Supporting Information

Evaluation of the GROMOS 56A$_{CARBO}$ Force Field for the Calculation of Structural, Volumetric and Dynamic Properties of Aqueous Glucose Systems

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Tables

Table S1 - Computed density as a function of glucose concentration estimated using the TIP3P water model and the $56A_{CARBO}$ force field for glucose at 303.15 K. Values in parentheses denote uncertainty related to the computational estimation.

$x_{glucose}$	ρ_{exp} [a] / kg.m^{-3}	ρ_{TIP3P} / kg.m^{-3}	AAD %
0.034	1081.8	1071.5	0.95
0.076	1125.7	1144.9	1.71
0.200	1177.7	1252.7	6.36

a) Comesaña et al., *J. Chem. Eng. Data*, **2003**, 48, 362-366 at *T*=303.15 K.

Table S2 - Computed density as a function of glucose concentration estimated using the SPC water model and the $56A_{CARBO}$ force field for glucose at 313.15 K. Values in parentheses denote uncertainty related to the computational estimation.

$x_{glucose}$	ρ_{exp} [a] / kg.m^{-3}	ρ_{SPC} / kg.m^{-3}	AAD %
0.034	1077.6	1056.7 (±0.2)	1.94
0.050	1100.6	1089.0 (±0.2)	1.05
0.076	1121.2	1130.6 (±0.1)	0.84
0.110	1139.9	1167.2 (±0.2)	2.39
0.150	1157.1	1206.0 (±0.3)	4.23
0.200[b]	1172.7	1241.0 (±0.4)	5.82
0.200[c]	1172.7	1241.4 (±0.2)	5.95
0.200[d]	1172.7	1242.5 (±0.2)	6.04

a) Comesaña et al., *J. Chem. Eng. Data*, **2003**, 48, 362-366 at *T*=313.15 K.

b) System with 42 glucose and 170 water molecules and cutoff = 0.9 nm. Density with SPC/E is 1251.3 ± 0.5 kg·m^{-3}.

c) System with 168 glucose and 680 water molecules and cutoff = 0.9 nm. Density with SPC/E is 1253.1 ± 0.6 kg·m^{-3}.

d) System with 168 glucose and 680 water molecules and cutoff = 1.4 nm. Density with SPC/E is 1253.1 ± 0.4 kg·m^{-3}.

Table S3 - Computed density as a function of glucose concentration estimated using the OPLS-AA force field for glucose and the SPC/E water model at 303.15 and 313.15 K. Values in parentheses denote uncertainty related to the computational estimation.

$x_{glucose}$	ρ_{exp} [a] / kg.m^{-3}	$\rho_{OPLS-AA}$ / kg.m^{-3}	AAD %
0.034	1081.8	1110.2 (±0.2)	2.62
0.050	1105.0	1151.4 (±0.4)	4.20
$x_{glucose}$	ρ_{exp} [b] / kg.m^{-3}	$\rho_{OPLS-AA}$ / kg.m^{-3}	AAD %
0.034	1077.6	1105.1 (±0.9)	2.55
0.050	1100.6	1147.7 (±0.4)	4.28
0.076	1121.2	1203.4 (±0.3)	7.33
0.110	1139.9	1253.4 (±0.2)	9.96
0.150	1157.1	1306.5 (±0.6)	12.91
0.200	1172.7	1355.5 (±0.8)	15.59

a) Comesaña et al., *J. Chem. Eng. Data*, **2003**, 48, 362-366 at *T*=303.15 K.
b) Comesaña et al., *J. Chem. Eng. Data*, **2003**, 48, 362-366 at *T*=313.15 K.

Table S4 - Computed density as a function of glucose concentration estimated using the OPLS-AA-SEI force field for glucose and the SPC/E water model at 313.15 K. Values in parentheses denote uncertainty related to the computational estimation.

$x_{glucose}$	ρ_{exp} [a] / kg.m^{-3}	$\rho_{OPLS-AA-SEI}$ / kg.m^{-3}	AAD %
0.034	1077.6	1093.8 (±0.1)	1.50
0.050	1100.6	1143.2 (±0.1)	3.87
0.076	1121.2	1197.6 (±0.2)	6.81
0.110	1139.9	1246.7 (±0.1)	9.37
0.150	1157.1	1298.4 (±0.2)	12.21
0.200	1172.7	1348.5 (±0.2)	14.99

e) Comesaña et al., *J. Chem. Eng. Data*, **2003**, 48, 362-366 at *T*=313.15 K.

Table S5 – Fitting parameters and decay times obtained using equation 3 of the main manuscript.

$x_{glucose}$	A	α	τ_1	τ_2
0.034	1412.22	1.32E-03	7.37E-02	7.03E-04
0.050	1479.54	3.13E-02	6.54E-03	7.96E-04
0.076	1025.62	6.12E-03	8.63E-02	2.17E-03
0.110	922.576	1.36E-02	1.06E-01	4.11E-03
0.150	1121.61	5.86E-02	6.70E-02	5.83E-03
0.200	1143.22	9.73E-02	9.43E-02	1.29E-02

Table S6 - Experimental and computational viscosity values estimated using the $56A_{CARBO}$ force field for glucose and the SPC water model at 313.15 K. Values in parentheses denote uncertainty related to the computational estimation.

$x_{glucose}$	η_{exp} [a] / mPa.s	η_{SPC} / mPa.s	AAD %
0.034	1.205	0.681 (±0.130)	43.52
0.050	1.475	1.018 (±0.204)	30.96
0.076	1.804	1.507 (±0.194)	7.41
0.110	2.182	2.911 (±0.270)	33.41
0.150	2.660	5.943 (±0.491)	123.41
0.200[b]	3.175	17.997 (±0.449)	466.85
0.200[c]	3.175	18.796 (±0.499)	492.00
0.200[d]	3.175	19.931 (±0.686)	527.75

a) Comesaña et al., *J. Chem. Eng. Data*, 2003, 48, 362-366.

b) System with 42 glucose and 170 water molecules and cutoff = 0.9 nm for nonbonded interactions.

c) System with 168 glucose and 680 water molecules and cutoff = 0.9 nm for nonbonded interactions.

d) System with 168 glucose and 680 water molecules and cutoff = 1.4 nm for nonbonded interactions.

Table S7 - Experimental and computational viscosity values estimated using OPLS-AA force field for glucose and SPC/E water model at 313.15 K for some selected glucose mole fractions. Values in parentheses denote uncertainty related to the computational estimation.

$x_{glucose}$	η_{exp} [a] / mPa.s	$\eta_{OPLS-AA}$ / mPa.s	AAD %
0.034	1.205	1.221 (±0.175)	1.34
0.050	1.475	2.269 (±0.238)	53.83
0.076	1.804	5.518 (±0.371)	205.86
0.110	2.182	13.905 (±0.601)	537.27

a) Comesaña et al., *J. Chem. Eng. Data*, 2003, 48, 362-366

Table S8 - Experimental and computational viscosity values estimated using the OPLS-AA-SEI force field for glucose and the SPC/E water model at 313.15 K. Values in parentheses denote uncertainty related to the computational estimation.

$x_{glucose}$	η_{exp} [a)] / mPa.s	$\eta_{OPLS\text{-}AA\text{-}SEI}$ / mPa.s	AAD %
0.034	1.205	1.010 (±0.159)	16.16
0.050	1.475	1.670 (±0.204)	13.24
0.076	1.804	3.619 (±0.274)	100.58
0.110	2.182	6.288 (±0.396)	188.18
0.150	2.660	19.262 (±0.696)	624.13
0.200	3.175	69.656 (±1.347)	2093.89

a) Comesaña et al., *J. Chem. Eng. Data*, 2003, 48, 362-366

Table S9 - Coordination number (CN) from the RDF peaks for water-water interactions, at each mixture considered.

$x_{glucose}$	reference_atom	atom2	CN
0.034	OW	OW	4.78
0.050			4.51
0.076			4.19
0.110			3.88
0.150			3.36
0.200			2.99

Table S10 - Coordination number (CN) from the RDF peaks for glucose-glucose interactions, at each mixture considered.

$x_{glucose}$	reference_atom	atom2	**CN**
0.034	O1	HO3	0.02
		HO6	0.02
		HO4	0.02
0.050	O1	HO3	0.02
		HO6	0.03
		HO4	0.03
0.076	O1	HO3	0.04
		HO6	0.05
		HO4	0.04
0.110	O1	HO3	0.05
		HO6	0.05
		HO4	0.05
0.150	O1	HO3	0.07
		HO6	0.07
		HO4	0.07
0.200	O1	HO3	0.09
		HO6	0.09
		HO4	0.08

Table S11 – Values for the hydrogen bonds established between glucose and water molecules and for water with water molecules.

$x_{glucose}$	H-Bonds water-water (per water basis)	H-Bonds glucose-water (per glucose basis)
0.034	1.49	8.04
0.050	1.43	7.58
0.076	1.36	7.19
0.110	1.23	6.45
0.150	1.18	6.12
0.200	0.96	5.00

Table S12 – Experimental and computational densities (ρ) for different glucose+water mixtures at 313.15 K. Values in parentheses denote the uncertainties (the standard deviation) estimated with the calculated results applying the scaling factor 0.8 to atomic charges. AAD represents the absolute deviations of the simulated data from the experimental values.

$x_{glucose}$	ρ_{exp} / kg·m^{-3}	ρ_{sim} / kg·m^{-3}	AAD %
0.034	1077.6	1061.2 (±0.3)	1.52
0.050	1100.6	1084.3 (±0.3)	1.48
0.076	1121.2	1113.5 (±0.4)	0.69
0.110	1139.9	1138.5 (±0.3)	0.12
0.150	1157.1	1164.6 (±0.4)	0.65
0.200	1172.7	1188.7 (±0.5)	1.36

Table S13 – Experimental and calculated viscosities (η) by applying the scaling factor 0.8 to atomic charges, at 313.15 K. Values in parentheses denote uncertainties estimated accordingly to equation 4 in the main text. AAD represents the absolute deviations of the simulated data from the experimental values.

$x_{glucose}$	η_{exp} / mPa·s	η_{sim} / mPa·s	AAD %
0.034	1.205	0.781 (±0.136)	35.20
0.050	1.475	1.075 (±0.164)	27.11
0.076	1.804	1.412 (±0.188)	21.71
0.110	2.182	2.371 (±0.244)	8.68
0.150	2.660	2.716 (±0.261)	2.09
0.200	3.175	4.030 (±0.317)	26.93

Figures

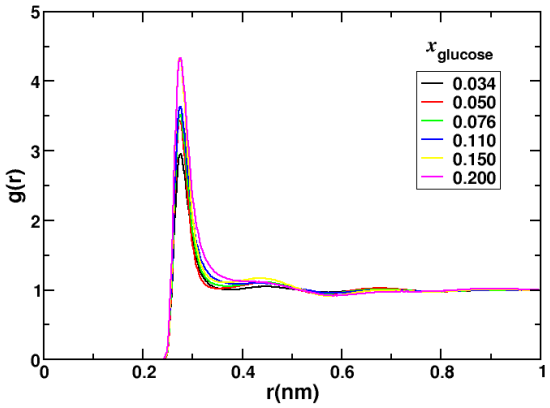

Figure S1. Radial distributions functions (RDFs) for water-water interactions, at six different glucose mole fractions ($x_{glucose}$) and temperature of 313.15 K.

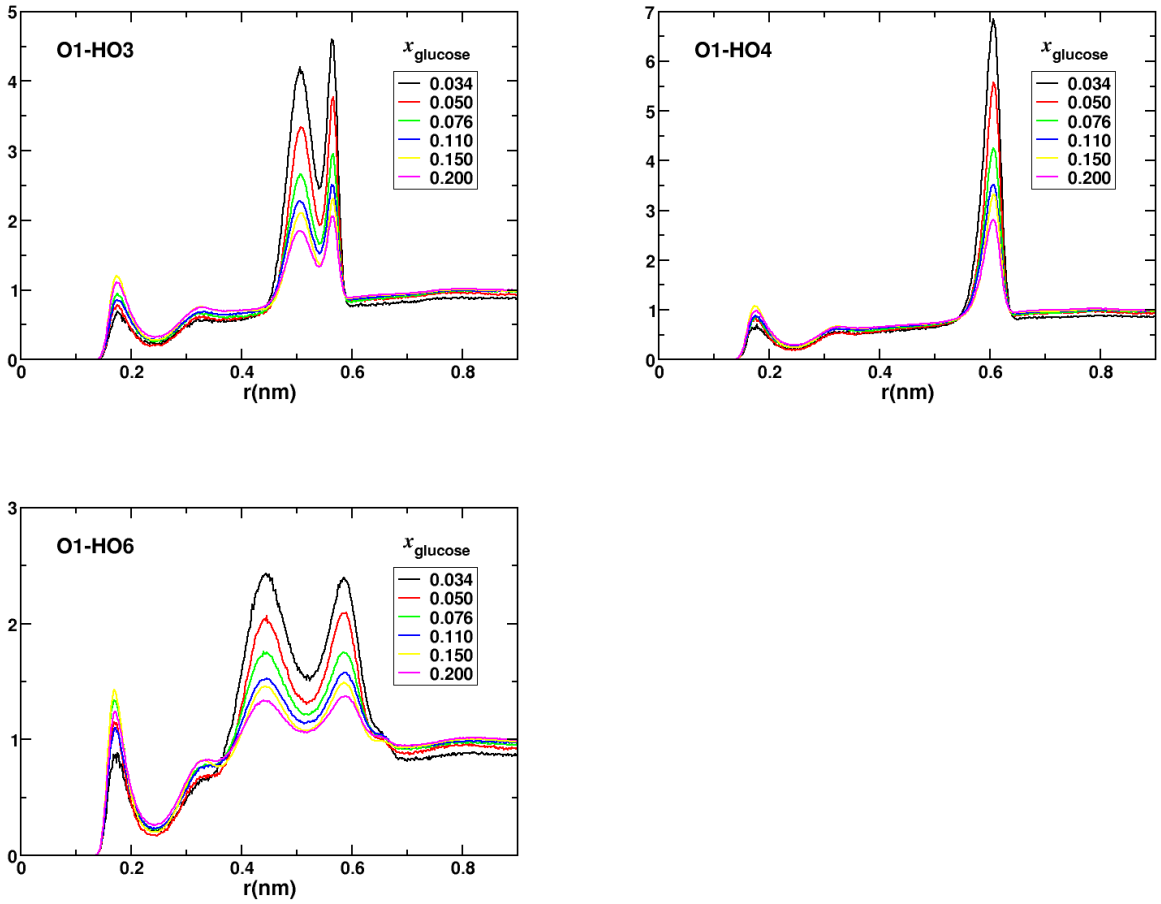

Figure S2 - Radial distributions functions (RDFs) for O1-HO3, O1-HO4 and O1-HO6 glucose-glucose interactions, at six different glucose mole fractions ($x_{glucose}$) and temperature of 313.15 K.