SUPPORTING INFORMATION

FOR

COMPETITIVE CATIONIC PATHWAYS AND THE ASYMMETRIC SYNTHESIS
OF ARYL-SUBSTITUTED CYCLOPROPANES

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Sample: BJM2017p Feb 07 2006

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

File: bjm2017p

INOVA-500 "bioch.chem.nd.edu"

Relax. delay 1.000 sec

Pulse 86.2 degrees

Acq. time 2.337 sec

Width 3506.0 Hz

92 repetitions

OBSERVE H1, 299.6993026 MHz

DATA PROCESSING

FT size 32768

Total time 7 min, 8 sec

S1

INDEX	FREQUENCY	PPM	HEIGHT
1	12601.465	167.218	14.1
2	11343.614	150.527	17.6
3	10150.218	134.691	33.8
4	9776.184	129.727	74.1
5	9758.605	129.494	6.2
6	9511.527	126.215	83.2
7	8856.234	117.520	29.8
8	5852.236	77.658	28.9
9	5820.985	77.243	26.0
10	5788.757	76.815	29.2
11	5655.941	75.053	24.4
12	3918.583	51.999	23.2
13	3420.521	45.389	38.0
14	1964.422	26.067	160.6
15	1958.562	25.990	9.1
16	1391.162	18.460	23.5

Sample: BJM2025p Feb 07 2006

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

File: bjm2025p

INOVA-500 "bloch.chem.nd.edu"

Relax. delay 1.000 sec

Pulse 86.2 degrees

Acq. time 2.337 sec

Width 3506.0 Hz

36 repetitions

OBSERVE H1, 299.6993026 MHz

DATA PROCESSING

FT size 32768

Total time 7 min, 8 sec

Sample: BJM2025p Feb 07 2006

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

User: 1-14-87

File: bjm2025p-cl3

INOVA-500 "bloch.chem.nd.edu"

Relax. delay 4.000 sec

Pulse 90.0 degrees

Acq. time 1.122 sec

Width 50000.0 Hz

44 repetitions

OBSERVE C13, 125.6901674 MHz

DECOUPLE H1, 499.8641580 MHz

Power 41 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 126 hr, 44 min, 42 sec

Sample: BJM2031p Feb 07 2006

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

File: BJM2031p

INOVA-500 "bloch.chem.nd.edu"

Relax. delay 1.000 sec

Pulse 90.0 degrees

Acq. time 2.022 sec

Width 8104.5 Hz

112 repetitions

OBSERVE H1, 499.8611708 MHz

DATA PROCESSING

FT size 32768

Total time 6 min, 28 sec

Sample: BJM2031p Feb 07 2006

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

User: 1-14-87

File: bjm2031p-C13

INOVA-500 "bloch.Chem.nd.edu"

Relax. delay 4.000 sec

Pulse 90.0 degrees

Acq. time 1.122 sec

Width 50000.0 Hz

56 repetitions

OBSERVE C13, 125.6901964 MHz

DECOUPLE H1, 499.8641580 MHz

Power 41 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 126 hr, 44 min, 42 sec

Sample: BJM2030p Feb 07 2006

Pulse Sequence: s2pul

Solvent: CDC13

Ambient temperature

File: bjm2030p

INOVA-500 "bloch.chem.nd.edu"

Relax. delay 1.000 sec

Pulse 90.0 degrees

Acq. time 2.022 sec

Width 8104.5 Hz

48 repetitions

OBSERVE H1, 499.8611708 MHz

DATA PROCESSING

FI size 32768

Total time 6 min, 28 sec

Sample: BJM2030p Feb 07 2006

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

User: 1-14-87

File: bjm2030p-C13

INOVA-500 "bioch.chem.nd.edu"

Relax. delay 4.000 sec

Pulse 90.0 degrees

Acq. time 1.122 sec

Width 50000.0 Hz

68 repetitions

OBSERVE C13, 125.6901811 MHz

DECOUPLE H1, 499.8641580 MHz

Power 41 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 1267 hr, 27 min, 41 sec

Sample: BJM2166p Dec 04 2005

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

UNITYplus-300 "nmr2a.chem.nd.edu"

Relax. delay 0.380 sec

pulse 70.4 degrees

Acq. time 3.620 sec

Width 4525.4 Hz

124 repetitions

OBSERVE H1, 299.9468799 MHz

DATA PROCESSING

FT size 65536

Total time 8 min, 33 sec

10

Sample: BJM2166p Dec 04 2005

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

User: 1-14-87

INOVA-500 "inova5"

Relax. delay 4.000 sec

Pulse 90.0 degrees

Acq. time 1.215 sec

Width 40000.0 Hz

44 repetitions

OBSERVE C13, 125.6901769 MHz

DECOUPLE H1, 499.8636612 MHz

Power 40 dB,

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 131072

Total time 12899 hr, 13 min, 16 sec

Sample: BJM2033p Feb 07 2006

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

File: bjm2033p

INOVA-500 "bloch.chem.nd.edu"

Relax. delay 1.000 sec

Pulse 90.0 degrees

Acq. time 2.022 sec

Width 8104.5 Hz

32 repetitions

OBSERVE H1, 499.8611713 MHz

DATA PROCESSING

FT size 32768

Total time 6 min, 28 sec

Sample: BJM2033p Feb 07 2006

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

User: 1-14-87

File: bjm2033p-C13

INOVA-500 "bloch.chem.nd.edu"

Relax. delay 4.000 sec

Pulse 90.0 degrees

Acq. time 1.122 sec

Width 50000.0 Hz

64 repetitions

OBSERVE C13, 125.6901811 MHz

DECOUPLE H1, 499.8641580 MHz

Power 41 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 126 hr, 44 min, 42 sec

Sample: BJM2269p Jan 16 2006

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

UNITYplus-300 "echo.chem.nd.edu"

Relax. delay 1.000 sec

Pulse 86.2 degrees

Acq. time 2.091 sec

Width 3918.5 Hz

36 repetitions

OBSERVE H1, 299.6993028 MHz

DATA PROCESSING

FT size 32788

Total time 6 min, 36 sec

Sample: BJM2269p Jan 17 2006

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

UNITYplus-300 "nmr2a.chem.nd.edu"

Relax. delay 6.000 sec

Pulse 92.2 degrees

Acq. time 0.957 sec

Width 40000.0 Hz

6760 repetitions

OBSERVE C13, 75.4216805 MHz

DECOUPLE H1, 299.9486241 MHz

Power 40 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 1935575 hr, 53 min, 7 sec

5d

Sample: BJM3200p Oct 18 2006

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

INOVA-500 "inova5"

Relax. delay 0.100 sec

Pulse 90.0 degrees

Acq. time 5.016 sec

Width 6533.3 Hz

16 repetitions

OBSERVE H1 499.8611751 MHz

DATA PROCESSING

FT size 65536

Total time 10 min, 55 sec

Sample: BJM3200p Oct 18 2006

Pulse Sequence: s2pul

Solvent: CDC13

Ambient temperature

User: 1-14-87

INOVA-500 "inova5"

Relax. delay 6.000 sec

Pulse 90.0 degrees

Acq. time 1.215 sec

Width 40000.0 Hz

288 repetitions

OBSERVE C13, 125.6901681 MHz

DECOUPLE H1, 499.8636612 MHz

Power 40 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

line broadening 1.0 Hz

FT size 131072

Total time 178374 hr, 56 min, 0 sec

Sample: BJM2168p Jan 17 2006

Pulse Sequence: s2pu1

Solvent: cdcl3

Ambient temperature

UNITYplus-300 "echo.chem.nd.edu"

Relax. delay 1.000 sec

Pulse 86.2 degrees

Acq. time 2.091 sec

Width 3918.5 Hz

24 repetitions

OBSERVE H1, 299.6993062 MHz

DATA PROCESSING

FT size 32768

Total time 6 min, 36 sec

Sample: BJM2168 Jan 18 2006

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

User: 1-14-87

INOVA-500 "inova5"

Relax. delay 4.000 sec

Pulse 90.0 degrees

Acq. time 1.215 sec

Width 40000.0 Hz

536 repetitions

OBSERVE C13, 125.6901726 MHz

DECOUPLE H1, 499.8636612 MHz

Power 40 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 131072

Total time 12899 hr, 13 min, 16 sec

Sample: BJM2258 Dec 04 2005

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

INOVA-500 "inova5"

Relax. delay 0.100 sec

Pulse 90.0 degrees

Acq. time 5.016 sec

Width 6533.3 Hz

20 repetitions

OBSERVE H1, 499.8611759 MHz

DATA PROCESSING

FT size 65536

Total time 10 min, 55 sec

Sample: BJM2258p Dec 04 2005

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

User: 1-14-87

INOVA-500 "inova5"

Relax. delay 4.000 sec

Pulse 90.0 degrees

Acq. time 1.215 sec

Width 40000.0 Hz

68 repetitions

OBSERVE C13, 125.6901659 MHz

DECOUPLE H1, 499.8636612 MHz

Power 40 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 131072

Total time 128992 hr, 13 min, 20 sec

5g

Sample: BJM2265 Mar 22 2006

Pulse Sequence: s2pul

Solvent: cdc13

Ambient temperature

UNITYplus-300 "echo.chem.nd.edu"

Relax. delay 1.000 sec

Pulse 86.2 degre

Acq. time 2.091 sec

Width 3918.5 Hz

24 repetitions 41 20

OBSERVE H1, 299.6993064 MHZ

DATA PROCESSING

FT size 32768

Total time 6 min, 36 sec

Sample: BJM2265p Dec 22 2005

Pulse Sequence: s2pul1

Solvent: cdcl3

Ambient temperature

UNITYplus-300 "nmr2a.chem.nd.edu"

Relax. delay 7.000 sec

Pulse 92.2 degrees

Acq. time 0.957 sec

Width 40000.0 Hz

4392 repetitions

OBSERVE C13, 75.4216778 MHz

DECOUPLE H1, 299.9486241 MHz

Power 40 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 196742 hr, 32 min, 32 sec

Sample: BJM2196 Mar 22 2006

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

File: BJM2196p
INOVA-500 "bloch.chem.nd.edu"

Relax. delay 1.000 sec

Pulse 86.2 degrees

Acq. time 2.091 sec

Width 3918.5 Hz

44 repetitions

OBSERVE H1, 299.6993028 MHz

DATA PROCESSING

FT size 32768

Total time 6 min, 36 sec

6b

Sample: BJM2196p Feb 07 2006

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

File: bjm2196-13C

INOVA-500 "bloch.chem.nd.edu"

Relax. delay 4.000 sec

Pulse 92.2 degrees

Acq. time 0.957 sec

Width 40000.0 Hz

300 repetitions

OBSERVE C13, 75.4216817 MHz

DECOUPLE H1, 299.9486241 MHz

Power 40 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 12266 hr, 50 min, 48 sec

Sample: BJM2197p Feb 07 2006

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

File: bjm2197p

INOVA-500 "b1och.chem.nd.edu"

Relax. delay 0.100 sec

Pulse 70.4 degrees

Acq. time 3.948 sec

Width 4150.2 Hz

48 repetitions

OBSERVE H1, 299.9468567 MHz

DATA PROCESSING

FT size 65536

Total time 8 min, 39 sec

Sample: BJM2197p Feb 07 2006

Pulse Sequence: s2pul

Solvent: CDC13

Ambient temperature

File: bjm2197-13C

INOVA-500 "biotech.chem.nd.edu"

Relax. delay 4.000 sec

Pulse 92.2 degrees

Acq. time 0.957 sec

Width 40000.0 Hz

268 repetitions

OBSERVE C13, 75.4216817 MHz

DECOUPLE H1, 299.9486241 MHz

Power 40 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 12266 hr, 50 min, 48 sec

Sample: BJM3174p Sept 18 2006

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

INOVA-500 "inova5"

Relax. delay 0.100 sec

Pulse 90.0 degrees

Acq. time 5.016 sec

Width 6533.3 Hz

24 repetitions

OBSERVE H1, 499.8611751 MHZ

DATA PROCESSING

FT size 65536

Total time 10 min, 55 sec

Sample: BJM3205p Oct 26 2006

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

User: 1-14-87

INNOVA-500 "inova5"

Relax. delay 6.000 sec
Pulse 90.0 degrees
Acq. time 1.215 sec
Width 40000.0 Hz
436 repetitions
OBSERVE C13, 125.6901659 MHz
DECOUPLE H1, 499.8636612 MHz
Power 40 dB
Continuously On
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 1783 hr, 44 min, 51 sec

Sample: BJM3038p Mar 20 2006

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

INOVA-500 "inova5"

Relax. delay 1.000 sec

Pulse 90.0 degrees

Acq. time 2.022 sec

Width 8104.5 Hz

56 repetitions

OBSERVE H1, 499.8611713 MHz

DATA PROCESSING

FT size 32768

Total time 6 min, 27 sec

sample: BJM3038 Mar 20 2006

Pulse Sequence: s2pu1

Solvent: CDCl3

Ambient temperature

User: i-14-87

INOVA-500 "nova5"

Relax. delay 4.000 sec

Pulse 90.0 degrees

Acq. time 1.215 sec

Width 40000.0 Hz

684 repetitions

OBSERVE C13, 125.6901677 MHz

DECOUPLE H1, 499.8636612 MHz

Power 40 dB,

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 131072

Total time 1289922 hr, 16 min, 7 sec

Sample: BJM3272 Feb 23 2007

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

UNITYplus-300 "echo.chem.nd.edu"

Relax. delay 1.000 sec

Pulse 86.2 degrees

Acq. time 2.091 sec

Width 3918.5 Hz

32 repetitions

OBSERVE H1, 299.6993062 MHz

DATA PROCESSING

FI size 32768

Total time 1 min, 39 sec

Sample: BJM3272 13 CNMR Feb 26 2007

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

User: l-lq-87

INOVA-500 "inova5"

Relax. delay 7.000 sec

Pulse 90.0 degrees

Acq. time 1.215 sec

Width 38004.8 Hz

60 repetitions

OBSERVE C13, 125.6901655 MHz

DECOUPLE H1, 499.8636612 MHz

Power 40 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 131072

Total time 2030 hr, 39 min, 57 sec

Sample: BJM3043p Apr 4 2006

Pulse Sequence: s2pu1

Solvent: CDCl3

Ambient temperature

INOVA-500 "inovaS"

Relax. delay 1.000 sec

Pulse 90.0 degrees

Acq. time 2.022 sec

Width 8104.5 Hz

32 repetitions

OBSERVE H1, 499.8611769 MHz

DATA PROCESSING

FT size 32768

Total time 6 min, 27 sec

7a

Sample: BJM3043p Apr 4 2006

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

User: 1-14-87

INOVA-500 "inova5"

Relax. delay 6.000 sec

Pulse 90.0 degrees

Acq. time 1.215 sec

Width 40000.0 Hz

2008 repetitions

OBSERVE C13, 125.6901891 MHz

DECOUPLE H1, 499.8636612 MHz

Power 40 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 131072

Total time 178374 hr, 56 min, 0 sec

7a

Sample: BJM2202p Feb 07 2006

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

File: bjm2202p

INOVA-500 "bloch.chem.nd.edu"

Relax. delay 0.100 sec

Pulse 70.4 degrees

Acq. time 3.948 sec

Width 4150.2 Hz

56 repetitions

OBSERVE H1, 299.9468586 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 8 min, 39 sec

7b

Sample: BJM2202p Feb 07 2006

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

File: bjm2202p-13C

INOVA-500 "bloch.chem.nd.edu"

Relax. delay 4.000 sec

Pulse 92.2 degrees

Acq. time 0.957 sec

Width 40000.0 Hz

228 repetitions

OBSERVE C13, 75.4216817 MHZ

DECOUPLE H1, 299.9486241 MHZ

Power 40 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 1226 hr, 41 min, 0 sec

7b

Sample: BJM 2093 Mar 30 2006

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

INOVA-500 "inova5"

Relax. delay 1.000 sec

Pulse 90.0 degrees

Acq. time 2.022 sec

Width 8104.5 Hz

36 repetitions

OBSERVE H1 489.8611759 MHZ

DATA PROCESSING

FT size 32768

Total time 6 min, 27 sec

Sample: BJM2093 Mar 30 2006

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

User: 1-14-87

INNOVA-500 "nova5"

Relax. delay 6.000 sec

Pulse 90.0 degrees

Acq. time 1.215 sec

Width 40000.0 Hz

996 Repetitions

OBSERVE C13, 125.6901565 MHz

DECOUPLE H1, 499.8636612 MHz

Power 40 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 131072

Total time 178374 hr, 56 min, 0 sec

Sample: BJM3209 Oct 28 2006

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

INOVA-500 "Inova5"

Relax. delay 0.100 sec

Pulse 90.0 degrees

Acq. time 5.016 sec

Width 6533.3 Hz

24 repetitions

OBSERVE H1, 499.8611751 MHz

DATA PROCESSING

FT size 55536

Total time 10 min, 55 sec

Sample: BJM3209 Oct 30 2006

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

User: 1-14-87

INOVA-500 "inova5"

Relax. delay 6.000 sec

Pulse 90.0 degrees

Acq. time 1.215 sec

Width 40000.0 Hz

568 repetitions

OBSERVE C13, 125.6901696 MHz

DECOUPLE H1, 499.8636812 MHz

Power 40 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 131072

Total time 1783 hr, 44 min, 51 sec

Sample: BJM2266p Feb 07 2006

Pulse Sequence: s2pul1

Solvent: CDCl3

Ambient temperature

File: bjm2266p

INOVA-500 "bloch.Chem.nd.edu"

Relax. delay 0.100 sec

Pulse 90.0 degrees

Acq. time 5.016 sec

Width 6533.3 Hz

40 repetitions

OBSERVE H1, 499.8611619 MHz

DATA PROCESSING

FT size 65536

Total time 10 min, 56 sec

Sample: BJM2266p Feb 07 2006

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

User: 1-14-87

File: bjm2266-13C

INOVA-500 "b1och.Chem.nd.edu"

Relax. delay 4.000 sec

Pulse 90.0 degrees

Acq. time 1.215 sec

Width 40000.0 Hz

496 repetitions

OBSERVE C13, 125.6901702 MHz

DECOUPLE H1, 499.8636612 MHz

Power 40 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 131072

Total time 12904 hr, 9 min, 36 sec

Sample: BJM3052 Apr 6 2006

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

INOVA-500 "inova5"

Relax. delay 1.000 sec

Pulse 90.0 degrees

Acq. time 2.022 sec

Width 8104.5 Hz

56 repetitions

OBSERVE H1, 499.8611764 MHz

DATA PROCESSING

FT size 32768

Total time 6 min, 27 sec

7g

Sample: BJM3052 Apr 6 2006

Pulse Sequence: s2pu1

Solvent: CDCl3

Ambient temperature

User: 1-14-87

INOVA-500 "inova5"

Relax. delay 6.000 sec

Pulse 90.0 degrees

Acq. time 1.215 sec

Width 40000.0 Hz

400 repetitions

OBSERVE C13, 125.6901659 MHz

DECOUPLE H1, 499.8636612 MHz

Power 40 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 131072

Total time 17837 hr, 29 min, 32 sec

7g

Sample: BJM3057p Apr 14 2006

Pulse Sequence: s2pul1

Solvent: CDCl3

Ambient temperature

INOVA-500 "inova5"

Relax. delay 0.100 sec

Pulse 90.0 degrees

Acq. time 5.016 sec

Width 6533.3 Hz

28 repetitions

OBSERVE H1 499.8611763 MHZ

DATA PROCESSING

Line broadening 0.1 Hz

FI size 85536

Total time 10 min, 55 sec

Sample: BJM3057p Apr 14 2006

Pulse Sequence: s2pul

Solvent: CDC13

Ambient temperature

User: 1-14-87

INOVA-500 "inova5"

Relax. delay 6.000 sec

Pulse 90.0 degrees

Acq. time 1.215 sec

Width 40000.0 Hz

740 repetitions

OBSERVE C13, 125.6901671 MHz

DECOUPLE H1, 499.8636612 MHz

Power 40 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 131072

Total time 1783 hr, 44 min, 51 sec

Sample: BJM2204p-trans Feb 07 2006

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

File: bjm2204-trans

INOVA-500 "bloch.chem.nd.edu"

Relax. delay 1.000 sec

Pulse 48.6 degrees

Acq. time 2.902 sec

Width 5645.3 Hz

44 repetitions

OBSERVE H1, 499.8611715 MHz

DATA PROCESSING

FT size 32768

Total time 8 min, 20 sec

8b

Sample: BJM2157 Mar 23 2006

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

UNITYplus-300 "nmr3a.chem.nd.edu"

Relax. delay 6.000 sec

Pulse 92.2 degrees

Acq. time 0.957 sec

Width 40000.0 Hz

1328 repetitions

OBSERVE C13, 75.4216811 MHz

DECOUPLE H1, 299.9486243 MHz

Power 40 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 17205 hr, 7 min, 4 sec

8b

Sample: BJM2211p Feb 07 2006

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

File: bjm2211p

INOVA-500 "bioch.chem.nd.edu"

Relax. delay 0.380 sec

Pulse 70.4 degrees

Acq. time 3.620 sec

Width 4525.4 Hz

48 repetitions

OBSERVE H1, 299.9468799 MHz

DATA PROCESSING

FT size 65536

Total time 8 min, 33 sec

44

Sample: BJM2211p Feb 07 2006

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

File: bjm2211p-13C

INOVA-500 "bloch.chem.nd.edu"

Relax. delay 4.000 sec

Pulse 92.2 degrees

Acq. time 0.957 sec

Width 40000.0 Hz

500 repetitions

OBSERVE C13, 75.4216841 MHz

DECOUPLE H1, 299.9486241 MHz

Power 40 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 1226 hr, 41 min, 0 sec

45

Sample: BJM3210p-trans Nov 10 2006

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

INOVA-500 "InovaS"

Relax. delay 0.100 sec

Pulse 90.0 degrees

Acq. time 5.016 sec

Width 6533.3 Hz

32 repetitions

OBSERVE H1, 499.8611757 MHz

DATA PROCESSING

FT size 65536

Total time 2 min, 43 sec

Sample: BJM3210-13C Nov 10 2006

Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-87
INOVA-500 "inova5"

Relax. delay 7.000 sec
Pulse 90.0 degrees
Acq. time 1.215 sec
Width 40000.0 Hz
44 repetitions
OBSERVE C13, 125.6901665 MHz
DECOUPLE H1, 499.8636612 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 2030 hr, 39 min, 39 sec

Sample: BJM3059p Apr 10 2006

Pulse Sequence: s2pu1

Solvent: CDCl3

Ambient temperature
INOVA-500 "inova5"

Relax. delay 0.100 sec

Pulse 90.0 degrees

Acq. time 5.016 sec

Width 6533.3 Hz

24 repetitions

OBSERVE H1 499.8611761 MHz

DATA PROCESSING

FT size 85536

Total time 10 min, 55 sec

Sample: BJM3059 Apr 10 2006

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

User: 1-14-87

INNOVA-500 "inova5"

Relax. delay 4.000 sec

Pulse 90.0 degrees

Acq. time 1.215 sec

Width 40000.0 Hz

92 repetitions

OBSERVE C13, 125.6901859 MHz

DECOUPLE H1, 499.8636612 MHz

Power 40 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 131072

Total time 11 min, 8 sec

STANDARD PROTON PARAMETERS

Pulse Sequence: s2pul

Solvent: CDC13

Ambient temperature

INOVA-500 "inova5"

Relax. delay 0.100 sec

Pulse 90.0 degrees

Acq. time 5.016 sec

Width 6533.3 Hz

56 repetitions

OBSERVE H1, 499.8611763 MHz

DATA PROCESSING

FT size 65536

Total time 10 min, 55 sec

8g

Sample: BJM3056p Apr 13 2006

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

User: 1-14-87

INOVA-500 "Inova5"

Relax. delay 6.000 sec

Pulse 90.0 degrees

Acq time 1.215 sec

Width 40000.0 Hz

988 repetitions

OBSERVE C13, 125.6901659 MHz

DECOUPLE H1, 499.8636612 MHz

Power 40 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 131072

Total time 1783 hr, 44 min, 51 sec

Sample: BJM3216p Nov 24 2006

Pulse Sequence: s2pul1

Solvent: cdcl3

Ambient temperature

UNITYplus-300 "echo.chem.nd.edu"

Relax. delay 1.000 sec

Pulse 86.2 degrees

Acq. time 2.091 sec

Width 3918.5 Hz

32 repetitions

OBSERVE H1 299.6993062 MHZ

DATA PROCESSING

FI size 32768

Total time 1 min, 39 sec

Sample: BJM3216 Nov 24 2006

Pulse Sequence: s2pu1

Solvent: CDCl3

Ambient temperature

User: l-14-87

INOVA-500 "nova5"

Relax. delay 7.000 sec

Pulse 90.0 degrees

Acq. time 1.215 sec

Width 40000.0 Hz

20 repetitions

OBSERVE C13, 125.6901891 MHz

DECOUPLE H1, 499.8636612 MHz

Power 40 dB,

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 131072

Total time 2030 hr, 39 min, 39 sec

Sample: BJM3233p Dec 10 2006

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

INOVA-500 "inova5"

Relax. delay 0.100 sec

Pulse 90.0 degrees

Acq. time 5.016 sec

Width 6533.3 Hz

40 repetitions

OBSERVE H1, 499.8611757 MHz

DATA PROCESSING

FT size 65536

Total time 10 min, 55 sec

Sample: BJM3233p 13C Dec 10 2006

Pulse Sequence: s2pul

Solvent: CDCl3
Ambient temperature
User: 1-14-87
INOVA-500 "inova5"

Relax. delay 6.000 sec
Pulse 90.0 degrees
Acq. time 1.215 sec
Width 40000.0 Hz
140 repetitions
OBSERVE C13, 125.6901659 MHz
DECOUPLE H1, 499.8636612 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FI size 131072
Total time 17837 hr, 29 min, 32 sec

Sample: BJM2241 19F NMR
 Pulse Sequence: s2pu1
 Solvent: CDCl3
 Ambient temperature
 File: bjm2241-19f
 INOVA-500 "bloch.chem.nd.edu"
 Relax. delay 2.000 sec
 Pulse 90.0 degrees
 Acq. time 1.092 sec
 Width 30007.5 Hz
 76 repetitions
 OBSERVE F19, 281.9990982 MHz
 DATA PROCESSING
 Resol. enhancement -0.0 Hz
 FT size 65536
 Total time 6 min, 37 sec