Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Insights into the solvation of glucose in water, Dimethyl sulfoxide (DMSO), Tetrahydrofuran (THF) and N,N-Dimethylformamide (DMF) and its possible implications on the conversion of glucose to platform chemicals

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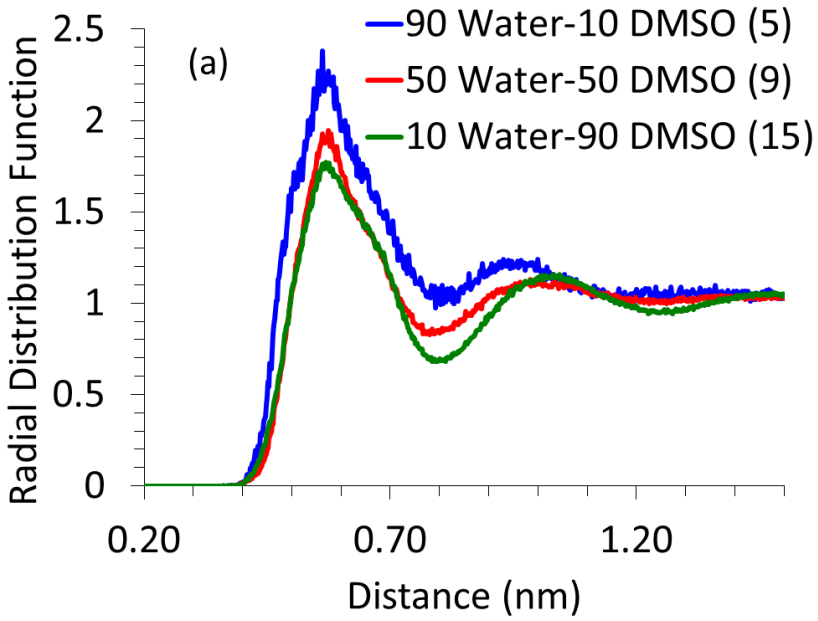
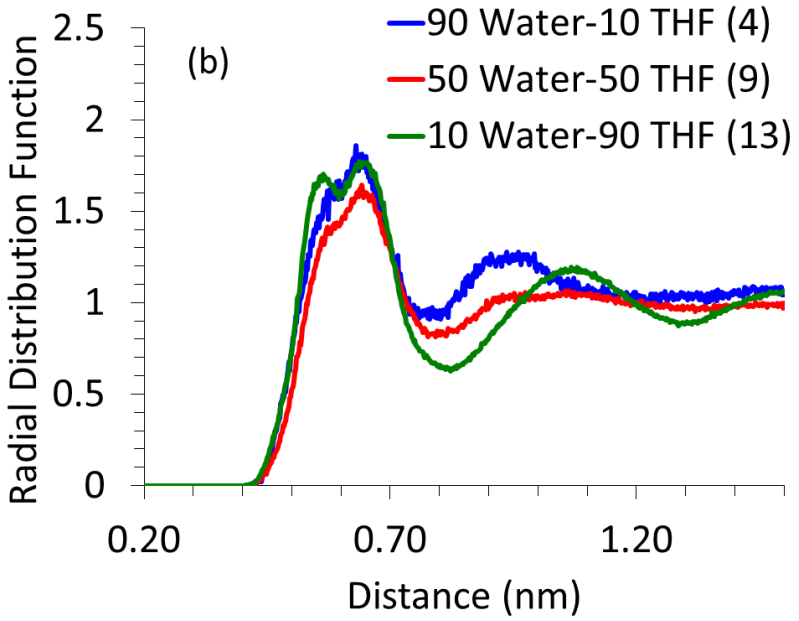




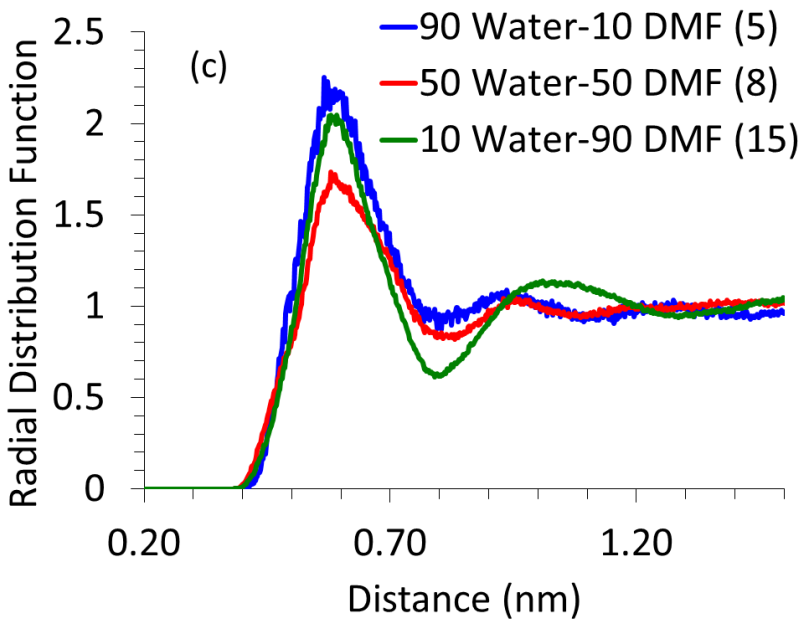
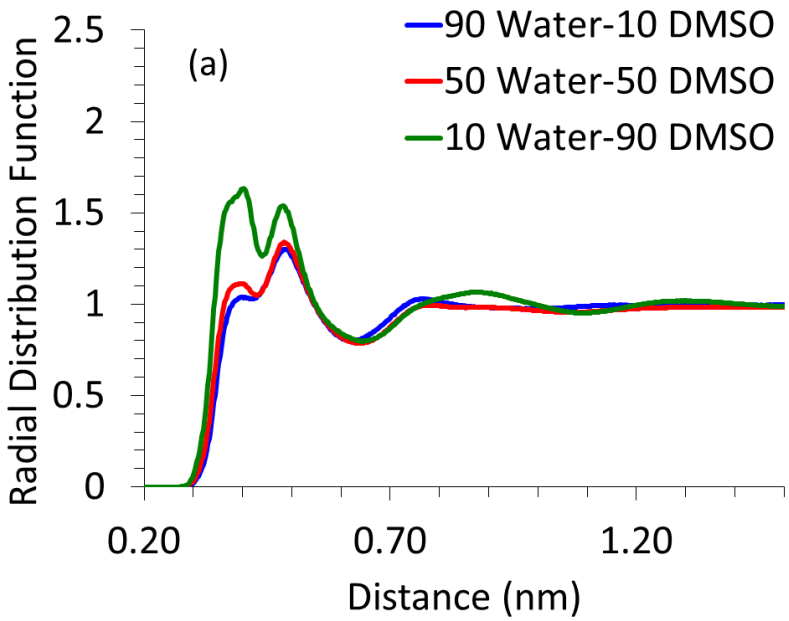
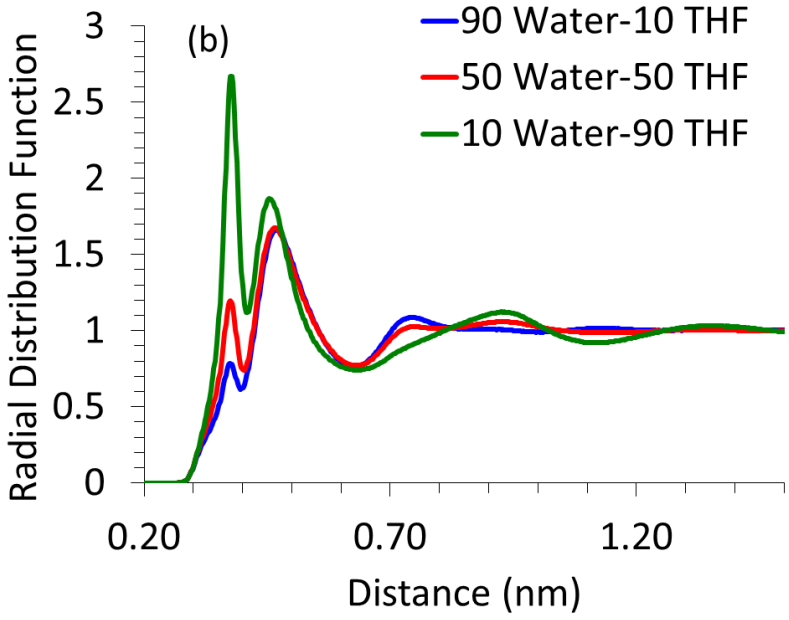


Figure S1. Center of mass radial pair distribution function of glucose with co-solvent in a) DMSO-water-glucose system; b) THF-water-glucose system; c) DMF-water-glucose system. The numbers in square brackets are first solvation shell coordination numbers.

The local arrangement of the co-solvent around glucose was studied using center of mass radial distribution functions (RDF) and are given in Fig S1. The local arrangement of the solvents did not change much as the solvent concentration changed. The increase in the first solvation shell co-ordination numbers is due to the increased number of co-solvent molecules present in the system.

To understand the water-co-solvent interactions the center of mass RDF between co-solvent and water molecules was calculated. The RDF curves are given in Figure S2. The RDF curves for the DMSO-water and THF-water systems show the presence of two significant solvation shells of water around the co-solvent molecules.


(a)
90 Water-10 DMSO
50 Water-50 DMSO
10 Water-90 DMSO
Radial Distribution Function
2.5
2
1.5
1
0.5
0
0.20
0.70
1.20
Distance (nm)


(b)
90 Water-10 THF
50 Water-50 THF
10 Water-90 THF
Radial Distribution Function
3
2.5
2
1.5
1
0.5
0
0.20
0.70
1.20
Distance (nm)

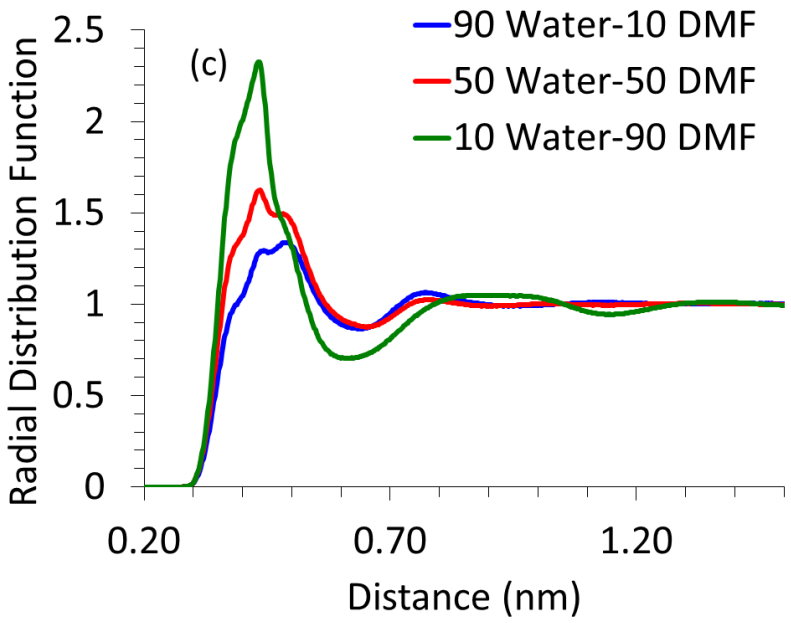
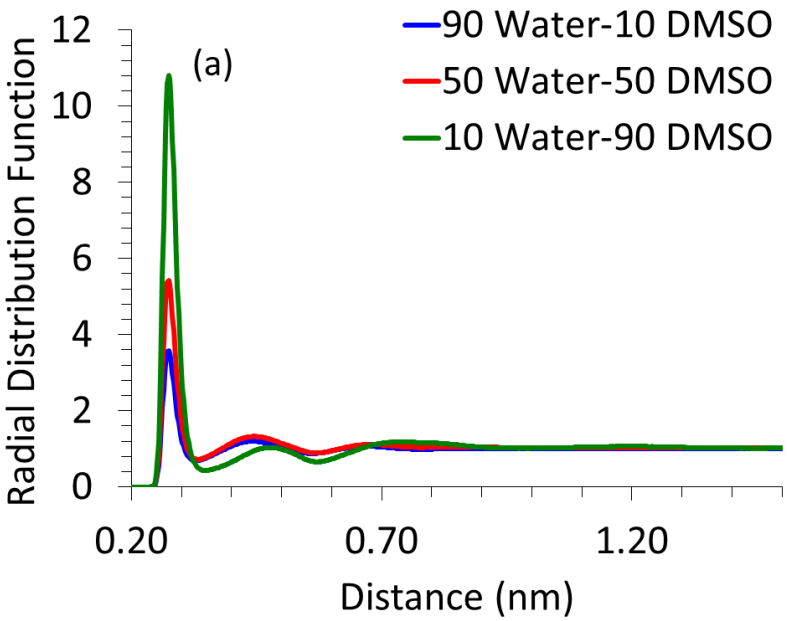
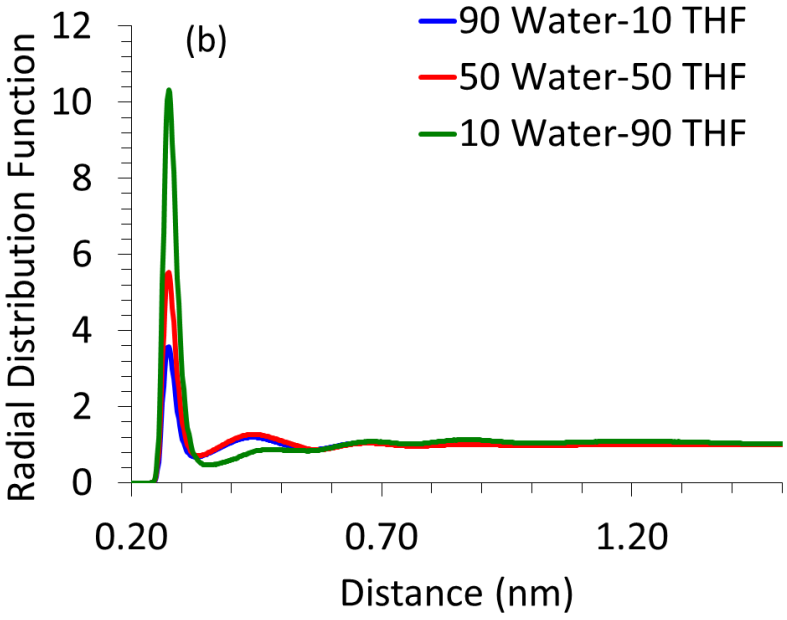


Figure S2. Center of mass Radial pair distribution function of co-solvent with water in a) DMSO-water-glucose system; b) THF-water-glucose system; c) DMF-water-glucose system.


(a)
90 Water-10 DMSO
50 Water-50 DMSO
10 Water-90 DMSO
Radial Distribution Function
12
10
8
6
4
2
0
0.20
0.70
1.20
Distance (nm)


(b)
90 Water-10 THF
50 Water-50 THF
10 Water-90 THF
Radial Distribution Function
12
10
8
6
4
2
0
0.20
0.70
1.20
Distance (nm)

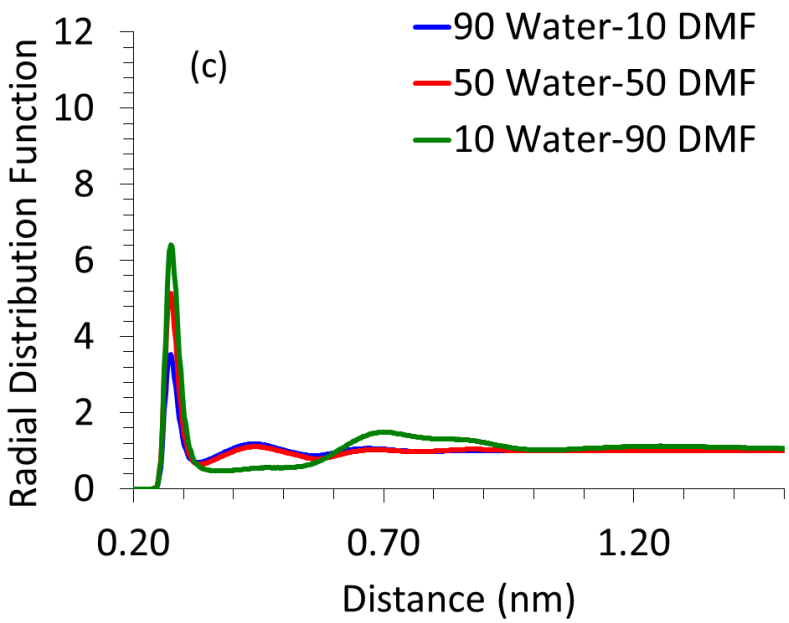


Figure S3. Center of mass Radial pair distribution function of water with water in a) DMSO-water-glucose system; b) THF-water-glucose system; c) DMF-water-glucose system.