Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

HCl-Mediated Cascade Cyclocondensation of Oxygenated Arylacetic Acids with Arylaldehydes. One-pot Synthesis of 1-Arylisoquinolines

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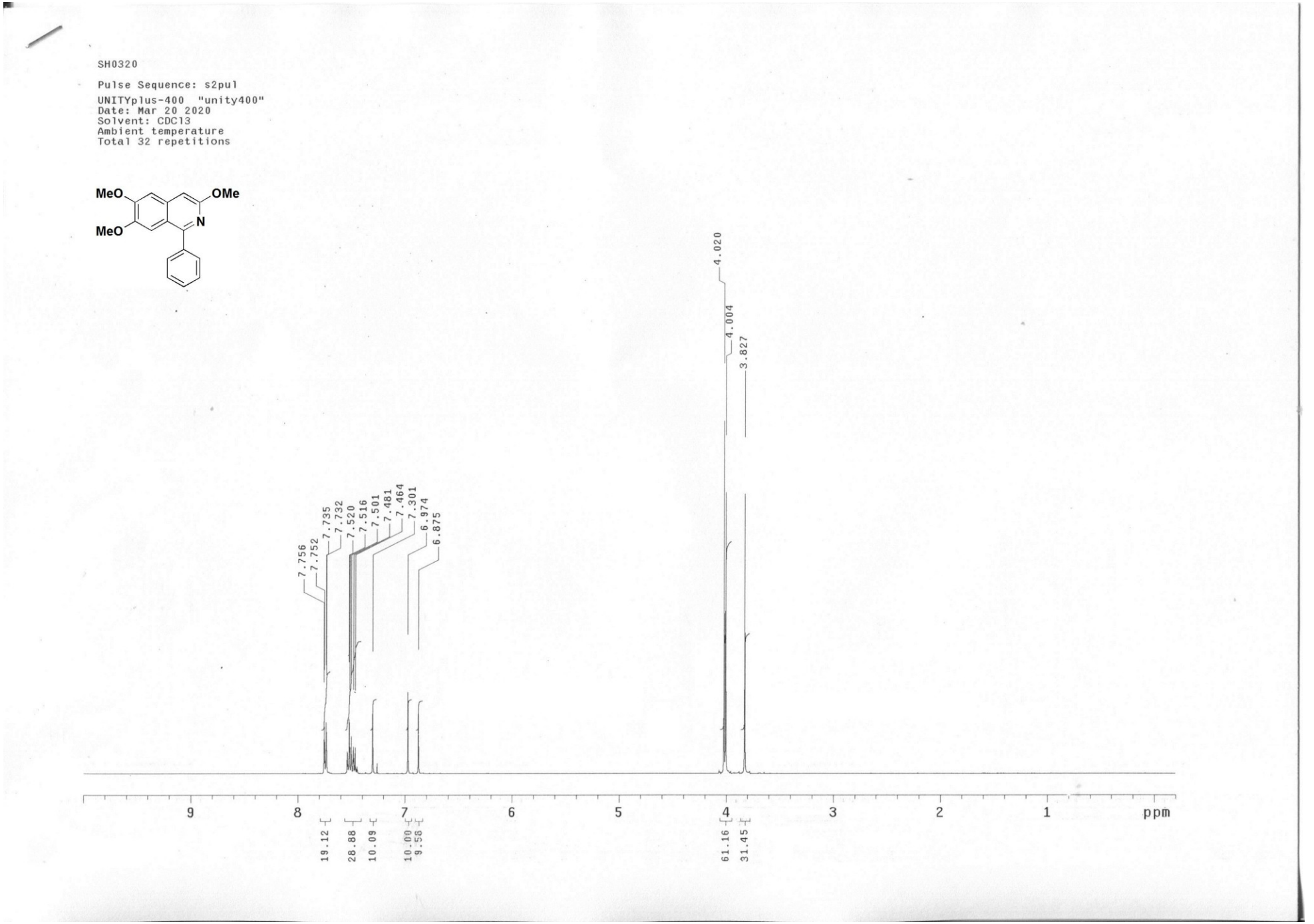
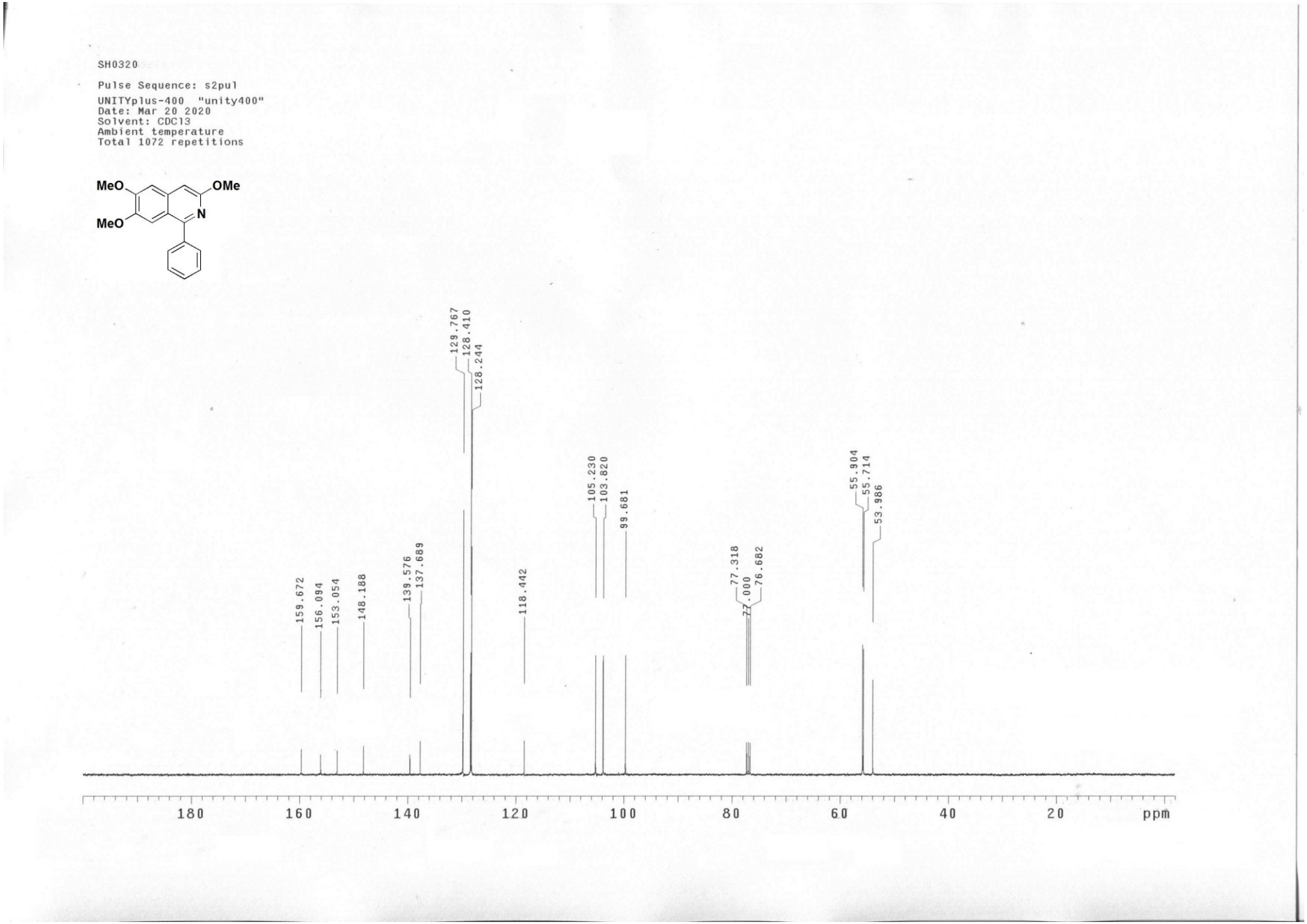
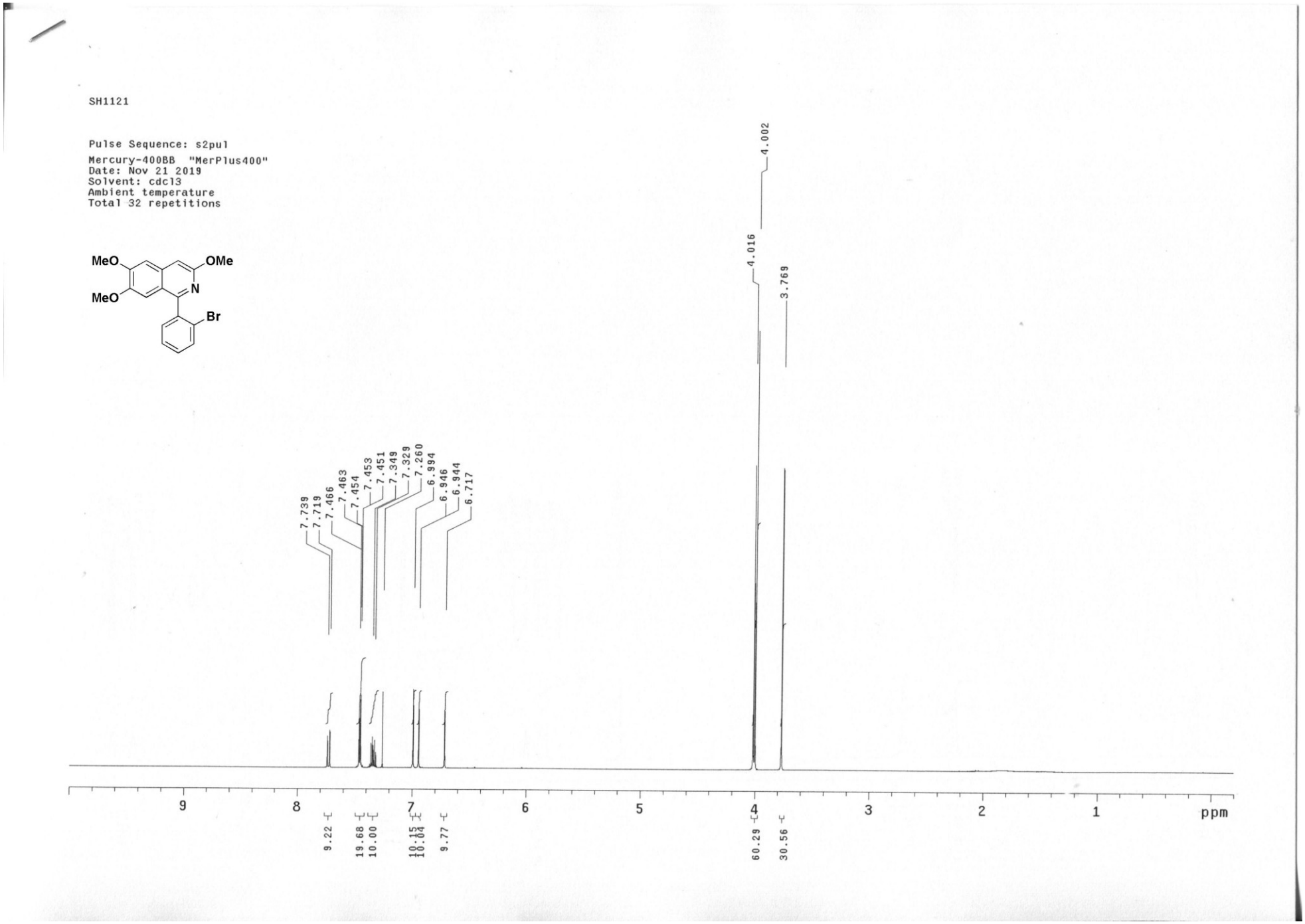
Compound 4a (^{1}H-NMR spectral data)



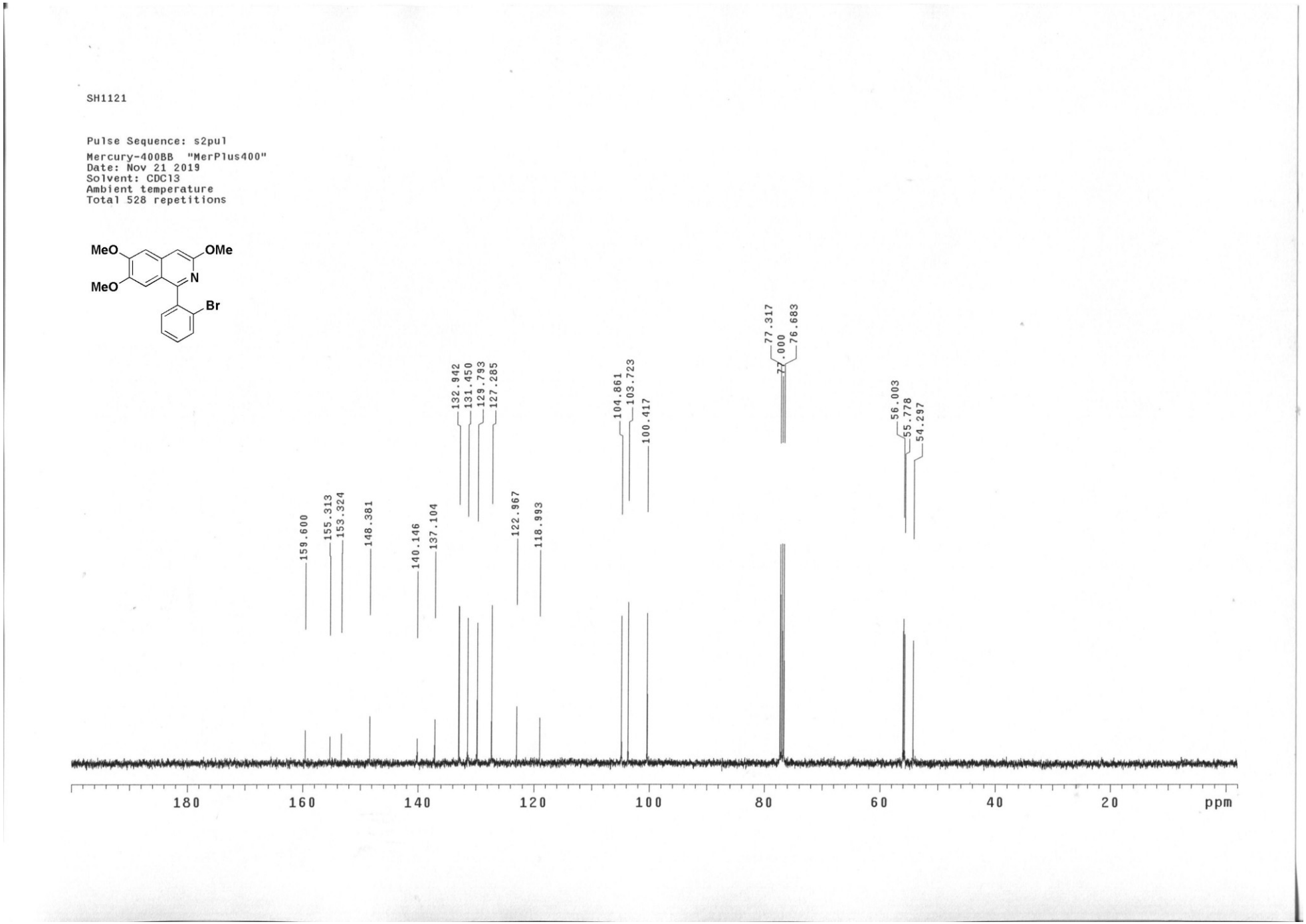
Compound 4a (^{13}C-NMR spectral data)



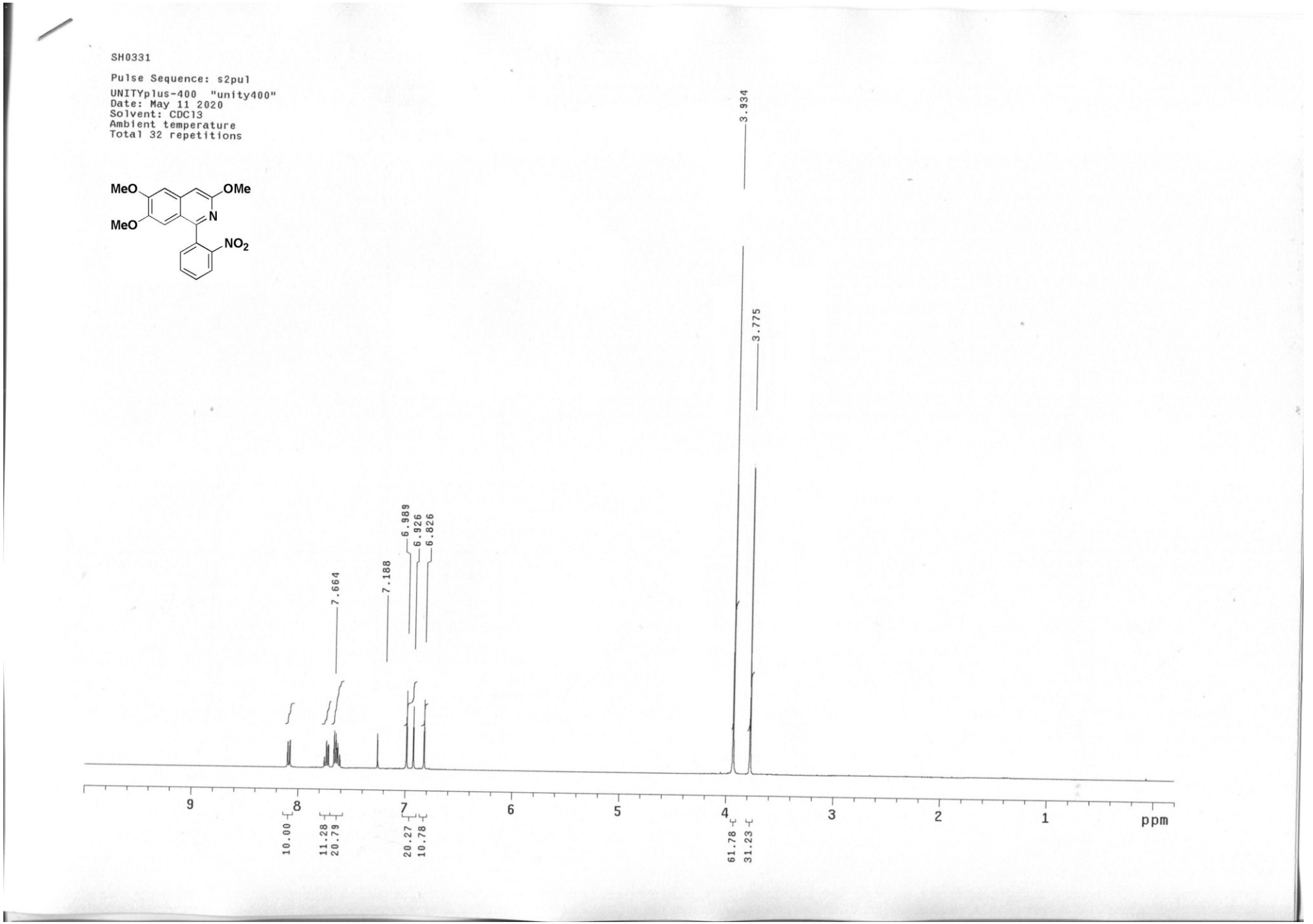
Compound 4b (^{1}H-NMR spectral data)



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



Compound 4c (^{1}H-NMR spectral data)

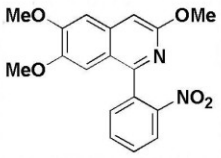


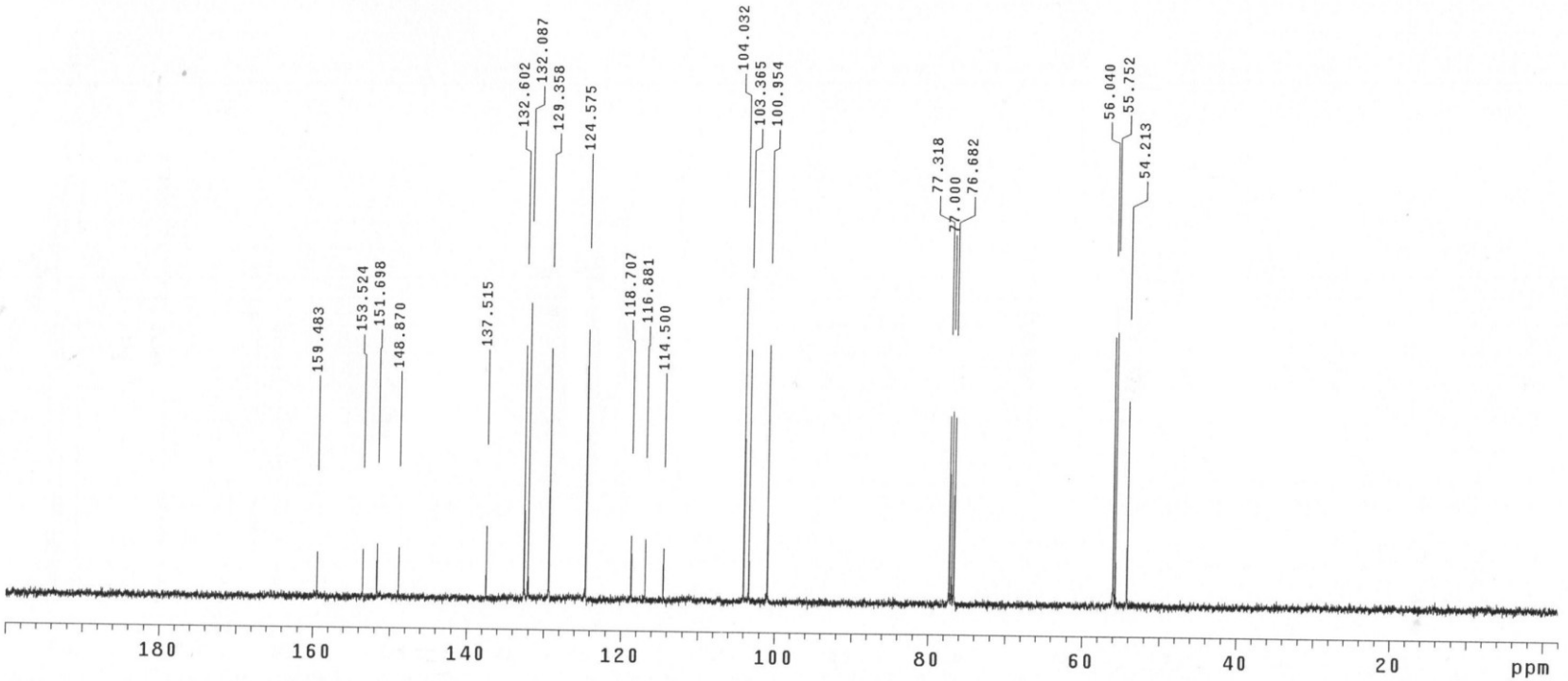
Compound 4c (^{13}C-NMR spectral data)

SH0331

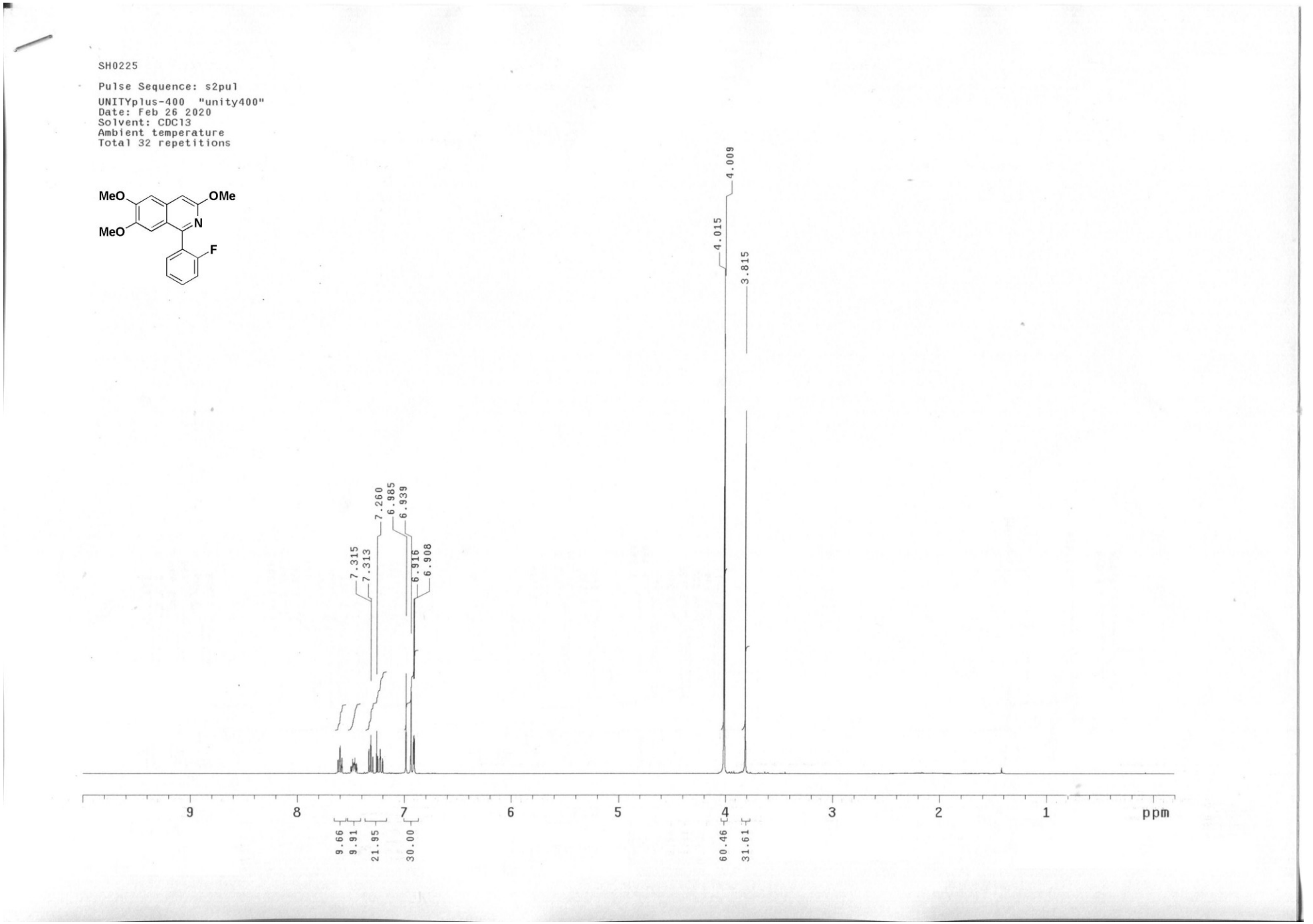
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 11 2020
Solvent: CDCl3
Ambient temperature
Total 3328 repetitions





Compound 4d (^{1}H-NMR spectral data)

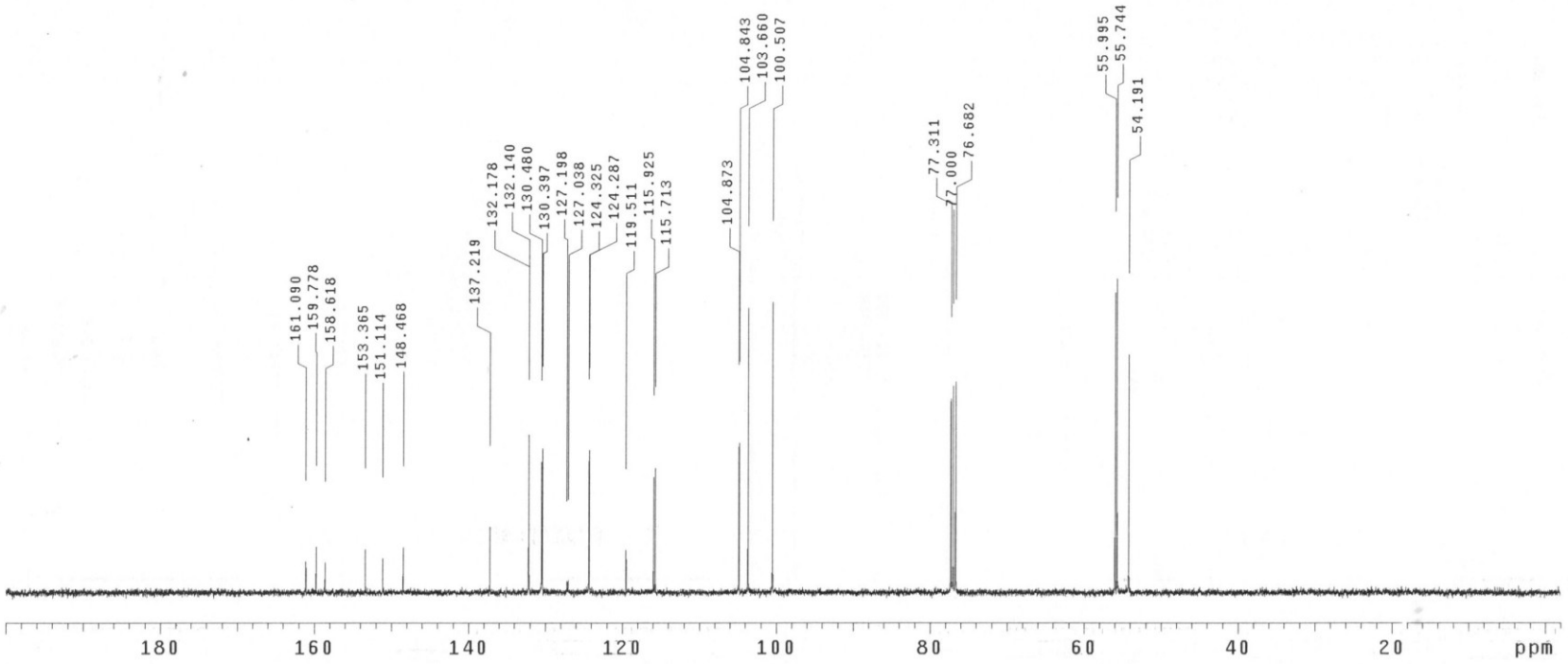


Compound 4d (^{13}C-NMR spectral data)

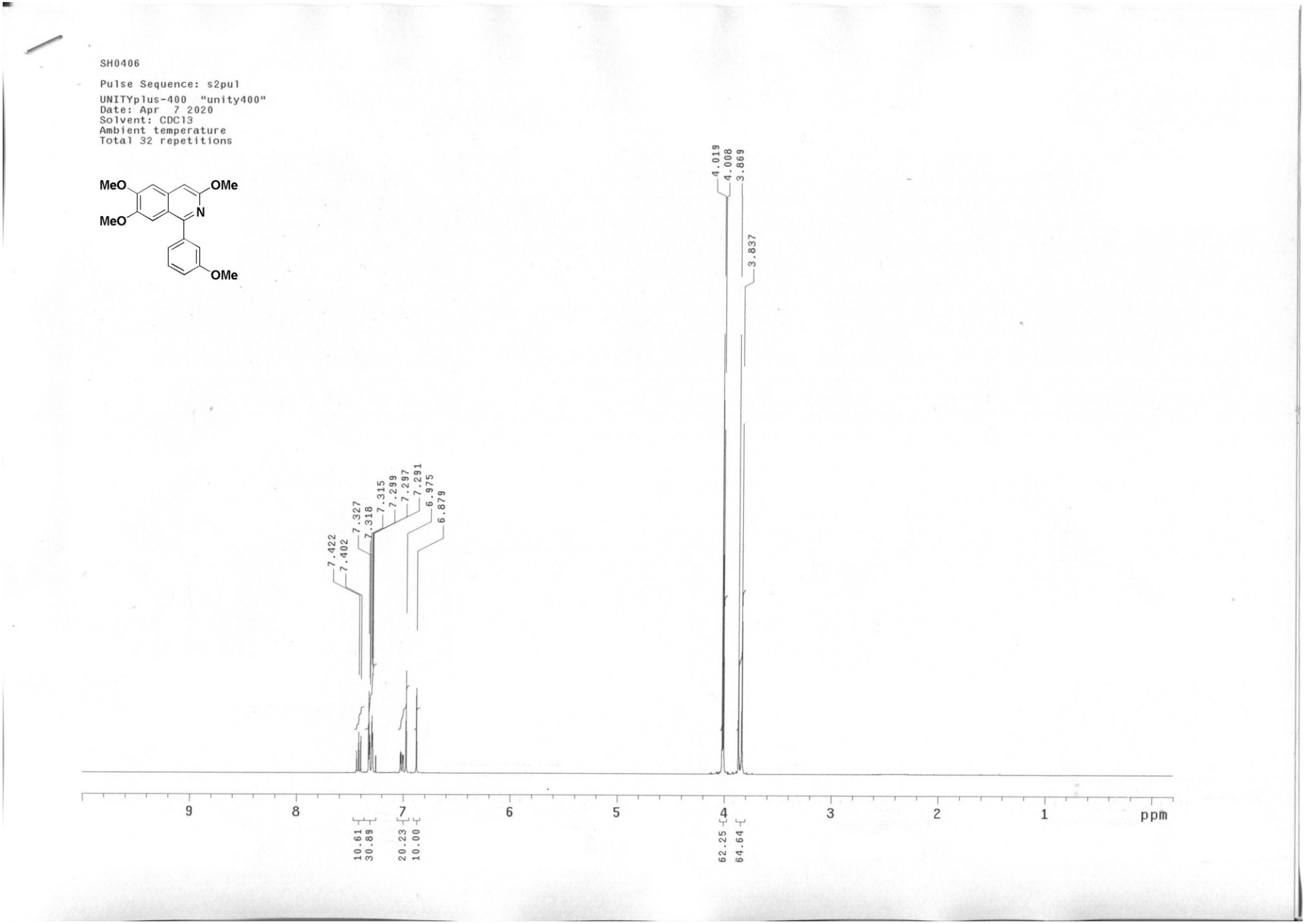
SH0225

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Feb 26 2020
Solvent: CDCl3
Ambient temperature
Total 3664 repetitions



Compound 4e (^{1}H-NMR spectral data)

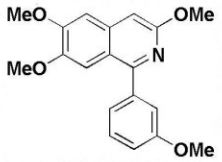


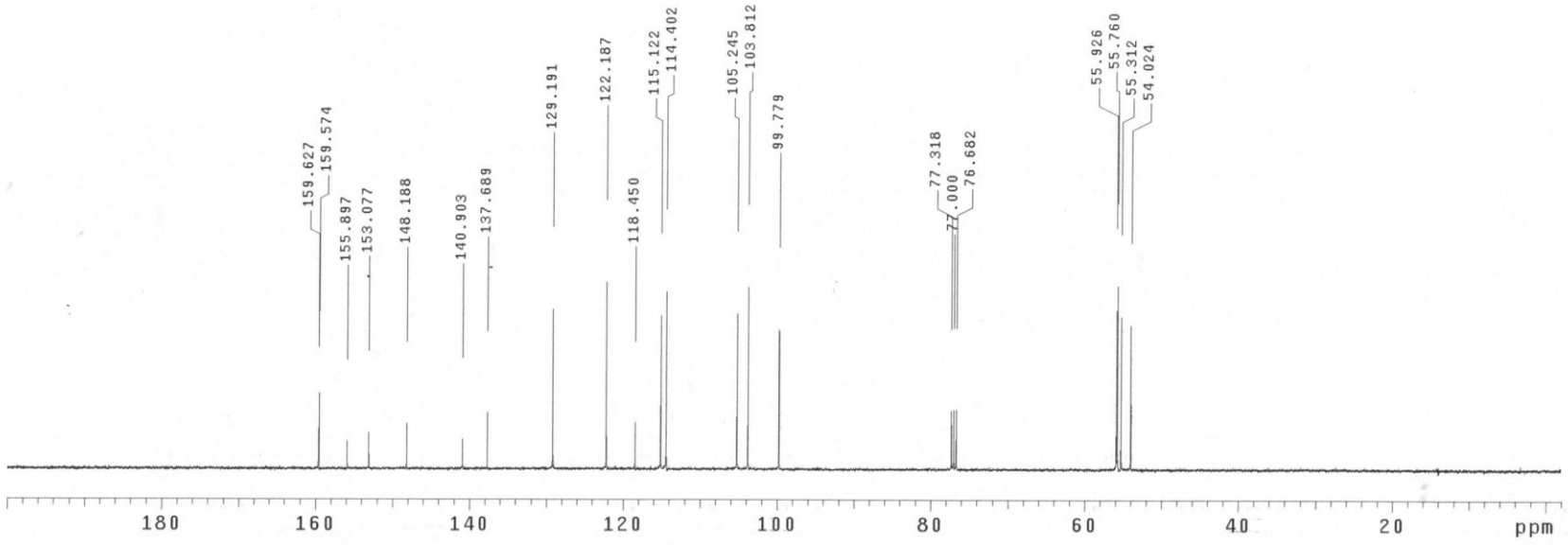
Compound 4e (^{13}C-NMR spectral data)

SH0406

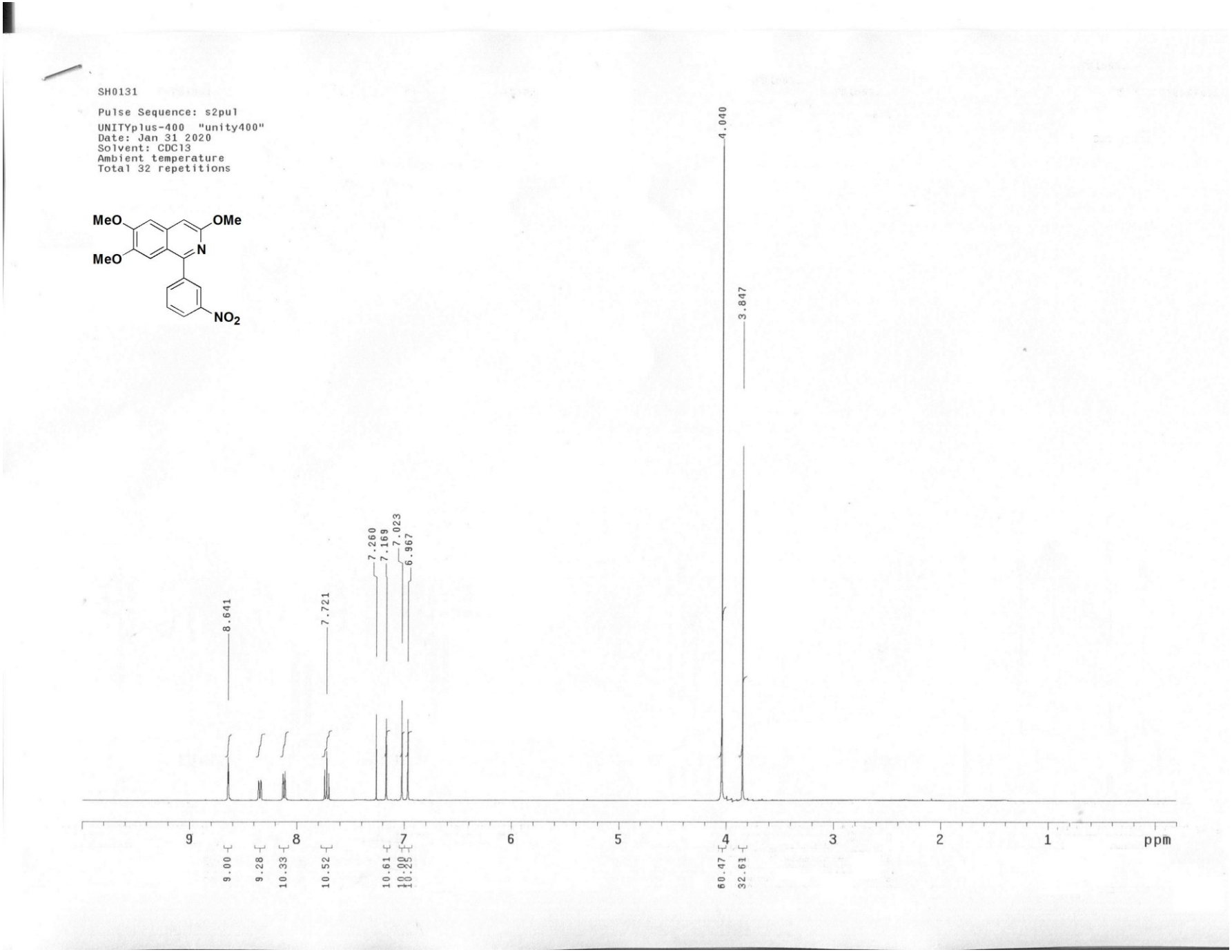
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Apr 7 2020
Solvent: CDCl3
Ambient temperature
Total 1568 repetitions

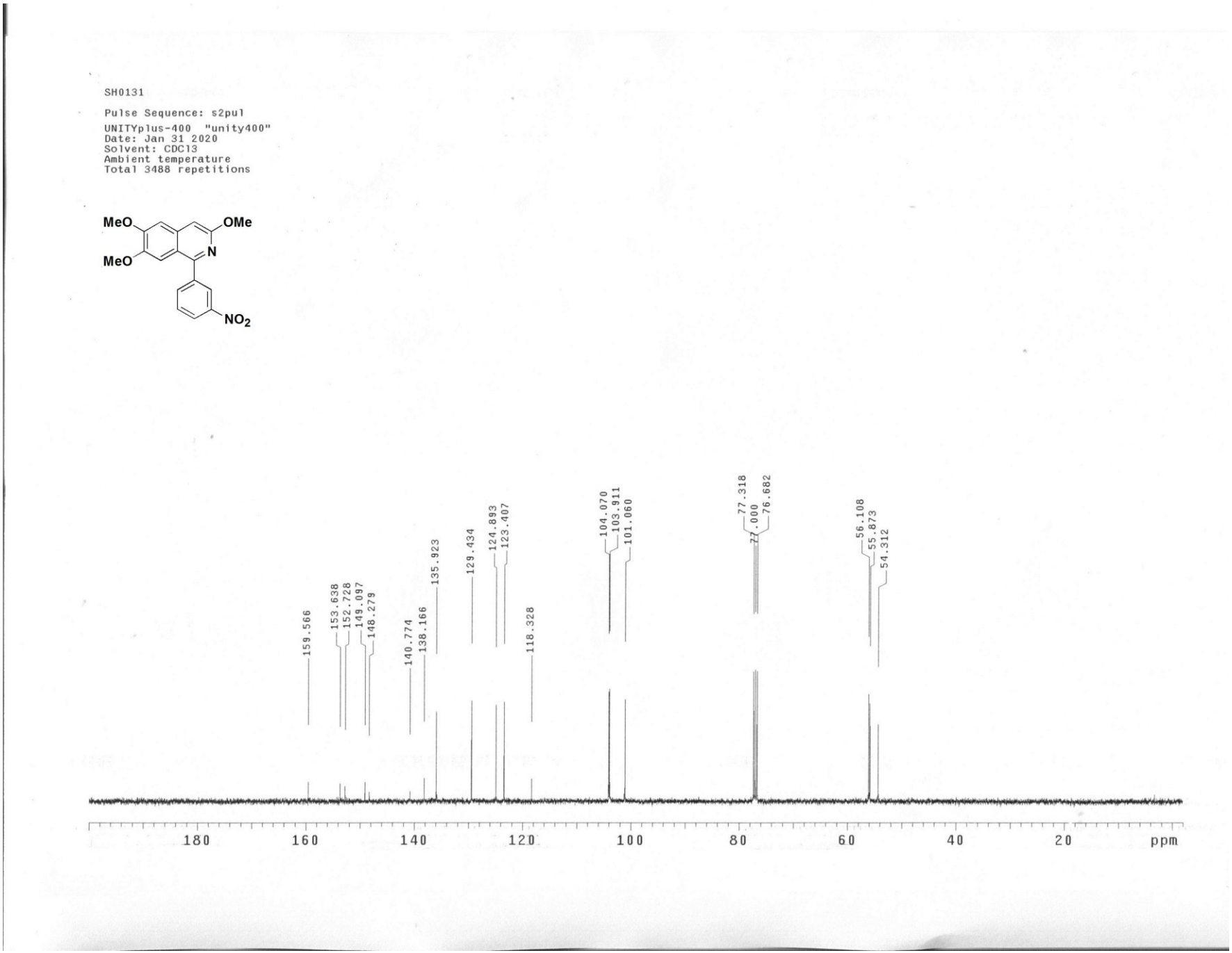




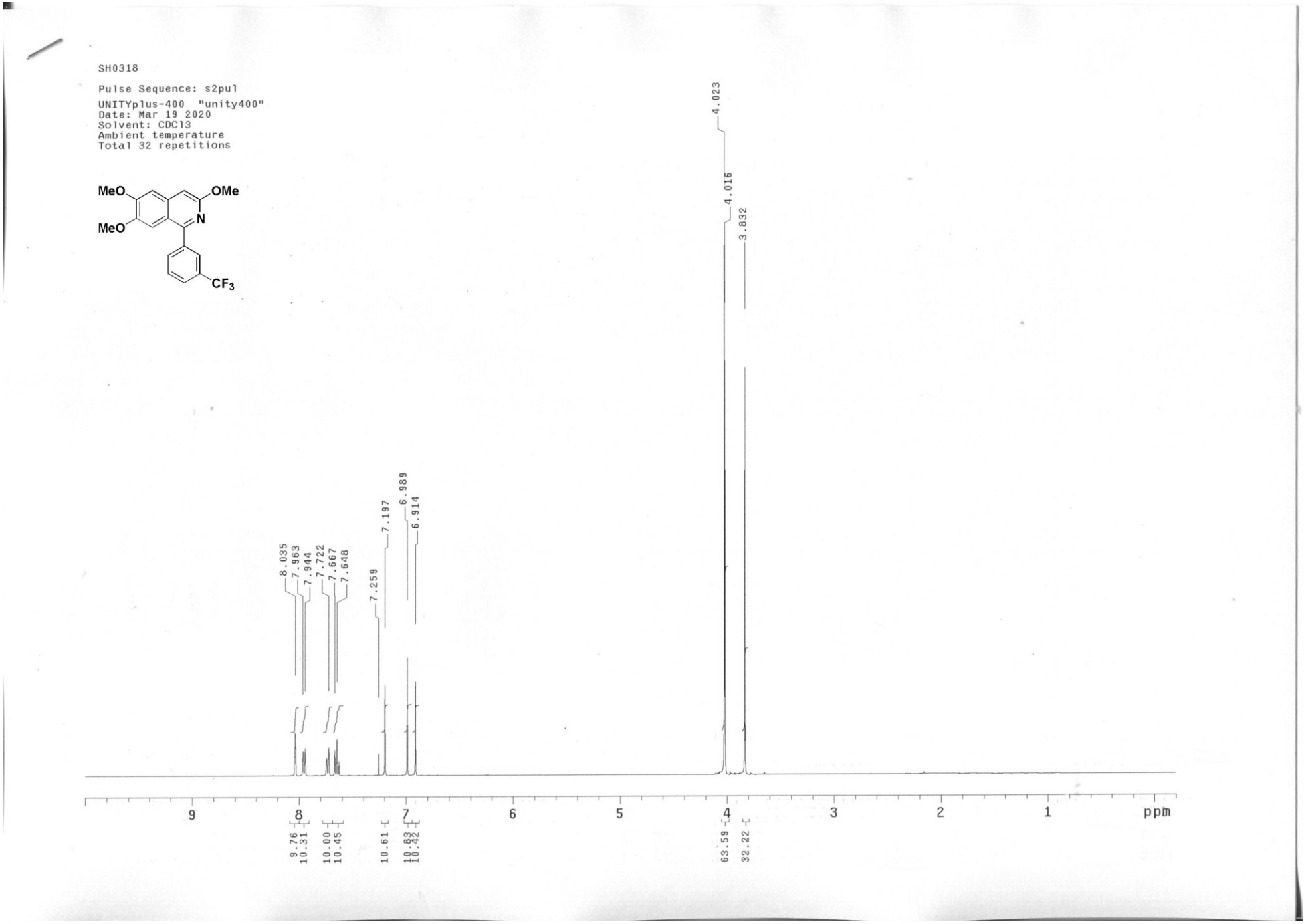
Compound 4f (^{1}H-NMR spectral data)



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



Compound 4g (^{1}H-NMR spectral data)

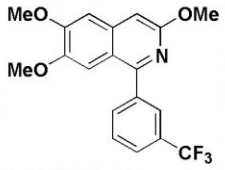


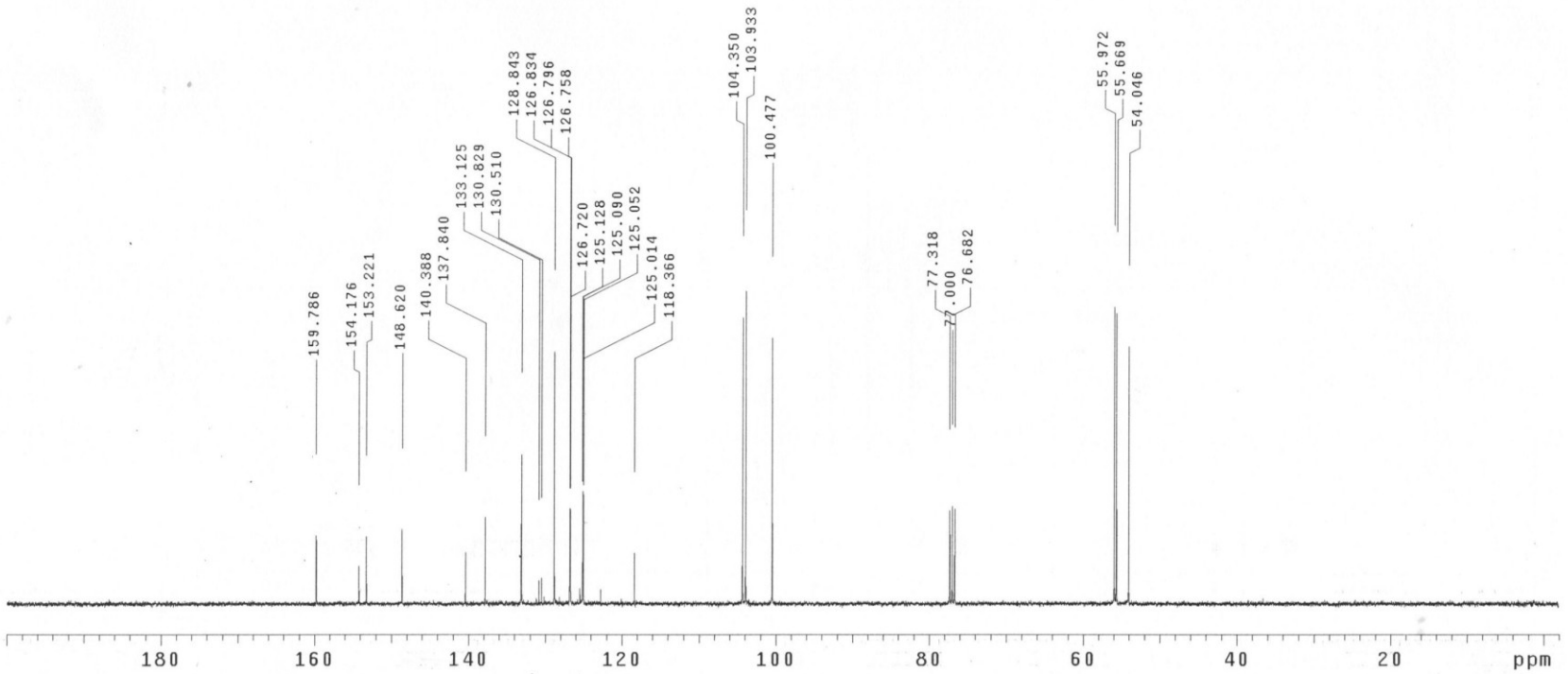
Compound 4g (^{13}C-NMR spectral data)

SH0318

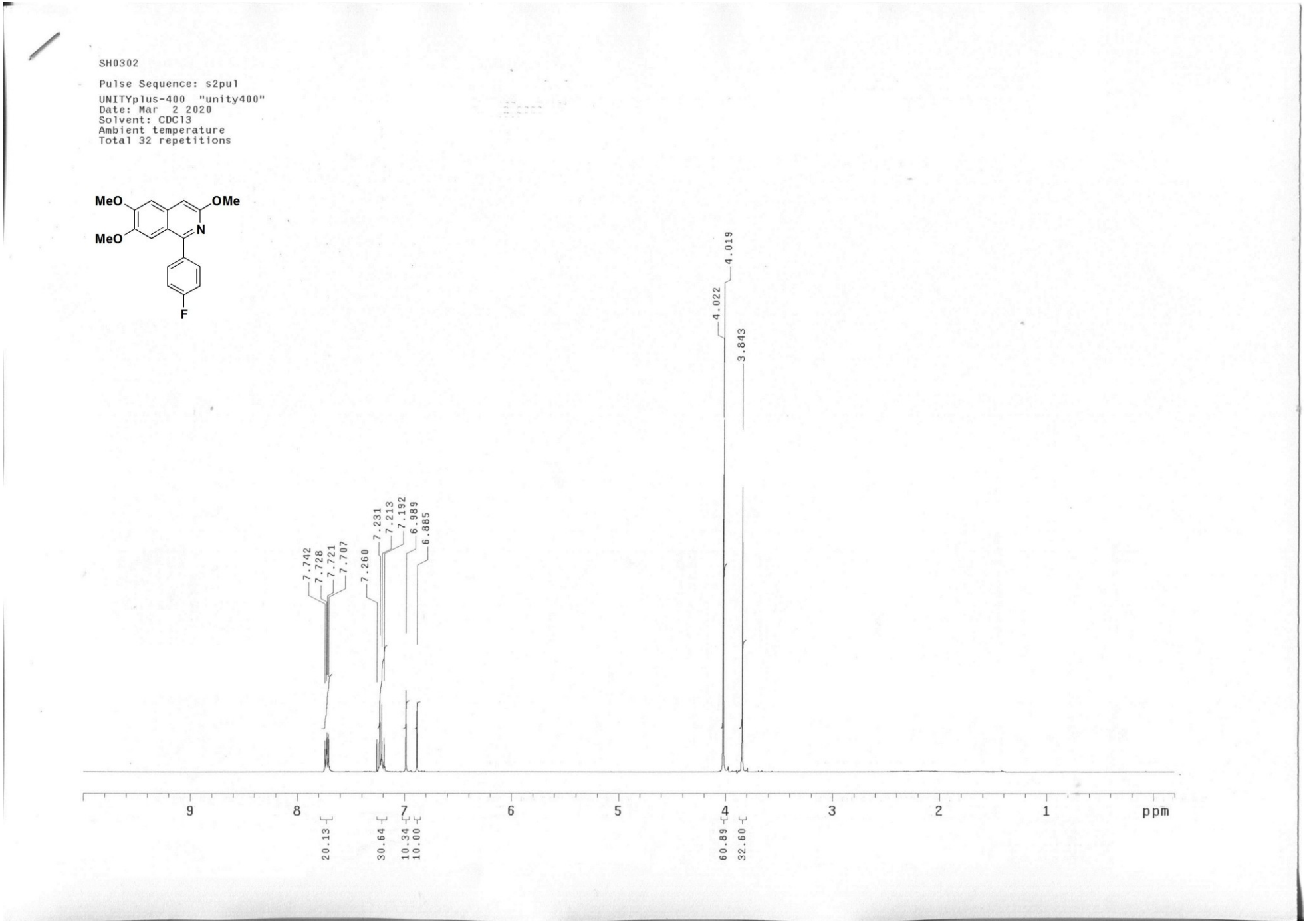
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Mar 19 2020
Solvent: CDCl3
Ambient temperature
Total 1792 repetitions





Compound 4h (^{1}H-NMR spectral data)

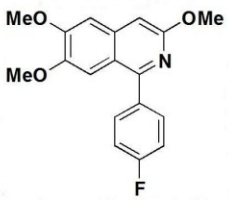


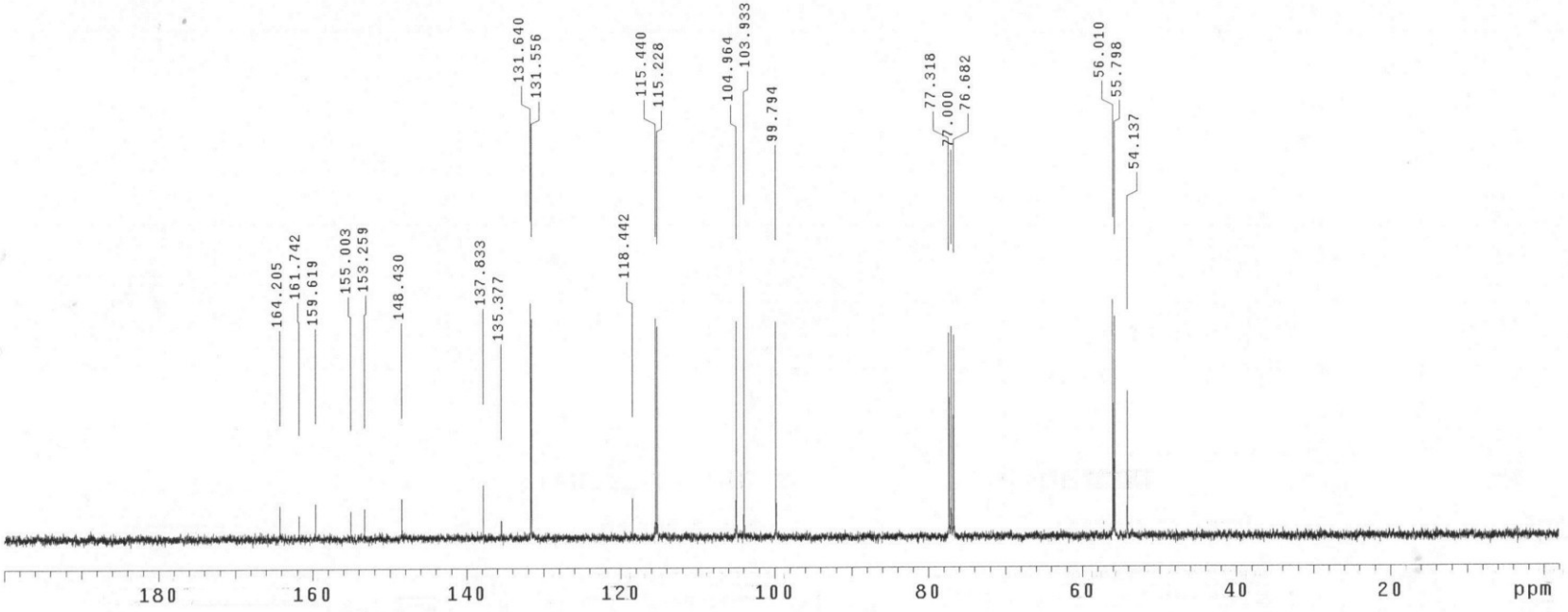
Compound 4h (^{13}C-NMR spectral data)

SH0302

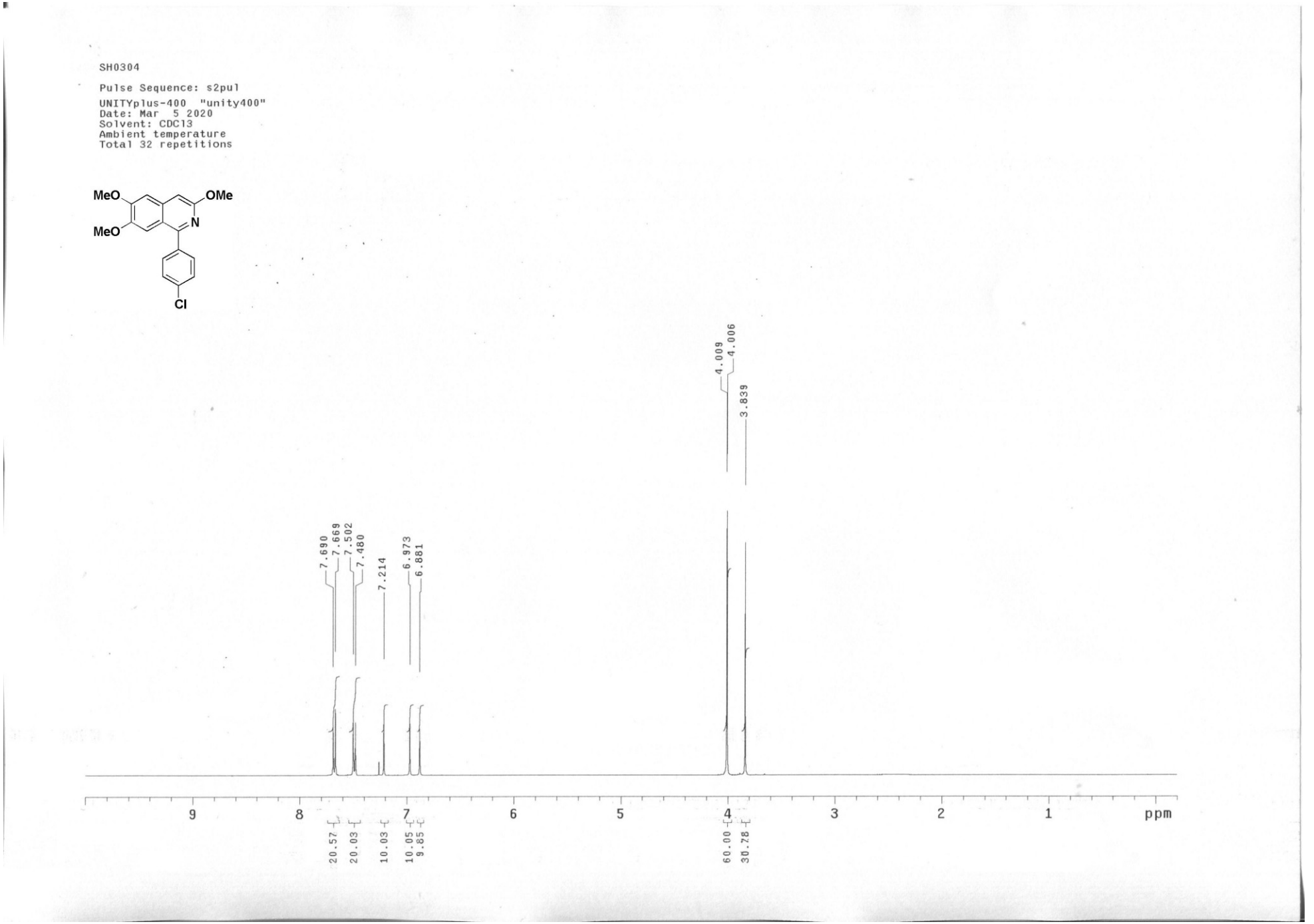
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Mar 2 2020
Solvent: CDCl3
Ambient temperature
Total 2080 repetitions





Compound 4i (^{1}H-NMR spectral data)

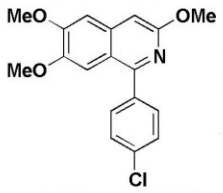


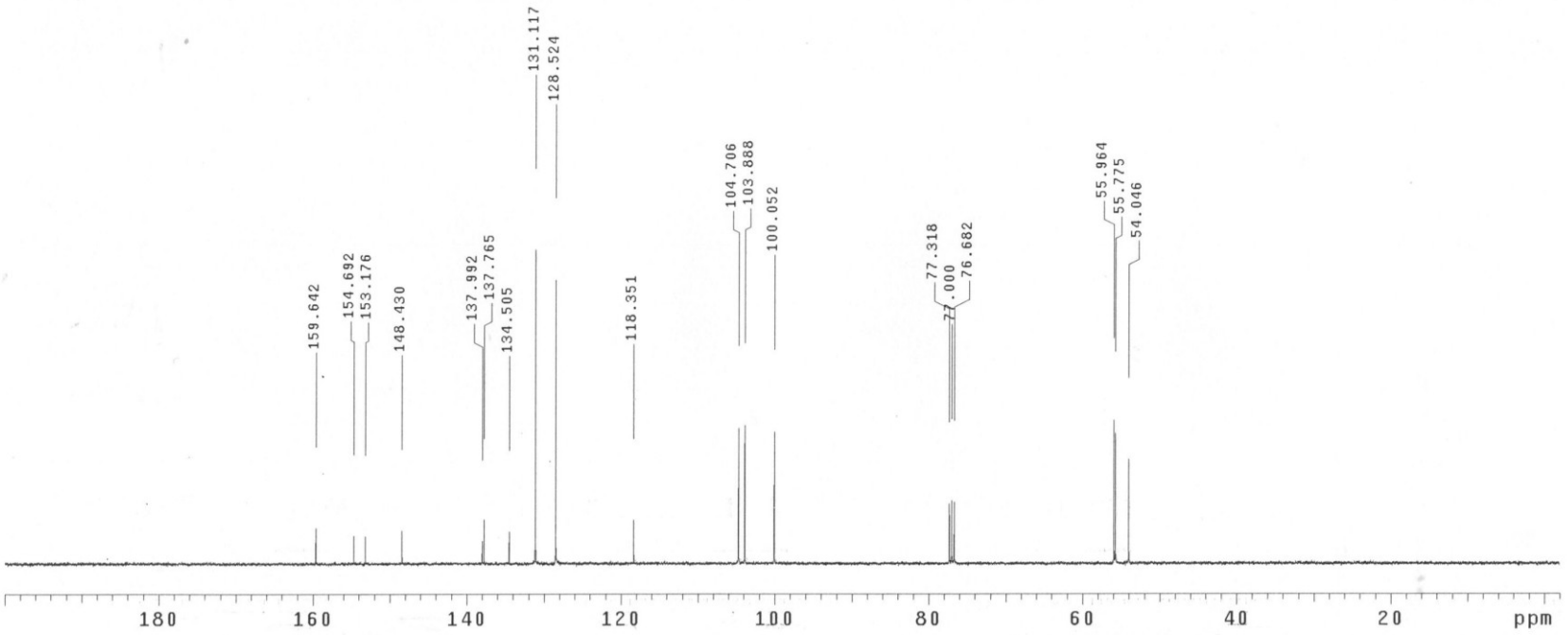
Compound 4i (^{13}C-NMR spectral data)

SH0304

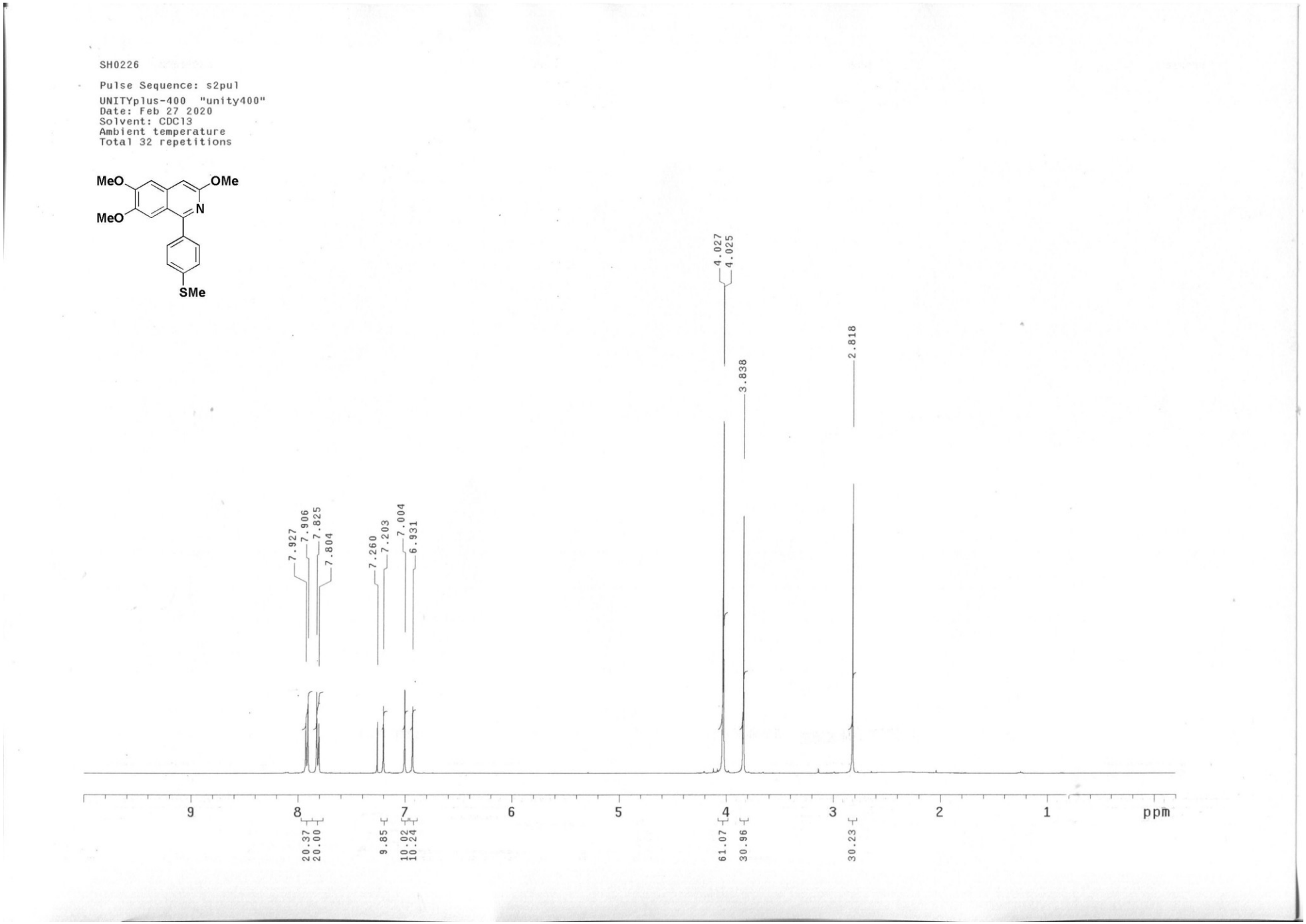
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Mar 5 2020
Solvent: CDCl3
Ambient temperature
Total 1200 repetitions





Compound 4j (^{1}H-NMR spectral data)

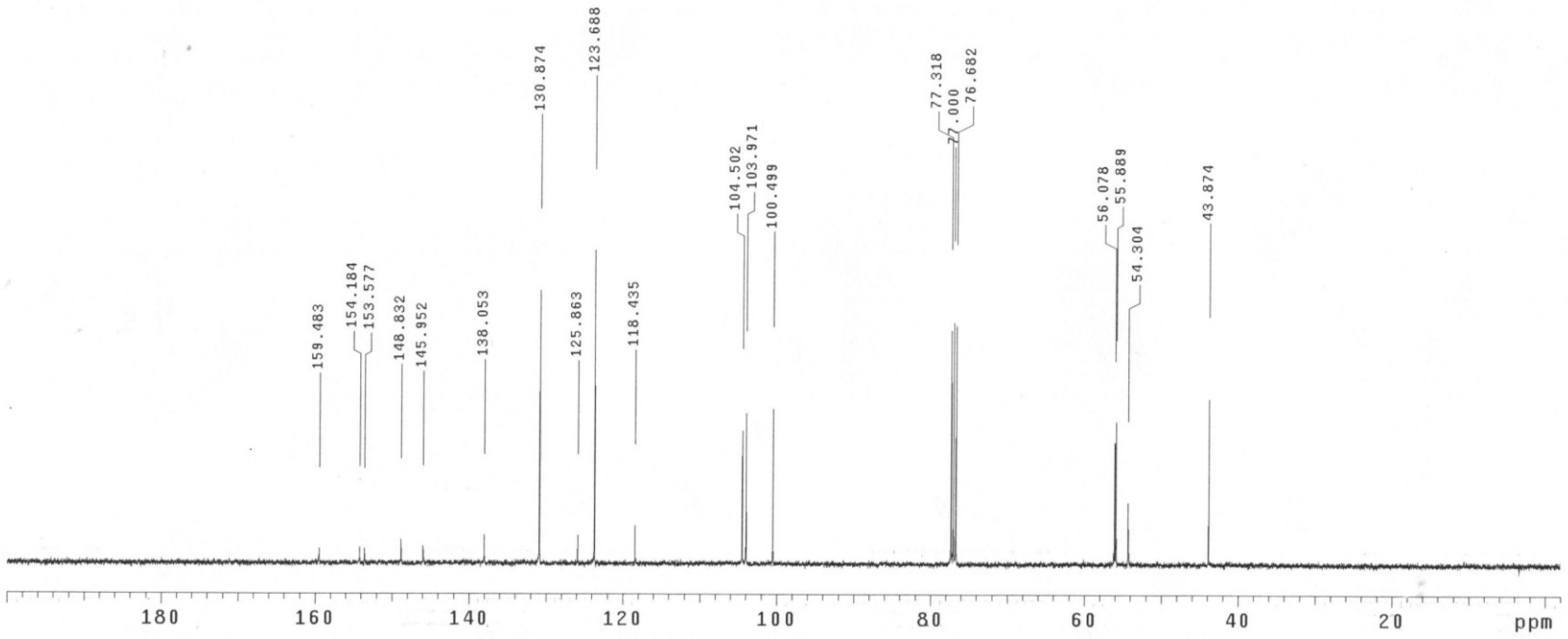


Compound 4j (^{13}C-NMR spectral data)

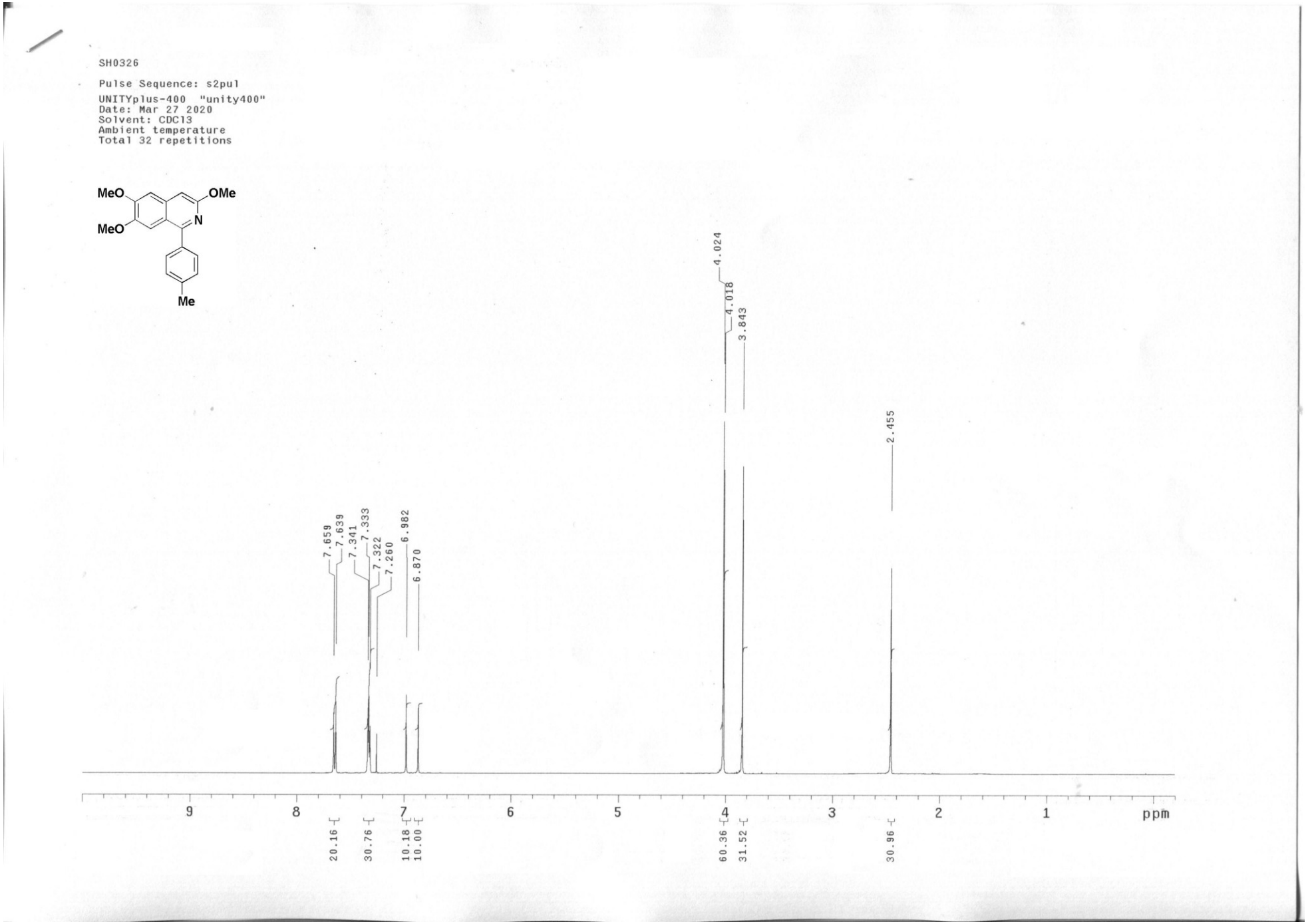
SH0226

Pulse Sequence: s2pul

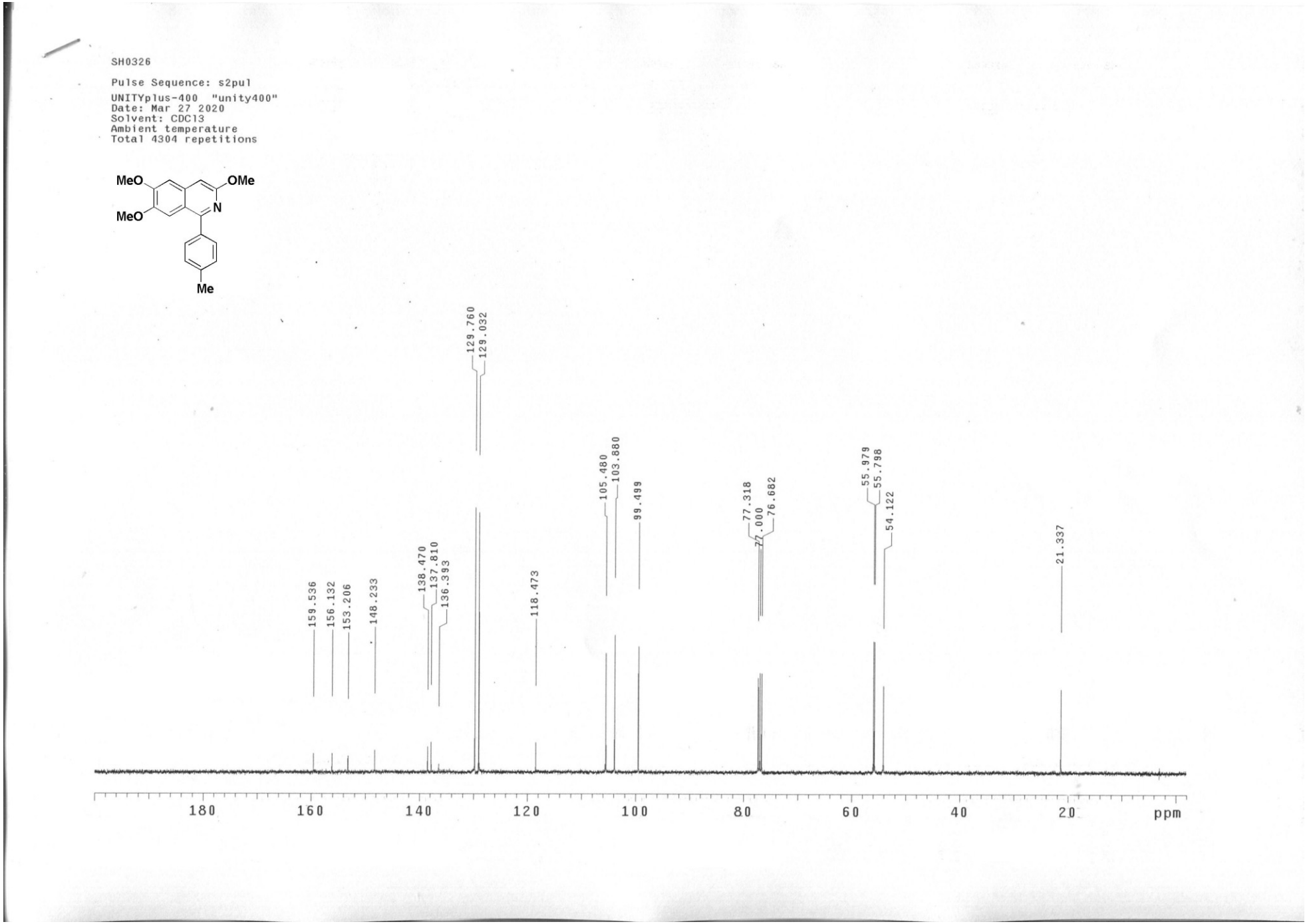
UNITYplus-400 "unity400"
Date: Feb 27 2020
Solvent: CDCl3
Ambient temperature
Total 8016 repetitions



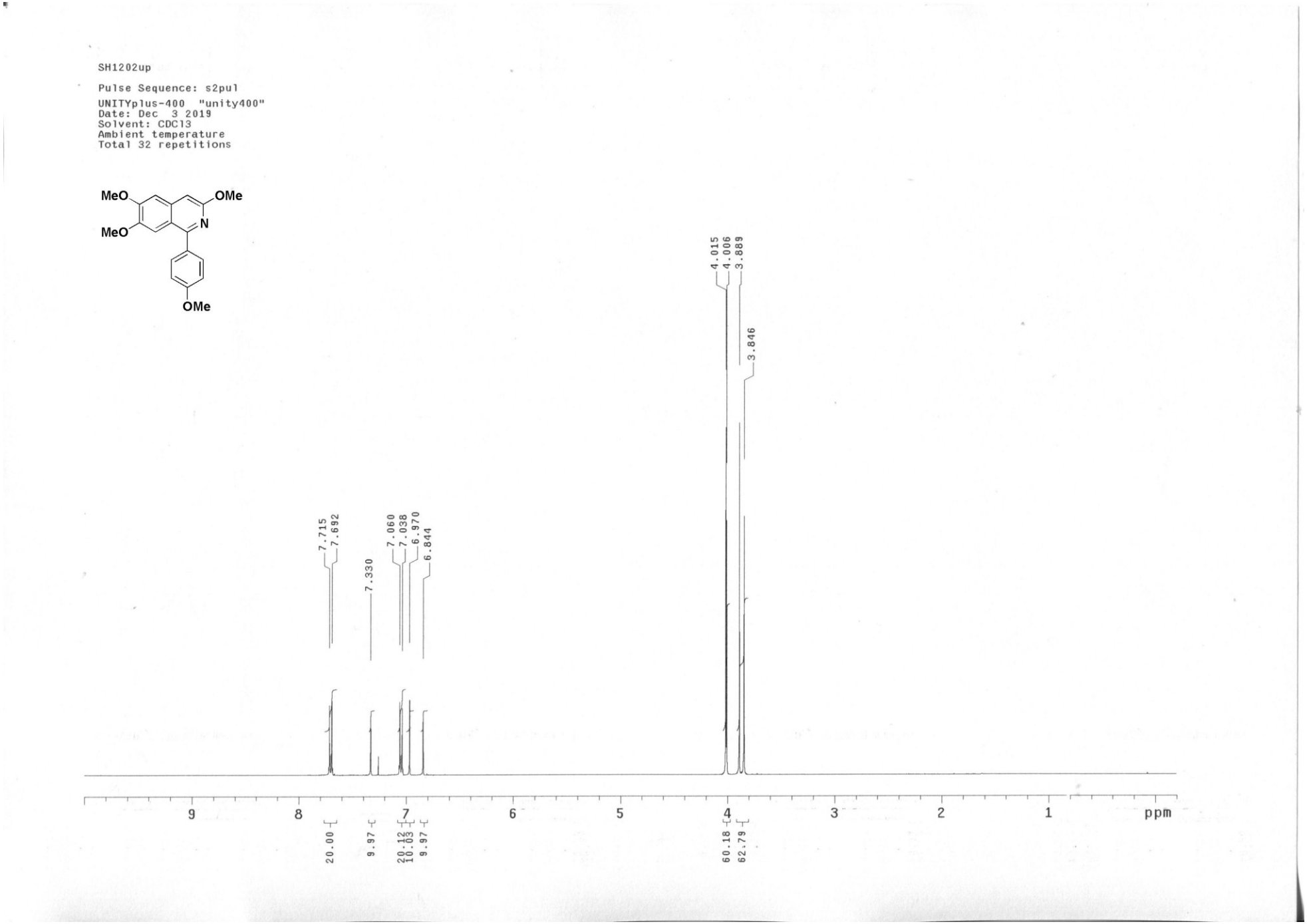
Compound 4k (^{1}H-NMR spectral data)



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



Compound 4l (^{1}H-NMR spectral data)

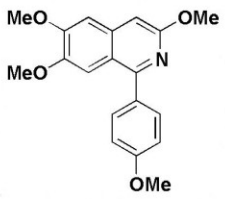


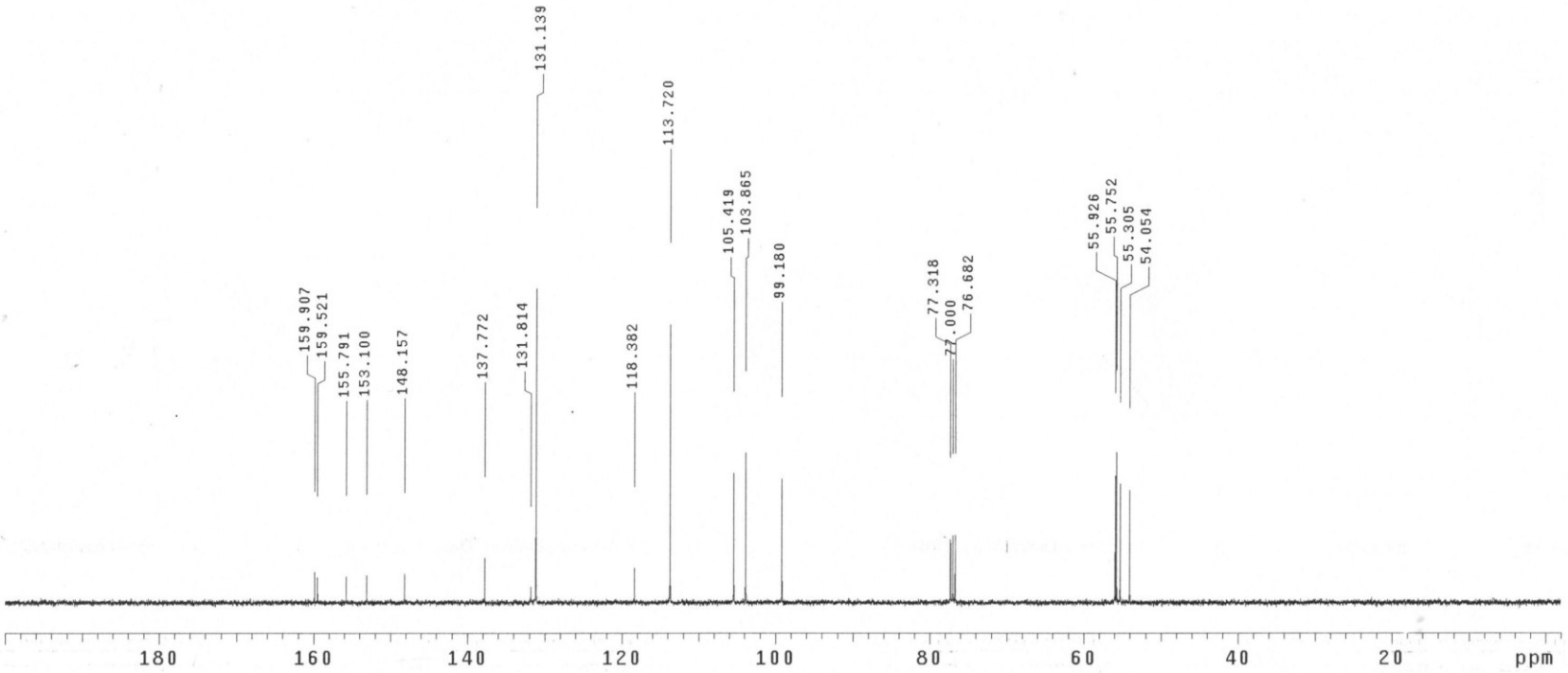
Compound 4l (^{13}C-NMR spectral data)

SH1202up

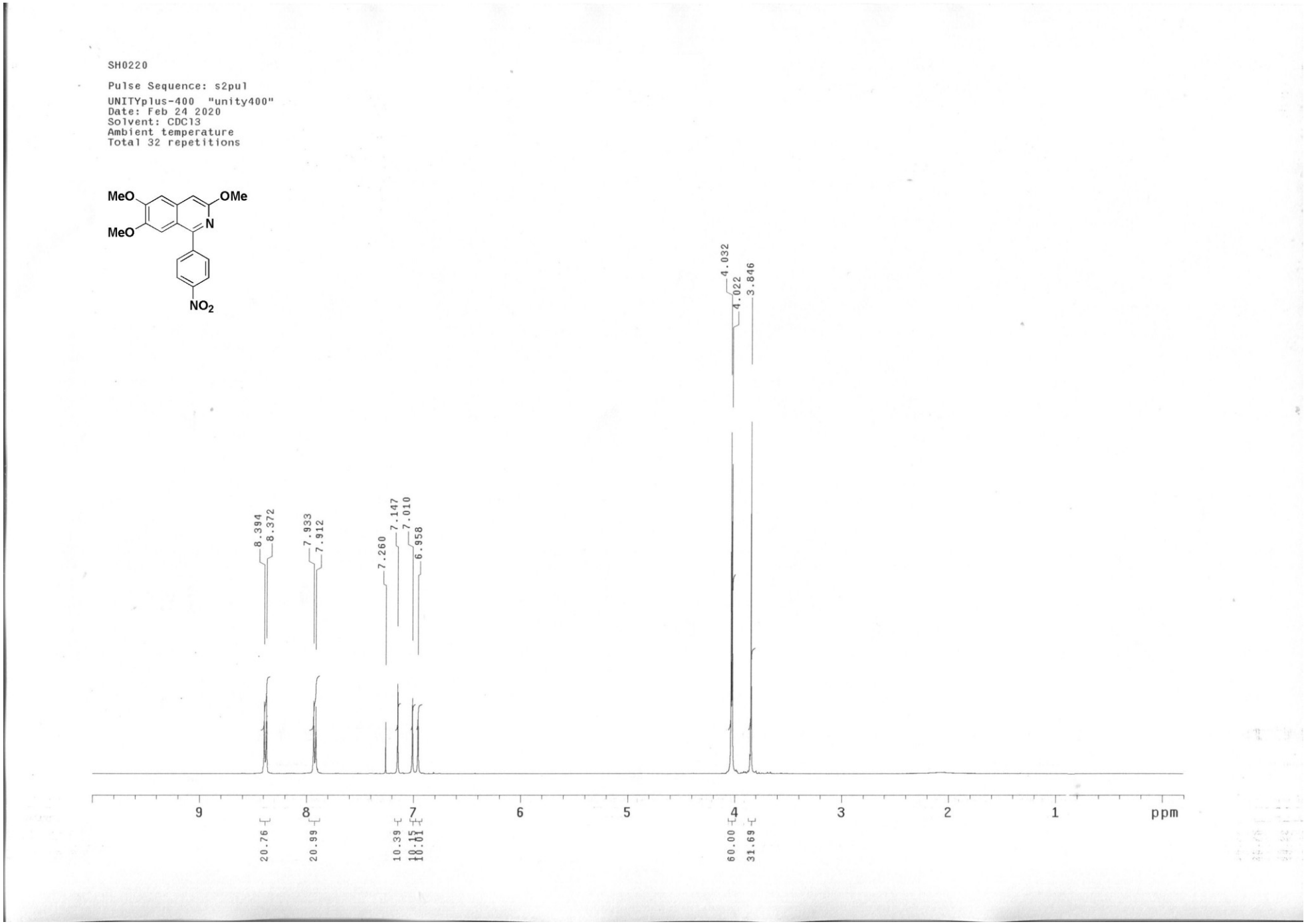
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Dec 3 2019
Solvent: CDCl3
Ambient temperature
Total 512 repetitions





Compound 4m (^{1}H-NMR spectral data)

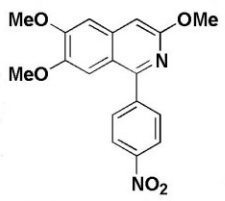


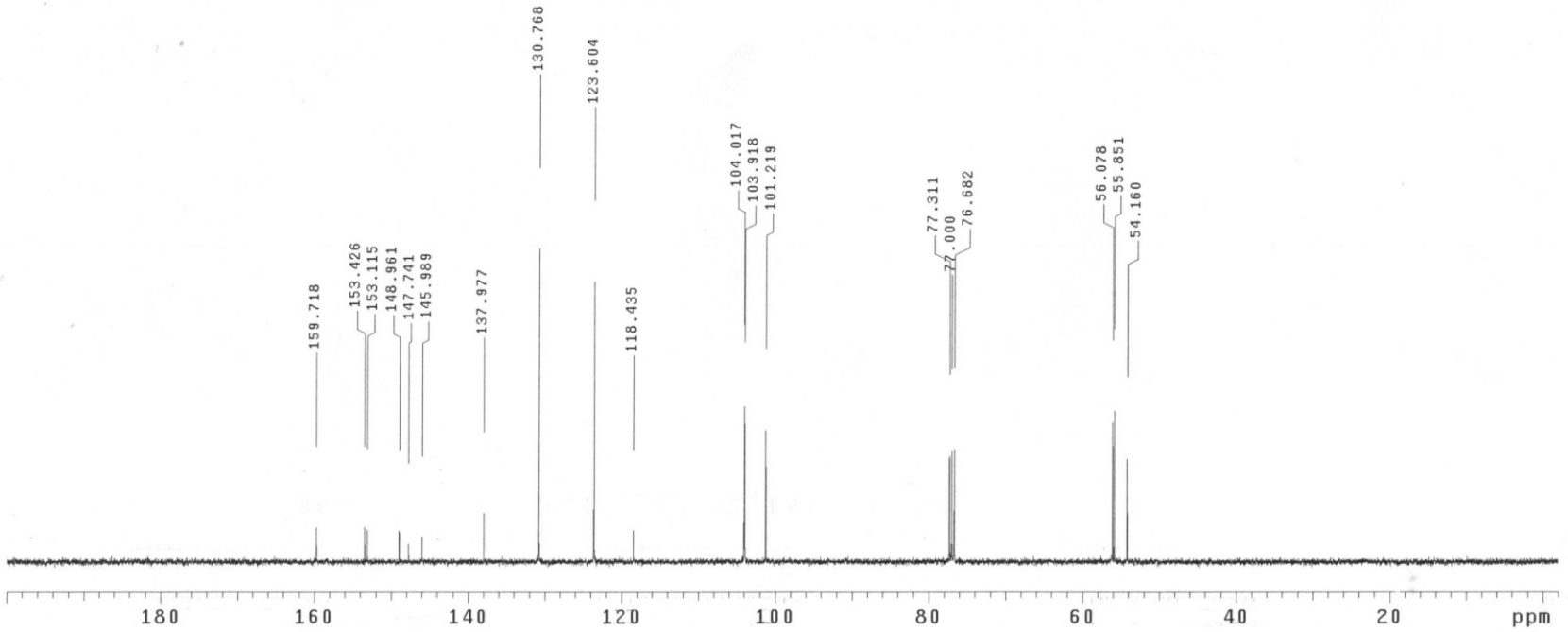
Compound 4m (^{13}C-NMR spectral data)

SH0220

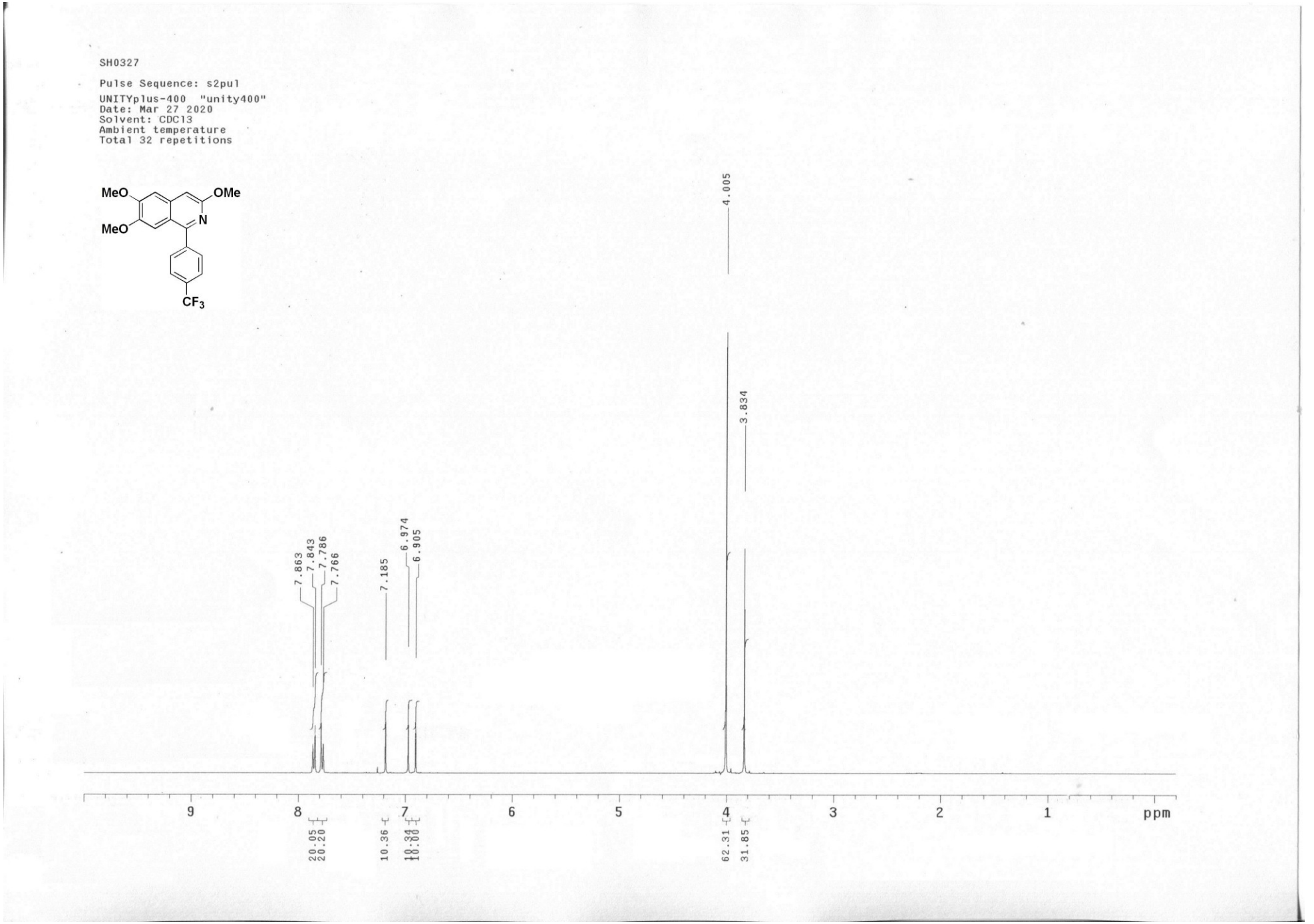
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Feb 24 2020
Solvent: CDCl3
Ambient temperature
Total 2272 repetitions





Compound 4n (^{1}H-NMR spectral data)

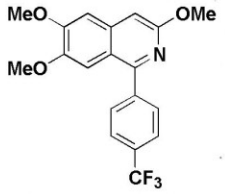


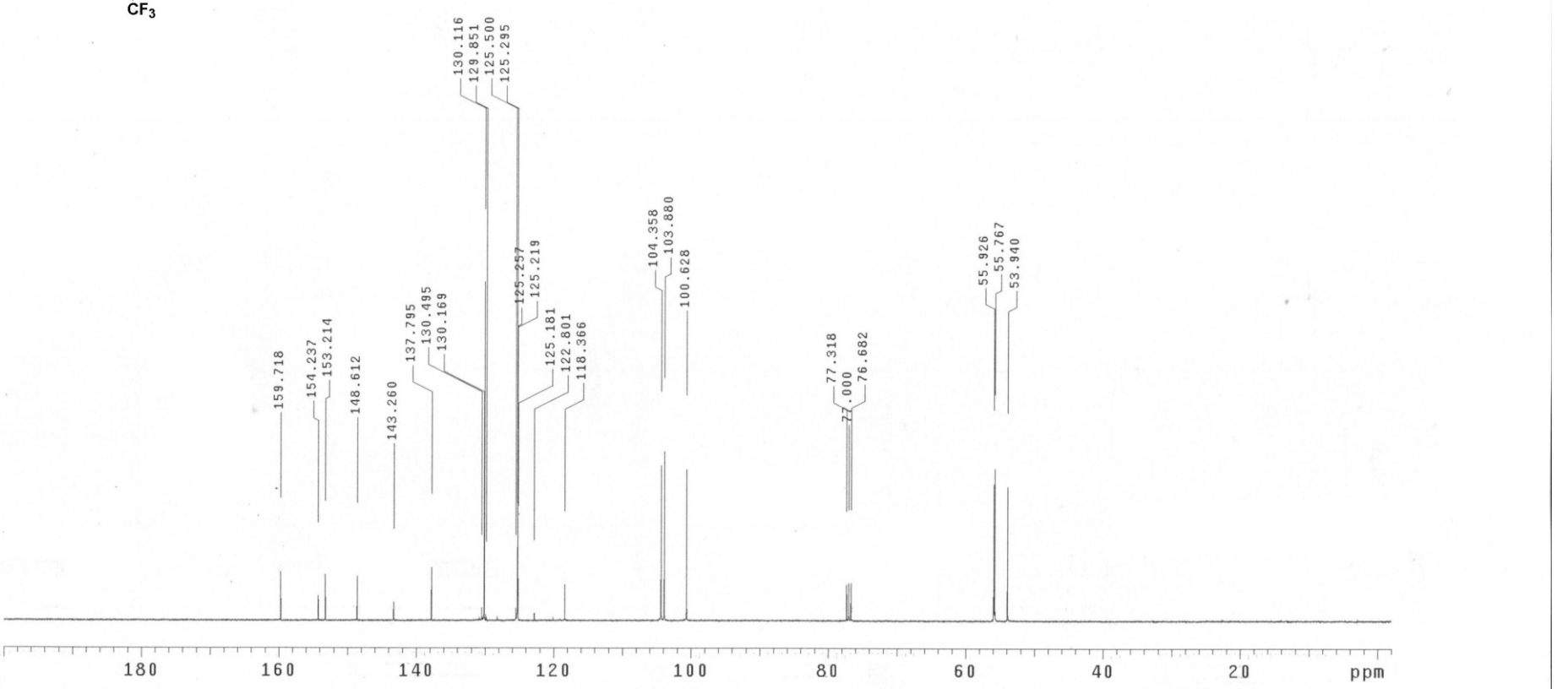
Compound 4n (^{13}C-NMR spectral data)

SH0327

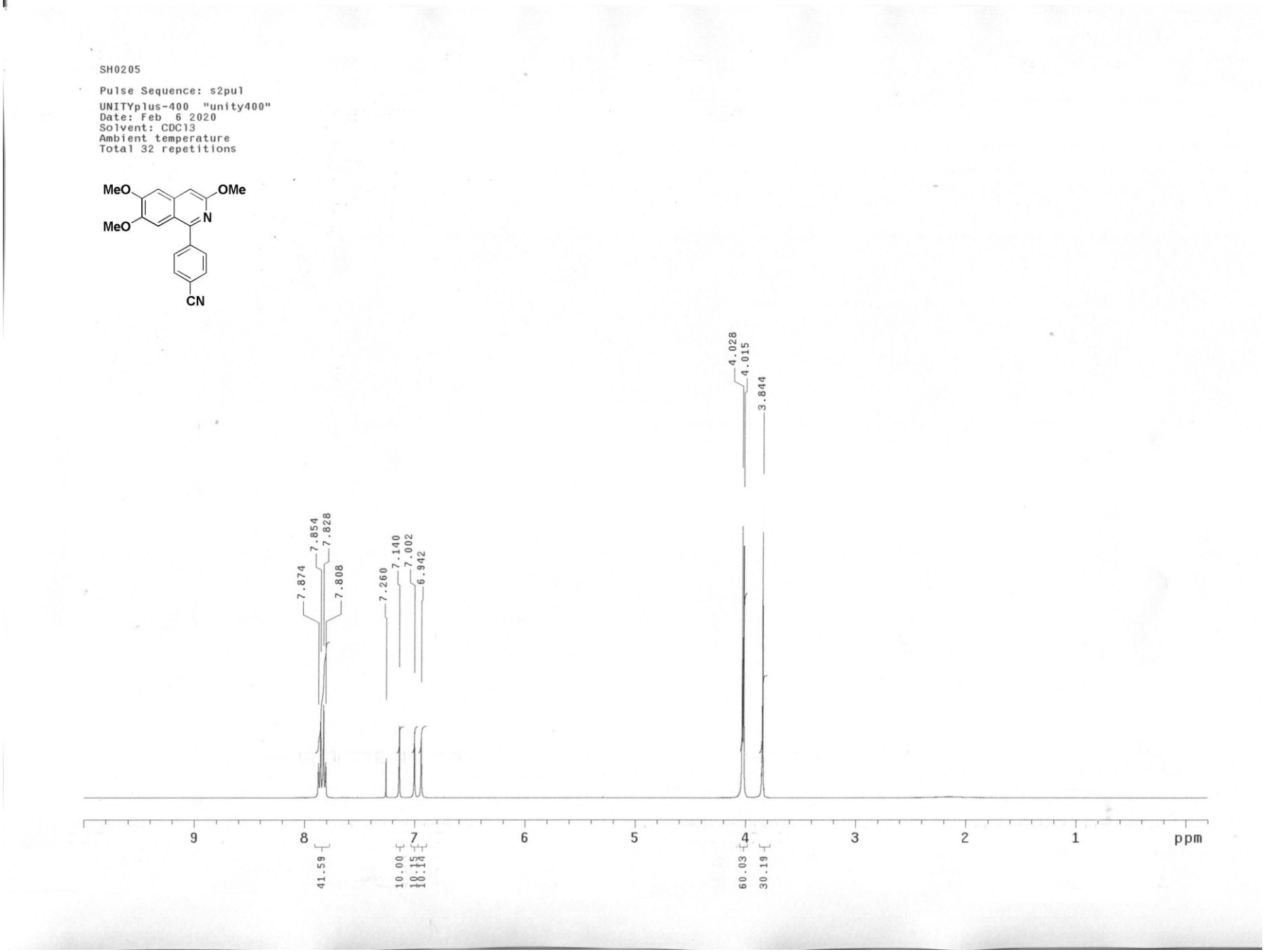
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Mar 27 2020
Solvent: CDCl3
Ambient temperature
Total 2704 repetitions

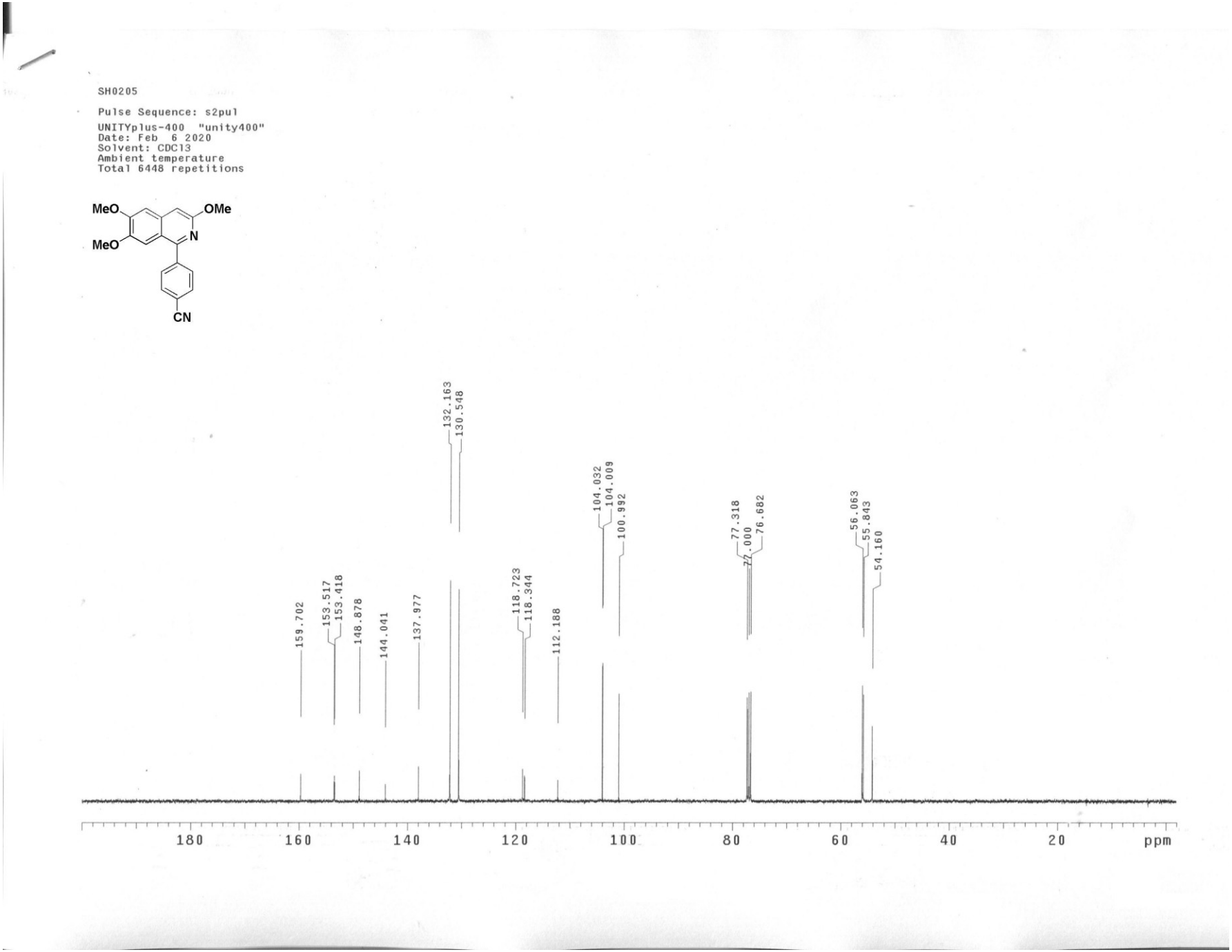




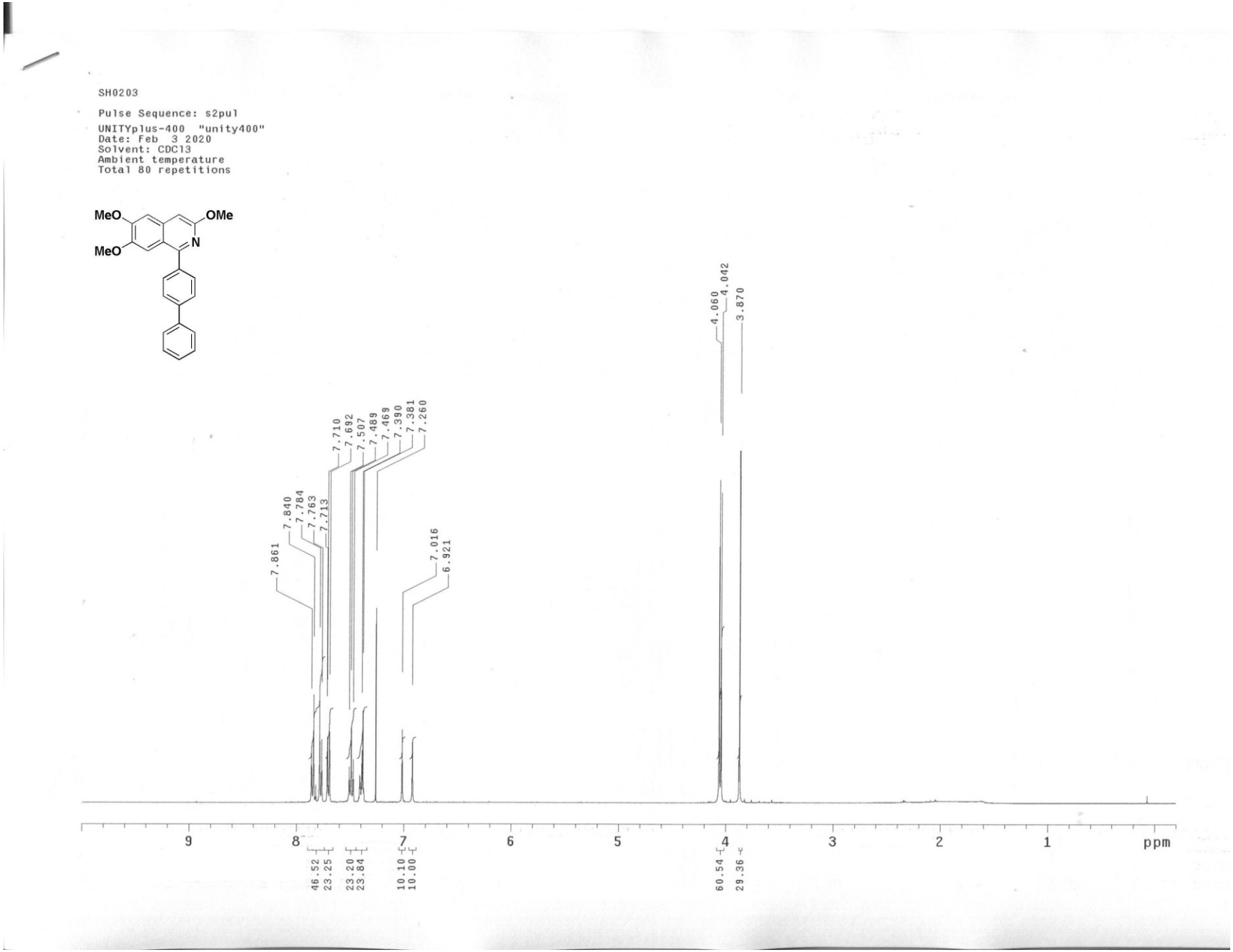
Compound 4o (^{1}H-NMR spectral data)



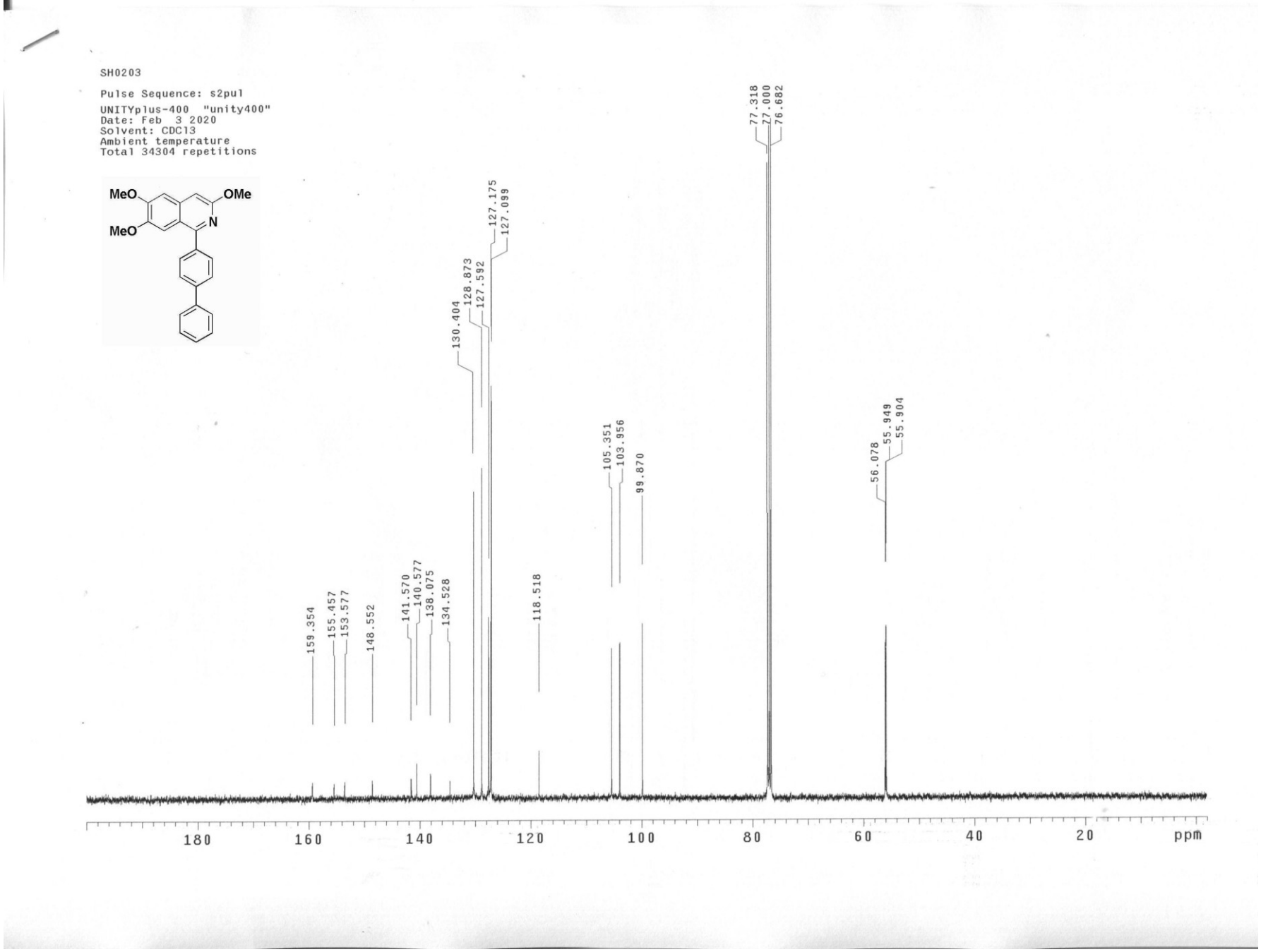
Compound 4o (^{13}C-NMR spectral data)



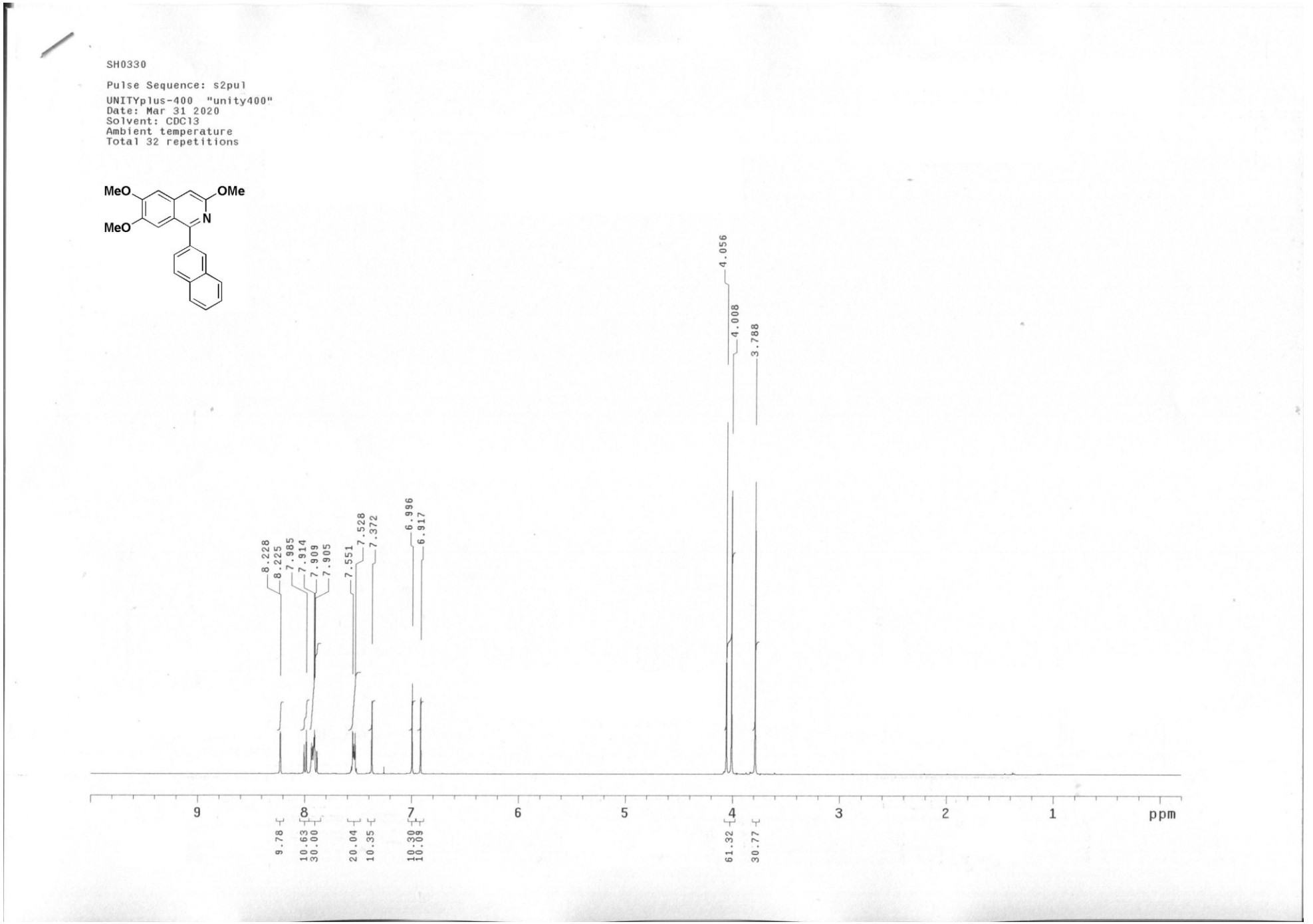
Compound 4p (^{1}H-NMR spectral data)



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



Compound 4q (^{1}H-NMR spectral data)

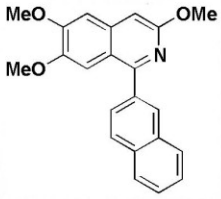


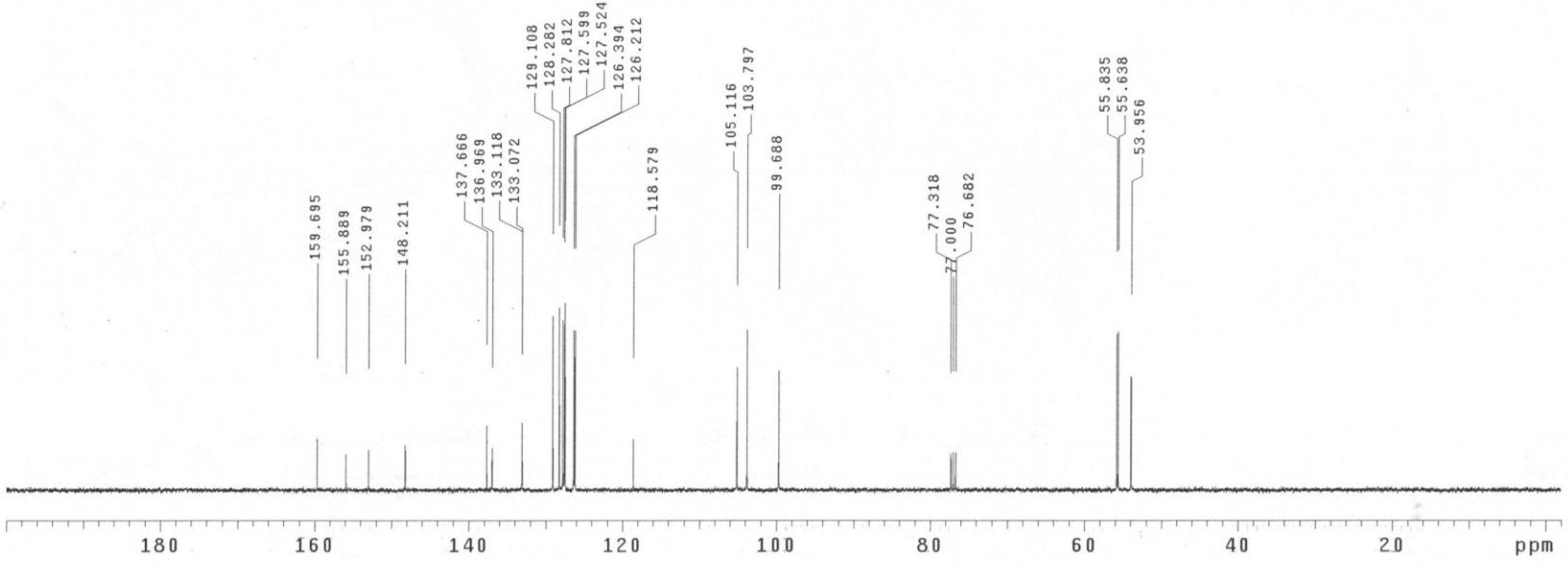
Compound 4q (^{13}C-NMR spectral data)

SH0330

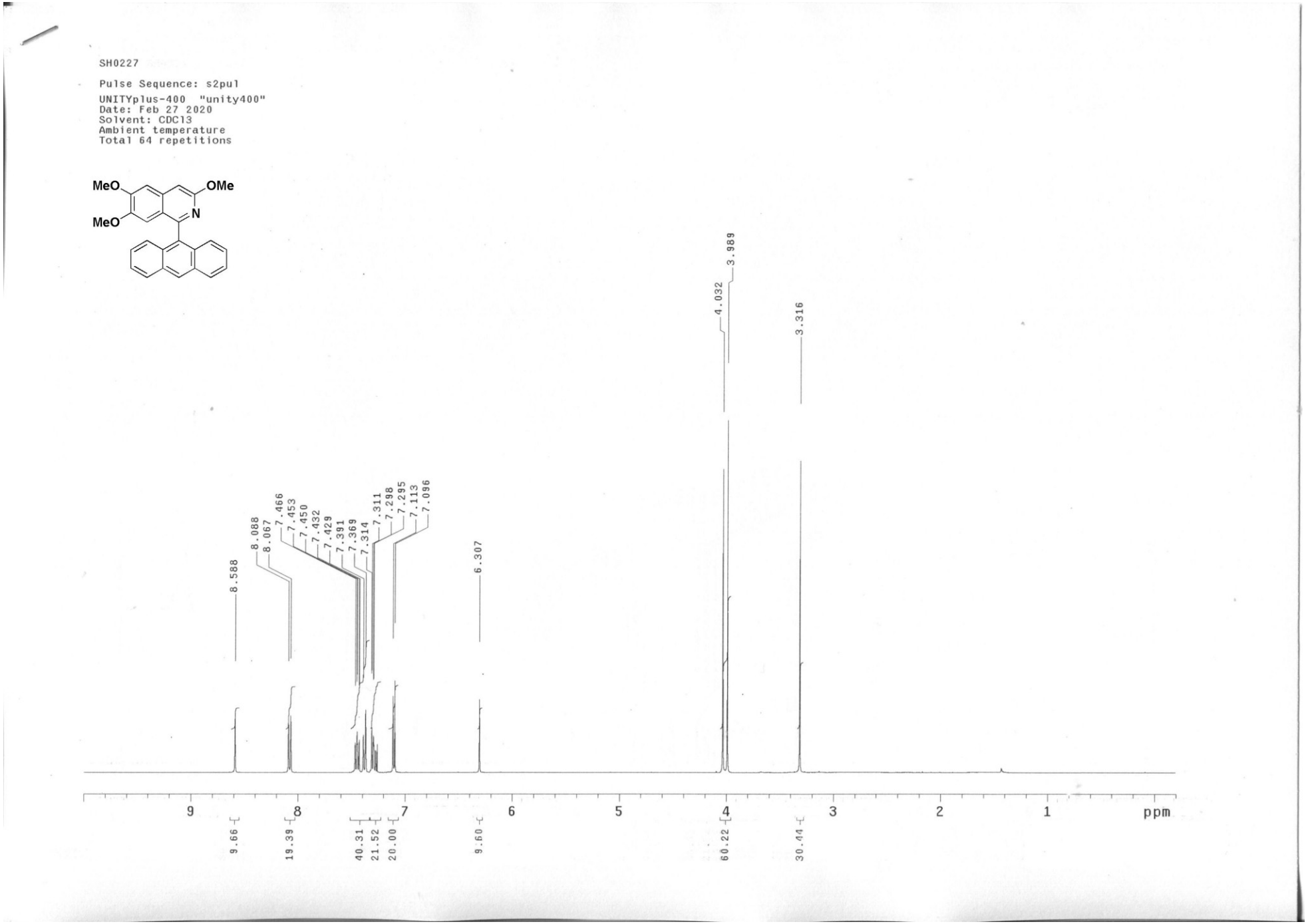
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Mar 31 2020
Solvent: CDCl3
Ambient temperature
Total 128 repetitions





Compound 4r (^{1}H-NMR spectral data)

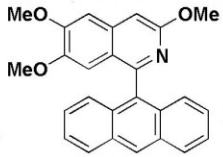


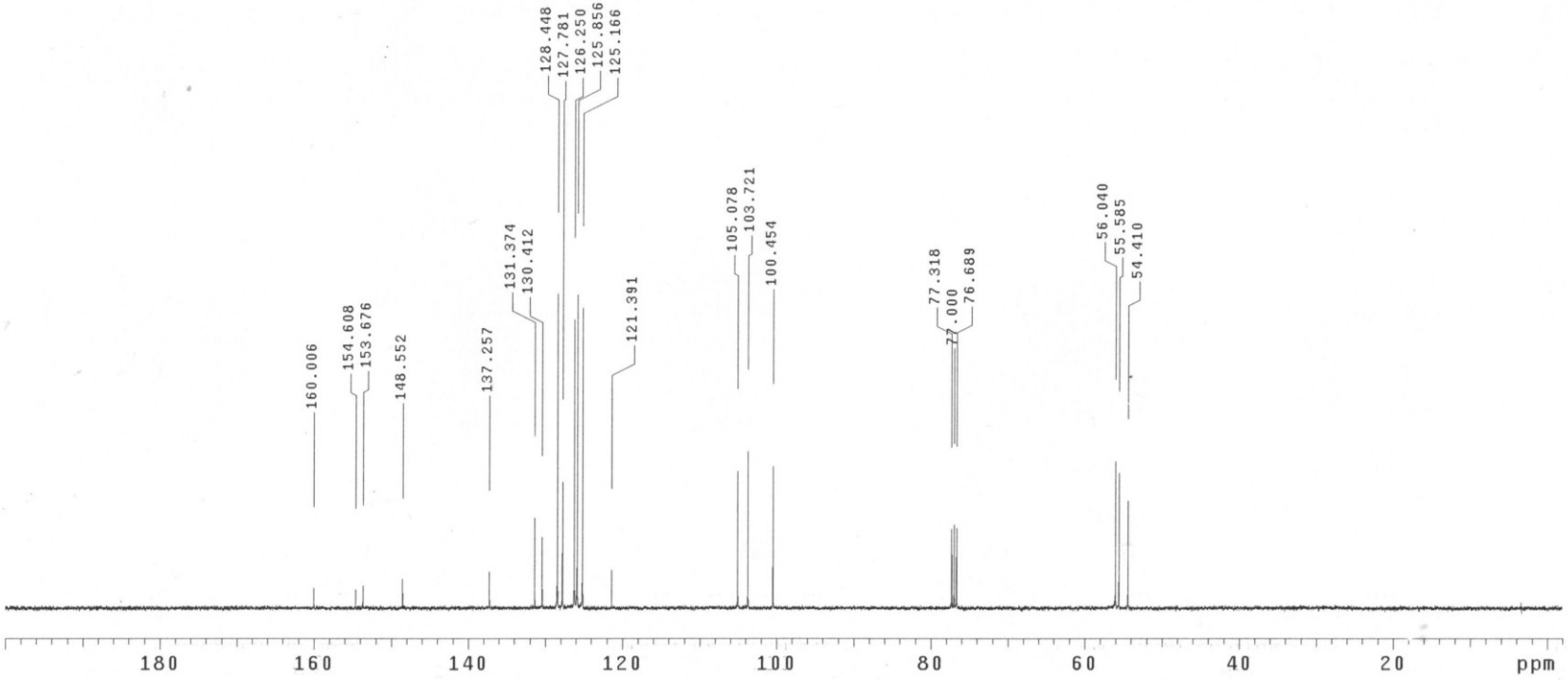
Compound 4r (^{13}C-NMR spectral data)

SH0227

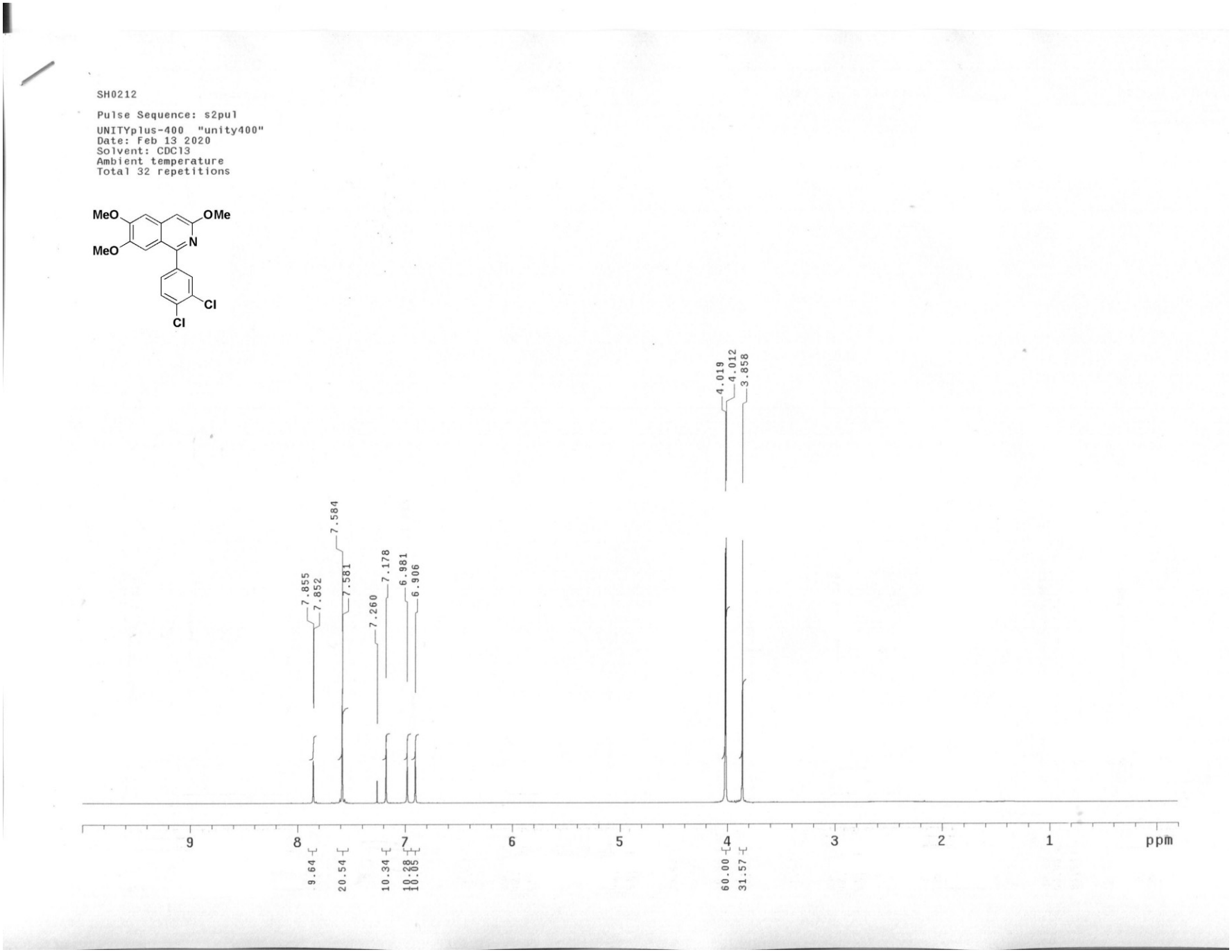
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Feb 27 2020
Solvent: CDCl3
Ambient temperature
Total 2640 repetitions

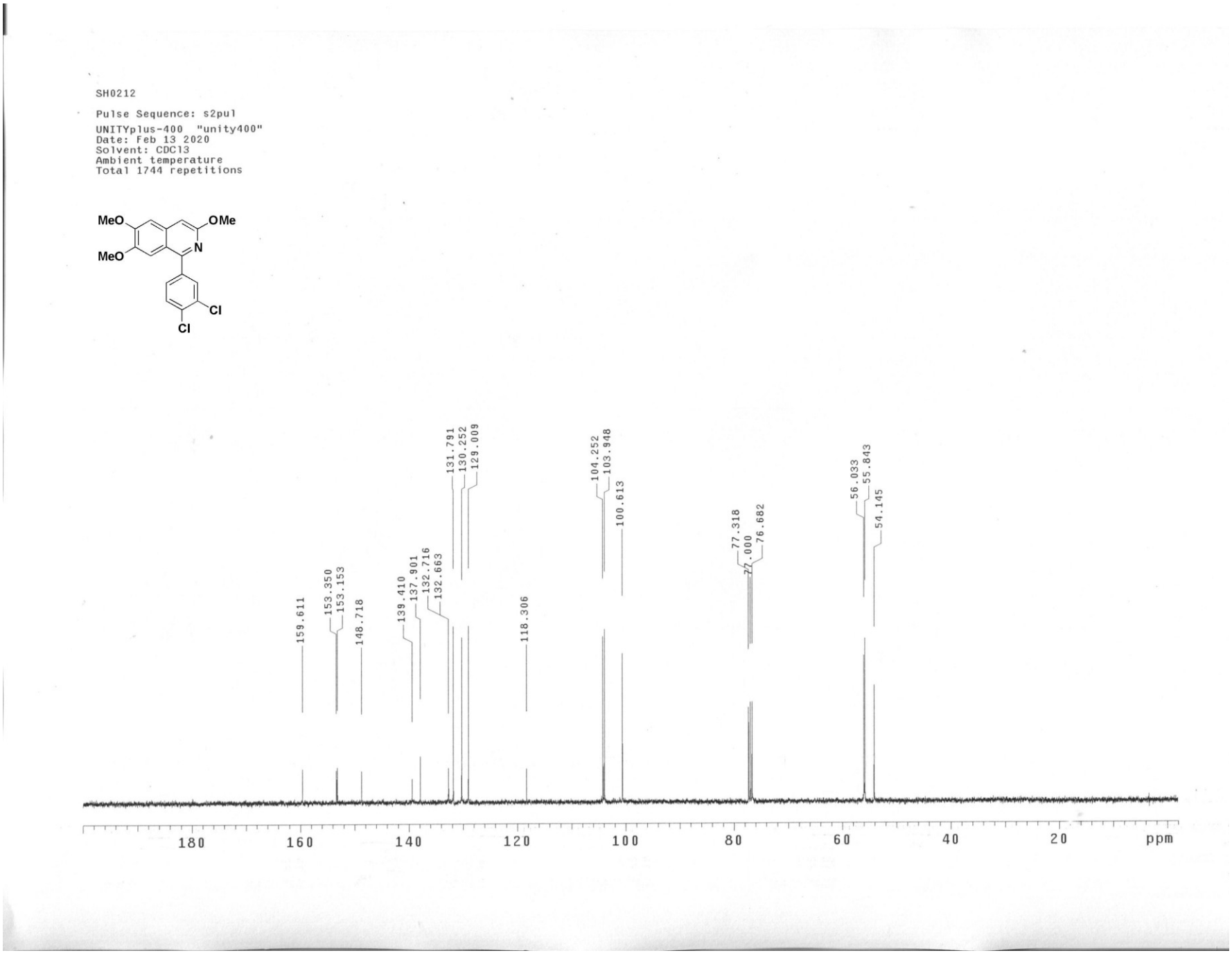




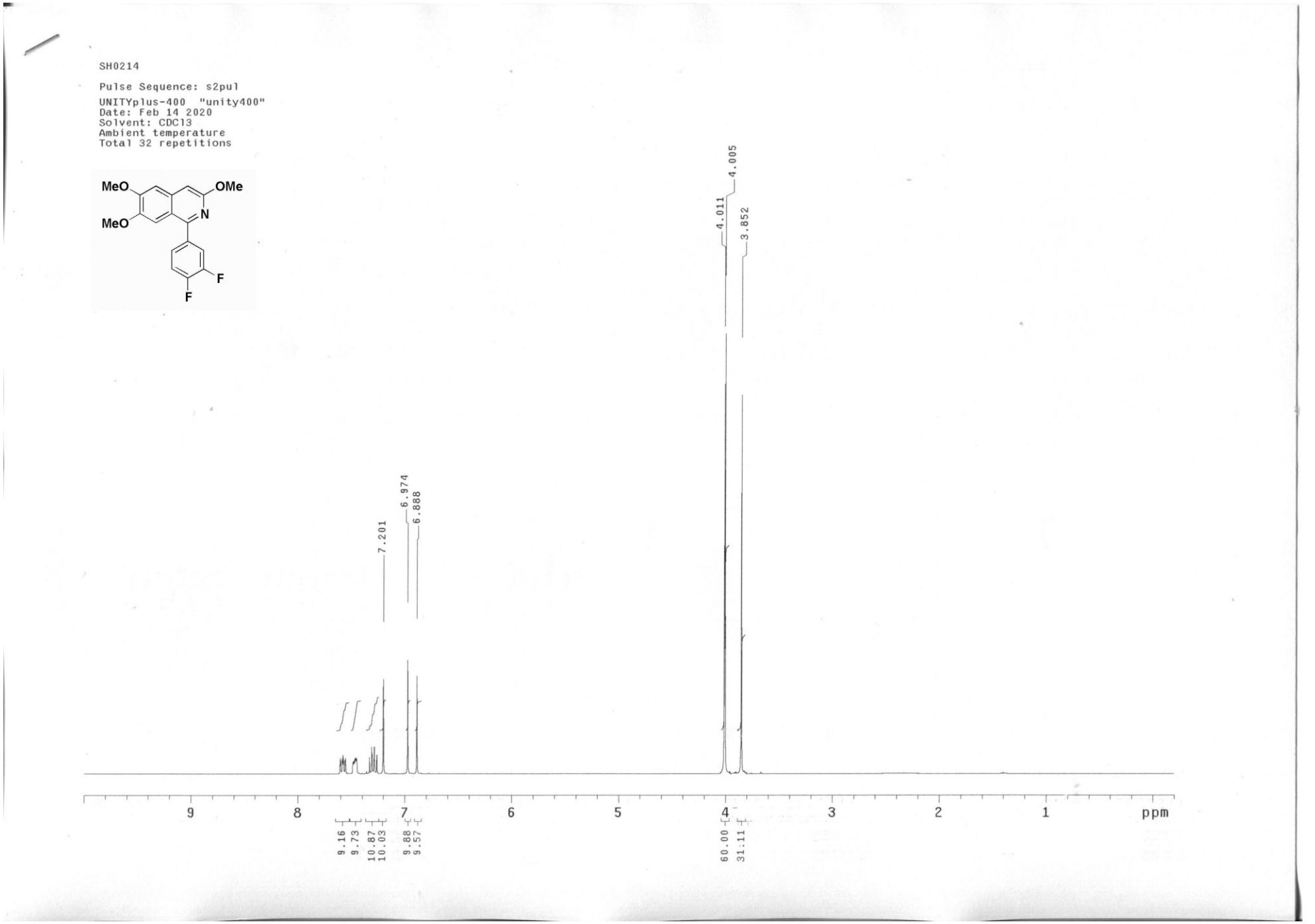
Compound 4s (^{1}H-NMR spectral data)



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



Compound 4t (^{1}H-NMR spectral data)

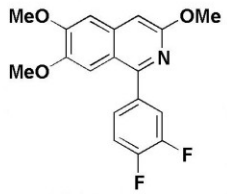


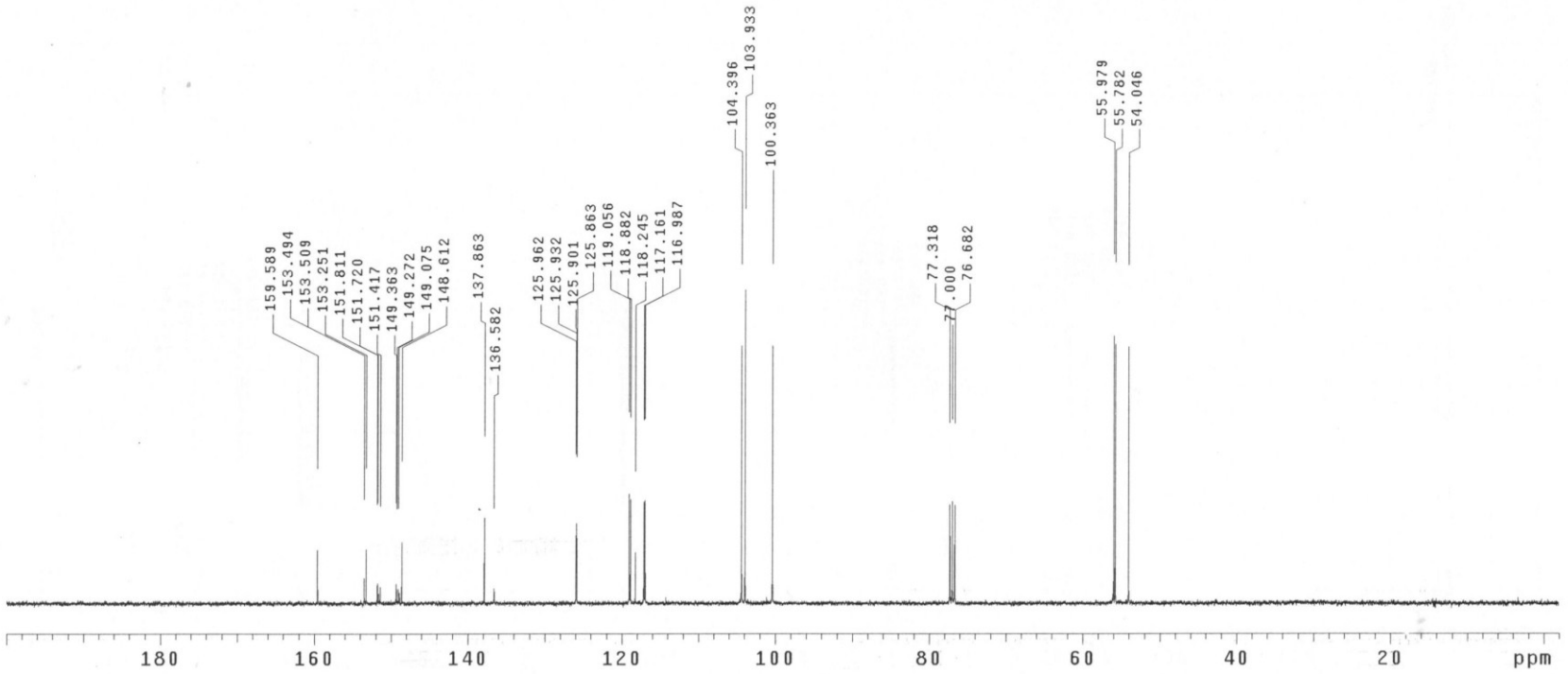
Compound 4t (^{13}C-NMR spectral data)

SH0214

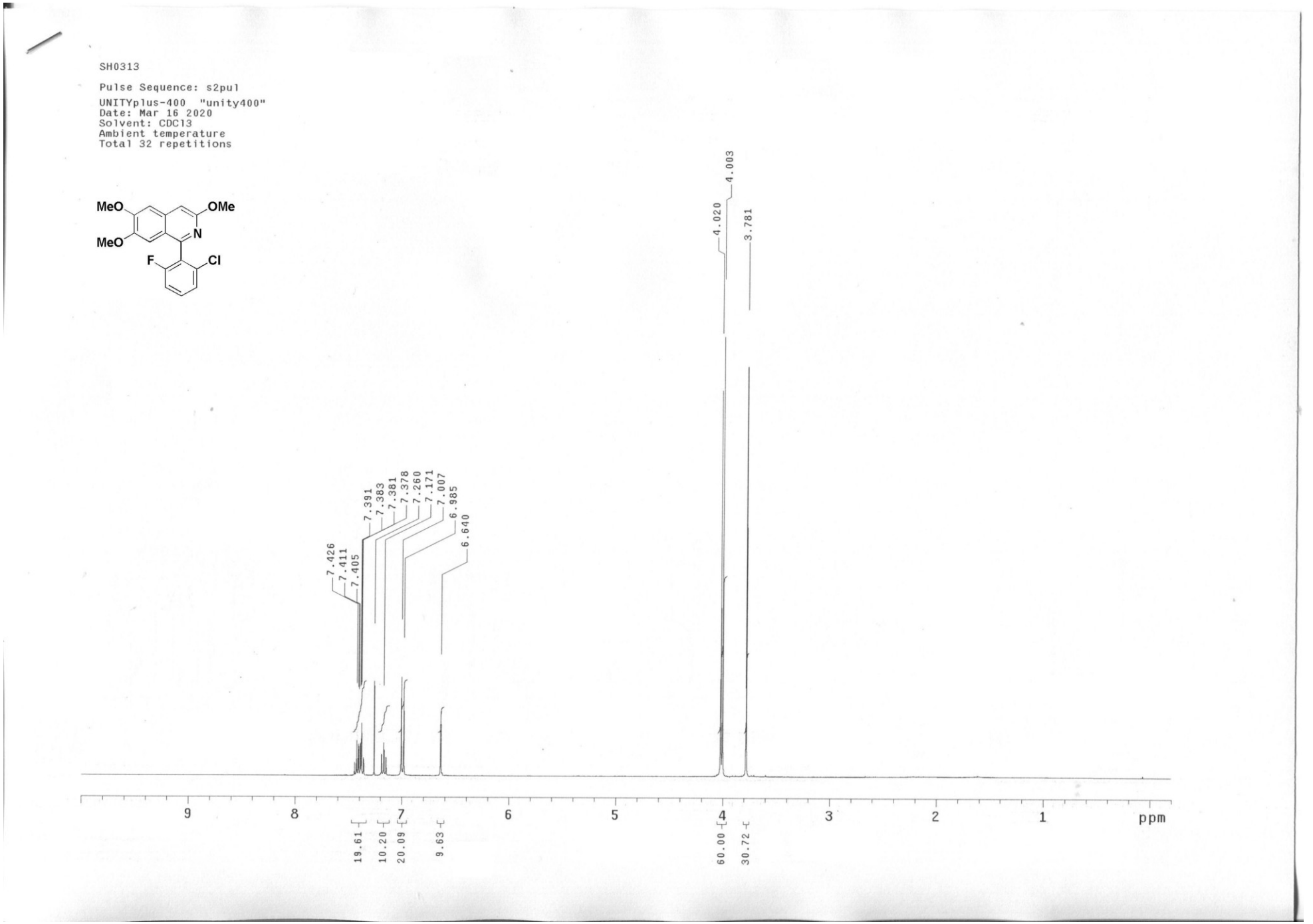
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Feb 14 2020
Solvent: CDCl3
Ambient temperature
Total 2096 repetitions





Compound 4u (^{1}H-NMR spectral data)

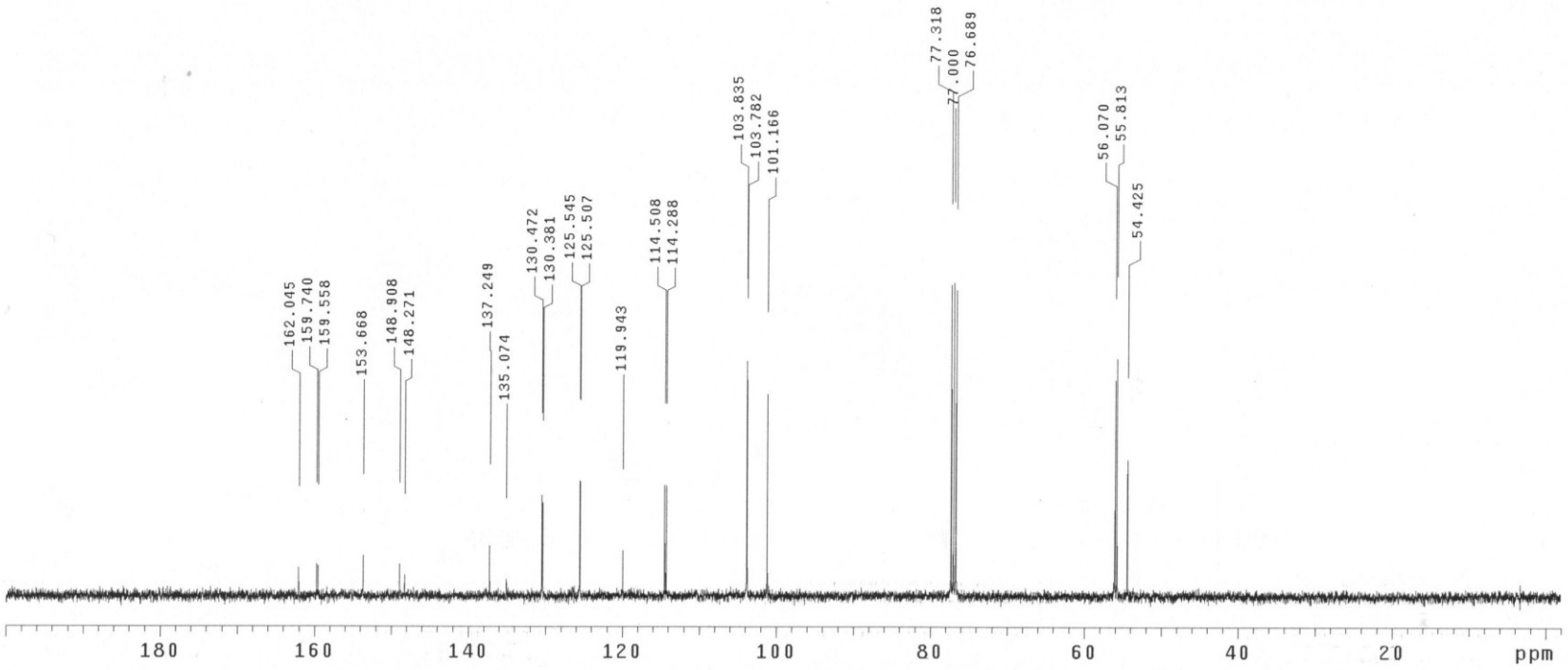


Compound 4u (^{13}C-NMR spectral data)

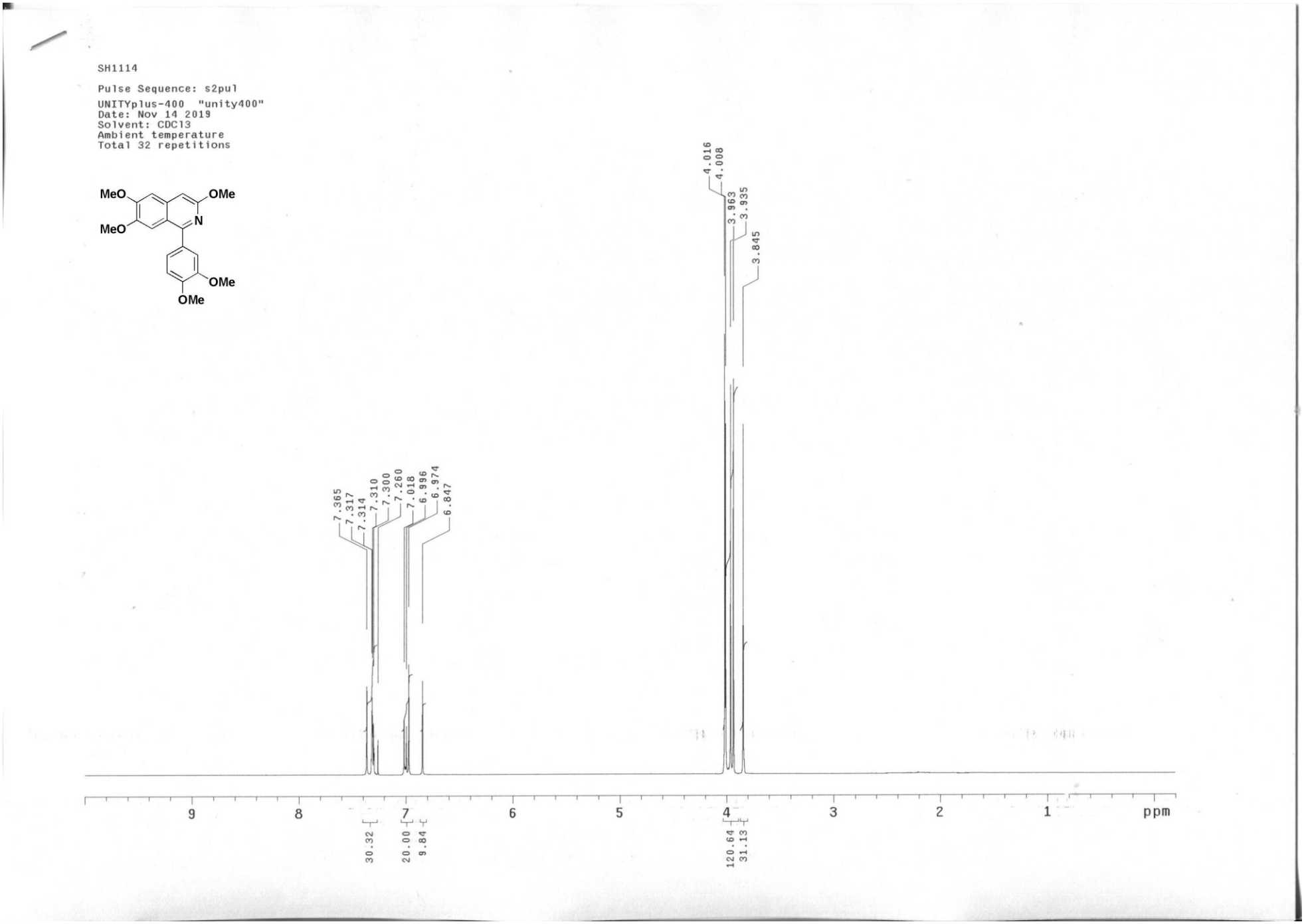
SH0313

Pulse Sequence: s2pul

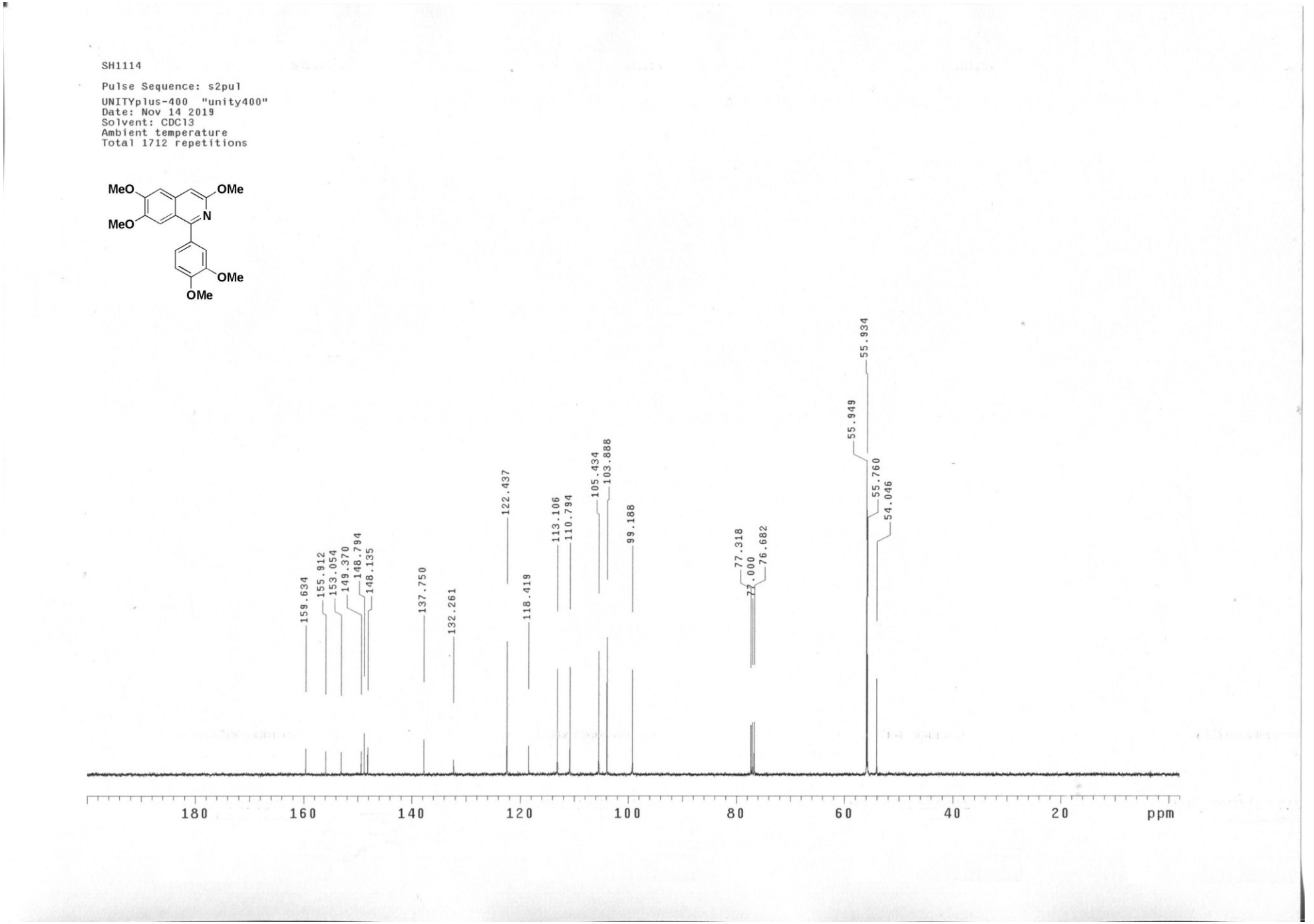
UNITYplus-400 "unity400"
Date: Mar 16 2020
Solvent: CDCl3
Ambient temperature
Total 5088 repetitions



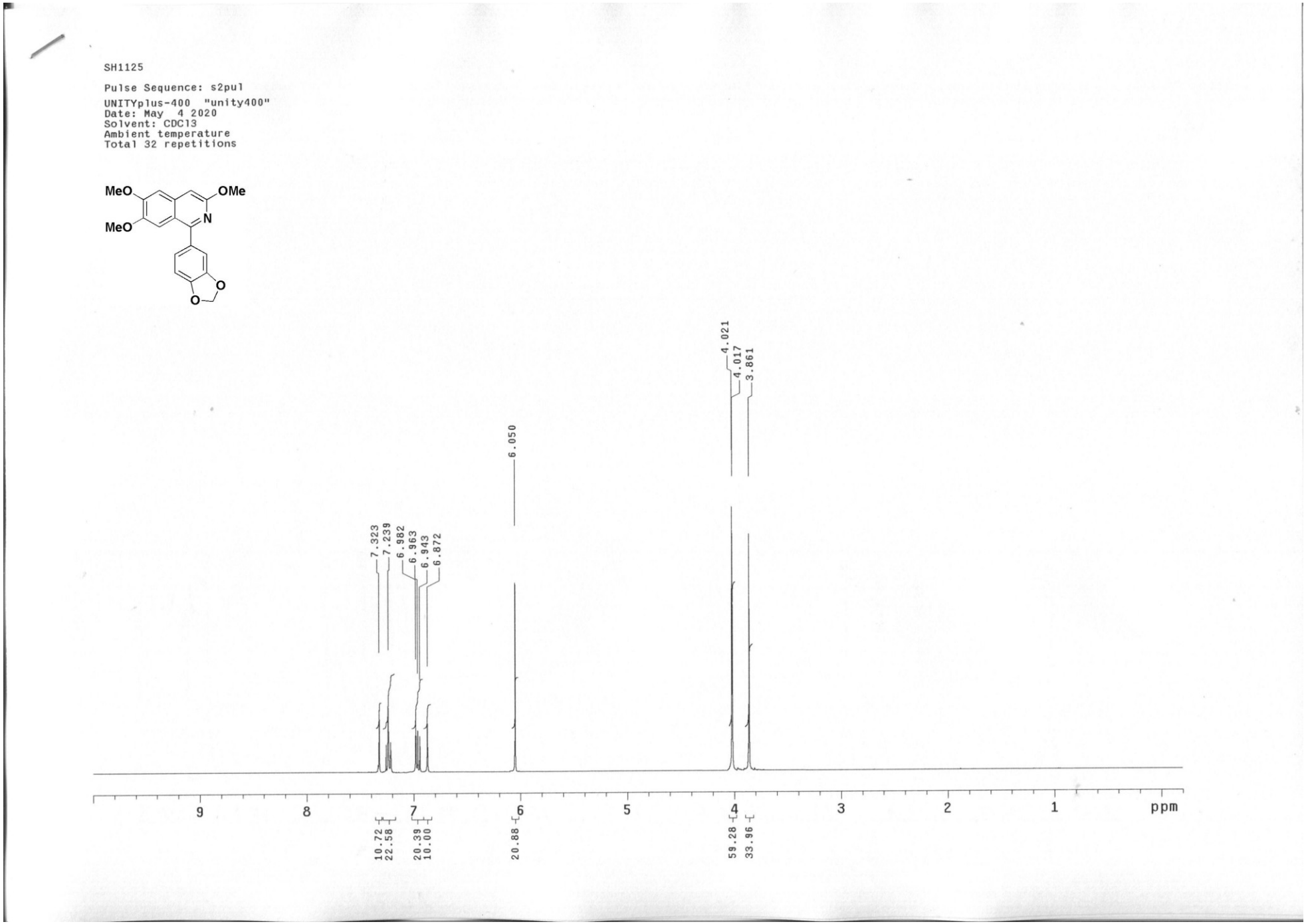
Compound 4v (^{1}H-NMR spectral data)



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



Compound 4w (^{1}H-NMR spectral data)

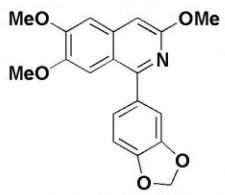


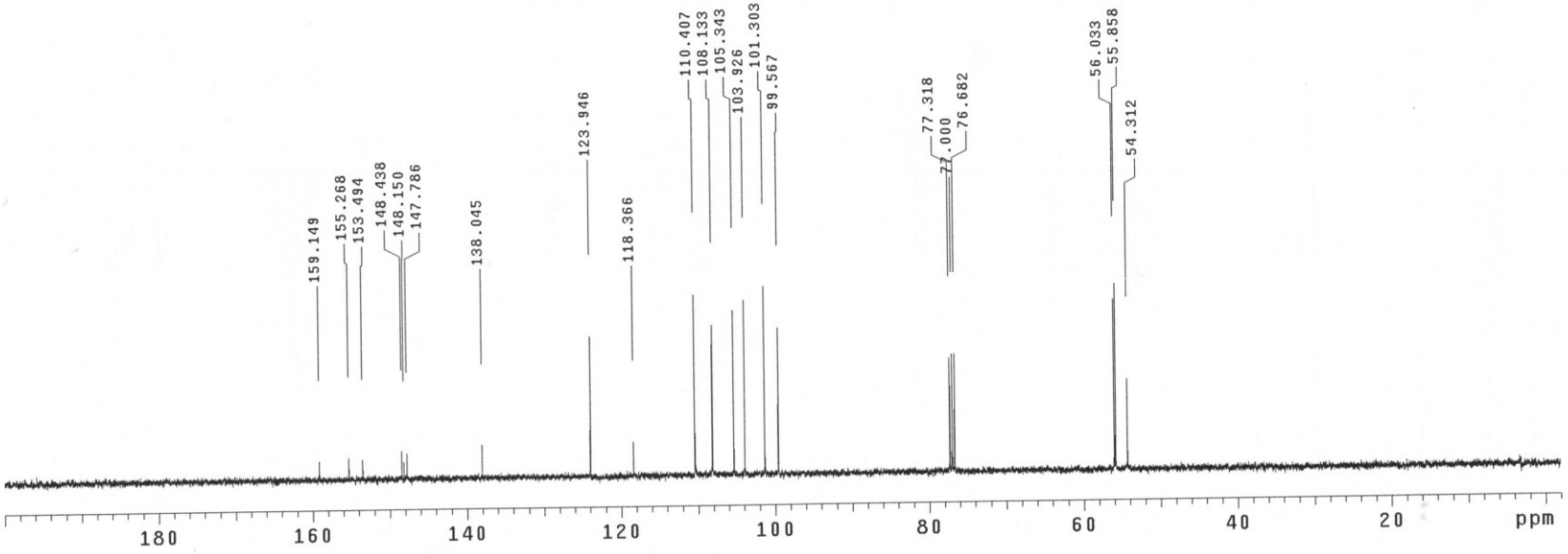
Compound 4w (^{13}C-NMR spectral data)

SH1125

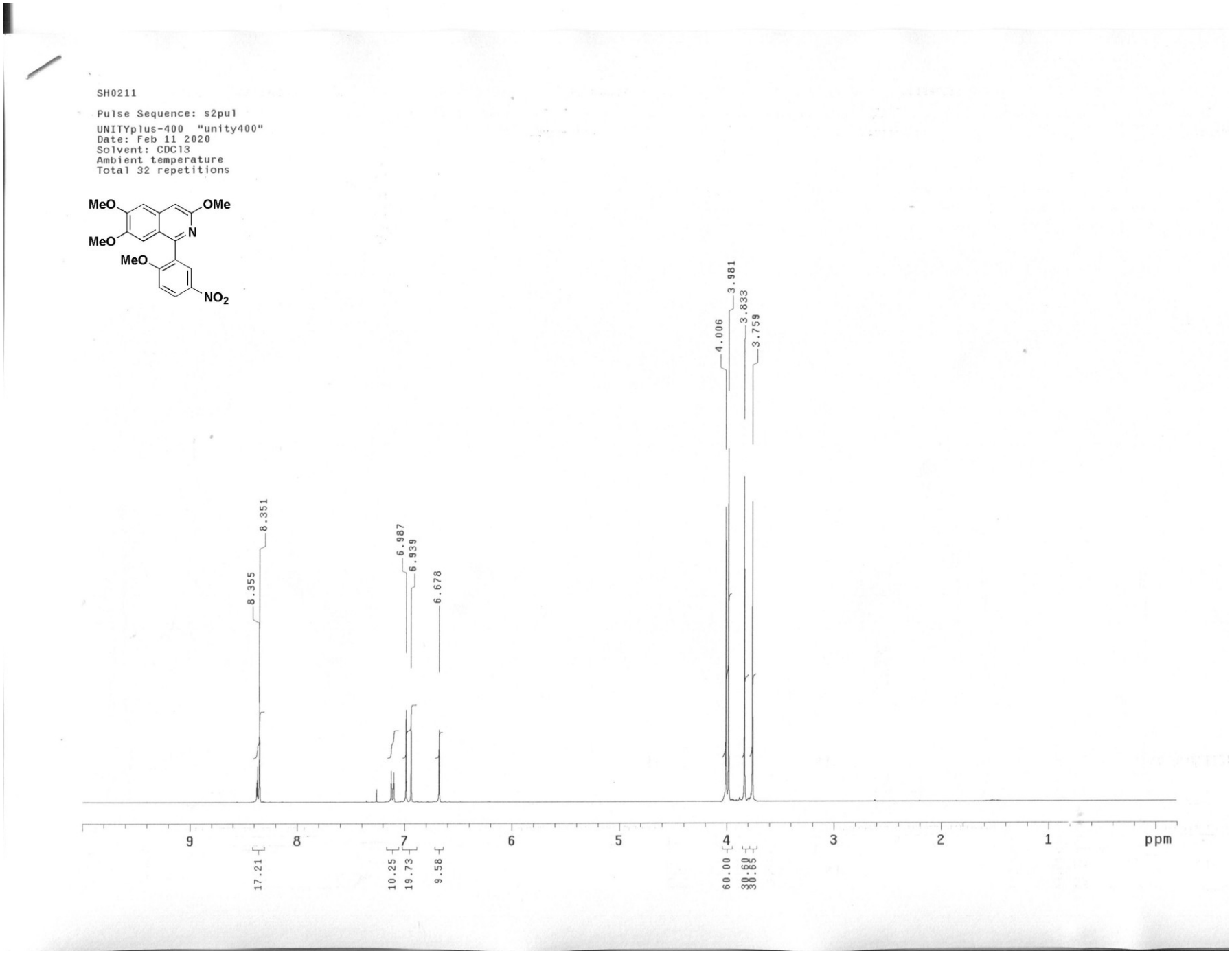
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 4 2020
Solvent: CDCl3
Ambient temperature
Total 1360 repetitions





Compound 4x (^{1}H-NMR spectral data)

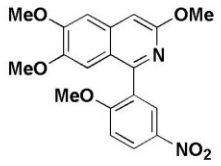


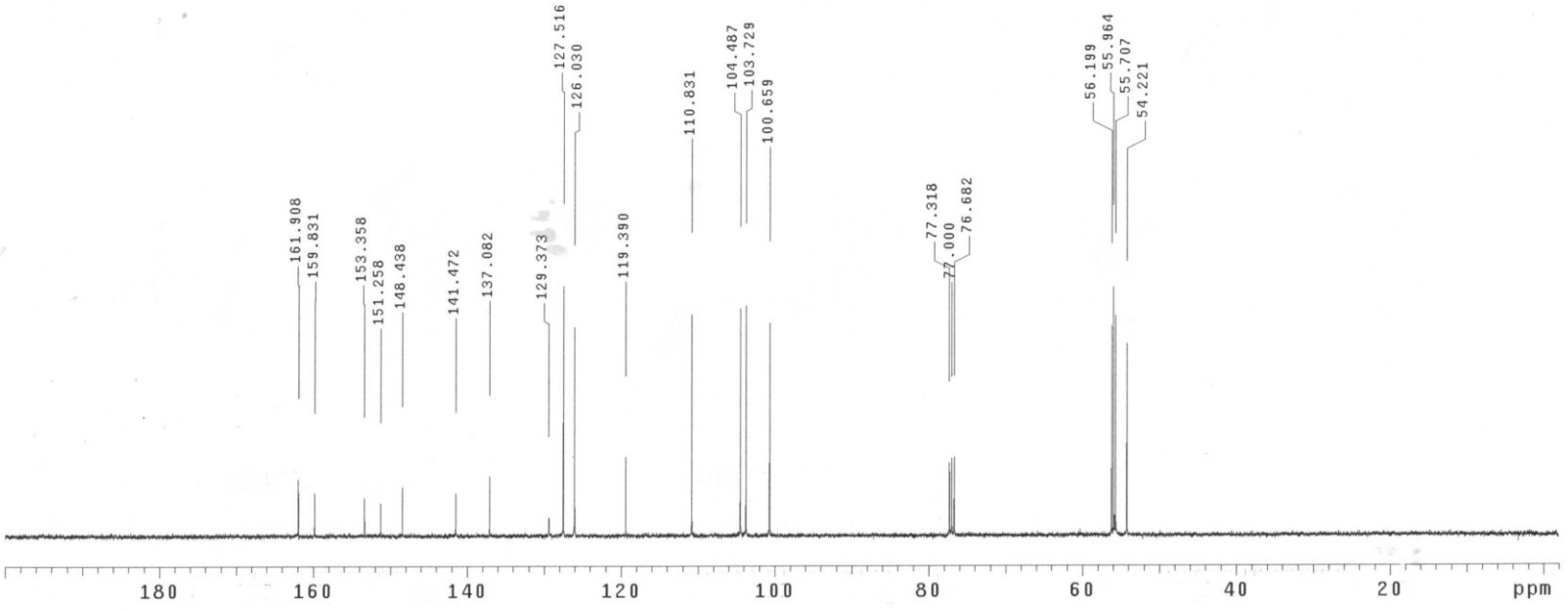
Compound 4x (^{13}C-NMR spectral data)

SH0211

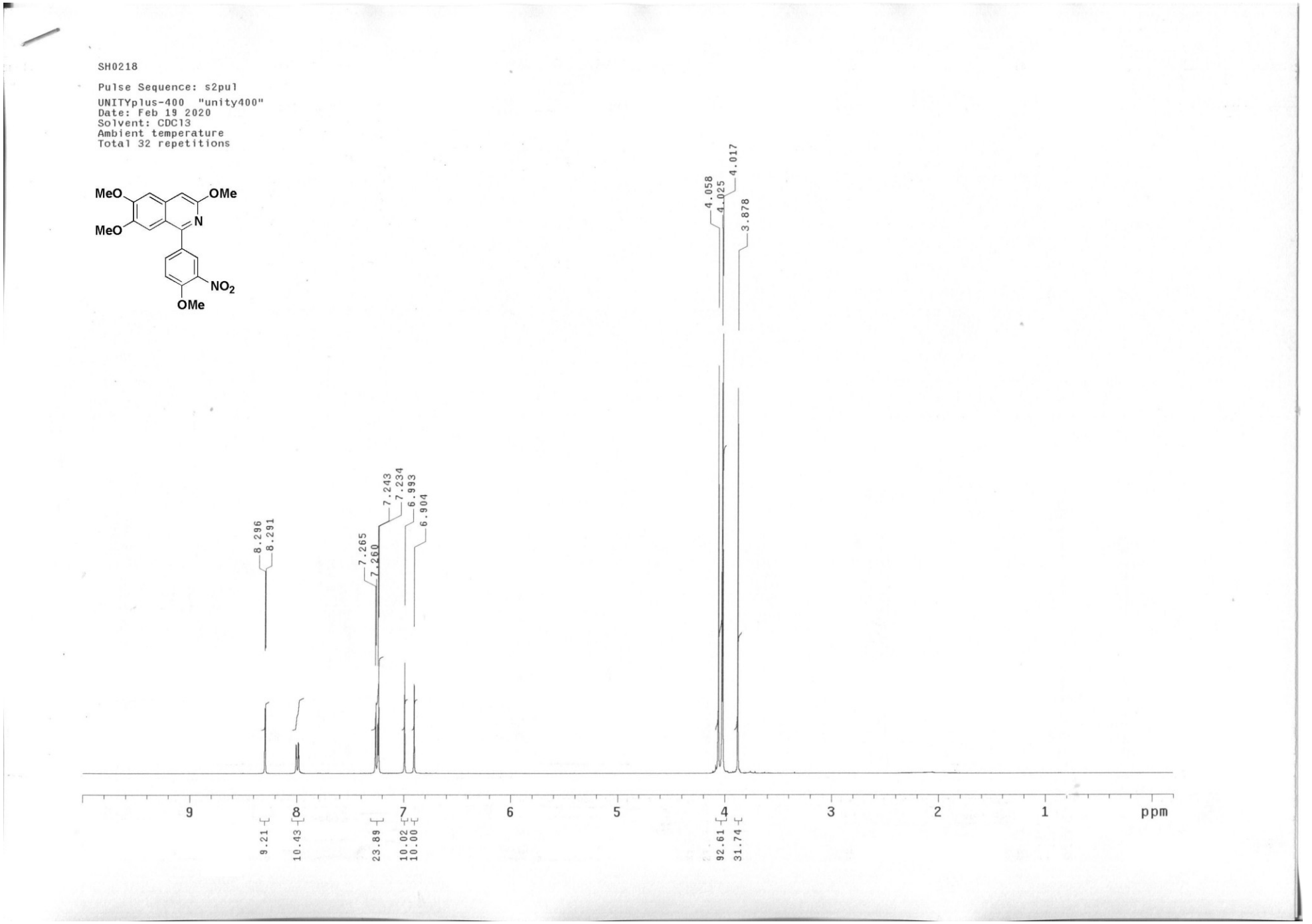
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Feb 11 2020
Solvent: CDCl3
Ambient temperature
Total 1120 repetitions





Compound 4y (^{1}H-NMR spectral data)

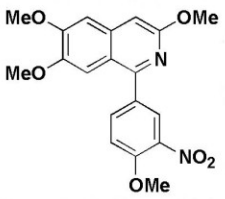


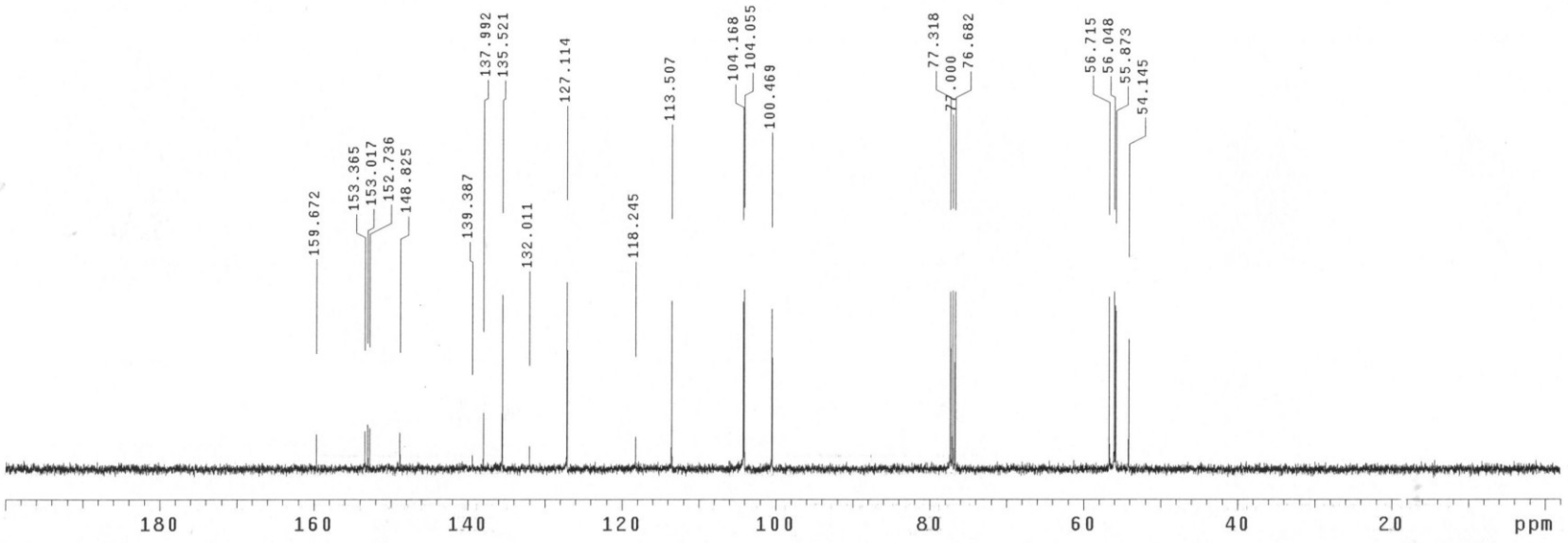
Compound 4y (^{13}C-NMR spectral data)

SH0218

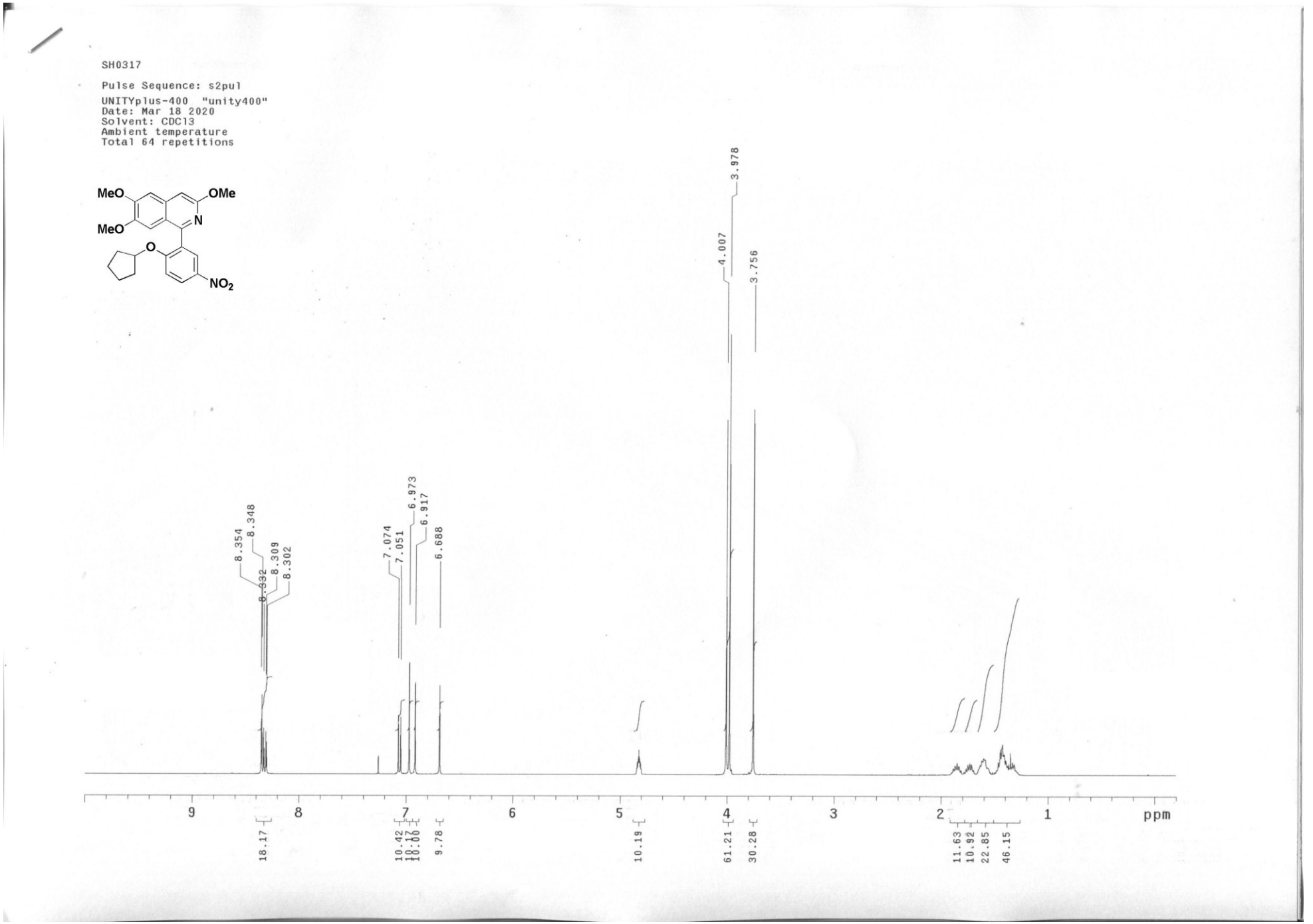
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Feb 19 2020
Solvent: CDCl3
Ambient temperature
Total 2352 repetitions

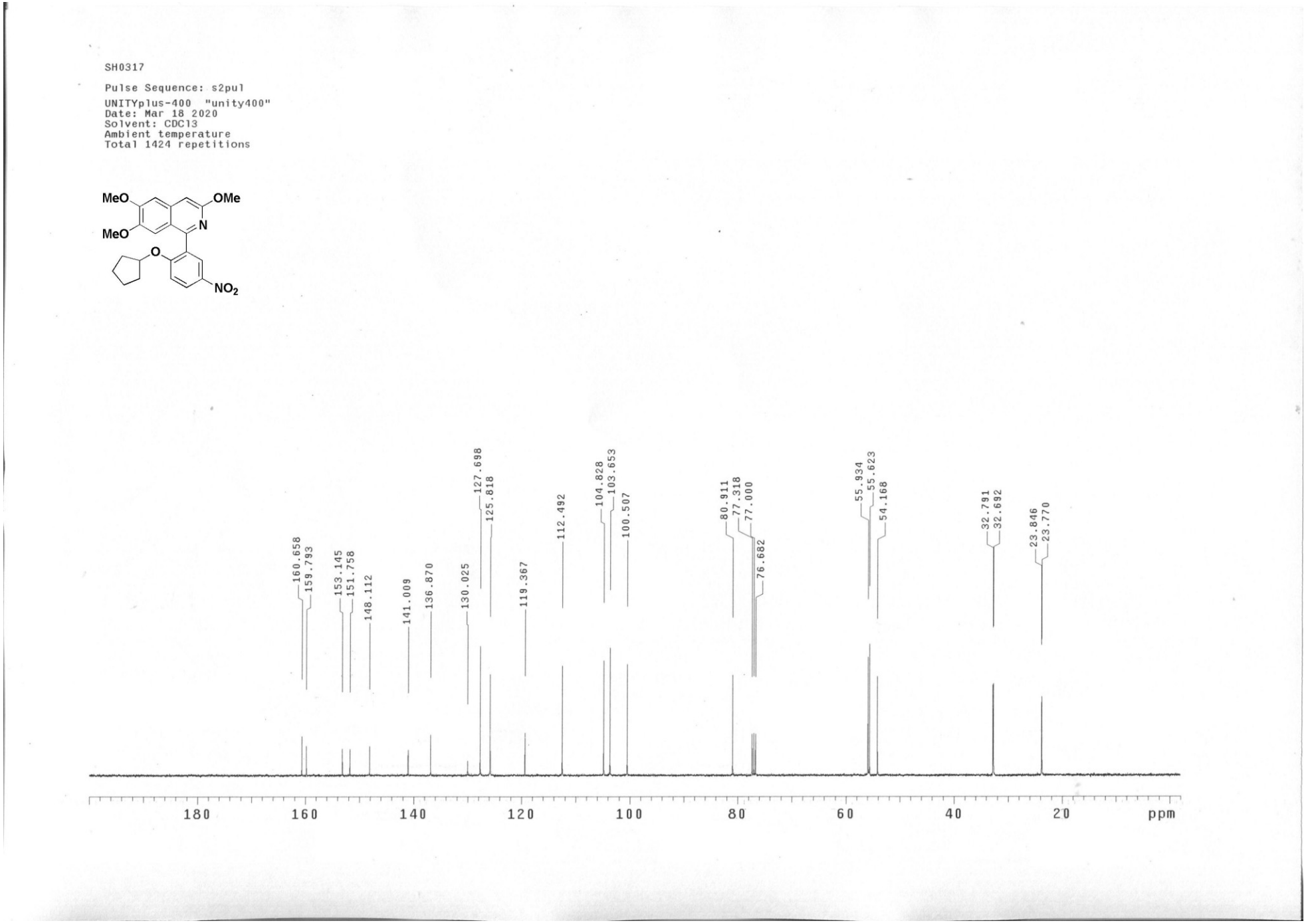




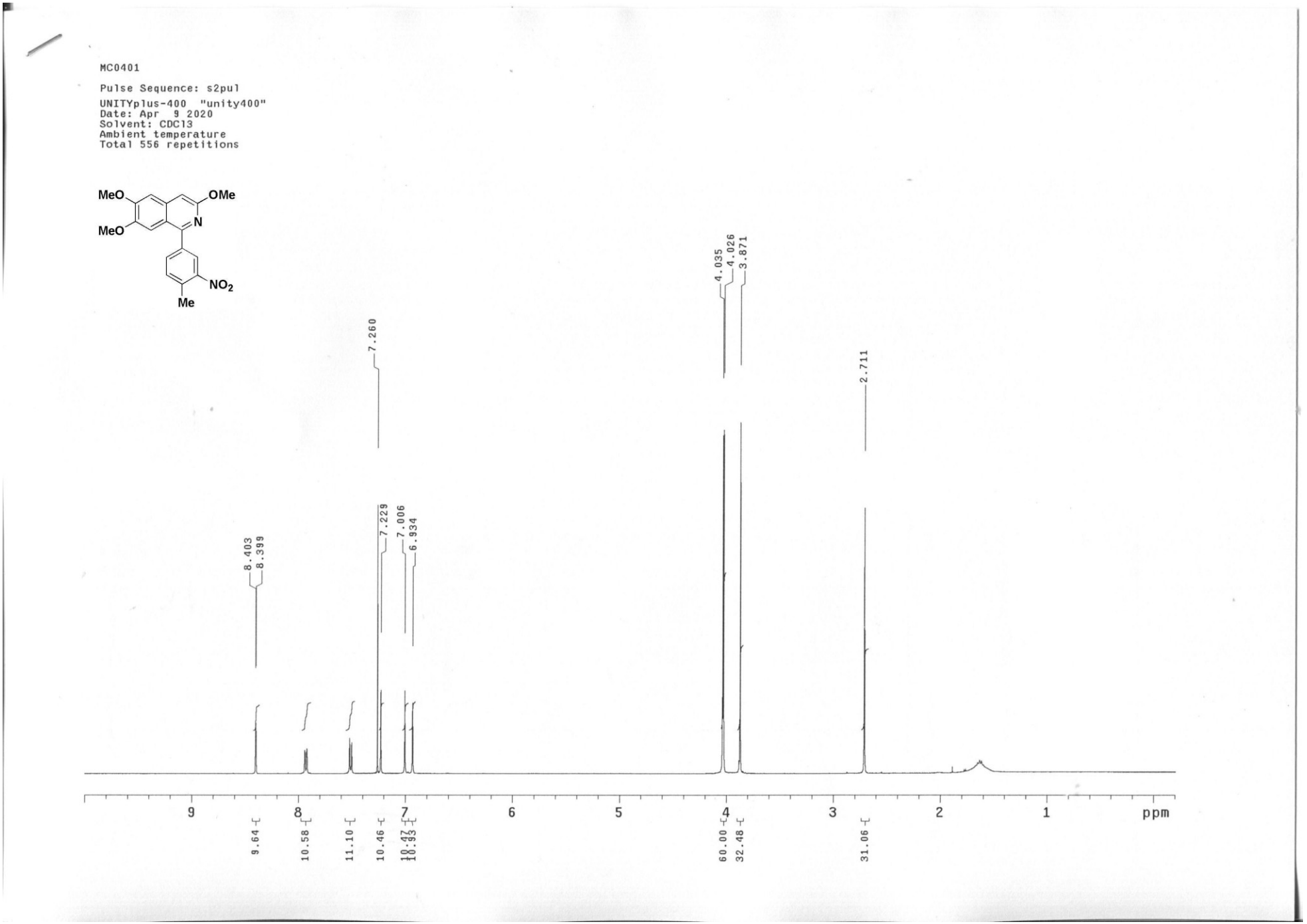
Compound 4z (^{1}H-NMR spectral data)



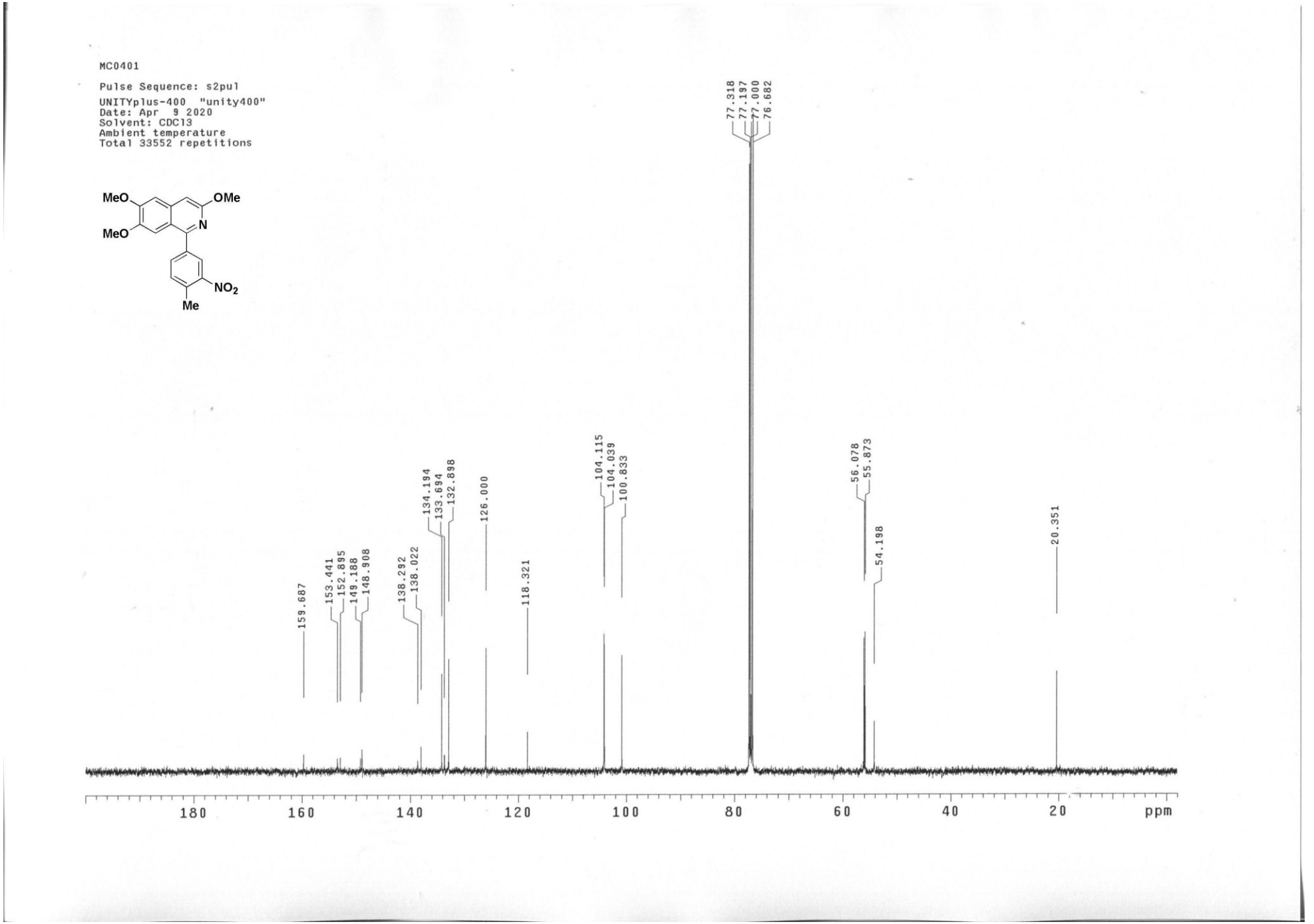
Compound 4z (^{13}C-NMR spectral data)



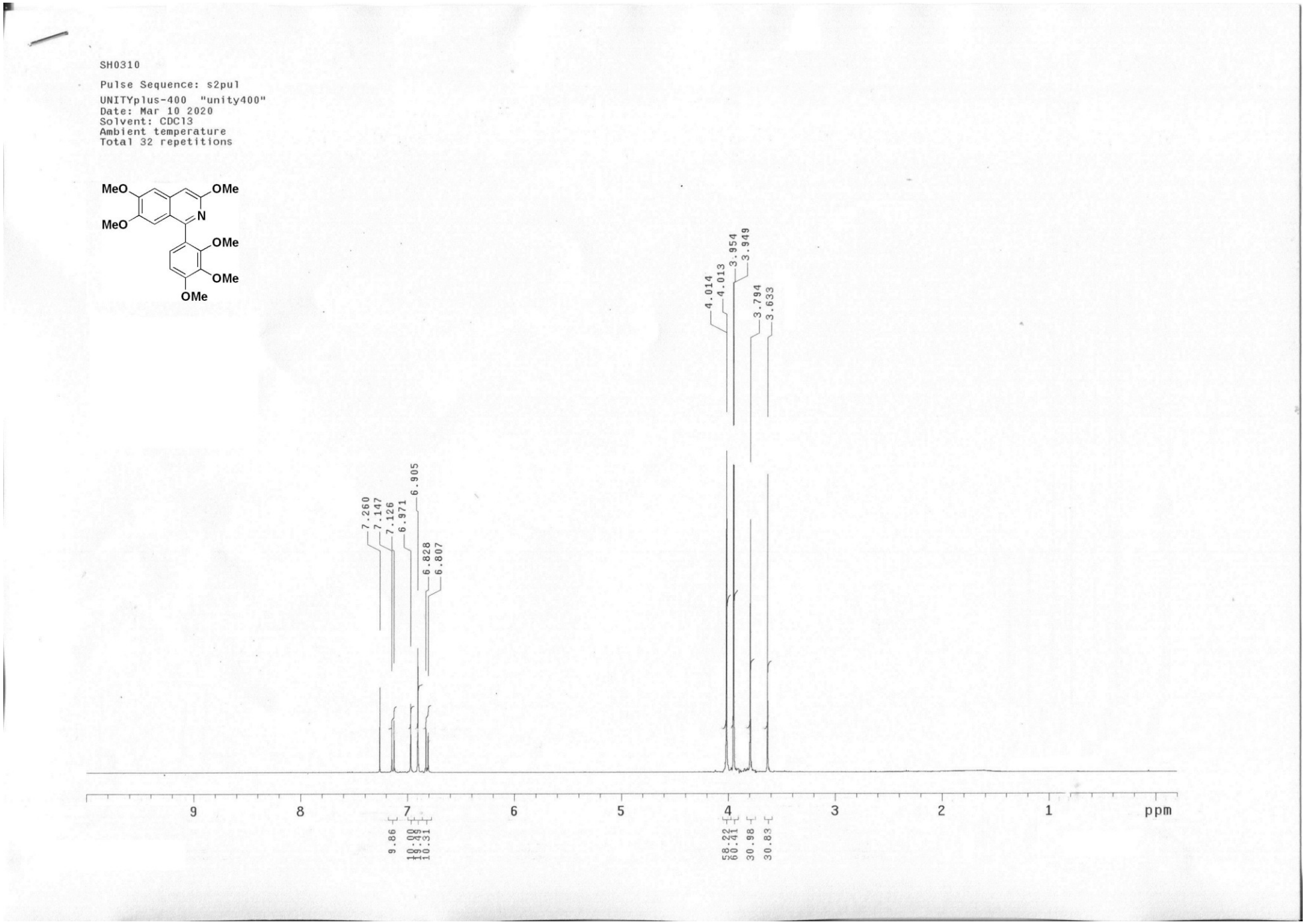
Compound 4aa (^{1}H-NMR spectral data)



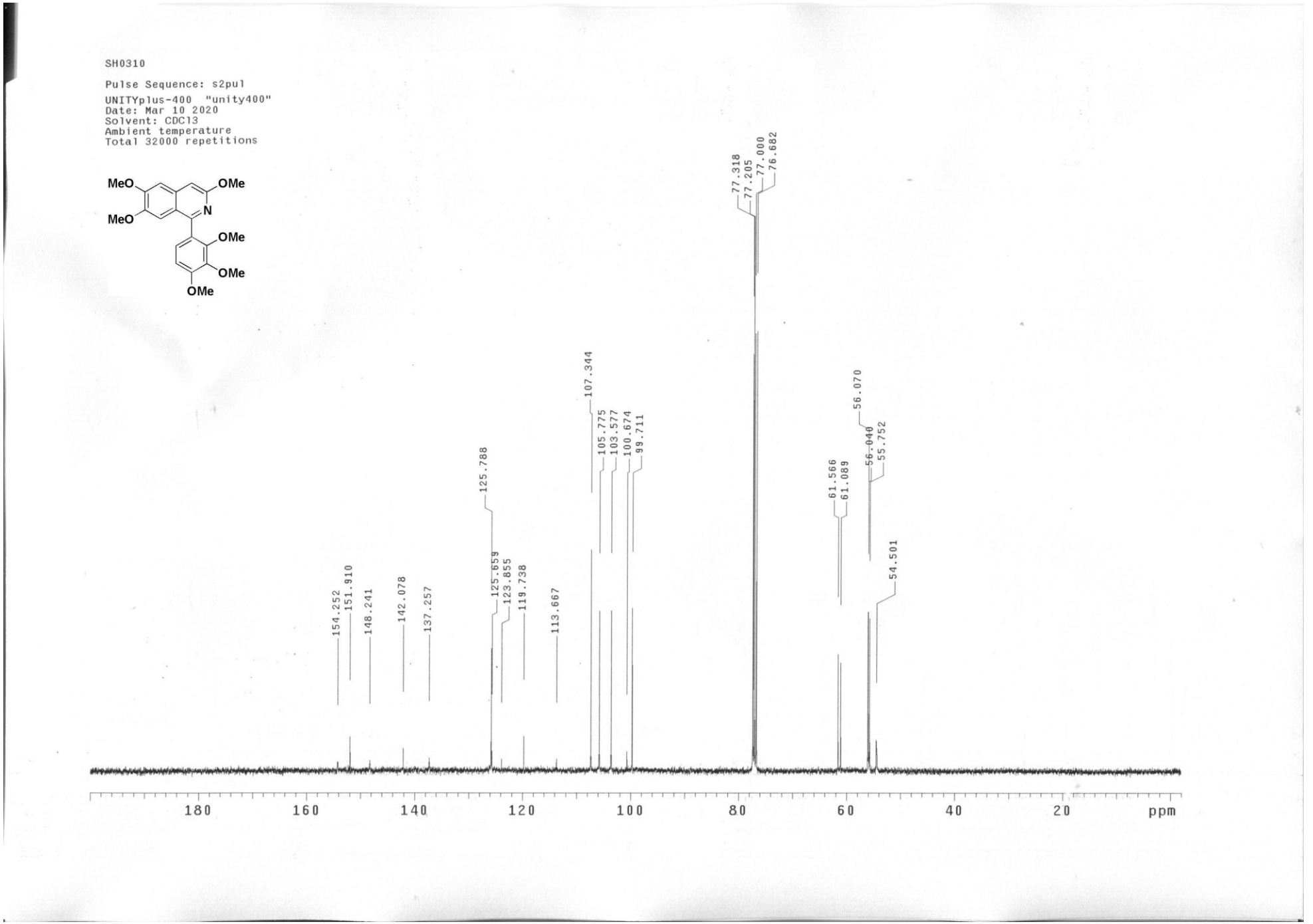
Compound 4aa (^{13}C-NMR spectral data)



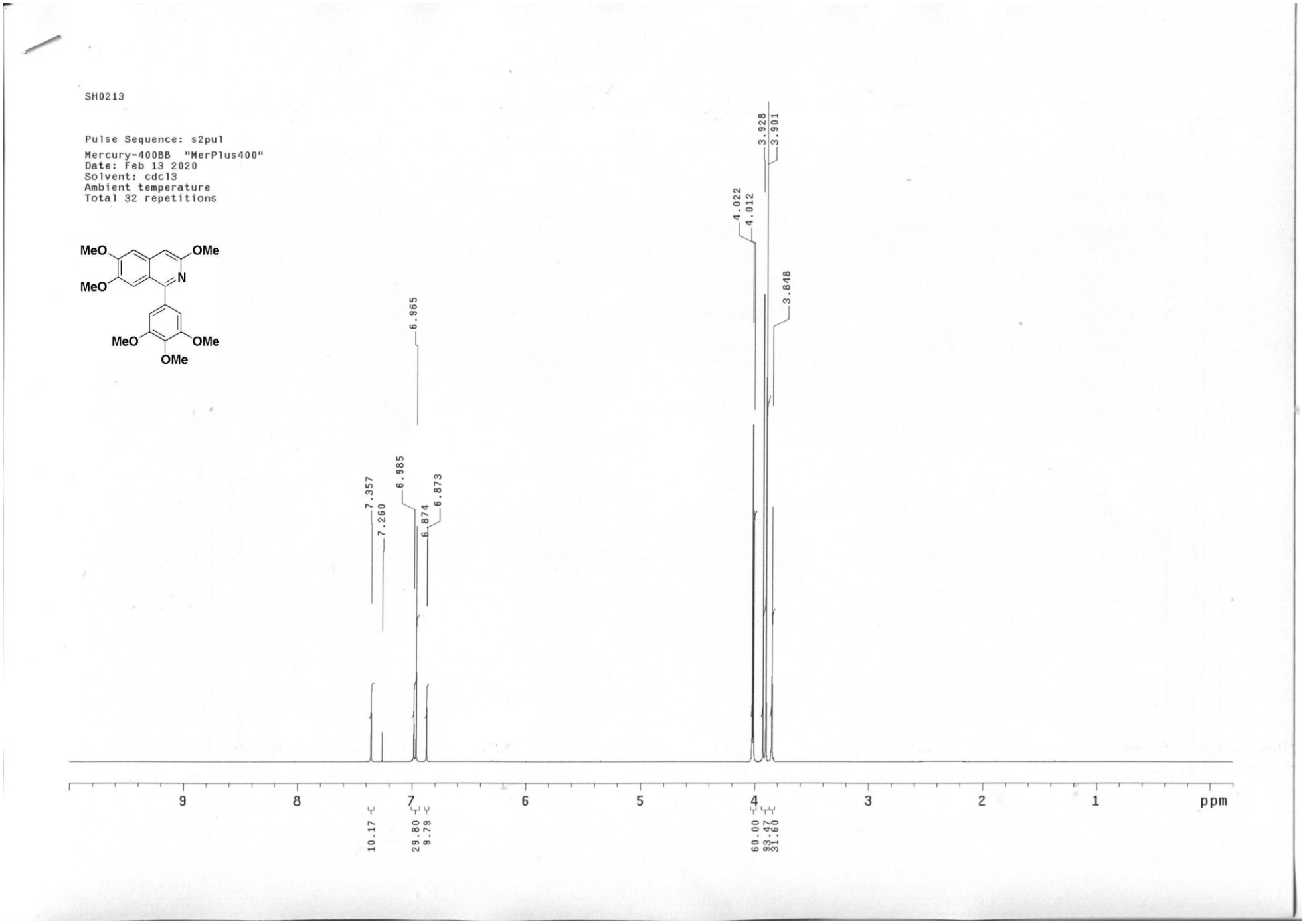
Compound 4ab (^{1}H-NMR spectral data)



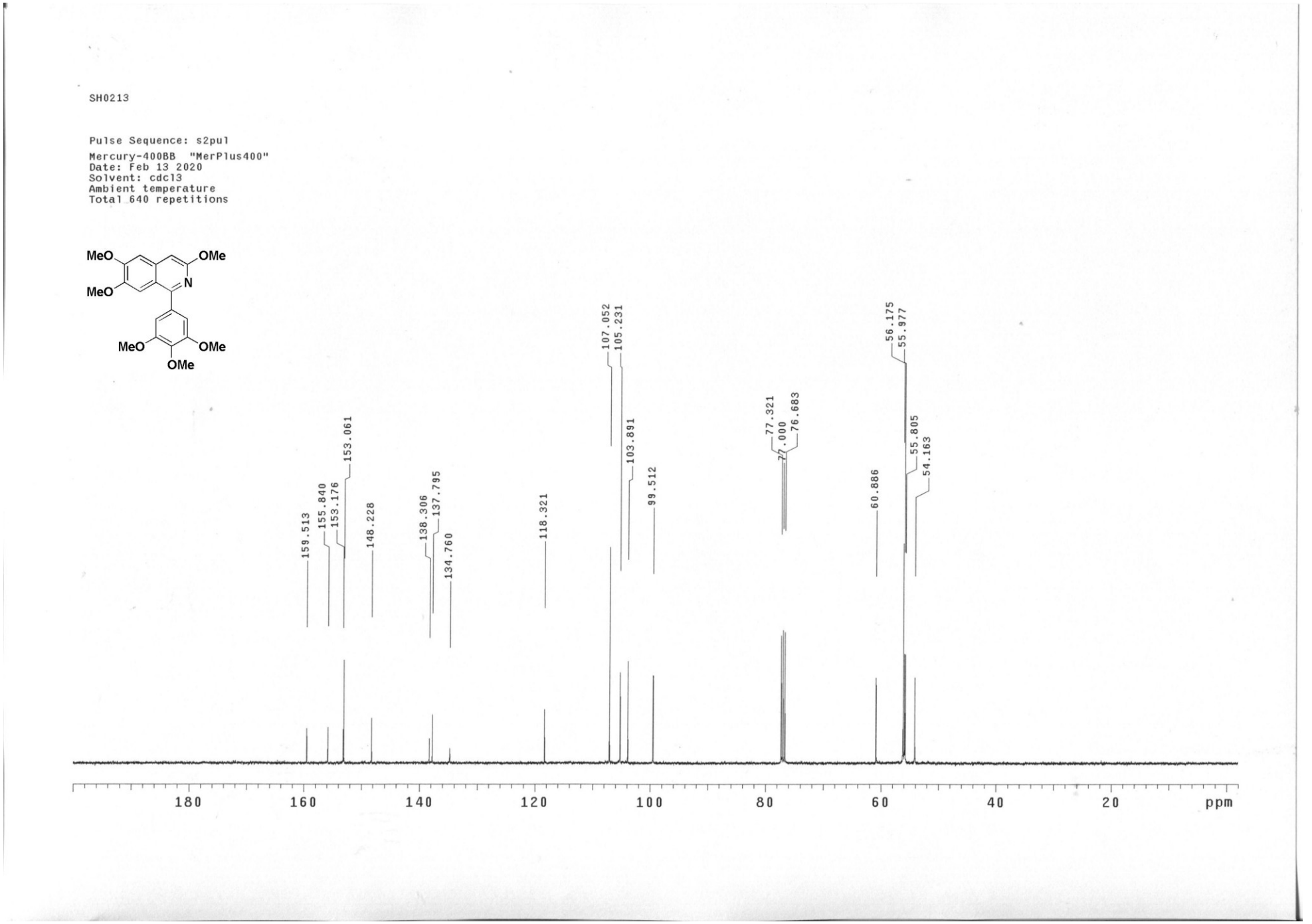
Compound 4ab (^{13}C-NMR spectral data)



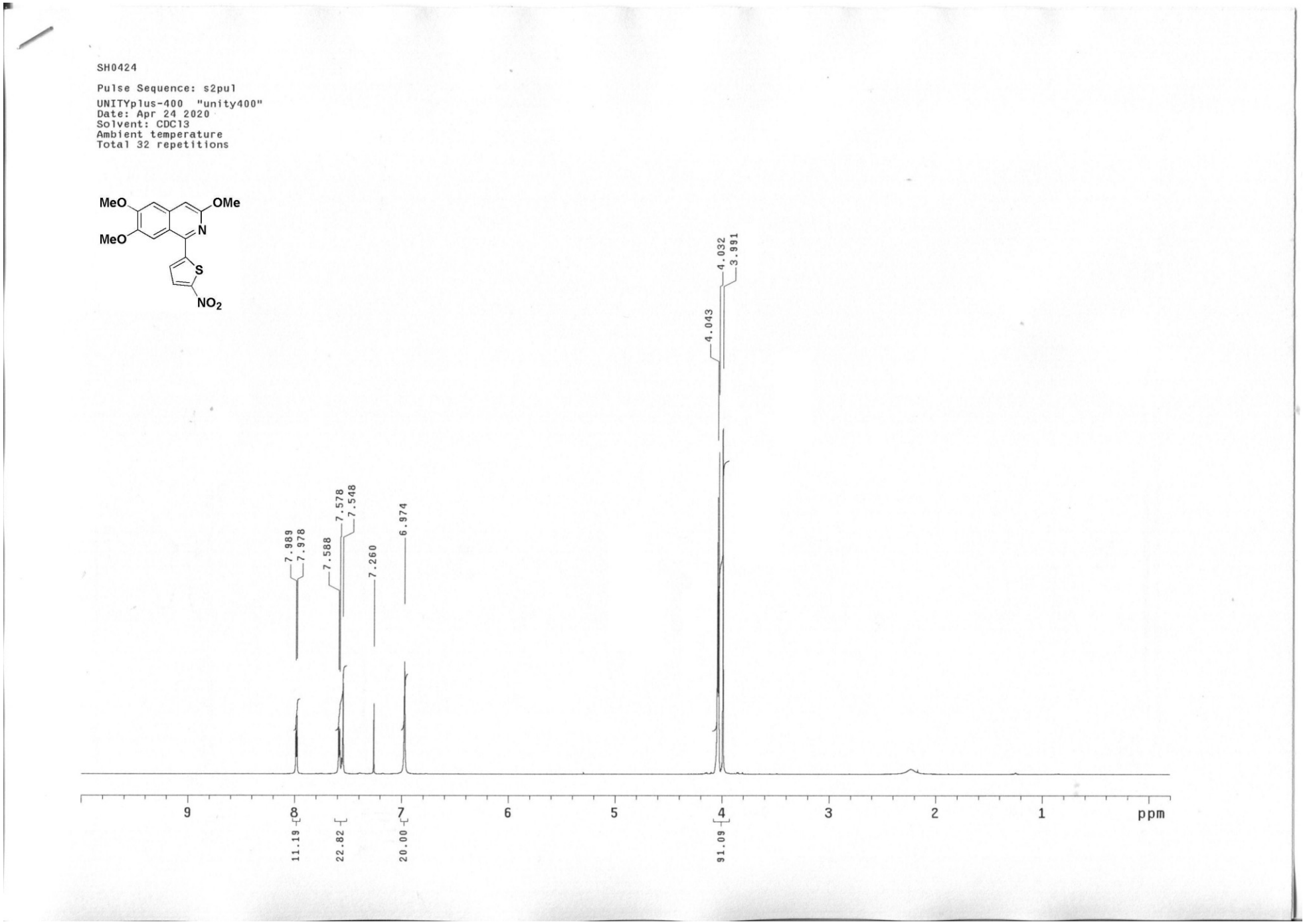
Compound 4ac (^{1}H-NMR spectral data)



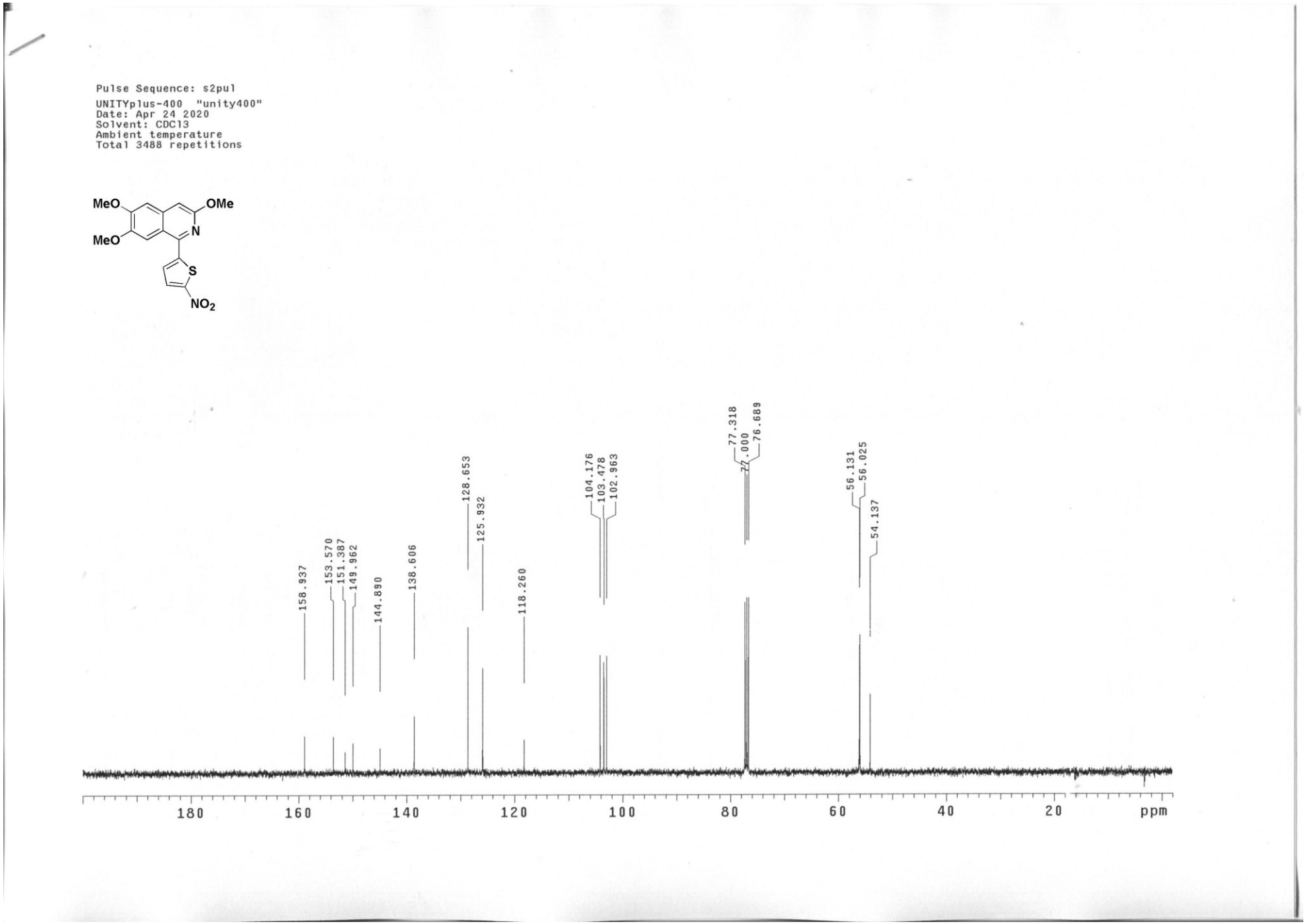
Compound 4ac (^{13}C-NMR spectral data)



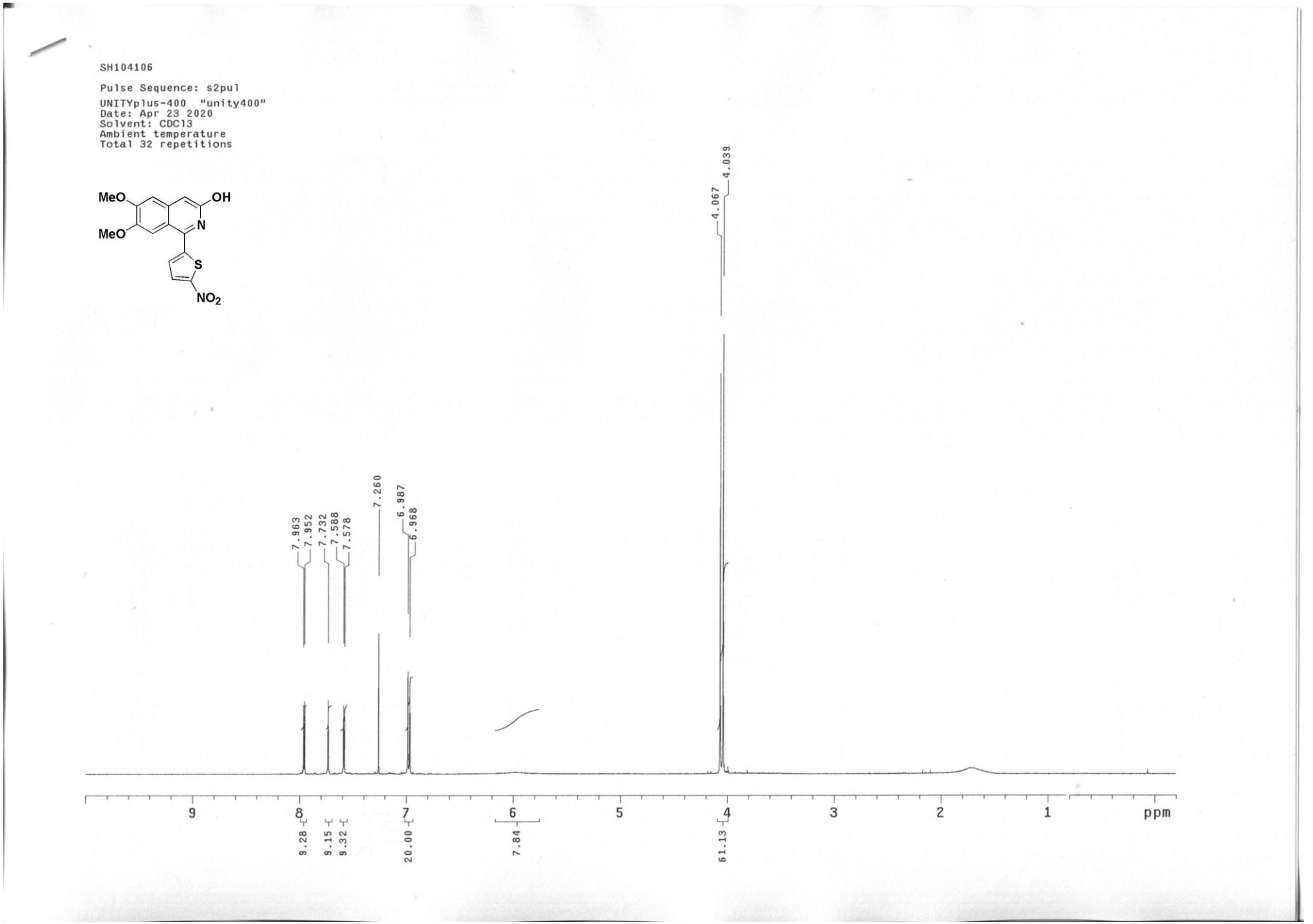
Compound 4ad (^{1}H-NMR spectral data)



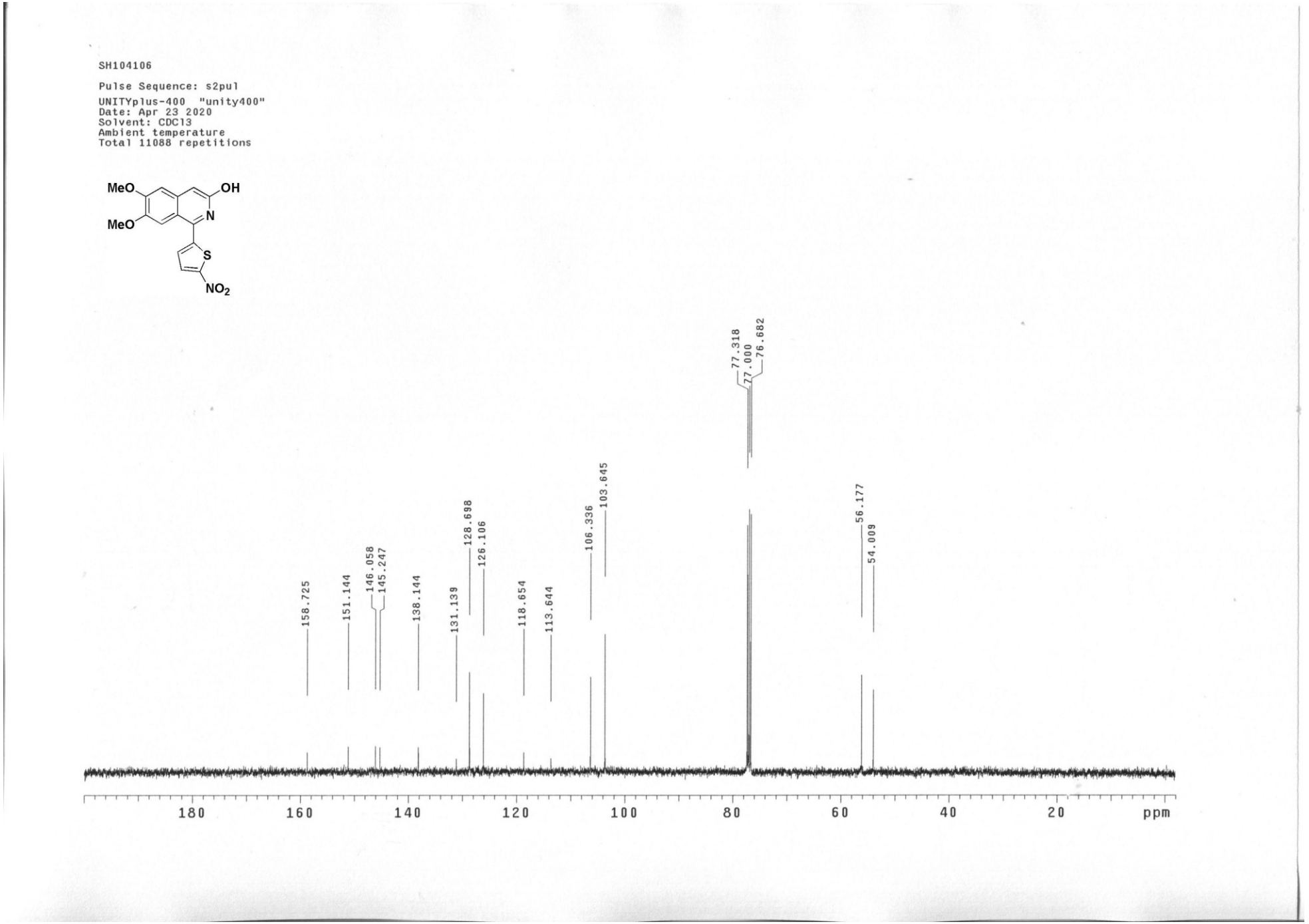
Compound 4ad (^{13}C-NMR spectral data)



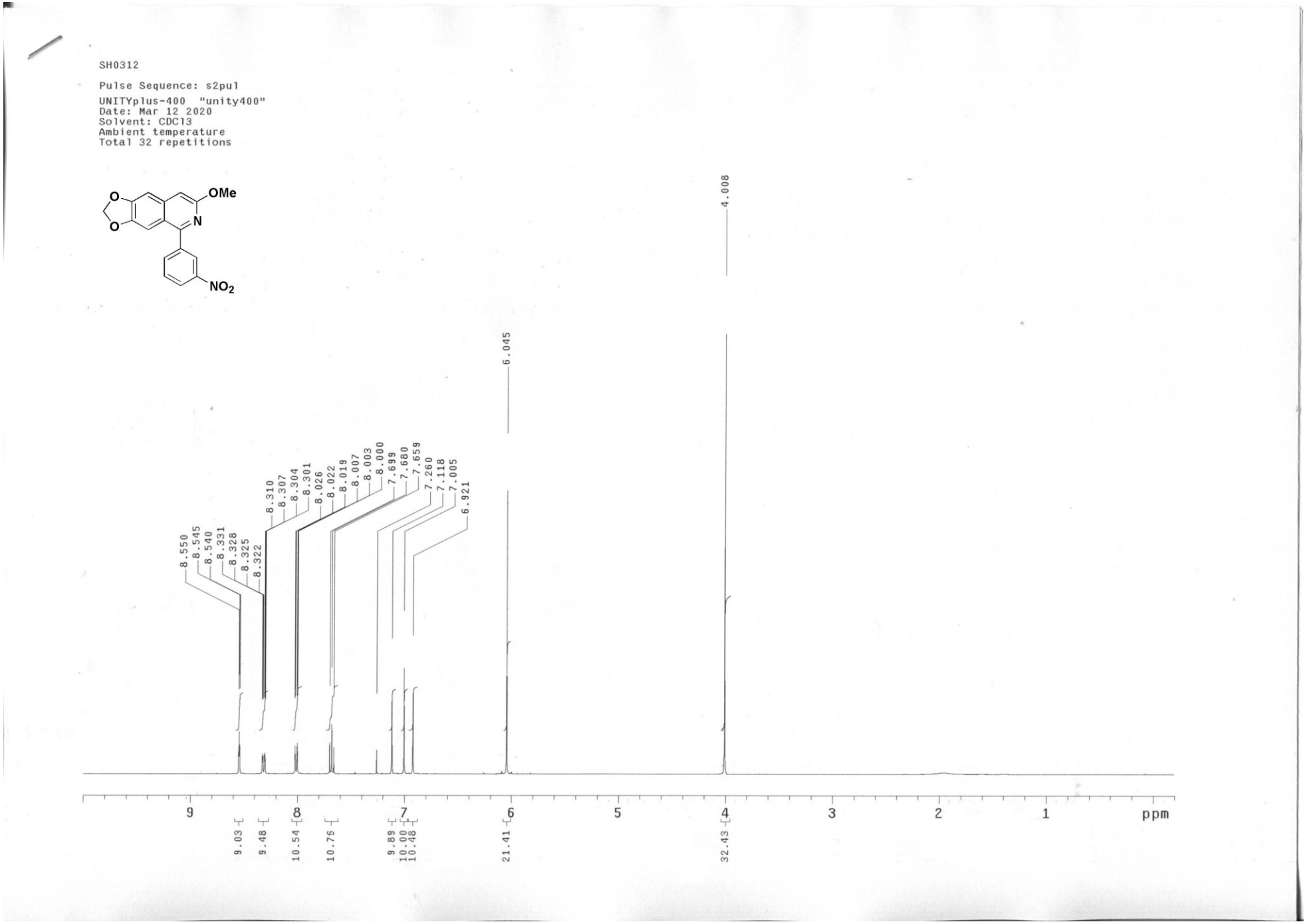
Compound 4ad-1 (^{1}H-NMR spectral data)



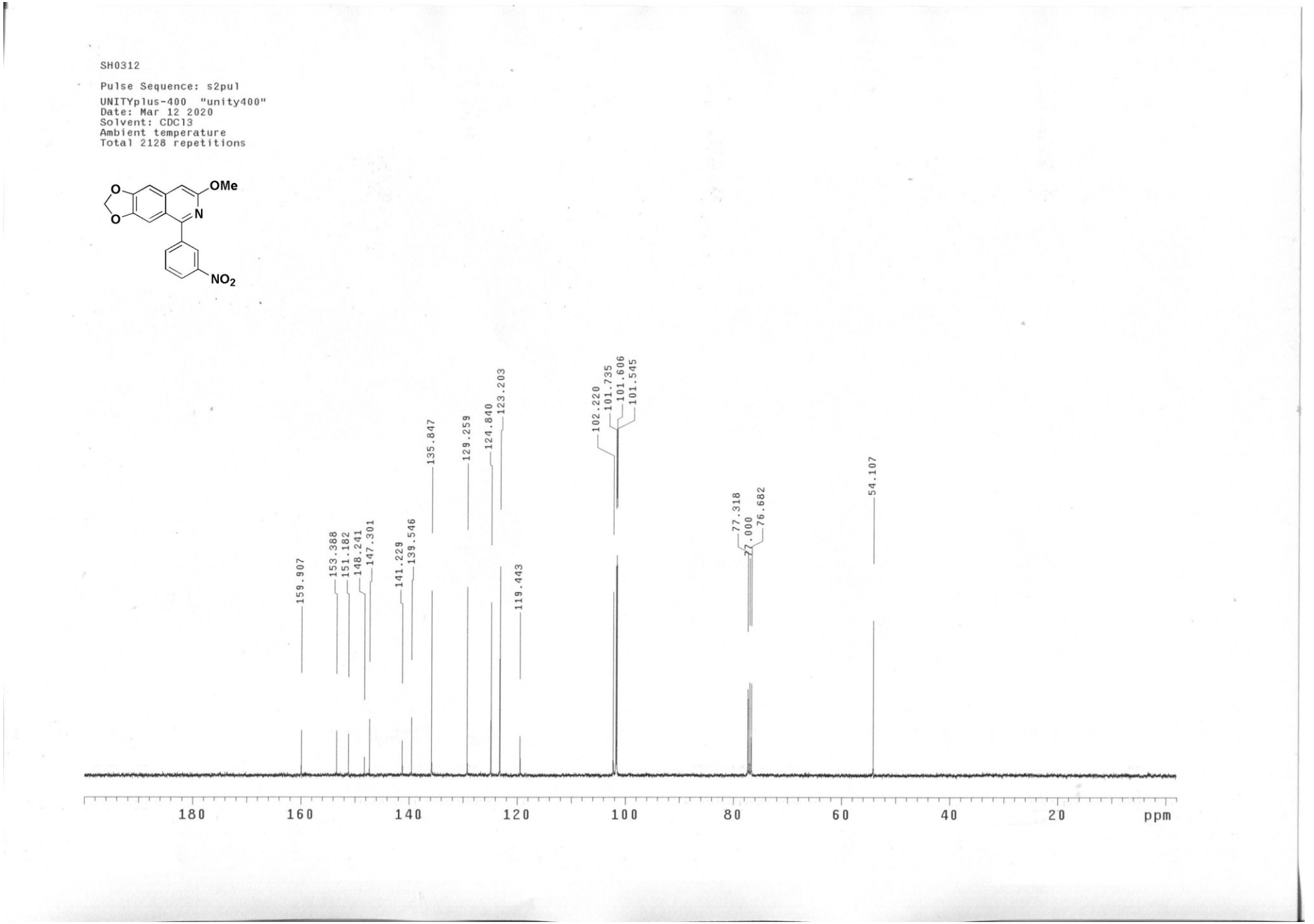
Compound 4ad-1 (^{13}C-NMR spectral data)



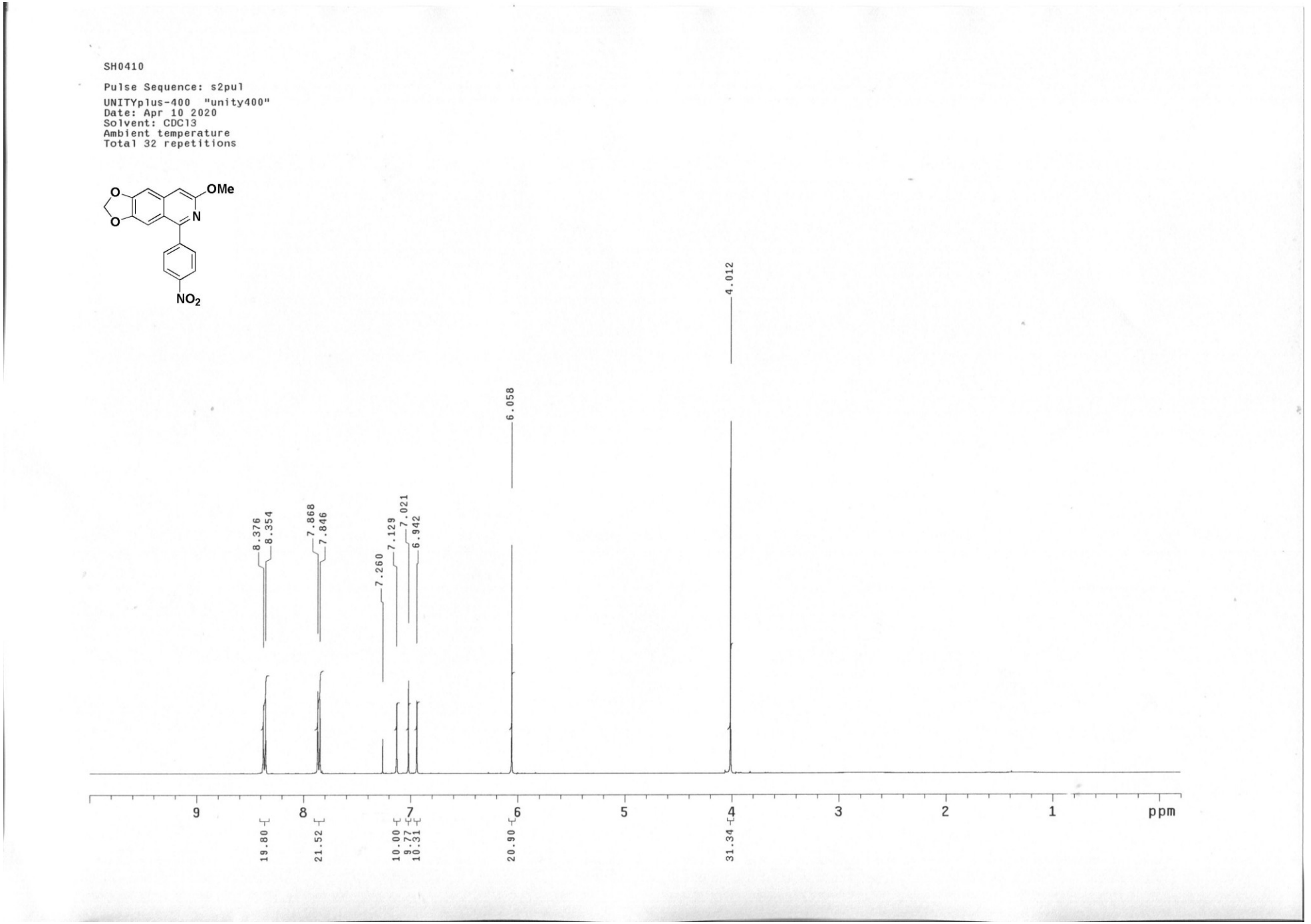
Compound 4ae (^{1}H-NMR spectral data)



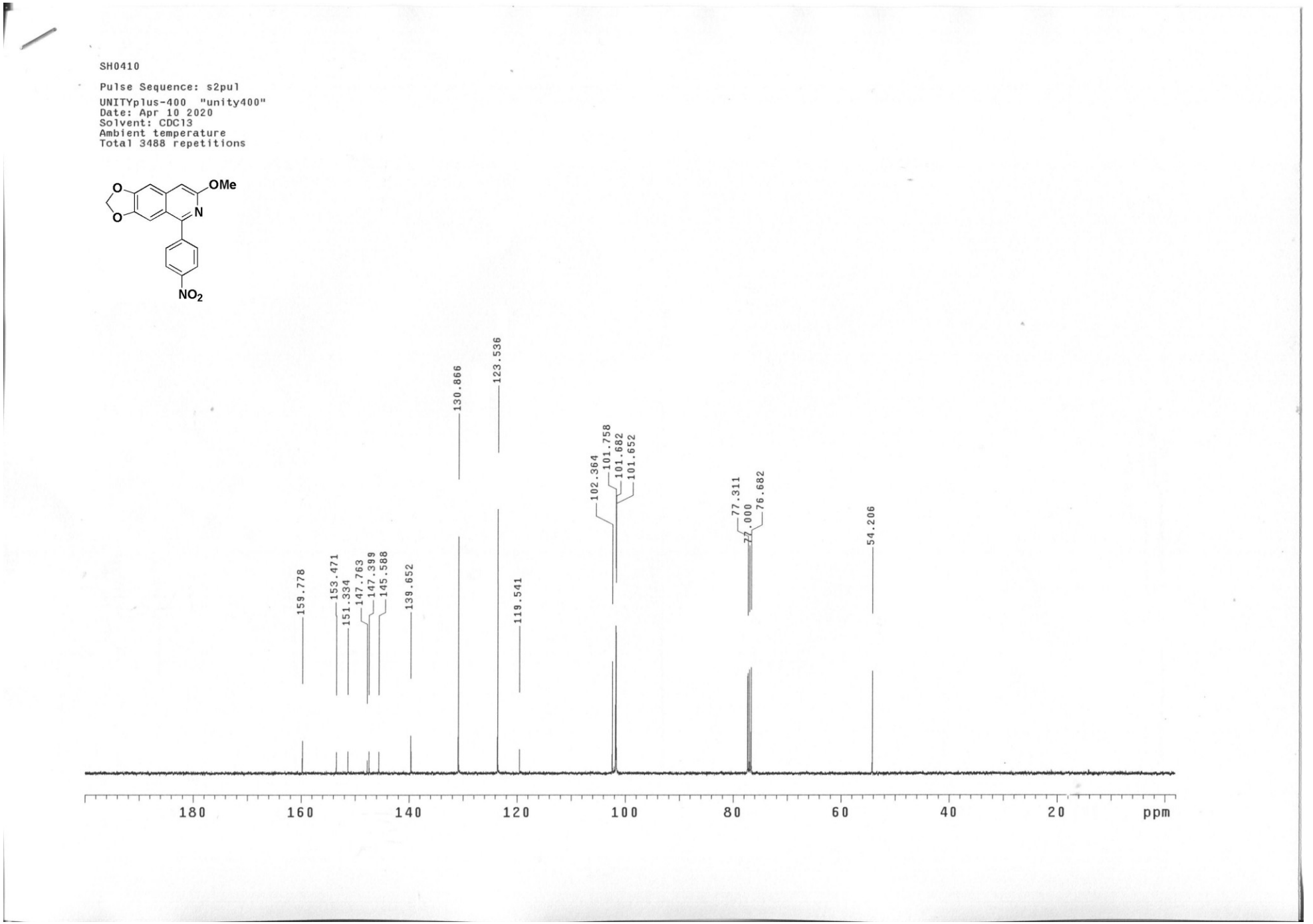
Compound 4ae (^{13}C-NMR spectral data)



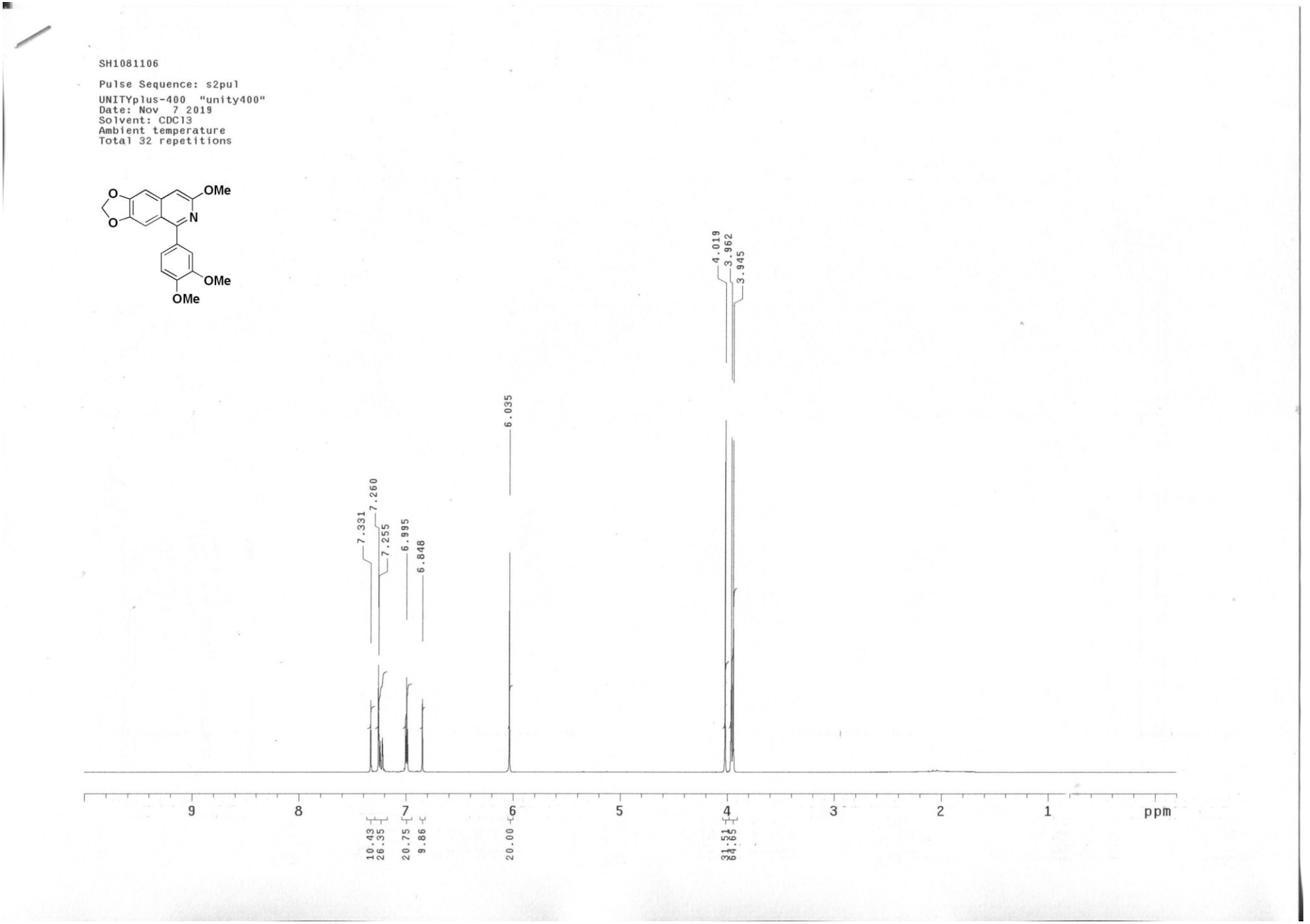
Compound 4af (^{1}H-NMR spectral data)



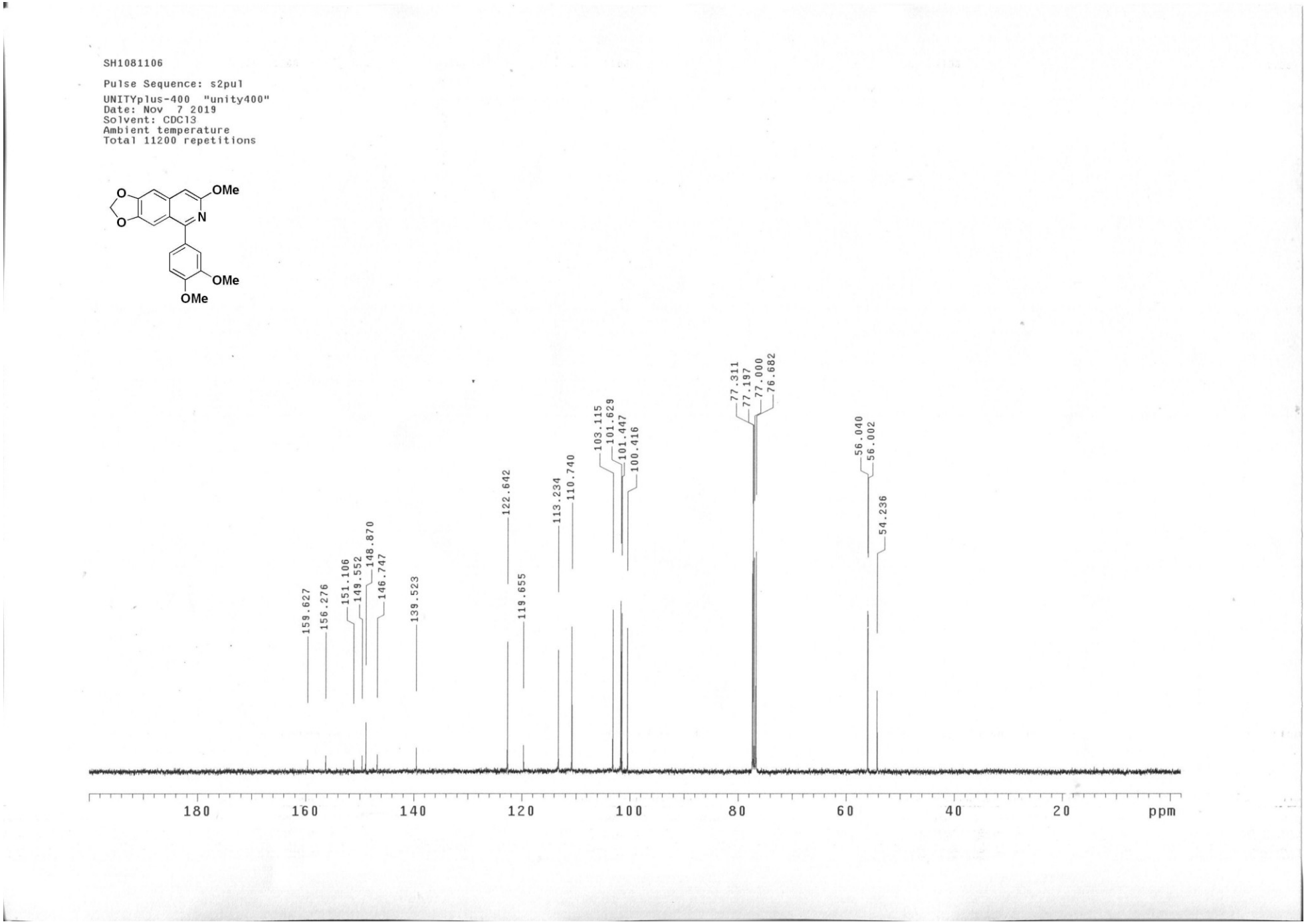
Compound 4af (^{13}C-NMR spectral data)



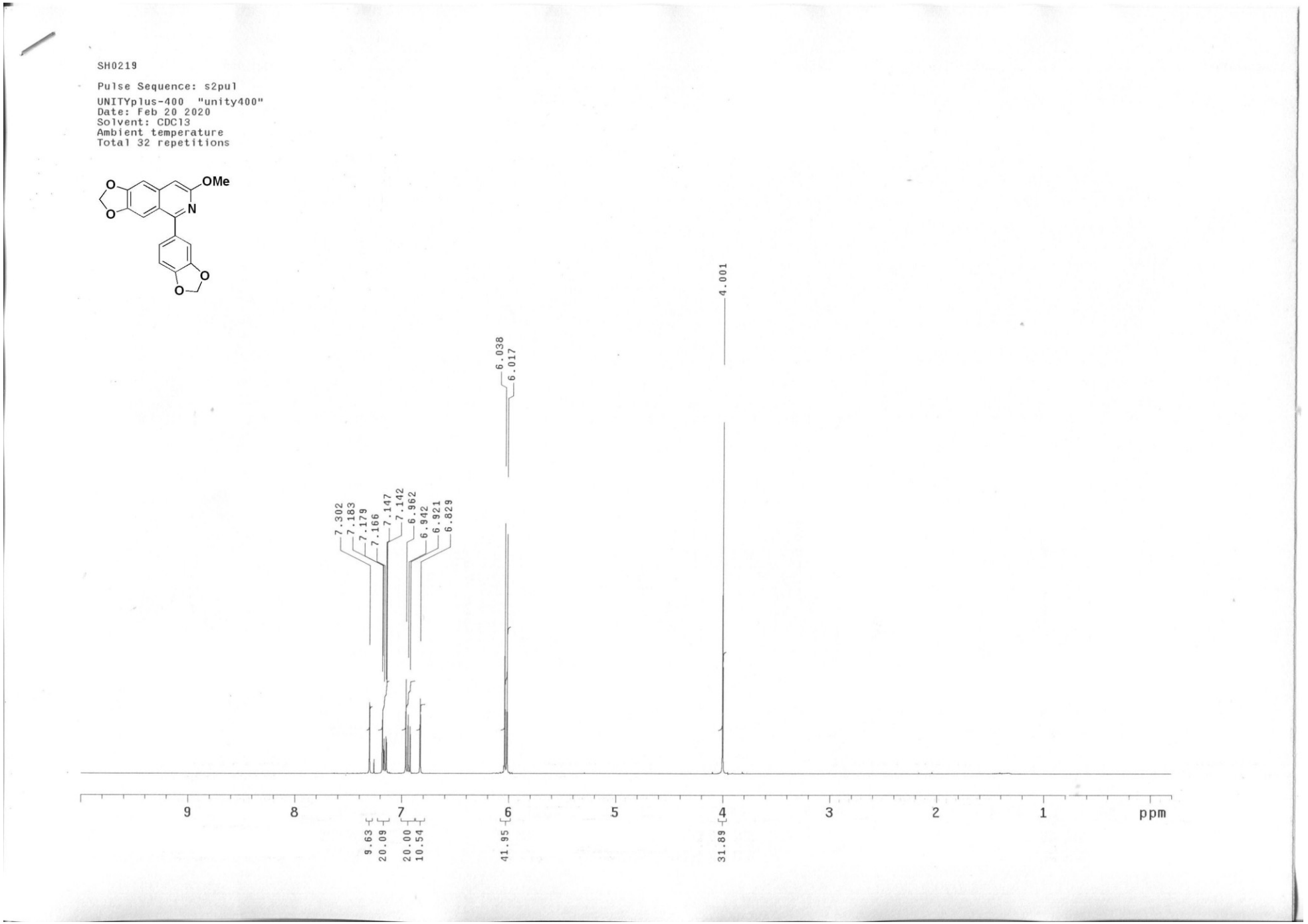
Compound 4ag (^{1}H-NMR spectral data)



Compound 4ag (^{13}C-NMR spectral data)



Compound 4ah (^{1}H-NMR spectral data)

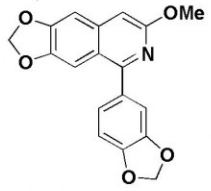


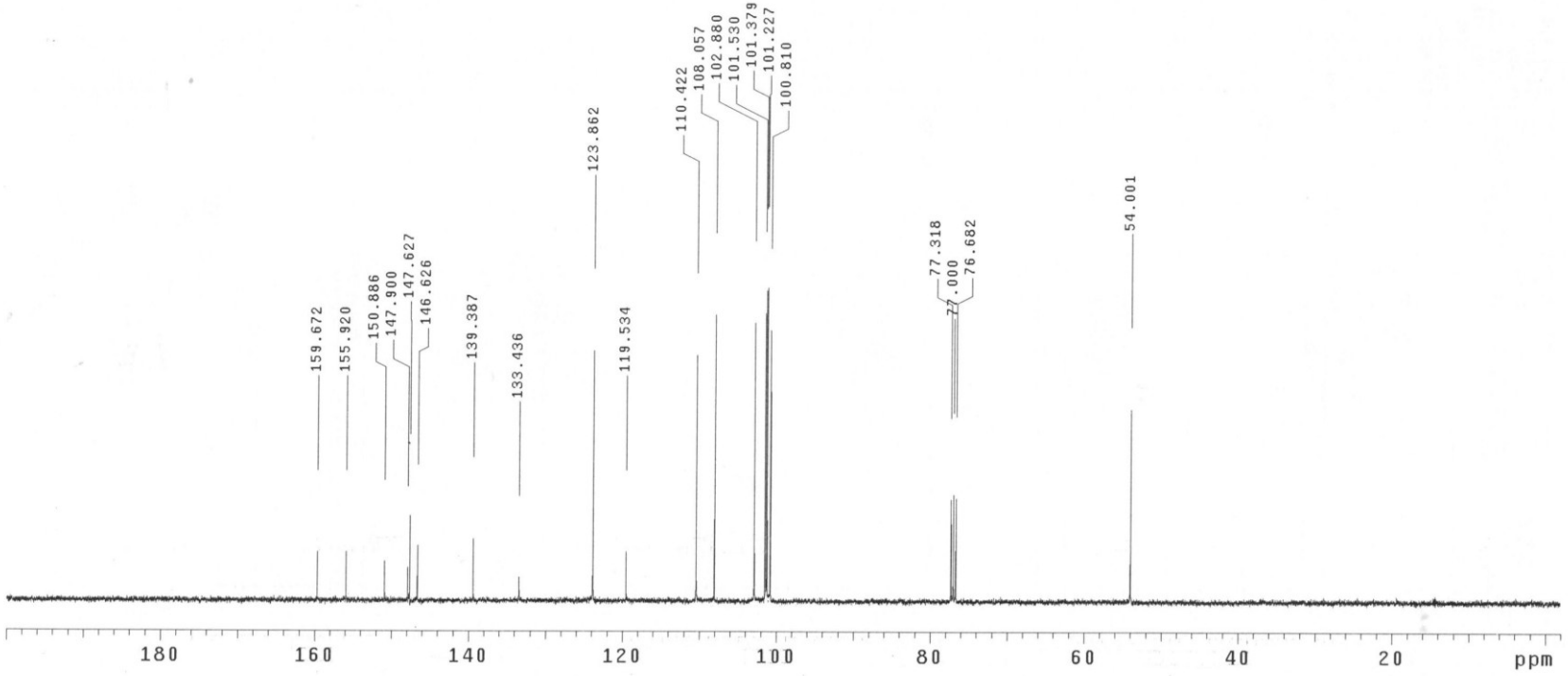
Compound 4ah (^{13}C-NMR spectral data)

SH0219

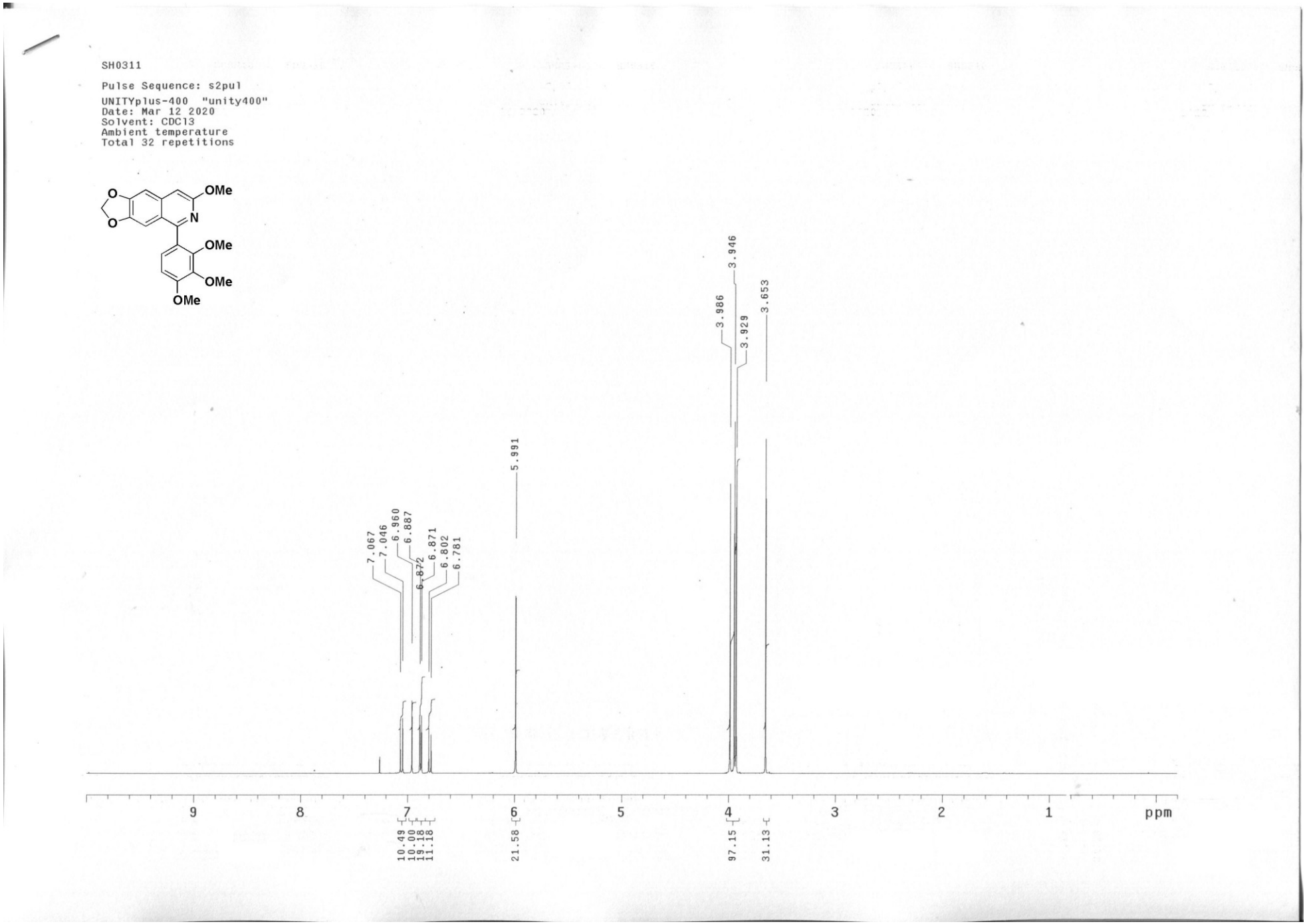
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Feb 20 2020
Solvent: CDCl3
Ambient temperature
Total 2128 repetitions





Compound 4ai (^{1}H-NMR spectral data)

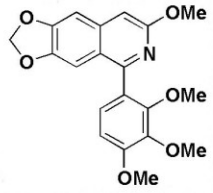


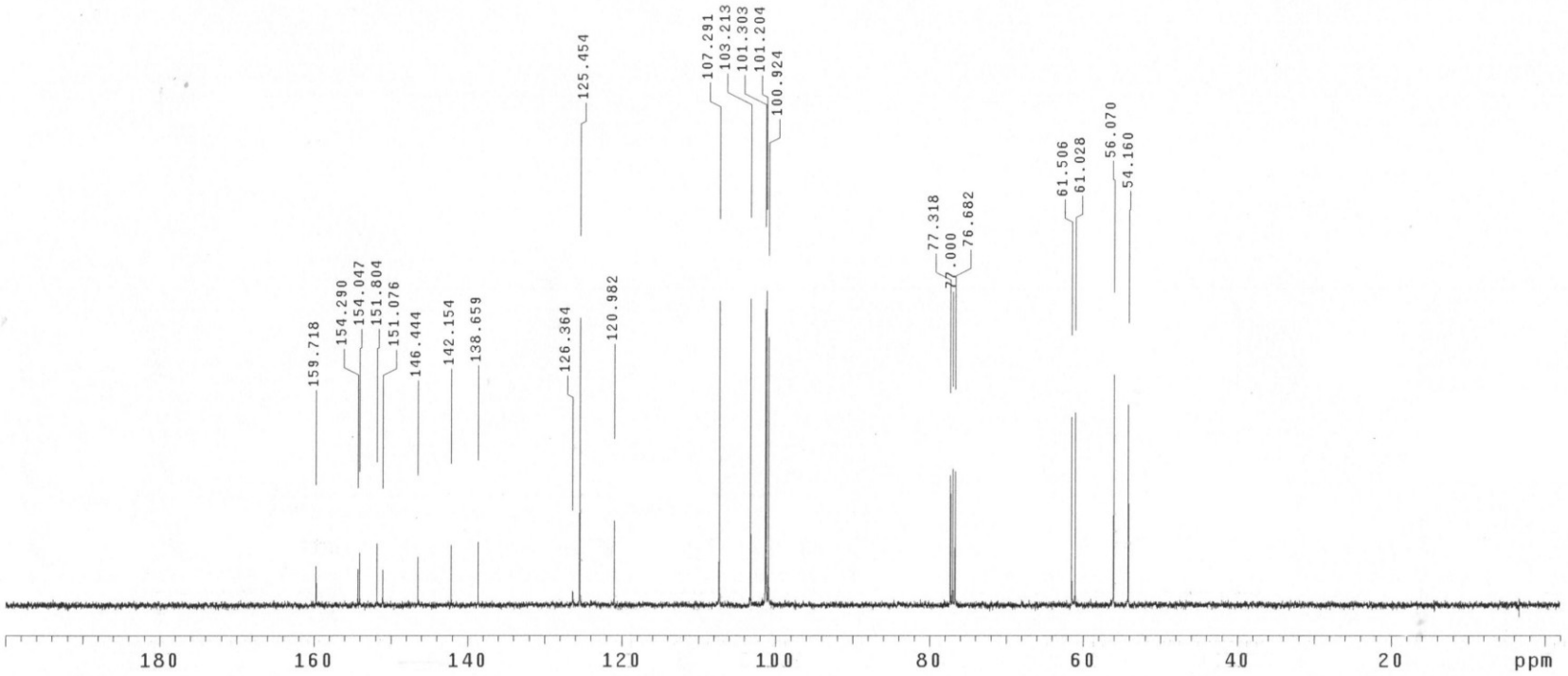
Compound 4ai (^{13}C-NMR spectral data)

SH0311

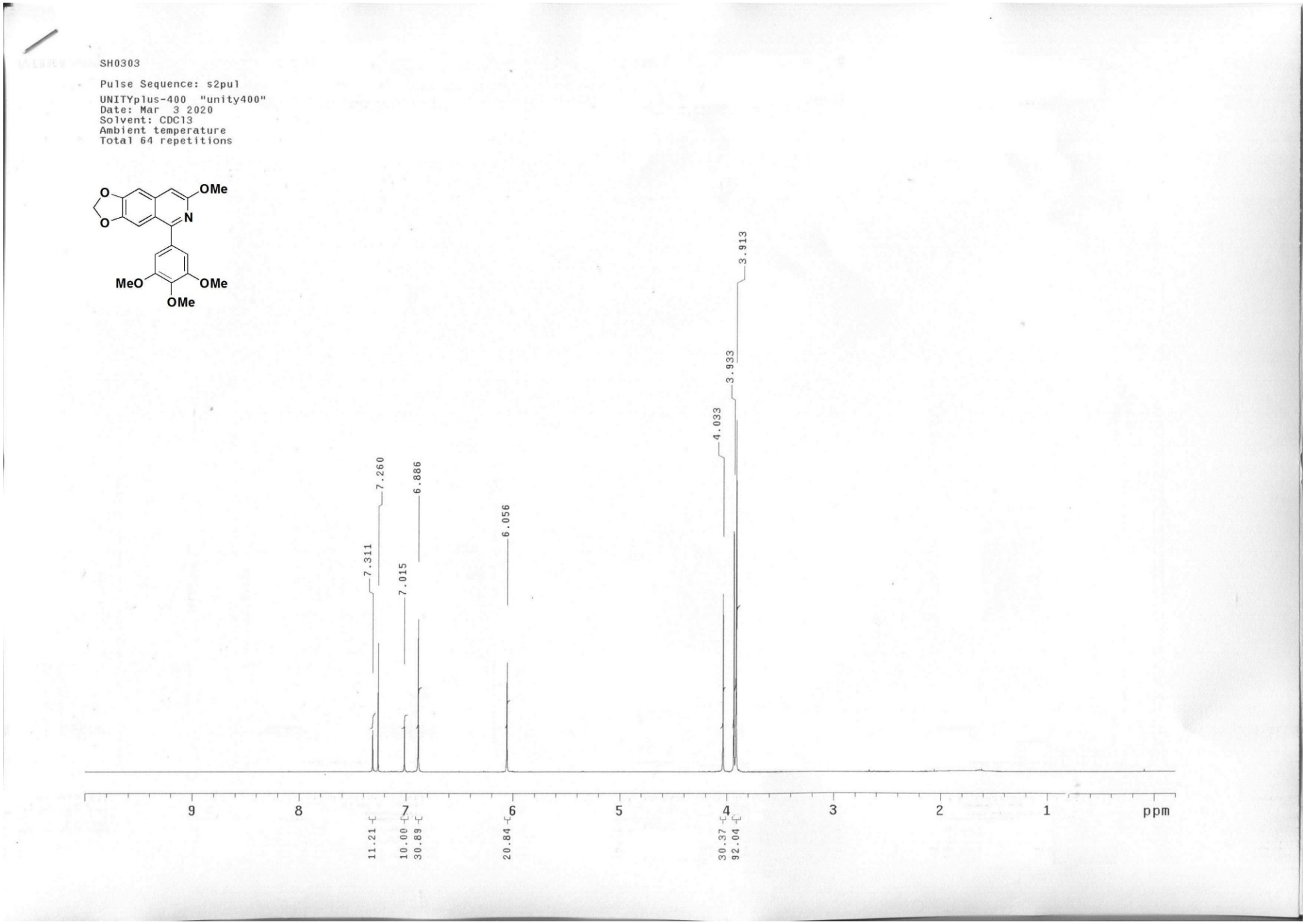
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Mar 12 2020
Solvent: CDCl3
Ambient temperature
Total 1712 repetitions

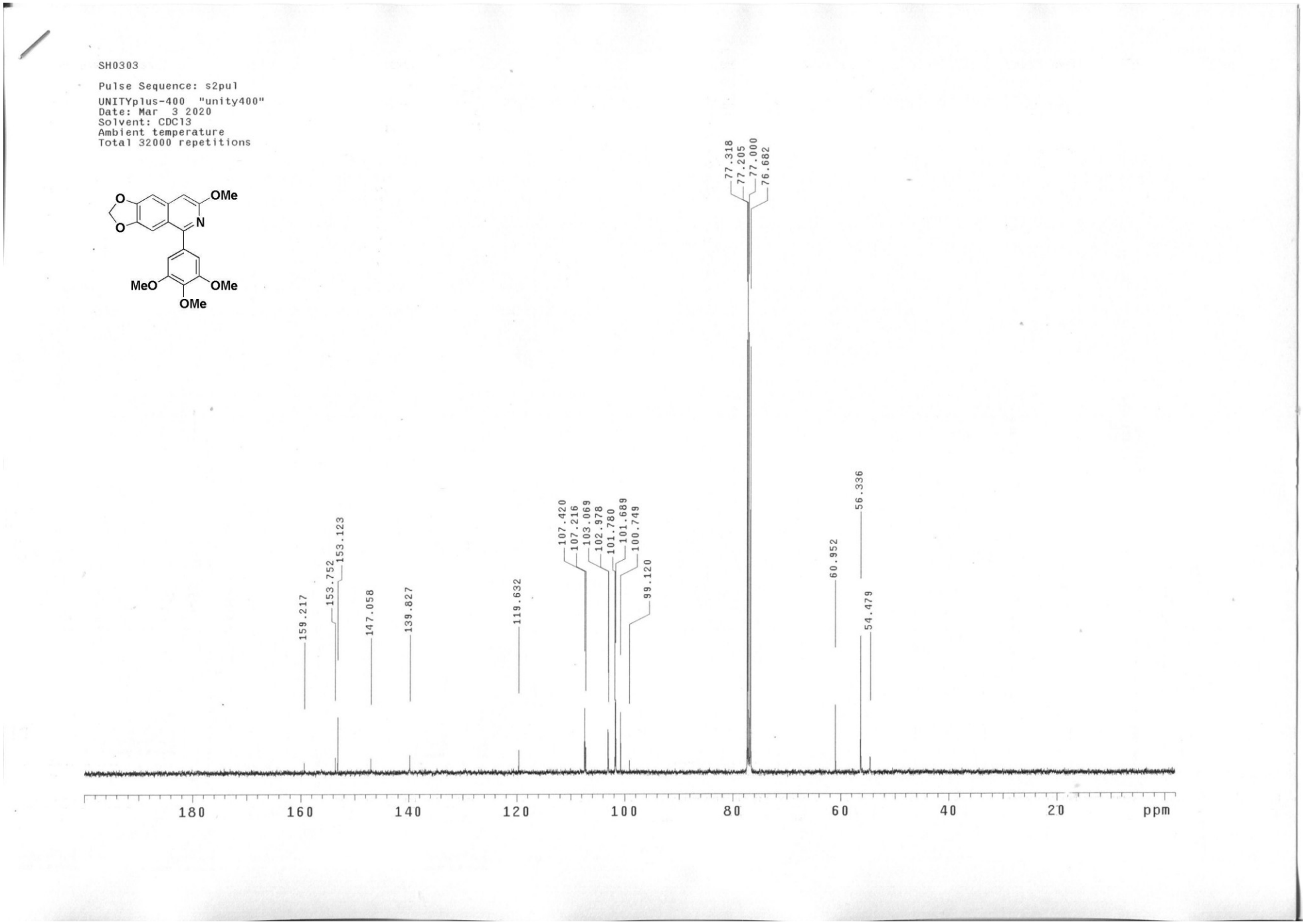




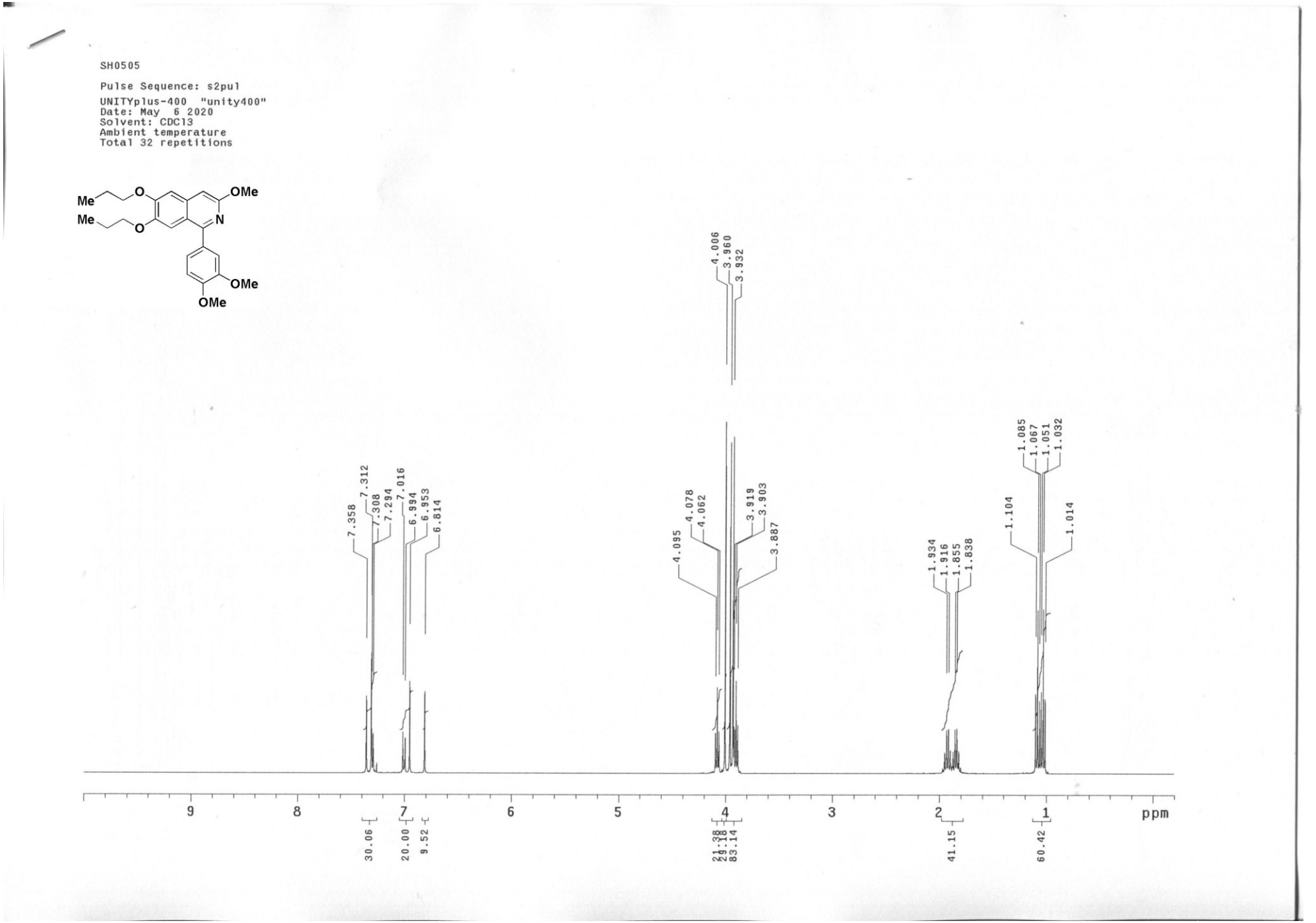
Compound 4aj (^{1}H-NMR spectral data)



Compound 4aj (^{13}C-NMR spectral data)



Compound 4ak (^{1}H-NMR spectral data)

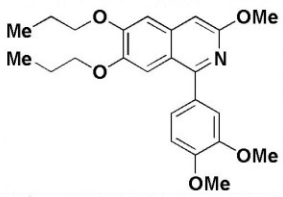


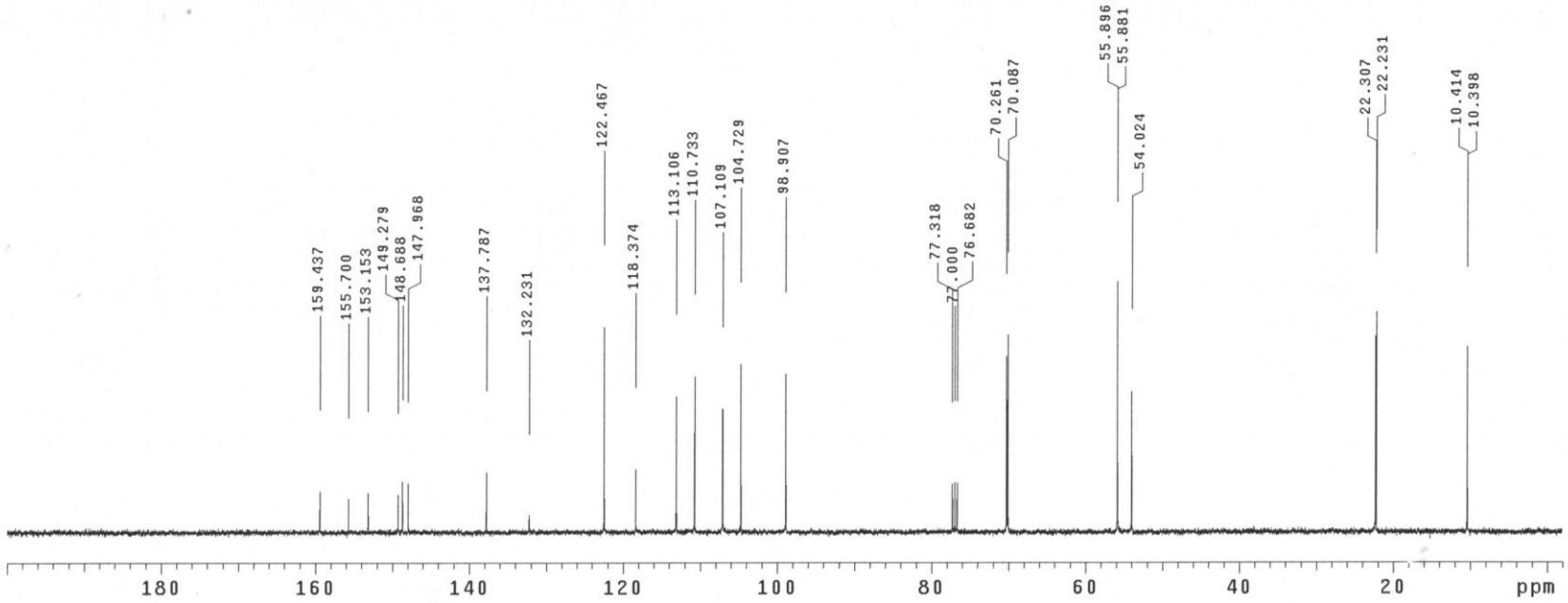
Compound 4ak (^{13}C-NMR spectral data)

SH0505

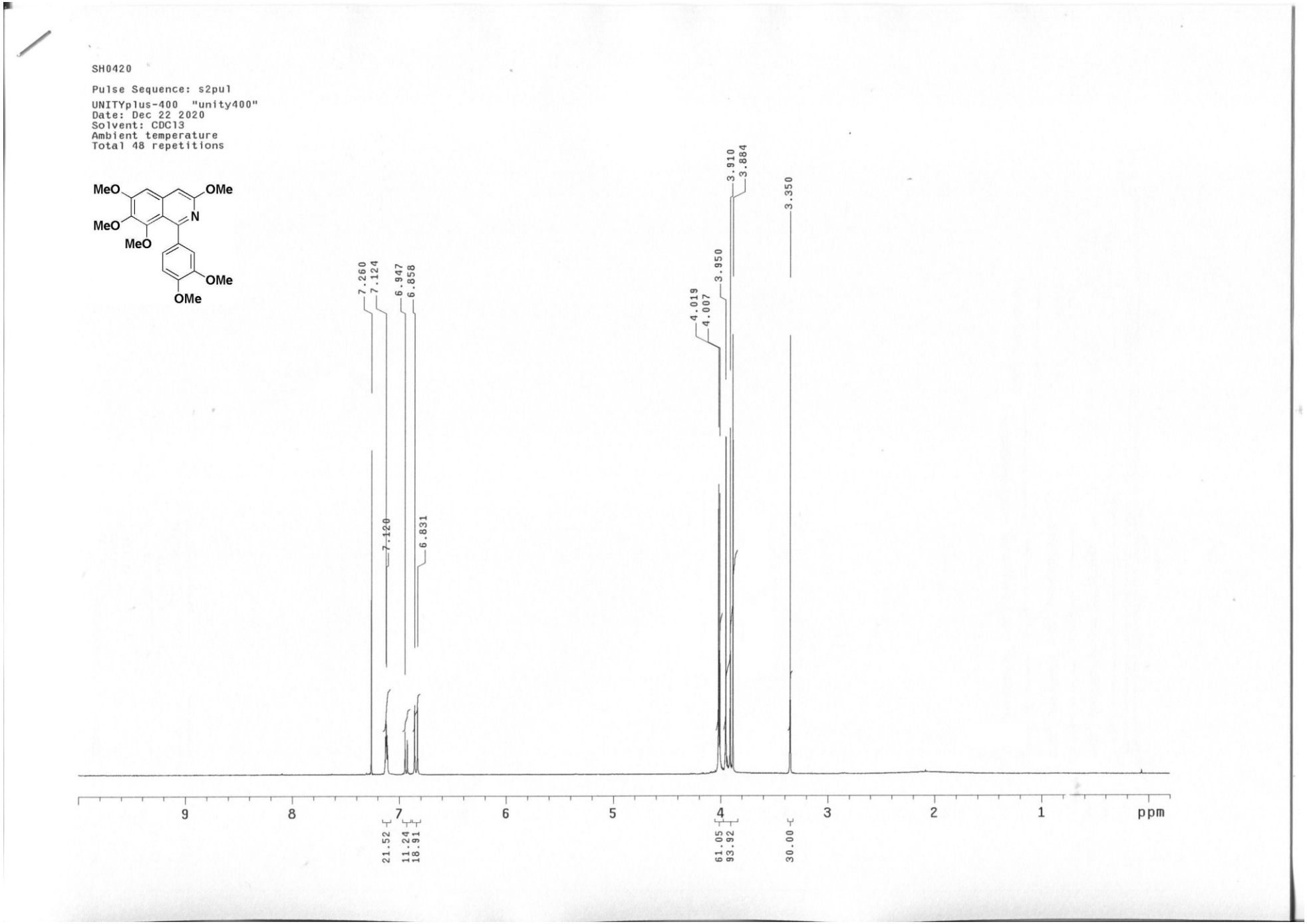
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 6 2020
Solvent: CDCl3
Ambient temperature
Total 512 repetitions

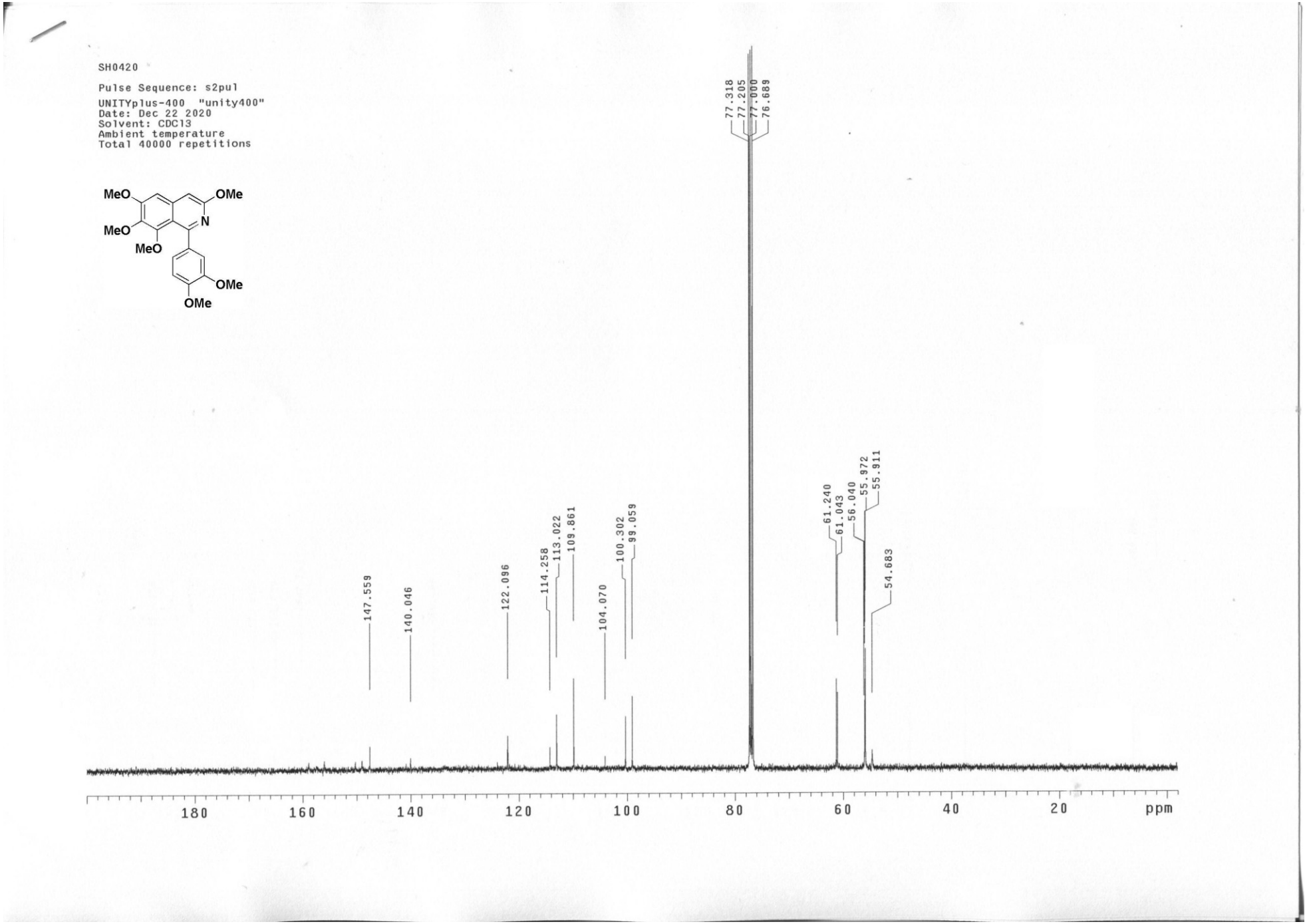




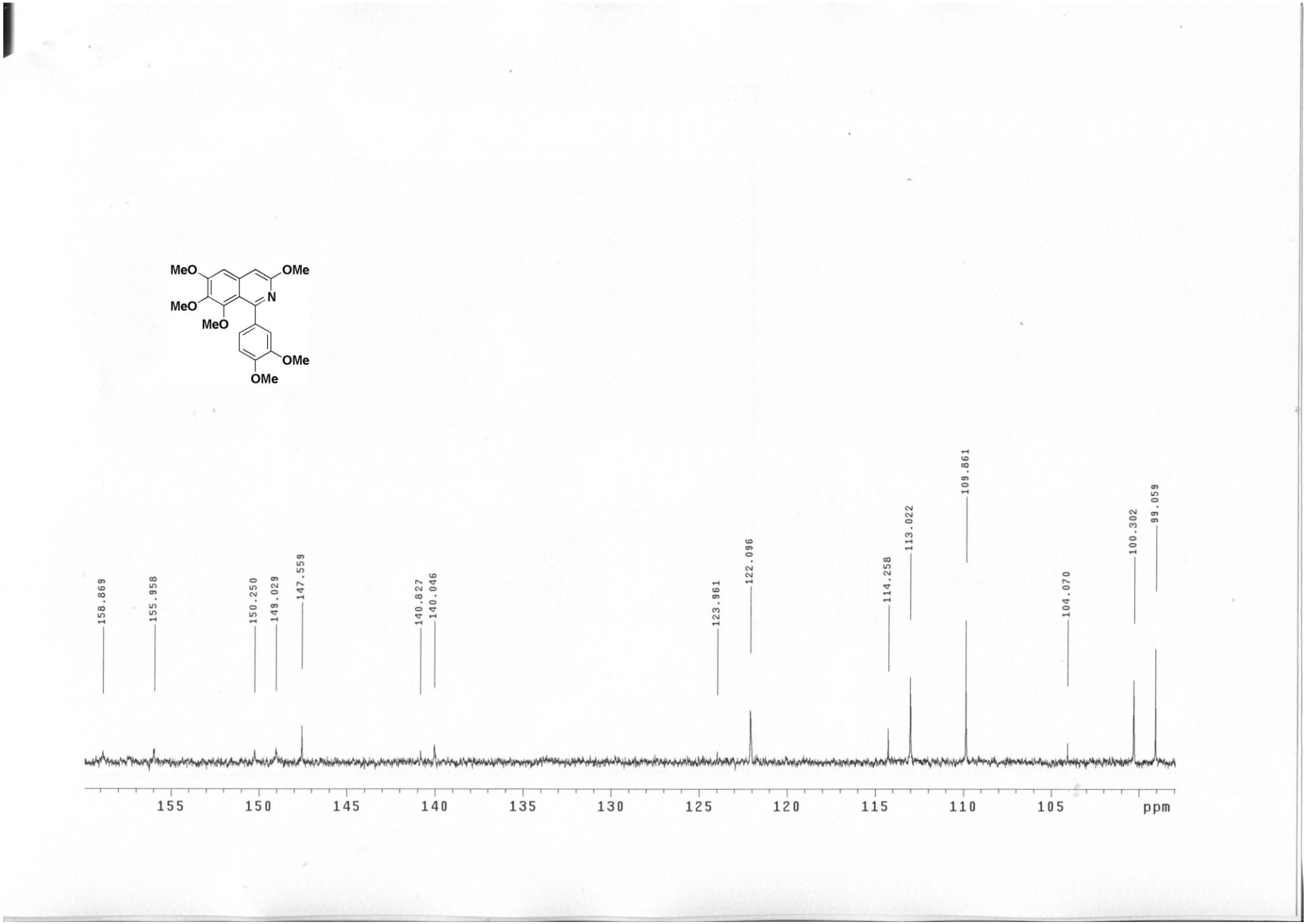
Compound 4al (^{1}H-NMR spectral data)



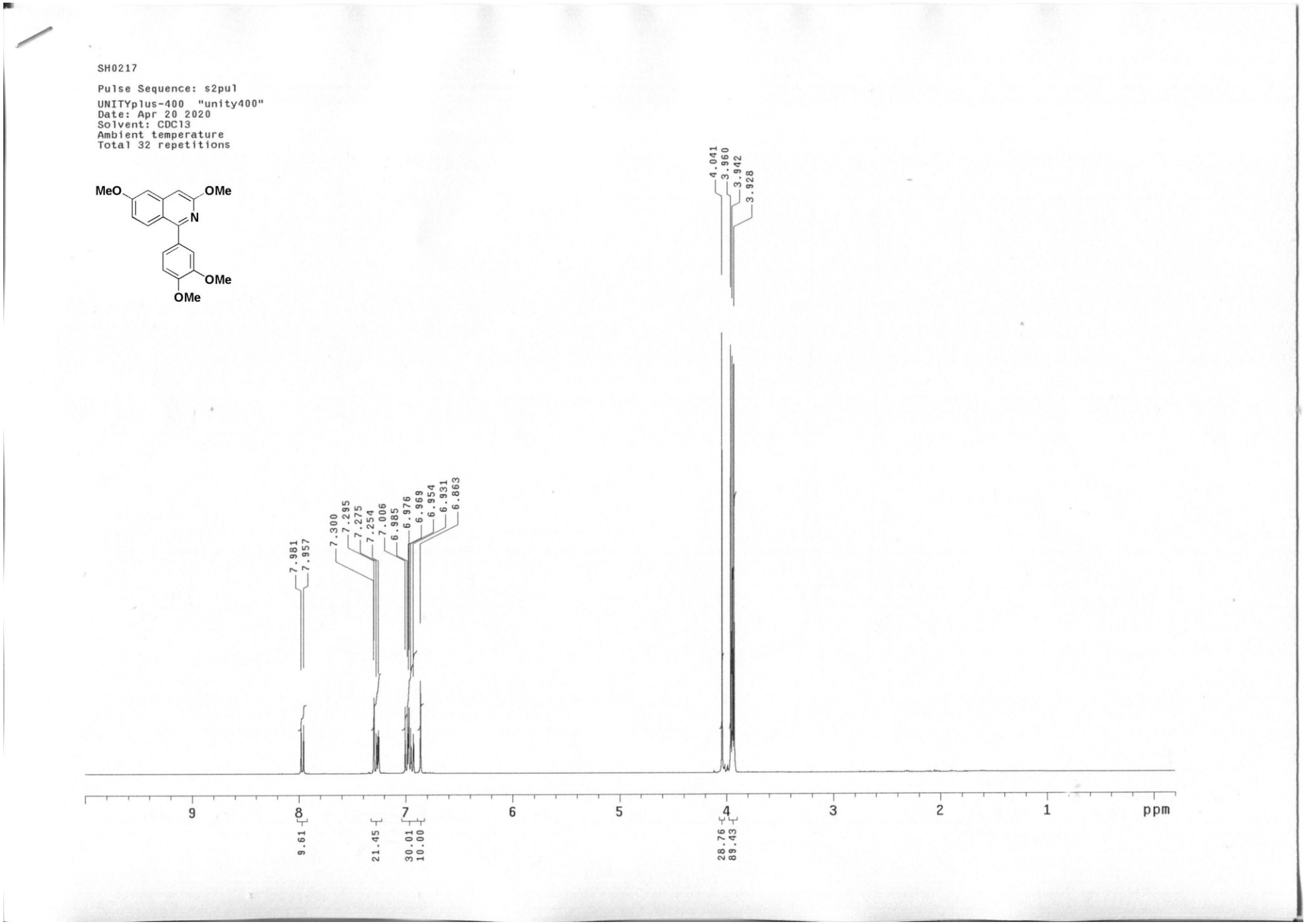
Compound 4al (^{13}C-NMR spectral data-1)



Compound 4al (^{13}C-NMR spectral data-2)



Compound 4am (^{1}H-NMR spectral data)

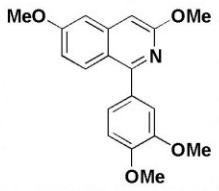


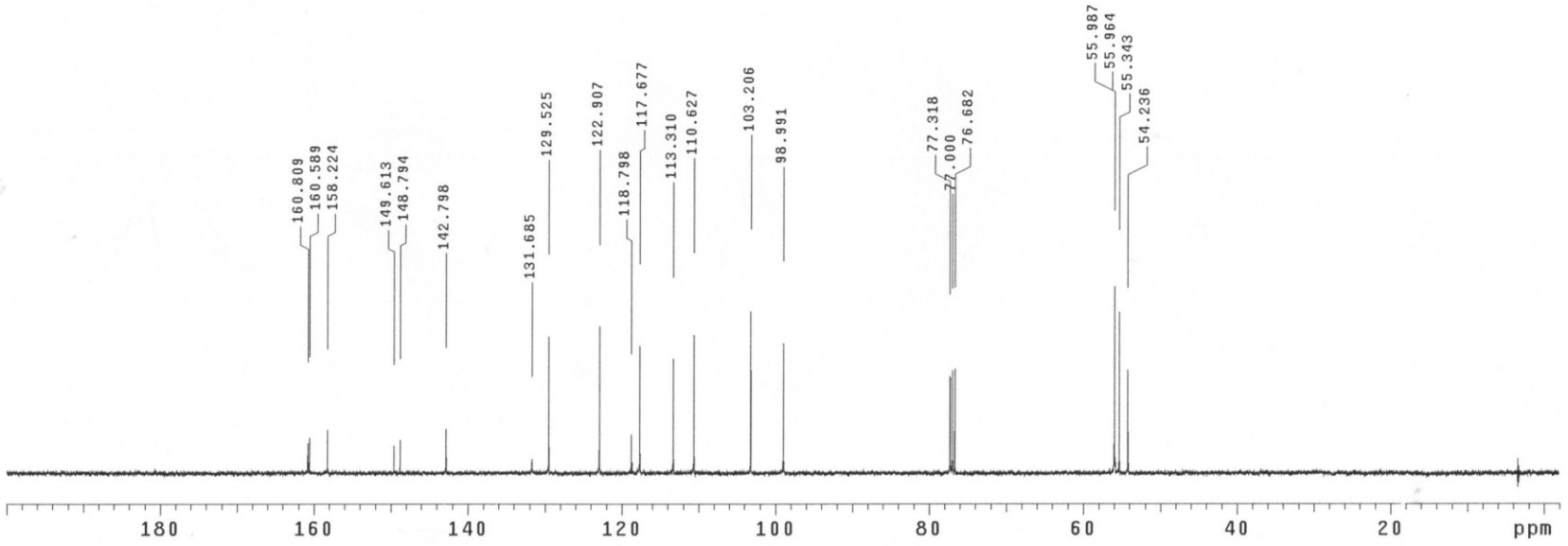
Compound 4am (^{13}C-NMR spectral data)

SH0217

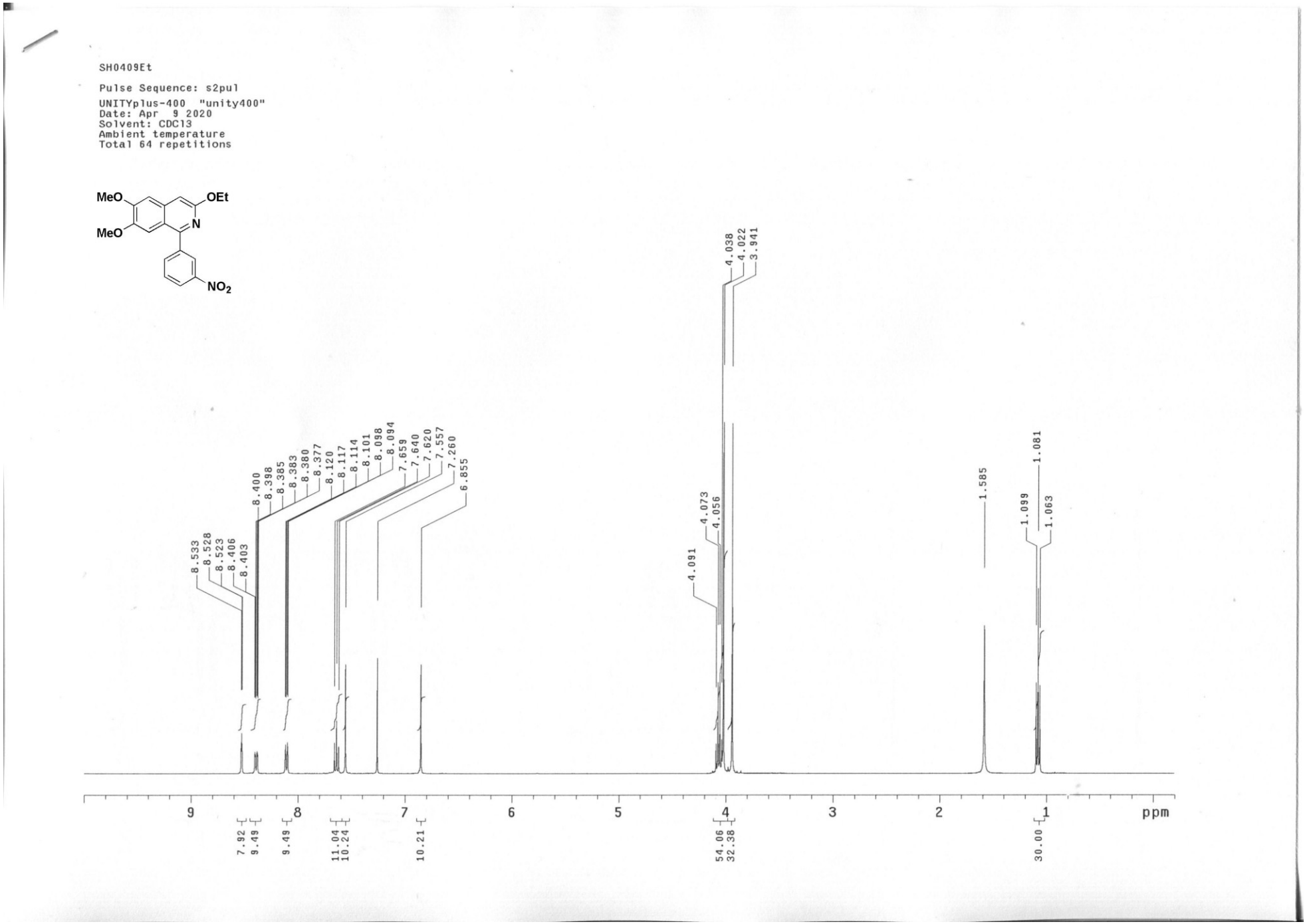
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Apr 20 2020
Solvent: CDCl3
Ambient temperature
Total 1536 repetitions

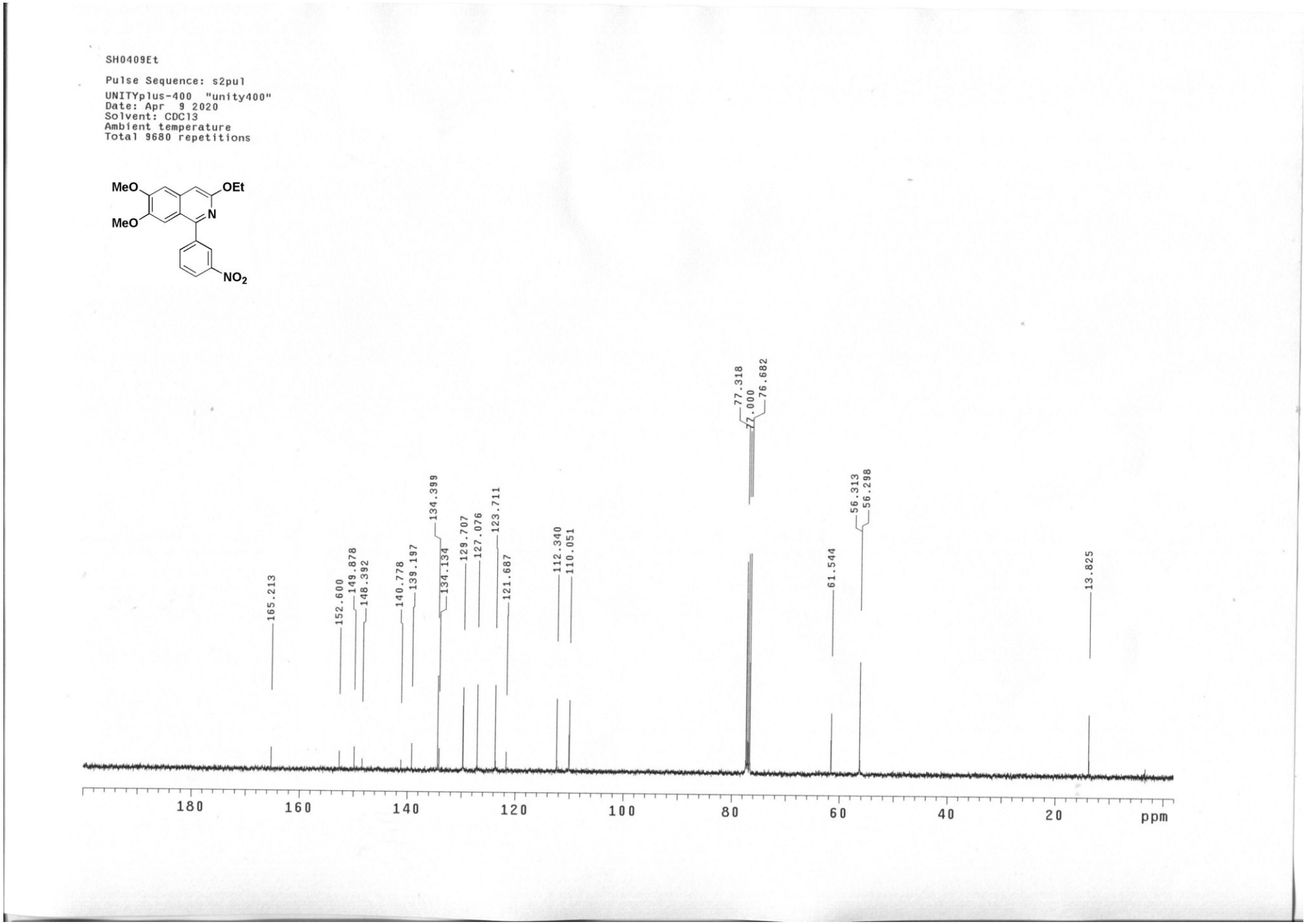




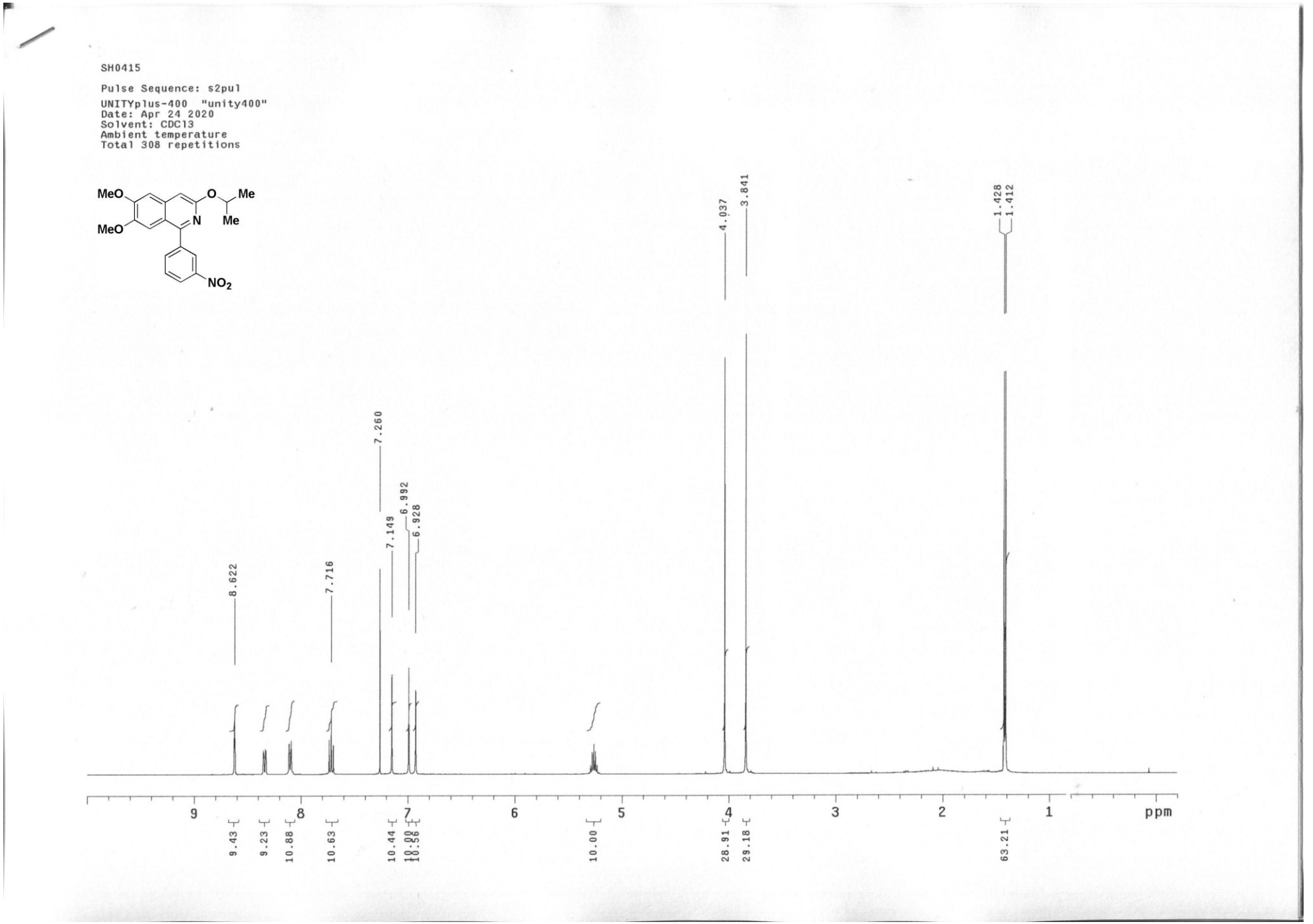
Compound 5a (^{1}H-NMR spectral data)



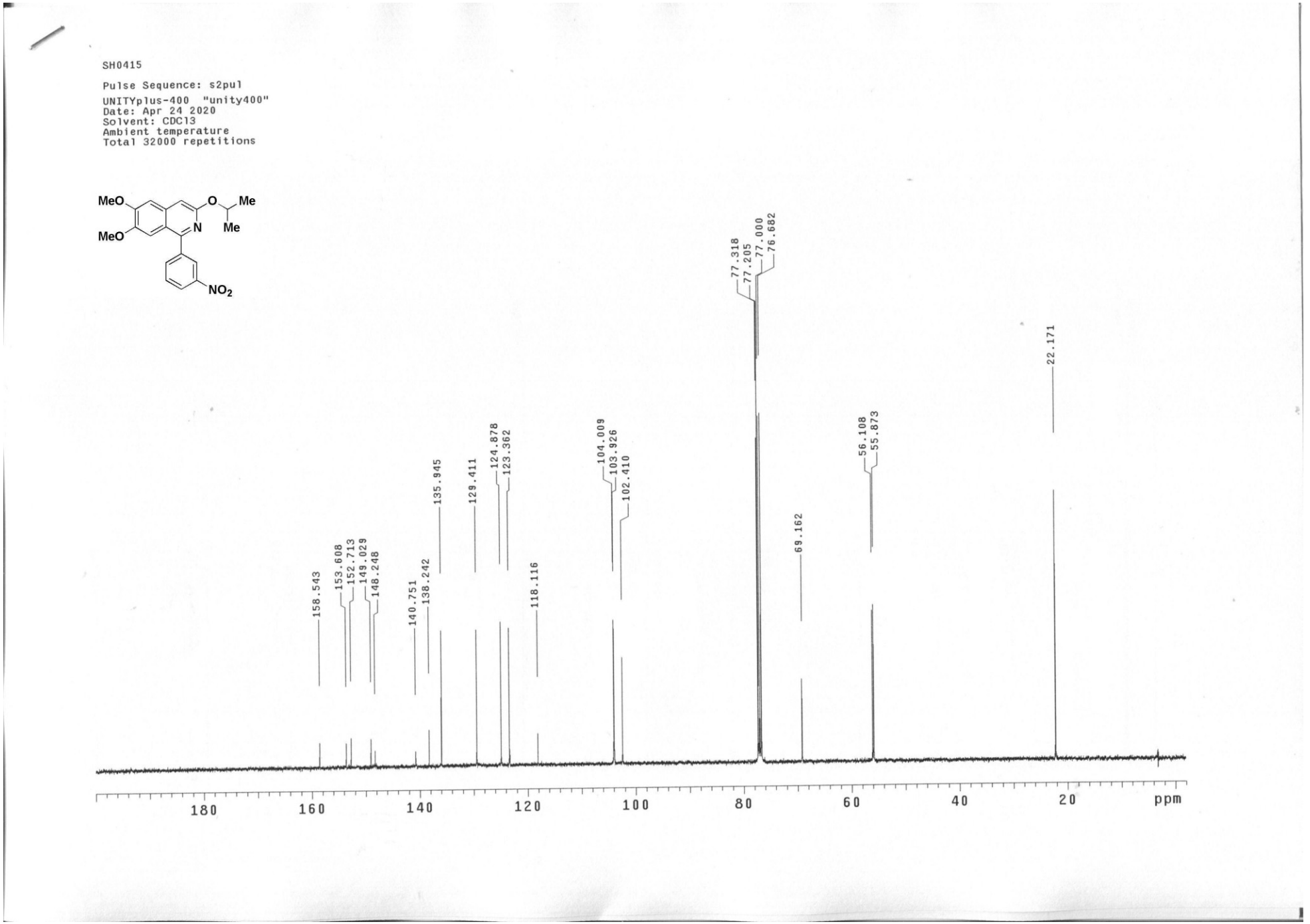
Compound 5a (^{13}C-NMR spectral data)



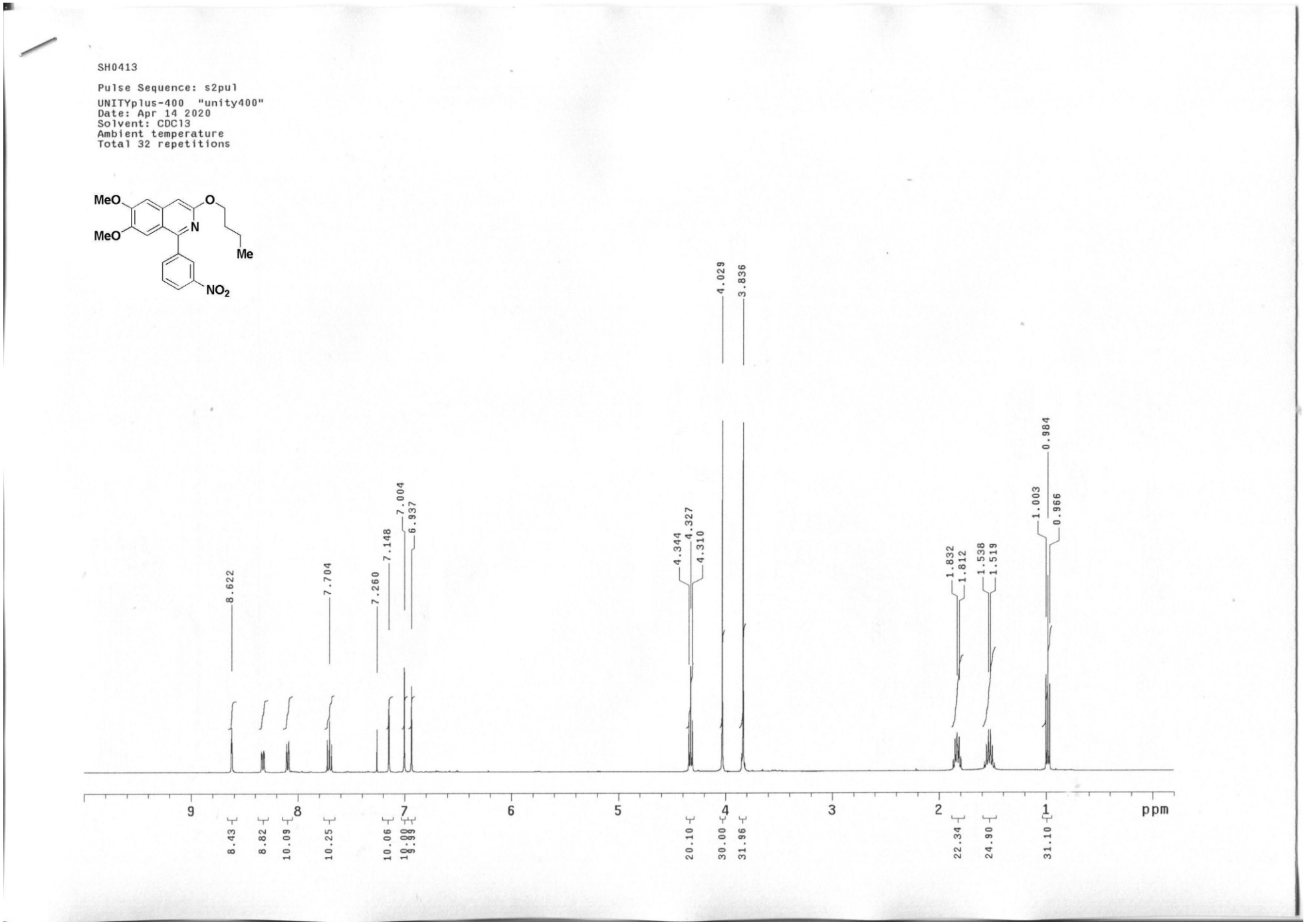
Compound 5b (^{1}H-NMR spectral data)



Compound 5b (^{13}C-NMR spectral data)



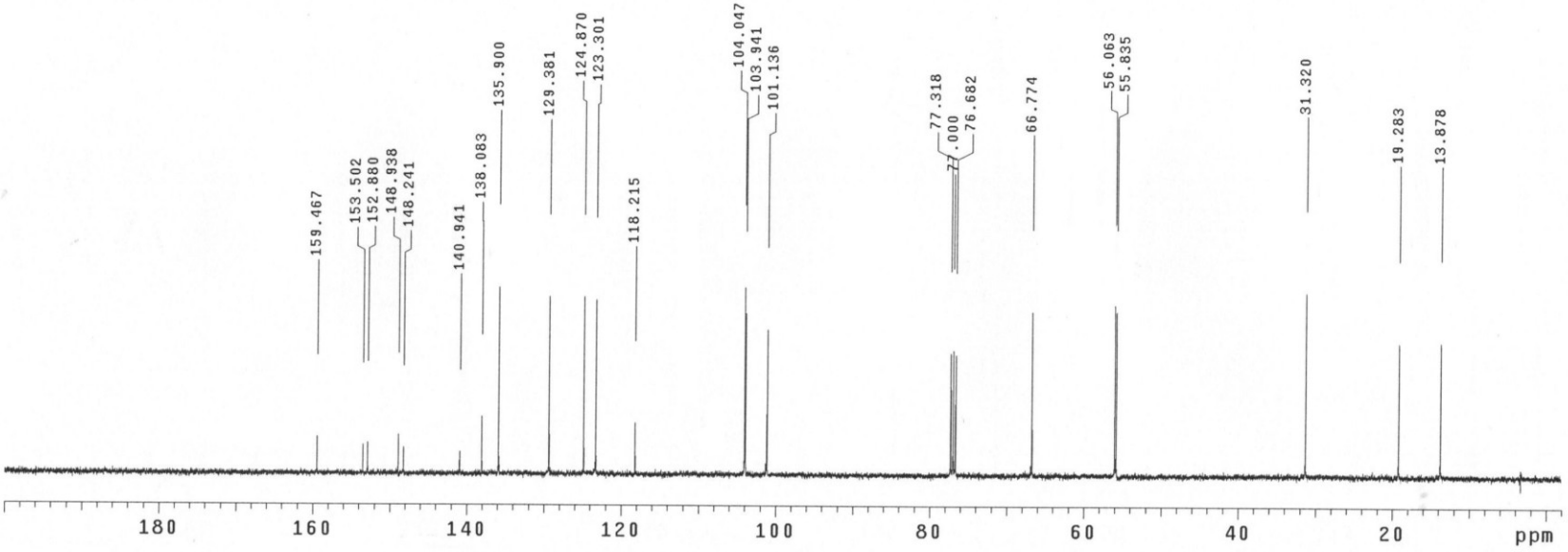
Compound 5c (^{1}H-NMR spectral data)



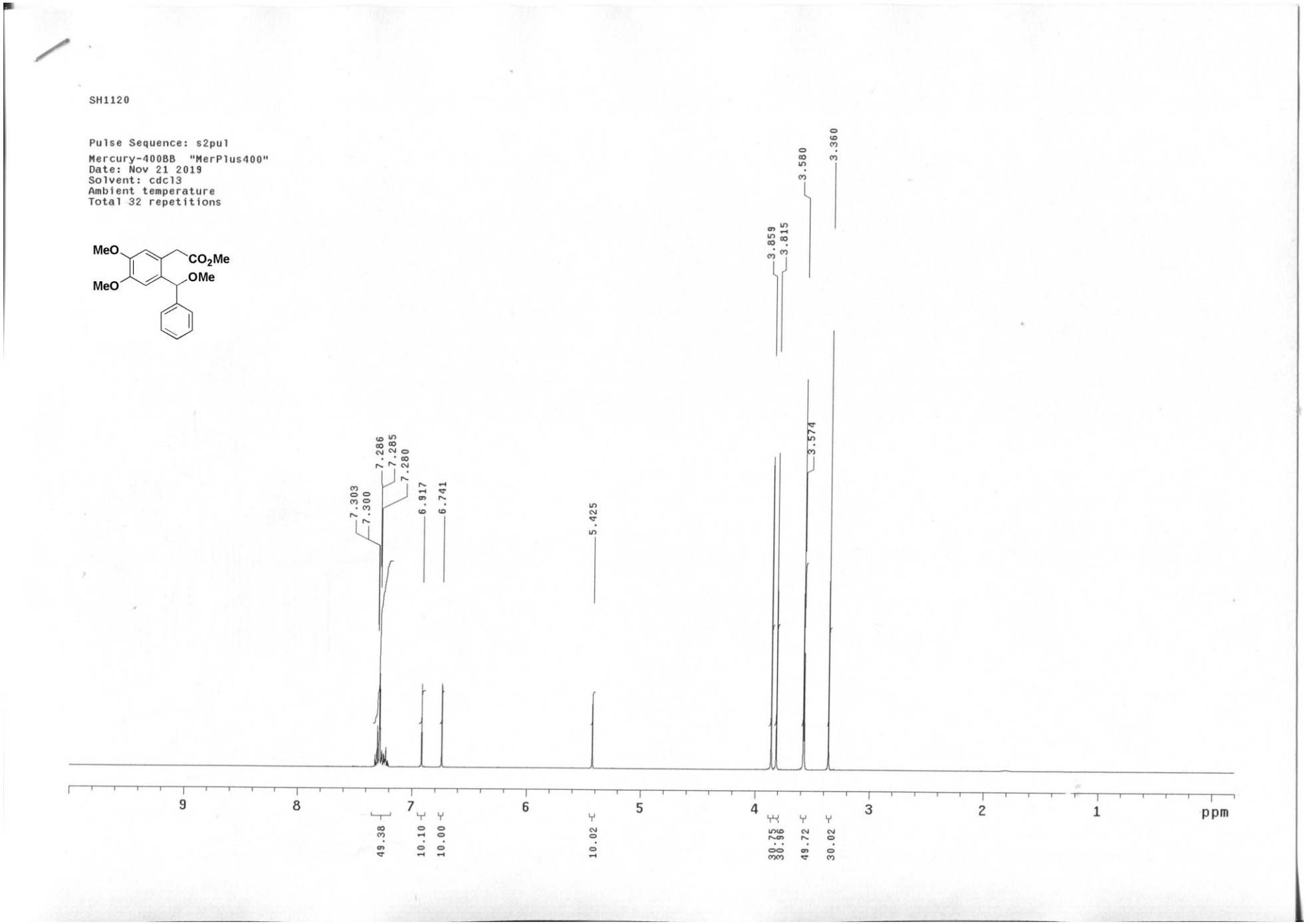
Compound 5c (^{13}C-NMR spectral data)

SH0413

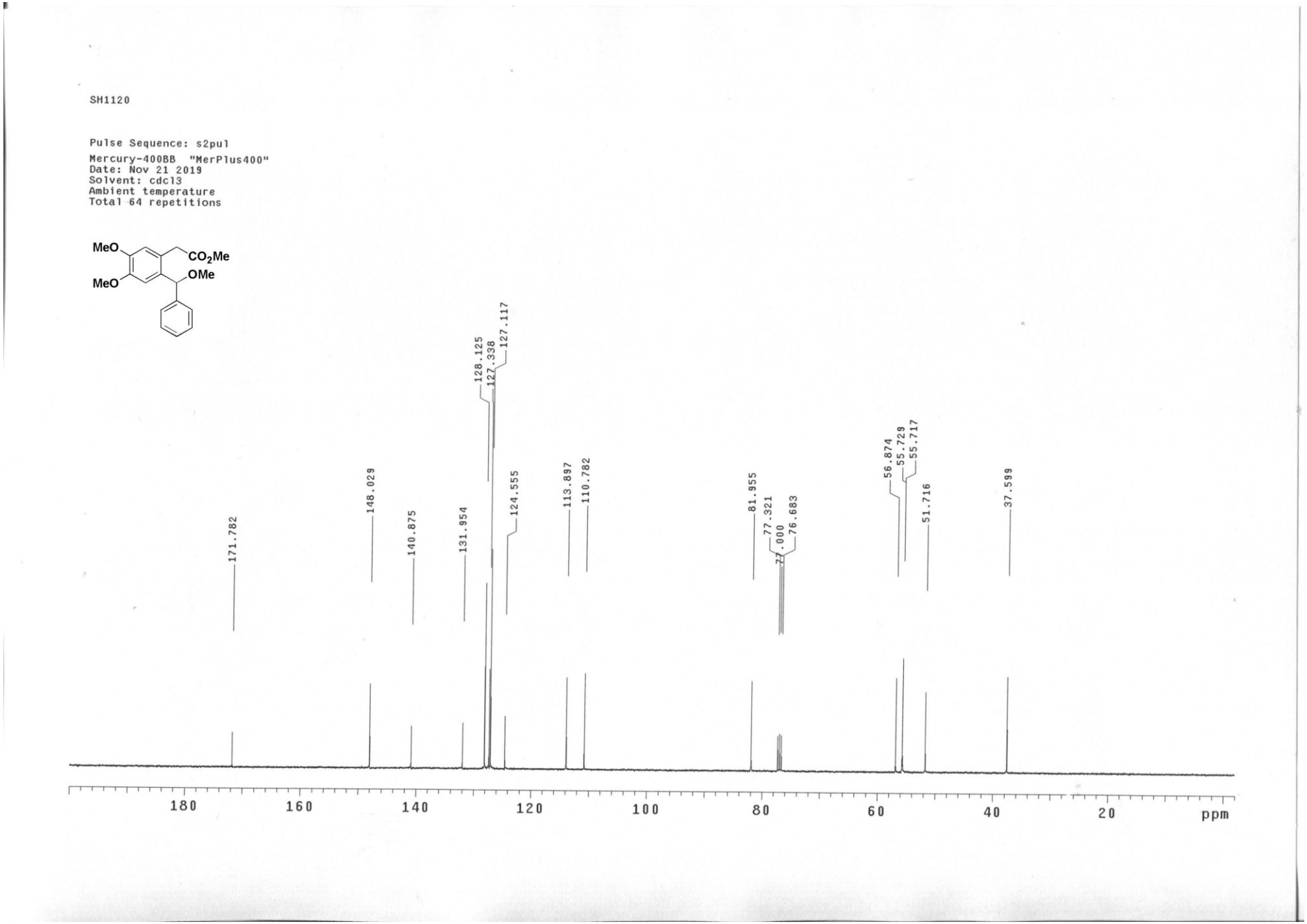
Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Apr 14 2020
Solvent: CDCl3
Ambient temperature
Total 3136 repetitions



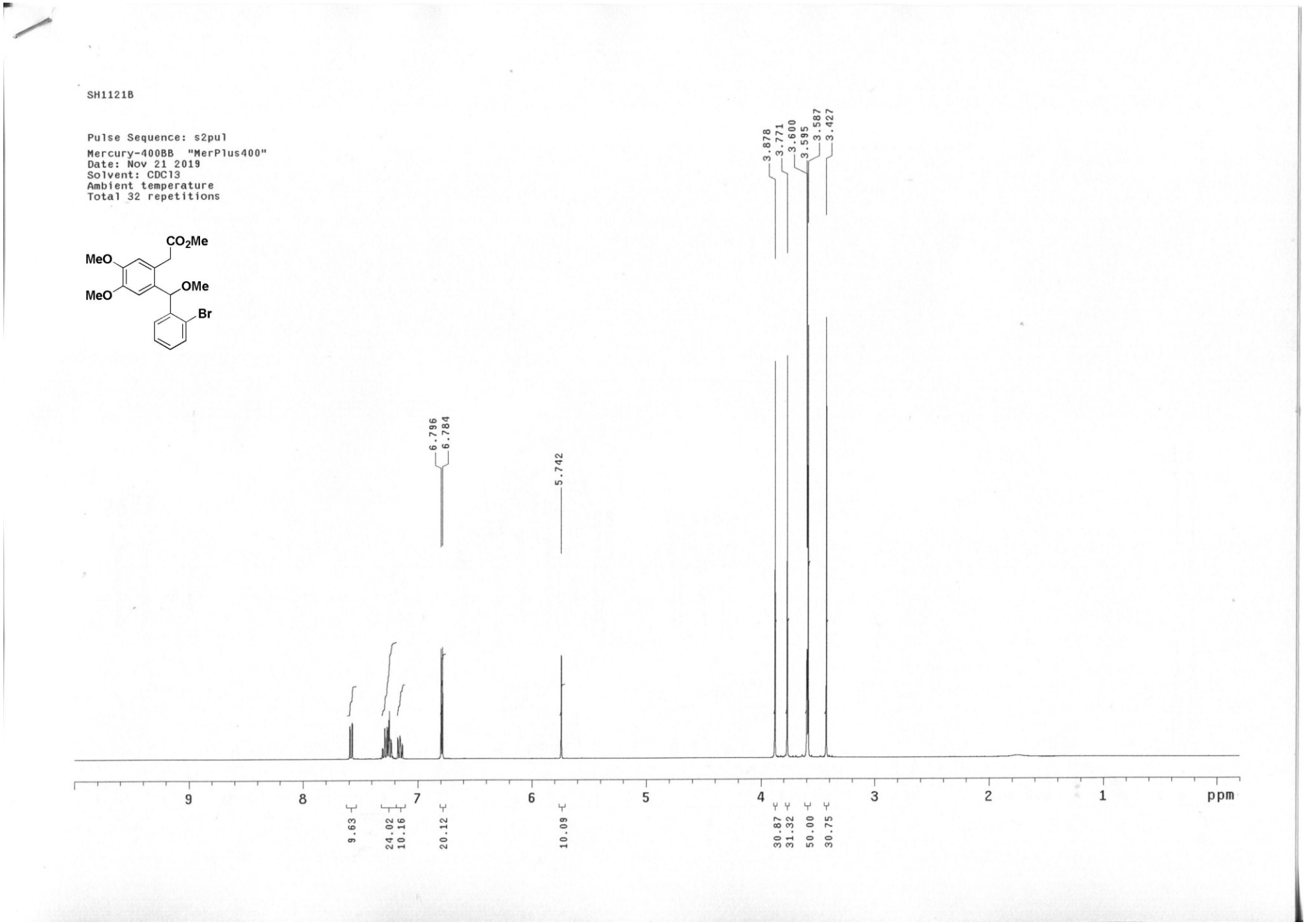
Compound 6a (^{1}H-NMR spectral data)



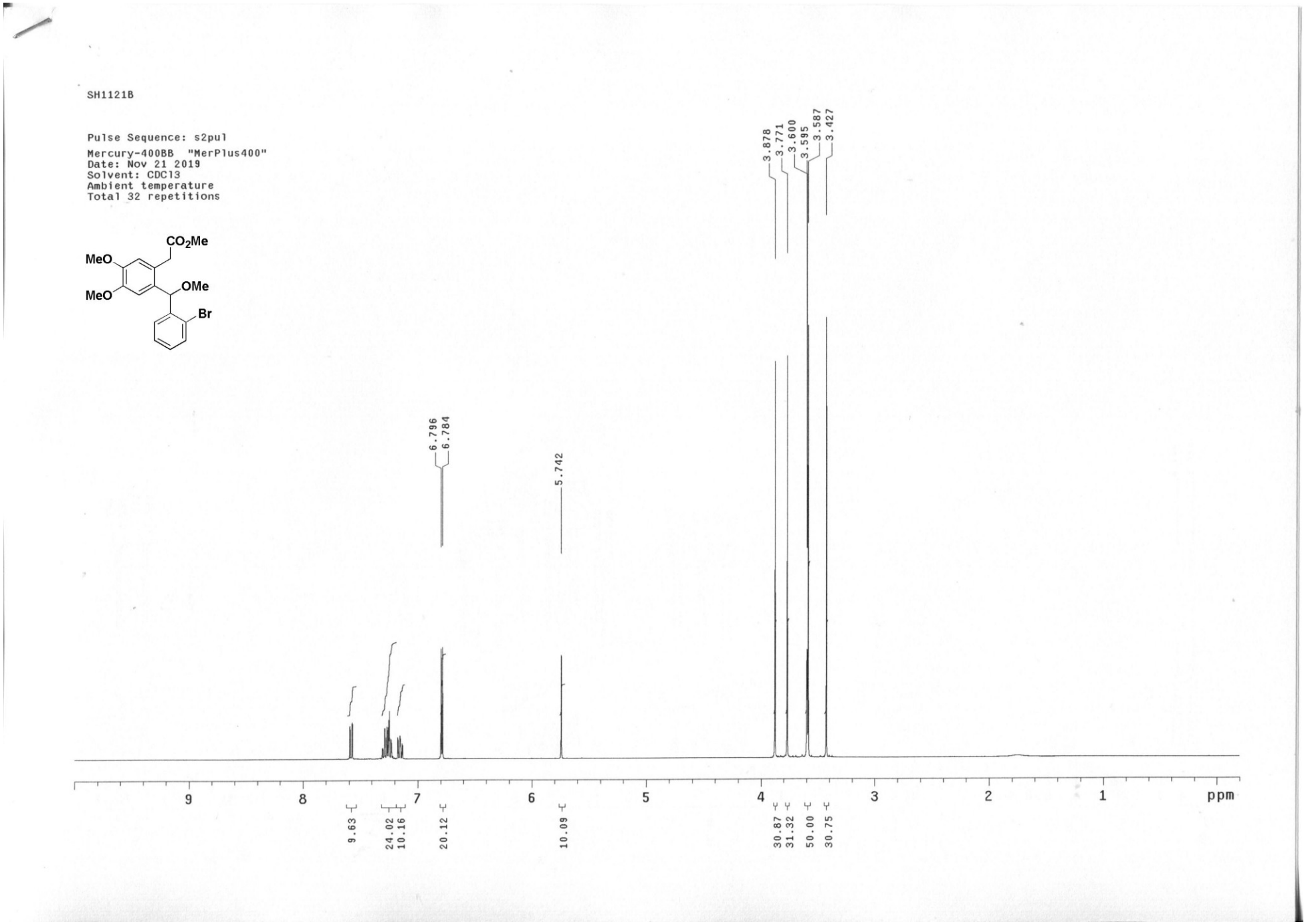
Compound 6a (^{13}C-NMR spectral data)



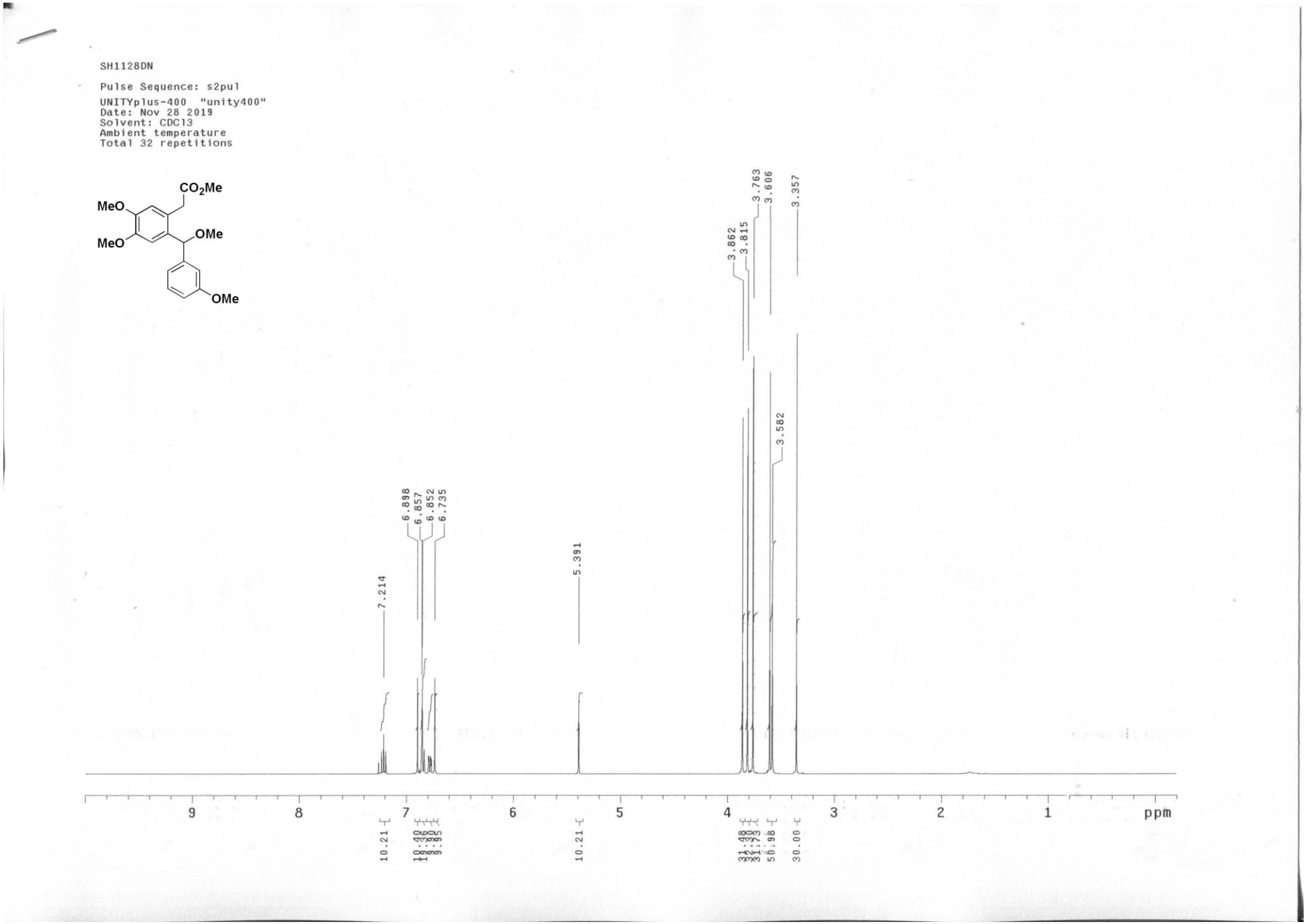
Compound 6b (^{1}H-NMR spectral data)



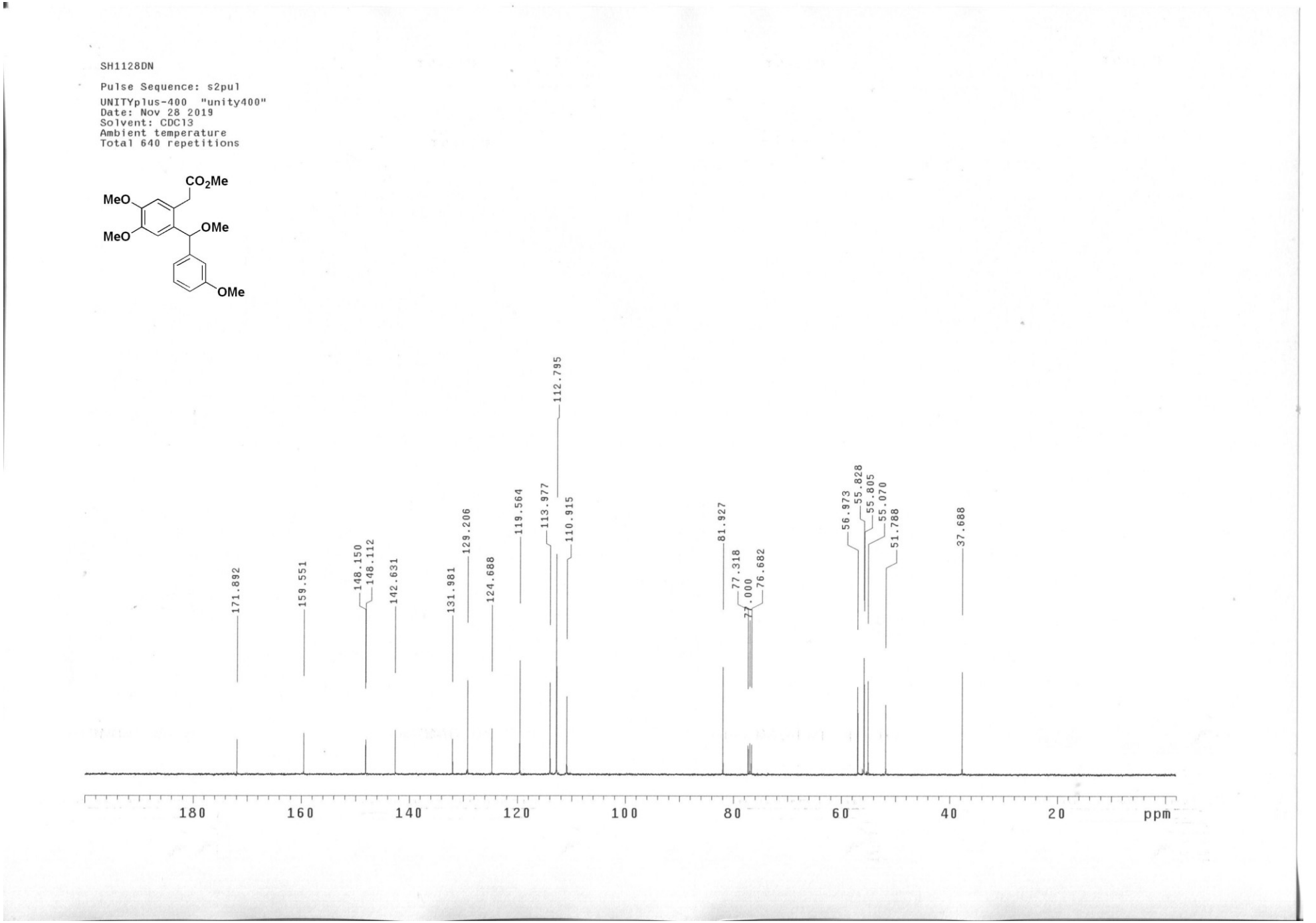
Compound 6b (^{13}C-NMR spectral data)



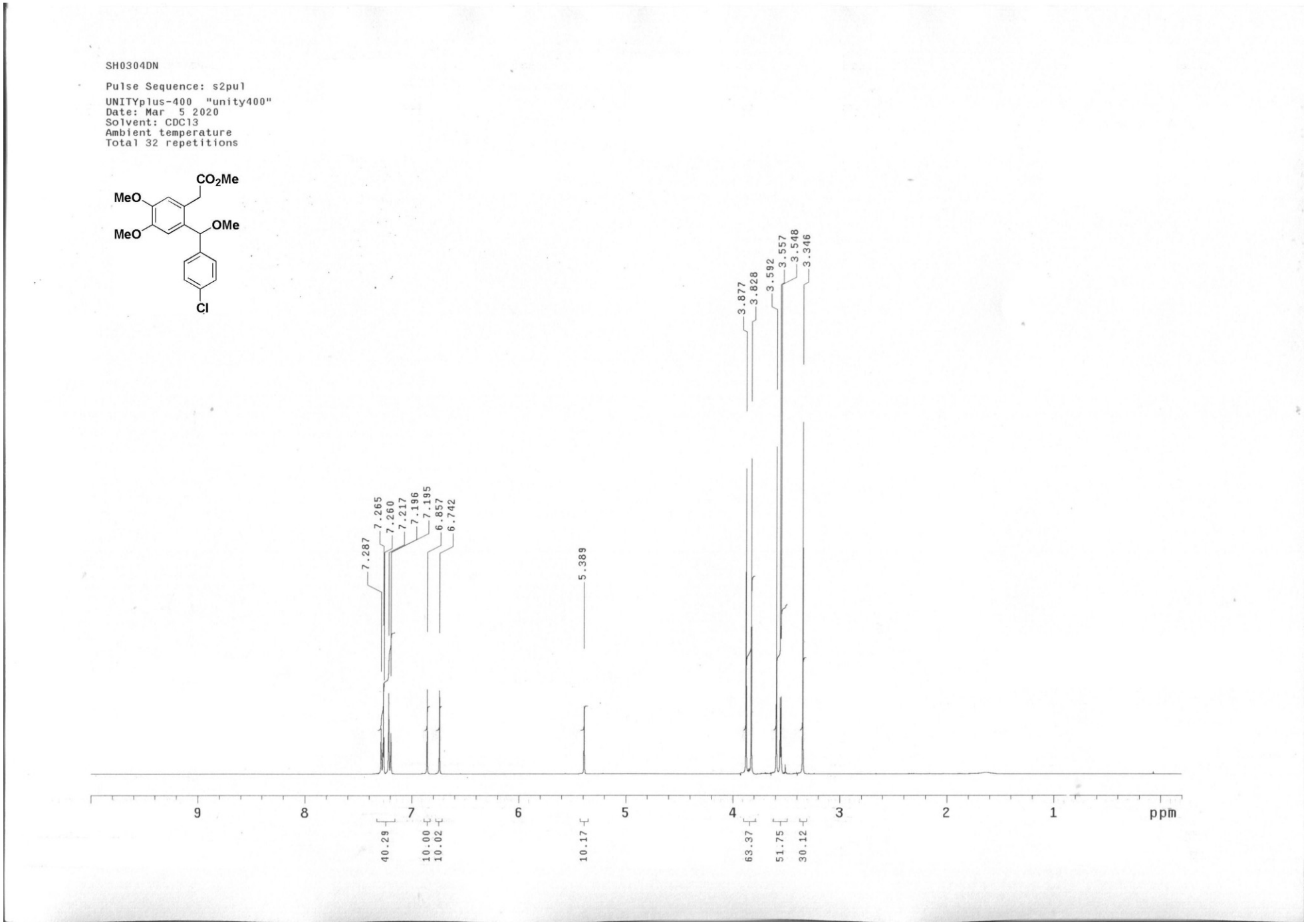
Compound 6c (^{1}H-NMR spectral data)



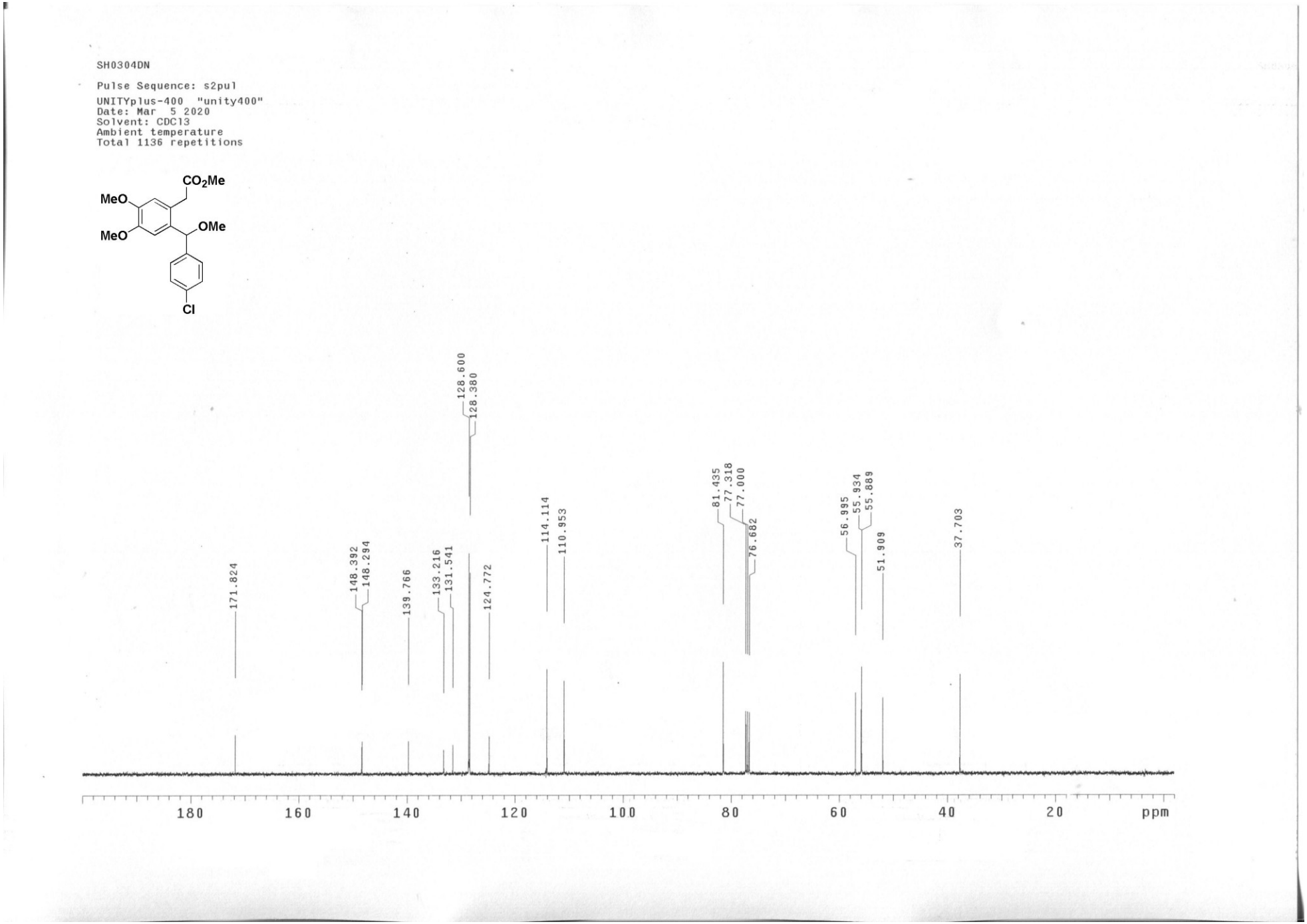
Compound 6c (^{13}C-NMR spectral data)



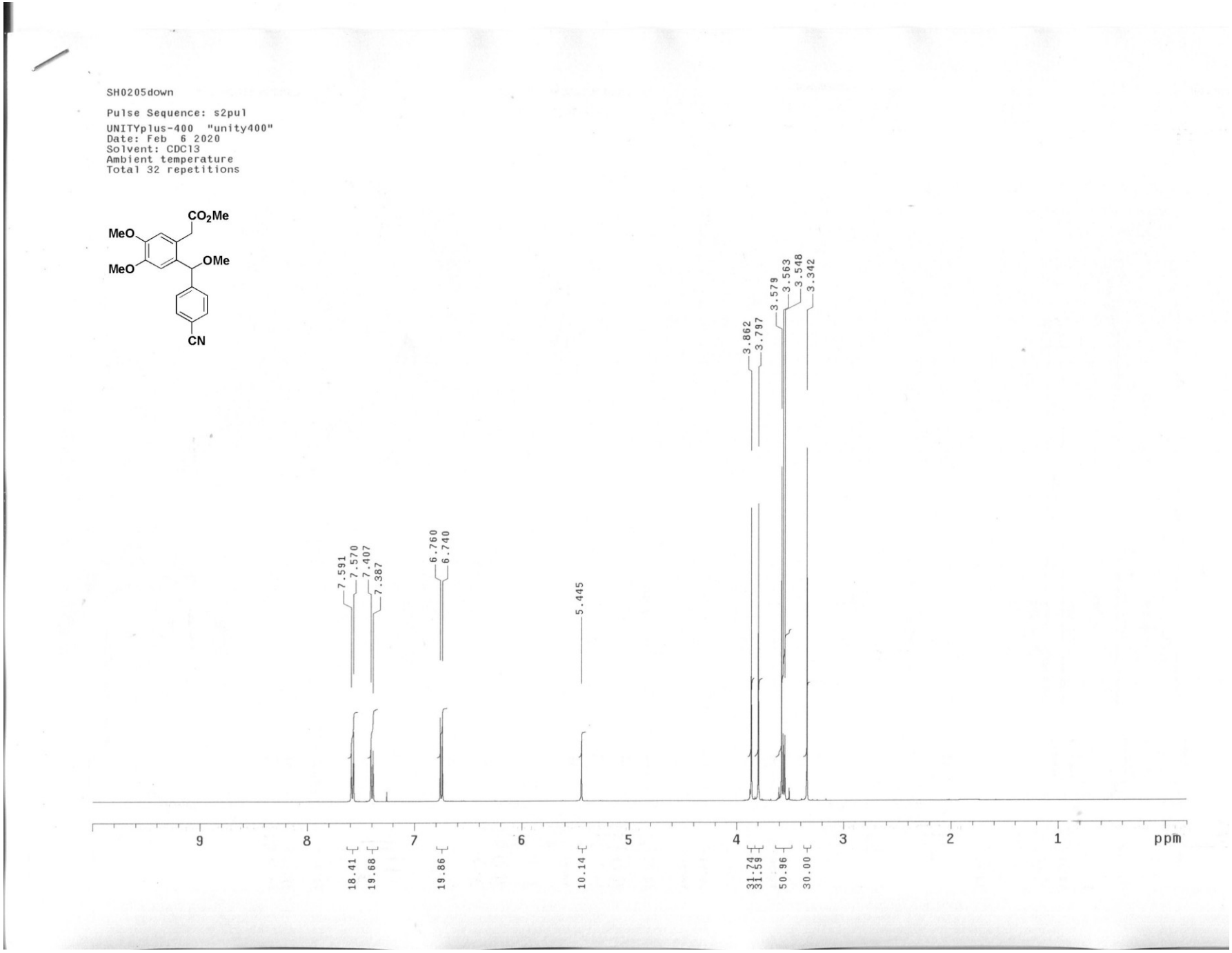
Compound 6d (^{1}H-NMR spectral data)



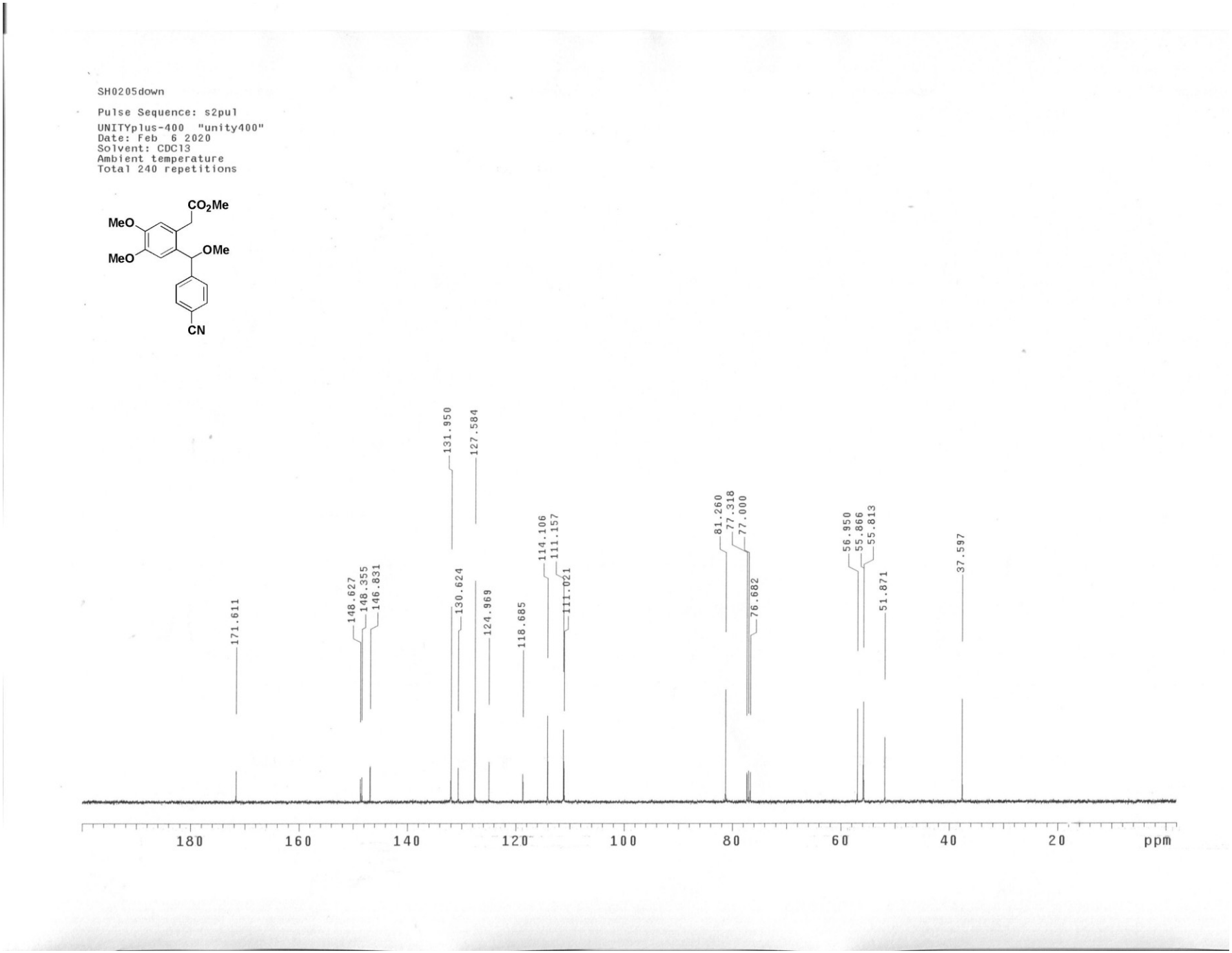
Compound 6d (^{13}C-NMR spectral data)



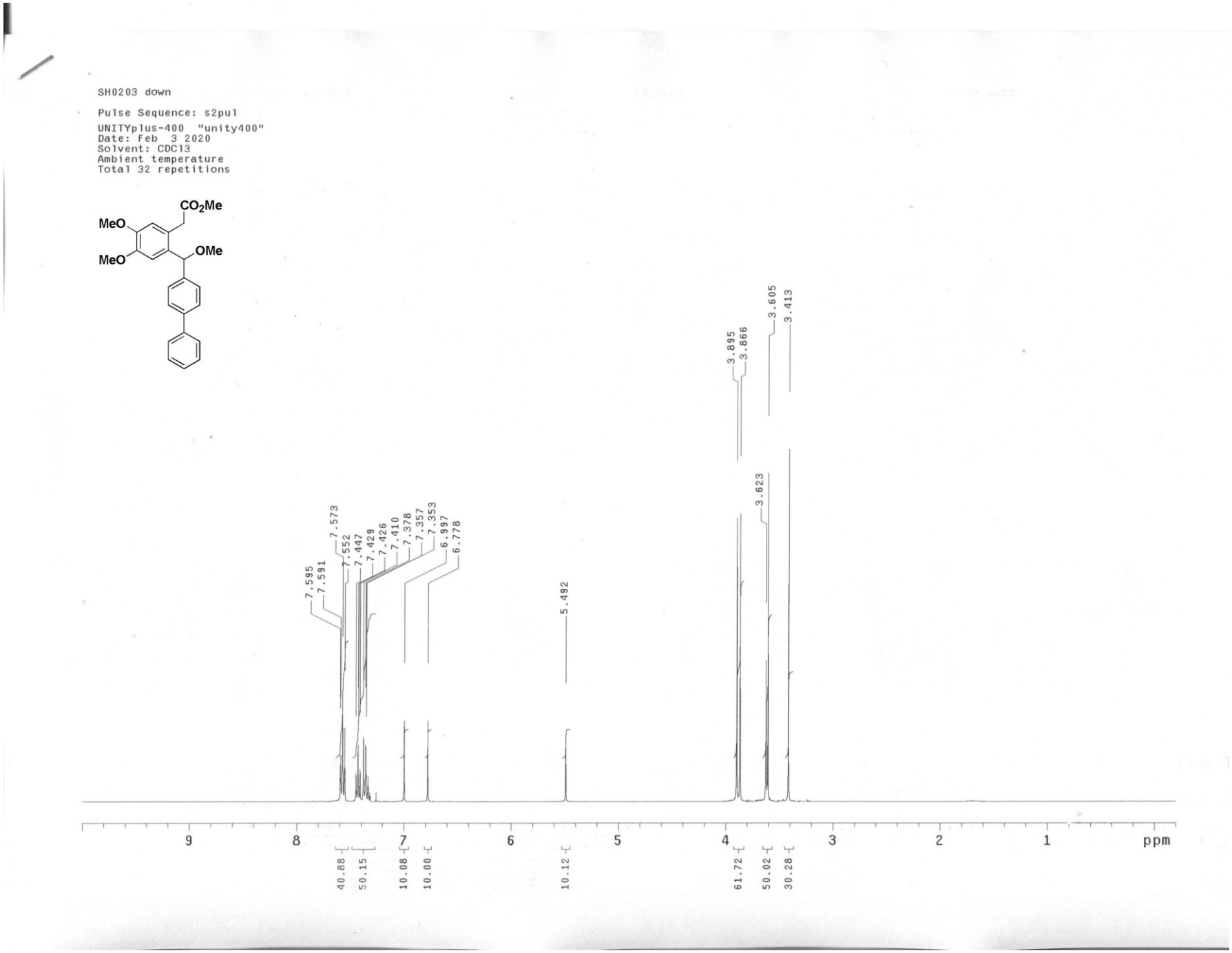
Compound 6e (^{1}H-NMR spectral data)



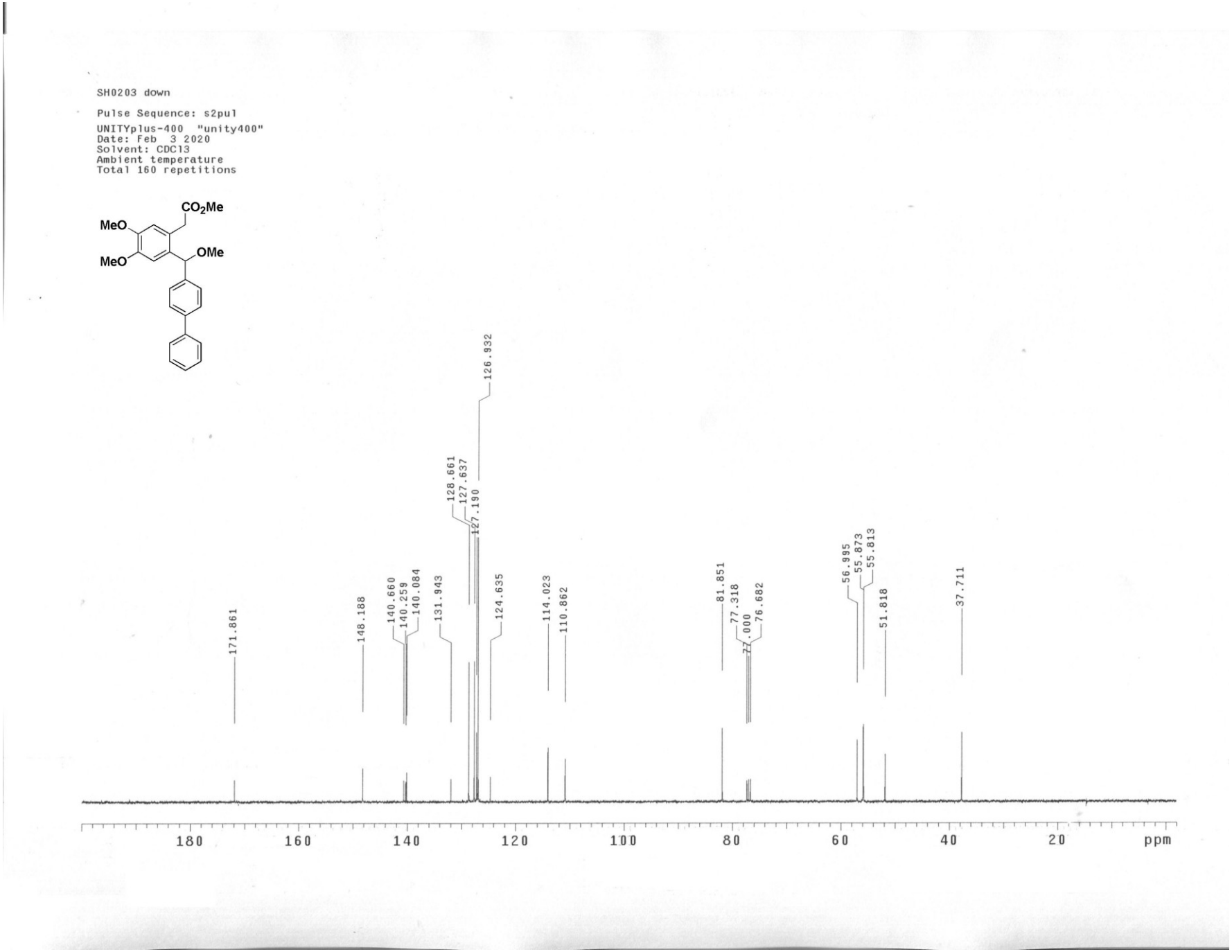
Compound 6e (^{13}C-NMR spectral data)



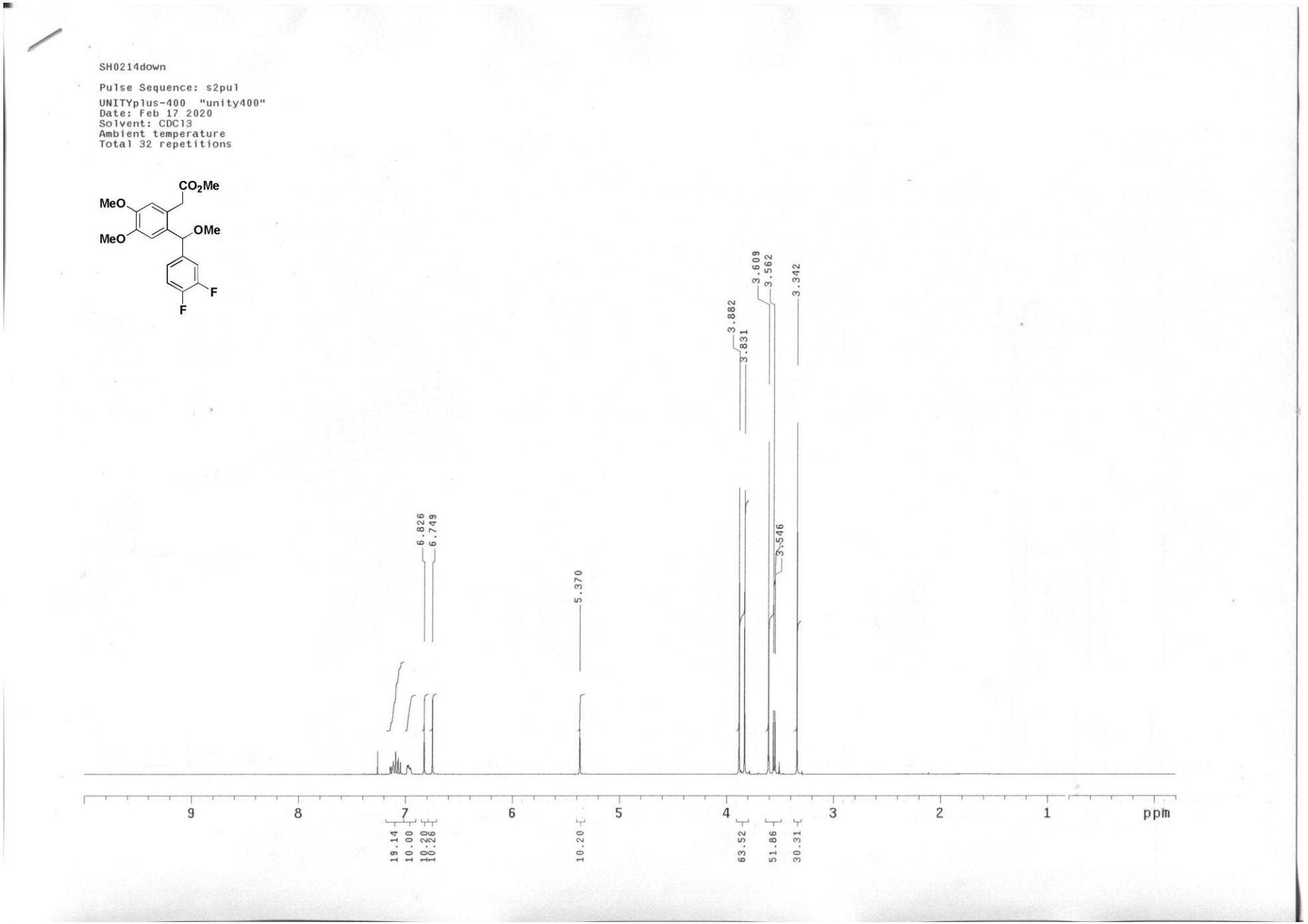
Compound 6f (^{1}H-NMR spectral data)



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



Compound 6g (^{1}H-NMR spectral data)

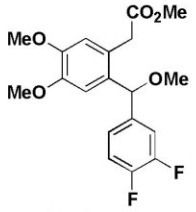


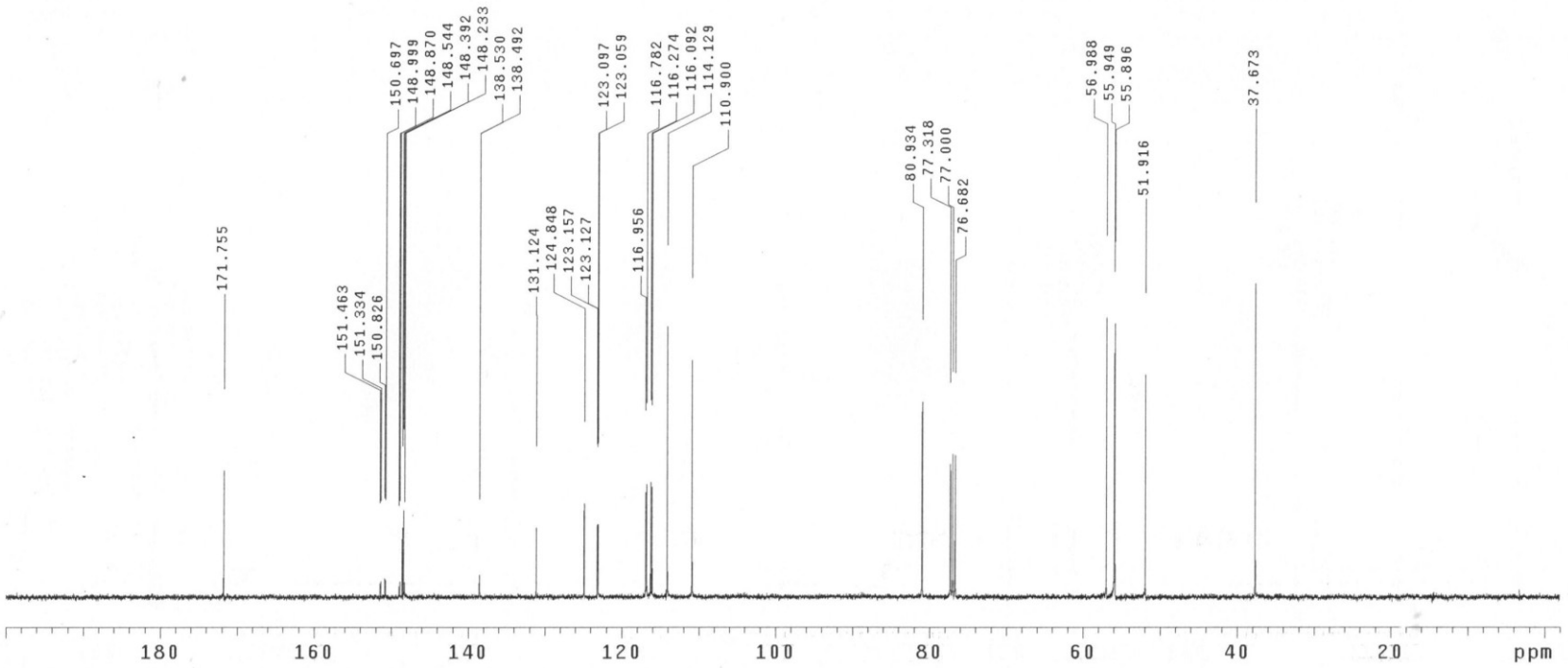
Compound 6g (^{13}C-NMR spectral data)

SH0214down

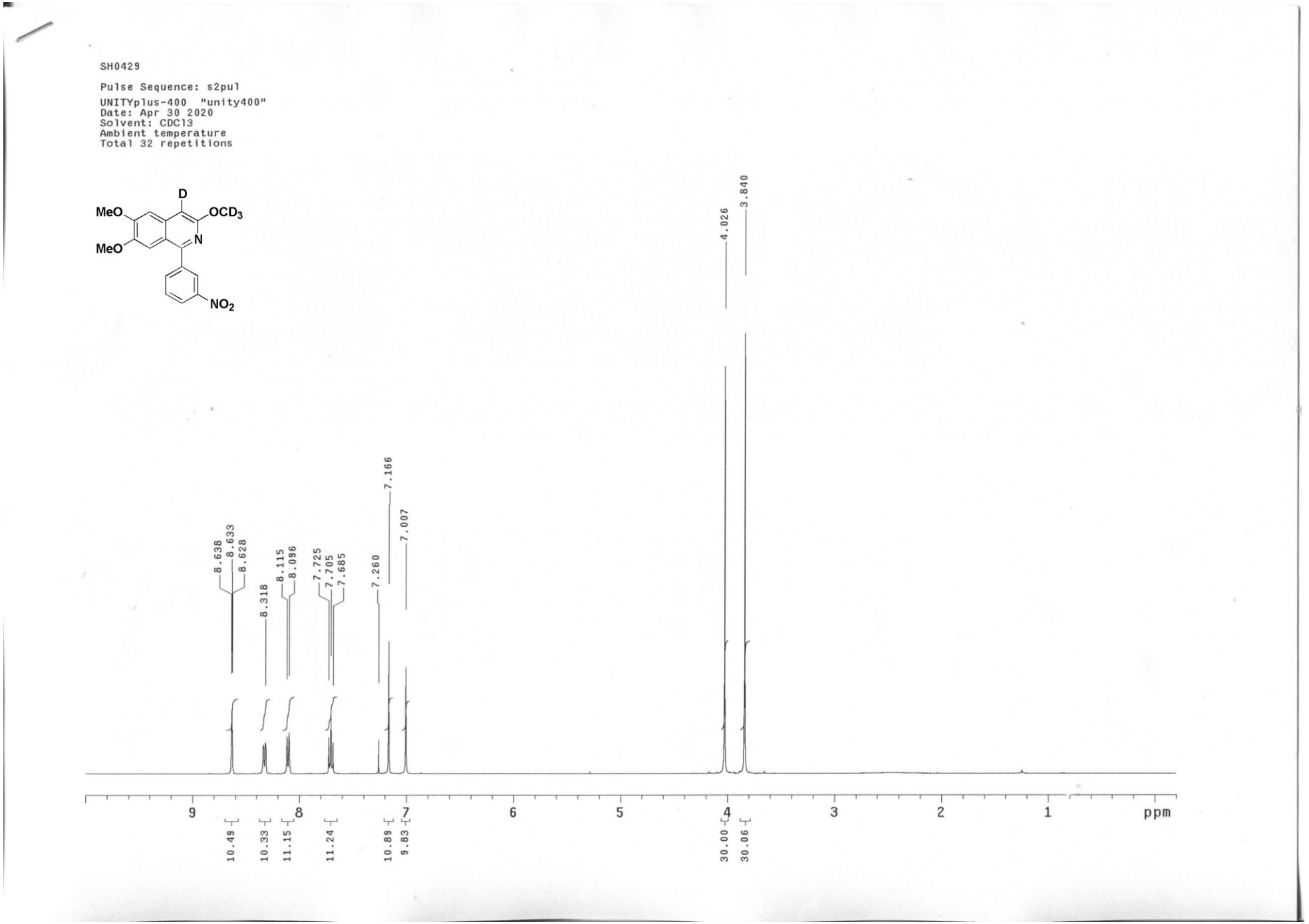
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Feb 17 2020
Solvent: CDCl3
Ambient temperature
Total 4048 repetitions

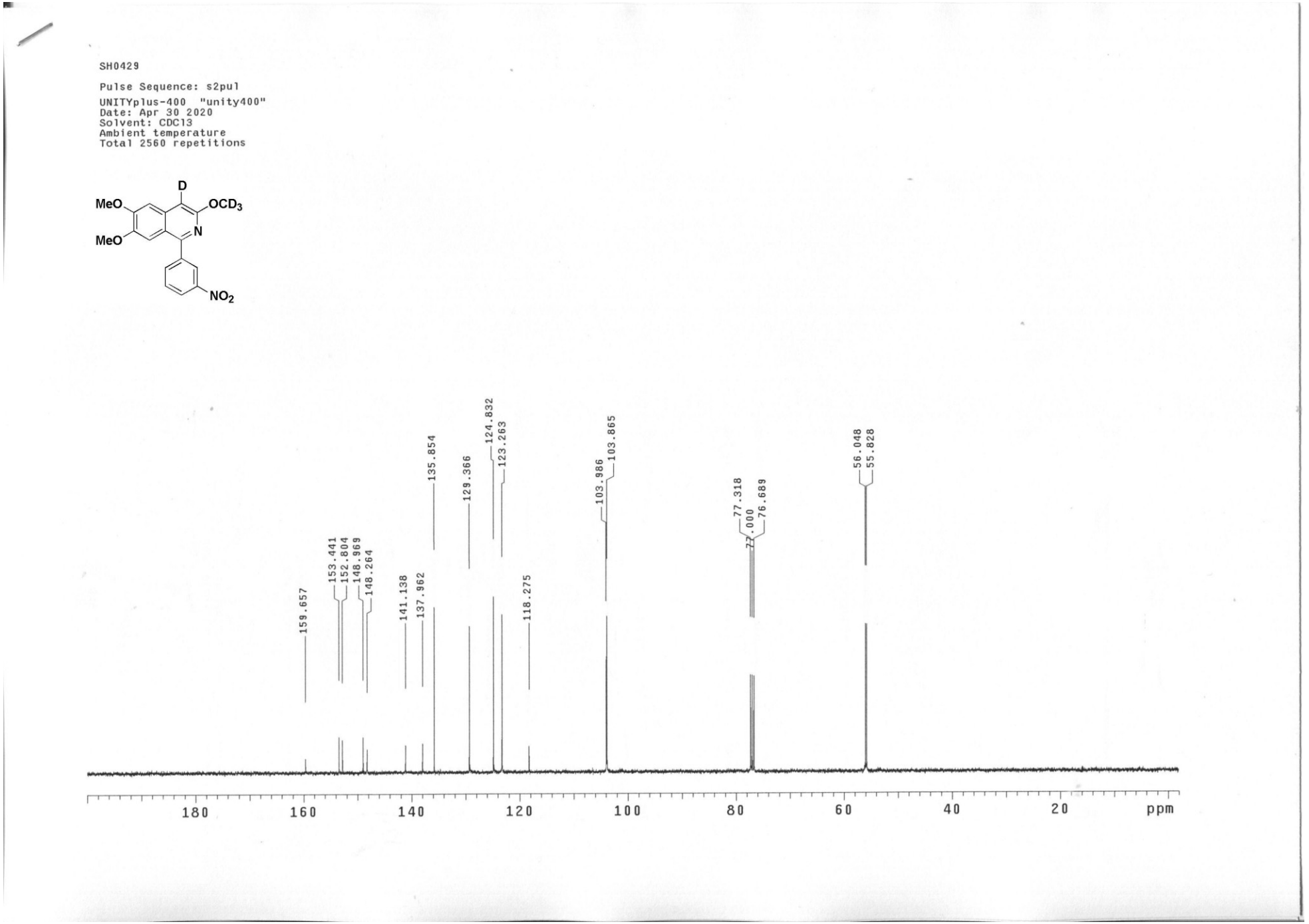




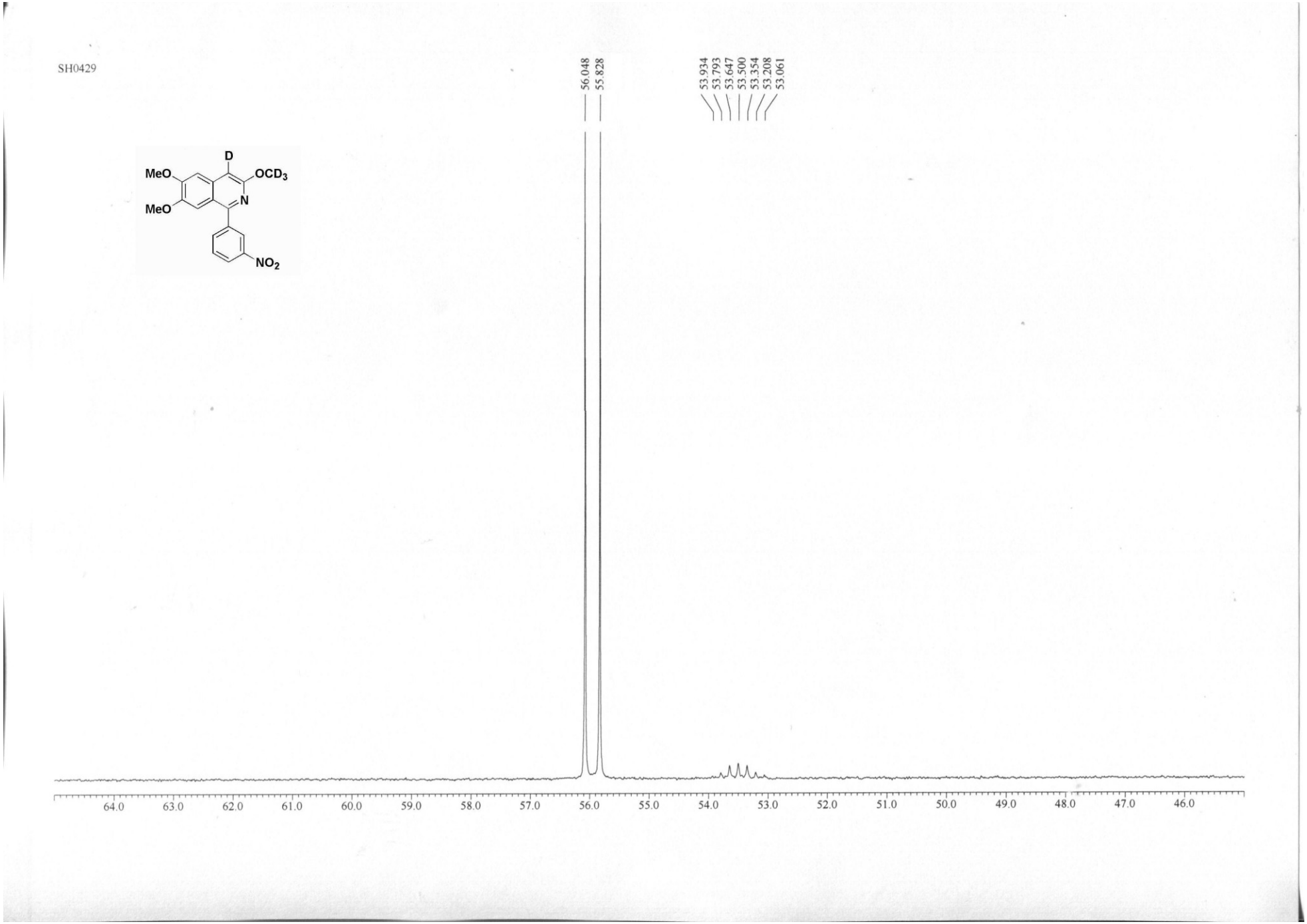
Compound 7 (^{1}H-NMR spectral data)



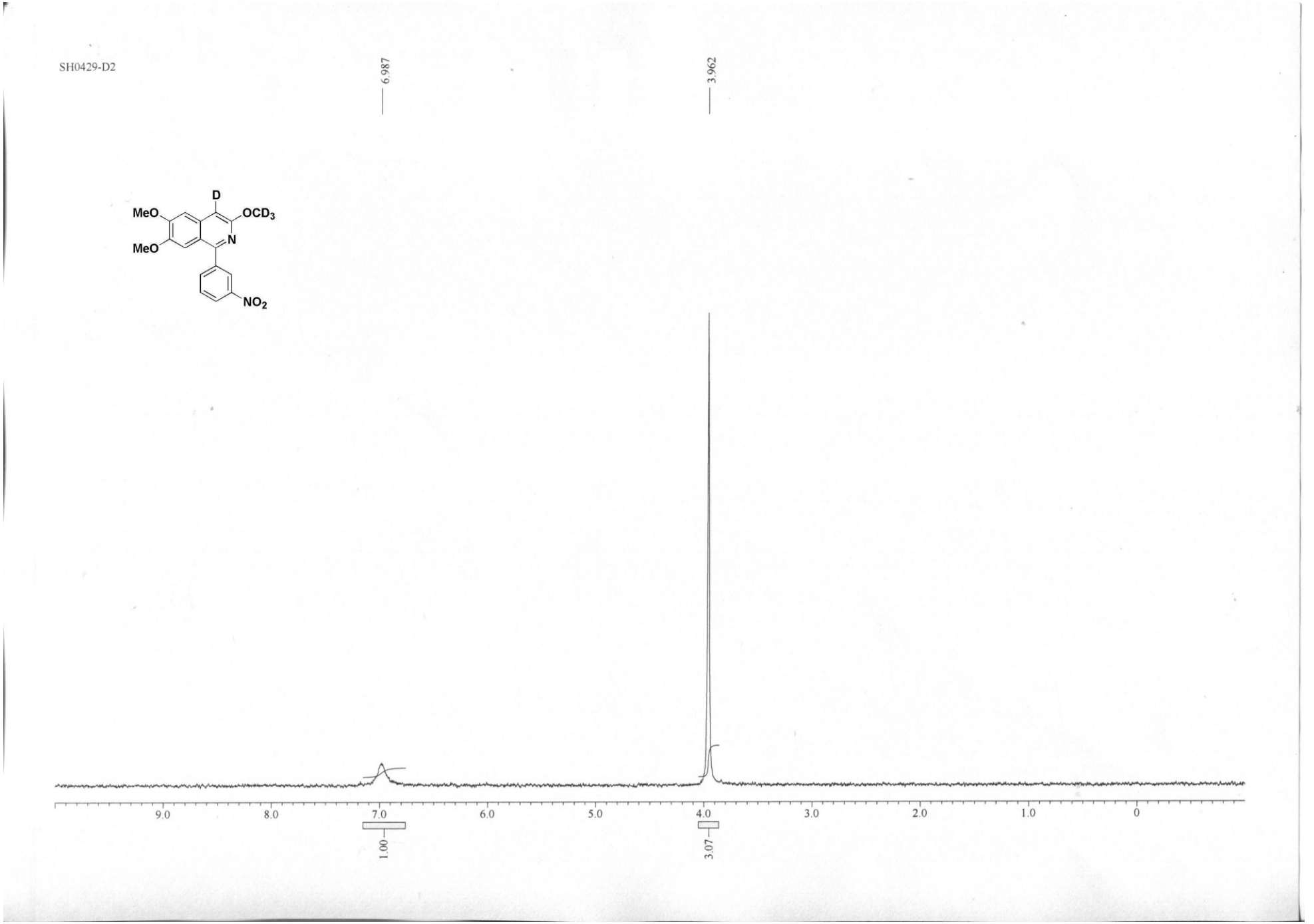
Compound 7 (^{13}C-NMR spectral data-1)



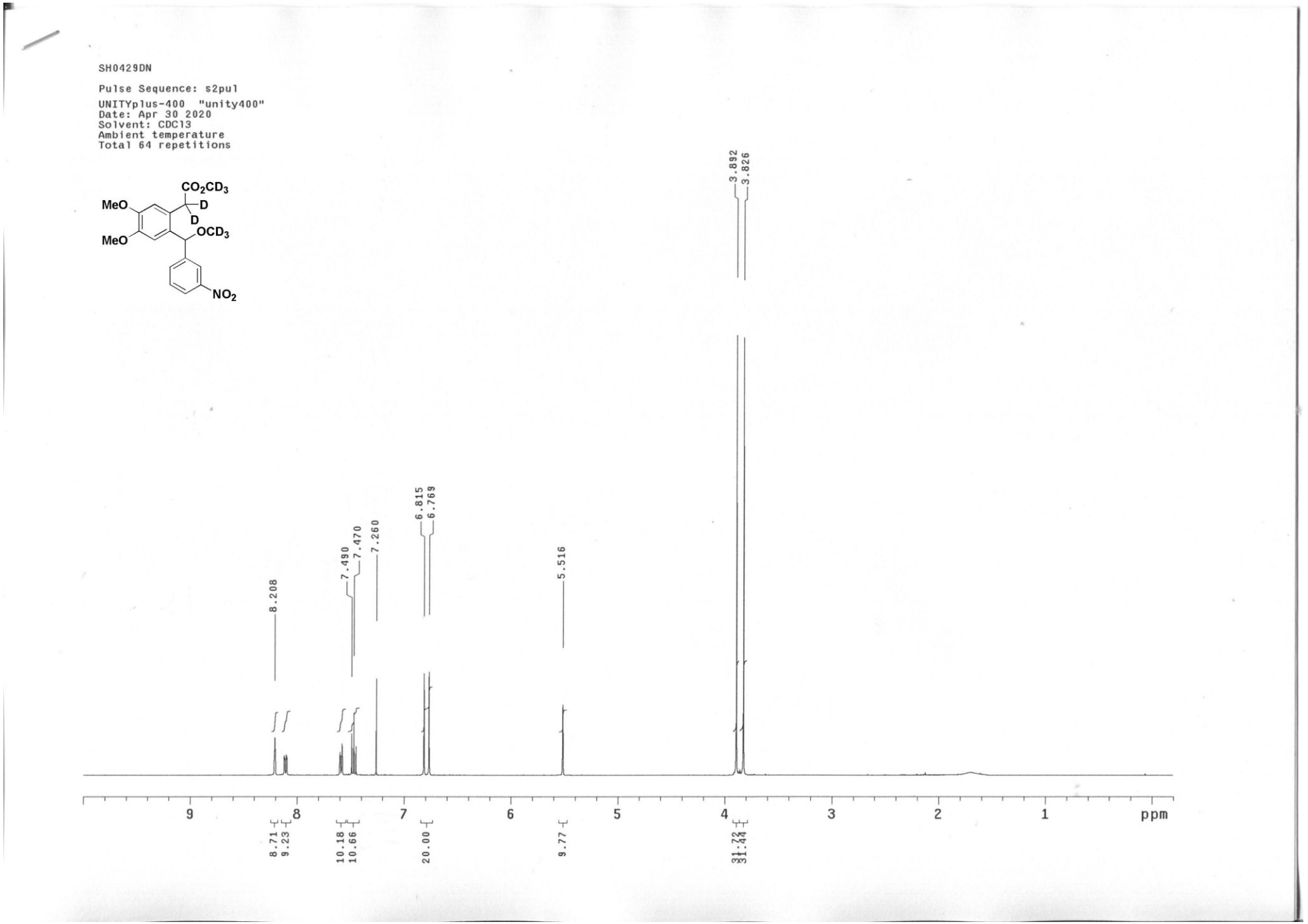
Compound 7 (^{13}C-NMR spectral data-2)



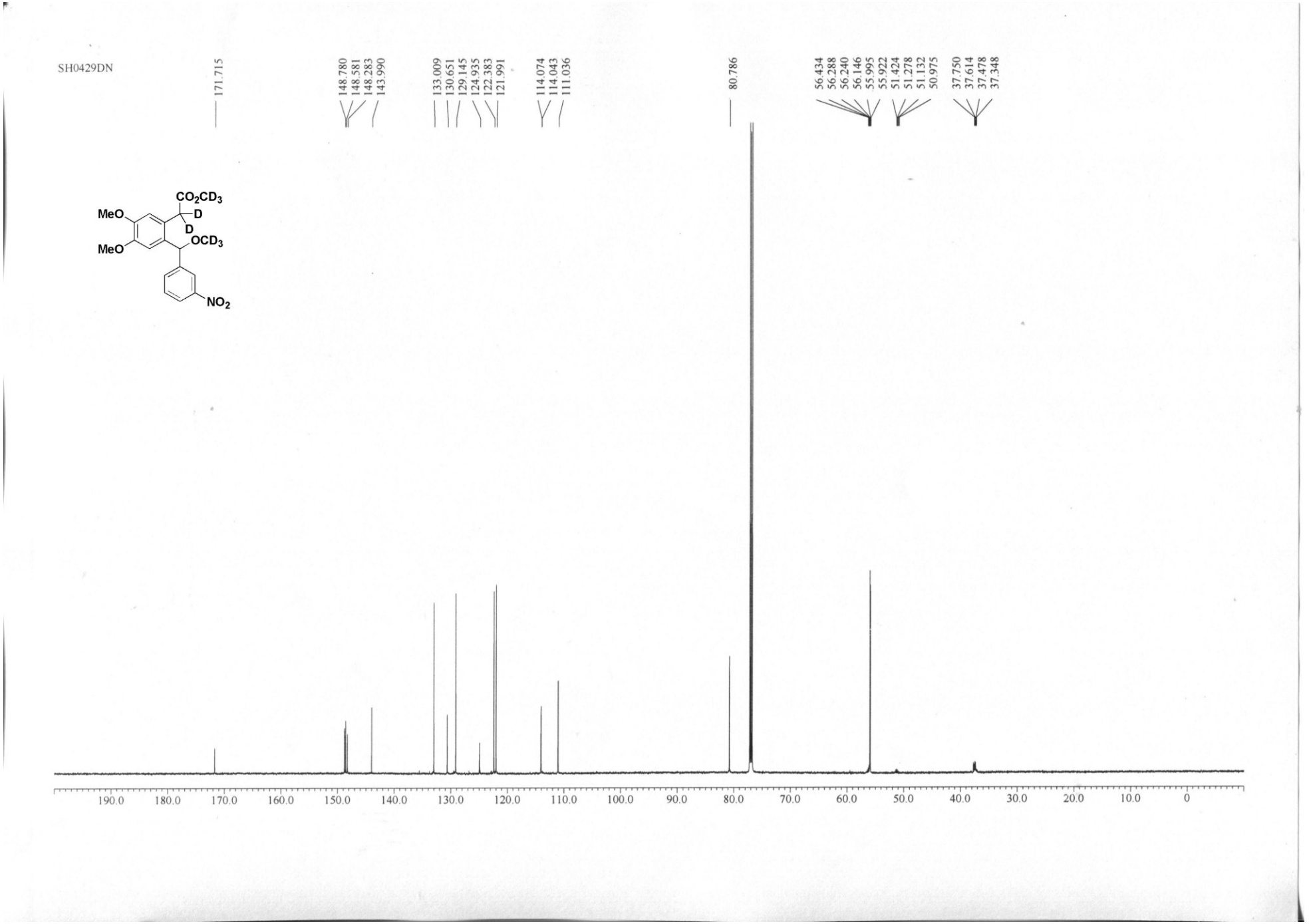
Compound 7 (^{2}H-NMR spectral data)



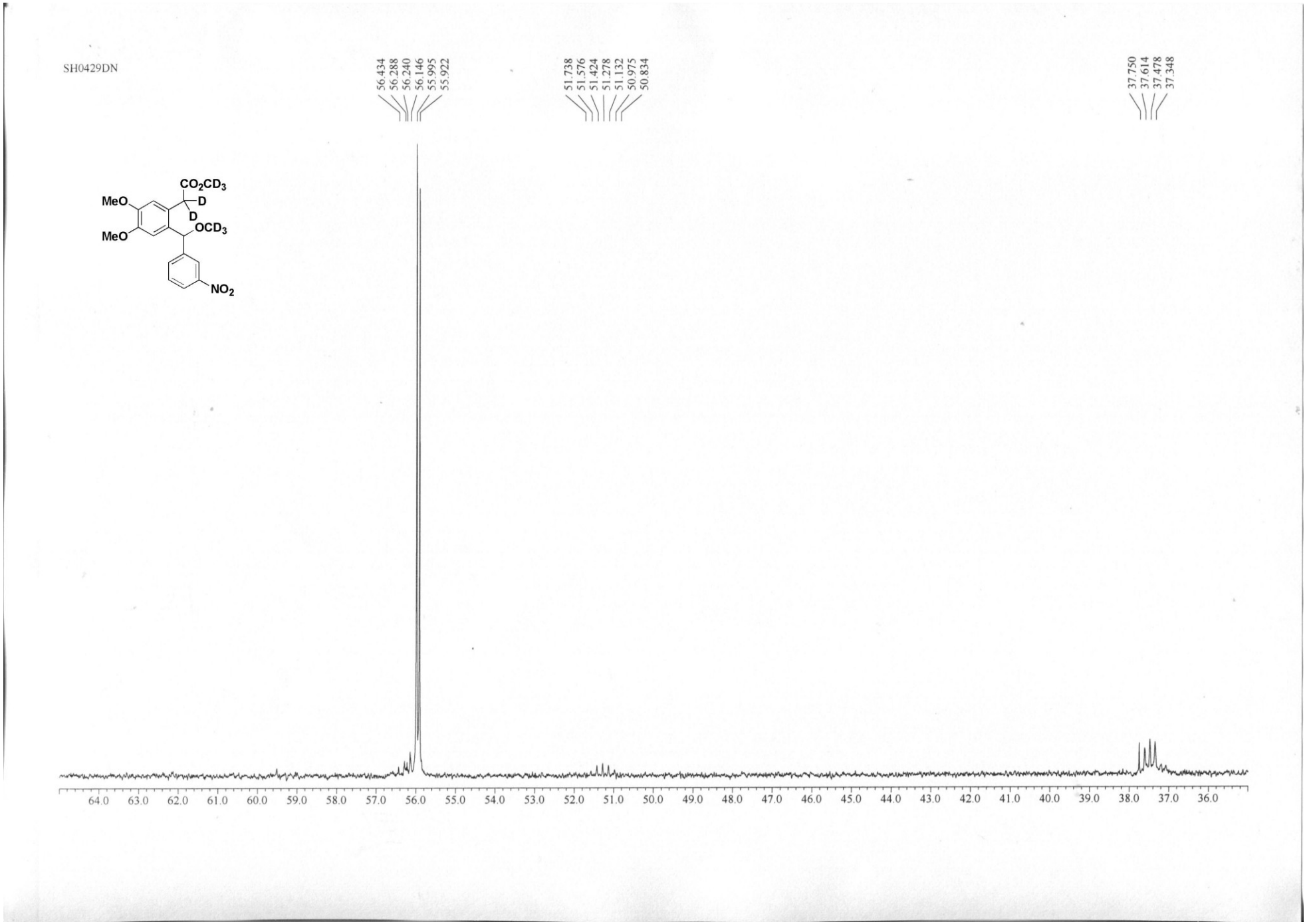
Compound 8 (^{1}H-NMR spectral data)



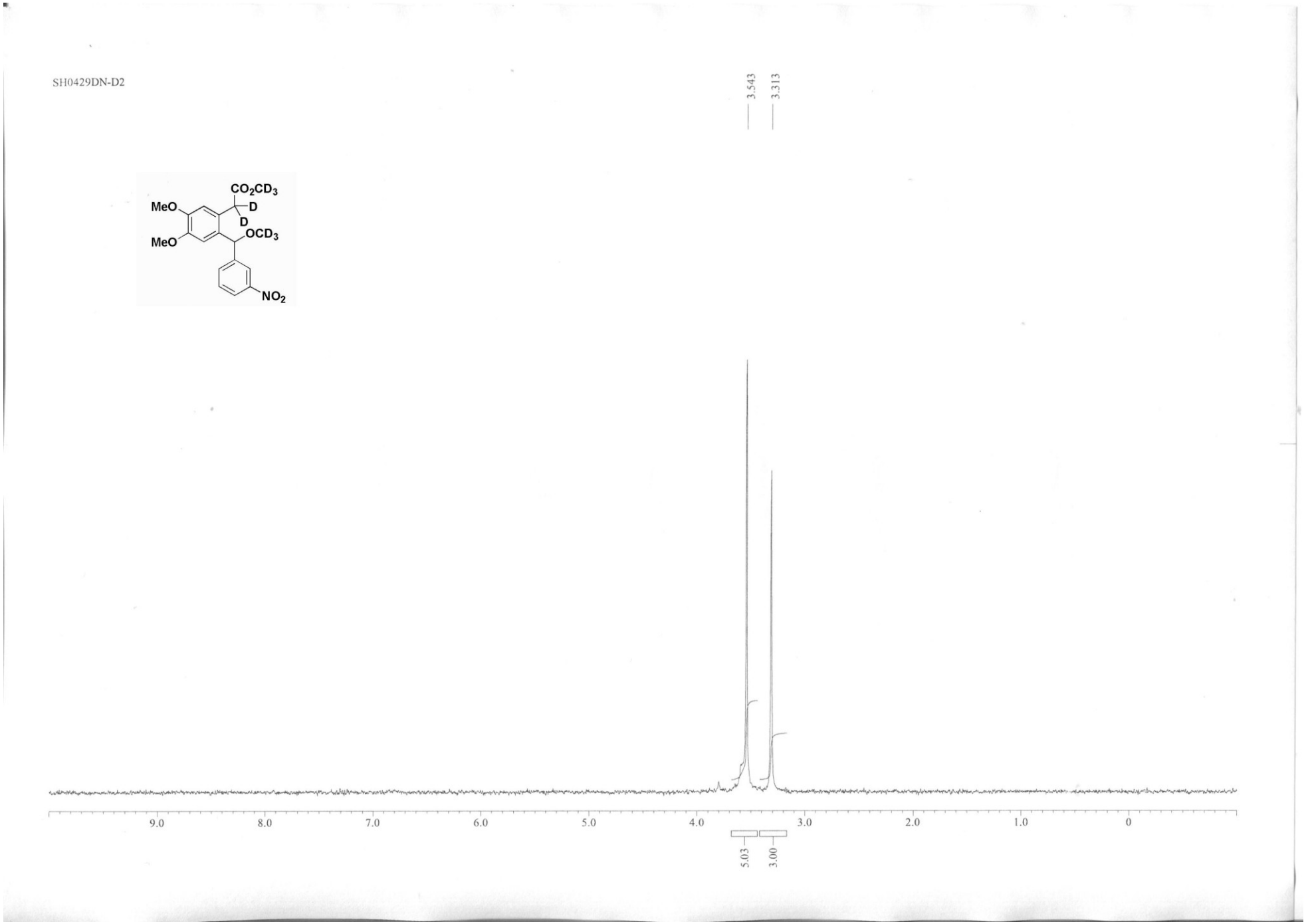
Compound 8 (^{13}C-NMR spectral data-1)



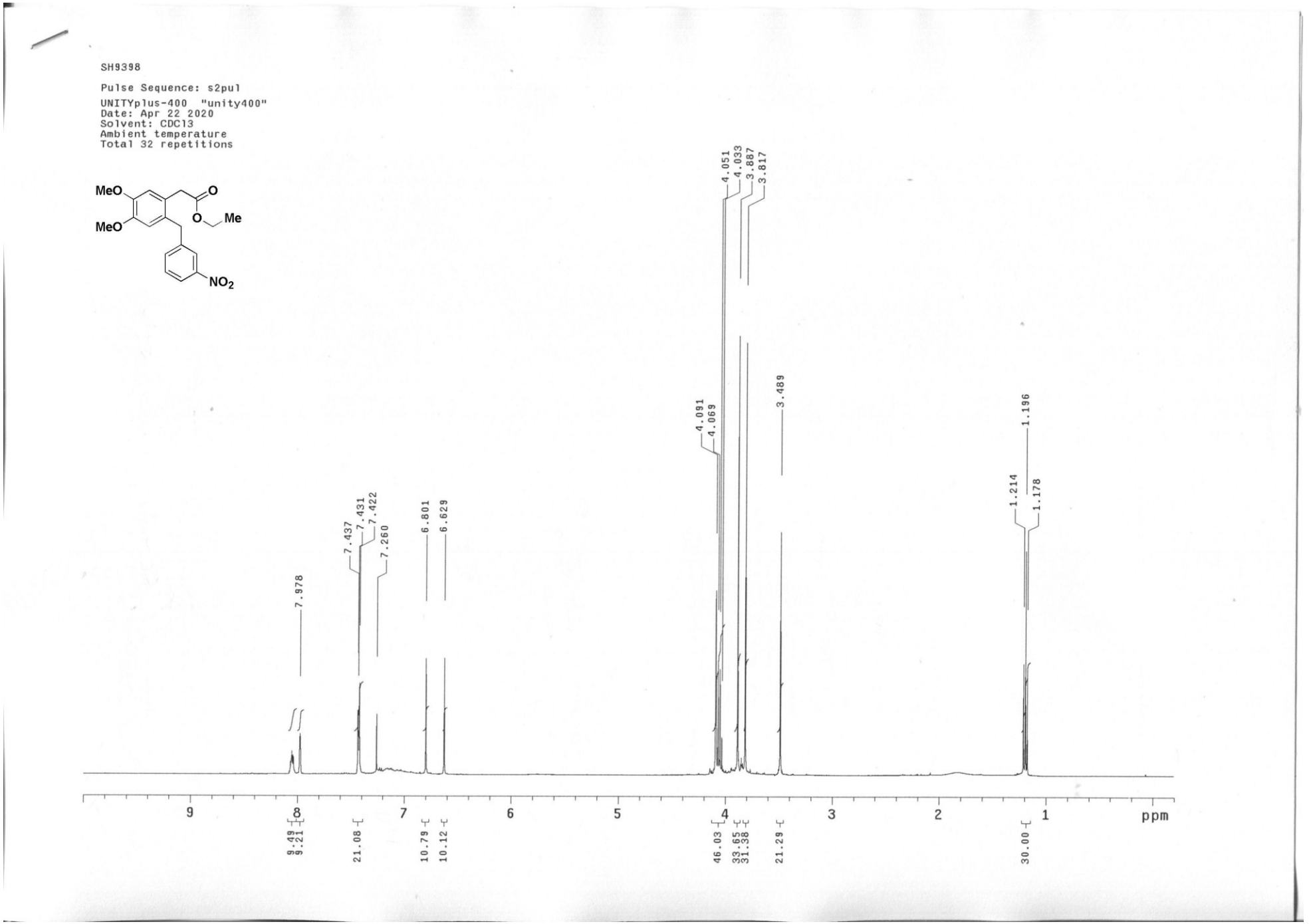
Compound 8 (^{13}C-NMR spectral data-2)



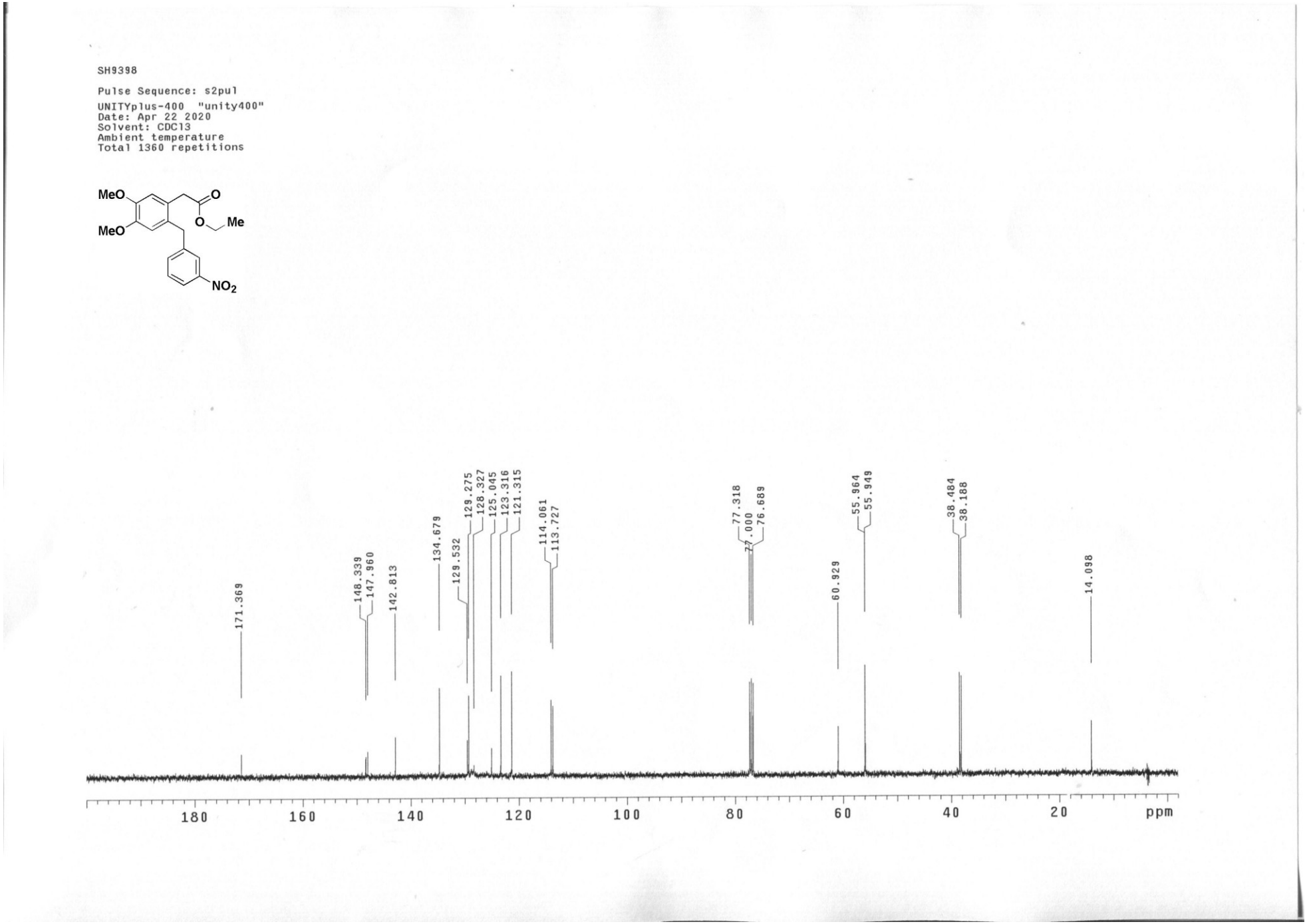
Compound 8 (^{2}H-NMR spectral data)



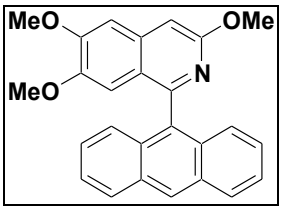
Compound 9 (^{1}H-NMR spectral data)



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

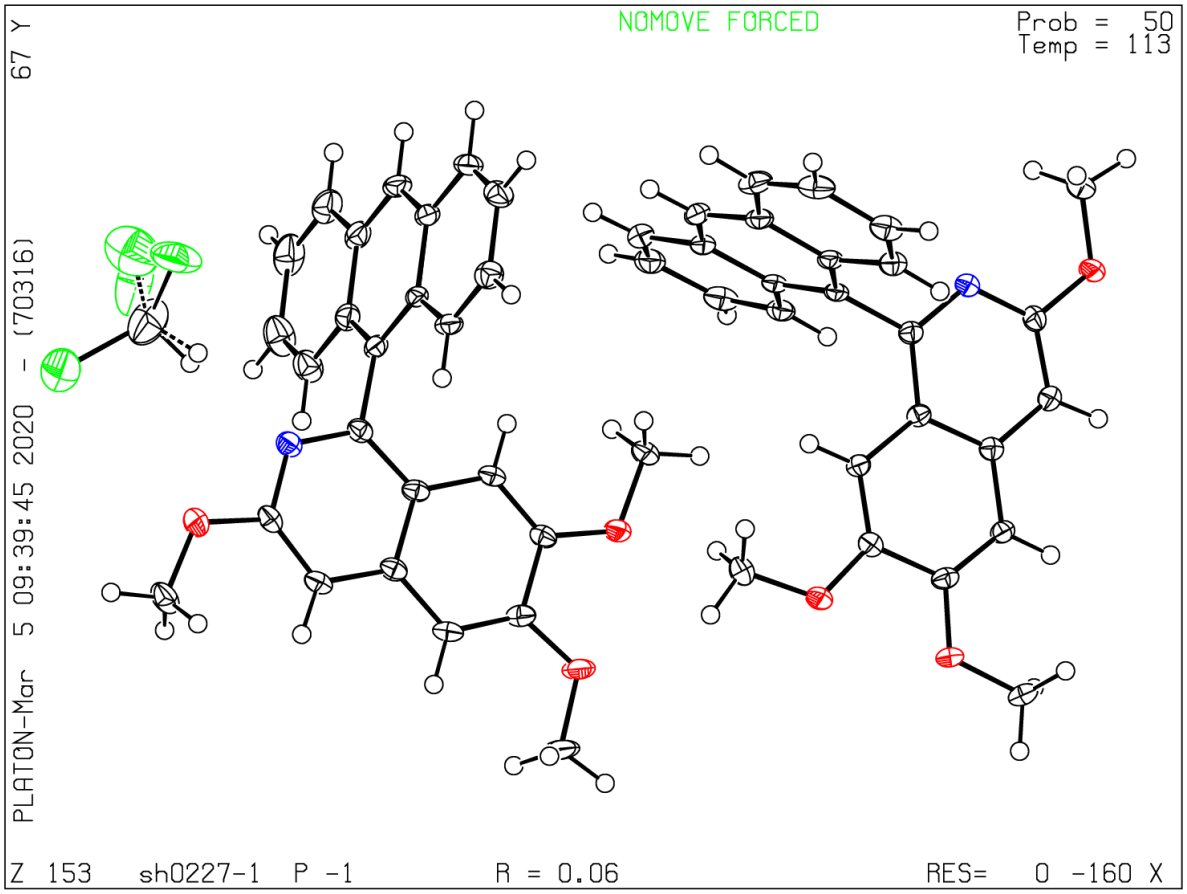


X-ray crystal data of compound 4r (CCDC 2000637)



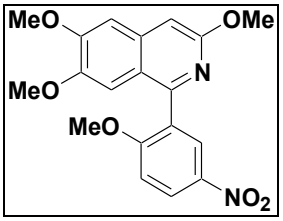
Sample preparation : A solution of compound **4r** (30 mg) in $CHCl_3$ (10 mL) was placed in a tube (10 mL). EtOAc (2 mL) was added slowly to the vial with a dropper. The vial was closed with little cotton and kept at room temperature for 2 days. Then, colorless prisms were observed.

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.



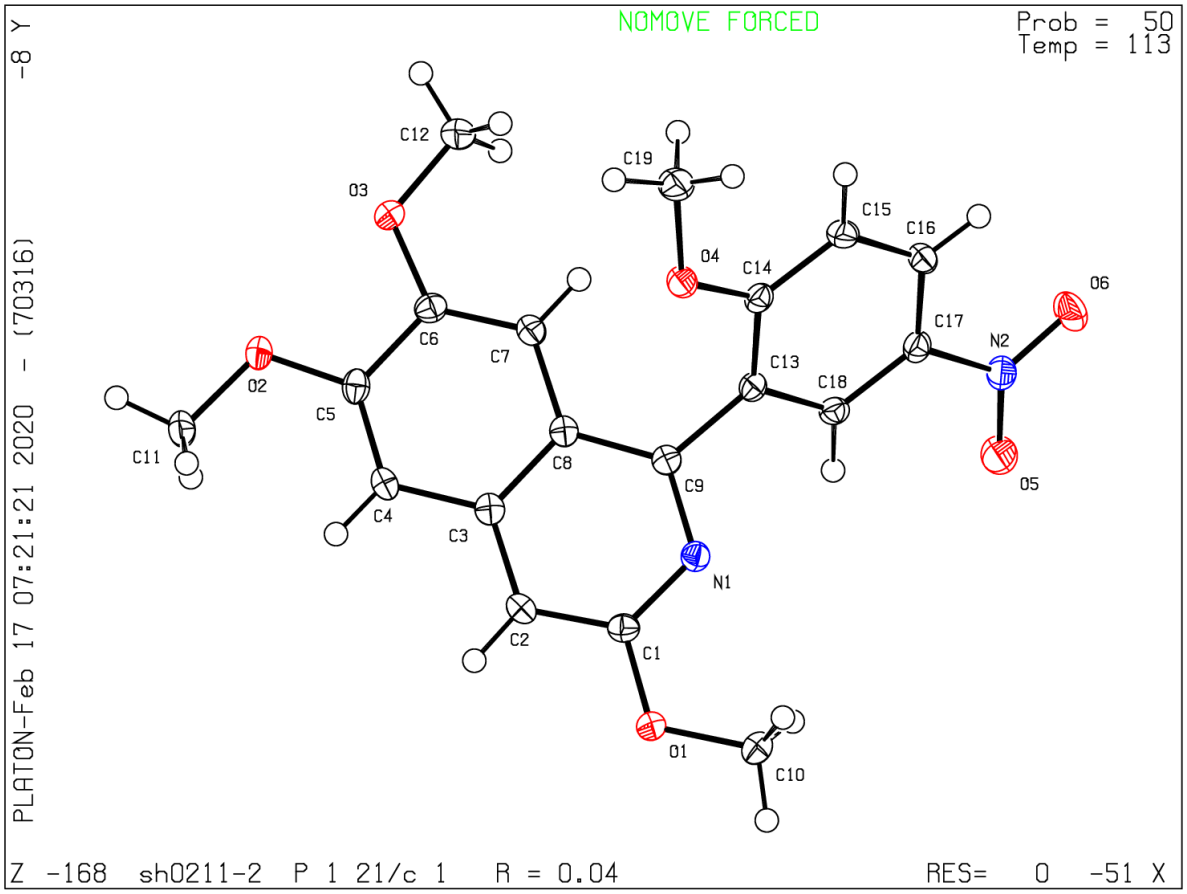
Empirical formula	$C_{53}H_{43}Cl_3N_2O_6$
Formula weight	910.24
Temperature/K	113(2)
Crystal system	triclinic
Space group	P-1
a/Å	9.82420(10)
b/Å	13.6944(2)
c/Å	17.0549(3)
α/°	83.0810(10)
β/°	83.3180(10)
γ/°	79.1050(10)
Volume/Å^3	2226.41(6)
Z	2
ρ_{calc}g/cm^3	1.358
μ/mm^{-1}	0.261
F(000)	948.0
Crystal size/mm^3	0.15 × 0.1 × 0.1
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.08 to 52
Index ranges	$-9 \leq h \leq 12$, $-16 \leq k \leq 16$, $-20 \leq l \leq 21$
Reflections collected	49820
Independent reflections	8704 [R_{int} = 0.0301, R_{sigma} = 0.0269]
Data/restraints/parameters	8704/0/602
Goodness-of-fit on F^2	1.048
Final R indexes [I>=2σ (I)]	R_1 = 0.0634, wR_2 = 0.1779
Final R indexes [all data]	R_1 = 0.0770, wR_2 = 0.1861
Largest diff. peak/hole / e Å^{-3}	1.42/-1.27

X-ray crystal data of compound 4x (CCDC 2000638)



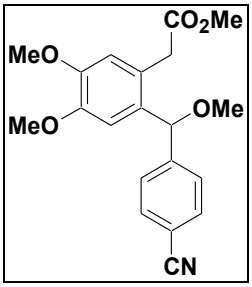
Sample preparation : A solution of compound **4x** (30 mg) in CH_2Cl_2 (10 mL) was placed in a tube (10 mL). EtOAc (2 mL) was added slowly to the vial with a dropper. The vial was closed with little cotton and kept at room temperature for 2 days. Then, colorless prisms were observed.

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



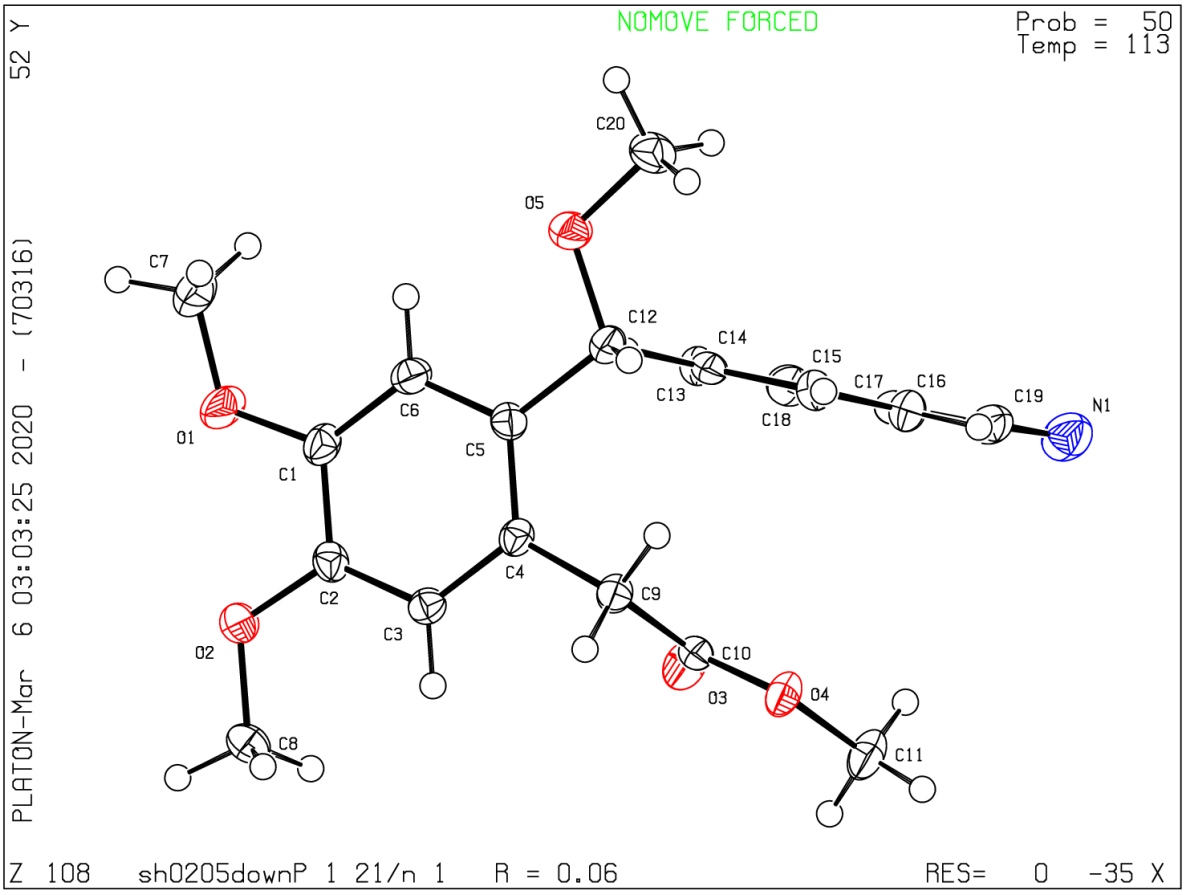
Empirical formula	$C_{19}H_{18}N_2O_6$
Formula weight	370.35
Temperature/K	113(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	10.5325(2)
b/Å	8.1523(2)
c/Å	19.8965(4)
α/°	90
β/°	94.680(2)
γ/°	90
Volume/Å^3	1702.70(6)
Z	4
ρ_{calc}g/cm^3	1.445
μ/mm^{-1}	0.109
F(000)	776.0
Crystal size/mm^3	0.2 × 0.15 × 0.1
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	3.88 to 54.028
Index ranges	$-13 \leq h \leq 13$, $-10 \leq k \leq 8$, $-19 \leq l \leq 25$
Reflections collected	13633
Independent reflections	3558 [R_{int} = 0.0245, R_{sigma} = 0.0272]
Data/restraints/parameters	3558/0/249
Goodness-of-fit on F^2	1.063
Final R indexes [I>=2σ (I)]	R_1 = 0.0353, wR_2 = 0.0893
Final R indexes [all data]	R_1 = 0.0440, wR_2 = 0.0939
Largest diff. peak/hole / e Å^{-3}	0.26/-0.22

X-ray crystal data of compound 6e (CCDC 2000639)



Sample preparation : A solution of compound **6e** (30 mg) in CH_2Cl_2 (10 mL) was placed in a tube (10 mL). EtOAc (2 mL) was added slowly to the vial with a dropper. The vial was closed with little cotton and kept at room temperature for 2 days. Then, colorless prisms were observed.

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



Empirical formula	$C_{20}H_{21}NO_5$
Formula weight	355.38
Temperature/K	113(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	8.6565(2)
b/Å	9.9527(2)
c/Å	20.7506(5)
α/°	90.00
β/°	96.235(2)
γ/°	90.00
Volume/Å^3	1777.20(7)
Z	4
ρ_{calc}g/cm^3	1.328
μ/mm^{-1}	0.096
F(000)	752.0
Crystal size/mm^3	0.25 × 0.2 × 0.2
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.54 to 52
Index ranges	$-10 \leq h \leq 10$, $-12 \leq k \leq 12$, $-25 \leq l \leq 17$
Reflections collected	28695
Independent reflections	3493 [R_{int} = 0.0488, R_{sigma} = 0.0285]
Data/restraints/parameters	3493/0/240
Goodness-of-fit on F^2	1.109
Final R indexes [I>=2σ (I)]	R_1 = 0.0636, wR_2 = 0.1507
Final R indexes [all data]	R_1 = 0.0728, wR_2 = 0.1550
Largest diff. peak/hole / e Å^{-3}	0.65/-0.32