

Supporting Information

Synthesis of 4-Sulfonyl-1,7-diesters via K₂CO₃-Mediated Alkylative Debenzoylation of α -Sulfonyl *o*-Hydroxyacetophenones with Acrylates

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Compound 6a (¹H-NMR spectral data)

PS1107

Pulse Sequence: s2pu1

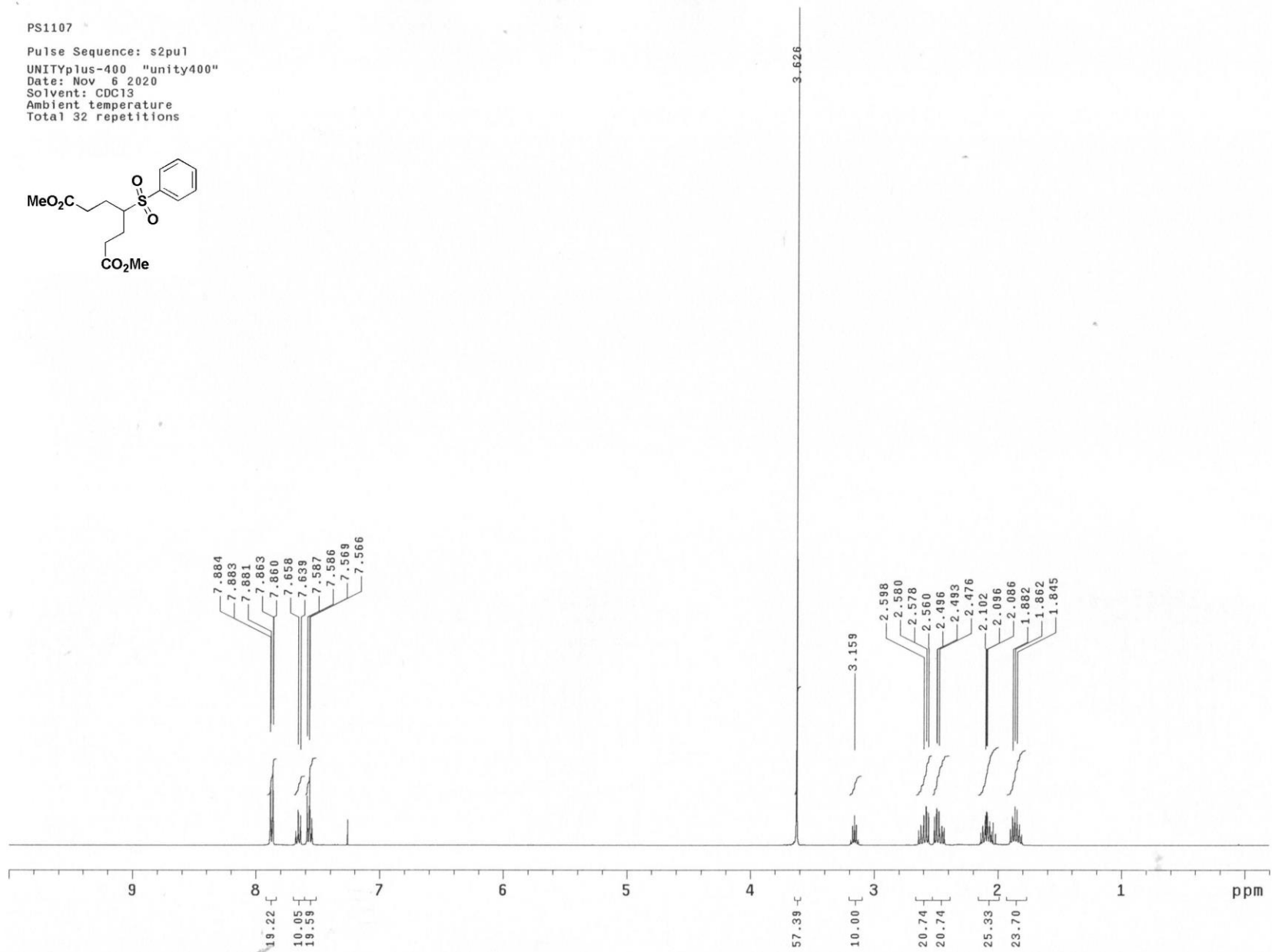
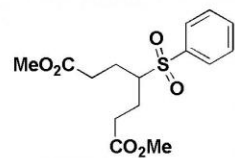
UNITYplus-400 "unity400"

Date: Nov 6 2020

Solvent: CDCl₃

Ambient temperature

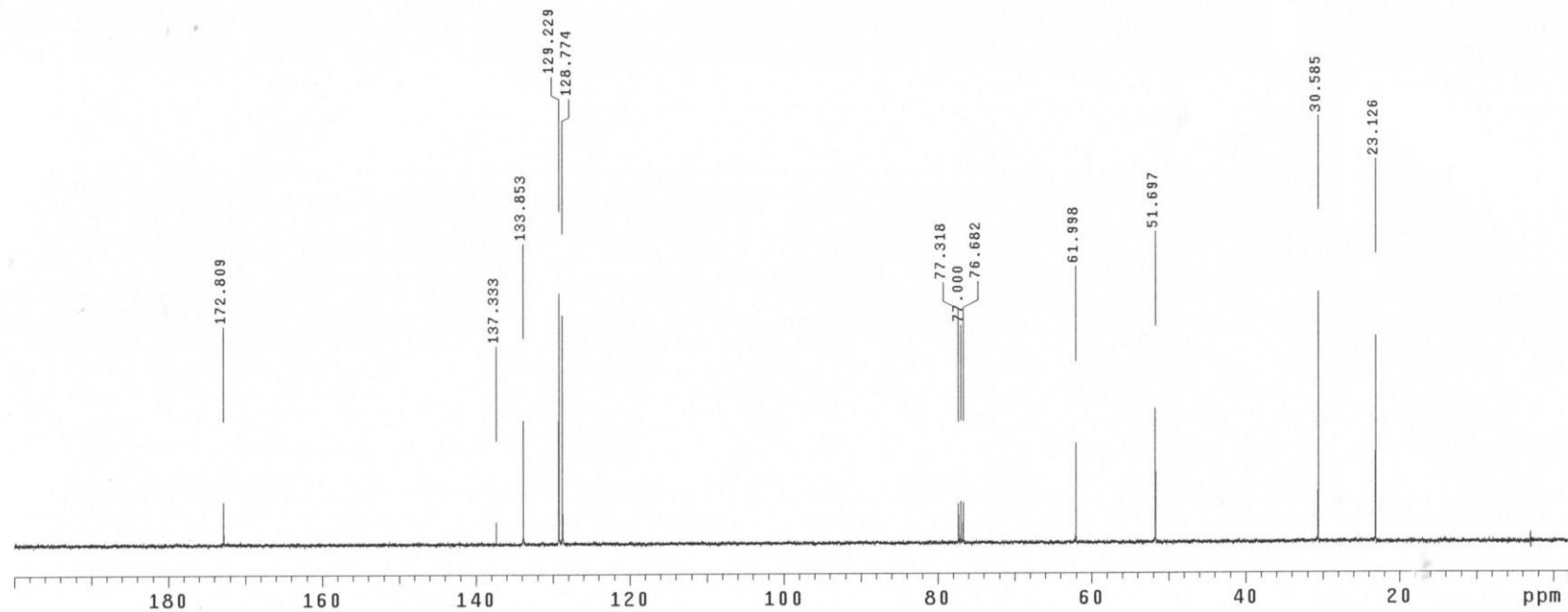
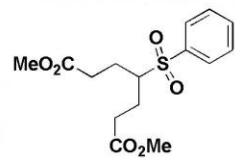
Total 32 repetitions



Compound 6a (¹³C-NMR spectral data)

PS1107

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Nov 6 2020
Solvent: CDCl₃
Ambient temperature
Total 672 repetitions



Compound 6b (¹H-NMR spectral data)

PS1105

Pulse Sequence: s2pu1

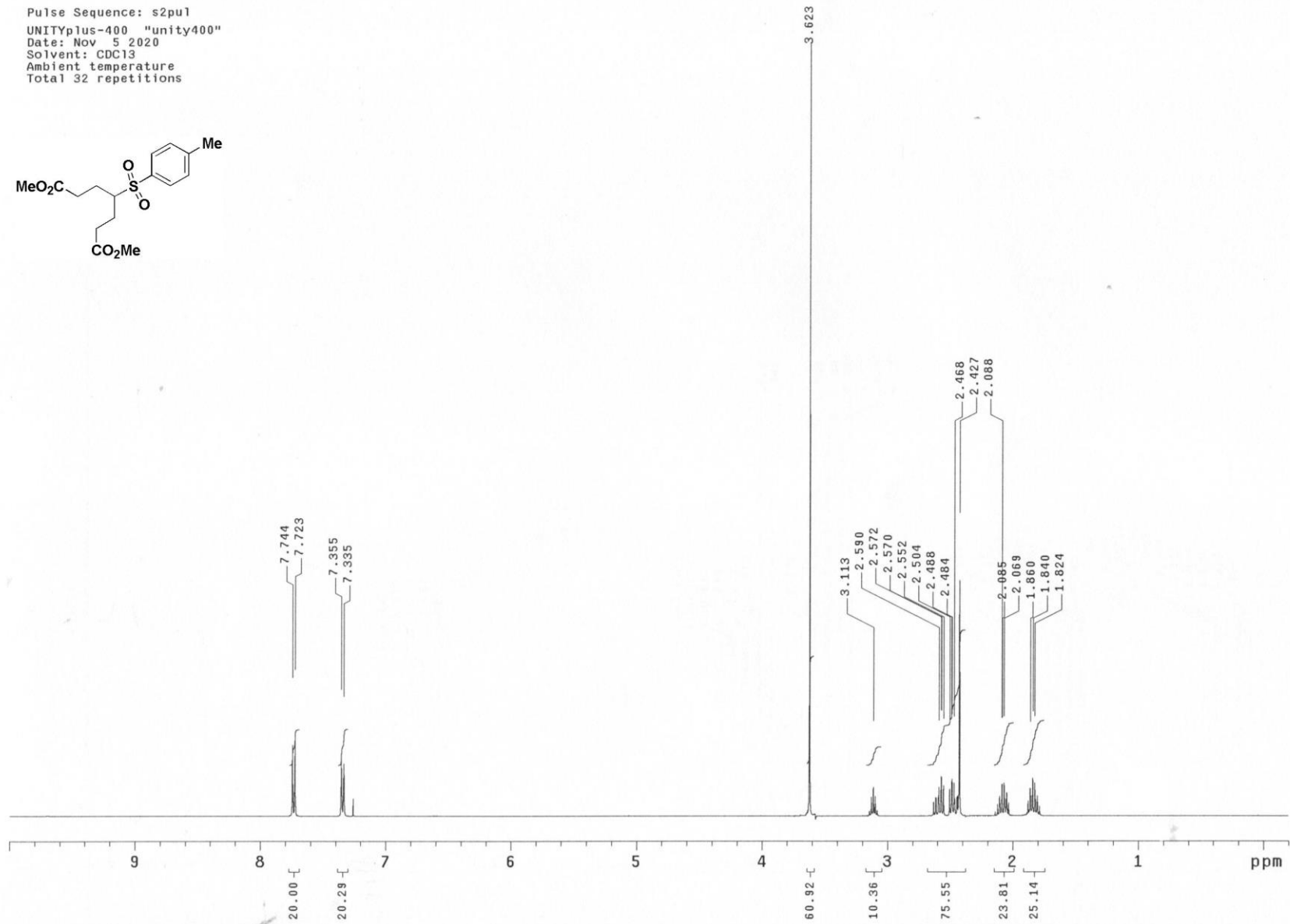
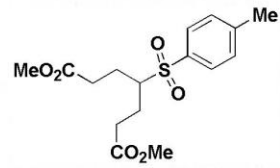
UNITYplus-400 "unity400"

Date: Nov 5 2020

Solvent: CDCl₃

Ambient temperature

Total 32 repetitions



Compound 6b (¹³C-NMR spectral data)

PS1105

Pulse Sequence: s2pu1

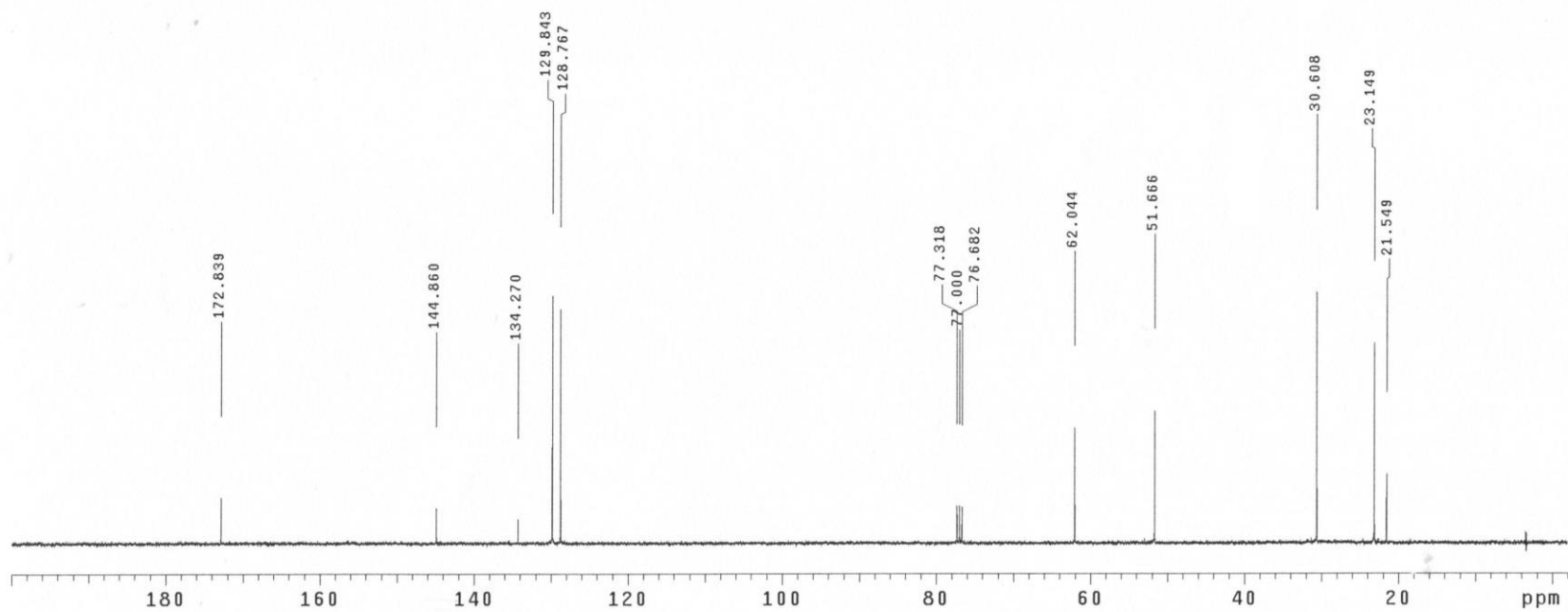
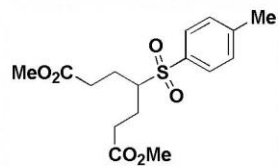
UNITYplus-400 "unity400"

Date: Nov 5 2020

Solvent: CDCl₃

Ambient temperature

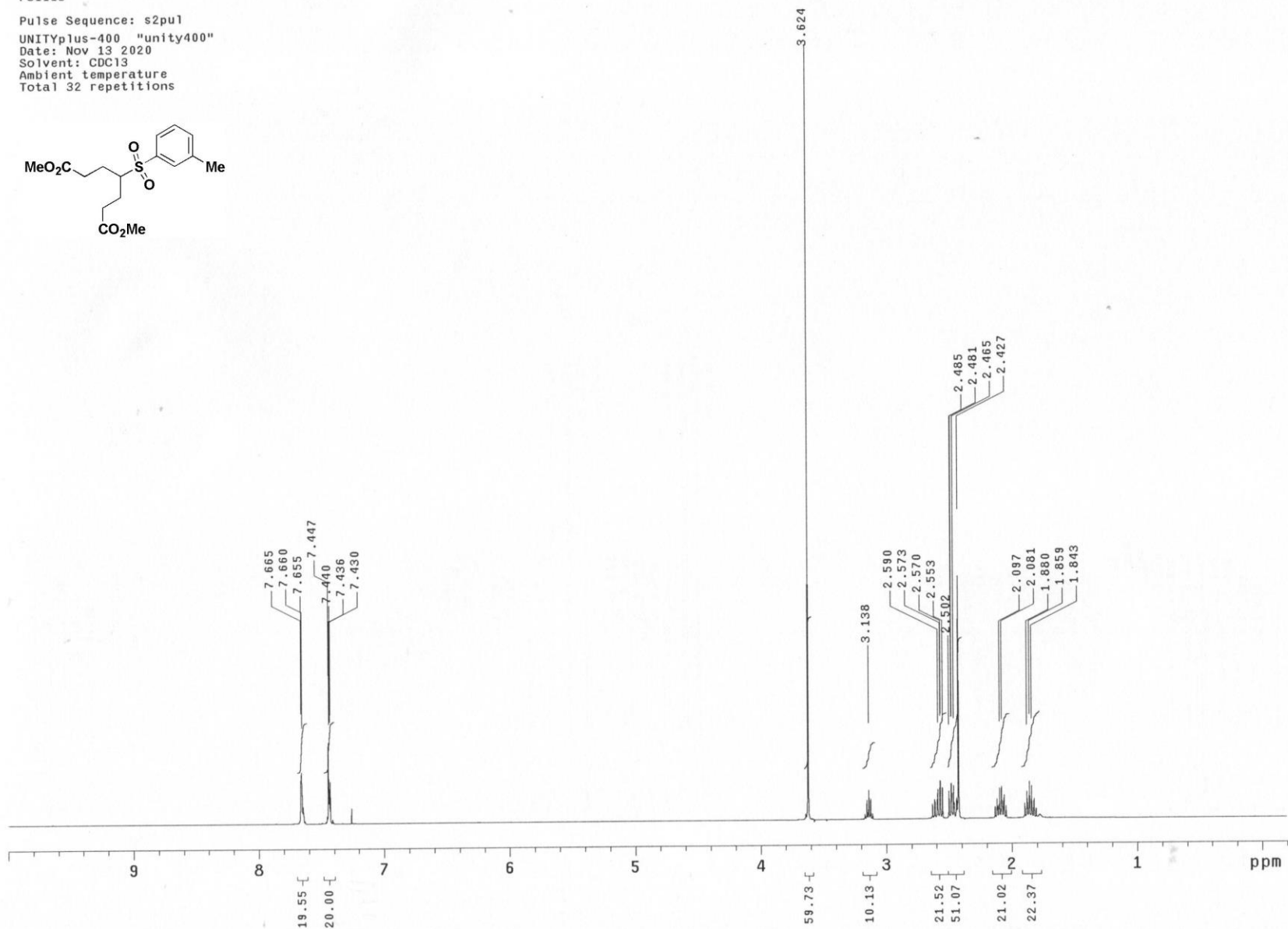
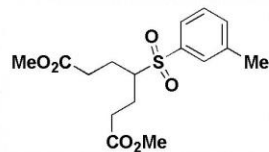
Total 432 repetitions



Compound 6c (¹H-NMR spectral data)

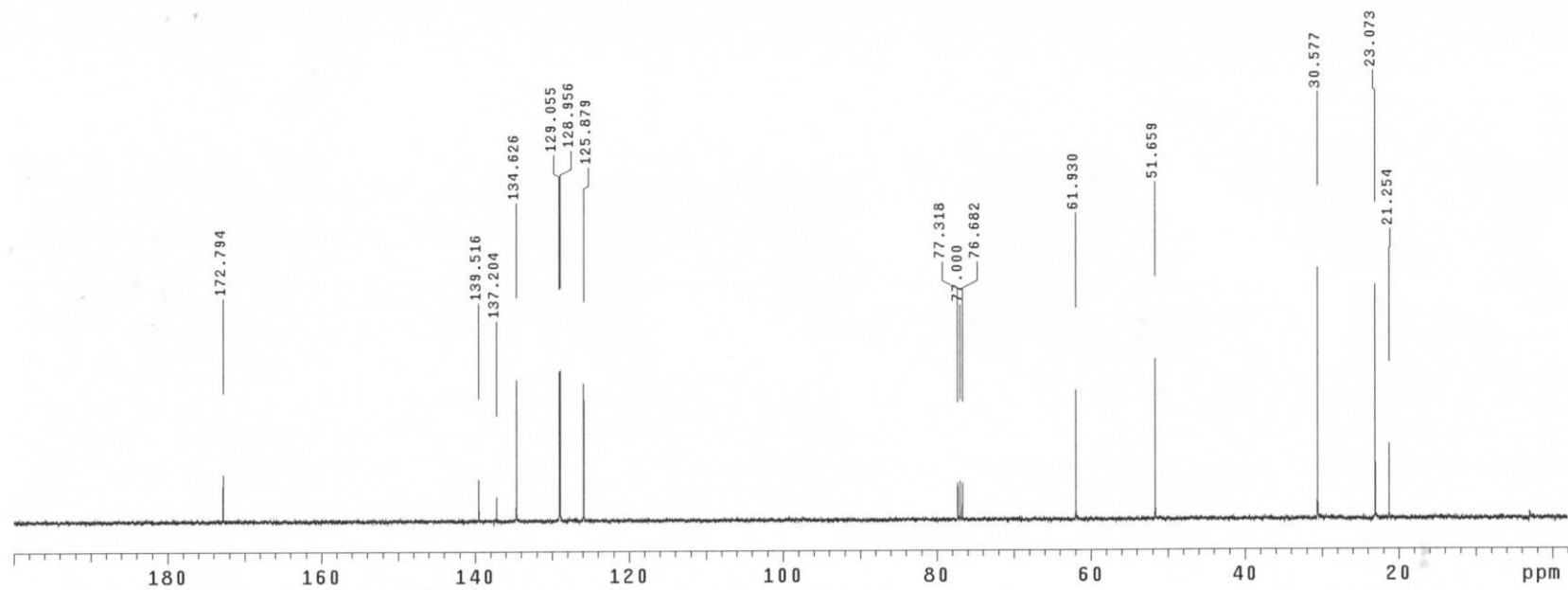
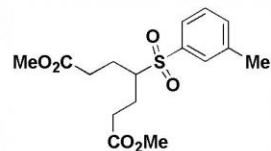
PS1113

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Nov 13 2020
Solvent: CDCl₃
Ambient temperature
Total 32 repetitions



Compound 6c (¹³C-NMR spectral data)

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Nov 13 2020
Solvent: CDCl₃
Ambient temperature
Total 368 repetitions



Compound 6d (¹H-NMR spectral data)

PS1120

Pulse Sequence: s2pu1

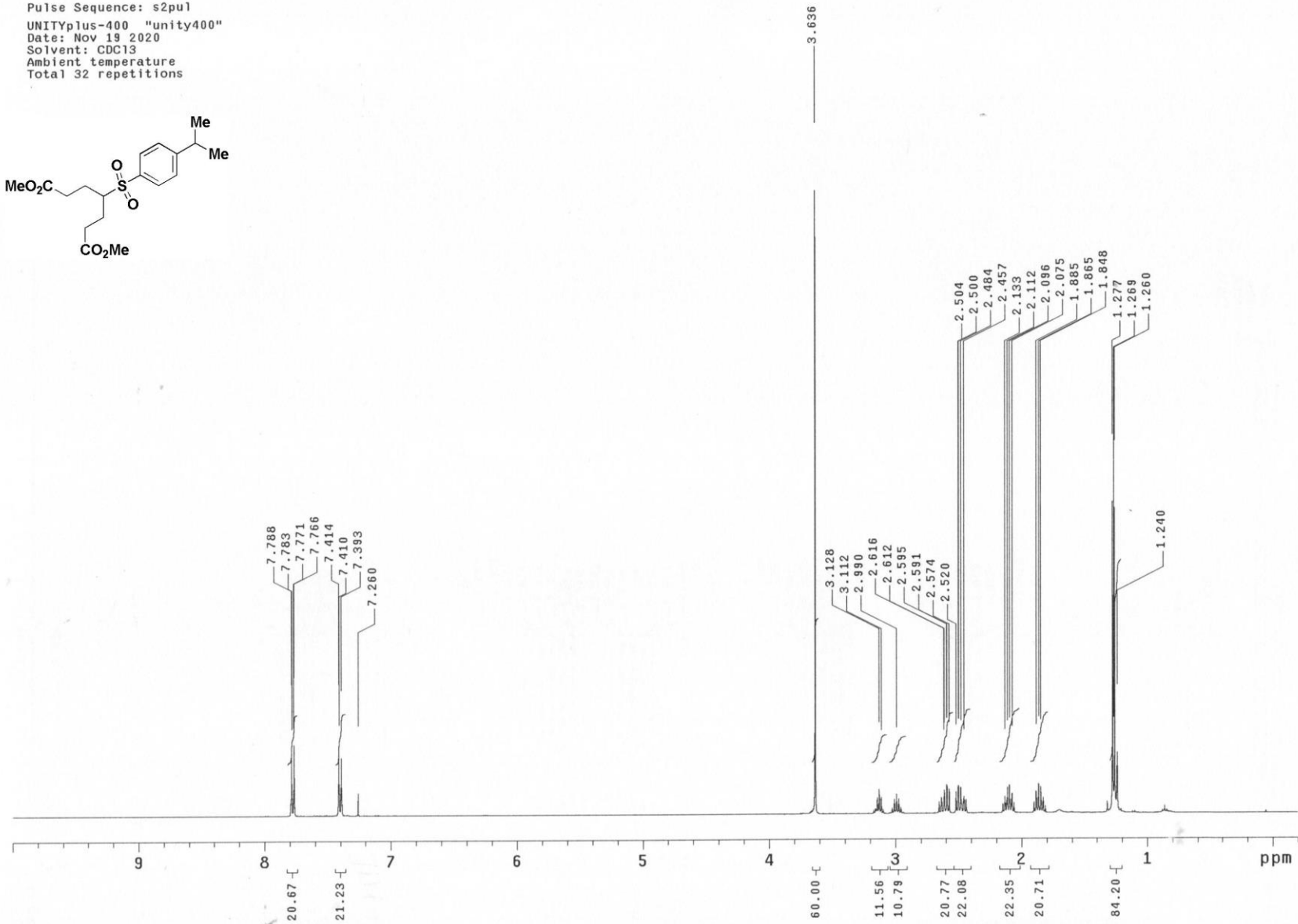
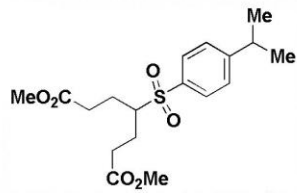
UNITYplus-400 "unity400"

Date: Nov 19 2020

Solvent: CDCl₃

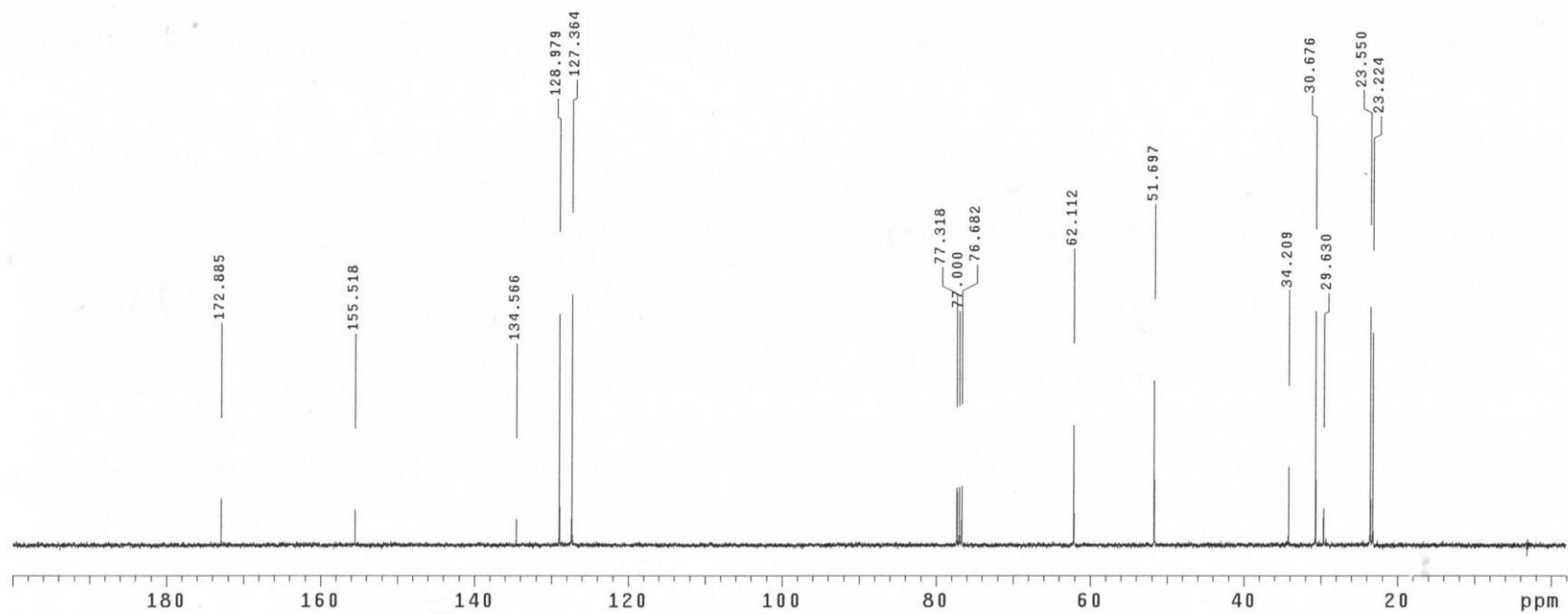
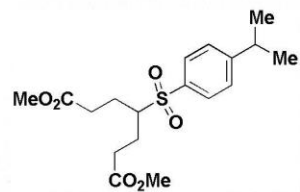
Ambient temperature

Total 32 repetitions



Compound 6d (¹³C-NMR spectral data)

PS1120
Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Nov 19 2020
Solvent: CDCl₃
Ambient temperature
Total 1008 repetitions



Compound 6e (¹H-NMR spectral data)

PS1125

Pulse Sequence: s2pu1

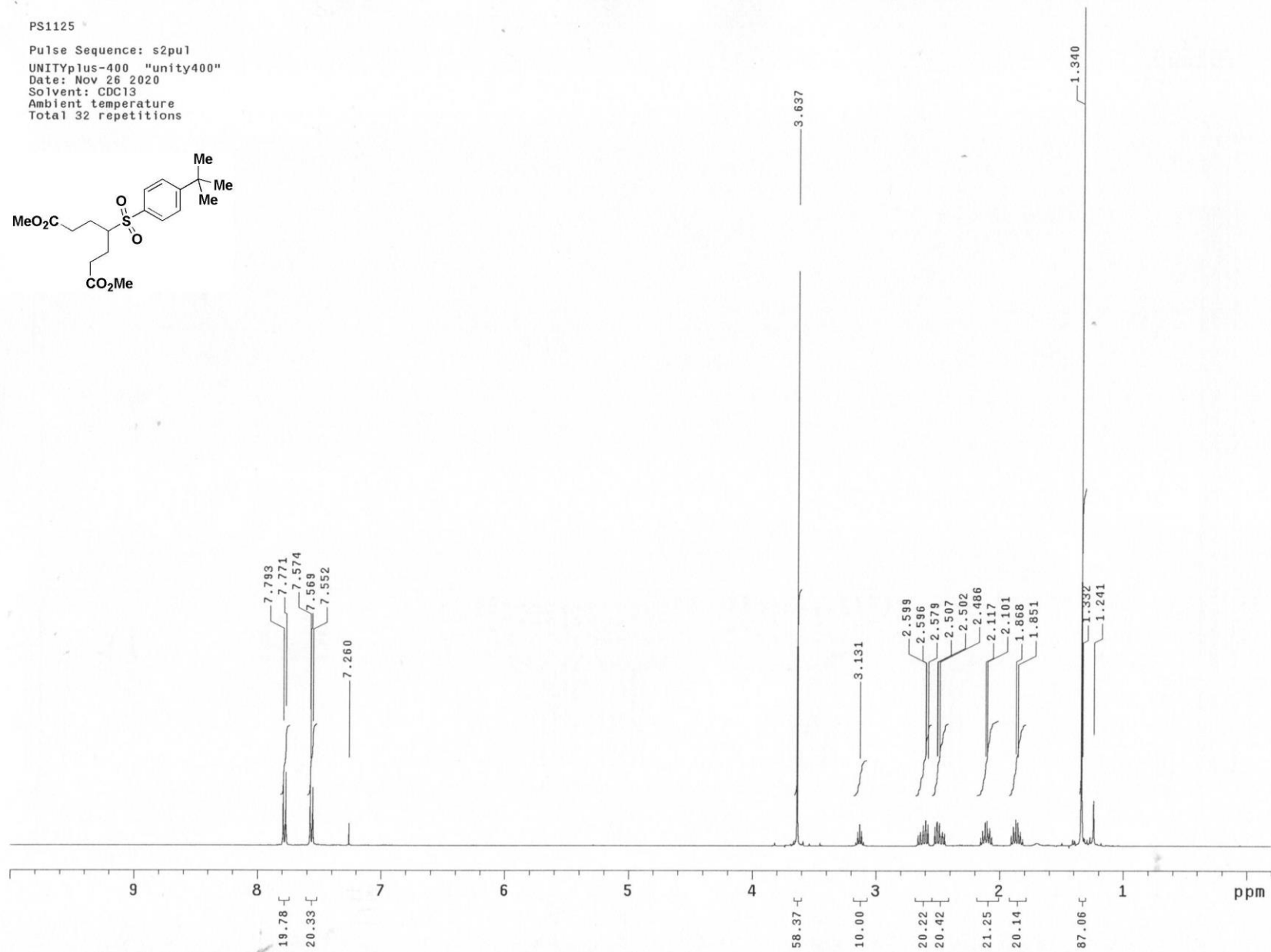
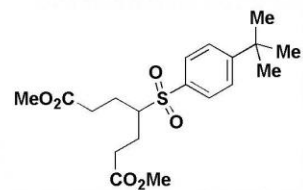
UNITYplus-400 "unity400"

Date: Nov 26 2020

Solvent: CDCl₃

Ambient temperature

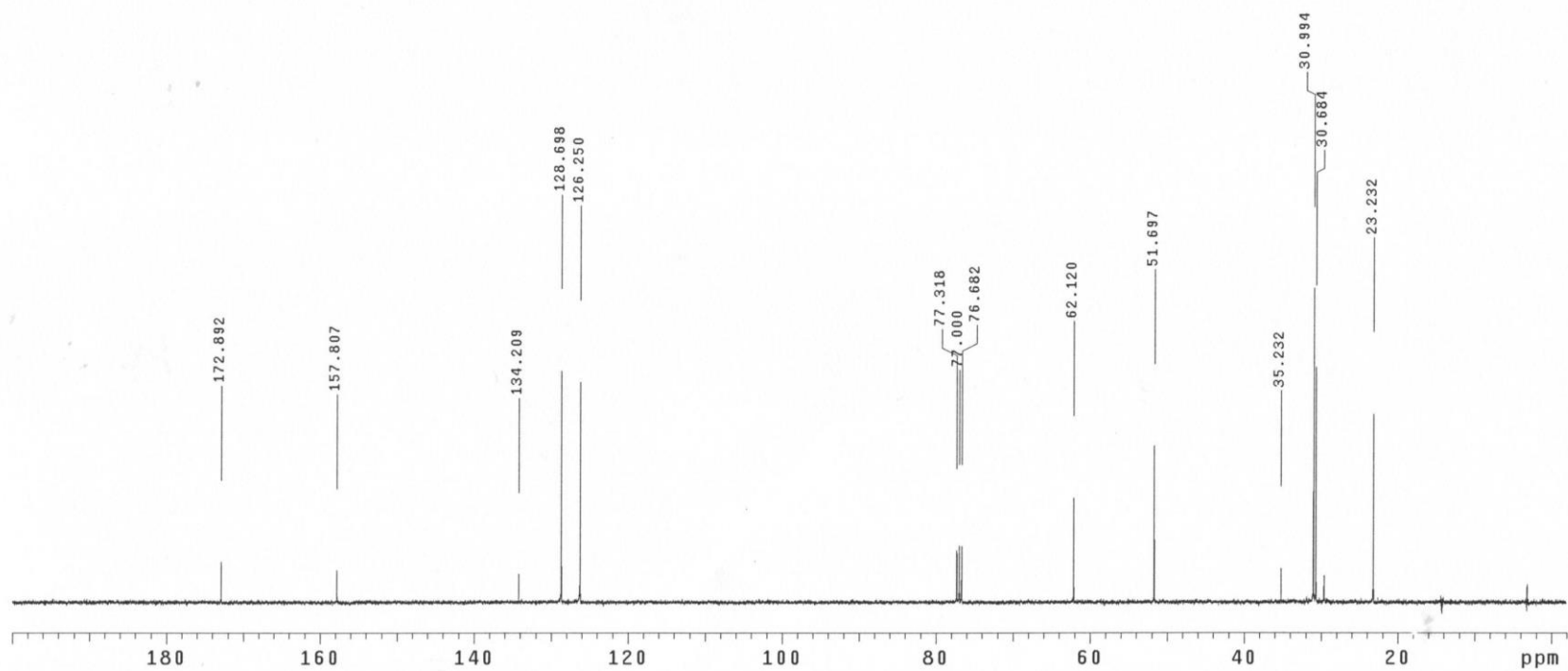
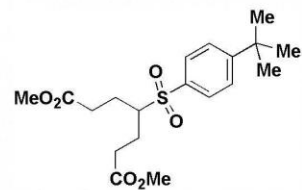
Total 32 repetitions



Compound 6e (¹³C-NMR spectral data)

PS1125

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Nov 26 2020
Solvent: CDCl₃
Ambient temperature
Total 1088 repetitions



Compound 6f (¹H-NMR spectral data)

PS1126

Pulse Sequence: s2pu1

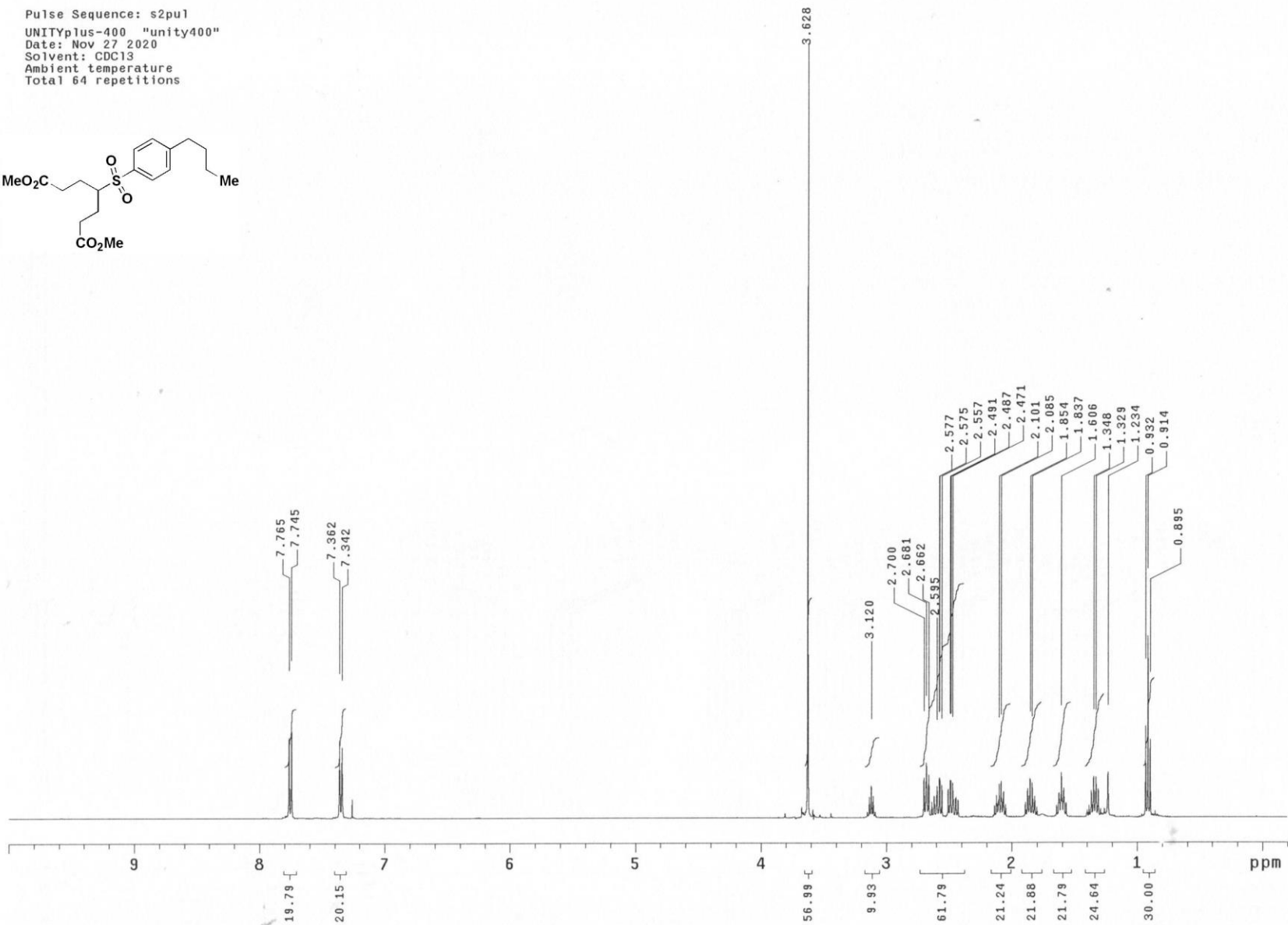
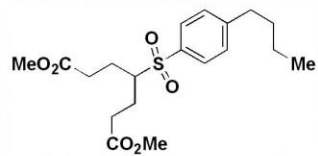
UNITYplus-400 "unity400"

Date: Nov 27 2020

Solvent: CDCl₃

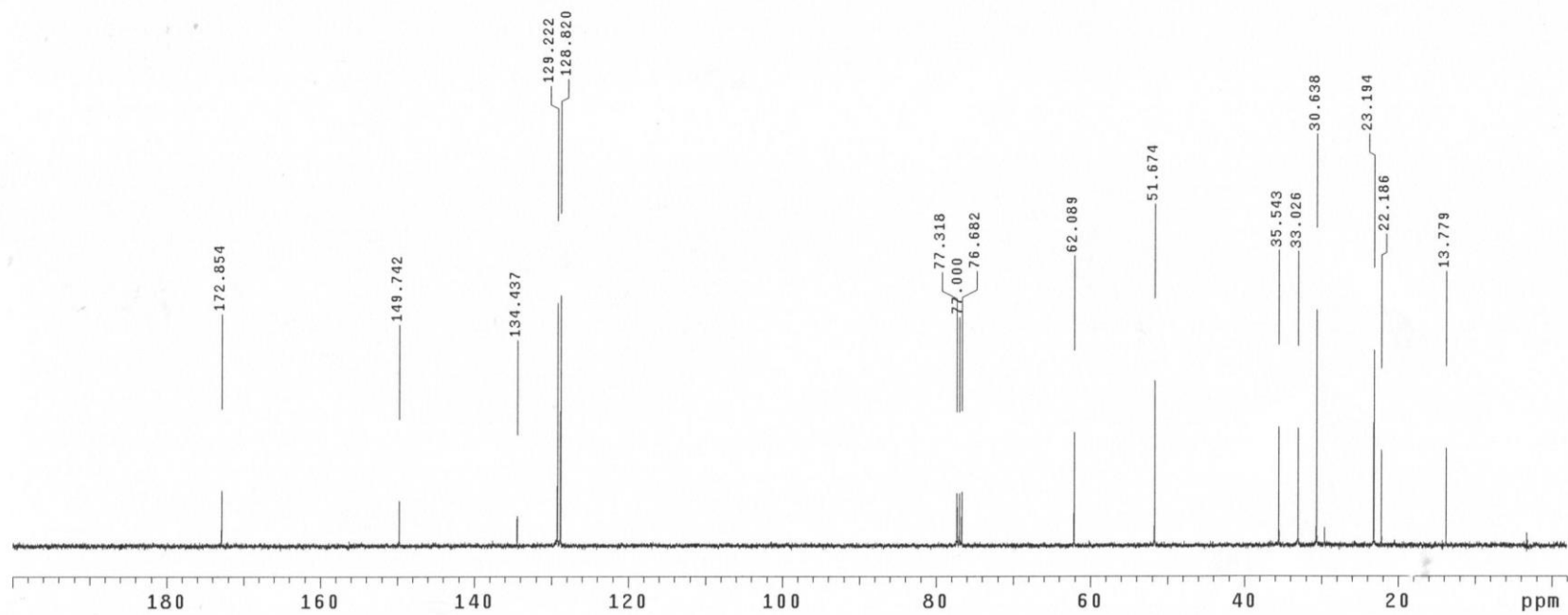
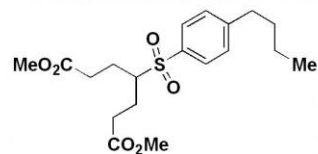
Ambient temperature

Total 64 repetitions



Compound 6f (¹³C-NMR spectral data)

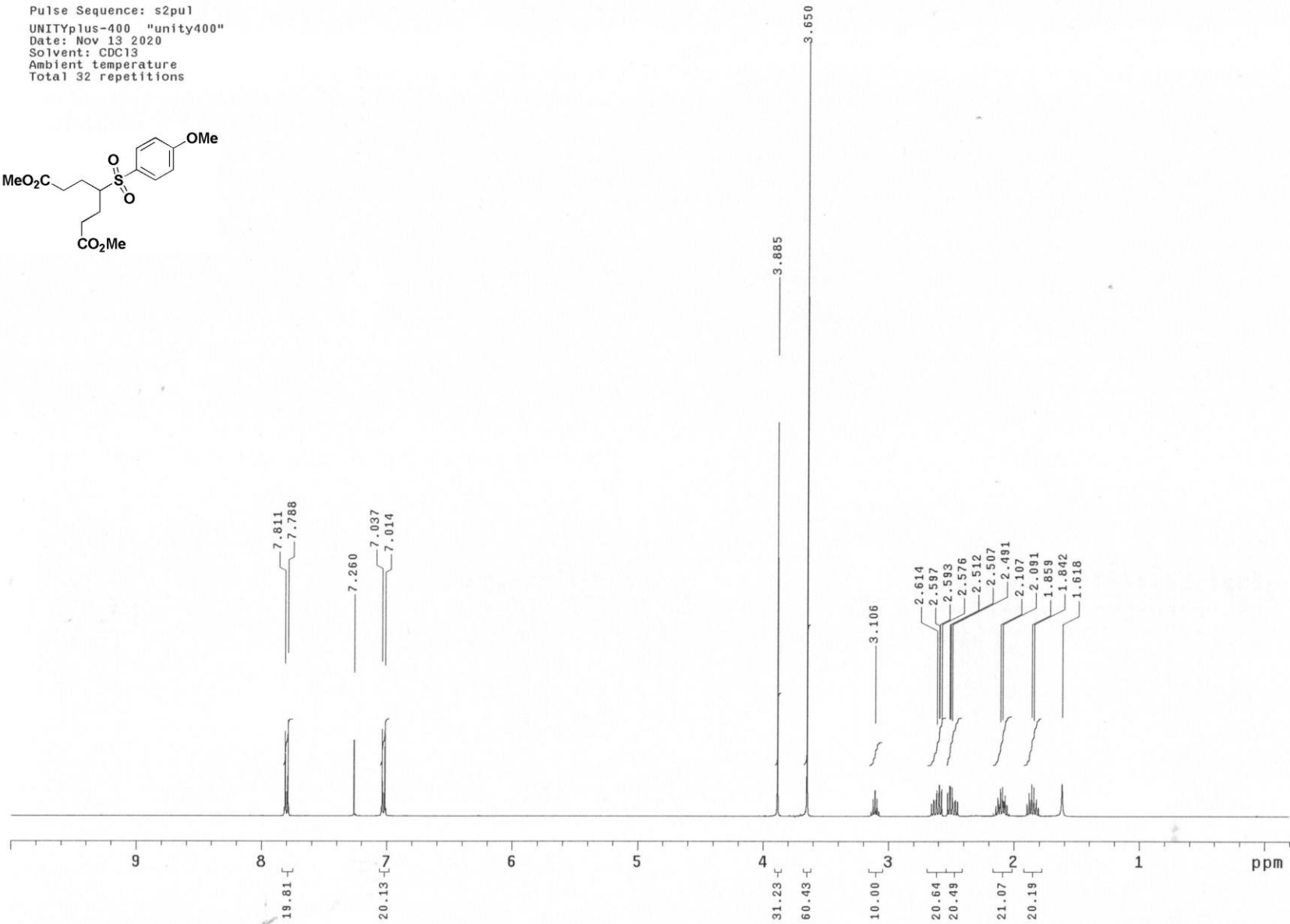
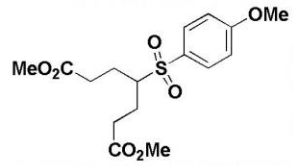
PS1126
Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Nov 27 2020
Solvent: CDC13
Ambient temperature
Total 512 repetitions



Compound 6g (¹H-NMR spectral data)

PS1112

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Nov 13 2020
Solvent: CDCl₃
Ambient temperature
Total 32 repetitions



Compound 6g (¹³C-NMR spectral data)

PS1112

Pulse Sequence: s2pu1

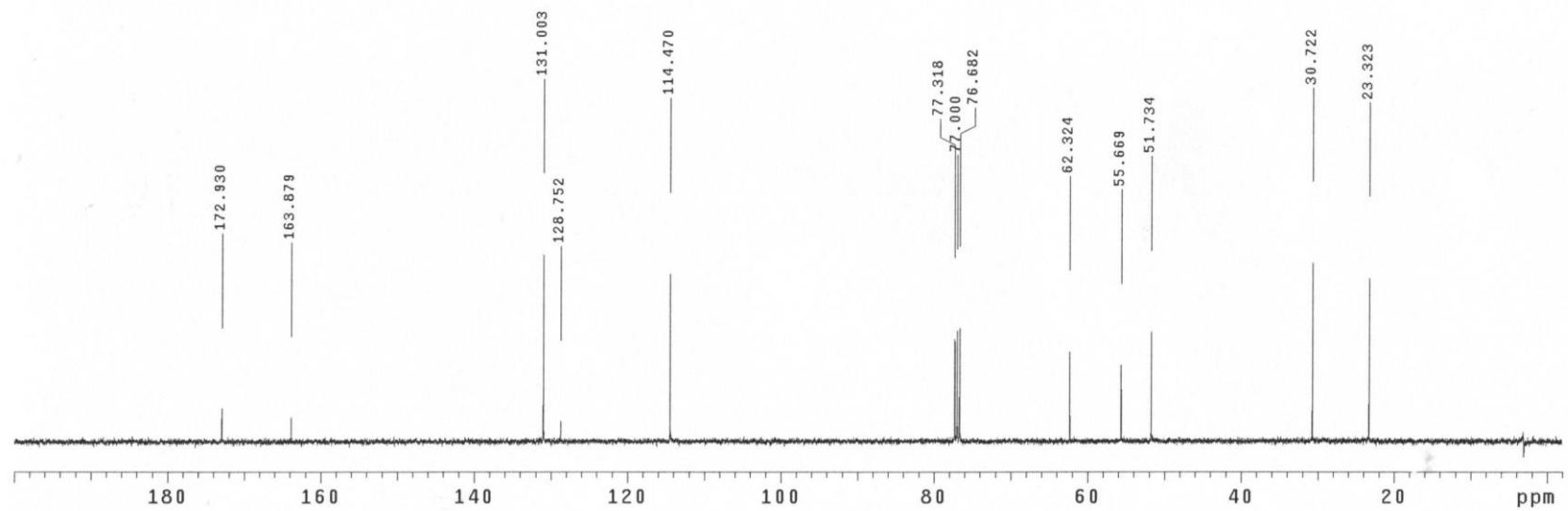
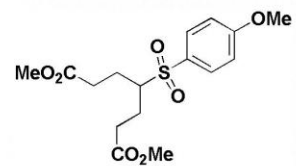
UNITYplus-400 "unity400"

Date: Nov 13 2020

Solvent: CDCl₃

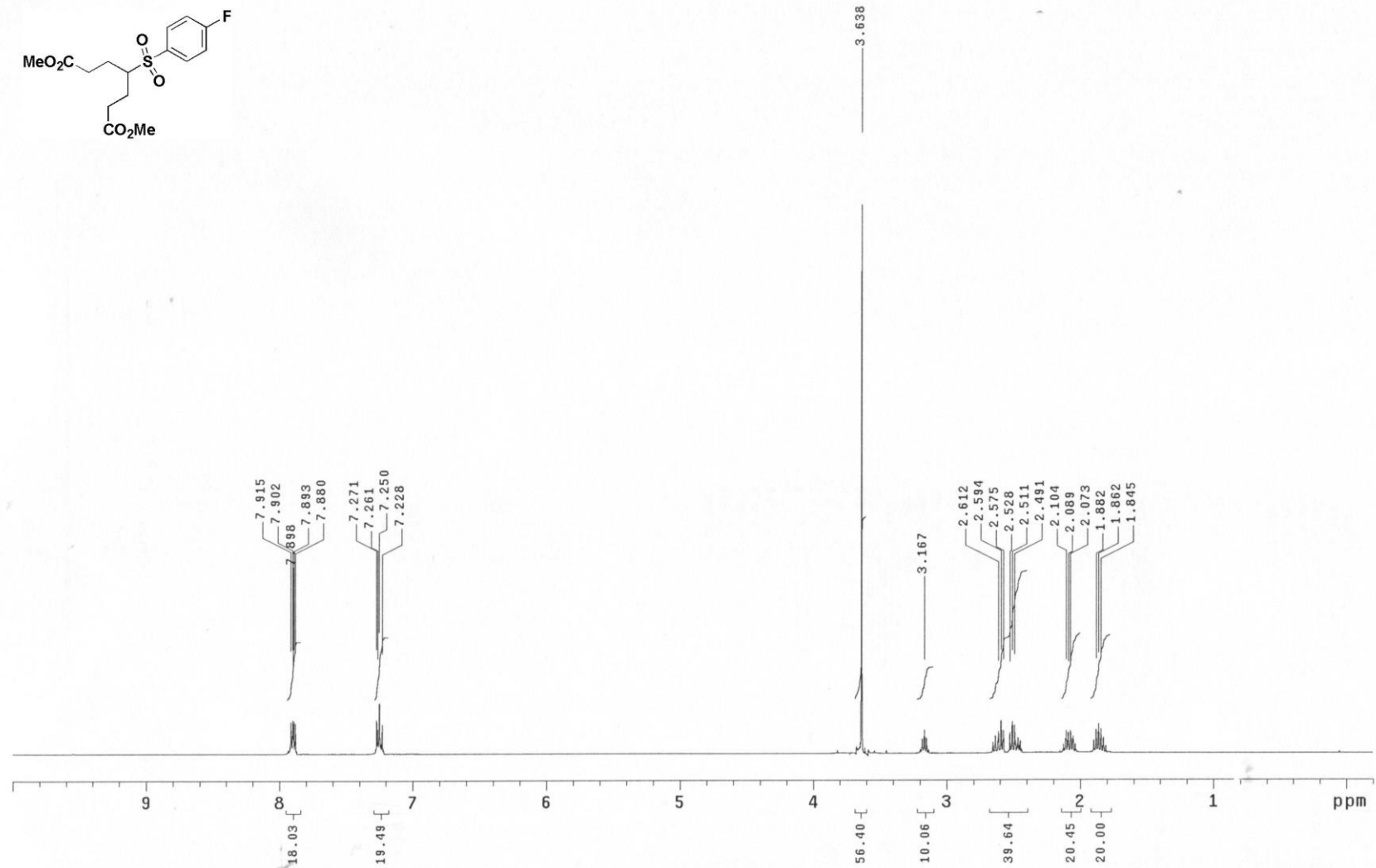
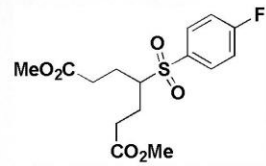
Ambient temperature

Total 2336 repetitions



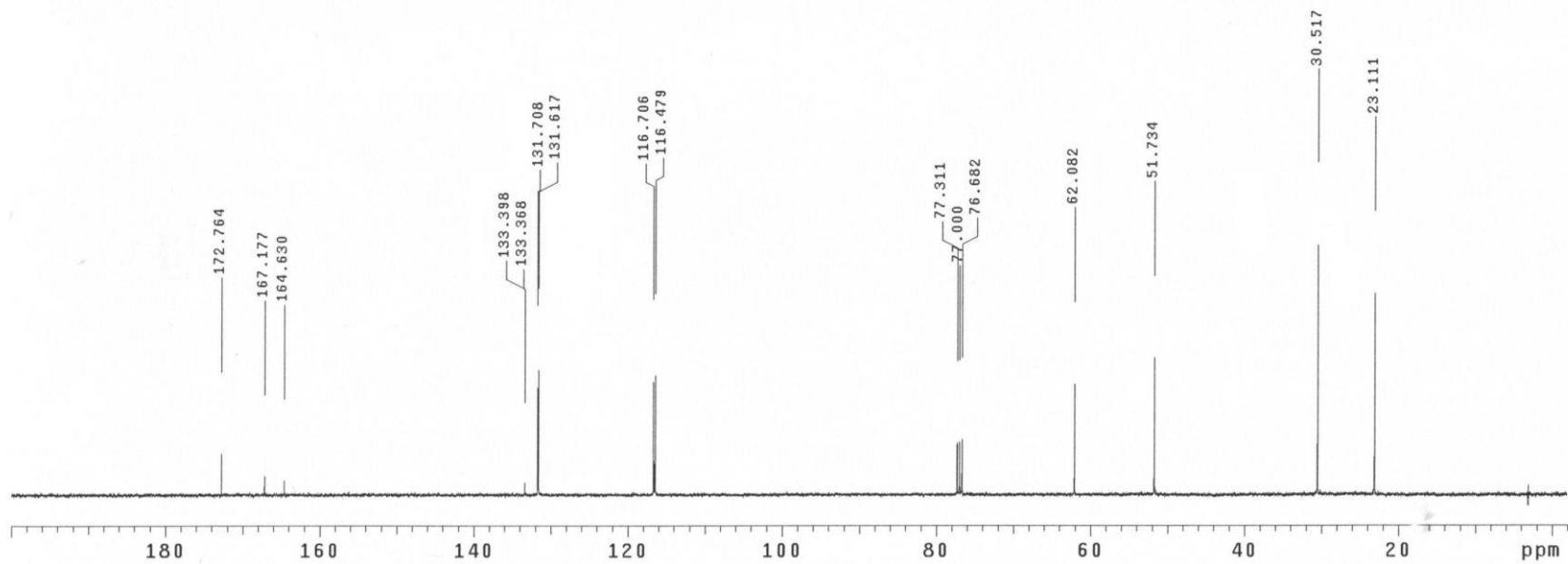
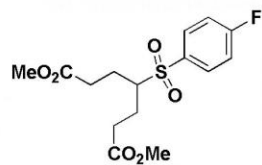
Compound 6h (¹H-NMR spectral data)

PS1117
Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Nov 19 2020
Solvent: CDCl3
Ambient temperature
Total 32 repetitions



Compound 6h (¹³C-NMR spectral data)

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Nov 19 2020
Solvent: CDCl₃
Ambient temperature
Total 1408 repetitions



Compound 6i (¹H-NMR spectral data)

PS1201

Pulse Sequence: s2pu1

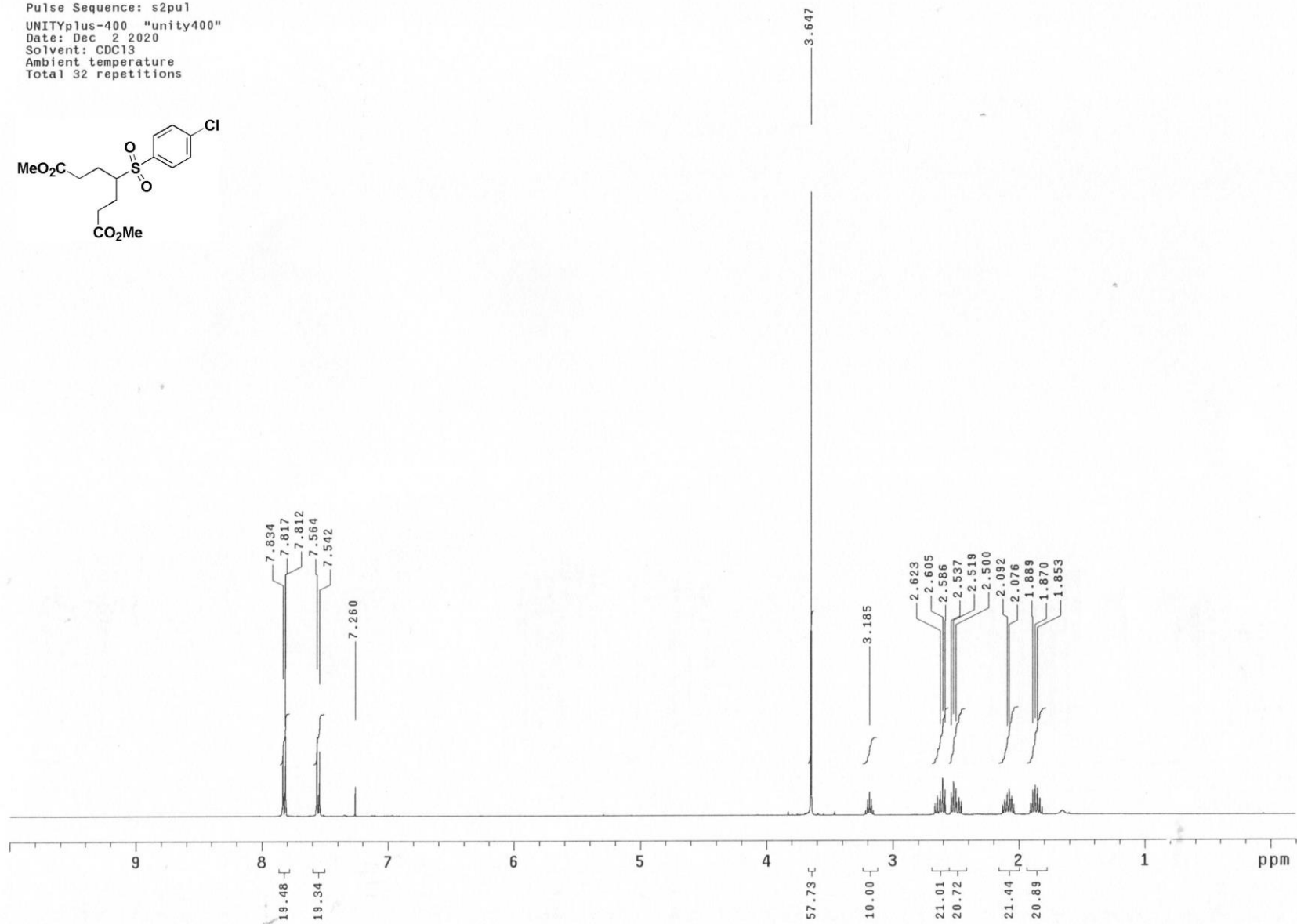
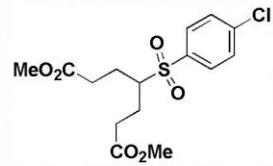
UNITYplus-400 "unity400"

Date: Dec 2 2020

Solvent: CDCl₃

Ambient temperature

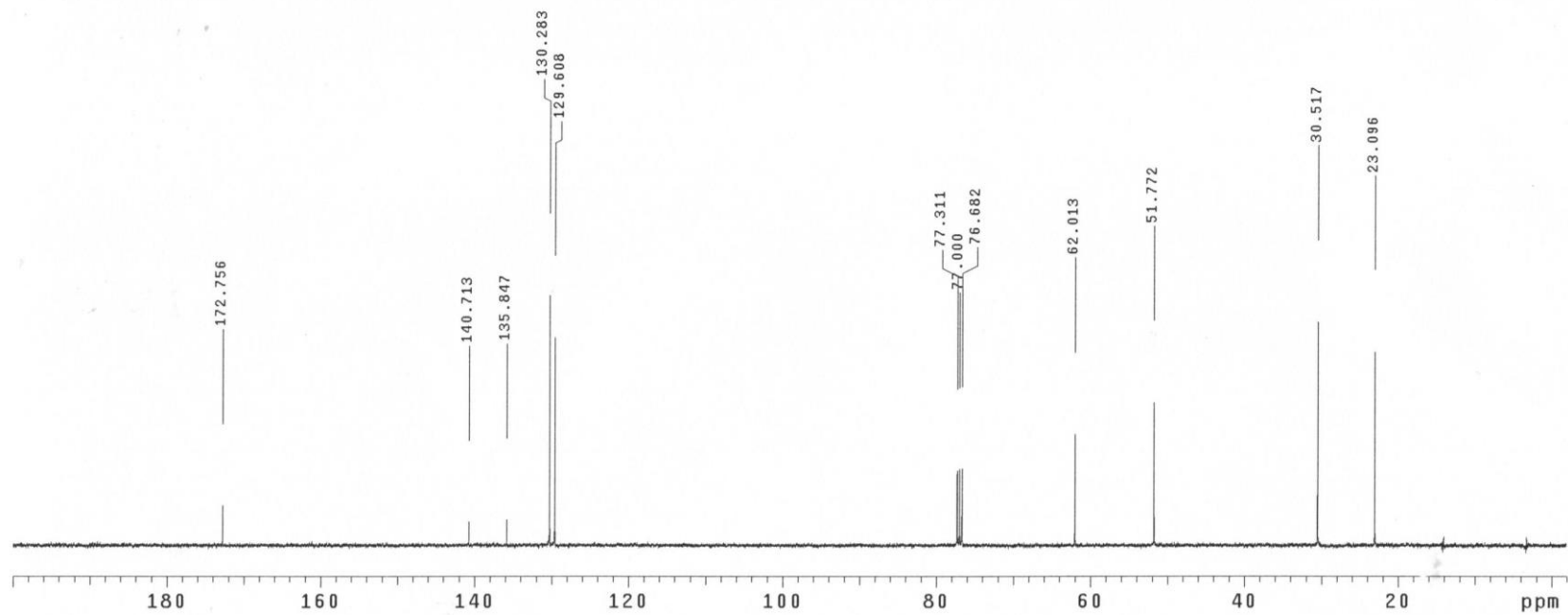
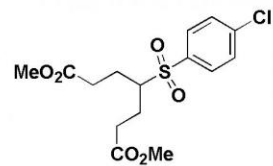
Total 32 repetitions



Compound 6i (¹³C-NMR spectral data)

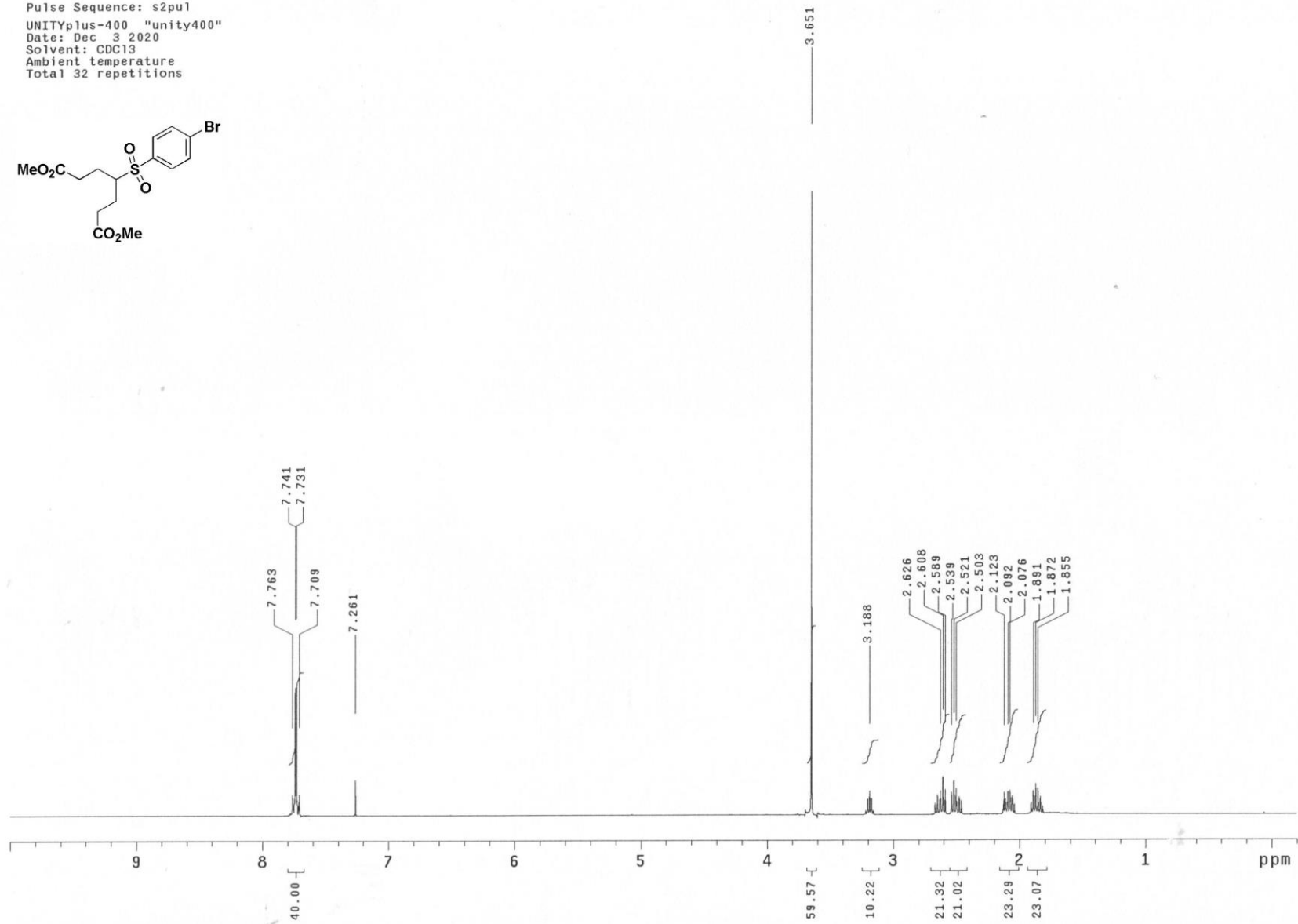
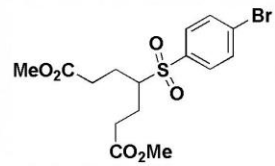
PS1201

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Dec 2 2020
Solvent: CDCl₃
Ambient temperature
Total 1792 repetitions



Compound 6j (¹H-NMR spectral data)

PS1202
Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Dec 3 2020
Solvent: CDCl₃
Ambient temperature
Total 32 repetitions



Compound 6j (¹³C-NMR spectral data)

PS1202

Pulse Sequence: s2pu1

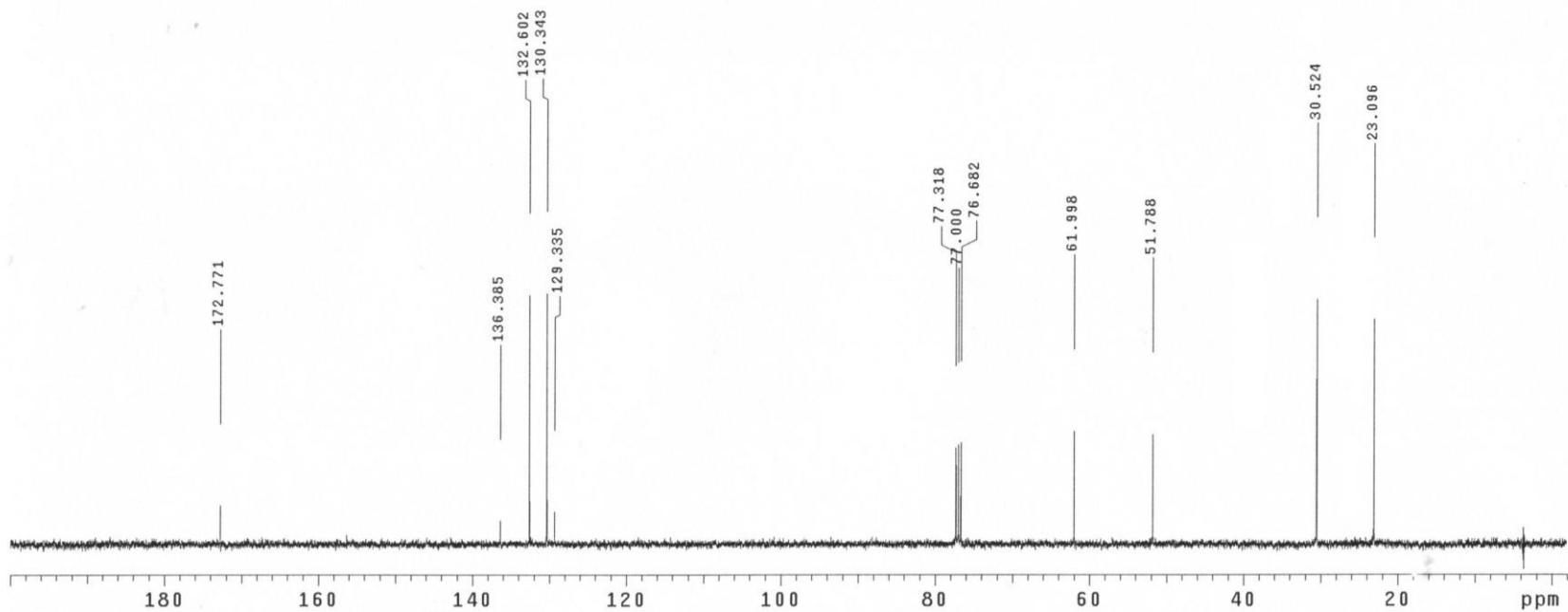
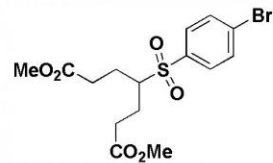
UNITYplus-400 "unity400"

Date: Dec 3 2020

Solvent: CDCl₃

Ambient temperature

Total 1024 repetitions



Compound 6k (¹H-NMR spectral data)

PS1217k

Pulse Sequence: s2pu1

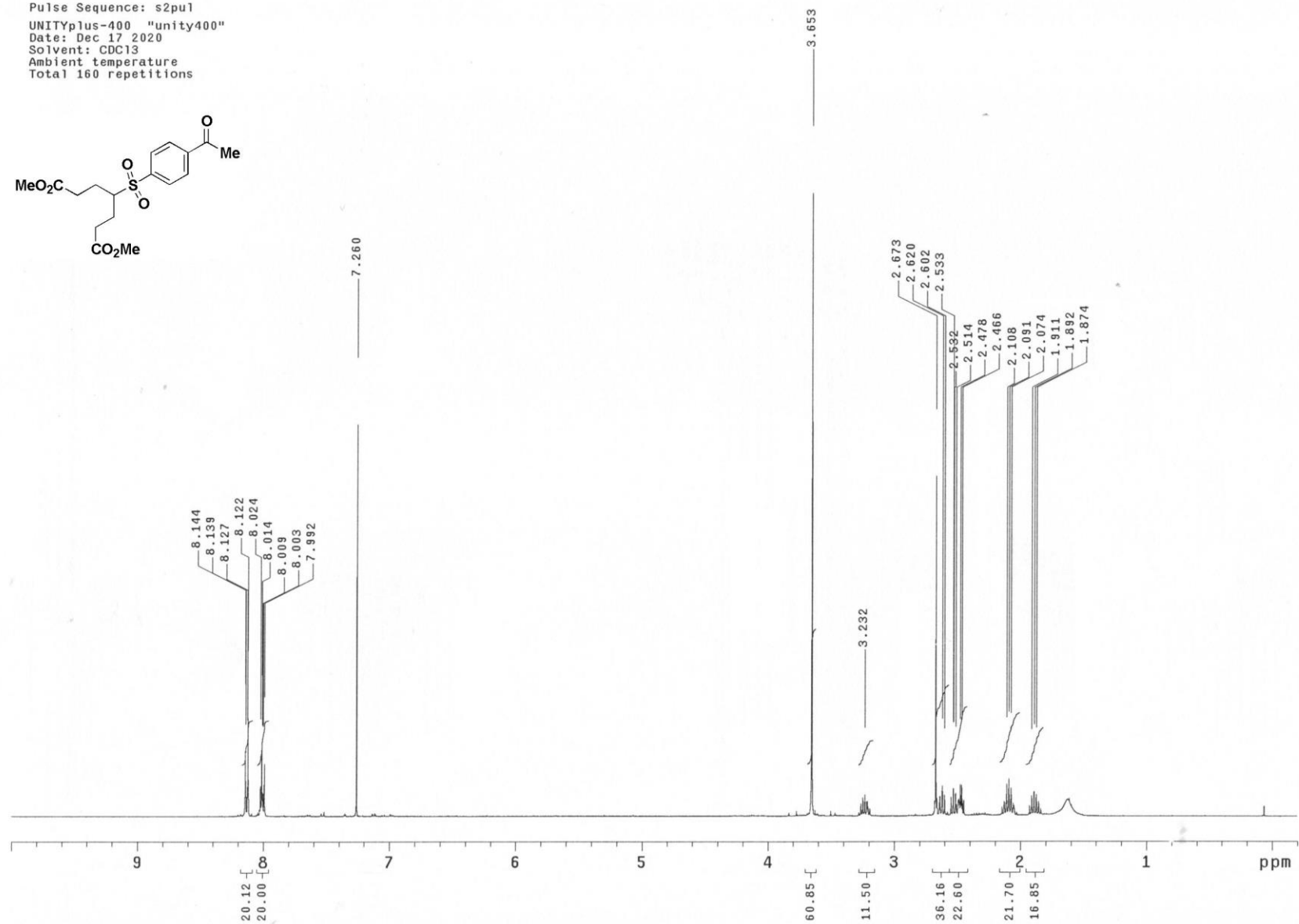
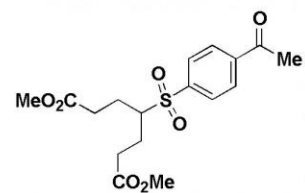
UNITYplus-400 "unity400"

Date: Dec 17 2020

Solvent: CDCl₃

Ambient temperature

Total 160 repetitions



Compound 6k (¹³C-NMR spectral data)

PS1217k

Pulse Sequence: s2pu1

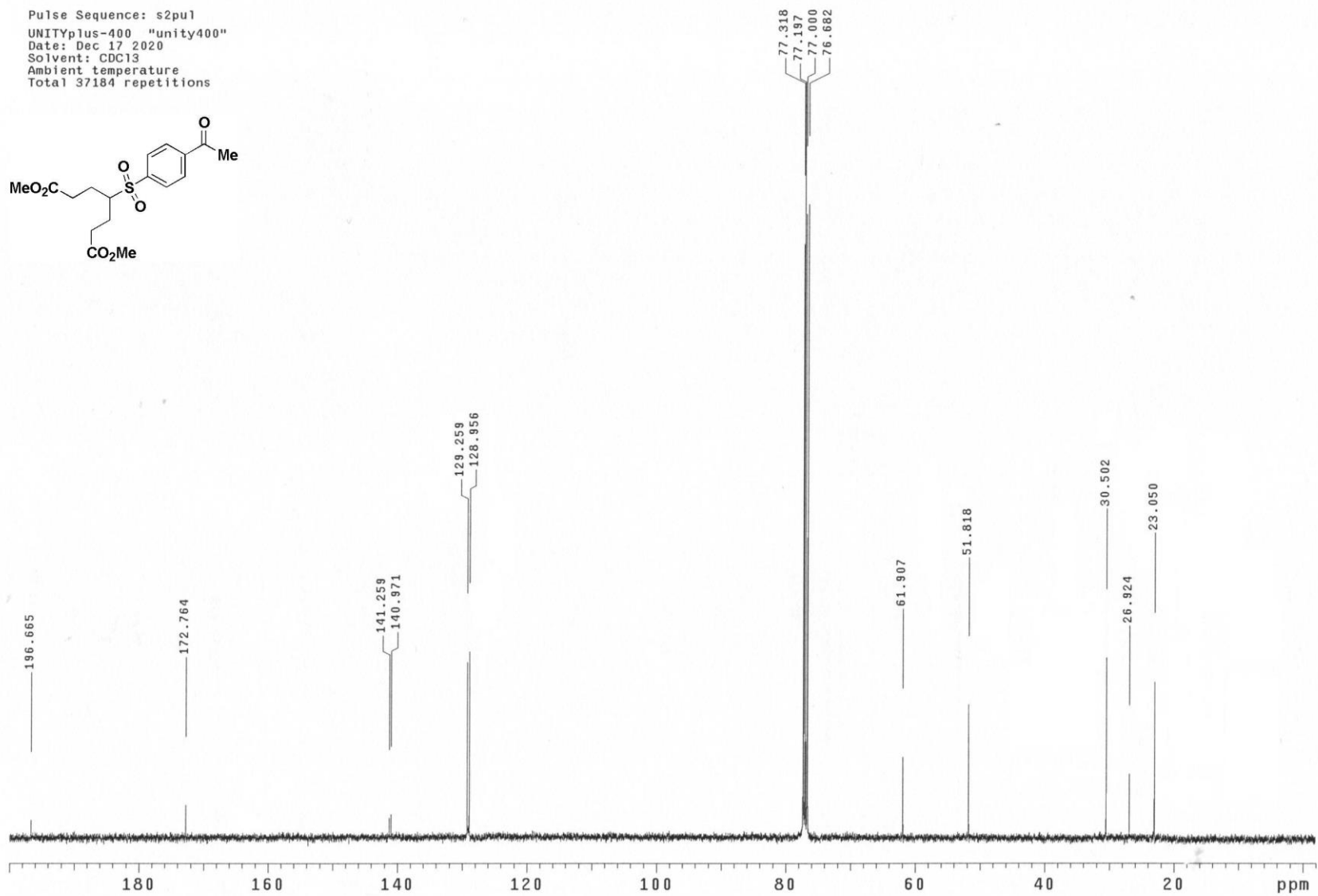
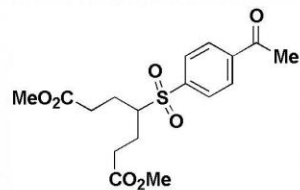
UNITYplus-400 "unity400"

Date: Dec 17 2020

Solvent: CDCl₃

Ambient temperature

Total 37184 repetitions



Compound 6I (¹H-NMR spectral data)

PS1203

Pulse Sequence: s2pu1

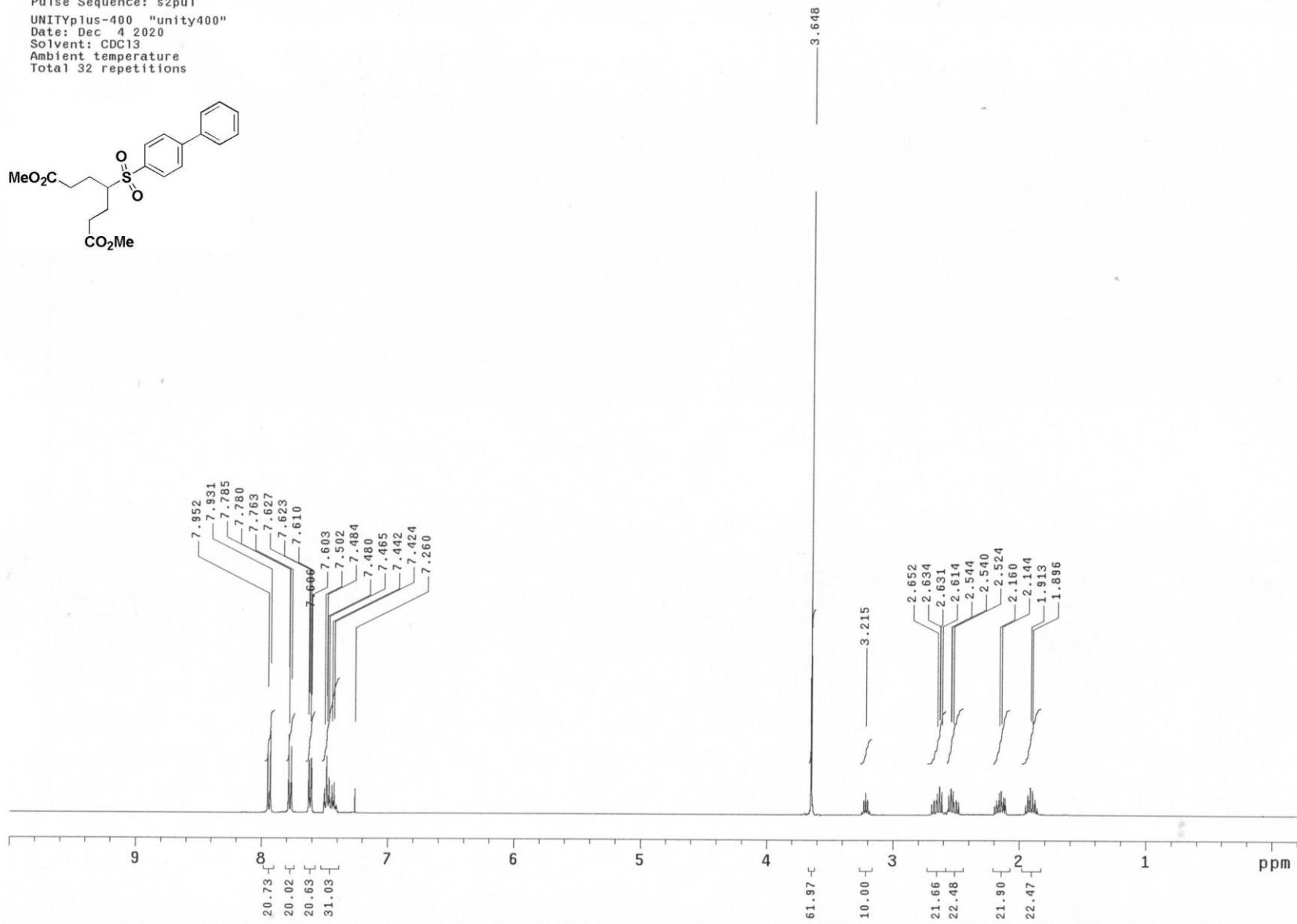
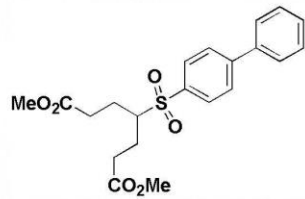
UNITYplus-400 "unity400"

Date: Dec 4 2020

Solvent: CDC13

Ambient temperature

Total 32 repetitions



Compound 6I (¹³C-NMR spectral data)

PS1203

Pulse Sequence: s2pu1

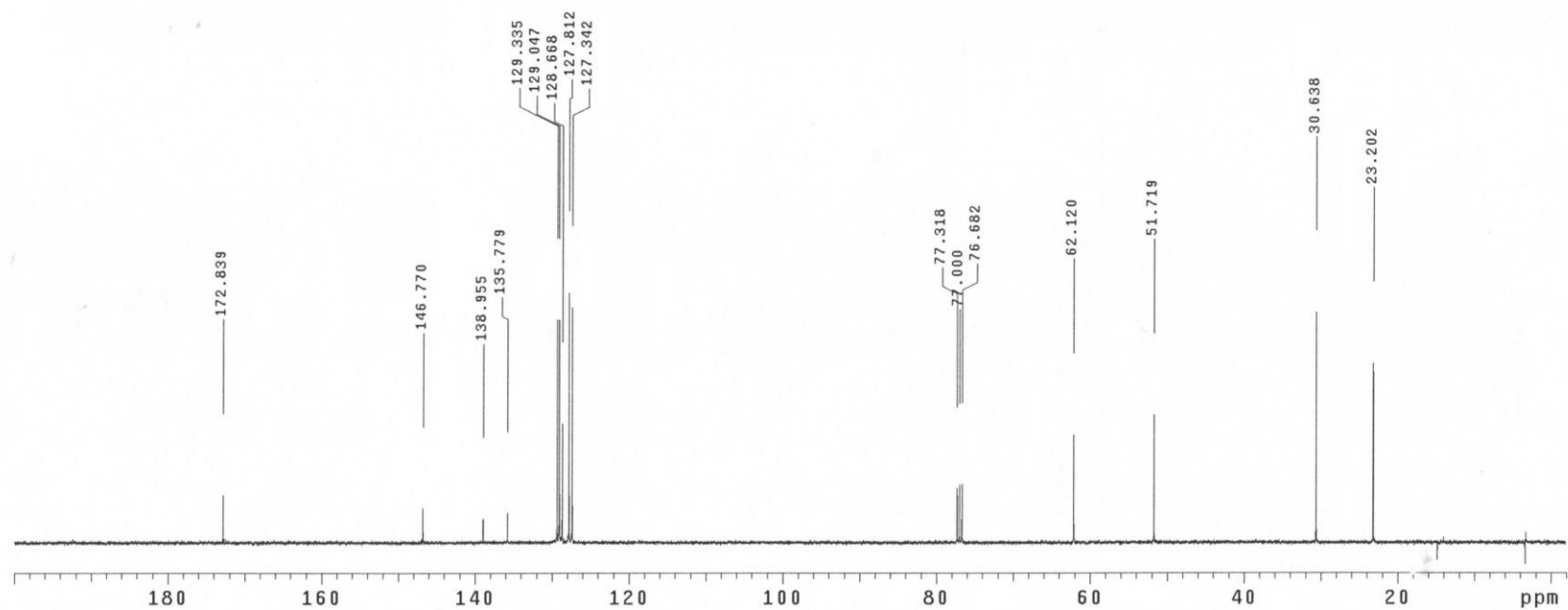
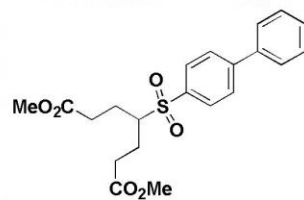
UNITYplus-400 "unity400"

Date: Dec 4 2020

Solvent: CDC13

Ambient temperature

Total 1392 repetitions



Compound 6m (¹H-NMR spectral data)

PS1208

Pulse Sequence: s2pu1

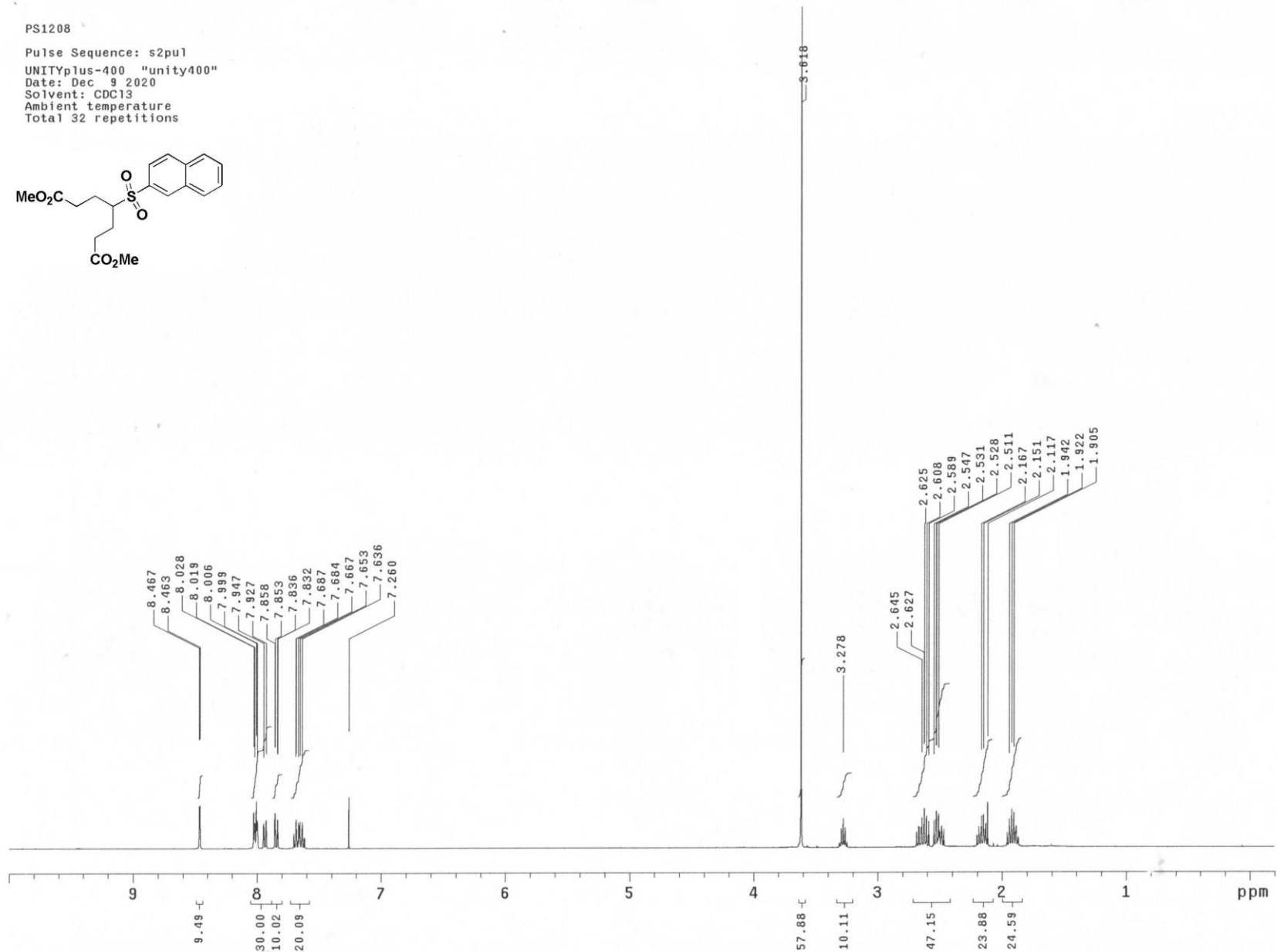
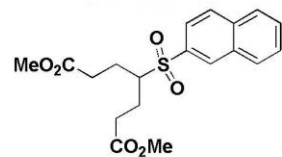
UNITYplus-400 "unity400"

Date: Dec 9 2020

Solvent: CDCl₃

Ambient temperature

Total 32 repetitions



Compound 6m (¹³C-NMR spectral data)

PS1208

Pulse Sequence: s2pu1

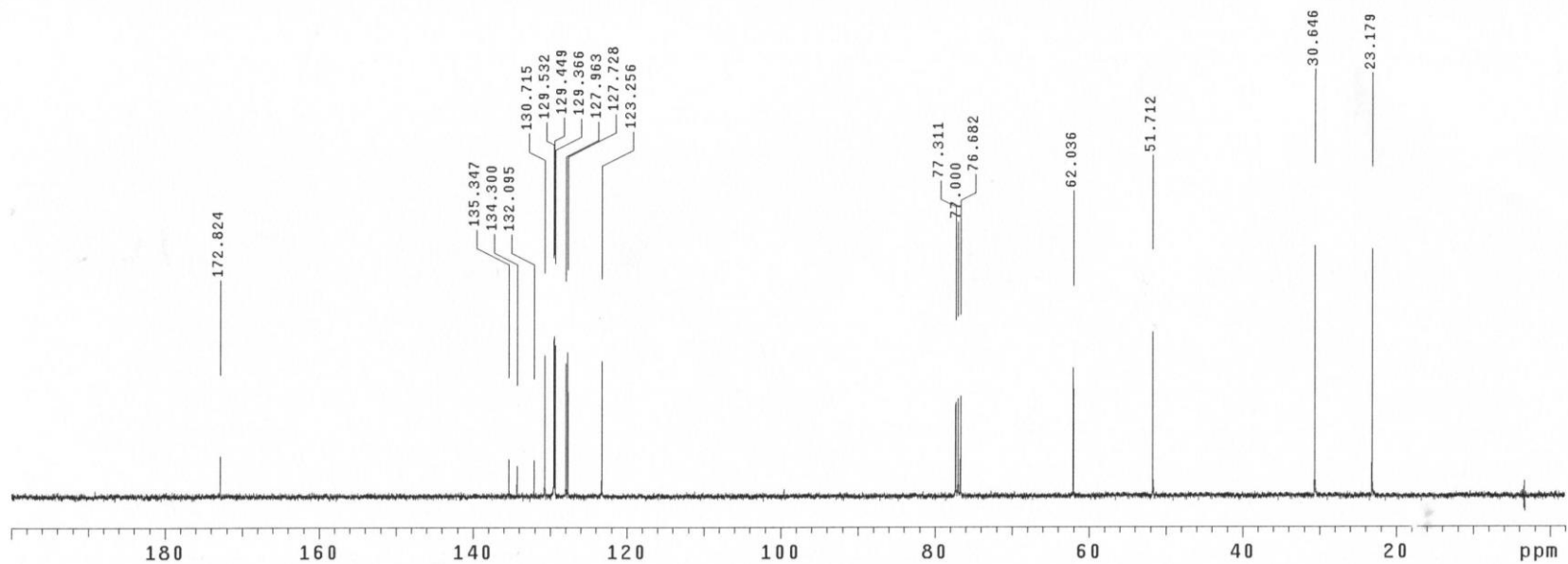
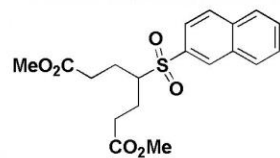
UNITYplus-400 "unity400"

Date: Dec 9 2020

Solvent: CDCl₃

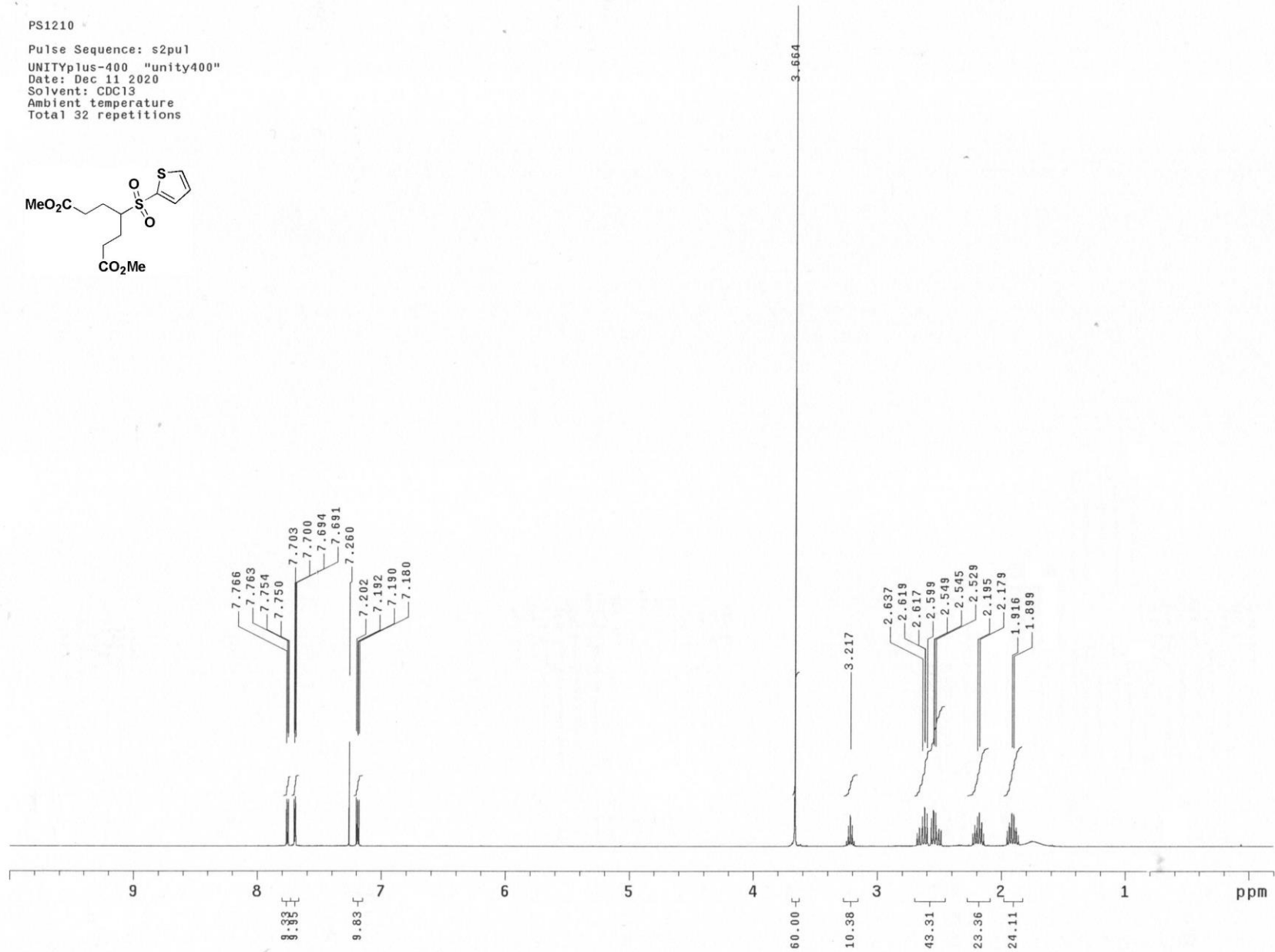
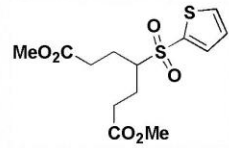
Ambient temperature

Total 1712 repetitions



Compound 6n (¹H-NMR spectral data)

PS1210
Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Dec 11 2020
Solvent: CDCl3
Ambient temperature
Total 32 repetitions



Compound 6n (¹³C-NMR spectral data)

PS1210

Pulse Sequence: s2pu1

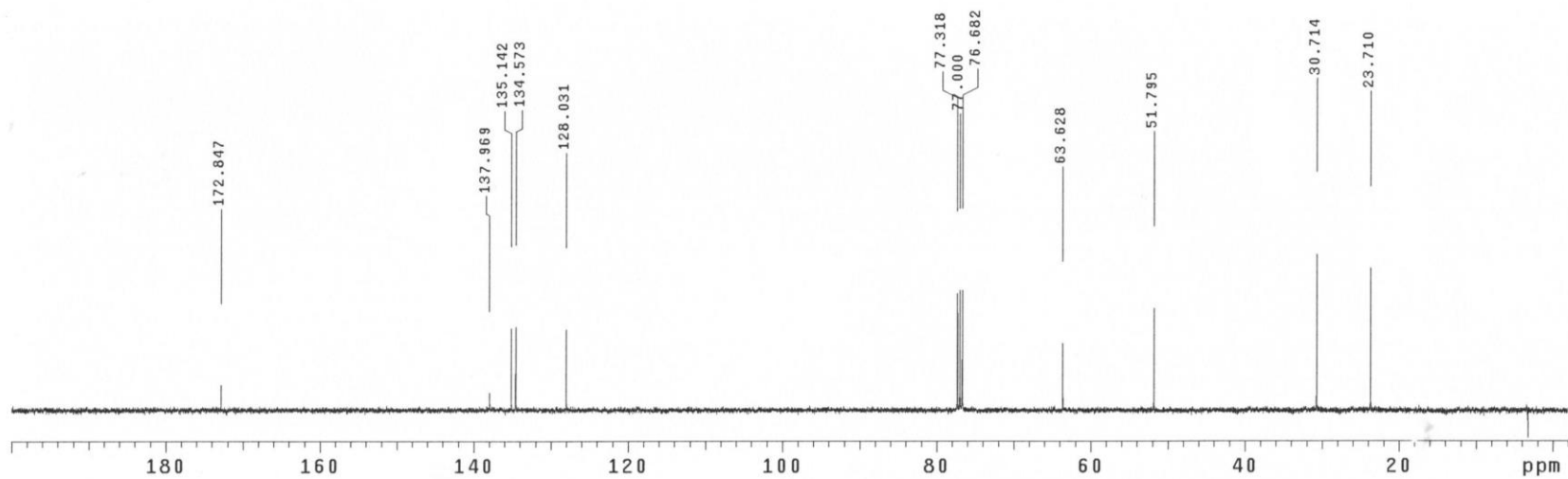
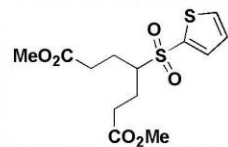
UNITYplus-400 "unity400"

Date: Dec 11 2020

Solvent: CDCl₃

Ambient temperature

Total 2720 repetitions



Compound 7a (¹H-NMR spectral data)

CRA0113

Pulse Sequence: s2pu1

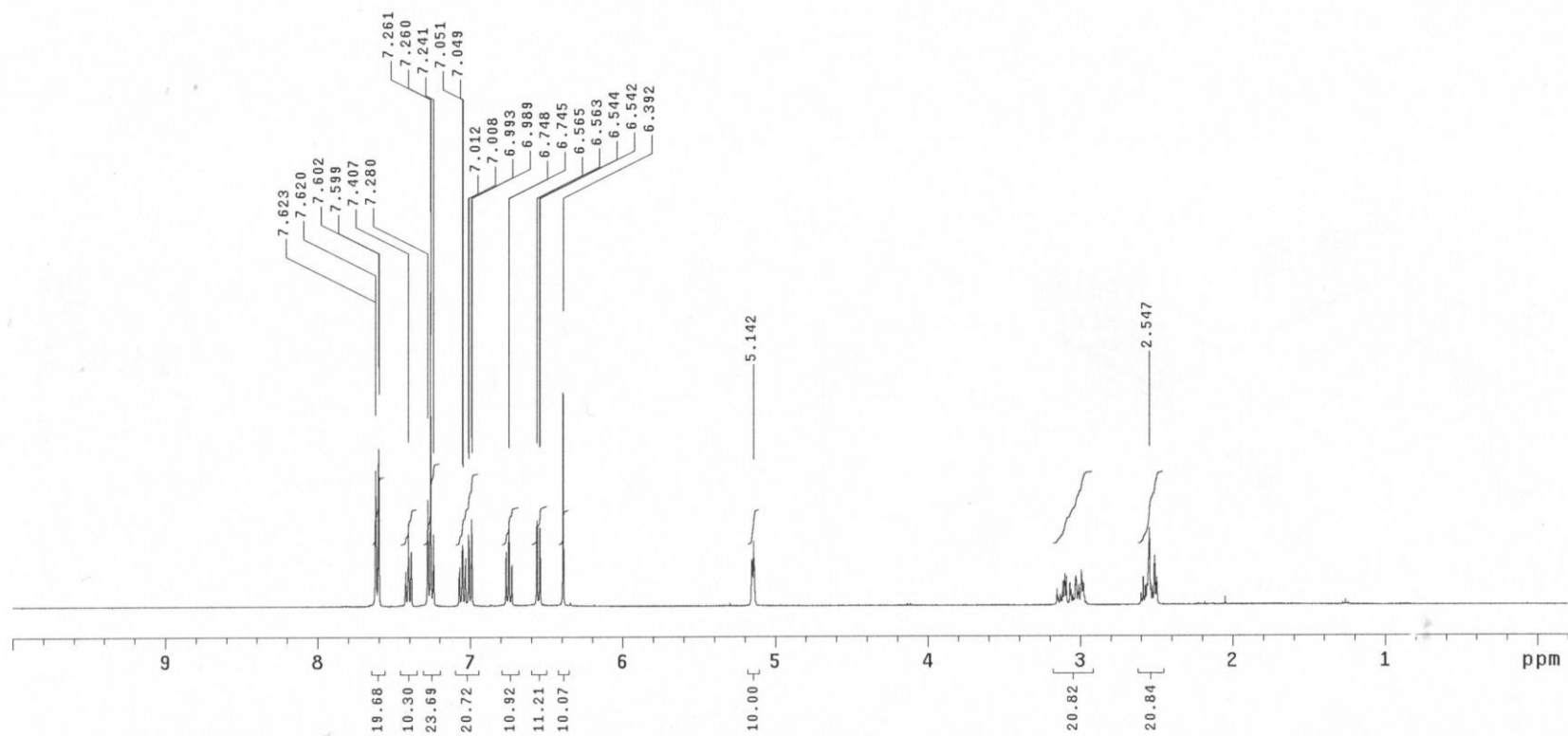
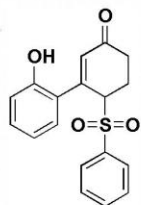
UNITYplus-400 "unity400"

Date: Jan 15 2021

Solvent: CDCl₃

Ambient temperature

Total 32 repetitions



Compound 7a (¹³C-NMR spectral data)

CRA0113

Pulse Sequence: s2pu1

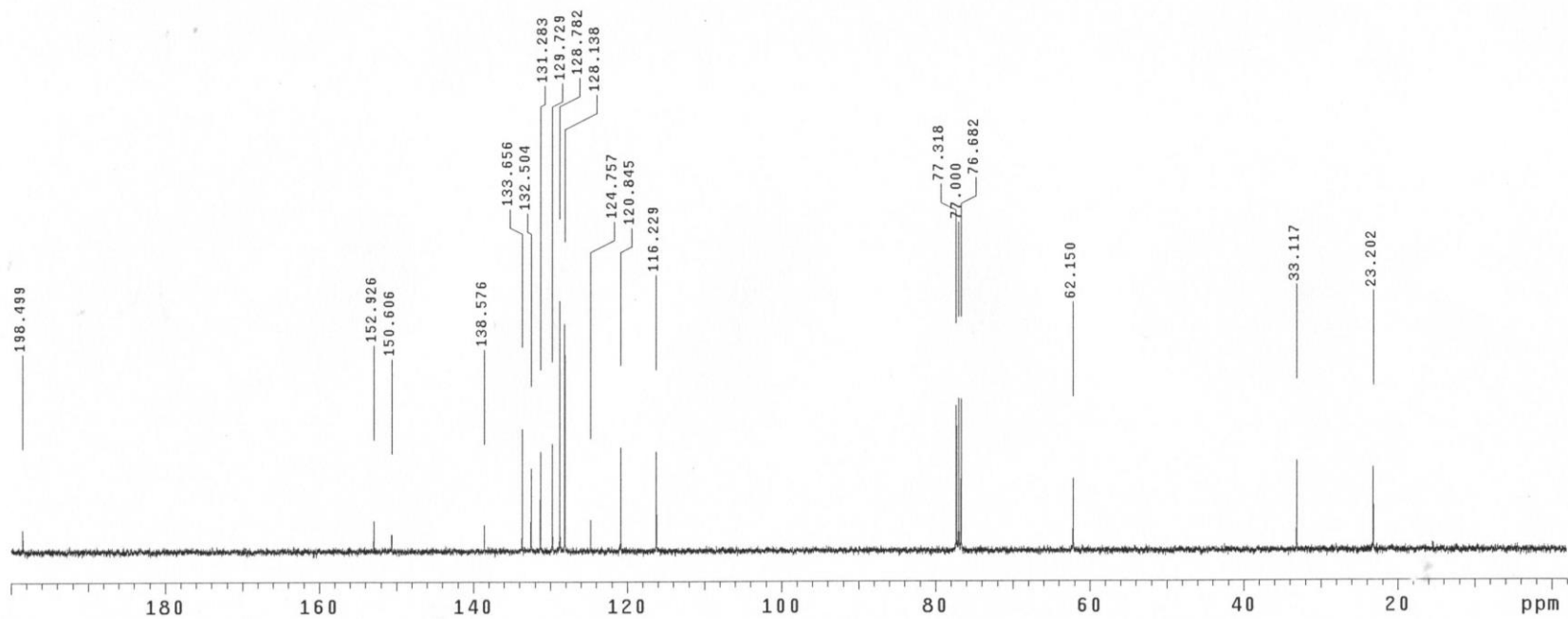
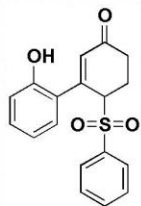
UNITYplus-400 "unity400"

Date: Jan 15 2021

Solvent: CDCl₃

Ambient temperature

Total 2128 repetitions



Compound 7b (¹H-NMR spectral data)

PSMVK103

Pulse Sequence: s2pu1

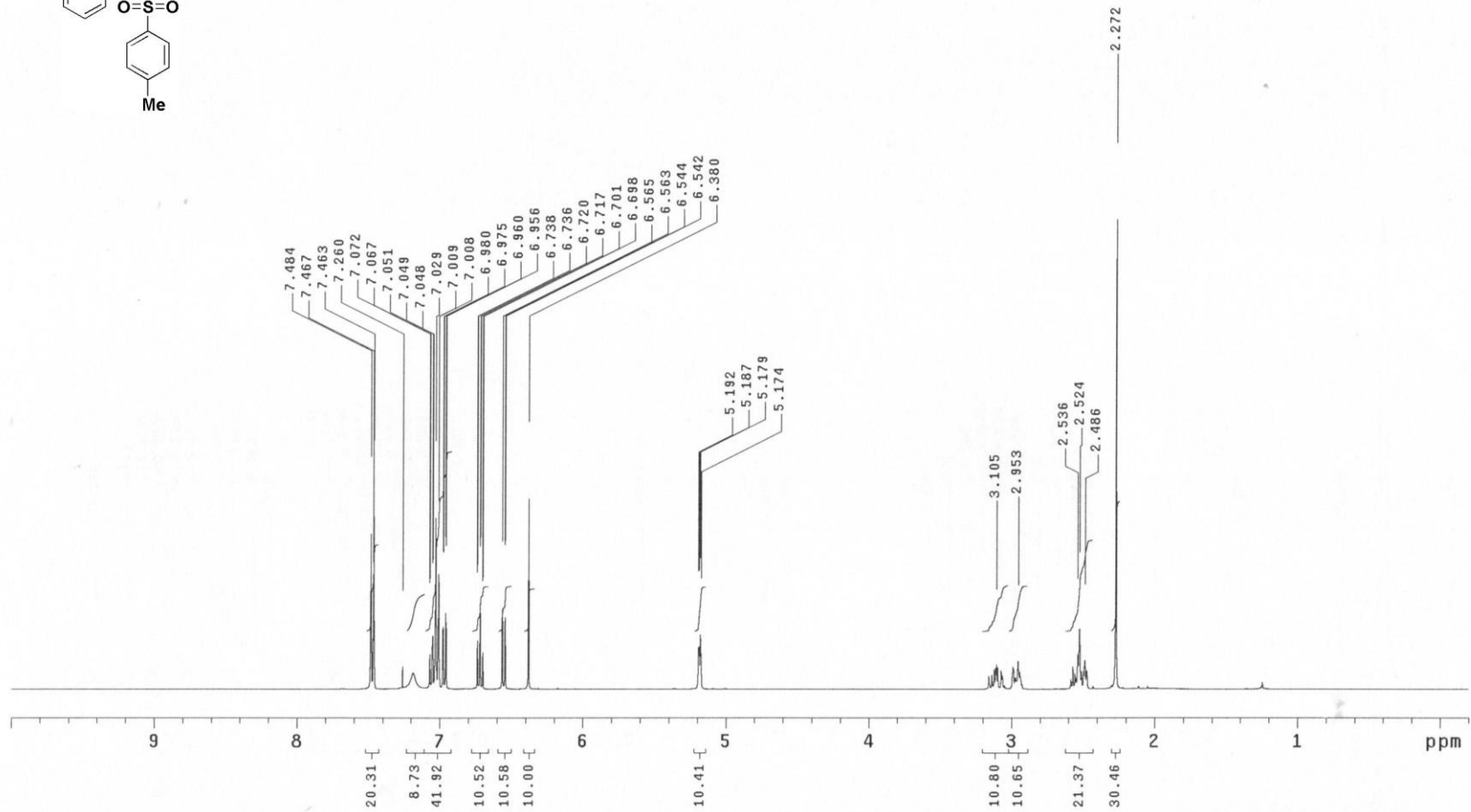
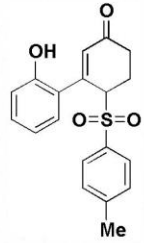
UNITYplus-400 "unity400"

Date: Dec 21 2020

Solvent: CDCl₃

Ambient temperature

Total 32 repetitions



Compound 7b (¹³C-NMR spectral data)

PSMVK103

Pulse Sequence: s2pu1

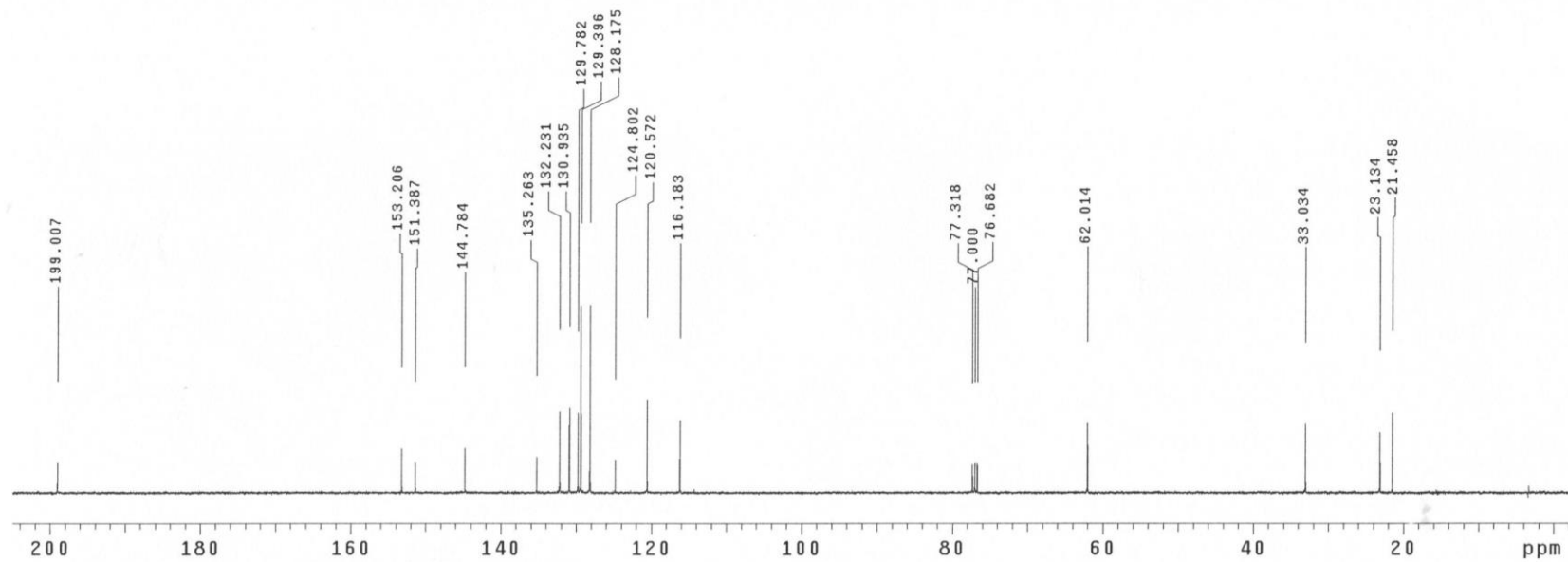
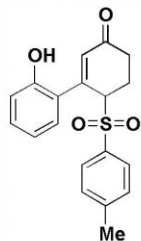
UNITYplus-400 "unity400"

Date: Dec 21 2020

Solvent: CDC13

Ambient temperature

Total 2208 repetitions



Compound 5a (¹H-NMR spectral data)

PS1106

Pulse Sequence: s2pu1

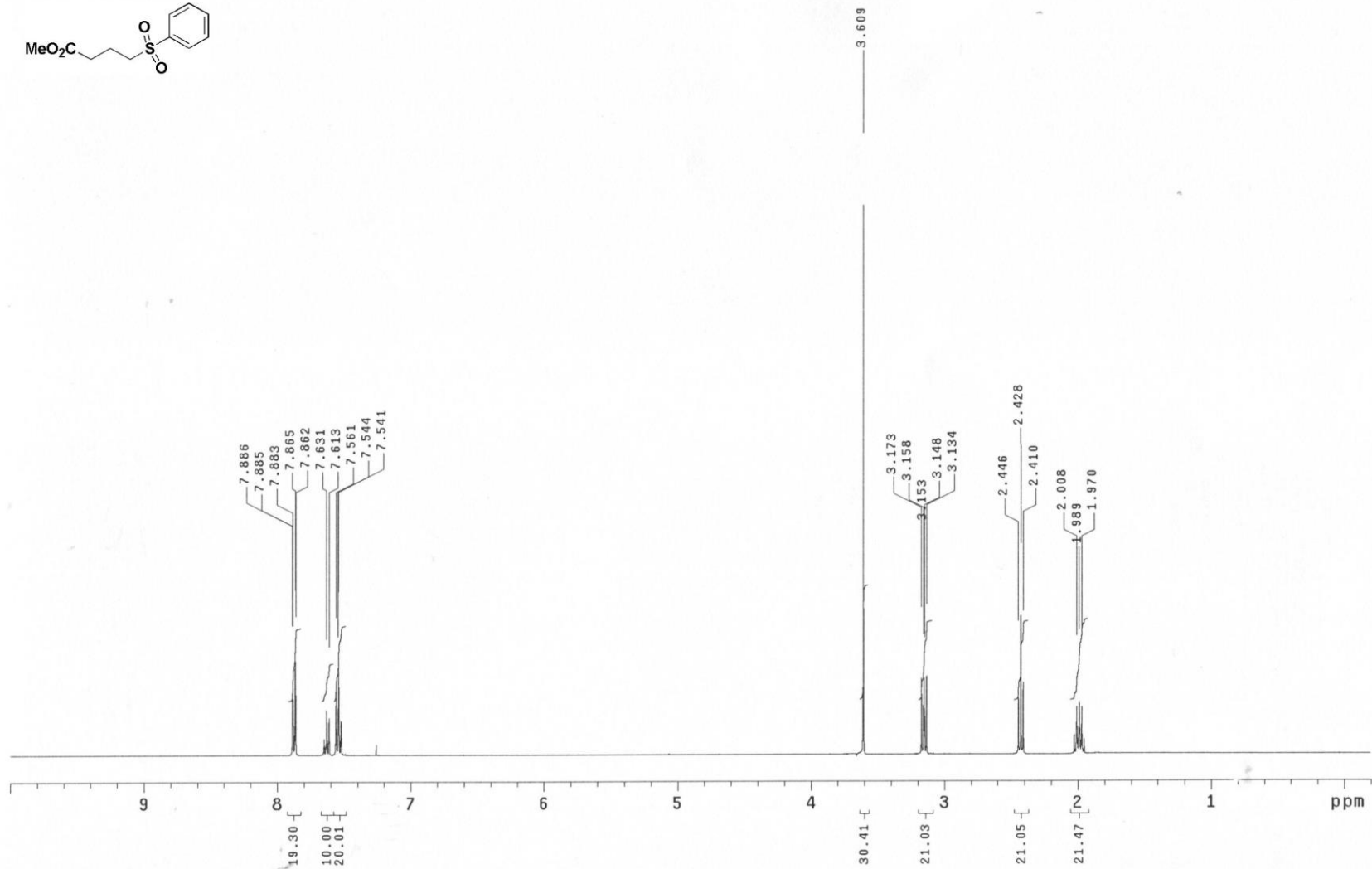
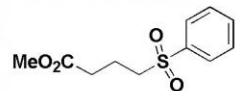
UNITYplus-400 "unity400"

Date: Nov 5 2020

Solvent: CDCl₃

Ambient temperature

Total 32 repetitions



Compound 5a (¹³C-NMR spectral data)

PS1106

Pulse Sequence: s2pu1

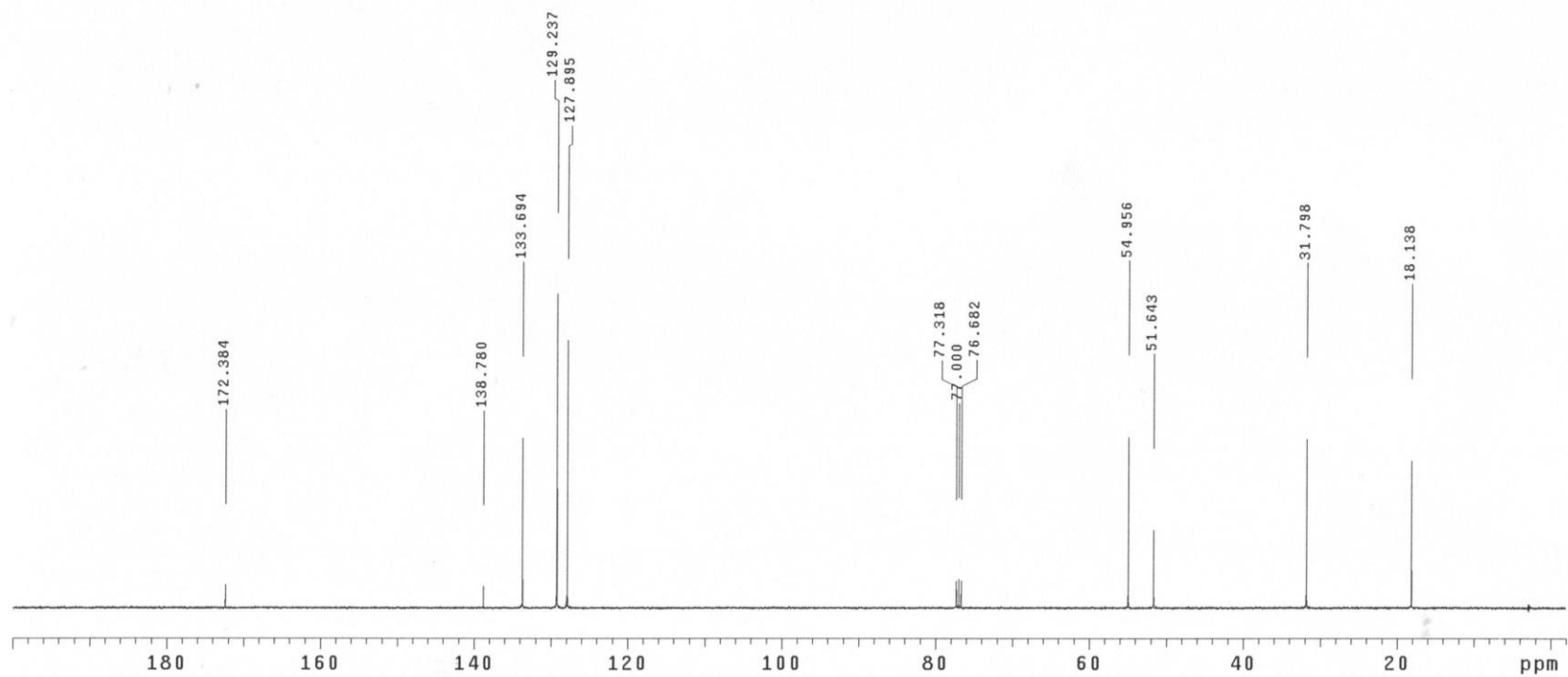
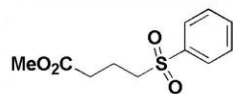
UNITYplus-400 "unity400"

Date: Nov 5 2020

Solvent: CDCl₃

Ambient temperature

Total 944 repetitions



Compound 5b (¹H-NMR spectral data)

PS1104

Pulse Sequence: s2pu1

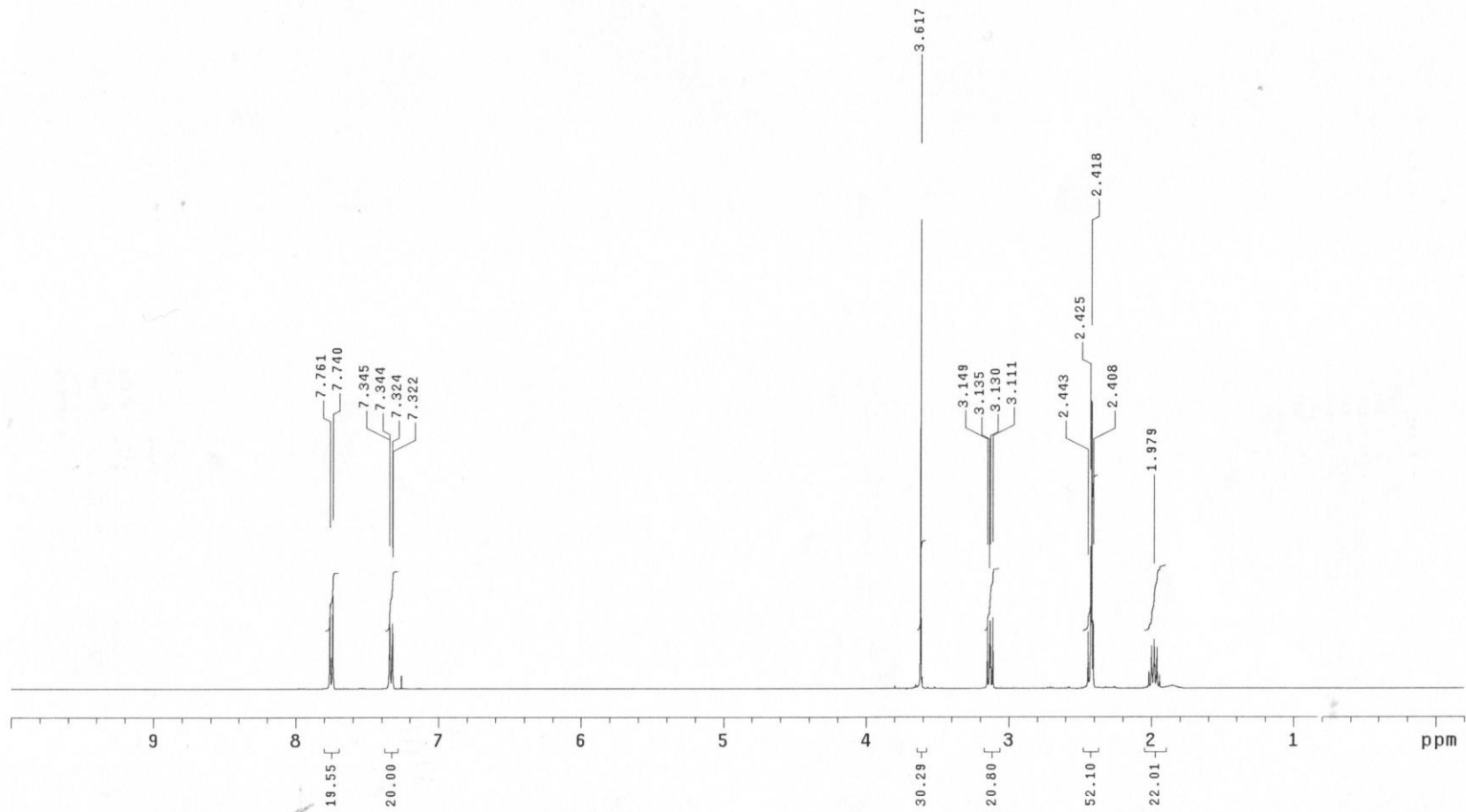
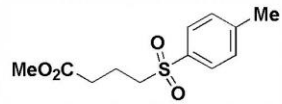
UNITYplus-400 "unity400"

Date: Nov 4 2020

Solvent: CDCl₃

Ambient temperature

Total 32 repetitions



Compound 5b (¹³C-NMR spectral data)

PS1104

Pulse Sequence: s2pu1

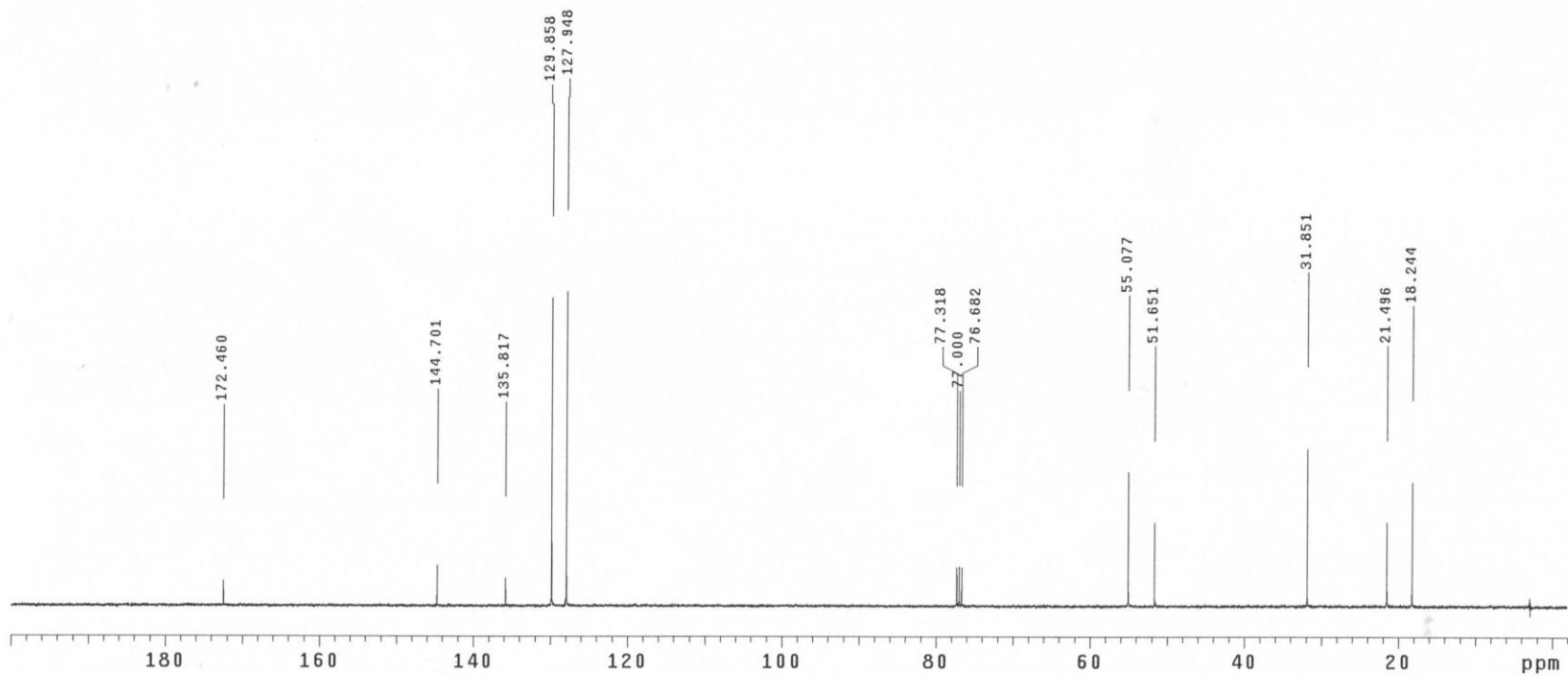
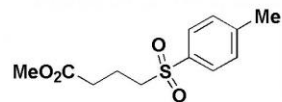
UNITYplus-400 "unity400"

Date: Nov 4 2020

Solvent: CDCl₃

Ambient temperature

Total 640 repetitions



Compound 5c (¹H-NMR spectral data)

PS1113-1

Pulse Sequence: s2pu1

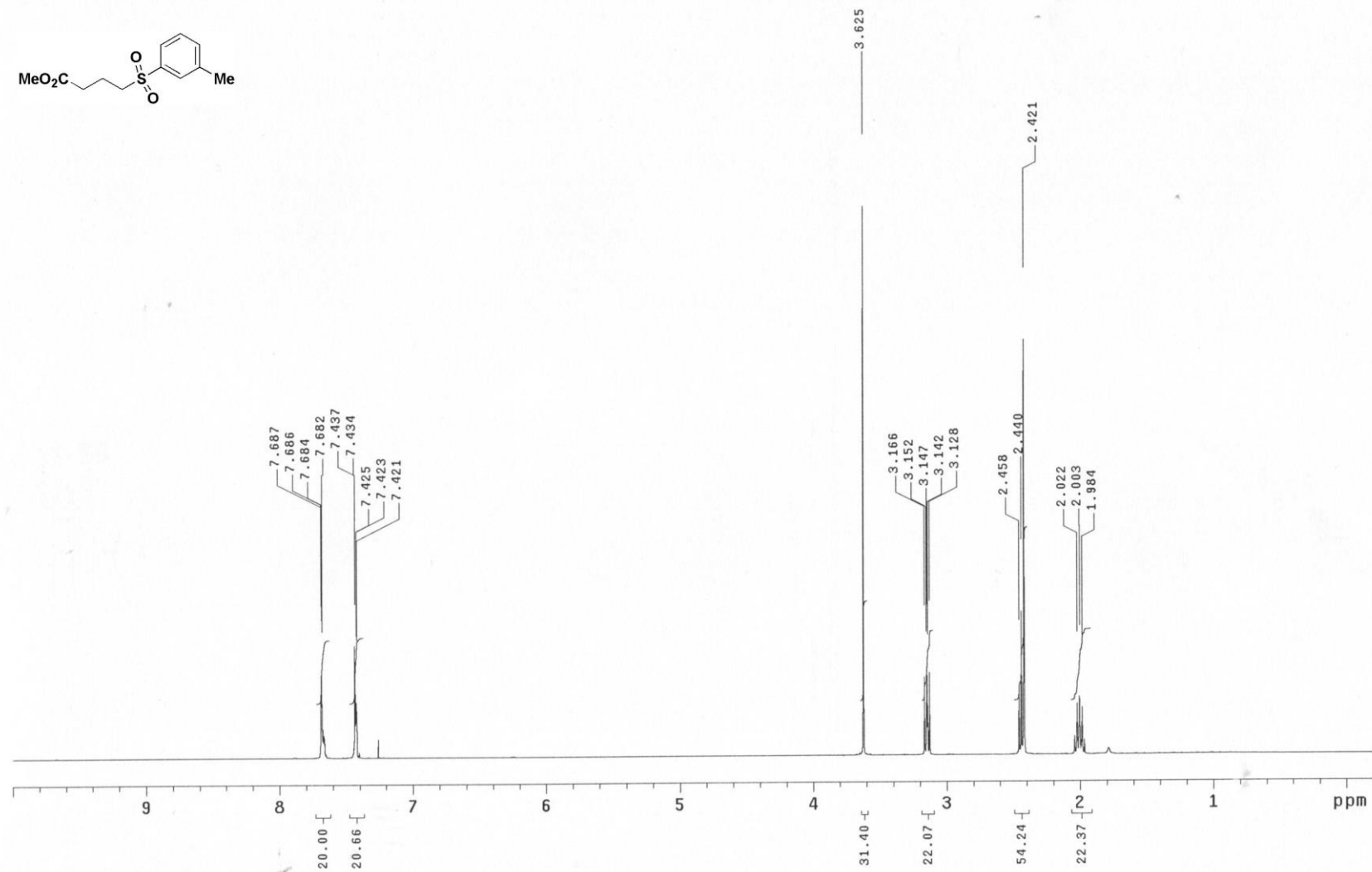
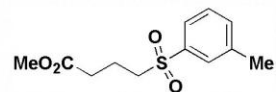
UNITYplus-400 "unity400"

Date: Nov 13 2020

Solvent: CDCl₃

Ambient temperature

Total 32 repetitions



Compound 5c (¹³C-NMR spectral data)

PS1113-1

Pulse Sequence: s2pu1

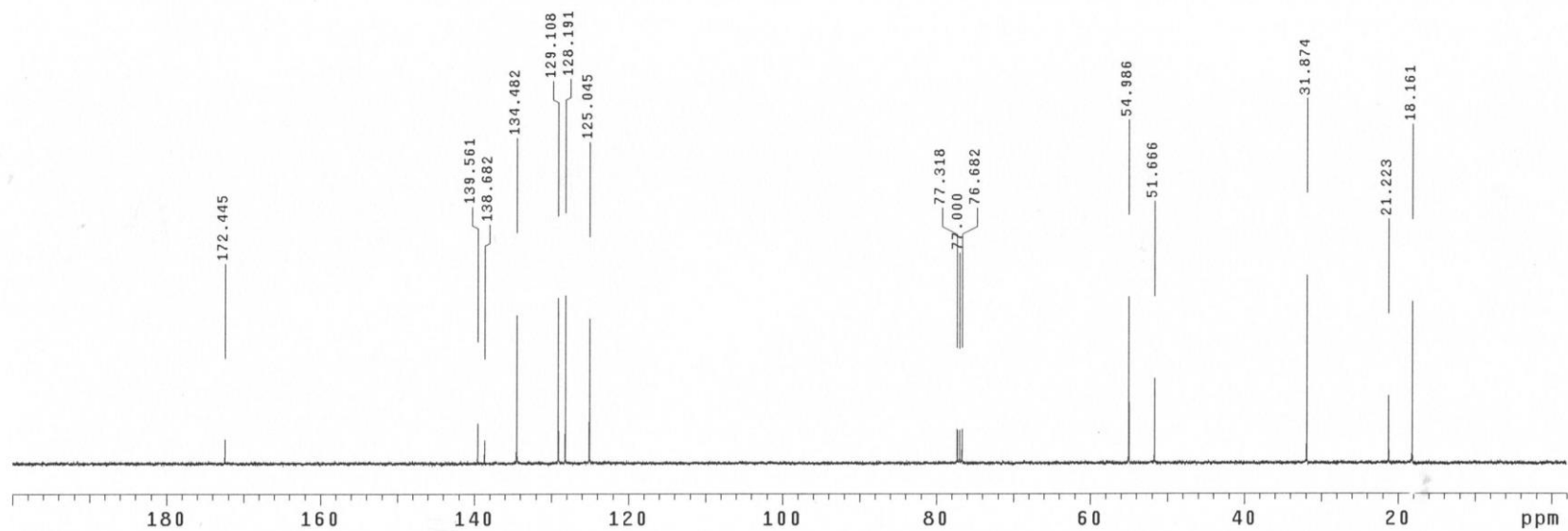
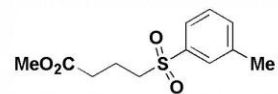
UNITYplus-400 "unity400"

Date: Nov 13 2020

Solvent: CDCl₃

Ambient temperature

Total 720 repetitions



Compound 5d (¹H-NMR spectral data)

PS1120-1

Pulse Sequence: s2pu1

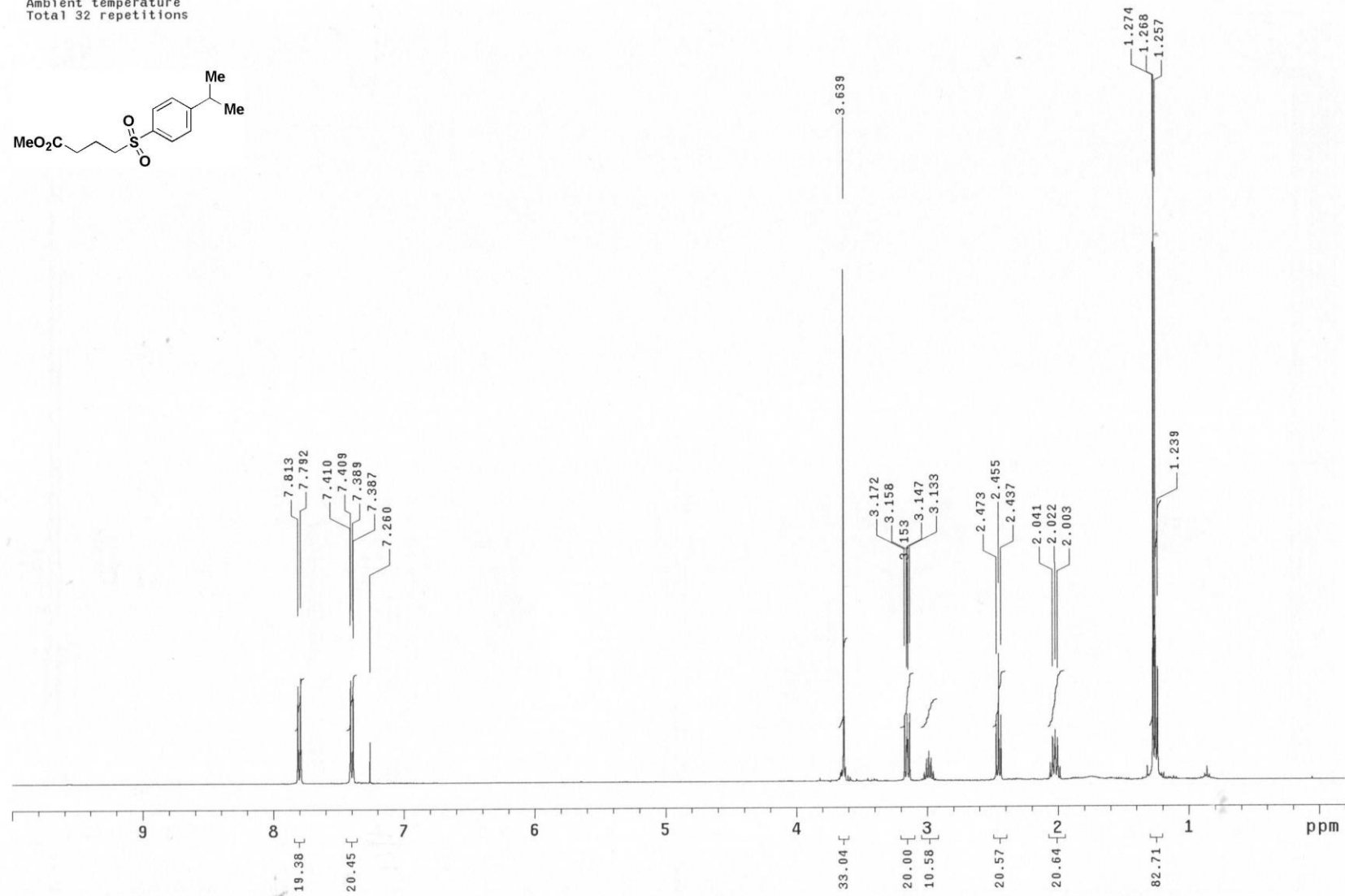
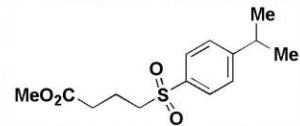
UNITYplus-400 "unity400"

Date: Nov 19 2020

Solvent: CDCl₃

Ambient temperature

Total 32 repetitions



Compound 5d (¹³C-NMR spectral data)

PS1120-1

Pulse Sequence: s2pu1

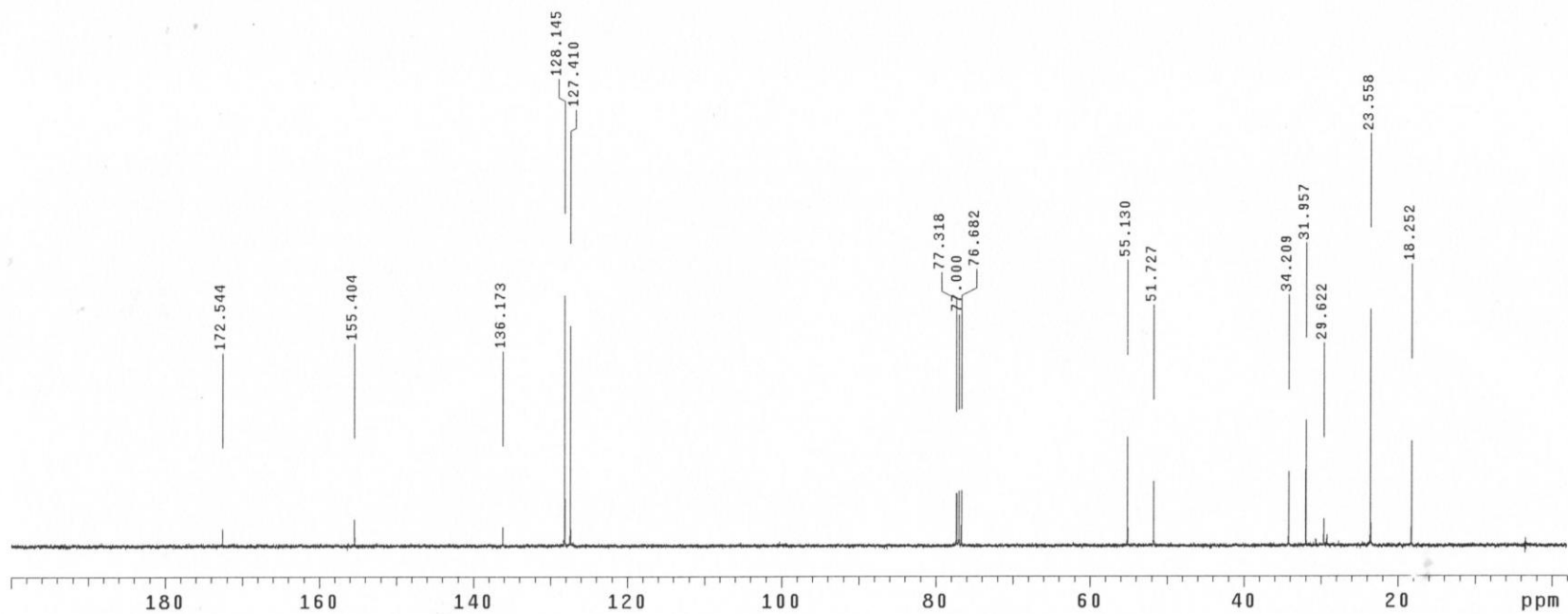
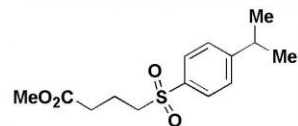
UNITYplus-400 "unity400"

Date: Nov 19 2020

Solvent: CDCl₃

Ambient temperature

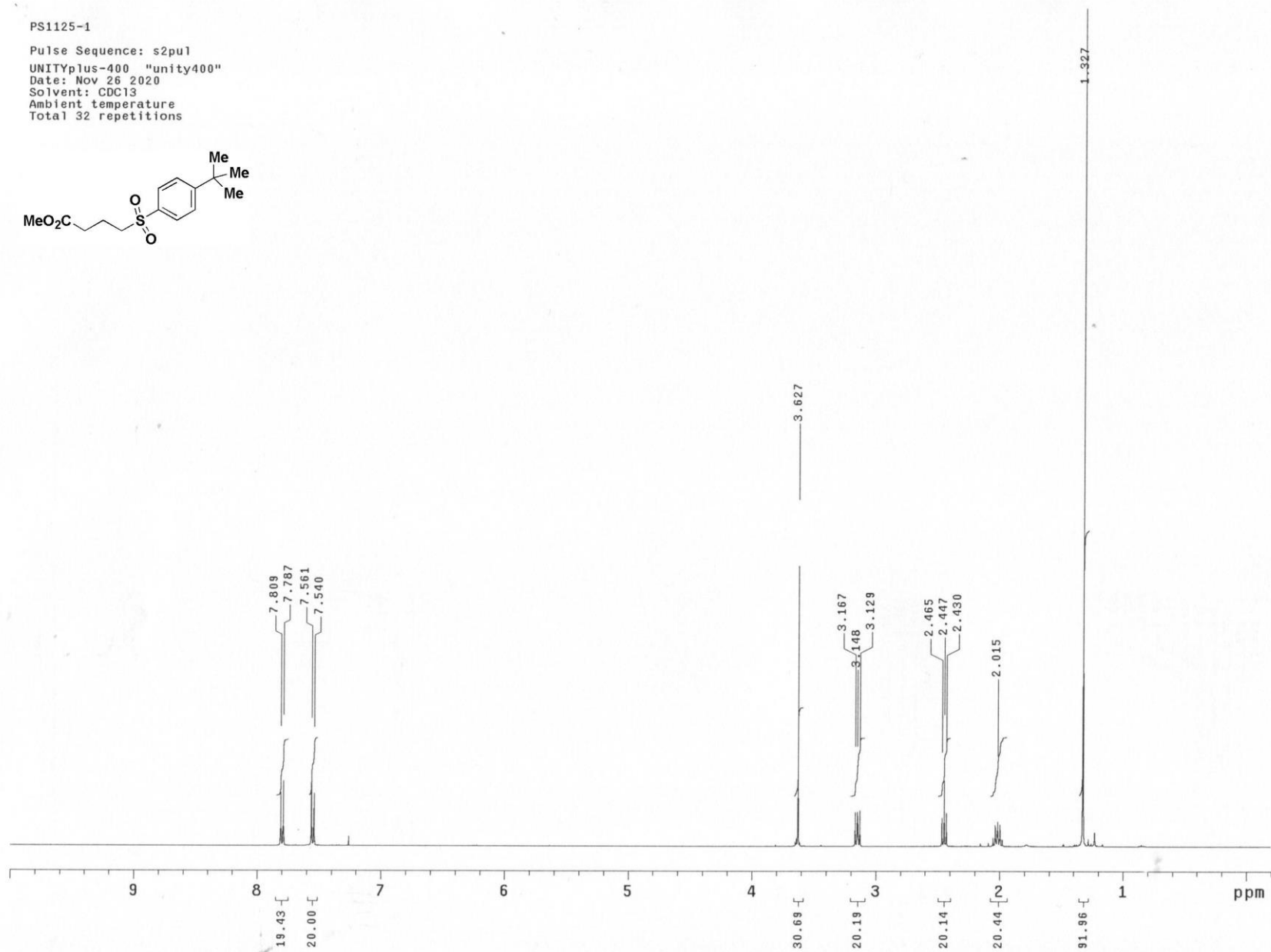
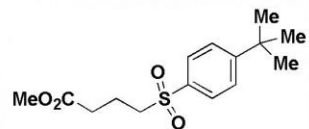
Total 1312 repetitions



Compound 5e (¹H-NMR spectral data)

PS1125-1

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Nov 26 2020
Solvent: CDC13
Ambient temperature
Total 32 repetitions



Compound 5e (¹³C-NMR spectral data)

PS1125-1

Pulse Sequence: s2pu1

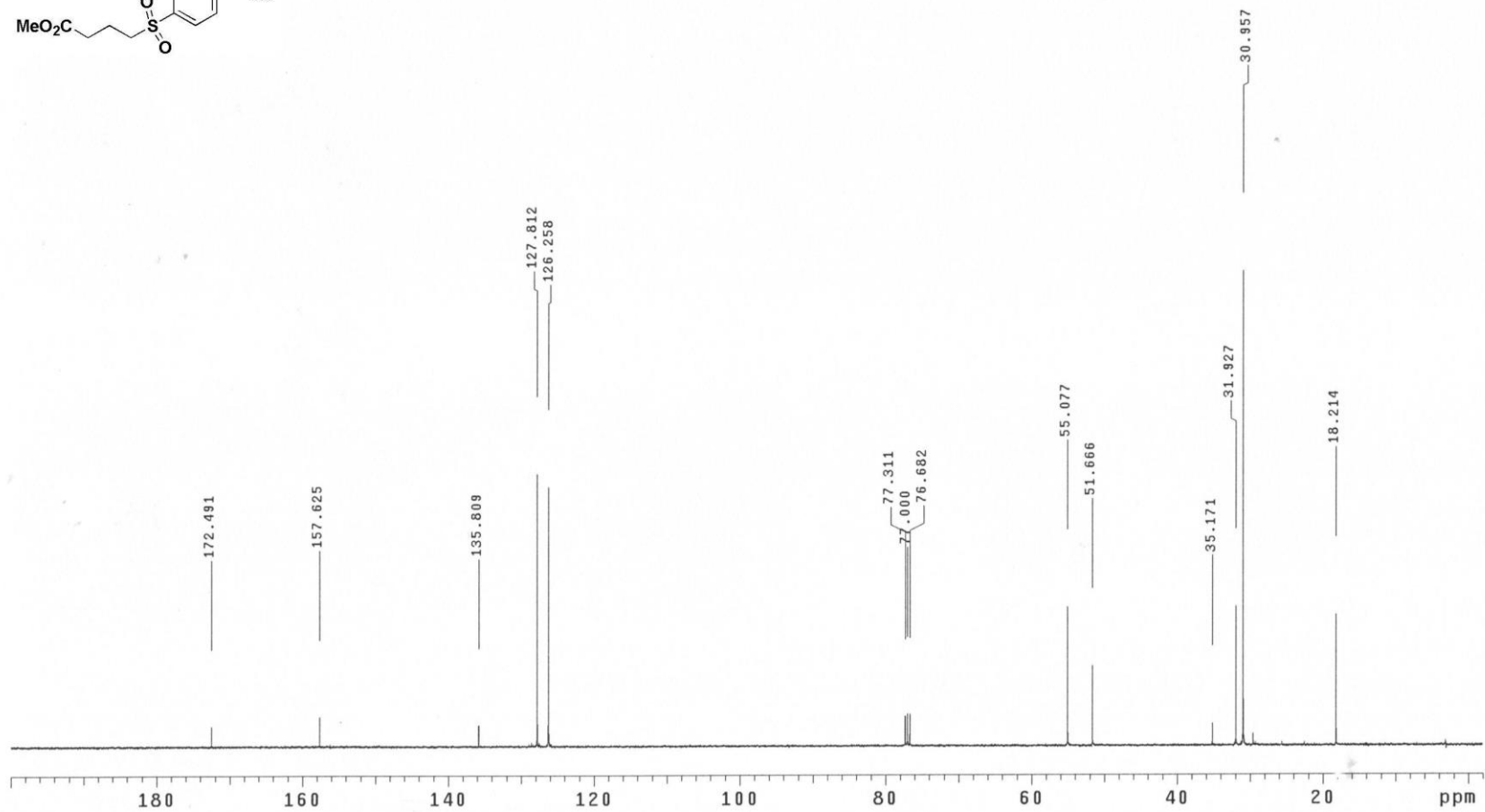
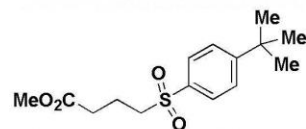
UNITYplus-400 "unity400"

Date: Nov 26 2020

Solvent: CDCl₃

Ambient temperature

Total 1408 repetitions



Compound 5f (¹H-NMR spectral data)

PS1126-1

Pulse Sequence: s2pu1

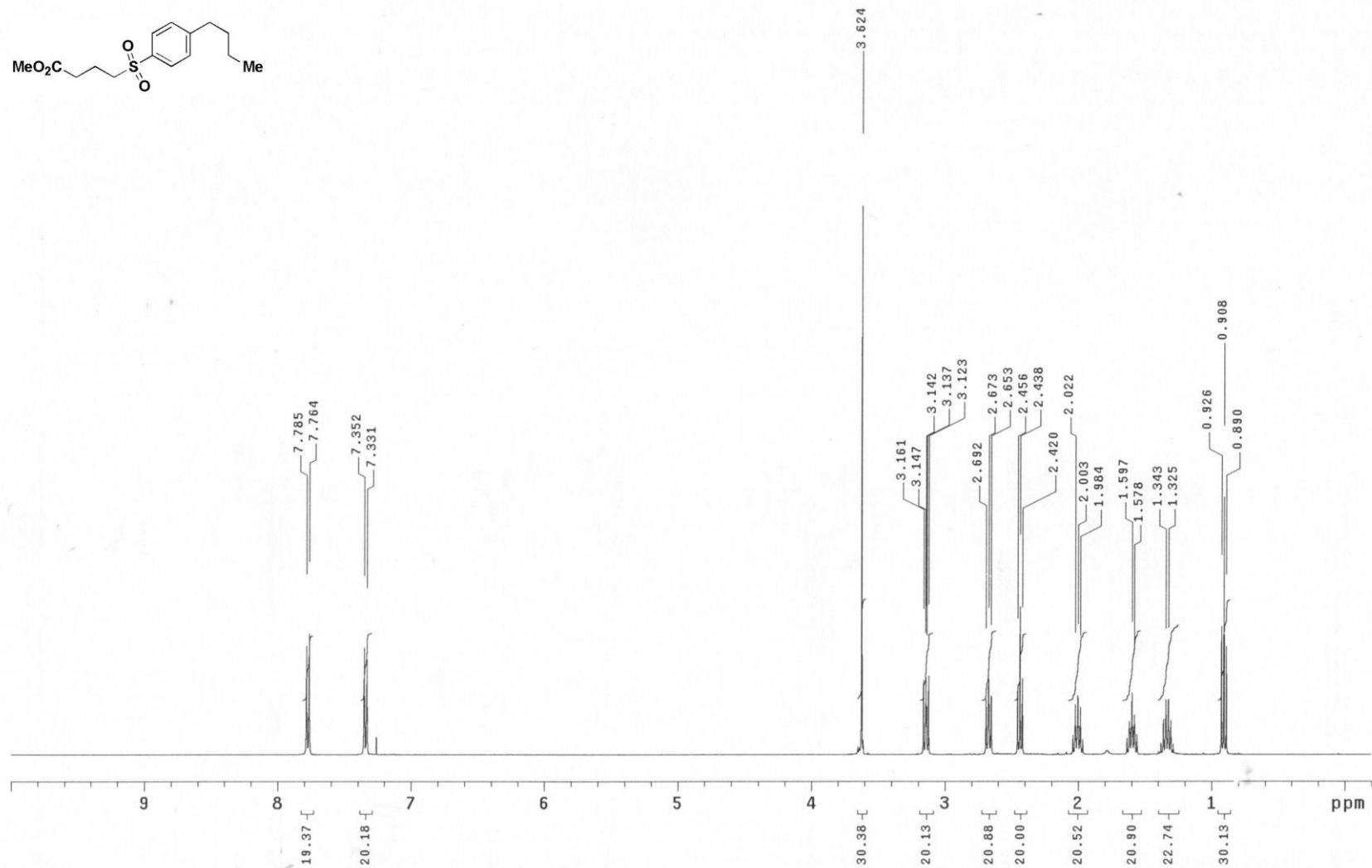
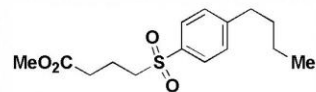
UNITYplus-400 "unity400"

Date: Nov 26 2020

Solvent: CDCl₃

Ambient temperature

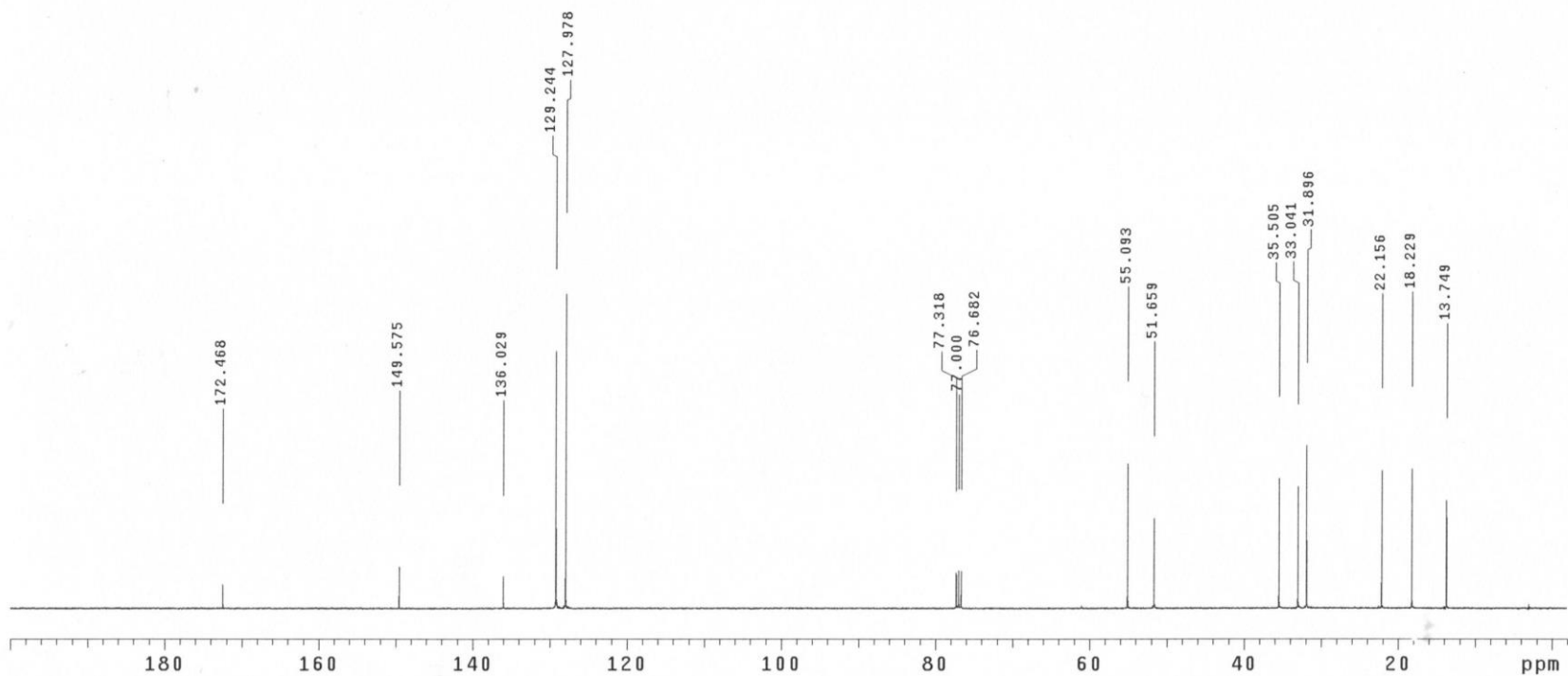
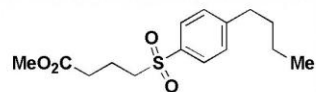
Total 32 repetitions



Compound 5f (¹³C-NMR spectral data)

PS1126-1

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Nov 26 2020
Solvent: CDC13
Ambient temperature
Total 64000 repetitions



Compound 5g (¹H-NMR spectral data)

PS1112-1

Pulse Sequence: s2pu1

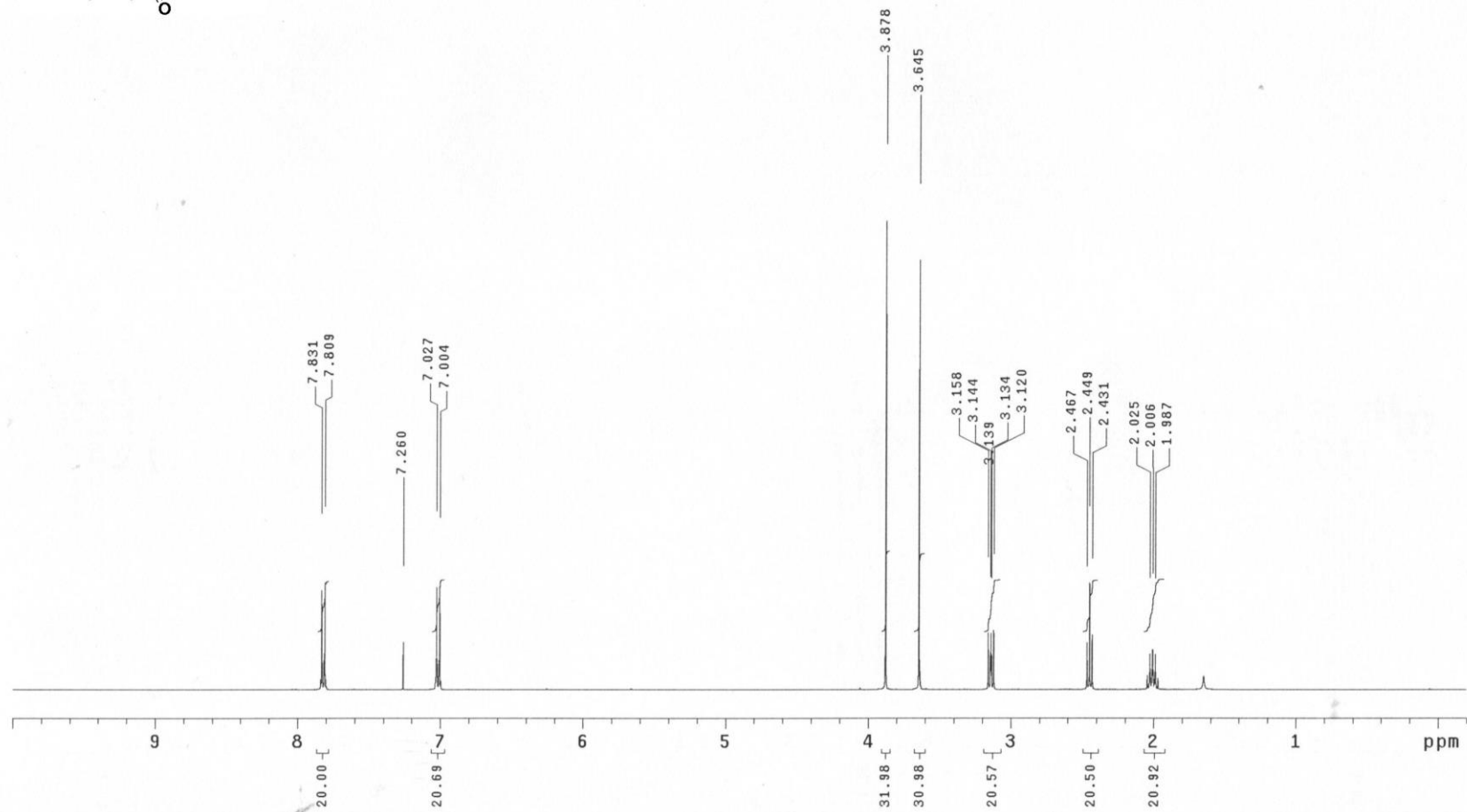
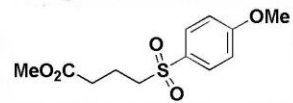
UNITYplus-400 "unity400"

Date: Nov 13 2020

Solvent: CDCl₃

Ambient temperature

Total 32 repetitions



Compound 5g (¹³C-NMR spectral data)

PS1112-1

Pulse Sequence: s2pu1

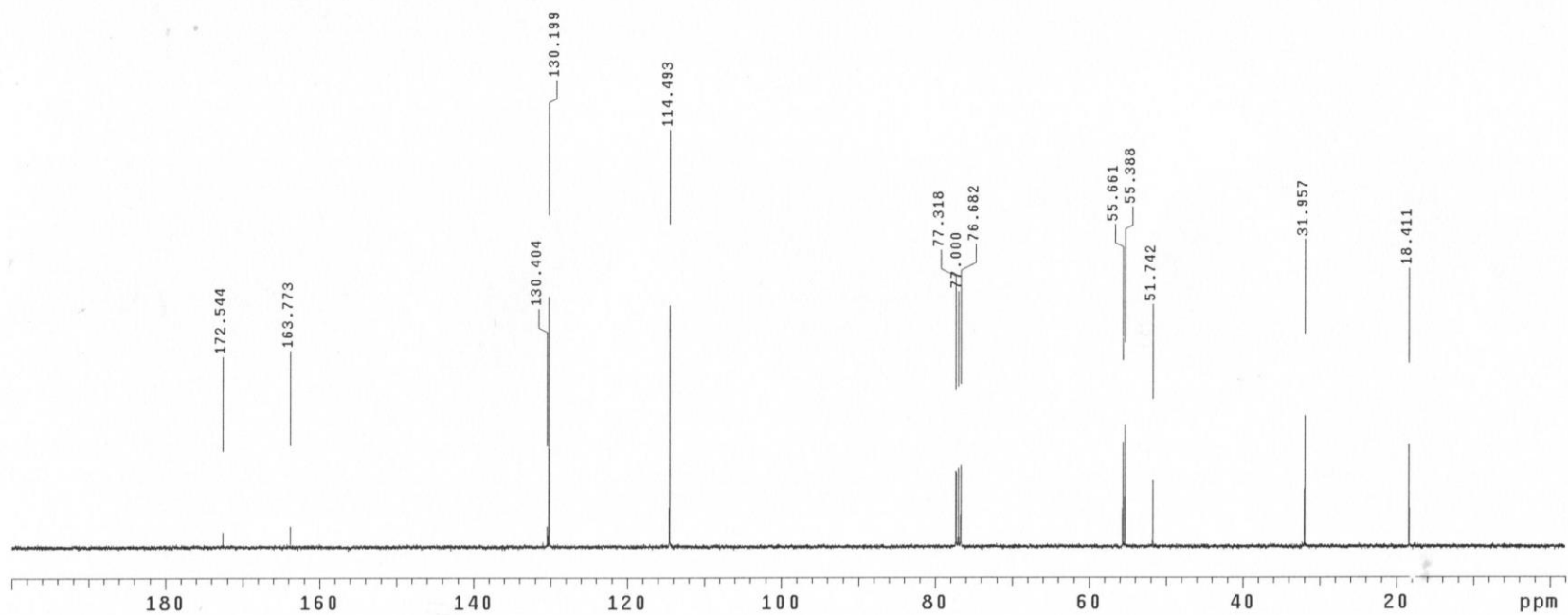
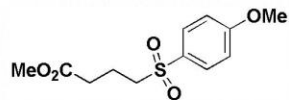
UNITYplus-400 "unity400"

Date: Nov 13 2020

Solvent: CDCl₃

Ambient temperature

Total 2128 repetitions



Compound 5h (¹H-NMR spectral data)

PS1117-1

Pulse Sequence: s2pu1

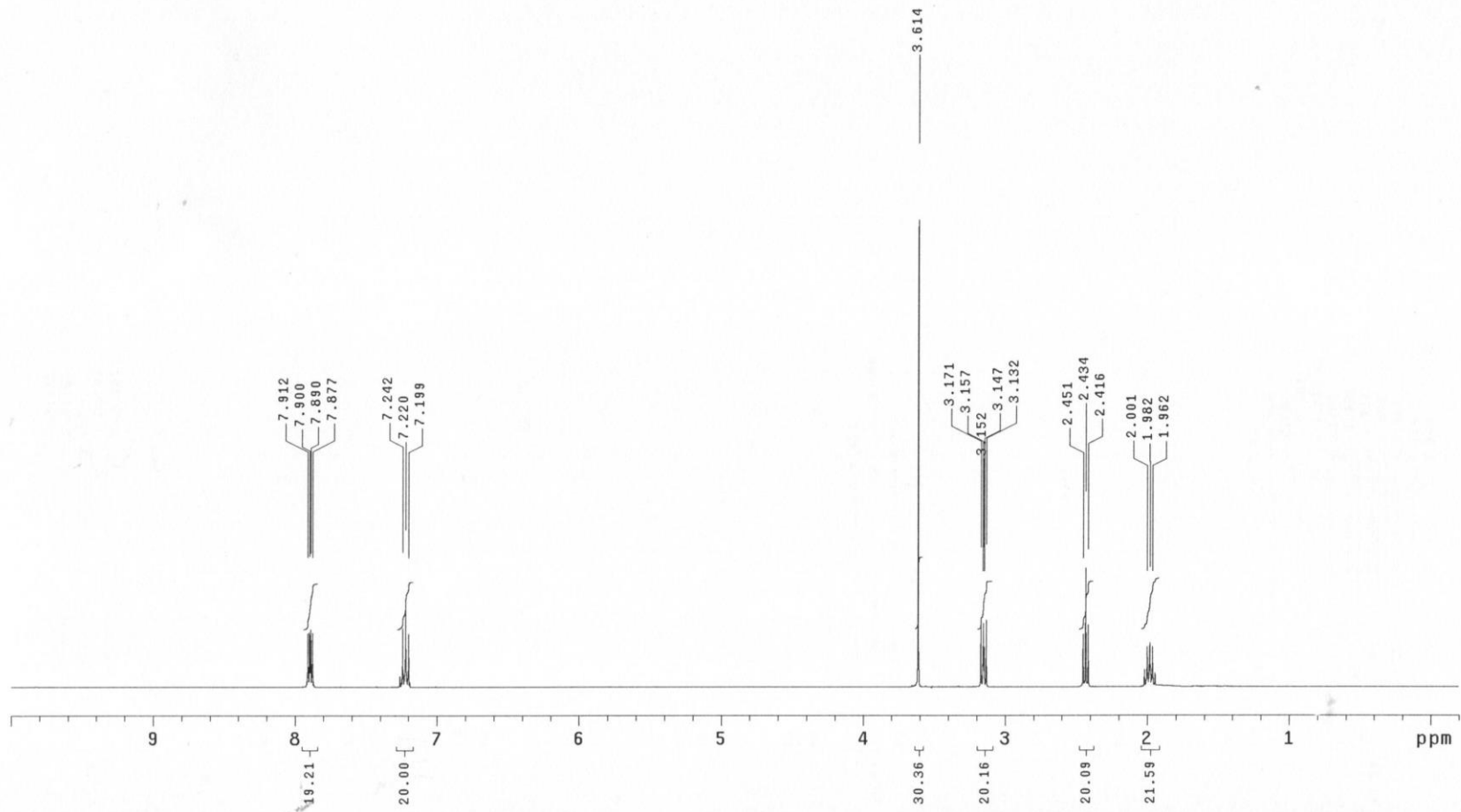
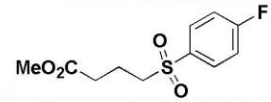
UNITYplus-400 "unity400"

Date: Nov 18 2020

Solvent: CDCl₃

Ambient temperature

Total 32 repetitions



Compound 5h (¹³C-NMR spectral data)

PS1117-1

Pulse Sequence: s2pu1

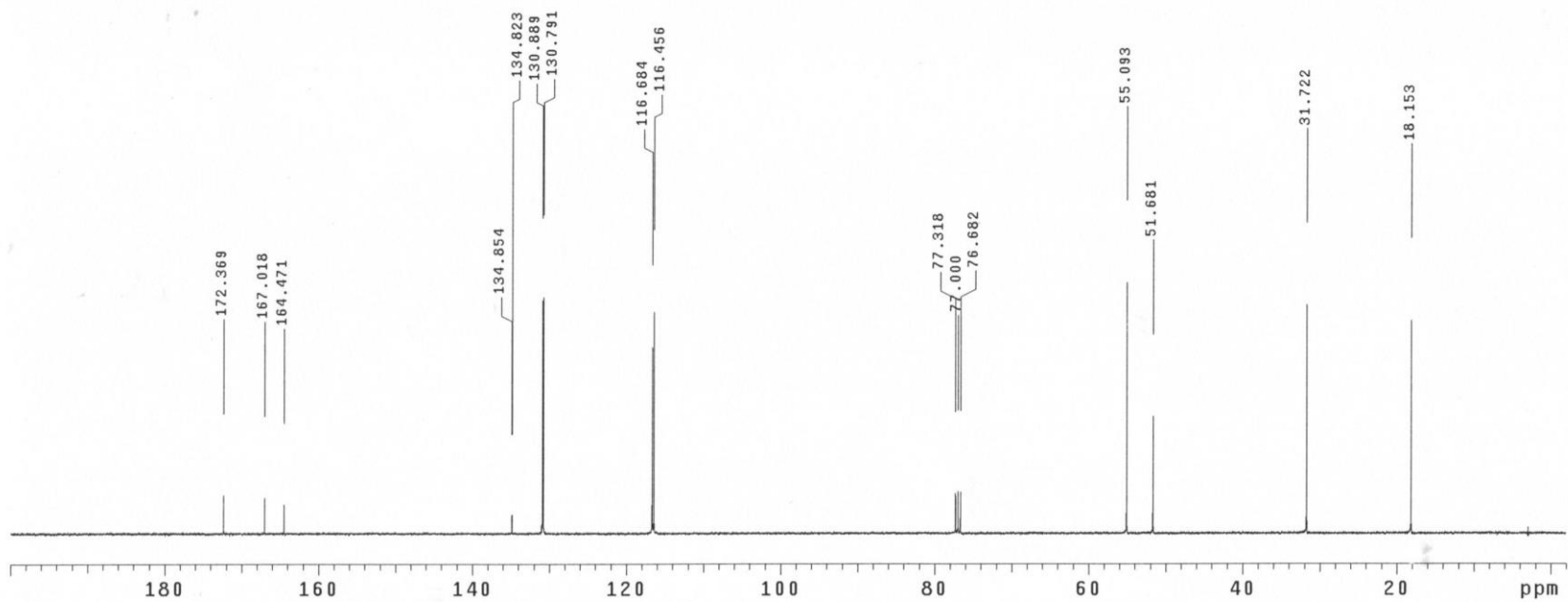
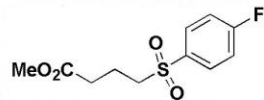
UNITYplus-400 "unity400"

Date: Nov 18 2020

Solvent: CDCl₃

Ambient temperature

Total 1616 repetitions



Compound 5i (¹H-NMR spectral data)

PS1201-1

Pulse Sequence: s2pu1

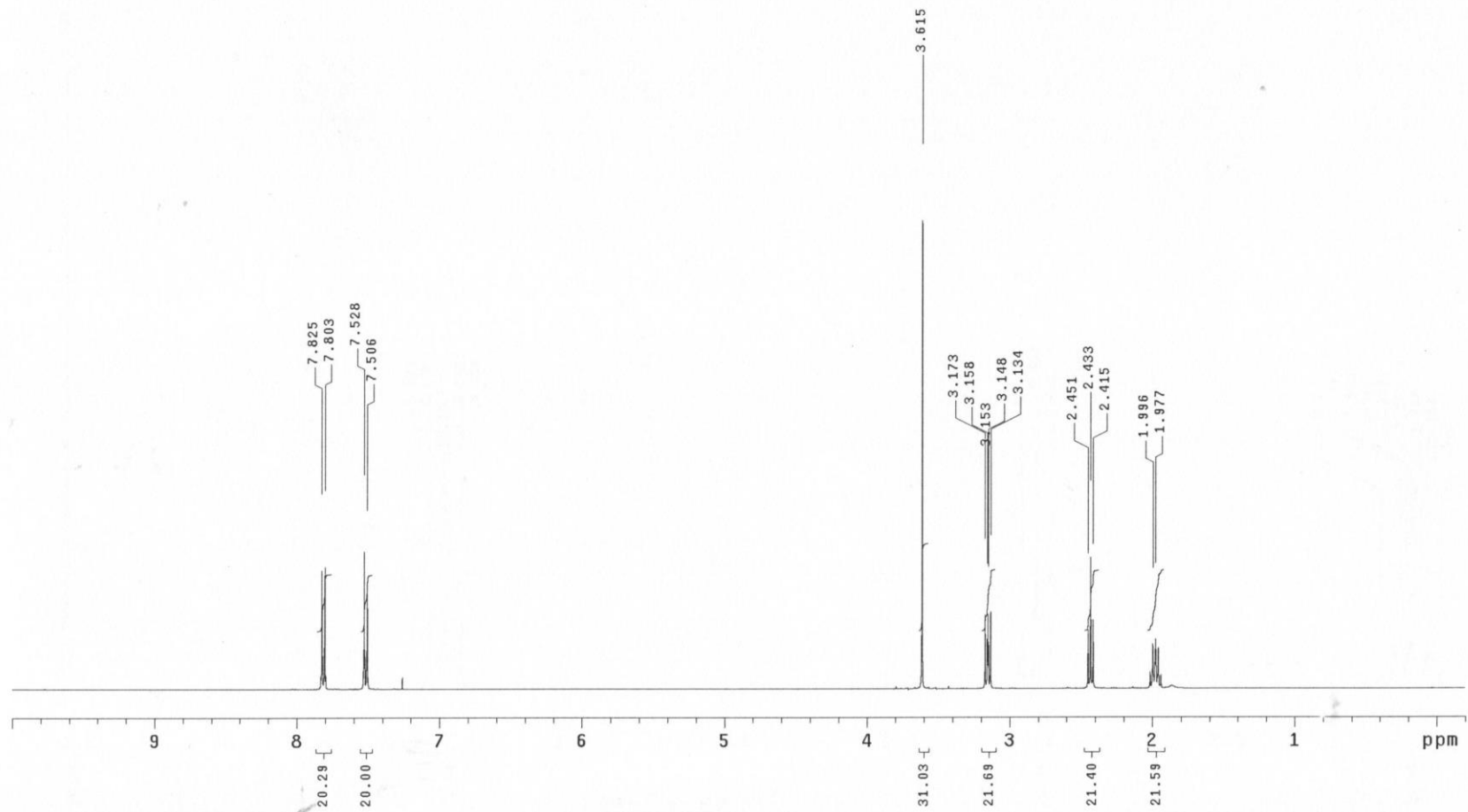
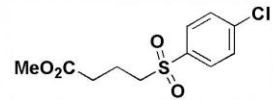
UNITYplus-400 "unity400"

Date: Dec 2 2020

Solvent: CDCl₃

Ambient temperature

Total 32 repetitions



Compound 5i (¹³C-NMR spectral data)

PS1201-1

Pulse Sequence: s2pu1

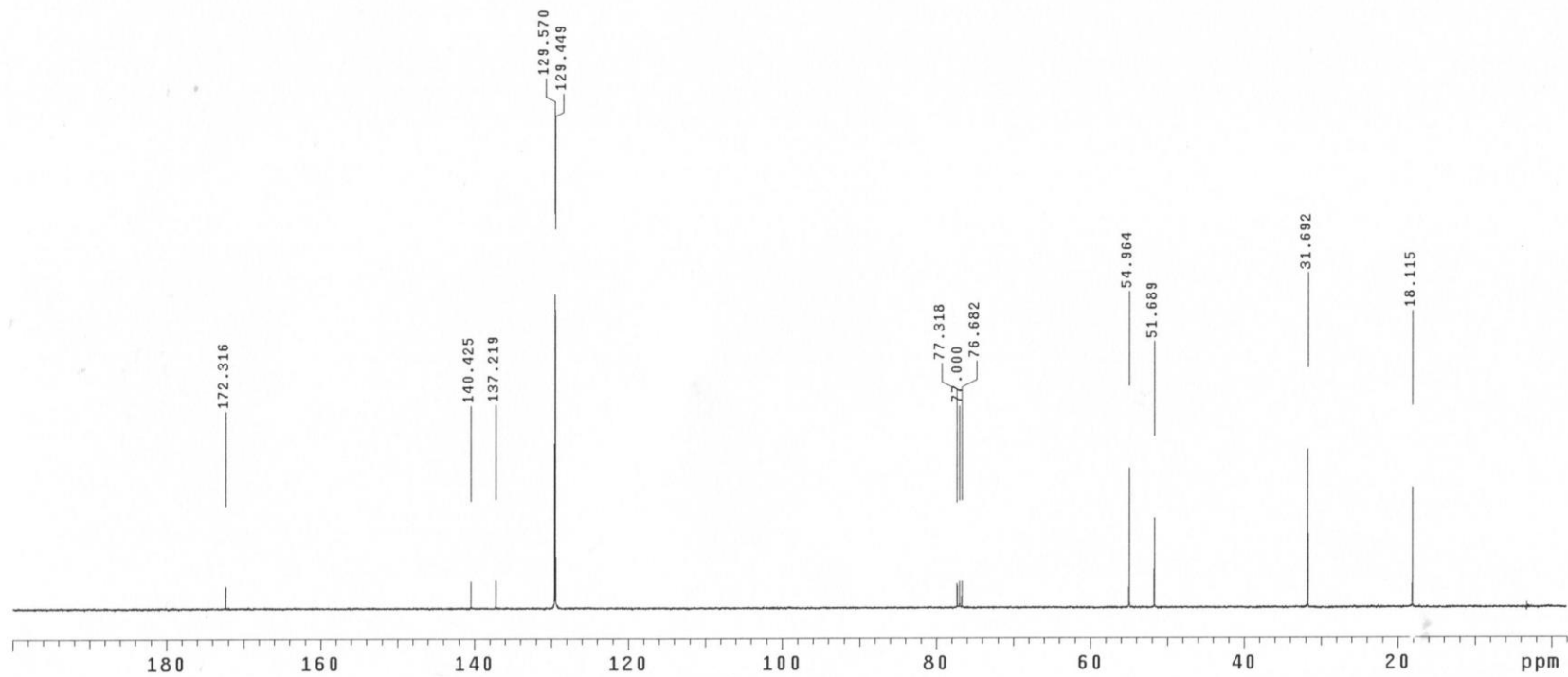
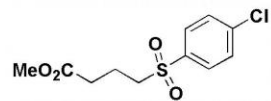
UNITYplus-400 "unity400"

Date: Dec 2 2020

Solvent: CDCl₃

Ambient temperature

Total 640 repetitions



Compound 5j (¹H-NMR spectral data)

PS1202-1

Pulse Sequence: s2pu1

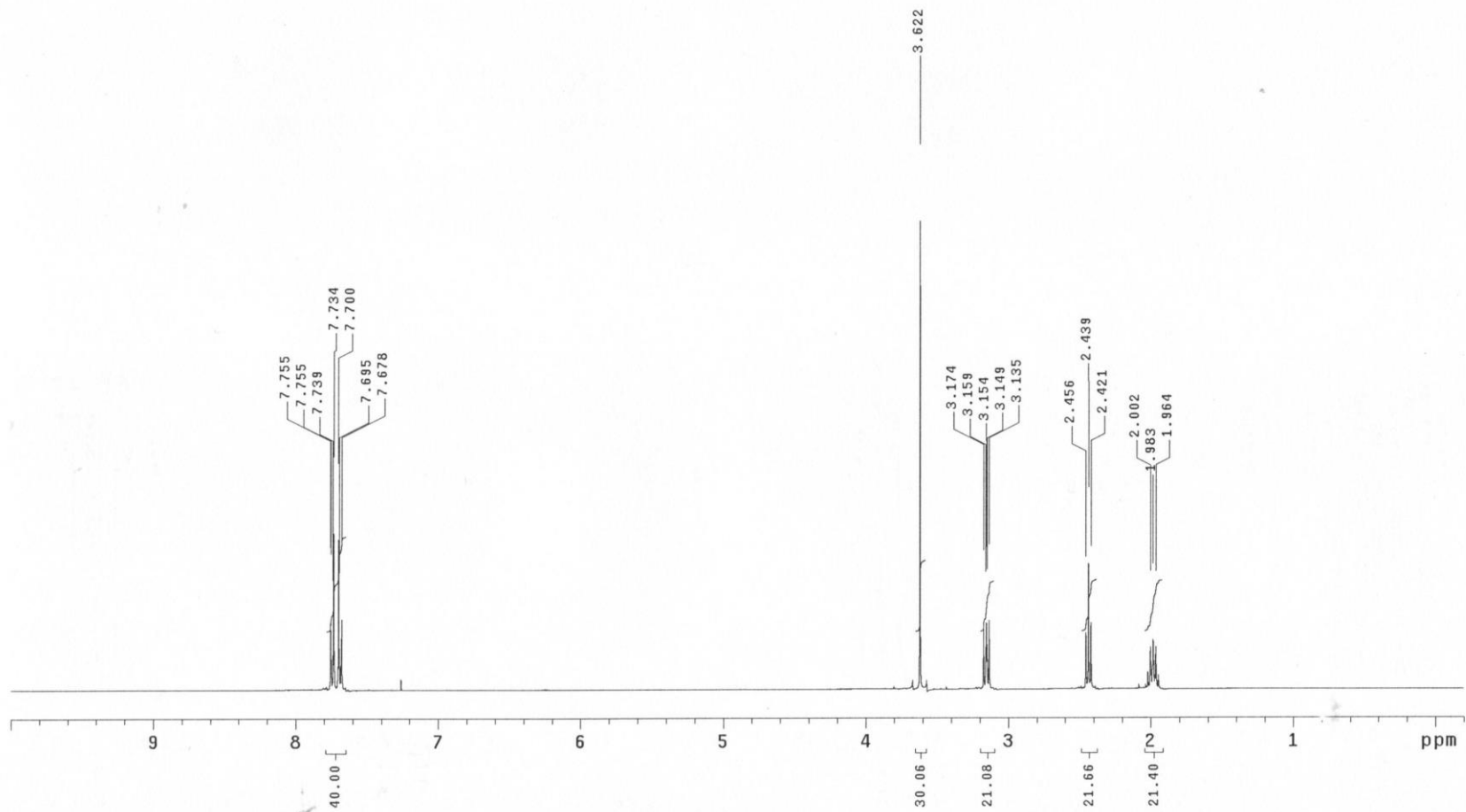
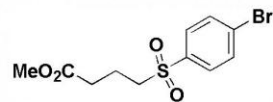
UNITYplus-400 "unity400"

Date: Dec 3 2020

Solvent: CDCl₃

Ambient temperature

Total 32 repetitions



Compound 5j (¹³C-NMR spectral data)

PS1202-1

Pulse Sequence: s2pu1

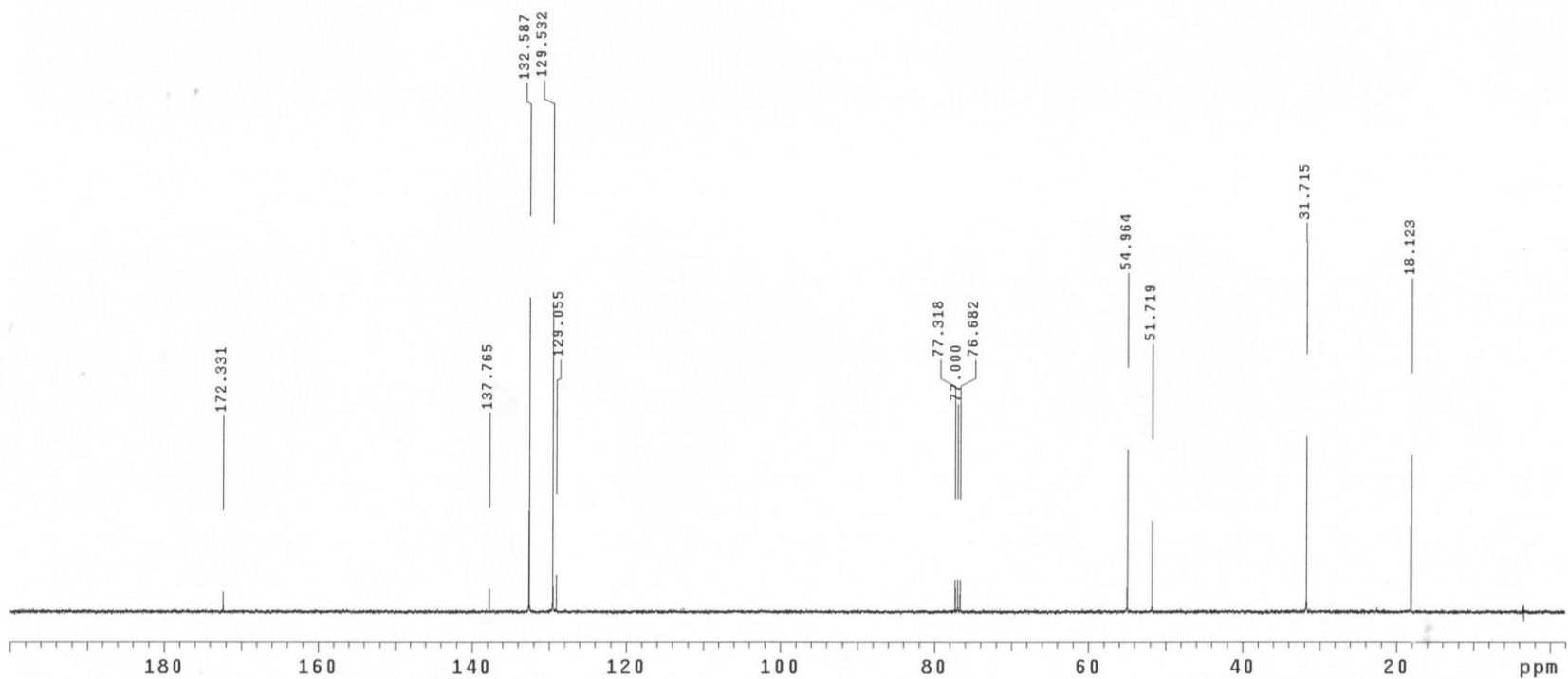
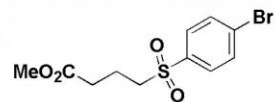
UNITYplus-400 "unity400"

Date: Dec 3 2020

Solvent: CDCl₃

Ambient temperature

Total 352 repetitions



Compound 5k (¹H-NMR spectral data)

PS1217-1

Pulse Sequence: s2pul

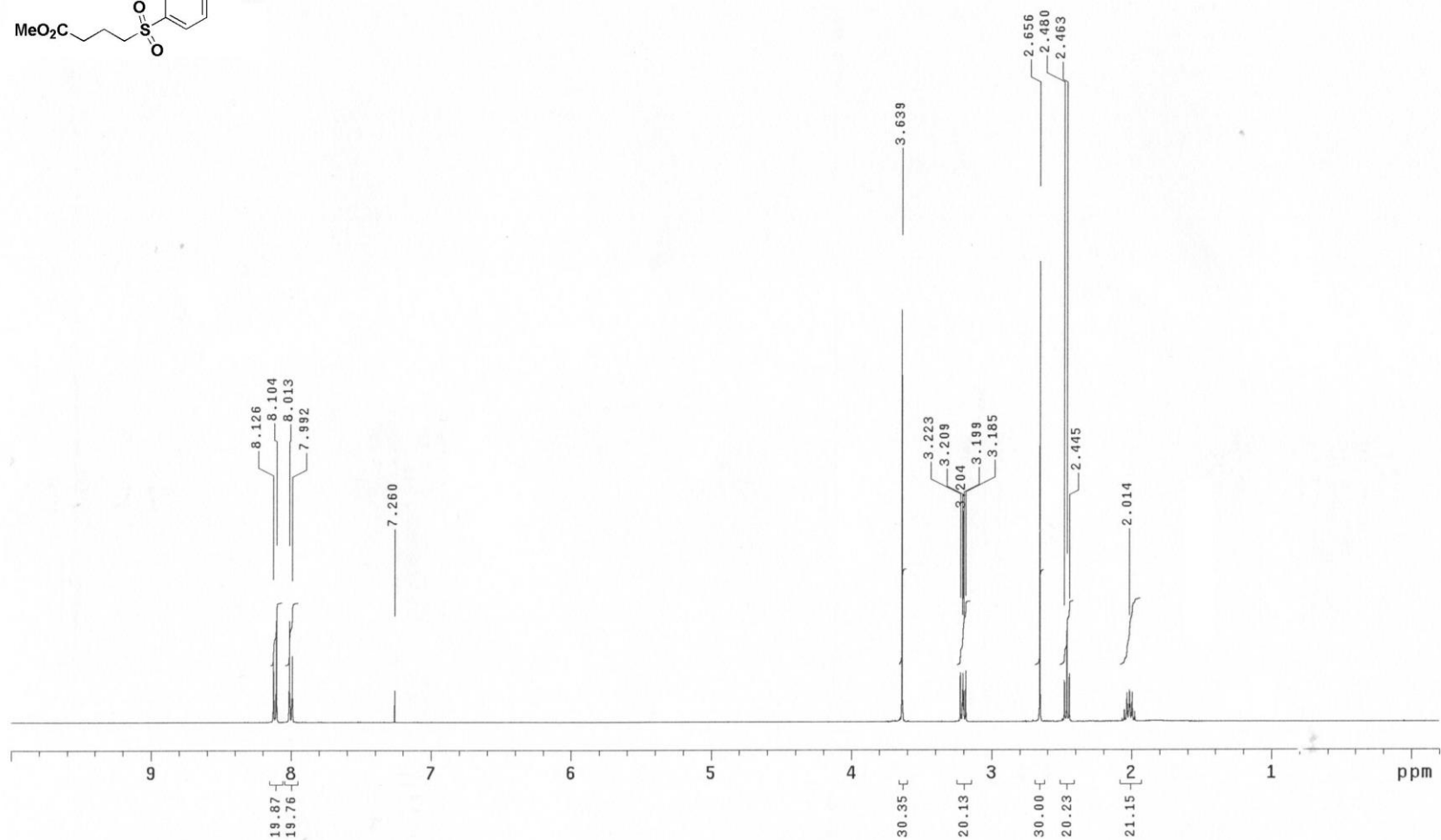
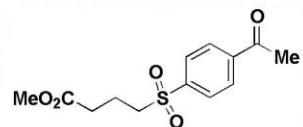
UNITYplus-400 "unity400"

Date: Dec 17 2020

Solvent: CDCl₃

Ambient temperature

Total 32 repetitions



Compound 5k (¹³C-NMR spectral data)

PS1217-1

Pulse Sequence: s2pu1

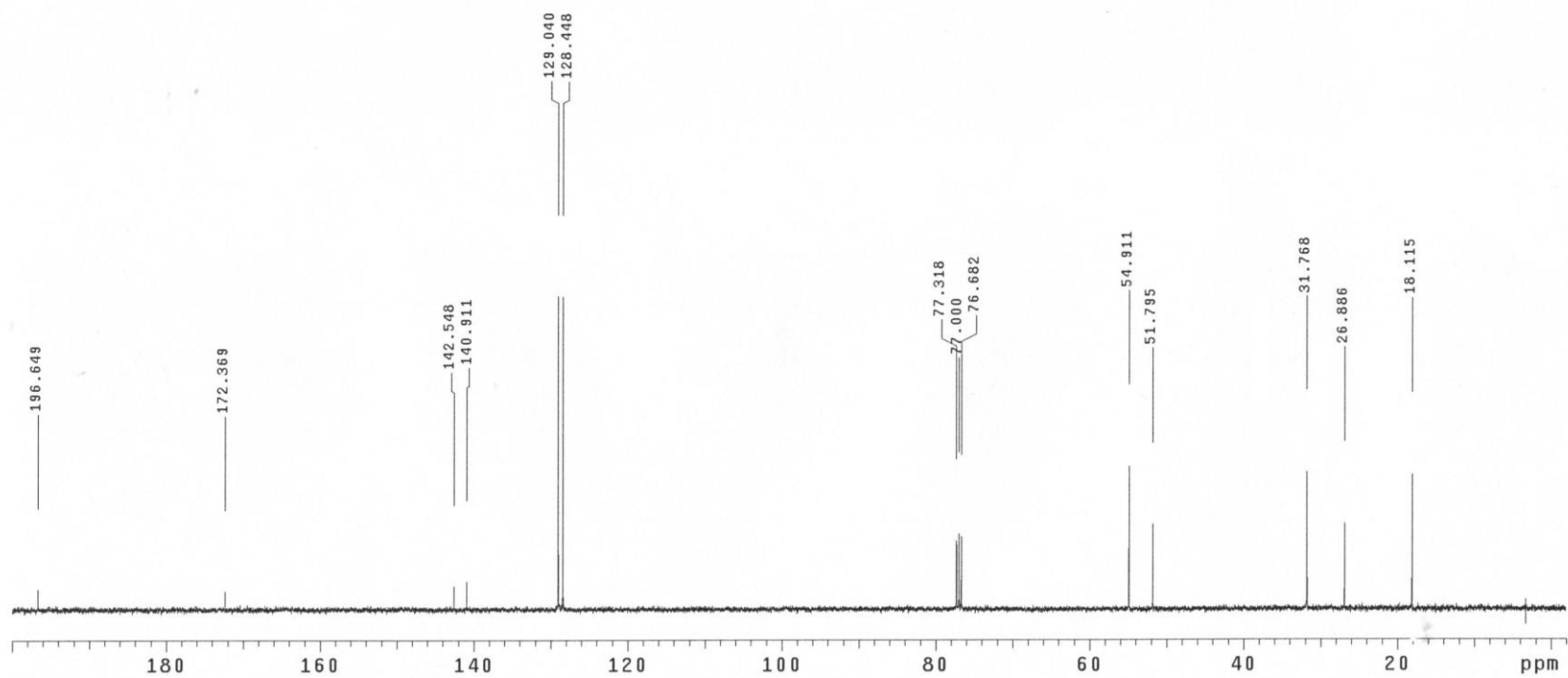
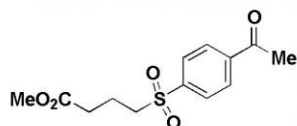
UNITYplus-400 "unity400"

Date: Dec 17 2020

Solvent: CDCl₃

Ambient temperature

Total 768 repetitions



Compound 5I (¹H-NMR spectral data)

PS1203-1

Pulse Sequence: s2pu1

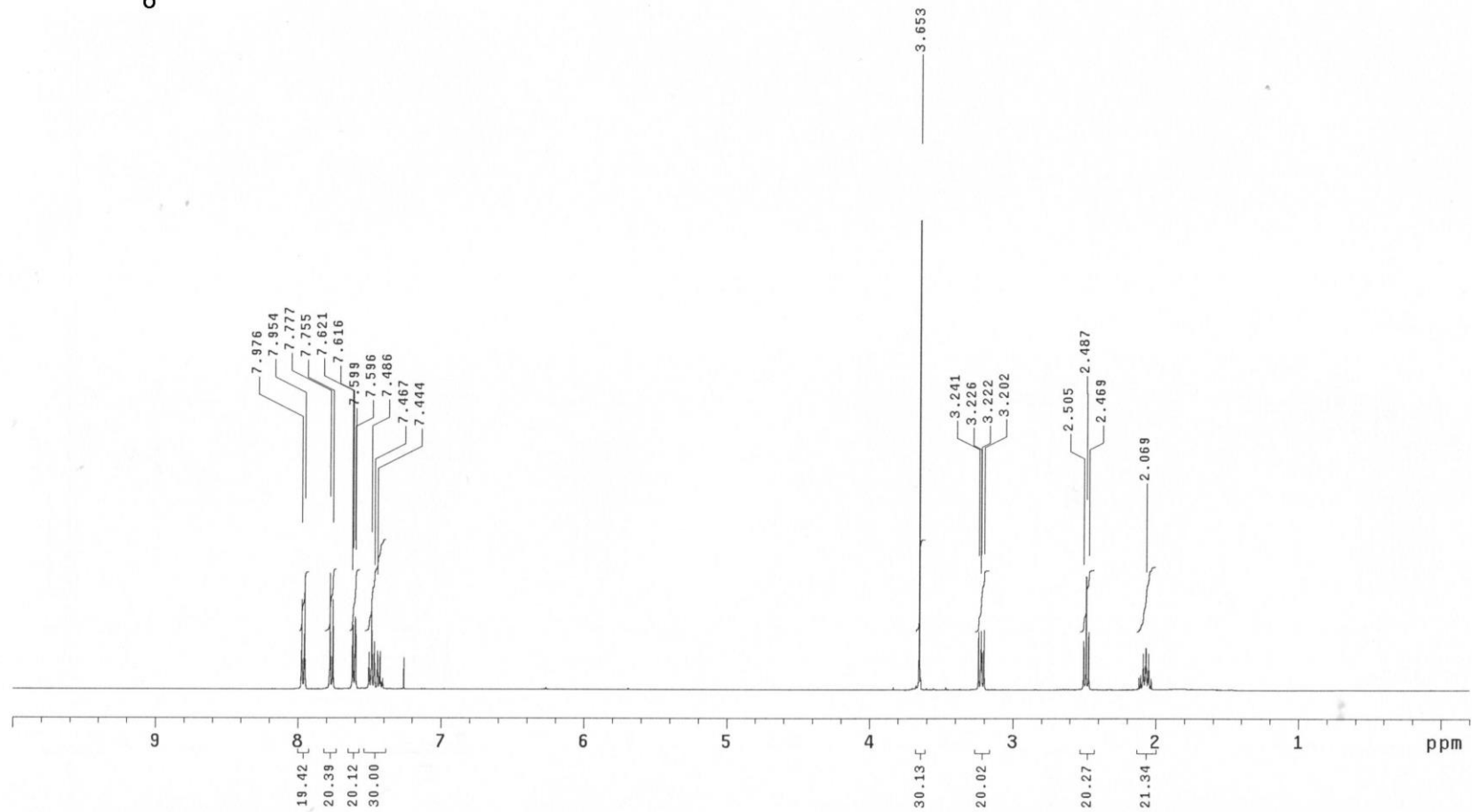
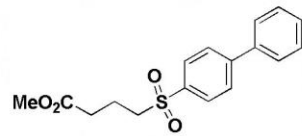
UNITYplus-400 "unity400"

Date: Dec 4 2020

Solvent: CDCl₃

Ambient temperature

Total 64 repetitions



Compound 5I (¹³C-NMR spectral data)

PS1203-1

Pulse Sequence: s2pu1

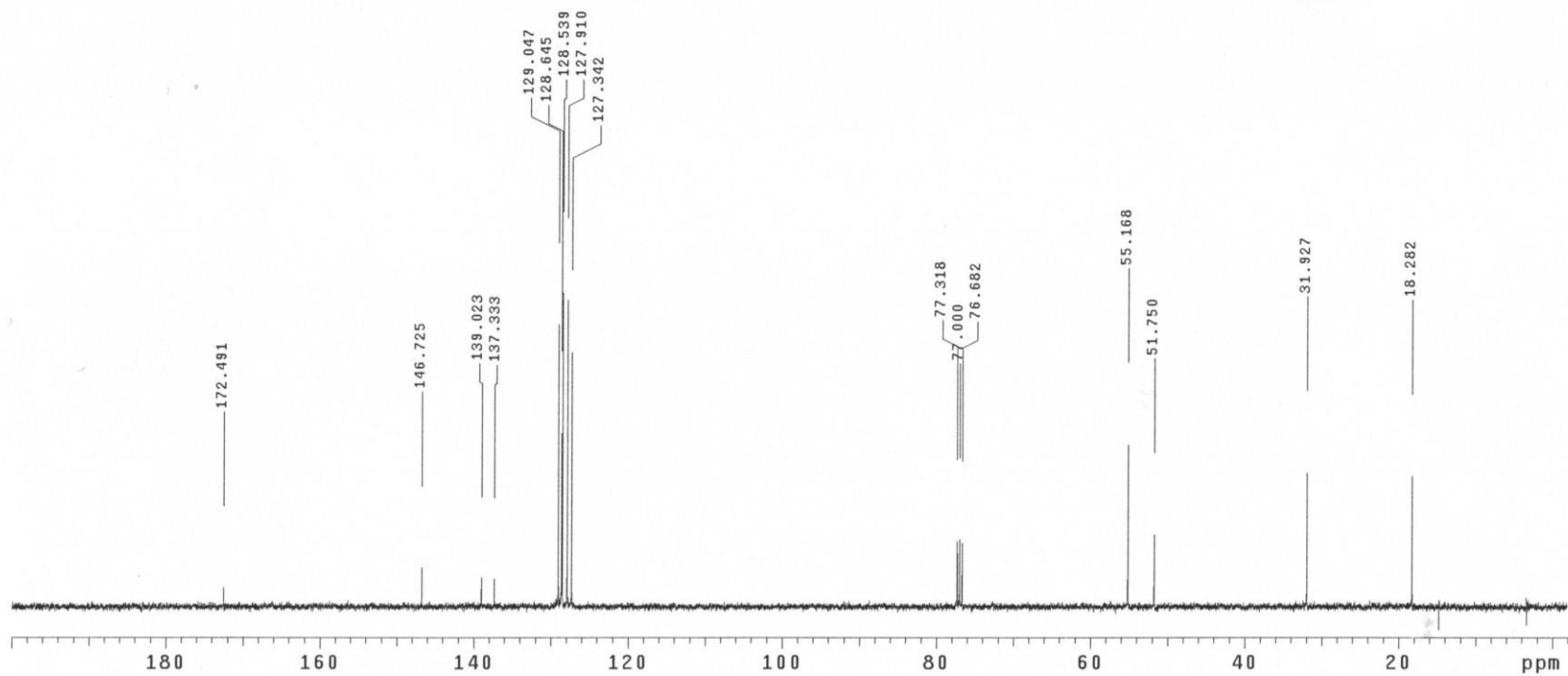
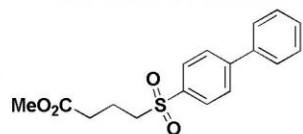
UNITYplus-400 "unity400"

Date: Dec 4 2020

Solvent: CDC13

Ambient temperature

Total 416 repetitions



Compound 5m (¹H-NMR spectral data)

PS1208-1

Pulse Sequence: s2pu1

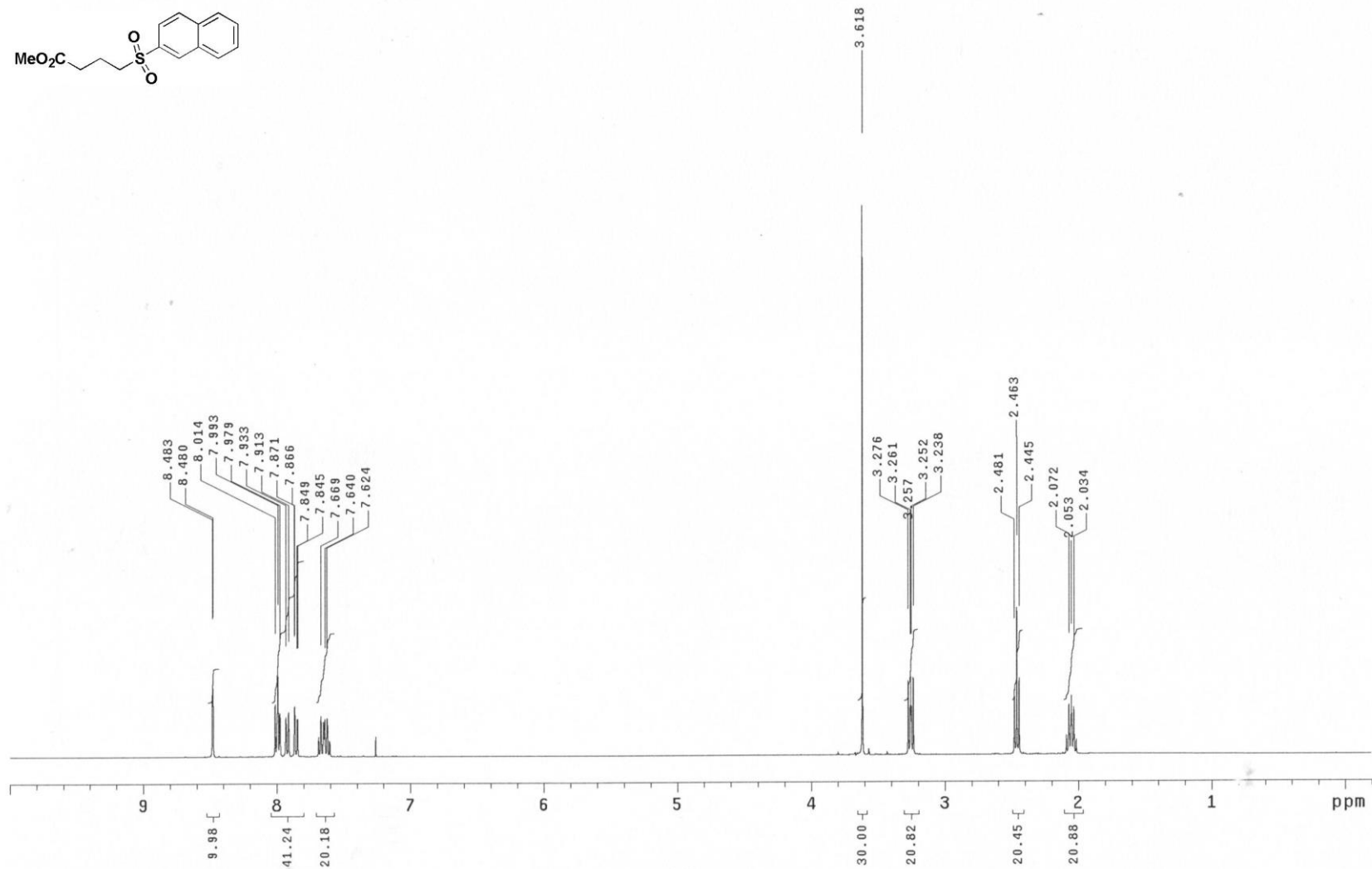
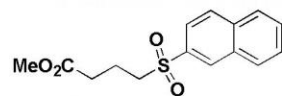
UNITYplus-400 "unity400"

Date: Dec 9 2020

Solvent: CDCl₃

Ambient temperature

Total 32 repetitions



Compound 5m (¹³C-NMR spectral data)

PS1208-1

Pulse Sequence: s2pu1

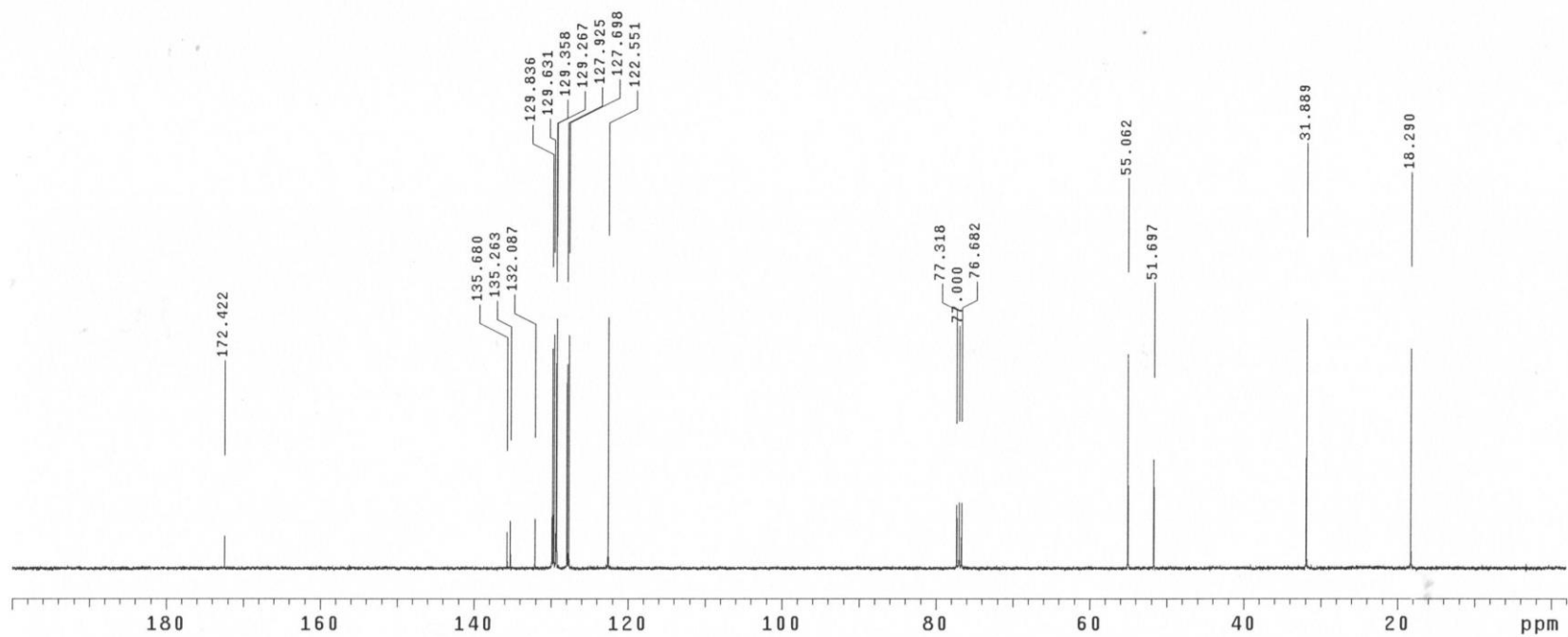
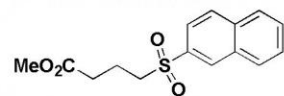
UNITYplus-400 "unity400"

Date: Dec 9 2020

Solvent: CDCl₃

Ambient temperature

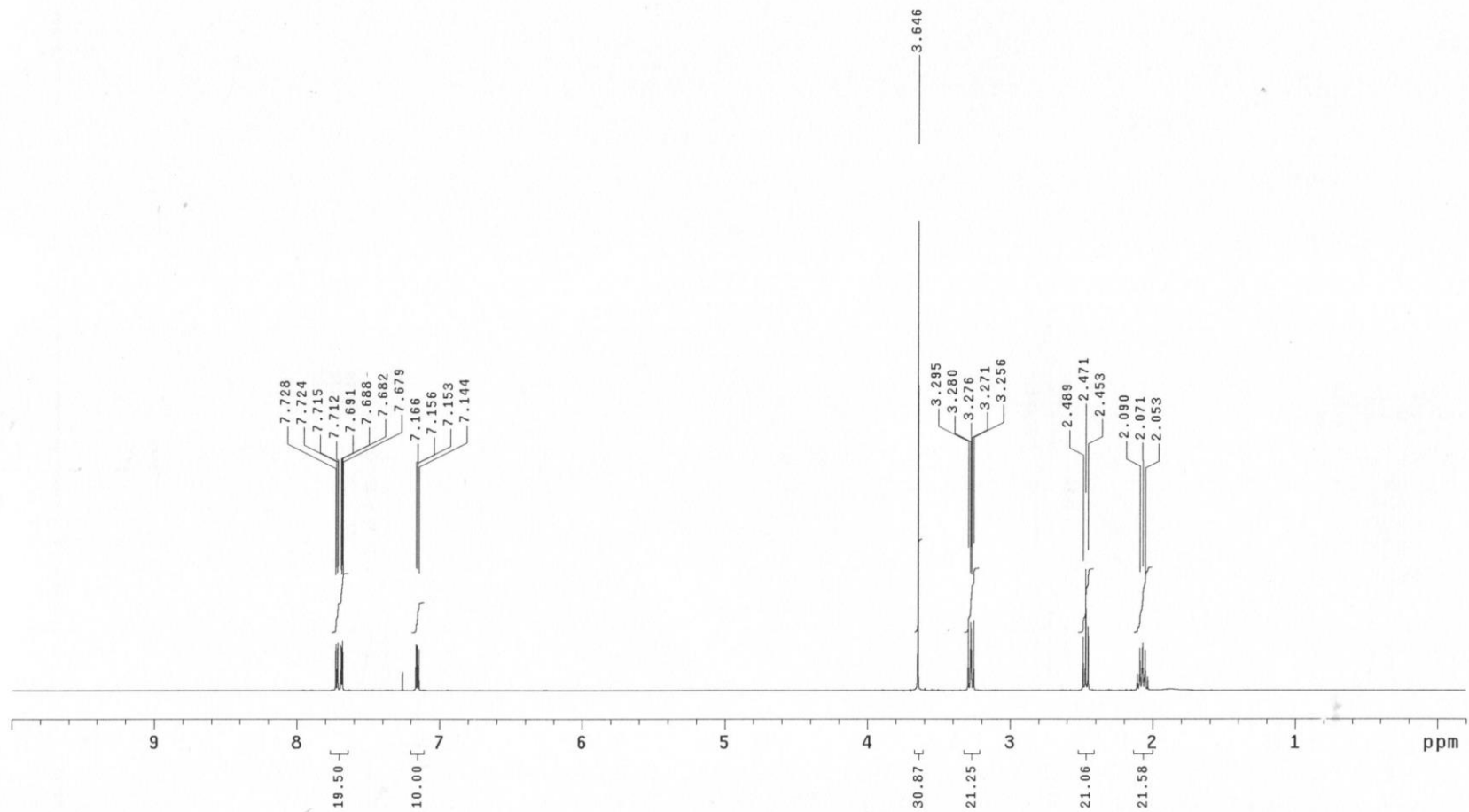
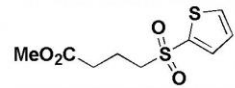
Total 2000 repetitions



Compound 5n (¹H-NMR spectral data)

PS1210-1

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Dec 11 2020
Solvent: CDCl₃
Ambient temperature
Total 24 repetitions



Compound 5n (¹³C-NMR spectral data)

PS1210-1

Pulse Sequence: s2pu1

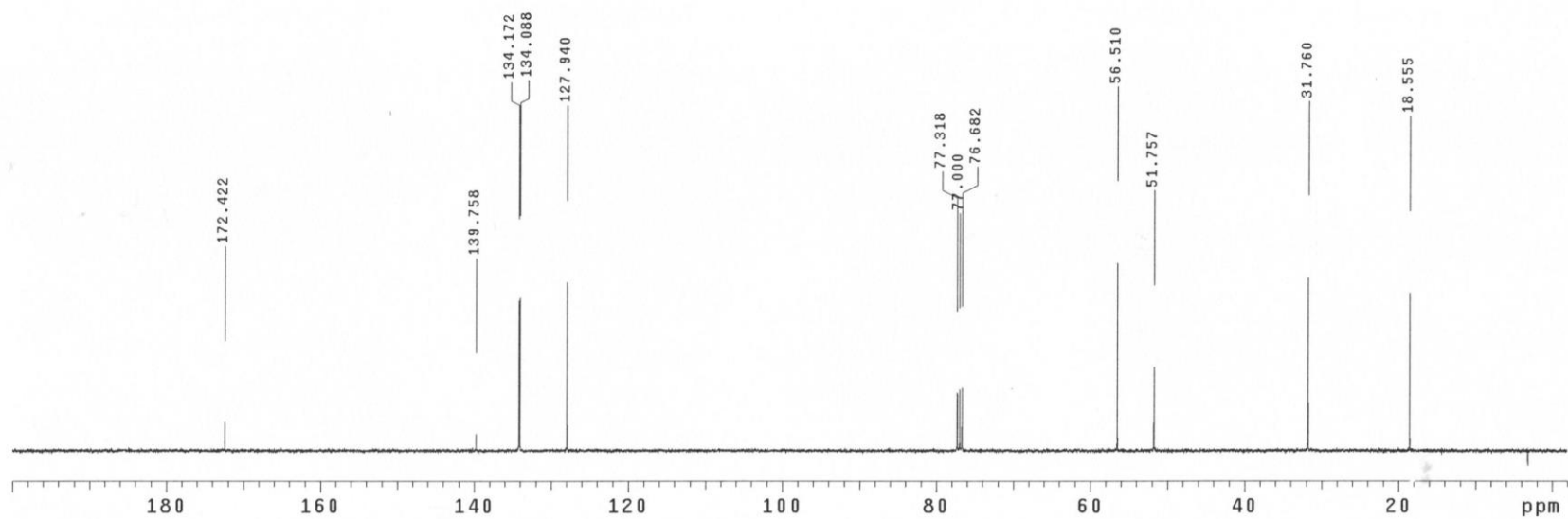
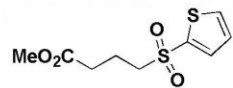
UNITYplus-400 "unity400"

Date: Dec 11 2020

Solvent: CDCl₃

Ambient temperature

Total 1296 repetitions



Compound 5o (¹H-NMR spectral data)

PS1209-1

Pulse Sequence: s2pu1

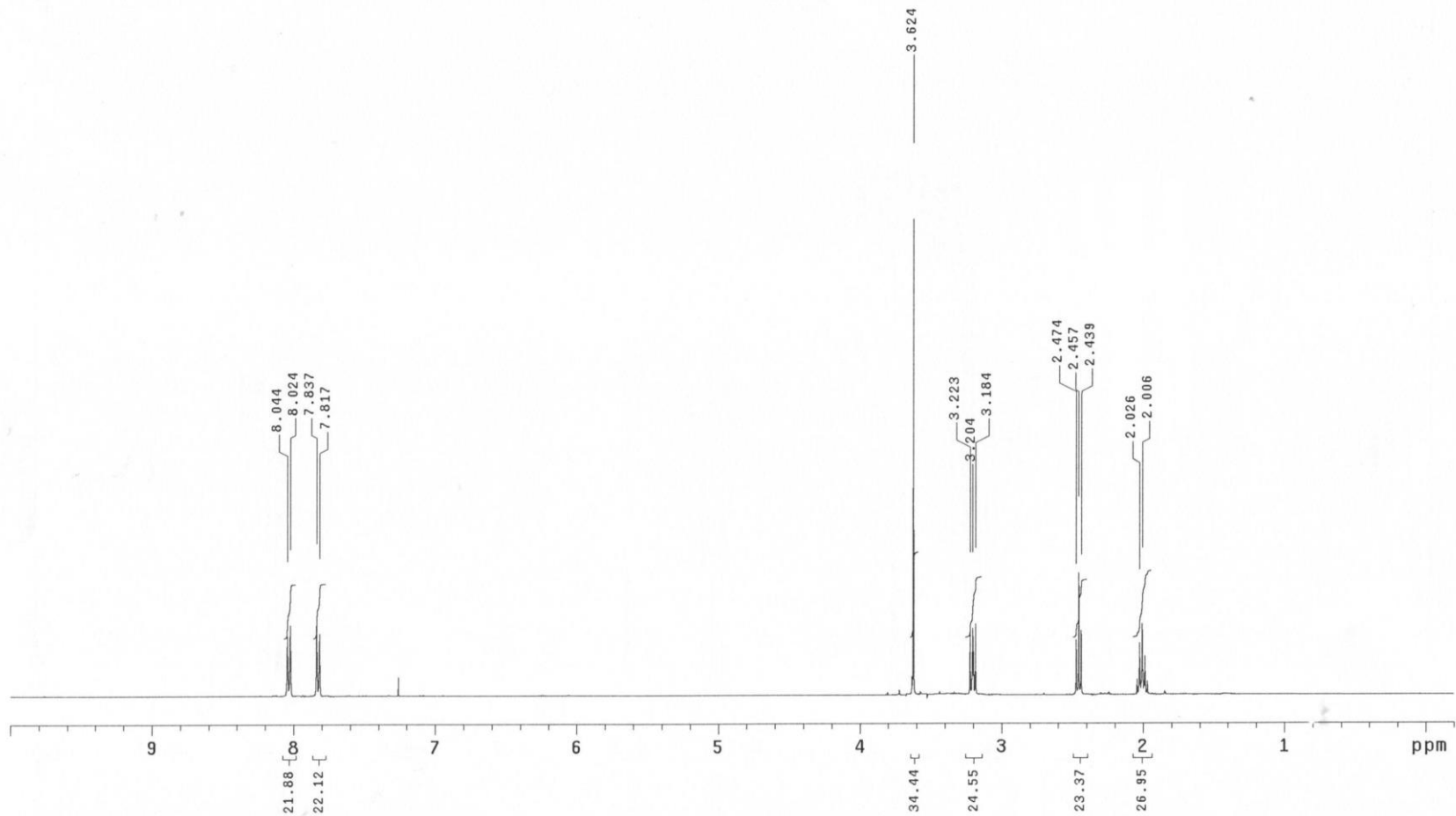
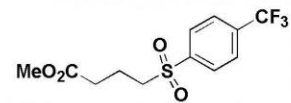
UNITYplus-400 "unity400"

Date: Dec 10 2020

Solvent: CDCl₃

Ambient temperature

Total 32 repetitions



Compound 5o (¹³C-NMR spectral data)

PS1209-1

Pulse Sequence: s2pu1

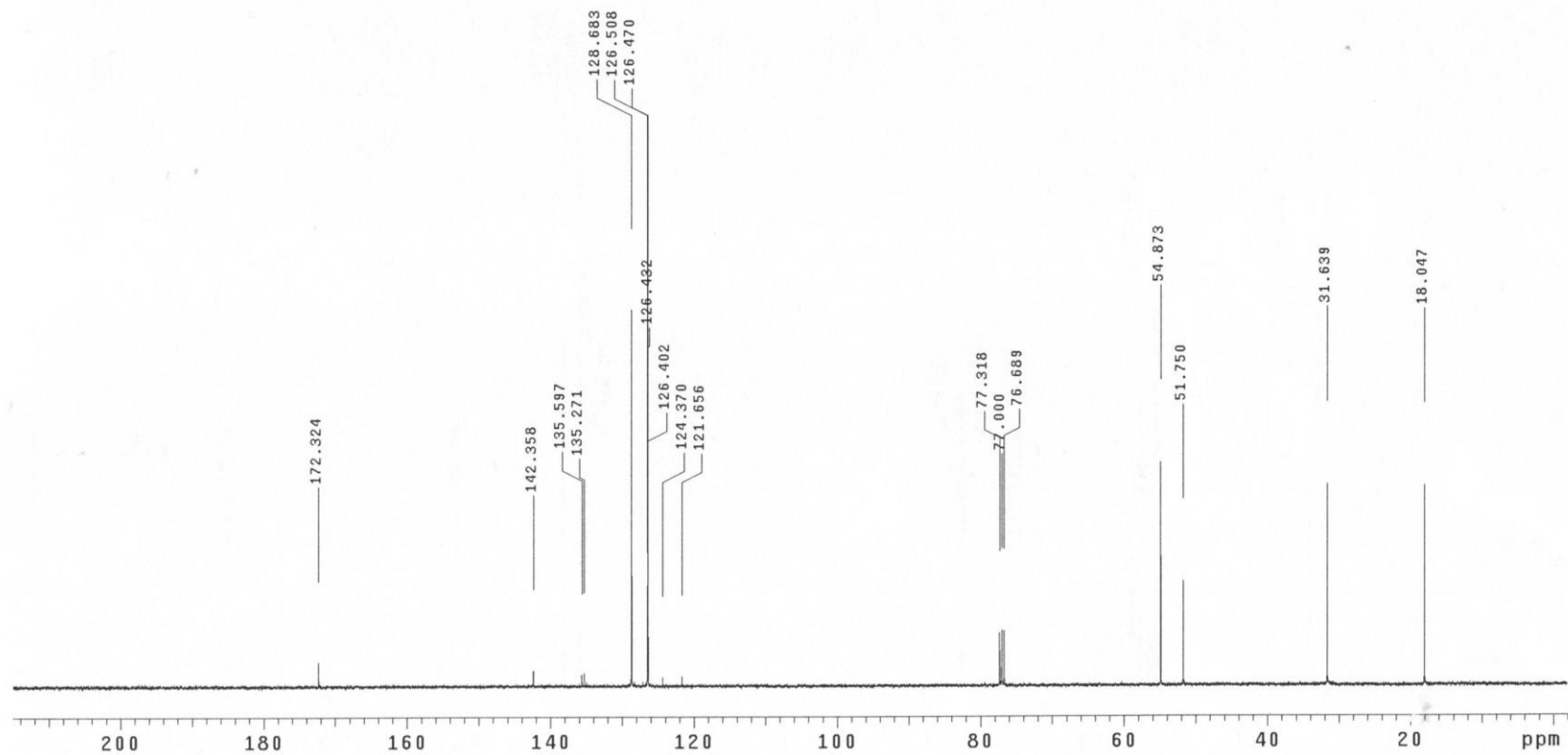
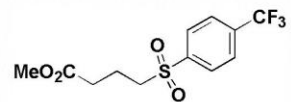
UNITYplus-400 "unity400"

Date: Dec 10 2020

Solvent: CDCl₃

Ambient temperature

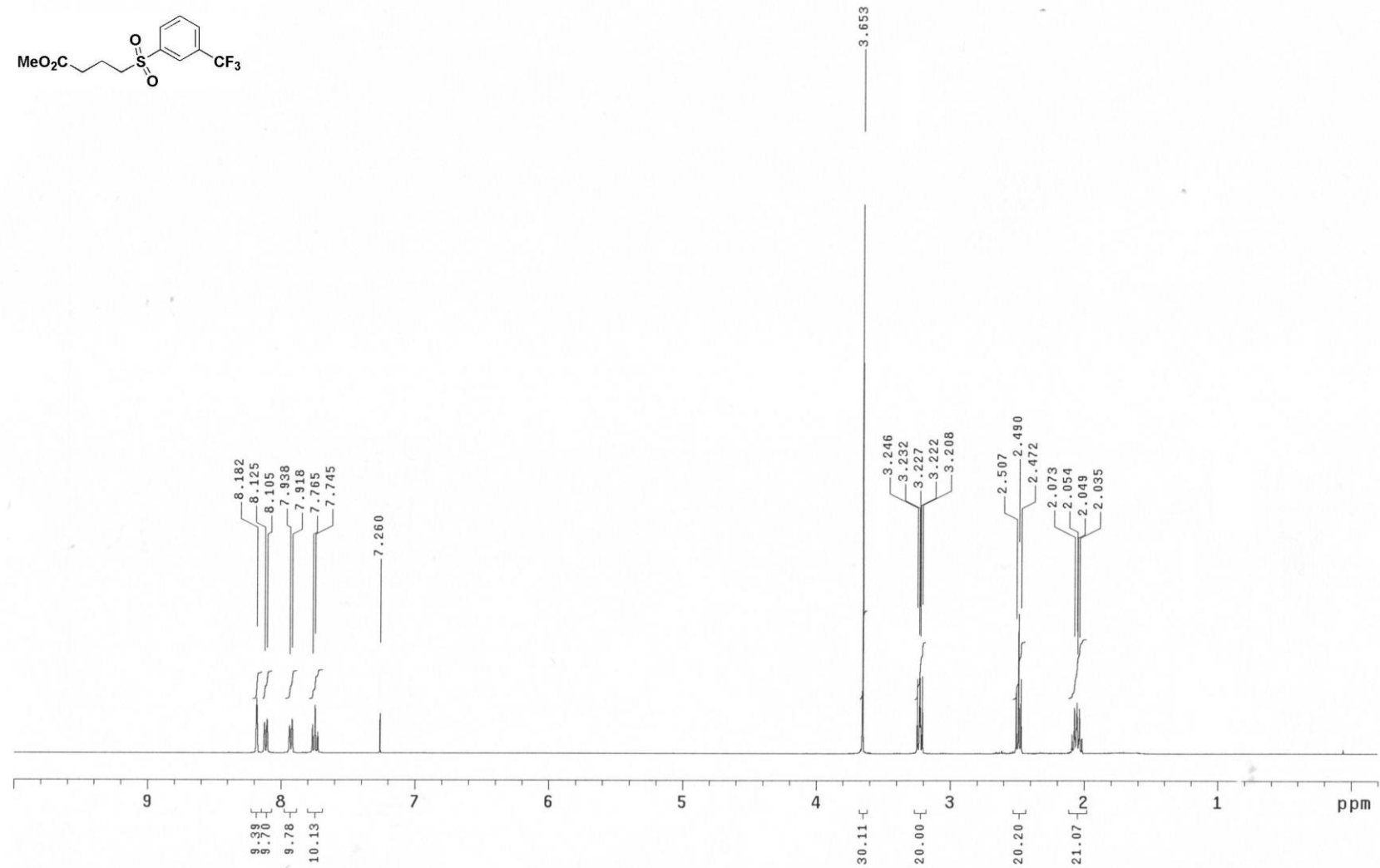
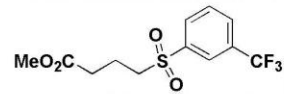
Total 1424 repetitions



Compound 5p (¹H-NMR spectral data)

PS1215-1

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Dec 16 2020
Solvent: CDCl3
Ambient temperature
Total 32 repetitions



Compound 5p (¹³C-NMR spectral data)

PS1215-1

Pulse Sequence: s2pu1

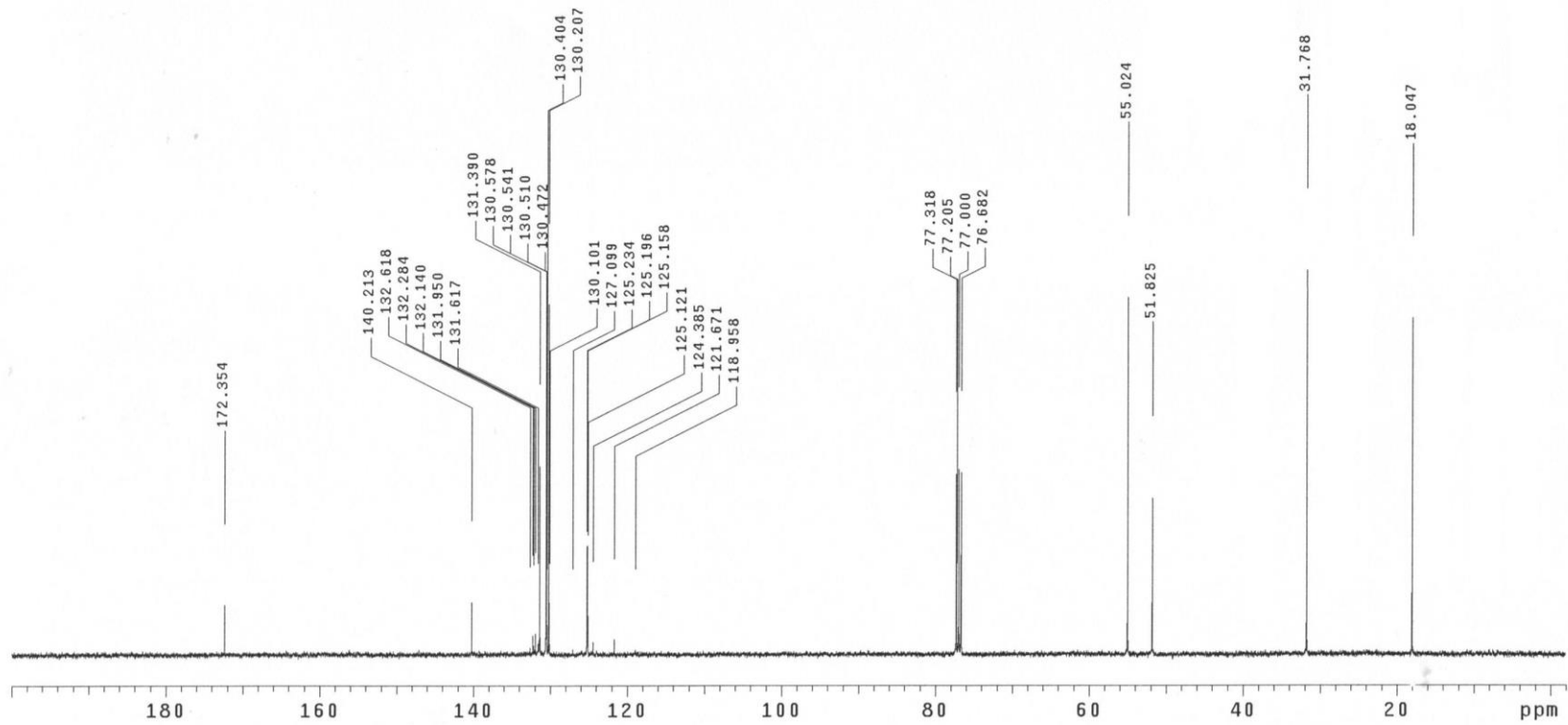
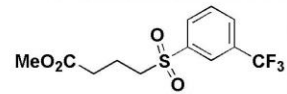
UNITYplus-400 "unity400"

Date: Dec 16 2020

Solvent: CDC13

Ambient temperature

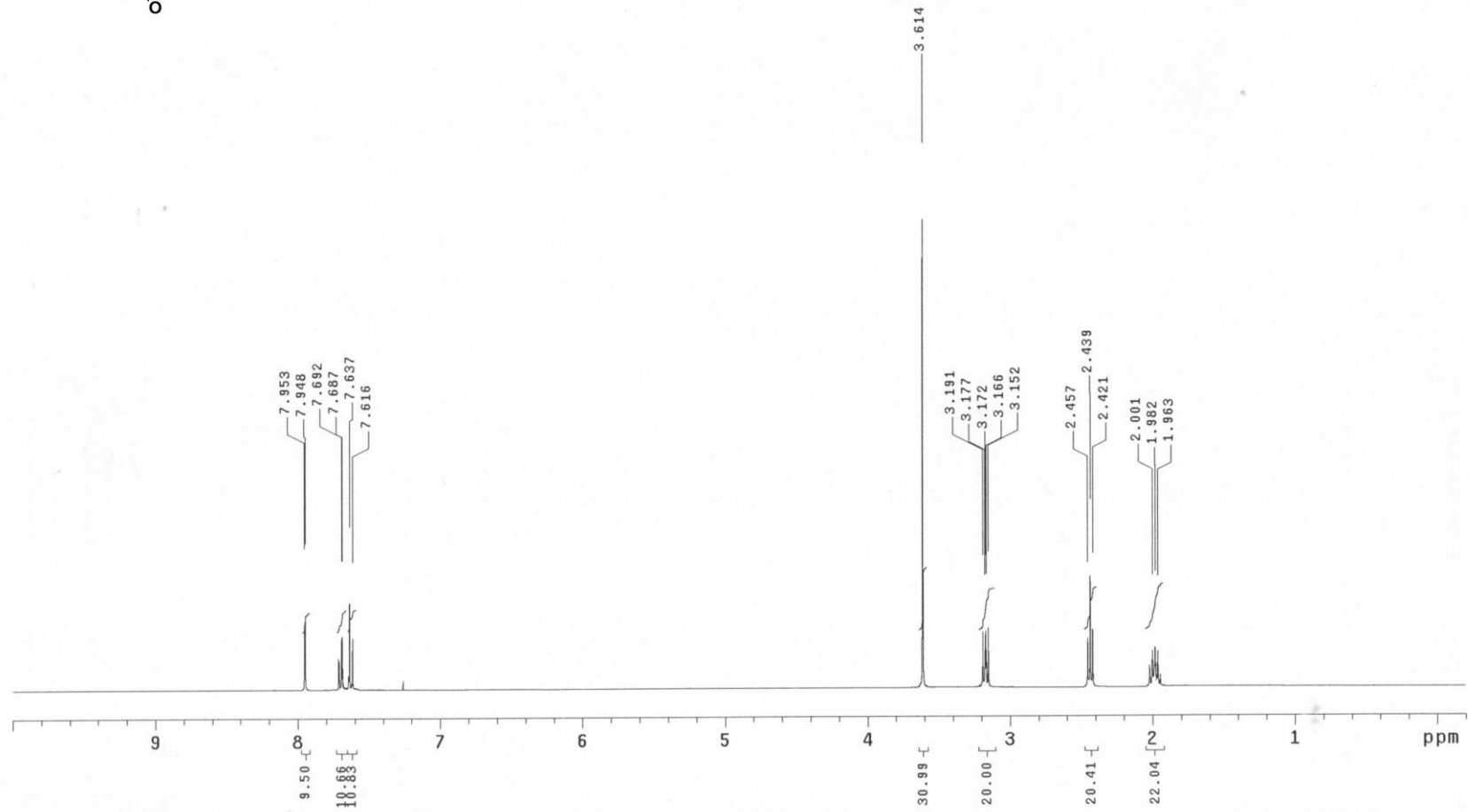
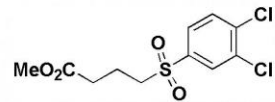
Total 7056 repetitions



Compound 5q (¹H-NMR spectral data)

PS0107-1

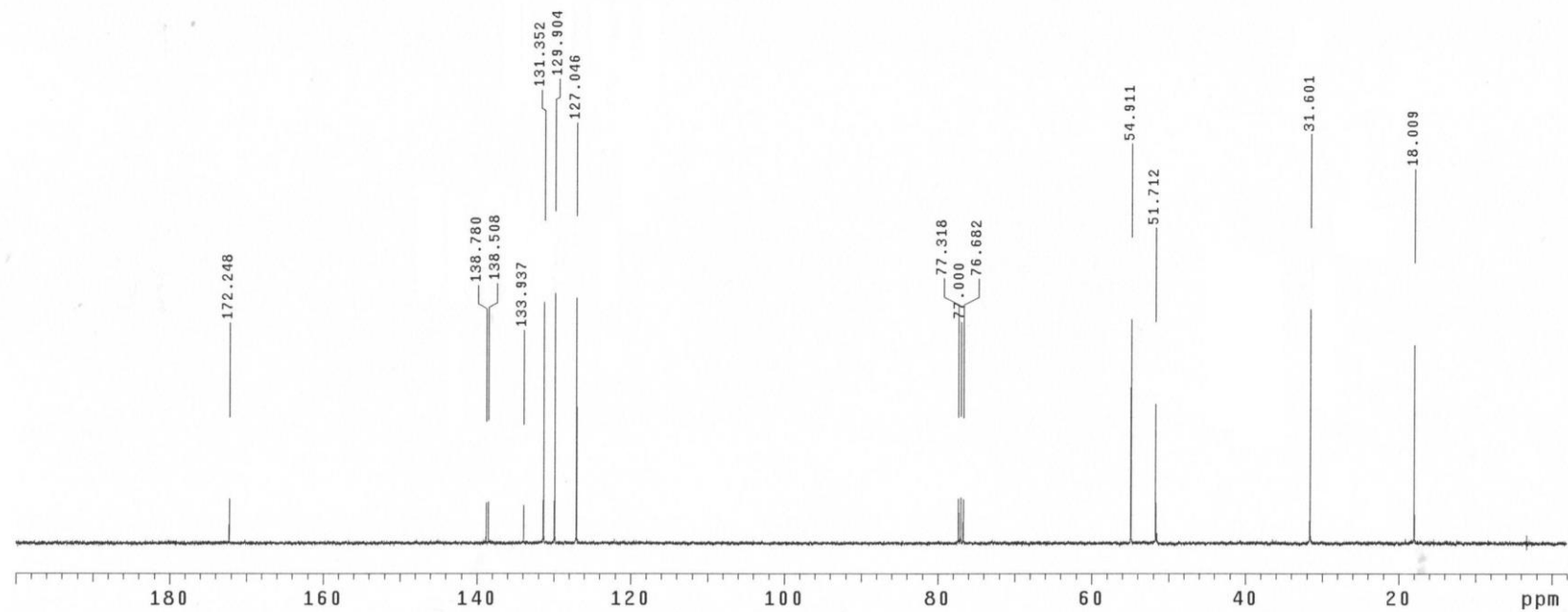
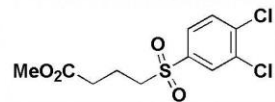
Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Jan 7 2021
Solvent: CDCl₃
Ambient temperature
Total 32 repetitions



Compound 5q (¹³C-NMR spectral data)

PS0107-1

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Jan 7 2021
Solvent: CDC13
Ambient temperature
Total 512 repetitions



Compound 5r (¹H-NMR spectral data)

PS1100122

Pulse Sequence: s2pu1

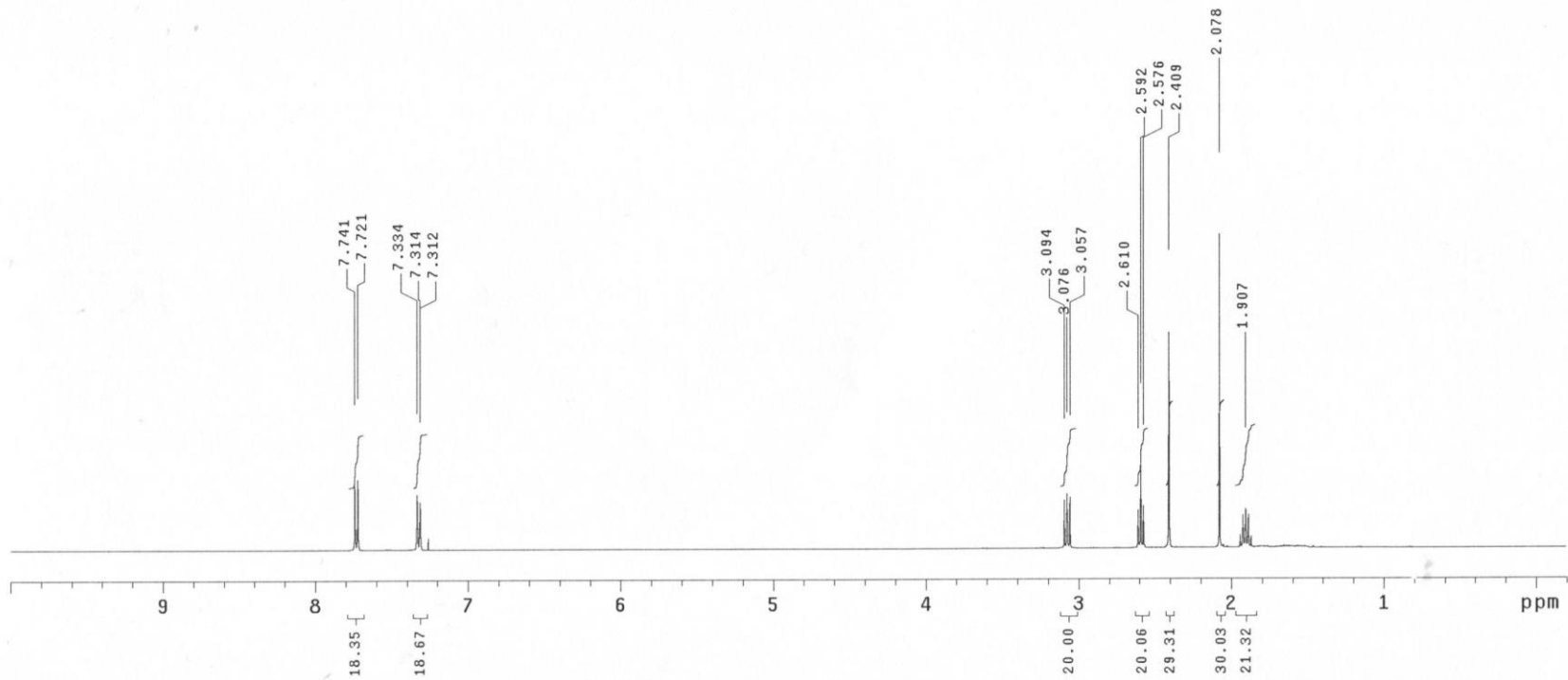
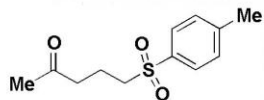
UNITYplus-400 "unity400"

Date: Jan 25 2021

Solvent: CDCl₃

Ambient temperature

Total 32 repetitions



Compound 5r (¹³C-NMR spectral data)

PS1100122

Pulse Sequence: s2pu1

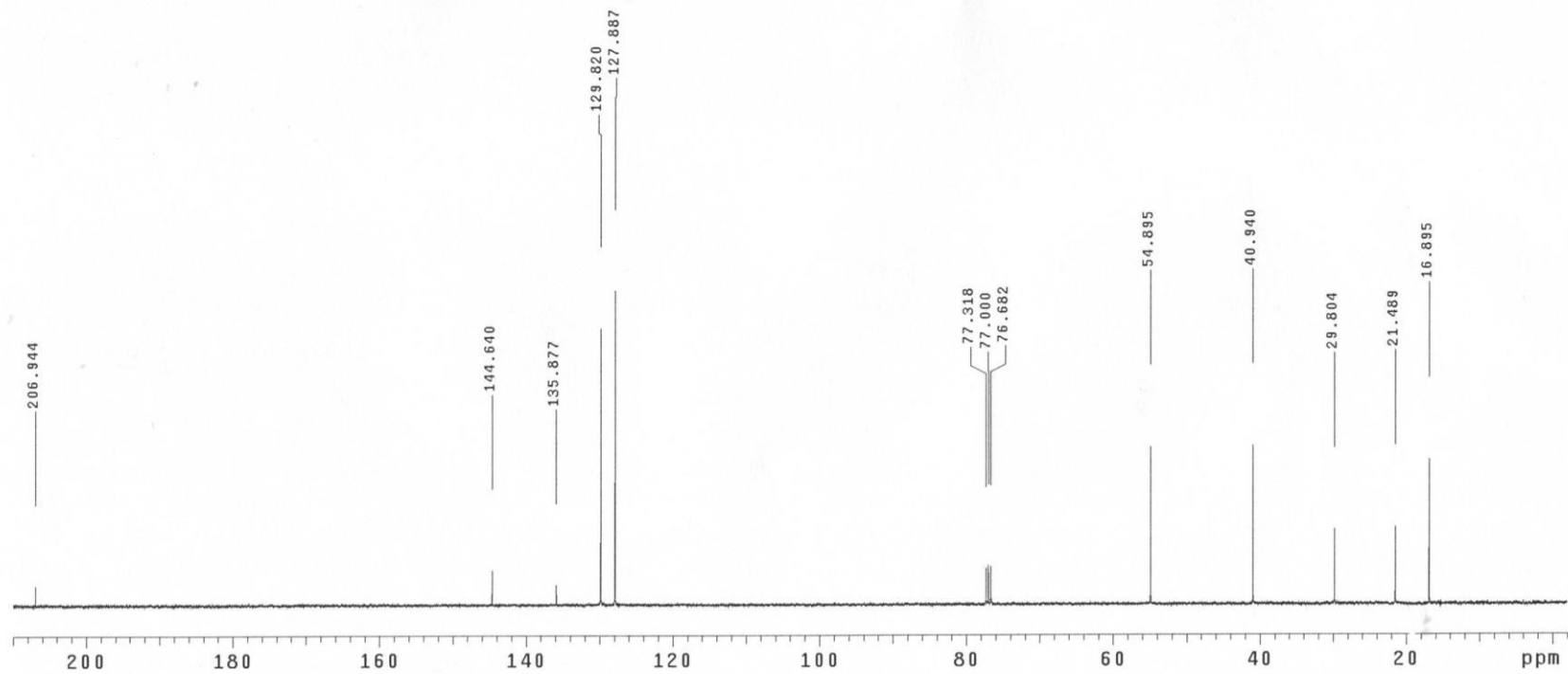
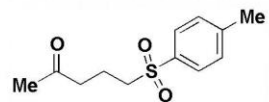
UNITYplus-400 "unity400"

Date: Jan 25 2021

Solvent: CDCl₃

Ambient temperature

Total 480 repetitions



Compound 5t (¹H-NMR spectral data)

PS0104-1

Pulse Sequence: s2pu1

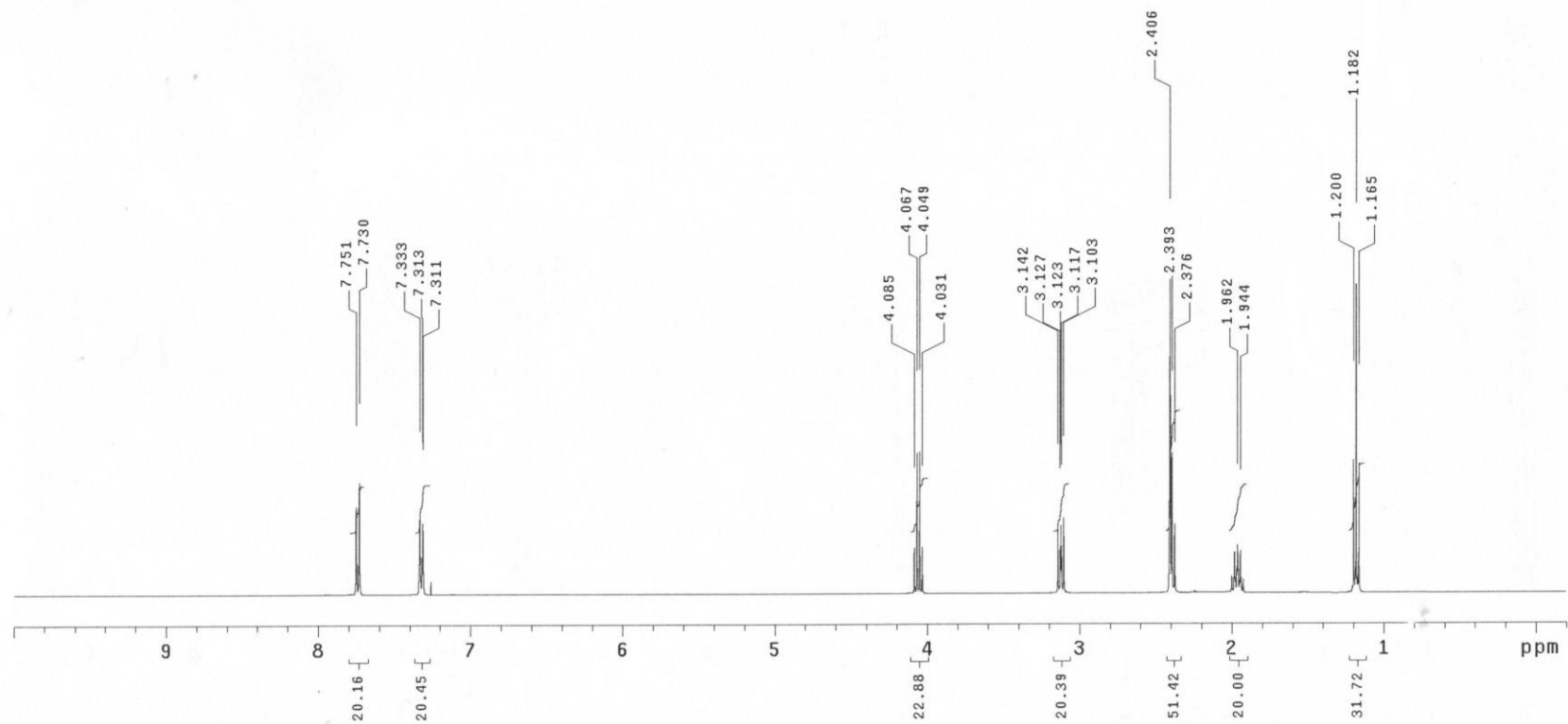
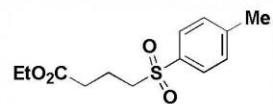
UNITYplus-400 "unity400"

Date: Jan 5 2021

Solvent: CDCl₃

Ambient temperature

Total 32 repetitions



Compound 5t (¹³C-NMR spectral data)

PS0104-1

Pulse Sequence: s2pu1

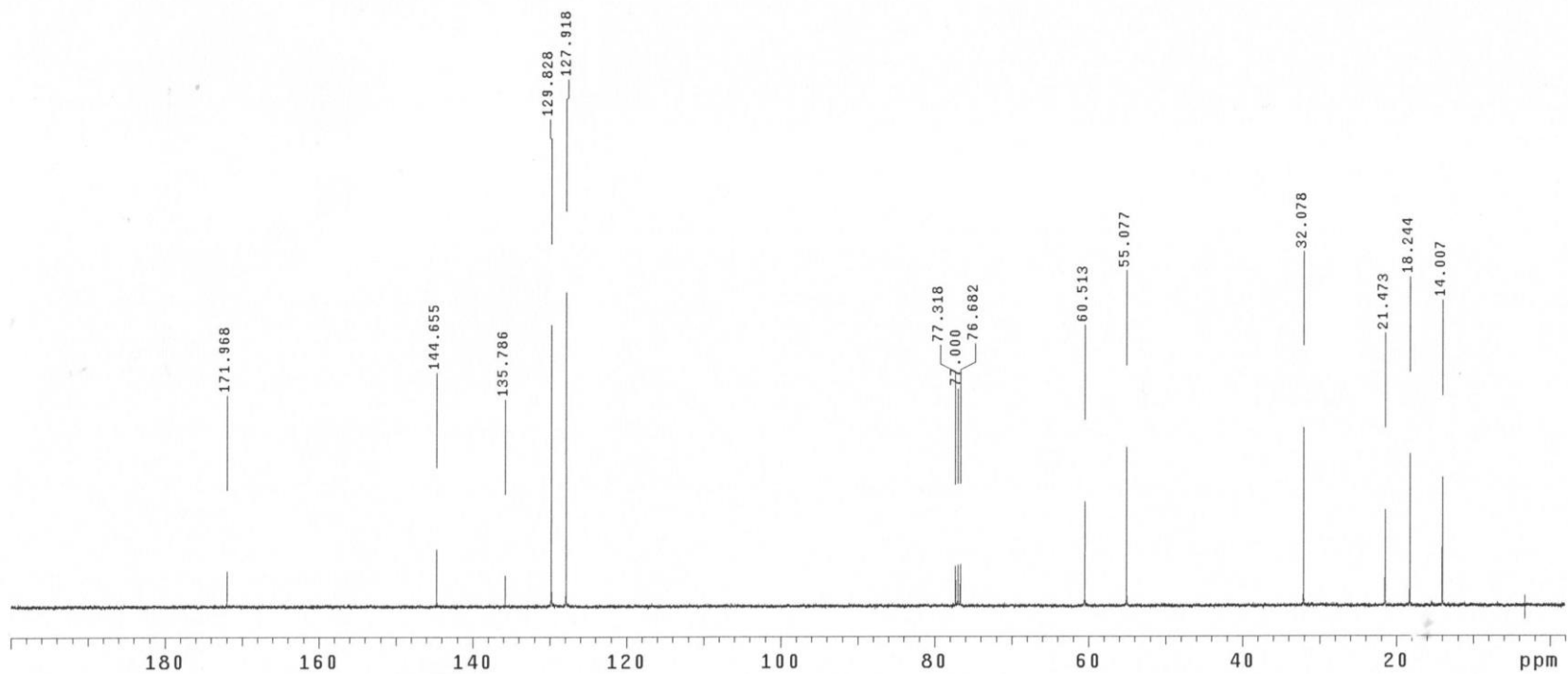
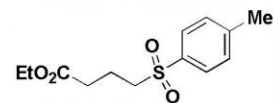
UNITYplus-400 "unity400"

Date: Jan 5 2021

Solvent: CDCl₃

Ambient temperature

Total 336 repetitions



Compound 5u (¹H-NMR spectral data)

PS1231-1

Pulse Sequence: s2pu1

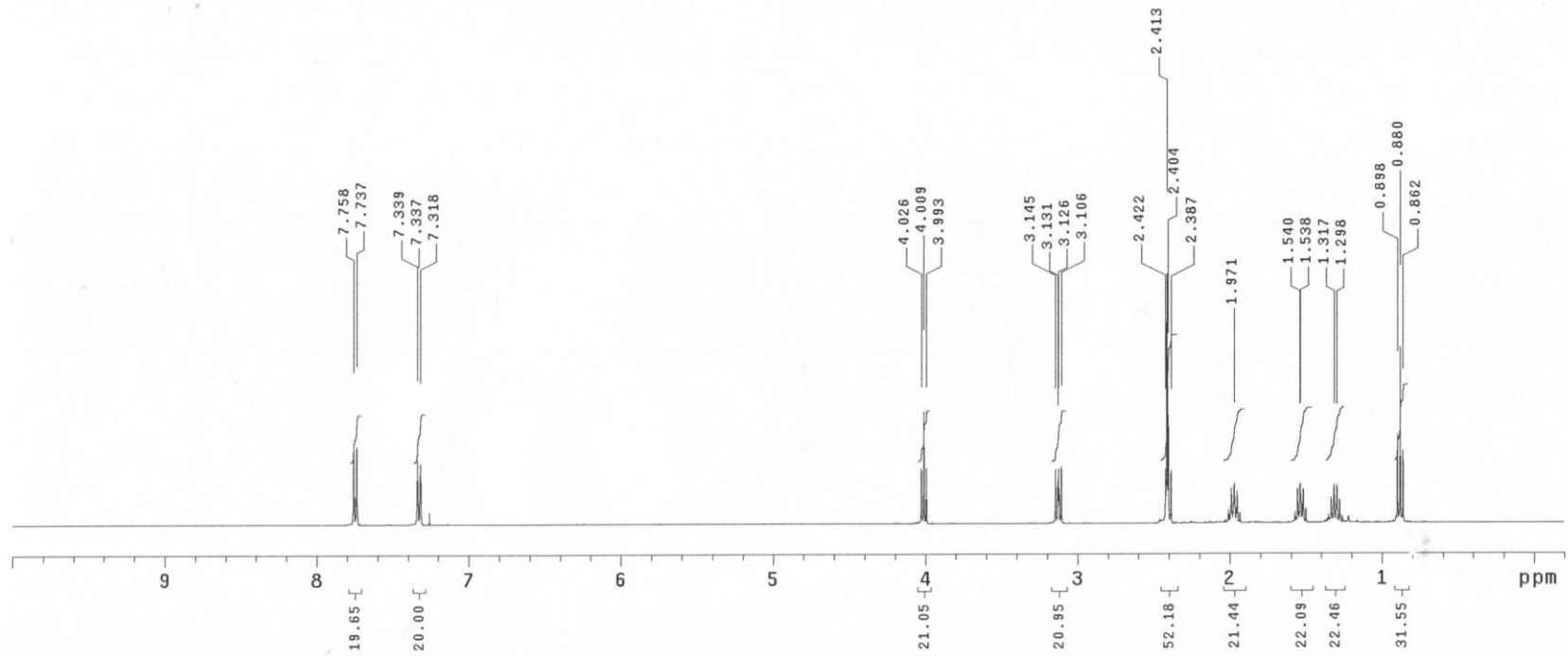
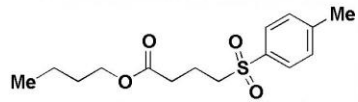
UNITYplus-400 "unity400"

Date: Dec 31 2020

Solvent: CDCl₃

Ambient temperature

Total 32 repetitions



Compound 5u (¹³C-NMR spectral data)

PS1231-1

Pulse Sequence: s2pu1

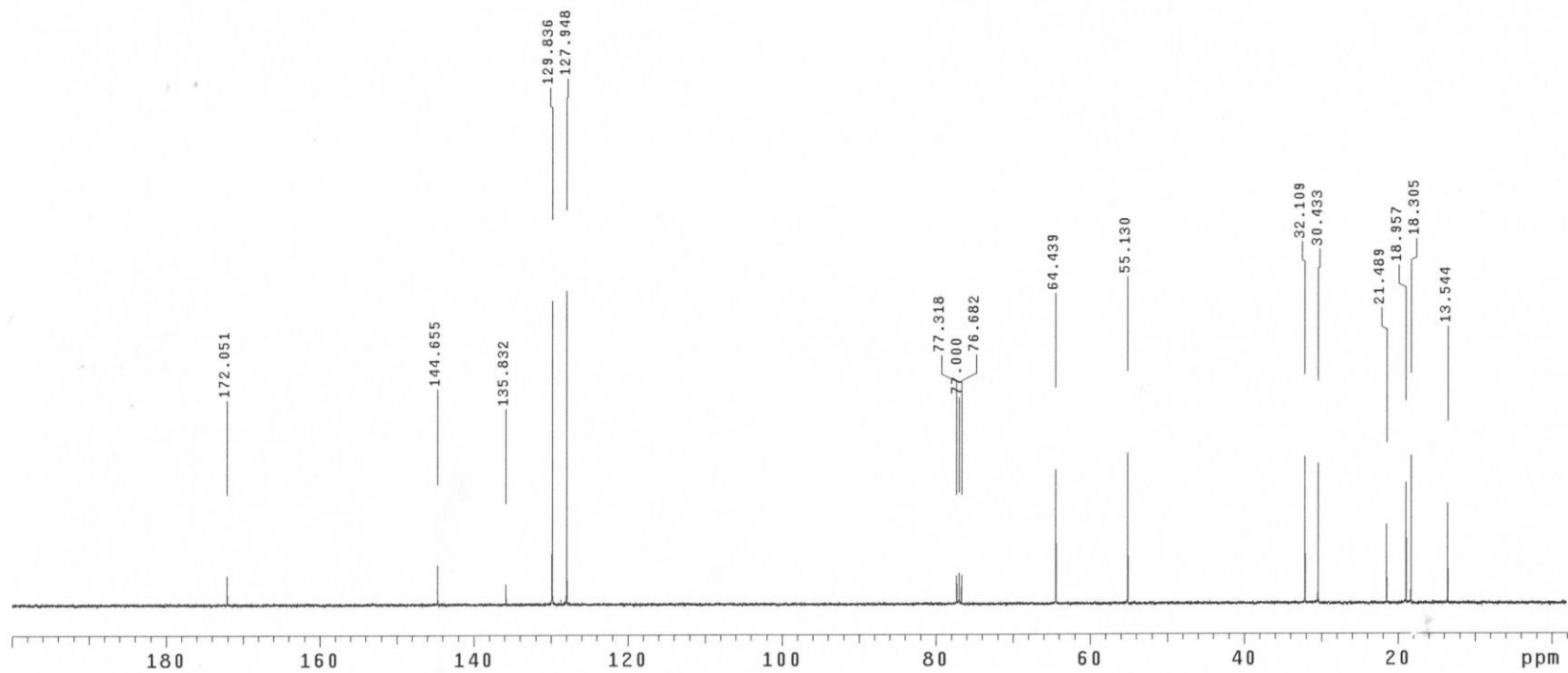
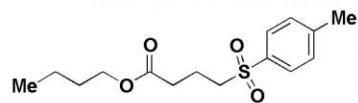
UNITYplus-400 "unity400"

Date: Dec 31 2020

Solvent: CDCl₃

Ambient temperature

Total 432 repetitions



Compound 5v (¹H-NMR spectral data)

PS0108-1

Pulse Sequence: s2pu1

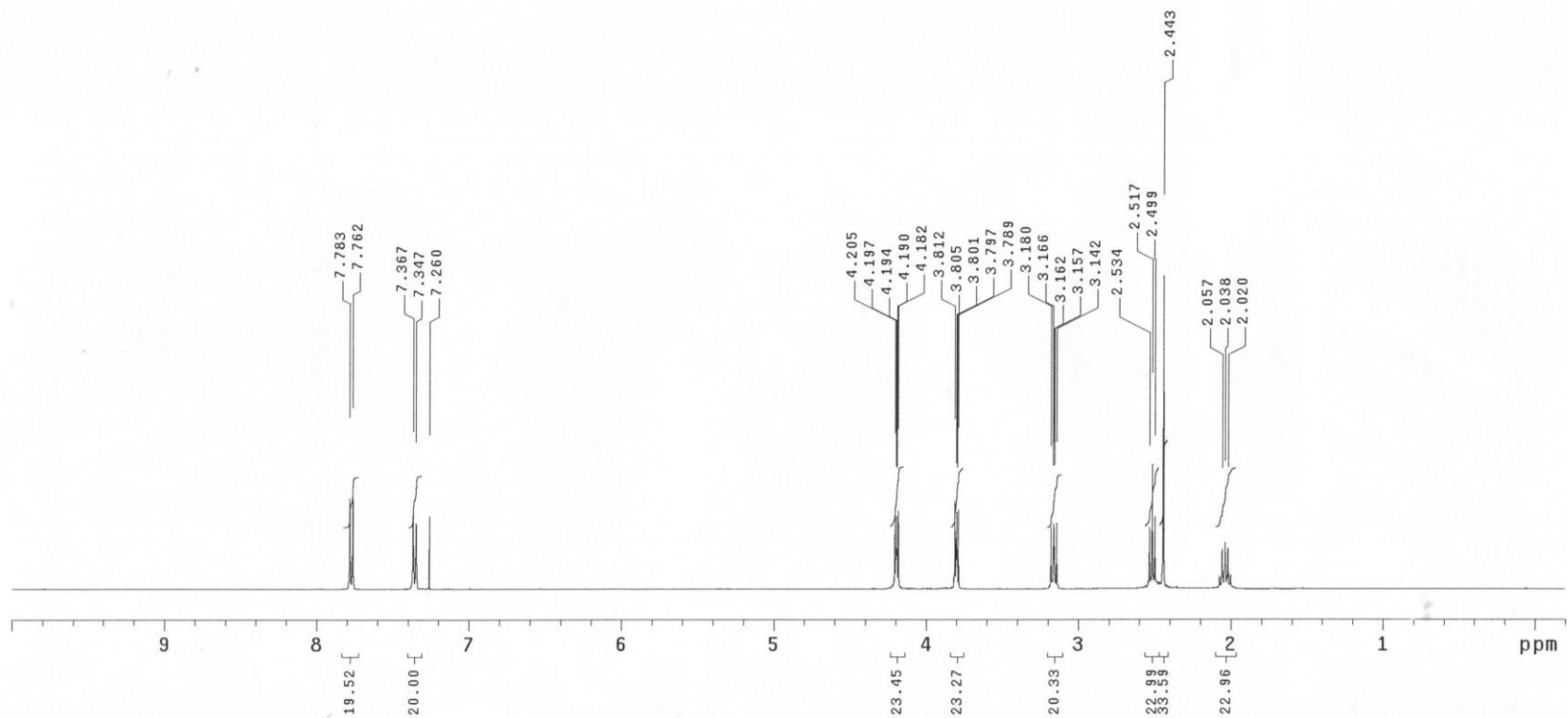
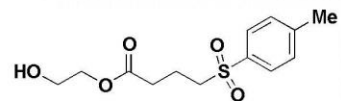
UNITYplus-400 "unity400"

Date: Jan 11 2021

Solvent: CDCl₃

Ambient temperature

Total 32 repetitions



Compound 5v (¹³C-NMR spectral data)

PS0108-1

Pulse Sequence: s2pu1

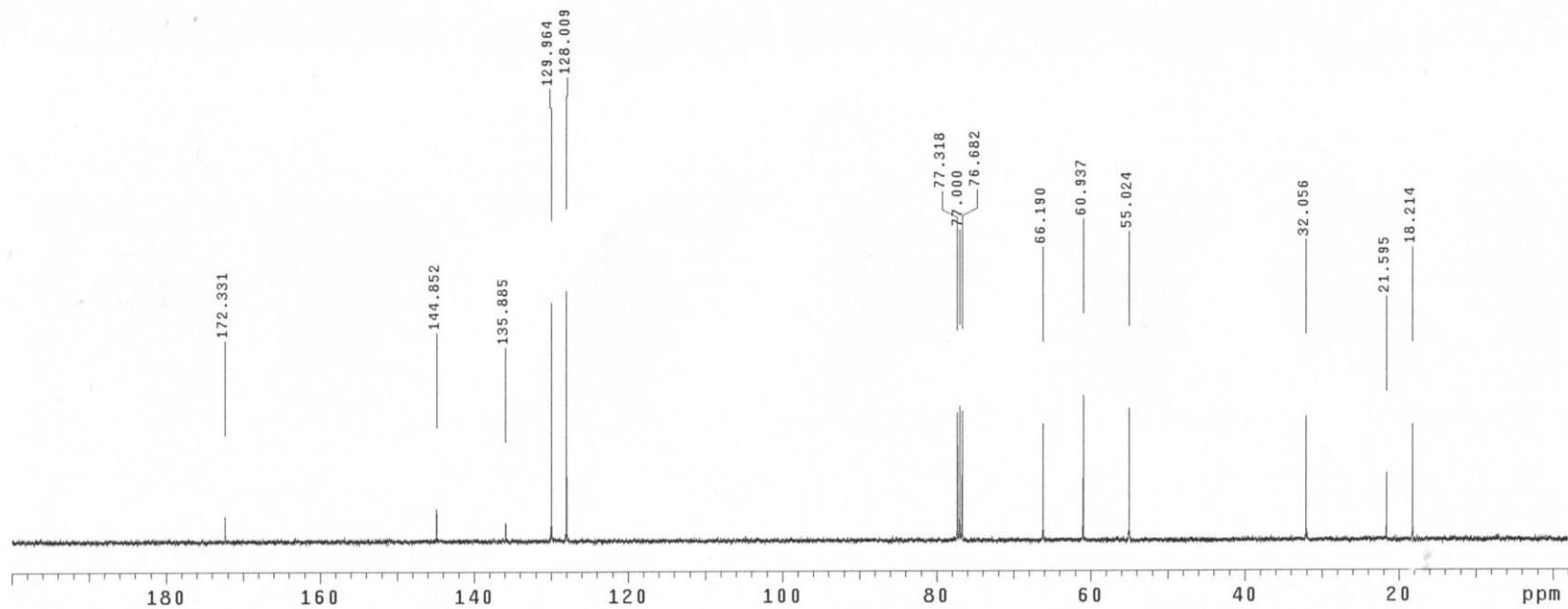
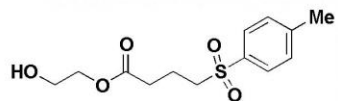
UNITYplus-400 "unity400"

Date: Jan 11 2021

Solvent: CDCl₃

Ambient temperature

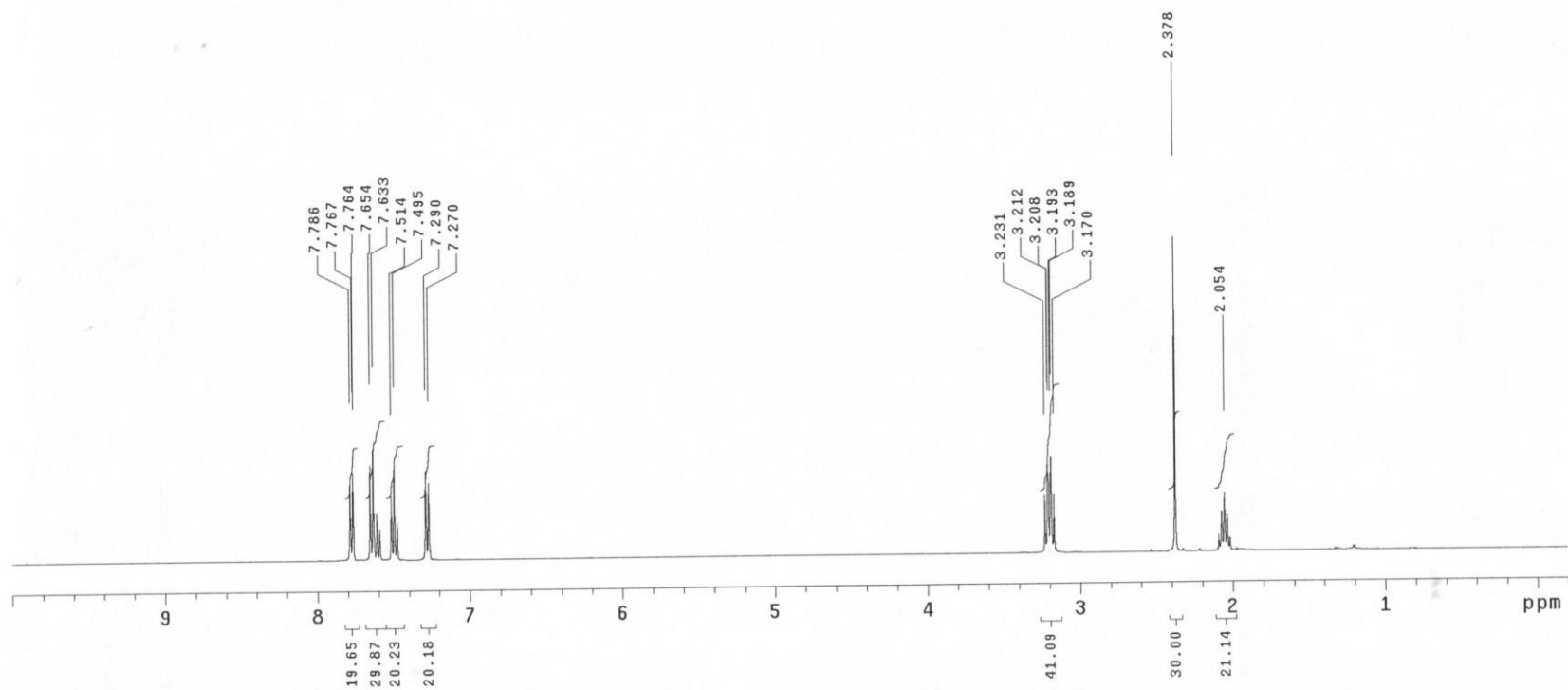
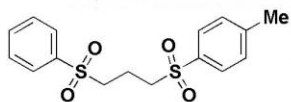
Total 3040 repetitions



Compound 5w (¹H-NMR spectral data)

PS0106-1

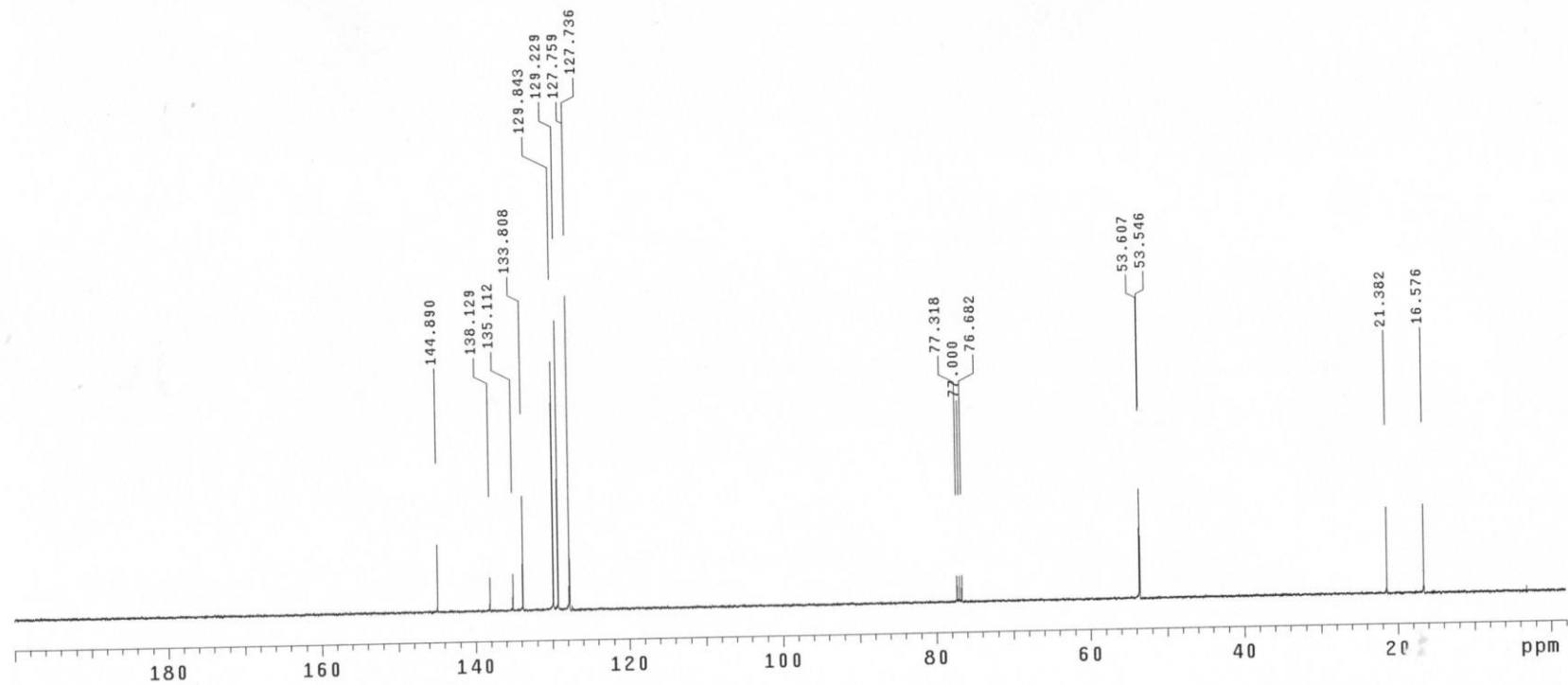
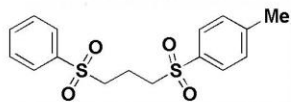
Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Jan 7 2021
Solvent: CDC13
Ambient temperature
Total 32 repetitions



Compound 5w (¹³C-NMR spectral data)

PS0106-1

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Jan 7 2021
Solvent: CDCl₃
Ambient temperature
Total 160 repetitions



Compound 5x (¹H-NMR spectral data)

PS1230-1

Pulse Sequence: s2pu1

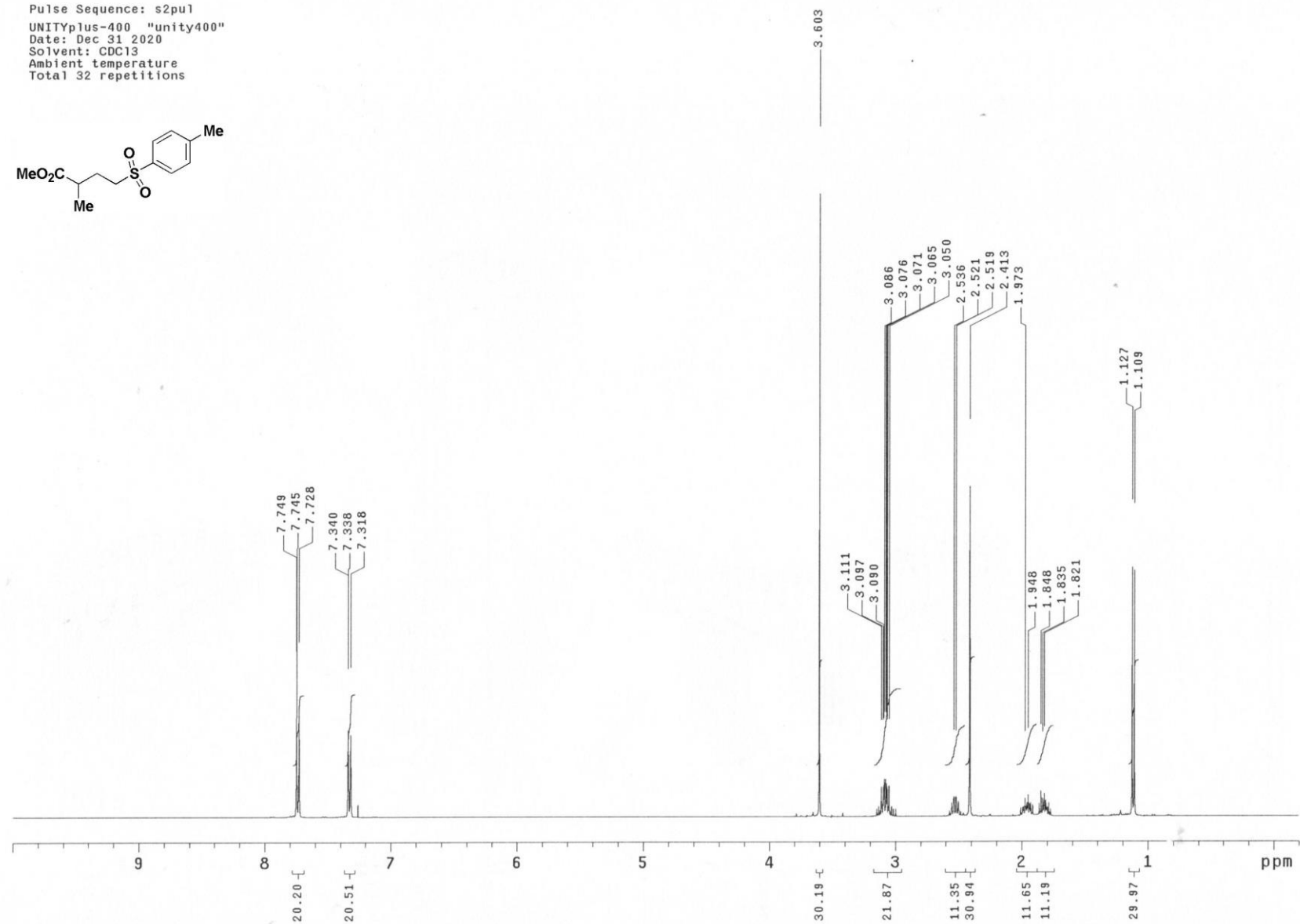
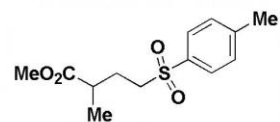
UNITYplus-400 "unity400"

Date: Dec 31 2020

Solvent: CDC13

Ambient temperature

Total 32 repetitions



Compound 5x (¹³C-NMR spectral data)

PS1230-1

Pulse Sequence: s2pu1

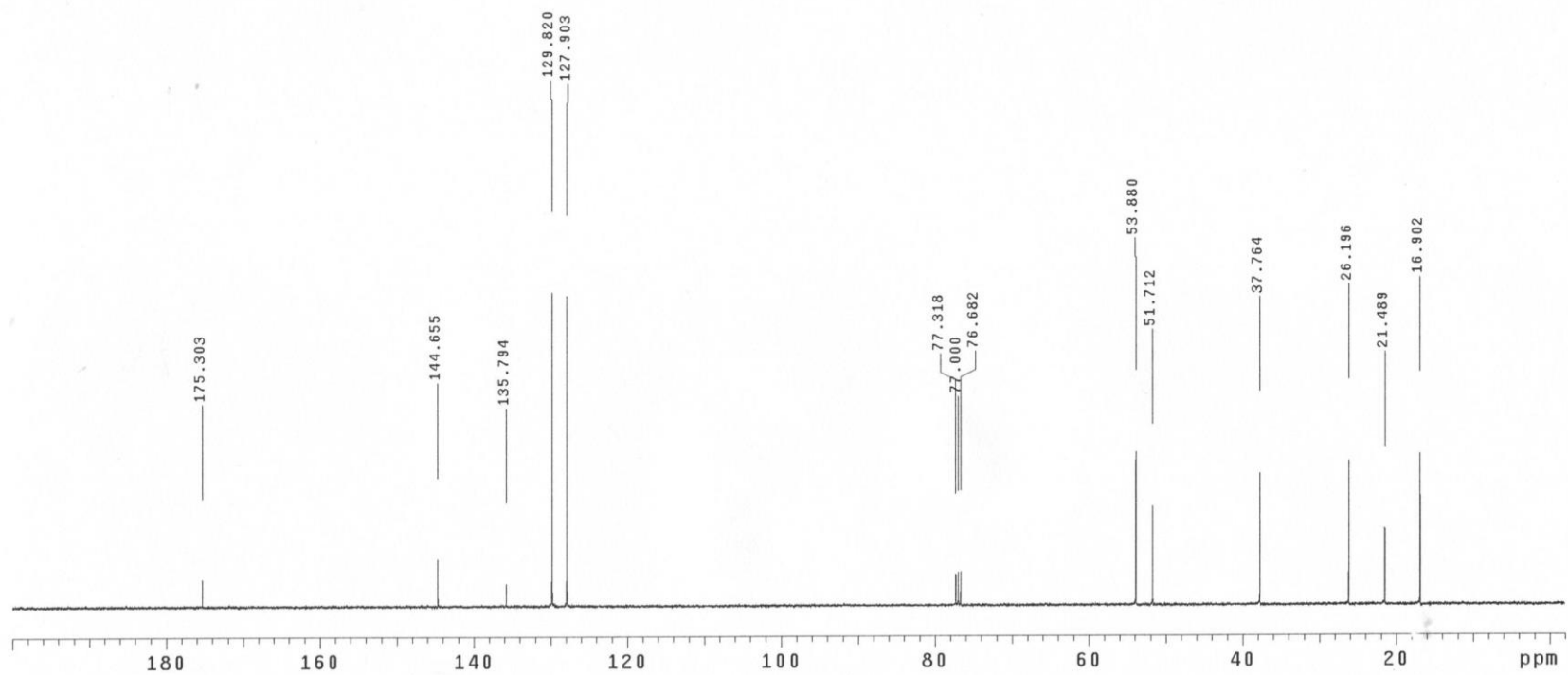
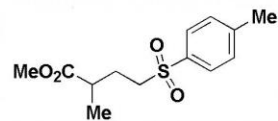
UNITYplus-400 "unity400"

Date: Dec 31 2020

Solvent: CDCl₃

Ambient temperature

Total 400 repetitions



Compound 5y (¹H-NMR spectral data)

PS0114-1

Pulse Sequence: s2pu1

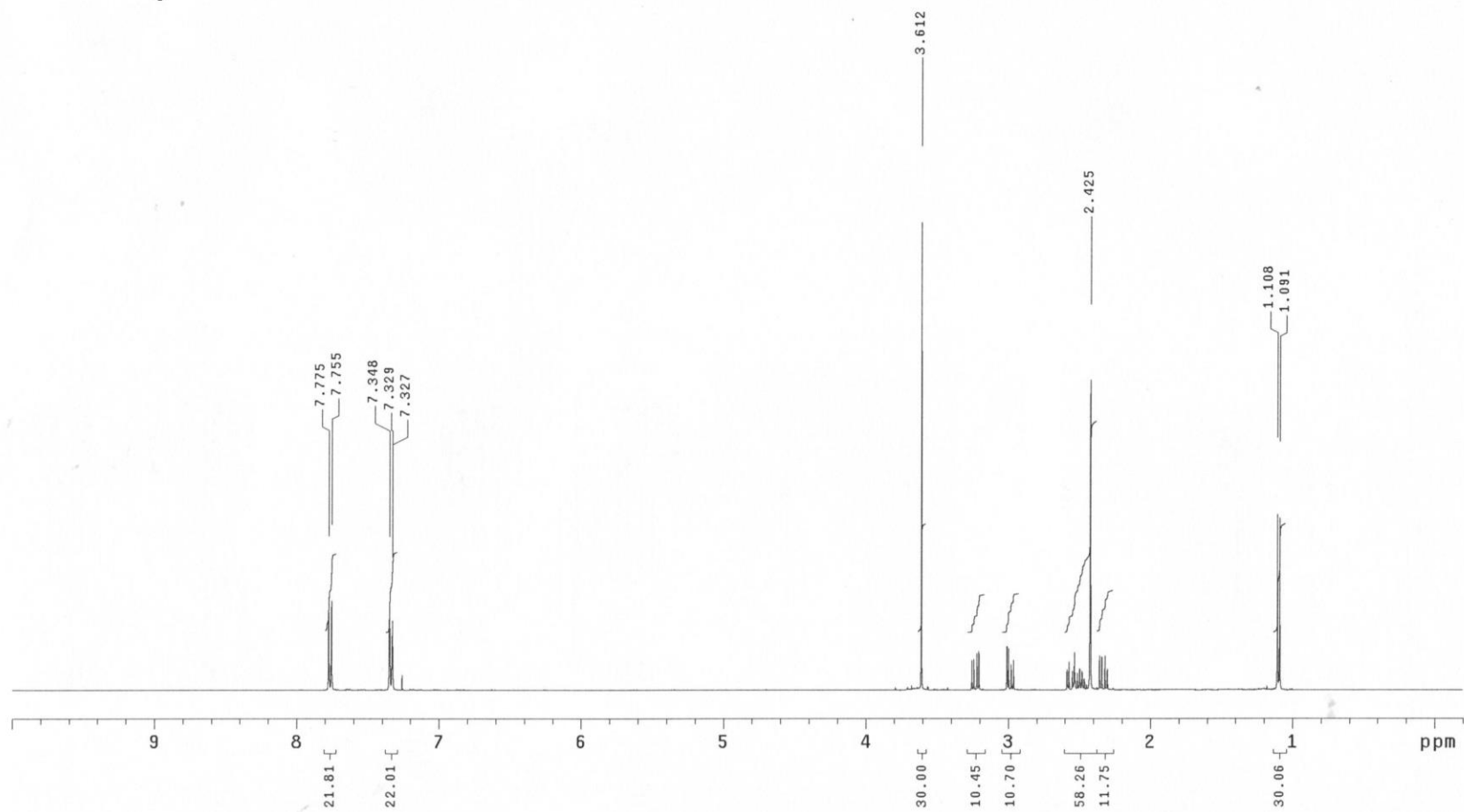
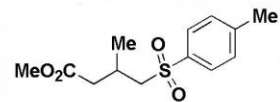
UNITYplus-400 "unity400"

Date: Jan 14 2021

Solvent: CDCl₃

Ambient temperature

Total 32 repetitions



Compound 5y (¹³C-NMR spectral data)

PS0114-1

Pulse Sequence: s2pu1

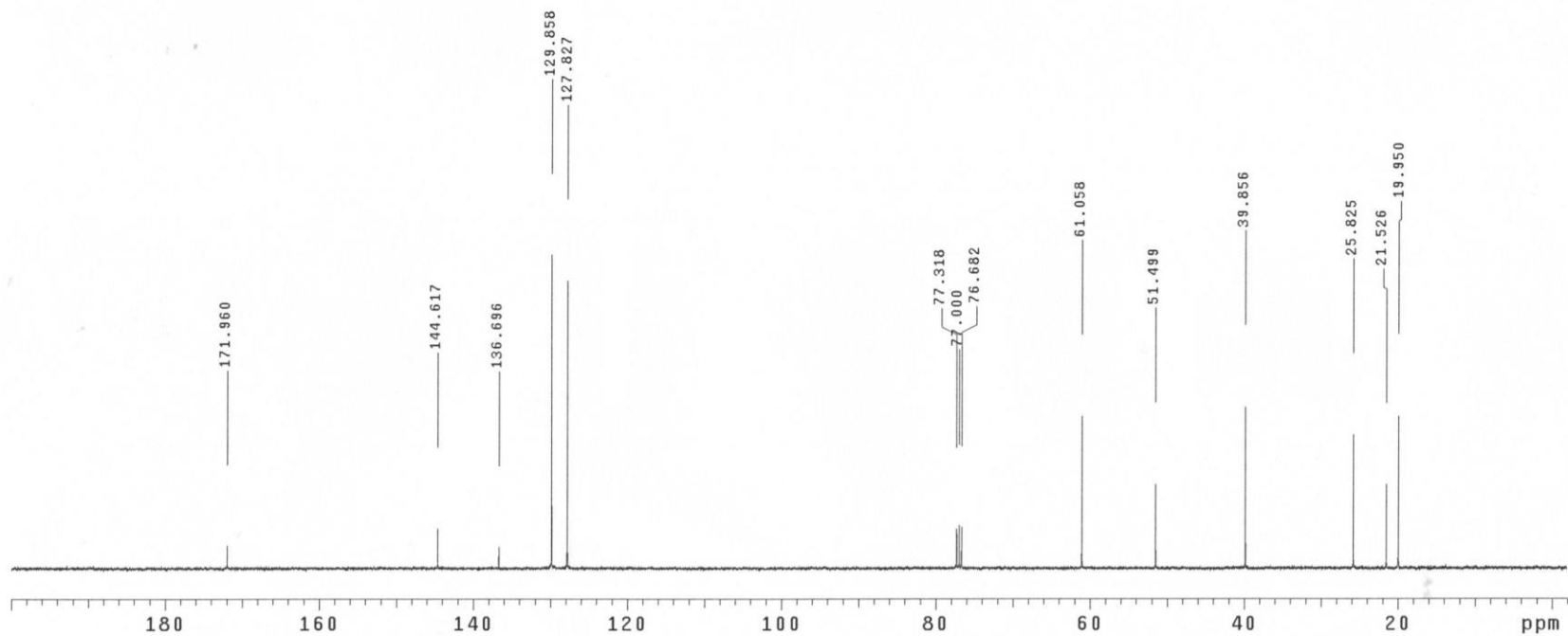
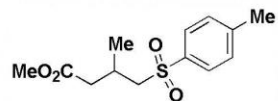
UNITYplus-400 "unity400"

Date: Jan 14 2021

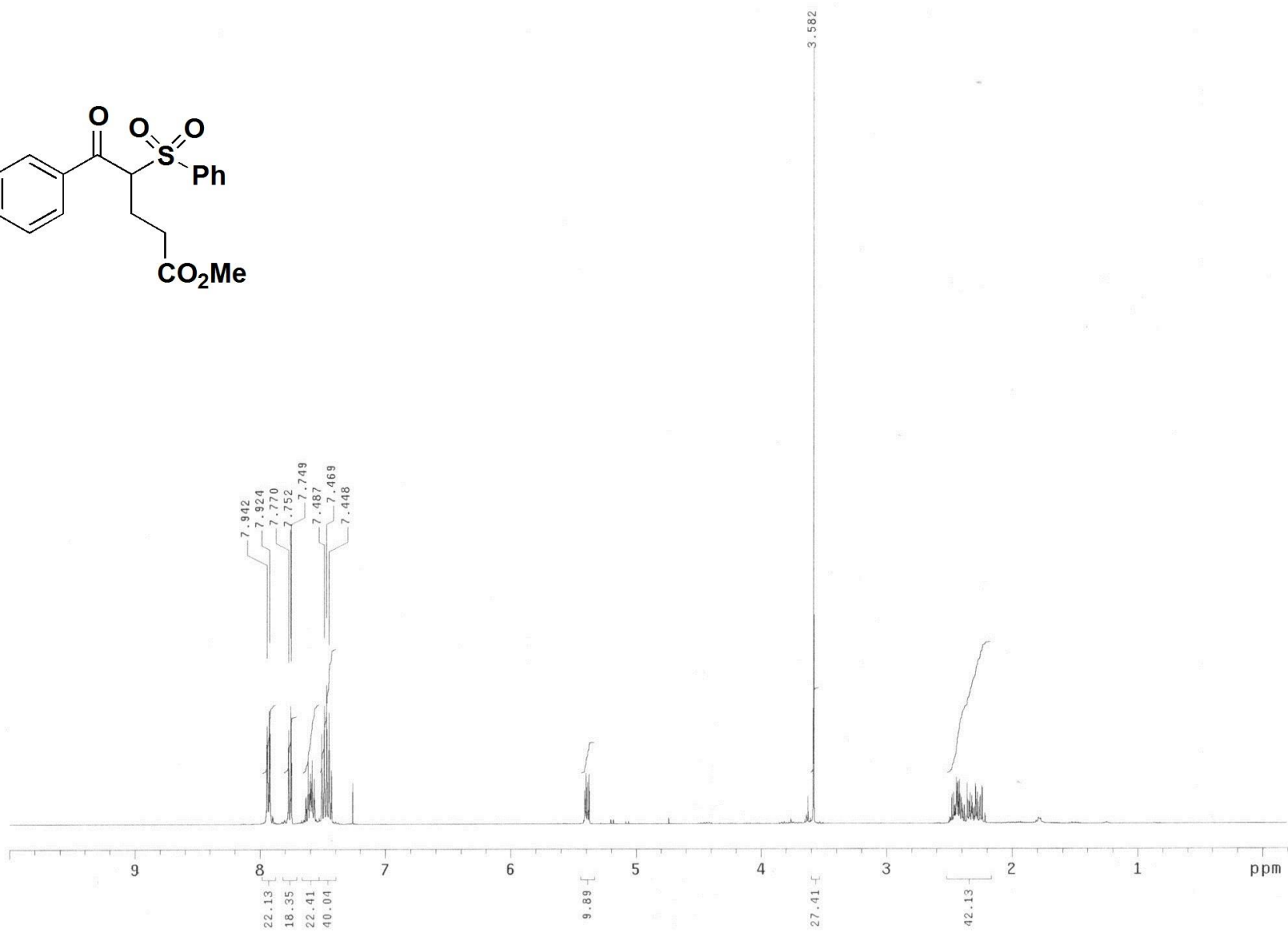
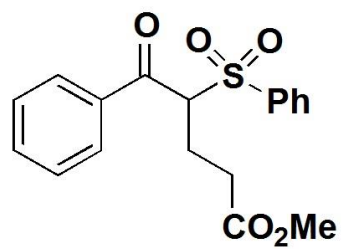
Solvent: CDCl₃

Ambient temperature

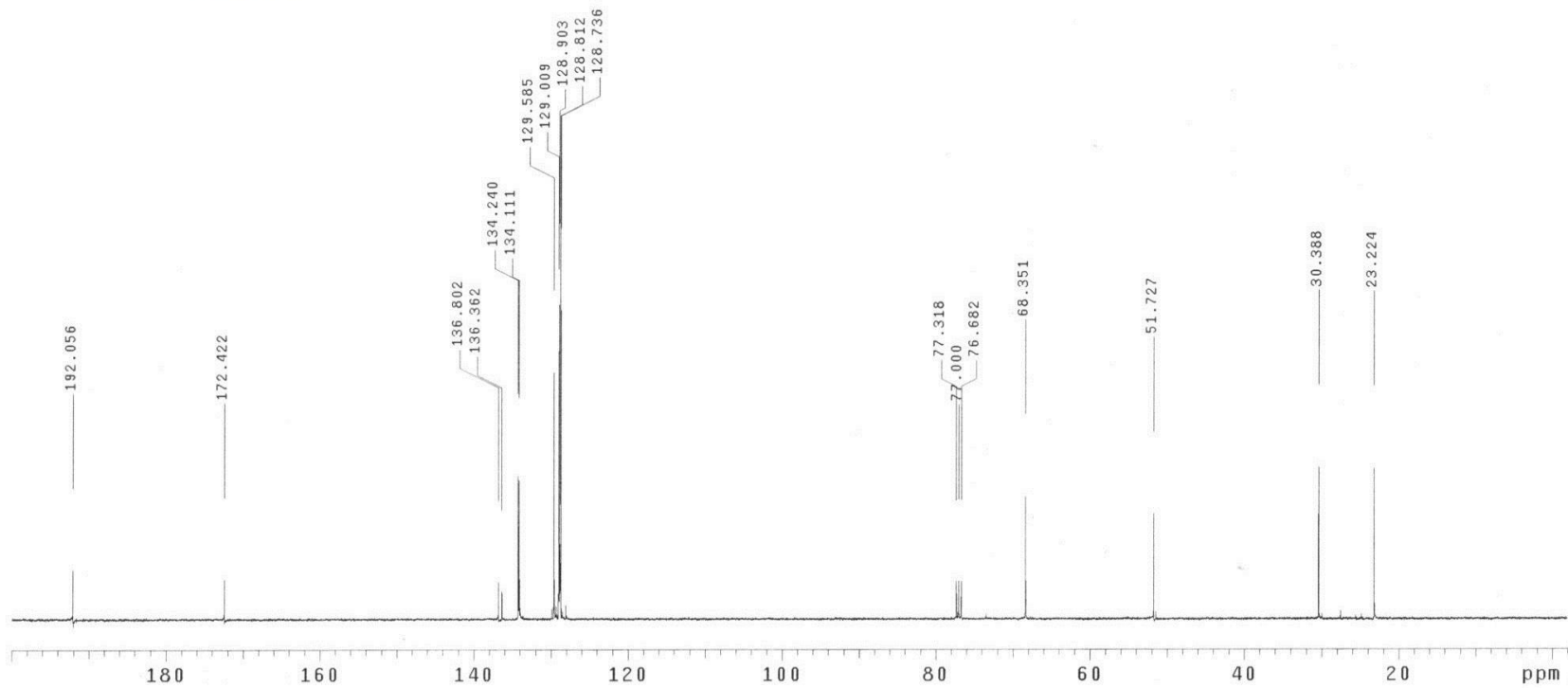
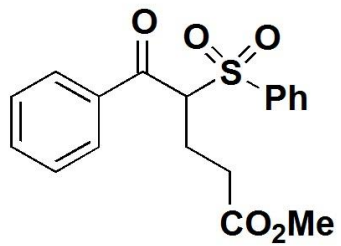
Total 800 repetitions



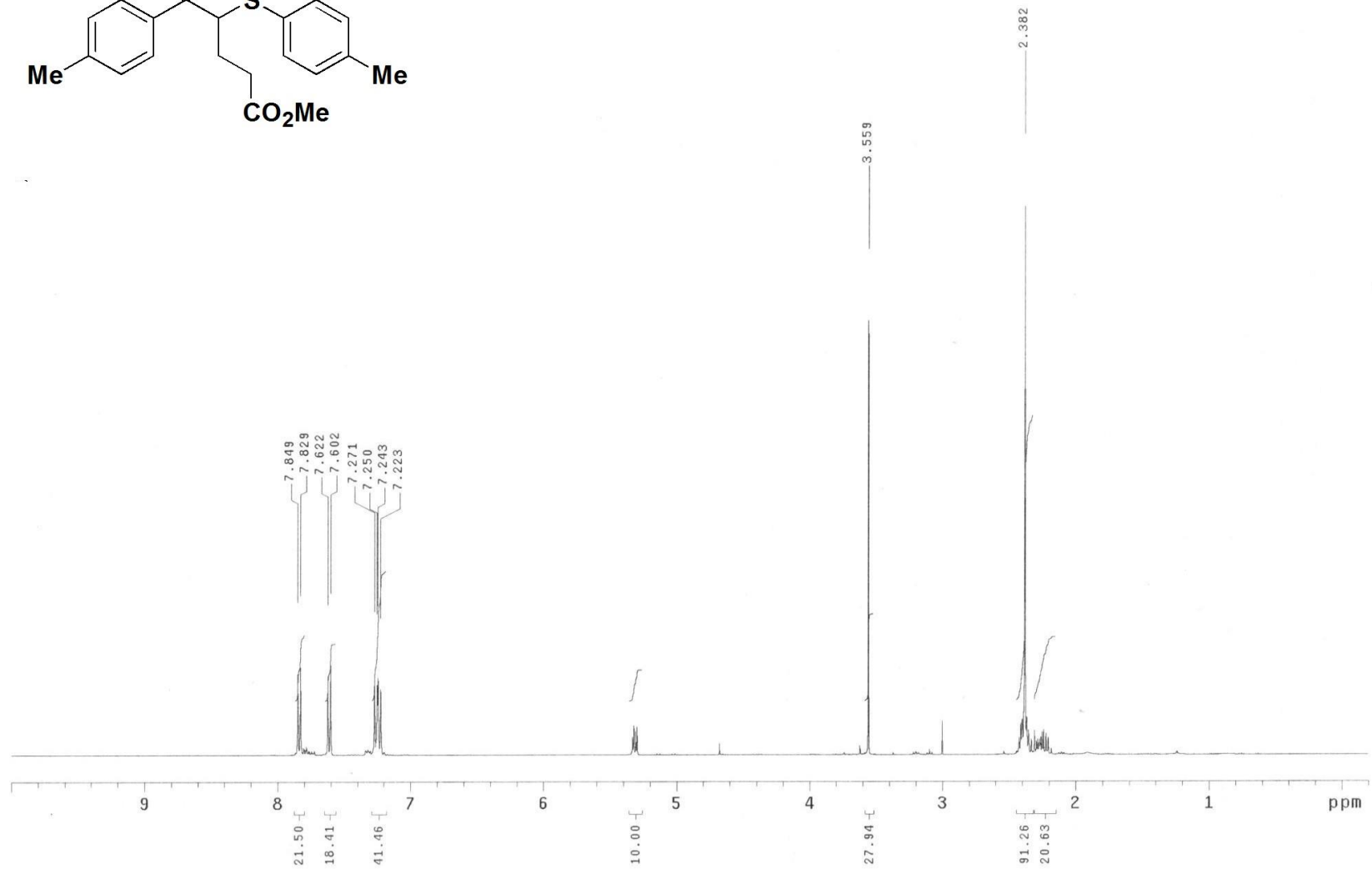
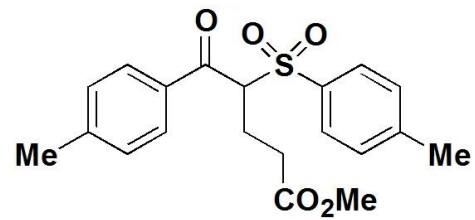
Compound 8a (¹H-NMR spectral data)



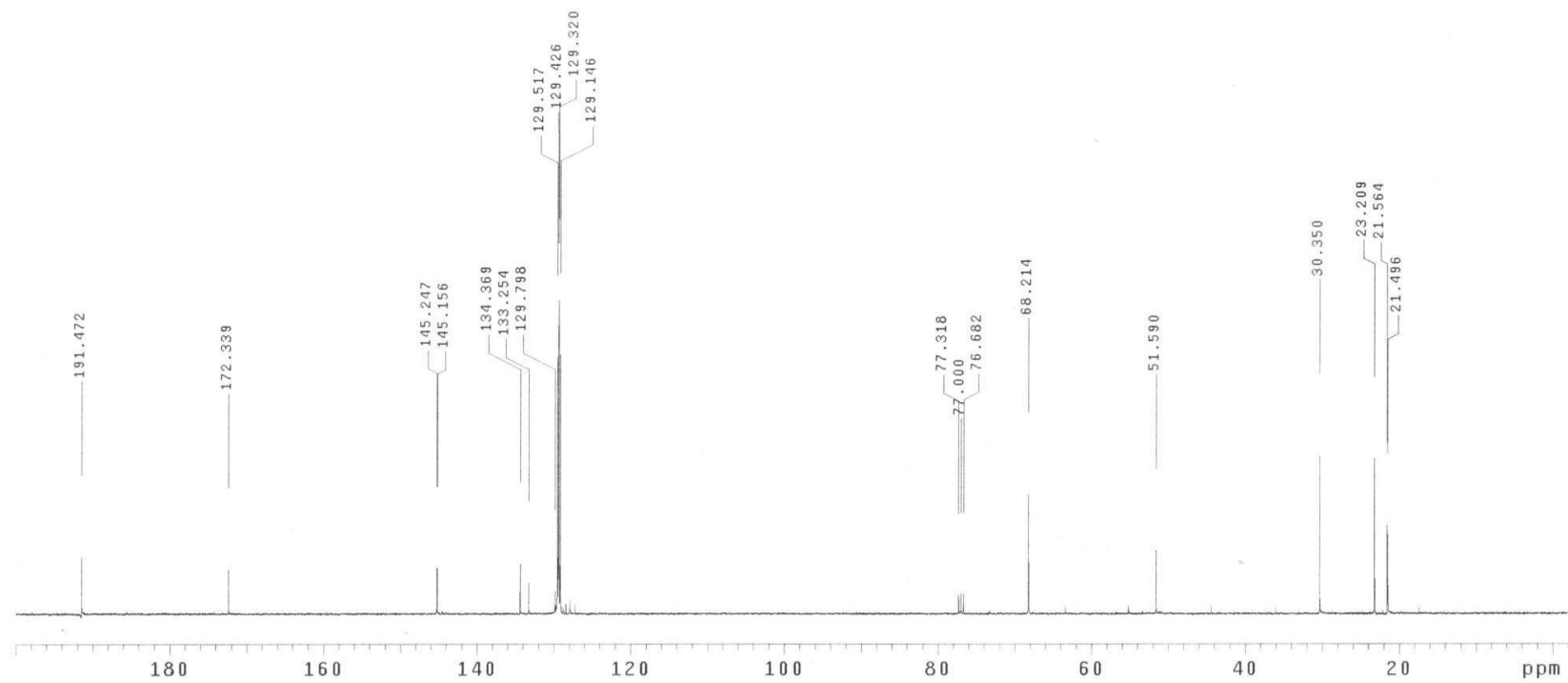
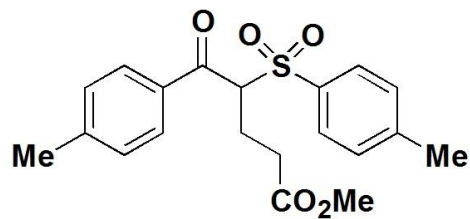
Compound 8a (¹³C-NMR spectral data)



Compound 8b (¹H-NMR spectral data)



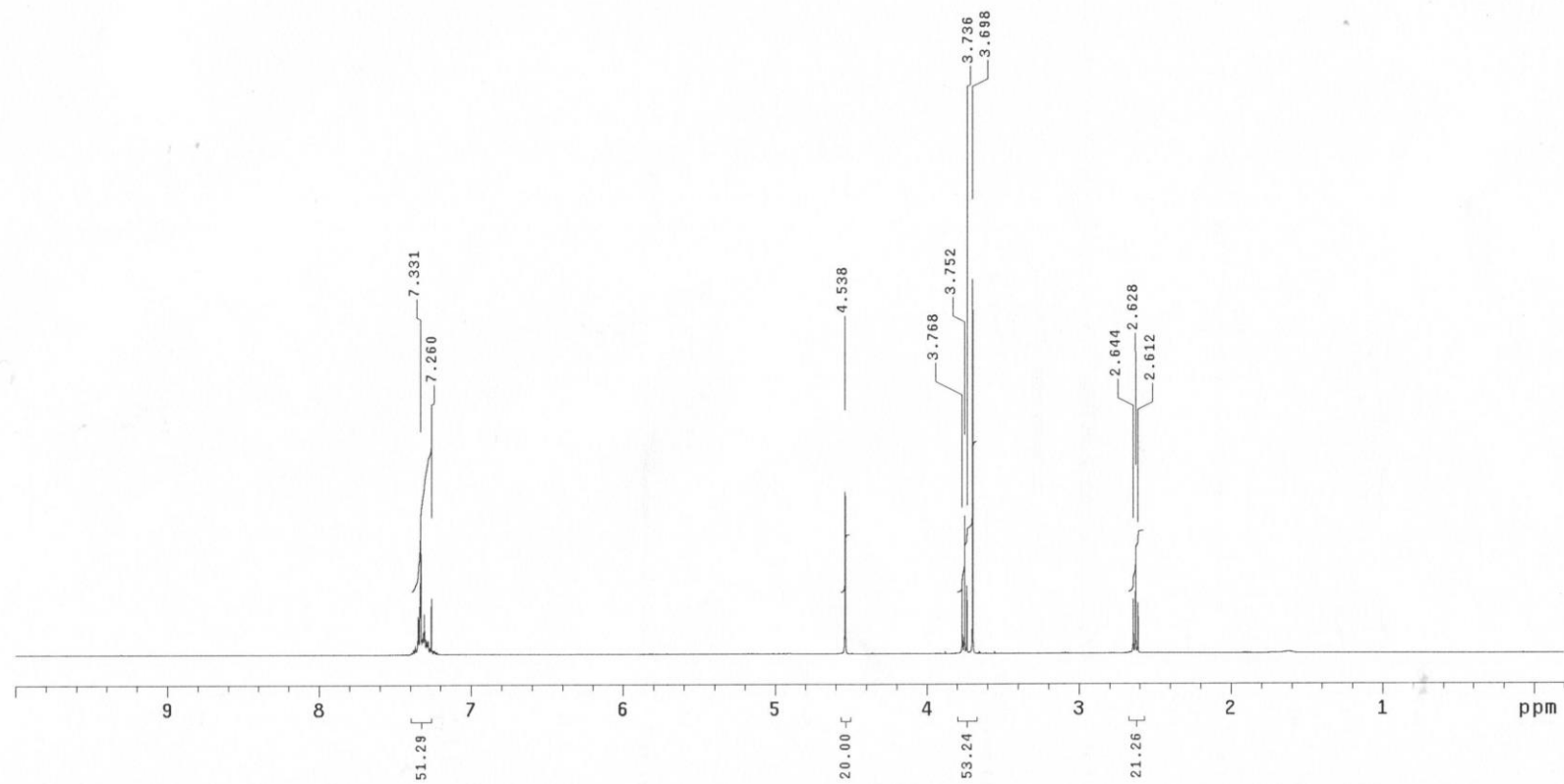
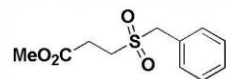
Compound 8b (¹³C-NMR spectral data)



Compound 9 (¹H-NMR spectral data)

PS0115-1

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Jan 14 2021
Solvent: CDCl₃
Ambient temperature
Total 32 repetitions



Compound 9 (¹³C-NMR spectral data)

PS0115-1

Pulse Sequence: s2pu1

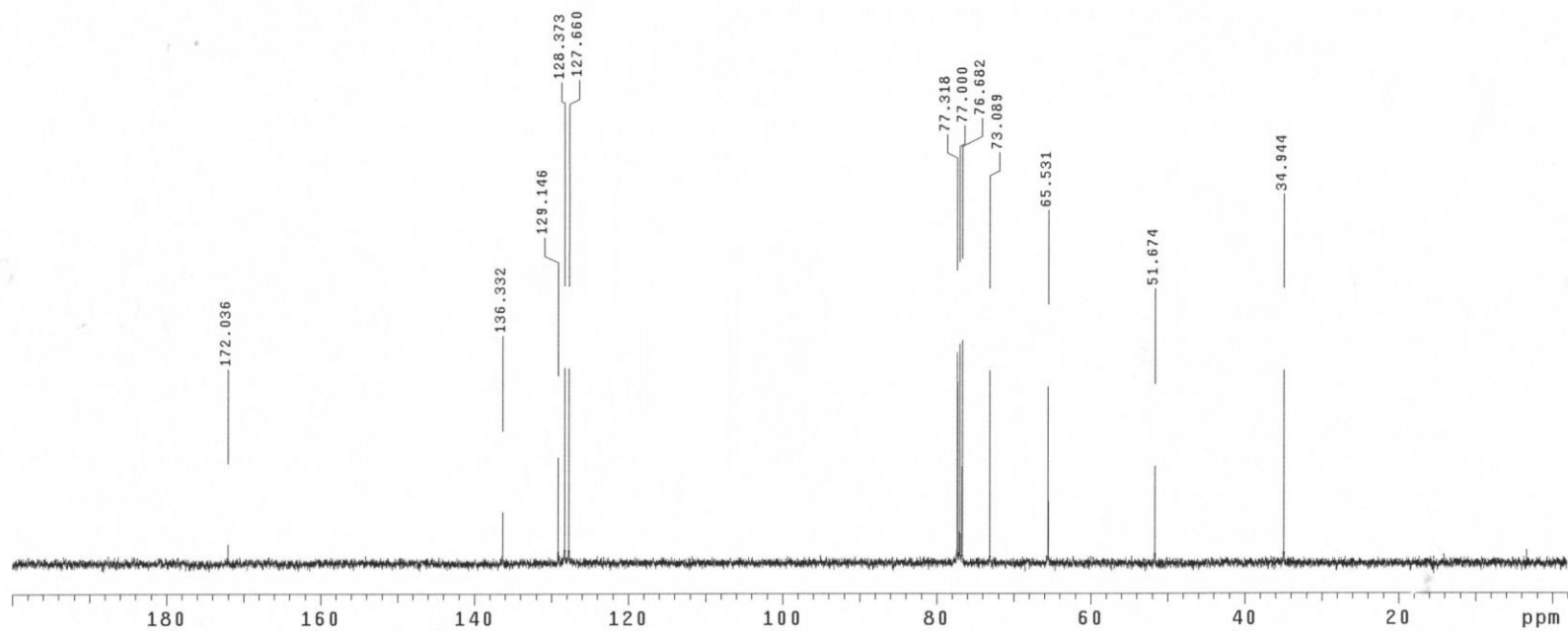
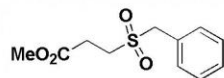
UNITYplus-400 "unity400"

Date: Jan 14 2021

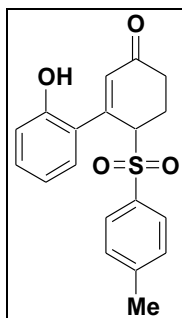
Solvent: CDCl₃

Ambient temperature

Total 2416 repetitions

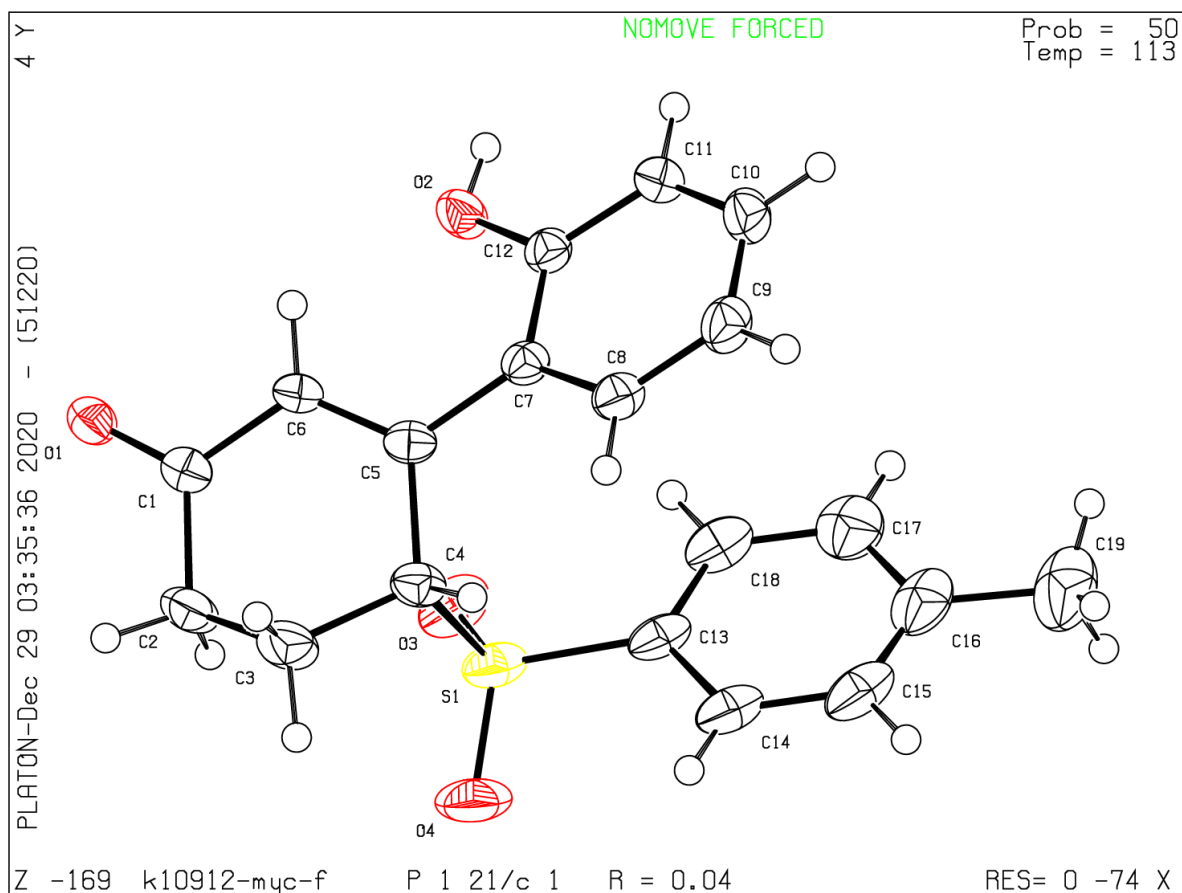


X-ray crystal data of compound 7b



Sample preparation : A solution of compound **7b** (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 ₁₉ H ₁₈ O ₄ S
Formula weight	342.39
Temperature/K	113(2)
Crystal system	monoclinic
Space group	P2 ₁ /c
a/Å	16.5325(5)
b/Å	5.5611(2)
c/Å	19.0631(6)
α/°	90
β/°	110.600(4)
γ/°	90
Volume/Å ³	1640.58(10)
Z	4
ρ _{calc} /cm ³	1.386
μ/mm ⁻¹	0.217
F(000)	720.0
Crystal size/mm ³	0.36 × 0.2 × 0.15
Radiation	Mo Kα (λ = 0.71073)
2θ range for data collection/°	4.394 to 54.05
Index ranges	-20 ≤ h ≤ 20, -7 ≤ k ≤ 4, -24 ≤ l ≤ 23
Reflections collected	15178
Independent reflections	3403 [R _{int} = 0.0316, R _{sigma} = 0.0333]
Data/restraints/parameters	3403/0/219
Goodness-of-fit on F ²	1.057
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0390, wR ₂ = 0.0973
Final R indexes [all data]	R ₁ = 0.0507, wR ₂ = 0.1031
Largest diff. peak/hole / e Å ⁻³	0.24/-0.37