# Supporting Information 

## The Journal of Organic Chemistry

## Synthesis of Substituted 2,3-Benzodiazepines

## Department of Medicinal and Applied Chemistry, and General Research Centers of R\&D office, Kaohsiung Medical University, Kaohsiung 807, Taiwan

Email: mychang@kmu.edu.tw
I. Scanned Photocopies of ${ }^{1} \mathrm{H}$ and ${ }^{13} \mathrm{C}$ NMR Spectra for Compounds 1a~1aa ..... S-2~S-109
II. Scanned Photocopies of ${ }^{1} \mathrm{H}$ and ${ }^{13} \mathrm{C}$ NMR Spectra for Compounds 6a $\sim \mathbf{6 a a}$ ..... S-110~S-217
III. Scanned Photocopies of ${ }^{1} \mathrm{H}$ and ${ }^{13} \mathrm{C}$ NMR Spectra for Compounds 8a $\mathbf{8} \mathbf{b}$ ..... S-218~S-221
IV. Scanned Photocopies of ${ }^{1} \mathrm{H}$ and ${ }^{13} \mathrm{C}$ NMR Spectra for Compounds 9a 9d ..... S-222~S-234
V. Scanned Photocopies of ${ }^{1} \mathrm{H}$ and ${ }^{13} \mathrm{C}$ NMR Spectra for Compound $\mathbf{1 0}$ ..... S-235~S-238
VI. Crystal Data for Compounds 1a, 1c, 1p, 7y and 9a ..... S-239~S-243

## Compound 1a

YR1040701
Pulse Sequence: s2pul
UNITYplus-400 "unity 400 "

Ambient temperature
Tota1 64
repetition


## Compound 1a

YR1040701
Pulse Sequence: s2pul
UNITYP Mus-400 "unity400"
Date: Ju1 ${ }^{2} 2015$
Solvent: ${ }^{2} 13$
Ambient temperature
Total 64 repetition


## Compound 1a



## Compound 1b



## Compound 1b



## Compound 1b

YL1040716
Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Jul
20 2015
Date: Jul $20{ }^{201}$
Solvent: $\operatorname{coc}^{2} 3$
Ambient
Total 2128 temperature
repetitions



## Compound 1b

YL1040716
Pulse Sequence: s2pul
UNTYP
Date: Jus-400
20
2015
Date: Jul $20{ }^{201}$
Solvent: ${ }^{20 C 13}$
${ }_{\text {Tombient }}^{\text {2 }}$ temperature


Compound 1b
${ }^{13} \mathrm{C}$ NMR $\left.\left(100 \mathrm{MHz}^{2} \mathrm{CDCL}\right)_{3}\right)$ spectra



## Compound 1c

YL1040906
Pulse Sequence: s2pul
UNITYPlus-400 "unity 400 "
Date: Sep ${ }^{\text {Sol }} 2015$
Solvent: ${ }^{2013}$
Ambient temperature
Total 64 repetitions



## Compound 1c

Yl1040906
Pulse Sequence: s2pul
Pulse Sequence: s2pu1
UNITYplus -400 "unity 400 "
UNITYplus-400
Date: Sep
Dan
Sole
Solvent: cocle
Ambient temperature
Total 64 repetitions


## Compound 1c

YL1040906
Pulise Sequence: s2pur
Pulse Sequence: sepul

Solvent: COC13
Ambiant temperature
Total 320 repetitions



## Compound 1d



## Compound 1d



## Compound 1d

Pulse Sequence: s2pul
UNITYP IUS-400 "unity 400 "
Date: Ju1 22.2015
Solvent: coc 13
Ambient temperature
Total 2080
repetitions

${ }^{13} \mathrm{C}$ NMR $\left(100 \mathrm{MHz}^{\text {CDC1 }}\right)$ spectra


## Compound 1d

YL1040717
Pulse Sequence: s2pul
UNITYPIuS-400 "unity400"
Oate: ${ }^{\text {Solvent: }} 222015$
Ambient temperature
Totai 2080 repetitions


Compound 1d
${ }^{13} \mathrm{C}$ NMR ( $100 \mathrm{MHz}, \mathrm{CDCl}_{3}$ ) spectra


## Compound 1e

Yt1040723
Pulse sequence: s2pul
UNITYplus-400 "unity 400 "

Ambient temperature
Total 64 repetitions


Compound 1 1e
${ }^{1} \mathrm{H}$ NMR $\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ spectra


## Compound 1e

YL1040723
Pulse Sequence: s2pul
UNITYP Ius-400 "uni ty 400"
Solvent: cocl3
Ambient
Total 64 temperature
repetitions


Compound 1
H NMR ( $400 \mathrm{MHz}, \mathrm{CDCl}_{3}$ ) spectra


## Compound 1e

YL1040723
Pulse Sequence: s2pul
UNITYPlus-400 "unity400"
Oate: Ju1 3022015
Ambient
Total 624 reperatitions

${ }^{13} \mathrm{C}$ NMR ( $100 \mathrm{MHz}, \mathrm{CDCl}_{3}$ ) spectra


## Compound 1f

YL1040729
Pulse Sequence: s2pul
UNITYPIUS-400 "unity400"
Date: Aus 5201
Ambient temperature
Total 64 repetitions


## Compound 1f

YL1040729
Pulse Sequence: s2pul
unityplus-400 "unity 400 "
Date: Aus 52015
Ambient temperature
Total 64 repetitions


## Compound 1f

YL1040729
Pulse Sequence: s2pul
UNITYplus-400 "unity 400 "
Date: Aug $5{ }^{201}$
Ambient temperature
Total 64 repetitions

${ }^{1} \mathrm{H}$ NMR ( $\left.400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ spectra


## Compound 1f



## Compound 1g

YL1040821
Pulse Sequence: s2pul
UNITYplus-400 "unity 400 "
Datvent: CDC13
Ambient temperature
Total 64 repetitions



## Compound 1g

YL1040821
Pulse Sequence: s2pul
UNITYplus-400 "unity 400
Date:
Date: Aug 242010
Solvent: CoCl ${ }^{201}$
Ambient temperature
Total 64 repetitions


## Compound 1g

YL1040821
Pulse Sequence: s2pul
UNITYPlus-400 "unity400"
Date: Aug 242015
Solvent: $\mathrm{CDCO}^{2} 3$



Compound 1 g
${ }^{1} \mathrm{H}$ NMR $\left(400 \mathrm{MHzz}, \mathrm{CDCl}_{3}\right)$ spectra


## Compound 1g

## YL1040821

Pulse Sequence: s2pul
UNITYPLUS-400 "unity400
UNITYPlus-400"
Date: Au9 24
Sole
Ambient temperature
Total 720 repetitions



## Compound 1h



## Compound 1h

YL1040831
Pulse Sequence: s2pul
UNITYPlus-400 "unity 400 "

Solvent: coc 13
Ambient temperature
Total 64 repetitions


## Compound 1h



## Compound 1i

Y11040825
Pulse Sequence: s2pul
UNITYPlus-400 "unity 400 "
Date: Aug $26{ }^{26} 201$
Solvent: cocis
Anbient temperature
Total 48 repetitions



## Compound 1i



## Compound 1i

Yi1040825
Pulse Sequence: s2pul
UNITYPlus-400 "unity 400
Date: Aug 26
2015
Solvent: CDCl 13
Ambient temperature
Ambient temperature
Total 48 repetitions


HMR ( $\left.400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)_{\text {spectra }}$


## Compound 1i

YL1040825
Pulse Sequence: s2pul
UNITYPlus-400 "unity 400 Cl
Date: Aug
26
2015
solvent: cocli
Ambient temperature
Total 400 repetitions


Compound 1 ii
${ }^{13} \mathrm{C}$ NMR $\left(100 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ spectra


## Compound 1i

Y 11040825
Pulse Sequence: s2pul
UNITYplus-400 "unity $400 "$
Date: Aug 26 2015
Solvent: COC13
Ambient
Ambient temperature
Total 400 repetitions


Compound 1 ii
${ }^{13} \mathrm{C}$ NMR ( $100 \mathrm{MHz}, \mathrm{CDCl}_{3}$ ) spectra


## Compound 1i

YL1040827
Pulse Sequence: s2pul
UNITYPIUS-400 "unity 400 "
UNTYP Lus- -400 "
Date: Au9
Dite
Solvent:


${ }^{1} \mathrm{H}$ NMR $\left(400 \mathrm{MHzound} \mathrm{CDCl}_{3}\right)$ spectra


## Compound 1i

YL1040827
Pulse Sequence: s2pul
UNITYPIus-400 "unity 400 "

Solvent: coll 13
Ambient temperature
Total 64 repetitions


## Compound 1i

Pulse Sequence: s2pul
UNITYplus-400 "unity 400 "
date: Aug ${ }^{31}{ }^{2015}$
Ambient temperature
Total 672 repetitions



## Compound 1k



## Compound 1k



## Compound 1k

YL1040730
Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Solvent: CDCl 13
Ambient $t$ emperatur
Ambient $\begin{gathered}\text { temperature } \\ \text { Total } 64 \\ \text { repetitions }\end{gathered}$




## Compound 1k

YL1040730
Pulse Sequence: s2pul
UNITYplus-400 "unity 400 "
Date: Aug ${ }^{5}{ }^{201}$
Solvent:
COC13
Ambient temperature


## Compound 11

YL1040822
Pulse Sequence: s2pul
UNITYplus-400 ${ }^{\text {unnity }}$
UNITYplus-400 "unity 400


| Ambient |
| :---: |
| Total $64 \begin{array}{c}\text { temperature } \\ \text { repetitions }\end{array}$ |

${ }^{1} \mathrm{H}$ NMR $\left(400 \mathrm{MHz}^{\text {Cond }} \mathrm{CDC}_{3}\right)$ spectra


YL1040822
Pulse Sequence: s2pul
UNITYplus-400 "unity $400 "$
Date: Aug
24
Date: Aug $24{ }^{2015}$
Solvent: ccclis
Ambient
Ambient temperature


## Compound 11

YL1040822
Pulse Sequence: s2pul
UNITYplus-400 "unity 400
Date: Aug 24201
Ambient temperature
Total 64 repetitions


Compound 11
H NMR ( $400 \mathrm{MHz}, \mathrm{CDCl}_{3}$ ) spectra


## Compound 11

YL. 1040822
Pulse Sequence: s2pul
UNITYplus-400 "uni ty 400 "
$\begin{array}{ll}\text { UNITYplus-400 } \\ \text { Date: Aug } & \text { "unity } \\ \text { 24 }\end{array}$
Solvent: cDC 13
Ambient
temperature
Ambient temperature
Total 704 repetitions


Compound 11


## Compound 1m



## Compound 1m

## YL1040832

Pulse Sequence: s2pul
UNITYplus-400 "unity 400 "



## Compound 1m

Pulse Sequence: s2pur
UNITYPIUs-400 "unity400"
Date: Sep $20{ }^{2015}$
Date: Sep coc 2013
${ }_{\text {Total }}^{\text {Ambient }}$ temperature



## Compound 1m

YL1040832
Pulse Sequence: s2pul
UNITYpTus-400
uunity
UNITYPIus-400 "unity400"
Date: Sep ${ }^{2}{ }^{2015}$
Solvent: $\operatorname{coc} 13$
${ }_{\text {Ambient }}^{\text {Total }} \mathbf{3 4 5 6}$ temperature


## Compound 1n

Pulse Sequence: s2pul
UNITYplus-400 "unity 400 "
Date: Aug
26
2015
Solvent: COC13
Ambient
Total 64 temperature
repetitions



## Compound 1n

```
YL1040826
Pulse Sequence: s2pul
UNITYPlus-400 "unity400"
Date: Aug 26 2015
Ambient temperature
```



## Compound 1n

YL1040826
Pulse Sequence: s2pul
UNITYplus-400 "unity 400 "
UNITYplus-400
Date: Au9
Sol
Solvent
2013
Ambient temperature
Total 64 repetitions


## Compound 1n

YL1040826
Pulse Sequence: s2pui
UNTTYPlus-400 "unity 400 "
Date: Aug
26
Date: Aug $26{ }^{20}{ }^{201}$
Solvent: coc 13
Ambient temperature
Total 64000 repetitions


Compound in
${ }^{13} \mathrm{C}$ NMR $\left(100 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ spectra


## Compound 1n

YL1040826
Pulse Sequence: s2pui
UNTYPIUs-400 "unity 400 "
Date: Aug 2612015
Solvent: ${ }^{26}{ }^{20 c} 13$
Ambient temperature
Total 64000 repetitions


Compound in
${ }^{13} \mathrm{C}$ NMR $\left(100 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ spectra


## Compound 10




## Compound 10

YL1040828
Pulse Sequence: s2pul
UNITYPlus-400 "unity $400 "$
Date: Aug ${ }^{31}{ }^{2015}$
Ambient
Total 64 temperature
repetitions

${ }^{1} \mathrm{H}$ NMR $\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ spectra


## Compound 10

YL1040828
Pulse Sequence: s2pul
UNITYplus-400 "unity 400 "
Date: Aug 312015
Solvent: $\operatorname{coc} 13$
Ambient temperature
Total 336 repetitions


Compound 10
${ }^{13} \mathrm{C}$ NMR $\left(100 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ spectra


## Compound 1p

YL1040805
Pulse Sequence: s2pul
UNITYp lus-400 "unity 400 "
Oate: ALH $200^{2015}$
Ambient temperature
Total 64 repetitions


## Compound 1p

YL1040805
Pulse Sequence: s2pul
UNITYplus-400 "unity 400 "
Solvent $\mathrm{CDCO}^{2015}$


## Compound 1p

YL1040805
Pulse Sequence: s2pul
UNITYplus-400 "unity 400
Date: ALG 20201
Solvent: ${ }^{20}{ }^{200} 13$
Ambient temperature
Total 64 repetitions




## Compound 1p

YL1040805
Pulse Sequence: s2pul
UNITYPlus-400 "unity 400 "
Date: Aug $20{ }^{201}$
Ambient temperature
Total 240 repetitions


## Compound 1q

YL1040823
Pulse Sequence: s2pul
Pulse Sequence: s2pul
UNITYplus-400 "unity 400 "
UNITYplus-400 "
Date: Aus
Sat
Sate
Solvent: Cocle
Ambient temperature
Total 64 repetitions


## Compound 19



## Compound 1q

YL1040823
Pulse Sequence: s2pul
UnITYplus-400 "unity 400 "
Oate: ALG 244201
Solvent: COC13
Ambient temperature
Total 64 repetitions




## Compound 1q



## Compound 1r



## Compound 1r



## Compound 1r

YL1040833
Pulse Sequence: s2pul
UNTYYPlus-400 "unity400"
Date:
Date: Sep ${ }^{2}$ 201vent: ${ }^{20 C 13}$
Ambient temprature
Total 320
repetitions


## Compound 1s



## Compound 1s

## YL1040827

Pulse Sequence: s2pul UNITYplus-400 "unity $400^{\prime \prime}$ Date: Aug $26{ }^{201}$
Solvent: $\mathrm{CDCl}_{3}{ }^{201}$ Ambient temperature




## Compound 1s

YL1040827
Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date:
Aug 26
2015
Date: Aug $26{ }^{201}$
Solvent: ${ }^{20 C l} 3$
Ambient temperature


Compound is
H NMR 400 NHz
${ }^{-} \mathrm{H}$ NMR $\left(400 \mathrm{mHz}, \mathrm{CDCl}_{3}\right)$ spectra


## Compound 1s

YL1040827
Pulse Sequence: s2pul
UNITYPlus-400 "unity 400 "
Date: Aug $26{ }^{2015}$
solvent: coclis $^{2015}$
Ambient temperature
Total 944 repetitions


Compound 1 s
${ }^{13} \mathrm{C}$ NMR $\left(100 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ spectra


## Compound 1s

YL1040827
Pulse Sequence: s2pul

solvent: cocli
Ambient
Total
g44
temperatiture
repetitions


Compound 1 s
${ }^{13} \mathrm{C}$ NMR $\left(100 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ spectra


## Compound 1t



## Compound 1t



## Compound 1t

YL1040829
Pulse sequence: s2pul
UNITYplus-400 "unity 400 "

Ambient $\begin{gathered}\text { Tomparature } \\ \text { Total } \\ \text { repetitions }\end{gathered}$


Compound it
${ }^{1} \mathrm{H}$ NMR $\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ spectra


## Compound 1t

## YL1040829

Pulse Sequence: s2pul
UNITYplus-409 "unity $400 "$
Date:
Date: Aug ${ }^{31}{ }^{2015}$
Ambient tenperature
Total 800 repetitions



## Compound 1u

YL1040814
Pulse Sequence: s2pur
UNTYP Lus-400 "unity 400 "
Date: Aug 20201
Ambient temperature


## Compound 1u

YL1040814
Pulse Sequence: s2pul
UNITYplus-400 "unity 400
Date: Aug 202015
Solvent: ${ }^{20} 13$
Ambient temperature
Total 32 repetitions




## Compound 1u

YL1040814
Pulse Sequence: s2pul
UNITYPlus-400 "unity 400 "
Date: Aug 202015
Solvent: ${ }^{20} 13$
Ambient temperature

${ }^{1} \mathrm{H}$ NMR $\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ spectra


## Compound 1u

YL1040814
Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Aug 202015
Solvent: $\operatorname{coc} 13$
Ambient tenperature
Total 208 repetitions


Compound $1 \mathbf{u n}$
${ }^{13} \mathrm{C}$ NMR (100 $\left.\mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ spectra


## Compound 1u

YL1040814
Pulse Sequence: s2pul
UNTYP
Date: Aug $20{ }^{2015}$
Ambient temperature
Total 208 repetitions

${ }^{13} \mathrm{C}$ NMR ( $100 \mathrm{mHzound}, \mathrm{CDC}_{13}$ ) spectra


## Compound 1v



## Compound 1v

YL1040908
Pulse Sequence: s2pul
UNITYplus-400 "unity 400
Date: Sep 111201
Solvent: COC13
Anbient
Total 64 temperature
repetitions



## Compound 1v

```
YL1040908
Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Sep 111 201 
Ambient temperature
```


Compound 1v


## Compound 1v

## YL1040908

Pulse Sequence: s2pul

Date: Sep ${ }^{11}{ }^{2015}$
Solvent:
Ambient
Ambient temperature
Total 448 repetitions


## Compound 1w

YL. 1040901
Pulse Sequence: s2pul
UNITYPIUS-400 "unity400

Ambient temperature
Total 64 repetitions


## Compound 1w

YL. 1040901
Pulse Sequence: s2pul
UNITYPIUS-400 "unity400
UNITY
Date: Sep
Dat
St
Ampient temperature
Total 64 repetition


## Compound 1w

## YL. 1040901

Pulse Sequence: s2pul
UNITYP Lus-400 "unity 400
Date: sep ${ }^{3}{ }^{3}{ }^{2015}$
Solvent: $\mathrm{CDCl}^{3}$
Ambient temperature
Total 64 repetition


## Compound 1w



## Compound 1w

> YL1040901
> Pulse Sequence: s2pul
$\begin{aligned} & \text { Date: Sep }{ }^{3}{ }^{201} \\ & \text { Solvent: CDC13 }\end{aligned}$
$\begin{aligned} & \text { Ambient } \\ & \text { Total } 1280 \text { temperature } \\ & \text { repetitions }\end{aligned}$


## Compound 1x

YL1040909
Pulse Sequence: s2pul
UNITYPlus-400 "unity400"
Date: Sep 112012
Solvent: $\mathbf{C D C O} 13$

| Ambient |
| :---: |
| Total $64 \begin{array}{c}\text { temperature } \\ \text { repetitions }\end{array}$ |



Compound $\frac{1 \mathrm{X}}{}$
(400 $\left.\mathrm{MHz}, \mathrm{CDC} \mathrm{C}_{3}\right)$ spectra


## Compound 1x



## Compound 1x

## YL1040909

Pulse Sequence: s2pul
UNITYplus-400 "unity 400
Date: Sep 11201
Solvent: 10 CDC 13
Ambient
Total
64
temperatiture
repetitions


Compound 1 x
${ }^{1} \mathrm{H}$ NMR $\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ spectra


## Compound 1x

YL1040909
Pulse Sequence: s2pul
UNITYplus-400 "unity 400 "
Date: Sep 112201
solvent: $\operatorname{coC} 13$
Solvent: Ciccle
Ambient terperature
Total 1312 repetitions


## Compound 1x

YL1040909
Pulse Sequence: s2pul
UNITYplus-400 "unity $400 "$
Date:
Date: Sep 1120
Solvent: coc 13
Ambient temperature
Total 1312 repetitions



## Compound 1y

YL1040830
Pulse sequence: s2pul
UNITYplus-400 "unity400"
Solvent: CDCl3
Ambient teemperature
Total 64 repetitions


## Compound 1y

## YL1040830

Pulse Sequence: s2pur
UNITYplus-400 "unity400"
Date: Sep ${ }^{1}{ }^{20}{ }^{20}$
Ambient
Total 64
temperatare
repetitions


## Compound 1y

YL1040830
Pulse Sequence: s2pul
Pulse Sequence: s2pu1
UNITYplus -400 "unity 400 n

Ambient: temperature
Total 704 repetitions


## Compound 1y

YL1040830
Pulse Sequence: s2pul
UNITYPlus-400 "unity400"
Solvent: cocil
Ambient temperature
Total 704 repetitions


Compound 1y
${ }^{13} \mathrm{C}$ NMR $\left(100 \mathrm{MHz}, \mathrm{CDCC}_{3}\right)$ spectra


## Compound 1z




S-102

## Compound 1z

YL1040916
Pulse sequence: s2pul
UNITYplus-400 "unity 400 "
Date: Sep $17{ }^{2015}$
Solvent: ${ }^{17} 1{ }^{2}{ }^{2}$
Ambient
Total 64 temperature
repetitions


Compound $\frac{12}{}$
${ }^{1} \mathrm{H}$ NMR (400 $\left.\mathrm{MHz}^{2} \mathrm{CDCl}_{3}\right)$ spectra


$\underset{\sim}{\sim}$

| 7.5 | 7.0 |  | 6.5 | 6.0 | 5.5 | 5.0 | 4.5 | 4.0 ppm |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\stackrel{\square}{*}$ |  |  |  |  |  |  | \% | $\stackrel{\square}{\circ}$ |
| $\stackrel{\square}{\square}$ | $\cdots$ | $\stackrel{\sim}{m}$ |  |  |  |  | $\stackrel{\circ}{-}$ | $\dot{\dagger}$ |

## Compound 1z



## Compound 1z



## Compound 1aa

YL1040915
Pulse Sequence: s2pul

Sate: Sep 162015
Solvent: ${ }^{16 C D 13}$
Ambient temperatur
Ambient temperature
Total 64 repetitions
1H NMR (400 MHz, CDCl3) spectra


S-106

## Compound 1aa

YL1040915
Pulse Sequence: s2pul

Solvent: COC13 ${ }^{2015}$
Ambient temperature


Compound 1aa
${ }^{1} \mathrm{H}$ NRR $\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ spectra


## Compound 1aa

YL1040915
Pulse Sequence: s2pul
UNITYplus-400 "unity 400 "
Date: Sep ${ }^{16}{ }^{2015}$
Solvent: ${ }^{2015}$
Ambient temperature
Total 736 repetitions

${ }^{13} \mathrm{C}$ Compound 1aa $\left(100 \mathrm{MHz}, \mathrm{CDC}_{3}\right)$ spectra


## Compound 1aa

YL1040915
Pulse Sequence: s2pul
UNITYplus-400 "unity 400 "
Solvent:
Ambient
CDCll
Ambient temperature


Compound 1aa
${ }^{13} \mathrm{C}$ NMR $\left(100 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ spectra


## Compound 6a


${ }^{1} \mathrm{H}$ NMR $\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ spectra ${ }^{\text {Com }}$

## Compound 6a



## Compound 6a

YLenon2a
Pulse Sequence: s2pu7
UNTYP US-400 "unity 400 "
Solvent: cocisar
Ambient temperature
Total 32 repetitions


Compound $\frac{6 a}{a}$
${ }^{1} \mathrm{H}$ NMR (400 MHz , $\left.\mathrm{CDCl}_{3}\right)^{3}$ spectra


## Compound 6a

YLenon2a
Pulse Sequence: s2pul
UNTYYPus-400 "unity 400 "
Date no $\operatorname{coc}^{2013}$
Ambentent temperature
Total 704 repetitions



## Compound 6b



## Compound 6b



## Compound 6b



## Compound 6c



## Compound 6c

YLenon2c
Pulse Sequence: s2pul
Pulse Sequence: s2pu1

Solvent: COCl13
Ambient
Total
64
temperature
repetitions


## Compound 6c



## Compound 6d



## Compound 6d



## Compound 6d

YLenon2d
Pulse Sequence: s2pul
UNTYP Lus-400 "unity400"
Date: Nov $23{ }^{201}$
Ambient temperature
Total 224 repetitions


Compound $\underline{6 d}$
${ }^{13} \mathrm{C}$ NMR $\left.(100 \mathrm{MHz}, \mathrm{CDCl}]_{3}\right)$ spectra


## Compound 6d

Ytenon2d
Pulse Sequence: s 2 pu
UNTYP Lus-400 "unity $400^{\prime \prime}$
Date: Nov 232015
Solvent: $\operatorname{coc} 13$
Ambient temperature
Total 224 repetitions


Compound $\underline{\text { bd }}$
${ }^{13} \mathrm{C}$ NMR $\left.(100 \mathrm{MHz}, \mathrm{CDCl})_{3}\right)$ spectra


## Compound 6e

YLenon2e
Pulse Sequence: s2pul
UNITYplus-400 "unity 400 "
Date: Nov 222015
Ambient temperature
Total 64 repetitions

5.



## Compound 6e

YLenon2e
Pulse Sequence: s2pul
UNTYYPIus-400 "unity 400 "
Solvent: CDCD 13
Ambient
Total 64
temperature
repetitions




## Compound 6e

YLenon2e
Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Nov 21201
Solvent: ${ }^{2}{ }^{2} 13$
Ambient temperature
Total 64 repetition


Compound 6 e
${ }^{1} \mathrm{H}$ NMR $\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ spectra


## Compound 6e

YLenon2e
Pulse Sequence: s2pul
UNITYP Lus-400 "unity 400
Date: Nov ${ }^{2}{ }^{201}$
Solvent: $\operatorname{coc}^{201}$
Ambient temperature
Total 2208
repetitions


Compound 6e



## Compound 6f

YLenon2f
Pulse Sequence: s2pur
Pulse Sequence: s2pul
UNITYplus -400 "unity 400 m

Solvent: coct 13
Ambint temperature
Total 64 repetitions


Compound 6 Ff


## Compound 6f

YLenon2f
Puise Sequence: s2pur
UNITYplus-400 "unity $400 "$
Date:
Oct 26
2015
Date: oct
Solvent: CDCC $^{26}$
Ambient
Total 64 reppetitions
$\underset{{ }^{1} \mathrm{H} \text { NMR }\left(400 \mathrm{MHzound} \text { 6f } \mathrm{CDCl}_{3}\right) \text { spectra }}{ }$


Total 64 repetitions

! ! ᄂ ! ! ! ! !


## Compound 6f



## Compound 6g



## Compound 6g

YLenon2g
Pulse Sequence: s2pul
UNITYplus-400 "unity 400 "
Date: Nov ${ }_{2}{ }_{2015}{ }^{2015}$
Solvent: cDC13
Ambient temperature
Total 64 repetitions


Compound 6 g
${ }^{1} \mathrm{H}$ NMR $\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ spectra


## Compound 6g

## YLenon2g

Pulse Sequence: s2pul
UNITYPLus-400
Date: Nov
2015
Date: Nov 212015
Solvent: cDC13
Ambient temperature
Totai 1008 repetitions

${ }^{13} \mathrm{C} \mathrm{CMR}\left(100 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ spectra


## Compound 6g

Pulse Sequence: s2pu1

Solvent: cDC 3 ,
Ambient
Ambient temperature
Total 1008 repetitions

${ }^{13} \mathrm{C} \mathrm{CMR}\left(100 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ spectra


## Compound 6h



## Compound 6h

YL1041223
Pulse Sequence: s2pul
UNITYplus-440 "unity 400 "
Date:
Dec 25
2015 Date: Dec 25201
Solvent: $\operatorname{coc} 13$ Ambient temperature
Total 64 repetitions


## Compound 6h



## Compound 6h


${ }^{13} \mathrm{C}$ NMR $\left(100 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ spectra



## Compound 6i



## Compound 6i

YLenon2i
Pulse Sequence: s2pul
UNITYplus-400 "unity400"
UNITYPlus-400 "unity 400
Date: Nove
Sat
Ambient
Total 64 temperature
repetitions


## Compound 6i

YLenon21
Pulse Sequence: s2pul
UNITYPlus-400 "unity 400
UNITYPlus-400 "un
Date. Nov 42015
Solvent: cocle
Ambient tenperature
Total 169 repetitions



## Compound 6j

YL. 1041023
Pulse Sequence: s2pul
UNITYplus-400 "unity400"

Solvent: CDC13
Ambient
Ambient
Total 64
temperature
repetitions


Compound $6 \mathfrak{i}$
$400 \mathrm{MHz}, \mathrm{CDC}_{3}$ ) spectra


## Compound 6j

YL1041023
Pulse Sequence: s2pul
Pulse

Solvent: c 0 cc 13
Ambient
temperatur
Ambient
Total 64
temperature
repetitions




## Compound 6j

## YL. 2041023

Pulse sequence: s2pul
UNITYPlus-400 "unity 400
Date: Nov $2{ }^{2} 2015$
Solvent: ${ }^{2}{ }^{2}{ }^{2} 13$
Ambient temperature
Total 64 repetition

$\underset{{ }^{1} \mathrm{H} \text { NMR }\left(400 \mathrm{MHPzond}, \mathrm{CDCl}_{3}\right) \text { spectra }}{\text { 6i }}$


## Compound 6i

## YL1041023

Pulse Sequence: s2pul
UNTYY Lus-400 "unity400"
Date: Nov 2015
Date: Nov ${ }^{2}{ }^{201}$
Solvent: $\operatorname{CDC}_{1}{ }^{3}$
Ambient temperature
Total 1312 repetitions



## Compound 6i


${ }^{13} \mathrm{C}$ NMR $\left(100 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ spectra


## Compound 6k

YLenon2K
Pulse Sequence: s2pul
UNITYPlus-400 "unity 400 "
UNITYplus-400 "unit
Date: Oct
Sit
Sile
Solvent: Coclis
Ambient temperature
Total $64 \begin{aligned} & \text { repetitions }\end{aligned}$


${ }^{1} \mathrm{H}$ NMR $\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ spectra


## Compound 6k

YLenon2K
Pulse Sequence: s2pul
UNITYplus-400 "unity 400 "

Solvent: Coct13
Ambient temperature
Total 64 repetitions


## Compound 6k

YLenon2K
Pulse Sequence: s2pul
UNITYplus-400 "unity 400 "
UNIIPlus-400 "unit
Date:
Oct
26
2015
Solvent: cocile
Ambient
Total 64
temperature
repetitions


Compound $\mathrm{G}_{\mathrm{k}}$
H NMR $\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ spectra


## Compound 6k

Pulse sequence: s2pul
UnITYplus-400 "unity 480 "
Date: Oct $26{ }^{2015}$
Solvent: coc ${ }^{201}$
Ambient temperature
Total 208 repetitions



## Compound 61

YLenon2 1
Pulse Sequence: s2pul
UNITYPlus-400 "unity400
UNITYplus-400
Date: Nov 2015
Ambient temperature
Total 64 repetitions



## Compound 61

YLenon2 1
Pulse Sequence: s2pul
UNITYPlus-400 "unity400

Ambient temperature
Total 64 repetitions


## Compound 61

YLenon2 1
Pulse Sequence: s 2 pul
UNITYPlus-400 "unity400
UNITYP Mus-400 ${ }^{\text {un }}$ unity 400
Date: Nov 22015
Ambient temperature
Total 64 repetitions

${ }^{1} \mathrm{H}$ NMR $\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ spectra


## Compound 61



## Compound 61

YLenon21
Pulse Sequence: s2pul
Pulse Sequence: s2pul
UNITYplus -400 "unity 400 M
UNITYPlus-400 "un
Date: Nov 20 2015
Solvent: CDC 13
Solvent: CDE13
Ambient temperature
Total 2464 repetitions



## Compound 6m



S-156

## Compound 6m

## YL1041224

Pulse Sequence: s2pul

Sate: Dec 252015
Solvent COC13
Ambient temperature
Total 64 repetitions


## Compound 6m



## Compound 6m



## Compound 6n

YLemon2n
Pulse Sequence: s2pul
UNITYplus-400 "unity 400 "
Sote: Nov ${ }^{\text {Solvent: }} \operatorname{cDC}_{13}{ }^{2015}$
Ambient temperature
Total
54
repetitions


Compound $\frac{6 \mathrm{n}}{}$
$\left.400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ spectra


## Compound 6n

YLenon2n
Puise Sequence: s2pul
UNITYPlus-400 "unity400"

Solvent:
Ambilint temperature
Total 64 repetitions


## Compound 6n

YLenon2n
Pulse Sequence: s2pul
UNITYplus-400 "unity 400 "

Ambient temperature
Total 64 repetitions


Compound $\frac{\mathrm{fn}}{}{ }^{1} \mathrm{HNRR}\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ spectra


S-162

## Compound 6n

YLemon2n
Pulse Sequence: s2pul
UNITYPIUS-400 "unity400"
Date: Nov ${ }^{4}{ }^{2015}$
Tmbient 2144 reperature
Totitions


Compound $\underline{6 n}$
${ }^{13} \mathrm{C}$ NMR $\left(100 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ spectra


## Compound 6n

YLenon2n
Purse sequence: s2pur
UNITYPIus-400 "unity 400 "
Date: Nov ${ }^{4}{ }^{201}{ }^{201}$
Ambient
Total 2144 remperature

${ }^{13} \mathrm{C}$ Compound 6 n
${ }^{13} \mathrm{C}$ NMR $\left(100 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ spectra


## Compound 60

Ylenon2o
Pulse Sequence: s2pul
UNITYPTus-400 "unity 400 "
Date: Nov $9{ }^{201}$
Solvent: $\operatorname{coc} 13$
Ambient temperature
Total 64 repetitions


## Compound 60

YLenon2o
Pulse Sequence: s2pu1

solvent: cDC13
Ambient temperature


## Compound 60

YLenon2o
Pulse Sequence: s2pul

Solvent: CDC13
Ambient temperature


Compound $\frac{60}{}{ }^{1} \mathrm{HNMR}\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ spectra


## Compound 60

YLenon2o
Pulse Sequence: s2pul

Date: Nov ${ }^{9}{ }^{201}{ }^{201}$
Solvent
Ambient temperature
Total 128 repetitions




## Compound 6p

YLenon2P
Pulse Sequence: s2pul
UNITYplus-400 "unity $400 "$
Date: Oct
Sol
Solvent: CDCl 13
Ambient
temperature
Ambient
Total 64 temperature
repetitions


Come
${ }^{1} \mathrm{H}$ NMR $\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ spectra


## Compound 6p



## Compound 6p

YLenon2P
Pulse Sequence: s2pul
UNTYPlus-400 "unity 400 "
Solvent: $\mathrm{CDCD}^{2} 3$
Ambient temperature
Total 64 repetitions


## Compound 6p

YLenon2P
Pulse Sequence: s2put
Purse Sequence: s2pul
UNITYplus-400 "unity $400 "$

Solvent: COCl 13
Ambient temperature
Total 256
repetitions


## Compound 6q

YLenon2Q
Pulse Sequence: s2pul
UNITYplus-400 "unity $400^{\prime \prime}$
UNITYplus-400 ${ }^{2}$ uni
Date. No 2 2 2015
Solvent: cDC 13
Ambient temperature
Total 64 repetitions

${ }^{1} \mathrm{H}$ NMR $\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ spectra


## Compound 6q

YLenon2Q
Pulse Sequence: s2pul
UnITYplus-400 "unity 400 "
Date: Nov $2{ }^{2015}$
Solvent: $\begin{aligned} & \text { CDC13 } \\ & \text { Ambient } \\ & \text { temperature }\end{aligned}$
Ambient
Total
64
temperature
repetitions


## Compound 6q

YLenon20
Pulse Sequence: s2pul
UNTYYP Lus-400 "unity 400 "
Solvent: CDC 13
Ambient
Total
64
temperature
repetitions


## Compound 6q




## Compound 6r

```
YL1041225
Pulse Sequence: s2pul
\(\begin{array}{ll}\text { UNITYPlus-400 "unity } 400 " \\ \text { Date: } \\ \text { Dec } & 25 \\ \text { 2015 }\end{array}\)
Date: Dec \(25{ }^{201}\)
Solvent cocl
\({ }^{\text {Ambient }}\) total 64 repperature
```



## Compound 6r

YL1041225
Pulse Sequence: s2pul
UNITYplus-400 "unity $400^{\circ}$
Solvent: cDC13
Ambient
Total
tomperature


## Compound 6r

YL1041225
Pulse Sequence: s2pul
UNITYPlus-400 "unity400"
Date: ${ }^{\text {Dec }} 25$
2015
Date: Dec $25{ }^{201}$
Solvent cocl
Ambient
Total 64
temperature
repetitions


## Compound 6r

```
YL1041225
Pulse Sequence: s2pu
UNITYPlus-400 "unity400"
Mate. Dec 25 2011
l
```



## Compound 6s

YLenon2s
Pulse Sequence: s2pul
unityplus-400 "unity 400
Date: Nov ${ }^{4}{ }^{2015}$
Ambient temperature
Total 64 repetitions



## Compound 6s



## Compound 6s

YLenon2s
Pulse Sequence: s2pul
UNITYplus-400 "unity 400
Date: Nov ${ }^{4}{ }^{2}{ }^{2015}$
Ambient temperature
Total 64 repetition


| Compound 6 S |
| :---: |

NMR ( 400 MHz . $\mathrm{CDCl}_{23}$ ) spectra


## Compound 6s

YLenon2s
Pulse sequence: s2pul
UnITYplus-400 "unity400"




Compound 6 s
${ }^{13} \mathrm{C}$ NMR ( $100 \mathrm{MHz}, \mathrm{CDC} \mathrm{Cl}_{3}$ ) spectra


## Compound 6t

YLenon2t
Pulse Sequence: s2pul

Solvent: cocli3
Ambient temperature


## Compound 6t

YLenon2t
Pulse Sequence: s2pu
UNTYYPUS-400 "unity400
solvent: coCl3
Ambient temperature


S-186

## Compound 6t

YLenon2t
Sequence: s2pul

Date: Nov ${ }^{9}{ }^{201}$
Solvent: ${ }^{20 C 13}$
Ambient temperature

${ }^{1}$ Compound


## Compound 6t

YLenon2t
Pulse Sequence: s2pul
UNITYP Lus-400 "unity400"
Date: Nov $9{ }^{2015}$
Solvent: cocl3
Ambient temperature
Total 1632 repetitions



## Compound 6u

YLenon2u
Pulse Sequence: s2pul
UNITYPIUS-400 "unity400"

Ambient temperature
Totâ 64 repetitions


## Compound 6u

YLenon2u
Pulse Sequence: s2pul

vent: $\operatorname{coc} 13$
Ambient temperature
Total 64 repetitions



ctra


## Compound 6u

YLenon2u
Pulse Sequence: s2pul
UNITYPlus-400 "unity400"
Date: Nov
2015
Solvent: CoCli3
Ambient temperature
Total 64 repetitions


## Compound 6u

YLenon2u
Pulse Sequence: s2pul
$\begin{array}{ll}\text { UNITYPlus-400 } \\ \text { Date: Nov } & 2015\end{array}$
Date: Nov ${ }^{2}{ }^{2015}$
Solvent: $\operatorname{coCl}^{2} 3$
Ambient tenperature
Total 3200 repetitions


## Compound 6v

YLenon2v
Pulse Sequence: s2pul
UNITYPLus-400 "unity400"
Solvent: $\mathrm{CDCD}^{2} 3$
Ambient
Total
64
temperature
repetitions


Compound 6 v
${ }^{1} \mathrm{HNMR}\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ spectra


## Compound 6v

YLenon2v
Pulse Sequence: s2pul
UNITYPlus-400 "unity400"
Date: Nov 13
Not
Solvent: COC13
Ambient
Total
temperater
repetitions


Compound 6 v
${ }^{1} \mathrm{HNMR}\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ spectra


## Compound 6v

YLenon2v
Pulse Sequence: s2pul
UNITYPlus-400 "unity $400 "$
Date: Nov
13
Oate: Nov ${ }^{13}{ }^{201}$
solvent: CDCl 13
Ambient temperature


Compound 6
${ }^{1} \mathrm{HNMR}\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ spectra


## Compound 6v

YLenon2v
Pulse Sequence: s2pul
UNITYPlus-400 "unity400
UNITYPlus-400
Date: Nov 13
Ambient
Total 512 temperature
retitions



## Compound 6v

YLenon2v
Pulse Sequence: s2pul
UNITYplus-400 "unity 400
Date: Nov 13201
Solvent: COC13
Ambient temperature
Tota1 512 repetitions



## Compound 6w

YLenon2w
Pulse Sequence: s2pul

Date: Nov $10{ }^{201}$
Solvent: ${ }^{20 C 13}$
Ambient temperature
Total 64 repetitions


## Compound 6w

YLenon2w
Pulse Sequence: s2pul

Date: Nov $10{ }^{2}$
Solvent: $\operatorname{coC} 13$
Ambient temperature
Total 64 repetitions


## Compound 6w

YLenon2w
Pulse Sequence: s2pul

Date: Nov $10{ }^{201}$
Solvent: $C$ COC13
Ambient temperature
Total 64 repetitions


## Compound 6w

YLenonaw
Pulse Sequence: s2pul

Date: No: $10{ }^{201}$
Solvent: $C O C 13$
Ambient temperature
Total 320 repetitions


## Compound 6w

YLenonzw
Pulse Sequence: s2pul
UNITYplus-400 "uni ty 400 "
Date: Nov $10{ }_{20}{ }^{2015}$
Oate: Nov $10{ }^{2015}$
Solvent: $\operatorname{CDC} 13$
Ambient
Total
320
temperature
repetitions




## Compound 6x




## Compound 6x

> Ylenon2x Pulse Sequence: s2pu1 UNTTYp, us - 400 "unity $400 "$ Date: Nov 42015

Sate: Nov ${ }^{4}{ }^{4}{ }^{201}$
${ }_{\text {Anbient }}$ temperature


## Compound 6x

YLenon2x
Pulse Sequence: s2pul

Date: Nov ${ }^{4}{ }^{2} 2015$
Solvent
CDCO 13
Ambient
Total 64 temperature
repetitions


Compound 6 x
${ }^{1} \mathrm{H}$ NMR $\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ spectra


## Compound 6x

YLenon2x
Pulse Sequence: s2pur
unityplus-400 "unity 400
Date: Nov ${ }^{4}{ }^{2015}$
Solvent: $\operatorname{coc} 13$
Ambient
Total 1728 emprature
repetitions

${ }^{13} \mathrm{C}$ NMR $\left(100 \mathrm{MHz}, \mathrm{CDCO}_{13}\right)$ spectra

## Compound 6x

YLenon2x
Pulse Sequence: s2pul
unityplus-400 "untty 400
Date: Nov ${ }^{4}{ }^{201}$
Solvent: ${ }^{201}$
Ambient temperature
Total 1728 repetitions


Compound $\underline{6 \mathrm{X}}$
${ }^{13} \mathrm{C}$ NMR $\left(100 \mathrm{MHz}, \mathrm{CDC} \mathrm{C}_{3}\right)$ spectra

## Compound 6y



## Compound 6y



## Compound 6y

YL1041024
Pulse Sequence: s2pul
UNITYPIUS-400 "unity 400
Date: Nov $2{ }^{201}$
Ambient temperature
Totai 64 repetitions


Compound 6 by
${ }^{1} \mathrm{H}$ NMR $\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ spectra


## Compound 6y

## YL1041024

Purse Sequence: s2pul
UNITYPIUS-400 "unity 400
UNTYPDus-400 ${ }^{\text {"un }}$
Date: Now
Solvent: ${ }^{2}{ }^{2015}$
Solvent:
Ambient temperature
Total 2176 repetitions



## Compound 6y

## YL1041024

Purse Sequence: s2pul
UNITYPIUS-400 "unity 400

Ambient tenperature
Total 2176 repetitions


Compound $6 y$
${ }^{13} \mathrm{C}$ NMR $\left(100 \mathrm{MHz}\right.$, $\left.\mathrm{CDC}_{3}\right)$ spectra


## Compound 6z



## Compound 6z



## Compound 6aa

YL1050423
Pulse Sequence: s2pul
UNITYplus-400 "unity 400
Solvent: CDCl $^{13}{ }^{\text {Date }}$
Ambient temperature
Total 32 repetitions



## Compound 6aa

YL1050423
Pulse sequence: s2pur
UNITYplus-400 "unity 400
27 2016
Ambient temperature
Total 32
repetitions



## Compound 6aa

YL1050423
Pulse Sequence: s2pul
UNITYplus-400 "unity 400 "
Date: Apr ${ }^{27}{ }^{2016}$
Solvent: ${ }^{20 C 13}$
Ambient temperature
Total $541 \begin{aligned} & \text { repetitions }\end{aligned}$



## Compound 8a



## Compound 8a

> SK1010808-2 Pulse sequence: s2pul unTryius

UNITYplus-400 "unity 400 "
ate: Sep $12{ }^{2012}$
solvent: CDCC
Ambient temperature

Compound 8 ga
${ }^{13} \mathrm{C}$ NMR $\left(100 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ spectra


## Compound 8b



## Compound 8b



## Compound 9a



## Compound 9a




## Compound 9b



## Compound 9b

## YL1040907

Pulse Sequence: s2pul
UnITYplus-400 "unity400"
Date: Sep 88201
Solvent: ${ }^{2}{ }^{2} 1{ }^{2}$
Ambient
Total 64 temperatition
tepetion


## Compound 9b

YL1040907
Pulse Sequence: s2pul
UNITYP Lus-480 "unity 400 "
Solvent: cocli3
Ambient temperature
Total 11728 repetitions


Compound 9 gb
${ }^{3} \mathrm{C}$ NMR ( $\left.100 \mathrm{MHz}, \mathrm{CDC} \mathrm{I}_{3}\right)$ spectra


## Compound 9b

YL1040907
Pulse Sequence: s2pul
UNITYPIus-400 "unity 400 "
Date: Sep ${ }^{8} 2015$
solvent: $\operatorname{coc} 13$
Ambient
Total 11728
temperature
repetitions




## Compound 9c

YL1040912
Pulse Sequence: s2pul

Date sep 144
Solvent: ${ }^{201}$
Smbient temperature
Tota1 64 repetitions




## Compound 9c



## Compound 9c

YL1040912
Pulse Sequence: s2pul

Date: Sep $14{ }^{201}$
Solvent: $C$ COC13
Ambient temperature
Total 4448 repetitions

${ }^{13} \mathrm{C}$ NMR ( $100 \mathrm{MHz}, \mathrm{CDC} \mathrm{I}_{3}$ ) spectra


## Compound 9d



## Compound 9d



## Compound 9d

YL1040931
Pulse Sequence: s2pul
UNITYPIus-400 "unity 400 "
Date: Oct ${ }^{6}{ }^{2015}$
solvent: $\operatorname{coc}^{2013}$
Ambient
Total $4272{ }^{\text {tenperature }}$ repetitions



## Compound 9d

YL1040931
Pulse Sequence: s2pul
UNITYplus-400 "unity 400 M
Solvent: COC13
Ambient
temperature
$\underset{\text { Total } 4272 \text { repetitions }}{\text { Ambient }}$



## Compound 10



## Compound 10

YL1041021
Pulse Sequence: s2pul
UNITYplus-400 "unity 400
ct
CDC 13
0 Ambient temperature
Total 64 repetitions


## Compound 10

YL1041021
Pulse sequence: s2pul
UnTYYplus-400 "unity400"
Date: Oct 222015
Solve
Ambient temperature
Total 12800 repetitions

${ }^{13} \mathrm{C}$ NMR $\left(100 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ spectra


## Compound 10

YL1041021
Pulse Sequence: s2pul
UNYTYplus-400
Date:
Oct
unity 42001
Date:
Solven
Ambien
Ambient temperature
Total 12800
repetitions

${ }^{13} \mathrm{C}$ NMR ( 100 MHPound , $\mathrm{CDCO}_{3}$ ) spectra


Crystal data and structure refinement for $\mathbf{1 a}$ (the thermal ellipsoid was drawn at the $50 \%$ probability level)


Crystal data and structure refinement for $\mathbf{1 c}$ (the thermal ellipsoid was drawn at the $50 \%$ probability level)

| (evel |  |
| :---: | :---: |
| Identification code | 150917_0m |
| Empirical formula | C19 H20 N2 O2 |
| Formula weight | 308.37 |
| Temperature | 296(2) K |
| Wavelength | 0.71073 Å |
| Crystal system, Space group | Monoclinic, P 21/c |
| Unit cell dimensions | $\begin{array}{ll} \mathrm{a}=7.1877(5) \AA & \alpha=90^{\circ} . \\ \mathrm{b}=25.1688(16) \AA & \beta=110.284(4)^{\circ} . \\ \mathrm{c}=9.8090(6) \AA & \gamma=90^{\circ} . \end{array}$ |
| Volume | 1664.46(19) $\AA^{3}$ |
| Z, Density (calculated) | $4,1.231 \mathrm{Mg} / \mathrm{m}^{3}$ |
| Absorption coefficient | $0.081 \mathrm{~mm}^{-1}$ |
| F(000) | 656 |
| Crystal size | $0.20 \times 0.15 \times 0.15 \mathrm{~mm}^{3}$ |
| Theta range for data collection | 1.618 to $26.408^{\circ}$. |
| Index ranges | $-8<=\mathrm{h}<=6,-31<=\mathrm{k}<=30,-12<=1<=12$ |
| Reflections collected | 13538 |
| Independent reflections | $3399[\mathrm{R}($ int $)=0.0362]$ |
| Completeness to theta $=25.242^{\circ}$ | 99.9 \% |
| Absorption correction | Semi-empirical from equivalents |
| Max. and min. transmission | 0.9485 and 0.8499 |
| Refinement method | Full-matrix least-squares on $\mathrm{F}^{2}$ |
| Data / restraints / parameters | 3399 / 0 / 212 |
| Goodness-of-fit on $\mathrm{F}^{2}$ | 1.030 |
| Final R indices [I>2sigma(I)] | $\mathrm{R} 1=0.0481, \mathrm{wR} 2=0.1186$ |
| R indices (all data) | $\mathrm{R} 1=0.0649, \mathrm{wR} 2=0.1299$ |
| Extinction coefficient | n/a |
| Largest diff. peak and hole | 0.166 and -0.167e. $\AA^{-3}$ |

Crystal data and structure refinement for $\mathbf{1 p}$ (the thermal ellipsoid was drawn at the $50 \%$ probability level)

| - |  |
| :---: | :---: |
| Identification code | mo_150908_0m |
| Empirical formula | C 23 H 26 N 2 O 3 |
| Formula weight | 378.46 |
| Temperature | 296(2) K |
| Wavelength | 0.71073 Å |
| Crystal system, Space group | Triclinic, P-1 |
| Unit cell dimensions | $a=8.4384(6) \AA \quad \alpha=70.841(2)^{\circ}$. |
|  | $\mathrm{b}=11.0458(8) \AA$ A $\quad \beta=77.317(2)^{\circ}$. |
|  | $\mathrm{c}=12.1243(8) \AA \quad \gamma=86.918(2)^{\circ}$. |
| Volume | 1041.25(13) $\AA^{3}$ |
| Z, Density (calculated) | $2,1.207 \mathrm{Mg} / \mathrm{m}^{3}$ |
| Absorption coefficient | $0.080 \mathrm{~mm}^{-1}$ |
| F(000) | 404 |
| Crystal size | $0.25 \times 0.20 \times 0.20 \mathrm{~mm}^{3}$ |
| Theta range for data collection | 1.820 to $26.514^{\circ}$. |
| Index ranges | $-10<=\mathrm{h}<=10,-13<=\mathrm{k}<=13,-11<=\mathrm{l}<=15$ |
| Reflections collected | 17072 |
| Independent reflections | $4298[\mathrm{R}(\mathrm{int})=0.0330]$ |
| Completeness to theta $=25.242^{\circ}$ | 99.8\% |
| Absorption correction | Semi-empirical from equivalents |
| Max. and min. transmission | 0.9485 and 0.8948 |
| Refinement method | Full-matrix least-squares on $\mathrm{F}^{2}$ |
| Data / restraints / parameters | 4298 / 180 / 302 |
| Goodness-of-fit on $\mathrm{F}^{2}$ | 1.040 |
| Final R indices [ $\mathrm{I}>2 \operatorname{sigma}(\mathrm{I})$ ] | $\mathrm{R} 1=0.0473, \mathrm{wR} 2=0.1277$ |
| R indices (all data) | $\mathrm{R} 1=0.0710, \mathrm{wR} 2=0.1461$ |
| Extinction coefficient | n/a |
| Largest diff. peak and hole | 0.253 and -0.175 e. $\AA^{-3}$ |

Crystal data and structure refinement for $\mathbf{7 y}$ (the thermal ellipsoid was drawn at the $50 \%$ probability level)


Crystal data and structure refinement for $\mathbf{9 a}$ (the thermal ellipsoid was drawn at the $50 \%$ probability level)

| (evel |  |
| :---: | :---: |
| Identification code | 1507081t_0m_a |
| Empirical formula | C12 H14 N2 O3 |
| Formula weight | 234.25 |
| Temperature | 100(2) K |
| Wavelength | 0.71073 Å |
| Crystal system, Space group | Monoclinic, P 21/n |
| Unit cell dimensions | $a=15.2093(9) \AA \AA^{\circ} \quad \alpha=90^{\circ}$. |
|  | $\mathrm{b}=4.0297(2) \AA \quad \beta=90.067(3)^{\circ}$. |
|  | $\mathrm{c}=18.2902(11) \AA \AA^{\text {A }} \quad \gamma=90^{\circ}$. |
| Volume | 1120.99(11) $\AA^{3}$ |
| Z, Density (calculated) | $4,1.388 \mathrm{Mg} / \mathrm{m}^{3}$ |
| Absorption coefficient | $0.101 \mathrm{~mm}^{-1}$ |
| F(000) | 496 |
| Crystal size | $0.20 \times 0.08 \times 0.08 \mathrm{~mm}^{3}$ |
| Theta range for data collection | 1.740 to $26.321^{\circ}$. |
| Index ranges | $-18<=\mathrm{h}<=18,-4<=\mathrm{k}<=5,-22<=\mathrm{l}<=22$ |
| Reflections collected | 9387 |
| Independent reflections | $2258[\mathrm{R}(\mathrm{int})=0.0243]$ |
| Completeness to theta $=25.242^{\circ}$ | 99.9 \% |
| Absorption correction | Semi-empirical from equivalents |
| Max. and min. transmission | 0.9485 and 0.8866 |
| Refinement method | Full-matrix least-squares on $\mathrm{F}^{2}$ |
| Data / restraints / parameters | 2258 / 0 / 157 |
| Goodness-of-fit on $\mathrm{F}^{2}$ | 1.098 |
| Final R indices [I>2sigma(I)] | $\mathrm{R} 1=0.0491, \mathrm{wR} 2=0.1559$ |
| R indices (all data) | $\mathrm{R} 1=0.0662, \mathrm{w} 2=0.1878$ |
| Extinction coefficient | n/a |
| Largest diff. peak and hole | 0.378 and -0.465 e. $\AA^{-3}$ |

