Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Molecular dynamics studies of native and substituted cyclodextrins in different media:

1. Charge derivation and force field performances

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SUPPLEMENTARY INFORMATION

CHARGE DERIVATION AND FORCE FIELD TOPOLOGY DATABASE

The molecular orientation of the optimized geometries was controlled before MEP calculation using the rigid-body reorientation algorithm (RBRA) implemented in the R.E.D. program. Charge derivation for these fragments was carried out in a single R.E.D. job following a highly consistent procedure summarized on Fig. 2 corresponding to a 34 "structure" (orientations and conformations) RESP fit. Eight molecules, namely methyl *α-D*-glucopyranoside, *β-N*-acetamido-*D*-mannoside, methyl *α-D*-mannoside, dimethyl ether, methyl acetate, benzyl methyl ether, methyl benzoate and *N*,*N'*-dimethylsuccinamide were considered. Two conformations were selected and optimized for monosaccharide-derived units since *D*-glucose and *D*-mannose derivatives show two main populations in solution relative to a *gg*/*gt* isomerism. Four molecular orientations based on the (C_1 C_3 C_5) and (C_2 C_4 O_5) sets of three atoms were considered in MEP computation. For each of the protective groups/ligands, a unique conformation corresponding to the lowest minimum obtained after geometry optimization was taken into account. Two orientations based on the connected C_{H3}-O-C atoms for the organic protective groups and based on the (C_1 C_2 C_3) atoms for *N*,*N'*-dimethylsuccinamide were considered.[1] No weighting factor to bias a conformation over another was applied during the charge derivation procedure. Inter- and intra-molecular charge constraints were used during the fitting step to rigorously define required molecular fragments. Inter-molecular charge constraints were set to a target value of zero between (i) the 2-hydroxyl, 3-hydroxyl and 6-hydroxyl groups of the methyl α-*D*-glucopyranoside and the methoxy group belonging to the different protective groups and (ii) the 3-hydroxyl, 4-hydroxyl and 6-hydroxyl groups of the β-*N*-acetamido-*D*-mannoside and the methyl group of α-*D*-mannoside. Intra-molecular charge constraints between the 4-hydroxyl and the methyl group of the methyl α-*D*-glucopyranoside as well as for one of the *NH*-methyl group of *N*,*N'*-dimethylsuccinamide and the acetyl group bound to β-*N*-acetamido-*D*-mannose were set to zero. For the sake of compatibility between the organic/carbohydrate and peptidic/carbohydrate connections, an additional intra-molecular charge constraint of 0.1980 *e* was imposed for the methyl group of *N*,*N'*-dimethylsuccinamide not involved in the intra-molecular charge constraint previously defined. A key aspect in the reported charge derivation procedure is that the number of constraints imposed during the fitting step is kept as minimal as possible. A RRMS (Relative Root Mean Square) value of 0.096 is obtained for the fit between the MEP calculated by quantum chemistry and that generated using the derived charge values. Intra- and inter-molecular constraints account for an increase of the RRMS value of only 0.004. The relative small difference of RRMS obtained in presence and in absence of inter- and intra-molecular constraints is a strong argument in favor of the accuracy of the reported charge fitting procedure.

[1] Molecular orientations for monosaccharide units are based on the (C1 C3 C5), (C5 C3 C1), (C2 C4 O5) and (O5 C4 C2) sets of three atoms. Molecular orientations for the organic protecting groups are based on the: (i) (CX OS CM) and (CM OS CX) sets of three atoms for dimethyl ether, (ii) (CX OS C) and (C OS CX) sets of three atoms for methyl acetate, (iii) (CX OS CM) and (CM OS CX) sets of three atoms for benzyl methyl ether, and (iv) (CX OS C) and (C OS CX) sets of three atoms for methyl benzoate. Molecular orientations for N,N'-dimethylsuccinamide are based on the (C1 C2 C3) and (C3 C2 C1) sets of three atoms. See the corresponding PDB files from the R.E.DD.B. website (project F-85) for atom naming convention.

SYNTHESIS

Hexakis(2,3,6 tri-*O*-methyl)*α*-cyclodextrin (TRIMEα)

NaH (8.1g, 340 mM) in solution in dry DMF was added to a solution of *α*-CD (2g, 2 mM) in dry DMF at 0°C. The mixture was stirred under nitrogen for 10 min and CH_3I (54 g, 380 mM) was added dropwise. The obtained mixture was stirred for a further 24h at room temperature. After evaporation of most of the solvent, the residue was extracted with CH_2Cl_2 (2*100mL). The fractions were washed with water (2*100mL), dried over sodium sulfate and concentrated under diminished pressure. The crude material was purified by flash-chromatography as a white powder (yield = 88 %).

RMN ^{13}C (125Mhz, $CDCl_3$): δ (ppm) 98.15 (C-1$^{I\text{-}VIII}$), 82.14 (C-3$^{I\text{-}VIII}$), 82.19 (C-2$^{I\text{-}VIII}$), 78.60 (C-4$^{I\text{-}VIII}$), 71.42 (C-6$^{I\text{-}VIII}$), 71.07 (C-5$^{I\text{-}VIII}$), 61.46, 59.11, 58.80 (CH_3).

^1H (500 Mhz, $CDCl_3$): δ (ppm): 5.217 (H-1$^{I\text{-}VIII}$, d, $J_{1,2}$= 3.50Hz), 3.842(H-6$^{I\text{-}VIII}$, d.d, $J_{5,6}$= *3.50Hz,* $J_{6,6'}$= *10.50Hz*), 3.741 (H-5$^{I\text{-}VIII}$, d.d.d, $J_{5,4}$= *10.0Hz*), 3.671 (H-4$^{I\text{-}VIII}$, t, $J_{3,4}$= *10.0Hz*), 3.525(H-3$^{I\text{-}VIII}$ and H-6$^{I\text{-}VIII}$, m), 3.196 (H-2$^{I\text{-}VIII}$, dd, $J_{2,3}$= *10.0Hz*), 3.636, 3.495, 3.555 ($CH_3^{i\text{-}VIII}$).

ESI-MS: m/z= 1247.5920 $[M+Na]^+$, $C_{54}H_{96}O_{30}Na$ requires 1247.5894

Octakis(2,3,6 tri-*O*-methyl)*γ*-cyclodextrin (TRIME*γ*)

NaH (6.11g, 254 mM) in solution in dry DMF was added to a solution of γ-CD (2g, 1.5 mM) in dry DMF at 0°C. The mixture was stirred under nitrogen for 10 min and CH_3I (40.54g, 285 mM) was added dropwise and the obtained mixture was stirred for a further 24h at room temperature. After evaporation of most of the solvent, the residue was extracted with CH_2Cl_2 (2*100mL). The fractions were washed with water (2*100mL), dried over sodium sulfate and concentrated under diminished pressure. The crude material was purified by flash-chromatography as a white powder (yield = 92 %).

RMN ^{13}C (125Mhz, $CDCl_3$): δ(ppm) 98.15 (C-1$^{I\text{-}VIII}$), 82.14 (C-3$^{I\text{-}VIII}$), 82.19 (C-2$^{I\text{-}VIII}$), 78.60 (C-4$^{I\text{-}VIII}$), 71.42 (C-6$^{I\text{-}VIII}$), 71.07 (C-5$^{I\text{-}VIII}$), 61.46, 59.11, 58.80 (CH_3).

^1H (500 Mhz, $CDCl_3$): δ (ppm): 5.217 (H-1$^{I\text{-}VIII}$, d, $J_{1,2}$= 3.50Hz), 3.842(H-6$^{I\text{-}VIII}$, d.d, $J_{5,6}$= *3.50Hz,* $J_{6,6'}$= *10.50Hz*), 3.741 (H-5$^{I\text{-}VIII}$, d.d.d, $J_{5,4}$= *10.0Hz*), 3.671 (H-4$^{I\text{-}VIII}$, t, $J_{3,4}$= *10.0Hz*), 3.525(H-3$^{I\text{-}VIII}$ and H-6$^{I\text{-}VIII}$, m), 3.196 (H-2$^{I\text{-}VIII}$, dd, $J_{2,3}$= *10.0Hz*), 3.636, 3.495, 3.555 ($CH_3^{i\text{-}VIII}$).

ESI-MS: m/z= 1655.7896 $[M+Na]^+$, $C_{72}H_{128}O_{40}Na$ requires 1655.7880

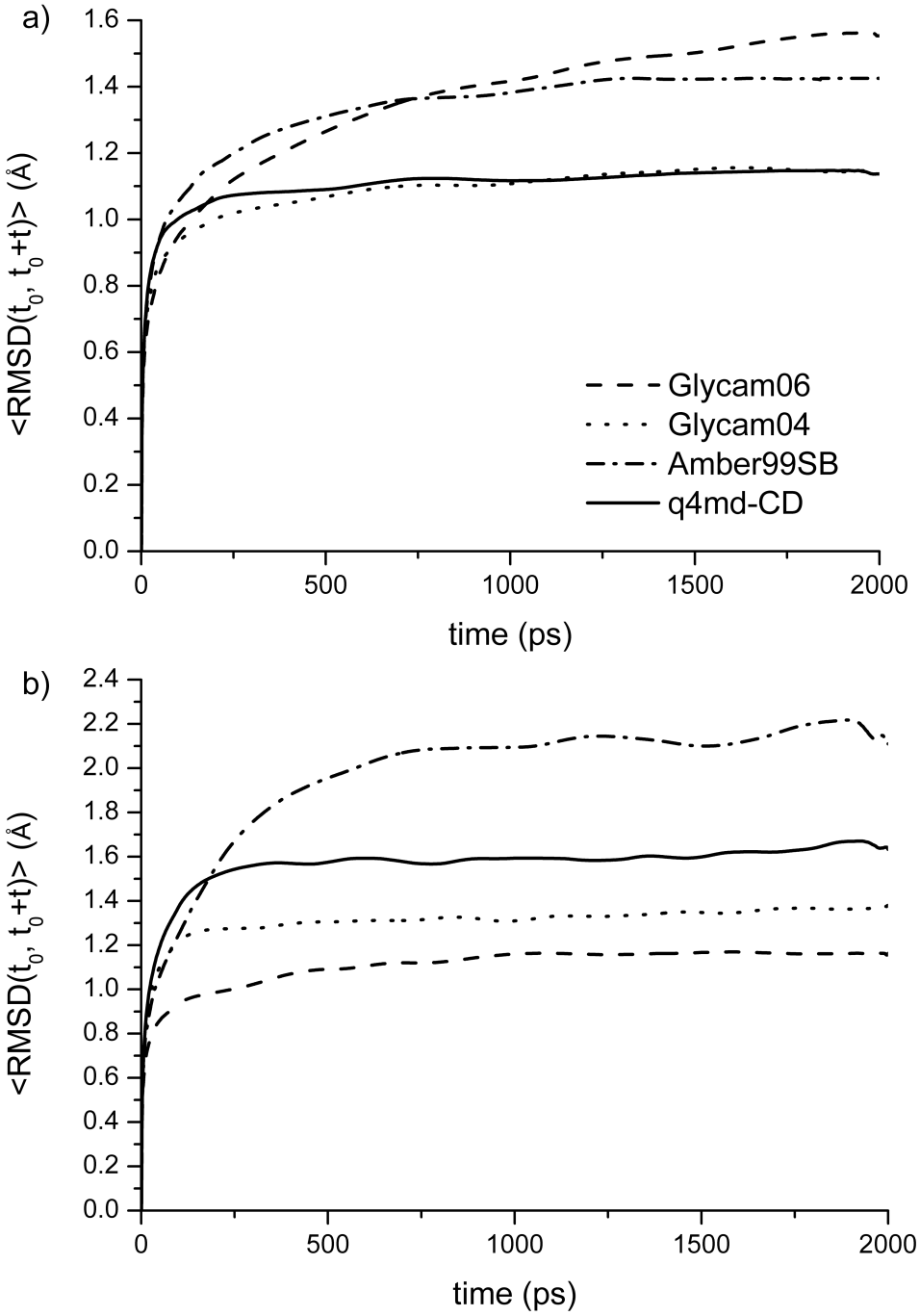

Figure S1. Time-evolution functions of the averaged RMSD for a) α-CD and b) γ-CD. Only heavy atoms have been taken into account for calculations. Each curve corresponds to an average over six independent trajectories of 50 ns.

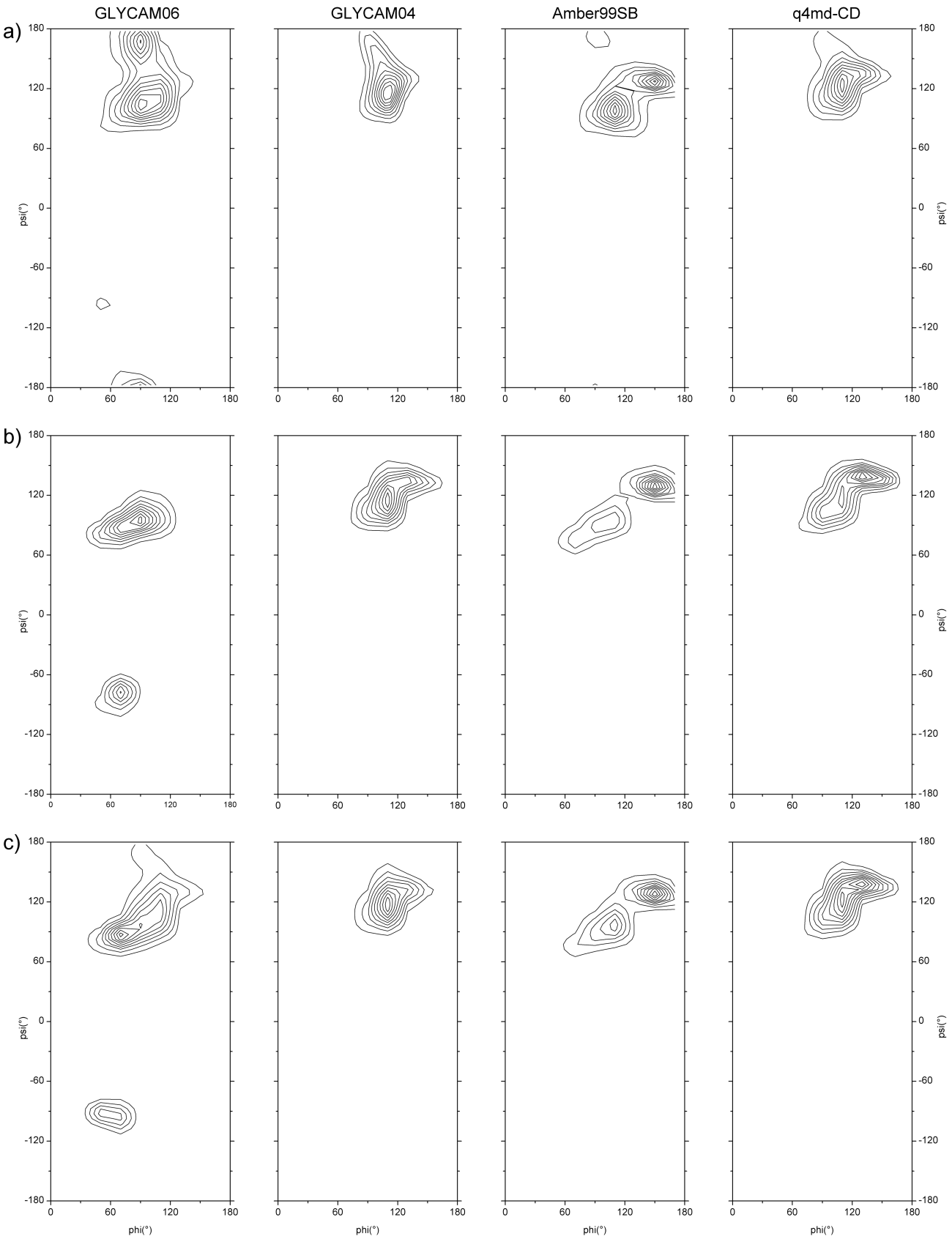

Figure S2. (φ,ψ) densities for a) α-CD b) β-CD and c) γ-CD calculated with the GLYCAM06, GLYCAM04, Amber99SB and q4md-CD force fields.

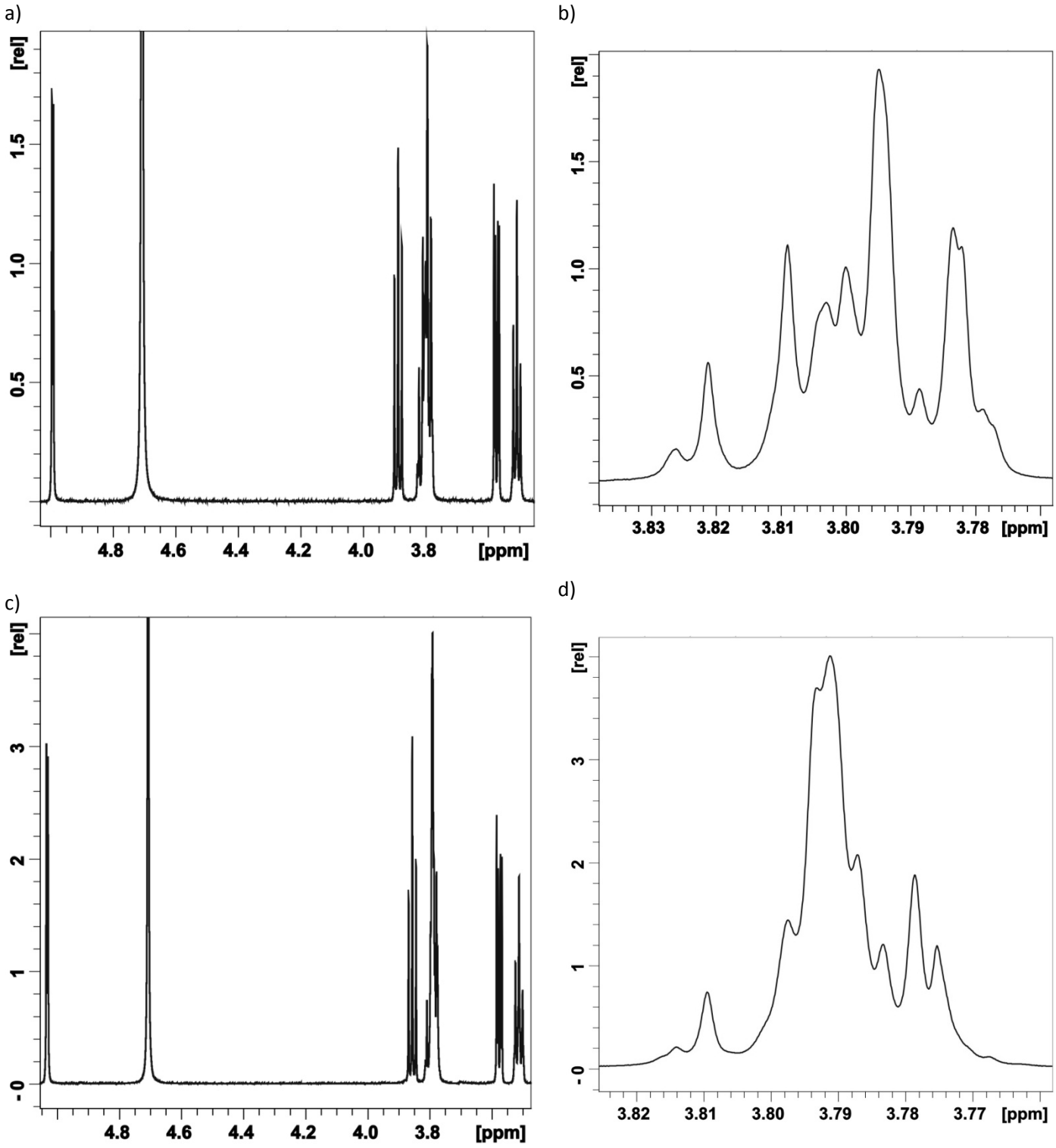

Figure S3. High order 1D ^{1}H NMR spectra recorded in D_2O at 800 MHz of CDs (10 mM, 298 K, pH = 7.5) of native CDs. *β*-CD: a) Whole spectrum and b) 3.77-3.84 ppm region. *γ*-CD: c) Whole spectrum and d) 3.76-3.82 ppm region. The overlapping of the H5, H6' and H6'' chemical shifts renders the accurate determination of the $^{3}J_{H5\text{-}H6'}$ and $^{3}J_{H5\text{-}H6''}$ coupling constants values complex. For the *β*-CD the coupling constants were nevertheless taken from ref. 1.

(1) Djedaïni, F., PhD thesis, University of Paris XI-Orsay, France, 1991.

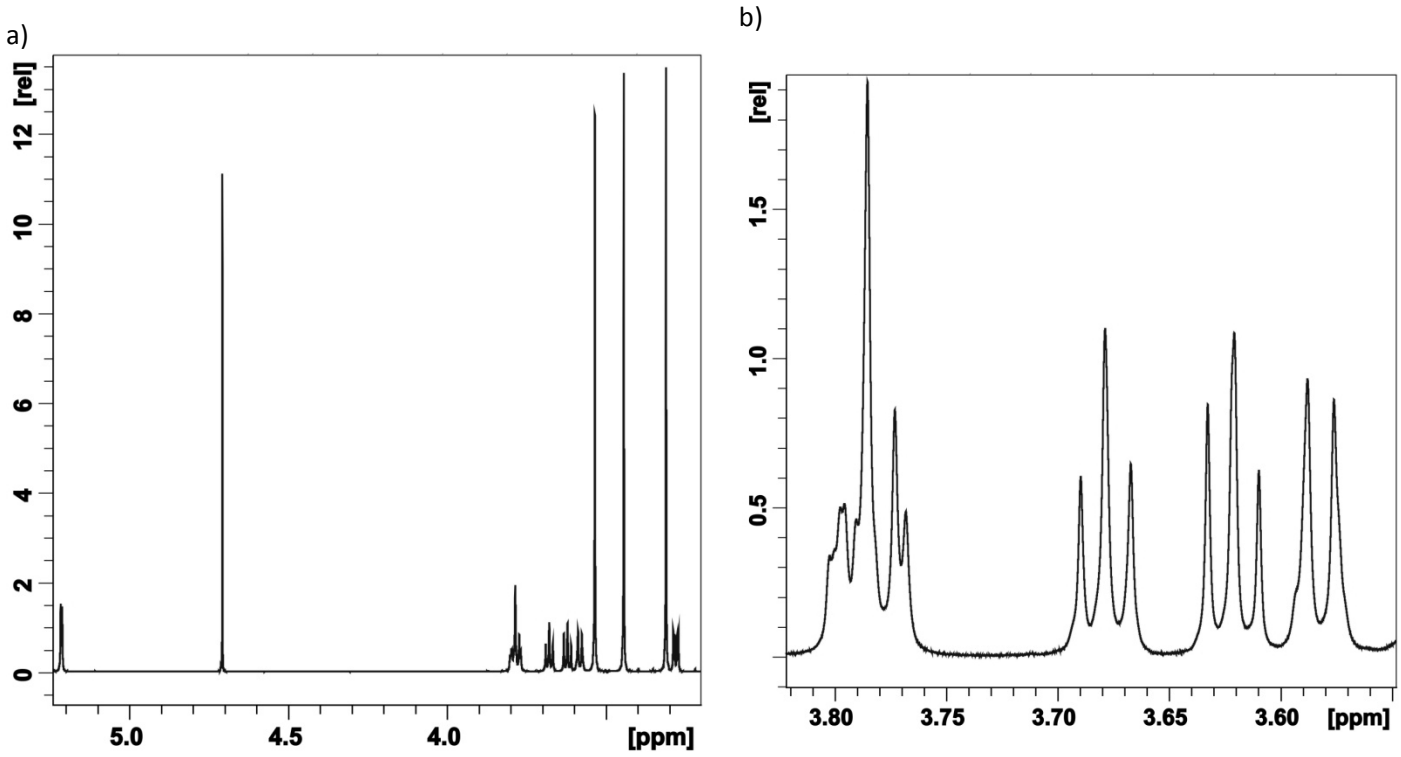

Figure S4. High order 1D ^{1}H NMR spectra of PM-*β*-CD recorded in D_2O at 800 MHz (10 mM, 298 K, pH = 7.5). a) Whole spectrum and b) 3.55-3.82 ppm region.

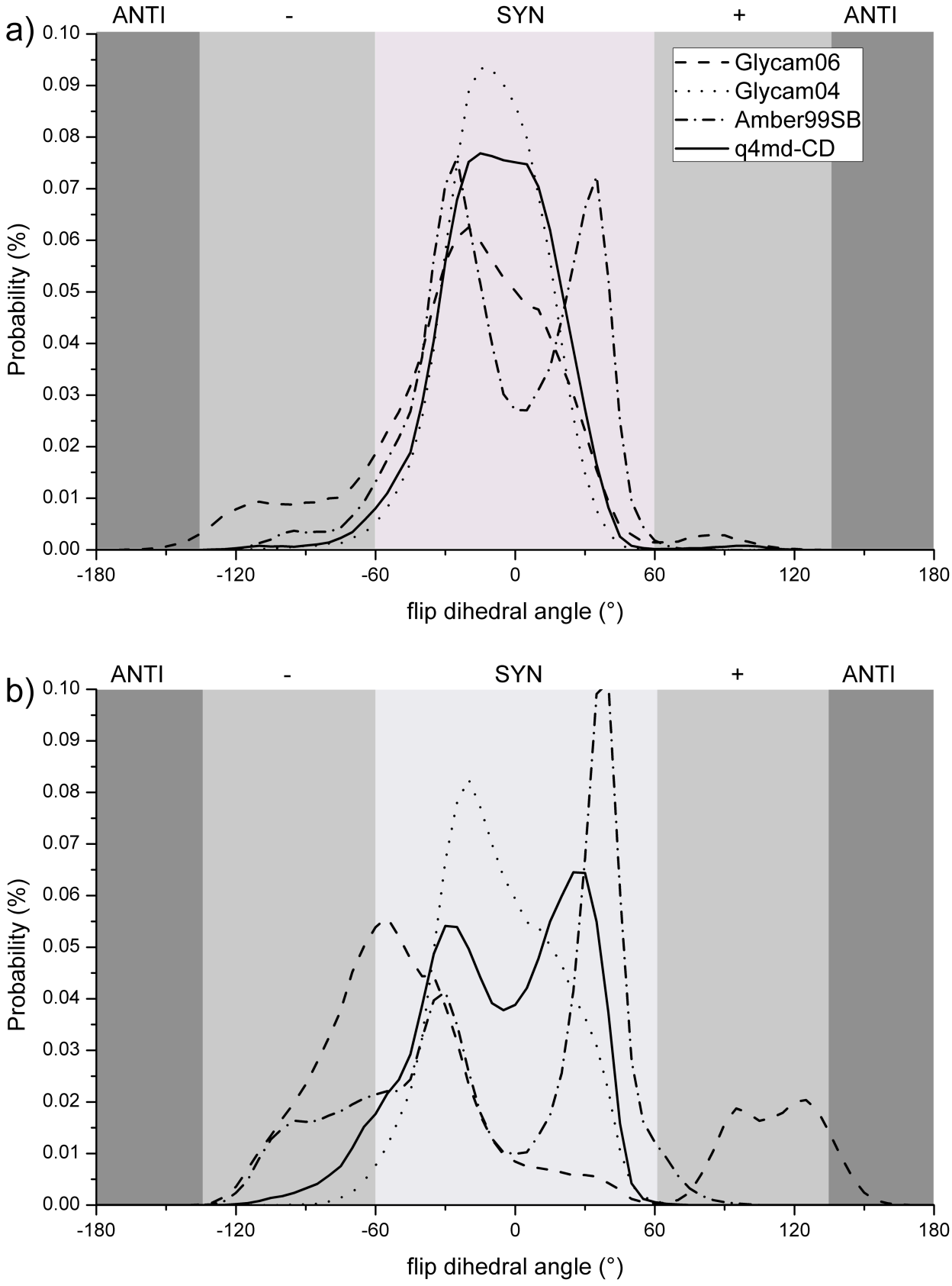

Figure S5. Distributions of the *flip* dihedral angle ($O3_n$-$C4_n$-$C1_{n+1}$-$O2_{n+1}$) for a) α-CD and b) γ-CD using the GLYCAM06, GLYCAM04, Amber99SB and q4md-CD force fields.

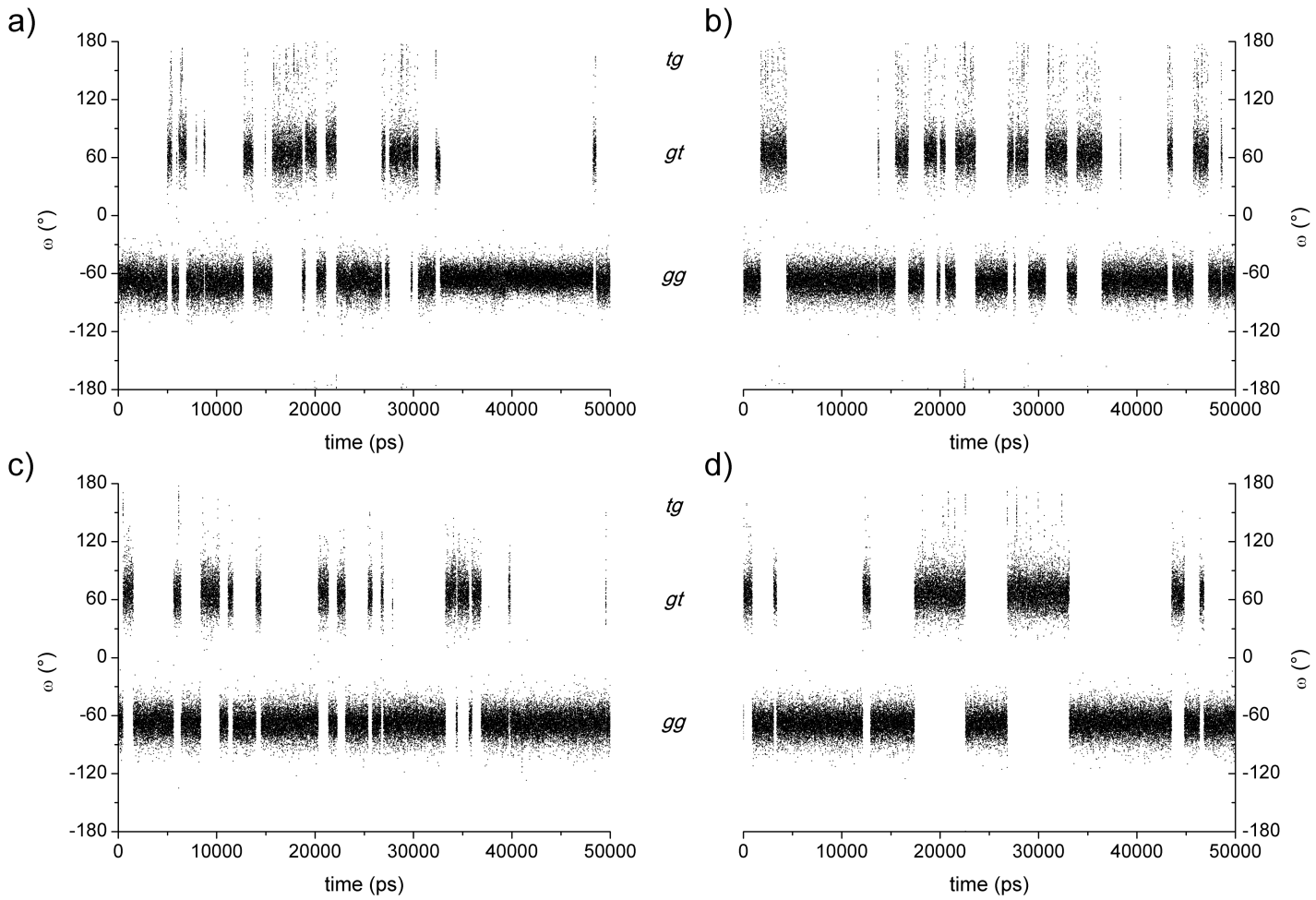

Figure S6. Time dependence of the *ω* torsion angle obtained with the a) GLYCAM04, b) GLYCAM06, c) Amber99SB and d) q4md-CD force fields for a representative *D*-glucose unit of *β*-CD over a 50 ns MD simulation. The averages over all *D*-glucose units and all MD simulations for the *ω* population are reported in Table 3. Similar patterns are observed for *α*- and *γ*-CDs.

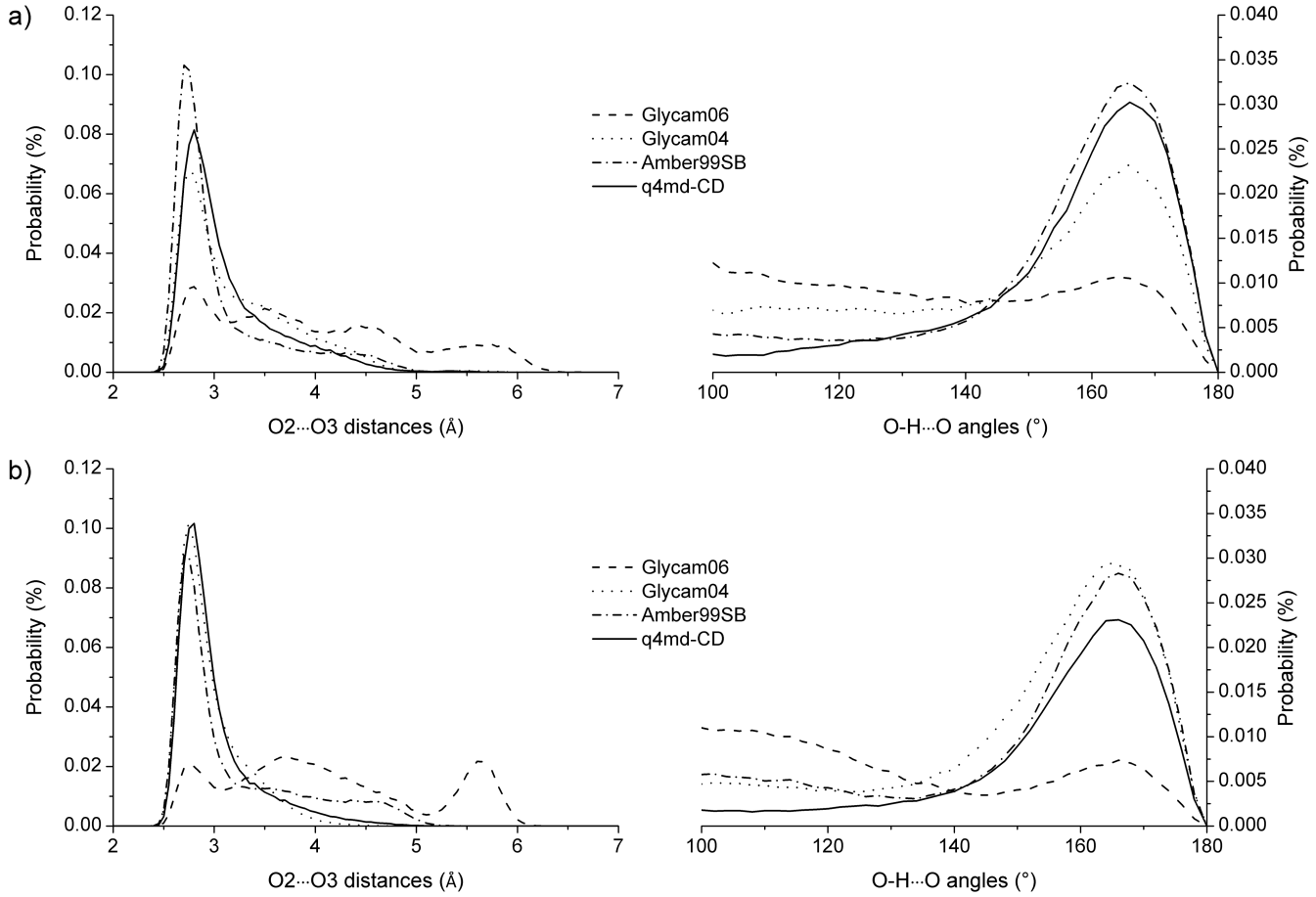

Figure S7. Distributions of the average $O2_n\cdots O3_{n-1}$ distances (left) and the average O-H···O angles (right) between two consecutive *n* and *n-1 D*-glucose units reflecting the establishment of stable HBs in a) *α*-CD and b) *γ*-CD. Each curve is the averaged result over the six and eight glucose units, respectively.

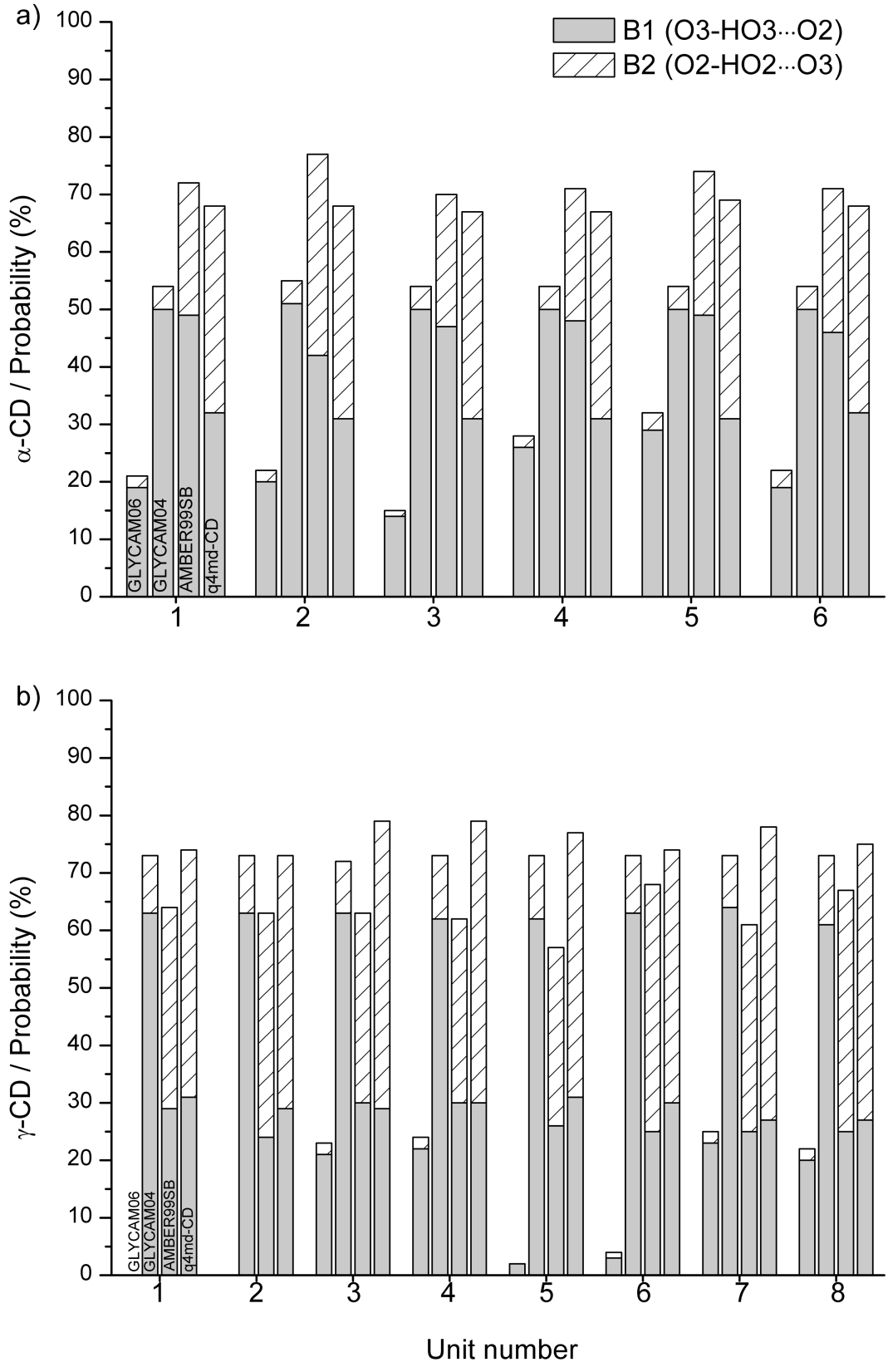

Figure S8. The percentage of HBs being in the B1 and B2 states for each inter-glucose $O2_n\cdots O3_{n-1}$ HB: a) *α*-CD and c) *γ*-CD. B1 corresponds to the $O3_{n-1}$-$HO3_{n-1}\cdots O2_n$ HB and B2 to the $O2_n$-$HO2_n\cdots O3_{n-1}$ one. Summing B1 and B2 gives the percentage of intra-glucosidic HBs. The remaining percentage corresponds to interactions with water molecules.

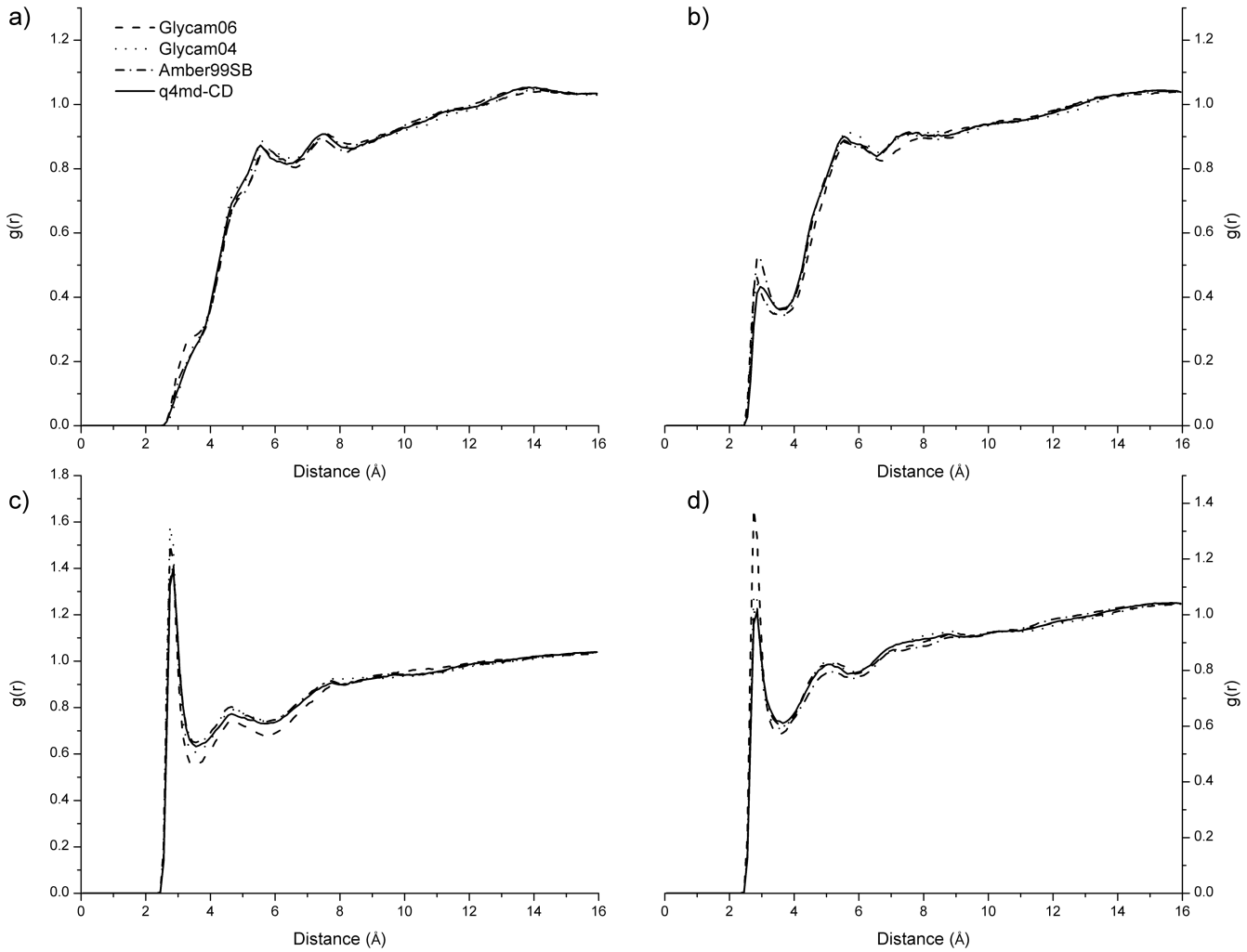

Figure S9. Radial distribution functions of water molecules around selected oxygens of *β*-CD obtained with the GLYCAM06, GLYCAM04, Amber99SB and q4md-CD force fields. a) *exo*-cyclic oxygen O4, b) *endo*-cyclic oxygen O5, c) primary hydroxyl oxygen O6 and d) secondary hydroxyl oxygens O2 and O3. Similar plots are observed for *α*- and *γ*-CDs.

Rdfs obtained with the GLYCAM06, GLYCAM04, Amber99SB and q4md-CD force fields show an identical behavior as the shape, width and location of their peaks are identical. For the hydroxyl oxygens the high and well-defined peaks relate to solvation shells where the solvent is ordered. Conversely, the rdfs relative to the *endo*-cyclic oxygens are poorly defined and show a shallow first minimum, indicating fewer and random interactions with water in the first solvation shell. The only accessible water molecules for the *endo*-cyclic oxygens are those within the cavity and the small height of the peaks demonstrates its relative hydrophobicity. The most noticeable difference between the curves obtained with the different force fields resides in the height of the peak corresponding to the 2- and 3-hydroxyls – water rdfs, where the GLYCAM06 force field describes more favorable interactions between these hydroxyls and water. Distributions related to $O2_n \cdots O3_{n-1}$ inter-glucose hydrogen bonding (*i. e.* flip-flop HBs) reported in the article showed that GLYCAM06 is not prone to form these HBs. Consequently the O2 and O3 atoms are more accessible to solvent interactions leading to an increased height of the corresponding rdf peak.

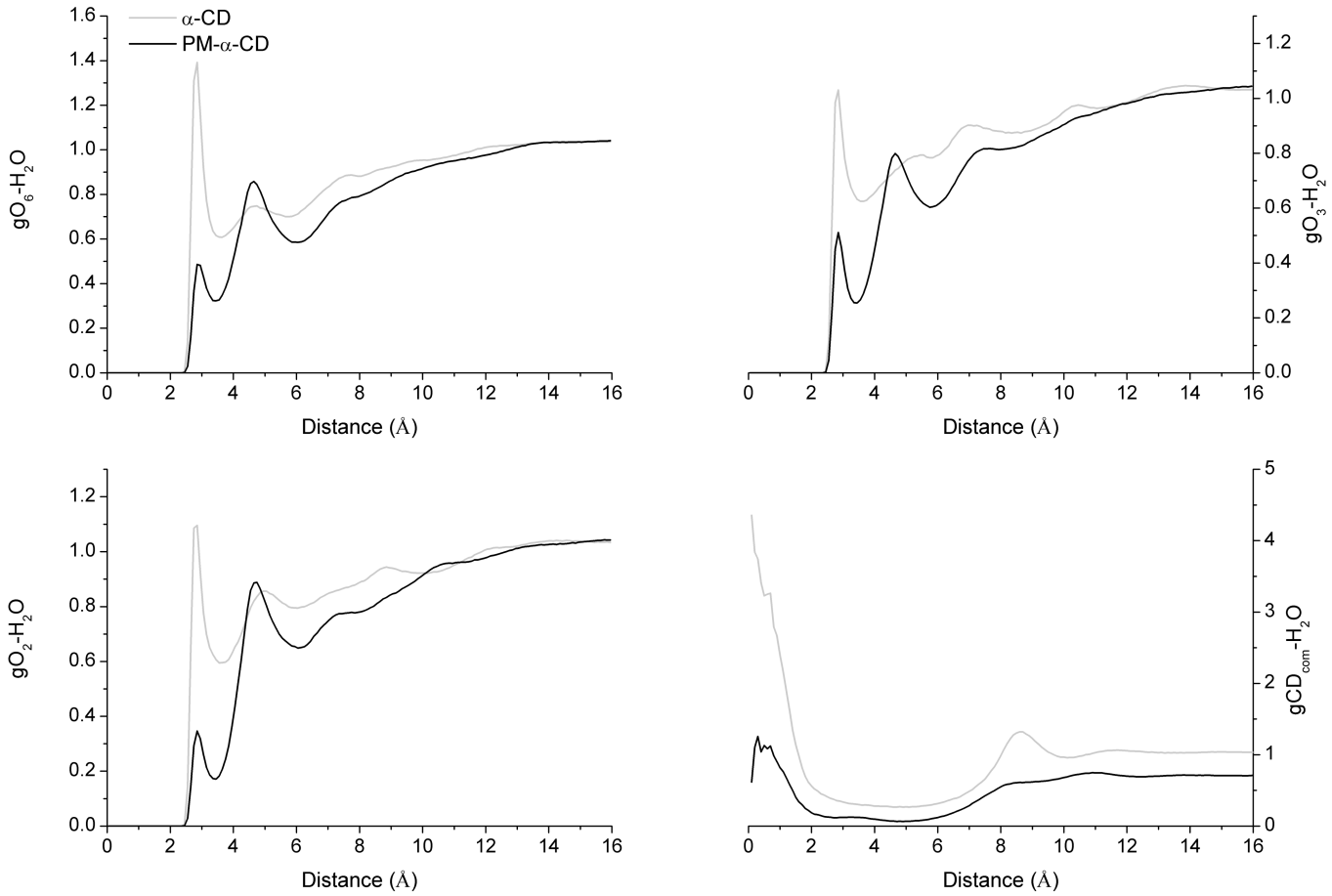

Figure S10. Radial distribution functions around selected oxygens a) O6, b) O3, c) O2 and around d) the center of mass for *α*-CD and PM-*α*-CD obtained with the q4md-CD force field.

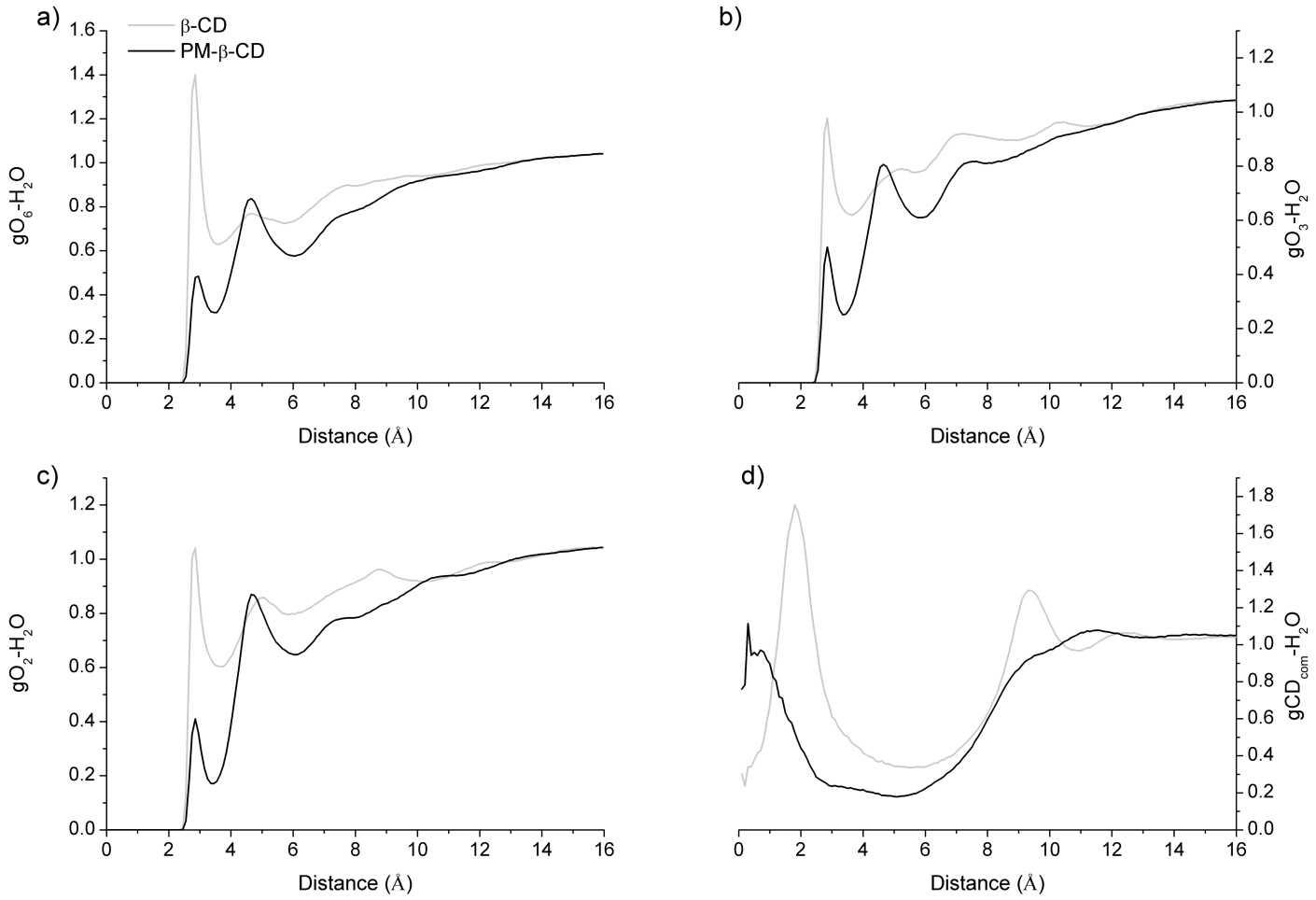

Figure S11. Radial distribution functions around selected oxygens a) O6, b) O3, c) O2 and around d) the center of mass for *β*-CD and PM-*β*-CD obtained with the q4md-CD force field.

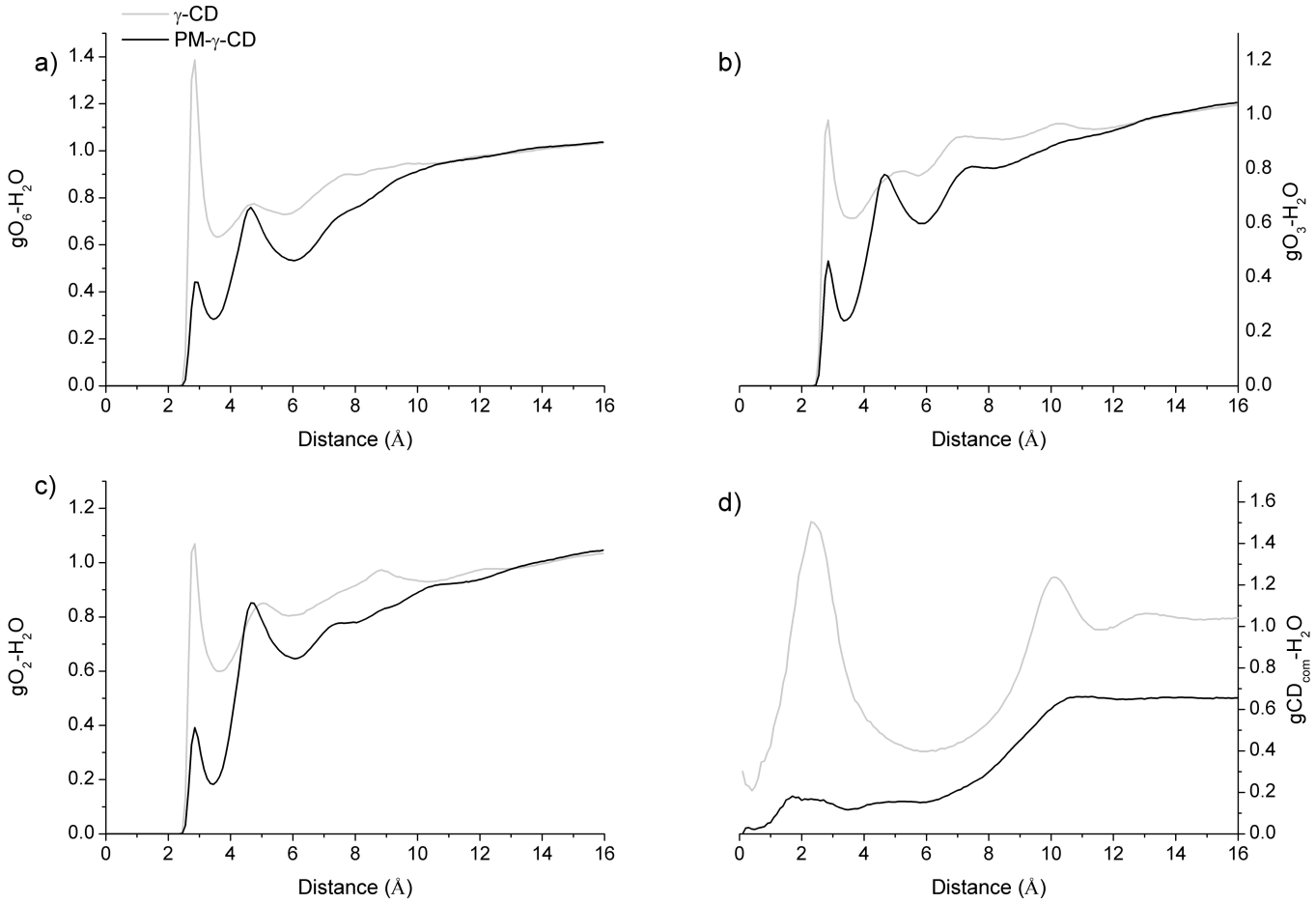

Figure S12. Radial distribution functions around selected oxygens a) O6, b) O3, c) O2 and around d) the center of mass for *γ*-CD and PM-*γ*-CD obtained with the q4md-CD force field.

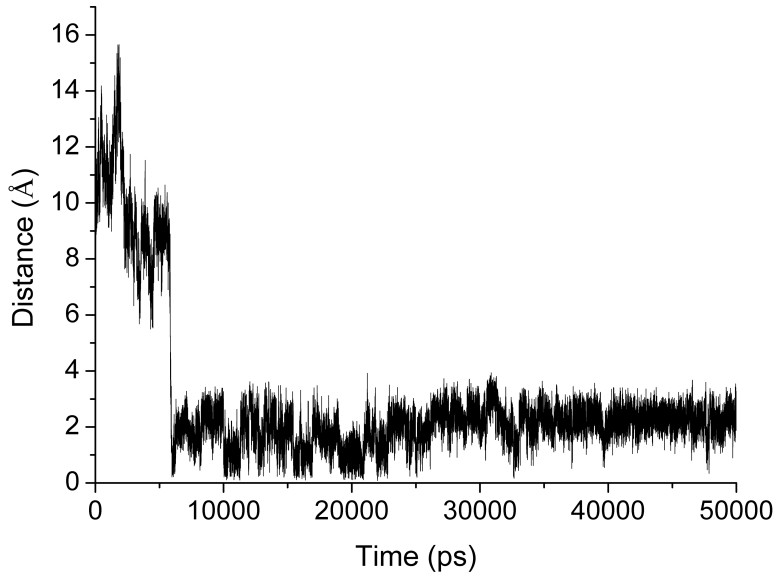

Figure S13. Distance between the CD_{com} and the ζ-carbon atom of tyrosine over a 50 ns MD run. The inclusion of tyrosine into the CD cavity happens after 5 ns of simulation. This is one representative simulation showing the self-complexation process.

The q4md-CD force field

```
# The q4md-CD Force Field
# C. Cezard & F.-Y. Dupradeau
#               R.E.DD.B. names                Description
# 1-MG2.mol2     tripos1.mol2       Fragment MG2 (w/ OH2) from a-OMe-D-Glucoside
# 1-MG3.mol2     tripos2.mol2       Fragment MG3 (w/ OH3) from a-OMe-D-Glucoside
# 1-MG6.mol2     tripos3.mol2       Fragment MG6 (w/ OH6) from a-OMe-D-Glucoside
# 1-MGA.mol2     tripos4.mol2       Fragment MGA (w/ OH3 & OH6) from a-OMe-D-Glucoside
# 1-MGB.mol2     tripos5.mol2       Fragment MGB (w/ OH2 & OH6) from a-OMe-D-Glucoside
# 1-MGC.mol2     tripos6.mol2       Fragment MGC (w/ OH2 & OH3) from a-OMe-D-Glucoside
# 1-MGO.mol2     tripos7.mol2       Fragment MGO (w/ all OHs but OH4) from a-OMe-D-
Glucoside
# 1-MGR.mol2     tripos8.mol2       Fragment MGR (w/o all OHs) from a-OMe-D-Glucoside
# 2-OAC.mol2     tripos9.mol2       Fragment OAc from Me-OAc
# 3-OBN.mol2     tripos10.mol2      Fragment OBn from Me-OBn
# 4-OBZ.mol2     tripos11.mol2      Fragment OBz from Me-OBz
# 5-OME.mol2     tripos12.mol2      Fragment OMe from Me-OMe
# 6-SCC.mol2     tripos13.mol2      Fragment SCC from N,N-dimethylsuccinamide
# 7-BM3.mol2     tripos14.mol2      Fragment BM3 (w/ OH2 & OH3) from b-N-acetamido-D-
Mannoside
# 7-BM4.mol2     tripos15.mol2      Fragment BM4 (w/ OH2 & OH4) from b-N-acetamido-D-
Mannoside
# 7-BM6.mol2     tripos16.mol2      Fragment BM6 (w/ OH2 & OH6) from b-N-acetamido-D-
Mannoside
# 7-BMA.mol2     tripos17.mol2      Fragment BMA (w/o OH3) from b-N-acetamido-D-
Mannoside
# 7-BMB.mol2     tripos18.mol2      Fragment BMB (w/o OH4) from b-N-acetamido-D-
Mannoside
# 7-BMC.mol2     tripos19.mol2      Fragment BMC (w/o OH6) from b-N-acetamido-D-
Mannoside
# 7-BMO.mol2     tripos20.mol2      Fragment BMO (w all OHs) from b-N-acetamido-D-
Mannoside
# 7-BMR.mol2     tripos21.mol2      Fragment BMR (w/o all OHs but OH2) from b-N-
acetamido-D-Mannoside
# 8-AMO.mol2     tripos22.mol2      Fragment AMO from a-OMe-D-Mannoside
#
# Ac = CH3CO // Bn = C6H5CH2 // Bz = C6H5CO // Me = CH3


##############################################################################
#                                                                            #
#                    Script file for Leap/xleap                              #
#                                                                            #
##############################################################################

addAtomTypes {
# Amber
        { "HZ"  "H" "sp3" }
        { "H"   "H" "sp3" }
        { "HO"  "H" "sp3" }
        { "H1"  "H" "sp3" }
        { "H2"  "H" "sp3" }
        { "HC"  "H" "sp3" }
        { "HA"  "H" "sp3" }
        { "HW"  "H" "sp3" }
        { "OW"  "O" "sp3" }
```

```
        { "OH"  "O" "sp3" }
        { "OS"  "O" "sp3" }
        { "O"   "O" "sp2" }
        { "O2"  "O" "sp2" }
        { "S"   "S" "sp3" }
        { "CT"  "C" "sp3" }
        { "CZ"  "C" "sp3" }
        { "C"   "C" "sp2" }
        { "CA"  "C" "sp2" }
        { "N"   "N" "sp2" }
        { "CL" "Cl" "sp3" }
# Glycam
        { "CG"  "C" "sp3" }
}

parm99 = loadamberparams parm99.dat
FF99SB = loadamberparams frcmod.ff99SB

loadoff all_amino94.lib
loadoff all_aminoct94.lib
loadoff all_aminont94.lib

loadoff solvents.lib

# Use Glycam
glycam04 = loadamberparams glycam04.dat

HOH = TP3
WAT = TP3

Q4MDCD = loadamberparams frcmod.q4md

################################
# LOAD ALL THE REQUIRED UNITS #
################################

# The central fragment - allows polymerisation of per-OR a(1,4)Glc (R = Me, Bn, Ac or
Bz)
# MGR = loadmol2 1-MGR.mol2
MGR = loadmol2 tripos8.mol2
set MGR name "MGR"
set MGR head MGR.1.C4
set MGR tail MGR.1.O1
set MGR.1 connect0 MGR.1.C4
set MGR.1 connect1 MGR.1.O1
set MGR.1 restype saccharide
set MGR.1 name "MGR"
# set FF atom types
set MGR.1.C1 type CG
set MGR.1.H1 type H2
set MGR.1.O1 type OS
set MGR.1.C2 type CG
set MGR.1.H2 type H1
set MGR.1.C3 type CG
set MGR.1.H3 type H1
set MGR.1.C4 type CG
set MGR.1.H4 type H1
```

```
set MGR.1.C5 type CG
set MGR.1.H5 type H1
set MGR.1.O5 type OS
set MGR.1.C6 type CG
set MGR.1.H61 type H1
set MGR.1.H62 type H1

# The central fragment - allows polymerisation of per-OH a(1,4)Glc
# MGO = loadmol2 1-MGO.mol2
MGO = loadmol2 tripos7.mol2
set MGO name "MGO"
set MGO head MGO.1.C4
set MGO tail MGO.1.O1
set MGO.1 connect0 MGO.1.C4
set MGO.1 connect1 MGO.1.O1
set MGO.1 restype saccharide
set MGO.1 name "MGO"
# set FF atom types
set MGO.1.C1 type CG
set MGO.1.H1 type H2
set MGO.1.O1 type OS
set MGO.1.C2 type CG
set MGO.1.H2 type H1
set MGO.1.O2 type OH
set MGO.1.HO2 type HO
set MGO.1.C3 type CG
set MGO.1.H3 type H1
set MGO.1.O3 type OH
set MGO.1.HO3 type HO
set MGO.1.C4 type CG
set MGO.1.H4 type H1
set MGO.1.C5 type CG
set MGO.1.H5 type H1
set MGO.1.O5 type OS
set MGO.1.C6 type CG
set MGO.1.H61 type H1
set MGO.1.H62 type H1
set MGO.1.O6 type OH
set MGO.1.HO6 type HO

# Fragment which allows linking between peptide arm & Glc
# MGC = loadmol2 1-MGC.mol2
MGC = loadmol2 tripos6.mol2
set MGC name "MGC"
set MGC head MGC.1.C6
set MGC tail MGC.1.O1
set MGC.1 connect0 MGC.1.C6
set MGC.1 connect1 MGC.1.O1
set MGC.1 restype saccharide
set MGC.1 name "MGC"
# set FF atom types
set MGC.1.C1 type CG
set MGC.1.H1 type H2
set MGC.1.O1 type OS
set MGC.1.C2 type CG
set MGC.1.H2 type H1
set MGC.1.O2 type OH
```

```
set MGC.1.HO2 type HO
set MGC.1.C3 type CG
set MGC.1.H3 type H1
set MGC.1.O3 type OH
set MGC.1.HO3 type HO
set MGC.1.C4 type CG
set MGC.1.H4 type H1
set MGC.1.C5 type CG
set MGC.1.H5 type H1
set MGC.1.O5 type OS
set MGC.1.C6 type CG
set MGC.1.H61 type H1
set MGC.1.H62 type H1

# OAc = loadmol2 2-OAC.mol2
OAc = loadmol2 tripos9.mol2
set OAc name "OAc"
set OAc head OAc.1.OS
set OAc.1 connect0 OAc.1.OS
set OAc.1 restype undefined
set OAc.1 name "OAc"
# set FF atom types
set OAc.1.OS type OS
set OAc.1.C type C
set OAc.1.O type O
set OAc.1.CM type CG
set OAc.1.HM1 type HC
set OAc.1.HM2 type HC
set OAc.1.HM3 type HC

# OBn = loadmol2 3-OBN.mol2
OBn = loadmol2 tripos10.mol2
set OBn name "OBn"
set OBn head OBn.1.OS
set OBn.1 connect0 OBn.1.OS
set OBn.1 restype undefined
set OBn.1 name "OBn"
# set FF atom types
set OBn.1.OS type OS
set OBn.1.CM type CG
set OBn.1.HM1 type H1
set OBn.1.HM2 type H1
set OBn.1.C1 type CA
set OBn.1.C2 type CA
set OBn.1.H2 type HA
set OBn.1.C3 type CA
set OBn.1.H3 type HA
set OBn.1.C4 type CA
set OBn.1.H4 type HA
set OBn.1.C5 type CA
set OBn.1.H5 type HA
set OBn.1.C6 type CA
set OBn.1.H6 type HA

# OBz = loadmol2 4-OBZ.mol2
OBz = loadmol2 tripos11.mol2
set OBz name "OBz"
```

```
set OBz name "OBz"
set OBz head OBz.1.OS
set OBz.1 connect0 OBz.1.OS
set OBz.1 restype undefined
set OBz.1 name "OBz"
# set FF atom types
set OBz.1.OS type OS
set OBz.1.C type C
set OBz.1.O type O
set OBz.1.C1 type CA
set OBz.1.C2 type CA
set OBz.1.H2 type HA
set OBz.1.C3 type CA
set OBz.1.H3 type HA
set OBz.1.C4 type CA
set OBz.1.H4 type HA
set OBz.1.C5 type CA
set OBz.1.H5 type HA
set OBz.1.C6 type CA
set OBz.1.H6 type HA

# OMe = loadmol2 5-OME.mol2
OMe = loadmol2 tripos12.mol2
set OMe name "OMe"
set OMe head OMe.1.OS
set OMe.1 connect0 OMe.1.OS
set OMe.1 restype undefined
set OMe.1 name "OMe"
# set FF atom types
set OMe.1.OS type OS
set OMe.1.CM type CG
set OMe.1.HM1 type H1
set OMe.1.HM2 type H1
set OMe.1.HM3 type H1

# Succinamide fragment
# SCC = loadmol2 6-SCC.mol2
SCC = loadmol2 tripos13.mol2
set SCC name "SCC"
set SCC head SCC.1.N1
set SCC tail SCC.1.C4
set SCC.1 connect0 SCC.1.N1
set SCC.1 connect1 SCC.1.C4
set SCC.1 restype protein
set SCC.1 name "SCC"
# set FF atom types
set SCC.1.N1  type N
set SCC.1.H1  type H
set SCC.1.C1  type C
set SCC.1.O1  type O
set SCC.1.C2  type CT
set SCC.1.H21 type HC
set SCC.1.H22 type HC
set SCC.1.C3  type CT
set SCC.1.H31 type HC
set SCC.1.H32 type HC
set SCC.1.C4  type C
```

```
set SCC.1.O4  type O

# Fragment Man-b-NH
# BM3 = loadmol2 7-BM3.mol2
BM3 = loadmol2 tripos14.mol2
set BM3 name "BM3"
set BM3 head BM3.1.C4
set BM3 tail BM3.1.NH1
set BM3.1 connect0 BM3.1.C4
set BM3.1 connect1 BM3.1.NH1
set BM3.1 restype saccharide
set BM3.1 name "BM3"
# set FF atom types
set BM3.1.C1 type CG
set BM3.1.H1 type H2
set BM3.1.NH1 type N
set BM3.1.HN1 type H
set BM3.1.C2 type CG
set BM3.1.H2 type H1
set BM3.1.O2 type OH
set BM3.1.HO2 type HO
set BM3.1.C3 type CG
set BM3.1.H3 type H1
set BM3.1.O3 type OH
set BM3.1.HO3 type HO
set BM3.1.C4 type CG
set BM3.1.H4 type H1
set BM3.1.C5 type CG
set BM3.1.H5 type H1
set BM3.1.O5 type OS
set BM3.1.C6 type CG
set BM3.1.H61 type H1
set BM3.1.H62 type H1

# Fragment Man-b-NH
# BM4 = loadmol2 7-BM4.mol2
BM4 = loadmol2 tripos15.mol2
set BM4 name "BM4"
set BM4 head BM4.1.C3
set BM4 tail BM4.1.NH1
set BM4.1 connect0 BM4.1.C3
set BM4.1 connect1 BM4.1.NH1
set BM4.1 restype saccharide
set BM4.1 name "BM4"
# set FF atom types
set BM4.1.C1 type CG
set BM4.1.H1 type H2
set BM4.1.NH1 type N
set BM4.1.HN1 type H
set BM4.1.C2 type CG
set BM4.1.H2 type H1
set BM4.1.O2 type OH
set BM4.1.HO2 type HO
set BM4.1.C3 type CG
set BM4.1.H3 type H1
set BM4.1.C4 type CG
set BM4.1.H4 type H1
```

```
set BM4.1.O4 type OH
set BM4.1.HO4 type HO
set BM4.1.C5 type CG
set BM4.1.H5 type H1
set BM4.1.O5 type OS
set BM4.1.C6 type CG
set BM4.1.H61 type H1
set BM4.1.H62 type H1

# Fragment Man-a terminal
# AMO = loadmol2 8-AMO.mol2
AMO = loadmol2 tripos22.mol2
set AMO name "AMO"
set AMO head AMO.1.C4
set AMO tail AMO.1.O1
set AMO.1 connect0 AMO.1.C4
set AMO.1 connect1 AMO.1.O1
set AMO.1 restype saccharide
set AMO.1 name "AMO"
# set FF atom types
set AMO.1.C1 type CG
set AMO.1.H1 type H2
set AMO.1.O1 type OS
set AMO.1.C2 type CG
set AMO.1.H2 type H1
set AMO.1.O2 type OH
set AMO.1.HO2 type HO
set AMO.1.C3 type CG
set AMO.1.H3 type H1
set AMO.1.O3 type OH
set AMO.1.HO3 type HO
set AMO.1.C4 type CG
set AMO.1.H4 type H1
set AMO.1.O4 type OH
set AMO.1.HO4 type HO
set AMO.1.C5 type CG
set AMO.1.H5 type H1
set AMO.1.O5 type OS
set AMO.1.C6 type CG
set AMO.1.H61 type H1
set AMO.1.H62 type H1
set AMO.1.O6 type OH
set AMO.1.HO6 type HO

################################
#       CREATE PER-OH CDs      #
################################

# per-OH alpha-cyclodextrin
ACDOH = sequence {MGO MGO MGO MGO MGO MGO}
set ACDOH head ACDOH.1.C4
set ACDOH tail ACDOH.6.O1
impose ACDOH {1 2 3 4 5 6} {{O5 C1 O1 C4 90.0}{C1 O1 C4 C5 -95.00}}
bond ACDOH.1.C4 ACDOH.6.O1

# per-OH beta-cyclodextrin
BCDOH = sequence {MGO MGO MGO MGO MGO MGO MGO}
```

```
set BCDOH head BCDOH.1.C4
set BCDOH tail BCDOH.7.O1
impose BCDOH {1 2 3 4 5 6 7} {{O5 C1 O1 C4 98.0}{C1 O1 C4 C5 -103.00}}
bond BCDOH.1.C4 BCDOH.7.O1

# per-OH gamma-cyclodextrin
GCDOH = sequence {MGO MGO MGO MGO MGO MGO MGO MGO}
set GCDOH head GCDOH.1.C4
set GCDOH tail GCDOH.8.O1
impose GCDOH {1 2 3 4 5 6 7 8} {{O5 C1 O1 C4 109.0}{C1 O1 C4 C5 -111.00}}
bond GCDOH.1.C4 GCDOH.8.O1

################################
#    CREATE PROTECTED CDs      #
################################

# per-OAc alpha-cyclodextrin
AAC = sequence {MGR MGR MGR MGR MGR MGR}
BAC = sequence {MGR MGR MGR MGR MGR MGR MGR}
GAC = sequence {MGR MGR MGR MGR MGR MGR MGR MGR}
set AAC tail AAC.1.C6
set BAC tail BAC.1.C6
set GAC tail GAC.1.C6
AAC1 = sequence {AAC OAc}
BAC1 = sequence {BAC OAc}
GAC1 = sequence {GAC OAc}
set AAC1 tail AAC1.1.C3
set BAC1 tail BAC1.1.C3
set GAC1 tail GAC1.1.C3
AAC2 = sequence {AAC1 OAc}
BAC2 = sequence {BAC1 OAc}
GAC2 = sequence {GAC1 OAc}
set AAC2 tail AAC2.1.C2
set BAC2 tail BAC2.1.C2
set GAC2 tail GAC2.1.C2
AAC3 = sequence {AAC2 OAc}
BAC3 = sequence {BAC2 OAc}
GAC3 = sequence {GAC2 OAc}
set AAC3 tail AAC3.2.C6
set BAC3 tail BAC3.2.C6
set GAC3 tail GAC3.2.C6
AAC4 = sequence {AAC3 OAc}
BAC4 = sequence {BAC3 OAc}
GAC4 = sequence {GAC3 OAc}
set AAC4 tail AAC4.2.C3
set BAC4 tail BAC4.2.C3
set GAC4 tail GAC4.2.C3
AAC5 = sequence {AAC4 OAc}
BAC5 = sequence {BAC4 OAc}
GAC5 = sequence {GAC4 OAc}
set AAC5 tail AAC5.2.C2
set BAC5 tail BAC5.2.C2
set GAC5 tail GAC5.2.C2
AAC6 = sequence {AAC5 OAc}
BAC6 = sequence {BAC5 OAc}
GAC6 = sequence {GAC5 OAc}
set AAC6 tail AAC6.3.C6
```

```
set BAC6 tail BAC6.3.C6
set GAC6 tail GAC6.3.C6
AAC7 = sequence {AAC6 OAc}
BAC7 = sequence {BAC6 OAc}
GAC7 = sequence {GAC6 OAc}
set AAC7 tail AAC7.3.C3
set BAC7 tail BAC7.3.C3
set GAC7 tail GAC7.3.C3
AAC8 = sequence {AAC7 OAc}
BAC8 = sequence {BAC7 OAc}
GAC8 = sequence {GAC7 OAc}
set AAC8 tail AAC8.3.C2
set BAC8 tail BAC8.3.C2
set GAC8 tail GAC8.3.C2
AAC9 = sequence {AAC8 OAc}
BAC9 = sequence {BAC8 OAc}
GAC9 = sequence {GAC8 OAc}
set AAC9 tail AAC9.4.C6
set BAC9 tail BAC9.4.C6
set GAC9 tail GAC9.4.C6
AAC10 = sequence {AAC9 OAc}
BAC10 = sequence {BAC9 OAc}
GAC10 = sequence {GAC9 OAc}
set AAC10 tail AAC10.4.C3
set BAC10 tail BAC10.4.C3
set GAC10 tail GAC10.4.C3
AAC11 = sequence {AAC10 OAc}
BAC11 = sequence {BAC10 OAc}
GAC11 = sequence {GAC10 OAc}
set AAC11 tail AAC11.4.C2
set BAC11 tail BAC11.4.C2
set GAC11 tail GAC11.4.C2
AAC12 = sequence {AAC11 OAc}
BAC12 = sequence {BAC11 OAc}
GAC12 = sequence {GAC11 OAc}
set AAC12 tail AAC12.5.C6
set BAC12 tail BAC12.5.C6
set GAC12 tail GAC12.5.C6
AAC13 = sequence {AAC12 OAc}
BAC13 = sequence {BAC12 OAc}
GAC13 = sequence {GAC12 OAc}
set AAC13 tail AAC13.5.C3
set BAC13 tail BAC13.5.C3
set GAC13 tail GAC13.5.C3
AAC14 = sequence {AAC13 OAc}
BAC14 = sequence {BAC13 OAc}
GAC14 = sequence {GAC13 OAc}
set AAC14 tail AAC14.5.C2
set BAC14 tail BAC14.5.C2
set GAC14 tail GAC14.5.C2
AAC15 = sequence {AAC14 OAc}
BAC15 = sequence {BAC14 OAc}
GAC15 = sequence {GAC14 OAc}
set AAC15 tail AAC15.6.C6
set BAC15 tail BAC15.6.C6
set GAC15 tail GAC15.6.C6
AAC16 = sequence {AAC15 OAc}
```

```
BAC16 = sequence {BAC15 OAc}
GAC16 = sequence {GAC15 OAc}
set AAC16 tail AAC16.6.C3
set BAC16 tail BAC16.6.C3
set GAC16 tail GAC16.6.C3
AAC17 = sequence {AAC16 OAc}
BAC17 = sequence {BAC16 OAc}
GAC17 = sequence {GAC16 OAc}
set AAC17 tail AAC17.6.C2
set BAC17 tail BAC17.6.C2
set GAC17 tail GAC17.6.C2
ACDOAC = sequence {AAC17 OAc}   # End
BAC18 = sequence {BAC17 OAc}
GAC18 = sequence {GAC17 OAc}
set BAC18 tail BAC18.7.C6
set GAC18 tail GAC18.7.C6
BAC19 = sequence {BAC18 OAc}
GAC19 = sequence {GAC18 OAc}
set BAC19 tail BAC19.7.C3
set GAC19 tail GAC19.7.C3
BAC20 = sequence {BAC19 OAc}
GAC20 = sequence {GAC19 OAc}
set BAC20 tail BAC20.7.C2
set GAC20 tail GAC20.7.C2
BCDOAC = sequence {BAC20 OAc}   # End
GAC21 = sequence {GAC20 OAc}
set GAC21 tail GAC21.8.C6
GAC22 = sequence {GAC21 OAc}
set GAC22 tail GAC22.8.C3
GAC23 = sequence {GAC22 OAc}
set GAC23 tail GAC23.8.C2
GCDOAC = sequence {GAC23 OAc}   # End
set ACDOAC head ACDOAC.1.C4
set ACDOAC tail ACDOAC.6.O1
impose ACDOAC {1 2 3 4 5 6} {{O5 C1 O1 C4 90.0}{C1 O1 C4 C5 -95.00}}
bond ACDOAC.1.C4 ACDOAC.6.O1
set BCDOAC head BCDOAC.1.C4
set BCDOAC tail BCDOAC.7.O1
impose BCDOAC {1 2 3 4 5 6 7} {{O5 C1 O1 C4 98.0}{C1 O1 C4 C5 -103.00}}
bond BCDOAC.1.C4 BCDOAC.7.O1
set GCDOAC head GCDOAC.1.C4
set GCDOAC tail GCDOAC.8.O1
impose GCDOAC {1 2 3 4 5 6 7 8} {{O5 C1 O1 C4 109.0}{C1 O1 C4 C5 -111.00}}
bond GCDOAC.1.C4 GCDOAC.8.O1

# per-OBn alpha-cyclodextrin
ABN = sequence {MGR MGR MGR MGR MGR MGR}
BBN = sequence {MGR MGR MGR MGR MGR MGR MGR}
GBN = sequence {MGR MGR MGR MGR MGR MGR MGR MGR}
set ABN tail ABN.1.C6
set BBN tail BBN.1.C6
set GBN tail GBN.1.C6
ABN1 = sequence {ABN OBn}
BBN1 = sequence {BBN OBn}
GBN1 = sequence {GBN OBn}
set ABN1 tail ABN1.1.C3
set BBN1 tail BBN1.1.C3
```

```
set GBN1 tail GBN1.1.C3
ABN2 = sequence {ABN1 OBn}
BBN2 = sequence {BBN1 OBn}
GBN2 = sequence {GBN1 OBn}
set ABN2 tail ABN2.1.C2
set BBN2 tail BBN2.1.C2
set GBN2 tail GBN2.1.C2
ABN3 = sequence {ABN2 OBn}
BBN3 = sequence {BBN2 OBn}
GBN3 = sequence {GBN2 OBn}
set ABN3 tail ABN3.2.C6
set BBN3 tail BBN3.2.C6
set GBN3 tail GBN3.2.C6
ABN4 = sequence {ABN3 OBn}
BBN4 = sequence {BBN3 OBn}
GBN4 = sequence {GBN3 OBn}
set ABN4 tail ABN4.2.C3
set BBN4 tail BBN4.2.C3
set GBN4 tail GBN4.2.C3
ABN5 = sequence {ABN4 OBn}
BBN5 = sequence {BBN4 OBn}
GBN5 = sequence {GBN4 OBn}
set ABN5 tail ABN5.2.C2
set BBN5 tail BBN5.2.C2
set GBN5 tail GBN5.2.C2
ABN6 = sequence {ABN5 OBn}
BBN6 = sequence {BBN5 OBn}
GBN6 = sequence {GBN5 OBn}
set ABN6 tail ABN6.3.C6
set BBN6 tail BBN6.3.C6
set GBN6 tail GBN6.3.C6
ABN7 = sequence {ABN6 OBn}
BBN7 = sequence {BBN6 OBn}
GBN7 = sequence {GBN6 OBn}
set ABN7 tail ABN7.3.C3
set BBN7 tail BBN7.3.C3
set GBN7 tail GBN7.3.C3
ABN8 = sequence {ABN7 OBn}
BBN8 = sequence {BBN7 OBn}
GBN8 = sequence {GBN7 OBn}
set ABN8 tail ABN8.3.C2
set BBN8 tail BBN8.3.C2
set GBN8 tail GBN8.3.C2
ABN9 = sequence {ABN8 OBn}
BBN9 = sequence {BBN8 OBn}
GBN9 = sequence {GBN8 OBn}
set ABN9 tail ABN9.4.C6
set BBN9 tail BBN9.4.C6
set GBN9 tail GBN9.4.C6
ABN10 = sequence {ABN9 OBn}
BBN10 = sequence {BBN9 OBn}
GBN10 = sequence {GBN9 OBn}
set ABN10 tail ABN10.4.C3
set BBN10 tail BBN10.4.C3
set GBN10 tail GBN10.4.C3
ABN11 = sequence {ABN10 OBn}
BBN11 = sequence {BBN10 OBn}
```

```
GBN11 = sequence {GBN10 OBn}
set ABN11 tail ABN11.4.C2
set BBN11 tail BBN11.4.C2
set GBN11 tail GBN11.4.C2
ABN12 = sequence {ABN11 OBn}
BBN12 = sequence {BBN11 OBn}
GBN12 = sequence {GBN11 OBn}
set ABN12 tail ABN12.5.C6
set BBN12 tail BBN12.5.C6
set GBN12 tail GBN12.5.C6
ABN13 = sequence {ABN12 OBn}
BBN13 = sequence {BBN12 OBn}
GBN13 = sequence {GBN12 OBn}
set ABN13 tail ABN13.5.C3
set BBN13 tail BBN13.5.C3
set GBN13 tail GBN13.5.C3
ABN14 = sequence {ABN13 OBn}
BBN14 = sequence {BBN13 OBn}
GBN14 = sequence {GBN13 OBn}
set ABN14 tail ABN14.5.C2
set BBN14 tail BBN14.5.C2
set GBN14 tail GBN14.5.C2
ABN15 = sequence {ABN14 OBn}
BBN15 = sequence {BBN14 OBn}
GBN15 = sequence {GBN14 OBn}
set ABN15 tail ABN15.6.C6
set BBN15 tail BBN15.6.C6
set GBN15 tail GBN15.6.C6
ABN16 = sequence {ABN15 OBn}
BBN16 = sequence {BBN15 OBn}
GBN16 = sequence {GBN15 OBn}
set ABN16 tail ABN16.6.C3
set BBN16 tail BBN16.6.C3
set GBN16 tail GBN16.6.C3
ABN17 = sequence {ABN16 OBn}
BBN17 = sequence {BBN16 OBn}
GBN17 = sequence {GBN16 OBn}
set ABN17 tail ABN17.6.C2
set BBN17 tail BBN17.6.C2
set GBN17 tail GBN17.6.C2
ACDOBN = sequence {ABN17 OBn}   # End
BBN18 = sequence {BBN17 OBn}
GBN18 = sequence {GBN17 OBn}
set BBN18 tail BBN18.7.C6
set GBN18 tail GBN18.7.C6
BBN19 = sequence {BBN18 OBn}
GBN19 = sequence {GBN18 OBn}
set BBN19 tail BBN19.7.C3
set GBN19 tail GBN19.7.C3
BBN20 = sequence {BBN19 OBn}
GBN20 = sequence {GBN19 OBn}
set BBN20 tail BBN20.7.C2
set GBN20 tail GBN20.7.C2
BCDOBN = sequence {BBN20 OBn}   # End
GBN21 = sequence {GBN20 OBn}
set GBN21 tail GBN21.8.C6
GBN22 = sequence {GBN21 OBn}
```

```
set GBN22 tail GBN22.8.C3
GBN23 = sequence {GBN22 OBn}
set GBN23 tail GBN23.8.C2
GCDOBN = sequence {GBN23 OBn}   # End
set ACDOBN head ACDOBN.1.C4
set ACDOBN tail ACDOBN.6.O1
impose ACDOBN {1 2 3 4 5 6} {{O5 C1 O1 C4 90.0}{C1 O1 C4 C5 -95.00}}
bond ACDOBN.1.C4 ACDOBN.6.O1
set BCDOBN head BCDOBN.1.C4
set BCDOBN tail BCDOBN.7.O1
impose BCDOBN {1 2 3 4 5 6 7} {{O5 C1 O1 C4 98.0}{C1 O1 C4 C5 -103.00}}
bond BCDOBN.1.C4 BCDOBN.7.O1
set GCDOBN head GCDOBN.1.C4
set GCDOBN tail GCDOBN.8.O1
impose GCDOBN {1 2 3 4 5 6 7 8} {{O5 C1 O1 C4 109.0}{C1 O1 C4 C5 -111.00}}
bond GCDOBN.1.C4 GCDOBN.8.O1

# per-OBz alpha-cyclodextrin
ABZ = sequence {MGR MGR MGR MGR MGR MGR}
BBZ = sequence {MGR MGR MGR MGR MGR MGR MGR}
GBZ = sequence {MGR MGR MGR MGR MGR MGR MGR MGR}
set ABZ tail ABZ.1.C6
set BBZ tail BBZ.1.C6
set GBZ tail GBZ.1.C6
ABZ1 = sequence {ABZ OBz}
BBZ1 = sequence {BBZ OBz}
GBZ1 = sequence {GBZ OBz}
set ABZ1 tail ABZ1.1.C3
set BBZ1 tail BBZ1.1.C3
set GBZ1 tail GBZ1.1.C3
ABZ2 = sequence {ABZ1 OBz}
BBZ2 = sequence {BBZ1 OBz}
GBZ2 = sequence {GBZ1 OBz}
set ABZ2 tail ABZ2.1.C2
set BBZ2 tail BBZ2.1.C2
set GBZ2 tail GBZ2.1.C2
ABZ3 = sequence {ABZ2 OBz}
BBZ3 = sequence {BBZ2 OBz}
GBZ3 = sequence {GBZ2 OBz}
set ABZ3 tail ABZ3.2.C6
set BBZ3 tail BBZ3.2.C6
set GBZ3 tail GBZ3.2.C6
ABZ4 = sequence {ABZ3 OBz}
BBZ4 = sequence {BBZ3 OBz}
GBZ4 = sequence {GBZ3 OBz}
set ABZ4 tail ABZ4.2.C3
set BBZ4 tail BBZ4.2.C3
set GBZ4 tail GBZ4.2.C3
ABZ5 = sequence {ABZ4 OBz}
BBZ5 = sequence {BBZ4 OBz}
GBZ5 = sequence {GBZ4 OBz}
set ABZ5 tail ABZ5.2.C2
set BBZ5 tail BBZ5.2.C2
set GBZ5 tail GBZ5.2.C2
ABZ6 = sequence {ABZ5 OBz}
BBZ6 = sequence {BBZ5 OBz}
GBZ6 = sequence {GBZ5 OBz}
```

```
set ABZ6 tail ABZ6.3.C6
set BBZ6 tail BBZ6.3.C6
set GBZ6 tail GBZ6.3.C6
ABZ7 = sequence {ABZ6 OBz}
BBZ7 = sequence {BBZ6 OBz}
GBZ7 = sequence {GBZ6 OBz}
set ABZ7 tail ABZ7.3.C3
set BBZ7 tail BBZ7.3.C3
set GBZ7 tail GBZ7.3.C3
ABZ8 = sequence {ABZ7 OBz}
BBZ8 = sequence {BBZ7 OBz}
GBZ8 = sequence {GBZ7 OBz}
set ABZ8 tail ABZ8.3.C2
set BBZ8 tail BBZ8.3.C2
set GBZ8 tail GBZ8.3.C2
ABZ9 = sequence {ABZ8 OBz}
BBZ9 = sequence {BBZ8 OBz}
GBZ9 = sequence {GBZ8 OBz}
set ABZ9 tail ABZ9.4.C6
set BBZ9 tail BBZ9.4.C6
set GBZ9 tail GBZ9.4.C6
ABZ10 = sequence {ABZ9 OBz}
BBZ10 = sequence {BBZ9 OBz}
GBZ10 = sequence {GBZ9 OBz}
set ABZ10 tail ABZ10.4.C3
set BBZ10 tail BBZ10.4.C3
set GBZ10 tail GBZ10.4.C3
ABZ11 = sequence {ABZ10 OBz}
BBZ11 = sequence {BBZ10 OBz}
GBZ11 = sequence {GBZ10 OBz}
set ABZ11 tail ABZ11.4.C2
set BBZ11 tail BBZ11.4.C2
set GBZ11 tail GBZ11.4.C2
ABZ12 = sequence {ABZ11 OBz}
BBZ12 = sequence {BBZ11 OBz}
GBZ12 = sequence {GBZ11 OBz}
set ABZ12 tail ABZ12.5.C6
set BBZ12 tail BBZ12.5.C6
set GBZ12 tail GBZ12.5.C6
ABZ13 = sequence {ABZ12 OBz}
BBZ13 = sequence {BBZ12 OBz}
GBZ13 = sequence {GBZ12 OBz}
set ABZ13 tail ABZ13.5.C3
set BBZ13 tail BBZ13.5.C3
set GBZ13 tail GBZ13.5.C3
ABZ14 = sequence {ABZ13 OBz}
BBZ14 = sequence {BBZ13 OBz}
GBZ14 = sequence {GBZ13 OBz}
set ABZ14 tail ABZ14.5.C2
set BBZ14 tail BBZ14.5.C2
set GBZ14 tail GBZ14.5.C2
ABZ15 = sequence {ABZ14 OBz}
BBZ15 = sequence {BBZ14 OBz}
GBZ15 = sequence {GBZ14 OBz}
set ABZ15 tail ABZ15.6.C6
set BBZ15 tail BBZ15.6.C6
set GBZ15 tail GBZ15.6.C6
```

```
ABZ16 = sequence {ABZ15 OBz}
BBZ16 = sequence {BBZ15 OBz}
GBZ16 = sequence {GBZ15 OBz}
set ABZ16 tail ABZ16.6.C3
set BBZ16 tail BBZ16.6.C3
set GBZ16 tail GBZ16.6.C3
ABZ17 = sequence {ABZ16 OBz}
BBZ17 = sequence {BBZ16 OBz}
GBZ17 = sequence {GBZ16 OBz}
set ABZ17 tail ABZ17.6.C2
set BBZ17 tail BBZ17.6.C2
set GBZ17 tail GBZ17.6.C2
ACDOBZ = sequence {ABZ17 OBz}   # End
BBZ18 = sequence {BBZ17 OBz}
GBZ18 = sequence {GBZ17 OBz}
set BBZ18 tail BBZ18.7.C6
set GBZ18 tail GBZ18.7.C6
BBZ19 = sequence {BBZ18 OBz}
GBZ19 = sequence {GBZ18 OBz}
set BBZ19 tail BBZ19.7.C3
set GBZ19 tail GBZ19.7.C3
BBZ20 = sequence {BBZ19 OBz}
GBZ20 = sequence {GBZ19 OBz}
set BBZ20 tail BBZ20.7.C2
set GBZ20 tail GBZ20.7.C2
BCDOBZ = sequence {BBZ20 OBz}   # End
GBZ21 = sequence {GBZ20 OBz}
set GBZ21 tail GBZ21.8.C6
GBZ22 = sequence {GBZ21 OBz}
set GBZ22 tail GBZ22.8.C3
GBZ23 = sequence {GBZ22 OBz}
set GBZ23 tail GBZ23.8.C2
GCDOBZ = sequence {GBZ23 OBz}   # End
set ACDOBZ head ACDOBZ.1.C4
set ACDOBZ tail ACDOBZ.6.O1
impose ACDOBZ {1 2 3 4 5 6} {{O5 C1 O1 C4 90.0}{C1 O1 C4 C5 -95.00}}
bond ACDOBZ.1.C4 ACDOBZ.6.O1
set BCDOBZ head BCDOBZ.1.C4
set BCDOBZ tail BCDOBZ.7.O1
impose BCDOBZ {1 2 3 4 5 6 7} {{O5 C1 O1 C4 98.0}{C1 O1 C4 C5 -103.00}}
bond BCDOBZ.1.C4 BCDOBZ.7.O1
set GCDOBZ head GCDOBZ.1.C4
set GCDOBZ tail GCDOBZ.8.O1
impose GCDOBZ {1 2 3 4 5 6 7 8} {{O5 C1 O1 C4 109.0}{C1 O1 C4 C5 -111.00}}
bond GCDOBZ.1.C4 GCDOBZ.8.O1

# per-OMe alpha-cyclodextrin
AME = sequence {MGR MGR MGR MGR MGR MGR}
BME = sequence {MGR MGR MGR MGR MGR MGR MGR}
GME = sequence {MGR MGR MGR MGR MGR MGR MGR MGR}
set AME tail AME.1.C6
set BME tail BME.1.C6
set GME tail GME.1.C6
AME1 = sequence {AME OMe}
BME1 = sequence {BME OMe}
GME1 = sequence {GME OMe}
set AME1 tail AME1.1.C3
```

```
set BME1 tail BME1.1.C3
set GME1 tail GME1.1.C3
AME2 = sequence {AME1 OMe}
BME2 = sequence {BME1 OMe}
GME2 = sequence {GME1 OMe}
set AME2 tail AME2.1.C2
set BME2 tail BME2.1.C2
set GME2 tail GME2.1.C2
AME3 = sequence {AME2 OMe}
BME3 = sequence {BME2 OMe}
GME3 = sequence {GME2 OMe}
set AME3 tail AME3.2.C6
set BME3 tail BME3.2.C6
set GME3 tail GME3.2.C6
AME4 = sequence {AME3 OMe}
BME4 = sequence {BME3 OMe}
GME4 = sequence {GME3 OMe}
set AME4 tail AME4.2.C3
set BME4 tail BME4.2.C3
set GME4 tail GME4.2.C3
AME5 = sequence {AME4 OMe}
BME5 = sequence {BME4 OMe}
GME5 = sequence {GME4 OMe}
set AME5 tail AME5.2.C2
set BME5 tail BME5.2.C2
set GME5 tail GME5.2.C2
AME6 = sequence {AME5 OMe}
BME6 = sequence {BME5 OMe}
GME6 = sequence {GME5 OMe}
set AME6 tail AME6.3.C6
set BME6 tail BME6.3.C6
set GME6 tail GME6.3.C6
AME7 = sequence {AME6 OMe}
BME7 = sequence {BME6 OMe}
GME7 = sequence {GME6 OMe}
set AME7 tail AME7.3.C3
set BME7 tail BME7.3.C3
set GME7 tail GME7.3.C3
AME8 = sequence {AME7 OMe}
BME8 = sequence {BME7 OMe}
GME8 = sequence {GME7 OMe}
set AME8 tail AME8.3.C2
set BME8 tail BME8.3.C2
set GME8 tail GME8.3.C2
AME9 = sequence {AME8 OMe}
BME9 = sequence {BME8 OMe}
GME9 = sequence {GME8 OMe}
set AME9 tail AME9.4.C6
set BME9 tail BME9.4.C6
set GME9 tail GME9.4.C6
AME10 = sequence {AME9 OMe}
BME10 = sequence {BME9 OMe}
GME10 = sequence {GME9 OMe}
set AME10 tail AME10.4.C3
set BME10 tail BME10.4.C3
set GME10 tail GME10.4.C3
AME11 = sequence {AME10 OMe}
```

```
BME11 = sequence {BME10 OMe}
GME11 = sequence {GME10 OMe}
set AME11 tail AME11.4.C2
set BME11 tail BME11.4.C2
set GME11 tail GME11.4.C2
AME12 = sequence {AME11 OMe}
BME12 = sequence {BME11 OMe}
GME12 = sequence {GME11 OMe}
set AME12 tail AME12.5.C6
set BME12 tail BME12.5.C6
set GME12 tail GME12.5.C6
AME13 = sequence {AME12 OMe}
BME13 = sequence {BME12 OMe}
GME13 = sequence {GME12 OMe}
set AME13 tail AME13.5.C3
set BME13 tail BME13.5.C3
set GME13 tail GME13.5.C3
AME14 = sequence {AME13 OMe}
BME14 = sequence {BME13 OMe}
GME14 = sequence {GME13 OMe}
set AME14 tail AME14.5.C2
set BME14 tail BME14.5.C2
set GME14 tail GME14.5.C2
AME15 = sequence {AME14 OMe}
BME15 = sequence {BME14 OMe}
GME15 = sequence {GME14 OMe}
set AME15 tail AME15.6.C6
set BME15 tail BME15.6.C6
set GME15 tail GME15.6.C6
AME16 = sequence {AME15 OMe}
BME16 = sequence {BME15 OMe}
GME16 = sequence {GME15 OMe}
set AME16 tail AME16.6.C3
set BME16 tail BME16.6.C3
set GME16 tail GME16.6.C3
AME17 = sequence {AME16 OMe}
BME17 = sequence {BME16 OMe}
GME17 = sequence {GME16 OMe}
set AME17 tail AME17.6.C2
set BME17 tail BME17.6.C2
set GME17 tail GME17.6.C2
ACDOME = sequence {AME17 OMe}   # End
BME18 = sequence {BME17 OMe}
GME18 = sequence {GME17 OMe}
set BME18 tail BME18.7.C6
set GME18 tail GME18.7.C6
BME19 = sequence {BME18 OMe}
GME19 = sequence {GME18 OMe}
set BME19 tail BME19.7.C3
set GME19 tail GME19.7.C3
BME20 = sequence {BME19 OMe}
GME20 = sequence {GME19 OMe}
set BME20 tail BME20.7.C2
set GME20 tail GME20.7.C2
BCDOME = sequence {BME20 OMe}   # End
GME21 = sequence {GME20 OMe}
set GME21 tail GME21.8.C6
```

```
GME22 = sequence {GME21 OMe}
set GME22 tail GME22.8.C3
GME23 = sequence {GME22 OMe}
set GME23 tail GME23.8.C2
GCDOME = sequence {GME23 OMe}   # End
set ACDOME head ACDOME.1.C4
set ACDOME tail ACDOME.6.O1
impose ACDOME {1 2 3 4 5 6} {{O5 C1 O1 C4 90.0}{C1 O1 C4 C5 -95.00}}
bond ACDOME.1.C4 ACDOME.6.O1
set BCDOME head BCDOME.1.C4
set BCDOME tail BCDOME.7.O1
impose BCDOME {1 2 3 4 5 6 7} {{O5 C1 O1 C4 98.0}{C1 O1 C4 C5 -103.00}}
bond BCDOME.1.C4 BCDOME.7.O1
set GCDOME head GCDOME.1.C4
set GCDOME tail GCDOME.8.O1
impose GCDOME {1 2 3 4 5 6 7 8} {{O5 C1 O1 C4 109.0}{C1 O1 C4 C5 -111.00}}
bond GCDOME.1.C4 GCDOME.8.O1

# Summarize a-, b- and g-cyclodextrin names (per-OH, per-OAc, per-OBn, per-OBz & per-
OMe)
#
# per-OH a-CD = ACDOH | per-OAc a-CD = ACDOAC | per-OBn a-CD = ACDOBN | per-OBz a-CD =
ACDOBZ | per-OMe a-CD = ACDOME
# per-OH b-CD = BCDOH | per-OAc b-CD = BCDOAC | per-OBn b-CD = BCDOBN | per-OBz b-CD =
BCDOBZ | per-OMe b-CD = BCDOME
# per-OH g-CD = GCDOH | per-OAc g-CD = GCDOAC | per-OBn g-CD = GCDOBN | per-OBz g-CD =
GCDOBZ | per-OMe g-CD = GCDOME

##############################################
#  CREATE PER-OH WITH PEPTIDO-MANNO ARM(S)  #
##############################################

# Define the peptidic arm-1
DIM1 = sequence { AMO BM3 }
set DIM1 head DIM1.2.C6
TIM1 = sequence { AMO DIM1 }
set TIM1 head TIM1.3.NH1
PEP1 = sequence { SCC TYR TIM1 }
set PEP1 tail PEP1.1.N1
CJG1 = sequence { PEP1 MGC }
set CJG1 head CJG1.6.C4
set CJG1 tail CJG1.6.O1

# Define the peptidic arm-2
DIM2 = sequence { AMO BM4 }
set DIM2 head DIM2.2.C6
TIM2 = sequence { AMO DIM2 }
set TIM2 head TIM2.3.NH1
PEP2 = sequence { SCC TYR TIM2 }
set PEP2 tail PEP2.1.N1
CJG2 = sequence { PEP2 MGC }
set CJG2 head CJG2.6.C4
set CJG2 tail CJG2.6.O1

# per-OH beta-cyclodextrin with one peptide arm
BCDOP1 = sequence {CJG1 MGO MGO MGO MGO MGO MGO}
set BCDOP1 head BCDOP1.6.C4
```

```
set BCDOP1 tail BCDOP1.12.O1
i BCDOP1 {5 6 7 8 9 10 11} {{O5 C1 O1 C4 98.0}{C1 O1 C4 C5 -103.00}}
#
bond BCDOP1.6.C4 BCDOP1.12.O1

# per-OH beta-cyclodextrin with one peptide arm
BCDOP2 = sequence {CJG2 MGO MGO MGO MGO MGO MGO}
set BCDOP2 head BCDOP2.6.C4
set BCDOP2 tail BCDOP2.12.O1
#
i BCDOP2 {6 7 8 9 10 11 12} {{O5 C1 O1 C4 98.0}{C1 O1 C4 C5 -103.00}}
#
bond BCDOP2.6.C4 BCDOP2.12.O1


##############################################################################
#                                                                            #
#                     The frcmod.q4md file for Leap/xleap                    #
#                                                                            #
##############################################################################


MASS

BOND
CA-CG  317.0    1.510                  Adapted from Parm99 = CA-CT

ANGL
OS-C -CG     95.0     110.80          From Glycam 2006
CG-OS-C      60.0     117.00          From Glycam 2006
CA-CG-H1     50.0     109.50          Adapted from Parm99 = CA-CT-HC
CA-CA-CG     70.0     120.00          Adapted from Parm99 = CA-CA-CT
CA-CG-OS     68.0     110.50          Adapted from GAFF   = ca-c3-os
CA-C -O      69.0     123.40          Adapted from GAFF   = ca-c -o
CA-C -OS     69.0     115.50          Adapted from GAFF   = ca-c -os

DIHEDRAL
OS-CG-CG-OH   1    0.144         0.0            -3          From parm98
              1    1.175         0.0             2
CG-OS-C -O    1   -3.20          0.0             2          From Glycam 2006
CG-C -OS-CG   1    3.00          0.0             2          From Glycam 2006
H1-CG-OS-C    1    0.00          0.0             3          From Glycam 2006
OS-C -CG-HC   1    0.00          0.0             3          From Glycam 2006
CG-CG-OS-C    1   -0.04          0.0            -3          From Glycam 2006
              1    0.47          0.0             1
CA-C -OS-CG   1    3.0           0.0             2          Adapted from Glycam 2006
(CG-C -OS-CG)
CA-CA-CA-CA   1    3.625       180.0             2          Adapted from Parm99
(14.5/4= 3.625)
CA-CA-CA-HA   1    3.625       180.0             2          Adapted from Parm99
CA-CA-CA-CA   1    3.625       180.0             2          Adapted from Parm99
HA-CA-CA-HA   1    3.625       180.0             2          Adapted from Parm99
HA-CA-CA-CG   1    3.625       180.0             2          Adapted from Parm99
CA-CA-CA-CG   1    3.625       180.0             2          Adapted from Parm99
HA-CA-CA-C    1    3.625       180.0             2          Adapted from Parm99
CA-CA-CA-C    1    3.625       180.0             2          Adapted from Parm99
CA-CA-C -O    1    3.625       180.0             2          Adapted from Parm99
```

```
CA-CA-C -OS    1    3.625       180.0             2          Adapted from Parm99
H1-CG-CA-CA    1    0.00          0.0             2          Adapted from Parm99
OS-CG-CA-CA    1    0.00          0.0             2          Adapted from Parm99
CA-CG-OS-CG    1    0.383         0.0            -3          Adapted from Parm99 (CT-
CT-OS-CT)
               1    0.1         180.0             2

IMPROPER
CG-O -C -OS          1.1         180.0             2          For acetate group
CA-CA-CA-CG          1.1         180.0             2          For benzyl group
CA-O -C -OS          1.1         180.0             2          For benzoyl group
CA-CA-CA-C           1.1         180.0             2          For benzoyl group

NONBOND

#########################################################################
#                                                                       #
#                     The 22 .mol2 files                                #
#                                                                       #
#########################################################################

@<TRIPOS>MOLECULE
MG2
   17    17     1     0     1
SMALL
USER_CHARGES
@<TRIPOS>ATOM
  1 C1          1.136334   -0.817888   -0.568646 C         1 MG2        0.0427 ****
  2 H1          1.629646   -1.347578   -1.380785 H         1 MG2        0.1610 ****
  3 O1          1.693018   -1.178781    0.641556 O         1 MG2       -0.3229 ****
  4 C2          1.286276    0.692637   -0.753039 C         1 MG2        0.1376 ****
  5 H2          0.893319    0.924482   -1.744331 H         1 MG2        0.0650 ****
  6 O2          2.610511    1.107081   -0.635813 O         1 MG2       -0.6346 ****
  7 HO2         3.115634    0.802626   -1.371102 H         1 MG2        0.4366 ****
  8 C3          0.447227    1.434454    0.283048 C         1 MG2        0.1224 ****
  9 H3          0.879881    1.235601    1.257571 H         1 MG2        0.1779 ****
 10 C4         -0.994062    0.923606    0.244390 C         1 MG2        0.0401 ****
 11 H4         -1.459363    1.220070   -0.688545 H         1 MG2        0.1595 ****
 12 C5         -1.054269   -0.606260    0.305489 C         1 MG2        0.0193 ****
 13 H5         -0.746412   -0.930062    1.299455 H         1 MG2        0.1156 ****
 14 O5         -0.202827   -1.180127   -0.659419 O         1 MG2       -0.3668 ****
 15 C6         -2.449769   -1.145415    0.061046 C         1 MG2        0.1918 ****
 16 H61        -3.093619   -0.804000    0.866610 H         1 MG2        0.0254 ****
 17 H62        -2.404699   -2.232005    0.089442 H         1 MG2        0.0254 ****
@<TRIPOS>BOND
    1    15    16 1
    2    15    17 1
    3    12    13 1
    4    12    14 1
    5    12    15 1
    6    10    11 1
    7    10    12 1
    8     8     9 1
    9     8    10 1
   10     6     7 1
   11     4     5 1
   12     4     6 1
```

```
   13     4     8 1
   14     1     2 1
   15     1     3 1
   16     1     4 1
   17     1    14 1
@<TRIPOS>SUBSTRUCTURE
      1  MG2              1 ****               0 ****  ****

-------------------------------------------------------------------------------
--

@<TRIPOS>MOLECULE
MG3
   17    17     1     0     1
SMALL
USER_CHARGES
@<TRIPOS>ATOM
  1 C1          1.136334   -0.817888   -0.568646 C         1 MG3        0.0427 ****
  2 H1          1.629646   -1.347578   -1.380785 H         1 MG3        0.1610 ****
  3 O1          1.693018   -1.178781    0.641556 O         1 MG3       -0.3229 ****
  4 C2          1.286276    0.692637   -0.753039 C         1 MG3        0.1376 ****
  5 H2          0.893319    0.924482   -1.744331 H         1 MG3        0.0650 ****
  6 C3          0.447227    1.434454    0.283048 C         1 MG3        0.1224 ****
  7 H3          0.879881    1.235601    1.257571 H         1 MG3        0.1779 ****
  8 O3          0.506247    2.818784    0.120021 O         1 MG3       -0.6200 ****
  9 HO3        -0.010885    3.082337   -0.624008 H         1 MG3        0.4220 ****
 10 C4         -0.994062    0.923606    0.244390 C         1 MG3        0.0401 ****
 11 H4         -1.459363    1.220070   -0.688545 H         1 MG3        0.1595 ****
 12 C5         -1.054269   -0.606260    0.305489 C         1 MG3        0.0193 ****
 13 H5         -0.746412   -0.930062    1.299455 H         1 MG3        0.1156 ****
 14 O5         -0.202827   -1.180127   -0.659419 O         1 MG3       -0.3668 ****
 15 C6         -2.449769   -1.145415    0.061046 C         1 MG3        0.1918 ****
 16 H61        -3.093619   -0.804000    0.866610 H         1 MG3        0.0254 ****
 17 H62        -2.404699   -2.232005    0.089442 H         1 MG3        0.0254 ****
@<TRIPOS>BOND
    1    15    16 1
    2    15    17 1
    3    12    13 1
    4    12    14 1
    5    12    15 1
    6    10    11 1
    7    10    12 1
    8     8     9 1
    9     6     7 1
   10     6     8 1
   11     6    10 1
   12     4     5 1
   13     4     6 1
   14     1     2 1
   15     1     3 1
   16     1     4 1
   17     1    14 1
@<TRIPOS>SUBSTRUCTURE
      1  MG3              1 ****               0 ****  ****

-------------------------------------------------------------------------------
--
```

```
@<TRIPOS>MOLECULE
MG6
   17    17     1     0     1
SMALL
USER_CHARGES
@<TRIPOS>ATOM
  1 C1          1.136334   -0.817888   -0.568646 C         1 MG6        0.0427 ****
  2 H1          1.629646   -1.347578   -1.380785 H         1 MG6        0.1610 ****
  3 O1          1.693018   -1.178781    0.641556 O         1 MG6       -0.3229 ****
  4 C2          1.286276    0.692637   -0.753039 C         1 MG6        0.1376 ****
  5 H2          0.893319    0.924482   -1.744331 H         1 MG6        0.0650 ****
  6 C3          0.447227    1.434454    0.283048 C         1 MG6        0.1224 ****
  7 H3          0.879881    1.235601    1.257571 H         1 MG6        0.1779 ****
  8 C4         -0.994062    0.923606    0.244390 C         1 MG6        0.0401 ****
  9 H4         -1.459363    1.220070   -0.688545 H         1 MG6        0.1595 ****
 10 C5         -1.054269   -0.606260    0.305489 C         1 MG6        0.0193 ****
 11 H5         -0.746412   -0.930062    1.299455 H         1 MG6        0.1156 ****
 12 O5         -0.202827   -1.180127   -0.659419 O         1 MG6       -0.3668 ****
 13 C6         -2.449769   -1.145415    0.061046 C         1 MG6        0.1918 ****
 14 H61        -3.093619   -0.804000    0.866610 H         1 MG6        0.0254 ****
 15 H62        -2.404699   -2.232005    0.089442 H         1 MG6        0.0254 ****
 16 O6         -2.912805   -0.695834   -1.180804 O         1 MG6       -0.6077 ****
 17 HO6        -3.815009   -0.942299   -1.293514 H         1 MG6        0.4097 ****
@<TRIPOS>BOND
    1    16    17 1
    2    13    14 1
    3    13    15 1
    4    13    16 1
    5    10    11 1
    6    10    12 1
    7    10    13 1
    8     8     9 1
    9     8    10 1
   10     6     7 1
   11     6     8 1
   12     4     5 1
   13     4     6 1
   14     1     2 1
   15     1     3 1
   16     1     4 1
   17     1    12 1
@<TRIPOS>SUBSTRUCTURE
      1  MG6             1 ****              0 ****  ****

-------------------------------------------------------------------------------
--

@<TRIPOS>MOLECULE
MGA
   19    19     1     0     1
SMALL
USER_CHARGES
@<TRIPOS>ATOM
  1 C1          1.136334   -0.817888   -0.568646 C         1 MGA        0.0427 ****
  2 H1          1.629646   -1.347578   -1.380785 H         1 MGA        0.1610 ****
  3 O1          1.693018   -1.178781    0.641556 O         1 MGA       -0.3229 ****
```

```
  4 C2          1.286276    0.692637   -0.753039 C         1 MGA        0.1376 ****
  5 H2          0.893319    0.924482   -1.744331 H         1 MGA        0.0650 ****
  6 C3          0.447227    1.434454    0.283048 C         1 MGA        0.1224 ****
  7 H3          0.879881    1.235601    1.257571 H         1 MGA        0.1779 ****
  8 O3          0.506247    2.818784    0.120021 O         1 MGA       -0.6200 ****
  9 HO3        -0.010885    3.082337   -0.624008 H         1 MGA        0.4220 ****
 10 C4         -0.994062    0.923606    0.244390 C         1 MGA        0.0401 ****
 11 H4         -1.459363    1.220070   -0.688545 H         1 MGA        0.1595 ****
 12 C5         -1.054269   -0.606260    0.305489 C         1 MGA        0.0193 ****
 13 H5         -0.746412   -0.930062    1.299455 H         1 MGA        0.1156 ****
 14 O5         -0.202827   -1.180127   -0.659419 O         1 MGA       -0.3668 ****
 15 C6         -2.449769   -1.145415    0.061046 C         1 MGA        0.1918 ****
 16 H61        -3.093619   -0.804000    0.866610 H         1 MGA        0.0254 ****
 17 H62        -2.404699   -2.232005    0.089442 H         1 MGA        0.0254 ****
 18 O6         -2.912805   -0.695834   -1.180804 O         1 MGA       -0.6077 ****
 19 HO6        -3.815009   -0.942299   -1.293514 H         1 MGA        0.4097 ****
@<TRIPOS>BOND
    1    18    19 1
    2    15    16 1
    3    15    17 1
    4    15    18 1
    5    12    13 1
    6    12    14 1
    7    12    15 1
    8    10    11 1
    9    10    12 1
   10     8     9 1
   11     6     7 1
   12     6     8 1
   13     6    10 1
   14     4     5 1
   15     4     6 1
   16     1     2 1
   17     1     3 1
   18     1     4 1
   19     1    14 1
@<TRIPOS>SUBSTRUCTURE
      1  MGA             1 ****              0 ****  ****

-------------------------------------------------------------------------------
--

@<TRIPOS>MOLECULE
MGB
   19    19     1     0     1
SMALL
USER_CHARGES
@<TRIPOS>ATOM
  1 C1          1.136334   -0.817888   -0.568646 C         1 MGB        0.0427 ****
  2 H1          1.629646   -1.347578   -1.380785 H         1 MGB        0.1610 ****
  3 O1          1.693018   -1.178781    0.641556 O         1 MGB       -0.3229 ****
  4 C2          1.286276    0.692637   -0.753039 C         1 MGB        0.1376 ****
  5 H2          0.893319    0.924482   -1.744331 H         1 MGB        0.0650 ****
  6 O2          2.610511    1.107081   -0.635813 O         1 MGB       -0.6346 ****
  7 HO2         3.115634    0.802626   -1.371102 H         1 MGB        0.4366 ****
  8 C3          0.447227    1.434454    0.283048 C         1 MGB        0.1224 ****
  9 H3          0.879881    1.235601    1.257571 H         1 MGB        0.1779 ****
```

```
 10 C4          -0.994062    0.923606    0.244390 C         1 MGB         0.0401 ****
 11 H4          -1.459363    1.220070   -0.688545 H         1 MGB         0.1595 ****
 12 C5          -1.054269   -0.606260    0.305489 C         1 MGB         0.0193 ****
 13 H5          -0.746412   -0.930062    1.299455 H         1 MGB         0.1156 ****
 14 O5          -0.202827   -1.180127   -0.659419 O         1 MGB        -0.3668 ****
 15 C6          -2.449769   -1.145415    0.061046 C         1 MGB         0.1918 ****
 16 H61         -3.093619   -0.804000    0.866610 H         1 MGB         0.0254 ****
 17 H62         -2.404699   -2.232005    0.089442 H         1 MGB         0.0254 ****
 18 O6          -2.912805   -0.695834   -1.180804 O         1 MGB        -0.6077 ****
 19 HO6         -3.815009   -0.942299   -1.293514 H         1 MGB         0.4097 ****
@<TRIPOS>BOND
    1    18    19 1
    2    15    16 1
    3    15    17 1
    4    15    18 1
    5    12    13 1
    6    12    14 1
    7    12    15 1
    8    10    11 1
    9    10    12 1
   10     8     9 1
   11     8    10 1
   12     6     7 1
   13     4     5 1
   14     4     6 1
   15     4     8 1
   16     1     2 1
   17     1     3 1
   18     1     4 1
   19     1    14 1
@<TRIPOS>SUBSTRUCTURE
      1  MGB              1 ****              0 ****  ****

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--

@<TRIPOS>MOLECULE
MGC
   19    19     1     0     1
SMALL
USER_CHARGES
@<TRIPOS>ATOM
  1 C1          1.136334   -0.817888   -0.568646 C         1 MGC         0.0427 ****
  2 H1          1.629646   -1.347578   -1.380785 H         1 MGC         0.1610 ****
  3 O1          1.693018   -1.178781    0.641556 O         1 MGC        -0.3229 ****
  4 C2          1.286276    0.692637   -0.753039 C         1 MGC         0.1376 ****
  5 H2          0.893319    0.924482   -1.744331 H         1 MGC         0.0650 ****
  6 O2          2.610511    1.107081   -0.635813 O         1 MGC        -0.6346 ****
  7 HO2         3.115634    0.802626   -1.371102 H         1 MGC         0.4366 ****
  8 C3          0.447227    1.434454    0.283048 C         1 MGC         0.1224 ****
  9 H3          0.879881    1.235601    1.257571 H         1 MGC         0.1779 ****
 10 O3          0.506247    2.818784    0.120021 O         1 MGC        -0.6200 ****
 11 HO3        -0.010885    3.082337   -0.624008 H         1 MGC         0.4220 ****
 12 C4         -0.994062    0.923606    0.244390 C         1 MGC         0.0401 ****
 13 H4         -1.459363    1.220070   -0.688545 H         1 MGC         0.1595 ****
 14 C5         -1.054269   -0.606260    0.305489 C         1 MGC         0.0193 ****
 15 H5         -0.746412   -0.930062    1.299455 H         1 MGC         0.1156 ****
```

```
 16 O5          -0.202827   -1.180127   -0.659419 O         1 MGC       -0.3668 ****
 17 C6          -2.449769   -1.145415    0.061046 C         1 MGC        0.1918 ****
 18 H61         -3.093619   -0.804000    0.866610 H         1 MGC        0.0254 ****
 19 H62         -2.404699   -2.232005    0.089442 H         1 MGC        0.0254 ****
@<TRIPOS>BOND
    1    17    18 1
    2    17    19 1
    3    14    15 1
    4    14    16 1
    5    14    17 1
    6    12    13 1
    7    12    14 1
    8    10    11 1
    9     8     9 1
   10     8    10 1
   11     8    12 1
   12     6     7 1
   13     4     5 1
   14     4     6 1
   15     4     8 1
   16     1     2 1
   17     1     3 1
   18     1     4 1
   19     1    16 1
@<TRIPOS>SUBSTRUCTURE
      1  MGC              1 ****              0 ****  ****

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--

@<TRIPOS>MOLECULE
MGO
   21    21     1     0     1
SMALL
USER_CHARGES
@<TRIPOS>ATOM
  1 C1           1.136334   -0.817888   -0.568646 C         1 MGO        0.0427 ****
  2 H1           1.629646   -1.347578   -1.380785 H         1 MGO        0.1610 ****
  3 O1           1.693018   -1.178781    0.641556 O         1 MGO       -0.3229 ****
  4 C2           1.286276    0.692637   -0.753039 C         1 MGO        0.1376 ****
  5 H2           0.893319    0.924482   -1.744331 H         1 MGO        0.0650 ****
  6 O2           2.610511    1.107081   -0.635813 O         1 MGO       -0.6346 ****
  7 HO2          3.115634    0.802626   -1.371102 H         1 MGO        0.4366 ****
  8 C3           0.447227    1.434454    0.283048 C         1 MGO        0.1224 ****
  9 H3           0.879881    1.235601    1.257571 H         1 MGO        0.1779 ****
 10 O3           0.506247    2.818784    0.120021 O         1 MGO       -0.6200 ****
 11 HO3         -0.010885    3.082337   -0.624008 H         1 MGO        0.4220 ****
 12 C4          -0.994062    0.923606    0.244390 C         1 MGO        0.0401 ****
 13 H4          -1.459363    1.220070   -0.688545 H         1 MGO        0.1595 ****
 14 C5          -1.054269   -0.606260    0.305489 C         1 MGO        0.0193 ****
 15 H5          -0.746412   -0.930062    1.299455 H         1 MGO        0.1156 ****
 16 O5          -0.202827   -1.180127   -0.659419 O         1 MGO       -0.3668 ****
 17 C6          -2.449769   -1.145415    0.061046 C         1 MGO        0.1918 ****
 18 H61         -3.093619   -0.804000    0.866610 H         1 MGO        0.0254 ****
 19 H62         -2.404699   -2.232005    0.089442 H         1 MGO        0.0254 ****
 20 O6          -2.912805   -0.695834   -1.180804 O         1 MGO       -0.6077 ****
 21 HO6         -3.815009   -0.942299   -1.293514 H         1 MGO        0.4097 ****
```

```
@<TRIPOS>BOND
    1     1     2 1
    2     1     3 1
    3     1     4 1
    4     1    16 1
    5     4     5 1
    6     4     6 1
    7     4     8 1
    8     6     7 1
    9     8     9 1
   10     8    10 1
   11     8    12 1
   12    10    11 1
   13    12    13 1
   14    12    14 1
   15    14    15 1
   16    14    16 1
   17    14    17 1
   18    17    18 1
   19    17    19 1
   20    17    20 1
   21    20    21 1
@<TRIPOS>SUBSTRUCTURE
      1  MGO             1 ****               0 ****  ****

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--

@<TRIPOS>MOLECULE
MGR
   15    15     1     0     1
SMALL
USER_CHARGES
@<TRIPOS>ATOM
  1 C1          1.136334   -0.817888   -0.568646 C         1 MGR        0.0427 ****
  2 H1          1.629646   -1.347578   -1.380785 H         1 MGR        0.1610 ****
  3 O1          1.693018   -1.178781    0.641556 O         1 MGR       -0.3229 ****
  4 C2          1.286276    0.692637   -0.753039 C         1 MGR        0.1376 ****
  5 H2          0.893319    0.924482   -1.744331 H         1 MGR        0.0650 ****
  6 C3          0.447227    1.434454    0.283048 C         1 MGR        0.1224 ****
  7 H3          0.879881    1.235601    1.257571 H         1 MGR        0.1779 ****
  8 C4         -0.994062    0.923606    0.244390 C         1 MGR        0.0401 ****
  9 H4         -1.459363    1.220070   -0.688545 H         1 MGR        0.1595 ****
 10 C5         -1.054269   -0.606260    0.305489 C         1 MGR        0.0193 ****
 11 H5         -0.746412   -0.930062    1.299455 H         1 MGR        0.1156 ****
 12 O5         -0.202827   -1.180127   -0.659419 O         1 MGR       -0.3668 ****
 13 C6         -2.449769   -1.145415    0.061046 C         1 MGR        0.1918 ****
 14 H61        -3.093619   -0.804000    0.866610 H         1 MGR        0.0254 ****
 15 H62        -2.404699   -2.232005    0.089442 H         1 MGR        0.0254 ****
@<TRIPOS>BOND
    1     1     2 1
    2     1     3 1
    3     1     4 1
    4     1    12 1
    5     4     5 1
    6     4     6 1
    7     6     7 1
```

```
     8     6     8 1
     9     8     9 1
    10     8    10 1
    11    10    11 1
    12    10    12 1
    13    10    13 1
    14    13    14 1
    15    13    15 1
@<TRIPOS>SUBSTRUCTURE
      1  MGR              1 ****               0 ****  ****

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--

@<TRIPOS>MOLECULE
OAc
    7     6     1     0     1
SMALL
USER_CHARGES
@<TRIPOS>ATOM
  1 OS          -0.546964   -0.695306   -0.000002 O         1 OAc       -0.3896 ****
  2 C            0.453509    0.175601   -0.000001 C         1 OAc        0.8849 ****
  3 O            0.294643    1.353062    0.000000 O         1 OAc       -0.6087 ****
  4 CM           1.786906   -0.518656    0.000000 C         1 OAc       -0.4521 ****
  5 HM1          1.867409   -1.153390   -0.874969 H         1 OAc        0.1225 ****
  6 HM2          2.577341    0.216914   -0.000018 H         1 OAc        0.1225 ****
  7 HM3          1.867423   -1.153357    0.874993 H         1 OAc        0.1225 ****
@<TRIPOS>BOND
     1     1     2 1
     2     2     3 1
     3     2     4 1
     4     4     5 1
     5     4     6 1
     6     4     7 1
@<TRIPOS>SUBSTRUCTURE
      1  OAc              1 ****               0 ****  ****

-------------------------------------------------------------------------------
--

@<TRIPOS>MOLECULE
OBn
   15    15     1     0     1
SMALL
USER_CHARGES
@<TRIPOS>ATOM
  1 OS          -2.184356    0.421976   -0.108366 O         1 OBn       -0.3527 ****
  2 CM          -1.364822   -0.683424    0.103455 C         1 OBn        0.1086 ****
  3 HM1         -1.568124   -1.451398   -0.643776 H         1 OBn        0.0382 ****
  4 HM2         -1.579314   -1.124511    1.078724 H         1 OBn        0.0382 ****
  5 C1           0.093002   -0.288060    0.038803 C         1 OBn        0.0662 ****
  6 C2           0.493032    1.039274    0.053176 C         1 OBn       -0.1410 ****
  7 H2          -0.249060    1.813380    0.086799 H         1 OBn        0.1140 ****
  8 C3           1.841606    1.363263    0.017153 C         1 OBn       -0.1639 ****
  9 H3           2.139056    2.397429    0.025972 H         1 OBn        0.1469 ****
 10 C4           2.801700    0.368610   -0.030441 C         1 OBn       -0.1467 ****
 11 H4           3.846517    0.623368   -0.058729 H         1 OBn        0.1382 ****
```

```
 12 C5          2.406879   -0.960553   -0.044720 C         1 OBn       -0.1639 ****
 13 H5          3.144597   -1.742817   -0.085177 H         1 OBn        0.1469 ****
 14 C6          1.062716   -1.283587   -0.012447 C         1 OBn       -0.1410 ****
 15 H6          0.765304   -2.319425   -0.029610 H         1 OBn        0.1140 ****
@<TRIPOS>BOND
    1     1     2 1
    2     2     3 1
    3     2     4 1
    4     2     5 1
    5     5     6 1
    6     5    14 1
    7     6     7 1
    8     6     8 1
    9     8     9 1
   10     8    10 1
   11    10    11 1
   12    10    12 1
   13    12    13 1
   14    12    14 1
   15    14    15 1
@<TRIPOS>SUBSTRUCTURE
      1  OBn              1 ****              0 ****  ****

-------------------------------------------------------------------------------
--

@<TRIPOS>MOLECULE
OBz
   14    14     1     0     1
SMALL
USER_CHARGES
@<TRIPOS>ATOM
  1 OS          -1.964676   -0.713969    0.000000 O         1 OBz       -0.3457 ****
  2 C           -1.233492    0.390187    0.000000 C         1 OBz        0.7379 ****
  3 O           -1.709192    1.482339    0.000000 O         1 OBz       -0.5479 ****
  4 C1           0.232373    0.120564    0.000000 C         1 OBz       -0.1094 ****
  5 C2           1.095370    1.210135    0.000000 C         1 OBz       -0.0927 ****
  6 H2           0.681925    2.200949    0.000000 H         1 OBz        0.1153 ****
  7 C3           2.463449    1.010110    0.000000 C         1 OBz       -0.1218 ****
  8 H3           3.129930    1.853899    0.000000 H         1 OBz        0.1282 ****
  9 C4           2.972673   -0.279553    0.000000 C         1 OBz       -0.1251 ****
 10 H4           4.037203   -0.435724    0.000000 H         1 OBz        0.1342 ****
 11 C5           2.115565   -1.368370    0.000000 C         1 OBz       -0.1218 ****
 12 H5           2.512756   -2.367641    0.000000 H         1 OBz        0.1282 ****
 13 C6           0.745635   -1.170861    0.000000 C         1 OBz       -0.0927 ****
 14 H6           0.077442   -2.010376    0.000000 H         1 OBz        0.1153 ****
@<TRIPOS>BOND
    1     1     2 1
    2     2     3 1
    3     2     4 1
    4     4     5 1
    5     4    13 1
    6     5     6 1
    7     5     7 1
    8     7     8 1
    9     7     9 1
   10     9    10 1
```

```
   11     9    11 1
   12    11    12 1
   13    11    13 1
   14    13    14 1
@<TRIPOS>SUBSTRUCTURE
      1  OBz              1 ****               0 ****  ****

-------------------------------------------------------------------------------
--

@<TRIPOS>MOLECULE
OMe
    5     4     1     0     1
SMALL
USER_CHARGES
@<TRIPOS>ATOM
  1 OS          -0.000011   -0.570627    0.000000 O         1 OMe       -0.3813 ****
  2 CM           1.166176    0.188570    0.000000 C         1 OMe        0.0123 ****
  3 HM1          1.230810    0.823246   -0.883390 H         1 OMe        0.0570 ****
  4 HM2          2.004450   -0.495460    0.000022 H         1 OMe        0.0570 ****
  5 HM3          1.230791    0.823278    0.883369 H         1 OMe        0.0570 ****
@<TRIPOS>BOND
    1     1     2 1
    2     2     3 1
    3     2     4 1
    4     2     5 1
@<TRIPOS>SUBSTRUCTURE
      1  OMe              1 ****               0 ****  ****

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--

@<TRIPOS>MOLECULE
SCC
   12    11     1     0     1
SMALL
USER_CHARGES
@<TRIPOS>ATOM
  1 N1           2.987211    0.617845   -0.179016 N         1 SCC       -0.5424 ****
  2 H1           2.831764    1.594953   -0.257116 H         1 SCC        0.3118 ****
  3 C1           1.925791   -0.192676    0.030327 C         1 SCC        0.5391 ****
  4 O1           2.047315   -1.369149    0.247703 O         1 SCC       -0.5628 ****
  5 C2           0.575148    0.497318   -0.029800 C         1 SCC        0.0540 ****
  6 H21          0.530205    1.132428   -0.908742 H         1 SCC       -0.0070 ****
  7 H22          0.485956    1.161628    0.823695 H         1 SCC       -0.0070 ****
  8 C3          -0.575148   -0.497320   -0.029781 C         1 SCC        0.0540 ****
  9 H31         -0.530210   -1.132458   -0.908704 H         1 SCC       -0.0070 ****
 10 H32         -0.485952   -1.161604    0.823734 H         1 SCC       -0.0070 ****
 11 C4          -1.925791    0.192675    0.030335 C         1 SCC        0.5391 ****
 12 O4          -2.047315    1.369149    0.247711 O         1 SCC       -0.5628 ****
@<TRIPOS>BOND
    1     1     2 1
    2     1     3 1
    3     3     4 1
    4     3     5 1
    5     5     6 1
    6     5     7 1
```

```
     7     5     8 1
     8     8     9 1
     9     8    10 1
    10     8    11 1
    11    11    12 1
@<TRIPOS>SUBSTRUCTURE
      1  SCC              1 ****               0 ****  ****

-------------------------------------------------------------------------------
--

@<TRIPOS>MOLECULE
BM3
    20    20     1     0     1
SMALL
USER_CHARGES
@<TRIPOS>ATOM
  1 C1          0.827809   -0.370435   -0.345635 C         1 BM3        0.0394 ****
  2 H1          0.968653   -0.402864   -1.420166 H         1 BM3        0.1574 ****
  3 NH1         2.111482   -0.431191    0.266074 N         1 BM3       -0.3845 ****
  4 HN1         2.093855   -0.507509    1.258340 H         1 BM3        0.3057 ****
  5 C2         -0.032022   -1.543880    0.103245 C         1 BM3       -0.0429 ****
  6 H2          0.388772   -2.474888   -0.273095 H         1 BM3        0.1057 ****
  7 O2         -0.066547   -1.550012    1.504047 O         1 BM3       -0.6107 ****
  8 HO2        -0.169873   -2.430813    1.819869 H         1 BM3        0.4591 ****
  9 C3         -1.447276   -1.406027   -0.459192 C         1 BM3        0.1591 ****
 10 H3         -1.386846   -1.477181   -1.549446 H         1 BM3        0.0516 ****
 11 O3         -2.273731   -2.420086    0.043691 O         1 BM3       -0.6480 ****
 12 HO3        -2.237300   -3.179543   -0.512596 H         1 BM3        0.4380 ****
 13 C4         -2.036990   -0.046228   -0.108559 C         1 BM3        0.0956 ****
 14 H4         -2.194702    0.003532    0.957447 H         1 BM3        0.2163 ****
 15 C5         -1.054804    1.057018   -0.523232 C         1 BM3        0.0020 ****
 16 H5         -0.982857    1.064561   -1.616764 H         1 BM3        0.0806 ****
 17 O5          0.216236    0.833997    0.022767 O         1 BM3       -0.2405 ****
 18 C6         -1.510421    2.439621   -0.100059 C         1 BM3        0.2171 ****
 19 H61        -0.744596    3.151988   -0.398264 H         1 BM3        0.0095 ****
 20 H62        -2.428896    2.673315   -0.630836 H         1 BM3        0.0095 ****
@<TRIPOS>BOND
    1    18    19 1
    2    18    20 1
    3    15    16 1
    4    15    17 1
    5    15    18 1
    6    13    14 1
    7    13    15 1
    8    11    12 1
    9     9    10 1
   10     9    11 1
   11     9    13 1
   12     7     8 1
   13     5     6 1
   14     5     7 1
   15     5     9 1
   16     3     4 1
   17     1     2 1
   18     1     3 1
   19     1     5 1
```

```
   20     1    17 1
@<TRIPOS>SUBSTRUCTURE
      1  BM3              1 ****               0 ****  ****

-------------------------------------------------------------------------------
--

@<TRIPOS>MOLECULE
BM4
   20    20     1     0     1
SMALL
USER_CHARGES
@<TRIPOS>ATOM
  1 C1          0.827809   -0.370435   -0.345635 C         1 BM4        0.0394 ****
  2 H1          0.968653   -0.402864   -1.420166 H         1 BM4        0.1574 ****
  3 NH1         2.111482   -0.431191    0.266074 N         1 BM4       -0.3845 ****
  4 HN1         2.093855   -0.507509    1.258340 H         1 BM4        0.3057 ****
  5 C2         -0.032022   -1.543880    0.103245 C         1 BM4       -0.0429 ****
  6 H2          0.388772   -2.474888   -0.273095 H         1 BM4        0.1057 ****
  7 O2         -0.066547   -1.550012    1.504047 O         1 BM4       -0.6107 ****
  8 HO2        -0.169873   -2.430813    1.819869 H         1 BM4        0.4591 ****
  9 C3         -1.447276   -1.406027   -0.459192 C         1 BM4        0.1591 ****
 10 H3         -1.386846   -1.477181   -1.549446 H         1 BM4        0.0516 ****
 11 C4         -2.036990   -0.046228   -0.108559 C         1 BM4        0.0956 ****
 12 H4         -2.194702    0.003532    0.957447 H         1 BM4        0.2163 ****
 13 O4         -3.286112    0.157568   -0.710207 O         1 BM4       -0.6309 ****
 14 HO4        -3.244560   -0.043291   -1.631267 H         1 BM4        0.4209 ****
 15 C5         -1.054804    1.057018   -0.523232 C         1 BM4        0.0020 ****
 16 H5         -0.982857    1.064561   -1.616764 H         1 BM4        0.0806 ****
 17 O5          0.216236    0.833997    0.022767 O         1 BM4       -0.2405 ****
 18 C6         -1.510421    2.439621   -0.100059 C         1 BM4        0.2171 ****
 19 H61        -0.744596    3.151988   -0.398264 H         1 BM4        0.0095 ****
 20 H62        -2.428896    2.673315   -0.630836 H         1 BM4        0.0095 ****
@<TRIPOS>BOND
    1    18    19 1
    2    18    20 1
    3    15    16 1
    4    15    17 1
    5    15    18 1
    6    13    14 1
    7    11    12 1
    8    11    13 1
    9    11    15 1
   10     9    10 1
   11     9    11 1
   12     7     8 1
   13     5     6 1
   14     5     7 1
   15     5     9 1
   16     3     4 1
   17     1     2 1
   18     1     3 1
   19     1     5 1
   20     1    17 1
@<TRIPOS>SUBSTRUCTURE
      1  BM4              1 ****               0 ****  ****
```

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@<TRIPOS>MOLECULE
BM6
   20    20     1     0     1
SMALL
USER_CHARGES
@<TRIPOS>ATOM
  1 C1          0.827809   -0.370435   -0.345635 C         1 BM6        0.0394 ****
  2 H1          0.968653   -0.402864   -1.420166 H         1 BM6        0.1574 ****
  3 NH1         2.111482   -0.431191    0.266074 N         1 BM6       -0.3845 ****
  4 HN1         2.093855   -0.507509    1.258340 H         1 BM6        0.3057 ****
  5 C2         -0.032022   -1.543880    0.103245 C         1 BM6       -0.0429 ****
  6 H2          0.388772   -2.474888   -0.273095 H         1 BM6        0.1057 ****
  7 O2         -0.066547   -1.550012    1.504047 O         1 BM6       -0.6107 ****
  8 HO2        -0.169873   -2.430813    1.819869 H         1 BM6        0.4591 ****
  9 C3         -1.447276   -1.406027   -0.459192 C         1 BM6        0.1591 ****
 10 H3         -1.386846   -1.477181   -1.549446 H         1 BM6        0.0516 ****
 11 C4         -2.036990   -0.046228   -0.108559 C         1 BM6        0.0956 ****
 12 H4         -2.194702    0.003532    0.957447 H         1 BM6        0.2163 ****
 13 C5         -1.054804    1.057018   -0.523232 C         1 BM6        0.0020 ****
 14 H5         -0.982857    1.064561   -1.616764 H         1 BM6        0.0806 ****
 15 O5          0.216236    0.833997    0.022767 O         1 BM6       -0.2405 ****
 16 C6         -1.510421    2.439621   -0.100059 C         1 BM6        0.2171 ****
 17 H61        -0.744596    3.151988   -0.398264 H         1 BM6        0.0095 ****
 18 H62        -2.428896    2.673315   -0.630836 H         1 BM6        0.0095 ****
 19 O6         -1.707325    2.461396    1.284348 O         1 BM6       -0.6280 ****
 20 HO6        -2.085921    3.285391    1.539200 H         1 BM6        0.4180 ****
@<TRIPOS>BOND
    1    19    20 1
    2    16    17 1
    3    16    18 1
    4    16    19 1
    5    13    14 1
    6    13    15 1
    7    13    16 1
    8    11    12 1
    9    11    13 1
   10     9    10 1
   11     9    11 1
   12     7     8 1
   13     5     6 1
   14     5     7 1
   15     5     9 1
   16     3     4 1
   17     1     2 1
   18     1     3 1
   19     1     5 1
   20     1    15 1
@<TRIPOS>SUBSTRUCTURE
      1  BM6             1 ****              0 ****  ****

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@<TRIPOS>MOLECULE
```

```
BMA
   22    22     1     0     1
SMALL
USER_CHARGES
@<TRIPOS>ATOM
  1 C1          0.827809   -0.370435   -0.345635 C         1 BMA        0.0394 ****
  2 H1          0.968653   -0.402864   -1.420166 H         1 BMA        0.1574 ****
  3 NH1         2.111482   -0.431191    0.266074 N         1 BMA       -0.3845 ****
  4 HN1         2.093855   -0.507509    1.258340 H         1 BMA        0.3057 ****
  5 C2         -0.032022   -1.543880    0.103245 C         1 BMA       -0.0429 ****
  6 H2          0.388772   -2.474888   -0.273095 H         1 BMA        0.1057 ****
  7 O2         -0.066547   -1.550012    1.504047 O         1 BMA       -0.6107 ****
  8 HO2        -0.169873   -2.430813    1.819869 H         1 BMA        0.4591 ****
  9 C3         -1.447276   -1.406027   -0.459192 C         1 BMA        0.1591 ****
 10 H3         -1.386846   -1.477181   -1.549446 H         1 BMA        0.0516 ****
 11 C4         -2.036990   -0.046228   -0.108559 C         1 BMA        0.0956 ****
 12 H4         -2.194702    0.003532    0.957447 H         1 BMA        0.2163 ****
 13 O4         -3.286112    0.157568   -0.710207 O         1 BMA       -0.6309 ****
 14 HO4        -3.244560   -0.043291   -1.631267 H         1 BMA        0.4209 ****
 15 C5         -1.054804    1.057018   -0.523232 C         1 BMA        0.0020 ****
 16 H5         -0.982857    1.064561   -1.616764 H         1 BMA        0.0806 ****
 17 O5          0.216236    0.833997    0.022767 O         1 BMA       -0.2405 ****
 18 C6         -1.510421    2.439621   -0.100059 C         1 BMA        0.2171 ****
 19 H61        -0.744596    3.151988   -0.398264 H         1 BMA        0.0095 ****
 20 H62        -2.428896    2.673315   -0.630836 H         1 BMA        0.0095 ****
 21 O6         -1.707325    2.461396    1.284348 O         1 BMA       -0.6280 ****
 22 HO6        -2.085921    3.285391    1.539200 H         1 BMA        0.4180 ****
@<TRIPOS>BOND
    1    21    22 1
    2    18    19 1
    3    18    20 1
    4    18    21 1
    5    15    16 1
    6    15    17 1
    7    15    18 1
    8    13    14 1
    9    11    12 1
   10    11    13 1
   11    11    15 1
   12     9    10 1
   13     9    11 1
   14     7     8 1
   15     5     6 1
   16     5     7 1
   17     5     9 1
   18     3     4 1
   19     1     2 1
   20     1     3 1
   21     1     5 1
   22     1    17 1
@<TRIPOS>SUBSTRUCTURE
      1  BMA              1 ****               0 ****  ****

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@<TRIPOS>MOLECULE
```

```
BMB
   22    22     1     0     1
SMALL
USER_CHARGES
@<TRIPOS>ATOM
  1 C1          0.827809   -0.370435   -0.345635 C         1 BMB        0.0394 ****
  2 H1          0.968653   -0.402864   -1.420166 H         1 BMB        0.1574 ****
  3 NH1         2.111482   -0.431191    0.266074 N         1 BMB       -0.3845 ****
  4 HN1         2.093855   -0.507509    1.258340 H         1 BMB        0.3057 ****
  5 C2         -0.032022   -1.543880    0.103245 C         1 BMB       -0.0429 ****
  6 H2          0.388772   -2.474888   -0.273095 H         1 BMB        0.1057 ****
  7 O2         -0.066547   -1.550012    1.504047 O         1 BMB       -0.6107 ****
  8 HO2        -0.169873   -2.430813    1.819869 H         1 BMB        0.4591 ****
  9 C3         -1.447276   -1.406027   -0.459192 C         1 BMB        0.1591 ****
 10 H3         -1.386846   -1.477181   -1.549446 H         1 BMB        0.0516 ****
 11 O3         -2.273731   -2.420086    0.043691 O         1 BMB       -0.6480 ****
 12 HO3        -2.237300   -3.179543   -0.512596 H         1 BMB        0.4380 ****
 13 C4         -2.036990   -0.046228   -0.108559 C         1 BMB        0.0956 ****
 14 H4         -2.194702    0.003532    0.957447 H         1 BMB        0.2163 ****
 15 C5         -1.054804    1.057018   -0.523232 C         1 BMB        0.0020 ****
 16 H5         -0.982857    1.064561   -1.616764 H         1 BMB        0.0806 ****
 17 O5          0.216236    0.833997    0.022767 O         1 BMB       -0.2405 ****
 18 C6         -1.510421    2.439621   -0.100059 C         1 BMB        0.2171 ****
 19 H61        -0.744596    3.151988   -0.398264 H         1 BMB        0.0095 ****
 20 H62        -2.428896    2.673315   -0.630836 H         1 BMB        0.0095 ****
 21 O6         -1.707325    2.461396    1.284348 O         1 BMB       -0.6280 ****
 22 HO6        -2.085921    3.285391    1.539200 H         1 BMB        0.4180 ****
@<TRIPOS>BOND
    1    21    22 1
    2    18    19 1
    3    18    20 1
    4    18    21 1
    5    15    16 1
    6    15    17 1
    7    15    18 1
    8    13    14 1
    9    13    15 1
   10    11    12 1
   11     9    10 1
   12     9    11 1
   13     9    13 1
   14     7     8 1
   15     5     6 1
   16     5     7 1
   17     5     9 1
   18     3     4 1
   19     1     2 1
   20     1     3 1
   21     1     5 1
   22     1    17 1
@<TRIPOS>SUBSTRUCTURE
      1  BMB             1 ****              0 ****  ****

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@<TRIPOS>MOLECULE
```

```
BMC
   22    22     1     0     1
SMALL
USER_CHARGES
@<TRIPOS>ATOM
  1 C1          0.827809   -0.370435   -0.345635 C         1 BMC        0.0394 ****
  2 H1          0.968653   -0.402864   -1.420166 H         1 BMC        0.1574 ****
  3 NH1         2.111482   -0.431191    0.266074 N         1 BMC       -0.3845 ****
  4 HN1         2.093855   -0.507509    1.258340 H         1 BMC        0.3057 ****
  5 C2         -0.032022   -1.543880    0.103245 C         1 BMC       -0.0429 ****
  6 H2          0.388772   -2.474888   -0.273095 H         1 BMC        0.1057 ****
  7 O2         -0.066547   -1.550012    1.504047 O         1 BMC       -0.6107 ****
  8 HO2        -0.169873   -2.430813    1.819869 H         1 BMC        0.4591 ****
  9 C3         -1.447276   -1.406027   -0.459192 C         1 BMC        0.1591 ****
 10 H3         -1.386846   -1.477181   -1.549446 H         1 BMC        0.0516 ****
 11 O3         -2.273731   -2.420086    0.043691 O         1 BMC       -0.6480 ****
 12 HO3        -2.237300   -3.179543   -0.512596 H         1 BMC        0.4380 ****
 13 C4         -2.036990   -0.046228   -0.108559 C         1 BMC        0.0956 ****
 14 H4         -2.194702    0.003532    0.957447 H         1 BMC        0.2163 ****
 15 O4         -3.286112    0.157568   -0.710207 O         1 BMC       -0.6309 ****
 16 HO4        -3.244560   -0.043291   -1.631267 H         1 BMC        0.4209 ****
 17 C5         -1.054804    1.057018   -0.523232 C         1 BMC        0.0020 ****
 18 H5         -0.982857    1.064561   -1.616764 H         1 BMC        0.0806 ****
 19 O5          0.216236    0.833997    0.022767 O         1 BMC       -0.2405 ****
 20 C6         -1.510421    2.439621   -0.100059 C         1 BMC        0.2171 ****
 21 H61        -0.744596    3.151988   -0.398264 H         1 BMC        0.0095 ****
 22 H62        -2.428896    2.673315   -0.630836 H         1 BMC        0.0095 ****
@<TRIPOS>BOND
    1    20    21 1
    2    20    22 1
    3    17    18 1
    4    17    19 1
    5    17    20 1
    6    15    16 1
    7    13    14 1
    8    13    15 1
    9    13    17 1
   10    11    12 1
   11     9    10 1
   12     9    11 1
   13     9    13 1
   14     7     8 1
   15     5     6 1
   16     5     7 1
   17     5     9 1
   18     3     4 1
   19     1     2 1
   20     1     3 1
   21     1     5 1
   22     1    19 1
@<TRIPOS>SUBSTRUCTURE
      1  BMC              1 ****              0 ****  ****

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--

@<TRIPOS>MOLECULE
```

```
BMO
    24    24     1     0     1
SMALL
USER_CHARGES
@<TRIPOS>ATOM
  1 C1          0.827809   -0.370435   -0.345635 C         1 BMO        0.0394 ****
  2 H1          0.968653   -0.402864   -1.420166 H         1 BMO        0.1574 ****
  3 NH1         2.111482   -0.431191    0.266074 N         1 BMO       -0.3845 ****
  4 HN1         2.093855   -0.507509    1.258340 H         1 BMO        0.3057 ****
  5 C2         -0.032022   -1.543880    0.103245 C         1 BMO       -0.0429 ****
  6 H2          0.388772   -2.474888   -0.273095 H         1 BMO        0.1057 ****
  7 O2         -0.066547   -1.550012    1.504047 O         1 BMO       -0.6107 ****
  8 HO2        -0.169873   -2.430813    1.819869 H         1 BMO        0.4591 ****
  9 C3         -1.447276   -1.406027   -0.459192 C         1 BMO        0.1591 ****
 10 H3         -1.386846   -1.477181   -1.549446 H         1 BMO        0.0516 ****
 11 O3         -2.273731   -2.420086    0.043691 O         1 BMO       -0.6480 ****
 12 HO3        -2.237300   -3.179543   -0.512596 H         1 BMO        0.4380 ****
 13 C4         -2.036990   -0.046228   -0.108559 C         1 BMO        0.0956 ****
 14 H4         -2.194702    0.003532    0.957447 H         1 BMO        0.2163 ****
 15 O4         -3.286112    0.157568   -0.710207 O         1 BMO       -0.6309 ****
 16 HO4        -3.244560   -0.043291   -1.631267 H         1 BMO        0.4209 ****
 17 C5         -1.054804    1.057018   -0.523232 C         1 BMO        0.0020 ****
 18 H5         -0.982857    1.064561   -1.616764 H         1 BMO        0.0806 ****
 19 O5          0.216236    0.833997    0.022767 O         1 BMO       -0.2405 ****
 20 C6         -1.510421    2.439621   -0.100059 C         1 BMO        0.2171 ****
 21 H61        -0.744596    3.151988   -0.398264 H         1 BMO        0.0095 ****
 22 H62        -2.428896    2.673315   -0.630836 H         1 BMO        0.0095 ****
 23 O6         -1.707325    2.461396    1.284348 O         1 BMO       -0.6280 ****
 24 HO6        -2.085921    3.285391    1.539200 H         1 BMO        0.4180 ****
@<TRIPOS>BOND
    1     1     2 1
    2     1     3 1
    3     1     5 1
    4     1    19 1
    5     3     4 1
    6     5     6 1
    7     5     7 1
    8     5     9 1
    9     7     8 1
   10     9    10 1
   11     9    11 1
   12     9    13 1
   13    11    12 1
   14    13    14 1
   15    13    15 1
   16    13    17 1
   17    15    16 1
   18    17    18 1
   19    17    19 1
   20    17    20 1
   21    20    21 1
   22    20    22 1
   23    20    23 1
   24    23    24 1
@<TRIPOS>SUBSTRUCTURE
      1  BMO             1 ****              0 ****  ****
```

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--------------------------------------------------------------------------------
--

@<TRIPOS>MOLECULE
BMR
   18    18     1     0     1
SMALL
USER_CHARGES
@<TRIPOS>ATOM
  1 C1          0.827809   -0.370435   -0.345635 C         1 BMR        0.0394 ****
  2 H1          0.968653   -0.402864   -1.420166 H         1 BMR        0.1574 ****
  3 NH1         2.111482   -0.431191    0.266074 N         1 BMR       -0.3845 ****
  4 HN1         2.093855   -0.507509    1.258340 H         1 BMR        0.3057 ****
  5 C2         -0.032022   -1.543880    0.103245 C         1 BMR       -0.0429 ****
  6 H2          0.388772   -2.474888   -0.273095 H         1 BMR        0.1057 ****
  7 O2         -0.066547   -1.550012    1.504047 O         1 BMR       -0.6107 ****
  8 HO2        -0.169873   -2.430813    1.819869 H         1 BMR        0.4591 ****
  9 C3         -1.447276   -1.406027   -0.459192 C         1 BMR        0.1591 ****
 10 H3         -1.386846   -1.477181   -1.549446 H         1 BMR        0.0516 ****
 11 C4         -2.036990   -0.046228   -0.108559 C         1 BMR        0.0956 ****
 12 H4         -2.194702    0.003532    0.957447 H         1 BMR        0.2163 ****
 13 C5         -1.054804    1.057018   -0.523232 C         1 BMR        0.0020 ****
 14 H5         -0.982857    1.064561   -1.616764 H         1 BMR        0.0806 ****
 15 O5          0.216236    0.833997    0.022767 O         1 BMR       -0.2405 ****
 16 C6         -1.510421    2.439621   -0.100059 C         1 BMR        0.2171 ****
 17 H61        -0.744596    3.151988   -0.398264 H         1 BMR        0.0095 ****
 18 H62        -2.428896    2.673315   -0.630836 H         1 BMR        0.0095 ****
@<TRIPOS>BOND
    1     1     2 1
    2     1     3 1
    3     1     5 1
    4     1    15 1
    5     3     4 1
    6     5     6 1
    7     5     7 1
    8     5     9 1
    9     7     8 1
   10     9    10 1
   11     9    11 1
   12    11    12 1
   13    11    13 1
   14    13    14 1
   15    13    15 1
   16    13    16 1
   17    16    17 1
   18    16    18 1
@<TRIPOS>SUBSTRUCTURE
      1  BMR              1 ****              0 ****  ****

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--

@<TRIPOS>MOLECULE
AMO
   23    23     1     0     1
SMALL
USER_CHARGES
```

```
@<TRIPOS>ATOM
  1 C1          -1.455580   -0.288327    0.514425 C         1 AMO        0.0129 ****
  2 H1          -2.067714   -0.558661    1.373011 H         1 AMO        0.1741 ****
  3 O1          -2.177352   -0.466724   -0.655076 O         1 AMO       -0.3502 ****
  4 C2          -1.067664    1.187016    0.591424 C         1 AMO        0.0834 ****
  5 H2          -1.966804    1.779189    0.419861 H         1 AMO        0.0964 ****
  6 O2          -0.502333    1.488044    1.831274 O         1 AMO       -0.6300 ****
  7 HO2         -1.082795    1.239753    2.531592 H         1 AMO        0.4350 ****
  8 C3          -0.033751    1.506820   -0.487912 C         1 AMO        0.1014 ****
  9 H3          -0.518240    1.346968   -1.452331 H         1 AMO        0.0585 ****
 10 O3           0.445853    2.812674   -0.396218 O         1 AMO       -0.6319 ****
 11 HO3         -0.264880    3.426264   -0.482494 H         1 AMO        0.4382 ****
 12 C4           1.149585    0.553515   -0.375330 C         1 AMO        0.2874 ****
 13 H4           1.680957    0.748629    0.542477 H         1 AMO        0.1699 ****
 14 O4           2.070504    0.736940   -1.415935 O         1 AMO       -0.6675 ****
 15 HO4          1.655277    0.577684   -2.248672 H         1 AMO        0.4202 ****
 16 C5           0.661992   -0.901640   -0.367411 C         1 AMO       -0.0272 ****
 17 H5           0.269625   -1.137489   -1.358508 H         1 AMO        0.1175 ****
 18 O5          -0.350533   -1.115613    0.590128 O         1 AMO       -0.3079 ****
 19 C6           1.775142   -1.889688   -0.079183 C         1 AMO        0.1411 ****
 20 H61          2.506865   -1.815827   -0.878366 H         1 AMO        0.0307 ****
 21 H62          1.352357   -2.892664   -0.089077 H         1 AMO        0.0307 ****
 22 O6           2.349480   -1.602189    1.162441 O         1 AMO       -0.6141 ****
 23 HO6          3.155555   -2.079464    1.260052 H         1 AMO        0.4214 ****
@<TRIPOS>BOND
    1     1     2 1
    2     1     3 1
    3     1     4 1
    4     1    18 1
    5     4     5 1
    6     4     6 1
    7     4     8 1
    8     6     7 1
    9     8     9 1
   10     8    10 1
   11     8    12 1
   12    10    11 1
   13    12    13 1
   14    12    14 1
   15    12    16 1
   16    14    15 1
   17    16    17 1
   18    16    18 1
   19    16    19 1
   20    19    20 1
   21    19    21 1
   22    19    22 1
   23    22    23 1
@<TRIPOS>SUBSTRUCTURE
      1  AMO             1 ****              0 ****  ****
```