Supporting Information

*m*CPBA-Mediated Intramolecular Oxidative Annulation of *ortho*-Crotyl or Cinnamyl Arylaldehydes. Synthesis of Benzofused Five-, Six- and Seven-Membered Oxacycles

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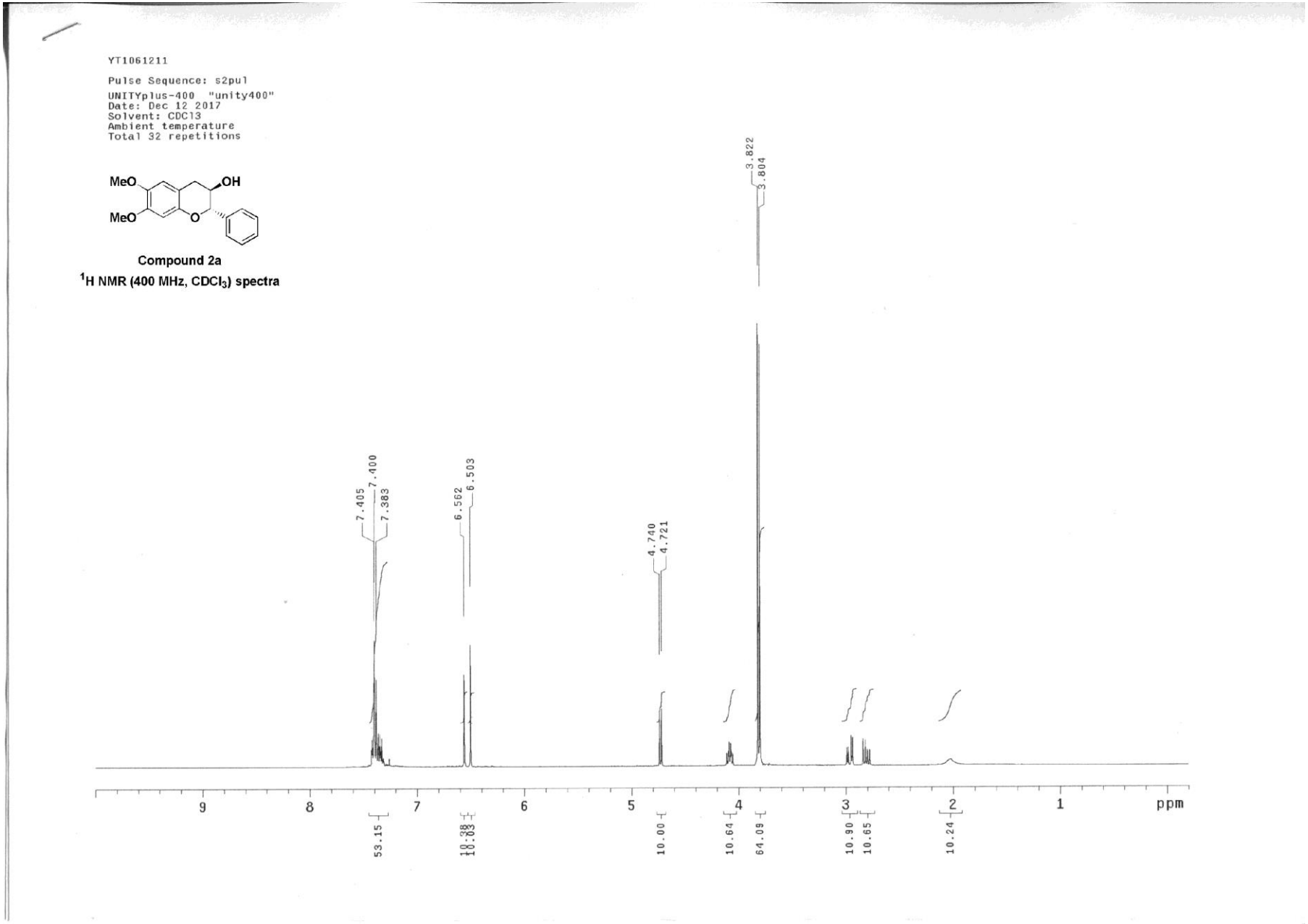
Compound 2a (^{1}H-NMR spectral data)

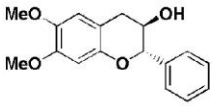


Compound 2a (^{1}H-NMR spectral data)

YT1061211

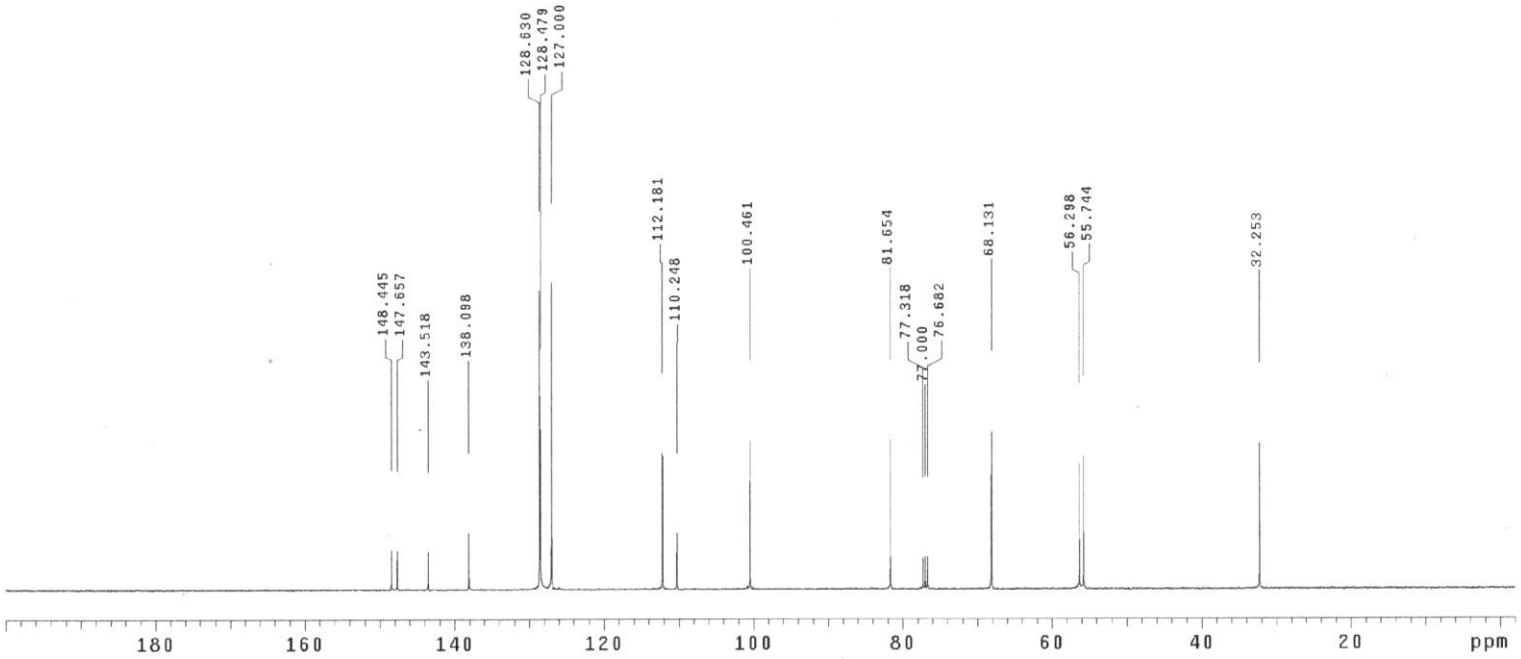
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Dec 12 2017
Solvent: CDCl3
Ambient temperature
Total 1392 repetitions



Compound 2a

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



Compound 2b (^{1}H-NMR spectral data)

YT1061227

Pulse Sequence: s2pul
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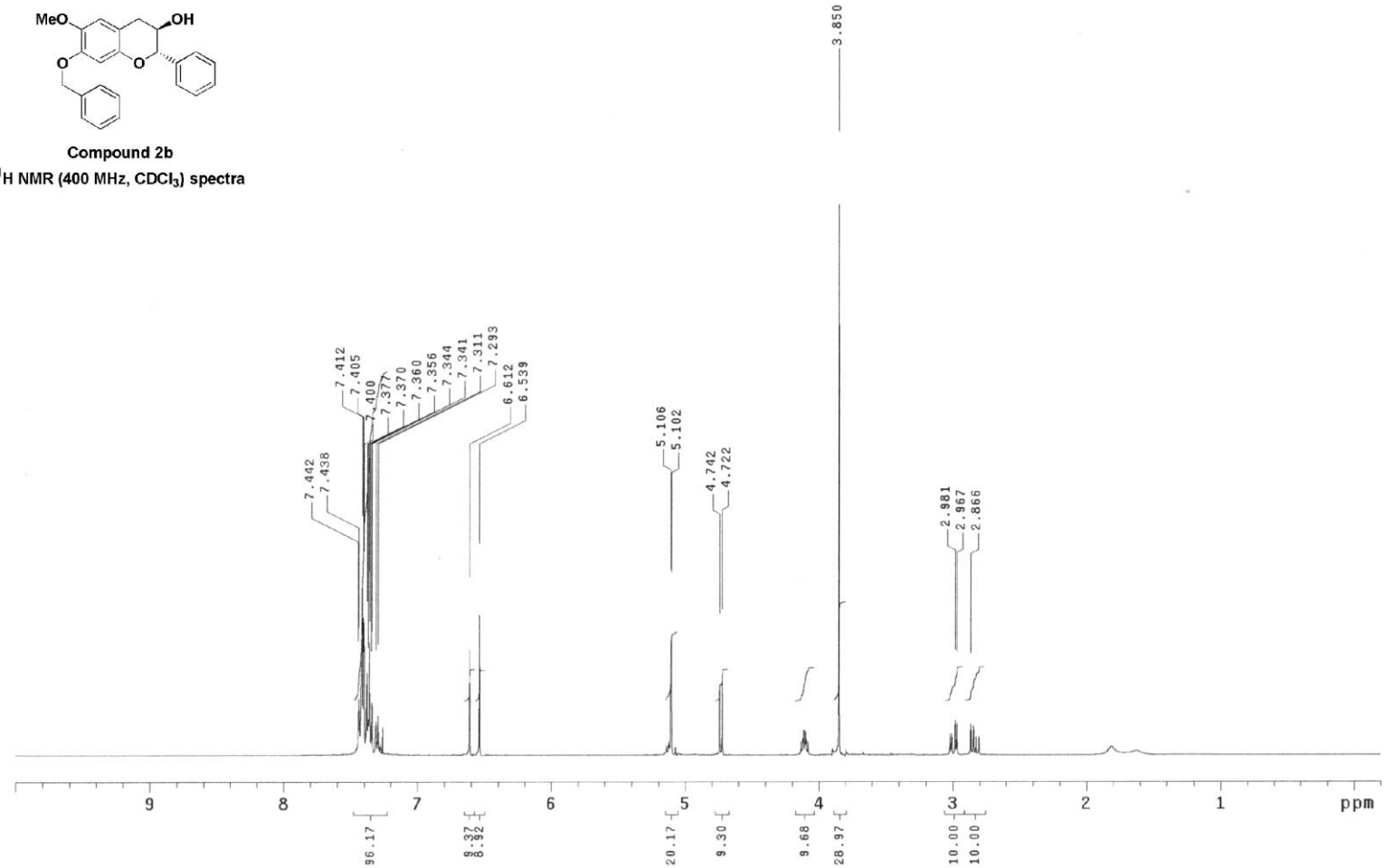
Date: Dec 26 2017
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

Compound 2b

^{1}H NMR (400 MHz, $CDCl_3$) spectra



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

YT1061227

Pulse Sequence: s2pul
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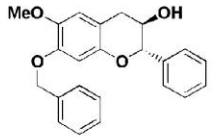
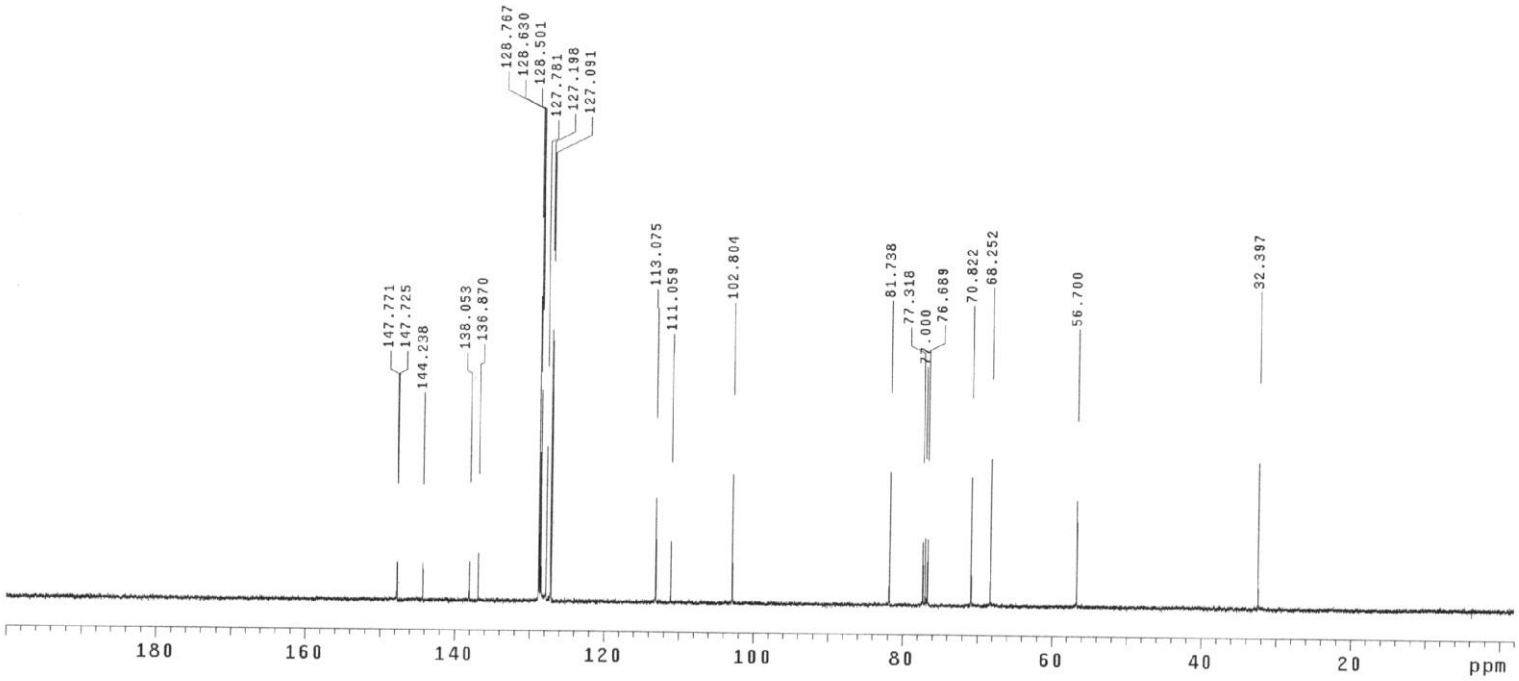
Date: Dec 26 2017
Solvent: CDCl3
Ambient temperature
Total 1232 repetitions

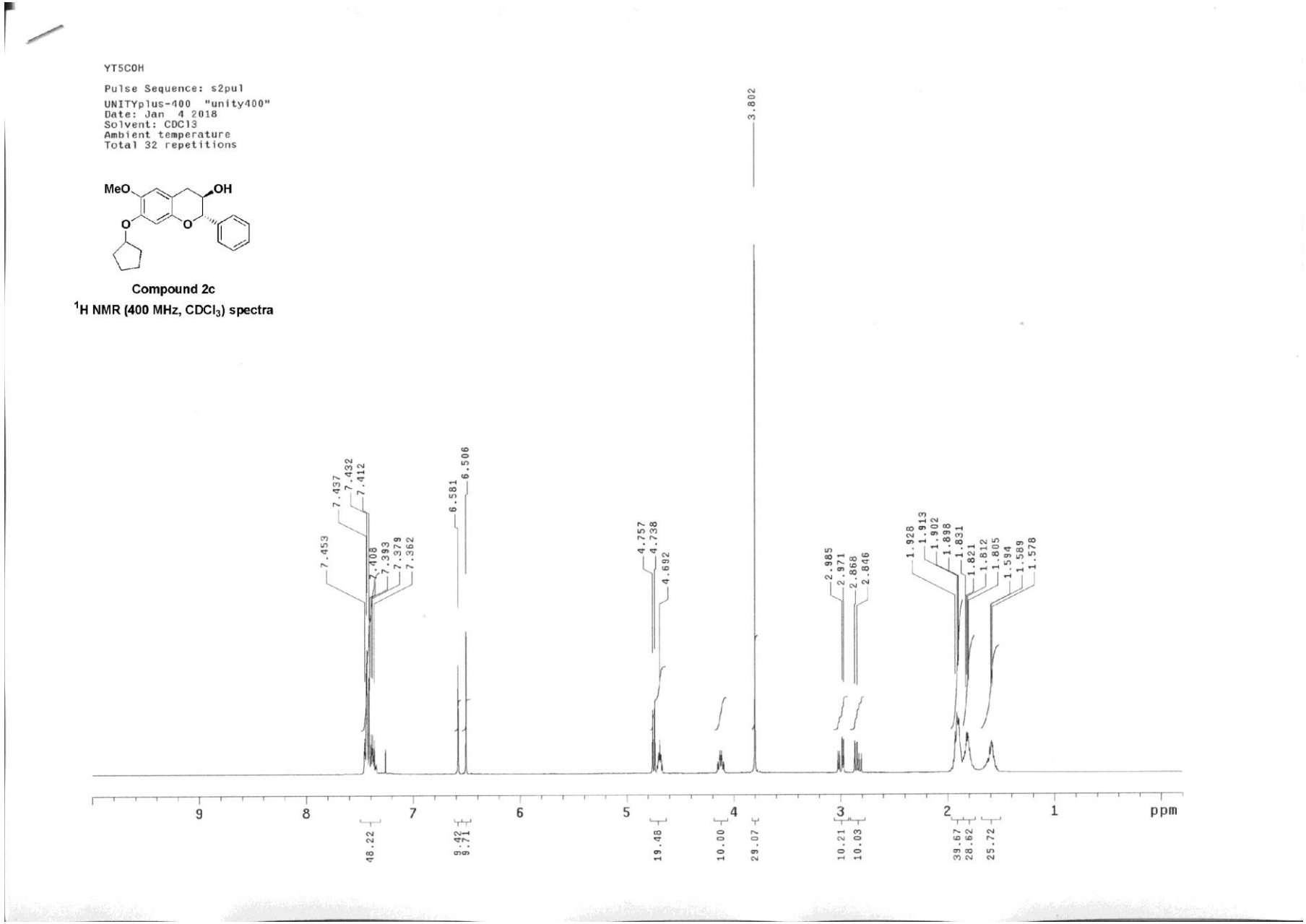


Compound 2b

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



Compound 2c (^{1}H-NMR spectral data)

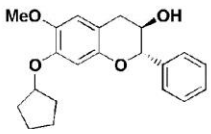


Compound 2c (^{13}C-NMR spectral data)

YT5COH

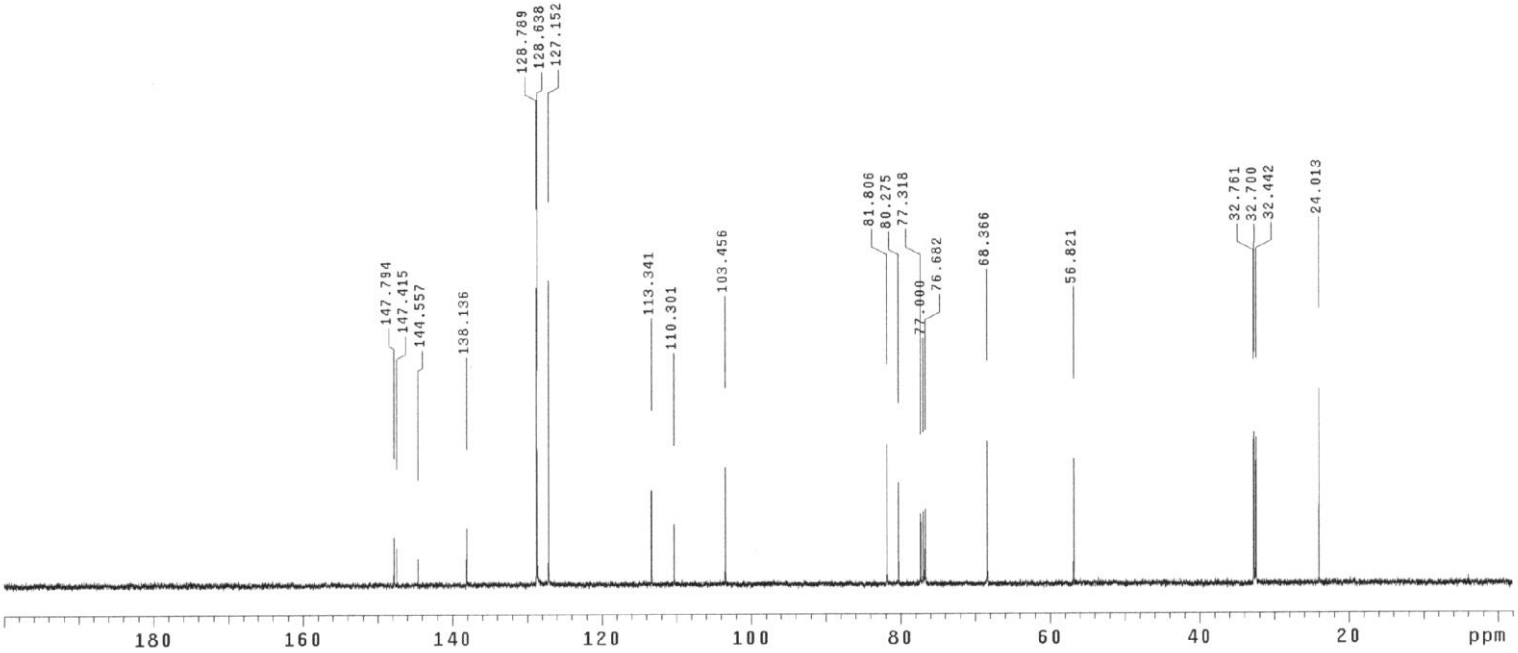
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jan 4 2018
Solvent: CDCl3
Ambient temperature
Total 768 repetitions

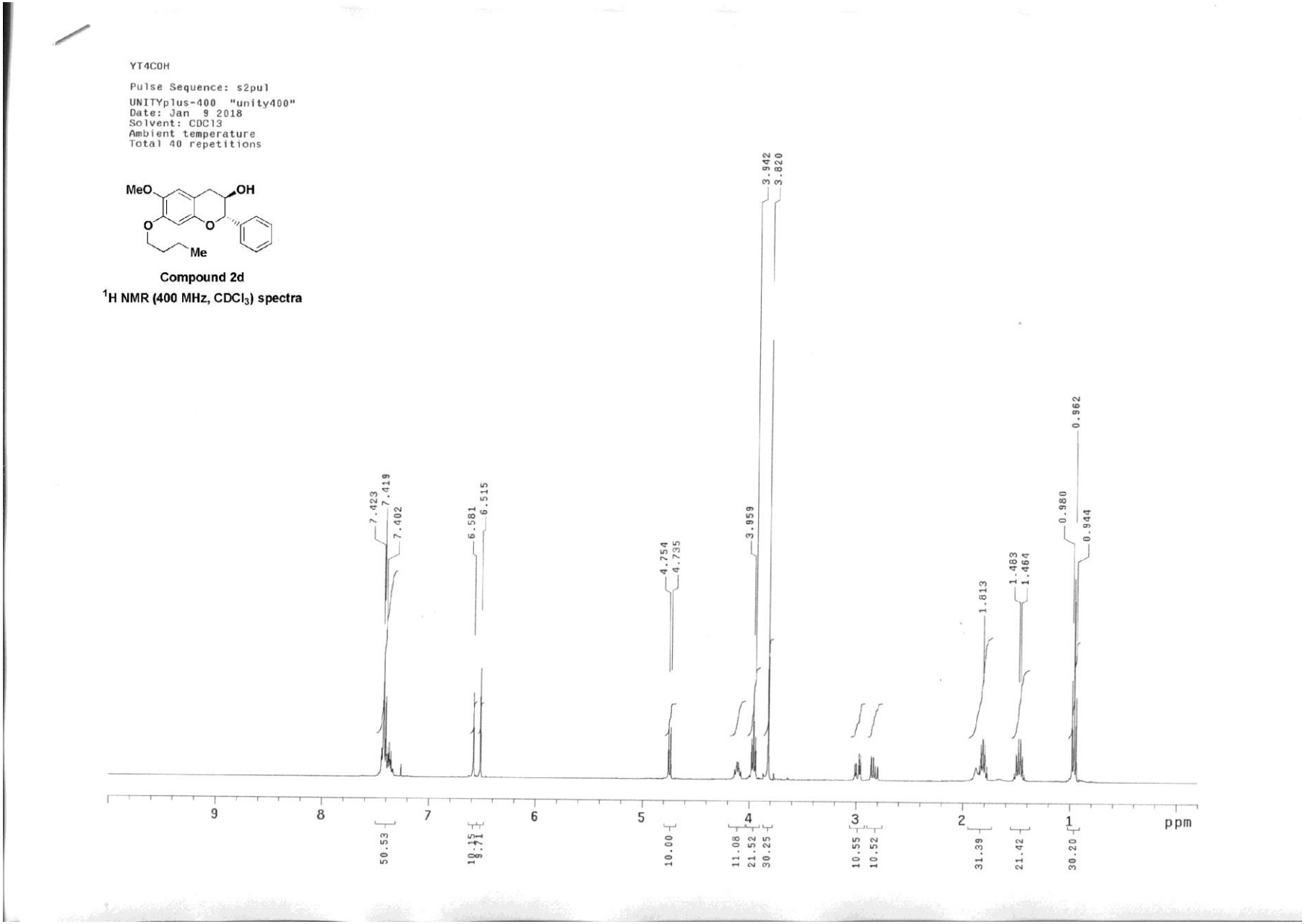


Compound 2c

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



Compound 2d (^{1}H-NMR spectral data)



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

YT4COH

Pulse Sequence: s2pul
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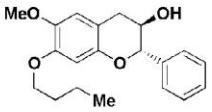
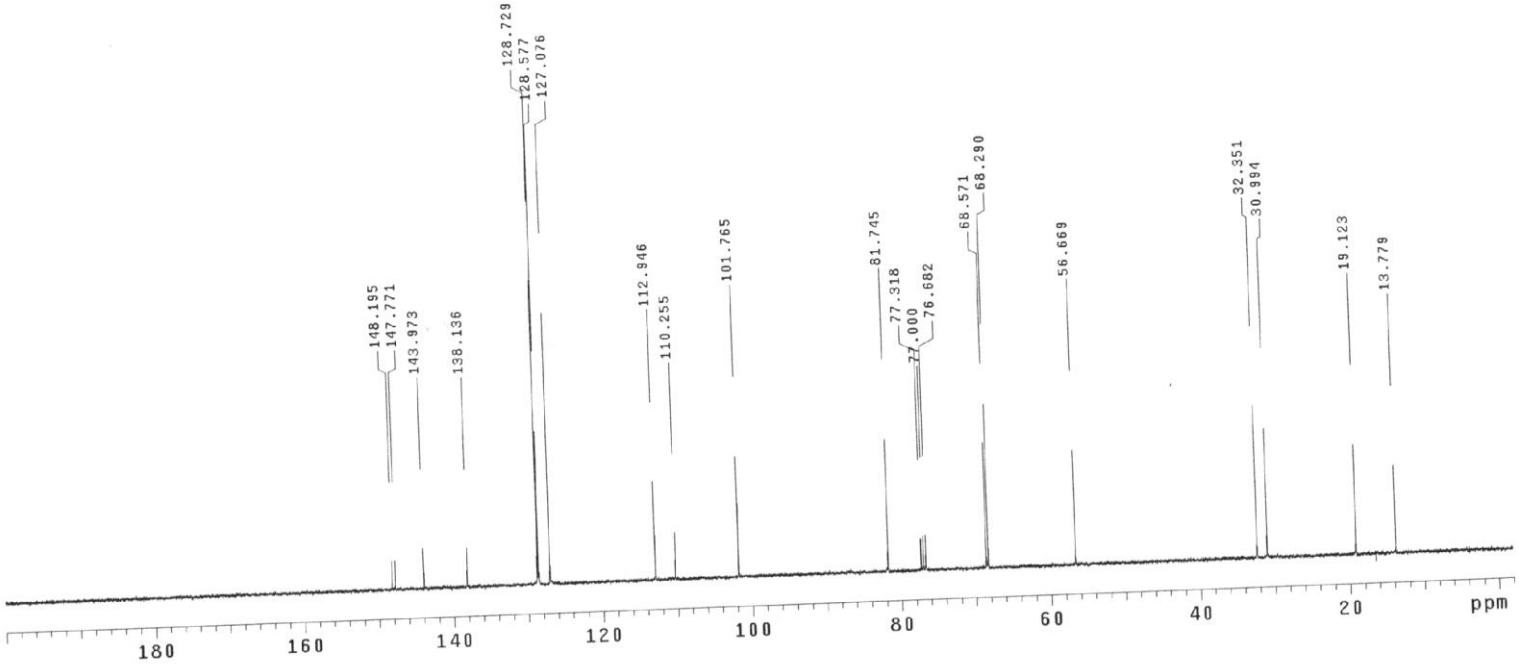
Solvent: CDCl3
Ambient temperature
Total 672 repetitions

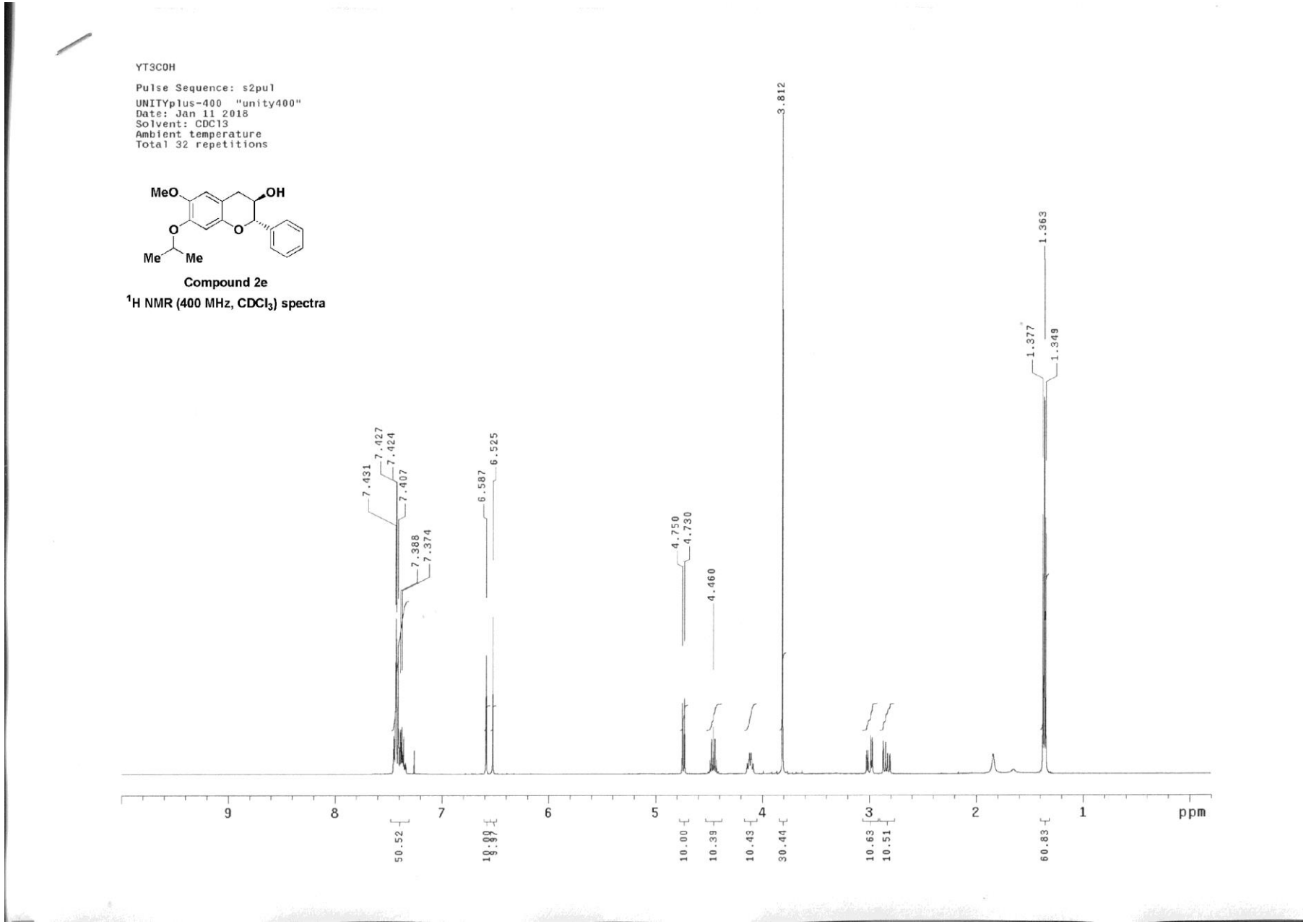


Compound 2d

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



Compound 2e (^{1}H-NMR sectral data)

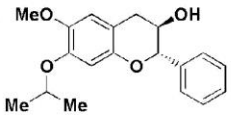


Compound 2e (^{13}C-NMR spectral data)

YT3COH

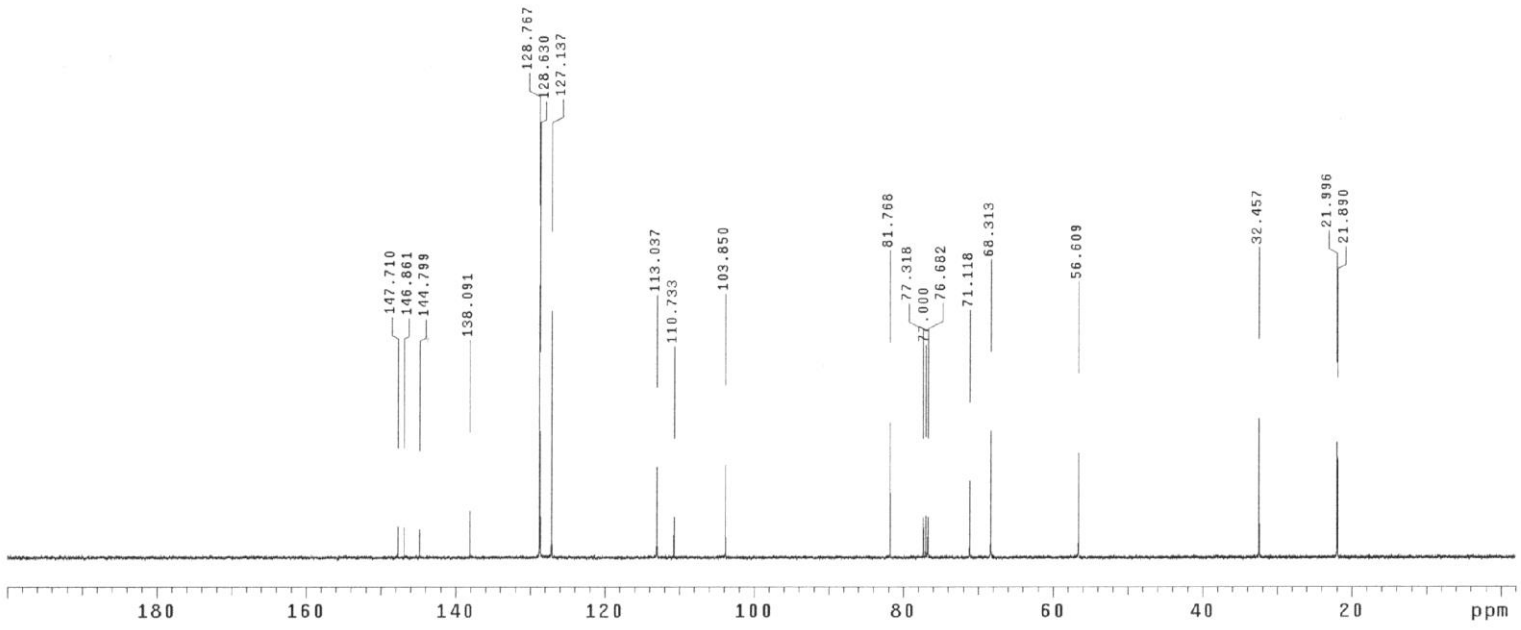
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jan 11 2018
Solvent: CDCl3
Ambient temperature
Total 736 repetitions

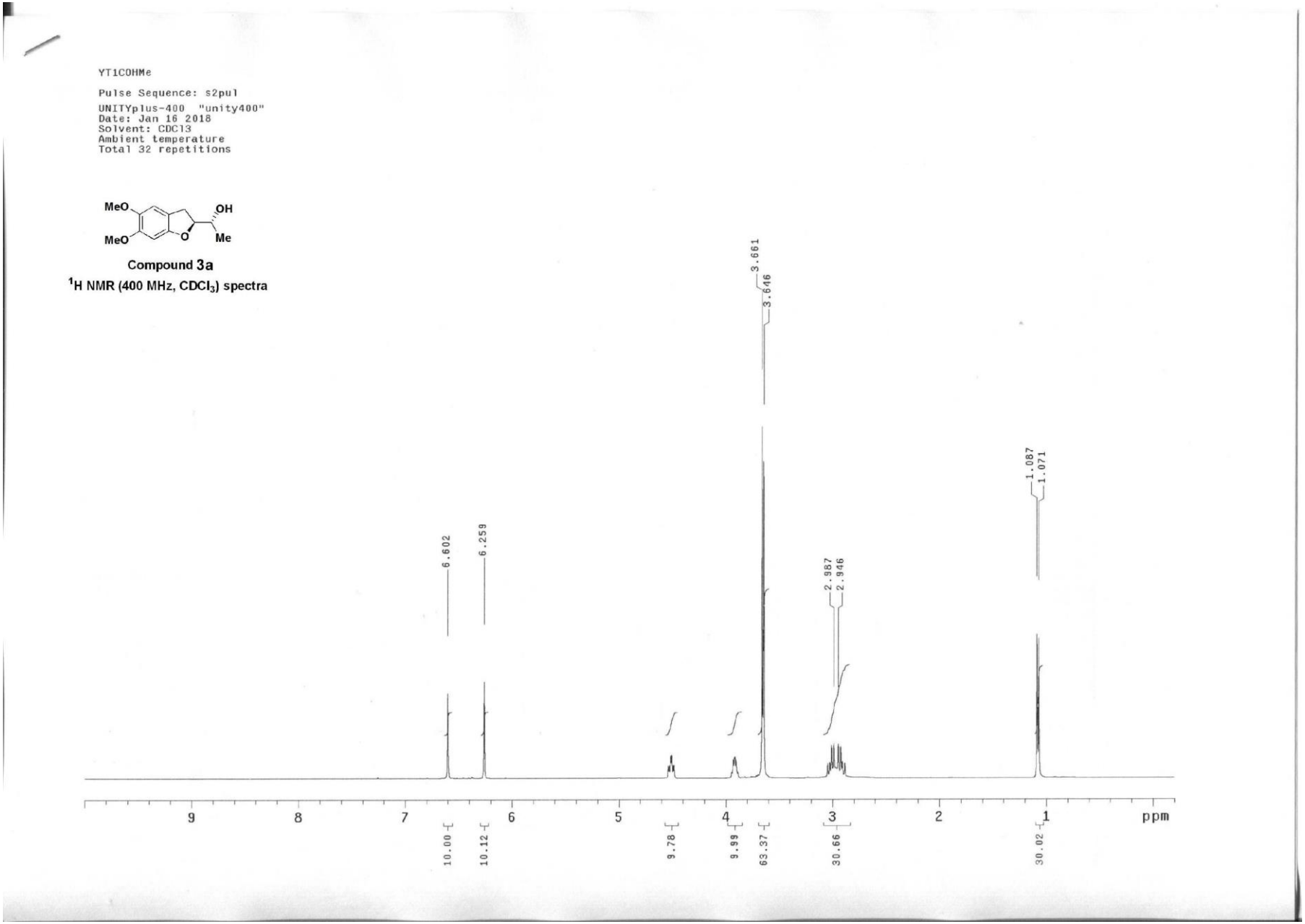


Compound 2e

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



Compound 3a (^{1}H-NMR spectral data)

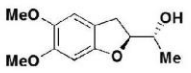


Compound 3a (^{13}C-NMR spectral data)

YT1COHMe

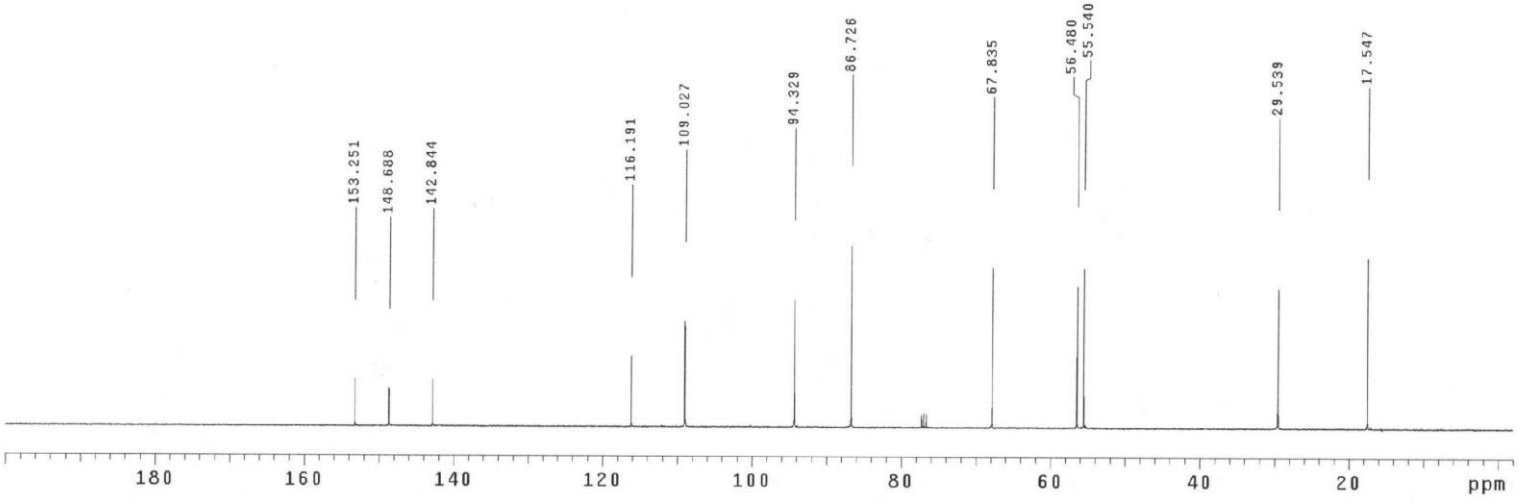
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jan 16 2018
Solvent: CDCl3
Ambient temperature
Total 176 repetitions



Compound 3a

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



Compound 3b (^{1}H-NMR spectral data)

YT7COH

Pulse Sequence: s2pul
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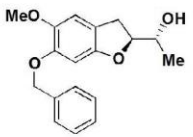
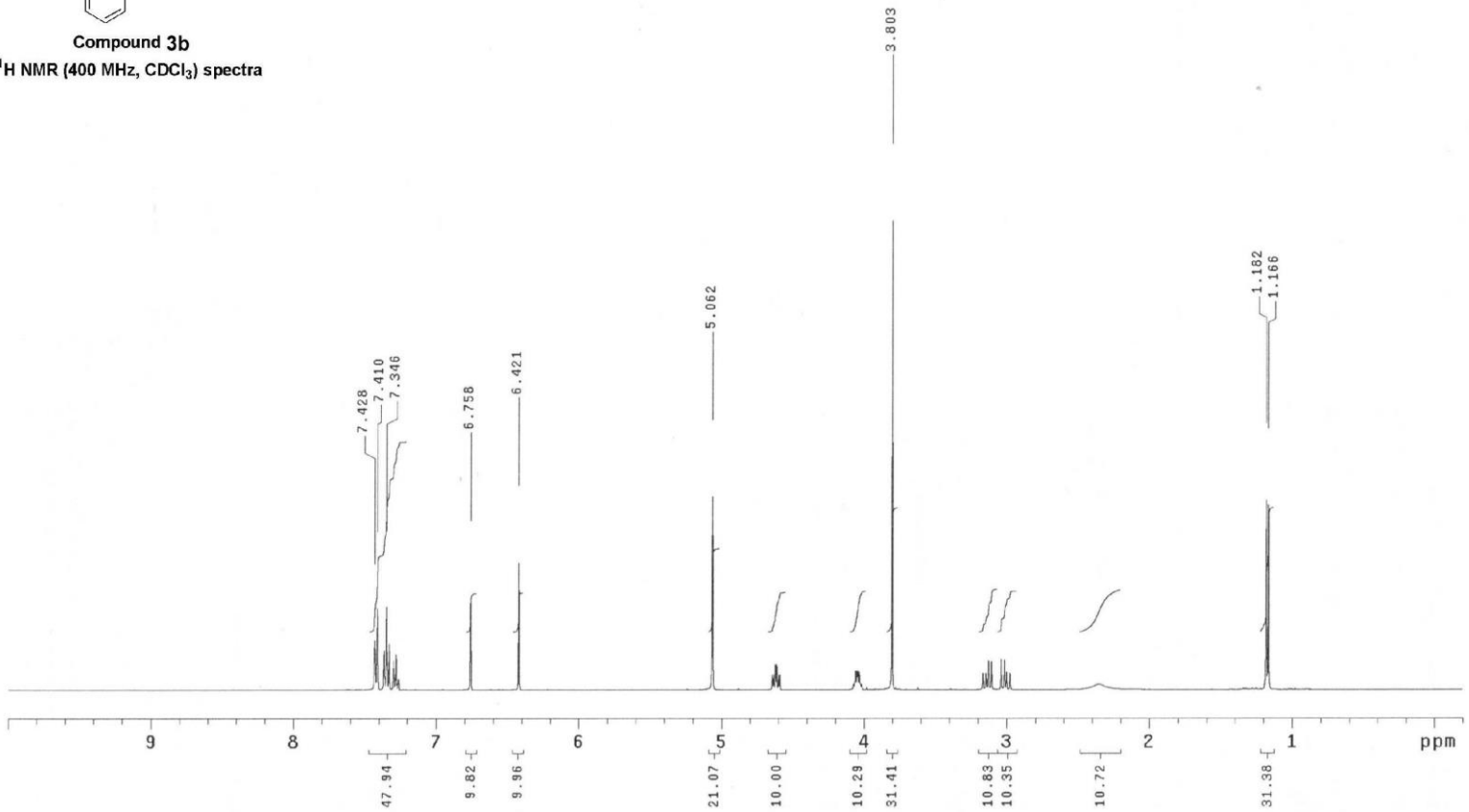
Date: Jan 22 2018
Solvent: CDCl3
Ambient temperature
Total 32 repetitions



Compound 3b

^{1}H NMR (400 MHz, $CDCl_3$) spectra



Compound 3b (^{13}C-NMR spectral data)

YT7COH

Pulse Sequence: s2pul
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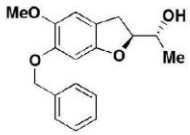
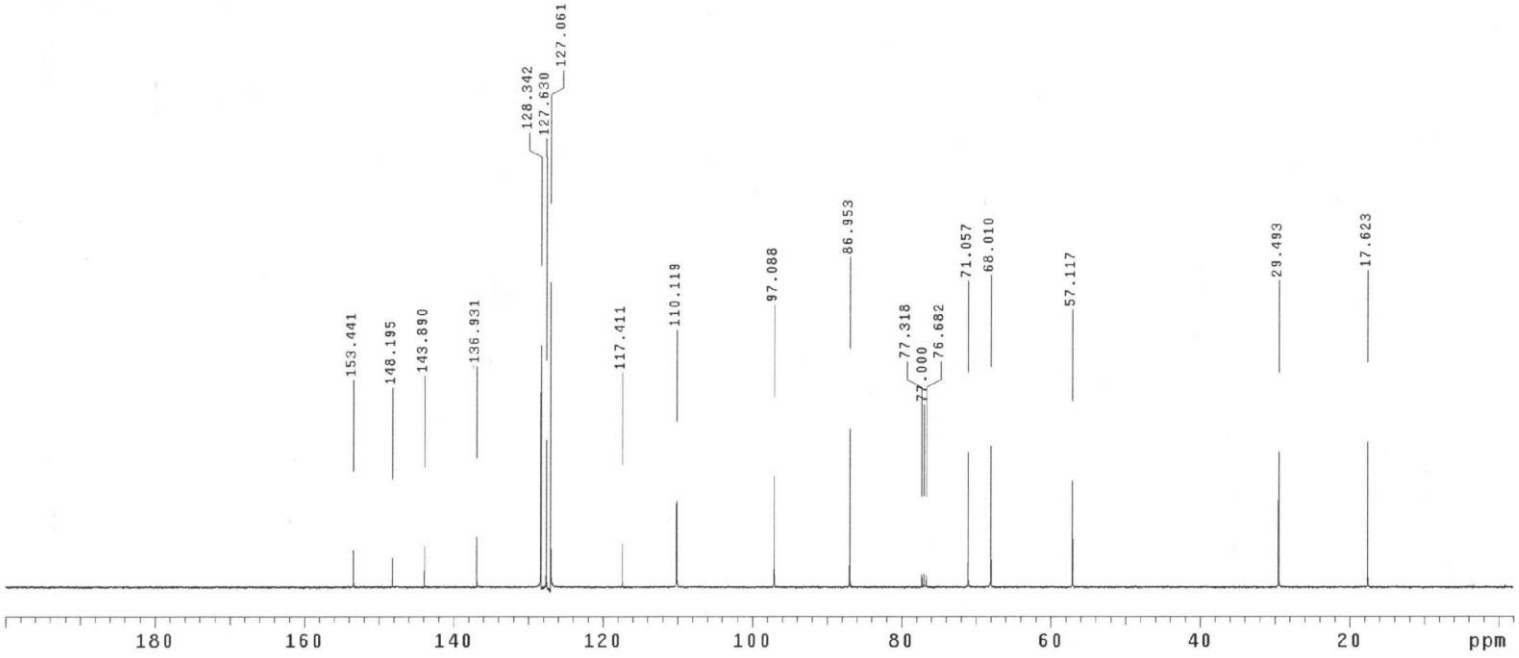
Date: Jan 22 2018
Solvent: CDCl3
Ambient temperature
Total 320 repetitions

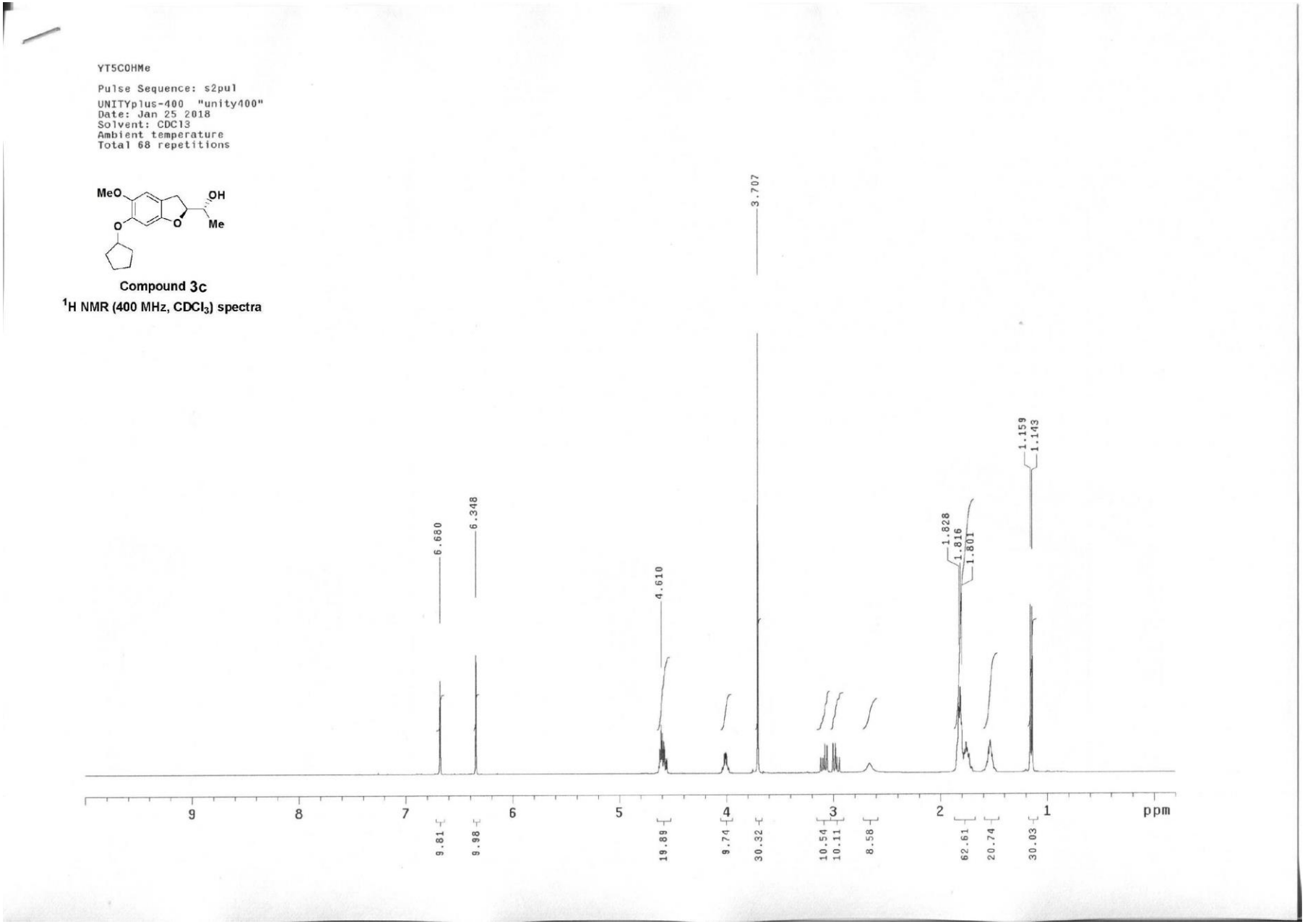


Compound 3b

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



Compound 3c (^{1}H-NMR spectral data)



Compound 3c (^{13}C-NMR spectral data)

YT5COHMe

Pulse Sequence: s2pul

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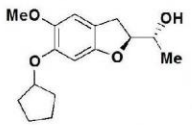
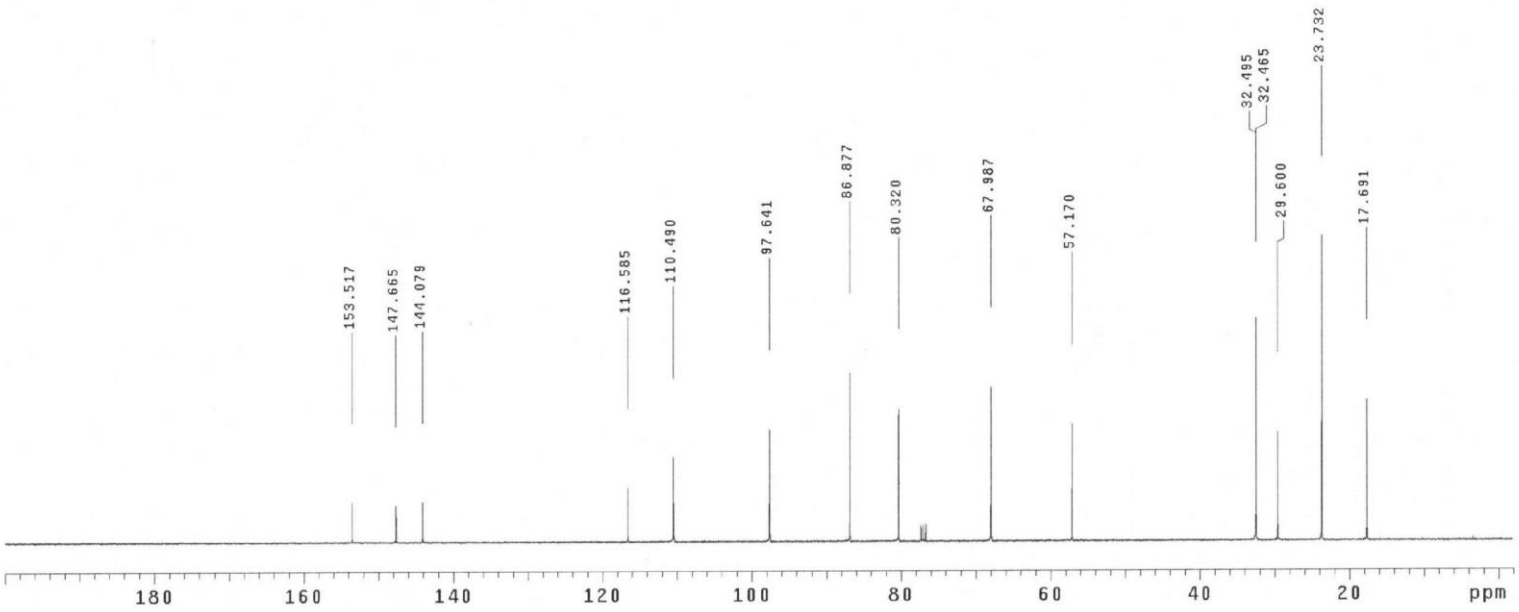
Date: Jan 25 2018
Solvent: CDCl3
Ambient temperature
Total 64000 repetitions

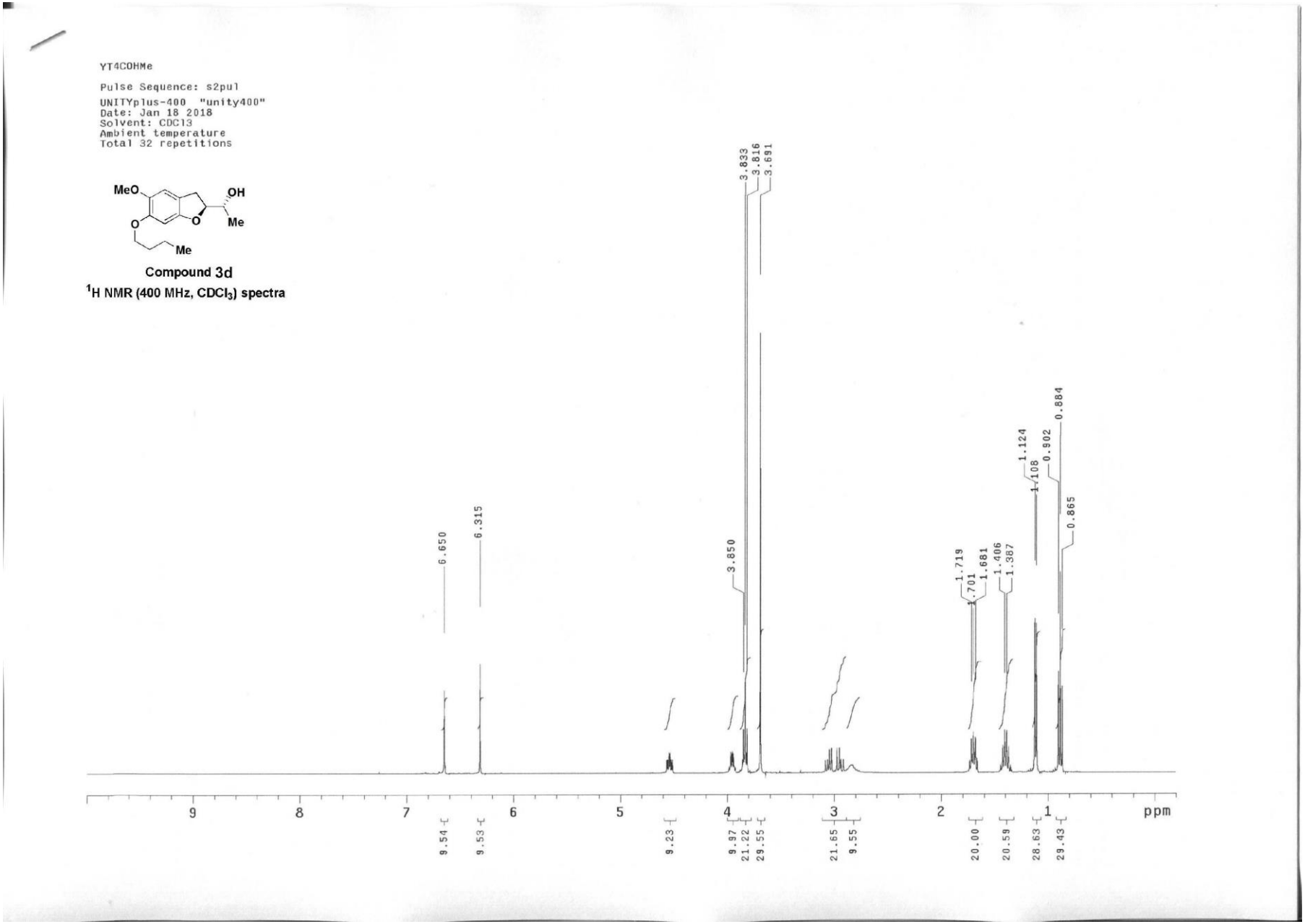


Compound 3c

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



Compound 3d (^{1}H-NMR sectral data)

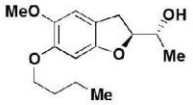


Compound 3d (^{13}C-NMR spectral data)

YT4COHMe

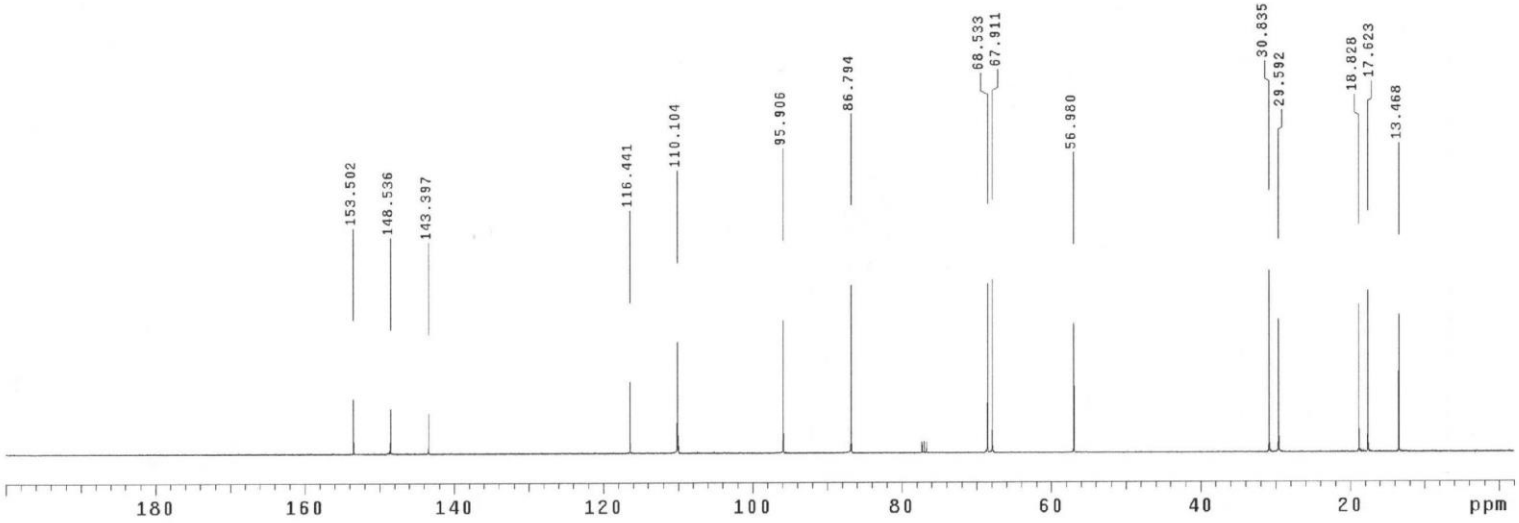
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jan 18 2018
Solvent: CDCl3
Ambient temperature
Total 96 repetitions

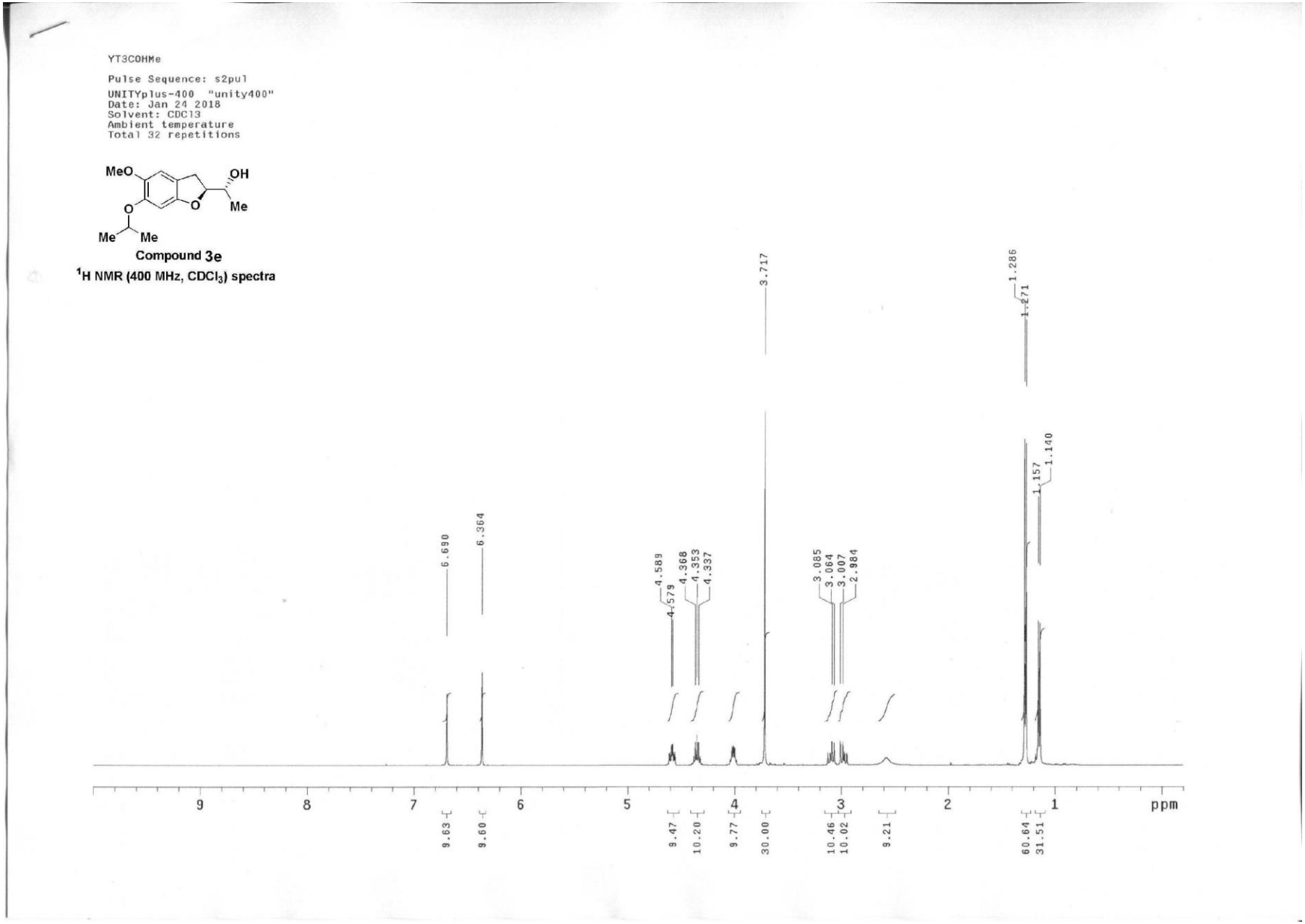


Compound 3d

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



Compound 3e (^{1}H-NMR spectral data)

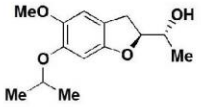


Compound 3e (^{13}C-NMR spectral data)

YT3COHMe

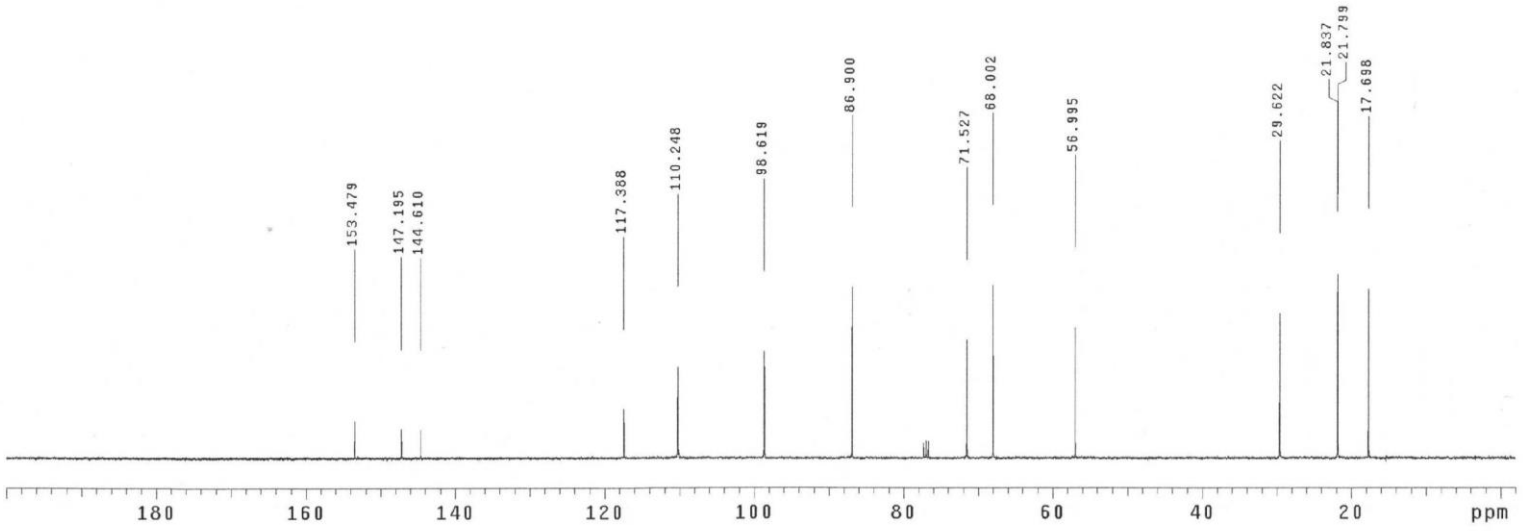
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jan 24 2018
Solvent: CDCl3
Ambient temperature
Total 80 repetitions

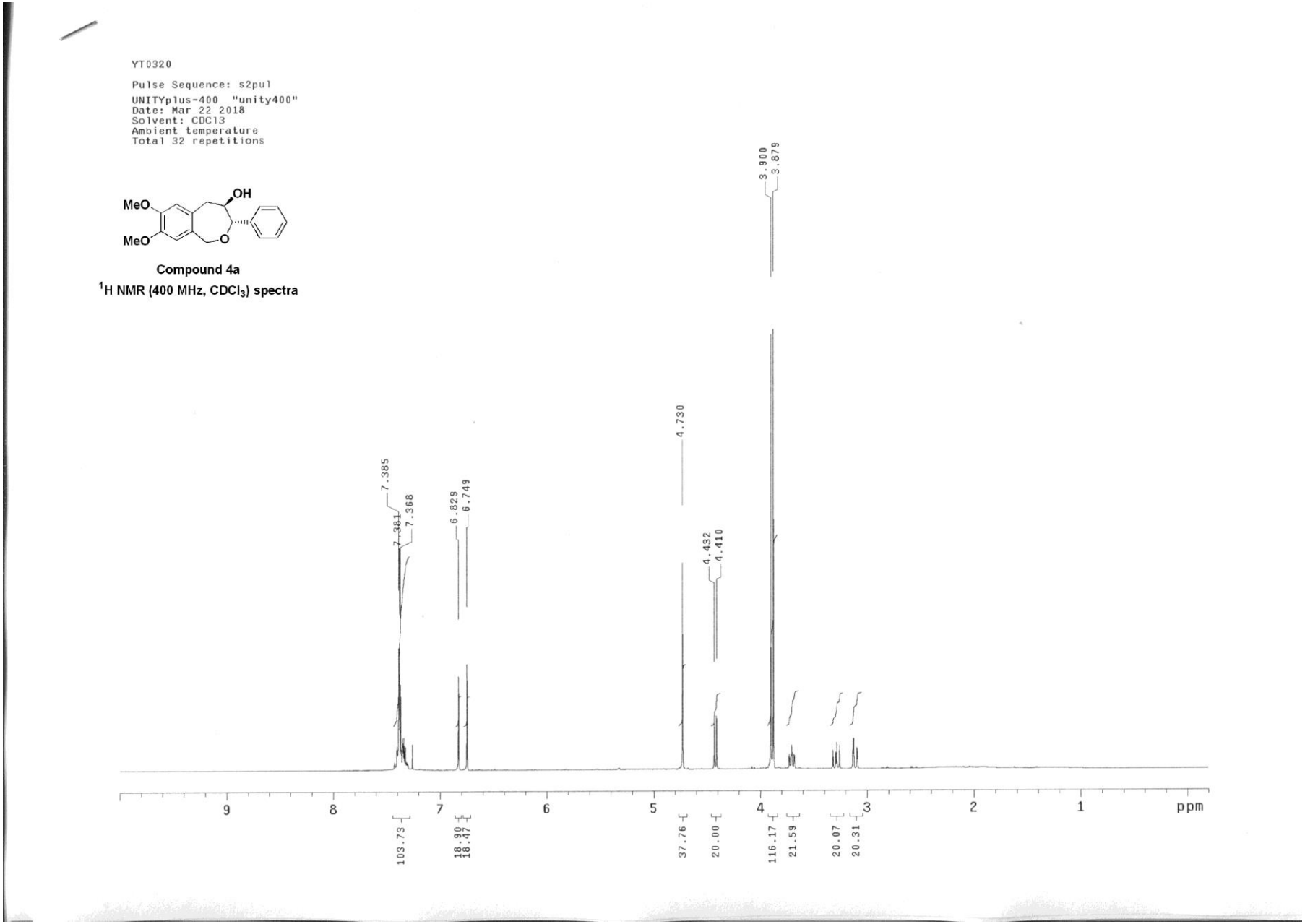


Compound 3e

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



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



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

YT0320

Pulse Sequence: s2pul

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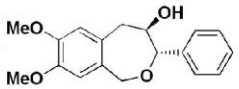
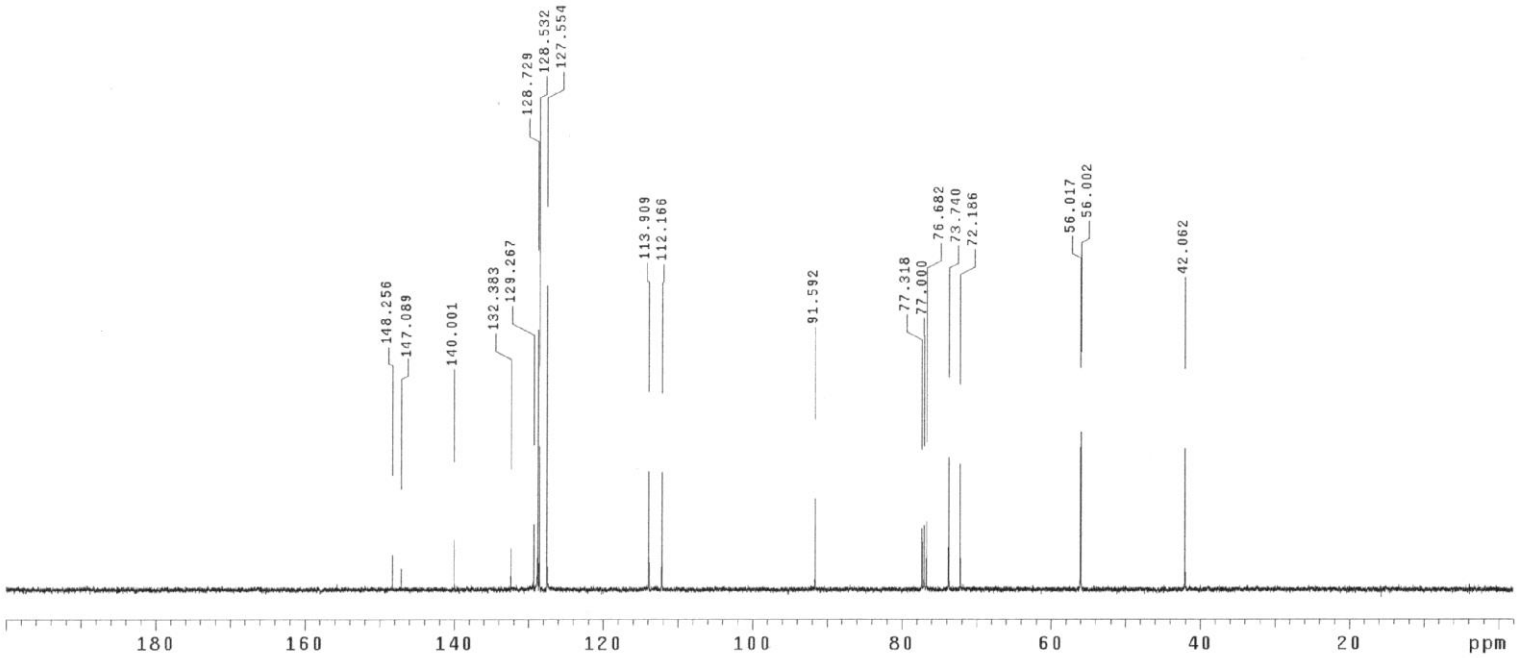
Date: Mar 22 2018
Solvent: CDCl3
Ambient temperature
Total 1024 repetitions



Compound 4a

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



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

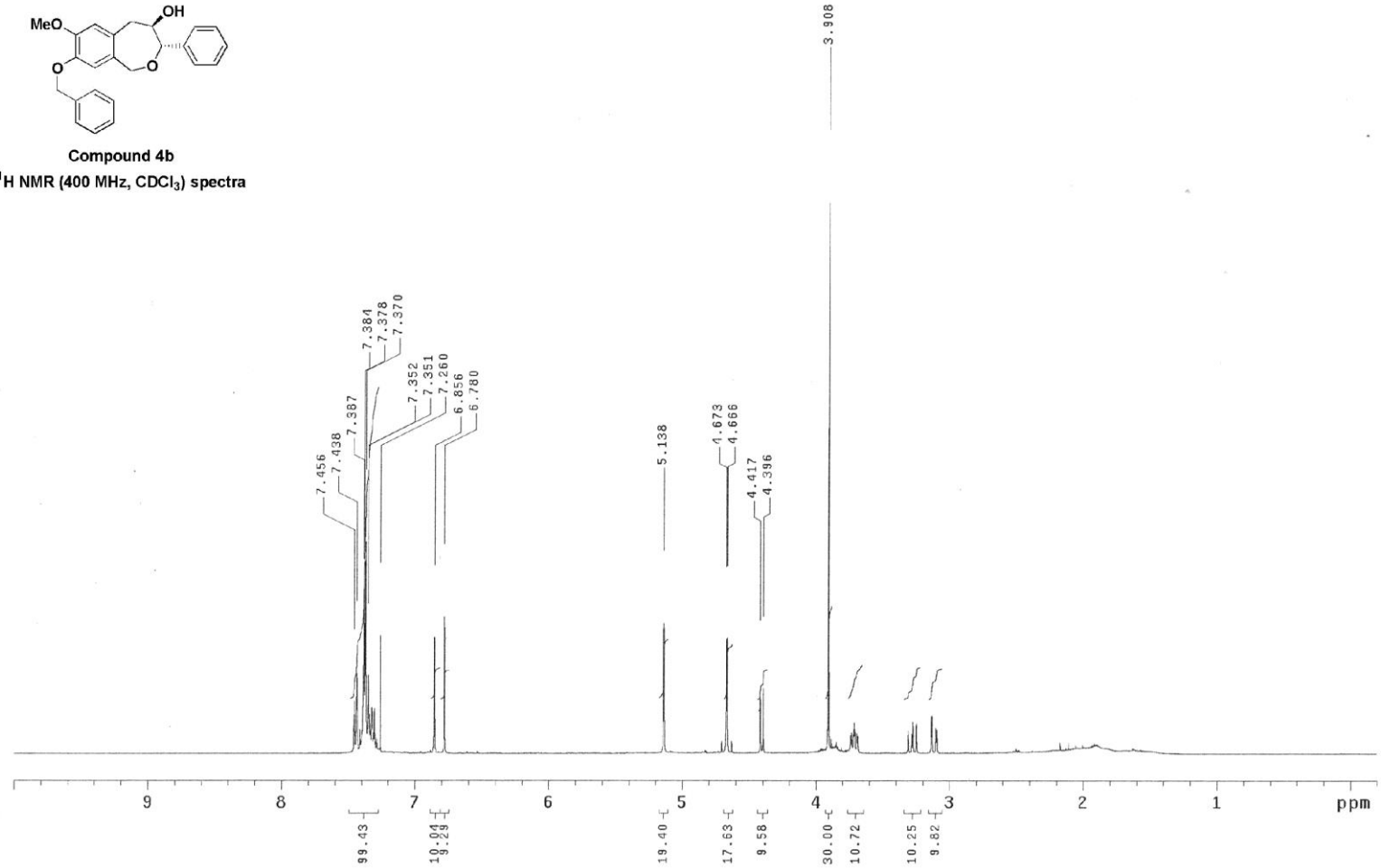
YT7CNaH

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Apr 18 2018
Solvent: CDCl3
Ambient temperature
Total 64 repetitions

Compound 4b

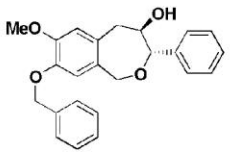
^{1}H NMR (400 MHz, $CDCl_3$) spectra



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

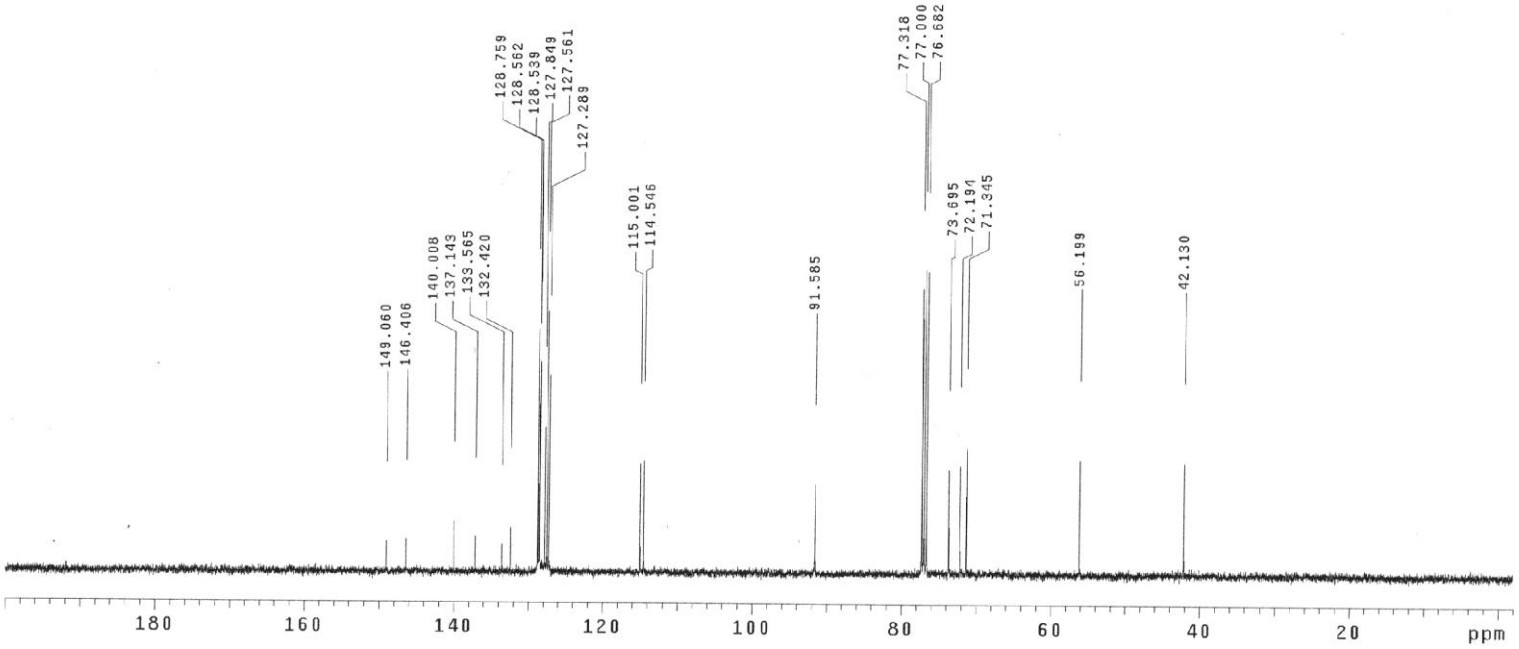
YT7CNaH

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Apr 18 2018
Solvent: CDCl3
Ambient temperature
Total 3232 repetitions

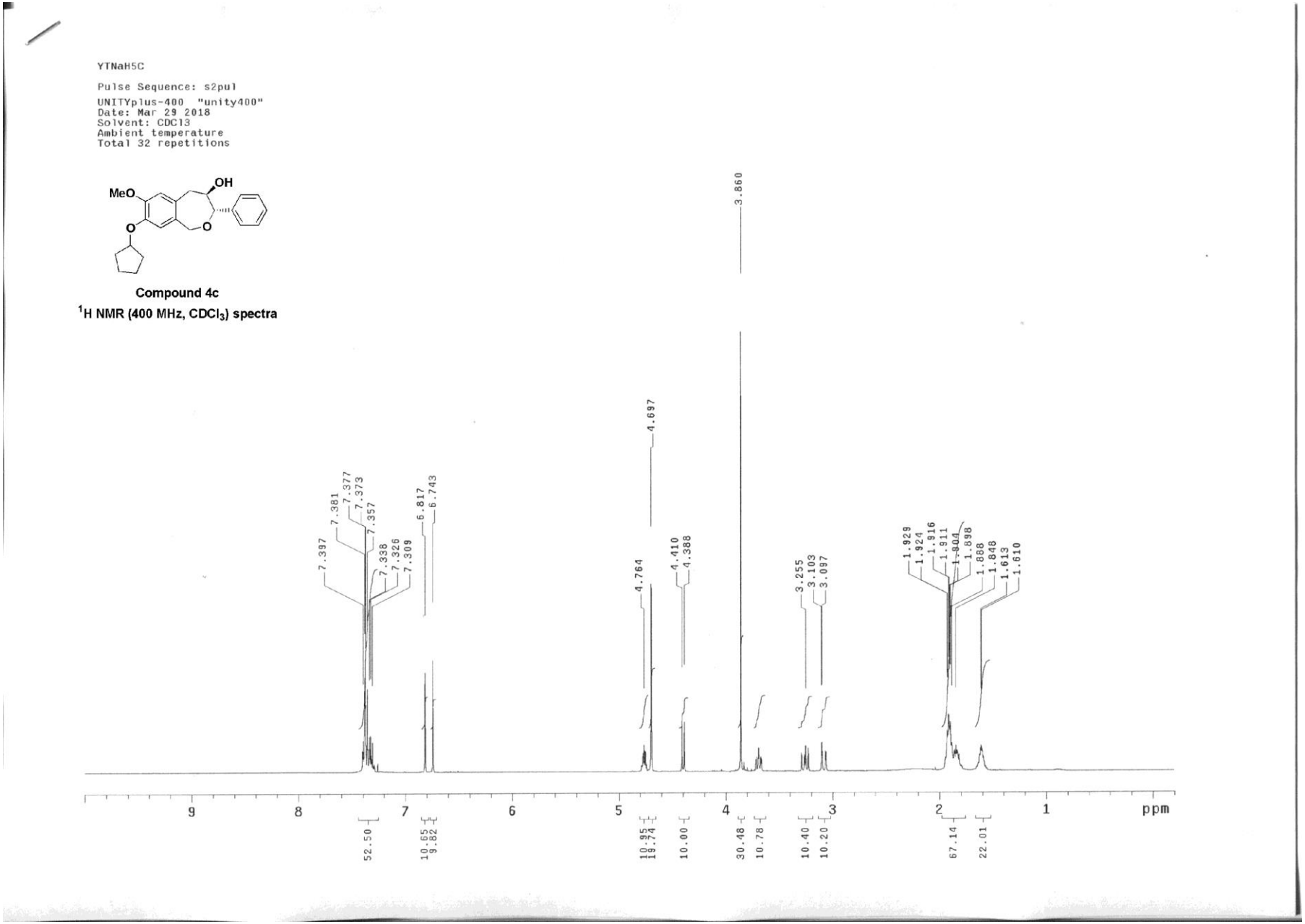


Compound 4b

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



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

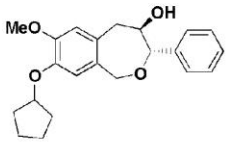


Compound 4c (^{13}C-NMR spectral data)

YTNaH5C

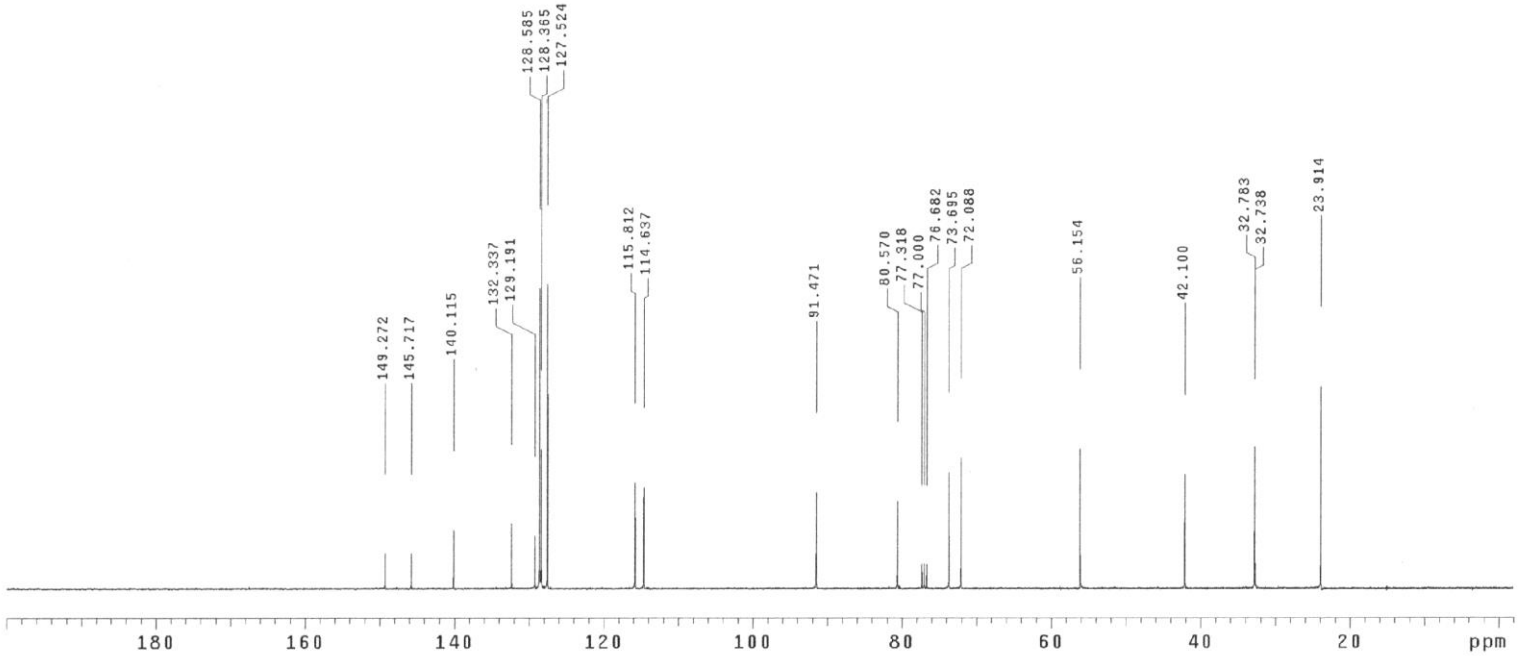
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Mar 29 2018
Solvent: CDCl3
Ambient temperature
Total 1024 repetitions

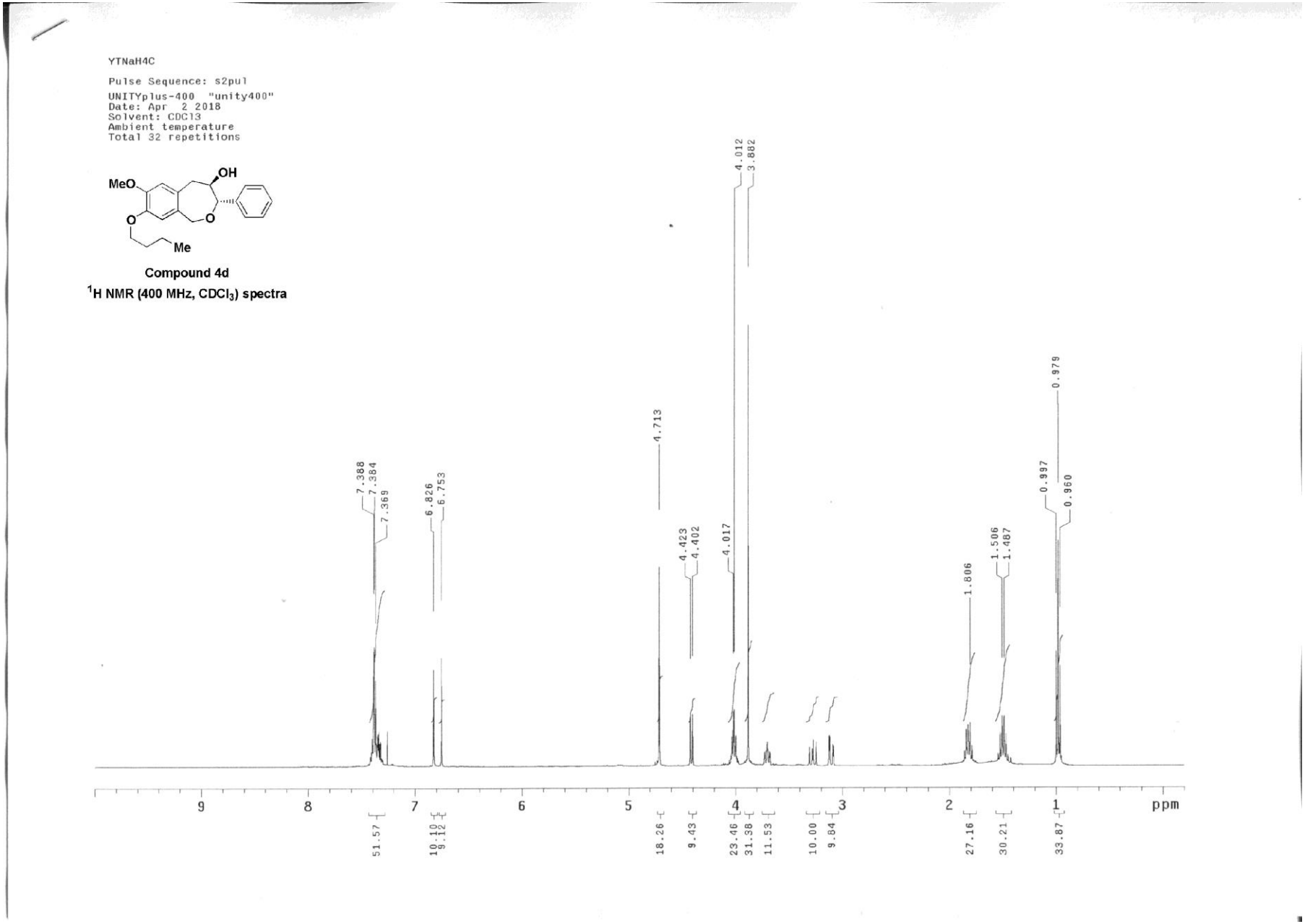


Compound 4c

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



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

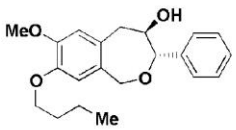


Compound 4d (^{13}C-NMR spectral data)

YTNaH4C

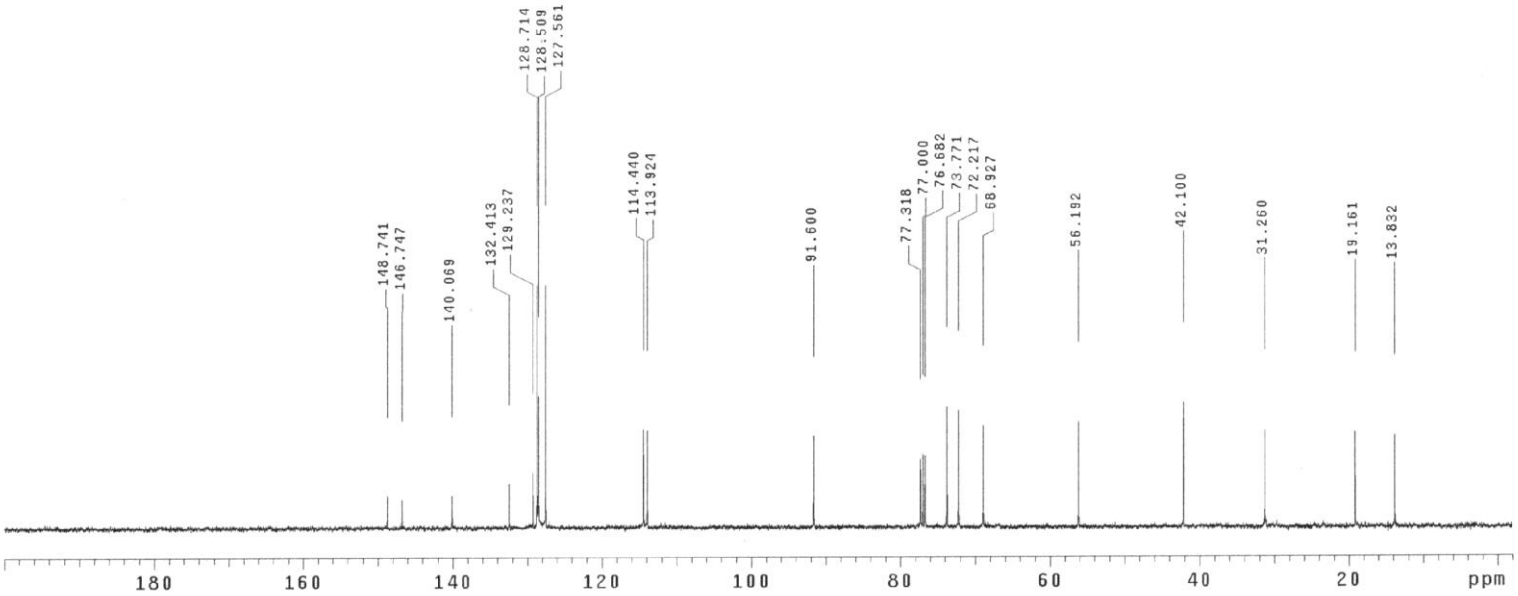
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Apr 2 2018
Solvent: CDCl3
Ambient temperature
Total 1632 repetitions



Compound 4d

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



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

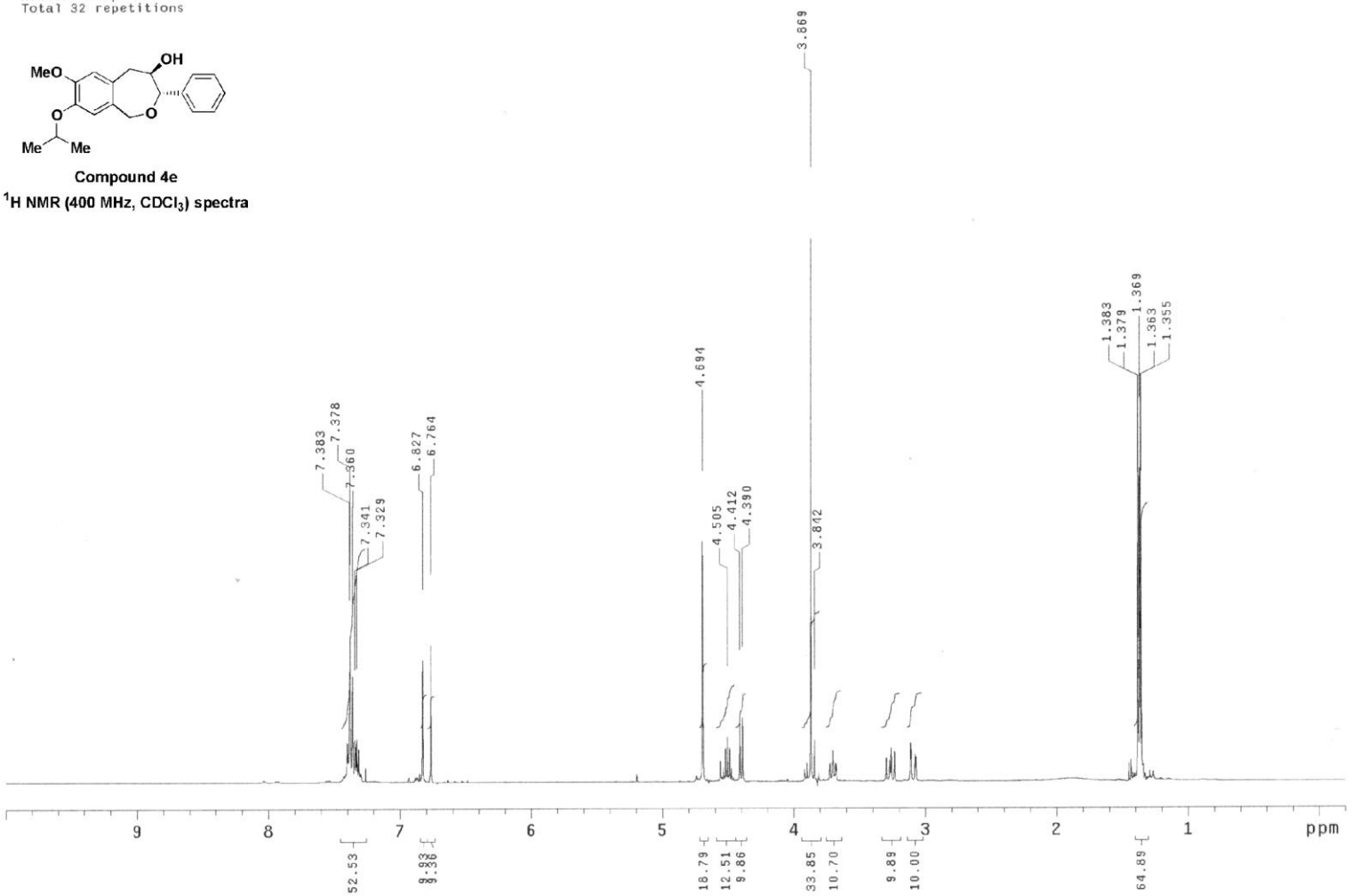
YTNaH3C

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Apr 2 2018
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

Compound 4e

^{1}H NMR (400 MHz, $CDCl_3$) spectra

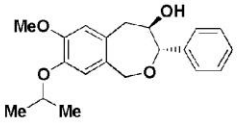


Compound 4e (^{13}C-NMR spectral data)

YTNaH3C

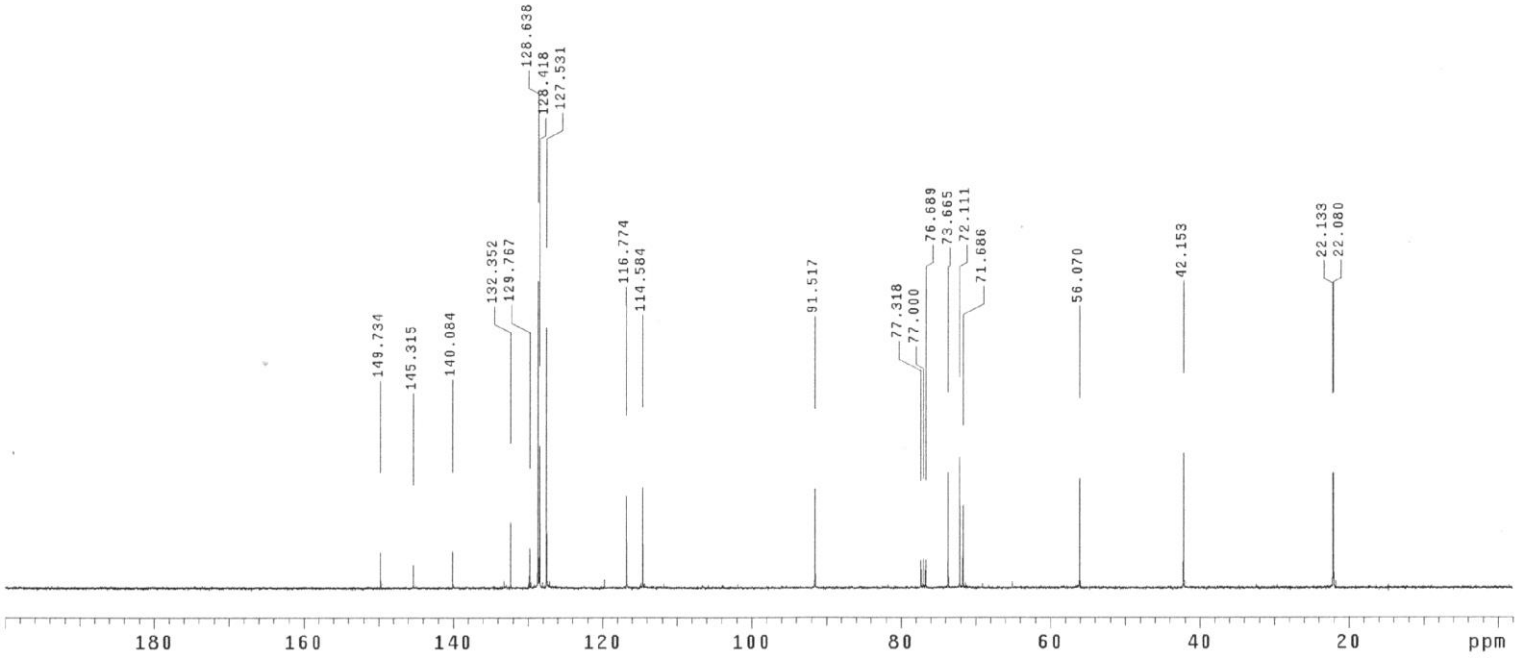
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Apr 2 2018
Solvent: CDCl3
Ambient temperature
Total 848 repetitions

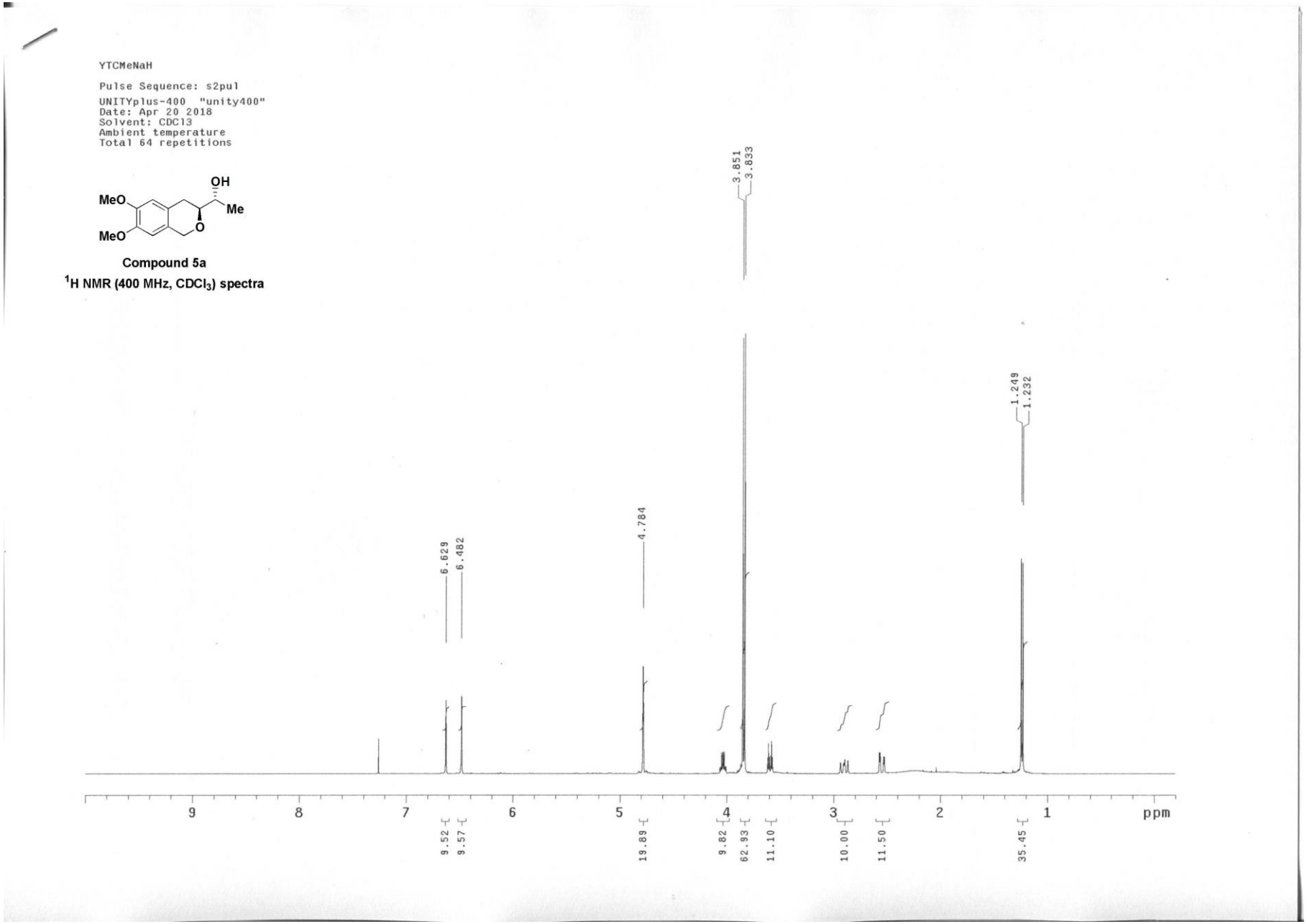


Compound 4e

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



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

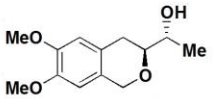


Compound 5a (^{13}C-NMR spectral data)

YTCMeNaH

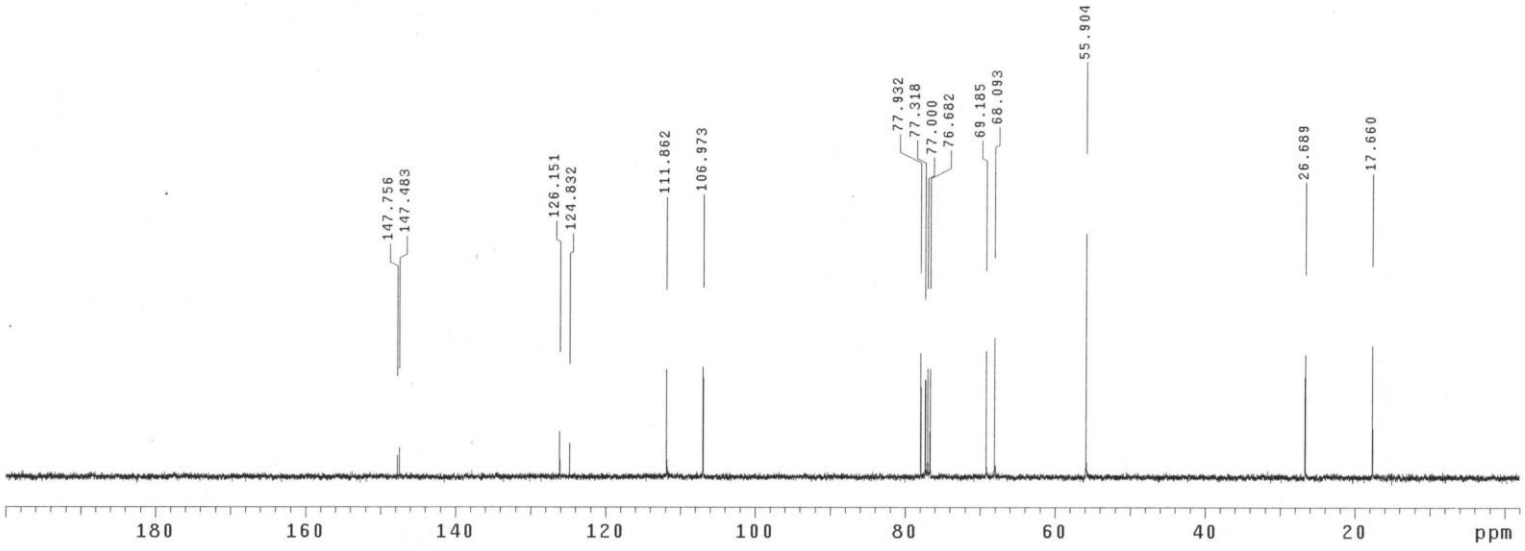
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Apr 20 2018
Solvent: CDCl3
Ambient temperature
Total 1072 repetitions

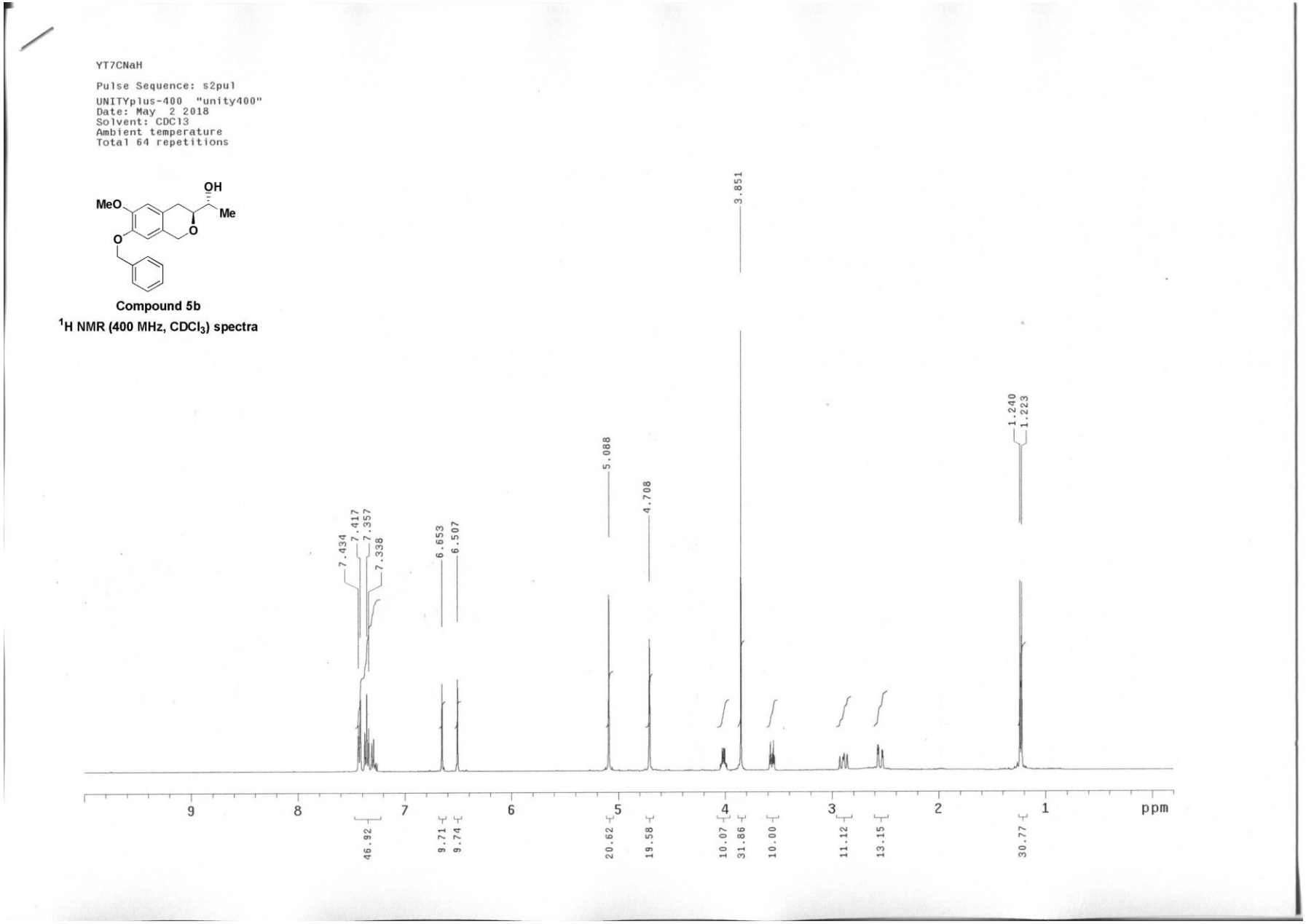


Compound 5a

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



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

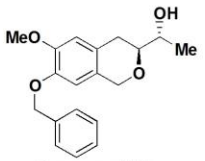


Compound 5b (^{13}C-NMR spectral data)

YT7CNaH

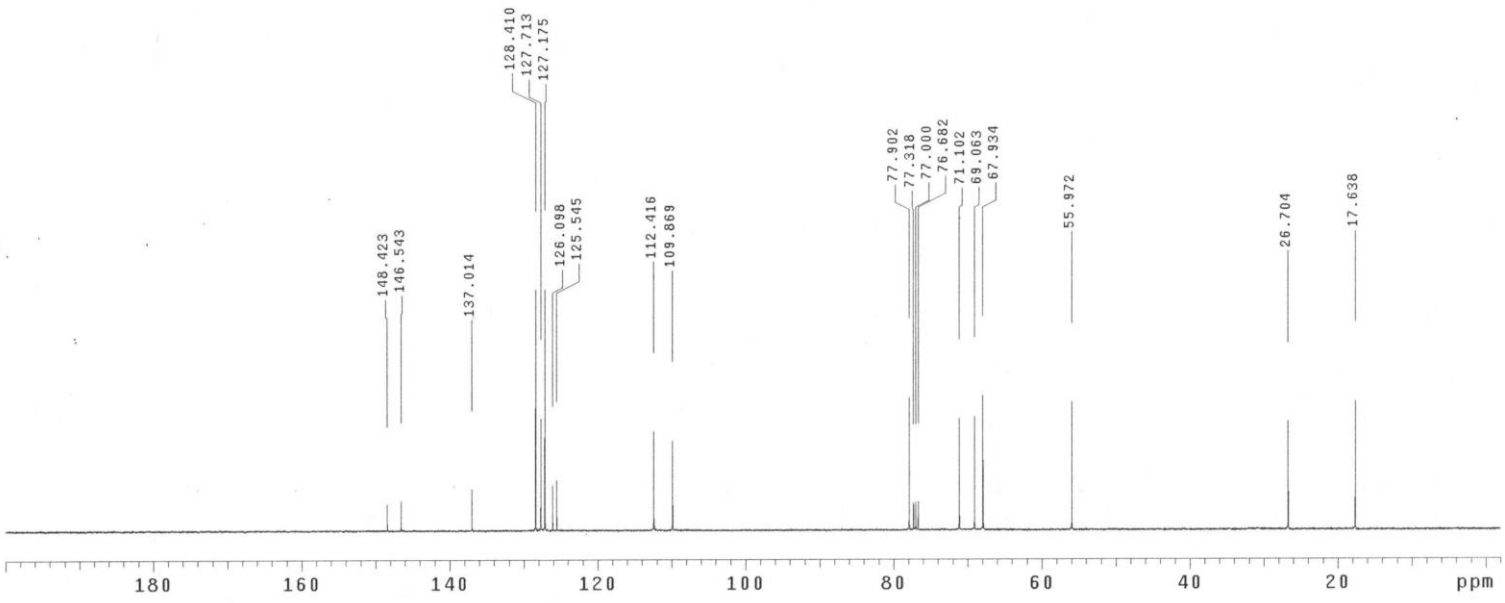
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 2 2018
Solvent: CDCl3
Ambient temperature
Total 576 repetitions

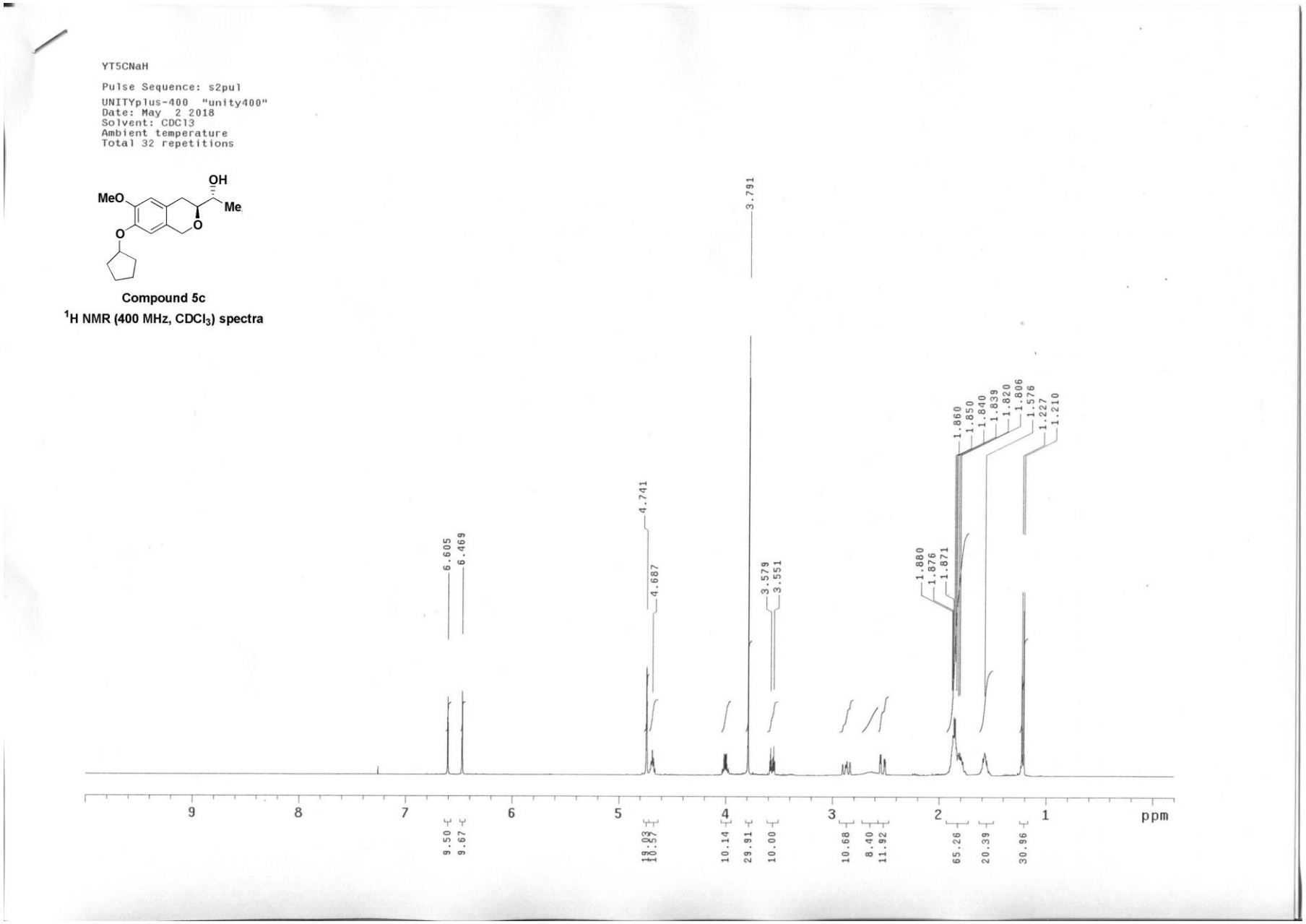


Compound 5b

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



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

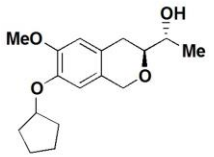


Compound 5c (^{13}C-NMR spectral data)

YT5CNaH

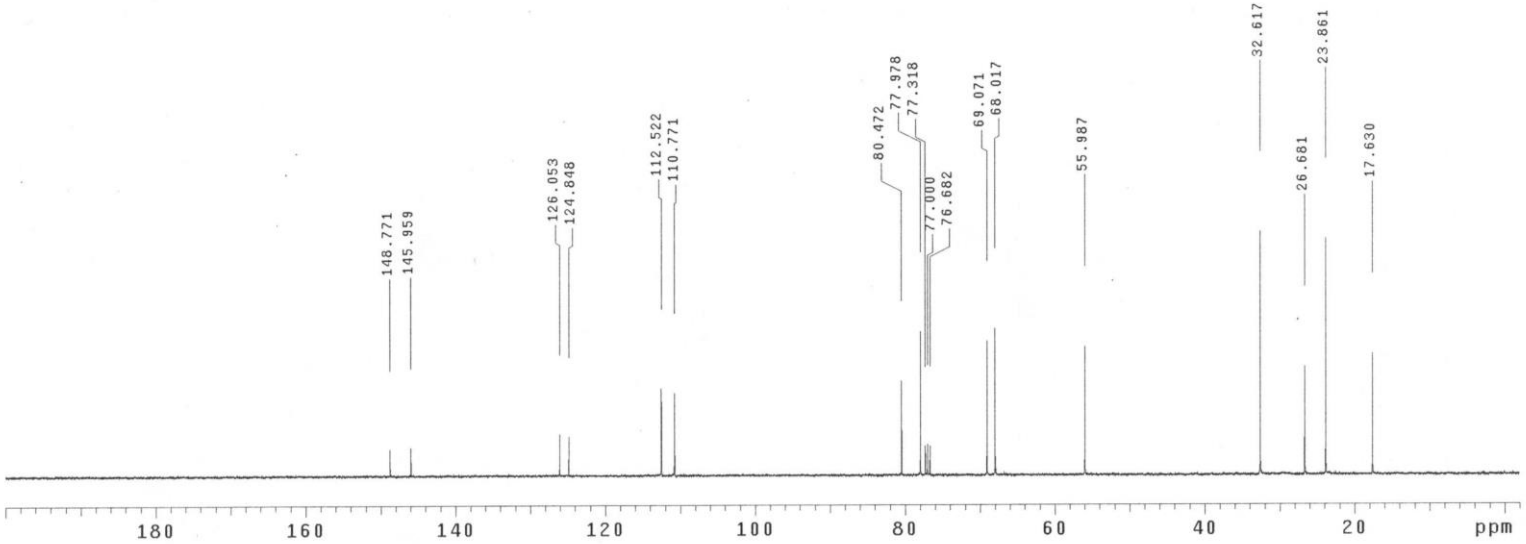
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 2 2018
Solvent: CDCl3
Ambient temperature
Total 208 repetitions

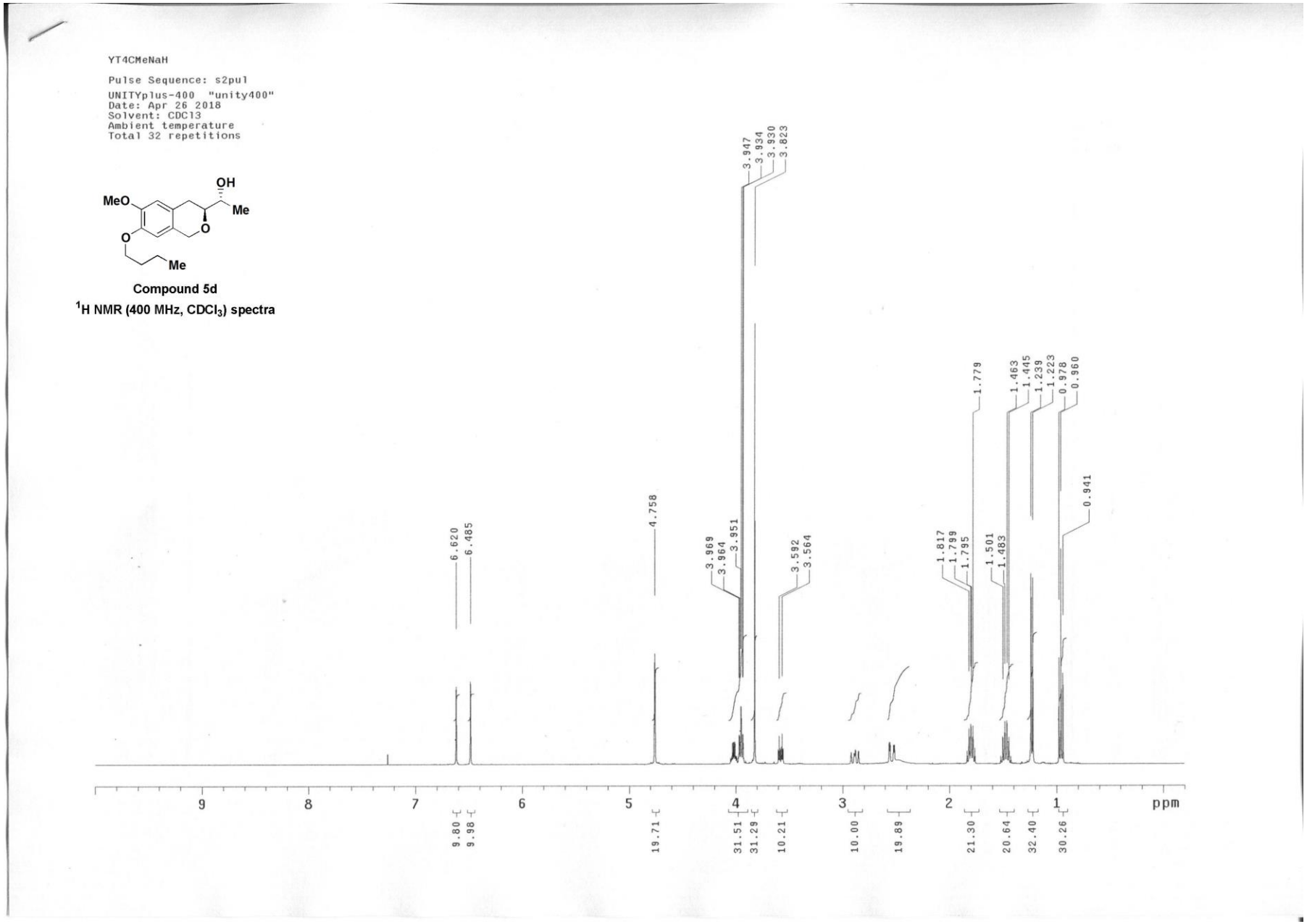


Compound 5c

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



Compound 5d (^{1}H-NMR sectral data)

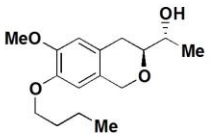


Compound 5d (^{13}C-NMR spectral data)

YT4CMeNaH

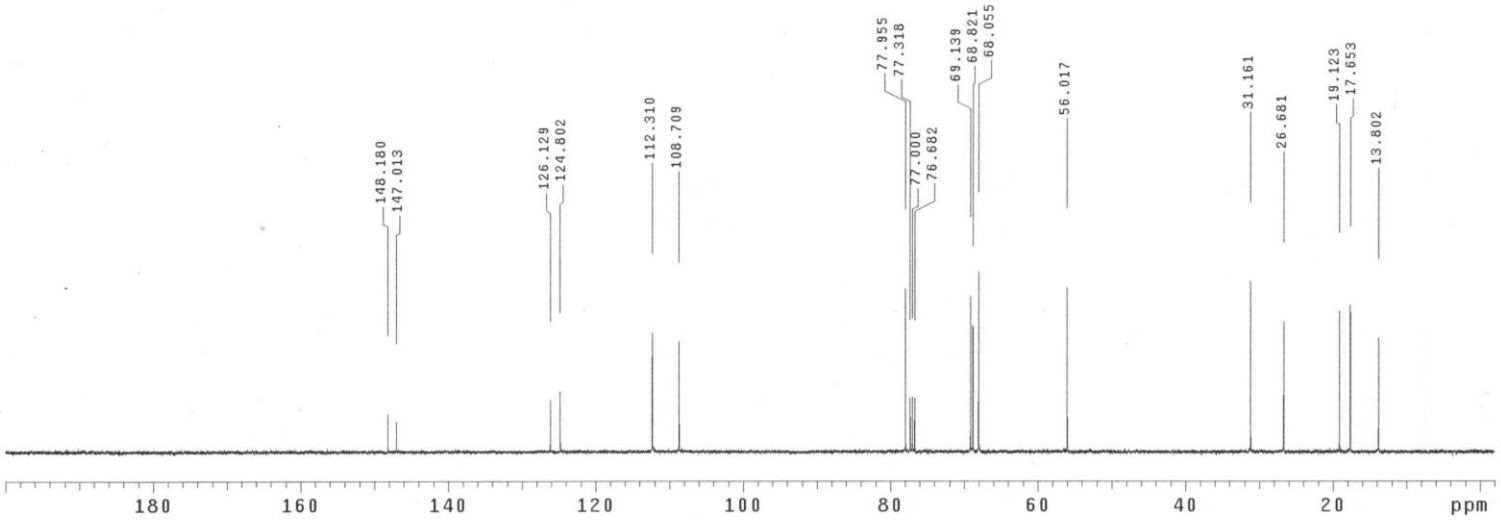
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Apr 26 2018
Solvent: CDCl3
Ambient temperature
Total 352 repetitions

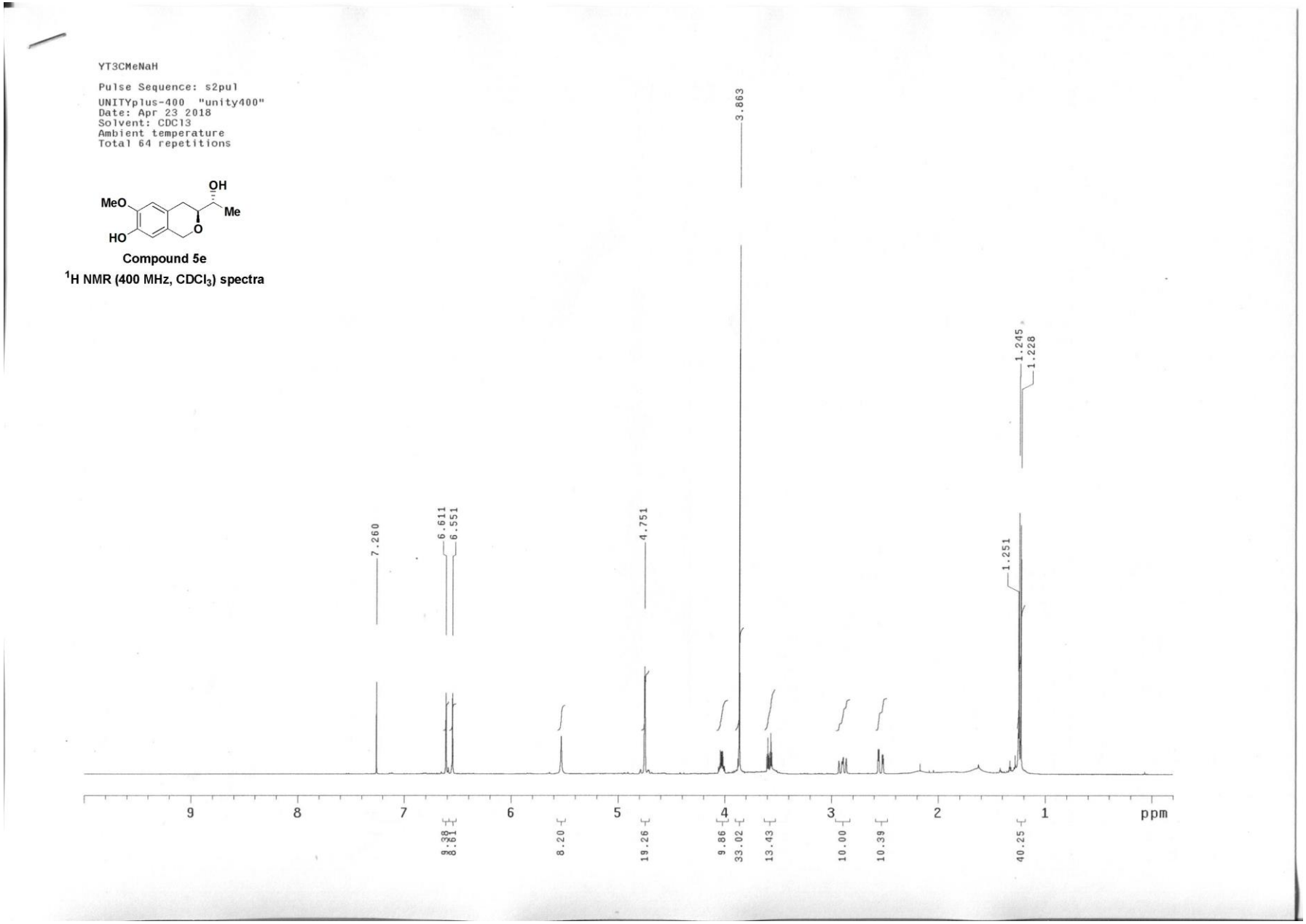


Compound 5d

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



Compound 5e (^{1}H-NMR sectral data)

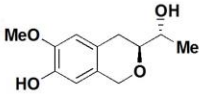


Compound 5e (^{13}C-NMR spectral data)

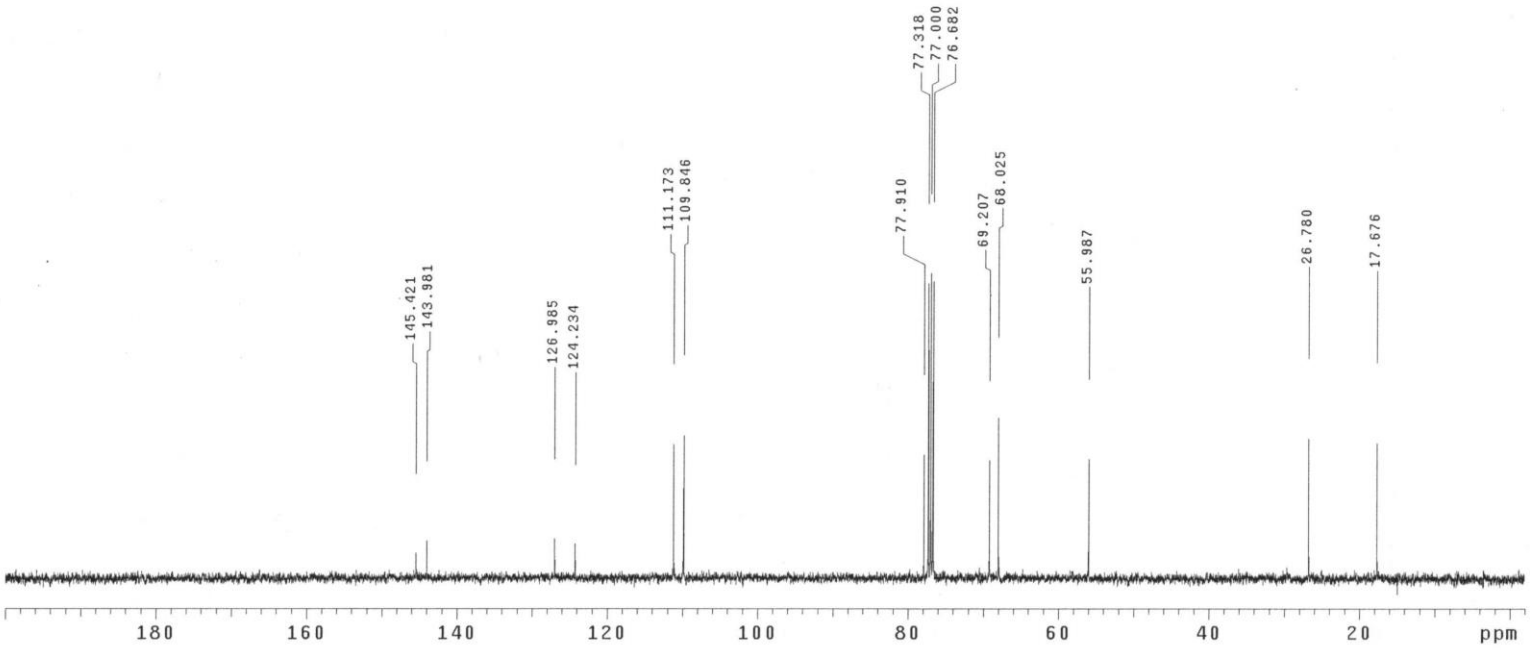
YT3CMeNaH

Pulse Sequence: s2pul

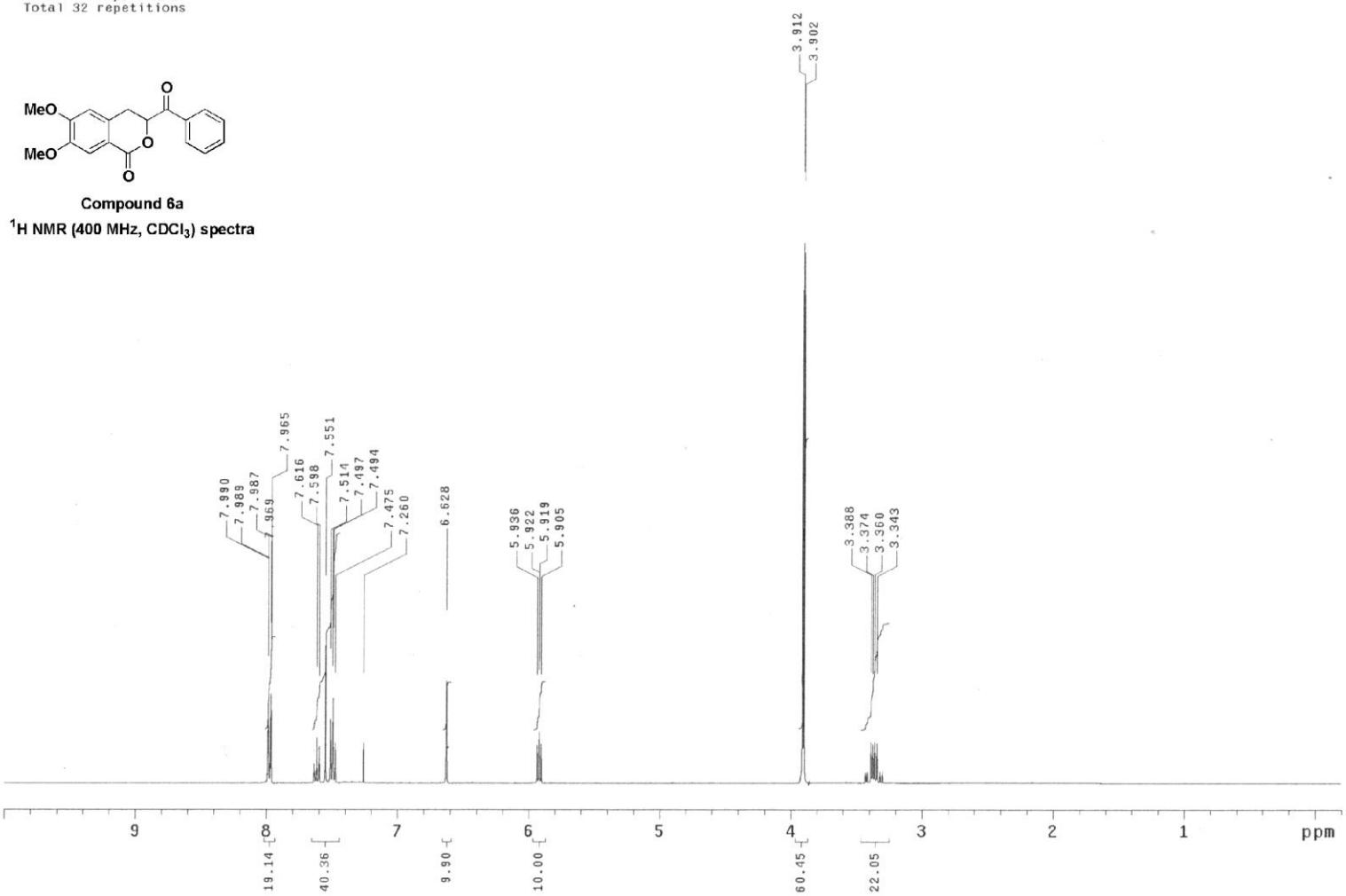
UNITYplus-400 "unity400"
Date: Apr 23 2018
Solvent: CDCl3
Ambient temperature
Total 2864 repetitions



Compound 5e
^{13}C NMR (100 MHz, $CDCl_3$) spectra



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

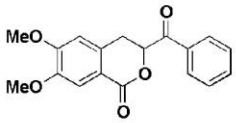


Compound 6a (^{13}C-NMR spectral data)

YTJones

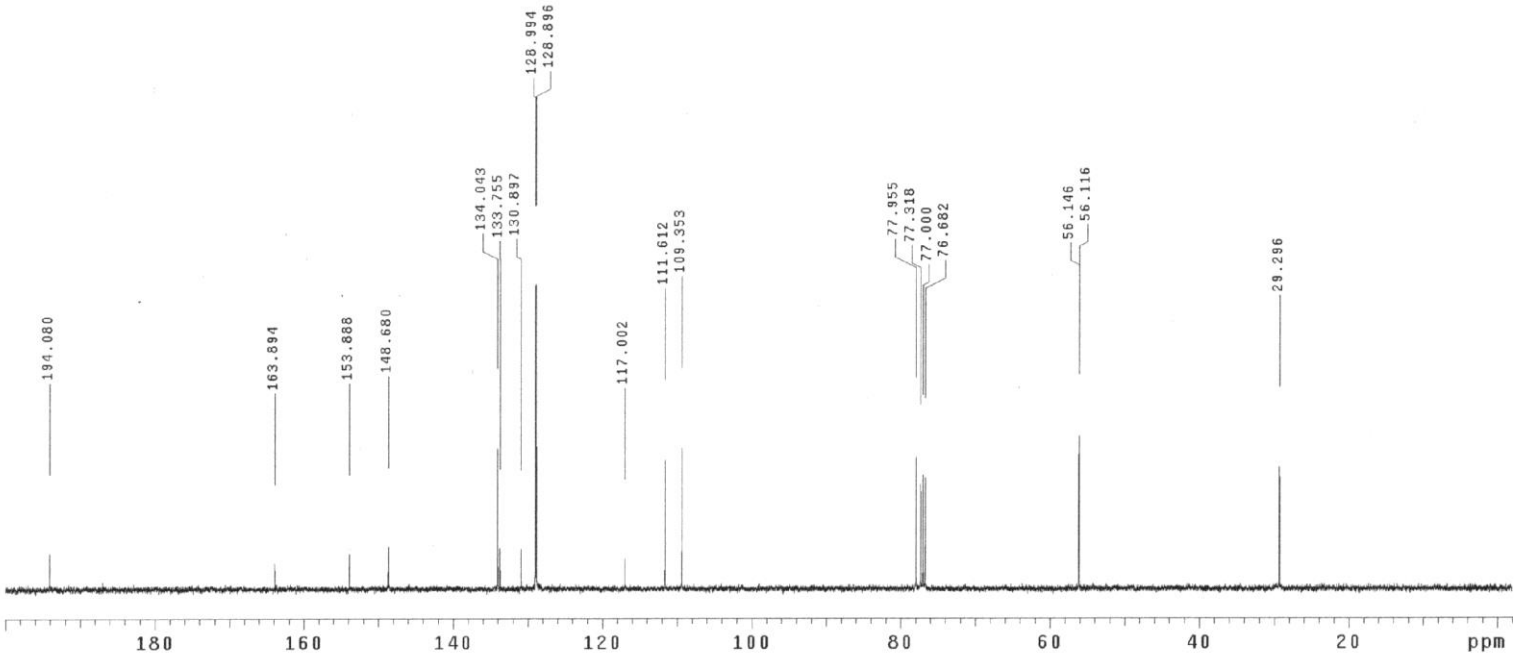
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Apr 27 2018
Solvent: CDCl3
Ambient temperature
Total 736 repetitions



Compound 6a

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

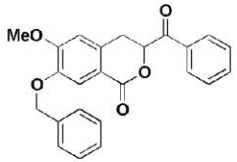


Compound 6b (^{1}H-NMR spectral data)

YTJBn

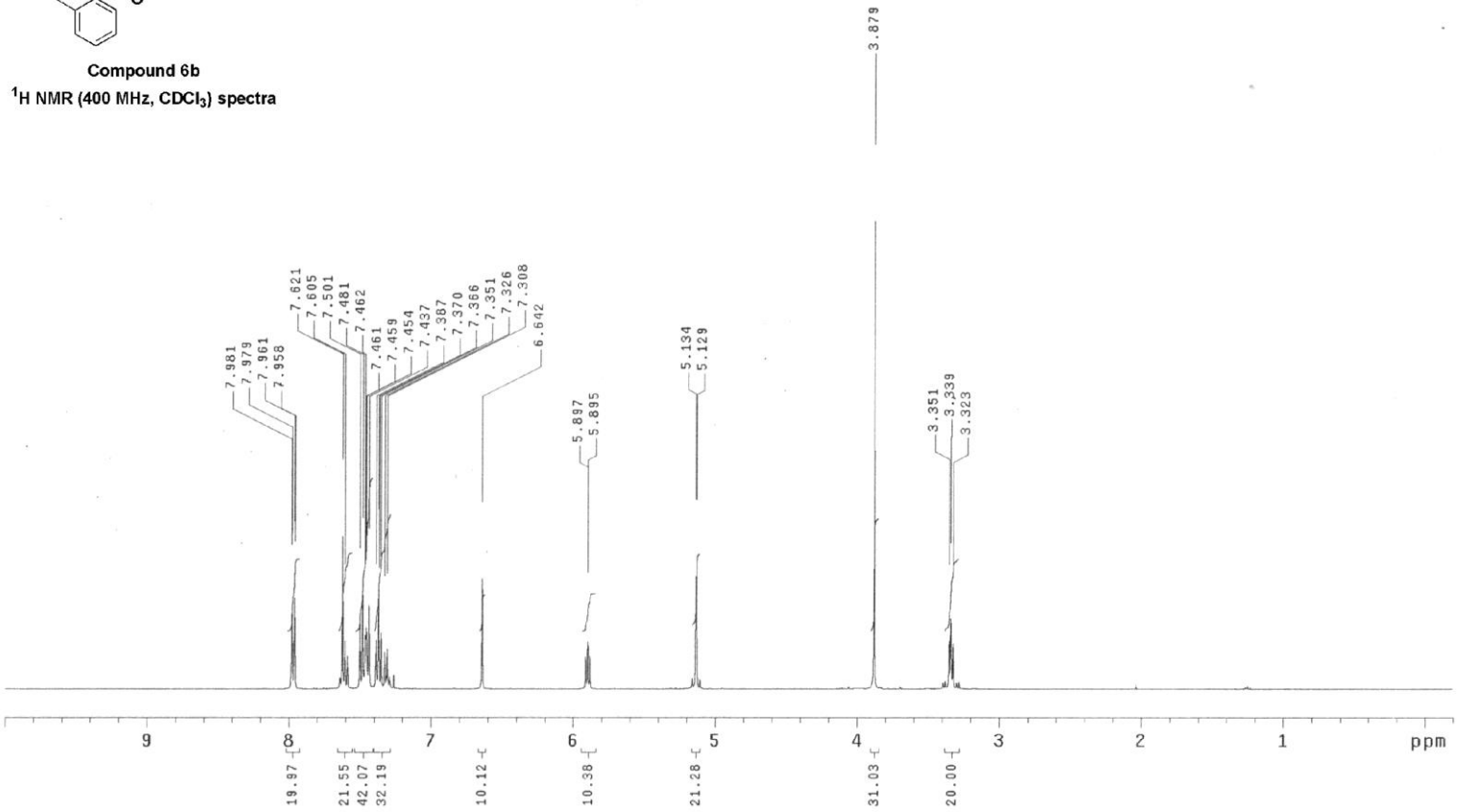
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 7 2018
Solvent: CDCl3
Ambient temperature
Total 32 repetitions



Compound 6b

^{1}H NMR (400 MHz, $CDCl_3$) spectra

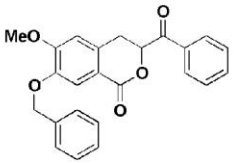


Compound 6b (^{13}C-NMR spectral data)

YTJBn

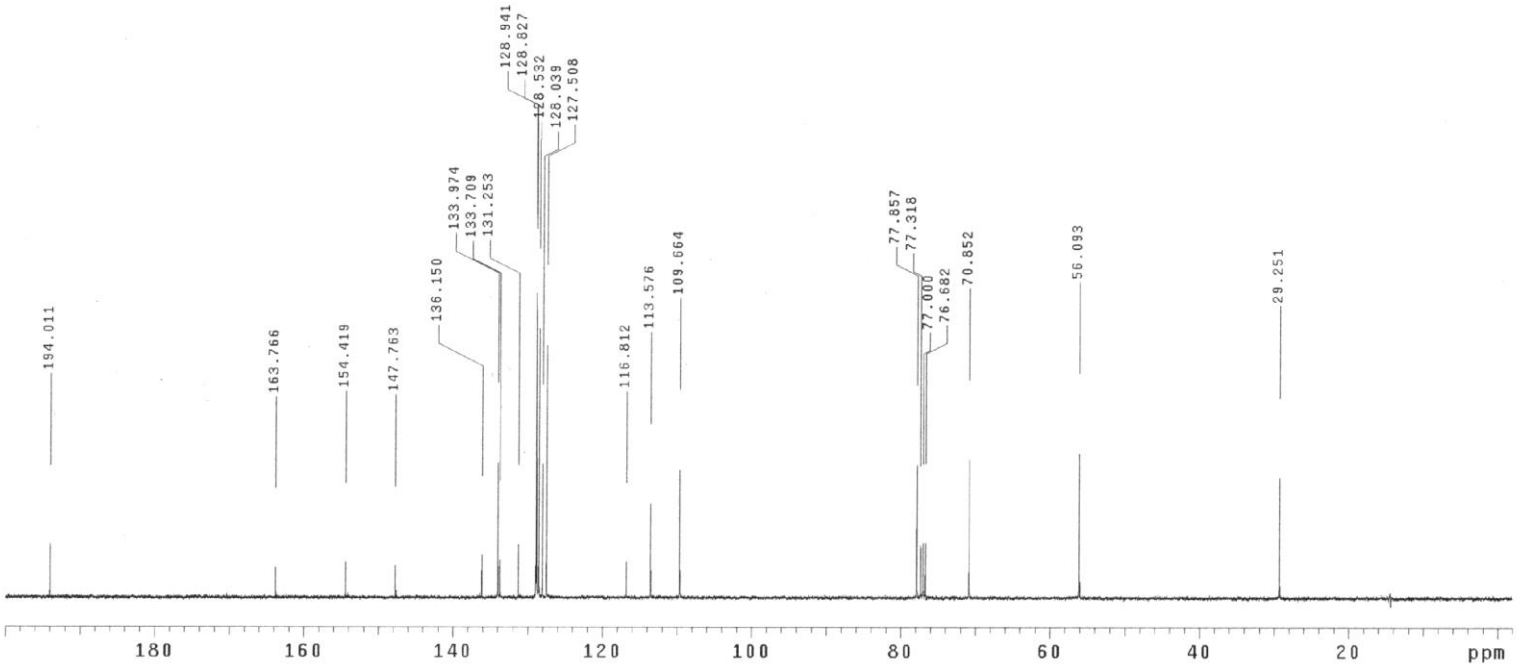
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 7 2018
Solvent: CDCl3
Ambient temperature
Total 400 repetitions



Compound 6b

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



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

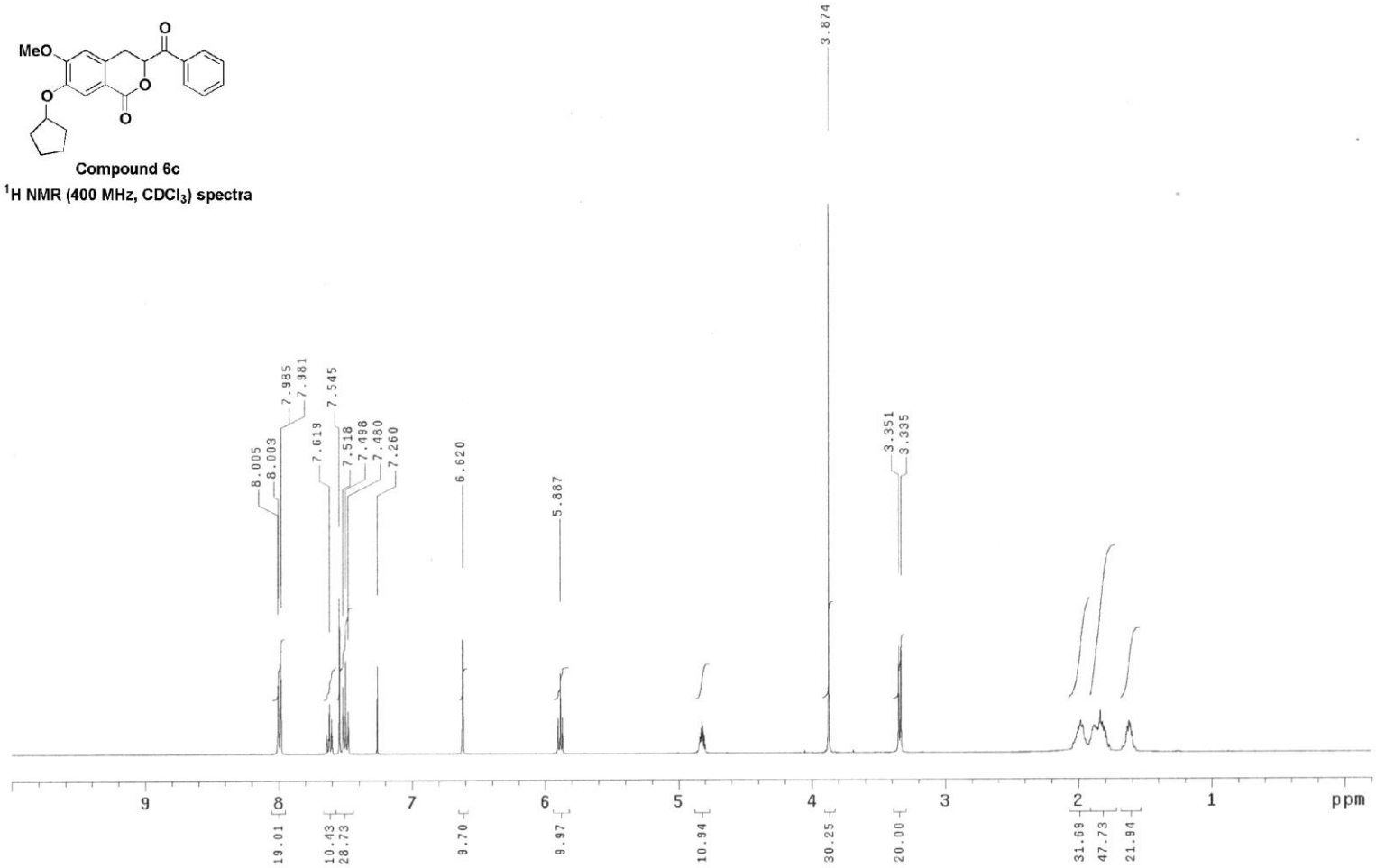
YTJ5C

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 28 2018
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

Compound 6c

^{1}H NMR (400 MHz, $CDCl_3$) spectra

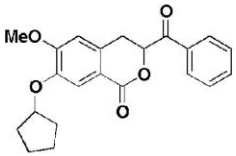


Compound 6c (^{13}C-NMR spectral data)

YTJ5C

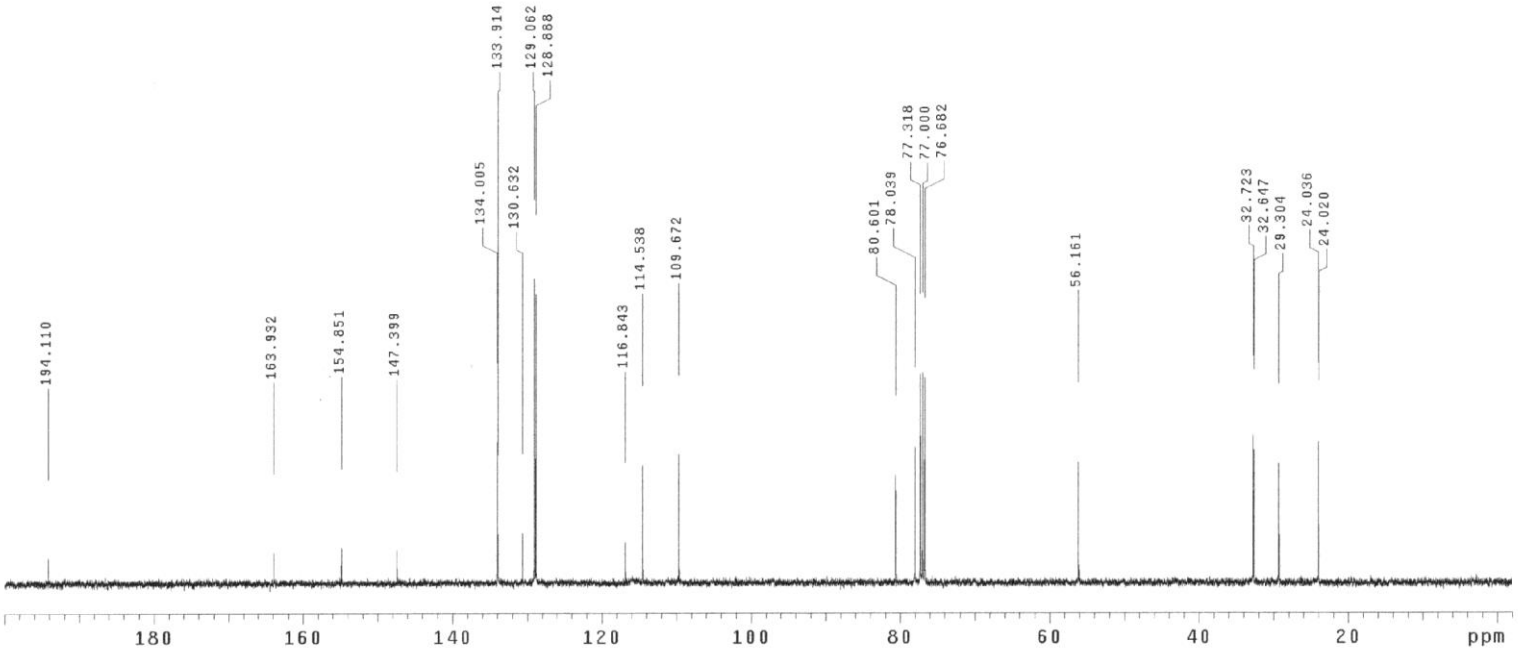
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 28 2018
Solvent: CDCl3
Ambient temperature
Total 2016 repetitions



Compound 6c

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

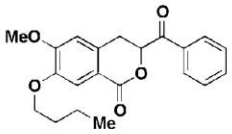


Compound 6d (^{1}H-NMR spectral data)

YTJ4C

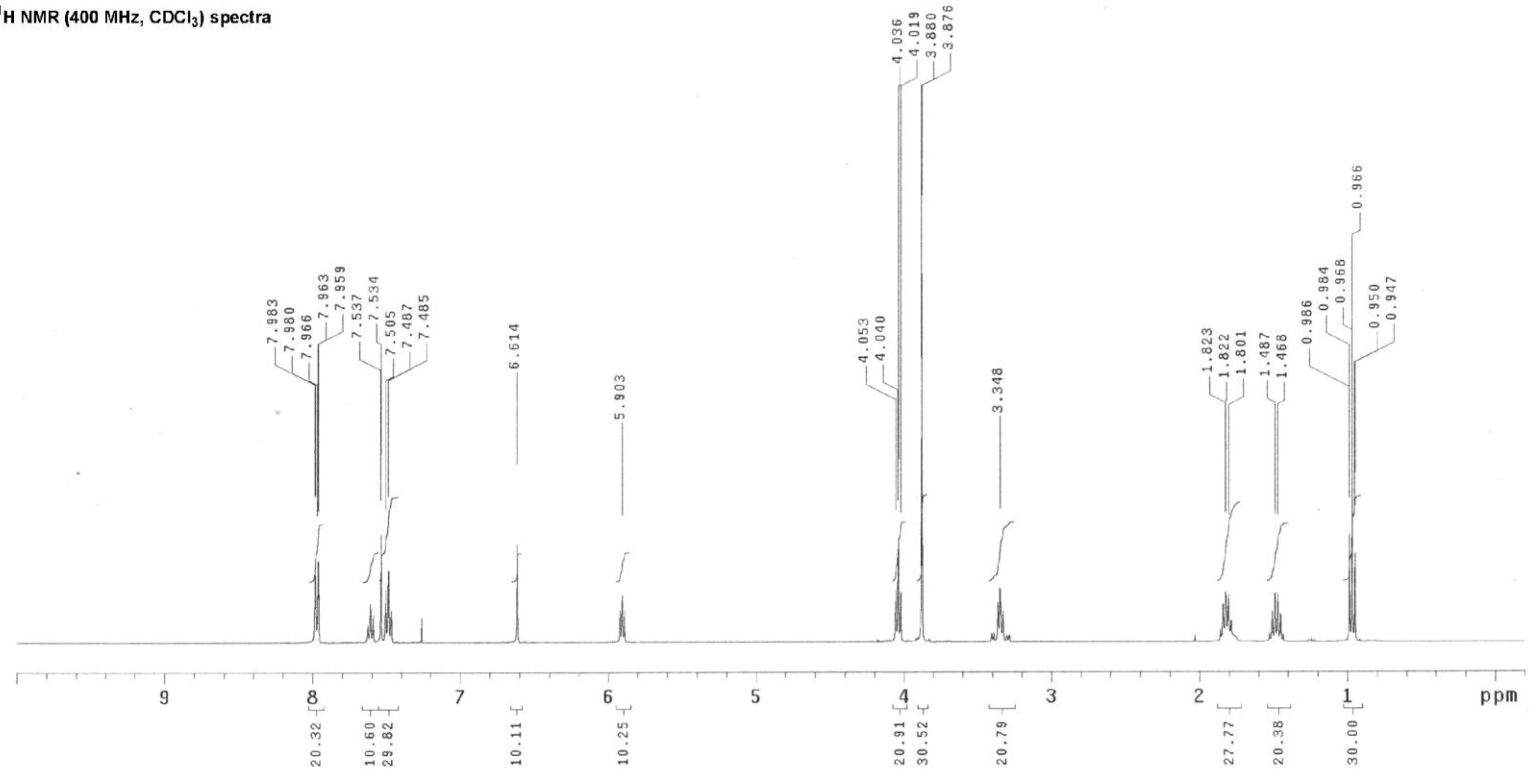
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 16 2018
Solvent: CDCl3
Ambient temperature
Total 32 repetitions



Compound 6d

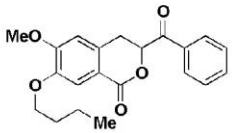
^{1}H NMR (400 MHz, $CDCl_3$) spectra



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

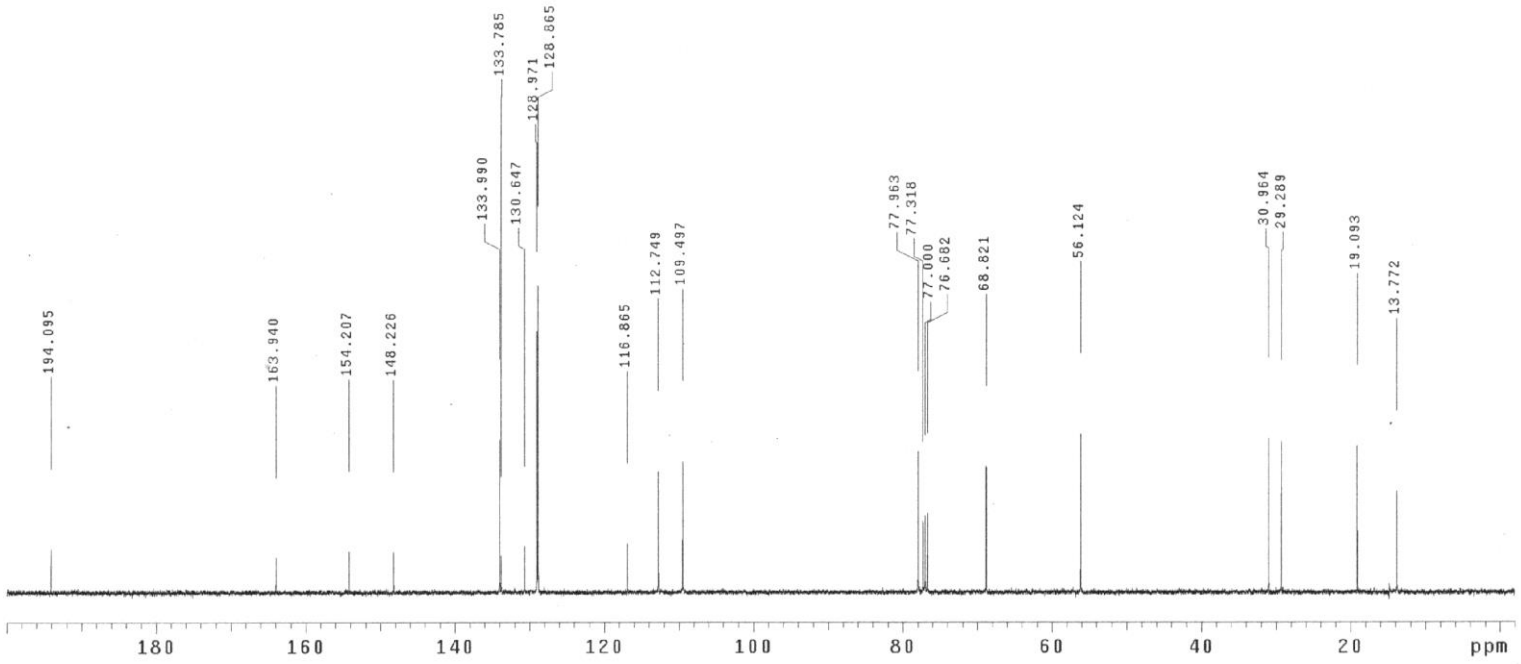
YTJ4C

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: May 16 2018
Solvent: CDCl3
Ambient temperature
Total 576 repetitions



Compound 6d

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



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

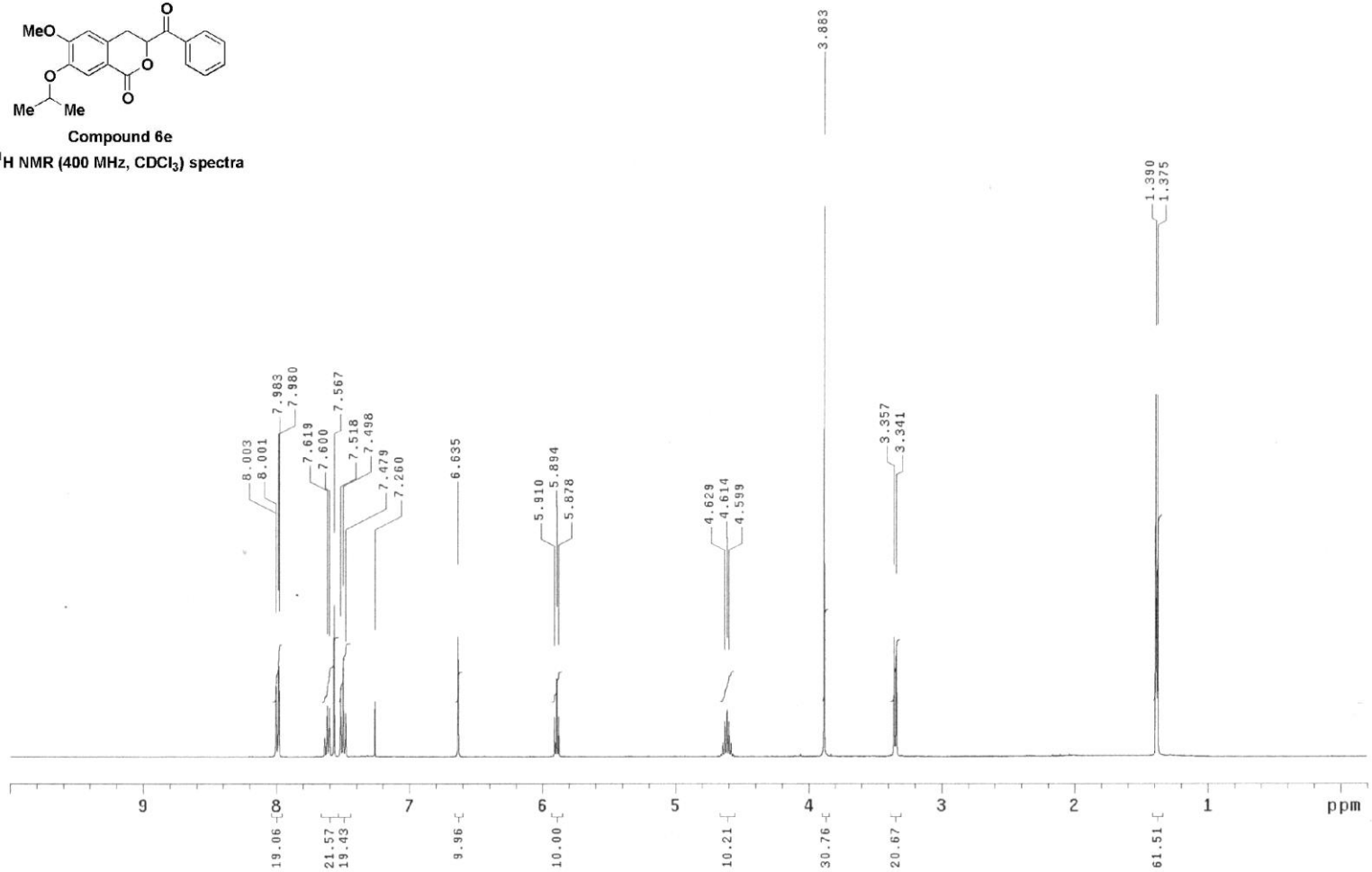
YTJ3CI

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 25 2018
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

Compound 6e

^{1}H NMR (400 MHz, $CDCl_3$) spectra

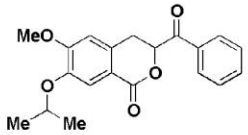


Compound 6e (^{13}C-NMR spectral data)

YTJ3CI

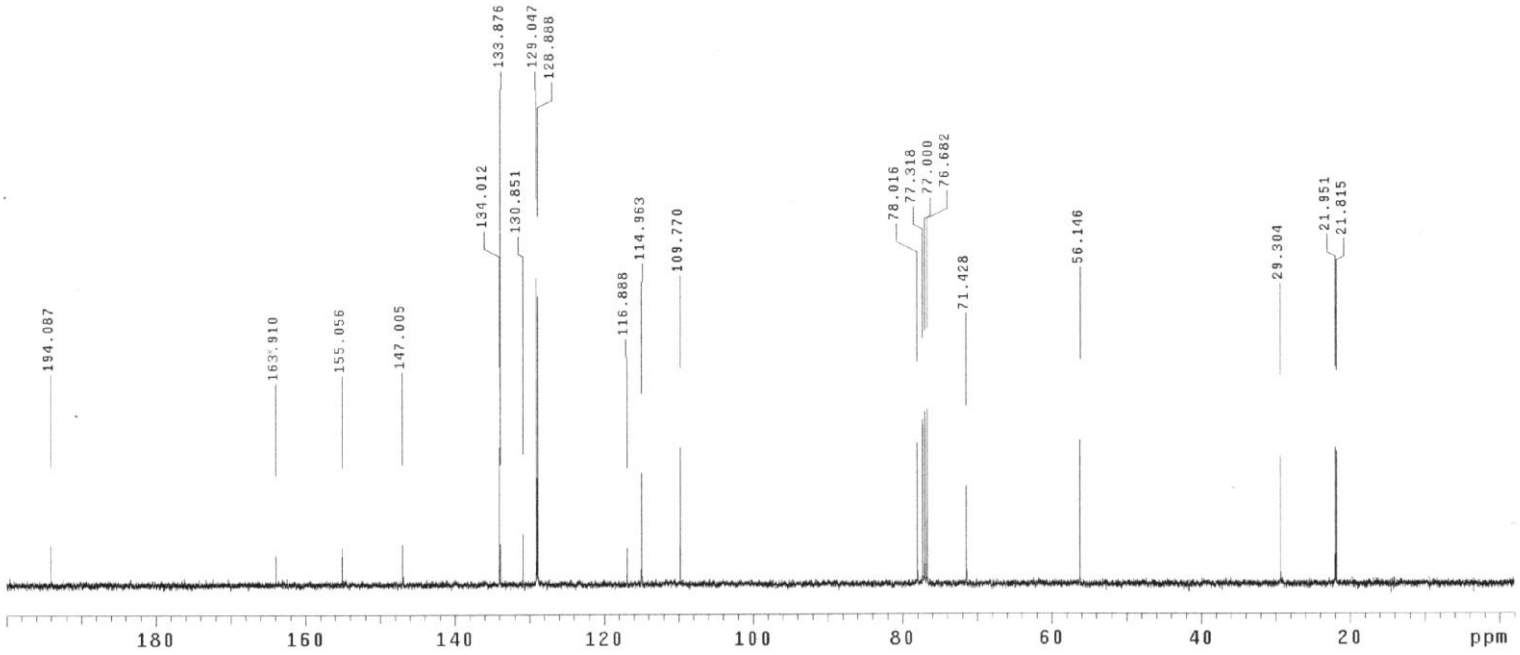
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 25 2018
Solvent: CDCl3
Ambient temperature
Total 1712 repetitions



Compound 6e

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

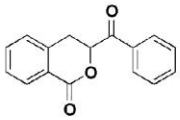


Compound 6f (^{1}H-NMR sectral data)

YTJPh

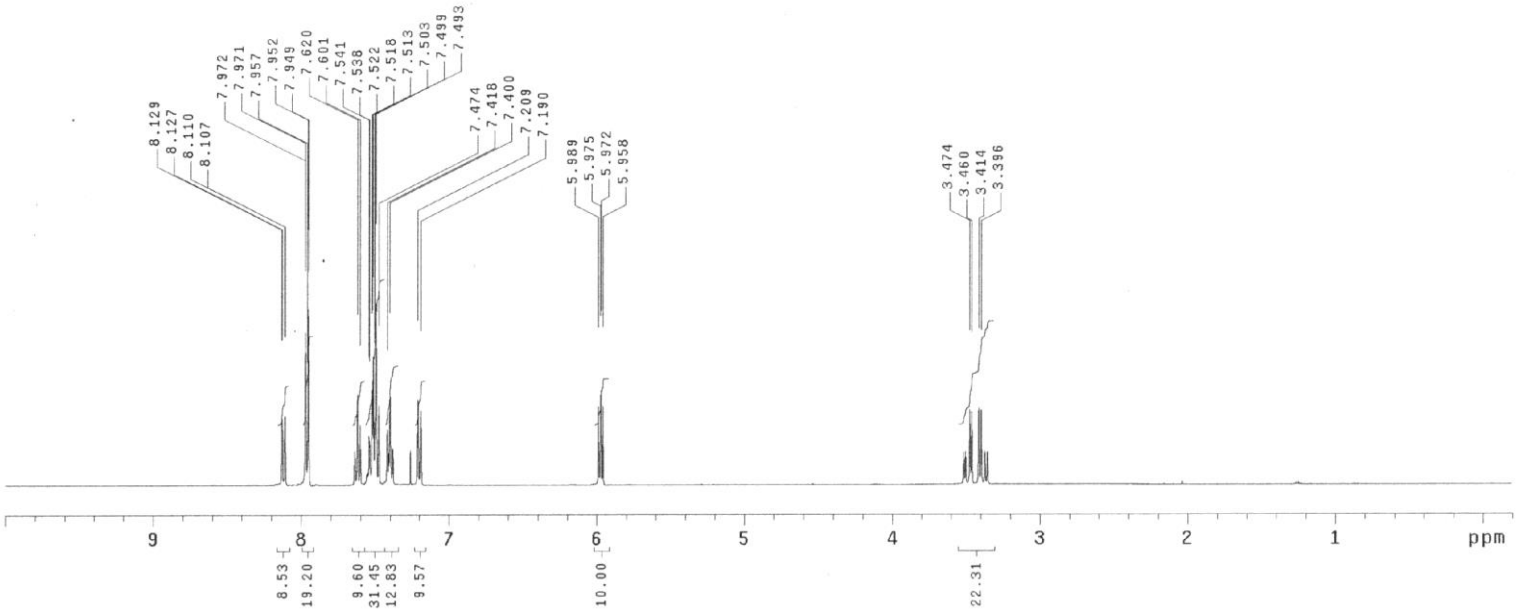
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 4 2018
Solvent: CDCl3
Ambient temperature
Total 32 repetitions



Compound 6f

^{1}H NMR (400 MHz, $CDCl_3$) spectra

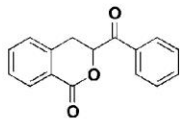


Compound 6f (^{13}C-NMR spectral data)

YTJPh

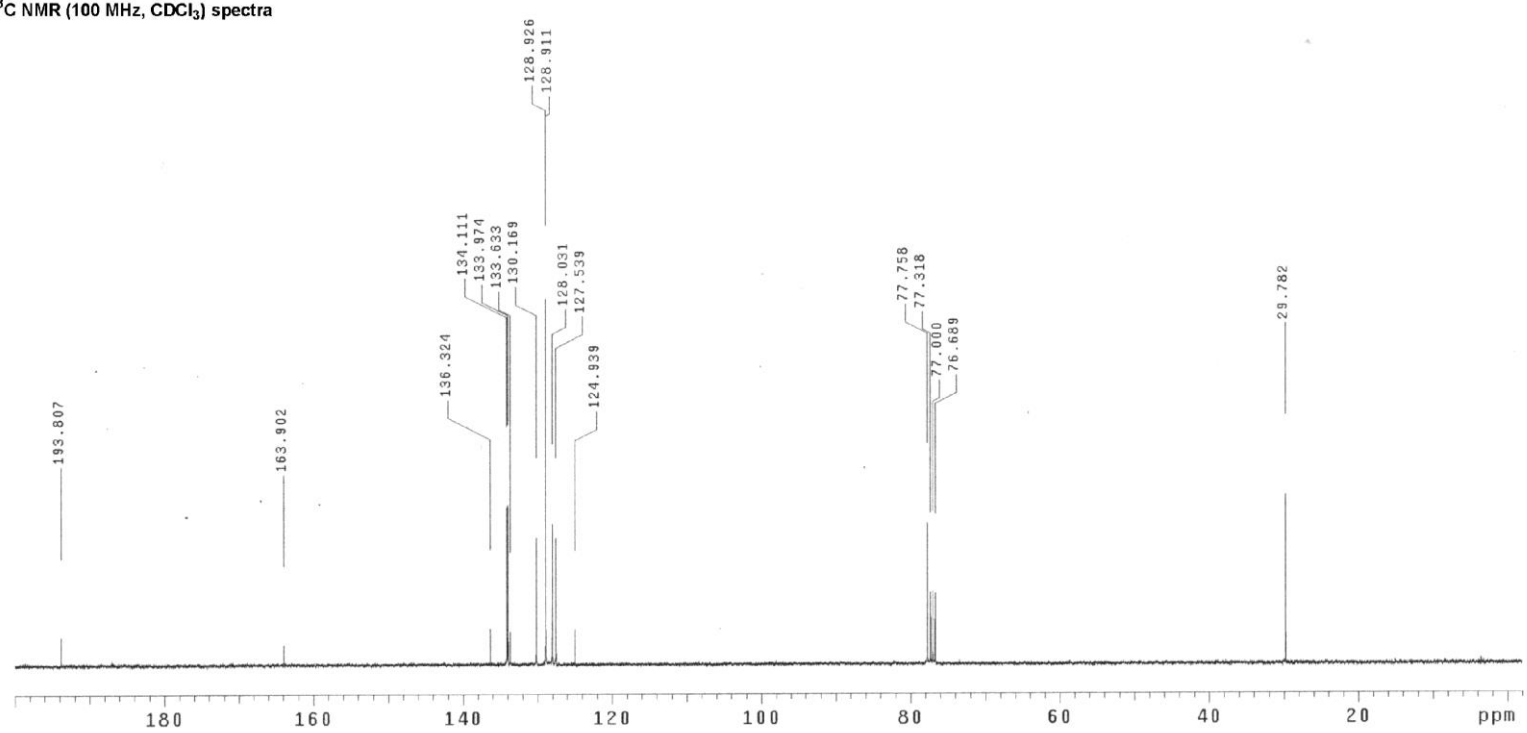
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 4 2018
Solvent: CDCl3
Ambient temperature
Total 816 repetitions



Compound 6f

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



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

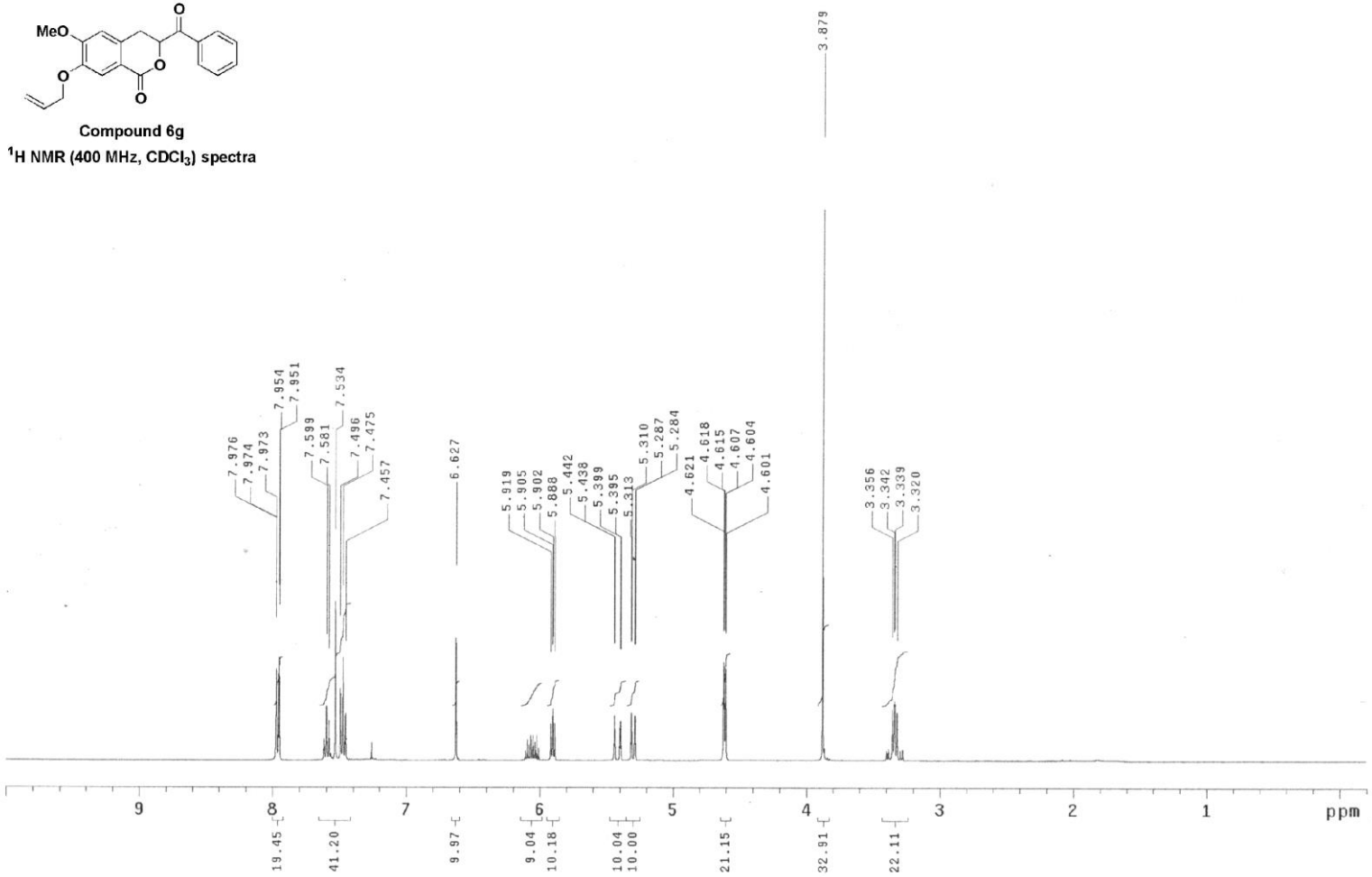
YTJ3CA

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 16 2018
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

Compound 6g

^{1}H NMR (400 MHz, $CDCl_3$) spectra

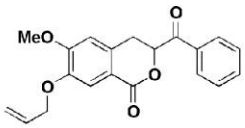


Compound 6g (^{13}C-NMR spectral data)

YTJ3CA

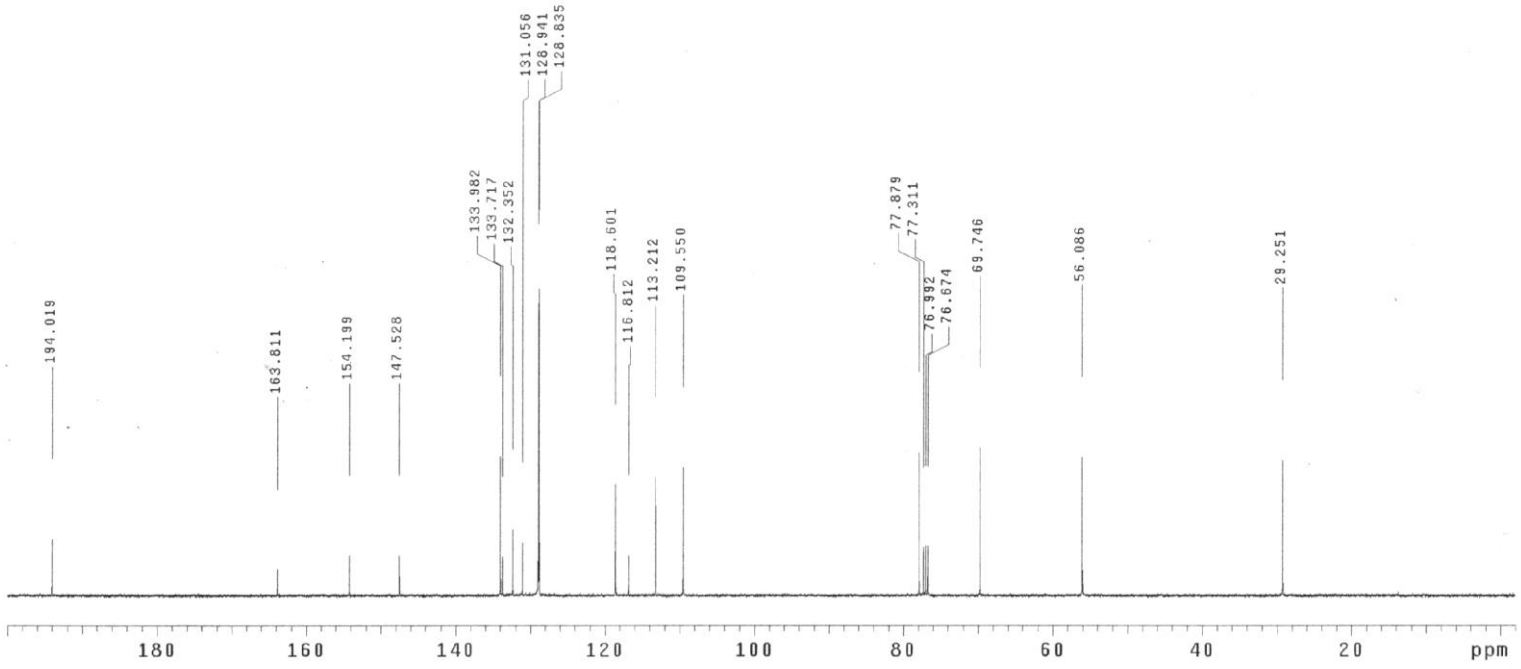
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 16 2018
Solvent: CDCl3
Ambient temperature
Total 864 repetitions



Compound 6g

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

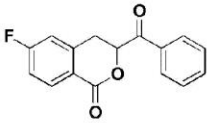


Compound 6h (^{1}H-NMR sectral data)

YTJ4F

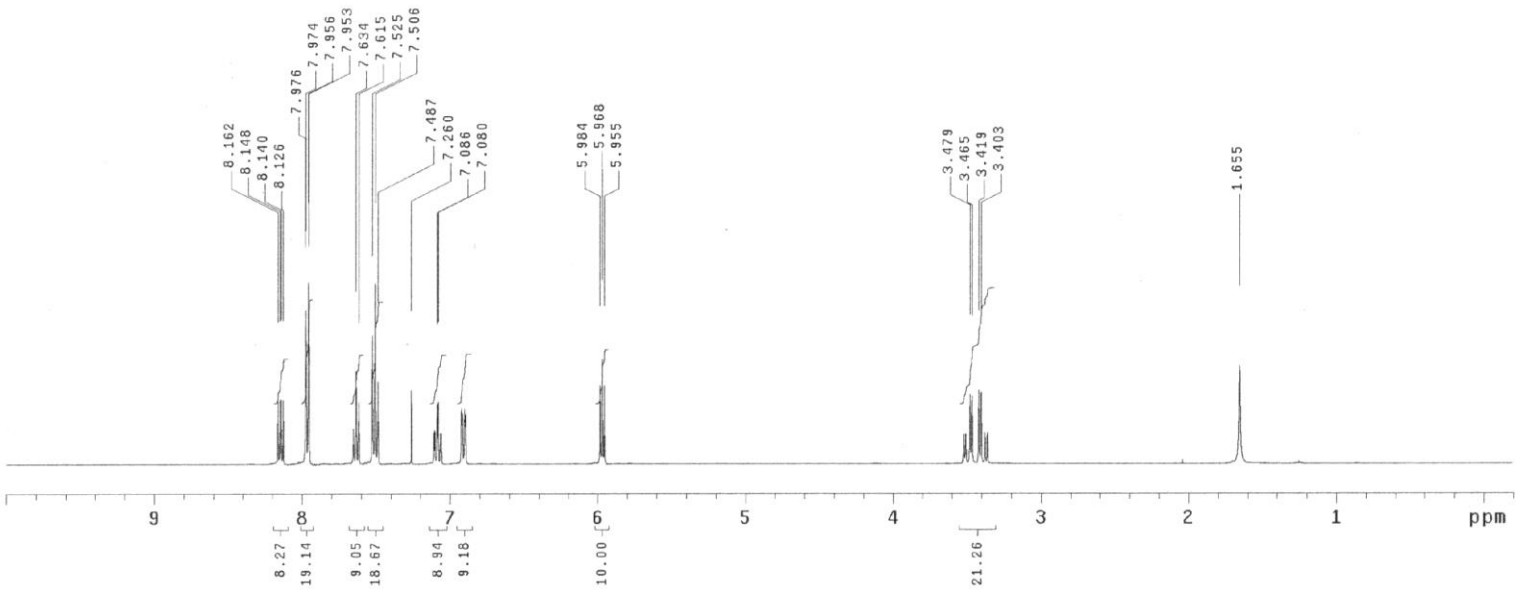
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 14 2018
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

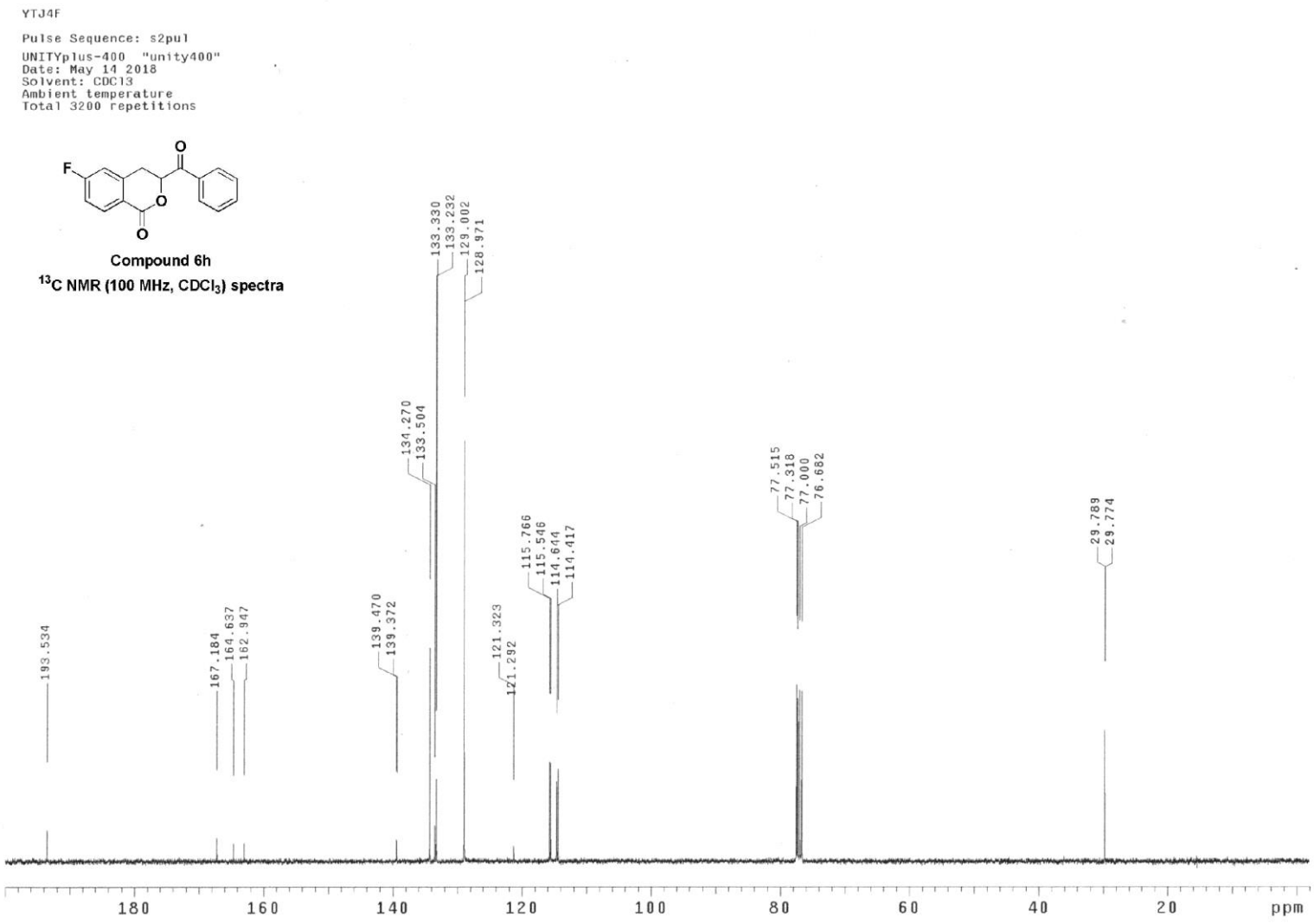


Compound 6h

^{1}H NMR (400 MHz, $CDCl_3$) spectra



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

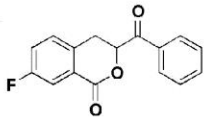


Compound 6i (^{1}H-NMR sectral data)

YTJ5F

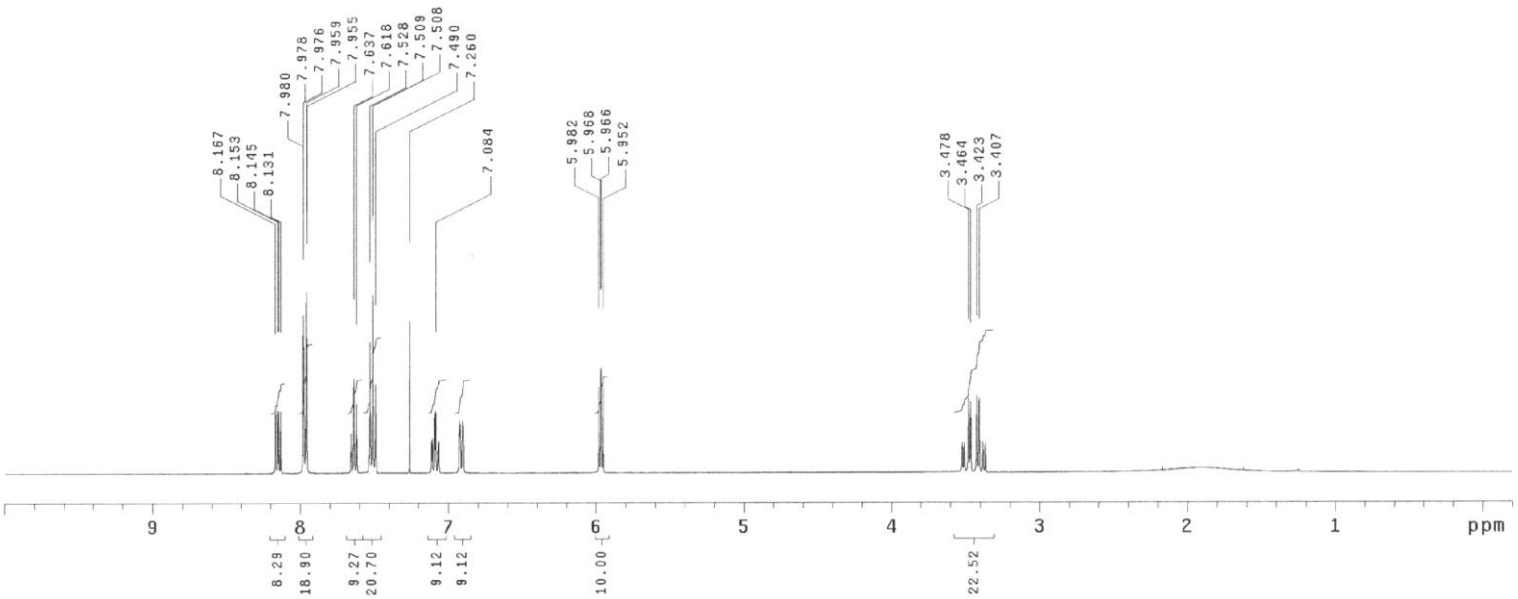
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 28 2018
Solvent: CDCl3
Ambient temperature
Total 64 repetitions

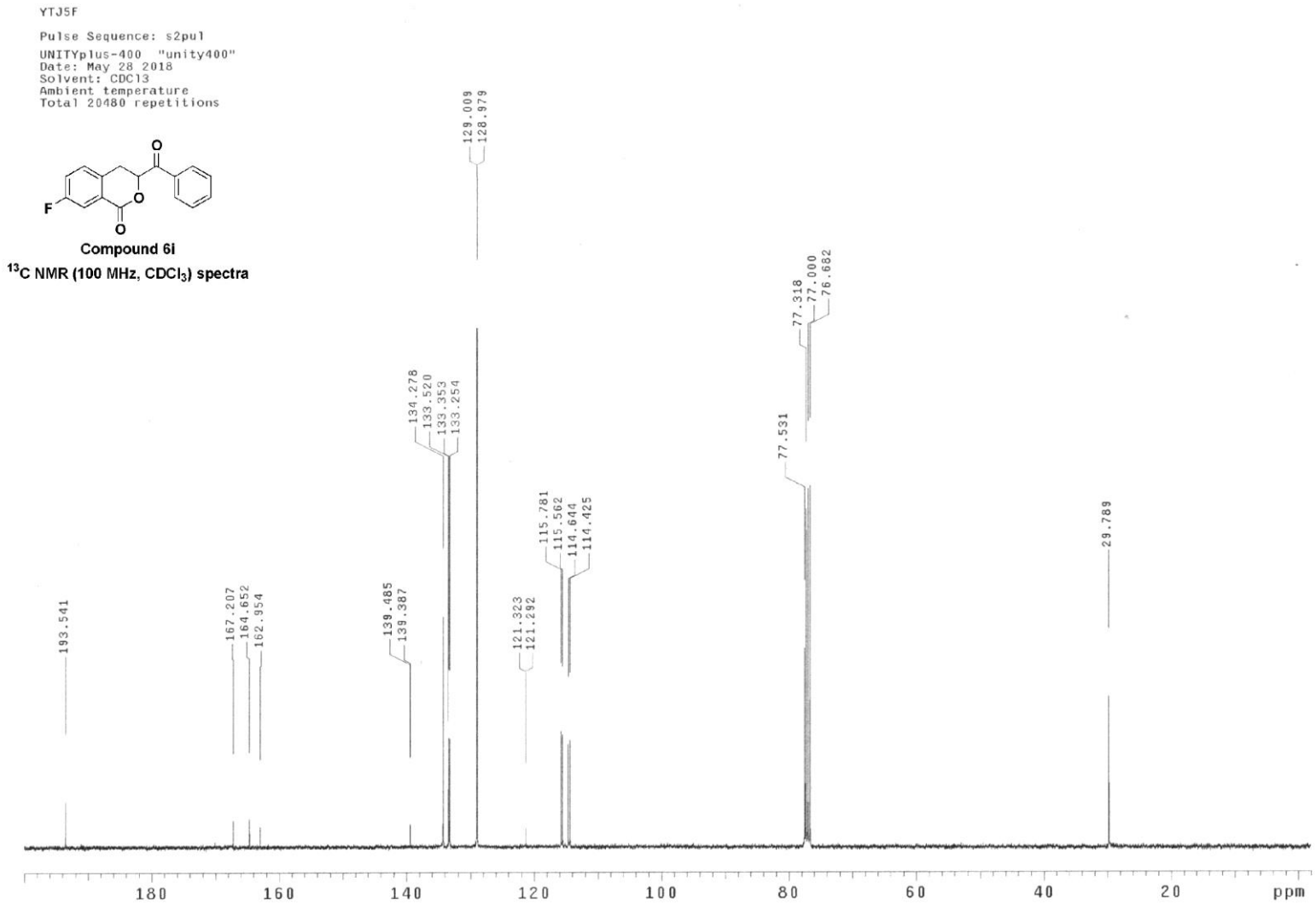


Compound 6i

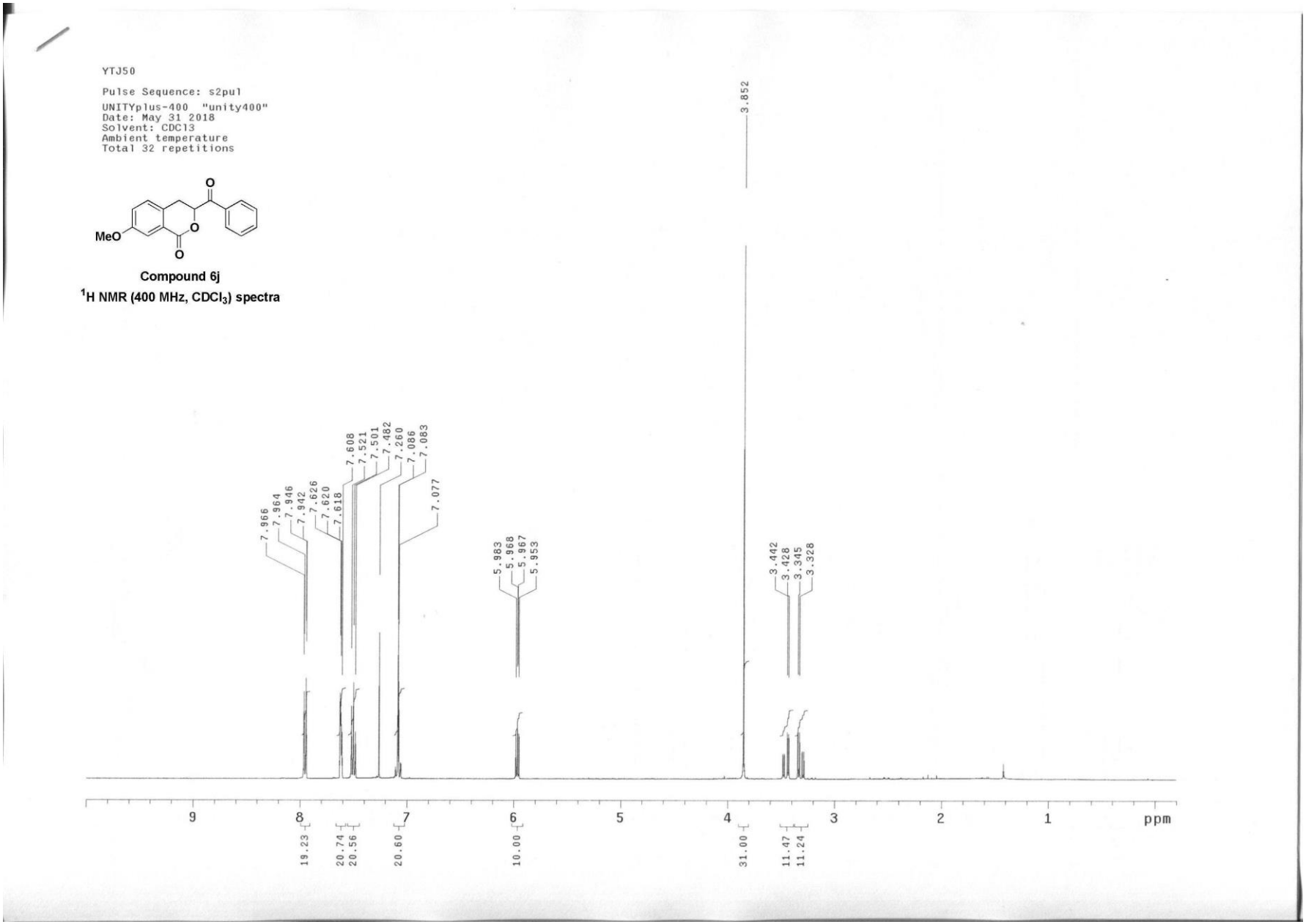
^{1}H NMR (400 MHz, $CDCl_3$) spectra



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



Compound 6j (^{1}H-NMR sectral data)

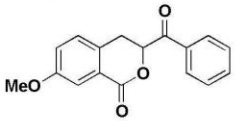


Compound 6j (^{13}C-NMR spectral data)

YTJ50

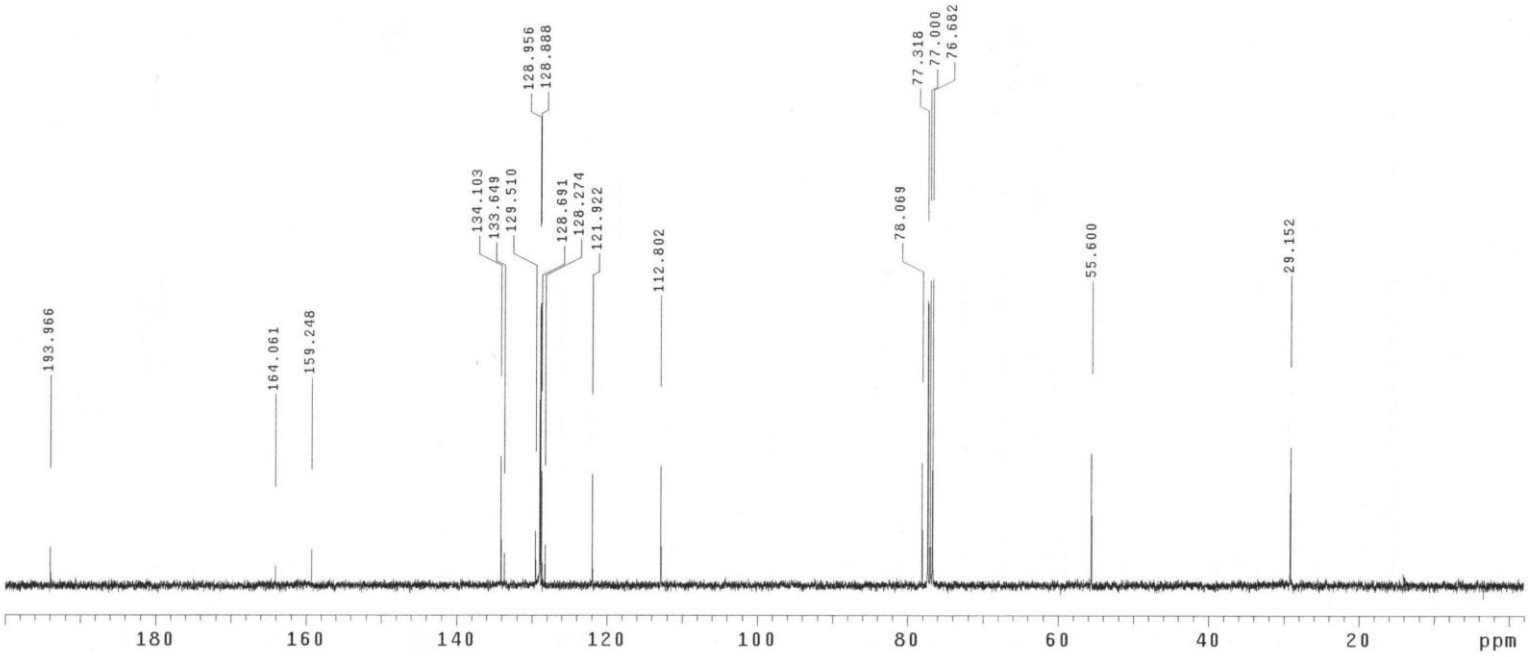
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 31 2018
Solvent: CDCl3
Ambient temperature
Total 2688 repetitions

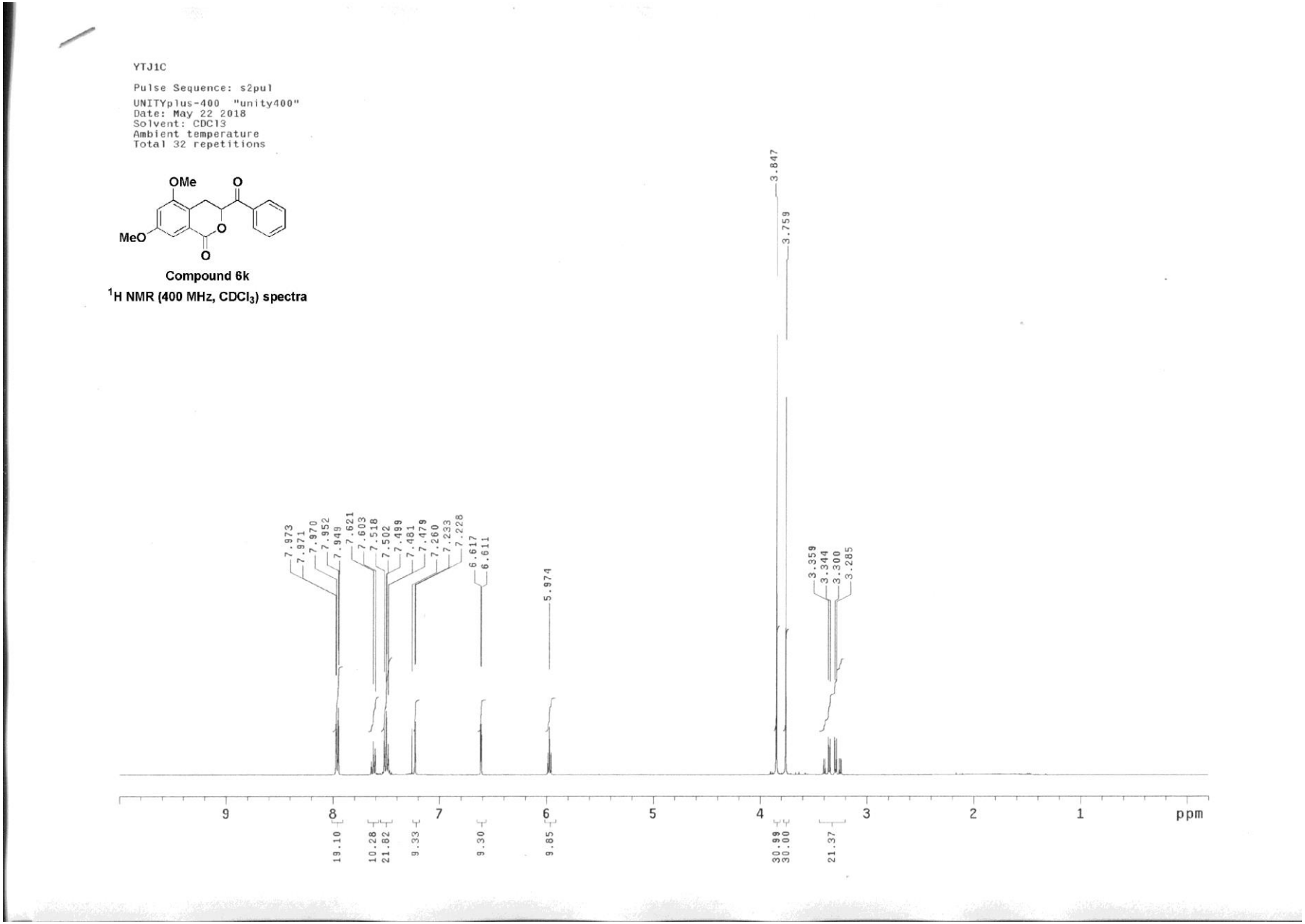


Compound 6j

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



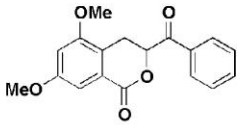
Compound 6k (^{1}H-NMR sectral data)



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

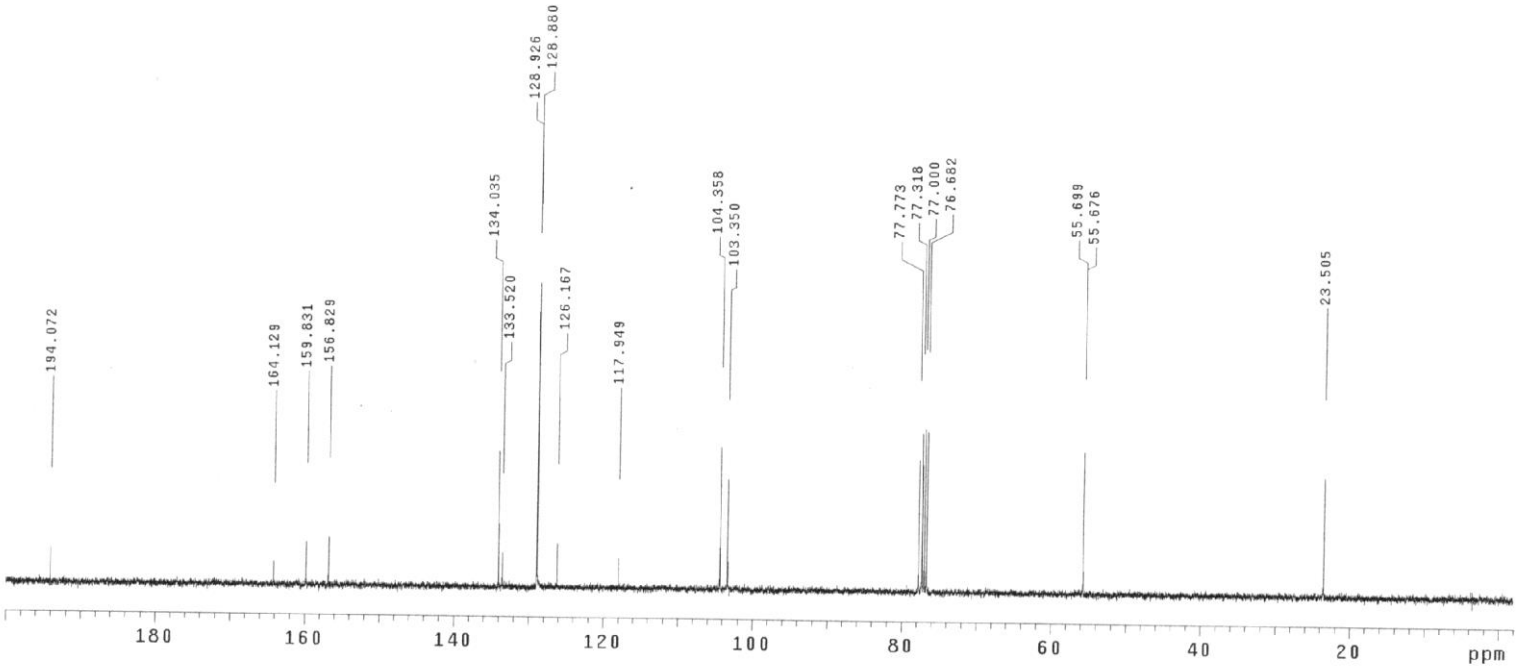
YTJ1C

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: May 22 2018
Solvent: CDCl3
Ambient temperature
Total 1328 repetitions



Compound 6k

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



Compound 6l (^{1}H-NMR sectral data)

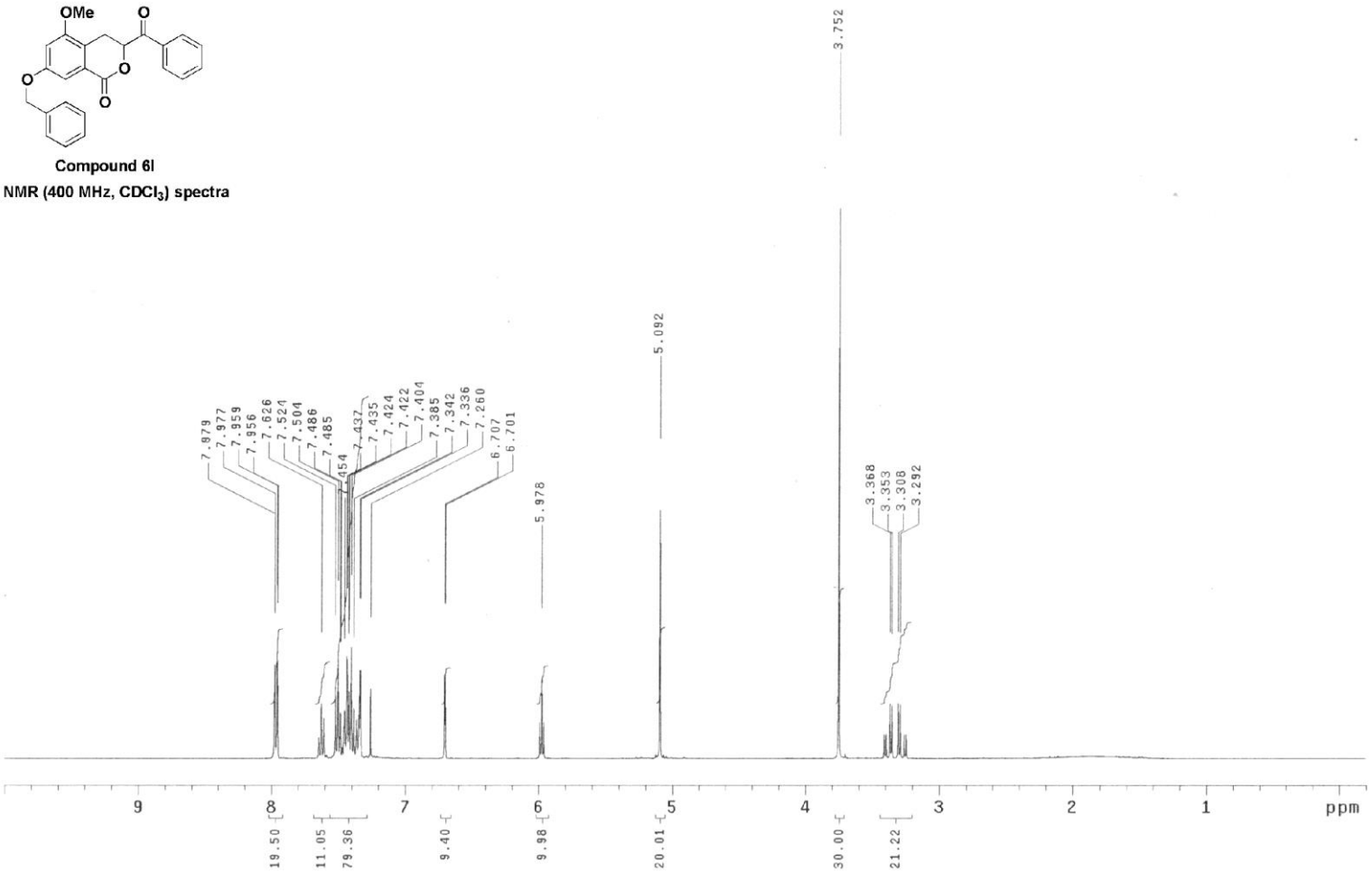
YTJ3Bn

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 11 2018
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

Compound 6l

^{1}H NMR (400 MHz, $CDCl_3$) spectra

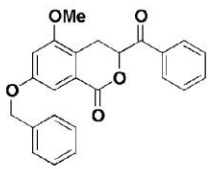


Compound 6l (^{13}C-NMR spectral data)

YTJ3Bn

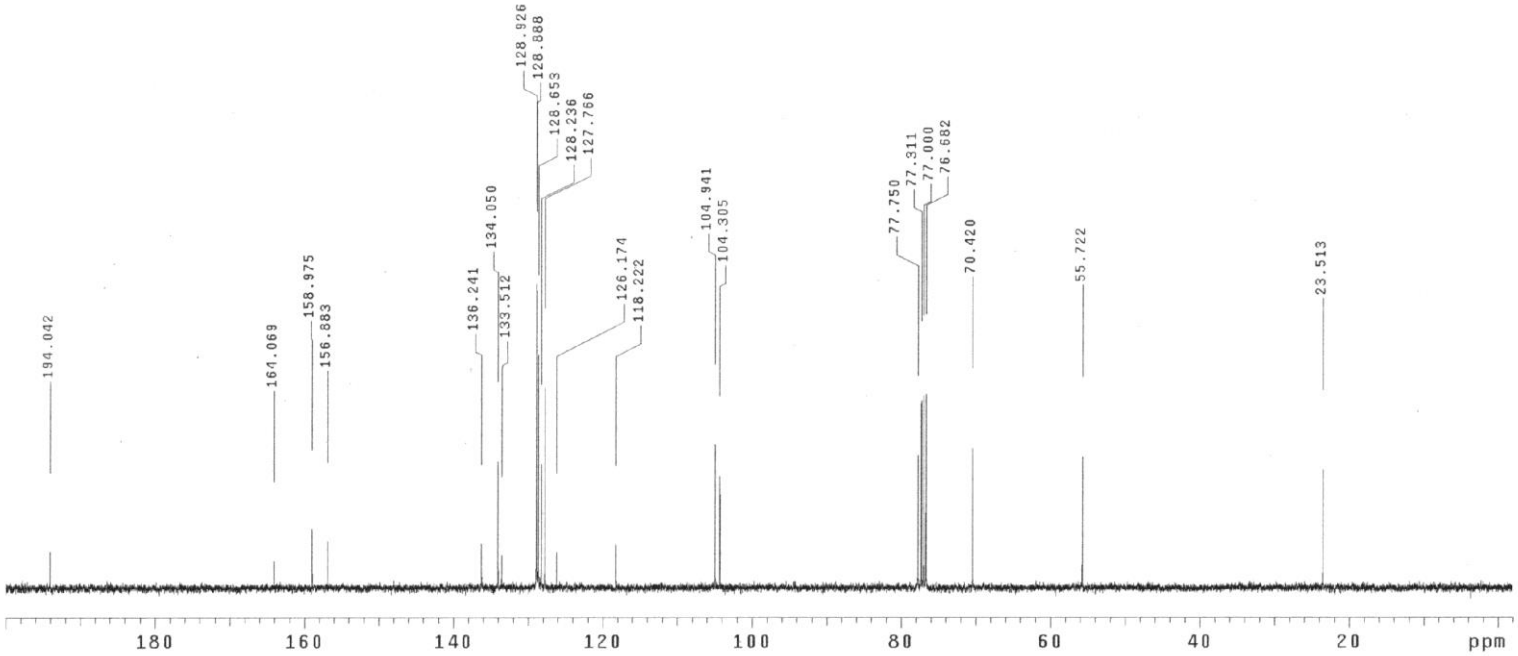
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 11 2018
Solvent: CDCl3
Ambient temperature
Total 1344 repetitions

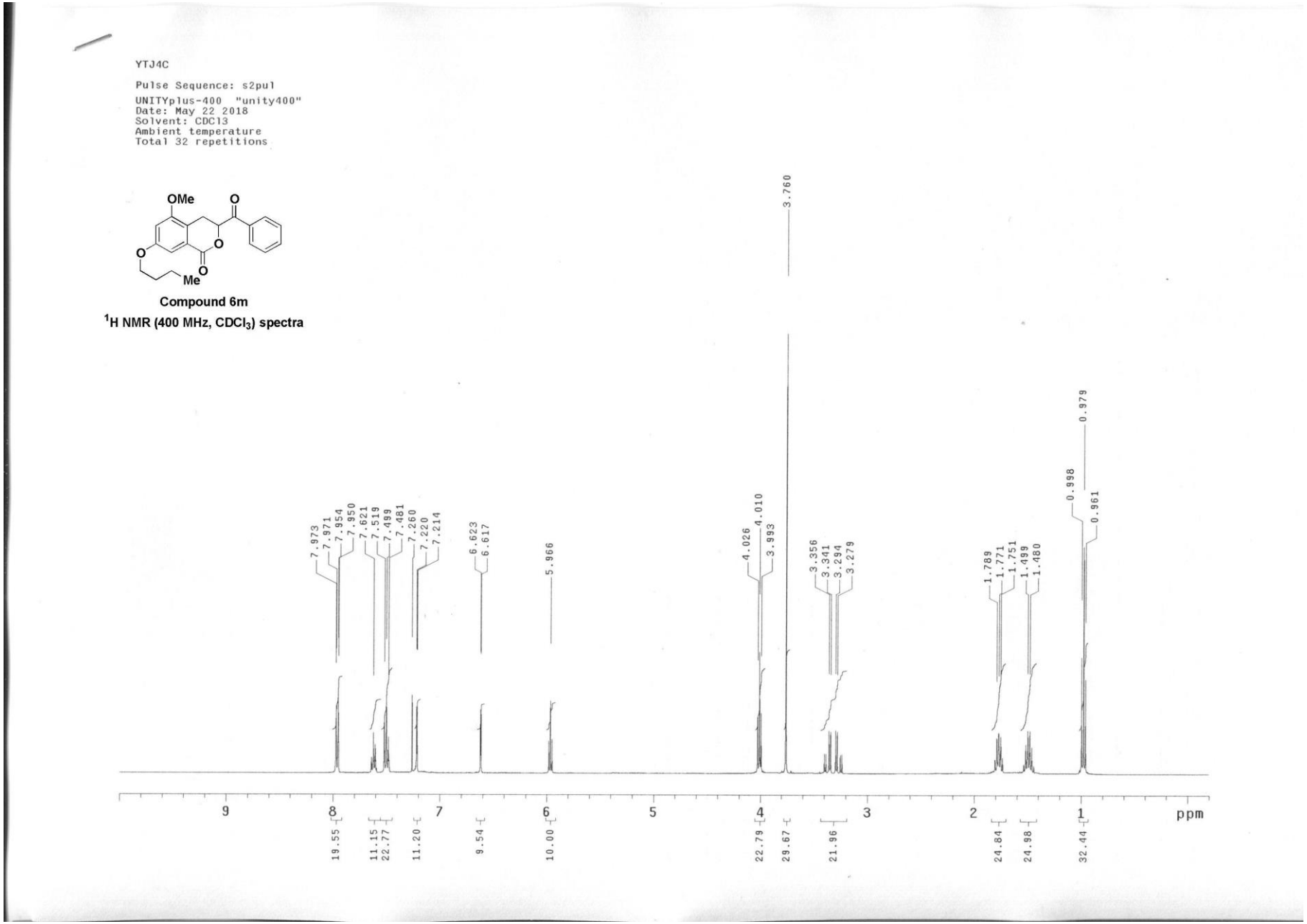


Compound 6l

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



Compound 6m (^{1}H-NMR sectral data)

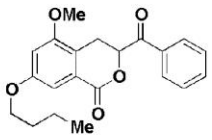


Compound 6m (^{13}C-NMR spectral data)

YTJ4C

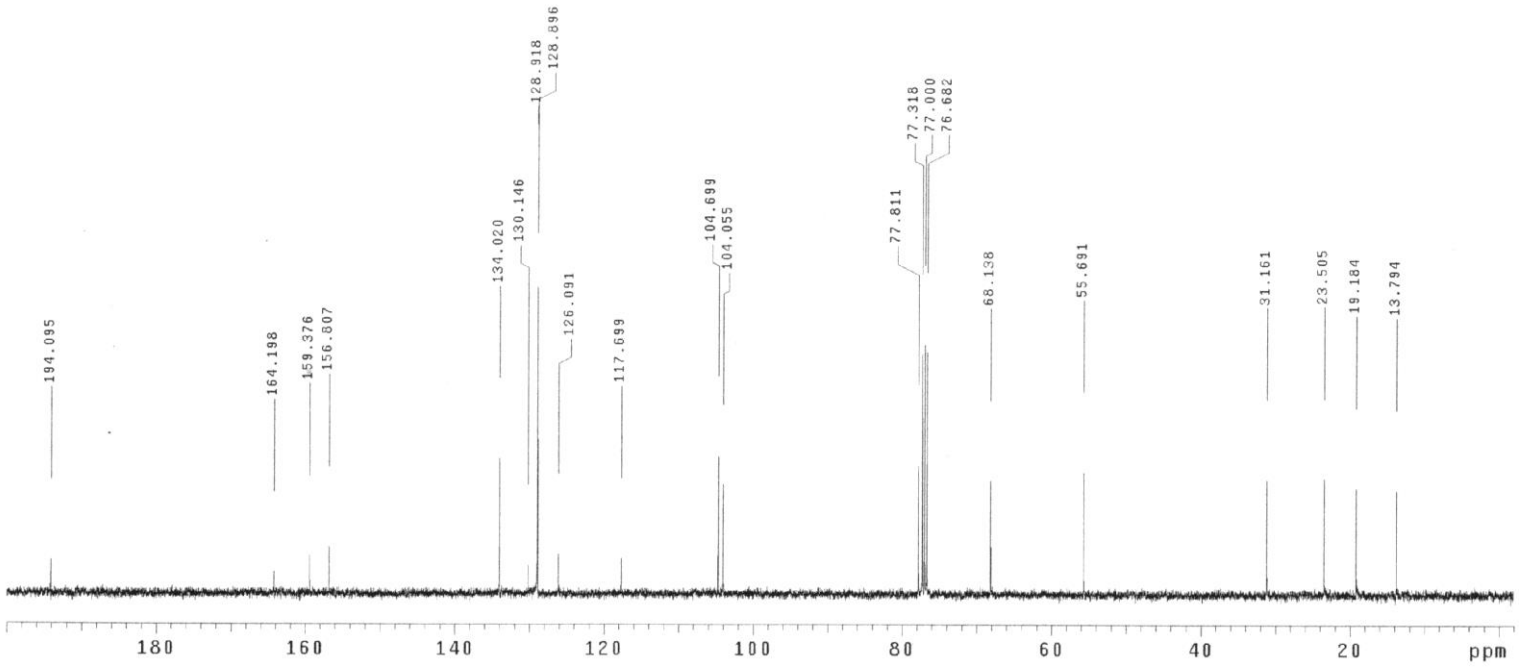
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 22 2018
Solvent: CDCl3
Ambient temperature
Total 1664 repetitions



Compound 6m

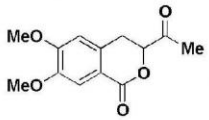
^{13}C NMR (100 MHz, $CDCl_3$) spectra



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

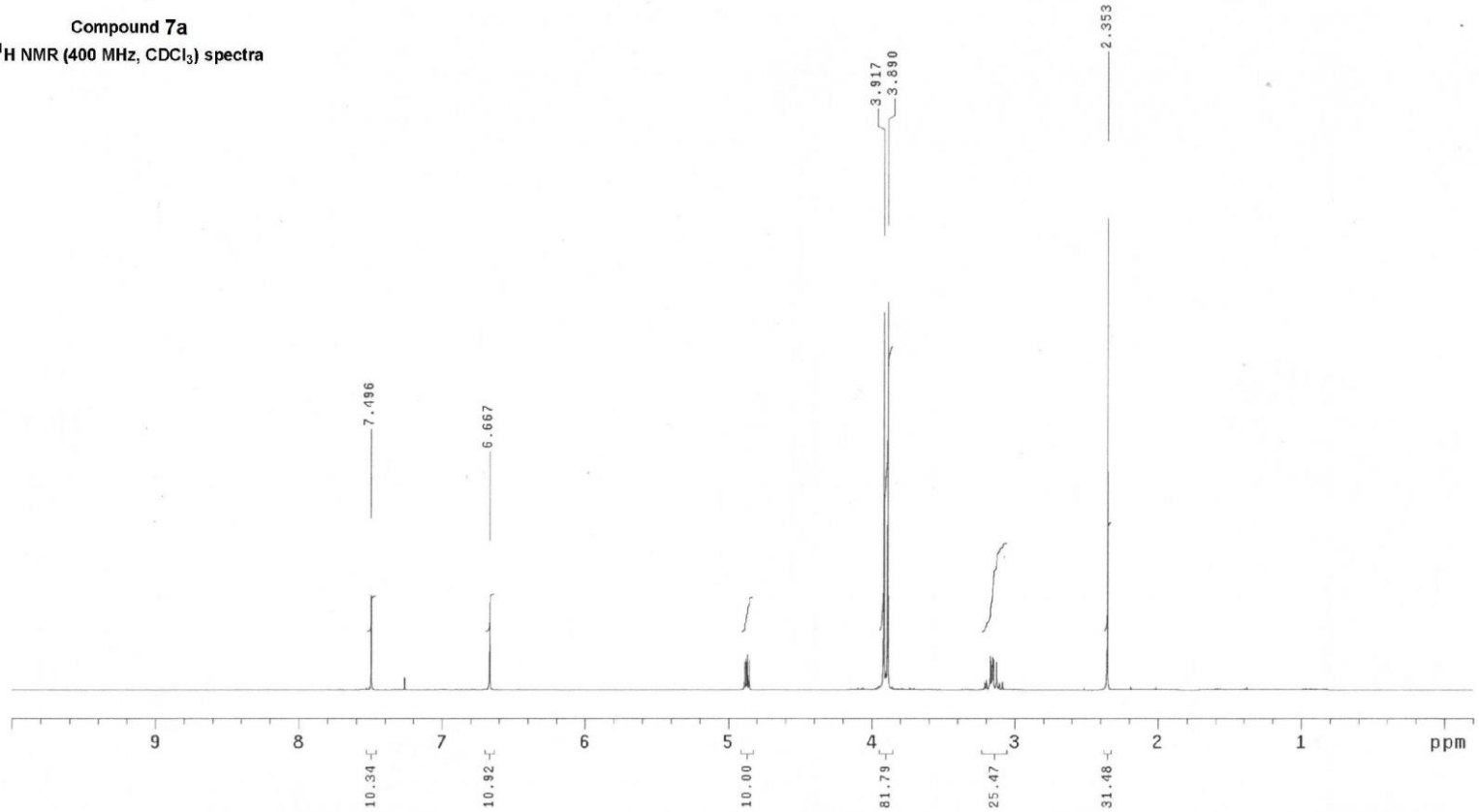
YTJMe

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: May 10 2018
Solvent: CDCl3
Ambient temperature
Total 32 repetitions



Compound 7a

^{1}H NMR (400 MHz, $CDCl_3$) spectra

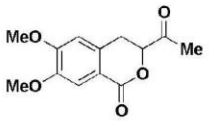


Compound 7a (^{13}C-NMR spectral data)

YTJMe

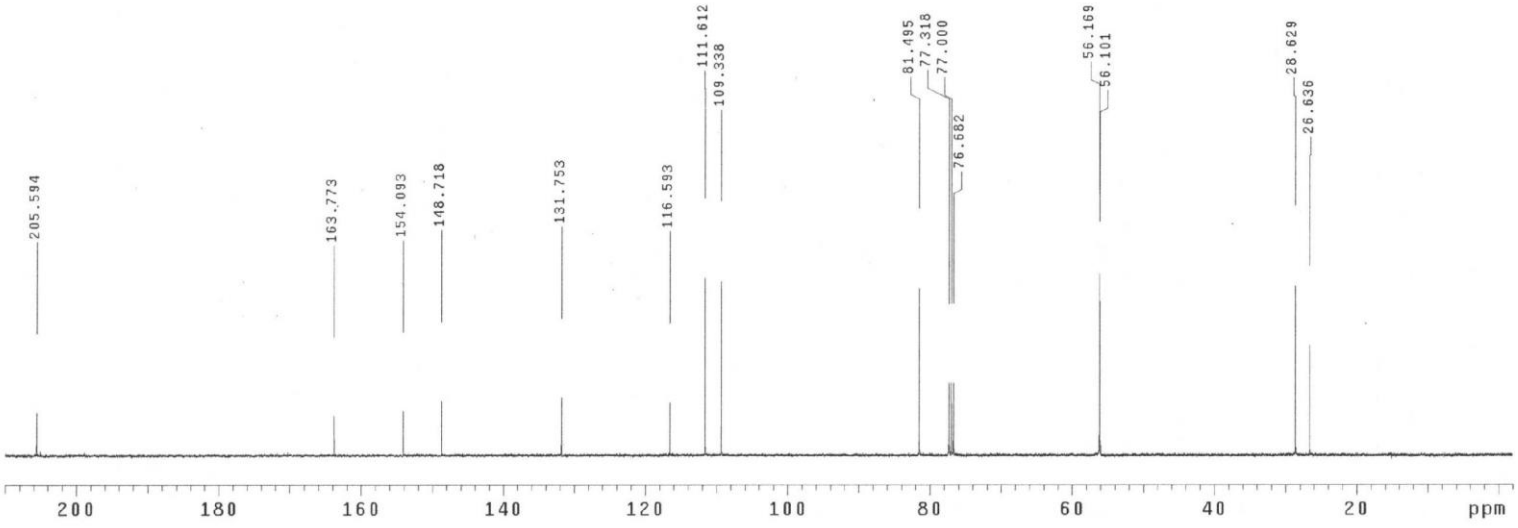
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 10 2018
Solvent: CDCl3
Ambient temperature
Total 1232 repetitions



Compound 7a

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

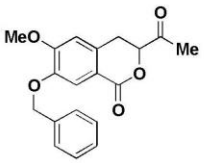


Compound 7b (^{1}H-NMR spectral data)

YTJ7CMe

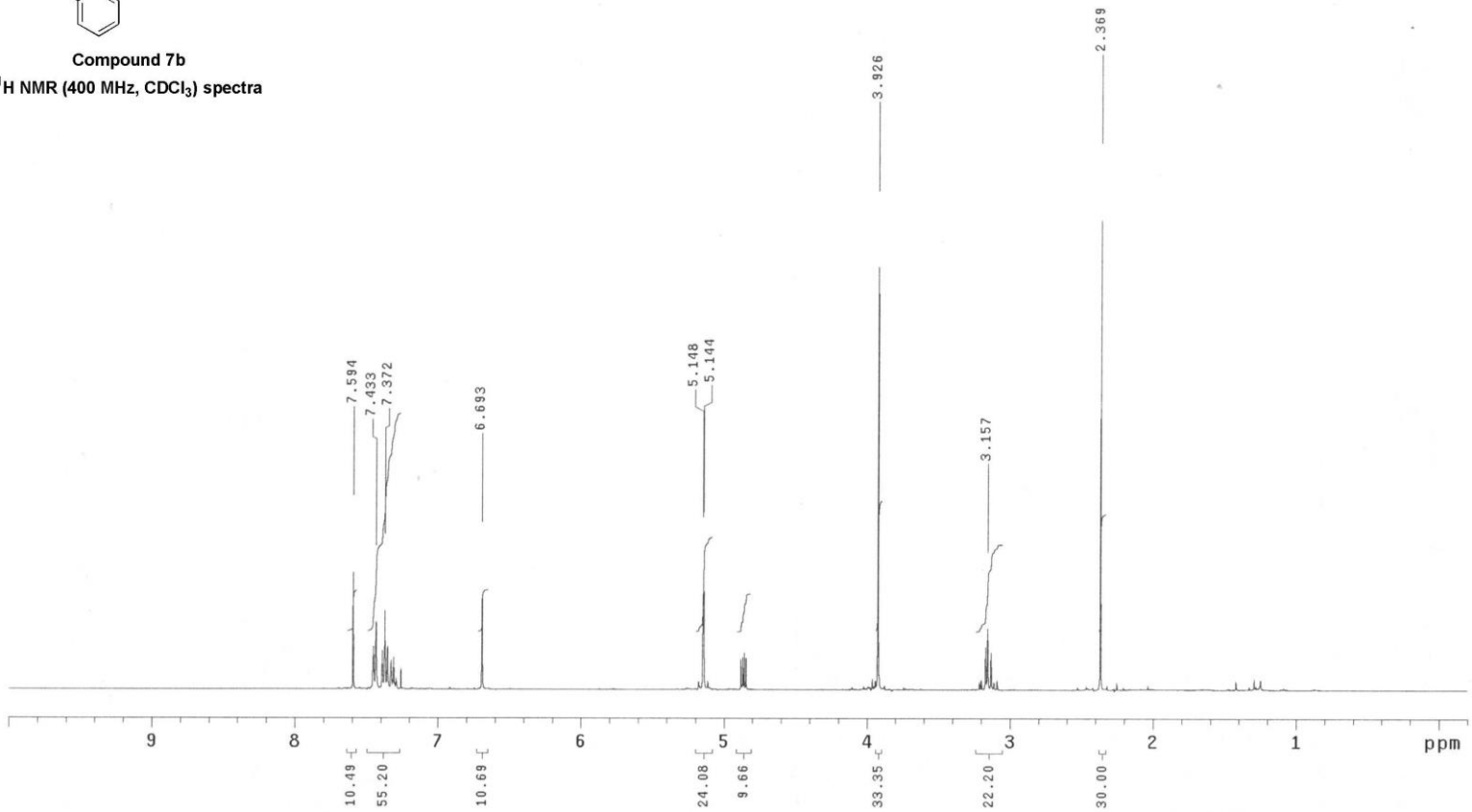
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jun 1 2018
Solvent: CDCl3
Ambient temperature
Total 32 repetitions



Compound 7b

^{1}H NMR (400 MHz, $CDCl_3$) spectra

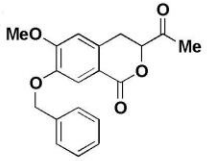


Compound 7b (^{13}C-NMR spectral data)

YTJ7CMe

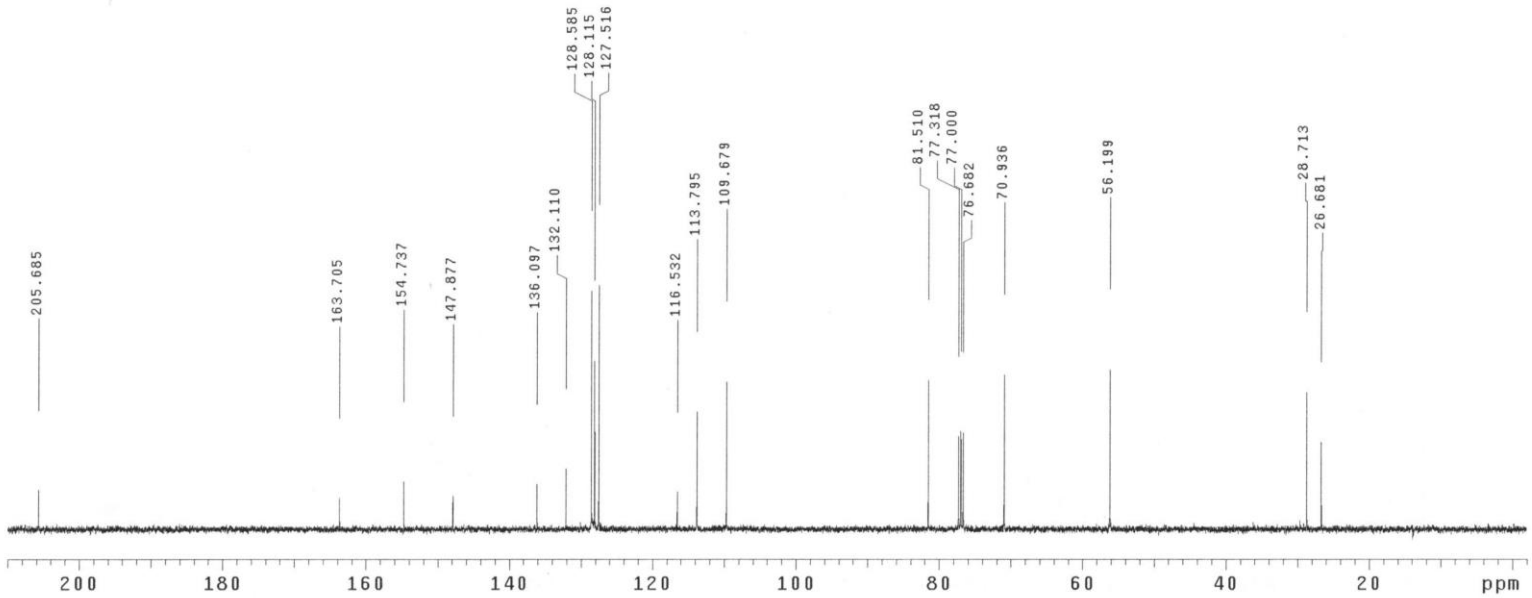
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jun 1 2018
Solvent: CDCl3
Ambient temperature
Total 608 repetitions

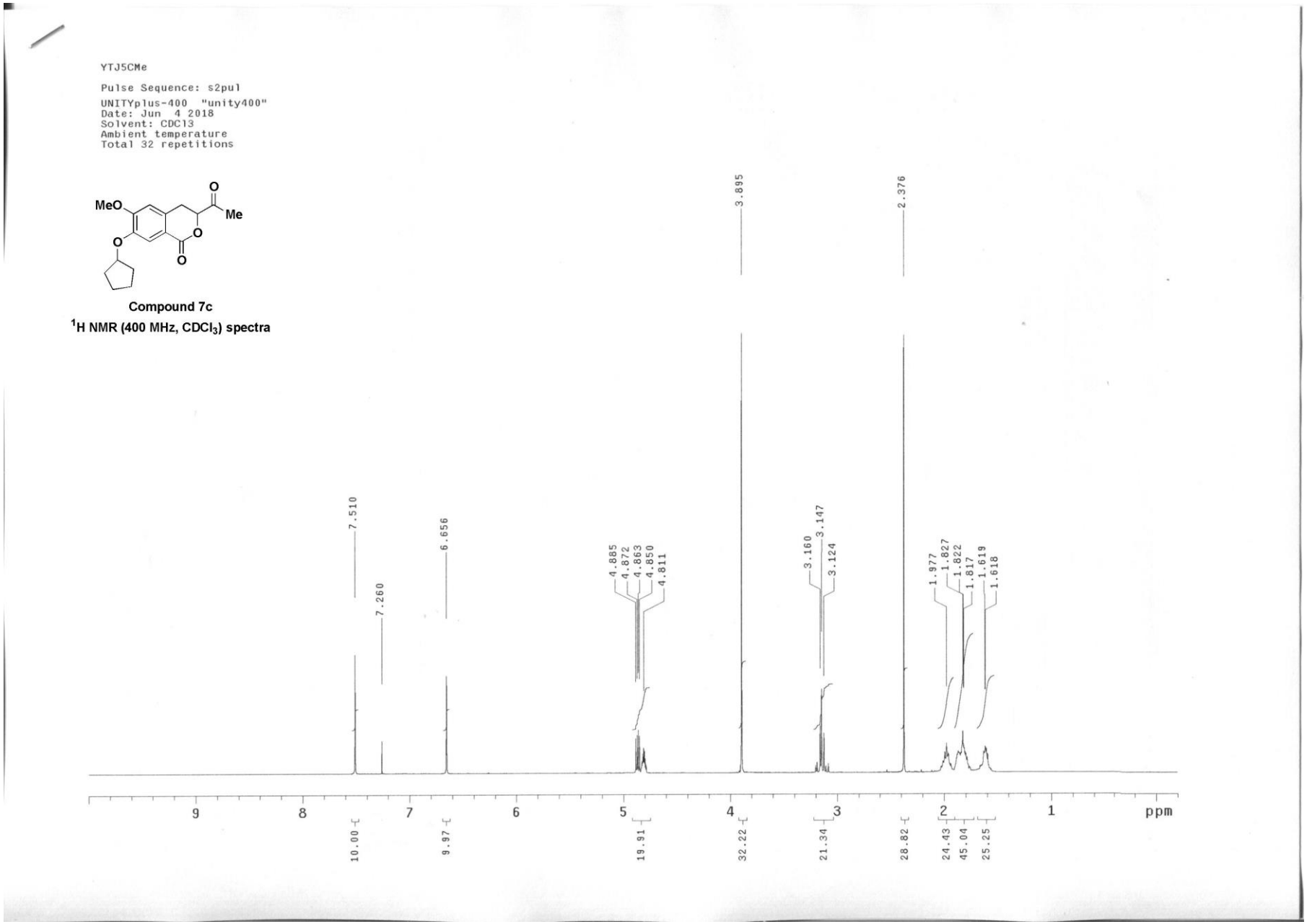


Compound 7b

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



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

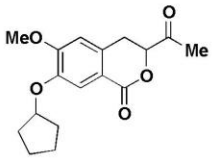


Compound 7c (^{13}C-NMR spectral data)

YTJ5CMe

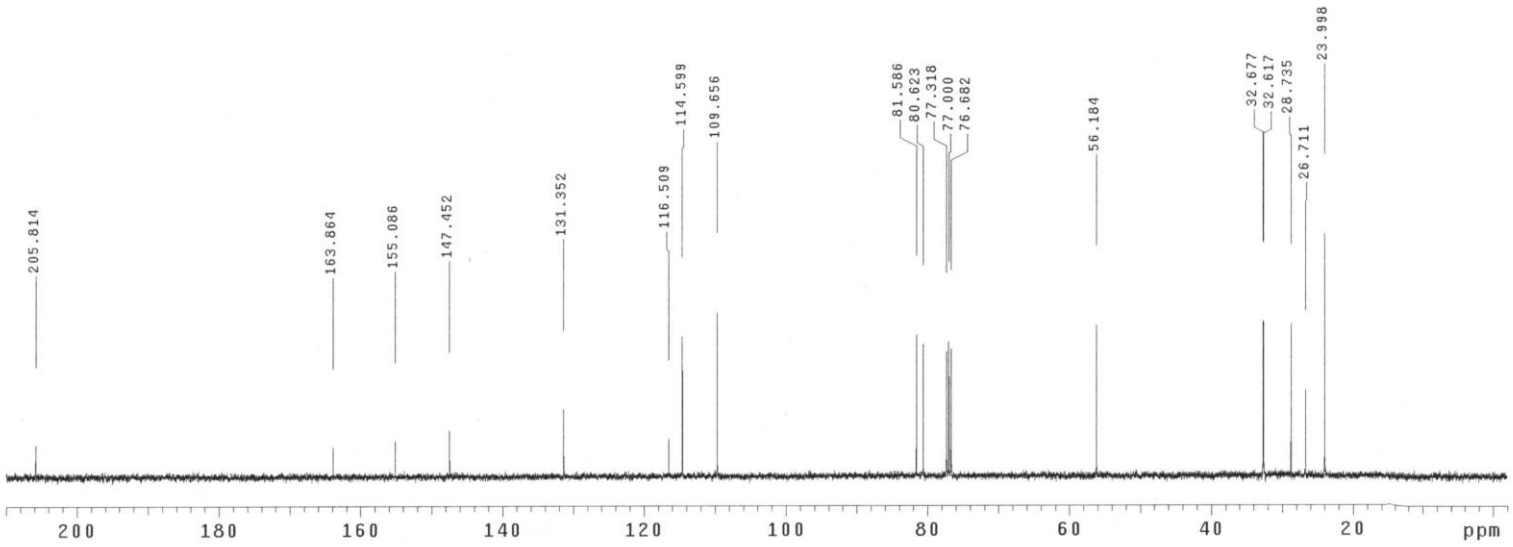
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jun 4 2018
Solvent: CDCl3
Ambient temperature
Total 928 repetitions

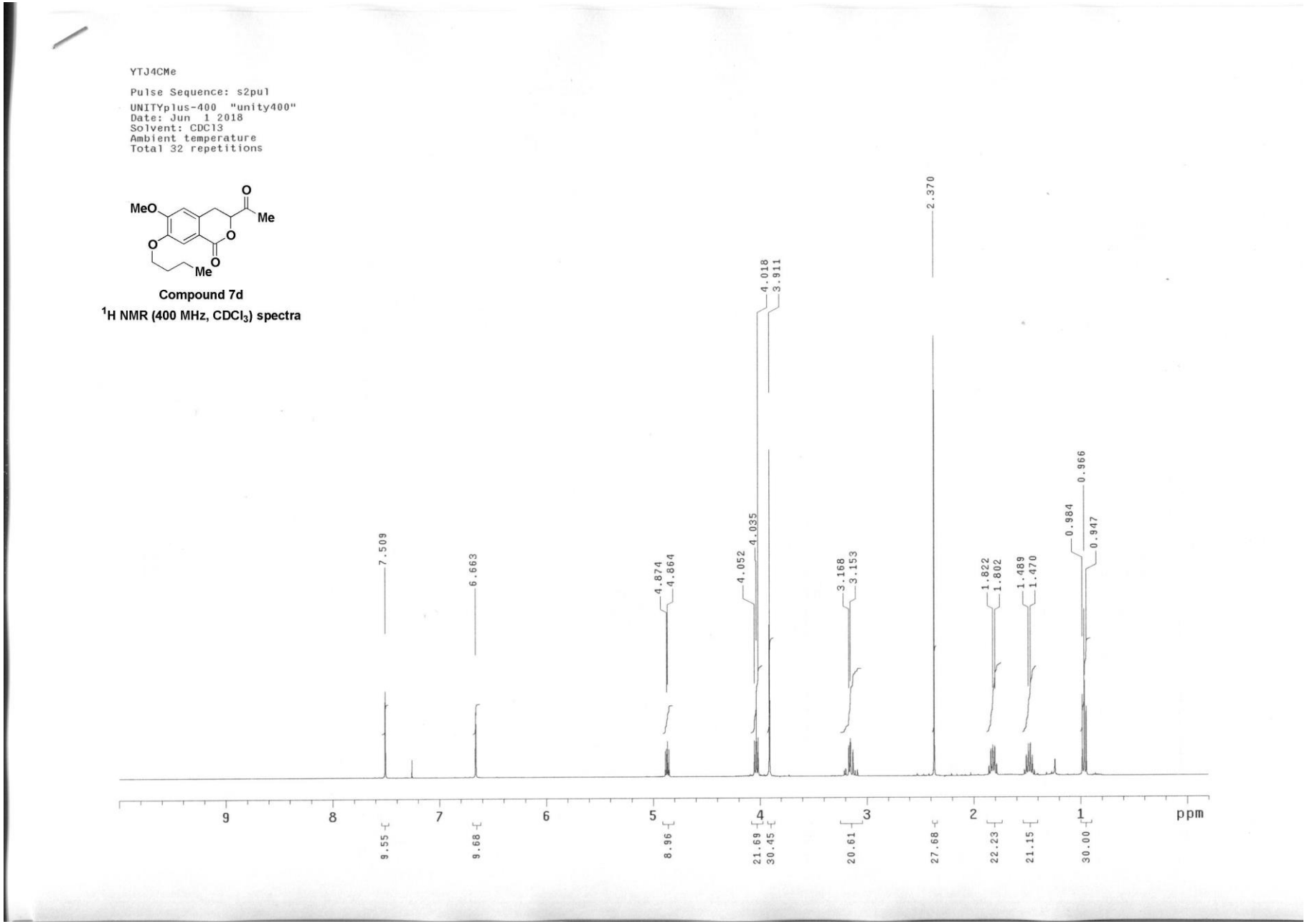


Compound 7c

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



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

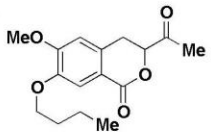


Compound 7d (^{13}C-NMR spectral data)

YTJ4CMe

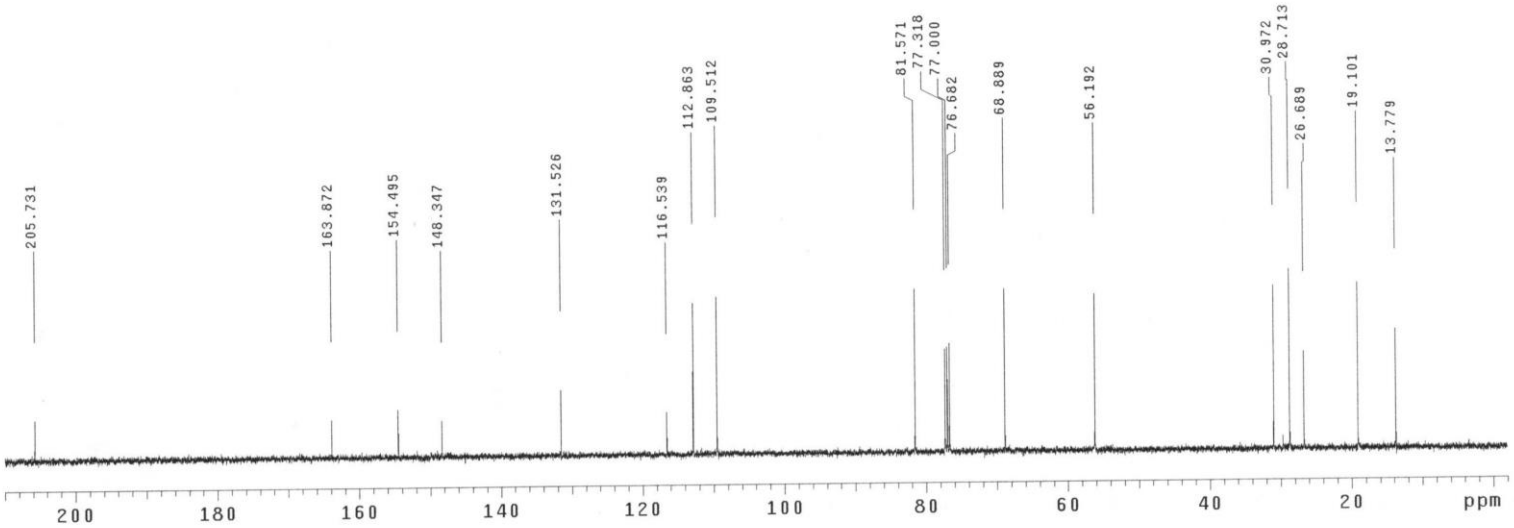
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jun 1 2018
Solvent: CDCl3
Ambient temperature
Total 608 repetitions

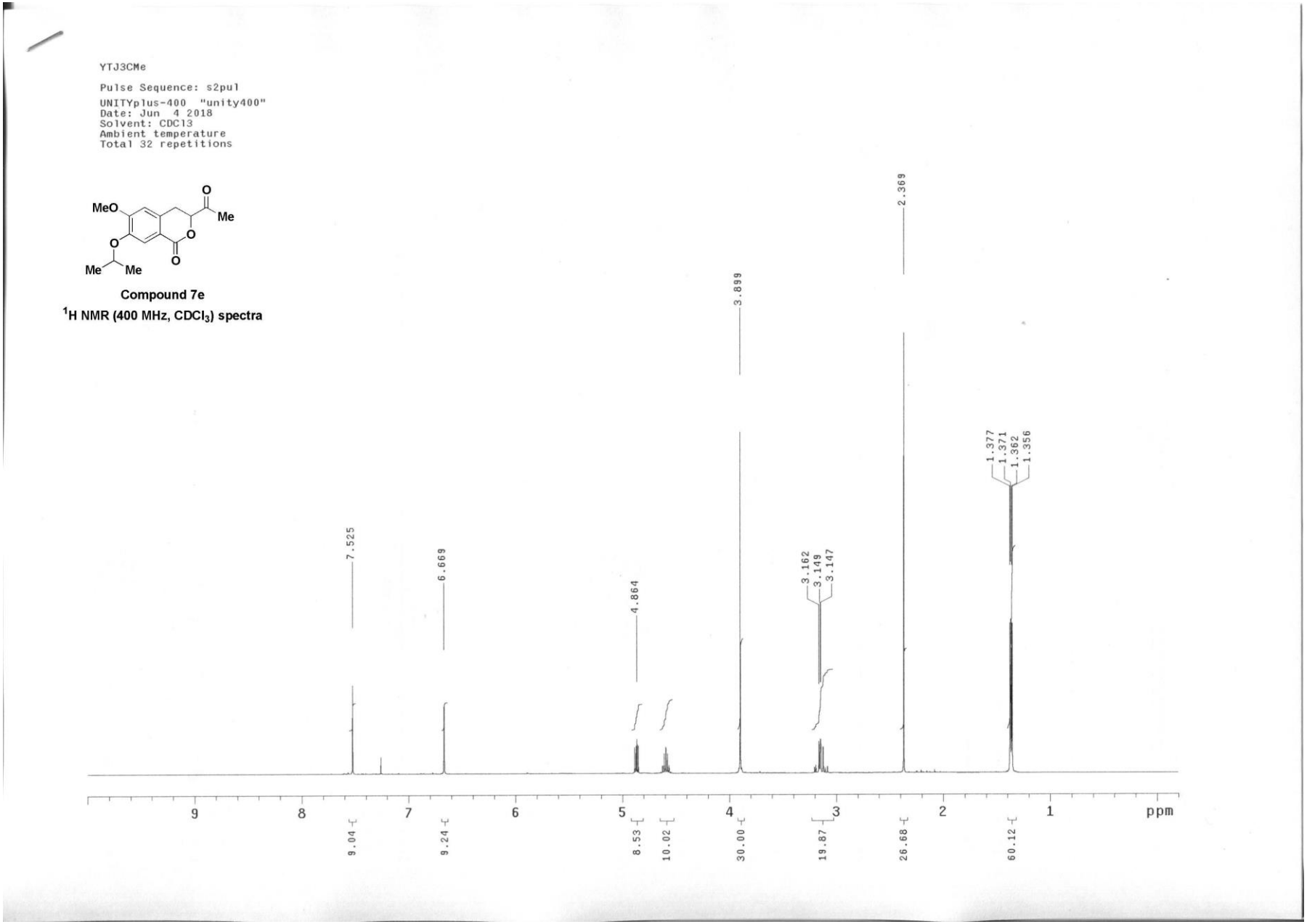


Compound 7d

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



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

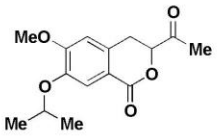


Compound 7e (^{13}C-NMR spectral data)

YTJ3CMe

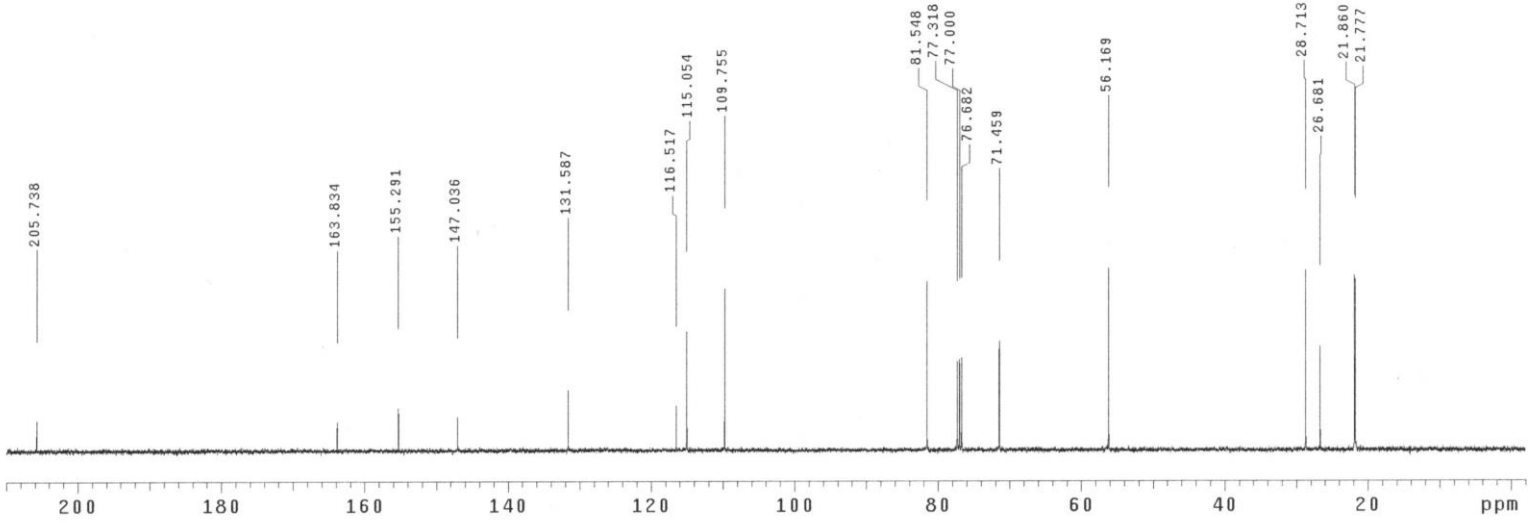
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jun 4 2018
Solvent: CDCl3
Ambient temperature
Total 1056 repetitions

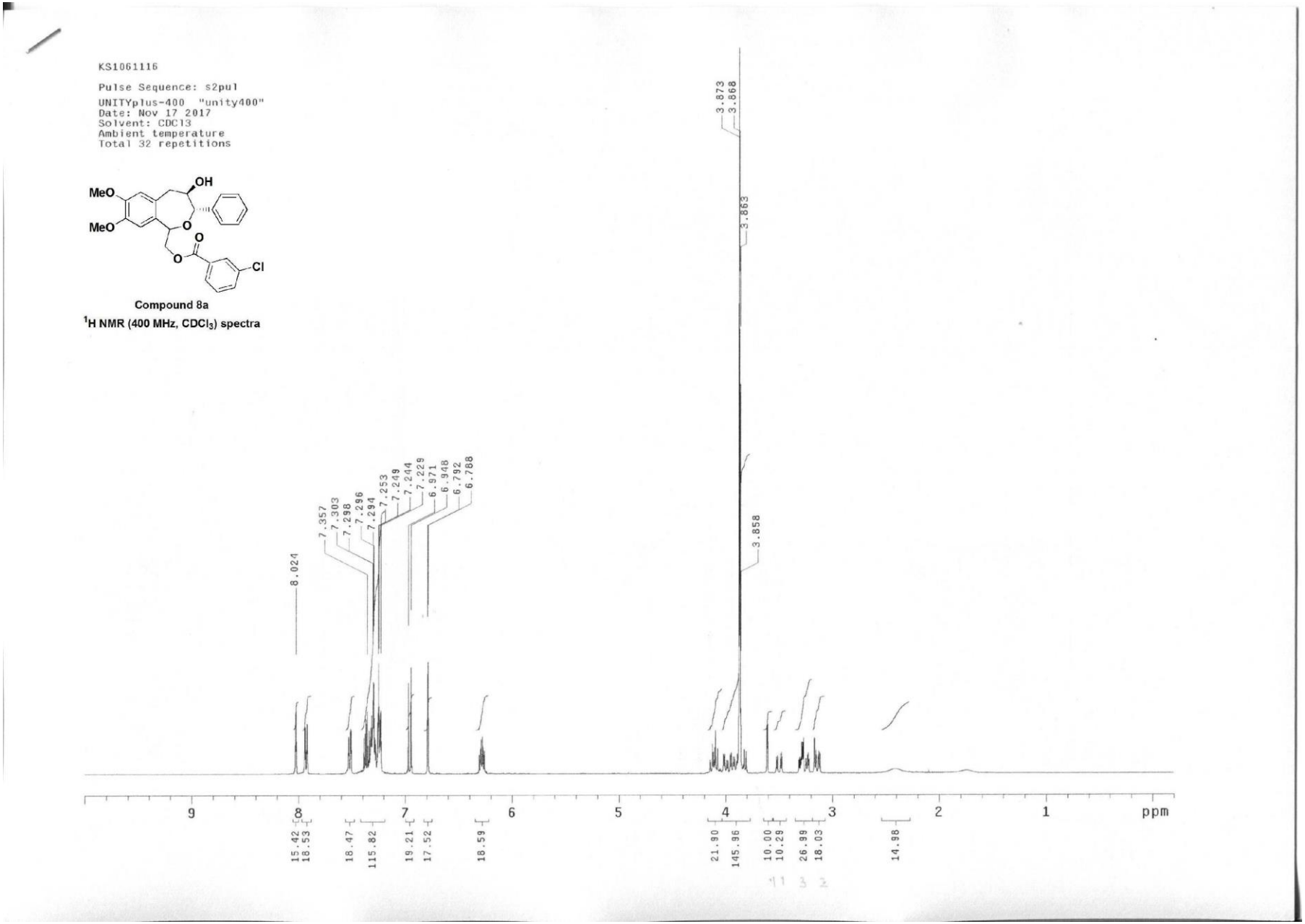


Compound 7e

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



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

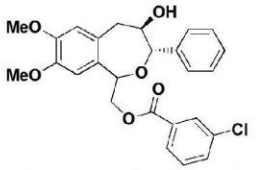


Compound 8a (^{13}C-NMR spectral data)

KS1061116

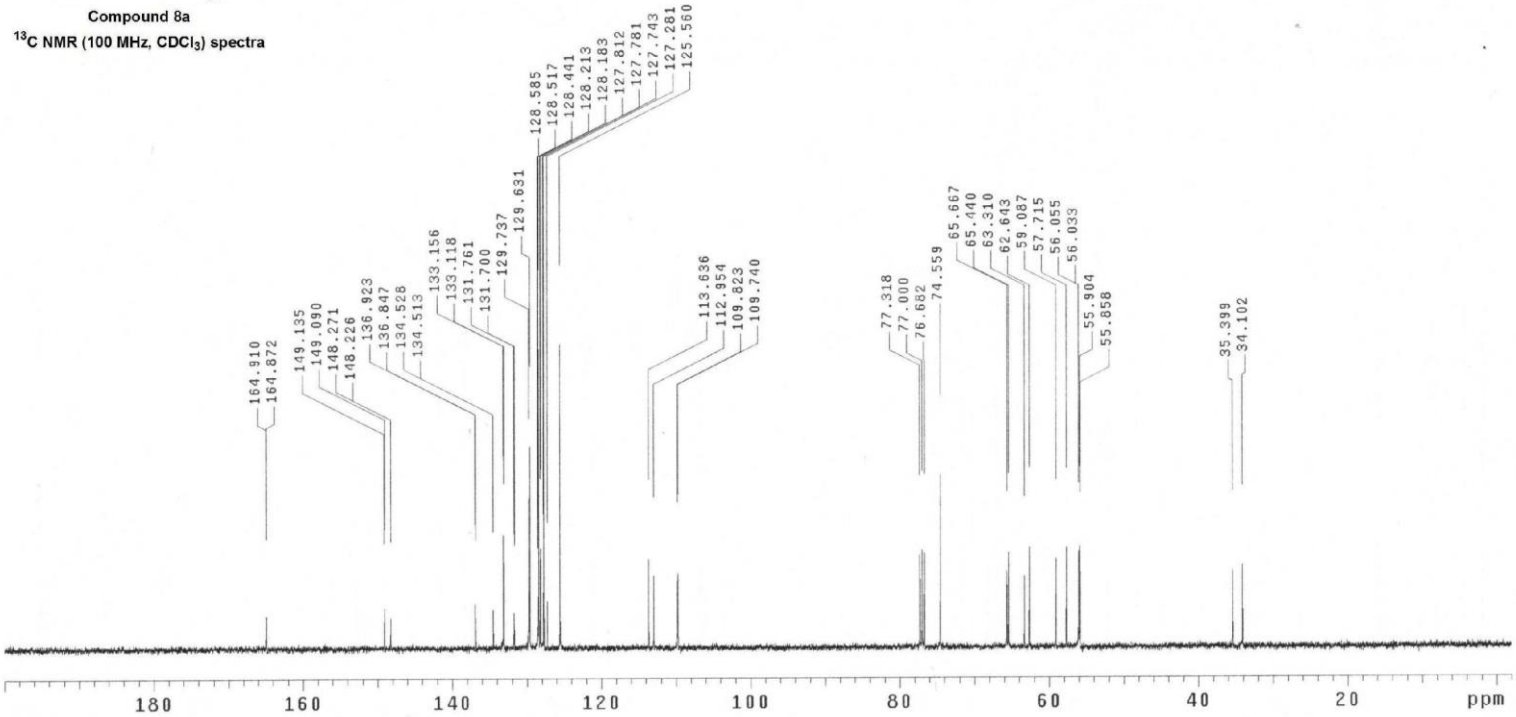
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Nov 17 2017
Solvent: CDCl3
Ambient temperature
Total 1104 repetitions

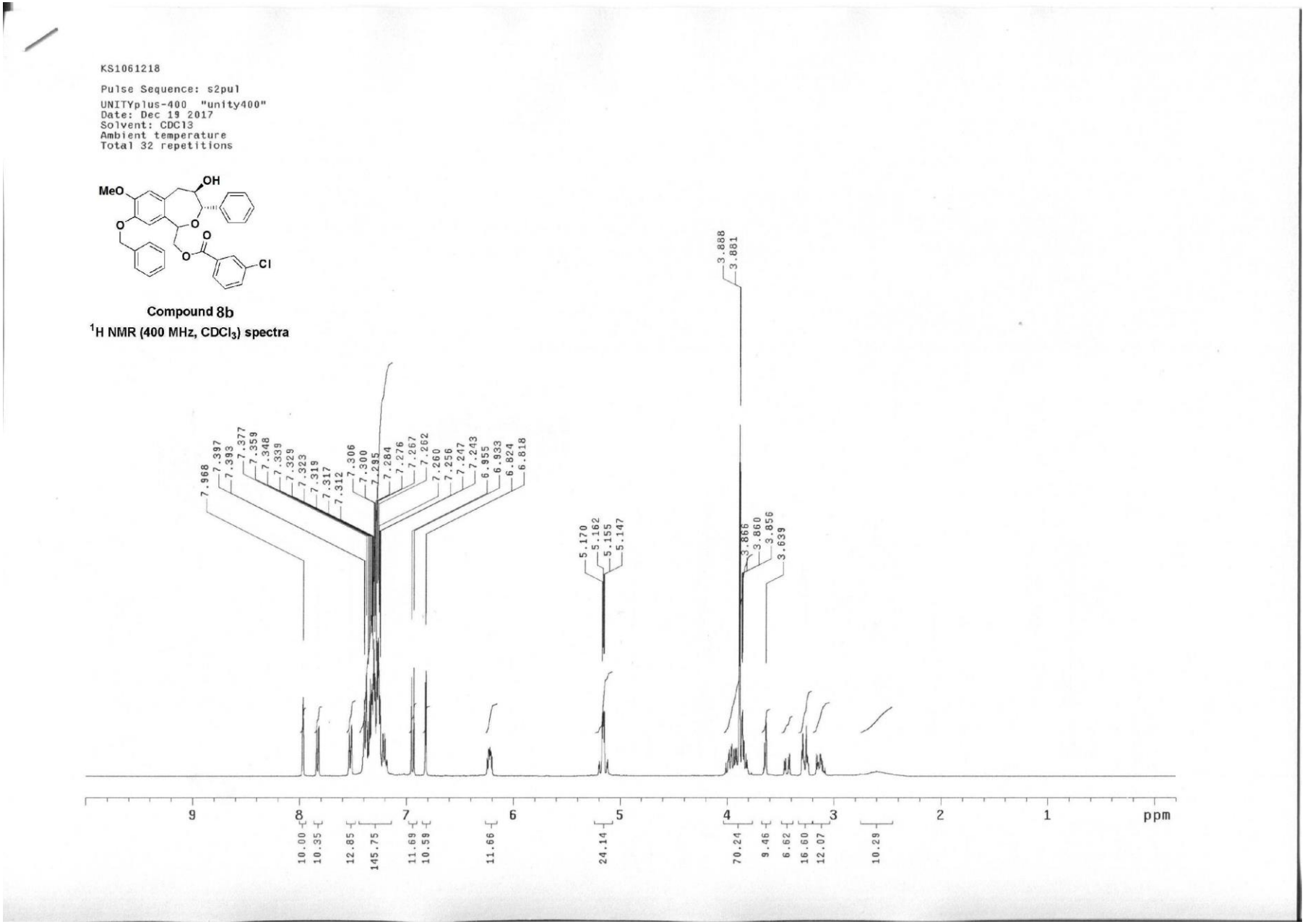


Compound 8a

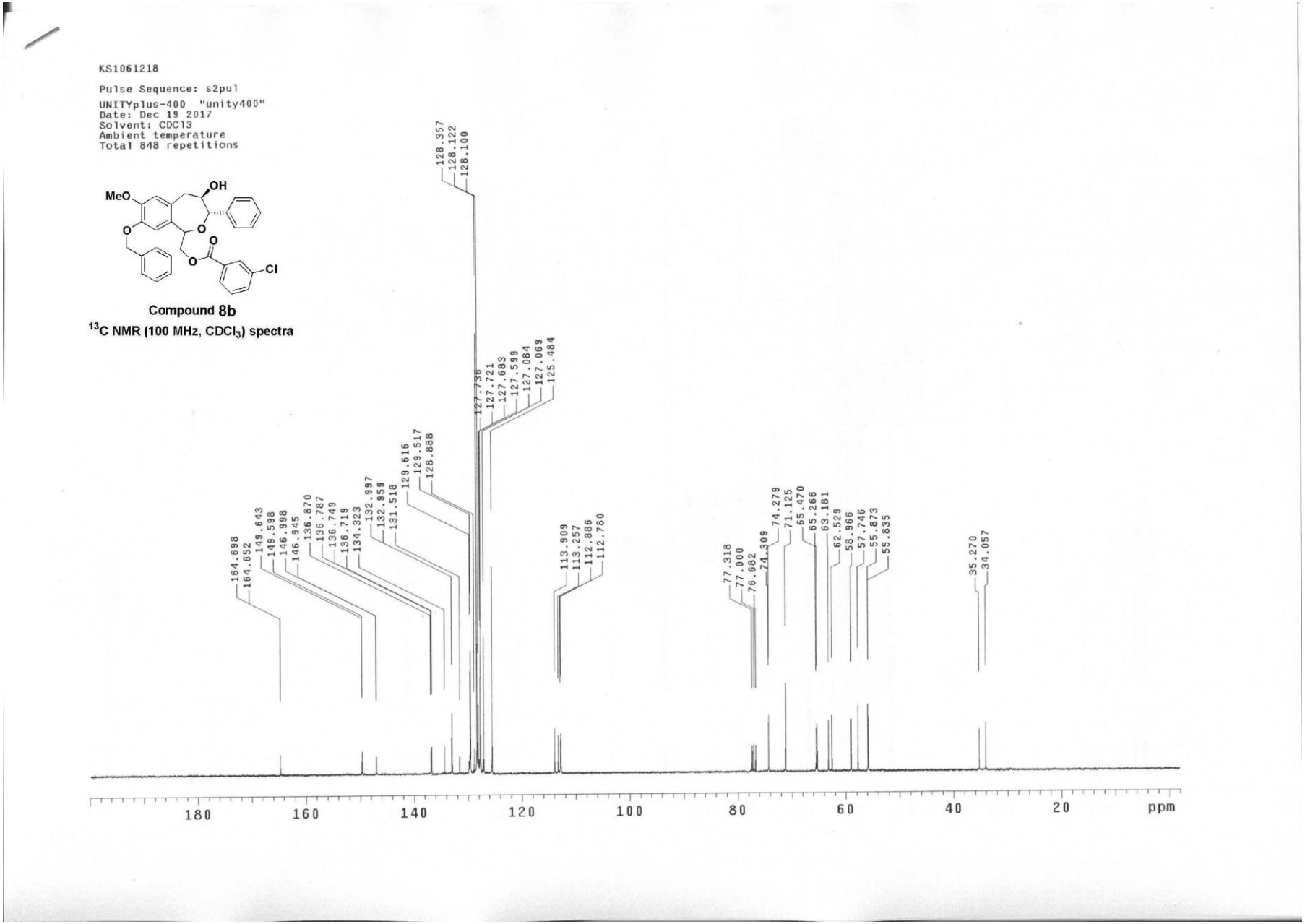
^{13}C NMR (100 MHz, $CDCl_3$) spectra



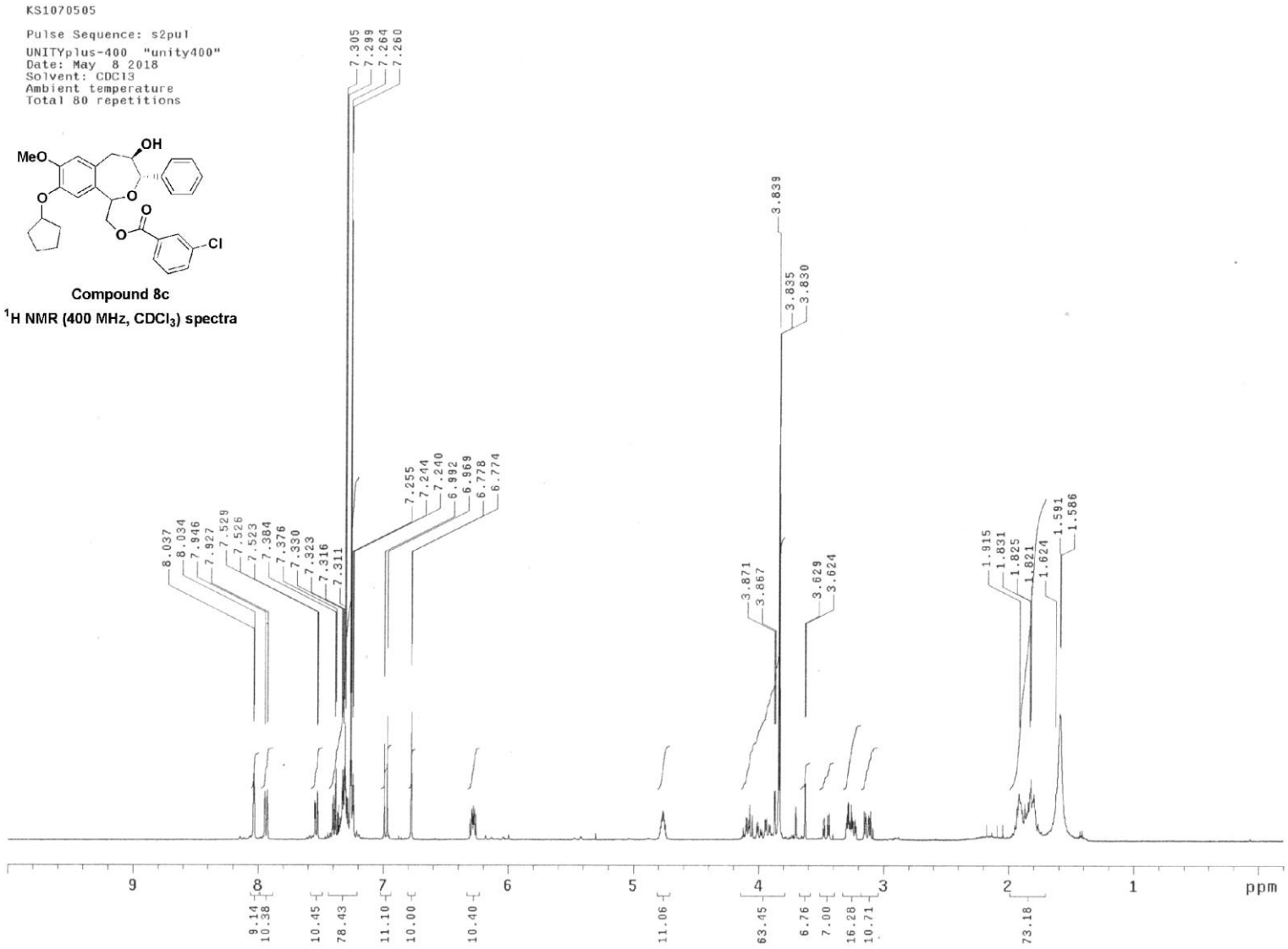
Compound 8b (^{1}H-NMR spectral data)



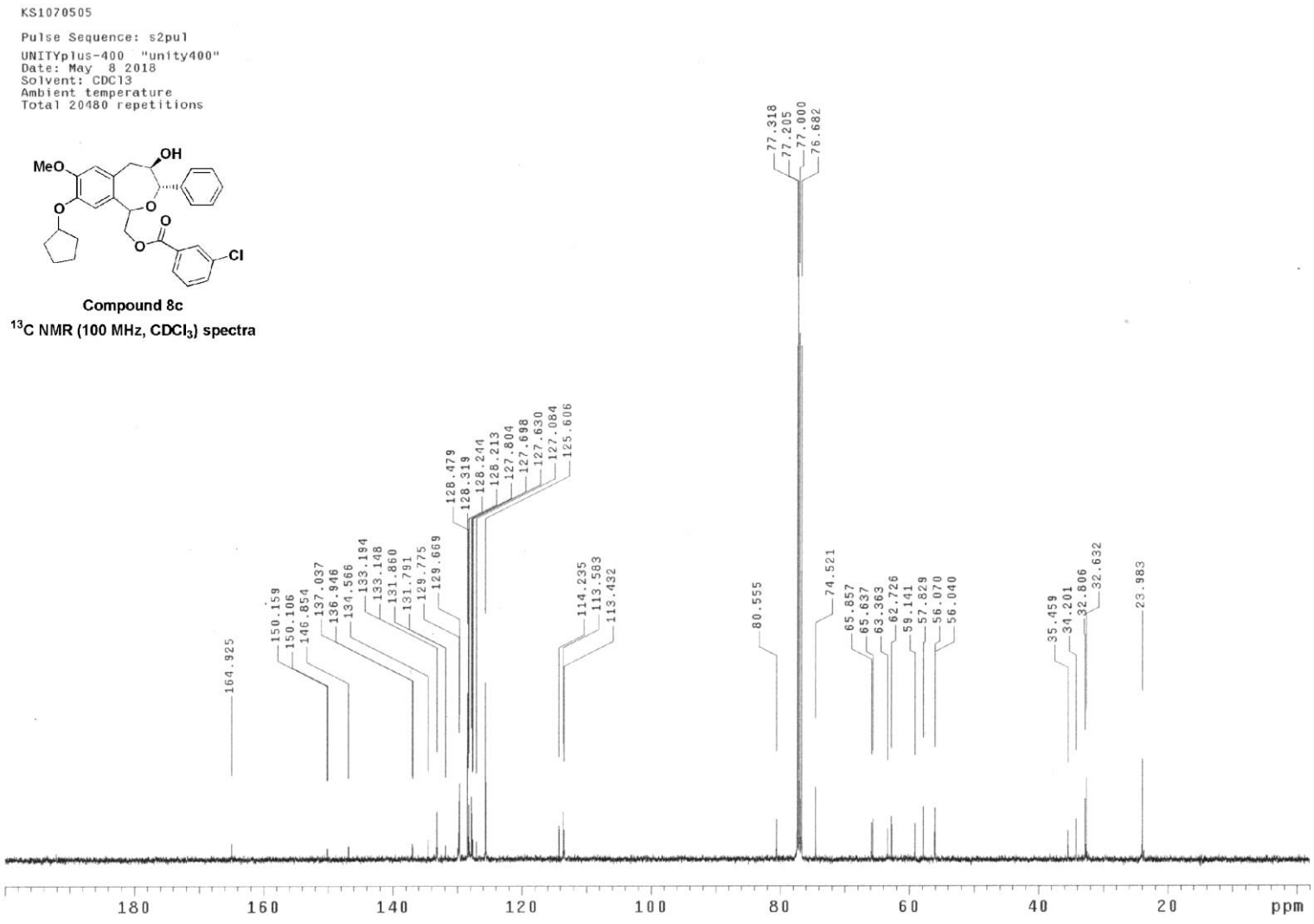
Compound 8b (^{13}C-NMR spectral data)



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



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

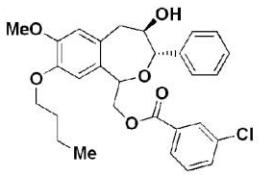


Compound 8d (^{1}H-NMR spectral data)

KS1070504

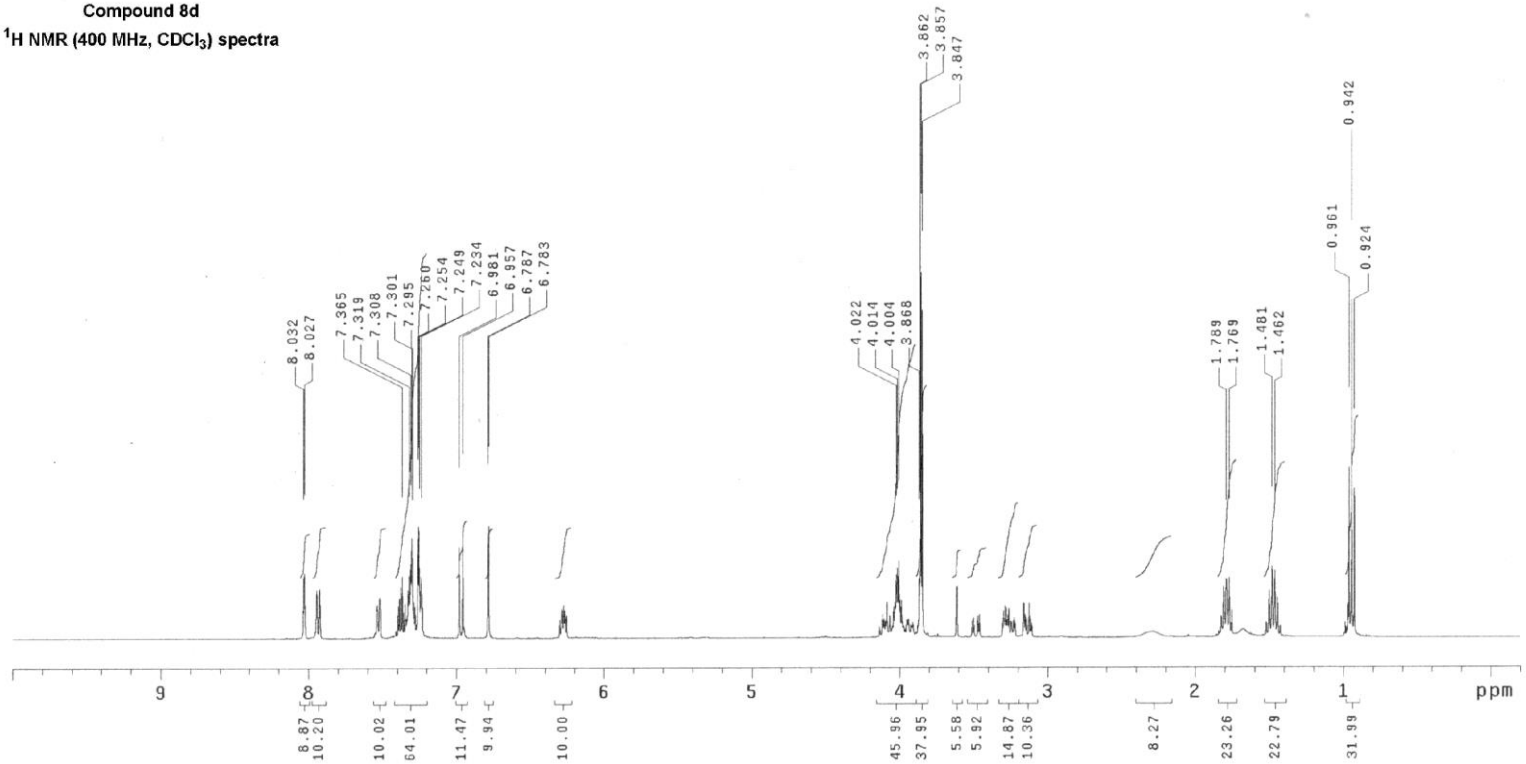
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 7 2018
Solvent: CDCl3
Ambient temperature
Total 32 repetitions



Compound 8d

^{1}H NMR (400 MHz, $CDCl_3$) spectra

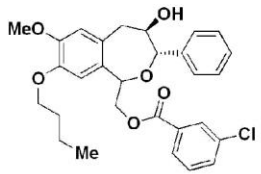


Compound 8d (^{13}C-NMR spectral data)

KS1070504

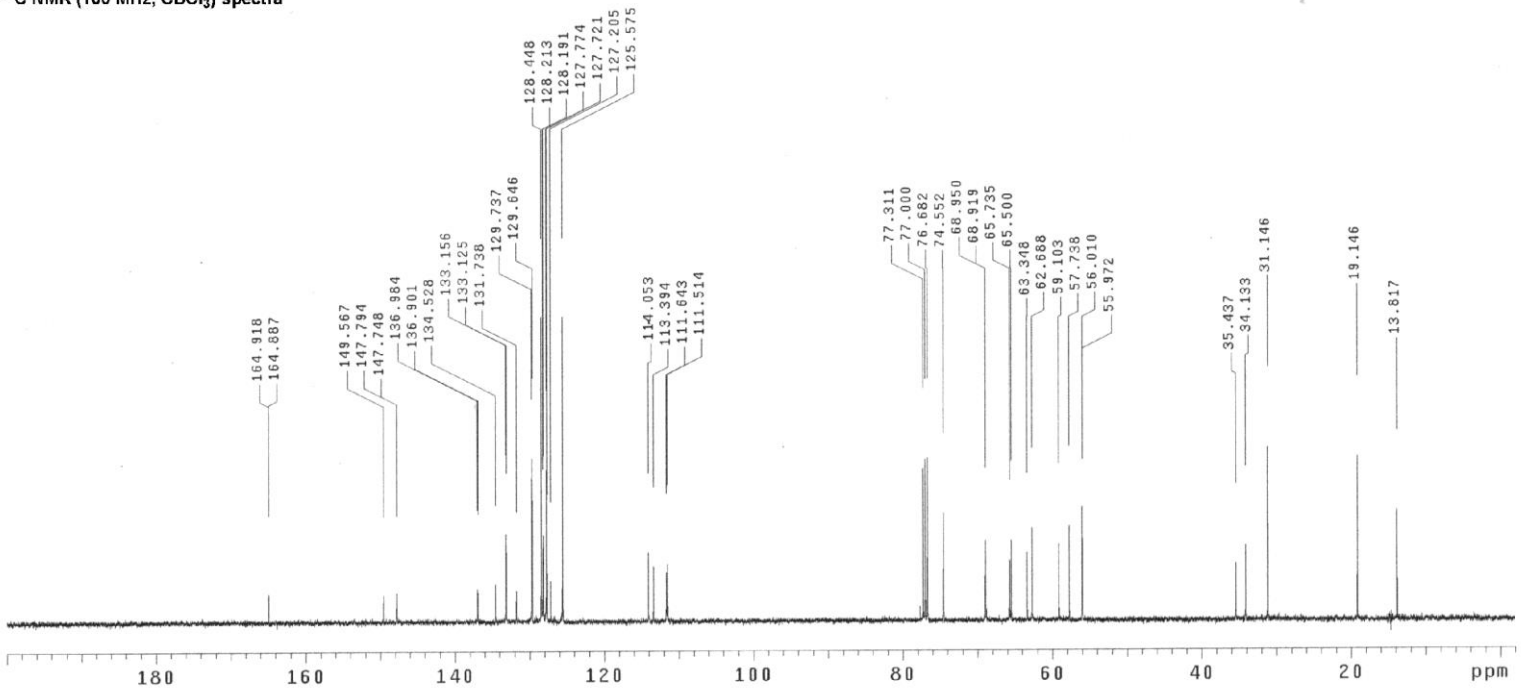
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 7 2018
Solvent: CDCl3
Ambient temperature
Total 1936 repetitions



Compound 8d

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

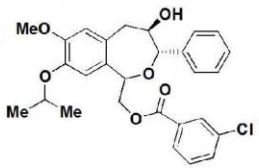


Compound 8e (^{1}H-NMR spectral data)

KS10651227-1

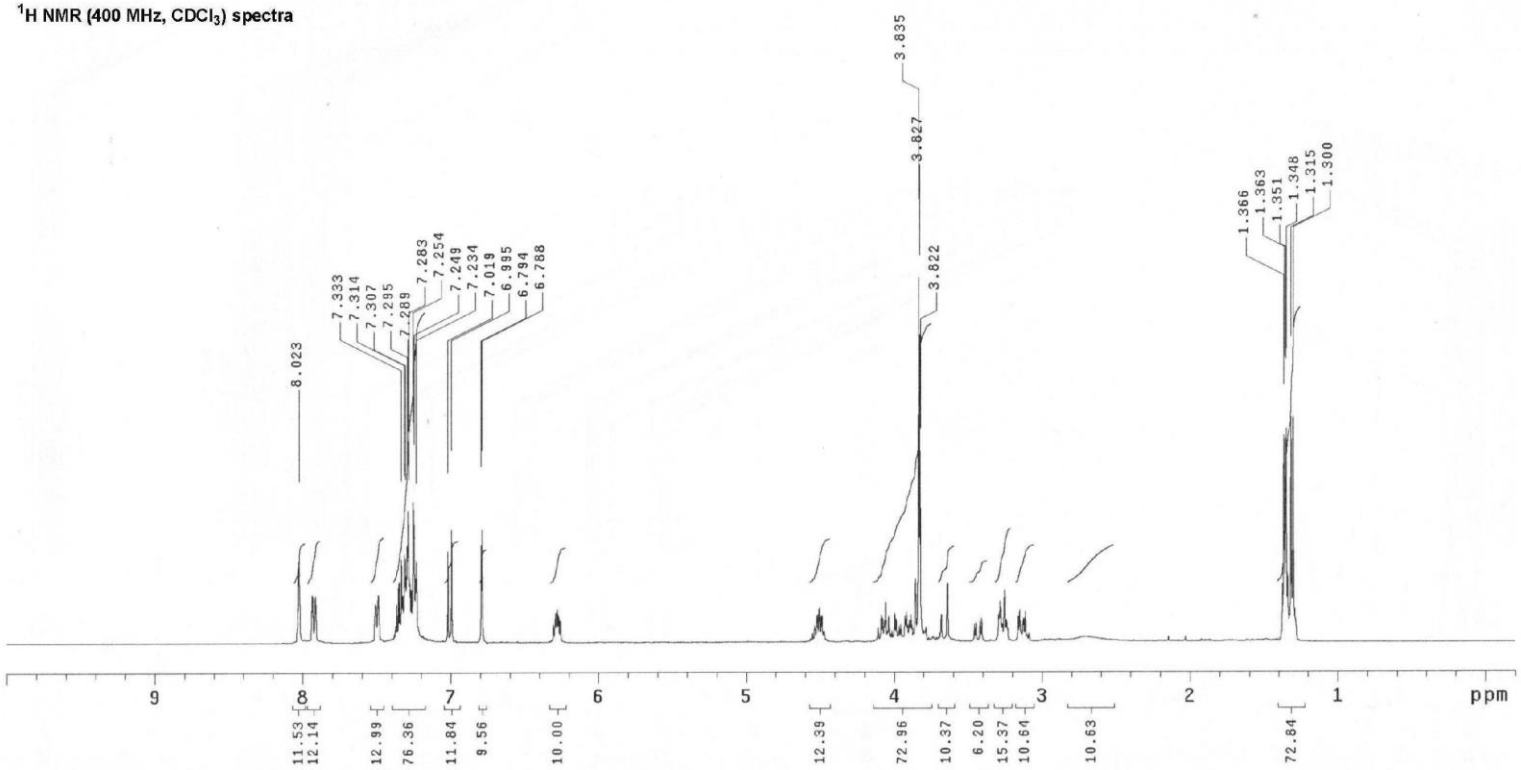
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Dec 28 2017
Solvent: CDCl3
Ambient temperature
Total 32 repetitions



Compound 8e

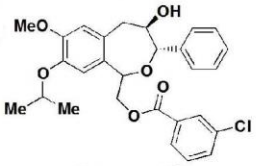
^{1}H NMR (400 MHz, $CDCl_3$) spectra



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

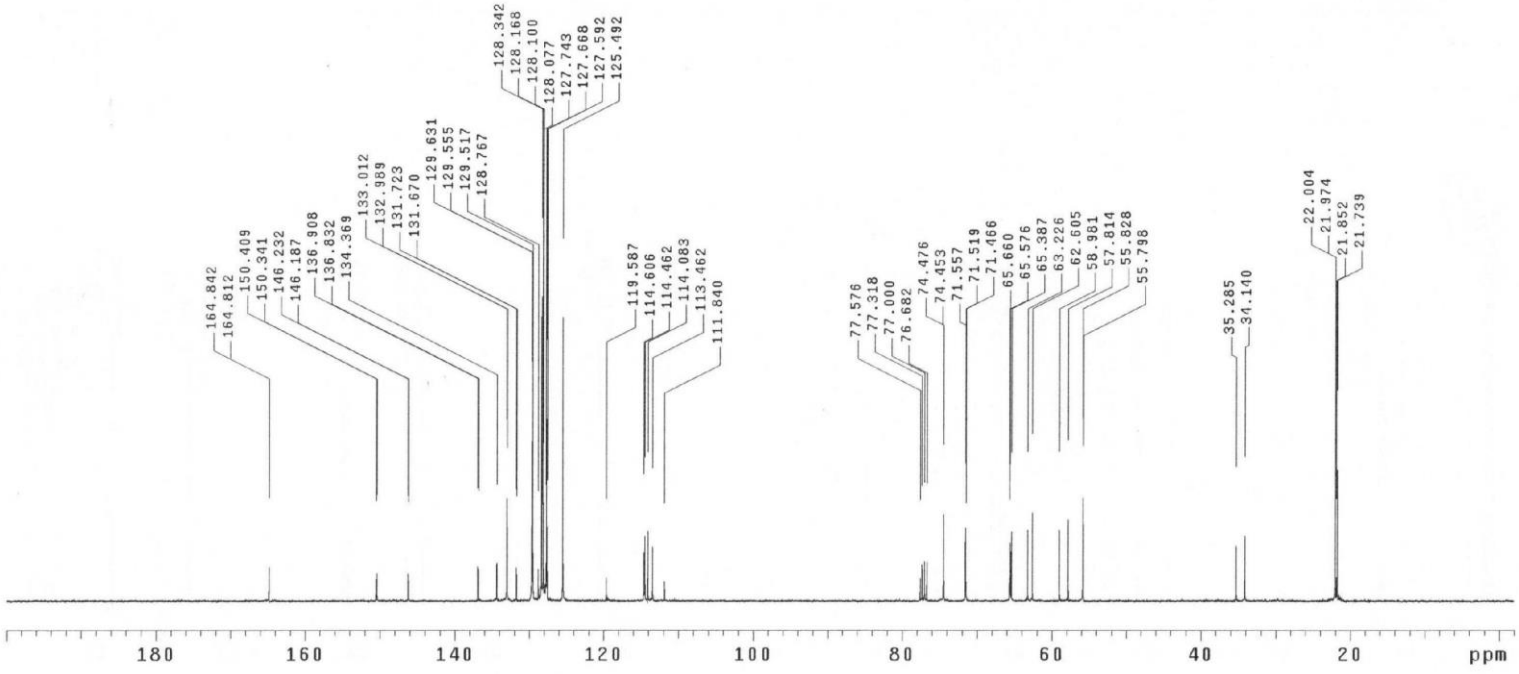
KS10651227-1

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Dec 28 2017
Solvent: CDCl3
Ambient temperature
Total 1744 repetitions



Compound 8e

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

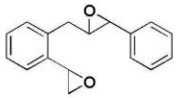


Compound 9a (^{1}H-NMR spectral data)

KS1070104

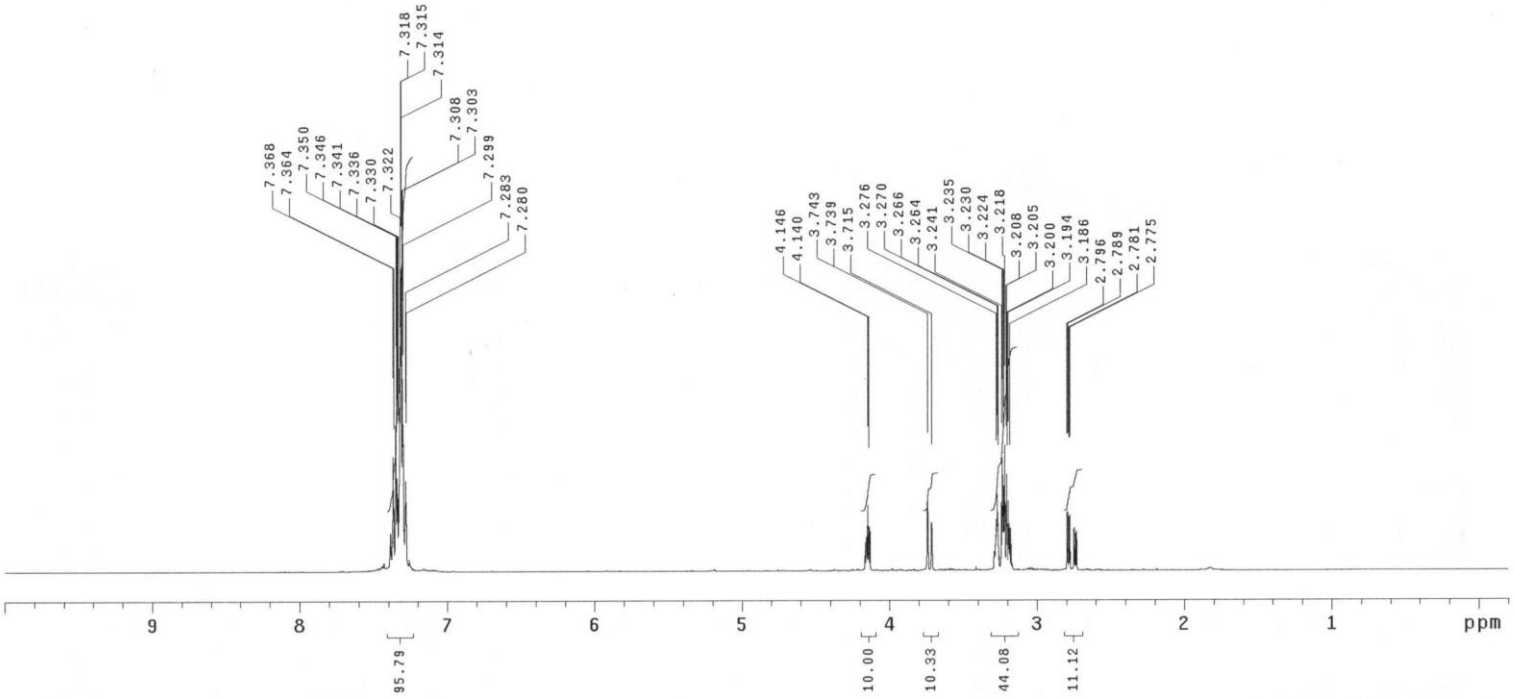
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jan 5 2018
Solvent: CDCl3
Ambient temperature
Total 32 repetitions



Compound 9a

^{1}H NMR (400 MHz, $CDCl_3$) spectra

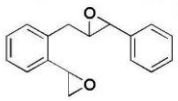


Compound 9a (^{13}C-NMR spectral data)

KS1070104

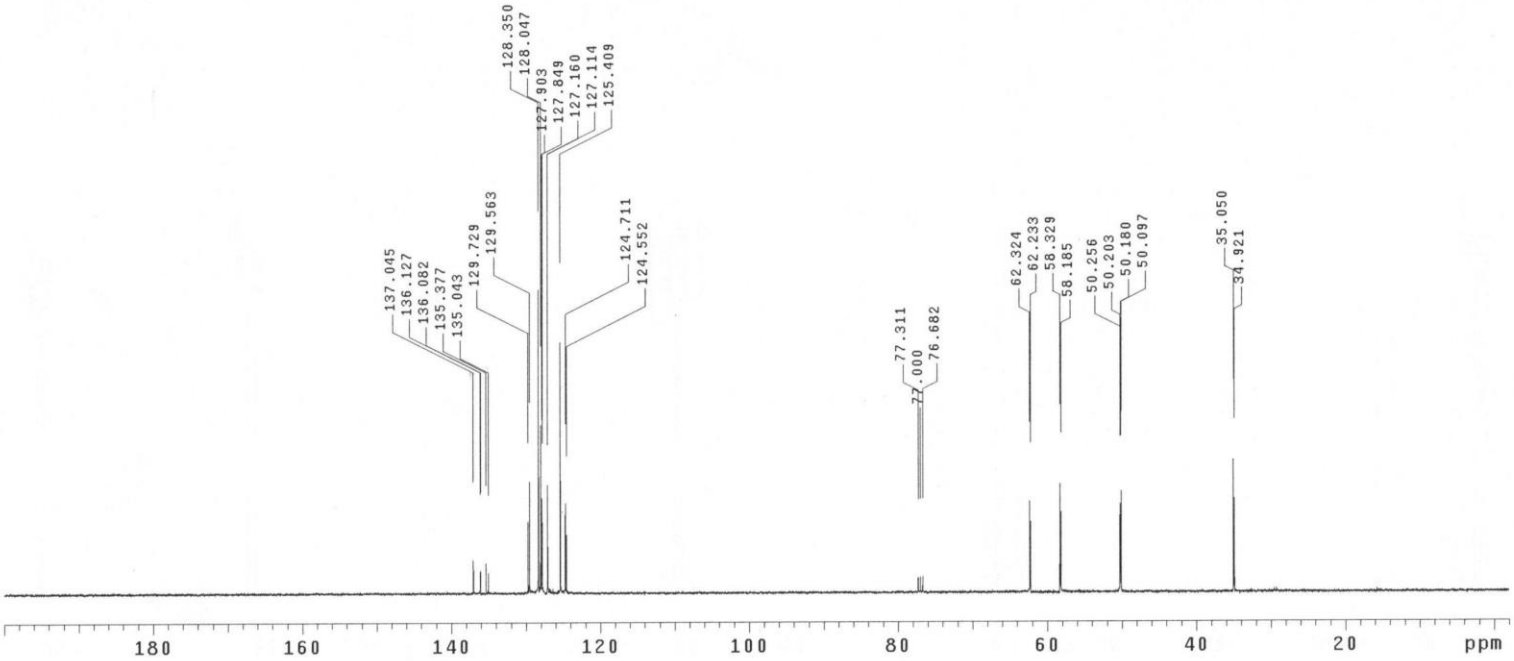
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jan 5 2018
Solvent: CDCl3
Ambient temperature
Total 256 repetitions

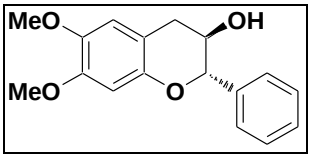


Compound 9a

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



X-ray crystal data of 2a



Empirical formula	C17 H18 O4	
Formula weight	286.31	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 8.0587(6) Å	α = 82.634(3)°.
	b = 8.8690(7) Å	β = 75.552(3)°.
	c = 10.2746(8) Å	γ = 88.084(3)°.
Volume	705.26(9) $Å^3$	
Z	2	
Density (calculated)	1.348 Mg/m^3	
Absorption coefficient	0.095 mm^{-1}	
F(000)	304	
Crystal size	0.20 x 0.17 x 0.04 mm^3	
Theta range for data collection	2.063 to 26.410°.	
Index ranges	-9<=h<=10, -8<=k<=11, -12<=l<=12	
Reflections collected	11247	
Independent reflections	2868 [R(int) = 0.0268]	
Completeness to theta = 25.242°	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9485 and 0.8864	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2868 / 0 / 193	
Goodness-of-fit on F^2	1.053	
Final R indices [I>2sigma(I)]	R1 = 0.0354, wR2 = 0.0889	
R indices (all data)	R1 = 0.0405, wR2 = 0.0928	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.253 and -0.215 e.$Å^{-3}$	

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 171209lt_0m_a

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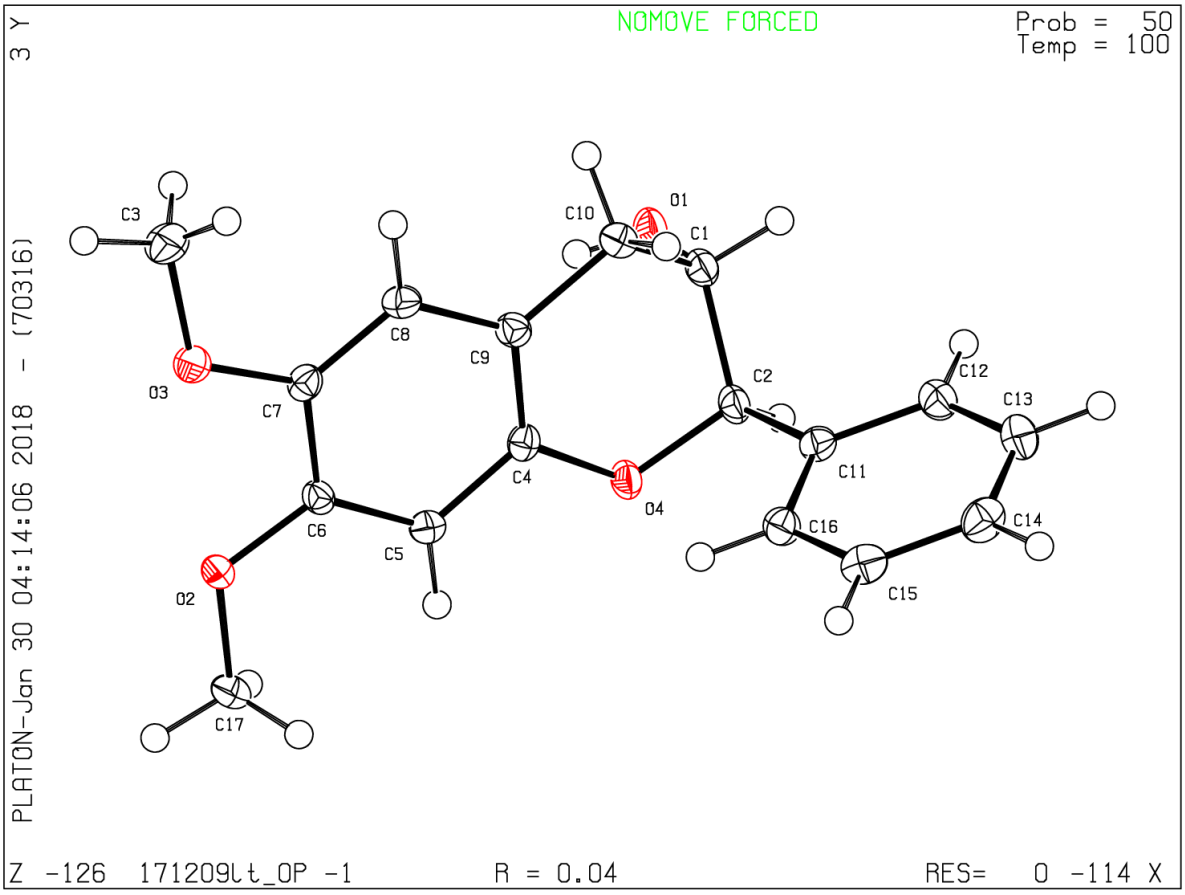
No syntax errors found. CIF dictionary Interpreting this report

Datablock: 171209lt_0m_a

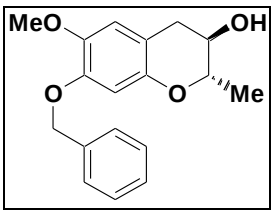
```
Bond precision:  C-C = 0.0017 A          Wavelength=0.71073

Cell:          a=8.0587(6)        b=8.8690(7)       c=10.2746(8)
               alpha=82.634(3)    beta=75.552(3)    gamma=88.084(3)
Temperature:   100 K

                Calculated                Reported
Volume          705.26(9)                 705.26(9)
Space group     P -1                      P -1
Hall group      -P 1                      -P 1
Moiety formula  C17 H18 O4                ?
Sum formula     C17 H18 O4                C17 H18 O4
Mr              286.31                    286.31
Dx,g cm-3       1.348                     1.348
Z               2                         2
Mu (mm-1)       0.095                     0.095
F000            304.0                     304.0
F000'           304.16
h,k,lmax        10,11,12                  10,11,12
Nref            2887                      2868
Tmin,Tmax       0.981,0.996               0.886,0.948
Tmin'           0.981

Correction method= # Reported T Limits: Tmin=0.886 Tmax=0.948
AbsCorr = MULTI-SCAN

Data completeness= 0.993          Theta(max)= 26.410

R(reflections)= 0.0354( 2508)     wR2(reflections)= 0.0928( 2868)

S = 1.053                  Npar= 193
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

The thermal ellipsoid was drawn at the 50% probability level



X-ray crystal data of 3b



Empirical formula	C18 H20 O4	
Formula weight	300.34	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 22.457(3) Å	α = 90°.
	b = 5.2177(7) Å	β = 95.828(4)°.
	c = 25.976(3) Å	γ = 90°.
Volume	3028.0(7) $Å^3$	
Z	8	
Density (calculated)	1.318 Mg/m^3	
Absorption coefficient	0.092 mm^{-1}	
F(000)	1280	
Crystal size	0.10 x 0.08 x 0.03 mm^3	
Theta range for data collection	1.576 to 26.616°.	
Index ranges	-28<=h<=28, -6<=k<=6, -32<=l<=32	
Reflections collected	28046	
Independent reflections	3174 [R(int) = 0.0585]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9485 and 0.8488	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3174 / 150 / 250	
Goodness-of-fit on F^2	1.057	
Final R indices [I>2sigma(I)]	R1 = 0.0561, wR2 = 0.1437	
R indices (all data)	R1 = 0.0983, wR2 = 0.1661	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.534 and -0.215 e.$Å^{-3}$	

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_180146LT_0m_a

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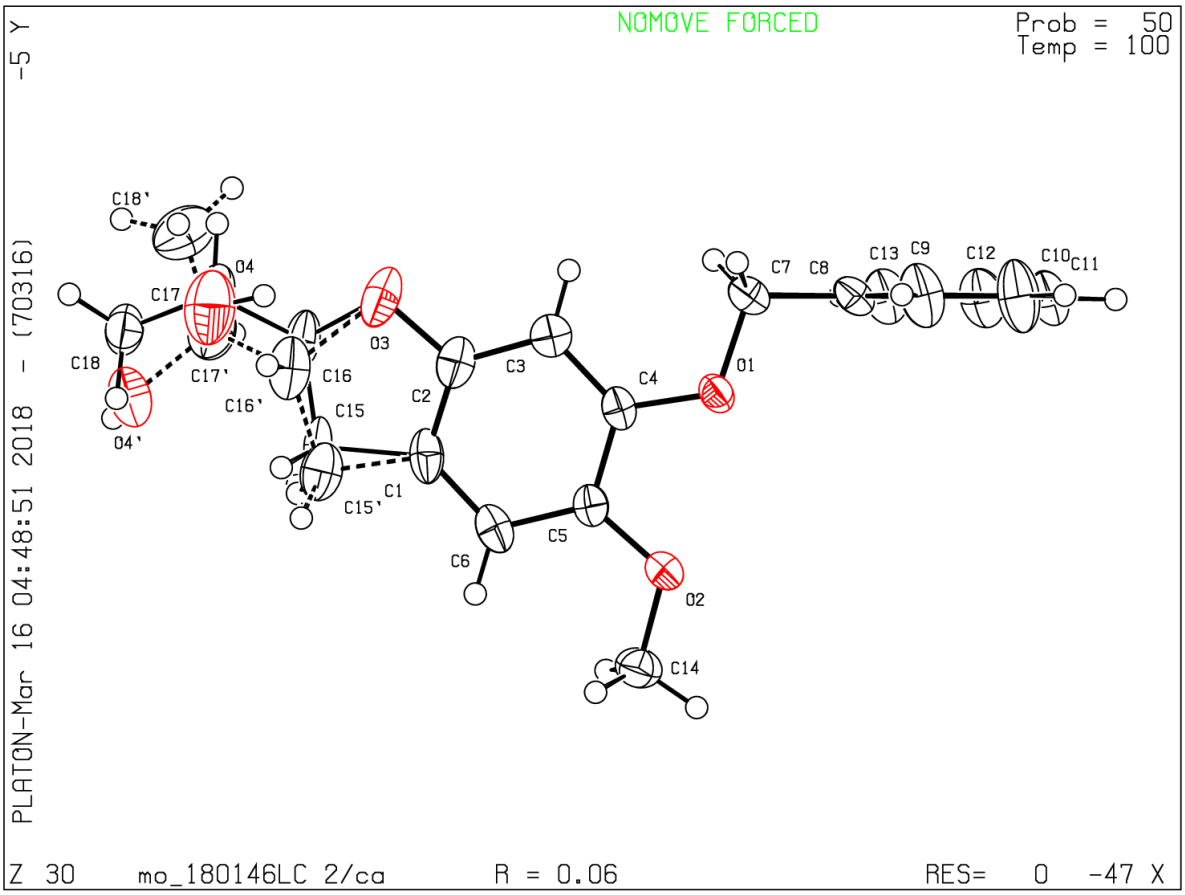
No syntax errors found. CIF dictionary Interpreting this report

Datablock: mo_180146LT_0m_a

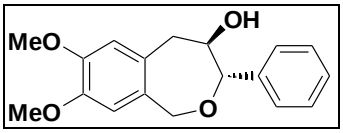
```
Bond precision:  C-C = 0.0035 A          Wavelength=0.71073

Cell:            a=22.457(3)     b=5.2177(7)         c=25.976(3)
                 alpha=90        beta=95.828(4)      gamma=90
Temperature:     100 K

                Calculated                Reported
Volume          3028.0(7)                 3028.0(7)
Space group     C 2/c                     C 2/c
Hall group      -C 2yc                    -C 2yc
Moiety formula  C18 H20 O4                ?
Sum formula     C18 H20 O4                C18 H20 O4
Mr              300.34                    300.34
Dx,g cm-3       1.318                     1.318
Z               8                         8
Mu (mm-1)       0.092                     0.092
F000            1280.0                    1280.0
F000'           1280.67
h,k,lmax        28,6,32                   28,6,32
Nref            3195                      3174
Tmin,Tmax       0.991,0.997               0.849,0.948
Tmin'           0.991

Correction method= # Reported T Limits: Tmin=0.849 Tmax=0.948
AbsCorr = MULTI-SCAN

Data completeness= 0.993          Theta(max)= 26.616

R(reflections)= 0.0561( 2079)     wR2(reflections)= 0.1661( 3174)

S = 1.057                  Npar= 250
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

The thermal ellipsoid was drawn at the 50% probability level



X-ray crystal data of 4a



Empirical formula	C18 H20 O4	
Formula weight	300.34	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 6.8432(2) Å	α = 90°.
	b = 18.7402(7) Å	β = 91.367(2)°.
	c = 11.7029(4) Å	γ = 90°.
Volume	1500.39(9) $Å^3$	
Z	4	
Density (calculated)	1.330 Mg/m^3	
Absorption coefficient	0.093 mm^{-1}	
F(000)	640	
Crystal size	0.20 x 0.18 x 0.10 mm^3	
Theta range for data collection	2.052 to 26.409°.	
Index ranges	-8<=h<=8, -23<=k<=23, -13<=l<=14	
Reflections collected	12349	
Independent reflections	3084 [R(int) = 0.0289]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9485 and 0.8686	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3084 / 0 / 204	
Goodness-of-fit on F^2	1.067	
Final R indices [I>2sigma(I)]	R1 = 0.0421, wR2 = 0.1042	
R indices (all data)	R1 = 0.0542, wR2 = 0.1116	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.279 and -0.248 e.$Å^{-3}$	

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 180414lt_0m

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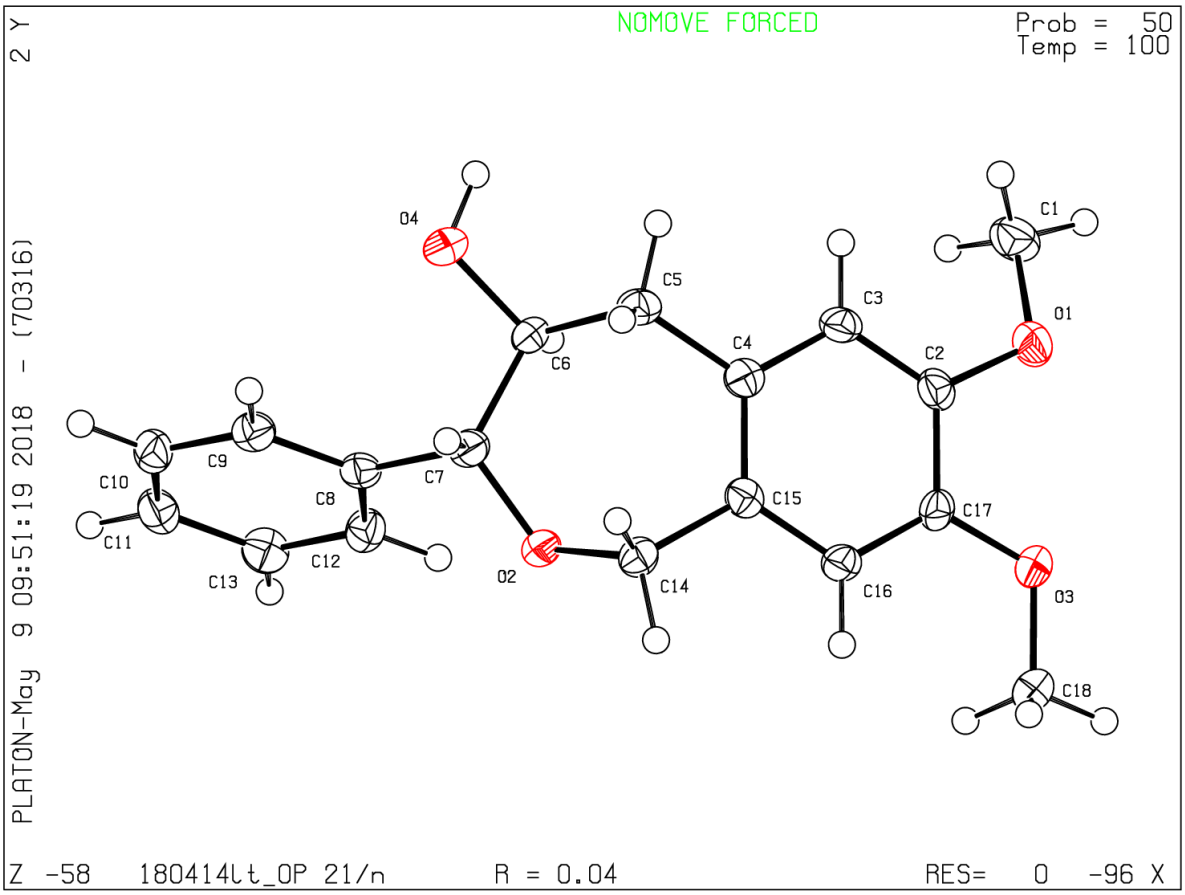
No syntax errors found. CIF dictionary Interpreting this report

Datablock: 180414lt_0m

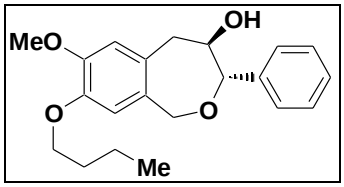
```
Bond precision:  C-C = 0.0020 A          Wavelength=0.71073

Cell:            a=6.8432(2)     b=18.7402(7)        c=11.7029(4)
                 alpha=90        beta=91.367(2)      gamma=90
Temperature:     100 K

                Calculated                Reported
Volume          1500.39(9)                1500.39(9)
Space group     P 21/n                    P 21/n
Hall group      -P 2yn                    -P 2yn
Moiety formula  C18 H20 O4                ?
Sum formula     C18 H20 O4                C18 H20 O4
Mr              300.34                    300.34
Dx,g cm-3       1.330                     1.330
Z               4                         4
Mu (mm-1)       0.093                     0.093
F000            640.0                     640.0
F000'           640.34
h,k,lmax        8,23,14                   8,23,14
Nref            3087                      3084
Tmin,Tmax       0.982,0.991               0.869,0.948
Tmin'           0.982

Correction method= # Reported T Limits: Tmin=0.869 Tmax=0.948
AbsCorr = MULTI-SCAN

Data completeness= 0.999          Theta(max)= 26.409

R(reflections)= 0.0421( 2510)     wR2(reflections)= 0.1116( 3084)

S = 1.067                  Npar= 204
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

The thermal ellipsoid was drawn at the 50% probability level



X-ray crystal data of 4d



Empirical formula	C21 H26 O4	
Formula weight	342.42	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 12.0101(14) Å	α = 90°.
	b = 10.6094(13) Å	β = 111.667(3)°.
	c = 15.9081(19) Å	γ = 90°.
Volume	1883.8(4) $Å^3$	
Z	4	
Density (calculated)	1.207 Mg/m^3	
Absorption coefficient	0.082 mm^{-1}	
F(000)	736	
Crystal size	0.25 x 0.23 x 0.22 mm^3	
Theta range for data collection	2.363 to 26.438°.	
Index ranges	-15<=h<=8, -13<=k<=13, -19<=l<=19	
Reflections collected	26303	
Independent reflections	3848 [R(int) = 0.0344]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9485 and 0.8852	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3848 / 0 / 231	
Goodness-of-fit on F^2	1.022	
Final R indices [I>2sigma(I)]	R1 = 0.0388, wR2 = 0.0968	
R indices (all data)	R1 = 0.0542, wR2 = 0.1079	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.320 and -0.242 e.$Å^{-3}$	

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Structure factors have been supplied for datablock(s) mo_180421lt_0m_a_sq

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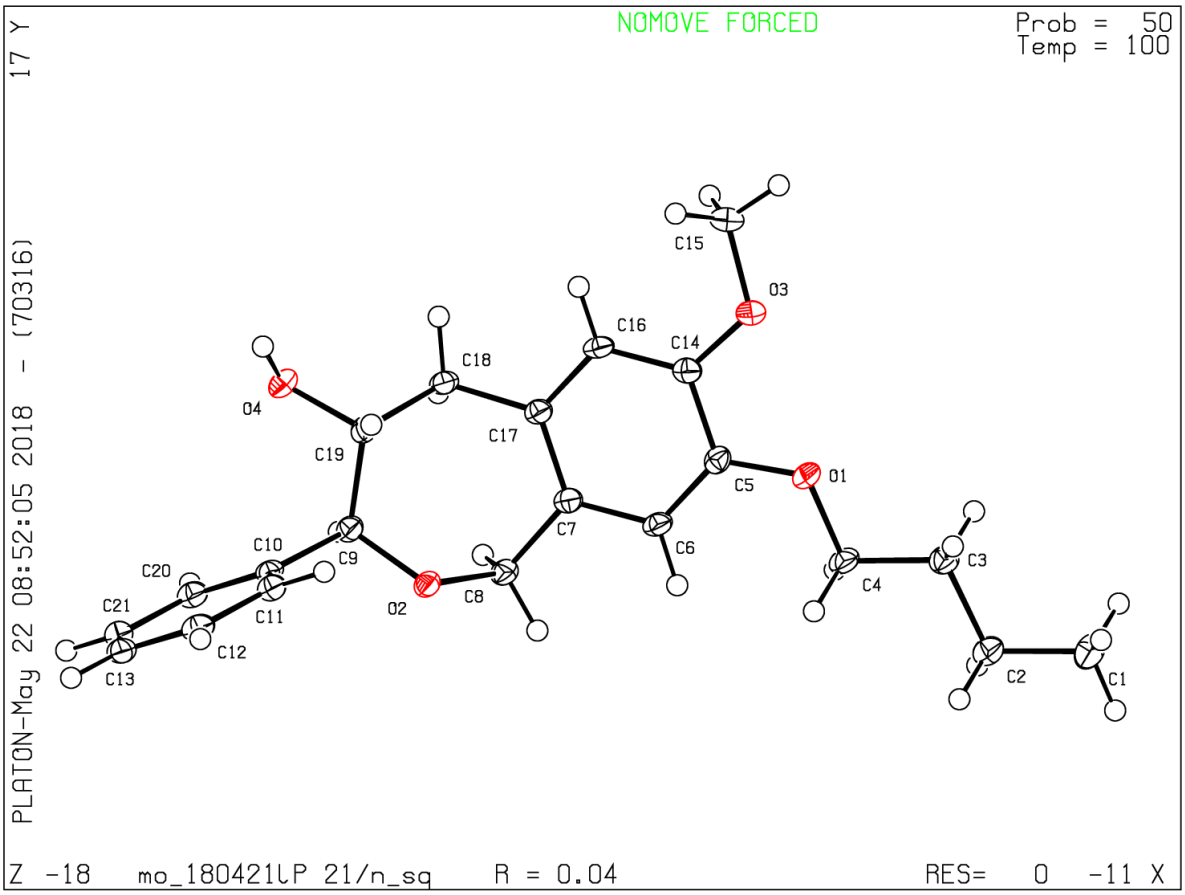
No syntax errors found. CIF dictionary Interpreting this report

Datablock: mo_180421lt_0m_a_sq

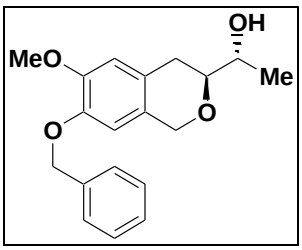
```
Bond precision:  C-C = 0.0021 A          Wavelength=0.71073

Cell:           a=12.0101(14)    b=10.6094(13)      c=15.9081(19)
                alpha=90         beta=111.667(3)    gamma=90
Temperature:    100 K

                Calculated                          Reported
Volume          1883.8(4)                           1883.8(4)
Space group     P 21/n                              P 21/n
Hall group      -P 2yn                              -P 2yn
Moiety formula  C21 H26 O4 [+ solvent]              ?
Sum formula     C21 H26 O4 [+ solvent]              C21 H26 O4
Mr              342.42                              342.42
Dx,g cm-3       1.207                               1.207
Z               4                                   4
Mu (mm-1)       0.082                               0.082
F000            736.0                               736.0
F000'           736.36
h,k,lmax        15,13,19                            15,13,19
Nref            3860                                3848
Tmin,Tmax       0.980,0.982                         0.885,0.948
Tmin'           0.980

Correction method= # Reported T Limits: Tmin=0.885 Tmax=0.948
AbsCorr = MULTI-SCAN

Data completeness= 0.997          Theta(max)= 26.438

R(reflections)= 0.0388( 3036)     wR2(reflections)= 0.1079( 3848)

S = 1.022                  Npar= 231
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

The thermal ellipsoid was drawn at the 50% probability level



X-ray crystal data of 5b



Empirical formula	C19 H23 O4.50	
Formula weight	323.37	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 35.856(6) Å	α = 90°.
	b = 5.1944(10) Å	β = 118.174(10)°.
	c = 19.808(3) Å	γ = 90°.
Volume	3252.1(10) $Å^3$	
Z	8	
Density (calculated)	1.321 Mg/m^3	
Absorption coefficient	0.093 mm^{-1}	
F(000)	1384	
Crystal size	0.20 x 0.15 x 0.15 mm^3	
Theta range for data collection	1.288 to 25.331°.	
Index ranges	-42<=h<=37, 0<=k<=6, 0<=l<=23	
Reflections collected	2882	
Independent reflections	2882 [R(int) = 0.0883]	
Completeness to theta = 25.000°	96.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9480 and 0.7442	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2882 / 177 / 217	
Goodness-of-fit on F^2	1.236	
Final R indices [I>2sigma(I)]	R1 = 0.1046, wR2 = 0.2618	
R indices (all data)	R1 = 0.1516, wR2 = 0.2804	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.511 and -0.400 e.$Å^{-3}$	

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) twin5

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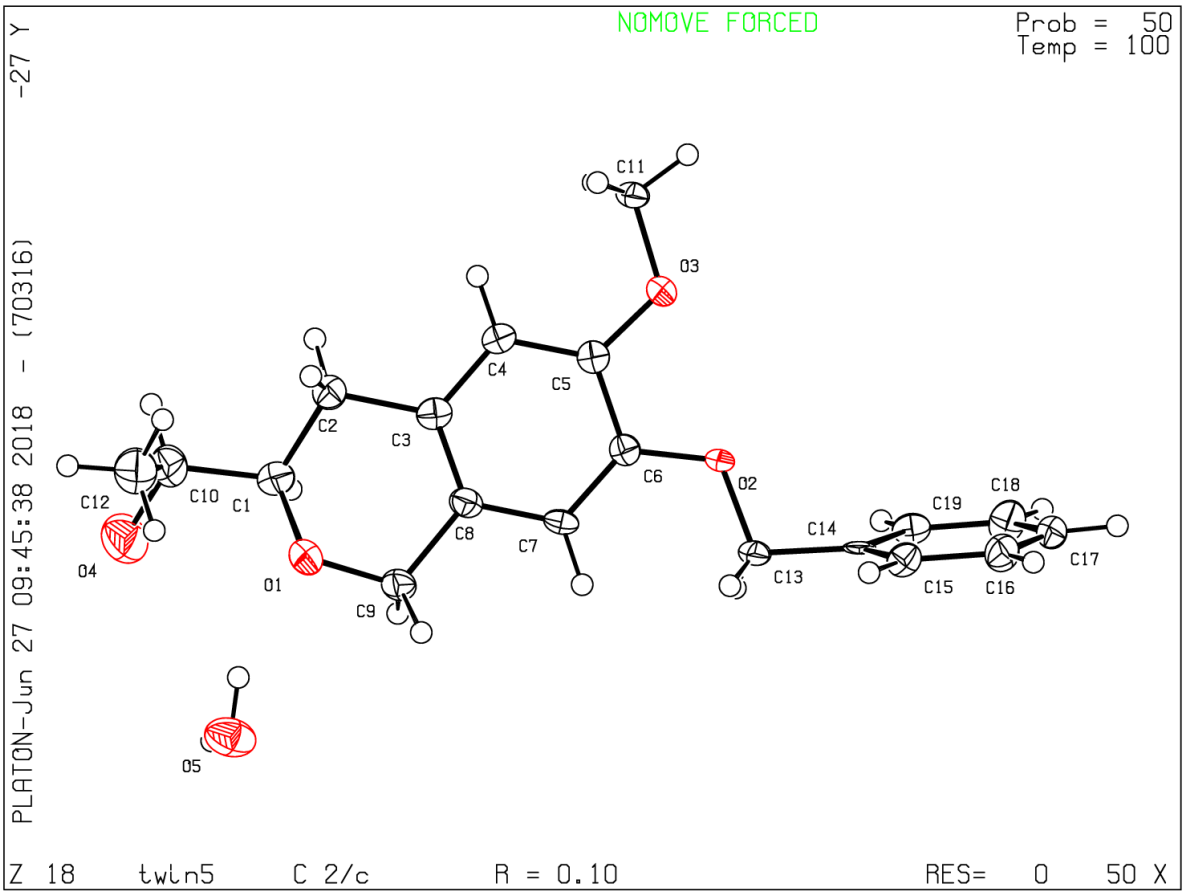
No syntax errors found. CIF dictionary Interpreting this report

Datablock: twin5

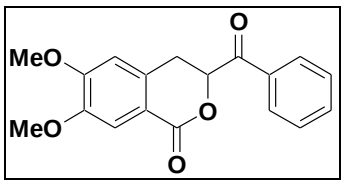
```
Bond precision:  C-C = 0.0148 A          Wavelength=0.71073

Cell:            a=35.856(6)    b=5.1944(10)          c=19.808(3)
                 alpha=90       beta=118.174(10)      gamma=90
Temperature:     100 K

                Calculated                Reported
Volume          3252.1(10)                3252.1(10)
Space group     C 2/c                     C 2/c
Hall group      -C 2yc                    -C 2yc
Moiety formula  2(C19 H22 O4), H2 O       ?
Sum formula     C38 H46 O9                C19 H23 O4.50
Mr              646.75                    323.37
Dx,g cm-3       1.321                     1.321
Z               4                         8
Mu (mm-1)       0.093                     0.093
F000            1384.0                    1384.0
F000'           1384.73
h,k,lmax        42,6,23                   42,6,23
Nref            2967                      2882
Tmin,Tmax       0.983,0.986               0.744,0.948
Tmin'           0.982

Correction method= # Reported T Limits: Tmin=0.744 Tmax=0.948
AbsCorr = MULTI-SCAN

Data completeness= 0.971          Theta(max)= 25.331

R(reflections)= 0.1046( 1937)     wR2(reflections)= 0.2804( 2882)

S = 1.236                  Npar= 217
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

The thermal ellipsoid was drawn at the 50% probability level



X-ray crystal data of 6a



Empirical formula	C18 H16 O5	
Formula weight	312.31	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 7.5282(6) Å	α = 93.465(4)°.
	b = 8.2601(7) Å	β = 104.206(3)°.
	c = 13.8286(12) Å	γ = 116.505(3)°.
Volume	731.54(11) $Å^3$	
Z	2	
Density (calculated)	1.418 Mg/m^3	
Absorption coefficient	0.104 mm^{-1}	
F(000)	328	
Crystal size	0.15 x 0.15 x 0.13 mm^3	
Theta range for data collection	2.810 to 26.406°.	
Index ranges	-9<=h<=9, -10<=k<=10, -17<=l<=16	
Reflections collected	12026	
Independent reflections	2958 [R(int) = 0.0274]	
Completeness to theta = 25.242°	98.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9485 and 0.8738	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2958 / 0 / 210	
Goodness-of-fit on F^2	1.134	
Final R indices [I>2sigma(I)]	R1 = 0.0392, wR2 = 0.1054	
R indices (all data)	R1 = 0.0427, wR2 = 0.1079	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.321 and -0.247 e.$Å^{-3}$	

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 180506LT_0m

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: 180506LT_0m

```
Bond precision:  C-C = 0.0020 A          Wavelength=0.71073

Cell:          a=7.5282(6)       b=8.2601(7)       c=13.8286(12)
               alpha=93.465(4)   beta=104.206(3)   gamma=116.505(3)
Temperature:   100 K

                Calculated                Reported
Volume          731.54(11)                731.54(11)
Space group     P -1                      P -1
Hall group      -P 1                      -P 1
Moiety formula  C18 H16 O5                ?
Sum formula     C18 H16 O5                C18 H16 O5
Mr              312.31                    312.31
Dx,g cm-3       1.418                     1.418
Z               2                         2
Mu (mm-1)       0.104                     0.104
F000            328.0                     328.0
F000'           328.19
h,k,lmax        9,10,17                   9,10,17
Nref            3018                      2958
Tmin,Tmax       0.985,0.987               0.874,0.948
Tmin'           0.985

Correction method= # Reported T Limits: Tmin=0.874 Tmax=0.948
AbsCorr = MULTI-SCAN

Data completeness= 0.980          Theta(max)= 26.406

R(reflections)= 0.0392( 2663)     wR2(reflections)= 0.1079( 2958)

S = 1.134                  Npar= 210
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

The thermal ellipsoid was drawn at the 50% probability level