Supporting information:

The Martini coarse grained force field: extension to carbohydrates

Cesar A. López[§], Andrzej J. Rzepiela[§], Alex H. de Vries[§], Lubbert Dijkhuizen[*], Philippe H. Hünenberger[†], Siewert J. Marrink[§*].

[§]Groningen Biomolecular Sciences and Biotechnology Institute & Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 4, 9747 AG Groningen, The Netherlands.

[*]Groningen Biomolecular Sciences and Biotechnology Institute (GBB), centre for Carbohydrate Bioprocessing, university of Groningen, Kerklaan 30, 9751 NN Haren, The Netherlands,

[†]Laboratorium für Physikalische Chemie, ETH Zürich, CH-8093 Zürich, Switzerland.

[*] Corresponding author e-mail: s.j.marrink@rug.nl

Table S1. Fructose parameters, Gromacs topology based. Note that the nomenclature for bonds, angles and dihedrals follows the convention adopted in[1].

```
[ moleculetype ]
; Name    nrexcl
FRU       3

[ atoms ]
;         nr        type      resnr     resid     atom      cgnr      charge    mass
          1         OA        1         FRU       O4        1         -0.642    15.9994
          2         H         1         FRU       H4        1         0.41      1.008
          3         CH1       1         FRU       C4        1         0.232     13.019
          4         CH1       1         FRU       C3        2         0.232     13.019
          5         OA        1         FRU       O3        2         -0.642    15.9994
          6         H         1         FRU       H3        2         0.41      1.008
          7         CH0       1         FRU       C2        4         0.293     12.011
          8         CH2       1         FRU       C1        3         0.232     14.027
          9         OA        1         FRU       O1        3         -0.642    15.9994
          10        H         1         FRU       H1        3         0.41      1.008
          11        OA        1         FRU       O2        4         -0.562    15.9994
          12        H         1         FRU       H2        4         0.41      1.008
          13        OA        1         FRU       O5        4         -0.434    15.9994
          14        CH1       1         FRU       C5        4         0.293     13.019
          15        CH2       1         FRU       C6        5         0.232     14.027
          16        OA        1         FRU       O6        5         -0.642    15.9994
          17        H         1         FRU       H6        5         0.41      1.008

[ bonds ]
;         ai        aj        fu        c0, c     1,
          1         2         2         gb_1      ;
          1         3         2         gb_20     ;
          3         4         2         gb_26     ;
          3         14        2         gb_26     ;
          4         5         2         gb_20     ;
          4         7         2         gb_26     ;
          5         6         2         gb_1      ;
          7         8         2         gb_26     ;
          7         11        2         gb_20     ;
          7         13        2         gb_20     ;
          8         9         2         gb_20     ;
          9         10        2         gb_1      ;
          11        12        2         gb_1      ;
          13        14        2         gb_20     ;
          14        15        2         gb_26     ;
          15        16        2         gb_20     ;
          16        17        2         gb_1      ;

[ pairs ]
;         ai        aj        fu    c0, c1, ...
          1         5         1         ;
          1         7         1         ;
          1         13        1         ;
          1         15        1         ;
          2         4         1         ;
          2         14        1         ;
          3         6         1         ;
          3         8         1         ;
          3         11        1         ;
          3         16        1         ;
          4         9         1         ;
          4         12        1         ;
          4         15        1         ;
          5         8         1         ;
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          5         11        1         ;
          5         13        1         ;
          5         14        1         ;
          6         7         1         ;
          7         10        1         ;
          7         15        1         ;
          8         12        1         ;
          8         14        1         ;
          9         11        1
          9         13        1         ;
          11        14        1         ;
          12        13
          13        16        1         ;
          14        17        1         ;
          11        13

[ angles ]
; ai  aj  ak  fu    c0, c1, ...

2         1         3         2         ga_12     ;
1         3         4         2         ga_9      ;
1         3         14        2         ga_9      ;
4         3         14        2         ga_6      ;
3         4         5         2         ga_9      ;
3         4         7         2         ga_6      ;
5         4         7         2         ga_9      ;
4         5         6         2         ga_12     ;
4         7         8         2         ga_9      ;
4         7         11        2         ga_9      ;
4         7         13        2         ga_7      ;
8         7         11        2         ga_9      ;
8         7         13        2         ga_9      ;
11        7         13        2         ga_9      ;
7         8         9         2         ga_9      ;
8         9         10        2         ga_12     ;
7         11        12        2         ga_12     ;
7         13        14        2         ga_10     ;
3         14        13        2         ga_7      ;
3         14        15        2         ga_9      ;
13        14        15        2         ga_9      ;
14        15        16        2         ga_9      ;
15        16        17        2         ga_12     ;

[ dihedrals ]
; ai        aj        ak        al        fu        c0, c1    ,         m, ...
3         4         1         14        2         gi_2      ;         imp       C4        O4        C5        C3
4         5         7         3         2         gi_2      ;         imp       C3        C4        O3        C2
7         13        8         4         2         gi_2      ;         imp       C2        C3        C1        O2
14        13        15        3         2         gi_2      ;         imp       C5        C6        C4        O5
7         8         11        5         2         gi_2      ;
; Hydrogens
2         1         3         4         1         gd_30
6         5         4         7         1         gd_30
10        9         8         7         1         gd_30
17        16        15        14        1         gd_30
12        11        7         13        1         gd_30
;Ring
4         3         14        13        1         gd_29
4         7         13        14        1         gd_29
13        4         7         3         1         gd_34
4         8         7         13        1         gd_34
11        7         4         5         1         gd_18
5         4         3         1         1         gd_18
3         4         7         11        1         gd_17
14        3         4         5         1         gd_17
7         4         3         1         1         gd_17
15        14        3         1         1         gd_17
```

8	7	4	5	1	gd_17
4	3	14	13	1	gd_17
13	14	15	16	1	gd_37
13	14	15	16	1	gd_5
13	7	8	9	1	gd_37
13	7	8	9	1	gd_5
13	7	11	12	1	gd_32
13	7	11	12	1	gd_2

Conformational analysis of fructose in water

A molecular dynamics simulation of β-D-fructofuranose in water using the parameters given above was carried on under NPT conditions for 50ns at 300K. The molecule showed a highly flexible conformation, with many ring orientations populated. We focus on the behaviour of the two principal alcohol groups, since from their dynamics; the mapping procedure would be affected (see mapping section in the article). Figure S1 depicts the history of the β-D-fructofuranose primary alcohol group orientations in aqueous solution from 50ns simulation: (a) O_1–C_1–C_2–O_5, (b) O_1–C_1–C_2–C_3, (c) O_6–C_6–C_5–O_5 and (d) O_6–C_6–C_5–C_4. As can be observed from the graphs, the alcohol groups adopted preferably the GT orientation. We compare our results with the data obtained by Costa et. al[2]. From our results we concluded that the parameters used for the simulation of fructose reproduce quiet well the behaviour of the molecule, at least for our purpose. We decided to continue using these parameters for the simulation of sucrose as well as for the parameterization of the CG model.

Figure S1.

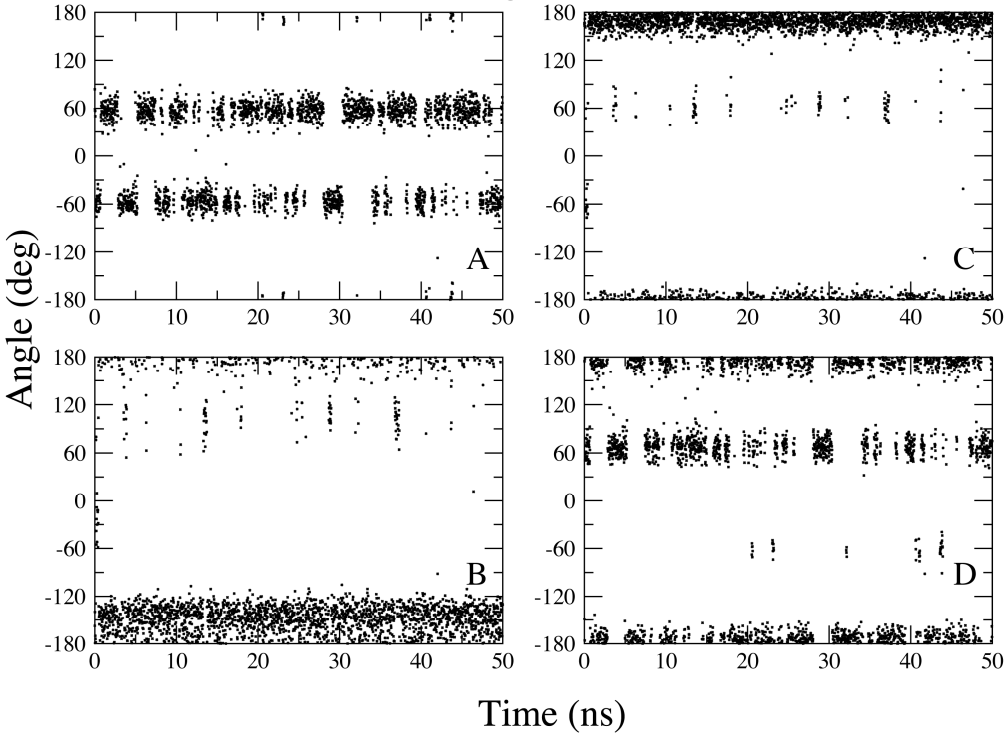


Table S2. Sucrose parameters, Gromacs topology based. Note that the nomenclature for bonds, angles and dihedrals follows the convention adopted in[1].

[moleculetype]

; Name nrexcl
SUC 3

[atoms]

;	nr	type	resnr	resid	atom	cgnr	charge	mass
	1	OA	1	SUC	O3'	1	-0.642	15.9994
	2	H	1	SUC	H3'	1	0.41	1.008
	3	CH1	1	SUC	C3'	1	0.232	13.019
	4	CH1	1	SUC	C4'	2	0.232	13.019
	5	OA	1	SUC	O4'	2	-0.642	15.9994
	6	H	1	SUC	H4'	2	0.41	1.008
	7	CH1	1	SUC	C5'	9	0.378	13.019
	8	CH2	1	SUC	C6'	3	0.232	14.027
	9	OA	1	SUC	O6'	3	-0.642	15.9994
	10	H	1	SUC	H6'	3	0.41	1.008
	11	OA	1	SUC	O5'	9	-0.45	15.9994
	12	CH0	1	SUC	C2'	9	0.242	12.011
	13	CH2	1	SUC	C1'	4	0.232	14.027
	14	OA	1	SUC	O1'	4	-0.642	15.9994
	15	H	1	SUC	H1'	4	0.41	1.008
	16	OA	1	SUC	O1	9	-0.34	15.9994
	17	CH1	1	SUC	C1	9	0.242	13.019
	18	OA	1	SUC	O5	9	-0.45	15.9994
	19	CH1	1	SUC	C5	9	0.378	13.019
	20	CH2	1	SUC	C6	5	0.232	14.027
	21	OA	1	SUC	O6	5	-0.642	15.9994
	22	H	1	SUC	H6	5	0.41	1.008
	23	CH1	1	SUC	C4	6	0.232	13.019
	24	OA	1	SUC	O4	6	-0.642	15.9994
	25	H	1	SUC	H4	6	0.41	1.008
	26	CH1	1	SUC	C3	7	0.232	13.019
	27	OA	1	SUC	O3	7	-0.642	15.9994
	28	H	1	SUC	H3	7	0.41	1.008
	29	CH1	1	SUC	C2	8	0.232	13.019
	30	OA	1	SUC	O2	8	-0.642	15.9994
	31	H	1	SUC	H2	8	0.41	1.008

[bonds]

;	ai	aj	fu	c0, c	1,	...	
	1	2	2	gb_1	;	O3'	H3'
	1	3	2	gb_20	;	O3'	C3'
	3	4	2	gb_26	;	C3'	C4'
	3	12	2	gb_26	;	C3'	C2'
	4	5	2	gb_20	;	C4'	O4'
	4	7	2	gb_26	;	CA'	C5'
	5	6	2	gb_1	;	O4'	H4'
	7	8	2	gb_26	;	C5'	C6'
	7	11	2	gb_20	;	C5'	O2'
	8	9	2	gb_20	;	C6'	O6'
	9	10	2	gb_1	;	O6'	H6'
	11	12	2	gb_20	;	O2'	C2'
	12	13	2	gb_26	;	C2'	C1'
	12	16	2	gb_20	;	C2'	O1'
	13	14	2	gb_20	;	C1'	O1'
	14	15	2	gb_1	;	O1'	H1'
	16	17	2	gb_20	;	O1	C1
	17	18	2	gb_20	;	C1	O5
	17	29	2	gb_26	;	C1	C2
	18	19	2	gb_20	;	O5	C5
	19	20	2	gb_26	;	C5	C6

19	23	2	gb_26	;	C5	C4
20	21	2	gb_20	;	C6	O6
21	22	2	gb_1	;	O6	H6
23	24	2	gb_20	;	C4	O4
23	26	2	gb_26	;	C4	C3
24	25	2	gb_1	;	O4	H4
26	27	2	gb_20	;	C3	O3
26	29	2	gb_26	;	C3	C2
27	28	2	gb_1	;	O3	H3
29	30	2	gb_20	;	C2	O2
30	31	2	gb_1	;	O2	H2

[pairs]
; ai aj fu c0, c1, ...

1	5	1	;	O3'	O4'	
1	7	1	;	O3'	C5'	
1	11	1	;	O3'	O2'	
1	13	1	;	O3'	C1'	
1	16	1	;	O3'	O1	;'
2	4	1	;	H67	C4'	;'
2	12	1	;	H67	C2'	;'
3	6	1	;	C3'	H68	;'
3	8	1	;	C3'	C6'	
3	14	1	;	C3'	O1'	
3	17	1	;	C3'	C1	;'
4	9	1	;	C4'	O6'	
4	13	1	;	C4'	C1'	
4	16	1	;	C4'	O1	;'
5	8	1	;	O4'	C6'	
5	11	1	;	O4'	O2'	
5	12	1	;	O4'	C2'	
6	7	1	;	H68	C5'	;'
7	10	1	;	C5'	H69	;'
7	13	1	;	C5'	C1'	
7	16	1	;	C5'	O1	;'
8	12	1	;	C6'	C2'	
9	11	1	;	O6'	O2'	
11	14	1	;	O2'	O1'	
11	17	1	;	O2'	C1	;'
12	15	1	;	C2'	H66	;'
12	18	1	;	C2'	O5	;'
12	29	1	;	C2'	C2	;'
13	17	1	;	C1'	C1	;'
14	16	1	;	O1'	O1	;'
16	19	1	;	O1	C5	
16	26	1	;	O1	C3	
16	30	1	;	O1	O2	
17	20	1	;	C1	C6	
17	23	1	;	C1	C4	
17	27	1	;	C1	O3	
17	31	1	;	C1	H22	
18	21	1	;	O5	O6	
18	24	1	;	O5	O4	
18	26	1	;	O5	C3	
18	30	1	;	O5	O2	
19	22	1	;	C5	H65	
19	25	1	;	C5	H42	
19	27	1	;	C5	O3	
19	29	1	;	C5	C2	
20	24	1	;	C6	O4	
20	26	1	;	C6	C3	
21	23	1	;	O6	C4	
23	28	1	;	C4	H32	
23	30	1	;	C4	O2	
24	27	1	;	O4	O3	
24	29	1	;	O4	C2	

```
25      26      1       ;       H42     C3
26      31      1       ;       C3      H22
27      30      1       ;       O3      O2
28      29      1       ;       H32     C2

[ angles ]
; ai  aj  ak  fu   c0, c1, ...

2       1       3       2       ga_12   ;       H3'     O3'     C3'
1       3       4       2       ga_9    ;       O3'     C3'     C4'
1       3       12      2       ga_9    ;       O3'     C3'     C2'
4       3       12      2       ga_6    ;       C4'     C3'     C2'
3       4       5       2       ga_9    ;       C3'     C4'     O4'
3       4       7       2       ga_6    ;       C3'     C4'     C5'
5       4       7       2       ga_9    ;       O4'     C4'     C5'
4       5       6       2       ga_12   ;       C4'     O4'     H4'
4       7       8       2       ga_9    ;       C4'     C5'     C6'
4       7       11      2       ga_9    ;       C4'     C5'     O2'
8       7       11      2       ga_7    ;       C6'     C5'     O2'
7       8       9       2       ga_9    ;       C5'     C6'     O6'
8       9       10      2       ga_12   ;       C6'     O6'     H6'
7       11      12      2       ga_10   ;       C5'     O2'     C2'
3       12      11      2       ga_7    ;       C3'     C2'     O2'
3       12      13      2       ga_9    ;       C3'     C2'     C1'
3       12      16      2       ga_9    ;       C3'     C2'     O1
11      12      13      2       ga_9    ;       O2'     C2'     C1'
11      12      16      2       ga_9    ;       O2'     C2'     O1
13      12      16      2       ga_9    ;       C1'     C2'     O1
12      13      14      2       ga_9    ;       C2'     C1'     O1'
13      14      15      2       ga_12   ;       C1'     O1'     H1'
12      16      17      2       ga_10   ;       C2'     O1      C1
16      17      18      2       ga_9    ;       O1      C1      O5
16      17      29      2       ga_9    ;       O1      C1      C2
18      17      29      2       ga_9    ;       O5      C1      C2
17      18      19      2       ga_10   ;       C1      O5      C5
18      19      20      2       ga_9    ;       O5      C5      C6
18      19      23      2       ga_9    ;       O5      C5      C4
20      19      23      2       ga_8    ;       C6      C5      C4
19      20      21      2       ga_9    ;       C5      C6      O6
20      21      22      2       ga_12   ;       C6      O6      H6
19      23      24      2       ga_9    ;       C5      C4      O4
19      23      26      2       ga_8    ;       C5      C4      C3
24      23      26      2       ga_9    ;       O4      C4      C3
23      24      25      2       ga_12   ;       C4      O4      H4
23      26      27      2       ga_9    ;       C4      C3      O3
23      26      29      2       ga_8    ;       C4      C3      C2
27      26      29      2       ga_9    ;       O3      C3      C2
26      27      28      2       ga_12   ;       C3      O3      H3
17      29      26      2       ga_8    ;       C1      C2      C3
17      29      30      2       ga_9    ;       C1      C2      O2
26      29      30      2       ga_9    ;       C3      C2      O2
29      30      31      2       ga_12   ;       C2      O2      H2

[ dihedrals ]

;       ai      aj      ak      al      fu      c0, c   1, m    , ...
        3       4       1       12      2       gi_2    ;       imp     C4      O4      C5      C3
        4       5       7       3       2       gi_2    ;       imp     C3      C4      O3      C2
        7       11      8       4       2       gi_2    ;       imp     C2      C3      C1      O2
        12      11      13      3       2       gi_2    ;       imp     C5      C6      C4      O5
        12      16      3       13      2       gi_2
        17      18      16      29      2       gi_2    ;
        29      30      26      17      2       gi_2
        26      27      29      23      2       gi_2
        23      26      24      19      2       gi_2
        19      18      20      23      2       gi_2
```

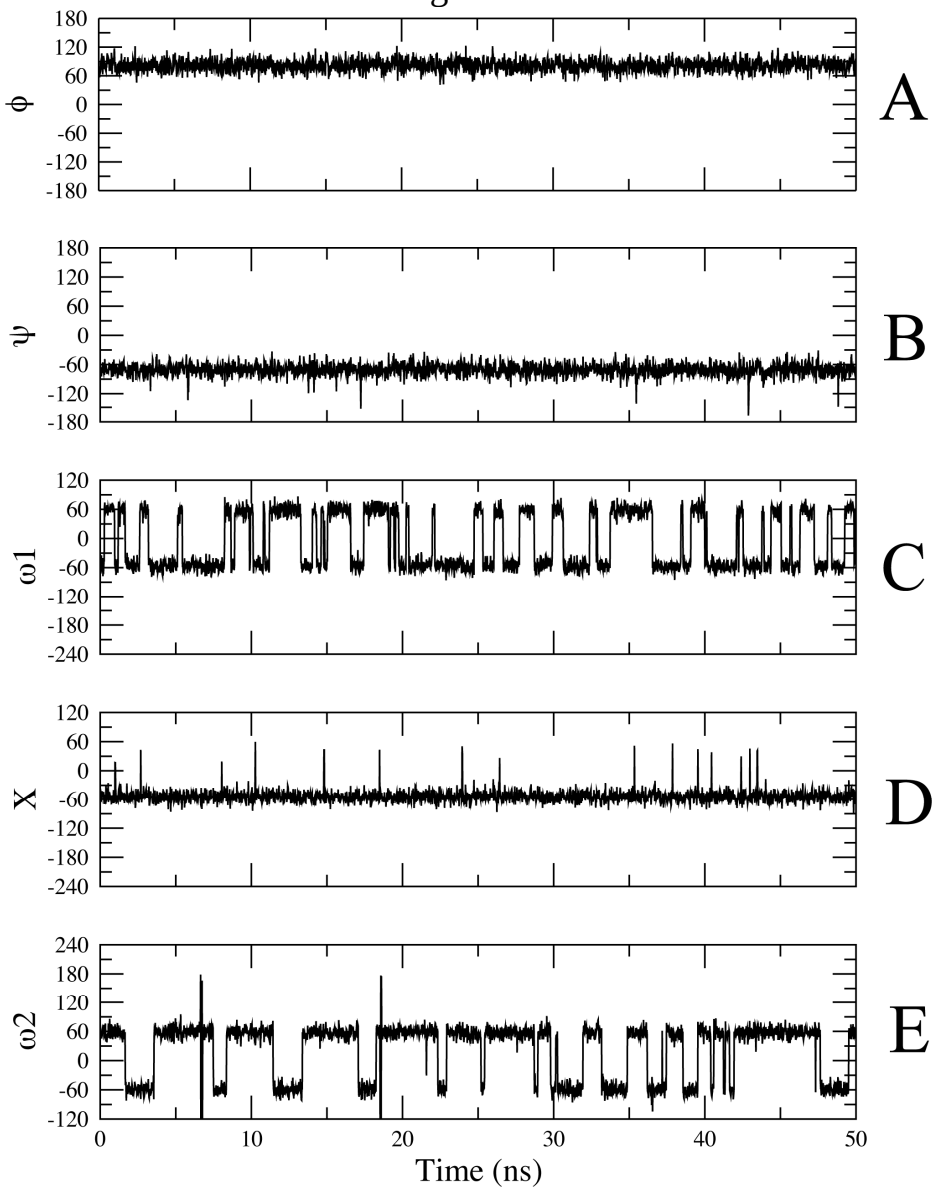
;Hydrogens

2	1	3	4	1	gd_30
6	5	4	7	1	gd_30
10	9	8	7	1	gd_30
15	14	13	12	1	gd_30
17	29	30	31	1	gd_30
29	26	27	28	1	gd_30
26	23	24	25	1	gd_30
19	20	21	22	1	gd_30
;ring					
7	4	3	12	1	gd_34
4	3	12	11	1	gd_34
16	12	3	1	1	gd_18
5	4	3	1	1	gd_18
4	3	12	16	1	gd_17
7	4	3	1	1	gd_17
2	3	4	5	1	gd_17
8	7	4	5	1	gd_17
13	12	3	1	1	gd_17
3	4	7	11	1	gd_17
11	7	8	9	1	gd_37
11	7	8	9	1	gd_5
11	12	13	14	1	gd_37
11	12	13	14	1	gd_5
11	12	16	17	1	gd_32 ; glycosidic link from fructose
11	12	16	17	1	gd_2 ; glycosidic link from fructose
29	17	18	19	1	gd_29
23	19	18	17	1	gd_29
17	29	26	23	1	gd_34
29	26	23	19	1	gd_34
26	29	17	18	1	gd_34
26	23	19	18	1	gd_34
16	17	29	30	1	gd_18
30	29	26	27	1	gd_18
27	26	23	24	1	gd_18
26	29	17	16	1	gd_17
23	26	29	30	1	gd_17
17	29	26	27	1	gd_17
19	23	26	27	1	gd_17
29	26	23	24	1	gd_17
20	19	23	24	1	gd_17
26	29	17	18	1	gd_17
26	23	19	18	1	gd_17
18	19	20	21	1	gd_37
18	19	20	21	1	gd_5
18	17	16	12	1	gd_28 ; for alpha glucose glycosidic link
18	17	16	12	1	gd_6 ; for alpha glucose glycosidic link

Conformational analysis of Sucrose in water

In order to assess the accuracy of our parameters, a simulation of sucrose was carried on under the same conditions as for fructose. In aqueous solution, the value for ω1 (primary alcohol group of the glucopyranose ring) was oscillating between the *gg* and *gt* configurations. The value for ω2 (primary alcohol group of the fructofuranose ring) also showed the same behavior. The value for X (primary hydroxyl group of the fructofuranose ring) populated the *gg* conformation. In general these results are in agreement with the ones obtained by Engelsen et. al[3]. For a best comparison, figure S2 depicts the time behaviour of the following dihedral angles: (Φ)=O_5-C_1-O_1-$C_{2'}$, (ψ)=C_1-O_1-$C_{2'}$-$O_{5'}$, (ω1)=O_5-C_5-C_6-O_6, (X)=$O_{5'}$-$C_{2'}$-$O_{1'}$-$C_{1'}$, (ω2)=$O_{5'}C_{5'}$-$O_{6'}$-$C_{6'}$. Panels A, B, C, D and E can be easily compared with the figure 5 of [3].

Figure S2



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