Electronic supplementary information (ESI)

Synthesis of *β-C*-Galactosyl D- and L-Alanines

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(Dedicated to Prof. M. S. Wadia on the occasion of his 75th birthday)

NAME   SSK-8-NT-07-1H
EXPNO   4
PROCNO   1
Date_   20111221
Time_   9.07
INSTRUM   spect
PROBHD   5 mm PABBO BB-
PULPROG   zgpg30
TD   65536
SOLVENT   CDCl3
NS   58
DS   4
SWH   24038.461 Hz
FIDRES   0.366798 Hz
AQ   1.3631988 sec
RG   2050
DW   20.800 usec
DE   6.50 usec
TE   295.5 K
D1   2.00000000 sec
D11   0.03000000 sec
TD0   1

======== CHANNEL f1 ========
NUC1   13C
P1   8.75 usec
PL1   -2.00 dB
PL1W   56.53121948 W
SFO1   100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2   waltz16
NUC2   1H
PCPD2   80.00 usec
PL2   -1.00 dB
PL12   14.50 dB
PL13   14.50 dB
PL2W   10.56200695 W
PL12W   0.29767781 W
PL13W   0.29767781 W
SFO2   400.1316005 MHz
SI   32768
SF   100.6127690 MHz
WDW   EM
SSB   0
LB   1.00 Hz
GB   0
PC   1.40

138.92
138.57
138.47
138.14
135.33
128.54
128.51
128.32
128.22
128.18
128.02
127.84
127.80
127.74
127.65
116.76

84.98
79.46
78.68
77.52
77.22
76.89
75.45
74.53
73.83
73.61
72.28
69.12

36.30

0.15

6

BnO⟍OBn
BnO
BnO
BnO

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

SSK-8-NT-36-C-13C

^{13}C NMR spectrum with peaks labeled: 138.64, 138.34, 138.25, 137.83, 135.70, 135.68, 133.59, 133.54, 129.76, 128.58, 128.56, 128.50, 128.38, 128.30, 128.22, 128.08, 127.94, 127.82, 127.79, 127.69, 84.55, 80.00, 78.93, 77.52, 77.40, 77.20, 76.88, 75.69, 74.62, 73.66, 72.43, 71.94, 69.02, 67.66, 35.24, 26.99, 19.34, 0.15

Structure label: 7 (BnO, BnO, BnO, O, OBn, OH, OTBDPS)

NAME   SSK-8-NT-19B-1H
EXPNO   5
PROCNO   1
Date_   20120119
Time   11.02
INSTRUM   spect
PROBHD   5 mm PABBO BB-
PULPROG   zg30
TD   65536
SOLVENT   CDCl3
NS   15
DS   0
SWH   9615.385 Hz
FIDRES   0.146719 Hz
AQ   3.4079220 sec
RG   32
DW   52.000 usec
DE   6.50 usec
TE   292.5 K
D1   1.00000000 sec
TD0   1

======== CHANNEL f1 ========
NUC1   1H
P1   13.50 usec
PL1   -1.00 dB
PL1W   10.5620695 W
SFO1   400.1324710 MHz
SI   32768
SF   400.1300188 MHz
WDW   EM
SSB   0
LB   0.00 Hz
GB   0
PC   1.00

SSK-8-NT-19B-1H

1.00 6.58 0.48 0.26 0.73 0.50 0.48 0.75 1.23 0.20 0.26 0.30 0.44 2.27 0.23 1.96

10 9 8 7 6 5 4 3 2 1 0 ppm

NAME SSX-8-NT-19B1-13C
EXPNO 9
PROCNO 1
Date_ 2011:228
Time 9.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 59
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======= CHANNEL f1 =======
NUC1 13C
P1 8.75 usec
PL1 -2.00 dB
PL1W 56.53121948 W
SFO1 100.6228298 MHz

======= CHANNEL f2 =======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 14.50 dB
PL13 14.50 dB
PL2W 10.56200695 W
PL12W 0.29767781 W
PL13W 0.29767781 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127624 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

138.78
138.44
138.01
135.70
133.36
129.87
128.57
128.45
128.40
128.36
128.16
128.04
127.92
127.87
127.76
127.73
127.69

84.87
78.78
77.52
77.40
77.20
77.04
76.86
76.81
75.47
74.62
73.58
72.35
68.88
68.82
68.18

35.11

26.99

19.37

0.17

8

S8

NAME   SSK-8-NT-34-C13
EXPNO   3
PROCNO   1
Date_   20110610
Time_   8.21
INSTRUM   spect
PROBHD   5 mm PABBO BB-
PULPROG   zgpg30
TD   65536
SOLVENT   CDC13
NS   620
DS   4
SWH   27173.912 Hz
FIDRES   0.414641 Hz
AQ   1.2059124 sec
RG   1030
DW   18.400 usec
DE   6.50 usec
TE   296.4 K
D1   1.00000000 sec
D11   0.03000000 sec
TD0   1

======== CHANNEL f1 ========
NUC1   13C
P1   8.75 usec
PL1   -2.00 dB
PL1W   56.53121948 W
SFO1   100.6233364 MHz

======== CHANNEL f2 ========
CPDPRG2   waltz16
NUC2   1H
PCPD2   80.00 usec
PL2   -1.00 dB
PL12   14.50 dB
PL13   14.50 dB
PL2W   10.56200695 W
PL12W   0.29767781 W
PL13W   0.29767781 W
SFO2   400.1316005 MHz
SI   32768
SF   100.6127567 MHz
WDW   EM
SSB   0
LB   1.00 Hz
GB   0
PC   1.40

138.94
138.74
137.99
135.85
135.73
135.68
133.70
133.56
129.85
129.82
128.58
128.56
128.49
128.34
128.13
127.94
127.86
127.82
127.72
127.55

82.60
80.35
80.29
79.45
78.49
77.51
77.19
76.87
75.45
73.74
72.30
69.23
66.17

30.83
26.97
19.46
0.17

10

BnO
BnO
OBn
OTBDPS

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

S14

SSK-8-NT-34-COSY

^{1}H-^{1}H COSY NMR

10

NAME   SSK-8-NT-92-1H
EXPNO   16
PROCNO   1
Date_   20120127
Time   13.06
INSTRUM   spect
PROBHD   5 mm PABBO BB-
PULPROG   zg30
TD   65536
SOLVENT   CDCl3
NS   10
DS   0
SWH   8223.685 Hz
FIDRES   0.125483 Hz
AQ   3.9846387 sec
RG   32
DW   60.800 usec
DE   6.50 usec
TE   293.6 K
D1   1.00000000 sec
TD0   1

======== CHANNEL f1 ========
NUC1   1H
P1   13.50 usec
PL1   -1.00 dB
PL1W   10.56200695 W
PLIW   400.1324710 MHz
SFO1   400.1324710 MHz
SI   32768
SF   400.1300298 MHz
WDW   EM
SSB   0
LB   0.00 Hz
GB   0
PC   1.00

SSK-8-NT-92-1H

S17

NAME   SSK-8-NT-109-1H
EXPNO   9
PROCNO   1
Date_   20111216
Time   11:29
INSTRUM   spect
PROBHD   5 mm PABBO BB-
PULPROG   zg30
TD   65536
SOLVENT   CDCl3
NS   11
DS   0
SWH   8223.685 Hz
FIDRES   0.125483 Hz
AQ   3.9846387 sec
RG   32
DW   60.800 usec
DE   6.50 usec
TE   294.2 K
D1   1.00000000 sec
TD0   1

======== CHANNEL f1 ========
NUC1   1H
P1   13.50 usec
PL1   -1.00 dB
PL1W   10.55200695 W
SFO1   400.1324710 MHz
SI   32768
SF   400.1300311 MHz
WDW   EM
SSB   0
LB   0.30 Hz
GB   0
PC   1.00

SSK-8-NT-109-1H

14

9.95 0.18 1.00 0.88 1.12 1.00 0.47 3.05 0.98 0.49 0.42 0.53 0.53 0.12 0.32 1.20

ppm 10 9 8 7 6 5 4 3 2 1

S19

SSK-8-NT-109-13C

NAME	SSK-8-NT-109-13C
EXPNO	10
PROCNO	1
Date_	20111216
Time	11.30
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	70
DS	2
SWH	27173.912 Hz
FIDRES	0.414641 Hz
AQ	1.2059124 sec
RG	912
DW	18.400 usec
DE	6.50 usec
TE	294.3 K
D1	1.00000000 sec
D11	0.03000000 sec
TD0	1

======== CHANNEL f1 ========
NUC1	13C
P1	8.75 usec
PL1	-2.00 dB
PL1W	56.53121948 W
SFO1	100.6238364 MHz

======== CHANNEL f2 ========
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-1.00 dB
PL12	14.50 dB
PL13	14.50 dB
PL2W	10.56200695 W
PL12W	0.29767781 W
PL13W	0.29767781 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127642 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

138.57
138.26
138.22
137.85
128.60
128.55
128.45
128.40
128.29
128.07
127.95
127.85
127.73

84.75
78.65
77.52
77.20
77.05
76.88
76.59
75.53
74.72
73.64
73.60
72.44
68.94
65.52
61.30

33.35

1.15
0.14

14

BnO OBn
BnO
BnO
O
N₃
OH

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 ppm

NAME   SSK-8-NT-111-1H
EXPNO   11
PROCNO   1
Date_   20111126
Time   12.04
INSTRUM   spect
PROBHD   5 mm PABBO BB-
PULPROG   zg30
TD   65536
SOLVENT   CDCl3
NS   22
DS   0
SWH   8223.685 Hz
FIDRES   0.125483 Hz
AQ   3.9846387 sec
RG   50.8
DW   60.800 usec
DE   6.50 usec
TE   293.1 K
D1   1.00000000 sec
TD0   1

======== CHANNEL f1 ========
NUC1   1H
P1   13.50 usec
PL1   -1.00 dB
PL1W   10.5620695 W
SFO1   400.1324710 MHz
SI   32768
SF   400.1300197 MHz
WDW   EM
SSB   0
LB   0.30 Hz
GB   0
PC   1.00

SSK-8-NT-111-1H

Integrations (right to left): 20.38, 2.00, 1.08, 3.06, 2.07, 1.02, 0.97, 2.91, 2.28, 2.99, 1.12, 1.06, 1.05, 3.59

SSK-8-NT-123C-1H

NAME	SSK-8-NT-123C-1H
EXPNO	5
PROCNO	1
Date_	20111220
Time	12.56
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65560
SOLVENT	CDCl3
NS	14
DS	0
SWH	10416.667 Hz
FIDRES	0.156500 Hz
AQ	3.1949301 sec
RG	32
DW	48.000 usec
DE	6.50 usec
TE	294.2 K
D1	1.00000000 sec
TD0	1

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

NUC1	1H
P1	13.50 usec
PL1	-1.00 dB
PL1W	10.56200695 W
SFO1	400.1320007 MHz
SI	32768
SF	400.1300207 MHz
WDW	EM
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

16

20.47 0.81 2.00 1.06 3.07 1.91 1.07 0.98 4.16 4.13 1.01 0.93 1.13 9.29 1.03 0.45 1.67 3.54

10 9 8 7 6 5 4 3 2 1 ppm

S23

SSK-8-NT-164-13C

NAME	SSK-8-NT-164-13C
EXPNO	6
PROCNO	1
Date_	20120229
Time	20.25
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1222
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	1030
DW	20.800 usec
DE	6.50 usec
TE	294.3 K
D1	1.00000000 sec
D11	0.03000000 sec
TD0	1

======== CHANNEL f1 ========
NUC1	13C
P1	8.75 usec
PL1	-2.00 dB
PL1W	56.53121948 W
SFO1	100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-1.00 dB
PL12	14.50 dB
PL13	14.50 dB
PL2W	10.56200695 W
PL12W	0.29767781 W
PL13W	0.29767781 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127539 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

174.14

156.23

81.21
80.32
78.72
77.98
77.52
77.40
77.20
76.88
76.32
75.18
71.40
69.79
62.04
61.47
52.67
50.74

29.84
28.51
28.38

0.14

1a

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

NAME   SSK-8-NT-18-1H
EXPNO   7
PROCNO   1
Date_   20111220
Time   11.11
INSTRUM   spect
PROBHD   5 mm PABBO BB-
PULPROG   zg30
TD   65560
SOLVENT   CDCl3
NS   15
DS   0
SWH   10416.667 Hz
FIDRES   0.156500 Hz
AQ   3.1449301 sec
RG   32
DW   48.000 usec
DE   6.50 usec
TE   294.6 K
D1   1.00000000 sec
TD0   1

======= CHANNEL f1 =======
NUC1   1H
P1   13.50 usec
PL1   1.00 dB
PL1W   10.56220695 W
SFO1   400.1320007 MHz
SI   32768
SF   400.1300283 MHz
WDW   EM
SSB   0
LB   0.00 Hz
GB   0
PC   1.00

SSK-8-NT-118-1H

SSK-8-NT-187A-1H

NAME   SSK-8-NT-187A-1H
EXPNO   1
PROCNO   5
Date_   20122418
Time_   21.51
INSTRUM   spect
PROBHD 5 mm PABBO BB-
PULPROG   zg30
TD   65536
SOLVENT   CDC13
NS   35
DS   0
SWH   8223.685 Hz
FIDRES   0.125483 Hz
AQ   3.9846387 sec
RG   71.8
DW   60.800 usec
DE   6.50 usec
TE   293.4 K
D1   1.00000000 sec
TD0   1

======== CHANNEL f1 ========
NUC1   1H
P1   13.50 usec
PL1   -1.00 dB
PL1W   10.56200695 W
SFO1   400.1324710 MHz
SI   32768
SF   400.1299993 MHz
WDW   EM
SSB   0
LB   0.30 Hz
GB   0
PC   1.00

S39

SSK-8-NT-187A-C13