Electronic supplementary information (ESI)

Chemoenzymatic synthesis of enantiopure hydroxy sulfoxides derived from substituted arenes

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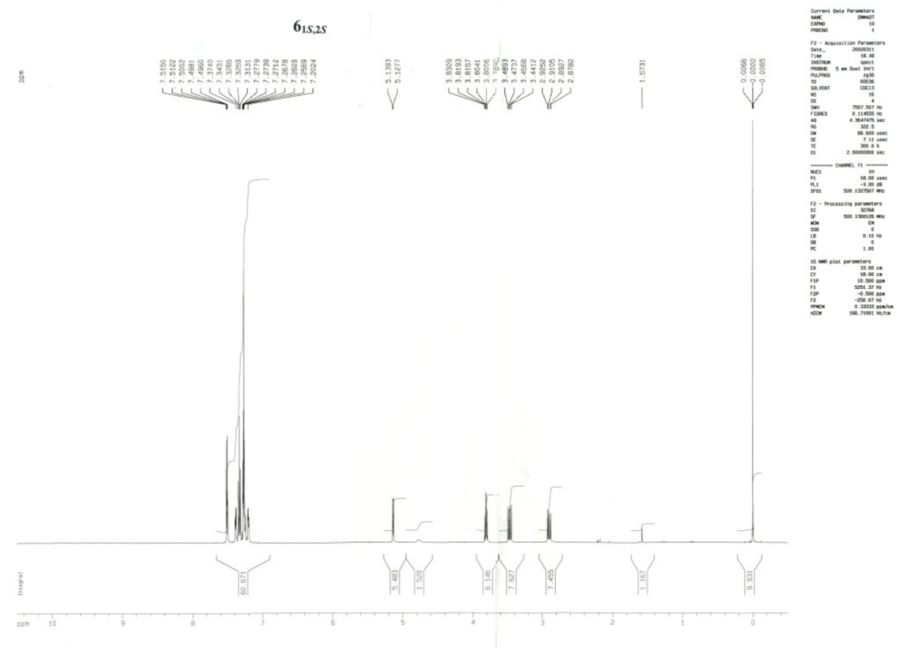
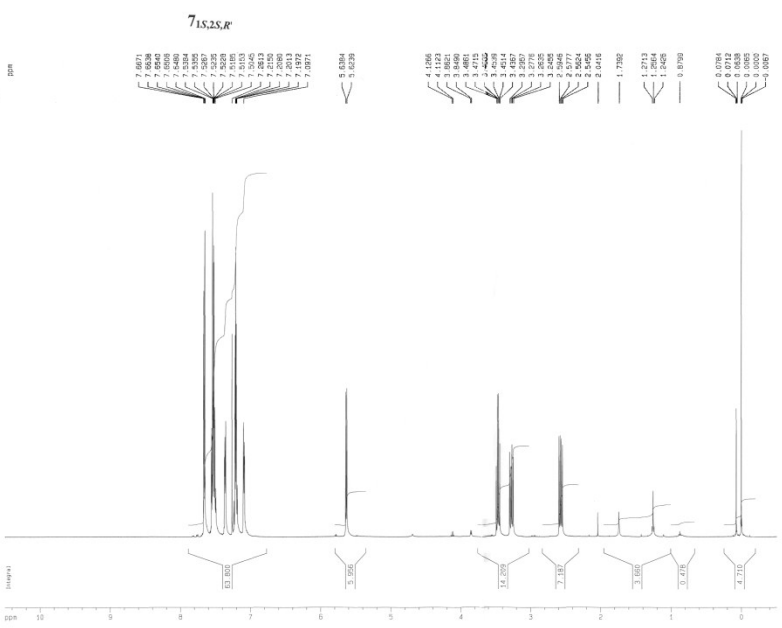
NMR spectra

ECD Spectra

$\mathbf{6}_{1S,2S}$



7$_{1S,2S,R'}$



Current Data Parameters
NAME DMIS57H
EXPNO 10
PROCNO 1

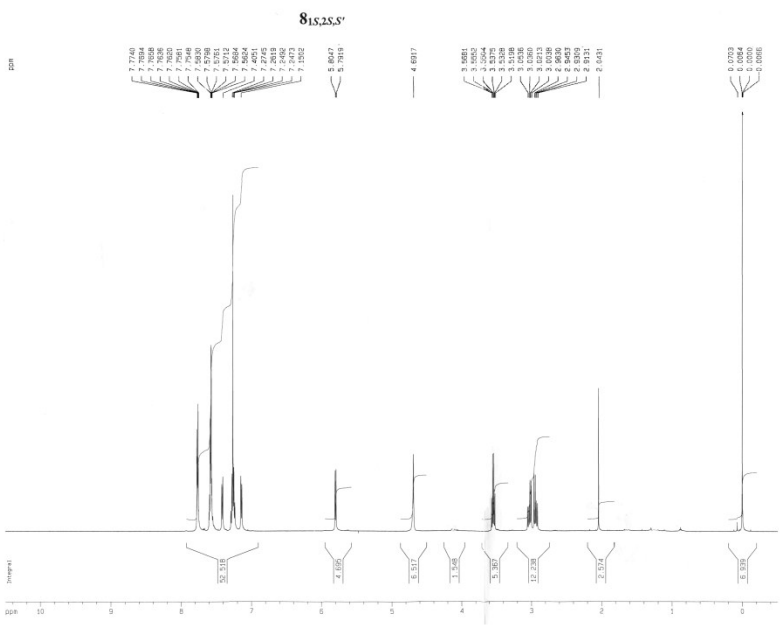
F2 - Acquisition Parameters
Date_ 20191015
Time 15.51
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 7507.507 Hz
FIDRES 0.114533 Hz
AQ 4.3647475 sec
RG 144.5
DW 66.600 usec
DE 7.11 usec
TE 300.0 K
D1 2.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 30.00 usec
PL1 -3.00 dB
SFO1 500.1327507 MHz

F2 - Processing parameters
SI 32768
SF 500.1300125 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 19.50 cm
CY 19.80 cm
F1P 11.500 ppm
F1 5251.37 Hz
F2P -0.500 ppm
F2 -250.07 Hz
PPMCM 0.33333 ppm/cm
HZCM 166.71001 Hz/cm

8$_{1S,2S,5'}$



Current Data Parameters
NAME DMSO1S_
EXPNO 10
PROCNO 1

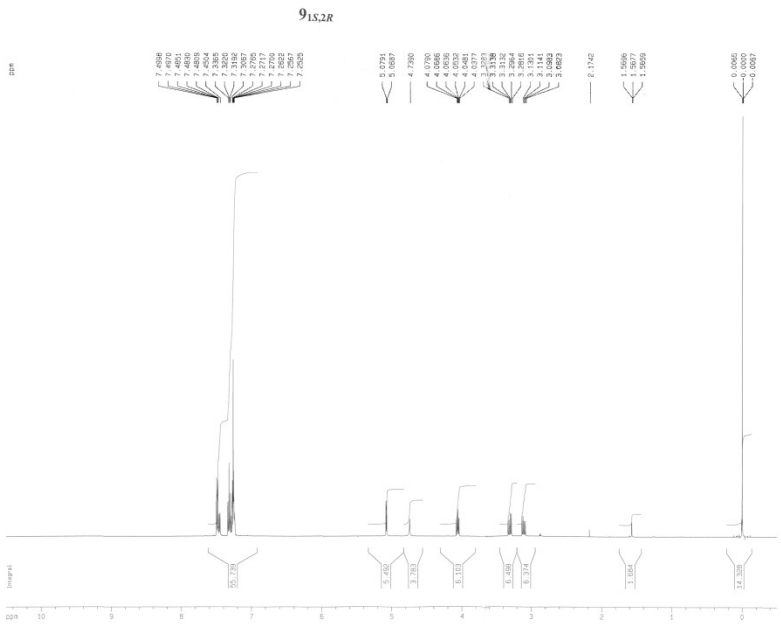
F2 - Acquisition Parameters
Date_ 20020319
Time 17.51
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 4
SWH 7567.567 Hz
FIDRES 0.114005 Hz
AQ 4.3647475 sec
RG 256
DW 66.000 usec
DE 7.11 usec
TE 300.0 K
D1 2.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 30.00 usec
PL1 -3.00 dB
SFO1 500.1327567 MHz

F2 - Processing parameters
SI 32768
SF 500.1300120 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 33.00 cm
CY 18.00 cm
F1P 10.500 ppm
F1 5253.37 Hz
F2P -0.500 ppm
F2 -250.07 Hz
PPMCM 0.31333 ppm/cm
HZCM 156.71001 Hz/cm

9*1S,2R*



Current Data Parameters
NAME DMMA2C
EXPNO 10
PROCNO 1

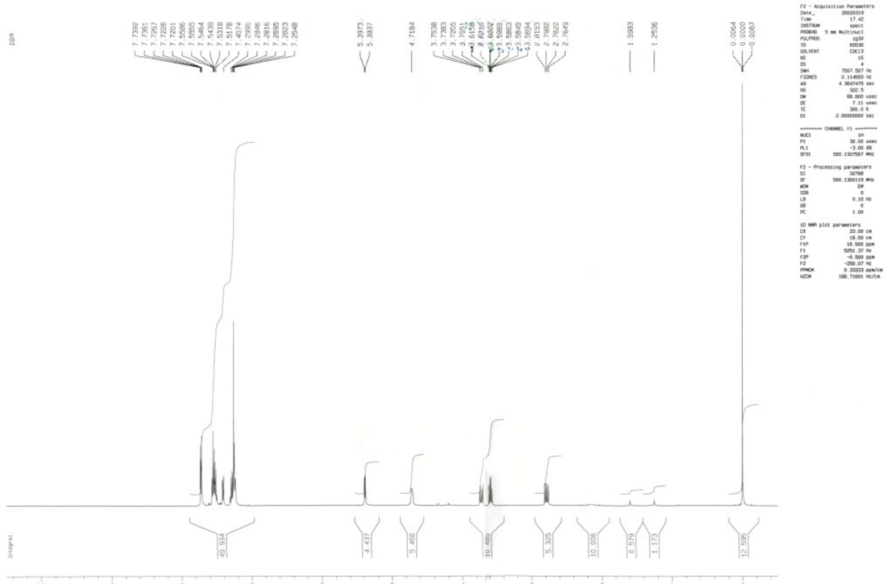
F2 - Acquisition Parameters
Date_ 20020301
Time 15.32
INSTRUM spect
PROBHD 5 mm Dual 1H/1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 4
SWH 7507.507 Hz
FIDRES 0.114555 Hz
AQ 4.3647475 sec
RG 362
DW 66.560 usec
DE 7.15 usec
TE 300.0 K
D1 2.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -3.00 dB
SFO1 500.1327507 MHz

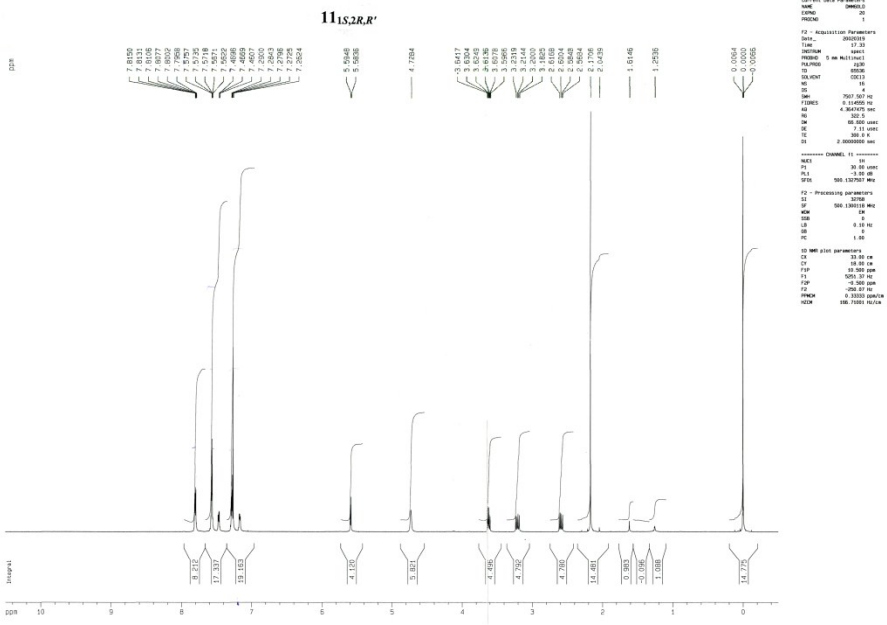
F2 - Processing parameters
SI 32768
SF 500.1300119 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 33.00 cm
CY 16.00 cm
F1P 10.500 ppm
F1 5251.37 Hz
F2P -0.500 ppm
F2 -250.07 Hz
PPMCM 0.31933 ppm/cm
HZCM 159.71901 Hz/cm

10$_{1S,2R,S}$



11$_{1S,2R,R'}$



Current Data Parameters
NAME DMMOLD
EXPNO 20
PROCNO 1

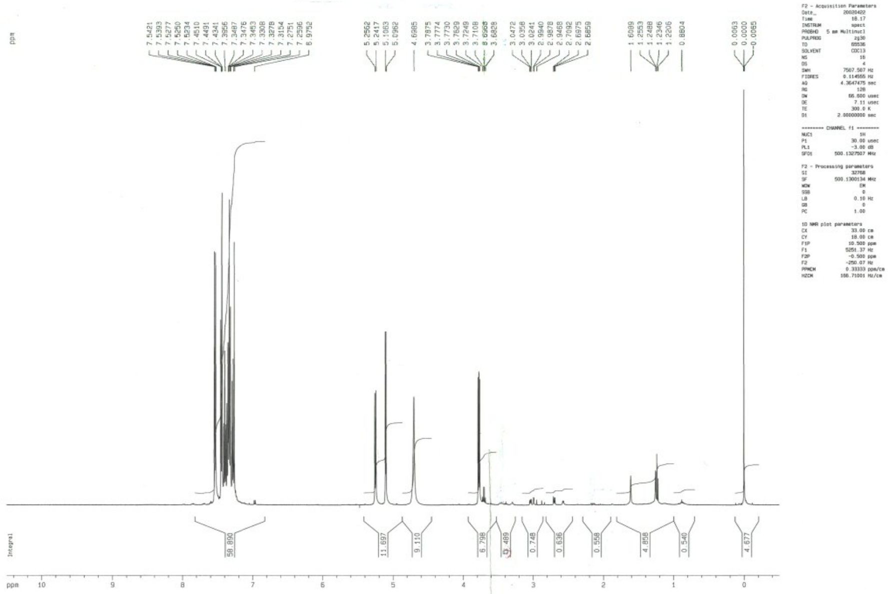
F2 - Acquisition Parameters
Date_ 20220315
Time 17.33
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 4
SWH 7507.507 Hz
FIDRES 0.114555 Hz
AQ 4.3647475 sec
RG 203
DW 66.500 usec
DE 7.11 usec
TE 300.0 K
D1 2.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 30.00 usec
PL1 -1.00 dB
SFO1 500.1327587 MHz

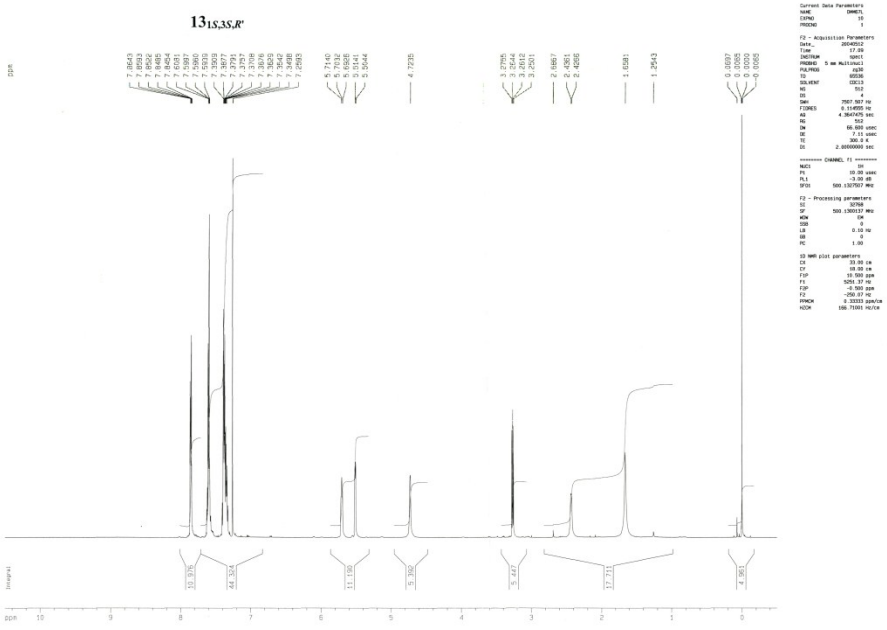
F2 - Processing parameters
SI 32768
SF 500.1300118 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 33.00 cm
CY 19.00 cm
F1P 10.000 ppm
F1 5255.37 Hz
F2P -0.500 ppm
F2 -250.07 Hz
PPMCM 0.33333 ppm/cm
HZCM 166.71003 Hz/cm

$\mathbf{12}_{1S,3S}$



13$_{1S,3S,R'}$



Current Data Parameters
NAME DMMEZL
EXPNO 10
PROCNO 1

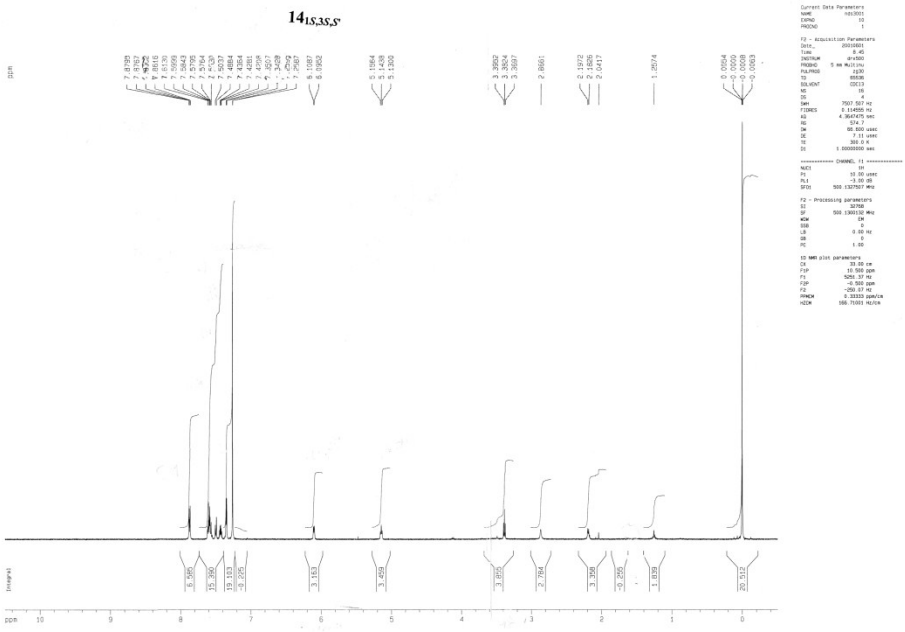
F2 - Acquisition Parameters
Date_ 20140512
Time 17.09
INSTRUM
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 7567.567 Hz
FIDRES 0.114955 Hz
AQ 4.3647475 sec
RG 512
DW 66.000 usec
DE 6.50 usec
TE 300.1 K
D1 2.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -3.00 dB
SFO1 500.1327007 MHz

F2 - Processing parameters
SI 32768
SF 500.1300137 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 33.00 cm
CY 18.00 cm
F1P 10.500 ppm
F1 5251.37 Hz
F2P -0.500 ppm
F2 -250.07 Hz
PPMCM 0.33337 ppm/cm
HZCM 166.71001 Hz/cm

$14_{1S,3S,5S}$



Current Data Parameters
NAME nmr3001
EXPNO 10
PROCNO 1

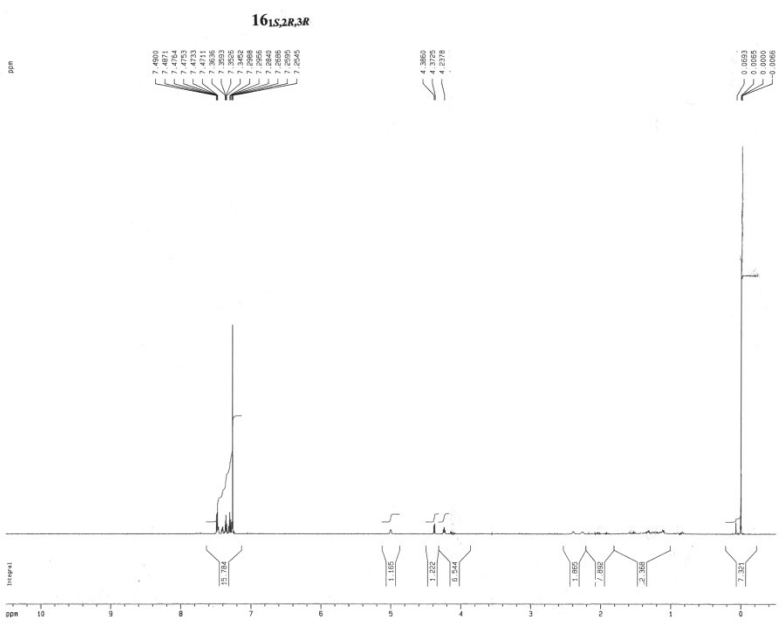
F2 - Acquisition Parameters
Date_ 20210601
Time 8.45
INSTRUM av500
PROBHD 5 mm Multinu
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 4
SWH 7507.507 Hz
FIDRES 0.114555 Hz
AQ 4.3647475 sec
RG 203
DW 66.600 usec
DE 7.11 usec
TE 300.0 K
D1 1.00000000 sec

========== CHANNEL f1 ==========
NUC1 1H
P1 10.00 usec
PL1 -3.00 dB
SFO1 500.1327557 MHz

F2 - Processing parameters
SI 32768
SF 500.1300132 MHz
WDW EM
SSB 0
LB 0.60 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 10.500 ppm
F1 5250.97 Hz
F2P -0.500 ppm
F2 -250.07 Hz
PPMCM 0.33333 ppm/cm
HZCM 166.71691 Hz/cm

16*1S,2R,3R*



Current Data Parameters
NAME DAN03.DF
EXPNO 10
PROCNO 1

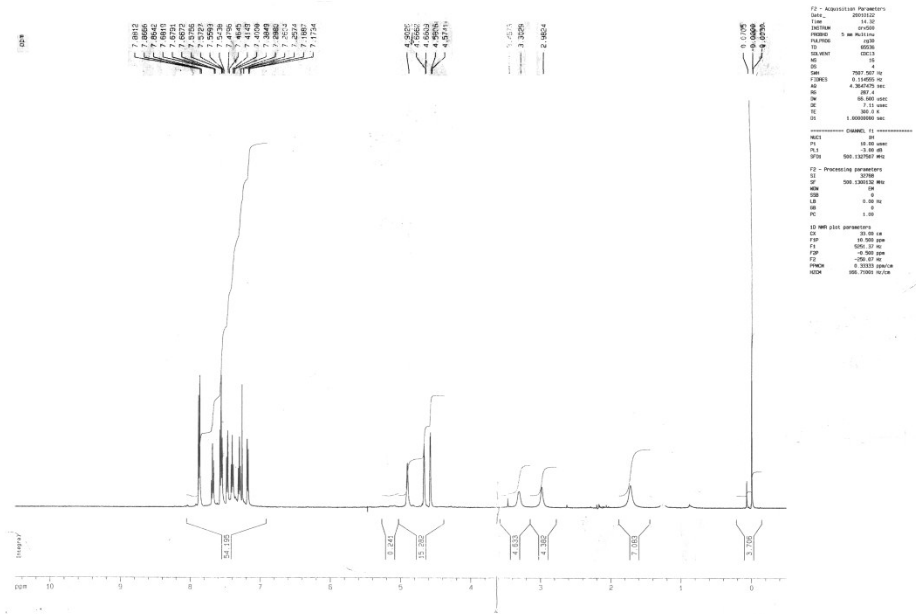
F2 - Acquisition Parameters
Date_ 20010930
Time 10.14
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 4
SWH 7507.507 Hz
FIDRES 0.114555 Hz
AQ 4.3647475 sec
RG 512
DW 66.600 usec
DE 6.11 usec
TE 300.0 K
D1 2.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -3.00 dB
SFO1 500.1327507 MHz

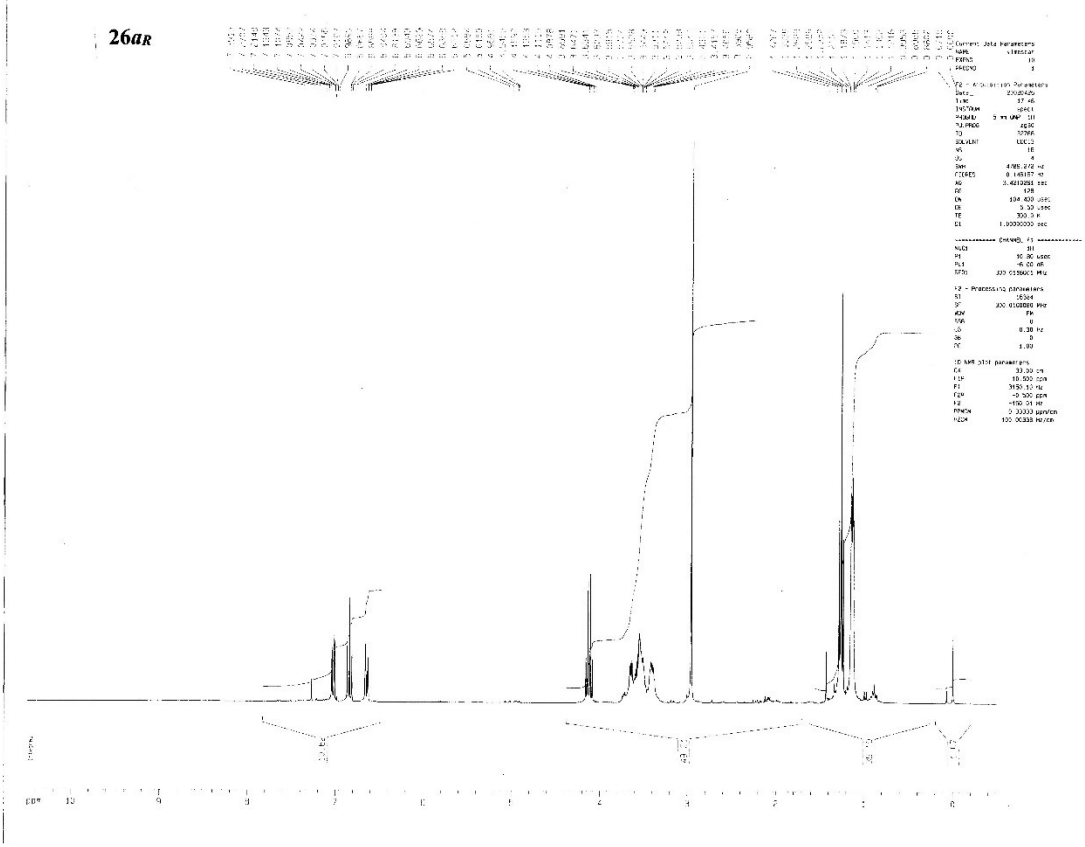
F2 - Processing parameters
SI 32768
SF 500.1300120 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

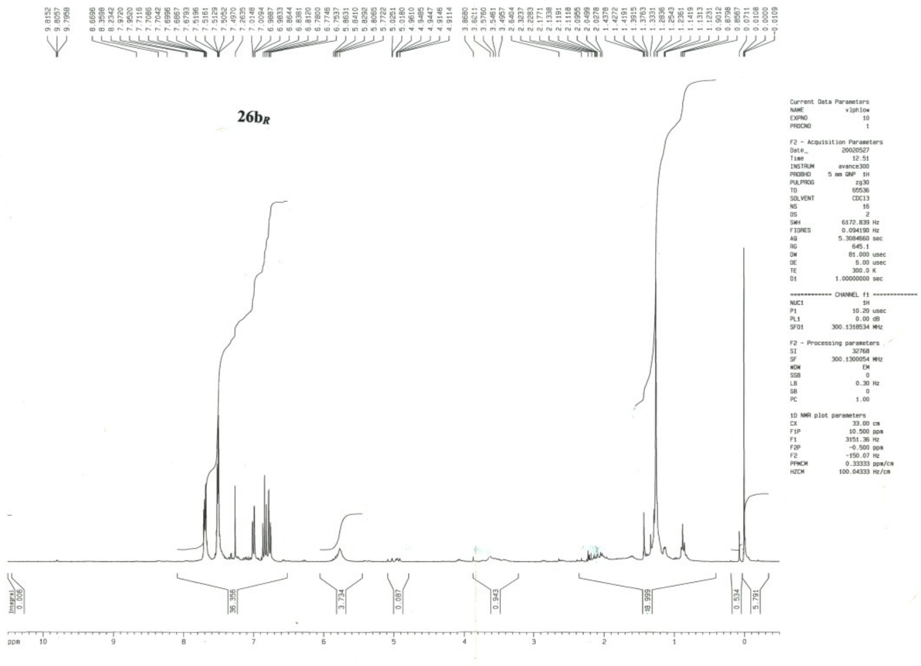
1D NMR plot parameters
CX 33.00 cm
CY 18.00 cm
F1P 10.500 ppm
F1 5254.37 Hz
F2P -0.500 ppm
F2 -250.07 Hz
PPMCM 0.33333 ppm/cm
HZCM 166.71601 Hz/cm

$17_{1S,2R,3R,R'}$

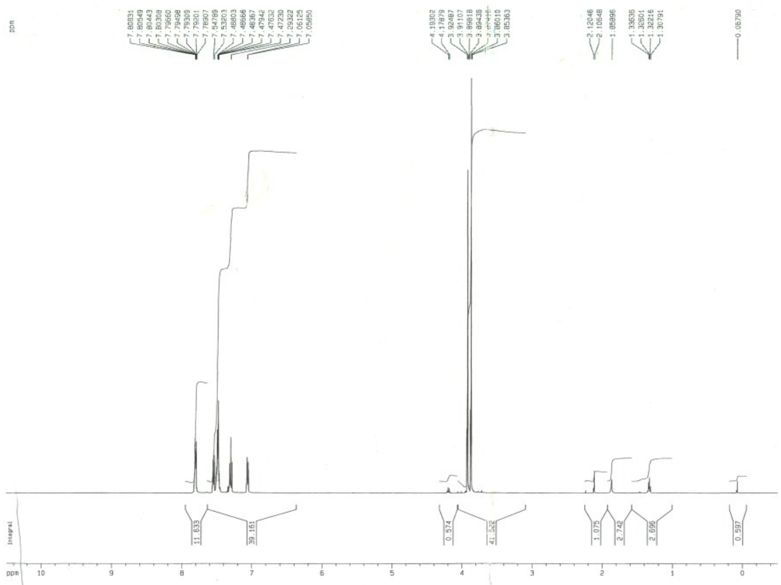

Current Data Parameters
NAME ndsohbyosph
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20010122
Time 14.32
INSTRUM drx500
PROBHD 5 mm Multinu
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 4
SWH 7507.507 Hz
FIDRES 0.114555 Hz
AQ 4.3647475 sec
RG 287.4
DW 66.600 usec
DE 7.11 usec
TE 300.0 K
D1 1.00000000 sec
============ CHANNEL f1 ============
NUC1 1H
P1 10.00 usec
PL1 -3.00 dB
SFO1 500.1327507 MHz
F2 - Processing parameters
SI 32768
SF 500.1300132 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 33.00 cm
F1P 10.500 ppm
F1 5251.37 Hz
F2P -0.500 ppm
F2 -250.07 Hz
PPMCM 0.33333 ppm/cm
HZCM 166.71001 Hz/cm
54.195
0.241
15.282
4.633
4.382
7.083
3.706
ppm 10 9 8 7 6 5 4 3 2 1 0

26a$_R$




26b$_R$
Current Data Parameters
NAME vlphlow
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20020527
Time 12.51
INSTRUM avance300
PROBHD 5 mm QNP 1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 645.1
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
============ CHANNEL f1 ============
NUC1 1H
P1 10.20 usec
PL1 0.00 dB
SFO1 300.1318534 MHz
F2 - Processing parameters
SI 32768
SF 300.1300054 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 33.00 cm
F1P 10.500 ppm
F1 3151.36 Hz
F2P -0.500 ppm
F2 -150.07 Hz
PPMCM 0.33333 ppm/cm
HZCM 100.04333 Hz/cm
ppm

27b$_R$

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Current Data Parameters
NAME          vlphminor
EXPNO                30   -> rs-30
PROCNO                1

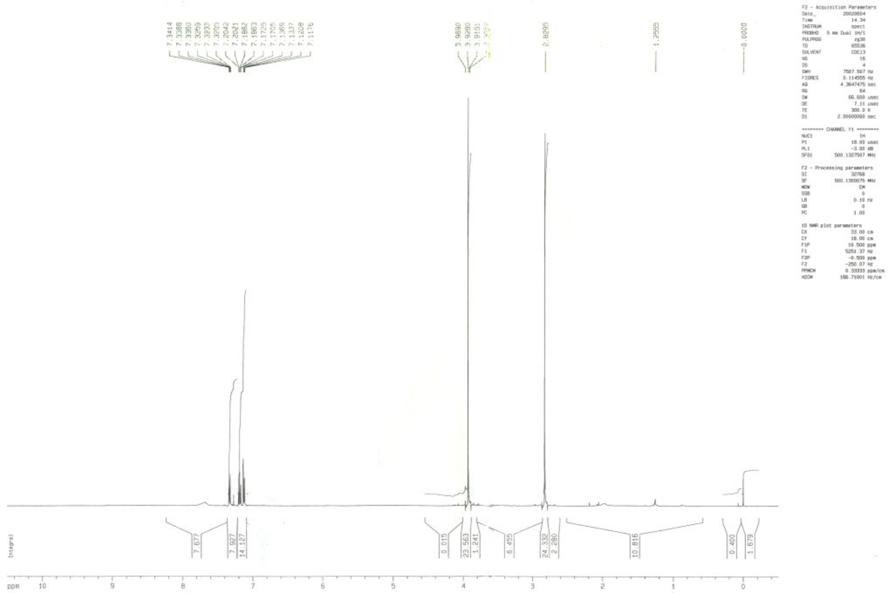
F2 - Acquisition Parameters
Date_          20020730
Time              13.48
INSTRUM           spect
PROBHD   5 mm Multinucl
PULPROG            zg30
TD                65536
SOLVENT            DMSO
NS                   16
DS                    4
SWH            7507.507 Hz
FIDRES         0.114555 Hz
AQ            4.3647475 sec
RG                 50.8
DW               66.600 usec
DE                 7.11 usec
TE                300.0 K
D1           2.00000000 sec

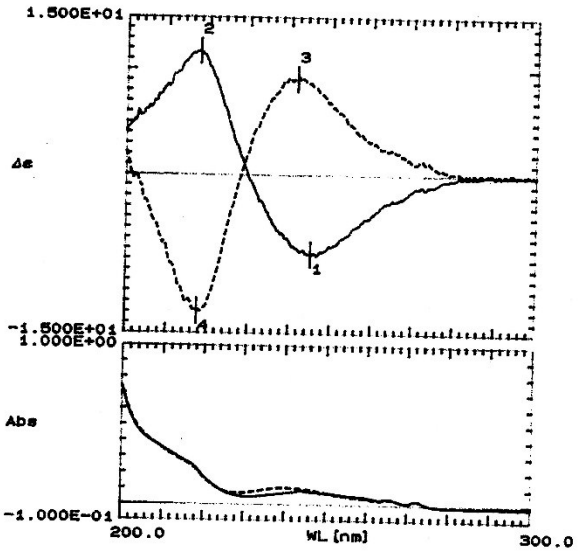
======== CHANNEL f1 ========
NUC1                 1H
P1                30.00 usec
PL1               -3.00 dB
SFO1        500.1327507 MHz

F2 - Processing parameters
SI                32768
SF          500.1299743 MHz
WDW                  EM
SSB                   0
LB                 0.10 Hz
GB                    0
PC                 1.00

1D NMR plot parameters
CX                33.00 cm
CY                18.00 cm
F1P              10.500 ppm
F1              5251.36 Hz
F2P              -0.500 ppm
F2              -250.06 Hz
PPMCM           0.33333 ppm/cm
HZCM          166.70999 Hz/cm
```

$29a_R$

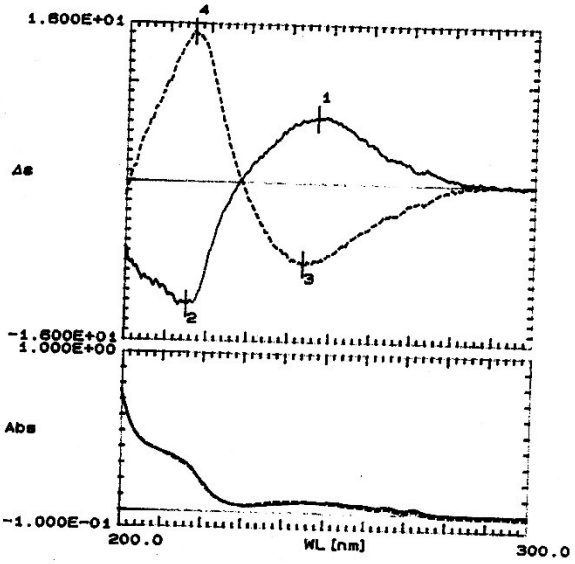




No.	Wavelength	Value
1	245.20 nm	-7.508E+00
2	217.80 nm	1.174E+01
3	241.60 nm	9.145E+00
4	217.60 nm	-1.291E+01

$8_{1S,2S,S'}$

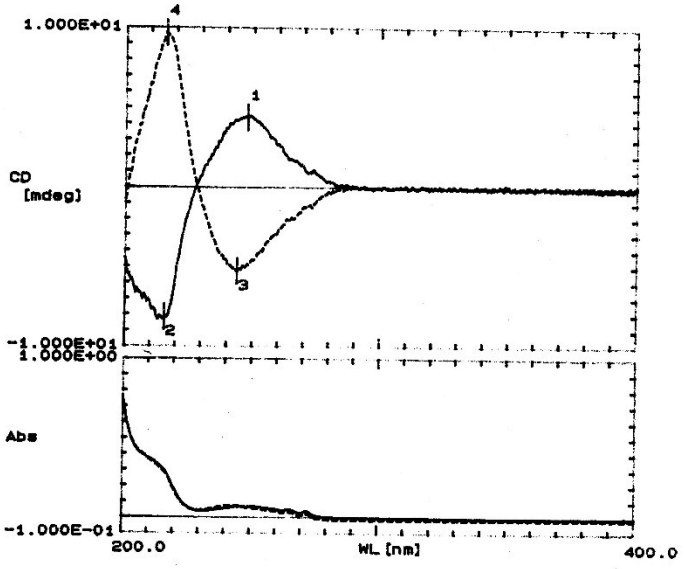
$7_{1S,2S,R'}$



No.	Wavelength	Value
1	246.60 nm	6.532E+00
2	215.20 nm	-1.235E+01
3	243.60 nm	-8.154E+00
4	216.20 nm	1.518E+01

$11_{1S,2R,R'}$

$10_{1S,2R,S'}$

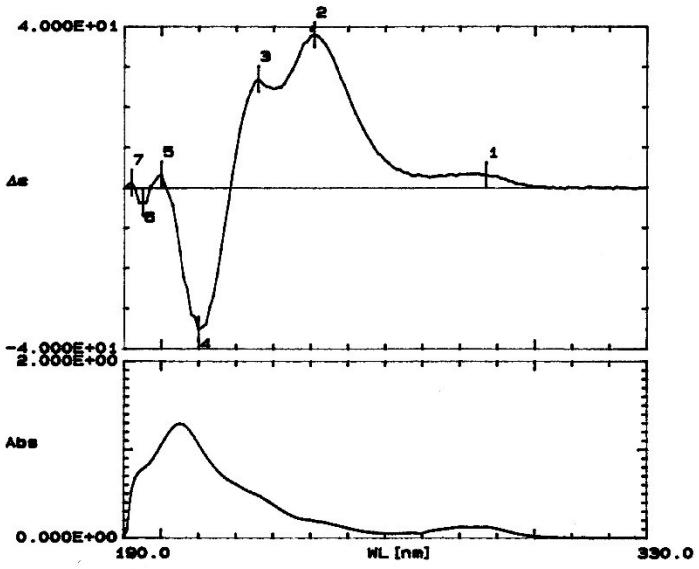


No.	Wavelength	Value
1	247.80 nm	4.402E+00
2	215.80 nm	-8.156E+00
3	244.00 nm	-5.284E+00
4	216.00 nm	9.671E+00

$13_{1S,3S,R}$

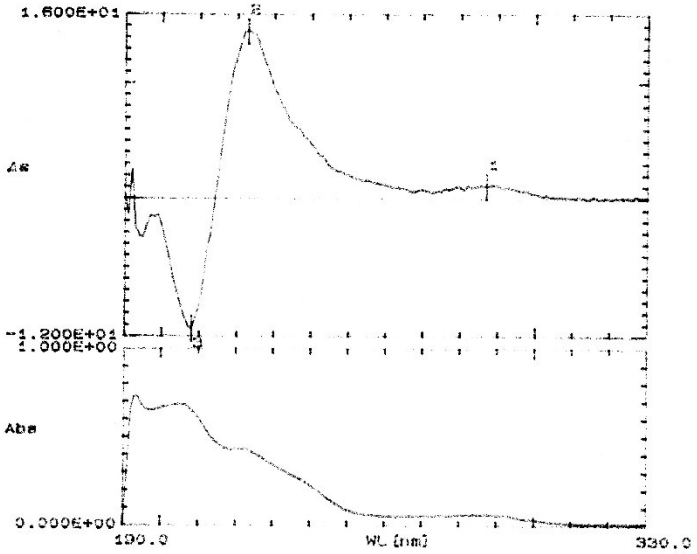
$14_{1S,3S,S}$

27a$_R$.



No.	Wavelength	Value
1	287.00 nm	3.152E+00
2	241.00 nm	3.808E+01
3	226.00 nm	2.711E+01
4	210.00 nm	-3.514E+01
5	200.00 nm	3.305E+00
6	195.00 nm	-3.717E+00
7	192.00 nm	1.308E+00

27b*R*



No.	Wavelength	Value
1	287.00 nm	1.0220E+00
2	223.00 nm	1.4628E+01
3	308.00 nm	-1.1356E+01