Evaluation of Chiral Oxazolines for the Highly Enantioselective Diethylzinc

Addition to *N*-(Diphenylphosphinoyl) imines**

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(Supporting Information)

Current Data Parameters
NAME sin
EXPNO 38
PROCNO 1

F2 - Acquisition Parameters
Date_ 20010528
Time 12:42
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 32
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 16
DM 111.200 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec

0.003
0.014
0.025
2.340
2.396
2.409
2.451
2.461
2.493
2.530
2.560
2.570
2.597
3.027
3.064
3.111
3.132
3.150
3.158
3.181
3.199
3.235
3.294
7.277
7.439
7.450
7.456
7.464
7.475
7.480
7.486
7.491
7.497
7.904
7.925
7.930
7.939
7.945
7.966
7.971
9.248
9.355

===== CHANNEL f1 =====
NUC1 1H
P1 4.50 usec
PL1 2.00 dB
SF01 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 300.1300010 MHz
WDW nc
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 10.518 ppm
F1 3156.91 Hz
F2P -0.706 ppm
F2 -212.04 Hz
PPMCM 0.56125 ppm/cm
HZCM 168.44734 Hz/cm

Current Data Parameters
NAME sin
EXPNO 9
PROCNO 1

F2 - Acquisition Parameters

Date_ 20010209
Time 10:55
INSTRUM gp300
PROBHD 5 mm Multinu
PULPROG zg30
TD 26976
SOLVENT CDCl3
NS 32
DS 0
SWH 4495.403 Hz
FIDRES 0.166682 Hz
AQ 2.9997811 sec
RG 24
DH 111.200 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====

NUC1 1H
P1 4.50 usec
PL1 2.00 dB
SF01 300.1312005 MHz

F2 - Processing parameters

SI 32768
SF 300.1300010 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters

CX 20.00 cm
F1P 8.789 ppm
F1 2637.92 Hz
F2P -0.349 ppm
F2 -104.66 Hz
PPMCM 0.45690 ppm/cm
HZCM 137.12912 Hz/cm

Current Data Parameters
NAME sin
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters

Date_ 20010215
Time 14.43
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zg30
TD 32768
SOLVENT D2O
NS 32
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 24
DM 111.200 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====

NUC1 1H
P1 4.50 usec
PL1 2.00 dB
SF01 300.1312005 MHz

F2 - Processing parameters

SI 32768
SF 300.1300010 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters

CX 20.00 cm
F1P 8.521 ppm
F1 2557.39 Hz
F2P -0.289 ppm
F2 -86.76 Hz
PPMCM 0.44050 ppm/cm
HZCM 132.20767 Hz/cm

Current Data Parameters
NAME sin
EXPNO 26
PROCNO 1

F2 - Acquisition Parameters

Date_ 20010426
Time 11.30
INSTRUM dpk300
PROBHD 5 mm Multinu
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 32
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 16
DW 111.200 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====

NUC1 1H
P1 4.50 usec
PL1 2.00 dB
SF01 300.1312005 MHz

F2 - Processing parameters

SI 32768
SF 300.1300010 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters

CX 20.00 cm
F1P 8.650 ppm
F1 2596.20 Hz
F2P -0.447 ppm
F2 -134.08 Hz
PPMCH 0.45485 ppm/cm
HZCM 136.51404 Hz/cm

Current Data Parameters
NAME sin
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20001214
Time 8.09
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SHH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 16
DM 111.200 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 ¹H
P1 4.50 usec
PL1 2.00 dB
SF01 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 300.1300010 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 8.372 ppm
F1 2512.65 Hz
F2P -0.483 ppm
F2 -144.93 Hz
PPMCM 0.44274 ppm/cm
HZCM 132.87878 Hz/cm

Current Data Parameters
NAME sin
EXPNO 34
PROCNO 1

F2 - Acquisition Parameters
Date_ 20010309
Time 12.01
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zg30
TO 32768
SOLVENT CDC13
NS 64
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 4
DM 111.200 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 4.50 usec
PL1 2.00 dB
SF01 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 300.1300010 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 8.804 ppm
F1 2642.40 Hz
F2P -0.140 ppm
F2 -42.02 Hz
PPMCM 0.44721 ppm/cm
HZCM 134.22099 Hz/cm

ZHL 01.06.21-A 1H NMR bbi probe

Current Data Parameters
NAME c-1367
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20021111
Time 11.37
INSTRUM dpx300
PROBHD 5 mm Dual 13
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 963
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 24
DM 111.200 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 4.50 usec
PL1 2.00 dB
SF01 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 300.1300010 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 8.494 ppm
F1 2549.35 Hz
F2P 0.678 ppm
F2 203.60 Hz
PPMCM 0.39079 ppm/cm
HZCM 117.28761 Hz/cm

ZHL-01.05.26 1H NMR bbi probe

Current Data Parameters
NAME c-1367
EXPNO 48
PROCNO 1

F2 - Acquisition Parameters
Date_ 20021126
Time 16.42
INSTRUM dpx300
PROBHD 5 mm Dual 13
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 32
DS 0
SWH 4006.410 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 24
DM 124.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 4.50 usec
PL1 2.00 dB
SF01 300.1315007 MHz

F2 - Processing parameters
SI 32768
SF 300.1300031 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 9.064 ppm
F1 2720.45 Hz
F2P -0.527 ppm
F2 -158.03 Hz
PPMCM 0.47954 ppm/cm
HZCM 143.92352 Hz/cm

ZHL-2 1H NMR bbi probe

Current Data Parameters
NAME sin
EXPNO 30
PROCNO 1

F2 - Acquisition Parameters
Date_ 20010623
Time 13.34
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 64
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 16
DW 111.200 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 4.50 usec
PL1 2.00 dB
SF01 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 300.1300010 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 8.635 ppm
F1 2591.69 Hz
F2P -0.387 ppm
F2 -116.06 Hz
PPMCM 0.45110 ppm/cm
HZCM 135.38768 Hz/cm

Current Data Parameters
NAME sin
EXPNO 9
PROCNO 1

F2 - Acquisition Parameters

Date_ 20001221
Time 11.34
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zg30
TD 26976
SOLVENT CDCl3
NS 32
DS 0
SWH 4496.403 Hz
FIDRES 0.166682 Hz
AQ 2.9997811 sec
RG 24
DM 111.200 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====

NUC1 1H
P1 4.50 usec
PL1 2.00 dB
SFO1 300.1312005 MHz

F2 - Processing parameters

SI 32768
SF 300.1300010 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters

CX 20.00 cm
F1P 8.342 ppm
F1 2503.70 Hz
F2P -0.304 ppm
F2 -91.24 Hz
PPMCM 0.43230 ppm/cm
HZCM 129.74696 Hz/cm

Current Data Parameters
NAME sin
EXPNO 9
PROCNO 1

F2 - Acquisition Parameters
Date_ 20010416
Time 17:27
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zg30
TD 26976
SOLVENT CDC13
NS 32
DS 0
SWH 4496.403 Hz
FIDRES 0.166682 Hz
AQ 2.9997811 sec
RG 24
DW 111.200 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 4.50 usec
PL1 2.00 dB
SF01 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 300.1300010 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 9.041 ppm
F1 2713.34 Hz
F2P -0.567 ppm
F2 -170.12 Hz
PPMCM 0.48037 ppm/cm
HZCM 144.17325 Hz/cm

Current Data Parameters
NAME sin
EXPNO 16
PROCNO 1

F2 - Acquisition Parameters

Date_ 20010322
Time 10.00
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 32
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6436515 sec
RG 24
DM 111.200 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 4.50 usec
PL1 2.00 dB
SF01 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 300.1300010 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
FIP 8.410 ppm
F1 2524.11 Hz
F2P -0.952 ppm
F2 -165.62 Hz
PPMCM 0.44809 ppm/cm
HZCM 134.48659 Hz/cm

Current Data Parameters
NAME Sin
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20010529
Time 16.44
INSTRUM dpx300
PROBHD 5 mm Multino
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 24
DM 111.200 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec

===== CHANNEL f1 =====

NUC1 1H
P1 4.50 usec
PL1 2.00 dB
SFO1 300.1318008 MHz

F2 - Processing parameters

SI 32768
SF 300.1300010 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters

CX 20.00 cm
F1P 9.795 ppm
F1 2939.65 Hz
F2P -0.623 ppm
F2 -187.11 Hz
PPMCM 0.52090 ppm/ci
HZCM 156.33789 Hz/cm

Current Data Parameters
NAME sin
EXPNO 30
PROCNO 1

F2 - Acquisition Parameters
Date_ 20010320
Time 10.38
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 32
DS 0
SWH 4495.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 16
DW 111.200 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 4.50 usec
PL1 2.00 dB
SF01 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 300.1300010 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 8.620 ppm
F1 2587.19 Hz
F2P -0.312 ppm
F2 -93.53 Hz
PPNCH 0.44659 ppm/cm
HZCM 134.03607 Hz/cm

4.136
4.162
4.166
4.169
4.188
4.191
4.256
4.269
4.274
4.287
4.291
4.312
4.317
4.356
4.581
4.591
4.599
7.278
7.401
7.403
7.429
7.434
7.439
7.450
7.454
7.459
7.976
7.981
8.005
8.009
ppm

Current Data Parameters
 NAME sin
 EXPNO 18
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20010514
 Time 16.25
 INSTRUM dpx300
 PROBHD 5 mm Multinu
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 32
 DS 0
 SWH 4496.403 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 40
 DW 111.200 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

===== CHANNEL f1 =====

NUC1 1H
 P1 4.50 usec
 PL1 2.00 dB
 SF01 300.1312005 MHz

F2 - Processing parameters

SI 32768
 SF 300.1300010 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters

CX 20.00 cm
 F1P 8.620 ppm
 F1 2587.19 Hz
 F2P -0.342 ppm
 F2 -102.54 Hz
 PPMCM 0.44809 ppm/cm
 HZCM 134.48659 Hz/cm

ZHL-01-06-5 1H-NMR bbi probe

Current Data Parameters

NAME sin
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters

Date_ 20010608
Time 11.28
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 32
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 24
DM 111.200 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====

NUC1 1H
P1 4.50 usec
PL1 2.00 dB
SF01 300.1312005 MHz

F2 - Processing parameters

SI 32768
SF 300.1300010 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters

CX 20.00 cm
F1P 8.605 ppm
F1 2582.68 Hz
F2P -0.657 ppm
F2 -197.16 Hz
PPMCM 0.46311 ppm/cm
HZCM 138.99203 Hz/cm

ZHL-010628 1H NMR bbi probe

Current Data Parameters

NAME sin
EXPNO 31
PROCNO 1

F2 - Acquisition Parameters

Date_ 20010628
Time 11.07
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 32
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 16
DM 111.200 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec

===== CHANNEL f1 =====

NUC1 1H
P1 4.50 usec
PL1 2.00 dB
SF01 300.1312005 MHz

F2 - Processing parameters

SI 32768
SF 300.1300010 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters

CX 20.00 cm
F1P 8.981 ppm
F1 2695.32 Hz
F2P -0.477 ppm
F2 -143.09 Hz
PPMCM 0.47286 ppm/cm
HZCM 141.92055 Hz/cm

ZHL-OX-6 1H NMR bbi probe

Current Data Parameters
NAME sin
EXPNO 29
PROCNO 1

F2 - Acquisition Parameters
Date_ 20020425
Time 18.01
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 32
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 16
OW 111.200 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 4.50 usec
PL1 2.00 dB
SF01 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 300.1300010 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 9.038 ppm
F1 2712.65 Hz
F2P -0.531 ppm
F2 -159.38 Hz
PPMCM 0.47847 ppm/cm
HZCM 143.60358 Hz/cm

ZHL-OX-3 1H NMR bbi probe

Current Data Parameters
NAME sin
EXPNO 31
PROCNO 1

F2 - Acquisition Parameters
Date_ 20020528
Time 11.34
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 32
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 16
OW 111.200 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 4.50 usec
PL1 2.00 dB
SF01 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 300.1300010 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 8.681 ppm
F1 2605.34 Hz
F2P -0.614 ppm
F2 -184.17 Hz
PPMCM 0.46472 ppm/cm
HZCM 139.47543 Hz/cm

ZHL-OX-5 1H NMR bbi probe

Current Data Parameters
NAME sin
EXPNO 16
PROCNO 1

F2 - Acquisition Parameters
Date_ 20020514
Time 17.43
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 24
DW 111.200 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 4.50 usec
PL1 2.00 dB
SFO1 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 300.1300010 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 8.371 ppm
F1 2512.52 Hz
F2P -0.126 ppm
F2 -37.90 Hz
PPMCM 0.42489 ppm/cm
HZCM 127.52112 Hz/cm

ZHL-OX-4 1H NMR Bb1 probe

Current Data Parameters
NAME sin
EXPNO 26
PROCNO 1

F2 - Acquisition Parameters
Date_ 20020524
Time 15.58
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 16
DW 111.200 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 4.50 usec
PL1 2.00 dB
SFO1 300.1318008 MHz

F2 - Processing parameters
SI 32768
SF 300.1300010 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 8.771 ppm
F1 2632.36 Hz
F2P -0.738 ppm
F2 -221.56 Hz
PPMCM 0.47545 ppm/cm
HZCM 142.69614 Hz/cm

X-ray structure of **4f**

X-ray structure of **4j**