Supplementary Information

Derivatization of Bufadienolides at Carbon-3 of the Steroid Core and Their Consequences for the Interaction with Na^+,K^+-ATPase

Lucy Kate Ladefoged [1,2,†], Birgit Schiøtt [2,‡] and Natalya U. Fedosova [1,*]

[1] Department of Biomedicine, Aarhus University, Høegh-Guldbergsgade 10, 8000 Aarhus C, Denmark
[2] Department of Chemistry, Aarhus University, Langelandsgade 140, 8000 Aarhus C, Denmark
* Correspondence: nf@biomed.au.dk
† Current affiliation: Raven Biosciences, Åbogade 15, 8200 Aarhus N, Denmark.
‡ Current affiliation: Faculty of Natural Sciences, Aarhus University, Ny Munkegade 116, 8000 Aarhus C, Denmark.

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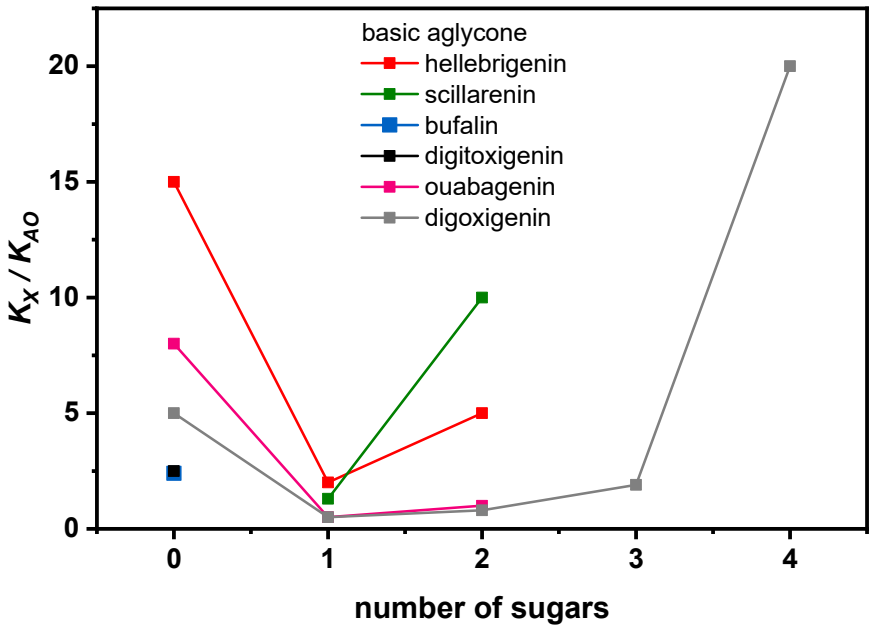
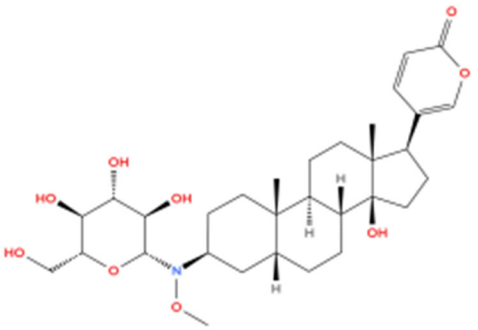
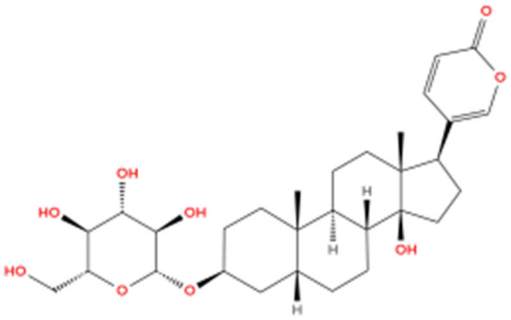


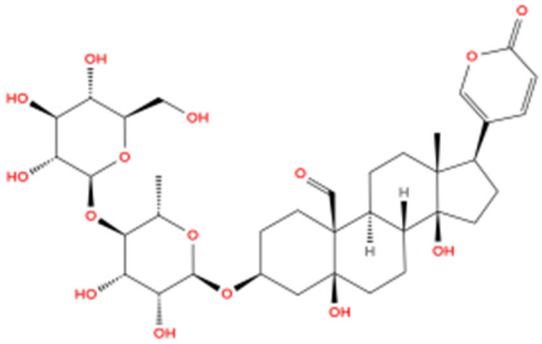
Supporting Figure S1. The ratio of the dissociation constants of CTS (K_x) to that of anthroylouabain (AO) (K_{AO}) as a function of a degree of glycosylation. Experiments were performed in His buffer and in the absence of K^+. All compounds are O-glycosylated.



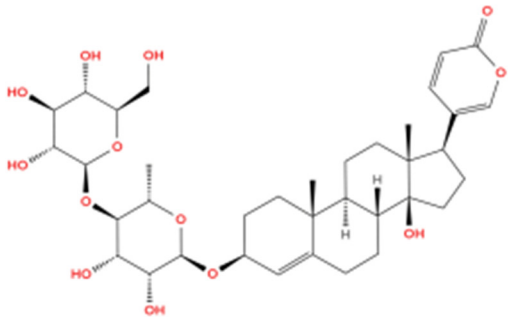
Bufalin-N-glucose



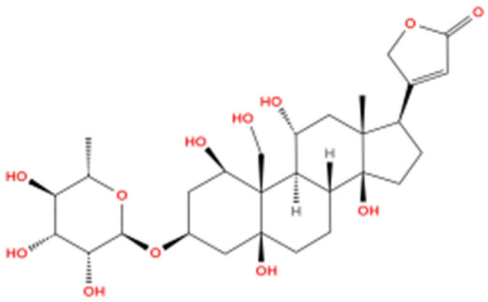
Bufalin-O-glucose



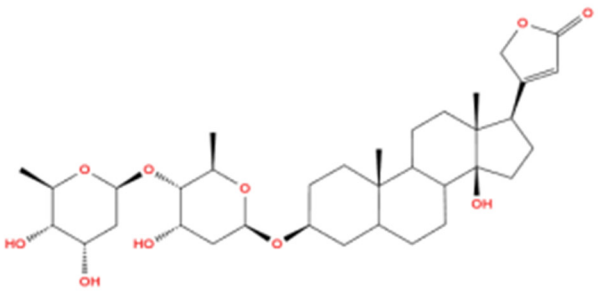
Hellebrin



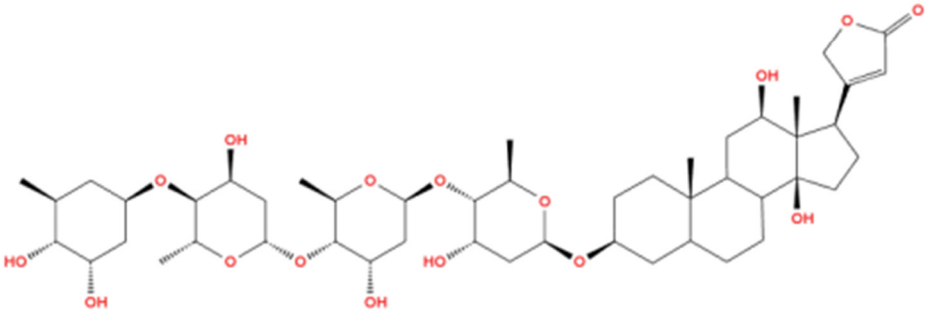
Scillaren A



Ouabain

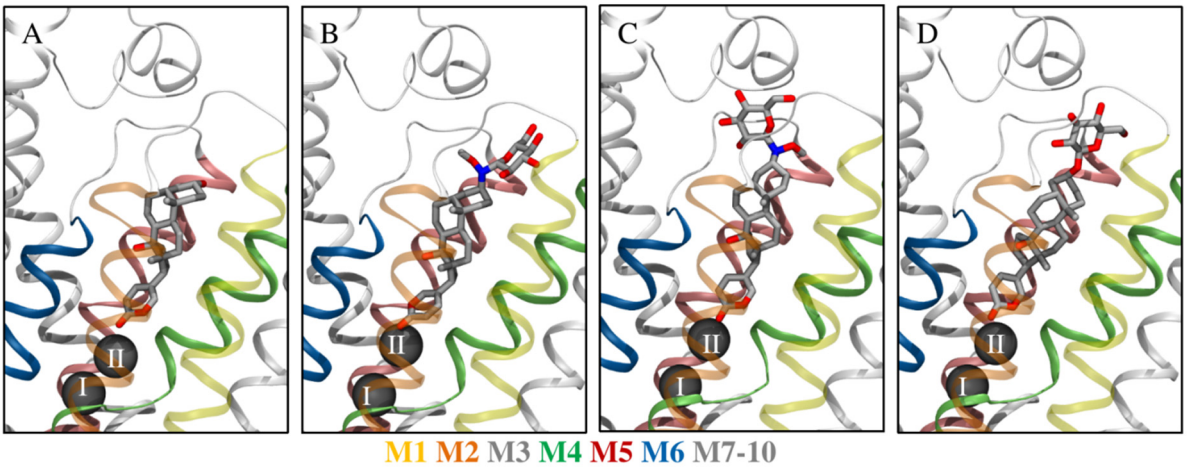


Digitoxigenin di-digitoxoside

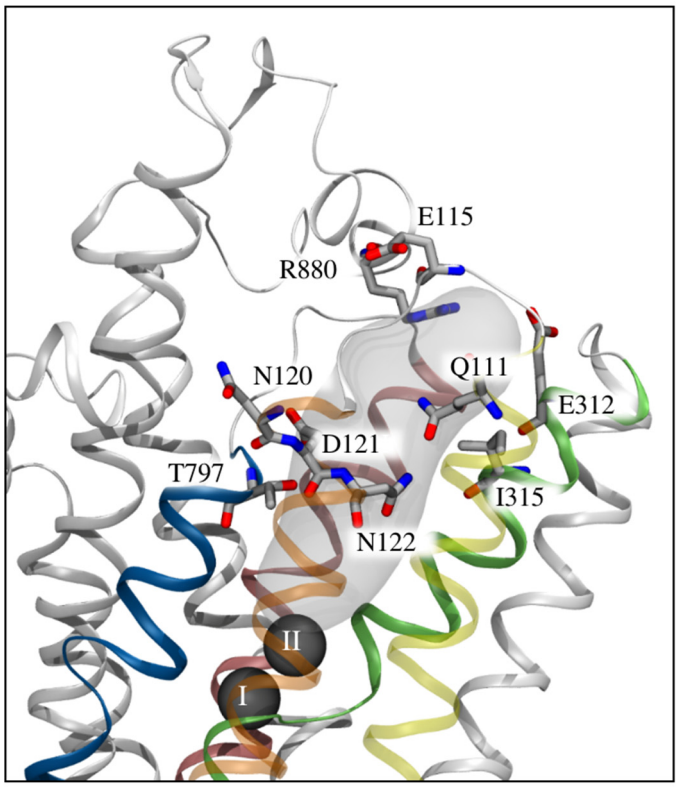


Digoxigenin tetra-digitoxose

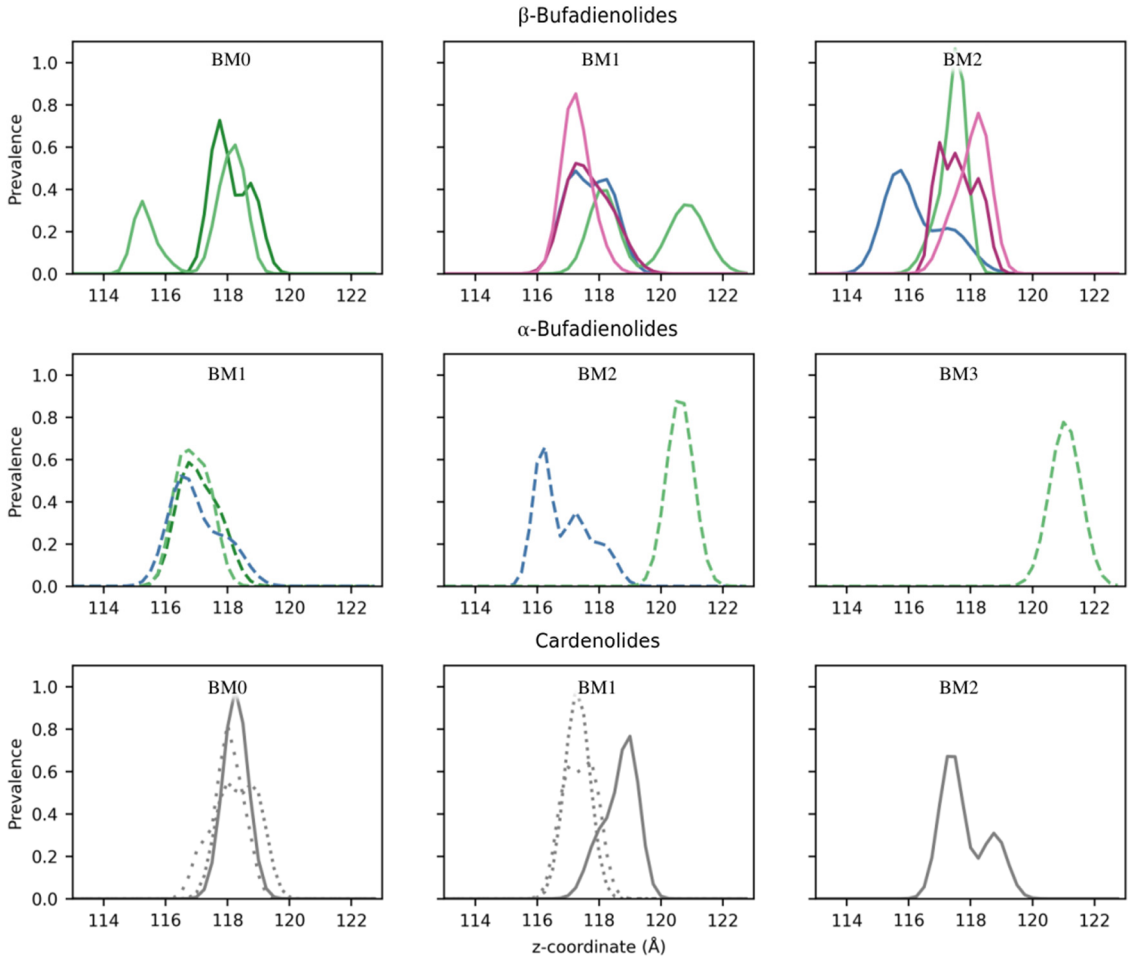
Supporting Figure S2. Chemical structures of CTS. For all shown CTS, the C3 carbon is in the S-configuration according to R/S nomenclature and the oxygen atom bound to C3 is axial relative to ring A of the steroid core.



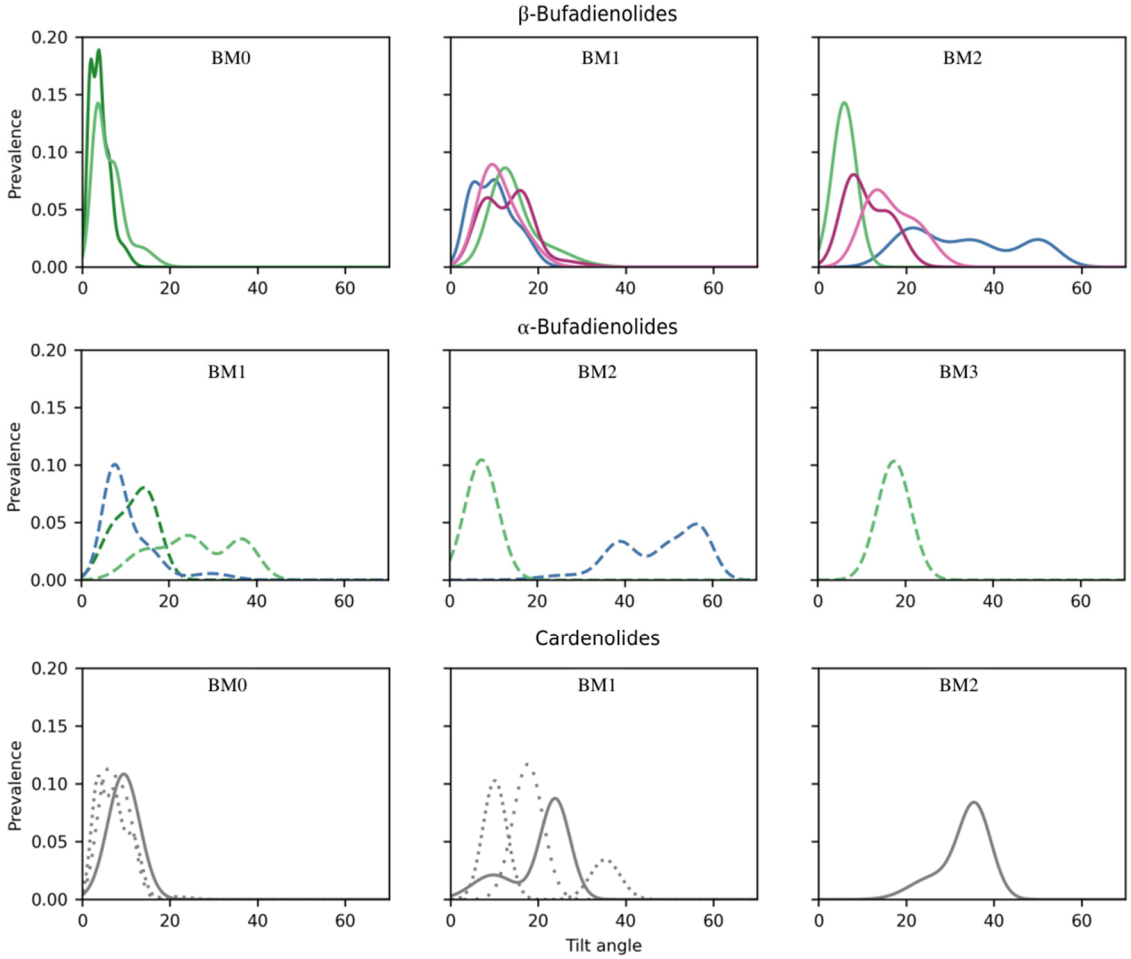
Supporting Figure S3. Starting conformations of bufalin derivatives for MD simulations. **(A)** α-bufalin, **(B)** β-bufalin-N-glucose, **(C)** α-bufalin-N-glucose, and **(D)** β-bufalin-O-glucose.



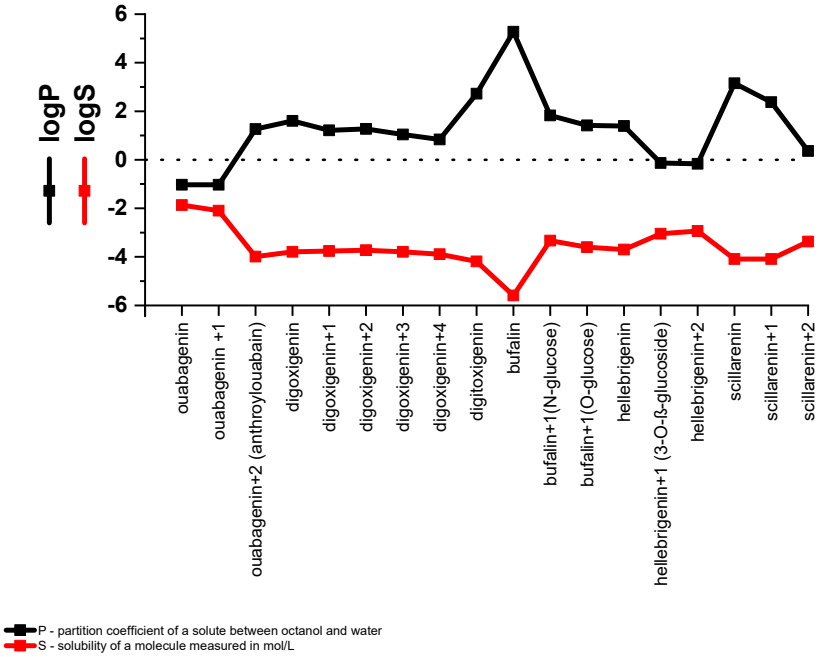
Supporting Figure S4. Overview of possible intermolecular hydrogen bonds between CTS and Na^+,K^+-ATPase. The density of the lactone ring and steroid core of bufalin is shown as gray mesh.



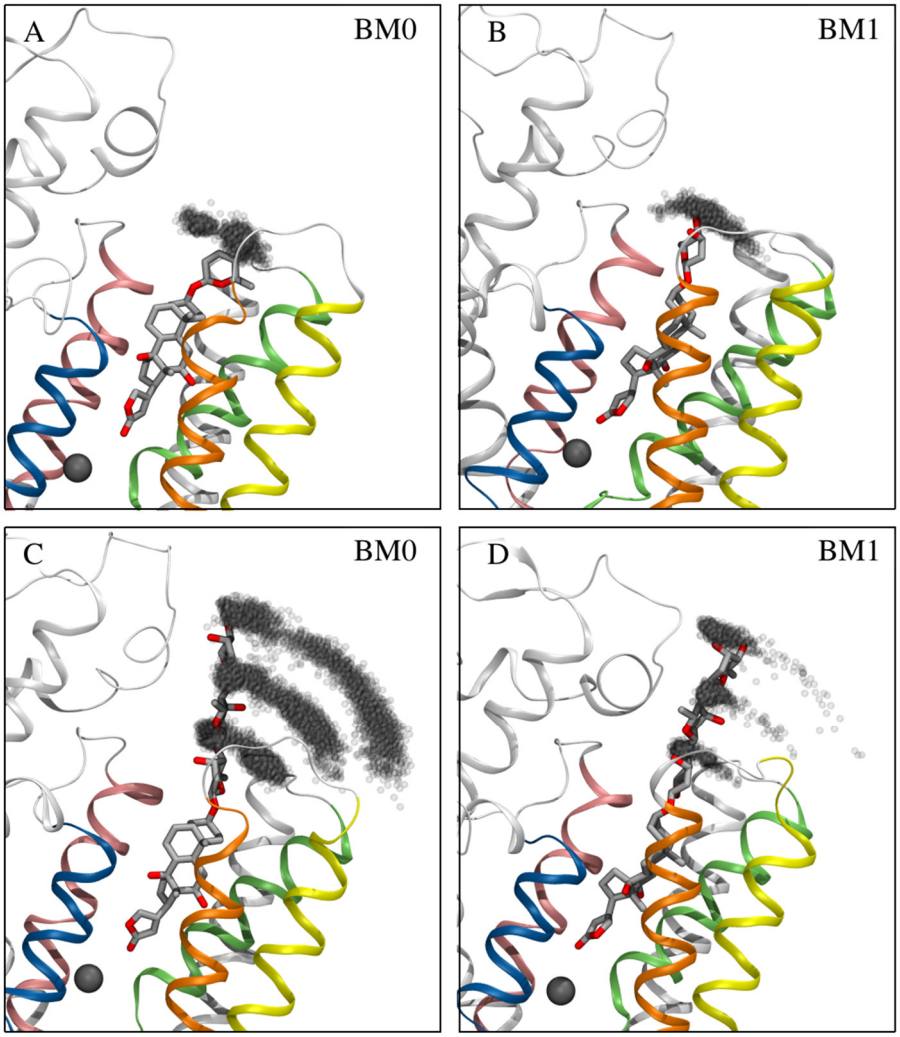
Supporting Figure S5. Ligand movement along the z-axis i.e. the longest axis of the binding site. The bufadienolides bufalin (blue), bufalin-N-glucose (green), and bufalin-O-glucose (magenta) are shown with β-isomers as solid lines and α-isomers as dashed lines. The results of simulations performed without ions in cation site I and II are shown in lighter hues. Cardenolides are all shown in gray; digoxigenin as a solid line, digoxin monodigitoxoside as a tightly dotted line, and digoxin as a loosely dotted line. Each distribution was calculated using a Gaussian Mixture model with the number of Gaussian components determined using the Bayesian information criterion. The z-coordinate represents the center-of-mass of the steroid core excl. the lactone ring. The lower the z-coord reflects position closer to the intracellular side. Before calculation, all frames were aligned by the alpha atoms of helices αM5-αM10. Only binding modes that are observed for more than 5% of the total simulation time are included.



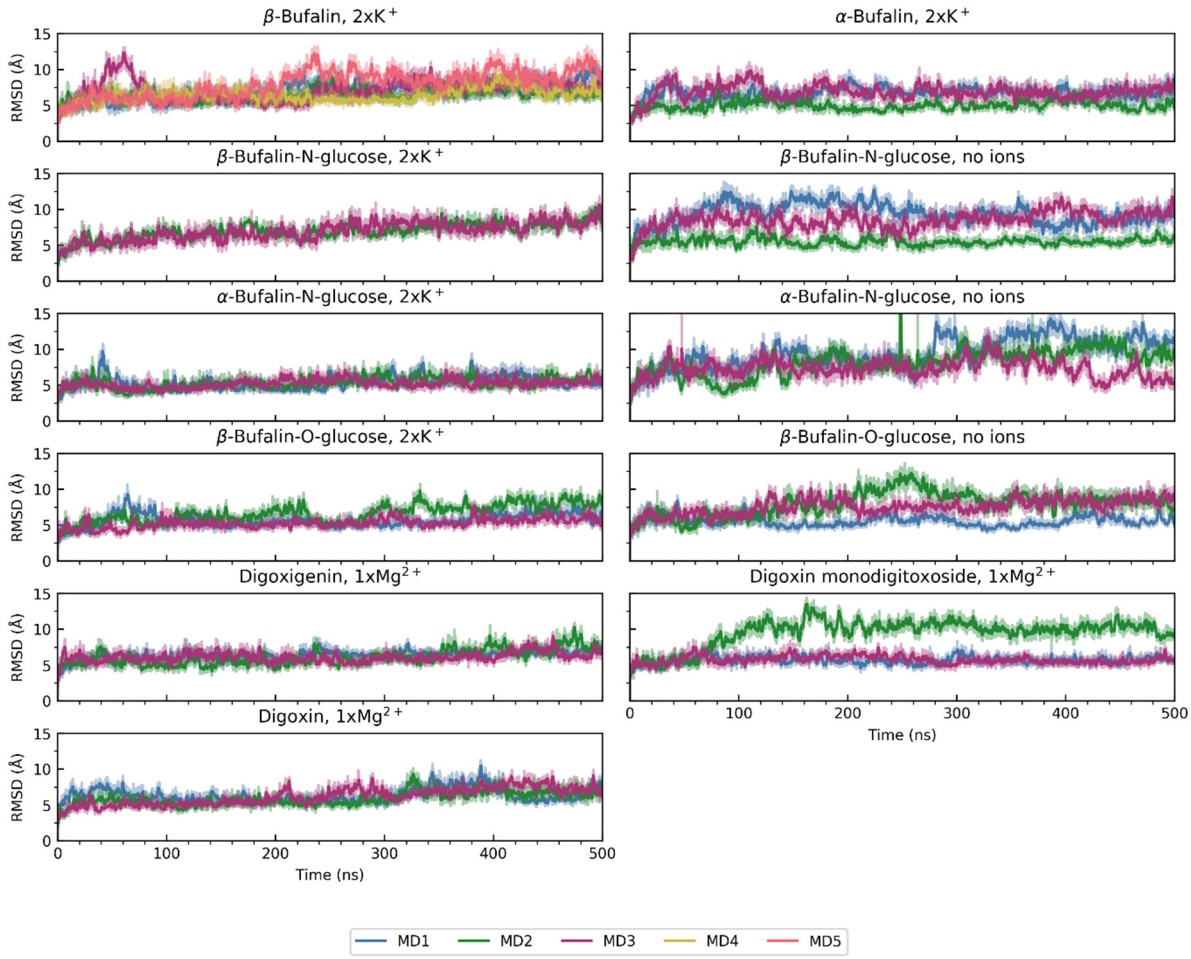
Supporting Figure S6. Distribution of tilt angles of the steroid core sampled for each ligand occupying BM0, BM1, BM2, and BM3. The bufadienolides bufalin (blue), bufalin-N-glucose (green), and bufalin-O-glucose (magenta) are shown with β-isomers as solid lines and α-isomers as dashed lines. Bufadienolide simulations performed without ions in cation site I and II are shown in lighter hues. Cardenolides are all shown in gray; digoxigenin as a solid line, digoxin monodigitoxoside as a tightly dotted line, and digoxin as a loosely dotted line. Each distribution was calculated using a Gaussian Mixture model with the number of Gaussian components determined using the Bayesian information criterion. Only binding modes that are observed for more than 5% of the total simulation time are included.



Supporting Figure S7. Estimated solubility (logS) and lipophilicity (logP) for each CTS calculated by ALOGPS 2.1.



Supporting Figure S8. Dynamic range of sugar moieties in **(A-B)** digoxigenin monodigitoxoside and **(C-D)** digoxin. Each gray dot is the location of the oxygen atom of the *para*-hydroxyl group. All trajectories are aligned on M1-6, and only frames representative of a given binding mode are included in each image.



Supporting Figure S9. RMSD progression of all simulated systems. The running average is shown in solid hues, while the raw data is shown in transparent hues. The RMSD was calculated for alpha residues of chain A following alignment of residues 760 to 1016.

Supporting Data File S1. Digoxin force field parameters.

#digoxin.pdb

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; atoms w Y: second/middle sugar moiety
; atoms w Z: third/terminal sugar moiety
; residue          1 digoxin rtp digoxin q         qsum
    1     CG321     1 digoxin    C1     1    -0.174     12.011   ;
    2     CG321     1 digoxin    C2     2    -0.194     12.011   ;
    3     CG311     1 digoxin    C3     3     0.090     12.011   ;
    4     OC301     1 digoxin    O3     4    -0.360     15.999   ;
    5     CG321     1 digoxin    C4     5    -0.178     12.011  ;
    6     CG311     1 digoxin    C5     6    -0.088     12.011   ;
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   16    CG3RC1     1 digoxin   C14    16     0.238     12.011   ;
   17     OG311     1 digoxin   O14    17    -0.652     15.999   ;
   18    CG3C52     1 digoxin   C15    18    -0.200     12.011   ;
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   21     CG331     1 digoxin   C18    21    -0.287     12.011   ;
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25    CC3162   1 digoxin   C1Z    25     0.290    12.011   ;
26    CG2R57   1 digoxin   C20    26    -0.013    12.011   ;
27    CG3C52   1 digoxin   C21    27     0.230    12.011   ;
28    OG3C51   1 digoxin   O21    28    -0.307    15.999   ;
29    CG2R51   1 digoxin   C22    29    -0.188    12.011   ;
30    CG2R53   1 digoxin   C23    30     0.290    12.011   ;
31    OG2D1    1 digoxin   O23    31    -0.430    15.999   ;
32    CC3261   1 digoxin   C2X    32    -0.180    12.011   ;
33    CC3261   1 digoxin   C2Y    33    -0.180    12.011   ;
34    CC3261   1 digoxin   C2Z    34    -0.180    12.011   ;
35    CC3161   1 digoxin   C3X    35     0.140    12.011   ;
36    OC311    1 digoxin   O3X    36    -0.650    15.999   ;
37    CC3161   1 digoxin   C3Y    37     0.140    12.011   ;
38    OC311    1 digoxin   O3Y    38    -0.650    15.999   ;
39    CC3161   1 digoxin   C3Z    39     0.140    12.011   ;
40    OC311    1 digoxin   O3Z    40    -0.650    15.999   ;
41    CC3161   1 digoxin   C4X    41     0.090    12.011   ;
42    OC301    1 digoxin   O4X    42    -0.360    15.999   ;
43    CC3161   1 digoxin   C4Y    43     0.090    12.011   ;
44    OC301    1 digoxin   O4Y    44    -0.360    15.999   ;
45    CC3161   1 digoxin   C4Z    45     0.140    12.011   ;
46    OC311    1 digoxin   O4Z    46    -0.650    15.999   ;
47    CC3163   1 digoxin   C5X    47     0.110    12.011   ;
48    OC3C61   1 digoxin   O5X    48    -0.400    15.999   ;
49    CC3163   1 digoxin   C5Y    49     0.110    12.011   ;
50    OC3C61   1 digoxin   O5Y    50    -0.400    15.999   ;
51    CC3163   1 digoxin   C5Z    51     0.110    12.011   ;
52    OC3C61   1 digoxin   O5Z    52    -0.400    15.999   ;
53    CC331    1 digoxin   C6X    53    -0.270    12.011   ;
54    CC331    1 digoxin   C6Y    54    -0.270    12.011   ;
55    CC331    1 digoxin   C6Z    55    -0.270    12.011   ;
56    HGA2     1 digoxin   H11    56     0.090     1.008   ;
57    HGA2     1 digoxin   H12    57     0.090     1.008   ;
58    HGA2     1 digoxin   H21    58     0.090     1.008   ;
59    HGA2     1 digoxin   H22    59     0.090     1.008   ;
60    HGA1     1 digoxin   H3     60     0.090     1.008   ;
61    HGA2     1 digoxin   H41    61     0.090     1.008   ;
62    HGA2     1 digoxin   H42    62     0.090     1.008   ;
63    HGA1     1 digoxin   H5     63     0.090     1.008   ;
64    HGA2     1 digoxin   H61    64     0.090     1.008   ;
65    HGA2     1 digoxin   H62    65     0.090     1.008   ;
66    HGA2     1 digoxin   H71    66     0.090     1.008   ;
67    HGA2     1 digoxin   H72    67     0.090     1.008   ;
68    HGA1     1 digoxin   H8     68     0.090     1.008   ;
69    HGA1     1 digoxin   H9     69     0.090     1.008   ;
70    HGA2     1 digoxin   H111   70     0.090     1.008   ;
71    HGA2     1 digoxin   H112   71     0.090     1.008   ;
72    HGA1     1 digoxin   H1     72     0.090     1.008   ;
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  73     HGP1    1 digoxin   HO12    73     0.419     1.008  ;
  74     HGP1    1 digoxin   HO14    74     0.420     1.008  ;
  75     HGA2    1 digoxin   H151    75     0.090     1.008  ;
  76     HGA2    1 digoxin   H152    76     0.090     1.008  ;
  77     HGA2    1 digoxin   H161    77     0.090     1.008  ;
  78     HGA2    1 digoxin   H162    78     0.090     1.008  ;
  79     HGA1    1 digoxin   H17     79     0.090     1.008  ;
  80     HGA3    1 digoxin   H181    80     0.090     1.008  ;
  81     HGA3    1 digoxin   H182    81     0.090     1.008  ;
  82     HGA3    1 digoxin   H183    82     0.090     1.008  ;
  83     HGA3    1 digoxin   H191    83     0.090     1.008  ;
  84     HGA3    1 digoxin   H192    84     0.090     1.008  ;
  85     HGA3    1 digoxin   H193    85     0.090     1.008  ;
  86     HCA1    1 digoxin   H1X     86     0.090     1.008  ;
  87     HCA1    1 digoxin   H1Y     87     0.090     1.008  ;
  88     HCA1    1 digoxin   H1Z     88     0.090     1.008  ;
  89     HGA2    1 digoxin   H211    89     0.090     1.008  ;
  90     HGA2    1 digoxin   H212    90     0.090     1.008  ;
  91     HGR51   1 digoxin   H2      91     0.263     1.008  ;
  92     HCA2    1 digoxin   H2X1    92     0.090     1.008  ;
  93     HCA2    1 digoxin   H2X2    93     0.090     1.008  ;
  94     HCA2    1 digoxin   H2Y1    94     0.090     1.008  ;
  95     HCA2    1 digoxin   H2Y2    95     0.090     1.008  ;
  96     HCA2    1 digoxin   H2Z1    96     0.090     1.008  ;
  97     HCA2    1 digoxin   H2Z2    97     0.090     1.008  ;
  98     HCA1    1 digoxin   H3X     98     0.090     1.008  ;
  99     HCP1    1 digoxin   HO3X    99     0.420     1.008  ;
 100     HCA1    1 digoxin   H3Y     100    0.090     1.008  ;
 101     HCP1    1 digoxin   HO3Y    101    0.420     1.008  ;
 102     HCA1    1 digoxin   H3Z     102    0.090     1.008  ;
 103     HCP1    1 digoxin   HO3Z    103    0.420     1.008  ;
 104     HCA1    1 digoxin   H4X     104    0.090     1.008  ;
 105     HCA1    1 digoxin   H4Y     105    0.090     1.008  ;
 106     HCA1    1 digoxin   H4Z     106    0.090     1.008  ;
 107     HCP1    1 digoxin   HO4Z    107    0.420     1.008  ;
 108     HCA1    1 digoxin   H5X     108    0.090     1.008  ;
 109     HCA1    1 digoxin   H5Y     109    0.090     1.008  ;
 110     HCA1    1 digoxin   H5Z     110    0.090     1.008  ;
 111     HCA3    1 digoxin   H6X1    111    0.090     1.008  ;
 112     HCA3    1 digoxin   H6X2    112    0.090     1.008  ;
 113     HCA3    1 digoxin   H6X3    113    0.090     1.008  ;
 114     HCA3    1 digoxin   H6Y1    114    0.090     1.008  ;
 115     HCA3    1 digoxin   H6Y2    115    0.090     1.008  ;
 116     HCA3    1 digoxin   H6Y3    116    0.090     1.008  ;
 117     HCA3    1 digoxin   H6Z1    117    0.090     1.008  ;
 118     HCA3    1 digoxin   H6Z2    118    0.090     1.008  ;
 119     HCA3    1 digoxin   H6Z3    119    0.090     1.008  ;
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#digoxin.prm

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[ bondtypes ]
;    i     j  func       b0          kb
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 CG2R57   CG3C51     1   0.15100000    292880.00
 CG2R57   CG3C52     1   0.15100000    292880.00
 CG3RC1    OG311     1   0.14200000    358150.40
 CC3261   CC3162     1   0.14800000    186188.00
  CG311    OC301     1    0.14150000    301248.00

[ angletypes ]
;    i       j       k  func       theta0       ktheta          ub0          kub
 CG2R53   CG2R51   CG2R57    5   116.500000   836.800000   0.00000000         0.00
 CG2R51   CG2R57   CG3C51    5   109.000000   962.320000   0.00000000         0.00
 CG2R51   CG2R57   CG3C52    5   109.000000   962.320000   0.00000000         0.00
 CG3C51   CG2R57   CG3C52    5   105.800000   753.120000   0.00000000         0.00
  CG311    CG311    OC311    5   109.700000   962.320000   0.00000000         0.00
  CG311    CG311   OG3C61    5   111.500000   376.560000   0.00000000         0.00
  CG321    CG311    OC311    5   109.700000   962.320000   0.00000000         0.00
  CG321    CG311    OC301    5   109.000000   376.560000   0.00000000         0.00
  CG321    CG311   OG3C61    5   111.500000   376.560000   0.00000000         0.00
  CG331    CG311   OG3C61    5   111.500000   376.560000   0.00000000         0.00
 OG3C61    CG311     HGA1    5   109.500000   376.560000   0.00000000         0.00
 CG2R57   CG3C51   CG3C52    5   106.000000   435.136000   0.00000000         0.00
 CG2R57   CG3C51   CG3RC1    5   106.000000   435.136000   0.00000000         0.00
 CG2R57   CG3C51     HGA1    5   112.600000   435.136000   0.00000000         0.00
 CG2R57   CG3C52   OG3C51    5   102.400000   627.600000   0.00000000         0.00
 CG2R57   CG3C52     HGA2    5   112.600000   435.136000   0.00000000         0.00
  CG311   CG3RC1    OG311    5   113.500000   488.272800   0.25610000      9338.69
 CG3C52   CG3RC1    OG311    5   110.000000   633.457600   0.00000000         0.00
 CG3RC1   CG3RC1    OG311    5   111.000000   446.432800   0.25610000      6694.40
 CC3162    OC301    CG311    5   109.200000   418.400000   0.00000000         0.00
 CG3RC1    OG311     HGP1    5   109.000000   418.400000   0.00000000         0.00
  CG311   OG3C61    CG311    5   109.700000   794.960000   0.00000000         0.00
 CC3261   CC3162     HCA1    5   110.100000   288.696000   0.21790000     18853.10
 CC3261   CC3162   OC3C61    5   106.000000   376.560000   0.00000000         0.00
  OC301    CG311     HGA1    5   109.500000   502.080000   0.00000000         0.00
 CC3261   CC3162    OC311    5   107.000000   633.457600   0.00000000         0.00
  OC301   CC3162   CC3261    5   105.000000   376.560000   0.00000000         0.00
 CC3162   CC3261   CC3161    5   111.000000   446.432800   0.25610000      6694.40
 CC3162   CC3261     HCA2    5   110.100000   288.696000   0.21790000     18853.10

[ dihedraltypes ]
;    i       j       k       l  func        phi0        kphi  mult
 CG2R57   CG2R51   CG2R53    OG2D1     9   180.000000     5.020800     2
 CG2R57   CG2R51   CG2R53   OG3C51     9   180.000000     1.715440     1
 CG2R53   CG2R51   CG2R57   CG3C51     9   180.000000    27.614400     2
 CG2R53   CG2R51   CG2R57   CG3C52     9   180.000000    27.614400     2
  HGR51   CG2R51   CG2R57   CG3C51     9   180.000000    12.133600     2
  HGR51   CG2R51   CG2R57   CG3C52     9   180.000000    12.133600     2
 CG2R51   CG2R57   CG3C51   CG3C52     9   180.000000     0.209200     3
 CG2R51   CG2R57   CG3C51   CG3RC1     9   180.000000     0.209200     3
 CG2R51   CG2R57   CG3C51     HGA1     9     0.000000     0.000000     3
 CG3C52   CG2R57   CG3C51   CG3C52     9     0.000000     9.916080     2
 CG3C52   CG2R57   CG3C51   CG3RC1     9     0.000000     9.916080     2
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CG3C52 CG2R57 CG3C51 HGA1 9 180.000000 0.000000 3
CG2R51 CG2R57 CG3C52 OG3C51 9 180.000000 1.171520 1
CG2R51 CG2R57 CG3C52 OG3C51 9 180.000000 4.100320 2
CG2R51 CG2R57 CG3C52 OG3C51 9 180.000000 7.322000 3
CG2R51 CG2R57 CG3C52 HGA2 9 0.000000 0.000000 3
CG3C51 CG2R57 CG3C52 OG3C51 9 180.000000 1.171520 1
CG3C51 CG2R57 CG3C52 OG3C51 9 180.000000 4.100320 2
CG3C51 CG2R57 CG3C52 OG3C51 9 180.000000 7.322000 3
CG3C51 CG2R57 CG3C52 HGA2 9 180.000000 0.000000 3
CG311 CG311 CG311 CG331 9 180.000000 2.092000 4
CG311 CG311 CG311 OG3C61 9 180.000000 0.794960 1
CG311 CG311 CG311 OG3C61 9 180.000000 4.184000 2
CG311 CG311 CG311 OG3C61 9 0.000000 2.510400 3
CG311 CG311 CG311 OG3C61 9 180.000000 0.334720 4
CG321 CG311 CG311 OG301 9 180.000000 0.836800 3
CG321 CG311 CG311 OC301 9 180.000000 0.836800 3
CG321 CG311 CG311 OG311 9 0.000000 0.585760 3
CG331 CG311 CG311 OG311 9 0.000000 0.585760 3
OG301 CG311 CG311 OG311 9 0.000000 0.836800 3
OG301 CG311 CG311 OG3C61 9 0.000000 0.836800 3
OC301 CG311 CG311 OG3C61 9 0.000000 0.836800 3
OG301 CG311 CG311 HGA1 9 0.000000 0.815880 3
OC301 CG311 CG311 HGA1 9 0.000000 0.815880 3
OG311 CG311 CG311 OG311 9 0.000000 0.836800 3
OG311 CG311 CG311 OG3C61 9 0.000000 0.836800 3
OG301 CG311 CG321 CG311 9 180.000000 0.669440 1
OG301 CG311 CG321 CG311 9 0.000000 1.631760 2
OC301 CG311 CG321 CG311 9 0.000000 0.836800 3
OC301 CG311 CG321 CG321 9 0.000000 0.836800 3
OG301 CG311 CG321 HGA2 9 0.000000 0.815880 3
OC301 CG311 CG321 HGA2 9 0.000000 0.815880 3
CG311 CG311 CG3RC1 OG311 9 0.000000 0.209200 3
CG321 CG311 CG3RC1 OG311 9 0.000000 0.209200 3
HGA1 CG311 CG3RC1 OG311 9 0.000000 0.209200 3
CG311 CG311 OG301 CG311 9 0.000000 1.673600 1
CG311 CG311 OG301 CG311 9 0.000000 2.050160 3
CG321 CG311 OC301 CC3162 9 180.000000 0.543920 1
CG321 CG311 OC301 CC3162 9 180.000000 1.046000 2
CG321 CG311 OC301 CC3162 9 180.000000 0.251040 3
HGA1 CG311 OG301 CG311 9 0.000000 1.188256 3
HGA1 CG311 OC301 CC3162 9 0.000000 1.188256 3
CG2R57 CG3C51 CG3C52 CG3C52 9 180.000000 15.480800 3
CG2R57 CG3C51 CG3C52 CG3C52 9 0.000000 9.414000 4
CG2R57 CG3C51 CG3C52 CG3C52 9 180.000000 0.962320 6
CG2R57 CG3C51 CG3C52 HGA2 9 0.000000 0.585760 3
CG2R57 CG3C51 CG3RC1 CG311 9 180.000000 15.480800 3
CG2R57 CG3C51 CG3RC1 CG311 9 0.000000 9.414000 4
CG2R57 CG3C51 CG3RC1 CG311 9 180.000000 0.962320 6
CG2R57 CG3C51 CG3RC1 CG331 9 180.000000 15.480800 3
CG2R57 CG3C51 CG3RC1 CG331 9 0.000000 9.414000 4
CG2R57 CG3C51 CG3RC1 CG331 9 180.000000 0.962320 6

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 CG2R57   CG3C51   CG3RC1   CG3RC1    9    0.000000    0.627600    3
 CG3C52   CG3C52   CG3RC1   OG311     9  180.000000    2.092000    1
 CG3C52   CG3C52   CG3RC1   OG311     9    0.000000    2.928800    2
 CG3C52   CG3C52   CG3RC1   OG311     9    0.000000    1.673600    3
 CG3C52   CG3C52   CG3RC1   OG311     9    0.000000    1.673600    5
  HGA2    CG3C52   CG3RC1   OG311     9  180.000000    0.815880    3
 CG2R57   CG3C52   OG3C51   CG2R53    9  180.000000    1.297040    1
 CG2R57   CG3C52   OG3C51   CG2R53    9    0.000000    1.171520    6
  CG311   CG3RC1   CG3RC1   OG311     9    0.000000   16.736000    3
  CG331   CG3RC1   CG3RC1   OG311     9    0.000000    0.209200    3
 CG3C51   CG3RC1   CG3RC1   OG311     9    0.000000    5.020800    3
  CG311   CG3RC1   OG311    HGP1      9    0.000000    1.213360    1
  CG311   CG3RC1   OG311    HGP1      9    0.000000    2.594080    2
  CG311   CG3RC1   OG311    HGP1      9    0.000000    0.209200    3
 CG3C52   CG3RC1   OG311    HGP1      9    0.000000    1.213360    1
 CG3C52   CG3RC1   OG311    HGP1      9    0.000000    2.594080    2
 CG3C52   CG3RC1   OG311    HGP1      9    0.000000    0.209200    3
 CG3RC1   CG3RC1   OG311    HGP1      9    0.000000    6.276000    1
 CG3RC1   CG3RC1   OG311    HGP1      9  180.000000    1.255200    2
 CG3RC1   CG3RC1   OG311    HGP1      9    0.000000    1.338880    3
 CG311    OC301    CC3162   OC3C61    9  180.000000    0.209200    1
 CG311    OC301    CC3162   OC3C61    9    0.000000    3.807440    2
 CG311    OC301    CC3162   OC3C61    9  180.000000    5.313680    3
 CC3161   CC3261   CC3162   OC301     9    0.000000    0.836800    3
 CC3261   CC3162   OC301    CG311     9  180.000000    1.715440    1
 CC3261   CC3162   OC301    CG311     9  180.000000    2.761440    2
 CC3261   CC3162   OC301    CG311     9    0.000000    6.694400    3
  CG311   OC301    CC3162   HCA1      9    0.000000    1.188256    3
 CC3161   CC3261   CC3162   OC3C61    9  180.000000    1.297040    3
 CC3161   CC3162   OC3C61   CC3163    9    0.000000    0.836800    3
  HCA1    CC3261   CC3162   OC3C61    9    0.000000    0.836800    3
    CC3261   CC3162   OC3C61   CC3163    9    0.000000    0.836800    3
  HCA2    CC3261   CC3162   OC3C61    9    0.000000    0.836800    3
  HCA2    CC3261   CC3162   OC301     9    0.000000    0.836800    3
  HCA1    CC3162   CC3261   CC3161    9    0.000000    0.836800    3
  HCA1    CC3162   CC3261   HCA2      9    0.000000    0.836800    3
 CC3261   CC3162   OC301    CC3161    9  180.000000    1.715440    1
 CC3261   CC3162   OC301    CC3161    9  180.000000    2.761440    2
 CC3261   CC3162   OC301    CC3161    9    0.000000    6.694400    3
 CC3161   CC3161   CC3261   CC3162    9  180.000000    0.794960    3
  HCA1    CC3161   CC3261   CC3162    9    0.000000    0.836800    3
 CC3162   CC3261   CC3161   OC311     9    0.000000    0.836800    3
 CC3261   CC3161   CC3161   OC301     9    0.000000    0.836800    3
 CC3261   CC3161   CC3161   OC311     9    0.000000    0.836800    3

[ dihedraltypes ]
; 'improper' dihedrals
;    i      j      k      l  func       phi0       kphi
```

Supporting Data File S2. Bufalin-N-glucose force field parameters.

#bufalin-N-glucose.pdb

```
ATOM      1  C18 bufaX2005      62.520  63.310 118.420  0.00  0.00
ATOM      2  C13 bufaX2005      61.600  64.550 118.520  0.00  0.00
ATOM      3  C12 bufaX2005      62.380  65.810 118.930  0.00  0.00
ATOM      4  C11 bufaX2005      62.890  65.720 120.360  0.00  0.00
ATOM      5  C9  bufaX2005      61.740  65.590 121.370  0.00  0.00
ATOM      6  C10 bufaX2005      62.210  65.470 122.840  0.00  0.00
ATOM      7  C19 bufaX2005      63.150  64.240 122.960  0.00  0.00
ATOM      8  C1  bufaX2005      63.050  66.690 123.310  0.00  0.00
ATOM      9  C2  bufaX2005      62.280  68.000 123.560  0.00  0.00
ATOM     10  C3  bufaX2005      61.160  67.880 124.620  0.00  0.00
ATOM     11  N11 bufaX2005      61.590  67.720 126.080  0.00  0.00
ATOM     12  C4  bufaX2005      60.260  66.700 124.130  0.00  0.00
ATOM     13  C5  bufaX2005      61.020  65.370 123.810  0.00  0.00
ATOM     14  C6  bufaX2005      60.040  64.250 123.390  0.00  0.00
ATOM     15  C7  bufaX2005      59.620  64.320 121.920  0.00  0.00
ATOM     16  C8  bufaX2005      60.870  64.360 121.000  0.00  0.00
ATOM     17  C14 bufaX2005      60.390  64.360 119.510  0.00  0.00
ATOM     18  O14 bufaX2005      59.680  63.160 119.200  0.00  0.00
ATOM     19  C15 bufaX2005      59.470  65.520 119.160  0.00  0.00
ATOM     20  C16 bufaX2005      59.710  65.810 117.660  0.00  0.00
ATOM     21  C17 bufaX2005      60.880  64.890 117.180  0.00  0.00
ATOM     22  C20 bufaX2005      60.510  63.750 116.260  0.00  0.00
ATOM     23  C22 bufaX2005      61.450  63.240 115.380  0.00  0.00
ATOM     24  C23 bufaX2005      61.200  62.190 114.510  0.00  0.00
ATOM     25  C24 bufaX2005      59.920  61.590 114.510  0.00  0.00
ATOM     26  O24 bufaX2005      59.500  60.830 113.640  0.00  0.00
ATOM     27  O21 bufaX2005      58.960  62.360 115.190  0.00  0.00
ATOM     28  C21 bufaX2005      59.270  63.170 116.270  0.00  0.00
ATOM     29 H181 bufaX2005      62.830  62.970 119.430  0.00  0.00
ATOM     30 H182 bufaX2005      62.020  62.460 117.920  0.00  0.00
ATOM     31 H183 bufaX2005      63.450  63.550 117.860  0.00  0.00
ATOM     32 H121 bufaX2005      63.260  65.910 118.260  0.00  0.00
ATOM     33 H122 bufaX2005      61.770  66.730 118.860  0.00  0.00
ATOM     34 H111 bufaX2005      63.490  66.630 120.570  0.00  0.00
ATOM     35 H112 bufaX2005      63.560  64.850 120.400  0.00  0.00
ATOM     36  H9  bufaX2005      61.110  66.500 121.300  0.00  0.00
ATOM     37 H191 bufaX2005      63.670  64.240 123.930  0.00  0.00
ATOM     38 H192 bufaX2005      62.590  63.290 122.880  0.00  0.00
ATOM     39 H193 bufaX2005      63.950  64.230 122.210  0.00  0.00
ATOM     40  H11 bufaX2005      63.480  66.410 124.290  0.00  0.00
ATOM     41  H12 bufaX2005      63.880  66.860 122.600  0.00  0.00
ATOM     42  H21 bufaX2005      61.800  68.280 122.600  0.00  0.00
ATOM     43  H22 bufaX2005      62.940  68.830 123.810  0.00  0.00
ATOM     44  H3  bufaX2005      60.560  68.810 124.610  0.00  0.00
ATOM     45  H41 bufaX2005      59.750  67.020 123.200  0.00  0.00
ATOM     46  H42 bufaX2005      59.470  66.500 124.870  0.00  0.00
ATOM     47  H5  bufaX2005      61.420  65.120 124.810  0.00  0.00
ATOM     48  H61 bufaX2005      60.500  63.250 123.570  0.00  0.00
```

```
ATOM     49  H62 bufaX2005     59.130  64.300 124.030  0.00  0.00
ATOM     50  H71 bufaX2005     59.000  65.230 121.770  0.00  0.00
ATOM     51  H72 bufaX2005     58.990  63.430 121.680  0.00  0.00
ATOM     52  H8  bufaX2005     61.440  63.420 121.140  0.00  0.00
ATOM     53 HO14 bufaX2005     60.310  62.450 119.030  0.00  0.00
ATOM     54 H151 bufaX2005     59.700  66.400 119.770  0.00  0.00
ATOM     55 H152 bufaX2005     58.420  65.280 119.370  0.00  0.00
ATOM     56 H161 bufaX2005     59.960  66.870 117.530  0.00  0.00
ATOM     57 H162 bufaX2005     58.790  65.650 117.090  0.00  0.00
ATOM     58  H17 bufaX2005     61.570  65.530 116.610  0.00  0.00
ATOM     59  H2  bufaX2005     62.440  63.710 115.380  0.00  0.00
ATOM     60  H23 bufaX2005     61.940  61.870 113.780  0.00  0.00
ATOM     61  H1  bufaX2005     58.570  63.380 117.080  0.00  0.00
ATOM     62  O62 bufaX2005     60.420  67.520 126.860  0.00  0.00
ATOM     63  C63 bufaX2005     60.490  66.370 127.690  0.00  0.00
ATOM     64  H64 bufaX2005     59.560  66.270 128.290  0.00  0.00
ATOM     65  H65 bufaX2005     60.580  65.450 127.070  0.00  0.00
ATOM     66  H66 bufaX2005     61.350  66.430 128.390  0.00  0.00
ATOM     67  H67 bufaX2005     62.530  68.380 127.860  0.00  0.00
ATOM     68  C68 bufaX2005     62.360  70.810 128.000  0.00  0.00
ATOM     69  O69 bufaX2005     61.870  70.070 126.860  0.00  0.00
ATOM     70  C70 bufaX2005     62.470  68.760 126.810  0.00  0.00
ATOM     71  C71 bufaX2005     63.920  68.980 126.400  0.00  0.00
ATOM     72  C72 bufaX2005     64.690  69.980 127.270  0.00  0.00
ATOM     73  C73 bufaX2005     63.860  71.100 127.870  0.00  0.00
ATOM     74  H74 bufaX2005     62.200  70.190 128.910  0.00  0.00
ATOM     75  C75 bufaX2005     61.530  72.070 128.180  0.00  0.00
ATOM     76  O76 bufaX2005     64.640  67.760 126.390  0.00  0.00
ATOM     77  H77 bufaX2005     63.940  69.420 125.380  0.00  0.00
ATOM     78  H78 bufaX2005     65.110  69.380 128.110  0.00  0.00
ATOM     79  H79 bufaX2005     63.940  71.980 127.190  0.00  0.00
ATOM     80  O80 bufaX2005     64.390  71.450 129.140  0.00  0.00
ATOM     81  H81 bufaX2005     61.790  72.820 127.400  0.00  0.00
ATOM     82  O82 bufaX2005     61.670  72.680 129.470  0.00  0.00
ATOM     83  H83 bufaX2005     60.460  71.800 128.060  0.00  0.00
ATOM     84  H84 bufaX2005     62.540  73.150 129.560  0.00  0.00
ATOM     85  H85 bufaX2005     64.630  67.370 127.300  0.00  0.00
ATOM     86  H86 bufaX2005     64.280  70.670 129.720  0.00  0.00
ATOM     87  O87 bufaX2005     65.850  70.500 126.610  0.00  0.00
ATOM     88  H88 bufaX2005     66.510  70.710 127.280  0.00  0.00
END
```

#bufalin-N-glucose.itp excerpt

```
[ atoms         ]

;               nr              type            resnr           residue         atom            cgnr
                charge          mass            typeB           chargeB         massB
;               residue         1               bufalin-N-glucose               rtp             bufalin-N-
glucose         q               qsum
                1               CTL3            1               bufalin-N-glucose               C18
                1               -0.268          12.011
```

2	CRL1	1	bufalin-N-glucose	C13
2	0.001	12.011		
3	CRL2	1	bufalin-N-glucose	C12
3	-0.183	12.011		
4	CRL2	1	bufalin-N-glucose	C11
4	-0.182	12.011		
5	CRL1	1	bufalin-N-glucose	C9
5	-0.09	12.011		
6	CRL1	1	bufalin-N-glucose	C10
6	-0.001	12.011		
7	CTL3	1	bufalin-N-glucose	C19
7	-0.274	12.011		
8	CRL2	1	bufalin-N-glucose	C1
8	-0.18	12.011		
9	CRL2	1	bufalin-N-glucose	C2
9	-0.179	12.011		
10	CRL1	1	bufalin-N-glucose	C3
10	0.135	12.011		
11	NG301	1	bufalin-N-glucose	N11
11	-0.391	14.007		
12	CRL2	1	bufalin-N-glucose	C4
12	-0.177	12.011		
13	CRL1	1	bufalin-N-glucose	C5
13	-0.09	12.011		
14	CRL2	1	bufalin-N-glucose	C6
14	-0.181	12.011		
15	CRL2	1	bufalin-N-glucose	C7
15	-0.181	12.011		
16	CRL1	1	bufalin-N-glucose	C8
16	-0.09	12.011		
17	CRL1	1	bufalin-N-glucose	C14
17	0.238	12.011		
18	OHL	1	bufalin-N-glucose	O14
18	-0.651	15.999		
19	CRL2	1	bufalin-N-glucose	C15
19	-0.181	12.011		
20	CRL2	1	bufalin-N-glucose	C16
20	-0.177	12.011		
21	CRL1	1	bufalin-N-glucose	C17
21	-0.039	12.011		
22	CG2R62	1	bufalin-N-glucose	C20
22	0.032	12.011		
23	CG2R62	1	bufalin-N-glucose	C22
23	-0.272	12.011		
24	CG2R62	1	bufalin-N-glucose	C23
24	-0.347	12.011		
25	CG2R63	1	bufalin-N-glucose	C24
25	0.49	12.011		
26	OG2D4	1	bufalin-N-glucose	O24
26	-0.46	15.999		

27	OG3R60	1	bufalin-N-glucose	O21
27	-0.362	15.999		
28	CG2R62	1	bufalin-N-glucose	C21
28	0.119	12.011		
29	HAL3	1	bufalin-N-glucose	H181
29	0.09	1.008		
30	HAL3	1	bufalin-N-glucose	H182
30	0.09	1.008		
31	HAL3	1	bufalin-N-glucose	H183
31	0.09	1.008		
32	HGA2	1	bufalin-N-glucose	H121
32	0.09	1.008		
33	HGA2	1	bufalin-N-glucose	H122
33	0.09	1.008		
34	HGA2	1	bufalin-N-glucose	H111
34	0.09	1.008		
35	HGA2	1	bufalin-N-glucose	H112
35	0.09	1.008		
36	HGA1	1	bufalin-N-glucose	H9
36	0.09	1.008		
37	HAL3	1	bufalin-N-glucose	H191
37	0.09	1.008		
38	HAL3	1	bufalin-N-glucose	H192
38	0.09	1.008		
39	HAL3	1	bufalin-N-glucose	H193
39	0.09	1.008		
40	HGA2	1	bufalin-N-glucose	H11
40	0.09	1.008		
41	HGA2	1	bufalin-N-glucose	H12
41	0.09	1.008		
42	HGA2	1	bufalin-N-glucose	H21
42	0.09	1.008		
43	HGA2	1	bufalin-N-glucose	H22
43	0.09	1.008		
44	HGA1	1	bufalin-N-glucose	H3
44	0.09	1.008		
45	HGA2	1	bufalin-N-glucose	H41
45	0.09	1.008		
46	HGA2	1	bufalin-N-glucose	H42
46	0.09	1.008		
47	HGA1	1	bufalin-N-glucose	H5
47	0.09	1.008		
48	HGA2	1	bufalin-N-glucose	H61
48	0.09	1.008		
49	HGA2	1	bufalin-N-glucose	H62
49	0.09	1.008		
50	HGA2	1	bufalin-N-glucose	H71
50	0.09	1.008		
51	HGA2	1	bufalin-N-glucose	H72
51	0.09	1.008		

52	HGA1	1	bufalin-N-glucose	H8
52	0.09	1.008		
53	HOL	1	bufalin-N-glucose	HO14
53	0.42	1.008		
54	HGA2	1	bufalin-N-glucose	H151
54	0.09	1.008		
55	HGA2	1	bufalin-N-glucose	H152
55	0.09	1.008		
56	HGA2	1	bufalin-N-glucose	H161
56	0.09	1.008		
57	HGA2	1	bufalin-N-glucose	H162
57	0.09	1.008		
58	HGA1	1	bufalin-N-glucose	H17
58	0.09	1.008		
59	HGR62	1	bufalin-N-glucose	H2
59	0.268	1.008		
60	HGR62	1	bufalin-N-glucose	H23
60	0.199	1.008		
61	HGR62	1	bufalin-N-glucose	H1
61	0.284	1.008		
62	OG301	1	bufalin-N-glucose	O62
62	-0.17	15.999		
63	CG331	1	bufalin-N-glucose	C63
63	-0.1	12.011		
64	HGA3	1	bufalin-N-glucose	H64
64	0.09	1.008		
65	HGA3	1	bufalin-N-glucose	H65
65	0.09	1.008		
66	HGA3	1	bufalin-N-glucose	H66
66	0.09	1.008		
67	HCA1	1	bufalin-N-glucose	H67
67	0.09	1.008		
68	CC3163	1	bufalin-N-glucose	C68
68	0.11	12.011		
69	OC3C61	1	bufalin-N-glucose	O69
69	-0.4	15.999		
70	CC3162	1	bufalin-N-glucose	C70
70	0.27	12.011		
71	CC3161	1	bufalin-N-glucose	C71
71	0.14	12.011		
72	CC3161	1	bufalin-N-glucose	C72
72	0.14	12.011		
73	CC3161	1	bufalin-N-glucose	C73
73	0.14	12.011		
74	HCA1	1	bufalin-N-glucose	H74
74	0.09	1.008		
75	CC321	1	bufalin-N-glucose	C75
75	0.05	12.011		
76	OC311	1	bufalin-N-glucose	O76
76	-0.65	15.999		

77	HCA1	1	bufalin-N-glucose	H77
77	0.09	1.008		
78	HCA1	1	bufalin-N-glucose	H78
78	0.09	1.008		
79	HCA1	1	bufalin-N-glucose	H79
79	0.09	1.008		
80	OC311	1	bufalin-N-glucose	O80
80	-0.65	15.999		
81	HCA2	1	bufalin-N-glucose	H81
81	0.09	1.008		
82	OC311	1	bufalin-N-glucose	O82
82	-0.65	15.999		
83	HCA2	1	bufalin-N-glucose	H83
83	0.09	1.008		
84	HCP1	1	bufalin-N-glucose	H84
84	0.42	1.008		
85	HCP1	1	bufalin-N-glucose	H85
85	0.42	1.008		
86	HCP1	1	bufalin-N-glucose	H86
86	0.42	1.008		
87	OC311	1	bufalin-N-glucose	O87
87	-0.65	15.999		
88	HCP1	1	bufalin-N-glucose	H88
88	0.42	1.008		

#bufalin-N-glucose.prm

```
[ bondtypes ]
;    i      j  func       b0          kb
  CG2R57   CG3C51     1   0.15100000    292880.00
  CG2R57   CG3C52     1   0.15100000    292880.00
  CG3RC1    OG311     1   0.14200000    358150.40
  CC3261   CC3162     1   0.14800000    186188.00
   CG311    OC301     1    0.14150000    301248.00

[ angletypes ]
;    i      j      k  func      theta0      ktheta         ub0         kub
  CG2R53   CG2R51   CG2R57    5   116.500000   836.800000   0.00000000       0.00
  CG2R51   CG2R57   CG3C51    5   109.000000   962.320000   0.00000000       0.00
  CG2R51   CG2R57   CG3C52    5   109.000000   962.320000   0.00000000       0.00
  CG3C51   CG2R57   CG3C52    5   105.800000   753.120000   0.00000000       0.00
   CG311    CG311    OC311    5   109.700000   962.320000   0.00000000       0.00
   CG311    CG311   OG3C61    5   111.500000   376.560000   0.00000000       0.00
   CG321    CG311    OC311    5   109.700000   962.320000   0.00000000       0.00
   CG321    CG311    OC301    5   109.000000   376.560000   0.00000000       0.00
   CG321    CG311   OG3C61    5   111.500000   376.560000   0.00000000       0.00
   CG331    CG311   OG3C61    5   111.500000   376.560000   0.00000000       0.00
  OG3C61    CG311     HGA1    5   109.500000   376.560000   0.00000000       0.00
  CG2R57   CG3C51   CG3C52    5   106.000000   435.136000   0.00000000       0.00
  CG2R57   CG3C51   CG3RC1    5   106.000000   435.136000   0.00000000       0.00
  CG2R57   CG3C51    HGA1     5   112.600000   435.136000   0.00000000       0.00
  CG2R57   CG3C52   OG3C51    5   102.400000   627.600000   0.00000000       0.00
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 CG2R57  CG3C52   HGA2    5  112.600000  435.136000  0.00000000      0.00
  CG311  CG3RC1   OG311   5  113.500000  488.272800  0.25610000   9338.69
 CG3C52  CG3RC1   OG311   5  110.000000  633.457600  0.00000000      0.00
 CG3RC1  CG3RC1   OG311   5  111.000000  446.432800  0.25610000   6694.40
 CC3162   OC301   CG311   5  109.200000  418.400000  0.00000000      0.00
 CG3RC1   OG311   HGP1    5  109.000000  418.400000  0.00000000      0.00
  CG311  OG3C61   CG311   5  109.700000  794.960000  0.00000000      0.00
 CC3261  CC3162   HCA1    5  110.100000  288.696000  0.21790000  18853.10
 CC3261  CC3162  OC3C61   5  106.000000  376.560000  0.00000000      0.00
  OC301   CG311   HGA1    5  109.500000  502.080000  0.00000000      0.00
 CC3261  CC3162   OC311   5  107.000000  633.457600  0.00000000      0.00
  OC301  CC3162  CC3261   5  105.000000  376.560000  0.00000000      0.00
 CC3162  CC3261  CC3161   5  111.000000  446.432800  0.25610000   6694.40
 CC3162  CC3261   HCA2    5  110.100000  288.696000  0.21790000  18853.10

[ dihedraltypes ]
;    i      j      k      l  func       phi0       kphi  mult
 CG2R57  CG2R51  CG2R53  OG2D1    9  180.000000   5.020800     2
 CG2R57  CG2R51  CG2R53  OG3C51   9  180.000000   1.715440     1
 CG2R53  CG2R51  CG2R57  CG3C51   9  180.000000  27.614400     2
 CG2R53  CG2R51  CG2R57  CG3C52   9  180.000000  27.614400     2
  HGR51  CG2R51  CG2R57  CG3C51   9  180.000000  12.133600     2
  HGR51  CG2R51  CG2R57  CG3C52   9  180.000000  12.133600     2
 CG2R51  CG2R57  CG3C51  CG3C52   9  180.000000   0.209200     3
 CG2R51  CG2R57  CG3C51  CG3RC1   9  180.000000   0.209200     3
 CG2R51  CG2R57  CG3C51   HGA1    9    0.000000   0.000000     3
 CG3C52  CG2R57  CG3C51  CG3C52   9    0.000000   9.916080     2
 CG3C52  CG2R57  CG3C51  CG3RC1   9    0.000000   9.916080     2
 CG3C52  CG2R57  CG3C51   HGA1    9  180.000000   0.000000     3
 CG2R51  CG2R57  CG3C52  OG3C51   9  180.000000   1.171520     1
 CG2R51  CG2R57  CG3C52  OG3C51   9  180.000000   4.100320     2
 CG2R51  CG2R57  CG3C52  OG3C51   9  180.000000   7.322000     3
 CG2R51  CG2R57  CG3C52   HGA2    9    0.000000   0.000000     3
 CG3C51  CG2R57  CG3C52  OG3C51   9  180.000000   1.171520     1
 CG3C51  CG2R57  CG3C52  OG3C51   9  180.000000   4.100320     2
 CG3C51  CG2R57  CG3C52  OG3C51   9  180.000000   7.322000     3
 CG3C51  CG2R57  CG3C52   HGA2    9  180.000000   0.000000     3
  CG311   CG311   CG311   CG331   9  180.000000   2.092000     4
  CG311   CG311   CG311  OG3C61   9  180.000000   0.794960     1
  CG311   CG311   CG311  OG3C61   9  180.000000   4.184000     2
  CG311   CG311   CG311  OG3C61   9    0.000000   2.510400     3
  CG311   CG311   CG311  OG3C61   9  180.000000   0.334720     4
  CG321   CG311   CG311   OG301   9  180.000000   0.836800     3
  CG321   CG311   CG311   OC301   9  180.000000   0.836800     3
  CG321   CG311   CG311   OG311   9    0.000000   0.585760     3
  CG331   CG311   CG311   OG311   9    0.000000   0.585760     3
  OG301   CG311   CG311   OG311   9    0.000000   0.836800     3
  OG301   CG311   CG311  OG3C61   9    0.000000   0.836800     3
  OC301   CG311   CG311  OG3C61   9    0.000000   0.836800     3
  OG301   CG311   CG311    HGA1   9    0.000000   0.815880     3
  OC301   CG311   CG311    HGA1   9    0.000000   0.815880     3
```

OG311 CG311 CG311 OG311 9 0.000000 0.836800 3
OG311 CG311 CG311 OG3C61 9 0.000000 0.836800 3
OG301 CG311 CG321 CG311 9 180.000000 0.669440 1
OG301 CG311 CG321 CG311 9 0.000000 1.631760 2
OC301 CG311 CG321 CG311 9 0.000000 0.836800 3
OC301 CG311 CG321 CG321 9 0.000000 0.836800 3
OG301 CG311 CG321 HGA2 9 0.000000 0.815880 3
OC301 CG311 CG321 HGA2 9 0.000000 0.815880 3
CG311 CG311 CG3RC1 OG311 9 0.000000 0.209200 3
CG321 CG311 CG3RC1 OG311 9 0.000000 0.209200 3
HGA1 CG311 CG3RC1 OG311 9 0.000000 0.209200 3
CG311 CG311 OG301 CG311 9 0.000000 1.673600 1
CG311 CG311 OG301 CG311 9 0.000000 2.050160 3
CG321 CG311 OC301 CC3162 9 180.000000 0.543920 1
CG321 CG311 OC301 CC3162 9 180.000000 1.046000 2
CG321 CG311 OC301 CC3162 9 180.000000 0.251040 3
HGA1 CG311 OG301 CG311 9 0.000000 1.188256 3
HGA1 CG311 OC301 CC3162 9 0.000000 1.188256 3
CG2R57 CG3C51 CG3C52 CG3C52 9 180.000000 15.480800 3
CG2R57 CG3C51 CG3C52 CG3C52 9 0.000000 9.414000 4
CG2R57 CG3C51 CG3C52 CG3C52 9 180.000000 0.962320 6
CG2R57 CG3C51 CG3C52 HGA2 9 0.000000 0.585760 3
CG2R57 CG3C51 CG3RC1 CG311 9 180.000000 15.480800 3
CG2R57 CG3C51 CG3RC1 CG311 9 0.000000 9.414000 4
CG2R57 CG3C51 CG3RC1 CG311 9 180.000000 0.962320 6
CG2R57 CG3C51 CG3RC1 CG331 9 180.000000 15.480800 3
CG2R57 CG3C51 CG3RC1 CG331 9 0.000000 9.414000 4
CG2R57 CG3C51 CG3RC1 CG331 9 180.000000 0.962320 6
CG2R57 CG3C51 CG3RC1 CG3RC1 9 0.000000 0.627600 3
CG3C52 CG3C52 CG3RC1 OG311 9 180.000000 2.092000 1
CG3C52 CG3C52 CG3RC1 OG311 9 0.000000 2.928800 2
CG3C52 CG3C52 CG3RC1 OG311 9 0.000000 1.673600 3
CG3C52 CG3C52 CG3RC1 OG311 9 0.000000 1.673600 5
HGA2 CG3C52 CG3RC1 OG311 9 180.000000 0.815880 3
CG2R57 CG3C52 OG3C51 CG2R53 9 180.000000 1.297040 1
CG2R57 CG3C52 OG3C51 CG2R53 9 0.000000 1.171520 6
CG311 CG3RC1 CG3RC1 OG311 9 0.000000 16.736000 3
CG331 CG3RC1 CG3RC1 OG311 9 0.000000 0.209200 3
CG3C51 CG3RC1 CG3RC1 OG311 9 0.000000 5.020800 3
CG311 CG3RC1 OG311 HGP1 9 0.000000 1.213360 1
CG311 CG3RC1 OG311 HGP1 9 0.000000 2.594080 2
CG311 CG3RC1 OG311 HGP1 9 0.000000 0.209200 3
CG3C52 CG3RC1 OG311 HGP1 9 0.000000 1.213360 1
CG3C52 CG3RC1 OG311 HGP1 9 0.000000 2.594080 2
CG3C52 CG3RC1 OG311 HGP1 9 0.000000 0.209200 3
CG3RC1 CG3RC1 OG311 HGP1 9 0.000000 6.276000 1
CG3RC1 CG3RC1 OG311 HGP1 9 180.000000 1.255200 2
CG3RC1 CG3RC1 OG311 HGP1 9 0.000000 1.338880 3
CG311 OC301 CC3162 OC3C61 9 180.000000 0.209200 1
CG311 OC301 CC3162 OC3C61 9 0.000000 3.807440 2
CG311 OC301 CC3162 OC3C61 9 180.000000 5.313680 3

```
  CC3161   CC3261   CC3162    OC301     9     0.000000     0.836800     3
  CC3261   CC3162    OC301    CG311     9   180.000000     1.715440     1
  CC3261   CC3162    OC301    CG311     9   180.000000     2.761440     2
  CC3261   CC3162    OC301    CG311     9     0.000000     6.694400     3
   CG311    OC301   CC3162     HCA1     9     0.000000     1.188256     3
  CC3161   CC3261   CC3162   OC3C61     9   180.000000     1.297040     3
  CC3161   CC3162   OC3C61   CC3163     9     0.000000     0.836800     3
   HCA1   CC3261   CC3162   OC3C61     9     0.000000     0.836800     3
  CC3261   CC3162   OC3C61   CC3163     9     0.000000     0.836800     3
   HCA2   CC3261   CC3162   OC3C61     9     0.000000     0.836800     3
   HCA2   CC3261   CC3162    OC301     9     0.000000     0.836800     3
   HCA1   CC3162   CC3261   CC3161     9     0.000000     0.836800     3
   HCA1   CC3162   CC3261    HCA2     9     0.000000     0.836800     3
  CC3261   CC3162    OC301   CC3161     9   180.000000     1.715440     1
  CC3261   CC3162    OC301   CC3161     9   180.000000     2.761440     2
  CC3261   CC3162    OC301   CC3161     9     0.000000     6.694400     3
  CC3161   CC3161   CC3261   CC3162     9   180.000000     0.794960     3
   HCA1   CC3161   CC3261   CC3162     9     0.000000     0.836800     3
  CC3162   CC3261   CC3161    OC311     9     0.000000     0.836800     3
  CC3261   CC3161   CC3161    OC301     9     0.000000     0.836800     3
  CC3261   CC3161   CC3161    OC311     9     0.000000     0.836800     3
```

```
[ dihedraltypes ]
; 'improper' dihedrals
;    i      j      k      l  func       phi0        kphi
```