Synthesis

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Supporting Information

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Supporting Information

$Cu(OAc)_2$-Mediated Synthesis of Sulfonyl 2-Aryl-2*H*-chromenes

Meng-Yang Chang,*[a,b] Yu-Hsin Chen[a] and Han-Yu Chen[a]

[a]*Department of Medicinal and Applied Chemistry, Kaohsiung Medical University, Kaohsiung 807, Taiwan* [b]*Department of Medical Research, Kaohsiung Medical University Hospital, Kaohsiung 807, Taiwan*

*Corresponding authors: mychang@kmu.edu.tw

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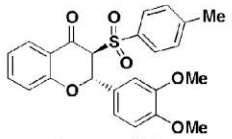
Compound 4a (^{1}H-NMR spectral data)

HAK1A1

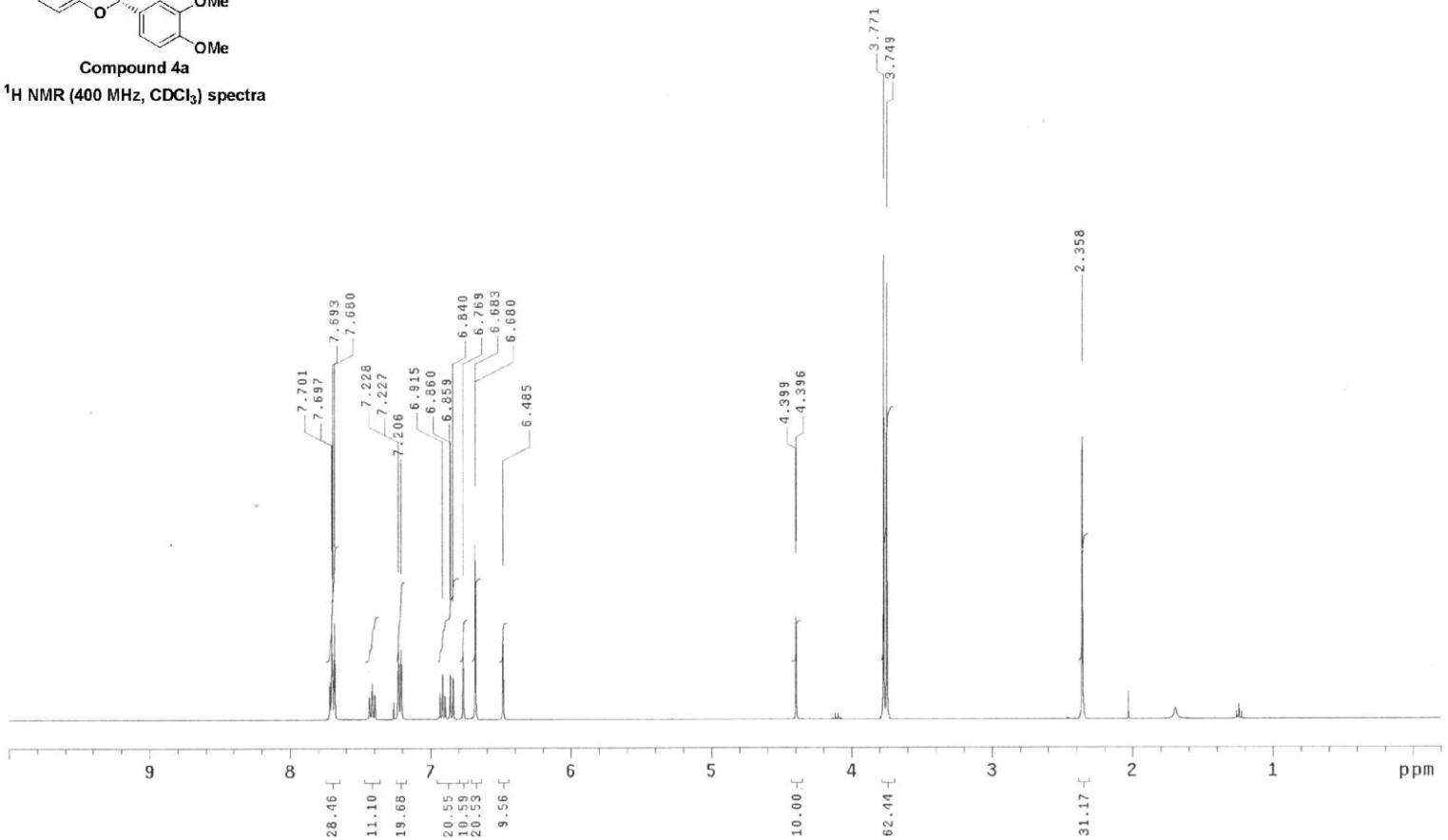
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Nov 8 2017
Solvent: CDCl3
Ambient temperature
Total 32 repetitions



Compound 4a

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

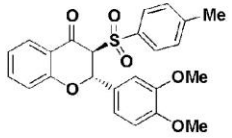


Compound 4a (^{13}C-NMR spectral data)

HAK1A1

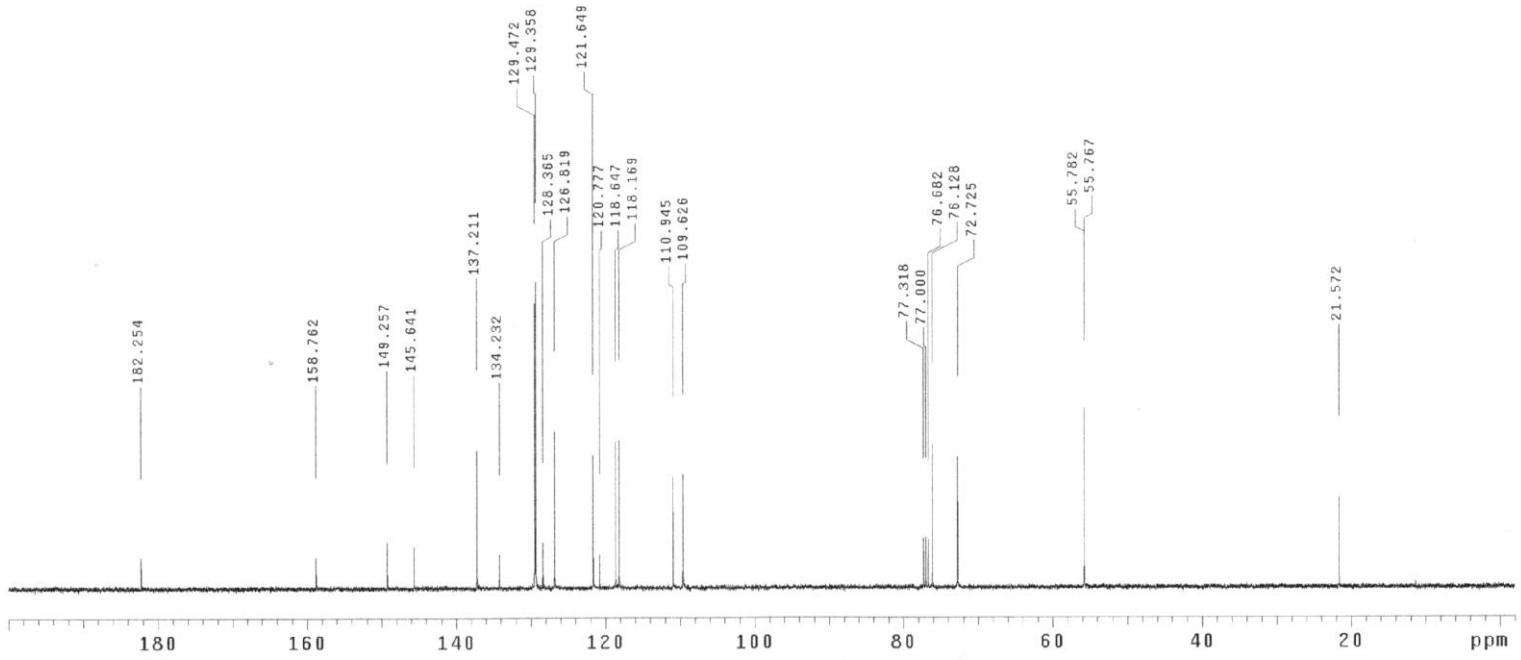
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Nov 8 2017
Solvent: CDCl3
Ambient temperature
Total 480 repetitions



Compound 4a

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

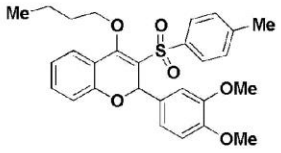


Compound 6a (^{1}H-NMR spectral data)

HA1K1Bu

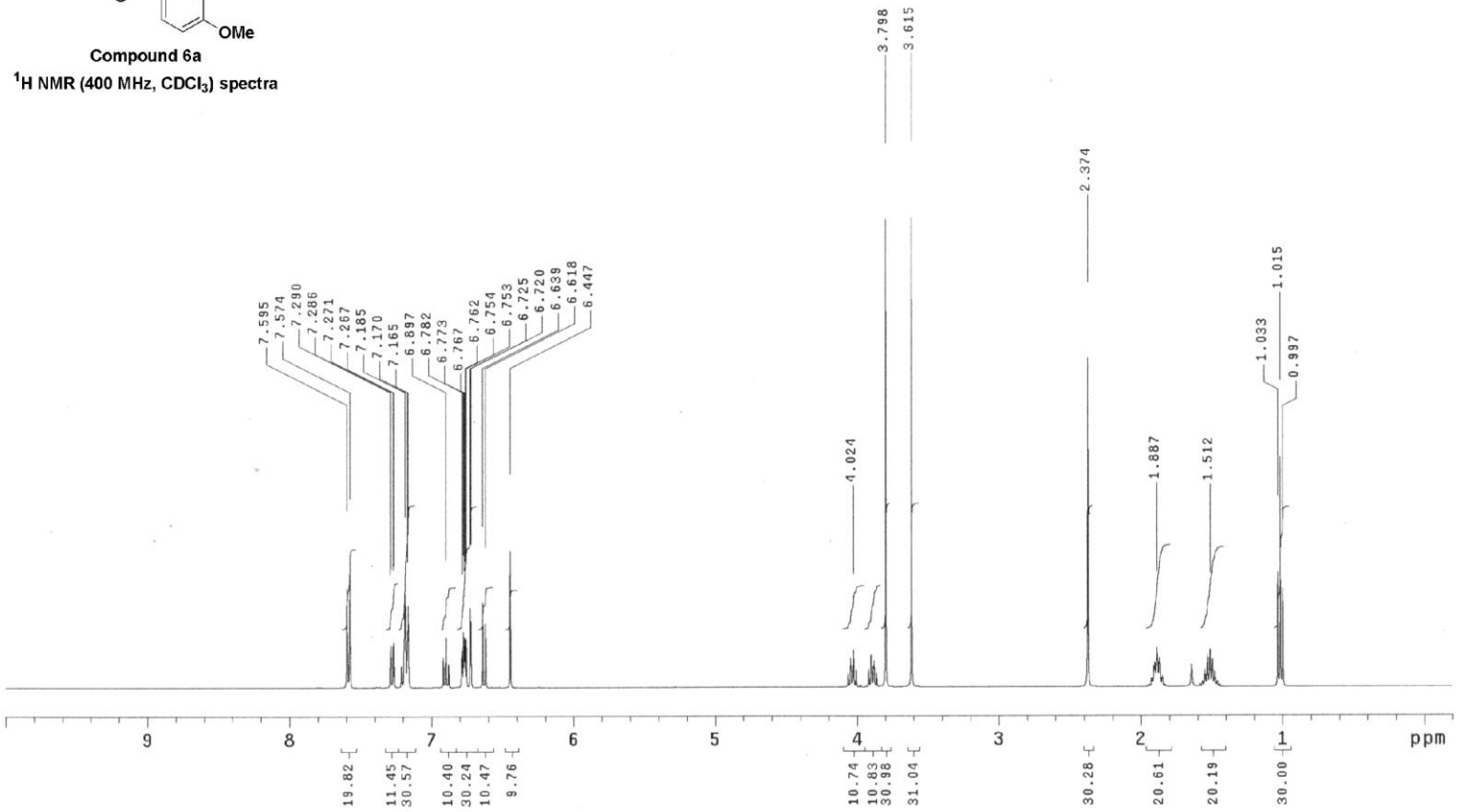
Pulse Sequence: s2pul

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



Compound 6a

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

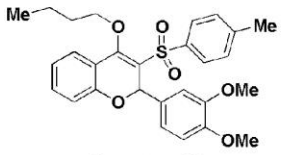


Compound 6a (^{13}C-NMR spectral data)

HA1K1Bu

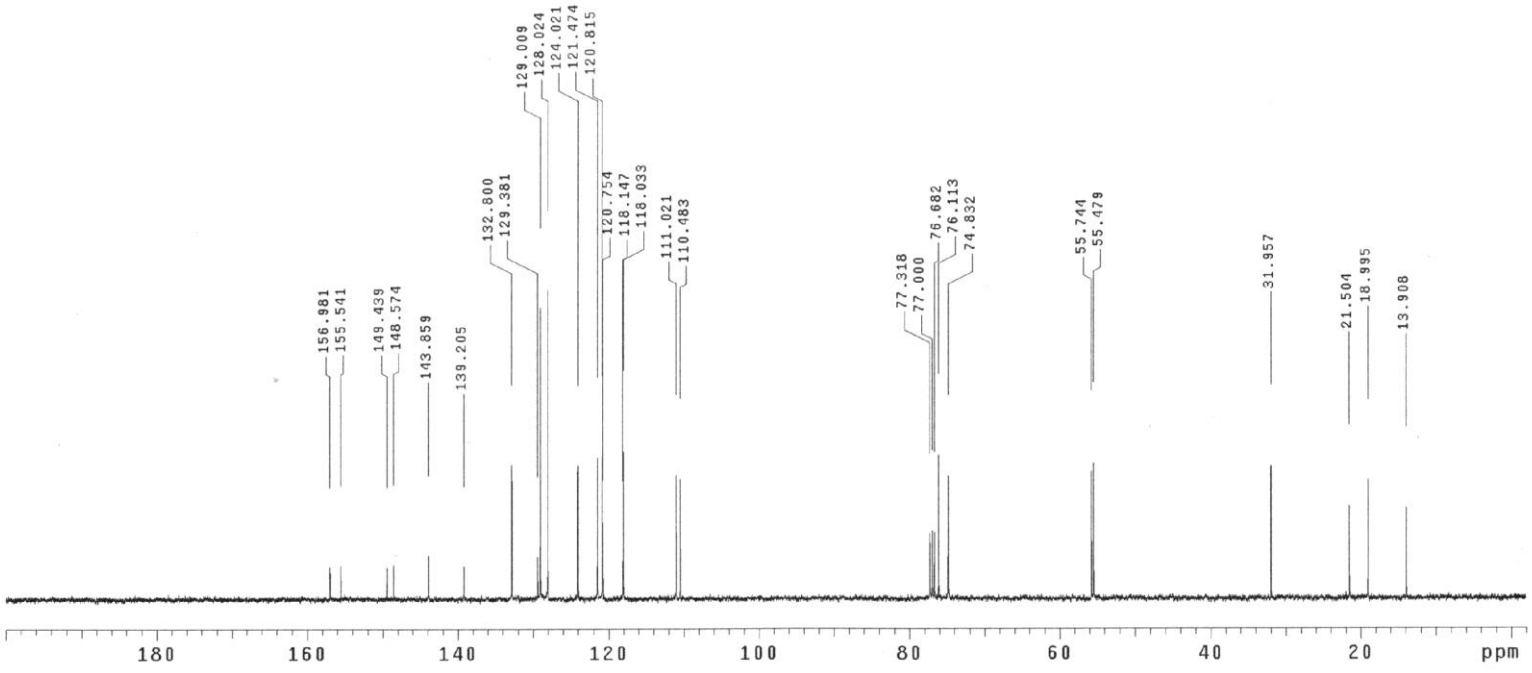
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Dec 11 2017
Solvent: CDCl3
Ambient temperature
Total 448 repetitions

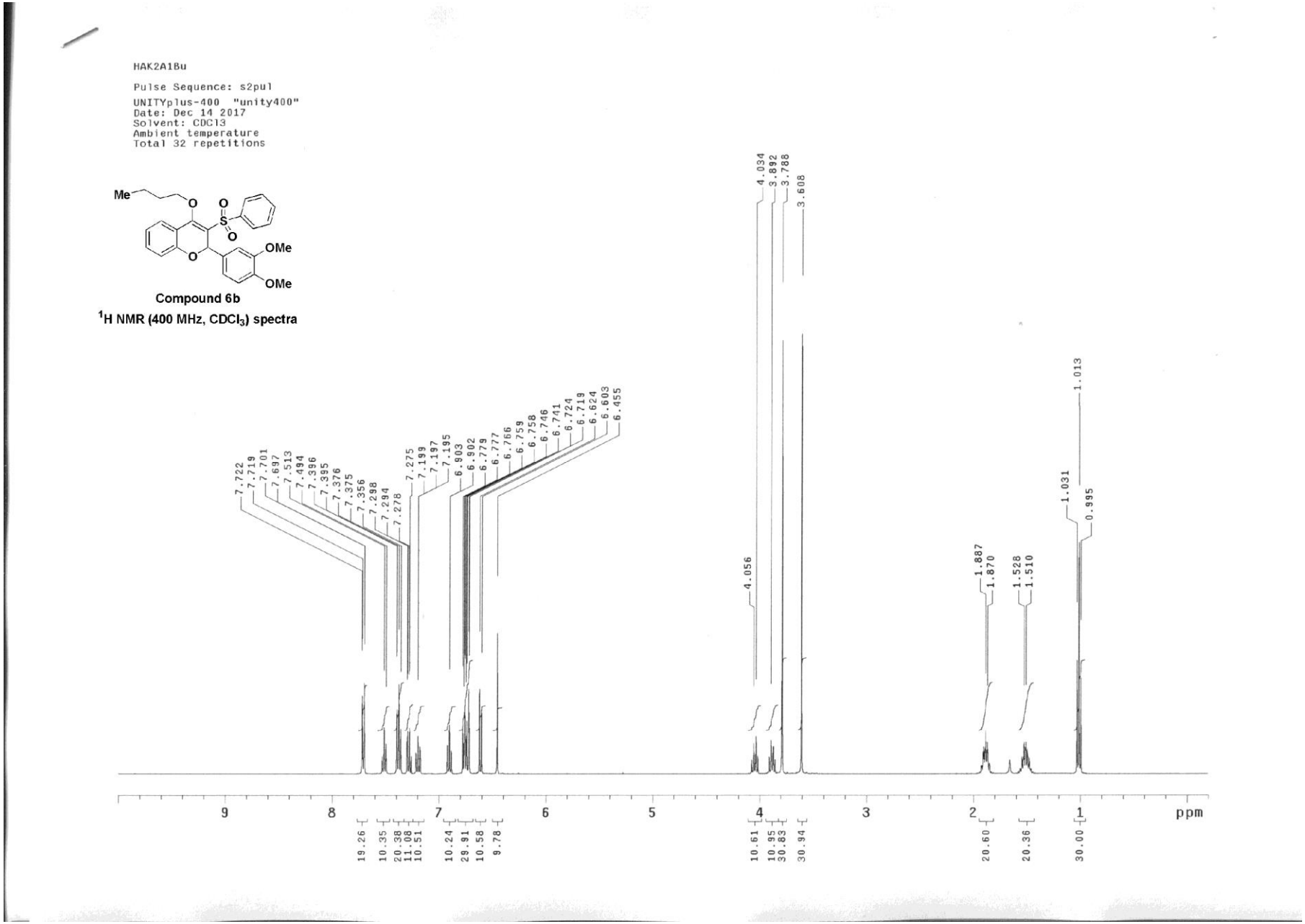


Compound 6a

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



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



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

HAK2A1Bu

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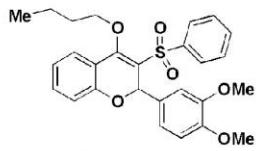
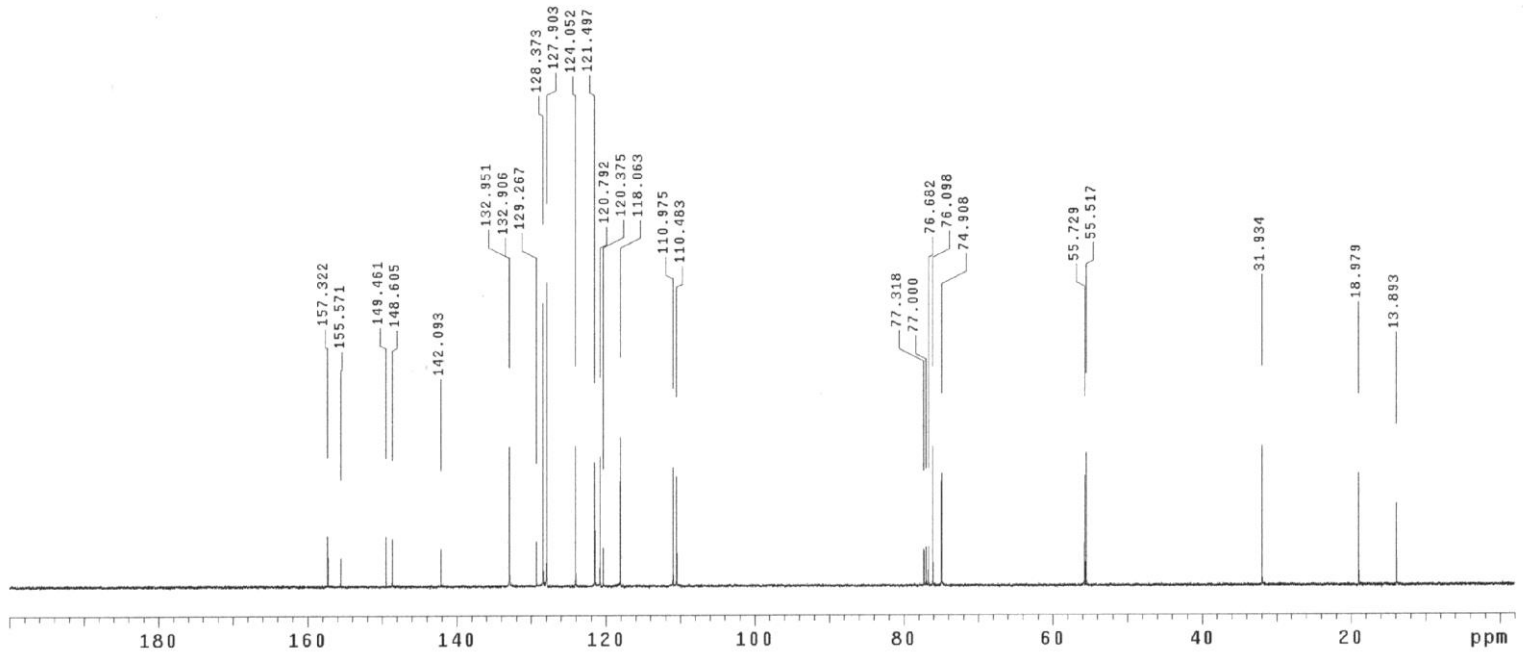
Date: Dec 14 2017
Solvent: CDCl3
Ambient temperature
Total 736 repetitions

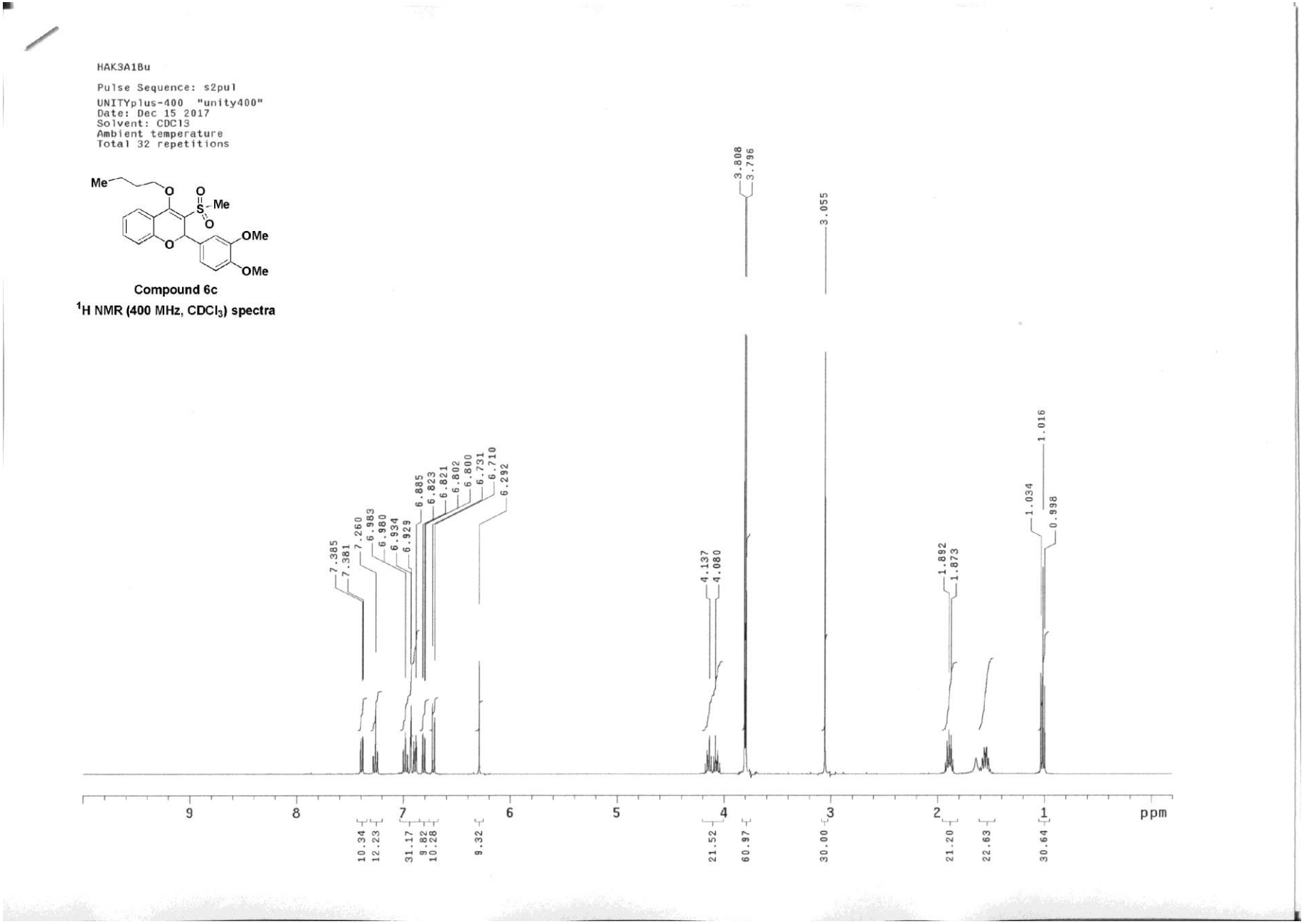


Compound 6b

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



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

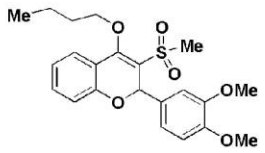


Compound 6c (^{13}C-NMR spectral data)

HAK3A1Bu

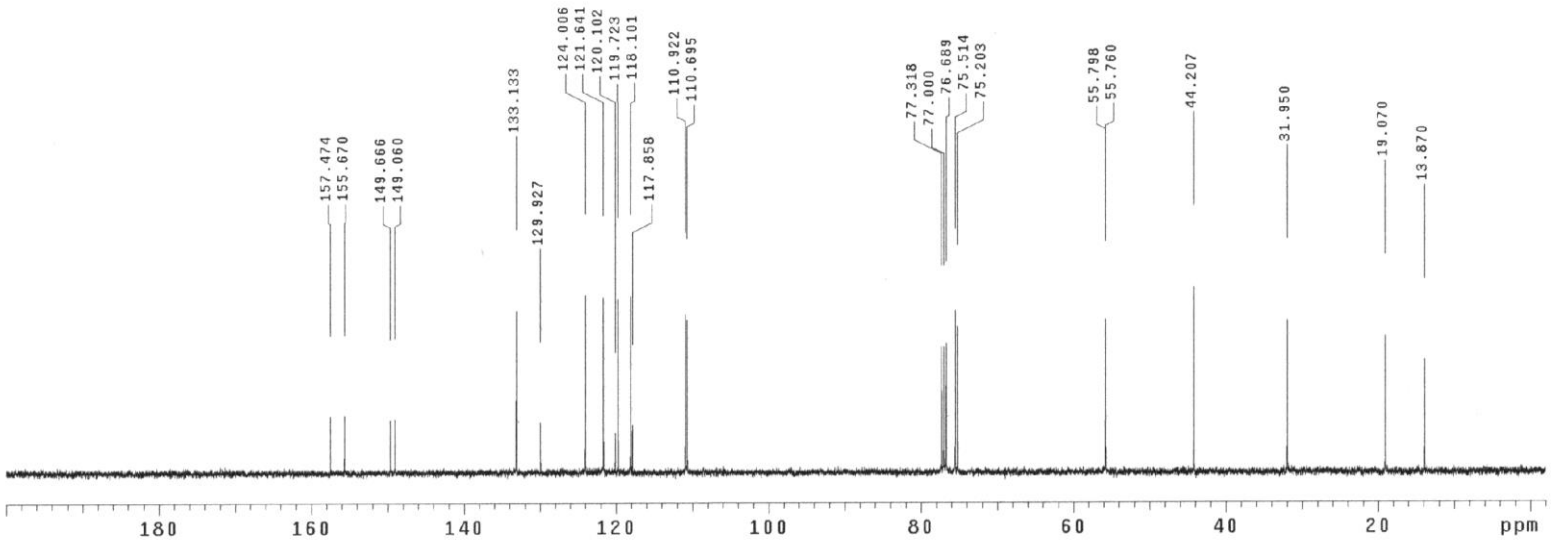
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Dec 15 2017
Solvent: CDCl3
Ambient temperature
Total 1904 repetitions

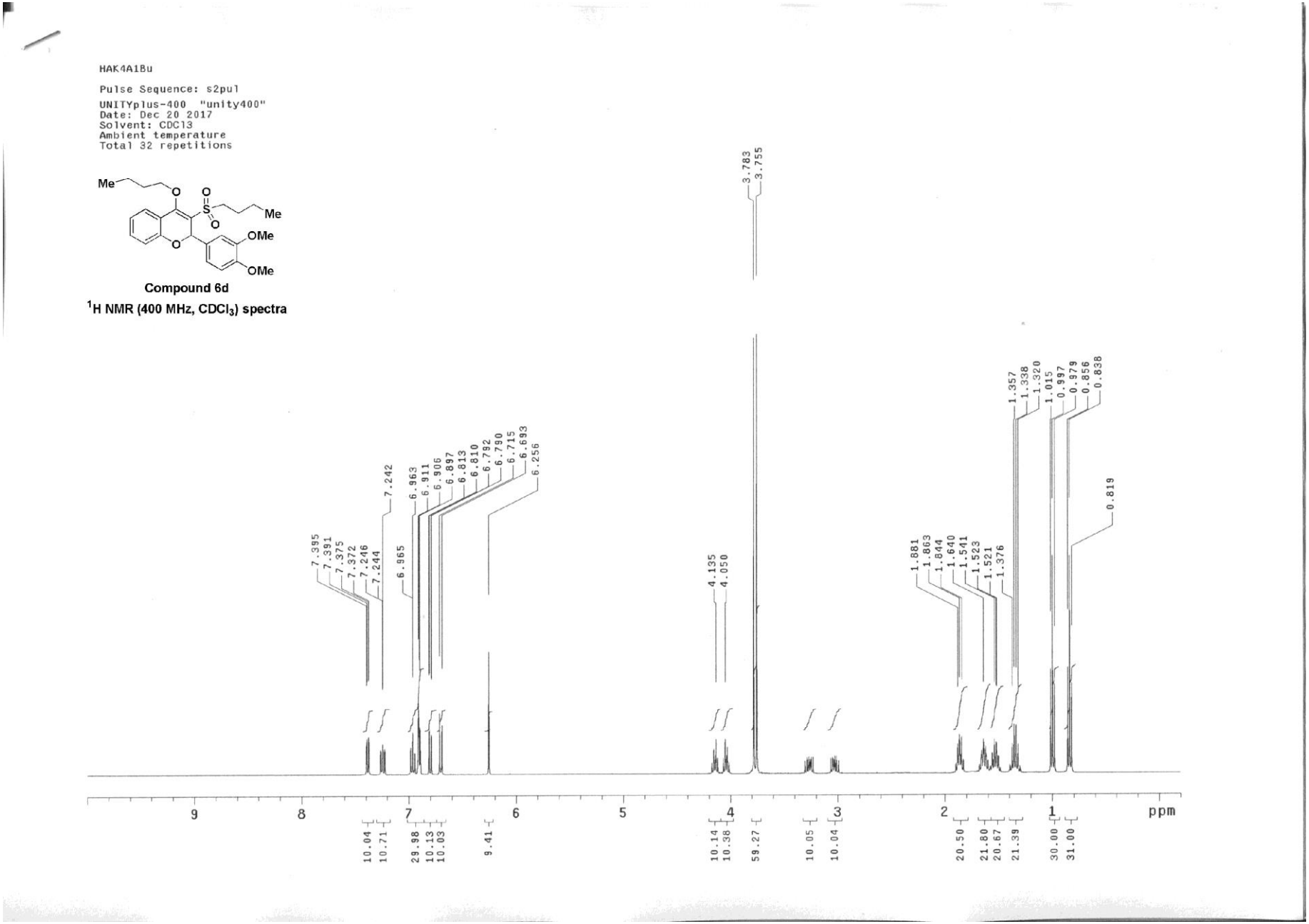


Compound 6c

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



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



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

HAK4A1Bu

Pulse Sequence: s2pul
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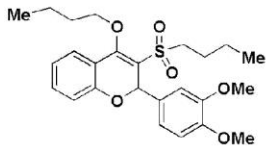
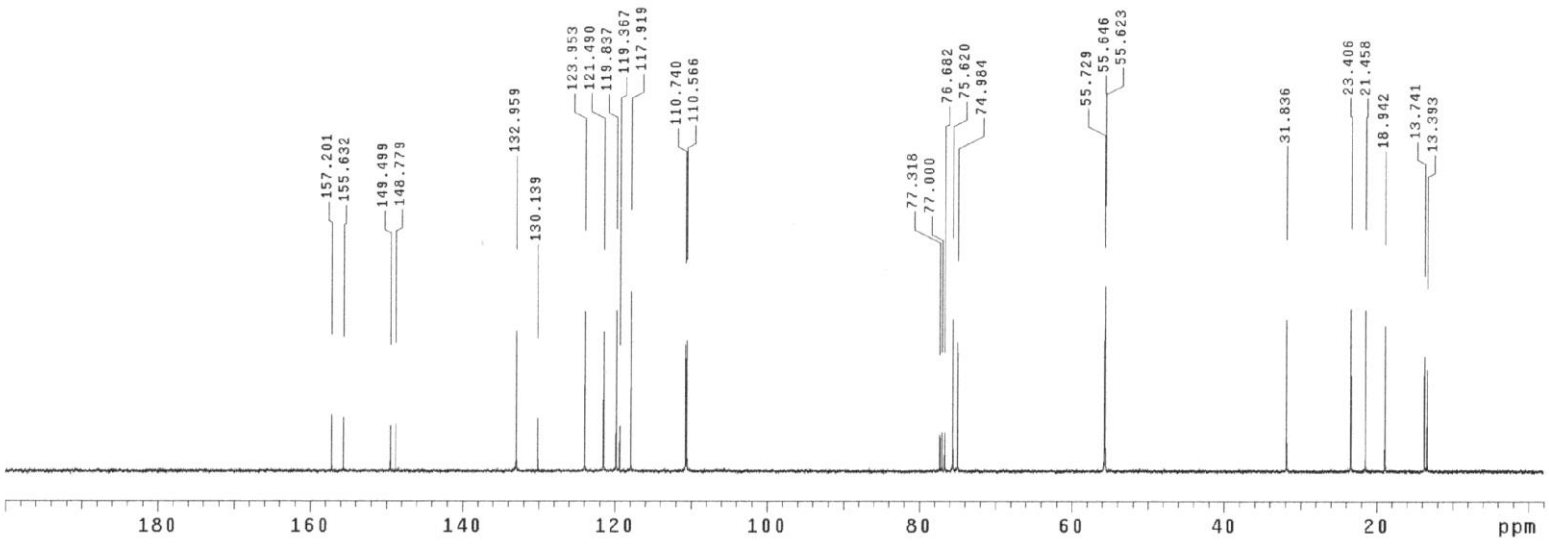
Date: Dec 20 2017
Solvent: CDCl3
Ambient temperature
Total 288 repetitions



Compound 6d

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



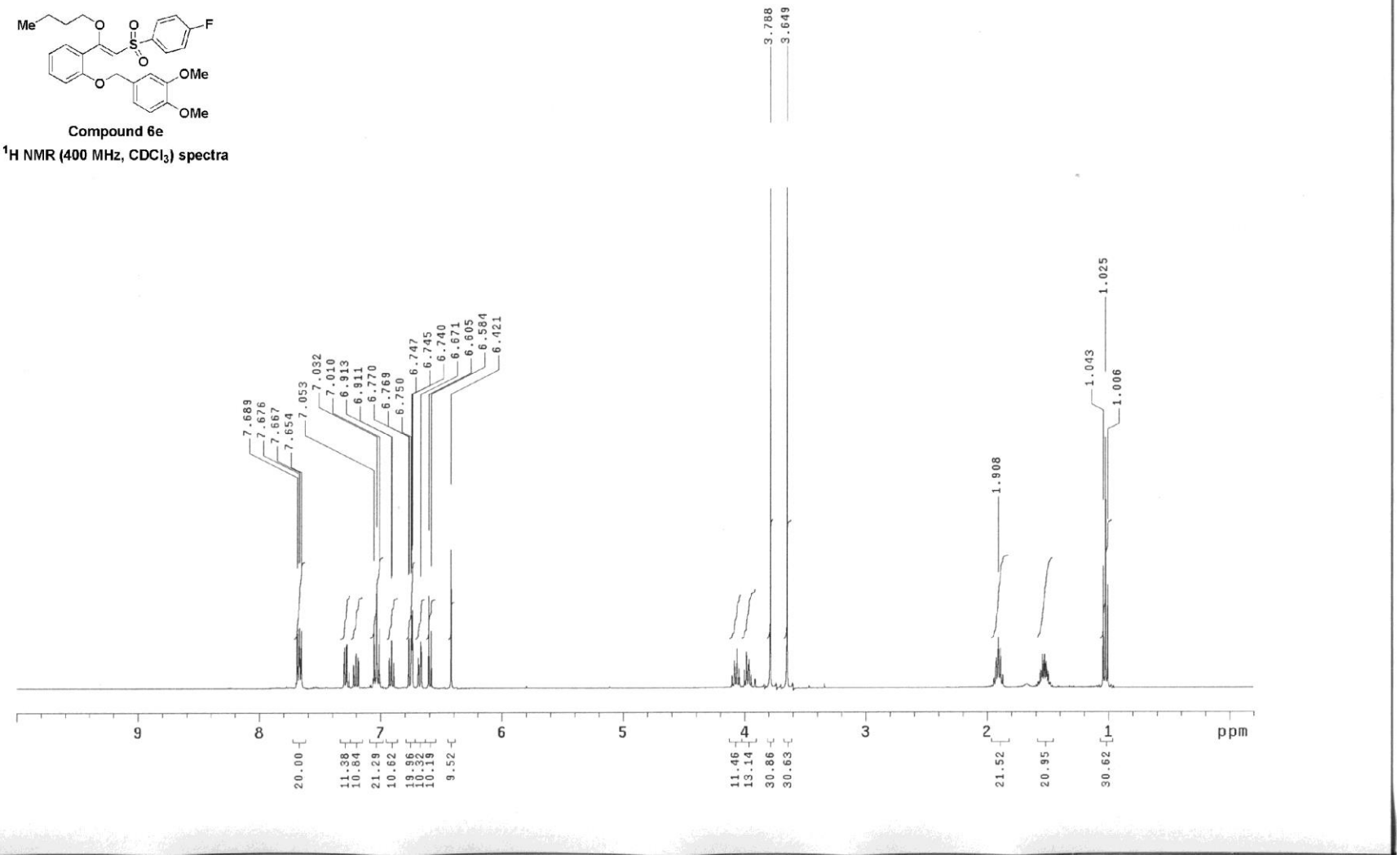
Compound 6e (^{1}H-NMR spectral data)

HAK5A1Bu

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Dec 27 2017
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

Compound 6e

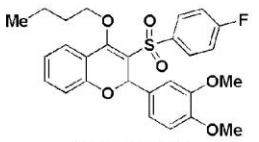
^{1}H NMR (400 MHz, $CDCl_3$) spectra



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

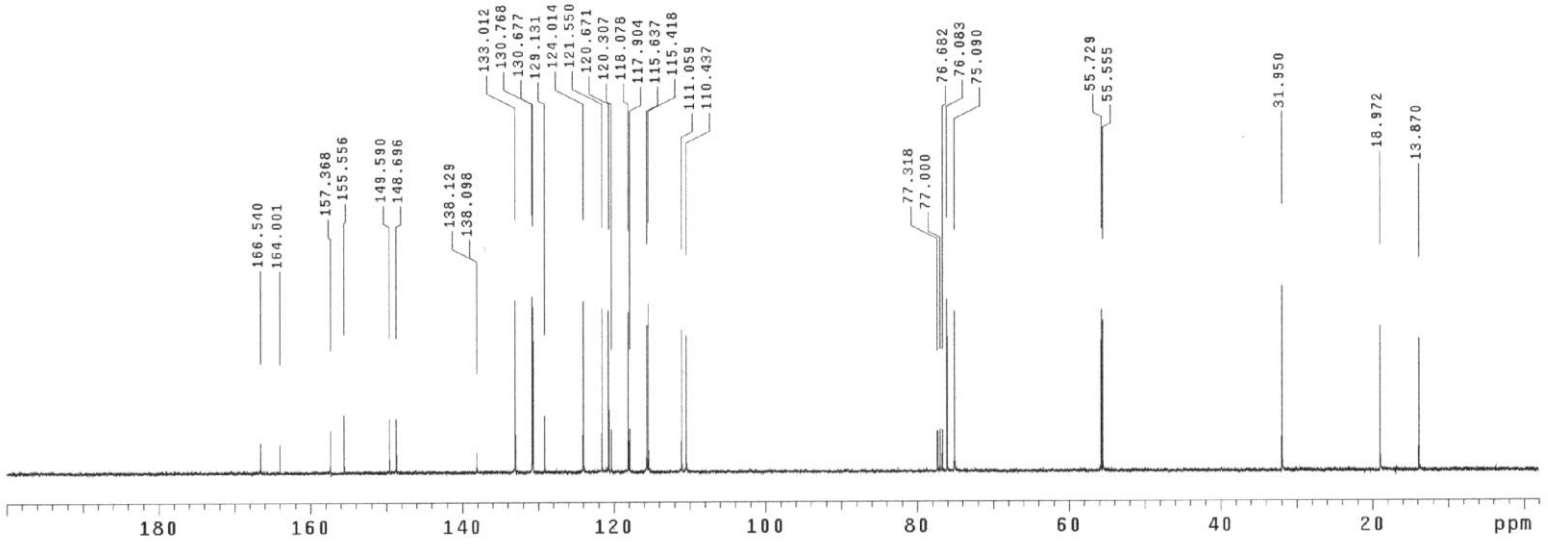
HAK5A1Bu

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Dec 27 2017
Solvent: CDCl3
Ambient temperature
Total 704 repetitions

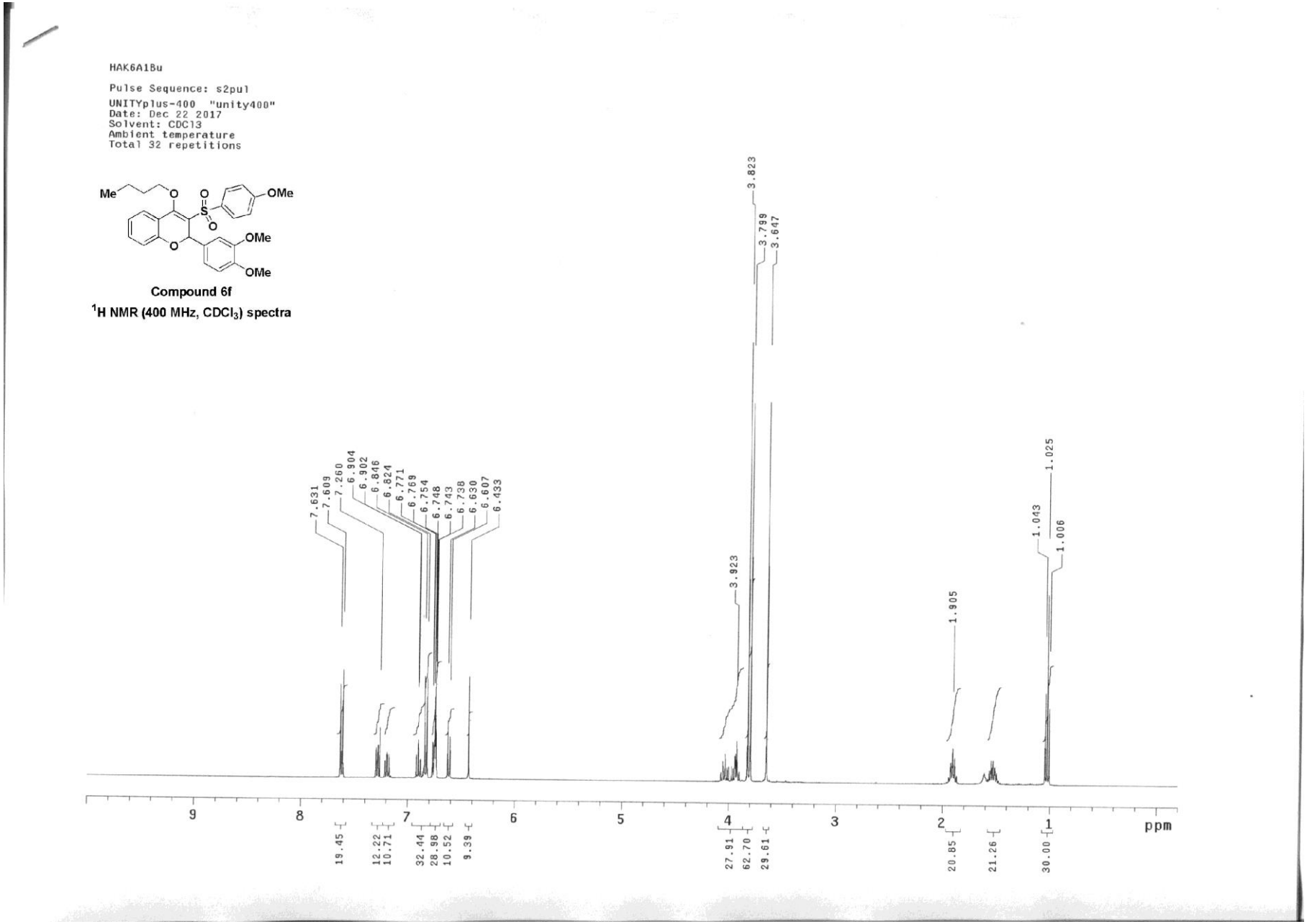


Compound 6e

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



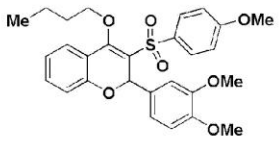
Compound 6f (^{1}H-NMR spectral data)



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

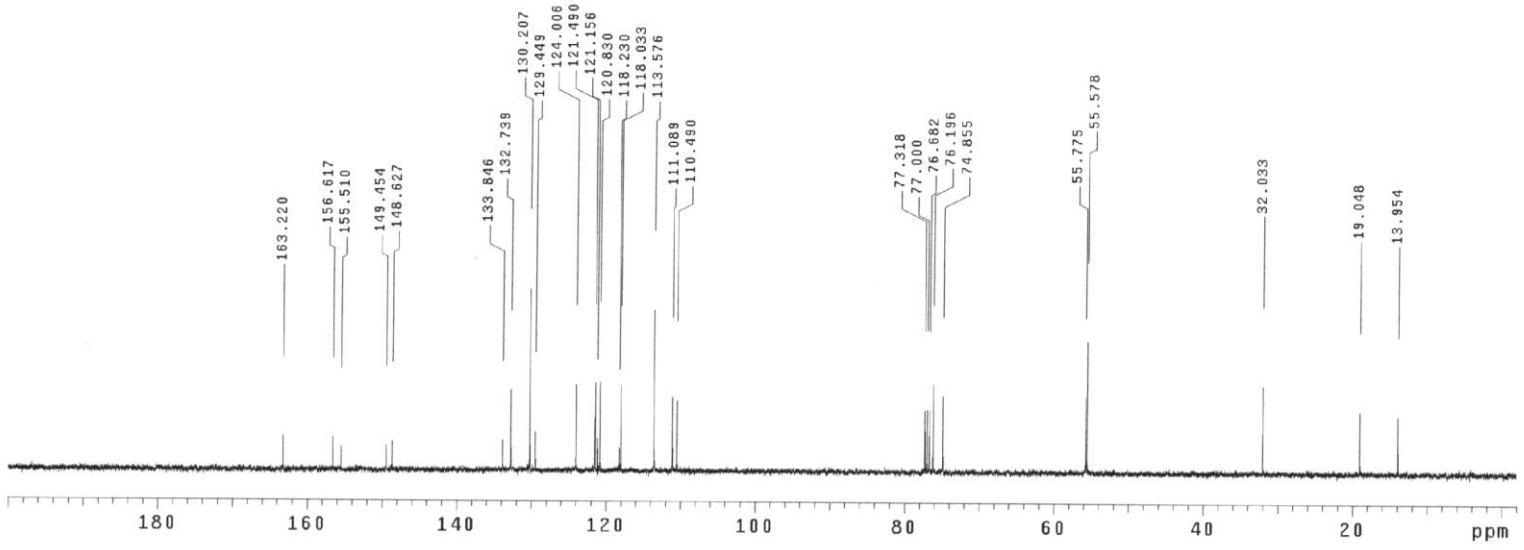
HAK6A1Bu

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Dec 22 2017
Solvent: CDCl3
Ambient temperature
Total 1056 repetitions



Compound 6f

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



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

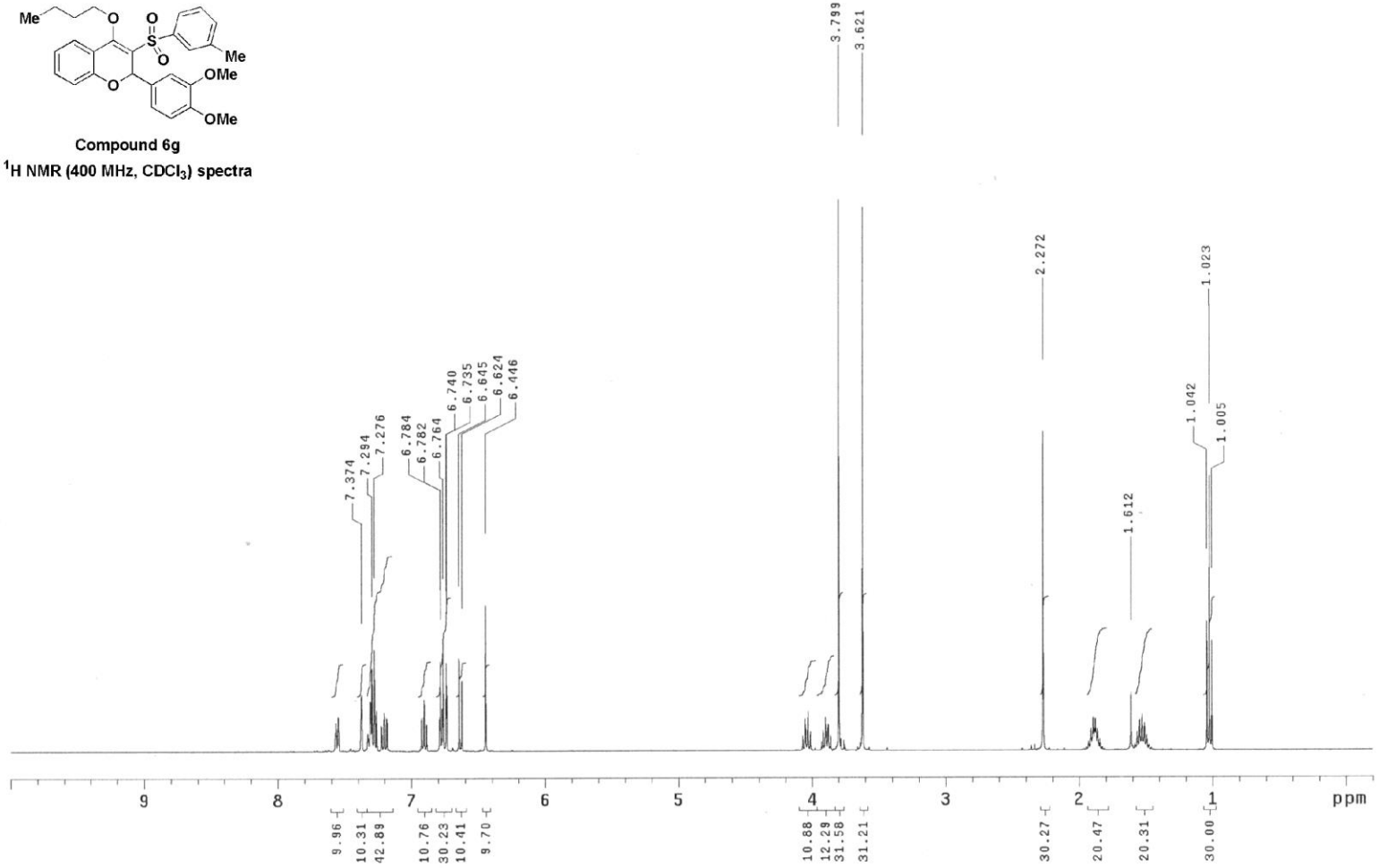
HAK1A7Bu

Pulse Sequence: s2pul

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

Compound 6g

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

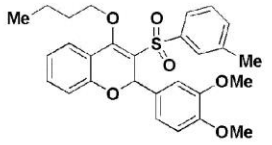


Compound 6g (^{13}C-NMR spectral data)

HAK1A7Bu

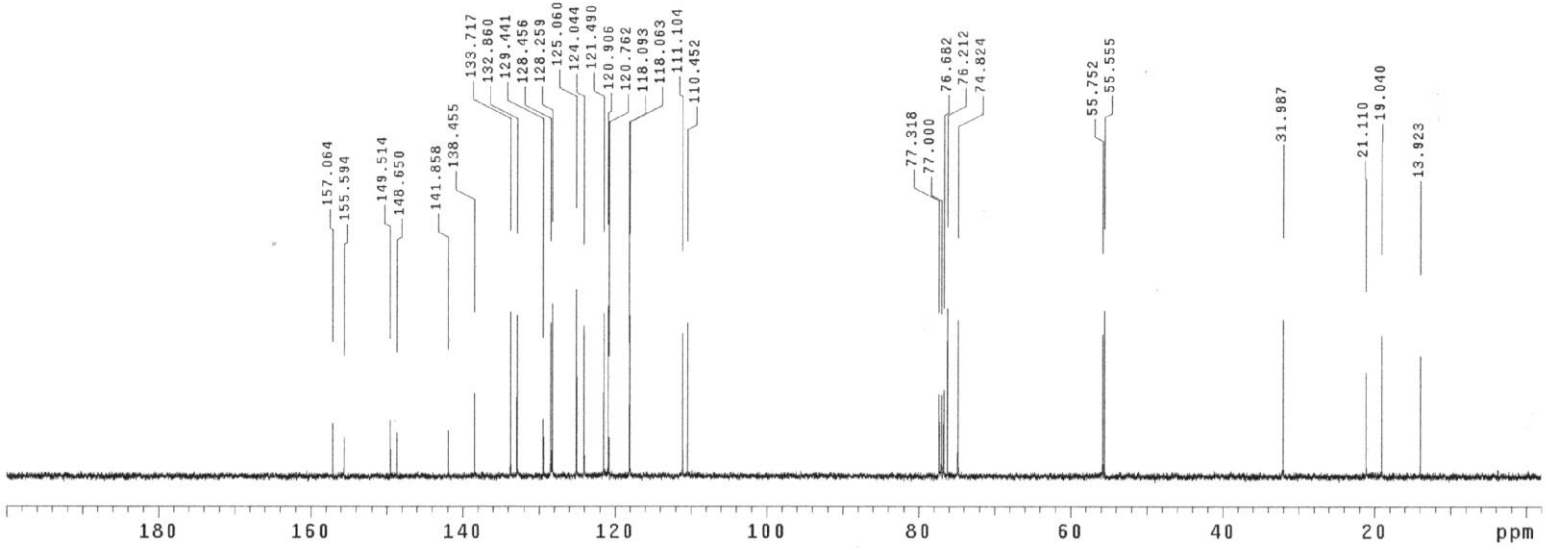
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Dec 28 2017
Solvent: CDCl3
Ambient temperature
Total 816 repetitions



Compound 6g

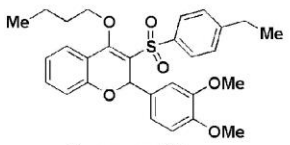
^{13}C NMR (100 MHz, $CDCl_3$) spectra



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

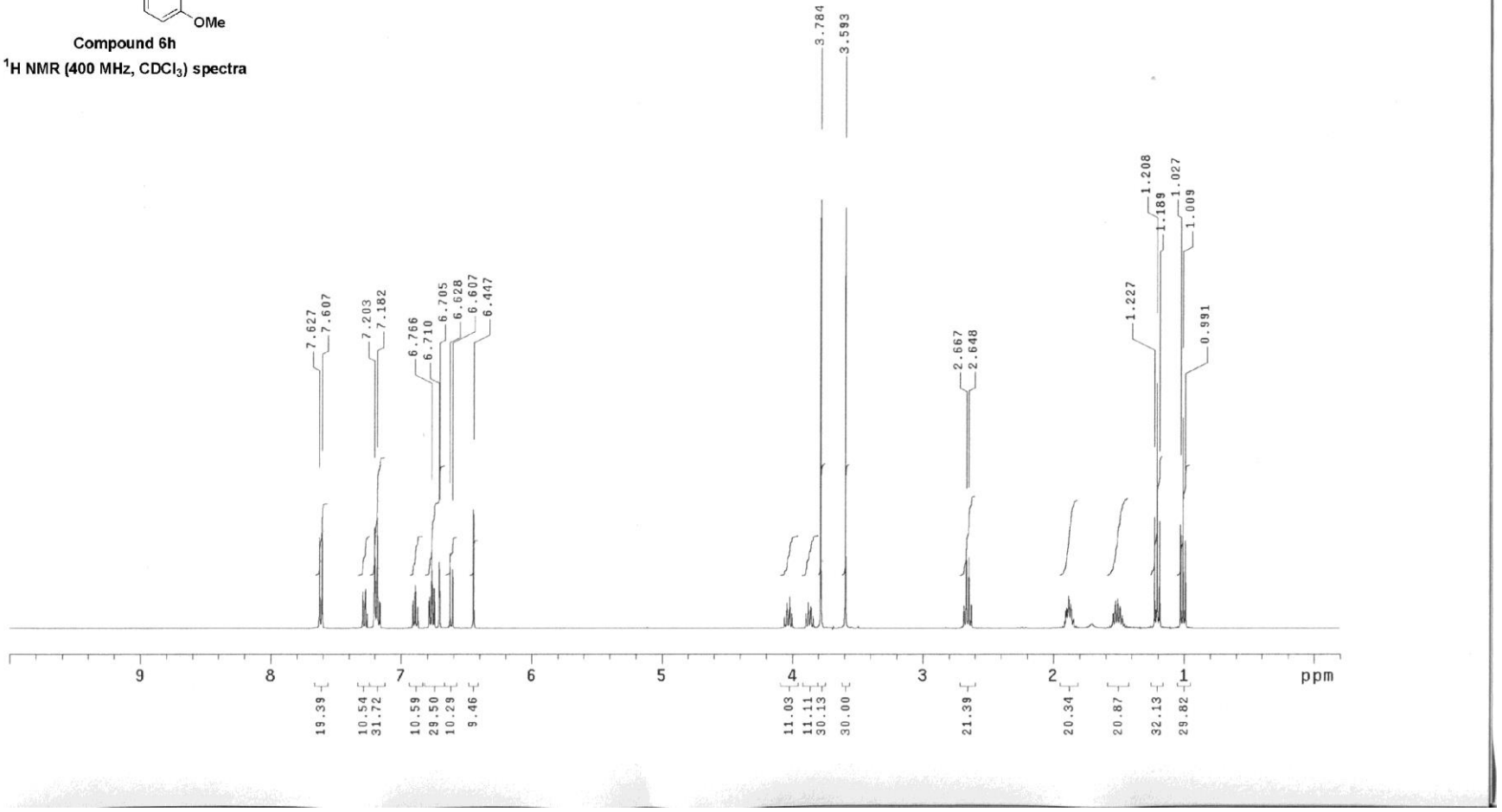
HAK1A8Bu

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Dec 26 2017
Solvent: CDCl3
Ambient temperature
Total 32 repetitions



Compound 6h

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



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

HAK1A8Bu

Pulse Sequence: s2pul
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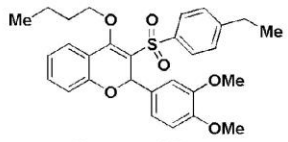
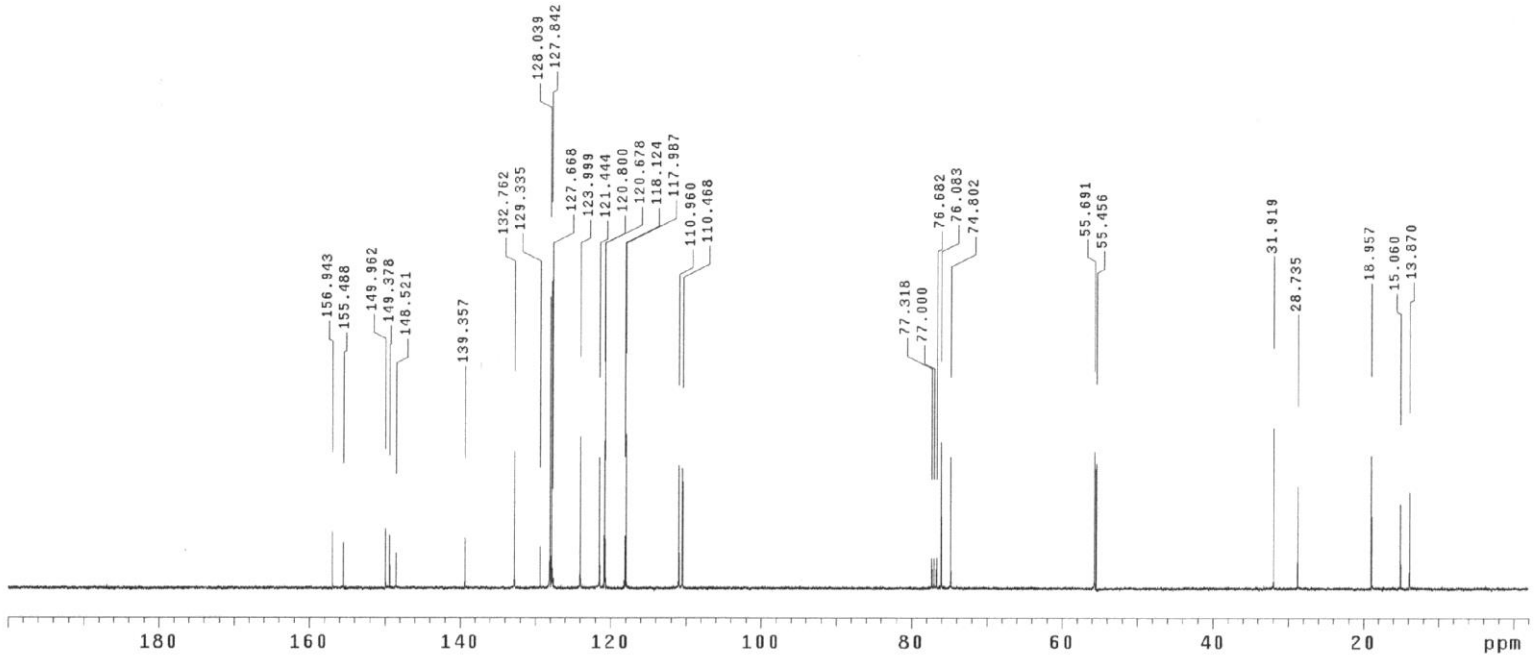
Date: Dec 26 2017
Solvent: CDCl3
Ambient temperature
Total 864 repetitions



Compound 6h

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

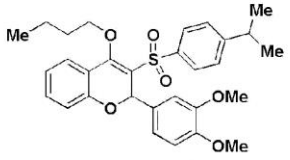


Compound 6i (^{1}H-NMR spectral data)

HAK9A1Bu

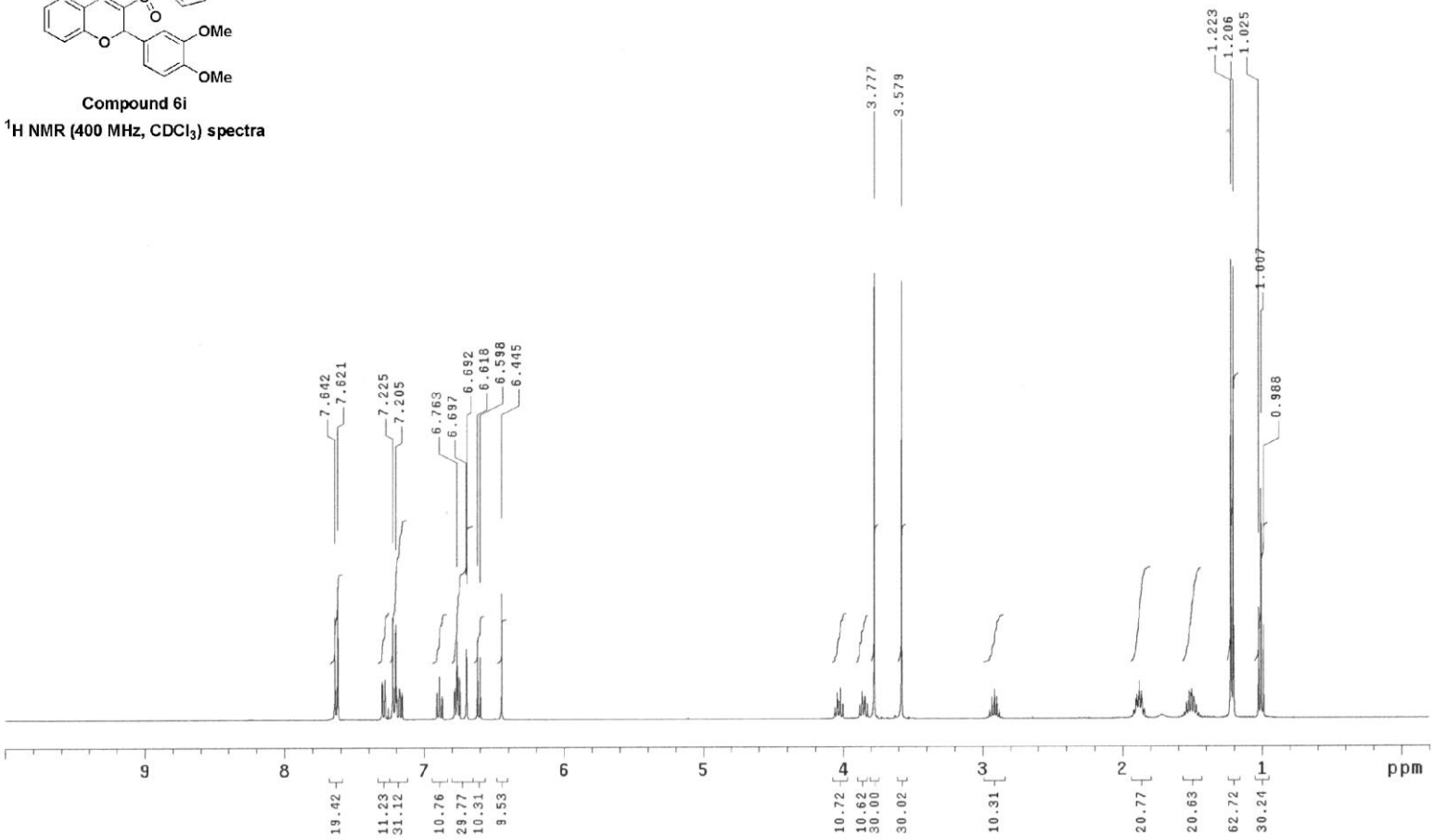
Pulse Sequence: s2pul

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



Compound 6i

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



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

HAK9A1Bu

Pulse Sequence: s2pul
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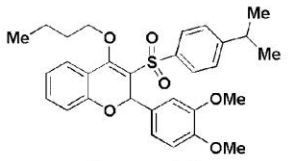
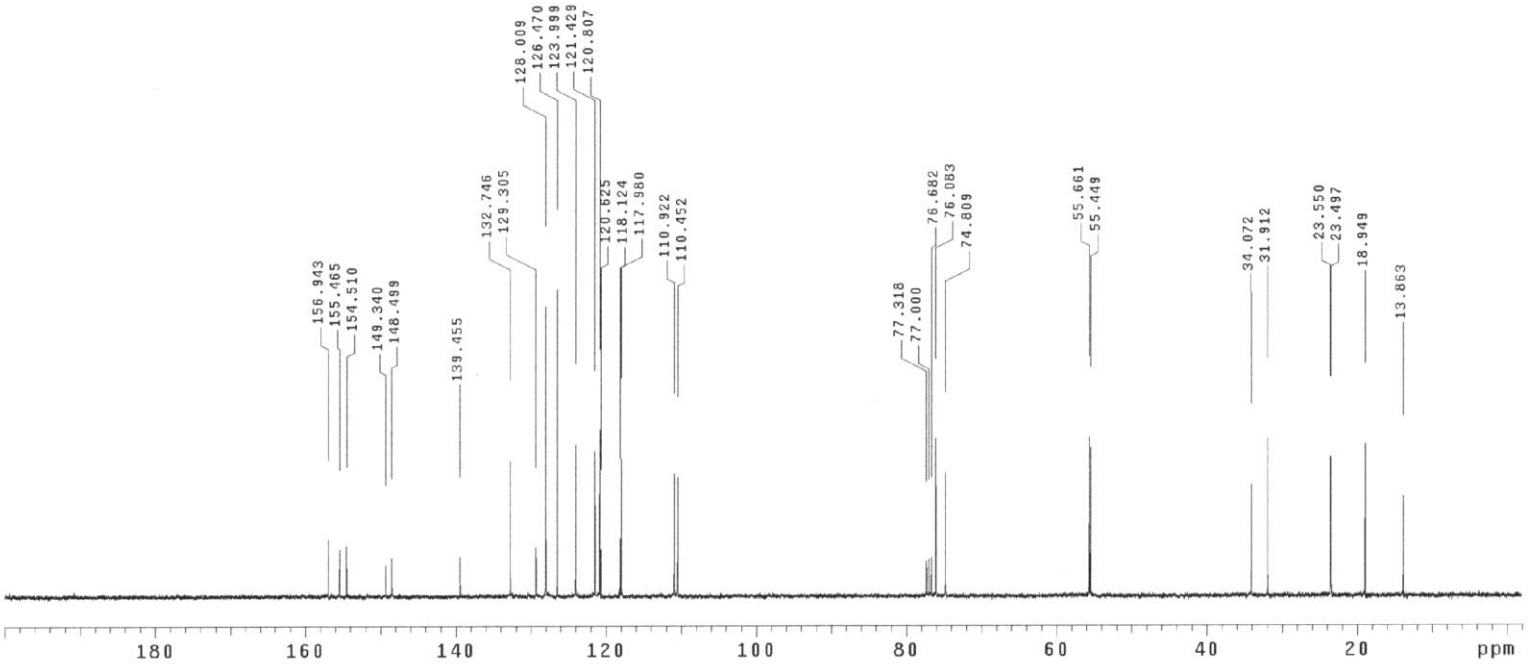
Date: Jan 5 2018
Solvent: CDCl3
Ambient temperature
Total 336 repetitions



Compound 6i

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



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

HAK10A1Bu

Pulse Sequence: s2pul

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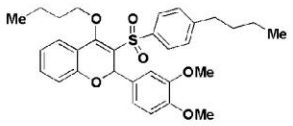
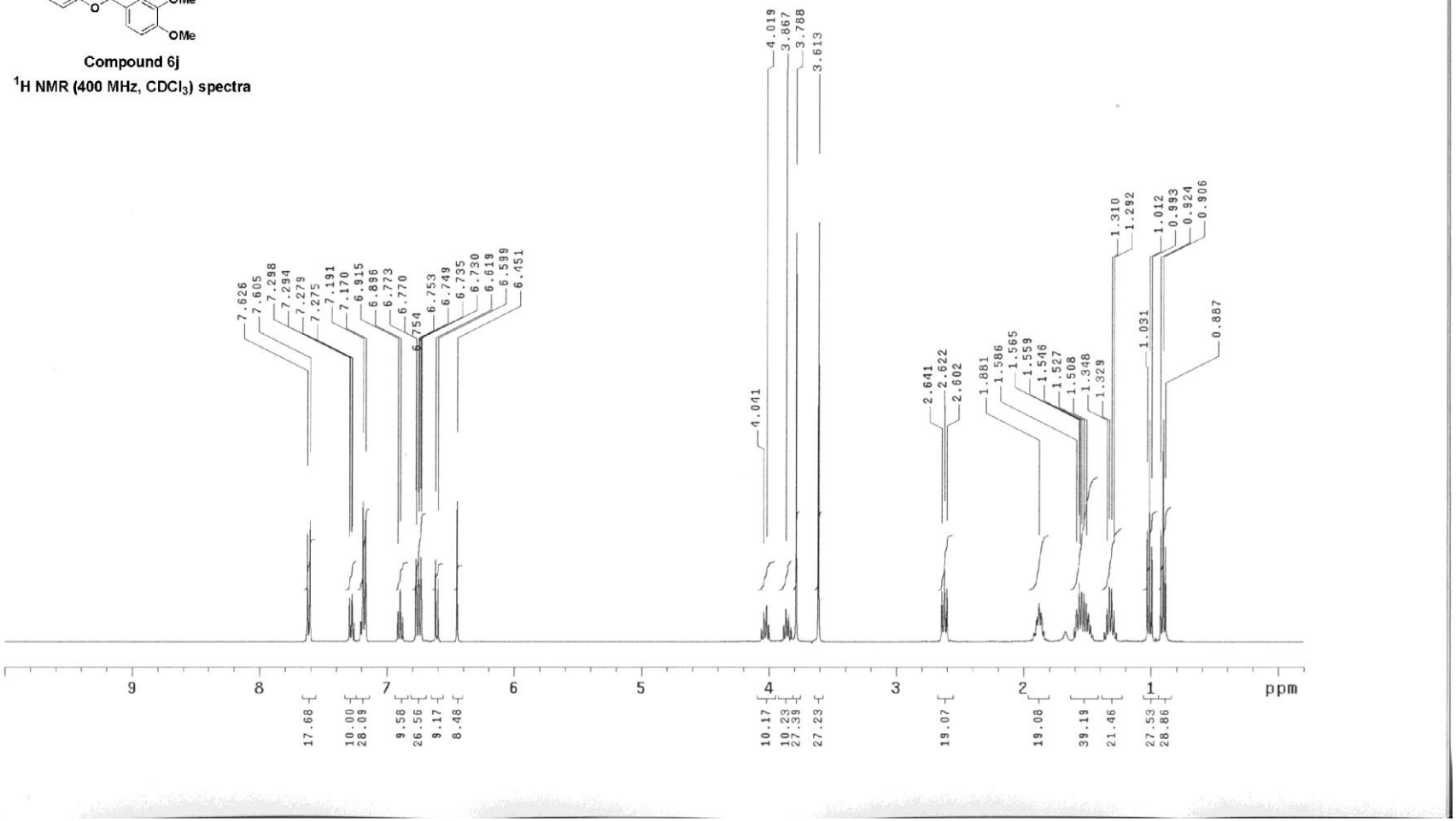
Date: Jan 8 2018
Solvent: CDCl3
Ambient temperature
Total 32 repetitions



Compound 6j

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



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

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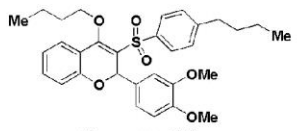
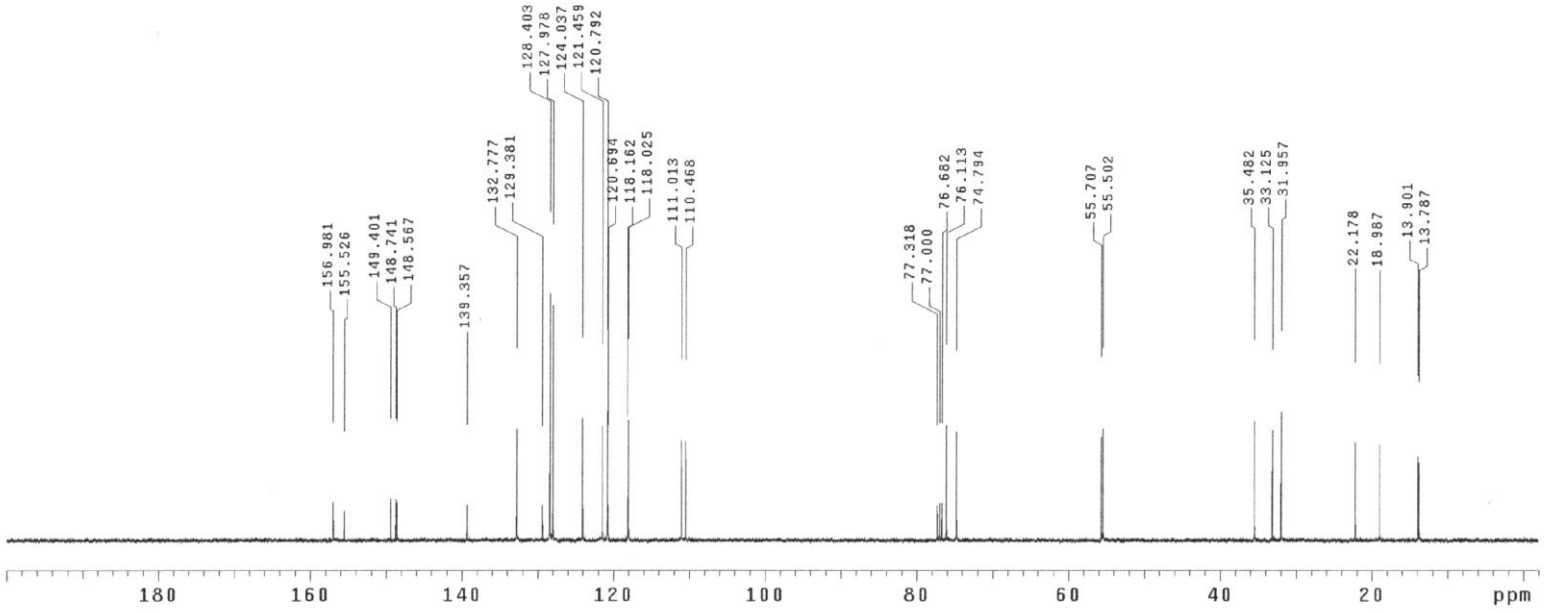
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jan 8 2018
Solvent: CDCl3
Ambient temperature
Total 608 repetitions

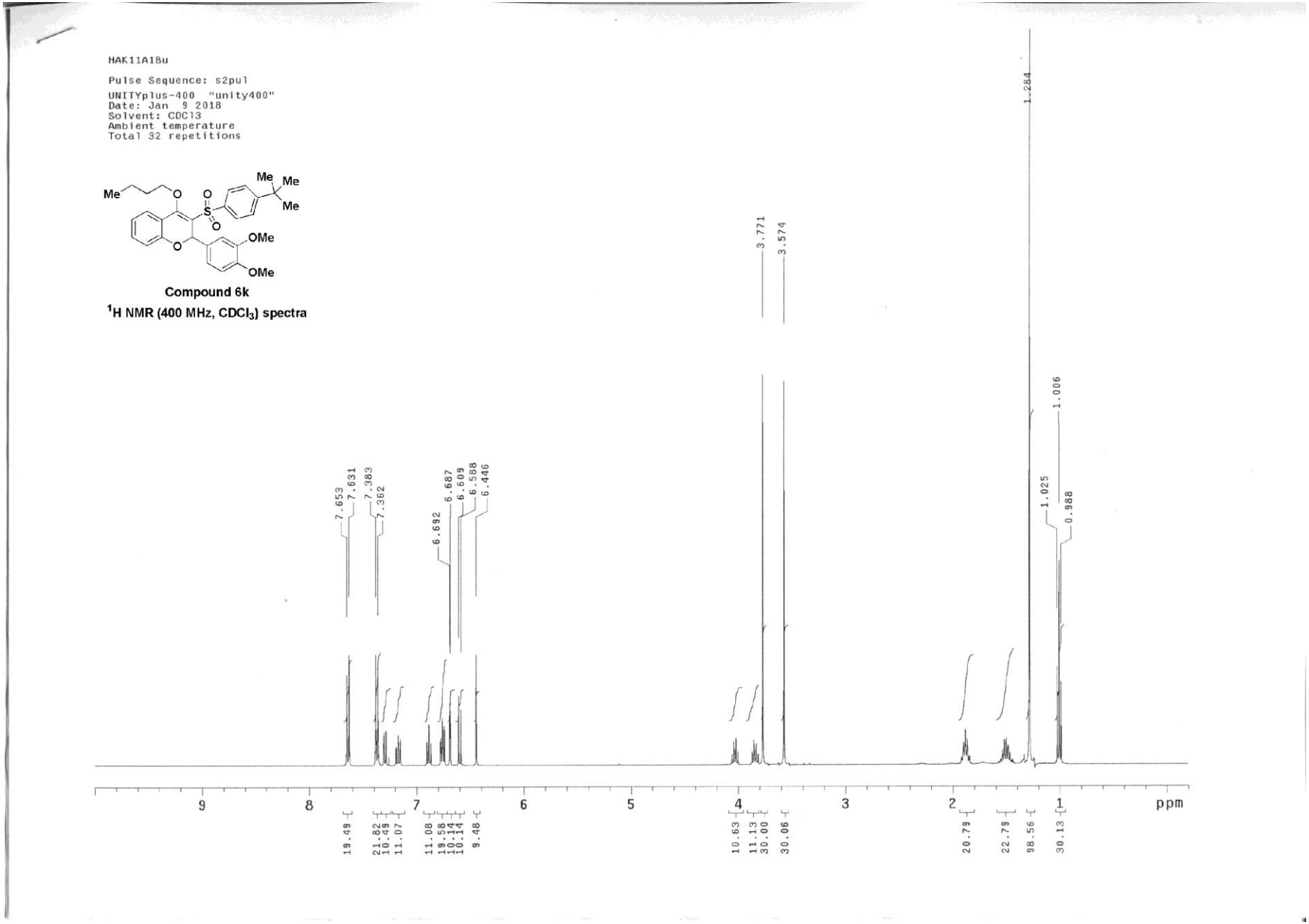


Compound 6j

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



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



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

HAK11A1Bu

Pulse Sequence: s2pul

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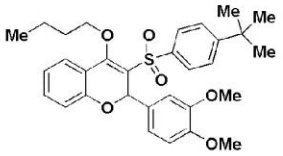
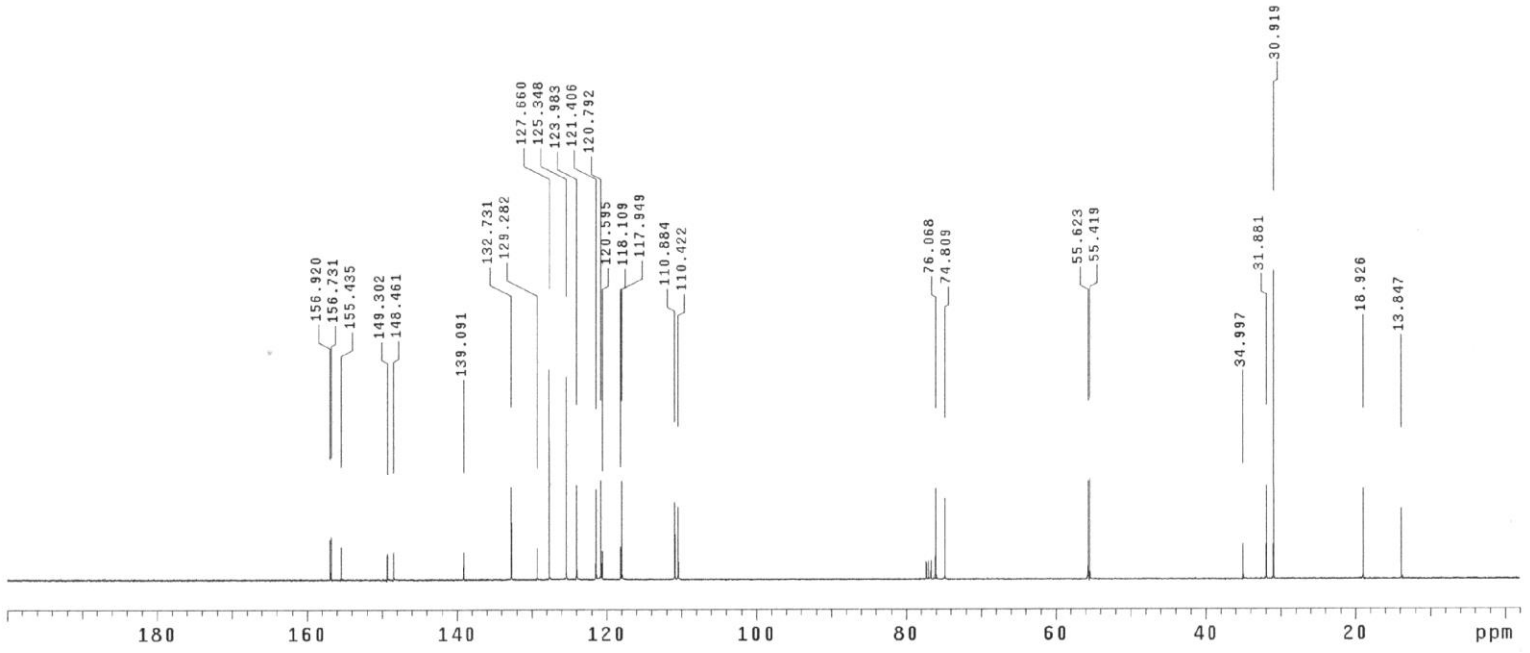
Date: Jan 9 2018
Solvent: CDCl3
Ambient temperature
Total 1136 repetitions



Compound 6k

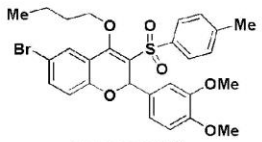
^{13}C NMR (100 MHz, $CDCl_3$) spectra



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

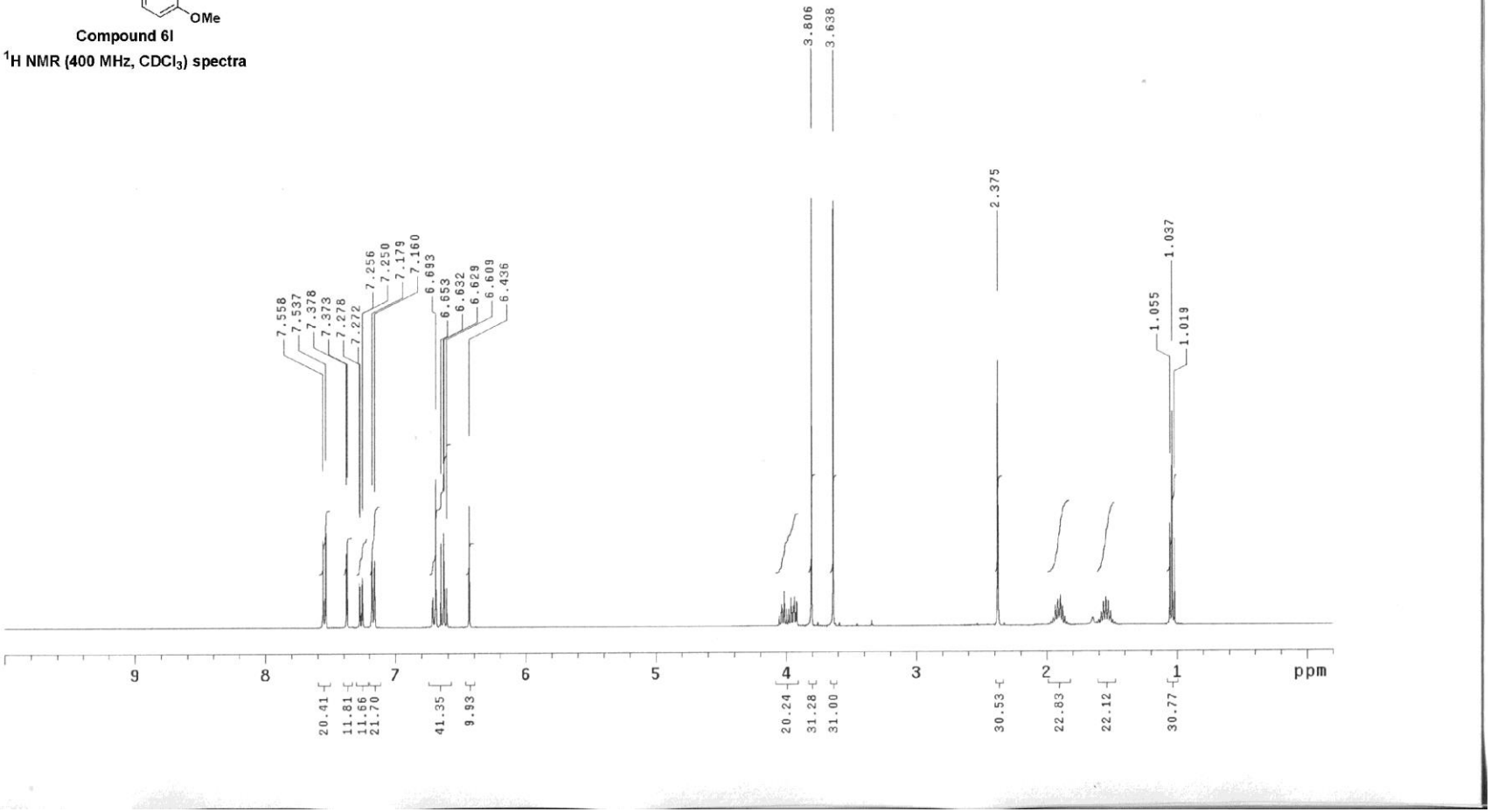
HAK12A1Bu

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Jan 11 2018
Solvent: CDCl3
Ambient temperature
Total 32 repetitions



Compound 6l

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



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

HAK12A1Bu

Pulse Sequence: s2pul
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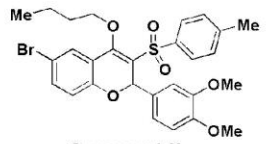
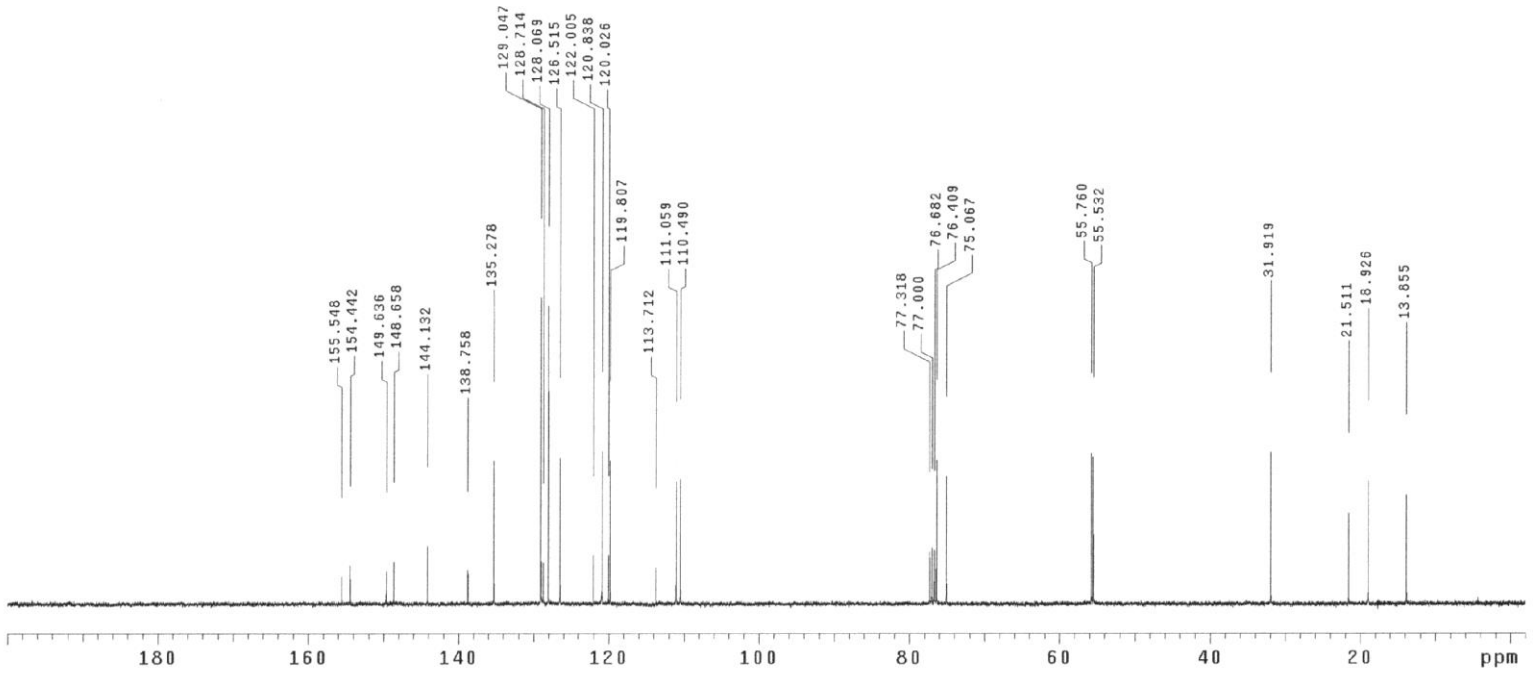
Date: Jan 11 2018
Solvent: CDCl3
Ambient temperature
Total 752 repetitions



Compound 6l

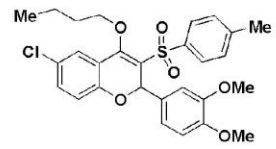
^{13}C NMR (100 MHz, $CDCl_3$) spectra



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

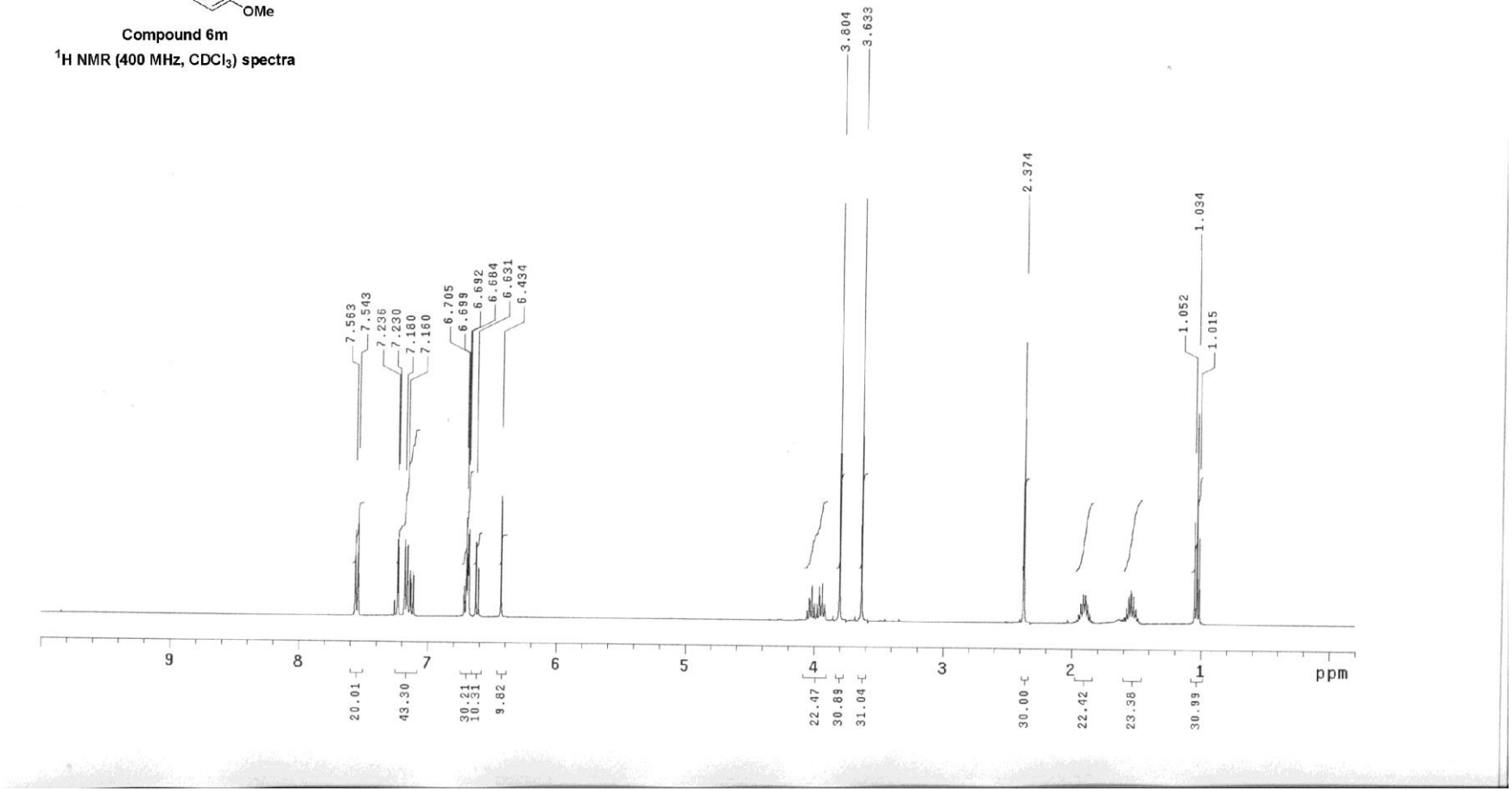
HAK13A1Bu

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Jan 15 2018
Solvent: CDCl3
Ambient temperature
Total 40 repetitions



Compound 6m

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

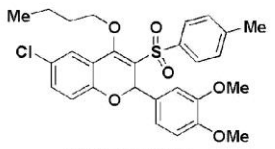


Compound 6m (^{13}C-NMR spectral data)

HAK13A1Bu

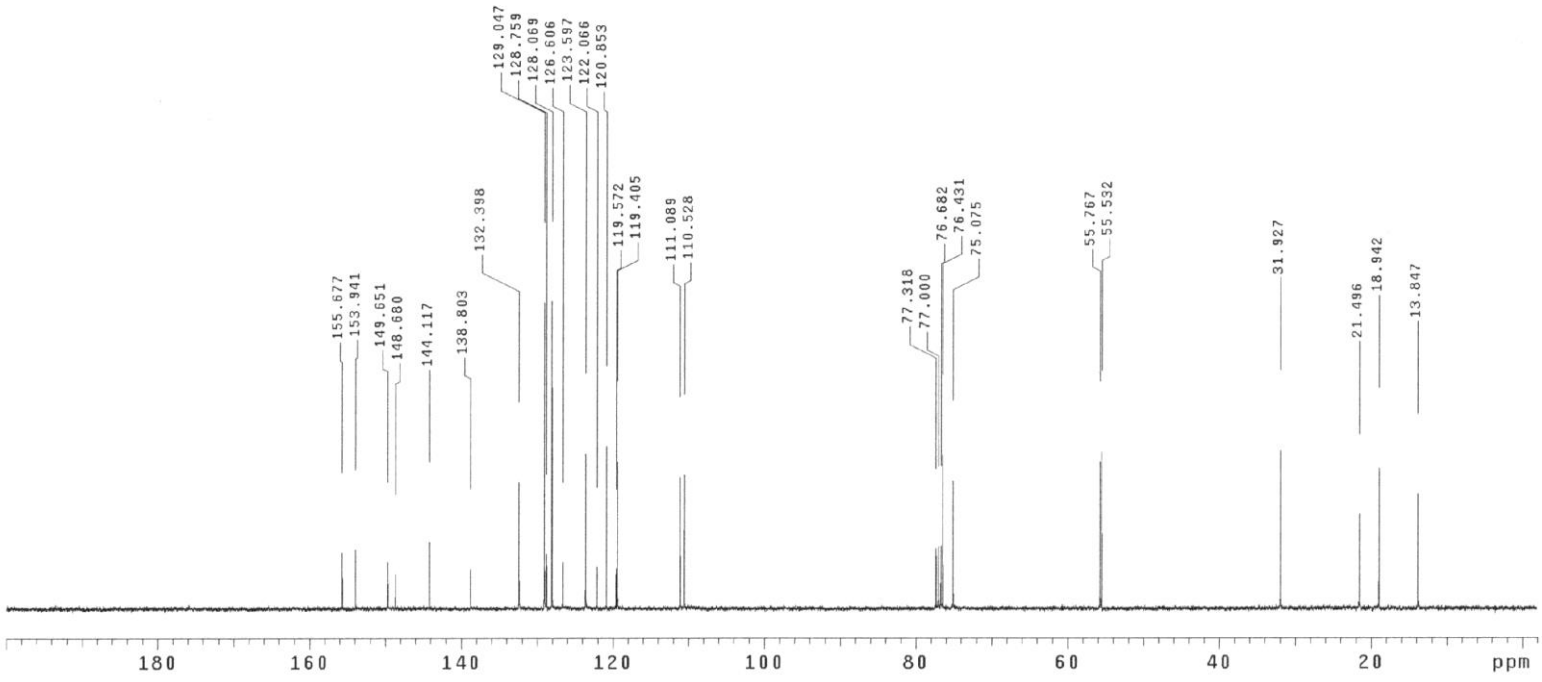
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jan 15 2018
Solvent: CDCl3
Ambient temperature
Total 752 repetitions



Compound 6m

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



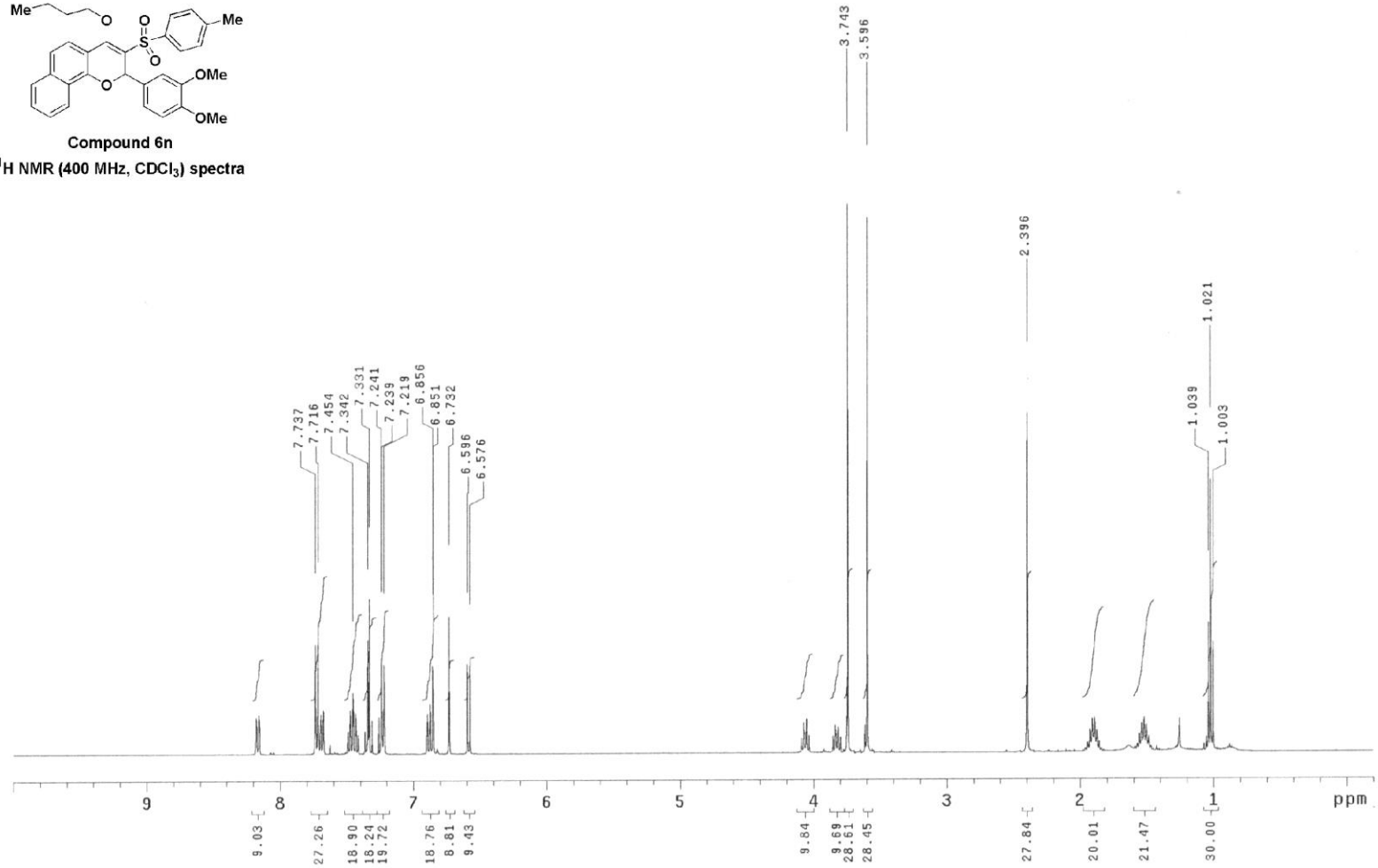
Compound 6n (^{1}H-NMR spectral data)

HAK14A1Bu

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Feb 26 2018
Solvent: CDCl3
Ambient temperature
Total 32 repetitions

Compound 6n

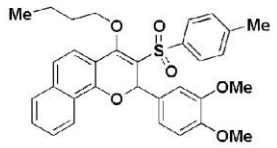
^{1}H NMR (400 MHz, $CDCl_3$) spectra



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

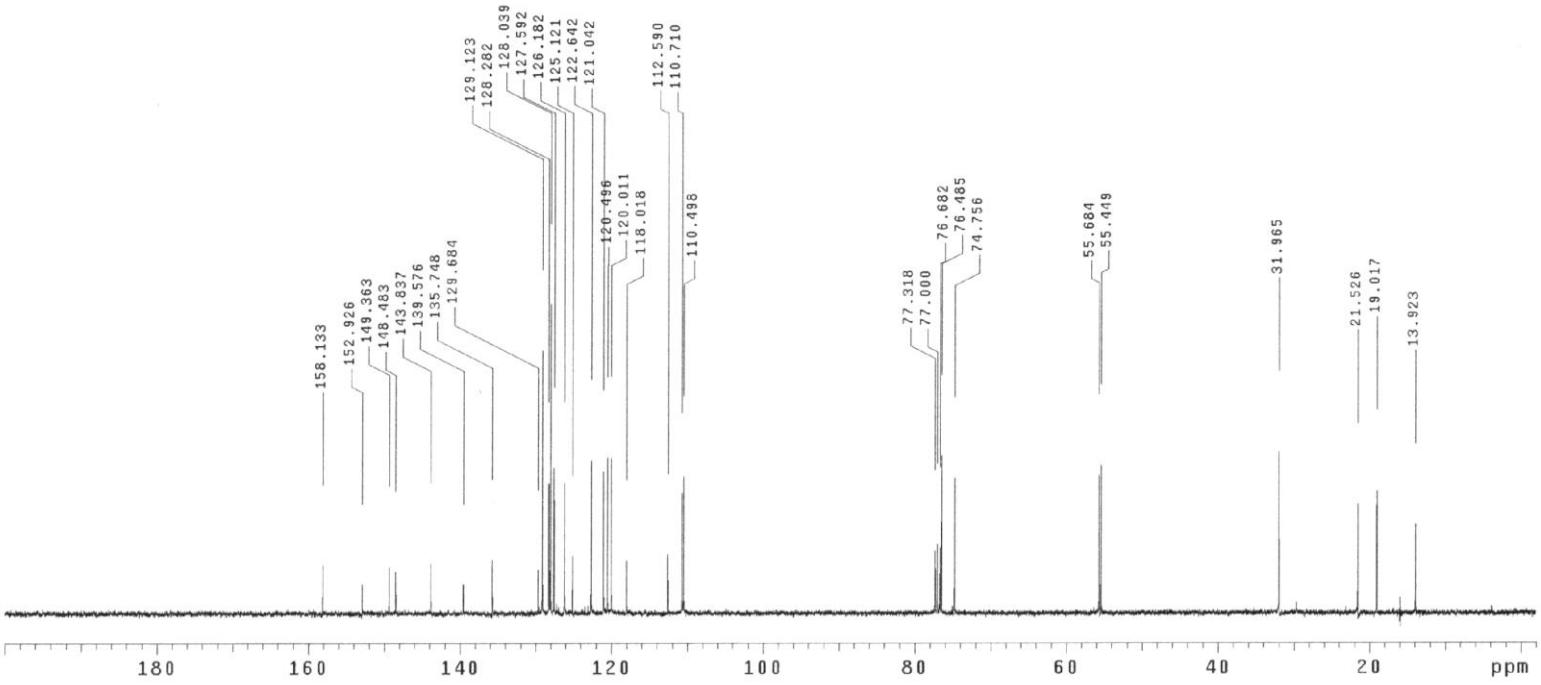
HAK14A1Bu

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Feb 26 2018
Solvent: CDCl3
Ambient temperature
Total 1152 repetitions



Compound 6n

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

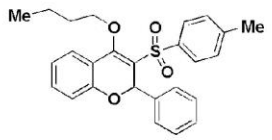


Compound 6o (^{1}H-NMR spectral data)

HAK1A2Bu

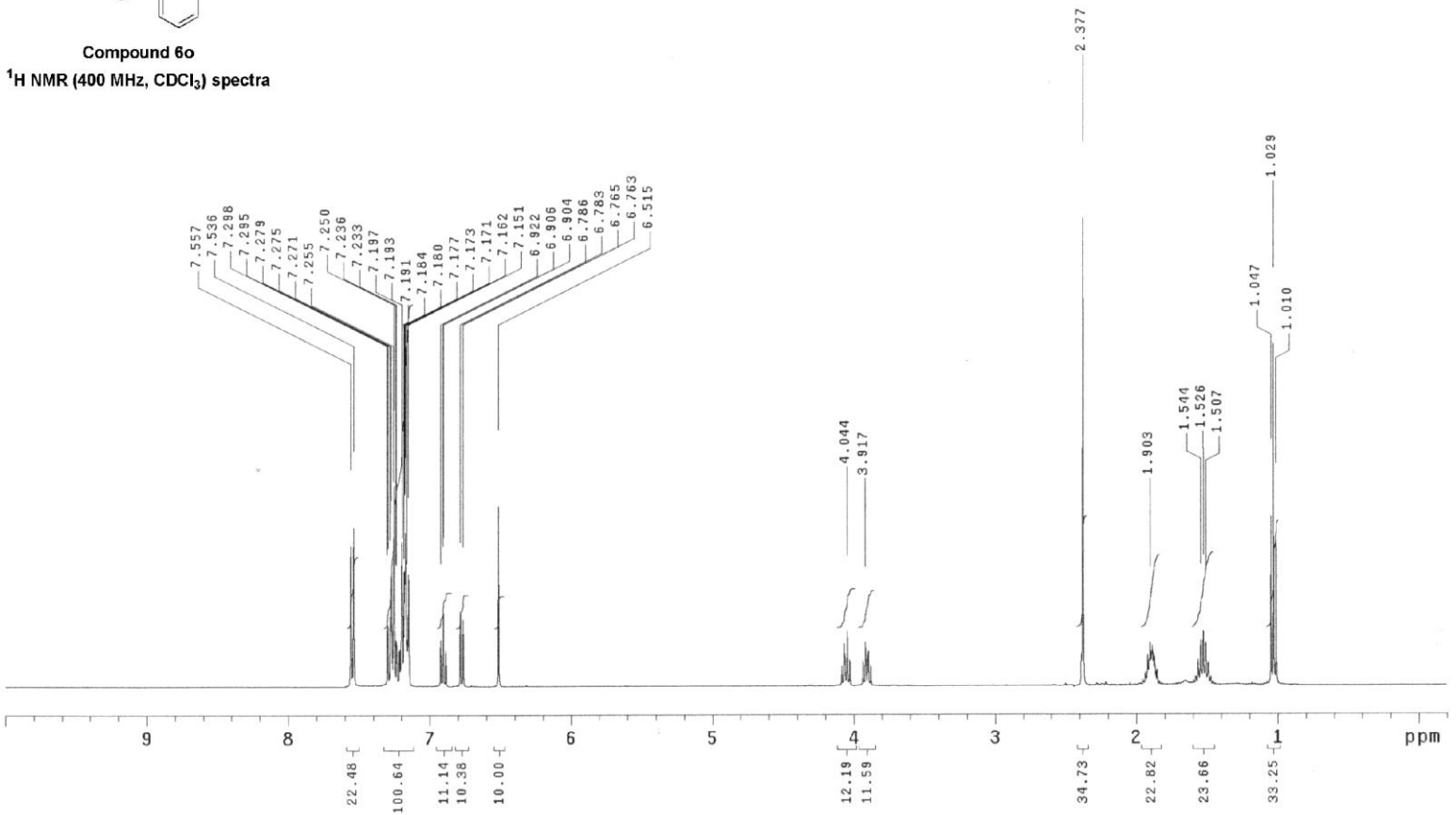
Pulse Sequence: s2pul

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



Compound 6o

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

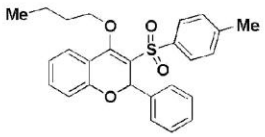


Compound 6o (^{13}C-NMR spectral data)

HAK1A2Bu

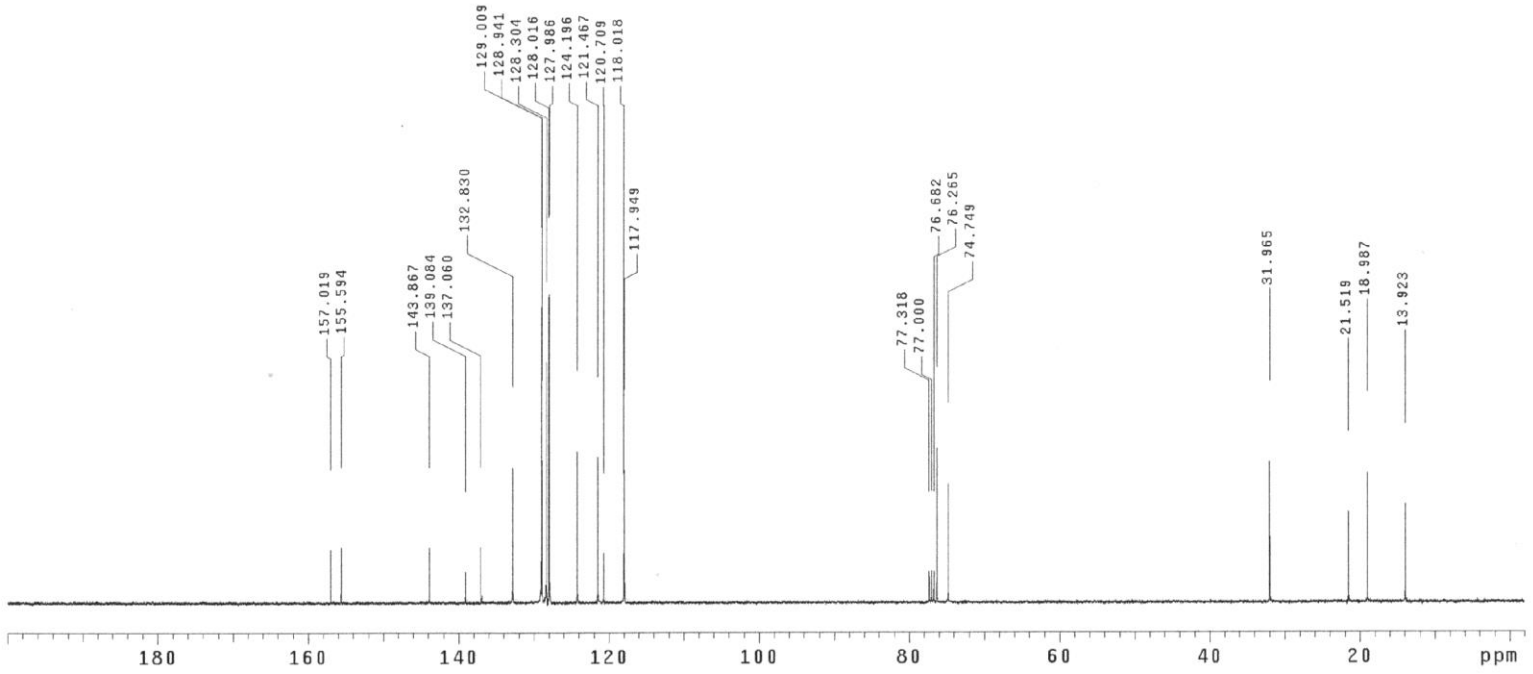
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jan 12 2018
Solvent: CDCl3
Ambient temperature
Total 848 repetitions



Compound 6o

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



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

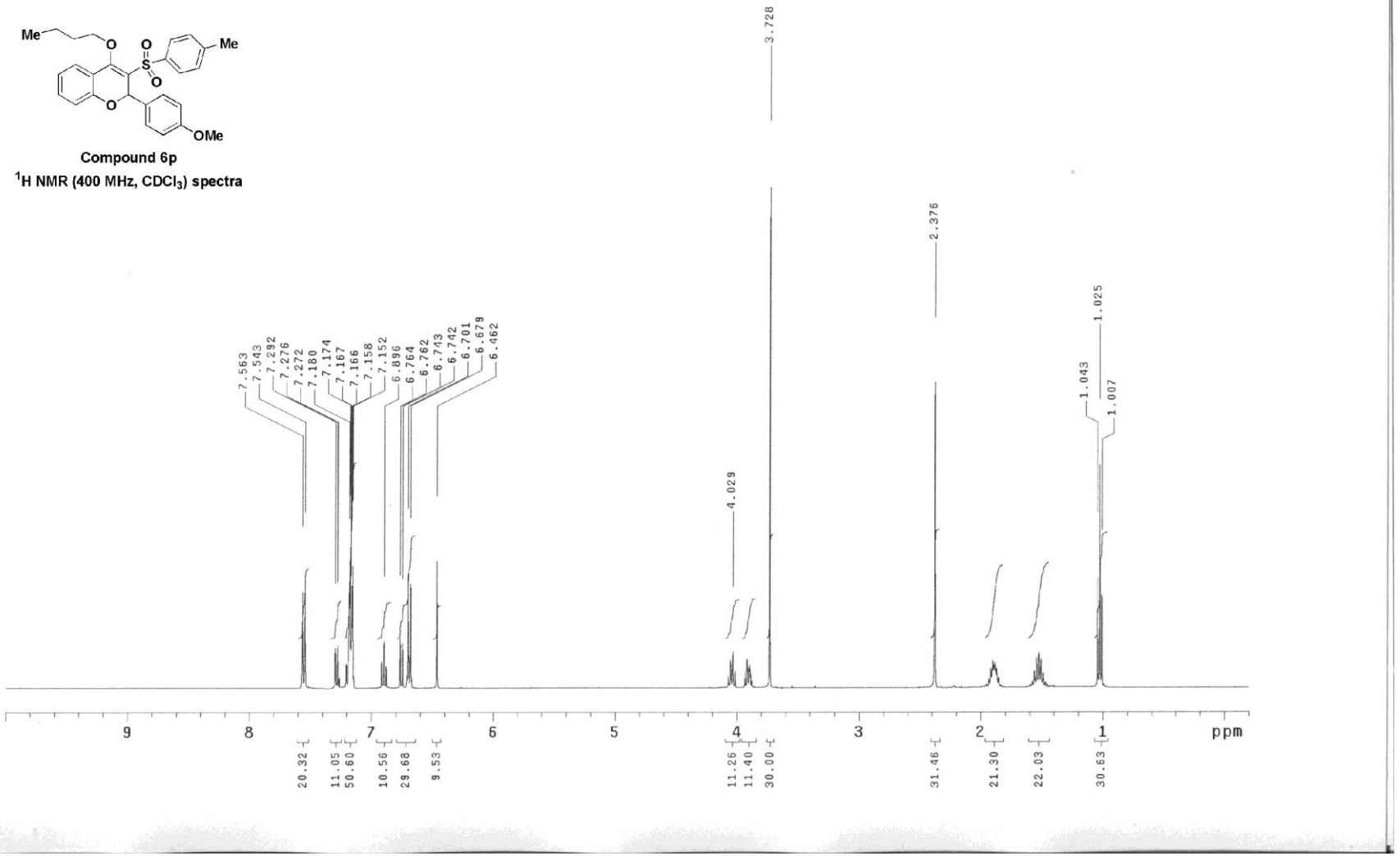
HAK1A4Bu

Pulse Sequence: s2pul

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

Compound 6p

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

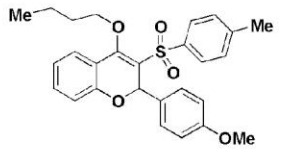


Compound 6p (^{13}C-NMR spectral data)

HAK1A4Bu

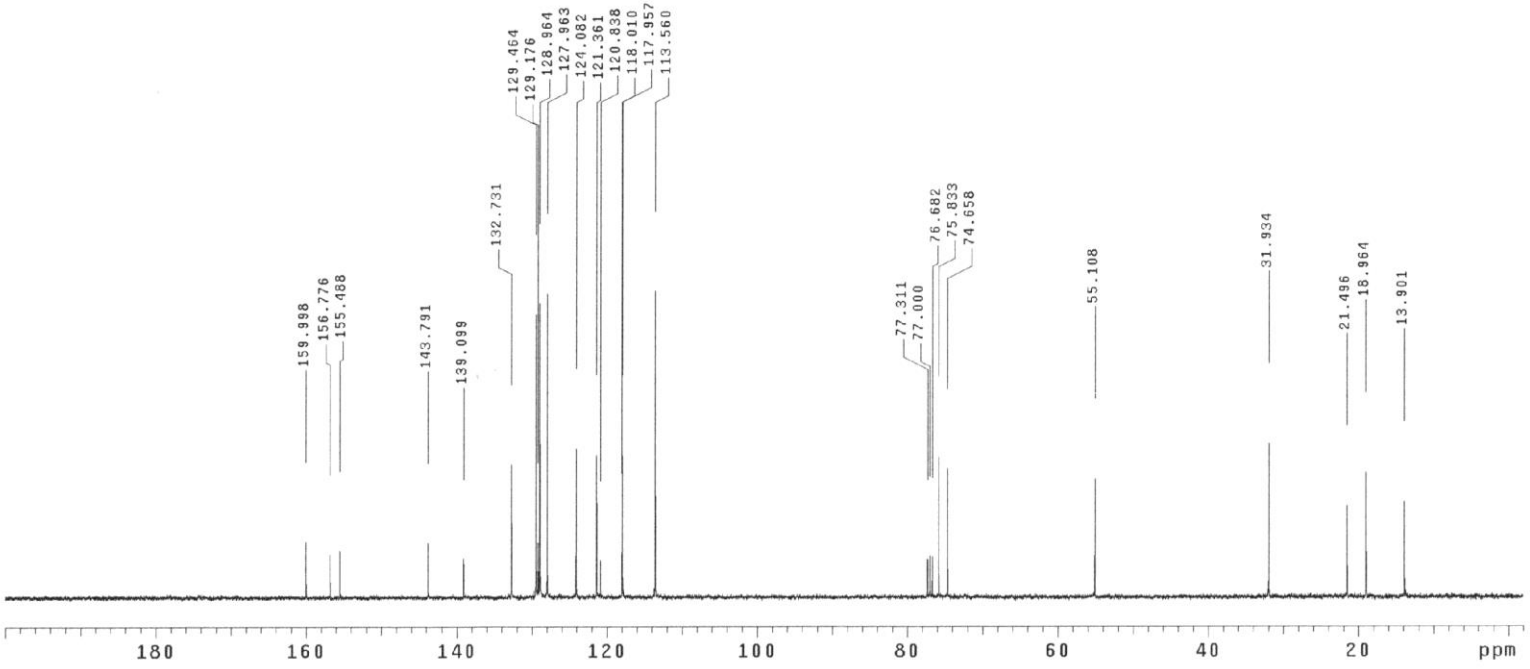
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jan 12 2018
Solvent: CDCl3
Ambient temperature
Total 208 repetitions



Compound 6p

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

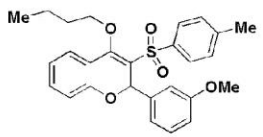


Compound 6q (^{1}H-NMR spectral data)

HAK1A3Bu

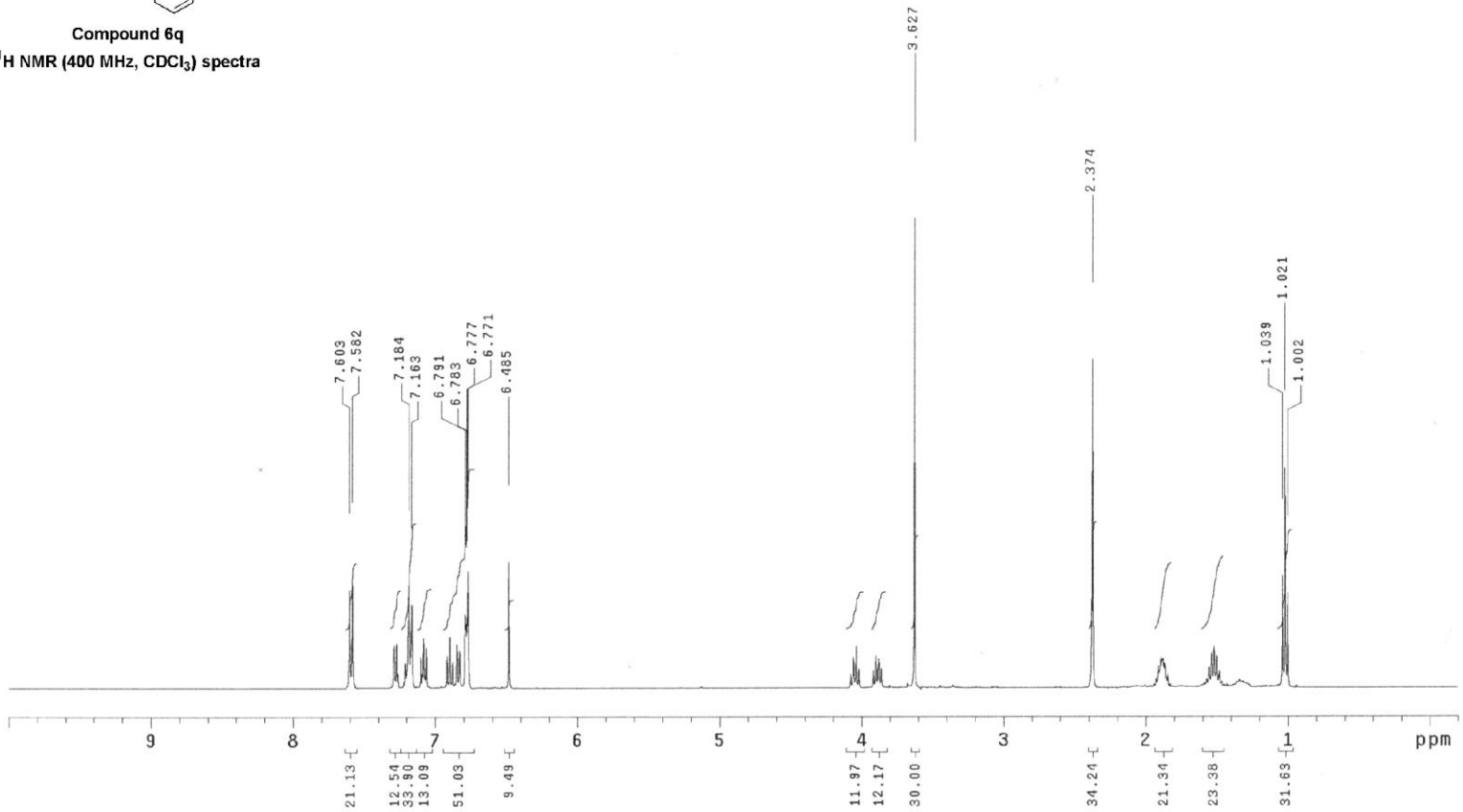
Pulse Sequence: s2pul

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



Compound 6q

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

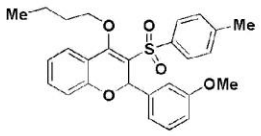


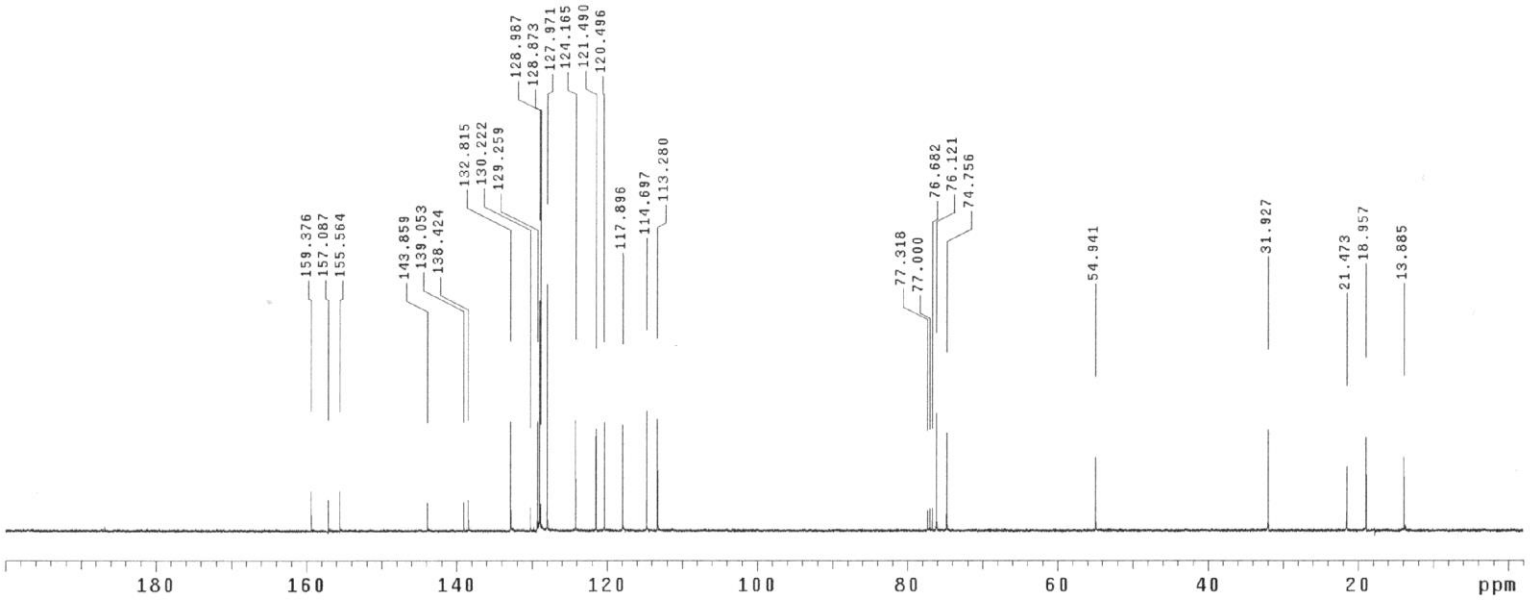
Compound 6q (^{13}C-NMR spectral data)

HAK1A3Bu

Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jan 12 2018
Solvent: CDCl3
Ambient temperature
Total 544 repetitions



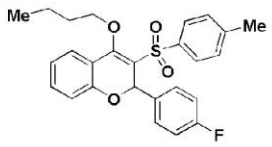


Compound 6r (^{1}H-NMR spectral data)

HAK1A5Bu

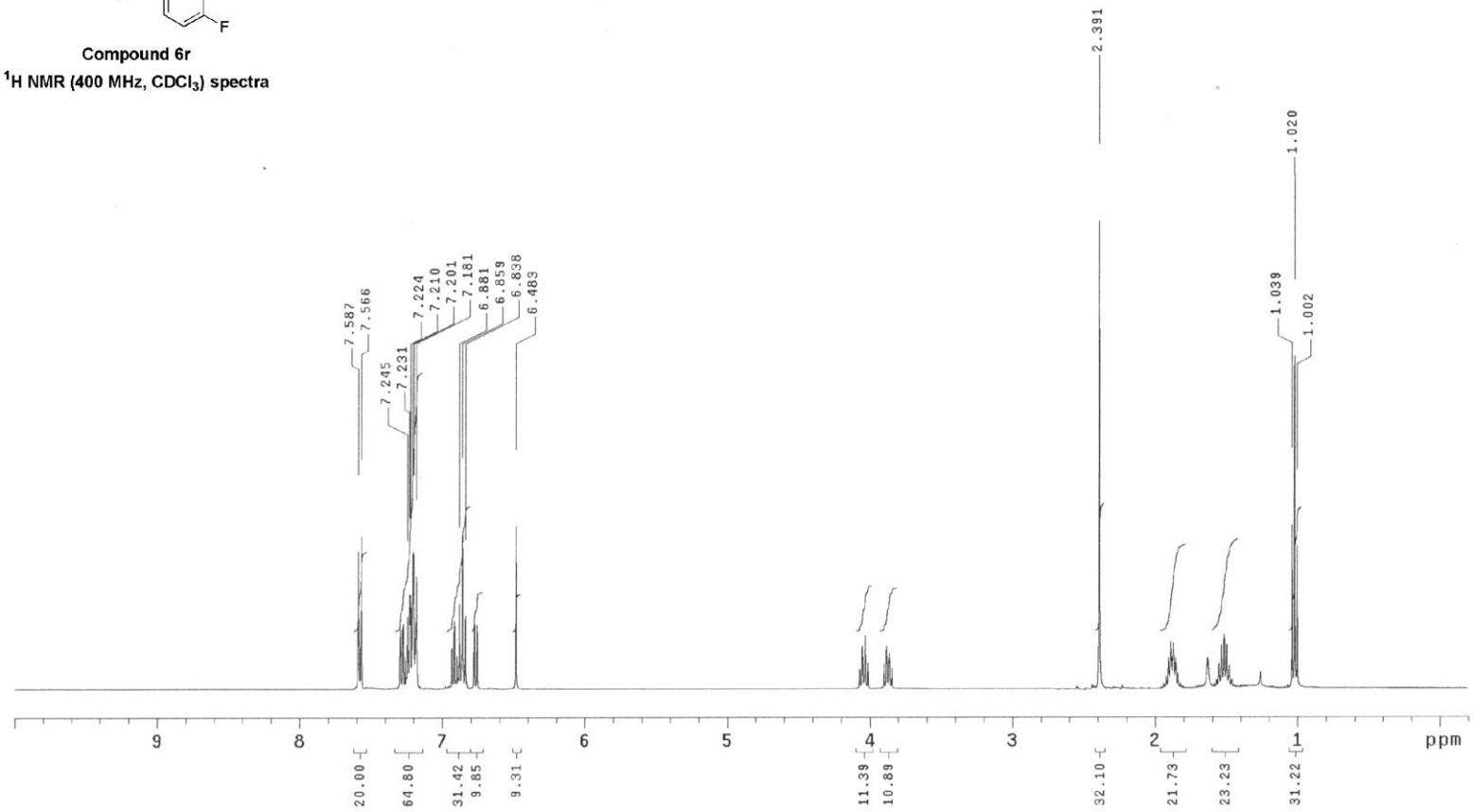
Pulse Sequence: s2pul

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



Compound 6r

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

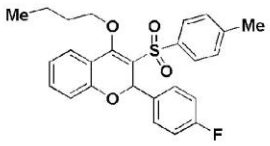


Compound 6r (^{13}C-NMR spectral data)

HAK1A5Bu

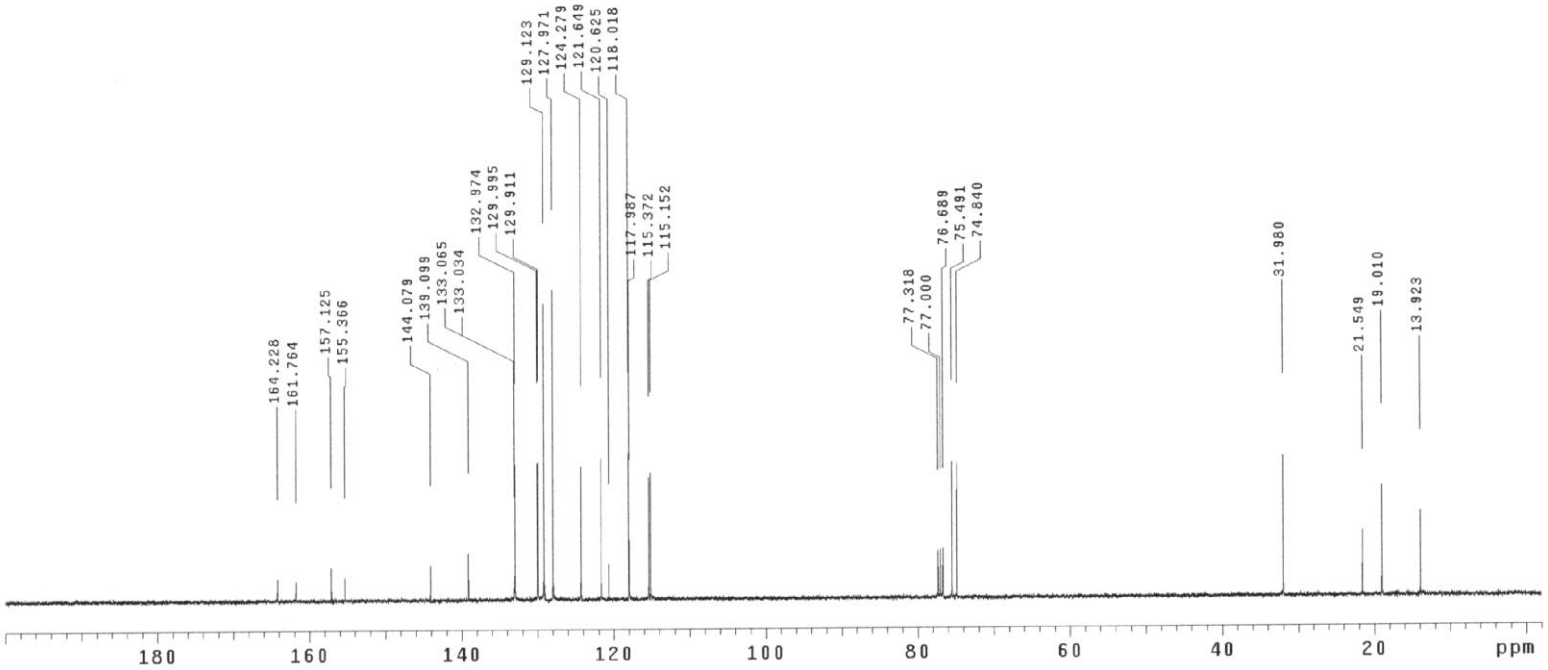
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jan 22 2018
Solvent: CDCl3
Ambient temperature
Total 1264 repetitions



Compound 6r

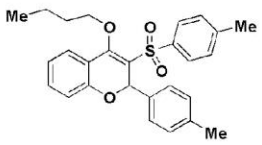
^{13}C NMR (100 MHz, $CDCl_3$) spectra



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

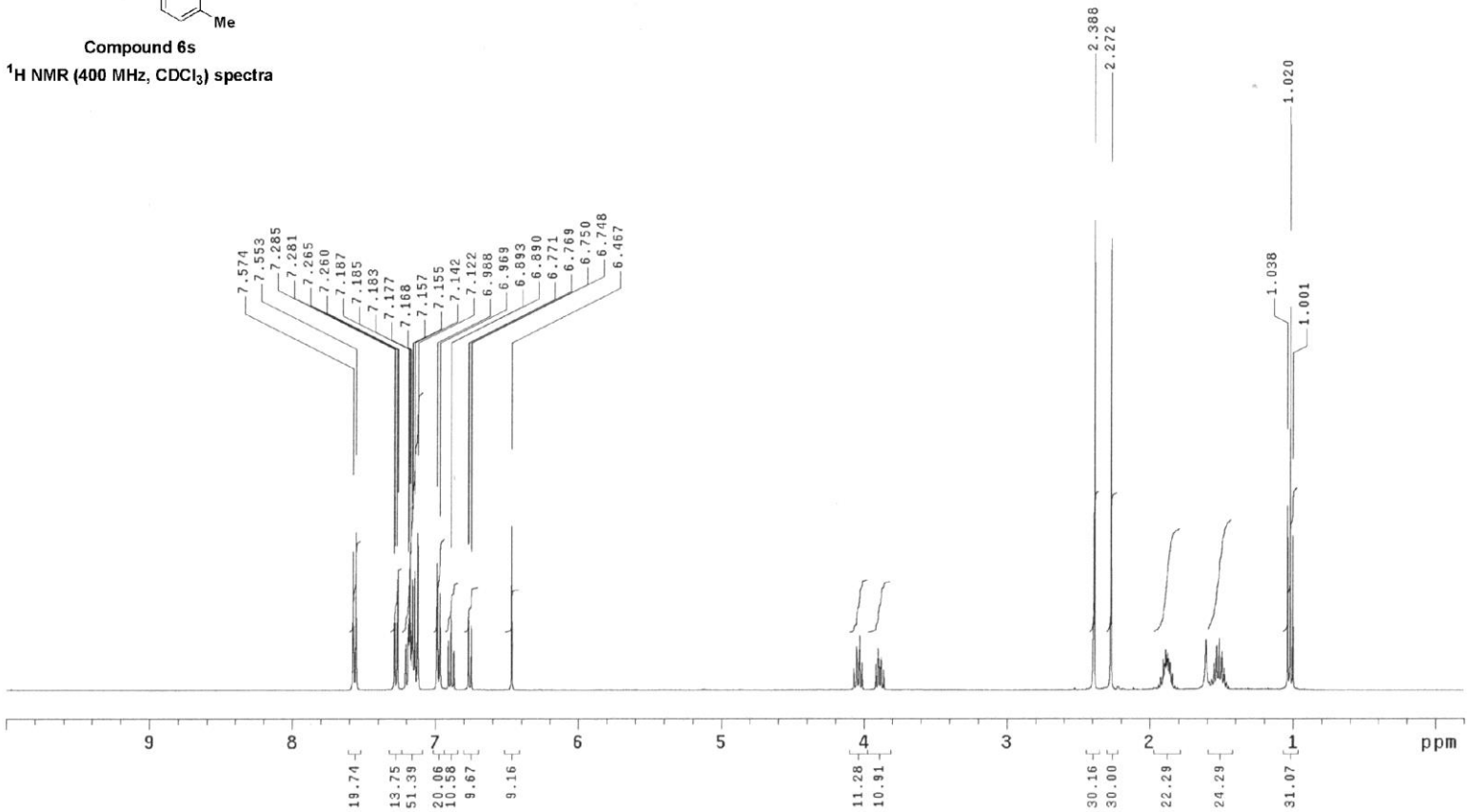
HAK1A6Bu

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



Compound 6s

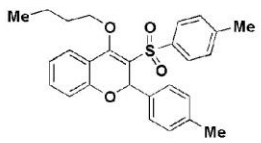
^{1}H NMR (400 MHz, $CDCl_3$) spectra



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

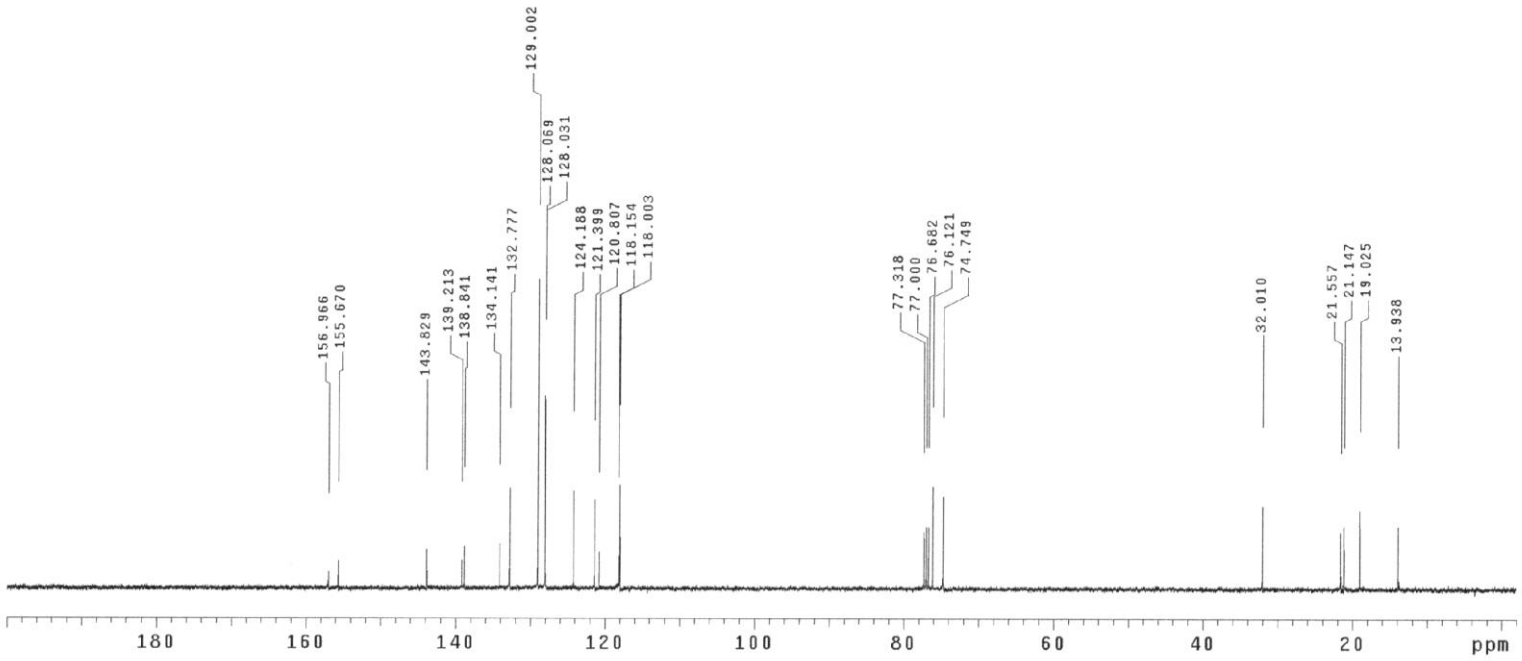
HAK1A6Bu

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Jan 22 2018
Solvent: CDCl3
Ambient temperature
Total 1600 repetitions

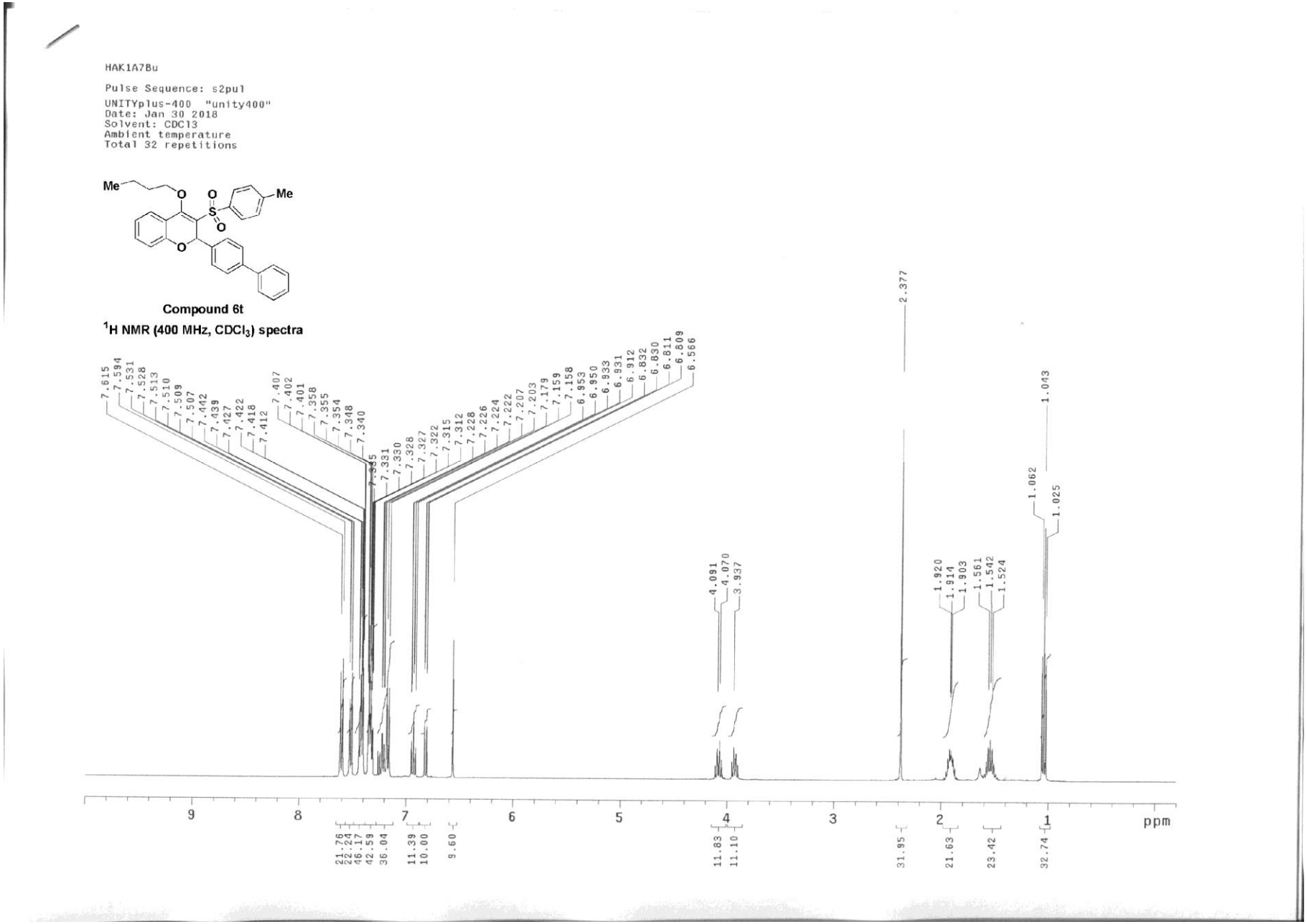


Compound 6s

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



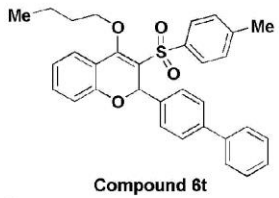
Compound 6t (^{1}H-NMR spectral data)



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

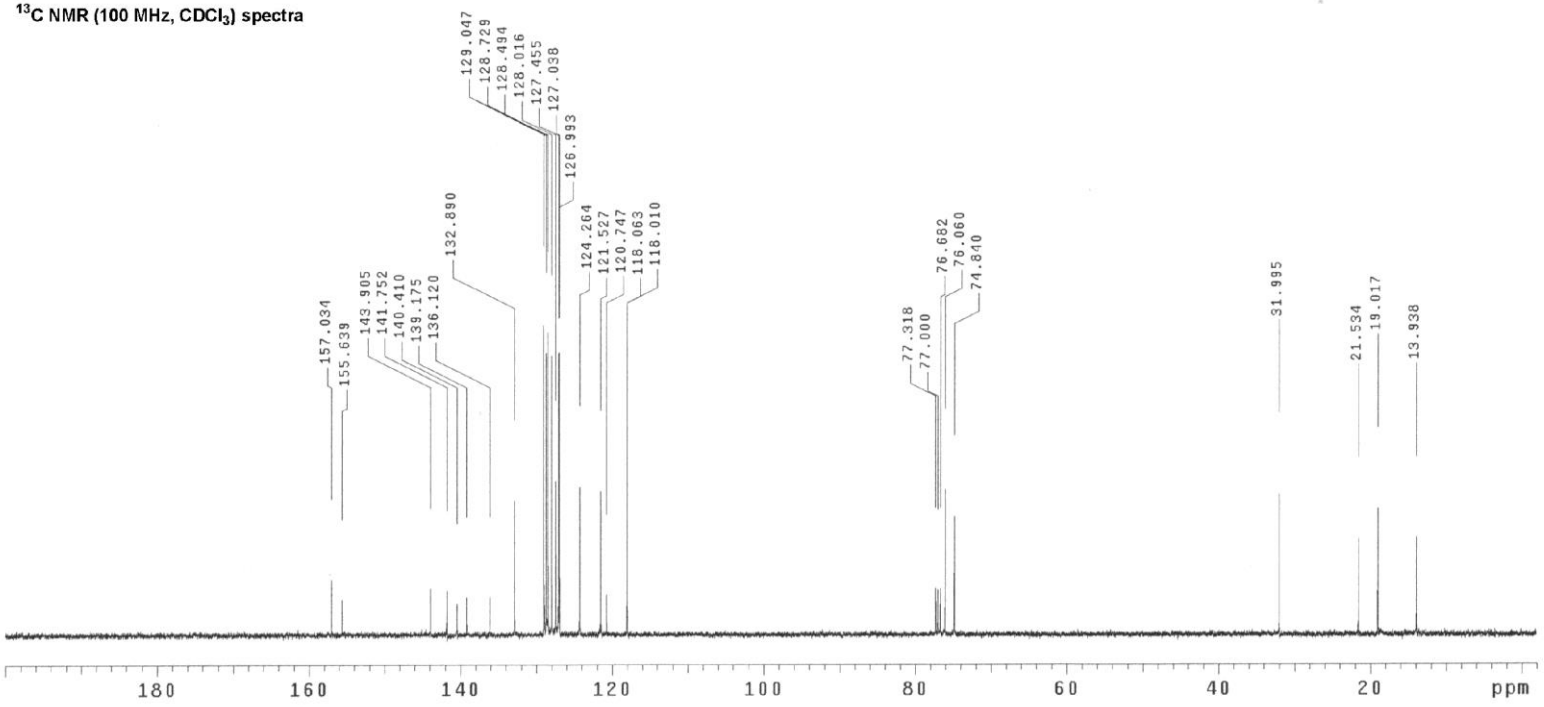
HAK1A7Bu

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Jan 30 2018
Solvent: CDCl3
Ambient temperature
Total 528 repetitions



Compound 6t

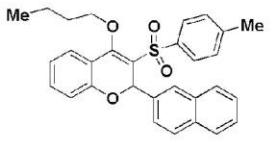
^{13}C NMR (100 MHz, $CDCl_3$) spectra



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

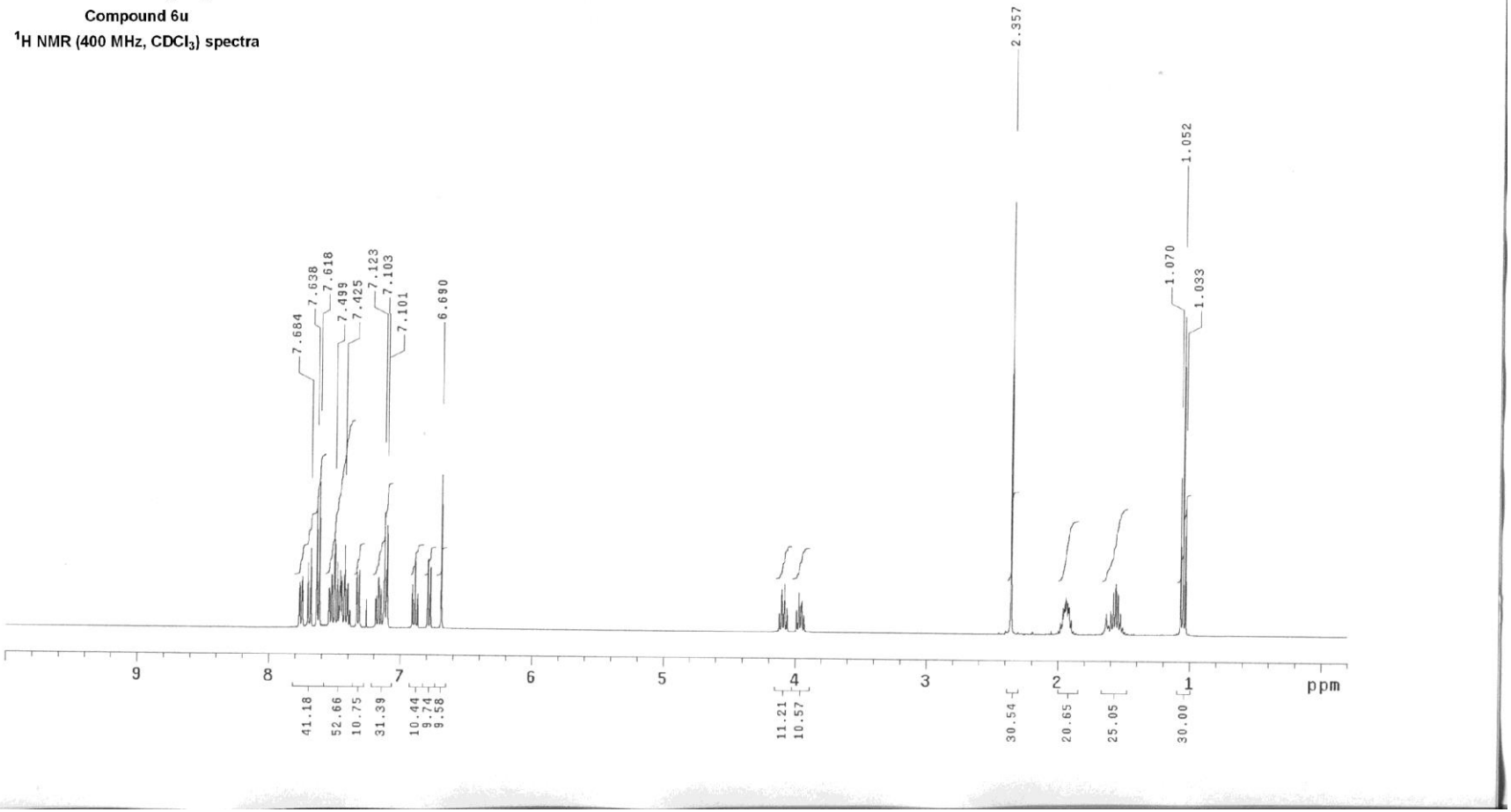
HAK1A8Bu

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Jan 30 2018
Solvent: CDCl3
Ambient temperature
Total 32 repetitions



Compound 6u

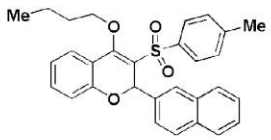
^{1}H NMR (400 MHz, $CDCl_3$) spectra



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

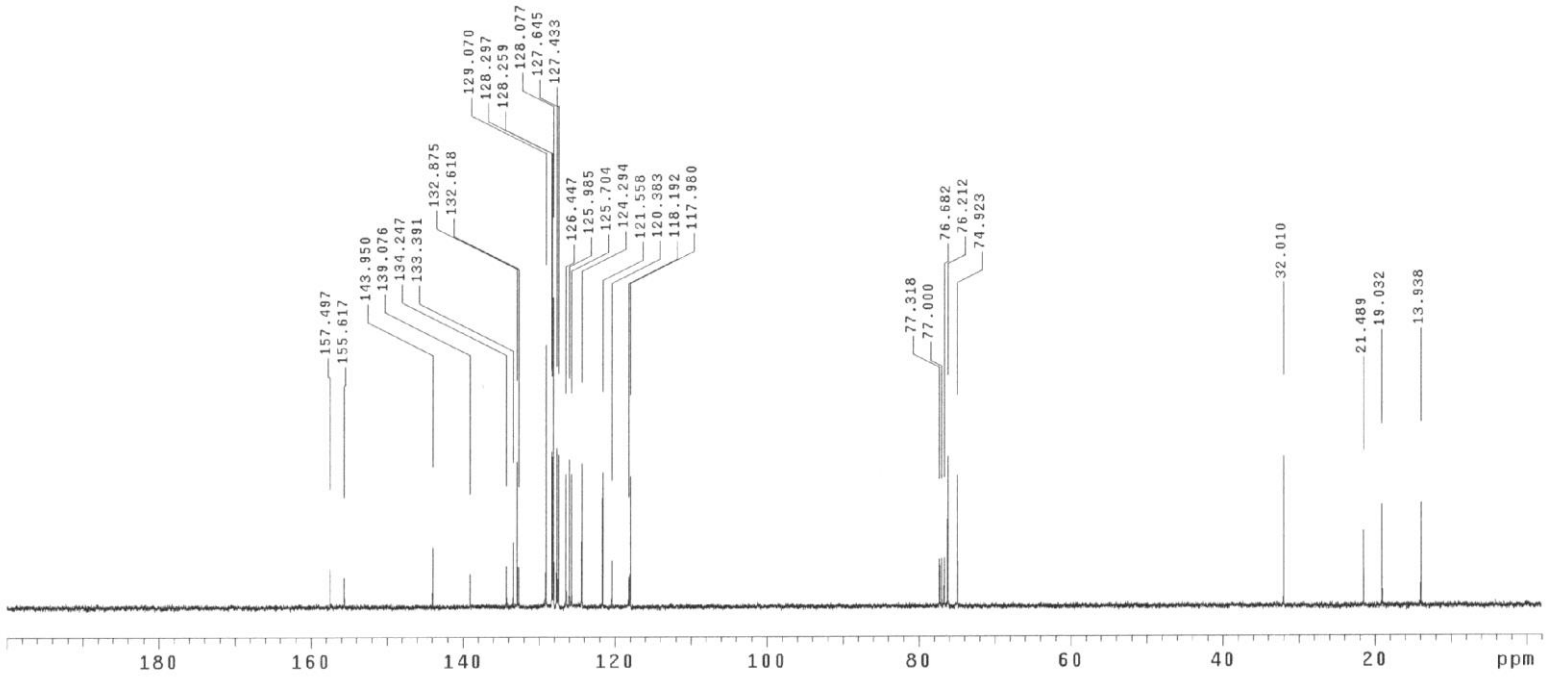
HAK1A8Bu

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Jan 30 2018
Solvent: CDCl3
Ambient temperature
Total 528 repetitions



Compound 6u

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

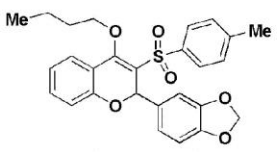


Compound 6v (^{1}H-NMR spectral data)

HAK1A9Bu

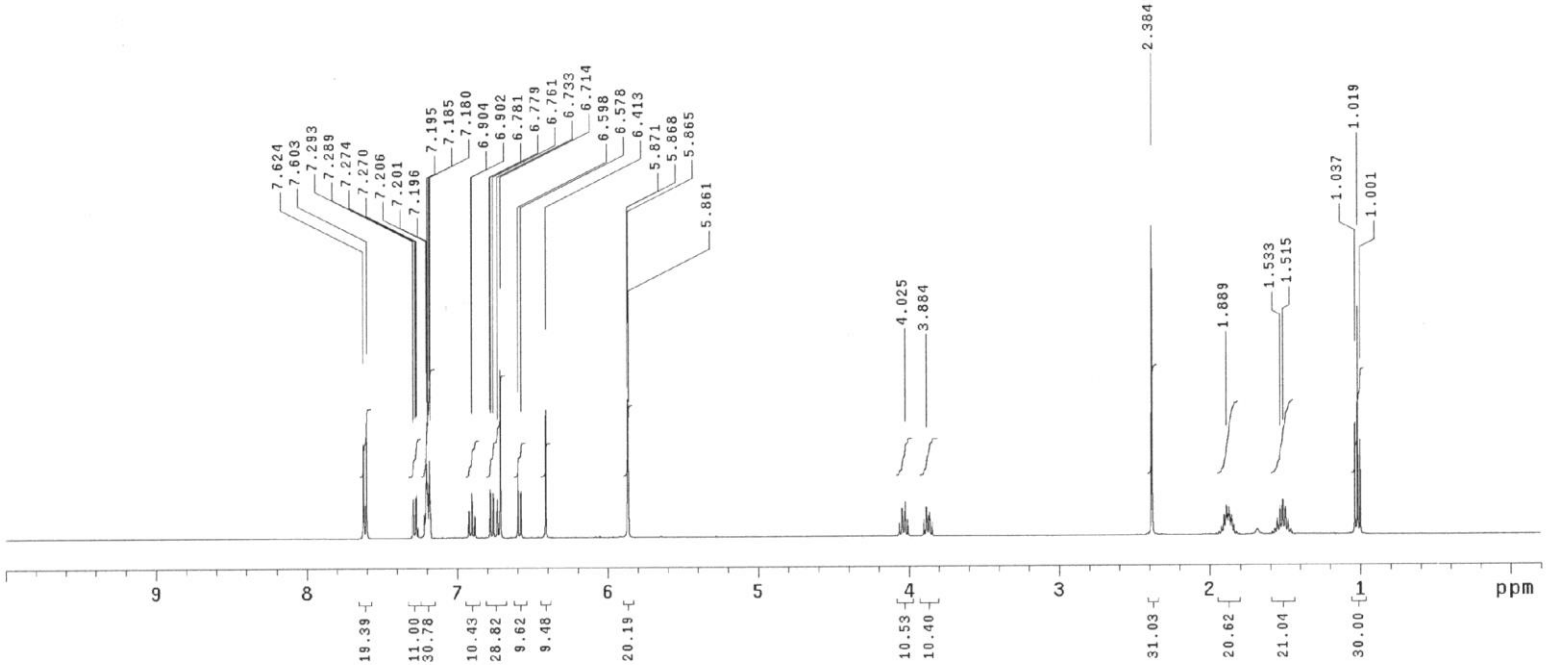
Pulse Sequence: s2pul

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



Compound 6v

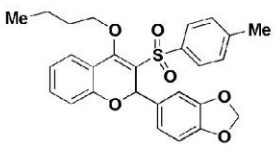
^{1}H NMR (400 MHz, $CDCl_3$) spectra



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

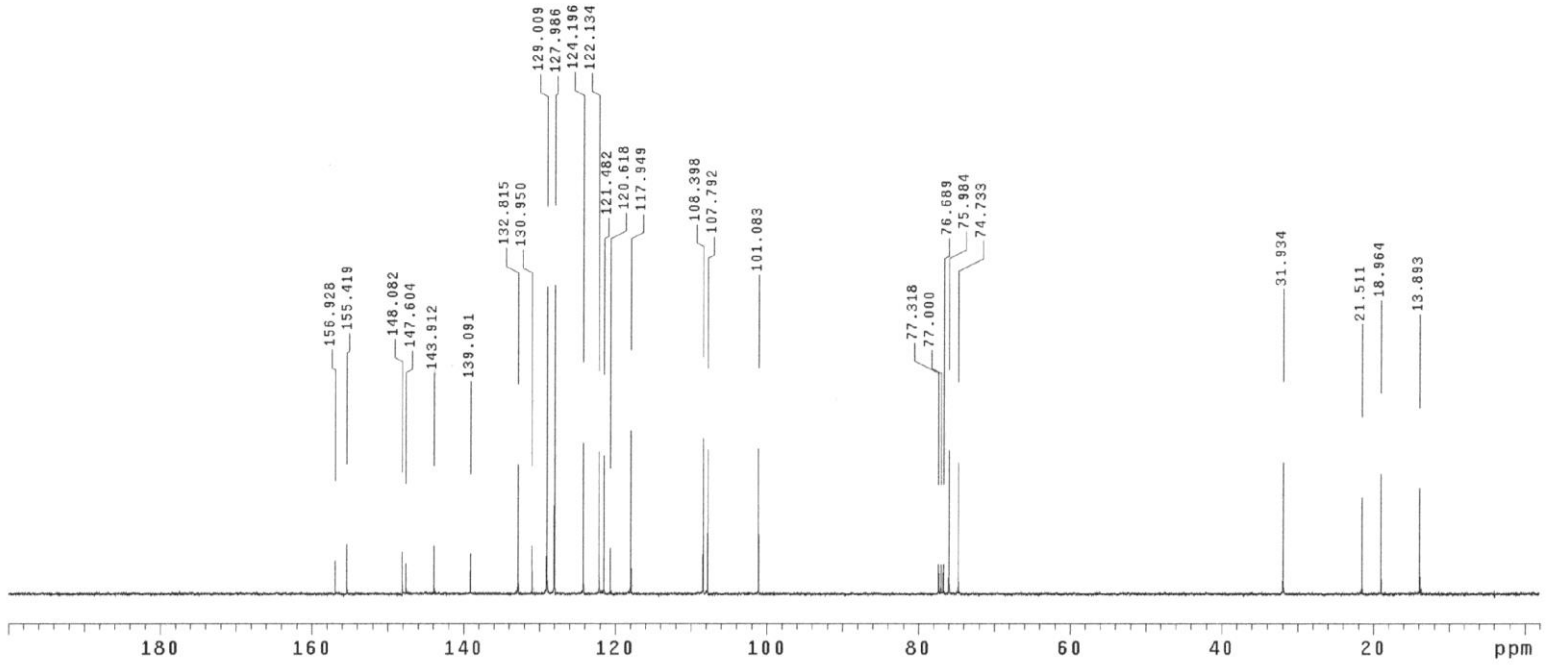
HAK1A9Bu

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Dec 28 2017
Solvent: CDCl3
Ambient temperature
Total 624 repetitions



Compound 6v

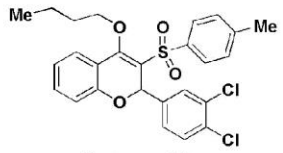
^{13}C NMR (100 MHz, $CDCl_3$) spectra



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

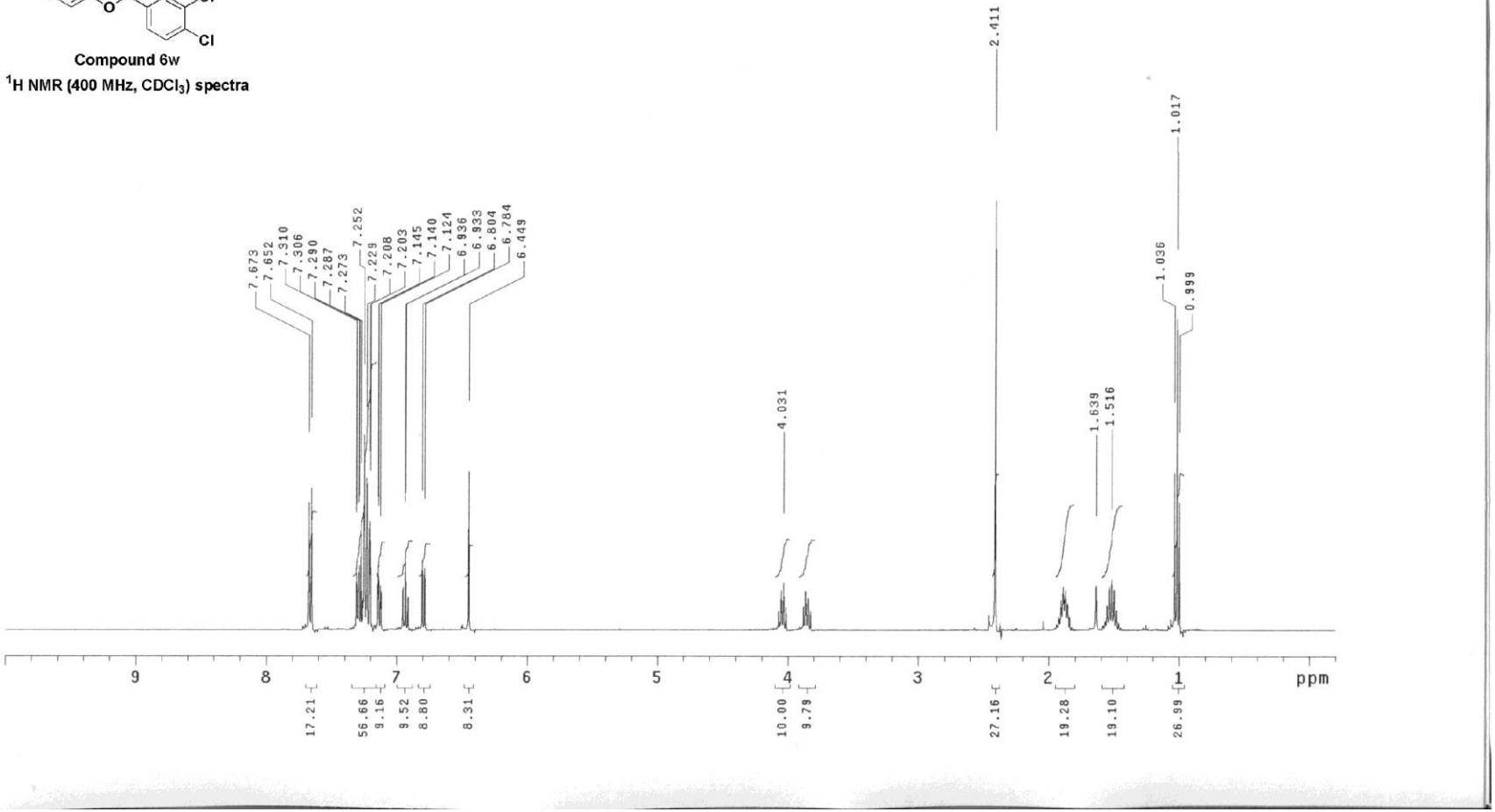
HAK1A10Bu

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Jan 8 2018
Solvent: CDCl3
Ambient temperature
Total 32 repetitions



Compound 6w

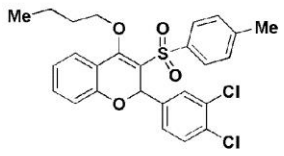
^{1}H NMR (400 MHz, $CDCl_3$) spectra



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

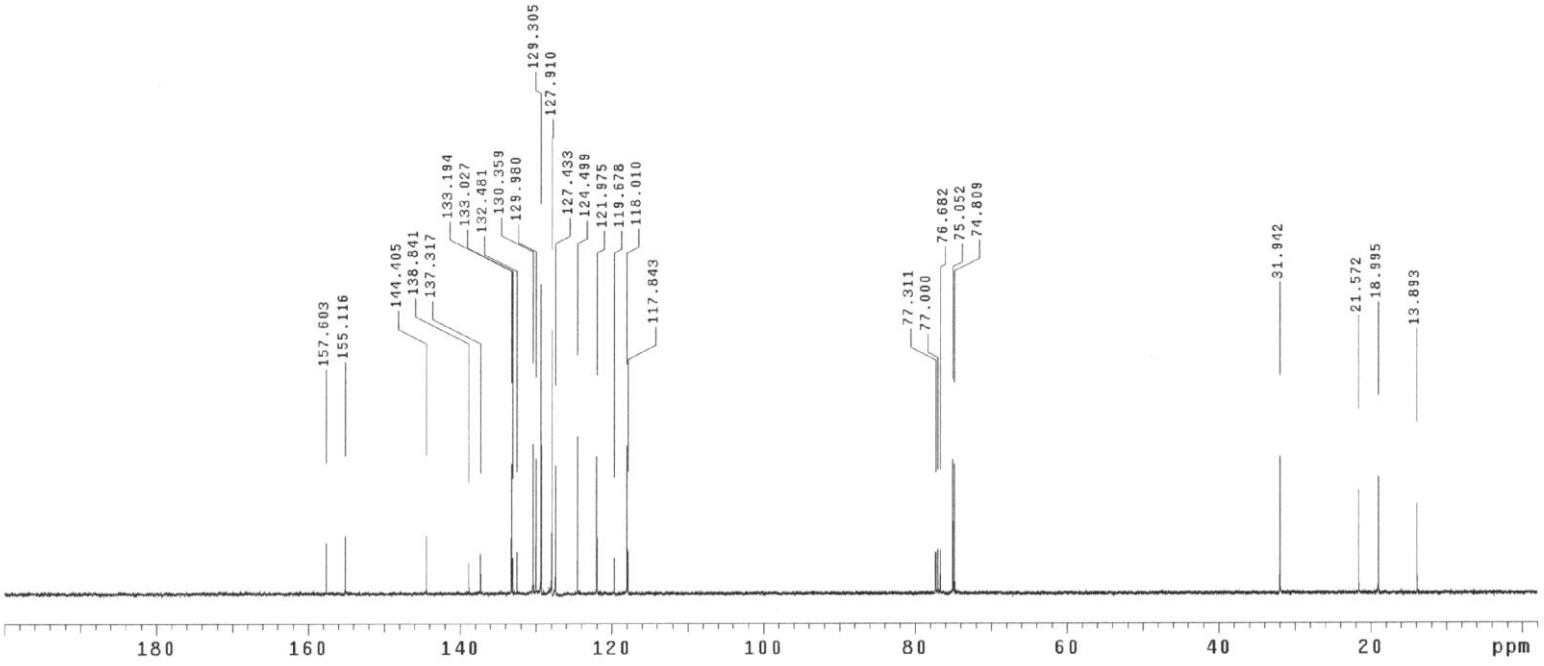
HAK1A10Bu

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Jan 8 2018
Solvent: CDCl3
Ambient temperature
Total 976 repetitions

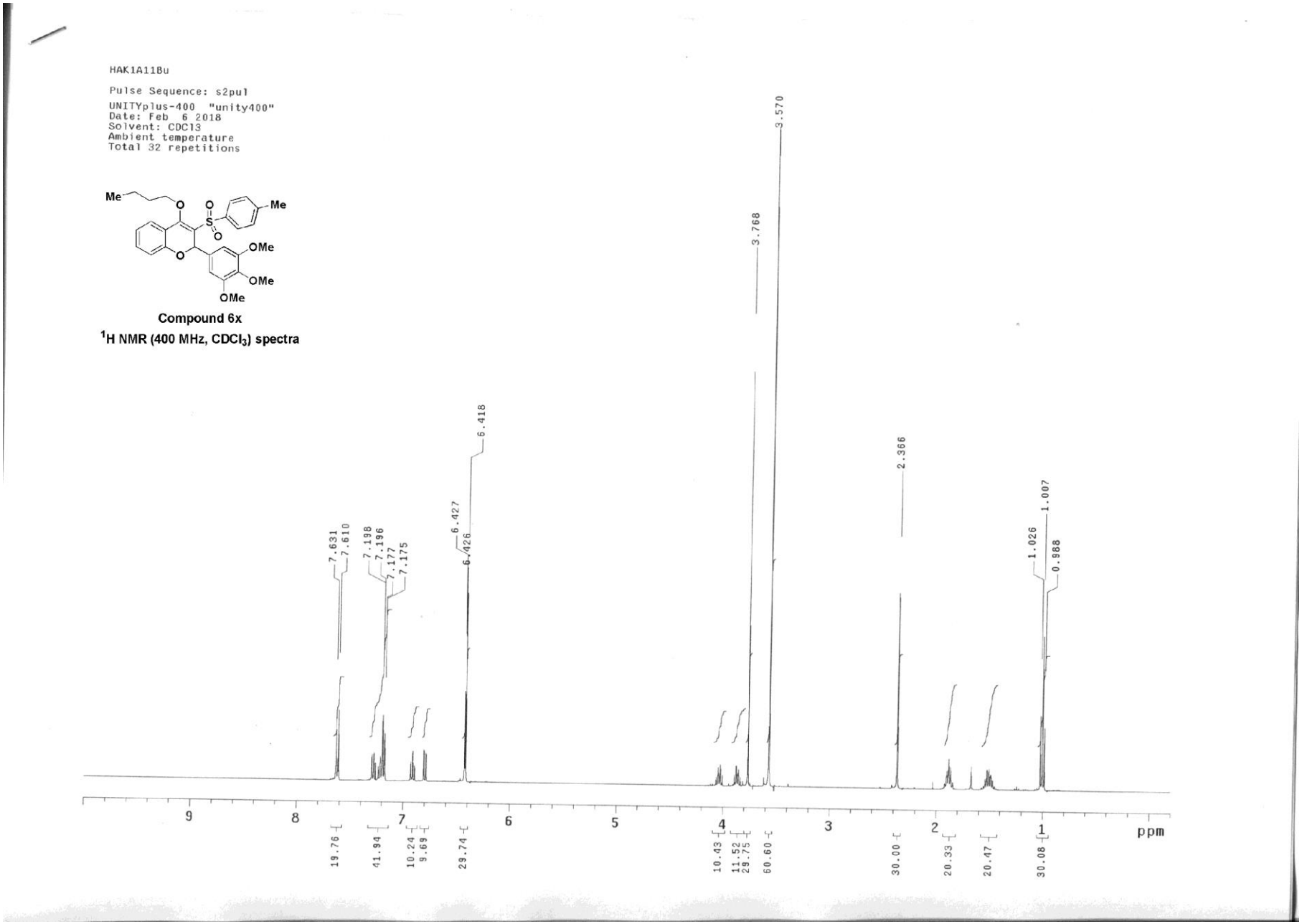


Compound 6w

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



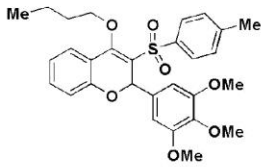
Compound 6x (^{1}H-NMR spectral data)



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

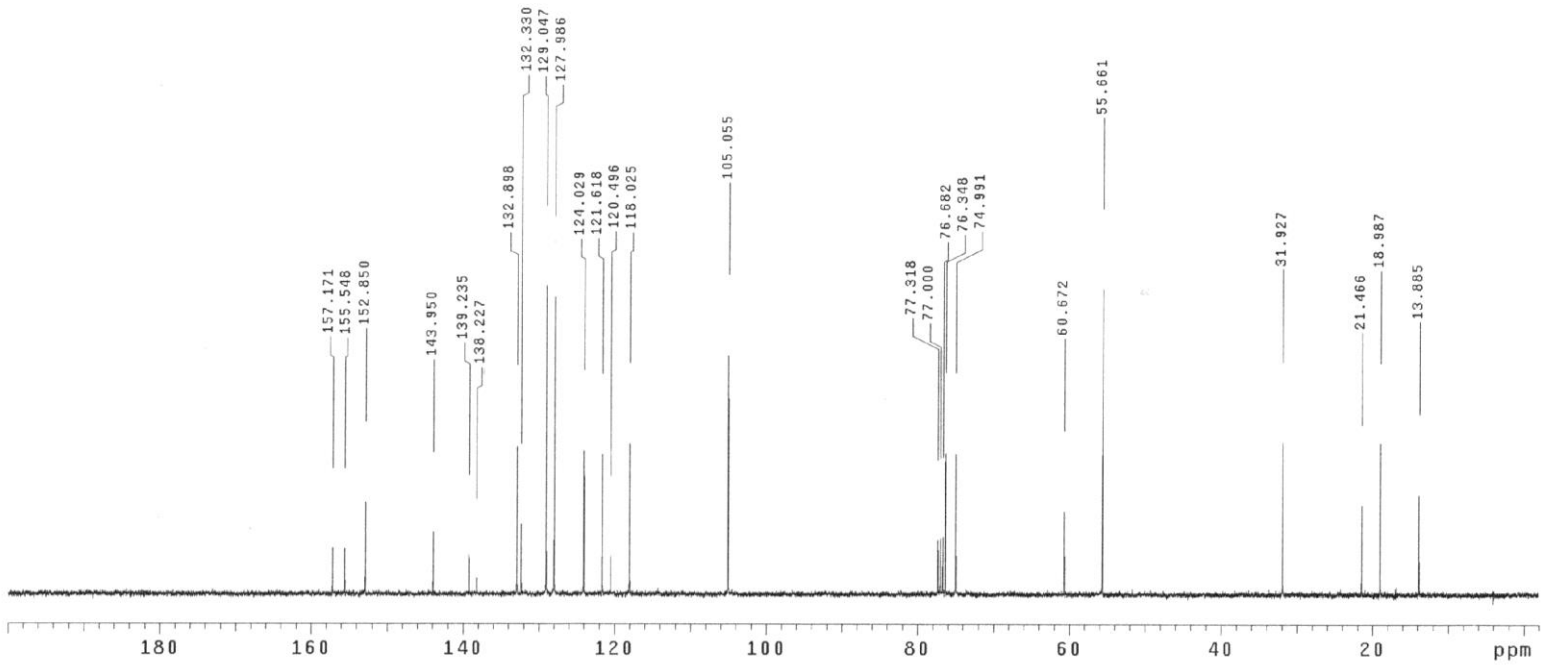
HAK1A11Bu

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Feb 6 2018
Solvent: CDCl3
Ambient temperature
Total 480 repetitions



Compound 6x

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



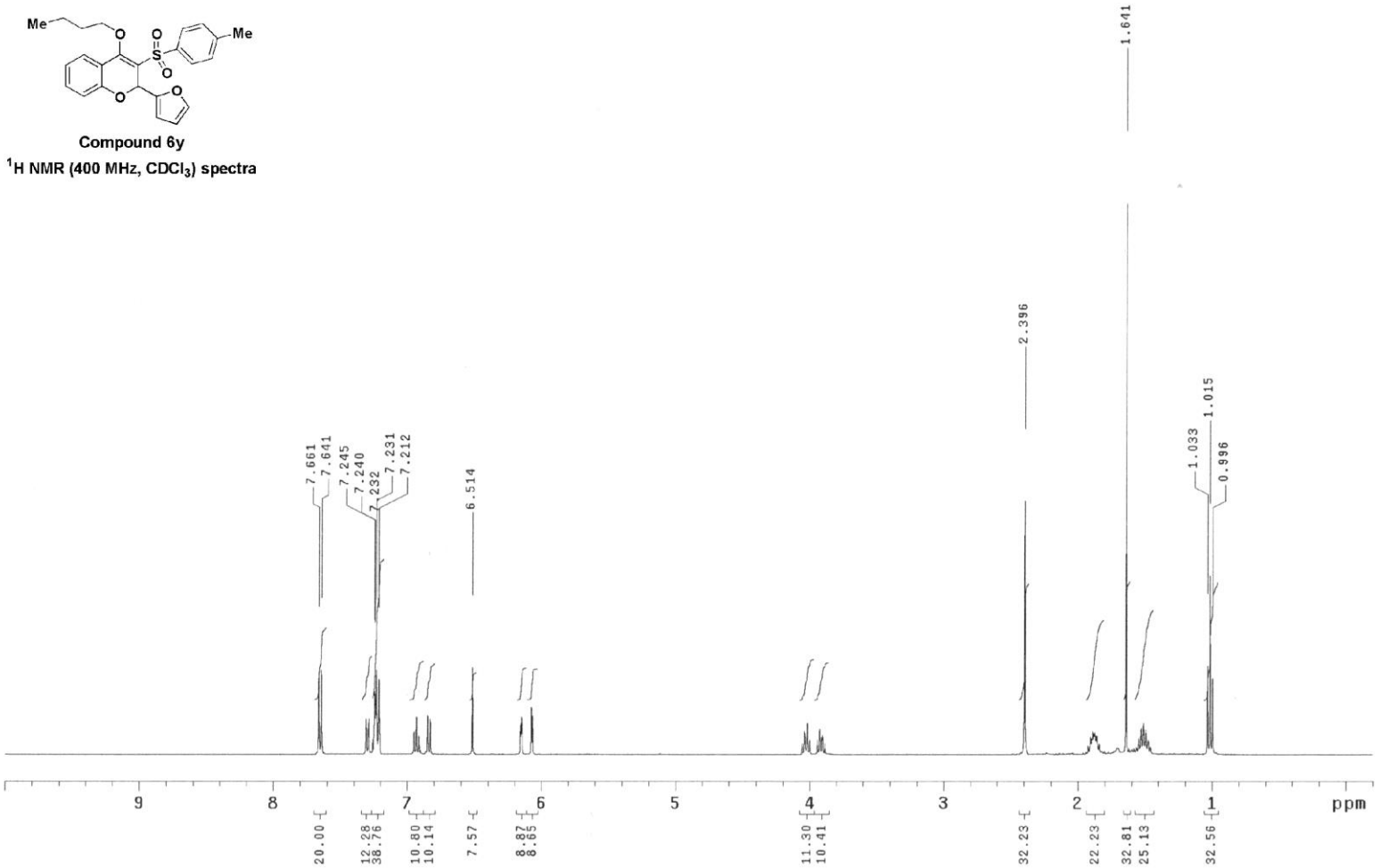
Compound 6y (^{1}H-NMR spectral data)

HAK1A12Bu

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

Compound 6y

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

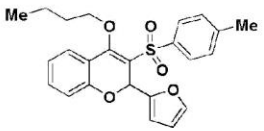


Compound 6y (^{13}C-NMR spectral data)

HAK1A12Bu

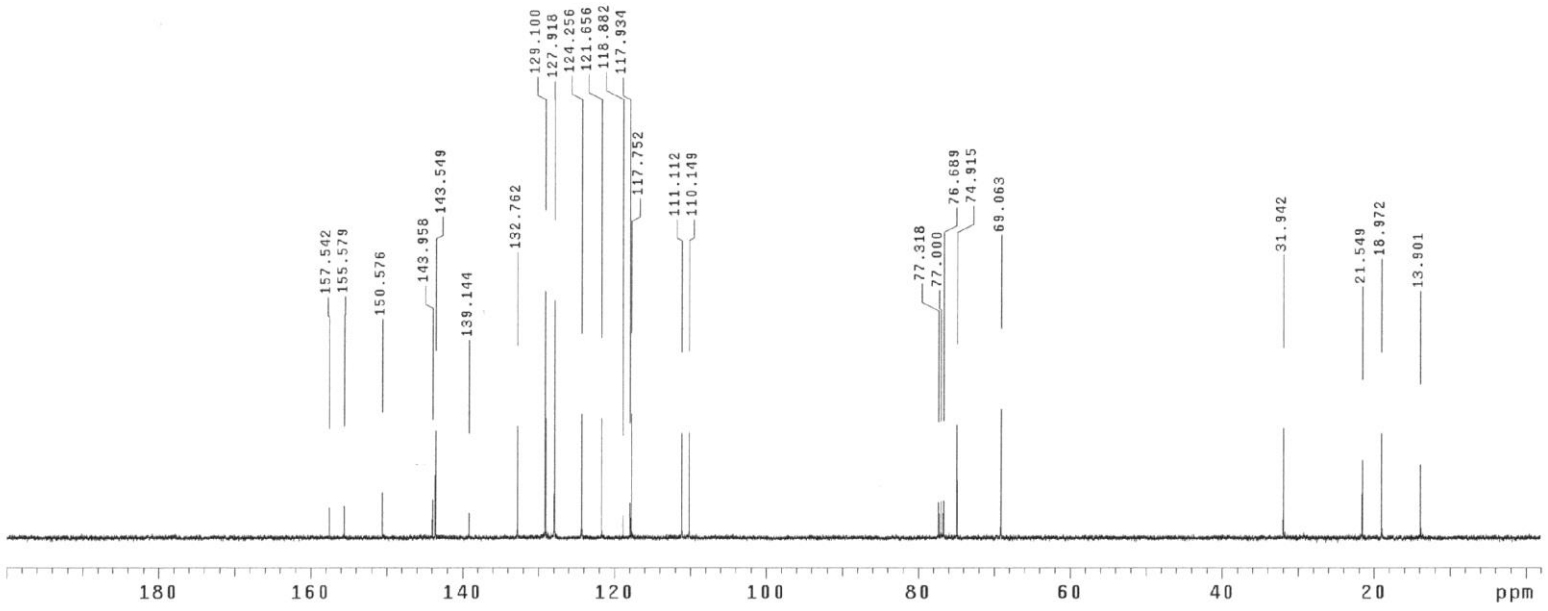
Pulse Sequence: s2pul

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



Compound 6y

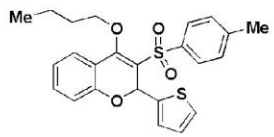
^{13}C NMR (100 MHz, $CDCl_3$) spectra



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

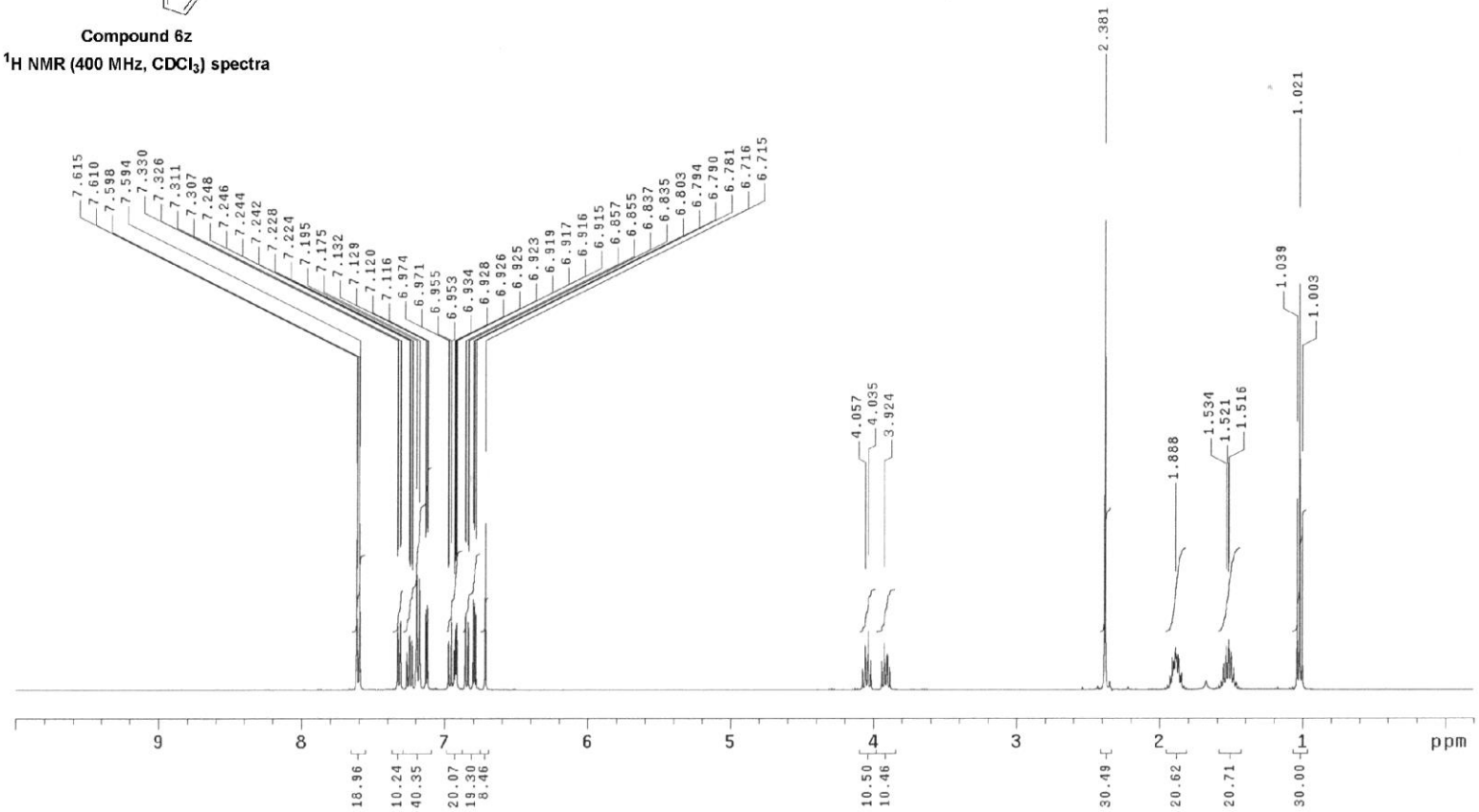
HAK1A13Bu

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



Compound 6z

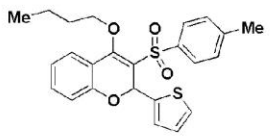
^{1}H NMR (400 MHz, $CDCl_3$) spectra



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

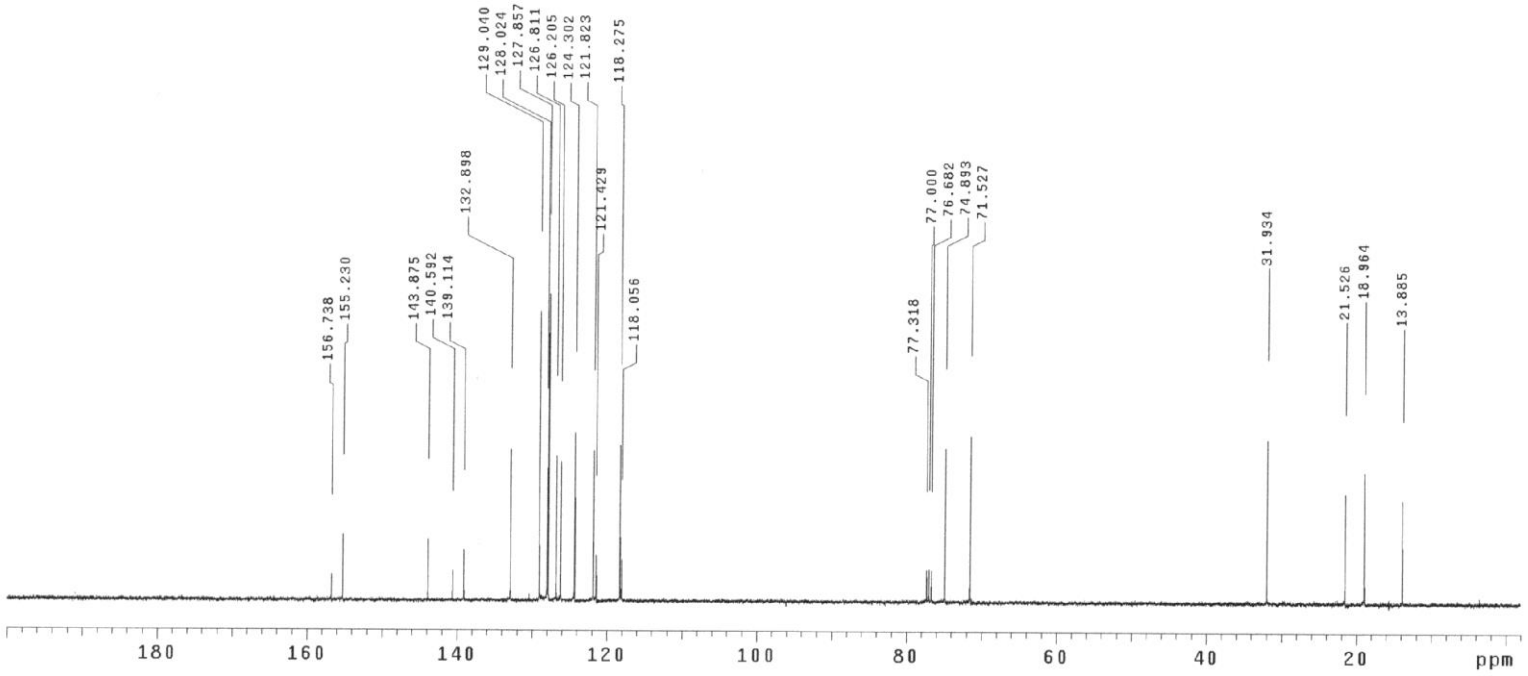
HAK1A13Bu

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Jan 19 2018
Solvent: CDCl3
Ambient temperature
Total 512 repetitions



Compound 6z

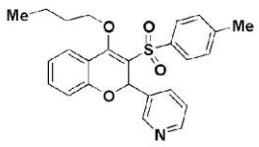
^{13}C NMR (100 MHz, $CDCl_3$) spectra



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

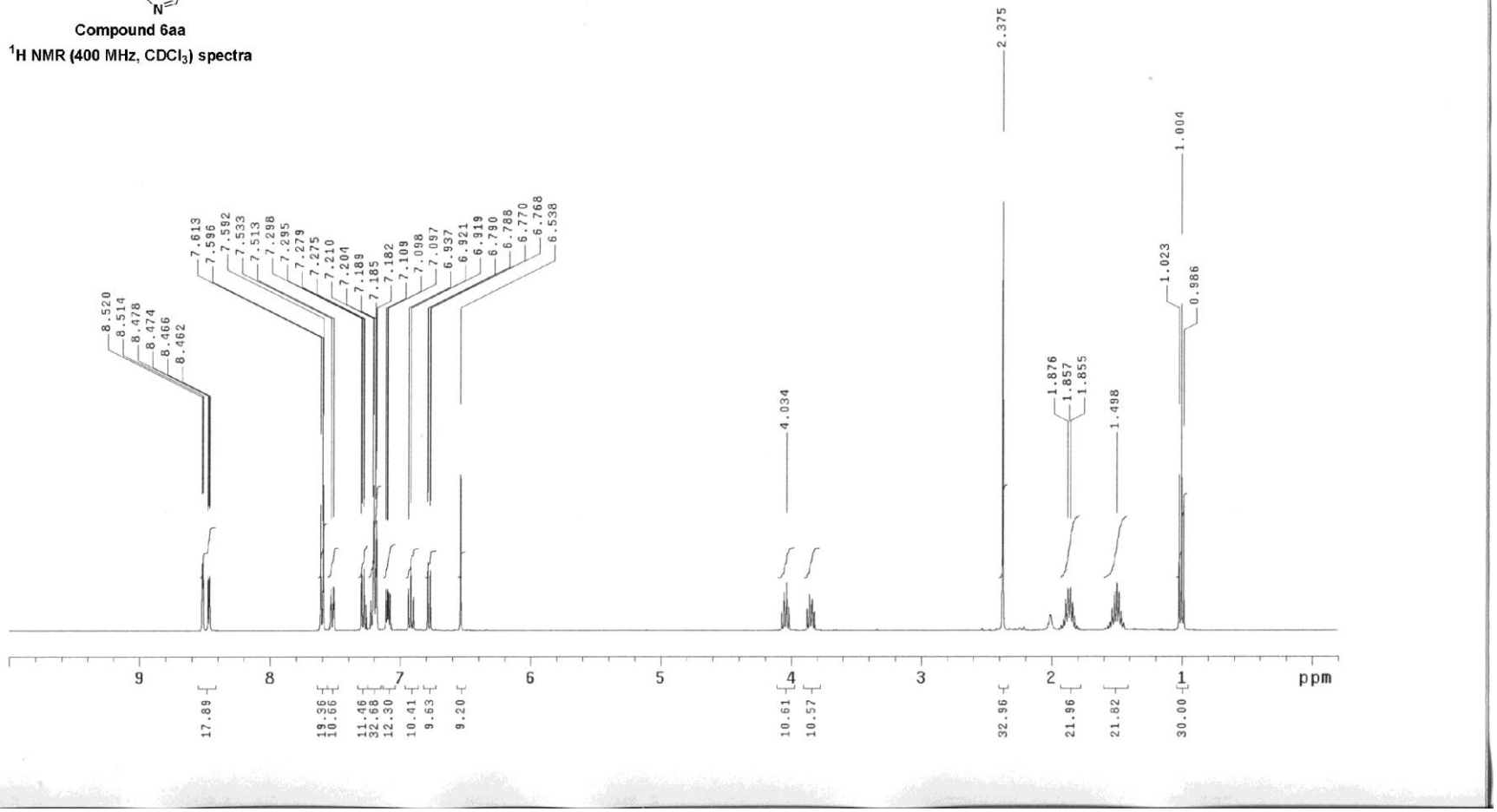
HAK1A14Bu

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Jan 23 2018
Solvent: CDCl3
Ambient temperature
Total 32 repetitions



Compound 6aa

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

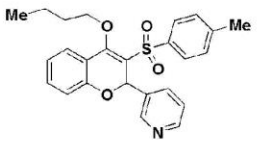


Compound 6aa (^{13}C-NMR spectral data)

HAK1A14Bu

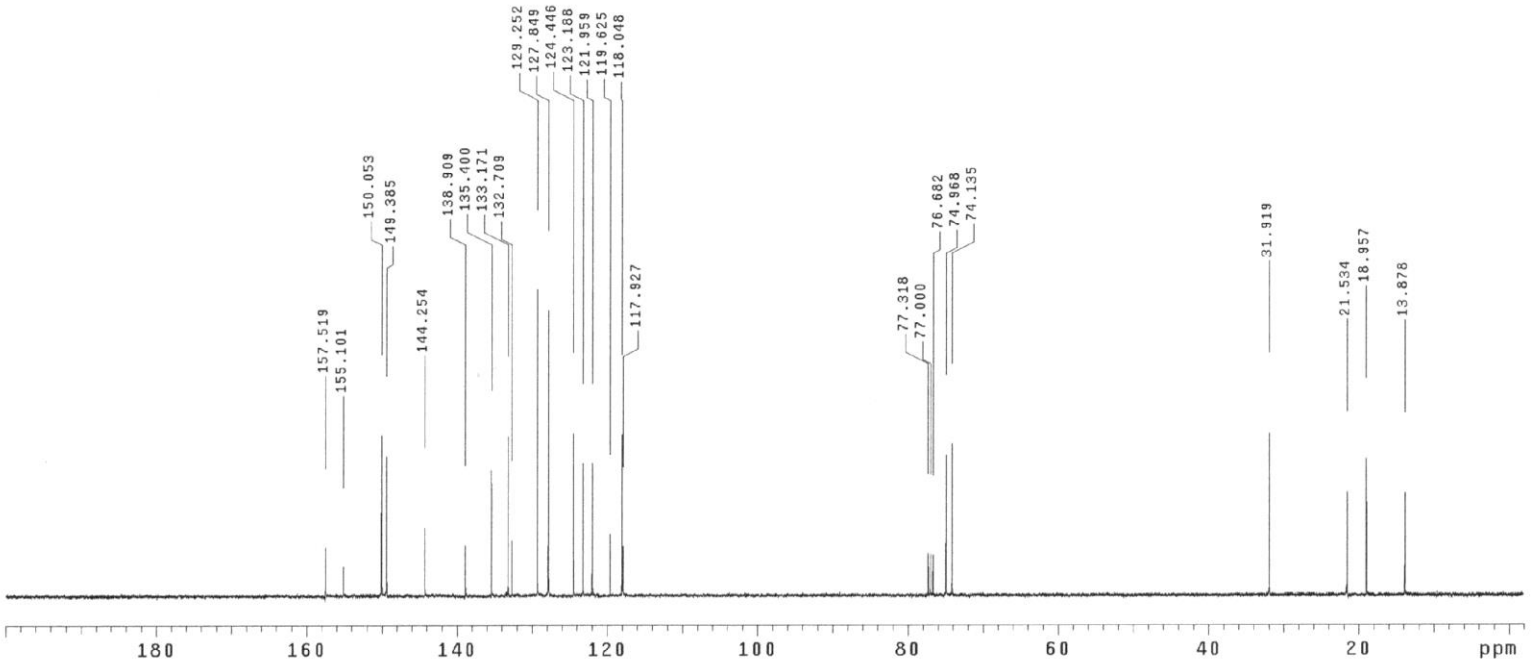
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Jan 23 2018
Solvent: CDCl3
Ambient temperature
Total 1040 repetitions



Compound 6aa

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

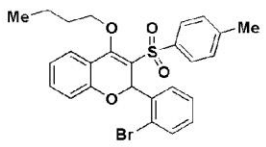


Compound 6ab (^{1}H-NMR spectral data)

HABrBu

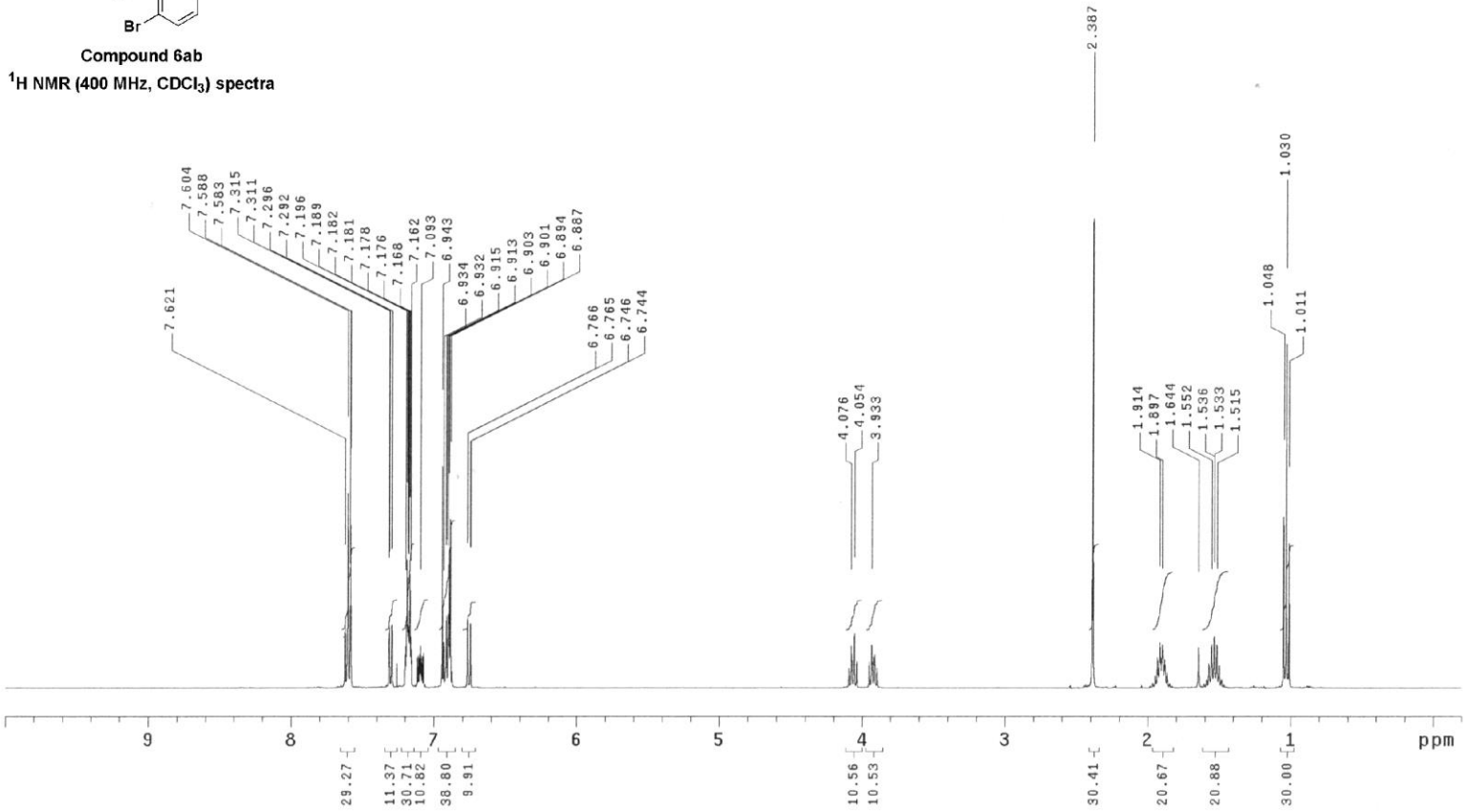
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Feb 7 2018
Solvent: CDCl3
Ambient temperature
Total 64 repetitions



Compound 6ab

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

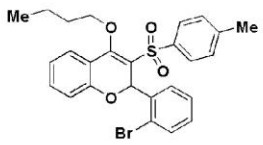


Compound 6ab (^{13}C-NMR spectral data)

HABrBu

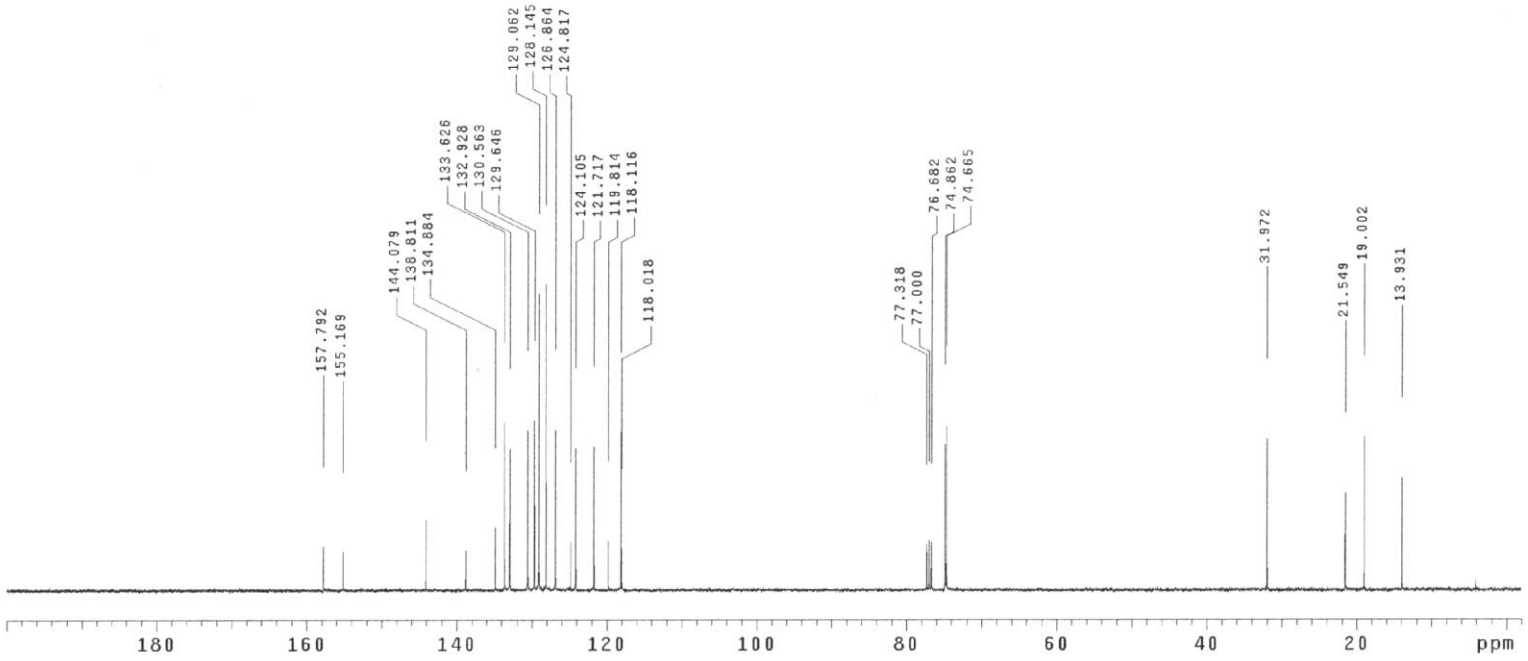
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Feb 7 2018
Solvent: CDCl3
Ambient temperature
Total 25600 repetitions



Compound 6ab

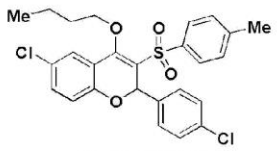
^{13}C NMR (100 MHz, $CDCl_3$) spectra



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

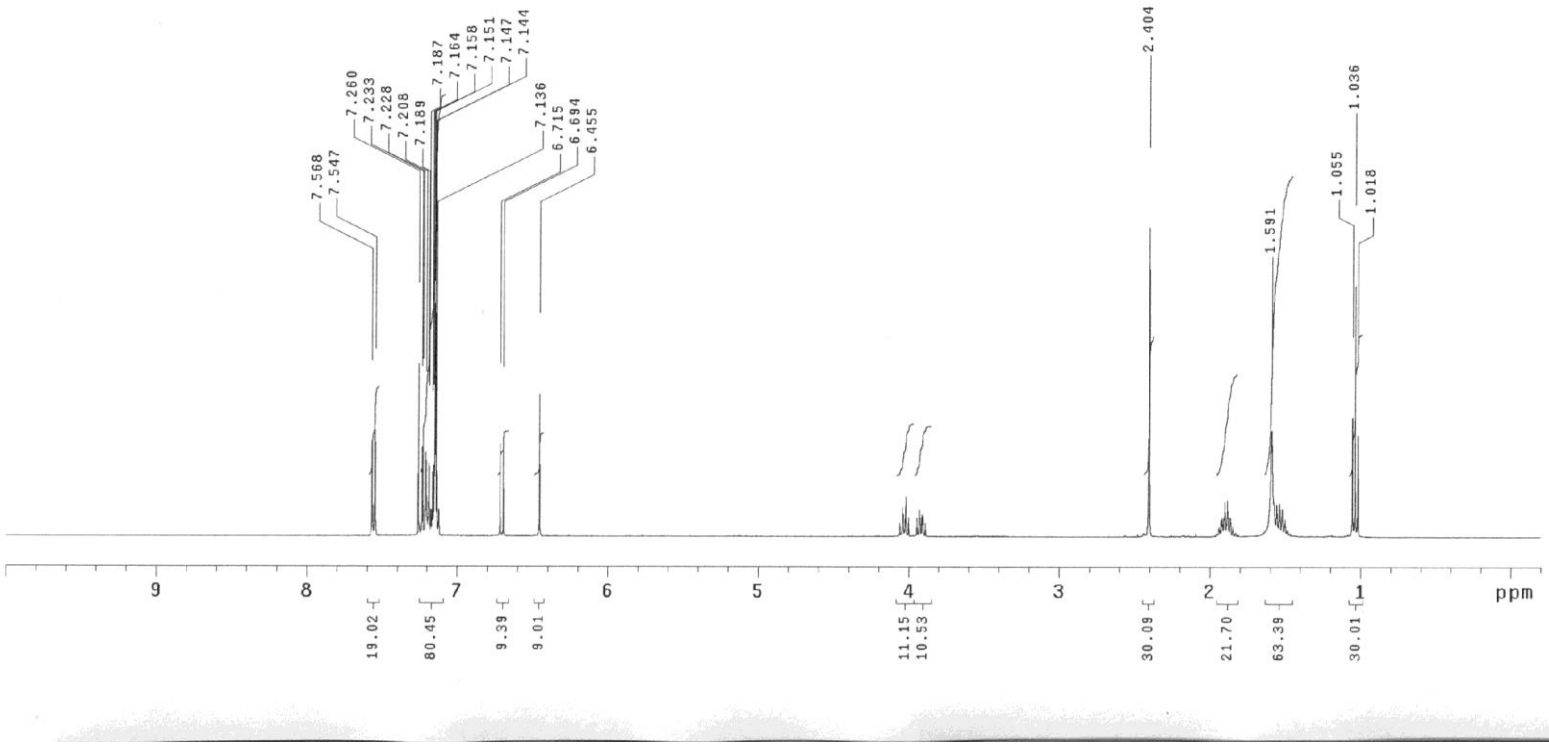
HAK21A12Bu

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Jan 19 2018
Solvent: CDCl3
Ambient temperature
Total 96 repetitions



Compound 6ac

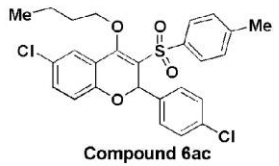
^{1}H NMR (400 MHz, $CDCl_3$) spectra



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

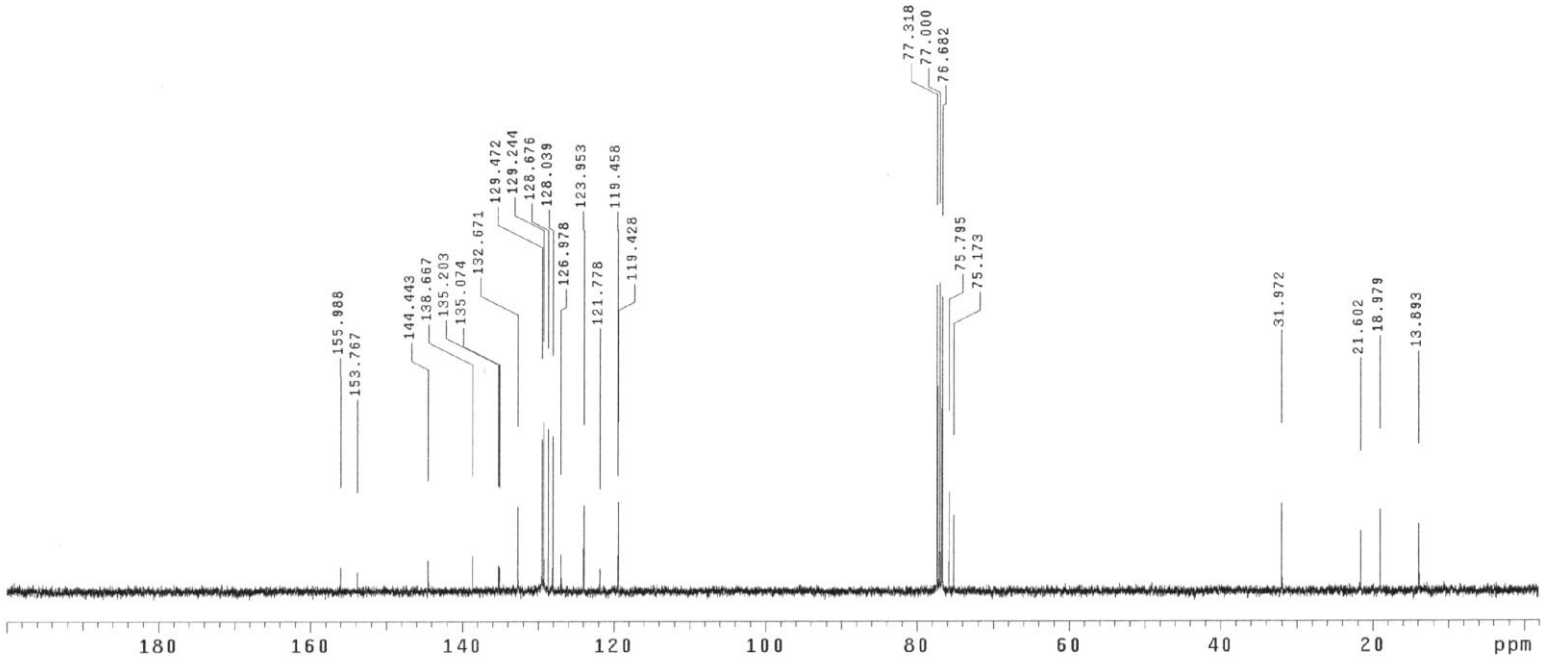
HAK21A12Bu

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Jan 19 2018
Solvent: CDCl3
Ambient temperature
File: U0032-20
Total 2432 repetitions

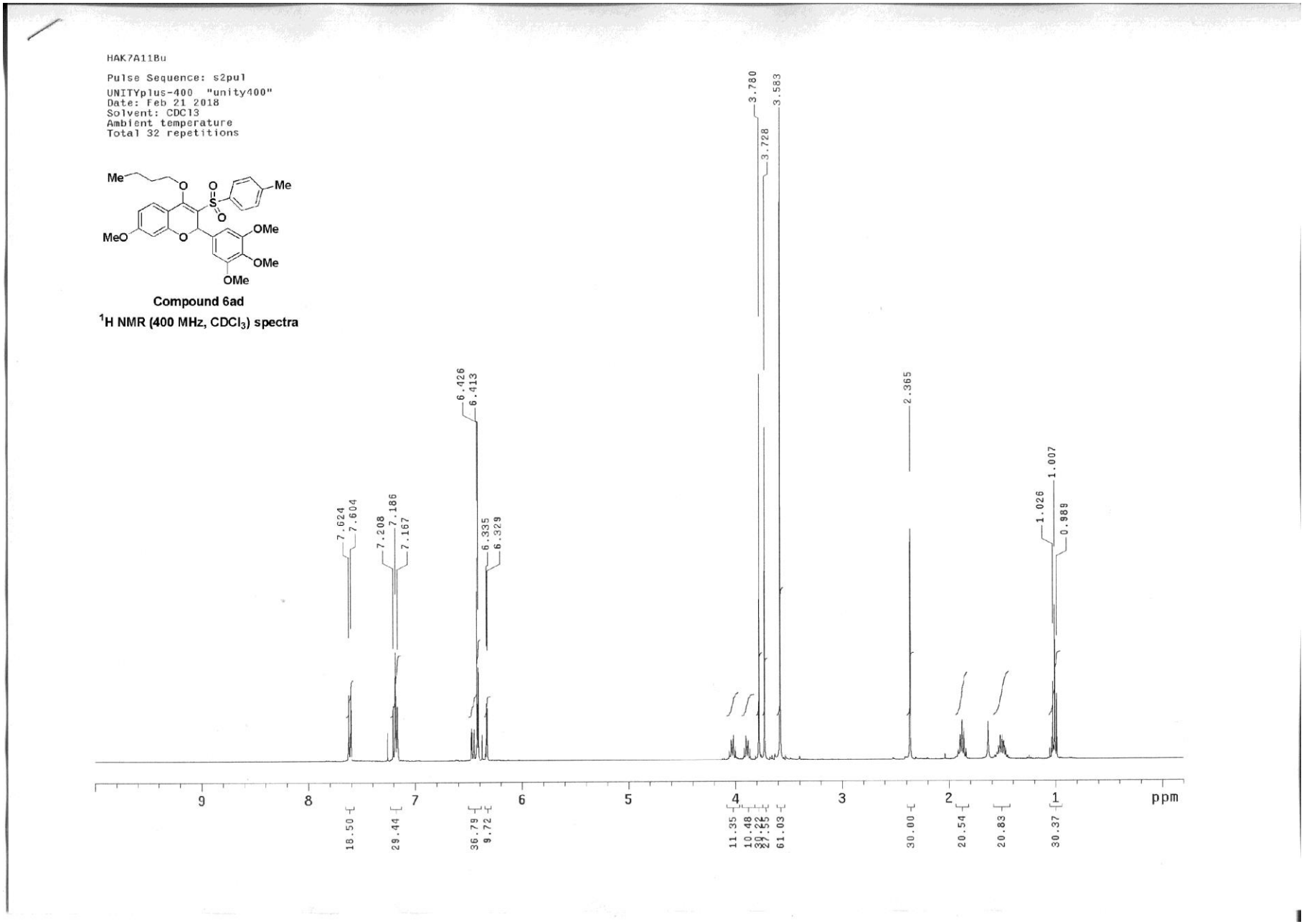


Compound 6ac

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



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

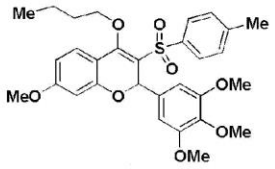


Compound 6ad (^{13}C-NMR spectral data)

HAK7A11Bu

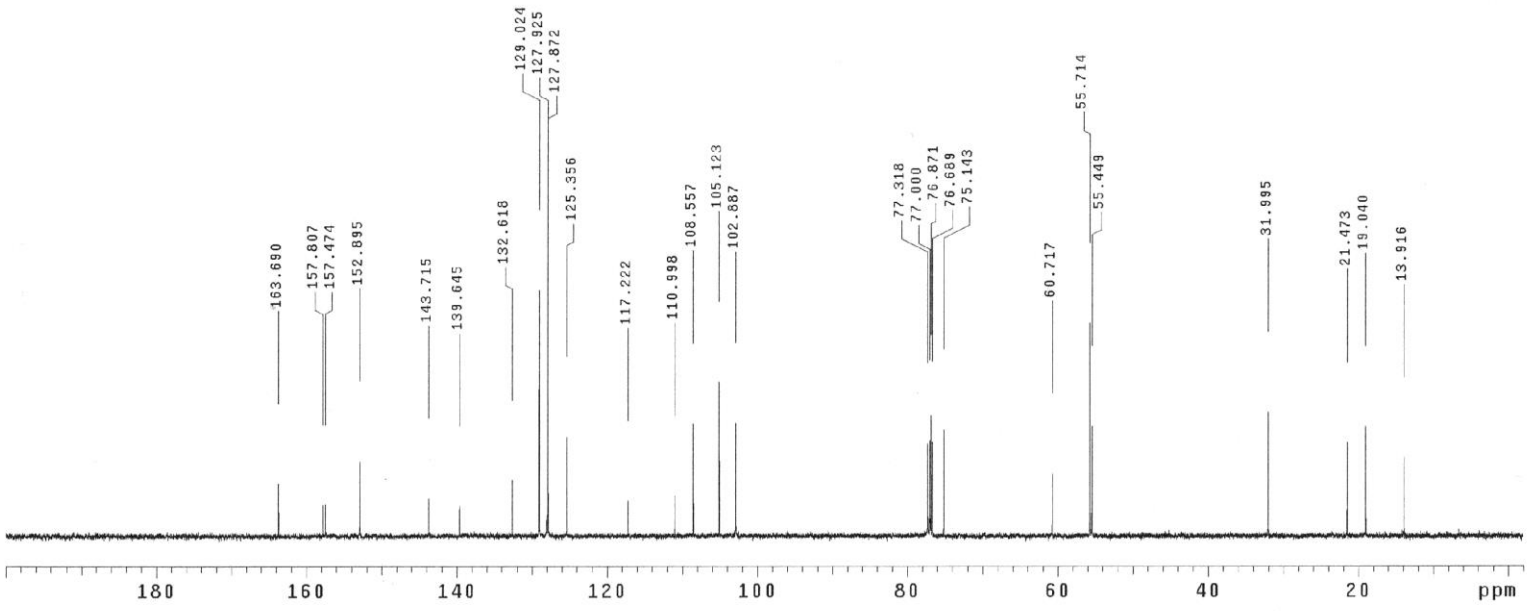
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Feb 21 2018
Solvent: CDCl3
Ambient temperature
Total 1312 repetitions



Compound 6ad

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

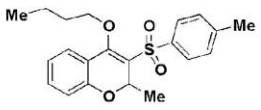


Compound 6ae (^{1}H-NMR spectral data)

HAK1A15Bu

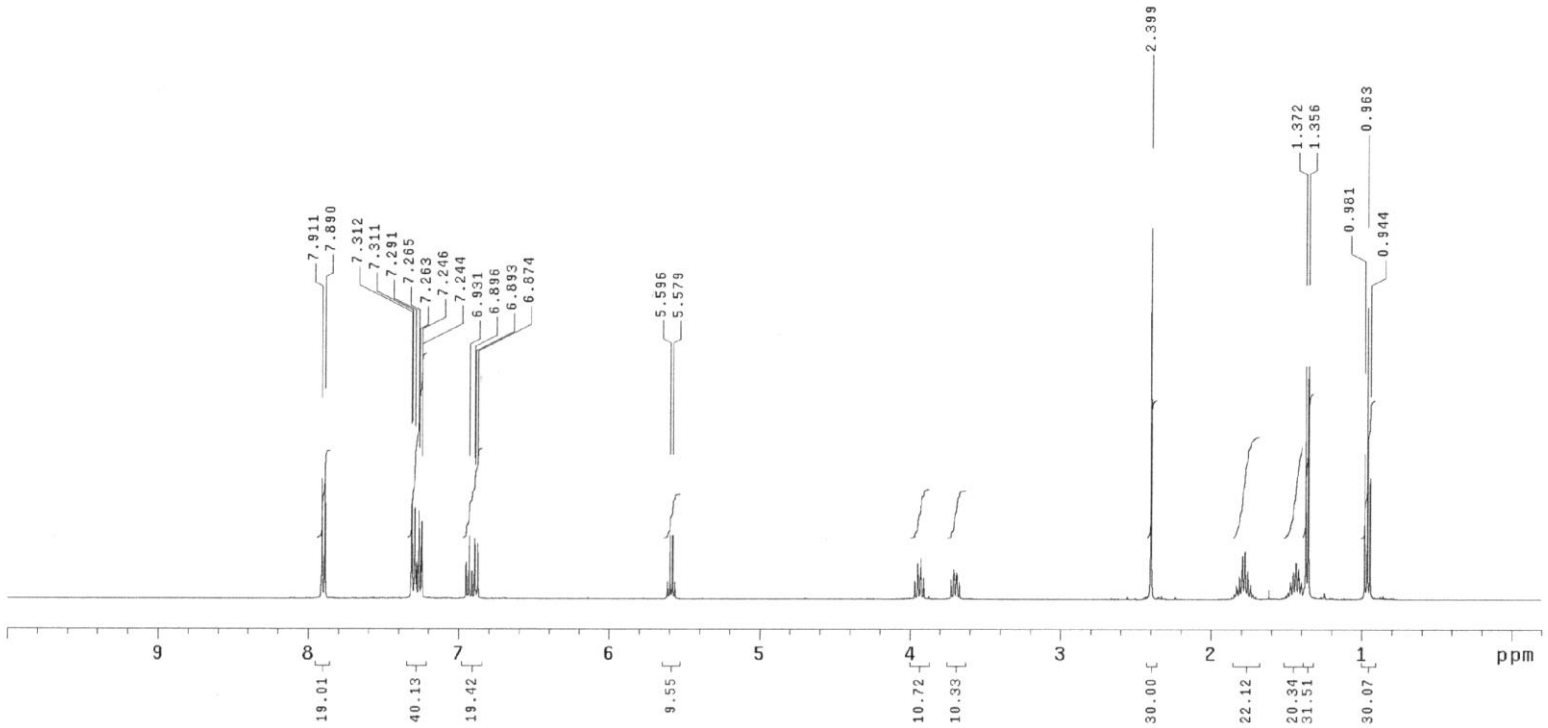
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Mar 6 2018
Solvent: CDCl3
Ambient temperature
Total 32 repetitions



Compound 6ae

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

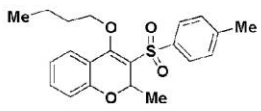


Compound 6ae (^{13}C-NMR spectral data)

HAK1A15Bu

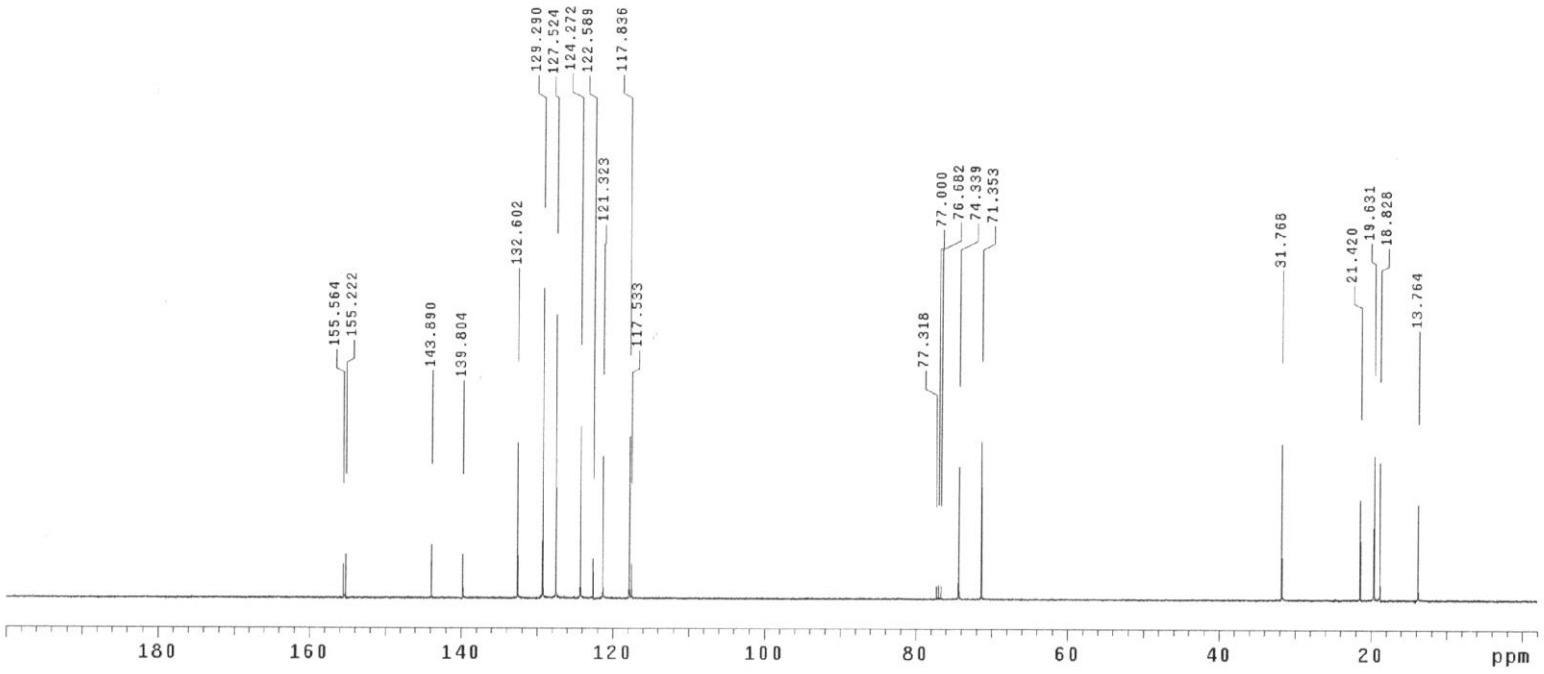
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Mar 6 2018
Solvent: CDCl3
Ambient temperature
Total 320 repetitions



Compound 6ae

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

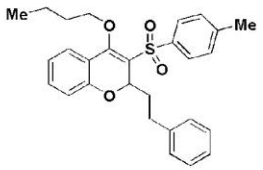


Compound 6af (^{1}H-NMR spectral data)

HA2CPhBu

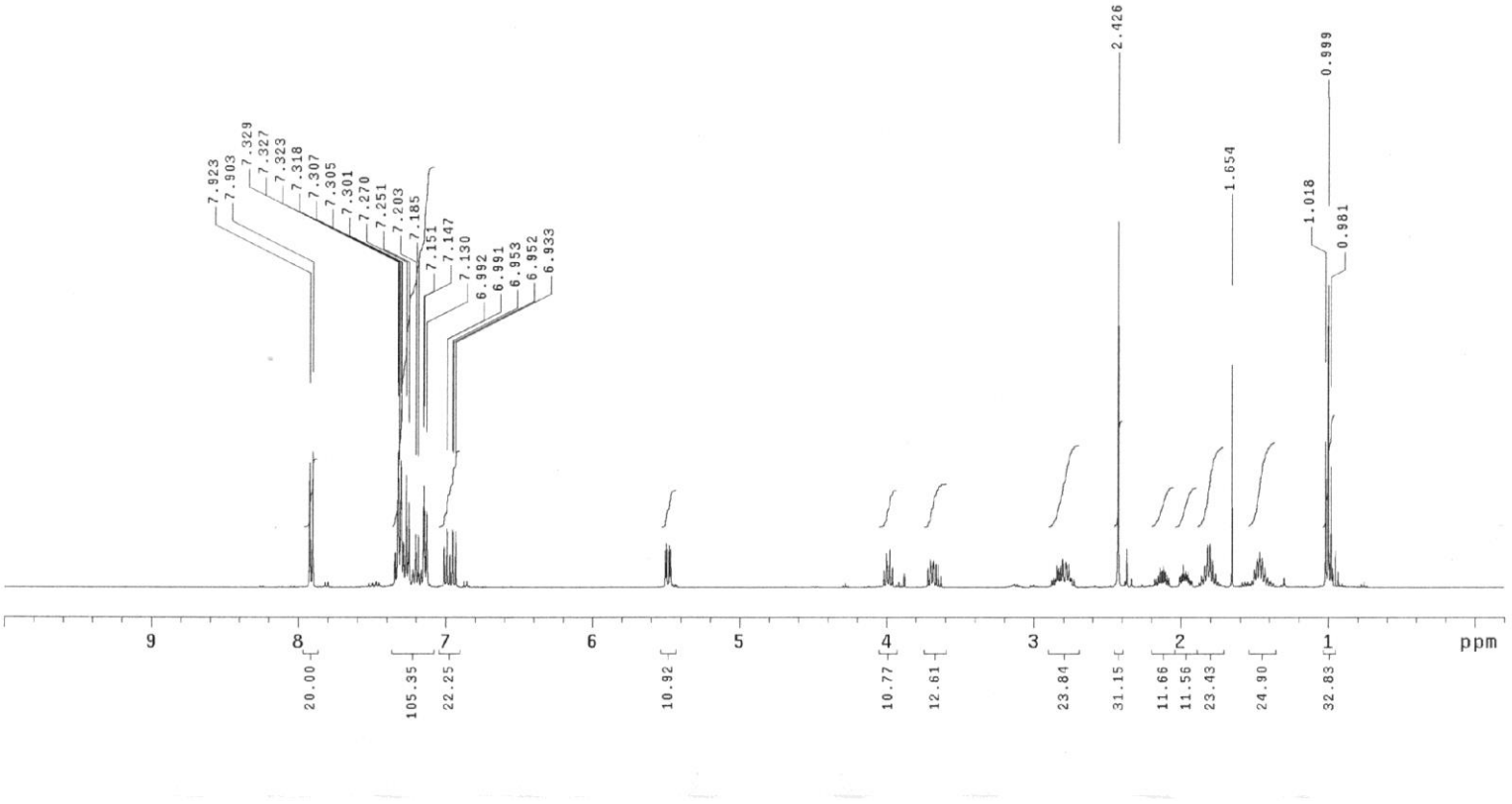
Pulse Sequence: s2pul

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



Compound 6af

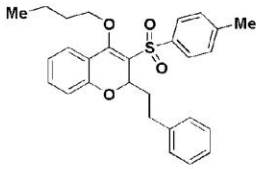
^{1}H NMR (400 MHz, $CDCl_3$) spectra



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

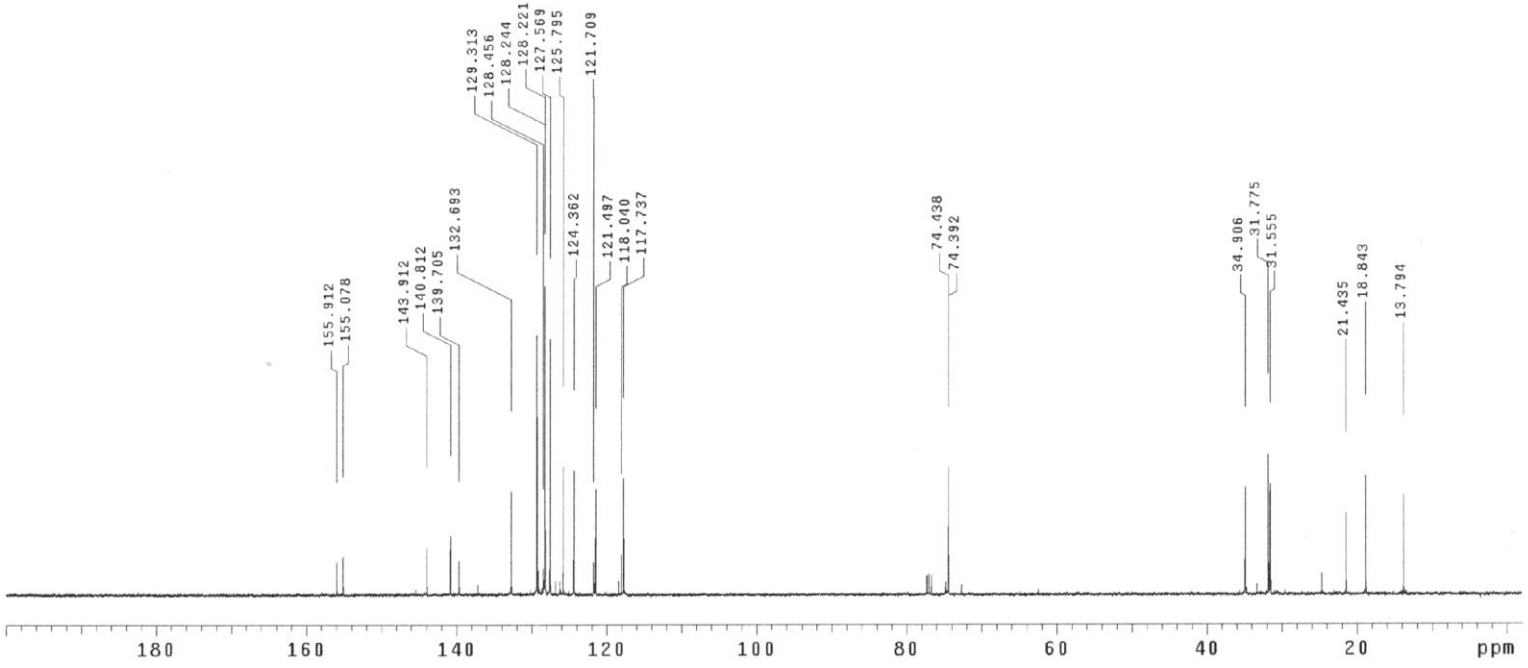
HA2CPhBu

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Mar 5 2018
Solvent: CDCl3
Ambient temperature
Total 128 repetitions



Compound 6af

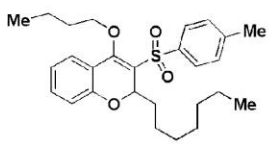
^{13}C NMR (100 MHz, $CDCl_3$) spectra



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

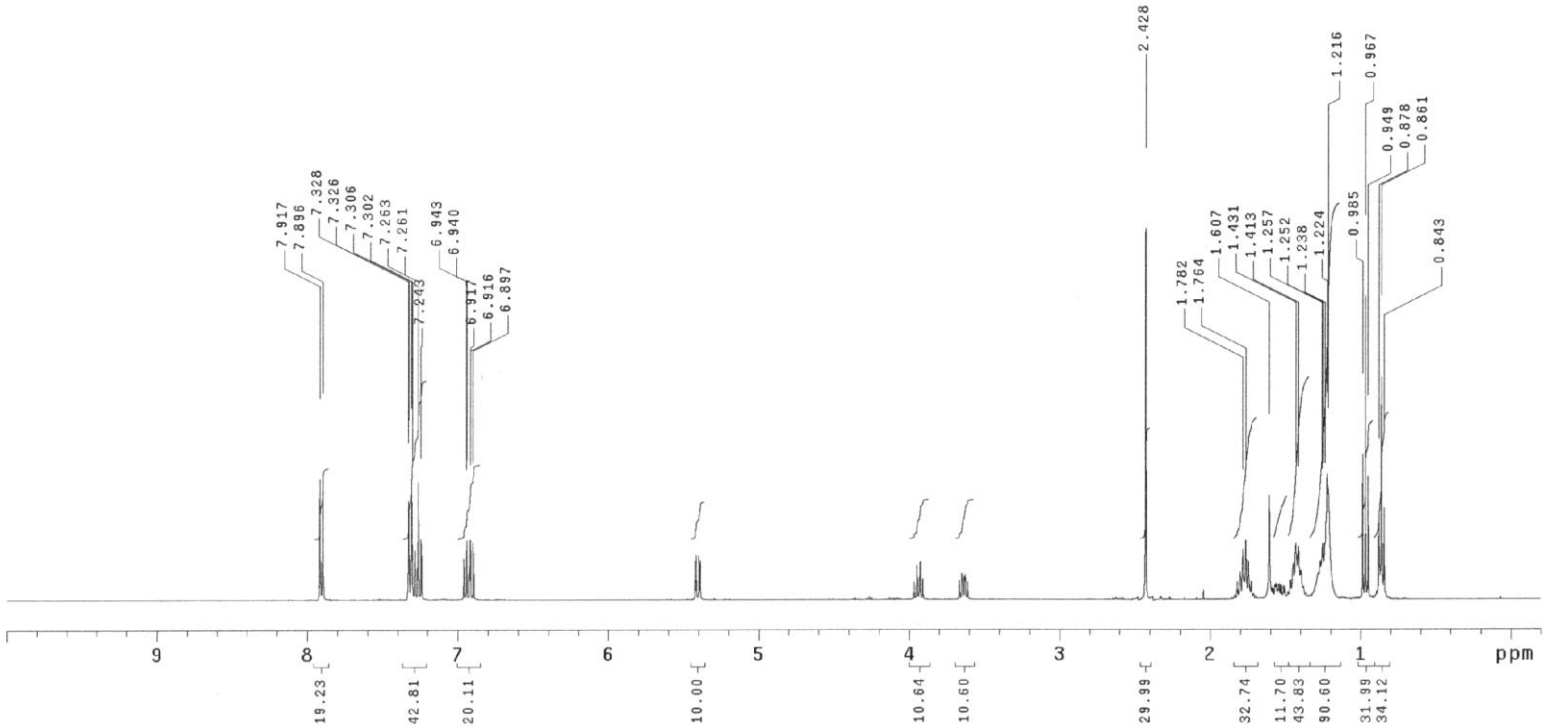
HA7CBu

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Mar 5 2018
Solvent: CDCl3
Ambient temperature
Total 32 repetitions



Compound 6ag

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

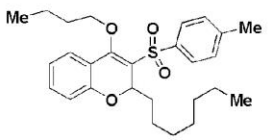


Compound 6ag (^{13}C-NMR spectral data)

HA7CBu

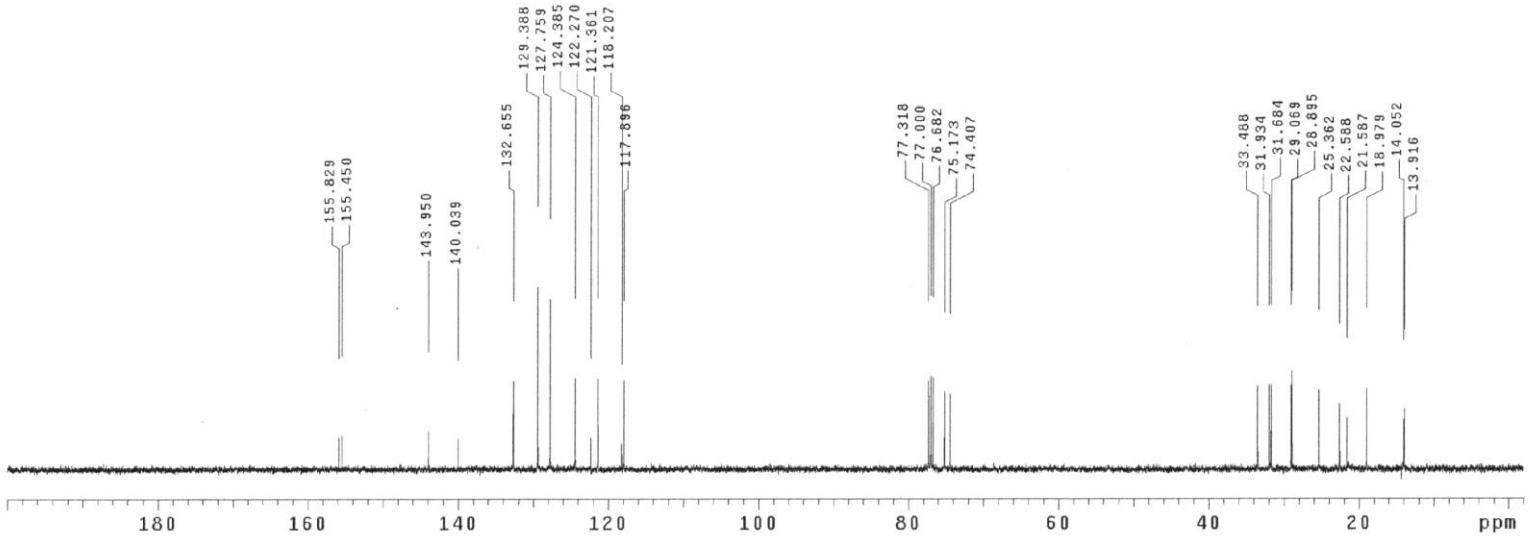
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Mar 5 2018
Solvent: CDCl3
Ambient temperature
Total 1056 repetitions

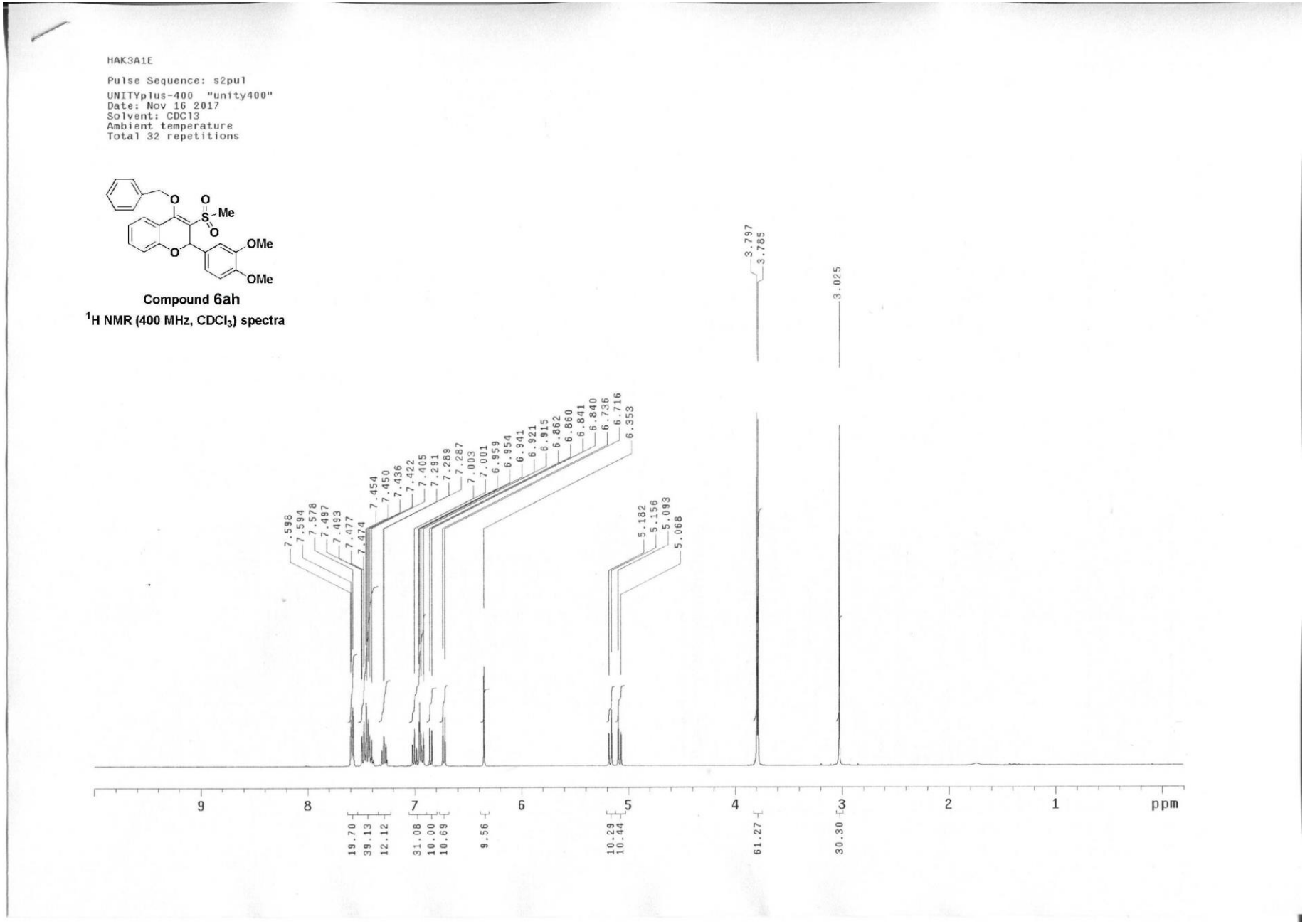


Compound 6ag

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



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

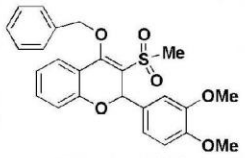


Compound 6ah (^{13}C-NMR spectral data)

HAK3A1E

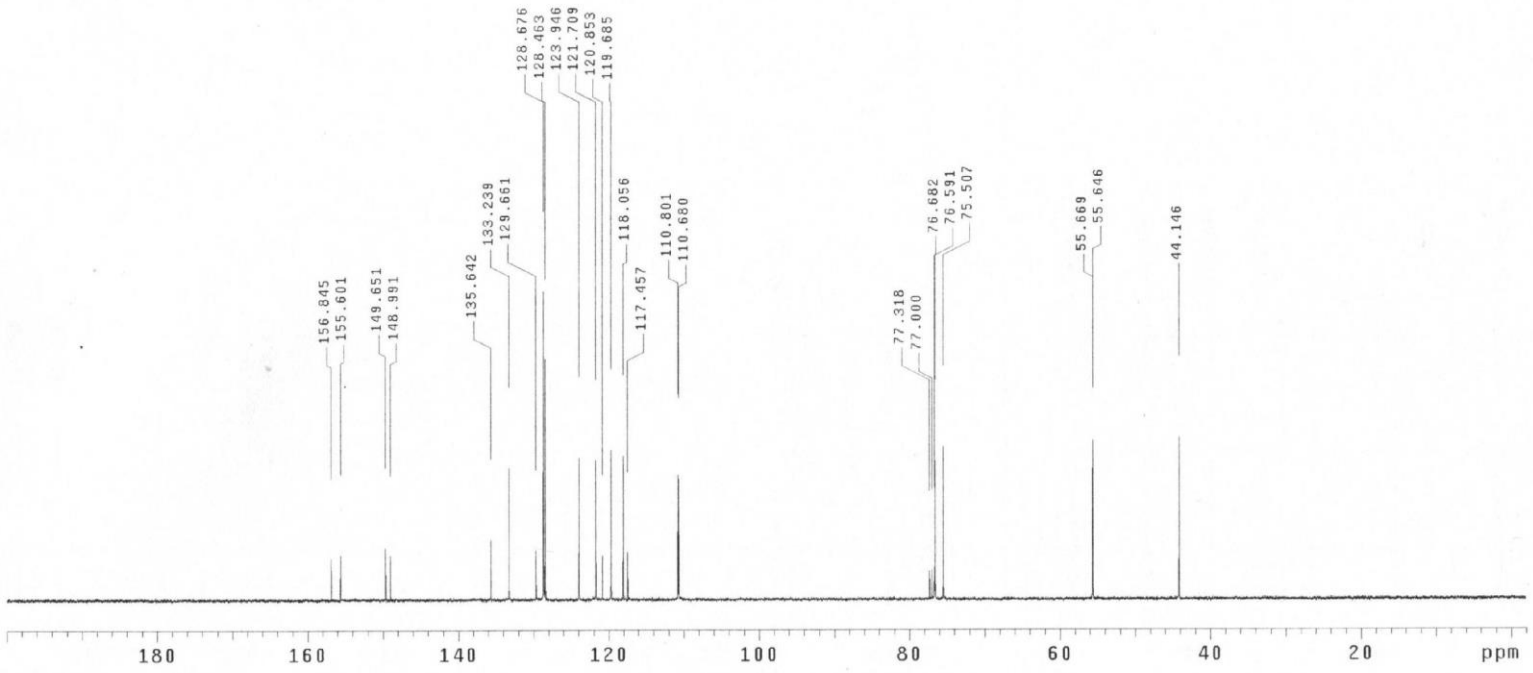
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Nov 16 2017
Solvent: CDCl3
Ambient temperature
Total 320 repetitions

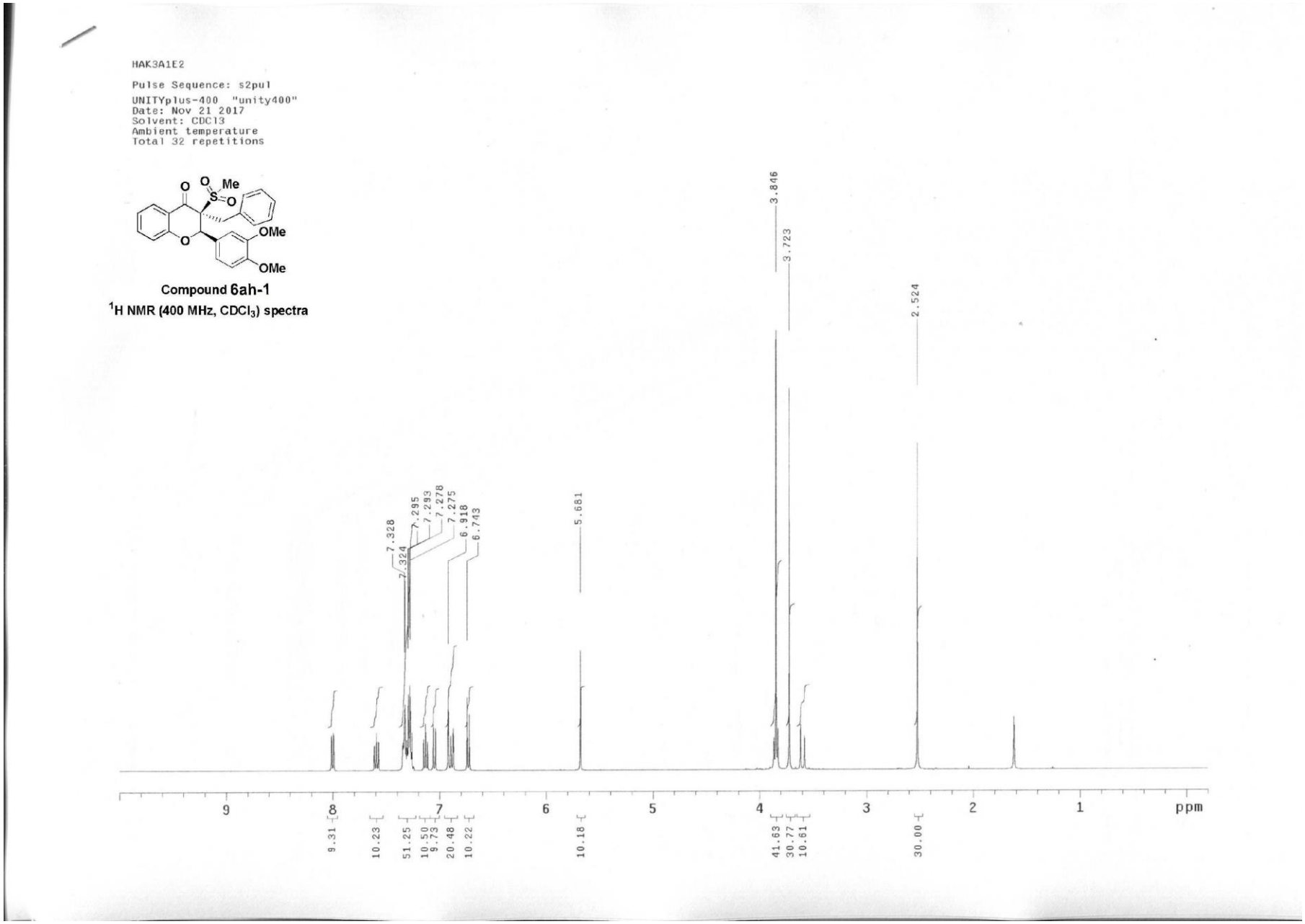


Compound **6ah**

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



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

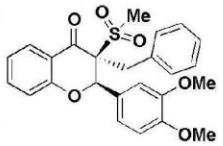


Compound 6ah-1 (^{13}C-NMR spectral data)

HAK3A1E2

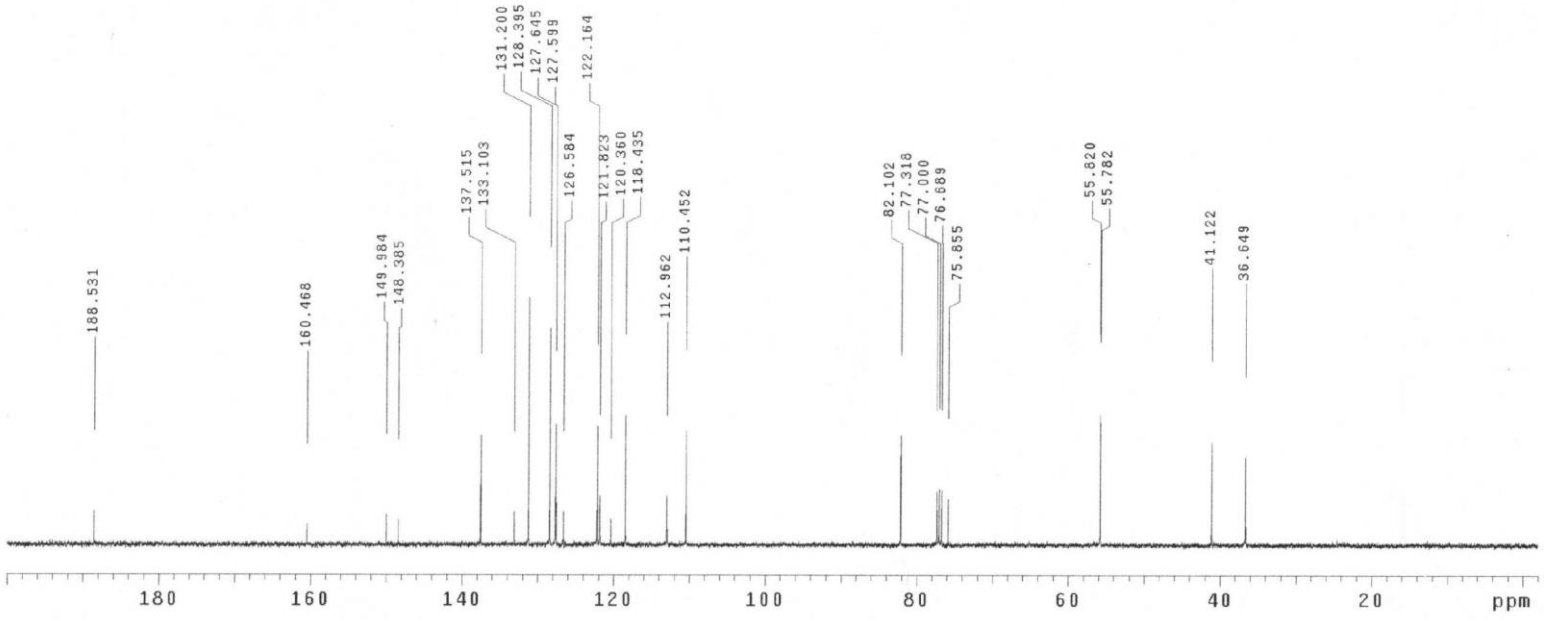
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Nov 21 2017
Solvent: CDCl3
Ambient temperature
Total 1264 repetitions



Compound **6ah-1**

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



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

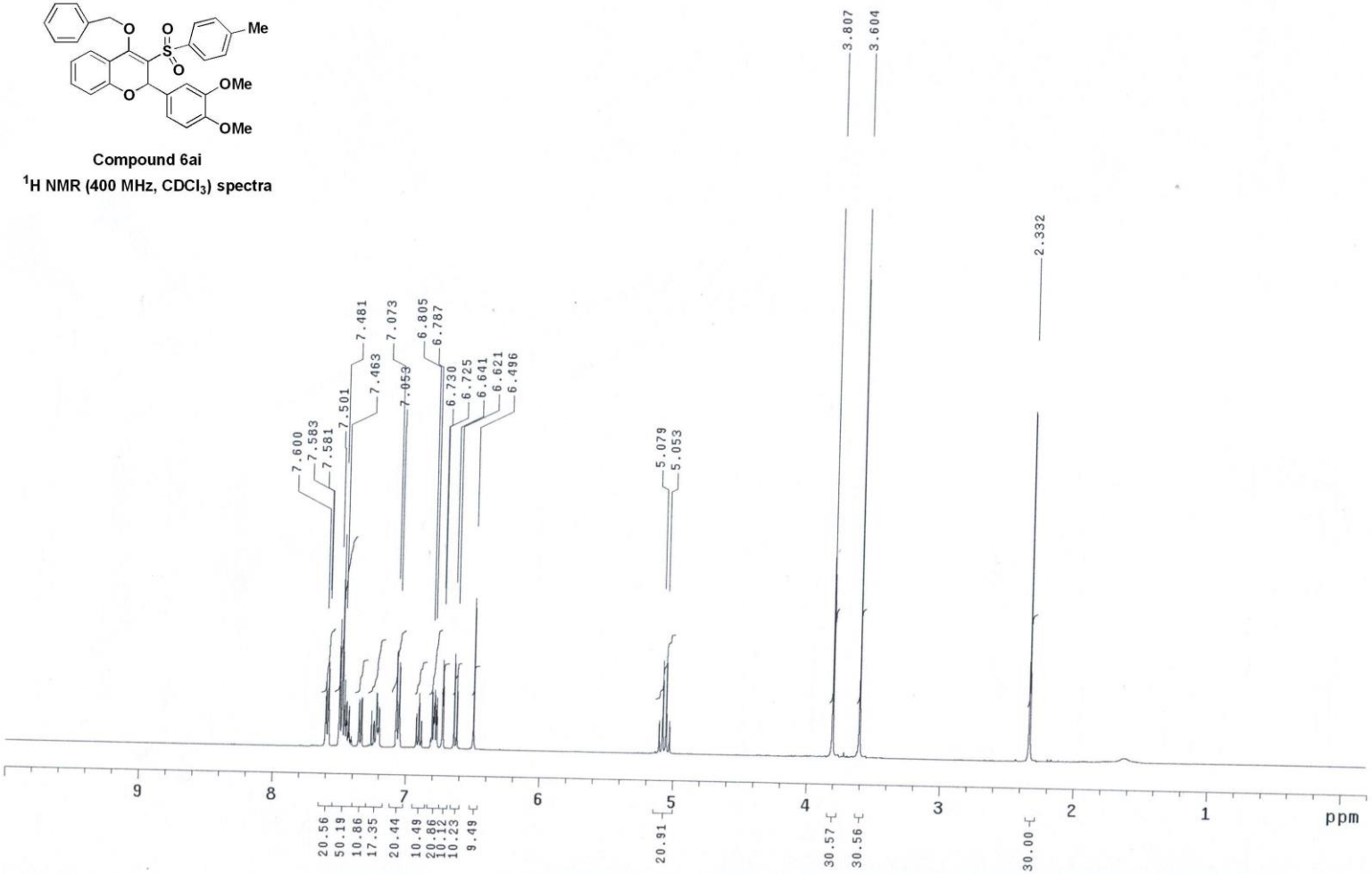
HAK1Bn

Pulse Sequence: s2pul

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

Compound 6ai

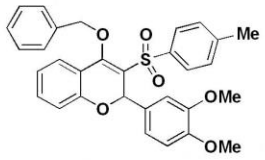
^{1}H NMR (400 MHz, $CDCl_3$) spectra



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

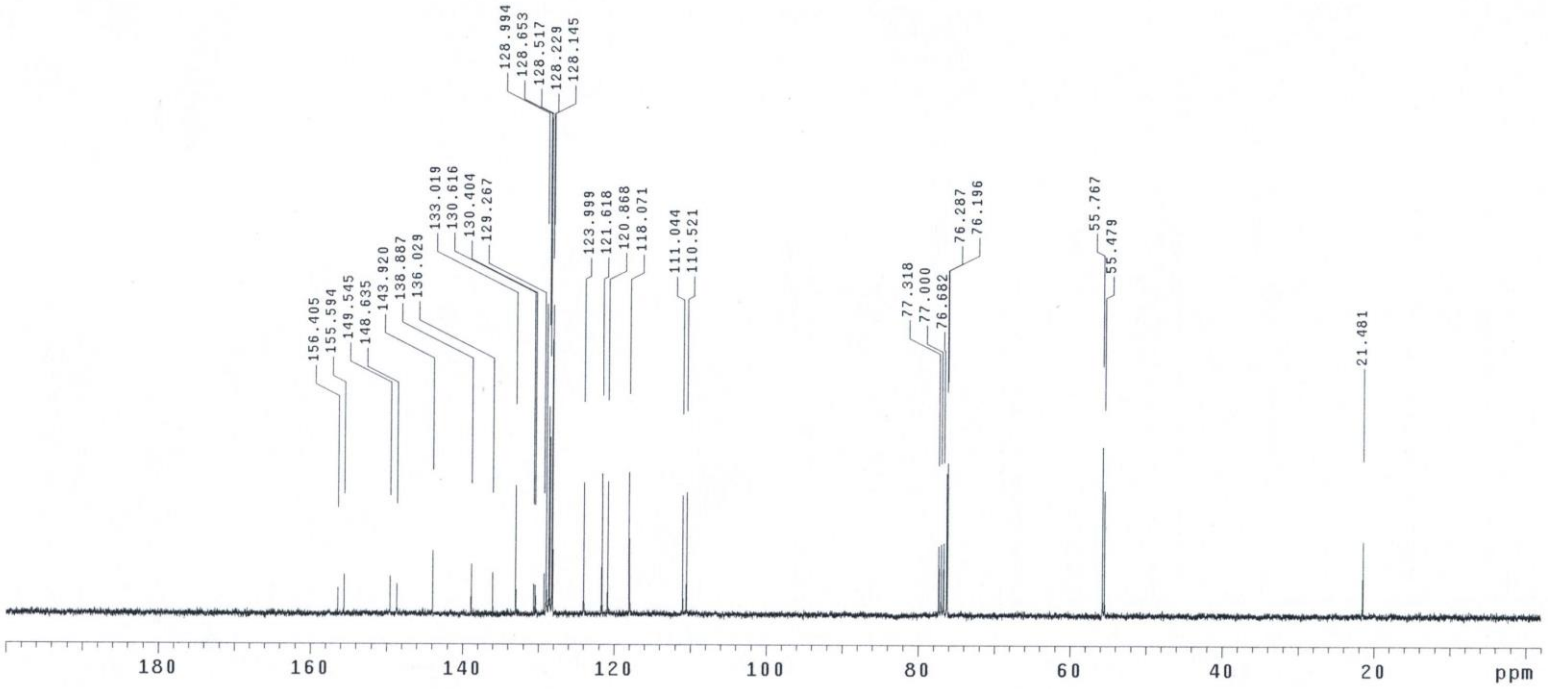
HAK1Bn

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Mar 14 2018
Solvent: CDCl3
Ambient temperature
Total 800 repetitions



Compound 6ai

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

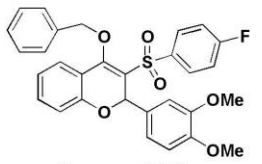


Compound 6aj (^{1}H-NMR spectral data)

HAK5BnF

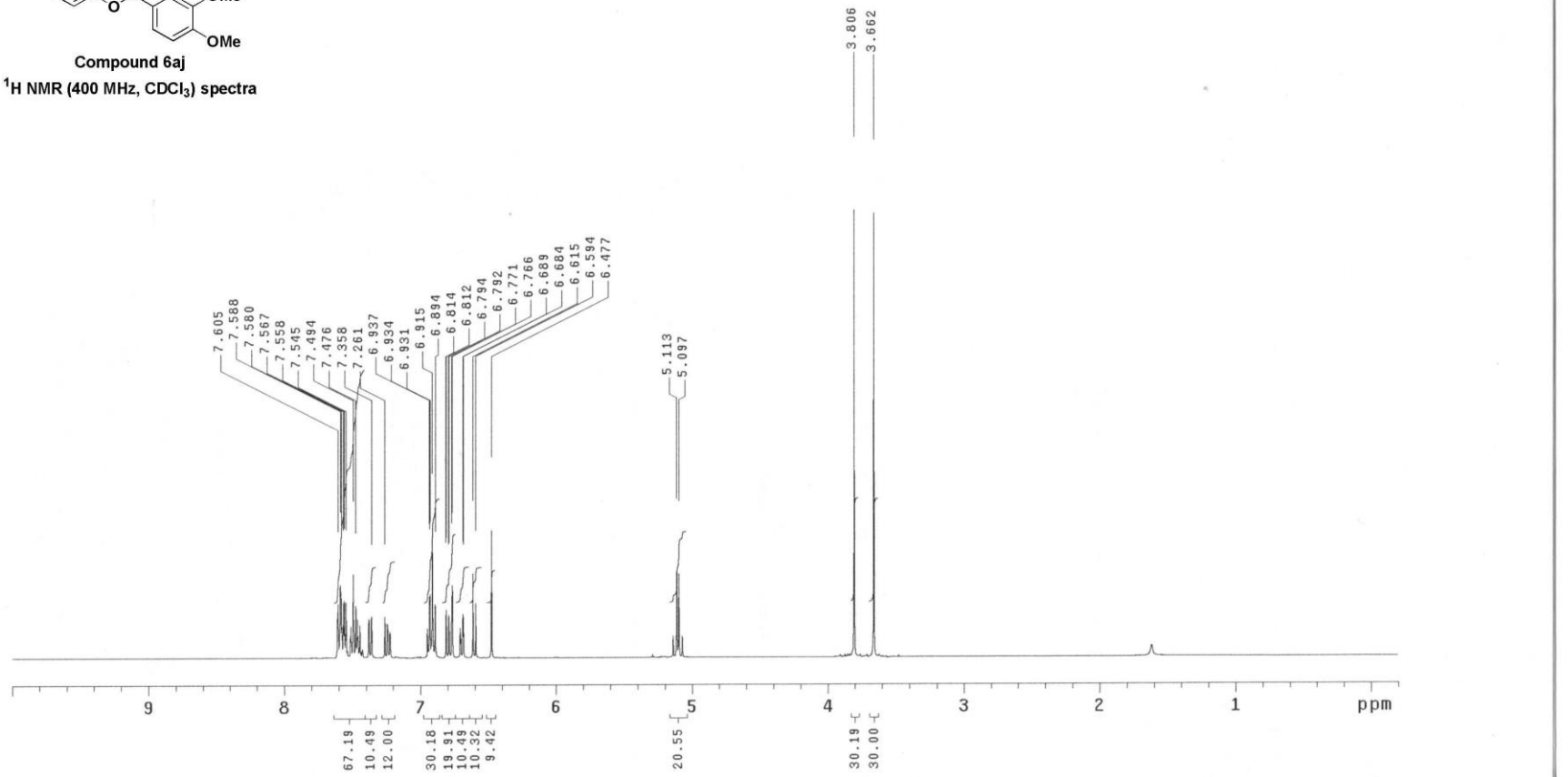
Pulse Sequence: s2pul

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



Compound 6aj

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

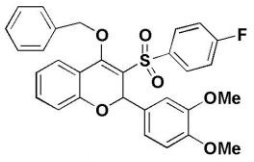


Compound 6aj (^{13}C-NMR spectral data)

HAK5BnF

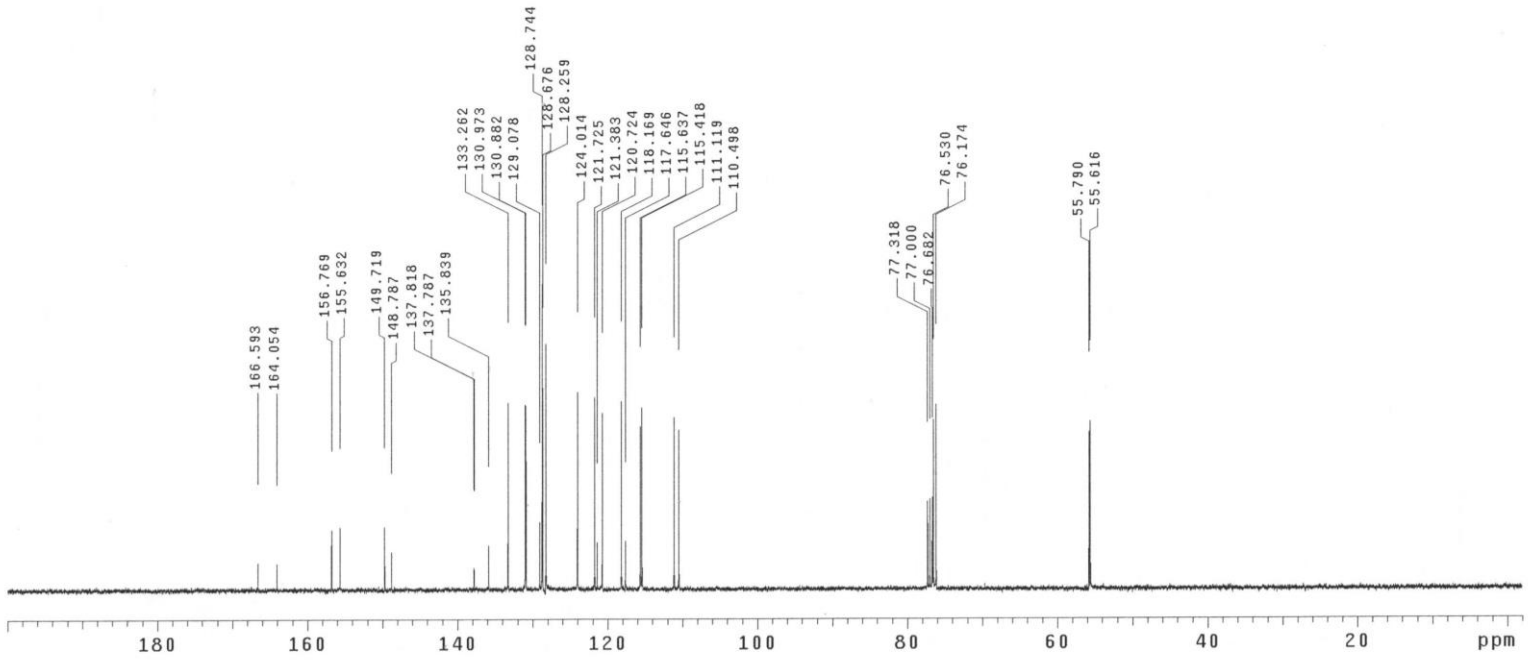
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: Mar 15 2018
Solvent: CDCl3
Ambient temperature
Total 2160 repetitions

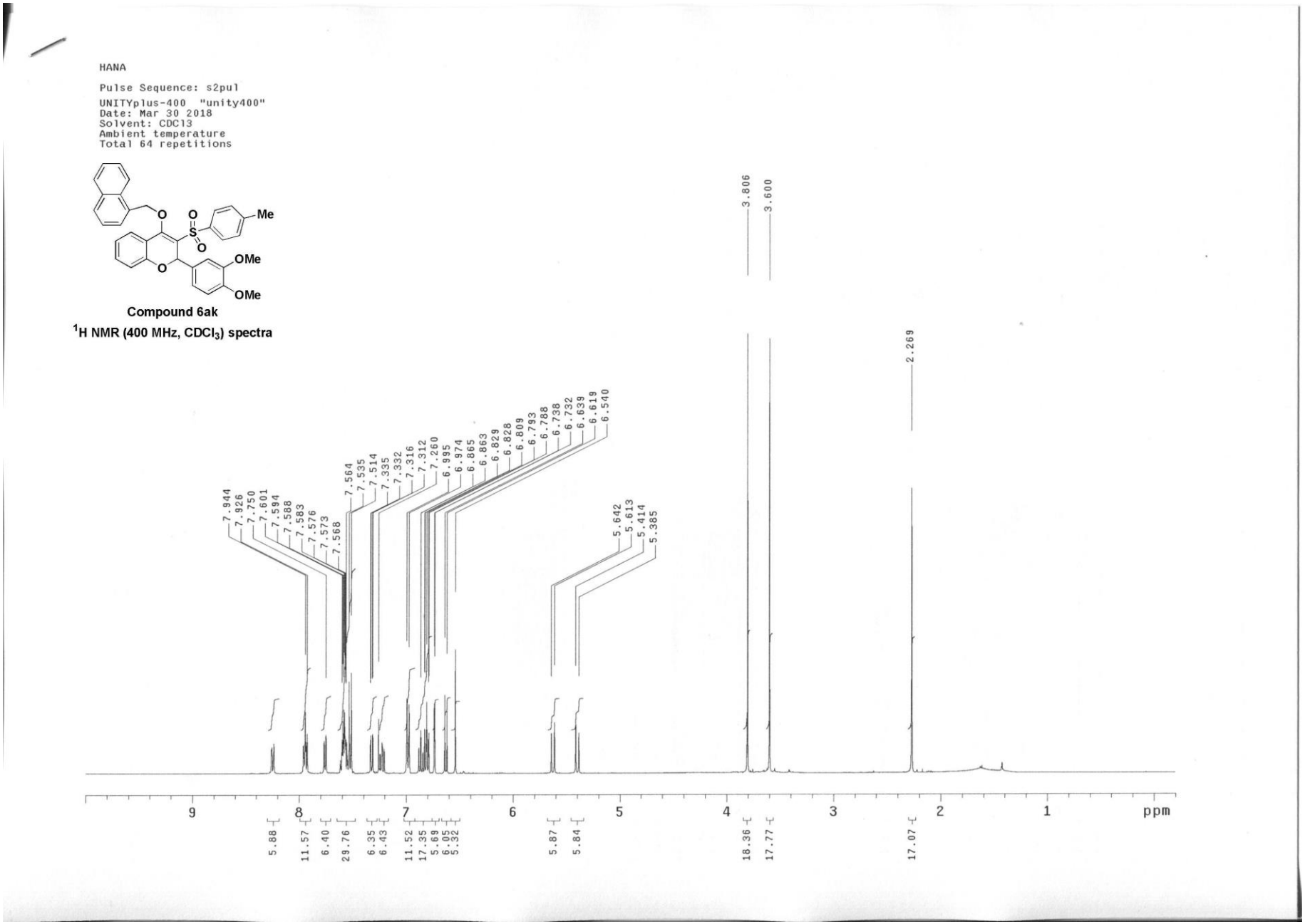


Compound 6aj

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



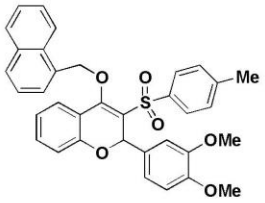
Compound 6ak (^{1}H-NMR spectral data)



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

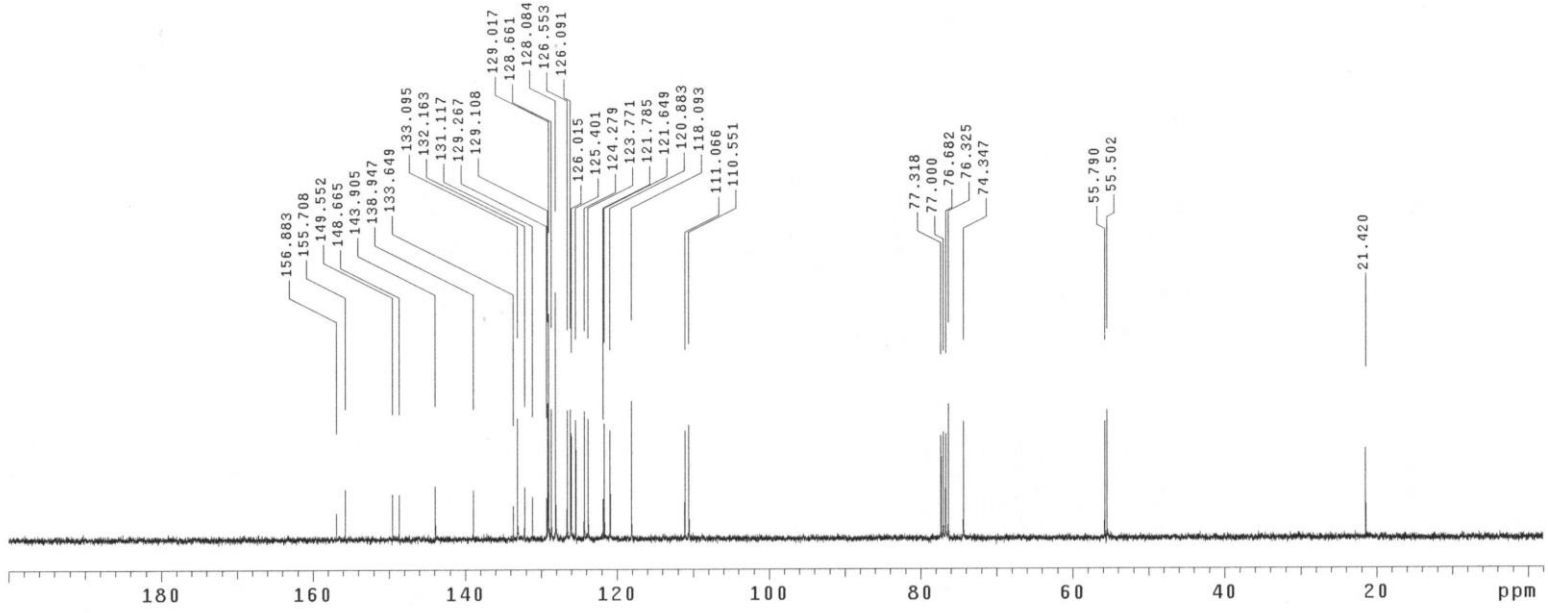
HANA

Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Mar 30 2018
Solvent: CDCl3
Ambient temperature
Total 2224 repetitions



Compound 6ak

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

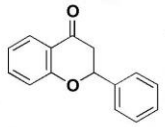


Compound 8a (^{1}H-NMR spectral data)

HAPhone

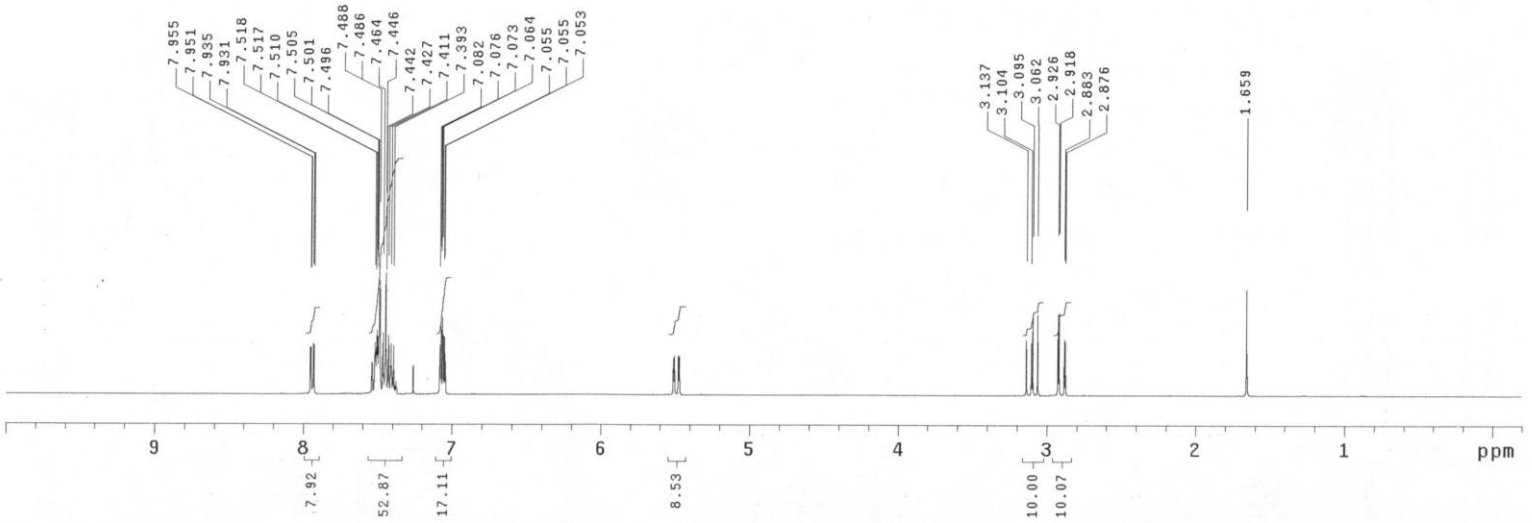
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 14 2019
Solvent: CDCl3
Ambient temperature
Total 32 repetitions



Compound 8a

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

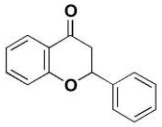


Compound 8a (^{13}C-NMR spectral data)

HAPhone

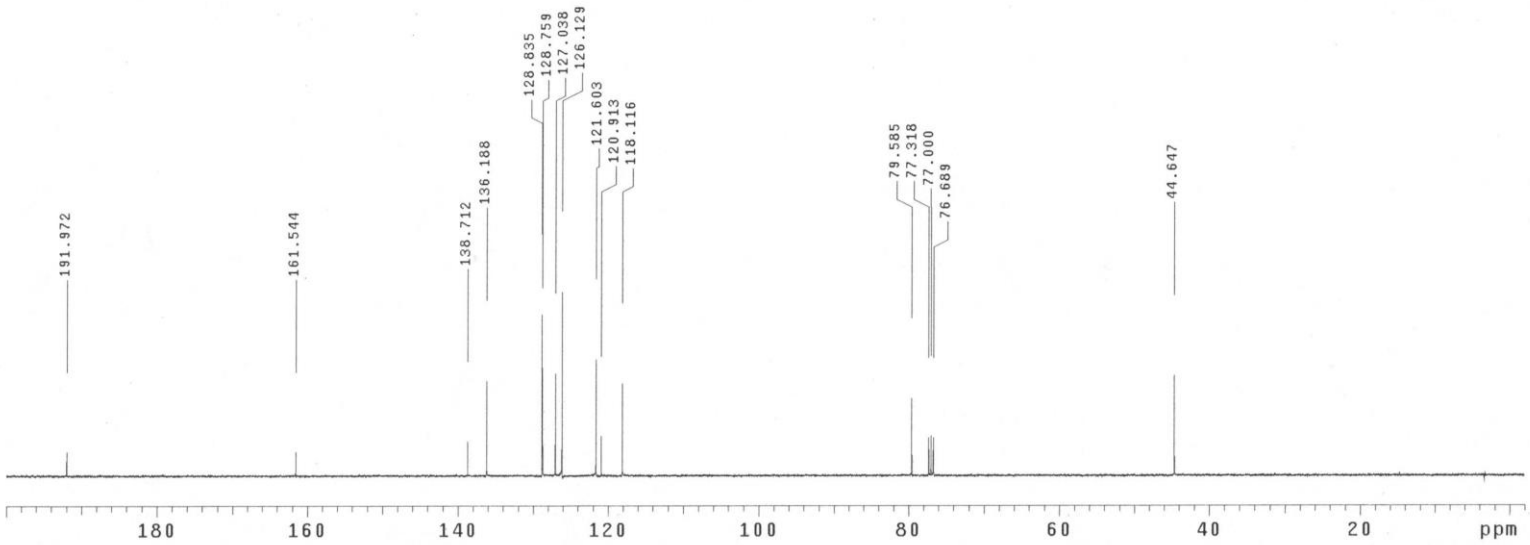
Pulse Sequence: s2pul

UNITYplus-400 "unity400"
Date: May 14 2019
Solvent: CDCl3
Ambient temperature
Total 2112 repetitions

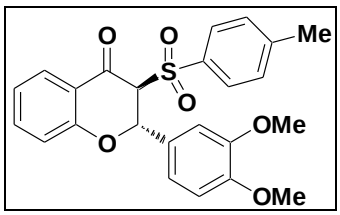


Compound 8a

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



X-ray crystal data of 4a



Empirical formula	C24 H22 O6 S	
Formula weight	438.47	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/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>2sigma(I)]	R1 = 0.0383, wR2 = 0.0960	
R indices (all data)	R1 = 0.0488, wR2 = 0.1084	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.291 and -0.358 e.$Å^{-3}$	

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 171121LT

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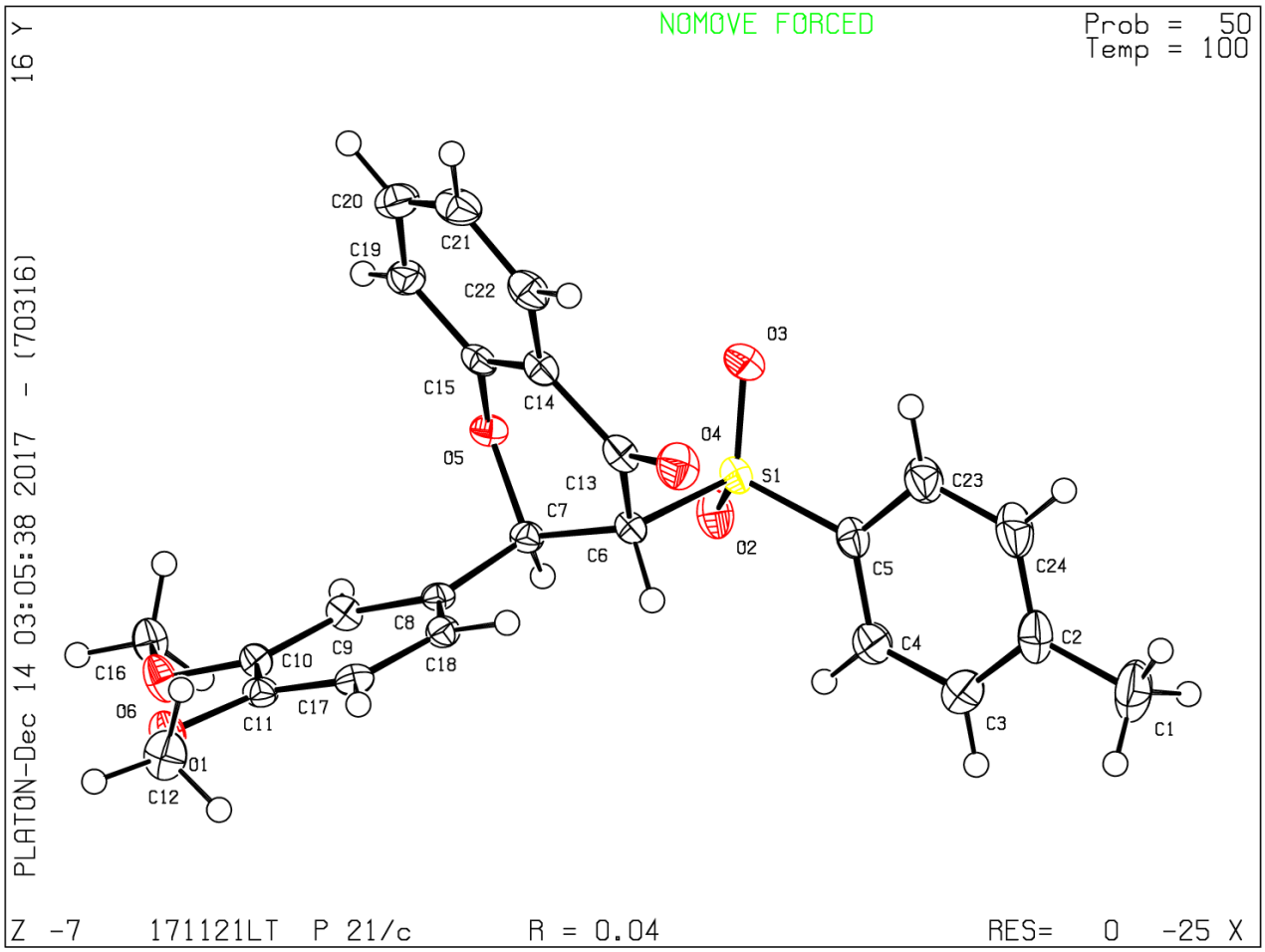
No syntax errors found. CIF dictionary Interpreting this report

Datablock: 171121LT

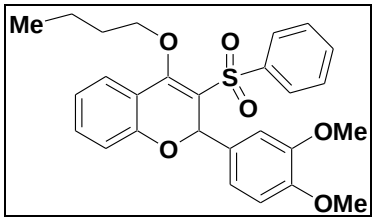
```
Bond precision:  C-C = 0.0026 A          Wavelength=0.71073

Cell:            a=21.002(3)     b=11.9195(15)      c=8.3067(11)
                 alpha=90        beta=97.290(5)     gamma=90
Temperature:     100 K

                 Calculated                Reported
Volume           2062.6(5)                 2062.6(5)
Space group      P 21/c                    P 21/c
Hall group       -P 2ybc                   -P 2ybc
Moiety formula   C24 H22 O6 S              ?
Sum formula      C24 H22 O6 S              C24 H22 O6 S
Mr               438.48                    438.47
Dx,g cm-3        1.412                     1.412
Z                4                         4
Mu (mm-1)        0.197                     0.197
F000             920.0                     920.0
F000'            920.97
h,k,lmax         26,14,10                  26,14,10
Nref             4275                      4236
Tmin,Tmax        0.965,0.988               0.893,0.948
Tmin'            0.965

Correction method= # Reported T Limits: Tmin=0.893 Tmax=0.948
AbsCorr = MULTI-SCAN

Data completeness= 0.991          Theta(max)= 26.475

R(reflections)= 0.0383( 3545)     wR2(reflections)= 0.1084( 4236)

S = 1.053                 Npar= 283
```

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

The thermal ellipsoid was drawn at the 50% probability level



X-ray crystal data of 6b



Empirical formula	C27 H28 O6 S	
Formula weight	480.55	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 12.1123(7) Å	α = 90°.
	b = 23.2762(17) Å	β = 102.201(3)°.
	c = 8.6774(7) Å	γ = 90°.
Volume	2391.1(3) $Å^3$	
Z	4	
Density (calculated)	1.335 Mg/m^3	
Absorption coefficient	0.176 mm^{-1}	
F(000)	1016	
Crystal size	0.25 x 0.22 x 0.20 mm^3	
Theta range for data collection	1.930 to 26.531°.	
Index ranges	-15<=h<=12, -28<=k<=29, -10<=l<=10	
Reflections collected	20929	
Independent reflections	4875 [R(int) = 0.0495]	
Completeness to theta = 25.242°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9485 and 0.8147	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4875 / 0 / 310	
Goodness-of-fit on F^2	1.040	
Final R indices [I>2sigma(I)]	R1 = 0.0410, wR2 = 0.1123	
R indices (all data)	R1 = 0.0489, wR2 = 0.1181	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.479 and -0.457 e.$Å^{-3}$	

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 171210LT

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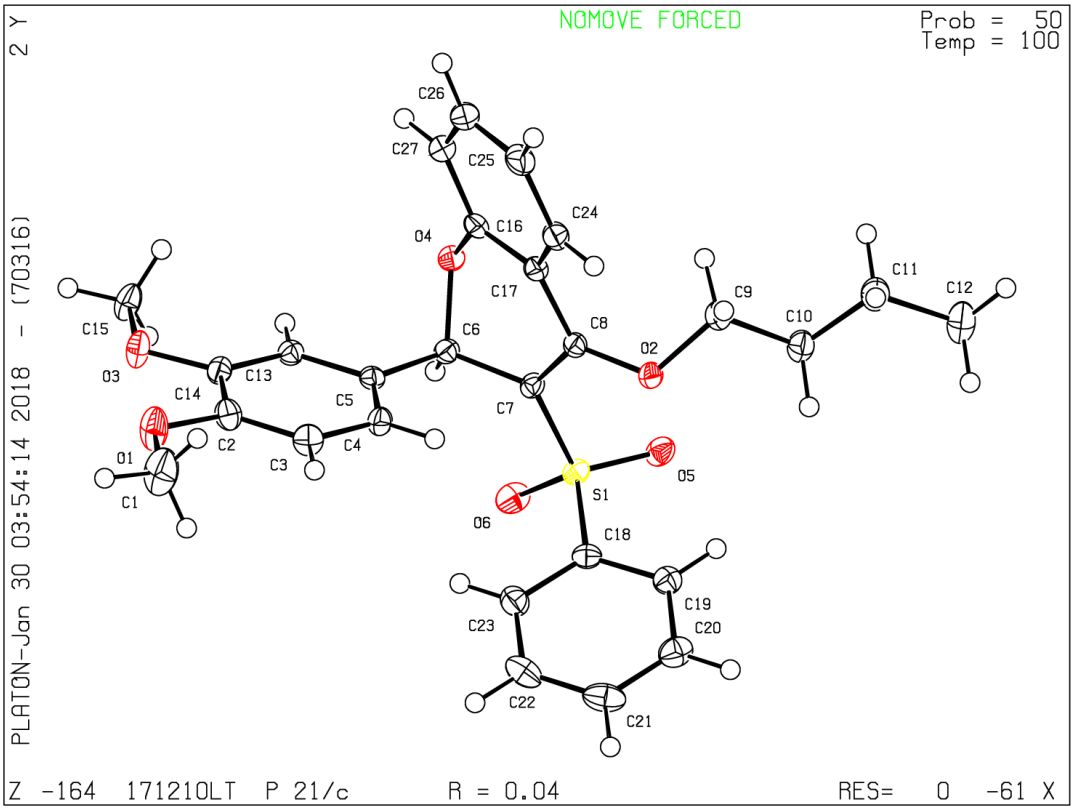
No syntax errors found. CIF dictionary Interpreting this report

Datablock: 171210LT

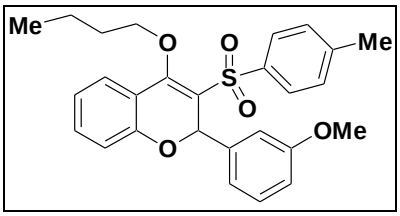
```
Bond precision:  C-C = 0.0023 A          Wavelength=0.71073

Cell:            a=12.1123(7)     b=23.2762(17)       c=8.6774(7)
                 alpha=90         beta=102.201(3)     gamma=90
Temperature:     100 K

                 Calculated                Reported
Volume           2391.2(3)                 2391.1(3)
Space group      P 21/c                    P 21/c
Hall group       -P 2ybc                   -P 2ybc
Moiety formula   C27 H28 O6 S              ?
Sum formula      C27 H28 O6 S              C27 H28 O6 S
Mr               480.55                    480.55
Dx,g cm-3        1.335                     1.335
Z                4                         4
Mu (mm-1)        0.176                     0.176
F000             1016.0                    1016.0
F000'            1017.00
h,k,lmax         15,29,10                  15,29,10
Nref             4966                      4875
Tmin,Tmax        0.957,0.965               0.815,0.948
Tmin'            0.957

Correction method= # Reported T Limits: Tmin=0.815 Tmax=0.948
AbsCorr = MULTI-SCAN

Data completeness= 0.982          Theta(max)= 26.531

R(reflections)= 0.0410( 4165)     wR2(reflections)= 0.1181( 4875)

S = 1.040                 Npar= 310
```

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

The thermal ellipsoid was drawn at the 50% probability level



X-ray crystal data of 6q



Empirical formula	C27 H28 O5 S	
Formula weight	464.55	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 6.727(3) Å	α = 90°.
	b = 12.012(5) Å	β = 90.175(15)°.
	c = 28.621(14) Å	γ = 90°.
Volume	2312.6(19) $Å^3$	
Z	4	
Density (calculated)	1.334 Mg/m^3	
Absorption coefficient	0.177 mm^{-1}	
F(000)	984	
Crystal size	0.18 x 0.15 x 0.13 mm^3	
Theta range for data collection	1.423 to 27.009°.	
Index ranges	-8<=h<=8, -15<=k<=13, -36<=l<=36	
Reflections collected	38185	
Independent reflections	4968 [R(int) = 0.1400]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9485 and 0.6855	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4968 / 0 / 302	
Goodness-of-fit on F^2	1.024	
Final R indices [I>2sigma(I)]	R1 = 0.0664, wR2 = 0.1537	
R indices (all data)	R1 = 0.1112, wR2 = 0.1804	
Extinction coefficient	0.0090(12)	
Largest diff. peak and hole	0.648 and -0.595 e.$Å^{-3}$	

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_180129LT_0m

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: mo_180129LT_0m

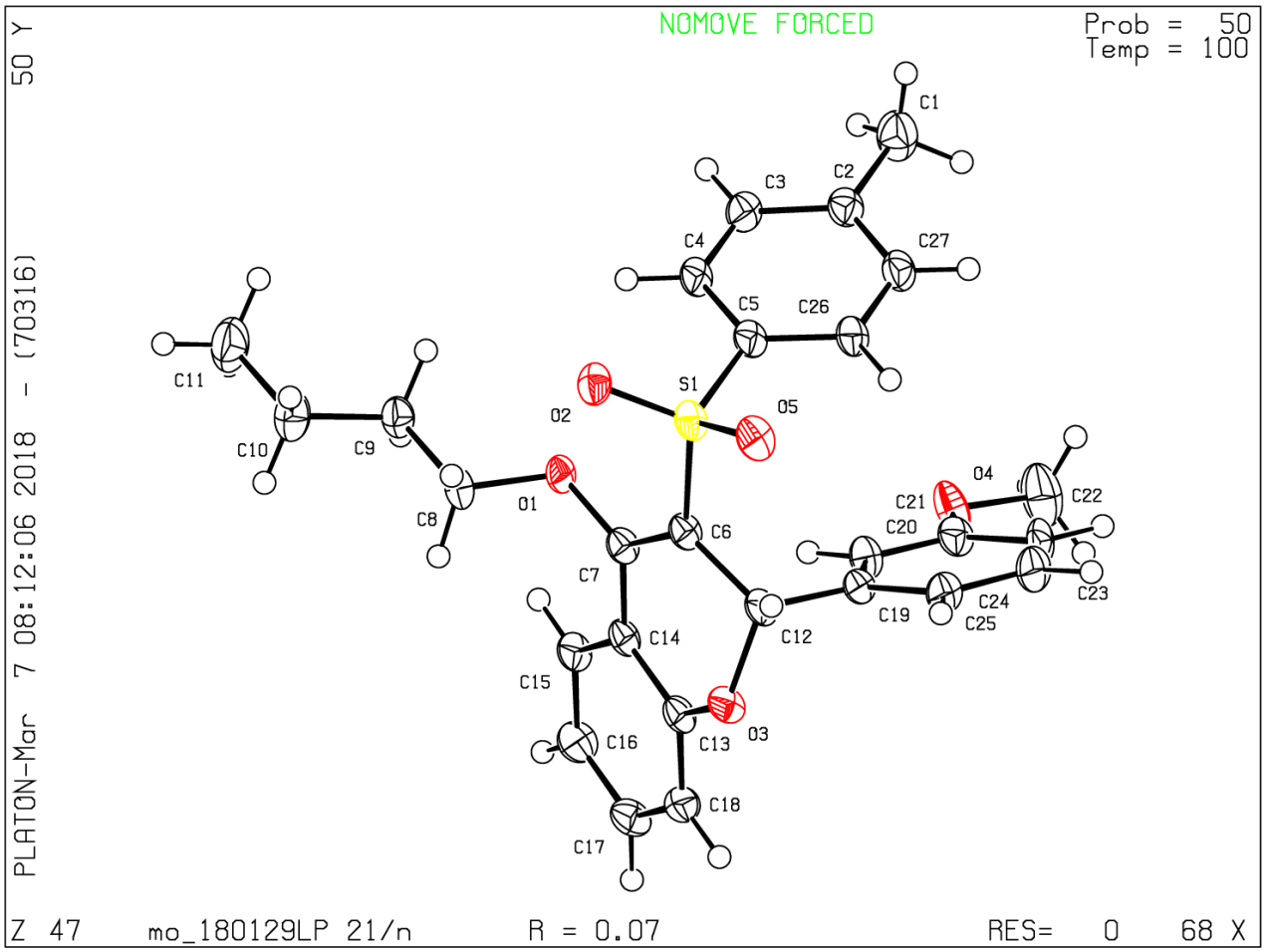
```
Bond precision:  C-C = 0.0049 A          Wavelength=0.71073

Cell:            a=6.727(3)    b=12.012(5)          c=28.621(14)
                 alpha=90      beta=90.175(15)      gamma=90
Temperature:     100 K
```

	Calculated	Reported
Volume	2312.7(18)	2312.6(19)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C27 H28 O5 S	?
Sum formula	C27 H28 O5 S	C27 H28 O5 S
Mr	464.55	464.55
Dx,g cm-3	1.334	1.334
Z	4	4
Mu (mm-1)	0.177	0.177
F000	984.0	984.0
F000'	984.96	
h,k,lmax	8,15,36	8,15,36
Nref	5068	4968
Tmin,Tmax	0.969,0.977	0.686,0.948
Tmin'	0.969	

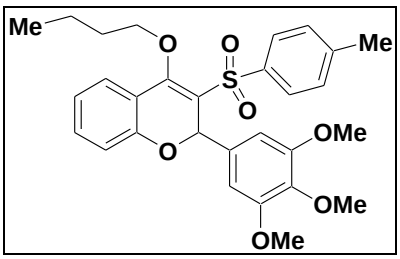
```
Correction method= # Reported T Limits: Tmin=0.686 Tmax=0.948
AbsCorr = MULTI-SCAN

Data completeness= 0.980          Theta(max)= 27.009

R(reflections)= 0.0664( 3246)     wR2(reflections)= 0.1804( 4968)

S = 1.024                 Npar= 302
```

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

The thermal ellipsoid was drawn at the 50% probability level



X-ray crystal data of 6x



Empirical formula	C29 H32 O7 S	
Formula weight	524.60	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 8.5862(10) Å	α = 90°.
	b = 11.7120(13) Å	β = 92.534(5)°.
	c = 26.193(3) Å	γ = 90°.
Volume	2631.5(5) $Å^3$	
Z	4	
Density (calculated)	1.324 Mg/m^3	
Absorption coefficient	0.169 mm^{-1}	
F(000)	1112	
Crystal size	0.10 x 0.08 x 0.06 mm^3	
Theta range for data collection	1.905 to 26.501°.	
Index ranges	-8<=h<=10, -11<=k<=14, -30<=l<=32	
Reflections collected	15533	
Independent reflections	5432 [R(int) = 0.0207]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9485 and 0.8441	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5432 / 0 / 339	
Goodness-of-fit on F^2	1.101	
Final R indices [I>2sigma(I)]	R1 = 0.0382, wR2 = 0.1074	
R indices (all data)	R1 = 0.0458, wR2 = 0.1176	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.821 and -0.566 e.$Å^{-3}$	

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 180205LT_2_0m

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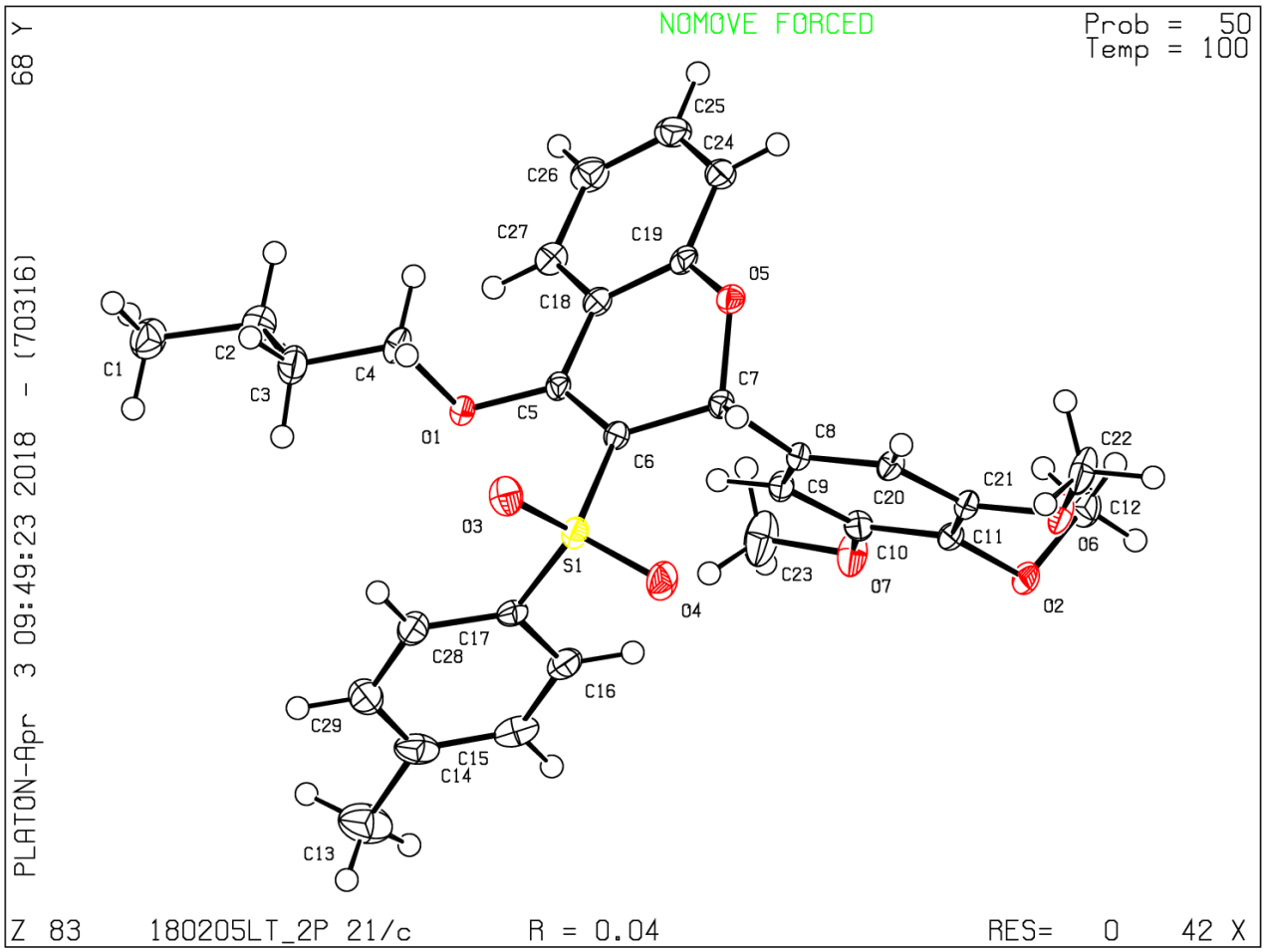
No syntax errors found. CIF dictionary Interpreting this report

Datablock: 180205LT_2_0m

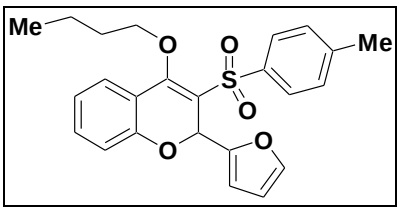
```
Bond precision:  C-C = 0.0022 A          Wavelength=0.71073

Cell:            a=8.5862(10)     b=11.7120(13)      c=26.193(3)
                 alpha=90         beta=92.534(5)     gamma=90
Temperature:     100 K

                 Calculated                Reported
Volume           2631.4(5)                 2631.5(5)
Space group      P 21/c                    P 21/c
Hall group       -P 2ybc                   -P 2ybc
Moiety formula   C29 H32 O7 S              ?
Sum formula      C29 H32 O7 S              C29 H32 O7 S
Mr               524.61                    524.60
Dx,g cm-3        1.324                     1.324
Z                4                         4
Mu (mm-1)        0.169                     0.169
F000             1112.0                    1112.0
F000'            1113.06
h,k,lmax         10,14,32                  10,14,32
Nref             5452                      5432
Tmin,Tmax        0.984,0.990               0.844,0.948
Tmin'            0.983

Correction method= # Reported T Limits: Tmin=0.844 Tmax=0.948
AbsCorr = MULTI-SCAN

Data completeness= 0.996          Theta(max)= 26.501

R(reflections)= 0.0382( 4817)     wR2(reflections)= 0.1176( 5432)

S = 1.101                 Npar= 339
```

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

The thermal ellipsoid was drawn at the 50% probability level



X-ray crystal data of 6y



Empirical formula	C24 H24 O5 S	
Formula weight	424.49	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 26.290(2) Å	α = 90°.
	b = 8.3391(7) Å	β = 108.275(2)°.
	c = 19.8288(16) Å	γ = 90°.
Volume	4128.0(6) $Å^3$	
Z	8	
Density (calculated)	1.366 Mg/m^3	
Absorption coefficient	0.191 mm^{-1}	
F(000)	1792	
Crystal size	0.20 x 0.17 x 0.15 mm^3	
Theta range for data collection	1.631 to 26.445°.	
Index ranges	-32<=h<=32, -10<=k<=10, -24<=l<=22	
Reflections collected	72376	
Independent reflections	4252 [R(int) = 0.0775]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9485 and 0.8957	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4252 / 159 / 321	
Goodness-of-fit on F^2	1.396	
Final R indices [I>2sigma(I)]	R1 = 0.1246, wR2 = 0.2901	
R indices (all data)	R1 = 0.1300, wR2 = 0.2920	
Extinction coefficient	0.00063(15)	
Largest diff. peak and hole	0.592 and -0.576 $e.Å^{-3}$	

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_180128lt_0m_a

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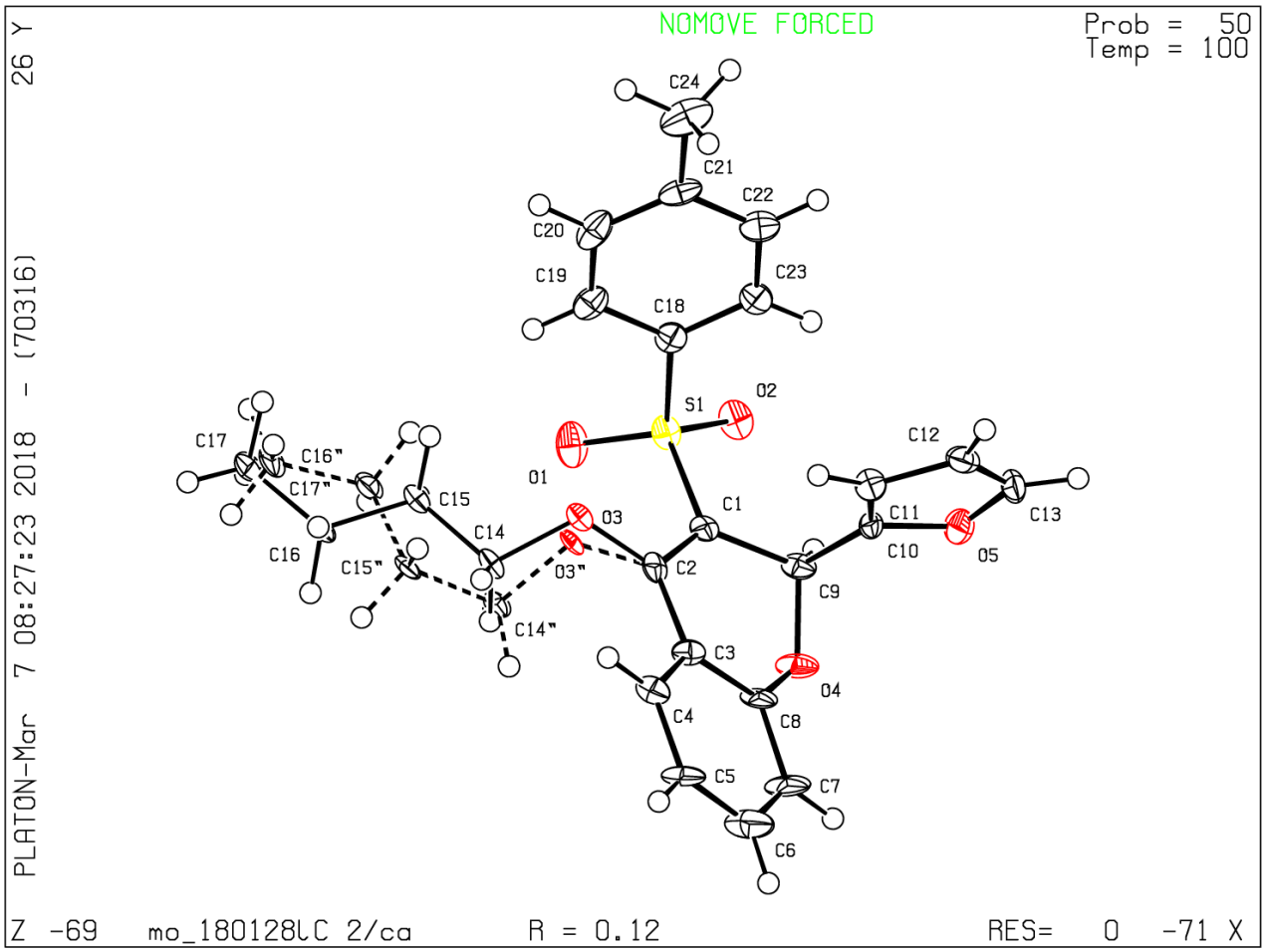
No syntax errors found. CIF dictionary Interpreting this report

Datablock: mo_180128lt_0m_a

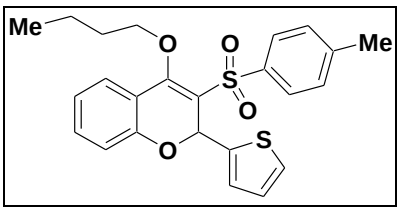
```
Bond precision:  C-C = 0.0110 A          Wavelength=0.71073

Cell:            a=26.290(2)    b=8.3391(7)         c=19.8288(16)
                 alpha=90       beta=108.275(2)     gamma=90
Temperature:     100 K

                 Calculated                 Reported
Volume           4127.9(6)                  4128.0(6)
Space group      C 2/c                      C 2/c
Hall group       -C 2yc                     -C 2yc
Moiety formula   C24 H24 O5 S               ?
Sum formula      C24 H24 O5 S               C24 H24 O5 S
Mr               424.49                     424.49
Dx,g cm-3        1.366                      1.366
Z                8                          8
Mu (mm-1)        0.191                      0.191
F000             1792.0                     1792.0
F000'            1793.87
h,k,lmax         32,10,24                   32,10,24
Nref             4263                       4252
Tmin,Tmax        0.963,0.972                0.896,0.948
Tmin'            0.963

Correction method= # Reported T Limits: Tmin=0.896 Tmax=0.948
AbsCorr = MULTI-SCAN

Data completeness= 0.997          Theta(max)= 26.445

R(reflections)= 0.1246( 3856)     wR2(reflections)= 0.2920( 4252)

S = 1.396                 Npar= 321
```

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

The thermal ellipsoid was drawn at the 50% probability level



X-ray crystal data of 6z



Empirical formula	C24 H24 O4 S2	
Formula weight	440.55	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 12.2582(7) Å	α= 90°.
	b = 8.5061(4) Å	β= 96.460(3)°.
	c = 21.0937(11) Å	γ = 90°.
Volume	2185.5(2) $Å^3$	
Z	4	
Density (calculated)	1.339 Mg/m^3	
Absorption coefficient	0.272 mm^{-1}	
F(000)	928	
Crystal size	0.20 x 0.18 x 0.18 mm^3	
Theta range for data collection	1.837 to 26.519°.	
Index ranges	-15<=h<=15, -10<=k<=10, -25<=l<=26	
Reflections collected	18659	
Independent reflections	4486 [R(int) = 0.0481]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9485 and 0.6826	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4486 / 0 / 273	
Goodness-of-fit on F^2	1.043	
Final R indices [I>2sigma(I)]	R1 = 0.0424, wR2 = 0.0960	
R indices (all data)	R1 = 0.0517, wR2 = 0.1010	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.433 and -0.363 $e.Å^{-3}$	

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 180139lt_0m

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

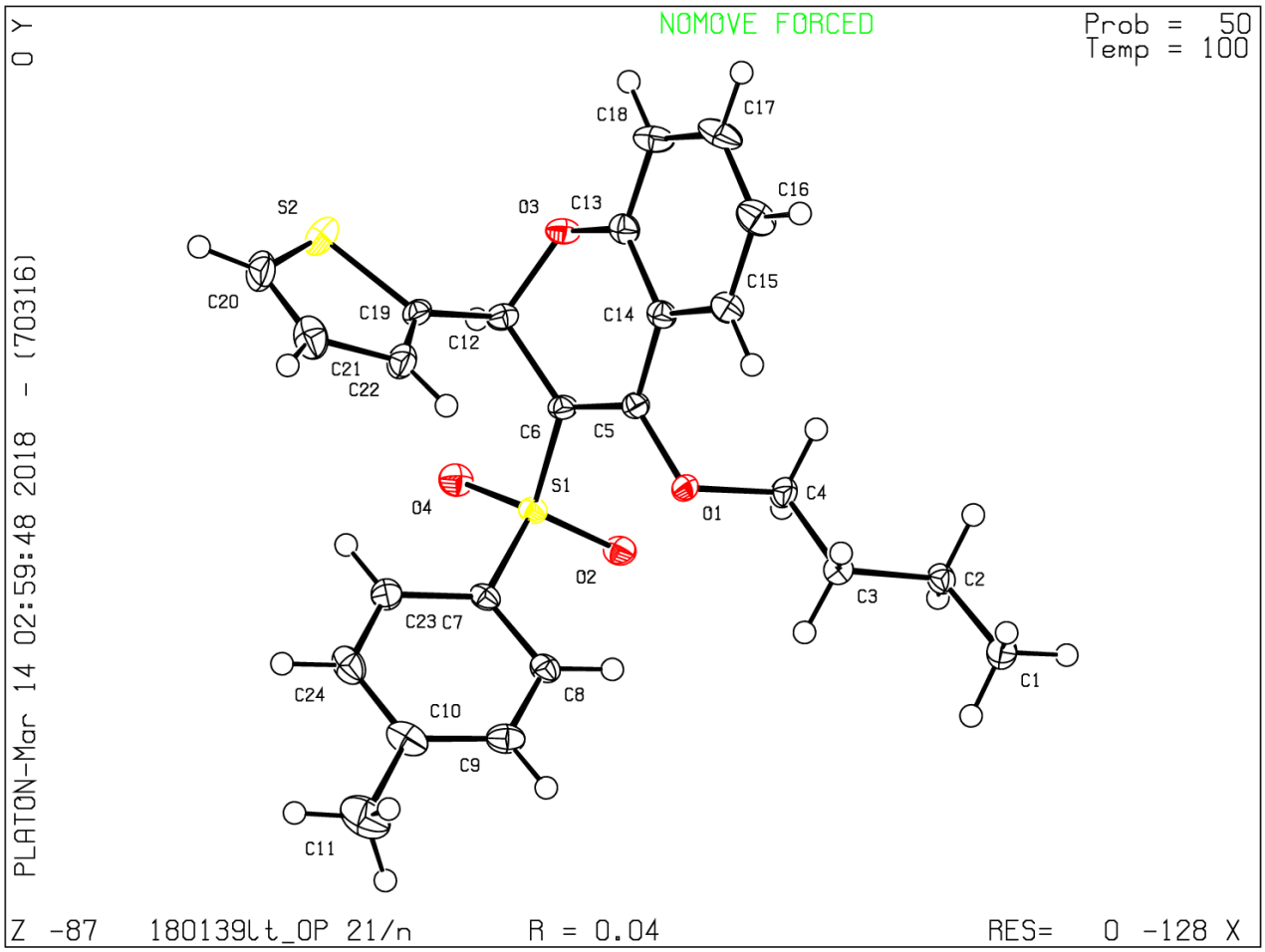
No syntax errors found. CIF dictionary Interpreting this report

Datablock: 180139lt_0m

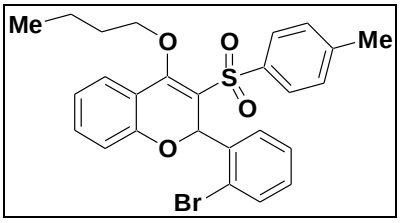
```
Bond precision:  C-C = 0.0029 A          Wavelength=0.71073

Cell:            a=12.2582(7)    b=8.5061(4)       c=21.0937(11)
                 alpha=90        beta=96.460(3)    gamma=90
Temperature:     100 K

                 Calculated                 Reported
Volume           2185.5(2)                  2185.5(2)
Space group      P 21/n                     P 21/n
Hall group       -P 2yn                     -P 2yn
Moiety formula   C24 H24 O4 S2              ?
Sum formula      C24 H24 O4 S2              C24 H24 O4 S2
Mr               440.55                     440.55
Dx,g cm-3        1.339                      1.339
Z                4                          4
Mu (mm-1)        0.272                      0.272
F000             928.0                      928.0
F000'            929.39
h,k,lmax         15,10,26                   15,10,26
Nref             4550                       4486
Tmin,Tmax        0.947,0.952                0.683,0.948
Tmin'            0.947

Correction method= # Reported T Limits: Tmin=0.683 Tmax=0.948
AbsCorr = MULTI-SCAN

Data completeness= 0.986          Theta(max)= 26.519

R(reflections)= 0.0424( 3820)     wR2(reflections)= 0.1010( 4486)

S = 1.043                 Npar= 273
```

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

The thermal ellipsoid was drawn at the 50% probability level



X-ray crystal data of 6ab



Empirical formula	C26 H25 Br O4 S	
Formula weight	513.43	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 12.2442(6) Å	α = 90°.
	b = 8.7485(4) Å	β = 98.628(2)°.
	c = 21.6094(11) Å	γ = 90°.
Volume	2288.57(19) Å^3	
Z	4	
Density (calculated)	1.490 Mg/m^3	
Absorption coefficient	1.919 mm^{-1}	
F(000)	1056	
Crystal size	0.18 x 0.16 x 0.15 mm^3	
Theta range for data collection	1.805 to 26.405°.	
Index ranges	-15<=h<=15, -9<=k<=10, -26<=l<=27	
Reflections collected	32769	
Independent reflections	4674 [R(int) = 0.0269]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9485 and 0.8720	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4674 / 0 / 291	
Goodness-of-fit on F^2	1.056	
Final R indices [I>2sigma(I)]	R1 = 0.0241, wR2 = 0.0611	
R indices (all data)	R1 = 0.0299, wR2 = 0.0634	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.367 and -0.347 e.Å^{-3}	

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_180206LT_0m

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

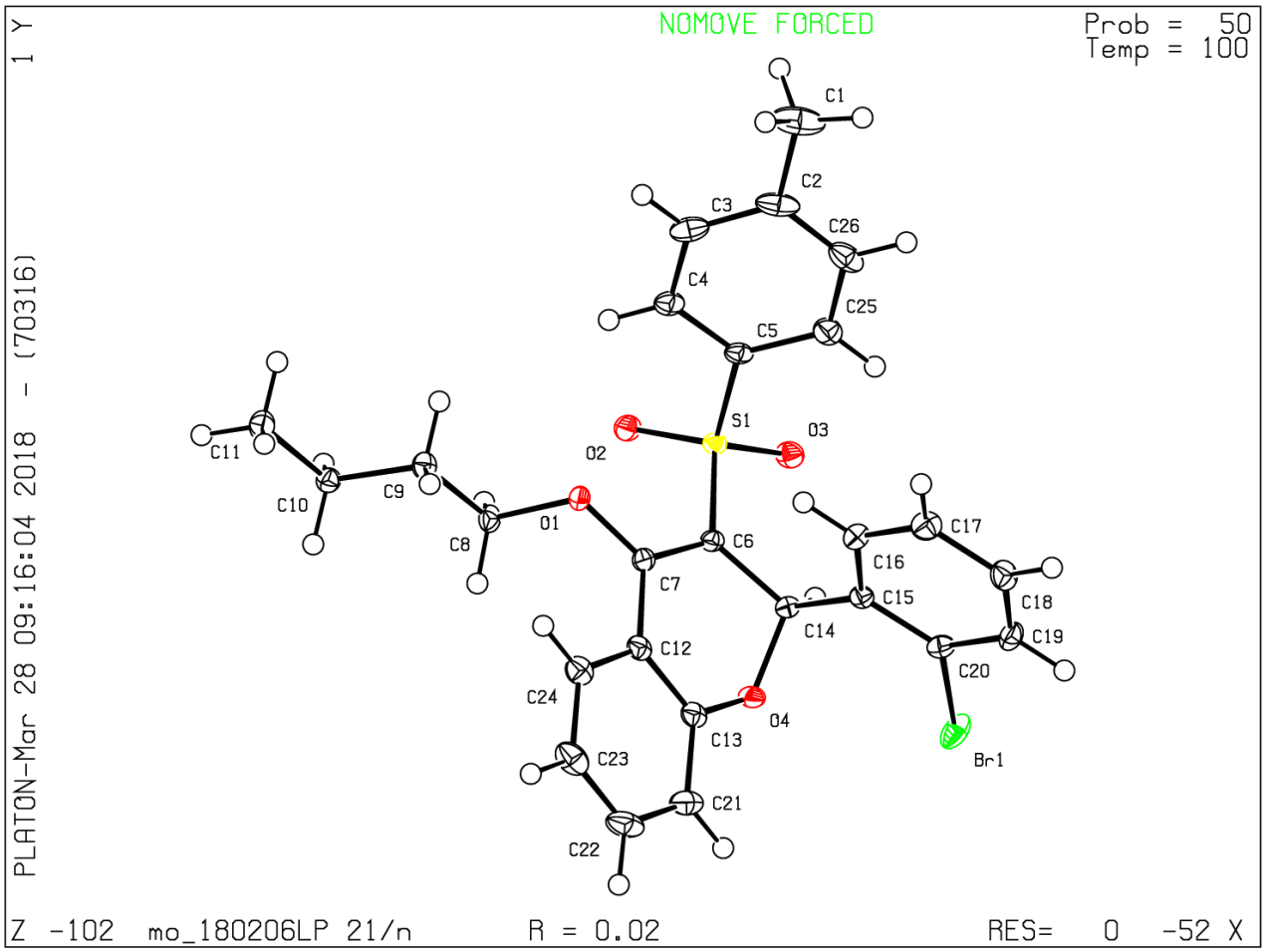
No syntax errors found. CIF dictionary Interpreting this report

Datablock: mo_180206LT_0m

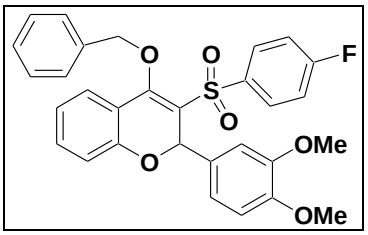
```
Bond precision:  C-C = 0.0022 A          Wavelength=0.71073

Cell:            a=12.2442(6)    b=8.7485(4)       c=21.6094(11)
                 alpha=90        beta=98.628(2)    gamma=90
Temperature:     100 K

                 Calculated                Reported
Volume           2288.57(19)               2288.57(19)
Space group      P 21/n                    P 21/n
Hall group       -P 2yn                    -P 2yn
Moiety formula   C26 H25 Br O4 S           ?
Sum formula      C26 H25 Br O4 S           C26 H25 Br O4 S
Mr               513.42                    513.43
Dx,g cm-3        1.490                     1.490
Z                4                         4
Mu (mm-1)        1.919                     1.919
F000             1056.0                    1056.0
F000'            1055.78
h,k,lmax         15,10,27                  15,10,27
Nref             4685                      4674
Tmin,Tmax        0.715,0.750               0.872,0.948
Tmin'            0.701

Correction method= # Reported T Limits: Tmin=0.872 Tmax=0.948
AbsCorr = MULTI-SCAN

Data completeness= 0.998          Theta(max)= 26.405

R(reflections)= 0.0241( 4093)     wR2(reflections)= 0.0634( 4674)

S = 1.056                 Npar= 291
```

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

The thermal ellipsoid was drawn at the 50% probability level



X-ray crystal data of 6aj



Empirical formula	C30 H25 F O6 S	
Formula weight	532.56	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 12.1195(4) Å	α = 90°.
	b = 16.7902(5) Å	β = 113.3580(10)°.
	c = 13.7432(5) Å	γ = 90°.
Volume	2567.39(15) $Å^3$	
Z	4	
Density (calculated)	1.378 Mg/m^3	
Absorption coefficient	0.177 mm^{-1}	
F(000)	1112	
Crystal size	0.12 x 0.10 x 0.09 mm^3	
Theta range for data collection	1.830 to 26.396°.	
Index ranges	-15<=h<=15, -20<=k<=20, -17<=l<=17	
Reflections collected	60350	
Independent reflections	5252 [R(int) = 0.0598]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9485 and 0.8552	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5252 / 0 / 345	
Goodness-of-fit on F^2	1.012	
Final R indices [I>2sigma(I)]	R1 = 0.0444, wR2 = 0.0960	
R indices (all data)	R1 = 0.0773, wR2 = 0.1101	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.245 and -0.359 e.$Å^{-3}$	

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_180346lt_0m

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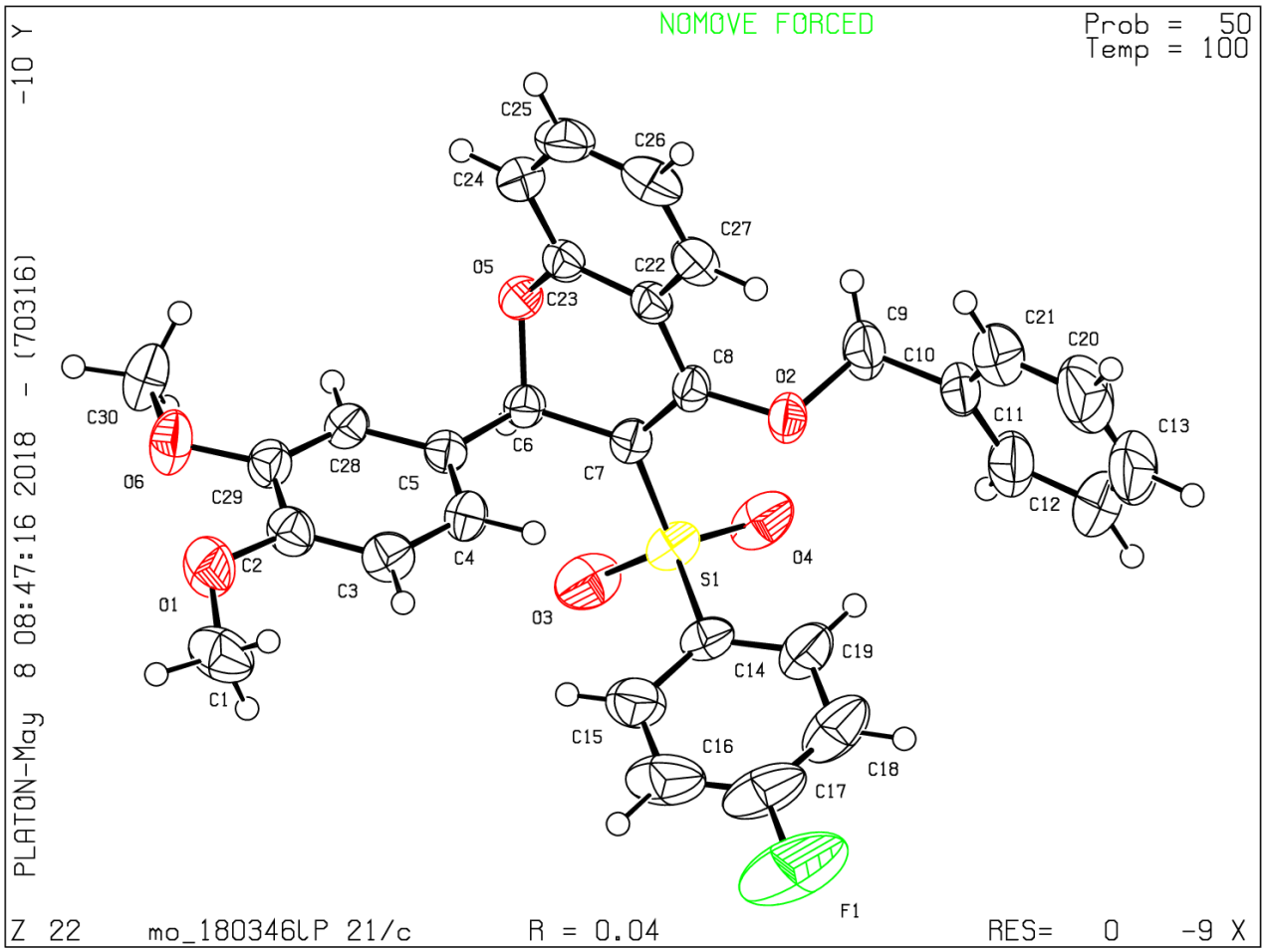
No syntax errors found. CIF dictionary Interpreting this report

Datablock: mo_180346lt_0m

```
Bond precision:  C-C = 0.0037 A          Wavelength=0.71073

Cell:            a=12.1195(4)    b=16.7902(5)        c=13.7432(5)
                 alpha=90        beta=113.358(1)     gamma=90
Temperature:     100 K

                 Calculated                  Reported
Volume           2567.40(15)                 2567.39(15)
Space group      P 21/c                      P 21/c
Hall group       -P 2ybc                     -P 2ybc
Moiety formula   C30 H25 F O6 S              ?
Sum formula      C30 H25 F O6 S              C30 H25 F O6 S
Mr               532.56                      532.56
Dx,g cm-3        1.378                       1.378
Z                4                           4
Mu (mm-1)        0.177                       0.177
F000             1112.0                      1112.0
F000'            1113.10
h,k,lmax         15,21,17                    15,20,17
Nref             5258                        5252
Tmin,Tmax        0.979,0.984                 0.855,0.948
Tmin'            0.979

Correction method= # Reported T Limits: Tmin=0.855 Tmax=0.948
AbsCorr = MULTI-SCAN

Data completeness= 0.999          Theta(max)= 26.396

R(reflections)= 0.0444( 3611)     wR2(reflections)= 0.1101( 5252)

S = 1.012                 Npar= 345
```

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

The thermal ellipsoid was drawn at the 50% probability level



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 171121LT

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 171121LT

```
Bond precision:  C-C = 0.0026 A          Wavelength=0.71073

Cell:            a=21.002(3)    b=11.9195(15)      c=8.3067(11)
                 alpha=90       beta=97.290(5)     gamma=90
Temperature:     100 K

                Calculated                Reported
Volume          2062.6(5)                 2062.6(5)
Space group     P 21/c                    P 21/c
Hall group      -P 2ybc                   -P 2ybc
Moiety formula  C24 H22 O6 S              ?
Sum formula     C24 H22 O6 S              C24 H22 O6 S
Mr              438.48                    438.47
Dx,g cm-3       1.412                     1.412
Z               4                         4
Mu (mm-1)       0.197                     0.197
F000            920.0                     920.0
F000'           920.97
h,k,lmax        26,14,10                  26,14,10
Nref            4275                      4236
Tmin,Tmax       0.965,0.988               0.893,0.948
Tmin'           0.965

Correction method= # Reported T Limits: Tmin=0.893 Tmax=0.948
AbsCorr = MULTI-SCAN

Data completeness= 0.991          Theta(max)= 26.475

R(reflections)= 0.0383( 3545)     wR2(reflections)= 0.1084( 4236)

S = 1.053                 Npar= 283
```

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

Alert level B

```
PLAT919_ALERT_3_B Reflection # Likely Affected by the Beamstop ...          2 Check
PLAT934_ALERT_3_B Number of (Iobs-Icalc)/SigmaW > 10 Outliers ....          2 Check
```

Alert level C

```
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .          1 Check
```

Alert level G

```
PLAT793_ALERT_4_G Model has Chirality at C6          (Centro SPGR)          R Verify
PLAT793_ALERT_4_G Model has Chirality at C7          (Centro SPGR)          R Verify
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         39 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         13 Info
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   2 ALERT level B = A potentially serious problem, consider carefully
   1 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   4 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   1 ALERT type 2 Indicator that the structure model may be wrong or deficient
   3 ALERT type 3 Indicator that the structure quality may be low
   3 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

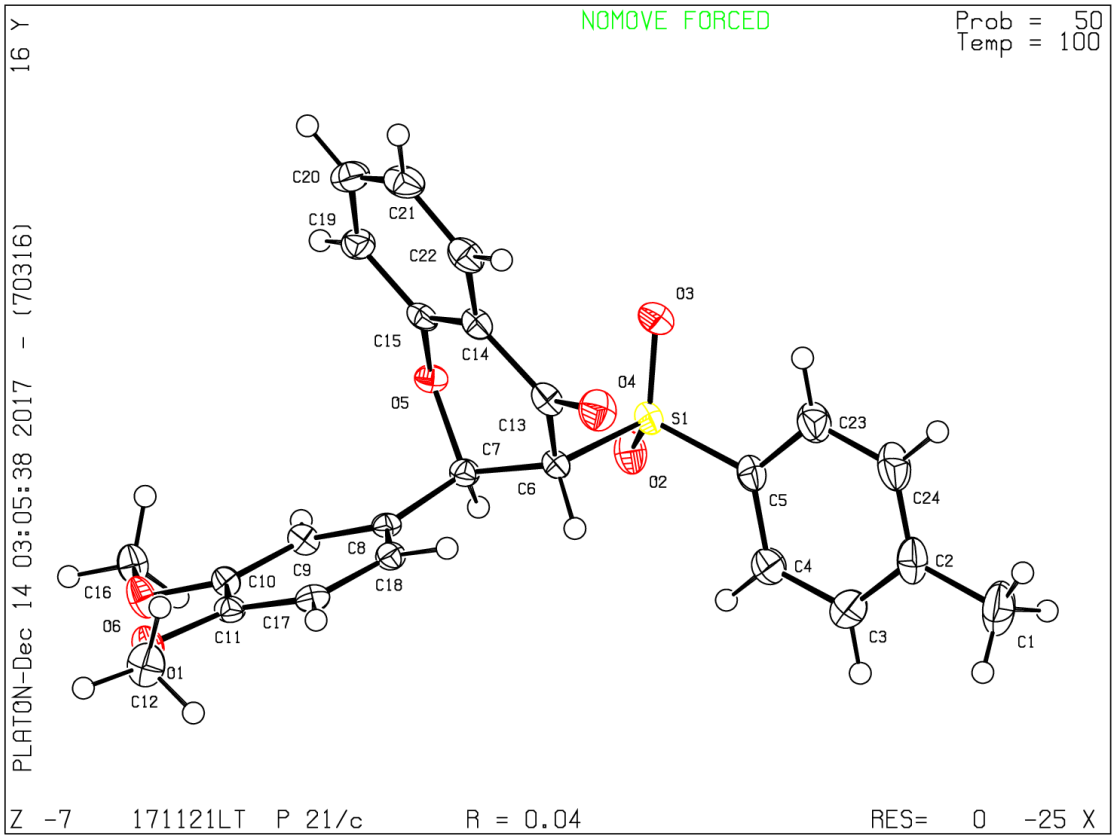
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 13/12/2017; check.def file version of 12/12/2017

Datablock 171121LT - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 171210LT

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: 171210LT

```
Bond precision:  C-C = 0.0023 A          Wavelength=0.71073

Cell:            a=12.1123(7)    b=23.2762(17)       c=8.6774(7)
                 alpha=90        beta=102.201(3)     gamma=90
Temperature:     100 K

                 Calculated                Reported
Volume           2391.2(3)                 2391.1(3)
Space group      P 21/c                    P 21/c
Hall group       -P 2ybc                   -P 2ybc
Moiety formula   C27 H28 O6 S              ?
Sum formula      C27 H28 O6 S              C27 H28 O6 S
Mr               480.55                    480.55
Dx,g cm-3        1.335                     1.335
Z                4                         4
Mu (mm-1)        0.176                     0.176
F000             1016.0                    1016.0
F000'            1017.00
h,k,lmax         15,29,10                  15,29,10
Nref             4966                      4875
Tmin,Tmax        0.957,0.965               0.815,0.948
Tmin'            0.957

Correction method= # Reported T Limits: Tmin=0.815 Tmax=0.948
AbsCorr = MULTI-SCAN

Data completeness= 0.982          Theta(max)= 26.531

R(reflections)= 0.0410( 4165)     wR2(reflections)= 0.1181( 4875)

S = 1.040                 Npar= 310
```

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

Alert level B

PLAT919_ALERT_3_B Reflection # Likely Affected by the Beamstop ... 1 Check
PLAT934_ALERT_3_B Number of (Iobs-Icalc)/SigmaW > 10 Outliers .... 2 Check

Alert level C

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.053 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 6 Report

Alert level G

PLAT793_ALERT_4_G Model has Chirality at C6 (Centro SPGR) R Verify
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 2 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 80 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF .... 1 Note
PLAT954_ALERT_1_G Reported (CIF) and Actual (FCF) Kmax Differ by . 1 Units
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 9 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
2 **ALERT level B** = A potentially serious problem, consider carefully
2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
6 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 ALERT type 2 Indicator that the structure model may be wrong or deficient
6 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

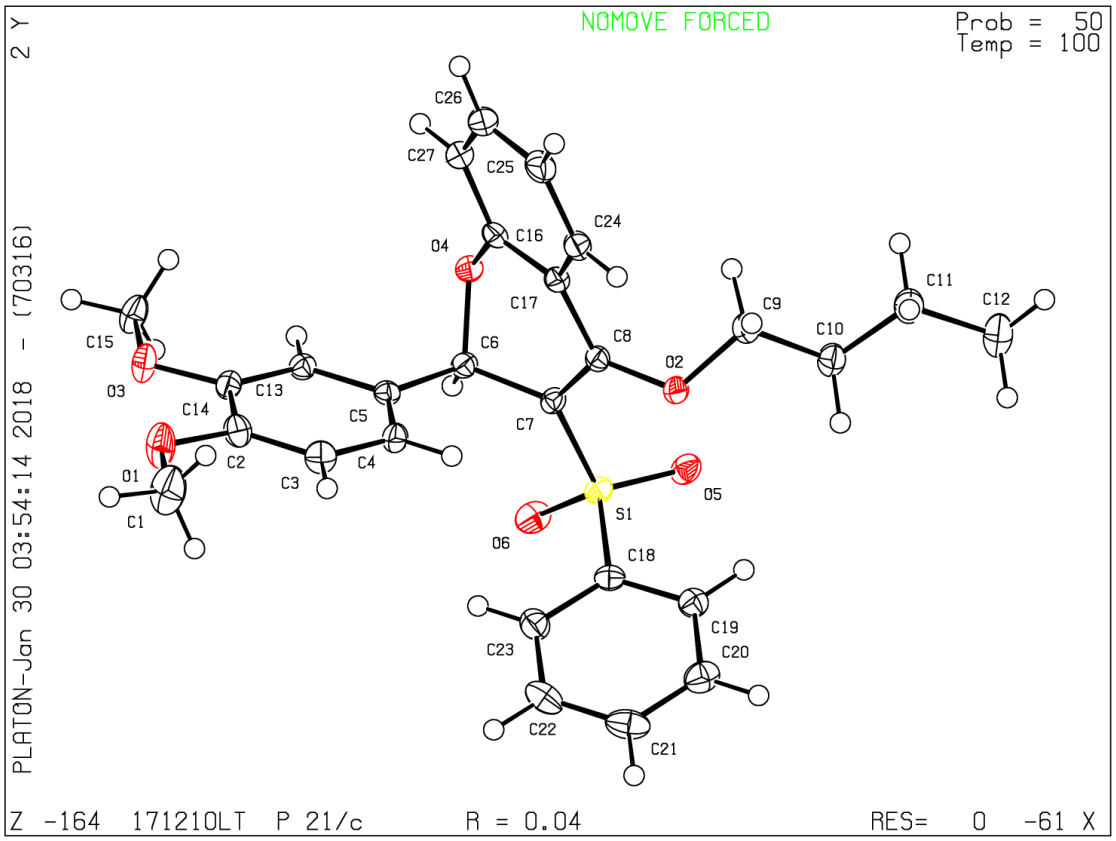
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 13/08/2017; check.def file version of 12/12/2017

Datablock 171210LT - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_180129LT_0m

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: mo_180129LT_0m

```
Bond precision:  C-C = 0.0049 A          Wavelength=0.71073

Cell:            a=6.727(3)    b=12.012(5)          c=28.621(14)
                 alpha=90      beta=90.175(15)      gamma=90
Temperature:     100 K

                Calculated                Reported
Volume          2312.7(18)                2312.6(19)
Space group     P 21/n                    P 21/n
Hall group      -P 2yn                    -P 2yn
Moiety formula  C27 H28 O5 S              ?
Sum formula     C27 H28 O5 S              C27 H28 O5 S
Mr              464.55                    464.55
Dx,g cm-3       1.334                     1.334
Z               4                         4
Mu (mm-1)       0.177                     0.177
F000            984.0                     984.0
F000'           984.96
h,k,lmax        8,15,36                   8,15,36
Nref            5068                      4968
Tmin,Tmax       0.969,0.977               0.686,0.948
Tmin'           0.969

Correction method= # Reported T Limits: Tmin=0.686 Tmax=0.948
AbsCorr = MULTI-SCAN

Data completeness= 0.980          Theta(max)= 27.009

R(reflections)= 0.0664( 3246)     wR2(reflections)= 0.1804( 4968)

S = 1.024                 Npar= 302
```

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

Alert level C

```
RINTA01_ALERT_3_C  The value of Rint is greater than 0.12
           Rint given   0.140
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00488 Ang.
```

Alert level G

```
PLAT020_ALERT_3_G The Value of Rint is Greater Than 0.12 .........      0.140 Report
PLAT793_ALERT_4_G Model has Chirality at C12         (Centro SPGR)          S Verify
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        100 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          3 Info
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   2 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   4 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   1 ALERT type 2 Indicator that the structure model may be wrong or deficient
   3 ALERT type 3 Indicator that the structure quality may be low
   2 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

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Publication of your CIF in IUCr journals

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Publication of your CIF in other journals

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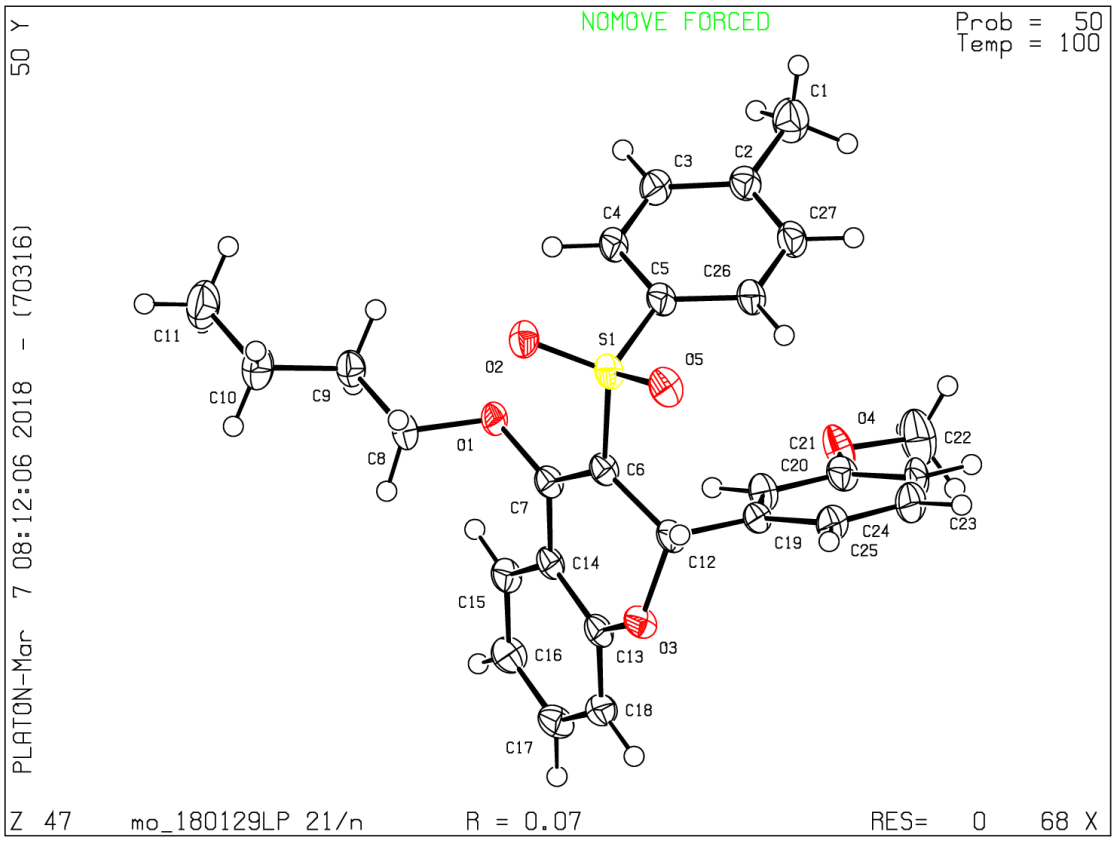
PLATON version of 30/01/2018; check.def file version of 30/01/2018

Datablock mo_180129LT_0m - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 180205LT_2_0m

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 180205LT_2_0m

```
Bond precision:  C-C = 0.0022 A          Wavelength=0.71073

Cell:            a=8.5862(10)     b=11.7120(13)      c=26.193(3)
                 alpha=90         beta=92.534(5)     gamma=90
Temperature:     100 K

                Calculated                Reported
Volume          2631.4(5)                 2631.5(5)
Space group     P 21/c                    P 21/c
Hall group      -P 2ybc                   -P 2ybc
Moiety formula  C29 H32 O7 S              ?
Sum formula     C29 H32 O7 S              C29 H32 O7 S
Mr              524.61                    524.60
Dx,g cm-3       1.324                     1.324
Z               4                         4
Mu (mm-1)       0.169                     0.169
F000            1112.0                    1112.0
F000'           1113.06
h,k,lmax        10,14,32                  10,14,32
Nref            5452                      5432
Tmin,Tmax       0.984,0.990               0.844,0.948
Tmin'           0.983

Correction method= # Reported T Limits: Tmin=0.844 Tmax=0.948
AbsCorr = MULTI-SCAN

Data completeness= 0.996          Theta(max)= 26.501

R(reflections)= 0.0382( 4817)     wR2(reflections)= 0.1176( 5432)

S = 1.101                 Npar= 339
```

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

Alert level A

PLAT939_ALERT_3_A Large Value of Not (SHELXL) Weight Optimized S . 4930.33 Check

Alert level B

PLAT919_ALERT_3_B Reflection # Likely Affected by the Beamstop ... 2 Check
PLAT934_ALERT_3_B Number of (Iobs-Icalc)/SigmaW > 10 Outliers .... 2 Check

Alert level C

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 3 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 1 Check

Alert level G

PLAT793_ALERT_4_G Model has Chirality at C7 (Centro SPGR) R Verify
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 16 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF .... 1 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 2 Info

---

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2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
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2 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

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Publication of your CIF in other journals

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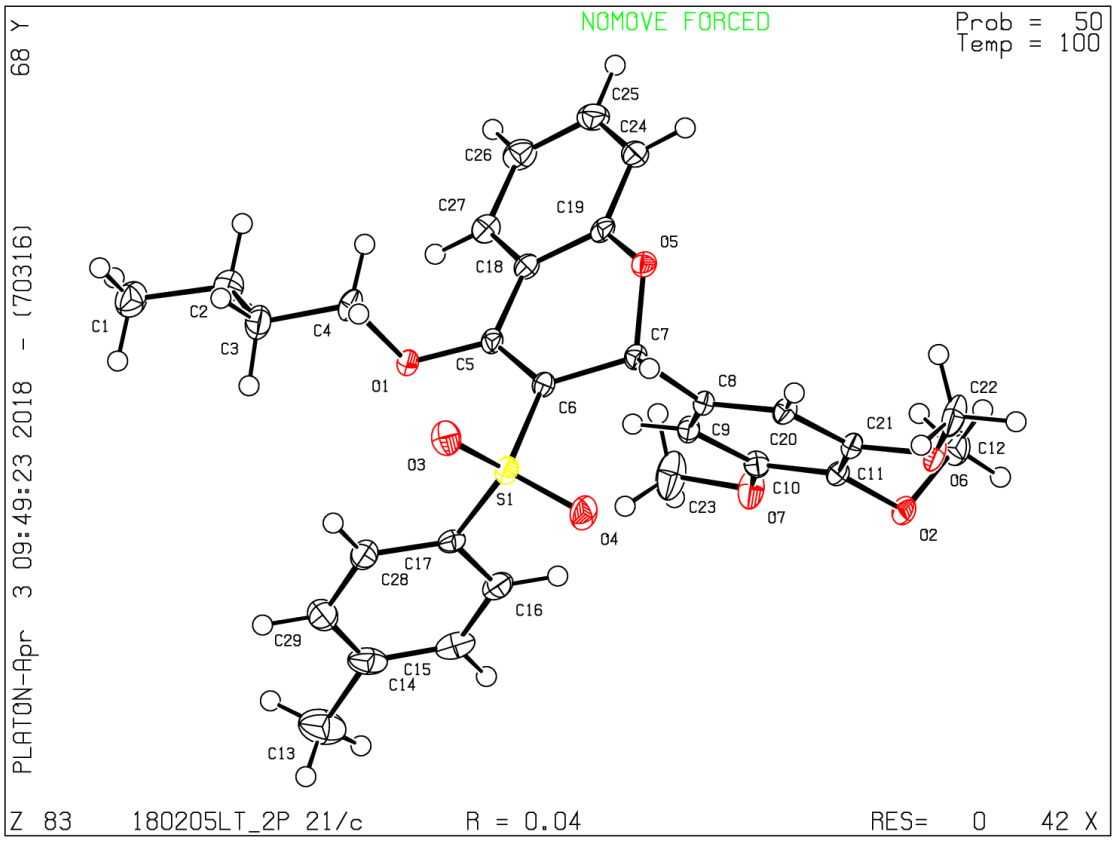
PLATON version of 30/01/2018; check.def file version of 30/01/2018

Datablock 180205LT_2_0m - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_180128lt_0m_a

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: mo_180128lt_0m_a

```
Bond precision:  C-C = 0.0110 A          Wavelength=0.71073

Cell:           a=26.290(2)    b=8.3391(7)         c=19.8288(16)
                alpha=90       beta=108.275(2)     gamma=90
Temperature:    100 K

                Calculated                Reported
Volume          4127.9(6)                 4128.0(6)
Space group     C 2/c                     C 2/c
Hall group      -C 2yc                    -C 2yc
Moiety formula  C24 H24 O5 S              ?
Sum formula     C24 H24 O5 S              C24 H24 O5 S
Mr              424.49                    424.49
Dx,g cm-3       1.366                     1.366
Z               8                         8
Mu (mm-1)       0.191                     0.191
F000            1792.0                    1792.0
F000'           1793.87
h,k,lmax        32,10,24                  32,10,24
Nref            4263                      4252
Tmin,Tmax       0.963,0.972               0.896,0.948
Tmin'           0.963

Correction method= # Reported T Limits: Tmin=0.896 Tmax=0.948
AbsCorr = MULTI-SCAN

Data completeness= 0.997          Theta(max)= 26.445

R(reflections)= 0.1246( 3856)     wR2(reflections)= 0.2920( 4252)

S = 1.396                 Npar= 321
```

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

Alert level B

PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.011 Ang.

Alert level C

PLAT082_ALERT_2_C High R1 Value ..... 0.12 Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..... 0.29 Report
PLAT213_ALERT_2_C Atom C7 has ADP max/min Ratio ..... 3.2 oblate
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 31.851 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 4.962 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.256 Check
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/SigmaW > 10 Outliers .... 1 Check
PLAT977_ALERT_2_C Check Negative Difference Density on H16A -0.36 eA-3

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 10 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 10 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 100.18 Why ?
PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records 1 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records 1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 17% Note
PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O5 106.2 Degree
PLAT432_ALERT_2_G Short Inter X...Y Contact O1 ..C14" 2.97 Ang.
PLAT793_ALERT_4_G Model has Chirality at C9 (Centro SPGR) R Verify
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 159 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 12 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 1 Info

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9 ALERT type 2 Indicator that the structure model may be wrong or deficient
8 ALERT type 3 Indicator that the structure quality may be low
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0 ALERT type 5 Informative message, check

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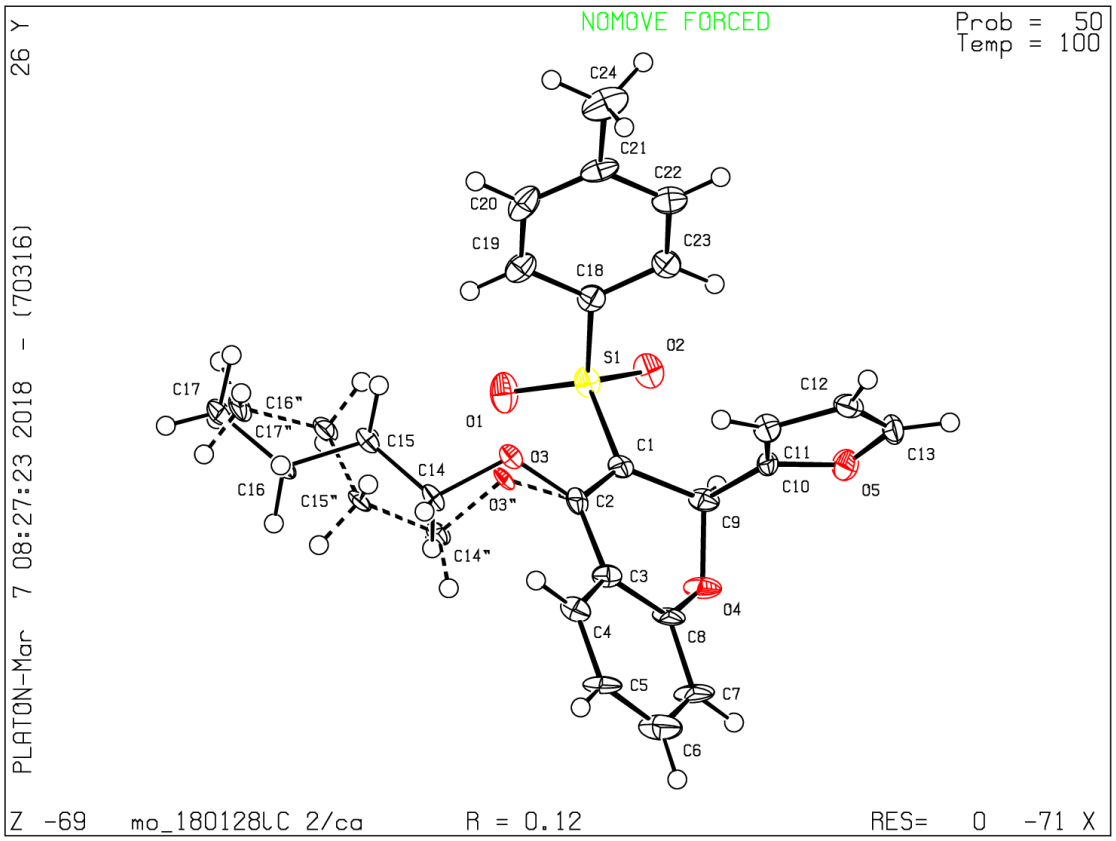
PLATON version of 30/01/2018; check.def file version of 30/01/2018

Datablock mo_180128lt_0m_a - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 180139lt_0m

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 180139lt_0m

```
Bond precision:  C-C = 0.0029 A          Wavelength=0.71073

Cell:           a=12.2582(7)    b=8.5061(4)       c=21.0937(11)
                alpha=90        beta=96.460(3)    gamma=90
Temperature:    100 K

                Calculated                Reported
Volume          2185.5(2)                 2185.5(2)
Space group     P 21/n                    P 21/n
Hall group      -P 2yn                    -P 2yn
Moiety formula  C24 H24 O4 S2             ?
Sum formula     C24 H24 O4 S2             C24 H24 O4 S2
Mr              440.55                    440.55
Dx,g cm-3       1.339                     1.339
Z               4                         4
Mu (mm-1)       0.272                     0.272
F000            928.0                     928.0
F000'           929.39
h,k,lmax        15,10,26                  15,10,26
Nref            4550                      4486
Tmin,Tmax       0.947,0.952               0.683,0.948
Tmin'           0.947

Correction method= # Reported T Limits: Tmin=0.683 Tmax=0.948
AbsCorr = MULTI-SCAN

Data completeness= 0.986          Theta(max)= 26.519

R(reflections)= 0.0424( 3820)     wR2(reflections)= 0.1010( 4486)

S = 1.043                 Npar= 273
```

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

Alert level C

```
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.595 Check
```

Alert level G

```
PLAT793_ALERT_4_G Model has Chirality at C12         (Centro SPGR)          R Verify
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         63 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          1 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         10 Info
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   1 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   4 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
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   2 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

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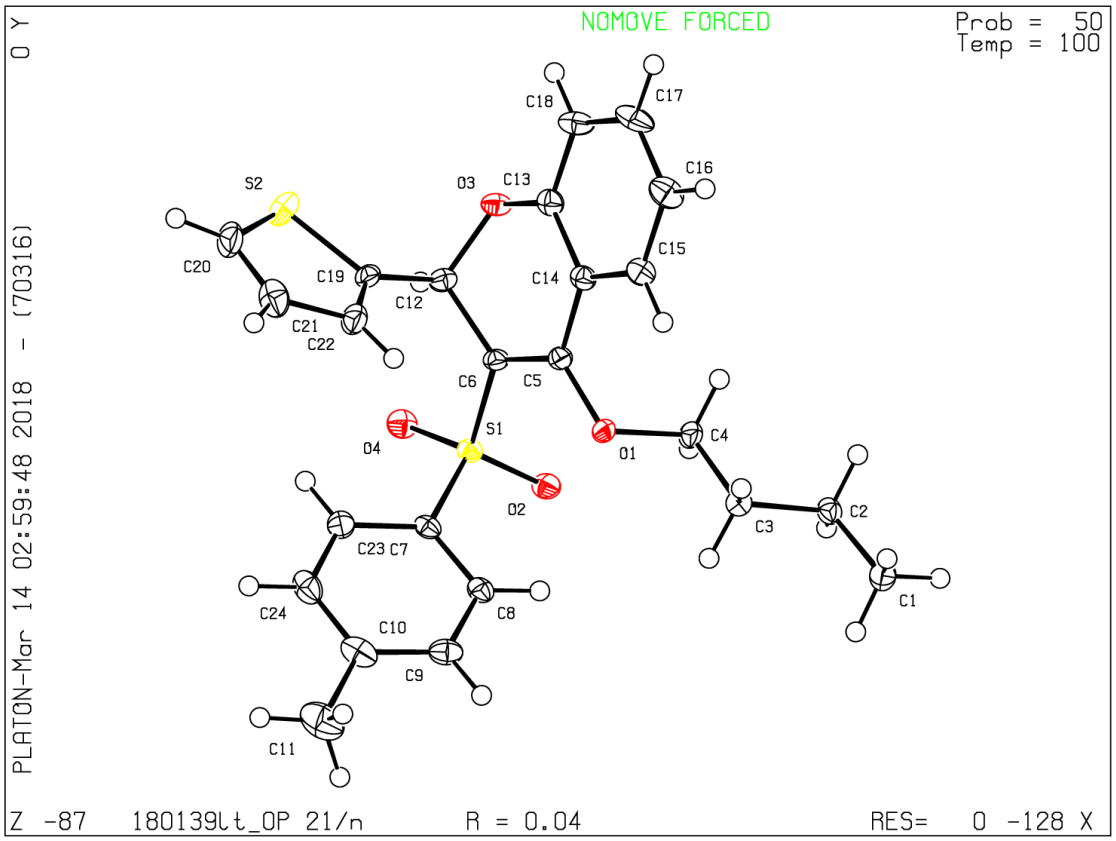
PLATON version of 30/01/2018; check.def file version of 30/01/2018

Datablock 180139lt_0m - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_180206LT_0m

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: mo_180206LT_0m

```
Bond precision:  C-C = 0.0022 A          Wavelength=0.71073

Cell:           a=12.2442(6)    b=8.7485(4)       c=21.6094(11)
                alpha=90        beta=98.628(2)    gamma=90
Temperature:    100 K

                Calculated                Reported
Volume          2288.57(19)               2288.57(19)
Space group     P 21/n                    P 21/n
Hall group      -P 2yn                    -P 2yn
Moiety formula  C26 H25 Br O4 S           ?
Sum formula     C26 H25 Br O4 S           C26 H25 Br O4 S
Mr              513.42                    513.43
Dx,g cm-3       1.490                     1.490
Z               4                         4
Mu (mm-1)       1.919                     1.919
F000            1056.0                    1056.0
F000'           1055.78
h,k,lmax        15,10,27                  15,10,27
Nref            4685                      4674
Tmin,Tmax       0.715,0.750               0.872,0.948
Tmin'           0.701

Correction method= # Reported T Limits: Tmin=0.872 Tmax=0.948
AbsCorr = MULTI-SCAN

Data completeness= 0.998          Theta(max)= 26.405

R(reflections)= 0.0241( 4093)     wR2(reflections)= 0.0634( 4674)

S = 1.056                 Npar= 291
```

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

Alert level C

```
PLAT220_ALERT_2_C Non-Solvent  Resd 1  C   Ueq(max)/Ueq(min) Range        3.1 Ratio
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          6 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....          5 Note
```

Alert level G

```
PLAT793_ALERT_4_G Model has Chirality at C14         (Centro SPGR)          R Verify
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          4 Note
PLAT955_ALERT_1_G Reported (CIF) and Actual (FCF) Lmax Differ by .          1 Units
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         16 Info
```

```
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   2 ALERT type 3 Indicator that the structure quality may be low
   2 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

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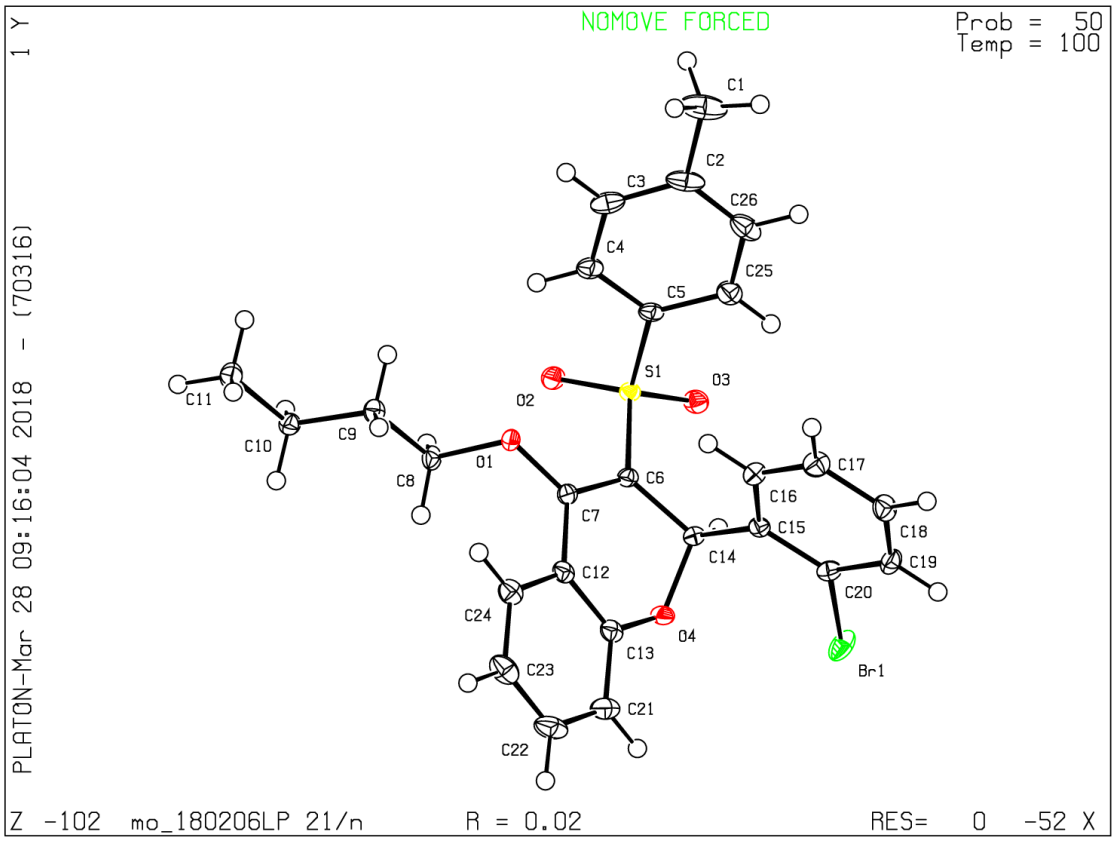
PLATON version of 30/01/2018; check.def file version of 30/01/2018

Datablock mo_180206LT_0m - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_180346lt_0m

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: mo_180346lt_0m

```
Bond precision:  C-C = 0.0037 A          Wavelength=0.71073

Cell:           a=12.1195(4)    b=16.7902(5)        c=13.7432(5)
                alpha=90        beta=113.358(1)     gamma=90
Temperature:    100 K

                Calculated                Reported
Volume          2567.40(15)               2567.39(15)
Space group     P 21/c                    P 21/c
Hall group      -P 2ybc                   -P 2ybc
Moiety formula  C30 H25 F O6 S            ?
Sum formula     C30 H25 F O6 S            C30 H25 F O6 S
Mr              532.56                    532.56
Dx,g cm-3       1.378                     1.378
Z               4                         4
Mu (mm-1)       0.177                     0.177
F000            1112.0                    1112.0
F000'           1113.10
h,k,lmax        15,21,17                  15,20,17
Nref            5258                      5252
Tmin,Tmax       0.979,0.984               0.855,0.948
Tmin'           0.979

Correction method= # Reported T Limits: Tmin=0.855 Tmax=0.948
AbsCorr = MULTI-SCAN

Data completeness= 0.999          Theta(max)= 26.396

R(reflections)= 0.0444( 3611)     wR2(reflections)= 0.1101( 5252)

S = 1.012                 Npar= 345
```

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

Alert level C

```
PLAT220_ALERT_2_C Non-Solvent  Resd 1  C   Ueq(max)/Ueq(min) Range        3.1 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for   C10      --C21       .        5.5 s.u.
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C10 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C17 Check
PLAT331_ALERT_2_C Small Average Phenyl C-C Dist C10      -C21           1.37 Ang.
PLAT334_ALERT_2_C Small Aver. Benzene C-C Dist C14      -C19            1.37 Ang.
PLAT431_ALERT_2_C Short Inter HL..A Contact  F1       ..O2              2.87 Ang.
```

Alert level G

```
PLAT793_ALERT_4_G Model has Chirality at C6          (Centro SPGR)          R Verify
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          7 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          4 Info
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   7 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   3 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   8 ALERT type 2 Indicator that the structure model may be wrong or deficient
   0 ALERT type 3 Indicator that the structure quality may be low
   2 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica, Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 23/04/2018; check.def file version of 23/04/2018

Datablock mo_180346lt_0m - ellipsoid plot