

Supporting Information

Gram-Scale Synthesis of 3-Sulfonyl Flavanones

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Table of Contents

1. ¹ H NMR and ¹³ C NMR spectra copies of 4a-4ao	S-2~S-83
2. X-ray crystal data of 4a , 4e , 4ab , 4af and 4aj	S-84~S-93

Compound 4a (¹H-NMR spectral data)

HAK1A1

Pulse Sequence: s2pu1

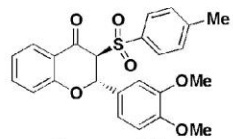
UNITYplus-400 "unity400"

Date: Nov 8 2017

Solvent: CDCl₃

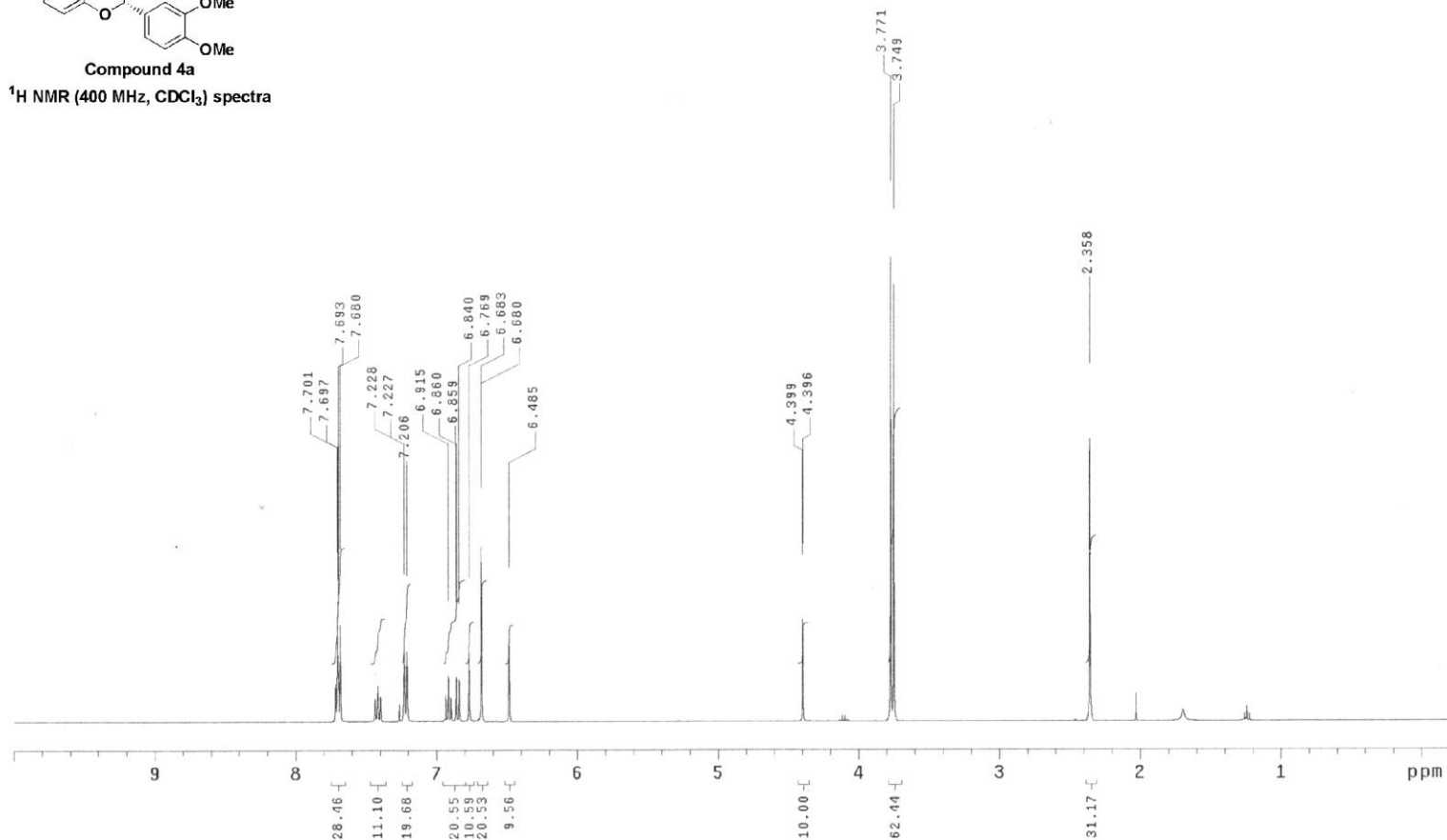
Ambient temperature

Total 32 repetitions



Compound 4a

¹H NMR (400 MHz, CDCl₃) spectra



Compound 4a (¹³C-NMR spectral data)

HAK1A1

Pulse Sequence: s2pu1

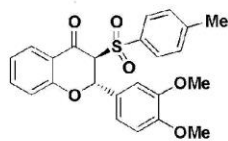
UNITYplus-400 "unity400"

Date: Nov 8 2017

Solvent: CDCl₃

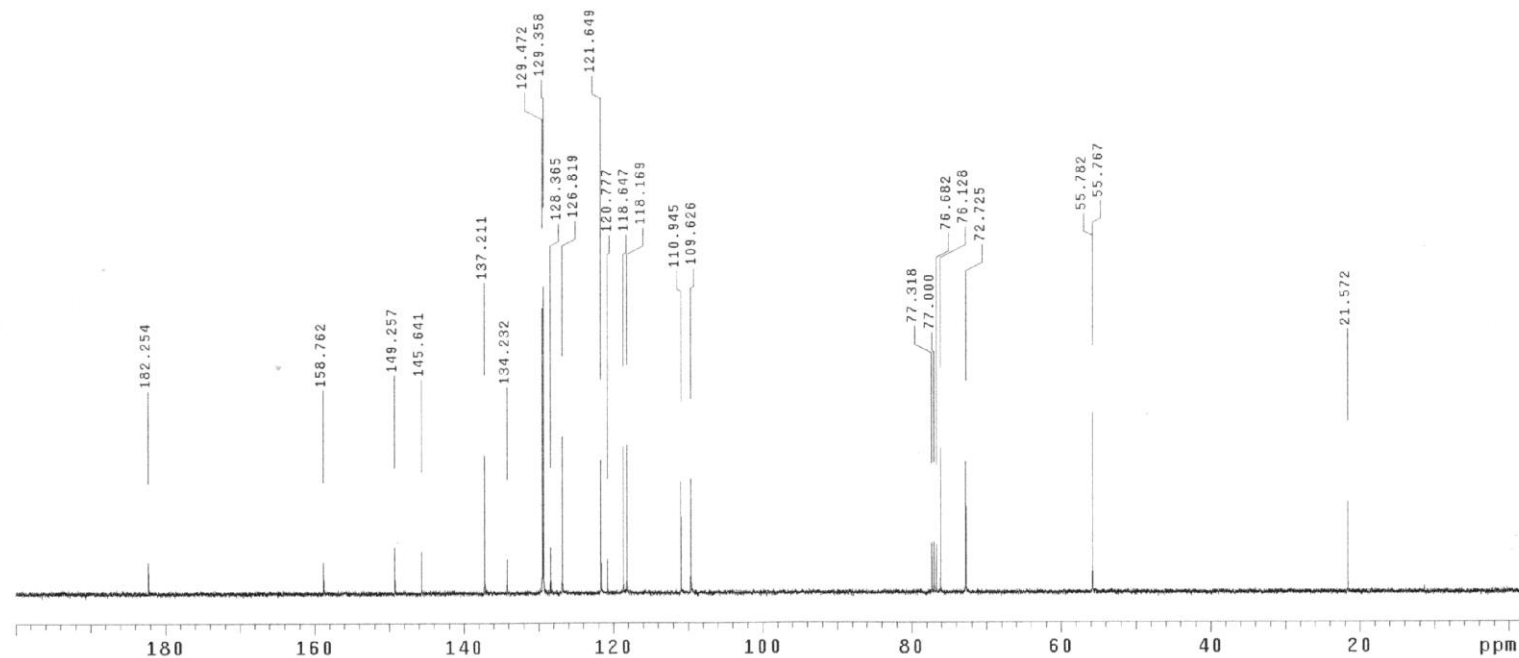
Ambient temperature

Total 480 repetitions



Compound 4a

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4b (¹H-NMR spectral data)

HAK2A1

Pulse Sequence: s2pul

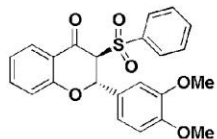
UNITYplus-400 "unity400"

Date: Nov 6 2017

Solvent: CDCl₃

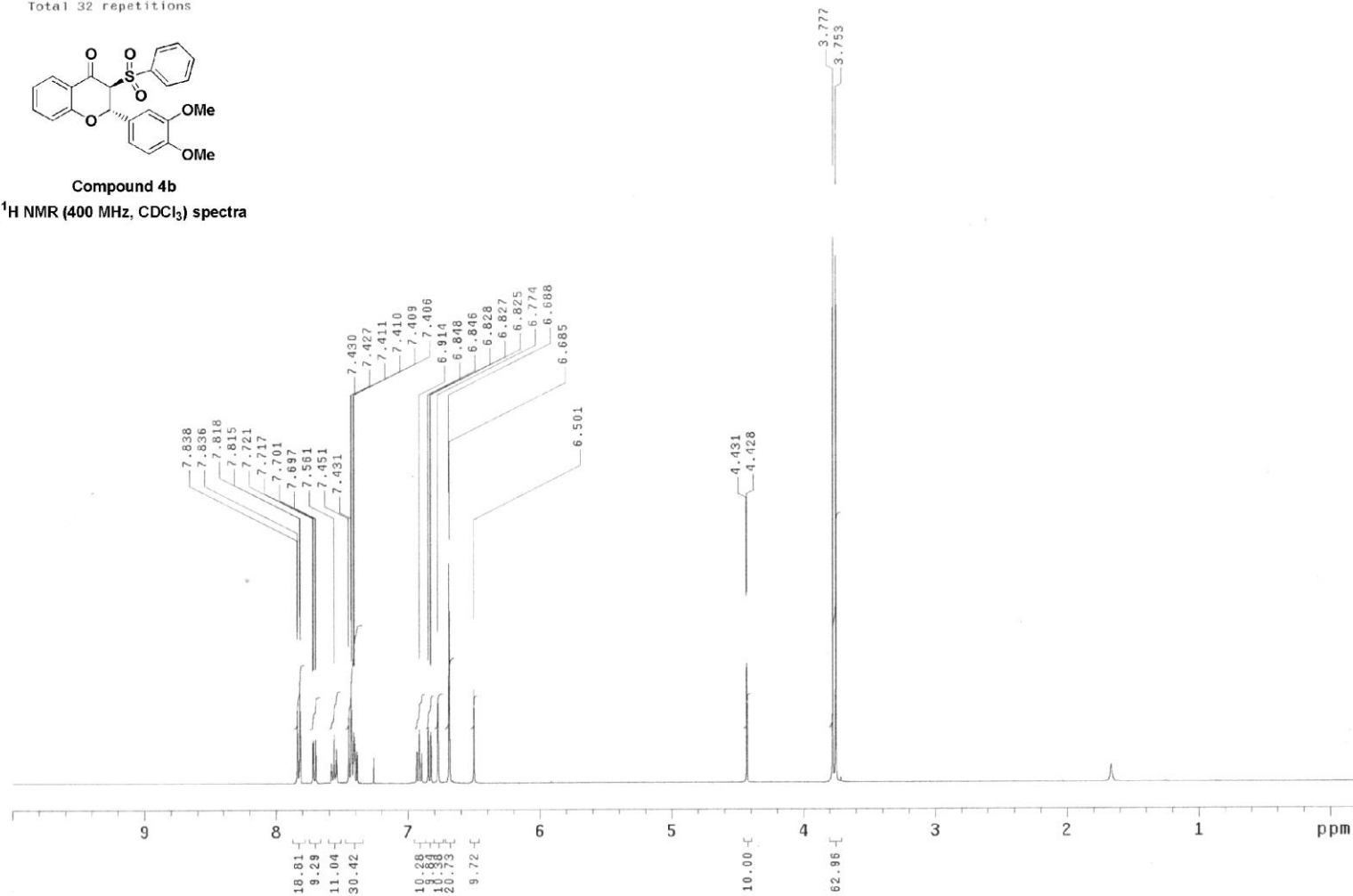
Ambient temperature

Total 32 repetitions



Compound 4b

¹H NMR (400 MHz, CDCl₃) spectra



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

HAK2A1

Pulse Sequence: s2pul

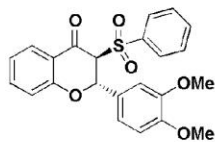
UNITYplus-400 "unity400"

Date: Nov 6 2017

Solvent: CDCl_3

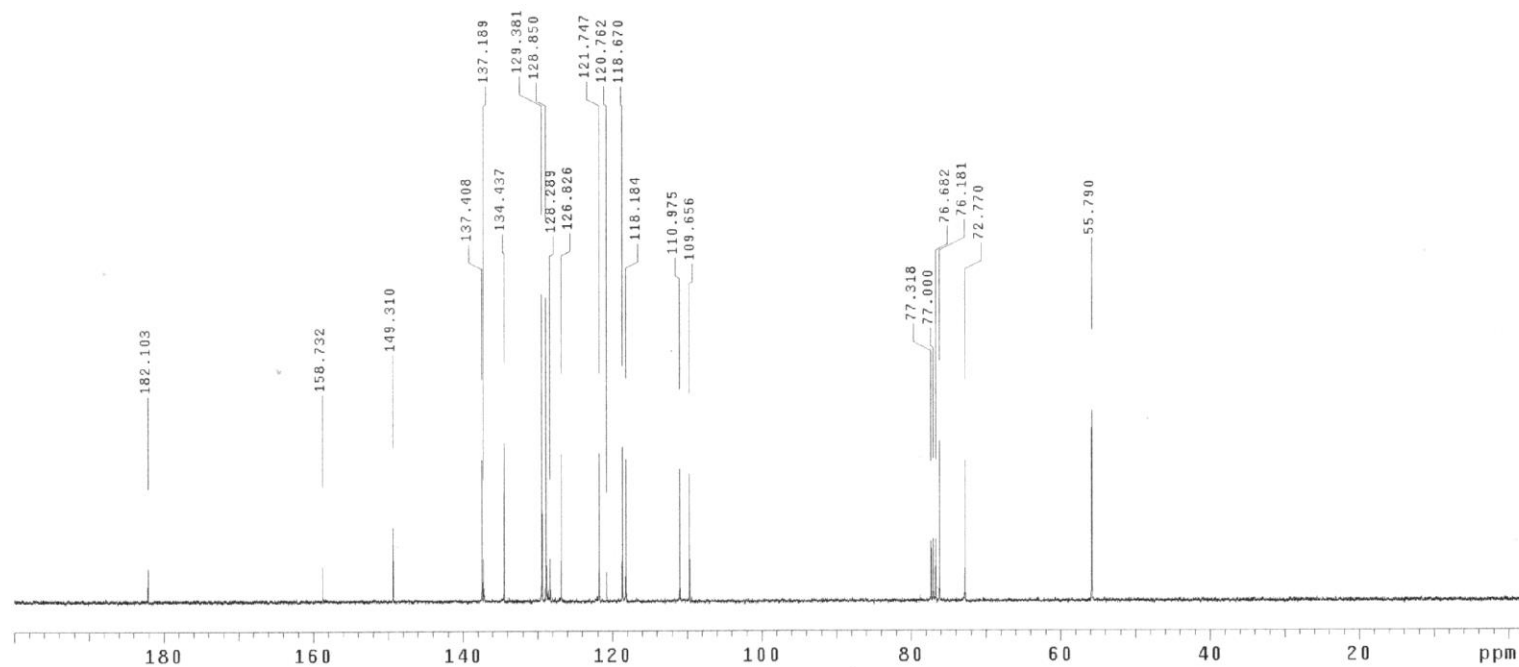
Ambient temperature

Total 1216 repetitions



Compound 4b

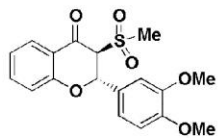
^{13}C NMR (100 MHz, CDCl_3) spectra



Compound 4c (¹H-NMR spectral data)

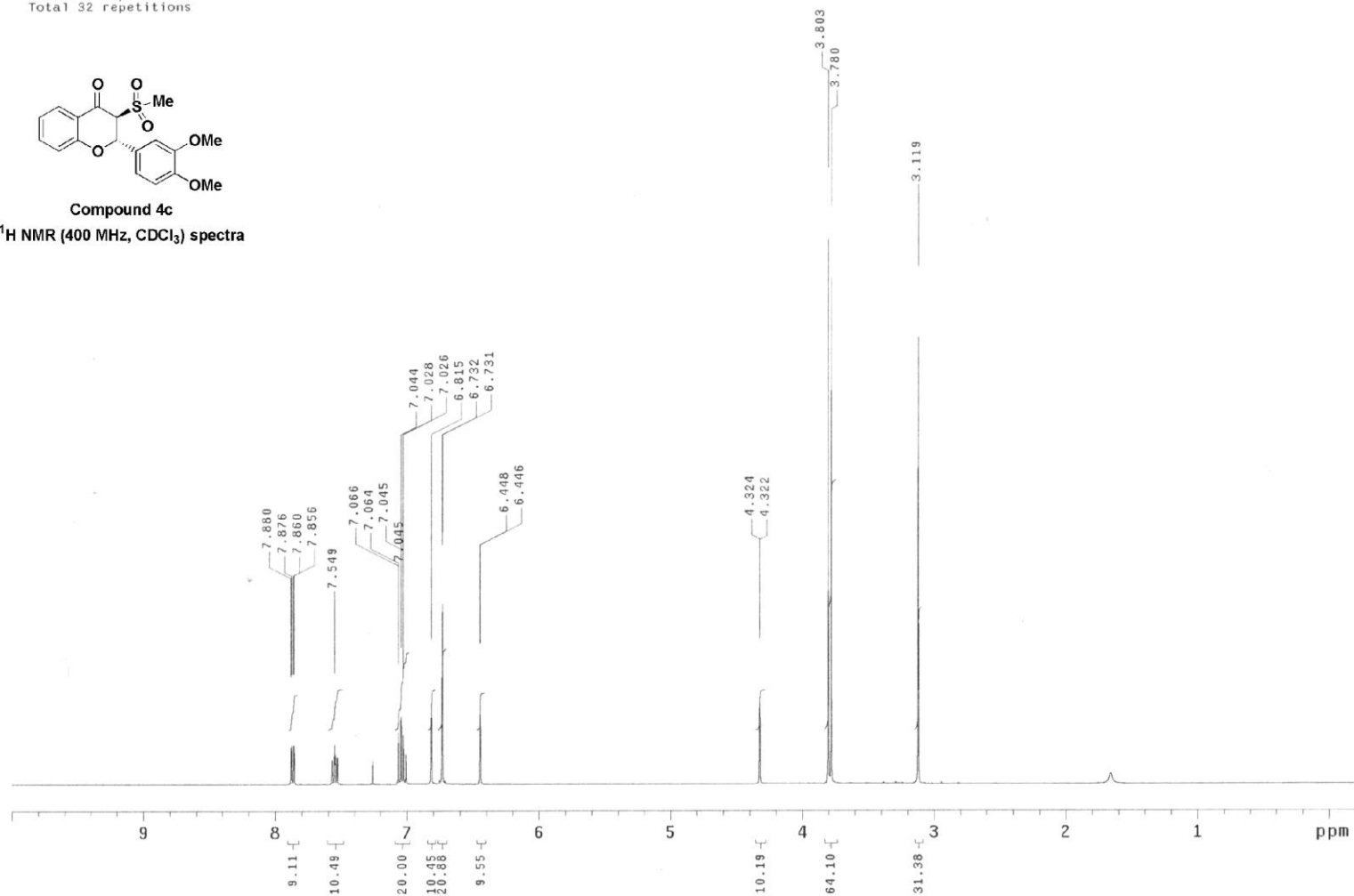
HAK3A1

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



Compound 4c

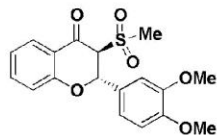
¹H NMR (400 MHz, CDCl₃) spectra



Compound 4c (¹³C-NMR spectral data)

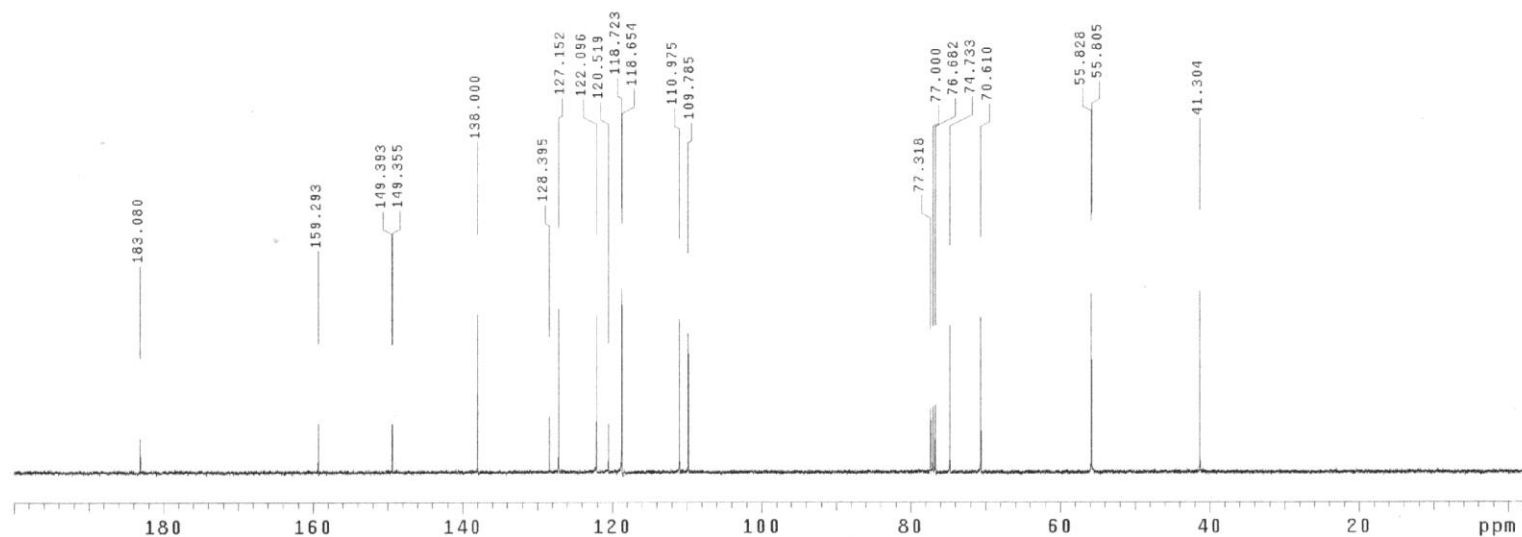
HAK3A1

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Nov 7 2017
Solvent: CDCl₃
Ambient temperature
Total 1280 repetitions



Compound 4c

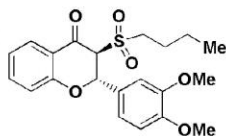
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4d (¹H-NMR spectral data)

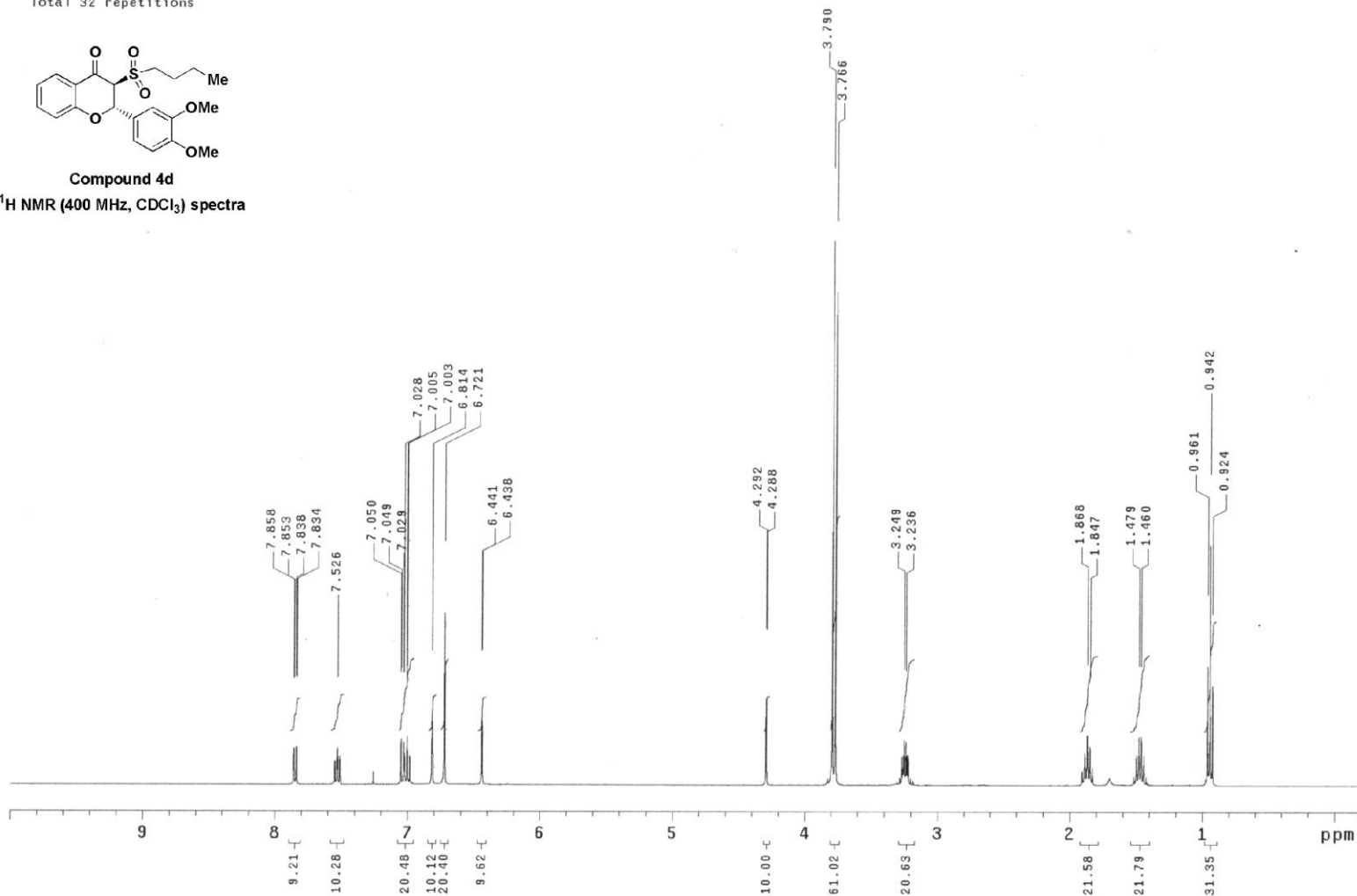
HAK4A1

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Nov 30 2017
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetitions



Compound 4d

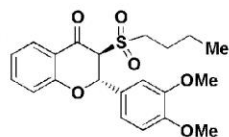
¹H NMR (400 MHz, CDCl₃) spectra



Compound 4d (¹³C-NMR spectral data)

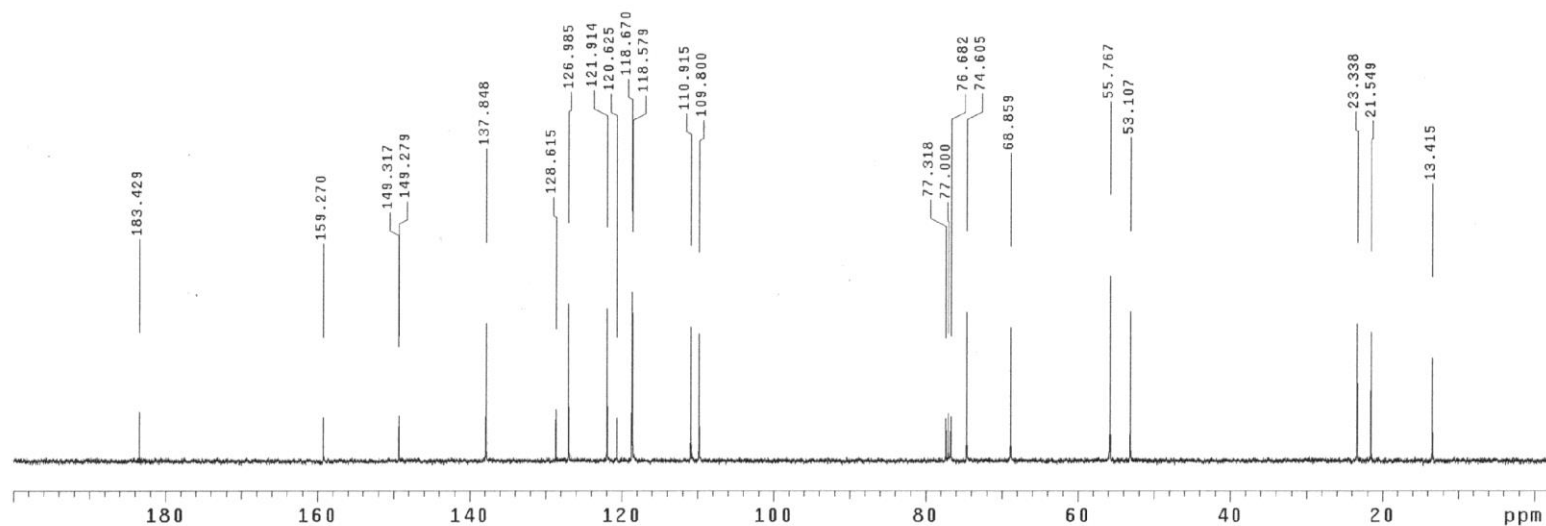
HAK4A1

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Nov 30 2017
Solvent: CDCl₃
Ambient temperature
Total 320 repetitions



Compound 4d

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4e (¹H-NMR spectral data)

HAK5A1

Pulse Sequence: s2pu1

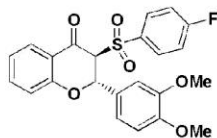
UNITYplus-400 "unity400"

Date: Nov 10 2017

Solvent: CDCl₃

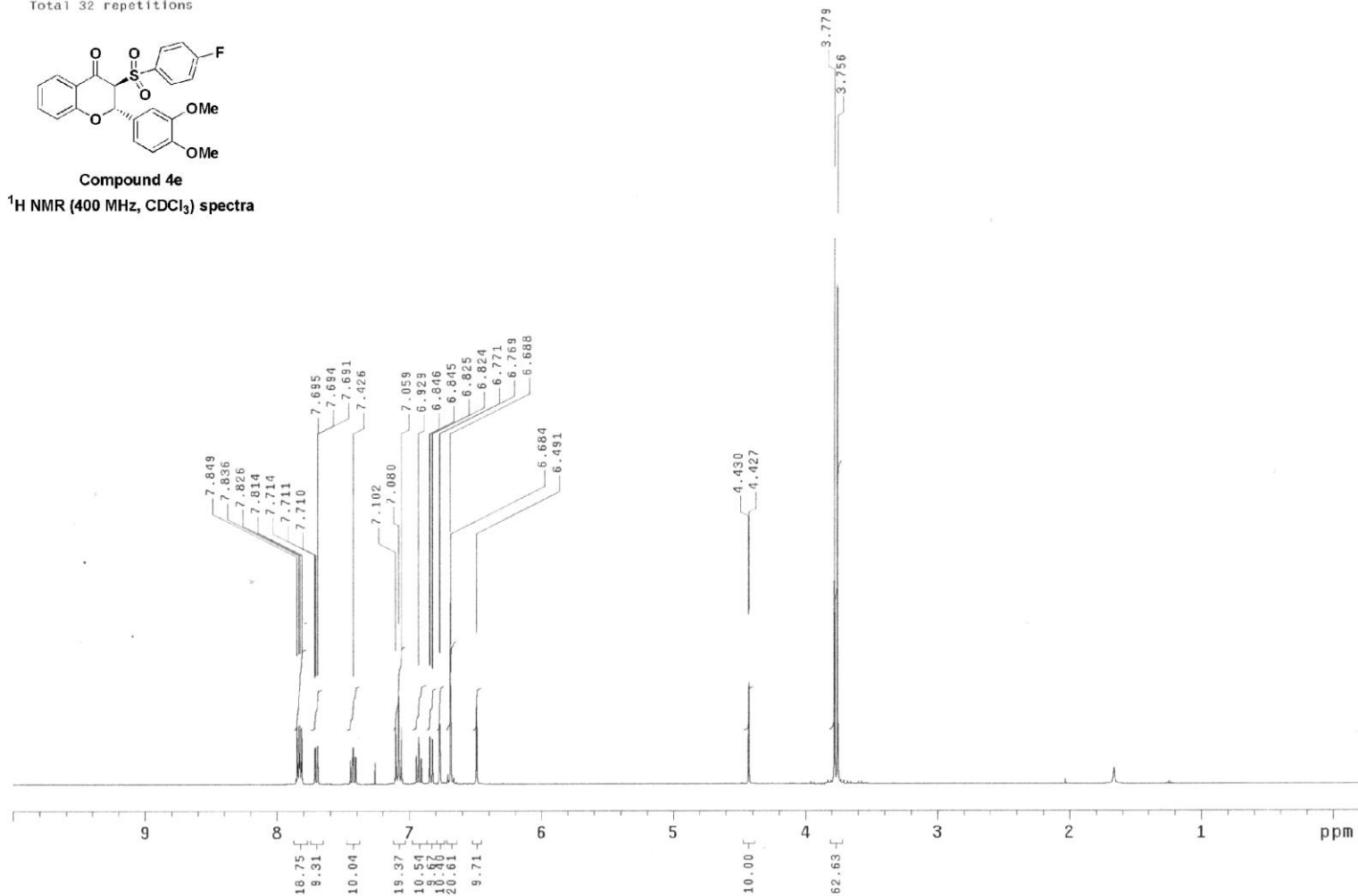
Ambient temperature

Total 32 repetitions



Compound 4e

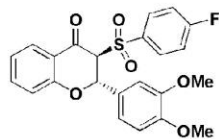
¹H NMR (400 MHz, CDCl₃) spectra



Compound 4e (¹³C-NMR spectral data)

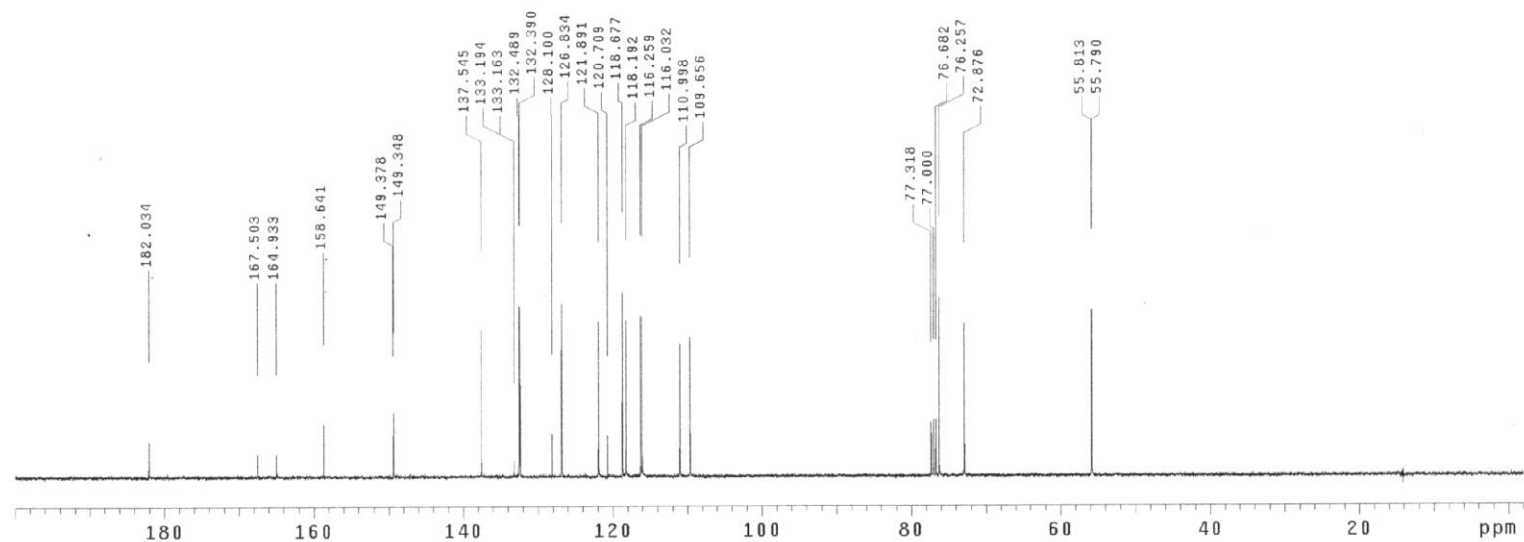
HAK5A1

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Nov 10 2017
Solvent: CDCl₃
Ambient temperature
Total 1264 repetitions



Compound 4e

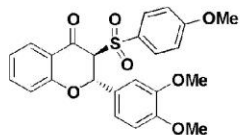
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4f (¹H-NMR spectral data)

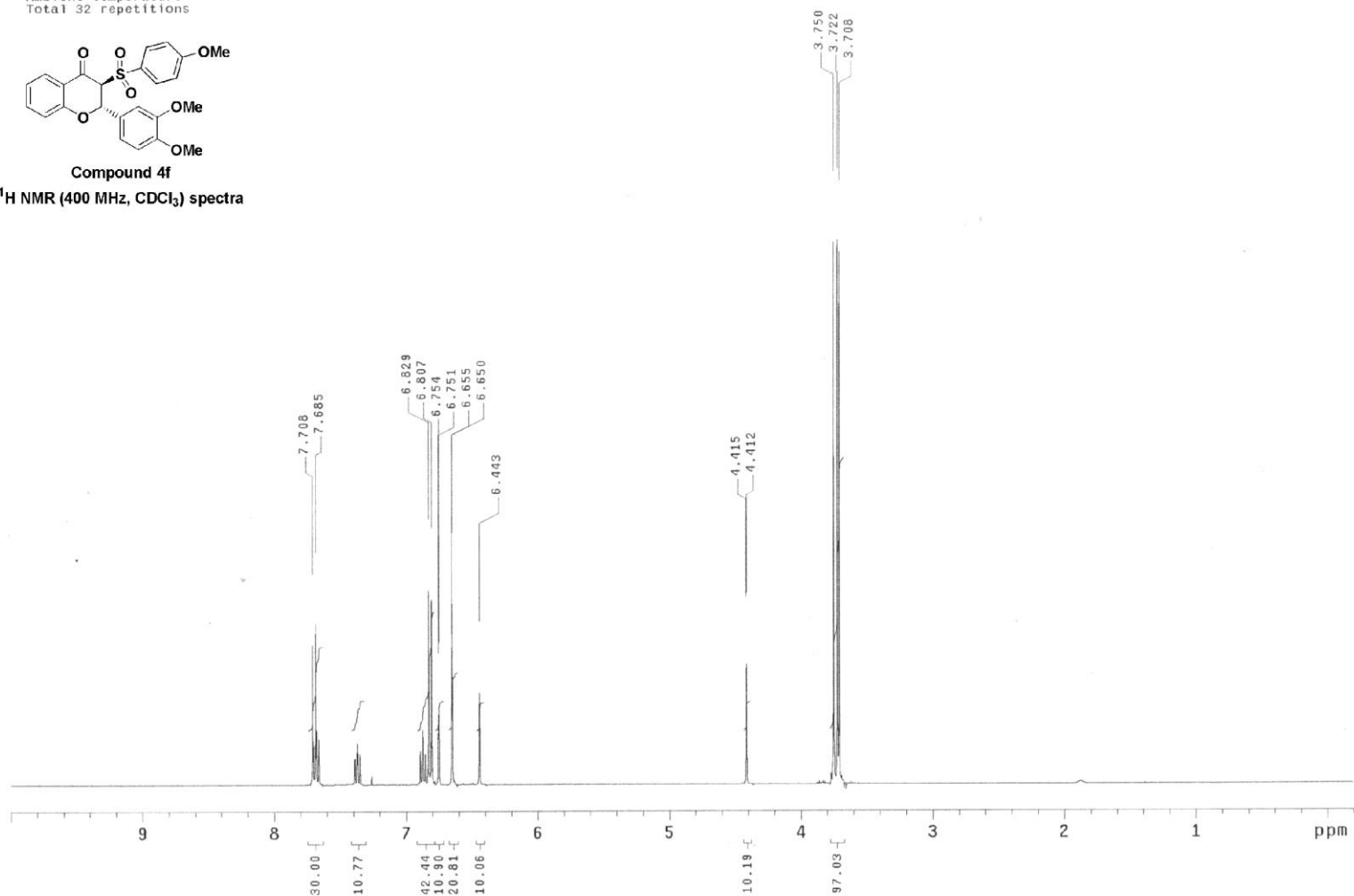
HAK6A1

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Nov 16 2017
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetitions



Compound 4f

¹H NMR (400 MHz, CDCl₃) spectra



Compound 4f (¹³C-NMR spectral data)

HAK6A1

Pulse Sequence: s2pu1

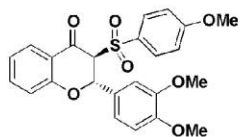
UNITYplus-400 "unity400"

Date: Nov 16 2017

Solvent: CDCl₃

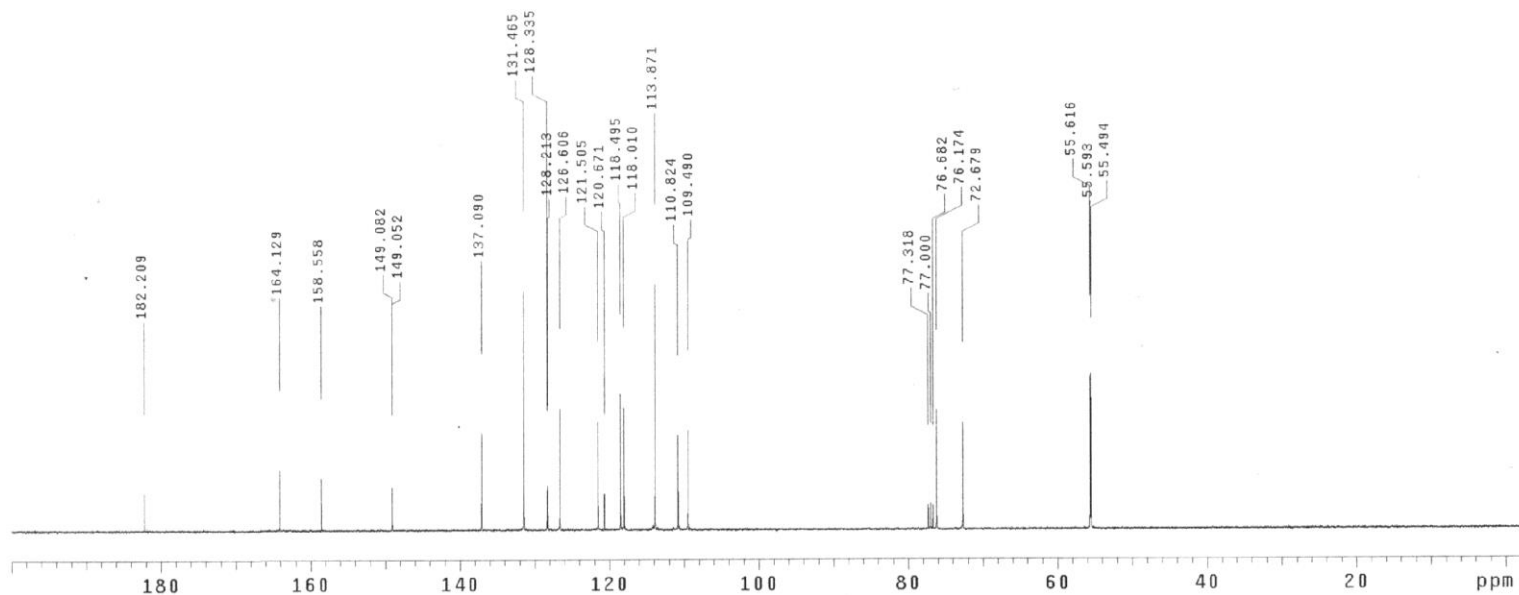
Ambient temperature

Total 256 repetitions



Compound 4f

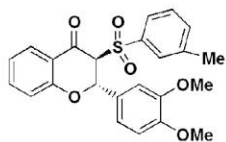
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4g (¹H-NMR spectral data)

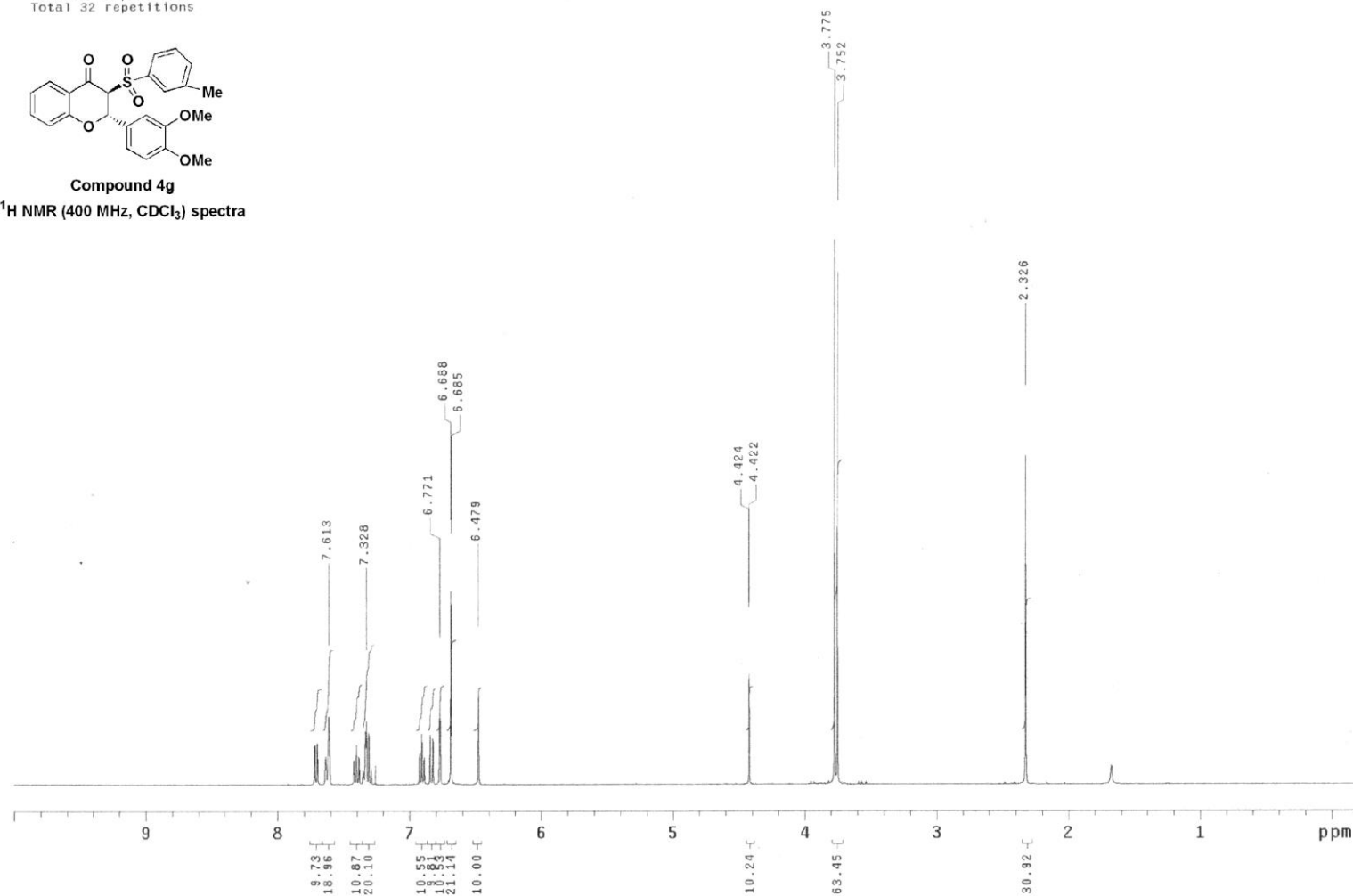
HAK7A1

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Nov 13 2017
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetitions



Compound 4g

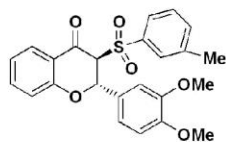
¹H NMR (400 MHz, CDCl₃) spectra



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

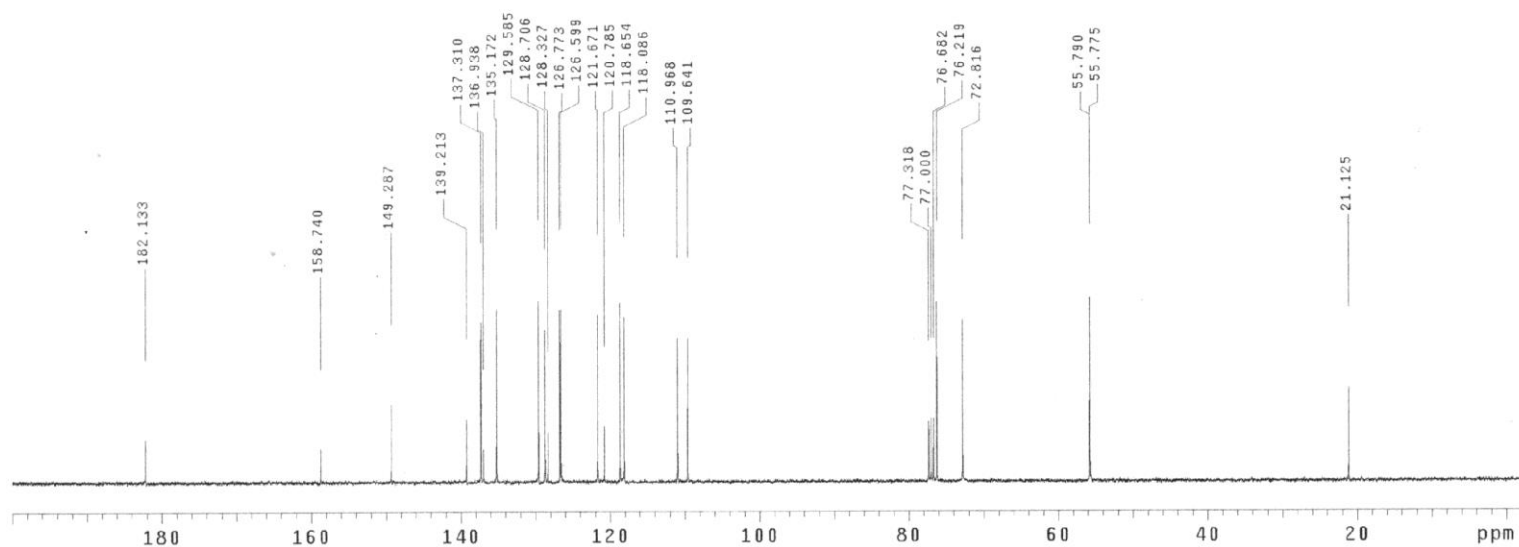
HAK7A1

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Nov 13 2017
Solvent: CDCl_3
Ambient temperature
Total 1072 repetitions



Compound 4g

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



Compound 4h (¹H-NMR spectral data)

HAK8A1

Pulse Sequence: s2pu1

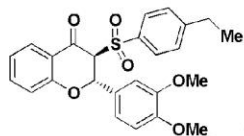
UNITYplus-400 "unity400"

Date: Nov 16 2017

Solvent: CDCl₃

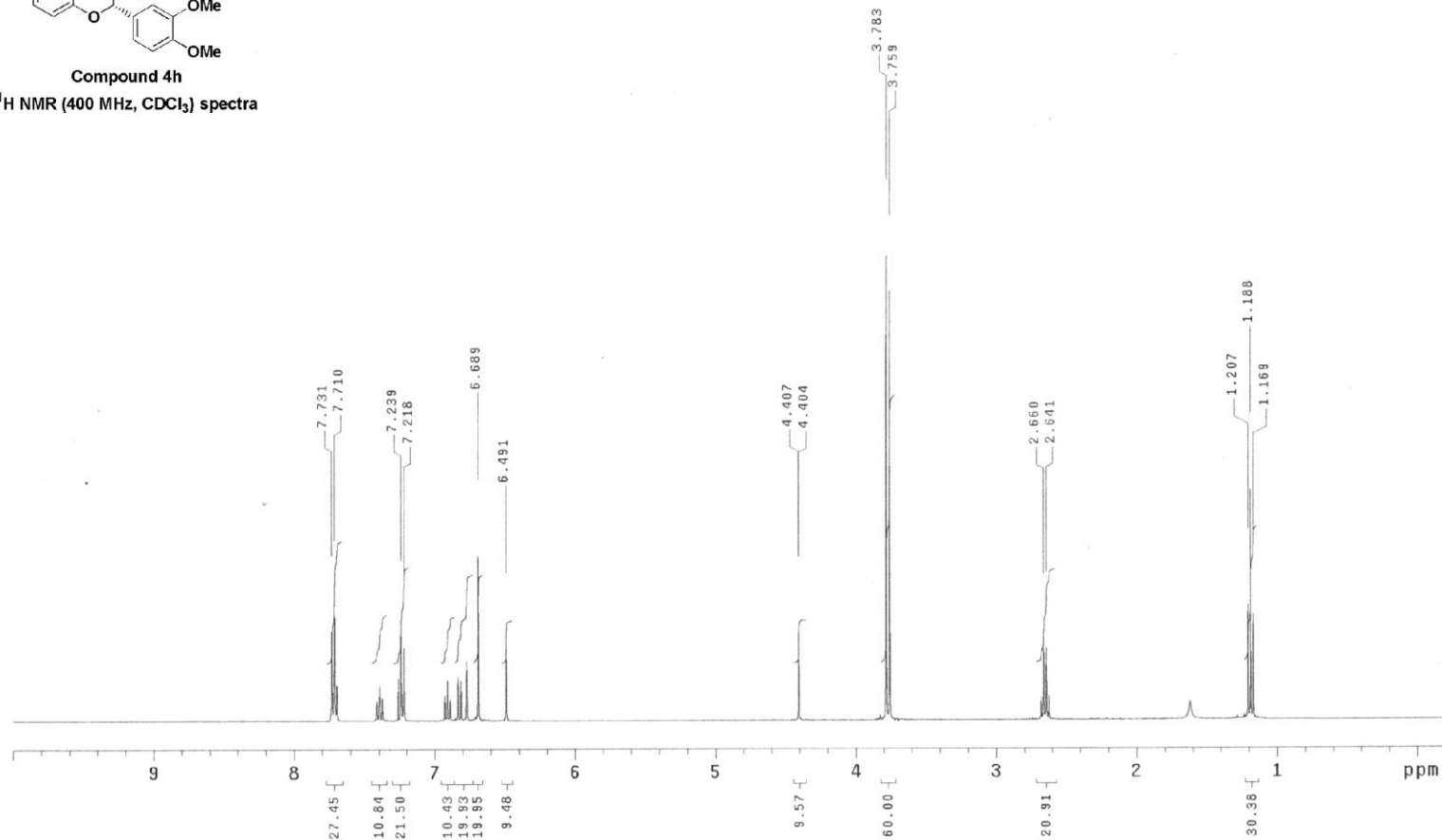
Ambient temperature

Total 32 repetitions



Compound 4h

¹H NMR (400 MHz, CDCl₃) spectra



Compound 4h (¹³C-NMR spectral data)

HAK8A1

Pulse Sequence: s2pu1

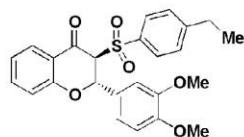
UNITYplus-400 "unity400"

Date: Nov 16 2017

Solvent: CDCl₃

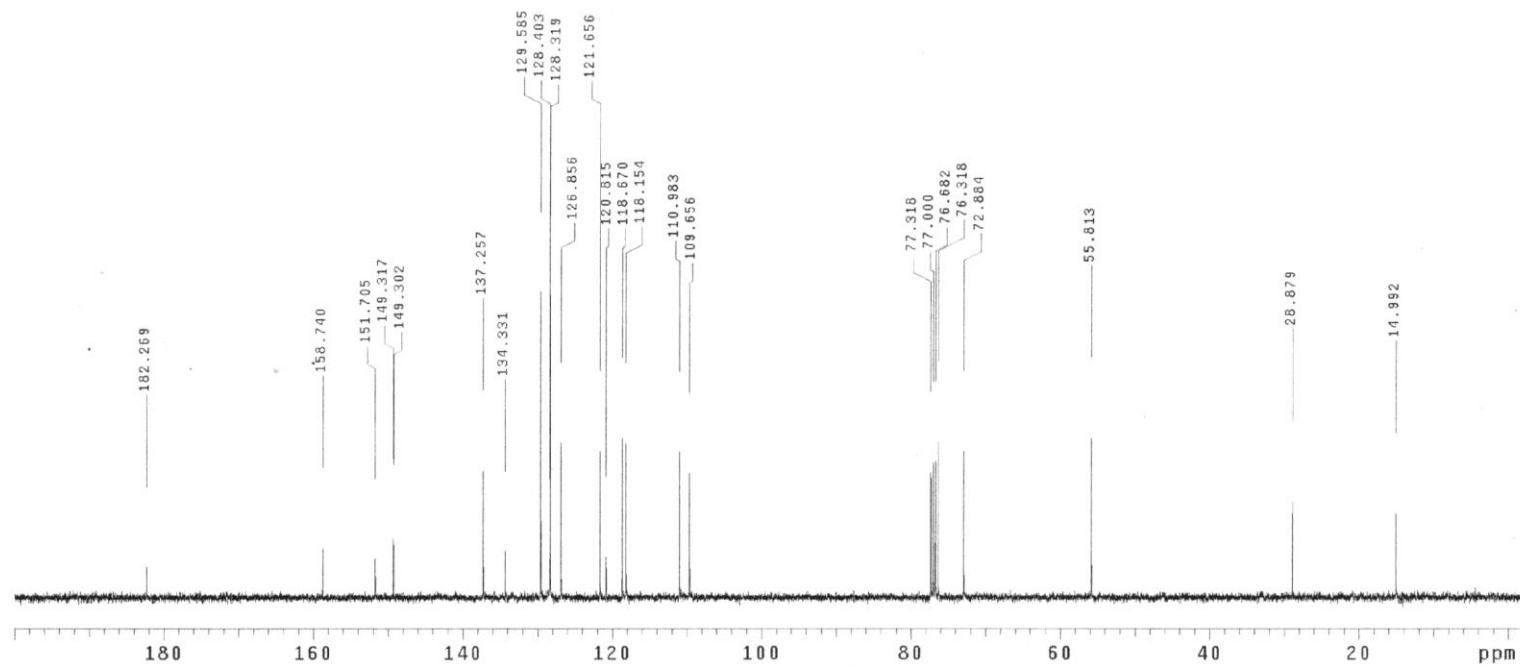
Ambient temperature

Total 1328 repetitions



Compound 4h

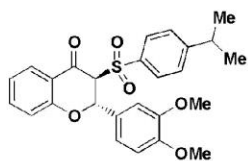
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4i (¹H-NMR spectral data)

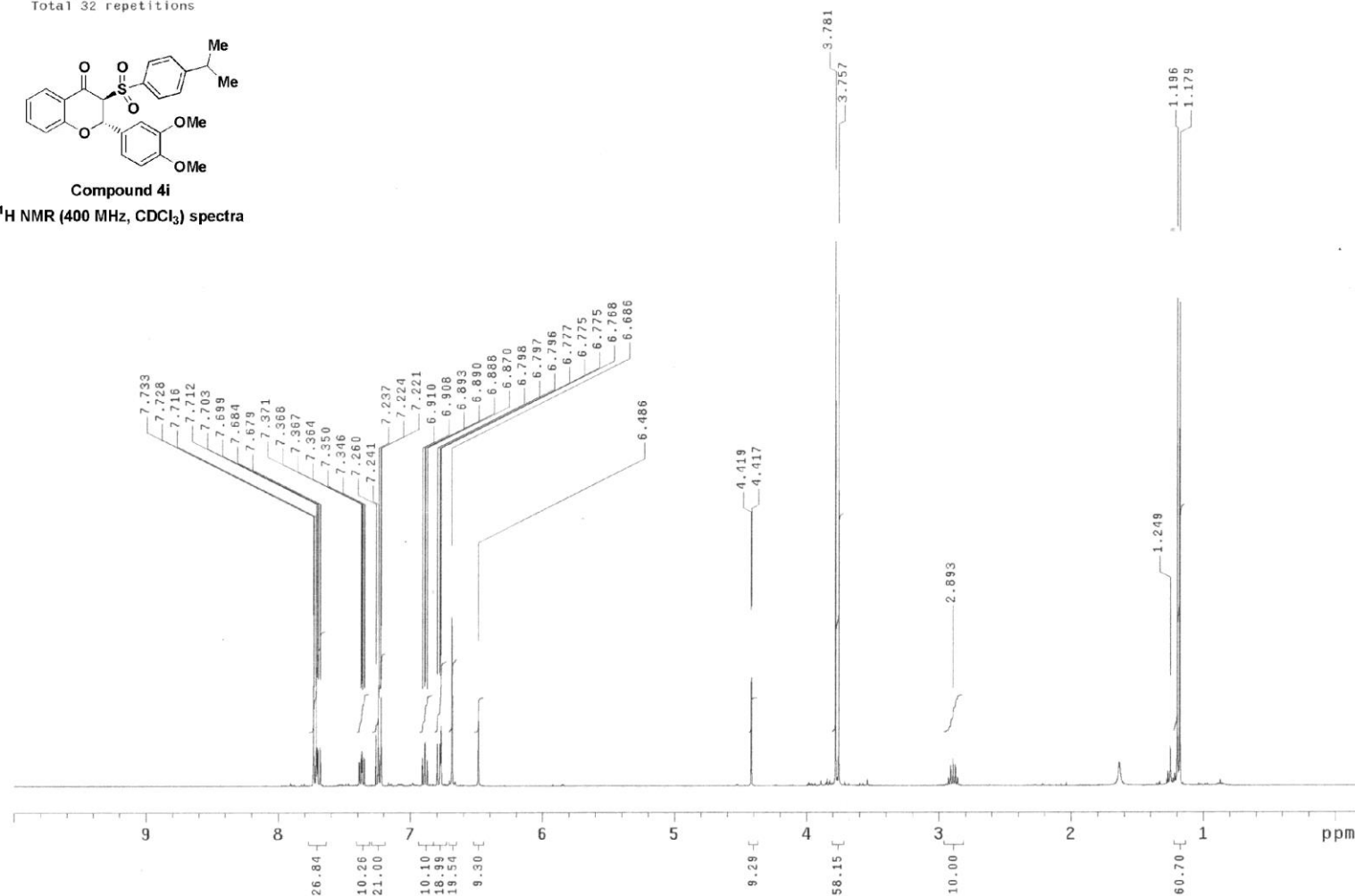
HAK9A1

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Nov 16 2017
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetitions



Compound 4i

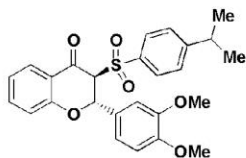
¹H NMR (400 MHz, CDCl₃) spectra



Compound 4i (¹³C-NMR spectral data)

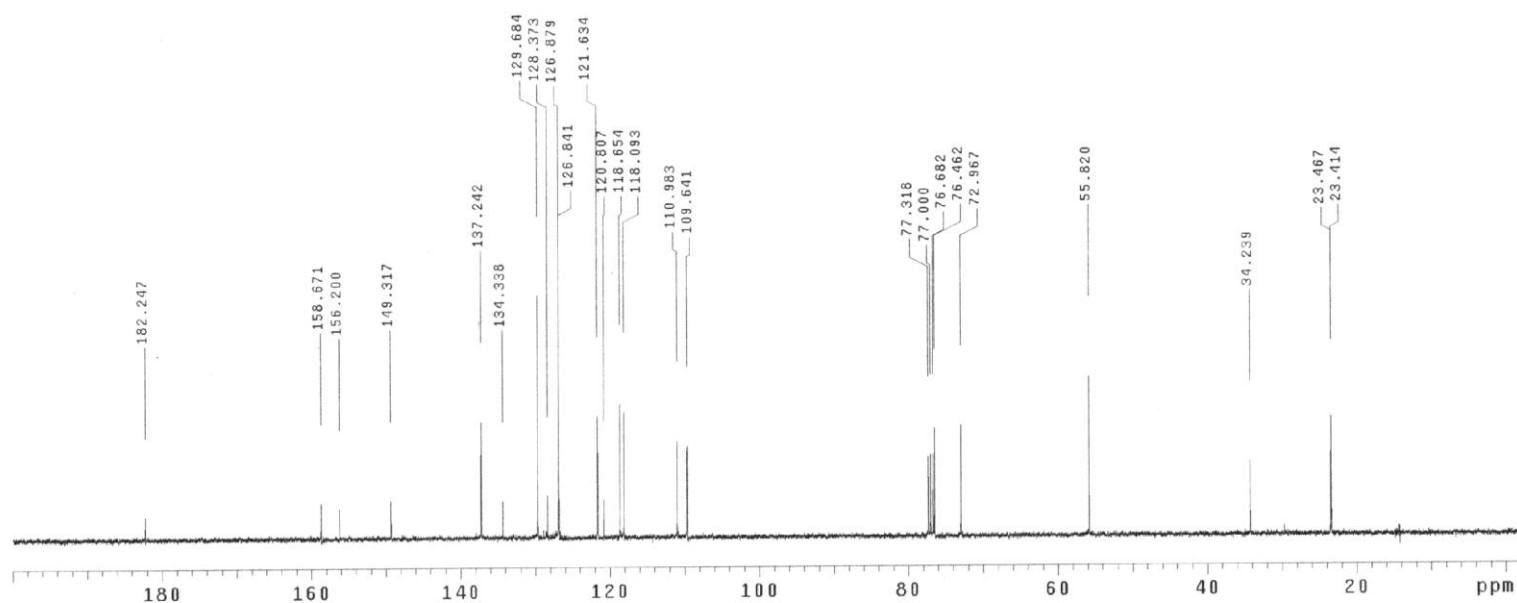
HAK9A1

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Nov 16 2017
Solvent: CDCl₃
Ambient temperature
Total 2080 repetitions



Compound 4i

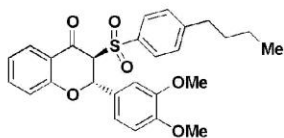
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4j (¹H-NMR spectral data)

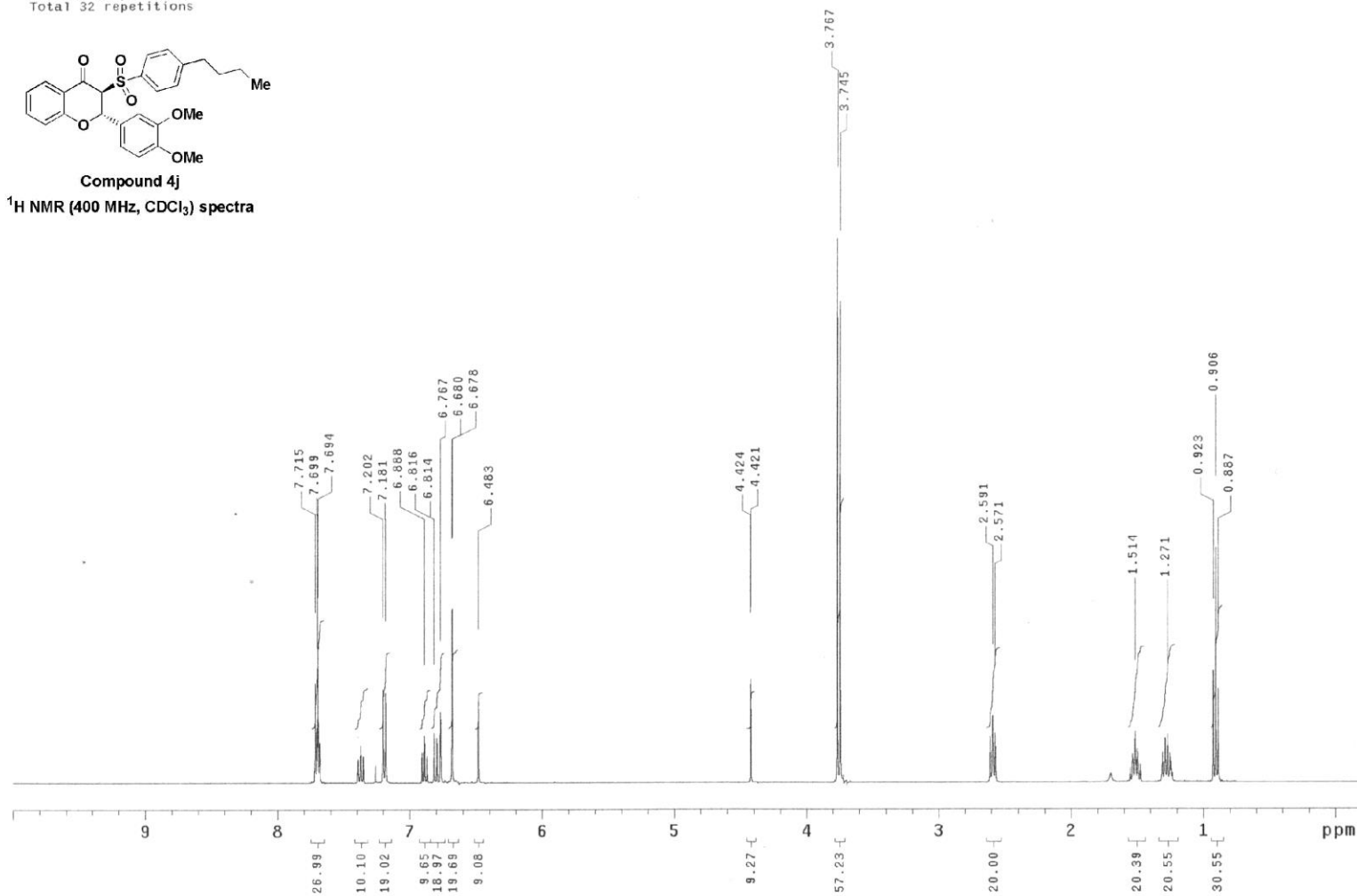
HAK10A1

Pulse Sequence: s2pul
 UNITYplus-400 "unity400"
 Date: Nov 23 2017
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetitions



Compound 4j

¹H NMR (400 MHz, CDCl₃) spectra



Compound 4j (¹³C-NMR spectral data)

HAK10A1

Pulse Sequence: s2pul

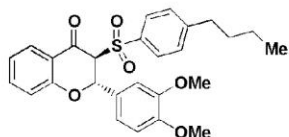
UNITYplus-400 "unity400"

Date: Nov 23 2017

Solvent: CDCl₃

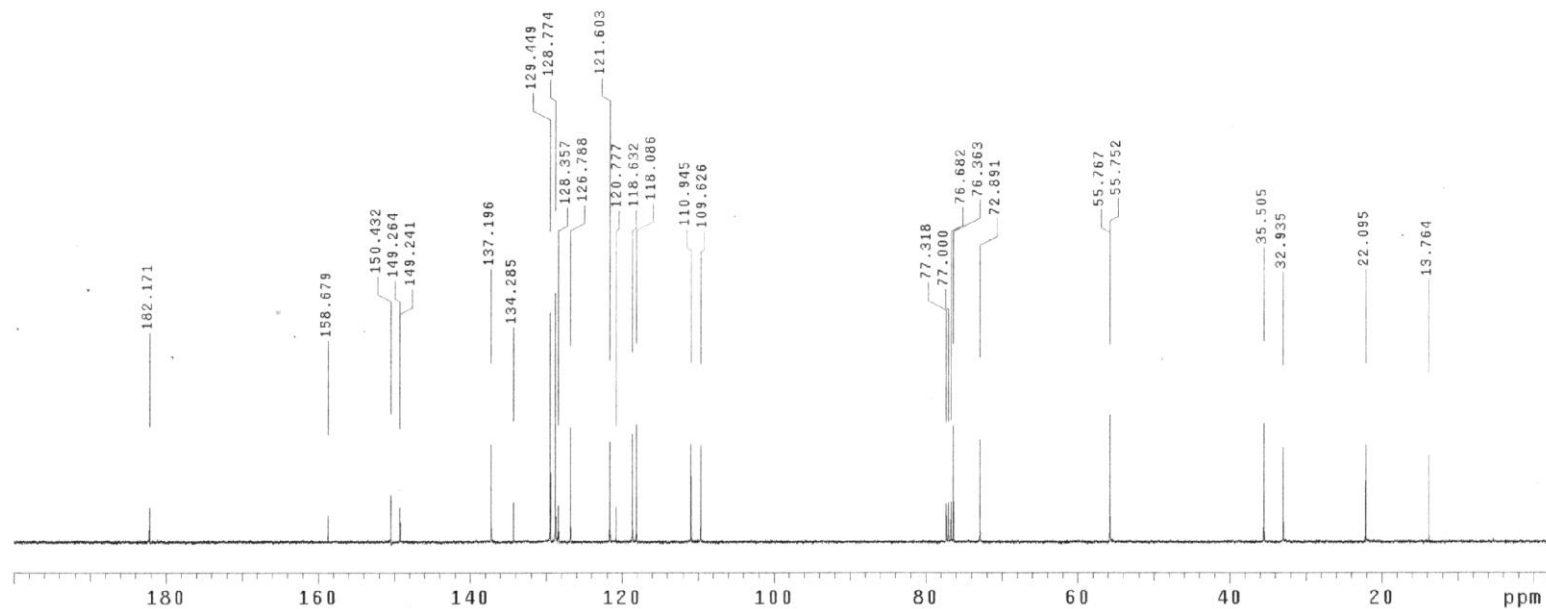
Ambient temperature

Total 640 repetitions



Compound 4j

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4k (¹H-NMR spectral data)

HAK11A1

Pulse Sequence: s2pu1

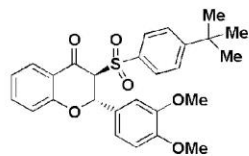
UNITYplus-400 "unity400"

Date: Nov 16 2017

Solvent: CDCl₃

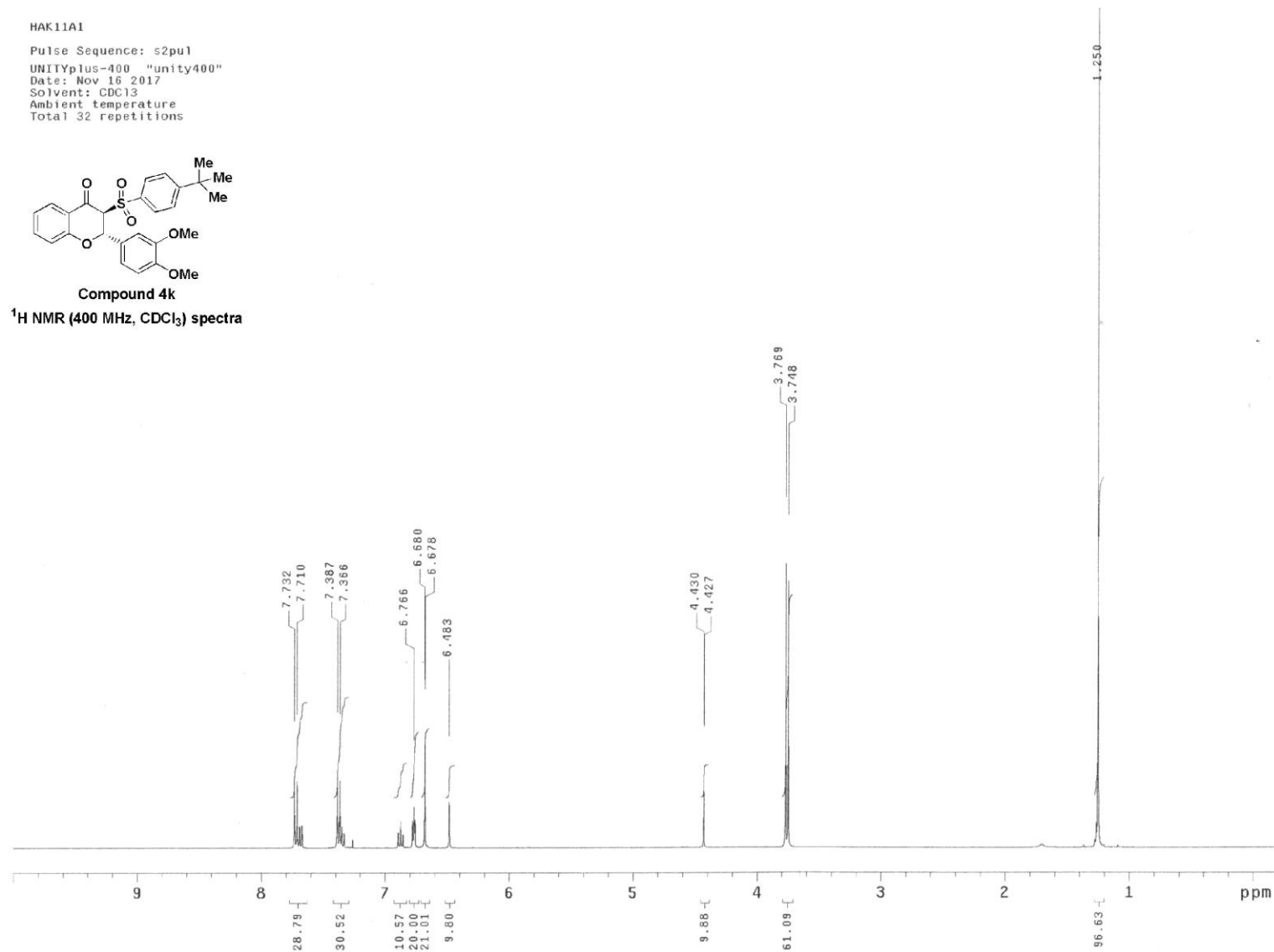
Ambient temperature

Total 32 repetitions



Compound 4k

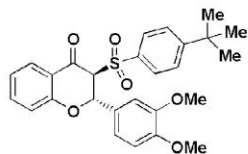
¹H NMR (400 MHz, CDCl₃) spectra



Compound 4k (¹³C-NMR spectral data)

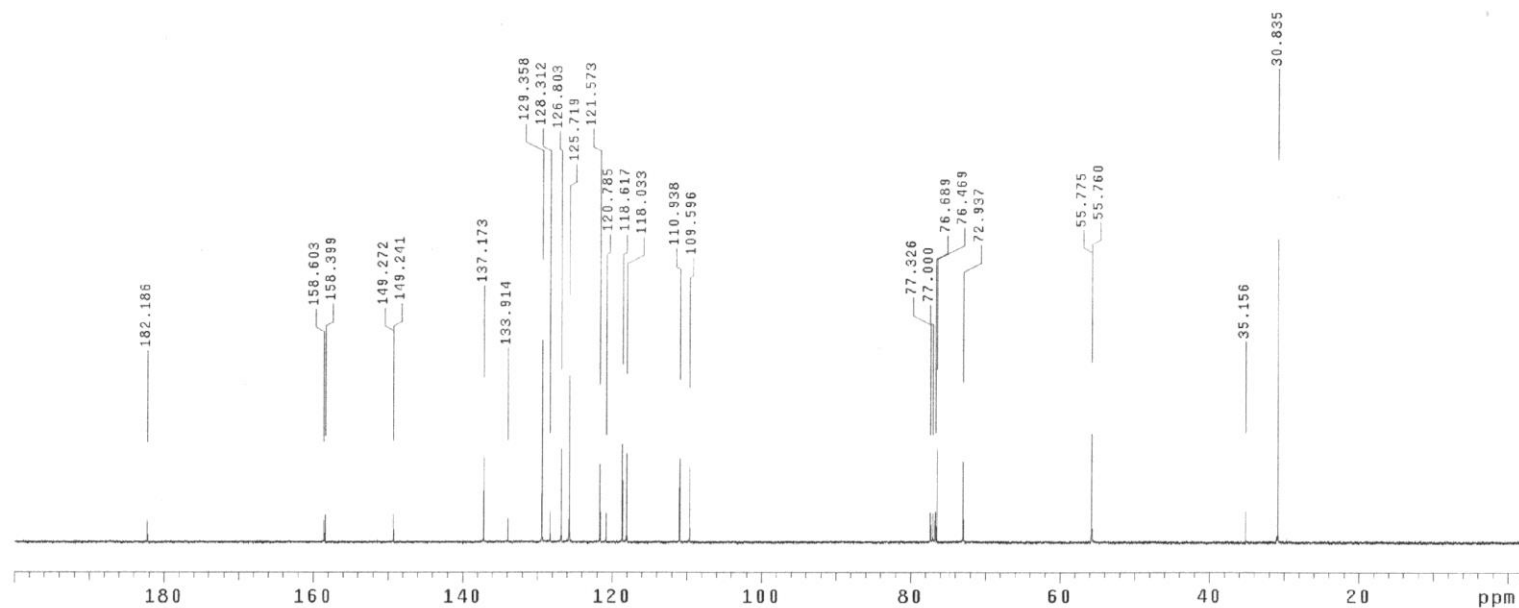
HAK11A1

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Nov 16 2017
 Solvent: CDCl₃
 Ambient temperature
 Total 720 repetitions



Compound 4k

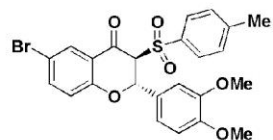
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4I (¹H-NMR spectral data)

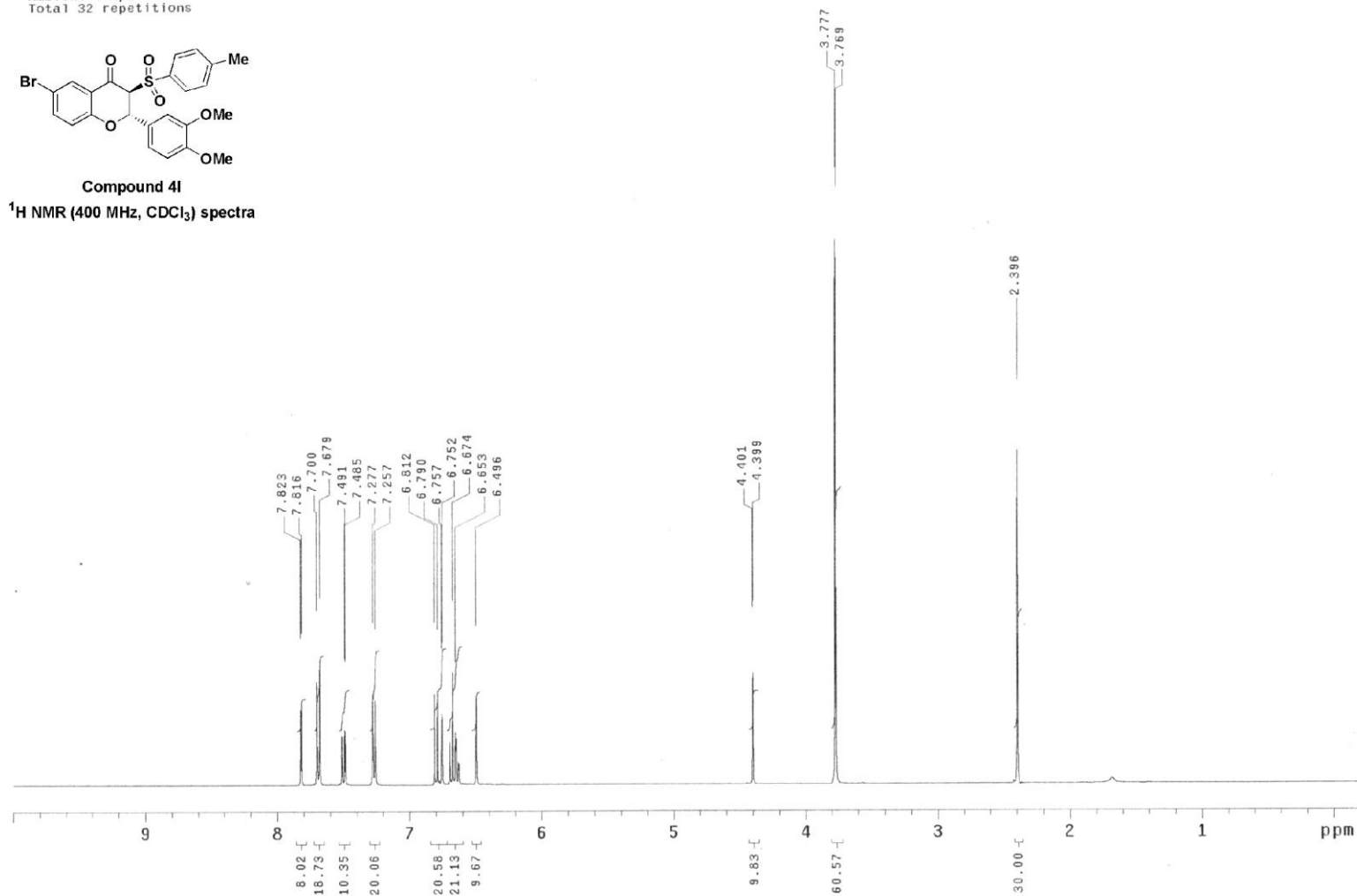
HAK12A1

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Nov 23 2017
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetitions



Compound 4I

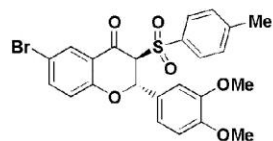
¹H NMR (400 MHz, CDCl₃) spectra



Compound 4I (¹³C-NMR spectral data)

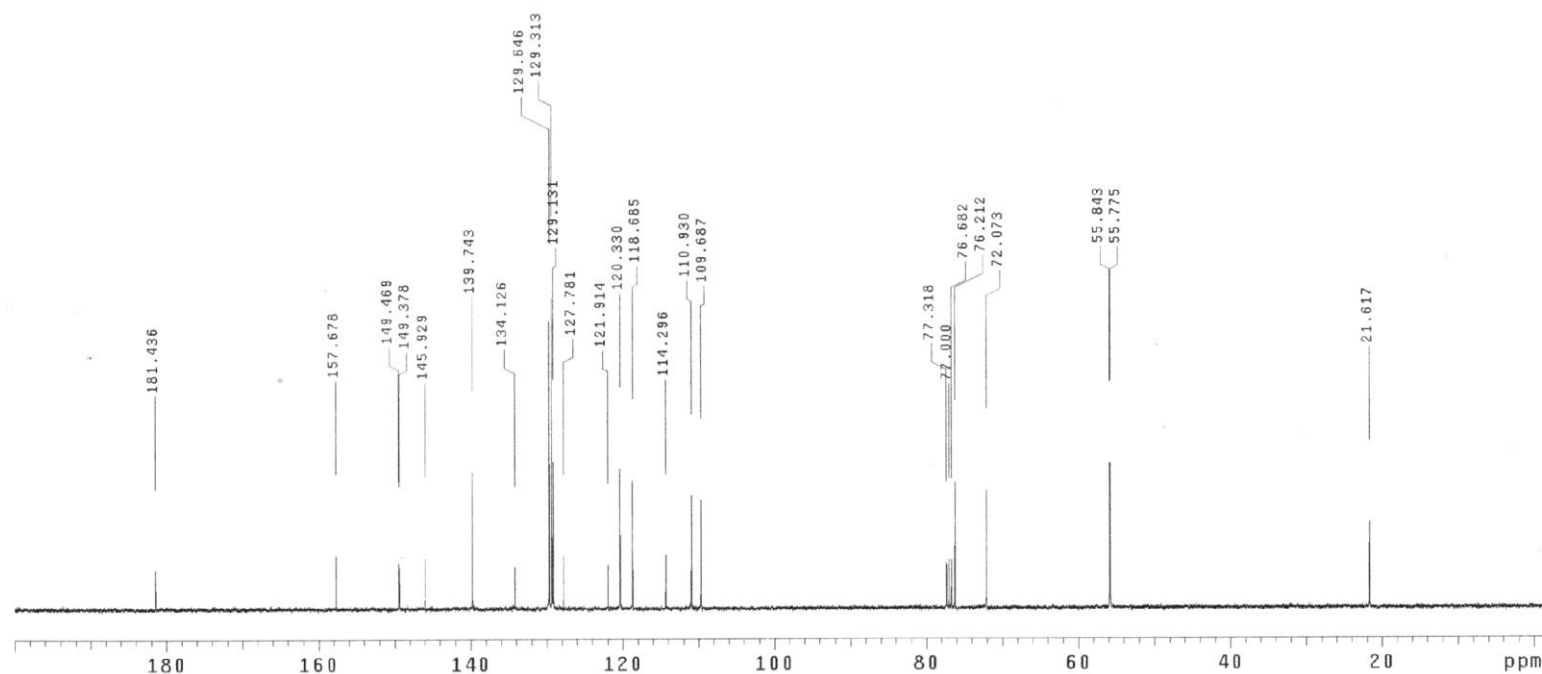
HAK12A1

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Nov 23 2017
 Solvent: CDCl₃
 Ambient temperature
 Total 512 repetitions



Compound 4I

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4m (¹H-NMR spectral data)

HAK13A1

Pulse Sequence: s2pu1

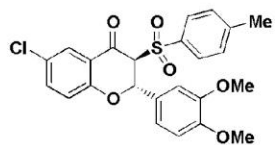
UNITYplus-400 "unity400"

Date: Nov 23 2017

Solvent: CDCl₃

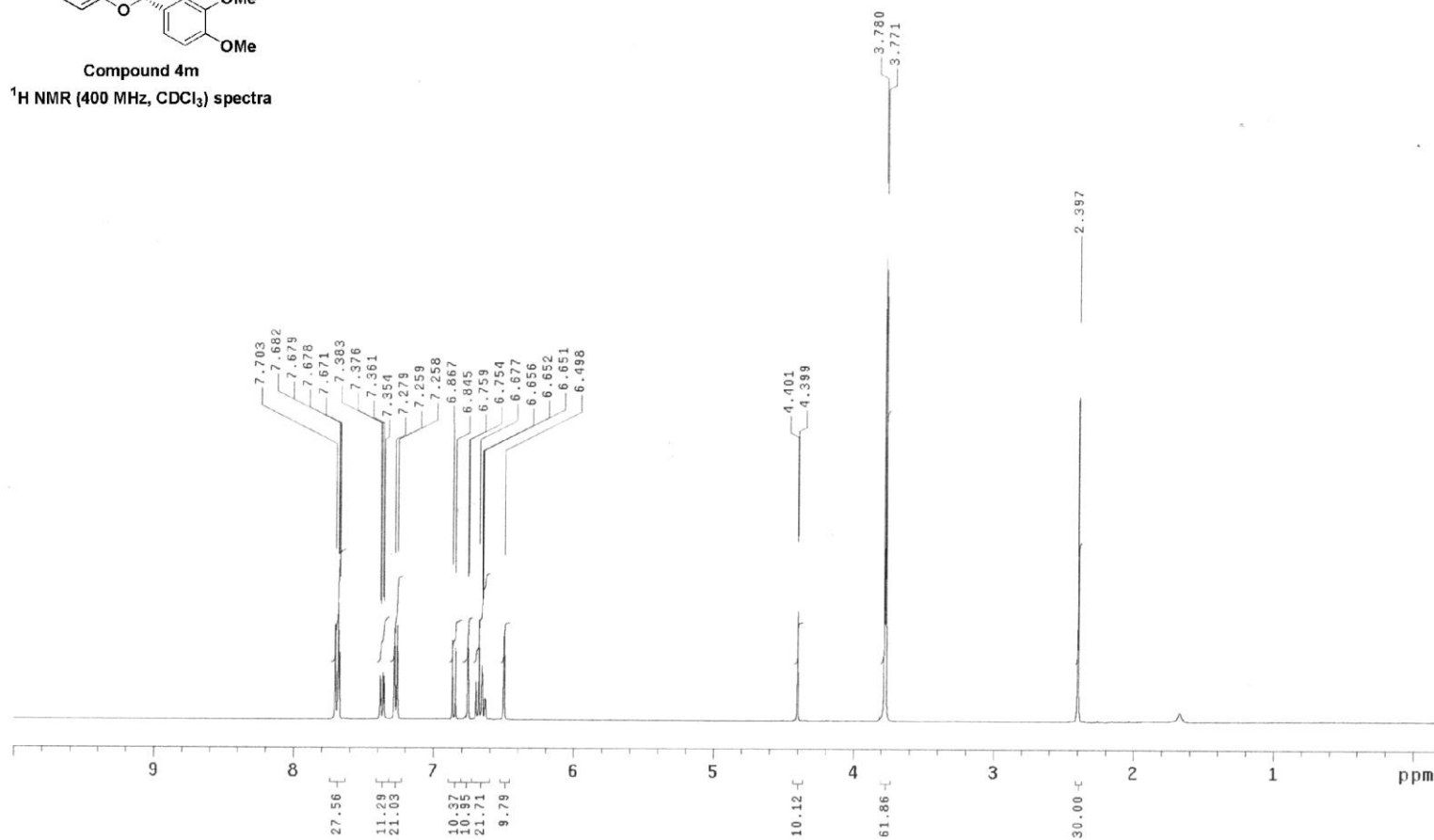
Ambient temperature

Total 32 repetitions



Compound 4m

¹H NMR (400 MHz, CDCl₃) spectra



Compound 4m (¹³C-NMR spectral data)

HAK13A1

Pulse Sequence: s2pu1

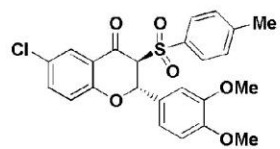
UNITYplus-400 "unity400"

Date: Nov 23 2017

Solvent: CDCl₃

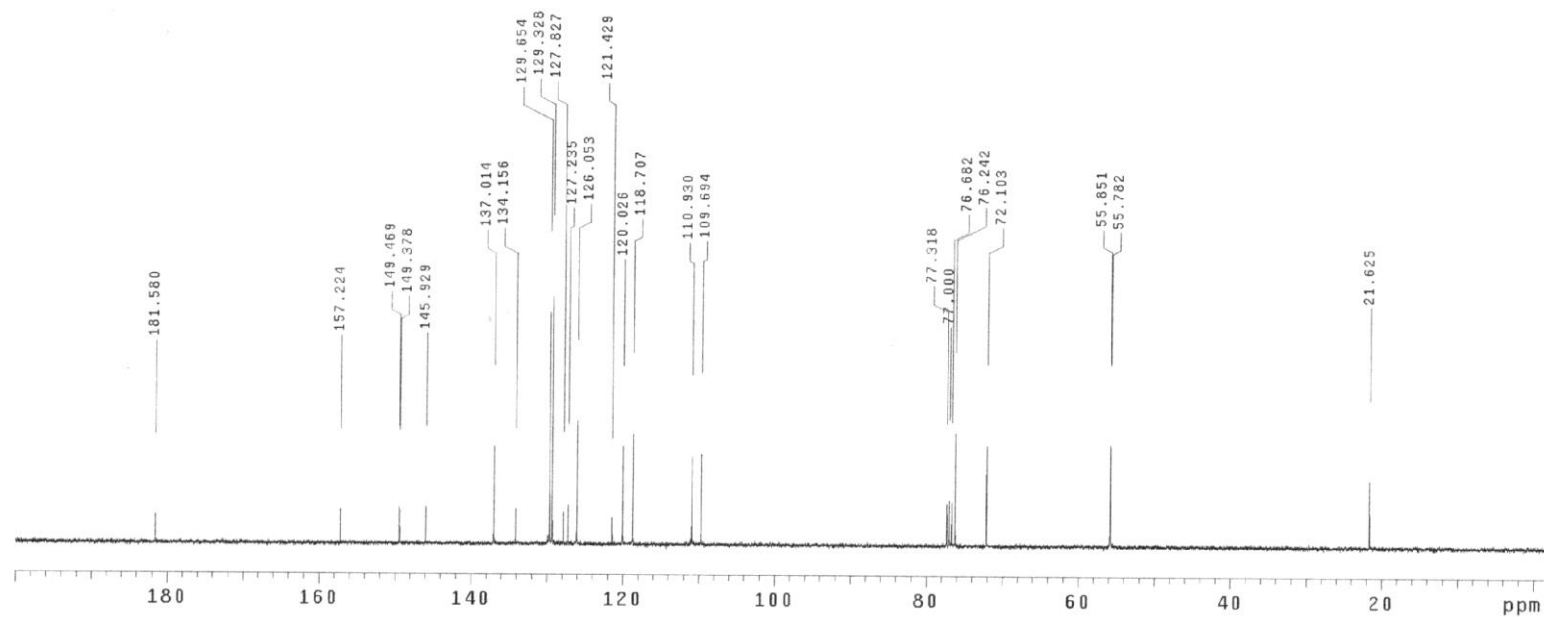
Ambient temperature

Total 464 repetitions



Compound 4m

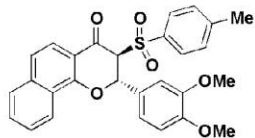
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4n (¹H-NMR spectral data)

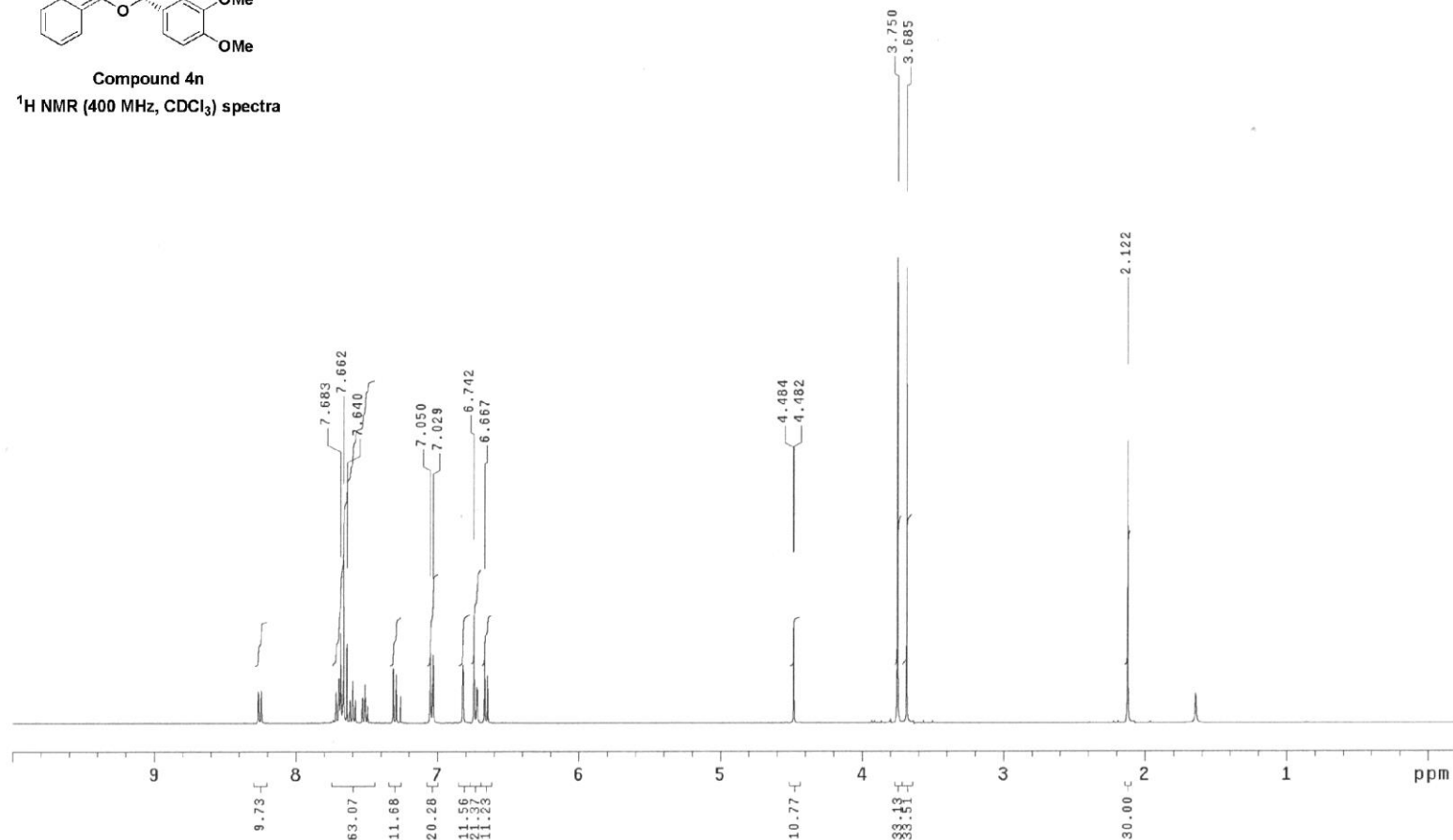
HAK14A1

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Jan 22 2018
Solvent: CDCl₃
Ambient temperature
Total 32 repetitions



Compound 4n

¹H NMR (400 MHz, CDCl₃) spectra



Compound 4n (¹³C-NMR spectral data)

HAK14A1

Pulse Sequence: s2pul

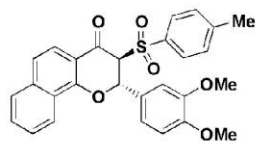
UNITYplus-400 "unity400"

Date: Jan 22 2018

Solvent: CDCl₃

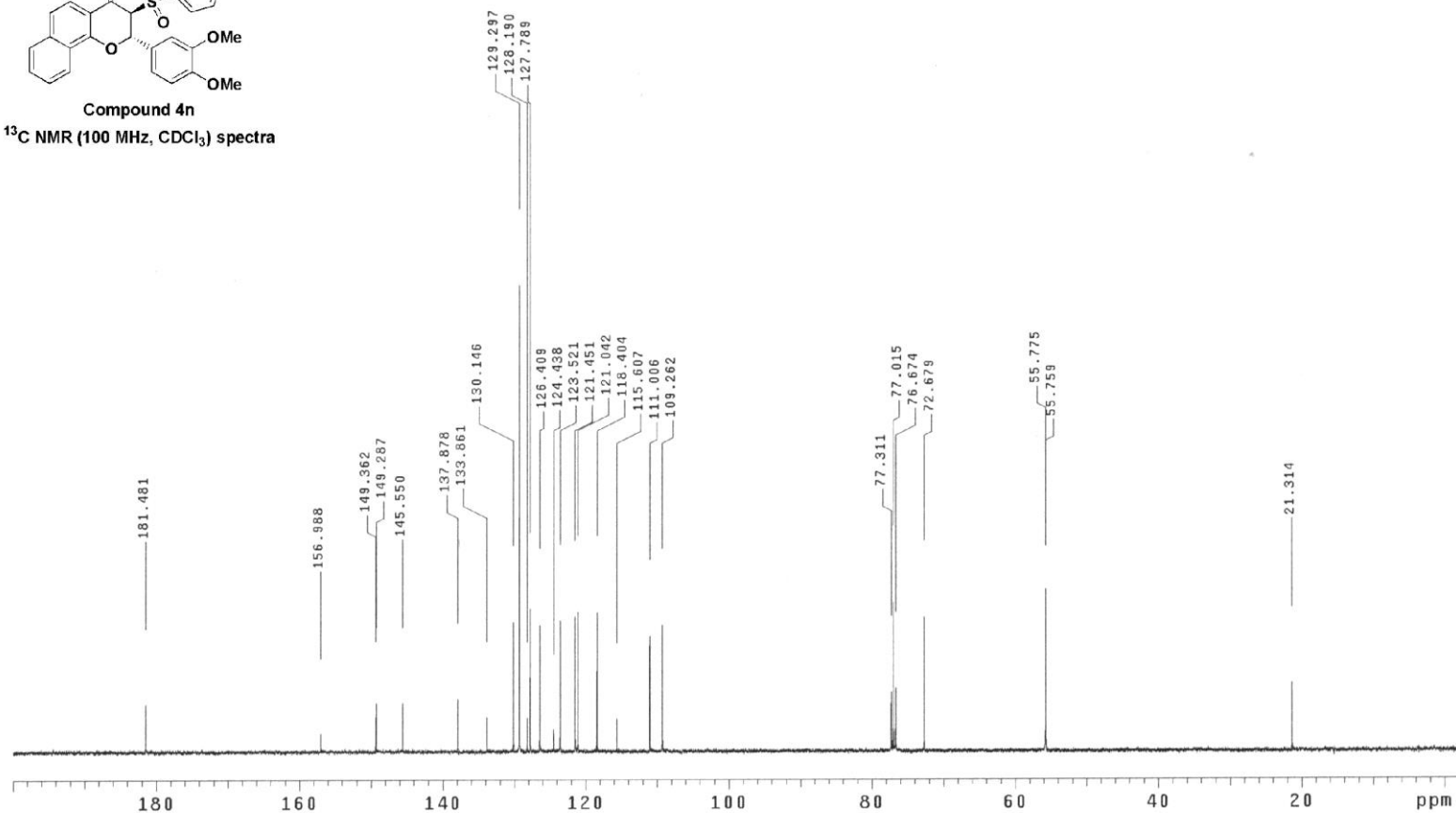
Ambient temperature

Total 2096 repetitions



Compound 4n

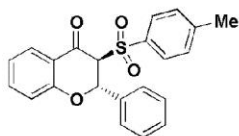
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4o (¹H-NMR spectral data)

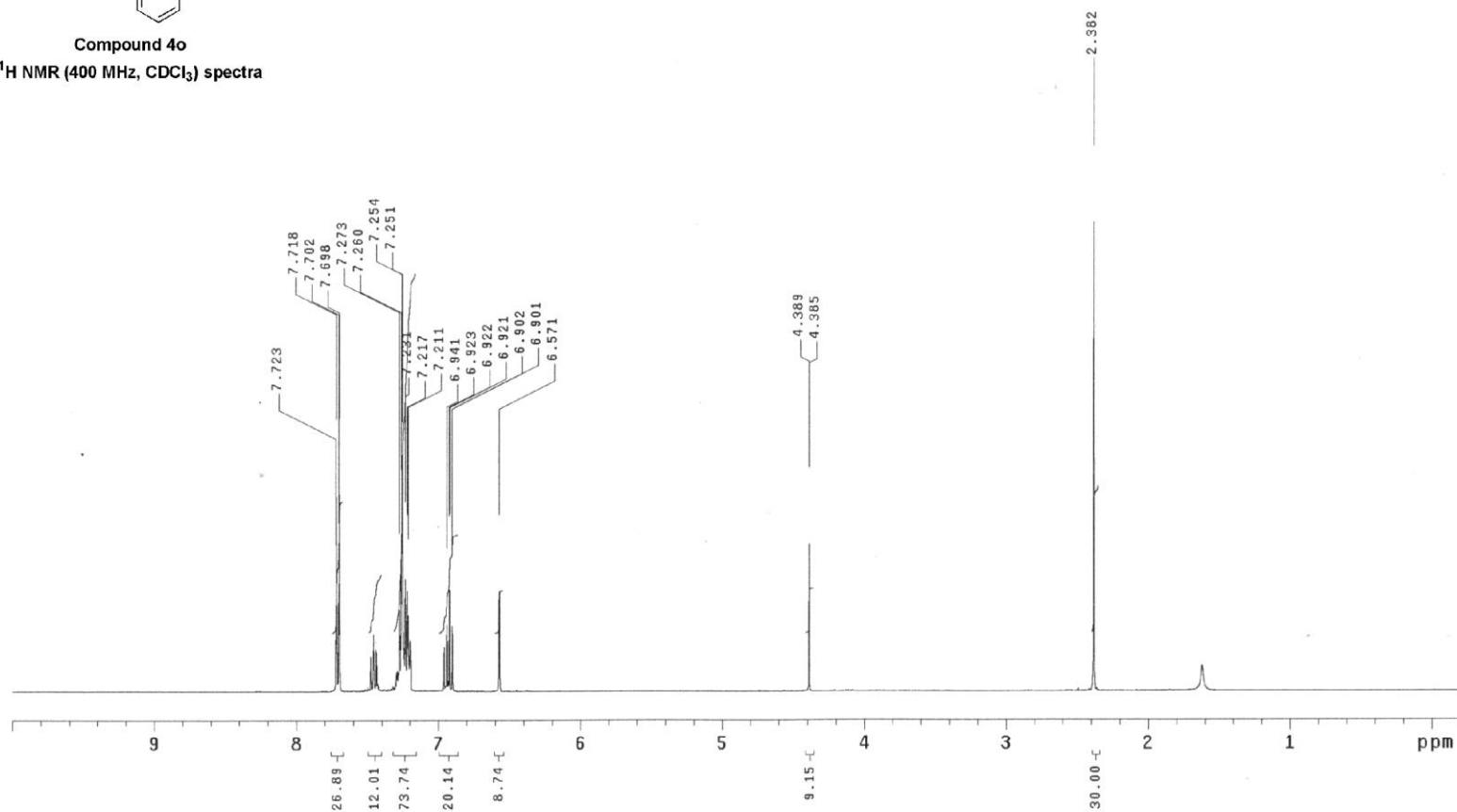
HAK15Ao

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Nov 30 2017
Solvent: CDCl₃
Ambient temperature
Total 32 repetitions



Compound 4o

¹H NMR (400 MHz, CDCl₃) spectra



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

HAK15Ao

Pulse Sequence: s2pu1

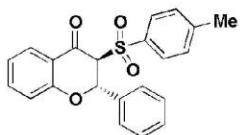
UNITYplus-400 "unity400"

Date: Nov 30 2017

Solvent: CDCl_3

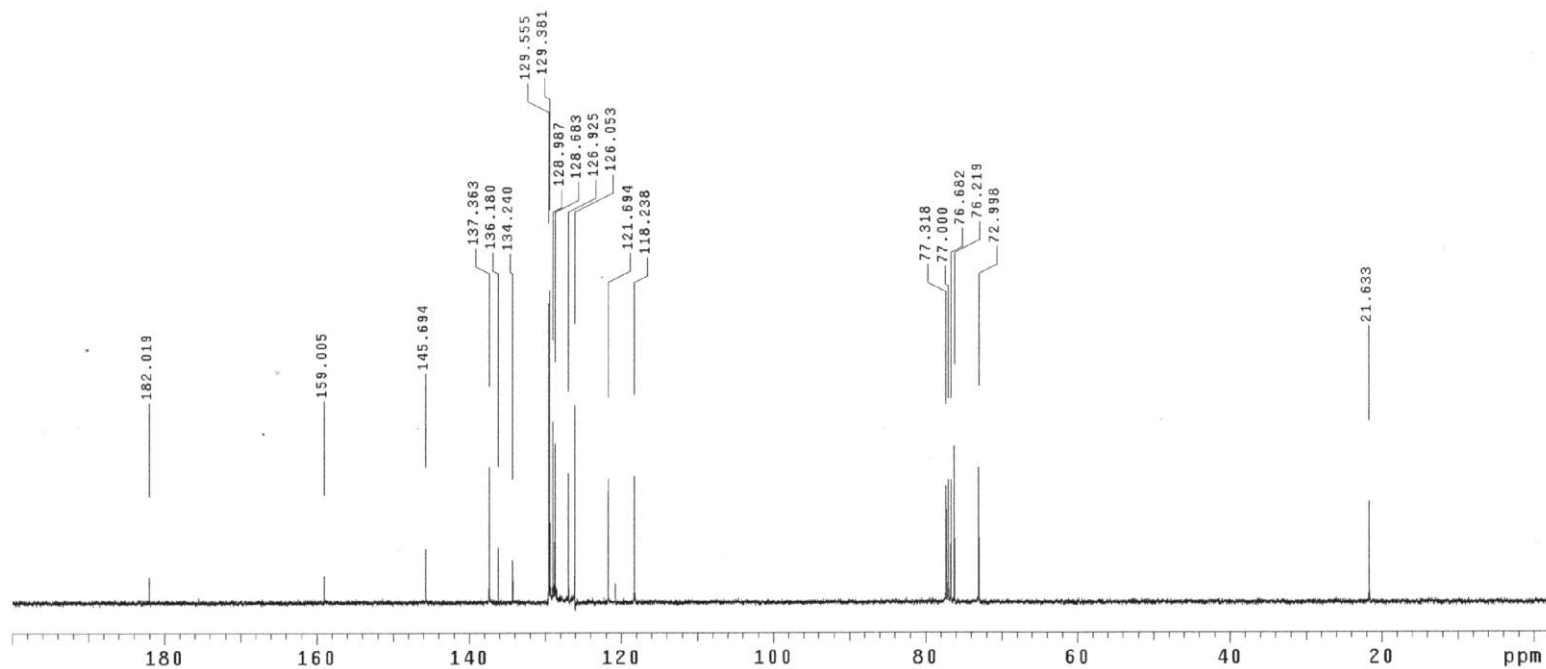
Ambient temperature

Total 3056 repetitions



Compound 4o

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



Compound 4p (¹H-NMR spectral data)

HAK1A4

Pulse Sequence: s2pu1

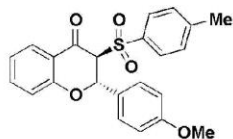
UNITYplus-400 "unity400"

Date: Dec 4 2017

Solvent: CDCl₃

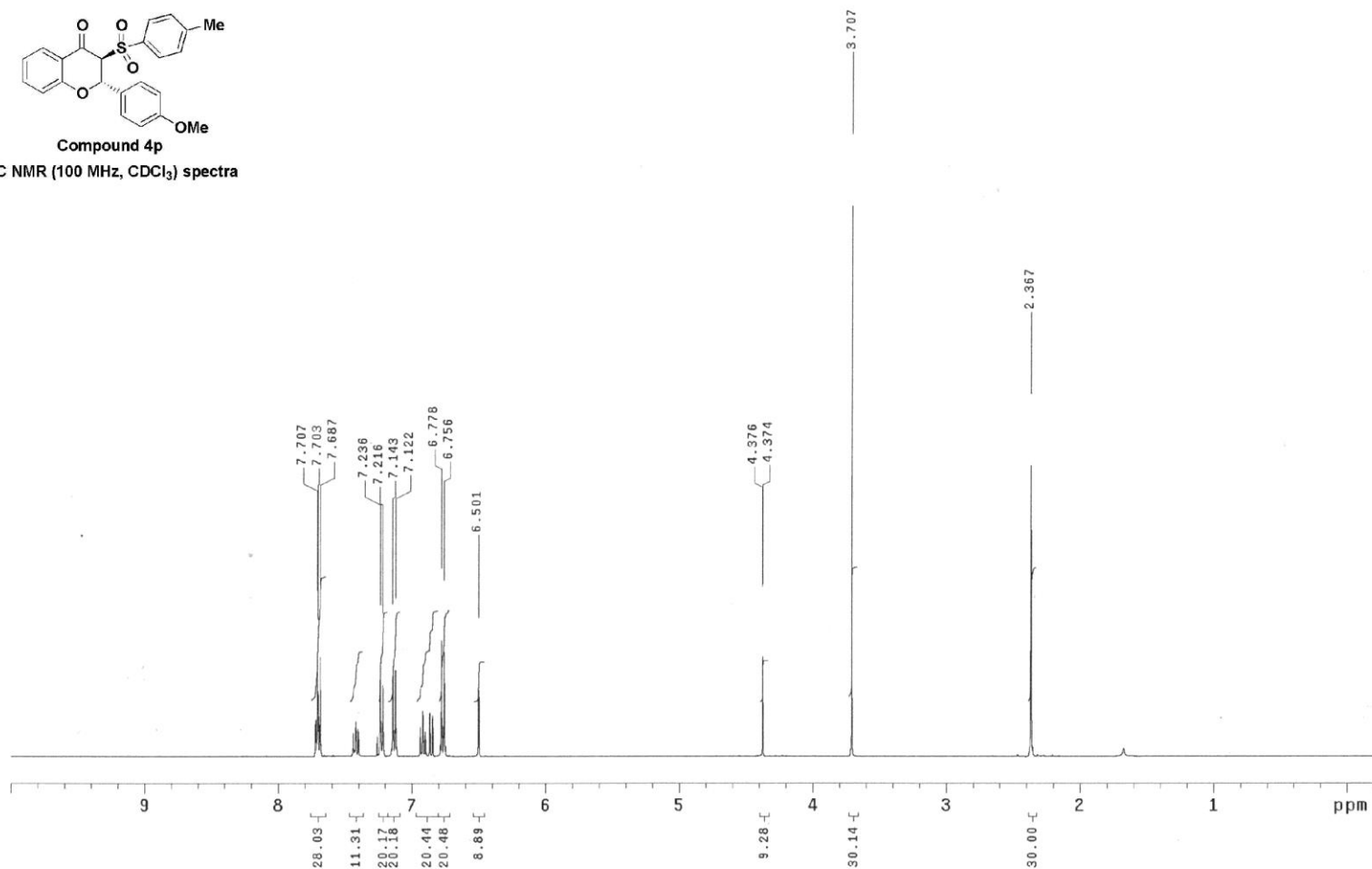
Ambient temperature

Total 32 repetitions



Compound 4p

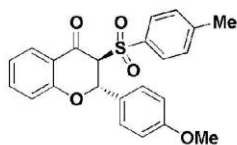
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4p (¹³C-NMR spectral data)

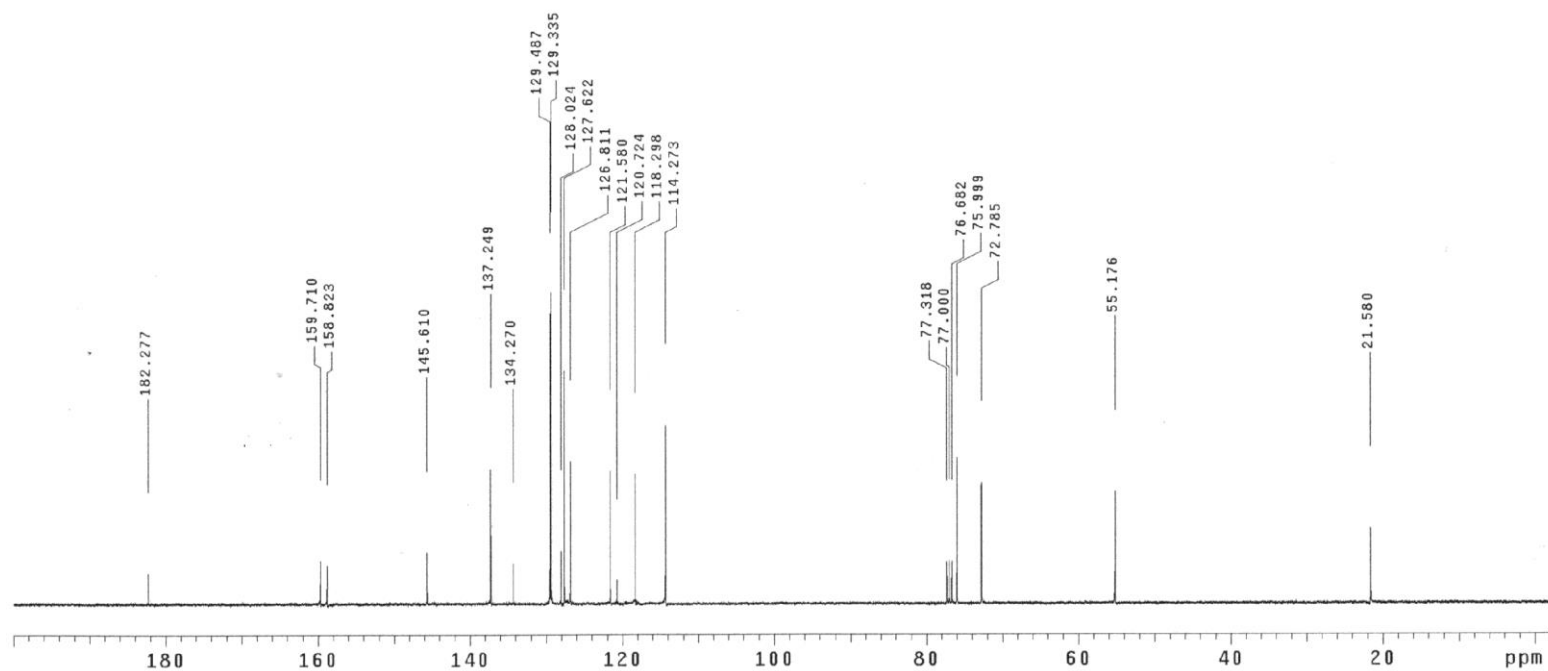
HAK1A4

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Dec 4 2017
 Solvent: CDCl₃
 Ambient temperature
 Total 1120 repetitions



Compound 4p

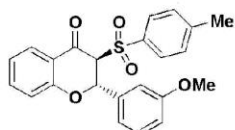
¹H NMR (400 MHz, CDCl₃) spectra



Compound 4q (¹H-NMR spectral data)

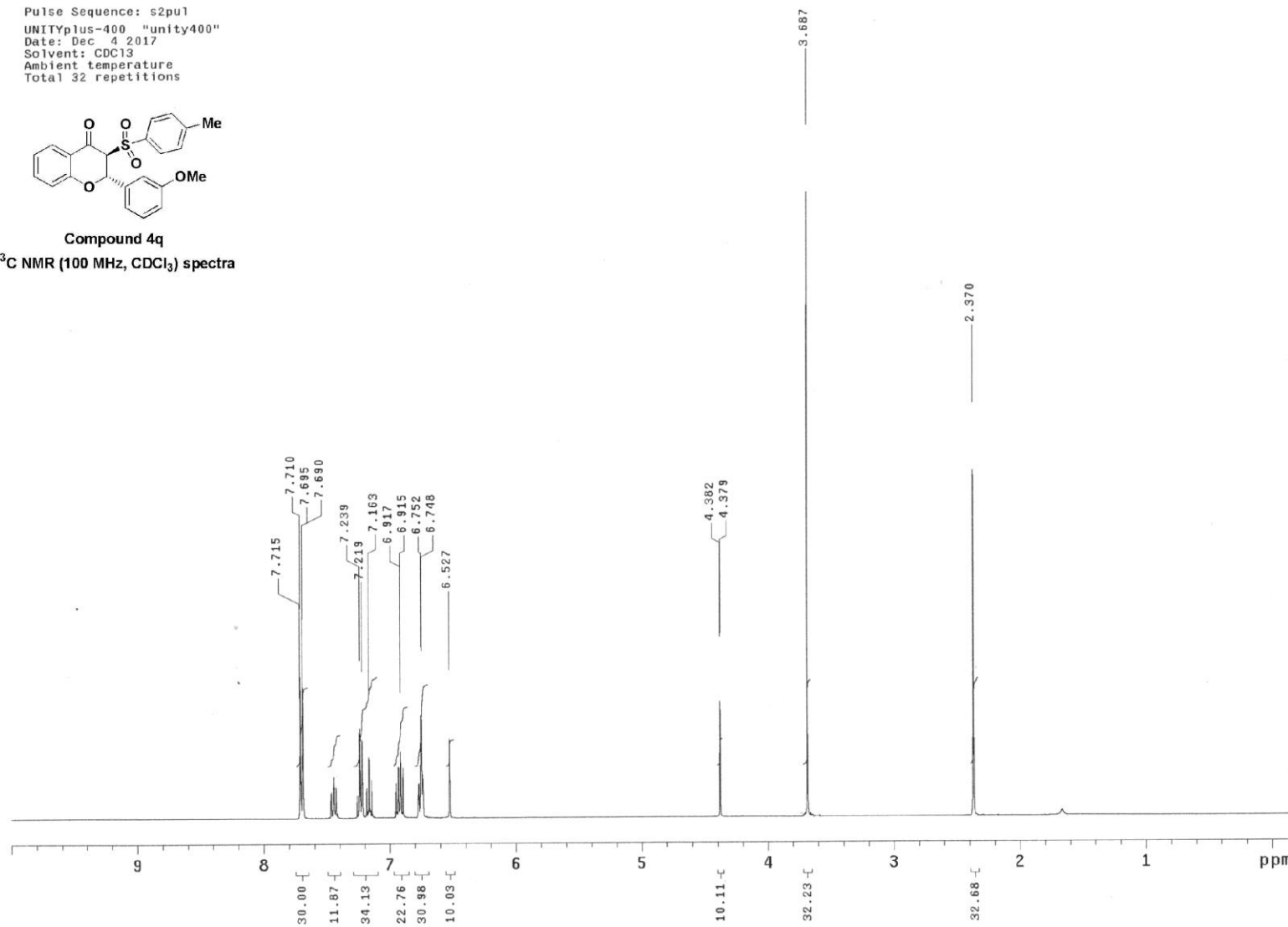
HAK1A3

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



Compound 4q

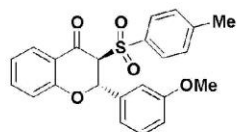
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4q (¹³C-NMR spectral data)

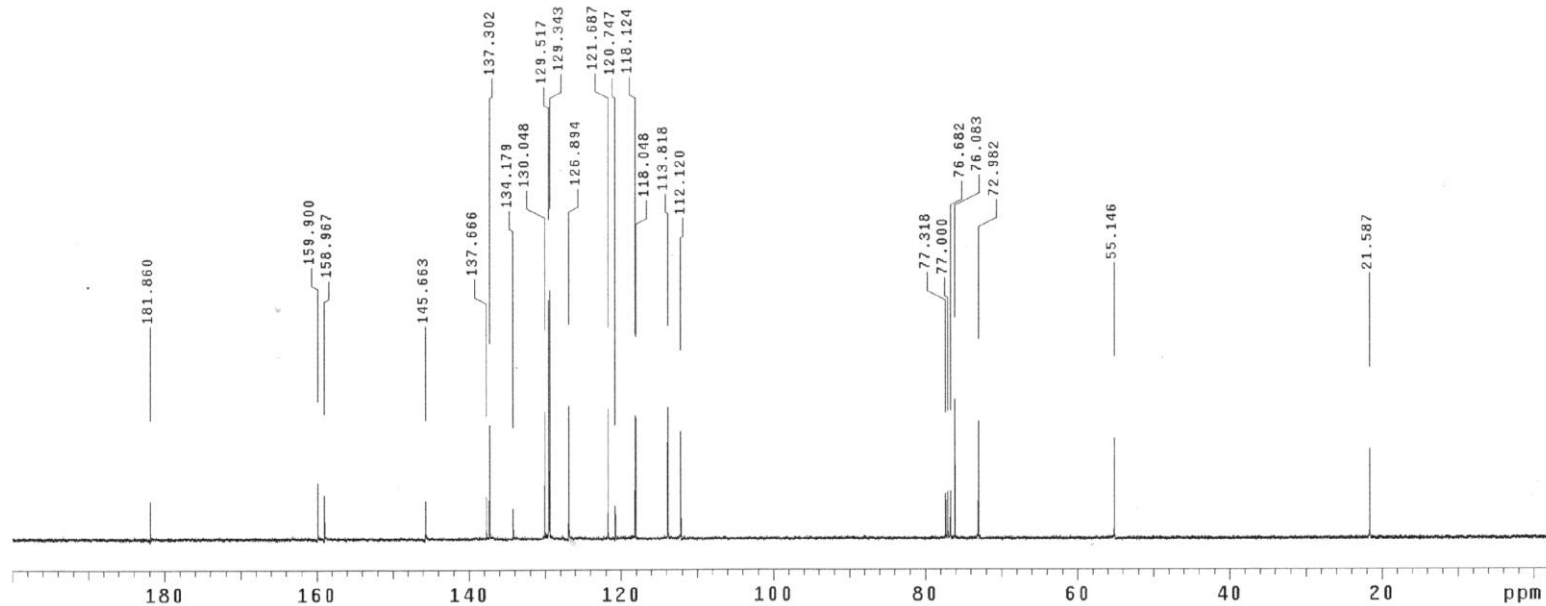
HAK1A3

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Dec 4 2017
 Solvent: CDCl₃
 Ambient temperature
 Total 848 repetitions



Compound 4q

¹H NMR (400 MHz, CDCl₃) spectra



Compound 4r (¹H-NMR spectral data)

HAK1A5

Pulse Sequence: s2pu1

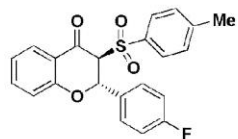
UNITYplus-400 "unity400"

Date: Dec 6 2017

Solvent: CDCl₃

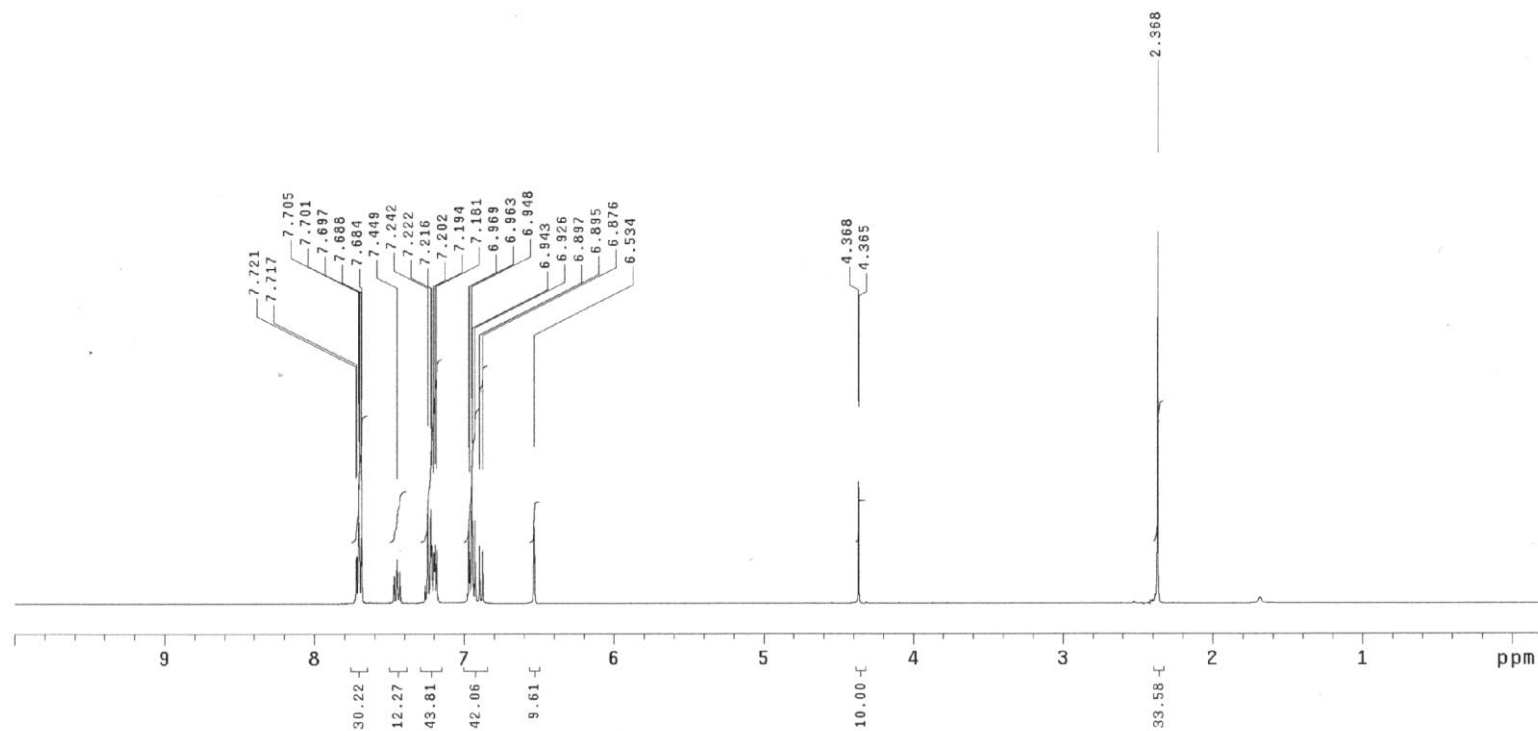
Ambient temperature

Total 32 repetitions



Compound 4r

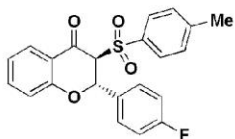
¹H NMR (400 MHz, CDCl₃) spectra



Compound 4r (¹³C-NMR spectral data)

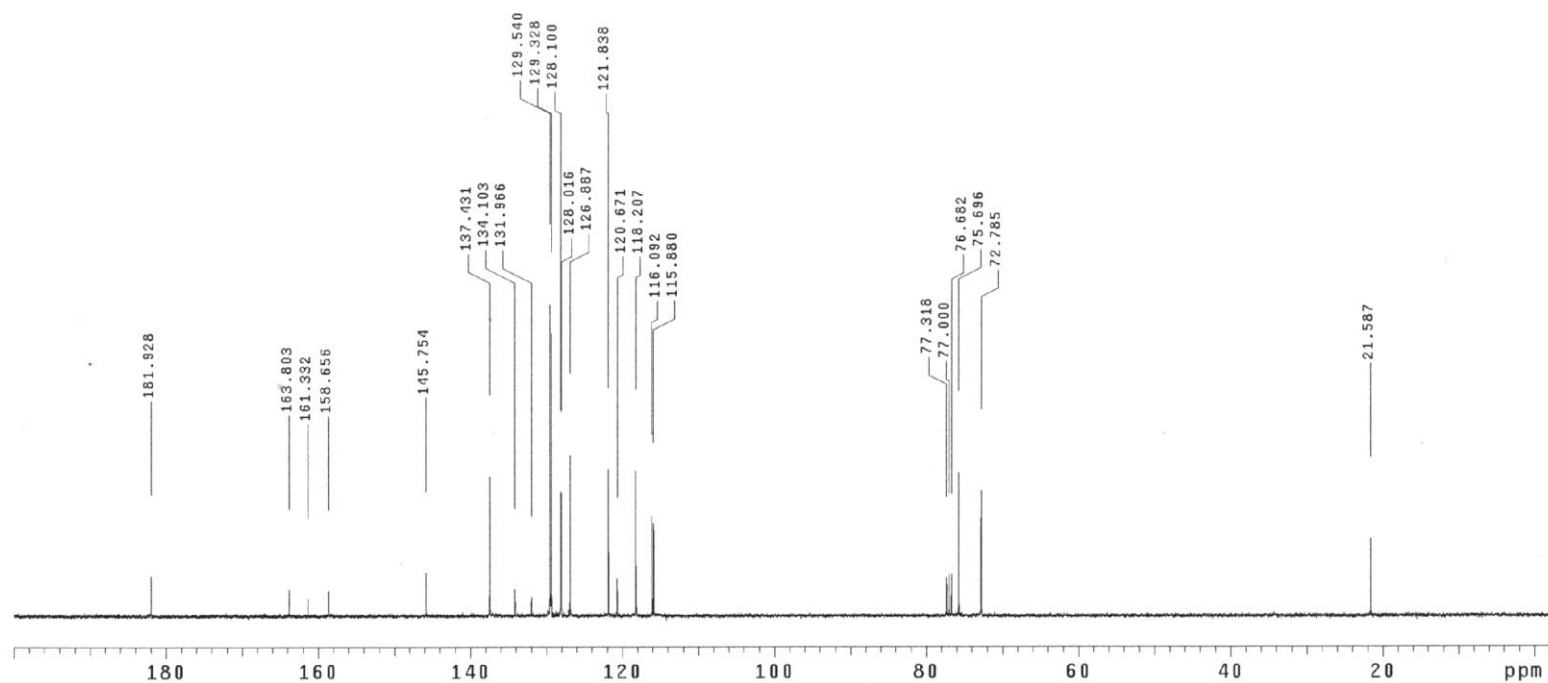
HAK1A5

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Dec 6 2017
Solvent: CDCl₃
Ambient temperature
Total 512 repetitions



Compound 4r

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4s (¹H-NMR spectral data)

HAK1A6

Pulse Sequence: s2pu1

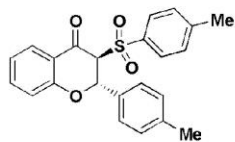
UNITYplus-400 "unity400"

Date: Dec 8 2017

Solvent: CDCl₃

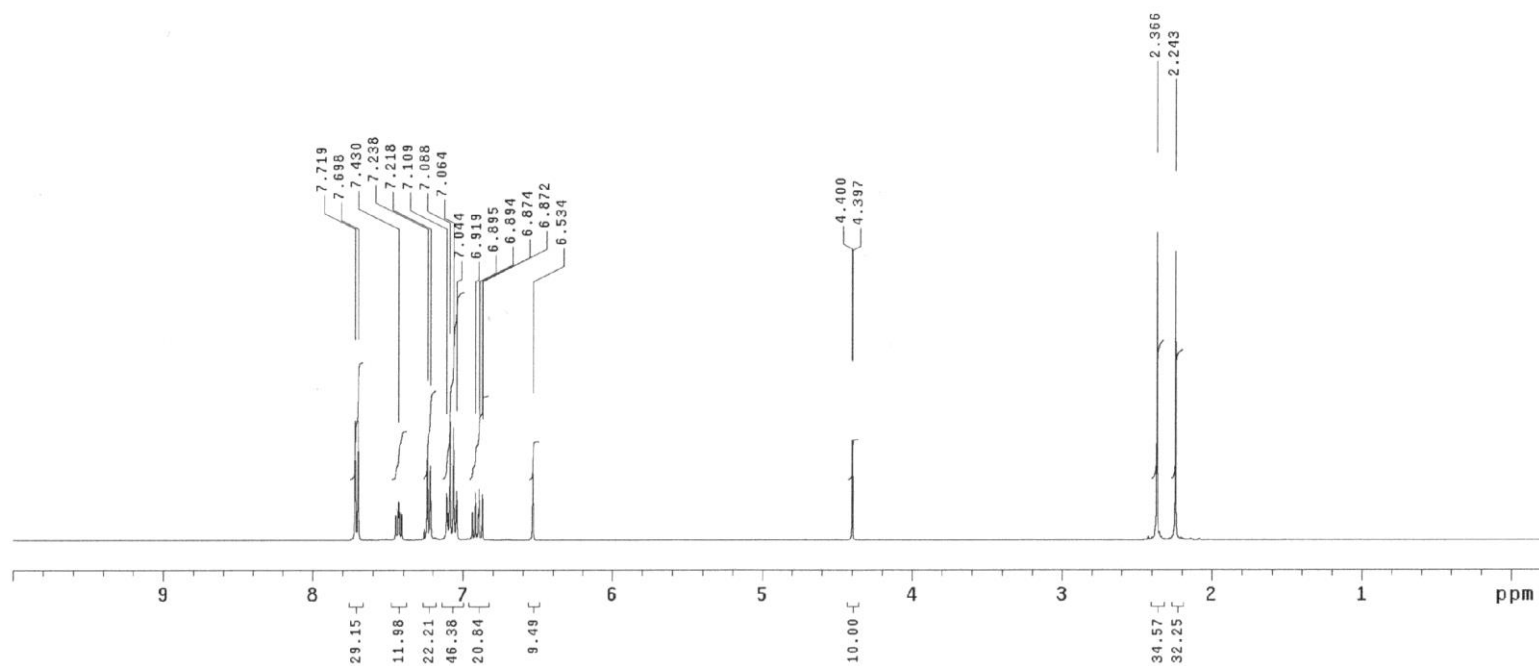
Ambient temperature

Total 32 repetitions



Compound 4s

¹H NMR (400 MHz, CDCl₃) spectra



Compound 4s (¹³C-NMR spectral data)

HAK1A6

Pulse Sequence: s2pu1

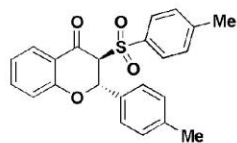
UNITYplus-400 "unity400"

Date: Dec 8 2017

Solvent: CDCl₃

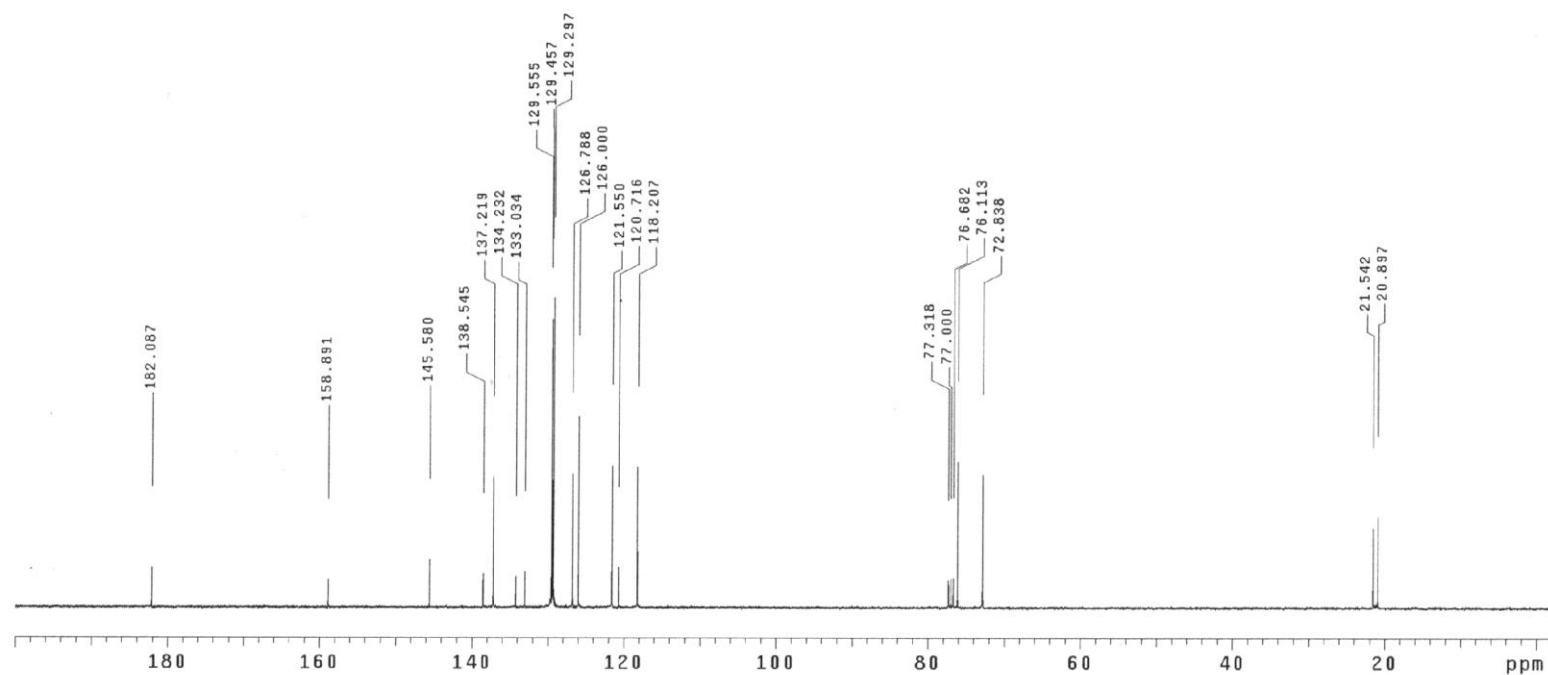
Ambient temperature

Total 736 repetitions



Compound 4s

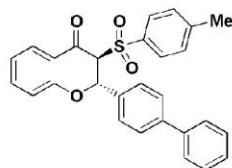
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4t (¹H-NMR spectral data)

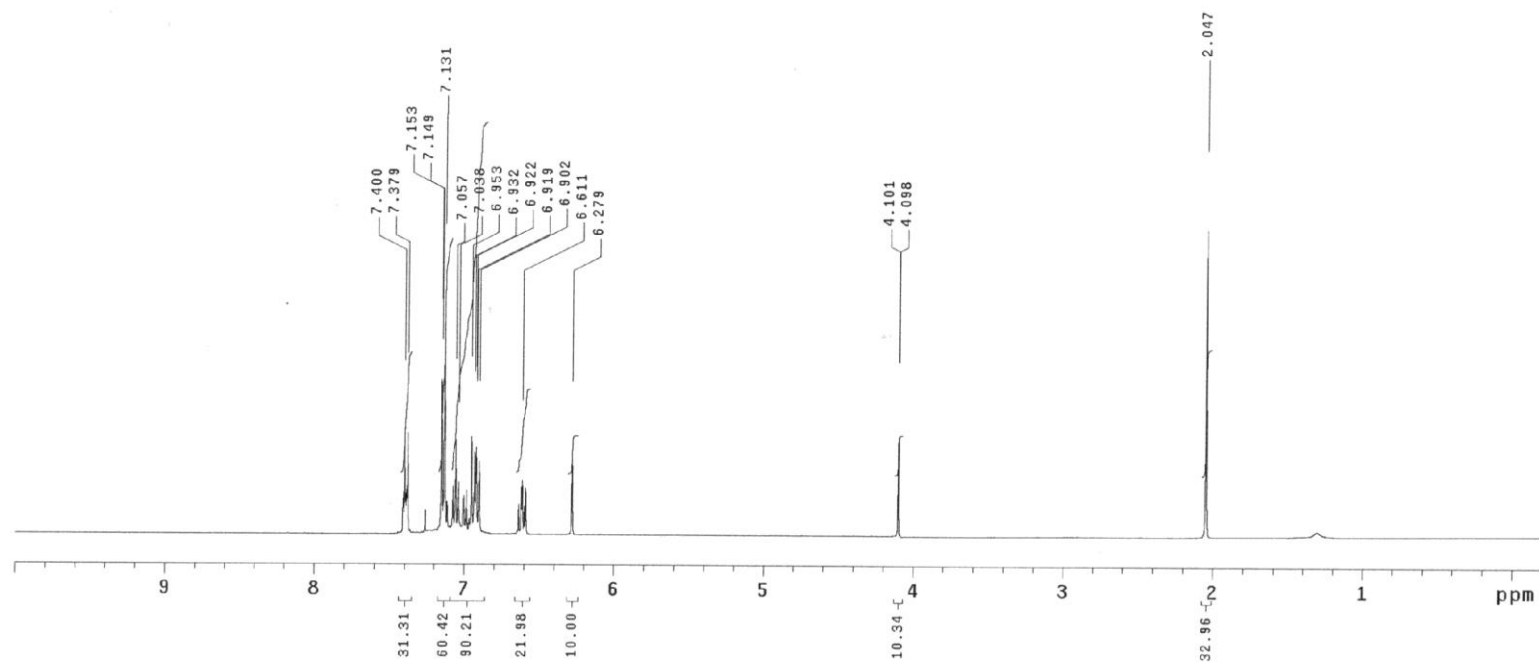
HAK1A7

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Dec 8 2017
Solvent: CDCl₃
Ambient temperature
Total 32 repetitions



Compound 4t

¹H NMR (400 MHz, CDCl₃) spectra



Compound 4t (¹³C-NMR spectral data)

HAK1A7

Pulse Sequence: s2pu1

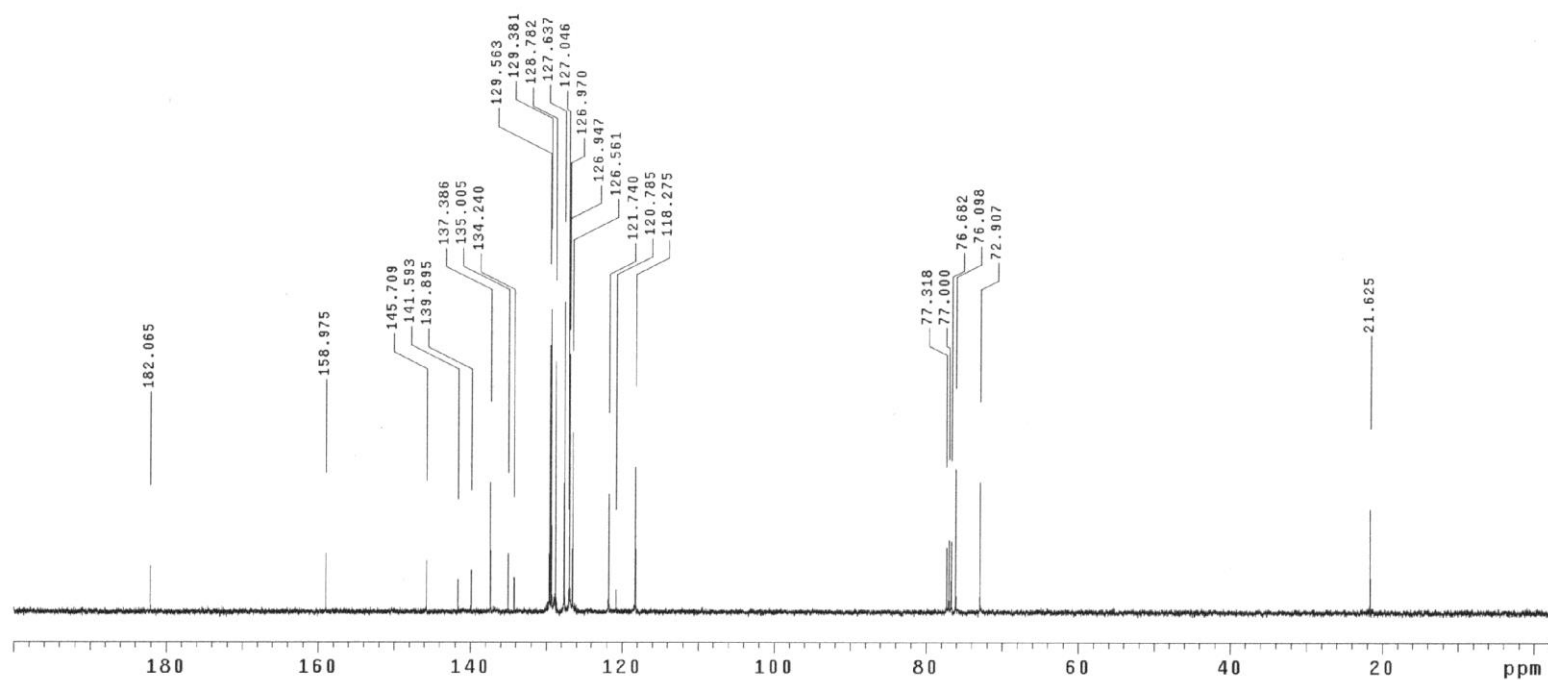
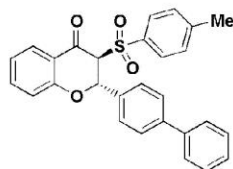
UNITYplus-400 "unity400"

Date: Dec 8 2017

Solvent: CDCl₃

Ambient temperature

Total 1408 repetitions



Compound 4u (¹H-NMR spectral data)

HAK1A8

Pulse Sequence: s2pu1

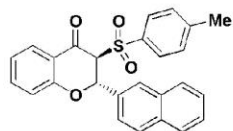
UNITYplus-400 "unity400"

Date: Dec 14 2017

Solvent: CDCl₃

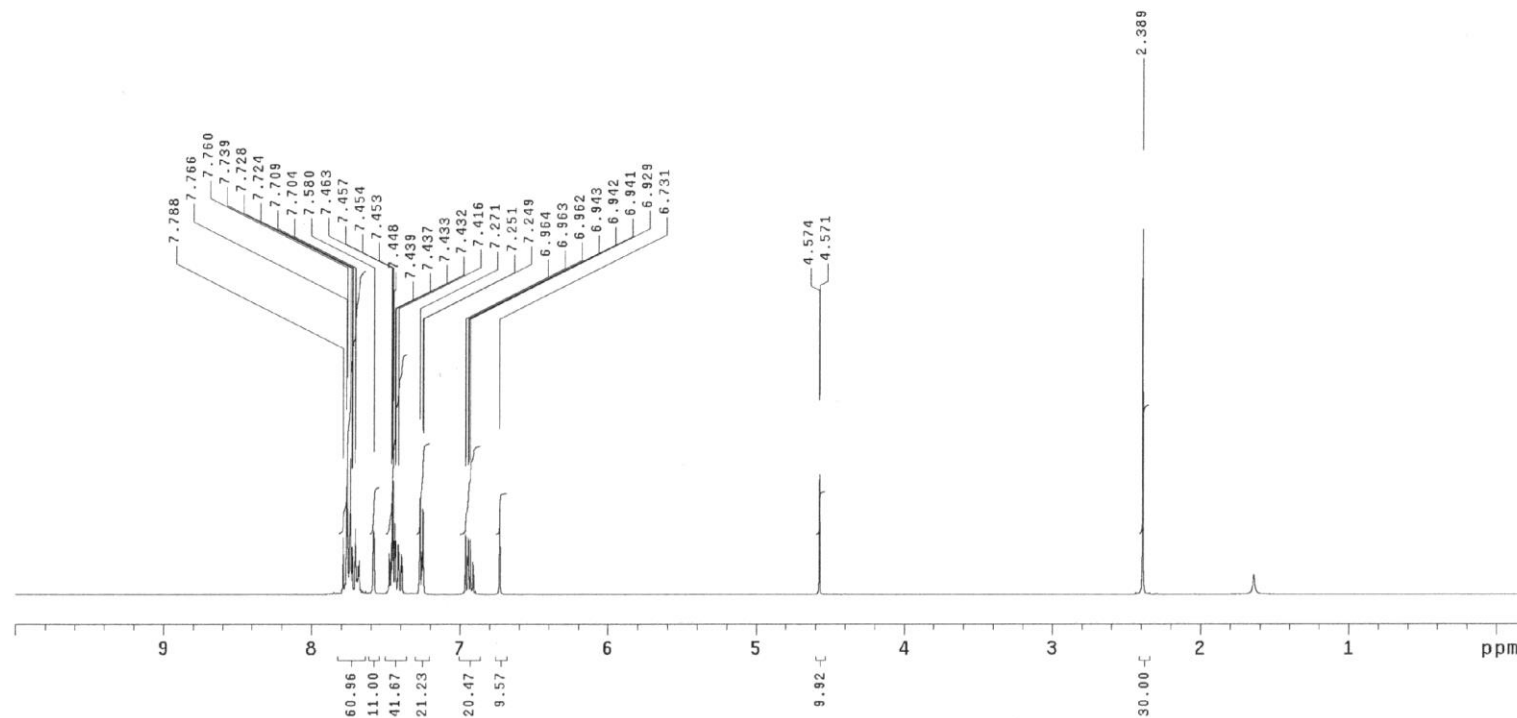
Ambient temperature

Total 32 repetitions



Compound 4u

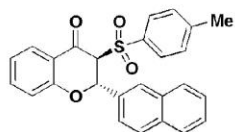
¹H NMR (400 MHz, CDCl₃) spectra



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

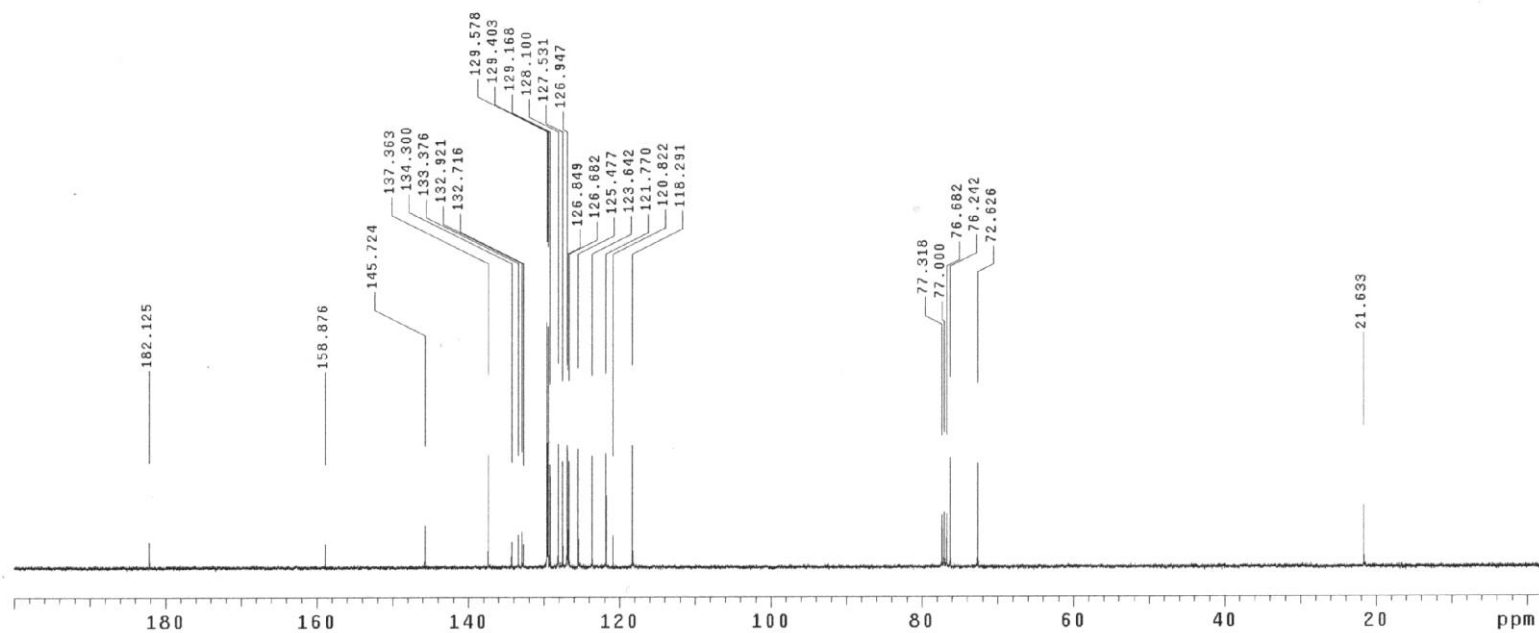
HAK1A8

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Dec 14 2017
Solvent: CDCl₃
Ambient temperature
Total 1056 repetitions



Compound 4u

^{13}C NMR (100 MHz, CDCl₃) spectra



Compound 4v (¹H-NMR spectral data)

HAK1A9

Pulse Sequence: s2pu1

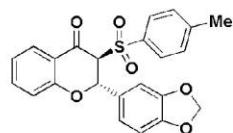
UNITYplus-400 "unity400"

Date: Dec 21 2017

Solvent: CDCl₃

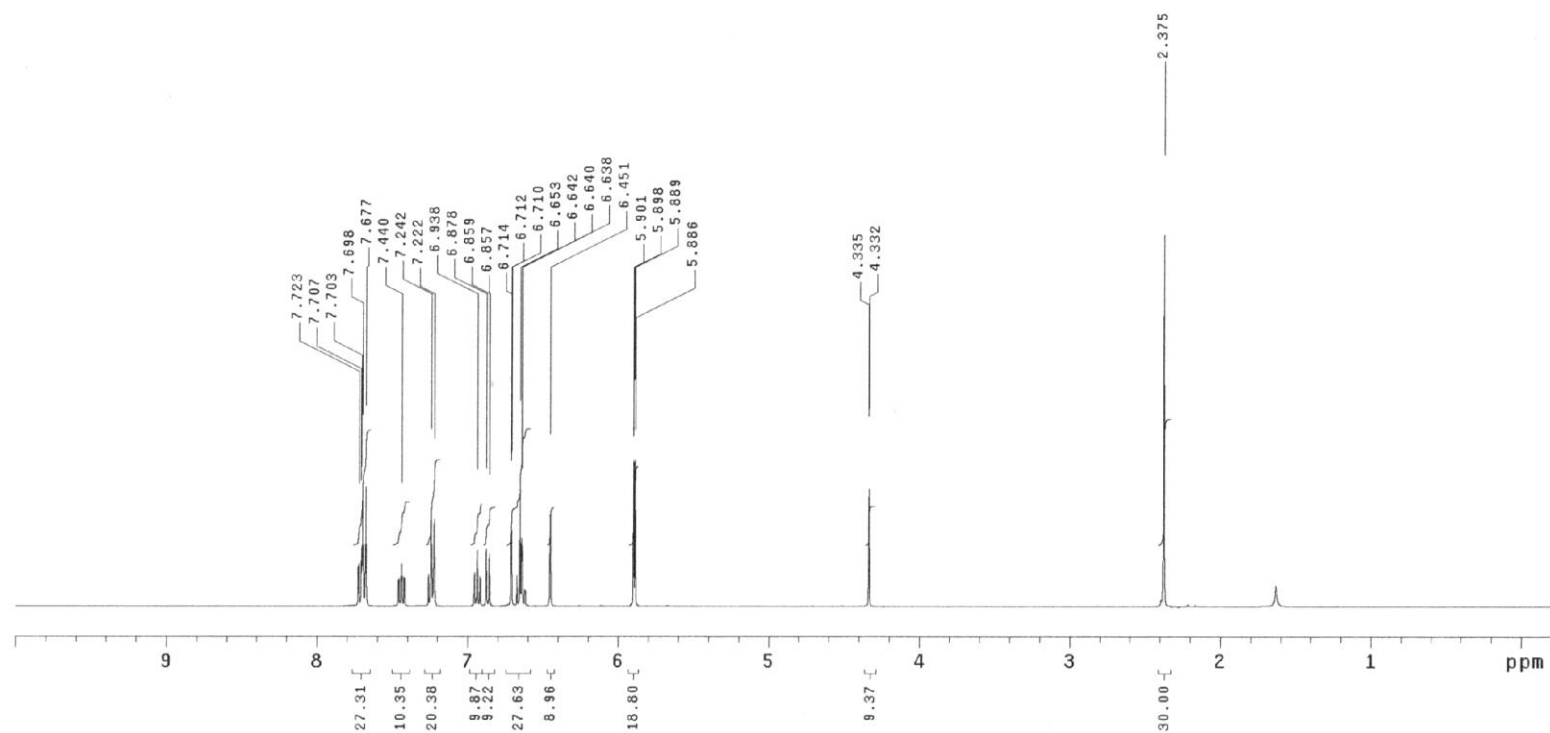
Ambient temperature

Total 32 repetitions



Compound 4v

¹H NMR (400 MHz, CDCl₃) spectra



Compound 4v (¹³C-NMR spectral data)

HAK1A9

Pulse Sequence: s2pu1

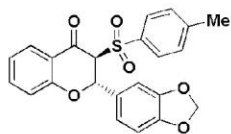
UNITYplus-400 "unity400"

Date: Dec 21 2017

Solvent: CDCl₃

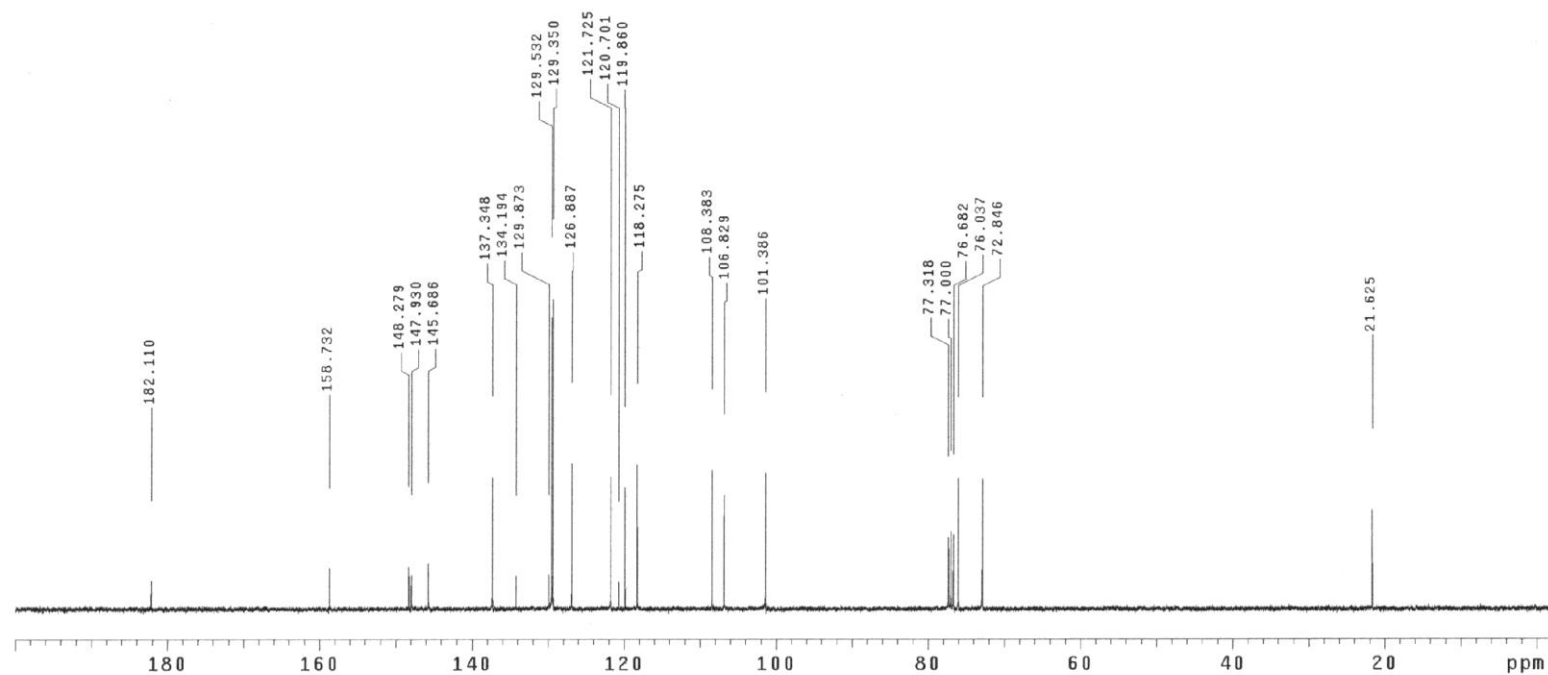
Ambient temperature

Total 1216 repetitions



Compound 4v

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4w (¹H-NMR spectral data)

HAK1A10

Pulse Sequence: s2pu1

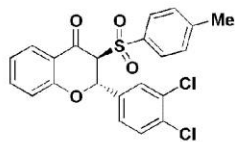
UNITYplus-400 "unity400"

Date: Dec 21 2017

Solvent: CDCl₃

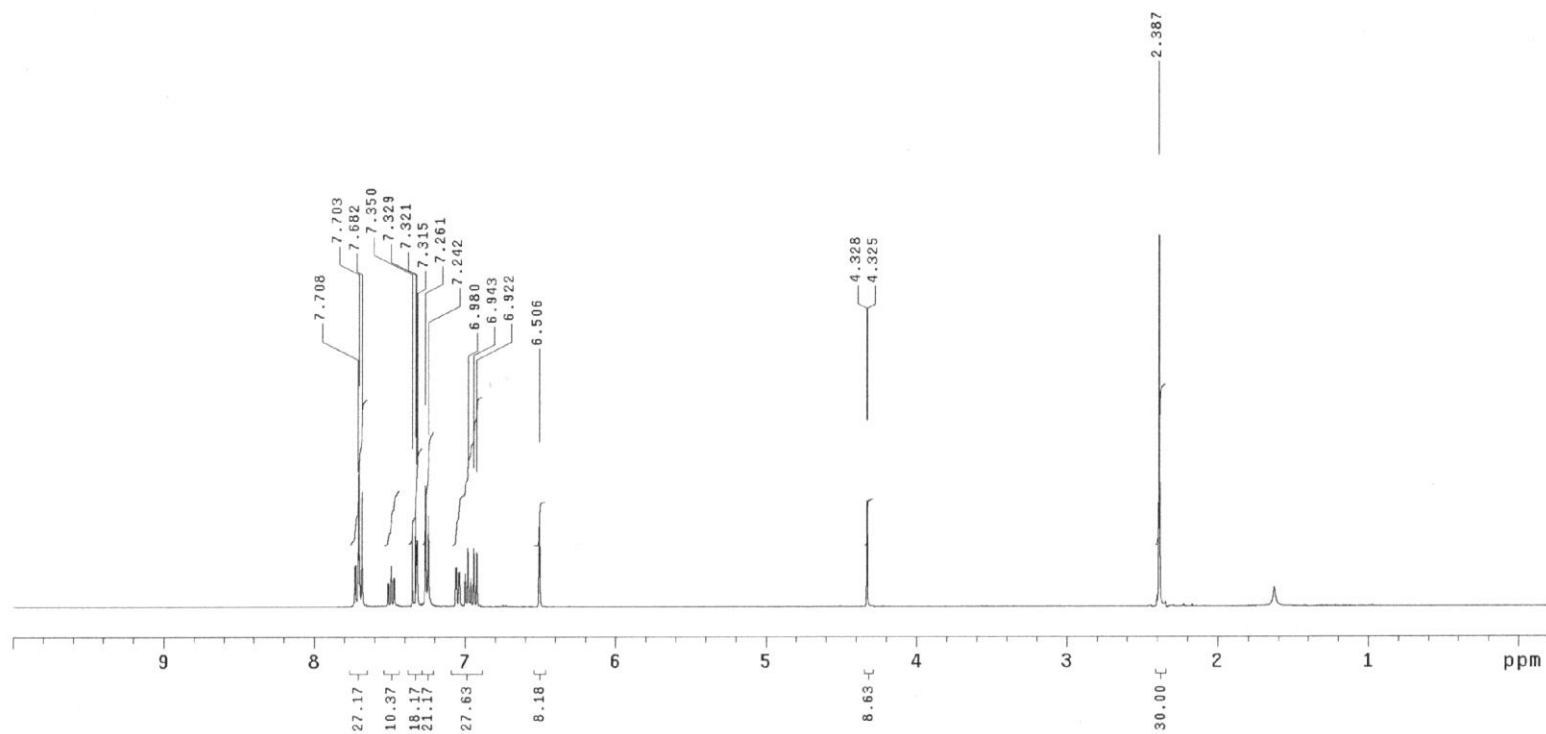
Ambient temperature

Total 32 repetitions



Compound 4w

¹H NMR (400 MHz, CDCl₃) spectra



Compound 4w (¹³C-NMR spectral data)

HAK1A10

Pulse Sequence: s2pu1

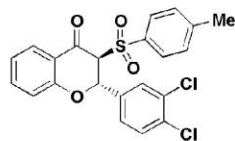
UNITYplus-400 "unity400"

Date: Dec 21 2017

Solvent: CDCl₃

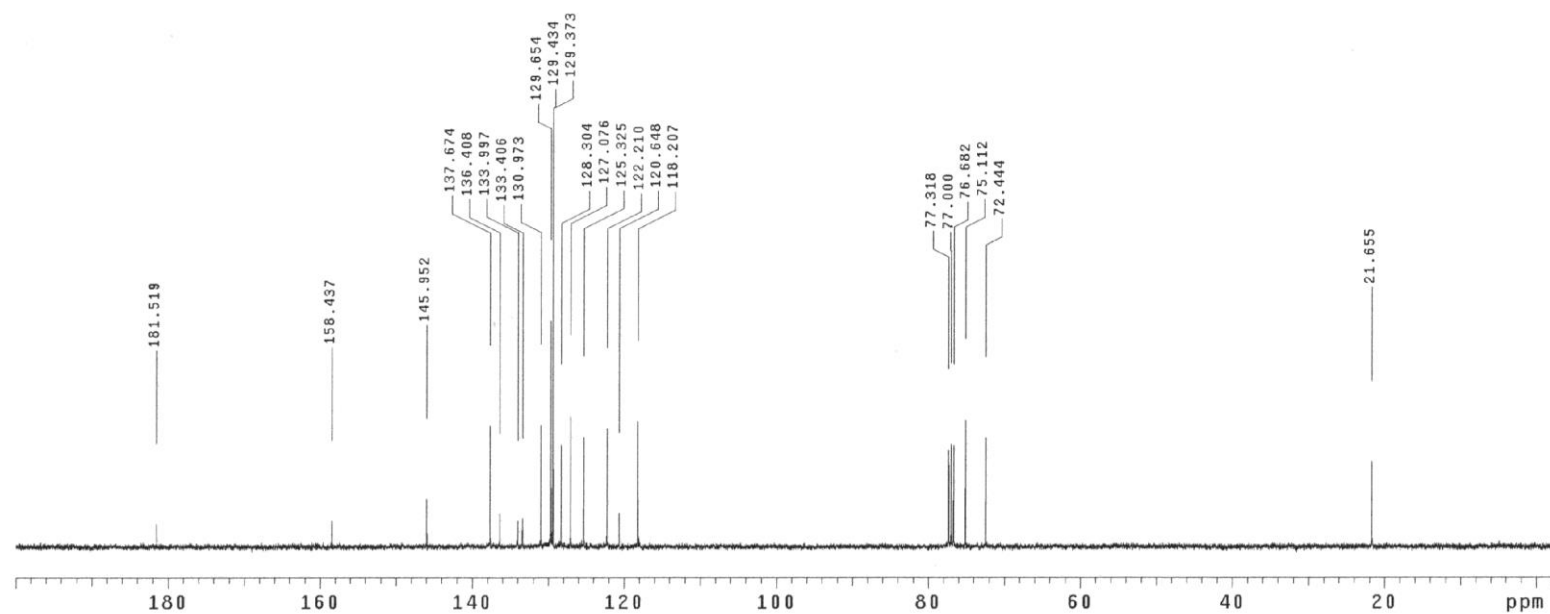
Ambient temperature

Total 1072 repetitions



Compound 4w

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4x (¹H-NMR spectral data)

HAK1A11

Pulse Sequence: s2pu1

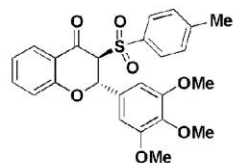
UNITYplus-400 "unity400"

Date: Dec 29 2017

Solvent: CDCl₃

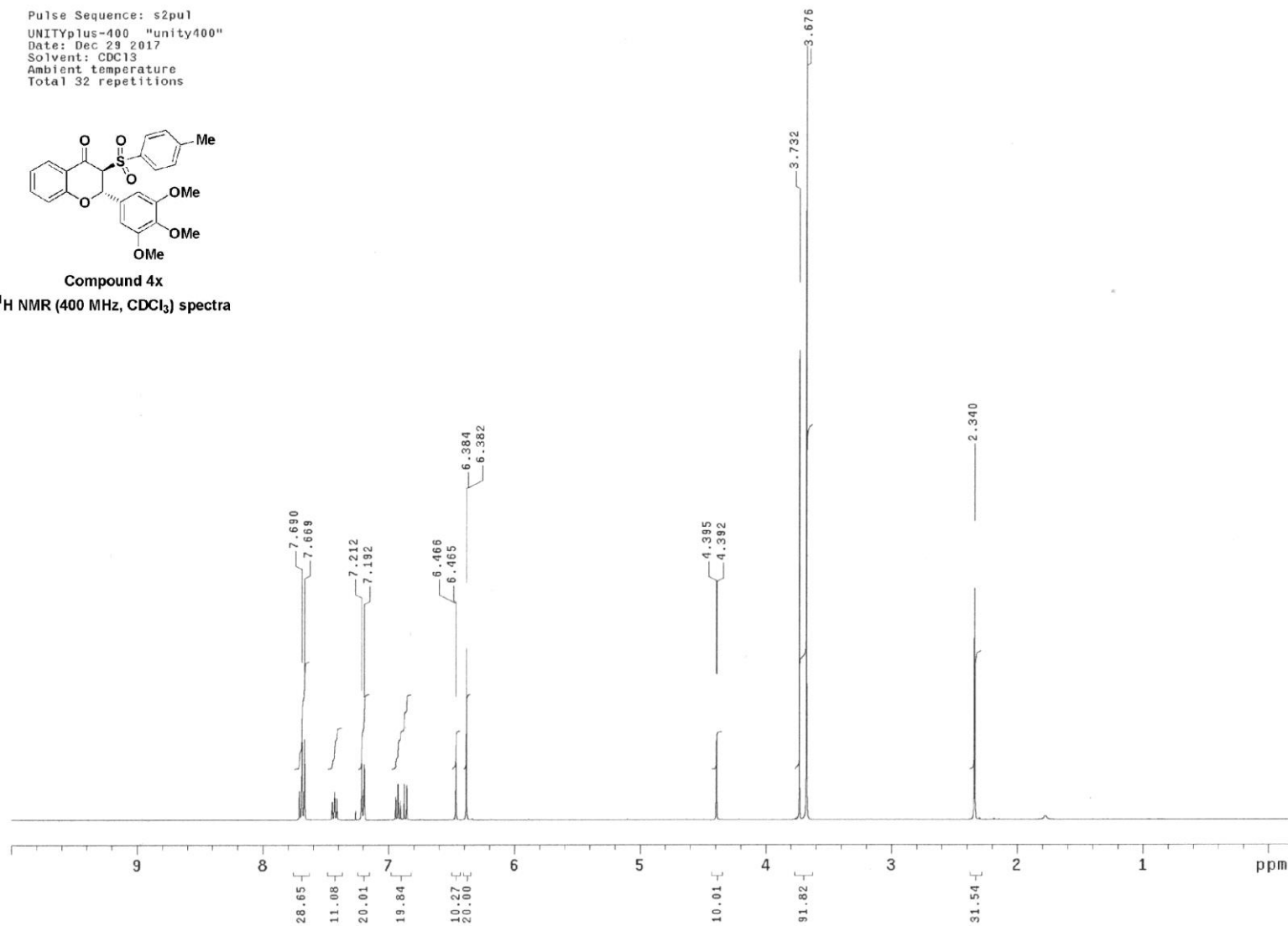
Ambient temperature

Total 32 repetitions



Compound 4x

¹H NMR (400 MHz, CDCl₃) spectra



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

HAK1A11

Pulse Sequence: s2pu1

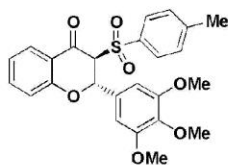
UNITYplus-400 "unity400"

Date: Dec 29 2017

Solvent: CDCl_3

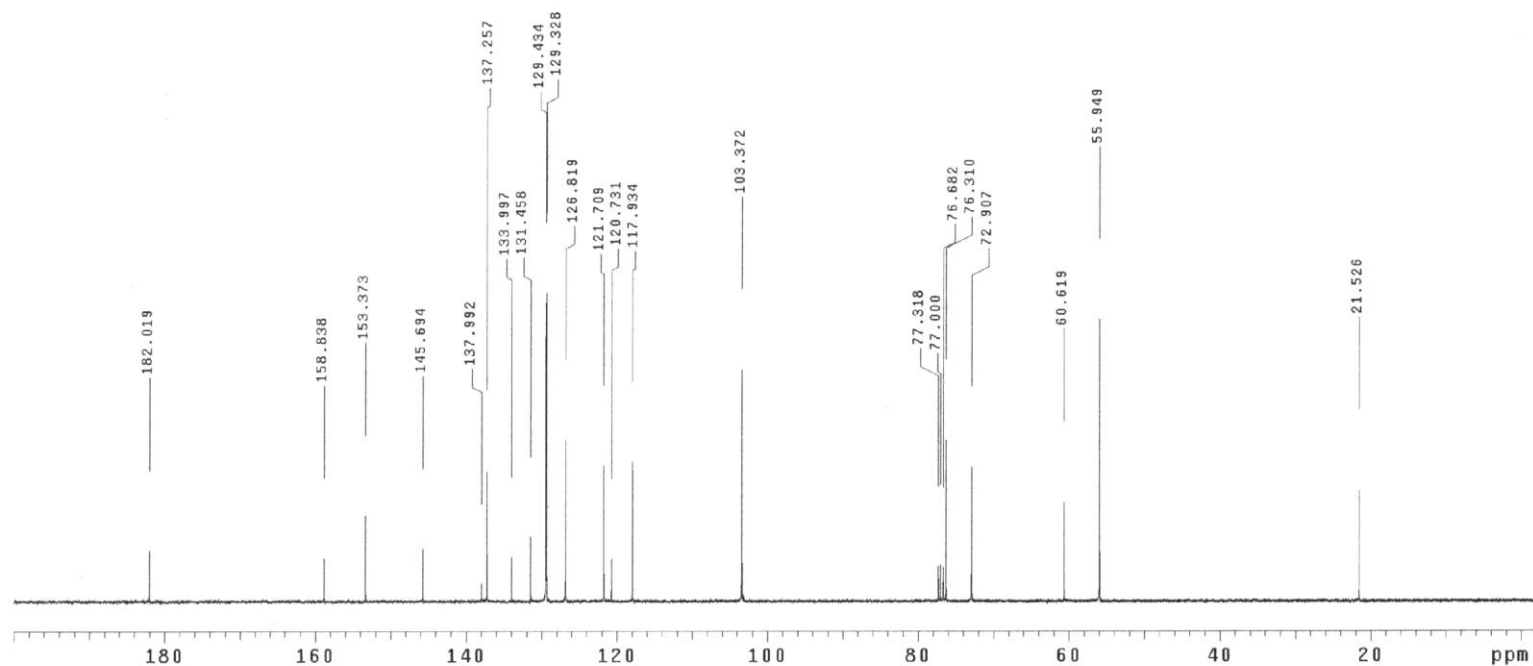
Ambient temperature

Total 576 repetitions



Compound 4x

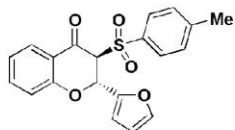
^{13}C NMR (100 MHz, CDCl_3) spectra



Compound 4y (¹H-NMR spectral data)

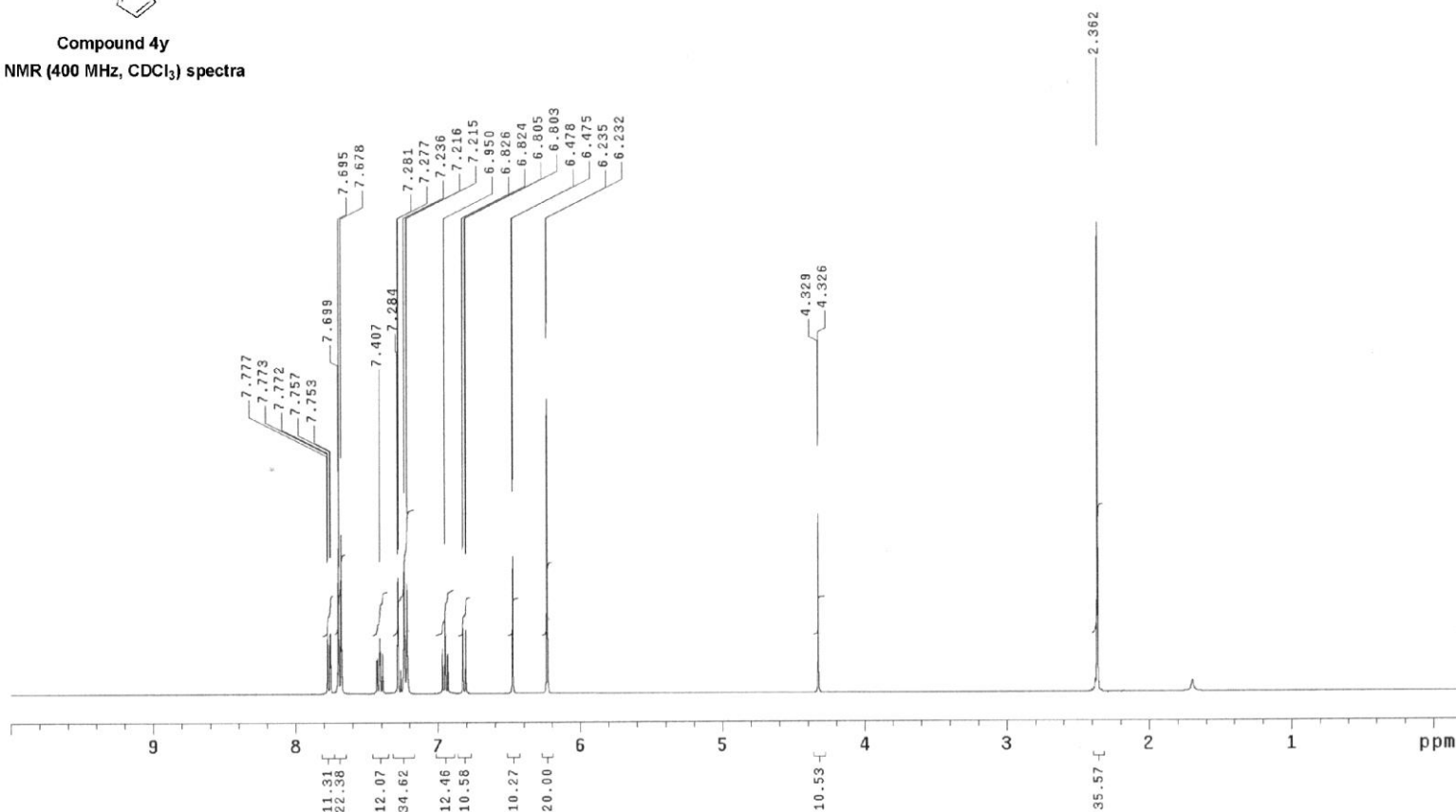
HAK1A12

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Jan 8 2018
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetitions



Compound 4y

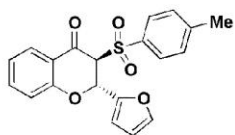
¹H NMR (400 MHz, CDCl₃) spectra



Compound 4y (¹³C-NMR spectral data)

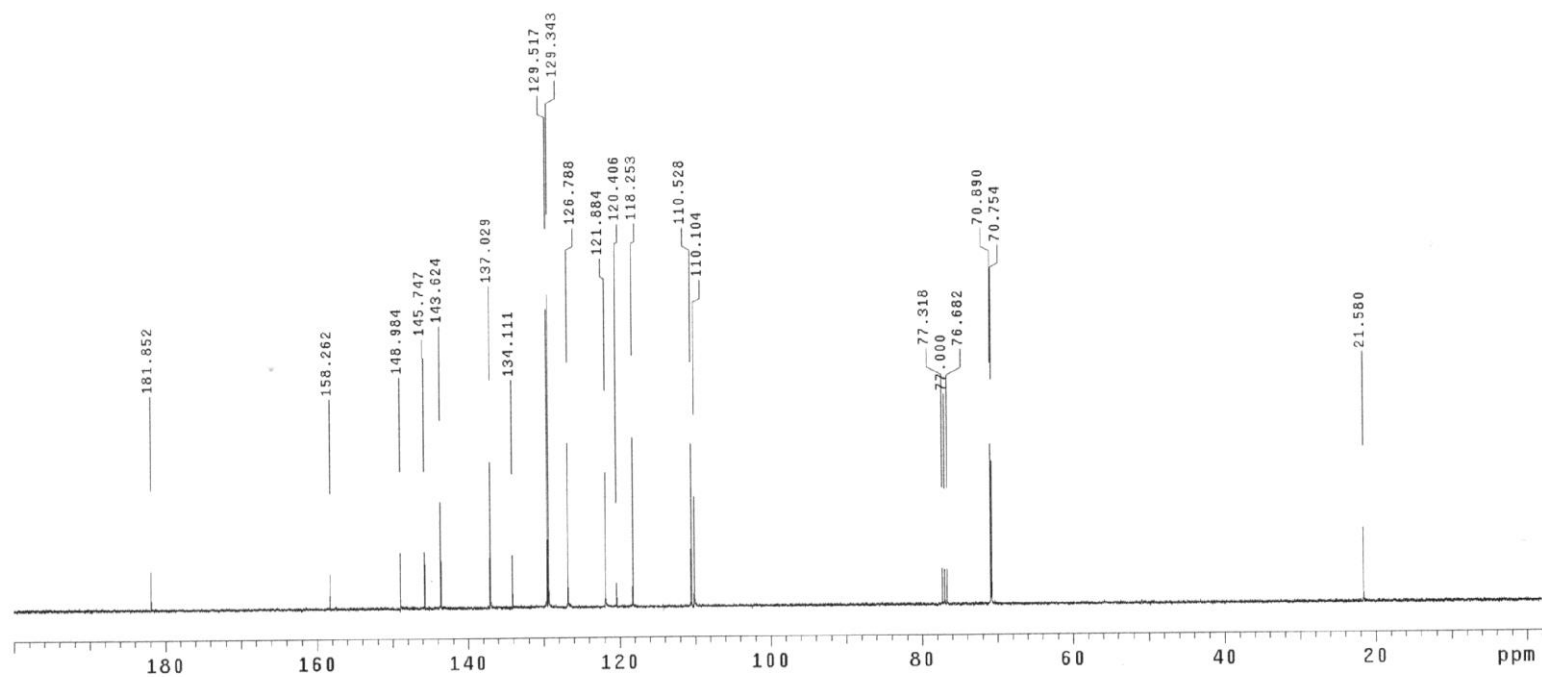
HAK1A12

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Jan 8 2018
 Solvent: CDCl₃
 Ambient temperature
 Total 928 repetitions



Compound 4y

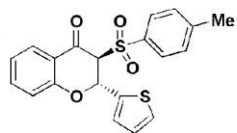
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4z (¹H-NMR spectral data)

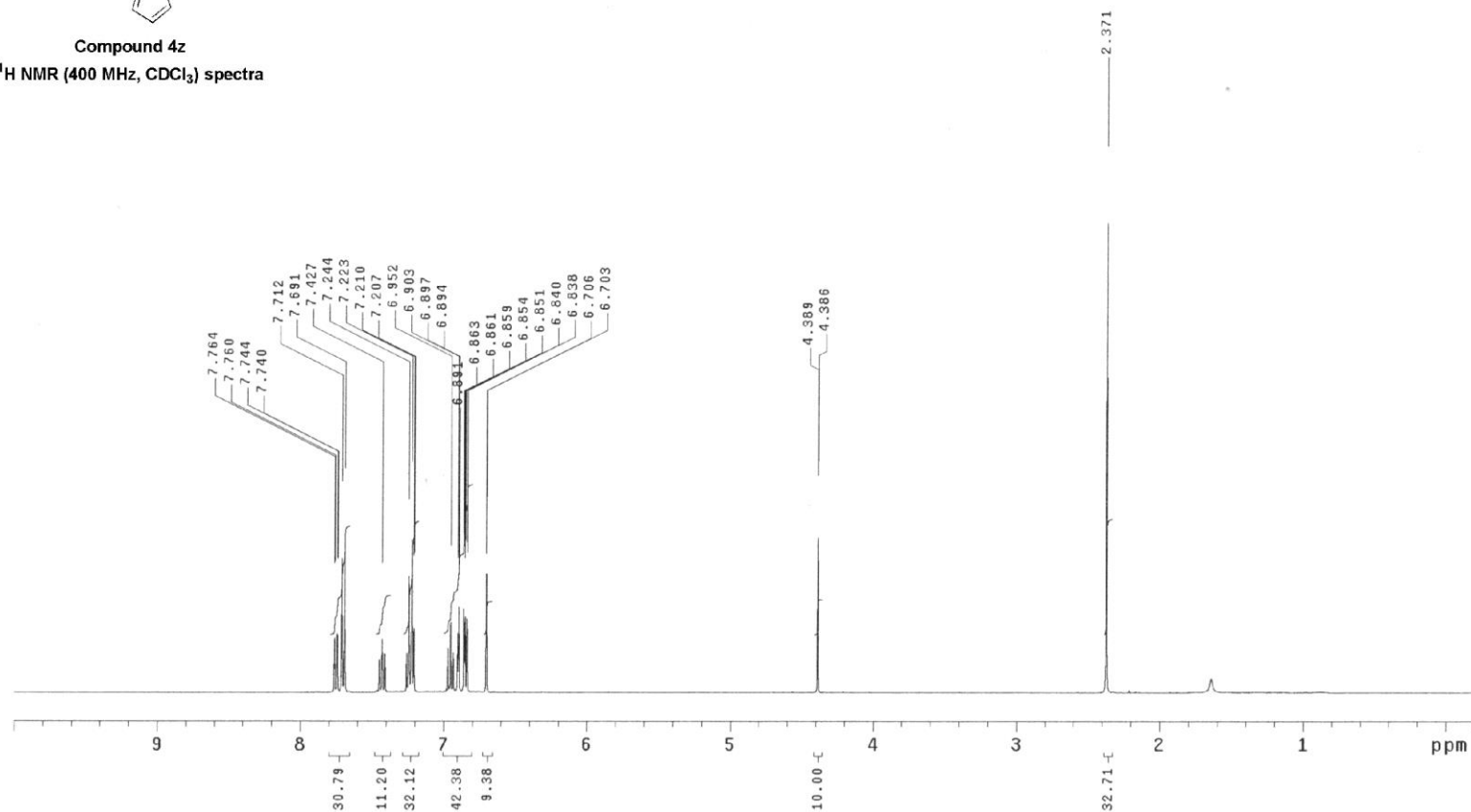
HAK1A13

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Jan 9 2018
 Solvent: CDCl₃
 Ambient temperature
 Total 32 repetitions



Compound 4z

¹H NMR (400 MHz, CDCl₃) spectra



Compound 4z (¹³C-NMR spectral data)

HAK1A13

Pulse Sequence: s2pu1

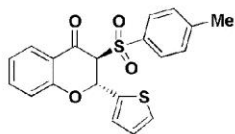
UNITYplus-400, "unity400"

Date: Jan 9 2018

Solvent: CDCl₃

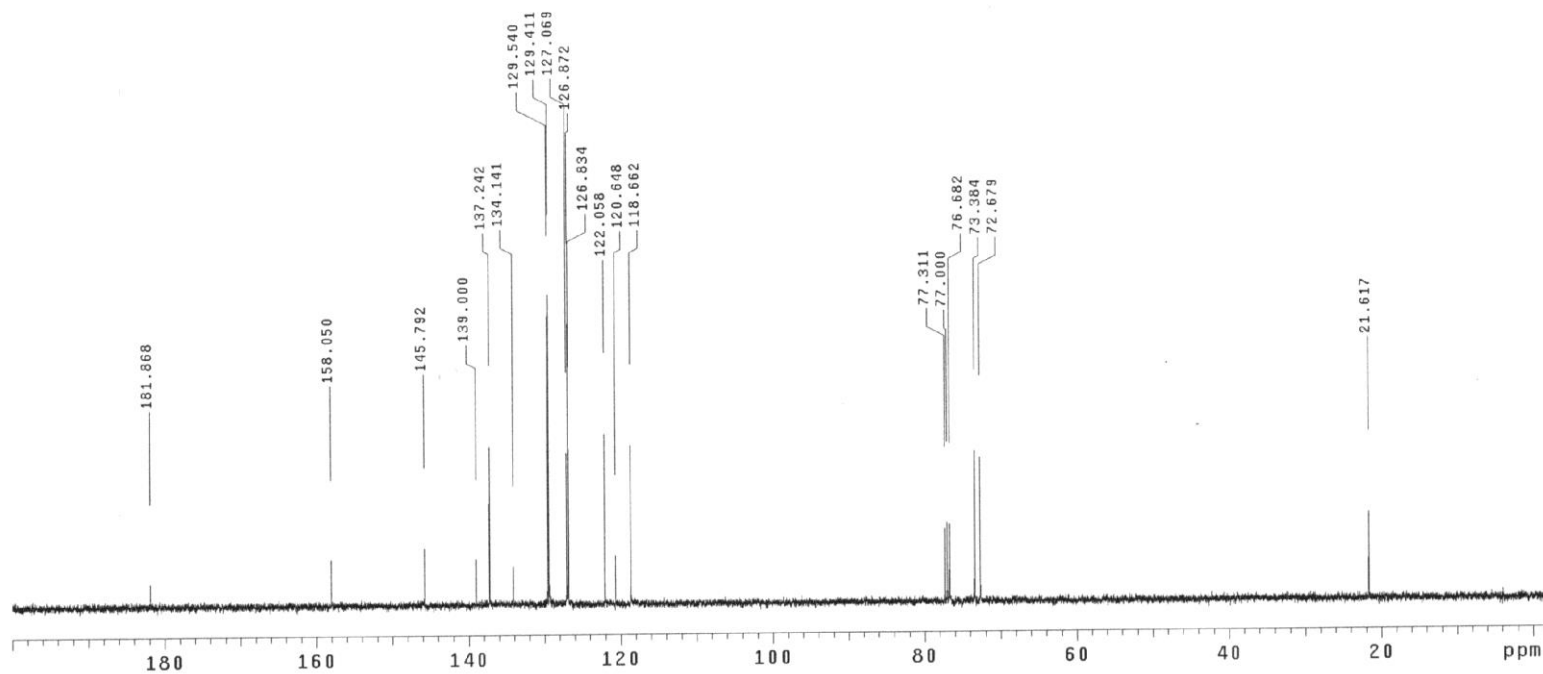
Ambient temperature

Total 576 repetitions



Compound 4z

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4aa (¹H-NMR spectral data)

HAK1A14

Pulse Sequence: s2pu1

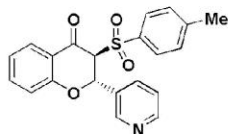
UNITYplus-400 "unity400"

Date: Jan 18 2018

Solvent: CDCl₃

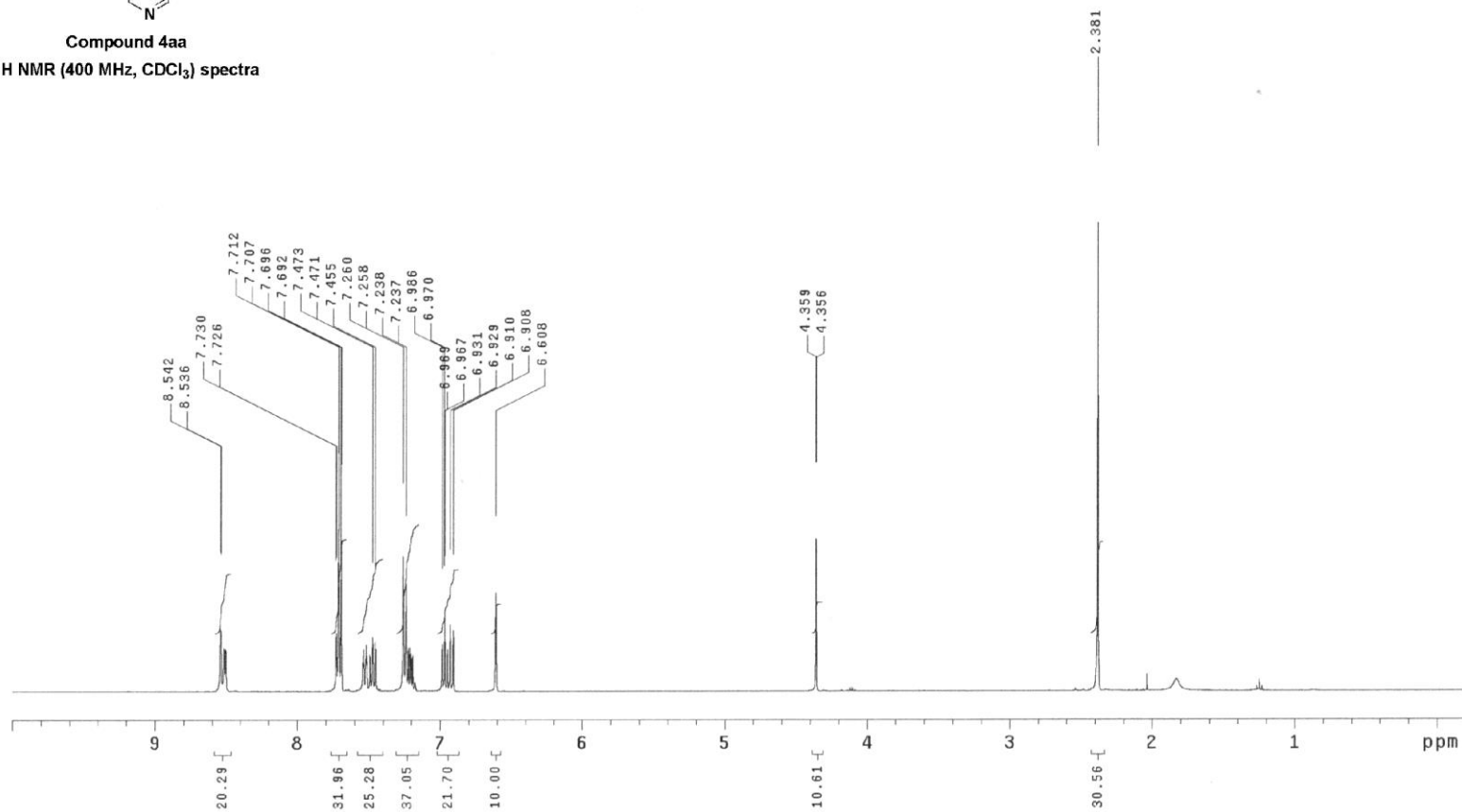
Ambient temperature

Total 32 repetitions



Compound 4aa

¹H NMR (400 MHz, CDCl₃) spectra



Compound 4aa (¹³C-NMR spectral data)

HAK1A14

Pulse Sequence: s2pu1

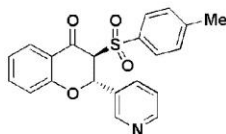
UNITYplus-400 "unity400"

Date: Jan 18 2018

Solvent: CDCl₃

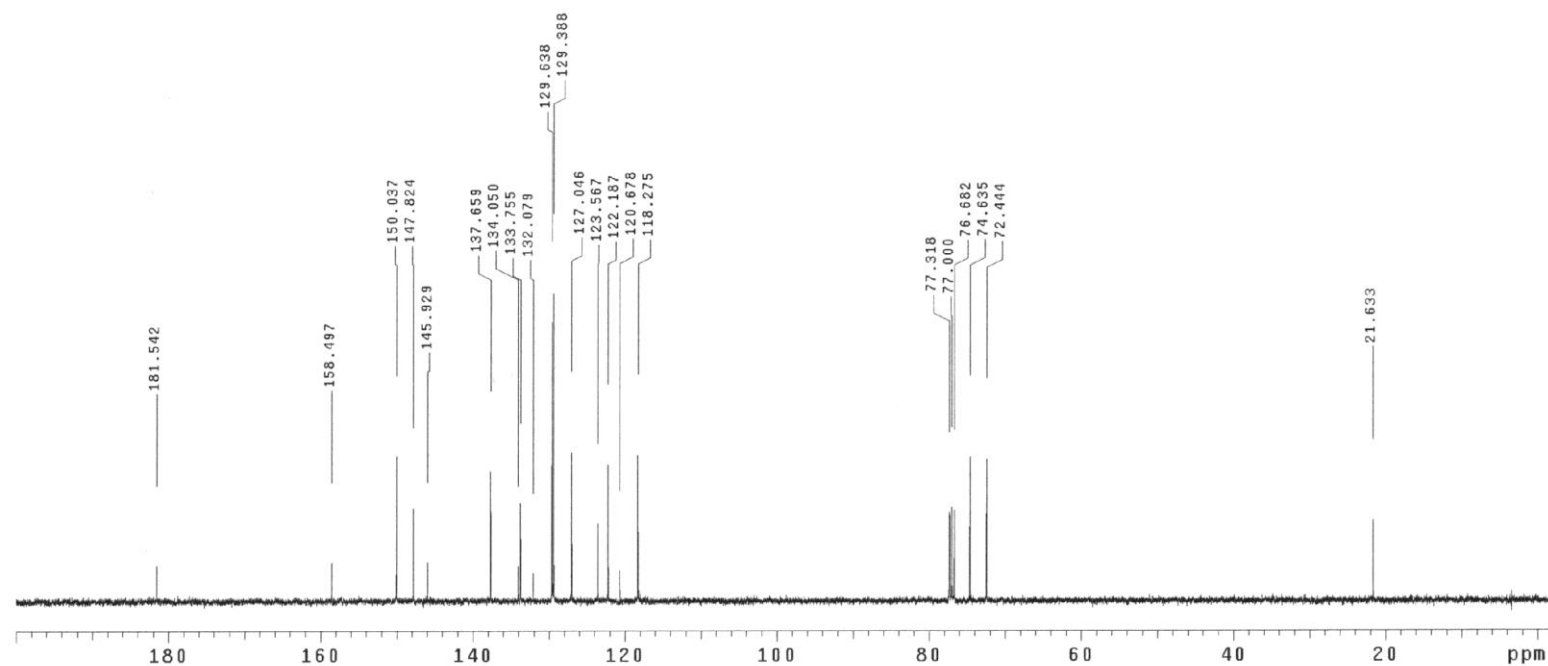
Ambient temperature

Total 880 repetitions



Compound 4aa

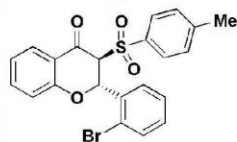
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4ab (¹H-NMR spectral data)

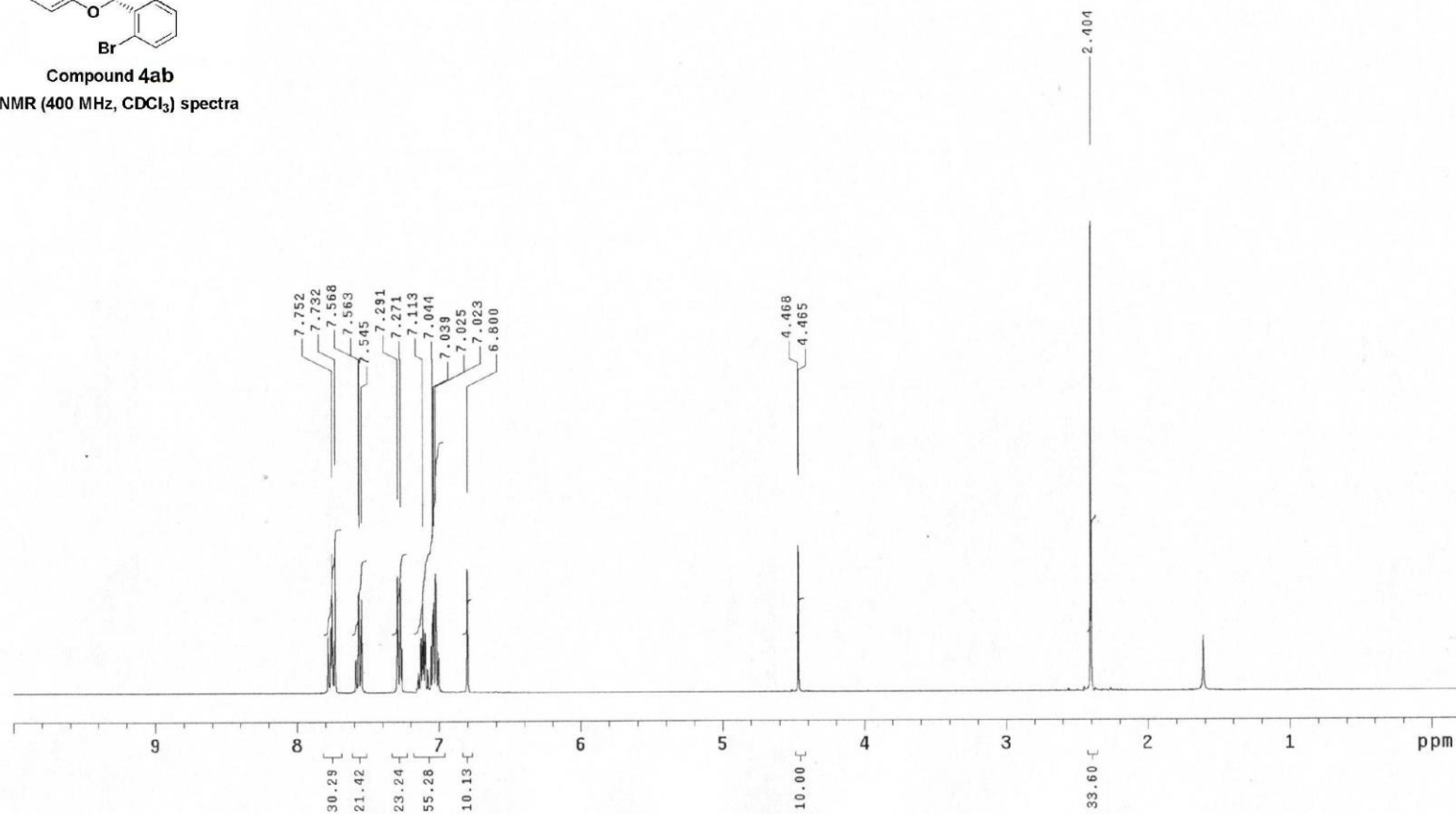
YTDS1

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



Compound 4ab

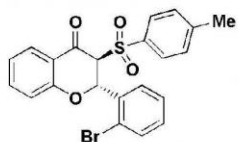
¹H NMR (400 MHz, CDCl₃) spectra



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

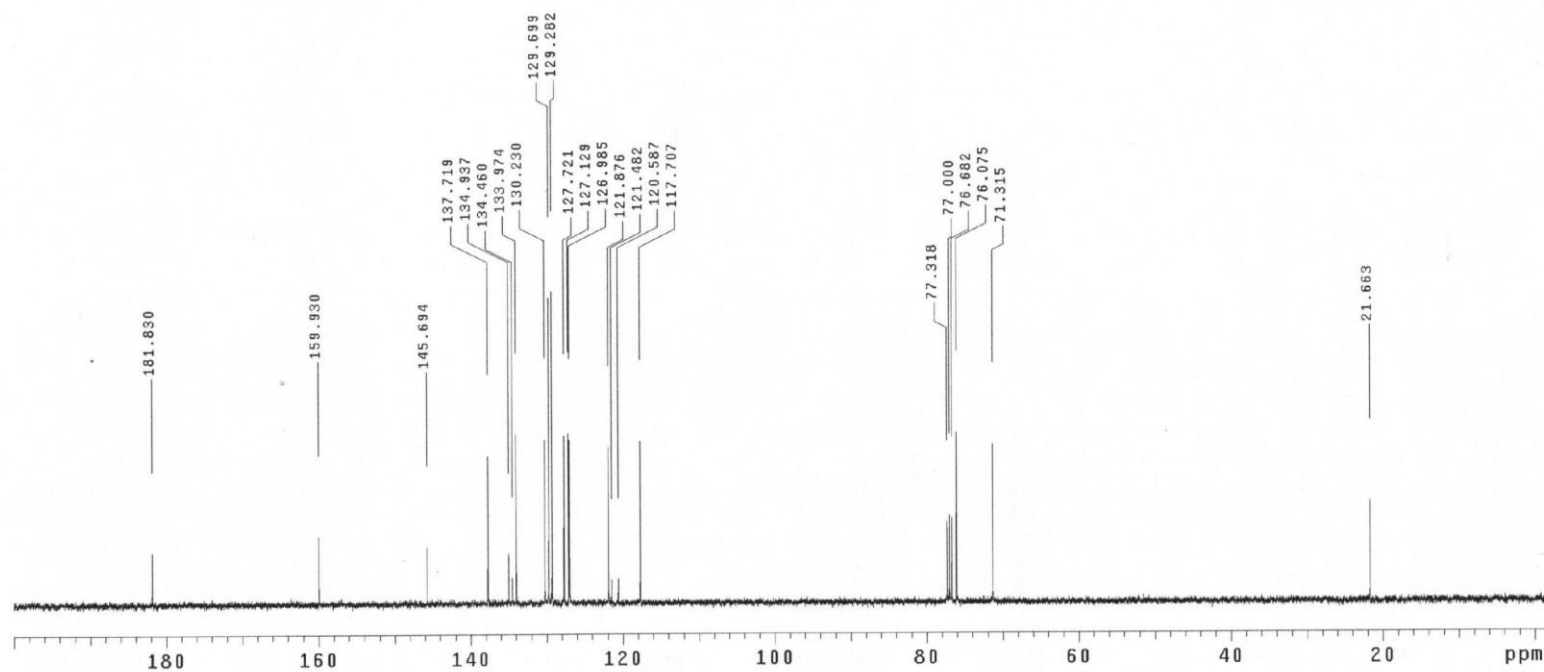
YTDS1

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Dec 4 2017
Solvent: CDCl₃
Ambient temperature
Total 880 repetitions



Compound 4ab

^{13}C NMR (100 MHz, CDCl₃) spectra



Compound 4ac (¹H-NMR spectral data)

HAK21A12

Pulse Sequence: s2pu1

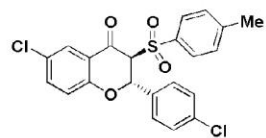
UNITYplus-400 "unity400"

Date: Jan 11 2018

Solvent: CDCl₃

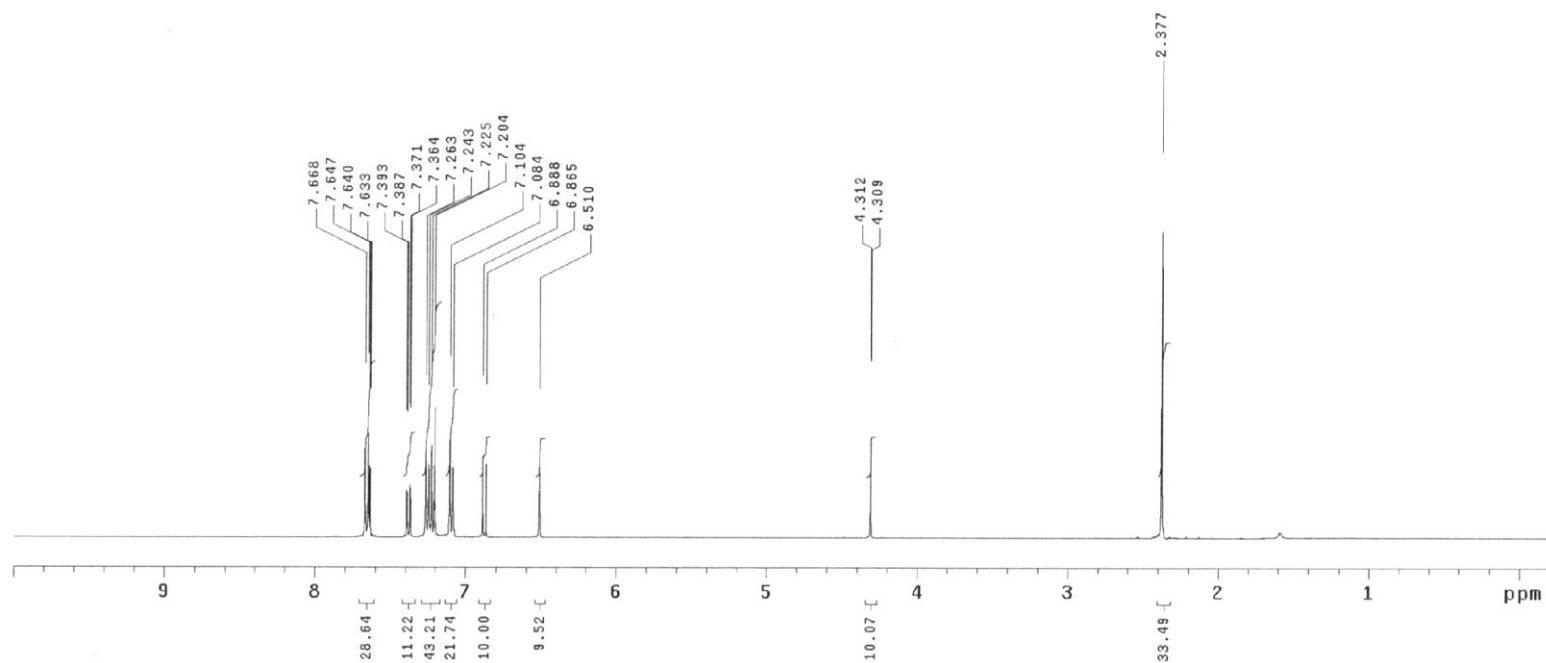
Ambient temperature

Total 32 repetitions



Compound 4ac

¹H NMR (400 MHz, CDCl₃) spectra



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

HAK21A12

Pulse Sequence: s2pu1

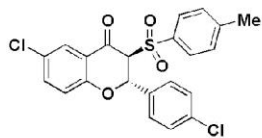
UNITYplus-400 "unity400"

Date: Jan 11 2018

Solvent: CDCl_3

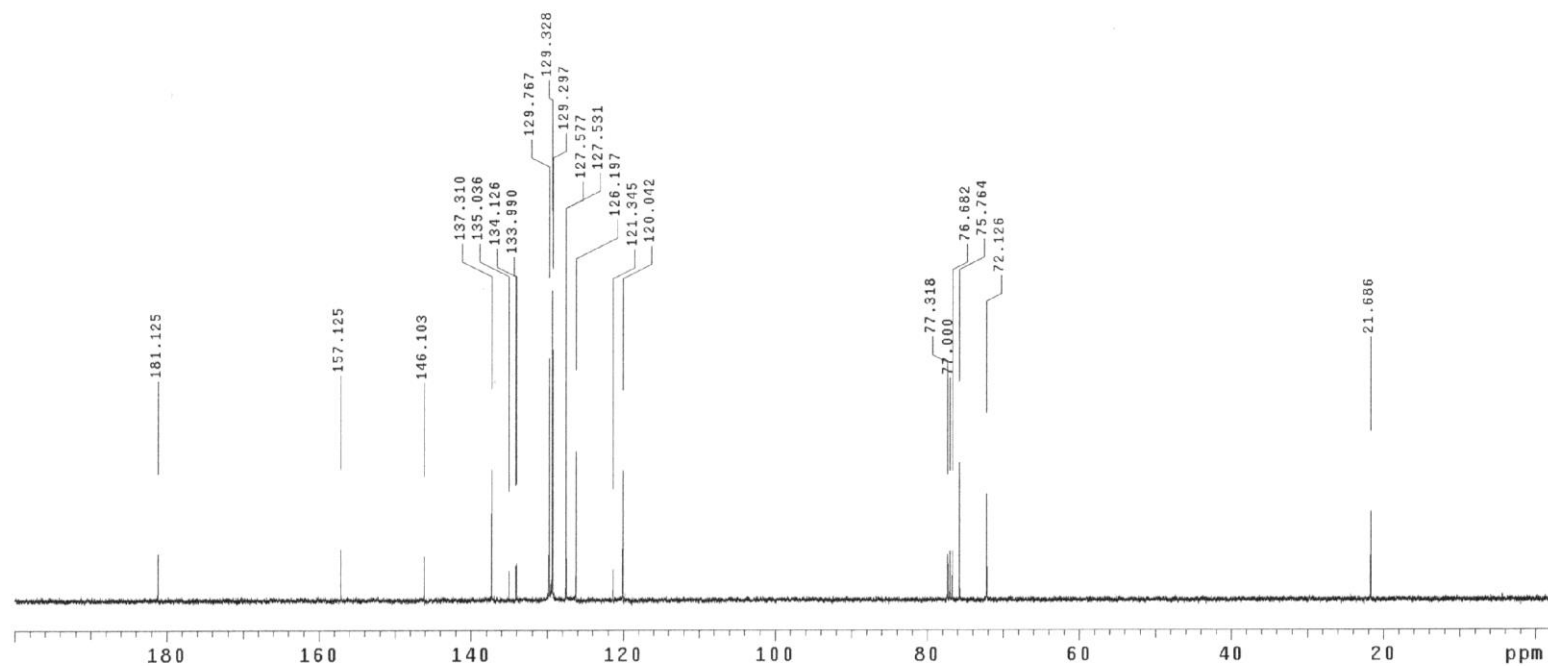
Ambient temperature

Total 752 repetitions



Compound 4ac

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



Compound 4ad (¹H-NMR spectral data)

HAK7A11

Pulse Sequence: s2pu1

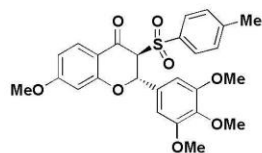
UNITYplus-400 "unity400"

Date: Feb 5 2018

Solvent: CDCl₃

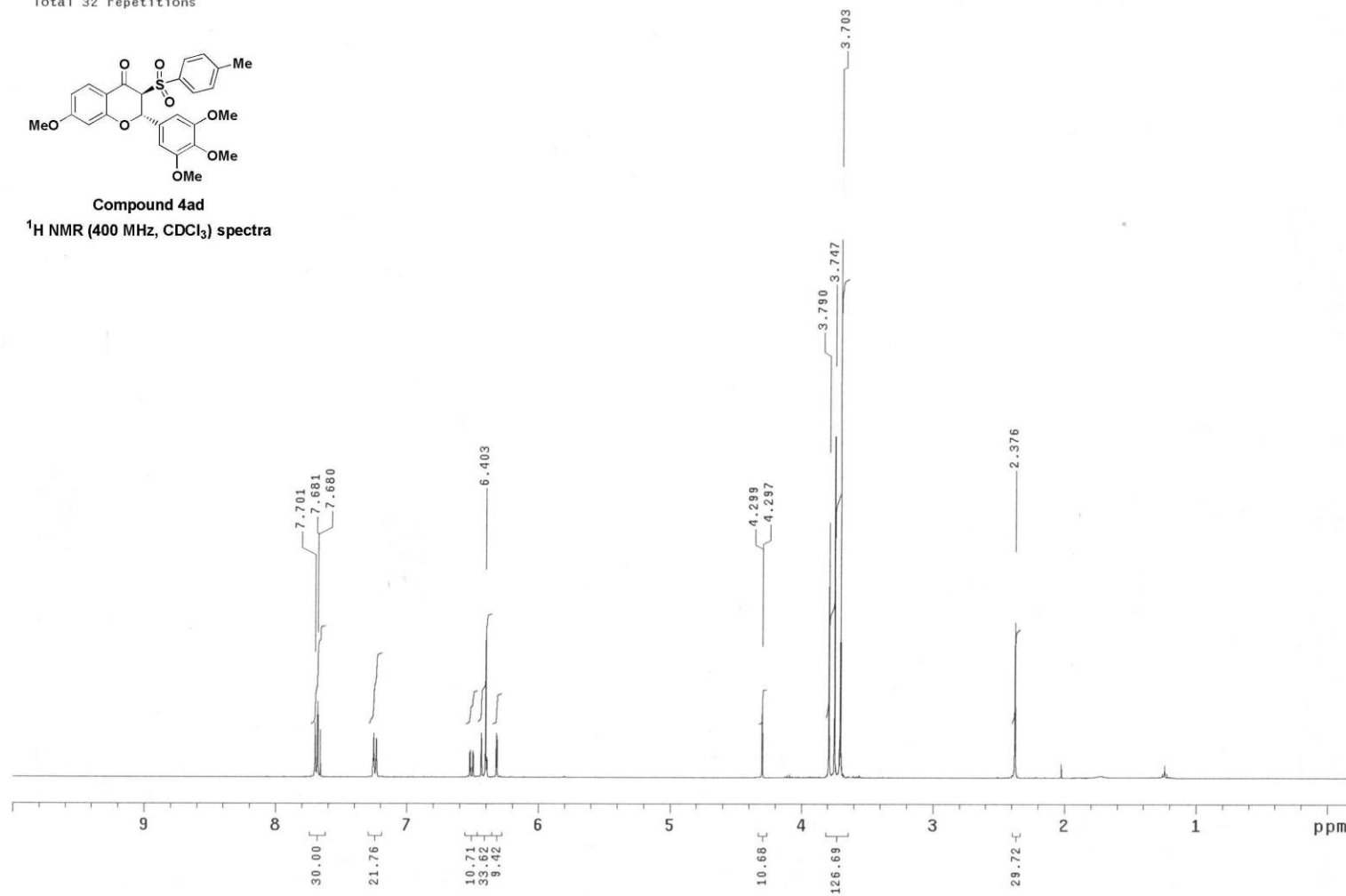
Ambient temperature

Total 32 repetitions



Compound 4ad

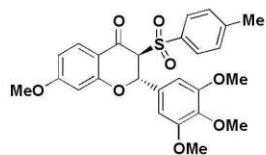
¹H NMR (400 MHz, CDCl₃) spectra



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

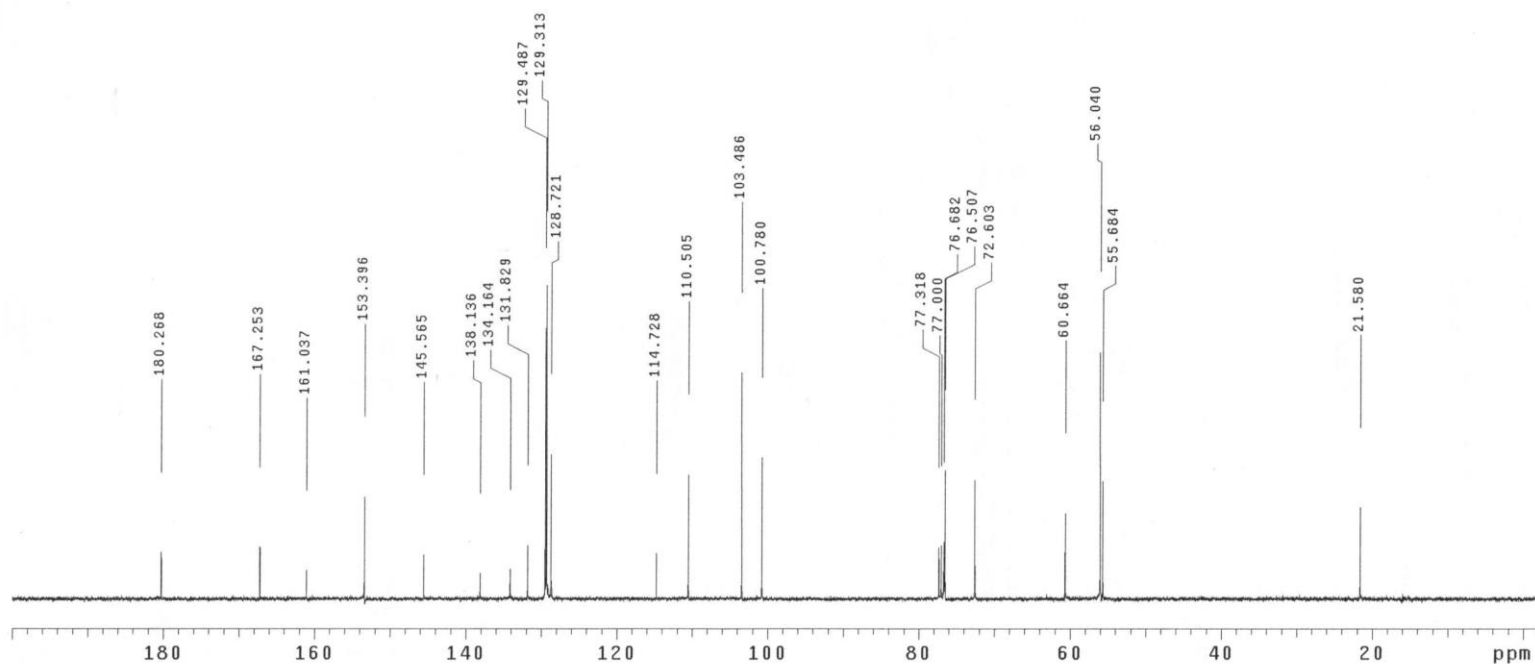
HAK7A11

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Feb 5 2018
Solvent: CDCl_3
Ambient temperature
Total 1136 repetitions



Compound 4ad

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



Compound 4ae (¹H-NMR spectral data)

YLMsCF3

Pulse Sequence: s2pu1

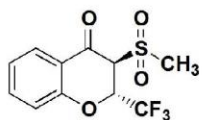
UNITYplus-400 "unity400"

Date: Jun 5 2017

Solvent: CDCl₃

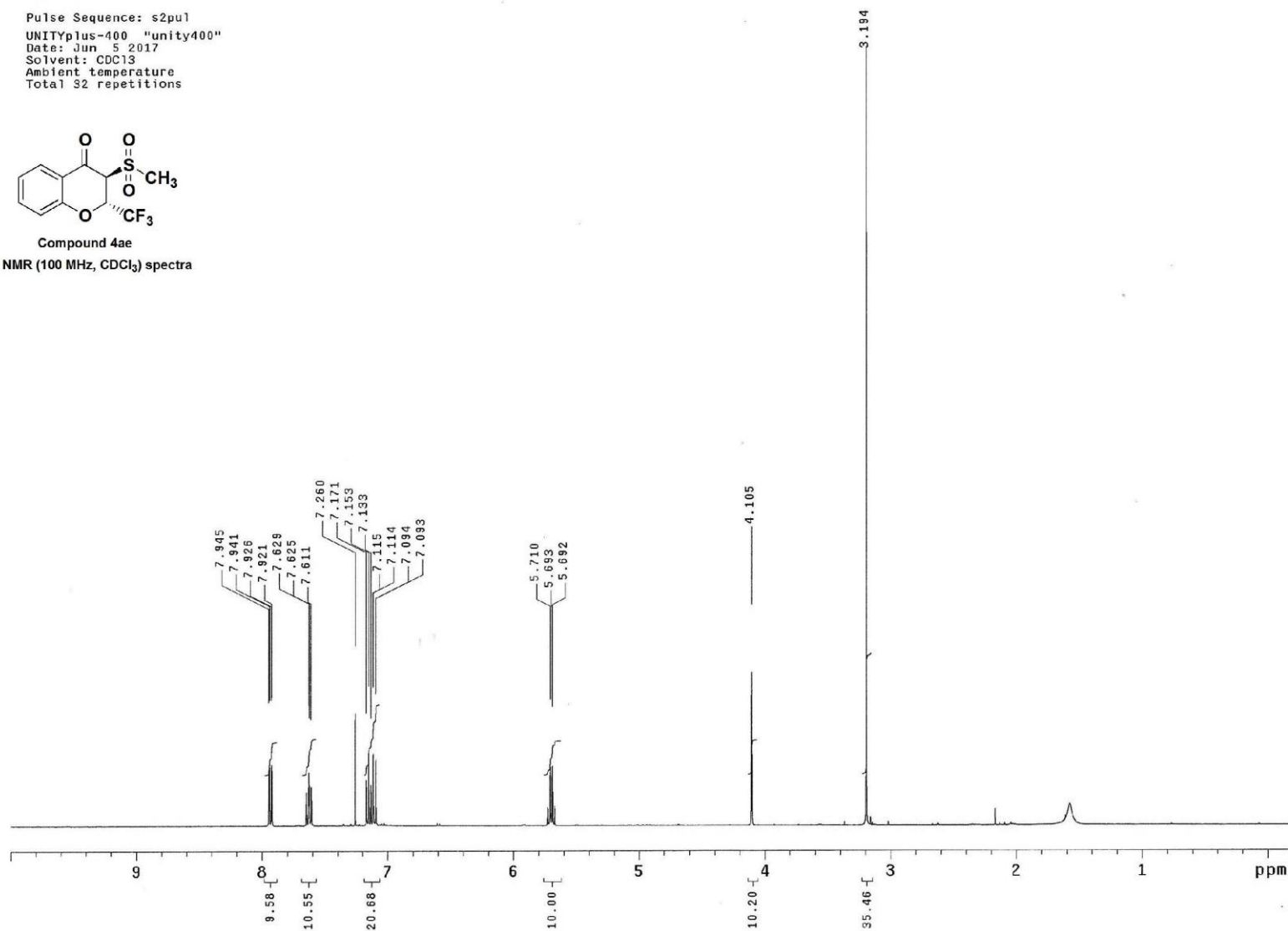
Ambient temperature

Total 32 repetitions



Compound 4ae

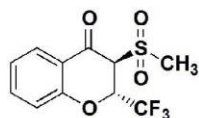
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4ae (¹³C-NMR spectral data)

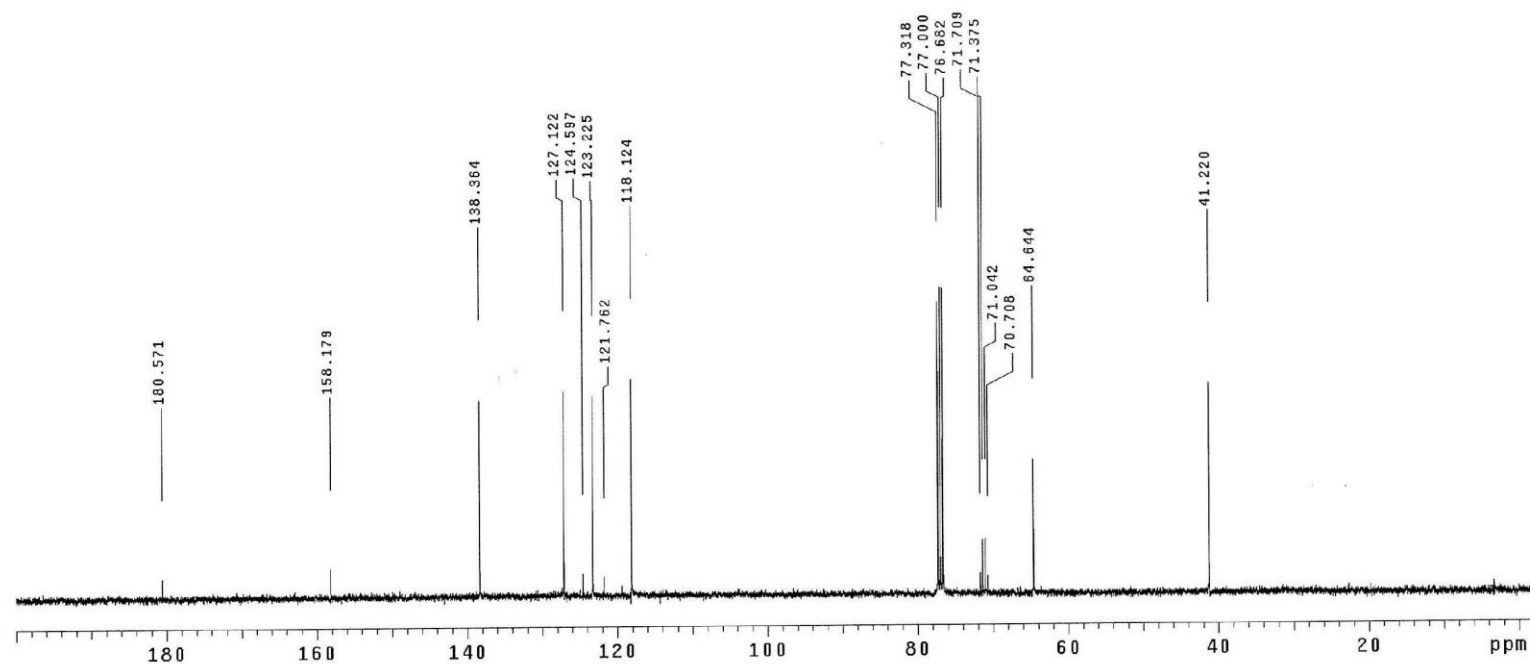
YLMsCF3

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Jun 5 2017
Solvent: CDCl₃
Ambient temperature
Total 17168 repetitions



Compound 4ae

¹H NMR (400 MHz, CDCl₃) spectra



Compound 4af (¹H-NMR spectral data)

YLBSCF3

Pulse Sequence: s2pu1

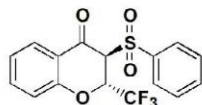
UNITYplus-400 "unity400"

Date: Apr 25 2017

Solvent: CDCl₃

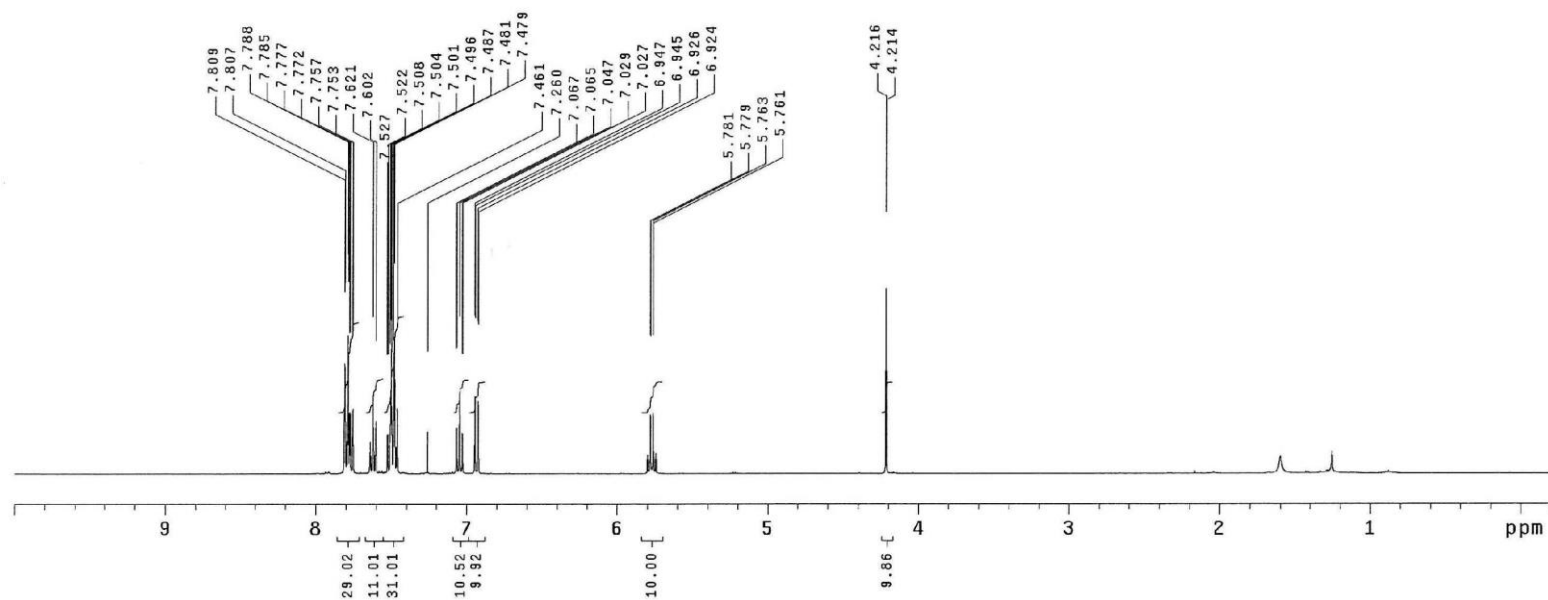
Ambient temperature

Total 32 repetitions



Compound 4af

¹H NMR (400 MHz, CDCl₃) spectra



Compound 4af (¹³C-NMR spectral data)

YLBSCF3

Pulse Sequence: s2pu1

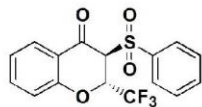
UNITYplus-400 "unity400"

Date: Apr 25 2017

Solvent: CDCl₃

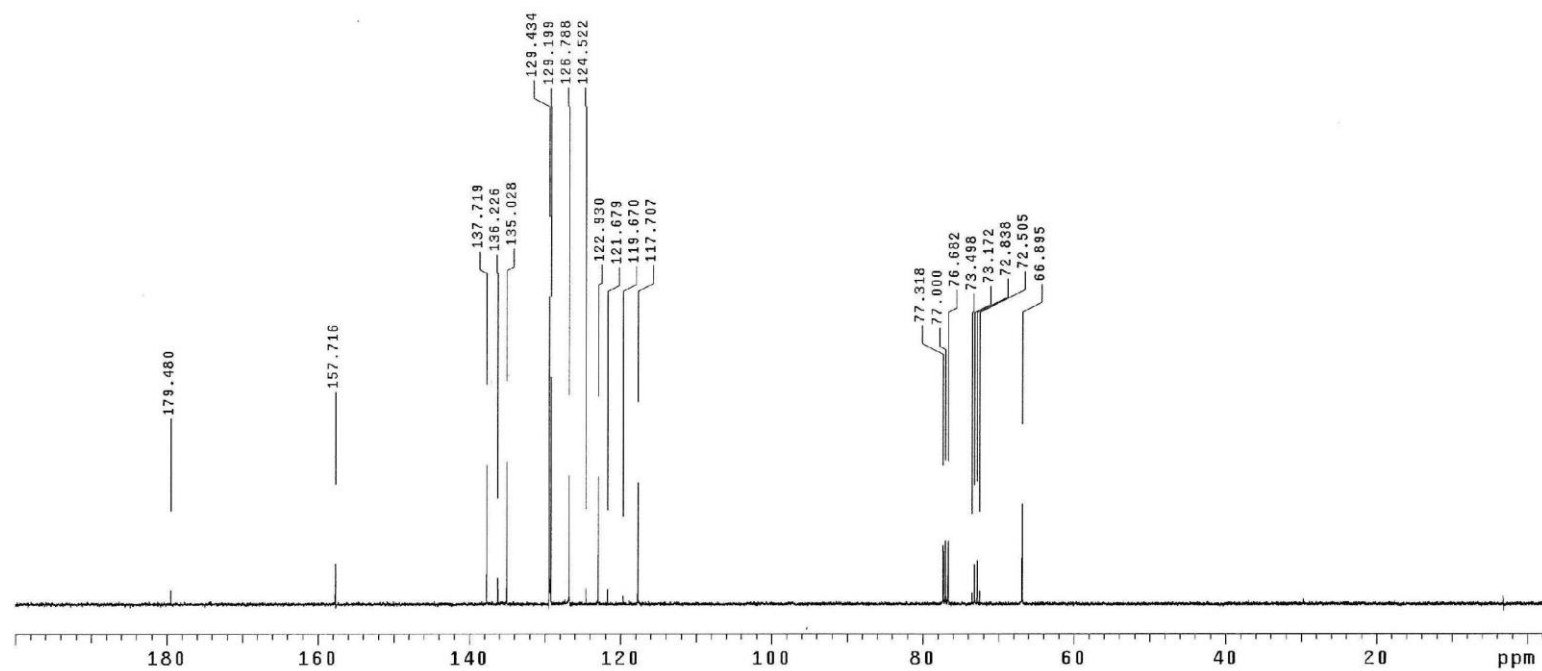
Ambient temperature

Total 1696 repetitions



Compound 4af

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4ag (¹H-NMR spectral data)

YLTsCF3

Pulse Sequence: s2pu1

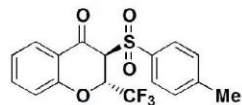
UNITYplus-400 "unity400"

Date: May 4 2017

Solvent: CDCl₃

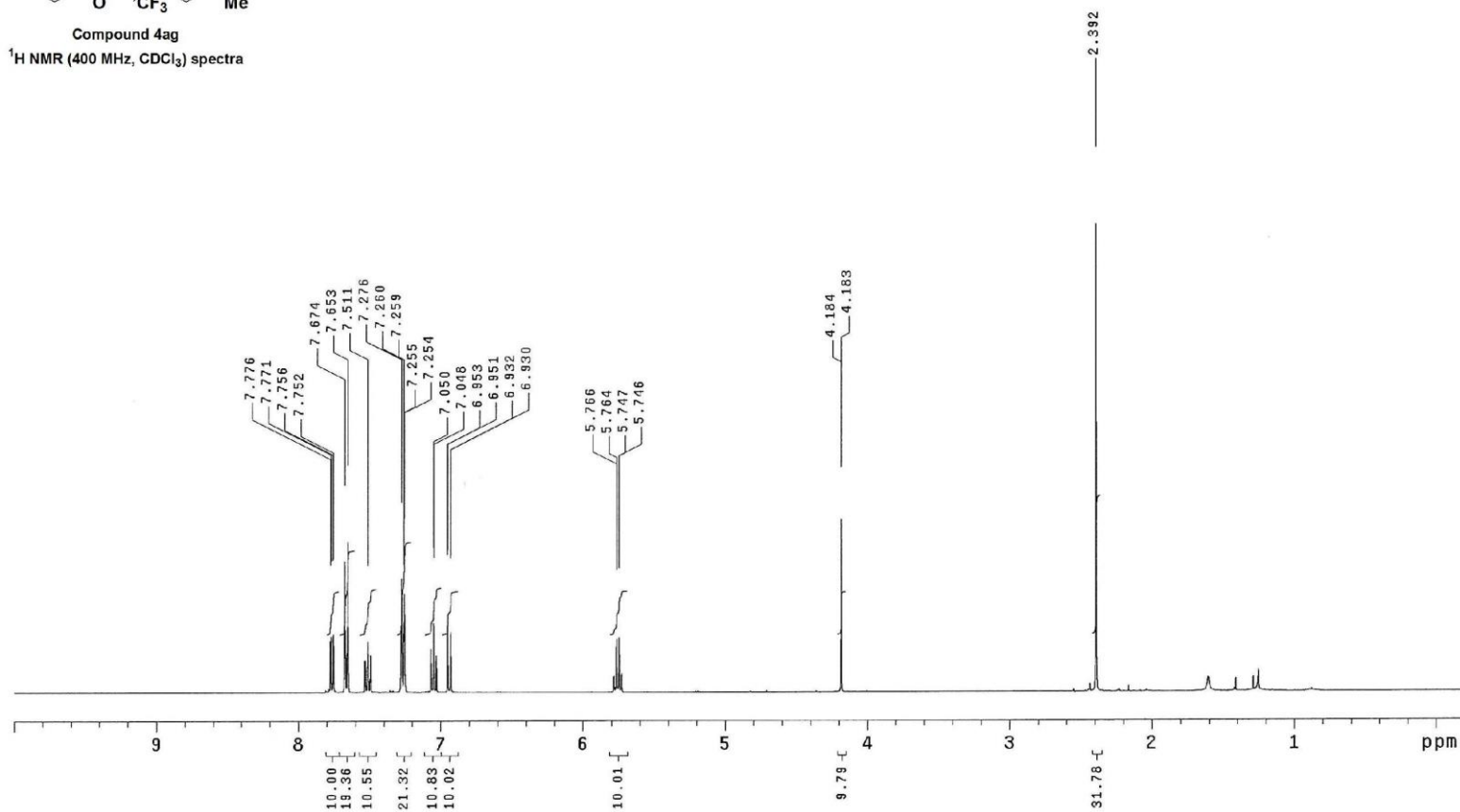
Ambient temperature

Total 32 repetitions



Compound 4ag

¹H NMR (400 MHz, CDCl₃) spectra



Compound 4ag (¹³C-NMR spectral data)

YLTsCF3

Pulse Sequence: s2pu1

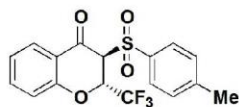
UNITYplus-400 "unity400"

Date: May 4 2017

Solvent: CDCl₃

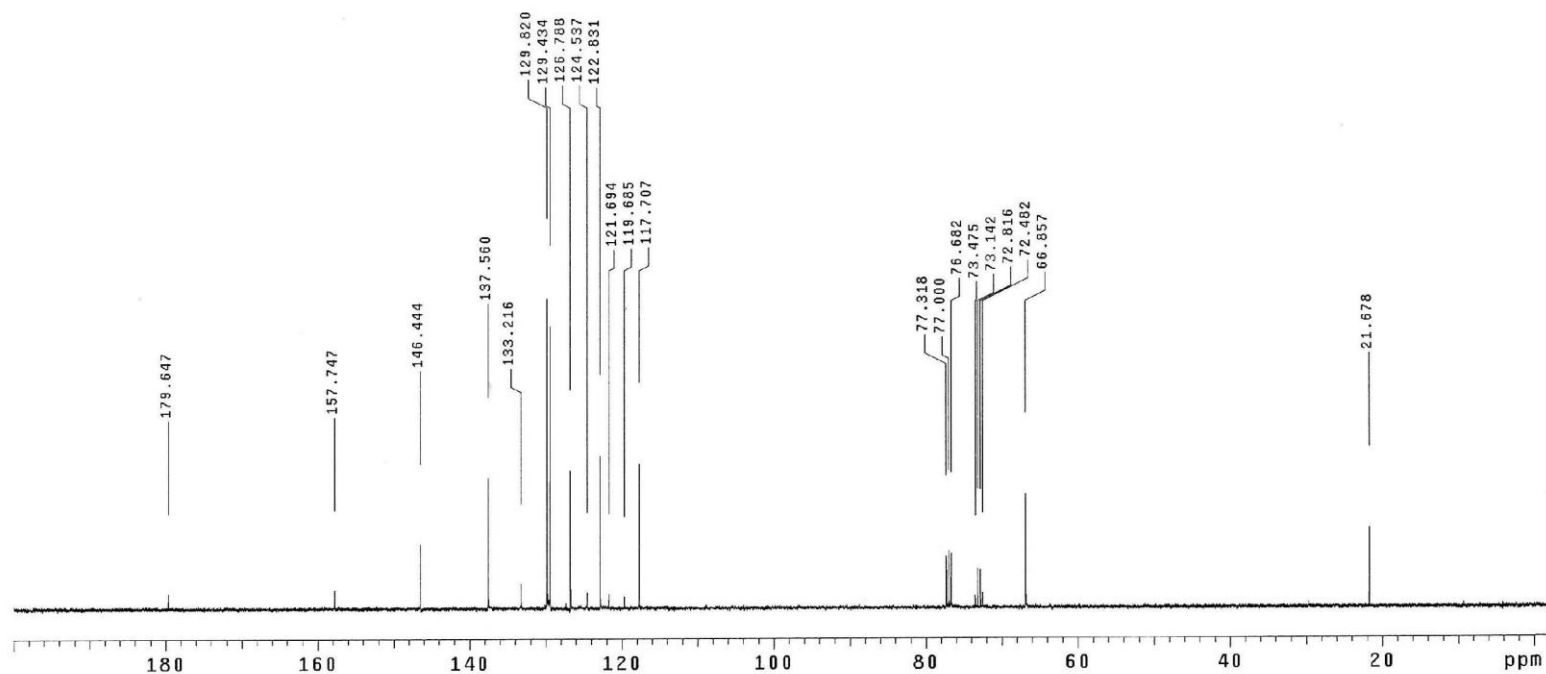
Ambient temperature

Total 2032 repetitions



Compound 4ag

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4ah (¹H-NMR spectral data)

YEFCF3

Pulse Sequence: s2pu1

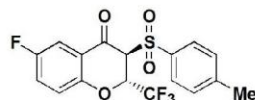
UNITYplus-400 "unity400"

Date: Jun 6 2017

Solvent: CDCl₃

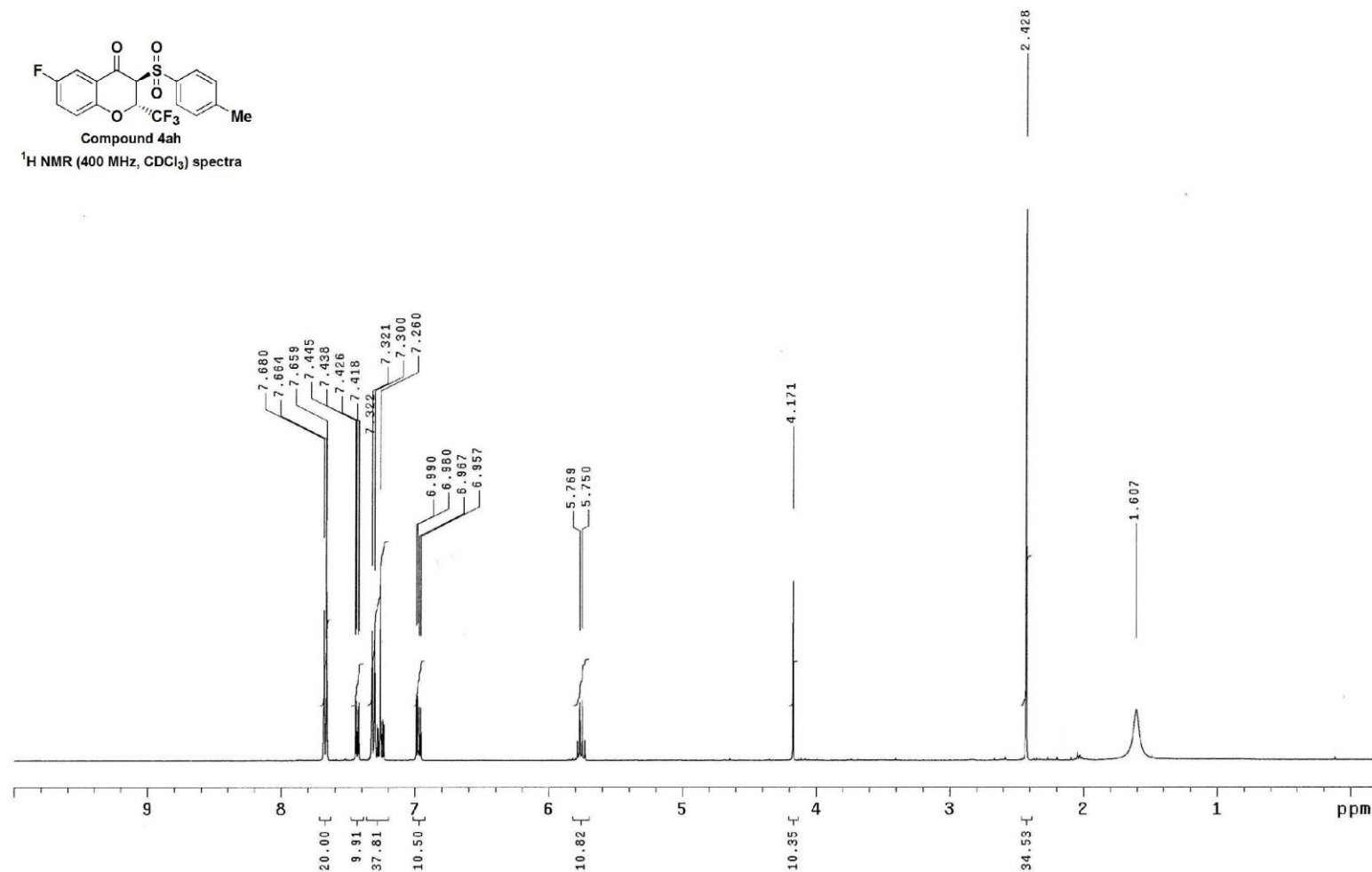
Ambient temperature

Total 64 repetitions



Compound 4ah

¹H NMR (400 MHz, CDCl₃) spectra



Compound 4ah (¹³C-NMR spectral data)

YEFCF3

Pulse Sequence: s2pu1

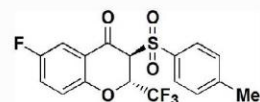
UNITYplus-400 "unity400"

Date: Jun 6 2017

Solvent: CDCl₃

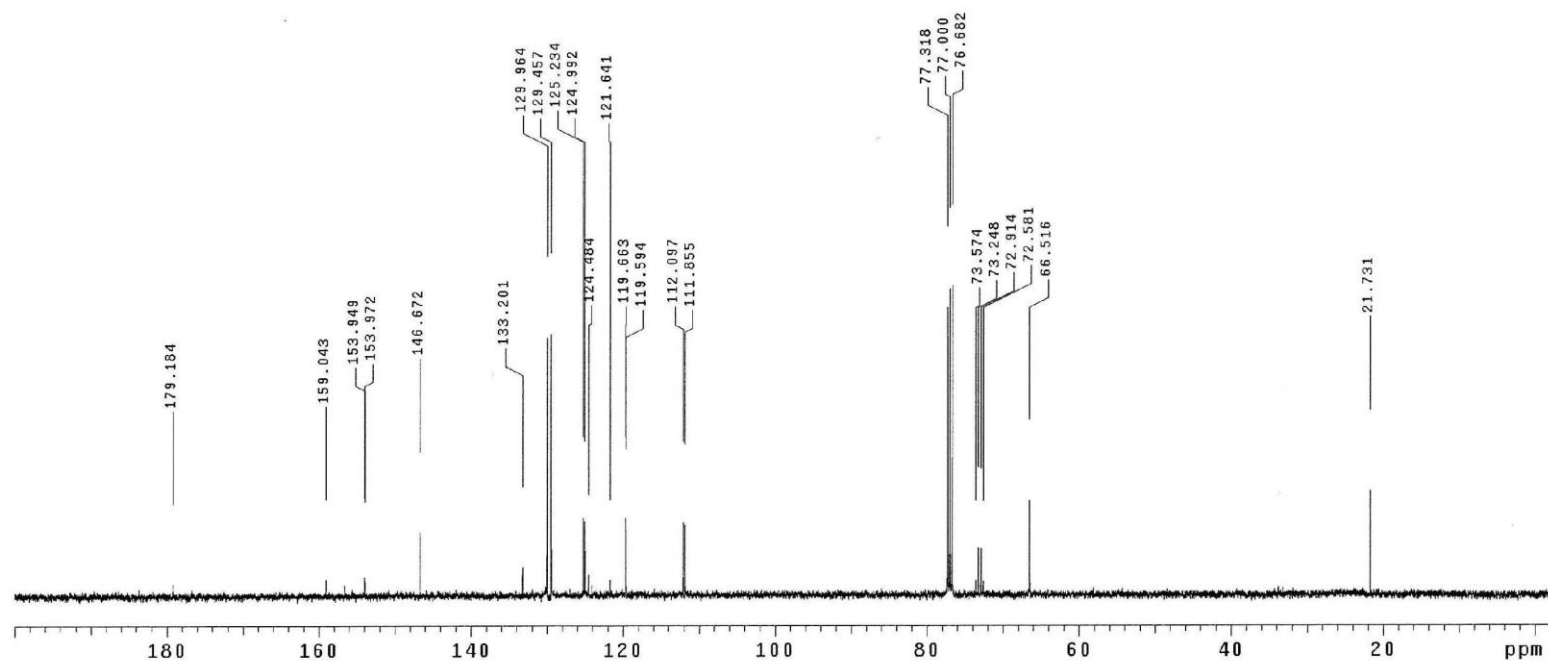
Ambient temperature

Total 15168 repetitions



Compound 4ah

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4ai (¹H-NMR spectral data)

YLTs0CF3

Pulse Sequence: s2pu1

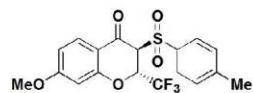
UNITYplus-400 "unity400"

Date: Apr 28 2017

Solvent: CDCl₃

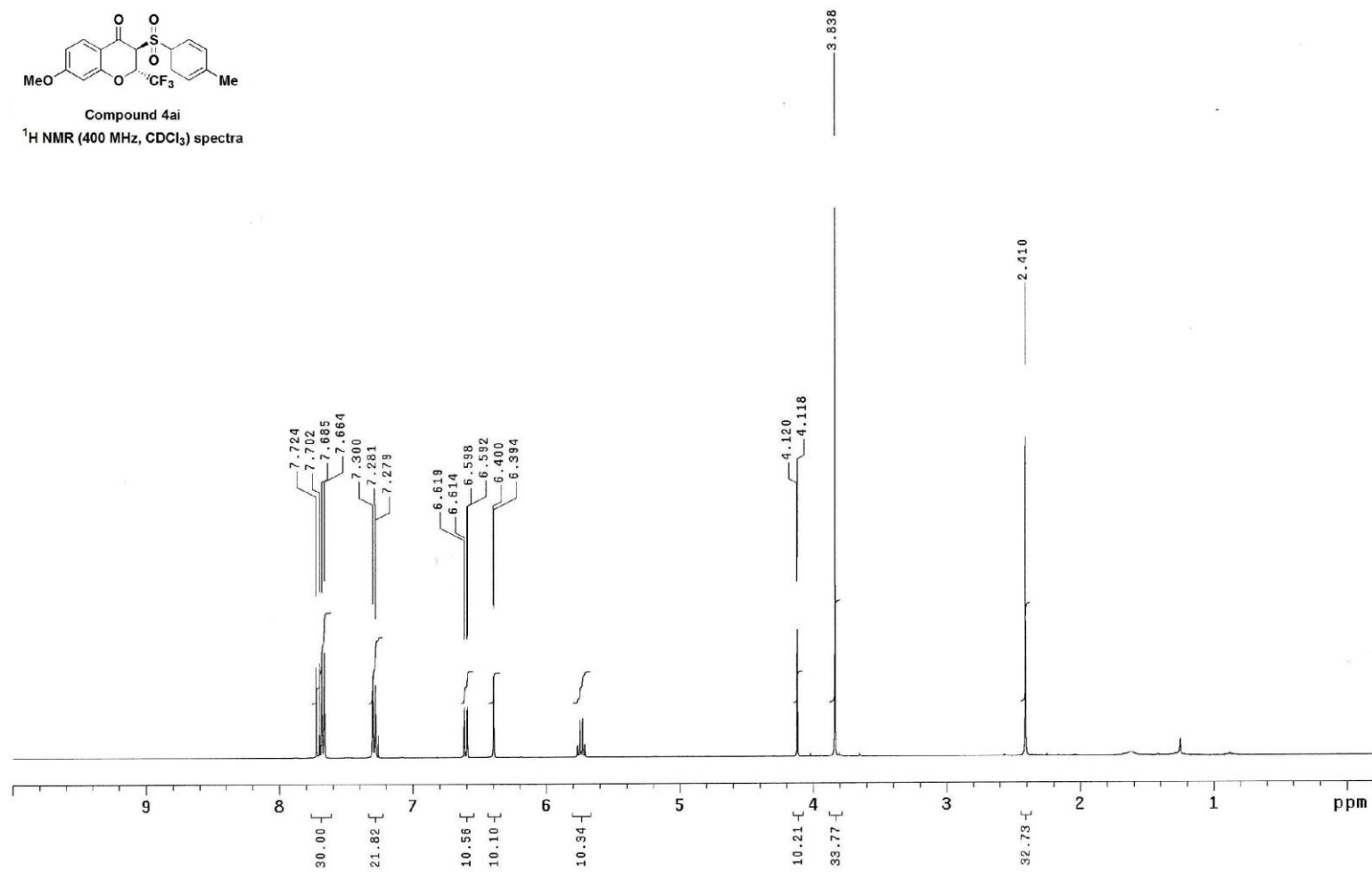
Ambient temperature

Total 32 repetitions



Compound 4ai

¹H NMR (400 MHz, CDCl₃) spectra



Compound 4ai (¹³C-NMR spectral data)

YLTsOCF3

Pulse Sequence: s2pul

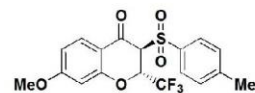
UNITYplus-400 "unity400"

Date: Apr 28 2017

Solvent: CDCl₃

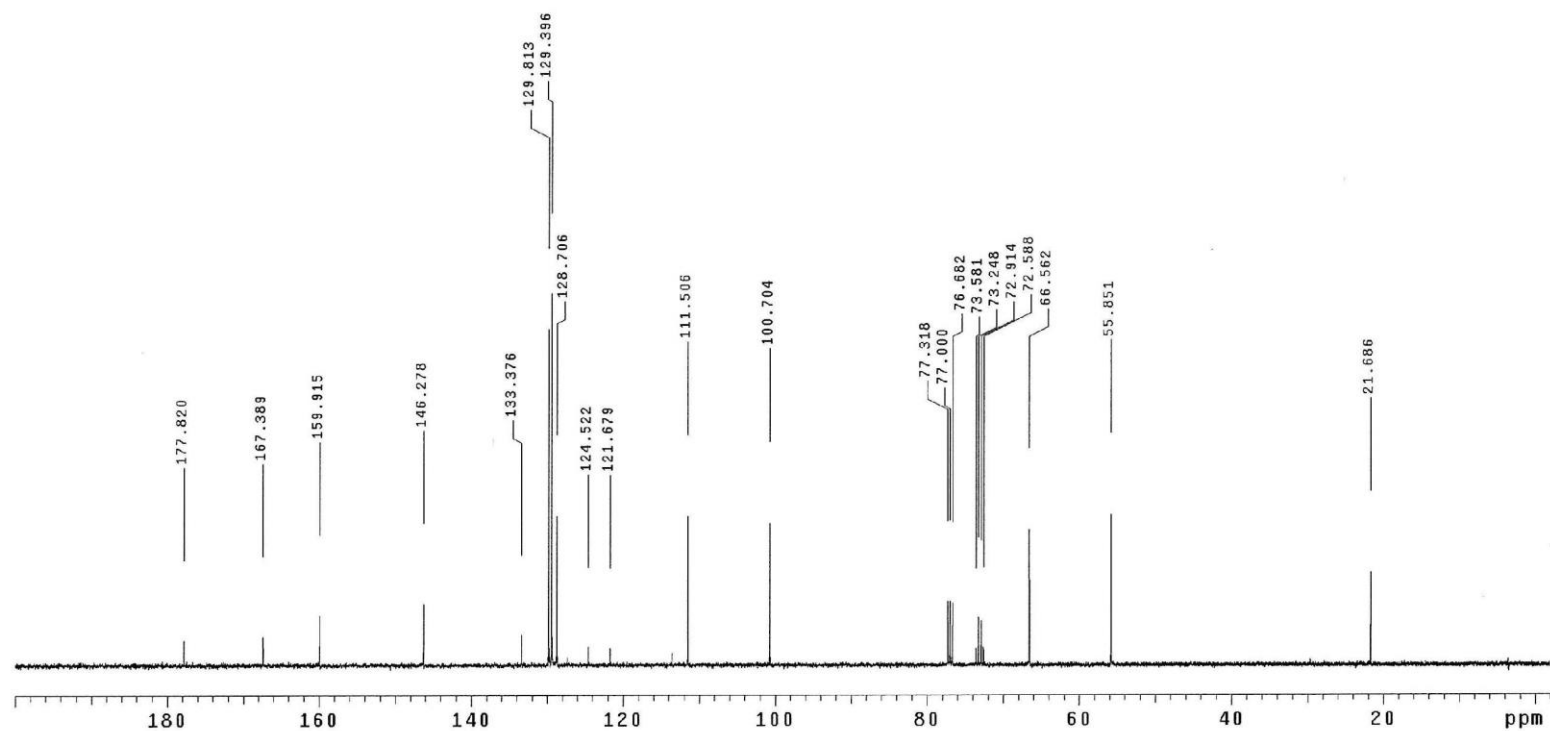
Ambient temperature

Total 1040 repetitions



Compound 4ai

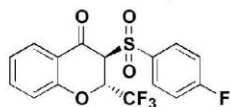
¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4aj (¹H-NMR spectral data)

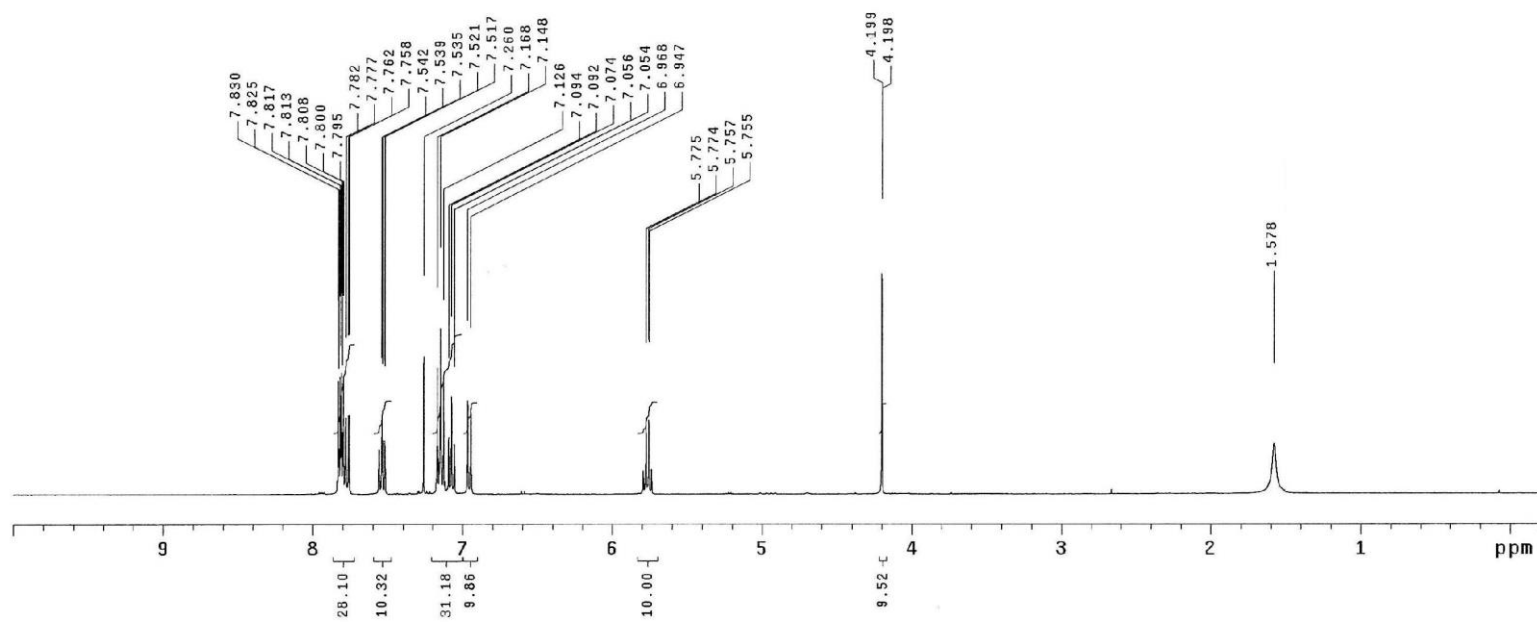
YLFCF3

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Jun 6 2017
Solvent: CDCl3
Ambient temperature
Total 64 repetitions



Compound 4aj

¹H NMR (400 MHz, CDCl₃) spectra



Compound 4aj (¹³C-NMR spectral data)

YLFCF3

Pulse Sequence: s2pu1

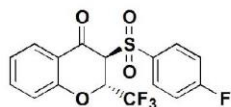
UNITYplus-400 "unity400"

Date: Jun 6 2017

Solvent: CDCl₃

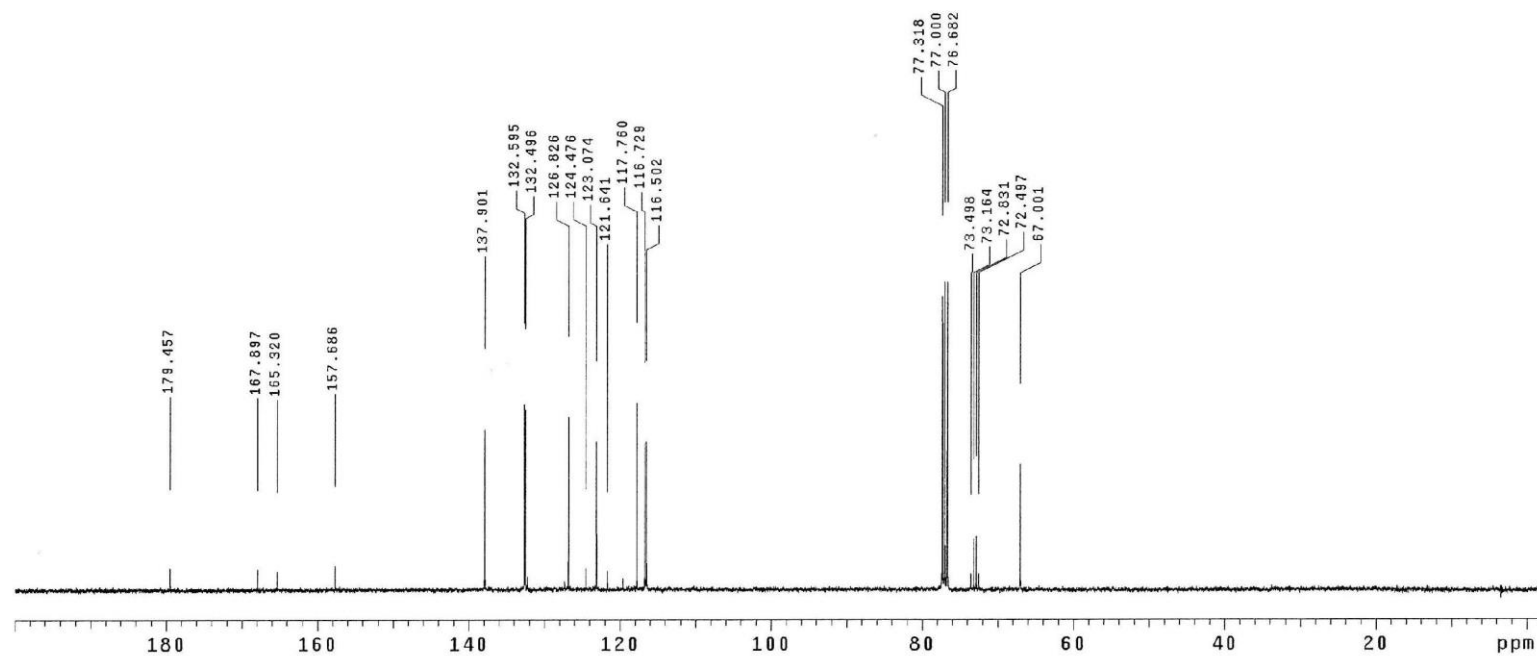
Ambient temperature

Total 20480 repetitions



Compound 4aj

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4ak (¹H-NMR spectral data)

YLRTsEt21

Pulse Sequence: s2pul

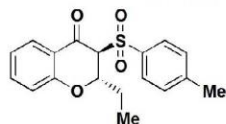
UNITYplus-400 "unity400"

Date: Nov 28 2017

Solvent: CDCl₃

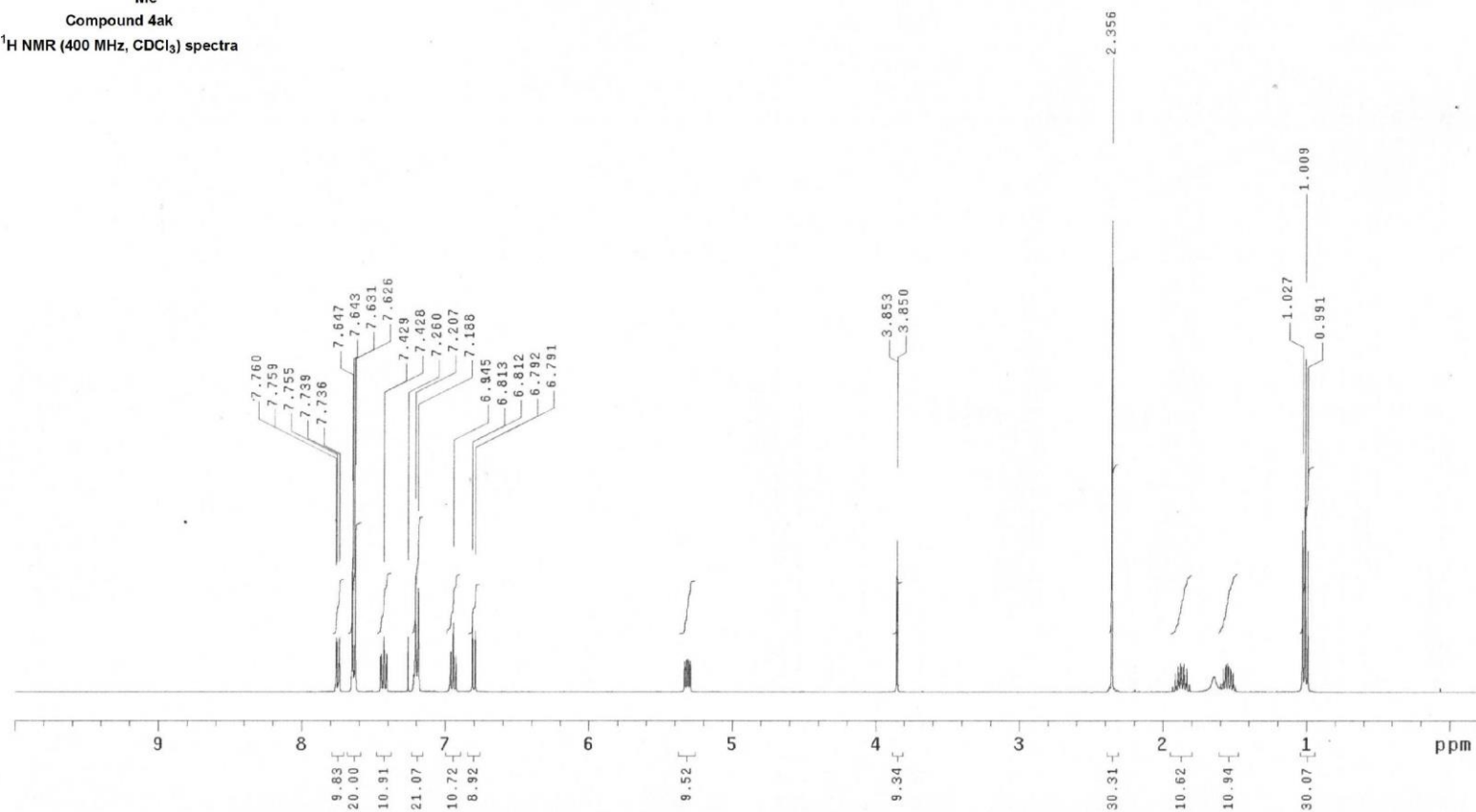
Ambient temperature

Total 32 repetitions



Compound 4ak

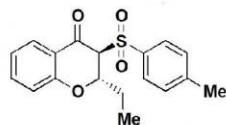
¹H NMR (400 MHz, CDCl₃) spectra



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

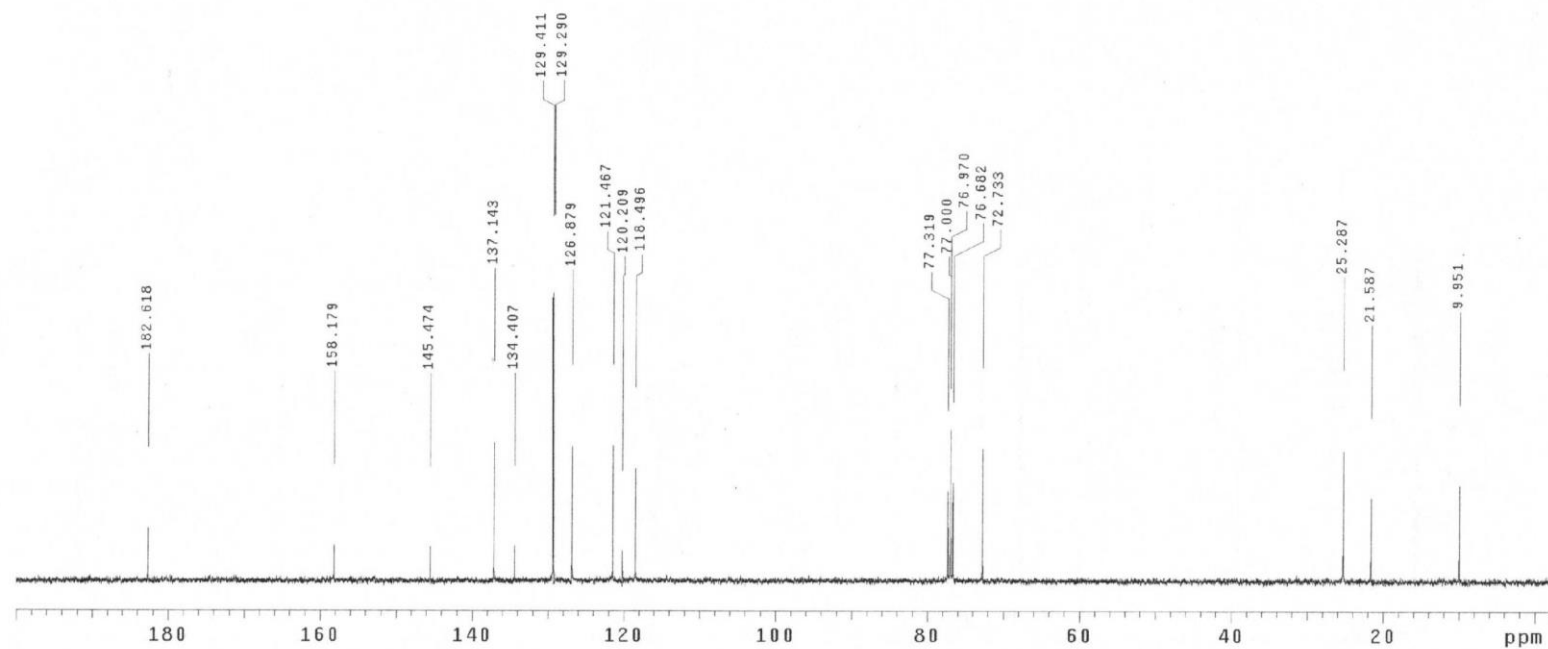
YLRTsEt21

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Nov 28 2017
Solvent: CDCl_3
Ambient temperature
Total 1728 repetitions



Compound 4ak

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



Compound 4al (¹H-NMR spectral data)

YLRF33

Pulse Sequence: s2pu1

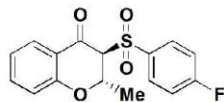
UNITYplus-400 "unity400"

Date: Jun 14 2017

Solvent: CDCl₃

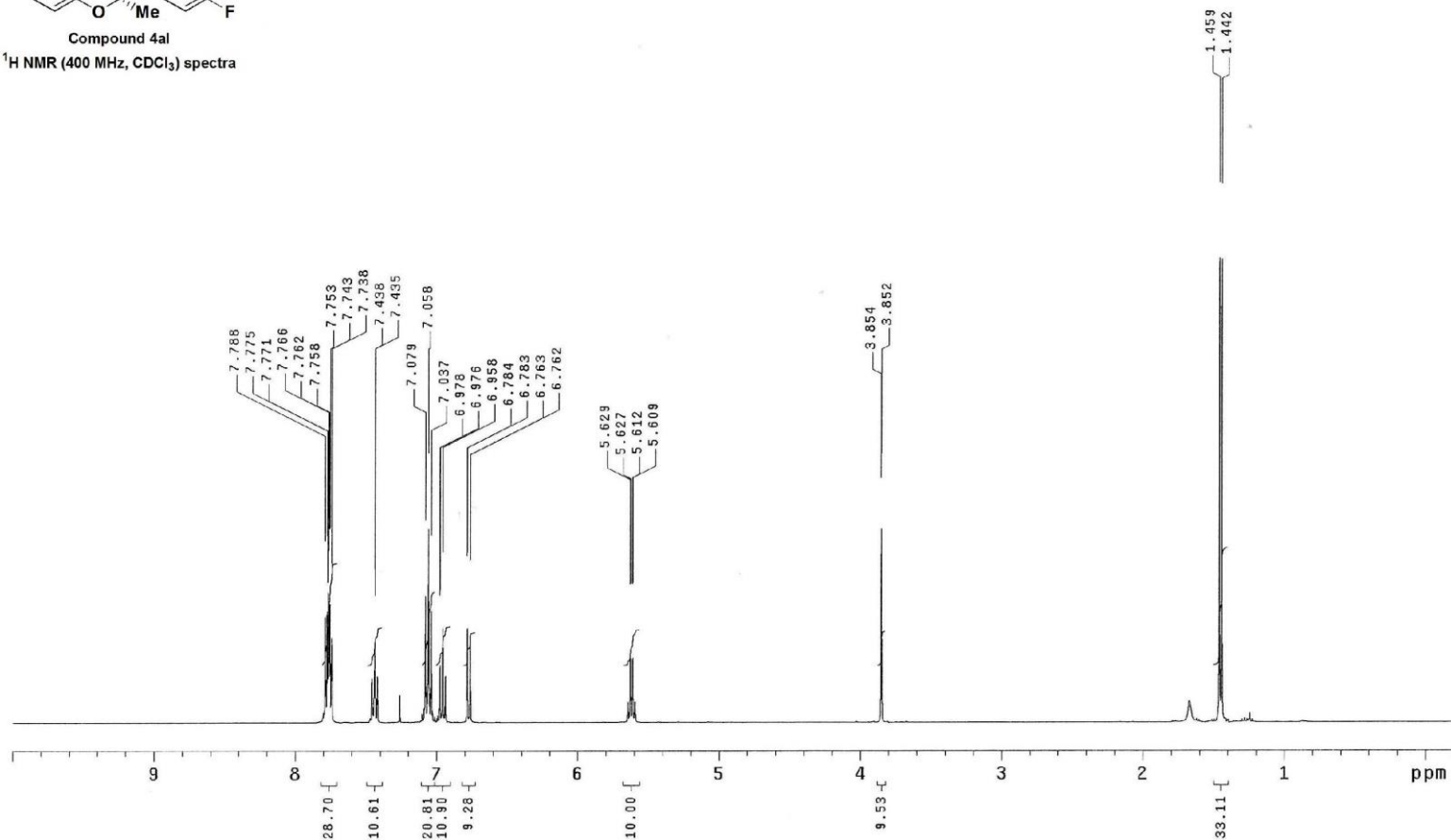
Ambient temperature

Total 32 repetitions



Compound 4al

¹H NMR (400 MHz, CDCl₃) spectra



Compound 4al (¹³C-NMR spectral data)

YLRF33

Pulse Sequence: s2pu1

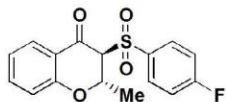
UNITYplus-400 "unity400"

Date: Jun 14 2017

Solvent: CDCl₃

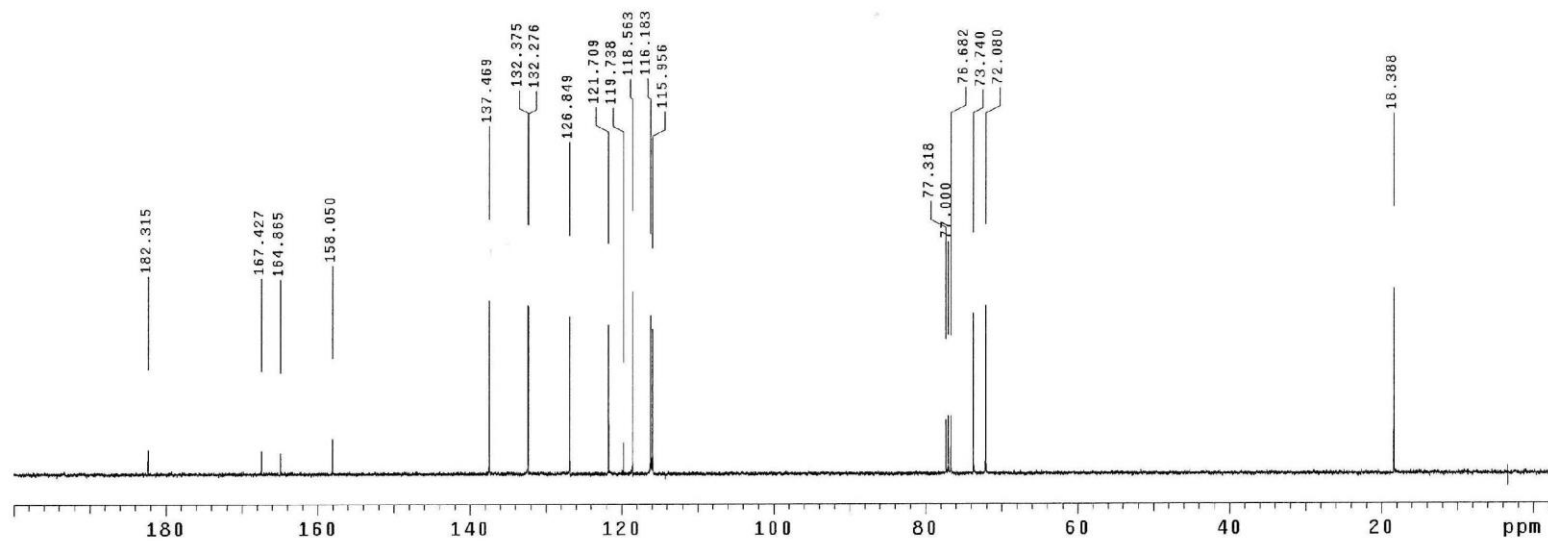
Ambient temperature

Total 1248 repetitions



Compound 4al

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4am (¹H-NMR spectral data)

HAK1A41

Pulse Sequence: s2pu1

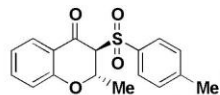
UNITYplus-400 "unity400"

Date: Feb 23 2018

Solvent: CDCl₃

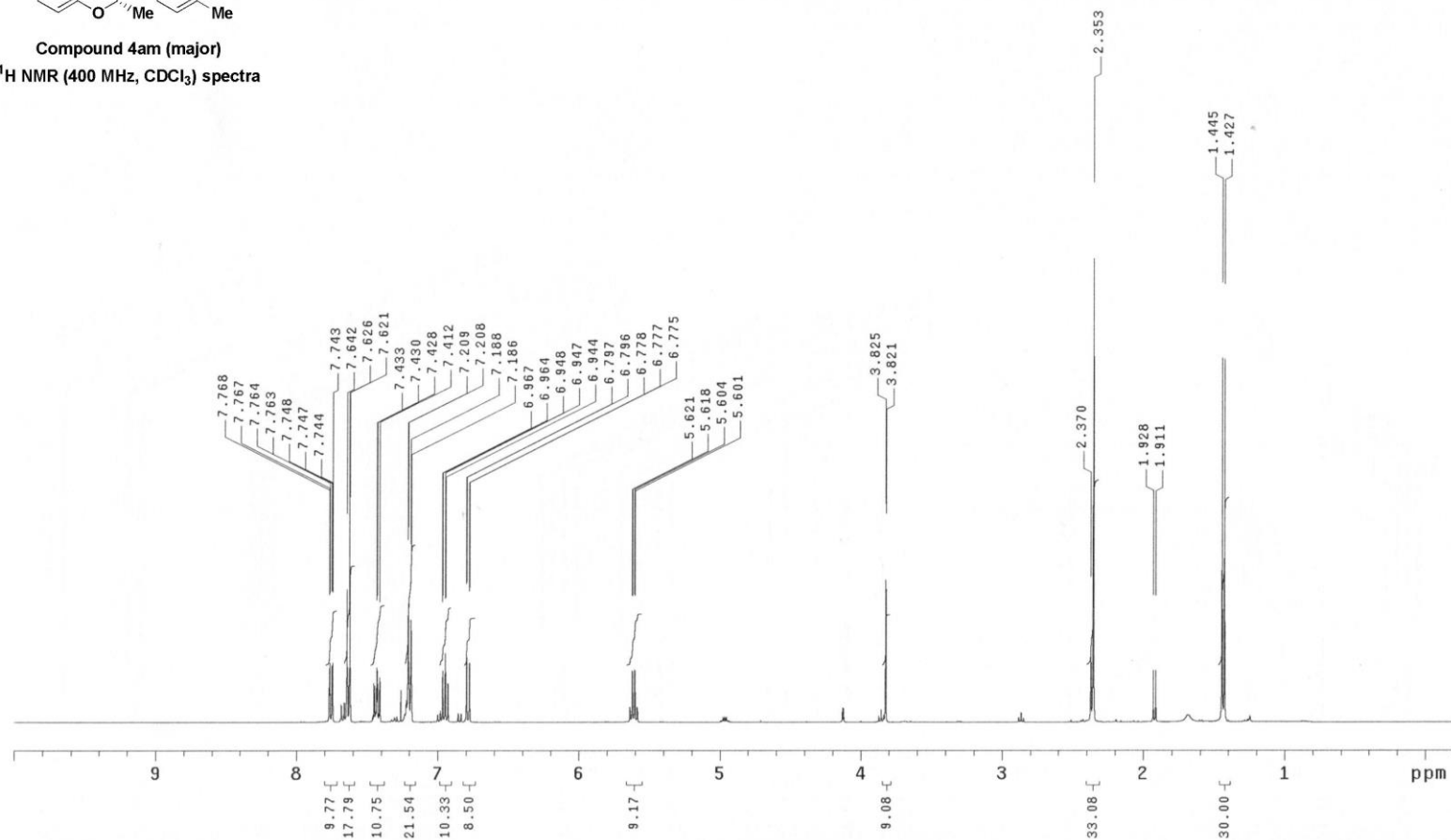
Ambient temperature

Total 32 repetitions



Compound 4am (major)

¹H NMR (400 MHz, CDCl₃) spectra



Compound 4am (¹³C-NMR spectral data)

HAK1A41

Pulse Sequence: s2pu1

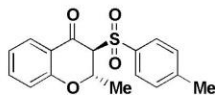
UNITYplus-400 "unity400"

Date: Feb 23 2018

Solvent: CDCl₃

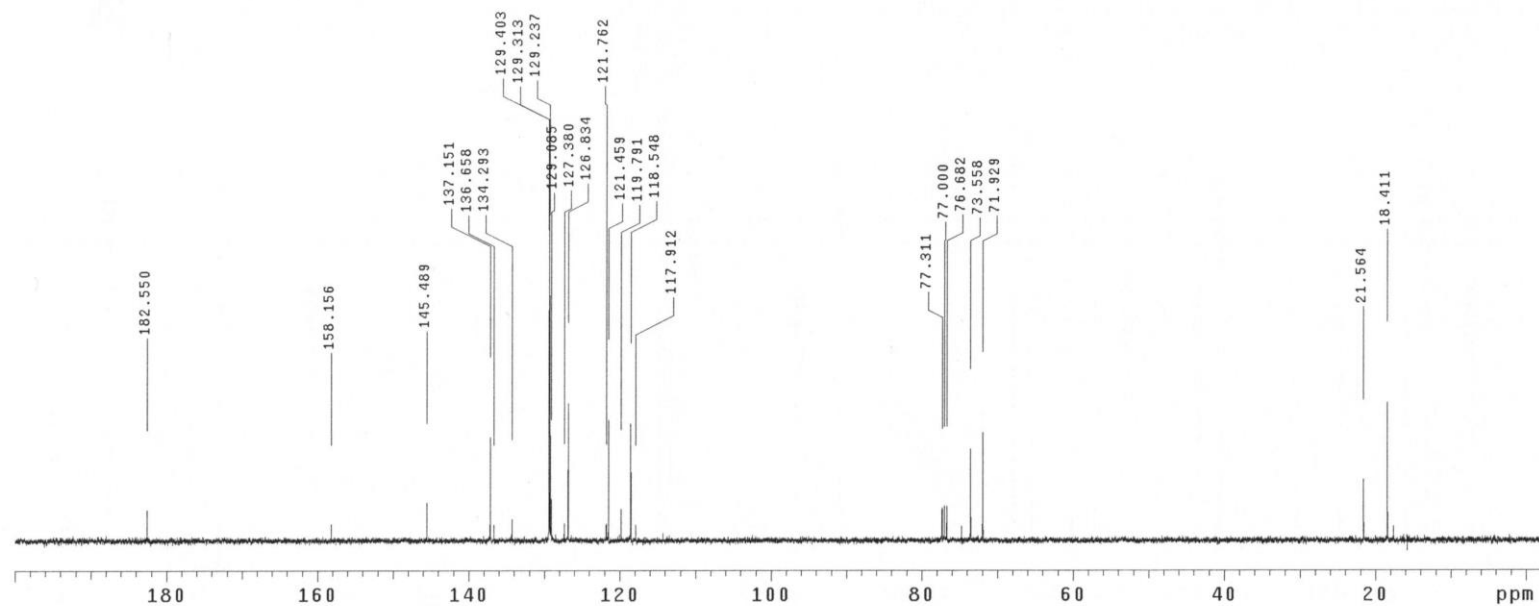
Ambient temperature

Total 320 repetitions



Compound 4am (major)

¹³C NMR (100 MHz, CDCl₃) spectra



Compound 4an (¹H-NMR spectral data)

HAK1A40

Pulse Sequence: s2pu1

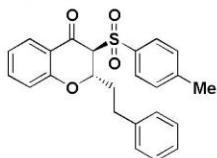
UNITYplus-400 "unity400"

Date: Feb 23 2018

Solvent: CDCl₃

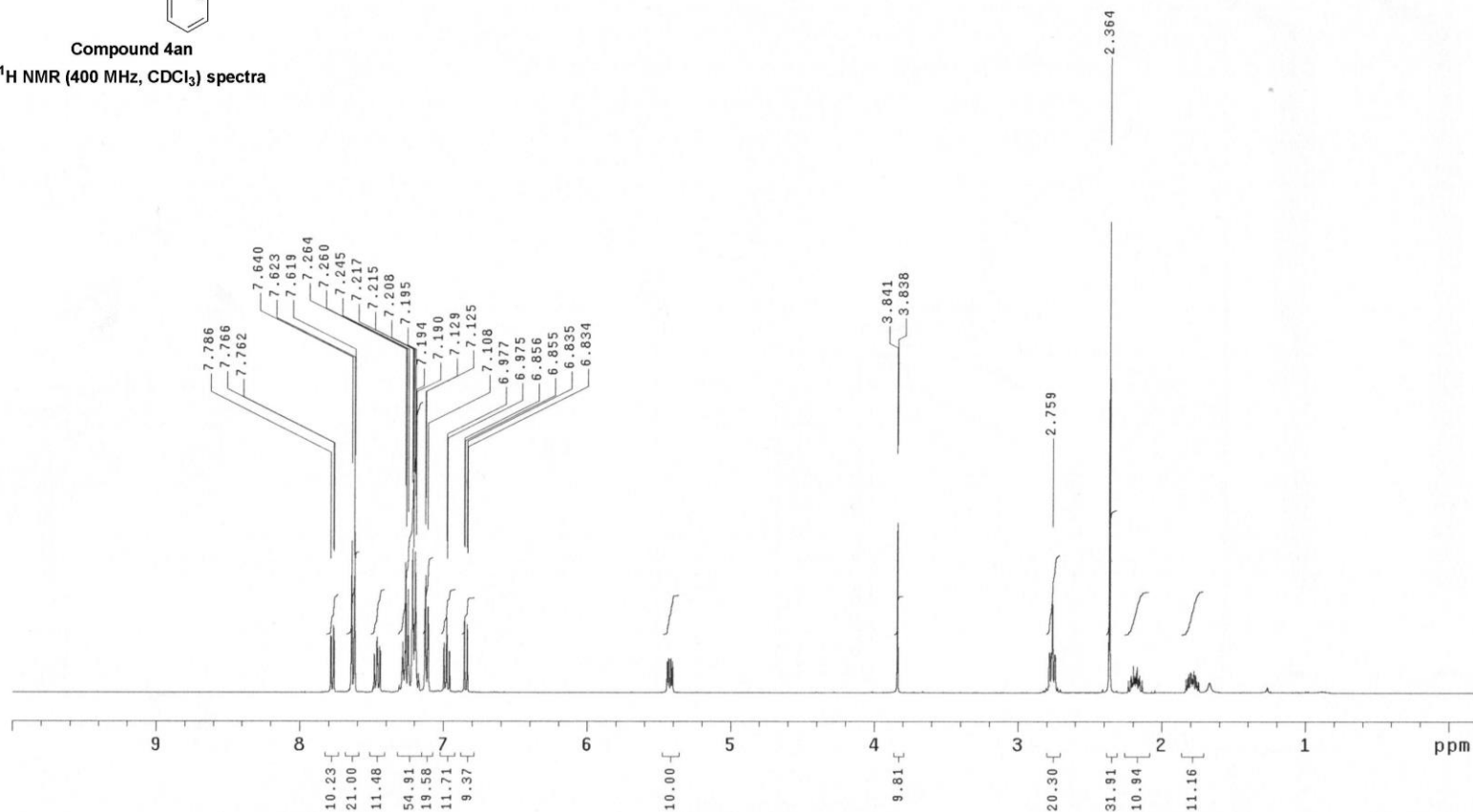
Ambient temperature

Total 32 repetitions



Compound 4an

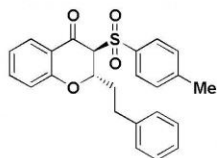
¹H NMR (400 MHz, CDCl₃) spectra



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

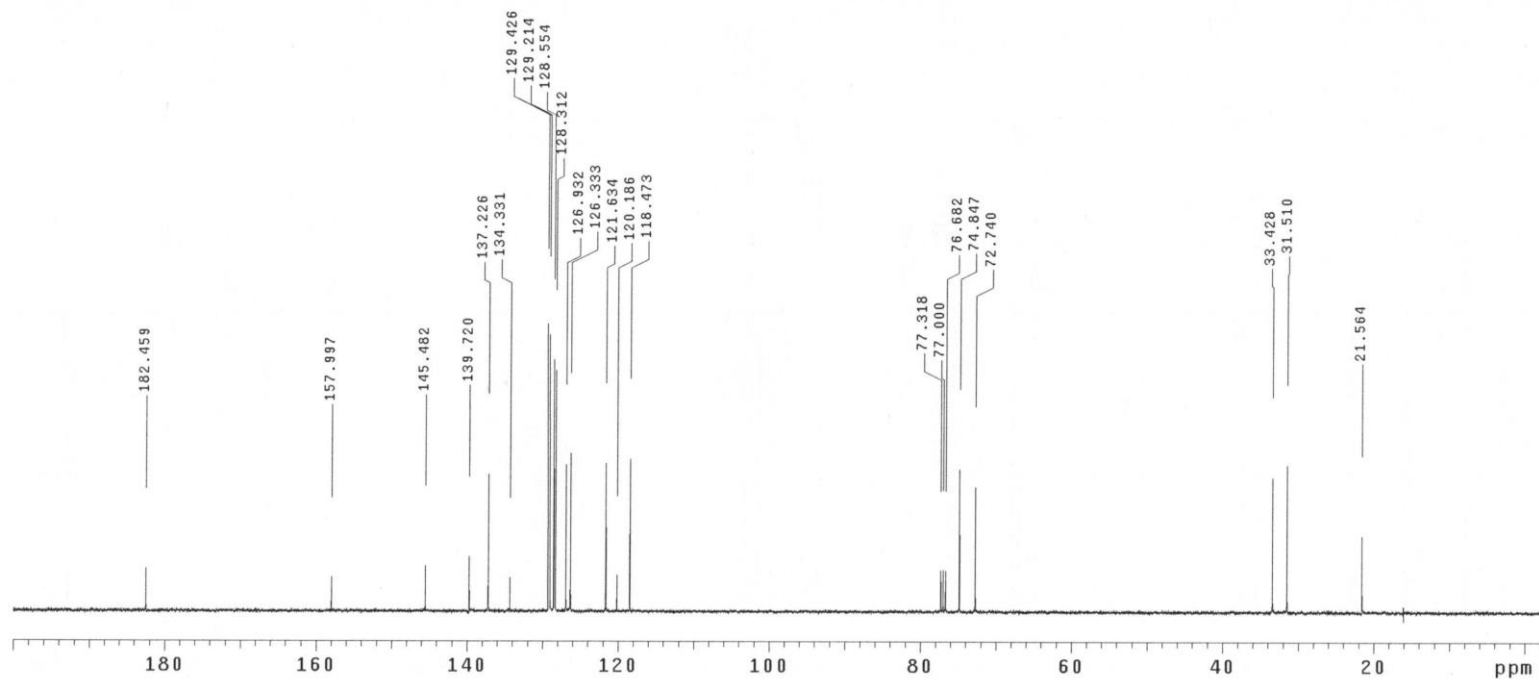
HAK1A40

Pulse Sequence: s2pu1
UNITYplus-400 "unity400"
Date: Feb 23 2018
Solvent: CDCl_3
Ambient temperature
Total 960 repetitions



Compound 4an

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



Compound 4ao (¹H-NMR spectral data)

HA7CDS

Pulse Sequence: s2pu1

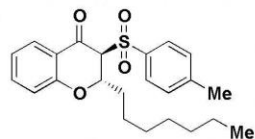
UNITYplus-400 "unity400"

Date: Feb 26 2018

Solvent: CDCl₃

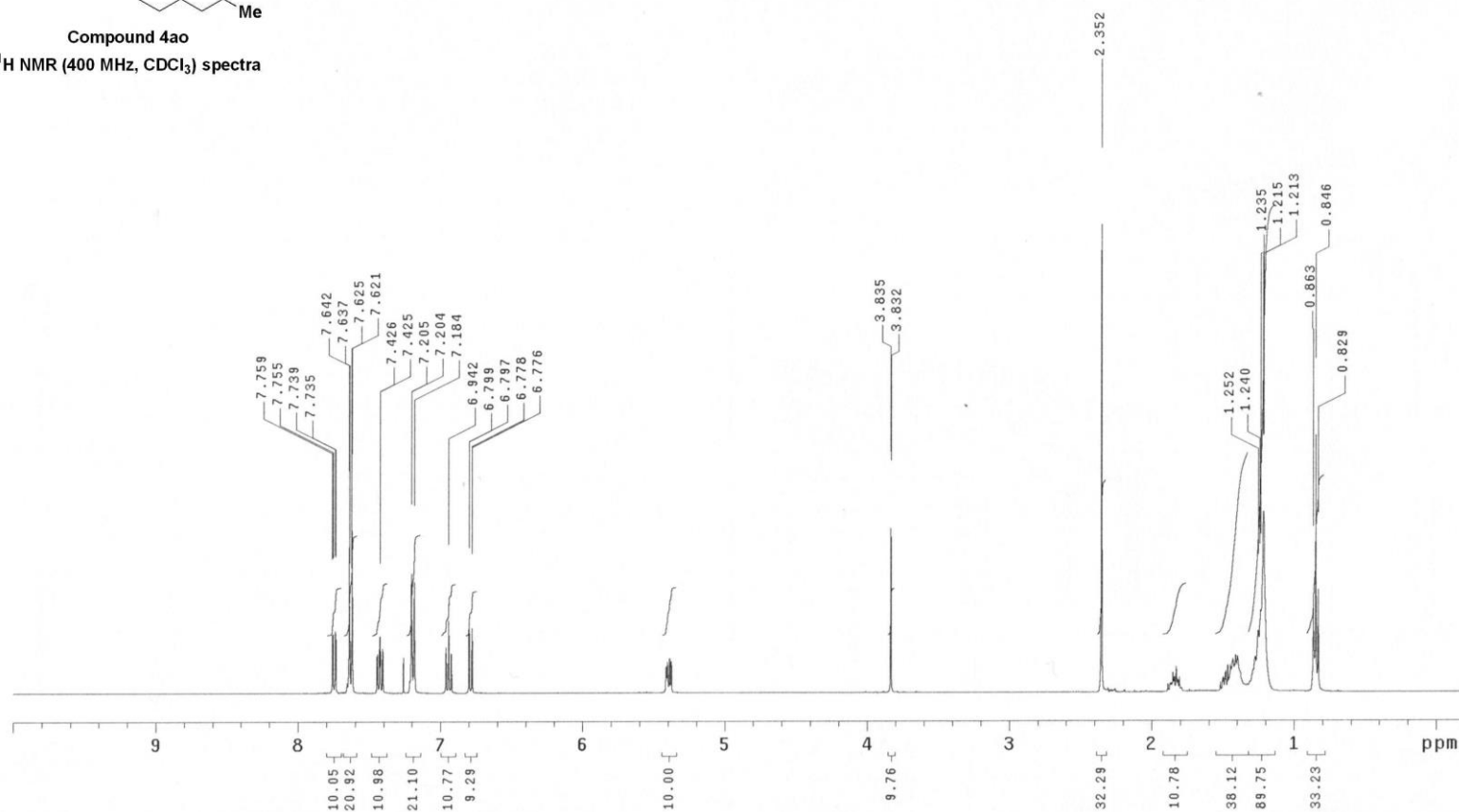
Ambient temperature

Total 32 repetitions



Compound 4ao

¹H NMR (400 MHz, CDCl₃) spectra



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

HA7CDS

Pulse Sequence: s2pu1

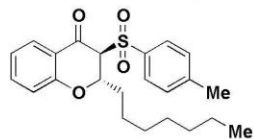
UNITYplus-400 "unity400"

Date: Feb 26 2018

Solvent: CDCl_3

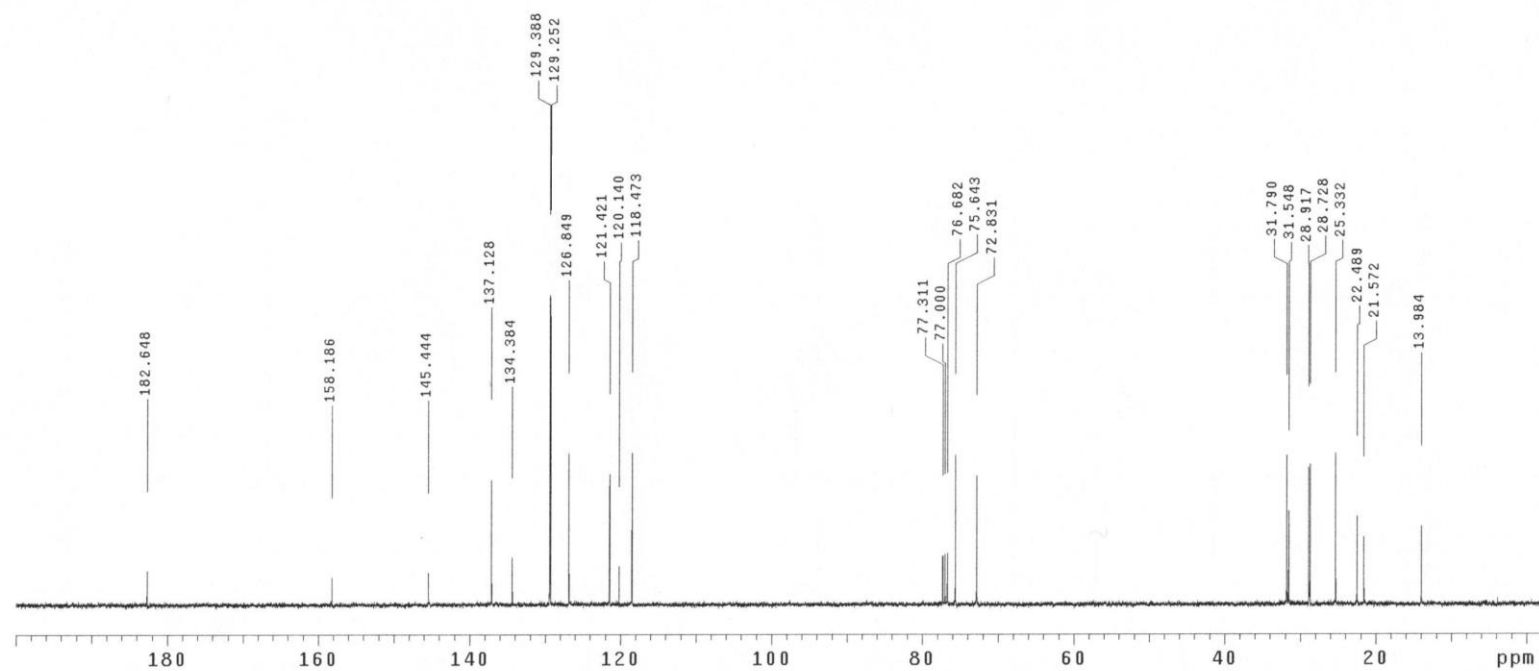
Ambient temperature

Total 912 repetitions

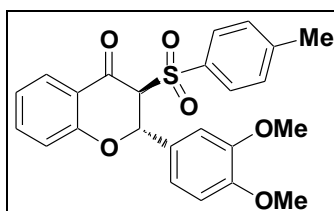


Compound 4ao

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

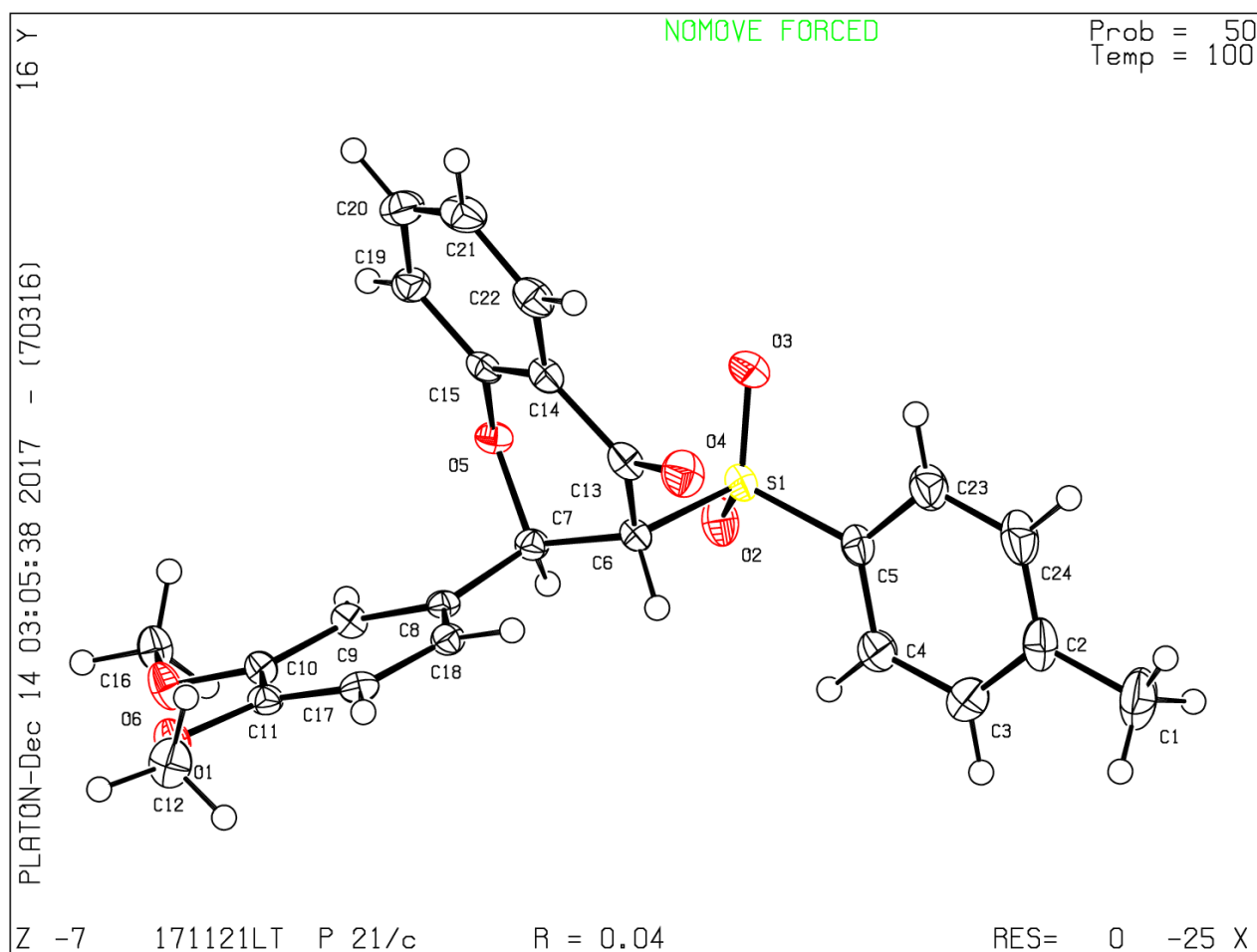


X-ray crystal data of compound 4a (CCDC 1811124)



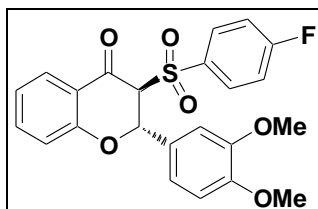
Sample preparation : A solution of compound **4a** (30 mg) in CH₂Cl₂ (10 mL) was placed in a tube (10 mL). EtOAc (2 mL) was added slowly to the vial with a dropper. The vial was closed with little cotton and kept at room temperature for 2 days. Then, colorless prisms were observed.

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.



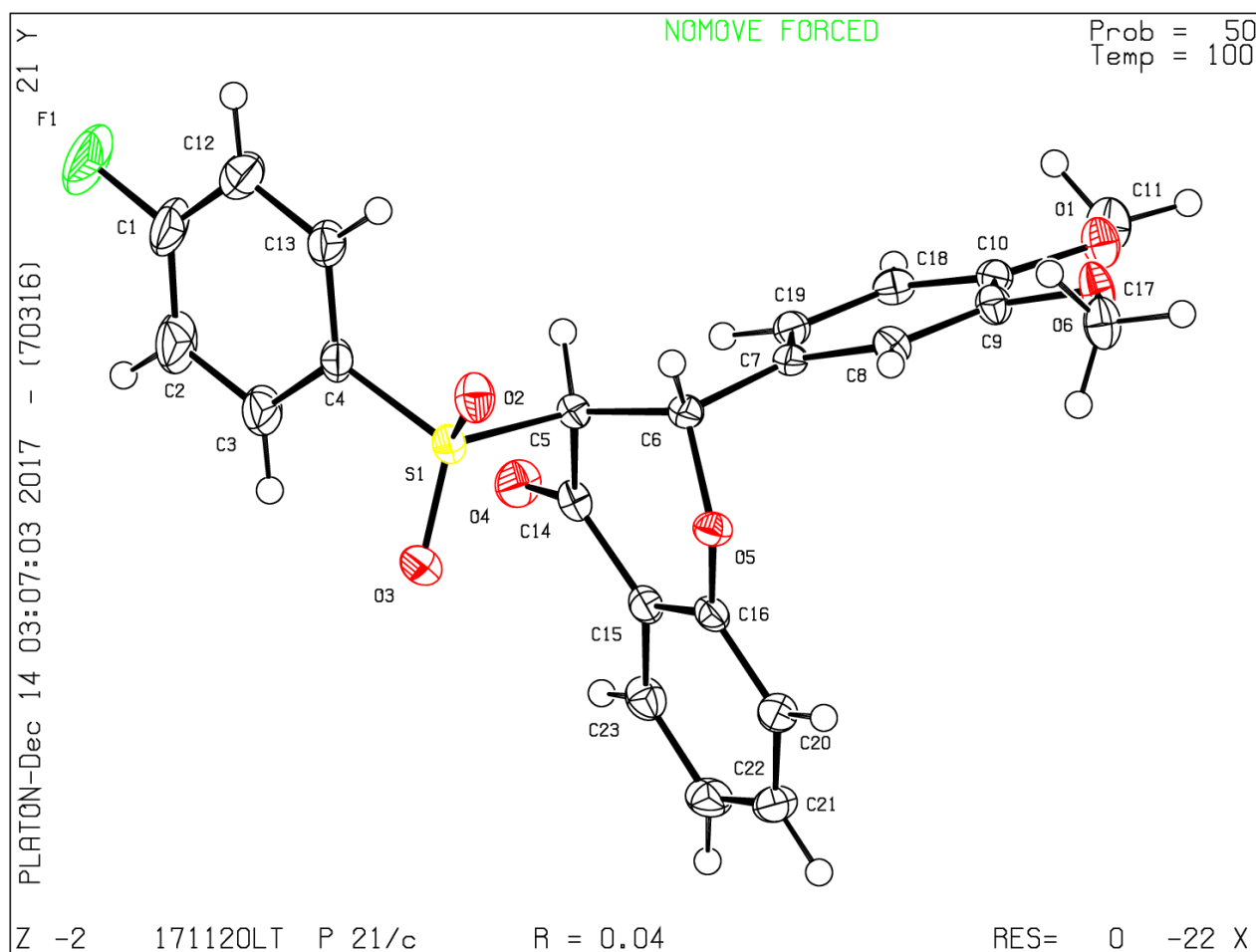
Empirical formula	C ₂₄ H ₂₂ O ₆ S
Formula weight	438.47
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P 2 ₁ /c
Unit cell dimensions	a = 21.002(3) Å α = 90°. b = 11.9195(15) Å β = 97.290(5)°. c = 8.3067(11) Å γ = 90°.
Volume	2062.6(5) Å ³
Z	4
Density (calculated)	1.412 Mg/m ³
Absorption coefficient	0.197 mm ⁻¹
F(000)	920
Crystal size	0.18 x 0.18 x 0.06 mm ³
Theta range for data collection	0.977 to 26.475°.
Index ranges	-23 ≤ h ≤ 26, -14 ≤ k ≤ 14, -9 ≤ l ≤ 10
Reflections collected	16553
Independent reflections	4236 [R(int) = 0.0349]
Completeness to theta = 25.242°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9485 and 0.8933
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	4236 / 0 / 283
Goodness-of-fit on F ²	1.053
Final R indices [I > 2σ(I)]	R ₁ = 0.0383, wR ₂ = 0.0960
R indices (all data)	R ₁ = 0.0488, wR ₂ = 0.1084
Extinction coefficient	n/a
Largest diff. peak and hole	0.291 and -0.358 e.Å ⁻³

X-ray crystal data of compound 4e (CCDC 1811125)



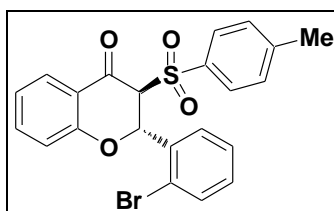
Sample preparation : A solution of compound **4e** (30 mg) in CH₂Cl₂ (10 mL) was placed in a tube (10 mL). EtOAc (2 mL) was added slowly to the vial with a dropper. The vial was closed with little cotton and kept at room temperature for 2 days. Then, colorless prisms were observed.

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.



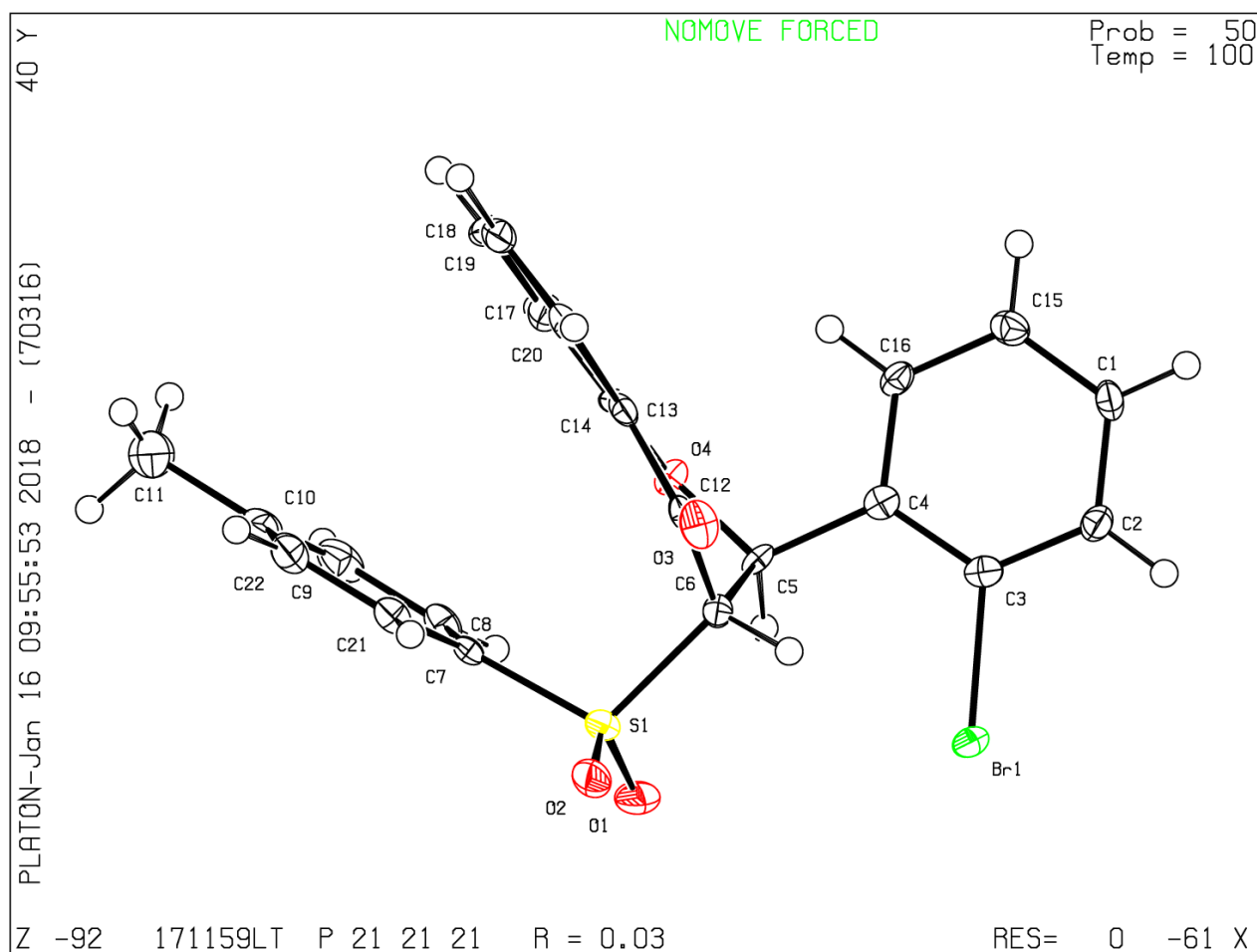
Empirical formula	C23 H19 F O6 S
Formula weight	442.44
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P 21/c
Unit cell dimensions	a = 20.5754(16) Å $\alpha = 90^\circ$.
b = 11.9457(8) Å	$\beta = 93.216(4)^\circ$.
c = 8.2774(6) Å	$\gamma = 90^\circ$.
Volume	2031.3(3) Å ³
Z	4
Density (calculated)	1.447 Mg/m ³
Absorption coefficient	0.208 mm ⁻¹
F(000)	920
Crystal size	0.15 x 0.13 x 0.10 mm ³
Theta range for data collection	0.991 to 26.478°.
Index ranges	-25 ≤ h ≤ 25, -14 ≤ k ≤ 14, -10 ≤ l ≤ 10
Reflections collected	16024
Independent reflections	4167 [R(int) = 0.0468]
Completeness to theta = 25.242°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9485 and 0.7484
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	4167 / 0 / 282
Goodness-of-fit on F ²	1.056
Final R indices [I > 2σ(I)]	R1 = 0.0380, wR2 = 0.0921
R indices (all data)	R1 = 0.0489, wR2 = 0.0997
Extinction coefficient	n/a
Largest diff. peak and hole	0.336 and -0.384 e.Å ⁻³

X-ray crystal data of compound 4ab (CCDC 1811128)



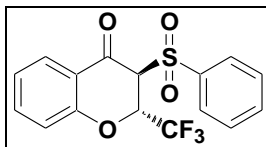
Sample preparation : A solution of compound **4ab** (30 mg) in CH₂Cl₂ (10 mL) was placed in a tube (10 mL). EtOAc (2 mL) was added slowly to the vial with a dropper. The vial was closed with little cotton and kept at room temperature for 2 days. Then, colorless prisms were observed.

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.



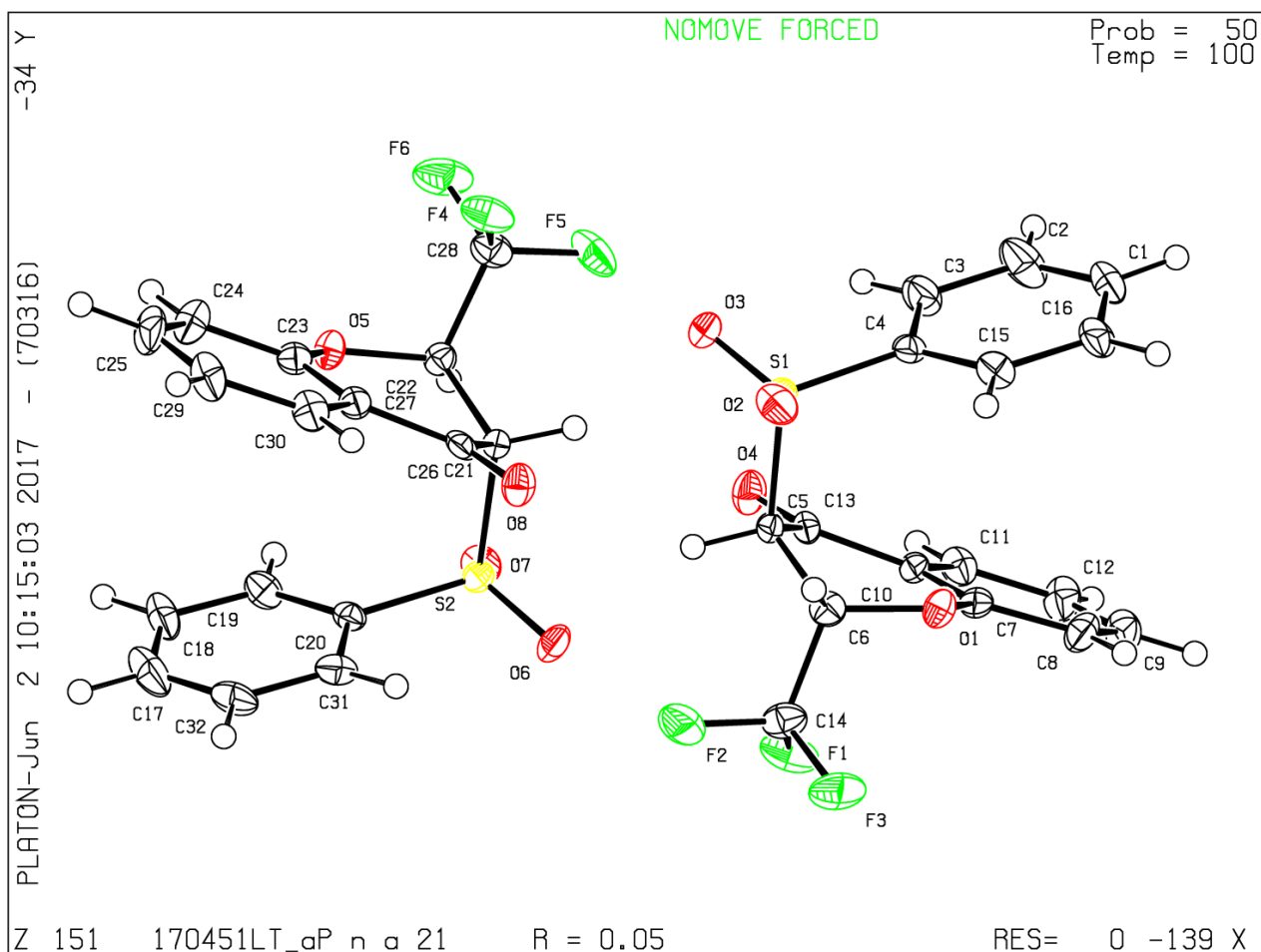
Empirical formula	C22 H17 Br O4 S
Formula weight	457.32
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	P 21 21 21
Unit cell dimensions	a = 8.6975(7) Å $\alpha = 90^\circ$. b = 11.1079(9) Å $\beta = 90^\circ$. c = 19.6779(17) Å $\gamma = 90^\circ$.
Volume	1901.1(3) Å ³
Z	4
Density (calculated)	1.598 Mg/m ³
Absorption coefficient	2.299 mm ⁻¹
F(000)	928
Crystal size	0.25 x 0.25 x 0.12 mm ³
Theta range for data collection	2.070 to 26.508°.
Index ranges	-9<=h<=10, -13<=k<=13, -24<=l<=24
Reflections collected	15695
Independent reflections	3914 [R(int) = 0.0483]
Completeness to theta = 25.242°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9485 and 0.8003
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3914 / 0 / 254
Goodness-of-fit on F ²	1.012
Final R indices [I>2sigma(I)]	R1 = 0.0283, wR2 = 0.0543
R indices (all data)	R1 = 0.0342, wR2 = 0.0561
Absolute structure parameter	0.011(6)
Extinction coefficient	n/a
Largest diff. peak and hole	0.445 and -0.277 e.Å ⁻³

X-ray crystal data of compound 4af (CCDC 1811129)



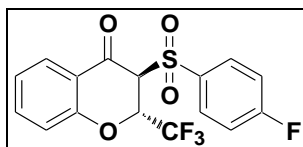
Sample preparation : A solution of compound **4af** (30 mg) in CH₂Cl₂ (10 mL) was placed in a tube (10 mL). EtOAc (2 mL) was added slowly to the vial with a dropper. The vial was closed with little cotton and kept at room temperature for 2 days. Then, colorless prisms were observed.

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.



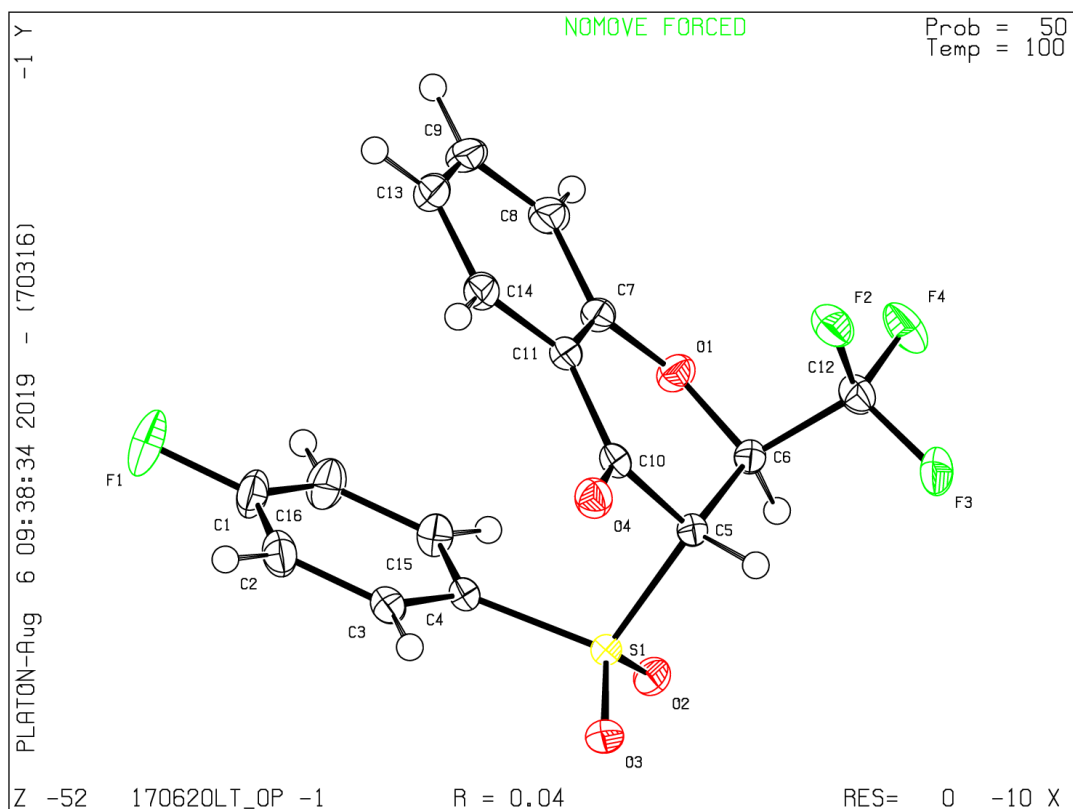
Empirical formula	C32 H22 F6 O8 S2
Formula weight	712.61
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	P n a 21
Unit cell dimensions	a = 24.1977(12) Å $\alpha = 90^\circ$. b = 9.9696(5) Å $\beta = 90^\circ$. c = 12.6028(6) Å $\gamma = 90^\circ$.
Volume	3040.3(3) Å ³
Z	4
Density (calculated)	1.557 Mg/m ³
Absorption coefficient	0.265 mm ⁻¹
F(000)	1456
Crystal size	0.22 x 0.20 x 0.16 mm ³
Theta range for data collection	1.683 to 26.419°.
Index ranges	-26<= <i>h</i> <=30, -12<= <i>k</i> <=11, -15<= <i>l</i> <=13
Reflections collected	24496
Independent reflections	6075 [R(int) = 0.0460]
Completeness to theta = 25.242°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9485 and 0.7454
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	6075 / 1 / 433
Goodness-of-fit on F ²	1.039
Final R indices [I>2sigma(I)]	R1 = 0.0543, wR2 = 0.1316
R indices (all data)	R1 = 0.0574, wR2 = 0.1359
Absolute structure parameter	0.04(4)
Extinction coefficient	n/a
Largest diff. peak and hole	1.821 and -0.385 e.Å ⁻³

X-ray crystal data of compound 4aj (CCDC 1811130)



Sample preparation : A solution of compound **4aj** (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	C16 H10 F4 O4 S
Formula weight	374.30
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 8.3801(12) Å $\alpha = 97.183(6)^\circ$. b = 9.4312(12) Å $\beta = 105.437(6)^\circ$. c = 11.0839(15) Å $\gamma = 113.837(6)^\circ$.
Volume	745.01(18) Å ³
Z	2
Density (calculated)	1.669 Mg/m ³
Absorption coefficient	0.284 mm ⁻¹
F(000)	380
Crystal size	0.20 x 0.15 x 0.15 mm ³
Theta range for data collection	1.976 to 26.815°.
Index ranges	-10 ≤ h ≤ 8, -11 ≤ k ≤ 11, -13 ≤ l ≤ 14
Reflections collected	10875
Independent reflections	3085 [R(int) = 0.0402]
Completeness to theta = 25.242°	99.2 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9485 and 0.8163
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3085 / 0 / 226
Goodness-of-fit on F ²	1.107
Final R indices [I > 2sigma(I)]	R1 = 0.0439, wR2 = 0.1125
R indices (all data)	R1 = 0.0489, wR2 = 0.1165
Extinction coefficient	n/a
Largest diff. peak and hole	0.434 and -0.611 e.Å ⁻³