

Supporting Information

In(OTf)₃-Catalyzed Intramolecular Hydroarylation of α -Phenylallyl β -Ketosulfones. Synthesis of Sulfonyl 1-Benzosuberones and 1-Tetralones

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Compound 4a (¹H-NMR spectral data-1)

KSYE7C

Pulse Sequence: s2pu1

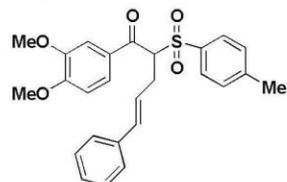
UNITYplus-400 "unity400"

Date: Aug 15 2018

Solvent: CDCl₃

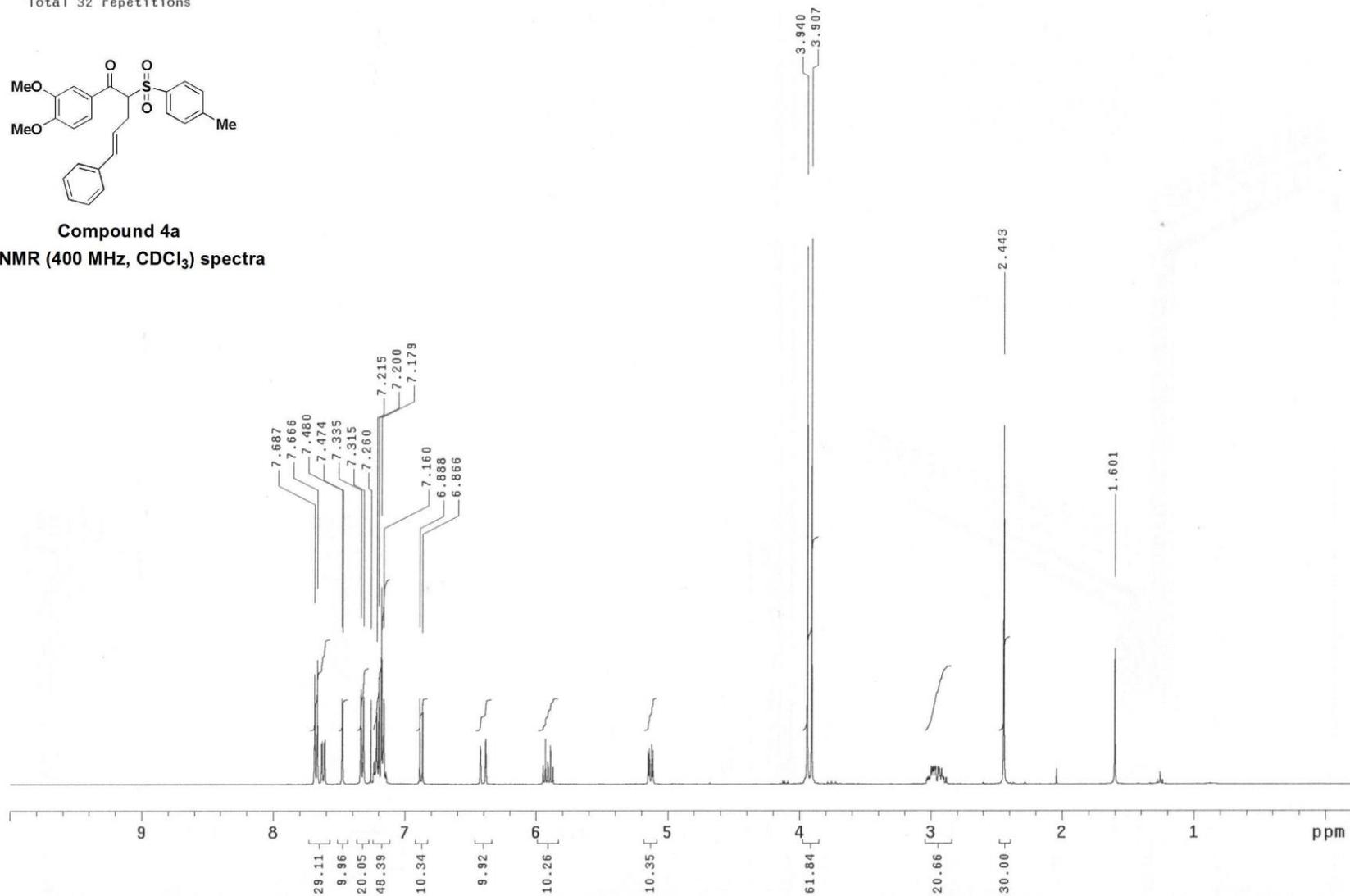
Ambient temperature

Total 32 repetitions

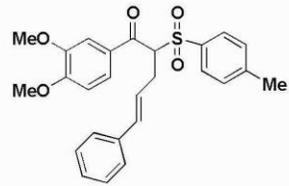


Compound 4a

¹H NMR (400 MHz, CDCl₃) spectra

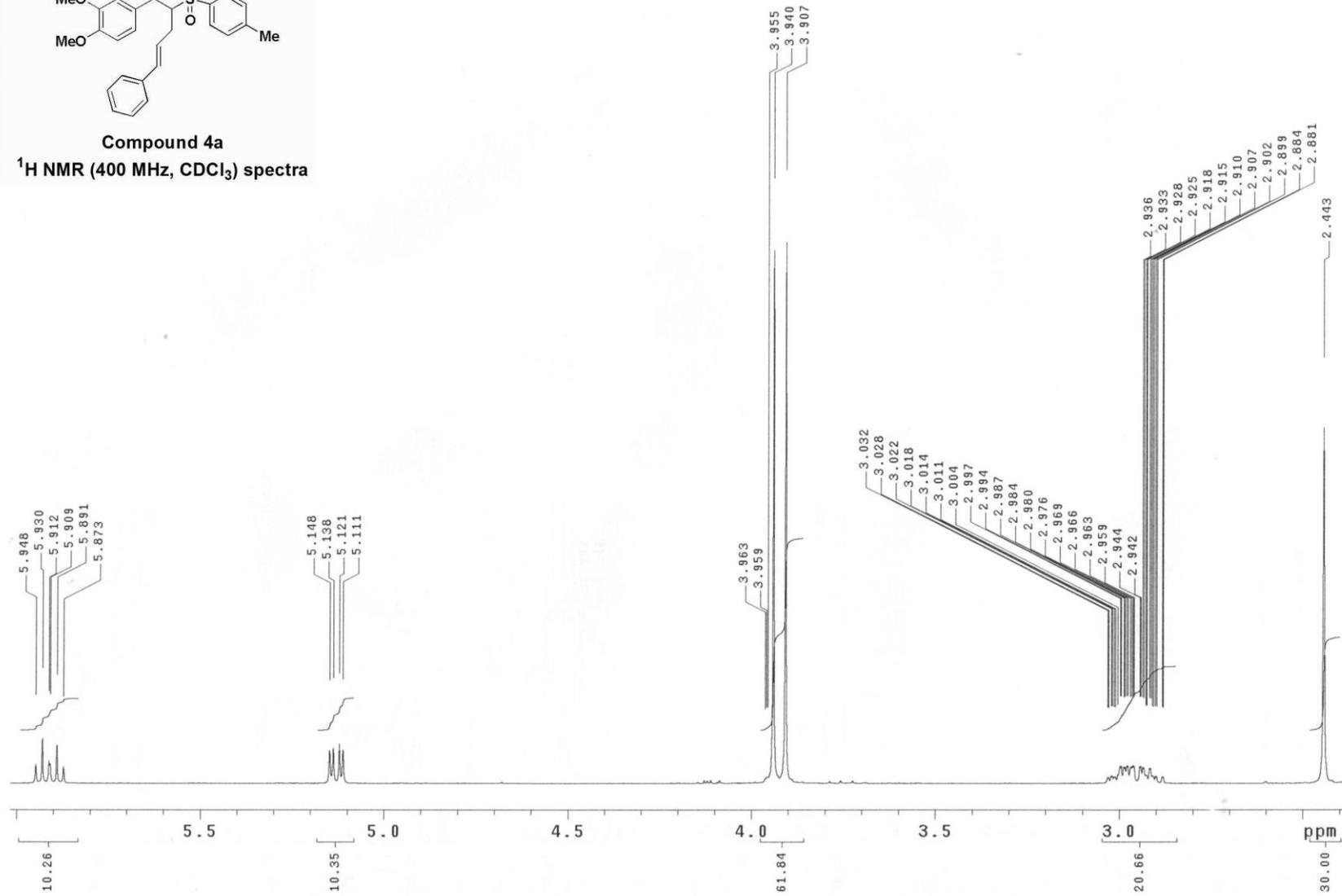


Compound 4a (¹H-NMR spectral data-2)



Compound 4a

¹H NMR (400 MHz, CDCl₃) spectra



Compound 4a (¹³C-NMR spectral data)

KSYE7C

Pulse Sequence: s2pu1

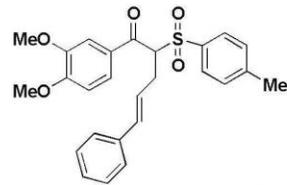
UNITYplus-400 "unity400"

Date: Aug 15 2018

Solvent: CDCl₃

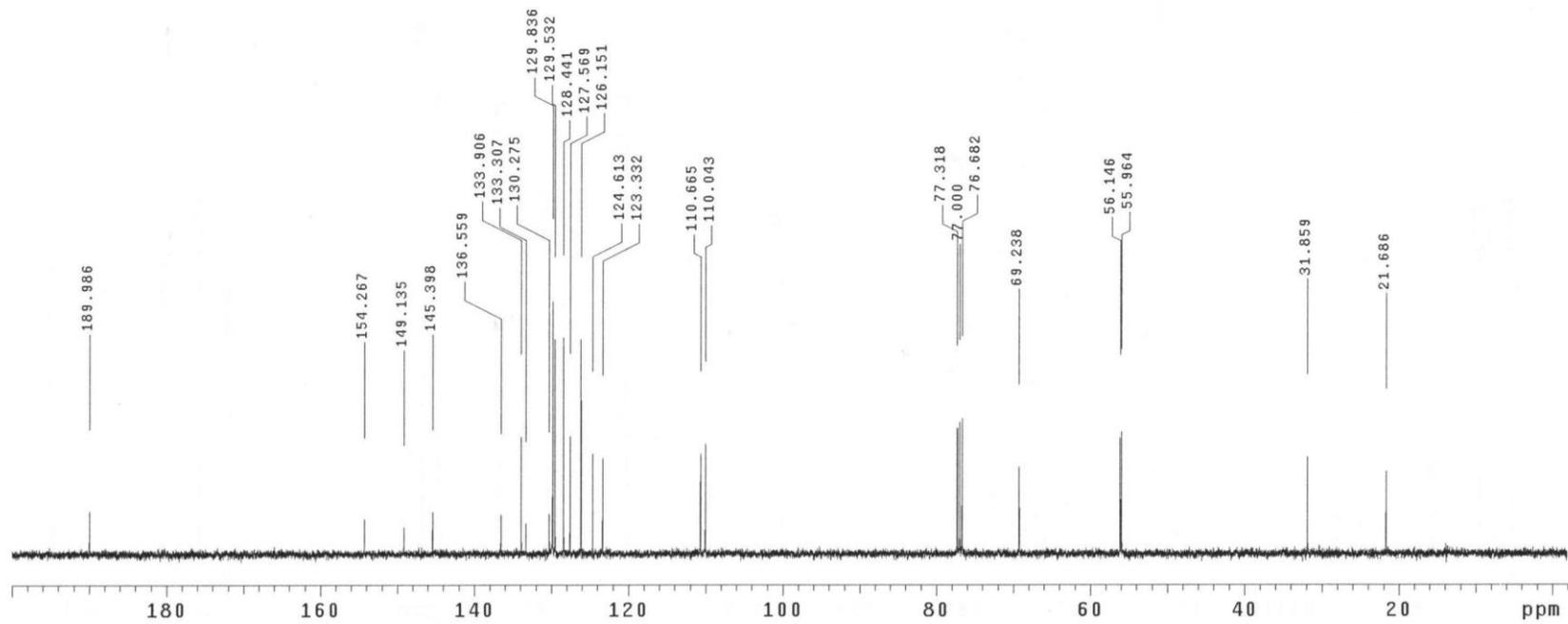
Ambient temperature

Total 720 repetitions



Compound 4a

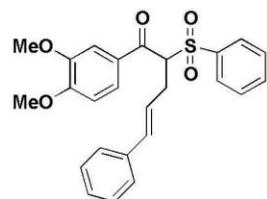
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4b (¹H-NMR spectral data-1)

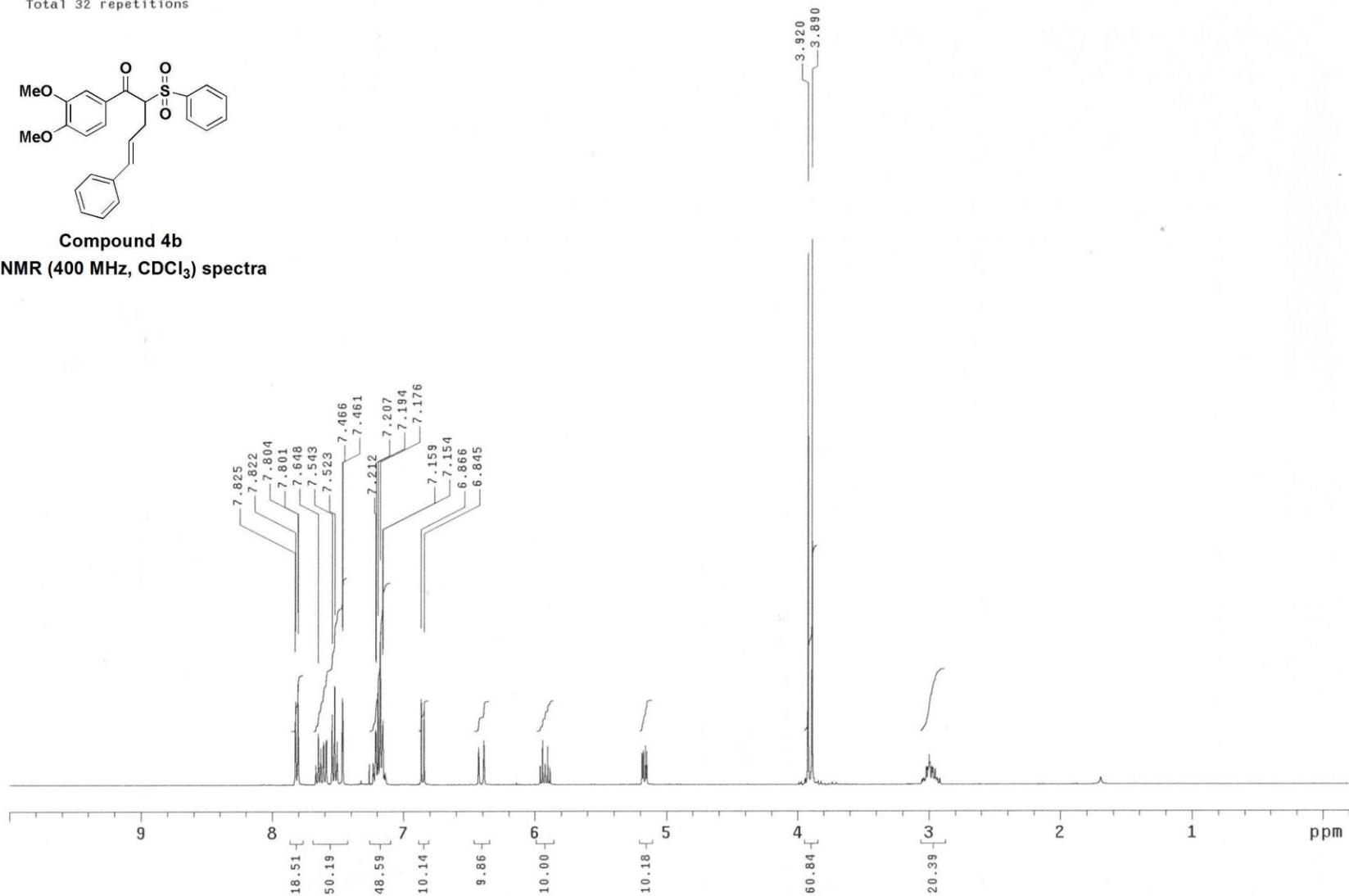
KSE8C

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Sep 11 2018
Solvent: CDCl₃
Ambient temperature
Total 32 repetitions

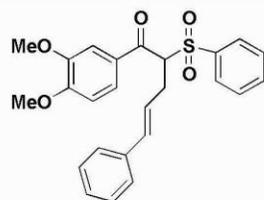


Compound 4b

¹H NMR (400 MHz, CDCl₃) spectra

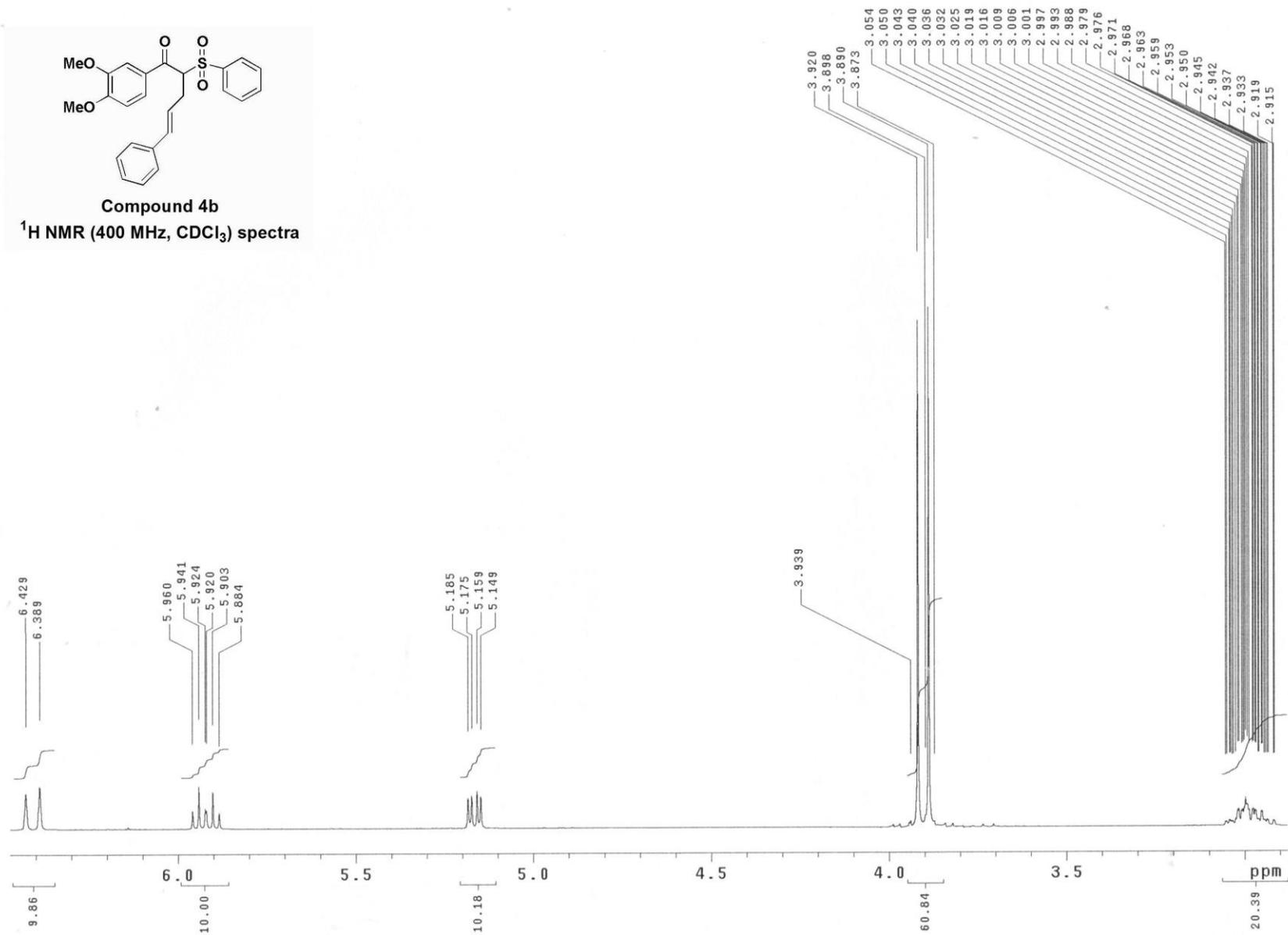


Compound 4b (¹H-NMR spectral data-2)



Compound 4b

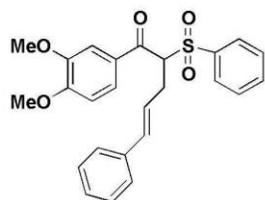
¹H NMR (400 MHz, CDCl₃) spectra



Compound 4b (¹³C-NMR spectral data)

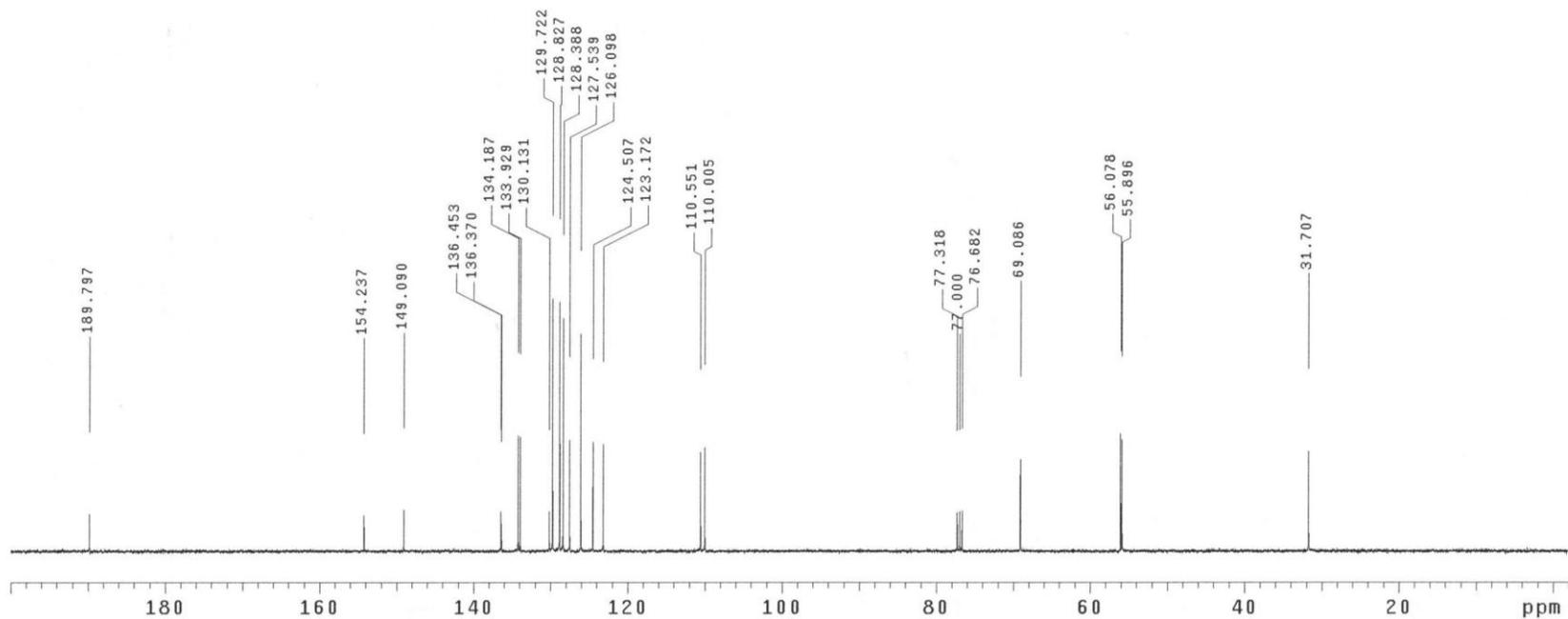
KSE8C

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Sep 11 2018
Solvent: CDCl₃
Ambient temperature
Total 432 repetitions



Compound 4b

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4c (¹H-NMR spectral data-1)

KSE11C

Pulse Sequence: s2pu1

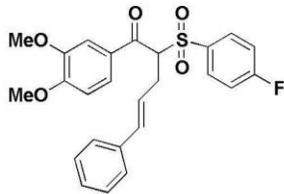
UNITYplus-400 "unity400"

Date: Nov 6 2018

Solvent: CDCl₃

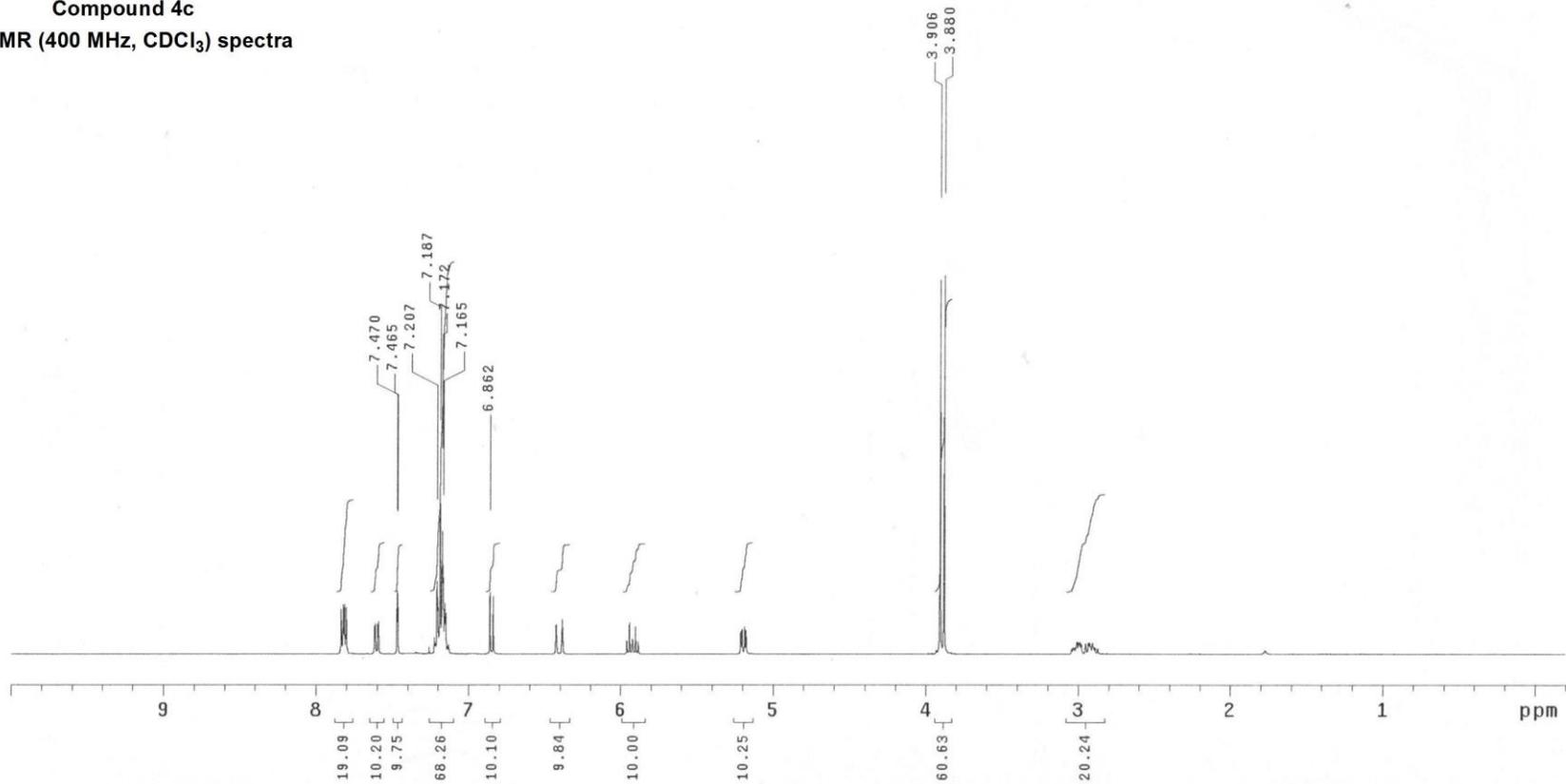
Ambient temperature

Total 32 repetitions

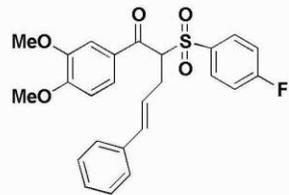


Compound 4c

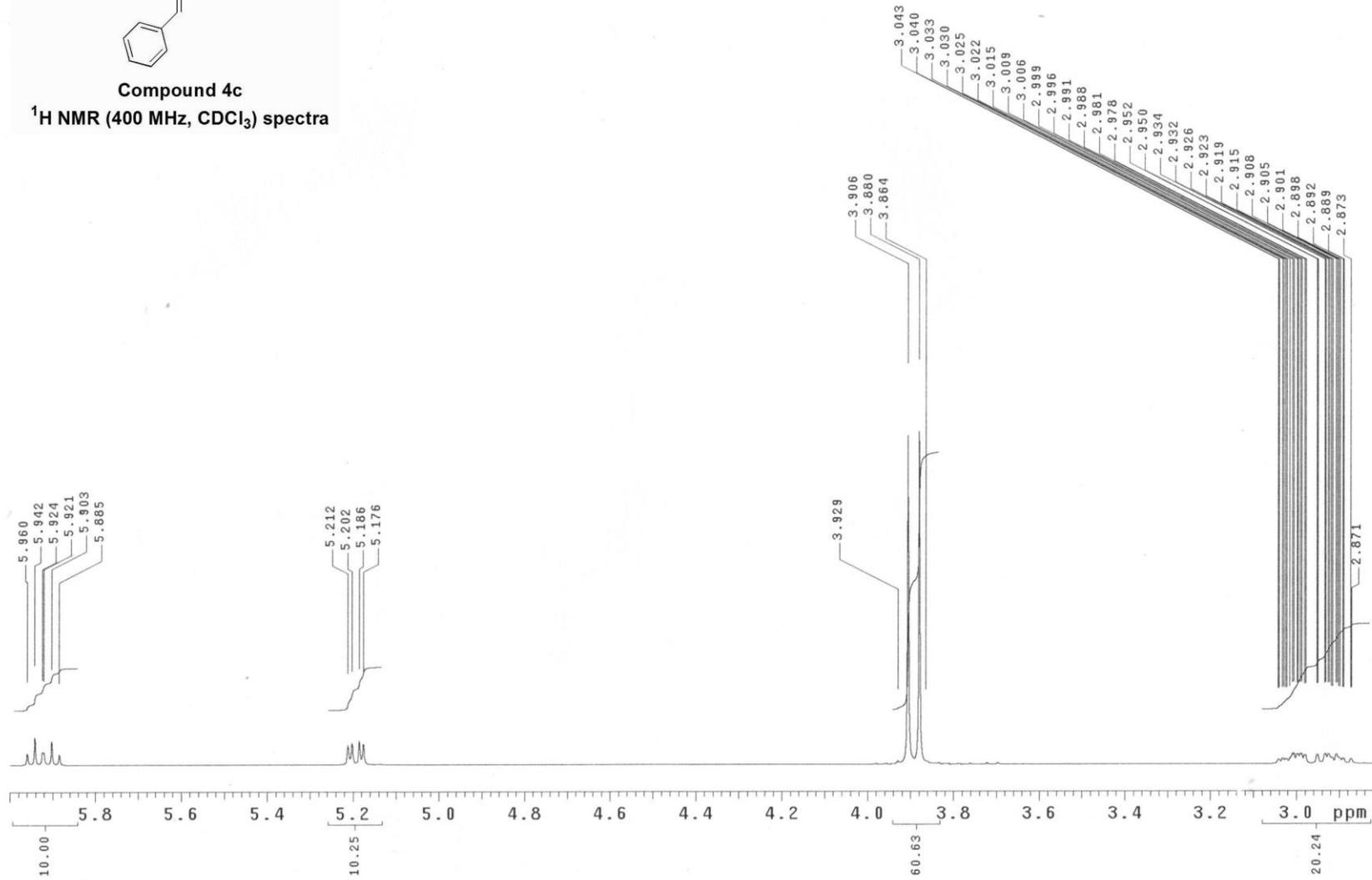
¹H NMR (400 MHz, CDCl₃) spectra



Compound 4c (¹H-NMR spectral data-2)



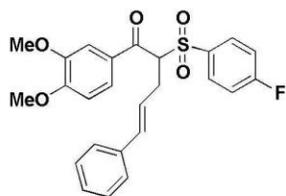
Compound 4c
¹H NMR (400 MHz, CDCl₃) spectra



Compound 4c (¹³C-NMR spectral data)

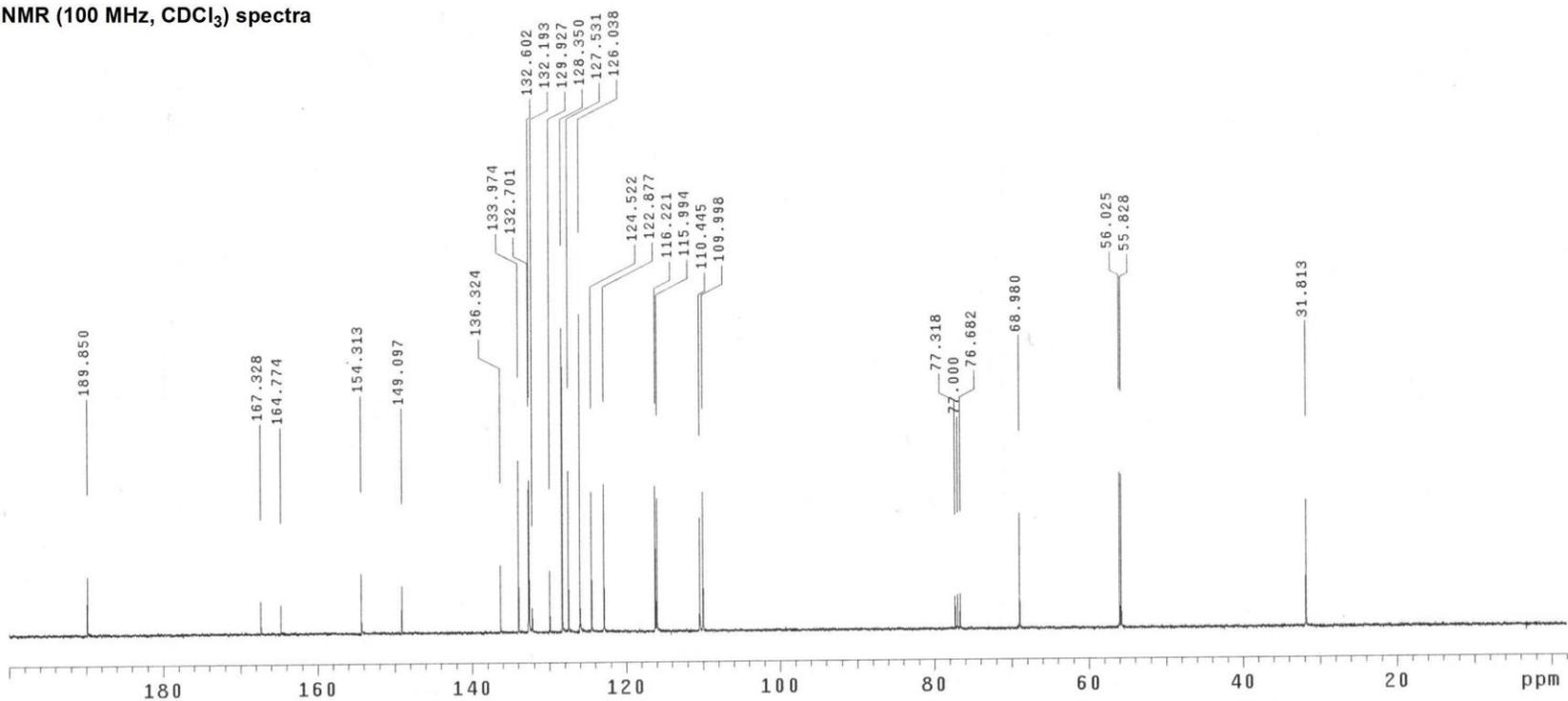
KSE11C

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Nov 6 2018
Solvent: CDCl₃
Ambient temperature
Total 288 repetitions



Compound 4c

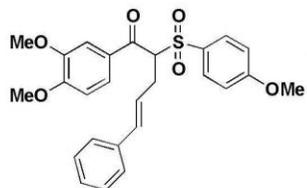
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4d (¹H-NMR spectral data-1)

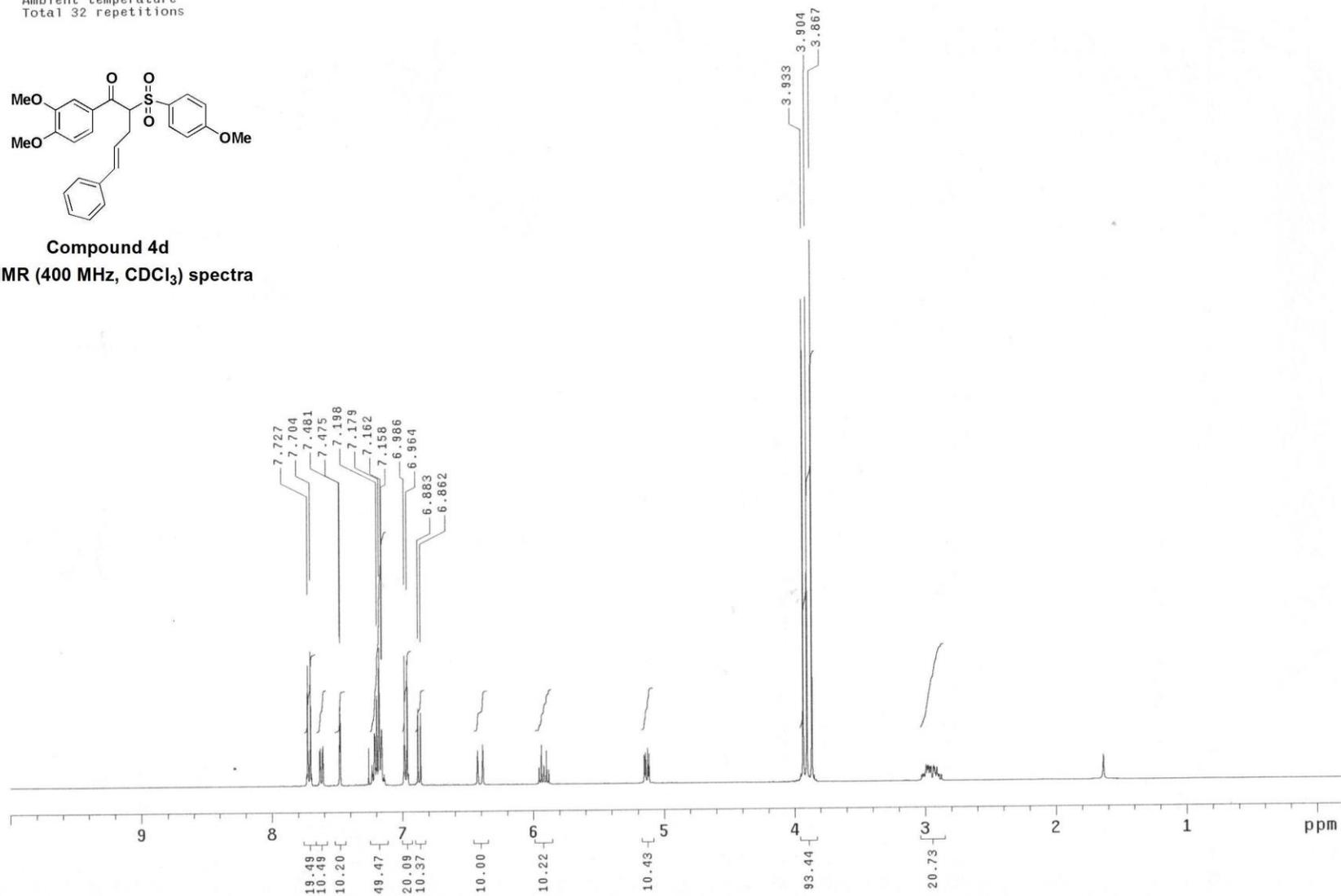
KSOMeC

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Nov 29 2018
Solvent: CDCl₃
Ambient temperature
Total 32 repetitions

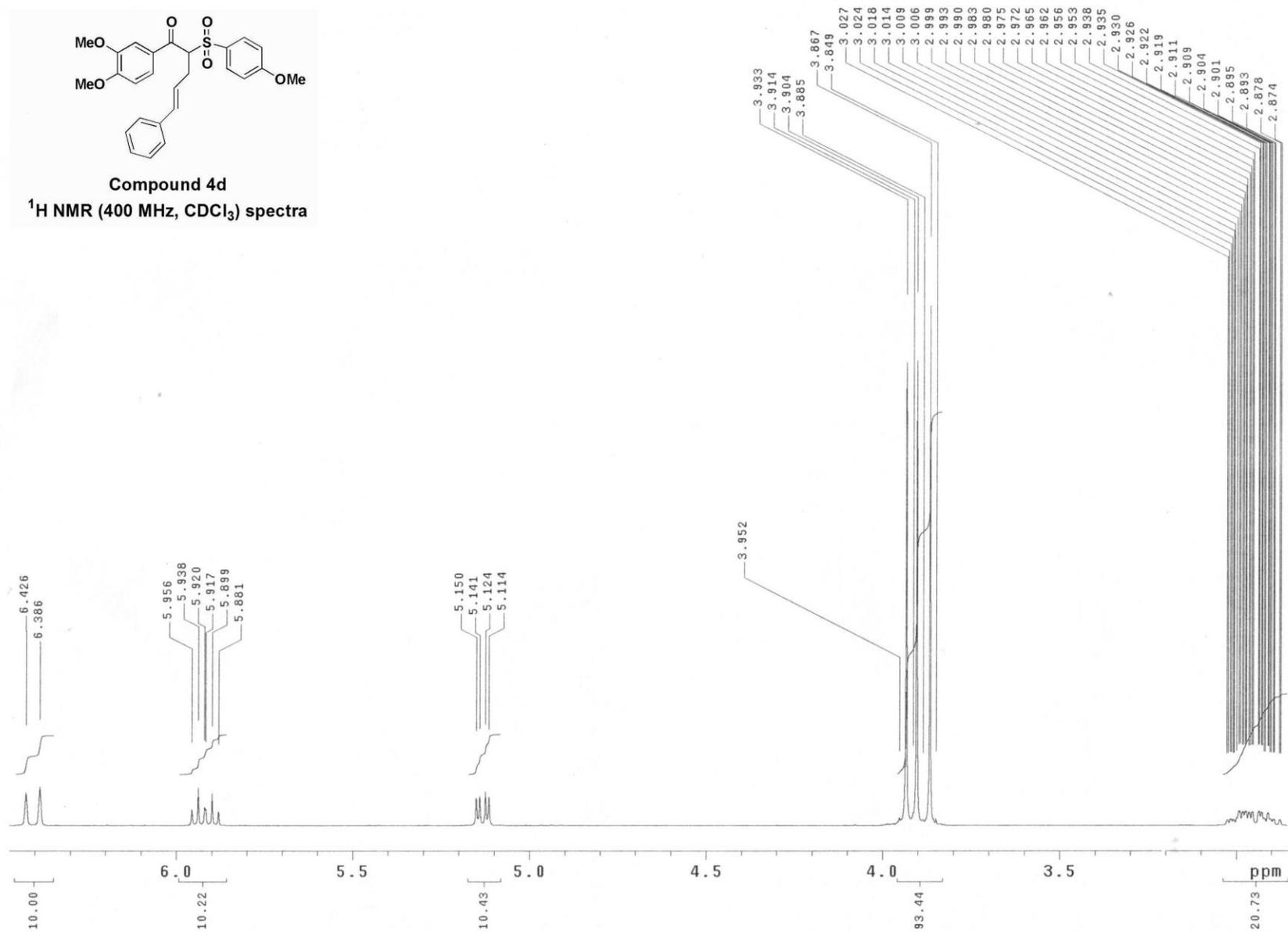
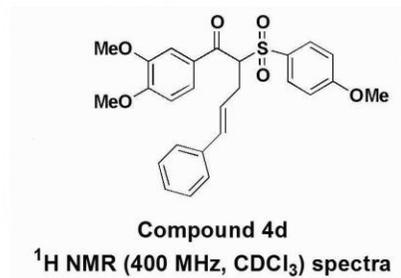


Compound 4d

¹H NMR (400 MHz, CDCl₃) spectra



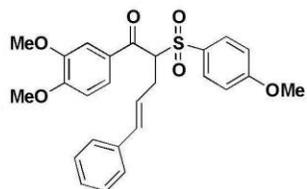
Compound 4d (¹H-NMR spectral data-2)



Compound 4d (¹³C-NMR spectral data)

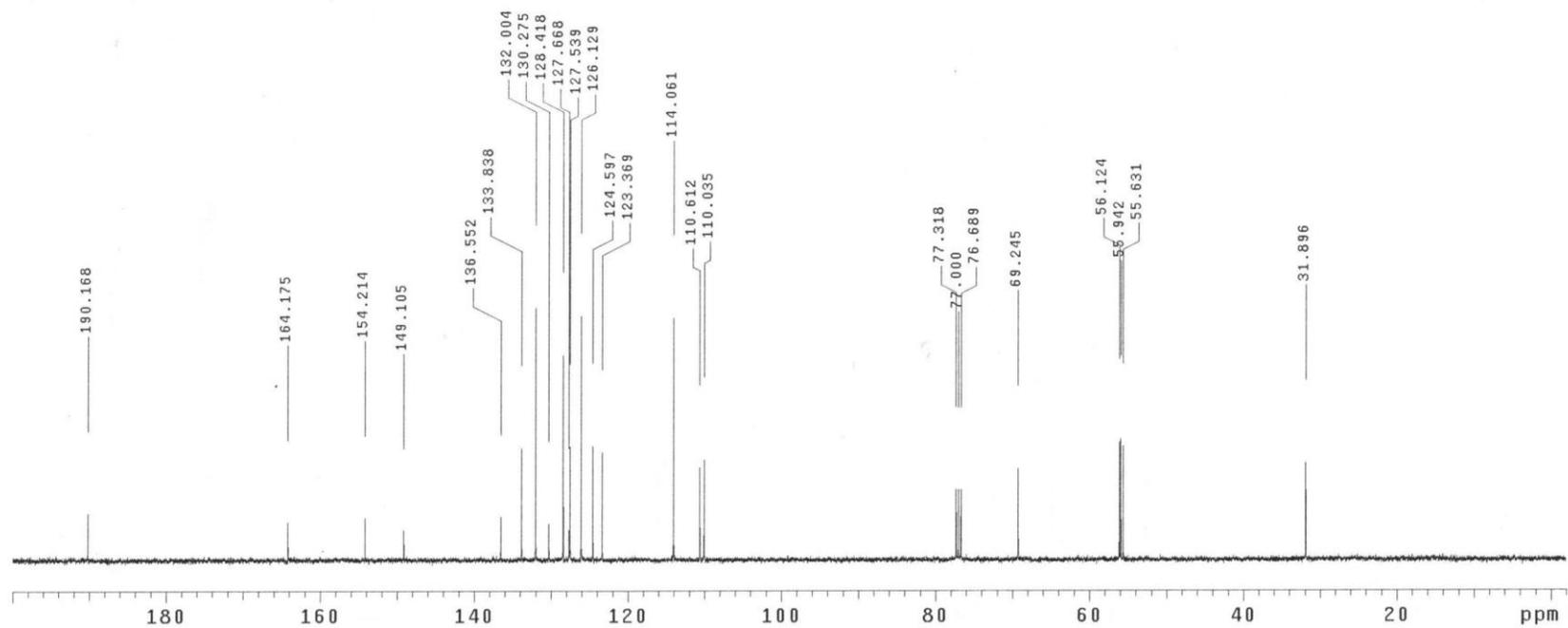
KSOMeC

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Nov 29 2018
Solvent: CDC13
Ambient temperature
Total 720 repetitions



Compound 4d

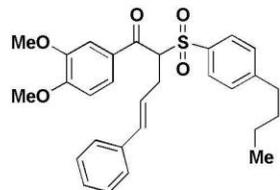
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4e (¹H-NMR spectral data-1)

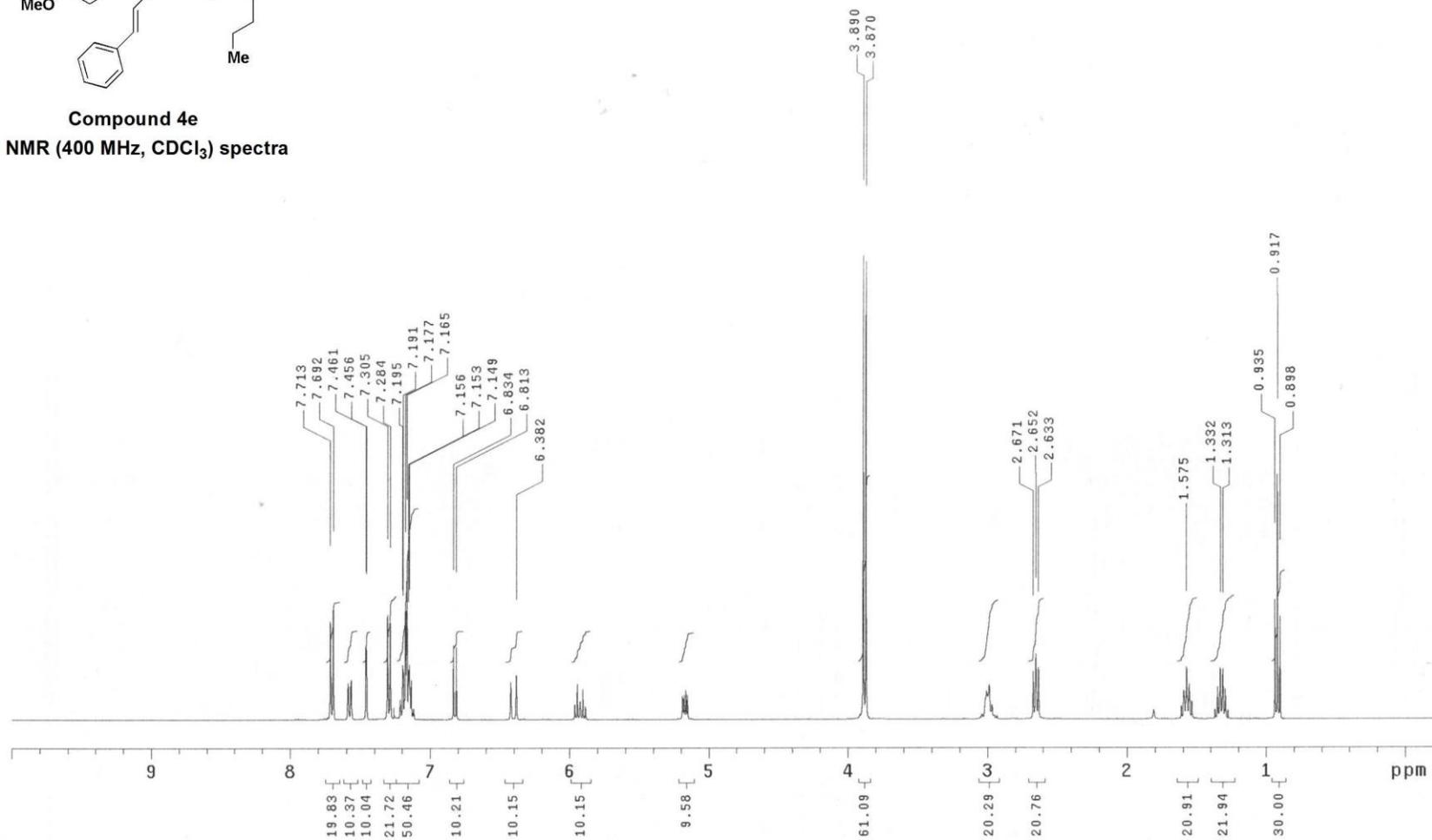
KSPhBuC

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Jan 8 2019
Solvent: CDCl₃
Ambient temperature
Total 32 repetitions

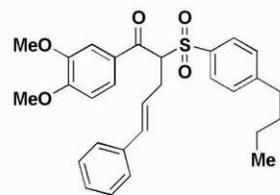


Compound 4e

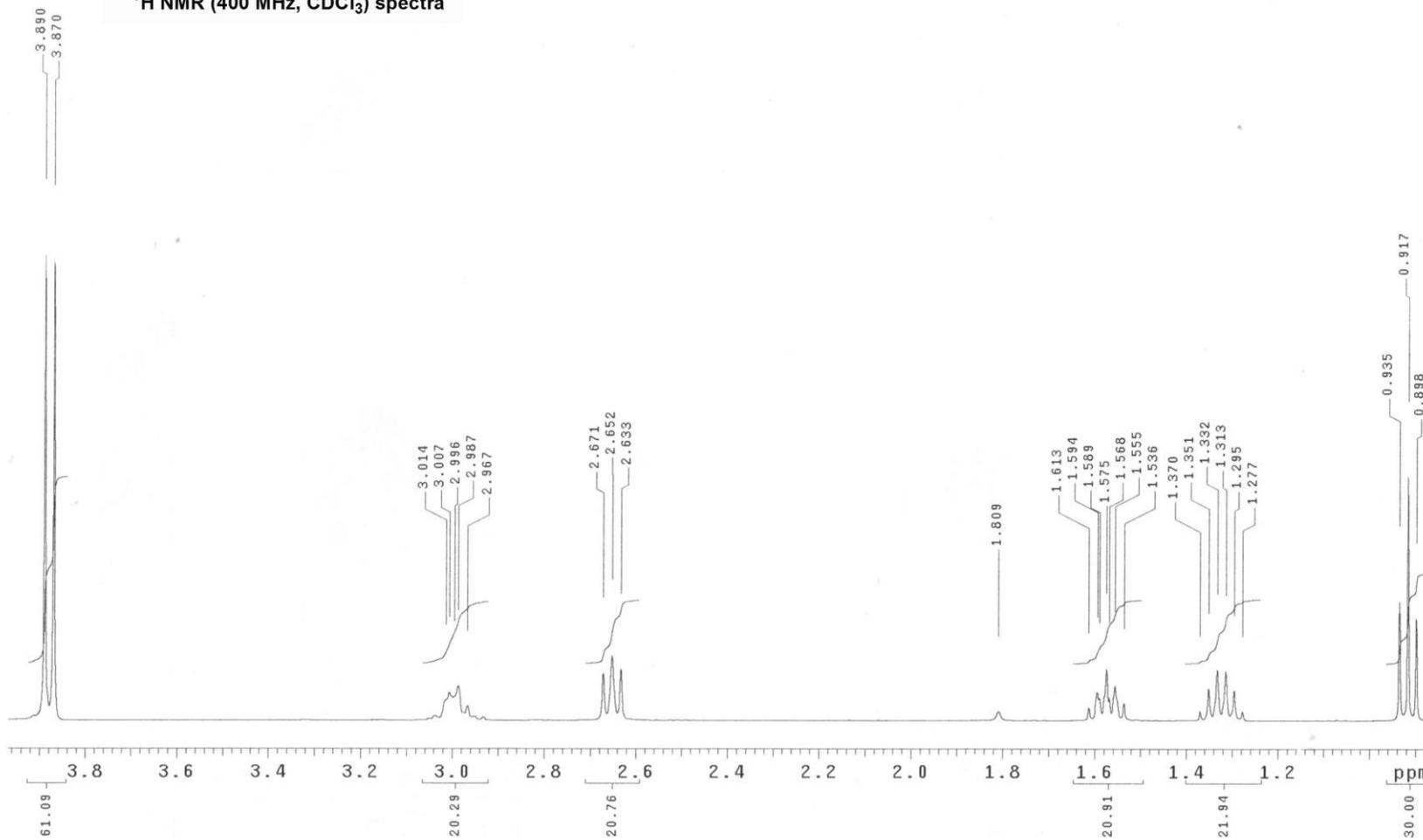
¹H NMR (400 MHz, CDCl₃) spectra



Compound 4e (¹H-NMR spectral data-2)



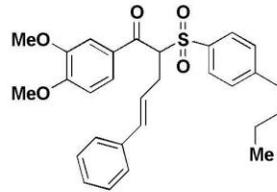
Compound 4e
¹H NMR (400 MHz, CDCl₃) spectra



Compound 4e (¹³C-NMR spectral data)

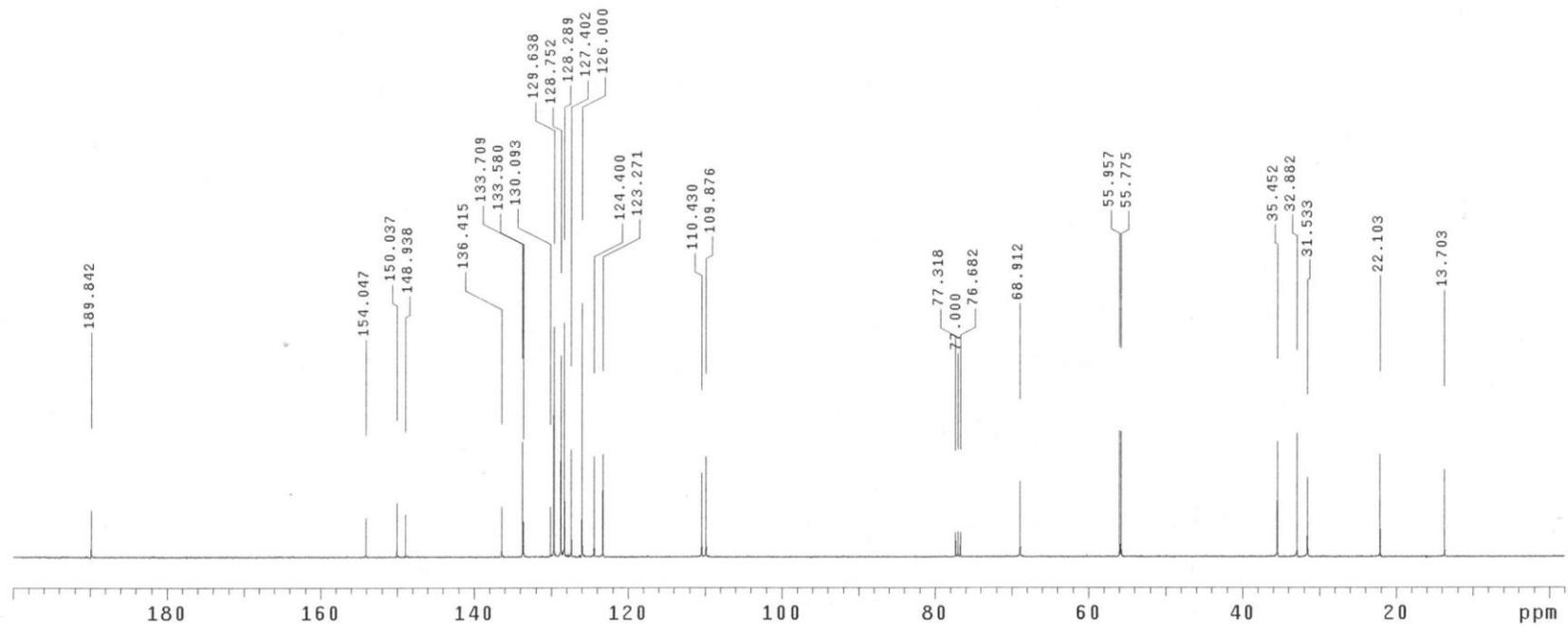
KSPHbuC

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Jan 8 2019
Solvent: CDC13
Ambient temperature
Total 1536 repetitions



Compound 4e

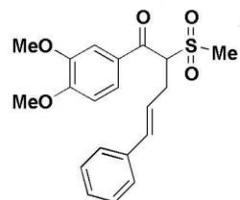
¹³C NMR (100 MHz, CDC1₃) spectra



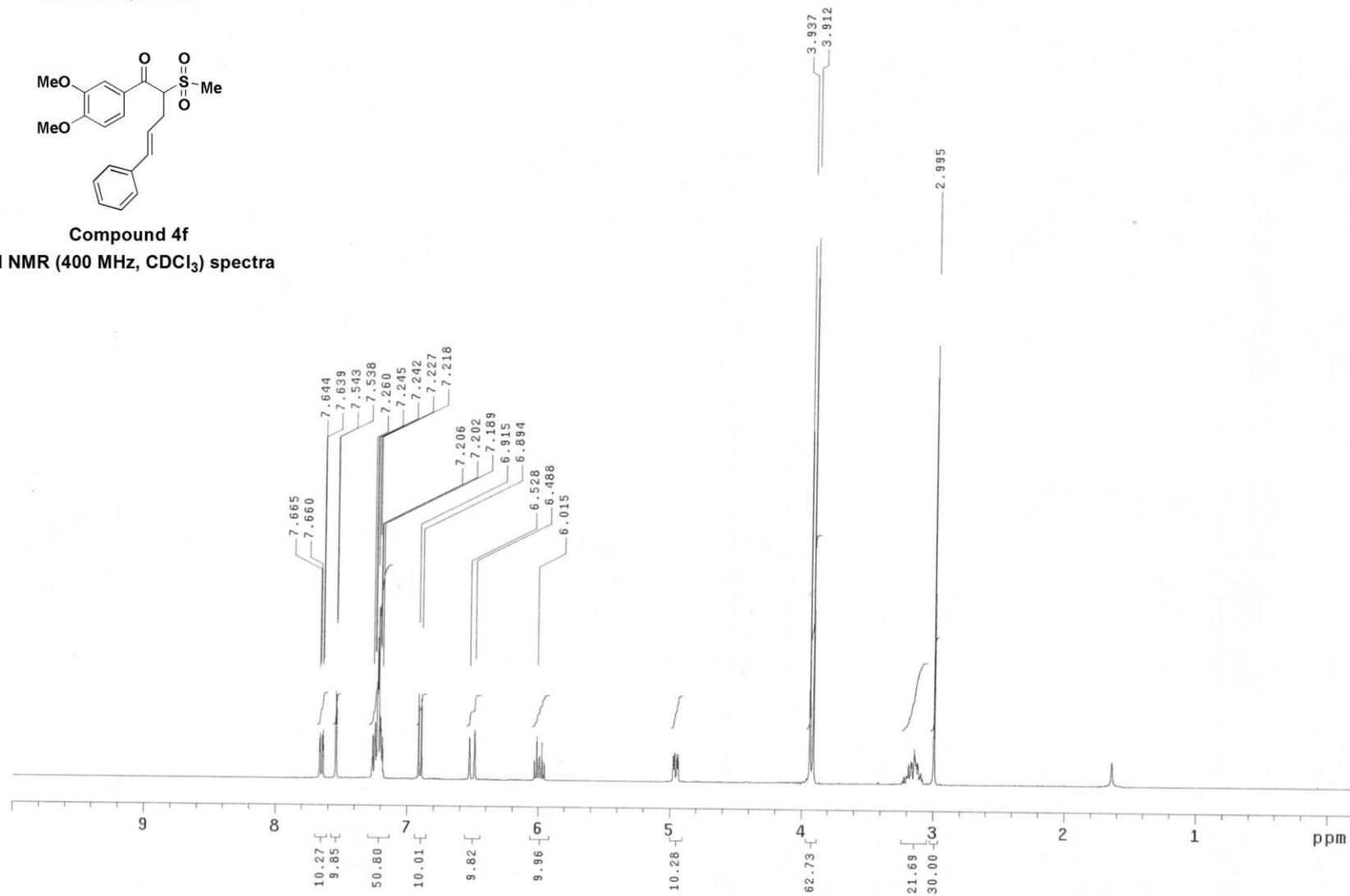
Compound 4f (¹H-NMR spectral data-1)

KSMsC

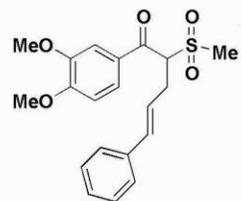
Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Dec 4 2018
Solvent: CDCl₃
Ambient temperature
Total 32 repetitions



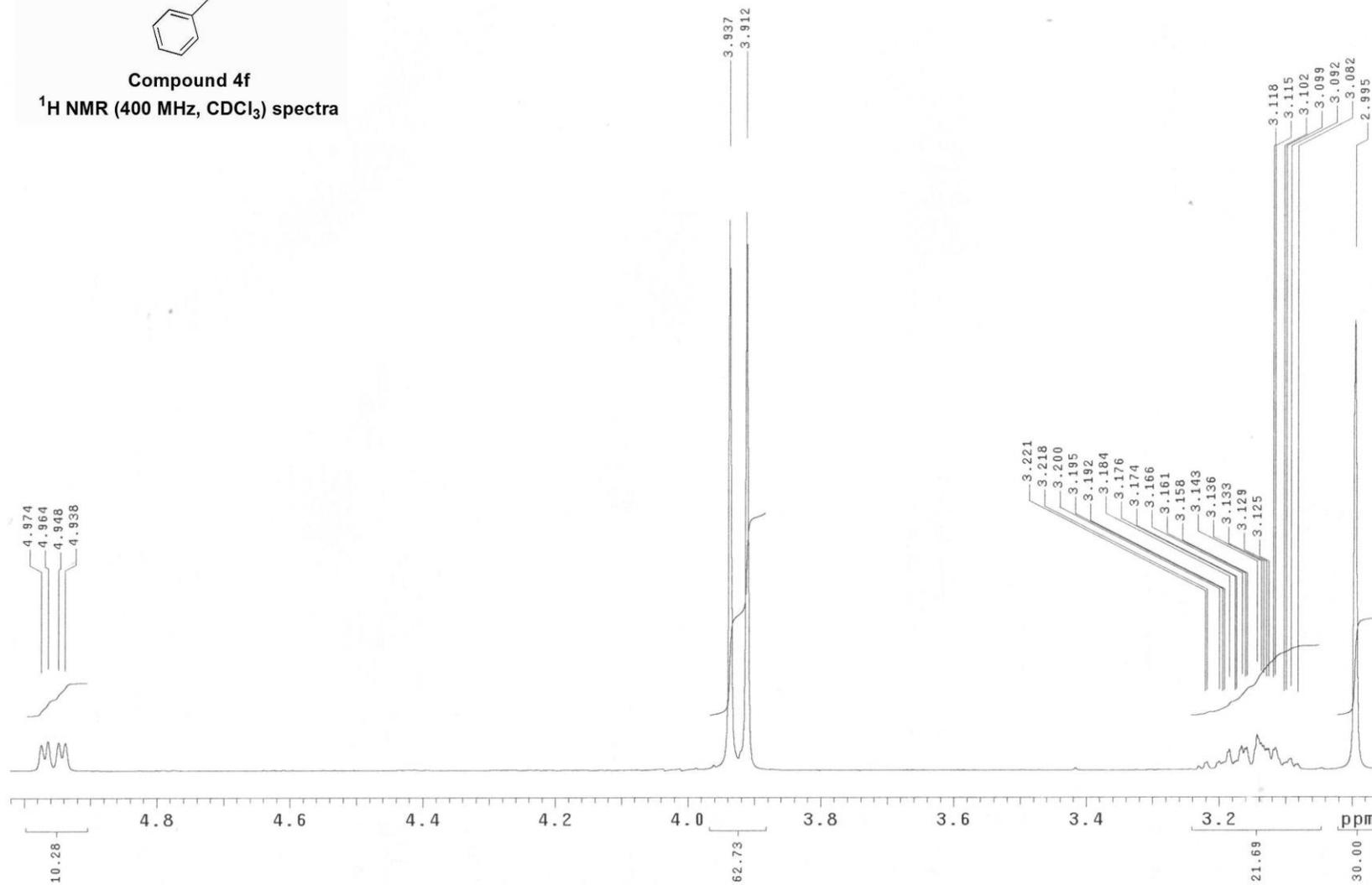
Compound 4f
¹H NMR (400 MHz, CDCl₃) spectra



Compound 4f (¹H-NMR spectral data-2)



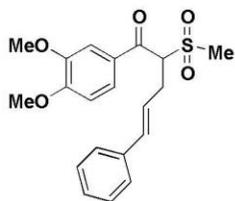
Compound 4f
¹H NMR (400 MHz, CDCl₃) spectra



Compound 4f (¹³C-NMR spectral data)

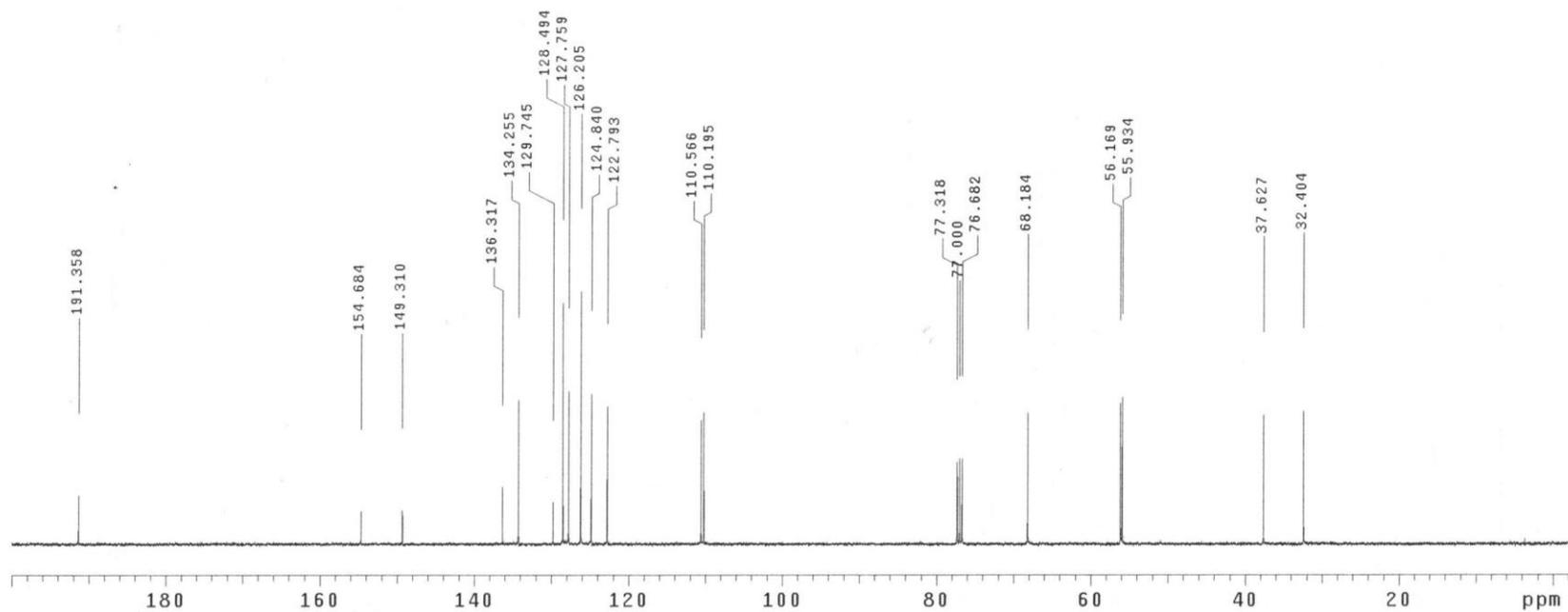
KSMsC

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Dec 4 2018
Solvent: CDCl₃
Ambient temperature
Total 2592 repetitions



Compound 4f

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4g (¹H-NMR spectral data-1)

KSBuC

Pulse Sequence: s2pu1

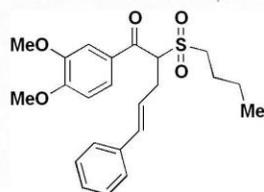
UNITYplus-400 "unity400"

Date: Nov 30 2018

Solvent: CDC13

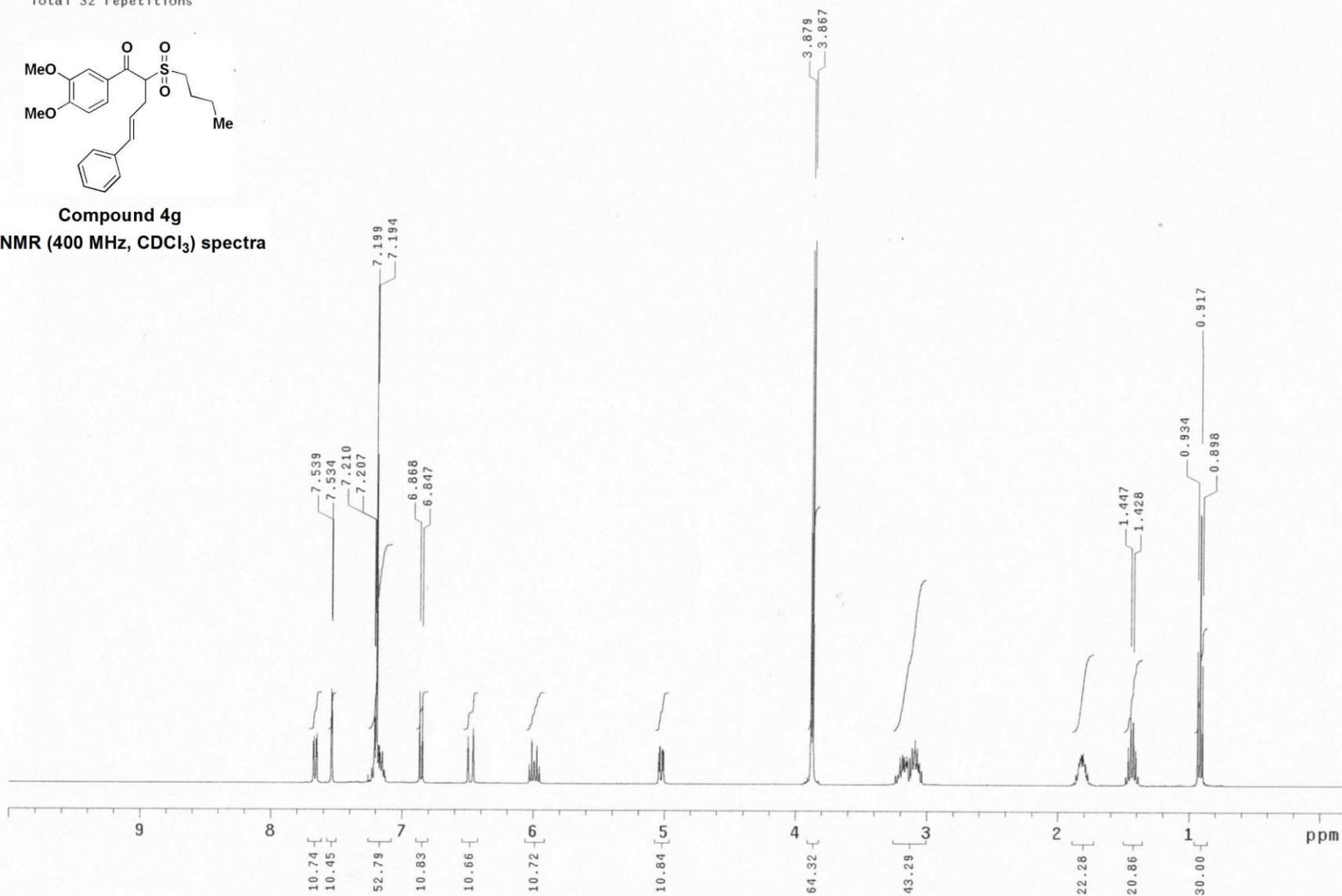
Ambient temperature

Total 32 repetitions

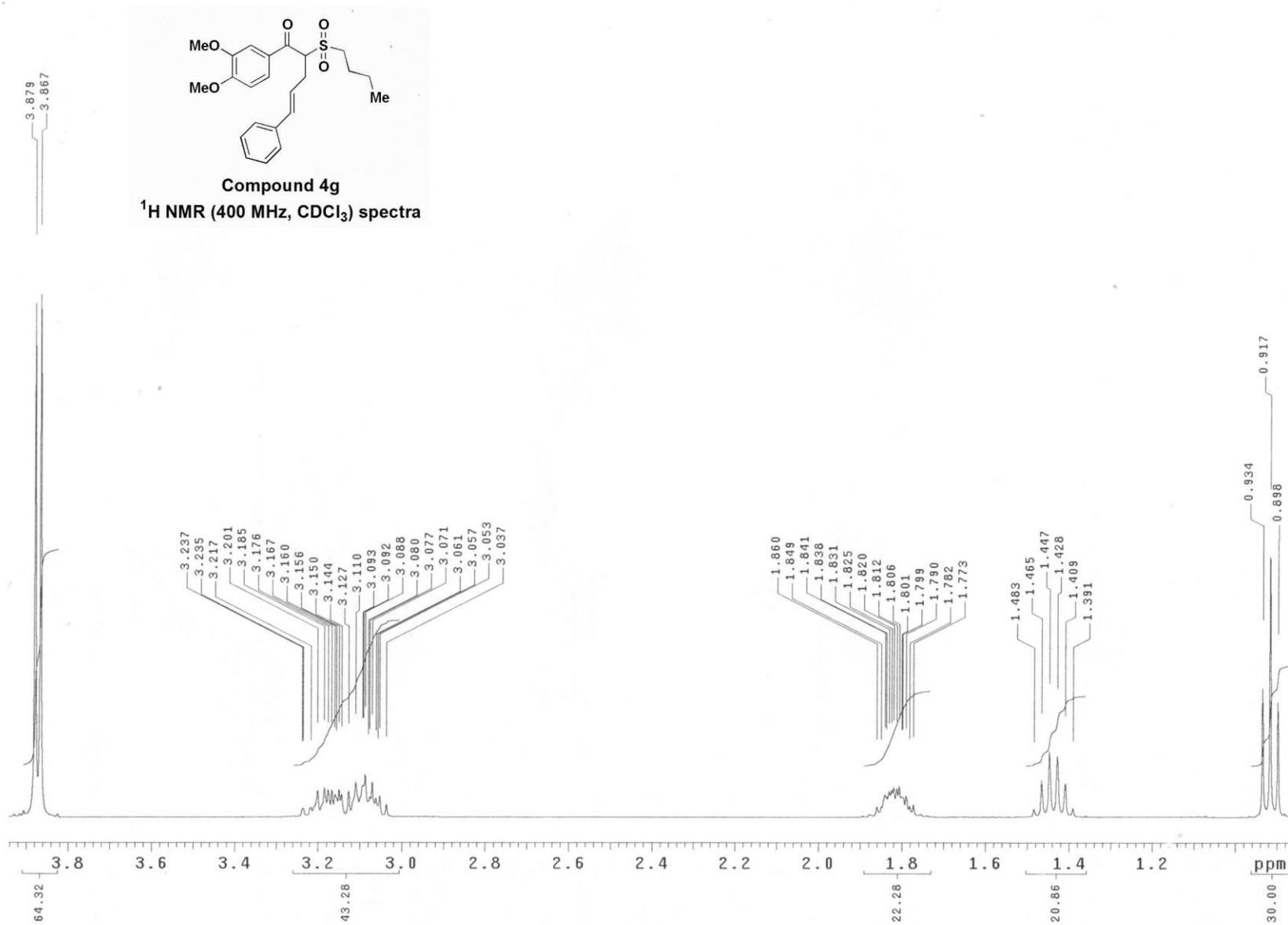


Compound 4g

¹H NMR (400 MHz, CDCl₃) spectra



Compound 4g (¹H-NMR spectral data-2)



Compound 4g (¹³C-NMR spectral data)

KSBUc

Pulse Sequence: s2pu1

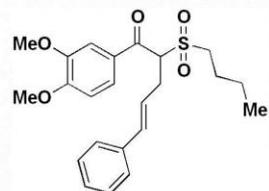
UNITYplus-400 "unity400"

Date: Nov 30 2018

Solvent: CDCl₃

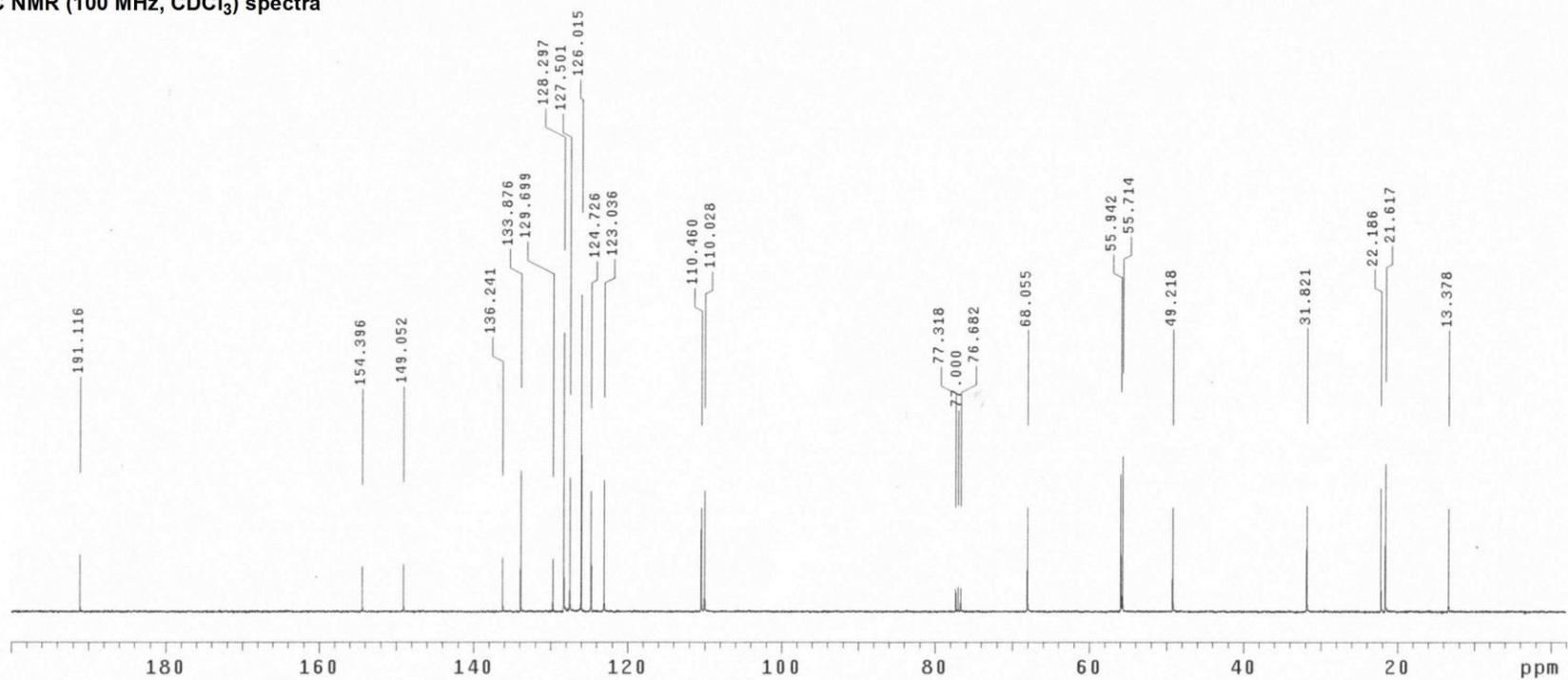
Ambient temperature

Total 320 repetitions



Compound 4g

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4h (¹H-NMR spectral data-1)

KSE1C

Pulse Sequence: s2pu1

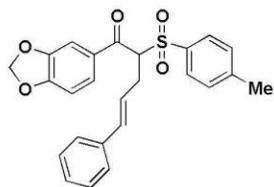
UNITYplus-400 "unity400"

Date: Aug 29 2018

Solvent: CDCl₃

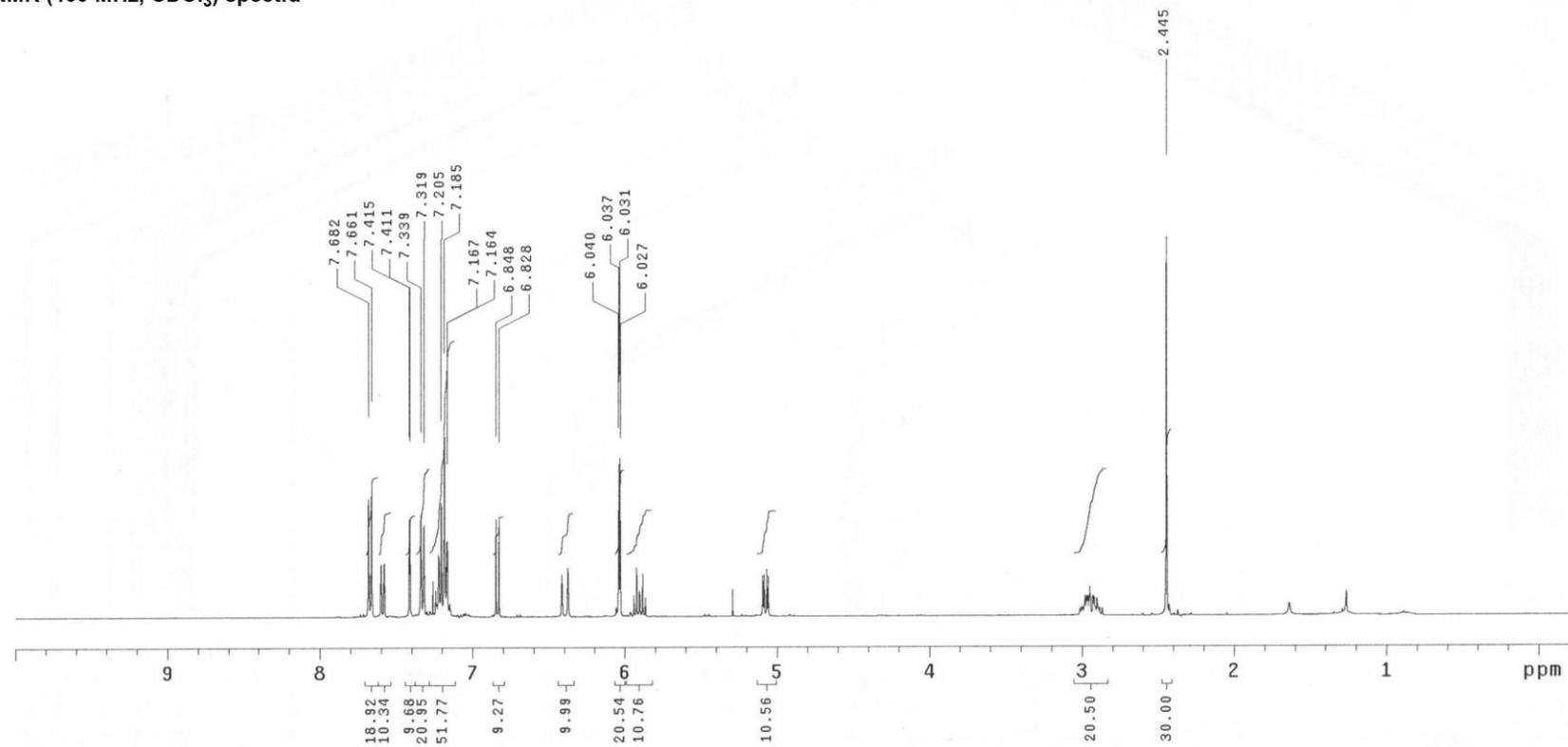
Ambient temperature

Total 32 repetitions

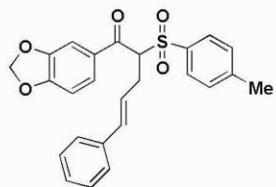


Compound 4h

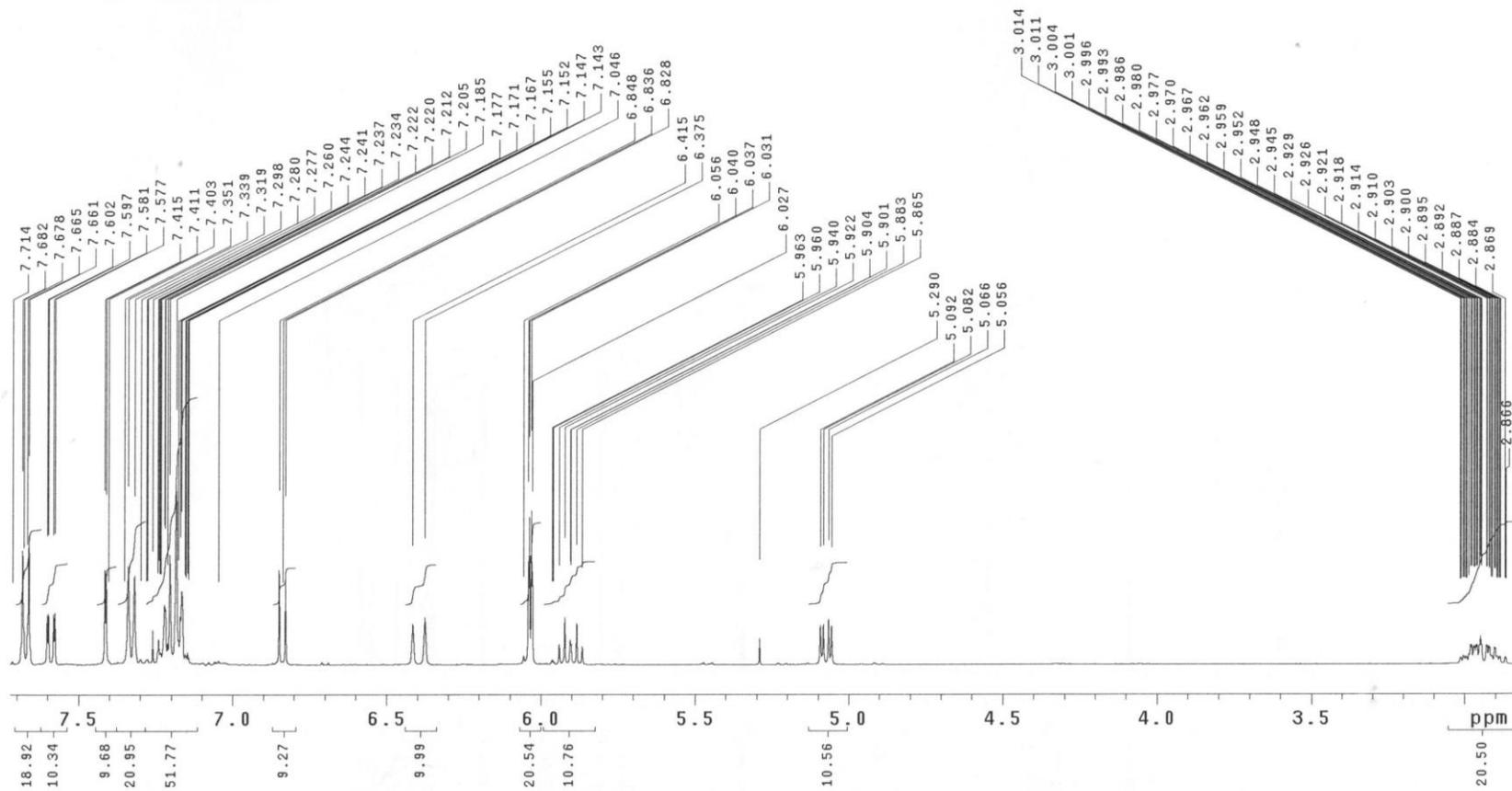
¹H NMR (400 MHz, CDCl₃) spectra



Compound 4h (¹H-NMR spectral data-2)



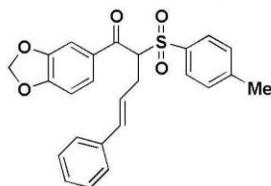
Compound 4h
¹H NMR (400 MHz, CDCl₃) spectra



Compound 4h (¹³C-NMR spectral data)

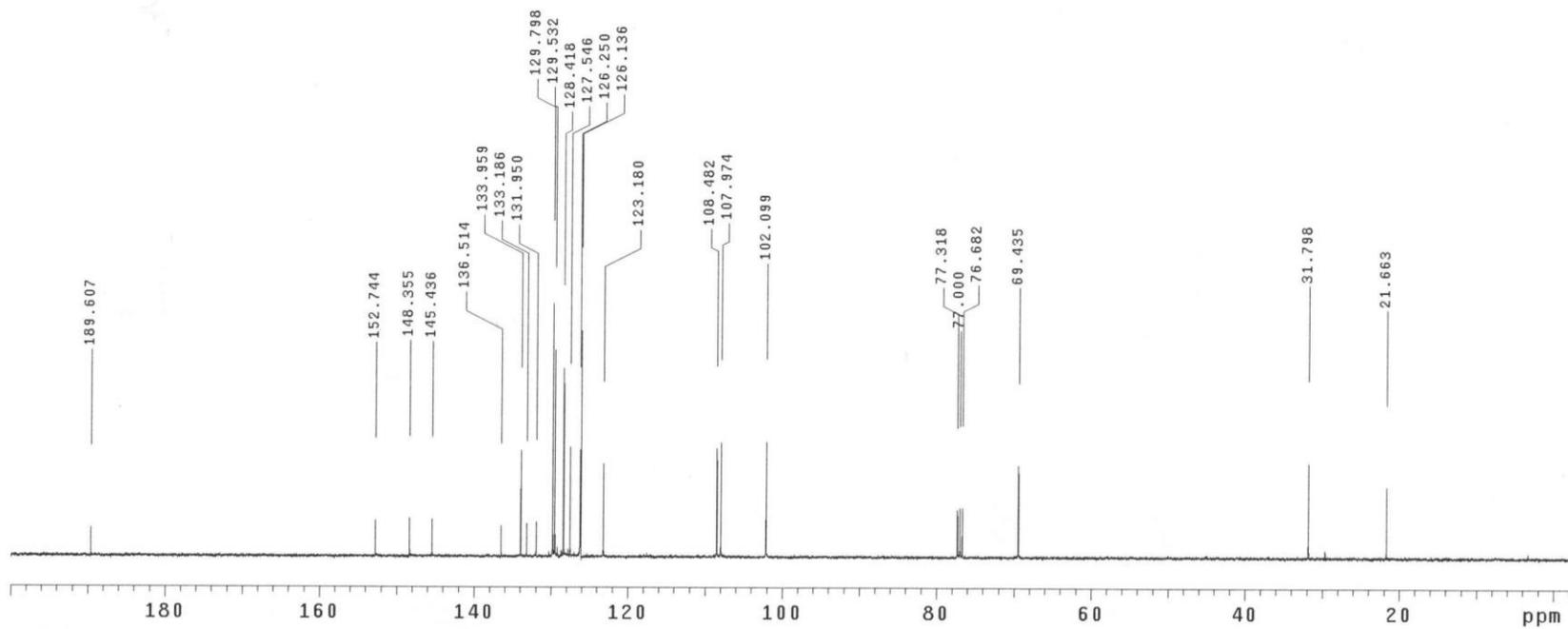
KSE1C

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Aug 29 2018
Solvent: CDCl₃
Ambient temperature
Total 1024 repetitions



Compound 4h

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4i (¹H-NMR spectral data-1)

KSE5C

Pulse Sequence: s2pu1

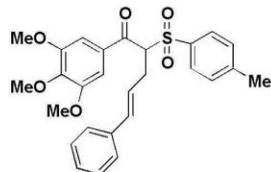
UNITYplus-400 "unity400"

Date: Sep 11 2018

Solvent: CDCl₃

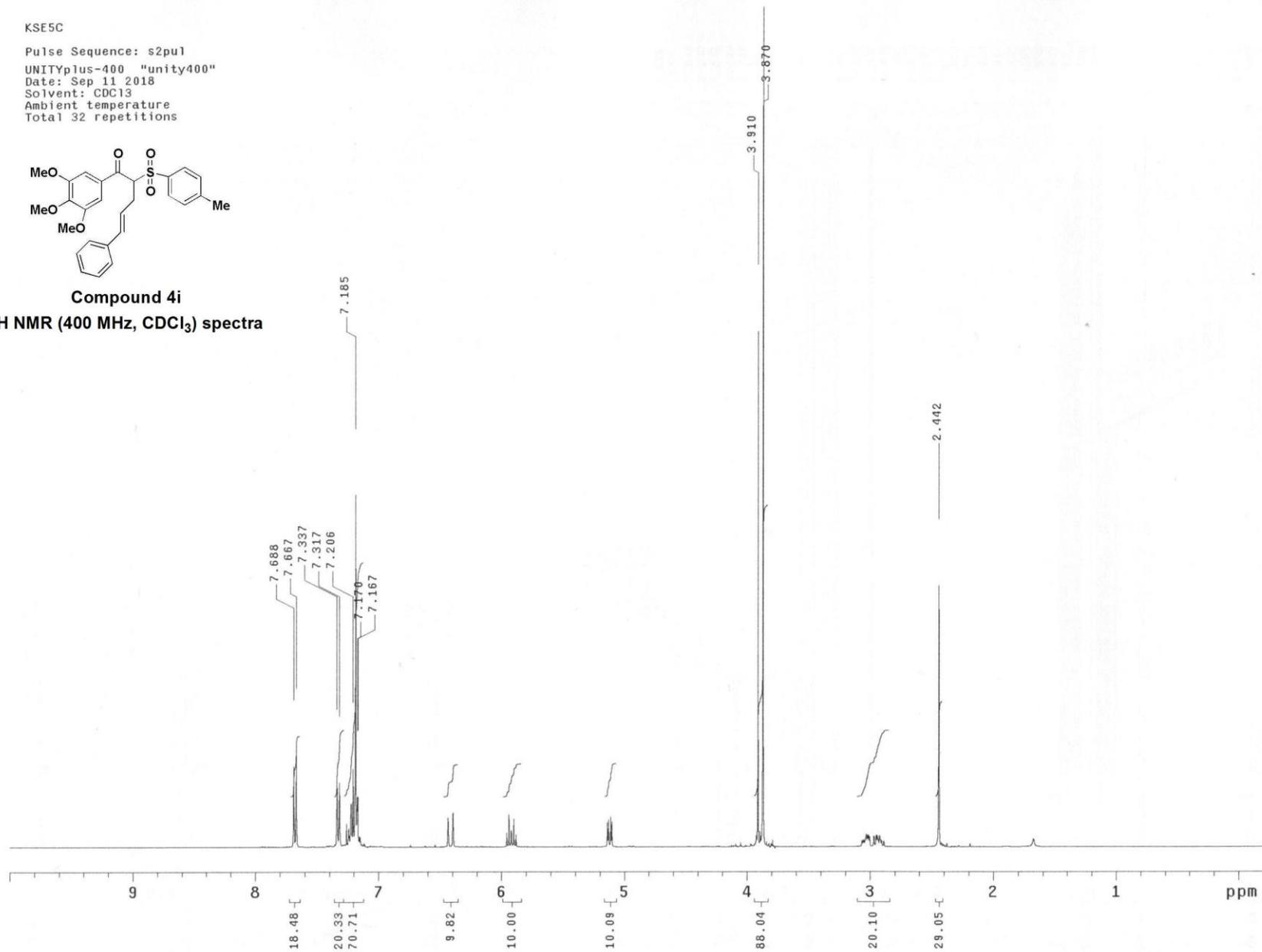
Ambient temperature

Total 32 repetitions

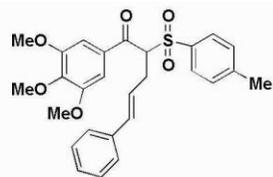


Compound 4i

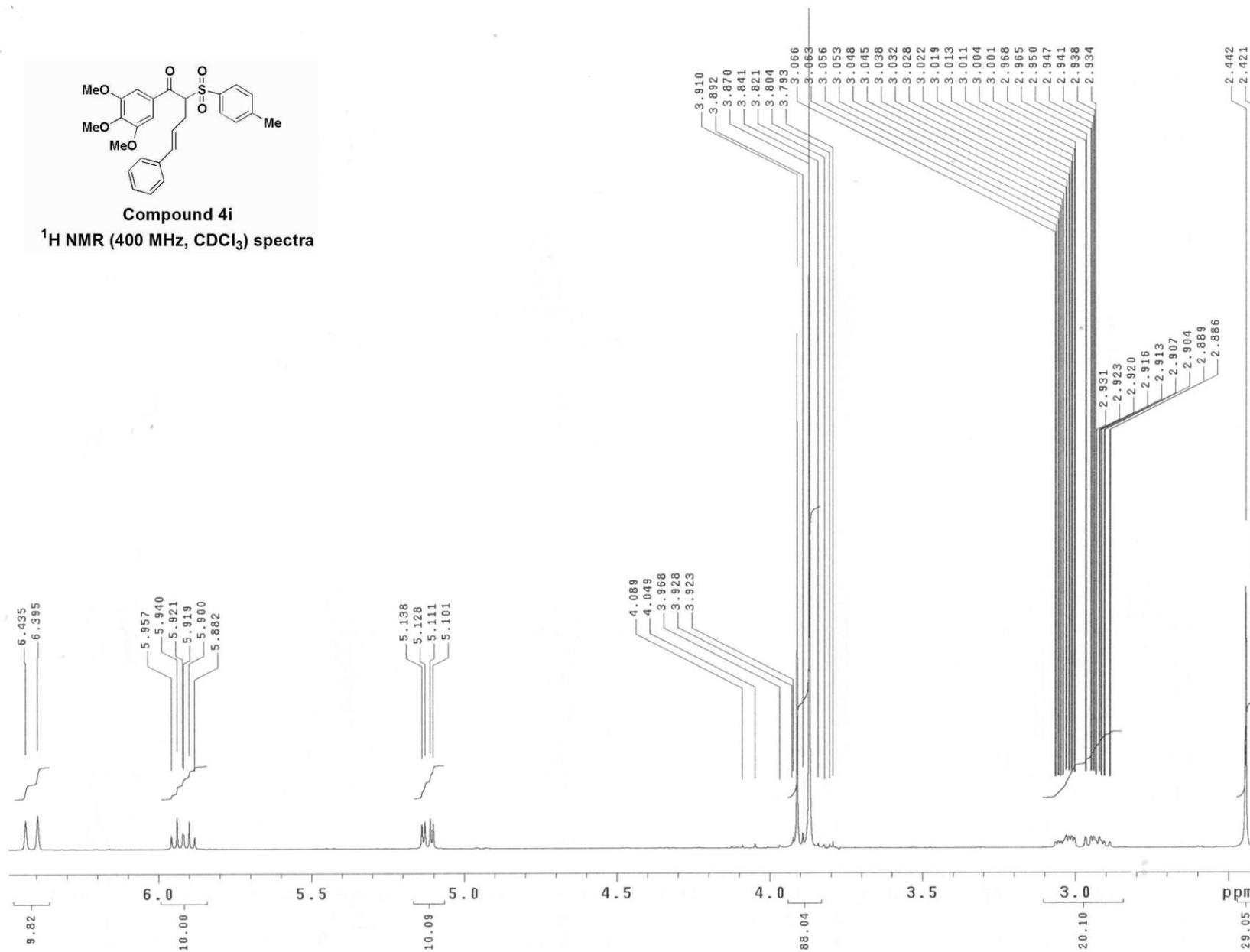
¹H NMR (400 MHz, CDCl₃) spectra



Compound 4i (¹H-NMR spectral data-2)



Compound 4i
¹H NMR (400 MHz, CDCl₃) spectra



Compound 4i (¹³C-NMR spectral data)

KSE5C

Pulse Sequence: s2pu1

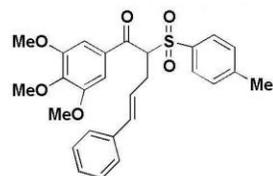
UNITYplus-400 "unity400"

Date: Sep 11 2018

Solvent: CDCl₃

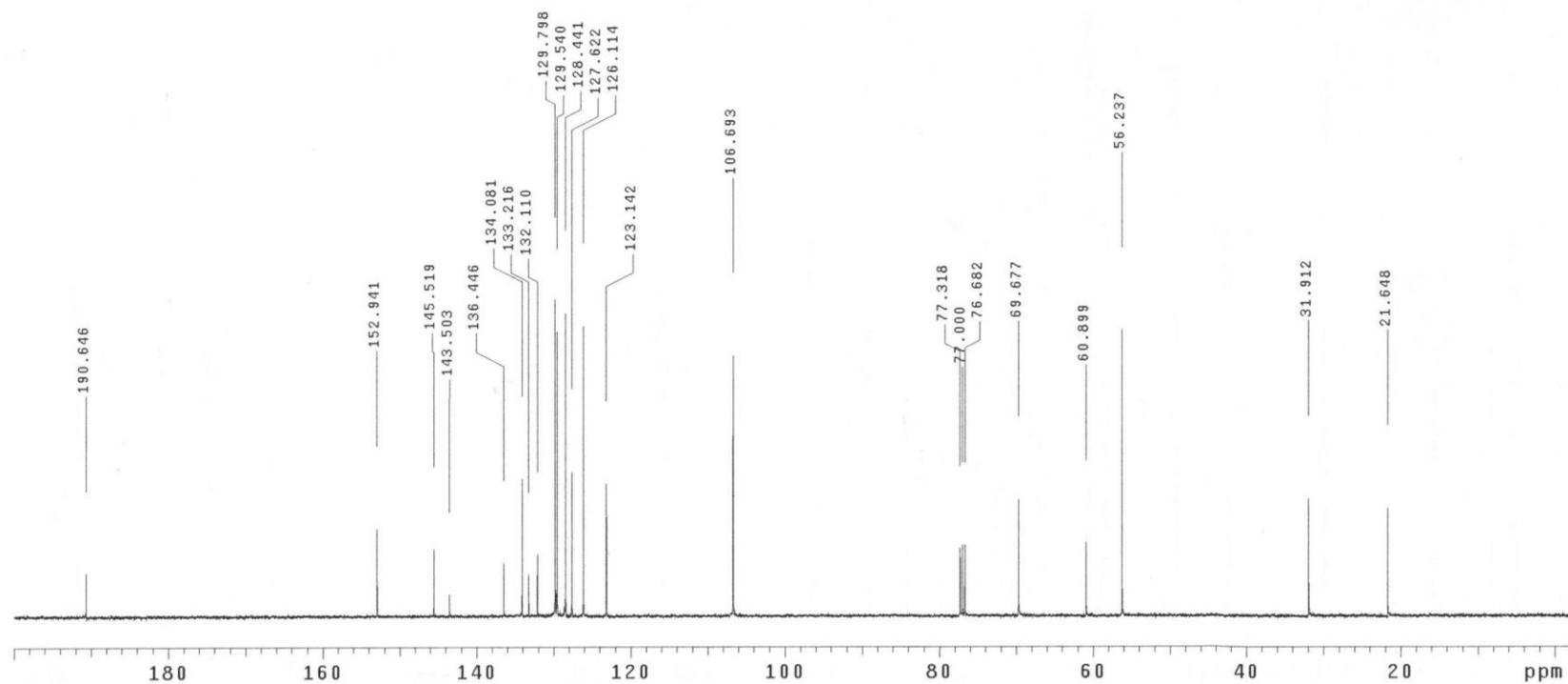
Ambient temperature

Total 1360 repetitions

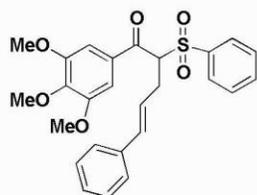


Compound 4i

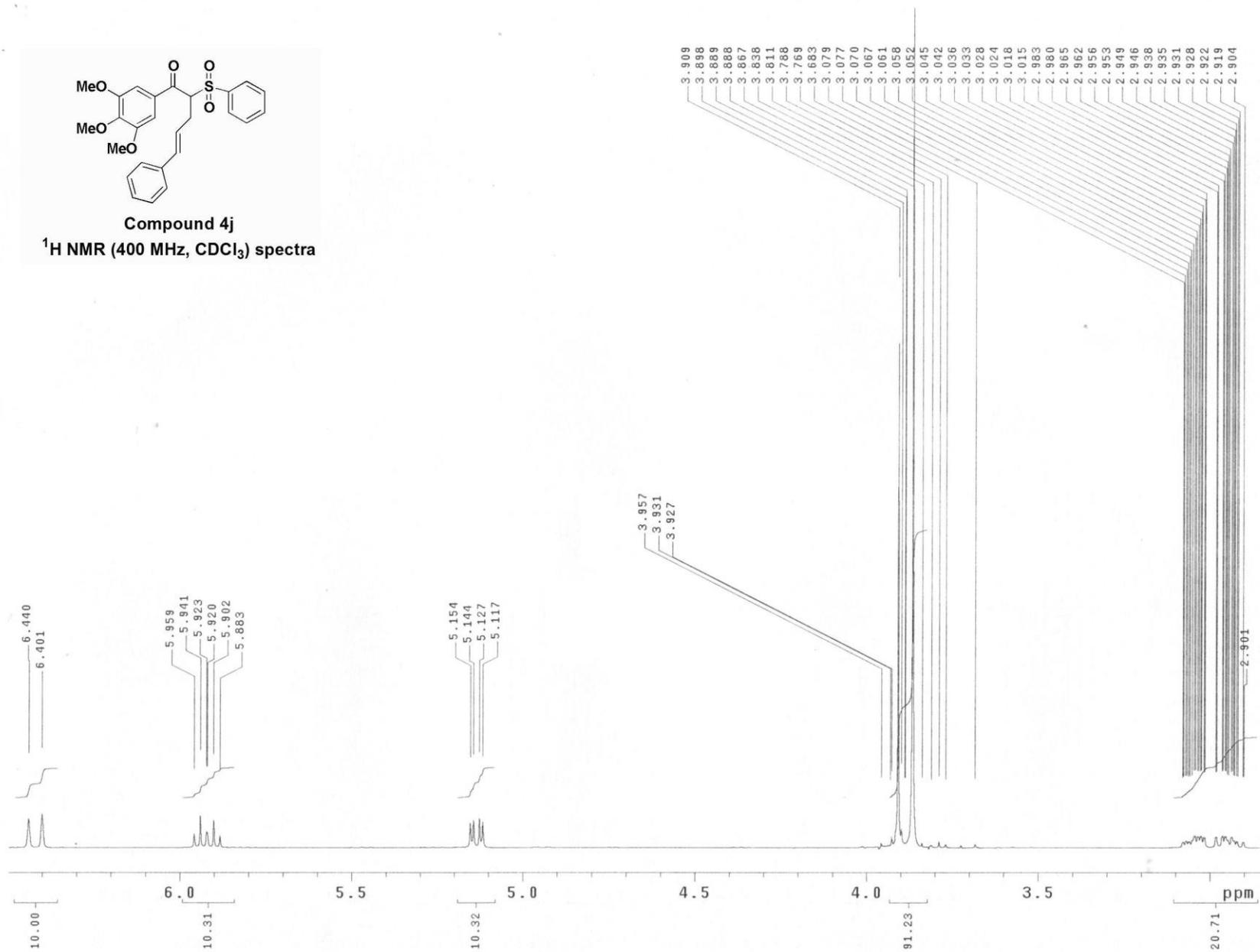
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4j (¹H-NMR spectral data-2)

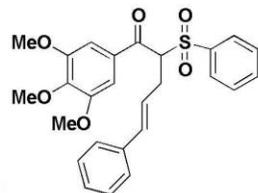


Compound 4j
¹H NMR (400 MHz, CDCl₃) spectra



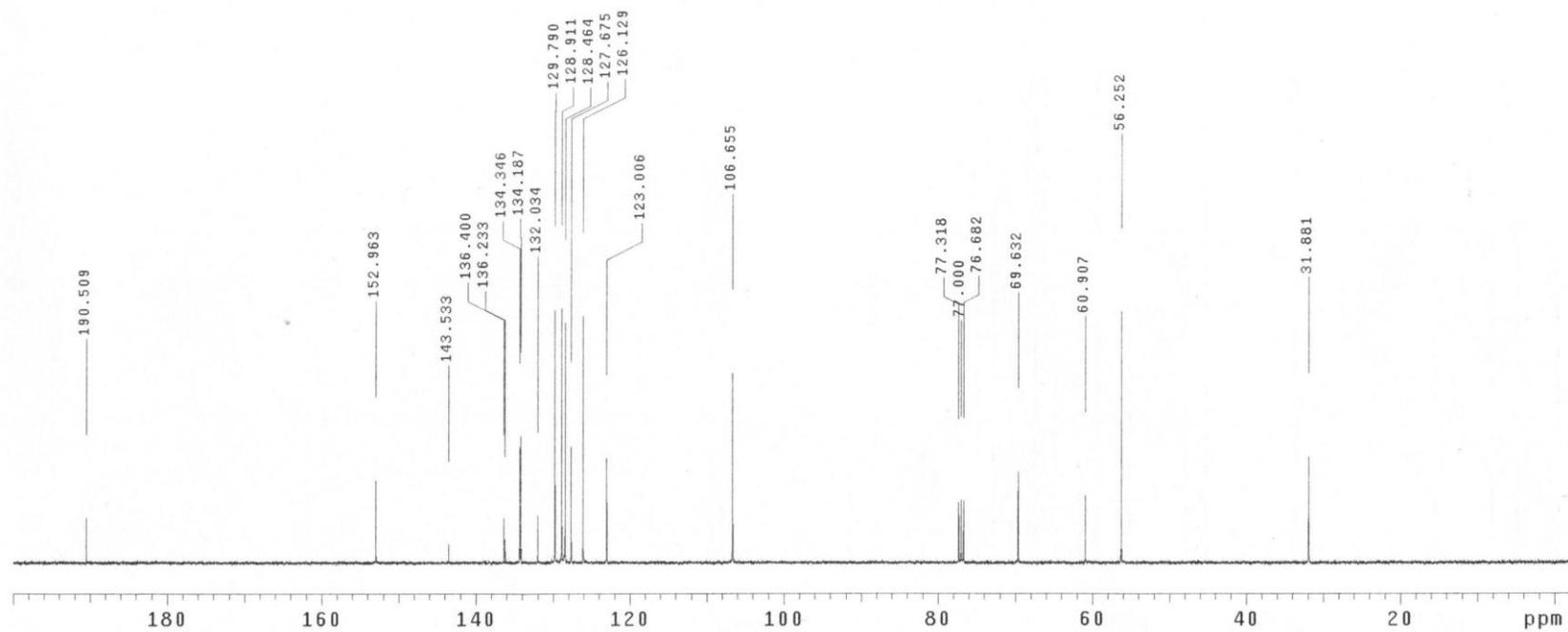
Compound 4j (¹³C-NMR spectral data)

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Feb 11 2019
Solvent: CDCl₃
Ambient temperature
Total 1424 repetitions



Compound 4j

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4k (¹H-NMR spectral data-1)

KS30MsC

Pulse Sequence: s2pu1

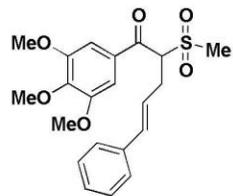
UNITYplus-400 "unity400"

Date: Jan 30 2019

Solvent: CDCl₃

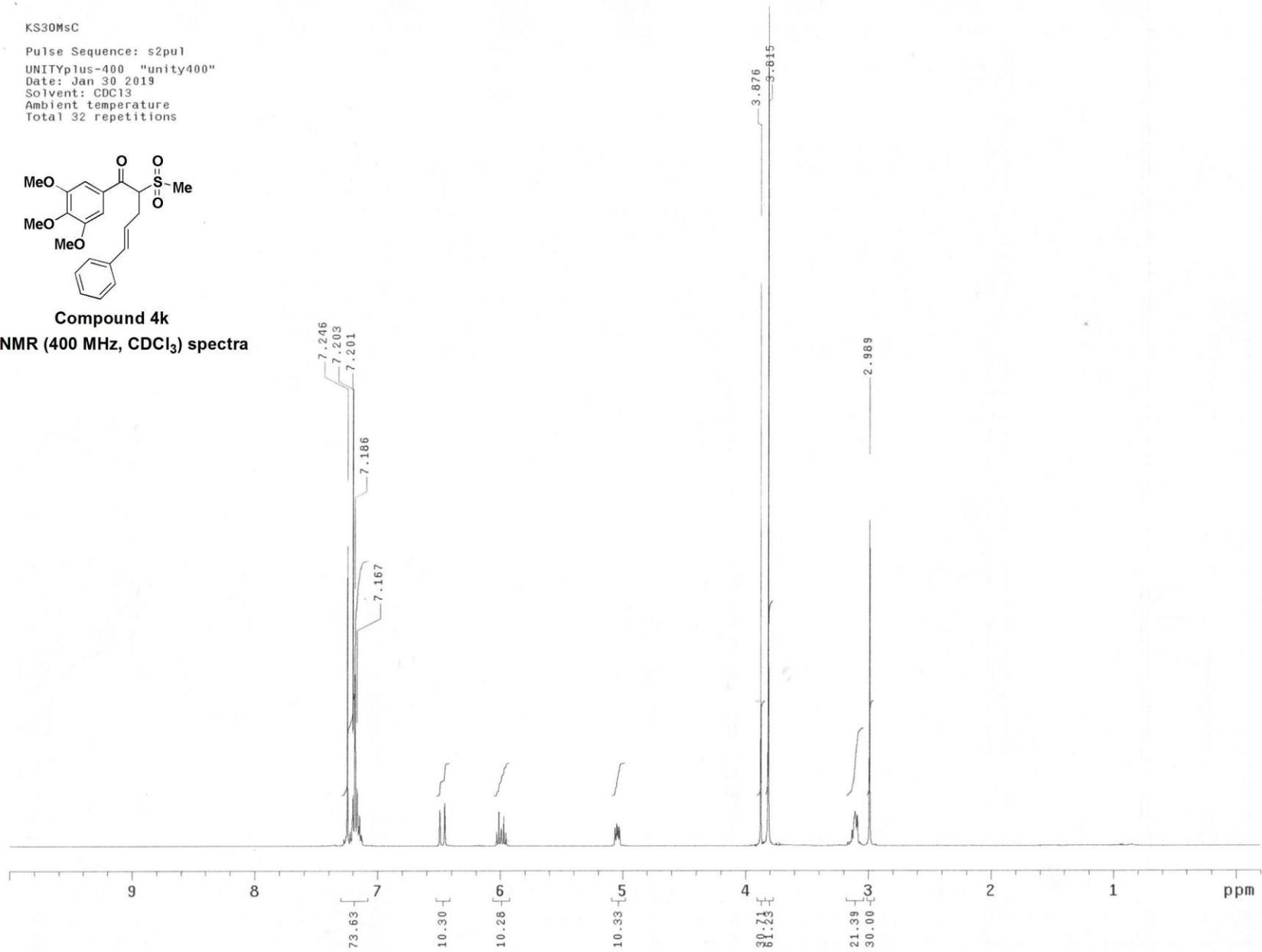
Ambient temperature

Total 32 repetitions

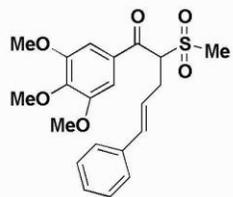


Compound 4k

¹H NMR (400 MHz, CDCl₃) spectra

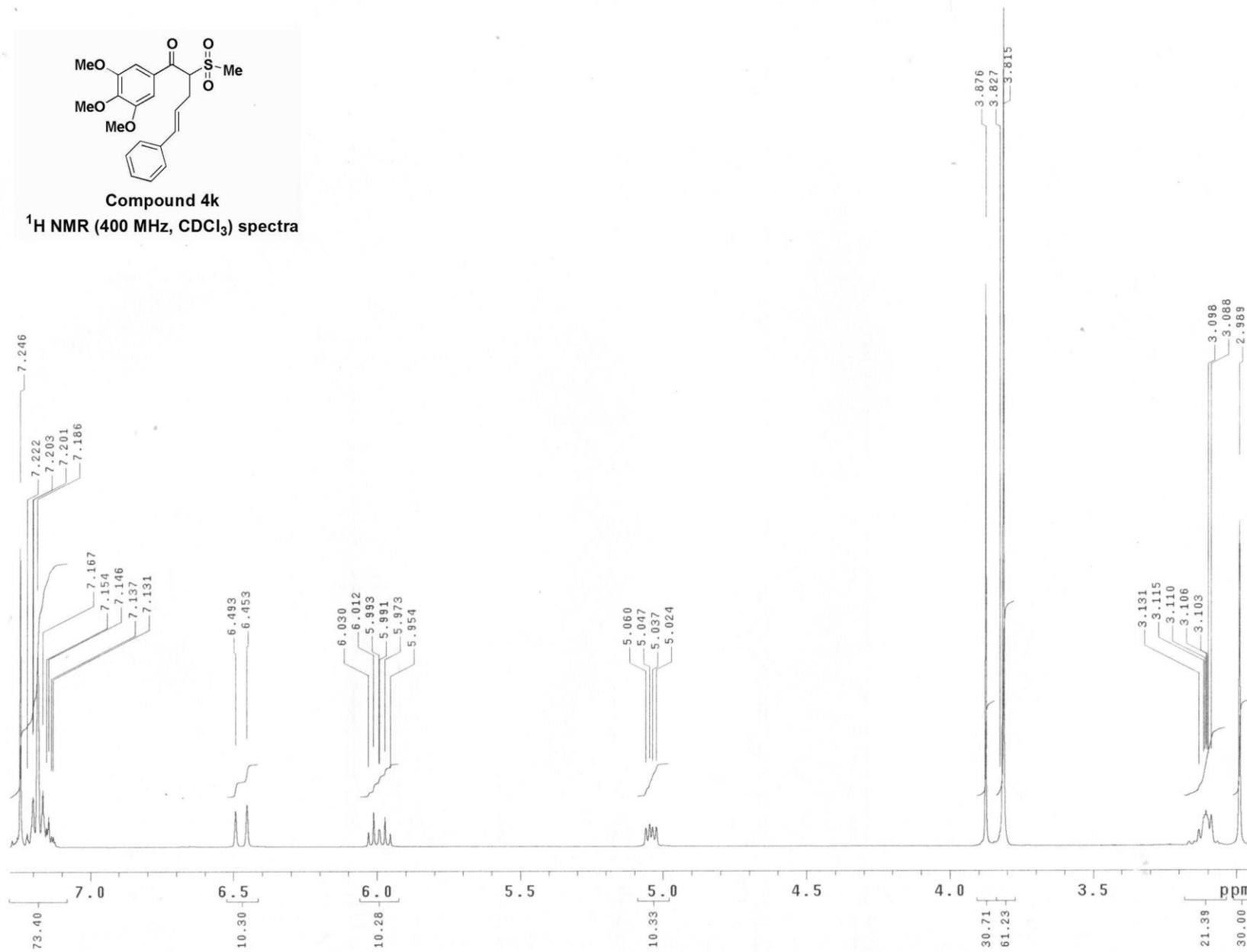


Compound 4k (¹H-NMR spectral data-2)



Compound 4k

¹H NMR (400 MHz, CDCl₃) spectra



Compound 4k (¹³C-NMR spectral data)

KS30MsC

Pulse Sequence: s2pu1

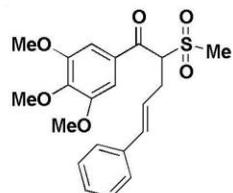
UNITYplus-400 "unity400"

Date: Jan 30 2019

Solvent: CDCl₃

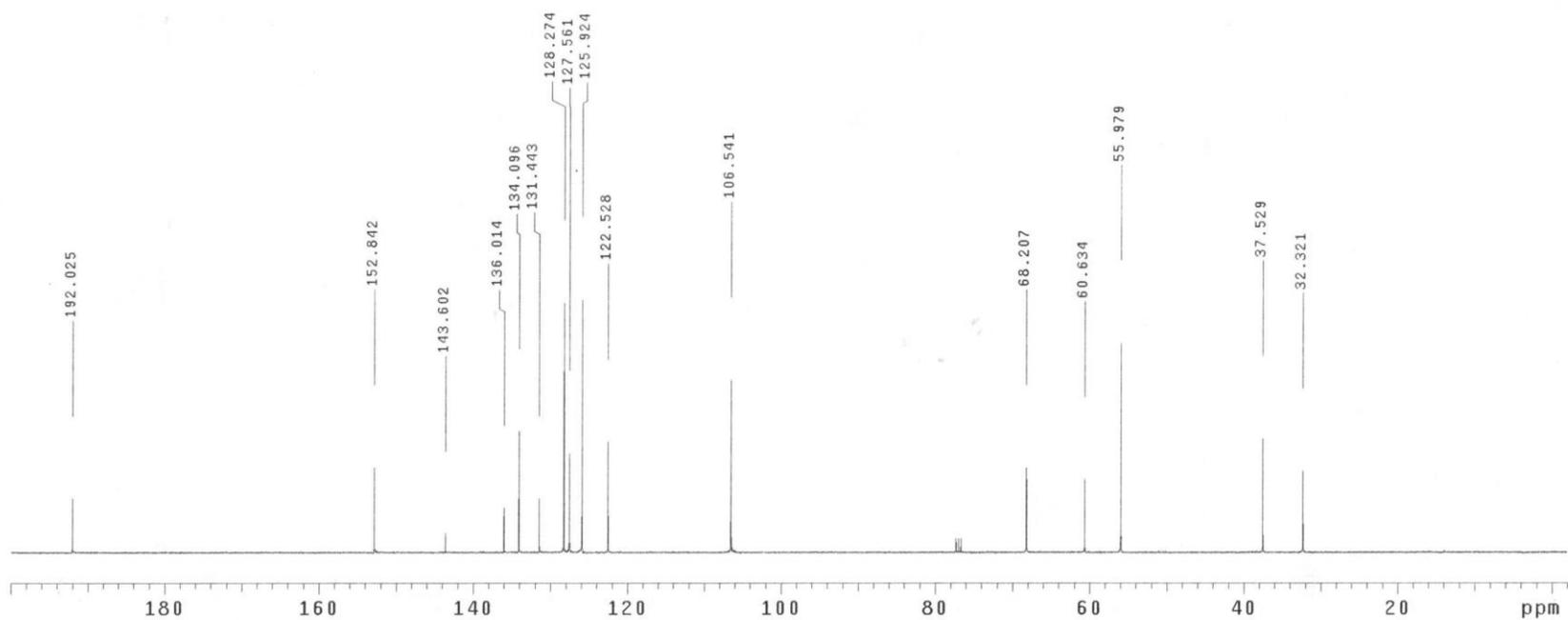
Ambient temperature

Total 368 repetitions



Compound 4k

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4l (¹H-NMR spectral data-1)

KSE2C

Pulse Sequence: s2pu1

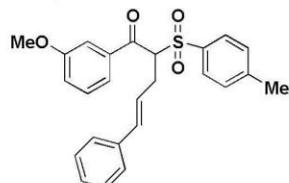
UNITYplus-400 "unity400"

Date: Aug 29 2018

Solvent: CDCl₃

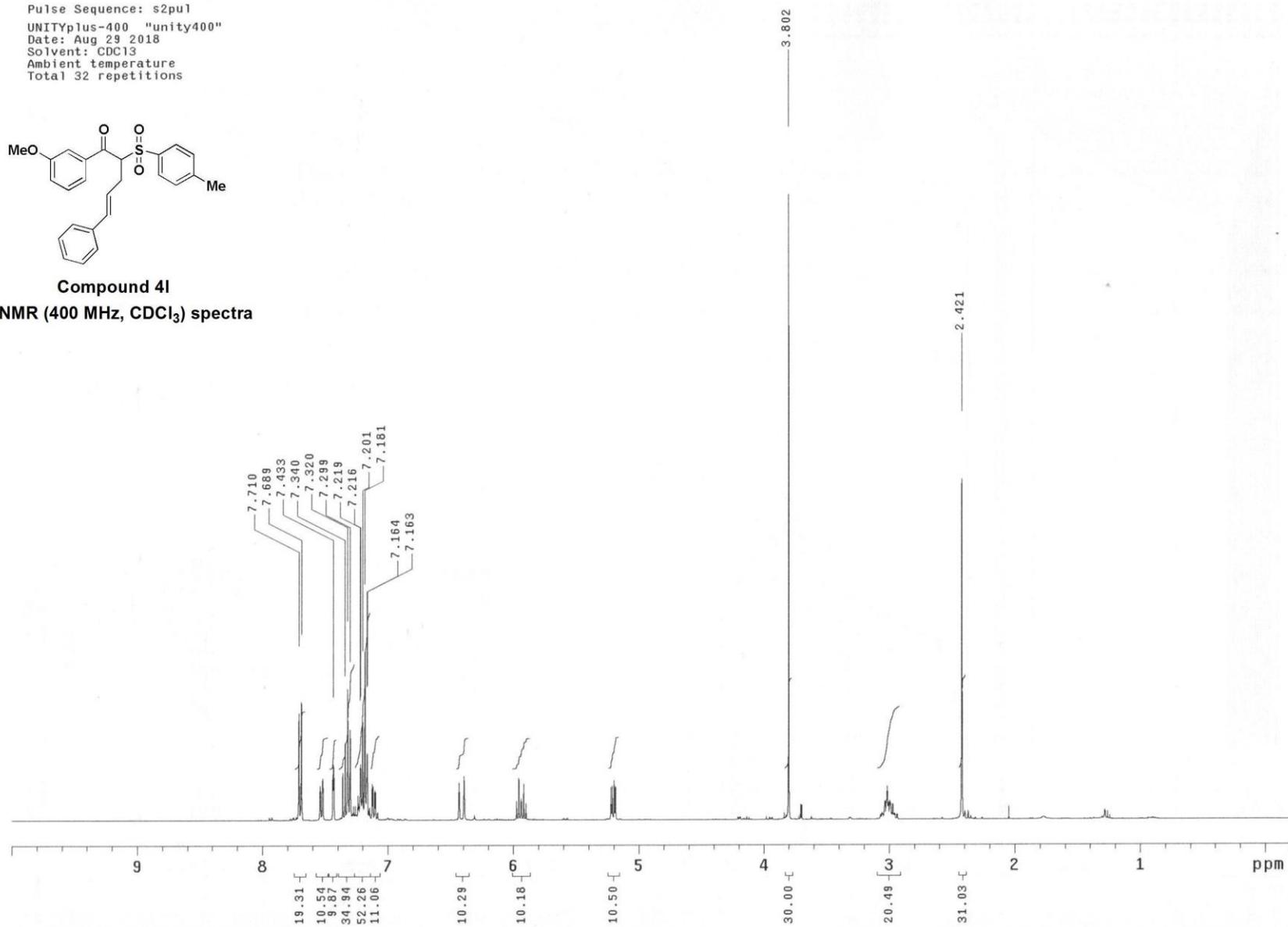
Ambient temperature

Total 32 repetitions

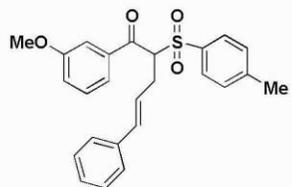


Compound 4l

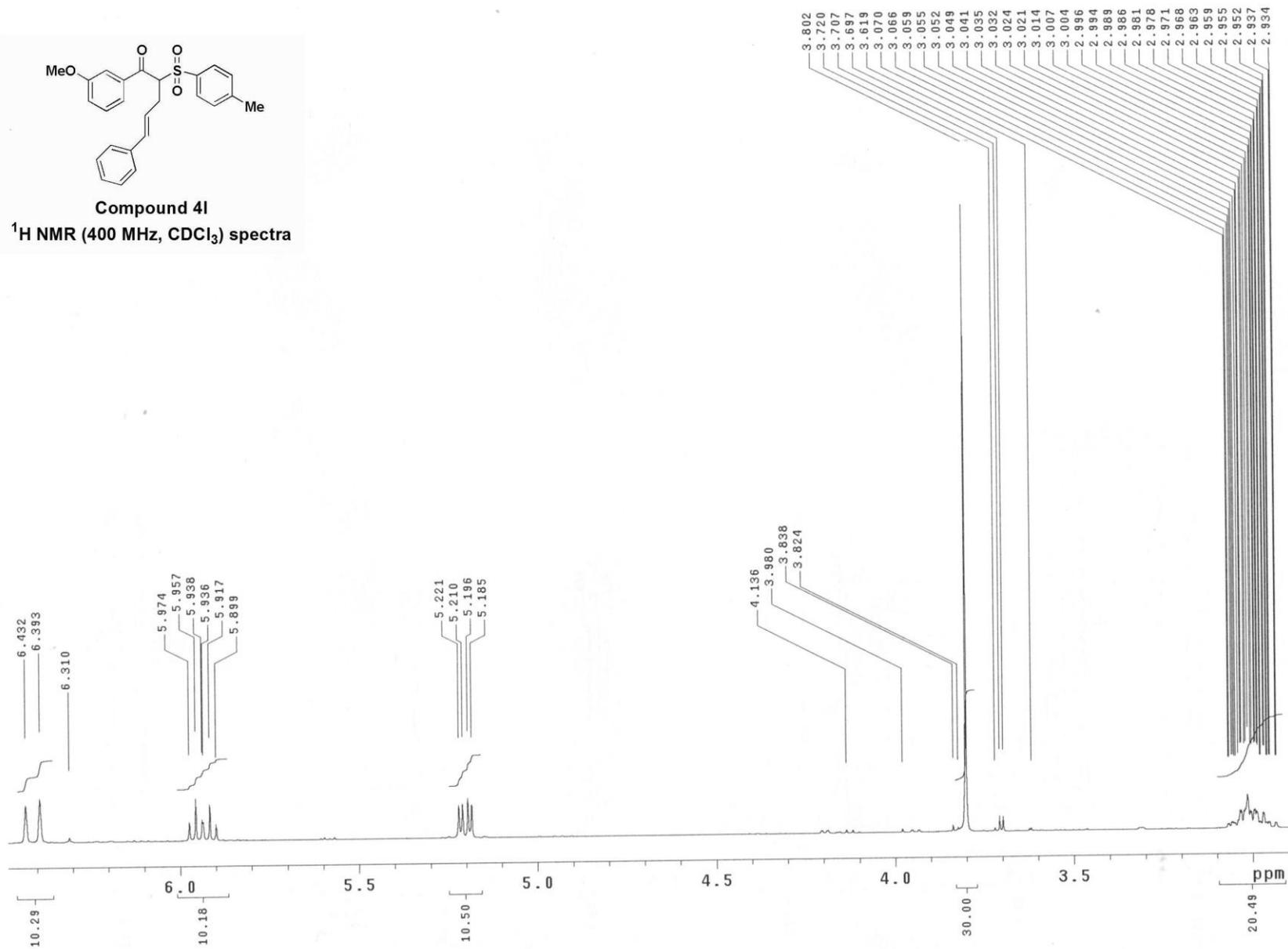
¹H NMR (400 MHz, CDCl₃) spectra



Compound 4I (¹H-NMR spectral data-2)



Compound 4I
¹H NMR (400 MHz, CDCl₃) spectra



Compound 4I (¹³C-NMR spectral data)

KSE2C

Pulse Sequence: s2pu1

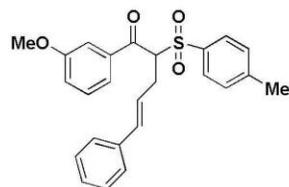
UNITYplus-400 "unity400"

Date: Aug 29 2018

Solvent: CDCl₃

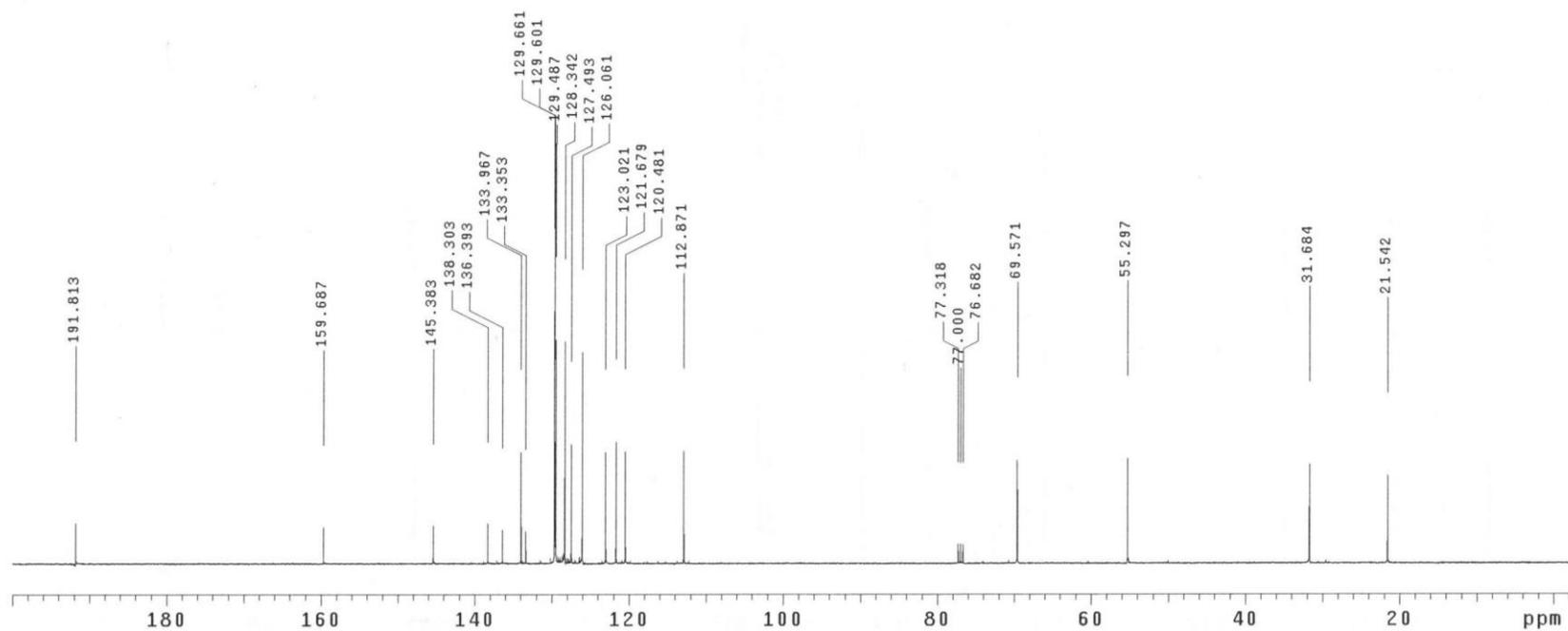
Ambient temperature

Total 1024 repetitions

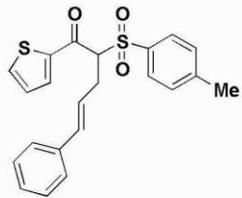


Compound 4I

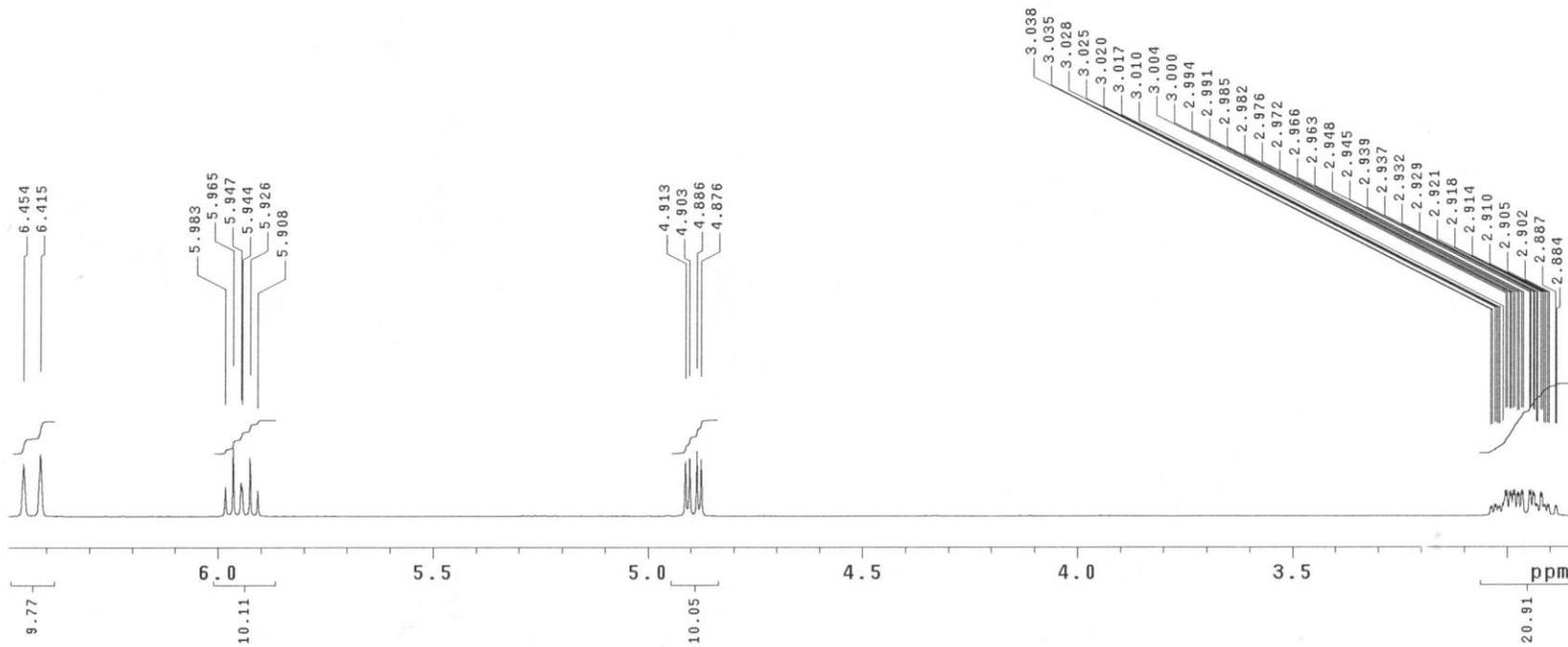
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4m (¹H-NMR spectral data-2)



Compound 4m
¹H NMR (400 MHz, CDCl₃) spectra



Compound 4m (¹³C-NMR spectral data)

KSE4C

Pulse Sequence: s2pu1

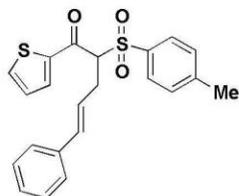
UNITYplus-400 "unity400"

Date: Sep 4 2018

Solvent: CDCl₃

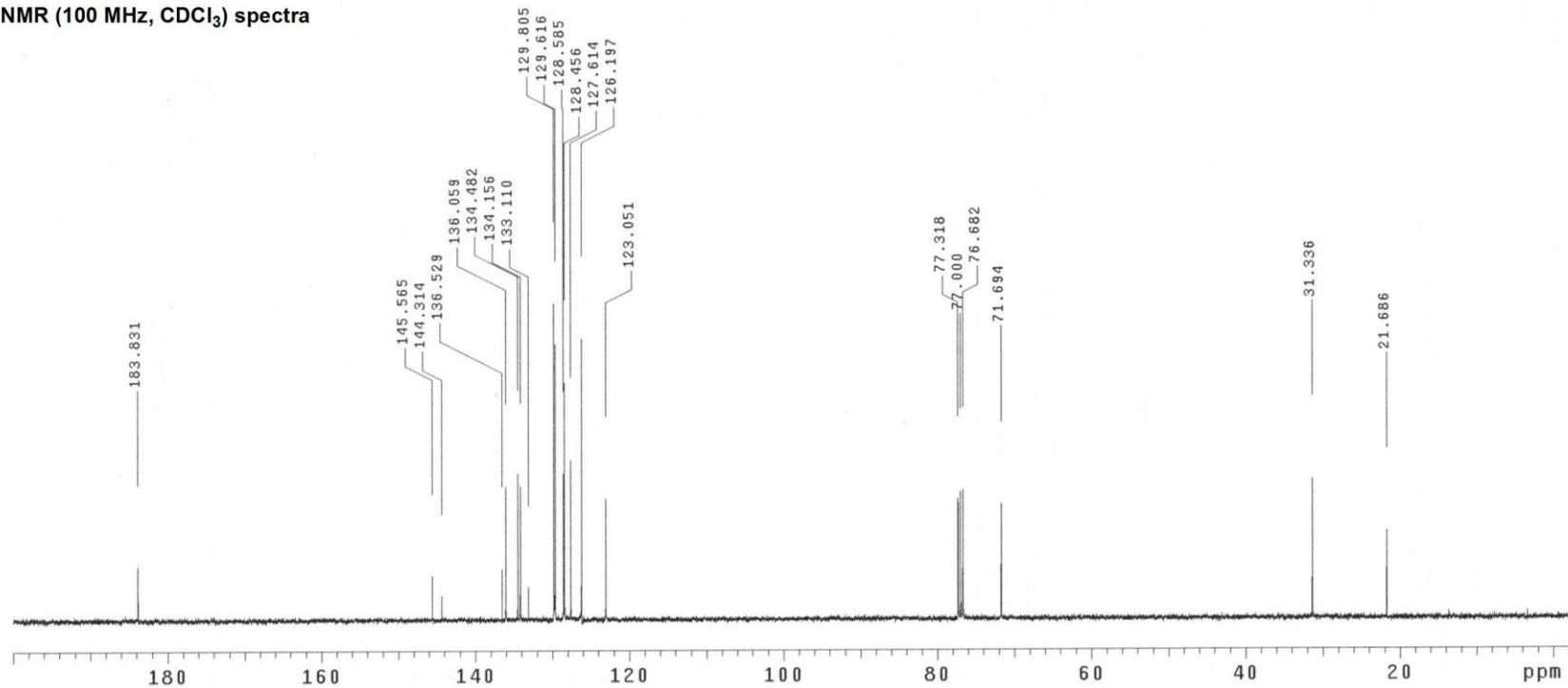
Ambient temperature

Total 1952 repetitions



Compound 4m

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4n (¹H-NMR spectral data-1)

KSE3C

Pulse Sequence: s2pu1

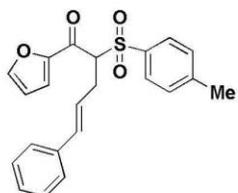
UNITYplus-400 "unity400"

Date: Sep 6 2018

Solvent: CDCl₃

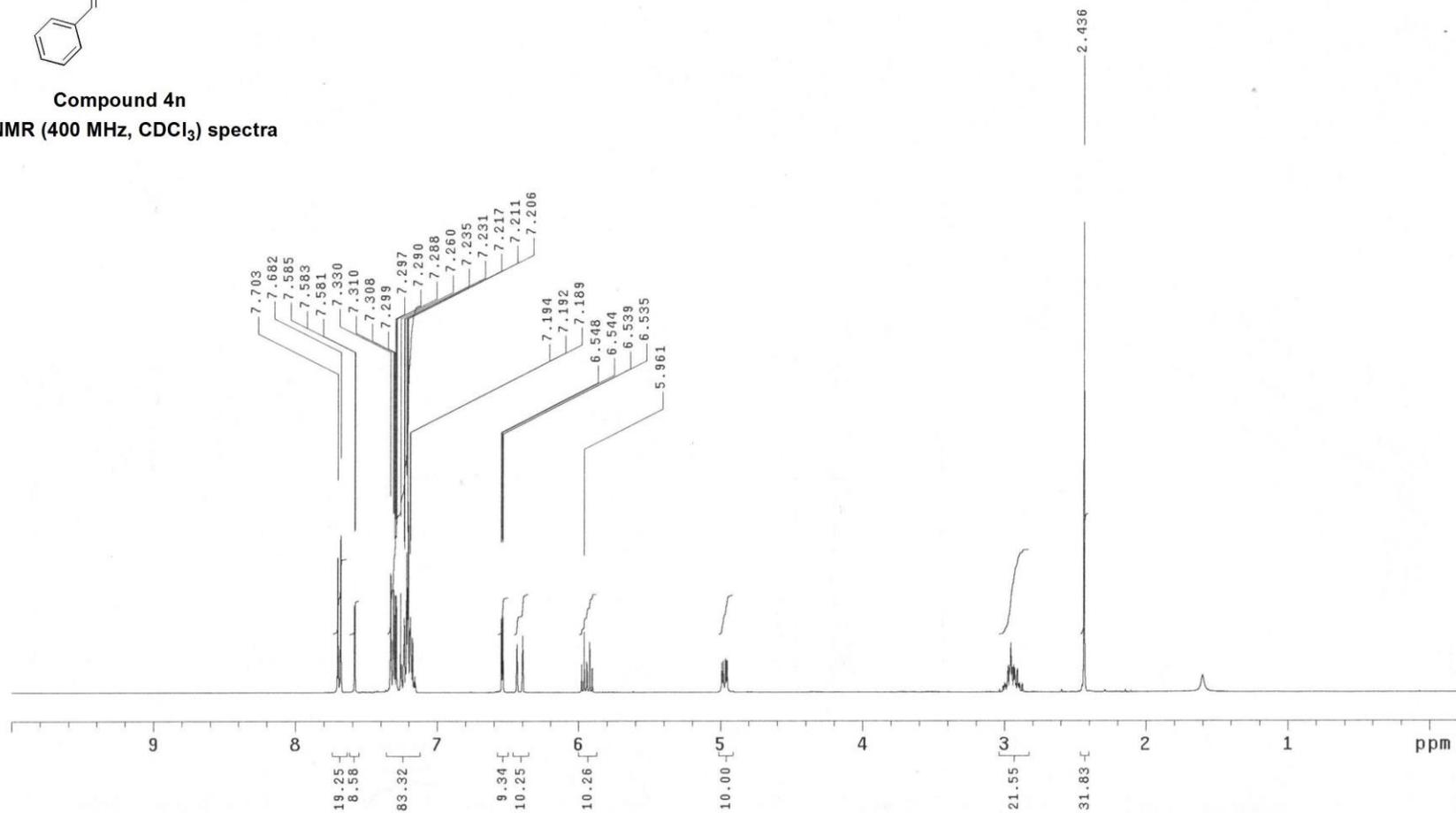
Ambient temperature

Total 32 repetitions

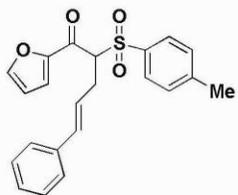


Compound 4n

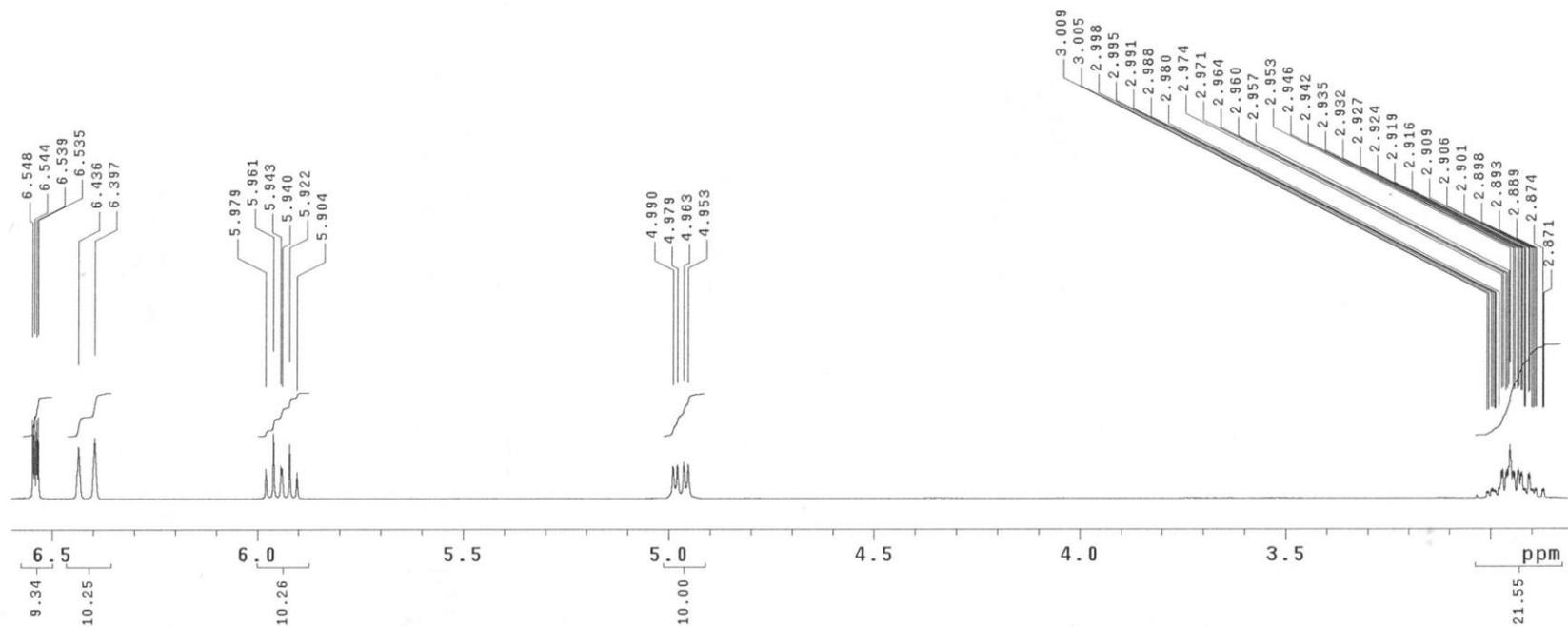
¹H NMR (400 MHz, CDCl₃) spectra



Compound 4n (¹H-NMR spectral data-2)

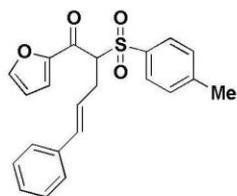


Compound 4n
¹H NMR (400 MHz, CDCl₃) spectra



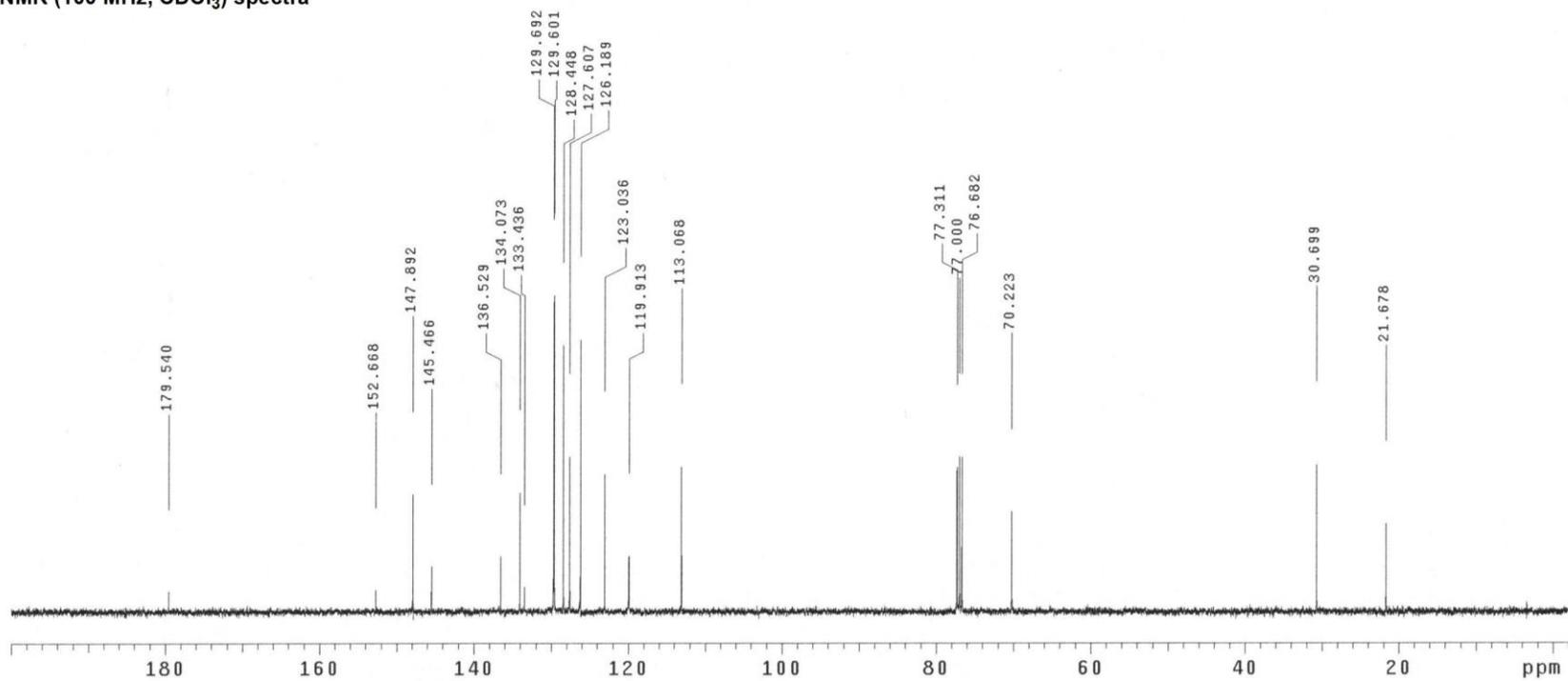
Compound 4n (¹³C-NMR spectral data)

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Sep 6 2018
Solvent: CDCl₃
Ambient temperature
Total 1408 repetitions



Compound 4n

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4o (¹H-NMR spectral data-1)

KSTSBr

Pulse Sequence: s2pu1

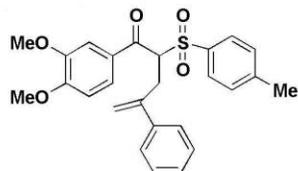
UNITYplus-400 "unity400"

Date: Feb 21 2019

Solvent: CDCl₃

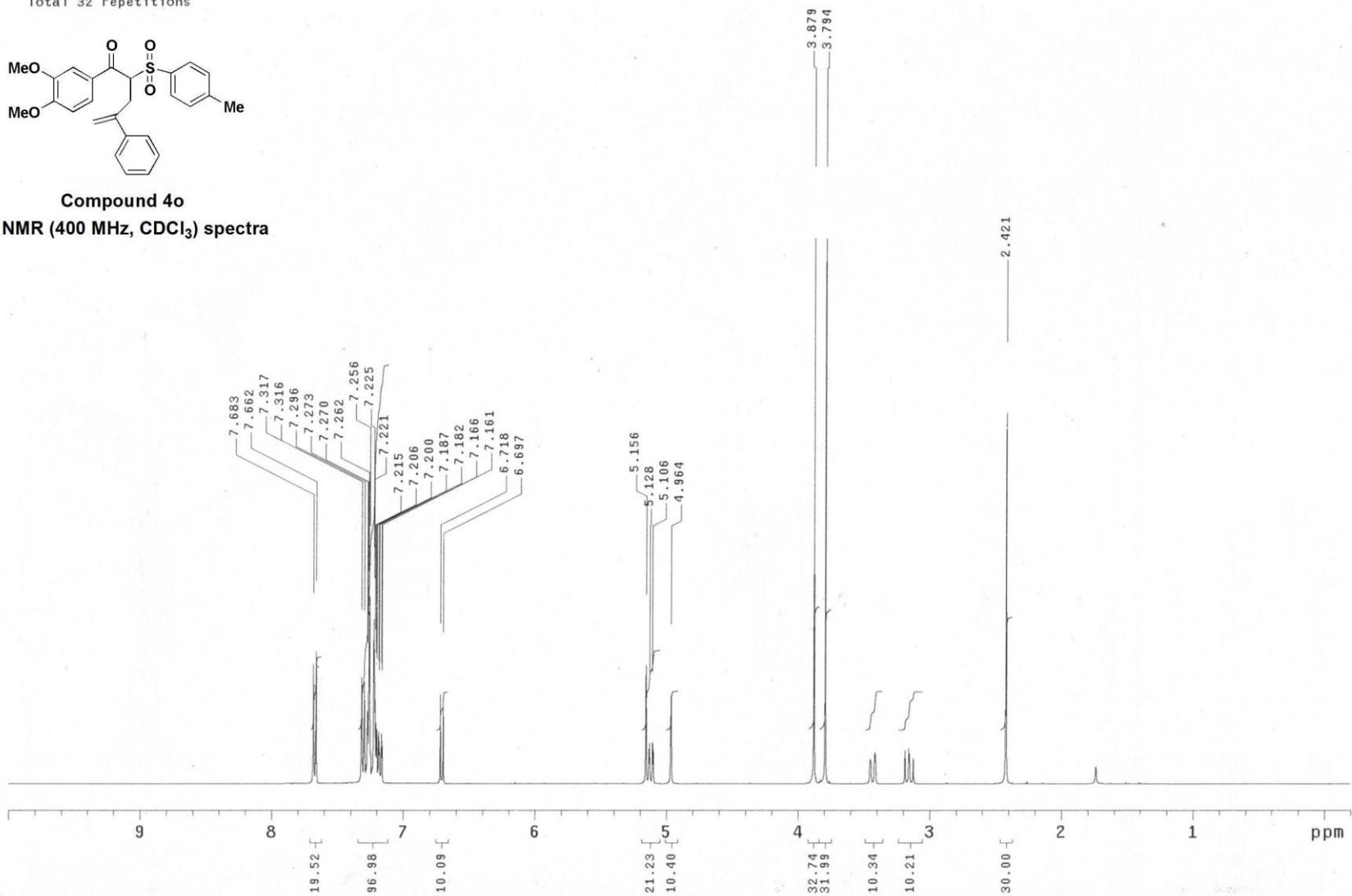
Ambient temperature

Total 32 repetitions



Compound 4o

¹H NMR (400 MHz, CDCl₃) spectra



Compound 4o (¹H-NMR spectral data-2)

KSTSBBr

Pulse Sequence: s2pu1

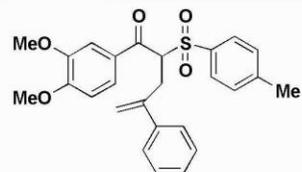
UNITYplus-400 "unity400"

Date: Feb 21 2019

Solvent: CDCl₃

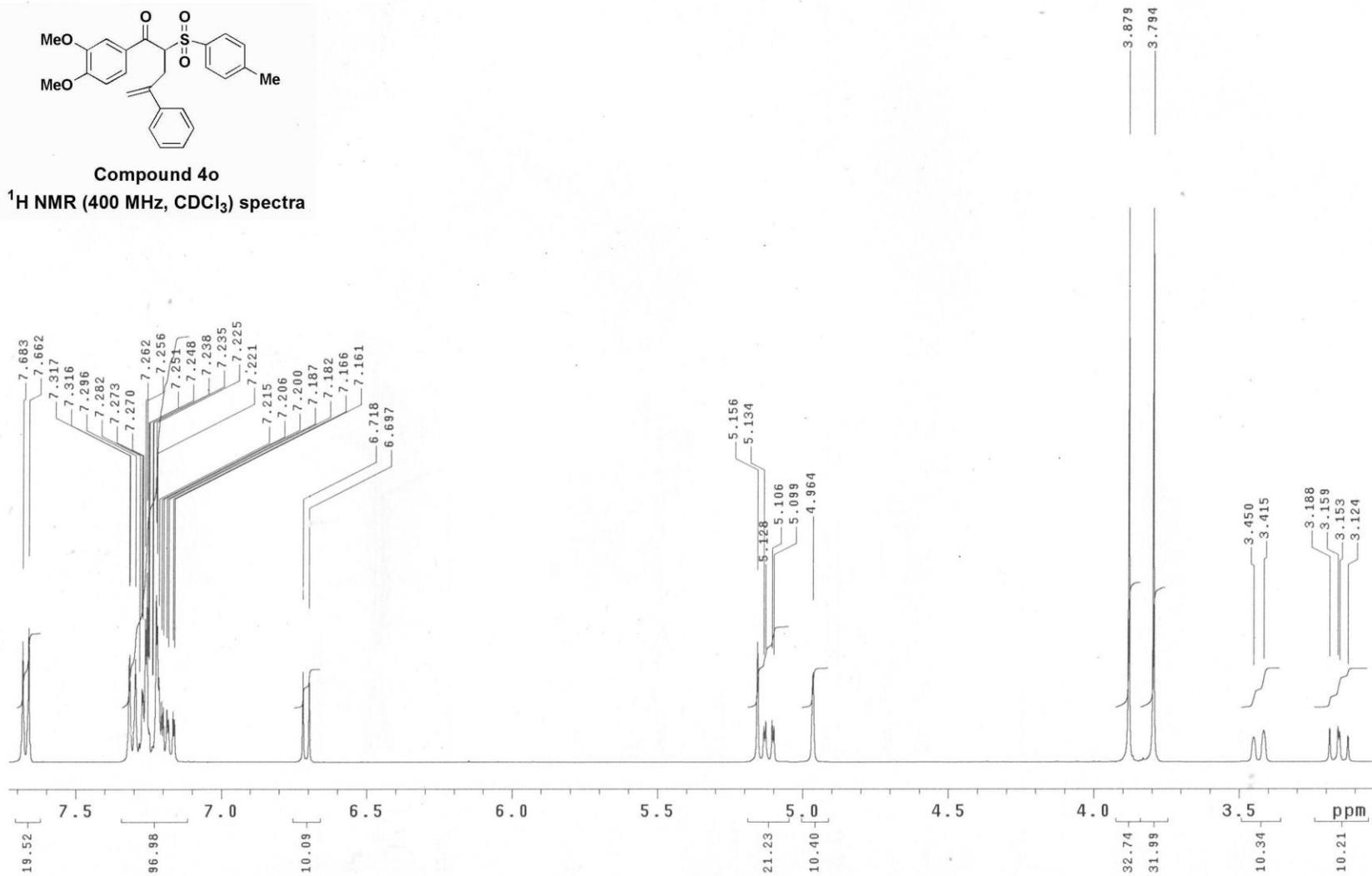
Ambient temperature

Total 32 repetitions



Compound 4o

¹H NMR (400 MHz, CDCl₃) spectra



Compound 4o (¹³C-NMR spectral data)

KSTSBr

Pulse Sequence: s2pu1

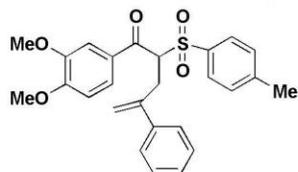
UNITYplus-400 "unity400"

Date: Feb 21 2019

Solvent: CDCl₃

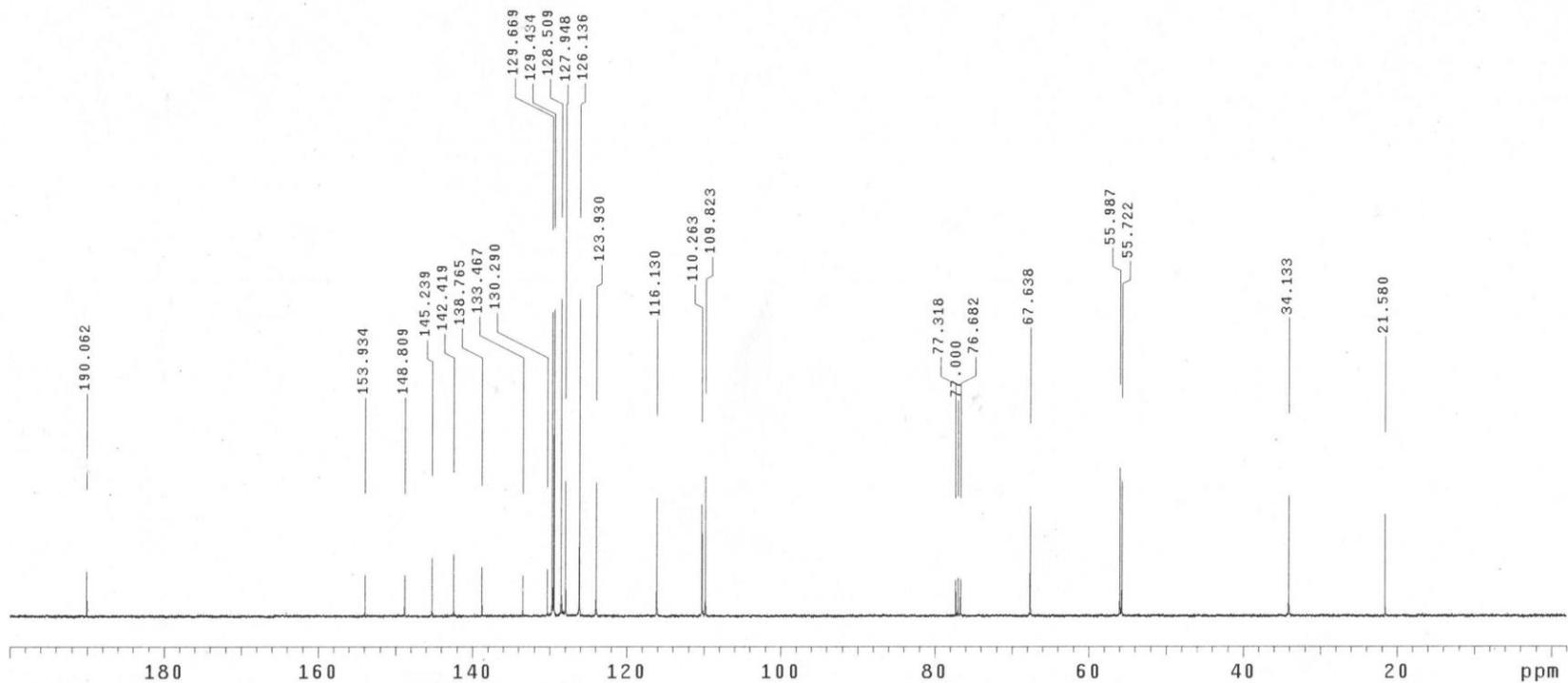
Ambient temperature

Total 560 repetitions



Compound 4o

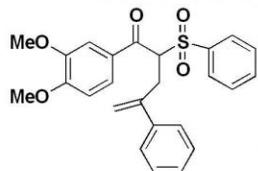
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4p (¹H-NMR spectral data-1)

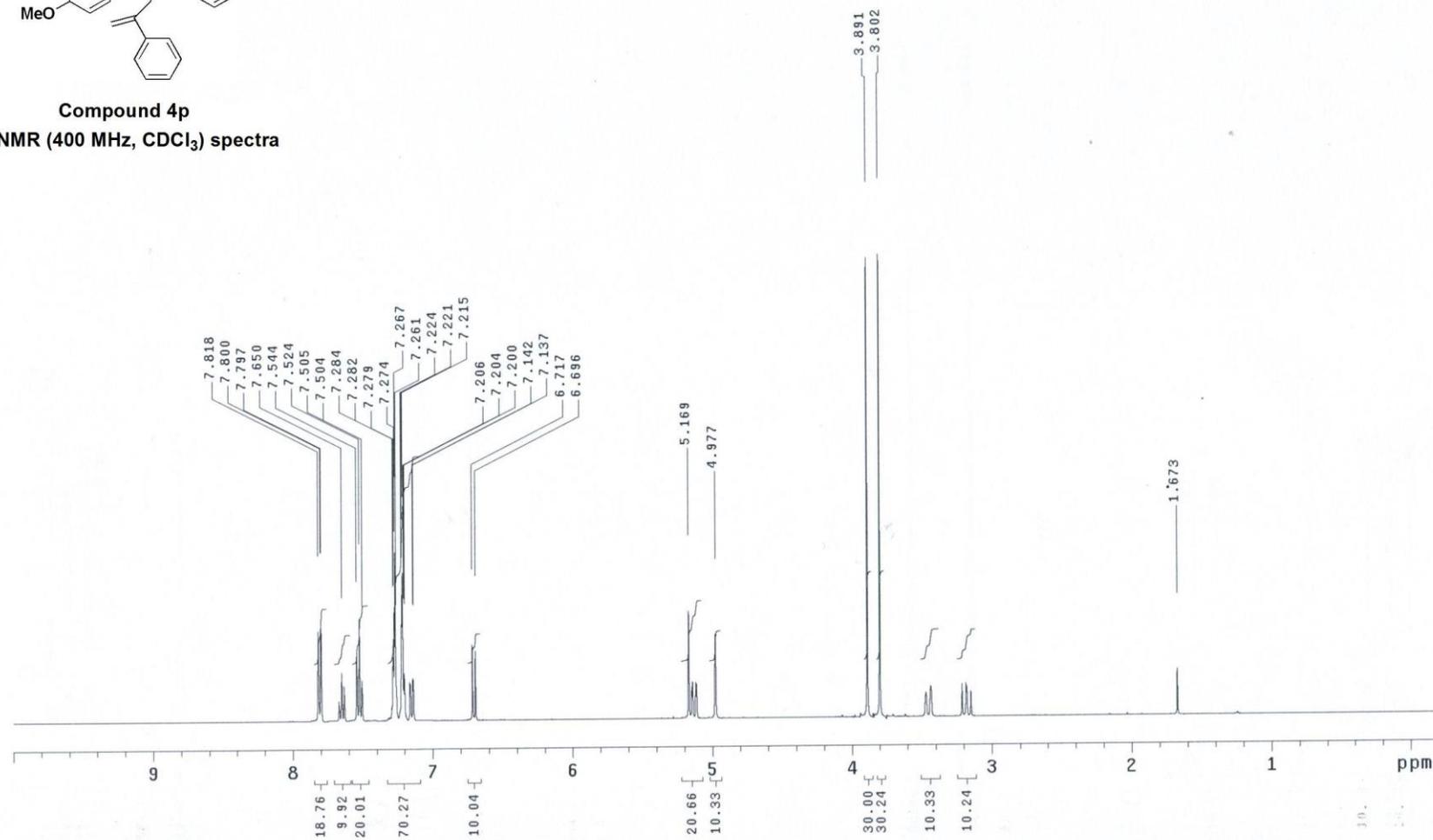
KSBSD

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Mar 8 2019
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

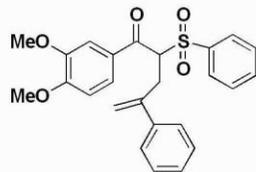


Compound 4p

¹H NMR (400 MHz, CDCl₃) spectra

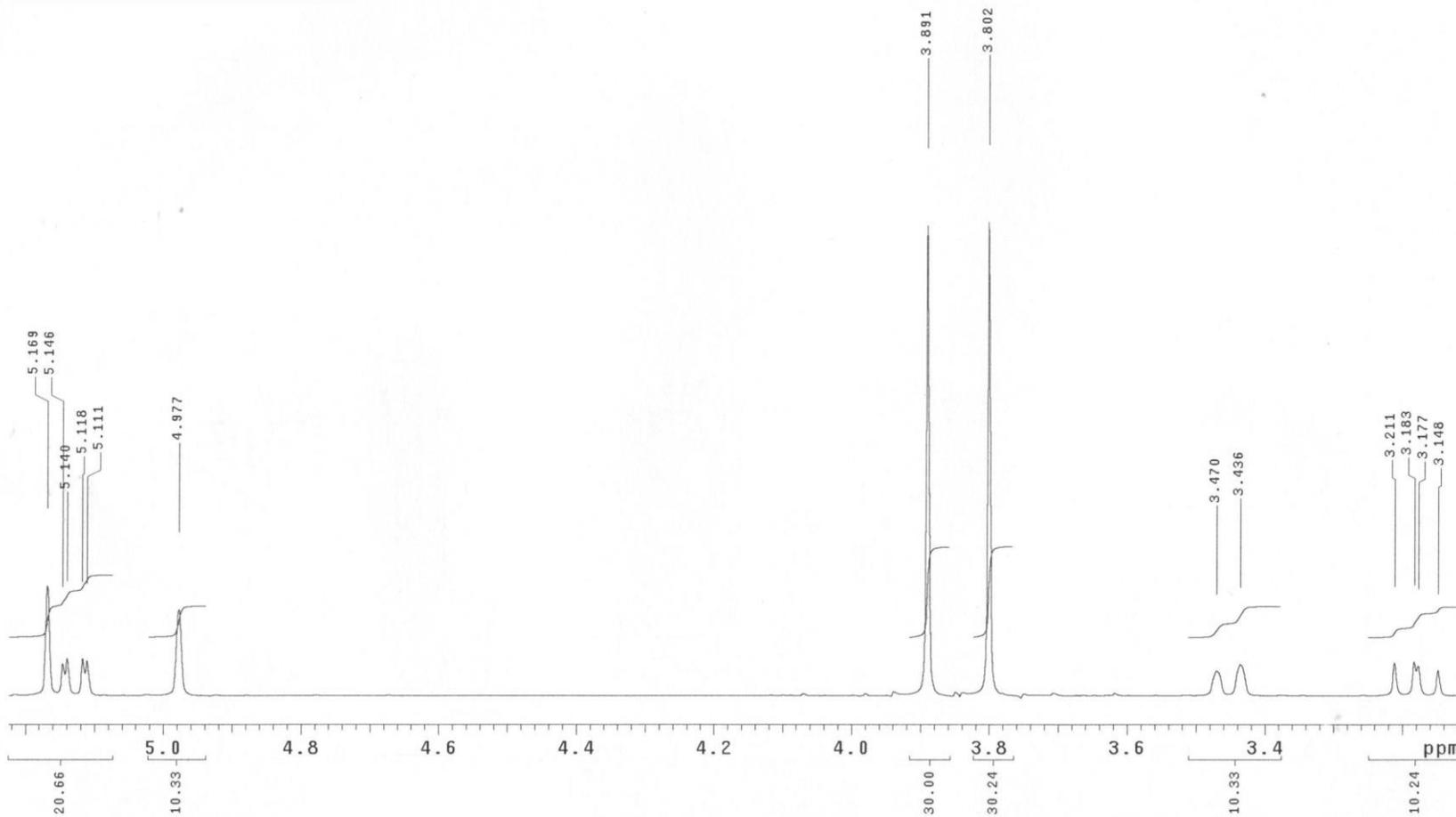


Compound 4p (¹H-NMR spectral data-2)



Compound 4p

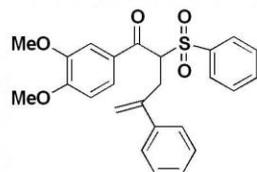
¹H NMR (400 MHz, CDCl₃) spectra



Compound 4p (¹³C-NMR spectral data)

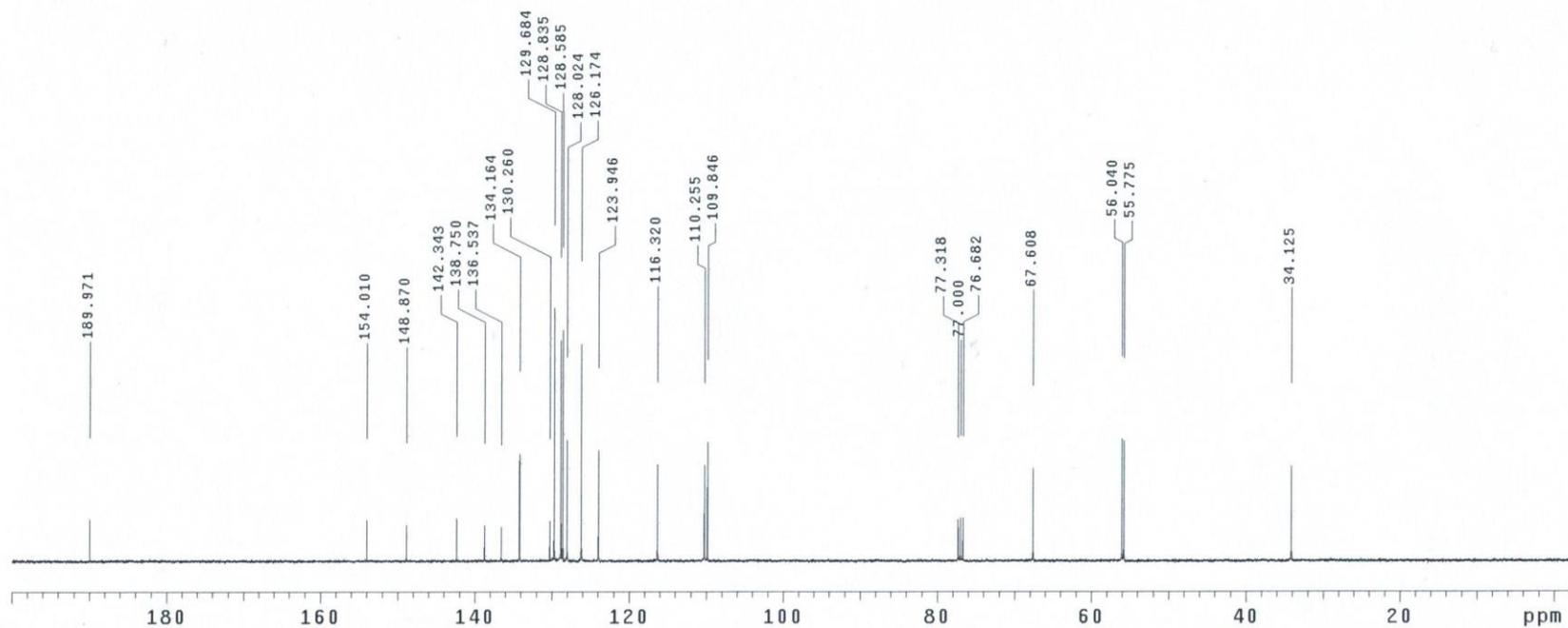
KSBSD

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Mar 8 2019
Solvent: CDCl₃
Ambient temperature
Total 800 repetitions



Compound 4p

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4q (¹H-NMR spectral data-1)

KSMSD

Pulse Sequence: s2pu1

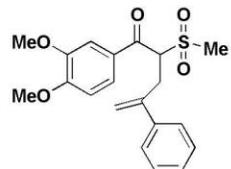
UNITYplus-400 "unity400"

Date: Mar 18 2019

Solvent: CDCl₃

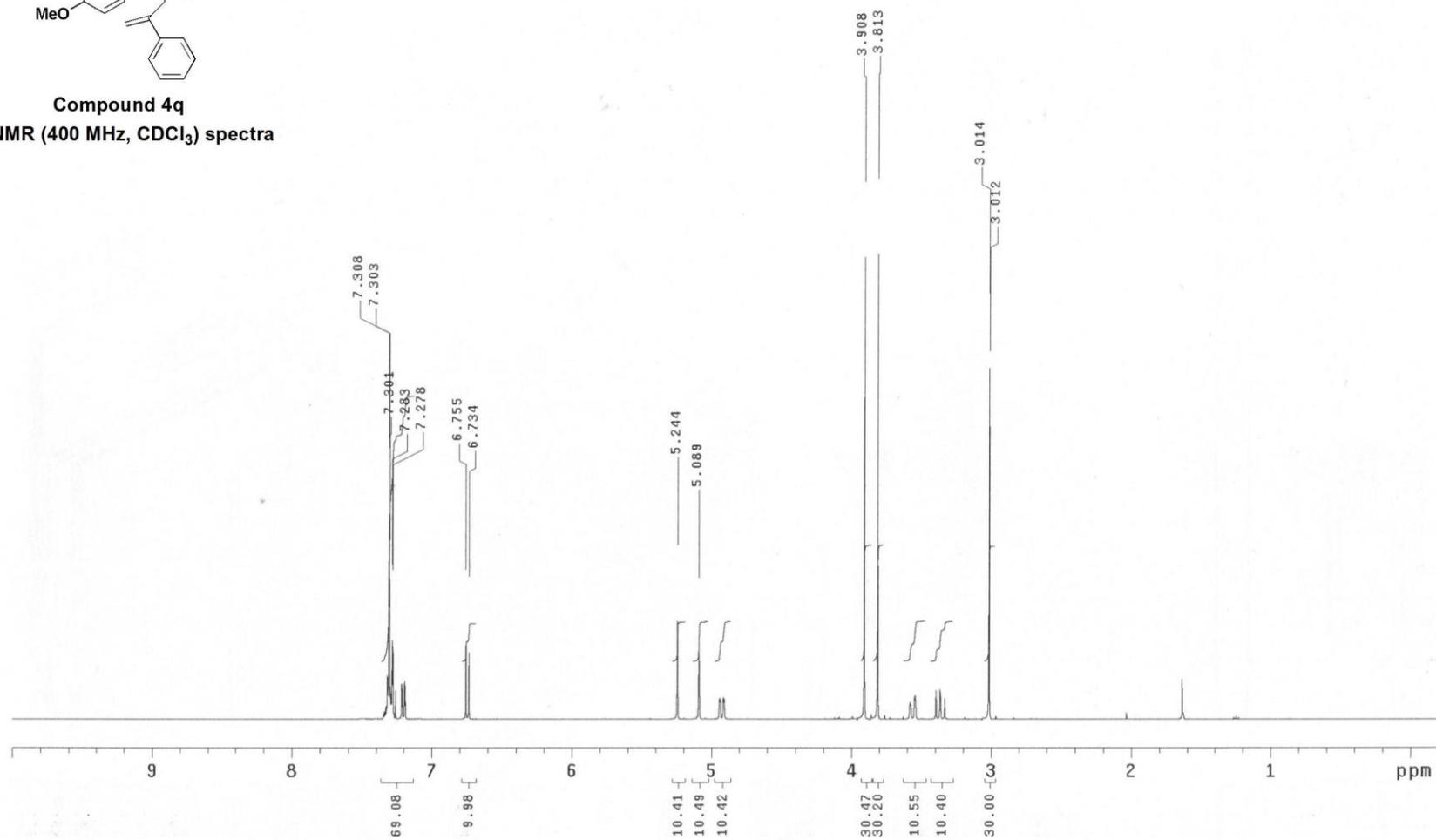
Ambient temperature

Total 32 repetitions

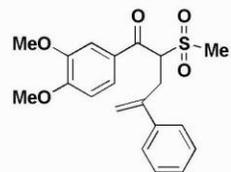


Compound 4q

¹H NMR (400 MHz, CDCl₃) spectra

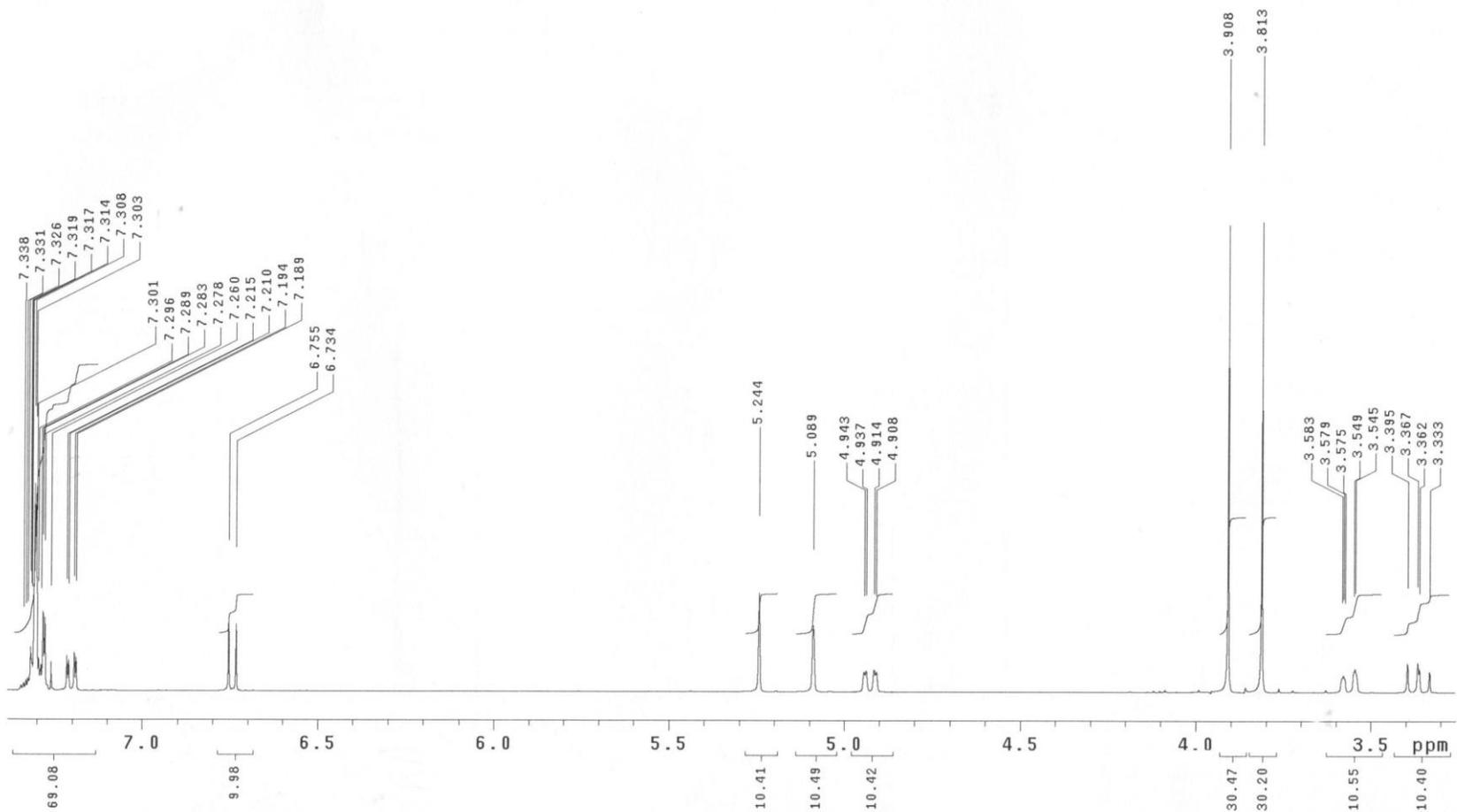


Compound 4q (¹H-NMR spectral data-2)



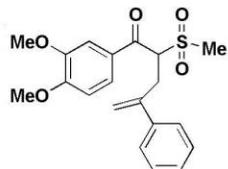
Compound 4q

¹H NMR (400 MHz, CDCl₃) spectra



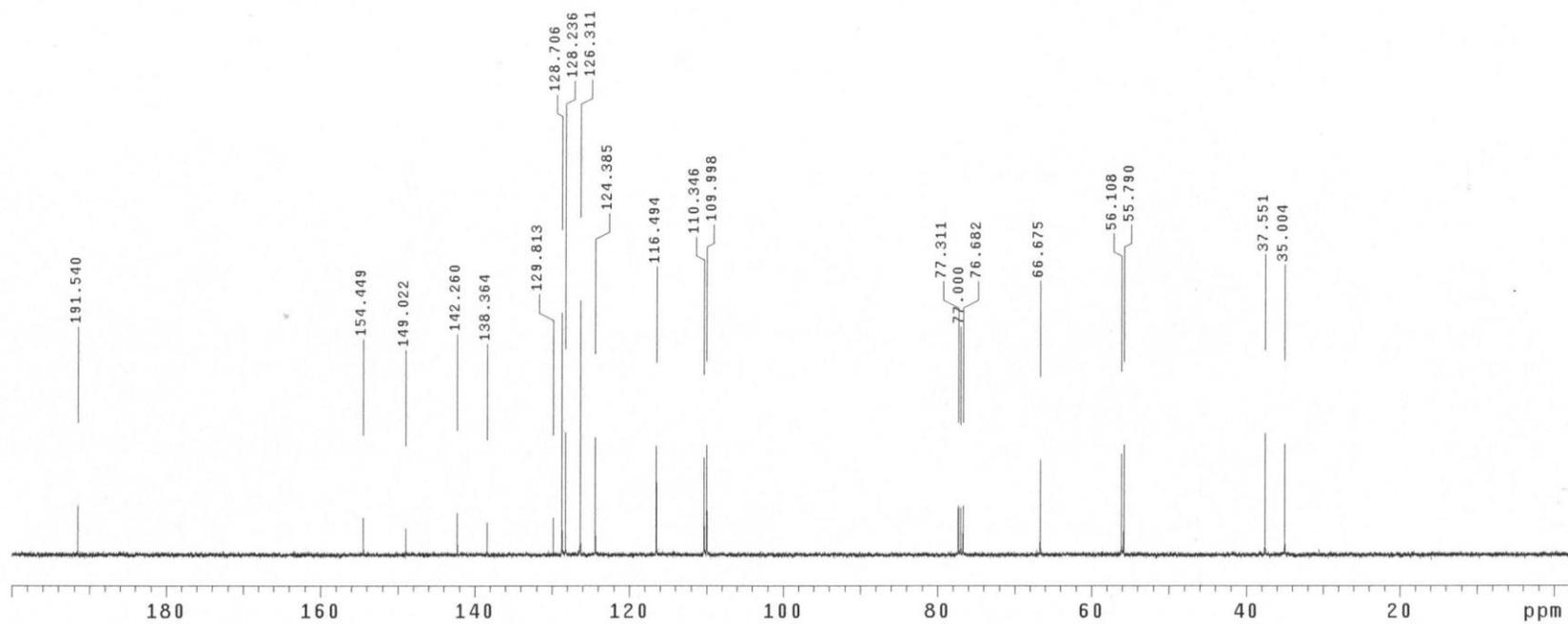
Compound 4q (¹³C-NMR spectral data)

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Mar 18 2019
Solvent: CDCl₃
Ambient temperature
Total 672 repetitions



Compound 4q

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4r (¹H-NMR spectral data-1)

KSmMeD

Pulse Sequence: s2pu1

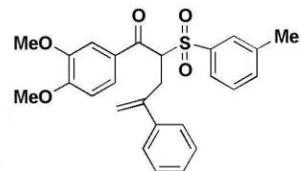
UNITYplus-400 "unity400"

Date: Mar 12 2019

Solvent: CDCl₃

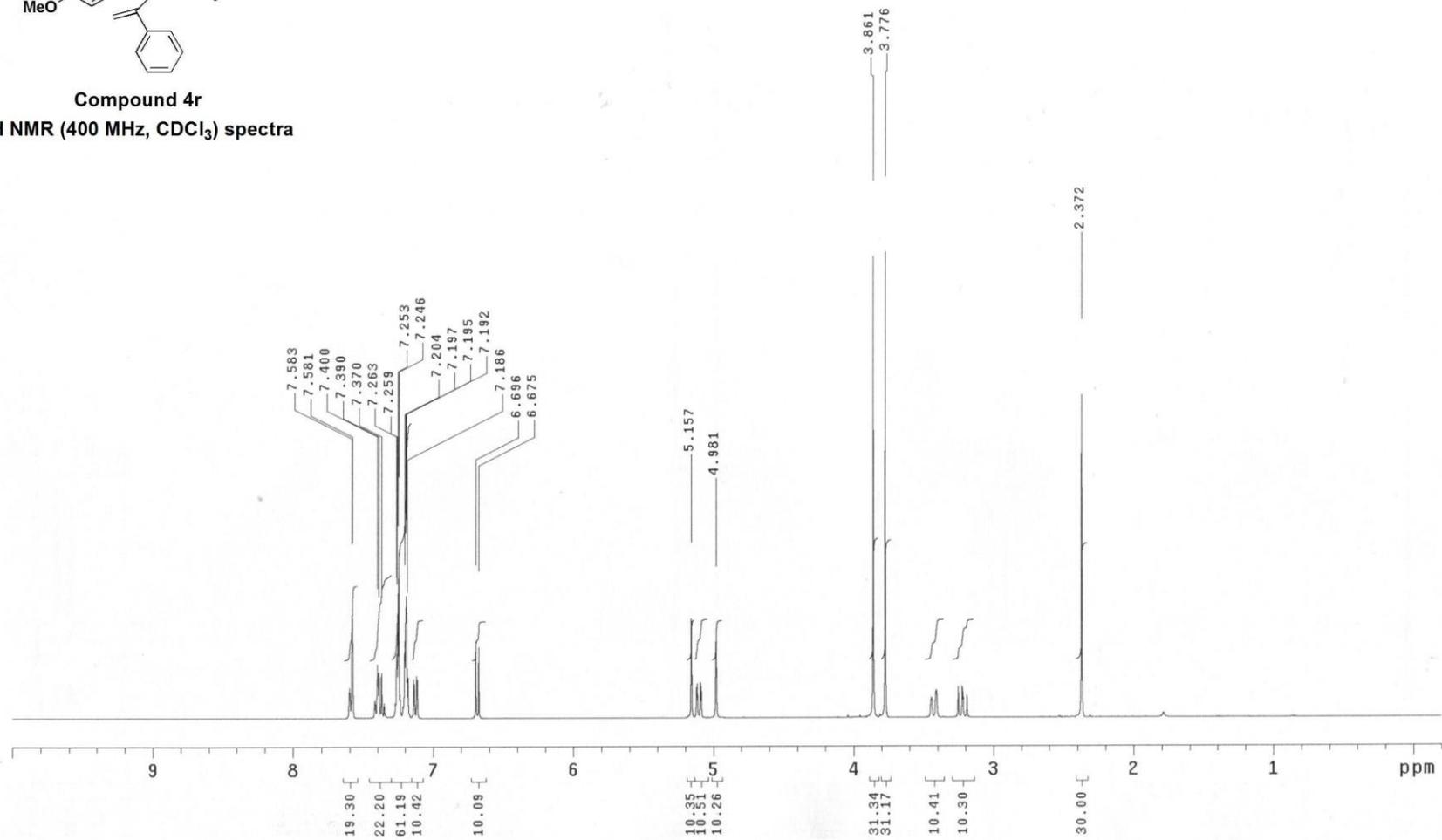
Ambient temperature

Total 32 repetitions

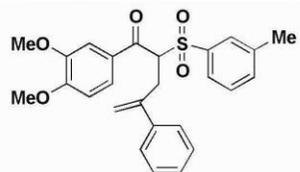


Compound 4r

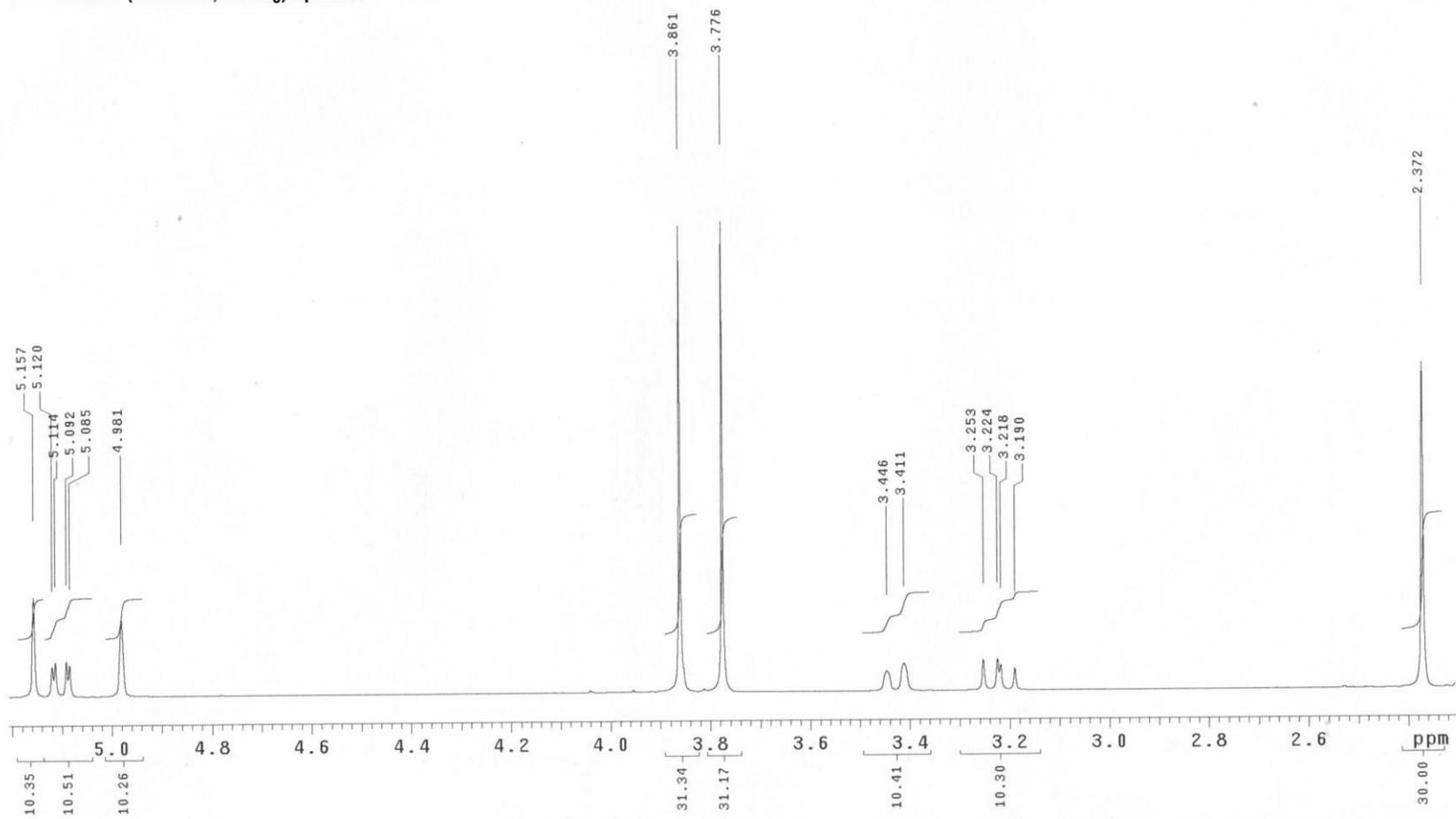
¹H NMR (400 MHz, CDCl₃) spectra



Compound 4r (¹H-NMR spectral data-2)



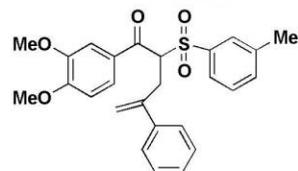
Compound 4r
¹H NMR (400 MHz, CDCl₃) spectra



Compound 4r (¹³C-NMR spectral data)

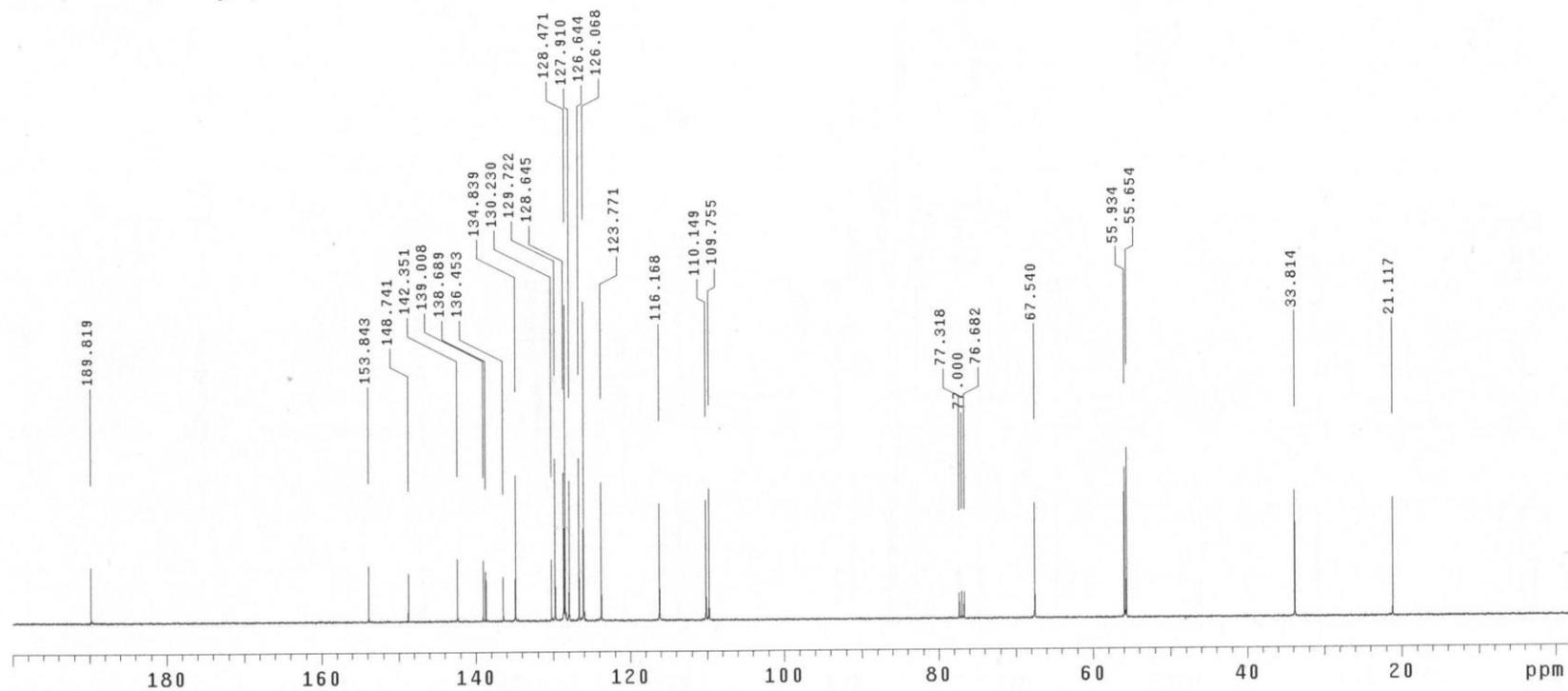
KSmMeD

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Mar 12 2019
Solvent: CDCl₃
Ambient temperature
Total 1024 repetitions



Compound 4r

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4s (¹H-NMR spectral data-1)

KS30MeD

Pulse Sequence: s2pu1

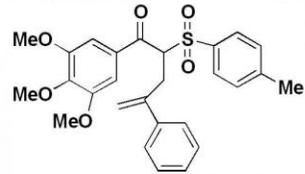
UNITYplus-400 "unity400"

Date: Mar 7 2019

Solvent: CDCl₃

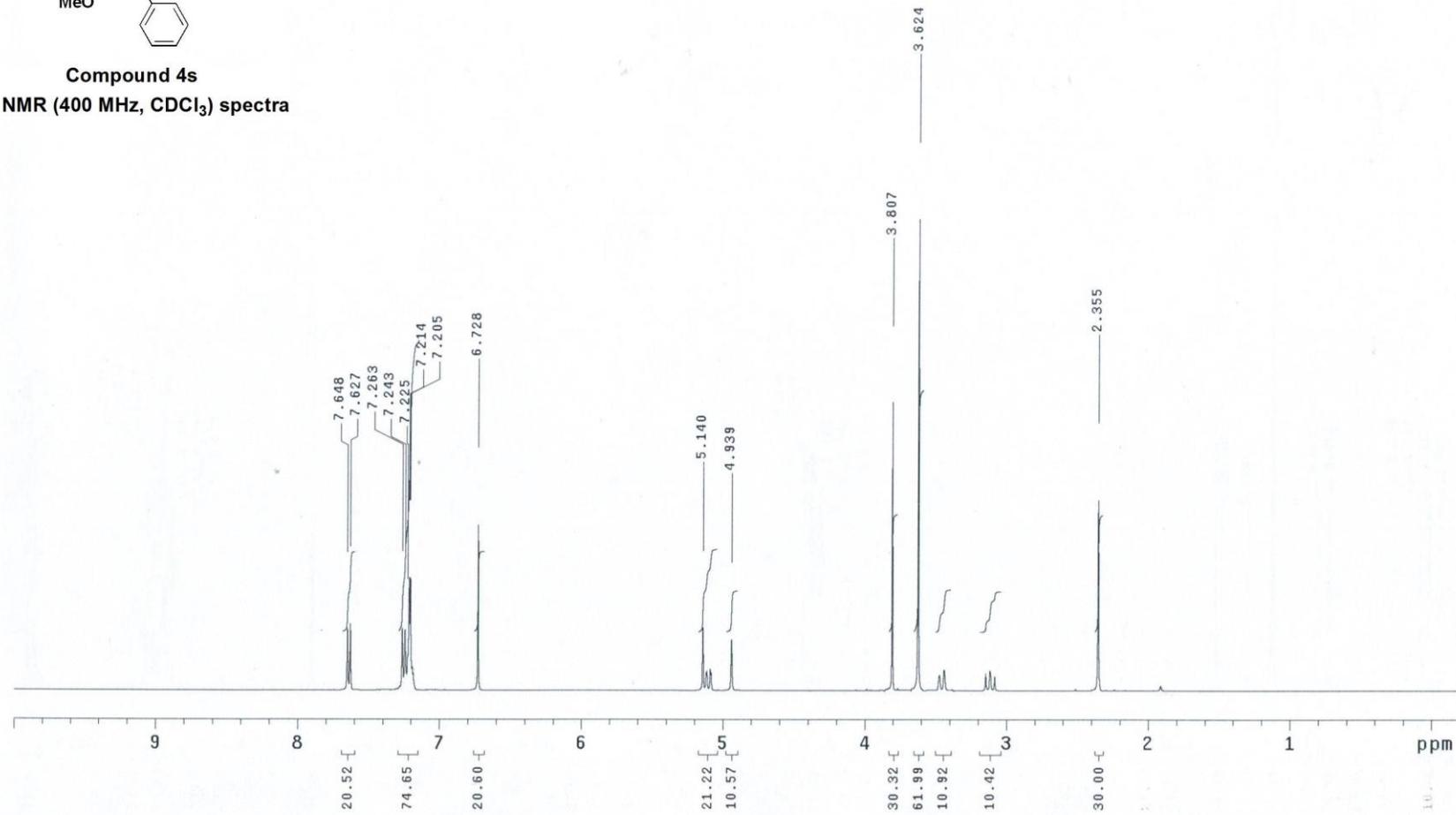
Ambient temperature

Total 32 repetitions

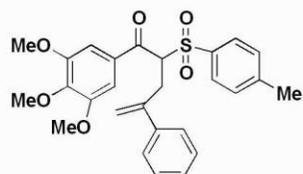


Compound 4s

¹H NMR (400 MHz, CDCl₃) spectra

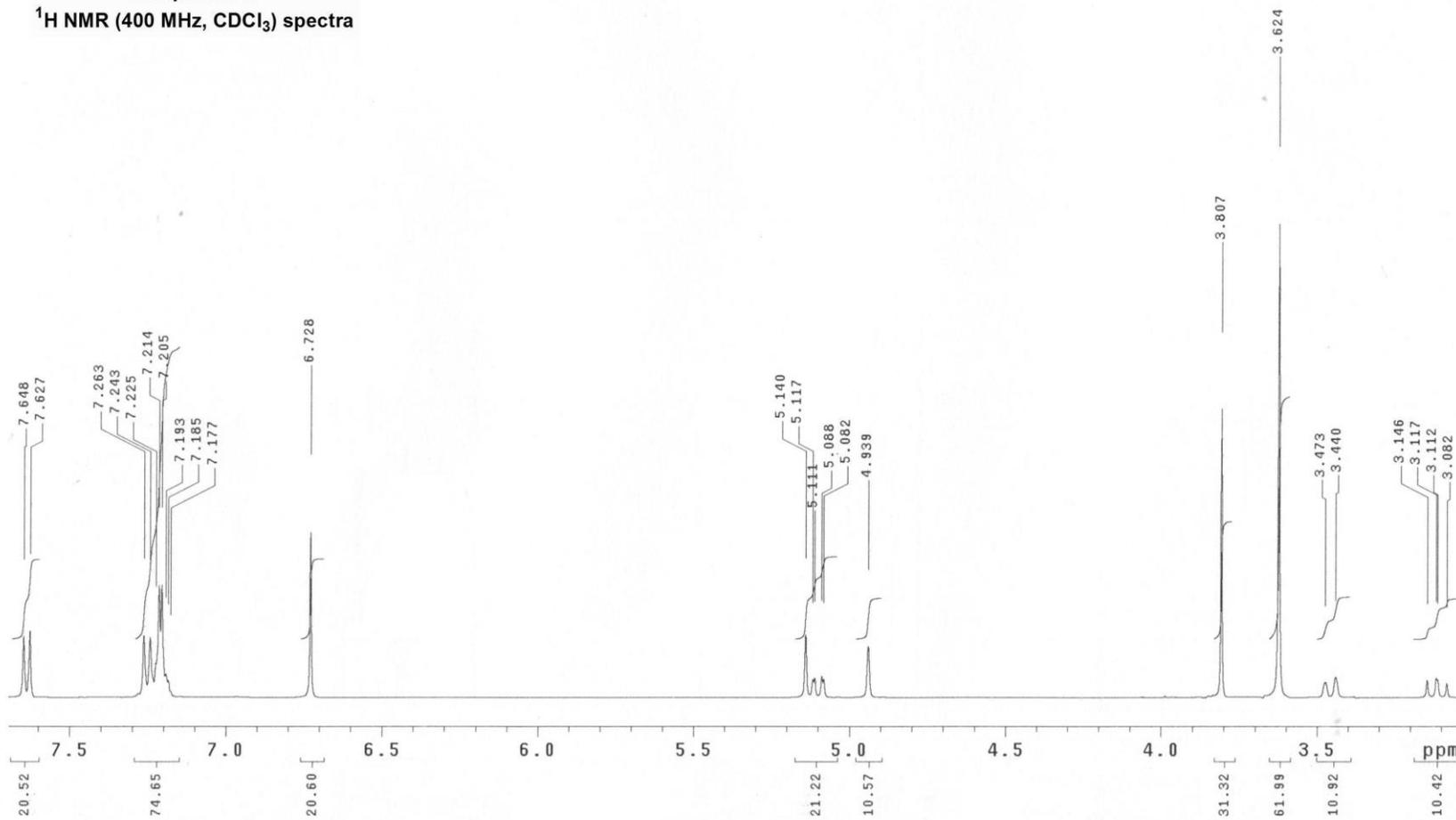


Compound 4s (¹H-NMR spectral data-2)



Compound 4s

¹H NMR (400 MHz, CDCl₃) spectra



Compound 4s (¹³C-NMR spectral data)

KS30MeD

Pulse Sequence: s2pu1

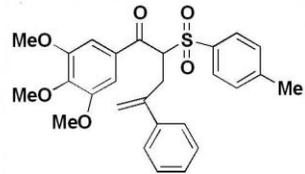
UNITYplus-400 "unity400"

Date: Mar 7 2019

Solvent: CDCl₃

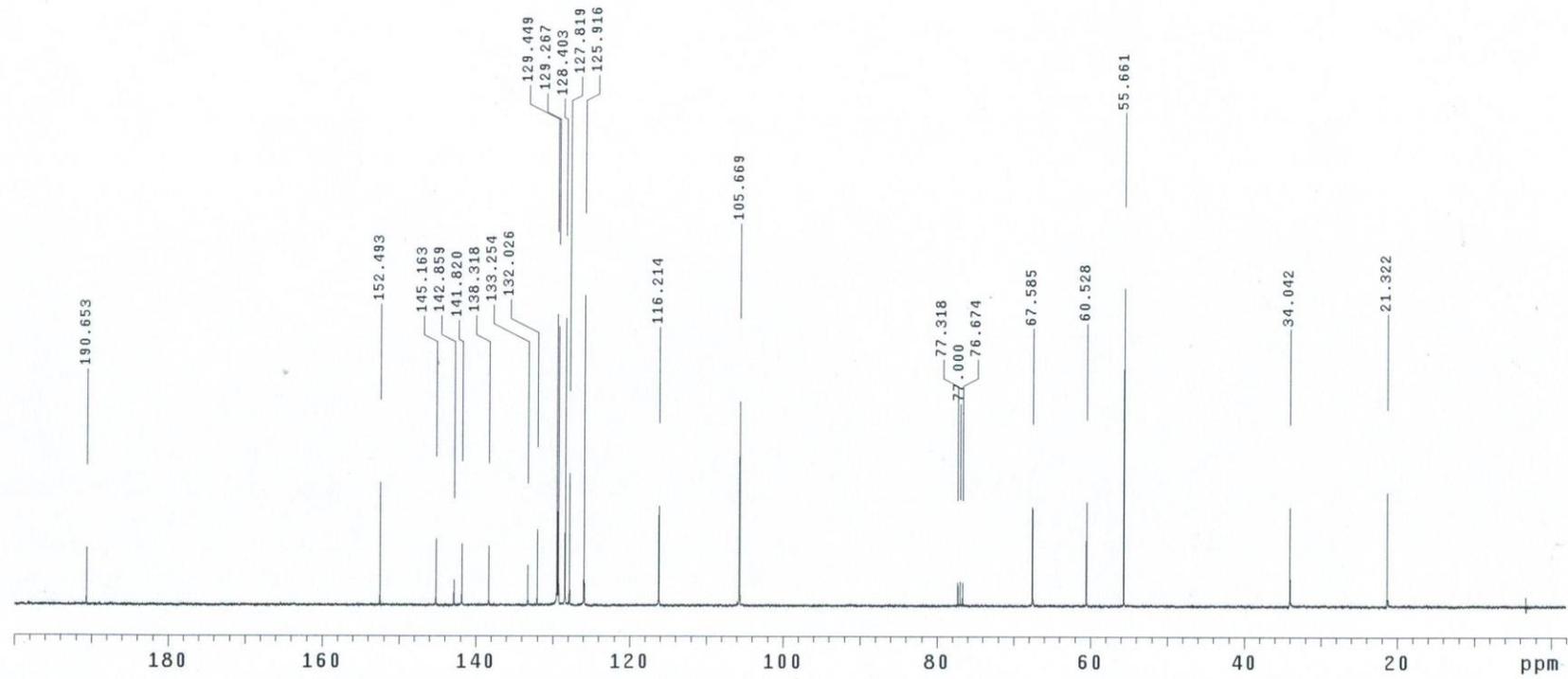
Ambient temperature

Total 160 repetitions



Compound 4s

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4t (¹H-NMR spectral data-1)

KSE7Cr

Pulse Sequence: s2pu1

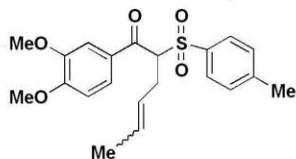
UNITYplus-400 "unity400"

Date: Nov 26 2018

Solvent: CDCl₃

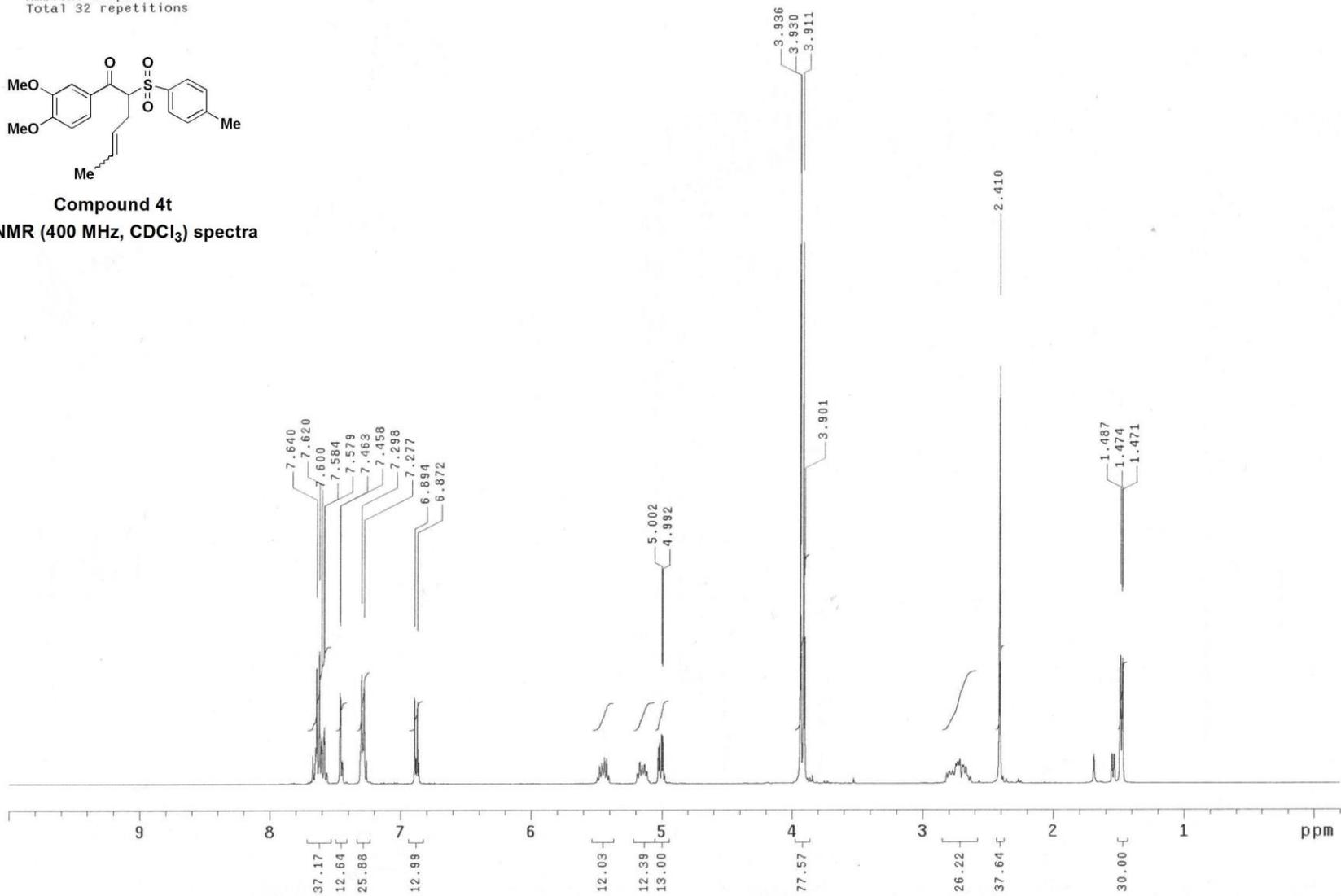
Ambient temperature

Total 32 repetitions

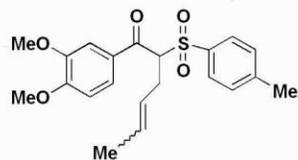


Compound 4t

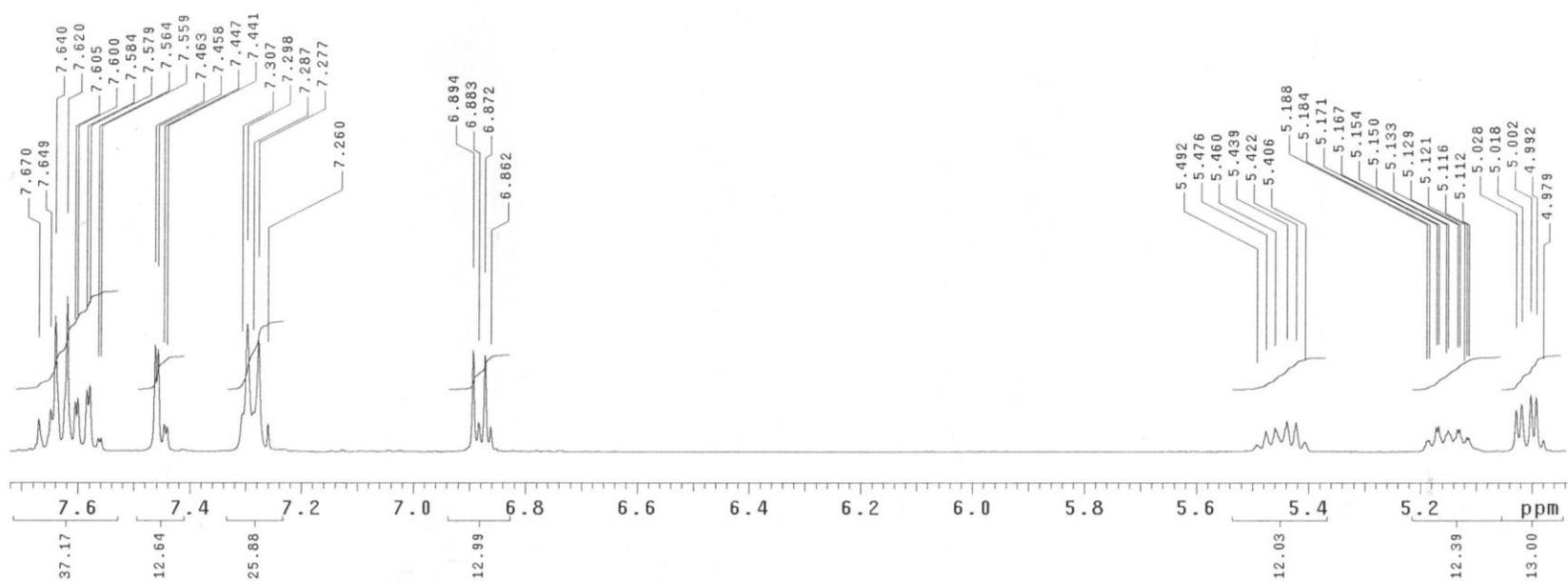
¹H NMR (400 MHz, CDCl₃) spectra



Compound 4t (¹H-NMR spectral data-2)



Compound 4t
¹H NMR (400 MHz, CDCl₃) spectra



Compound 4t (¹³C-NMR spectral data)

KSE7Cr

Pulse Sequence: s2pu1

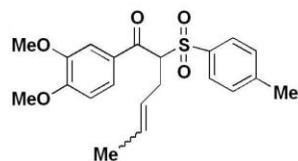
UNITYplus-400 "unity400"

Date: Nov 26 2018

Solvent: CDCl₃

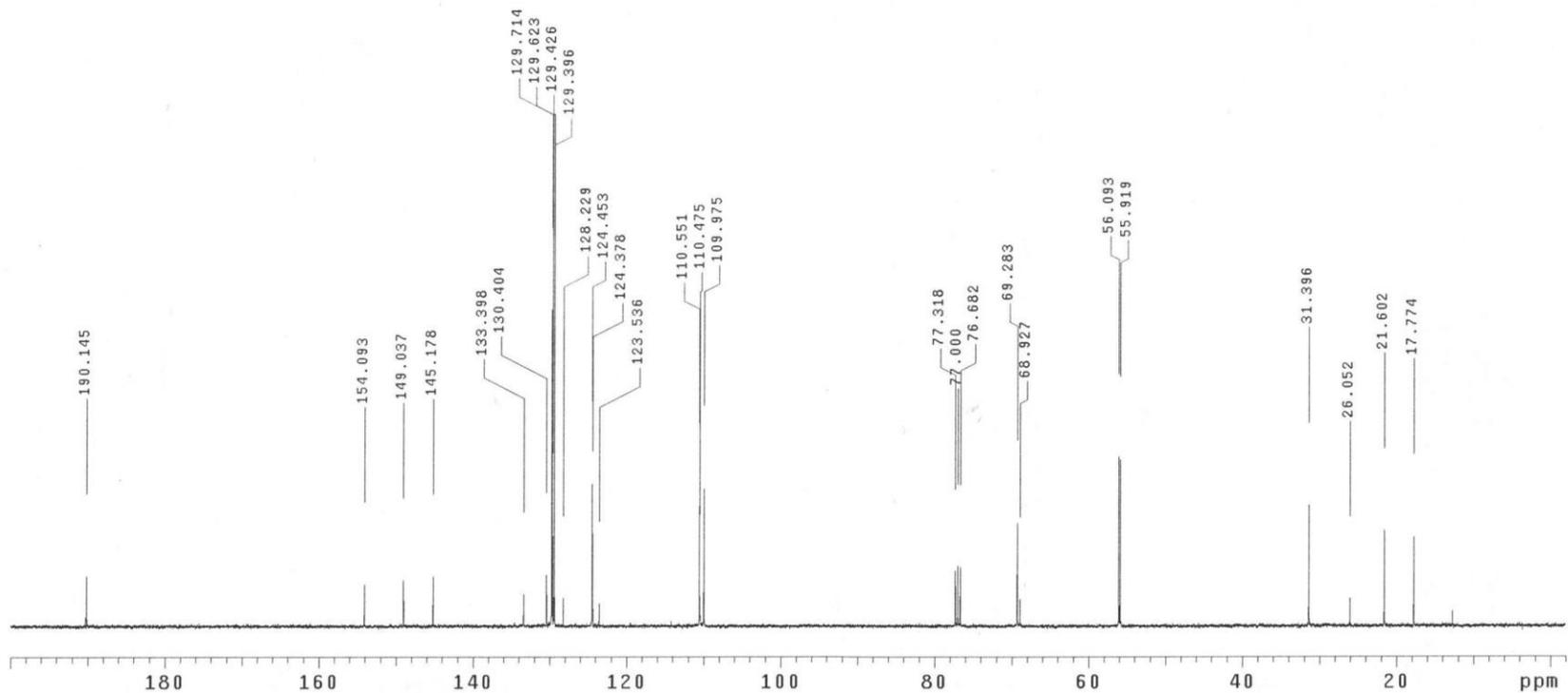
Ambient temperature

Total 848 repetitions



Compound 4t

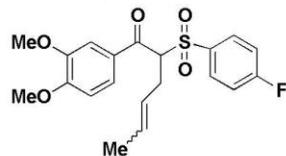
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4u (¹H-NMR spectral data-1)

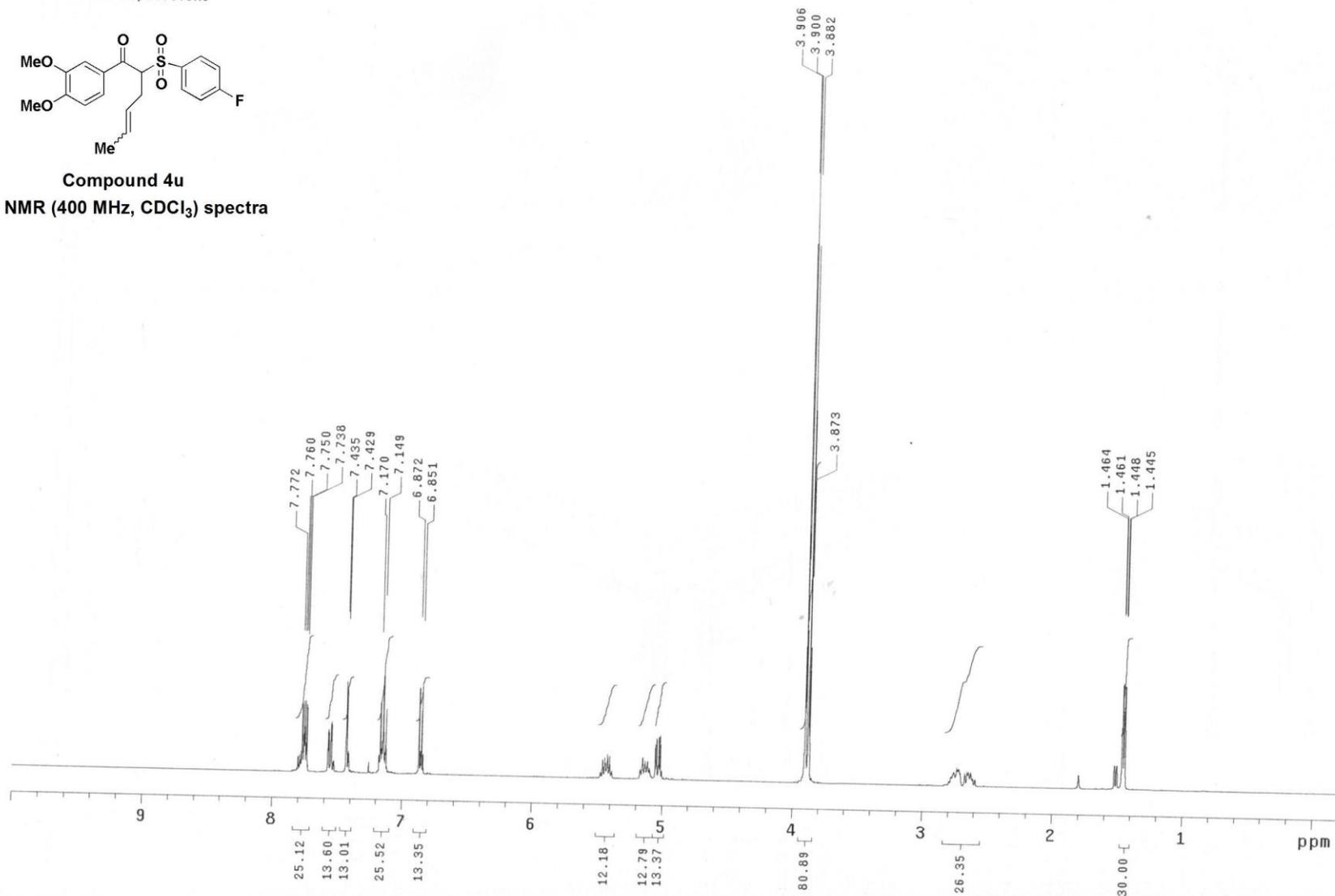
KSFCr

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Dec 24 2018
Solvent: CDCl₃
Ambient temperature
Total 32 repetitions



Compound 4u

¹H NMR (400 MHz, CDCl₃) spectra



Compound 4u (¹³C-NMR spectral data)

KSFCr

Pulse Sequence: s2pu1

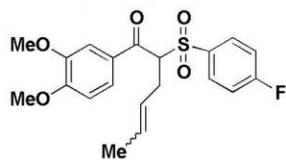
UNITYplus-400 "unity400"

Date: Dec 24 2018

Solvent: CDCl₃

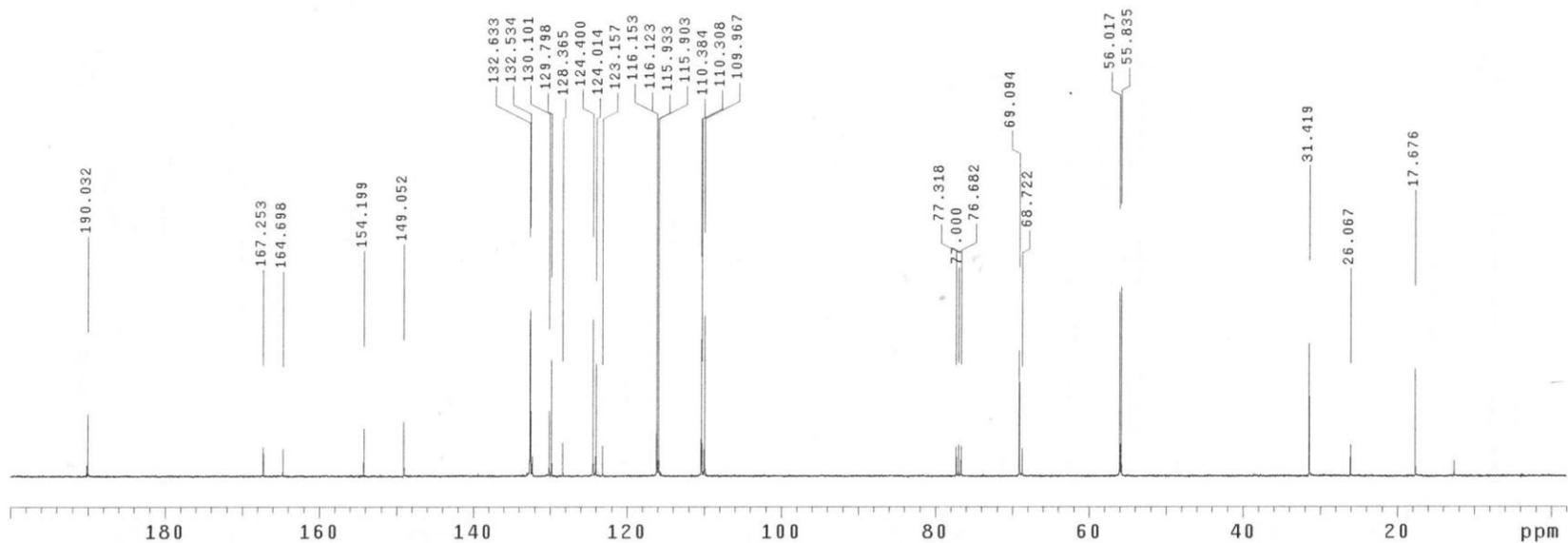
Ambient temperature

Total 800 repetitions



Compound 4u

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4v (¹H-NMR spectral data-1)

KSOMeCr

Pulse Sequence: s2pu1

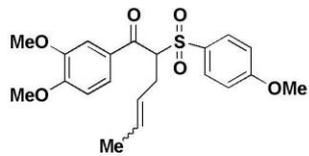
UNITYplus-400 "unity400"

Date: Jan 3 2019

Solvent: CDCl₃

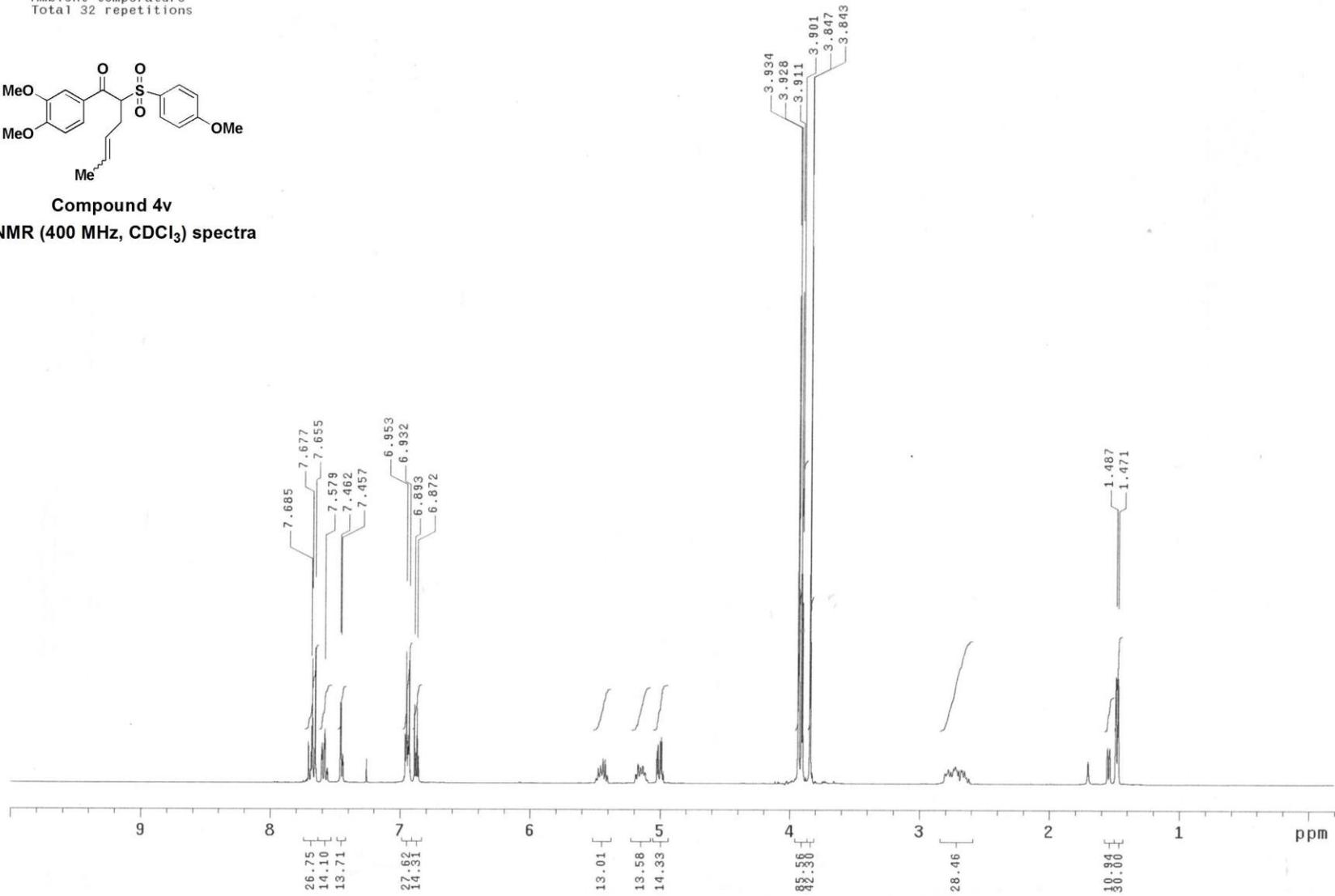
Ambient temperature

Total 32 repetitions

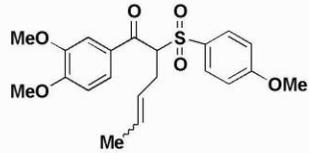


Compound 4v

¹H NMR (400 MHz, CDCl₃) spectra

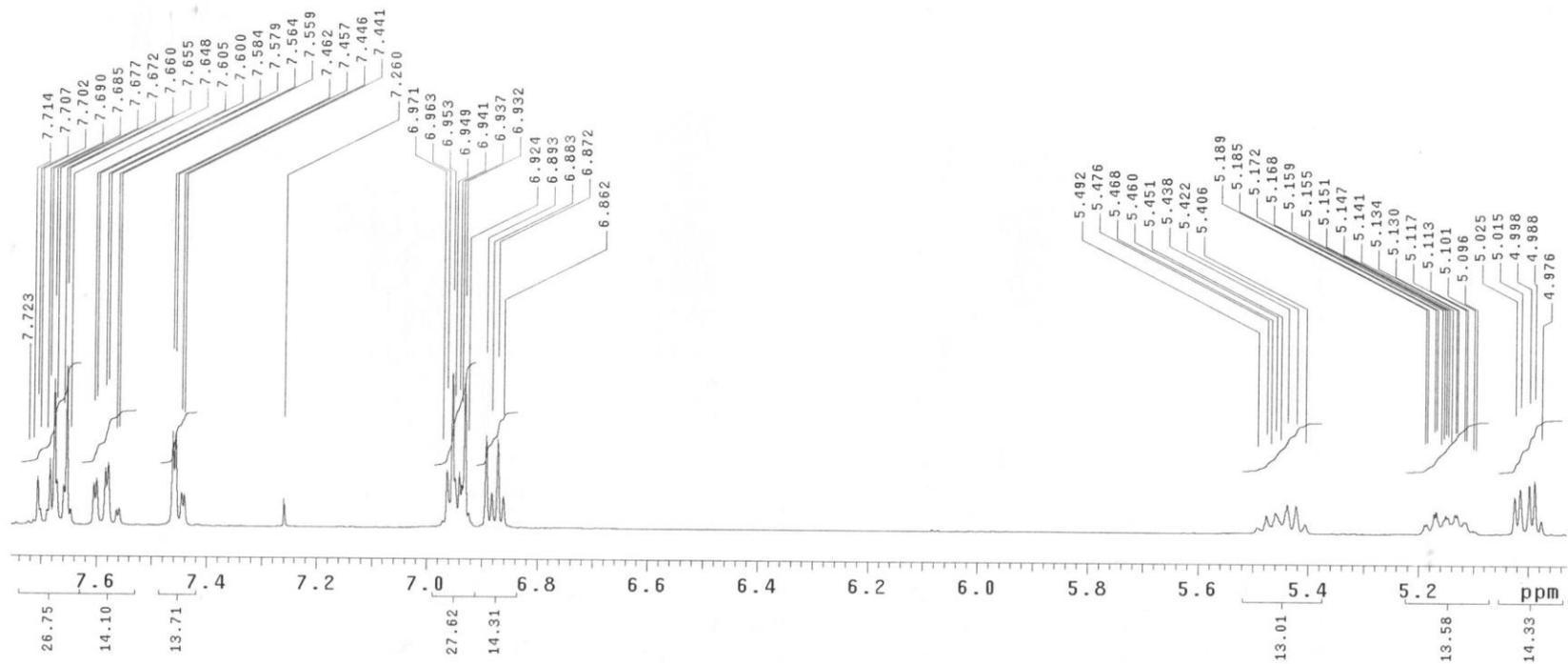


Compound 4v (¹H-NMR spectral data-2)



Compound 4v

¹H NMR (400 MHz, CDCl₃) spectra



Compound 4v (¹³C-NMR spectral data)

KSOMeCr

Pulse Sequence: s2pu1

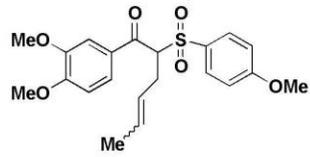
UNITYplus-400 "unity400"

Date: Jan 3 2019

Solvent: CDCl₃

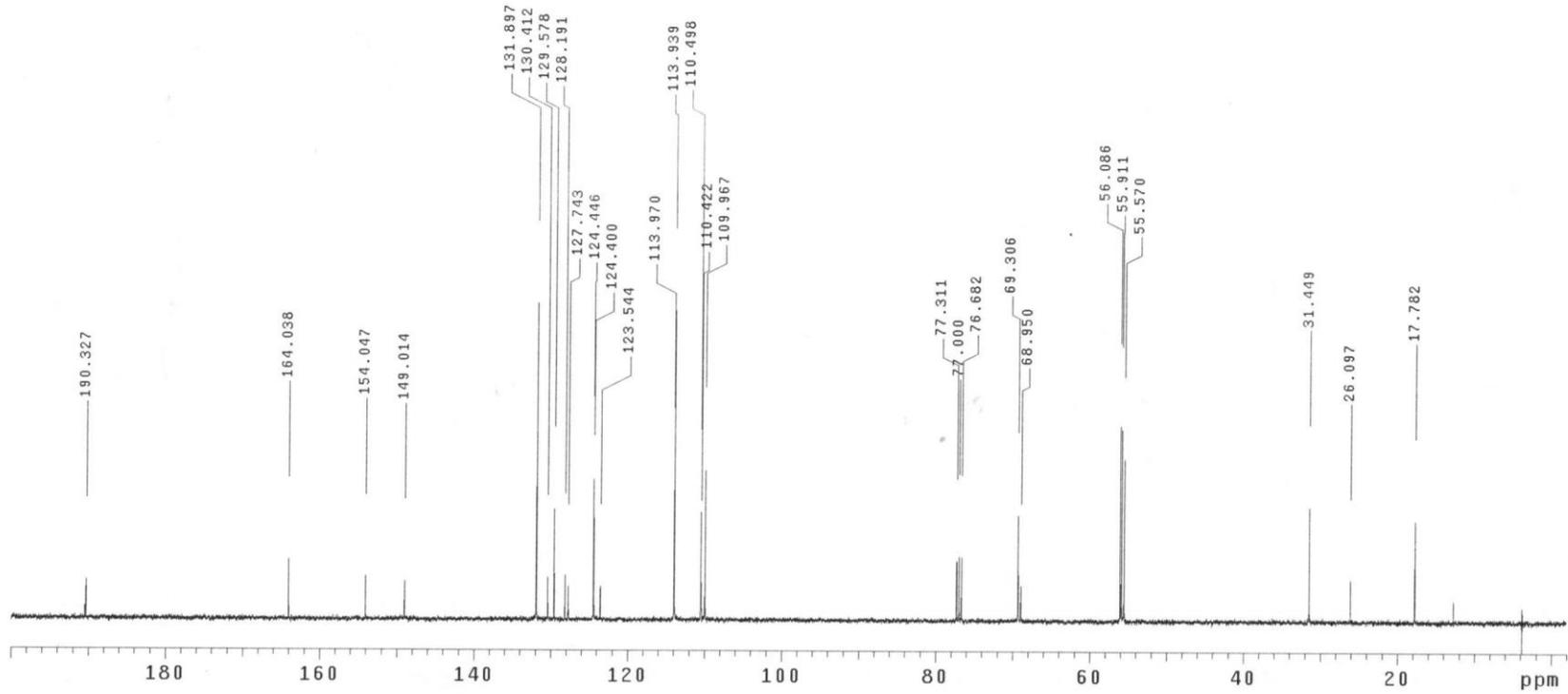
Ambient temperature

Total 528 repetitions



Compound 4v

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4w (¹H-NMR spectral data-1)

KSPHbUCr

Pulse Sequence: s2pu1

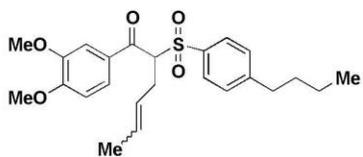
UNITYplus-400 "unity400"

Date: Jan 3 2019

Solvent: CDCl₃

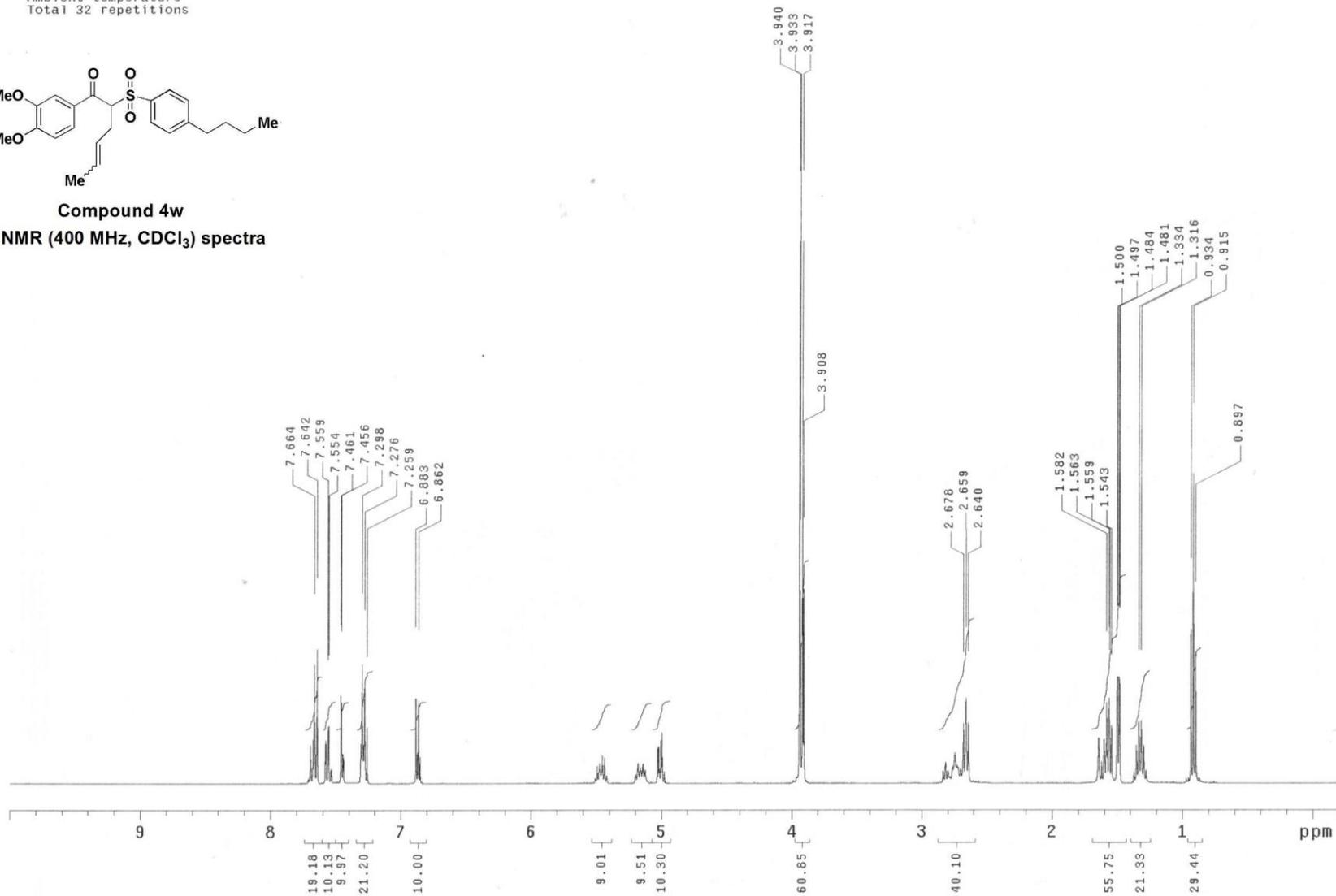
Ambient temperature

Total 32 repetitions

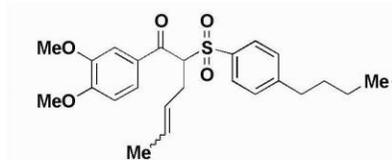


Compound 4w

¹H NMR (400 MHz, CDCl₃) spectra

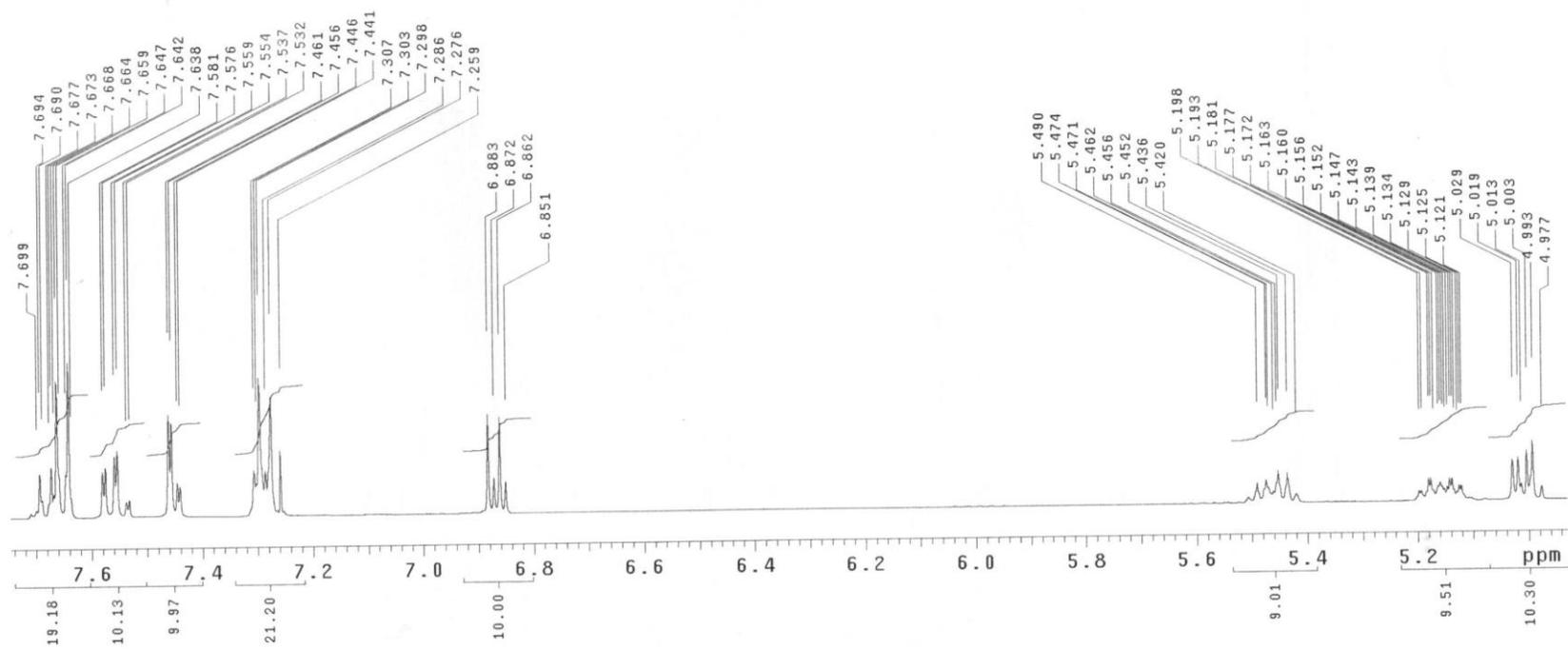


Compound 4w (¹H-NMR spectral data-2)



Compound 4w

¹H NMR (400 MHz, CDCl₃) spectra



Compound 4w (¹³C-NMR spectral data)

KSPHbuCr

Pulse Sequence: s2pu1

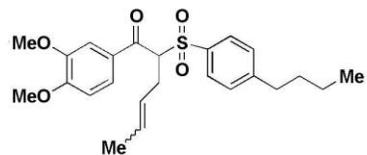
UNITYplus-400 "unity400"

Date: Jan 3 2019

Solvent: CDCl₃

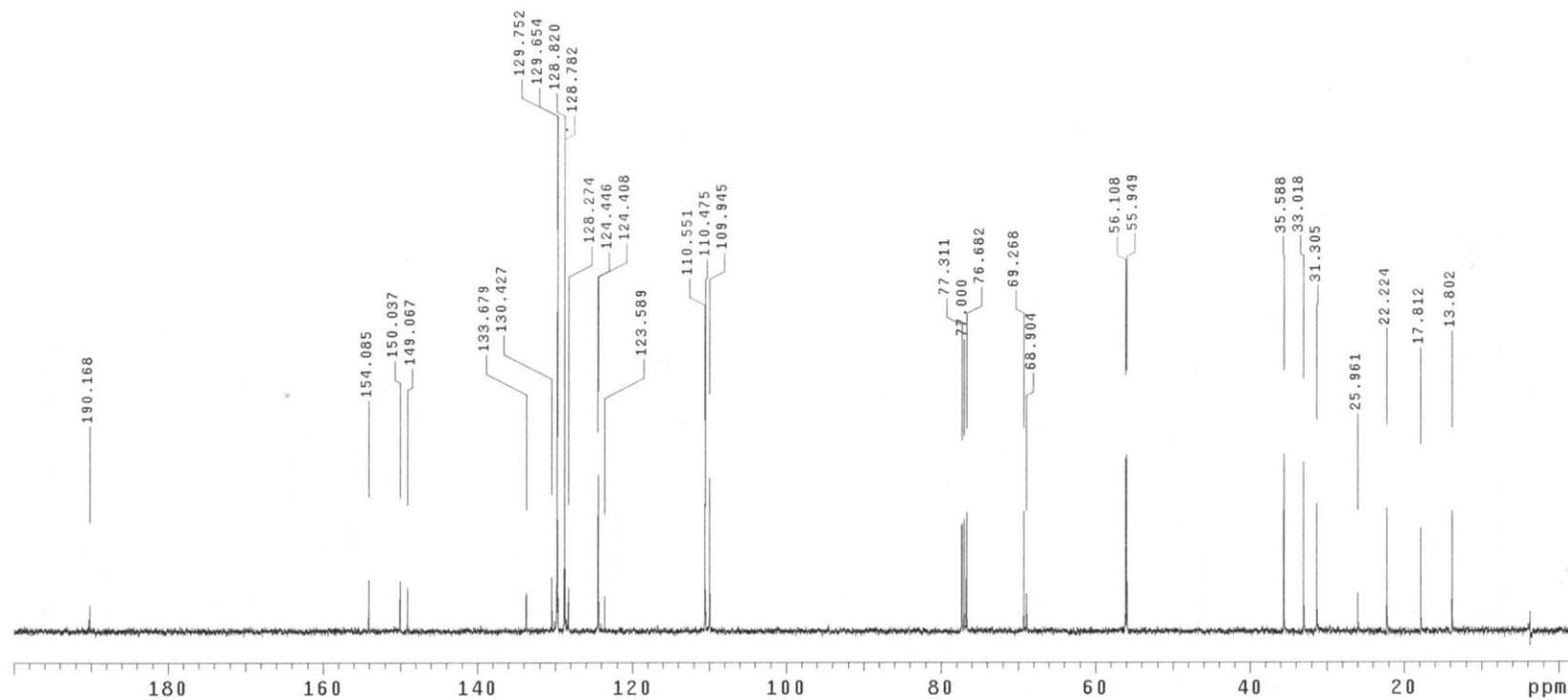
Ambient temperature

Total 1248 repetitions



Compound 4w

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4x (¹H-NMR spectral data-1)

KSTsPr

Pulse Sequence: s2pu1

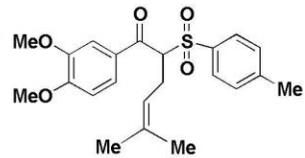
UNITYplus-400 "unity400"

Date: Jan 9 2019

Solvent: CDCl₃

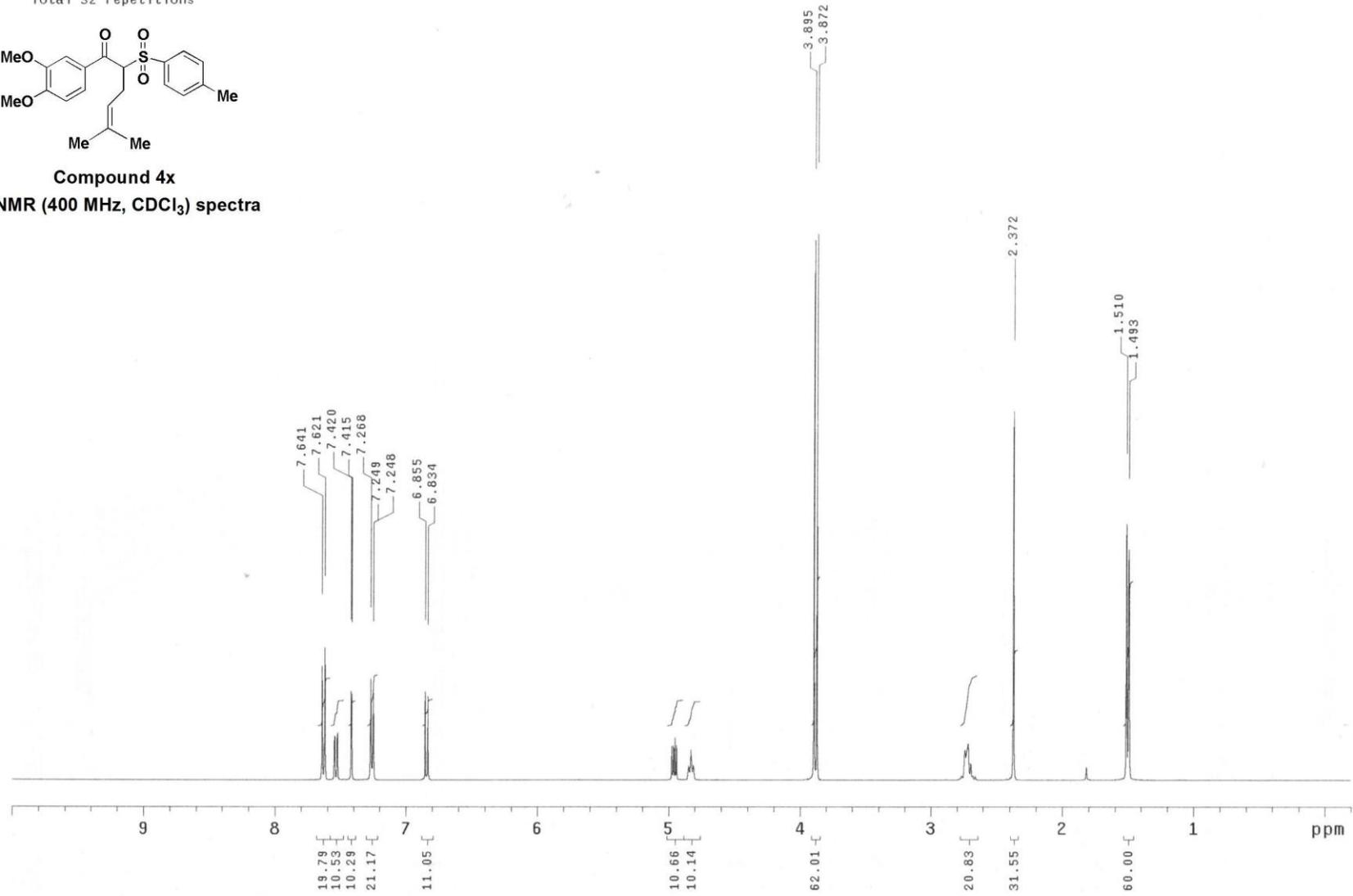
Ambient temperature

Total 32 repetitions

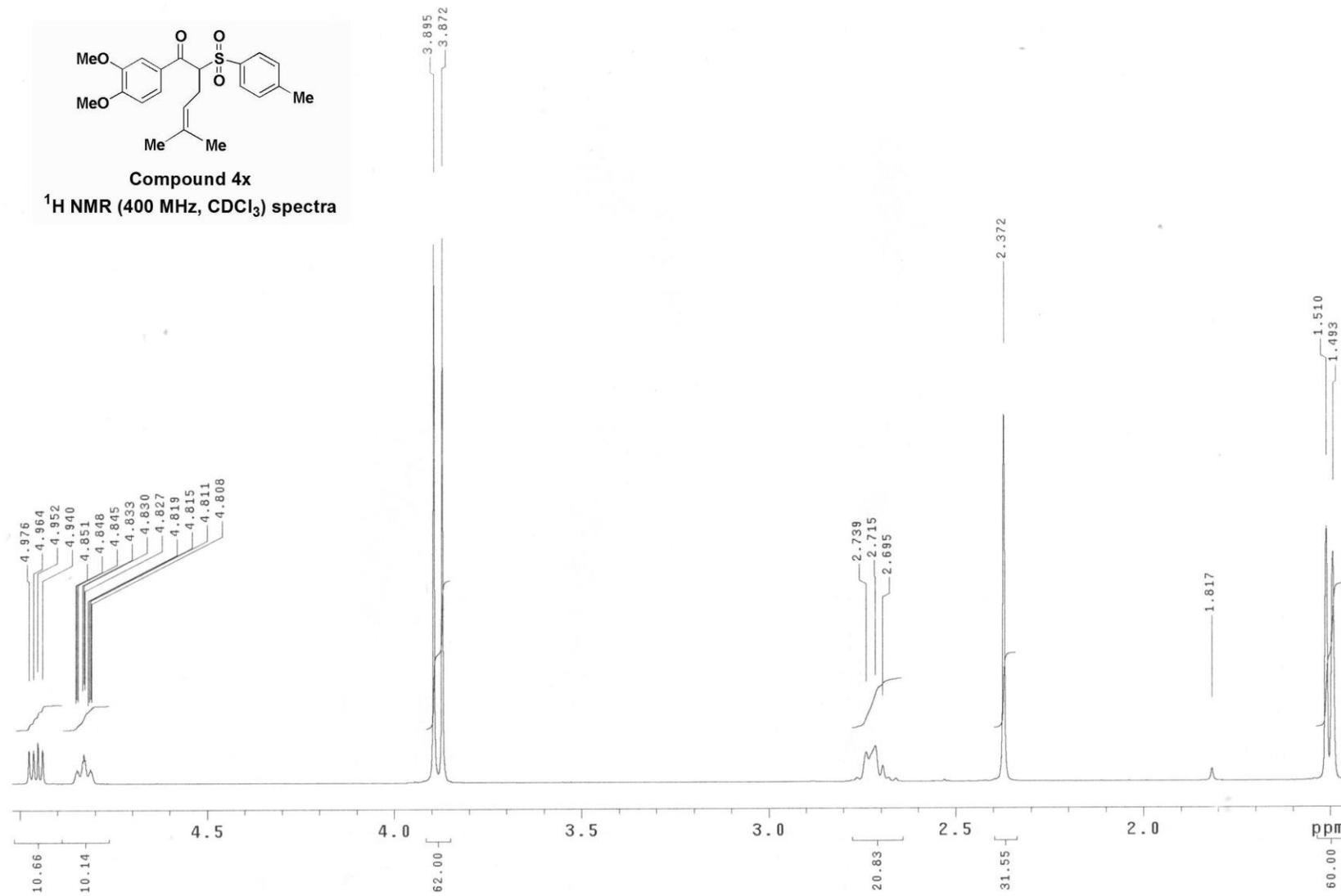


Compound 4x

¹H NMR (400 MHz, CDCl₃) spectra



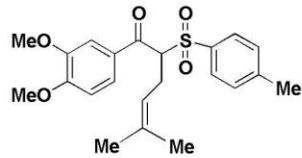
Compound 4x (¹H-NMR spectral data-2)



Compound 4x (¹³C-NMR spectral data)

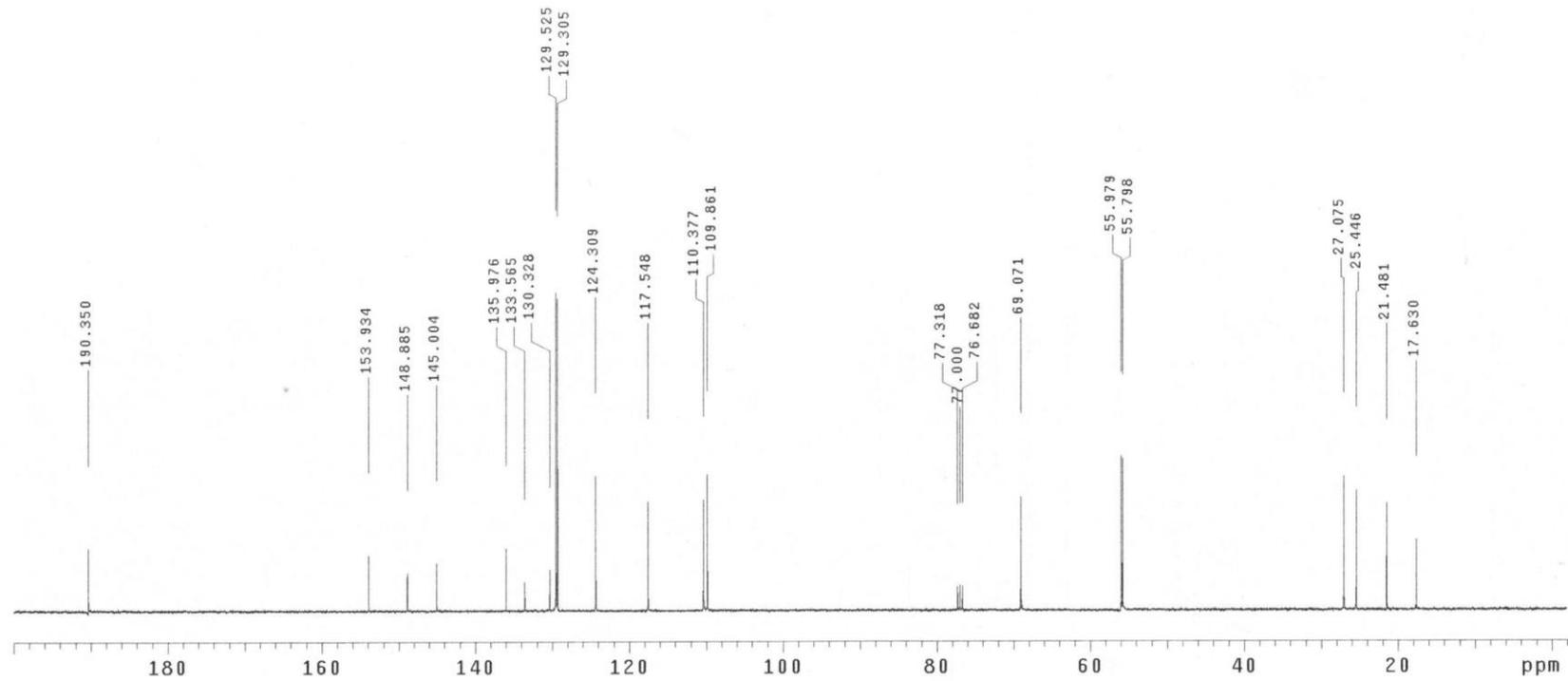
KSTsPr

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Jan 9 2019
Solvent: CDCl₃
Ambient temperature
Total 336 repetitions



Compound 4x

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4y (¹H-NMR spectral data-1)

KS4y

Pulse Sequence: s2pu1

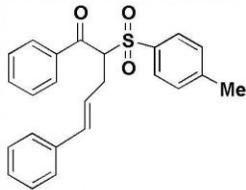
UNITYplus-400 "unity400"

Date: May 4 2020

Solvent: CDCl₃

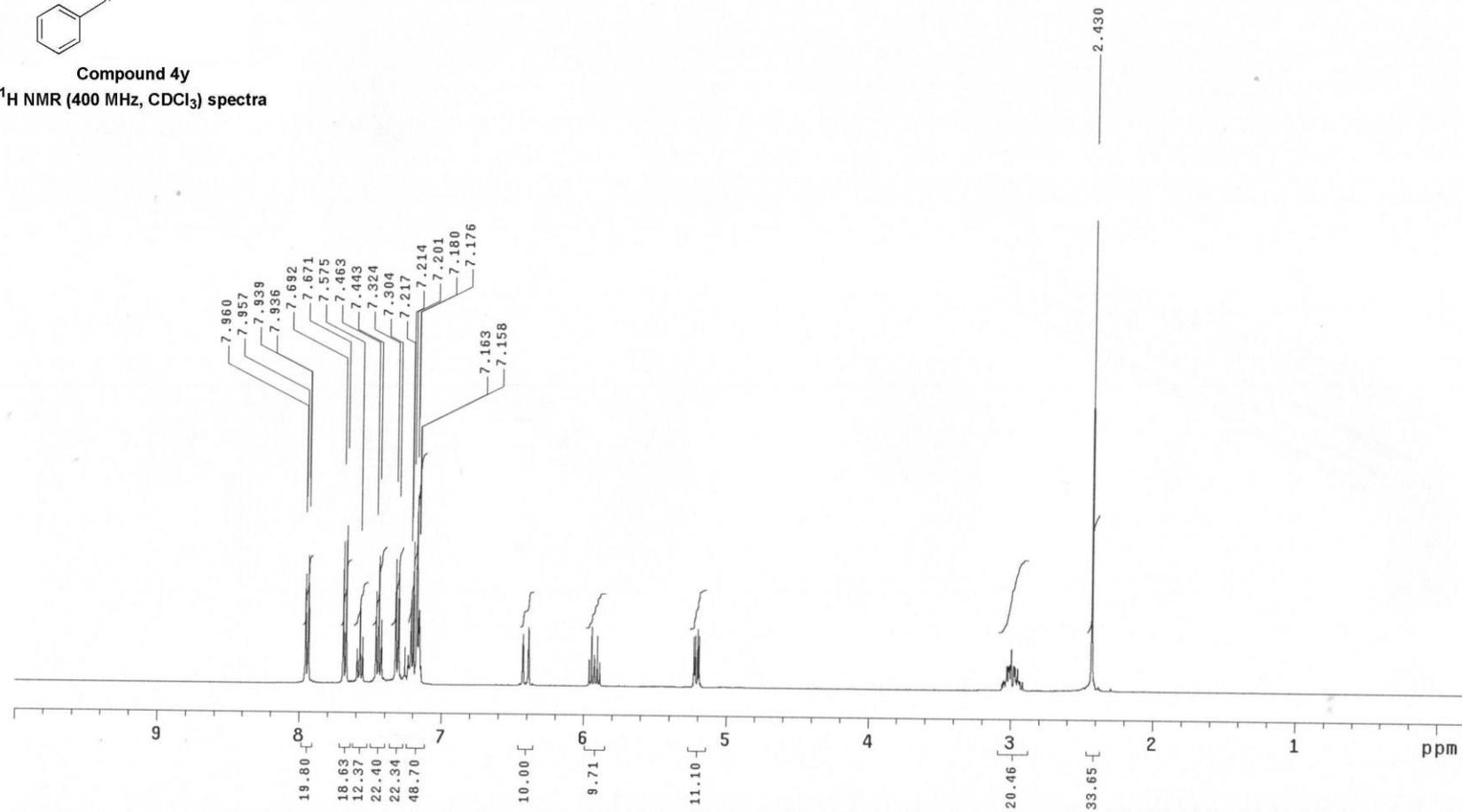
Ambient temperature

Total 32 repetitions

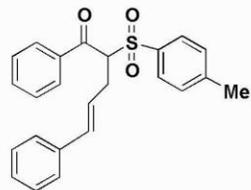


Compound 4y

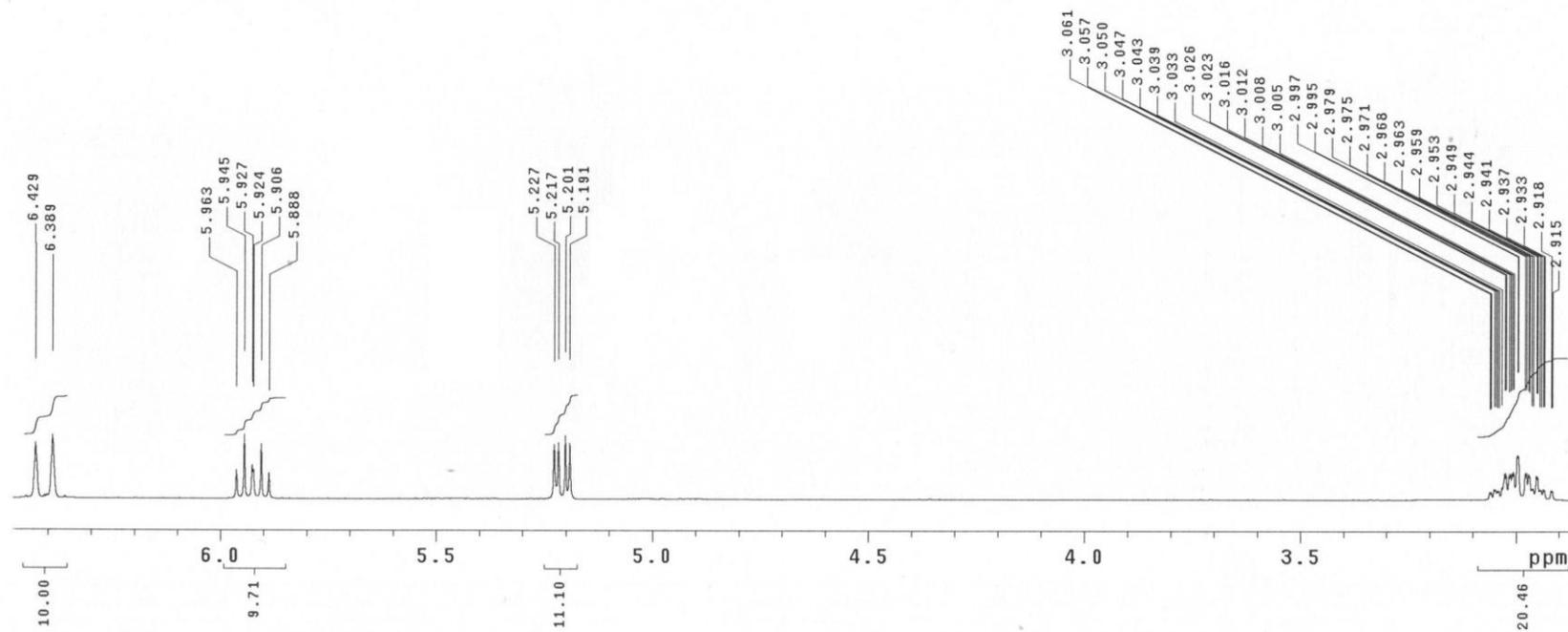
¹H NMR (400 MHz, CDCl₃) spectra



Compound 4y (¹H-NMR spectral data-2)



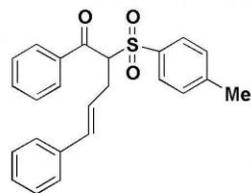
Compound 4y
¹H NMR (400 MHz, CDCl₃) spectra



Compound 4y (¹³C-NMR spectral data)

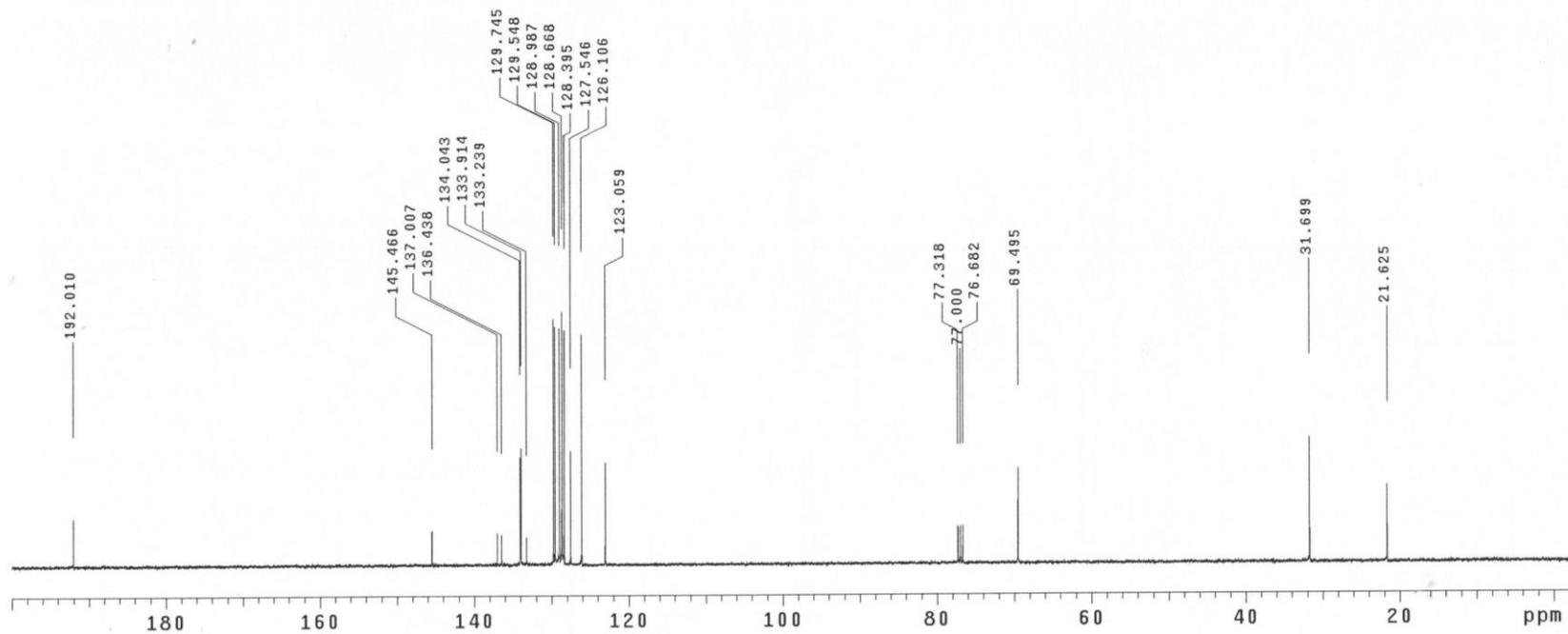
KS4y

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: May 4 2020
Solvent: CDCl₃
Ambient temperature
Total 704 repetitions



Compound 4y

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 5a (¹H-NMR spectral data-1)

KSTSCrB

Pulse Sequence: s2pu1

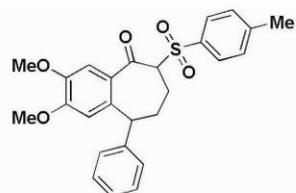
UNITYplus-400 "unity400"

Date: Apr 17 2020

Solvent: CDCl₃

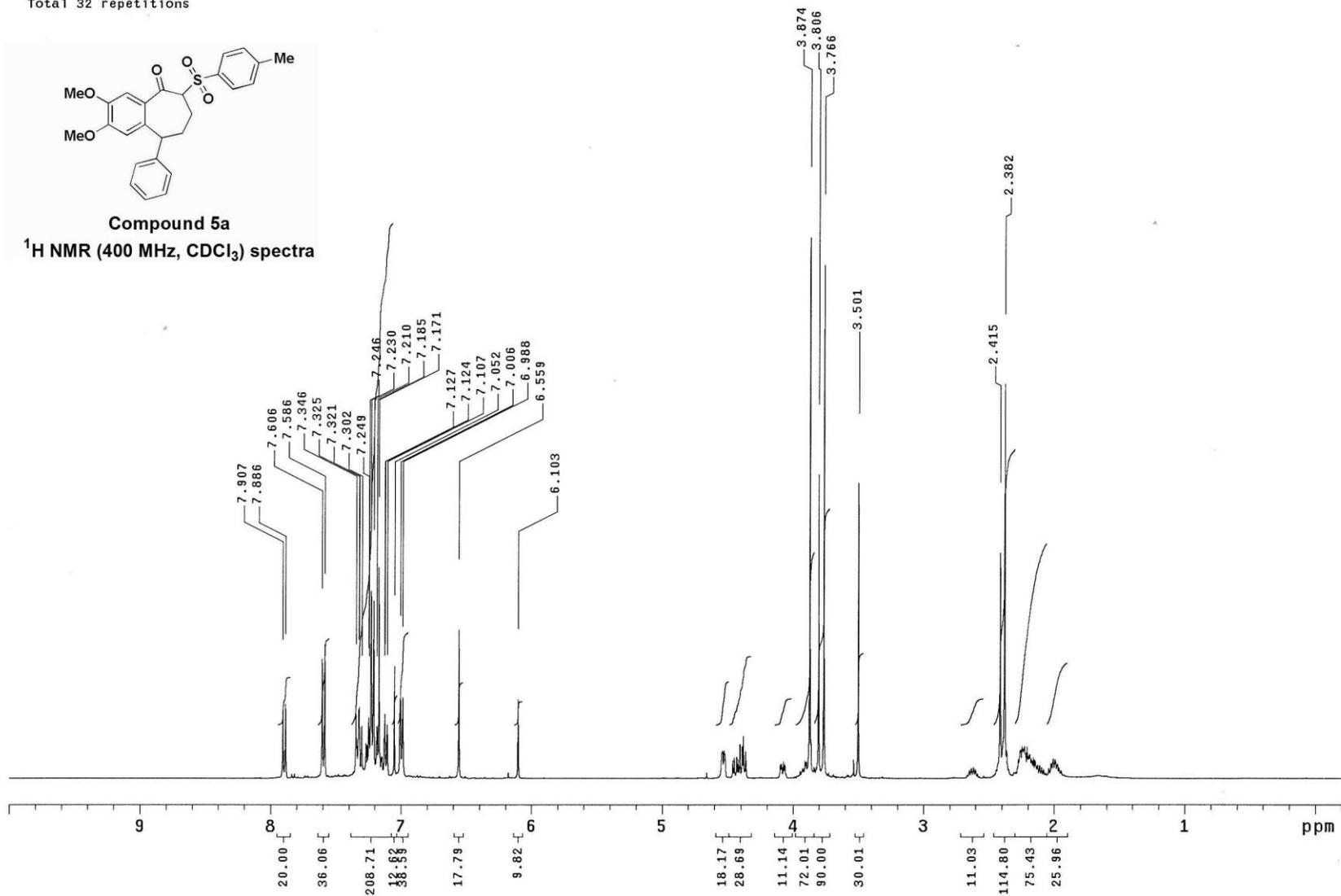
Ambient temperature

Total 32 repetitions

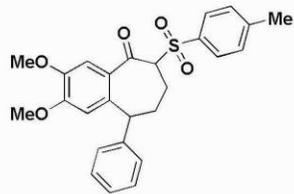


Compound 5a

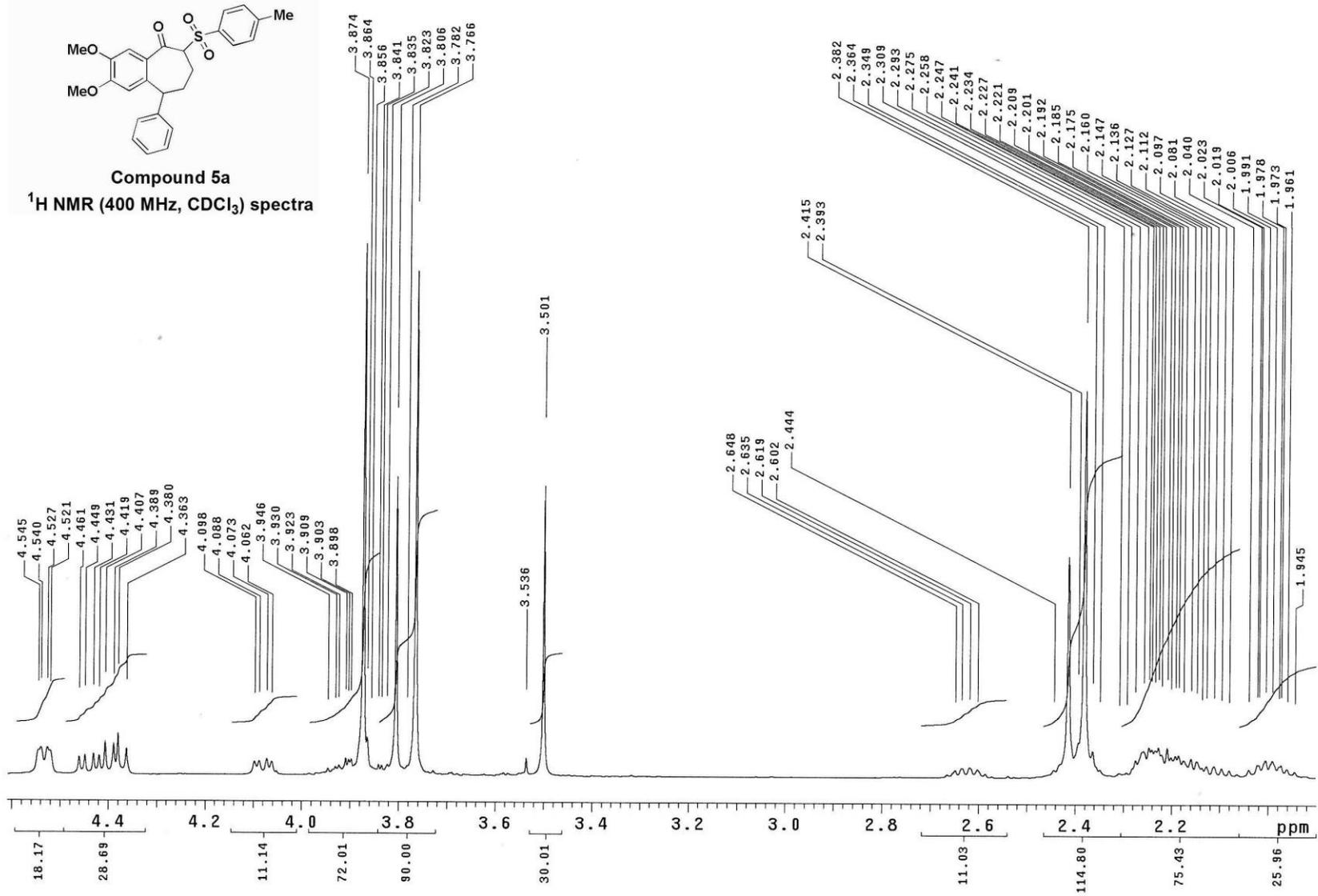
¹H NMR (400 MHz, CDCl₃) spectra



Compound 5a (¹H-NMR spectral data-2)



Compound 5a
¹H NMR (400 MHz, CDCl₃) spectra



Compound 5a (¹³C-NMR spectral data)

KSTSCrB

Pulse Sequence: s2pu1

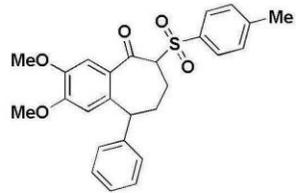
UNITYplus-400 "unity400"

Date: Apr 17 2020

Solvent: CDCl₃

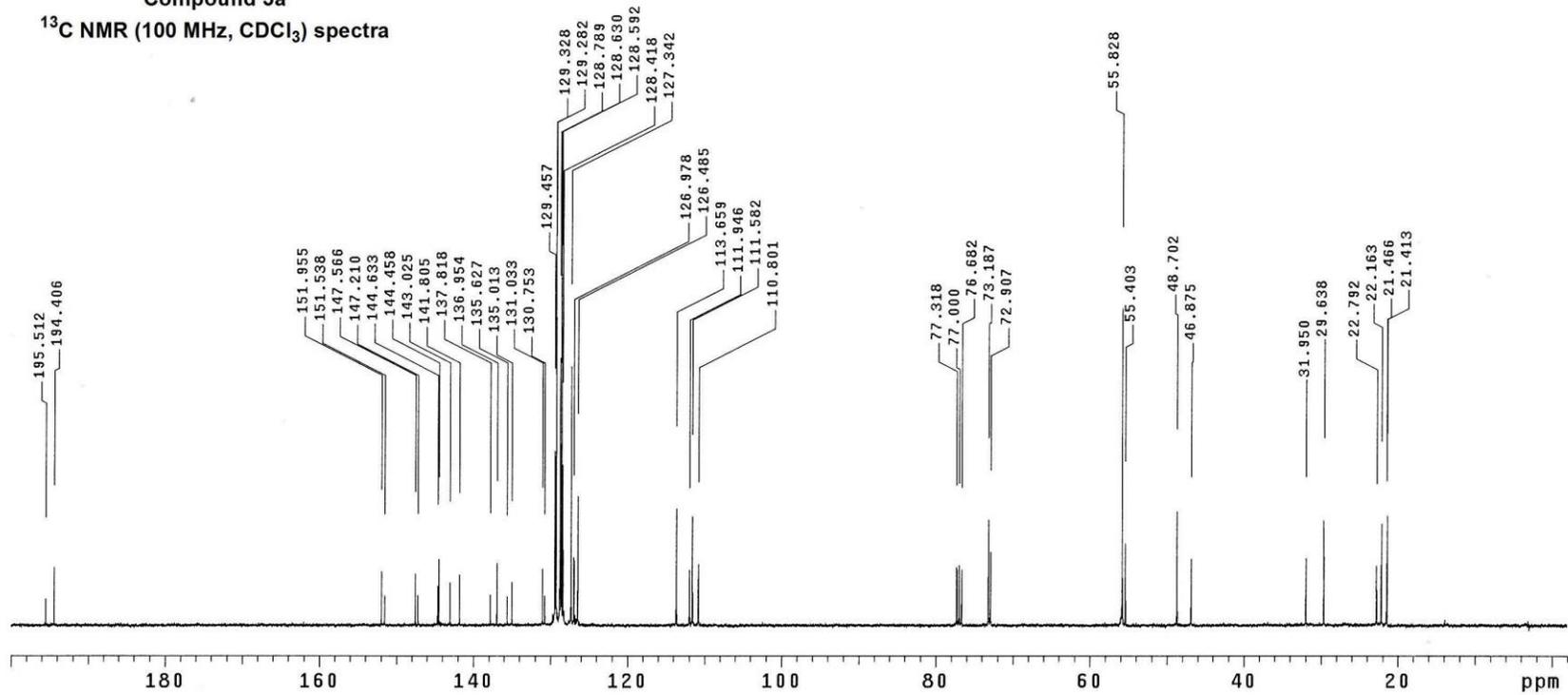
Ambient temperature

Total 800 repetitions



Compound 5a

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 5b (¹H-NMR spectral data-1)

KSE8CBF

Pulse Sequence: s2pu1

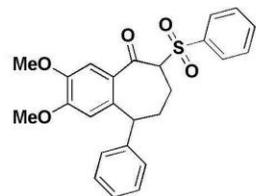
UNITYplus-400 "unity400"

Date: Sep 20 2018

Solvent: CDCl₃

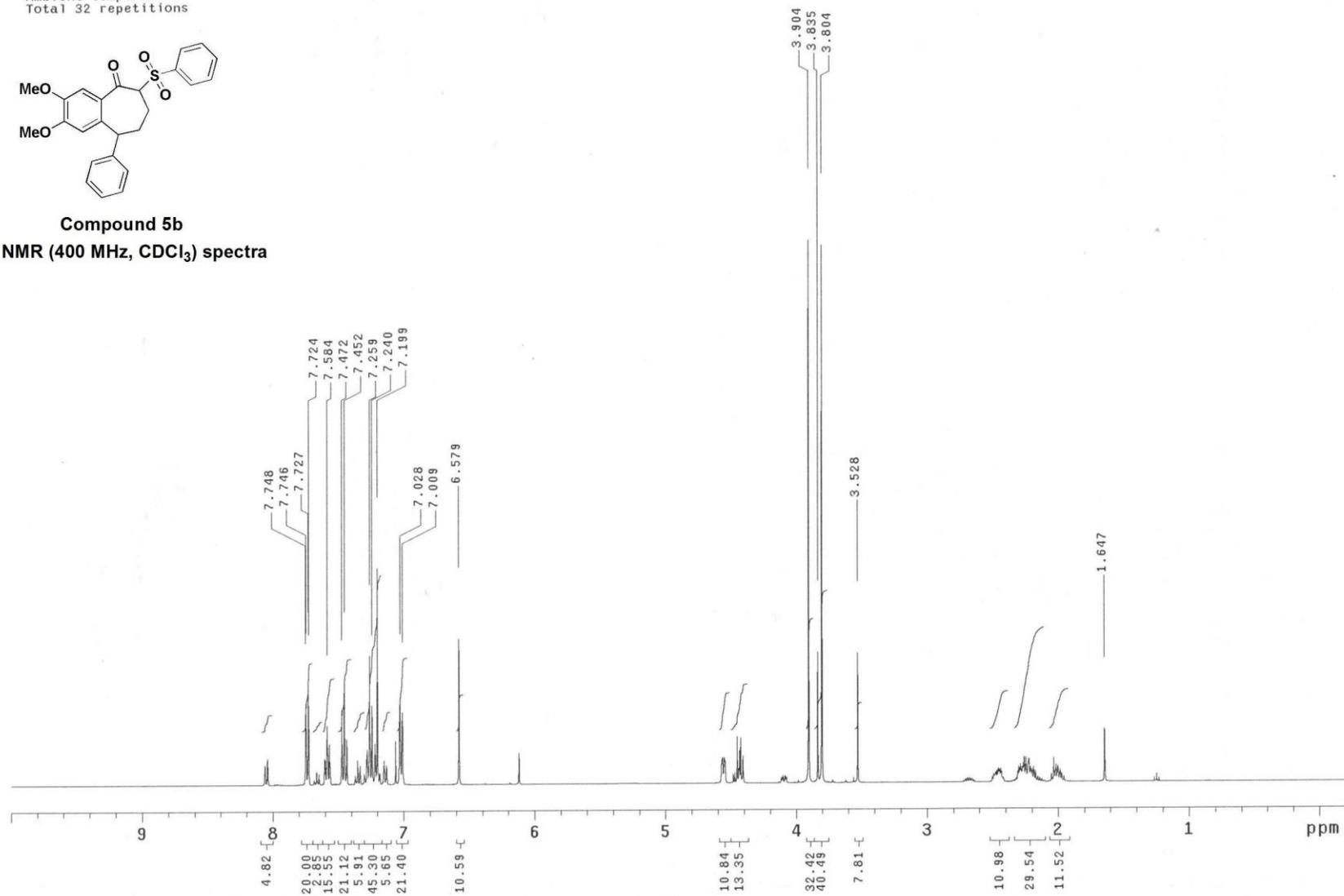
Ambient temperature

Total 32 repetitions

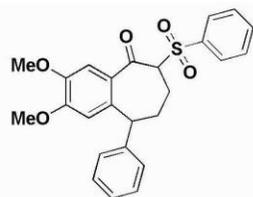


Compound 5b

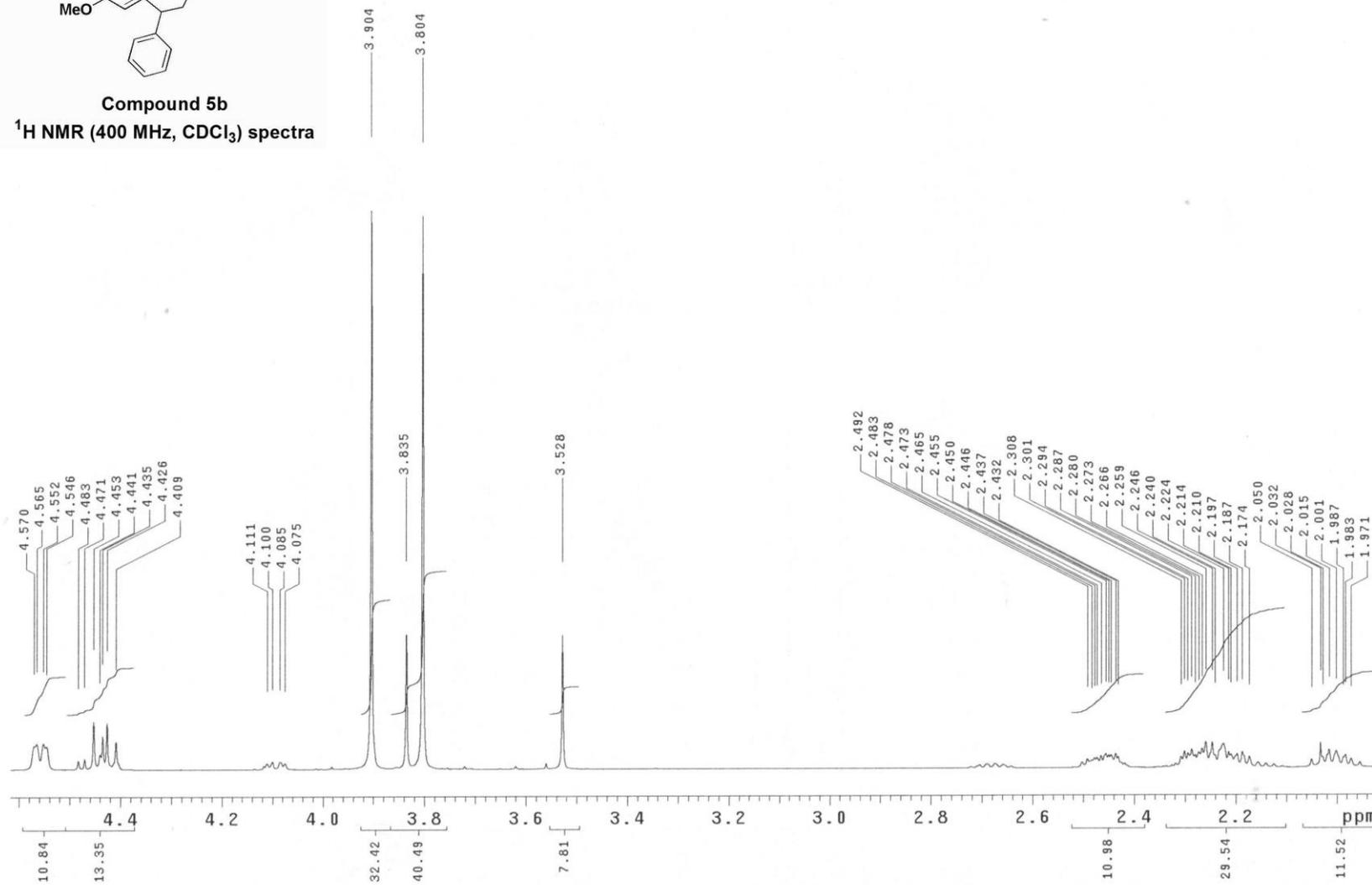
¹H NMR (400 MHz, CDCl₃) spectra



Compound 5b (¹H-NMR spectral data-2)



Compound 5b
¹H NMR (400 MHz, CDCl₃) spectra



Compound 5b (¹³C-NMR spectral data)

KSE8CBF

Pulse Sequence: s2pu1

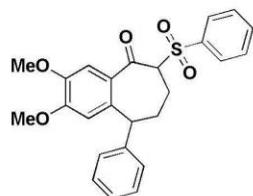
UNITYplus-400 "unity400"

Date: Sep 20 2018

Solvent: CDCl₃

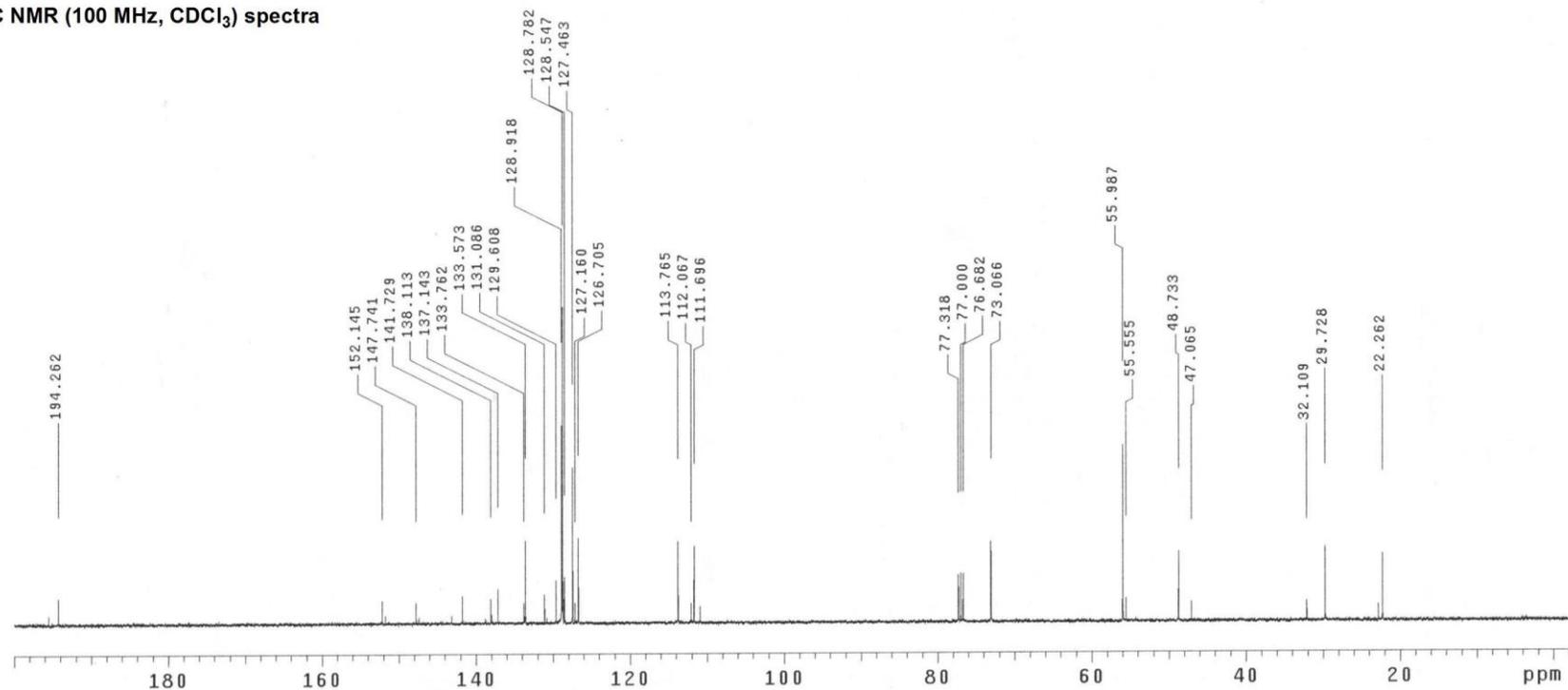
Ambient temperature

Total 640 repetitions



Compound 5b

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 5c (¹H-NMR spectral data-1)

KSSC

Pulse Sequence: s2pu1

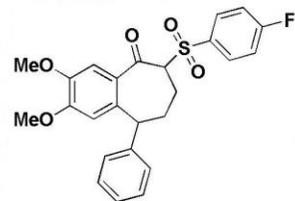
UNITYplus-400 "unity400"

Date: May 4 2020

Solvent: CDCl₃

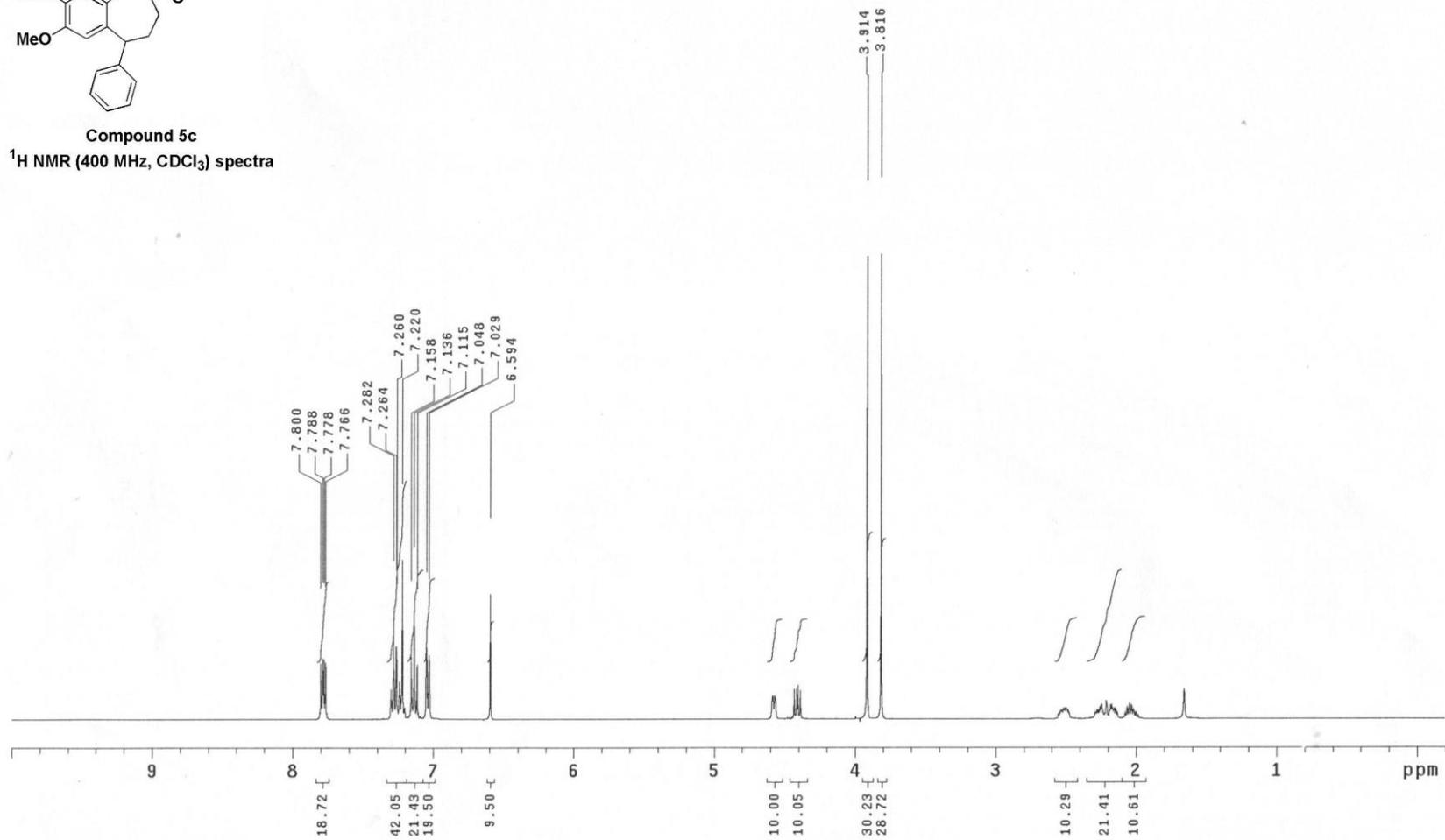
Ambient temperature

Total 32 repetitions

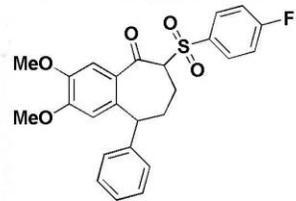


Compound 5c

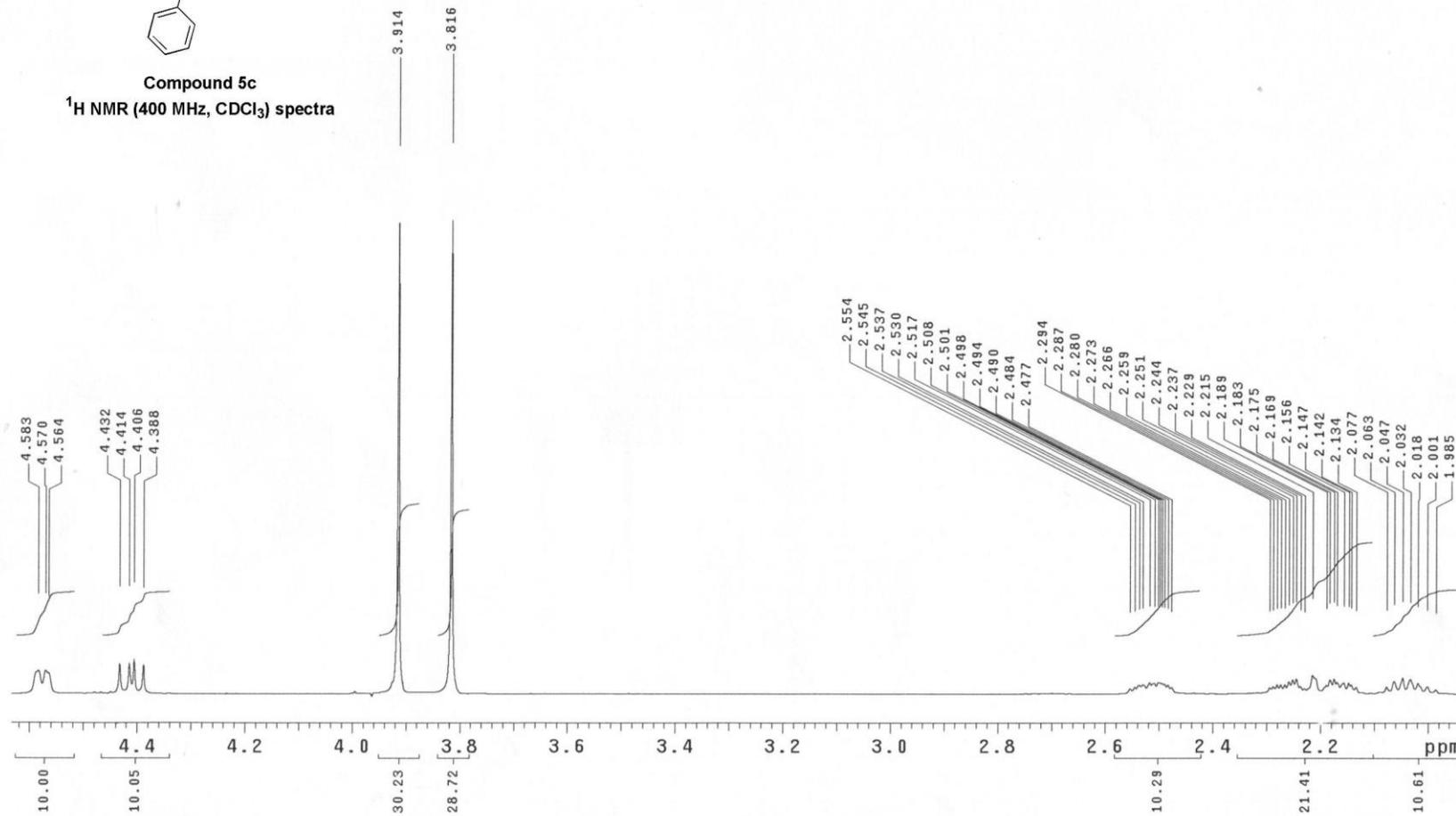
¹H NMR (400 MHz, CDCl₃) spectra



Compound 5c (¹H-NMR spectral data-2)



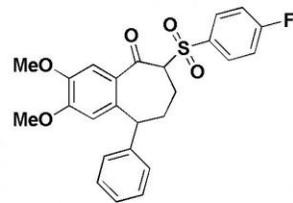
Compound 5c
¹H NMR (400 MHz, CDCl₃) spectra



Compound 5c (¹³C-NMR spectral data)

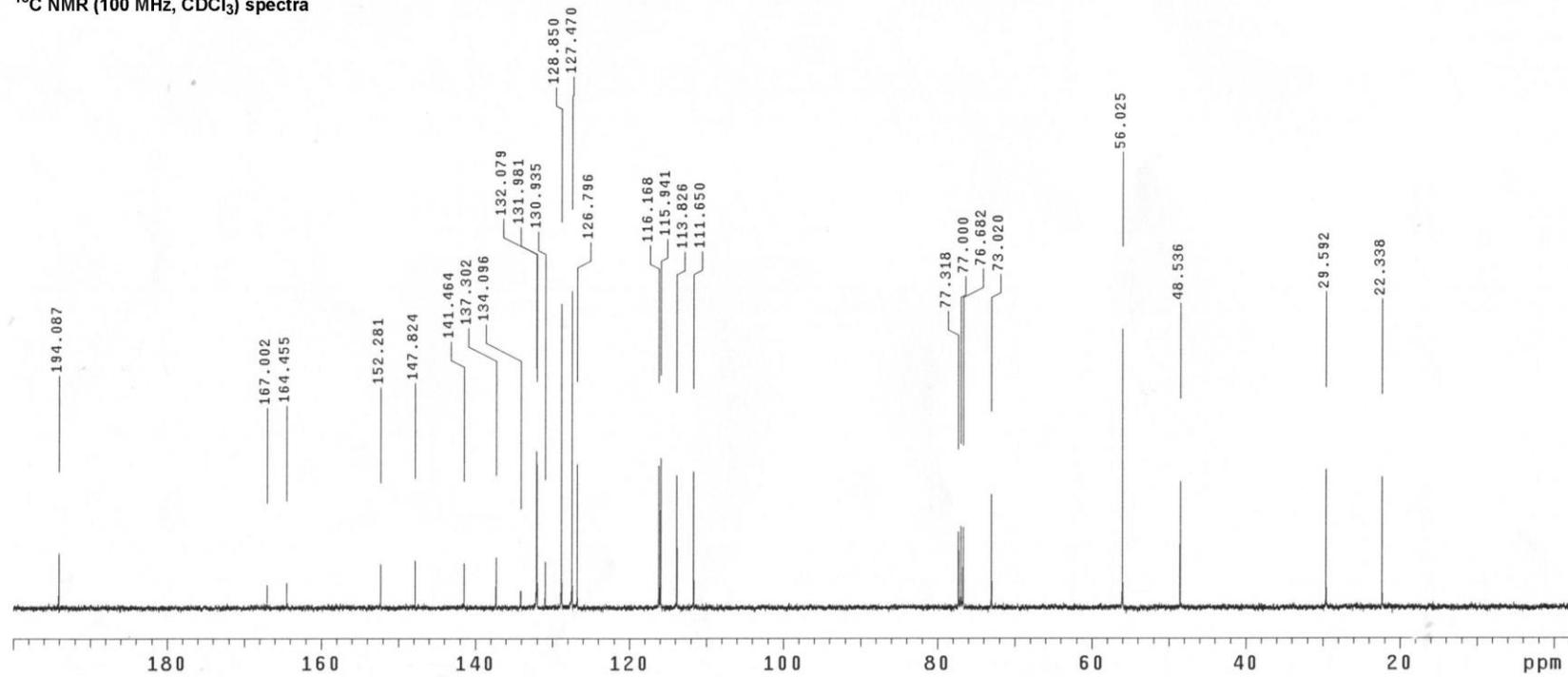
KS5C

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: May 4 2020
Solvent: CDCl₃
Ambient temperature
Total 1088 repetitions



Compound 5c

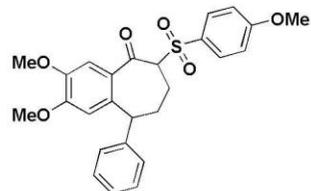
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 5d (¹H-NMR spectral data-1)

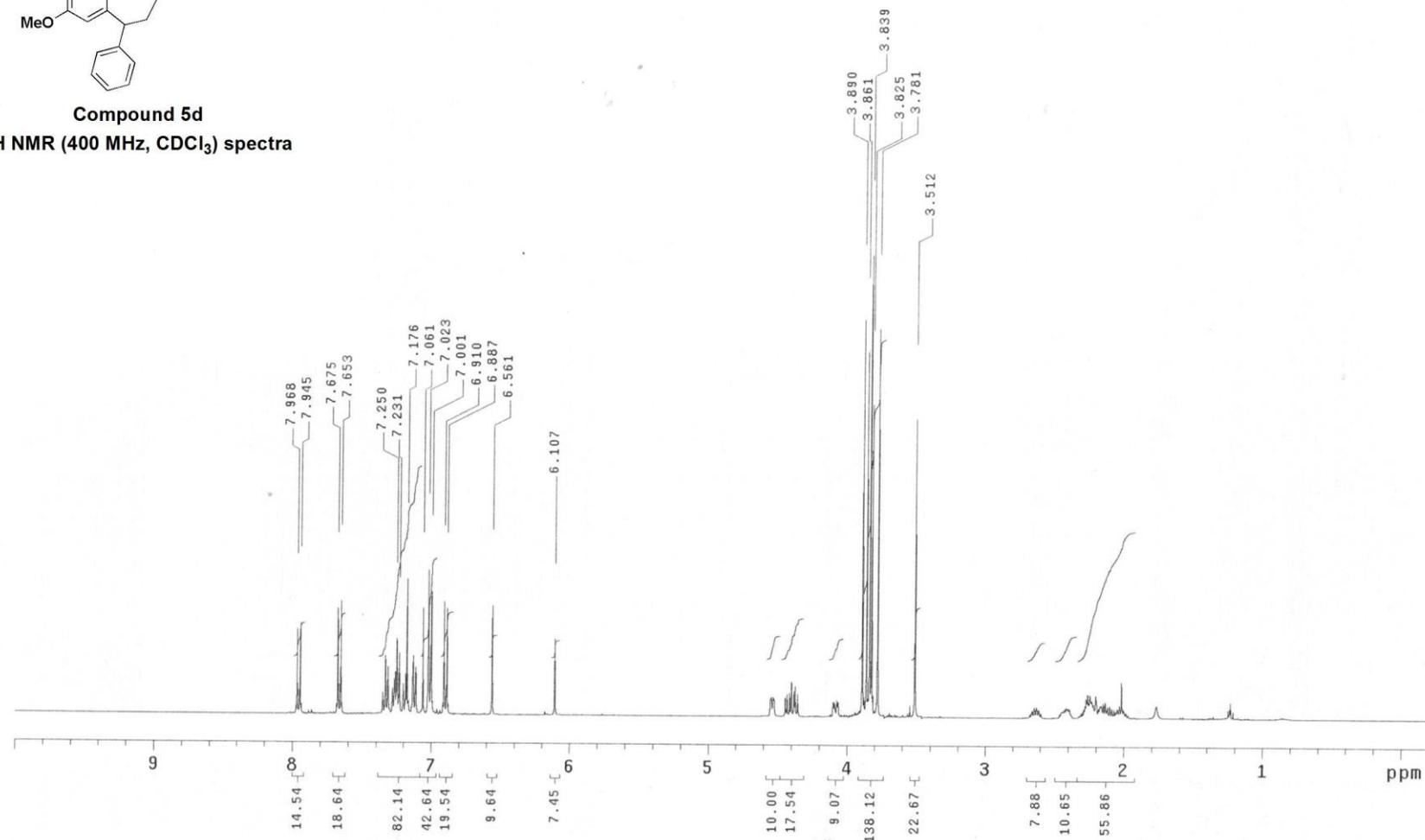
KSOMeCBF

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Dec 27 2018
Solvent: CDCl₃
Ambient temperature
Total 32 repetitions

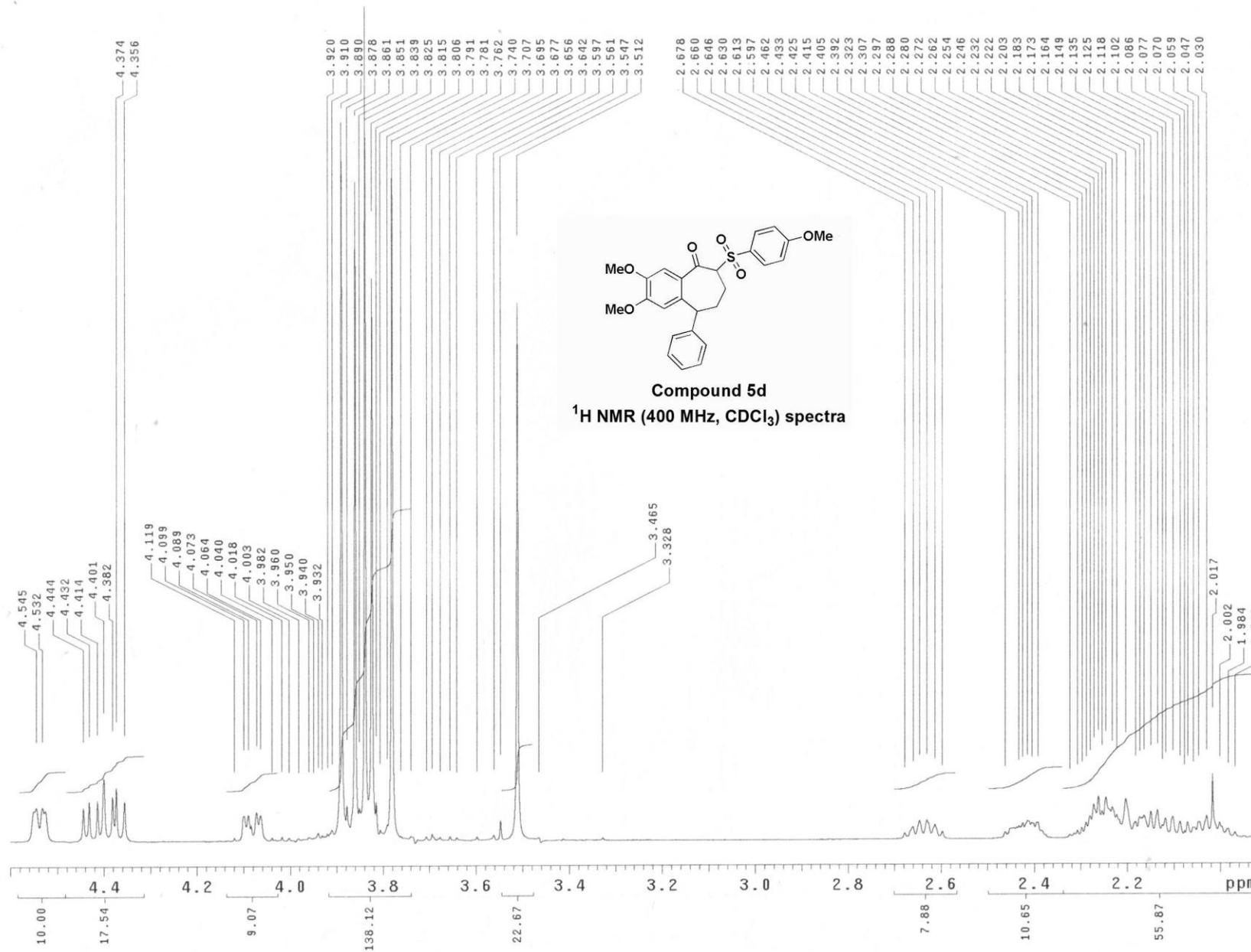


Compound 5d

¹H NMR (400 MHz, CDCl₃) spectra



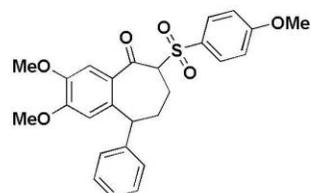
Compound 5d (¹H-NMR spectral data-2)



Compound 5d (¹³C-NMR spectral data)

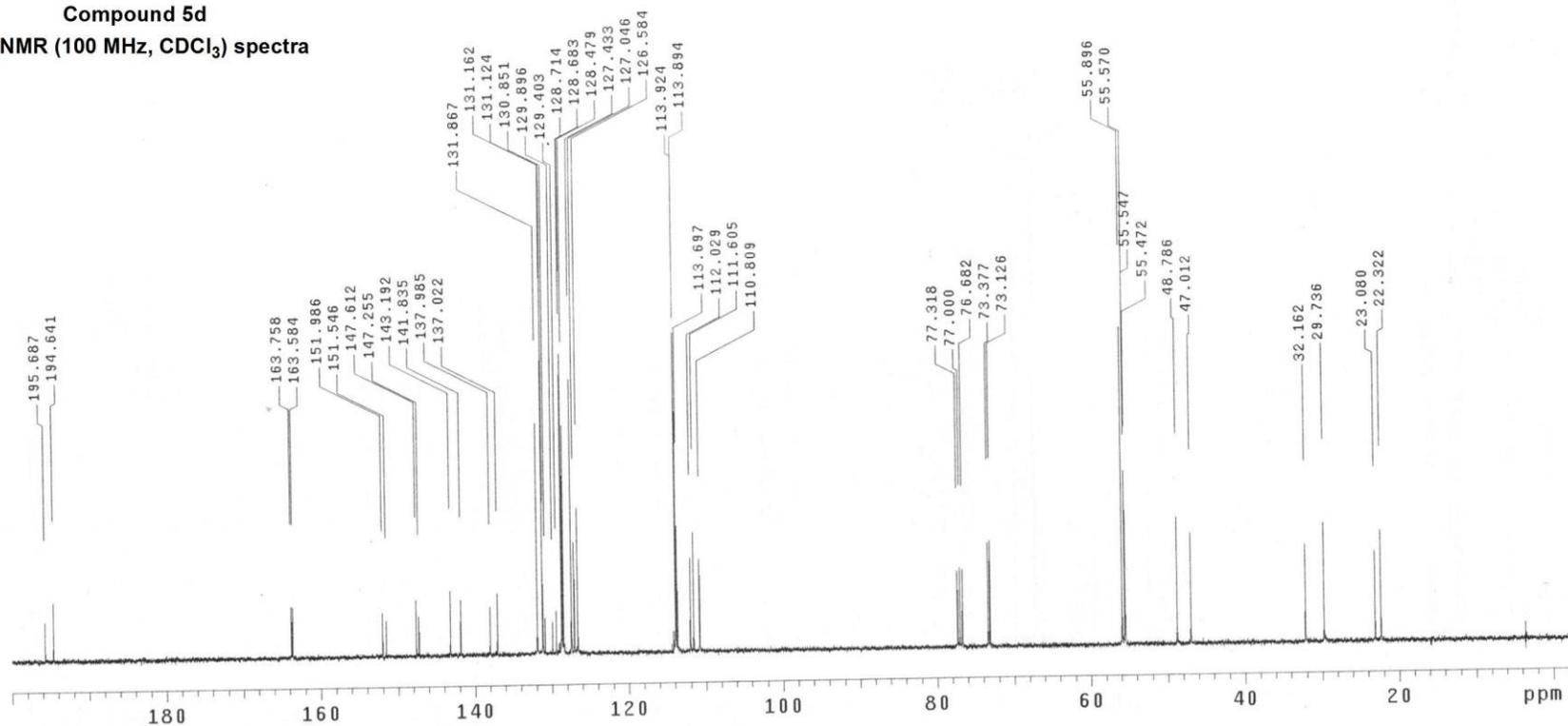
KS0MeCBF

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Dec 27 2018
Solvent: CDCl₃
Ambient temperature
Total 752 repetitions



Compound 5d

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 5e (¹H-NMR spectral data-1)

KSPHbuCBF

Pulse Sequence: s2pu1

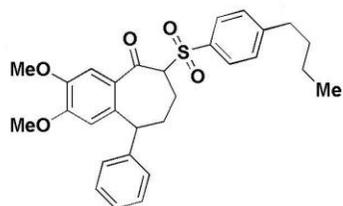
UNITYplus-400 "unity400"

Date: Jan 14 2019

Solvent: CDCl₃

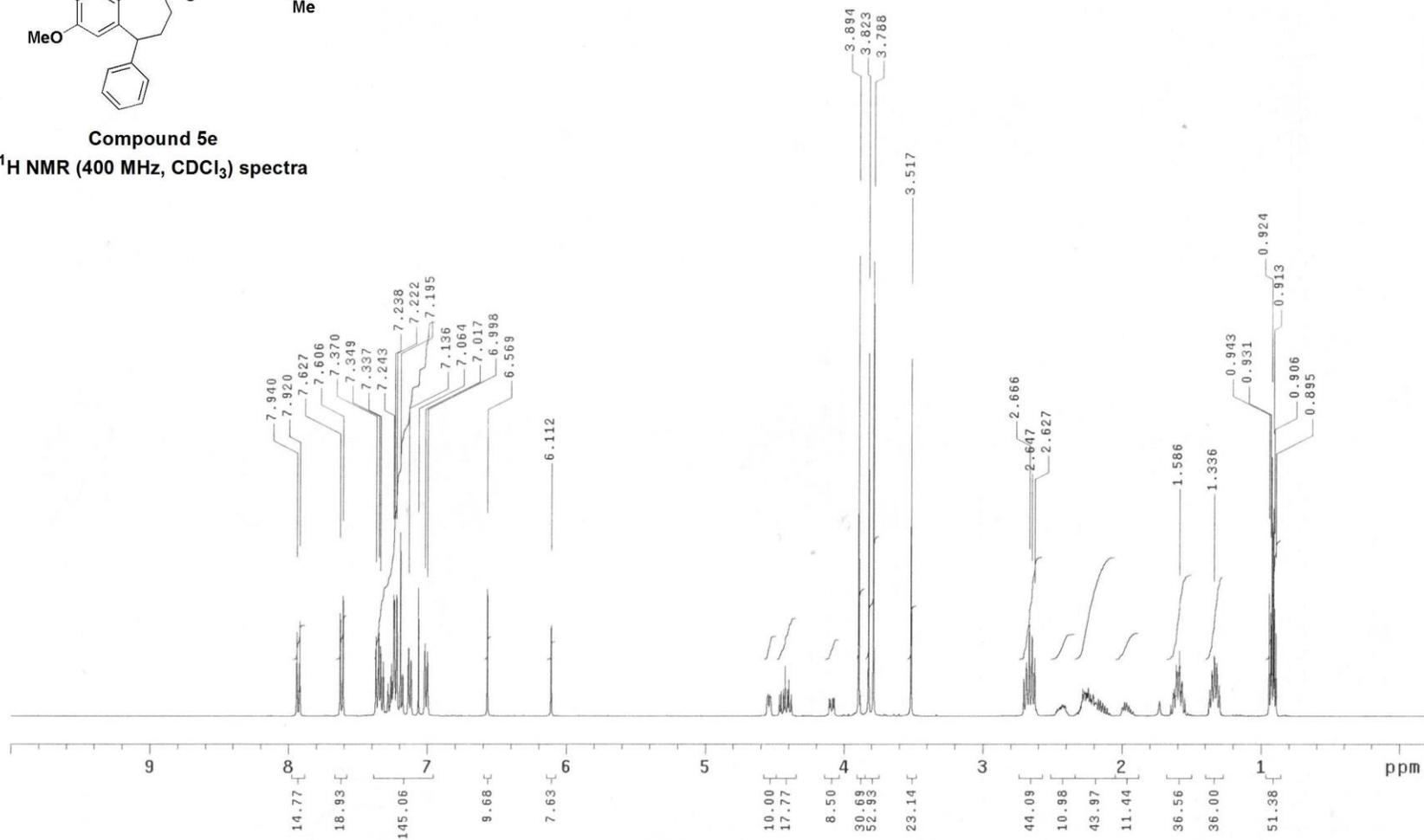
Ambient temperature

Total 32 repetitions

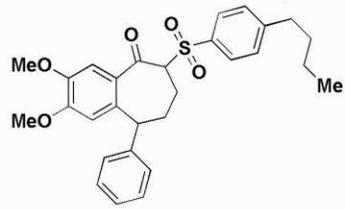


Compound 5e

¹H NMR (400 MHz, CDCl₃) spectra

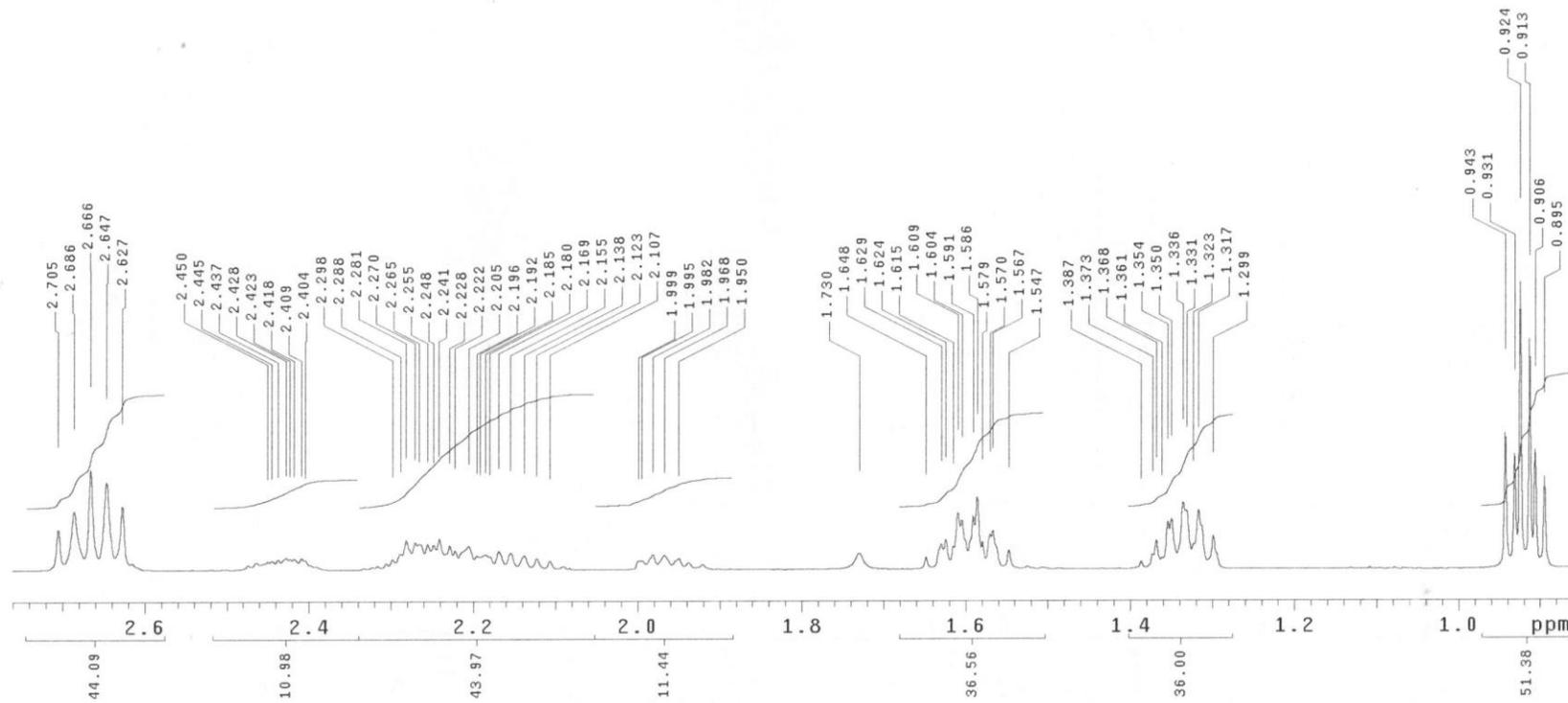


Compound 5e (¹H-NMR spectral data-2)

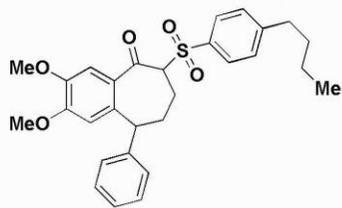


Compound 5e

¹H NMR (400 MHz, CDCl₃) spectra

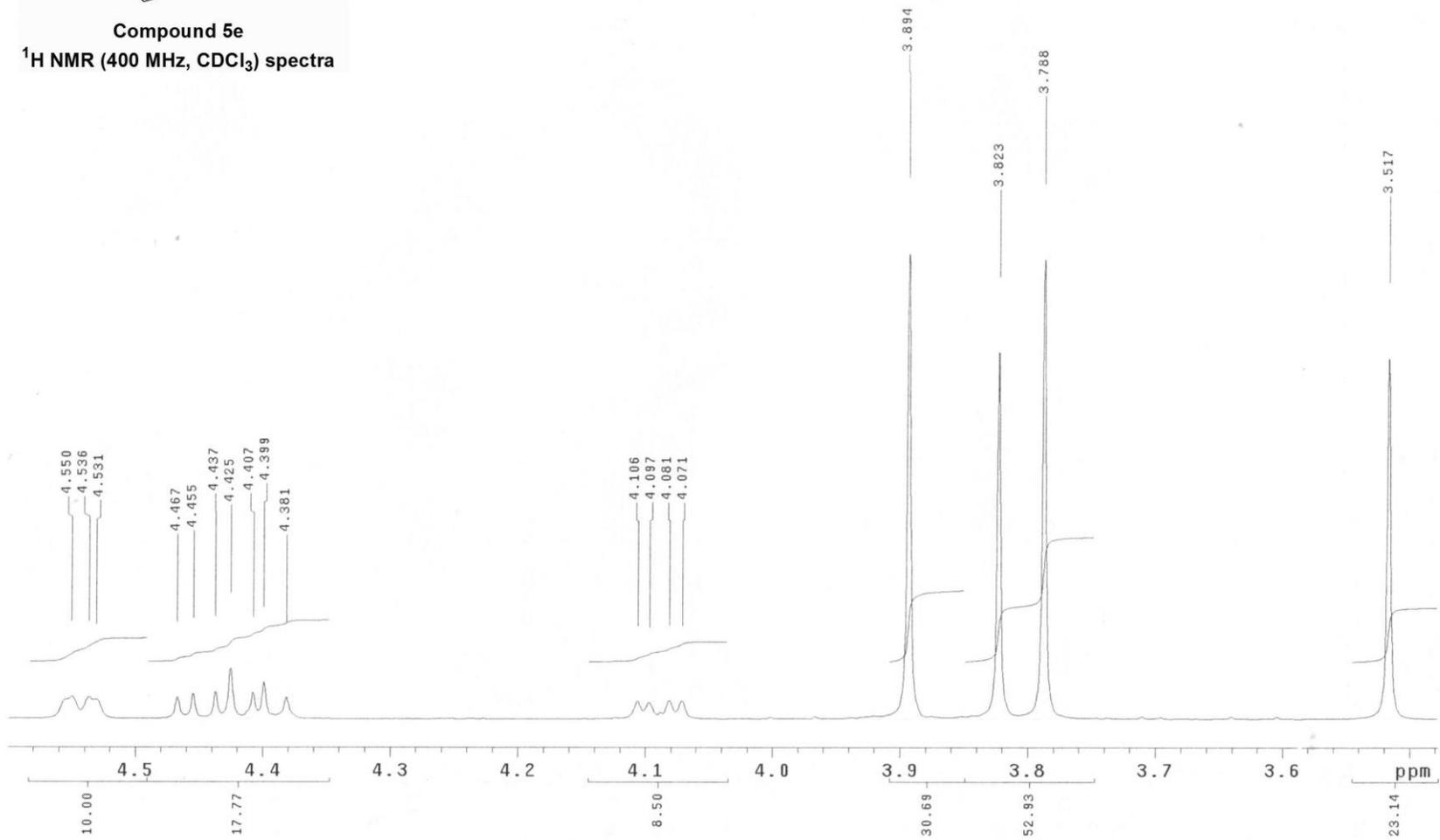


Compound 5e (¹H-NMR spectral data-3)



Compound 5e

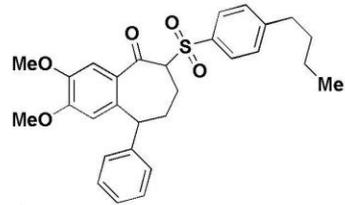
¹H NMR (400 MHz, CDCl₃) spectra



Compound 5e (¹³C-NMR spectral data)

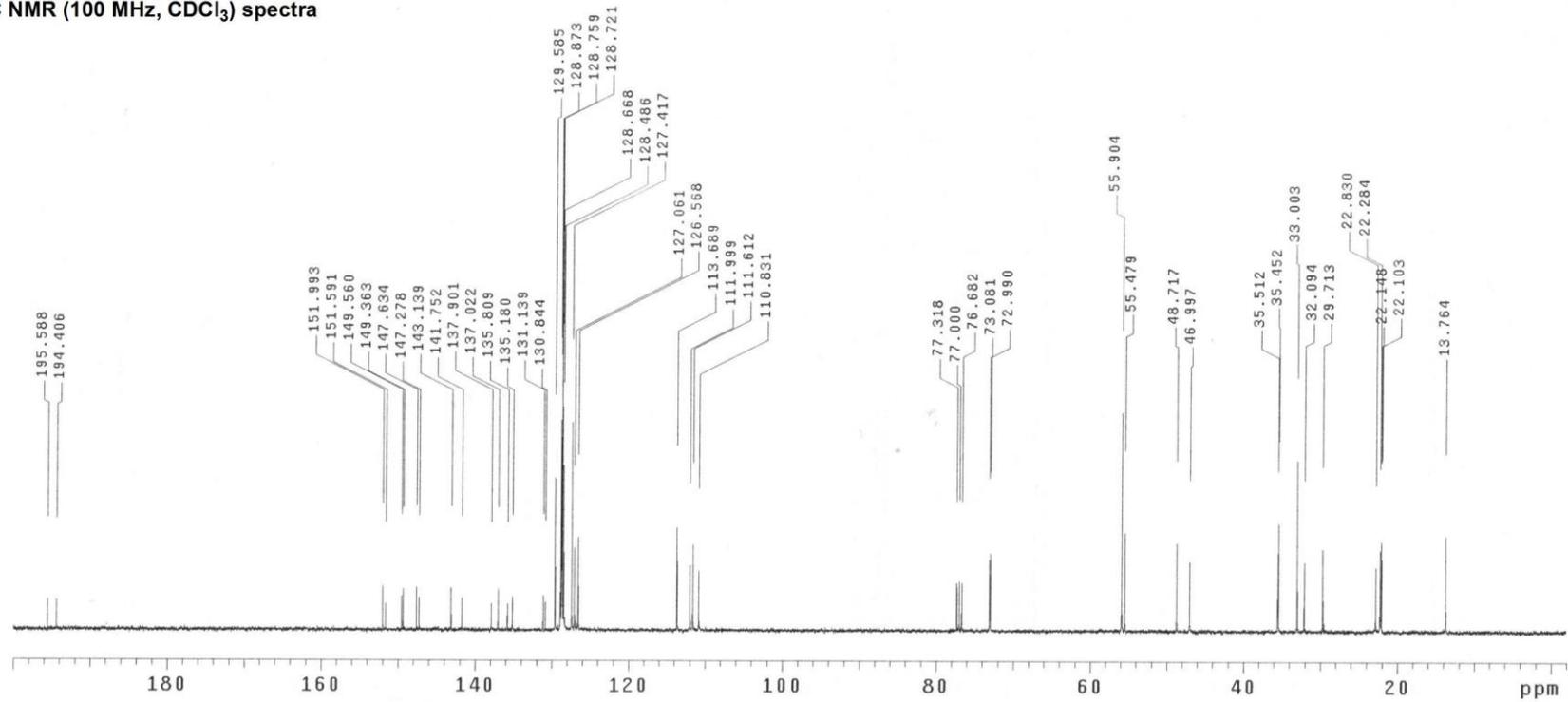
KSPHbuCBF

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Jan 14 2019
Solvent: CDCl₃
Ambient temperature
Total 672 repetitions



Compound 5e

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 5f (¹H-NMR spectral data-1)

KSMSCBF

Pulse Sequence: s2pu1

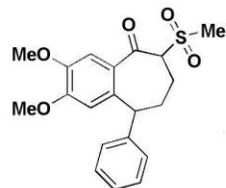
UNITYplus-400 "unity400"

Date: Dec 17 2018

Solvent: CDCl₃

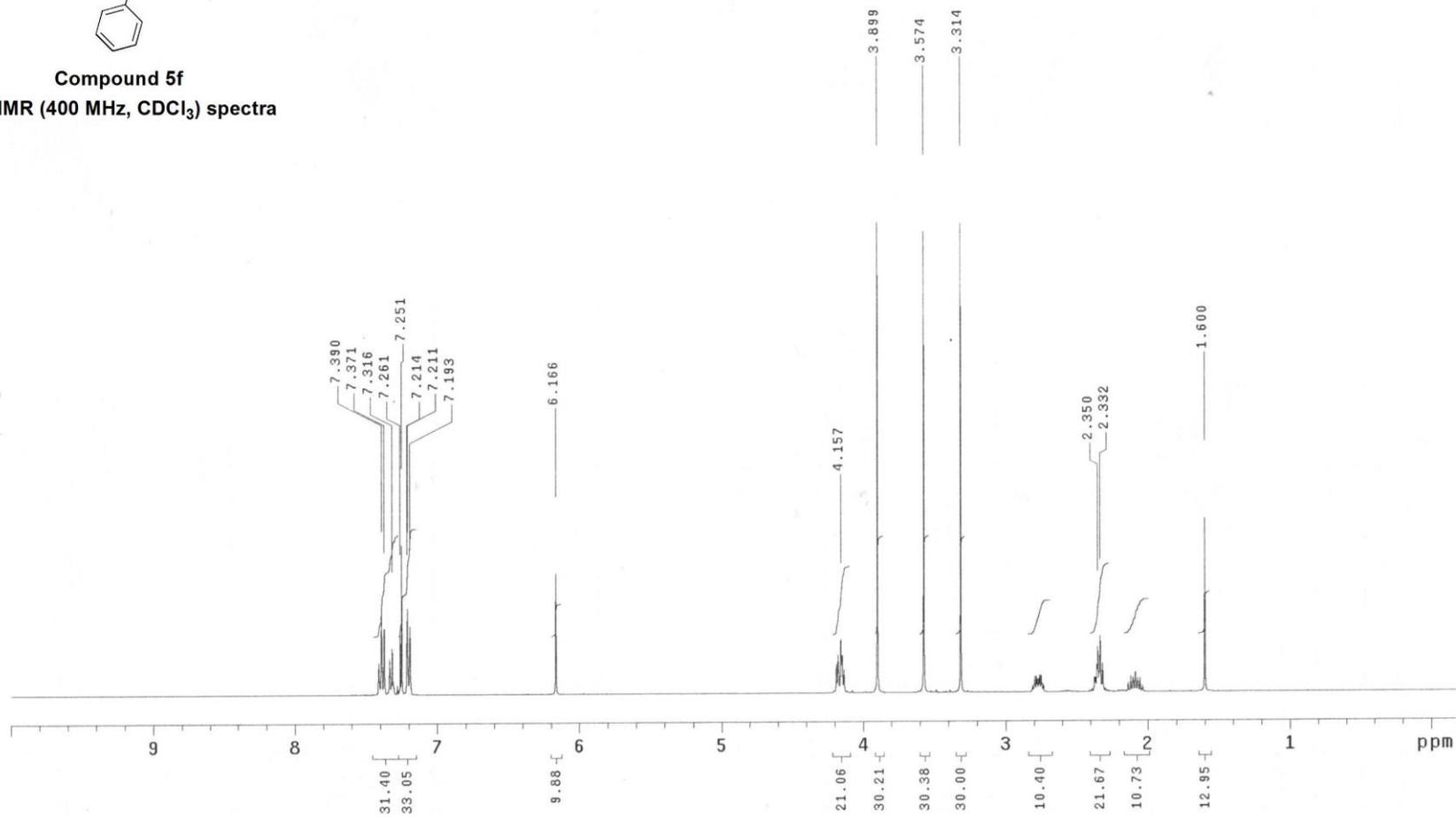
Ambient temperature

Total 32 repetitions

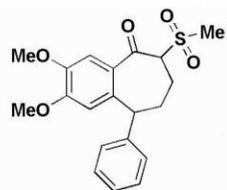


Compound 5f

¹H NMR (400 MHz, CDCl₃) spectra

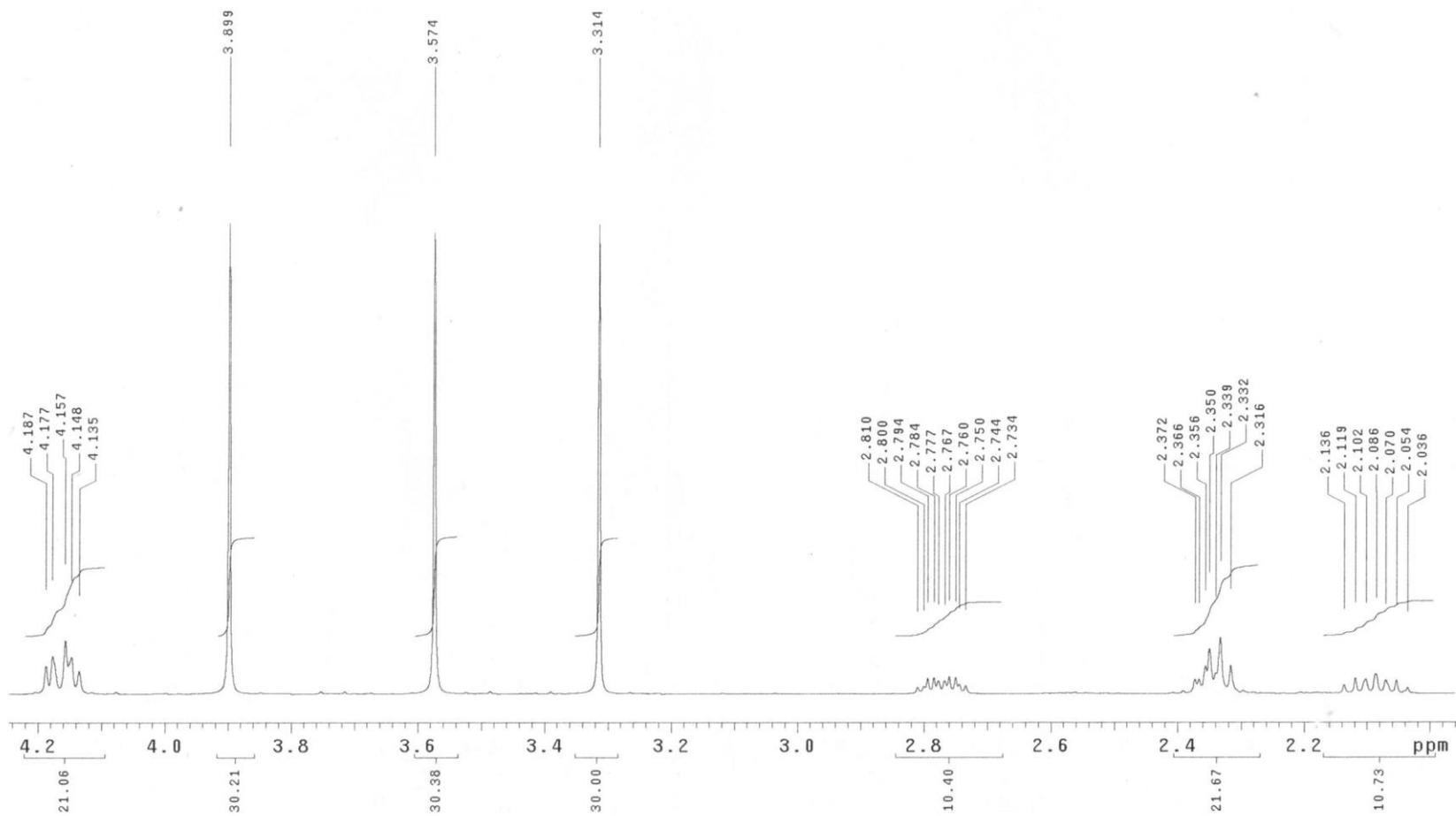


Compound 5f (¹H-NMR spectral data-2)



Compound 5f

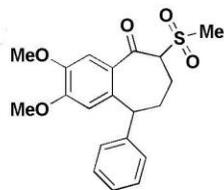
¹H NMR (400 MHz, CDCl₃) spectra



Compound 5f (¹³C-NMR spectral data)

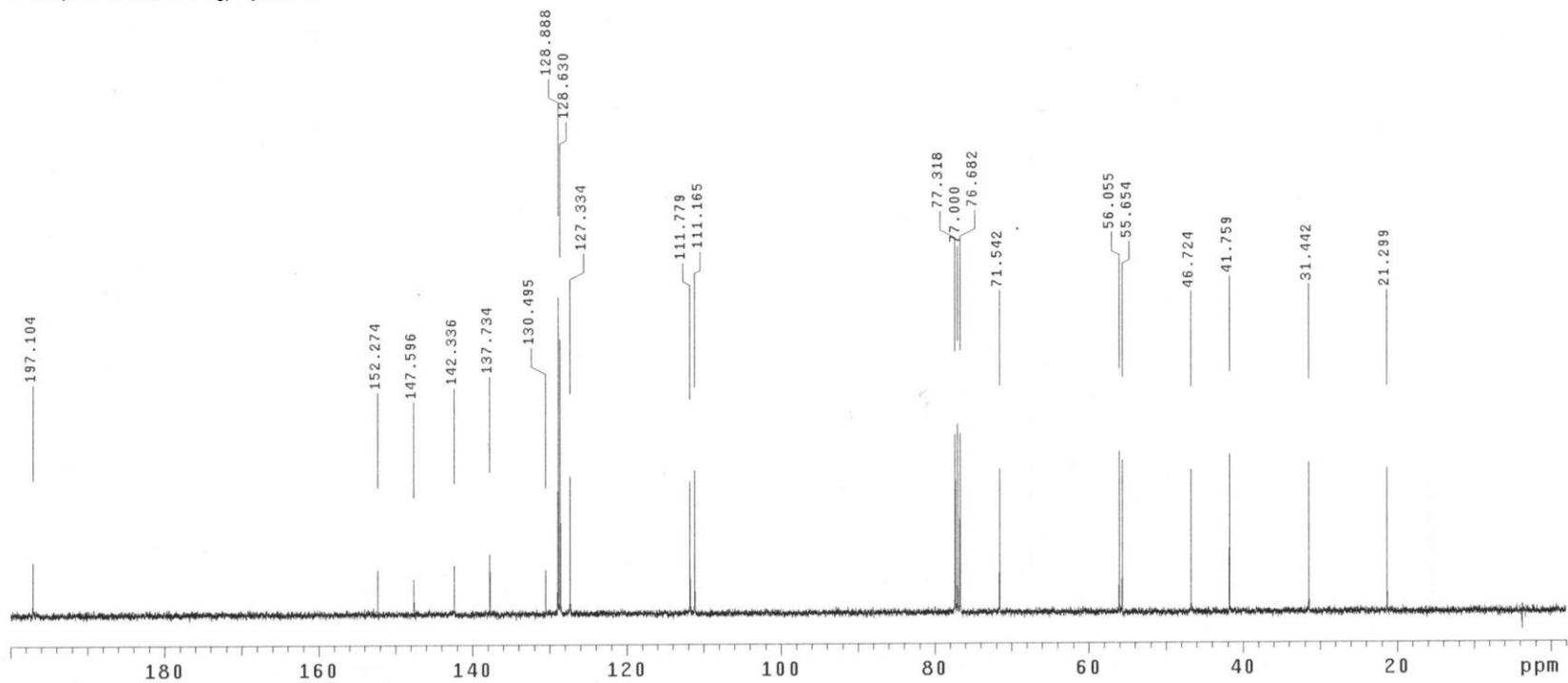
KSMSCBF

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Dec 17 2018
Solvent: CDCl₃
Ambient temperature
Total 2464 repetitions



Compound 5f

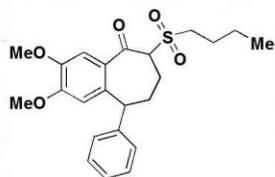
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 5g (¹H-NMR spectral data-1)

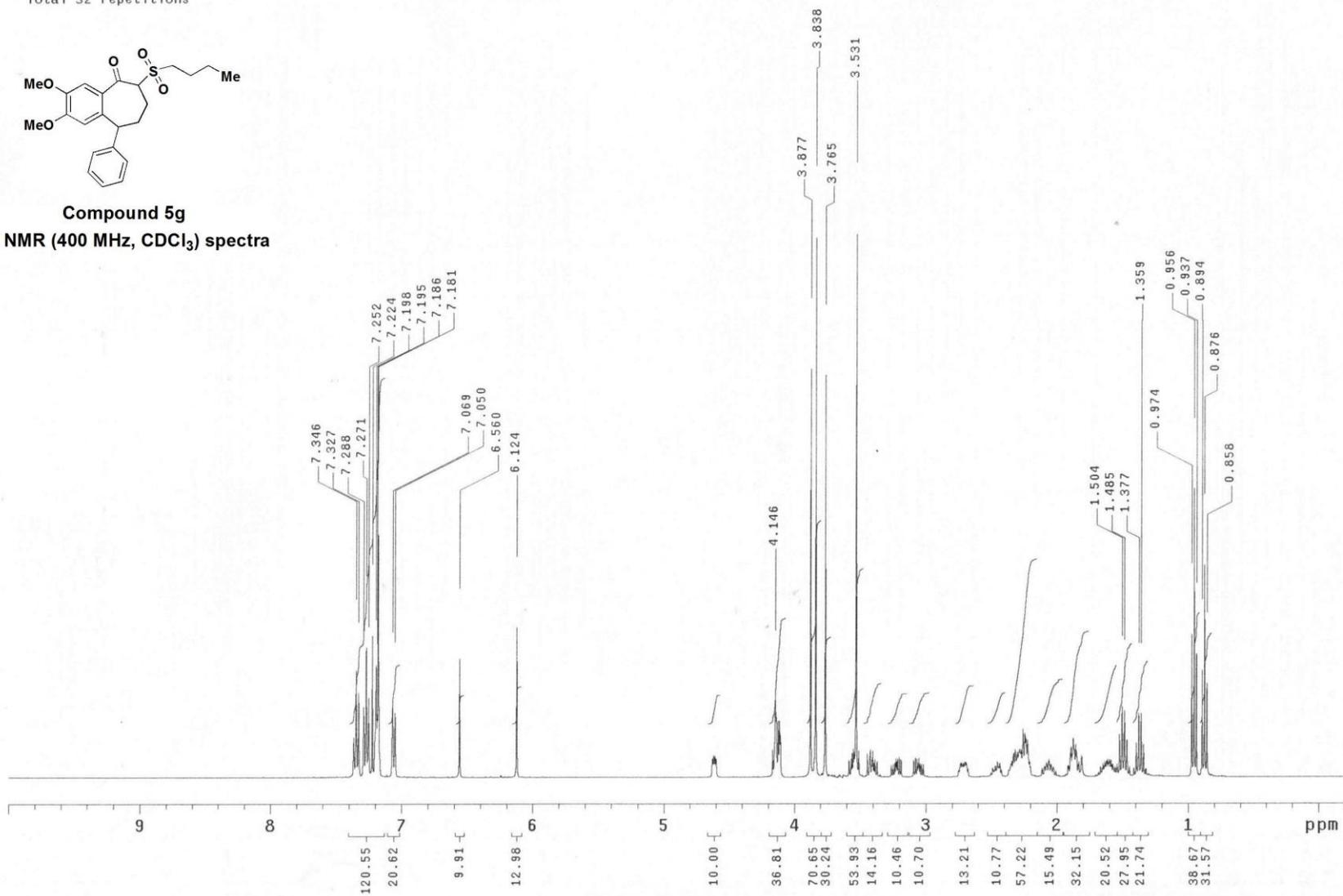
KSBuCBF

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Dec 21 2018
Solvent: CDCl₃
Ambient temperature
Total 32 repetitions

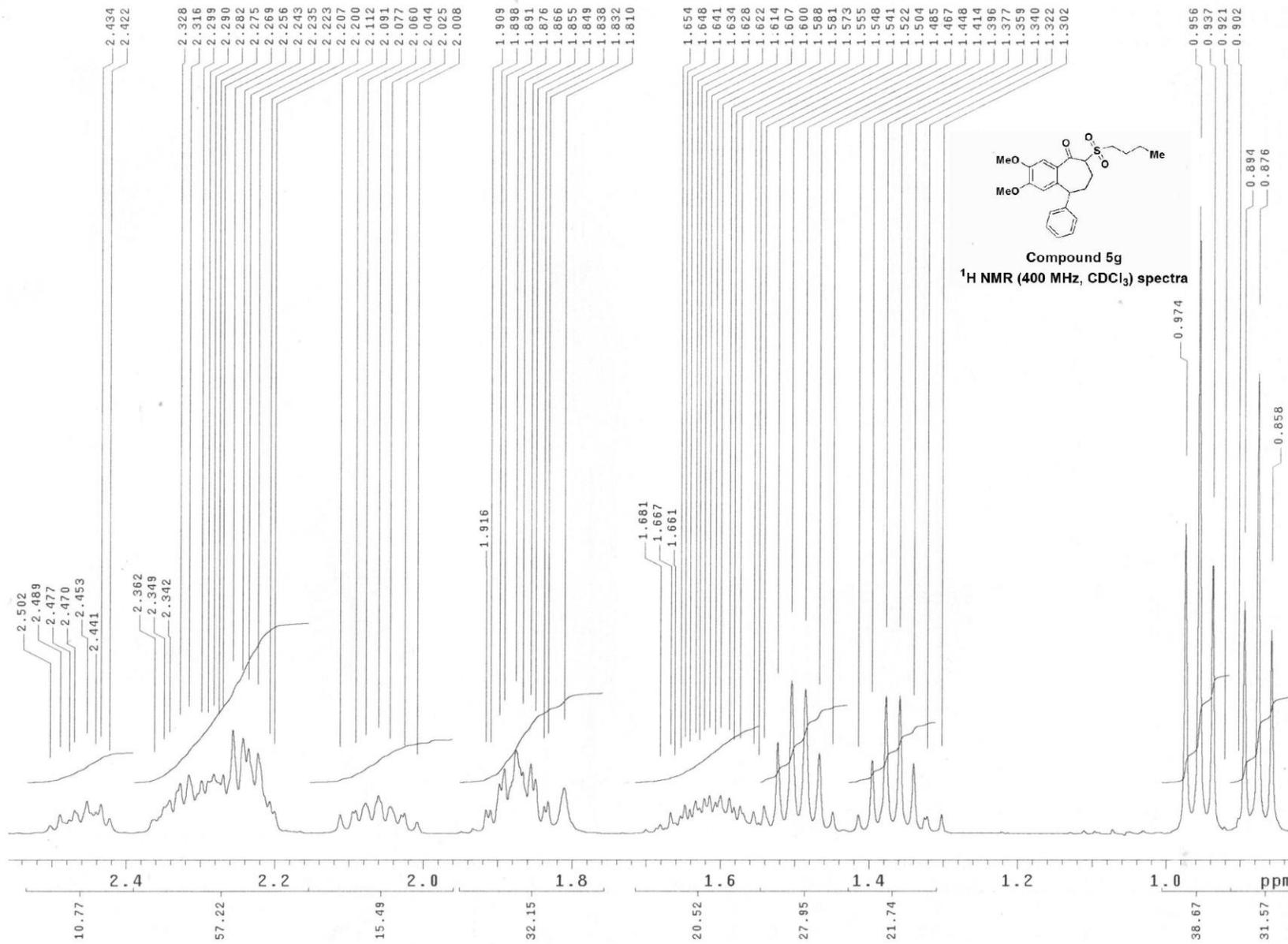


Compound 5g

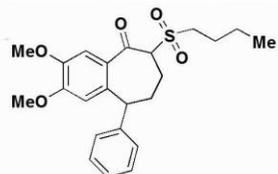
¹H NMR (400 MHz, CDCl₃) spectra



Compound 5g (¹H-NMR spectral data-2)

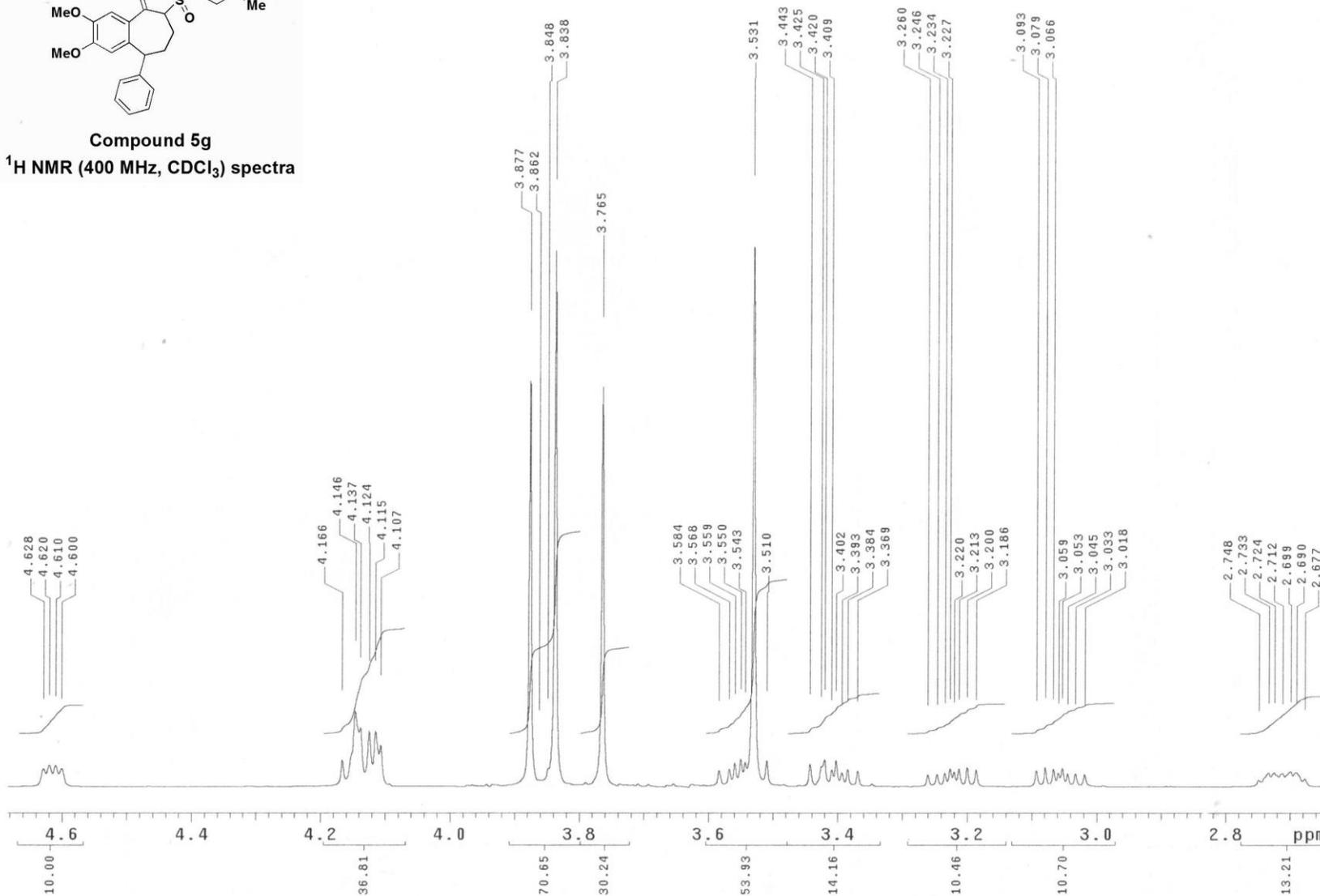


Compound 5g (¹H-NMR spectral data-3)



Compound 5g

¹H NMR (400 MHz, CDCl₃) spectra



Compound 5g (¹³C-NMR spectral data)

KSBuCBF

Pulse Sequence: s2pu1

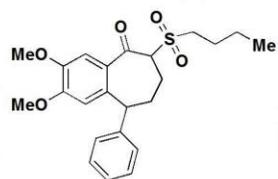
UNITYplus-400 "unity400"

Date: Dec 21 2018

Solvent: CDCl₃

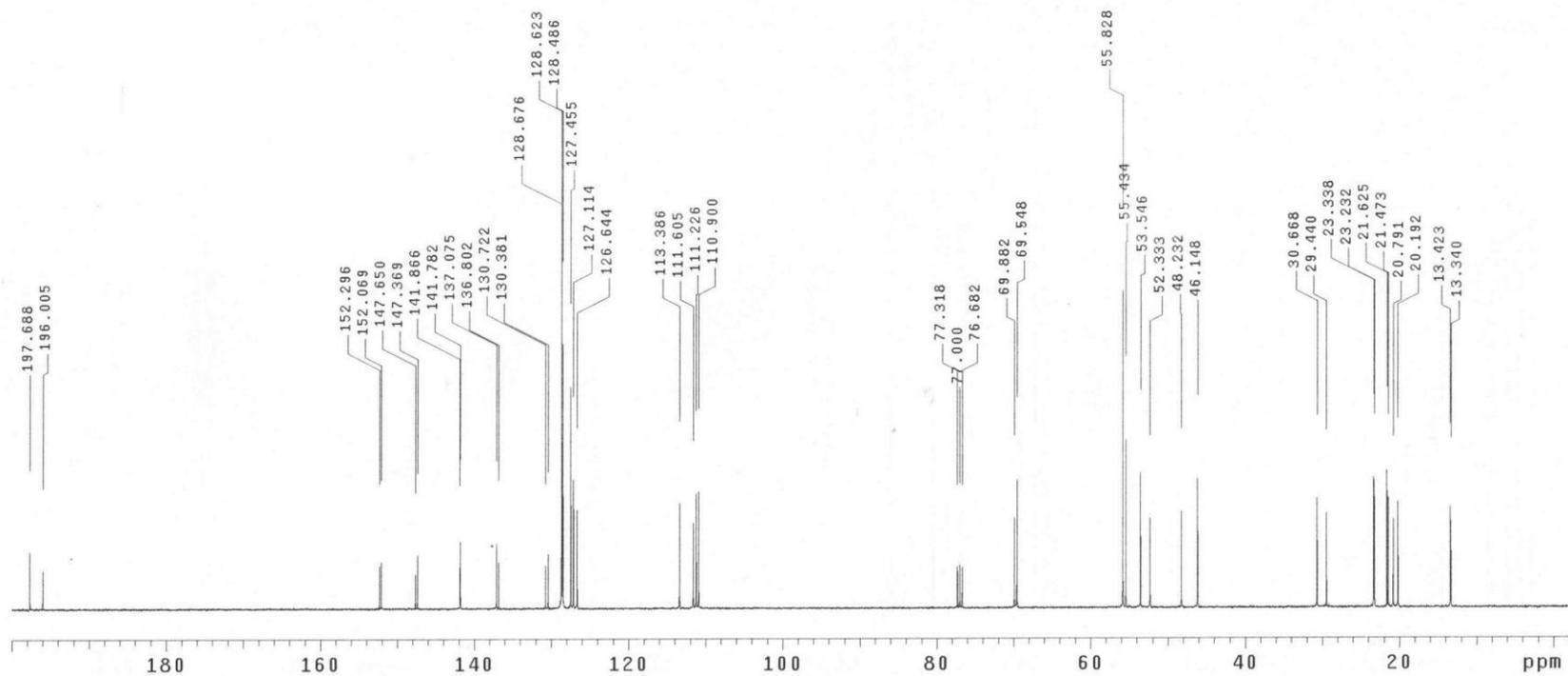
Ambient temperature

Total 1392 repetitions



Compound 5g

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 5h (¹H-NMR spectral data-1)

KSE1CBF

Pulse Sequence: s2pu1

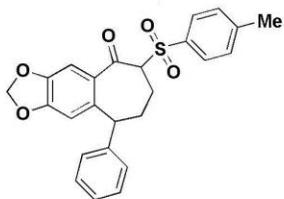
UNITYplus-400 "unity400"

Date: Jan 16 2019

Solvent: CDC13

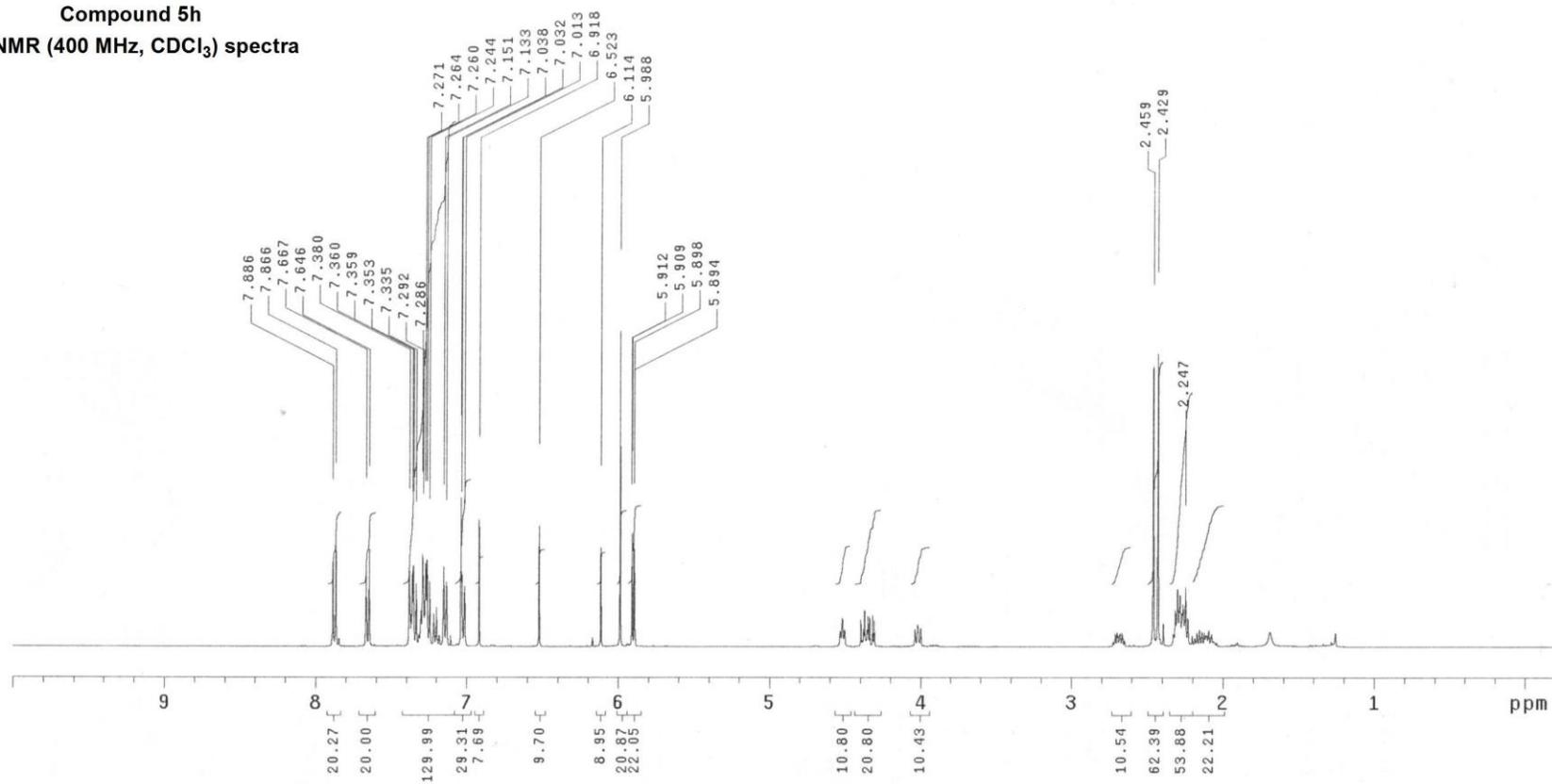
Ambient temperature

Total 64 repetitions

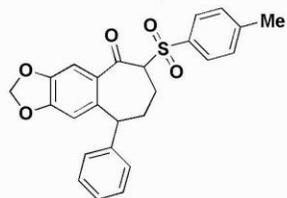


Compound 5h

¹H NMR (400 MHz, CDCl₃) spectra

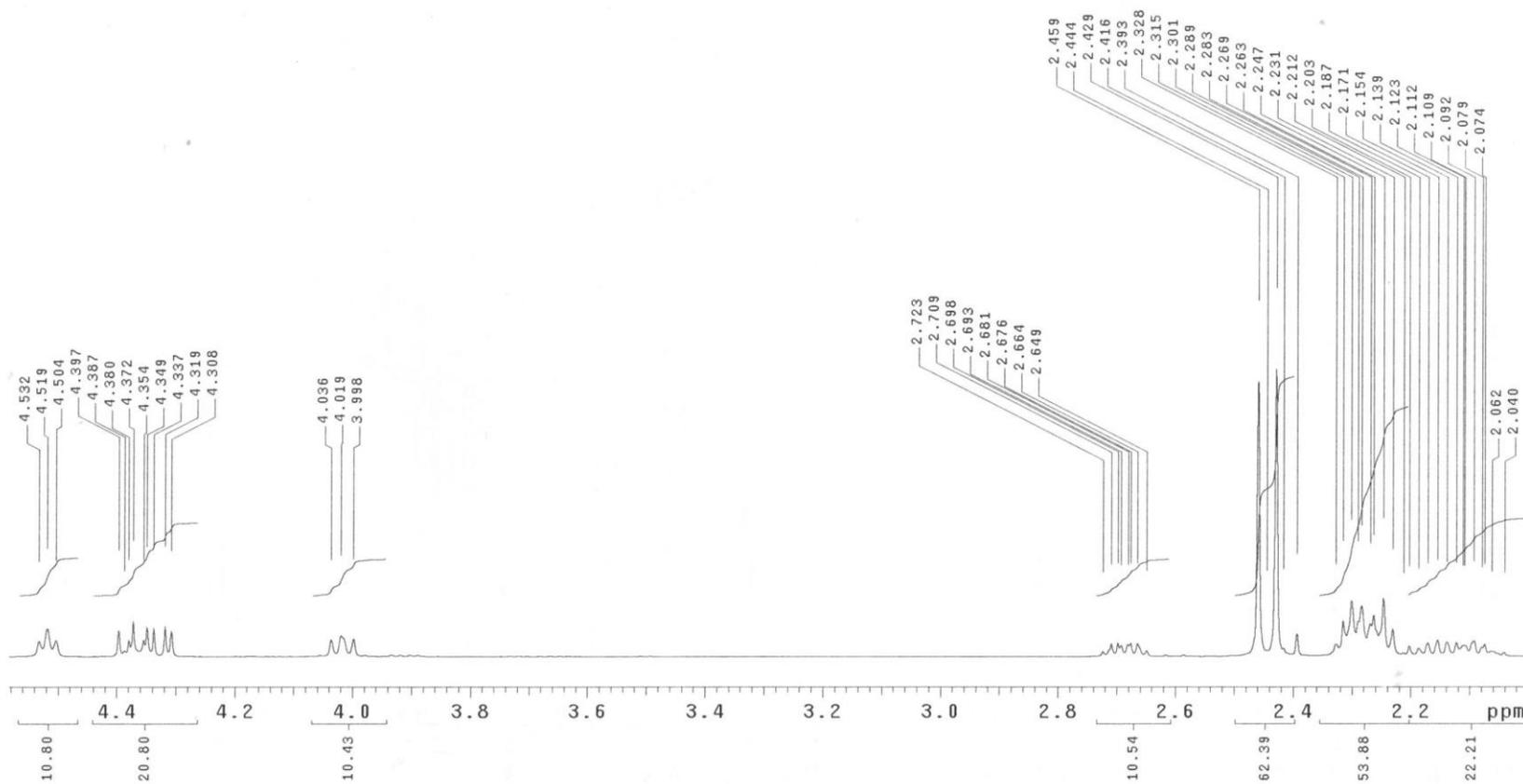


Compound 5h (¹H-NMR spectral data-2)



Compound 5h

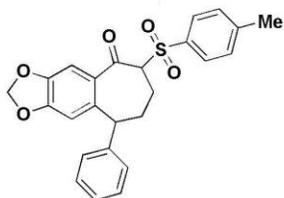
¹H NMR (400 MHz, CDCl₃) spectra



Compound 5h (¹³C-NMR spectral data)

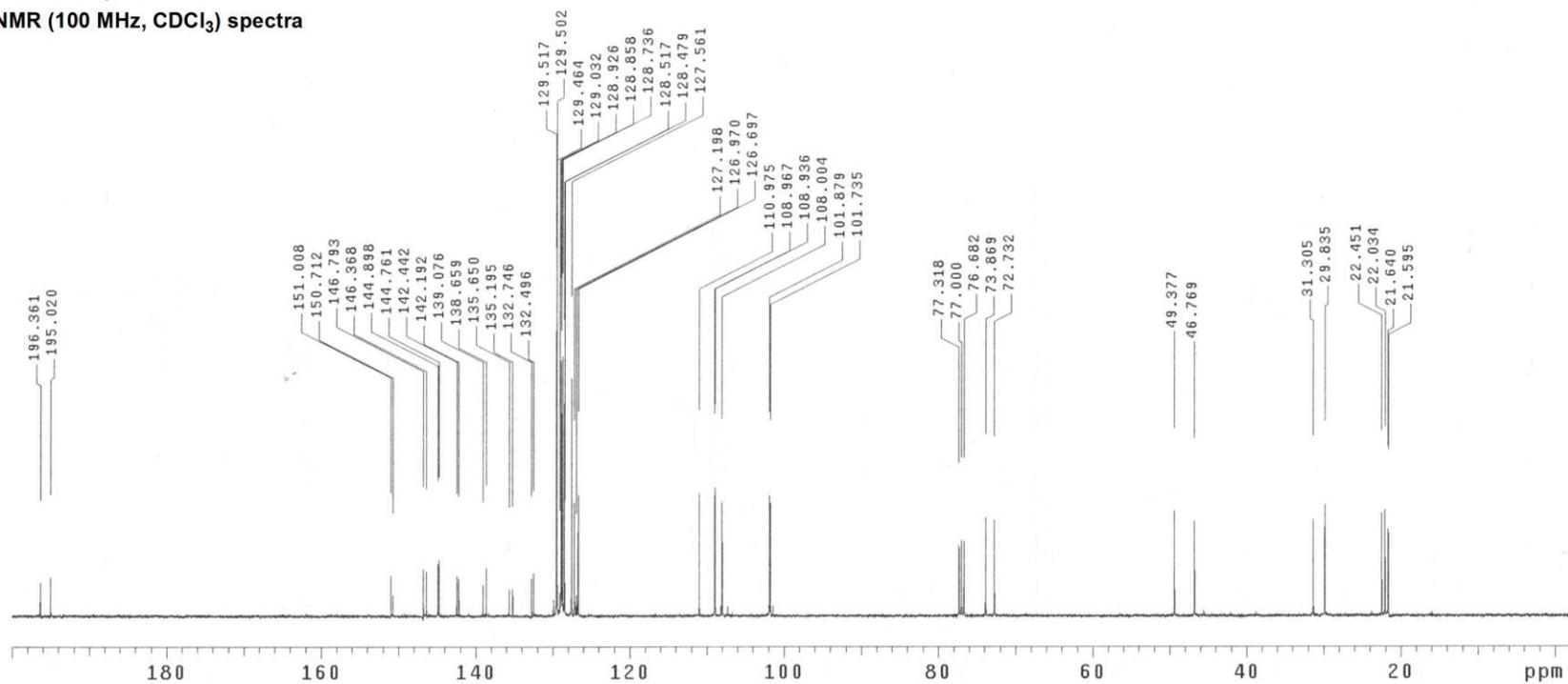
KSE1CBF

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Jan 16 2019
Solvent: CDCl₃
Ambient temperature
Total 4096 repetitions



Compound 5h

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 5i (¹H-NMR spectral data-1)

KSE8CBF

Pulse Sequence: s2pu1

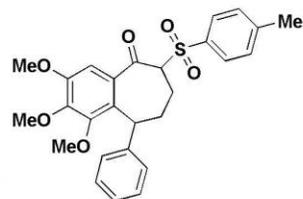
UNITYplus-400 "unity400"

Date: Jan 29 2019

Solvent: CDCl₃

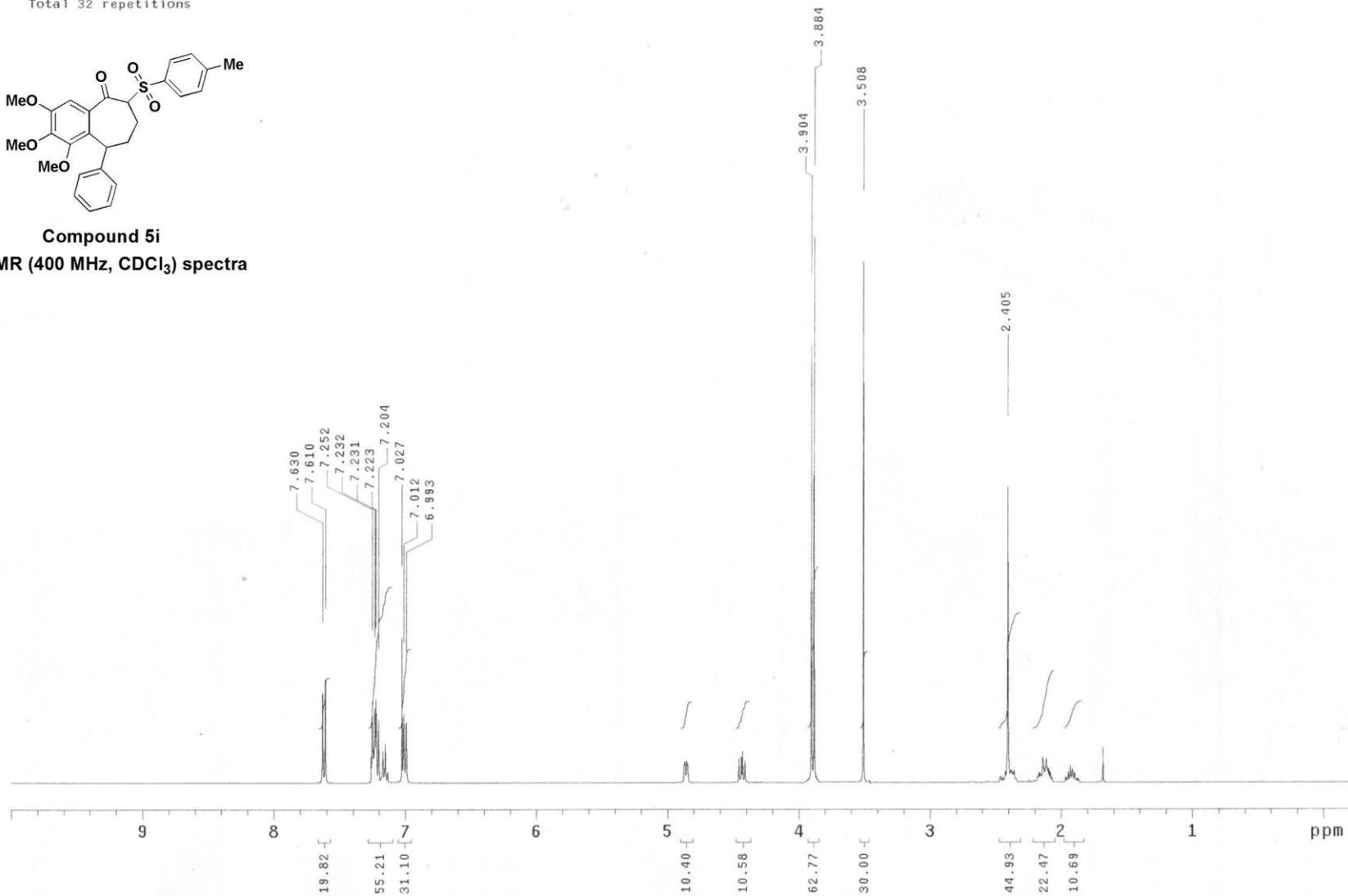
Ambient temperature

Total 32 repetitions

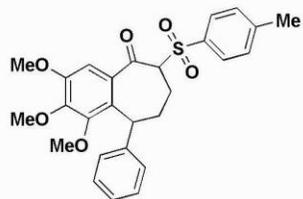


Compound 5i

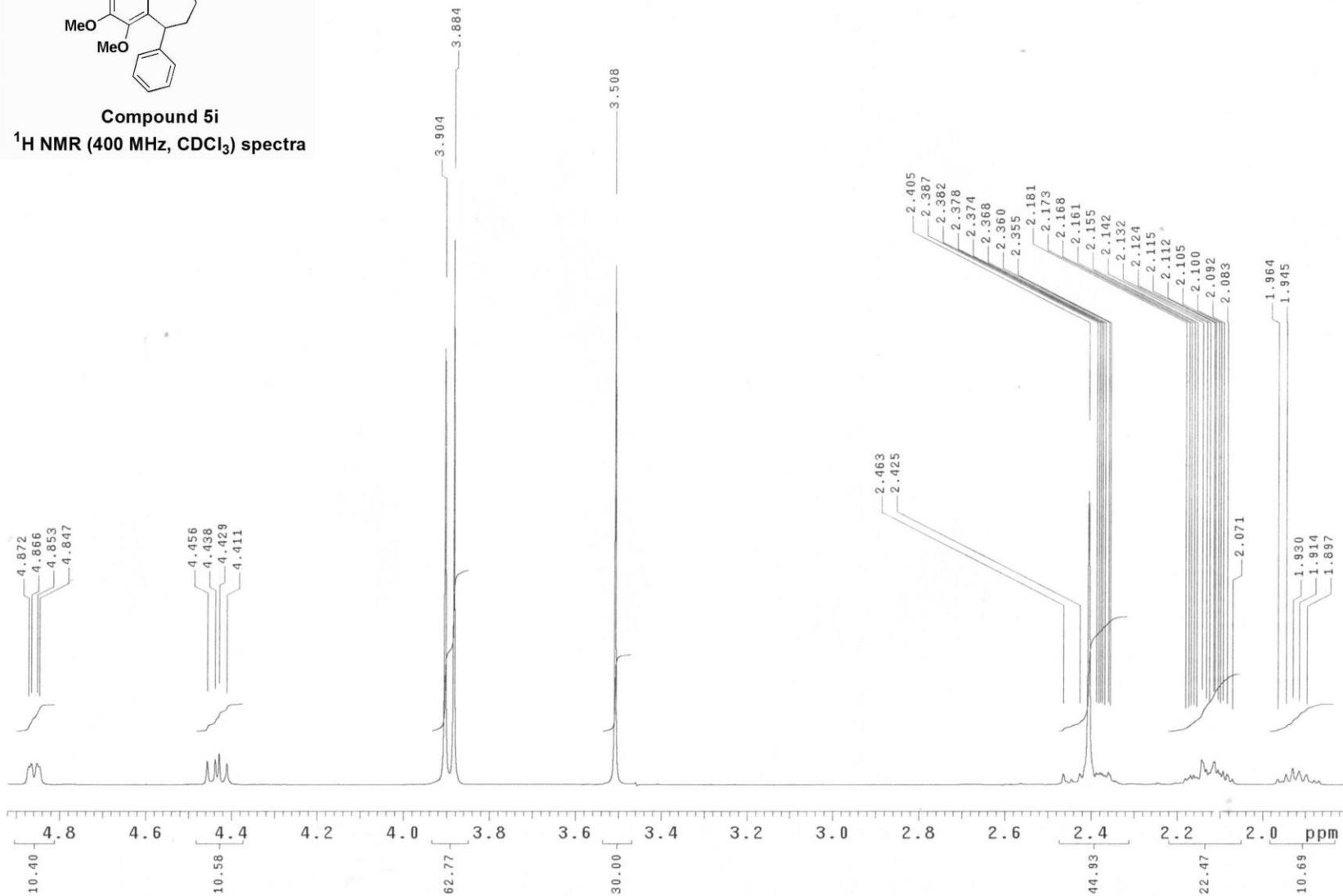
¹H NMR (400 MHz, CDCl₃) spectra



Compound 5i (¹H-NMR spectral data-2)



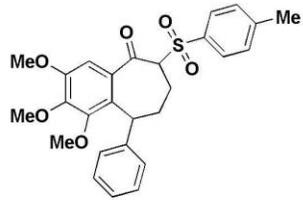
Compound 5i
¹H NMR (400 MHz, CDCl₃) spectra



Compound 5i (¹³C-NMR spectral data)

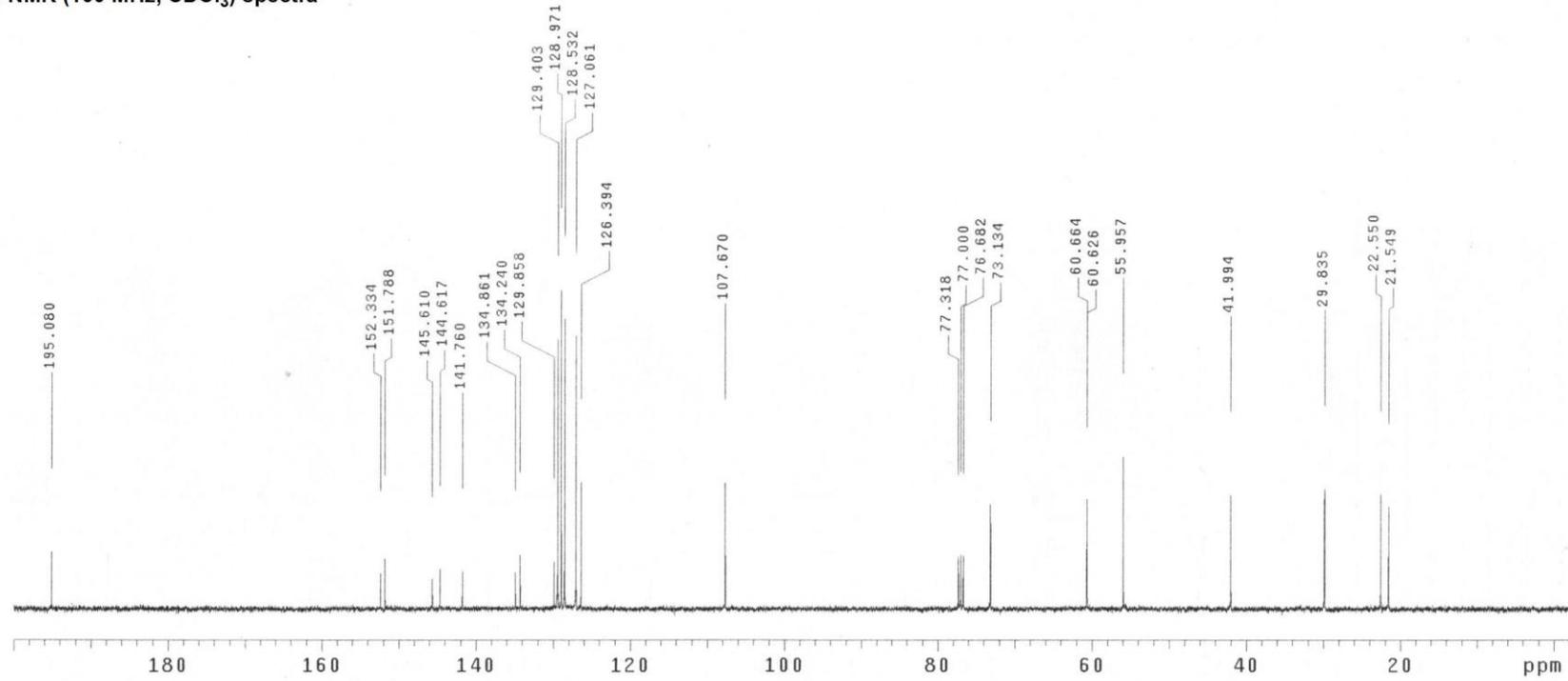
KSE8CBF

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Jan 29 2019
Solvent: CDCl₃
Ambient temperature
Total 480 repetitions



Compound 5i

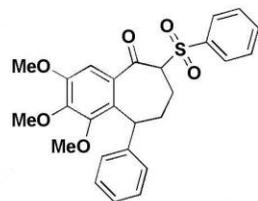
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 5j (¹H-NMR spectral data-1)

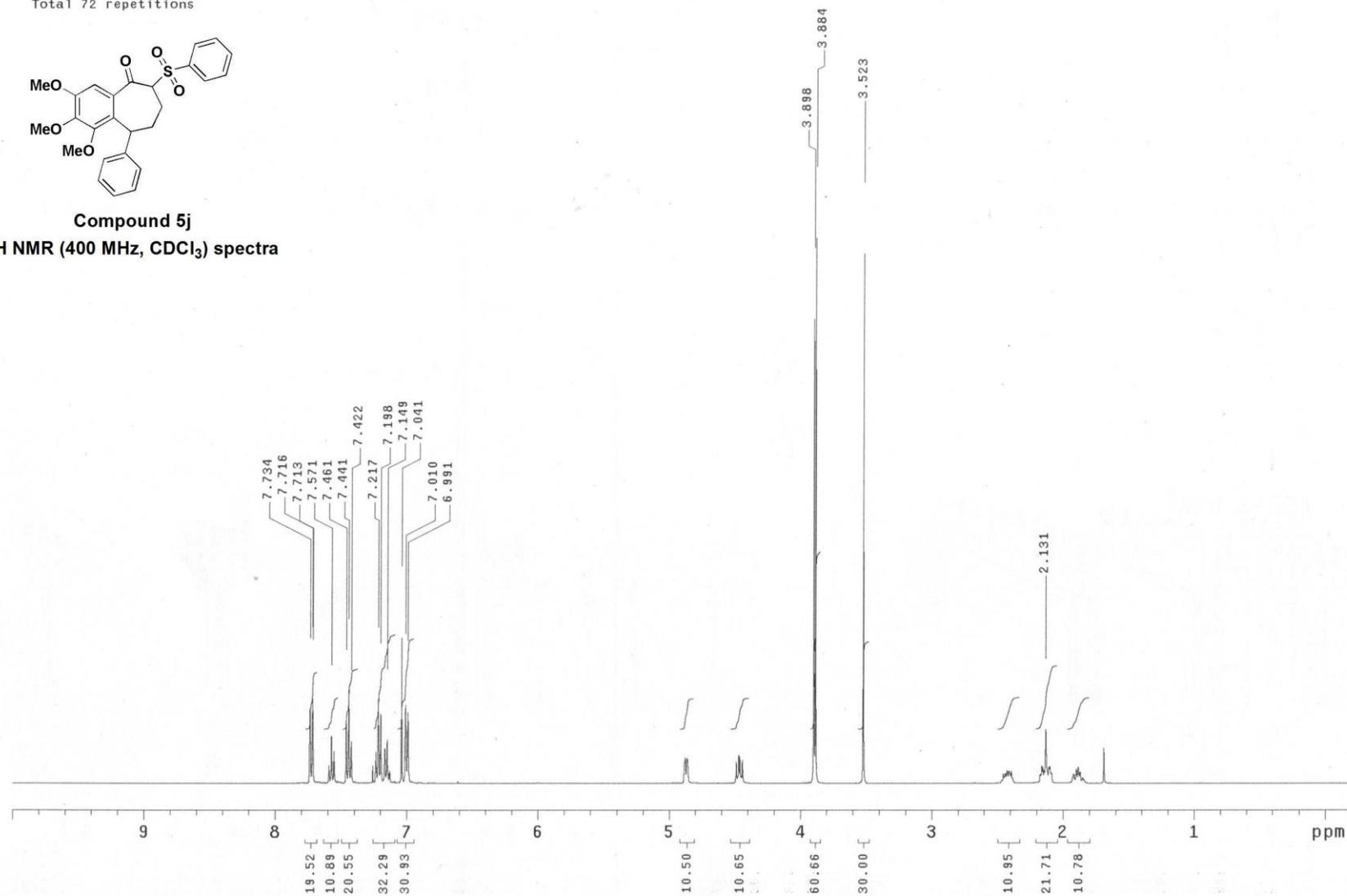
KS30BSCBF

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Feb 19 2019
Solvent: CDCl₃
Ambient temperature
Total 72 repetitions

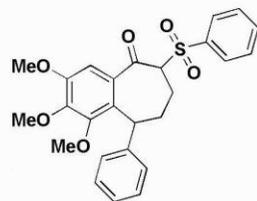


Compound 5j

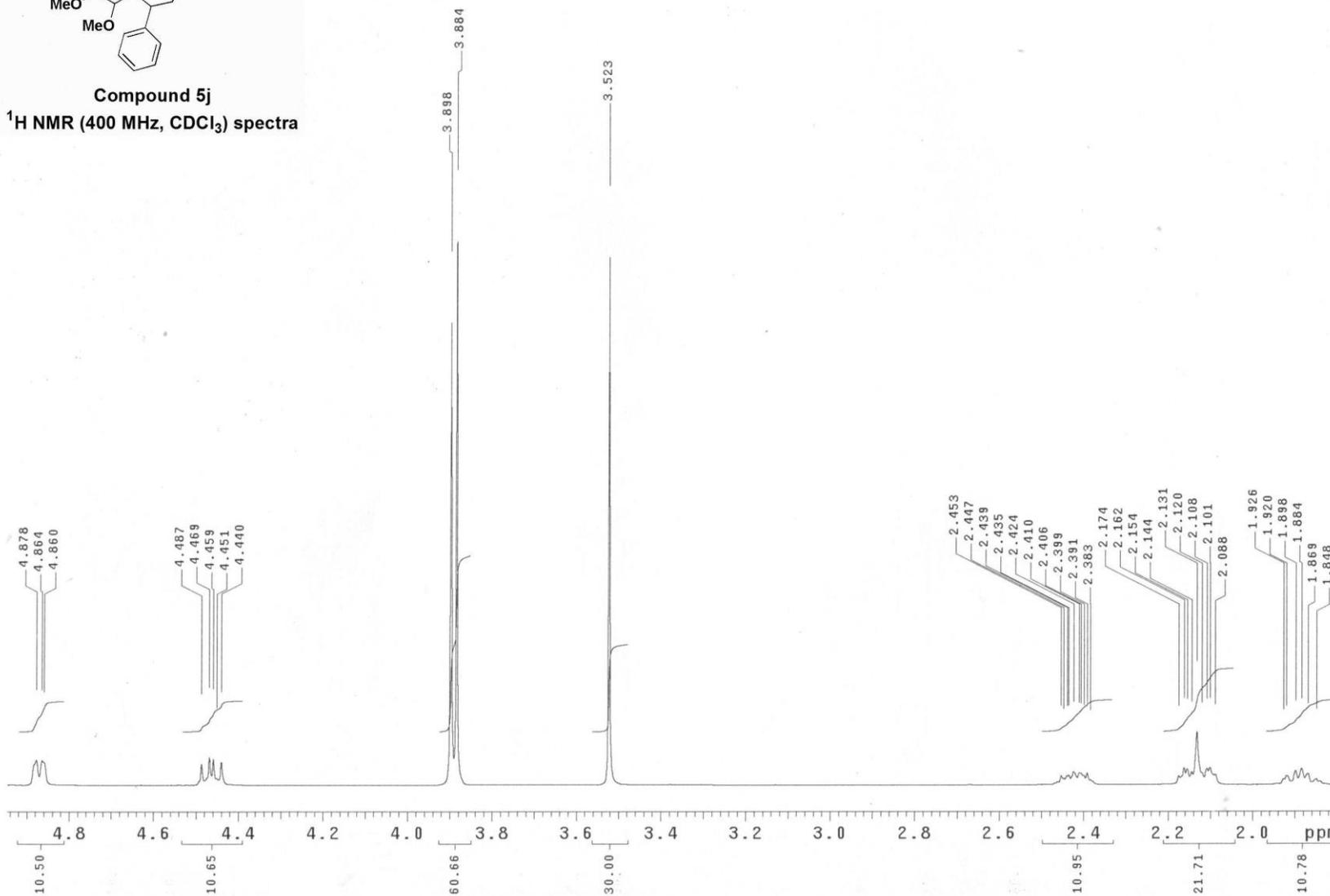
¹H NMR (400 MHz, CDCl₃) spectra



Compound 5j (¹H-NMR spectral data-2)



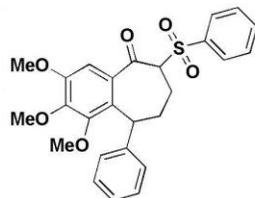
Compound 5j
¹H NMR (400 MHz, CDCl₃) spectra



Compound 5j (¹³C-NMR spectral data)

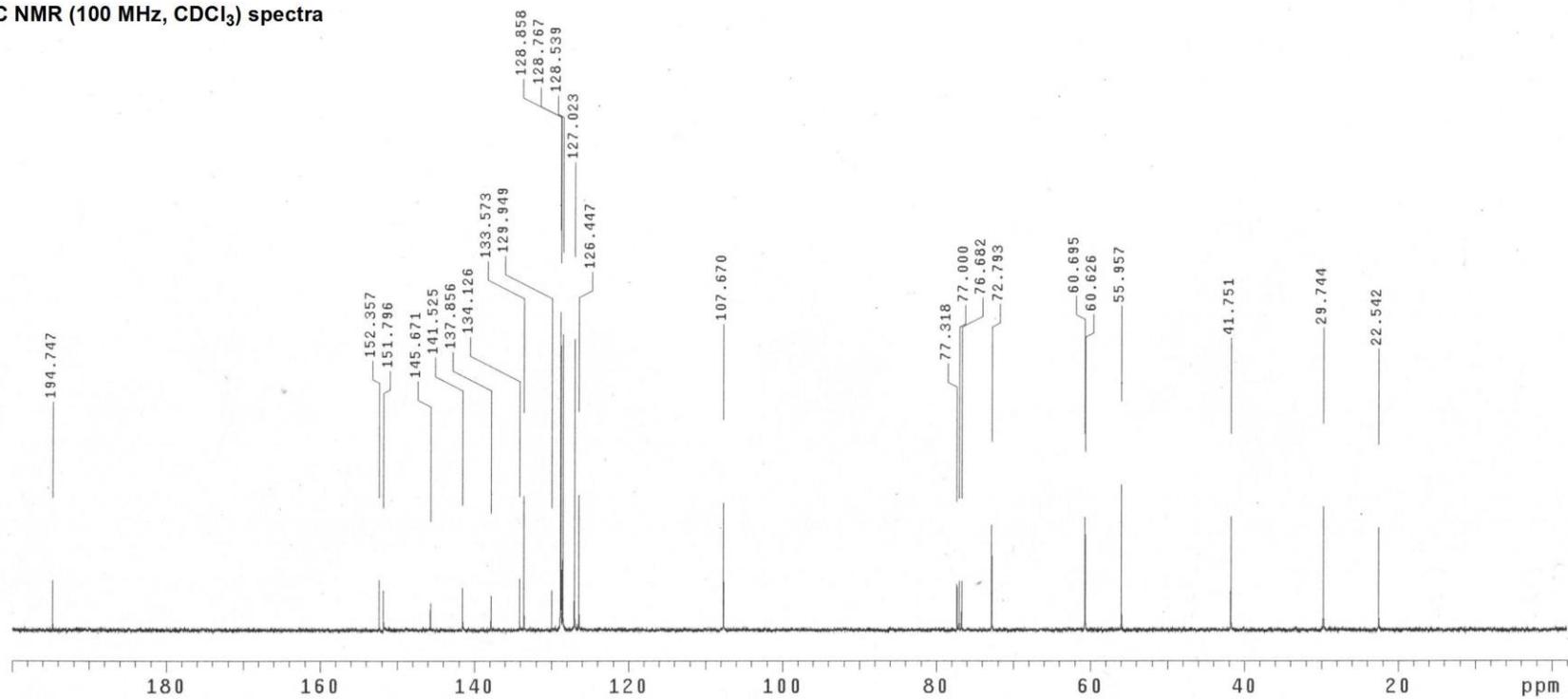
KS30BSCBF

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Feb 19 2019
Solvent: CDCl₃
Ambient temperature
Total 480 repetitions



Compound 5j

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 5k (¹H-NMR spectral data-1)

KS30MsCBF

Pulse Sequence: s2pu1

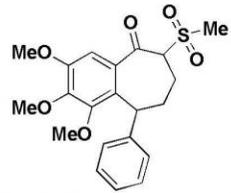
UNITYplus-400 "unity400"

Date: Feb 13 2019

Solvent: CDCl₃

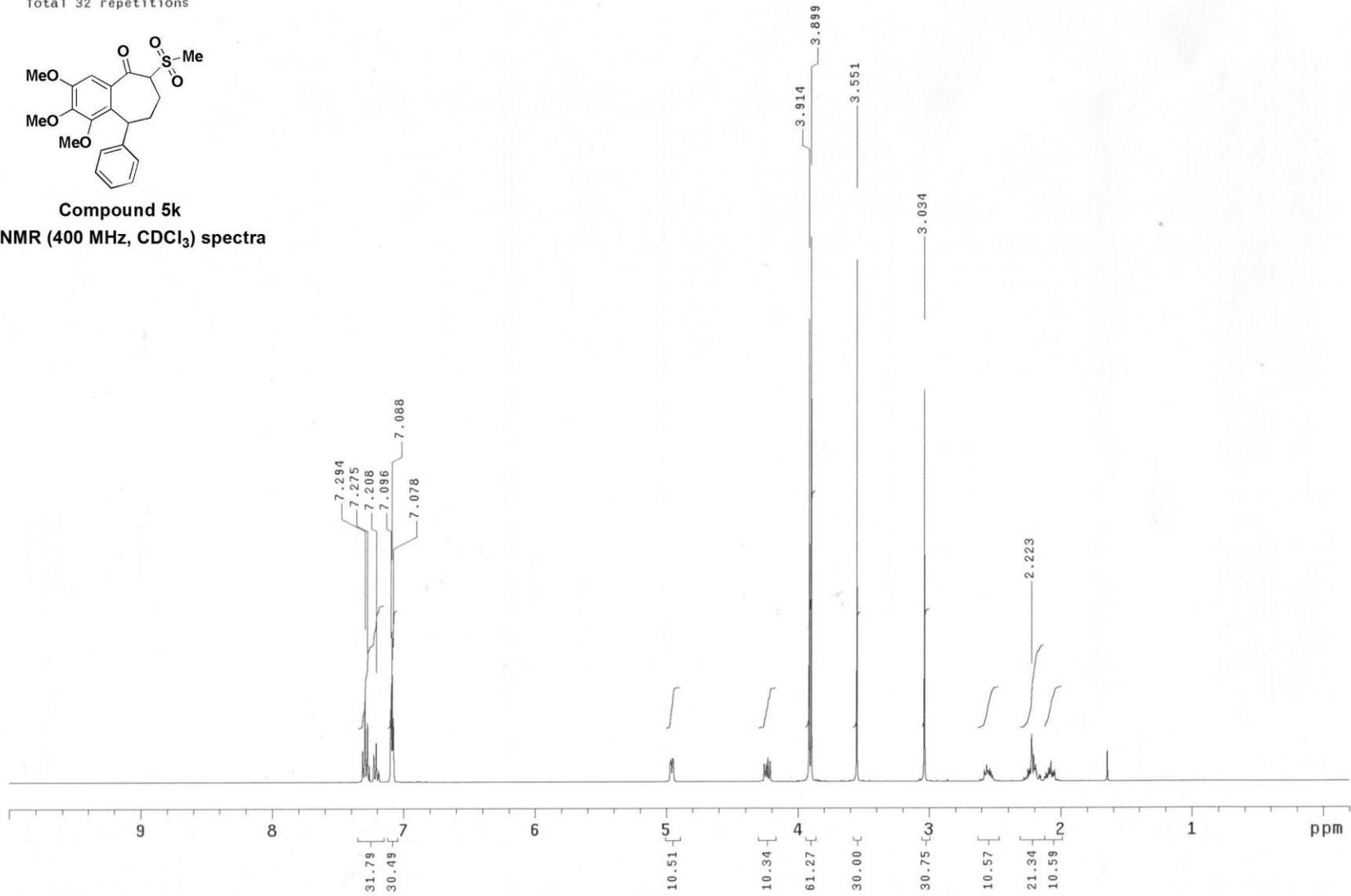
Ambient temperature

Total 32 repetitions

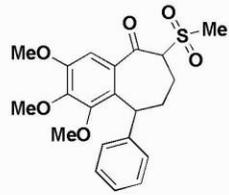


Compound 5k

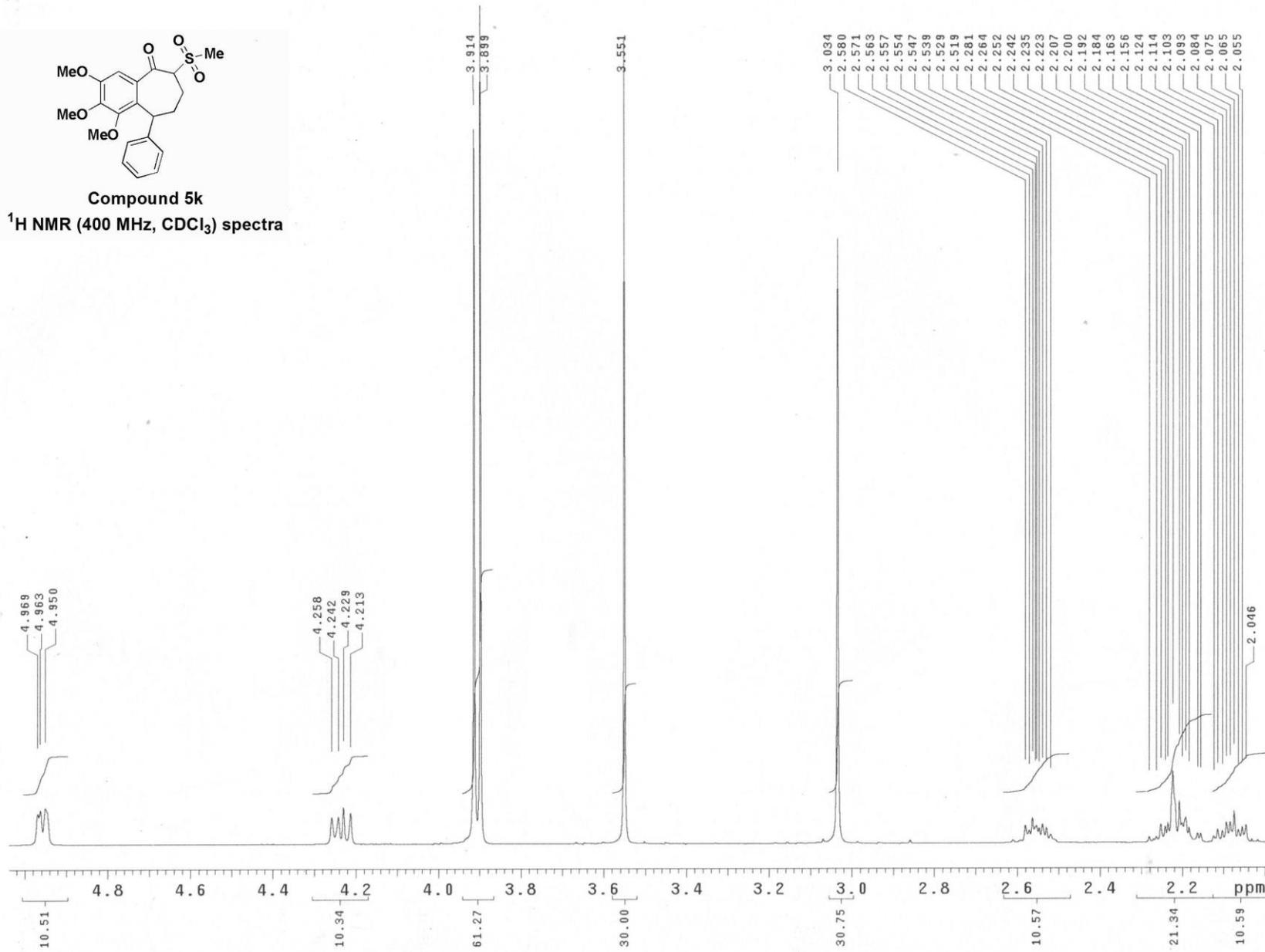
¹H NMR (400 MHz, CDCl₃) spectra



Compound 5k (¹H-NMR spectral data-2)



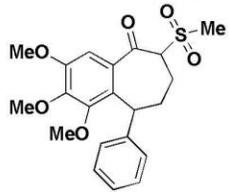
Compound 5k
¹H NMR (400 MHz, CDCl₃) spectra



Compound 5k (¹³C-NMR spectral data)

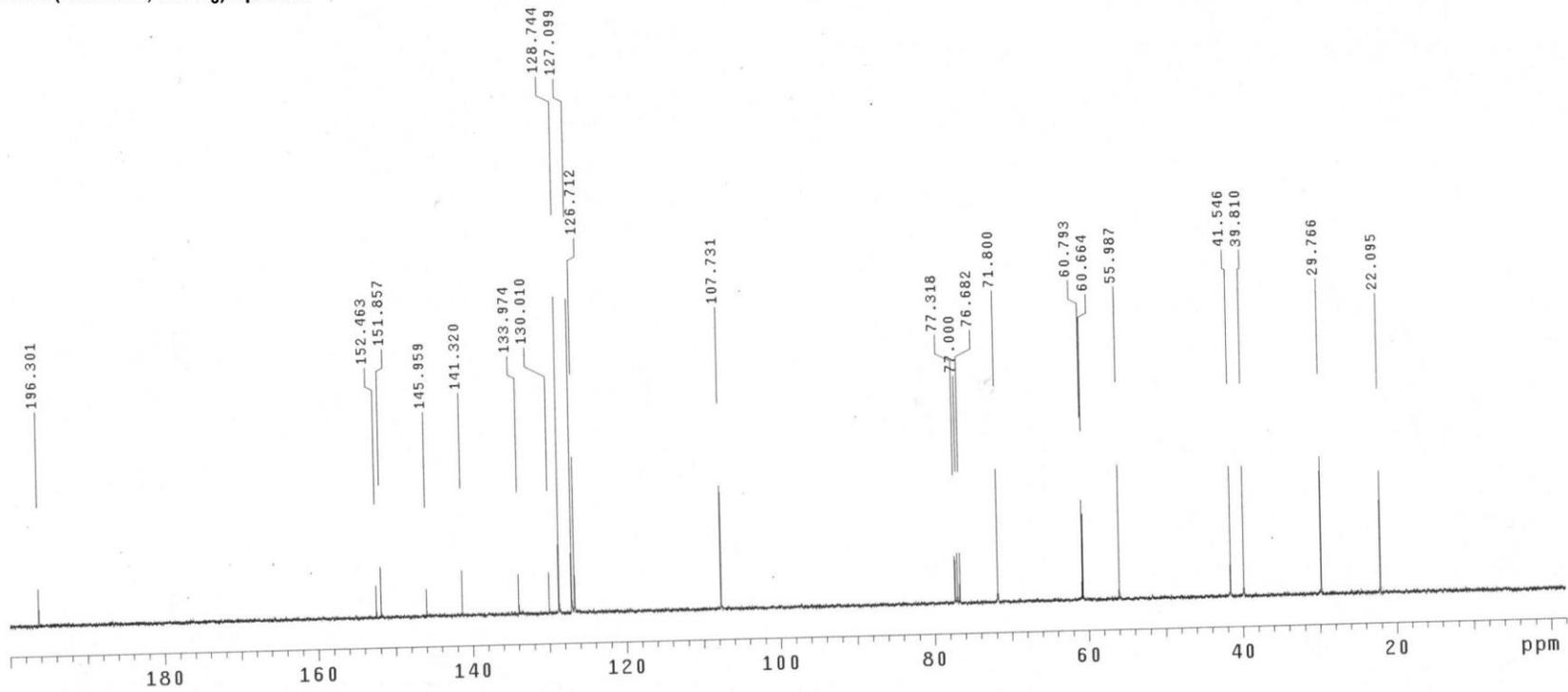
KS30MsCBF

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Feb 13 2019
Solvent: CDCl₃
Ambient temperature
Total 576 repetitions



Compound 5k

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 5I (¹H-NMR spectral data-1)

KSE2CBF

Pulse Sequence: s2pu1

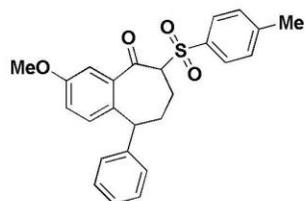
UNITYplus-400 "unity400"

Date: Dec 3 2018

Solvent: CDCl₃

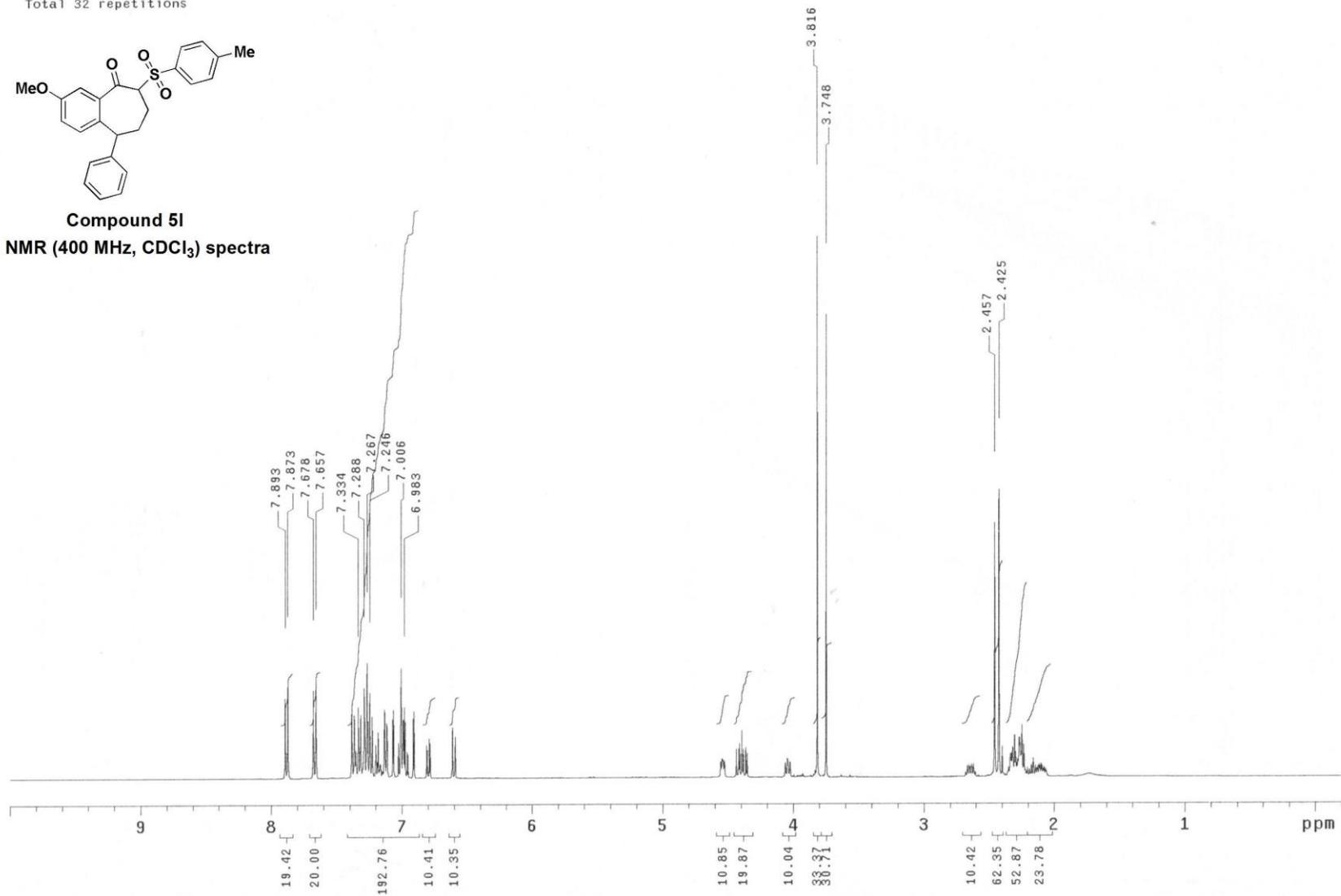
Ambient temperature

Total 32 repetitions

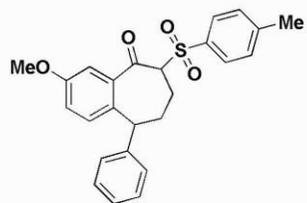


Compound 5I

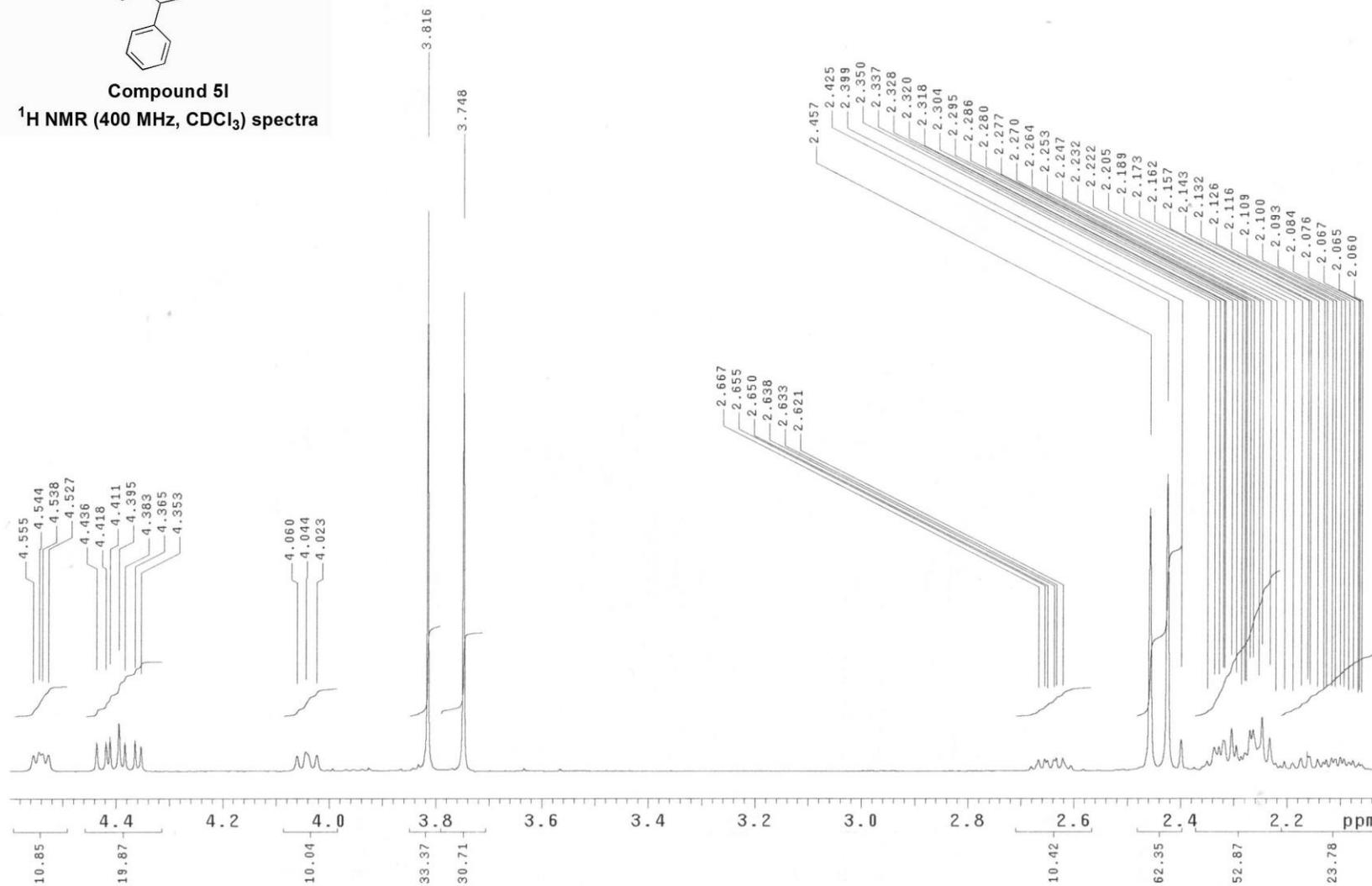
¹H NMR (400 MHz, CDCl₃) spectra



Compound 5I (¹H-NMR spectral data-2)



Compound 5I
¹H NMR (400 MHz, CDCl₃) spectra



Compound 5I (¹³C-NMR spectral data)

KSE2CBF

Pulse Sequence: s2pu1

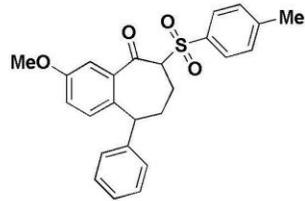
UNITYplus-400 "unity400"

Date: Dec 3 2018

Solvent: CDCl₃

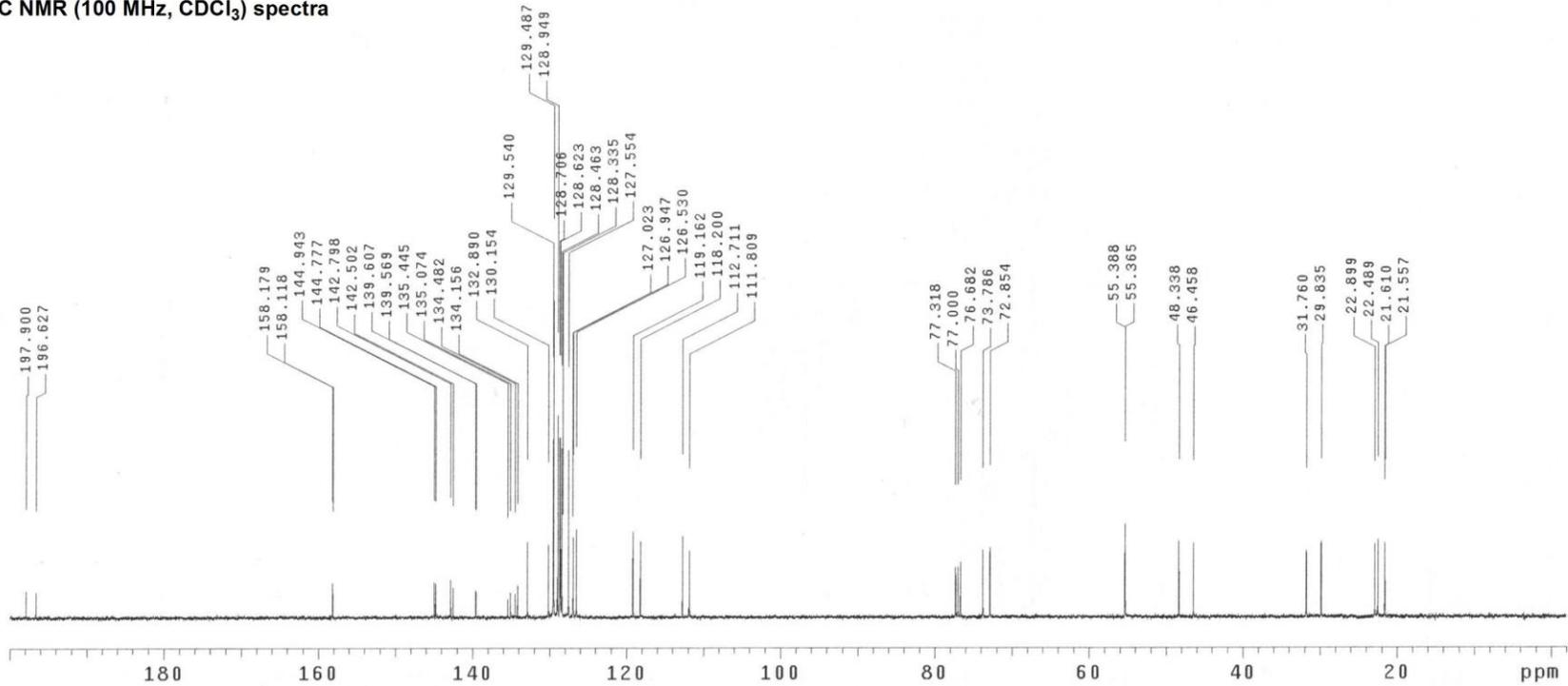
Ambient temperature

Total 544 repetitions



Compound 5I

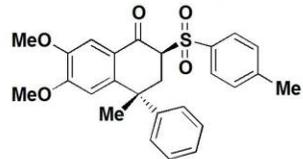
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 6a (¹H-NMR spectral data-1)

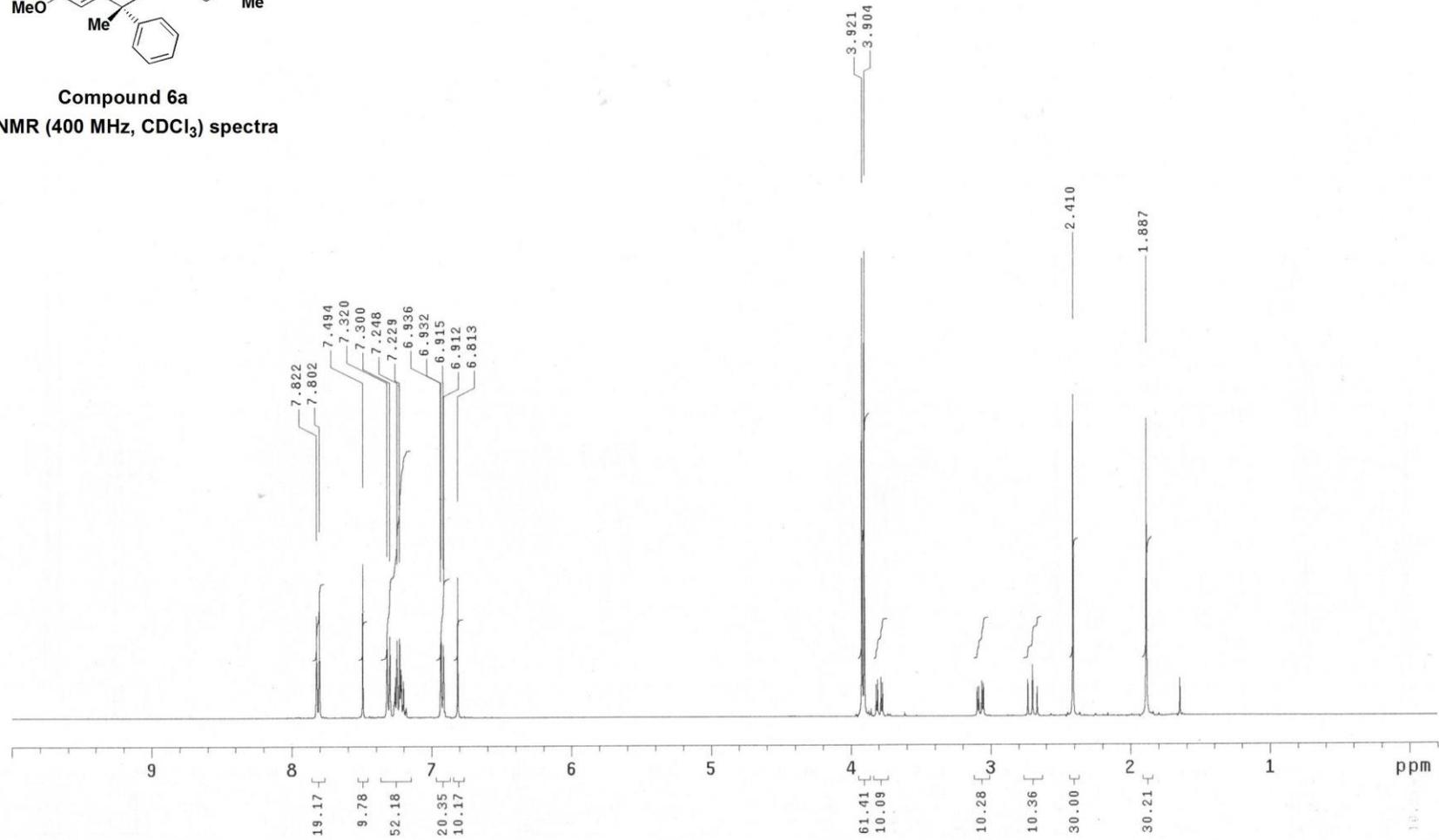
KSTsDBF

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Mar 4 2019
Solvent: CDCl₃
Ambient temperature
Total 32 repetitions

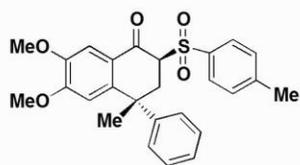


Compound 6a

¹H NMR (400 MHz, CDCl₃) spectra

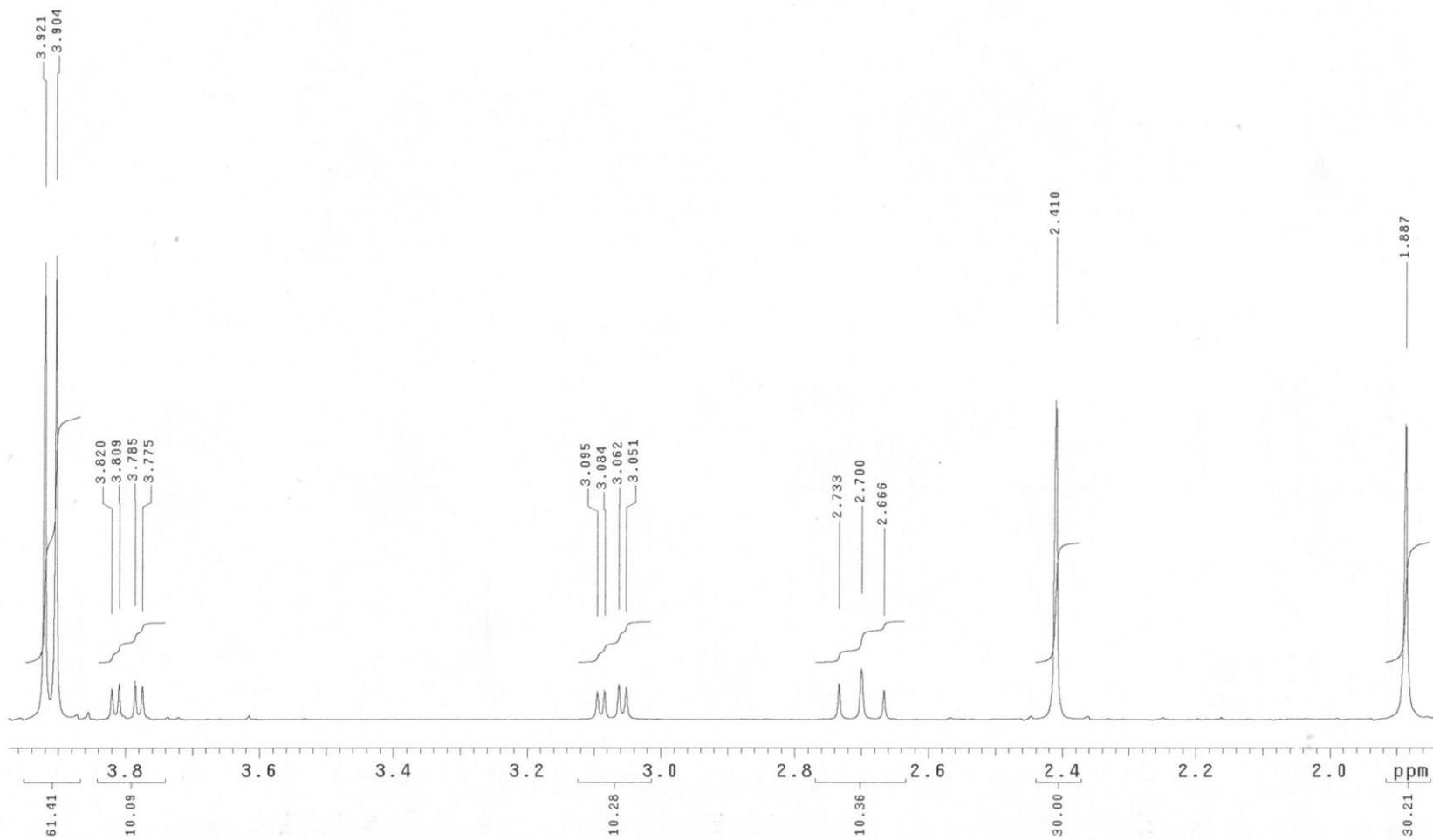


Compound 6a (¹H-NMR spectral data-2)



Compound 6a

¹H NMR (400 MHz, CDCl₃) spectra



Compound 6a (¹³C-NMR spectral data)

KSTsDBF

Pulse Sequence: s2pu1

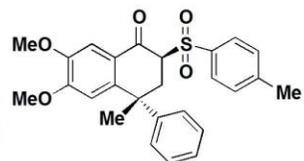
UNITYplus-400 "unity400"

Date: Mar 4 2019

Solvent: CDCl₃

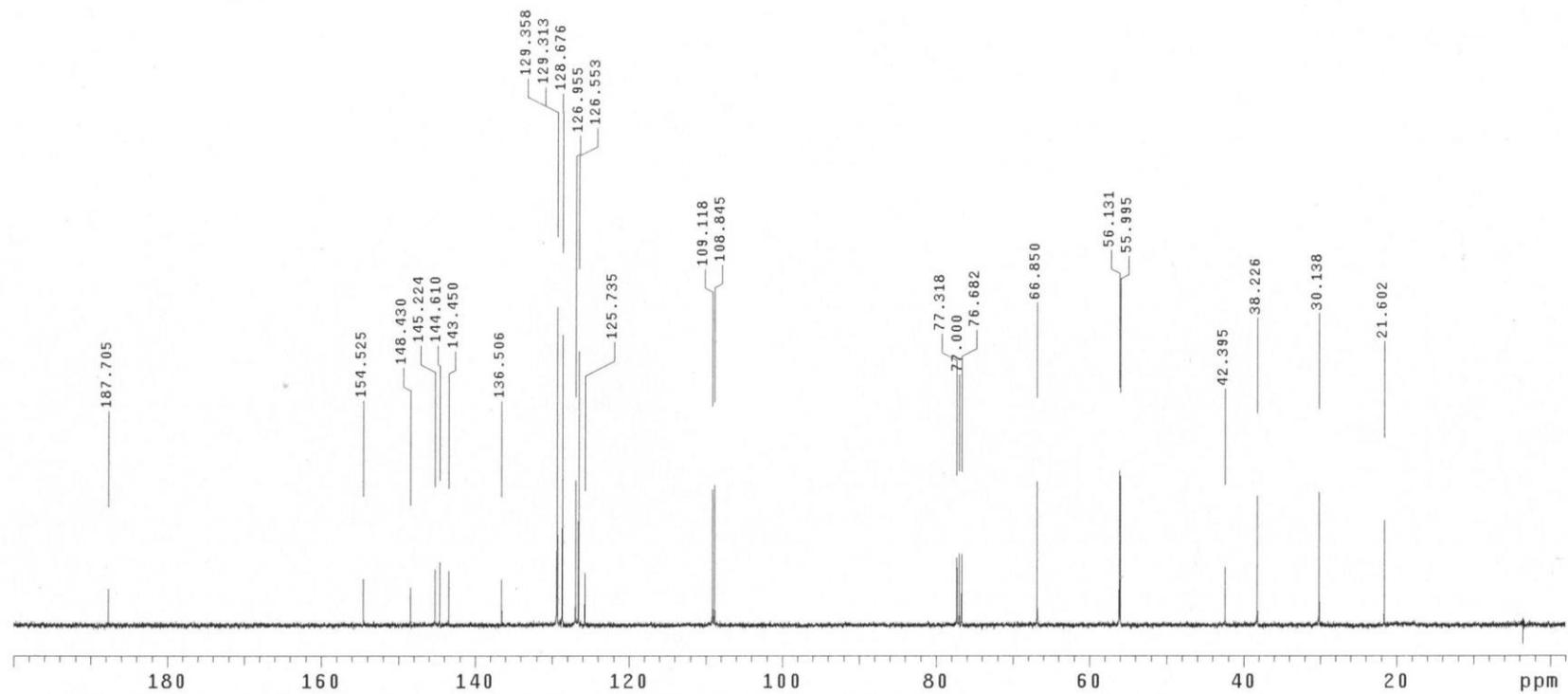
Ambient temperature

Total 1024 repetitions



Compound 6a

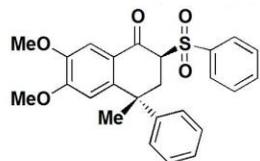
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 6b (¹H-NMR spectral data-1)

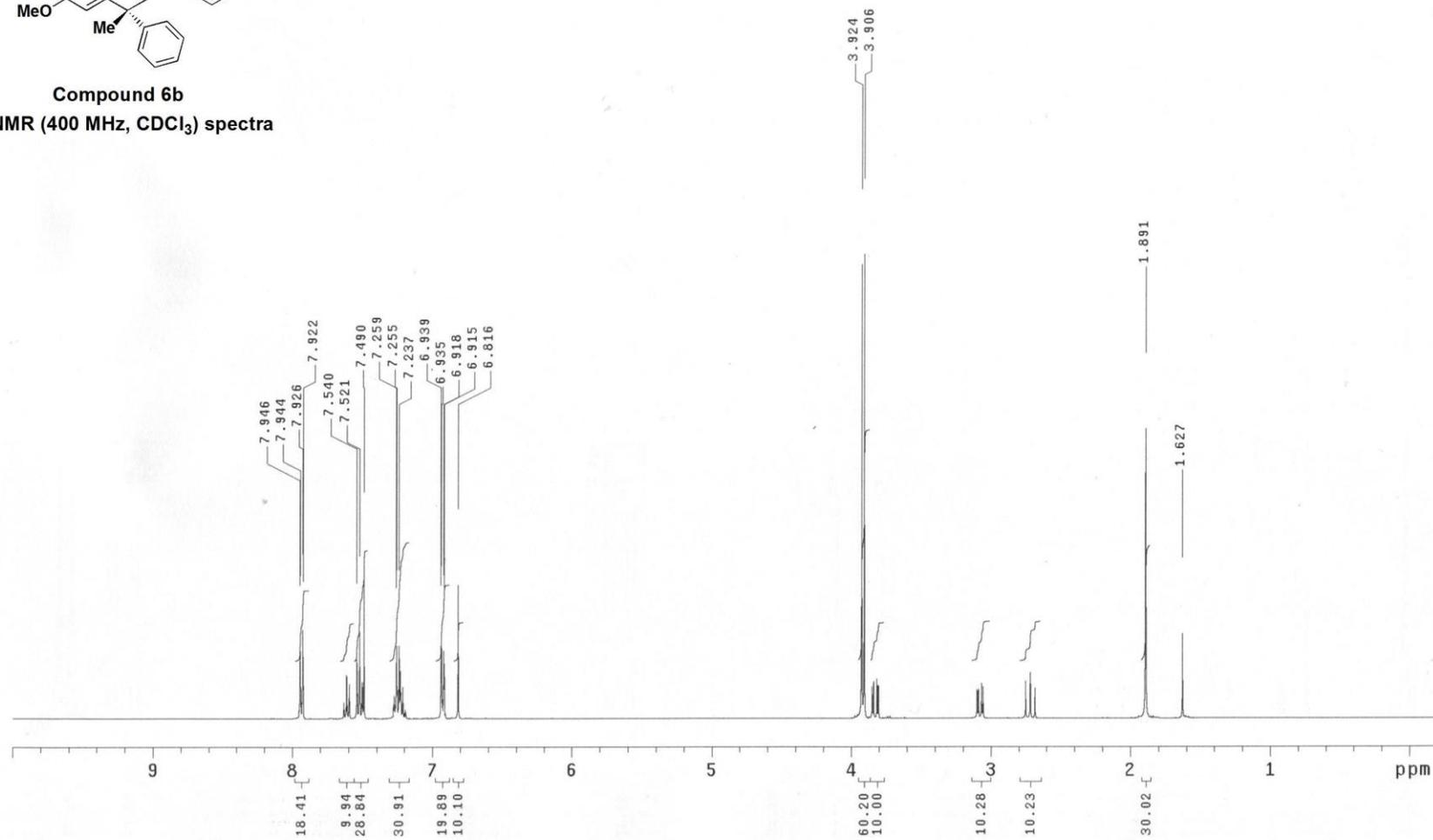
KSBSDBF

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Mar 14 2019
Solvent: CDCl₃
Ambient temperature
Total 32 repetitions

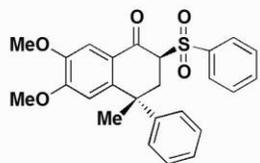


Compound 6b

¹H NMR (400 MHz, CDCl₃) spectra

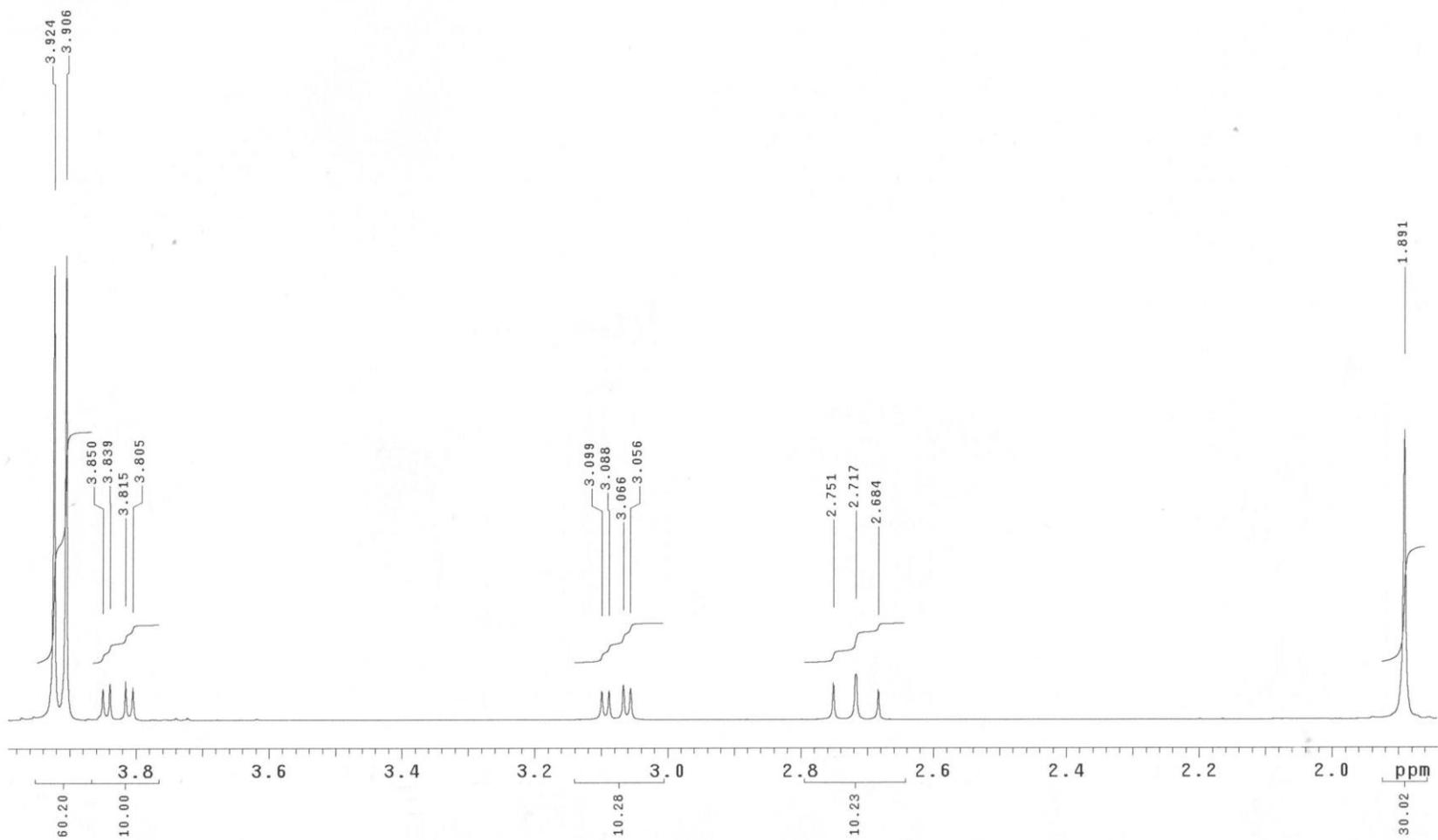


Compound 6b (¹H-NMR spectral data-2)



Compound 6b

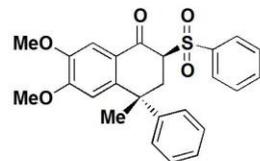
¹H NMR (400 MHz, CDCl₃) spectra



Compound 6b (¹³C-NMR spectral data)

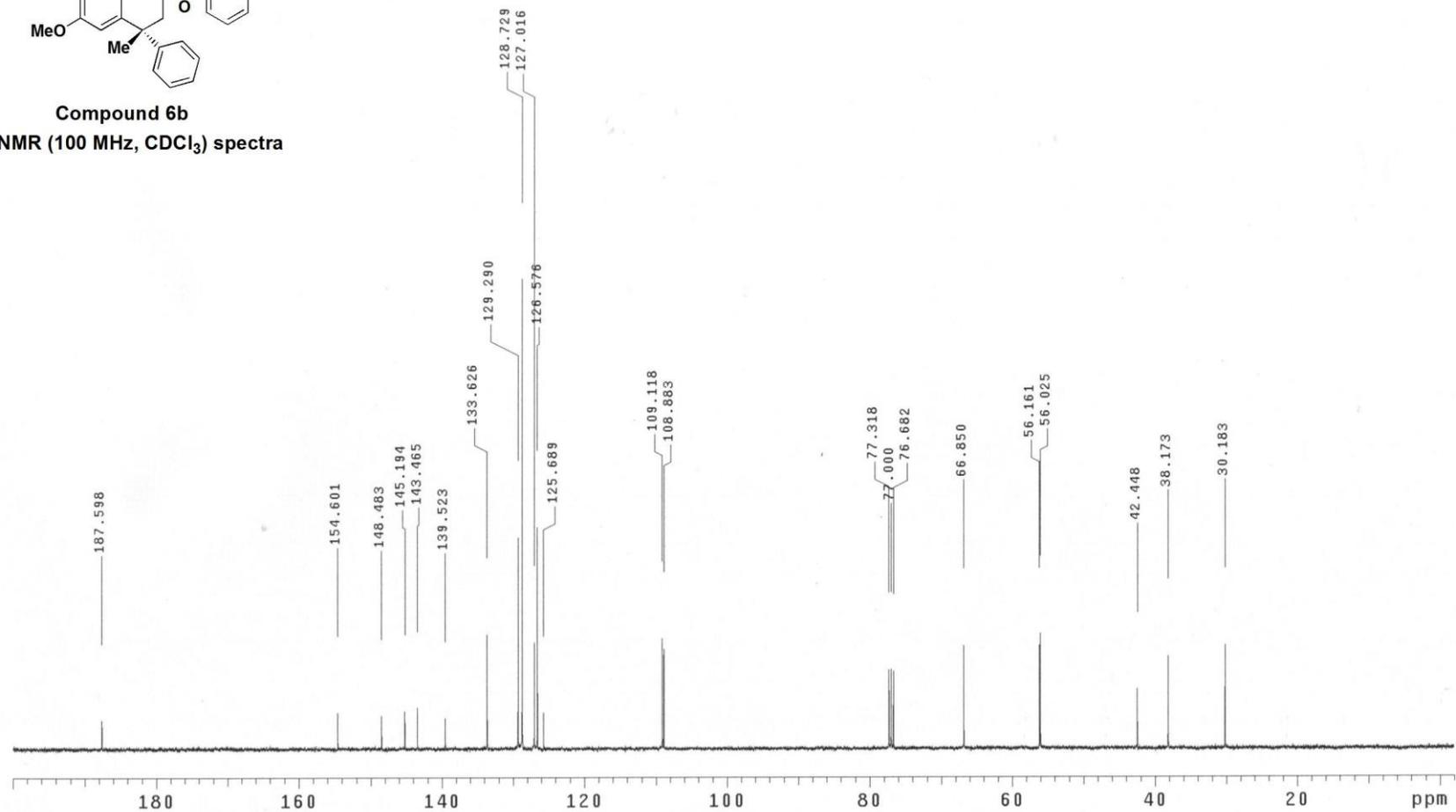
KSBSDBF

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Mar 14 2019
Solvent: CDCl₃
Ambient temperature
Total 1712 repetitions



Compound 6b

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 6c (¹H-NMR spectral data-1)

KSMSDBF

Pulse Sequence: s2pu1

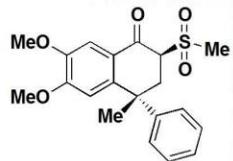
UNITYplus-400 "unity400"

Date: Mar 22 2019

Solvent: CDCl₃

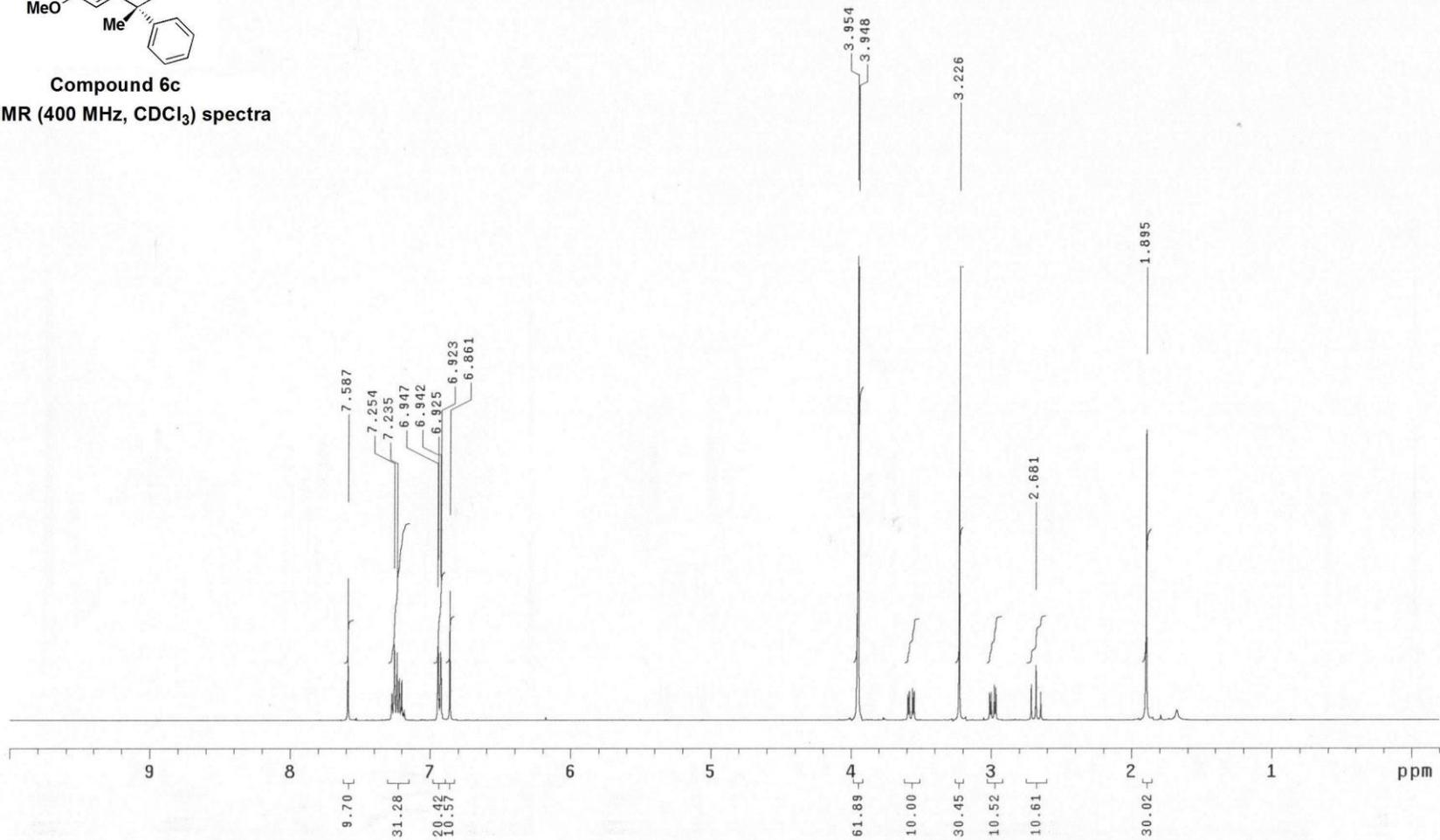
Ambient temperature

Total 32 repetitions

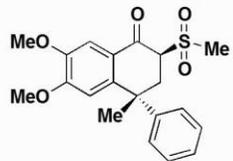


Compound 6c

¹H NMR (400 MHz, CDCl₃) spectra

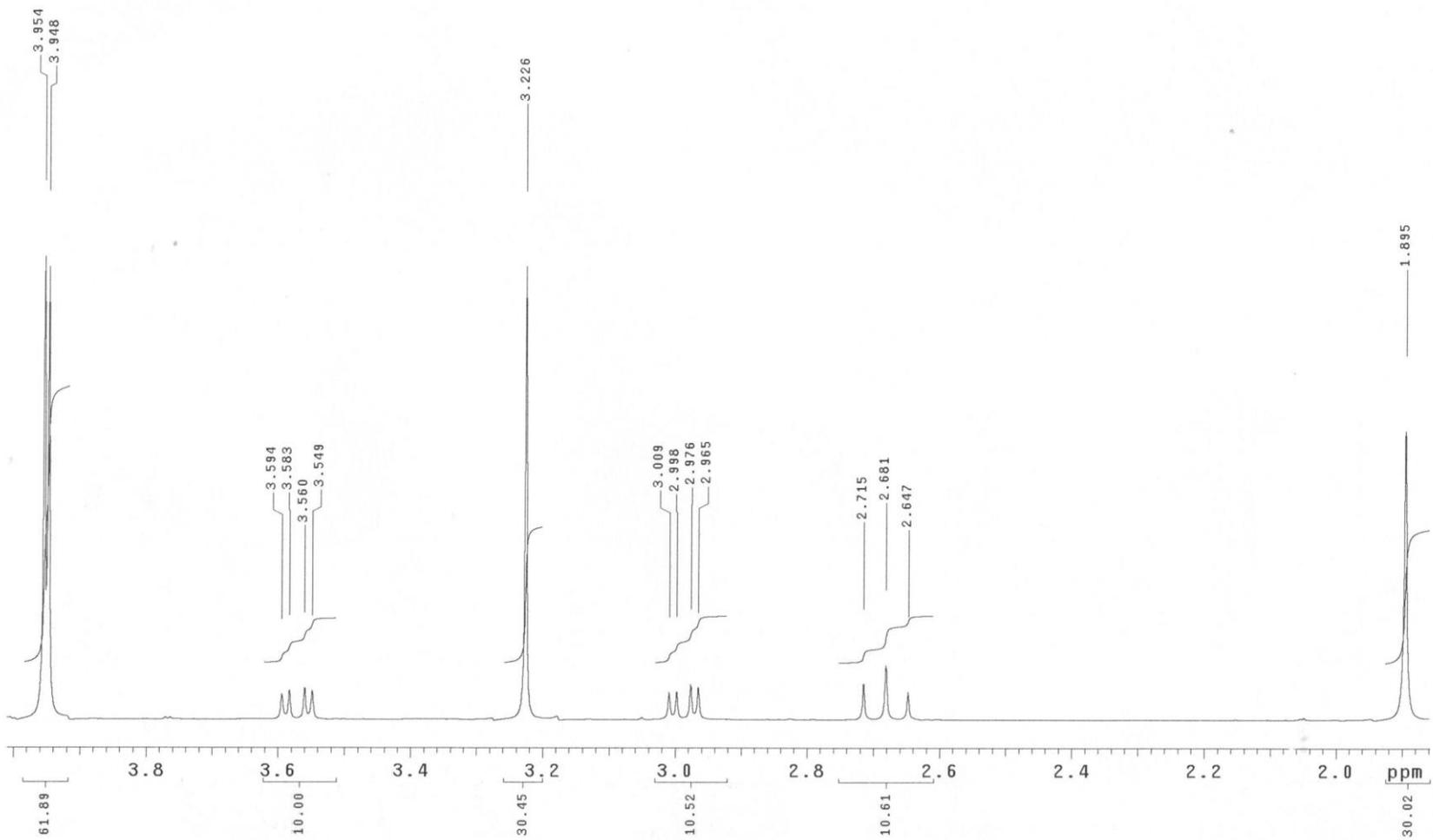


Compound 6c (¹H-NMR spectral data-2)



Compound 6c

¹H NMR (400 MHz, CDCl₃) spectra



Compound 6c (¹³C-NMR spectral data)

KSMSDBF

Pulse Sequence: s2pu1

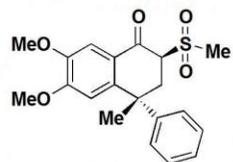
UNITYplus-400 "unity400"

Date: Mar 22 2019

Solvent: CDCl₃

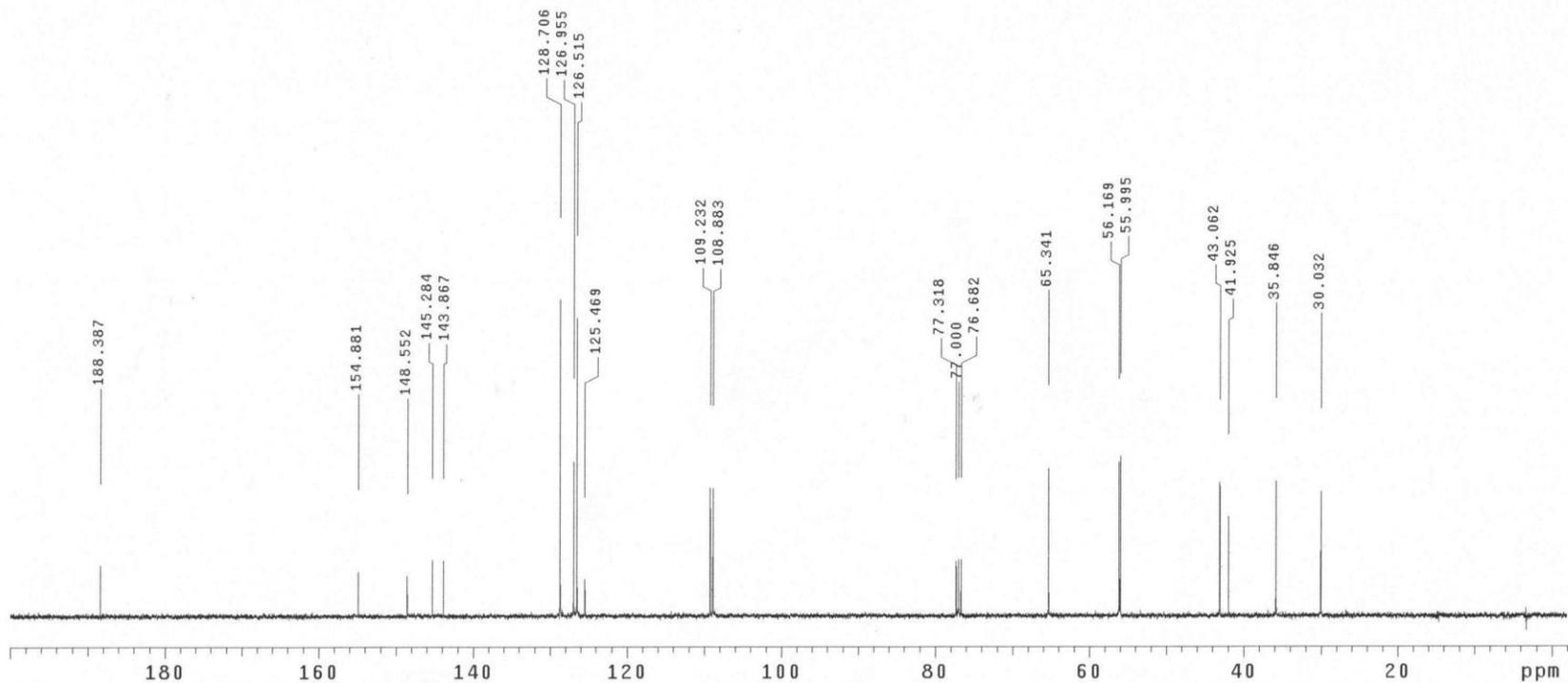
Ambient temperature

Total 432 repetitions



Compound 6c

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 6d (¹H-NMR spectral data-1)

KSmMeDBF

Pulse Sequence: s2pu1

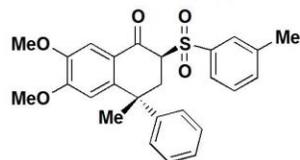
UNITYplus-400 "unity400"

Date: Mar 18 2019

Solvent: CDCl₃

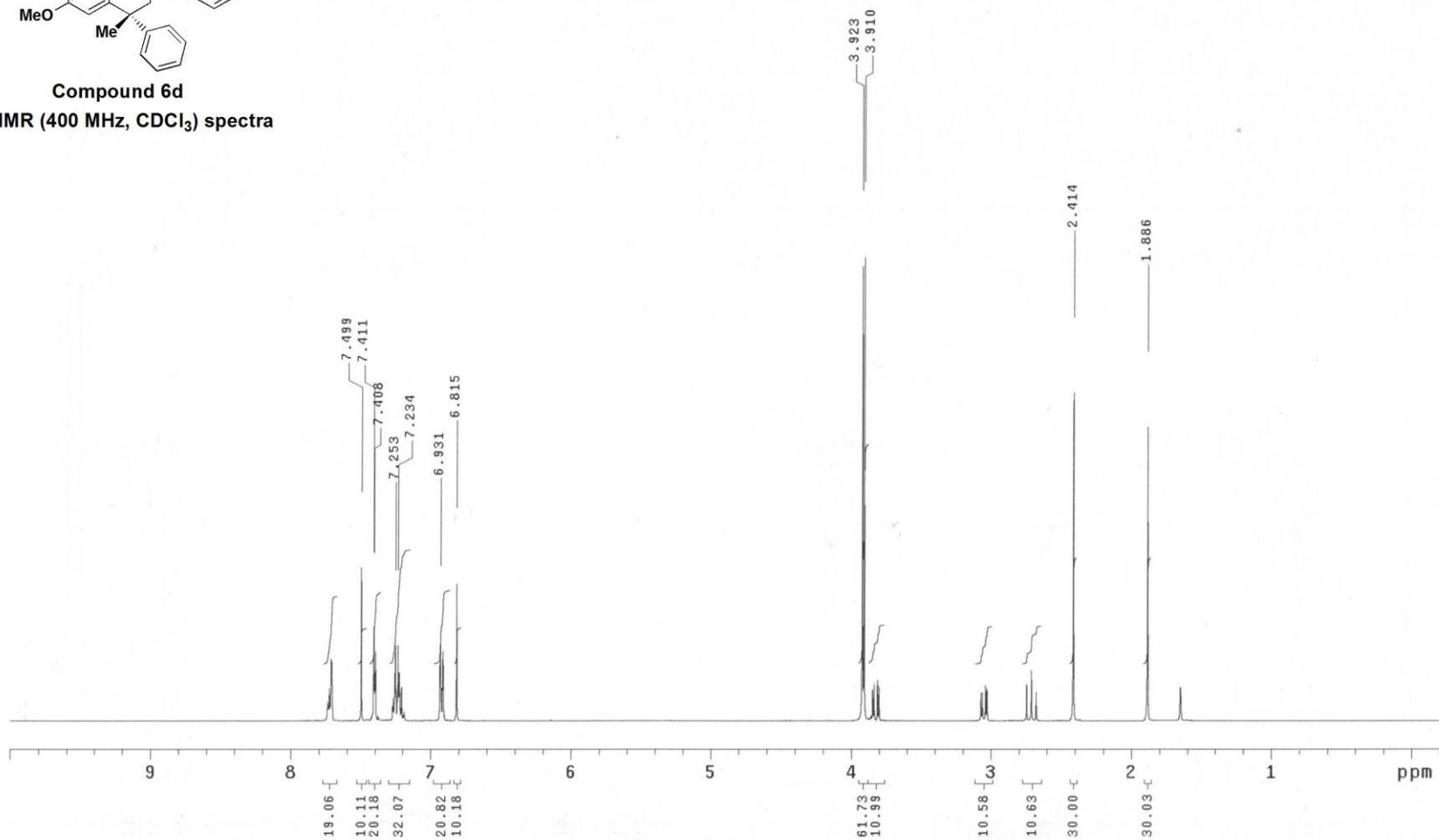
Ambient temperature

Total 32 repetitions

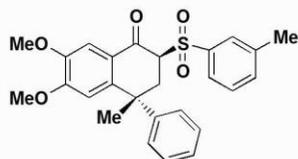


Compound 6d

¹H NMR (400 MHz, CDCl₃) spectra

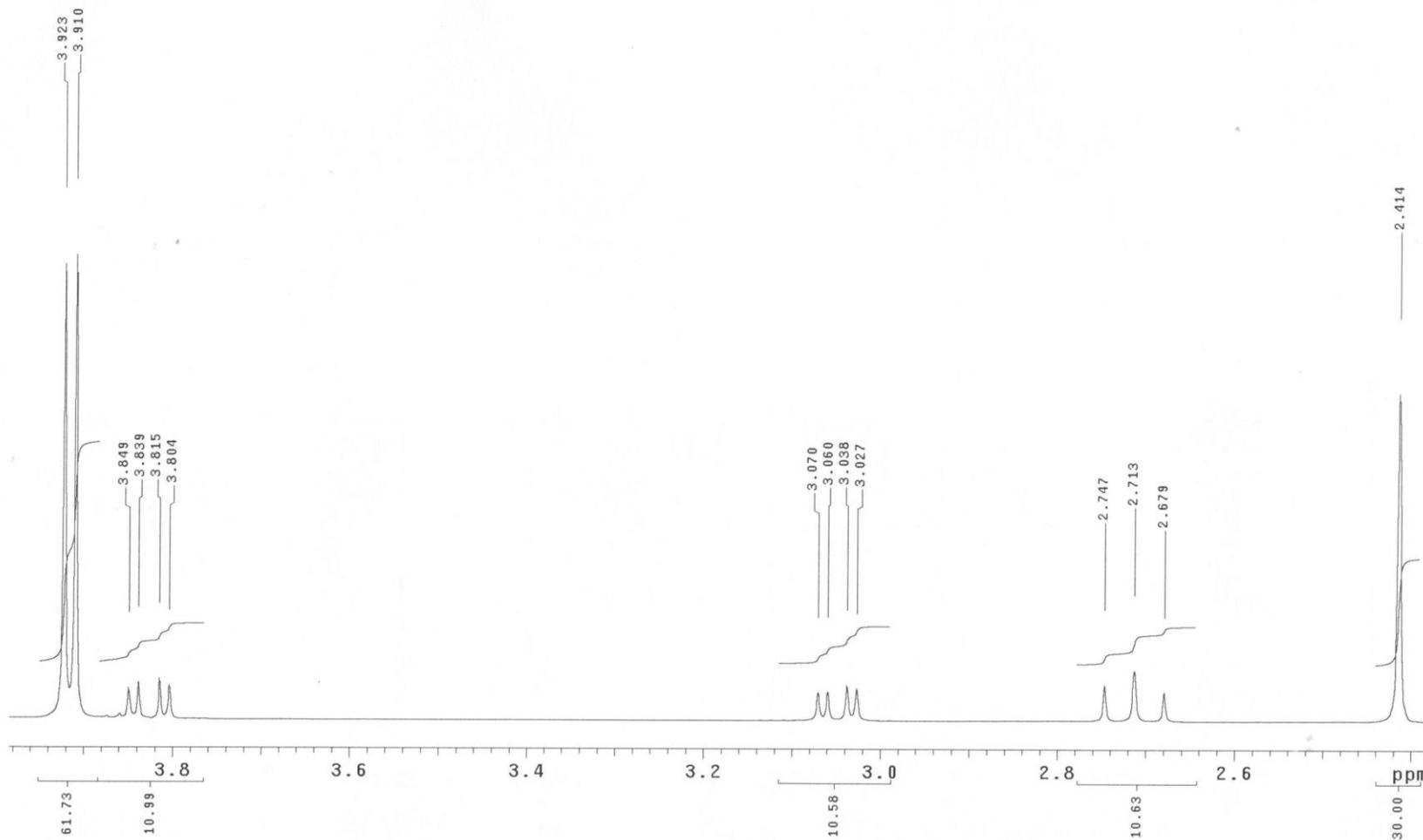


Compound 6d (¹H-NMR spectral data-2)



Compound 6d

¹H NMR (400 MHz, CDCl₃) spectra



Compound 6d (¹³C-NMR spectral data)

KSmMeDBF

Pulse Sequence: s2pu1

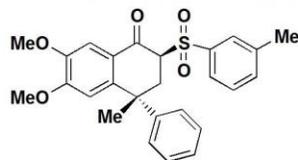
UNITYplus-400 "unity400"

Date: Mar 18 2019

Solvent: CDCl₃

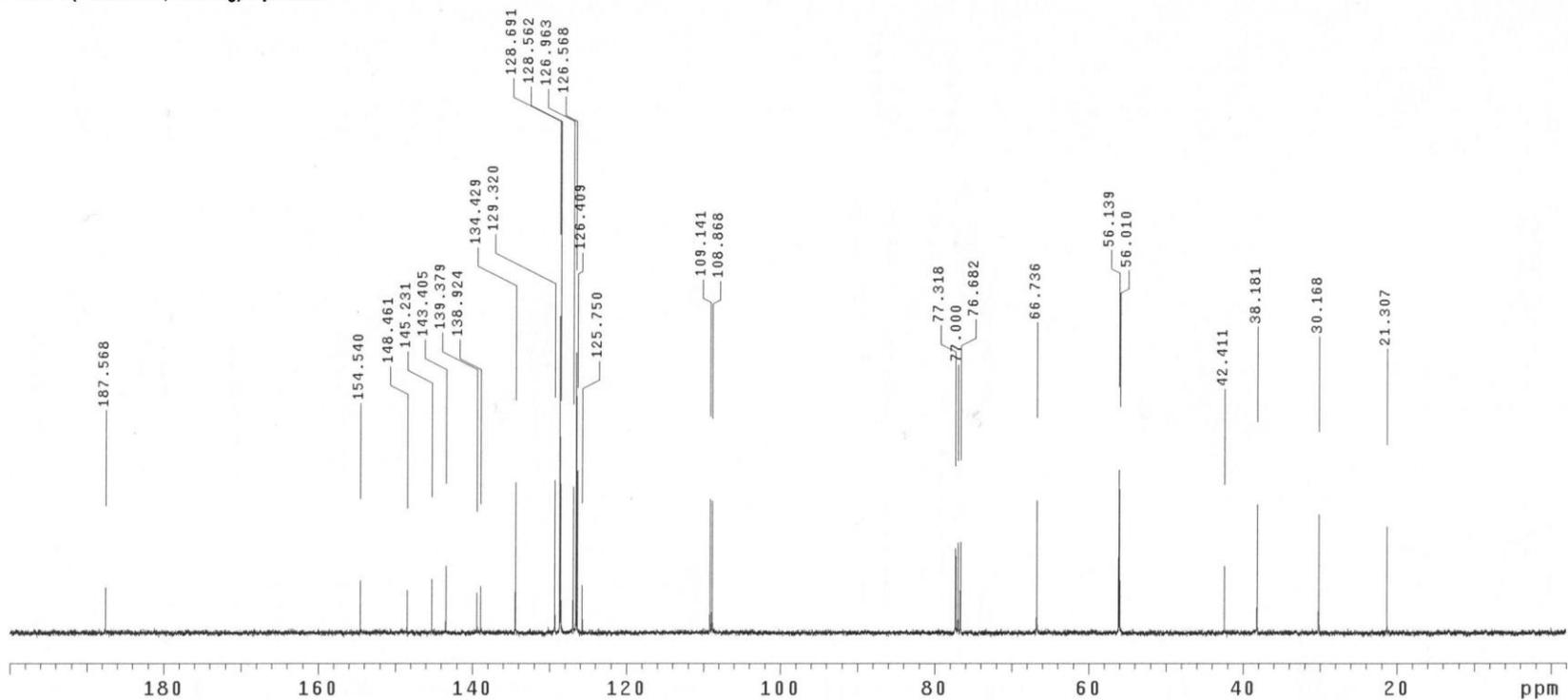
Ambient temperature

Total 1024 repetitions



Compound 6d

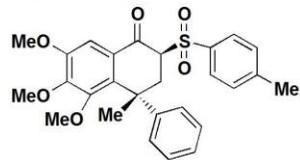
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 6e (¹H-NMR spectral data-1)

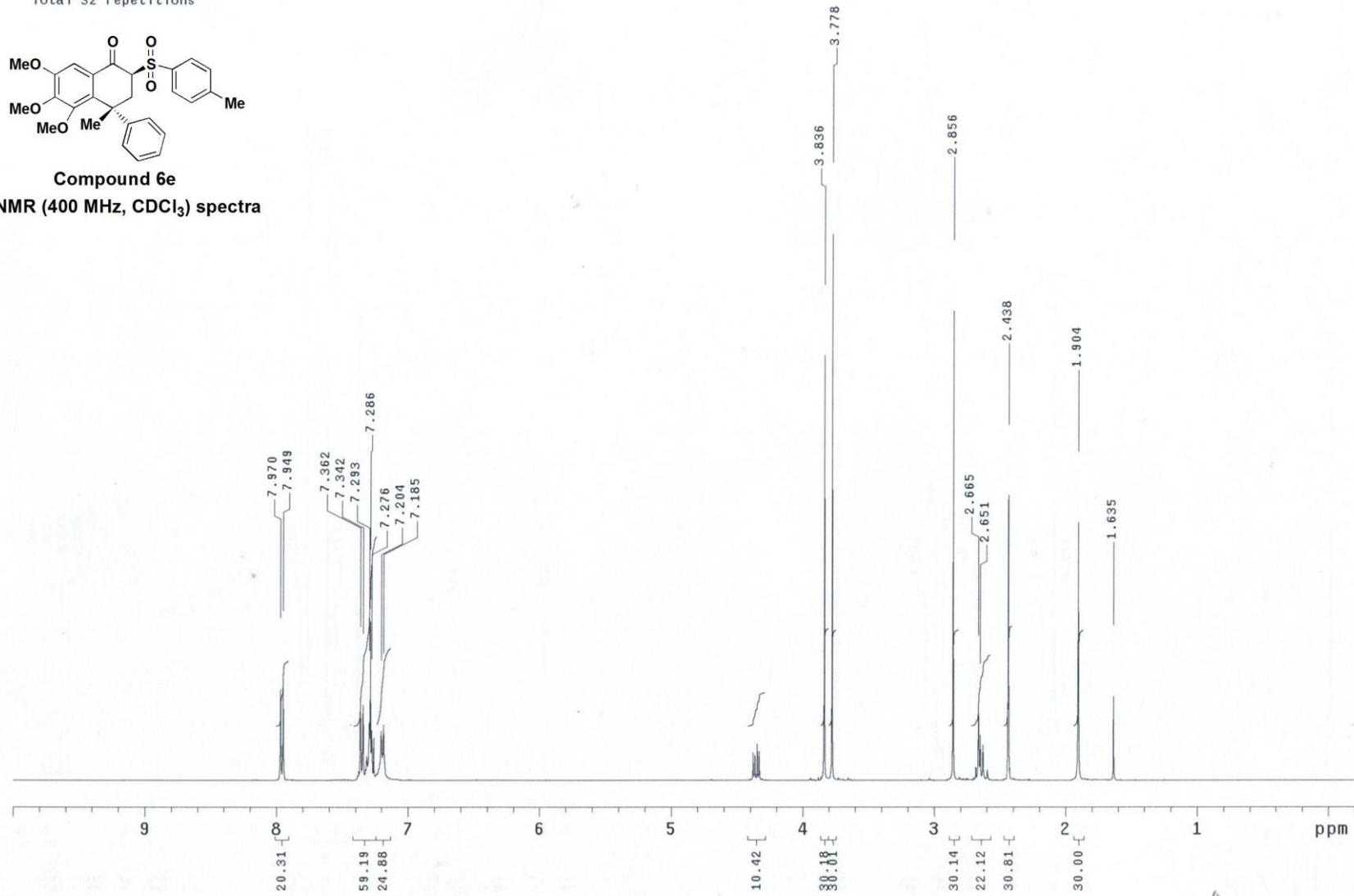
KS3Me0BF

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Mar 11 2019
Solvent: CDCl₃
Ambient temperature
Total 32 repetitions

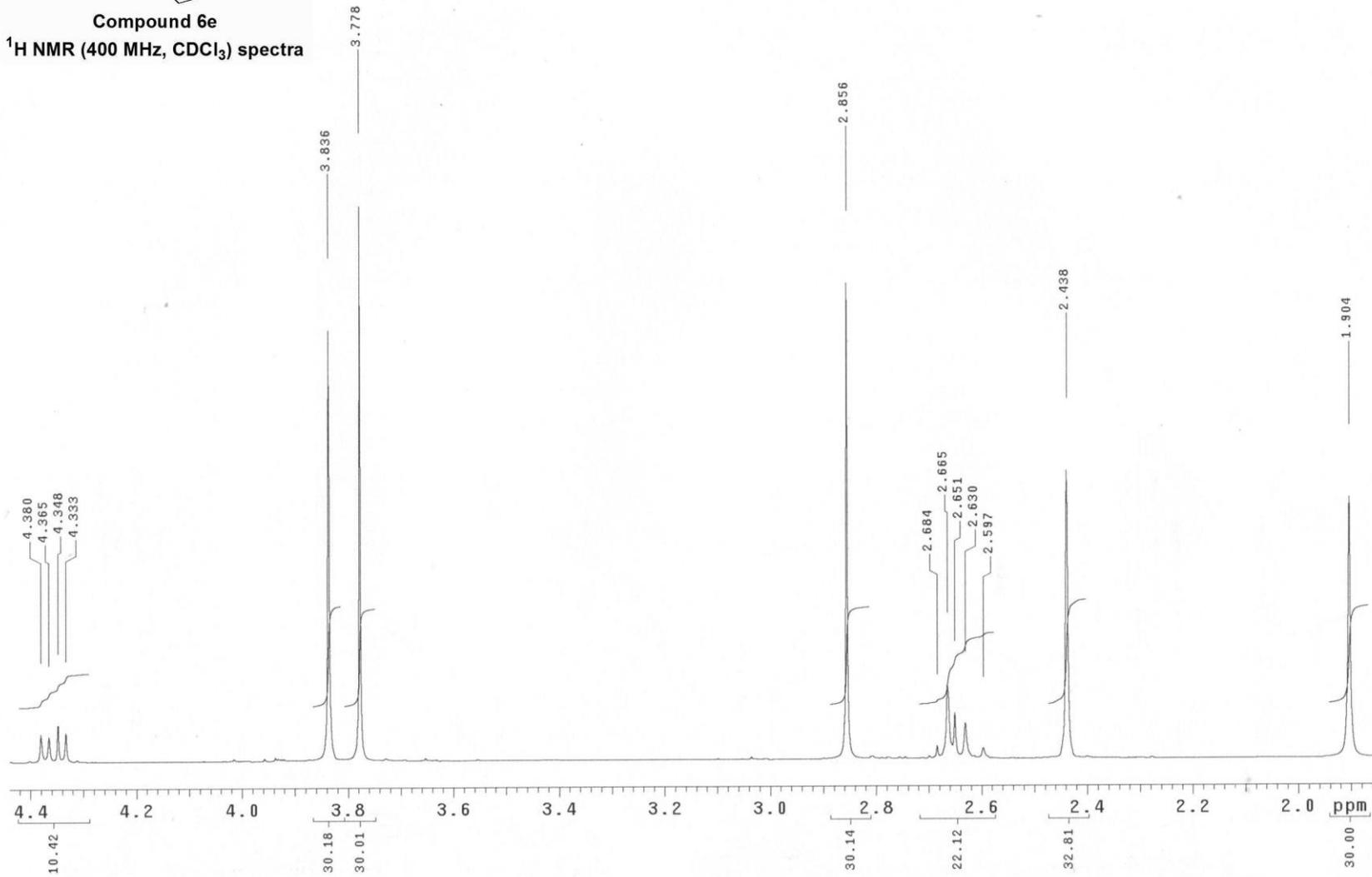
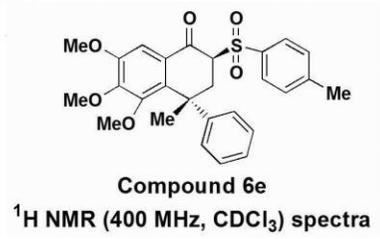


Compound 6e

¹H NMR (400 MHz, CDCl₃) spectra



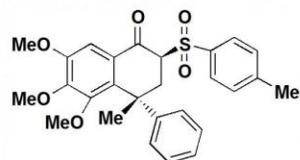
Compound 6e (¹H-NMR spectral data-2)



Compound 6e (¹³C-NMR spectral data)

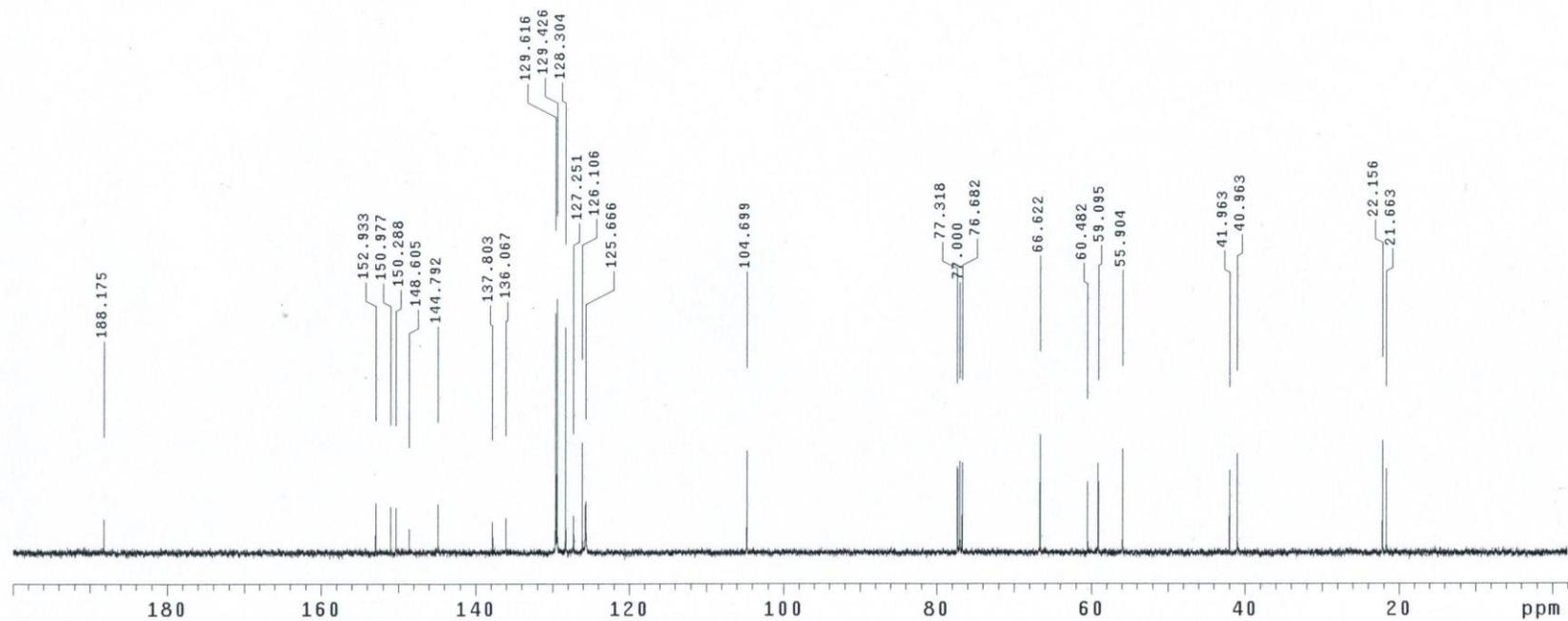
KS3Me0BF

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Mar 11 2019
Solvent: CDCl₃
Ambient temperature
Total 640 repetitions



Compound 6e

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 7a (¹H-NMR spectral data-1)

KSTScrBF

Pulse Sequence: s2pu1

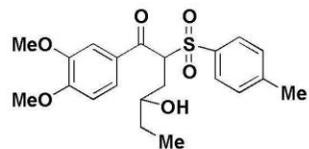
UNITYplus-400 "unity400"

Date: Jan 17 2019

Solvent: CDCl₃

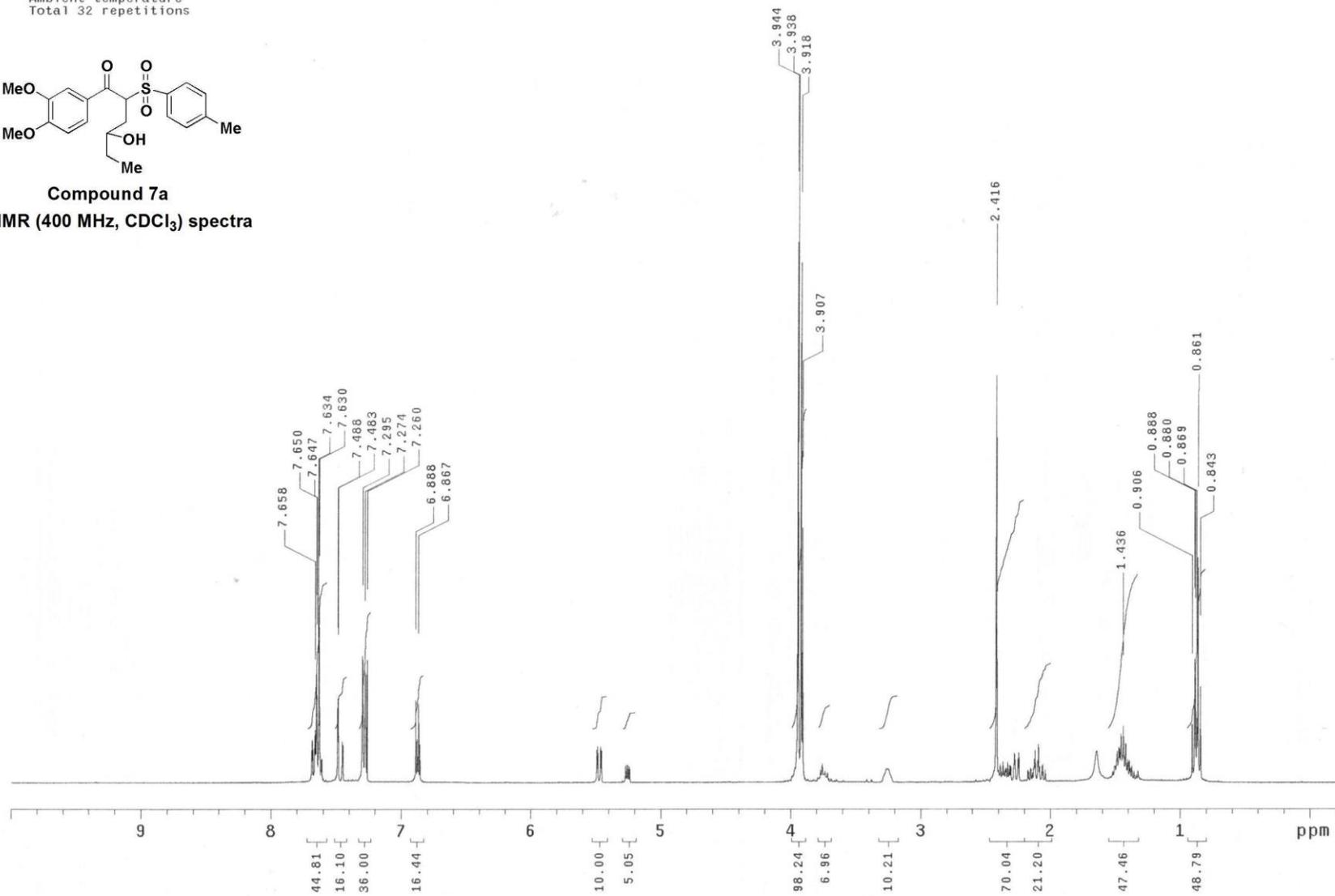
Ambient temperature

Total 32 repetitions

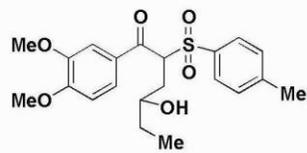


Compound 7a

¹H NMR (400 MHz, CDCl₃) spectra

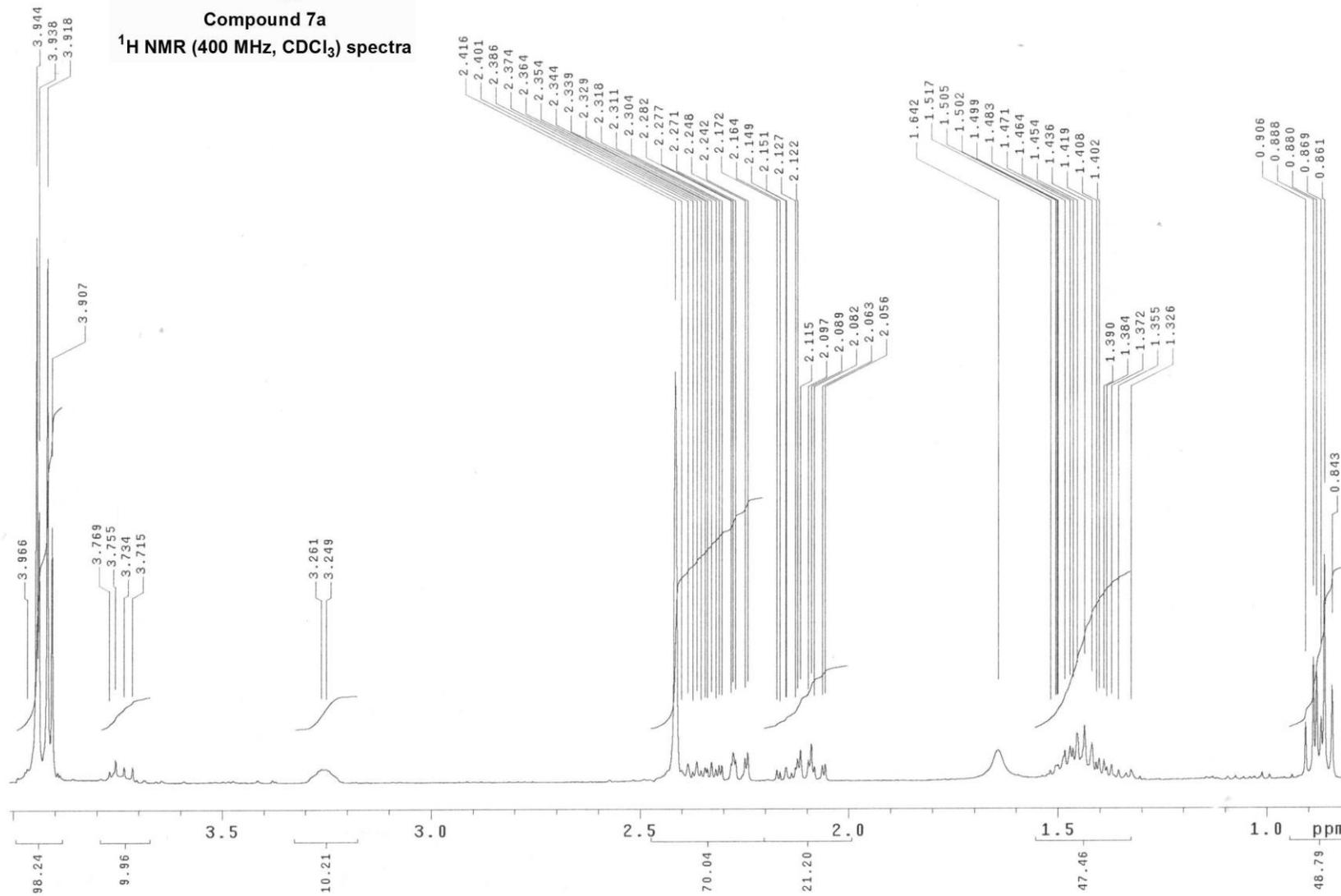


Compound 7a (¹H-NMR spectral data-2)

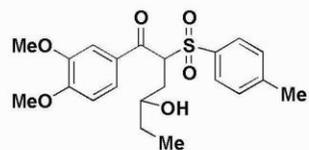


Compound 7a

¹H NMR (400 MHz, CDCl₃) spectra

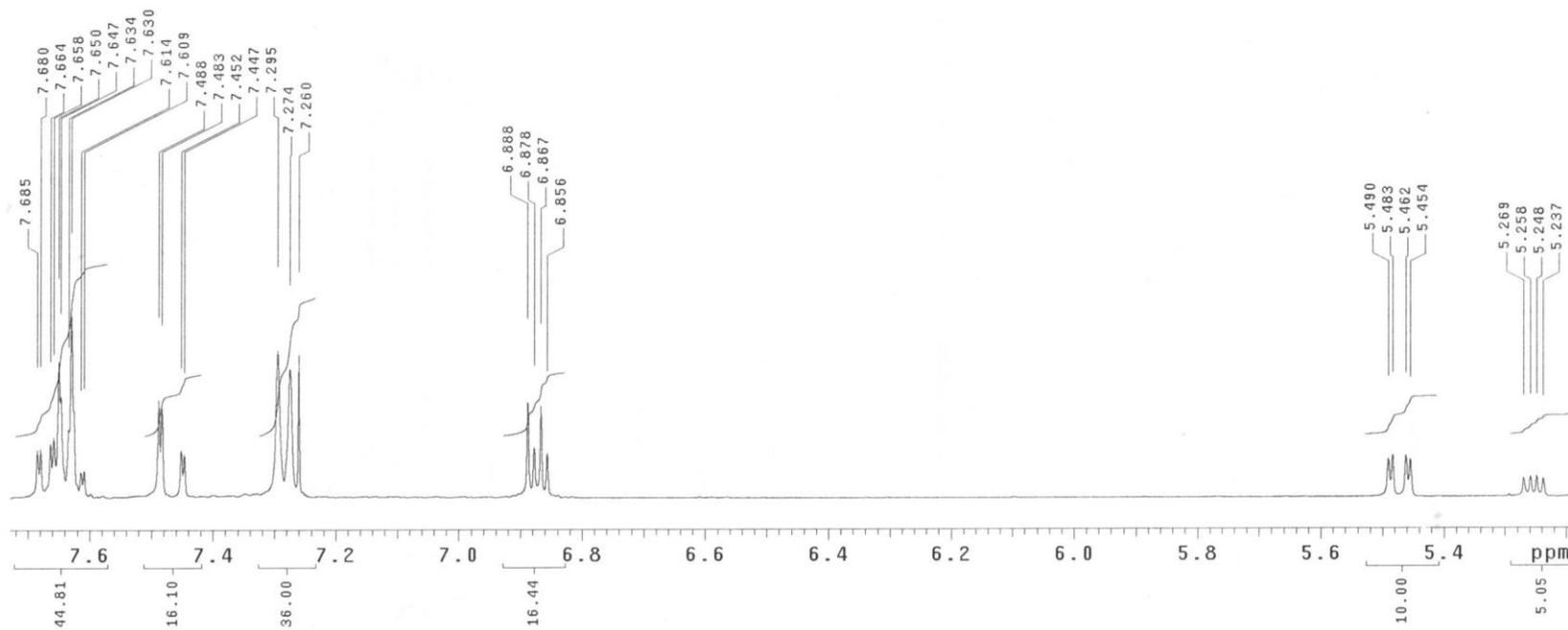


Compound 7a (¹H-NMR spectral data-3)



Compound 7a

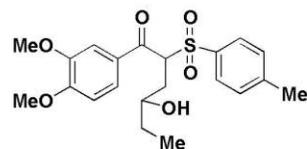
¹H NMR (400 MHz, CDCl₃) spectra



Compound 7a (¹³C-NMR spectral data)

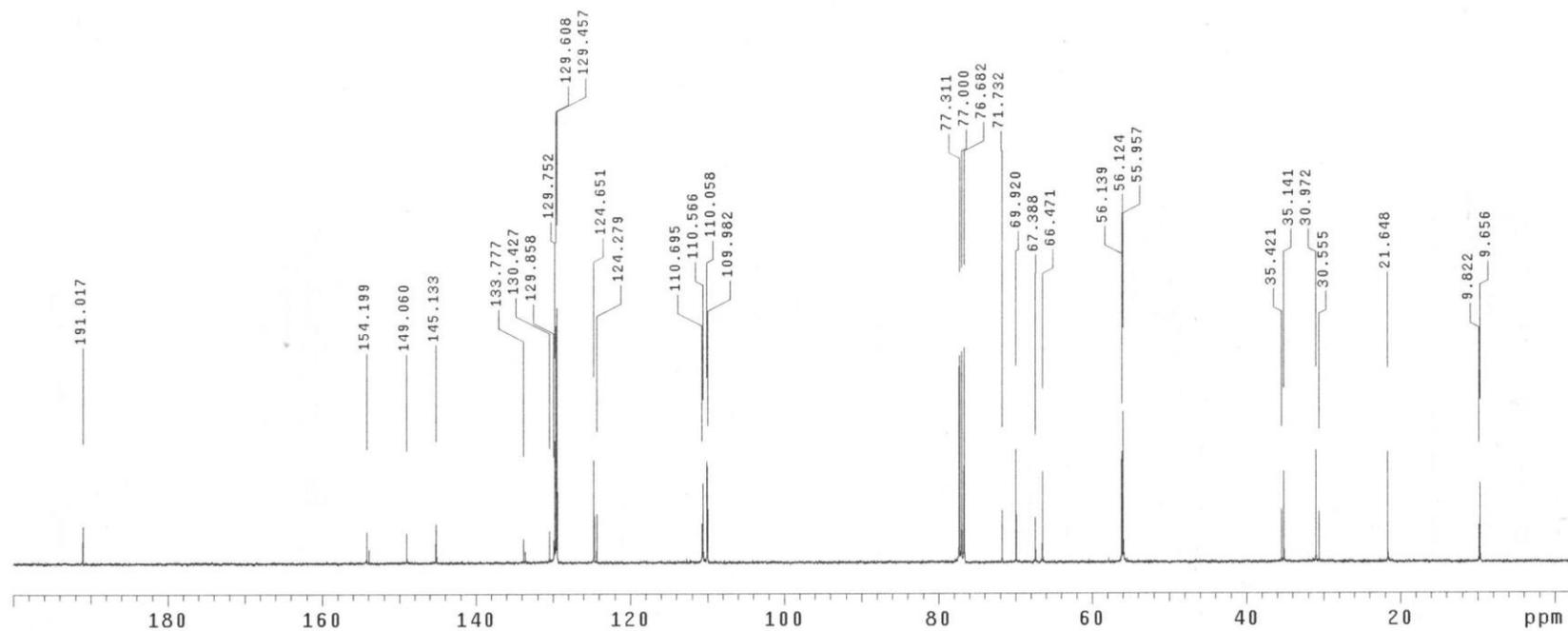
KSTSCrBF

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Jan 17 2019
Solvent: CDCl₃
Ambient temperature
Total 32000 repetitions



Compound 7a

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 7b (¹H-NMR spectral data-1)

KSFcrBF

Pulse Sequence: s2pu1

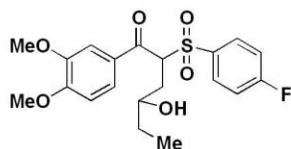
UNITYplus-400 "unity400"

Date: Dec 27 2018

Solvent: CDCl₃

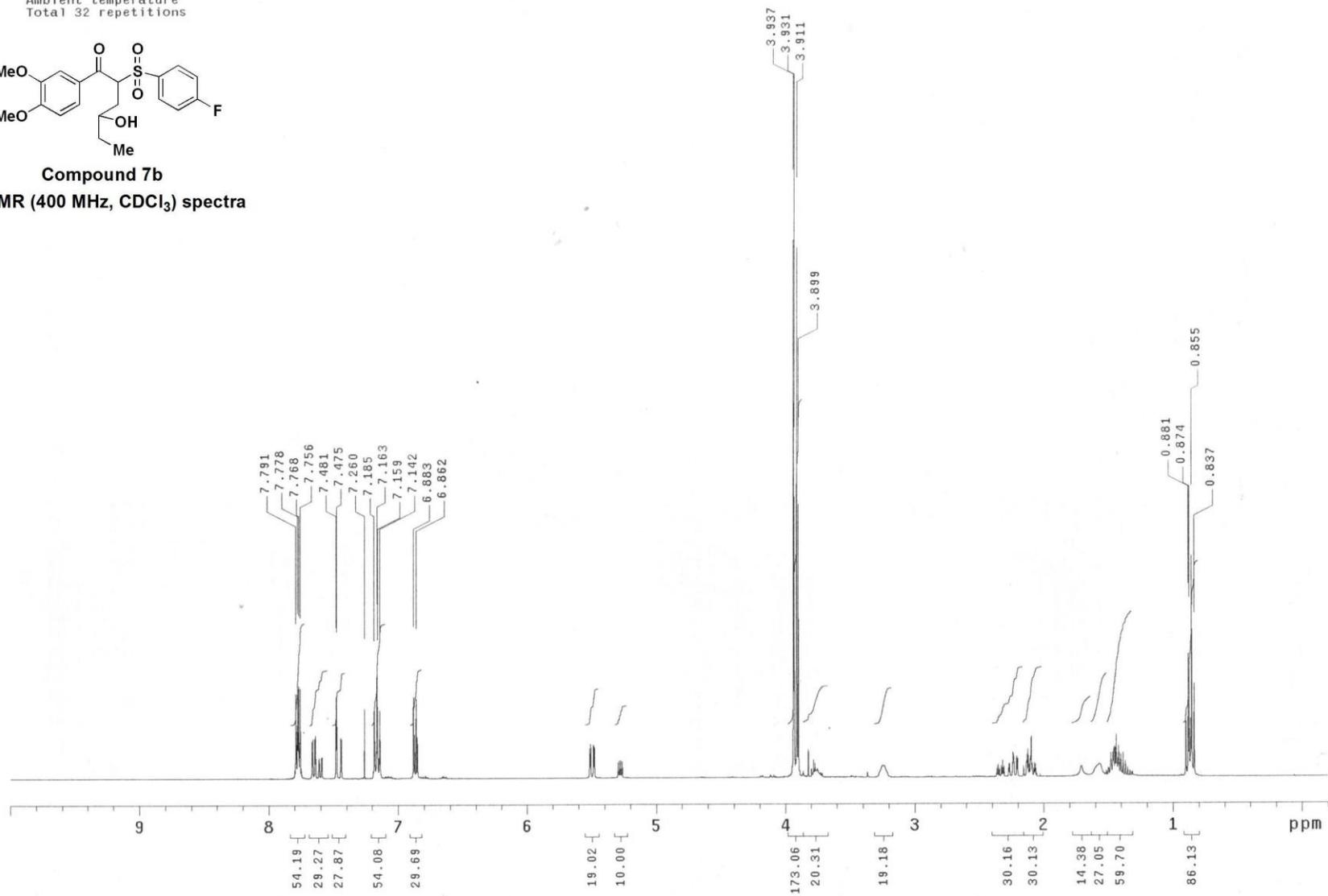
Ambient temperature

Total 32 repetitions

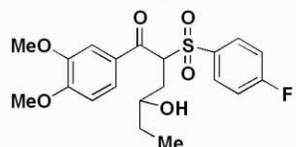


Compound 7b

¹H NMR (400 MHz, CDCl₃) spectra

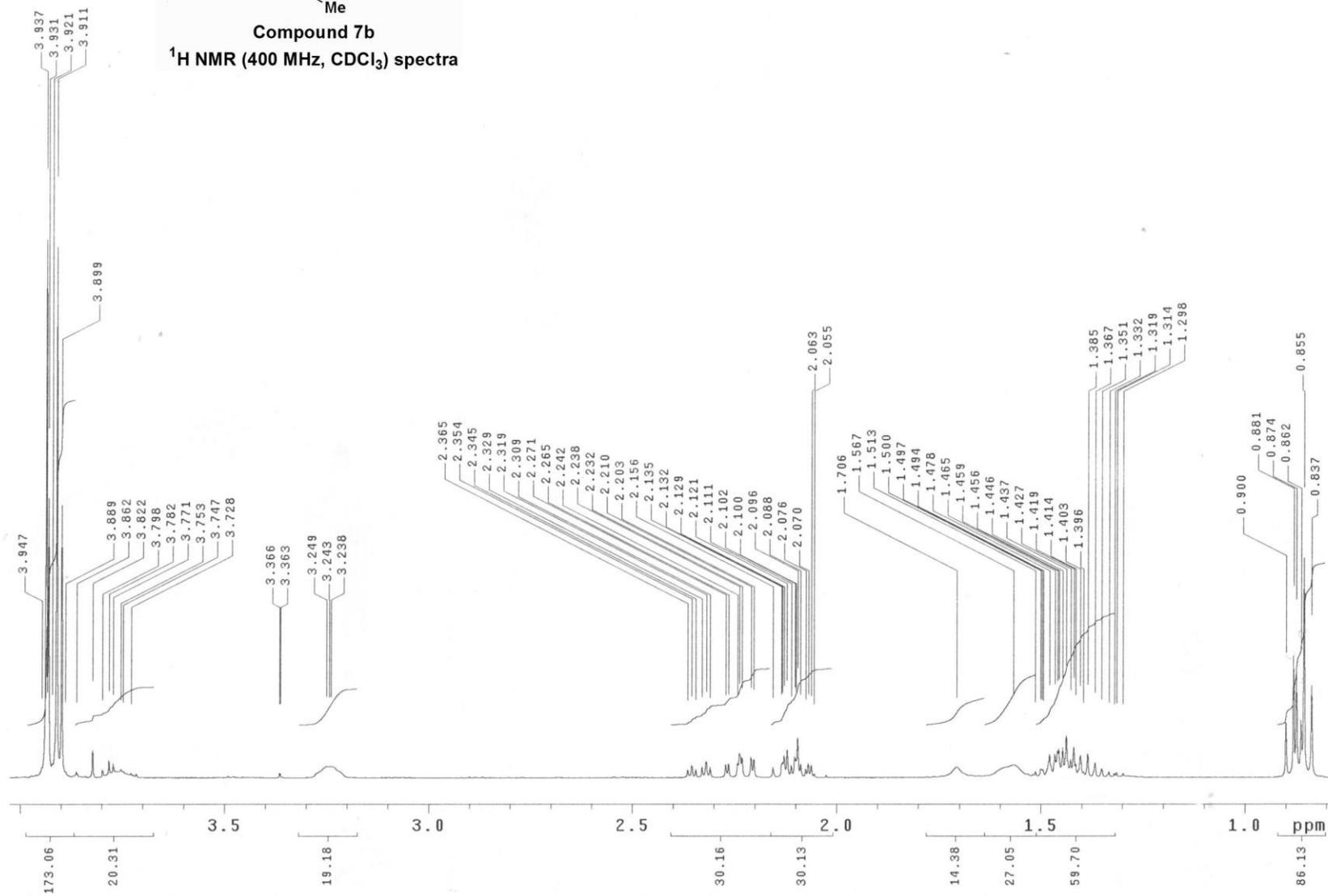


Compound 7b (¹H-NMR spectral data-2)

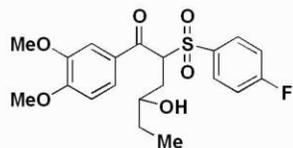


Compound 7b

¹H NMR (400 MHz, CDCl₃) spectra

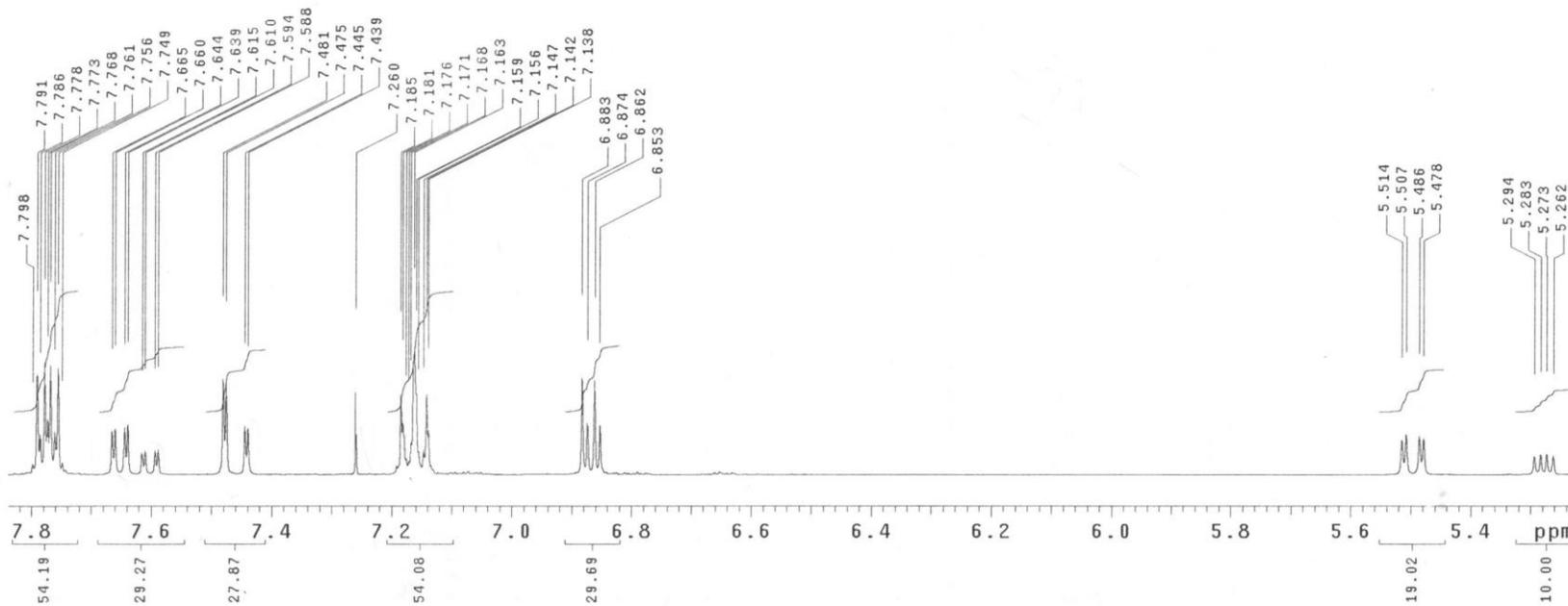


Compound 7b (¹H-NMR spectral data-3)



Compound 7b

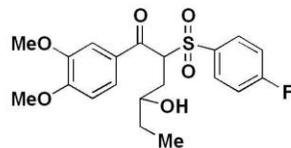
¹H NMR (400 MHz, CDCl₃) spectra



Compound 7b (¹³C-NMR spectral data)

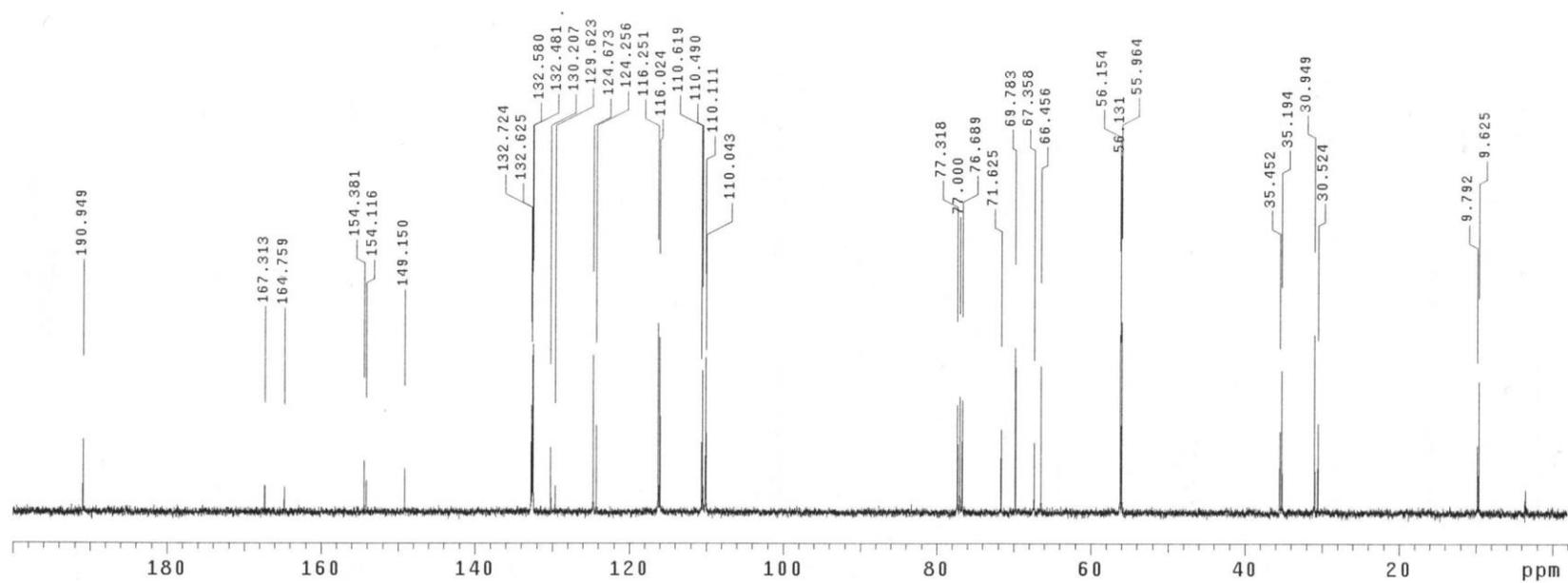
KSFcrBF

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Dec 27 2018
Solvent: CDCl₃
Ambient temperature
Total 1024 repetitions



Compound 7b

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 7c (¹H-NMR spectral data-1)

KSOMeCrBF

Pulse Sequence: s2pu1

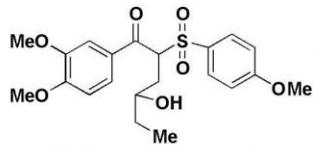
UNITYplus-400 "unity400"

Date: Jan 14 2019

Solvent: CDCl₃

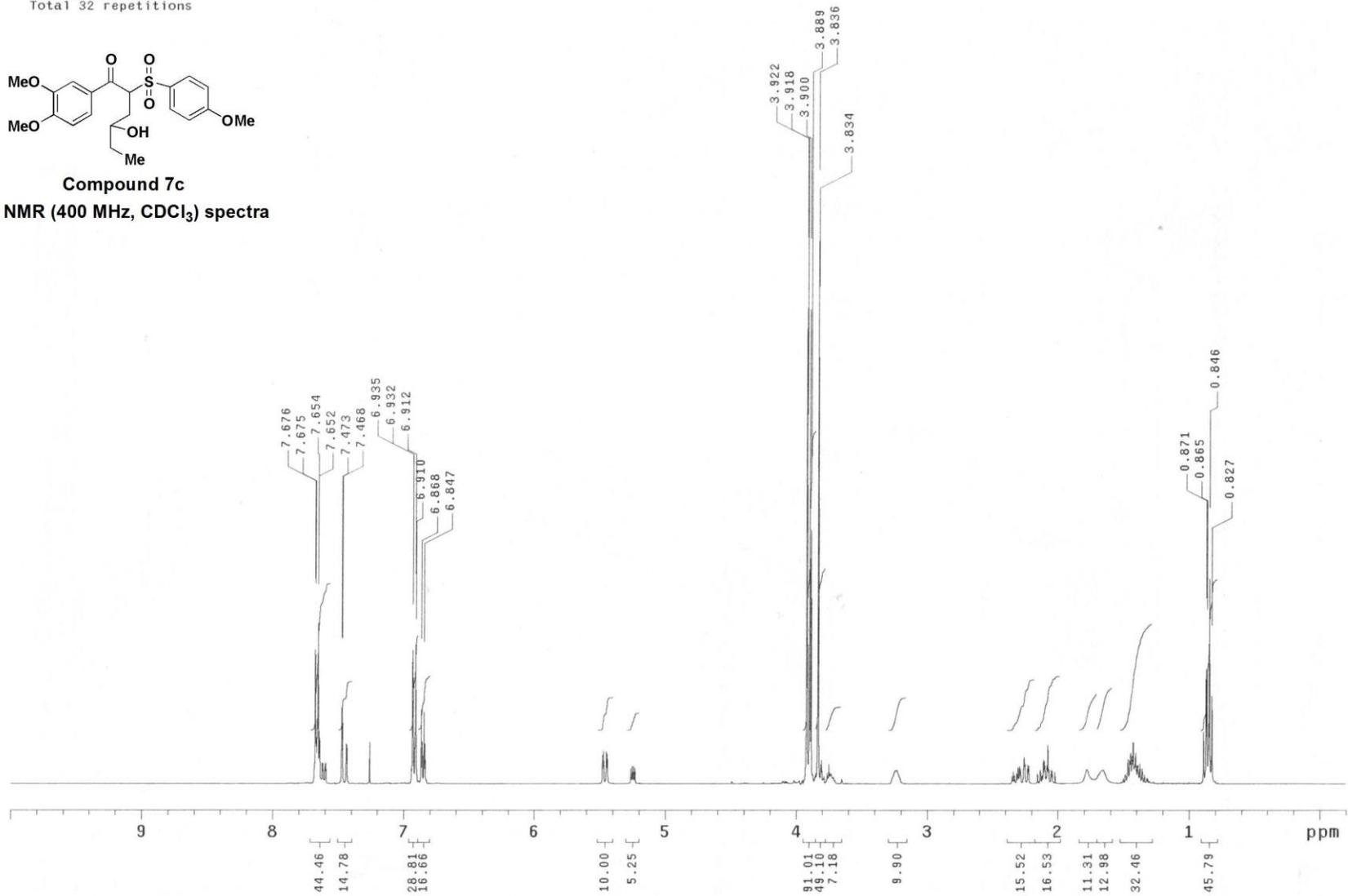
Ambient temperature

Total 32 repetitions

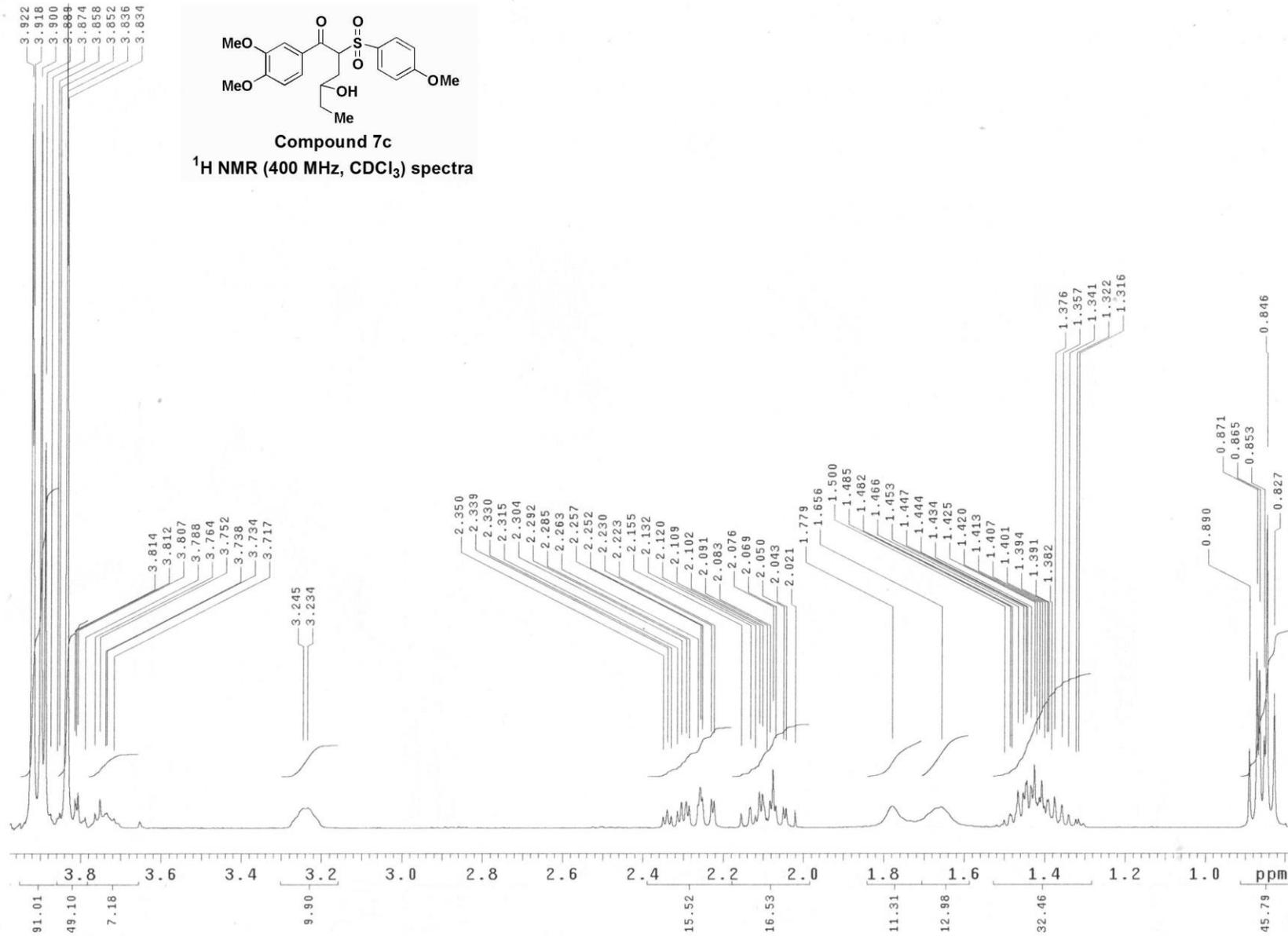


Compound 7c

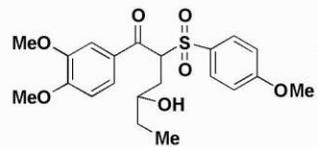
¹H NMR (400 MHz, CDCl₃) spectra



Compound 7c (¹H-NMR spectral data-2)

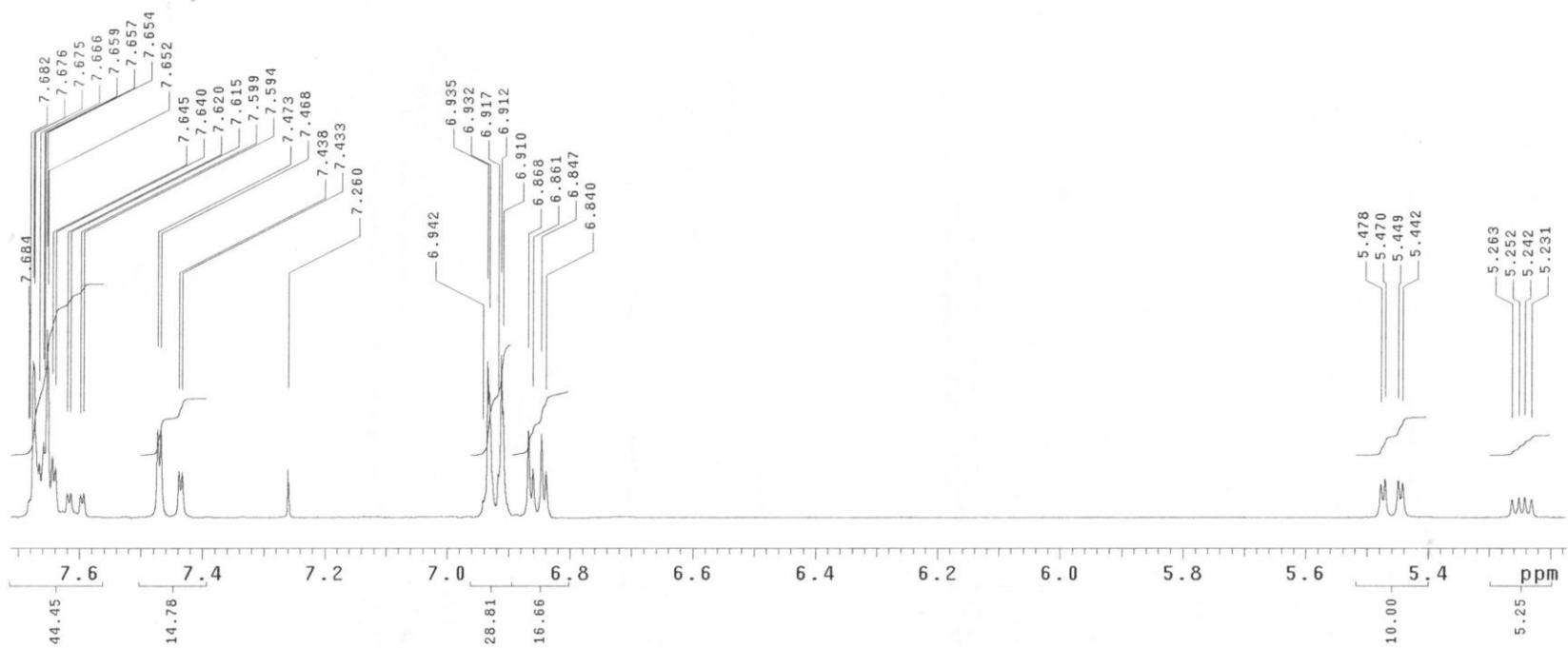


Compound 7c (¹H-NMR spectral data-3)



Compound 7c

¹H NMR (400 MHz, CDCl₃) spectra



Compound 7c (¹³C-NMR spectral data)

KSOMeCrBF

Pulse Sequence: s2pu1

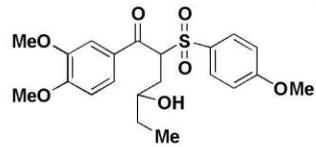
UNITYplus-400 "unity400"

Date: Jan 14 2019

Solvent: CDCl₃

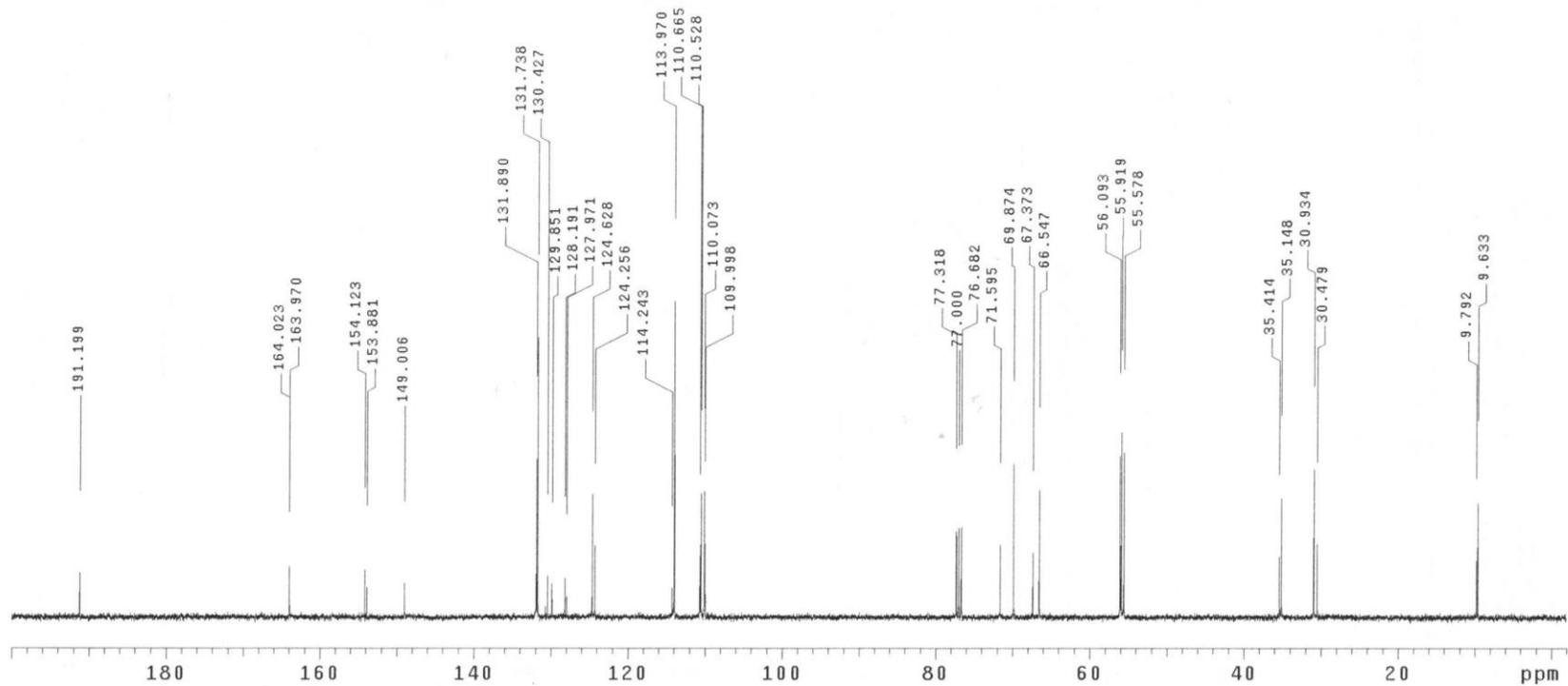
Ambient temperature

Total 1056 repetitions



Compound 7c

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 7d (¹H-NMR spectral data-1)

KSPHbuCrBF

Pulse Sequence: s2pu1

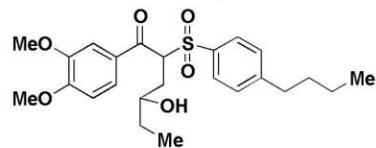
UNITYplus-400 "unity400"

Date: Jan 11 2019

Solvent: CDCl₃

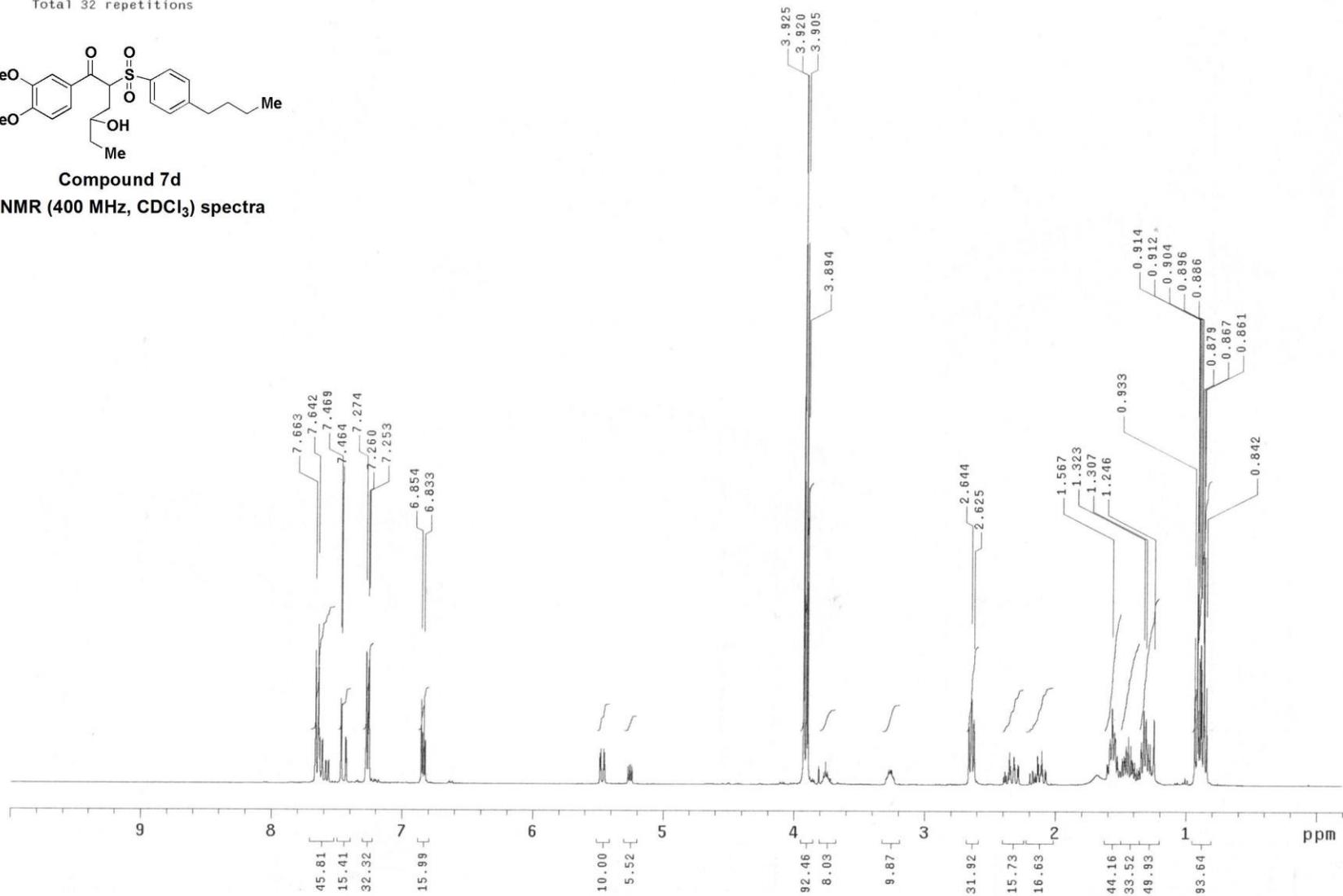
Ambient temperature

Total 32 repetitions

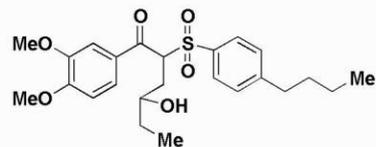


Compound 7d

¹H NMR (400 MHz, CDCl₃) spectra

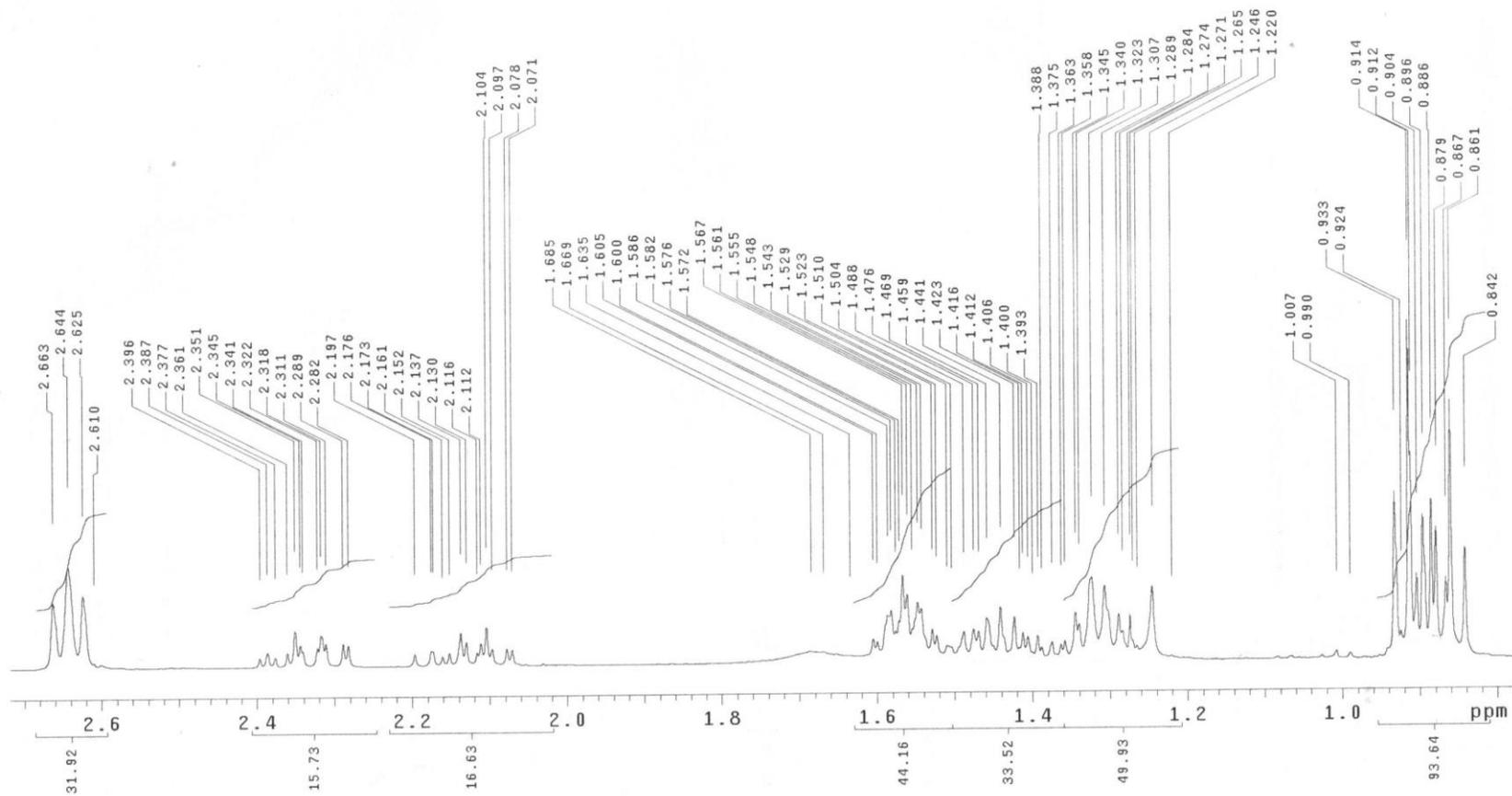


Compound 7d (¹H-NMR spectral data-2)

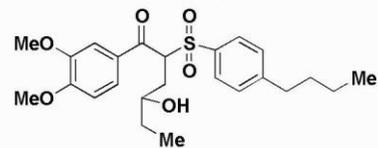


Compound 7d

¹H NMR (400 MHz, CDCl₃) spectra

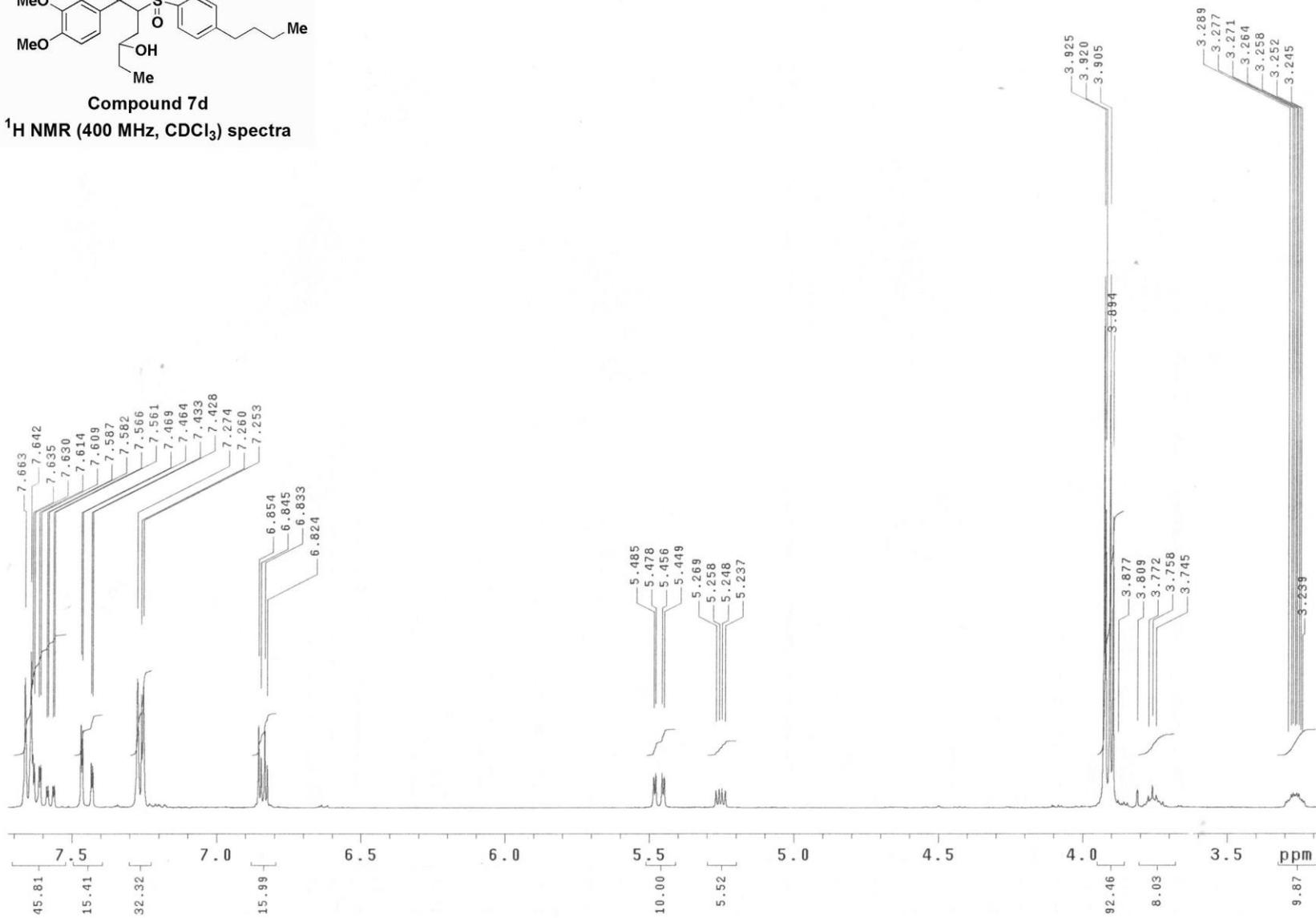


Compound 7d (¹H-NMR spectral data-3)



Compound 7d

¹H NMR (400 MHz, CDCl₃) spectra



Compound 7d (¹³C-NMR spectral data)

KSPHbUCrBF

Pulse Sequence: s2pu1

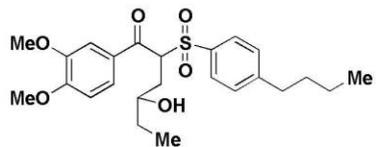
UNITYplus-400 "unity400"

Date: Jan 11 2019

Solvent: CDCl₃

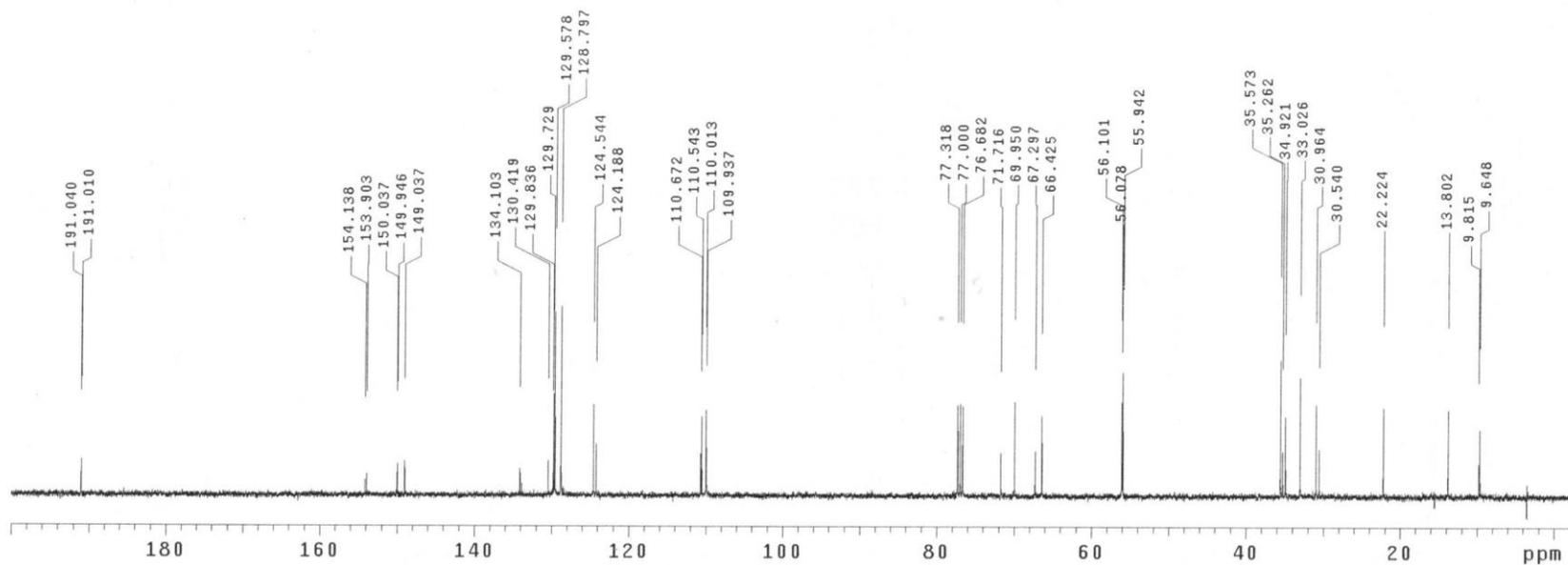
Ambient temperature

Total 1280 repetitions



Compound 7d

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 10a (¹H-NMR spectral data-1)

Kuo1009

Pulse Sequence: s2pu1

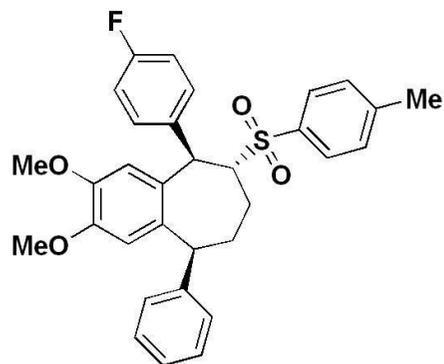
UNITYplus-400 "unity400"

Date: Nov 6 2015

Solvent: CDCl₃

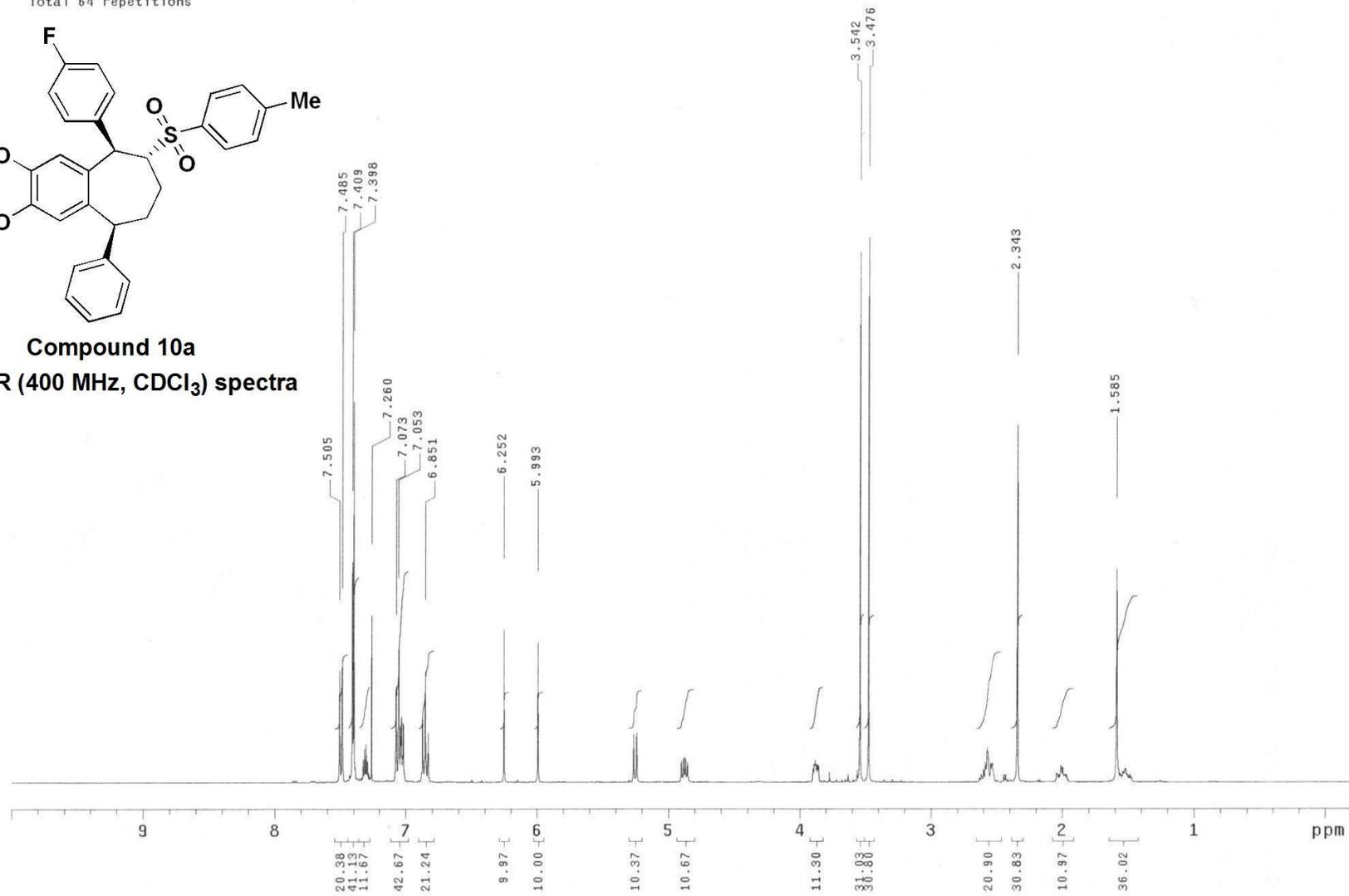
Ambient temperature

Total 64 repetitions

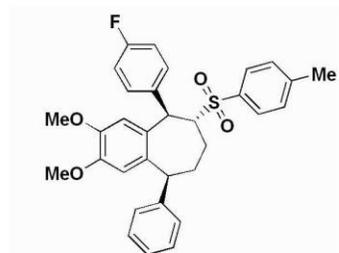


Compound 10a

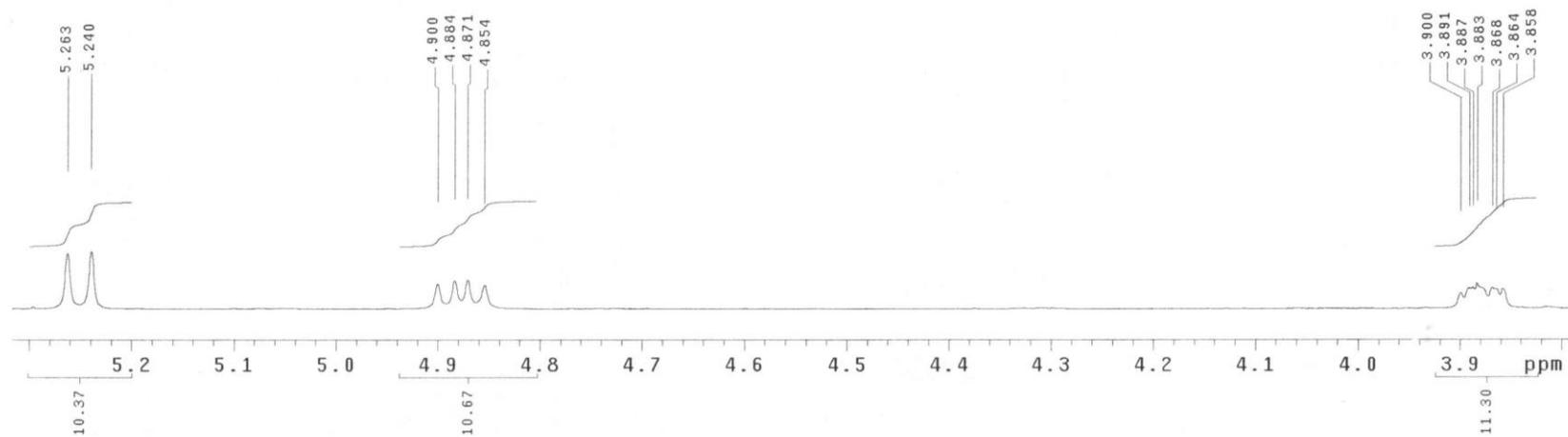
¹H NMR (400 MHz, CDCl₃) spectra



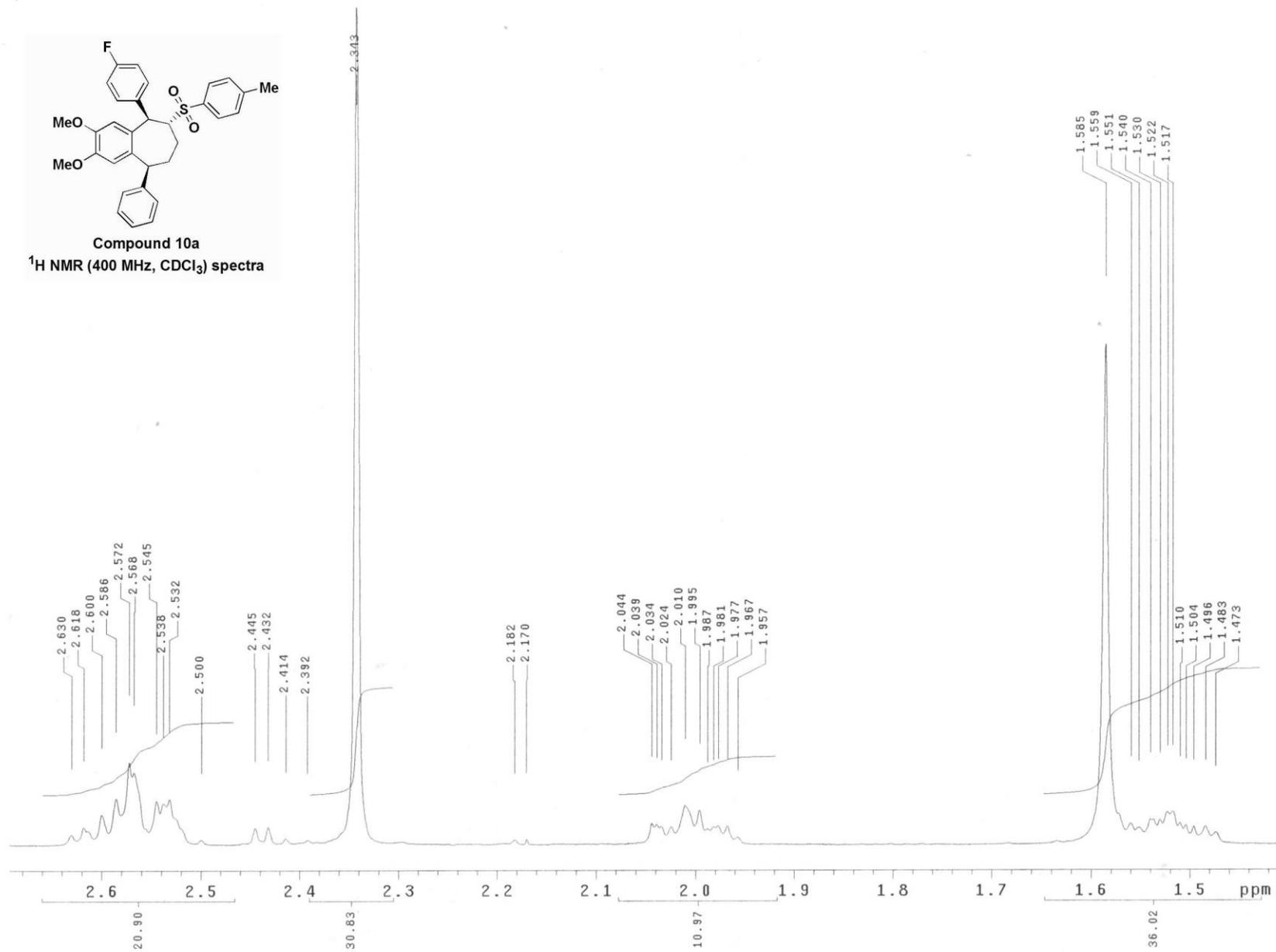
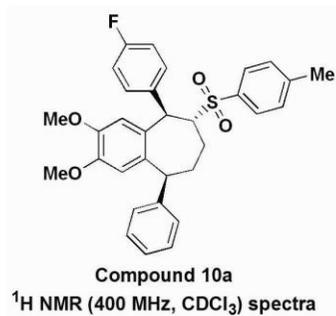
Compound 10a (¹H-NMR spectral data-2)



Compound 10a
¹H NMR (400 MHz, CDCl₃) spectra



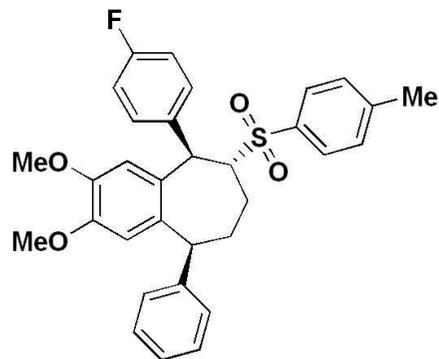
Compound 10a (¹H-NMR spectral data-3)



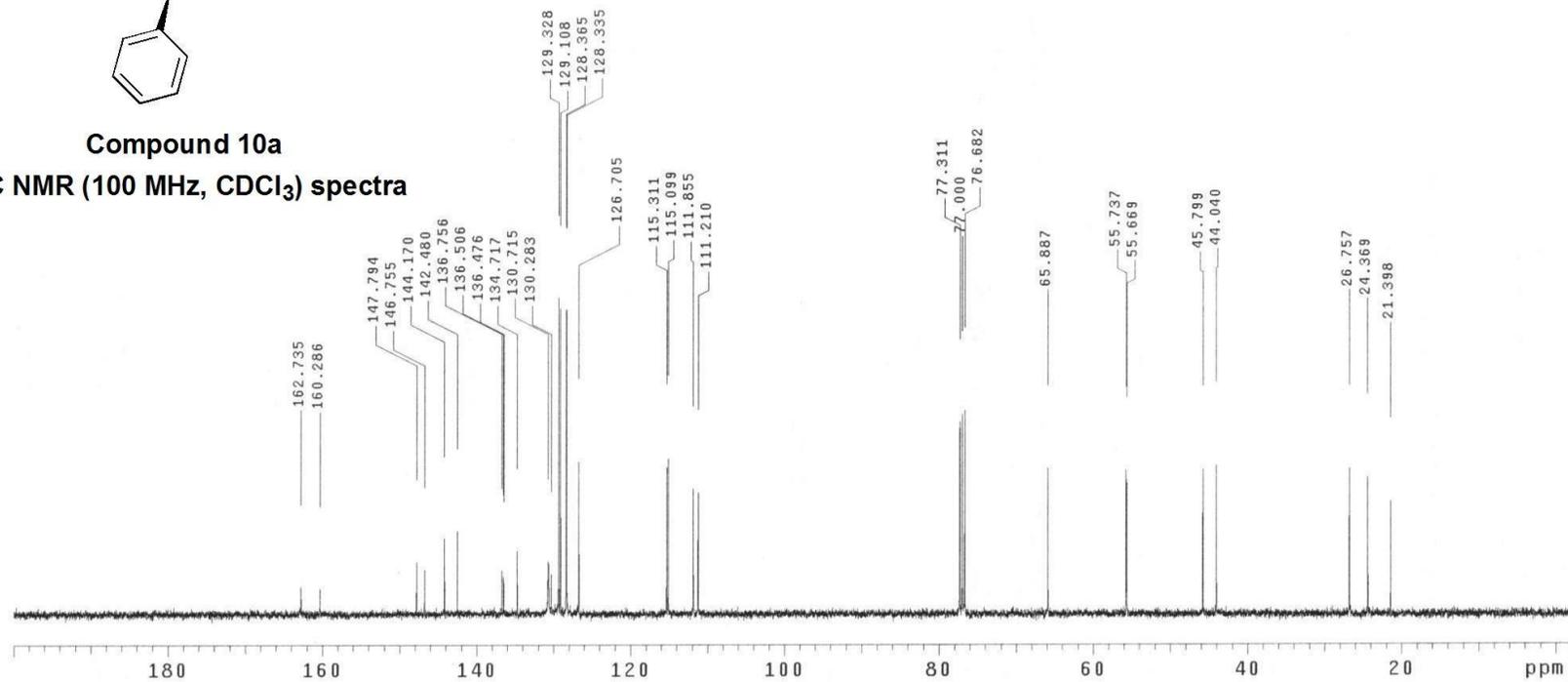
Compound 10a (¹³C-NMR spectral data)

Kuo1009

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Nov 6 2015
Solvent: CDCl₃
Ambient temperature
Total 5024 repetitions



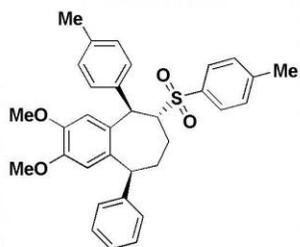
Compound 10a
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 10b (¹H-NMR spectral data-1)

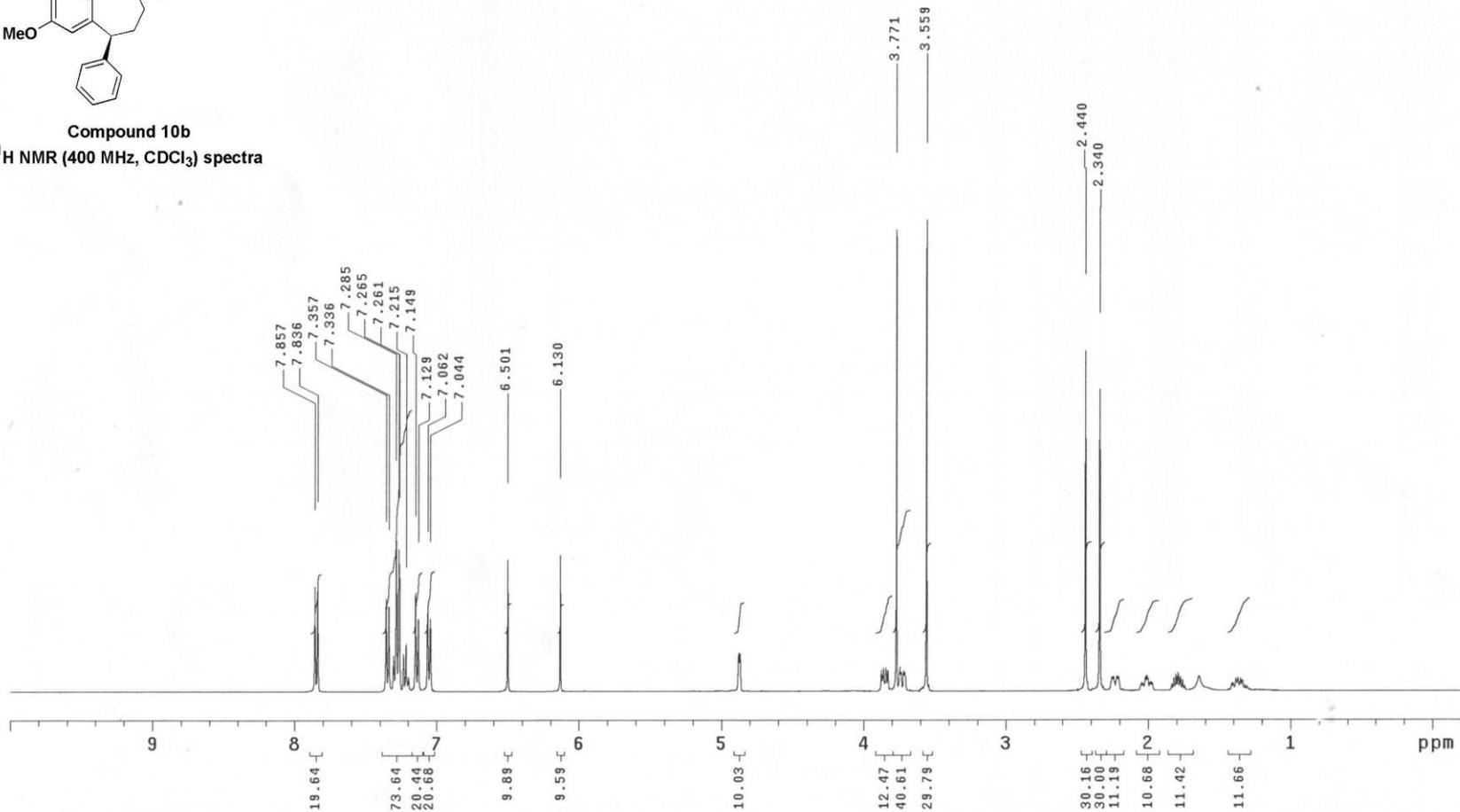
KS10b

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

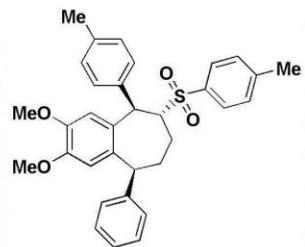


Compound 10b

¹H NMR (400 MHz, CDCl₃) spectra

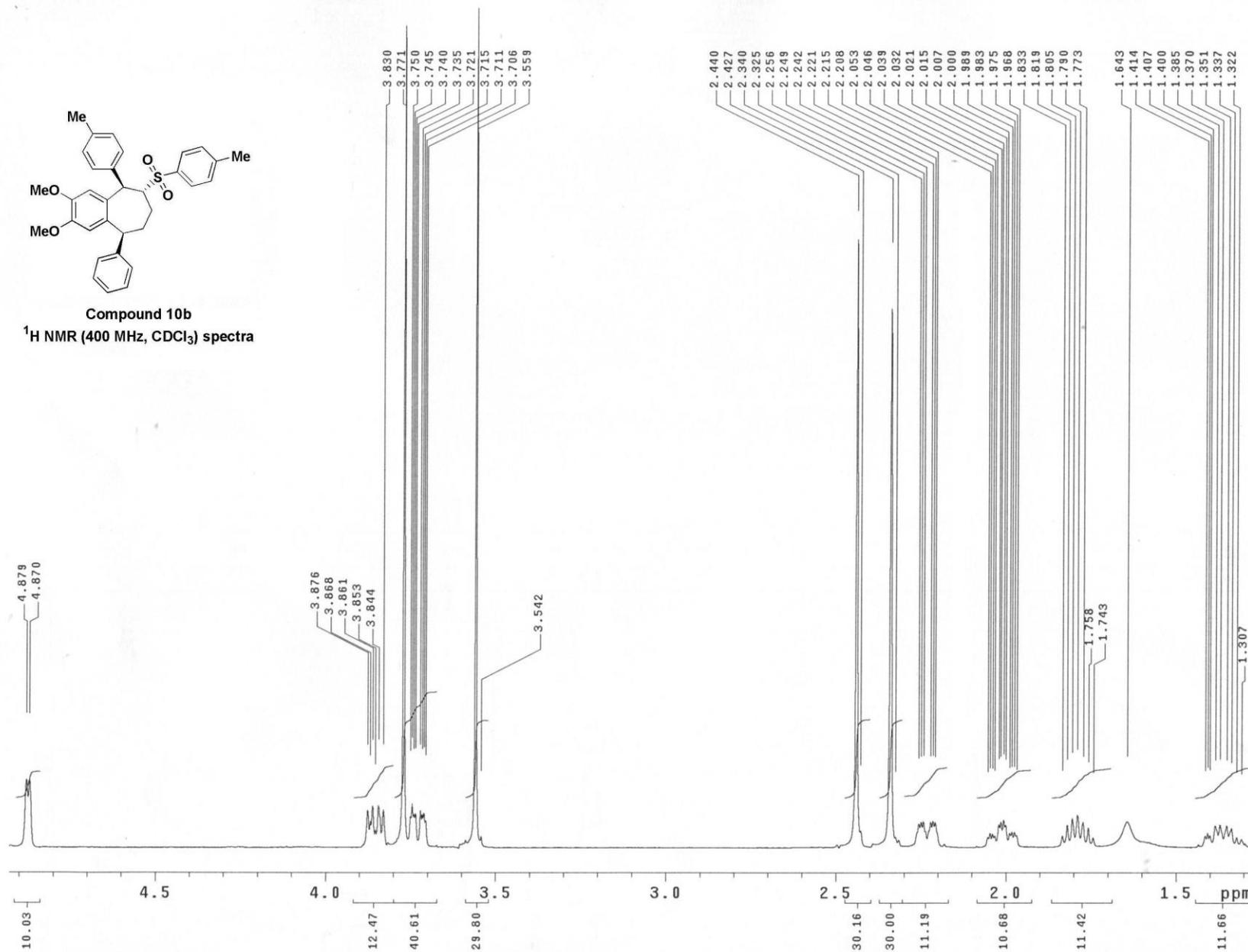


Compound 10b (¹H-NMR spectral data-2)



Compound 10b

¹H NMR (400 MHz, CDCl₃) spectra



Compound 10b (¹³C-NMR spectral data)

KS10b

Pulse Sequence: s2pu1

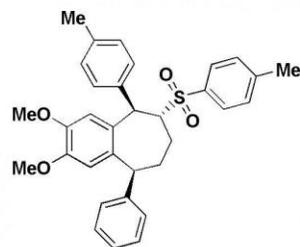
UNITYplus-400 "unity400"

Date: May 4 2020

Solvent: CDCl₃

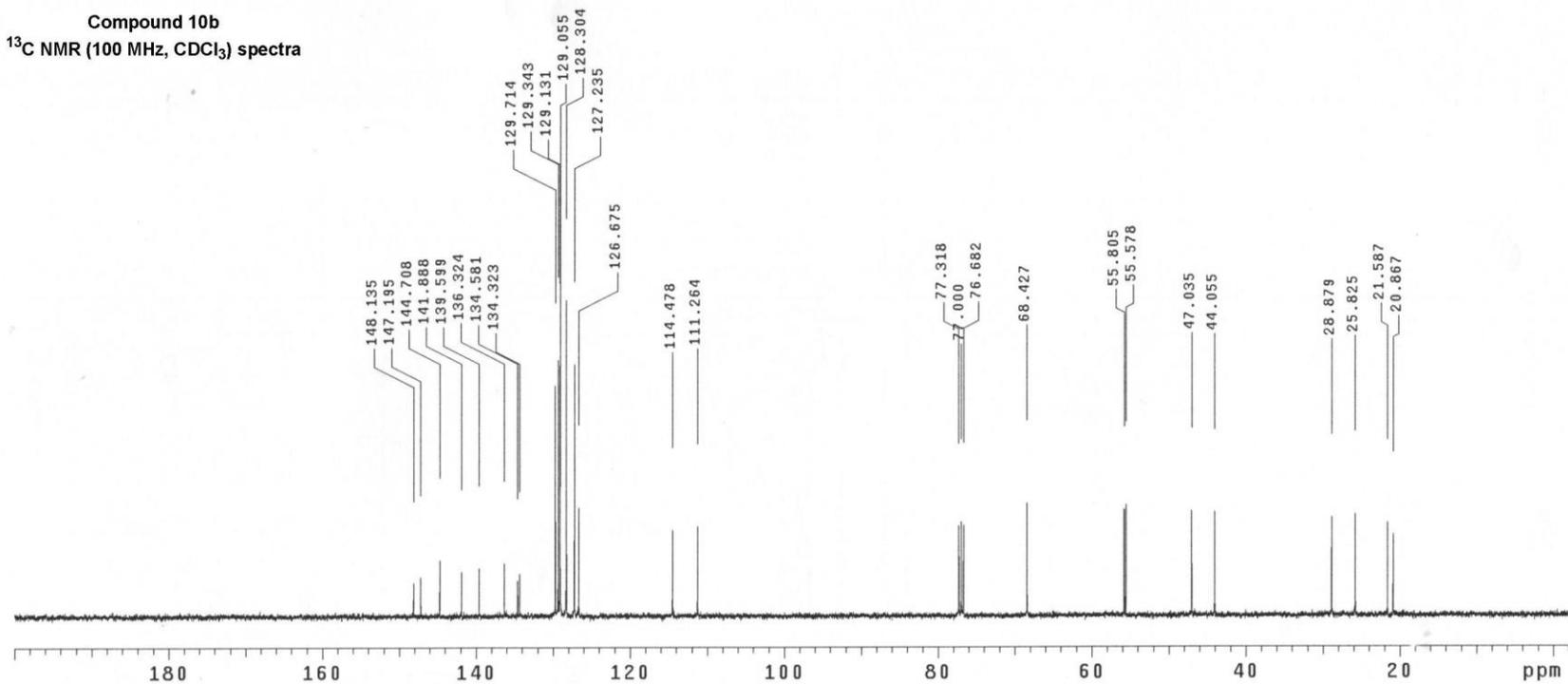
Ambient temperature

Total 1600 repetitions



Compound 10b

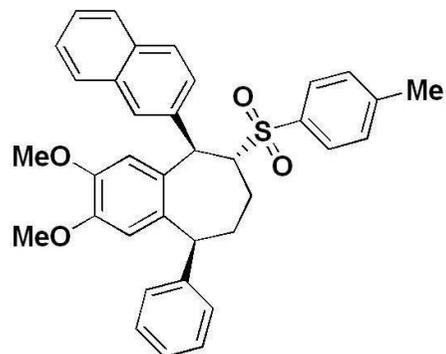
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 10c (¹H-NMR spectral data-1)

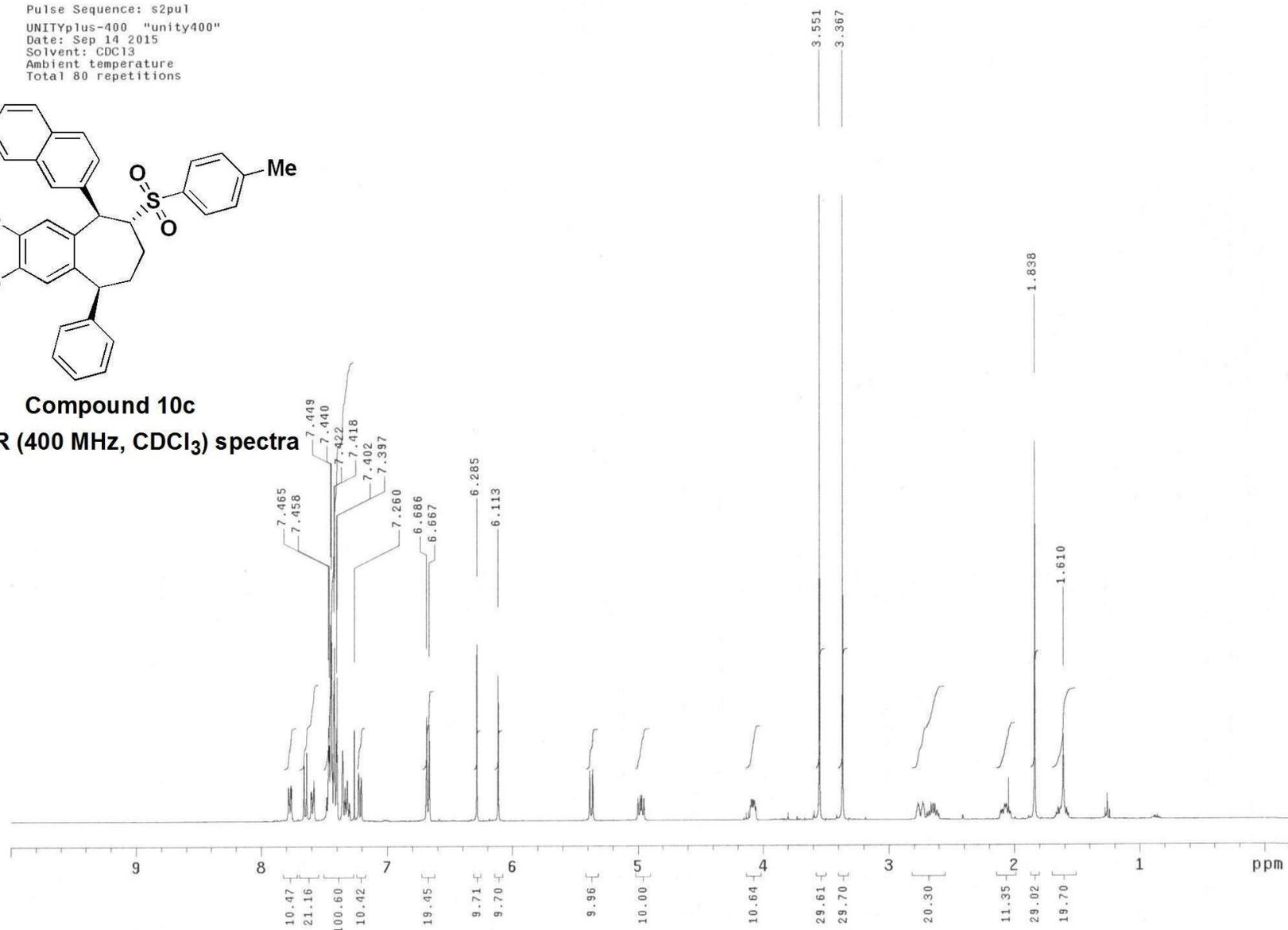
Kuo0904

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Sep 14 2015
Solvent: CDCl₃
Ambient temperature
Total 80 repetitions

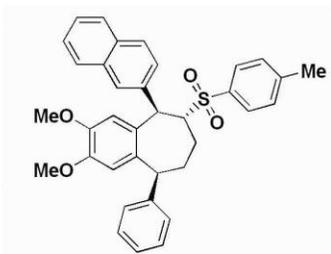


Compound 10c

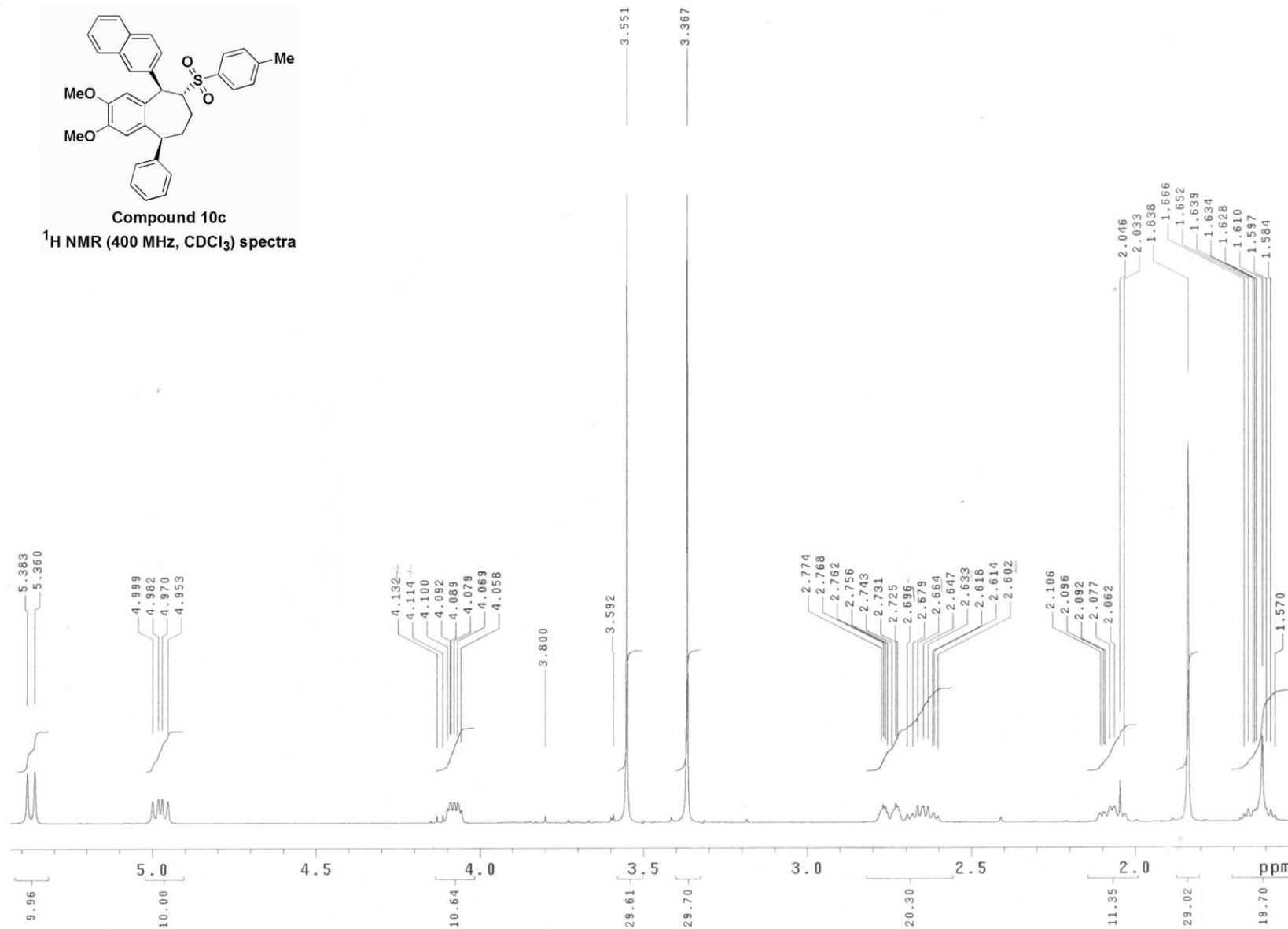
¹H NMR (400 MHz, CDCl₃) spectra



Compound 10c (¹H-NMR spectral data-2)



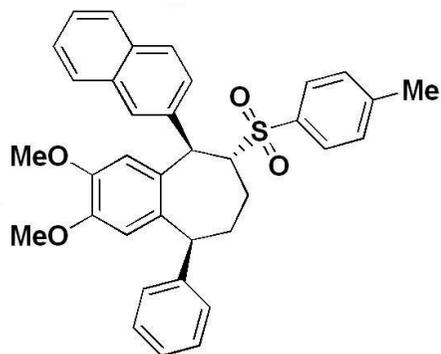
Compound 10c
¹H NMR (400 MHz, CDCl₃) spectra



Compound 10c (¹³C-NMR spectral data)

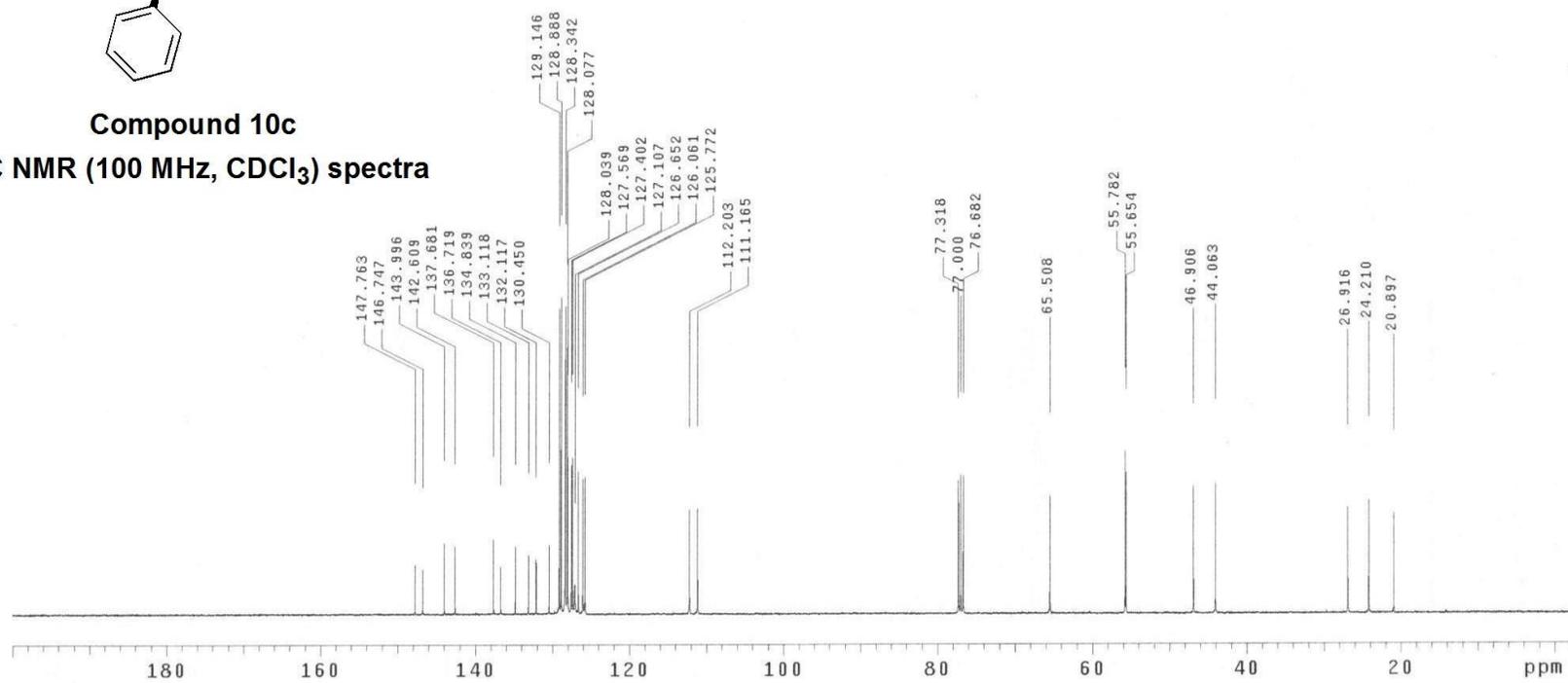
Kuo0904

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Sep 14 2015
Solvent: CDCl₃
Ambient temperature
Total 12800 repetitions

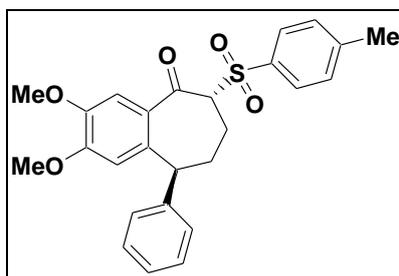


Compound 10c

¹³C NMR (100 MHz, CDCl₃) spectra

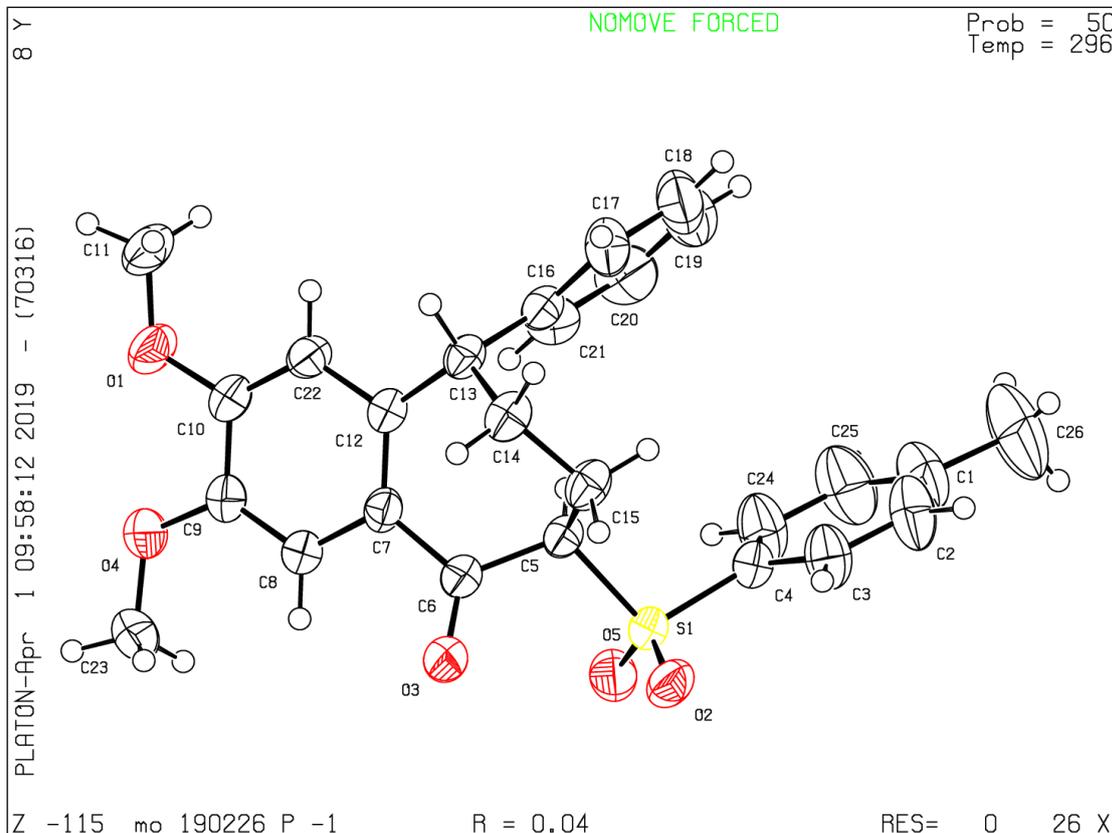


X-ray crystal data of compound 5a (CCDC 1915762)



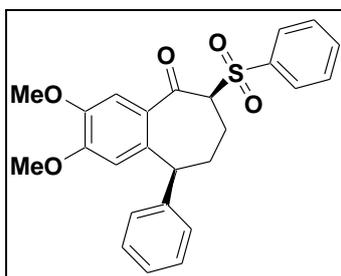
Sample preparation : A solution of compound **5a** (30 mg) in CH₂Cl₂ (10 mL) was placed in a tube (10 mL). EtOAc (2 mL) was added slowly to the vial with a dropper. The vial was closed with little cotton and kept at room temperature for 2 days. Then, colorless prisms were observed.

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



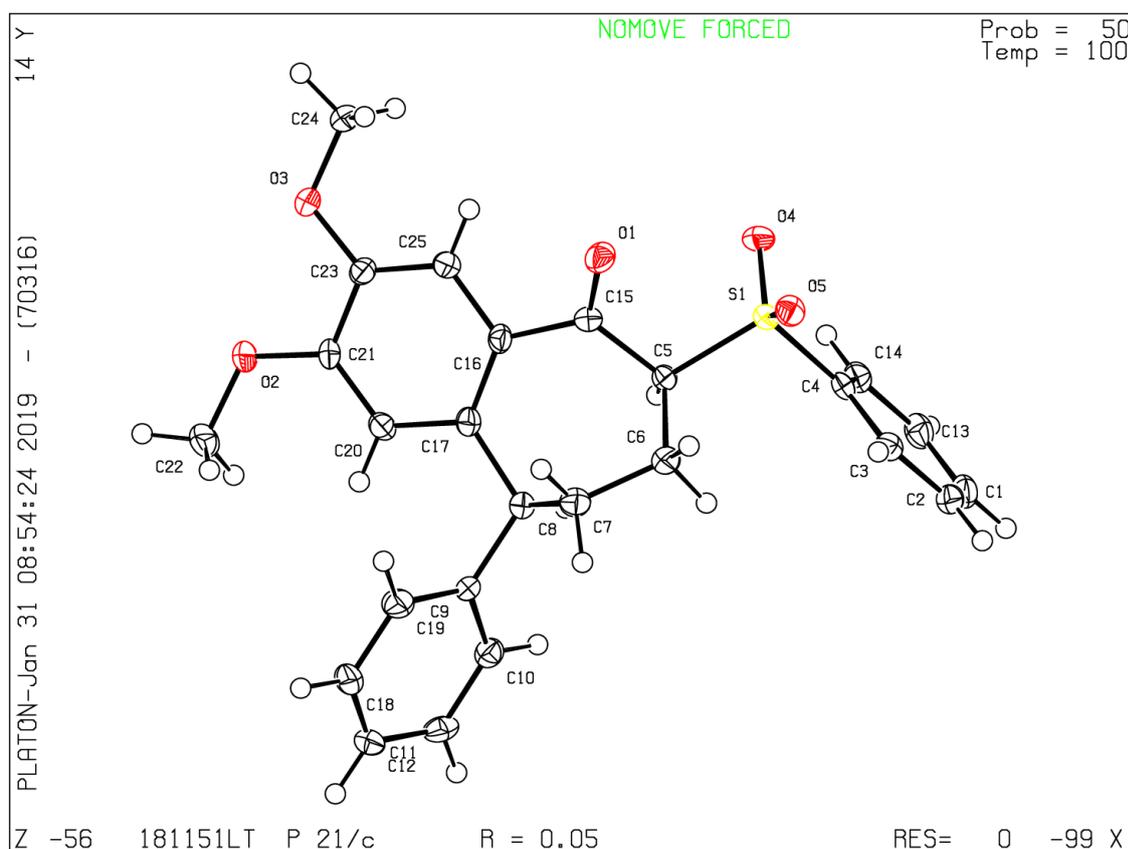
| | | |
|-----------------------------------|--|------------------|
| Empirical formula | C ₂₆ H ₂₆ O ₅ S | |
| Formula weight | 450.53 | |
| Temperature | 296(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Triclinic | |
| Space group | P-1 | |
| Unit cell dimensions | a = 8.6479(4) Å | α = 114.461(2)°. |
| | b = 11.7181(6) Å | β = 90.355(3)°. |
| | c = 12.4402(7) Å | γ = 96.581(3)°. |
| Volume | 1137.93(10) Å ³ | |
| Z | 2 | |
| Density (calculated) | 1.315 Mg/m ³ | |
| Absorption coefficient | 0.177 mm ⁻¹ | |
| F(000) | 476 | |
| Crystal size | 0.24 x 0.20 x 0.19 mm ³ | |
| Theta range for data collection | 1.802 to 26.452°. | |
| Index ranges | -10<=h<=10, -13<=k<=14, -15<=l<=15 | |
| Reflections collected | 28716 | |
| Independent reflections | 4674 [R(int) = 0.0331] | |
| Completeness to theta = 25.242° | 100.0 % | |
| Absorption correction | Semi-empirical from equivalents | |
| Max. and min. transmission | 0.7454 and 0.7128 | |
| Refinement method | Full-matrix least-squares on F ² | |
| Data / restraints / parameters | 4674 / 0 / 292 | |
| Goodness-of-fit on F ² | 1.039 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0434, wR2 = 0.1020 | |
| R indices (all data) | R1 = 0.0662, wR2 = 0.1136 | |
| Extinction coefficient | n/a | |
| Largest diff. peak and hole | 0.223 and -0.289 e.Å ⁻³ | |

X-ray crystal data of compound 5b (CCDC 1915763)



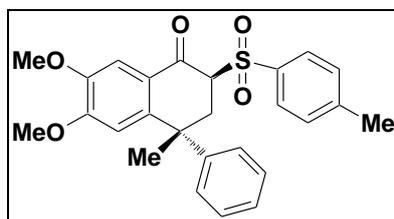
Sample preparation : A solution of compound **5b** (30 mg) in CH₂Cl₂ (10 mL) was placed in a tube (10 mL). EtOAc (2 mL) was added slowly to the vial with a dropper. The vial was closed with little cotton and kept at room temperature for 2 days. Then, colorless prisms were observed.

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



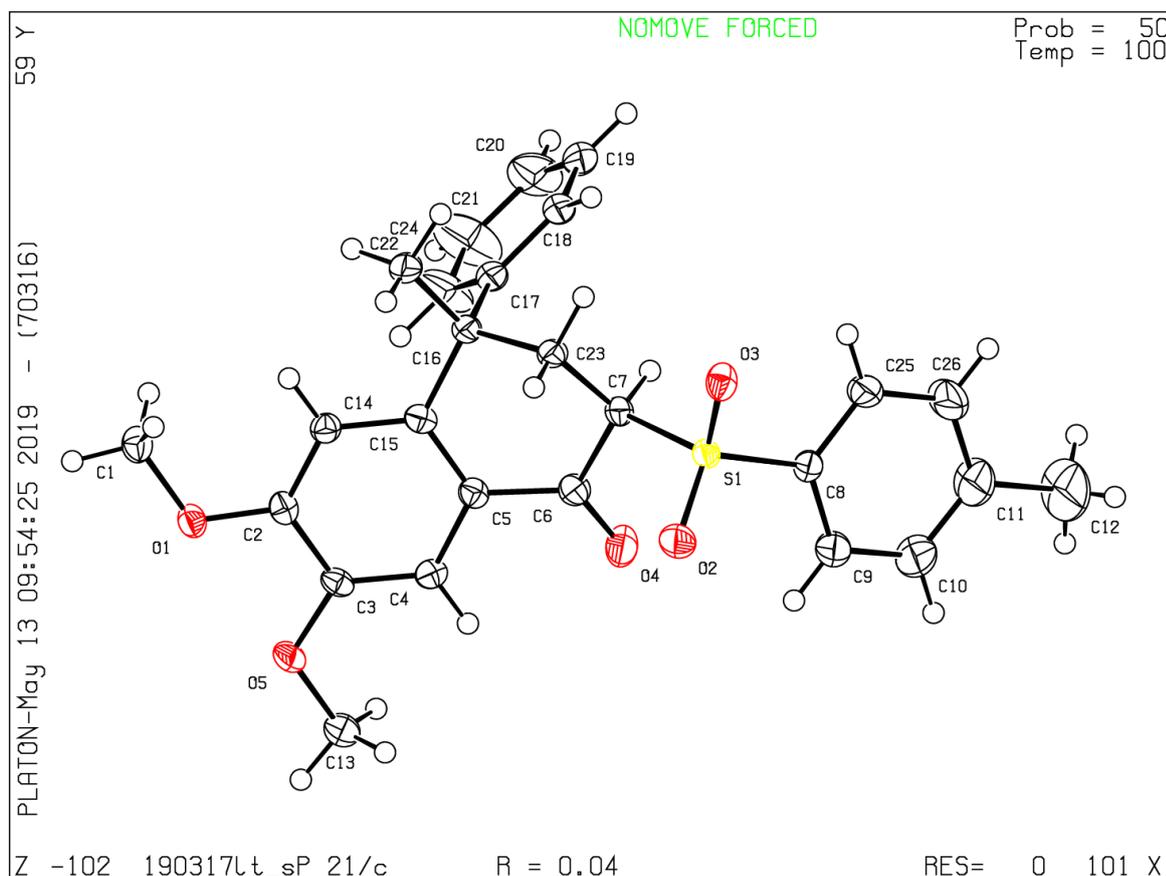
| | | |
|-----------------------------------|--|------------------|
| Empirical formula | C ₂₅ H ₂₄ O ₅ S | |
| Formula weight | 436.50 | |
| Temperature | 100(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Monoclinic | |
| Space group | P 21/c | |
| Unit cell dimensions | a = 12.2830(19) Å | α = 90°. |
| | b = 19.038(4) Å | β = 107.381(9)°. |
| | c = 9.2274(14) Å | γ = 90°. |
| Volume | 2059.2(6) Å ³ | |
| Z | 4 | |
| Density (calculated) | 1.408 Mg/m ³ | |
| Absorption coefficient | 0.194 mm ⁻¹ | |
| F(000) | 920 | |
| Crystal size | 0.10 x 0.08 x 0.08 mm ³ | |
| Theta range for data collection | 1.737 to 26.458°. | |
| Index ranges | -15 ≤ h ≤ 15, -22 ≤ k ≤ 23, -11 ≤ l ≤ 11 | |
| Reflections collected | 14957 | |
| Independent reflections | 4226 [R(int) = 0.0578] | |
| Completeness to theta = 25.242° | 100.0 % | |
| Absorption correction | Semi-empirical from equivalents | |
| Max. and min. transmission | 0.7454 and 0.6271 | |
| Refinement method | Full-matrix least-squares on F ² | |
| Data / restraints / parameters | 4226 / 0 / 282 | |
| Goodness-of-fit on F ² | 1.034 | |
| Final R indices [I > 2σ(I)] | R1 = 0.0471, wR2 = 0.1017 | |
| R indices (all data) | R1 = 0.0745, wR2 = 0.1146 | |
| Extinction coefficient | n/a | |
| Largest diff. peak and hole | 0.441 and -0.461 e.Å ⁻³ | |

X-ray crystal data of compound 6a (CCDC 1915765)



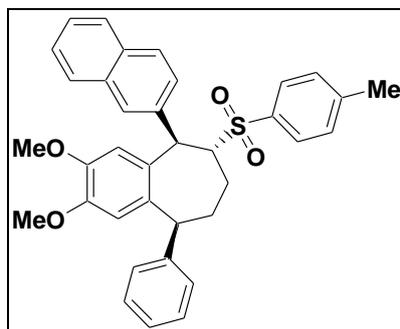
Sample preparation : A solution of compound **6a** (30 mg) in CH₂Cl₂ (10 mL) was placed in a tube (10 mL). EtOAc (2 mL) was added slowly to the vial with a dropper. The vial was closed with little cotton and kept at room temperature for 2 days. Then, colorless prisms were observed.

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



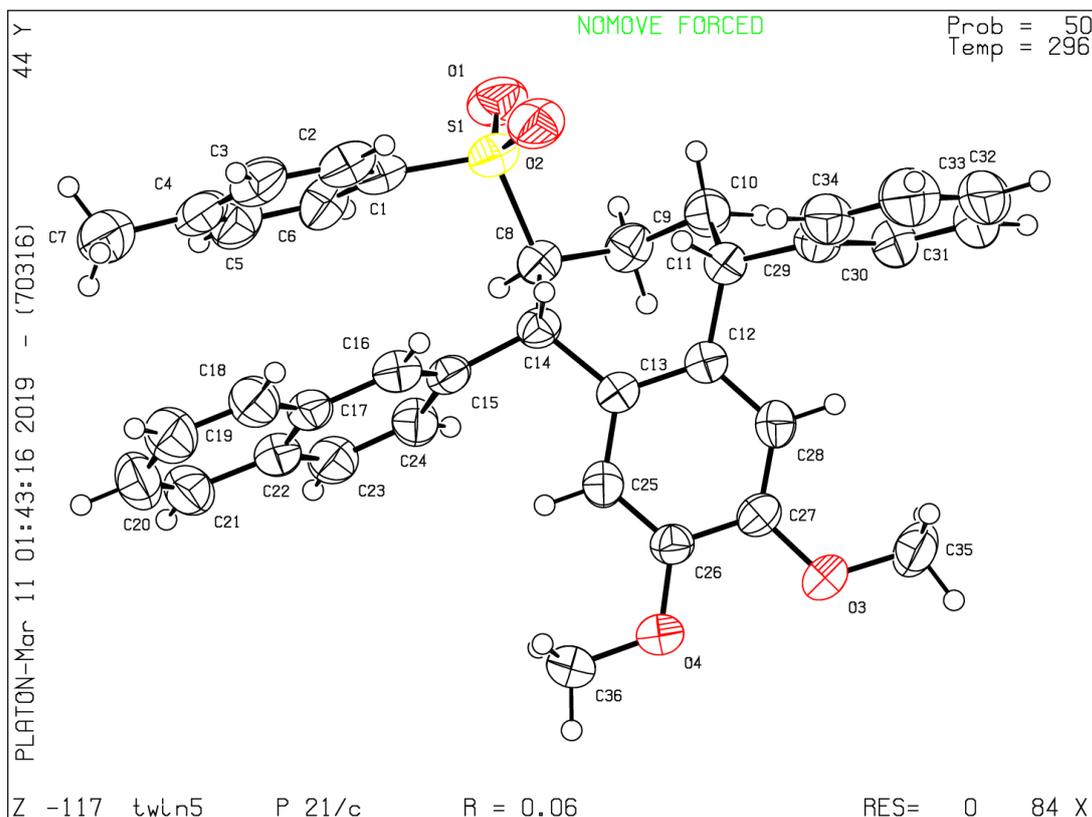
| | | |
|-----------------------------------|--|------------------|
| Empirical formula | C ₂₆ H ₂₆ O ₅ S | |
| Formula weight | 450.53 | |
| Temperature | 100(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Monoclinic | |
| Space group | P2 ₁ /c | |
| Unit cell dimensions | a = 17.4857(9) Å | α = 90°. |
| | b = 9.6877(5) Å | β = 118.713(3)°. |
| | c = 17.1467(9) Å | γ = 90°. |
| Volume | 2547.4(2) Å ³ | |
| Z | 4 | |
| Density (calculated) | 1.175 Mg/m ³ | |
| Absorption coefficient | 0.159 mm ⁻¹ | |
| F(000) | 952 | |
| Crystal size | 0.10 x 0.08 x 0.03 mm ³ | |
| Theta range for data collection | 2.376 to 26.419°. | |
| Index ranges | -21 ≤ h ≤ 21, -12 ≤ k ≤ 12, -21 ≤ l ≤ 21 | |
| Reflections collected | 22006 | |
| Independent reflections | 5222 [R(int) = 0.0316] | |
| Completeness to theta = 25.242° | 100.0 % | |
| Absorption correction | Semi-empirical from equivalents | |
| Max. and min. transmission | 0.7454 and 0.7144 | |
| Refinement method | Full-matrix least-squares on F ² | |
| Data / restraints / parameters | 5222 / 0 / 293 | |
| Goodness-of-fit on F ² | 1.032 | |
| Final R indices [I > 2σ(I)] | R1 = 0.0395, wR2 = 0.0935 | |
| R indices (all data) | R1 = 0.0524, wR2 = 0.1009 | |
| Extinction coefficient | n/a | |
| Largest diff. peak and hole | 0.372 and -0.379 e.Å ⁻³ | |

X-ray crystal data of compound 10c (CCDC 1915767)



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

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



| | | |
|-----------------------------------|--|------------------|
| Empirical formula | C ₃₆ H ₃₄ O ₄ S | |
| Formula weight | 562.69 | |
| Temperature | 296(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Monoclinic | |
| Space group | P 21/c | |
| Unit cell dimensions | a = 15.699(4) Å | α = 90°. |
| | b = 7.434(2) Å | β = 98.529(16)°. |
| | c = 24.908(8) Å | γ = 90°. |
| Volume | 2874.6(14) Å ³ | |
| Z | 4 | |
| Density (calculated) | 1.300 Mg/m ³ | |
| Absorption coefficient | 0.153 mm ⁻¹ | |
| F(000) | 1192 | |
| Crystal size | 0.18 x 0.15 x 0.06 mm ³ | |
| Theta range for data collection | 1.312 to 25.146°. | |
| Index ranges | -18 ≤ h ≤ 18, 0 ≤ k ≤ 8, 0 ≤ l ≤ 29 | |
| Reflections collected | 5423 | |
| Independent reflections | 5423 [R(int) = 0.0753] | |
| Completeness to theta = 25.000° | 100.0 % | |
| Absorption correction | Semi-empirical from equivalents | |
| Max. and min. transmission | 0.9484 and 0.5049 | |
| Refinement method | Full-matrix least-squares on F ² | |
| Data / restraints / parameters | 5423 / 0 / 374 | |
| Goodness-of-fit on F ² | 1.047 | |
| Final R indices [I > 2σ(I)] | R1 = 0.0641, wR2 = 0.1662 | |
| R indices (all data) | R1 = 0.1166, wR2 = 0.1989 | |
| Extinction coefficient | n/a | |
| Largest diff. peak and hole | 0.339 and -0.291 e.Å ⁻³ | |