Supporting Information

The dynamics of the conformational changes in the hexopyranose ring: a transition path sampling approach

Wojciech Plazinski[1] [+], Mateusz Drach[2]

[1] *Institute of Catalysis and Surface Chemistry, Polish Academy of Sciences, ul. Niezapominajek 8, 30-239 Cracow, Poland*

[2] *Department of Theoretical Chemistry, Faculty of Chemistry, UMCS, pl. M. Curie-Sklodowskiej 3, 20-031 Lublin, Poland*

[+] Corresponding author. Tel.: +48815375685; fax: +48815375685.
E-mail addresses: wojtek_plazinski@o2.pl; wojtek@vega.umcs.lublin.pl

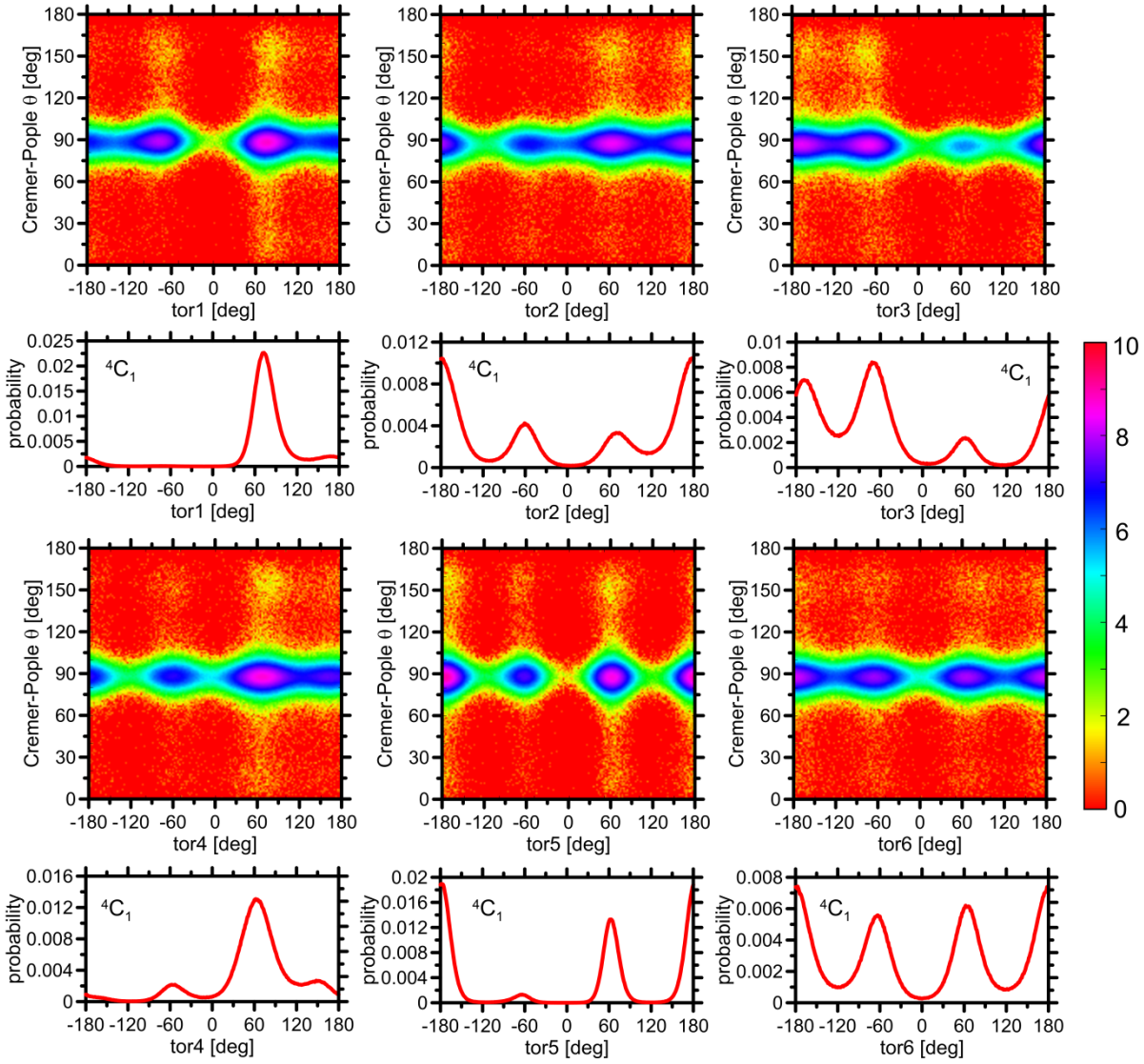

Fig. S1. Path density plots obtained from the TPS trajectories and reflecting the orientation of the exocyclic groups (tor1-tor6 dihedral angles in the molecule of GlcA) dependent on the progress of the $^4C_1 \rightarrow {}^1C_4$ transition, expressed as the value of θ. The bin dimension was 2.4×1.2 deg^2 and the scale on the right corresponds to the logarithm of the number of configurations per one bin. Note that not entire phase space is sampled, which results in the lack of data corresponding to the two chair conformers. The tor1-tor6 dihedral angle distributions obtained during unbiased MD simulations and representing the $^4C_1$ conformation are given as line plots. Further details are given in the main manuscript.

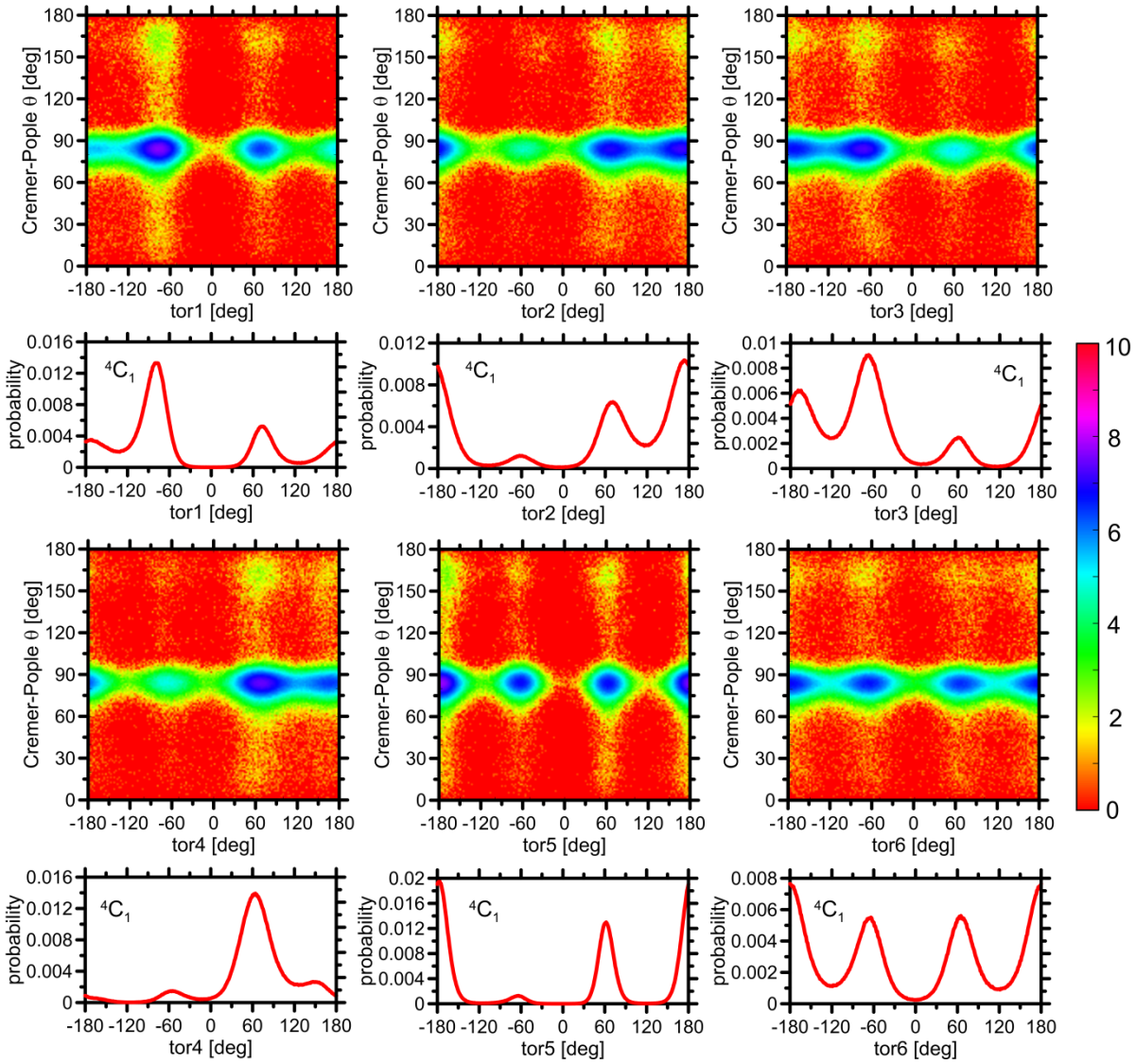

Fig. S2. Path density plots obtained from the TPS trajectories and reflecting the orientation of the exocyclic groups (tor1-tor6 dihedral angles in the molecule of GlcA) dependent on the progress of the $^4C_1 \rightarrow {}^1C_4$ transition, expressed as the value of θ. The rest of the details as in Fig. S1.

The coordinates of the four structures identified as transition states of GlcA (PDB data):

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CRYST1   30.145   30.145   30.145  90.00  90.00  90.00 P 1
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ATOM      1  C4  GLC     1      12.400  23.130  16.640  1.00  0.00
ATOM      2  O4  GLC     1      11.090  23.640  16.380  1.00  0.00
ATOM      3  HO4 GLC     1      10.380  23.030  16.760  1.00  0.00
ATOM      4  C3  GLC     1      13.530  23.170  15.620  1.00  0.00
ATOM      5  O3  GLC     1      13.600  21.930  14.900  1.00  0.00
ATOM      6  HO3 GLC     1      13.960  21.960  13.970  1.00  0.00
ATOM      7  C2  GLC     1      14.910  23.600  16.080  1.00  0.00
ATOM      8  O2  GLC     1      14.970  25.020  15.850  1.00  0.00
ATOM      9  HO2 GLC     1      15.840  25.450  16.070  1.00  0.00
ATOM     10  C6  GLC     1      12.240  22.460  19.040  1.00  0.00
ATOM     11  O6  GLC     1      12.810  21.140  19.030  1.00  0.00
ATOM     12  HO6 GLC     1      12.220  20.470  18.600  1.00  0.00
ATOM     13  C5  GLC     1      12.830  23.460  18.060  1.00  0.00
ATOM     14  O5  GLC     1      14.190  23.750  18.420  1.00  0.00
ATOM     15  C1  GLC     1      15.100  23.110  17.510  1.00  0.00
ATOM     16  O1  GLC     1      16.410  23.470  17.960  1.00  0.00
ATOM     17  HO1 GLC     1      16.540  24.460  17.880  1.00  0.00

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ATOM      1  C4  GLC     1      13.750  17.560  19.870  1.00  0.00
ATOM      2  O4  GLC     1      14.160  17.100  18.580  1.00  0.00
ATOM      3  HO4 GLC     1      14.010  16.130  18.420  1.00  0.00
ATOM      4  C3  GLC     1      14.510  18.790  20.340  1.00  0.00
ATOM      5  O3  GLC     1      14.680  19.170  21.720  1.00  0.00
ATOM      6  HO3 GLC     1      15.540  19.650  21.900  1.00  0.00
ATOM      7  C2  GLC     1      13.900  20.040  19.740  1.00  0.00
ATOM      8  O2  GLC     1      13.930  20.180  18.310  1.00  0.00
ATOM      9  HO2 GLC     1      14.730  20.700  18.040  1.00  0.00
ATOM     10  C6  GLC     1      11.780  16.480  20.430  1.00  0.00
ATOM     11  O6  GLC     1      10.350  16.450  20.580  1.00  0.00
ATOM     12  HO6 GLC     1      10.070  17.010  21.370  1.00  0.00
ATOM     13  C5  GLC     1      12.260  17.850  19.960  1.00  0.00
ATOM     14  O5  GLC     1      11.720  19.050  20.540  1.00  0.00
ATOM     15  C1  GLC     1      12.510  20.220  20.320  1.00  0.00
ATOM     16  O1  GLC     1      11.610  21.160  19.710  1.00  0.00
ATOM     17  HO1 GLC     1      11.330  21.850  20.370  1.00  0.00

TITLE     Generated by trjconv : UNNAMED in water t= 162.10001
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MODEL        1
ATOM      1  C4  GLC     1      11.220  20.120  19.050  1.00  0.00
ATOM      2  O4  GLC     1      11.960  21.340  18.910  1.00  0.00
ATOM      3  HO4 GLC     1      12.160  21.490  17.940  1.00  0.00
ATOM      4  C3  GLC     1      12.040  18.870  19.270  1.00  0.00
ATOM      5  O3  GLC     1      11.750  17.760  18.410  1.00  0.00
ATOM      6  HO3 GLC     1      11.740  18.000  17.440  1.00  0.00
ATOM      7  C2  GLC     1      12.130  18.390  20.710  1.00  0.00
ATOM      8  O2  GLC     1      12.930  19.240  21.550  1.00  0.00
ATOM      9  HO2 GLC     1      13.190  18.730  22.370  1.00  0.00
ATOM     10  C6  GLC     1       8.960  20.910  19.430  1.00  0.00
ATOM     11  O6  GLC     1       7.940  21.340  20.350  1.00  0.00
ATOM     12  HO6 GLC     1       7.710  20.550  20.920  1.00  0.00
ATOM     13  C5  GLC     1      10.180  20.350  20.140  1.00  0.00
ATOM     14  O5  GLC     1       9.810  19.360  21.110  1.00  0.00
ATOM     15  C1  GLC     1      10.660  18.210  21.080  1.00  0.00
ATOM     16  O1  GLC     1      10.560  17.510  22.330  1.00  0.00
ATOM     17  HO1 GLC     1       9.640  17.270  22.640  1.00  0.00

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MODEL        1
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ATOM      2  O4  GLC     1      19.090  16.760  14.920  1.00  0.00
ATOM      3  HO4 GLC     1      19.330  17.670  14.560  1.00  0.00
ATOM      4  C3  GLC     1      18.050  14.740  14.110  1.00  0.00
ATOM      5  O3  GLC     1      17.820  13.950  12.930  1.00  0.00
ATOM      6  HO3 GLC     1      18.650  13.760  12.420  1.00  0.00
ATOM      7  C2  GLC     1      16.870  14.490  15.030  1.00  0.00
ATOM      8  O2  GLC     1      17.230  14.420  16.420  1.00  0.00
ATOM      9  HO2 GLC     1      17.320  13.470  16.720  1.00  0.00
ATOM     10  C6  GLC     1      17.280  17.130  11.860  1.00  0.00
ATOM     11  O6  GLC     1      18.620  17.380  11.430  1.00  0.00
ATOM     12  HO6 GLC     1      18.650  17.330  10.430  1.00  0.00
ATOM     13  C5  GLC     1      17.170  16.900  13.360  1.00  0.00
ATOM     14  O5  GLC     1      15.890  16.310  13.630  1.00  0.00
ATOM     15  C1  GLC     1      15.680  15.360  14.680  1.00  0.00
ATOM     16  O1  GLC     1      15.200  16.110  15.810  1.00  0.00
ATOM     17  HO1 GLC     1      15.030  15.350  16.440  1.00  0.00
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