Total 64 repetitions



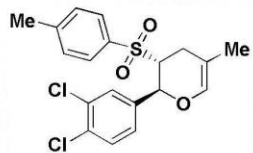
(¹H NMR, 400 MHz, CDCl₃)



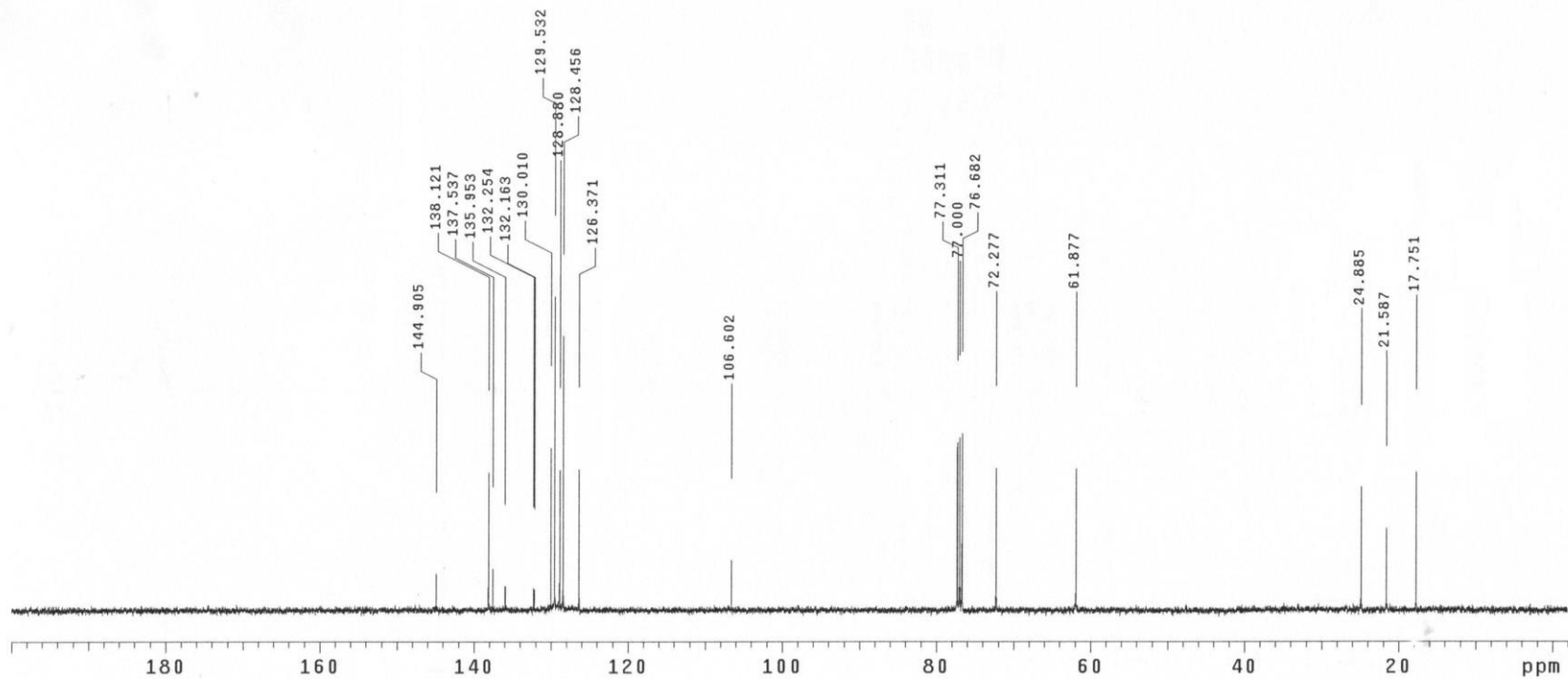
Compound 5u-1 (¹³C-NMR spectral data)

KT0804NB-1

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Oct 14 2020
Solvent: CDCl₃
Ambient temperature
Total 5008 repetitions



(¹³C NMR, 100 MHz, CDCl₃)



Compound 5v (¹H-NMR spectral data)

KT0810NB

Pulse Sequence: s2pu1

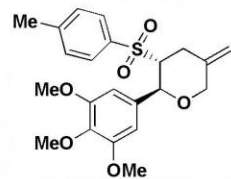
UNITYplus-400 "unity400"

Date: Sep 21 2020

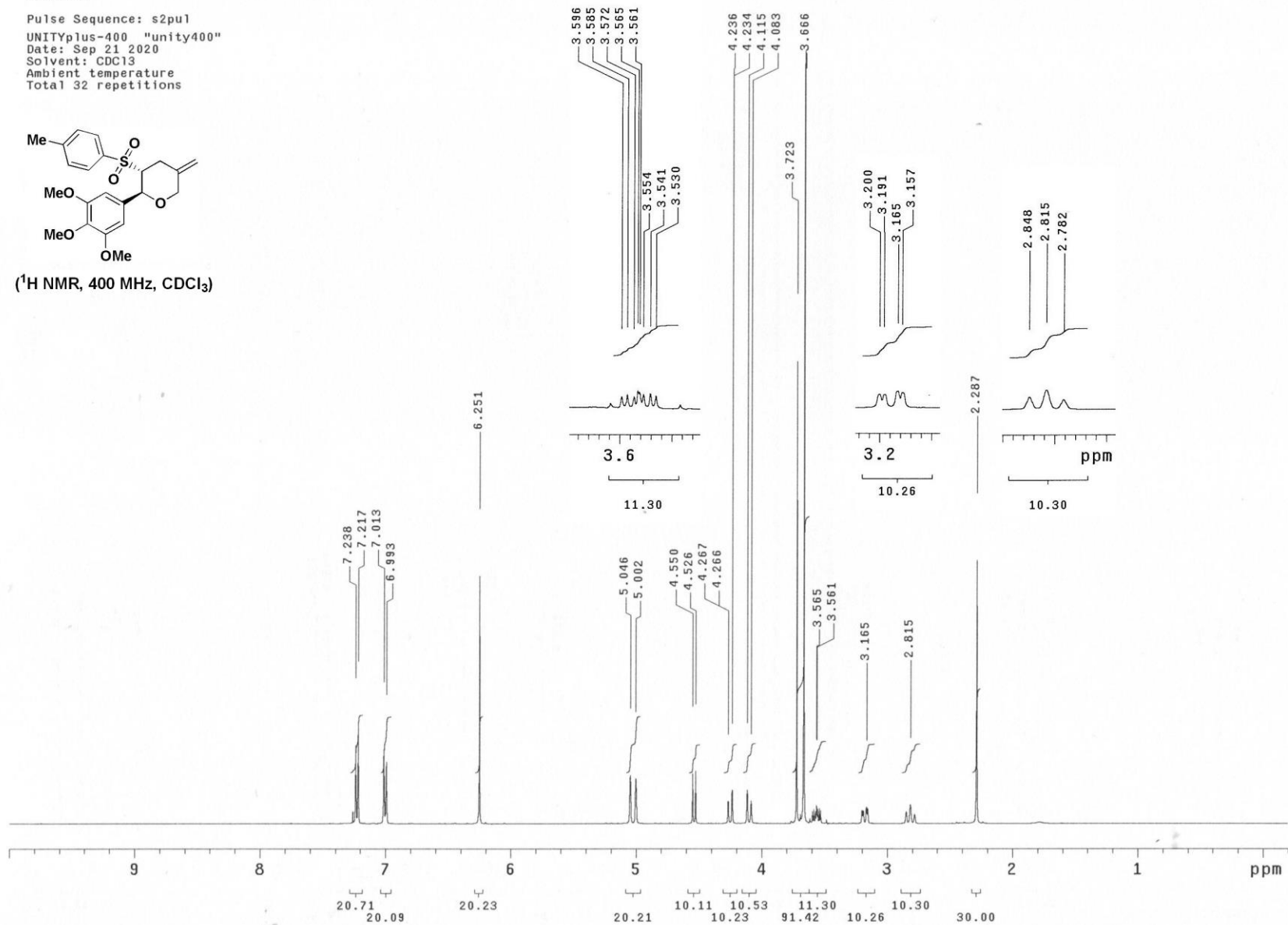
Solvent: CDCl₃

Ambient temperature

Total 32 repetitions



(¹H NMR, 400 MHz, CDCl₃)



Compound 5v (¹³C-NMR spectral data)

KT0810NB

Pulse Sequence: s2pu1

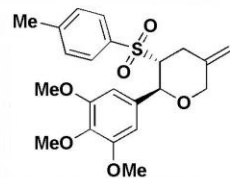
UNITYplus-400 "unity400"

Date: Sep 21 2020

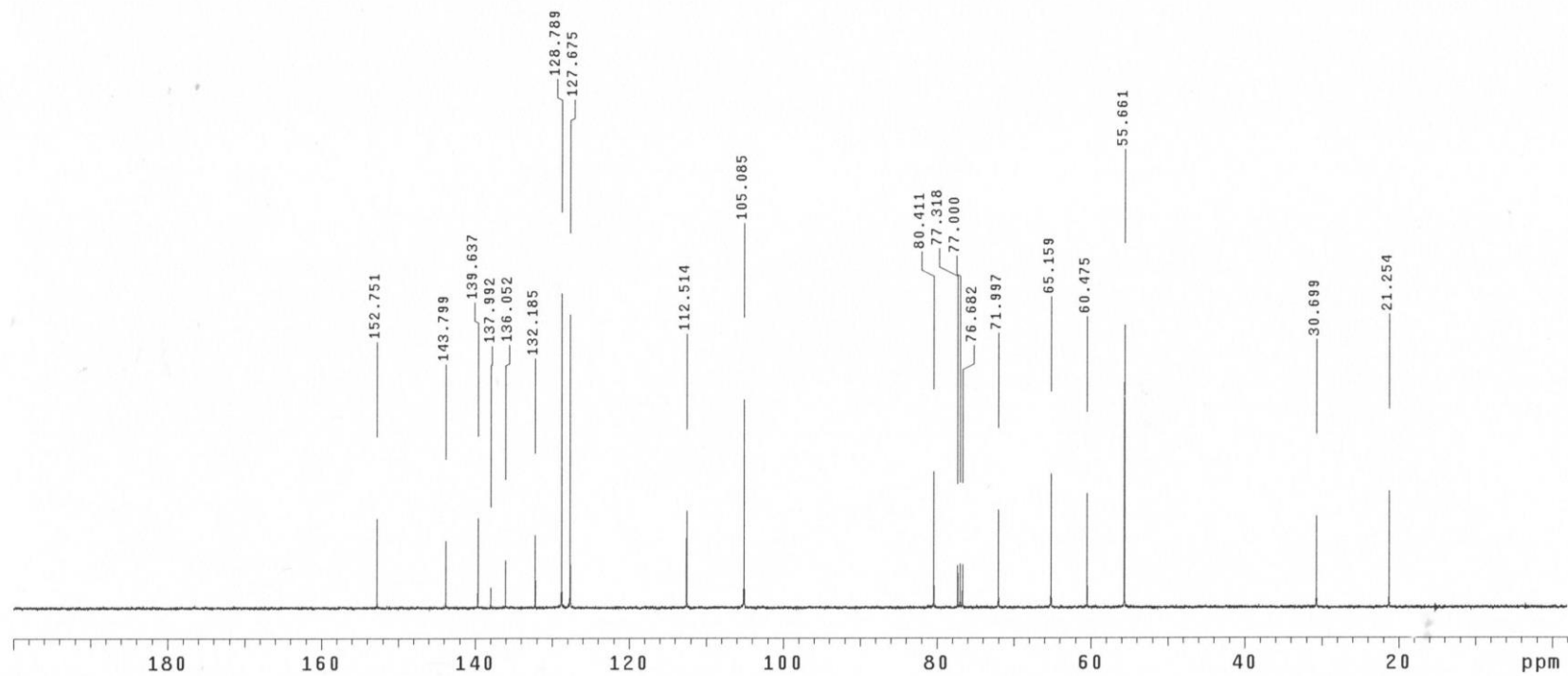
Solvent: CDCl₃

Ambient temperature

Total 720 repetitions



(¹³C NMR, 100 MHz, CDCl₃)



Compound 5w (¹H-NMR spectral data)

KT0813NB

Pulse Sequence: s2pu1

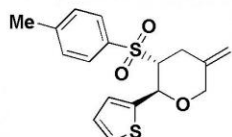
UNITYplus-400 "unity400"

Date: Aug 27 2020

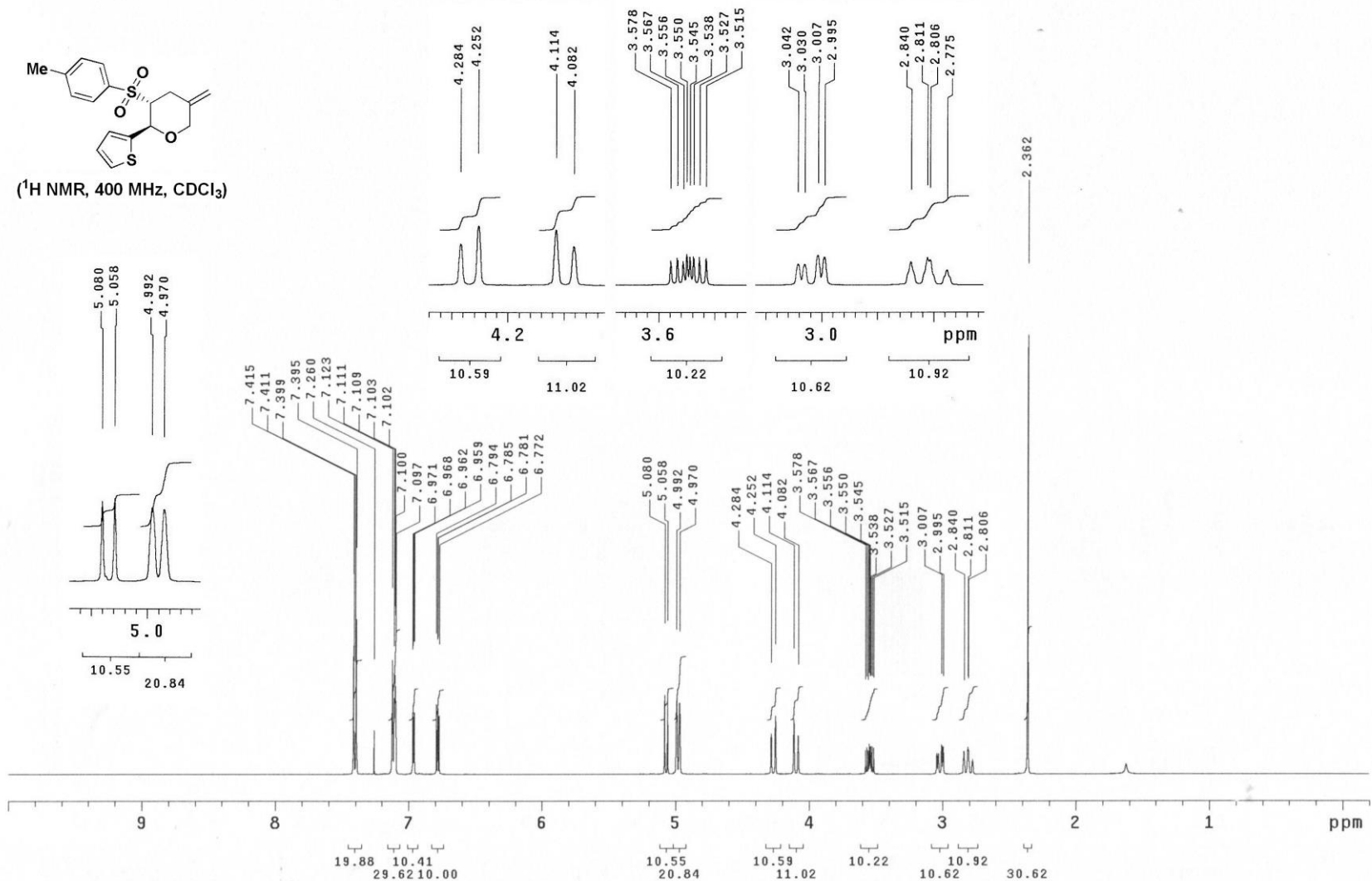
Solvent: CDCl₃

Ambient temperature

Total 32 repetitions



(¹H NMR, 400 MHz, CDCl₃)



Compound 5w (¹³C-NMR spectral data)

KT0813NB

Pulse Sequence: s2pu1

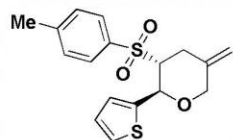
UNITYplus-400 "unity400"

Date: Aug 27 2020

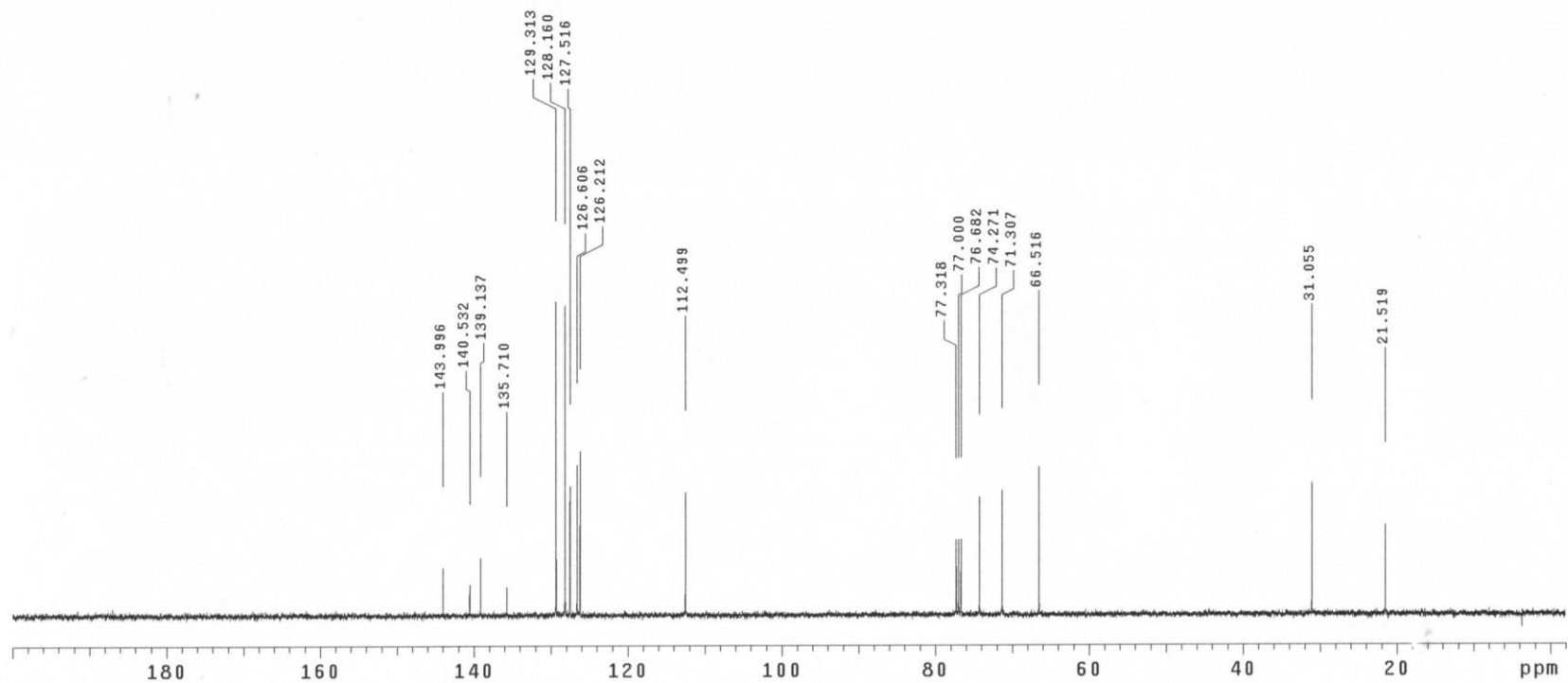
Solvent: CDCl₃

Ambient temperature

Total 576 repetitions



(¹³C NMR, 100 MHz, CDCl₃)



Compound 7a (¹H-NMR spectral data)

KT0416

Pulse Sequence: s2pu1

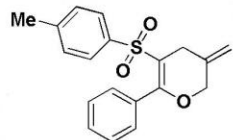
UNITYplus-400 "unity400"

Date: Apr 16 2020

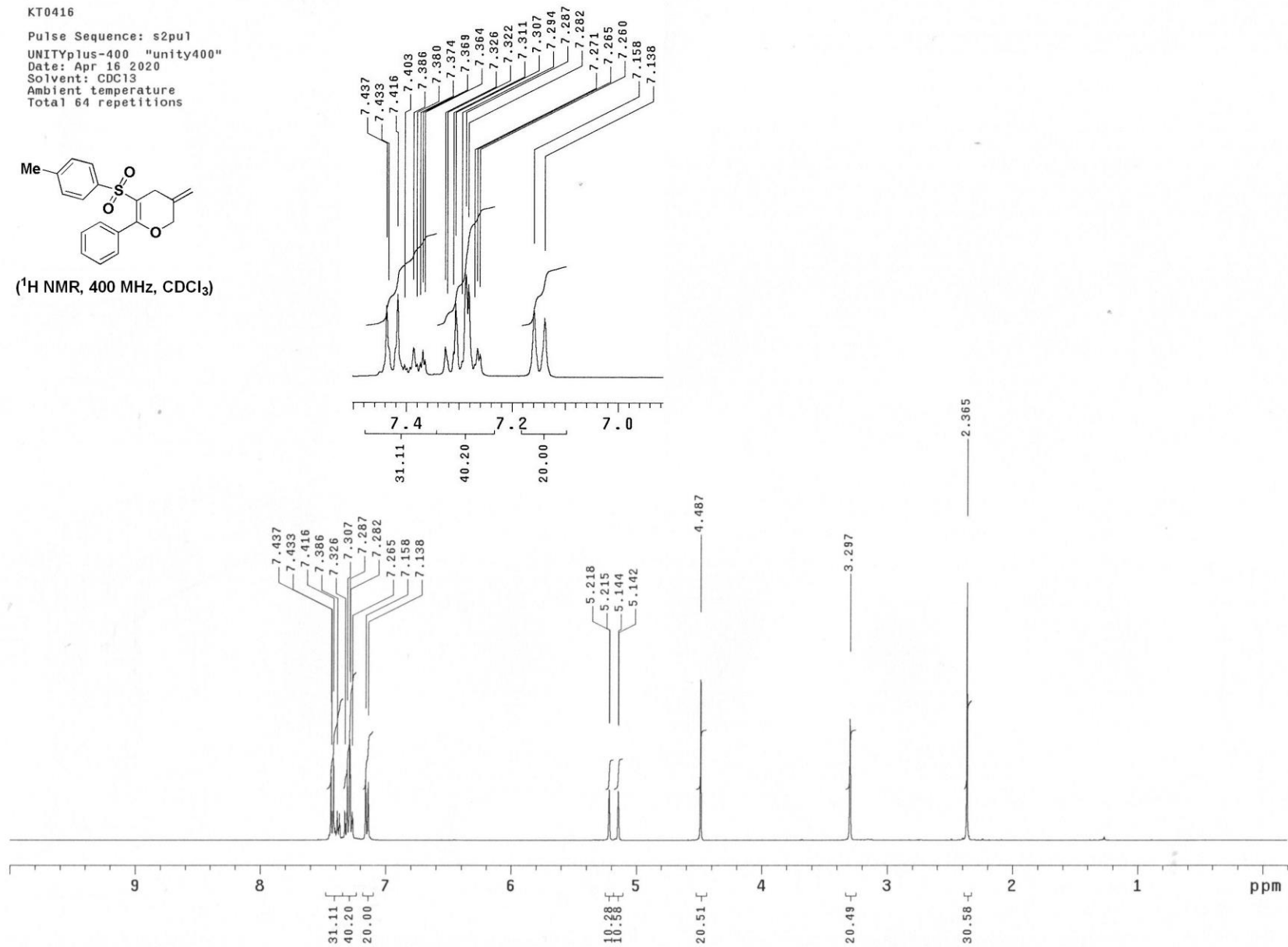
Solvent: CDCl₃

Ambient temperature

Total 64 repetitions



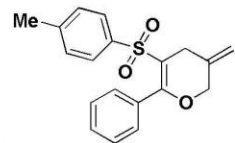
(¹H NMR, 400 MHz, CDCl₃)



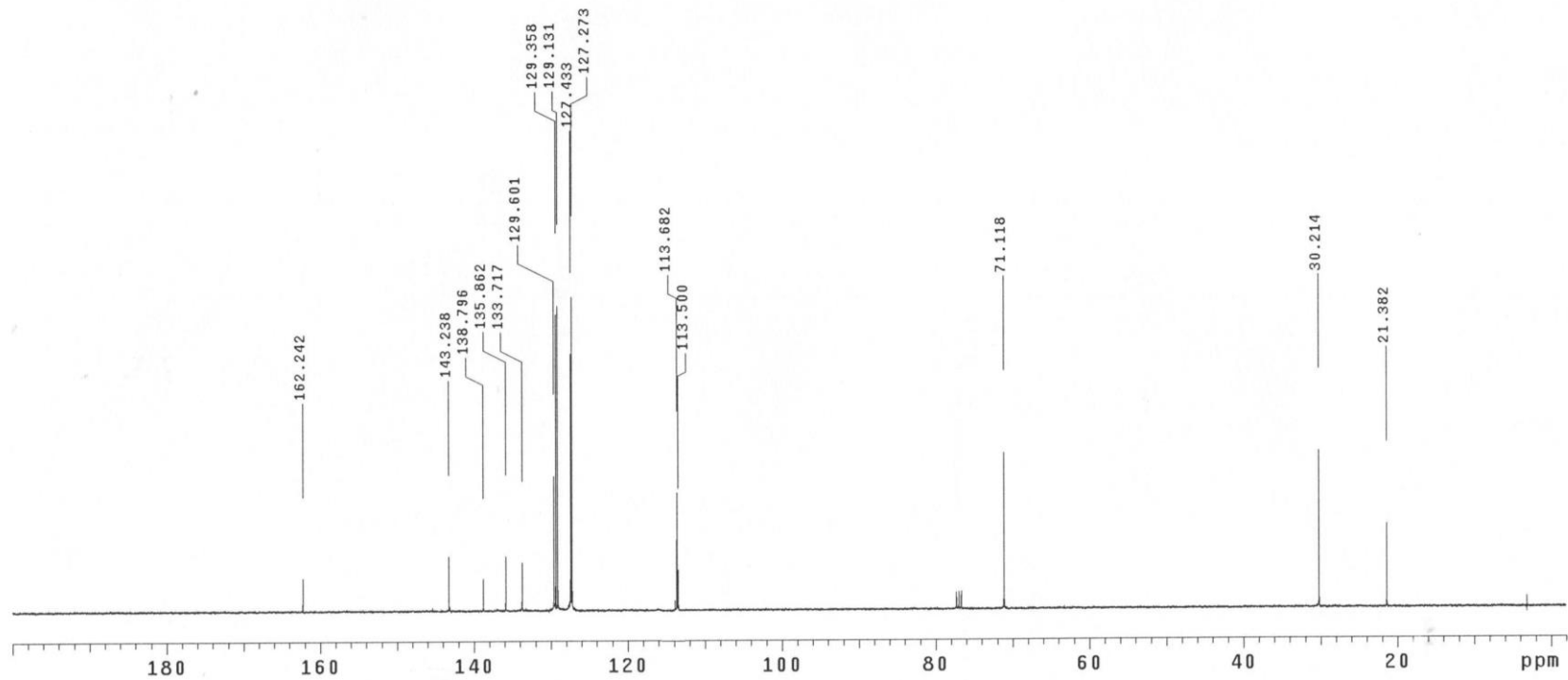
Compound 7a (¹³C-NMR spectral data)

KT0416

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Apr 16 2020
Solvent: CDCl₃
Ambient temperature
Total 800 repetitions



(¹³C NMR, 100 MHz, CDCl₃)



Compound 7b (¹H-NMR spectral data)

KT0506-6

Pulse Sequence: s2pu1

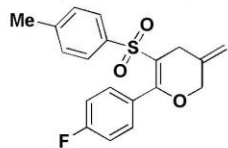
UNITYplus-400 "unity400"

Date: May 12 2020

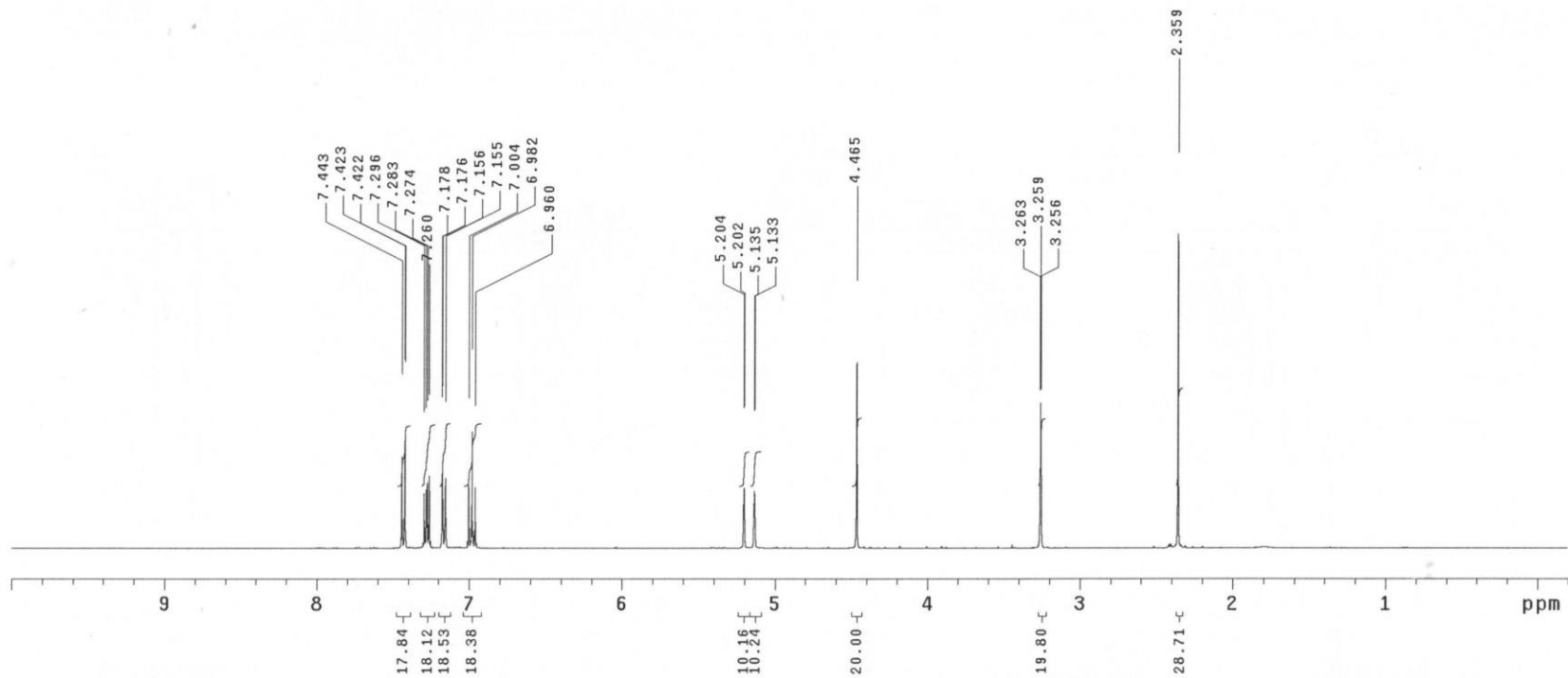
Solvent: CDCl₃

Ambient temperature

Total 32 repetitions



(¹H NMR, 400 MHz, CDCl₃)



Compound 7b (¹³C-NMR spectral data)

KT0506-6

Pulse Sequence: s2pu1

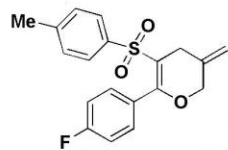
UNITYplus-400 "unity400"

Date: May 12 2020

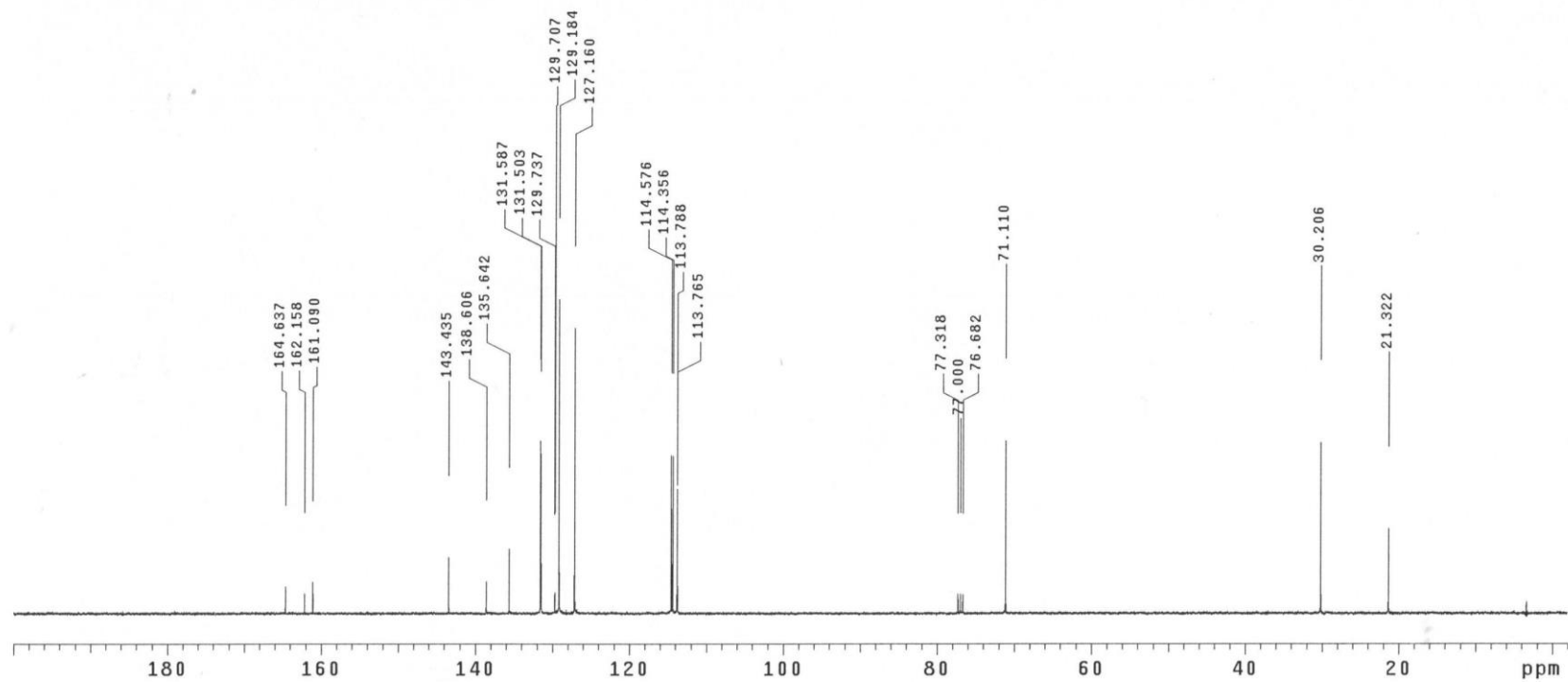
Solvent: CDCl₃

Ambient temperature

Total 240 repetitions



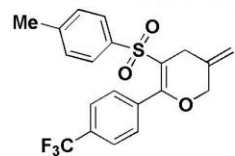
(¹³C NMR, 100 MHz, CDCl₃)



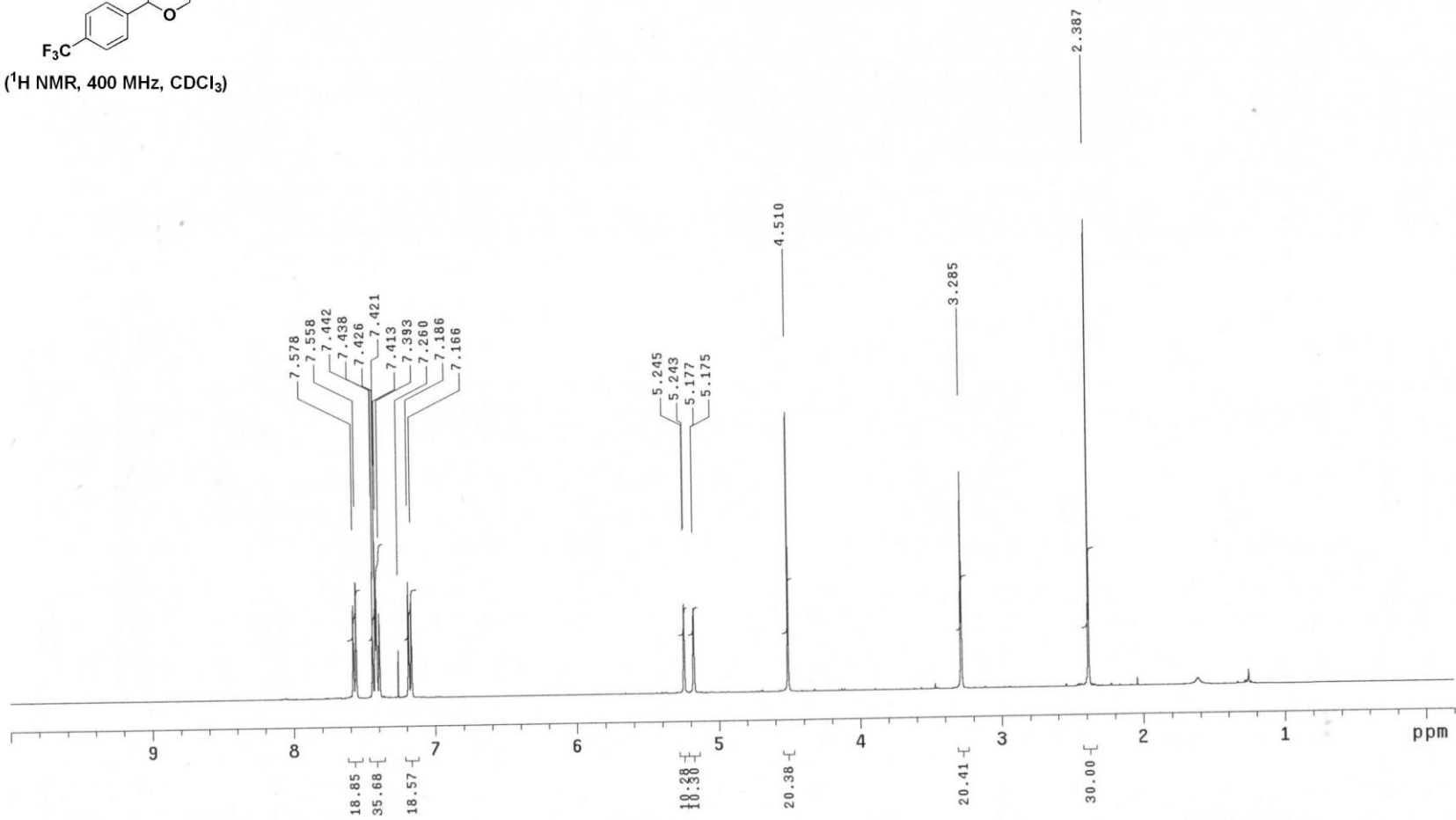
Compound 7c (¹H-NMR spectral data)

KT0423

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Apr 23 2020
Solvent: CDCl₃
Ambient temperature
Total 32 repetitions



(¹H NMR, 400 MHz, CDCl₃)



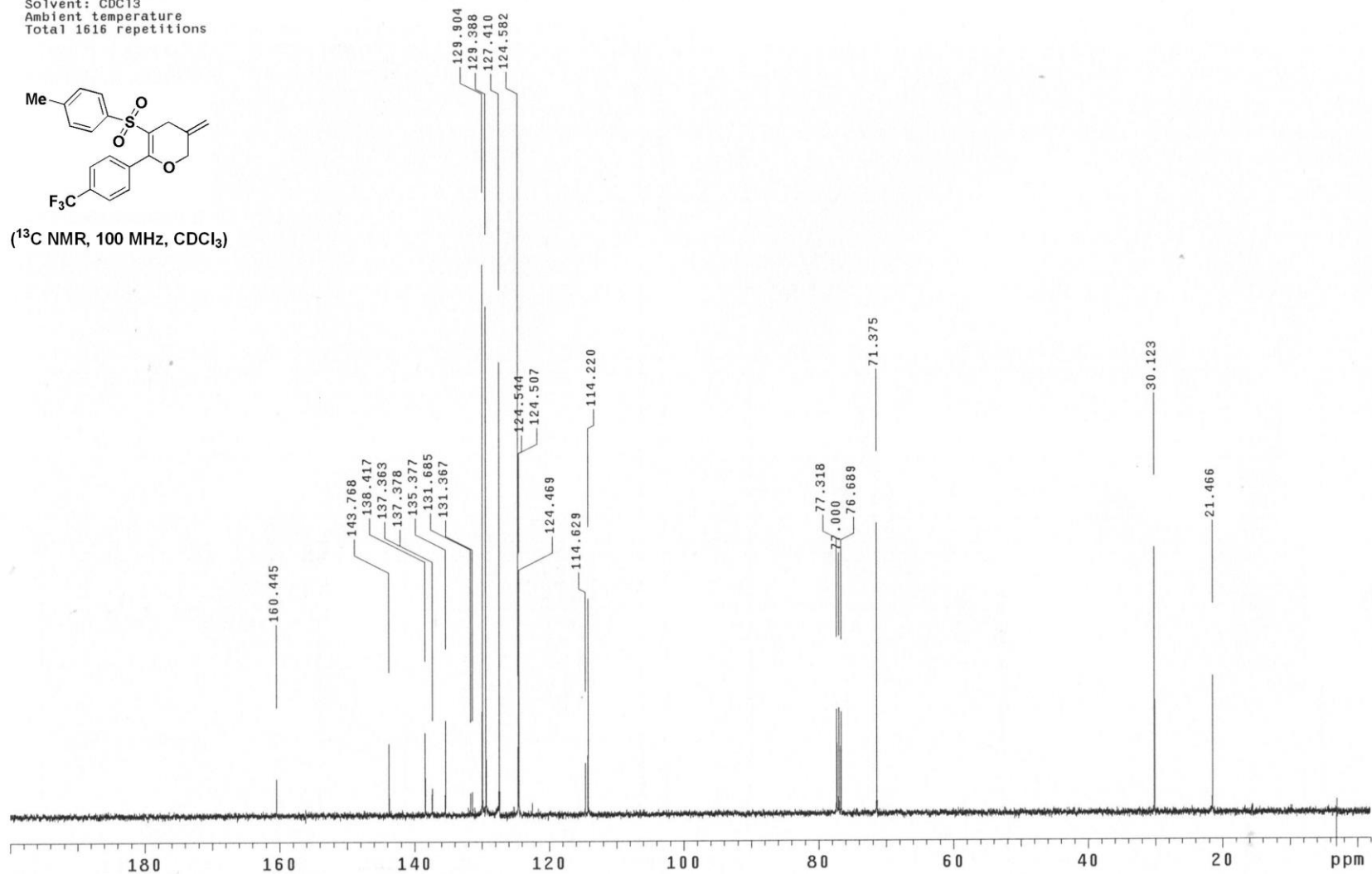
Compound 7c (^{13}C -NMR spectral data)

KT0423

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Apr 23 2020
Solvent: CDCl_3
Ambient temperature
Total 1616 repetitions



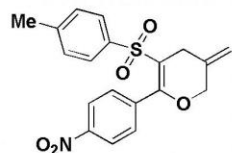
(^{13}C NMR, 100 MHz, CDCl_3)



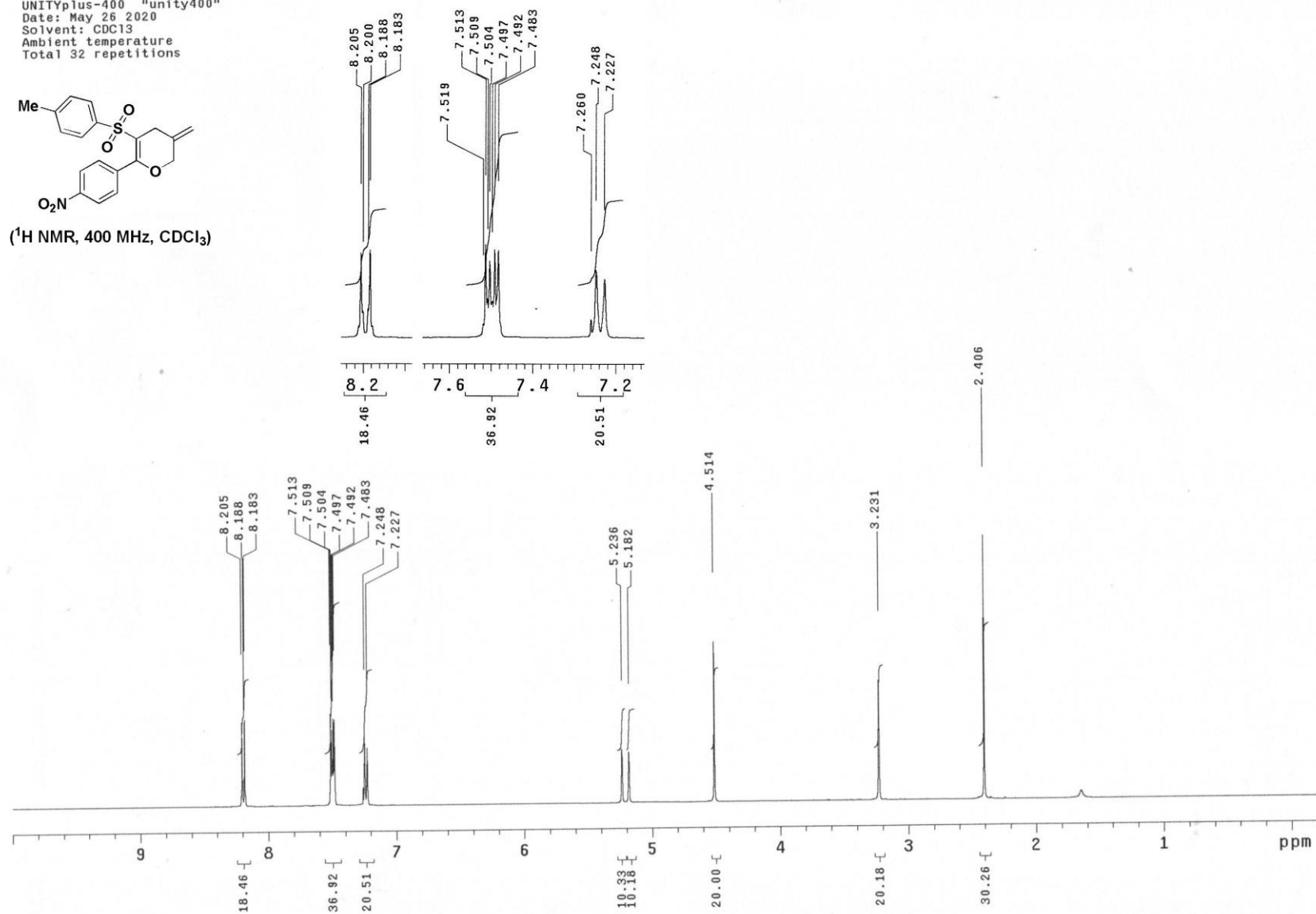
Compound 7d (¹H-NMR spectral data)

KT0526-6

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: May 26 2020
Solvent: CDCl₃
Ambient temperature
Total 32 repetitions



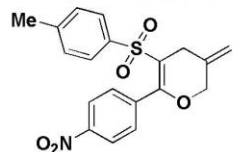
(¹H NMR, 400 MHz, CDCl₃)



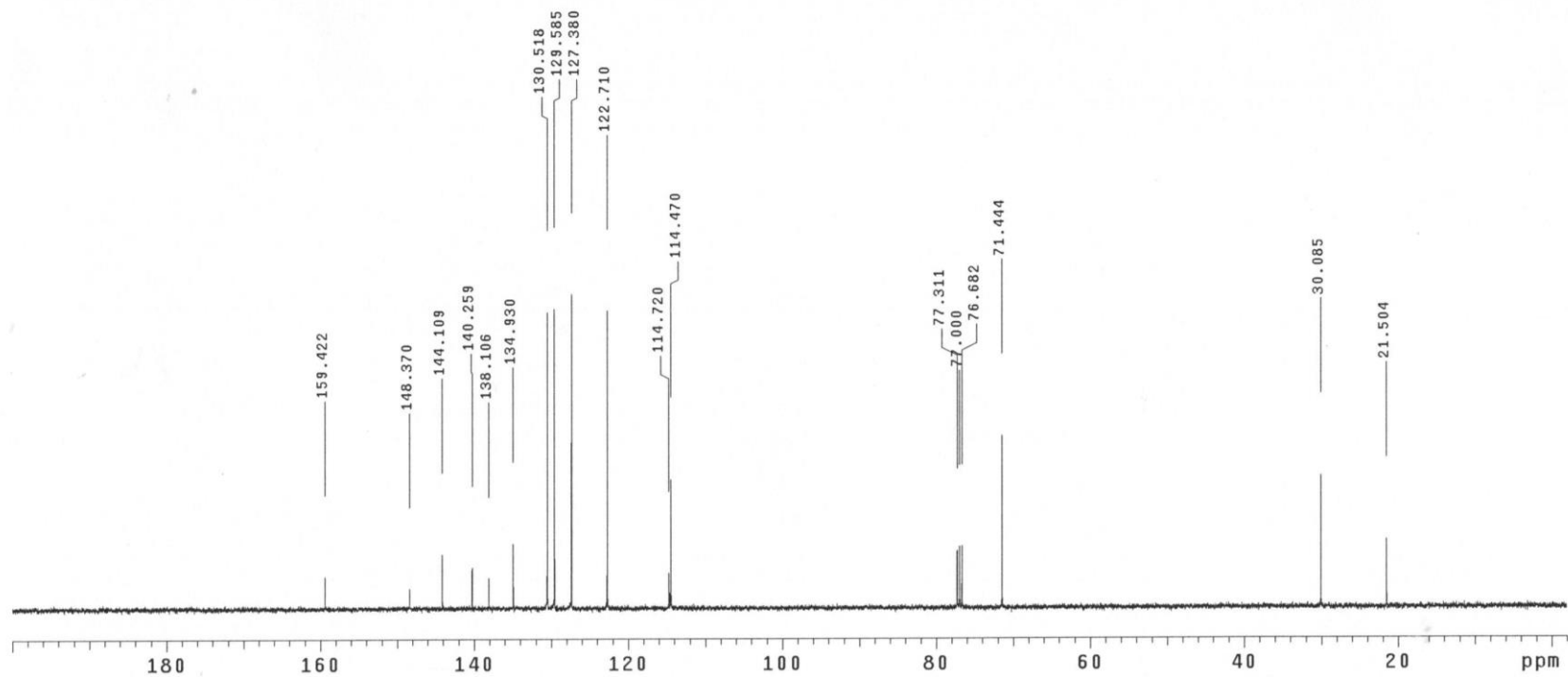
Compound 7d (¹³C-NMR spectral data)

KT0526-6

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: May 26 2020
Solvent: CDCl₃
Ambient temperature
Total 640 repetitions



(¹³C NMR, 100 MHz, CDCl₃)



Compound 7e (¹H-NMR spectral data)

KT0804-6

Pulse Sequence: s2pu1

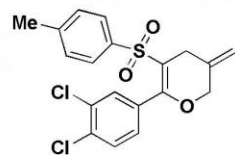
UNITYplus-400 "unity400"

Date: Aug 5 2020

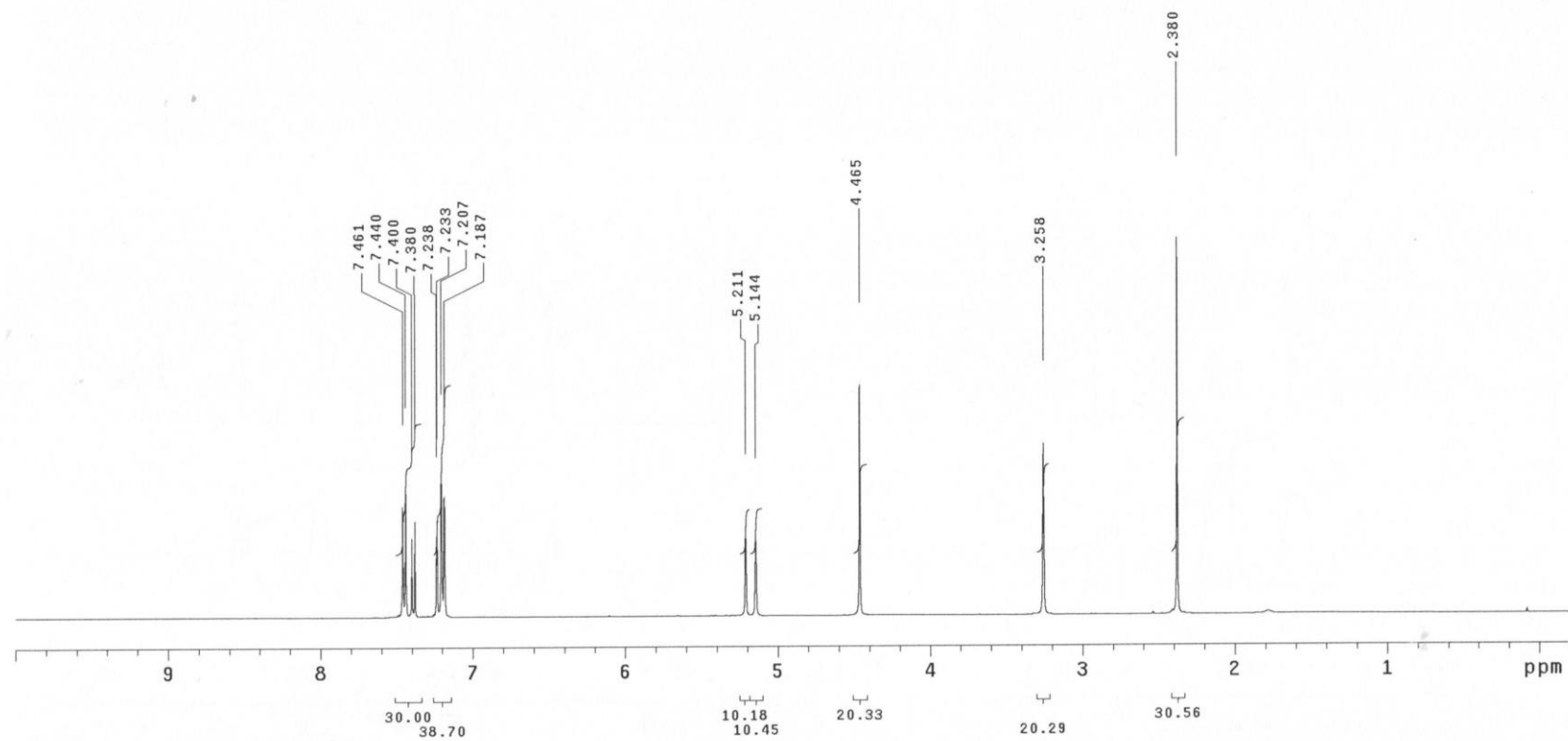
Solvent: CDCl₃

Ambient temperature

Total 32 repetitions



(¹H NMR, 400 MHz, CDCl₃)



Compound 7e (¹³C-NMR spectral data)

KT0804-6

Pulse Sequence: s2pu1

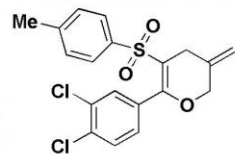
UNITYplus-400 "unity400"

Date: Aug 5 2020

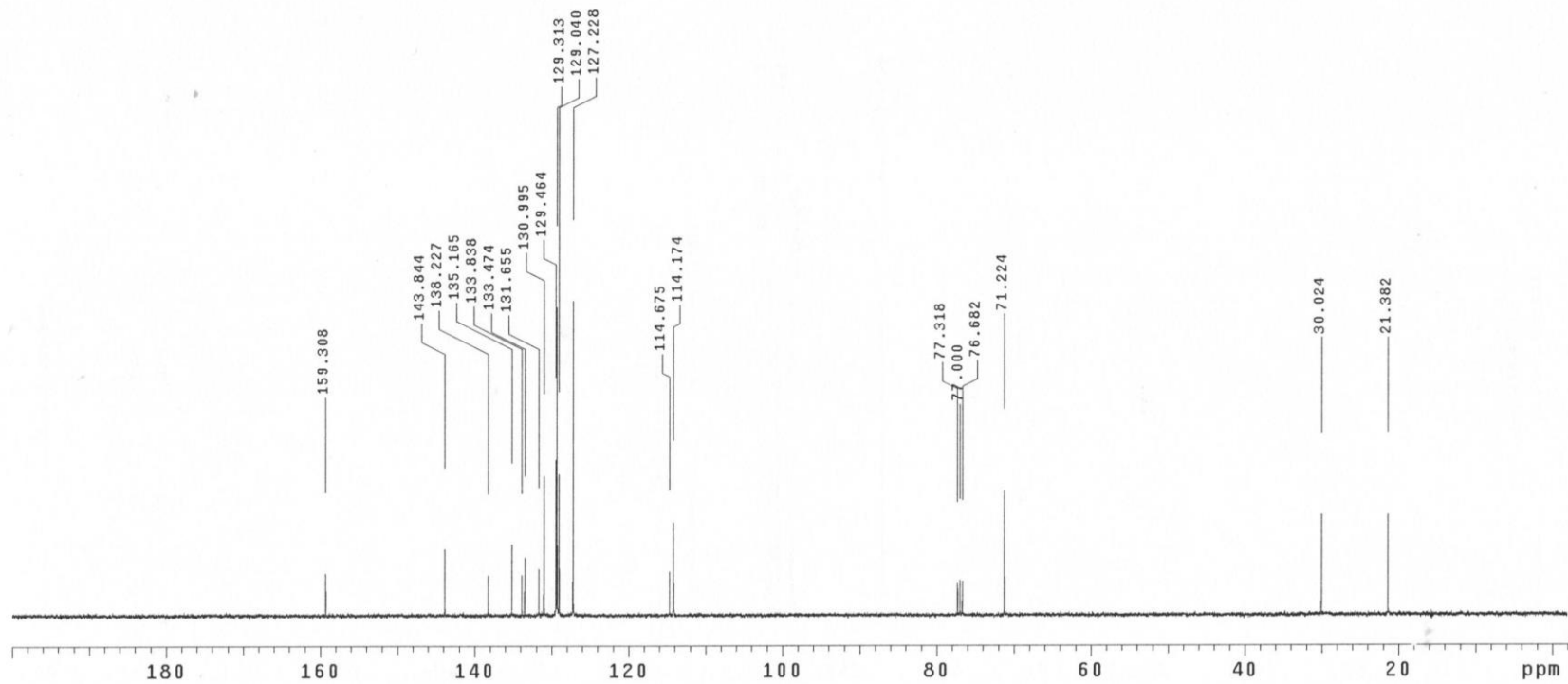
Solvent: CDCl₃

Ambient temperature

Total 112 repetitions



(¹³C NMR, 100 MHz, CDCl₃)



Compound 8 (¹H-NMR spectral data)

KT1090519-1

Pulse Sequence: s2pu1

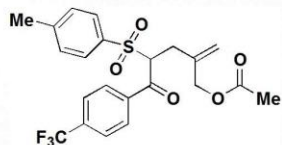
UNITYplus-400 "unity400"

Date: May 19 2020

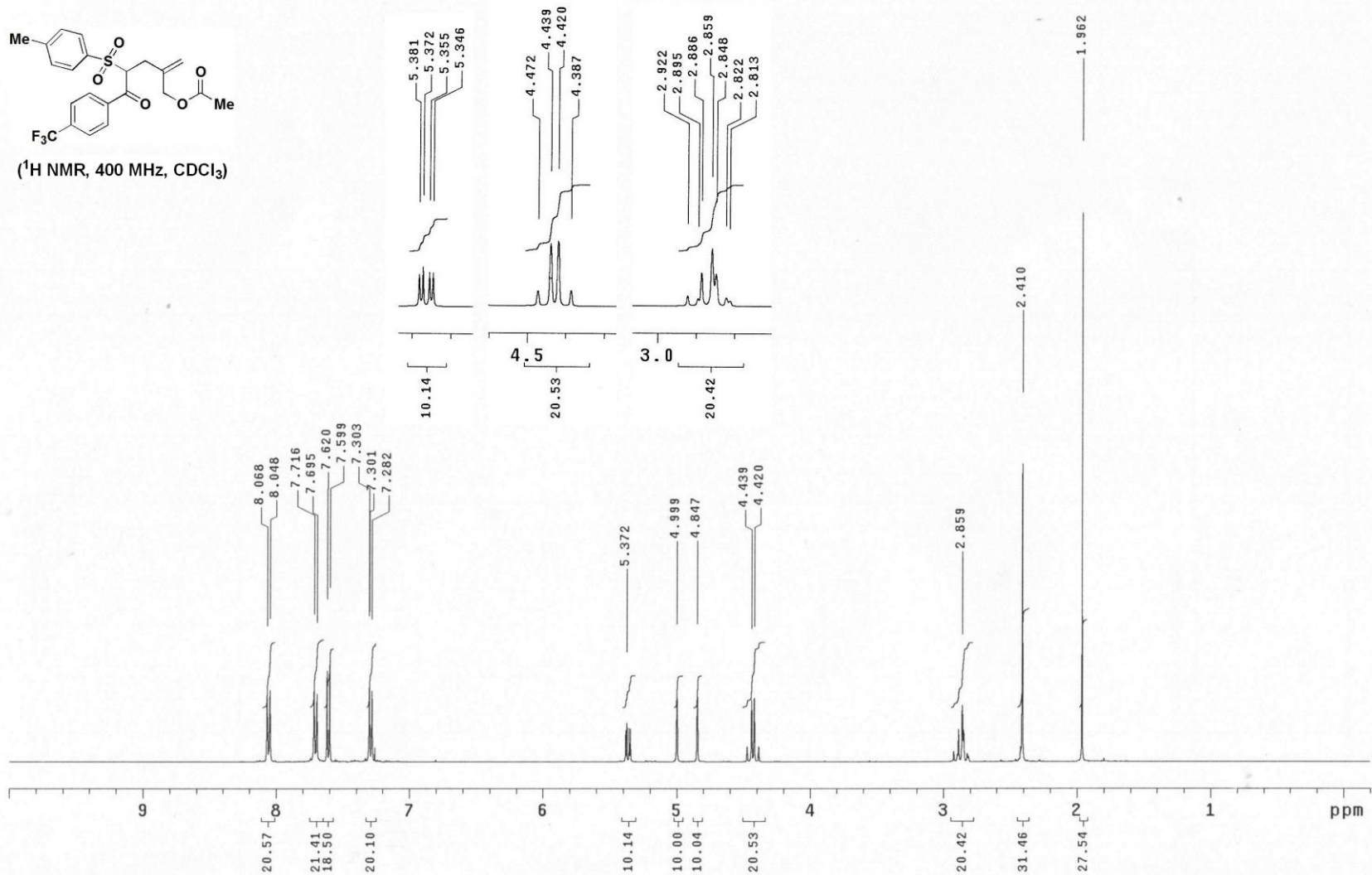
Solvent: CDCl₃

Ambient temperature

Total 32 repetitions



(¹H NMR, 400 MHz, CDCl₃)



Compound 8 (¹³C-NMR spectral data)

KT1090519-1

Pulse Sequence: s2pu1

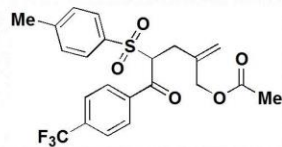
UNITYplus-400 "unity400"

Date: May 19 2020

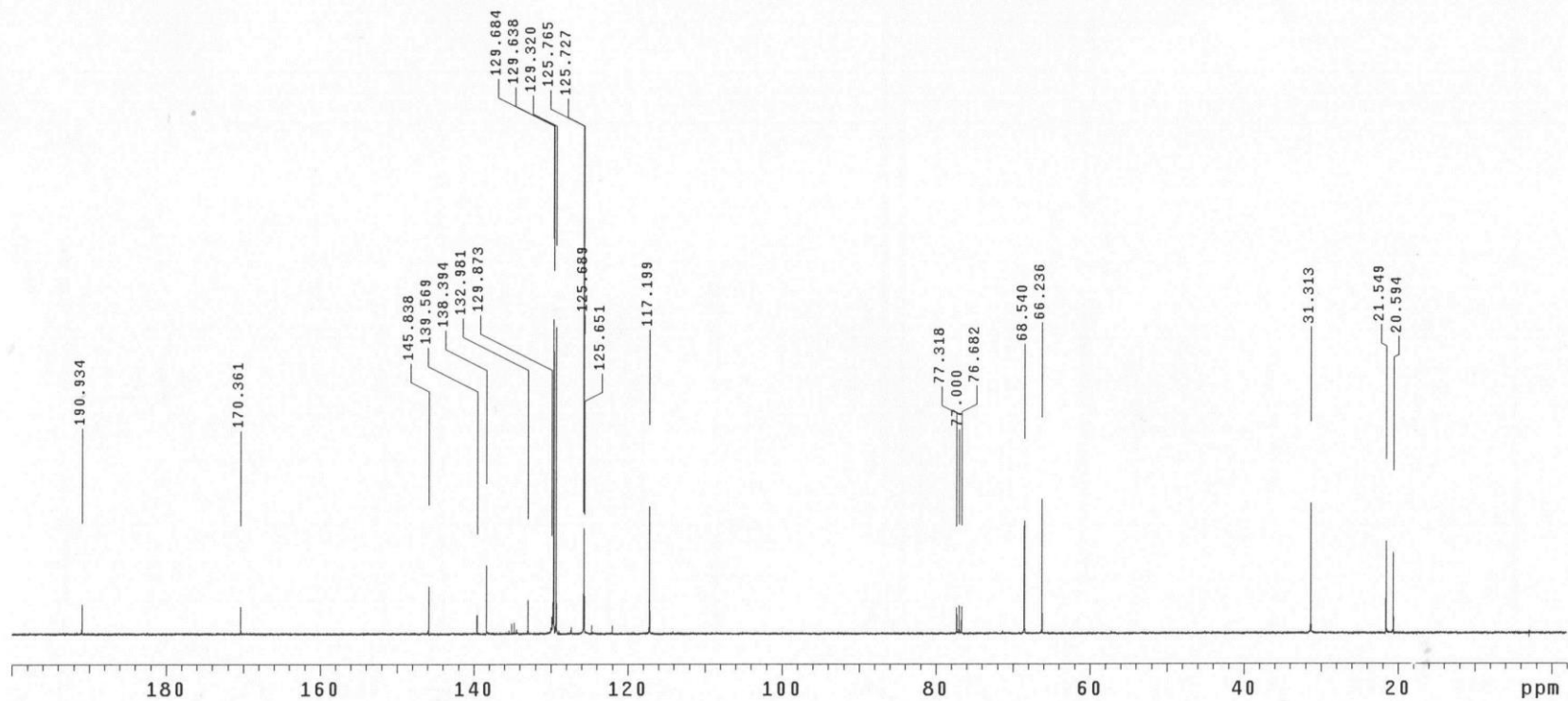
Solvent: CDCl₃

Ambient temperature

Total 1536 repetitions



(¹³C NMR, 100 MHz, CDCl₃)



Compound 9 (¹H-NMR spectral data)

KT0505NB-1

Pulse Sequence: s2pu1

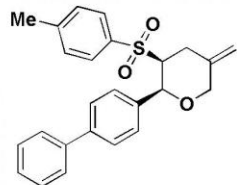
UNITYplus-400 "unity400"

Date: May 19 2020

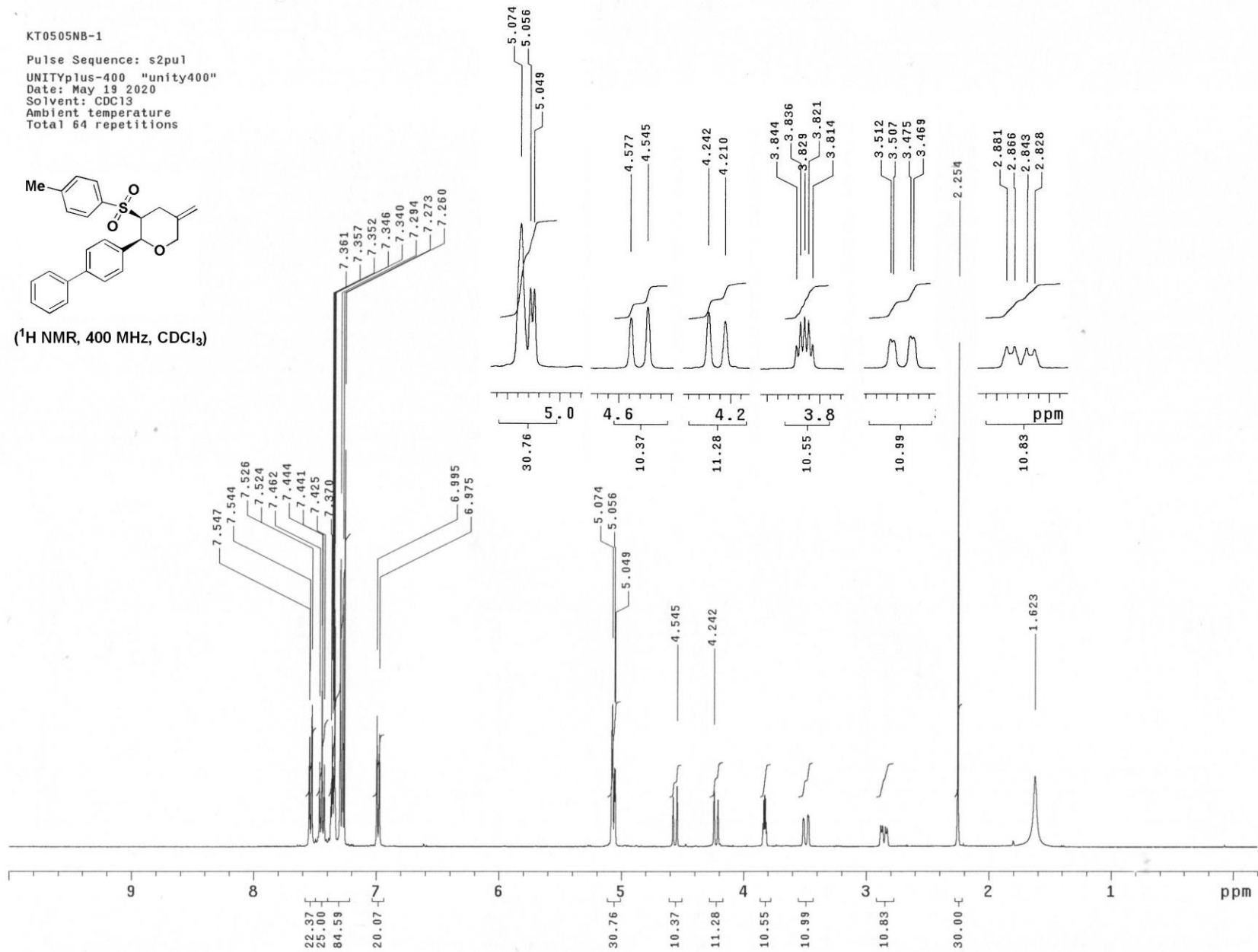
Solvent: CDCl₃

Ambient temperature

Total 64 repetitions



(¹H NMR, 400 MHz, CDCl₃)



Compound 9 (¹³C-NMR spectral data)

KT0505NB-1

Pulse Sequence: s2pu1

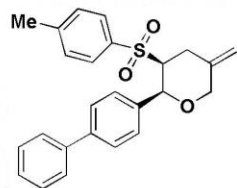
UNITYplus-400 "unity400"

Date: May 19 2020

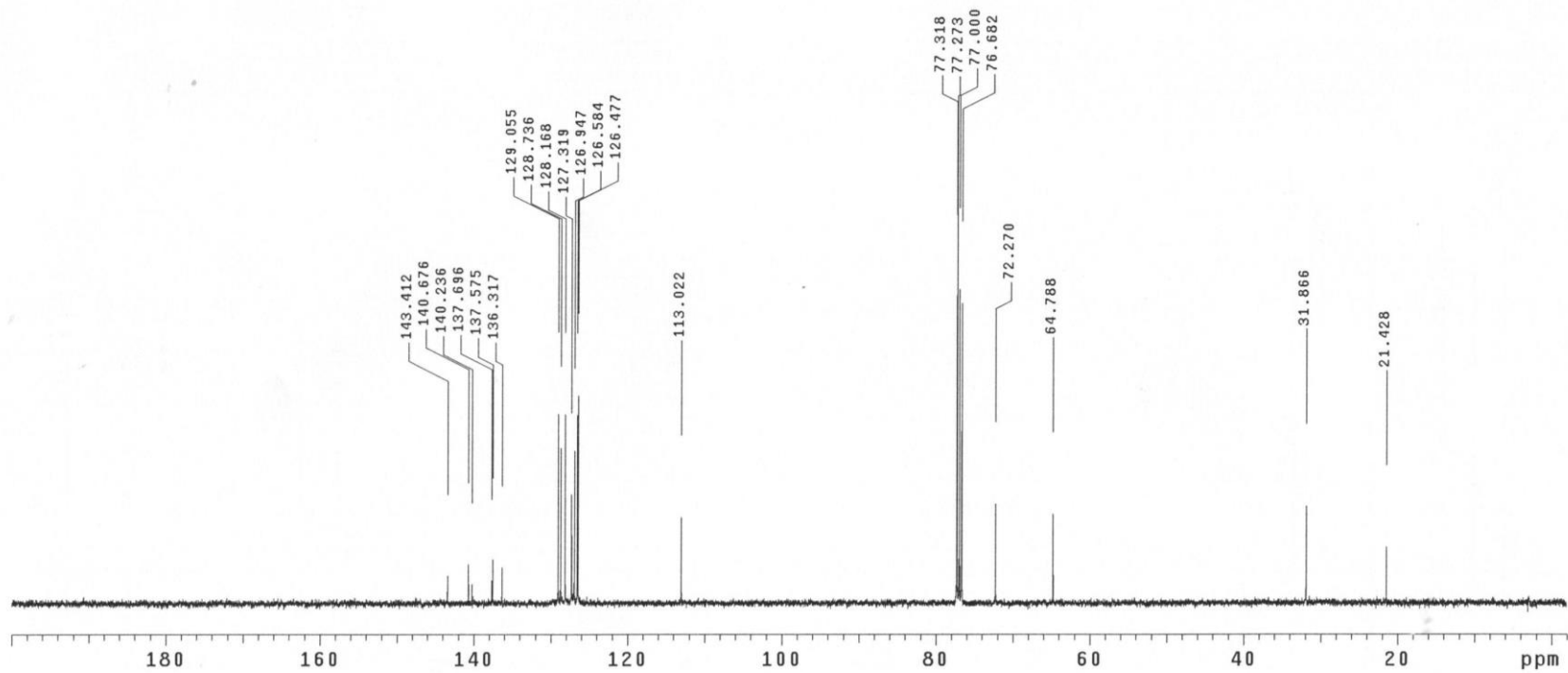
Solvent: CDCl₃

Ambient temperature

Total 11968 repetitions



(¹³C NMR, 100 MHz, CDCl₃)



Compound 11 (¹H-NMR spectral data)

PS1030

Pulse Sequence: s2pu1

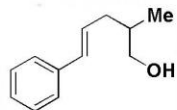
UNITYplus-400 "unity400"

Date: Oct 30 2020

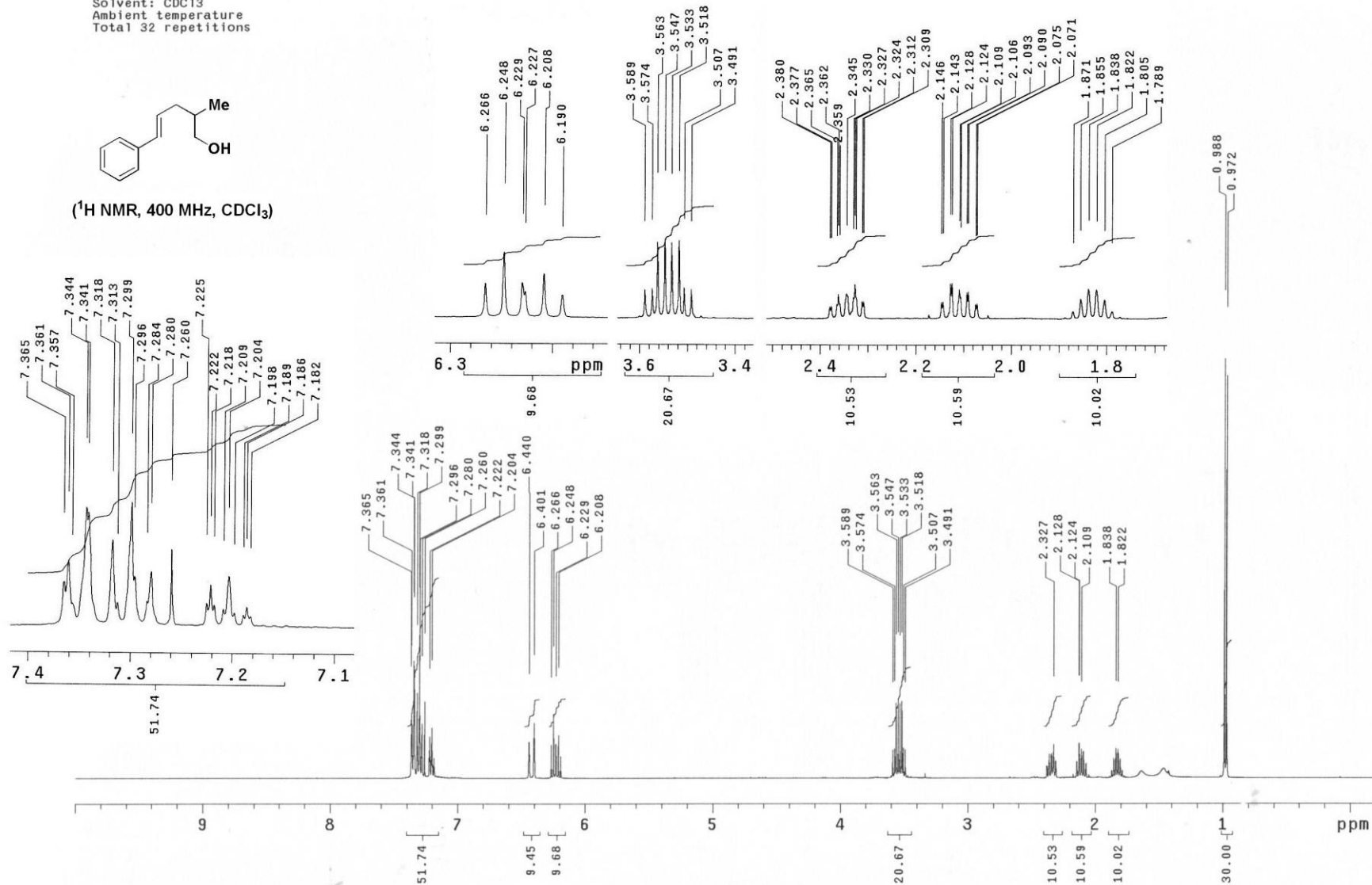
Solvent: CDC13

Ambient temperature

Total 32 repetitions



(¹H NMR, 400 MHz, CDCl₃)



Compound 11 (¹³C-NMR spectral data)

PS1030

Pulse Sequence: s2pu1

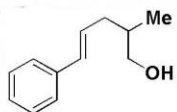
UNITYplus-400 "unity400"

Date: Oct 30 2020

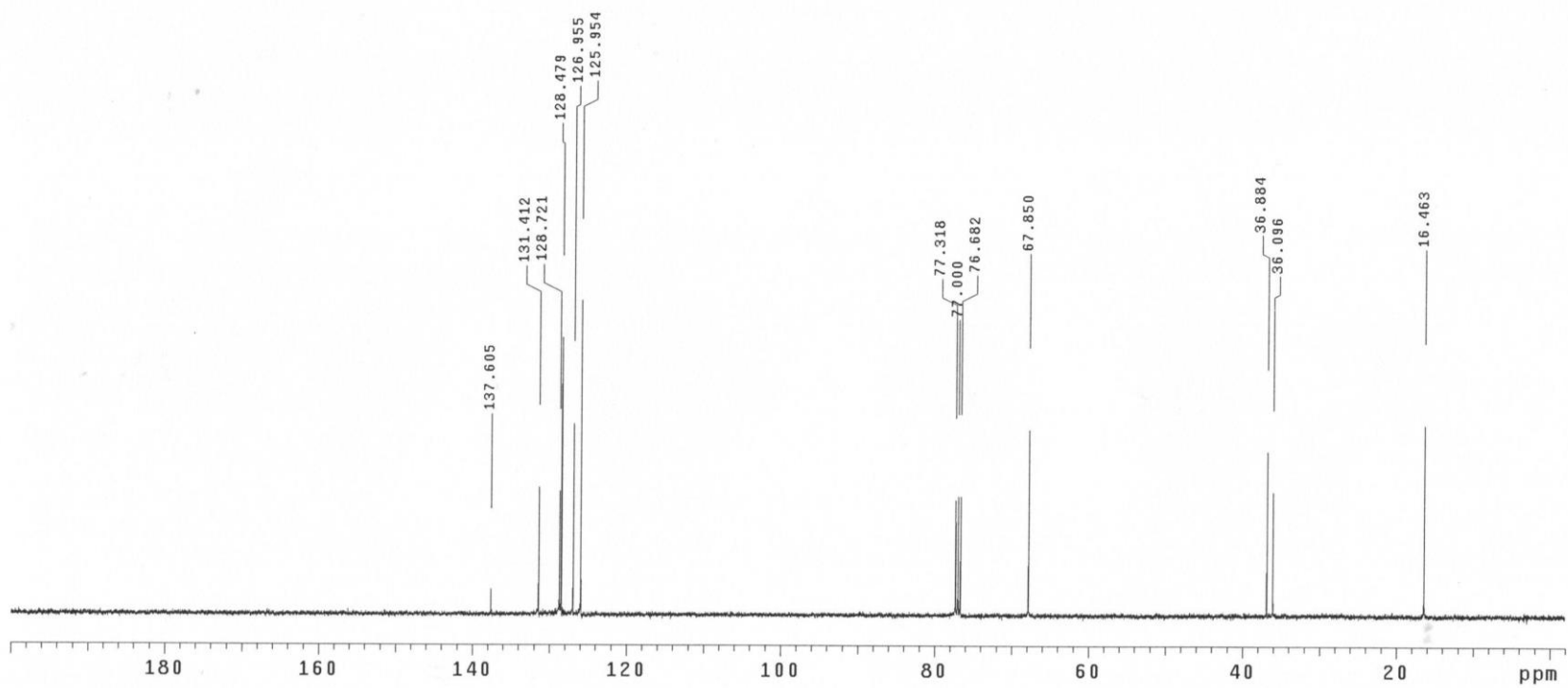
Solvent: CDCl₃

Ambient temperature

Total 4352 repetitions



(¹³C NMR, 100 MHz, CDCl₃)



Compound 12 (¹H-NMR spectral data)

KT1090501

Pulse Sequence: s2pu1

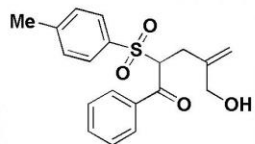
UNITYplus-400 "unity400"

Date: May 22 2020

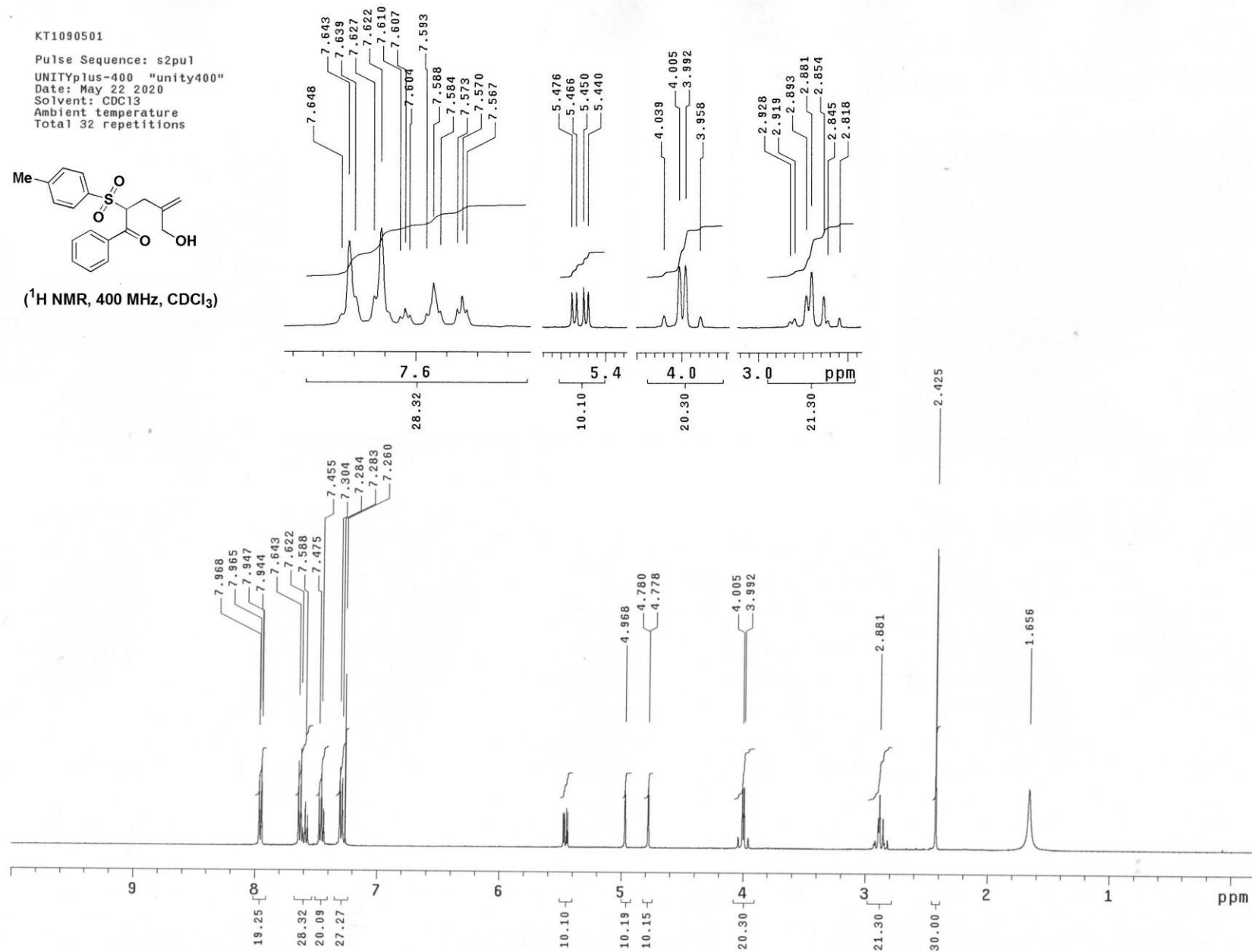
Solvent: CDCl₃

Ambient temperature

Total 32 repetitions



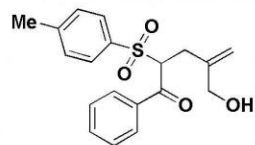
(¹H NMR, 400 MHz, CDCl₃)



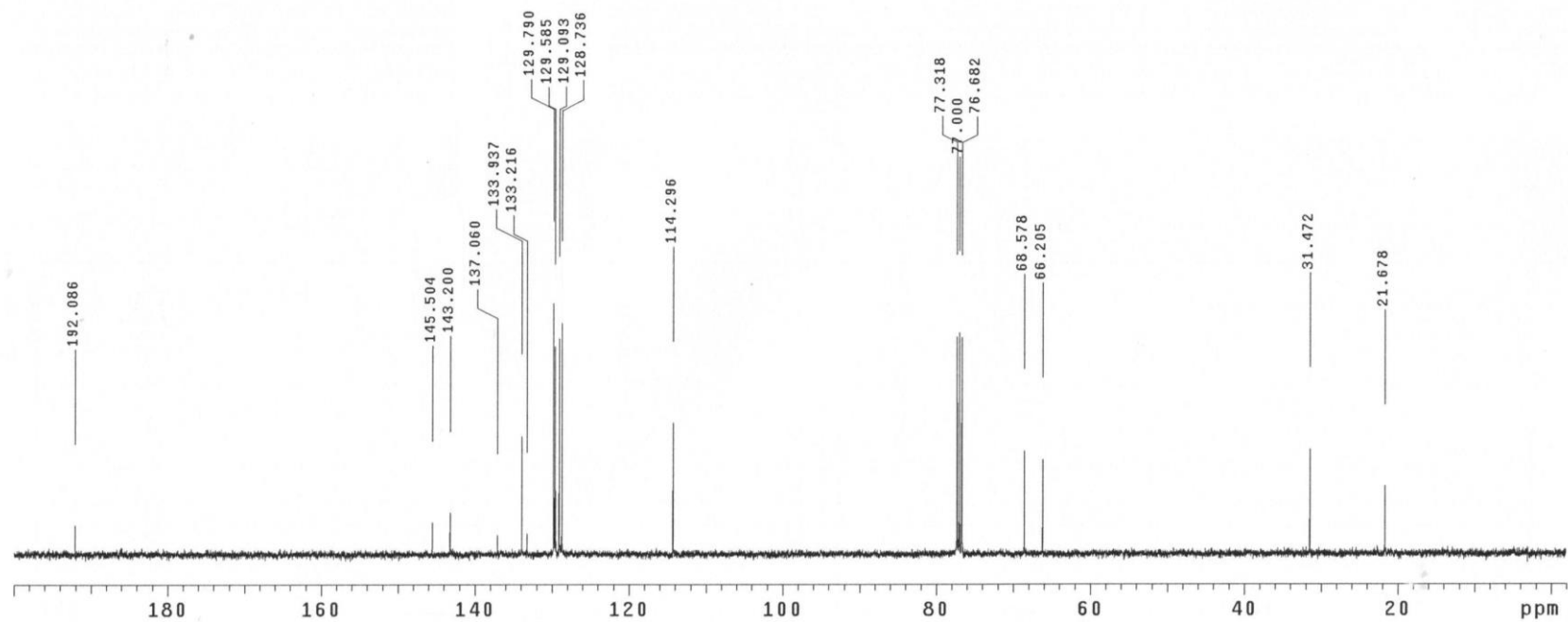
Compound 12 (¹³C-NMR spectral data)

KT1090501

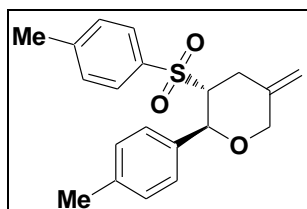
Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: May 22 2020
Solvent: CDCl₃
Ambient temperature
Total 5760 repetitions



(¹³C NMR, 100 MHz, CDCl₃)

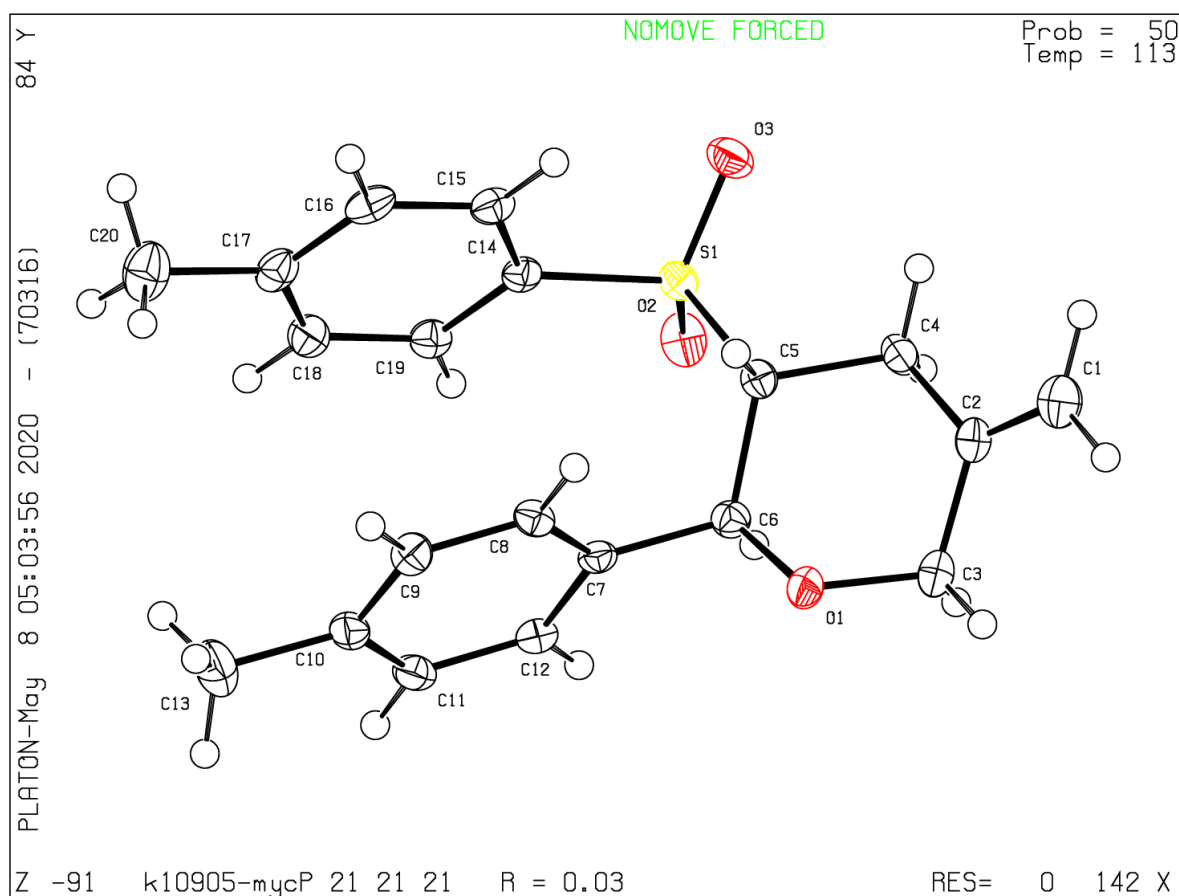


X-ray crystal data of compound 5m



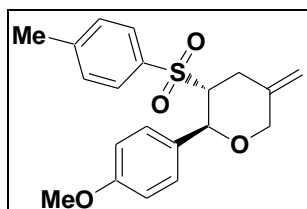
Sample preparation : A solution of compound **5m** (30 mg) in CH₂Cl₂ (10 mL) was placed in a tube (10 mL). EtOAc (2 mL) was added slowly to the vial with a dropper. The vial was closed with little cotton and kept at room temperature for 2 days. Then, colorless prisms were observed.

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.



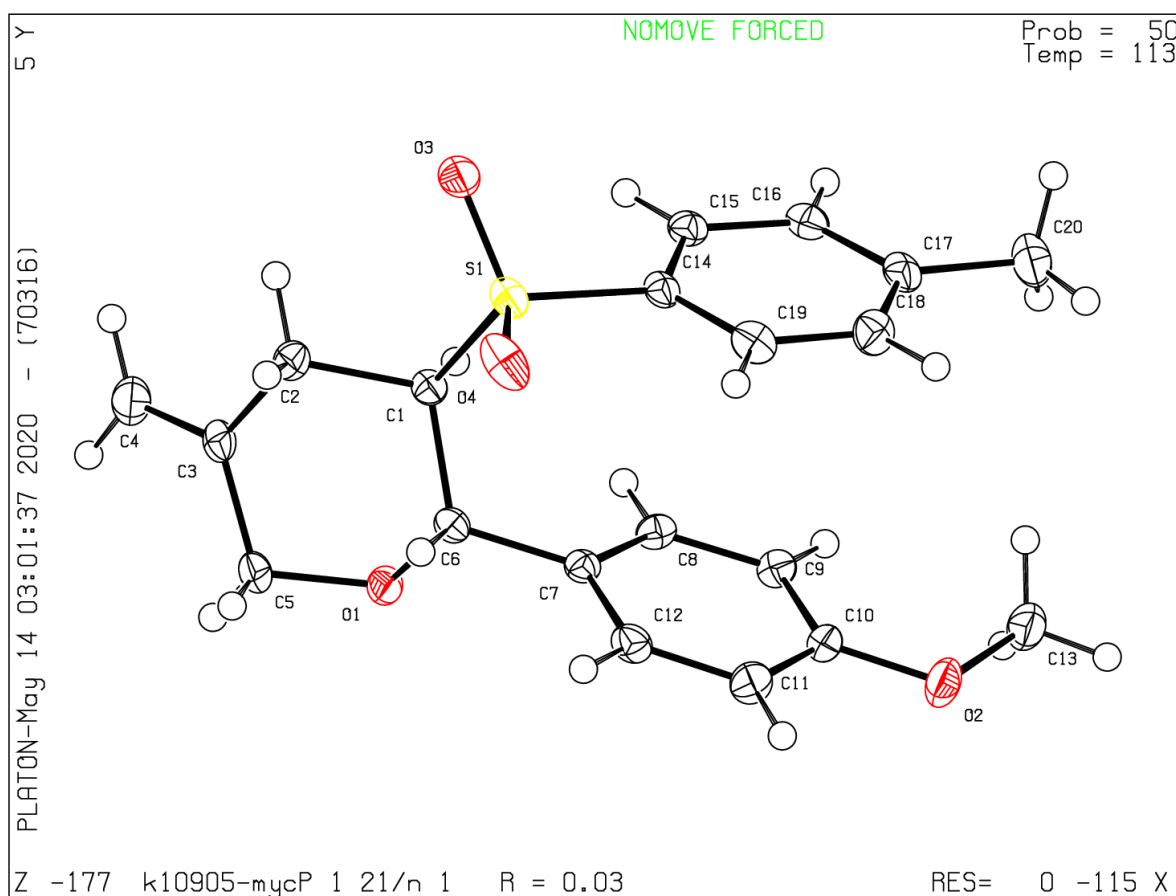
Empirical formula	C ₂₀ H ₂₂ O ₃ S
Formula weight	342.43
Temperature	113(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	P2 ₁ 2 ₁ 2 ₁
Unit cell dimensions	a = 5.61670(10) Å α = 90°. b = 15.9231(4) Å β = 90°. c = 19.6051(4) Å γ = 90°.
Volume	1753.39(6) Å ³
Z	4
Density (calculated)	1.297 Mg/m ³
Absorption coefficient	0.199 mm ⁻¹
F(000)	728
Crystal size	0.2 x 0.2 x 0.2 mm ³
Theta range for data collection	2.078 to 27.006°.
Index ranges	-6 ≤ h ≤ 7, -20 ≤ k ≤ 20, -25 ≤ l ≤ 20
Reflections collected	14002
Independent reflections	3611 [R(int) = 0.0344]
Completeness to theta = 25.242°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.75025
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3611 / 0 / 228
Goodness-of-fit on F ²	1.024
Final R indices [I > 2σ(I)]	R1 = 0.0320, wR2 = 0.0711
R indices (all data)	R1 = 0.0354, wR2 = 0.0727
Absolute structure parameter	0.03(3)
Extinction coefficient	0.0039(11)
Largest diff. peak and hole	0.258 and -0.287 e.Å ⁻³

X-ray crystal data of compound 5n



Sample preparation : A solution of compound **5n** (30 mg) in CH₂Cl₂ (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 ₂₀ H ₂₂ O ₄ S
Formula weight	358.43
Temperature/K	113(2)
Crystal system	monoclinic
Space group	P2 ₁ /n
a/Å	12.4097(3)
b/Å	9.8815(2)
c/Å	14.6434(3)
α/°	90
β/°	98.892(2)
γ/°	90
Volume/Å ³	1774.09(7)
Z	4
ρ _{calc} /cm ³	1.342
μ/mm ⁻¹	0.204
F(000)	760.0
Crystal size/mm ³	0.2 × 0.2 × 0.2
Radiation	Mo Kα (λ = 0.71073)
2θ range for data collection/°	4.008 to 54.124
Index ranges	-15 ≤ h ≤ 15, -12 ≤ k ≤ 7, -18 ≤ l ≤ 18
Reflections collected	20613
Independent reflections	3723 [R _{int} = 0.0273, R _{sigma} = 0.0235]
Data/restraints/parameters	3723/0/229
Goodness-of-fit on F ²	1.076
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0334, wR ₂ = 0.0860
Final R indexes [all data]	R ₁ = 0.0395, wR ₂ = 0.0890
Largest diff. peak/hole / e Å ⁻³	0.32/-0.36