

Supporting Information

Stereocontrolled Construction of 1-Vinyllindanes via Intramolecular Cyclization of o-Cinnamyl Chalcones

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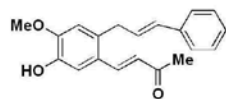
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Compound 4a (¹H-NMR spectral data)

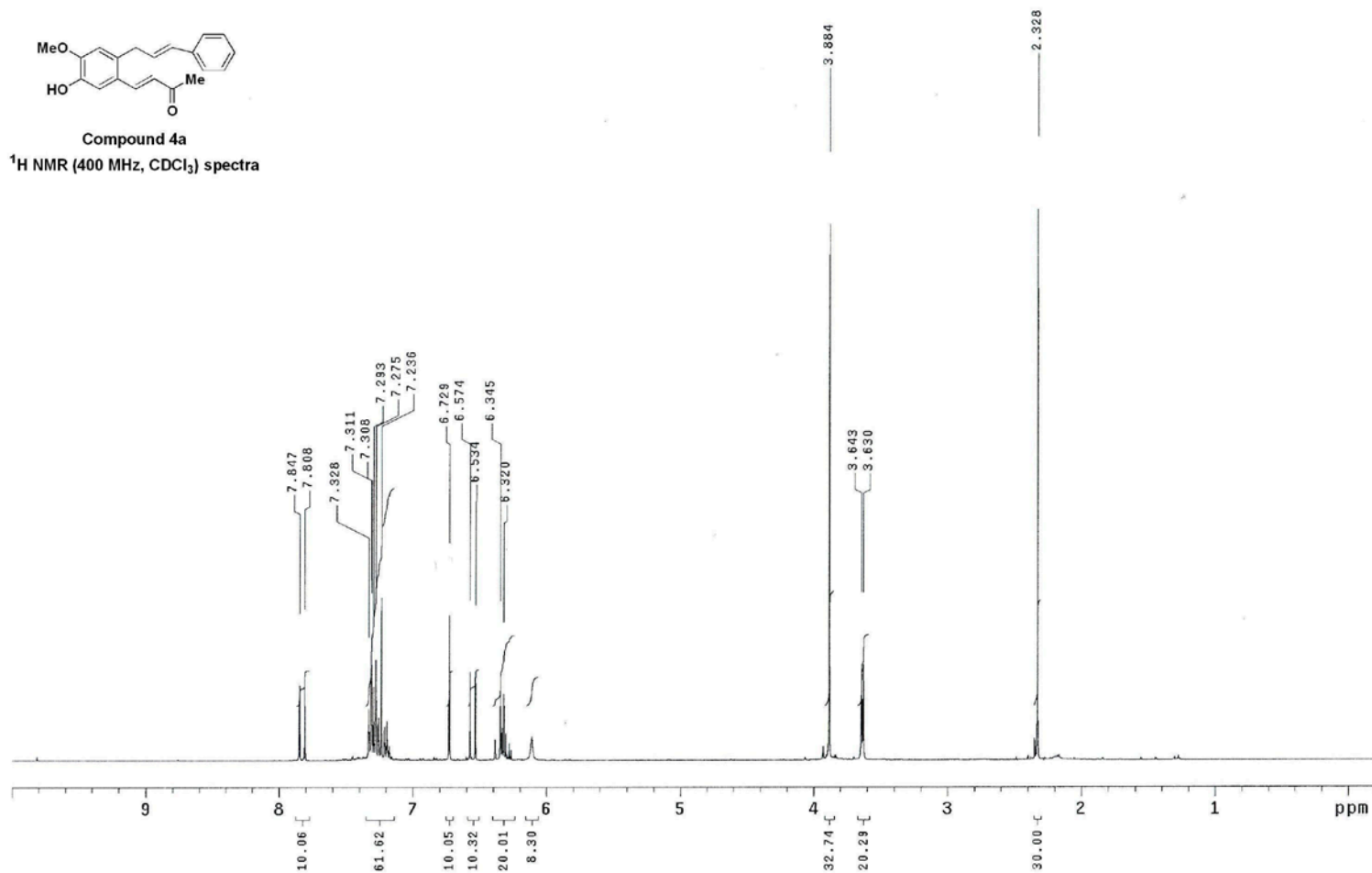
KS1060822

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Aug 24 2017
Solvent: CDCl₃
Ambient temperature
Total 32 repetitions



Compound 4a

¹H NMR (400 MHz, CDCl₃) spectra



Compound 4a (¹³C-NMR spectral data)

KS1060822

Pulse Sequence: s2pu1

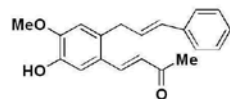
UNITYplus-400 "unity400"

Date: Aug 24 2017

Solvent: CDCl₃

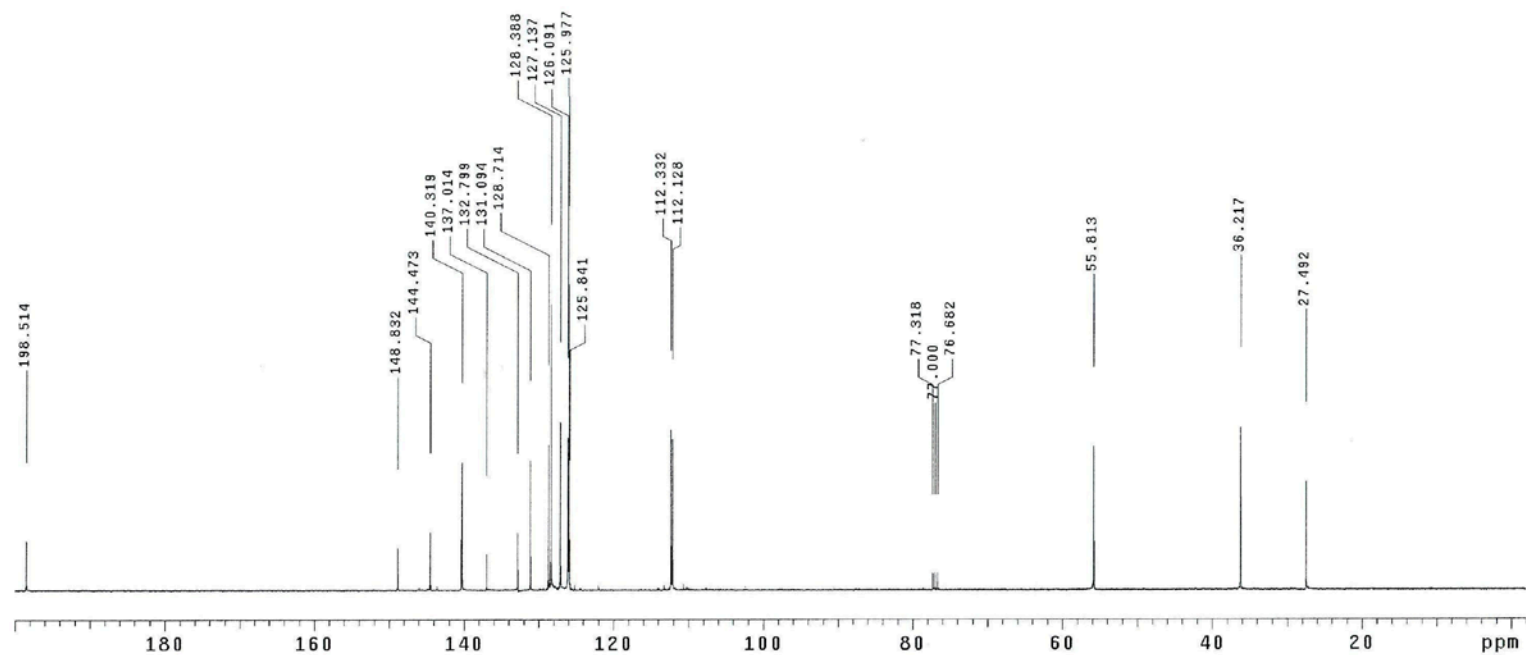
Ambient temperature

Total 1312 repetitions



Compound 4a

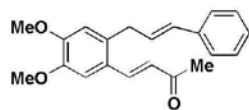
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4b (¹H-NMR spectral data)

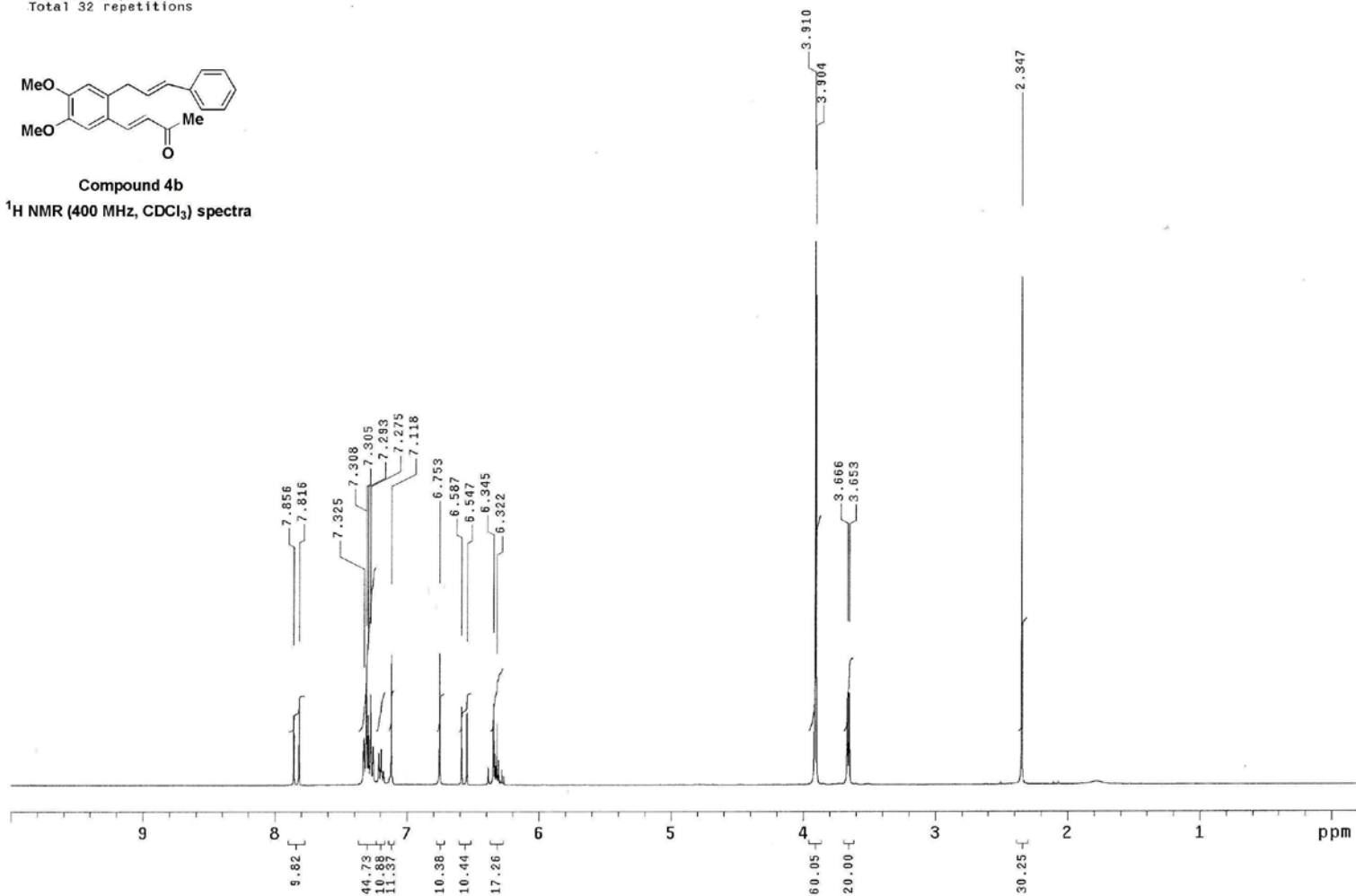
NC1060904

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Sep 4 2017
Solvent: CDCl₃
Ambient temperature
Total 32 repetitions



Compound 4b

¹H NMR (400 MHz, CDCl₃) spectra



Compound 4b (¹³C-NMR spectral data)

NC1060904

Pulse Sequence: s2pu1

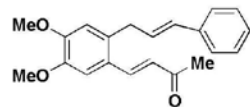
UNITYplus-400 "unity400"

Date: Sep 4 2017

Solvent: CDCl₃

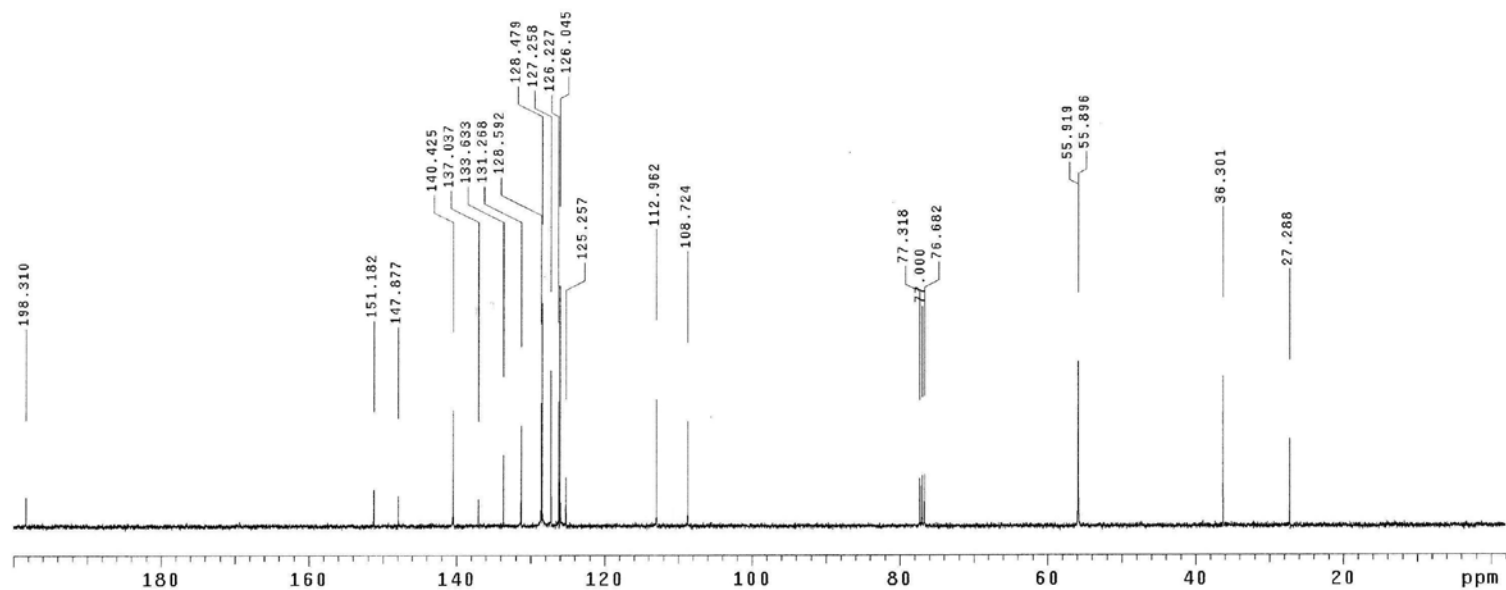
Ambient temperature

Total 544 repetitions



Compound 4b

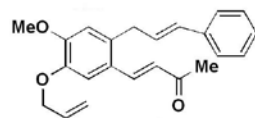
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4c (¹H-NMR spectral data)

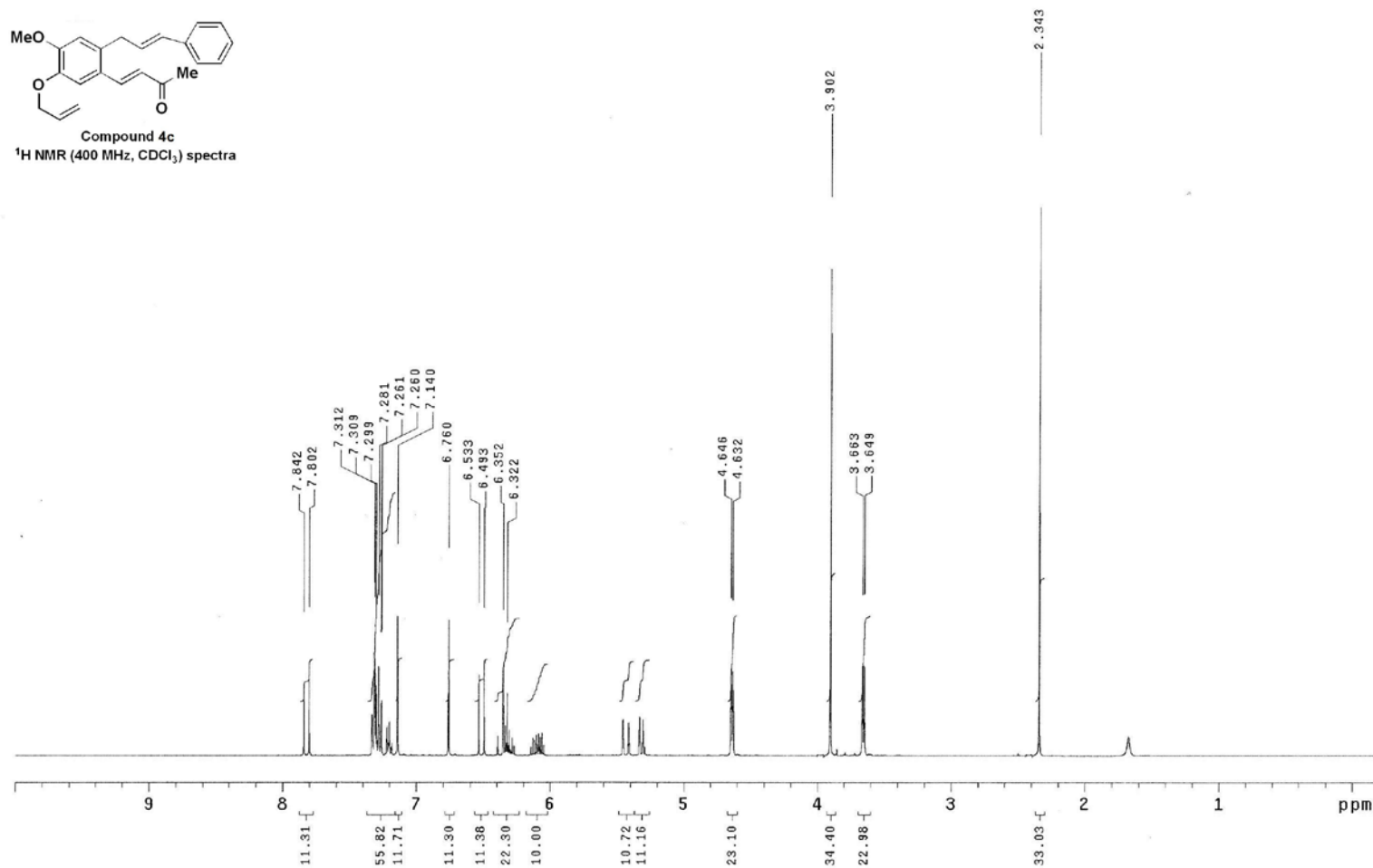
KSA01

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Sep 22 2017
Solvent: CDCl₃
Ambient temperature
Total 32 repetitions



Compound 4c

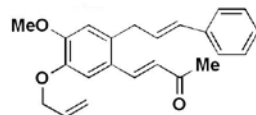
¹H NMR (400 MHz, CDCl₃) spectra



Compound 4c (¹³C-NMR spectral data)

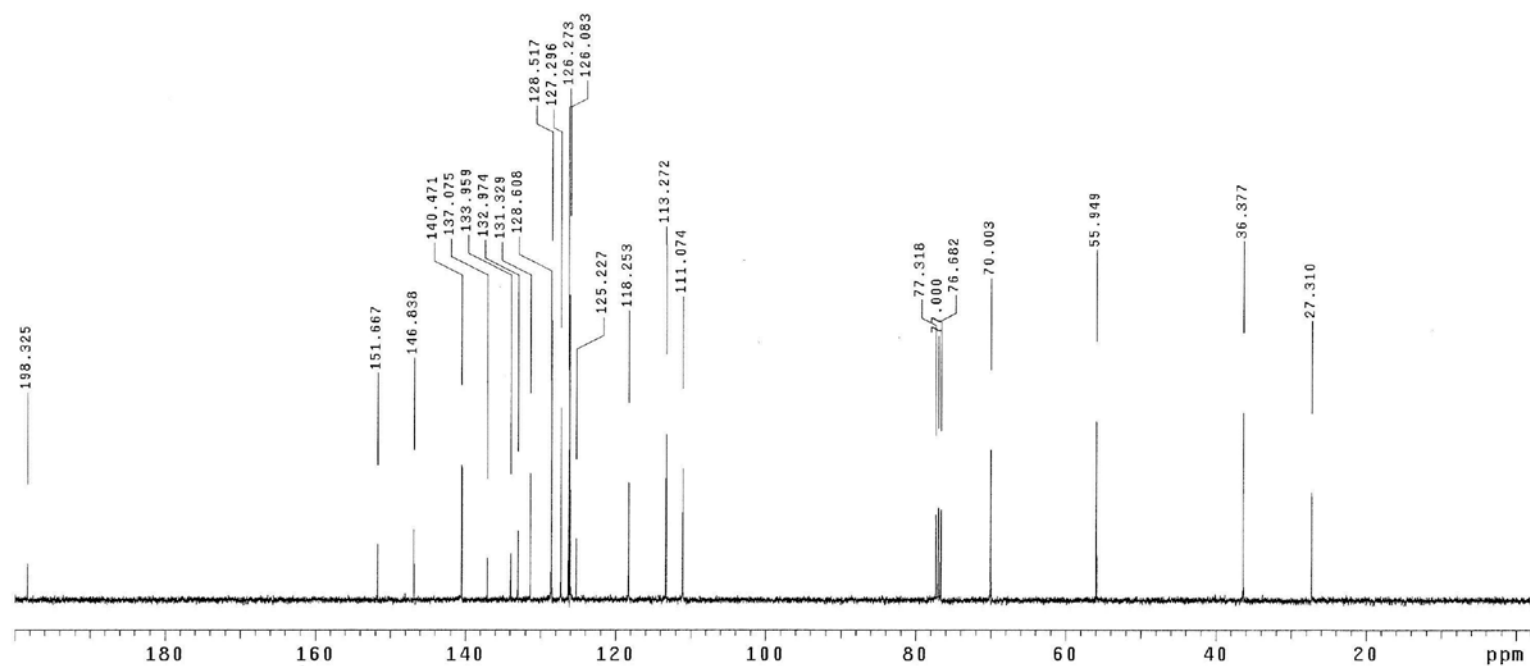
KSA01

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Sep 22 2017
Solvent: CDCl₃
Ambient temperature
Total 1056 repetitions



Compound 4c

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4d (¹H-NMR spectral data)

KSA03

Pulse Sequence: s2pu1

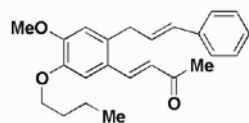
UNITYplus-400 "unity400"

Date: Sep 28 2017

Solvent: CDCl₃

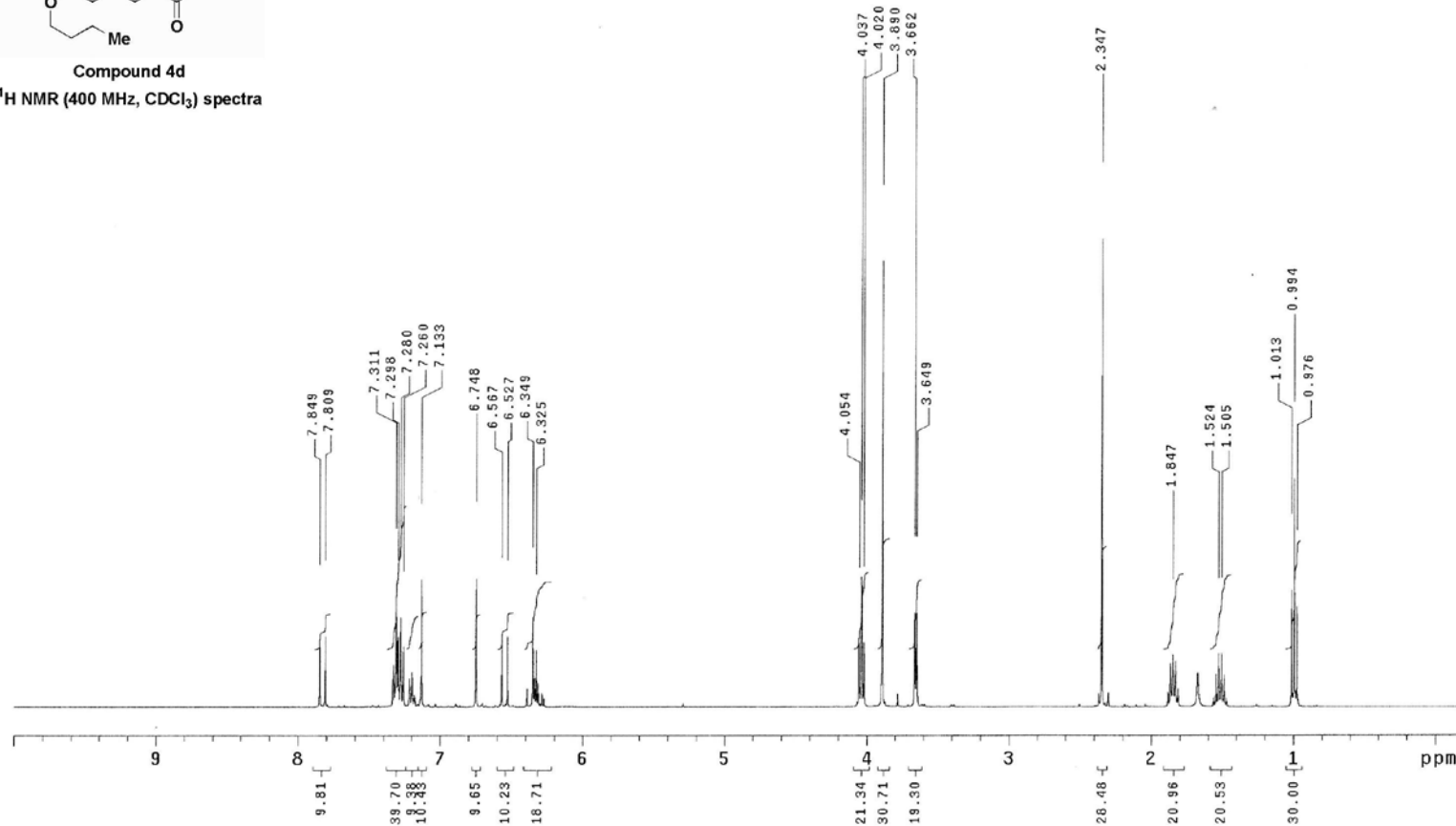
Ambient temperature

Total 32 repetitions



Compound 4d

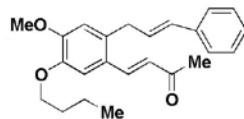
¹H NMR (400 MHz, CDCl₃) spectra



Compound 4d (¹³C-NMR spectral data)

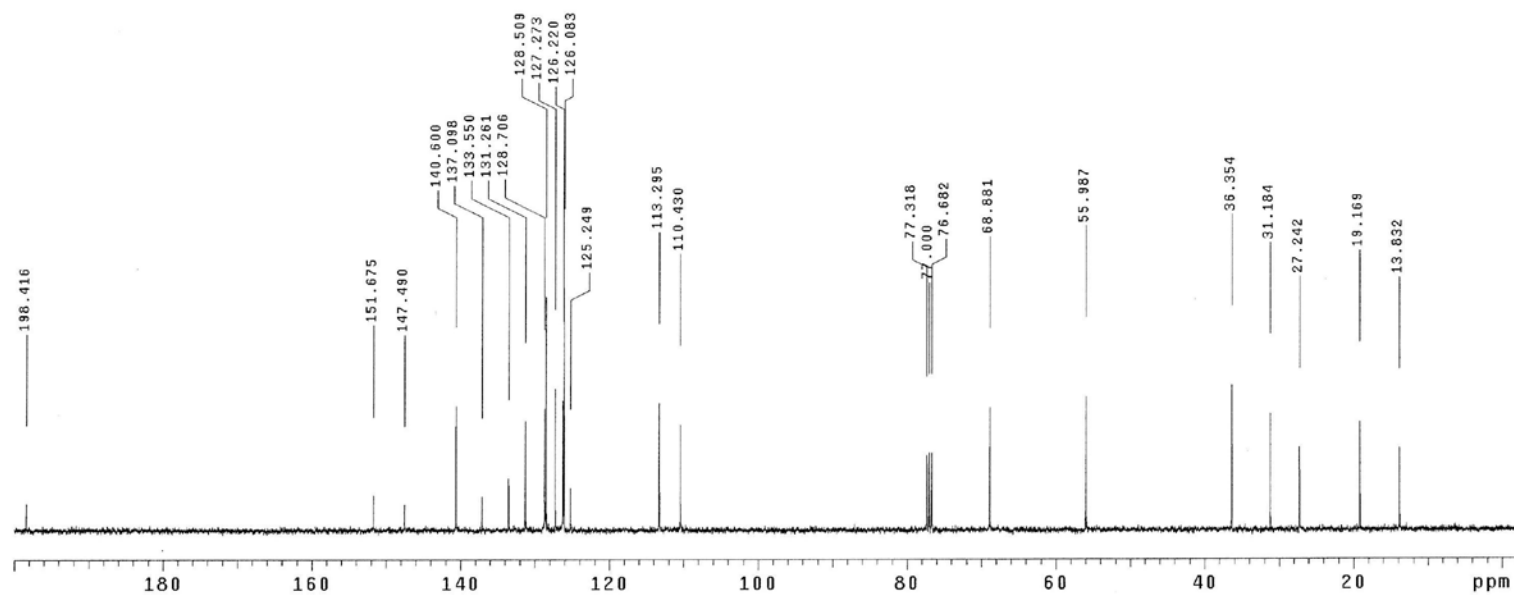
KSA03

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Sep 28 2017
Solvent: CDCl₃
Ambient temperature
Total 1040 repetitions



Compound 4d

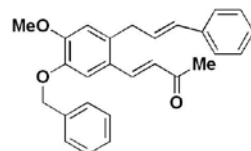
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4e (¹H-NMR spectral data)

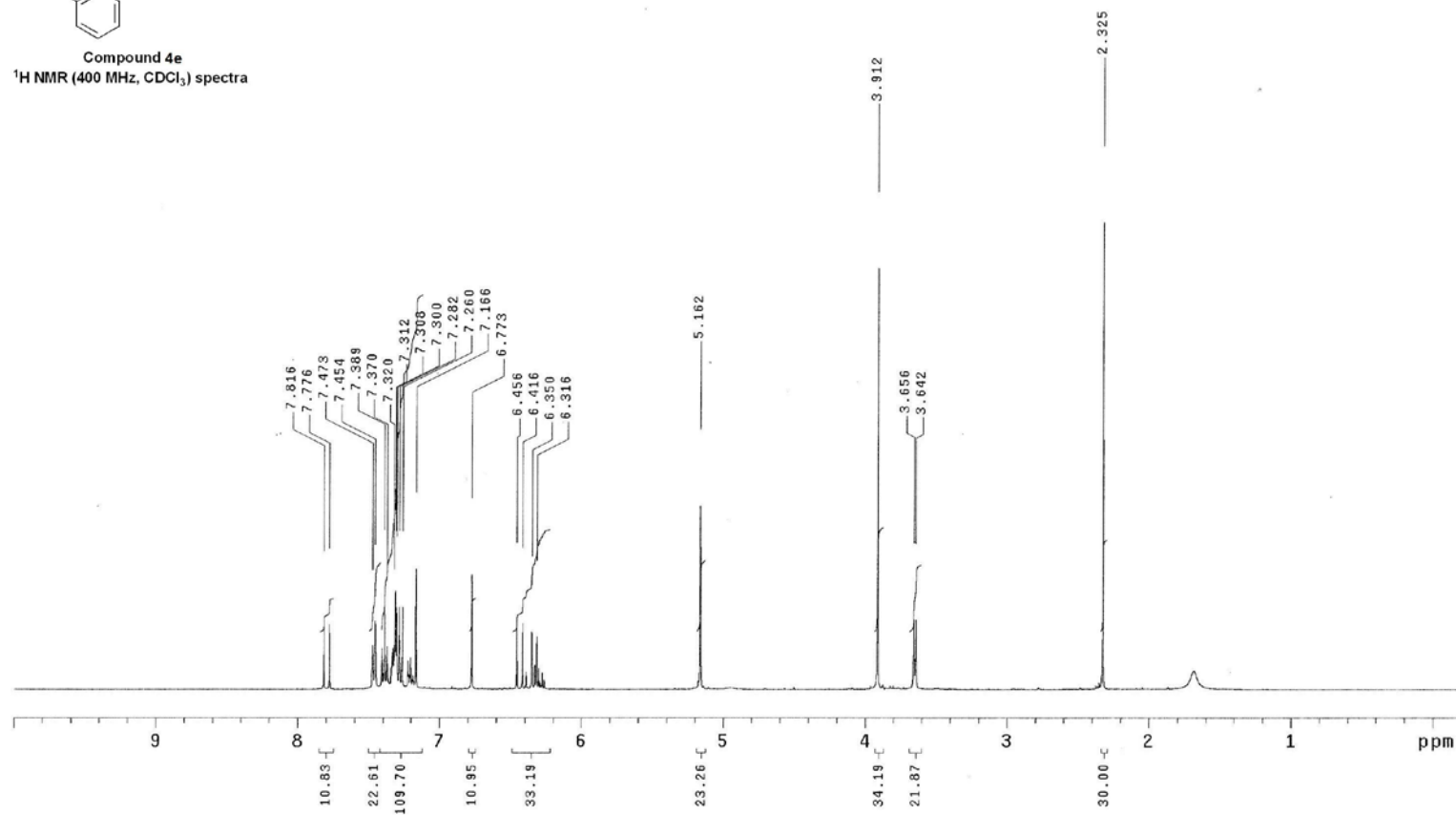
KSA02

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Sep 22 2017
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetitions



Compound 4e

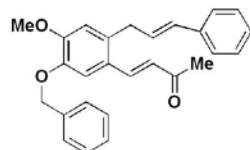
¹H NMR (400 MHz, CDCl₃) spectra



Compound 4e (¹³C-NMR spectral data)

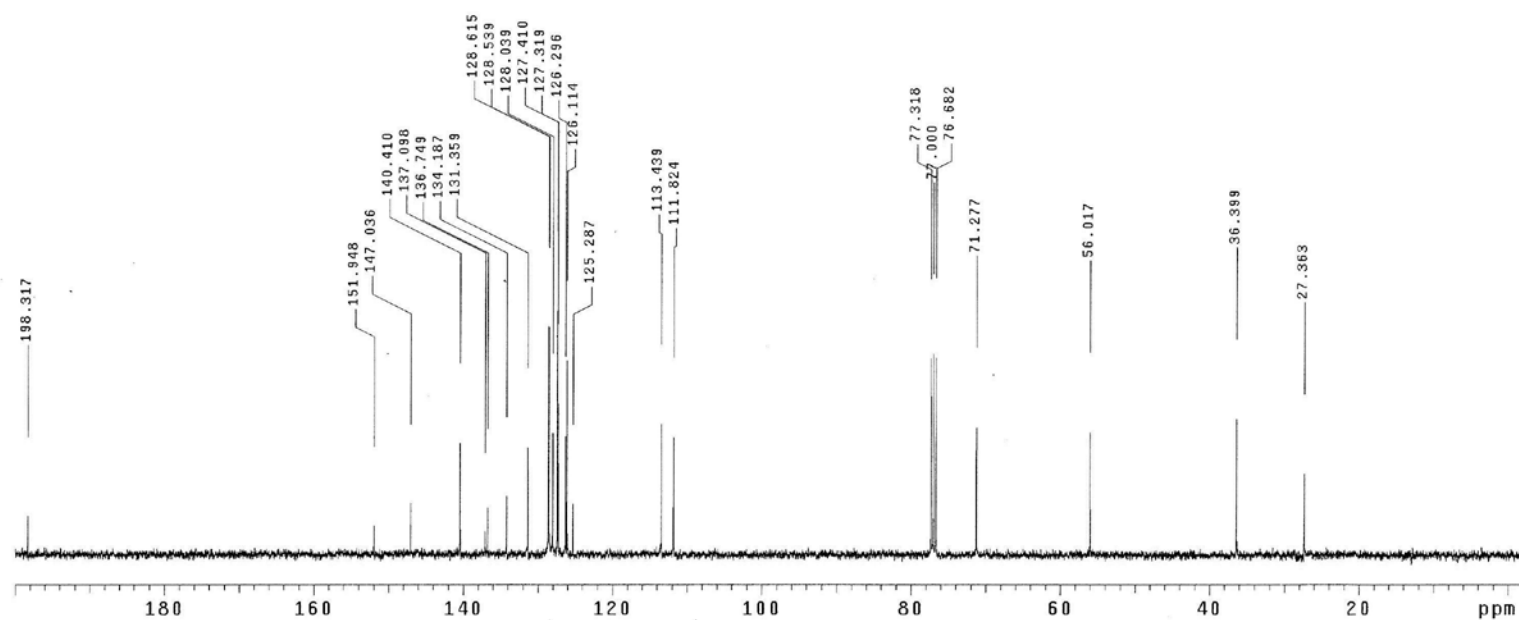
KSA02

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Sep 22 2017
Solvent: CDCl₃
Ambient temperature
Total 2608 repetitions



Compound 4e

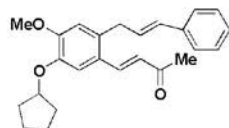
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4f (¹H-NMR spectral data)

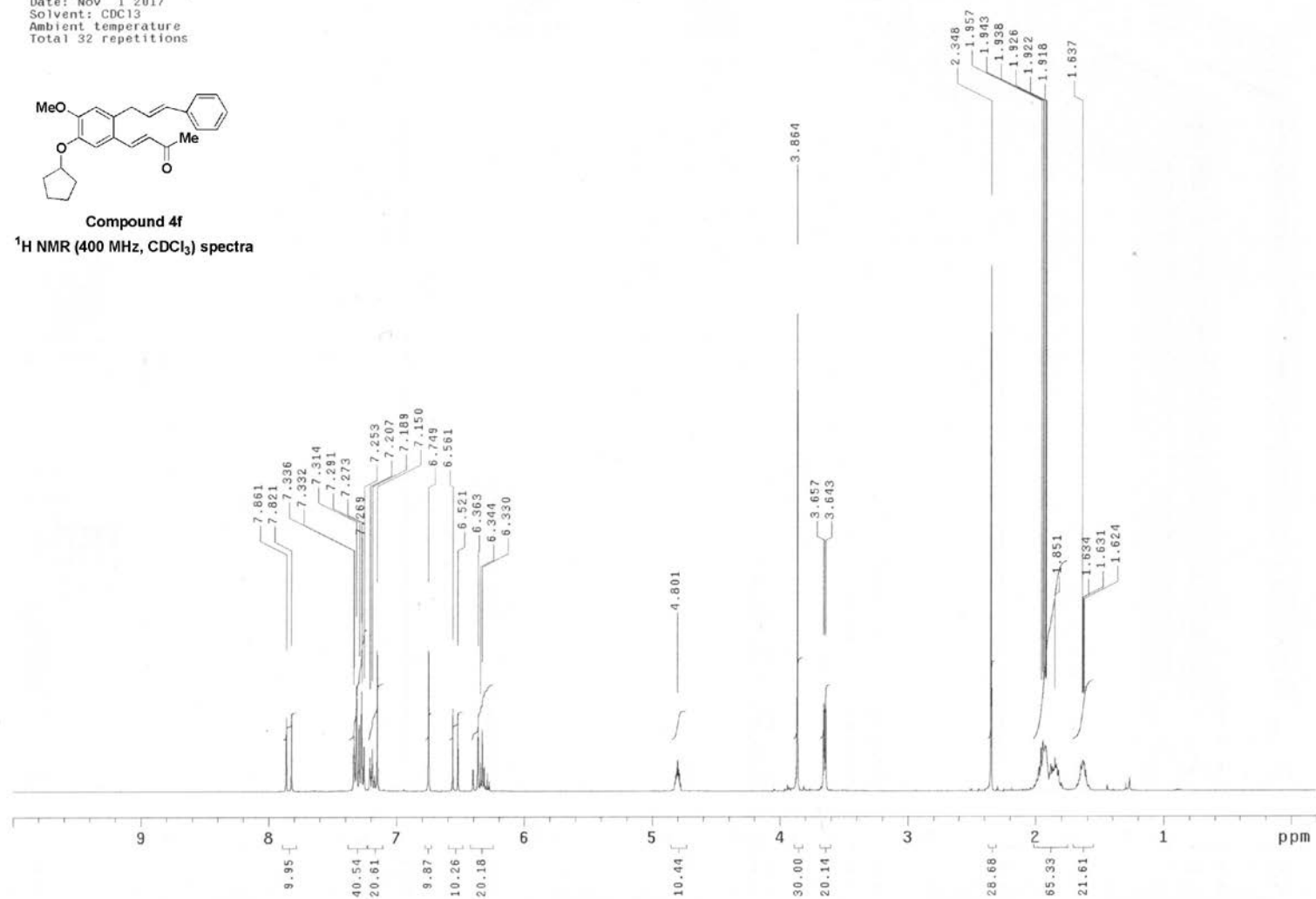
KS1061031

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Nov 1 2017
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetitions



Compound 4f

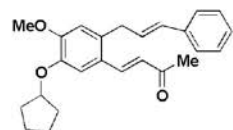
¹H NMR (400 MHz, CDCl₃) spectra



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

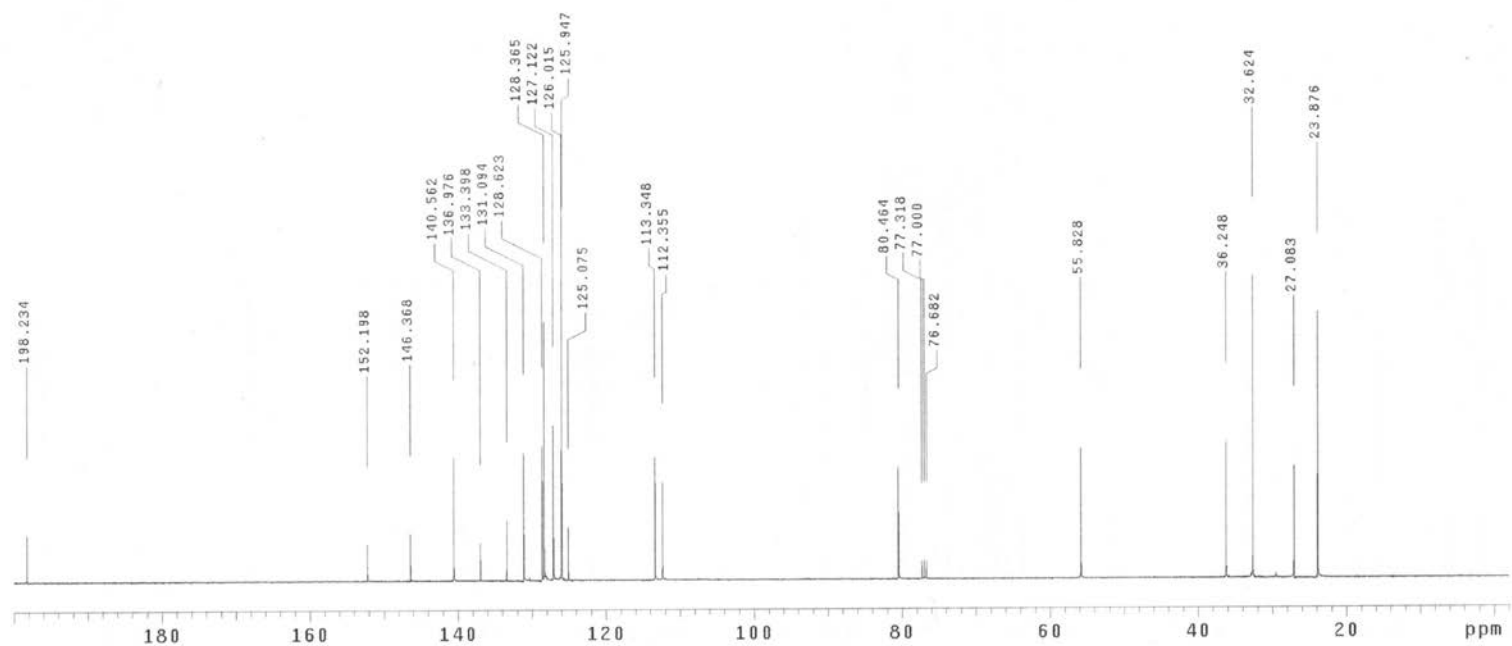
KS1061031

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Nov 1 2017
Solvent: CDCl₃
Ambient temperature
Total 32000 repetitions



Compound 4f

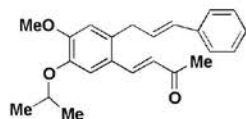
^{13}C NMR (100 MHz, CDCl₃) spectra



Compound 4g (¹H-NMR spectral data)

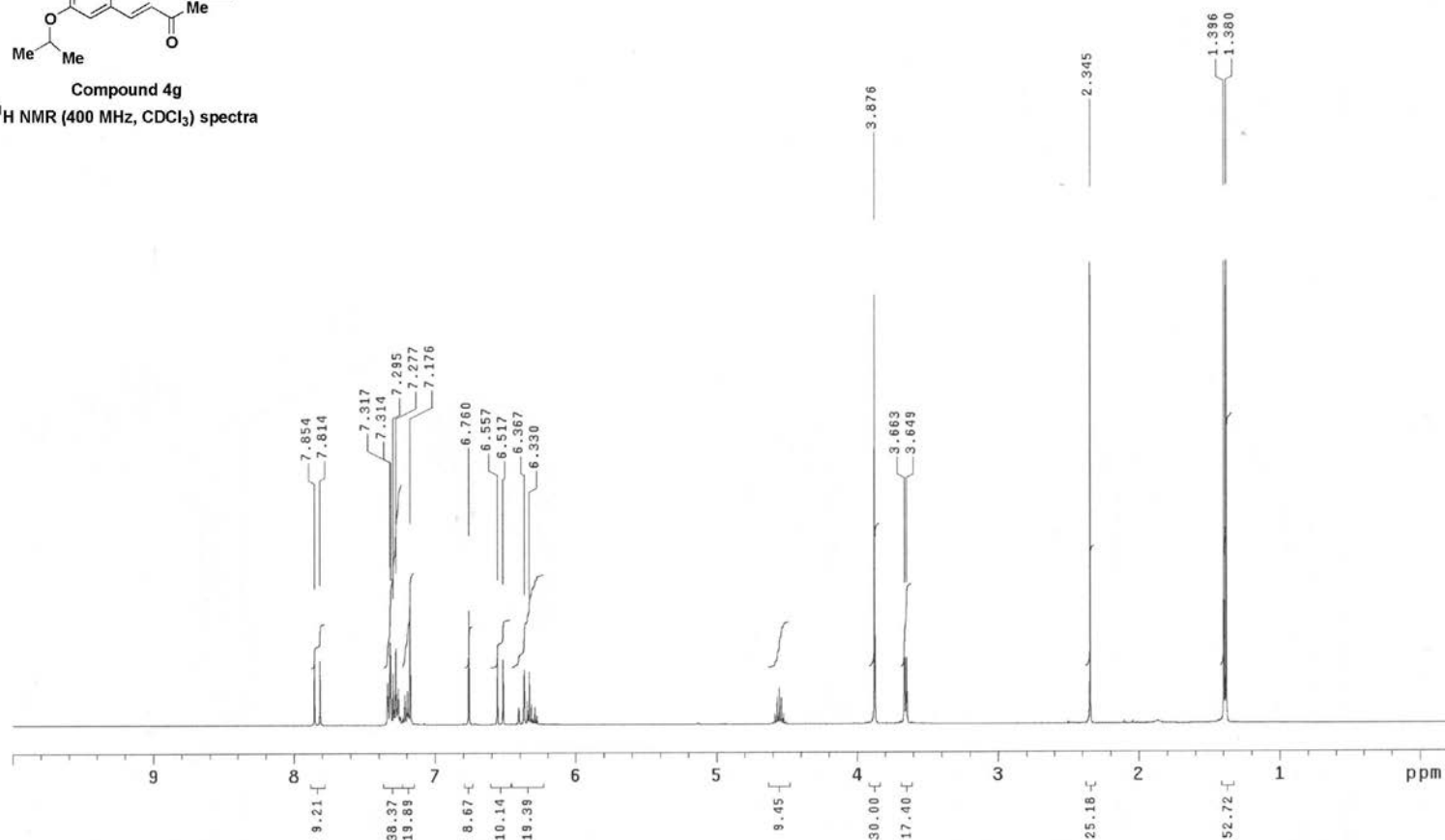
NC1070103

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Jan 4 2018
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetitions



Compound 4g

¹H NMR (400 MHz, CDCl₃) spectra



Compound 4g (¹³C-NMR spectral data)

NC1070103

Pulse Sequence: s2pu1

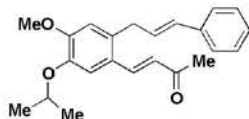
UNITYplus-400 "unity400"

Date: Jan 4 2018

Solvent: CDCl₃

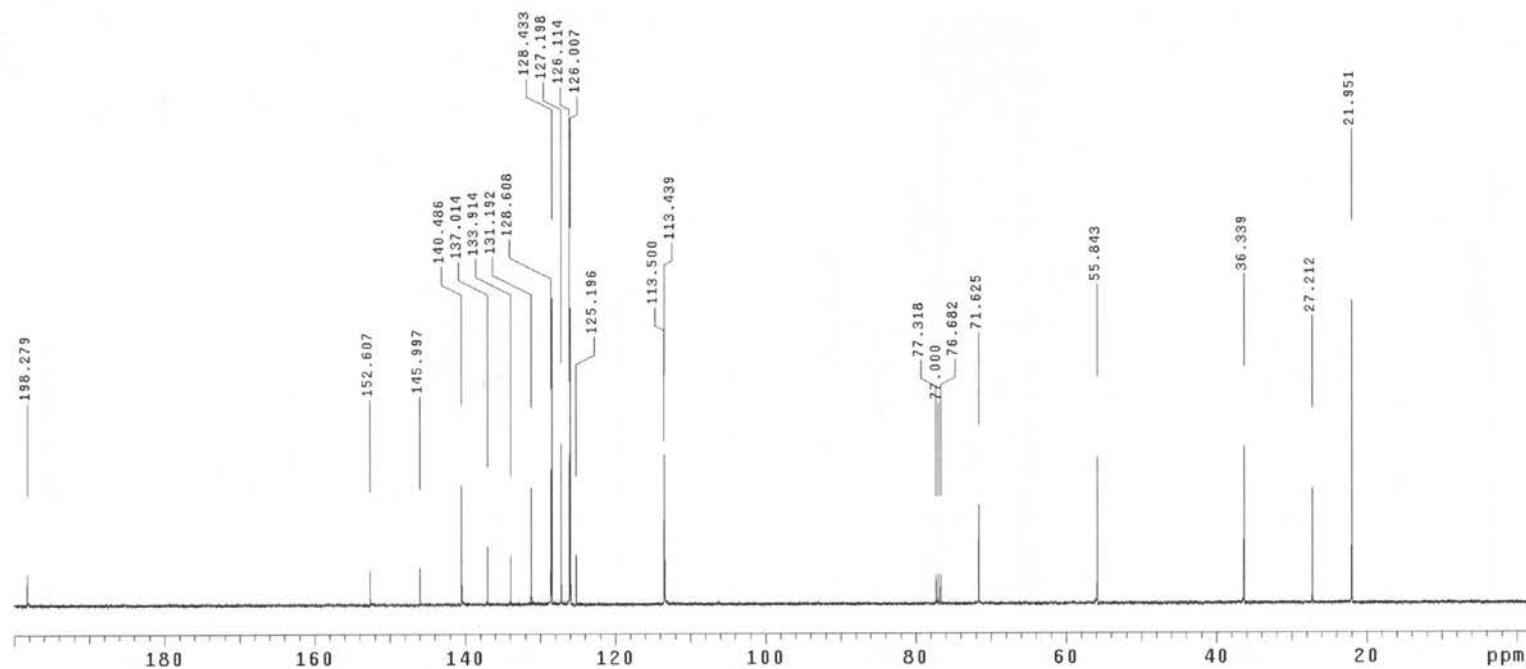
Ambient temperature

Total 512 repetitions



Compound 4g

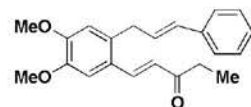
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4h (¹H-NMR spectral data)

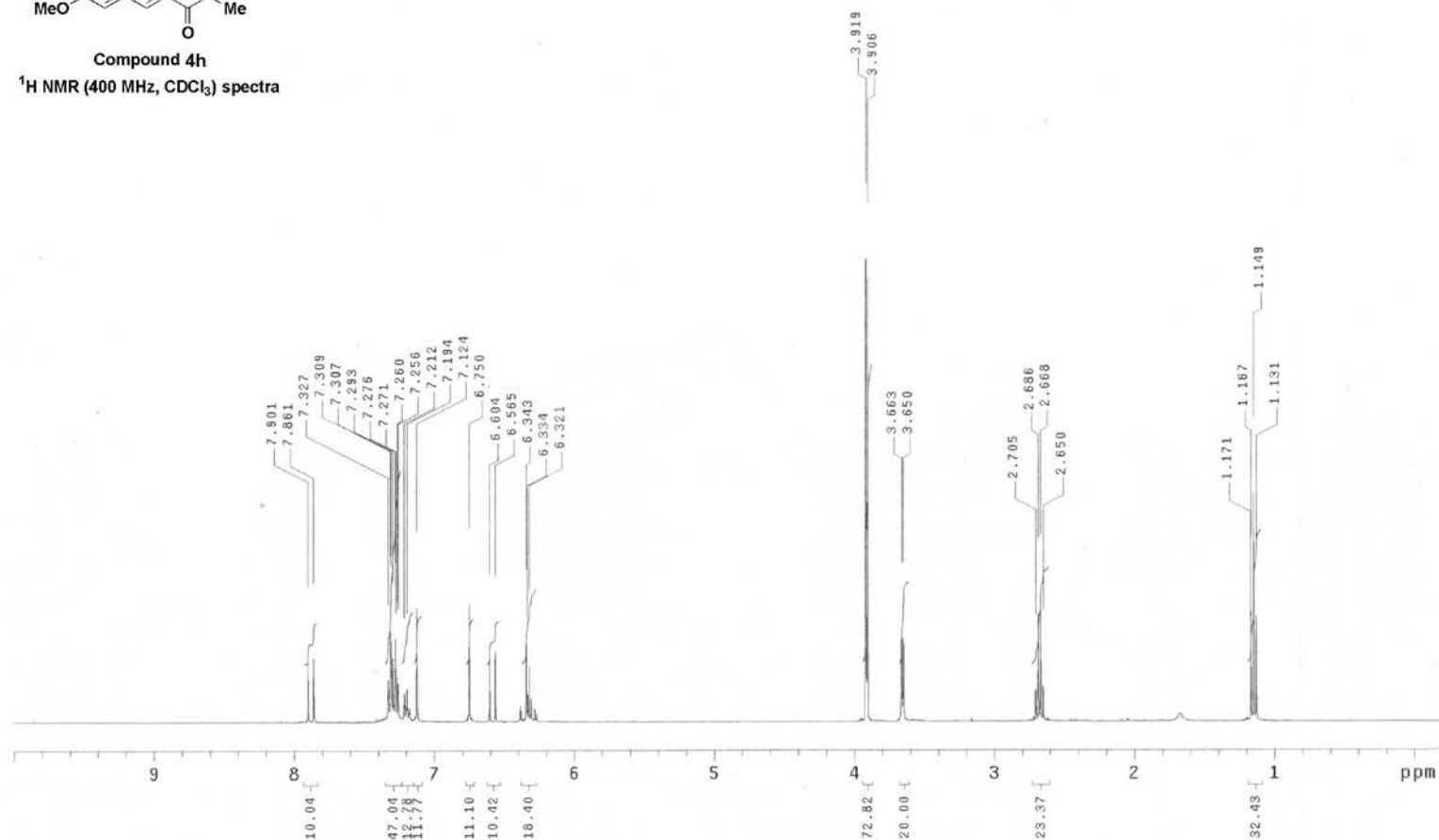
KS1061106

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Nov 7 2017
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetitions



Compound 4h

¹H NMR (400 MHz, CDCl₃) spectra



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

KS1061106

Pulse Sequence: s2pu1

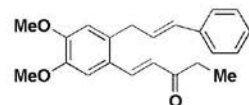
UNITYplus-400 "unity400"

Date: Nov 7 2017

Solvent: CDCl_3

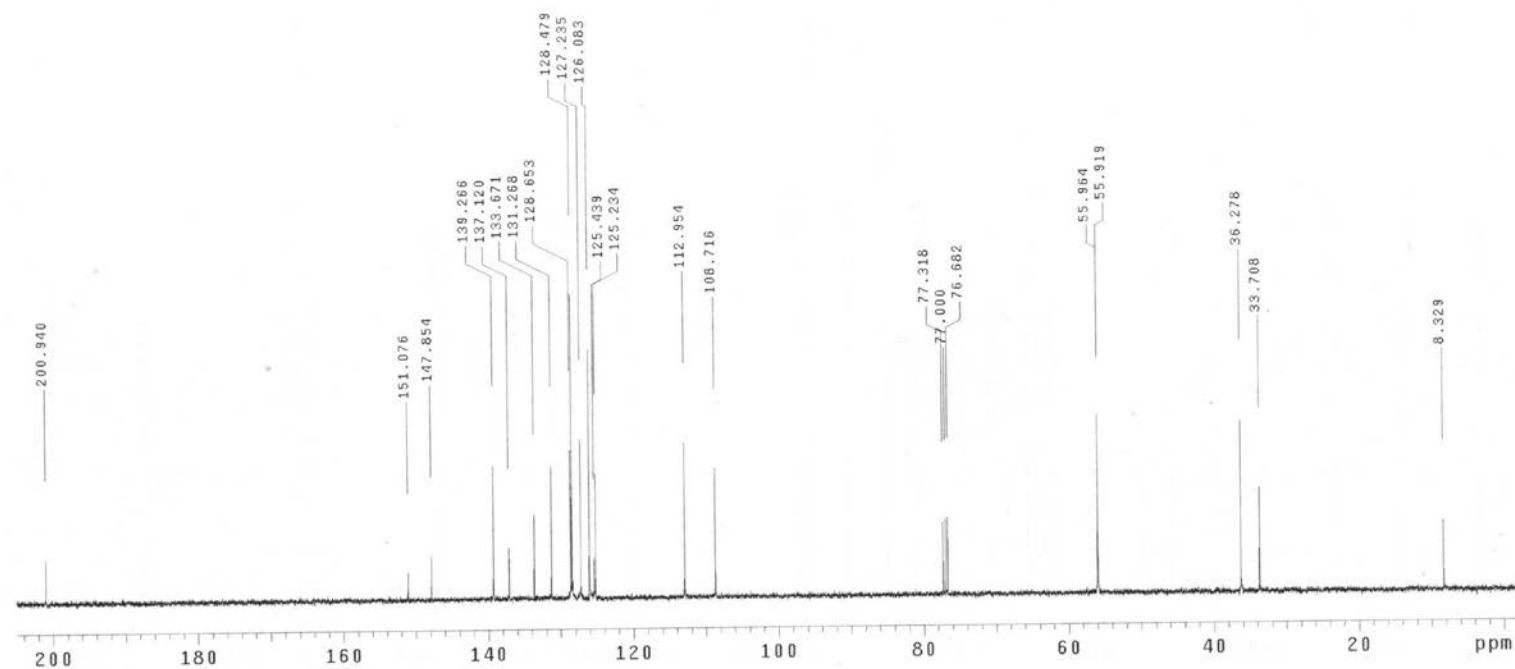
Ambient temperature

Total 1408 repetitions



Compound 4h

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



Compound 4i (¹H-NMR spectral data)

KS1061113

Pulse Sequence: s2pu1

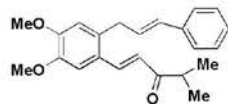
UNITYplus-400 "unity400"

Date: Nov 14 2017

Solvent: CDCl₃

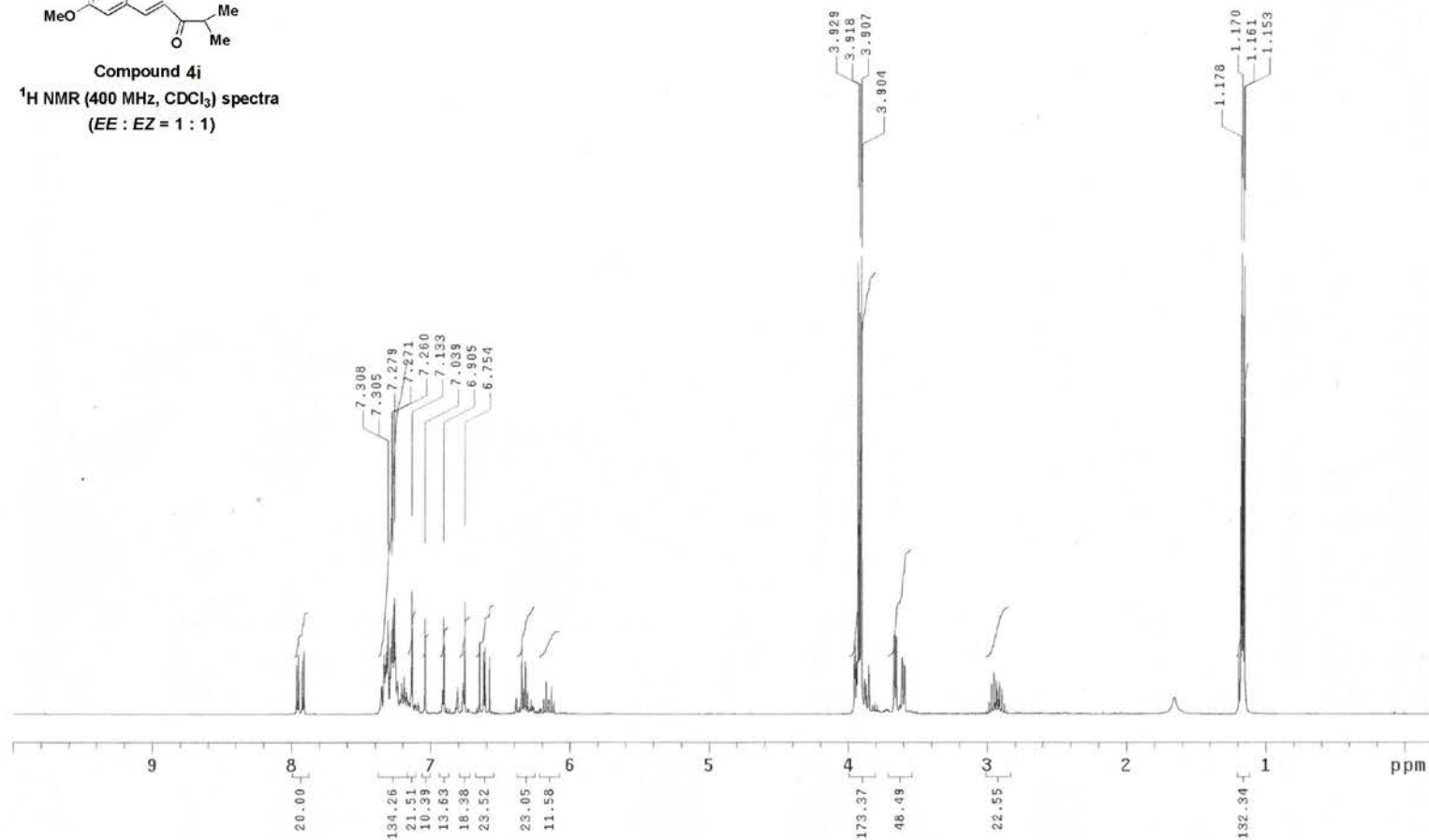
Ambient temperature

Total 32 repetitions



Compound 4i

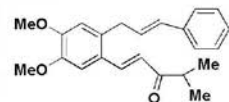
¹H NMR (400 MHz, CDCl₃) spectra
(EE : EZ = 1 : 1)



Compound 4i (¹³C-NMR spectral data)

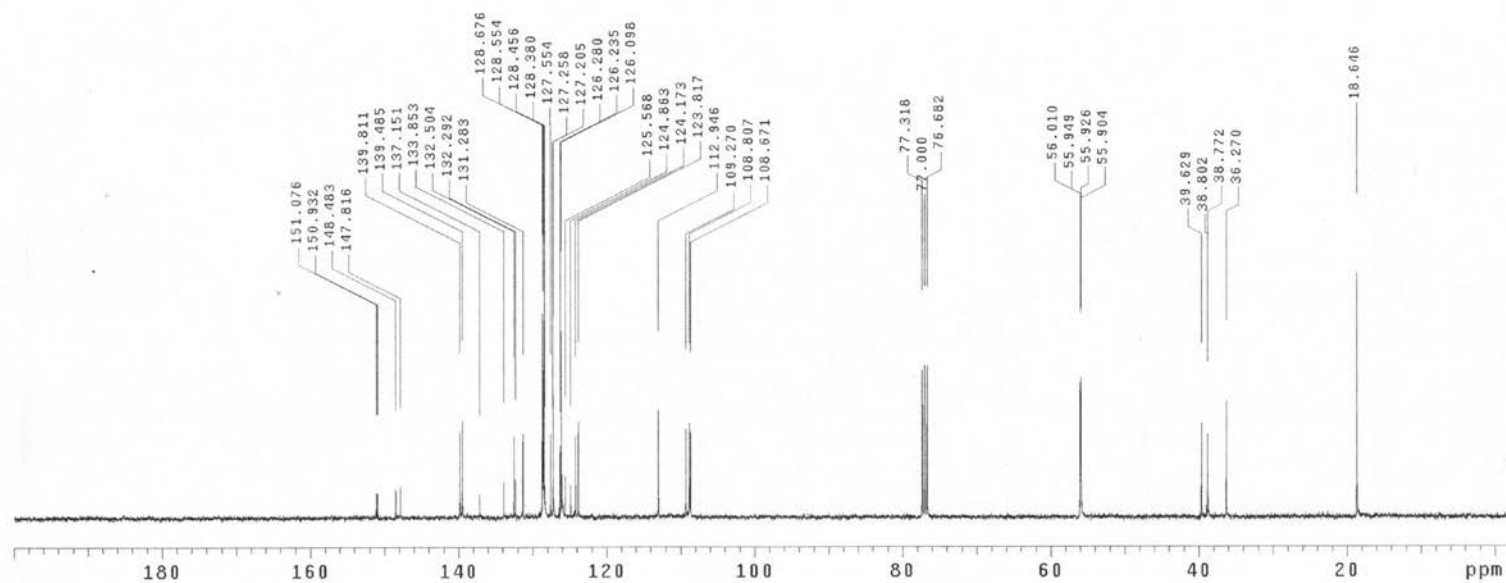
KS1061113

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Nov 14 2017
Solvent: CDCl₃
Ambient temperature
Total 4896 repetitions



Compound 4i

¹³C NMR (100 MHz, CDCl₃) spectra
(EE : EZ = 1 : 1)



Compound 4j (¹H-NMR spectral data)

KS1061108

Pulse Sequence: s2pul

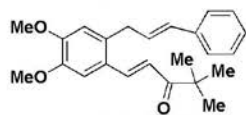
UNITYplus-400 "unity400"

Date: Nov 16 2017

Solvent: CDCl₃

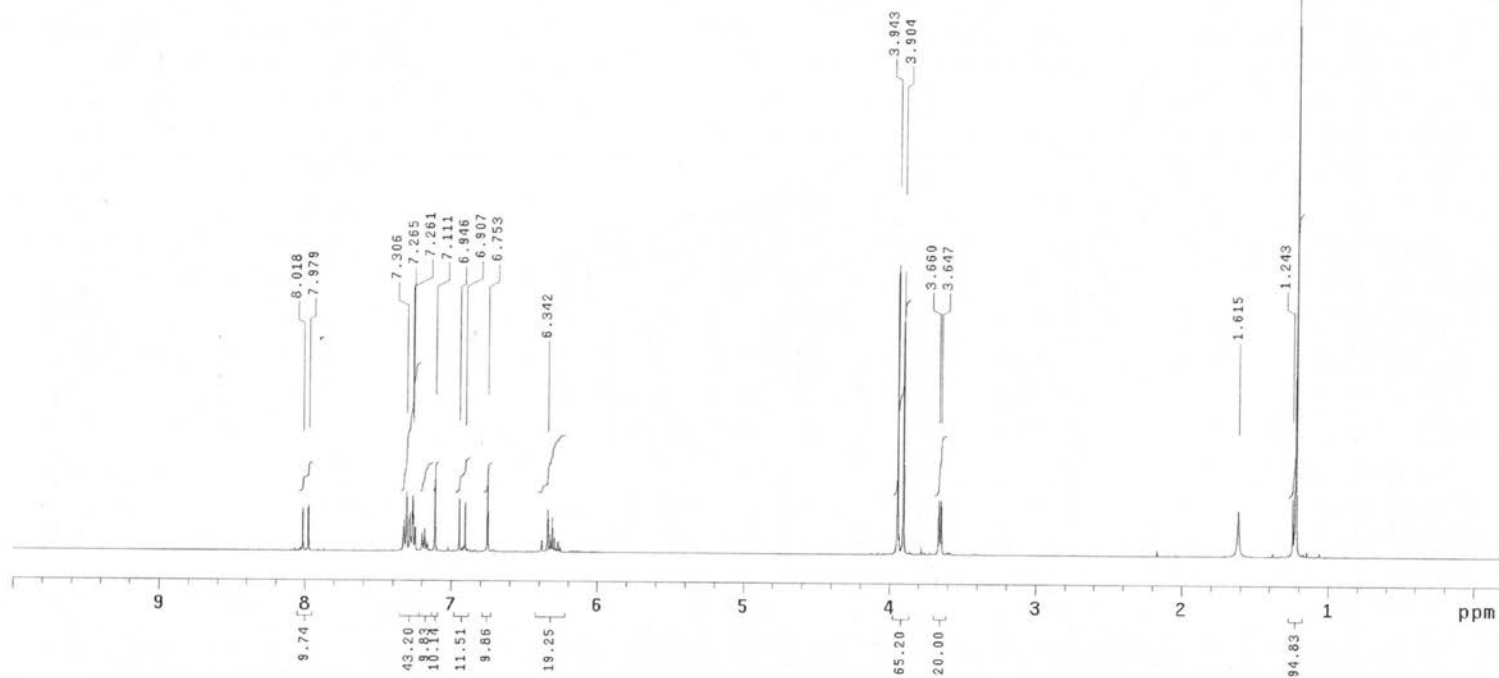
Ambient temperature

Total 32 repetitions



Compound 4j

¹H NMR (400 MHz, CDCl₃) spectra



Compound 4j (¹³C-NMR spectral data)

KS1061108

Pulse Sequence: s2pu1

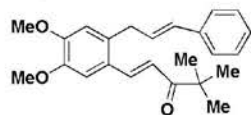
UNITYplus-400 "unity400"

Date: Nov 16 2017

Solvent: CDCl₃

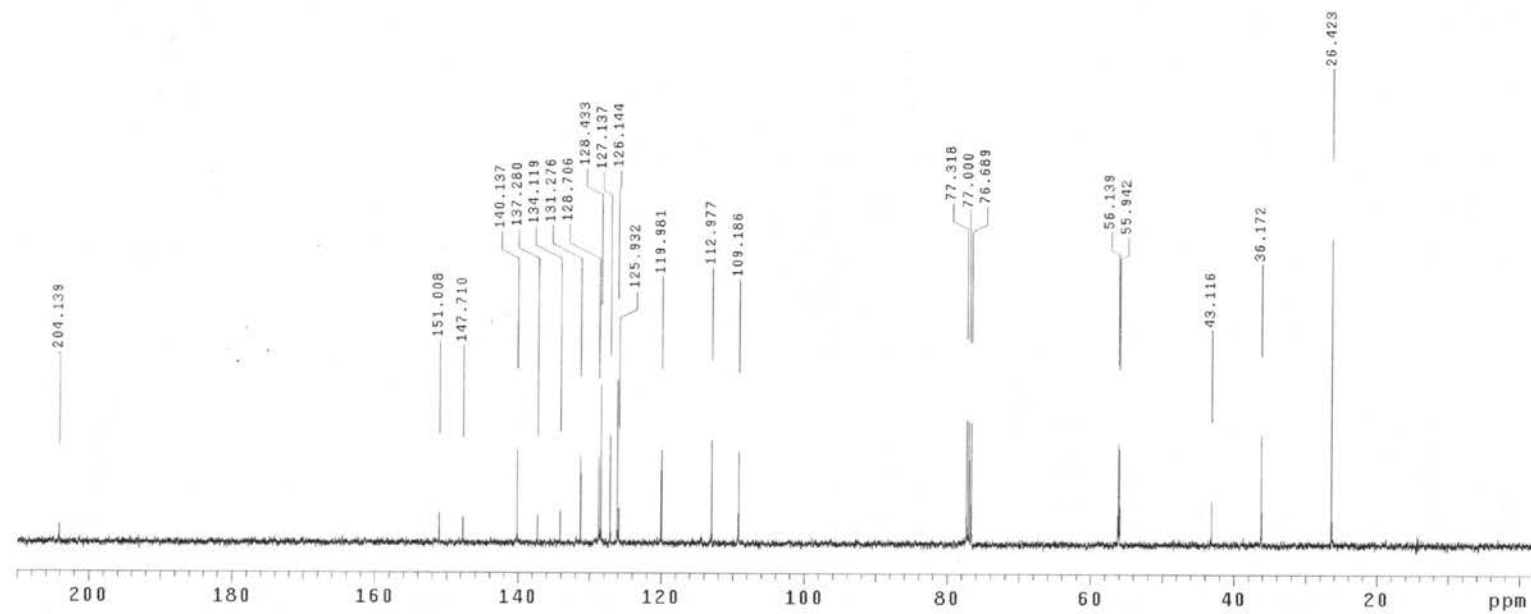
Ambient temperature

Total 1824 repetitions



Compound 4j

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4k (¹H-NMR spectral data)

KS1061129

Pulse Sequence: s2pu1

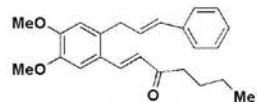
UNITYplus-400 "unity400"

Date: Dec 1 2017

Solvent: CDCl₃

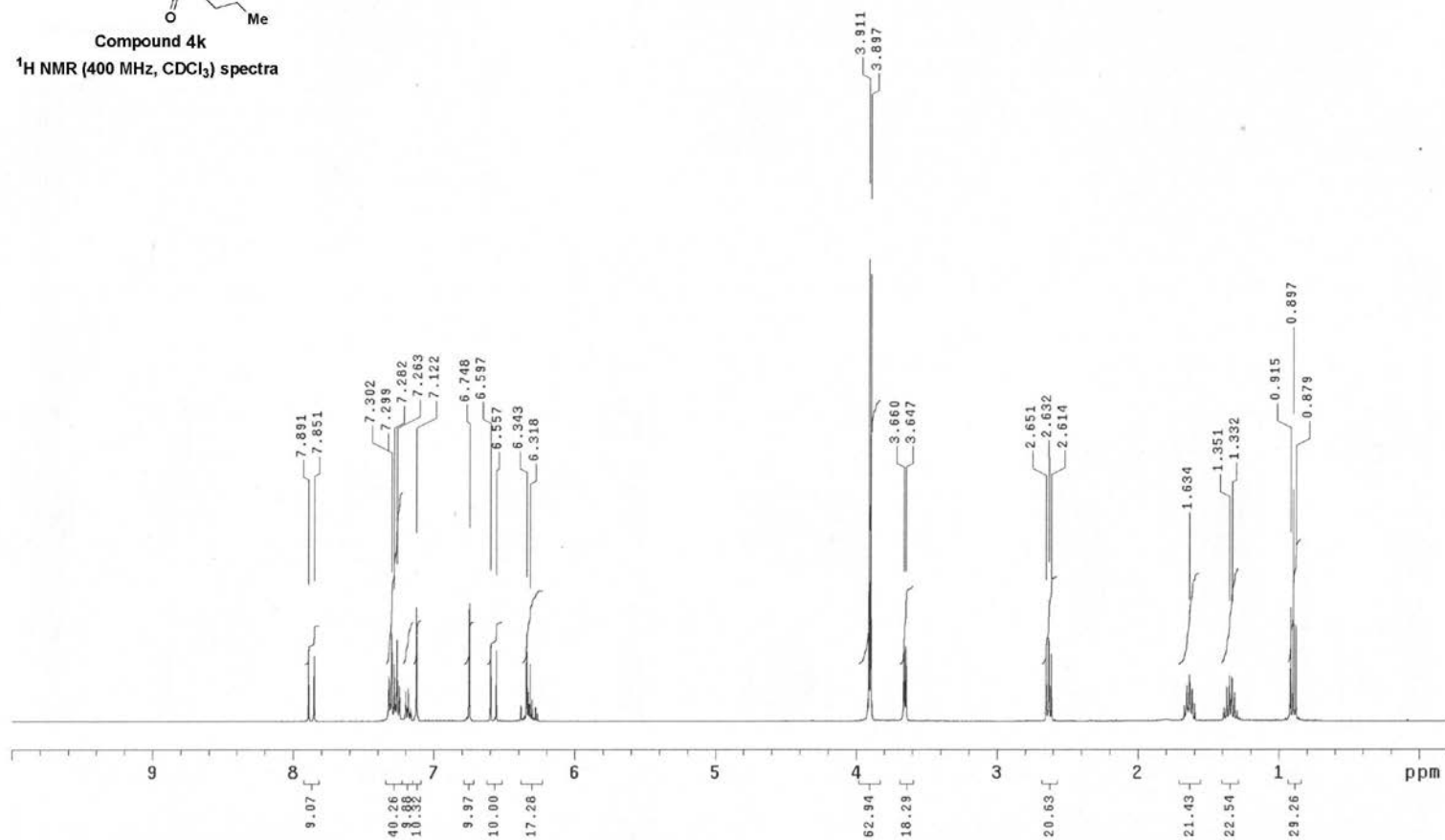
Ambient temperature

Total 32 repetitions



Compound 4k

¹H NMR (400 MHz, CDCl₃) spectra



Compound 4k (¹³C-NMR spectral data)

KS1061129

Pulse Sequence: s2pul

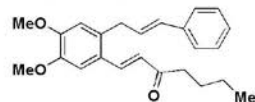
UNITYplus-400 "unity400"

Date: Dec 1 2017

Solvent: CDCl₃

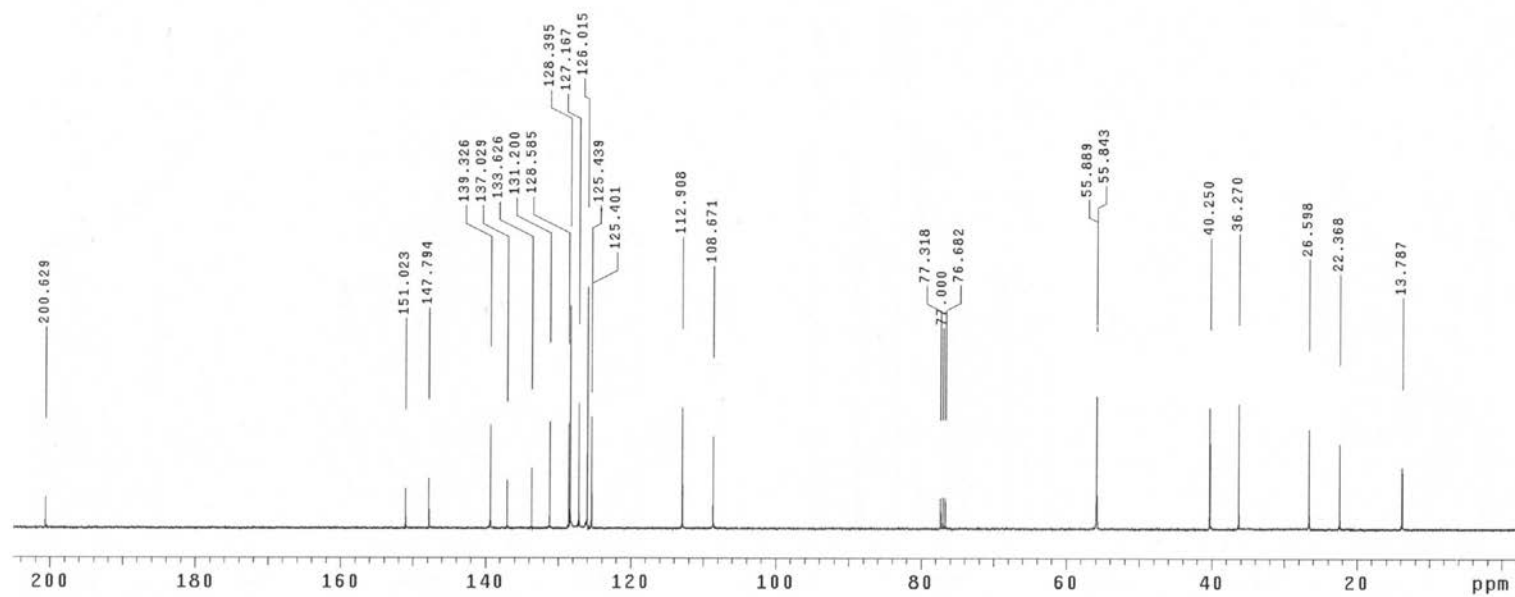
Ambient temperature

Total 1120 repetitions



Compound 4k

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4I (¹H-NMR spectral data)

KS1061130

Pulse Sequence: s2pu1

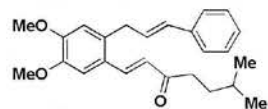
UNITYplus-400 "unity400"

Date: Dec 1 2017

Solvent: CDCl₃

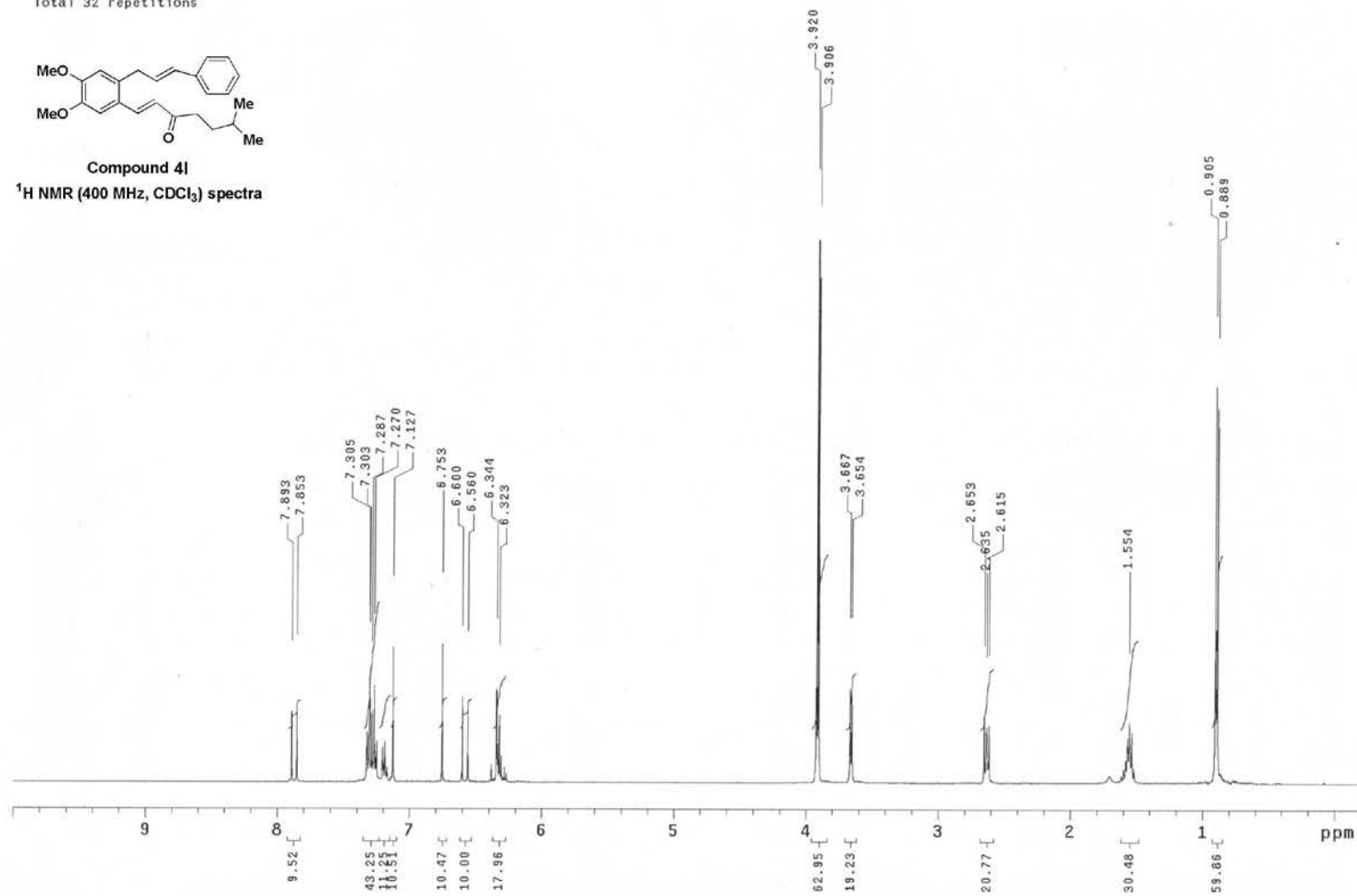
Ambient temperature

Total 32 repetitions



Compound 4I

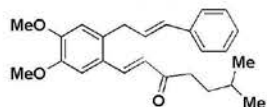
¹H NMR (400 MHz, CDCl₃) spectra



Compound 4I (¹³C-NMR spectral data)

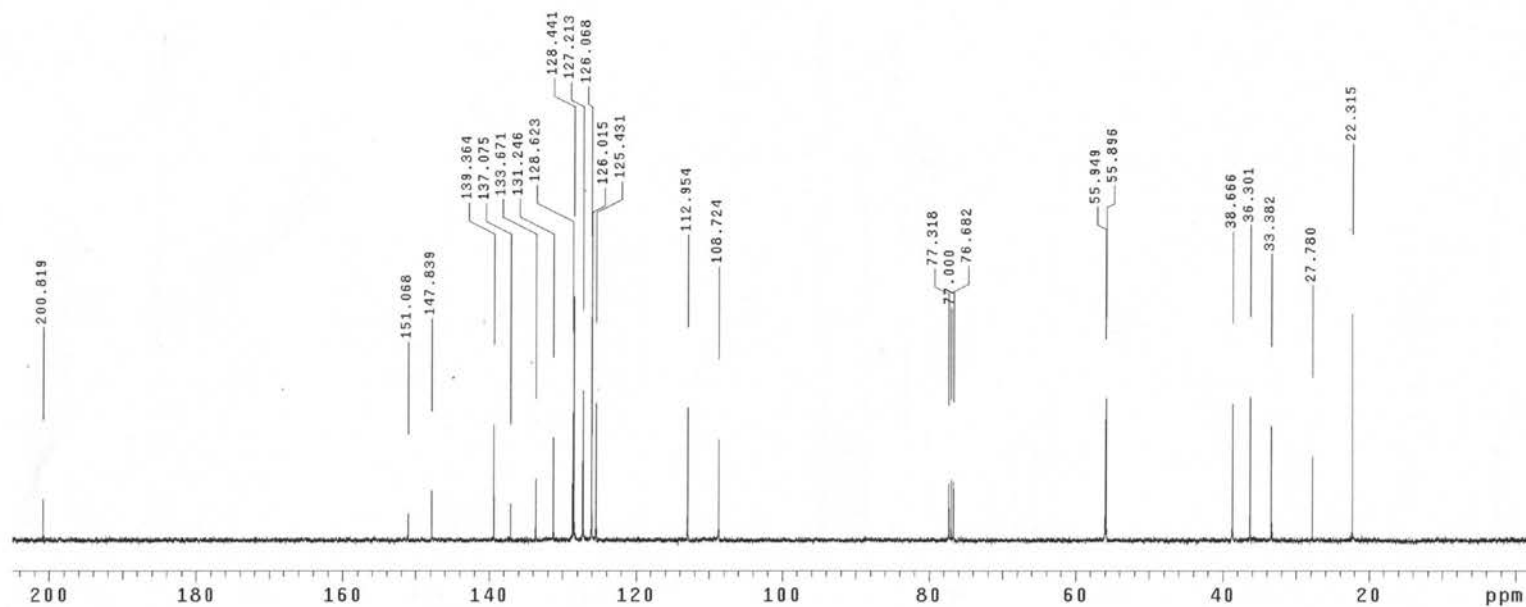
KS1061130

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Dec 1 2017
Solvent: CDCl₃
Ambient temperature
Total 672 repetitions



Compound 4I

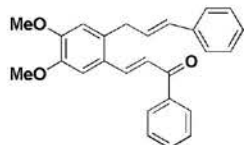
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4m (¹H-NMR spectral data)

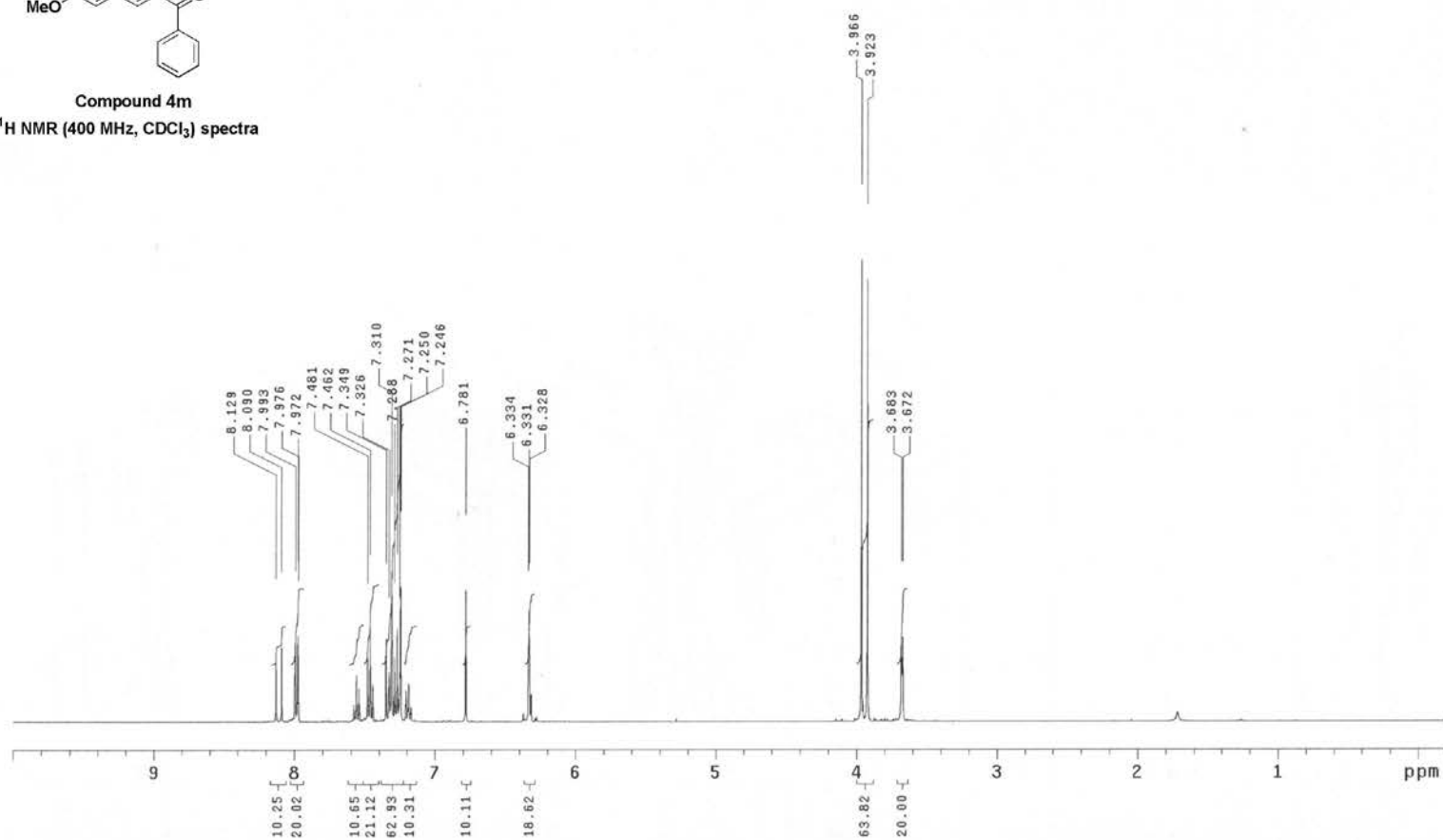
KS1061210

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Dec 11 2017
Solvent: CDCl₃
Ambient temperature
Total 32 repetitions



Compound 4m

¹H NMR (400 MHz, CDCl₃) spectra



Compound 4m (¹³C-NMR spectral data)

KS1061210

Pulse Sequence: s2pu1

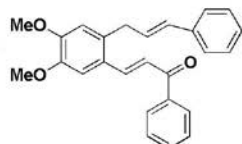
UNITYplus-400 "unity400"

Date: Dec 11 2017

Solvent: CDCl₃

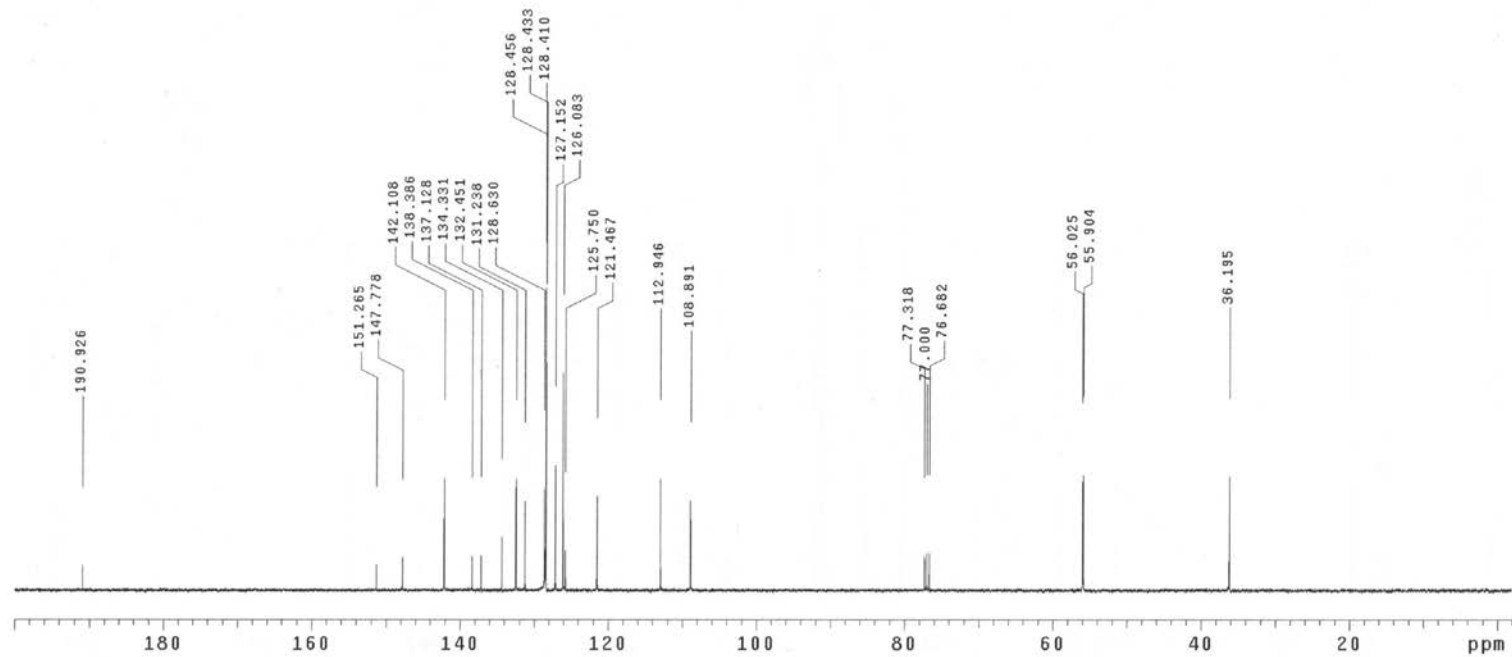
Ambient temperature

Total 640 repetitions



Compound 4m

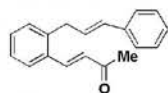
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4n (¹H-NMR spectral data)

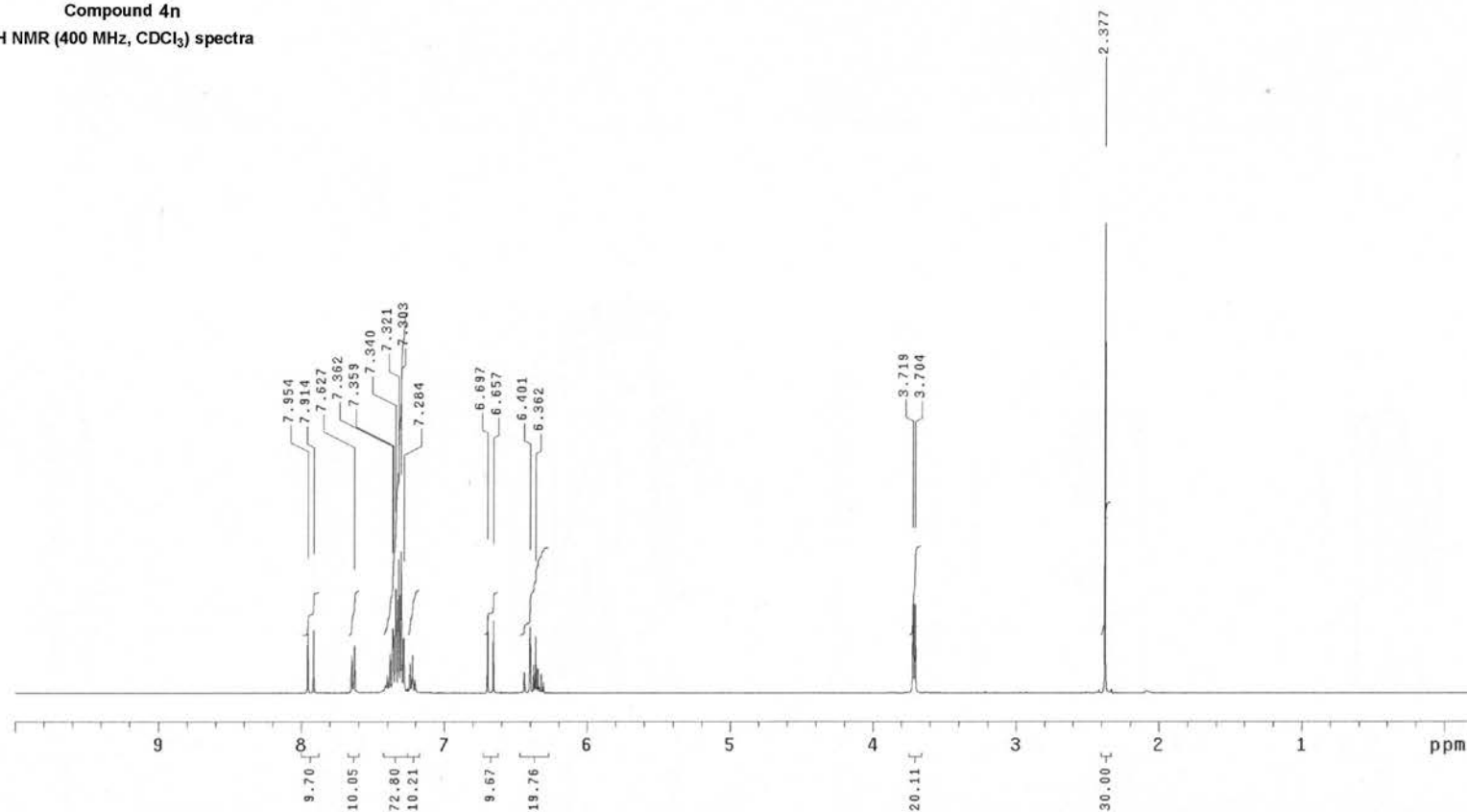
KS1061214

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Dec 15 2017
Solvent: CDCl₃
Ambient temperature
Total 32 repetitions



Compound 4n

¹H NMR (400 MHz, CDCl₃) spectra



Compound 4n (¹³C-NMR spectral data)

KS1061214

Pulse Sequence: s2pu1

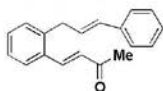
UNITYplus-400 "unity400"

Date: Dec 15 2017

Solvent: CDCl₃

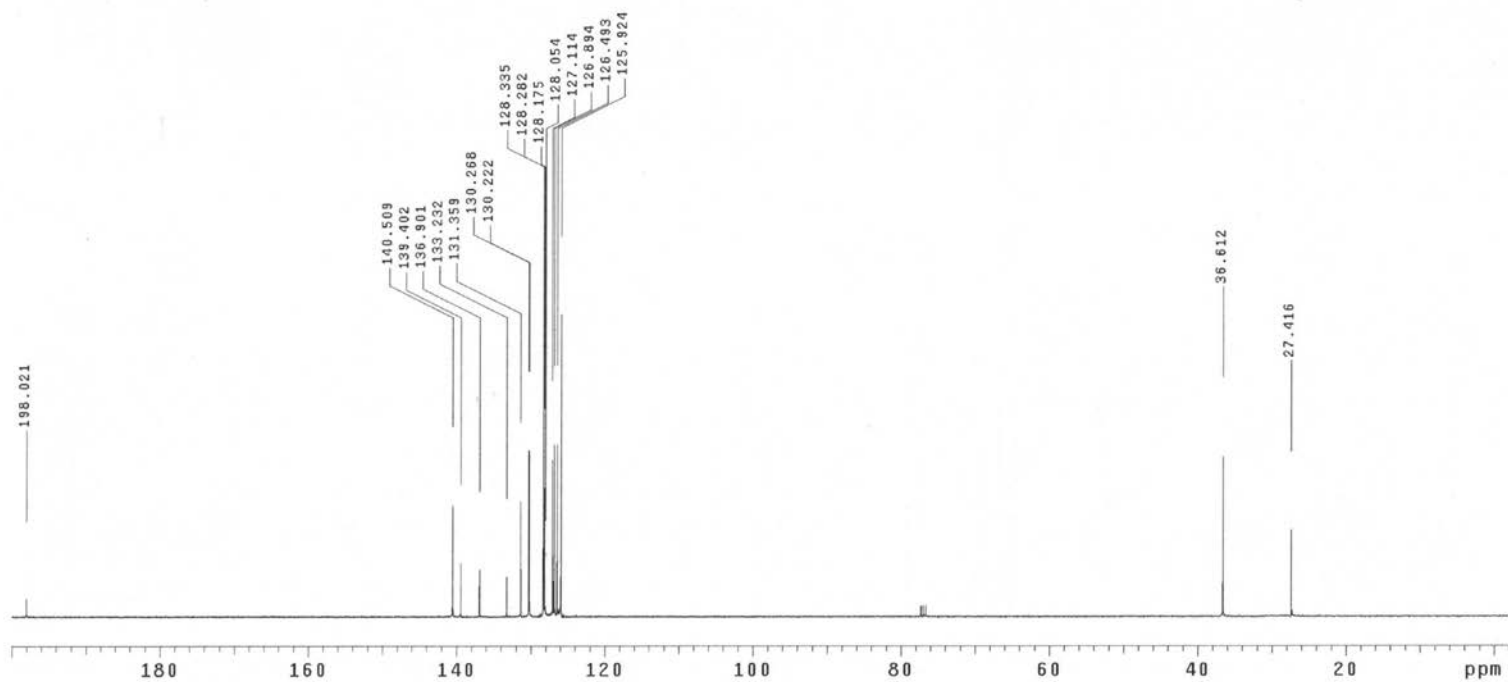
Ambient temperature

Total 432 repetitions



Compound 4n

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4o (¹H-NMR spectral data)

KS1061207

Pulse Sequence: s2pu1

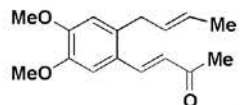
UNITYplus-400 "unity400"

Date: Dec 8 2017

Solvent: CDCl₃

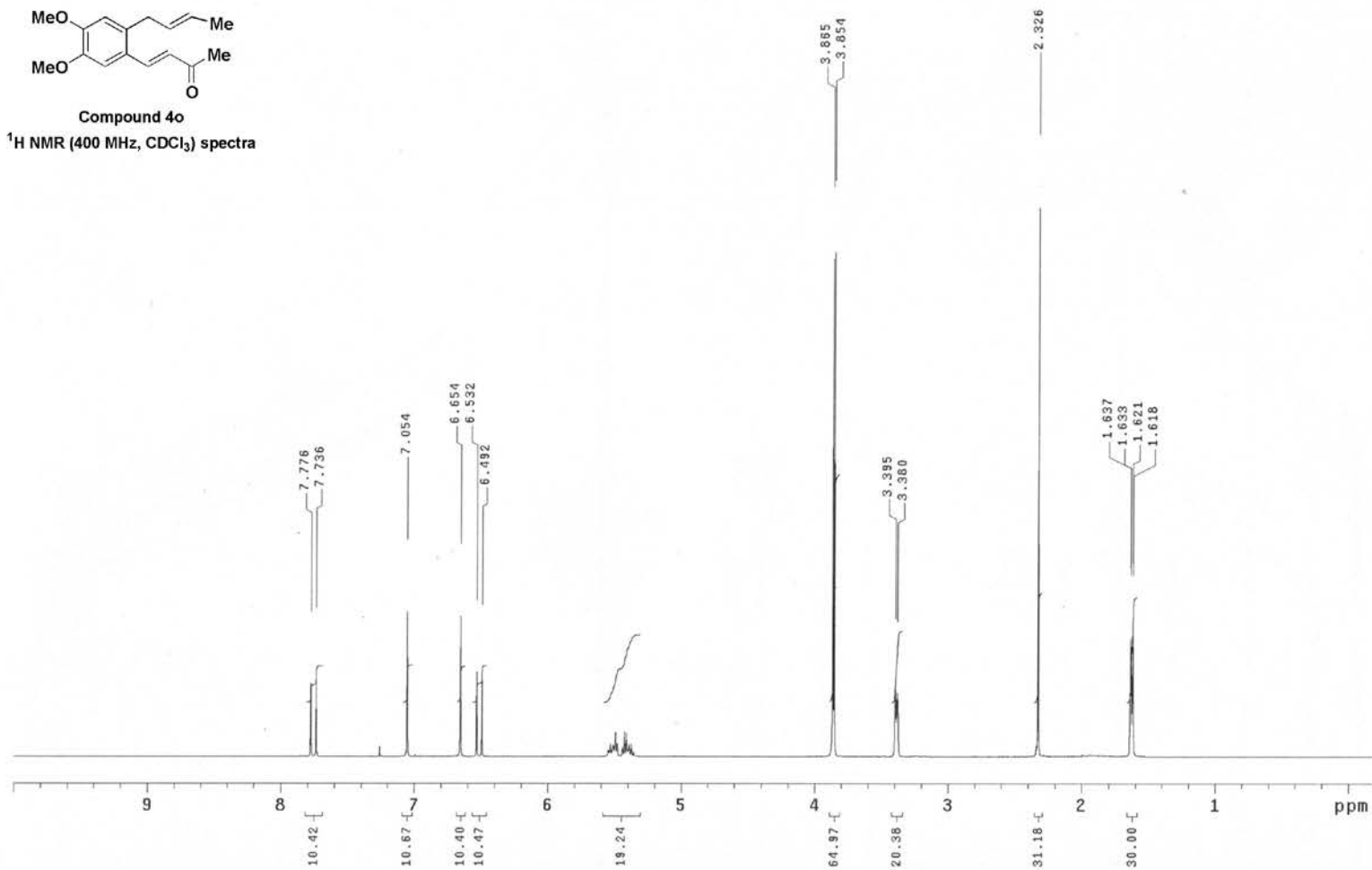
Ambient temperature

Total 32 repetitions



Compound 4o

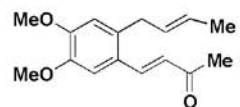
¹H NMR (400 MHz, CDCl₃) spectra



Compound 4o (¹³C-NMR spectral data)

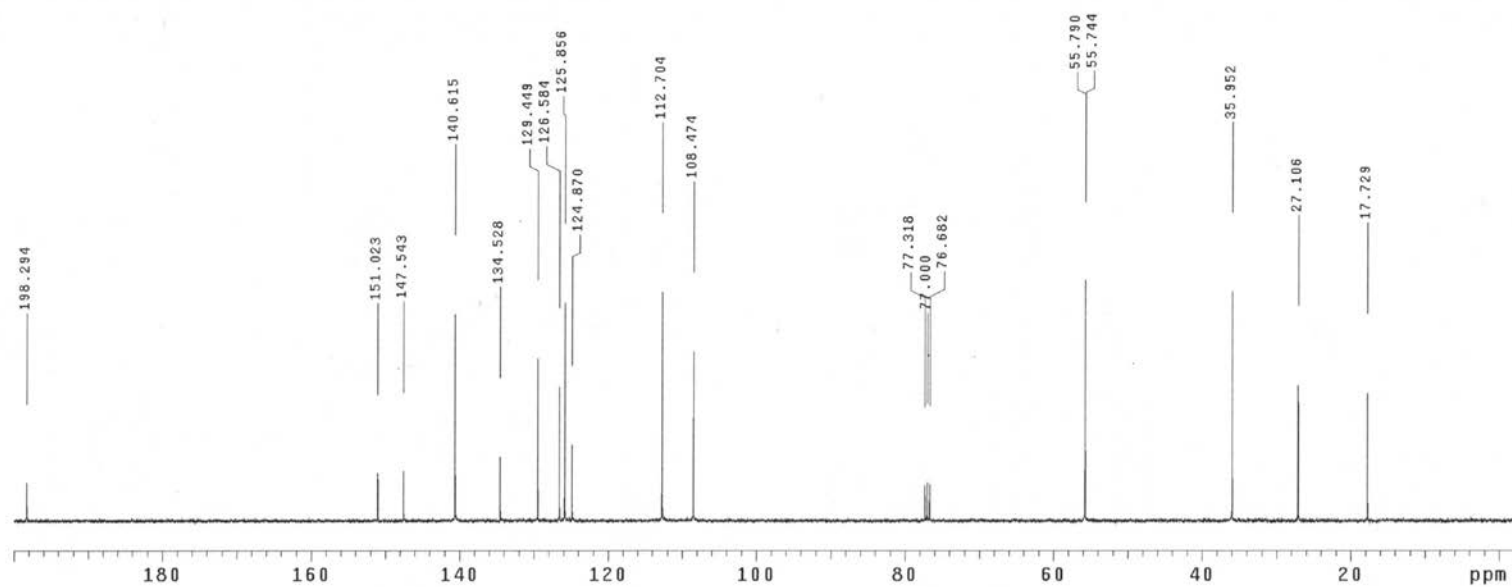
KS1061207

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Dec 8 2017
Solvent: CDCl₃
Ambient temperature
Total 480 repetitions



Compound 4o

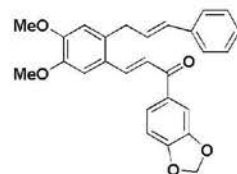
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4p (¹H-NMR spectral data)

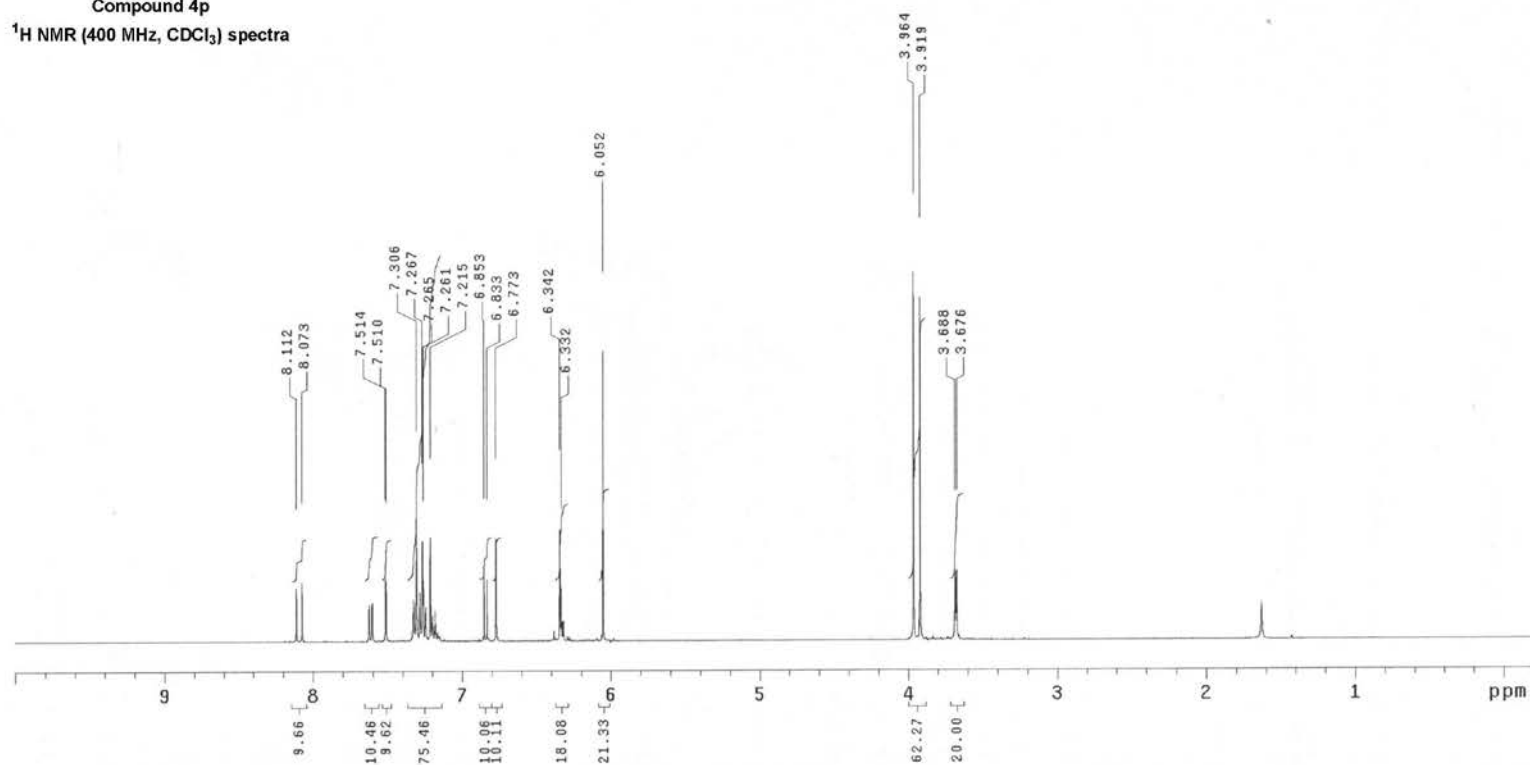
KS1070115

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Jan 16 2018
Solvent: CDCl₃
Ambient temperature
Total 32 repetitions



Compound 4p

¹H NMR (400 MHz, CDCl₃) spectra



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

KS1070115

Pulse Sequence: s2pu1

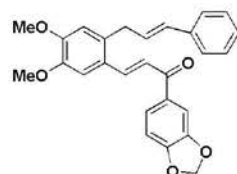
UNITYplus-400 "unity400"

Date: Jan 16 2018

Solvent: CDCl_3

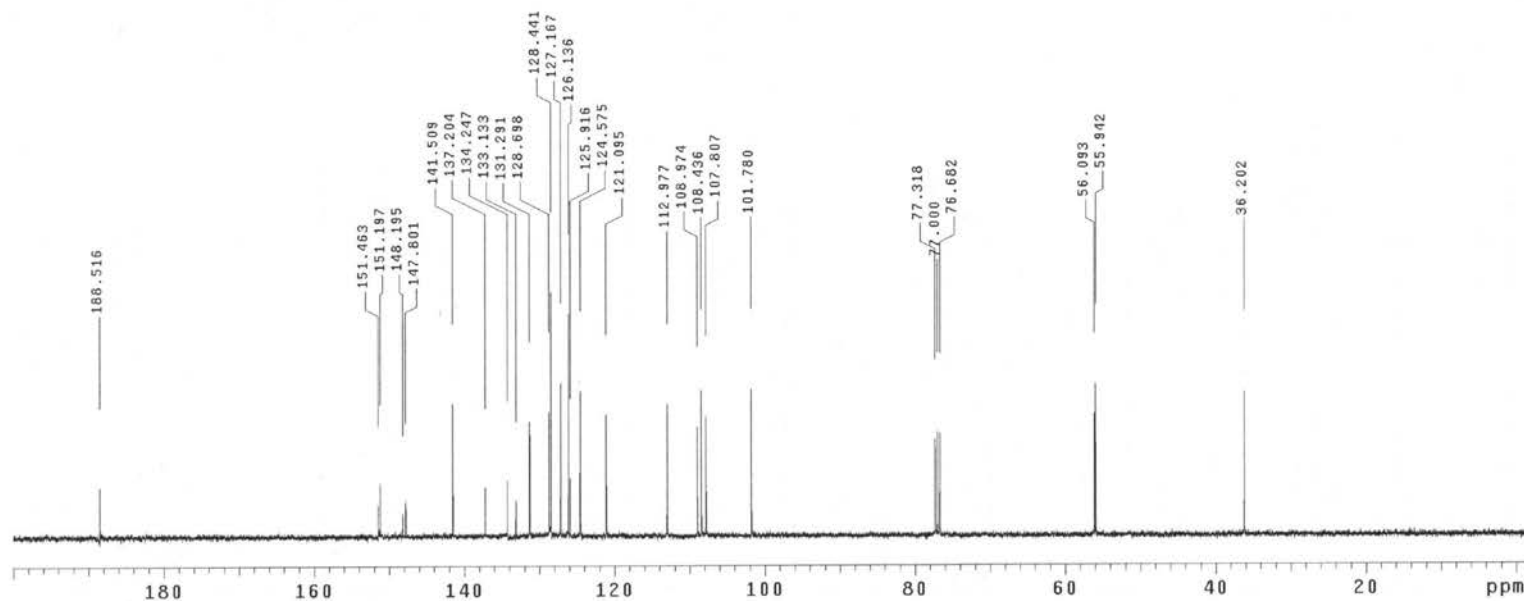
Ambient temperature

Total 2448 repetitions



Compound 4p

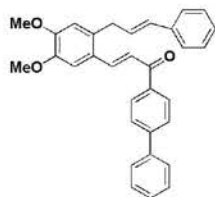
^{13}C NMR (100 MHz, CDCl_3) spectra



Compound 4q (¹H-NMR spectral data)

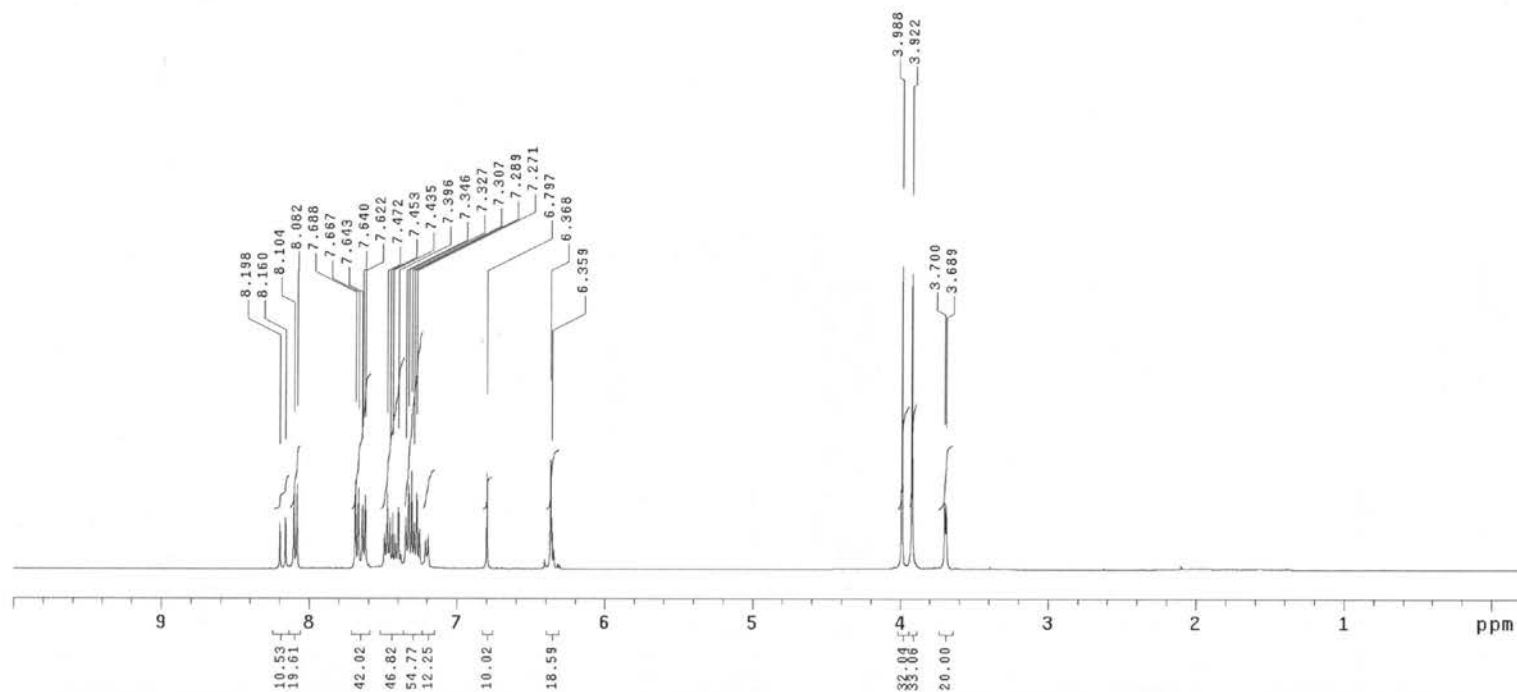
KS1070116

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Jan 16 2018
Solvent: CDCl₃
Ambient temperature
Total 32 repetitions



Compound 4q

¹H NMR (400 MHz, CDCl₃) spectra



Compound 4q (¹³C-NMR spectral data)

KS1070116

Pulse Sequence: s2pu1

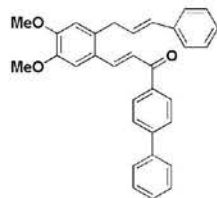
UNITYplus-400 "unity400"

Date: Jan 15 2018

Solvent: CDCl₃

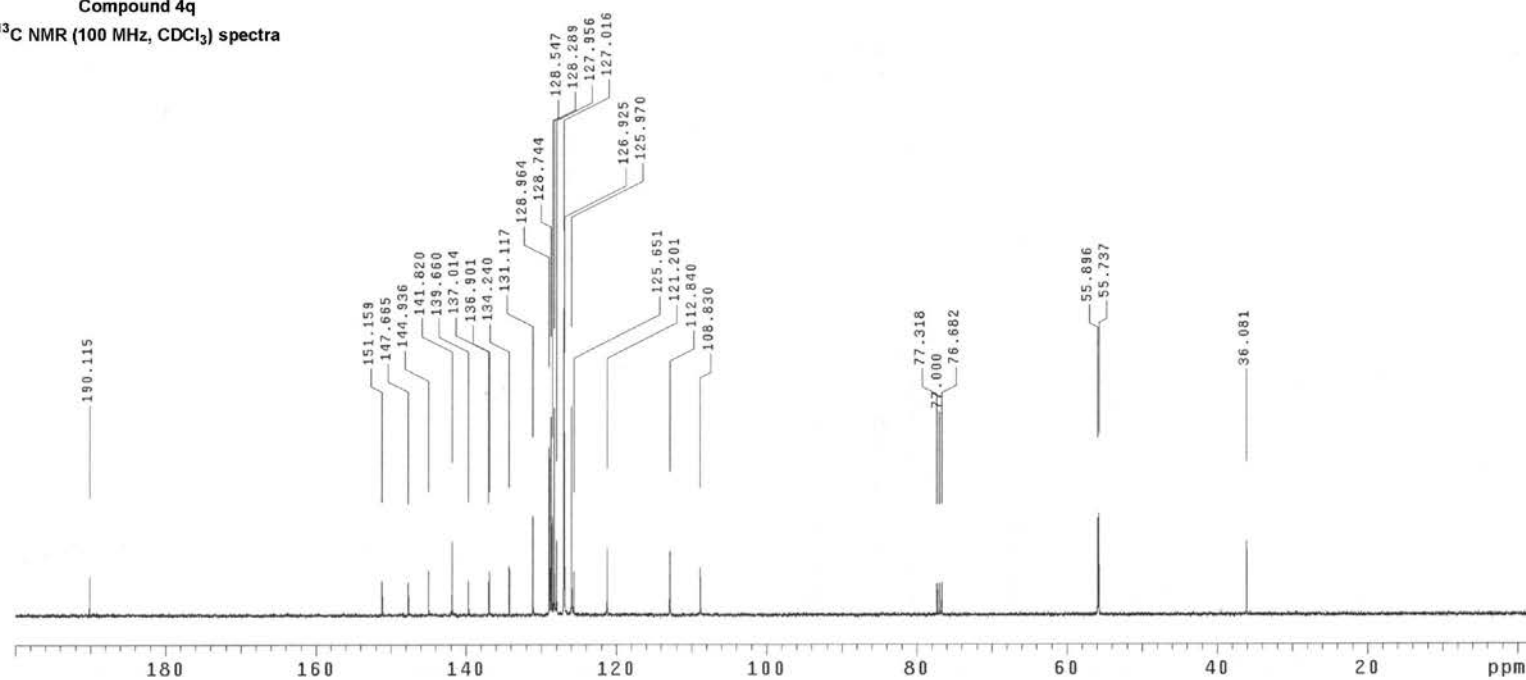
Ambient temperature

Total 80 repetitions



Compound 4q

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4r (¹H-NMR spectral data)

KSA08

Pulse Sequence: s2pu1

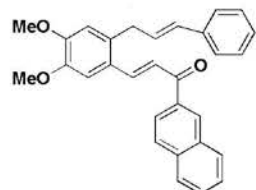
UNITYplus-400 "unity400"

Date: Oct 6 2017

Solvent: CDCl₃

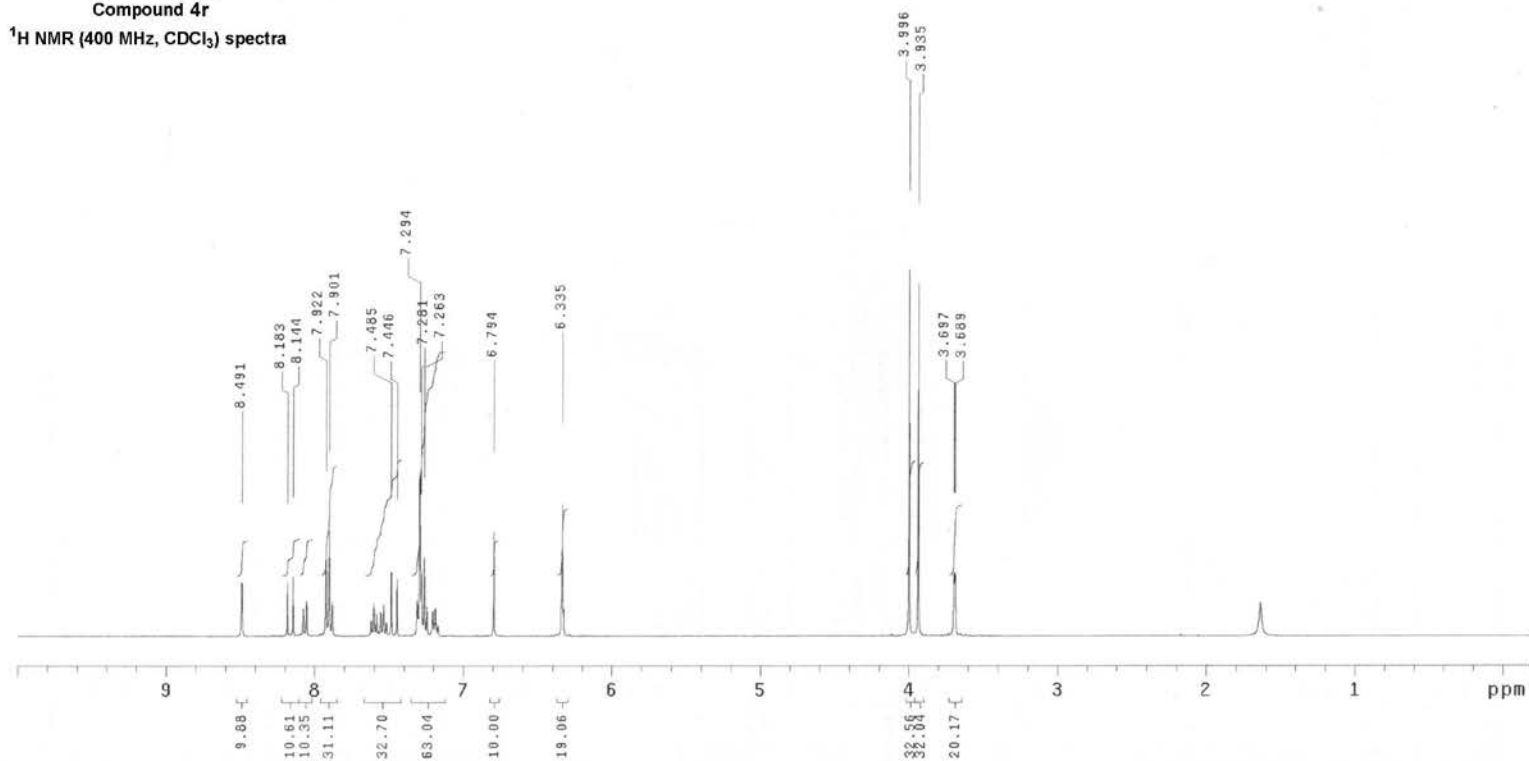
Ambient temperature

Total 32 repetitions



Compound 4r

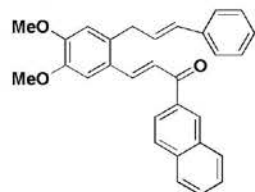
¹H NMR (400 MHz, CDCl₃) spectra



Compound 4r (¹³C-NMR spectral data)

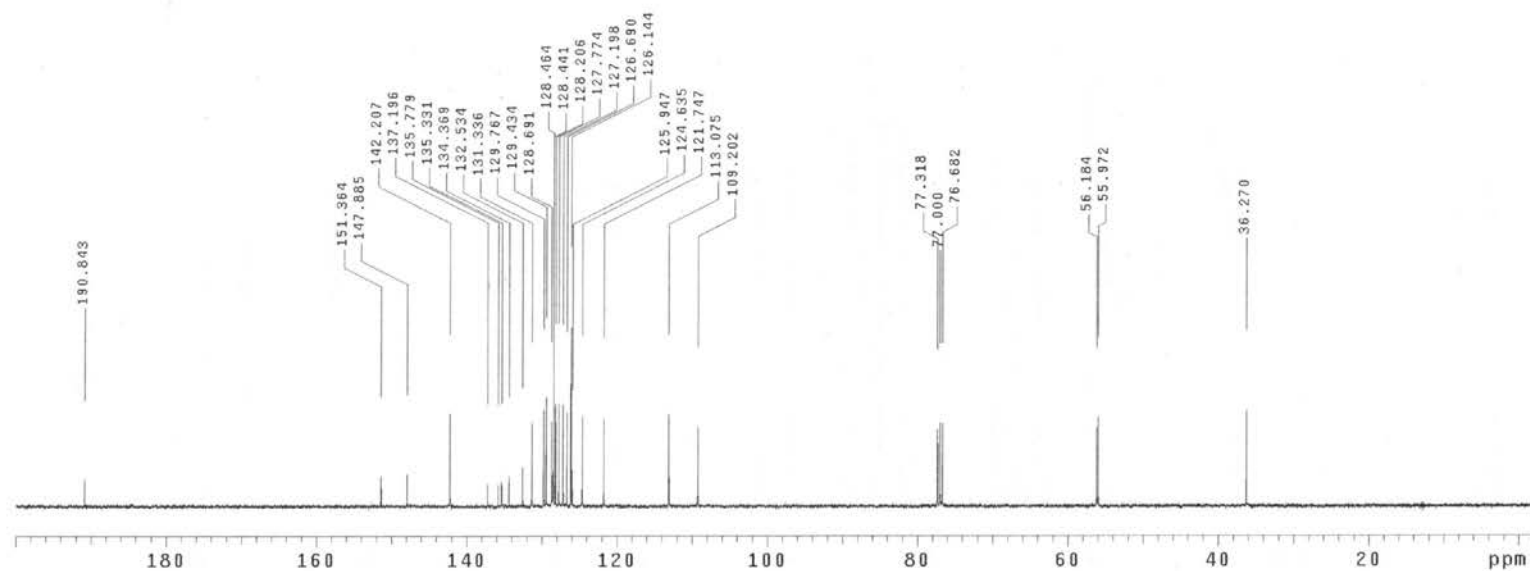
KSA08

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Oct 6 2017
Solvent: CDCl₃
Ambient temperature
Total 2176 repetitions



Compound 4r

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4s (¹H-NMR spectral data)

KSA09-1

Pulse Sequence: s2pu1

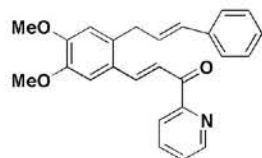
UNITYplus-400 "unity400"

Date: Oct 8 2017

Solvent: CDCl₃

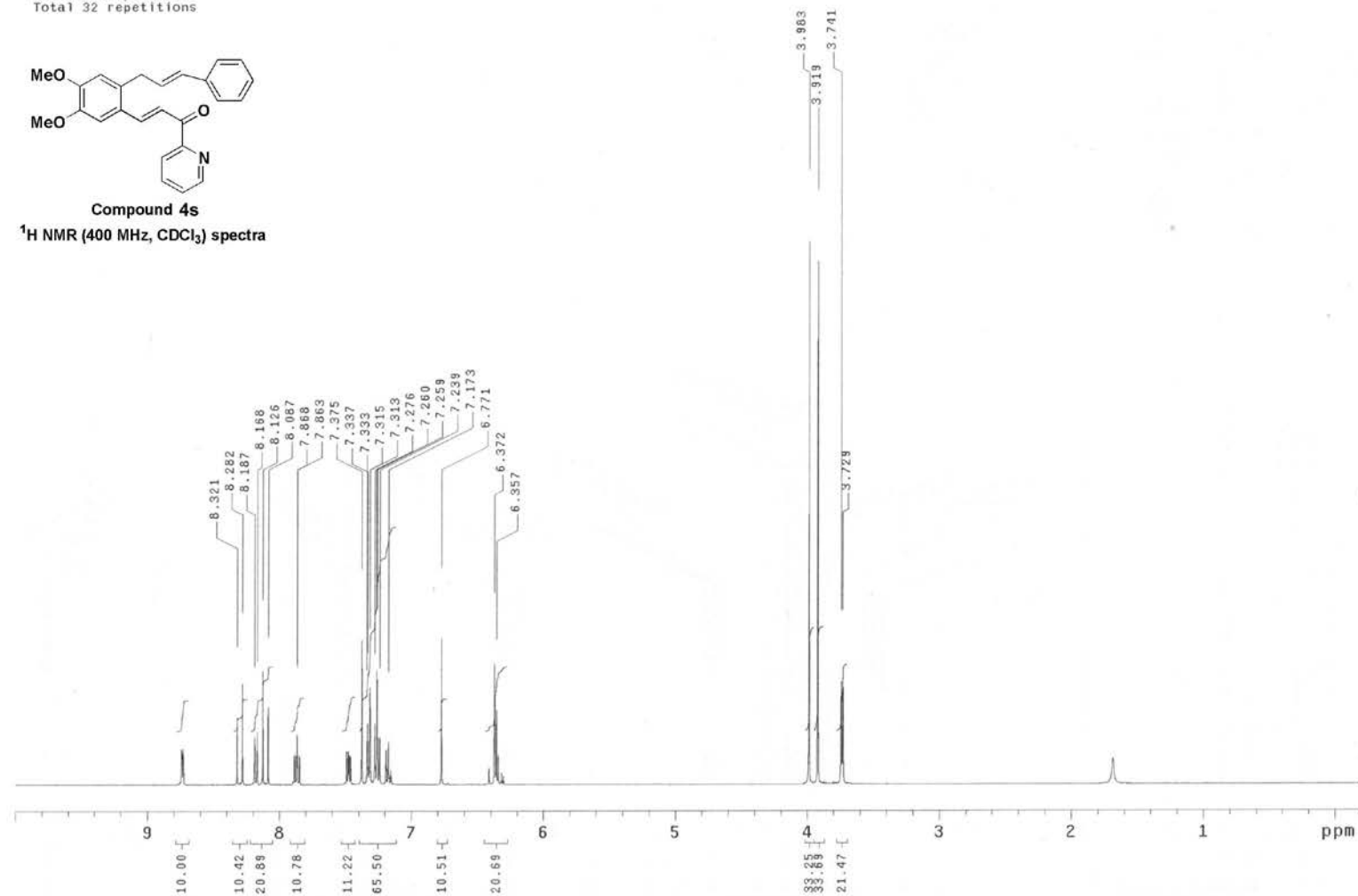
Ambient temperature

Total 32 repetitions



Compound 4s

¹H NMR (400 MHz, CDCl₃) spectra



Compound 4s (¹³C-NMR spectral data)

KSA09-1

Pulse Sequence: s2pu1

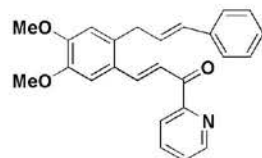
UNITYplus-400 "unity400"

Date: Oct 6 2017

Solvent: CDCl₃

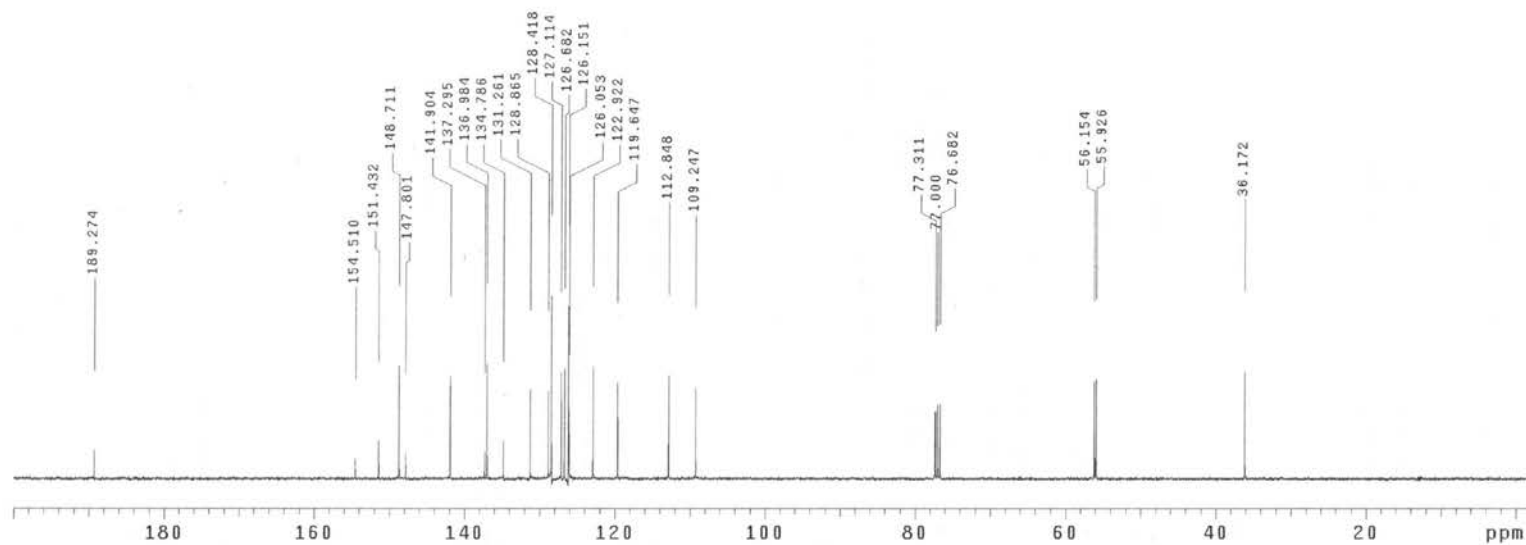
Ambient temperature

Total 3056 repetitions



Compound 4s

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4t (¹H-NMR spectral data)

KS1070118

Pulse Sequence: s2pu1

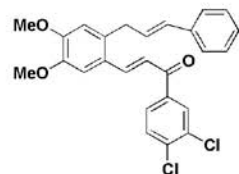
UNITYplus-400 "unity400"

Date: Jan 19 2018

Solvent: CDCl₃

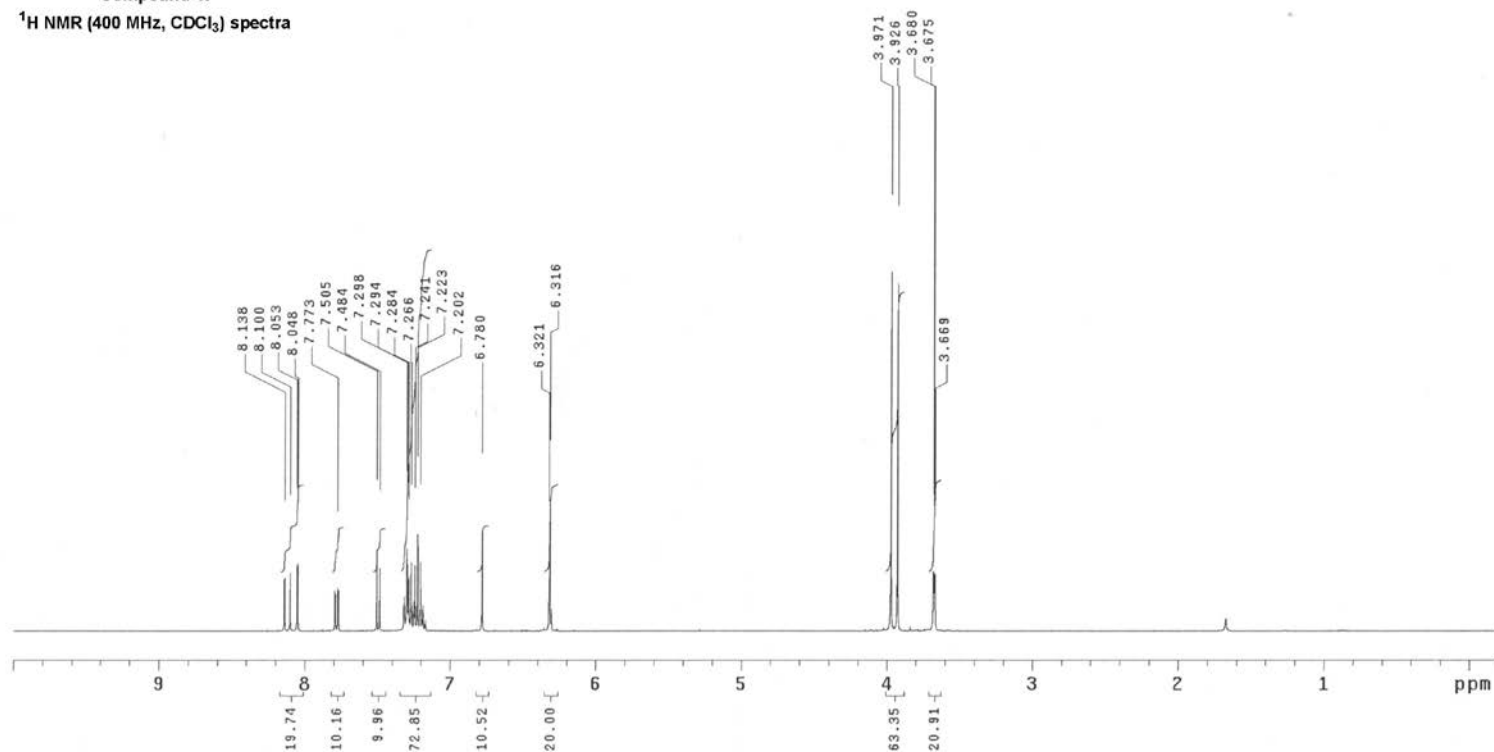
Ambient temperature

Total 32 repetitions



Compound 4t

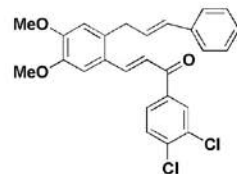
¹H NMR (400 MHz, CDCl₃) spectra



Compound 4t (¹³C-NMR spectral data)

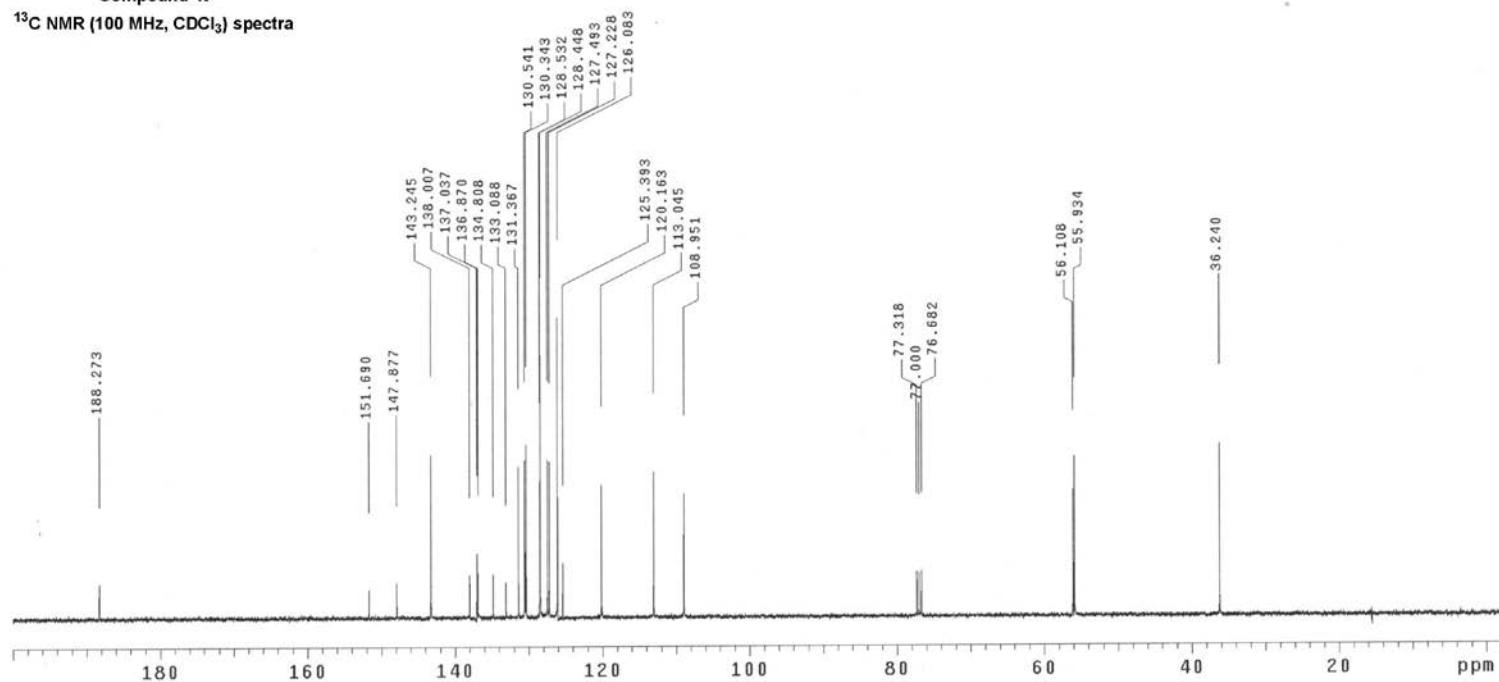
KS1070118

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Jan 19 2018
 Solvent: CDCl₃
 Ambient temperature
 Total 816 repetitions



Compound 4t

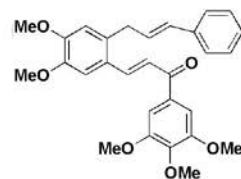
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4u (¹H-NMR spectral data)

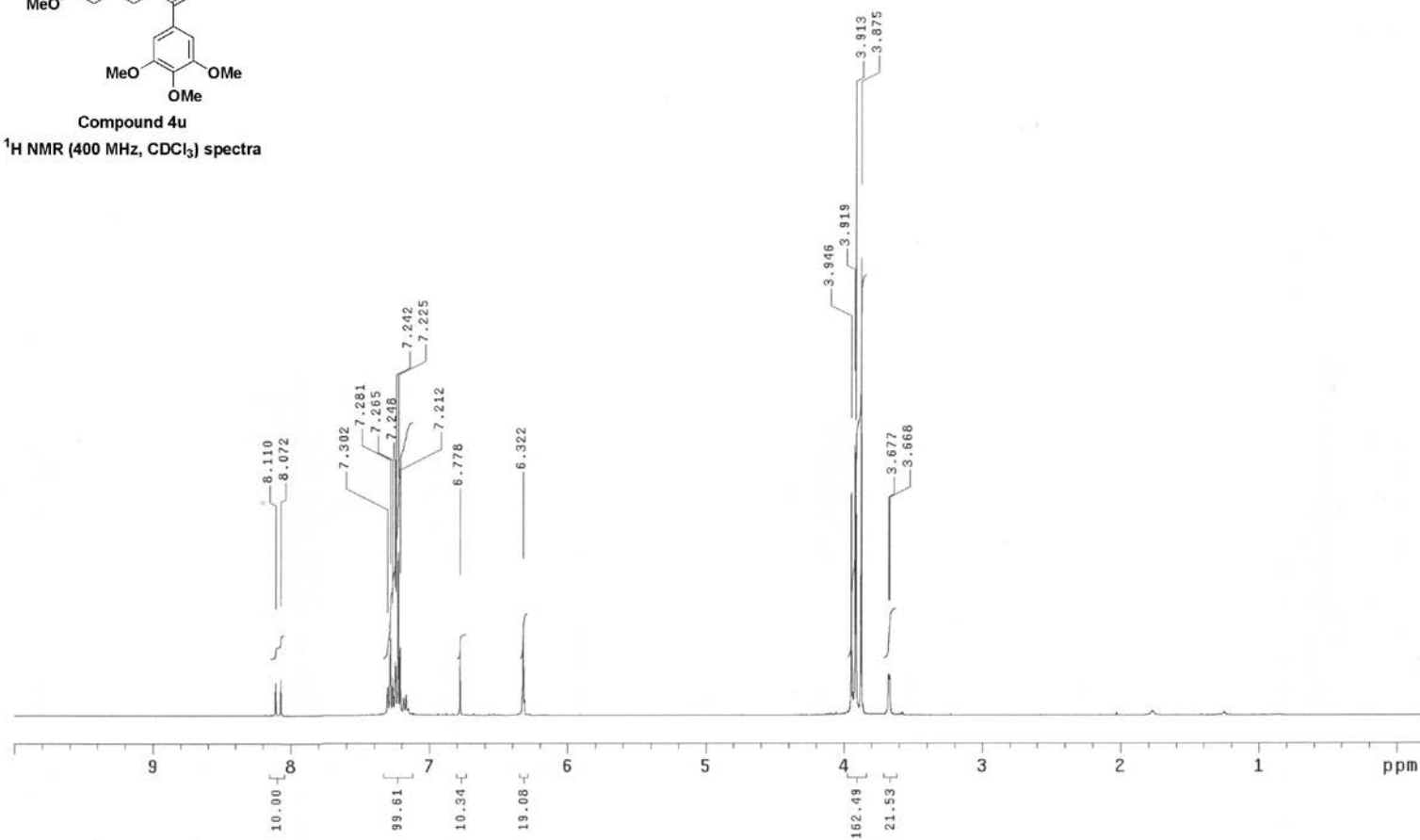
KS1070117

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Jan 18 2018
Solvent: CDCl₃
Ambient temperature
Total 32 repetitions



Compound 4u

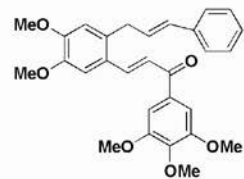
¹H NMR (400 MHz, CDCl₃) spectra



Compound 4u (¹³C-NMR spectral data)

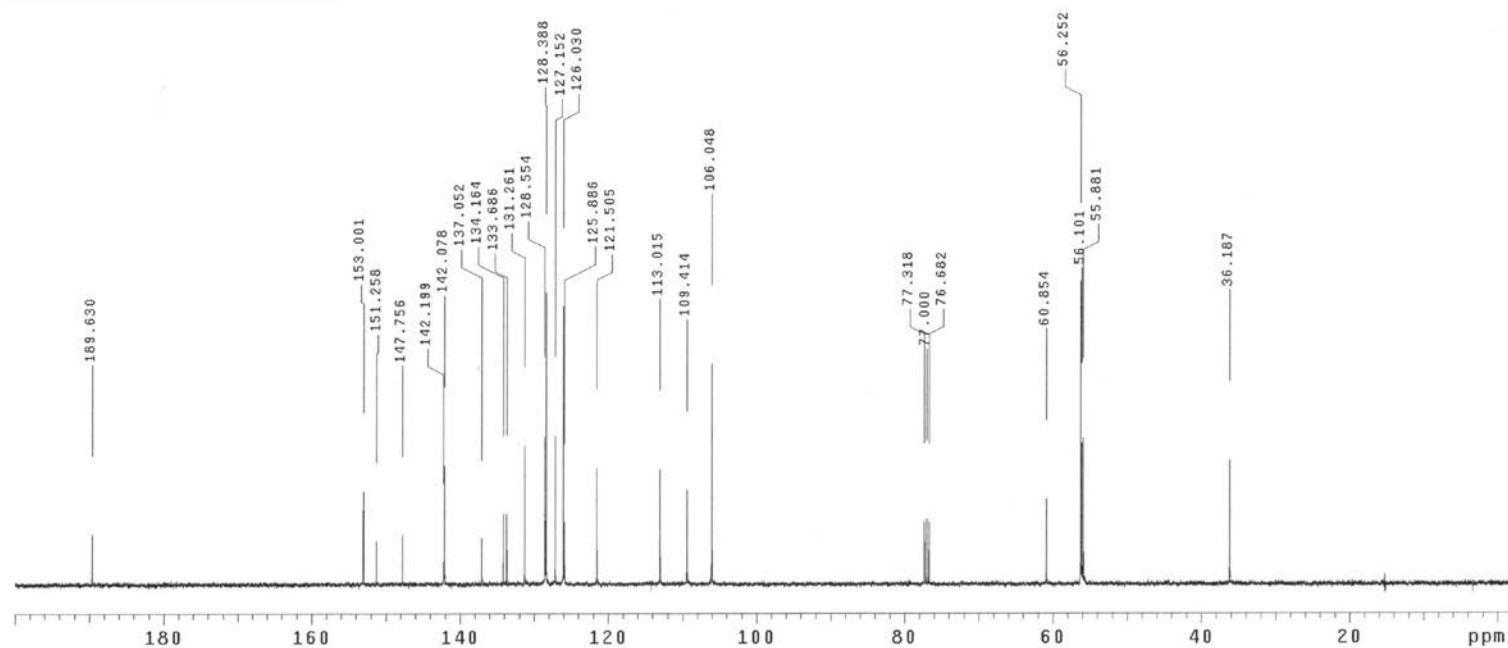
KS1070117

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Jan 18 2018
Solvent: CDCl₃
Ambient temperature
Total 64000 repetitions



Compound 4u

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4v (¹H-NMR spectral data)

KS1070207

Pulse Sequence: s2pu1

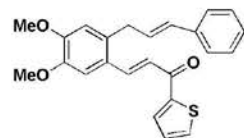
UNITYplus-400 "unity400"

Date: Feb 8 2018

Solvent: CDCl₃

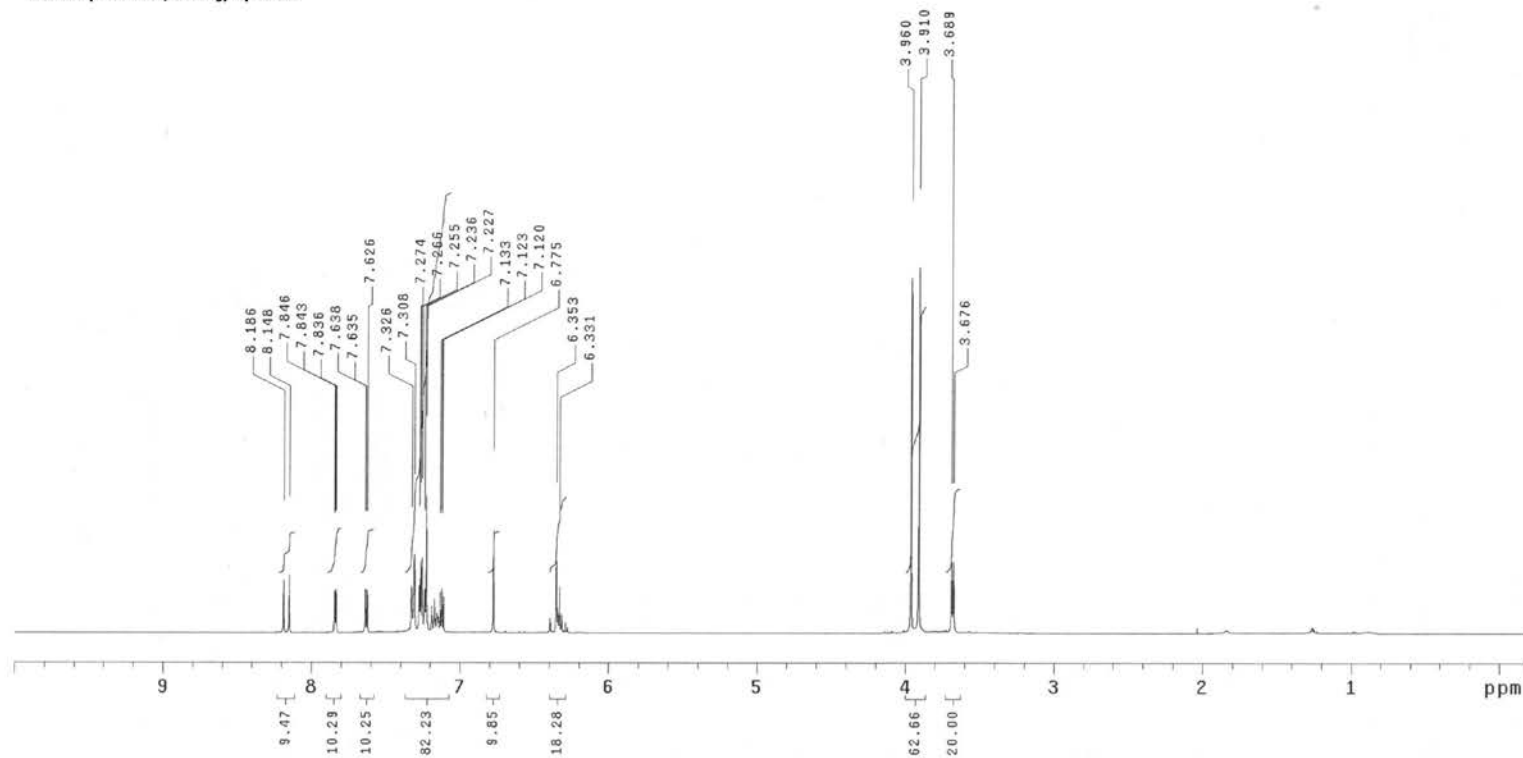
Ambient temperature

Total 32 repetitions



Compound 4v

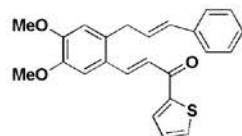
¹H NMR (400 MHz, CDCl₃) spectra



Compound 4v (¹³C-NMR spectral data)

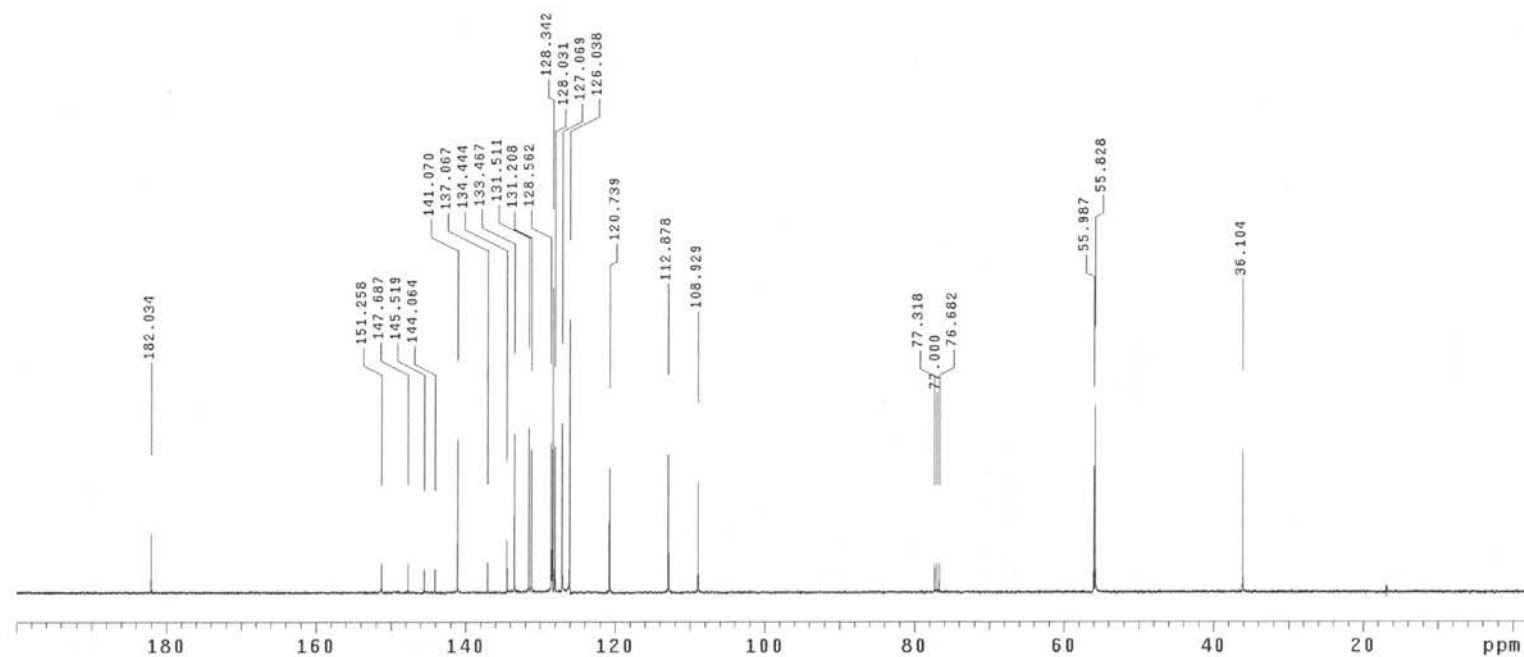
KS1070207

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Feb 8 2018
Solvent: CDCl₃
Ambient temperature
Total 1024 repetitions



Compound 4v

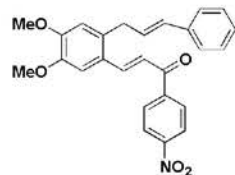
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4w (¹H-NMR spectral data)

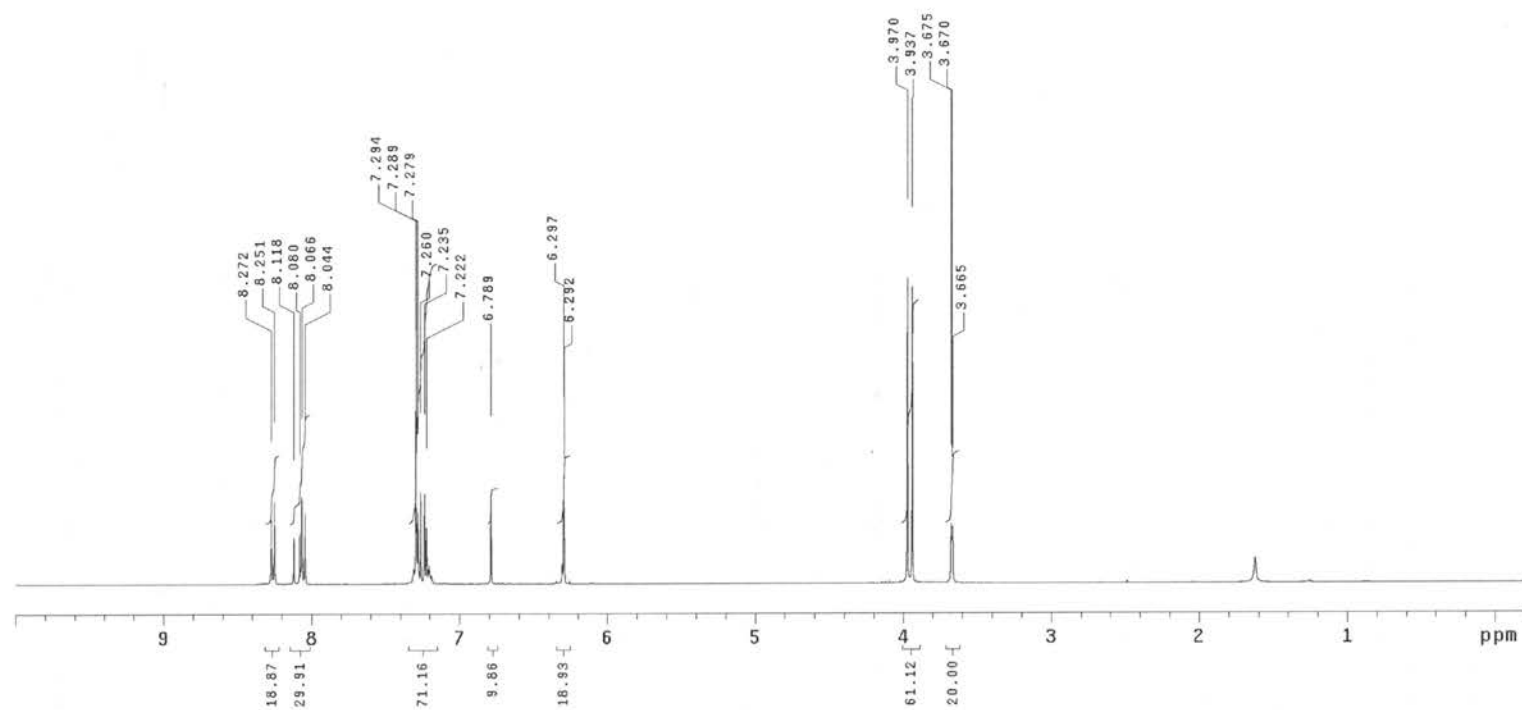
KS1070124

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Jan 25 2018
Solvent: CDCl₃
Ambient temperature
Total 32 repetitions



Compound 4w

¹H NMR (400 MHz, CDCl₃) spectra



Compound 4w (¹³C-NMR spectral data)

KS1070124

Pulse Sequence: s2pu1

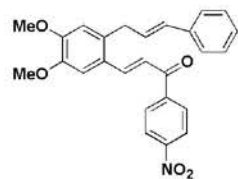
UNITYplus-400 "unity400"

Date: Jan 25 2018

Solvent: CDCl₃

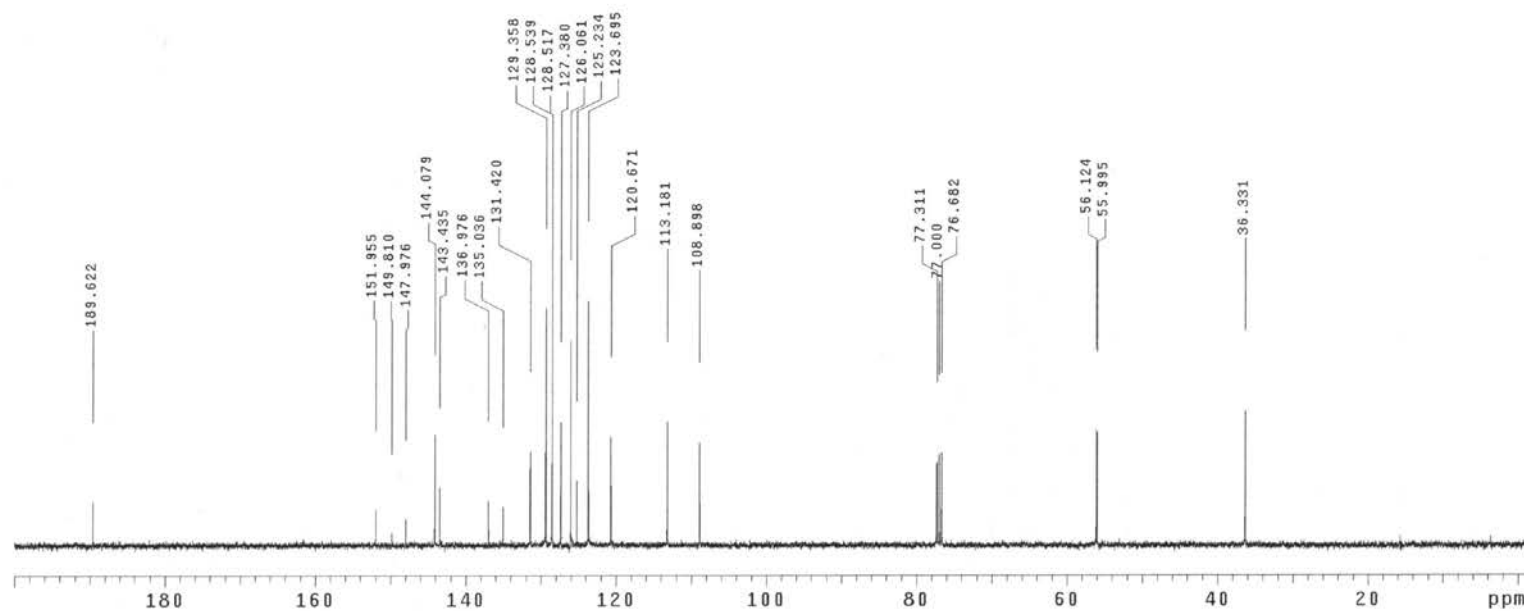
Ambient temperature

Total 1472 repetitions



Compound 4w

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4x (¹H-NMR spectral data)

KS1070307

Pulse Sequence: s2pu1

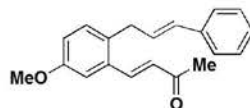
UNITYplus-400 "unity400"

Date: Mar 7 2018

Solvent: CDCl₃

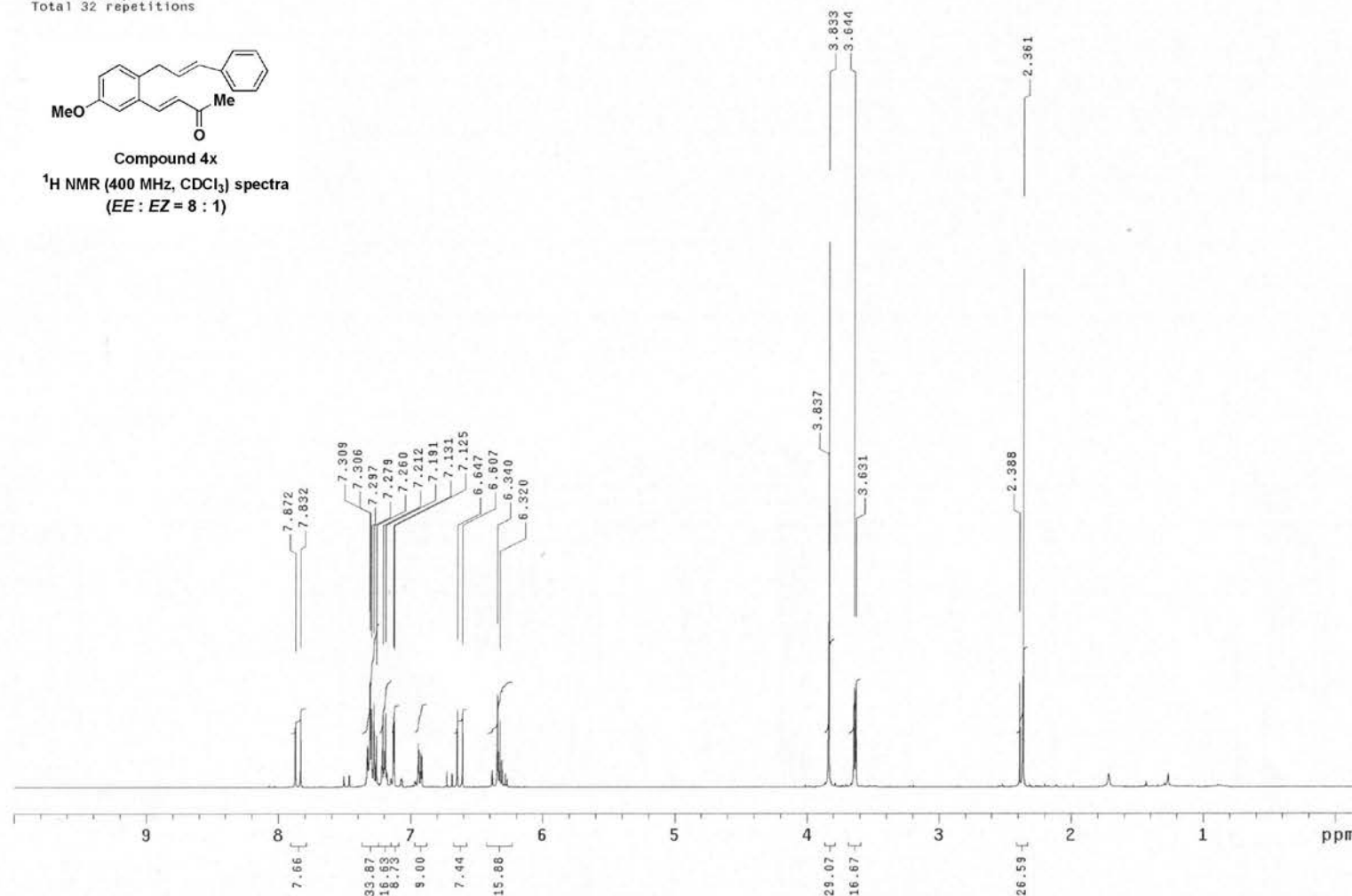
Ambient temperature

Total 32 repetitions



Compound 4x

¹H NMR (400 MHz, CDCl₃) spectra
(*EE* : *EZ* = 8 : 1)



Compound 4x (¹³C-NMR spectral data)

KS1070307

Pulse Sequence: s2pu1

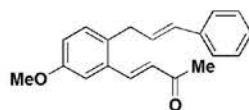
UNITYplus-400 "unity400"

Date: Mar 7 2016

Solvent: CDCl₃

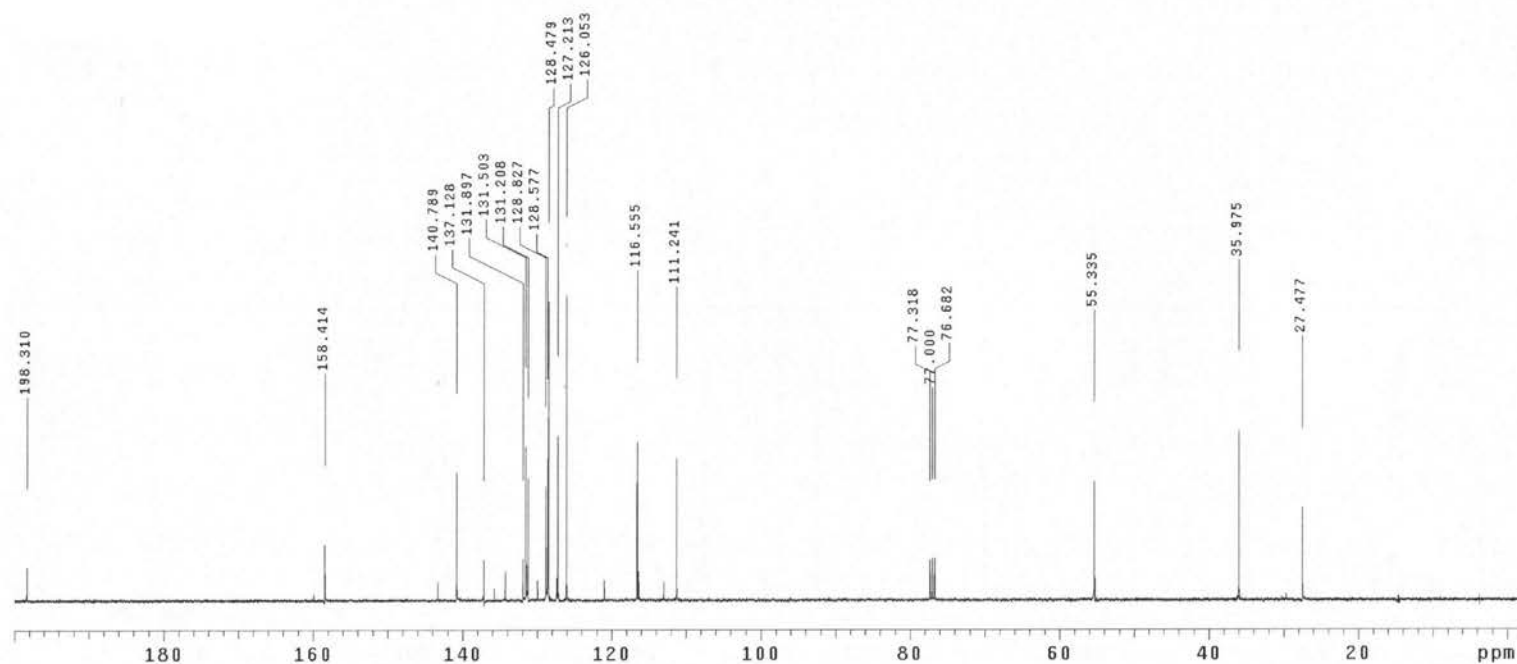
Ambient temperature

Total 2016 repetitions



Compound 4x

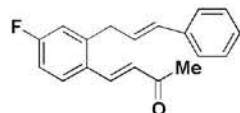
¹³C NMR (100 MHz, CDCl₃) spectra
(EE : EZ = 8 : 1)



Compound 4y (¹H-NMR spectral data)

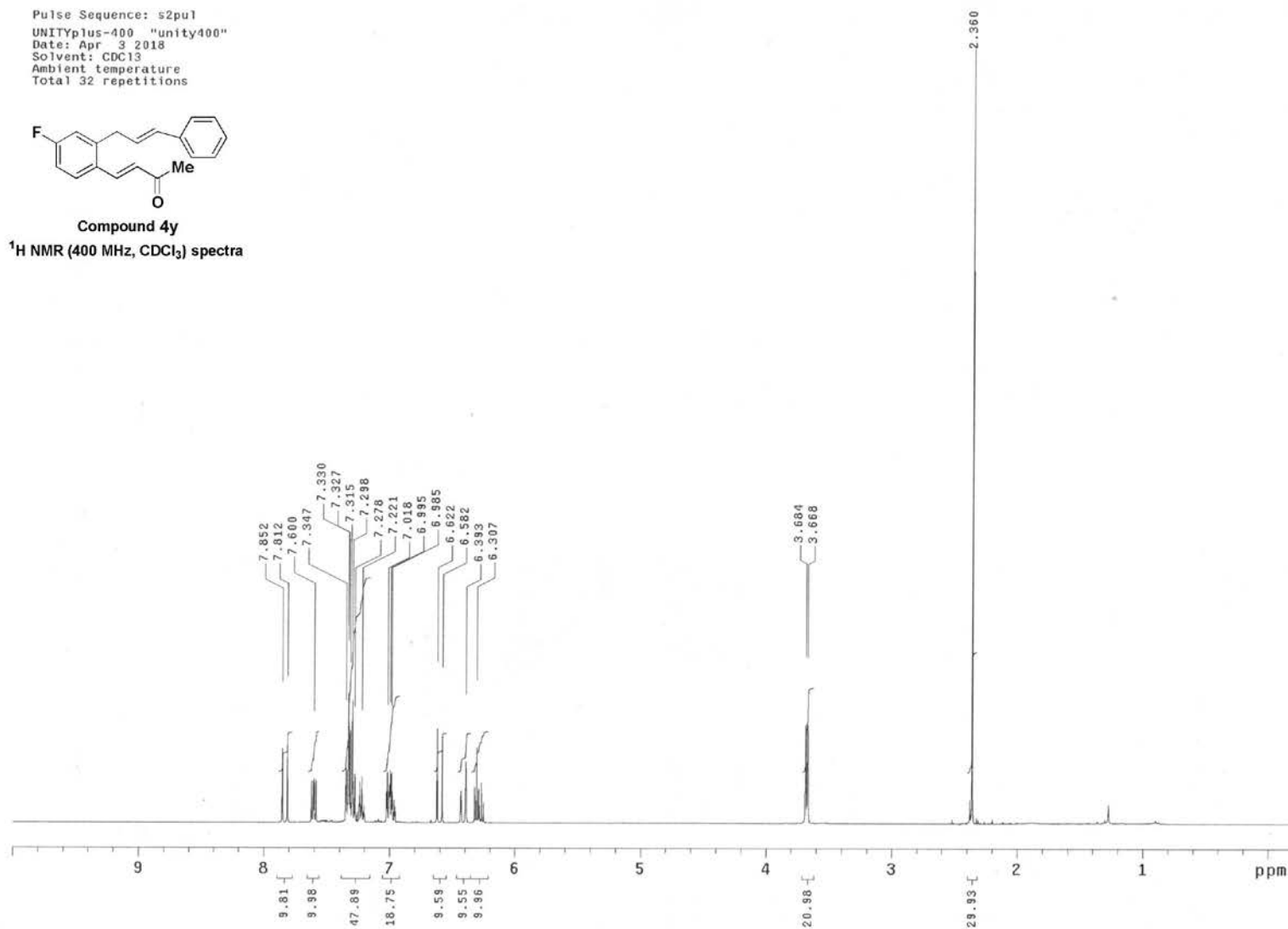
KS1070403

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Apr 3 2018
Solvent: CDCl₃
Ambient temperature
Total 32 repetitions



Compound 4y

¹H NMR (400 MHz, CDCl₃) spectra



Compound 4y (¹³C-NMR spectral data)

KS1070403

Pulse Sequence: s2pu1

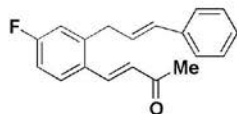
UNITYplus-400 "unity400"

Date: Apr 3 2018

Solvent: CDCl₃

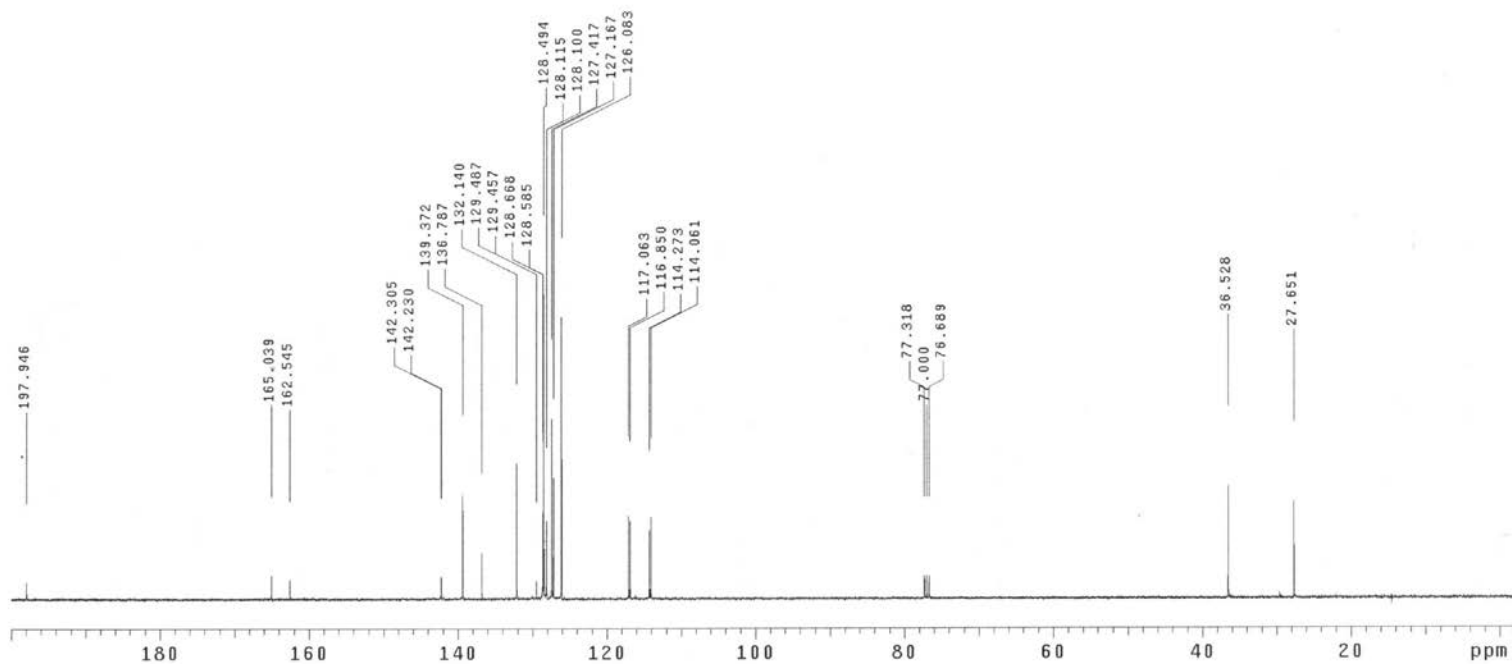
Ambient temperature

Total 336 repetitions



Compound 4y

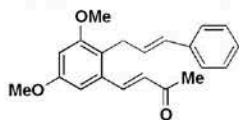
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4z (¹H-NMR spectral data)

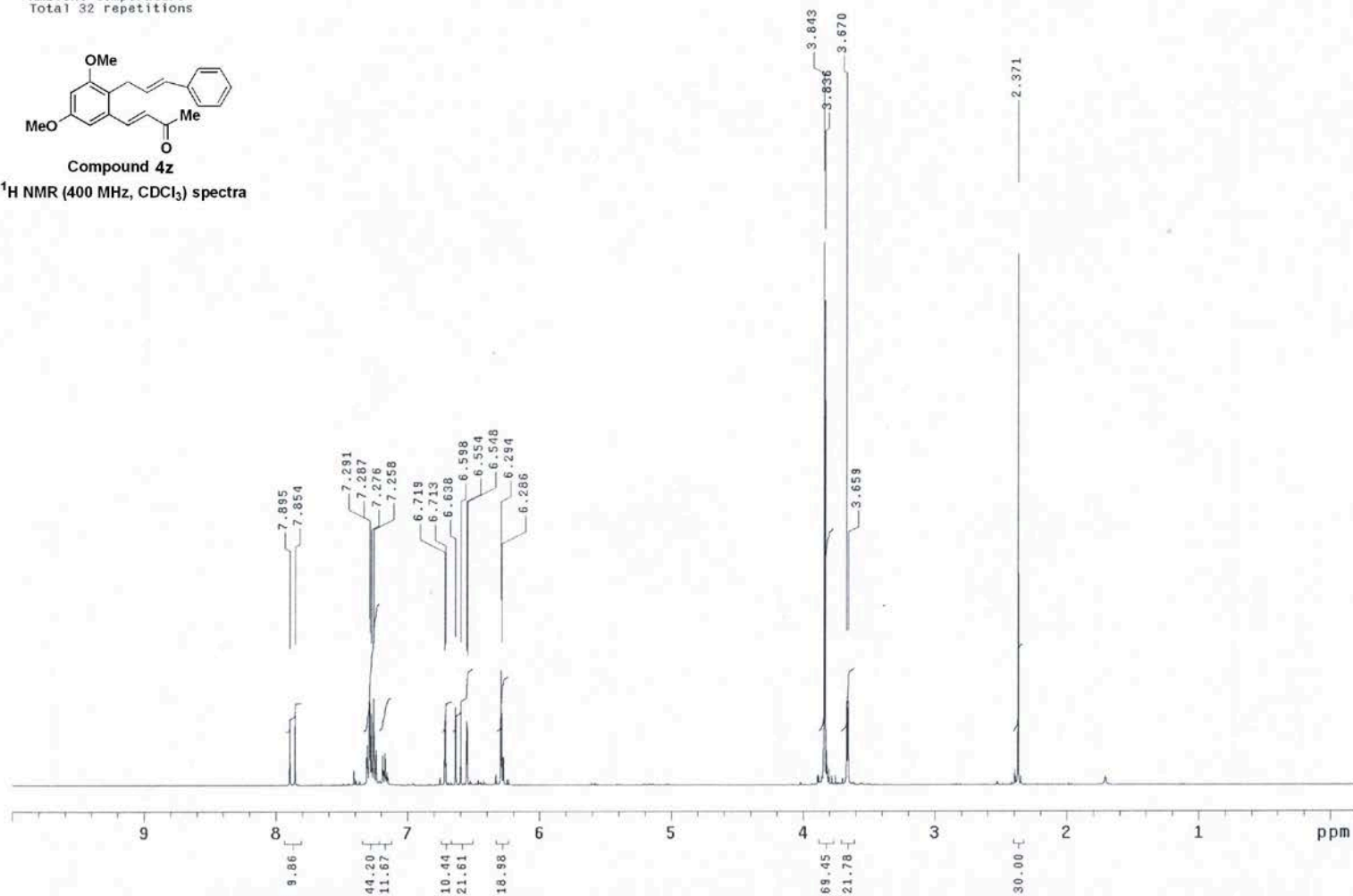
KS1070313

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Mar 14 2018
Solvent: CDCl₃
Ambient temperature
Total 32 repetitions



Compound 4z

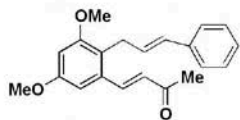
¹H NMR (400 MHz, CDCl₃) spectra



Compound 4z (¹³C-NMR spectral data)

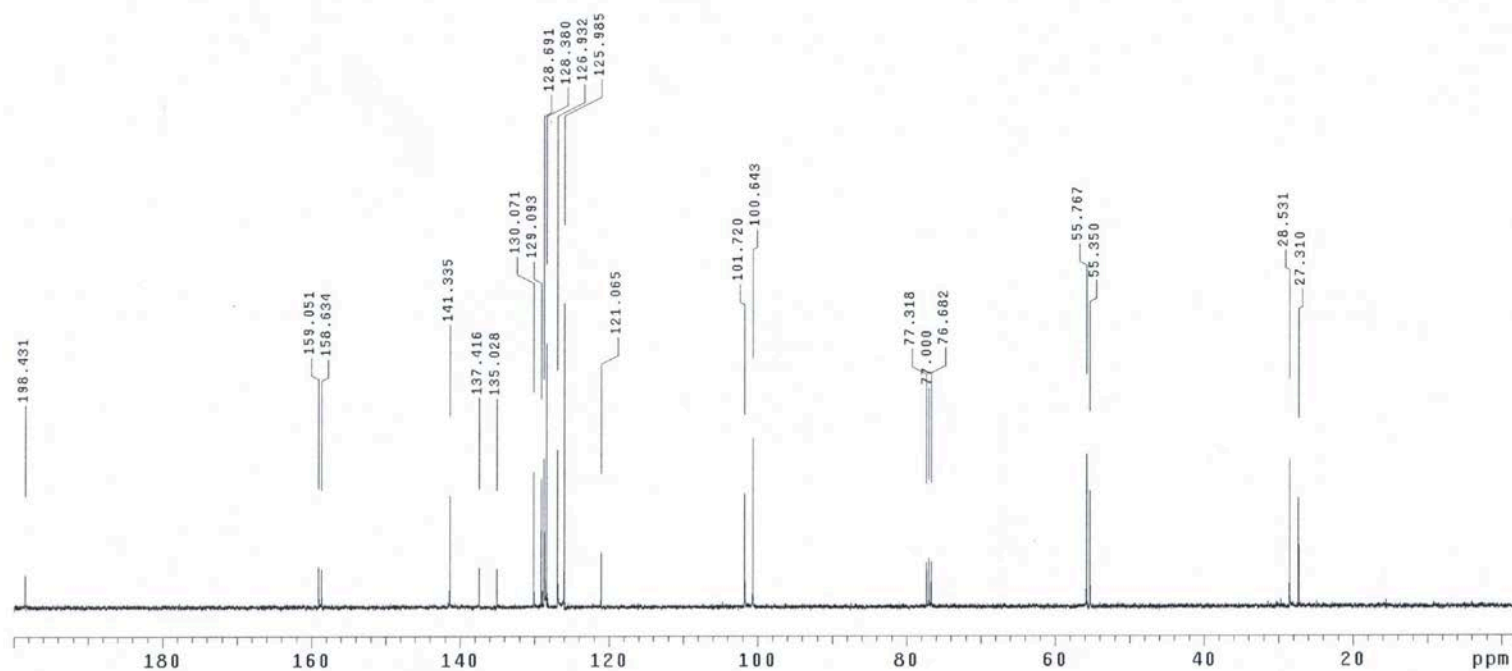
KS1070313

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Mar 14 2018
Solvent: CDCl₃
Ambient temperature
Total 720 repetitions



Compound 4z

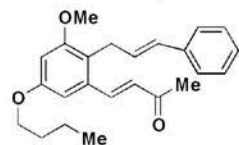
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4aa (¹H-NMR spectral data)

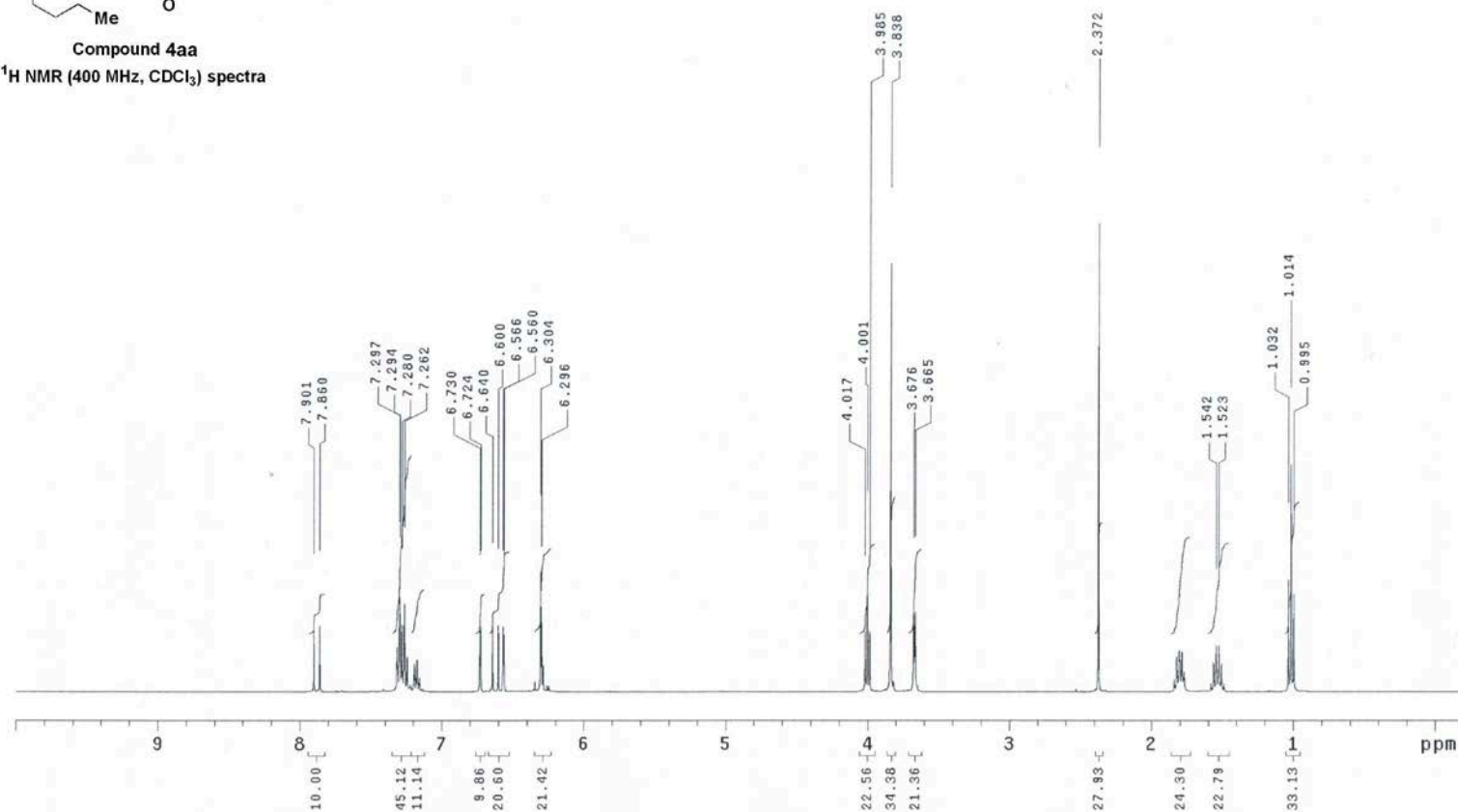
KS1070315

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Mar 15 2018
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetitions



Compound 4aa

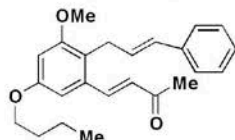
¹H NMR (400 MHz, CDCl₃) spectra



Compound 4aa (¹³C-NMR spectral data)

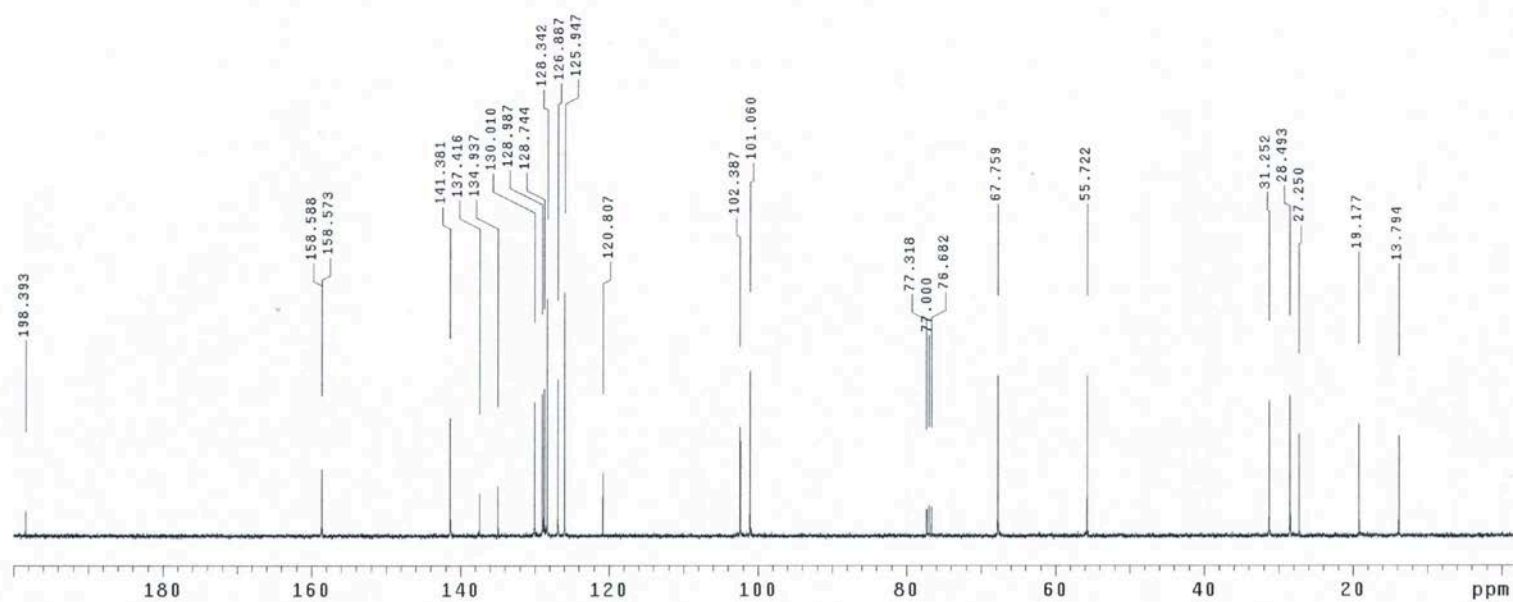
KS1070315

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Mar 15 2018
 Solvent: CDCl₃
 Ambient temperature
 Total 272 repetitions



Compound 4aa

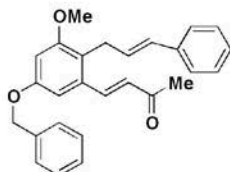
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4ab (¹H-NMR spectral data)

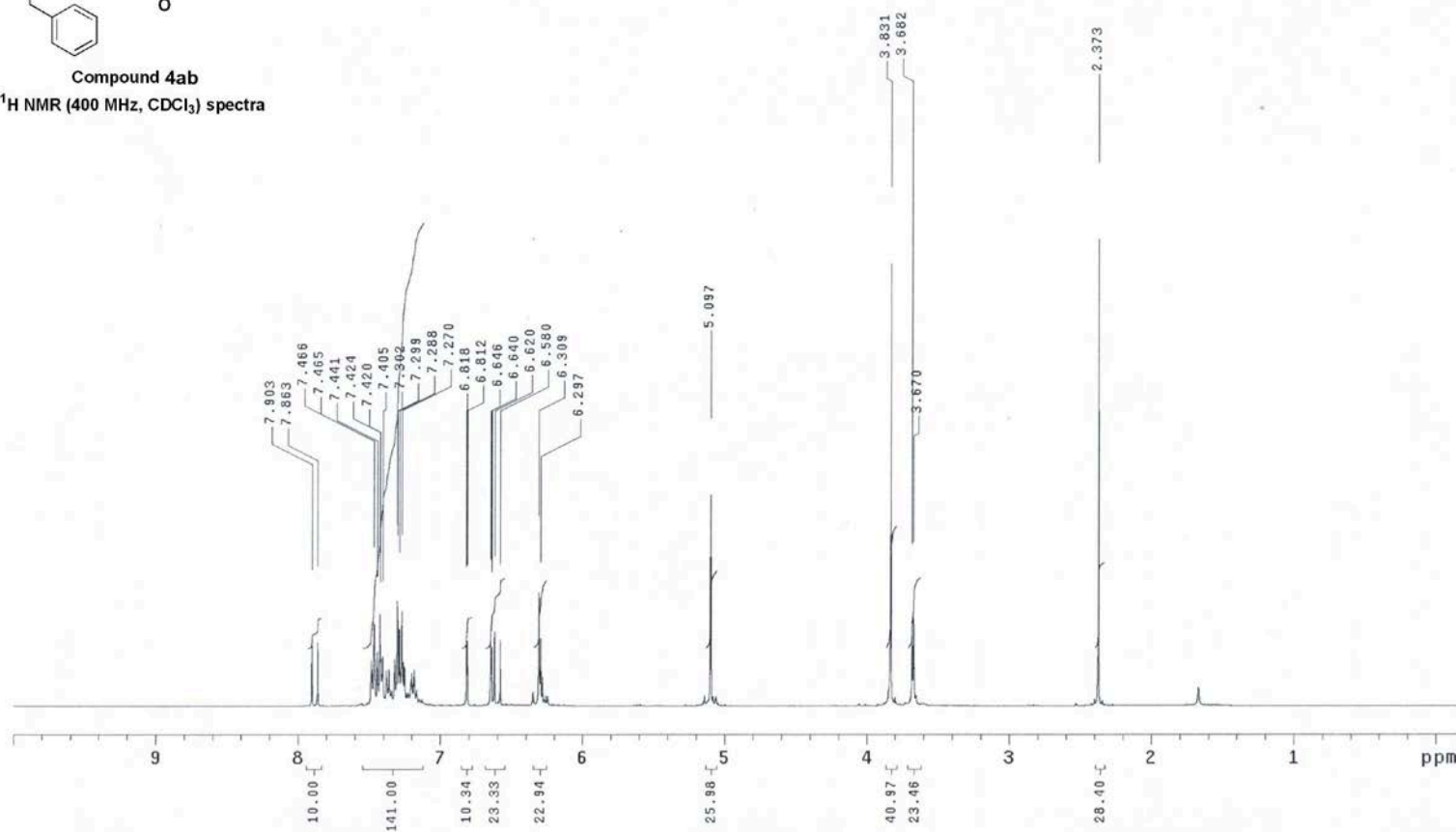
KS1070314

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Mar 14 2018
Solvent: CDCl₃
Ambient temperature
Total 32 repetitions



Compound 4ab

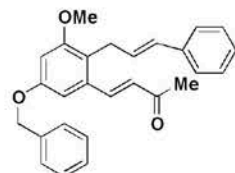
¹H NMR (400 MHz, CDCl₃) spectra



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

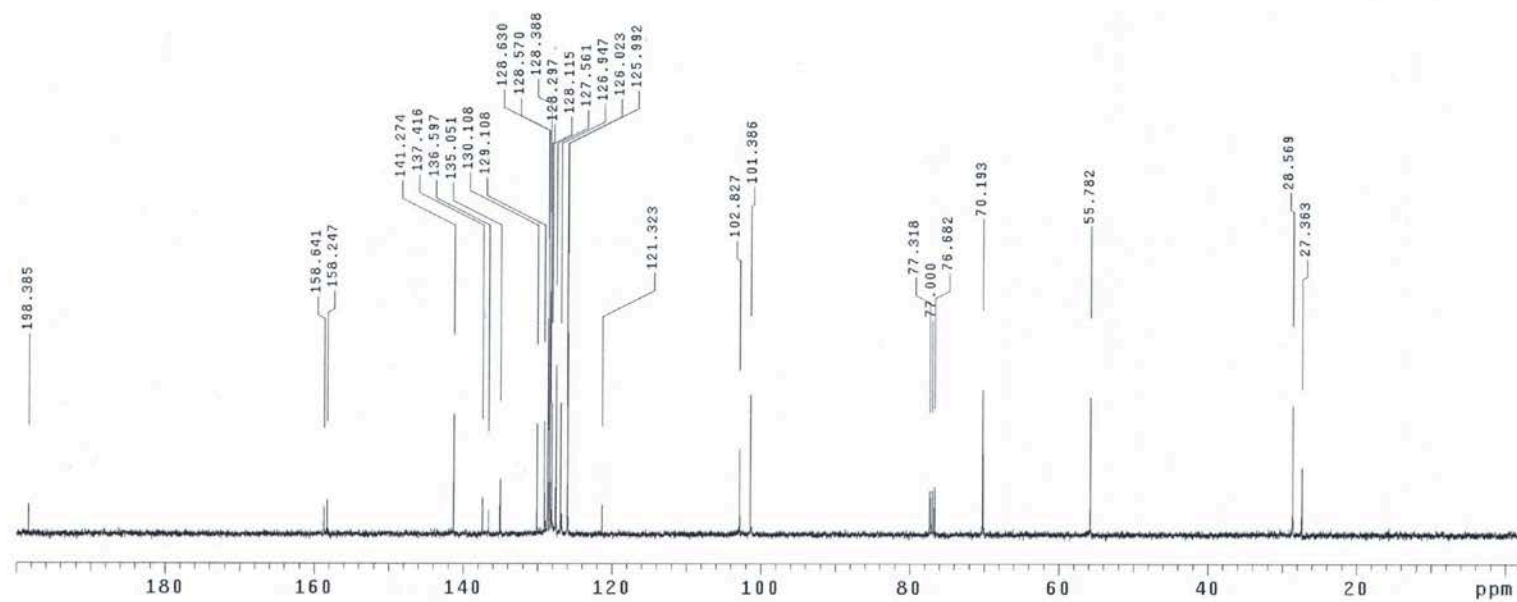
KS1070314

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Mar 14 2018
Solvent: CDCl_3
Ambient temperature
Total 576 repetitions



Compound 4ab

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



Compound 6a (¹H-NMR spectral data)

NC1060824

Pulse Sequence: s2pu1

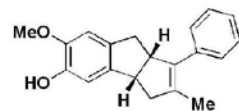
UNITYplus-400 "unity400"

Date: Aug 28 2017

Solvent: CDCl₃

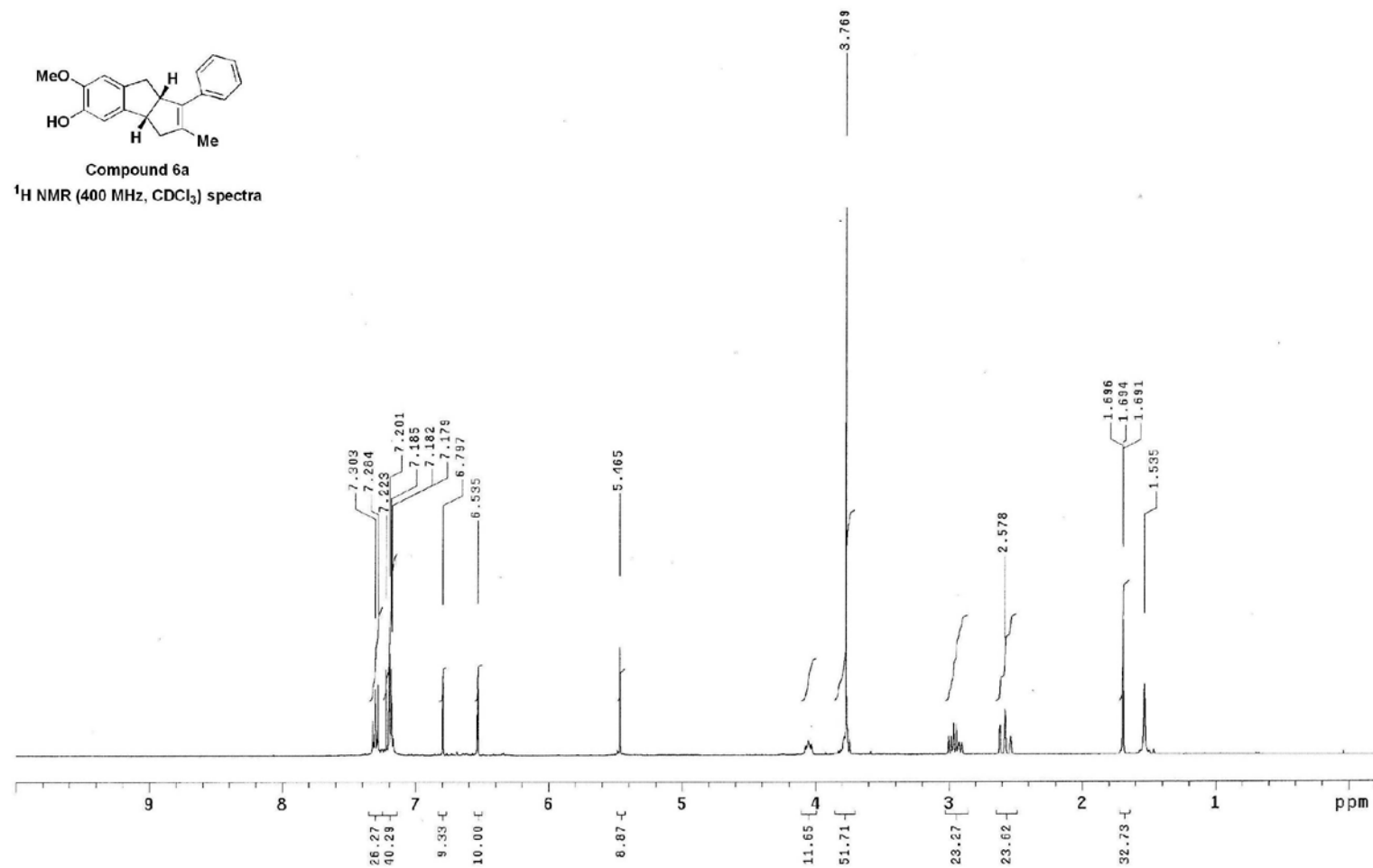
Ambient temperature

Total 64 repetitions



Compound 6a

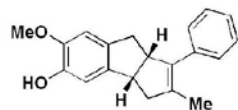
¹H NMR (400 MHz, CDCl₃) spectra



Compound 6a (¹³C-NMR spectral data)

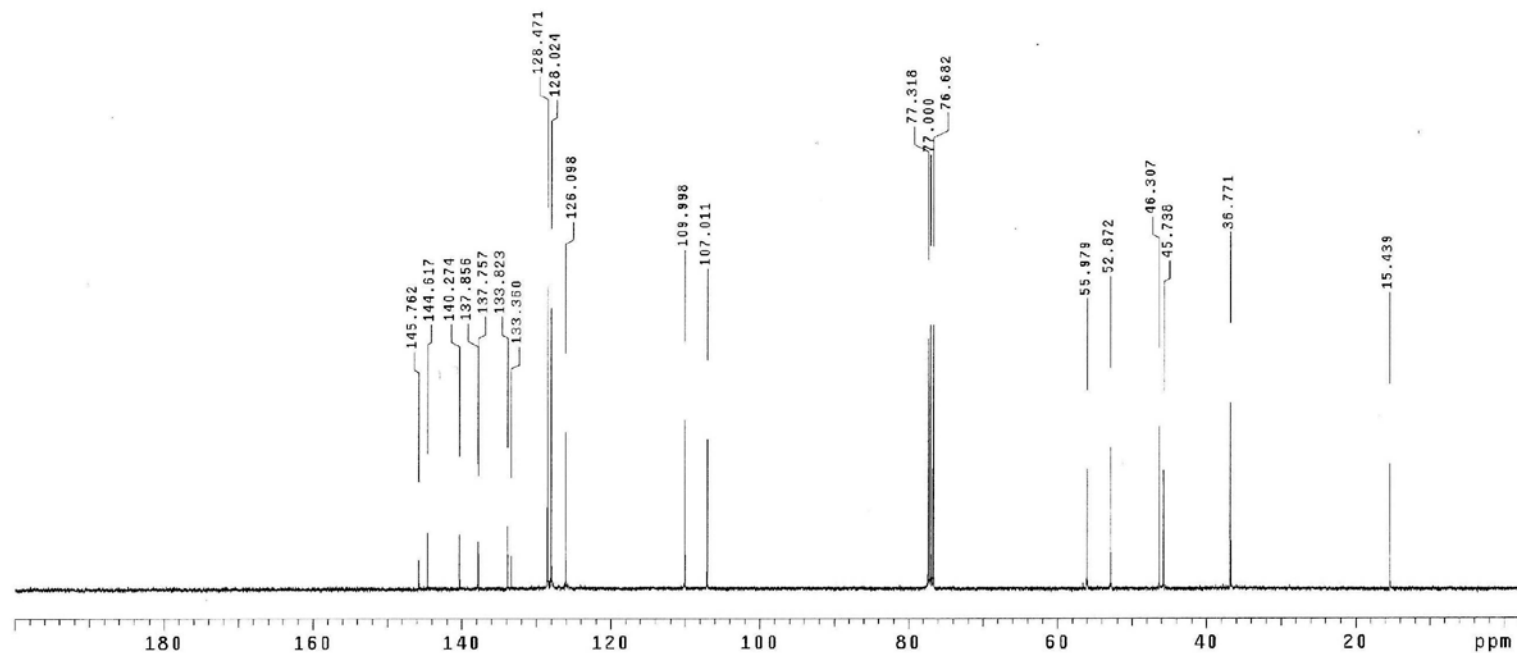
NC1060824

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Aug 28 2017
Solvent: CDCl₃
Ambient temperature
Total 20480 repetitions



Compound 6a

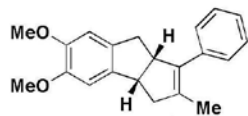
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 6b (¹H-NMR spectral data)

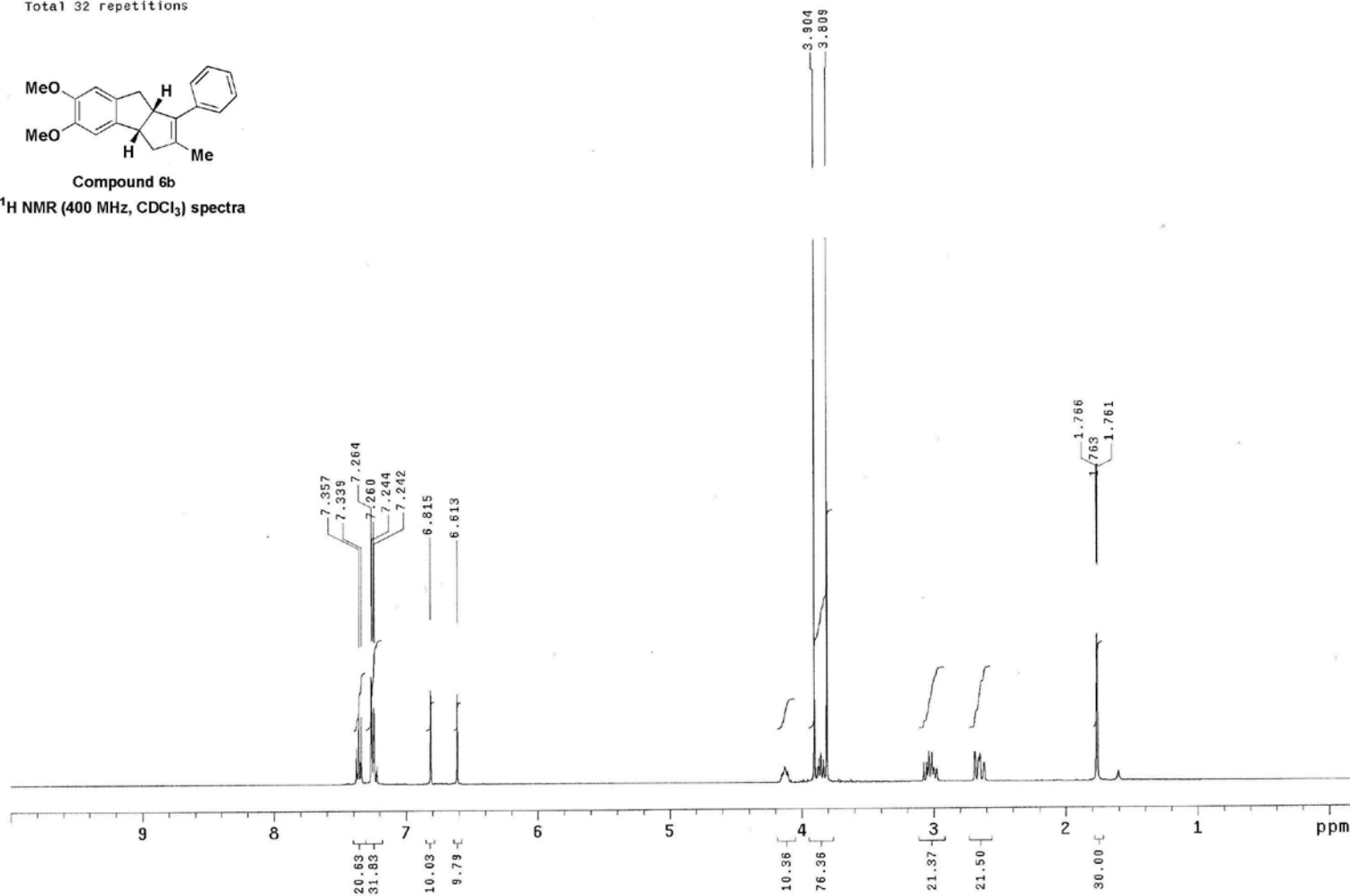
NC1060906

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Sep 7 2017
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetitions



Compound 6b

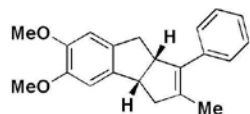
¹H NMR (400 MHz, CDCl₃) spectra



Compound 6b (¹³C-NMR spectral data)

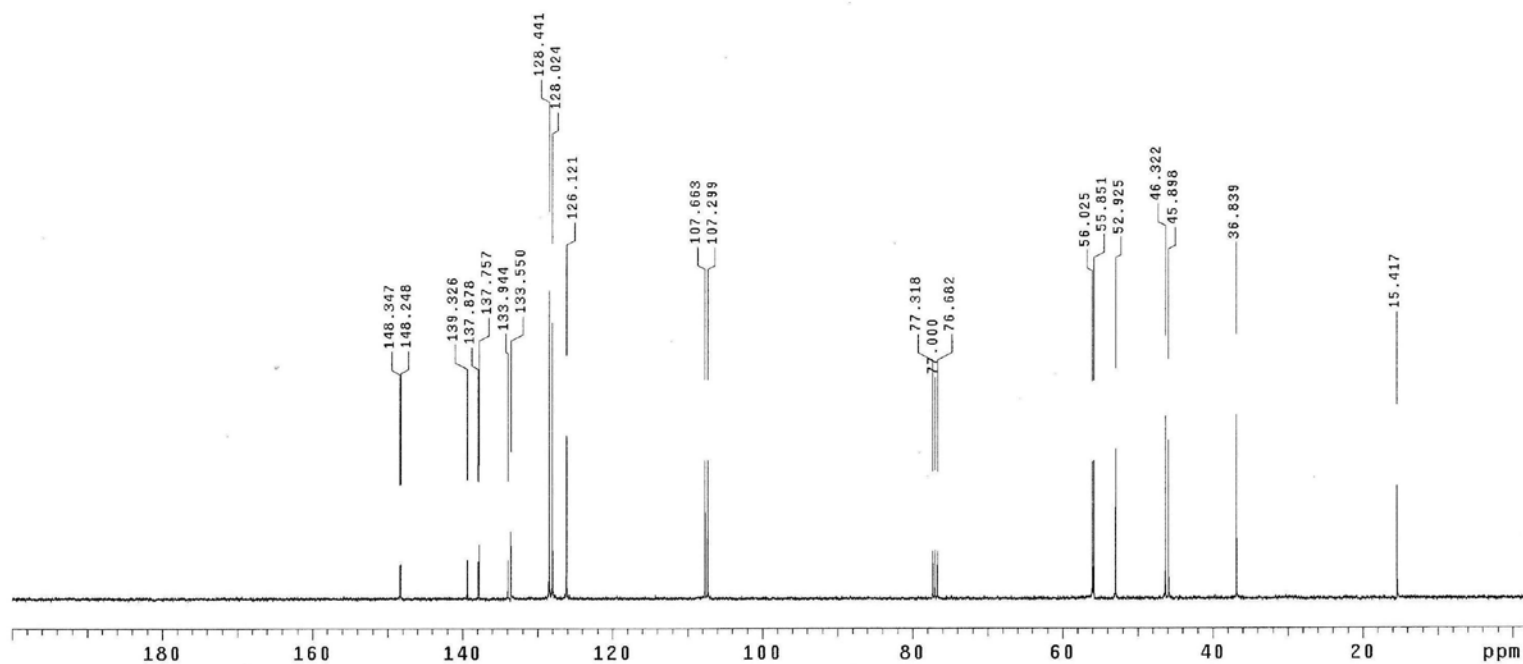
NC1060906

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Sep 7 2017
Solvent: CDCl₃
Ambient temperature
Total 1024 repetitions



Compound 6b

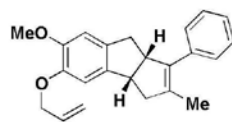
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 6c (¹H-NMR spectral data)

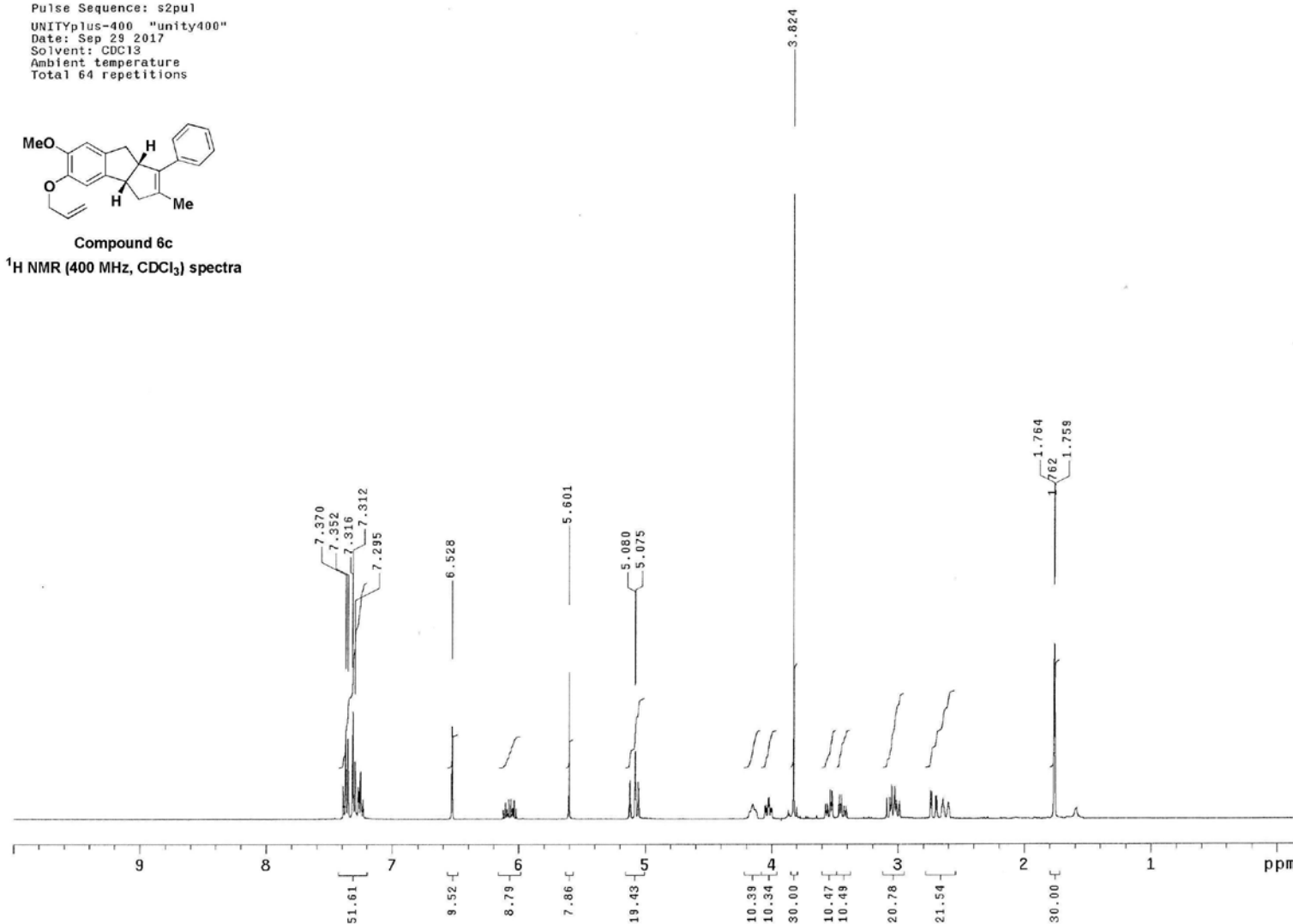
NC1060928

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Sep 29 2017
 Solvent: CDCl₃
 Ambient temperature
 Total 64 repetitions



Compound 6c

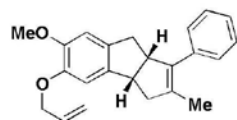
¹H NMR (400 MHz, CDCl₃) spectra



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

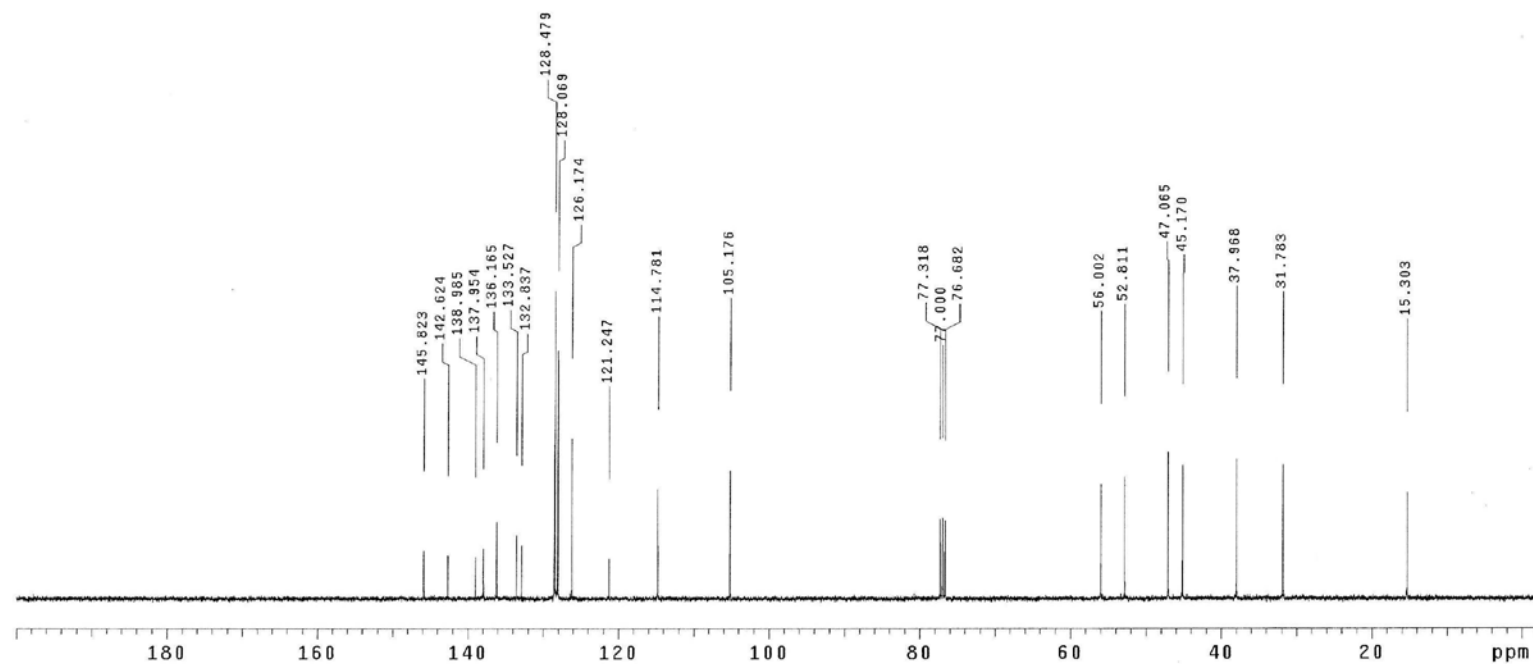
NC1060928

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Sep 29 2017
Solvent: CDCl_3
Ambient temperature
Total 736 repetitions



Compound 6c

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



Compound 6d (¹H-NMR spectral data)

NC1061002

Pulse Sequence: s2pu1

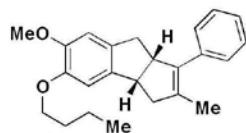
UNITYplus-400 "unity400"

Date: Oct 2 2017

Solvent: CDCl₃

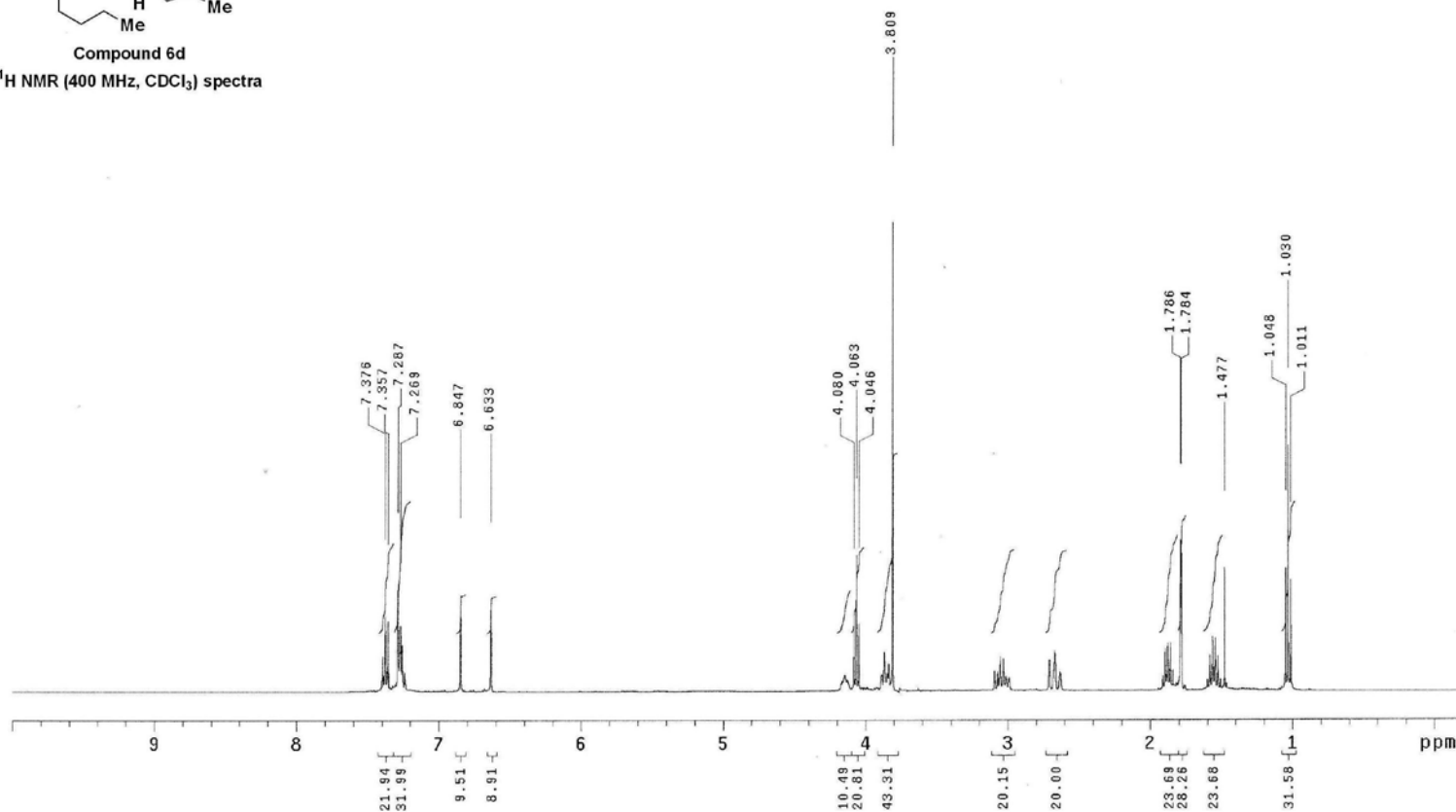
Ambient temperature

Total 32 repetitions



Compound 6d

¹H NMR (400 MHz, CDCl₃) spectra



Compound 6d (¹³C-NMR spectral data)

NC1061002

Pulse Sequence: s2pu1

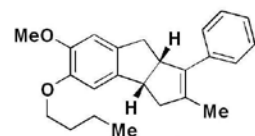
UNITYplus-400 "unity400"

Date: Oct 2 2017

Solvent: CDCl₃

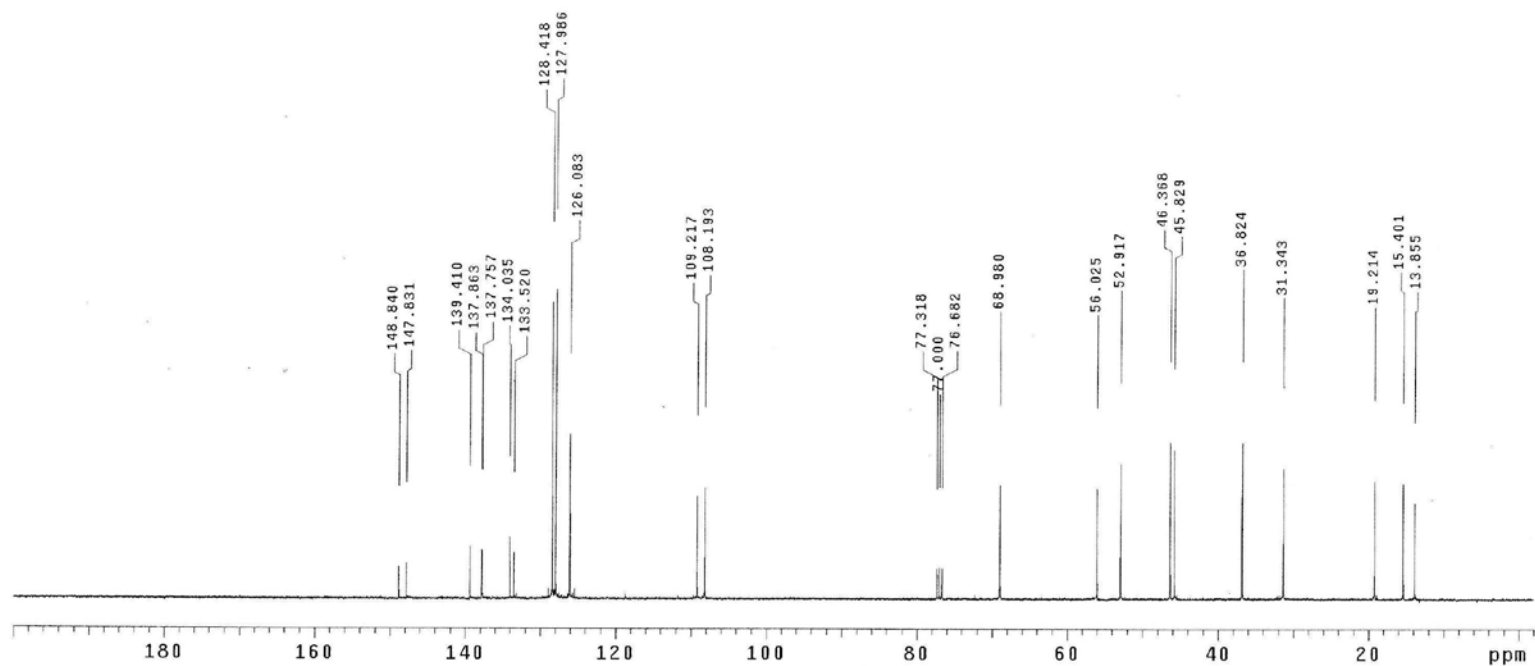
Ambient temperature

Total 864 repetitions



Compound 6d

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 6e (¹H-NMR spectral data)

NC1061127

Pulse Sequence: s2pu1

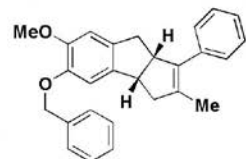
UNITYplus-400 "unity400"

Date: Nov 28 2017

Solvent: CDCl₃

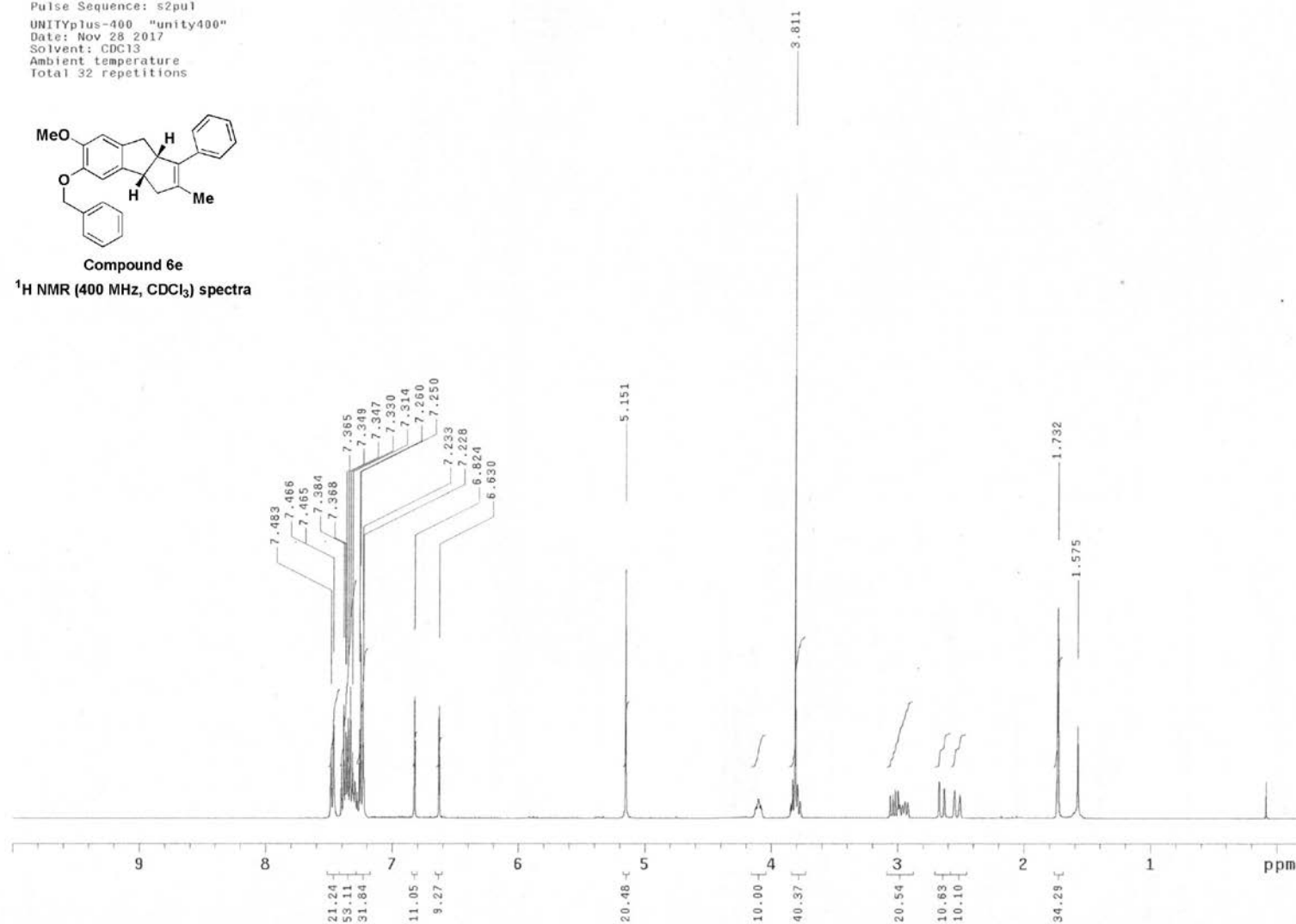
Ambient temperature

Total 32 repetitions



Compound 6e

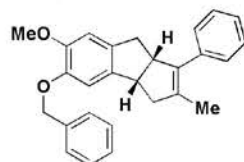
¹H NMR (400 MHz, CDCl₃) spectra



Compound 6e (¹³C-NMR spectral data)

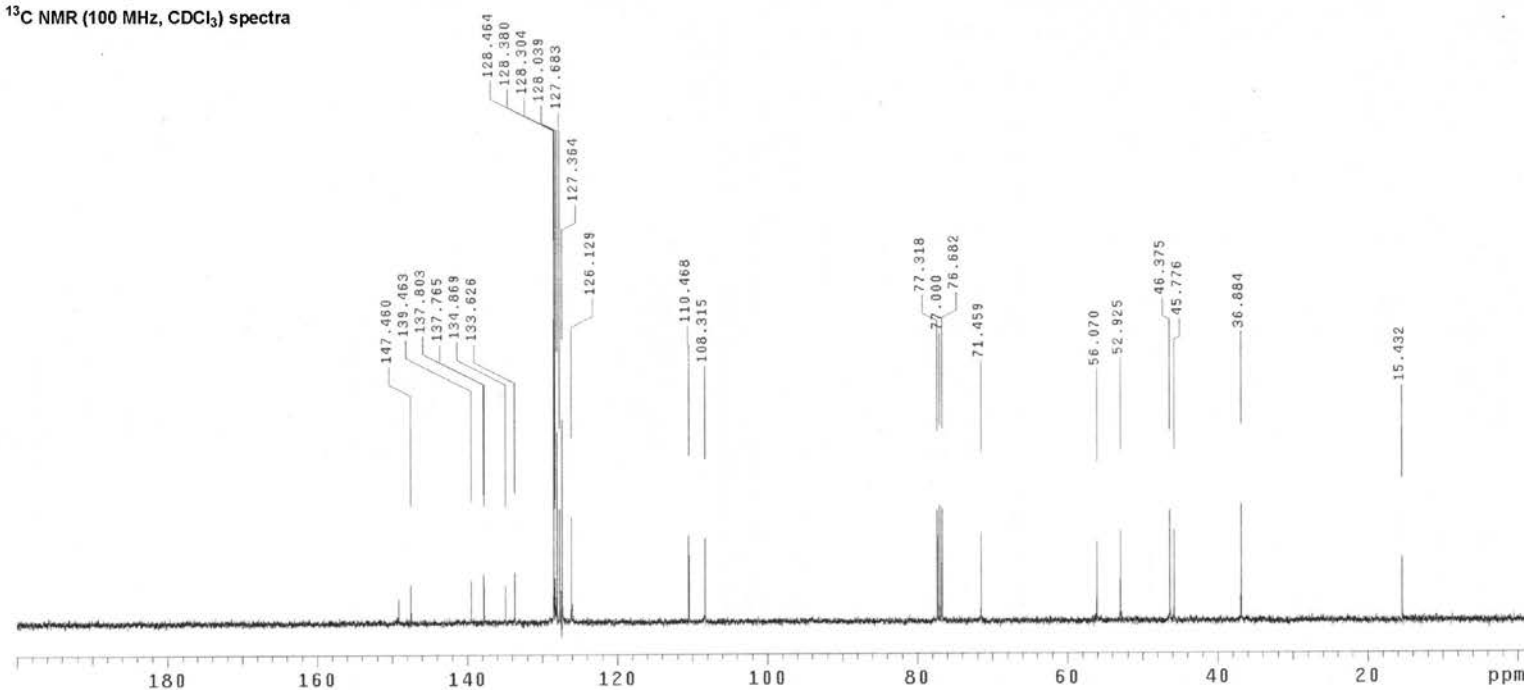
NC1061127

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Nov 28 2017
 Solvent: CDCl₃
 Ambient temperature
 Total 2096 repetitions



Compound 6e

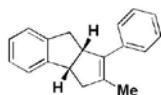
¹³C NMR (100 MHz, CDCl₃) spectra



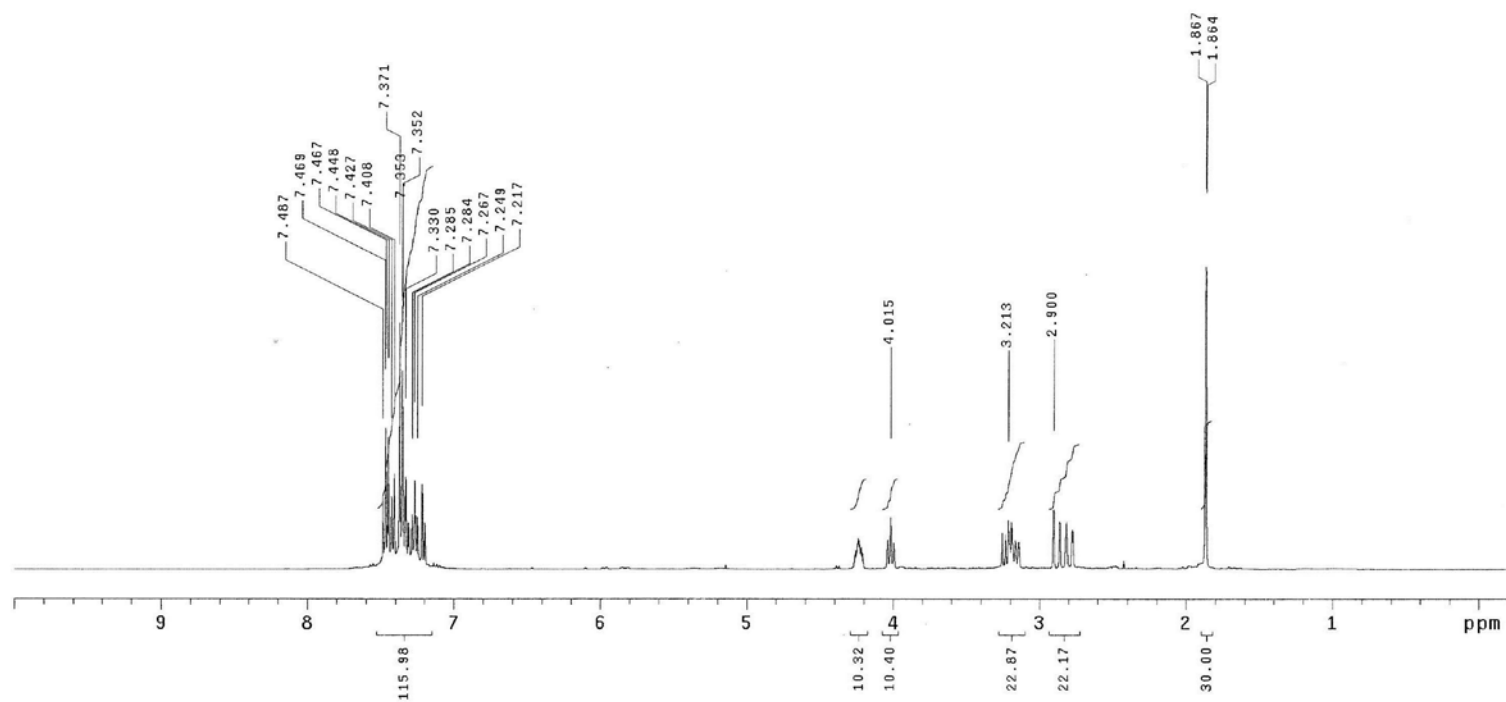
Compound 6n (¹H-NMR spectral data)

NC1060926

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Sep 26 2017
Solvent: CDCl₃
Ambient temperature
Total 32 repetitions



Compound 6n
¹H NMR (400 MHz, CDCl₃) spectra



Compound 6n (¹³C-NMR spectral data)

NC1060926

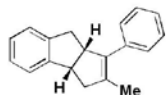
Pulse Sequence: s2pu1

UNITYplus-400 "unity400"

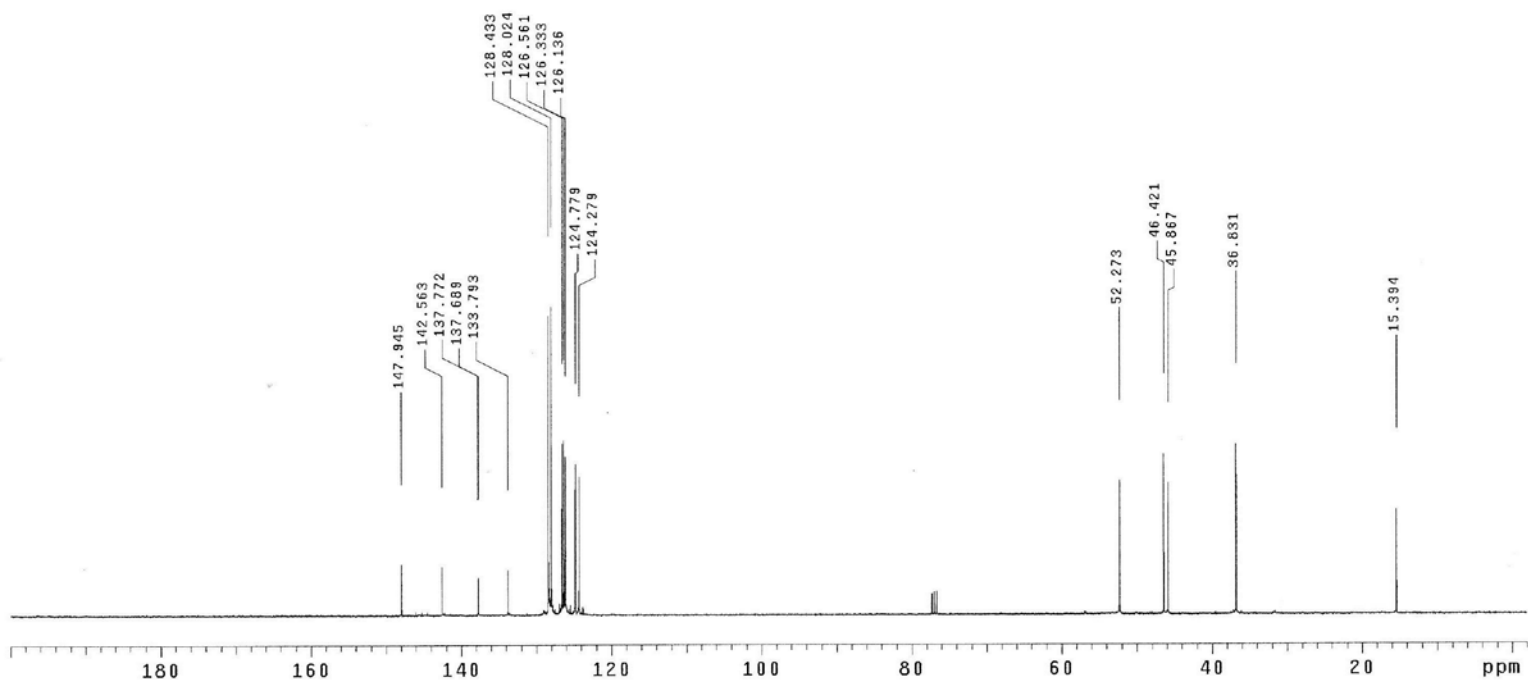
Date: Sep 26 2017

Solvent: CDCl₃
Ambient temperature

Ambient temperature
Total 432 repetitions



Compound 6n

¹³C NMR (100 MHz, CDCl₃) spectra

Compound 6y (¹H-NMR spectral data)

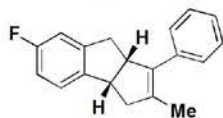
Pulse Sequence: s2pu1

UNITYplus-400 "unity400"

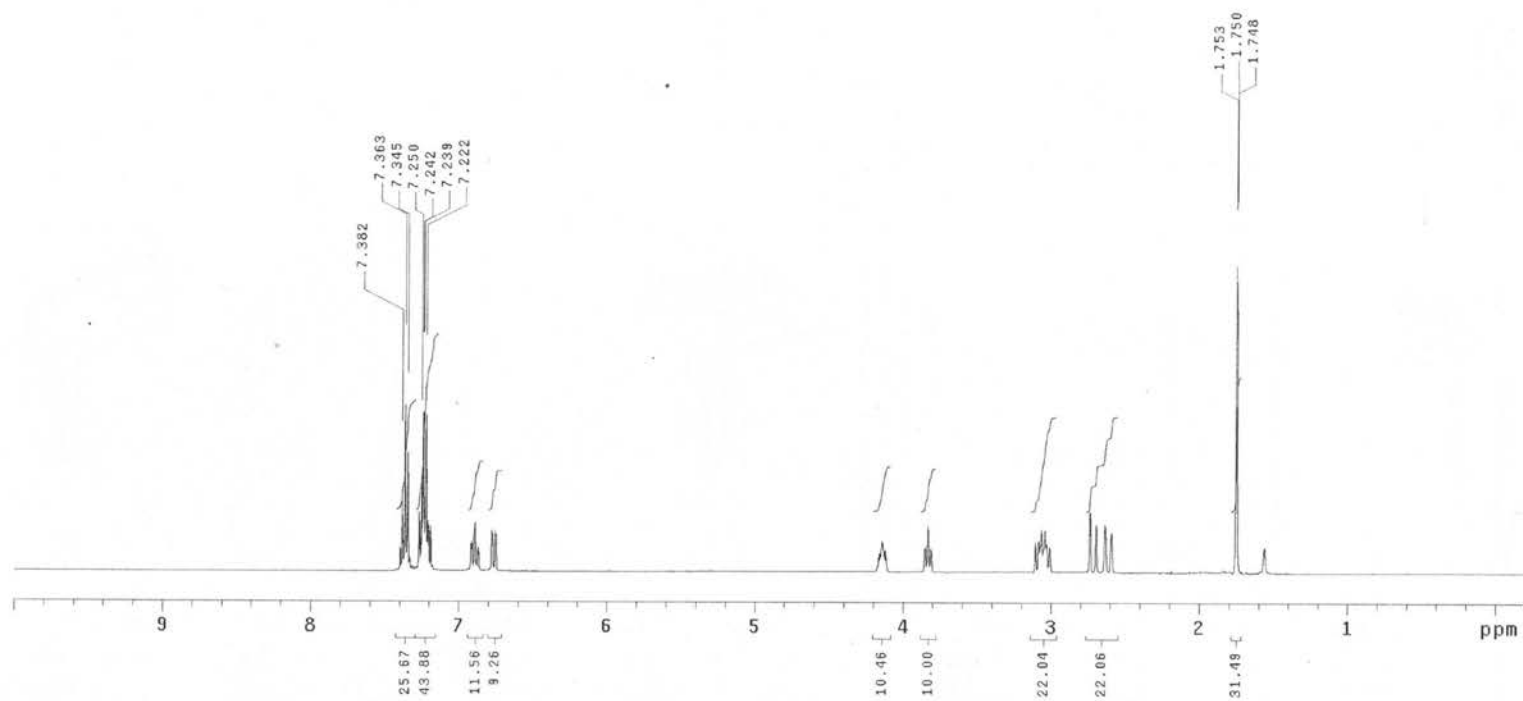
Date: Nov 23 2017

Solvent: CDCl₃
Ambient temperature

Ambient temperature
Total 64 repetitions



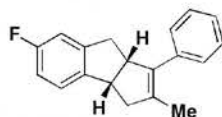
Compound 6y

¹H NMR (400 MHz, CDCl₃) spectra

Compound 6y (¹³C-NMR spectral data)

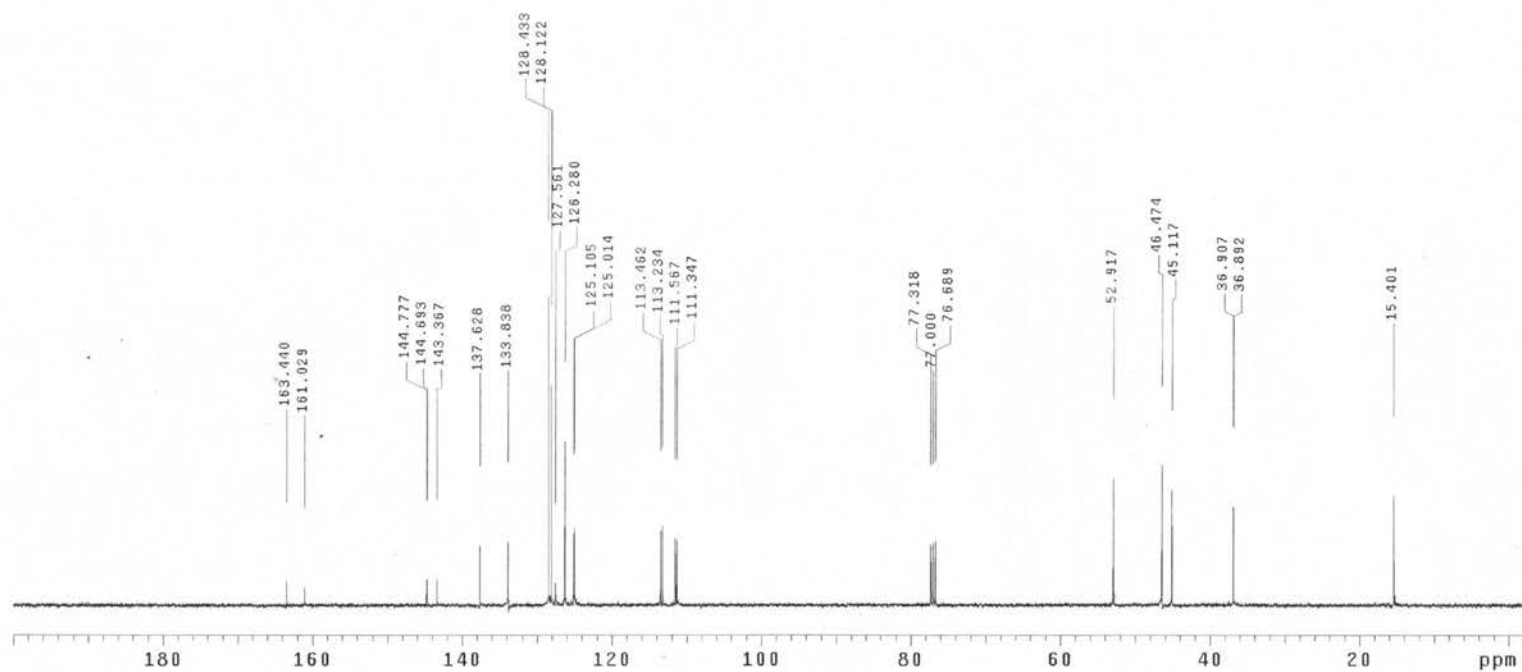
NC1061122

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Nov 23 2017
Solvent: CDCl₃
Ambient temperature
Total 2080 repetitions



Compound 6y

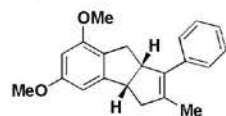
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 6z (¹H-NMR spectral data)

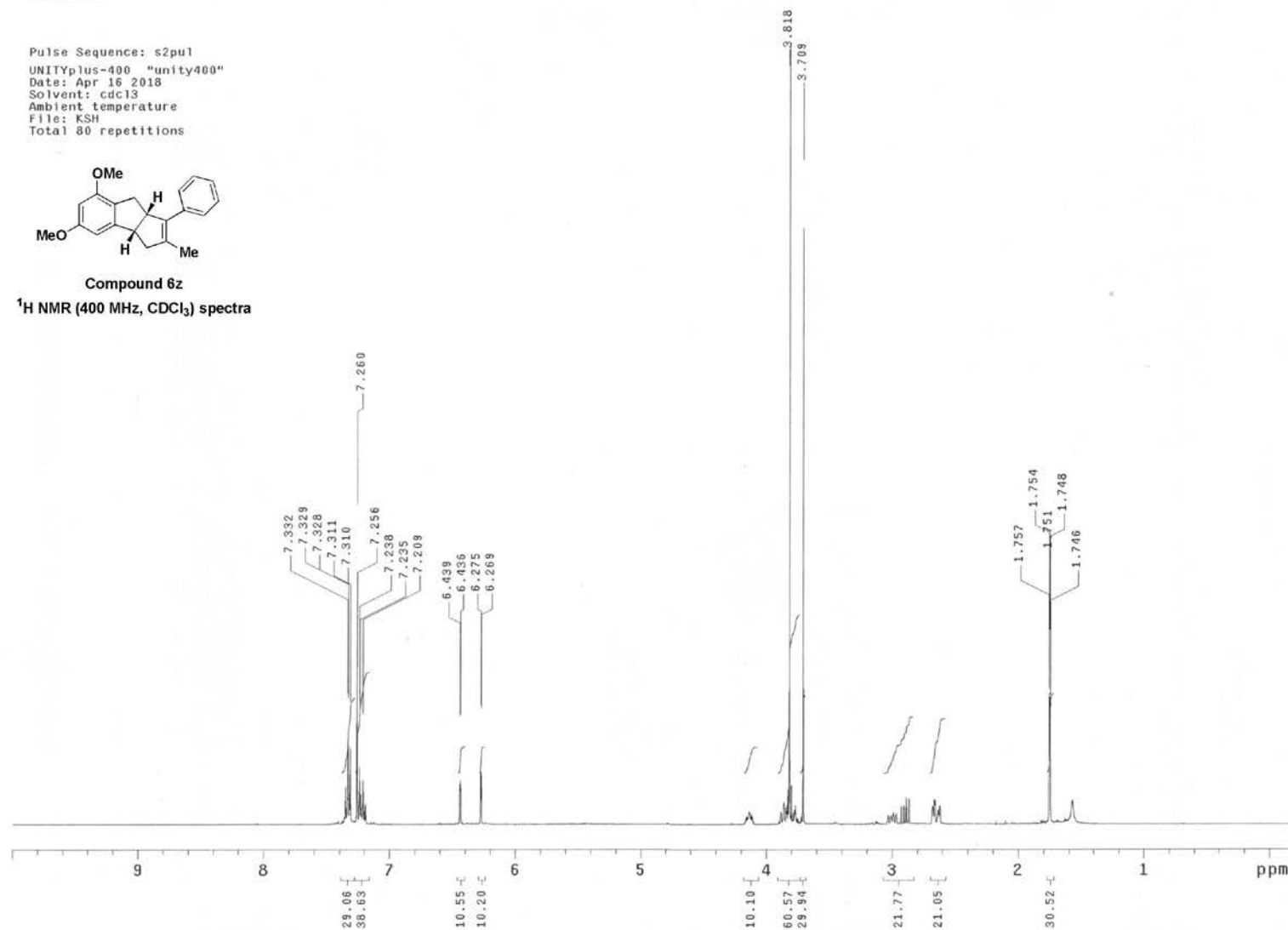
KS1070413

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Apr 16 2018
Solvent: cdcl3
Ambient temperature
File: KSH
Total 80 repetitions



Compound 6z

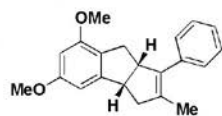
¹H NMR (400 MHz, CDCl₃) spectra



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

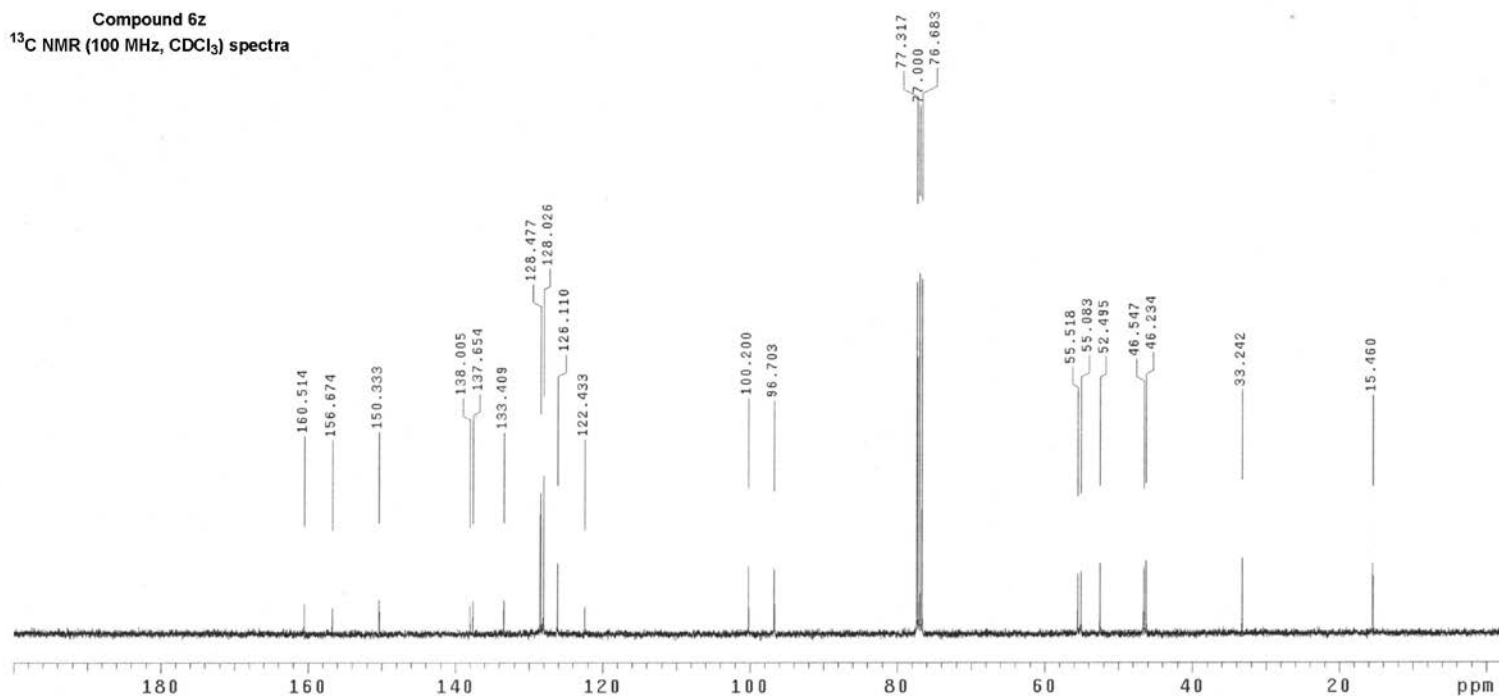
KS1070413

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Apr 16 2018
Solvent: CDCl_3
Ambient temperature
File: KSC
Total 624 repetitions

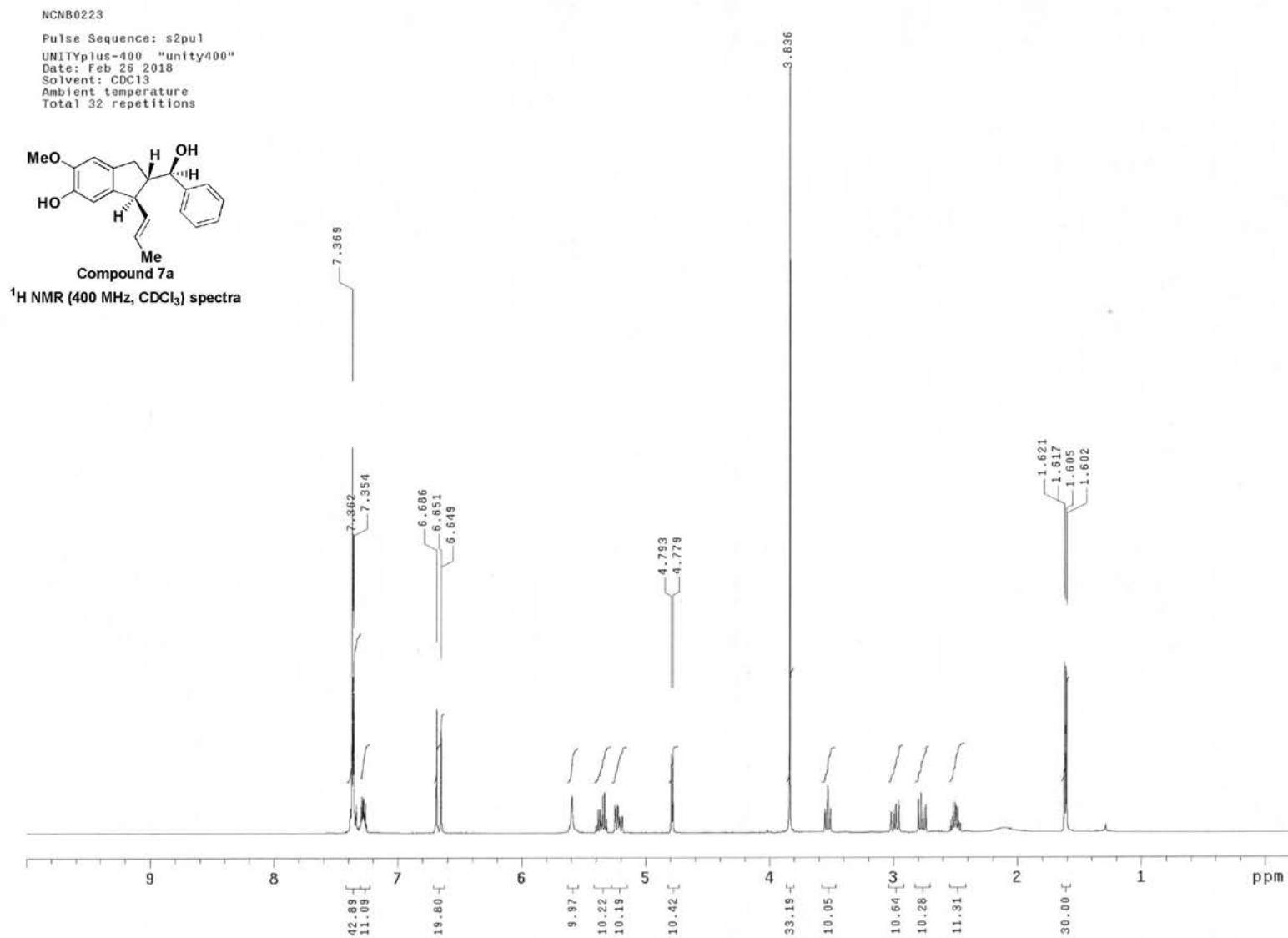


Compound 6z

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



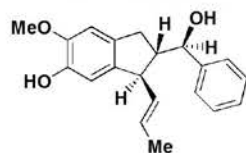
Compound 7a (¹H-NMR spectral data)



Compound 7a (¹³C-NMR spectral data)

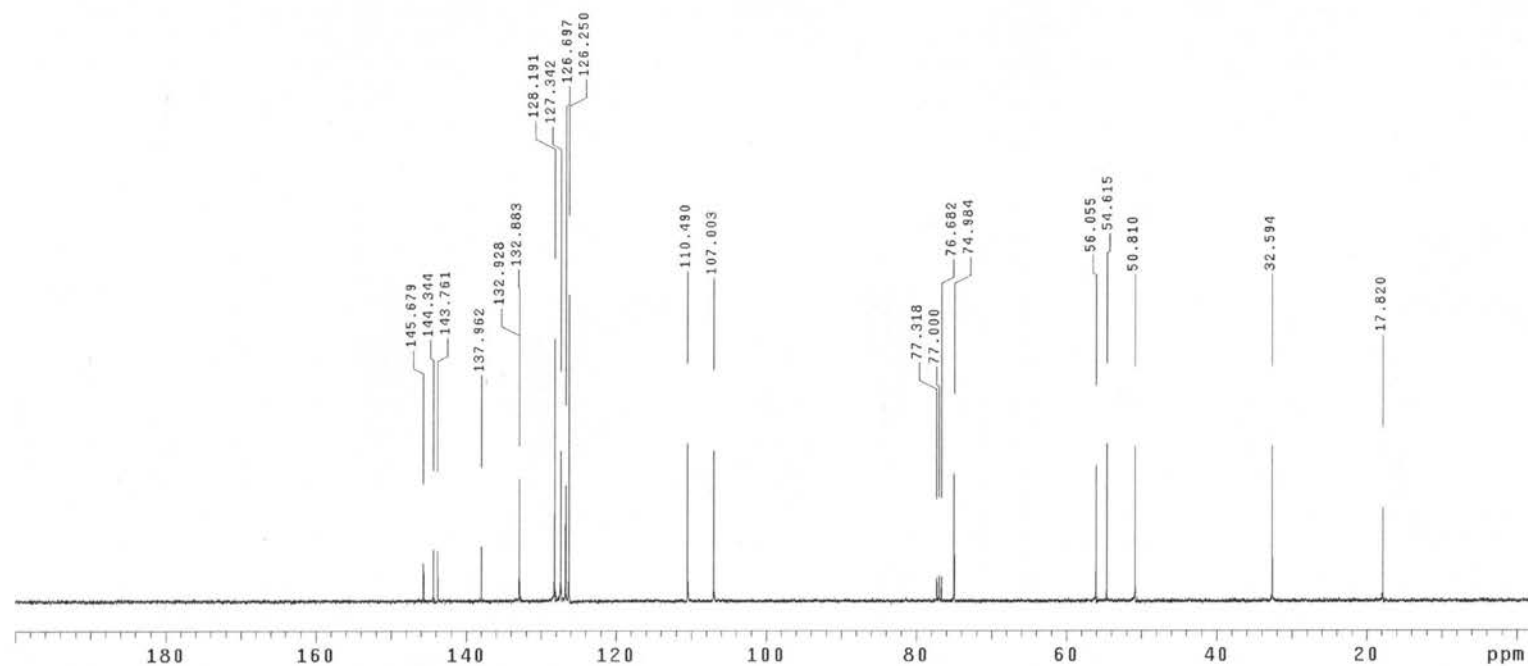
NCNB0223

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Feb 26 2018
 Solvent: CDCl₃
 Ambient temperature
 Total 320 repetitions



Compound 7a

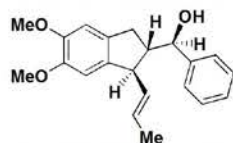
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 7b (¹H-NMR spectral data)

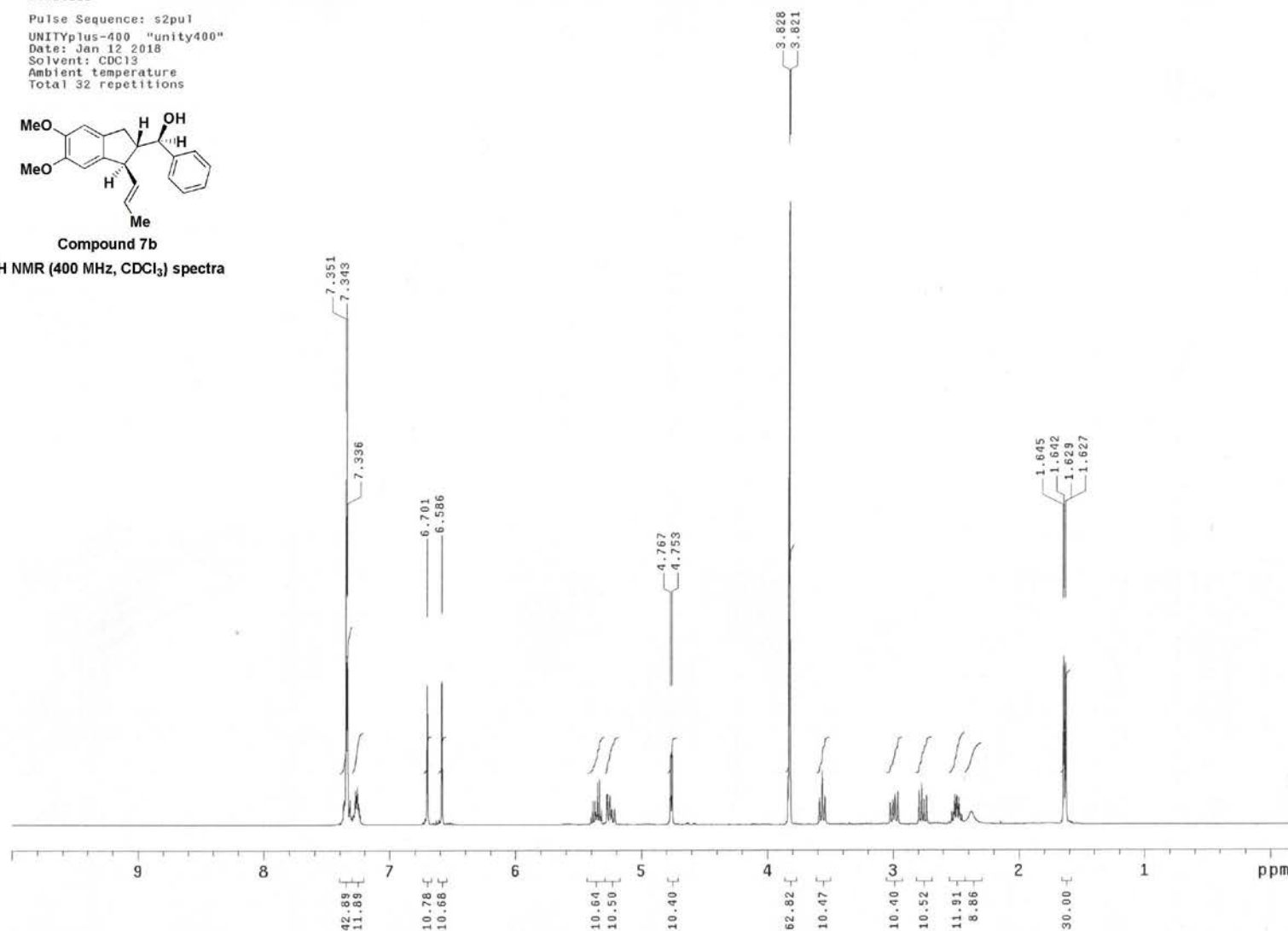
NCNB0111

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Jan 12 2018
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetitions



Compound 7b

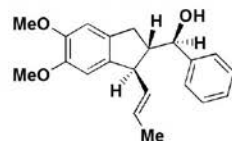
¹H NMR (400 MHz, CDCl₃) spectra



Compound 7b (¹³C-NMR spectral data)

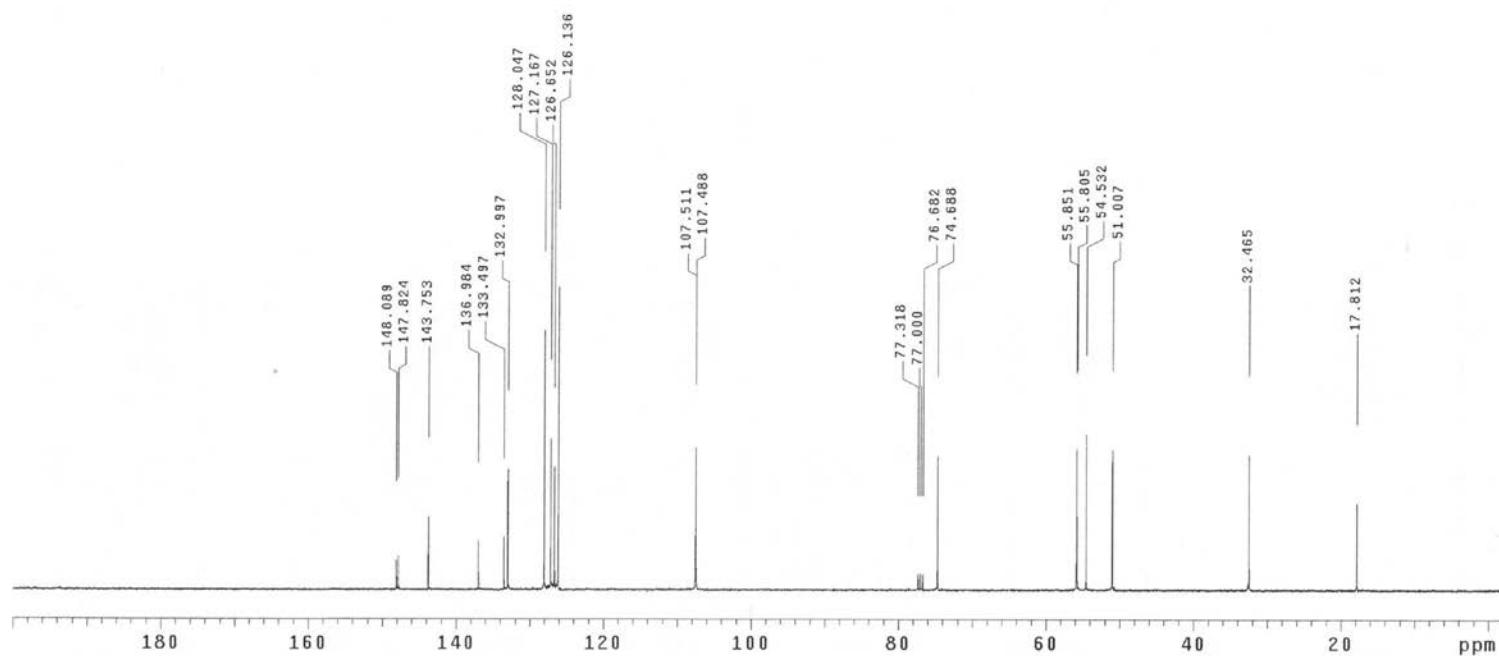
NCNB0111

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Jan 12 2018
Solvent: CDCl₃
Ambient temperature
Total 352 repetitions



Compound 7b

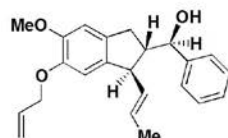
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 7c (¹H-NMR spectral data)

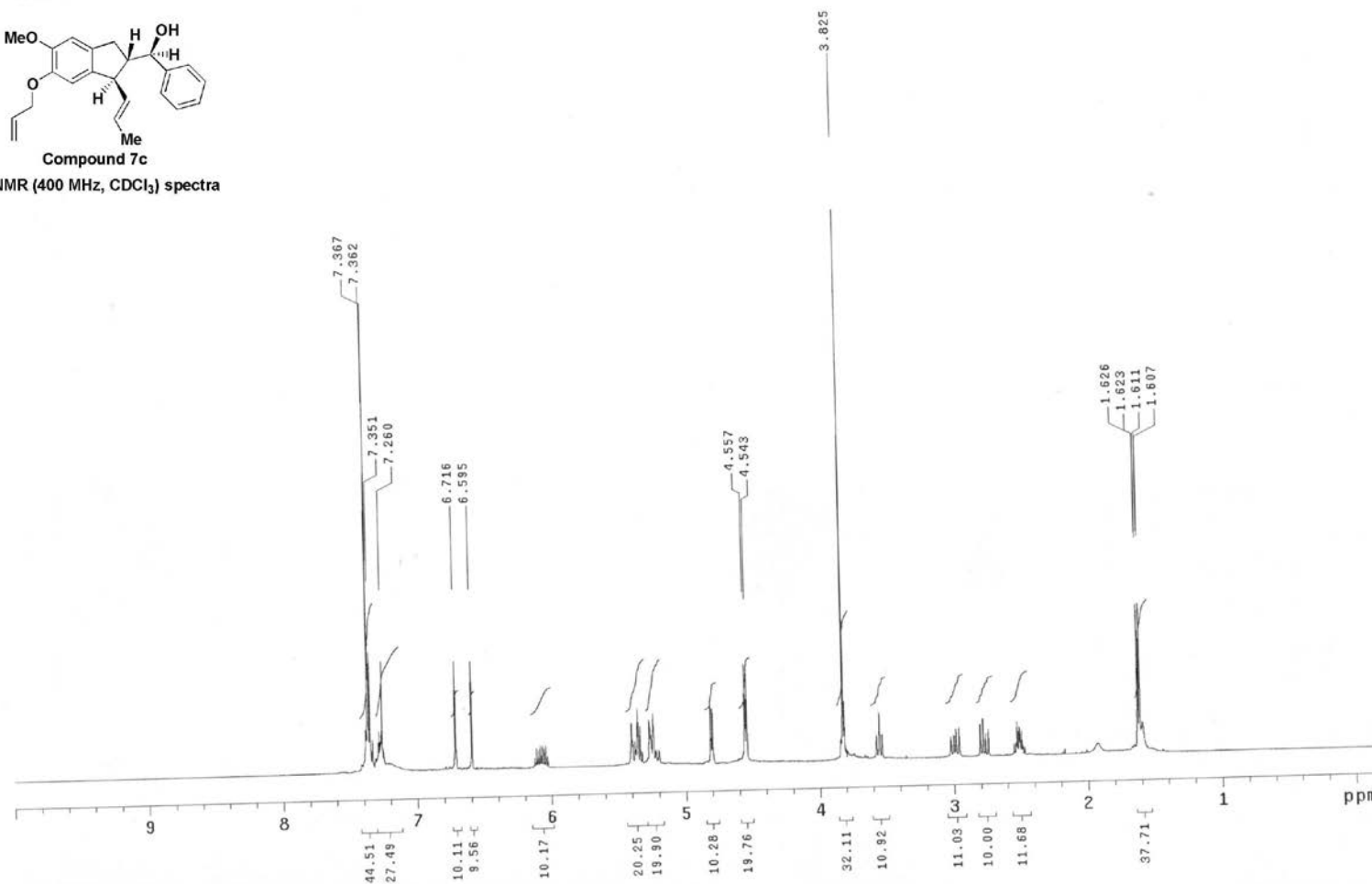
NCNB0131

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Feb 5 2018
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetitions



Compound 7c

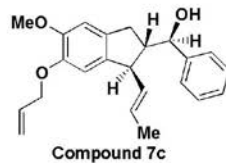
¹H NMR (400 MHz, CDCl₃) spectra



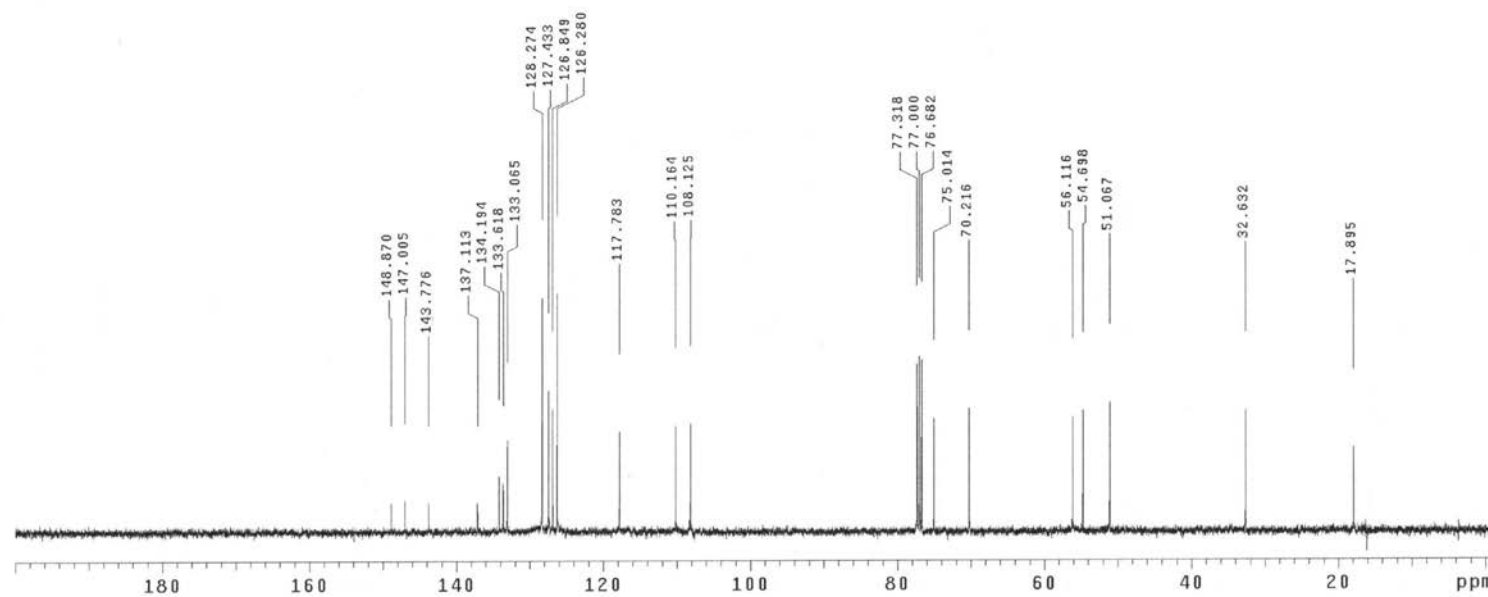
Compound 7c (^{13}C -NMR spectral data)

NCNB0131

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Feb 5 2018
Solvent: CDCl₃
Ambient temperature
Total 3280 repetitions



^{13}C NMR (100 MHz, CDCl₃) spectra



Compound 7d (¹H-NMR spectral data)

NCNB0129

Pulse Sequence: s2pu1

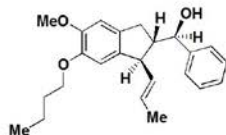
UNITYplus-400 "unity400"

Date: Jan 30 2018

Solvent: CDC13

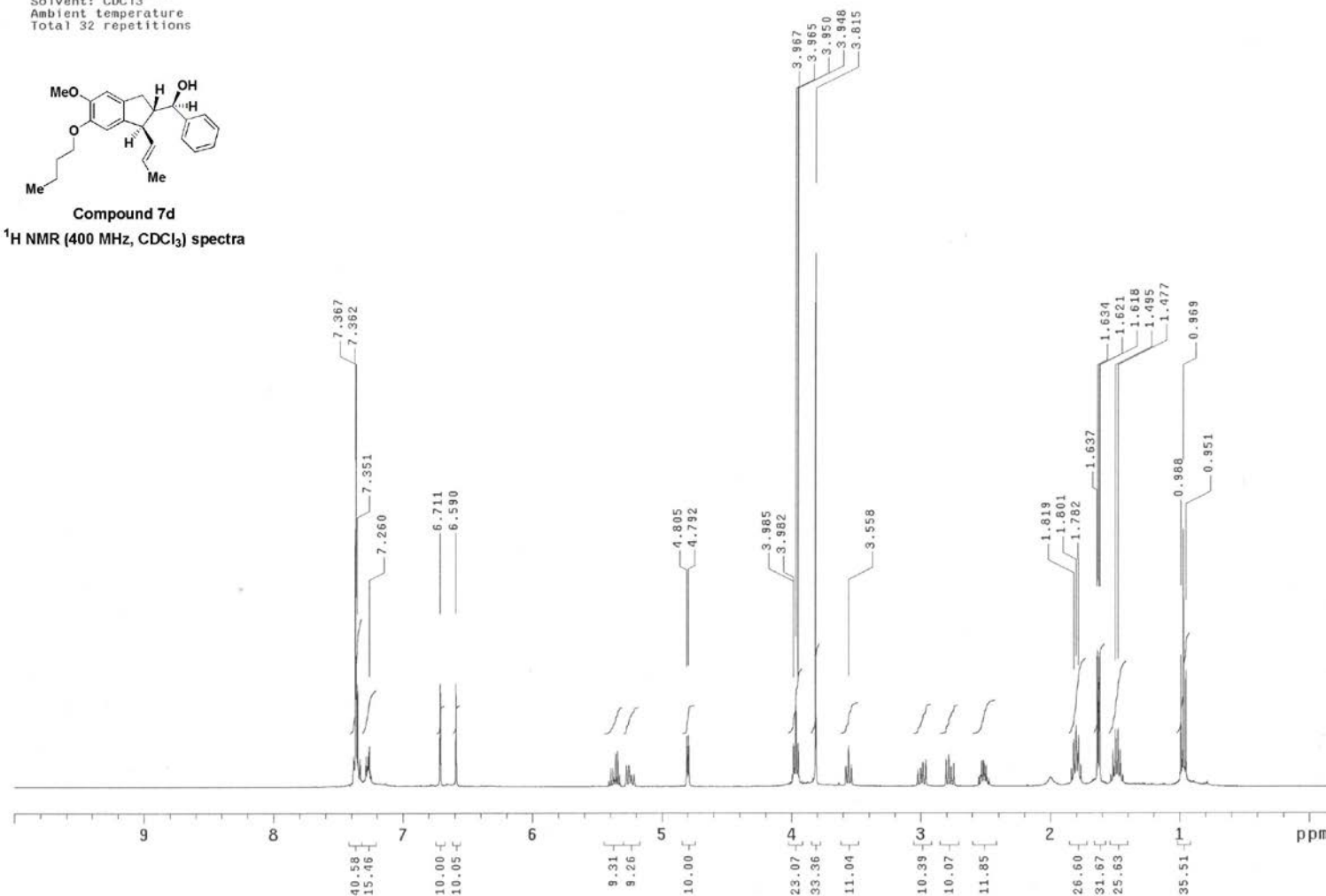
Ambient temperature

Total 32 repetitions



Compound 7d

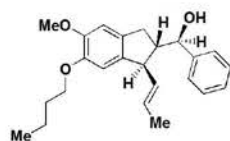
¹H NMR (400 MHz, CDCl₃) spectra



Compound 7d (¹³C-NMR spectral data)

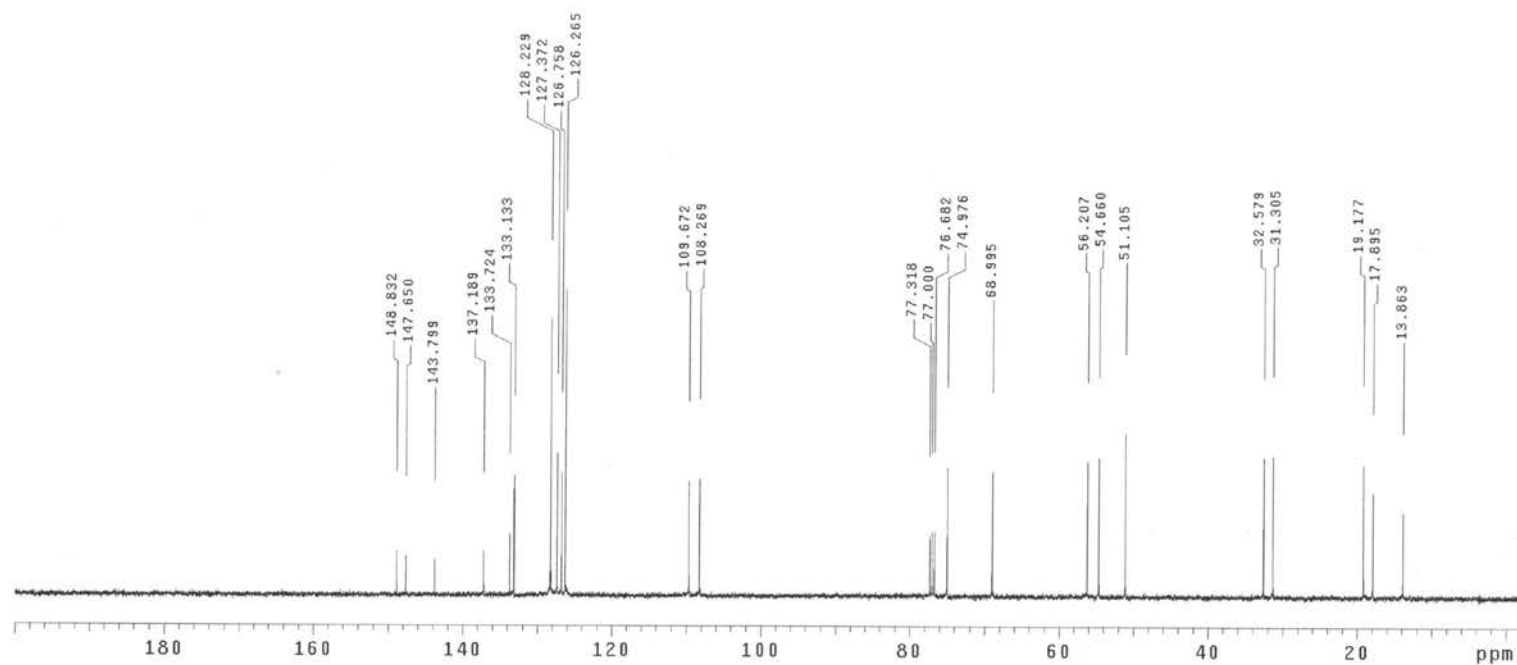
NCNB0129

Pulse Sequence: s2pul
 UNITYplus-400 "unity400"
 Date: Jan 30 2018
 Solvent: CDCl₃
 Ambient temperature
 Total 1168 repetitions



Compound 7d

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 7e (¹H-NMR spectral data)

NCNB0130

Pulse Sequence: s2pul

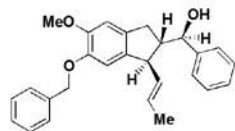
UNITYplus-400 "unity400"

Date: Jan 30 2018

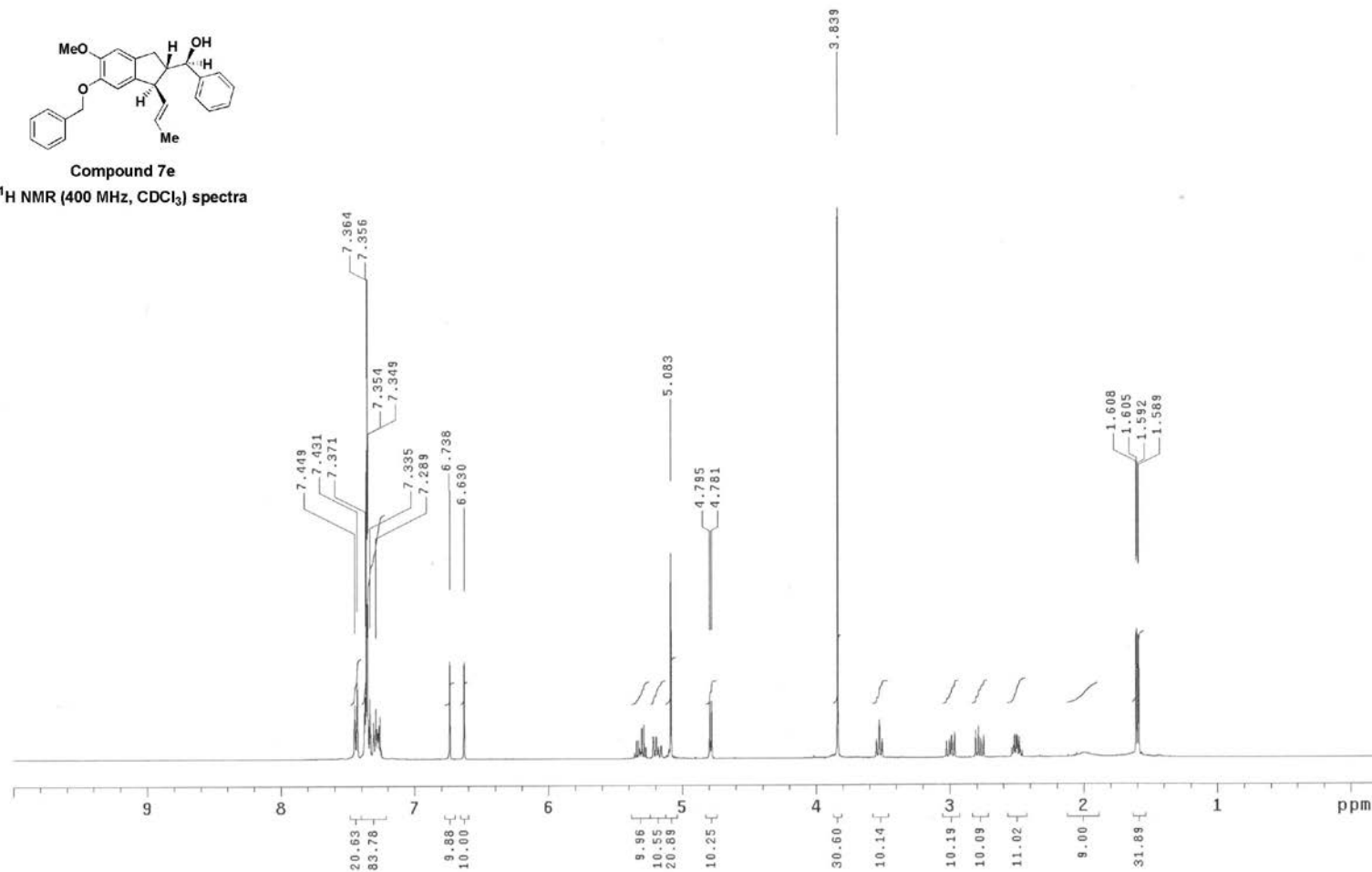
Solvent: CDCl₃

Ambient temperature
Tested 22 repetitions

Total 32 repetitions



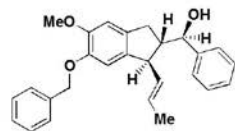
Compound 7e

¹H NMR (400 MHz, CDCl₃) spectra

Compound 7e (¹³C-NMR spectral data)

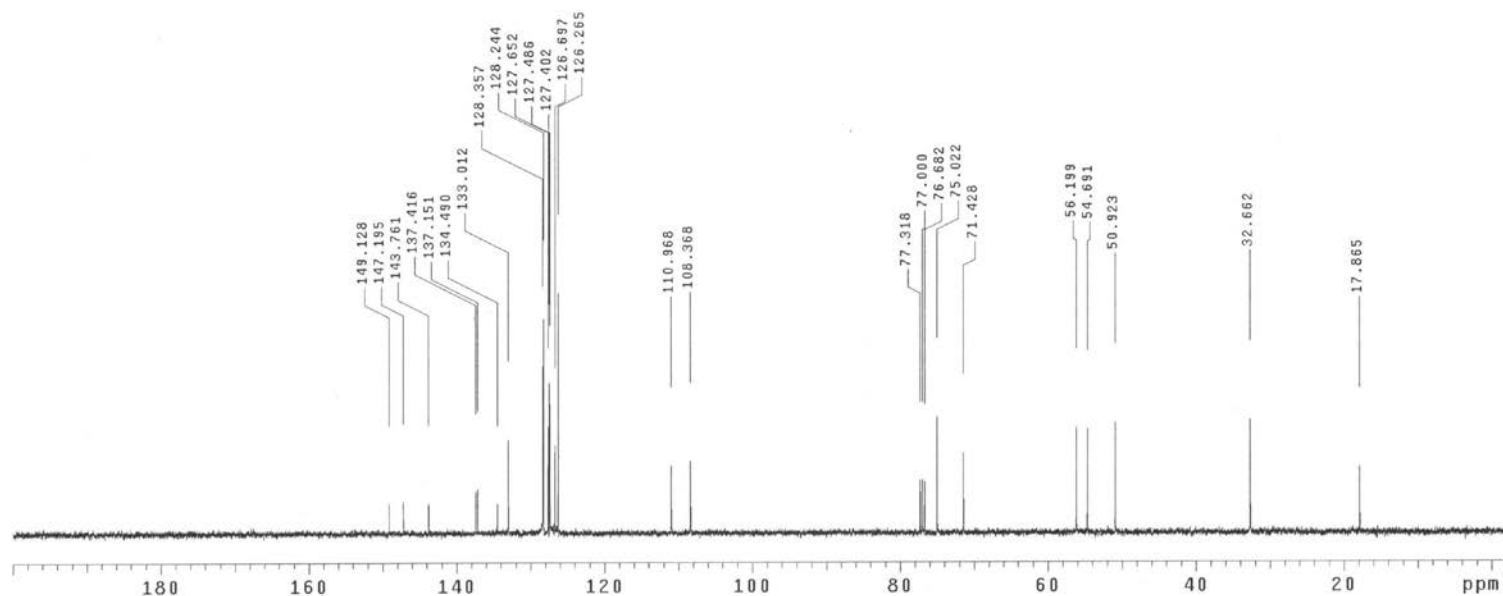
NCNB0130

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Jan 30 2018
Solvent: CDCl₃
Ambient temperature
Total 432 repetitions



Compound 7e

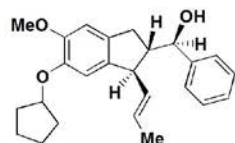
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 7f (¹H-NMR spectral data)

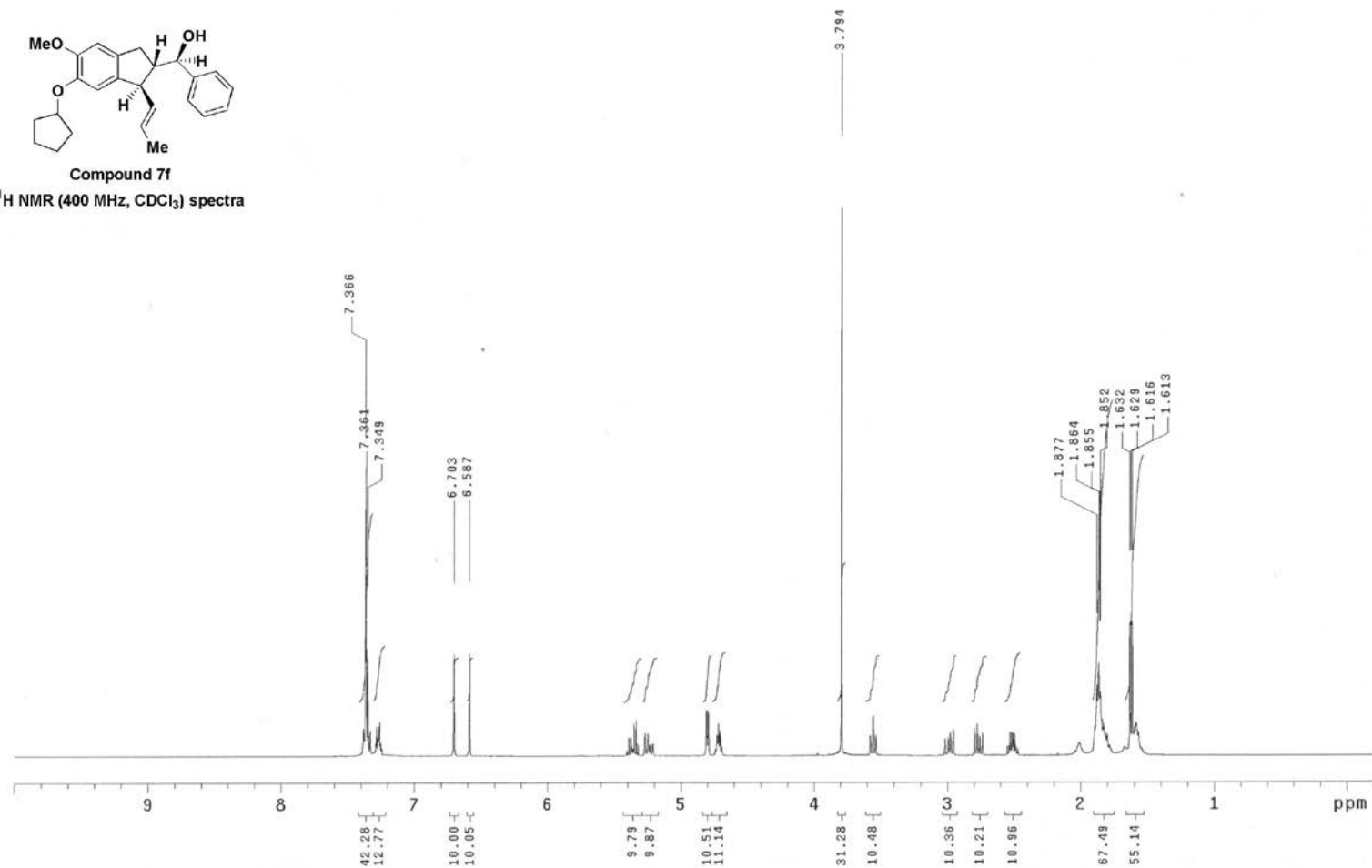
NCNB0116

Pulse Sequence: s2pul
 UNITYplus-400 "unity400"
 Date: Jan 18 2018
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetitions



Compound 7f

¹H NMR (400 MHz, CDCl₃) spectra



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

NCNB0116

Pulse Sequence: s2pu1

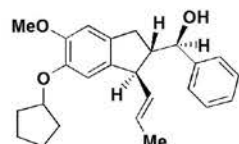
UNITYplus-400 "unity400"

Date: Jan 18 2018

Solvent: CDCl_3

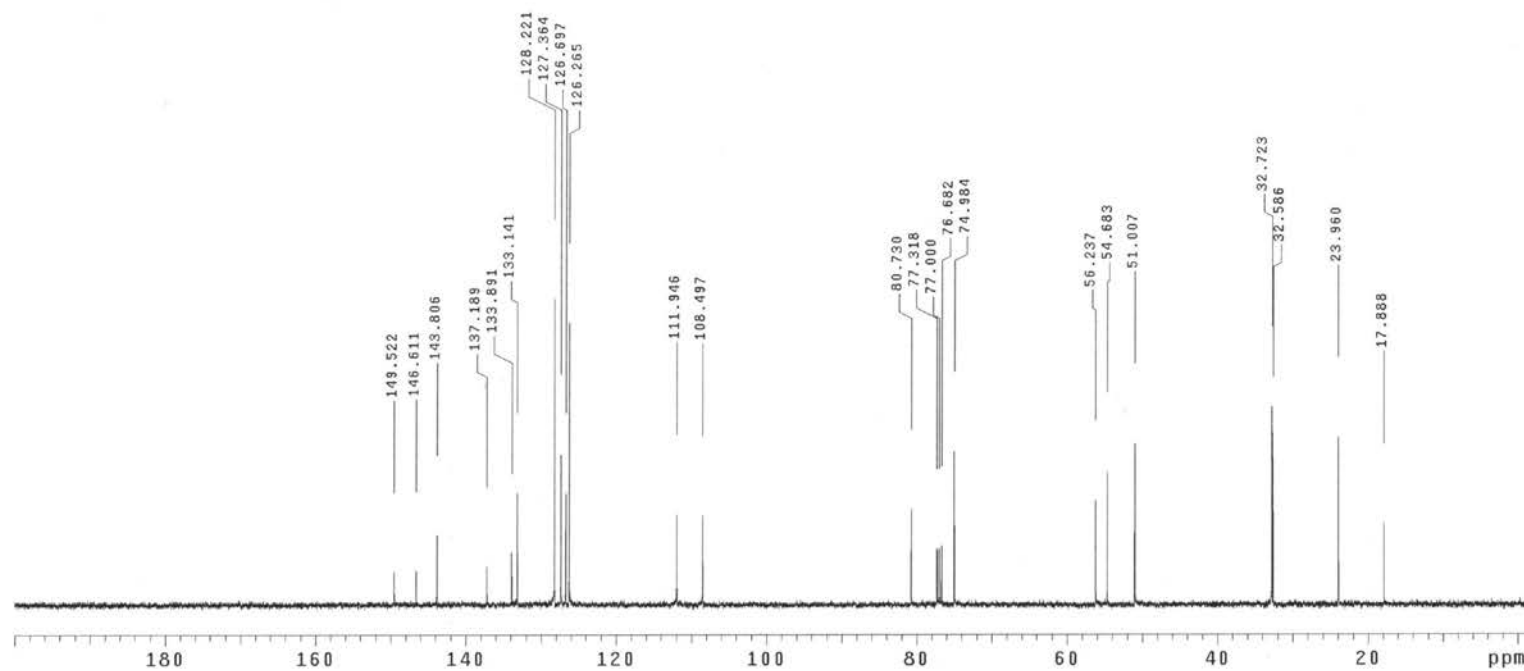
Ambient temperature

Total 640 repetitions



Compound 7f

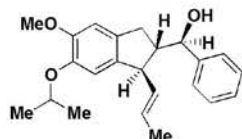
^{13}C NMR (100 MHz, CDCl_3) spectra



Compound 7g (¹H-NMR spectral data)

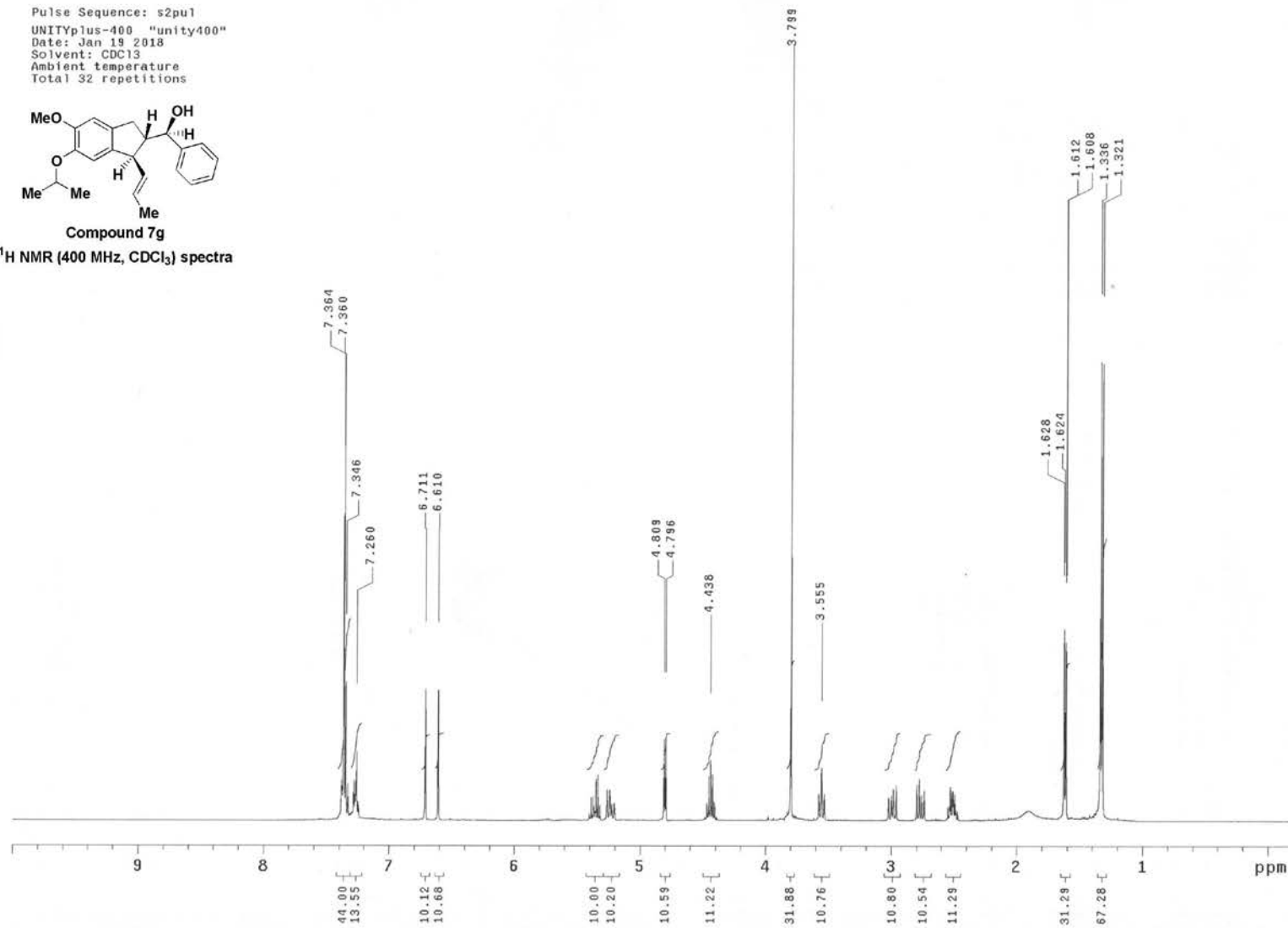
NCNB0118

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Jan 19 2018
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetitions



Compound 7g

¹H NMR (400 MHz, CDCl₃) spectra



Compound 7g (¹³C-NMR spectral data)

NCNB0118

Pulse Sequence: s2pu1

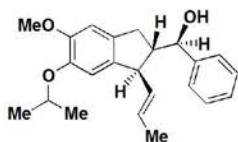
UNITYplus-400 "unity400"

Date: Jan 19 2018

Solvent: CDCl₃

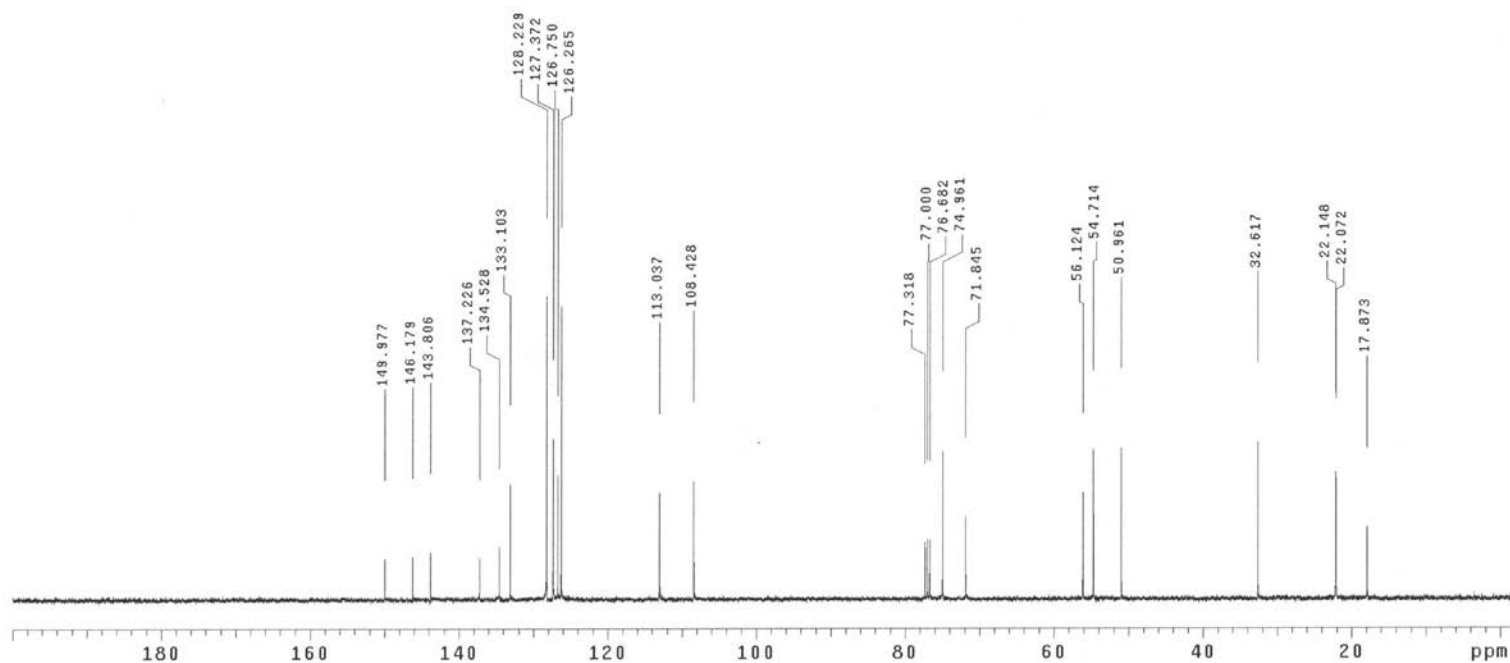
Ambient temperature

Total 1184 Repetitions

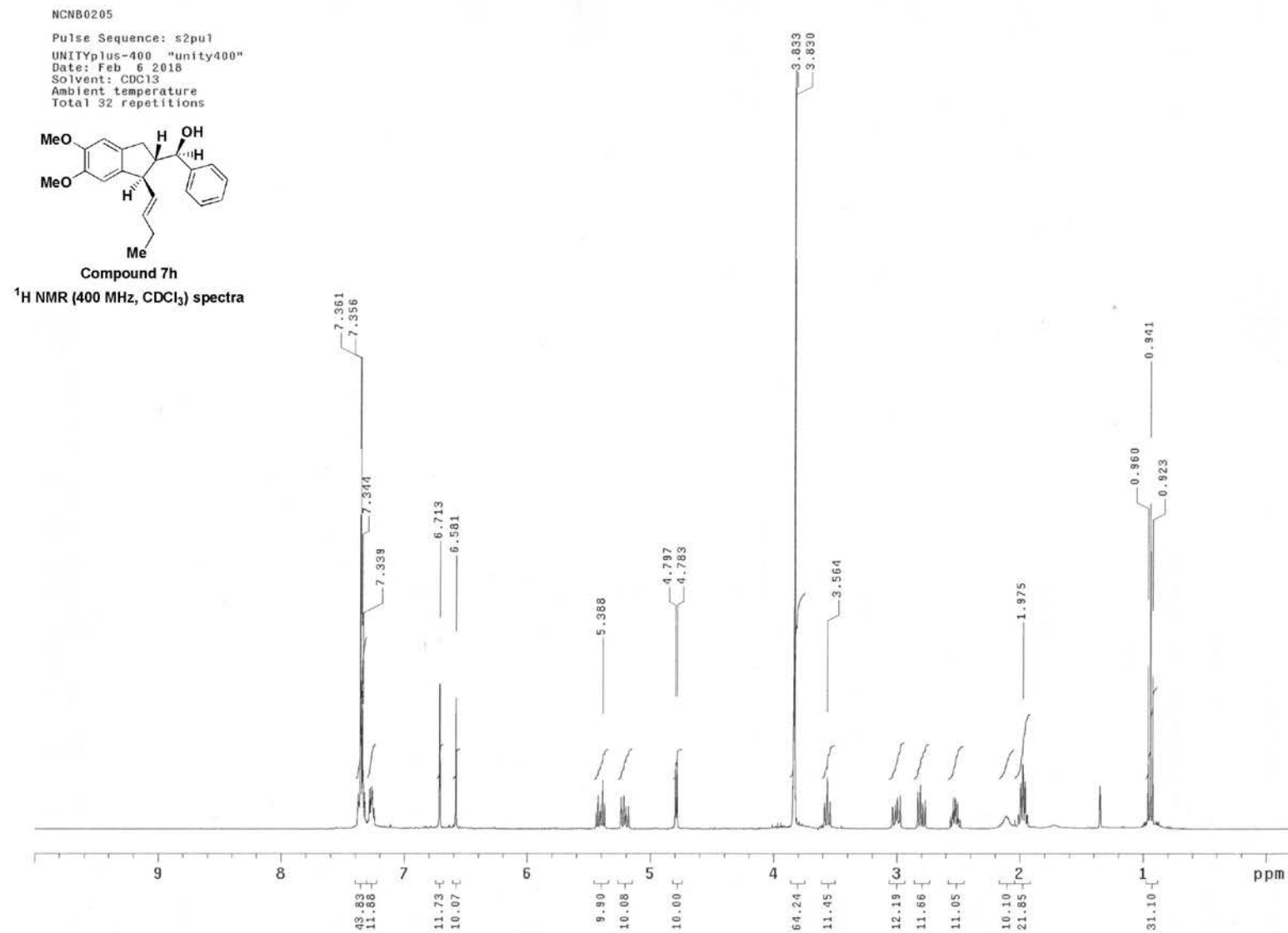


Compound 7g

¹³C NMR (100 MHz, CDCl₃) spectra



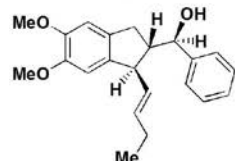
Compound 7h (¹H-NMR spectral data)



Compound 7h (¹³C-NMR spectral data)

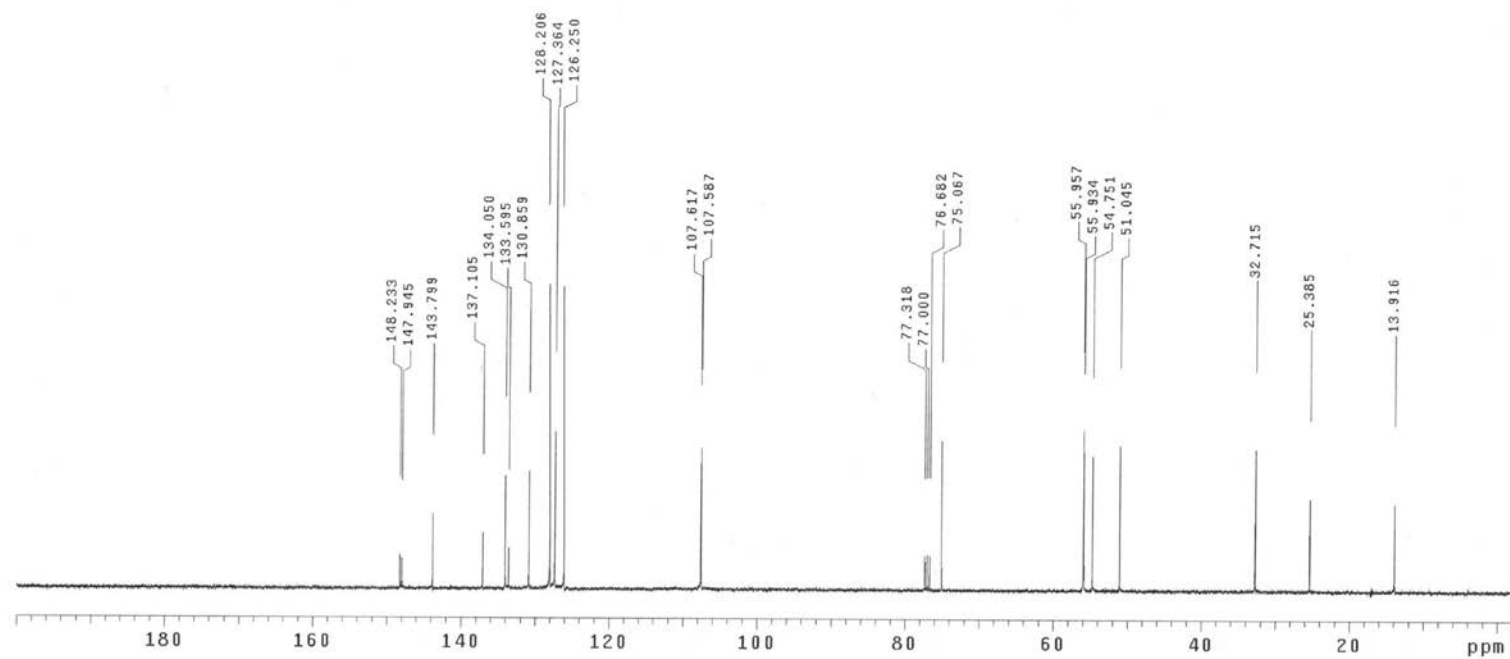
NCN80205

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Feb 6 2018
 Solvent: CDCl₃
 Ambient temperature
 Total 640 repetitions



Compound 7h

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 7i (¹H-NMR spectral data)

NCNB0315

Pulse Sequence: s2pu1

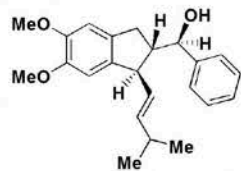
UNITYplus-400 "unity400"

Date: Mar 16 2018

Solvent: CDCl₃

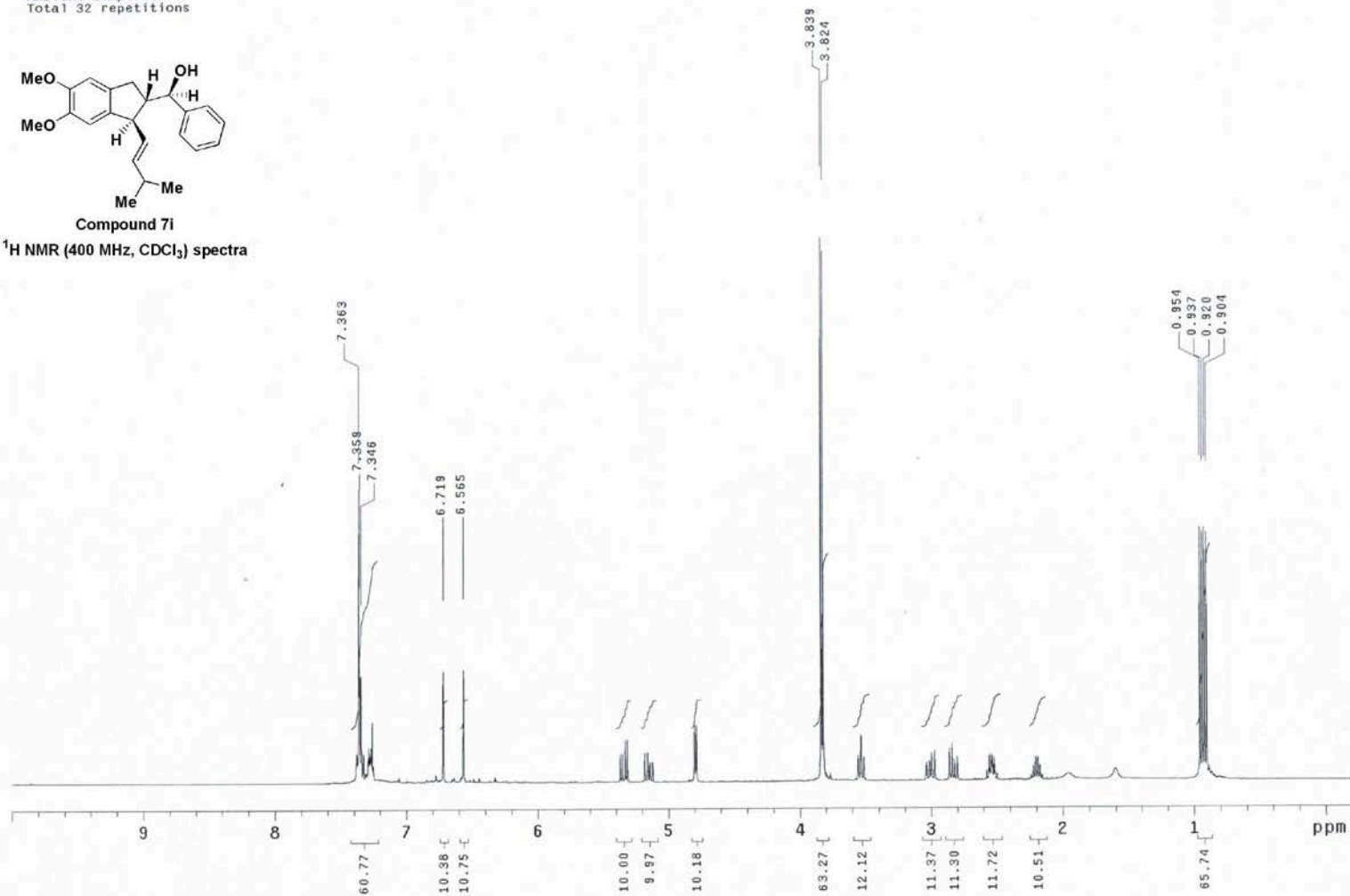
Ambient temperature

Total 32 repetitions



Compound 7i

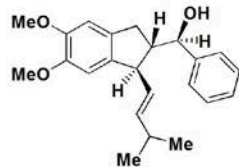
¹H NMR (400 MHz, CDCl₃) spectra



Compound 7i (¹³C-NMR spectral data)

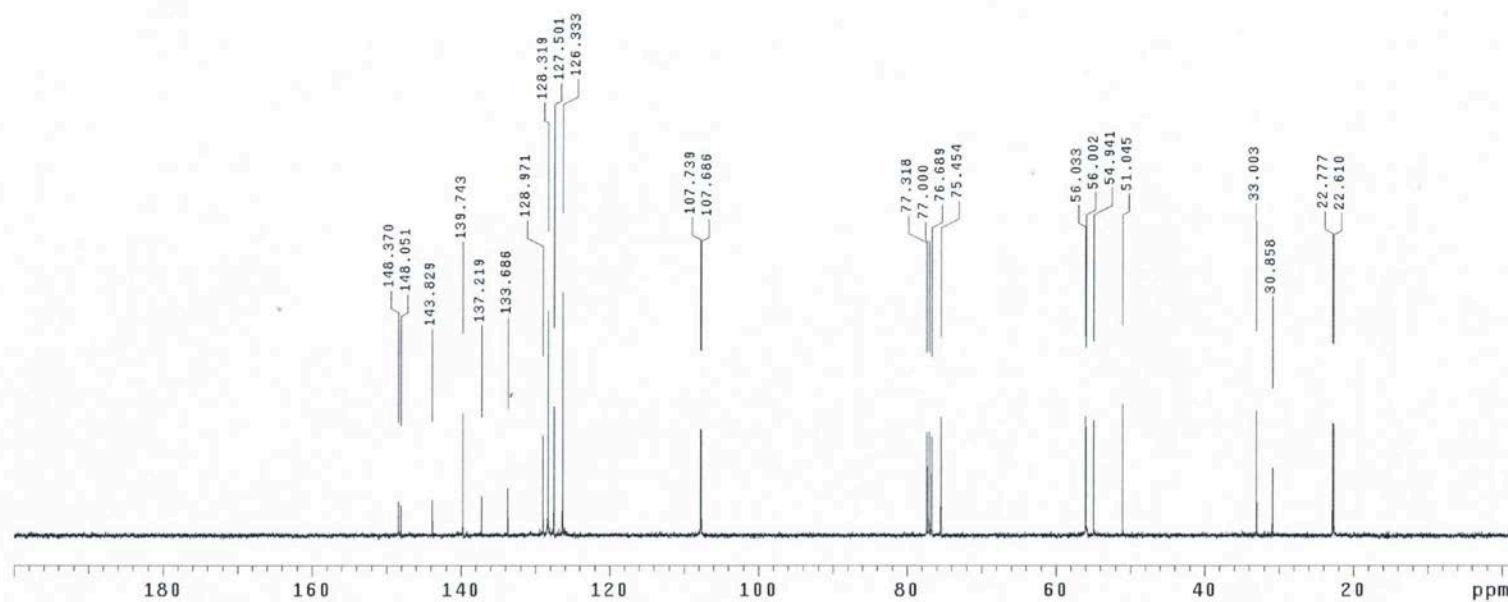
NCNB0315

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Mar 16 2018
Solvent: CDCl₃
Ambient temperature
Total 3216 repetitions



Compound 7i

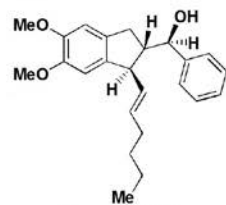
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 7k (¹H-NMR spectral data)

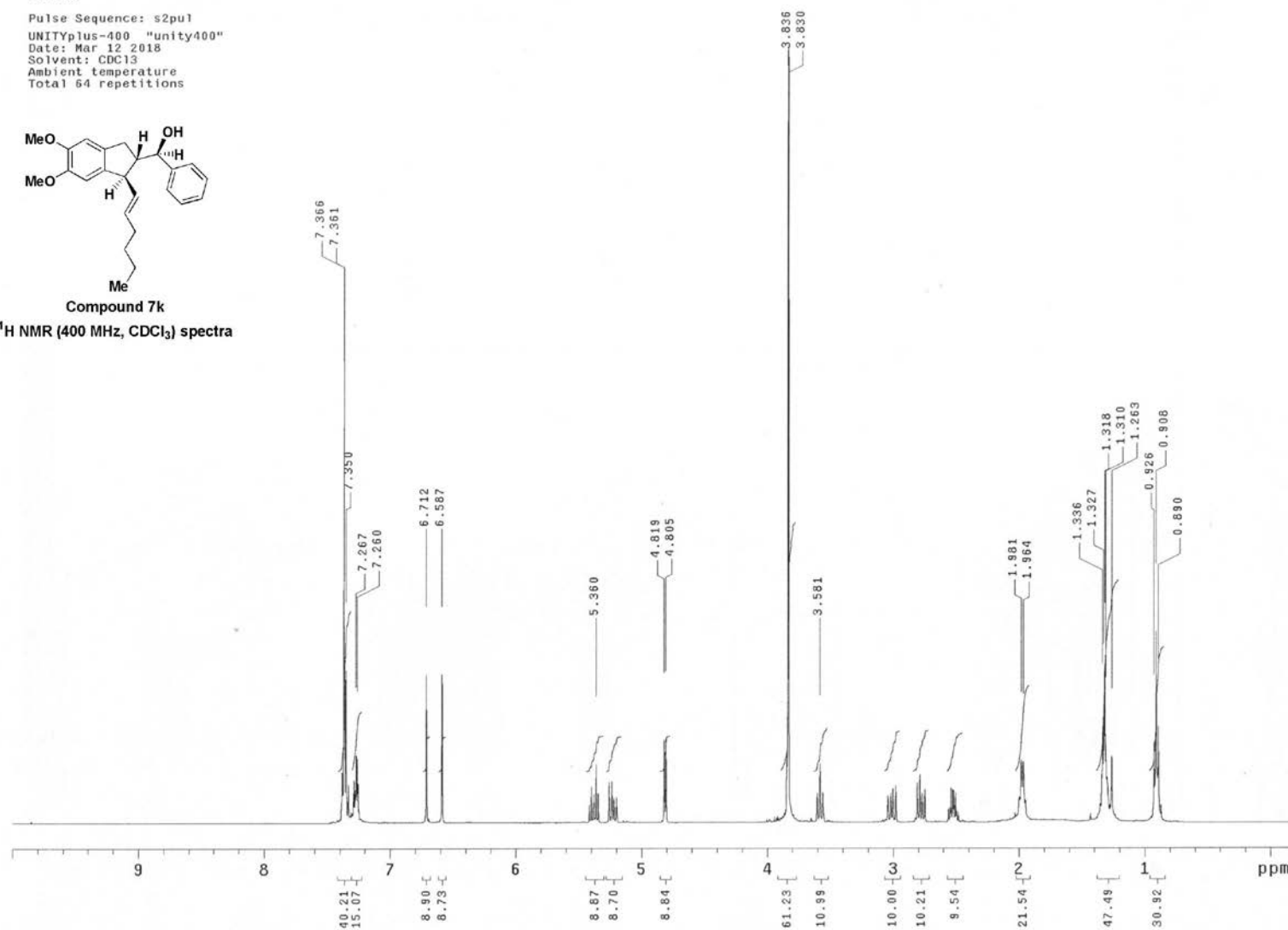
NCN84C

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Mar 12 2018
 Solvent: CDCl₃
 Ambient temperature
 Total 64 repetitions



Compound 7k

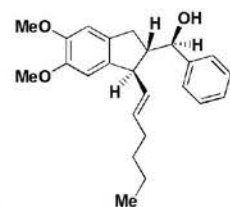
¹H NMR (400 MHz, CDCl₃) spectra



Compound 7k (¹³C-NMR spectral data)

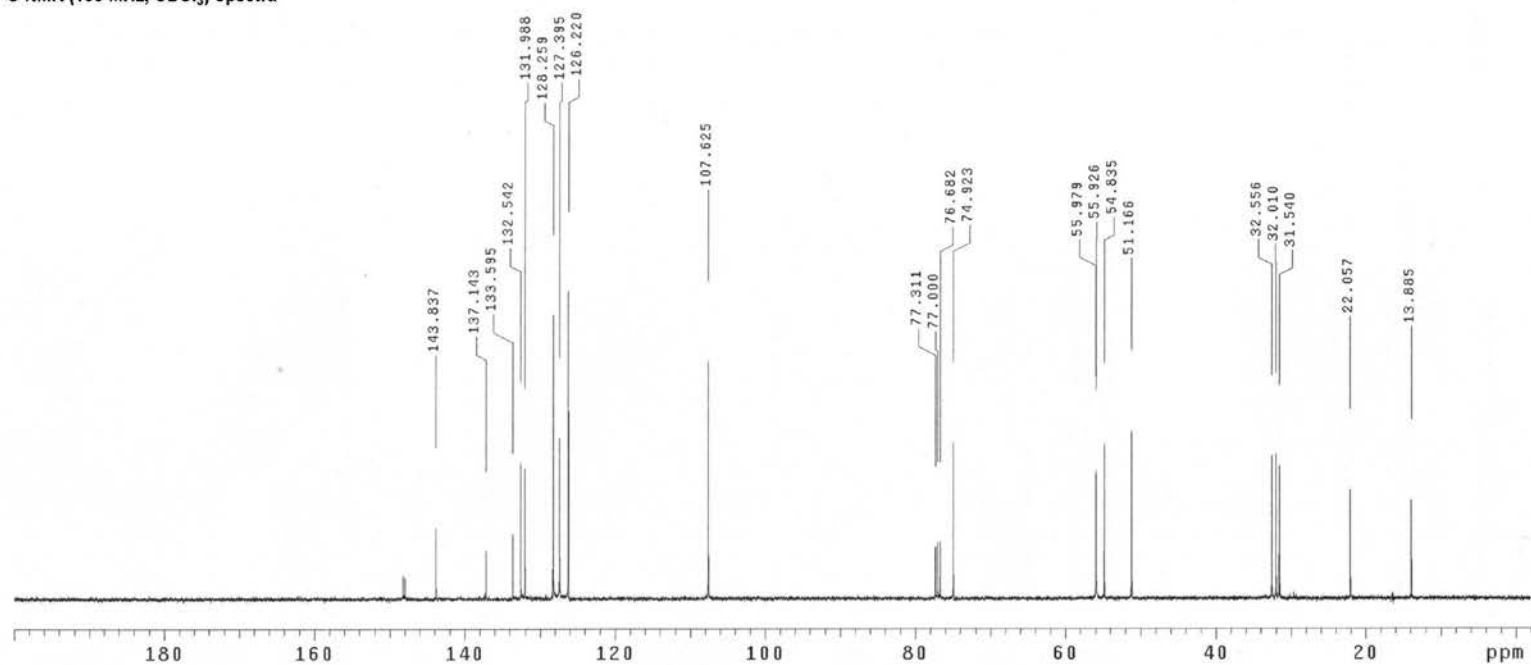
NCNB4C

Pulse Sequence: s2pul
 UNITYplus-400 "unity400"
 Date: Mar 12 2018
 Solvent: CDCl₃
 Ambient temperature
 Total 1600 repetitions

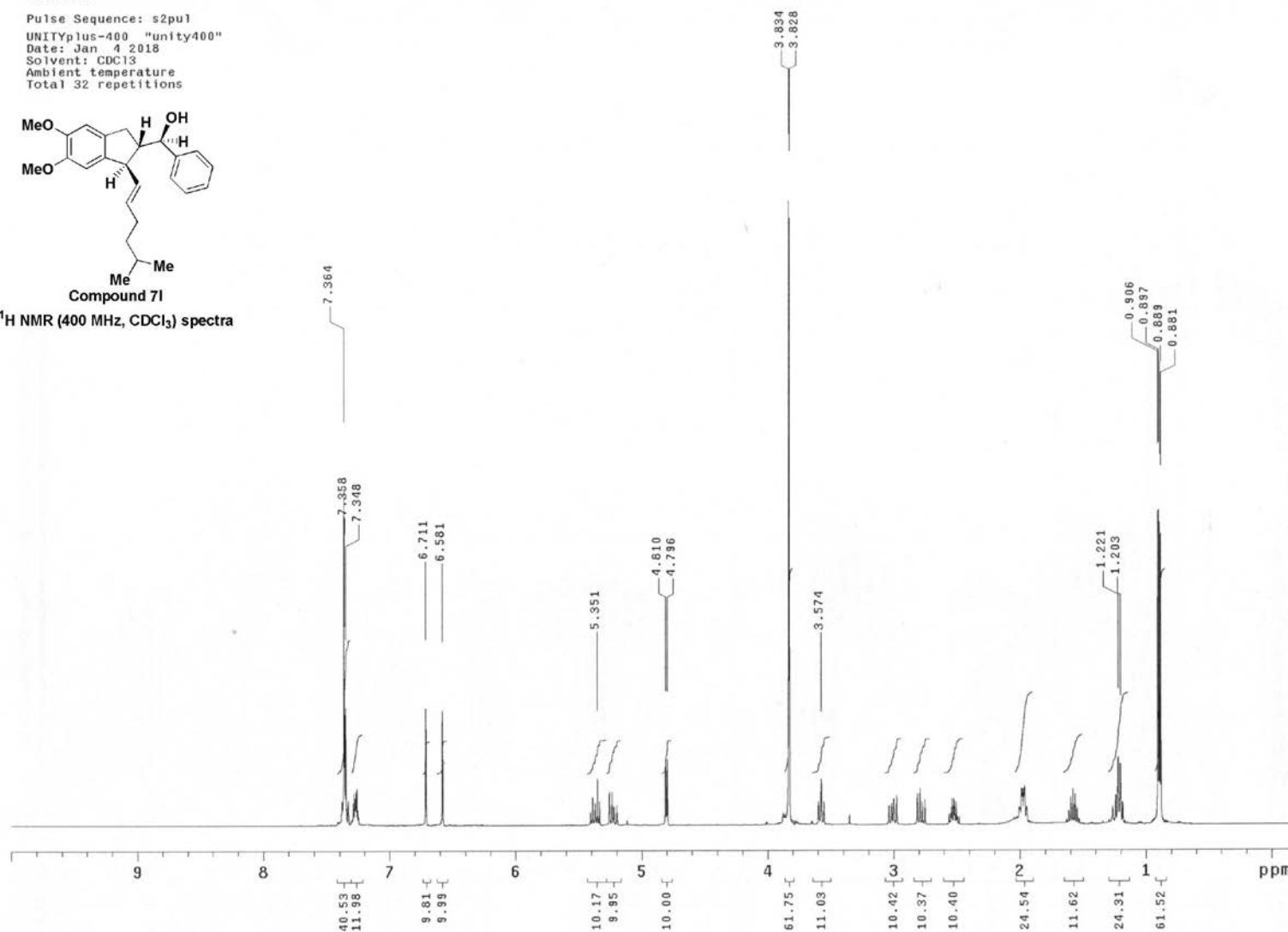
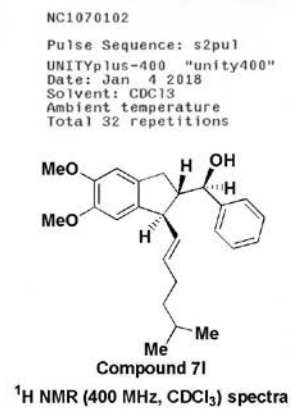


Compound 7k

¹³C NMR (100 MHz, CDCl₃) spectra



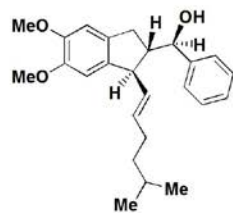
Compound 7I (¹H-NMR spectral data)



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

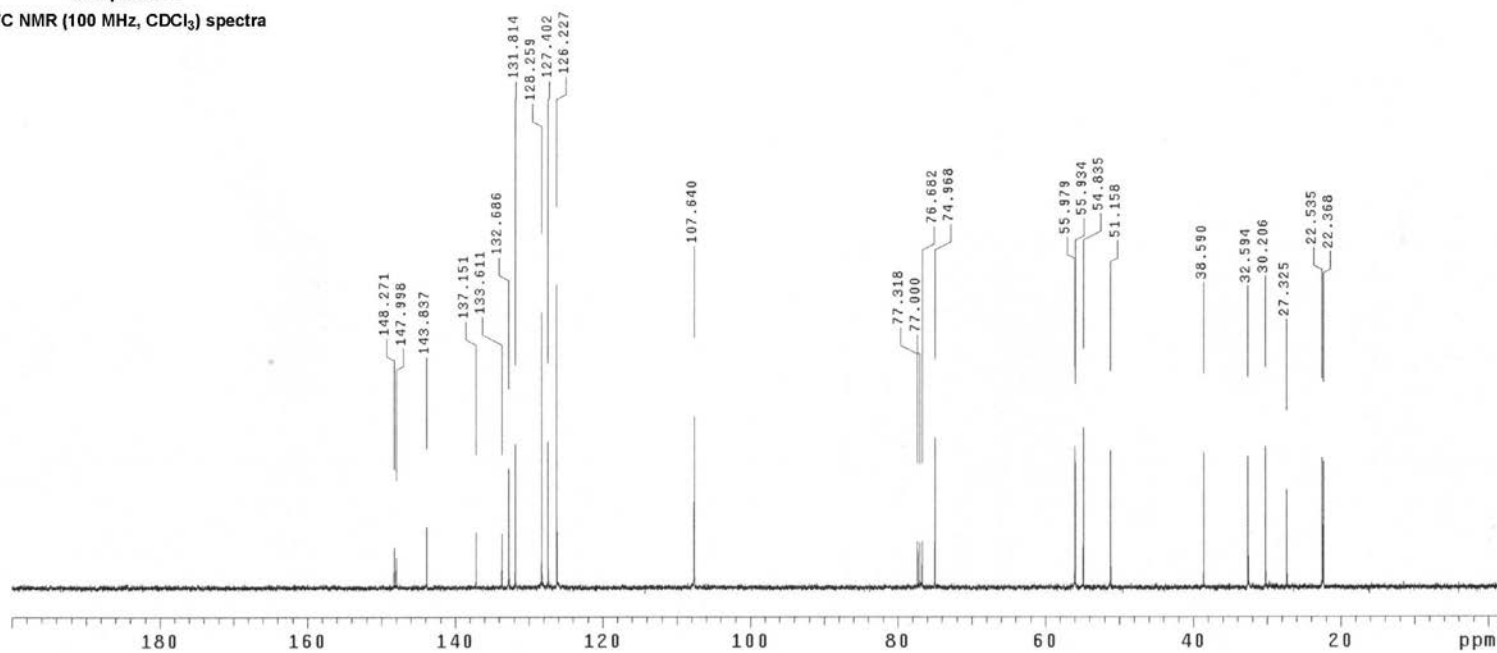
NC1070102

Pulse Sequence: s2pul
 UNITYplus-400 "unity400"
 Date: Jan 4 2018
 Solvent: CDCl_3
 Ambient temperature
 Total 512 repetitions



Compound 7I

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



Compound 7m (¹H-NMR spectral data)

NCPHNB

Pulse Sequence: s2pu1

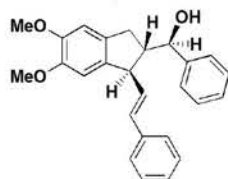
UNITYplus-400 "unity400"

Date: Jan 4 2018

Solvent: CDCl₃

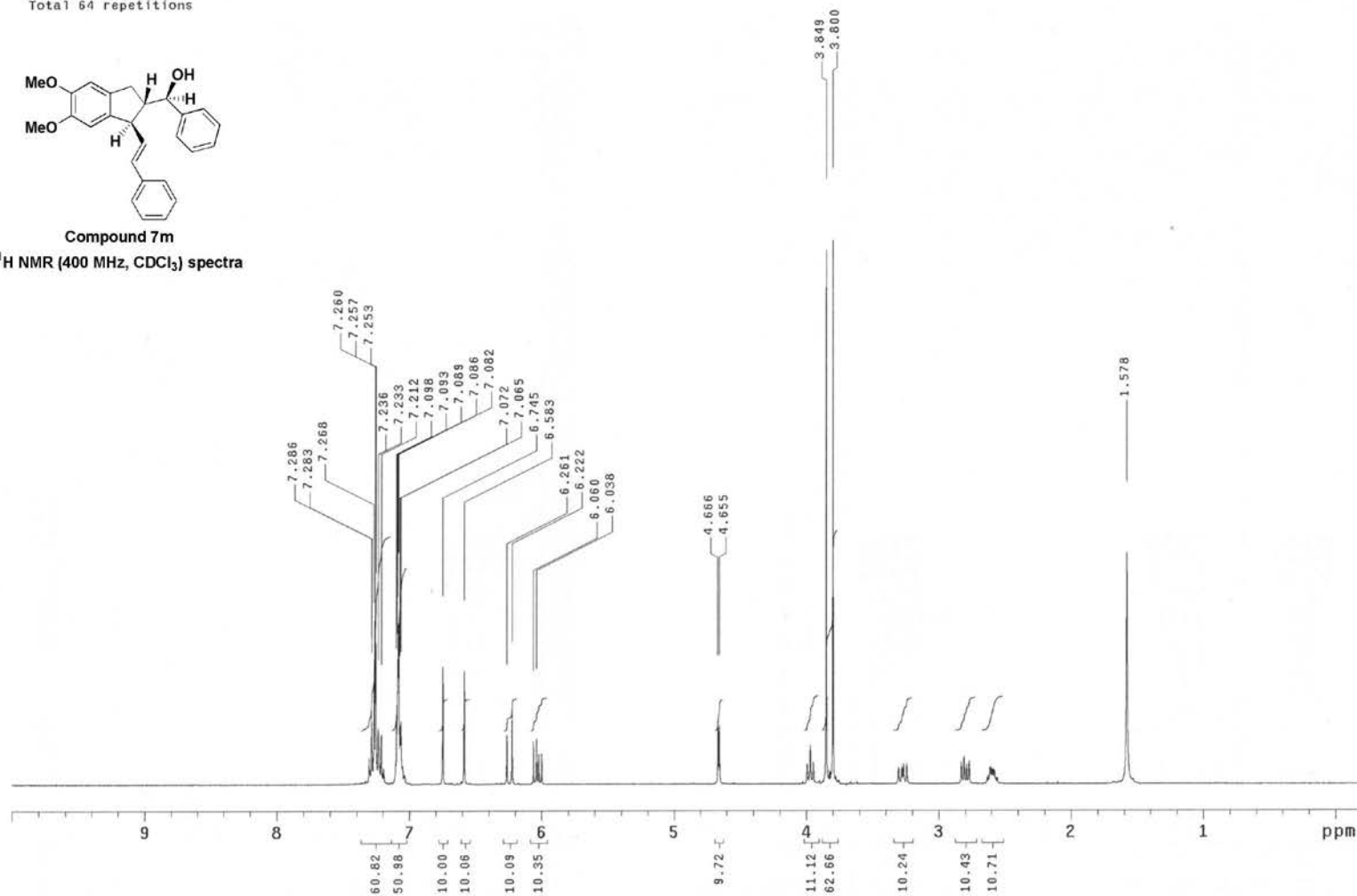
Ambient temperature

Total 64 repetitions



Compound 7m

¹H NMR (400 MHz, CDCl₃) spectra



Compound 7m (¹³C-NMR spectral data)

NCPbNB

Pulse Sequence: s2pu1

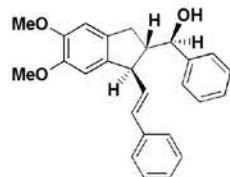
UNITYplus-400 "unity400"

Date: Jan 4 2018

Solvent: CDCl₃

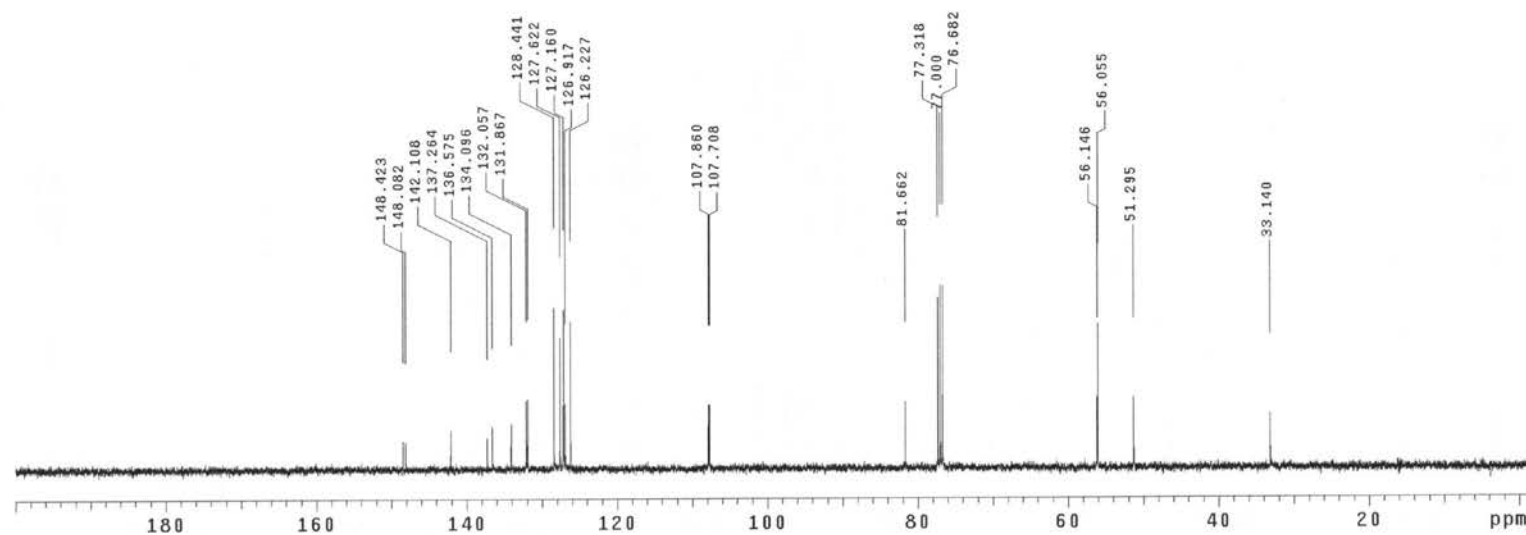
Ambient temperature

Total 5200 repetitions



Compound 7m

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 7n (¹H-NMR spectral data)

NCNB0206

Pulse Sequence: s2pu1

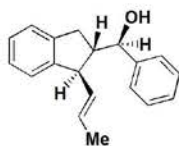
UNITYplus-400 "unity400"

Date: Feb 6 2018

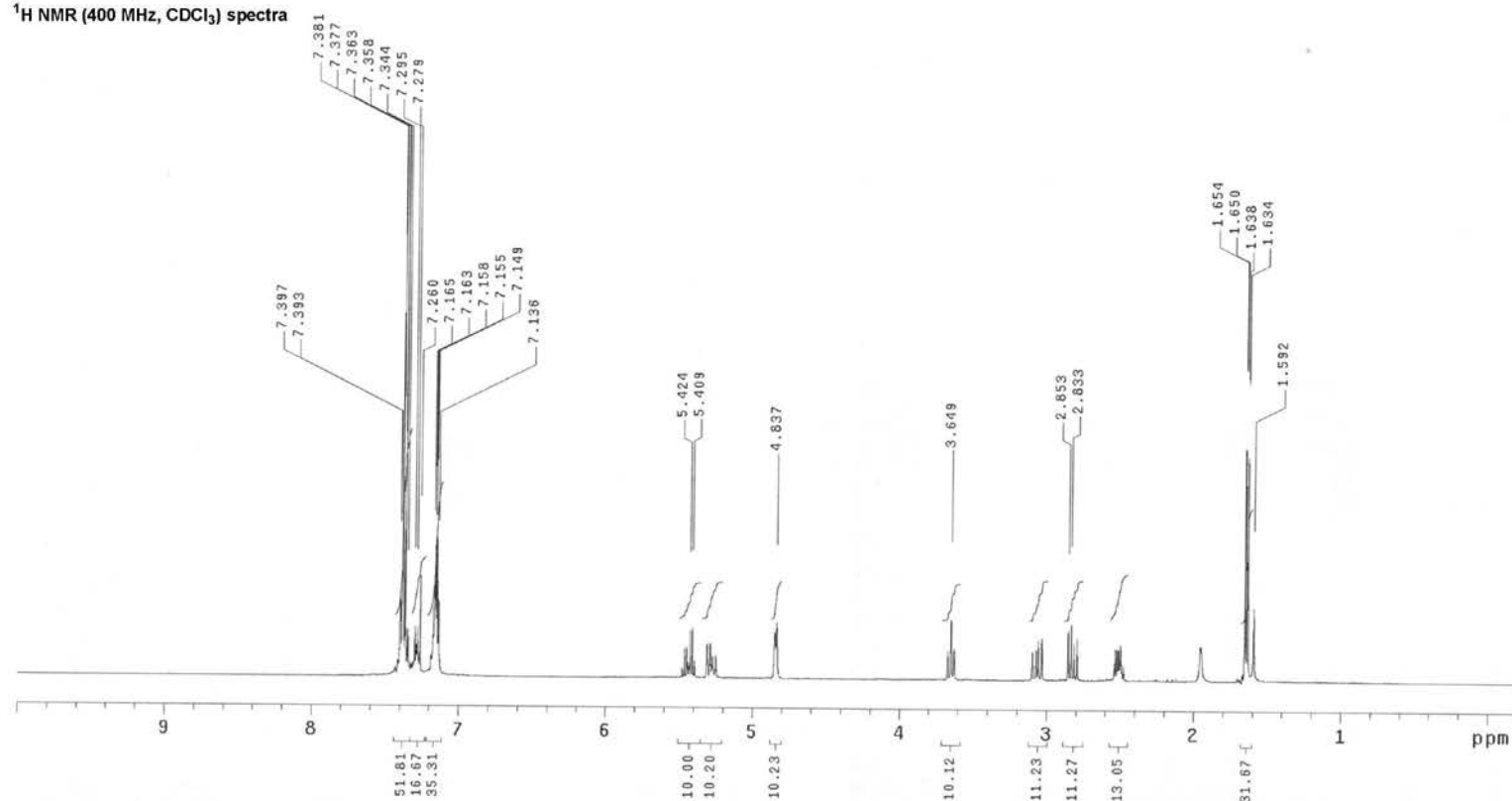
Solvent: CDCl₃

Ambient temperature

Total 32 repetitions



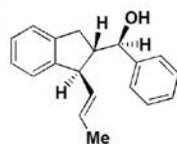
¹H NMR (400 MHz, CDCl₃) spectra



Compound 7n (¹³C-NMR spectral data)

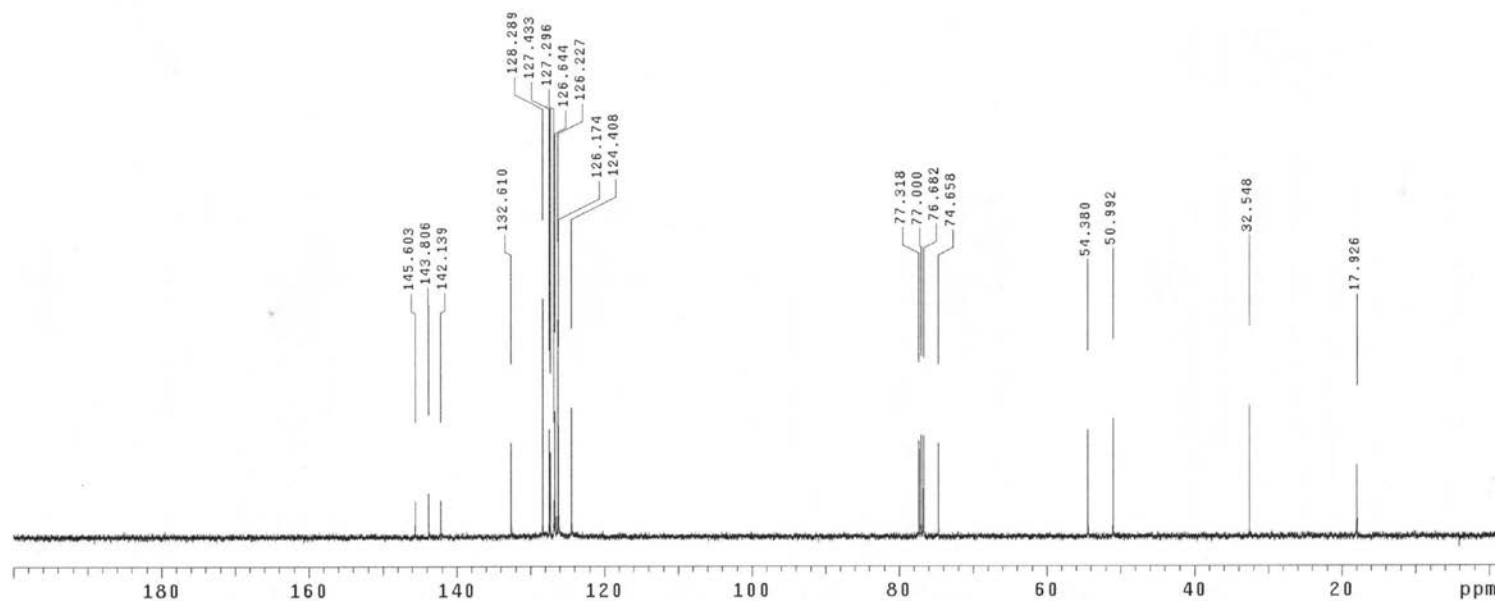
NCN80206

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Feb 6 2018
Solvent: CDCl₃
Ambient temperature
Total 1024 repetitions



Compound 7n

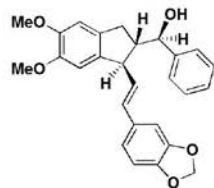
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 7p (¹H-NMR spectral data)

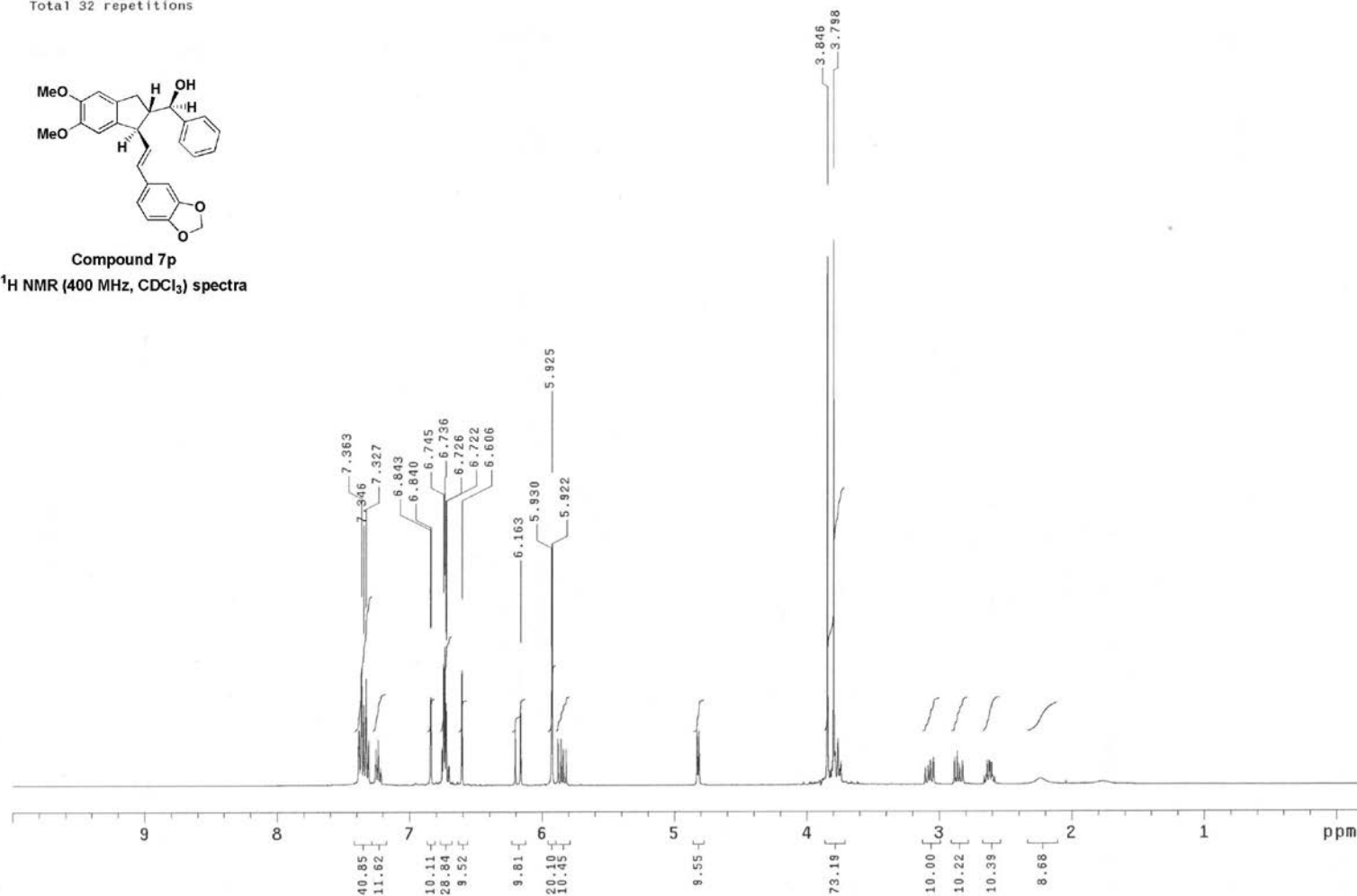
KS1070120

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Jan 22 2018
Solvent: CDCl₃
Ambient temperature
Total 32 repetitions



Compound 7p

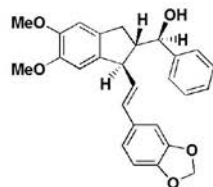
¹H NMR (400 MHz, CDCl₃) spectra



Compound 7p (¹³C-NMR spectral data)

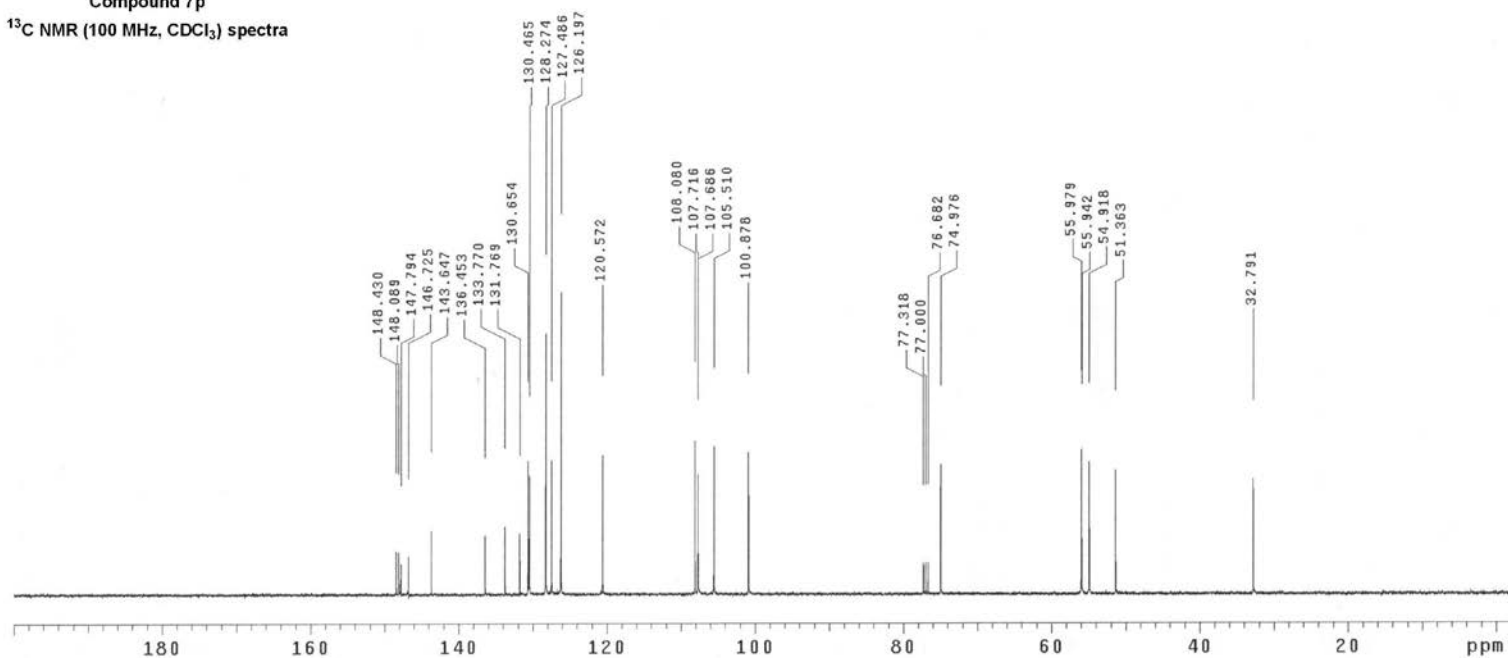
KS1070120

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Jan 22, 2018
Solvent: CDCl₃
Ambient temperature
Total 576 repetitions



Compound 7p

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 7q (¹H-NMR spectral data)

NCNB0126

Pulse Sequence: s2pu1

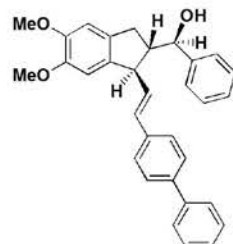
UNITYplus-400 "unity400"

Date: Jan 29 2018

Solvent: CDCl₃

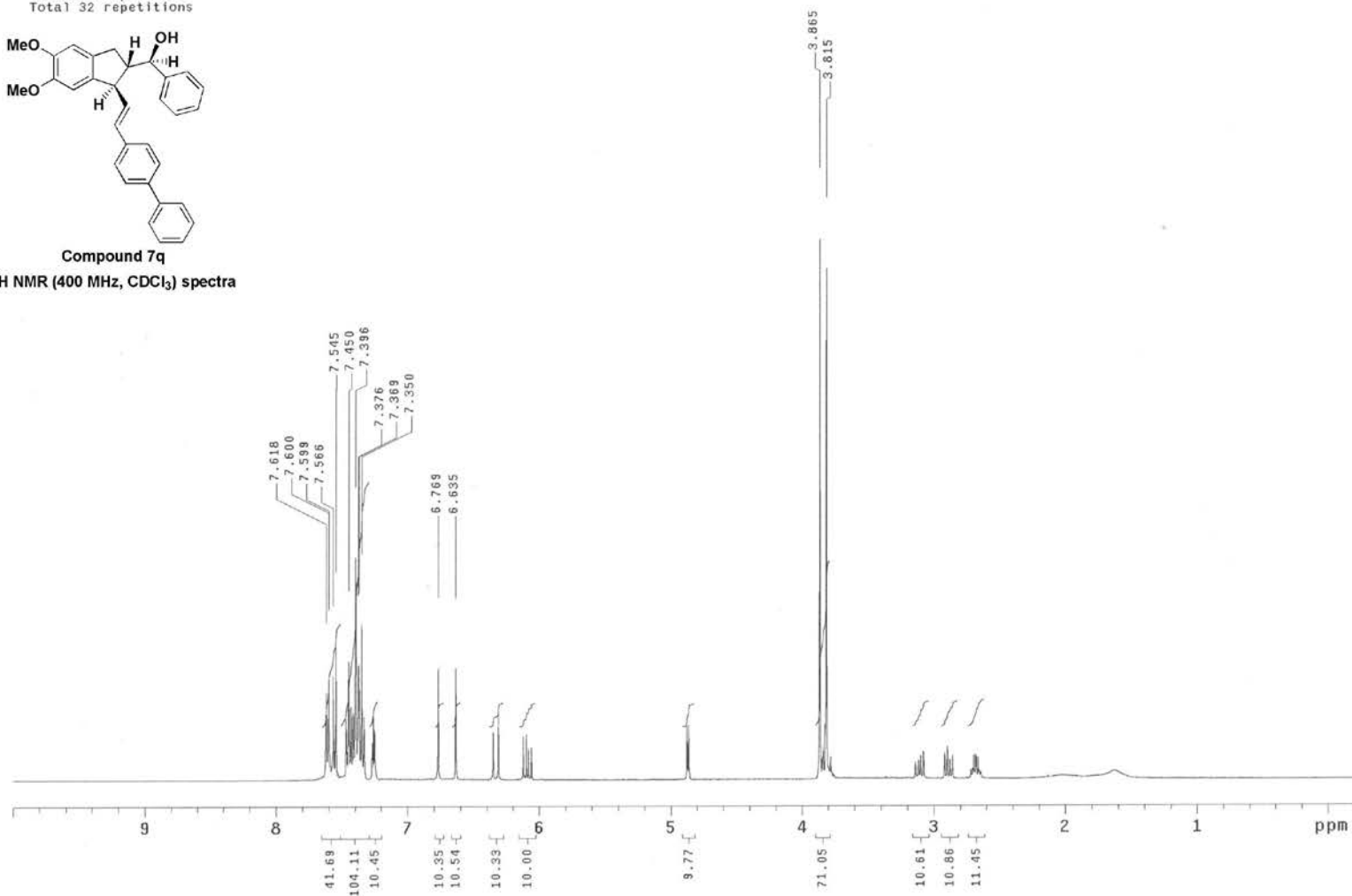
Ambient temperature

Total 32 repetitions



Compound 7q

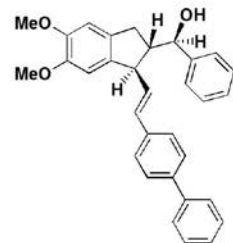
¹H NMR (400 MHz, CDCl₃) spectra



Compound 7q (¹³C-NMR spectral data)

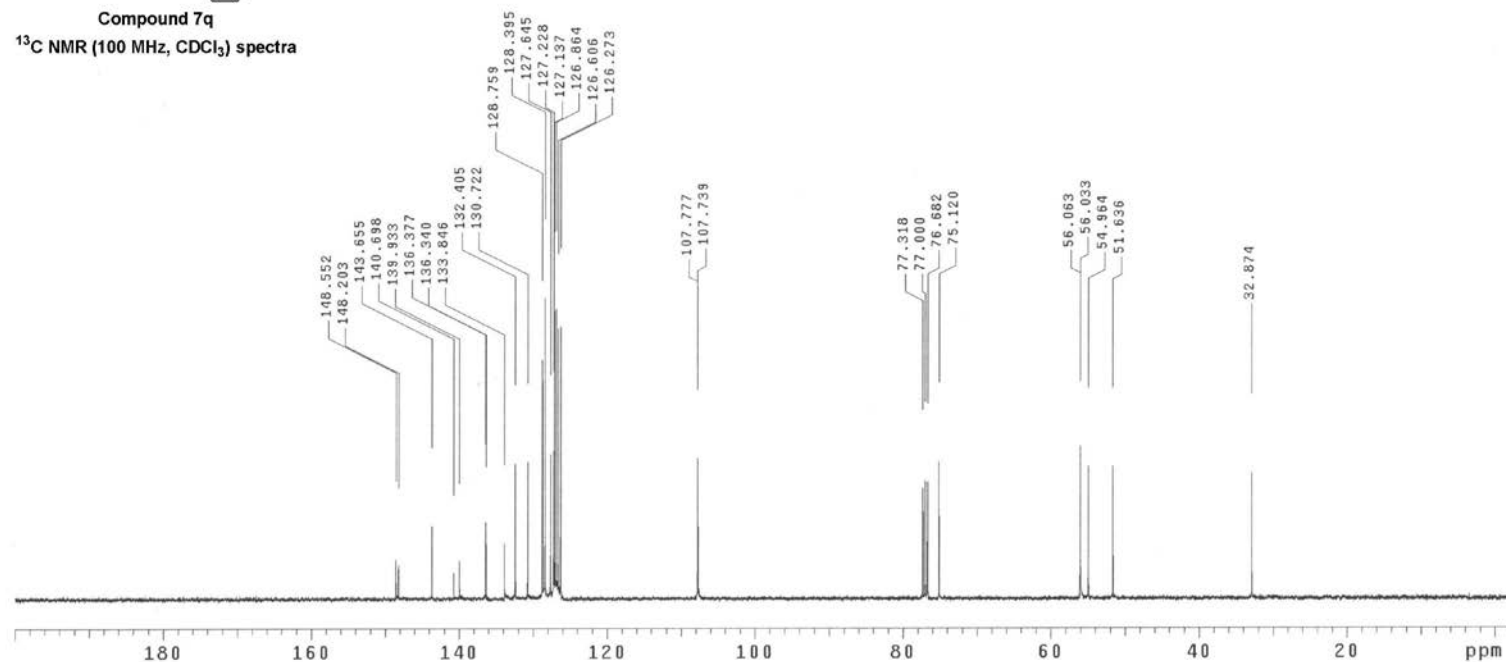
NCNB0126

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Jan 29 2018
 Solvent: CDCl₃
 Ambient temperature
 Total 5584 repetitions



Compound 7q

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 7r (¹H-NMR spectral data)

KS1070122

Pulse Sequence: s2pu1

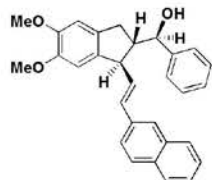
UNITYplus-400 "unity400"

Date: Feb 5 2018

Solvent: CDCl₃

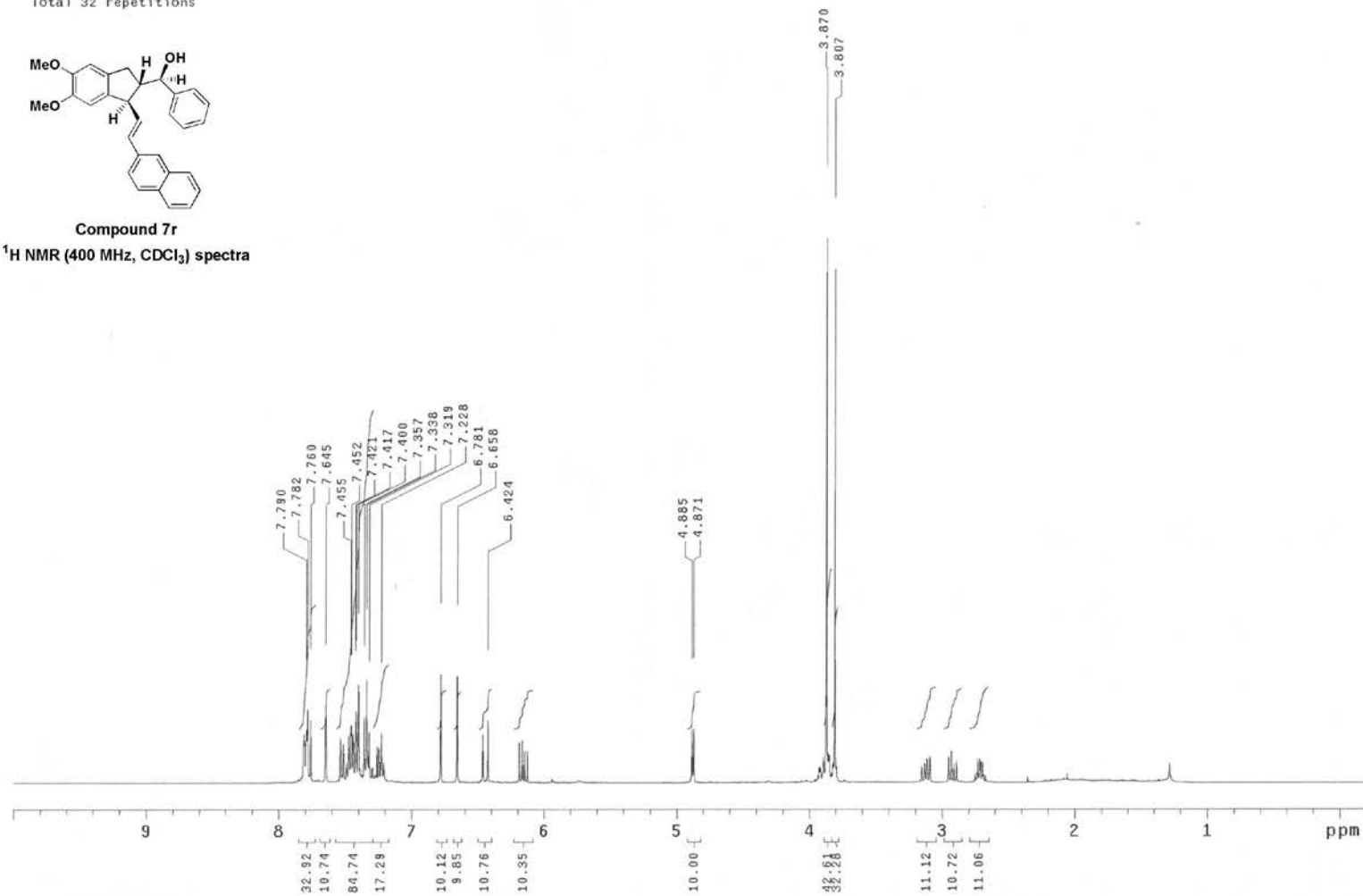
Ambient temperature

Total 32 repetitions



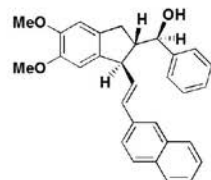
Compound 7r

¹H NMR (400 MHz, CDCl₃) spectra

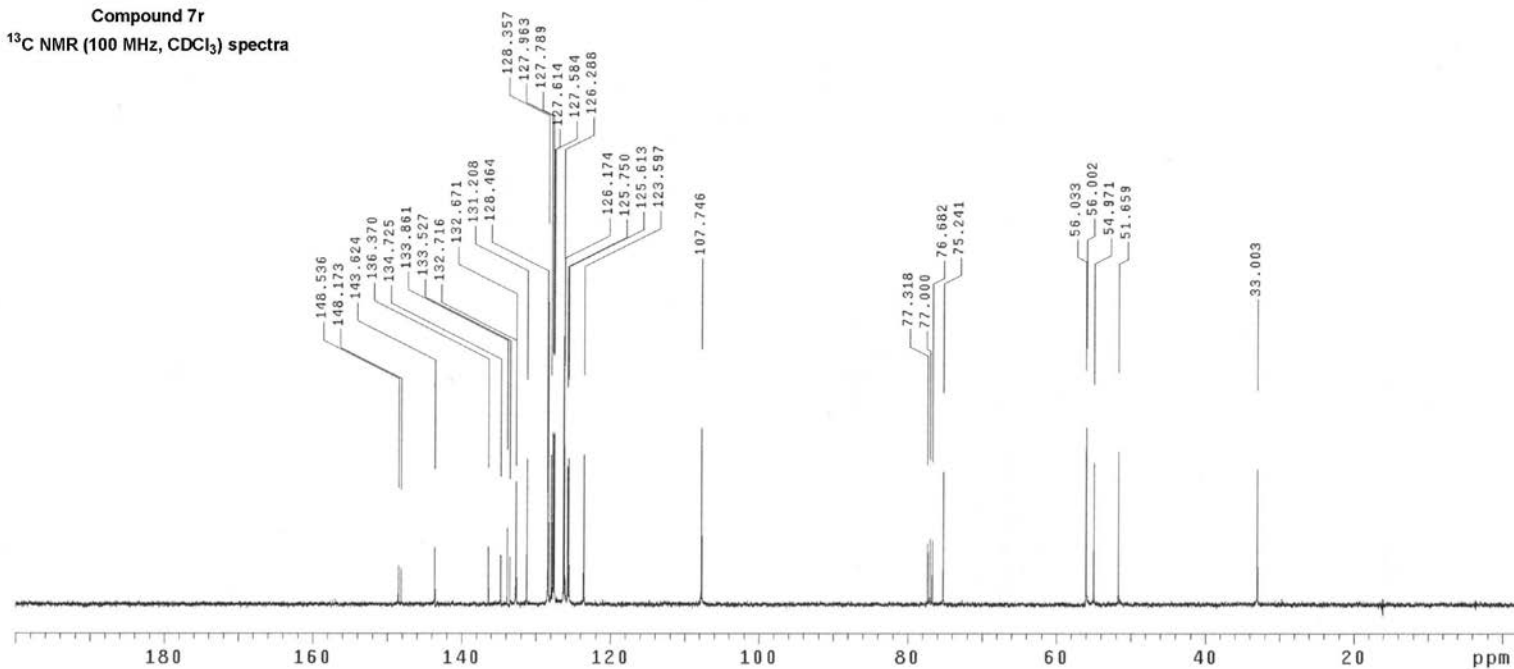


Compound 7r (¹³C-NMR spectral data)

KS1070122
Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Feb 5 2018
Solvent: CDCl₃
Ambient temperature
Total 1328 repetitions



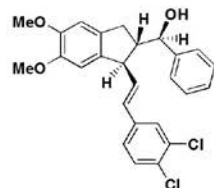
Compound 7r
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 7t (¹H-NMR spectral data)

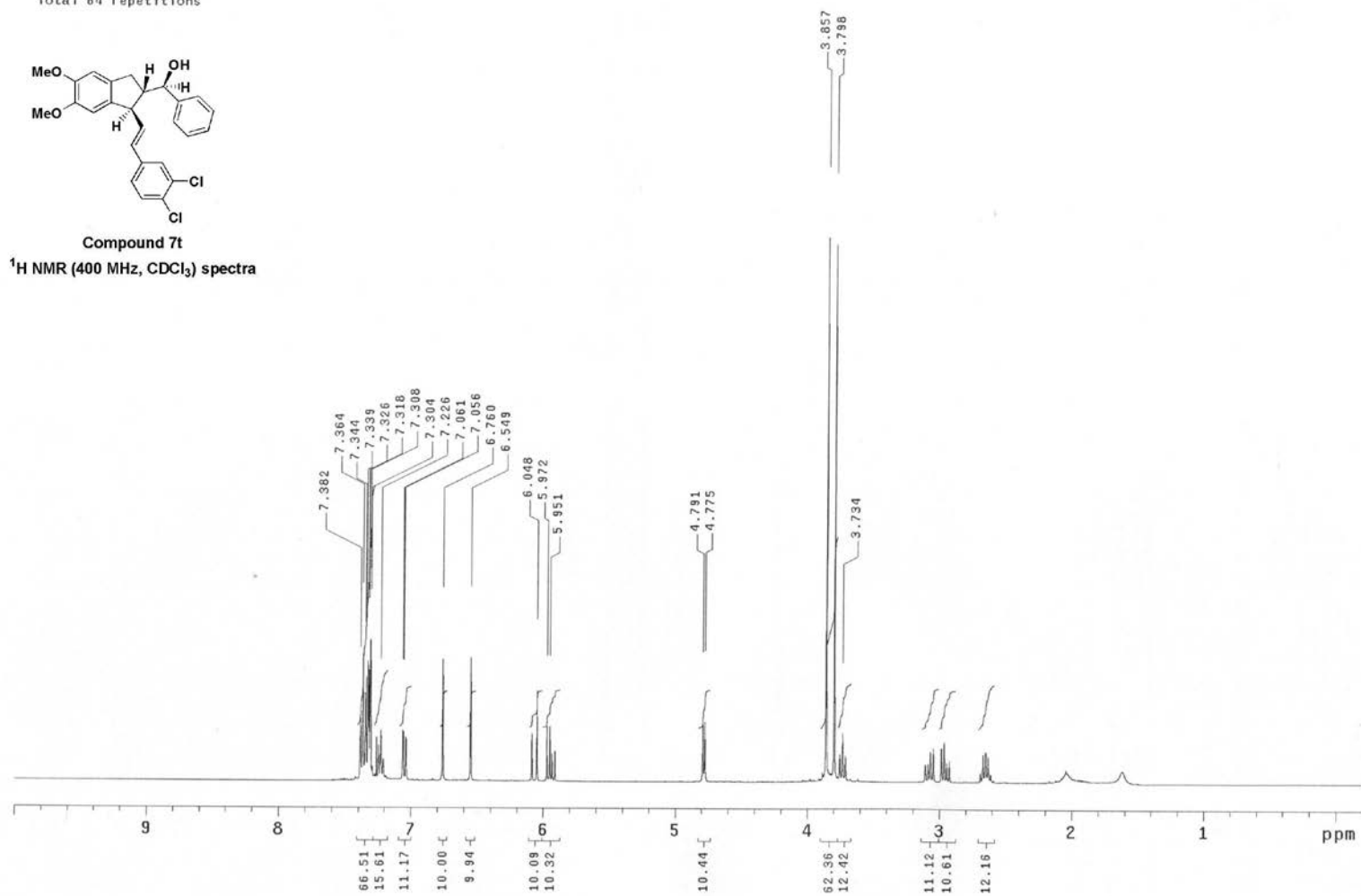
NCNB0308

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Mar 9 2018
 Solvent: CDCl₃
 Ambient temperature
 Total 64 repetitions



Compound 7t

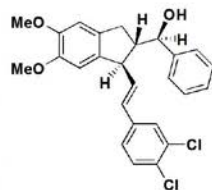
¹H NMR (400 MHz, CDCl₃) spectra



Compound 7t (¹³C-NMR spectral data)

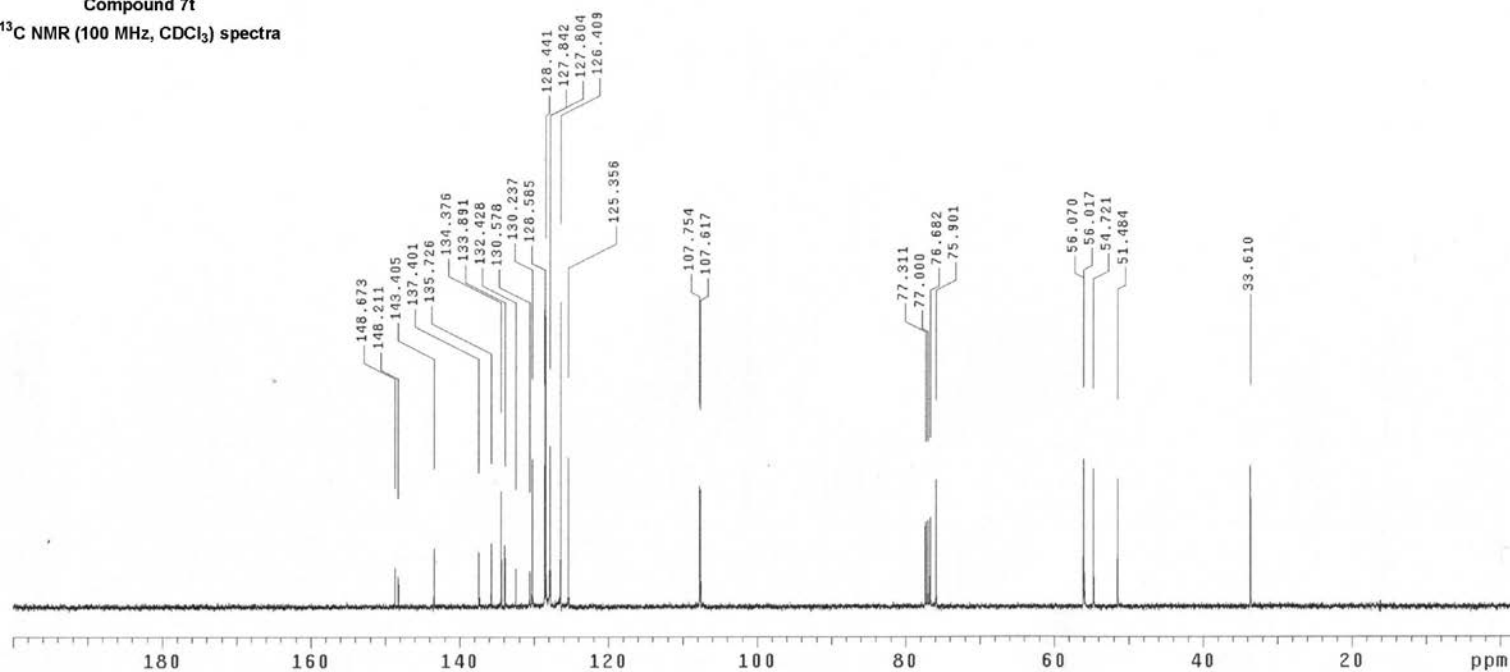
NCN80308

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Mar 9 2018
Solvent: CDCl₃
Ambient temperature
Total 2048 repetitions



Compound 7t

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 7u (¹H-NMR spectral data)

NCNB30Me

Pulse Sequence: s2pu1

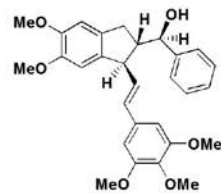
UNITYplus-400 "unity400"

Date: Jan 25 2018

Solvent: CDCl₃

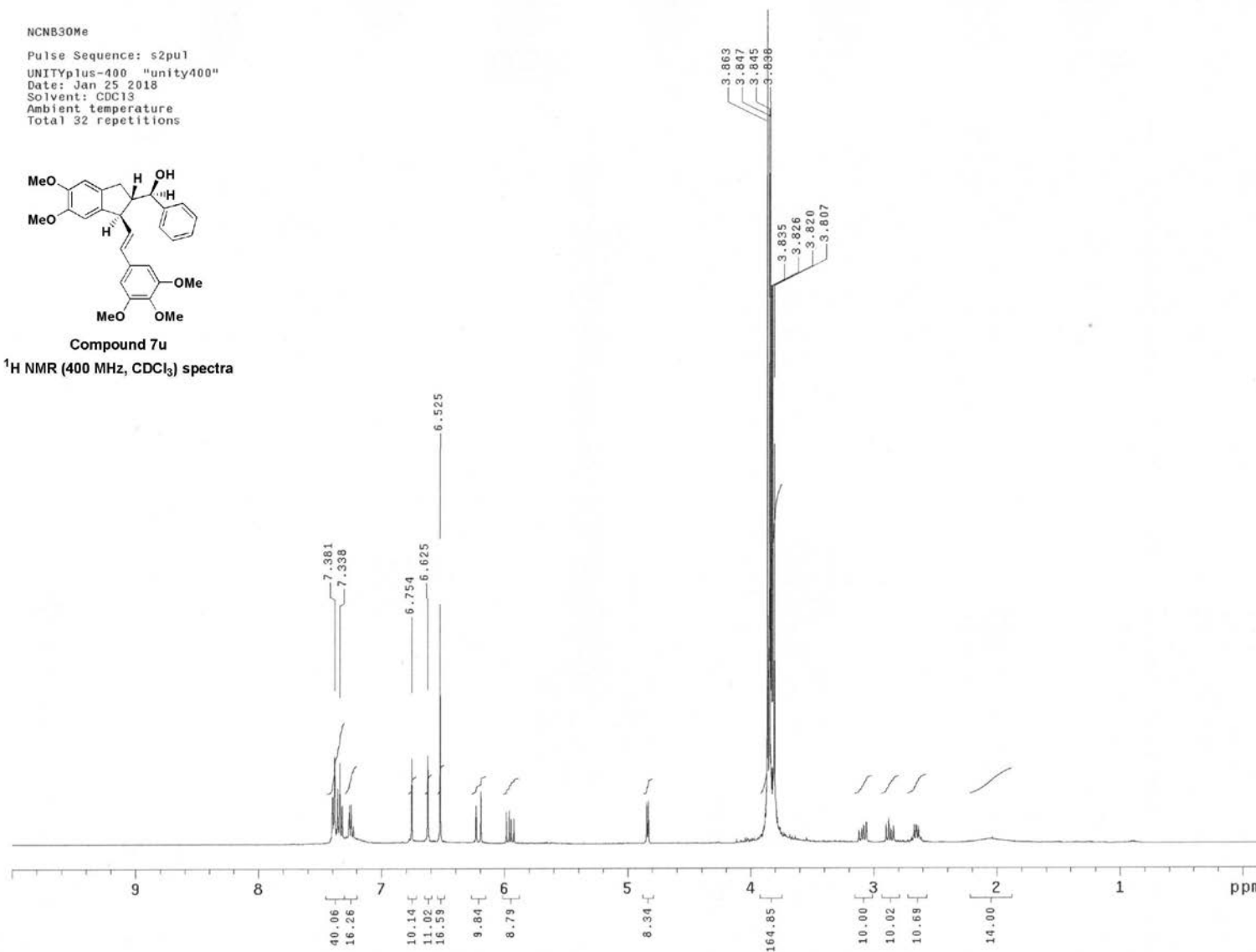
Ambient temperature

Total 32 repetitions



Compound 7u

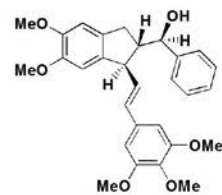
¹H NMR (400 MHz, CDCl₃) spectra



Compound 7u (¹³C-NMR spectral data)

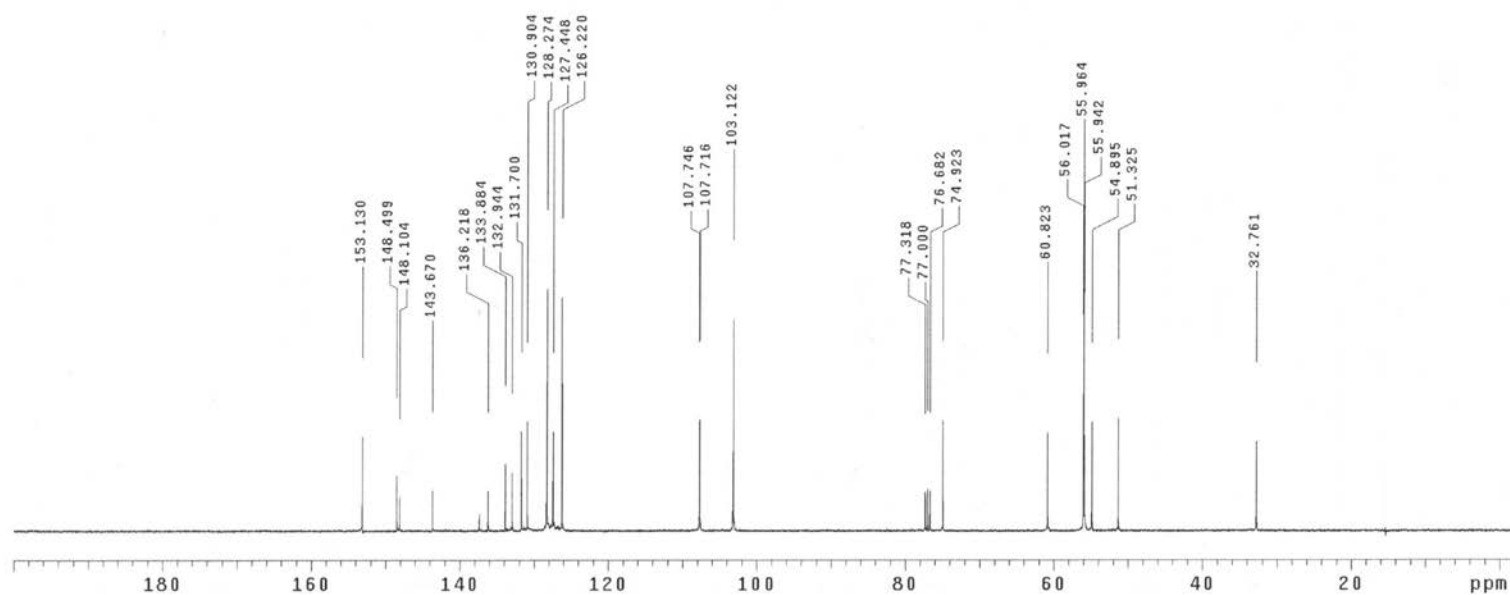
NCN830Me

Pulse Sequence: s2pul
 UNITYplus-400 "unity400"
 Date: Jan 25 2018
 Solvent: CDCl₃
 Ambient temperature
 Total 3040 repetitions



Compound 7u

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 7v (¹H-NMR spectral data)

NCNB0226

Pulse Sequence: s2pu1

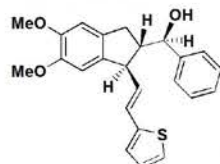
UNITYplus-400 "unity400"

Date: Feb 26 2018

Solvent: CDCl₃

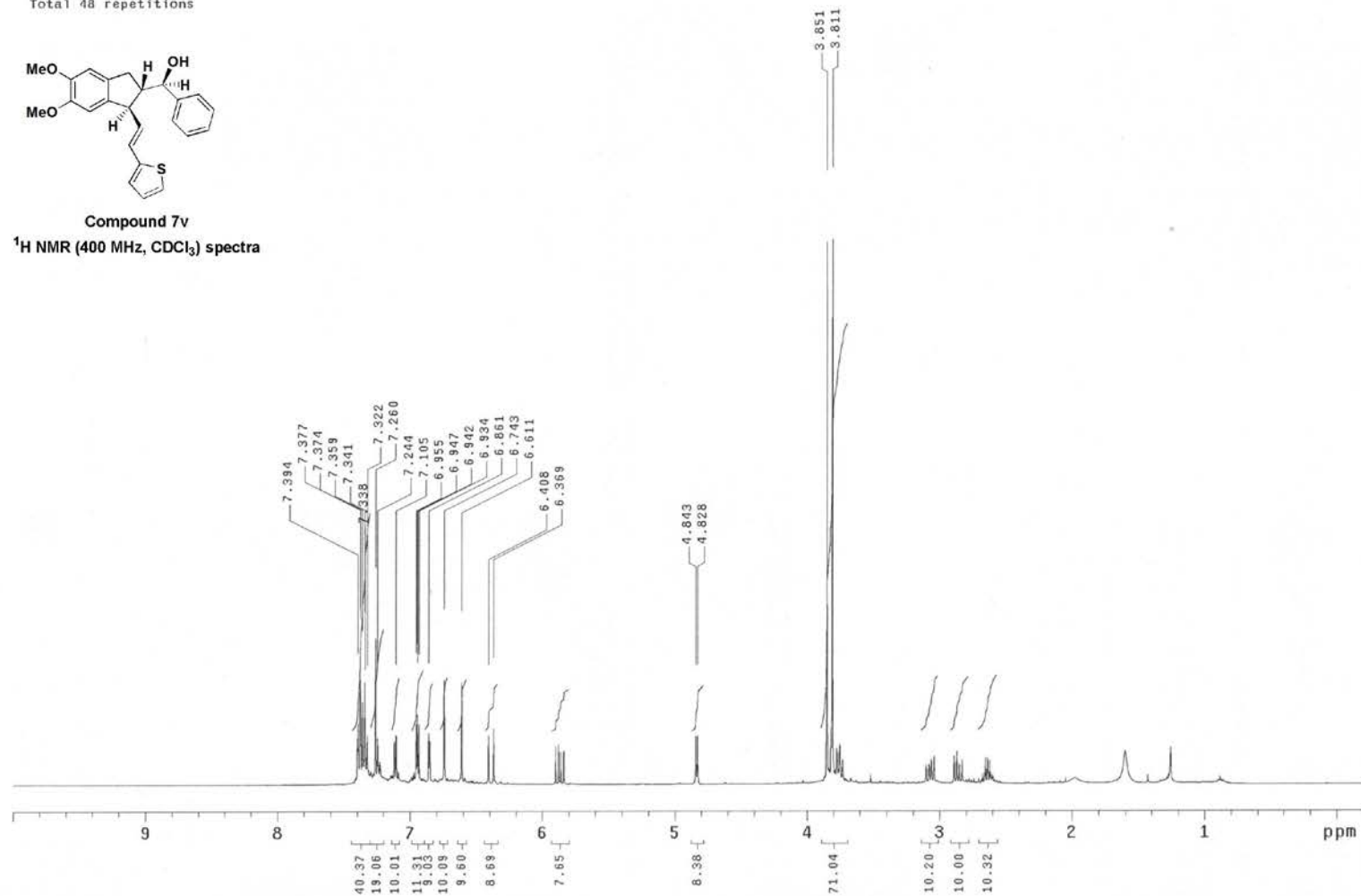
Ambient temperature

Total 48 repetitions



Compound 7v

¹H NMR (400 MHz, CDCl₃) spectra



Compound 7v (¹³C-NMR spectral data)

NCNB0226

Pulse Sequence: s2pu1

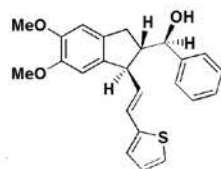
UNITYplus-400 "unity400"

Date: Feb 26 2018

Solvent: CDCl₃

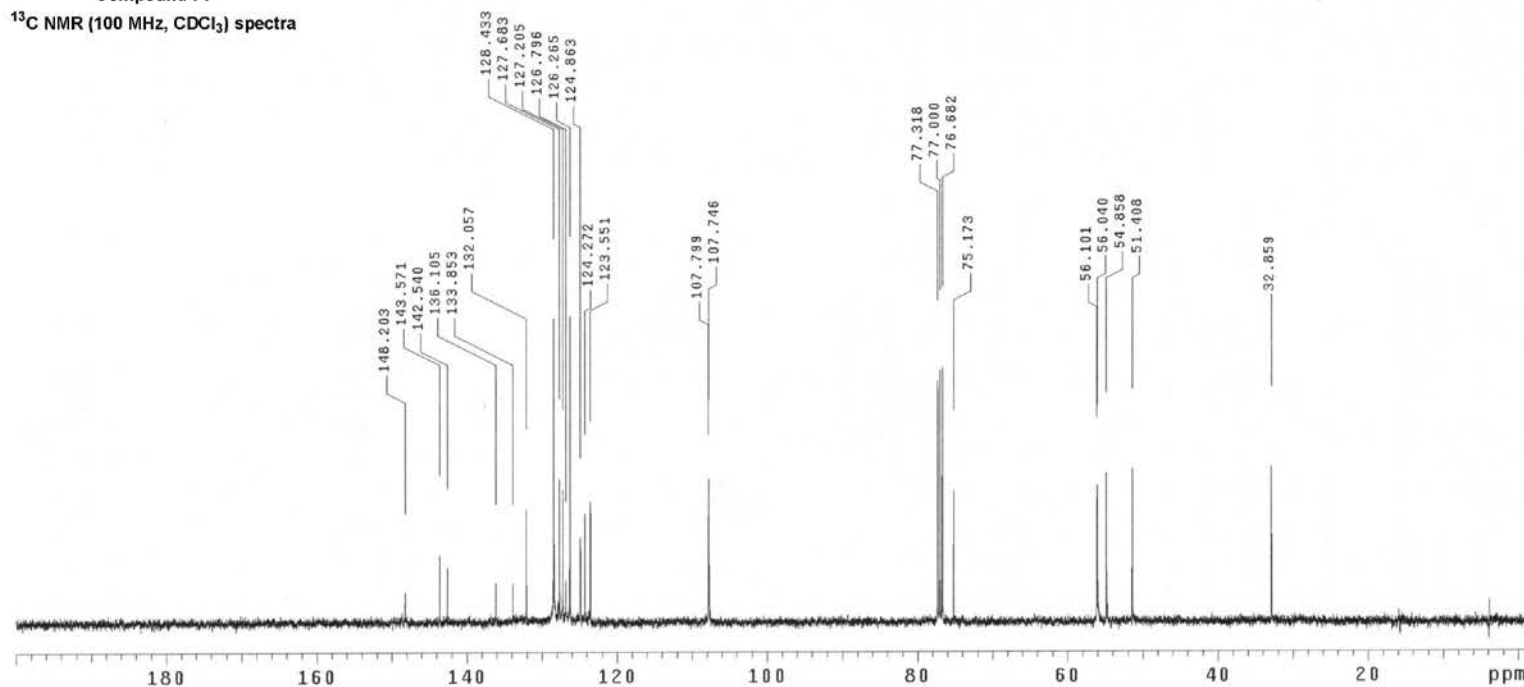
Ambient temperature

Total 6720 repetitions



Compound 7v

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 7w (¹H-NMR spectral data)

NCNB0207

Pulse Sequence: s2pu1

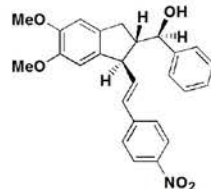
UNITYplus-400 "unity400"

Date: Feb 8 2018

Solvent: CDCl₃

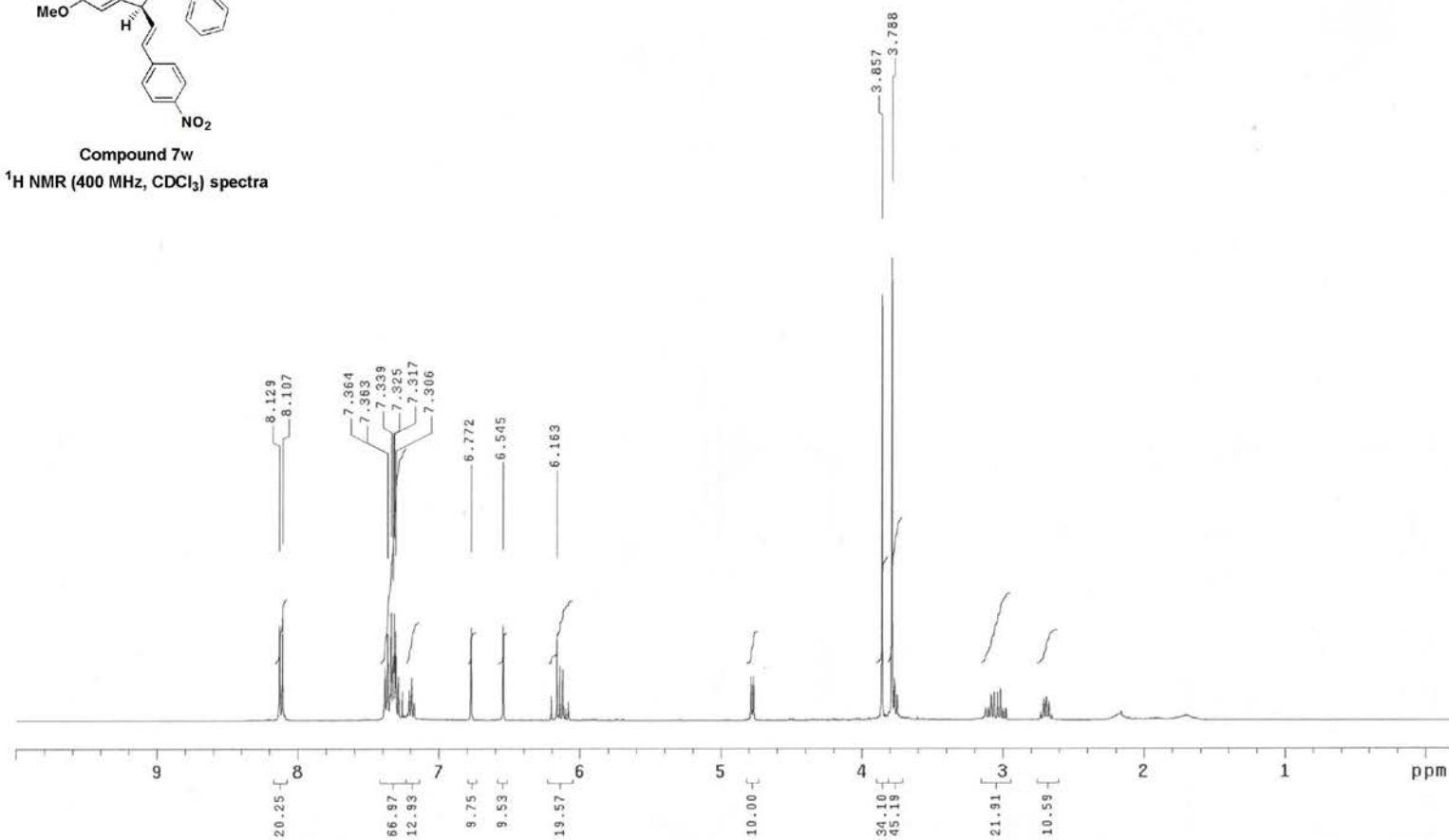
Ambient temperature

Total 32 repetitions



Compound 7w

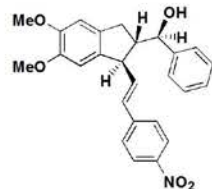
¹H NMR (400 MHz, CDCl₃) spectra



Compound 7w (¹³C-NMR spectral data)

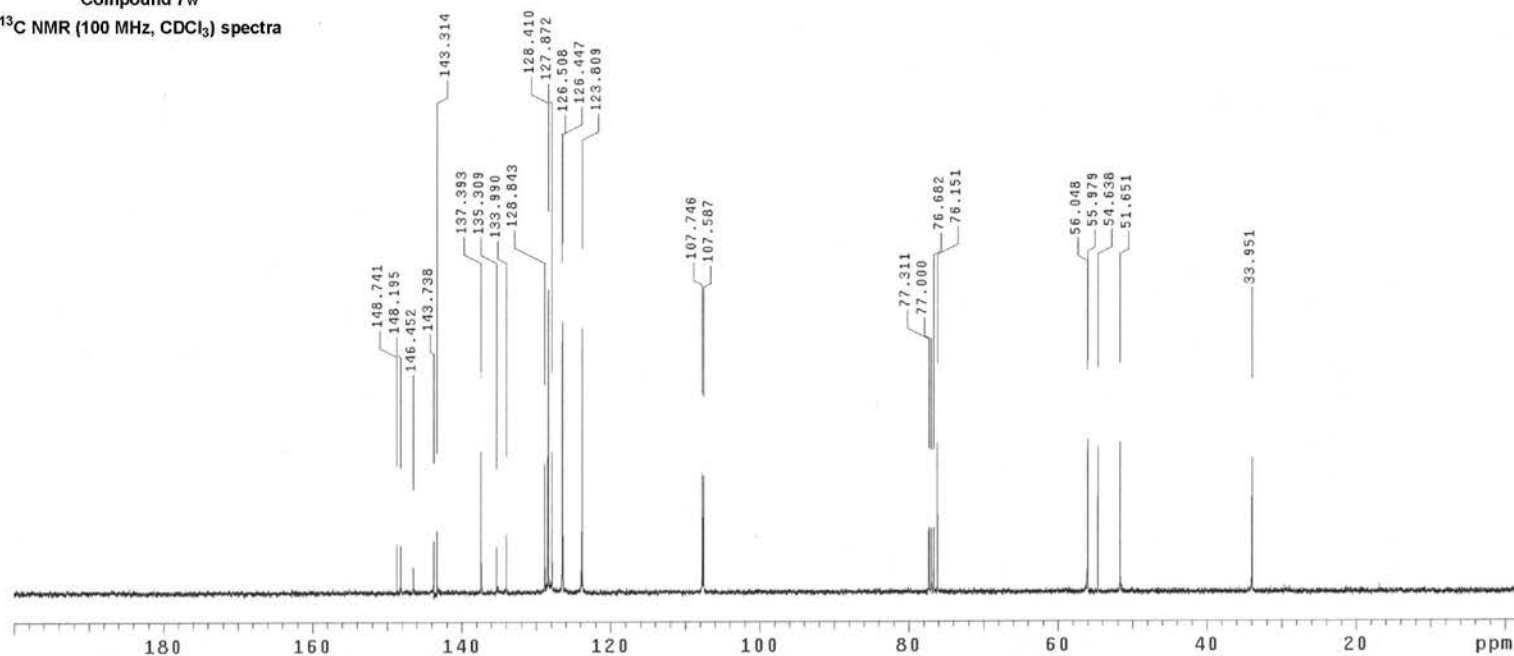
NCNB0207

Pulse Sequence: s2pul
 UNITYplus-400 "unity400"
 Date: Feb 8 2018
 Solvent: CDCl₃
 Ambient temperature
 Total 880 repetitions



Compound 7w

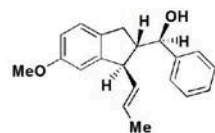
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 7x (¹H-NMR spectral data)

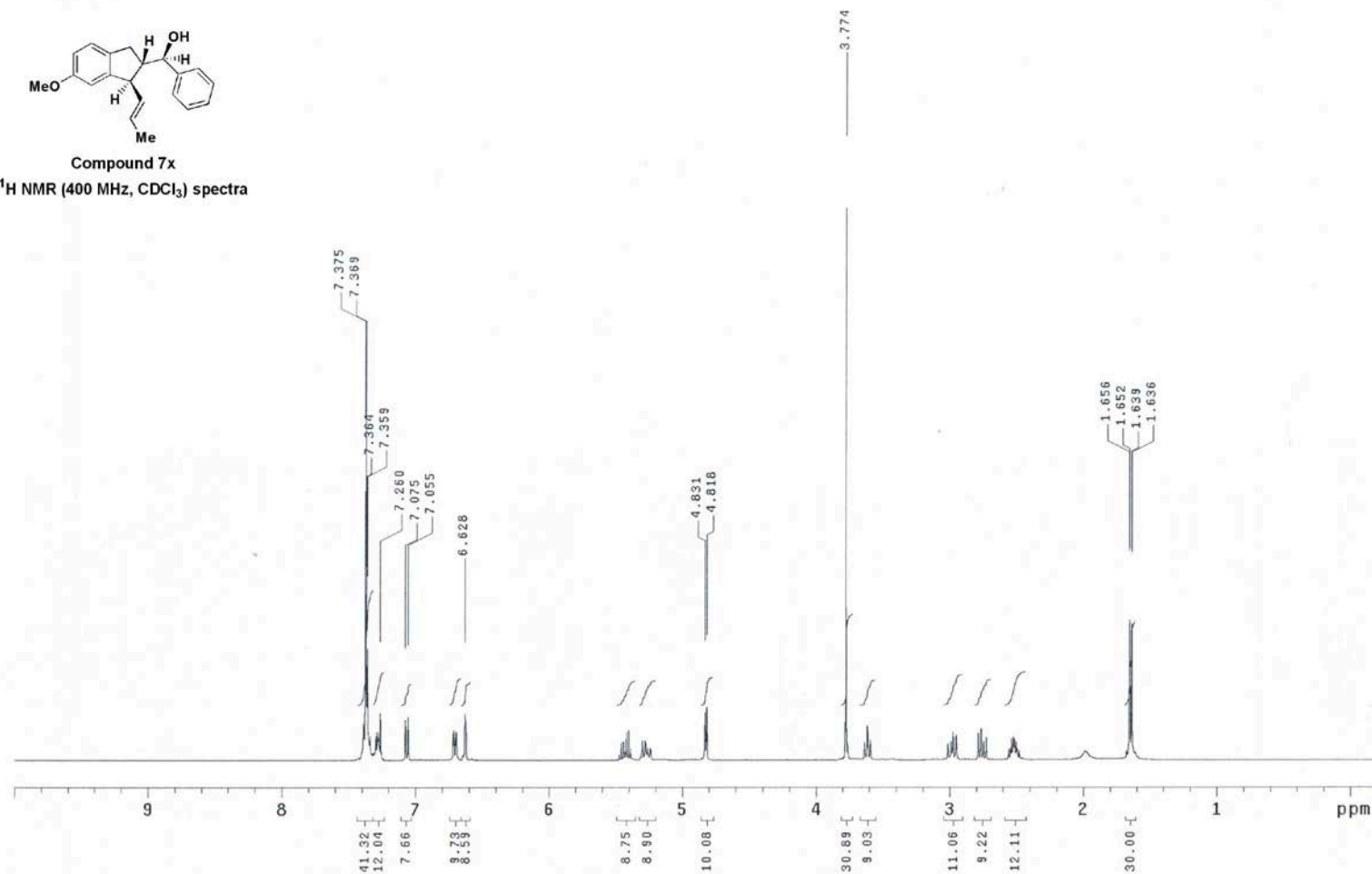
NCNB0314

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Mar 15 2018
 Solvent: CDCl₃
 Ambient temperature
 Total 64 repetitions



Compound 7x

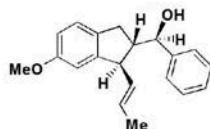
¹H NMR (400 MHz, CDCl₃) spectra



Compound 7x (¹³C-NMR spectral data)

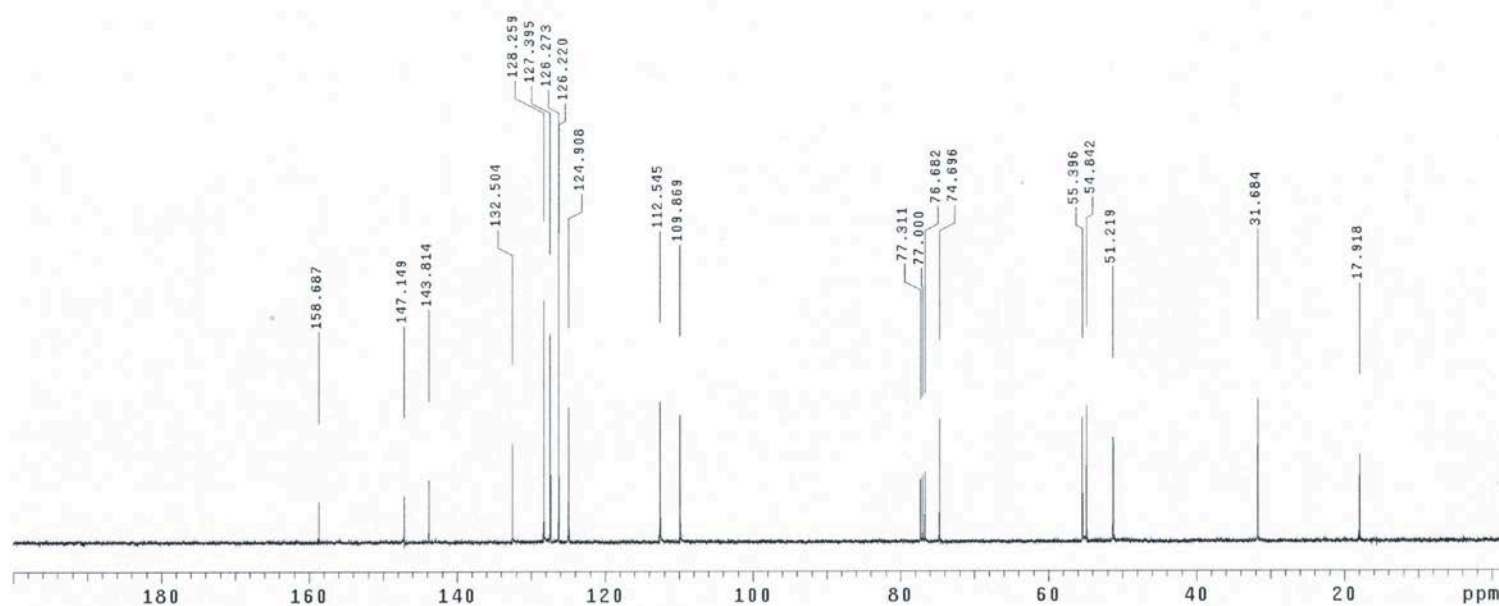
NCNB0314

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Mar 15 2018
Solvent: CDCl₃
Ambient temperature
Total 2304 repetitions



Compound 7x

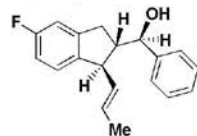
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 7y (¹H-NMR spectral data)

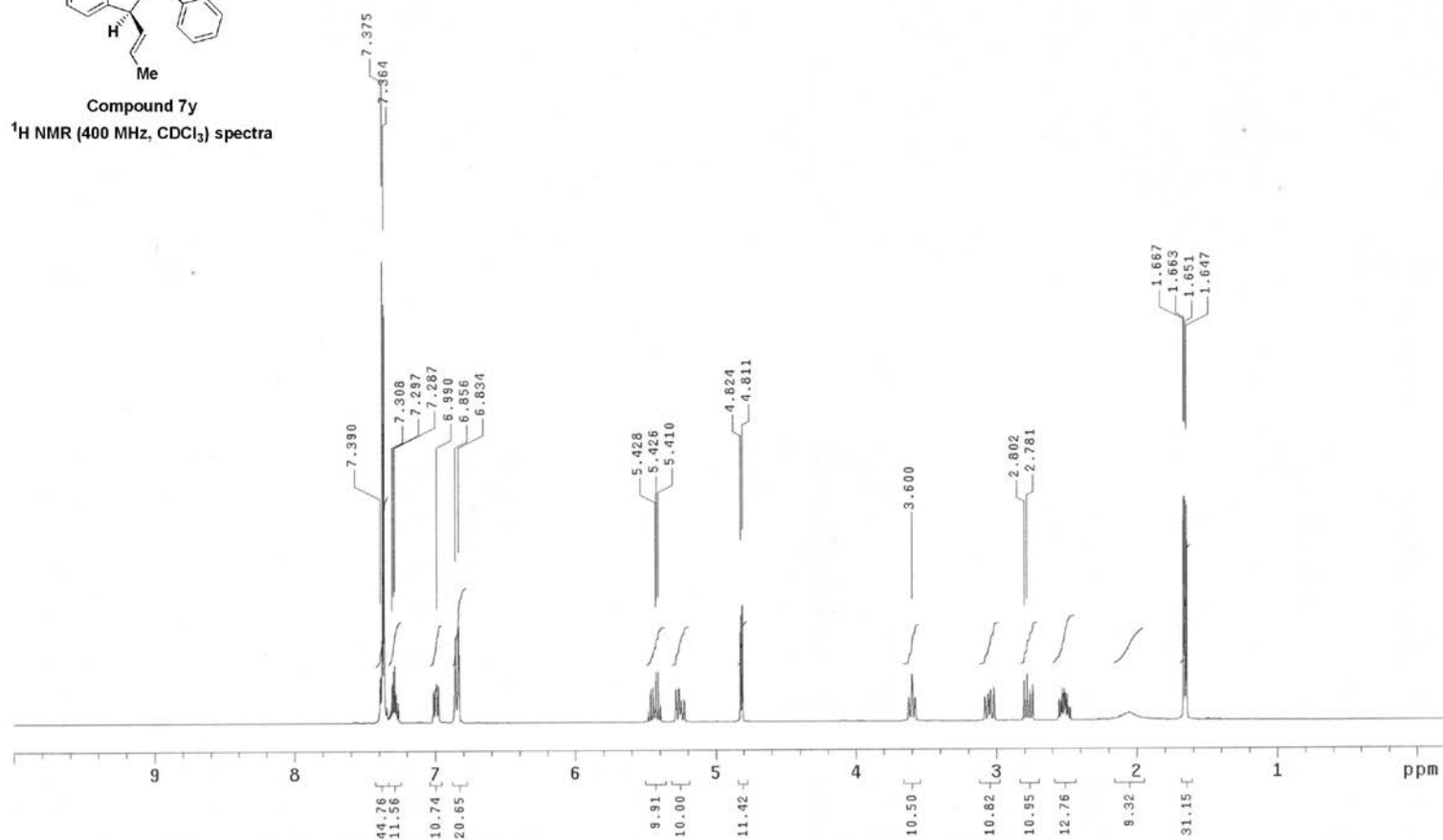
KS1070410

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Apr 12 2018
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetitions



Compound 7y

¹H NMR (400 MHz, CDCl₃) spectra



Compound 7y (¹³C-NMR spectral data)

KS1070410

Pulse Sequence: s2pu1

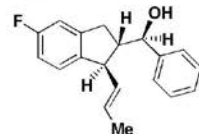
UNITYplus-400 "unity400"

Date: Apr 12 2018

Solvent: CDCl₃

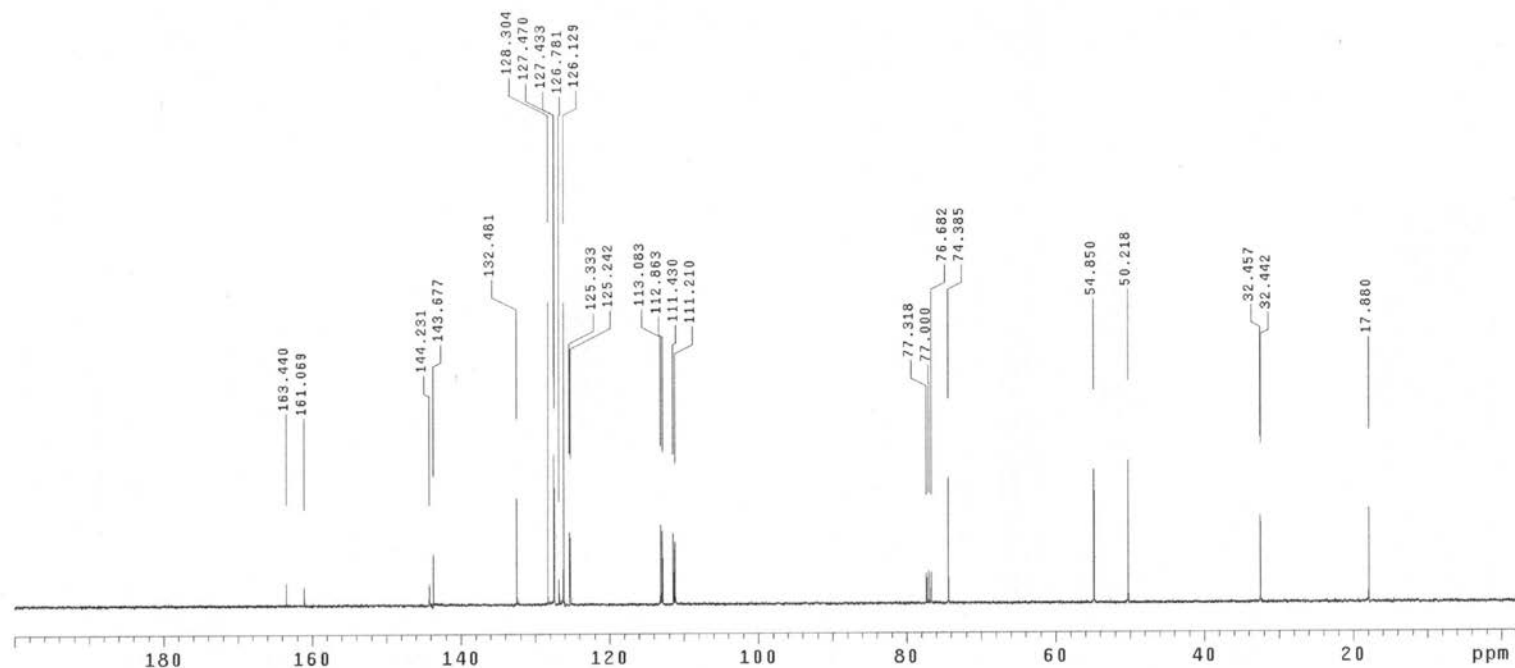
Ambient temperature

Total 528 repetitions



Compound 7y

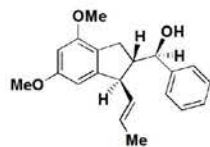
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 7z (¹H-NMR spectral data)

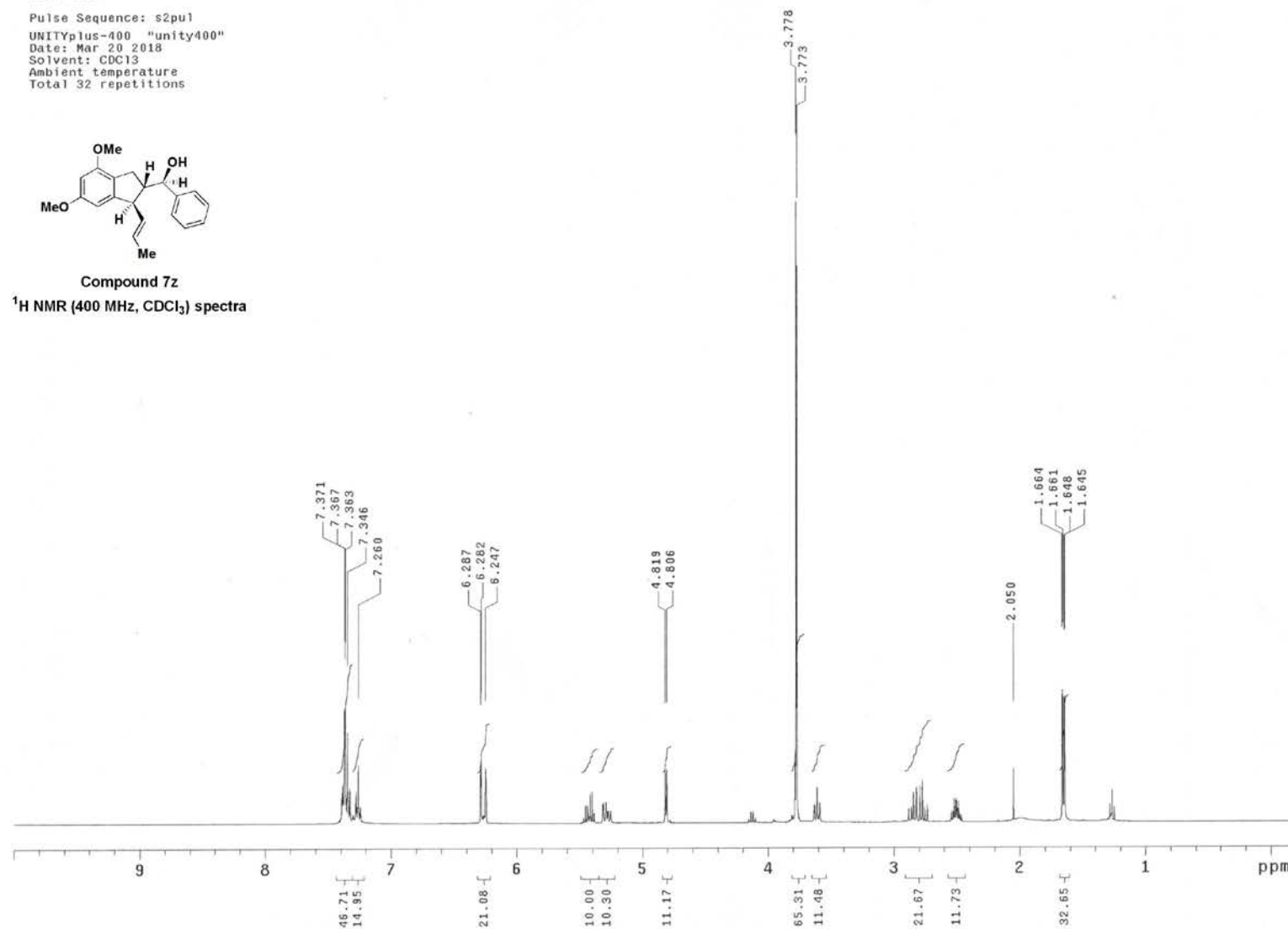
KS1070320

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Mar 20 2018
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetitions



Compound 7z

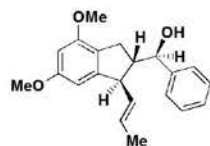
¹H NMR (400 MHz, CDCl₃) spectra



Compound 7z (¹³C-NMR spectral data)

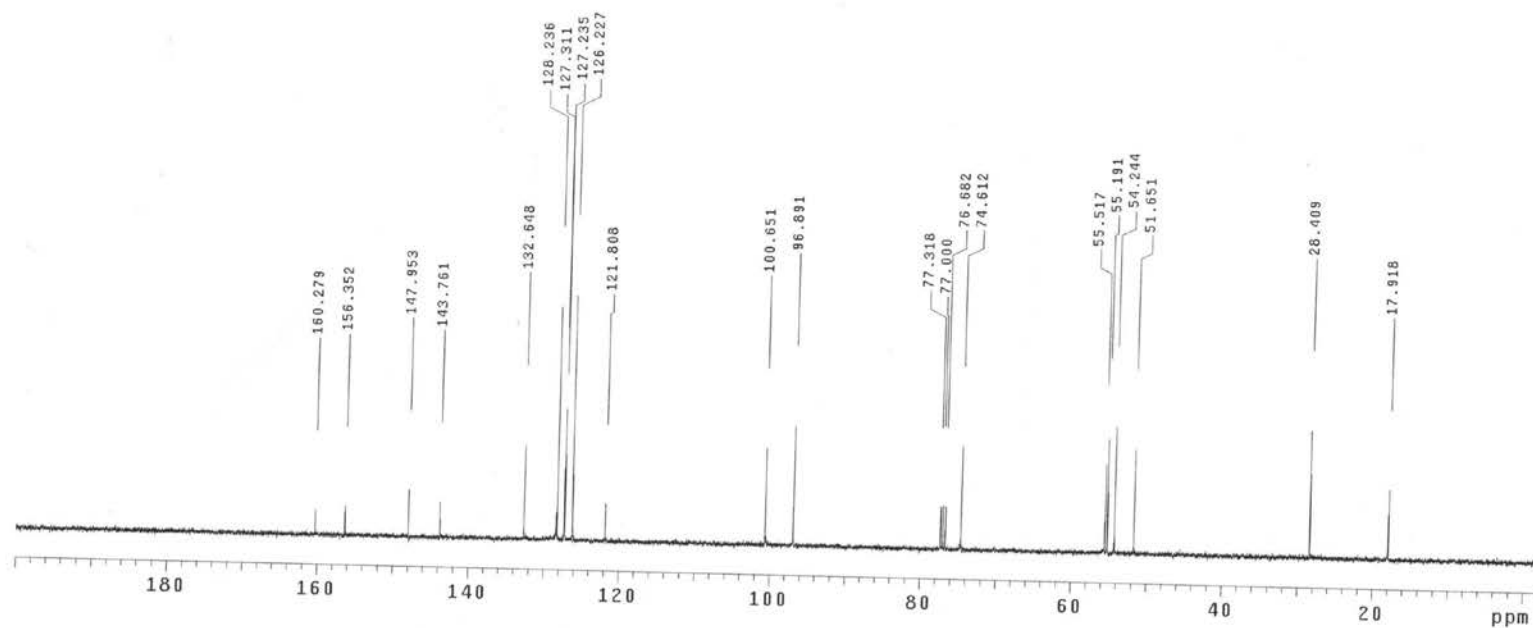
KS1070320

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Mar 20 2018
Solvent: CDCl₃
Ambient temperature
Total 672 repetitions



Compound 7z

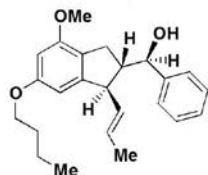
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 7aa (¹H-NMR spectral data)

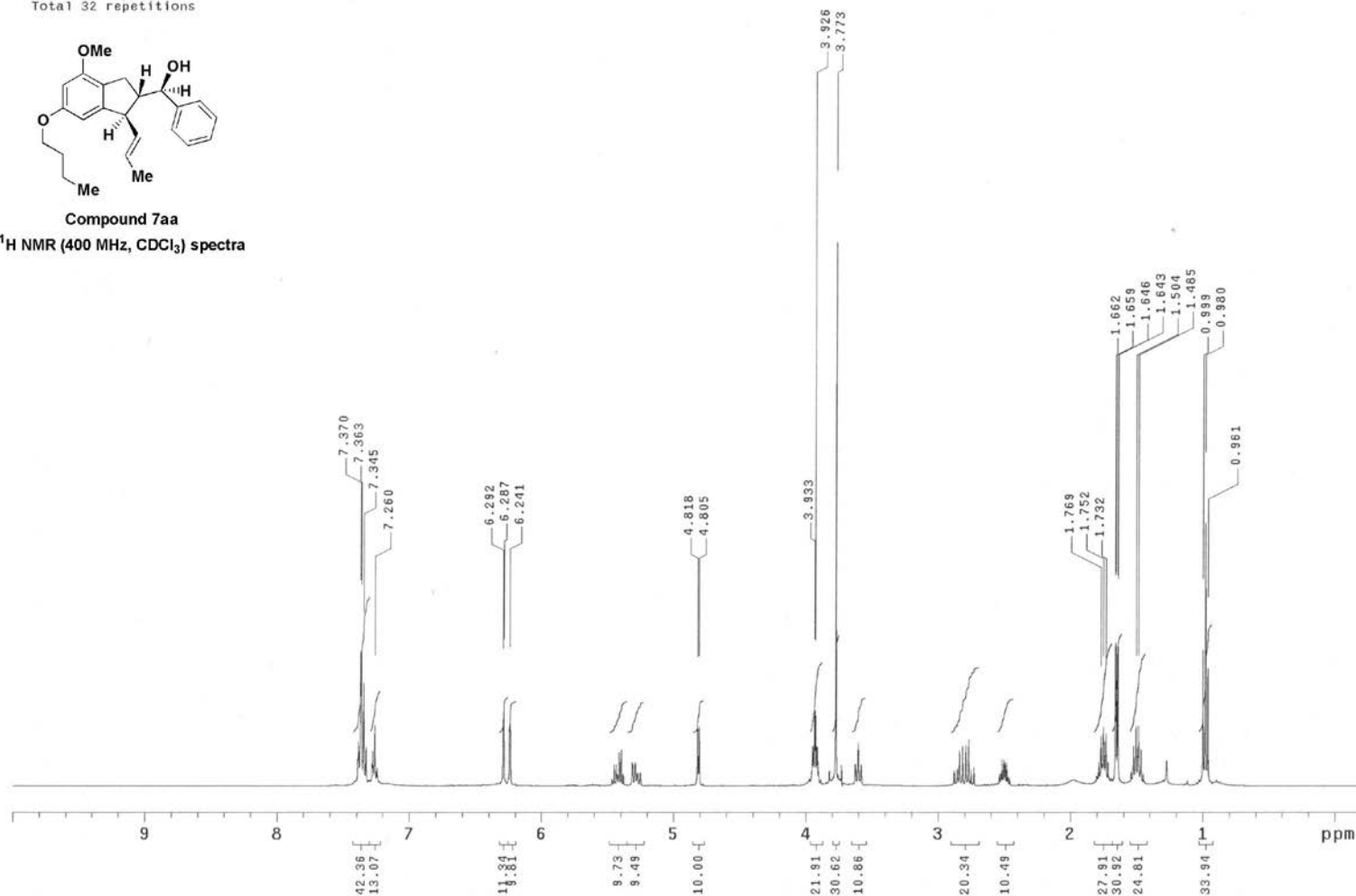
KS1070319

Pulse Sequence: s2pul
 UNITYplus-400 "unity400"
 Date: Mar 19 2018
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetitions



Compound 7aa

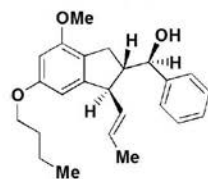
¹H NMR (400 MHz, CDCl₃) spectra



Compound 7aa (¹³C-NMR spectral data)

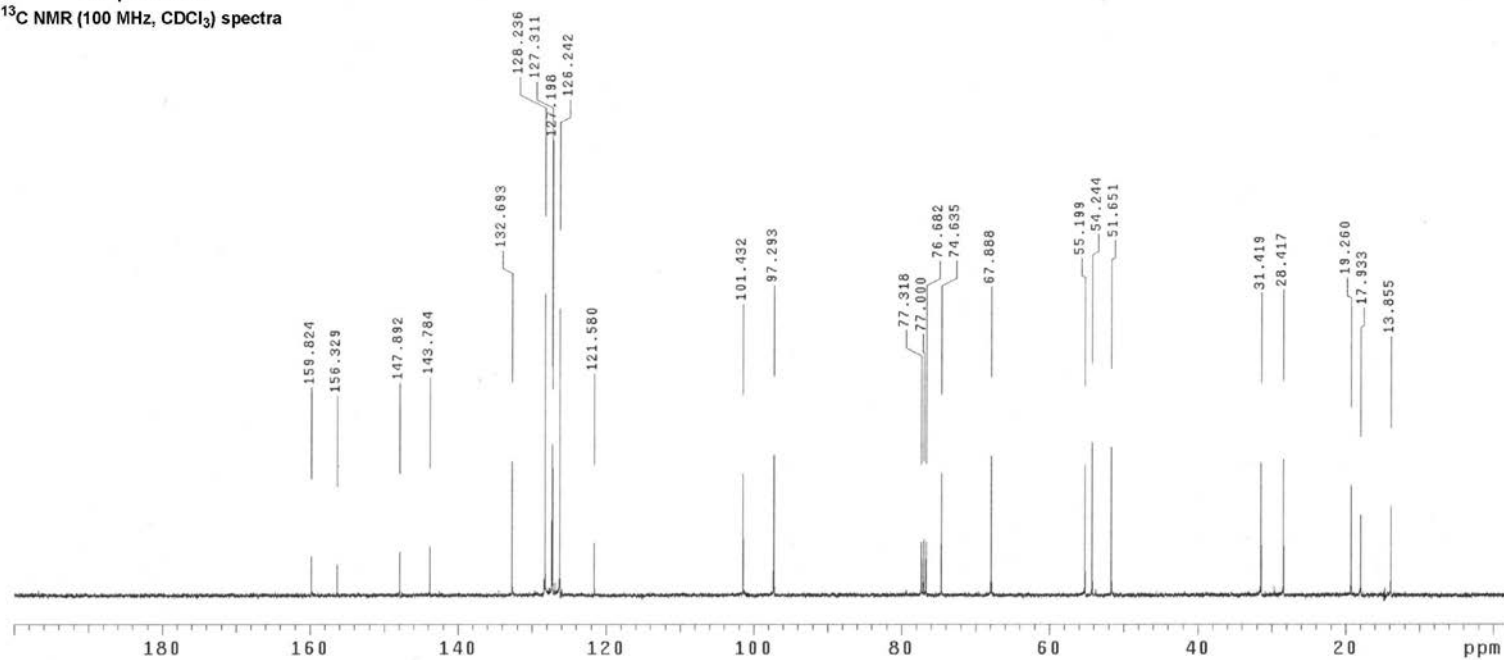
KS1070319

Pulse Sequence: s2pul
 UNITYplus-400 "unity400"
 Date: Mar 19 2018
 Solvent: CDCl₃
 Ambient temperature
 Total 1200 repetitions

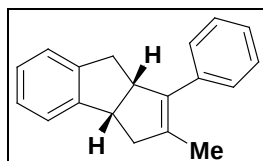


Compound 7aa

¹³C NMR (100 MHz, CDCl₃) spectra



X-ray crystal data of 6n



Empirical formula	C ₁₉ H ₁₈	
Formula weight	246.33	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P b c a	
Unit cell dimensions	a = 11.1361(7) Å	$\alpha = 90^\circ$.
	b = 7.7797(4) Å	$\beta = 90^\circ$.
	c = 30.9551(19) Å	$\gamma = 90^\circ$.
Volume	2681.8(3) Å ³	
Z	8	
Density (calculated)	1.220 Mg/m ³	
Absorption coefficient	0.069 mm ⁻¹	
F(000)	1056	
Crystal size	0.20 x 0.15 x 0.06 mm ³	
Theta range for data collection	1.316 to 26.379°.	
Index ranges	-13 ≤ h ≤ 13, -5 ≤ k ≤ 9, -38 ≤ l ≤ 38	
Reflections collected	14887	
Independent reflections	2735 [R(int) = 0.0345]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9485 and 0.9008	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	2735 / 0 / 173	
Goodness-of-fit on F ²	1.077	
Final R indices [I > 2σ(I)]	R ₁ = 0.0411, wR ₂ = 0.0947	
R indices (all data)	R ₁ = 0.0522, wR ₂ = 0.1114	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.206 and -0.203 e.Å ⁻³	

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 171013LT

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: 171013LT

Bond precision: C-C = 0.0021 Å Wavelength=0.71073

Cell: a=11.1361(7) b=7.7797(4) c=30.9551(19)
 alpha=90 beta=90 gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	2681.8(3)	2681.8(3)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C19 H18	?
Sum formula	C19 H18	C19 H18
Mr	246.33	246.33
Dx, g cm ⁻³	1.220	1.220
Z	8	8
Mu (mm ⁻¹)	0.069	0.069
F000	1056.0	1056.0
F000'	1056.37	
h,k,lmax	13,9,38	13,9,38
Nref	2737	2735
Tmin,Tmax	0.988,0.996	0.901,0.948
Tmin'	0.986	

Correction method= # Reported T Limits: Tmin=0.901 Tmax=0.948
AbsCorr = MULTI-SCAN

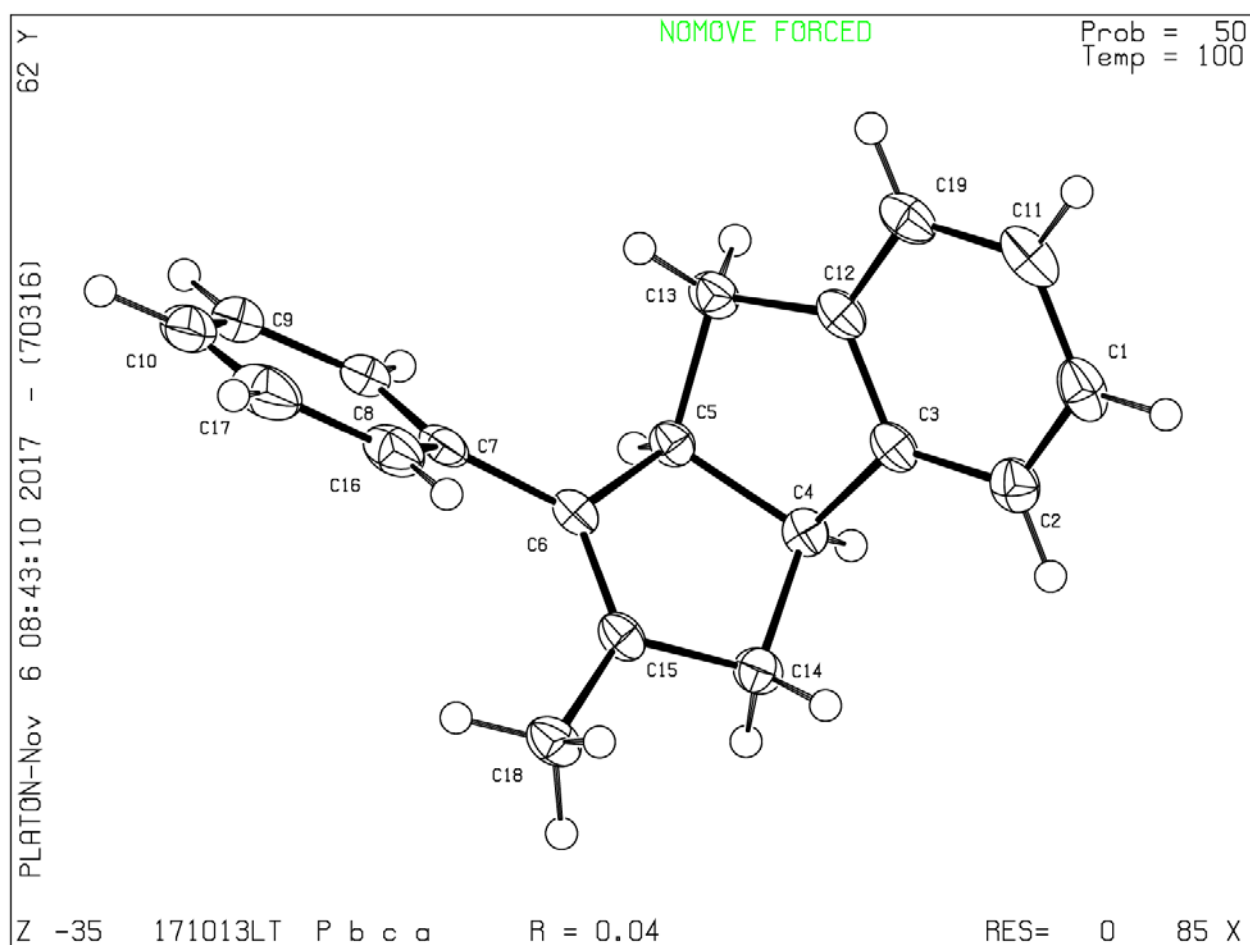
Data completeness= 0.999 Theta(max)= 26.379

R(reflections)= 0.0411(2275) wR2(reflections)= 0.1114(2735)

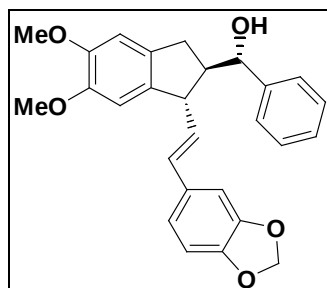
S = 1.077 Npar= 173

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 7p



Empirical formula	C ₃₁ H ₃₄ O ₆	
Formula weight	502.58	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 2 ₁ /c	
Unit cell dimensions	a = 11.796(3) Å	α = 90°.
	b = 17.150(5) Å	β = 110.944(7)°.
	c = 13.523(4) Å	γ = 90°.
Volume	2554.9(12) Å ³	
Z	4	
Density (calculated)	1.307 Mg/m ³	
Absorption coefficient	0.090 mm ⁻¹	
F(000)	1072	
Crystal size	0.23 x 0.22 x 0.18 mm ³	
Theta range for data collection	1.849 to 26.565°.	
Index ranges	-11 ≤ h ≤ 14, -21 ≤ k ≤ 21, -16 ≤ l ≤ 16	
Reflections collected	40644	
Independent reflections	5269 [R(int) = 0.0886]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9485 and 0.7968	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	5269 / 0 / 339	
Goodness-of-fit on F ²	1.126	
Final R indices [I > 2σ(I)]	R ₁ = 0.0642, wR ₂ = 0.1510	
R indices (all data)	R ₁ = 0.0956, wR ₂ = 0.1677	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.378 and -0.375 e.Å ⁻³	

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_180217LT_0m

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: mo_180217LT_0m

Bond precision: C-C = 0.0040 Å Wavelength=0.71073

Cell: a=11.796(3) b=17.150(5) c=13.523(4)
 alpha=90 beta=110.944(7) gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	2555.0(13)	2554.9(12)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C27 H26 O5, C4 H8 O	?
Sum formula	C31 H34 O6	C31 H34 O6
Mr	502.58	502.58
Dx, g cm ⁻³	1.307	1.307
Z	4	4
Mu (mm ⁻¹)	0.090	0.090
F000	1072.0	1072.0
F000'	1072.54	
h,k,lmax	14,21,17	14,21,16
Nref	5336	5269
Tmin,Tmax	0.980,0.984	0.797,0.948
Tmin'	0.980	

Correction method= # Reported T Limits: Tmin=0.797 Tmax=0.948
AbsCorr = MULTI-SCAN

Data completeness= 0.987 Theta(max)= 26.565

R(reflections)= 0.0642(3781) wR2(reflections)= 0.1677(5269)

S = 1.126 Npar= 339

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

