Synthesis of Deuterated 1,2,3-Triazoles

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TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>Information</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>500 MHz $^1$H NMR spectrum of 3-((triisopropylsilyl)ethynyl)pyridine in CDCl$_3$ (intermediate in the synthesis of $9$-$D$ and $9$-$H$)</td>
<td>S-4</td>
</tr>
<tr>
<td>125 MHz $^{13}$C NMR spectrum of 3-((triisopropylsilyl)ethynyl)pyridine in CDCl$_3$ (intermediate in the synthesis of $9$-$D$ and $9$-$H$)</td>
<td>S-5</td>
</tr>
<tr>
<td>500 MHz $^1$H NMR spectrum of 3-ethynylpyridine in CDCl$_3$ (intermediate in the synthesis of $9$-$D$ and $9$-$H$)</td>
<td>S-6</td>
</tr>
<tr>
<td>500 MHz $^1$H NMR spectrum of triisopropyl(phenylethynyl)silane-$D_5$ in CDCl$<em>3$ (intermediate in the synthesis of $13$-$D_6$ and $14$-$D</em>{11}$)</td>
<td>S-7</td>
</tr>
<tr>
<td>125 MHz $^{13}$C NMR spectrum of triisopropyl(phenylethynyl)silane-$D_5$ in CDCl$<em>3$ (intermediate in the synthesis of $13$-$D_6$ and $14$-$D</em>{11}$)</td>
<td>S-8</td>
</tr>
<tr>
<td>77 MHz $^2$H NMR spectrum of triisopropyl(phenylethynyl)silane-$D_5$ in CDCl$<em>3$ (intermediate in the synthesis of $13$-$D_6$ and $14$-$D</em>{11}$)</td>
<td>S-9</td>
</tr>
<tr>
<td>500 MHz $^1$H NMR spectrum of ethynylbenzene-$D_5$ in CDCl$<em>3$ (intermediate in the synthesis of $13$-$D_6$ and $14$-$D</em>{11}$)</td>
<td>S-10</td>
</tr>
<tr>
<td>77 MHz $^2$H NMR spectrum of ethynylbenzene-$D_5$ in CDCl$<em>3$ (intermediate in the synthesis of $13$-$D_6$ and $14$-$D</em>{11}$)</td>
<td>S-11</td>
</tr>
<tr>
<td>500 MHz $^1$H NMR spectrum of 4-(t-butyl)phenyl azide in CDCl$_3$ (intermediate in the synthesis of $6$-$D$)</td>
<td>S-12</td>
</tr>
<tr>
<td>500 MHz $^1$H NMR spectrum of $m$-azidobenzonitrile in CDCl$_3$ (intermediate in the synthesis of $9$-$D$)</td>
<td>S-13</td>
</tr>
<tr>
<td>77 MHz $^2$H NMR spectrum of phenyl azide-$D_5$ in CDCl$<em>3$ (intermediate in the synthesis of $12$-$D_6$ and $14$-$D</em>{11}$)</td>
<td>S-14</td>
</tr>
<tr>
<td>500 MHz $^1$H NMR spectrum of $1$-$D$ in CDCl$_3$</td>
<td>S-15</td>
</tr>
<tr>
<td>125 MHz $^{13}$C NMR spectrum of $1$-$D$ in CDCl$_3$</td>
<td>S-16</td>
</tr>
<tr>
<td>77 MHz $^2$H NMR spectrum of $1$-$D$ in CDCl$_3$</td>
<td>S-17</td>
</tr>
<tr>
<td>500 MHz $^1$H NMR spectrum of $2$-$D$ in CDCl$_3$</td>
<td>S-18</td>
</tr>
<tr>
<td>125 MHz $^{13}$C NMR spectrum of $2$-$D$ in CDCl$_3$</td>
<td>S-19</td>
</tr>
<tr>
<td>77 MHz $^2$H NMR spectrum of $2$-$D$ in CDCl$_3$</td>
<td>S-20</td>
</tr>
<tr>
<td>500 MHz $^1$H NMR spectrum of $3$-$D$ in CDCl$_3$</td>
<td>S-21</td>
</tr>
<tr>
<td>125 MHz $^{13}$C NMR spectrum of $3$-$D$ in CDCl$_3$</td>
<td>S-22</td>
</tr>
</tbody>
</table>
77 MHz $^2$H NMR spectrum of 3-D in CDCl$_3$  
500 MHz $^1$H NMR spectrum of 4-D in CDCl$_3$  
125 MHz $^{13}$C NMR spectrum of 4-D in CDCl$_3$  
77 MHz $^2$H NMR spectrum of 4-D in CDCl$_3$  
282 MHz $^{19}$F NMR spectrum of 4-D in CDCl$_3$  
500 MHz $^1$H NMR spectrum of 5-D in CDCl$_3$  
125 MHz $^{13}$C NMR spectrum of 5-D in CDCl$_3$  
77 MHz $^2$H NMR spectrum of 5-D in CDCl$_3$  
500 MHz $^1$H NMR spectrum of 6-D in CDCl$_3$  
125 MHz $^{13}$C NMR spectrum of 6-D in CDCl$_3$  
77 MHz $^2$H NMR spectrum of 6-D in CDCl$_3$  
500 MHz $^1$H NMR spectrum of 7-D in CDCl$_3$  
125 MHz $^{13}$C NMR spectrum of 7-D in CDCl$_3$  
77 MHz $^2$H NMR spectrum of 7-D in CDCl$_3$  
500 MHz $^1$H NMR spectrum of 8-D in CDCl$_3$  
125 MHz $^{13}$C NMR spectrum of 8-D in CDCl$_3$  
77 MHz $^2$H NMR spectrum of 8-D in CDCl$_3$  
500 MHz $^1$H NMR spectrum of 9-H in CDCl$_3$  
125 MHz $^{13}$C NMR spectrum of 9-H in CD$_3$OD  
500 MHz $^1$H NMR spectrum of 9-D in CDCl$_3$  
125 MHz $^{13}$C NMR spectrum of 9-D in CD$_3$OD  
77 MHz $^2$H NMR spectrum of 9-D in CDCl$_3$  
500 MHz $^1$H NMR spectrum of 10-D in CDCl$_3$  
500 MHz gCOSY NMR spectrum of 10-D in CDCl$_3$  
125 MHz $^{13}$C NMR spectrum of 10-D in CDCl$_3$  
77 MHz $^2$H NMR spectrum of 10-D in CDCl$_3$  
500 MHz $^1$H NMR spectrum of 11-D in CDCl$_3$  
500 MHz gCOSY NMR spectrum of 11-D in CDCl$_3$  
125 MHz $^{13}$C NMR spectrum of 11-D in CDCl$_3$  
77 MHz $^2$H NMR spectrum of 11-D in CDCl$_3$  
500 MHz $^1$H NMR spectrum of 12-D$_6$ in CDCl$_3$  
125 MHz $^{13}$C NMR spectrum of 12-D$_6$ in CDCl$_3$  
77 MHz $^2$H NMR spectrum of 12-D$_6$ in CDCl$_3$  
500 MHz $^1$H NMR spectrum of 13-D$_6$ in CDCl$_3$  
125 MHz $^{13}$C NMR spectrum of 13-D$_6$ in CDCl$_3$  
77 MHz $^2$H NMR spectrum of 13-D$_6$ in CDCl$_3$
125 MHz $^{13}$C NMR spectrum of $\mathbf{14-D}_{11}$ in CDCl$_3$  
S-59

77 MHz $^2$H NMR spectrum of $\mathbf{14-D}_{11}$ in CDCl$_3$  
S-60

500 MHz $^1$H NMR spectrum (in CDCl$_3$) of $\mathbf{1-H}$ and $\mathbf{1-D}$ obtained in the competition experiment performed in 1:1 H$_2$O/D$_2$O  
S-61
1203-HK-03-22

Pulse Sequence: s2pul
Solvent: CDC13
Temp. 25.0 C / 298.1 K
Operator: mk1
File: 1203-HK-03-22
INOVA-500, "riga"

Pulse 38.6 degrees
Acq. time 1.892 sec
Width 8000.0 Hz
132 repetitions
OBSERVE H1, 499.7707095 MHz
DATA PROCESSING
FT size 32768
Total time 6 min, 20 sec

3-((Triisopropylsilyl)ethynyl)pyridine
Intermediate in the synthesis of 9-D and 9-H
3-((Trisopropylsilyl)ethyl)pyridine
Intermediate in the synthesis of 9-D and 9-H
1203-HK-03-pure

Pulse Sequence: s2pul

Solvent: CDC13
Temp. 24.0 C / 297.1 K
Operator: mkp
File: 1203-HK-03-23-pure
INOVA-500 "riga"

Pulse 38.6 degrees
Acq. time 1.892 sec
Width 8000.0 Hz
73 repetitions
OBSERVE H1, 499.7707095 MHz
DATA PROCESSING
FT size 32768
Total time 6 min, 20 sec

3-Ethynyl)pyridine
Intermediate in the synthesis of 9-D and 9-H
Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 24.0 C / 297.1 K
Operator: mkl
File: 1203-HK-04-21-1H-pure
INOVA-500 "riga"

Pulse 38.6 degrees
Acq. time 1.892 sec
Width 8000.0 Hz
44 repetitions
OBSERVE H1, 499.7707202 MHz
DATA PROCESSING
FT size 32768
Total time 6 min, 20 sec

Triisopropyl(phenylethynyl)silane-D$_5$
Intermediate in the synthesis of 13-D$_6$ and 14-D$_{11}$
Triisopropyl(phenylethynyl)silane-D$_5$
Intermediate in the synthesis of 13-$D_6$ and 14-$D_{11}$
1203-HK-04-20-2Deuterium

Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
Operator: mkl
File: 1203-HK-04-20-2Deuterium
INNOVA-500 "riga"

Relax. delay 1.000 sec
Pulse 516.7 degrees
Acq. time 1.780 sec
Width 1150.8 Hz
100 repetitions

OBSERVE 1H, 76.7178480 MHz
DECOUPLE 1H, 499.7732084 MHz
Power 39 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.1 Hz
Gauss apodisation 0.400 sec
FT size 8192
Total time 5 min, 56 sec

Triisopropyl(phenylethynyl)silane-\(D_5\)
Intermediate in the synthesis of \(13-D_6\) and \(14-D_{11}\)
Pulse Sequence: s2pul
Solvent: CDC13
Temp. 24.0 C / 297.1 K
Operator: mkl
File: 1203-HK-04-25-1H-pure
INOVA-500 "riga"

Pulse 38.6 degrees
Acq. time 1.892 sec
Width 8000.0 Hz
18 repetitions
OBSERVE H1, 499.7707207 MHz
DATA PROCESSING
FT size 32768
Total time 6 min, 20 sec

Ethynylbenzene-D₅
Intermediate in the synthesis of 13-D₅ and 14-D₁₁
Ethynylbenzene-\(D_5\)
Intermediate in the synthesis of \(13-D_6\) and \(14-D_{11}\)

1203-HK-04-25-2Deutirium

Pulse Sequence: n2pul
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
Operator: mkl
File: 1203-HK-04-25-2Deutirium
INOVA-500 "riga"

Relax. delay 1.000 sec
Pulse 516.7 degrees
Acq. time 1.780 sec
Width 1150.8 Hz
108 repetitions
OBSERVE 1k, 76.7178492 MHz
DECOUPLE H1, 499.7732084 MHz
Power 39 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.1 Hz
Gauss apodization 0.400 sec
FT size 8192
Total time 18 min, 35 sec
Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 24.0 °C / 297.1 K
Operator: mkl
File: 1203-HK-02-45
INOVA-500 "riga"

Pulse 38.6 degrees
Acq. time 1.892 sec
Width 8000.0 Hz
75 repetitions
OBSERVE H1, 499.7707212 MHz
DATA PROCESSING
FT size 32768
Total time 6 min, 20 sec
m-Azidobenzonitrile
Intermediate in the synthesis of $9-D$ and $9-H$

Pulse Sequence: m2pul
Solvent: dcd13
Temp. 25.0 C / 298.1 K
Operator: mkl
File: 1203-HK-03-15
INOVA-500 'riga'

Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8000.0 Hz
63 repetitions

OBSERVE $E1$, 499.7707095 MHz
DATA PROCESSING
Resol. enhancement 0.5 Hz
Gauss apodization 0.600 sec
FT size 32768
Total time 5 min, 43 sec
Phenyl azide-$D_5$
Intermediate in the synthesis of $12-D_6$ and $14-D_{11}$
Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
Operator: mkl
File: 1203-HK-04-30-d1-3
INOVA-500 "riga"

Relax. delay 3.000 sec
Pulse 38.6 degrees
Acq. time 1.892 sec
Width 8000.0 Hz
16 repetitions

OBSERVE H1, 499.7707202 MHz
DATA PROCESSING
FT size 32768
Total time 1 min, 18 sec
Pulse Sequence: s2pu1
Solvent: CDC13
Temp. 24.0 C / 297.1 K
Operator: skl
File: 1203-NK-02-63-13C-final
INOVA-500 “rigs”

Relax. delay 4.000 sec
Pulse 52.1 degrees
Acq. time 1.300 sec
Width 29996.3 Hz
1676 repetitions

OBSERVE C13, 125.6674132 MHz
DECOUPLE H1, 499.7743279 MHz
Power 42 dB
on during acquisition
WALTZ-16 modulated

DATA PROCESSING
Line broadening 1.0 Hz
Gauss apodization 0.200 sec
FT size 131072
Total time 117 hr, 59 min, 33 sec

1-D

\[ \text{N} = \text{N} \]

\[ \text{Me} \]
Pulse Sequence: s2pel
Solvent: CDC13
Ambient temperature
Operator: mkl
File: 1203-HK-02-07-Deuterium
INOVA-500 "riga"

Relax. delay 4.000 sec
Pulse 1000.0 degrees
Acq. time 2.636 sec
Width 1534.7 Hz
32 repetitions
OWSERVE 1L, 76.7178670 MHz
DECOUPLE H1, 495.7732084 MHz
Power 60 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
FT size 8192
Total time 3 min, 32 sec
1203-HX-02-62

Pulse Sequence: s2pul
Solvent: dcl3
Temp. 25.0 C / 298.1 K
Operator: mkl
File: 1203-HX-02-62
INOVA-500 'riga'

Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8000.0 Hz
8 repetitions

OBSERVE H1, 499.7707207 MHz
DATA PROCESSING
Resol. enhancement 0.5 Hz
Gauss apodisation 0.600 sec
FT size 32768
Total time 5 min, 43 sec
1203-HK-02-63-13C-pure

Archive directory: /export/home/mkl/vnmrsys/data
Sample directory:

Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 24.0 °C / 297.1 K
Operator: mkl
File: 1203-HK-02-62-13C-pure
IMRVA-500 "riga"

Relax. delay 4.000 sec
Pulse 52.1 degrees
Acq. time 1.300 sec
Width 299.9 Hz
1629 repetitions
OBSERVE C13, 125.6674123 MHz
DECOUPLE H1, 499.7743279 MHz
Power 62 dB
on during acquisition
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
Gauss apodization 0.200 sec
FT size 131072
Total time 117 hr, 59 min, 33 sec
1203-HK-02-62-2Deuterium

Pulse Sequence: n2pul
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
Operator: mk1
File: 1203-HK-02-62-2Deuterium
INOVES-500 "riga"

Relax. delay 1.000 sec
Pulse 516.7 degrees
Acq. time 1.780 sec
Width 1150.8 Hz
146 repetitions

OBSERVE 1H, 75.7178478 MHz
DECouple 1H, 599.7732086 MHz
Power 39 dB
continuously on
WALTZ-16 modulated

DATA PROCESSING
Line broadening 0.1 Hz
Gauss apodisation 0.400 sec
FT size 8192
Total time 9 min, 17 sec
Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: mkl
File: 1203-HK-02-49-1H
INOV3500 "riga"

Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8000.0 Hz
14 repetitions
OBEERVE H1, 699.7707095 MHz
DATA PROCESSING
Resol. enhancement 0.5 Hz
Gauss apodization 0.600 sec
FT size 32768
Total time 5 min, 43 sec
1203-HX-02-49

Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Operator: mkl
File: 1203-HX-02-49-13C-final
INOSA-500 "riga"

Pulse 70.1 degrees
Acq. time 1.300 sec
Width 25000.0 Hz
40624 repetitions
OBSERVE C13, 125.6674255 MHz
DECOUPLE H1, 699.7732084 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 18 hr, 11 min, 9 sec
1203-EK-02-49-2Deuterium

Pulse Sequence: s2pul
Solvent: CDC13
Temp. 25.0 C / 298.1 K
Operator: mkl
File: 1203-EK-02-49-2Deuterium
INOVA-500 "rigs"

Relax. delay 1.000 sec
Pulse 516.7 degrees
Acq. time 1.780 sec
Width 1150.8 Hz
200 repetitions

OBSERVE 1x, 76.7178489 MHz
DECOUPLE H1, 499.7732084 MHz
Power 39 dB
continuously on
WALTZ-16 modulated

DATA PROCESSING
Line broadening 0.1 Hz
Gauss apodisation 0.400 sec
FT size 8192
Total time 9 min, 17 sec
Pulse Sequence: n2pul

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: mkl

File: 1203-HK-02-59

Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8000.0 Hz

13 repetitions

OBSERVE H1, 499.7707197 MHz

DATA PROCESSING

Resol. enhancement 0.5 Hz
Gauss apodization 0.600 sec

FT size 32768

Total time 5 min, 43 sec
1203-HK-02-59-13C-pure

Archive directory: /export/home/mkl/Vmnrays/data
Sample directory:

Pulse Sequence: s2pul
Solvent: CDC13
Temp. 24.0 C / 297.1 K
Operator: mkl
File: 1203-HK-02-59-13C-pure
INOVA-500 "riga"

Relax. delay 4.000 sec
Pulse 52.1 degrees
Acq. time 1.300 sec
Width 29996.3 Hz
10981 repetitions
ON-SERVE C13, 125.6674190 MHz
DECOUPLE H1, 499.7743279 MHz
Power 62 dB
on during acquisition
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
Gauss apodization 0.200 sec
FT size 131072
Total time 117 hr, 59 min, 33 sec
1203-EK-02-59-2Deuterium

Pulse Sequence: n2pul
Solvent: CDCl3
Temp. 25.0 °C / 298.1 K
Operator: mk1
File: 1203-EK-02-59-2Deuterium
INOVA-500 'riga'

Relax. delay 1.000 sec
Pulse 516.7 degrees
Acq. time 1.780 sec
Width 1150.8 Hz
130 repetitions

Observe 1H, 76.7178480 MHz
Decouple H1, 499.7712084 MHz
Power 39 dB
Continuously on

WALTZ-16 modulated

Data Processing
Line broadening 0.1 Hz
Gauss apodisation 0.400 sec
FT size 8192
Total time 9 min, 17 sec
Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 24.0 C / 297.1 K
Operator: mlk
File: 1203-HK-02-48-13C-final
INOVA-500 "riga"

Relax. delay 4.000 sec
Pulse 52.1 degrees
Acq. time 1.300 sec
Width 29996.3 Hz
1305 repetitions
OBSERVE C13, 128.6674132 MHz
DECouple H1, 499.7743279 MHz
Power 42 dB
on during acquisition
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
Gauss apodization 0.200 sec
FT size 131072
Total time 117 hr, 59 min, 33 sec
1203-HK-02-48-2Deuterium

Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
Operator: nkl
File: 1203-HK-02-48-2Deuterium
INOVA-500 "riga"

Relax. delay 1.000 sec
Pulse 516.7 degrees
Acq. time 1.780 sec
Width 1150.8 Hz
128 repetitions

OBSERVE 1k, 76.7178478 MHz
DECOUPLE E1, 499.7732084 MHz
Power 39 dB
continuously on
WALZ-16 modulated

DATA PROCESSING
Line broadening 0.1 Hz
Gauss apodization 0.400 sec
FT size 8192
Total time 5 min, 56 sec
Pulse Sequence: n2pul
Solvent: cdc13
Temp. 25.0 C / 298.1 K
Operator: mlk
File: 1203-HK-02-57
INOV4-500 "riga"

Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8000.0 Hz
24 repetitions
OBSERVE H1, 499.7707202 MHz
DATA PROCESSING
Resol. enhancement 0.5 Hz
Gauss apodization 0.600 sec
FT size 32768
Total time 5 min, 43 sec
**1203-EK-02-57-2Deuterium**

**Pulse Sequence:** n2pul

**Solvent:** CDC13

**Temp.** 25.0 C / 298.1 K

**Operator:** mk1

**File:** 1203-EK-02-57-2Deuterium INNOVA-500 "riga"

- Relax. delay 1.000 sec
- Pulse 516.7 degrees
- Acq. time 1.780 sec
- Width 1150.8 Hz
- 200 repetitions

**OBSERVE** 1H, 76.7178489 MHz

**DECORRELATE** 2H, 499.7732084 MHz

Power 39 dB

- continuously on
- WALTZ-16 modulated

**DATA PROCESSING**
- Line broadening 0.1 Hz
- Gaussian apodization 0.100 sec
- FT size 8192
- Total time 9 min, 17 sec

**Chemical Structure:**

![Chemical Structure](image)

**ppm:**

![ppm Scale](image)
Pulse Sequence: s2pul
Solvent: cdc13
Temp. 25.0 C / 298.1 K
Operator: mkl
File: 1203-HK-02-61
INOVA-500 "riga"

Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8000.0 Hz
11 repetitions

OBSEVE H1, 499.7707202 MHz
DATA PROCESSING
Resol. enhancement 0.5 Hz
Gauss apodization 0.600 sec
FT size 32768
Total time 5 min, 43 sec

0.08 11.27 1.00
0.96
1203-HK-02-61-13C-pure

Archive directory: /export/home/mkl/vnmrjgs/data
Sample directory:

Pulse Sequence: a2pul
Solvent: CDC13
Temp. 24.0 C / 297.1 K
Operator: mkl
File: 1203-HK-02-61-13C-pure
INOVA-500 “riga”

Relax. delay 4.000 sec
Pulse 52.1 degrees
Acq. time 1.300 sec
Width 29996.3 Hz
1429 repetitions

OBSERVE C13, 125.8674196 MHz
DECouple H1, 499.7743279 MHz
Power 42 dB
on during acquisition
WALTZ-16 modulated

DATA PROCESSING
Line broadening 1.0 Hz
Gauss apodisation 0.200 sec
FT size 131072
Total time 117 hr, 59 min, 33 sec
1203-HK-02-61-2Deuterium

Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
Operator: mkI
File: 1203-HK-02-61-2Deuterium
INOVA-500 "riga"

Relax. delay 1.000 sec
Pulse 516.7 degrees
Acq. time 1.780 sec
Width 1150.8 Hz
112 repetitions
OBSERVE 1k, 76.7178470 MHz
DECouple H1, 499.7732084 MHz
Power 39 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.1 Hz
Gauss apodization 0.800 sec
FT size 8192
Total time 9 min, 17 sec
Pulse Sequence: s2pul

Solvent: cdcl3

Temp. 25.0 °C / 298.1 K

Operator: mkl

File: 1203-HK-02-58

INova-600 "riga"

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

20 repetitions

OBSERVE H1, 499.7707207 MHz

DATA PROCESSING

Resol. enhancement 0.5 Hz

Gauss apodization 0.600 sec

FT size 32768

Total time 5 min, 43 sec
1203-HK-02-58-2Deuterium

Pulse Sequence: s2pul

Solvent: CDCl3
Temp. 25.0 C / 298.1 K
Operator: ml1
File: 1203-HK-02-58-2Deuterium
INOVA-300 'riga'

Relax. delay 1.000 sec
Pulse 516.7 degrees
Acq. time 1.780 sec
Width 1150.8 Hz
149 repetitions

OBSERVE 1k, 76.7178478 MHz
DEC couple H1, 499.7732088 MHz
Power 39 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.1 Hz
Gauss apodisation 0.400 sec
FT size 8192
Total time 9 min, 17 sec

8-D
1203-HK-02-45

Pulse Sequence: s2pu1
Solvent: CDC13
Temp. 24.0 C / 297.1 K
Operator: mkl
File: 1203-HK-03-24-1H-pure
INOVA-500 "riga"

Pulse 38.6 degrees
Acq. time 1.892 sec
Width 8000.0 Hz
200 repetitions
OBSERVE H1, 499.7707212 MHz
DATA PROCESSING
Resol. enhancement -0.0 Hz
FT size 32768
Total time 6 min, 20 sec

-40  9
Pulse Sequence: s2pul
Solvent: CD3OD
Temp. 55.0 C / 328.1 K
Operator: mkl
File: 1203-HK-03-24-13C-CD3OD
INOVA-500 "riya"

Relax, delay 3.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 28996.0 Hz
3824 repetitions

OBSERVE C13, 125.6677457 MHz
DECOUPLE H1, 499.7749775 MHz
Power 42 dB
on during acquisition
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 133072
Total time 16 hr, 45 min, 31 sec
1203-HK-03-24D

Pulse Sequence: s2pul

Solvent: CDC13
Temp. 25.0 C / 297.1 K
Operator: mkl
File: 1203-HK-03-24D
INOVA-500 “riga”

Pulse 38.6 degrees
Acq. time 1.892 sec
Width 8000.0 Hz
121 repetitions
OBSERVE E1, 499.7707226 MHz
DATA PROCESSING
FT size 32768
Total time 6 min, 20 sec
1203-HK-03-24D-13C

Pulse Sequence: s2pul
Solvent: CD3OD
Temp. 55.0 C / 328.1 K
Operator: mk1
File: 1203-HK-03-24D-13C-CD3OD
INova-500 “rign”

Relax. delay 3.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 28996.0 Hz
13840 repetitions
OBSERVE C13, 125.6677437 MHz
DECOPLE B1, 499.7749775 MHz
Power 42 dB
on during acquisition
WALTZ-16 modulated
DATA PROCESSING
Line broadening 8.0 Hz
FT size 131072
Total time 16 hr, 45 min, 31 sec
Pulse Sequence: s2pul
Solvent: CDC13
Temp. 25.0 C / 298.1 K
Operator: mkl
File: 1203-NK-03-24D-2deuterium
IMOSA-500 “riga”

Relax. delay 1.000 sec
Pulse 516.7 degrees
Acq. time 1.780 sec
Width 1150.8 Hz
400 repetitions
OBSERVE 1k, 76.7178613 MHz
DECOPLEX H1, 499.7732084 MHz
Power 39 dB
continuously on
WALTZ-16 modulated

DATA PROCESSING
Line broadening 0.1 Hz
Gauss apodization 0.400 sec
FT size 8192
Total time 18 min, 35 sec
1203-HK-02-71-1H-Pure
Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 °C / 298.1 K
Operator: nkl
File: 1203-HK-02-71-1H-pure
INova-500 "riga"

Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8000.0 Hz
28 repetitions
OBSERVE Hi, 499.7707212 MHz
DATA PROCESSING
Resol. enhancement 0.5 Hz
Gauss apodization 0.600 sec
FT size 32768
Total time 13 min, 0 sec
500 MHz gCOSY NMR spectrum of 10-D

10-D
Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 25.0 °C / 298.1 K
Operator: mkl
File: 1203-HK-02-71-2Deuterium
INOVA-500 "riga"

Relax. delay 1.000 sec
Pulse 516.7 degrees
Acq. time 1.780 sec
Width 1150.8 Hz
200 repetitions
OBSERVE 1k, 75.7178480 MHz
DECOUPLE H1, 499.7732084 MHz
Power 39 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.1 Hz
Gauss apodization 0.400 sec
FT size 8192
Total time 9 min, 17 sec
1203-HX-02-70
Pulse Sequence: n2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: mkl
File: 1203-HX-02-70
INOVA-500 ‘riga’

Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8000.0 Hz
26 repetitions
OBSERVE H1, 499.7707095 MHz
DATA PROCESSING
Resol. enhancement 0.5 Hz
Gauss apodization 0.600 sec
FT size 32768
Total time 5 min, 43 sec
500 MHz gCOSY NMR spectrum of 11-D
Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 24.0 C / 297.1 K
Operator: mk1
File: 1203-HX-02-70-13C
INOVa-500 "riga"

Relax. delay 4.000 sec
Pulse 52.1 degrees
Acq. time 1.300 sec
Width 29996.3 Hz
11663 repetitions
OBSERVE C13, 125.6674095 MHz
DECouple B1, 499.7743279 MHz
Power 42 db
on during acquisition
WAL22-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
Gaus apodization 0.200 sec
FT size 131072
Total time 117 hr, 59 min, 33 sec
Pulse Sequence: s2ps1

Solvent: CDCl3
Temp. 29.0 C / 297.1 K
Operator: skl
File: 1203-HX-04-23-2-13C
INova-500 "riga"

Relax. delay 4.000 sec
Pulse 52.1 degrees
Acq. time 1.300 sec
Width 29996.3 Hz
11833 repetitions

OBSERVE: C13, 125.6674205 MHz
DECOUPLE: N1, 499.7743279 MHz
Power 42 dB
on during acquisition

WALTZ-16 modulated

DATA PROCESSING
Line broadening 1.0 Hz
Gauss apodization 0.200 sec
FT size 111072
Total time 117 hr, 59 min, 33 sec
Pulse Sequence: s2pul
Solvent: CDC13
Temp. 25.0 C / 298.1 K
Operator: mkl
File: 1203-MK-04-23-2deutirium-1
INOVIA-500 "riga"

Relax. delay 1.000 sec
Pulse 516.7 degrees
Acq. time 1.780 sec
Width 1150.8 Hz
200 repetitions

OBSERVE 1k, 76.7178689 MHz
DECUPLE HD, 499.7732084 MHz
Power 39 db
continuously on
WALTZ-16 modulated

DATA PROCESSING
line broadening 0.1 Hz
Gauss apodisation 0.400 sec
FT size 8192
Total time 9 min, 17 sec
1203-HK-04-26-1H-pure

Pulse Sequence: s2pul
Solvent: CDC13
Temp. 24.0 C / 297.1 K
Operator: mkl
File: 1203-HK-04-26-1H-pure
INOVA-500 "riga"

Pulse 38.6 degrees
Acq. time 1.892 sec
Width 8000.0 Hz
146 repetitions
OBSERVE H1, 499.7707212 MHz
DATA PROCESSING
PT size 32768
Total time 6 min, 20 sec
Pulse Sequence: s2pel
Solvent: CDCl3
Temp. 24.0 C / 297.1 K
Operator: mkl
File: 1203-HK-04-26-13C-final
INOVA-500 "riga"

Relax. delay 4.000 sec
Pulse 52.1 degrees
Acq. time 1.301 sec
Width 34995.6 Hz
11759 repetitions
OBSERVE C13, 125.6674218 MHz
DECOUPLE H1, 499.7743279 MHz
Power 42 dB
on during acquisition
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
Gauss apodization 0.200 sec
FT size 131072
Total time 17 hr, 42 min, 14 sec
1203-HK-04-26-2deutirium

Pulse Sequence: s2pul
Solvent: CDC13
Temp. 25.0 C / 298.1 K
Operator: mh
File: 1203-HK-04-26-2deutirium
INOVA-500 "riga"

Relax. delay 1.000 sec
Pulse 516.7 degrees
Acq. time 1.780 sec
Width 1150.8 Hz
200 repetitions

OBSERVE 1x, 76.7178500 MHz
DECOUPLE H1, 499.7732084 MHz
Power 39 dB
continuously on
WALTZ-16 modulated

DATA PROCESSING
Line broadening 0.1 Hz
Gauss apodisation 0.400 sec
FT size 8192
Total time 9 min, 17 sec
1203-HK-04-27-13C

Archive directory: /export/home/mkl/vsmrsys/data
Sample directory:

Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 24.0 C / 297.1 K
Operator: mkl
File: 1203-HK-04-27-13C
INOVA-500 "riga"

Relax. delay 4.000 sec
Pulse 52.1 degrees
Acq. time 1.300 sec
Width 29996.3 Hz
10500 repetitions

OBSERVE C13, 125.6674196 MHz
DECouple H1, 499.7743279 MHz
Power 42 dB
on during acquisition
WALZ-16 modulated

DATA PROCESSING
Line broadening 1.0 Hz
Gauss apodization 0.200 sec
FT size 131072
Total time 117 hr, 59 min, 33 sec
Pulse Sequence: s2pul

Solvent: CDC13
Temp. 25.0 C / 298.1 K
Operator: mk1
File: 1203-HK-04-31-d1-3
INOVA-500 "riga"

Relax. delay 3.000 sec
Pulse 38.6 degrees
Acq. time 1.892 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.7707222 MHz
DATA PROCESSING
PT size 32768
Total time 1 min, 18 sec

1203-HK-04-31-d1-3

CuSO4
H2O/D2O

1:1

1-H

1-D