Supporting Information

Approach toward Convergence into Single Enantiomer in Enzyme-catalyzed Kinetic Resolution of Racemic Mixture

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Pulse Sequence: s2pul
Solvent: d6d13
Ambient temperature
Sample #3, Operator: walkup
File: 100115-p57-12-pure
VNMRS-400 "400NMR"

Relax. delay 1.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6410.3 Hz
16 repetitions
OBSERVE H1, 399.8698550 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 1 min, 20 sec

13c
Pulse Sequence: z2pul
solvent: ddeo13
Ambient temperature
Operator: wandup
File: 120114-p200-12a-pure-C
INOVA-500 "INOVAS500"

Relax. delay 0.700 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 50188.7 Hz
512 repetitions
OBSERVE C13, 125.7745771 MHz
DECOUPLE H1, 500.1992491 MHz
Power 41 dB continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 17 min, 8 sec
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
Operator: walkup
File: Proton_02
INOVA-500 "INOVAS00"

Relax. delay 1.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 9003.2 Hz
16 repetitions
OBSERVE M1, 500.1967481 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 1 min, 20 sec

(+)-9c
Pulse Sequence: a2pul
Solvent: cdcl3
Ambient temperature
Operator: walkup
File: 22-iBu-pure
VNMRS-400 "400MR"

Relax. delay 0.700 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 24509.8 Hz
512 repetitions
OBSERVE C13, 100.5458808 MHz
DECUPLE H1, 399.8659914 MHz
Power 37 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 17 min, 9 sec
Pulse Sequence: z2pul
Solvent: cdcl3
Ambient temperature
Operator: walkup
File: 110627-p154-crude
VNMRS-400 "400MR"

Relax. delay 1.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6410.3 Hz
16 repetitions
OBSERVE  H1, 399.8639921 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 1 min, 20 sec
Pulse Sequence: a2pul
Solvent: odo13
Ambient temperature
Operator: walkup
File: 120120-21-iPr-pure-C
VNMRS-400 "400MR"

Relax. delay 0.700 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 24509.8 Hz
15000 repetitions
OBSERVE C13, 106.5458608 MHz
DESCOUPLE H1, 399.8659914 MHz
Power 37 dB
continuously on
WAFFE-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 8 hr, 22 min, 13 sec

(±)-9d
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
Operator: walkup
File: 120204-22-pure
INOVA-500 "INOVASOHO"

Relax. delay 1.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 8003.2 Hz
16 repetitions
OBSERVE H1, 500.1967587 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 1 min, 20 sec

(±)-12a
Pulse Sequence: s2ps1
Solvent: cdcl3
Ambient temperature
Operator: walkup
File: Carbon_02
INOVA-500 "INOVA500"

Relax. delay 0.700 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 30166.7 Hz
20000 repetitions

OBSERVE C13, 125.7745724 MHz
DECOUPLE H1, 500.1992491 MHz
Power 35 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 11 hr, 9 min, 36 sec

(±)-12a
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
Operator: walkup
File: 120105-p197-crude
VNMRS-400 "400MR"

Relax. delay 1.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6410.3 Hz
16 repetitions
OBSERVE H1, 399.8639921 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 1 min, 20 sec
Pulse Sequence: z2pul
Solvent: dcdcl3
Ambient temperature
Operator: walkup
File: 120126-p198-crude-C
Vnmrs=400 "400MR"

Relax. delay 0.700 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 24509.8 Hz
20000 repetitions
COSBNERE C13, 100.5458808 MHz
DECOPLE N1, 399.6659914 MHz
Power 37 dB
continuously on
MULTI-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 11 hr, 9 min, 38 sec
Pulse Sequence: a2pul
Solvent: odol3
 Ambient temperature
Operator: walkup
File: 150623_exp673_1H
INOVA-500 "INOVASO"

Relax. delay 1.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 8000.2 Hz
16 repetitions
OBSERVE H1, 500.1967586 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 1 min, 20 sec
Pulse Sequence: a2pul
Solvent: cdcl3
Ambient temperature
Operator: walkup
File: 150623_exp673_13C
INOVIA-500 "INOVIA500"

Relax. delay 0.700 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 30188.7 Hz
1000 repetitions

OBSERVE C13, 125.7745724 MHz
DECOPUPE H1, 500.1592451 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 33 min. 28 sec
Pulse Sequence: z2pul
Solvent: cdcl3
Ambient temperature
Operator: walkup
File: 150601_exp680
VINMRS-400 "400MR"

Relax. delay 1.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6410.3 Hz
16 repetitions

OBserve: H1, 399.8646434 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 1 min, 20 sec

(-)-14b 3:1 (+)-15