

SUPPORTING INFORMATION

_E- or Z-Selective synthesis of 4-fluorovinyl-1,2,3-triazoles with fluorinated second-generation Julia-Kocienski reagents_

Rakesh Kumar, a Govindra Singh, a Louis J. Todaro, b Lijia Yang, a and Barbara Zajc** a

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**TABLE OF CONTENTS**

<table>
<thead>
<tr>
<th>Information</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>^1^H NMR of 2-[1-fluoro-3-(trimethylsilyl)prop-2-ynylsulfonfonyl]benzo[d]thiazole (1)</td>
<td>3</td>
</tr>
<tr>
<td>^1^3^C NMR of 2-[1-fluoro-3-(trimethylsilyl)prop-2-ynylsulfonfonyl]benzo[d]thiazole (1)</td>
<td>4</td>
</tr>
<tr>
<td>^1^H NMR of 2-[[fluoro(1-phenyl-1H-1,2,3-triazole-4-yl)methyl]sulfonfonyl]benzo[d]thiazole (2)</td>
<td>5</td>
</tr>
<tr>
<td>^1^3^C NMR of 2-[[fluoro(1-phenyl-1H-1,2,3-triazole-4-yl)methyl]sulfonfonyl]benzo[d]thiazole (2)</td>
<td>6</td>
</tr>
<tr>
<td>^1^H NMR of 2-[[fluoro(1-(naphthalen-2-yl)-1H-1,2,3-triazole-4-yl)methyl]sulfonfonyl]benzo[d]thiazole (3)</td>
<td>7</td>
</tr>
<tr>
<td>^1^3^C NMR of 2-[[fluoro(1-(naphthalen-2-yl)-1H-1,2,3-triazole-4-yl)methyl]sulfonfonyl]benzo[d]thiazole (3)</td>
<td>8</td>
</tr>
<tr>
<td>^1^H NMR of 2-[[fluoro(1-(4-methoxyphenyl)-1H-1,2,3-triazole-4-yl)methylsulfonfonyl]benzo[d]-thiazole (4)</td>
<td>9</td>
</tr>
<tr>
<td>^1^3^C NMR of 2-[[fluoro(1-(4-methoxyphenyl)-1H-1,2,3-triazole-4-yl)methylsulfonfonyl]benzo[d]-thiazole (4)</td>
<td>10</td>
</tr>
<tr>
<td>^1^H NMR of 2-[[fluoro(1-(4-phenoxyphenyl)-1H-1,2,3-triazole-4-yl)methylsulfonfonyl]benzo[d]thiazole (5)</td>
<td>11</td>
</tr>
<tr>
<td>^1^3^C NMR of 2-[[fluoro(1-(4-phenoxyphenyl)-1H-1,2,3-triazole-4-yl)methylsulfonfonyl]benzo[d]thiazole (5)</td>
<td>12</td>
</tr>
<tr>
<td>^1^H NMR of 2-[[fluoro(1-(4-nitrophenyl)-1H-1,2,3-triazole-4-yl)methyl]sulfonfonyl]benzo[d]thiazole (6)</td>
<td>13</td>
</tr>
<tr>
<td>^1^3^C NMR of 2-[[fluoro(1-(4-nitrophenyl)-1H-1,2,3-triazole-4-yl)methyl]sulfonfonyl]benzo[d]thiazole (6)</td>
<td>14</td>
</tr>
<tr>
<td>^1^H NMR of 2-[[1-(adamantan-1-yl)-1H-1,2,3-triazole-4-yl]fluoromethyl]sulfonfonyl]benzo[d]thiazole (7)</td>
<td>15</td>
</tr>
<tr>
<td>^1^3^C NMR of 2-[[1-(adamantan-1-yl)-1H-1,2,3-triazole-4-yl]fluoromethyl]sulfonfonyl]benzo[d]thiazole (7)</td>
<td>16</td>
</tr>
<tr>
<td>^1^H NMR of 2-[[1-decyl-1H-1,2,3-triazole-4-yl]fluoromethylsulfonfonyl]benzo[d]thiazole (8)</td>
<td>17</td>
</tr>
<tr>
<td>^1^3^C NMR of 2-[[1-decyl-1H-1,2,3-triazole-4-yl]fluoromethylsulfonfonyl]benzo[d]thiazole (8)</td>
<td>18</td>
</tr>
<tr>
<td>^1^H NMR of 2-[[fluoro(1-(3-phenylpropyl)-1H-1,2,3-triazole-4-yl)methyl]sulfonfonyl]benzo[d]-thiazole (9)</td>
<td>19</td>
</tr>
<tr>
<td>^1^3^C NMR of 2-[[fluoro(1-(3-phenylpropyl)-1H-1,2,3-triazole-4-yl)methyl]sulfonfonyl]benzo[d]-thiazole (9)</td>
<td>20</td>
</tr>
<tr>
<td>^1^H NMR of 2-[[fluoro(1-(ferrocenyl)-1H-1,2,3-triazole-4-yl)methyl]sulfonfonyl]benzo[d]thiazole (10)</td>
<td>21</td>
</tr>
<tr>
<td>^1^3^C NMR of 2-[[fluoro(1-(ferrocenyl)-1H-1,2,3-triazole-4-yl)methyl]sulfonfonyl]benzo[d]thiazole (10)</td>
<td>22</td>
</tr>
<tr>
<td>^1^H NMR of E/Z-11 by method B</td>
<td>23</td>
</tr>
<tr>
<td>^1^H NMR of E/Z-12 by method A</td>
<td>24</td>
</tr>
<tr>
<td>^1^H NMR of E/Z-13 by method A</td>
<td>25</td>
</tr>
</tbody>
</table>
$^1$H NMR of E/Z-14 by method A
$^1$H NMR of E/Z-15 by method B
$^1$H NMR of E/Z-16 by method A
$^1$H NMR of E/Z-17 by method A
$^1$H NMR of E/Z-18 by method A
$^1$H NMR of E/Z-19 by method B
$^1$H NMR of E/Z-20 by method B
$^1$H NMR of E/Z-21 by method B
$^1$H NMR of E/Z-22 by method B
$^1$H NMR of E/Z-23 by method B
$^1$H NMR of E/Z-24 by method B
$^1$H NMR of E/Z-25 by method B
$^1$H NMR of 26
$^{13}$C NMR of 26
$^1$H NMR of 27
$^{13}$C NMR of 27
$^1$H NMR of 28: Major isomer
$^{13}$C NMR of 28: Major isomer
$^1$H NMR of 28: Minor isomer
$^{13}$C NMR of 28: Minor isomer
$^1$H NMR of Z-29: Major isomer
$^{13}$C NMR of Z-29: Major isomer
$^1$H NMR of E-29: Minor isomer
$^{13}$C NMR of E-29: Minor isomer
$^1$H NMR of 30
$^{13}$C NMR of 30
Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
Operator: barbara
File: 1222-RK-02-144-13C
INOVA-500 "riga"

Relax. delay 4.000 sec
Pulse 52.1 degrees
Acq. time 1.300 sec
Width 29996.3 Hz
100 repetitions
OBSERVE C13, 125.6676411 MHz
DECOUPLE H1, 499.7732084 MHz
Power 42 dB
on during acquisition
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 9 min, 12 sec

125 MHz, CDCl3

[Chemical structure image]
 Archive directory: /export/home/mkl/vnmrsys/data
 Sample directory: auto_13Dec2004

 Pulse Sequence: s2pul
 Solvent: cdcl3
 Temp. 25.0 C / 298.1 K
 Operator: barbara
 File: 1222-RK-04-259-pure
 INOVA-500 "riga"

 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.892 sec
 Width 7544.3 Hz
 20 repetitions
 OBSERVE H1, 499.7707212 MHz
 DATA PROCESSING
 Line broadening 0.1 Hz
 FT size 32768
 Total time 1 min, 32 sec

 500 MHz, CDCl3

 ppm

 9 8 7 6 5 4 3 2 1
1222-RK-04-259-13C-1

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

Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
Operator: barbara
File: 1222-RK-04-259-13C-1
INOVA-500 "riga"

Relax. delay 4.000 sec
Pulse 52.1 degrees
Acq. time 1.300 sec
Width 29996.3 Hz
1892 repetitions
OBSERVE C13, 125.6674182 MHz
DECOUPLE H1, 499.7732084 MHz
Power 42 dB
on during acquisition
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 29 hr, 30 min, 9 sec

125 MHz, CDCl3

![Chemical structure](image)
1222-RK-04-257-PURE

Archive directory: /export/home/mkl/vnmrsys/data
Sample directory: auto_13Dec2004

Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: barbara
File: 1222-RK-04-257-PURE
INova-500 "riga"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7544.3 Hz
16 repetitions
OBSERVE H1, 499.7707207 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 1 min, 32 sec

500 MHz, CDCl₃
1222-RK-04-258-13C

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

Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
Operator: barbara
File: 1222-RK-04-257-13C
INOVA-500 "riga"

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

OBSERVE C13, 125.6674218 MHz
DECOUPLE H1, 499.7732084 MHz

Power 42 dB
on during acquisition
WALTZ-16 modulated

DATA PROCESSING
Line broadening 4.0 Hz
FT size 131072
Total time 44 min, 35 sec

125 MHz, CDCl3

125 MHz, CDCl3
Pulse Sequence: s2pul
Solvent: dcd13
Temp. 25.0 C / 298.1 K
Operator: barbara
File: 1222-RX-04-246-pure-1M
INOVA-500 "riga"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 756.3 Hz
52 repetitions
OBSERVE 71, 499.7707216 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 9 min, 40 sec

500 MHz, CDCl3
1222-RK-04-246-pure

Archive directory: /export/home/barbara/vnmrsys/data

Pulse Sequence: s2pul
Solvent: CDCl₃
Temp. 25.0 C / 298.1 K
Operator: barbara
File: 1222-RK-04-246-pure
INOVA-500 "riga"

Relax. delay 25.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 3121.8 Hz
512 repetitions
OBSERVE C13, 125.6674148 MHz
DECOUPLE H1, 499.7732084 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 4.0 Hz
FT size 131072
Total time 7 hr, 18 min, 29 sec

125 MHz, CDCl₃
1222-RK-04-242-2ndfraction

Archive directory: /export/home/mkl/vnmrsys/data
Sample directory: auto_13Dec2004

Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: barbara
File: 1222-RK-04-242-2ndfraction
INOVA-500 "riga"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7544.3 Hz
24 repetitions
OBSERVE H1, 499.7707212 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 1 min, 32 sec
Archive directory: /export/home/barbara/vnmrsys/data
Sample directory: Pulsed Sequence: s2pul
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
Operator: barbara
File: 1222-RK-04-242-13C
INOVA-500 "riga"

Relax. delay 4.000 sec
Pulse 52.1 degrees
Acq. time 1.300 sec
Width 29996.3 Hz
296 repetitions
OBSERVE C13, 125.6674218 MHz
DECOUPLE H1, 499.7732084 MHz
Power 42 dB
on during acquisition
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 131072
Total time 44 min, 35 sec

125 MHz, CDCl3

5

1222-RK-04-242-13C
Archive directory: /export/home/mkl/vnmrsys/data
Sample directory: auto_13Dec2004

Pulse Sequence: s2pul
Solvent: dms
Temp. 25.0 C / 298.1 K
Operator: barbara
File: 1222-RK-04-304-2-pure-DMSO
INOVA-500 "riga"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7544.3 Hz
28 repetitions

OBSERVE H1, 499.7730861 MHz

DATA PROCESSING
Line broadening 0.0 Hz
FT size 32768
Total time 1 min, 32 sec
1222-RK-04-304-13C-DMSO

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

Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
Operator: barbara
File: 1222-RK-04-304-13C-DMSO
INOVA-500 "riga"

Relax. delay 4.000 sec
Pulse 52.1 degrees
Acq. time 1.300 sec
Width 29996.3 Hz
388 repetitions
OBSERVE C13, 125.6674526 MHz
DECOUPLE H1, 499.7732084 MHz
Power 42 dB
on during acquisition
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 53 min, 26 sec
1222-RK-04-247-pure

Archive directory: /export/home/mkl/vnmrsys/data
Sample directory: auto_13Dec2004

Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: barbara
File: 1222-RK-04-247-pure
INOVA-500 "riga"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7444.3 Hz
20 repetitions
OBSERVE H1, 499.7707212 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 1 min, 32 sec
1222-RK-04-247-13C

Pulse Sequence: s2pul
Solvent: CDCl₃
Temp. 25.0 °C / 298.1 K
Operator: barbara
File: 1222-RK-04-247-13C
INOVA-500 "riga"

Relax. delay 4.000 sec
Pulse 52.1 degrees
Acq. time 1.300 sec
Width 29996.3 Hz
84 repetitions
OBSERVE C13, 125.6674273 MHz
DECOUPLE H1, 499.7732084 MHz
Power 42 dB
on during acquisition
WALTZ-16 modulated
DATA PROCESSING
Line broadening 3.0 Hz
FT size 131072
Total time 18 min, 3 sec

125 MHz, CDCl₃
1222-RK-04-270-pure

Archive directory: /export/home/mkl/vnmrsys/data
Sample directory: auto_13Dec2004

Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: barbara
File: 1222-RK-04-270-pure
INOVA-500 "riga"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7444.3 Hz
16 repetitions
OBSERVE H1, 499.7707212 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 1 min, 32 sec

500 MHz, CDCl₃
Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 25.0 °C / 298.1 K
Operator: barbara
File: 1222-RK-04-270-13C
INOVA-500 "riga"

Relax. delay 4.000 sec
Pulse 52.1 degrees
Acq. time 1.300 sec
Width 29996.3 Hz
64 repetitions
OBSERVE C13, 125.6674571 MHz
DECOUPLE H1, 499.7732084 MHz
Power 42 dB
on during acquisition
WALTZ-16 modulated

DATA PROCESSING
Line broadening 3.0 Hz
FT size 131072
Total time 18 min, 3 sec
**1H NMR Spectroscopy**

Sample: **F**

- **Solvent:** CDCl₃
- **Temp:** 25 °C
- **Freq:** 500 MHz
- **Pulse:** 90°
- **Acquisition Time:** 1.000 sec
- **Number of Repeats:** 32

**Chemical Shifts:**

- **9.9** ppm

**Structure:**

- Molecular formula: `C₉H₈FNO₃S`
- Functional groups: S, N, O, F, N

**Additional Details:**

- **Relaxation Delay:** 1.000 sec
- **Data Processing:** 0.1 Hz
- **Total Time:** 1 min, 32 sec
Archive directory: /export/home/mkl/vnmrsys/data
Sample directory: auto_13Dec2004
Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: barbara
File: 1222-RK-04-254-1stfraction
INOVA-500 "riga"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7544.3 Hz
12 repetitions
OBSERVE H1, 499.7707212 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 1 min, 32 sec
1222-RK-04-254-13C

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

Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 25.0 °C / 298.1 K
Operator: barbara
File: 1222-RK-04-254-pure-13C
INOVA-500 “riga”

Relax. delay 4.000 sec
Pulse 52.1 degrees
Acq. time 1.300 sec
Width 29996.3 Hz
856 repetitions
OBSERVE C13, 125.6674205 MHz
DECOUPLE H1, 499.7732084 MHz
Power 42 dB
on during acquisition
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 131072
Total time 14 hr, 45 min, 15 sec
Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: barbara
File: 1222-RK-04-288
INOVA-500 "riga"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 10000.0 Hz
J2 repetitions
OBSERVE H1, 499.7707209 MHz
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 1 min, 32 sec
1222-RK-04-301-pure

Archive directory: /export/home/mkl/vnmrsys/data
Sample directory: auto_13Dec2004

Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: barbara
File: 1222-RK-04-301-pure
INOVA-500 "riga"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7544.3 Hz
144 repetitions

OBSERVE H1, 499.7707198 MHz

DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 9 min, 40 sec
1222-RK-05-365-pure

Archive directory: /export/home/mkl/vnmrsys/data
Sample directory: auto_13Dec2004

Pulse Sequence: s2pul
Solvent: dms
Temp. 25.0 C / 298.1 K
Operator: barbara
File: 1222-RK-05-365-pure
INOVA-500 "riga"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7544.3 Hz
J2 repetitions
OBSERVE H1, 499.7730834 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 1 min, 32 sec
1222-RK-04-308-pure

Archive directory: /export/home/mkl/vnmrsys/data
Sample directory: auto_13Dec2004

Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: barbara
File: 1222-RK-04-308-pure
INOVA-500 "riga"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7544.3 Hz
48 repetitions
OBSERVE H1, 499.7707198 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 9 min, 40 sec
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Operator: barbara
File: 1222-RK-11-851-pure
INOVA-500 "riga"

Pulse 48.0 degrees
Acq. time 1.892 sec
Width 8000.0 Hz
44 repetitions
OBSERVE H1, 499.7707217 MHz
DATA PROCESSING
FT size 32768
Total time 6 min, 20 sec
1231-RK-15-09-pure

Archive directory: /export/home/mkl/vnmrsys/data
Sample directory: auto_13Dec2004

Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 24.0 C / 297.1 K
Operator: barbara
File: 1231-RK-15-09-pure
INOVA-500 "riga"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7544.3 Hz
28 repetitions
OBSERVE H1, 499.7707216 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 9 min, 40 sec

E/Z-16 by method A
500 MHz, CDCl3

OMe
F
F
N
F
N

IN

9 8 7 6 5 4 3 2 1 ppm

IN

F3C
1231-RK-14-85-pure

Archive directory: /export/home/mkl/vnmrsys/data
Sample directory: auto_13Dec2004

Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
Operator: barbara
File: 1231-RK-14-85-pure
INOVA-500 "riga"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7544.3 Hz
12 repetitions

OBSERVE H1, 499.7707221 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 9 min, 40 sec
1231-RK-14-86-pure

Archive directory: /export/home/mkl/vnmrsys/data
Sample directory: auto_13Dec2004

Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
Operator: barbara
File: 1231-RK-14-86-pure
INOVA-500 "riga"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7544.3 Hz
12 repetitions

OBSERVE H1, 499.7707221 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 9 min, 40 sec

E/Z-18 by methodA
500 MHz, CDCl3

F3C

F

N

N

F

3

2

1

ppm
1222-RK-04-314-pure

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

Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 °C / 298.1 K
Operator: barbara
File: 1222-RK-04-314-pure
INOVA-500 "riga"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7544.3 Hz
64 repetitions
OBSERVE $^{1}H$, 499.7707189 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 9 min, 40 sec

EIZ-19 by method B
500 MHz, CDCl$_3$
1222-RK-04-328-1stfraction

Archive directory: /export/home/mkl/vnmrsys/data
Sample directory: auto_13Dec2004

Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: barbara
File: 1222-RK-04-328-1stfraction
INOVA-500 "riga"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7544.3 Hz
20 repetitions
OBSERVE H1, 499.7707189 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 1 min, 32 sec

E/Z-20 by method B
500 MHz, CDCl3
1222-RK-05-346-pure

Archive directory: /export/home/mkl/vnmrsys/data
Sample directory: auto_13Dec2004

Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: barbara
File: 1222-RK-05-346-pure
INOVA-500 "riga"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7544.3 Hz
12 repetitions

OBSERVE H1, 499.7707207 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 9 min, 40 sec
1222-RK-04-312-pure-2

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

Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: barbara
File: 1222-RK-04-312-pure-2
INOVA-500 "riga"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7544.3 Hz
36 repetitions
OBSERVE H1, 499.7707193 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 9 min, 40 sec

E/Z-22 by method B
500 MHz, CDCl3
Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 °C / 298.1 K
Operator: barbara
File: 1222-RK-05-352
INOVA-500 "riga"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7544.3 Hz
20 repetitions

OBSERVE H1, 499.7707198 MHz
DATA PROCESSING
FT size 32768
Total time 1 min, 32 sec
Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: barbara
File: 1222-RK-05-349
INOVA-500 "riga"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 10000.0 Hz
48 repetitions

OBSERVE H1, 499.7707203 MHz

DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 4 min, 50 sec
1222-RK-05-336

Archive directory: /export/home/mkl/vnmrsys/data
Sample directory: auto_13Dec2004
File: 1222-RK-05-336

Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: barbara
File: 1222-RK-05-336
INOVA-500 "capella500"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7544.3 Hz
16 repetitions
OBSERVE H1, 499.7707226 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 9 min, 40 sec

E/Z-25 by method B
500 MHz, CDCl₃
 Archive directory: /export/home/mkl/vnmrsys/data
Sample directory: auto_13Dec2004
Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Pulse 45.0 degrees
Acq. time 1.892 sec
OBSERVE   H1, 499.7707212 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 65536
Total time 1 min, 32 sec

26.500 MHz, CDCl3

OMe

26

0,0,

F

N

N

N

N

250:500 MHz, CDCl3
1222-RK-05-392-p-13C

Archive directory: /export/home/barbara/vnmrsys/data
File: 1222-RK-05-392-p-13C

Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
Operator: barbara
File: 1222-RK-05-392-p-13C
INOVA-500 "capella500"

Relax. delay 4.000 sec
Pulse 52.1 degrees
Acq. time 1.300 sec
Width 29996.3 Hz
320 repetitions
OBSERVE C13, 125.6674218 MHz
DECOUPLE H1, 499.7732084 MHz
Power 42 dB
on during acquisition
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 131072
Total time 2 hr, 57 min, 20 sec

26: 125 MHz, CDCl3
1231-RK-15-30-pure

Archive directory: /export/home/mkl/vnmrsys/data
Sample directory: auto_13Dec2004

Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: barbara
File: 1231-RK-15-30-pure
INOVA-500 "riga"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7544.3 Hz
20 repetitions
OBSERVE H1, 499.7707212 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 9 min, 40 sec

27: 500 MHz, CDCl₃
Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: barbara
File: 1231-Rk-15-30-13C
INOVA-500  "riga"
Relax. delay 4.000 sec
Pulse delay 6.000 sec
Acq. time 1.300 sec
Width 29996.3 Hz
8472 repetitions
Power 42 dB
on during acquisition
Line broadening 3.0 Hz
FT size 131072
Total time 14 hr, 45 min, 15 sec
Frequency 27.125 MHz, CDCl3

N
N
N
N

C13, 125.6674095 MHz
1222-RK-05-381-1

Archive directory: /export/home/mkl/vnmrsys/data
Sample directory: auto_13Dec2004

Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: barbara
File: 1222-RK-05-381-pure
INOVA-500 "riga"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7544.3 Hz
16 repetitions

OBSERVE H1, 499.7707184 MHz
DATA PROCESSING
FT size 32768
Total time 9 min, 40 sec

28: Major isomer
500 MHz, CDCl₃
1222-RK-05-381-13C

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

Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
Operator: barbara
File: 1222-RK-05-381-13C
INOVA-500 "riga"

Relax. delay 4.000 sec
Pulse 52.1 degrees
Acq. time 1.300 sec
Width 29996.3 Hz
176 repetitions
OBSERVE C13, 125.6674214 MHz
DECOUPLE H1, 499.7732084 MHz
Power 42 dB
on during acquisition
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 131072
Total time 2 hr, 57 min, 20 sec

28: Major isomer
125 MHz, CDCl3
1222-RK-05-fraction2

Archive directory: /export/home/mkl/vnmrsys/data
Sample directory: auto_13Dec2004

Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: barbara
File: 1222-RK-05-381-fraction2
INOVA-500 "riga"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 10000.0 Hz
20 repetitions
OBSERVE H1, 499.7707212 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 65536
Total time 9 min, 40 sec

28: Minor isomer
500 MHz, CDCl₃
Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: barbara
File: 1231-RK-05-381-fraction2-13C
INOVA-500 "riga"

Relax. delay 4.000 sec
Pulse 52.1 degrees
Acq. time 1.300 sec
Width 29996.3 Hz
10228 repetitions
OBSERVE C13, 125.6674191 MHz
DECOUPLE H1, 499.7732084 MHz
Power 42 dB
on during acquisition
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 29 hr, 30 min, 9 sec

28: Minor isomer
125 MHz, CDCl3
Archive directory: /export/home/mkl/vnmrsys/data
Sample directory: auto_13Dec2004

Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: barbara
File: 1231-RK-15-31-fraction1
INOVA-500 "riga"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7544.3 Hz
32 repetitions

DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 9 min, 40 sec
1231-RK-15-31-fraction1-13C

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

Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
Operator: barbara
File: 1231-RK-15-31-fraction1-13C
INOVA-500 "riga"

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

OBSERVE C13, 125.6674246 MHz
DECOUPLE H1, 499.7732084 MHz
Power 42 dB
on during acquisition
WALTZ-16 modulated

DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 2 hr, 57 min, 20 sec
1231-RK-15-31-fraction2

Archive directory: /export/home/mkl/vnmrsys/data
Sample directory: auto_13Dec2004

Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: barbara
File: 1231-RK-15-31-fraction2
INOVA-500 "riga"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7544.3 Hz
76 repetitions
OBSERVE H1, 499.7707221 MHz

DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 9 min, 40 sec

500 MHz, CDCl3
1231-RK-15-31-fraction2-13C

Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: barbara
File: 1231-RK-15-31-fraction2-13C
INOVA-500 "riga"

Relax. delay 4.000 sec
Pulse 52.1 degrees
Acq. time 1.300 sec
Width 29996.3 Hz
10000 repetitions
OBSERVE C13, 125.6674177 MHz
DECOUPLE H1, 499.7732084 MHz
Power 42 dB
on during acquisition
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 14 hr, 45 min, 15 sec
Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
Operator: barbara
File: GS-1231-03-209-pure1
INOVA-500 "riga"

Pulse 57.9 degrees
Acq. time 1.892 sec
Width 8000.0 Hz
60 repetitions
OBSERVE H1, 499.7707217 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 3 min, 10 sec
GS-1231-03-209-pure-c13-cdcl3

Pulse Sequence: s2pul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: barbara
File: GS-1231-03-209-pure-c13-cdcl3
INOVA-500 "riga"

Relax. delay 2.500 sec
Pulse 52.1 degrees
Acq. time 1.300 sec
Width 29996.3 Hz
15188 repetitions
OBSERVE C13, 125.6674223 MHz
DECOUPLE H1, 499.7732084 MHz
Power 42 dB
on during acquisition
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 131072
Total time 17 hr, 59 min, 35 sec

125 MHz, CDCl₃