

Supporting information for

Introduction of C-alkyl branches to L-iminosugars changes their active site binding orientation

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Figure S1 docking score top 10 poses generated by the docking analyses.

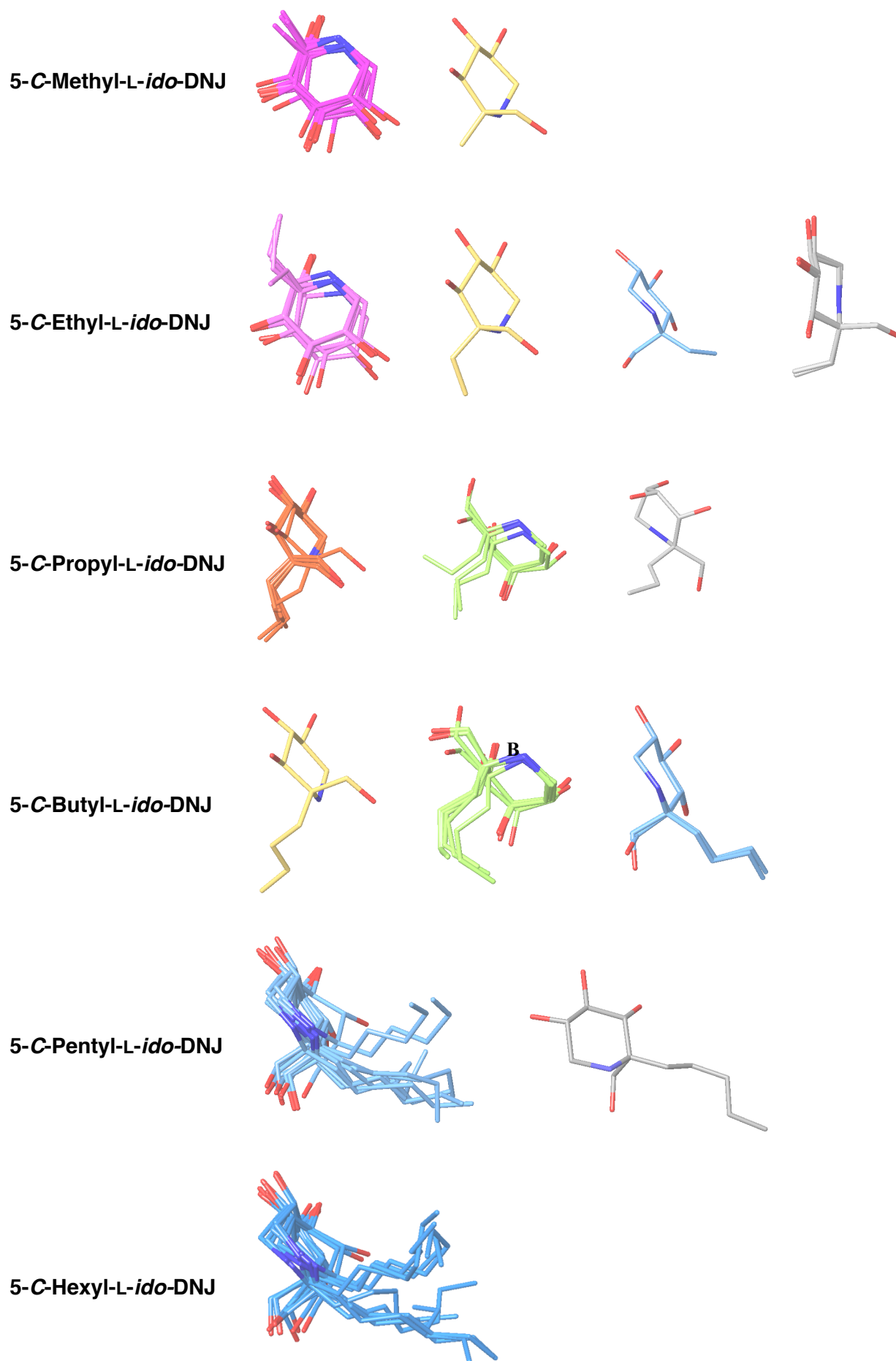
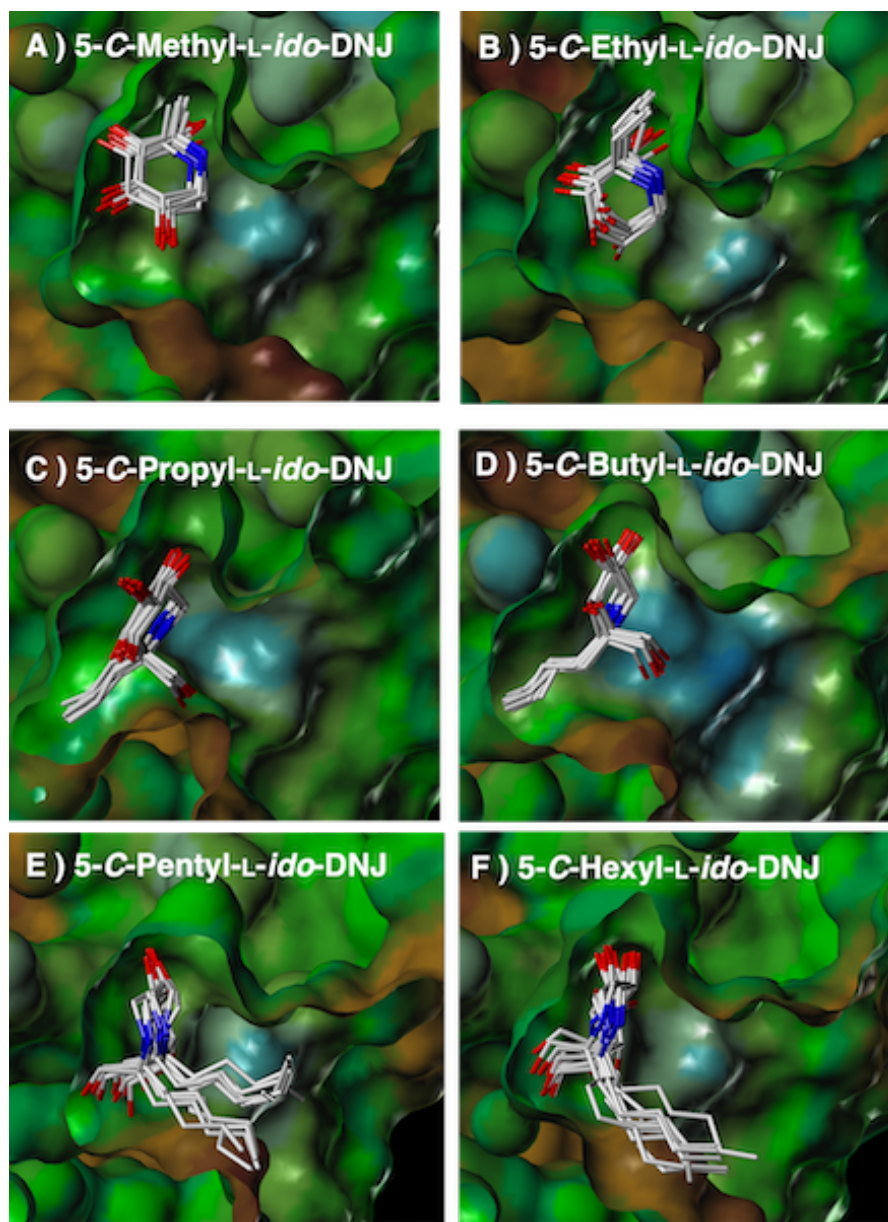


Figure S2 The binding poses of 5-C-alkyl-L-ido-DNJ's extracted from the MD trajectory.

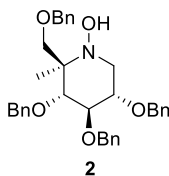


The molecular surfaces of GAA are rendered by lipophilic potential.

The 10 binding poses sampled from the MD trajectory are shown.

Compound 2

768a

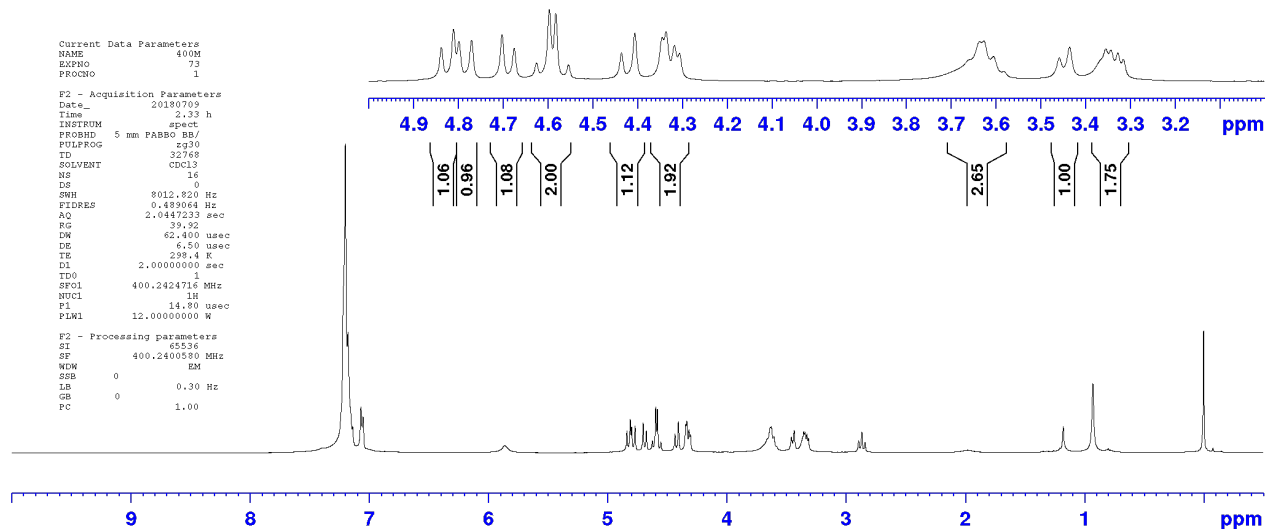
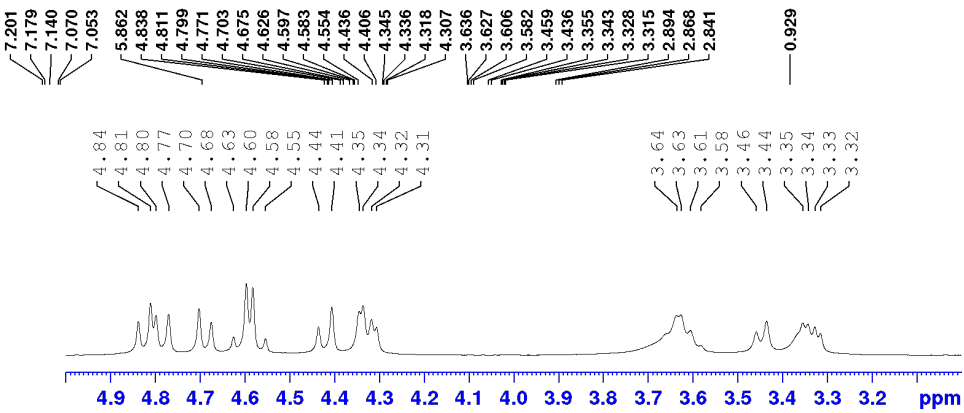


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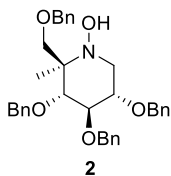
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PROCNO   1

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PULPROG  zg30
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SOLVENT  CDCl3
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DE       6.50 usec
TE       298.4 K
DL       2.00000000 sec
TDO      1
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PLM1     12.00000000 W

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768a

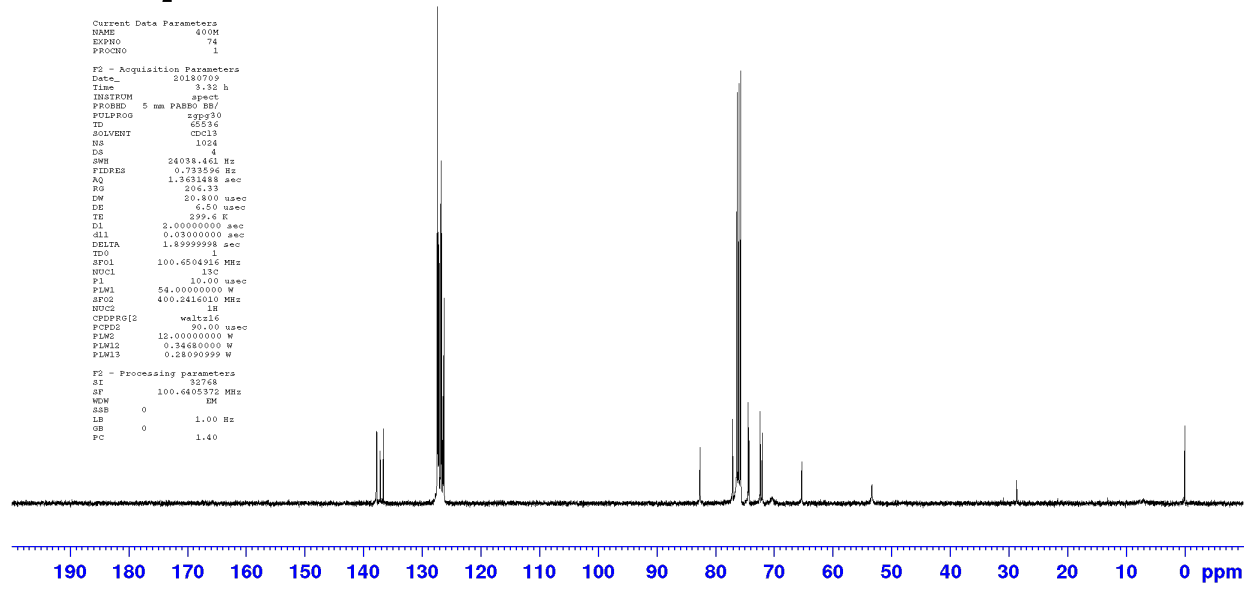
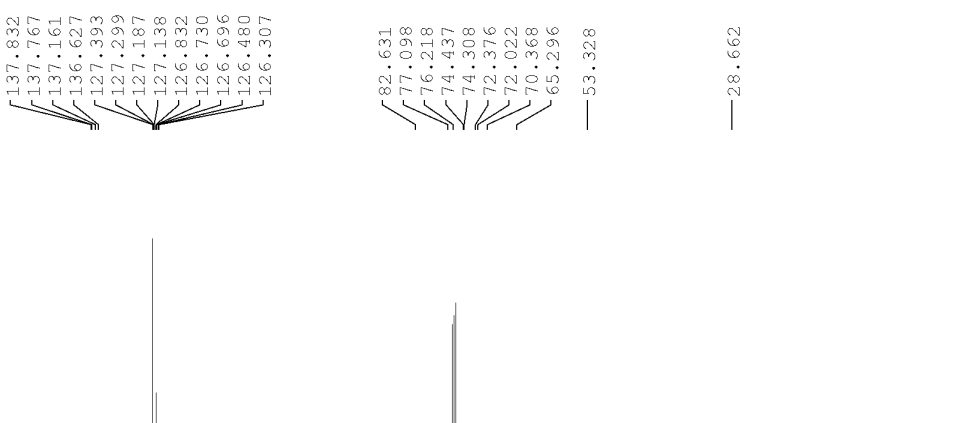


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EXPNO    74
PROCNO   1

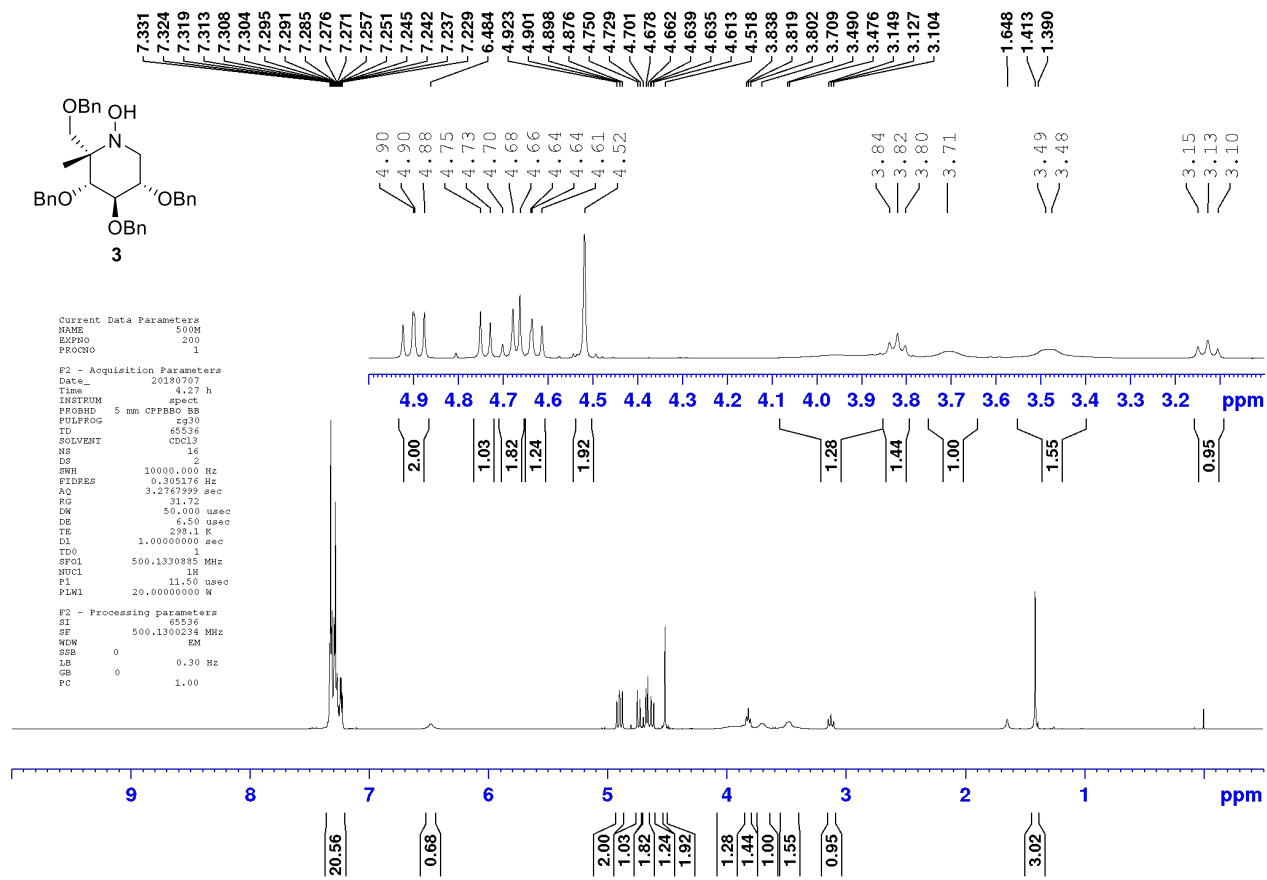
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PULPROG  zg30
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FIDRES   0.733594 Hz
AQ       1.363448 sec
RG       206.233
DM       20.800 usec
DE       6.50 usec
TE       299.6 K
DL       2.00000000 sec
SLL      0.03000000 sec
DELTA    4.89999998 sec
TDO      1
SFO1     100.6254916 MHz
NUC1     13C
P1       10.00 usec
PLM1     54.00000000 W
SFO2     400.2416010 MHz
NUC2     1H
CPDPRG2  waltz16
PCPDW    90.00 usec
PLM2     12.00000000 W
PLM3     0.34800000 W
PLM13    0.28090999 W

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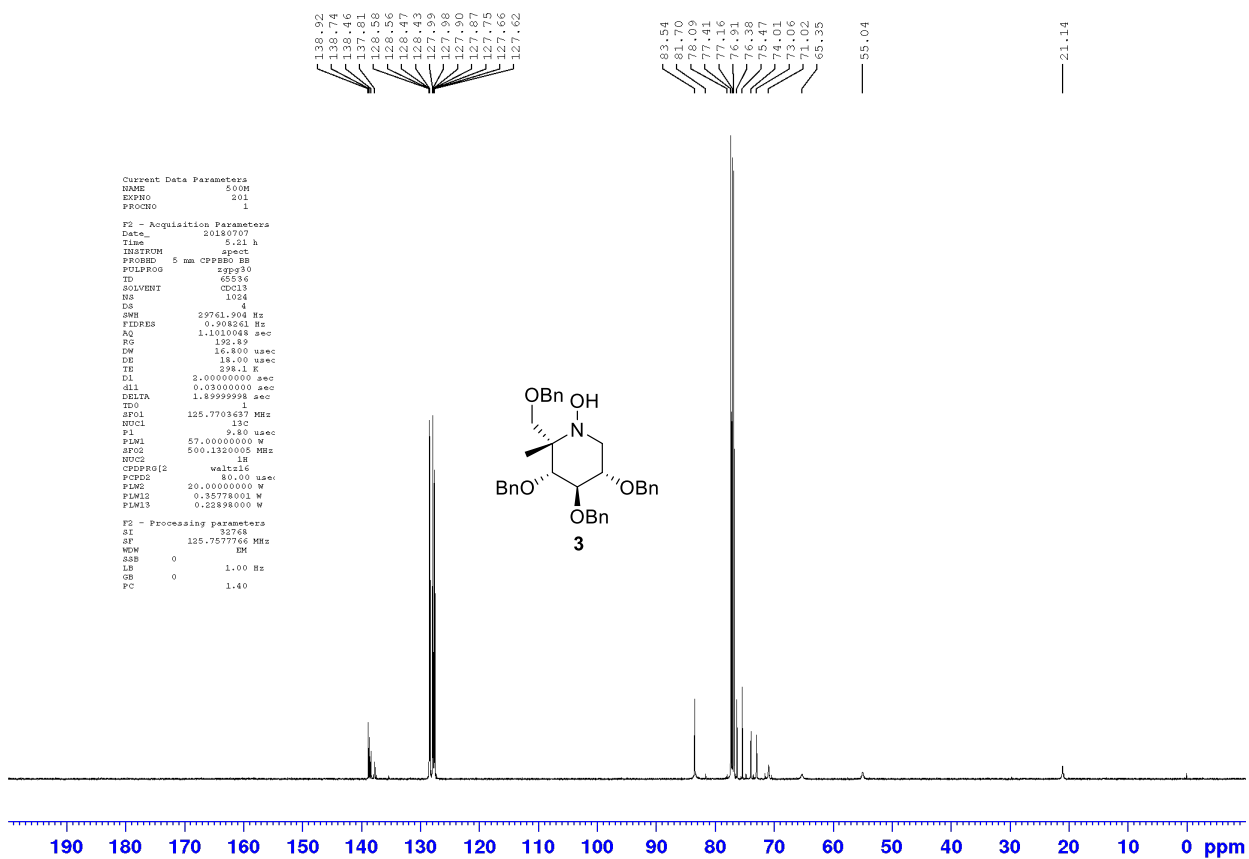


Compound 3

768b

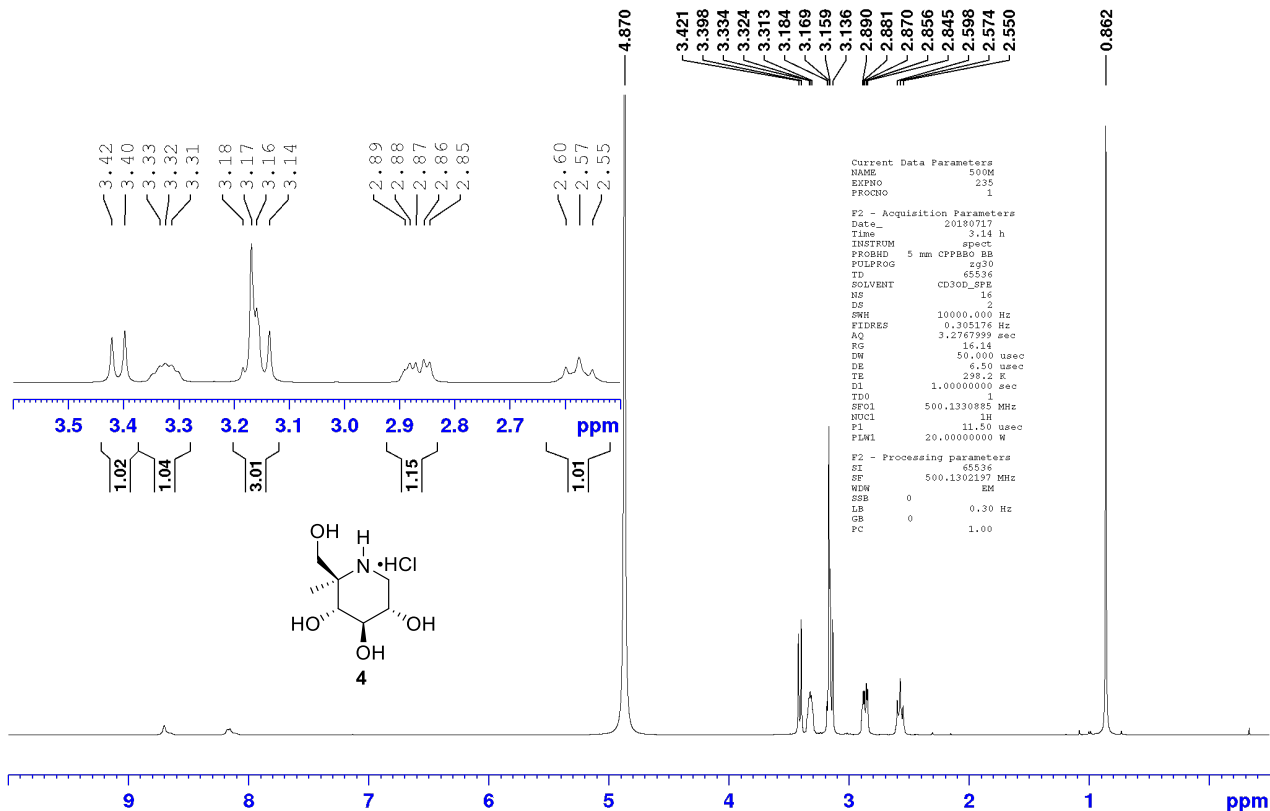


768b

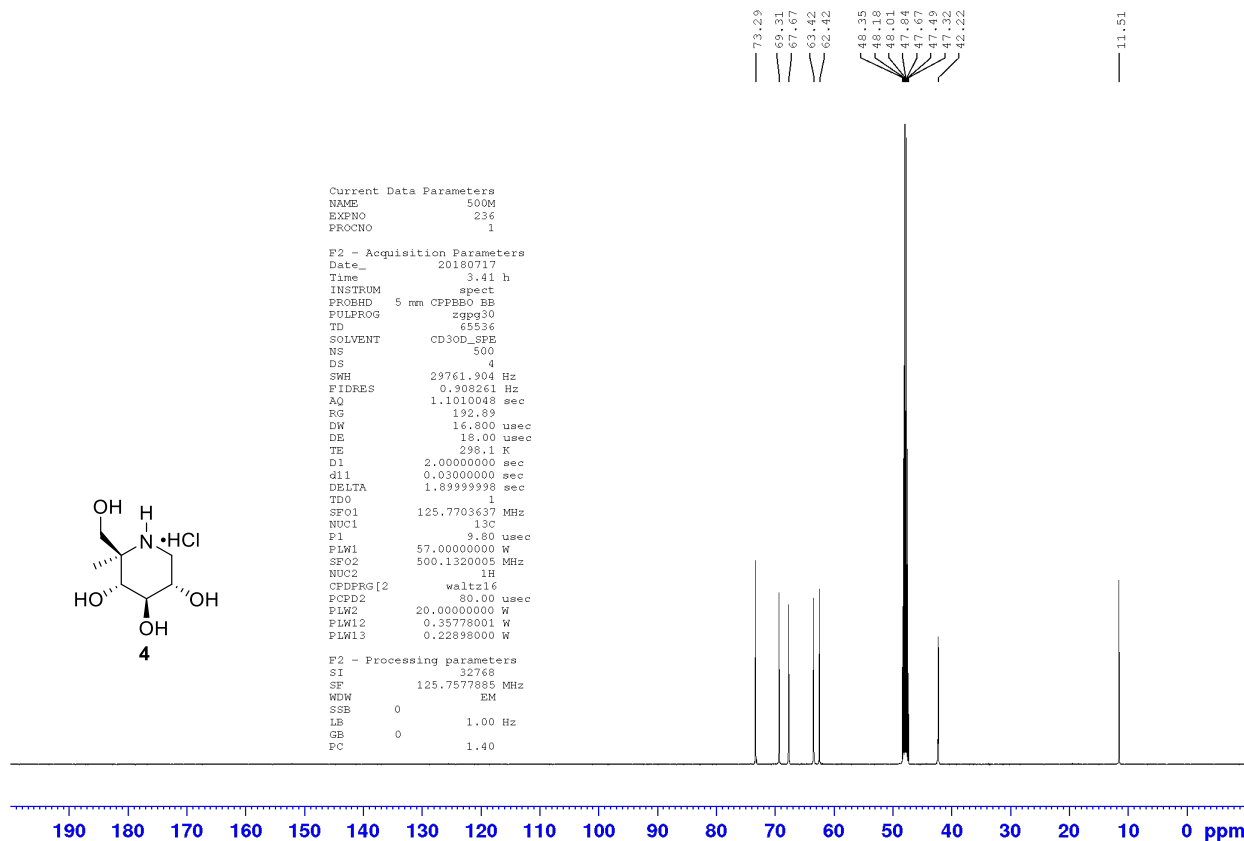


Compound 4

778

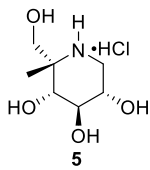


778



Compound 5

779

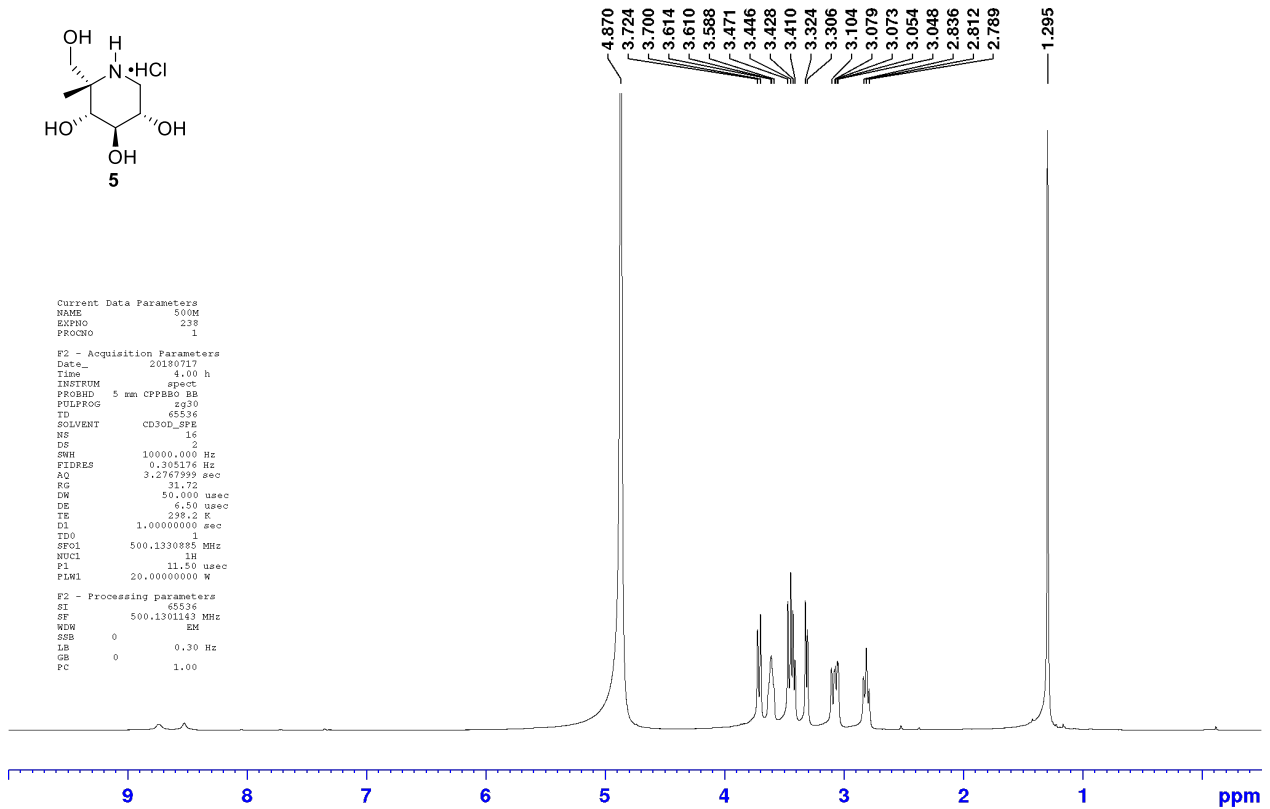


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Current Data Parameters
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EXPNO         239
PROCNO        1

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PULPROG       zgpg30
TD            65536
SOLVENT       CD3OD_SFE
NS            16
DS            4
SWH           10000.000 Hz
FIDRES        0.305176 Hz
AQ            3.2767999 sec
RG            31.72
DW            50.000 usec
DE            6.50 usec
TE            298.2 K
D1            1.00000000 sec
TDO           1
SFO1          500.1330885 MHz
NUC1          1H
P1            11.50 usec
PLW1          20.00000000 W

F2 - Processing parameters
SI            65536
SF            500.1301143 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
    
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779

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Current Data Parameters
NAME          500M
EXPNO         239
PROCNO        1

F2 - Acquisition Parameters
Date_         20180717
Time          4.27 h
INSTRUM       spect
PROBHD        5 mm CPPBBO BB
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TD            65536
SOLVENT       CD3OD_SFE
NS            500
DS            4
SWH           29761.904 Hz
FIDRES        0.908261 Hz
AQ            1.1010048 sec
RG            192.89
DW            16.800 usec
DE            18.00 usec
TE            298.1 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TDO           1
SFO1          125.7703637 MHz
NUC1          13C
P1            9.80 usec
PLW1          57.00000000 W
SFO2          500.1320005 MHz
NUC2          1H
CPDPRG[2]    waltz16
PCPD2         80.00 usec
PLW2          20.00000000 W
PLW12         0.35778001 W
PLW13         0.22898000 W

F2 - Processing parameters
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LB            1.00 Hz
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