Solvent-dependent iodide interactions in LiO_2 electrolytes – a molecular dynamics study
Electronic supplementary information

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1 Composition of simulation boxes

Table 1: The number of Li, I^-, TFSI and solvent molecules in the simulation boxes

				Solvents			
System	Li^+	I^-	TFSI	G1	G2	G3	G4
50 mM	160	20	140	3850	2790	2210	1815
100 mM	160	40	120	3850	2790	2210	1815
200 mM	160	80	80	3850	2790	2210	1815
300 mM	160	120	40	3850	2790	2210	1815
400 mM	160	160	0	3850	2790	2210	1815

Table 2: The number of water molecules in the simulation boxes

	Water
Neat	0
1,000 ppm	40
5,000 ppm	115
20,000 ppm	530

2 Radial Distribution Functions and their CN plots

Each of the following subsections are structured so that they start with an overview plot. These overview plots show the coordination number as a function of [I−] at a fixed distance between the reference atom (either I^- or Li^+) and the atom(s) of interest. The figures are then followed by the radial distribution functions and the coordination numbers plots of each system. To make comparison easier, these plots were collated around the glymes.

2.1 I^- – H-H_2O

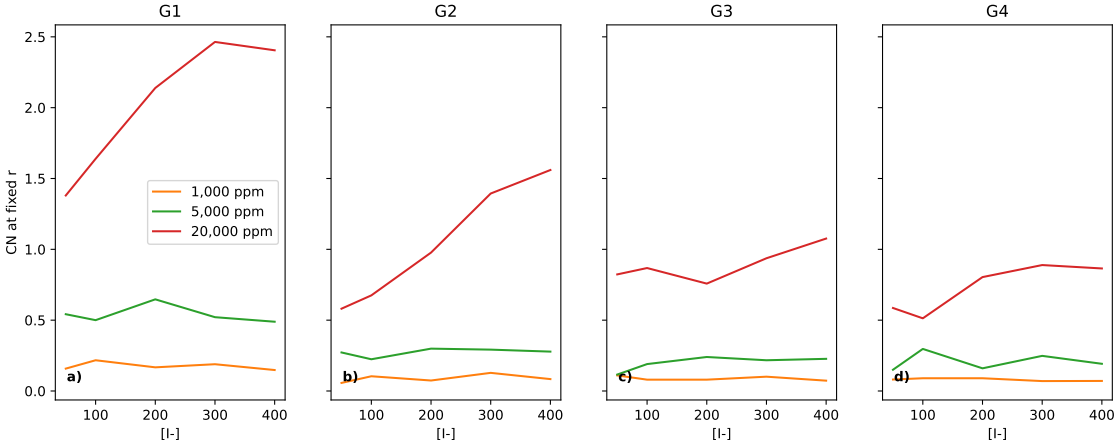


Figure 1: Coordination number of I^- to H (of H_2O) at a fixed distance of 3 Å, for the three different water containing systems (1,000 ppm = yellow, 5,000 ppm = green and 20,000 ppm = red) studied here, across the four different solvents (with a): G1, b): G2, c:) G3 and d): G4).

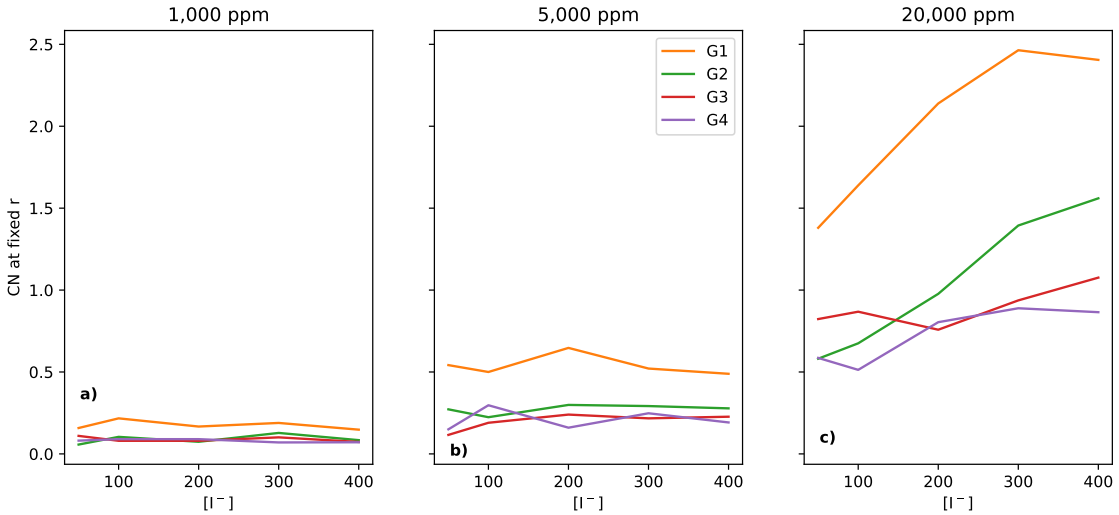
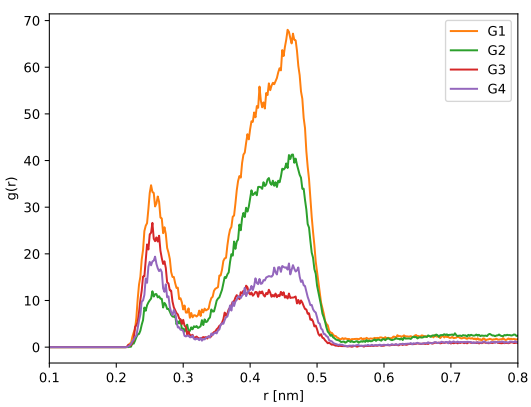
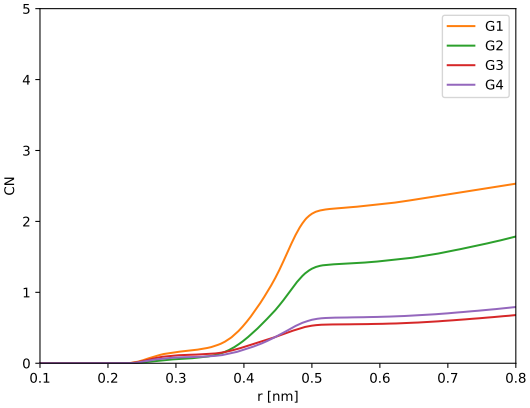


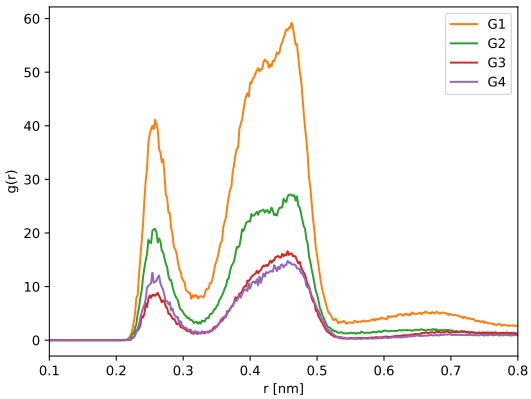
Figure 2: Coordination number of I^- to H (of H_2O) at a fixed distance of 3 Å, for the four different glymes (G1 = yellow, G2 = green, G3 = red, G4 = purple) studied here, across the three different water containing systems (with a): 1,000, b): 5,000, c): 20,000 ppm of water).

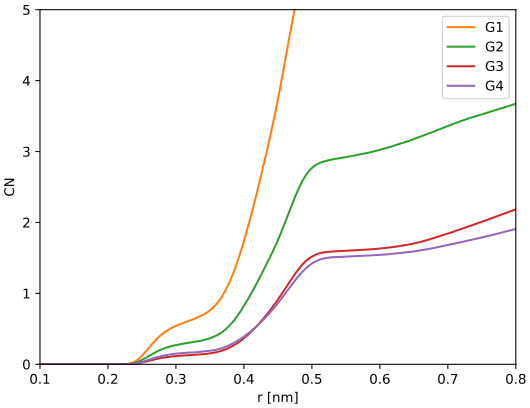
I^- – H-H_2O 50mM 1,000 ppm



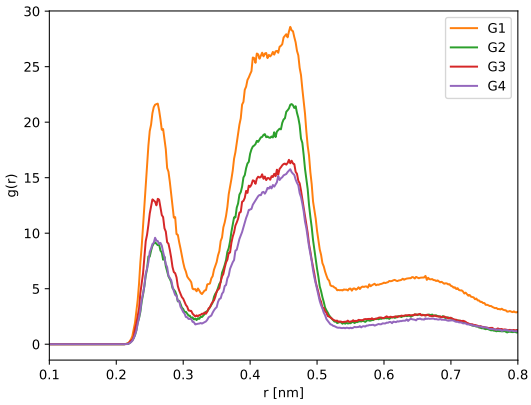


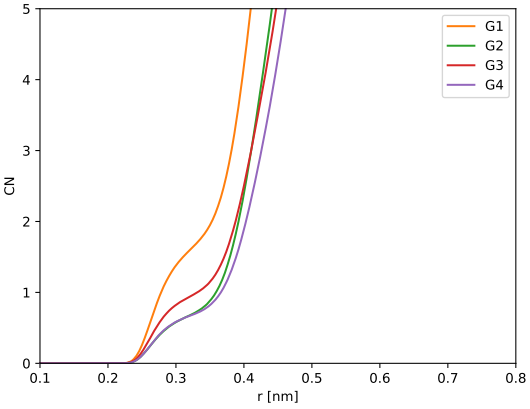
I^- – H-H_2O 50mM 5,000 ppm



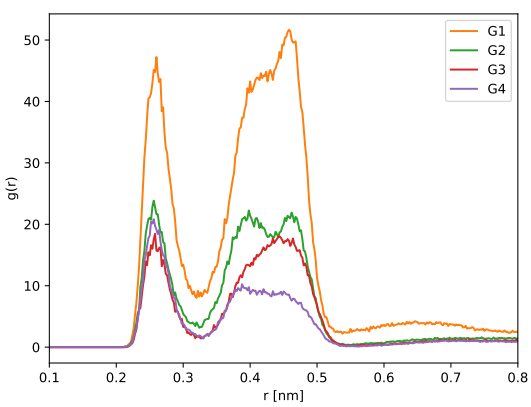


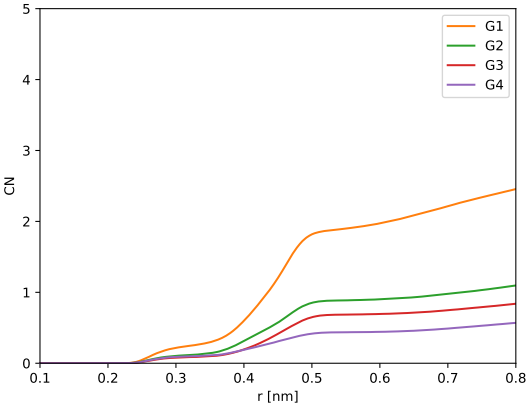
I^- – H-H_2O 50mM 20,000 ppm



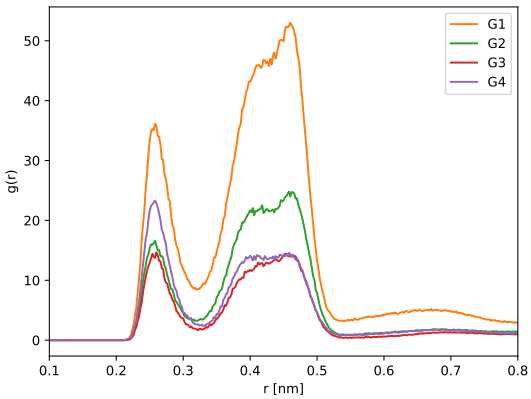


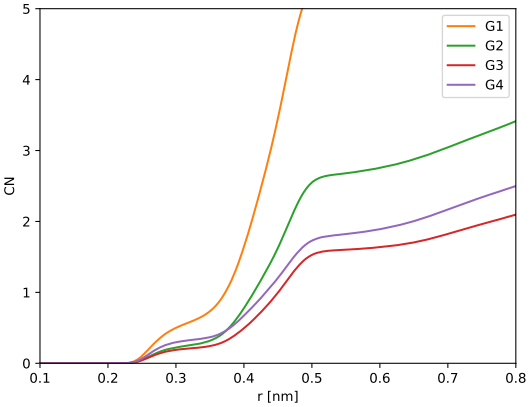
I^- – H-H_2O 100mM 1,000 ppm



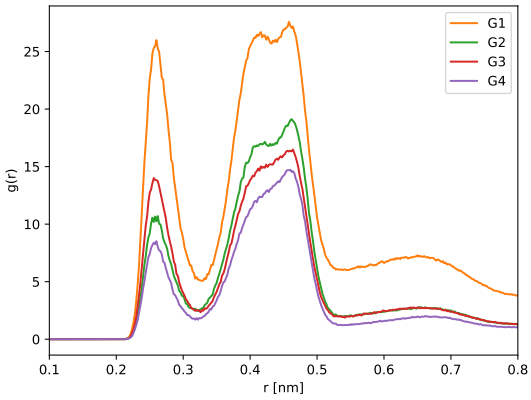


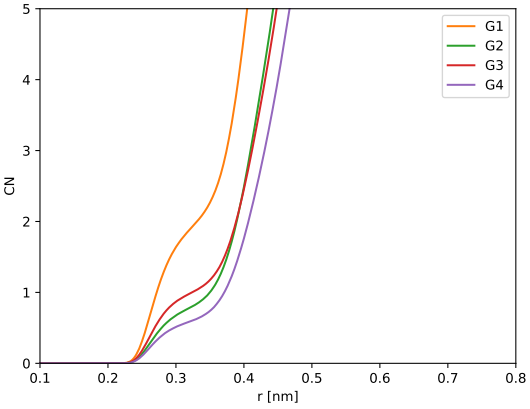
I^- – H-H_2O 100mM 5,000 ppm



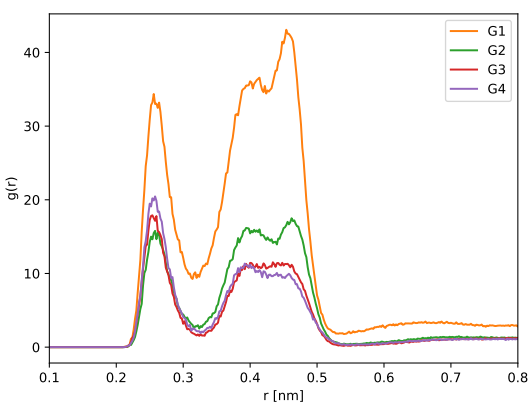


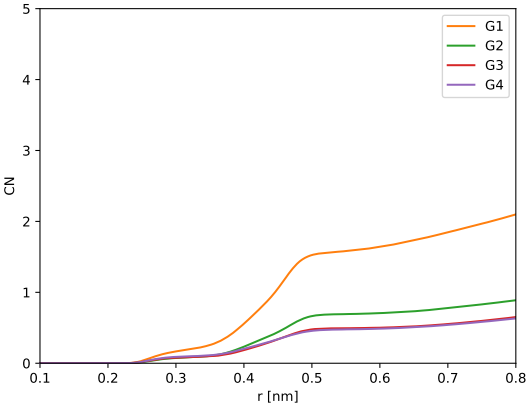
I^- – H-H_2O 100mM 20,000 ppm



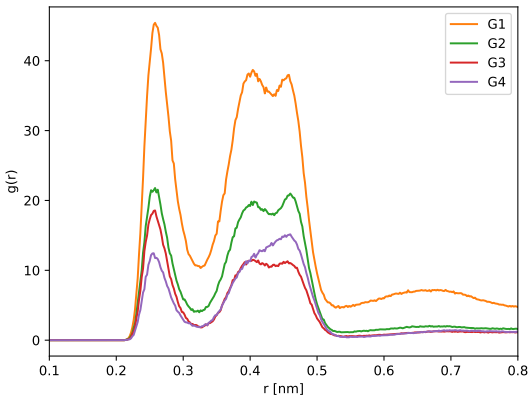


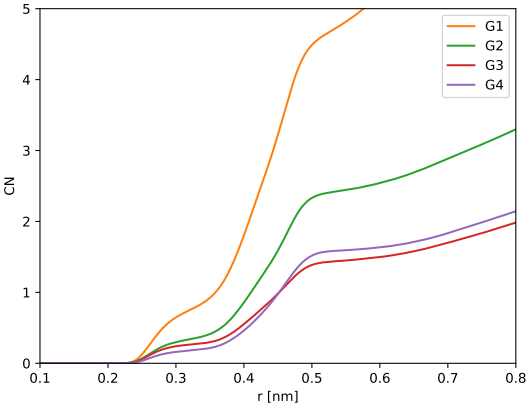
I^- – H-H_2O 200mM 1,000 ppm



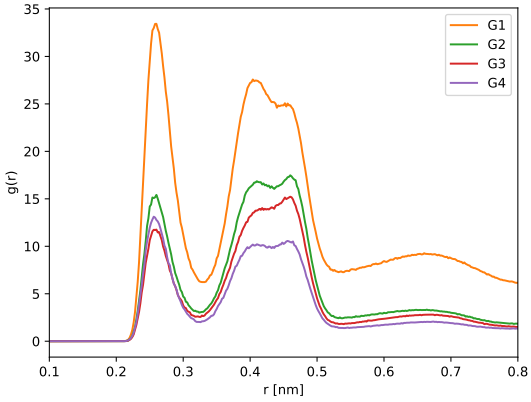


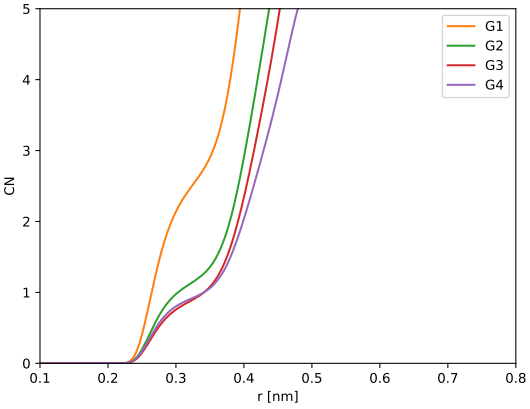
I^- – H-H_2O 200mM 5,000 ppm



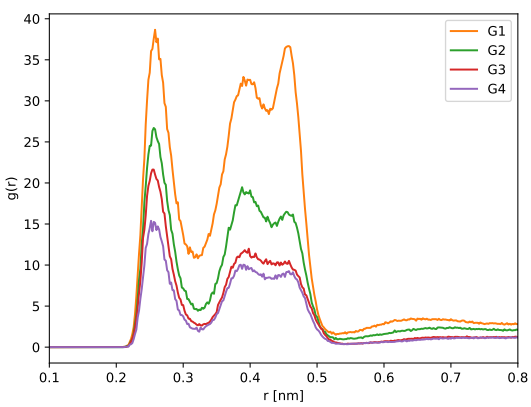


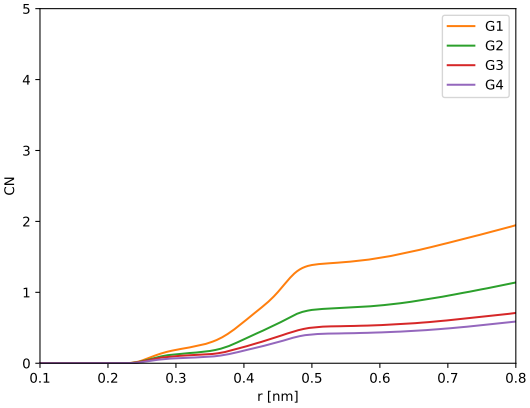
I^- – H-H_2O 200mM 20,000 ppm



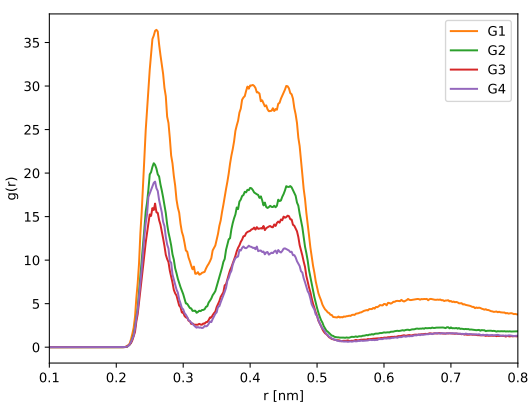


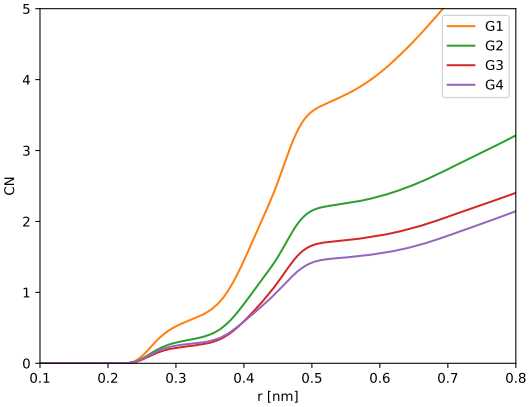
I^- – H-H_2O 300mM 1,000 ppm



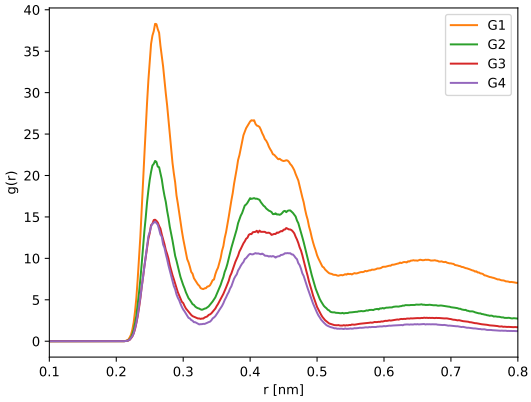


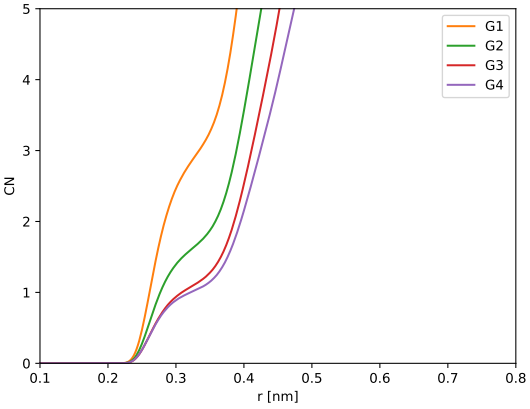
I^- – H-H_2O 300mM 5,000 ppm



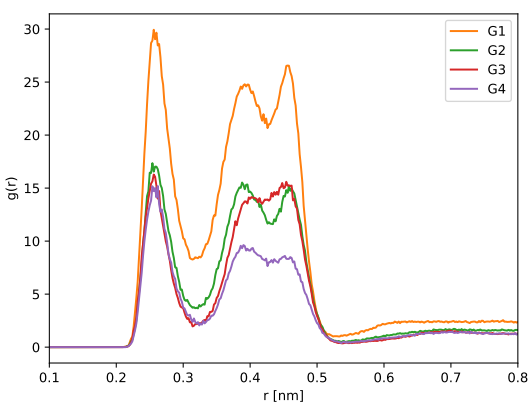


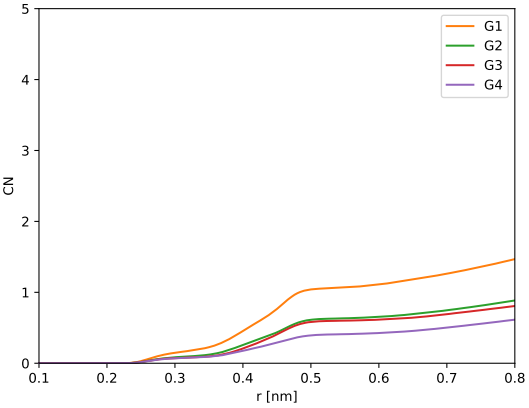
I^- – H-H_2O 300mM 20,000 ppm



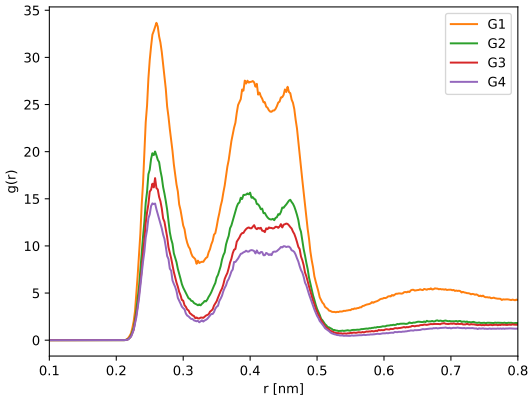


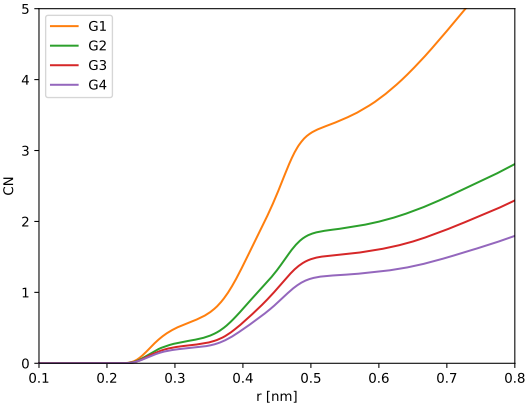
I^- – H-H_2O 400mM 1,000 ppm



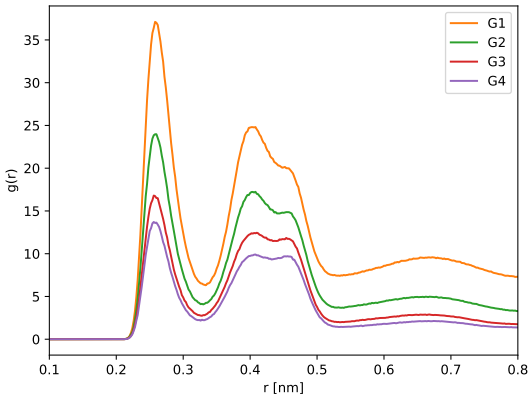


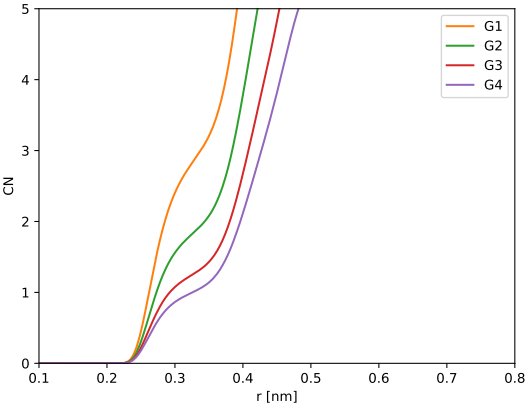
I^- – H-H_2O 400mM 5,000 ppm





I^- – H-H_2O 400mM 20,000 ppm





2.2 I^- – H-solvent

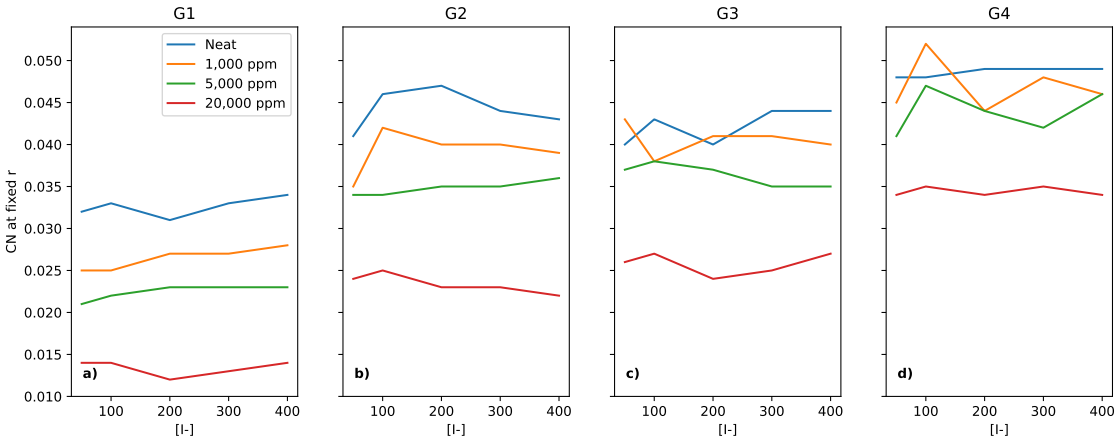


Figure 3: Coordination number of I^- to H (of the solvent) at a fixed distance of 3 Å, for the four different water containing systems (neat = blue, 1,000 ppm = yellow, 5,000 ppm = green and 20,000 ppm = red) studied here, across the four different solvents (with a): G1, b): G2, c): G3 and d): G4).

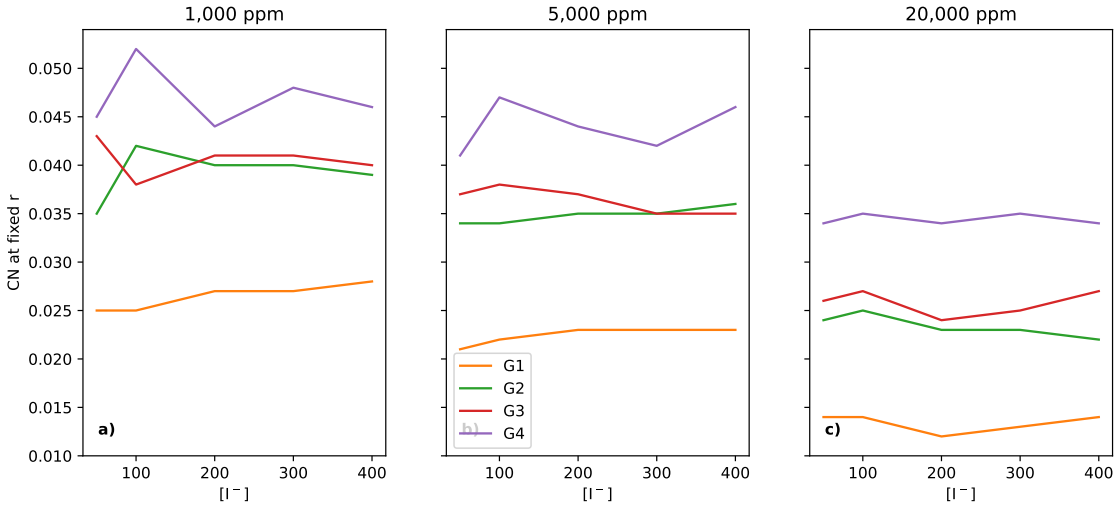
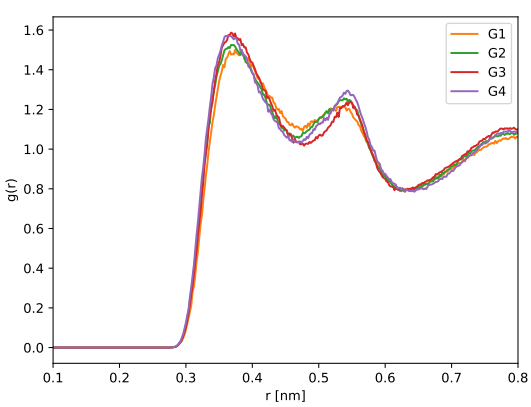
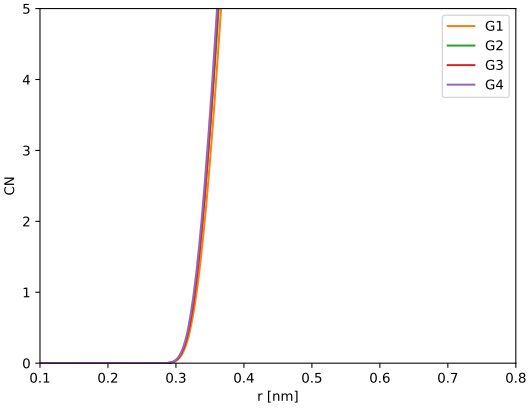


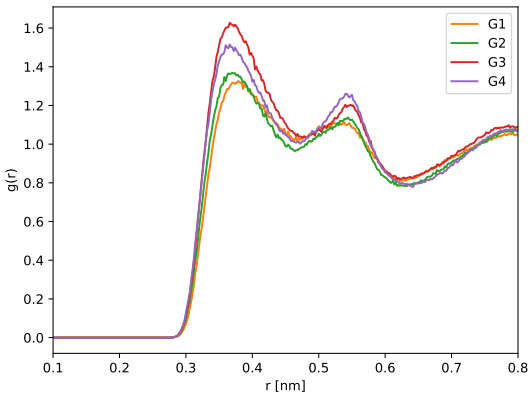
Figure 4: Coordination number of I^- to H (of the solvent) at a fixed distance of 3 Å, for the four different glymes (G1 = yellow, G2 = green, G3 = red, G4 = purple) studied here, across the four different water concentrations (with a): neat, b): 1,000, c): 5,000, d): 20,000 ppm of water).

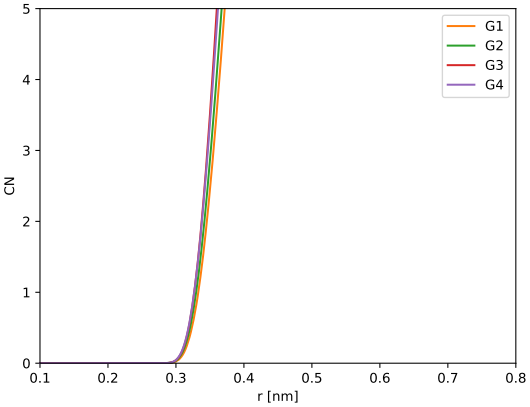
I^- – H-solvent 50mM neat



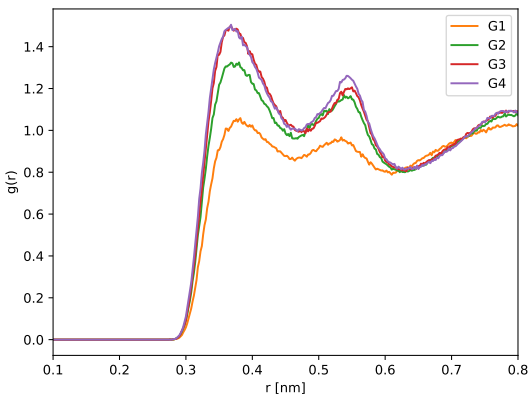


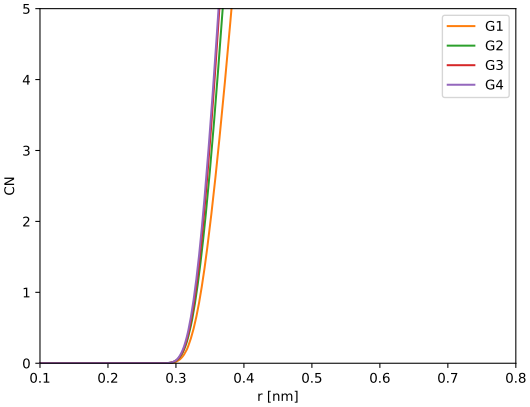
I^- – H-solvent 50mM 1,000 ppm



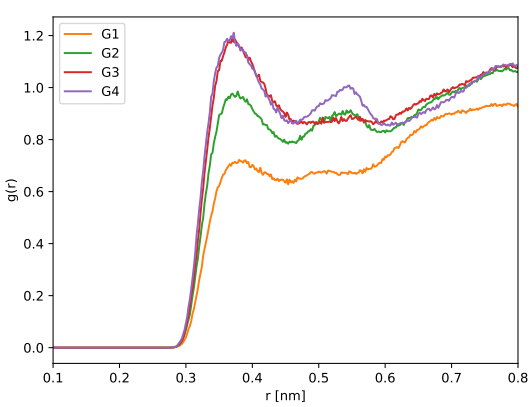


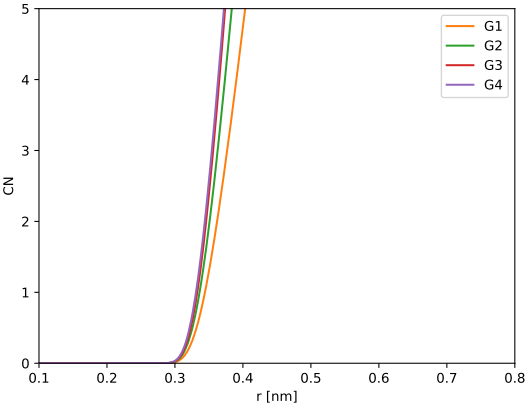
I^- – H-solvent 50mM 5,000 ppm



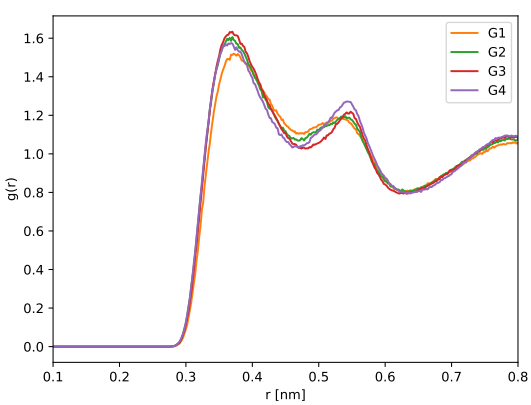


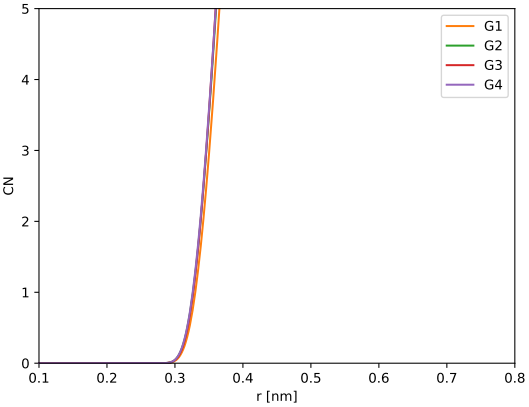
I^- – H-solvent 50mM 20,000 ppm



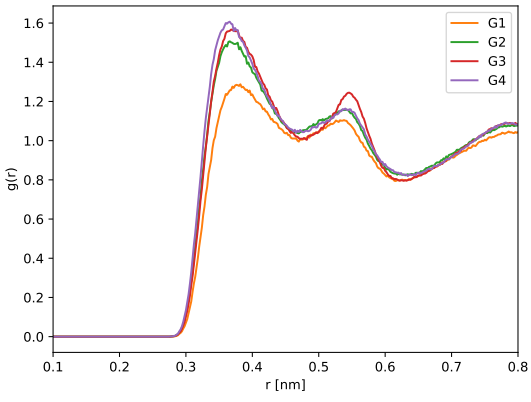


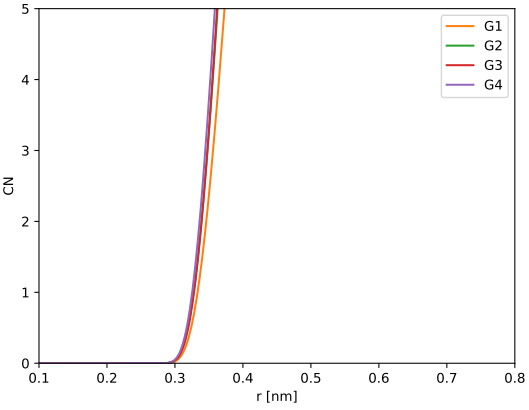
I^- – H-solvent 100mM neat



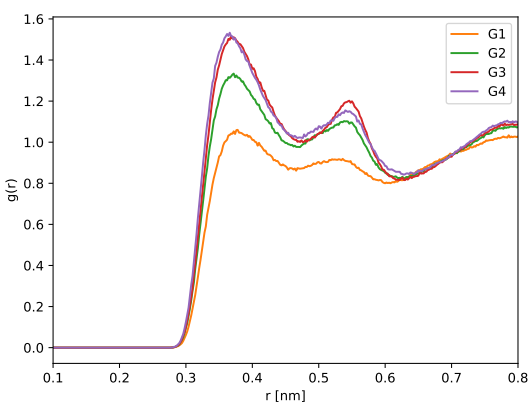


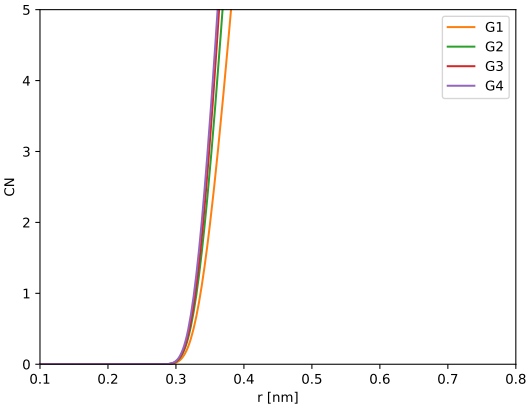
I^- – H-solvent 100mM 1,000 ppm



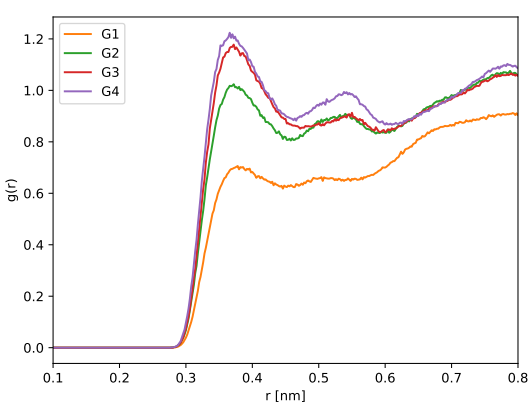


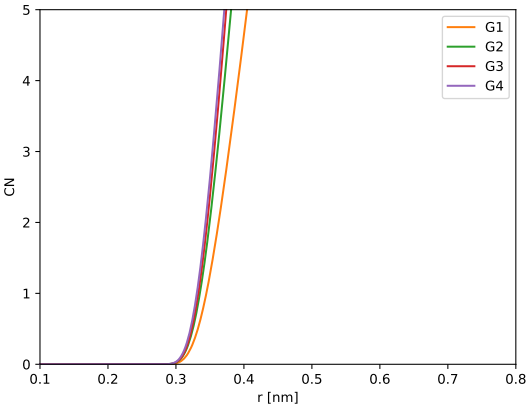
I^- – H-solvent 100mM 5,000 ppm



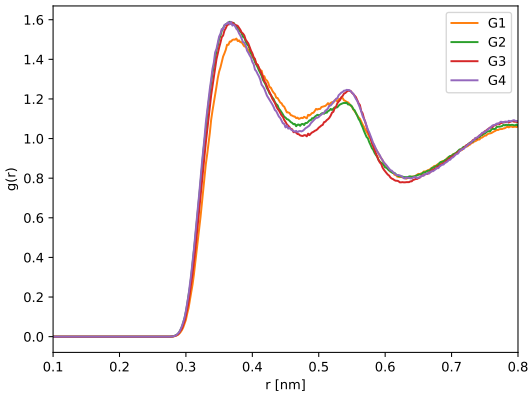


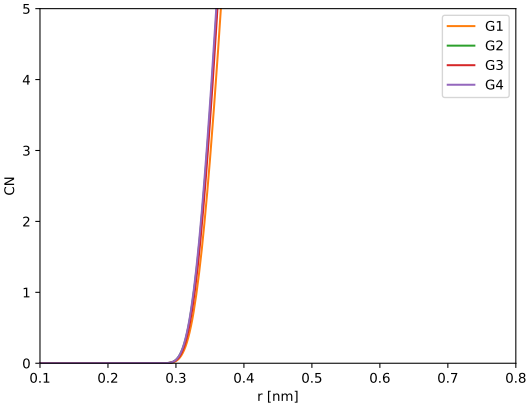
I^- – H-solvent 100mM 20,000 ppm



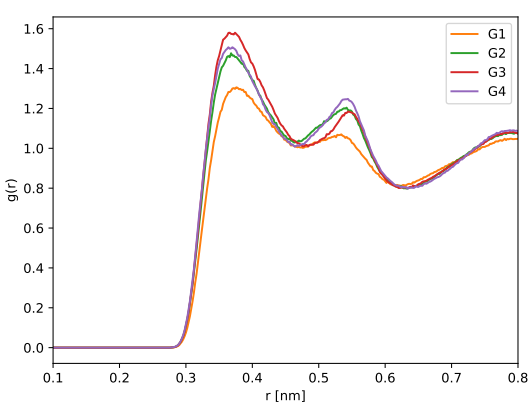


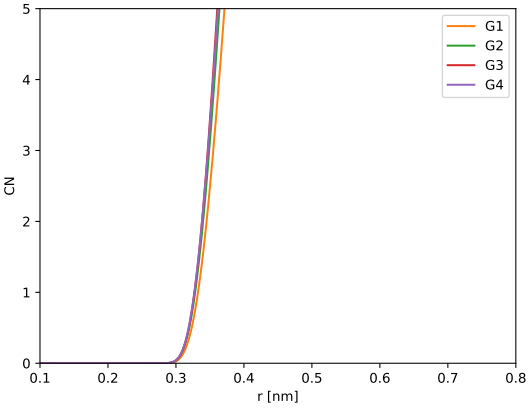
I^- – H-solvent 200mM neat



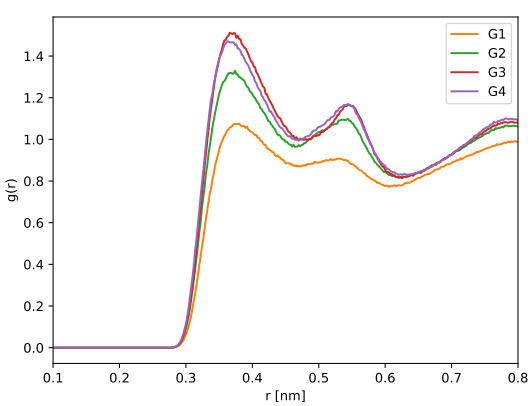


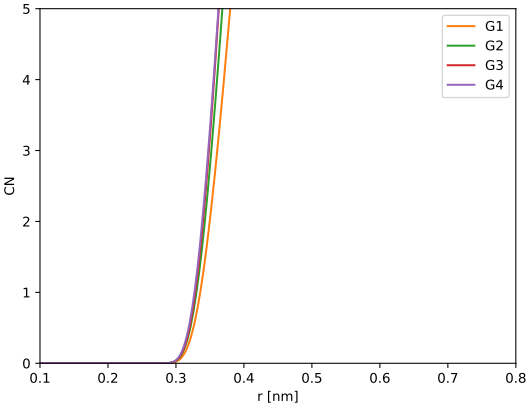
I^- – H-solvent 200mM 1,000 ppm



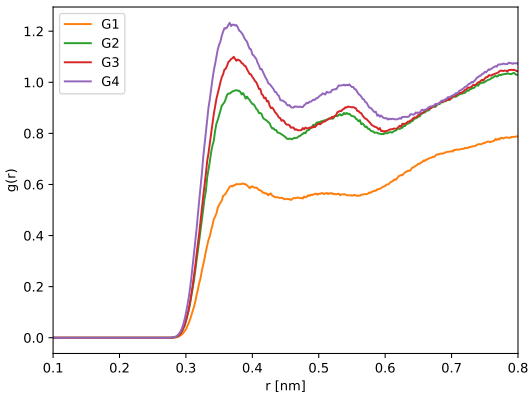


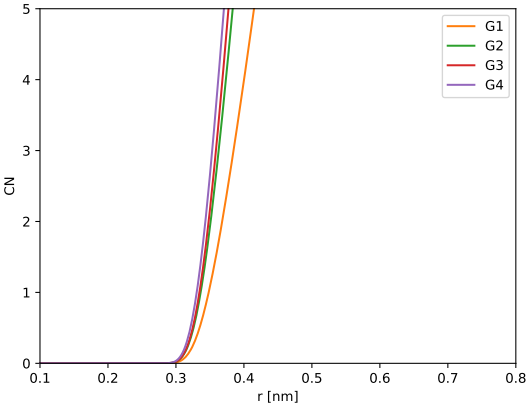
I^- – H-solvent 200mM 5,000 ppm



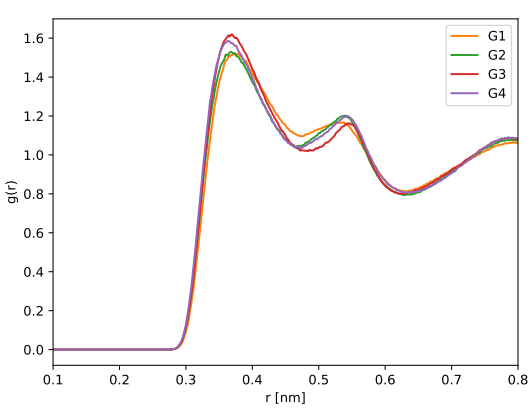


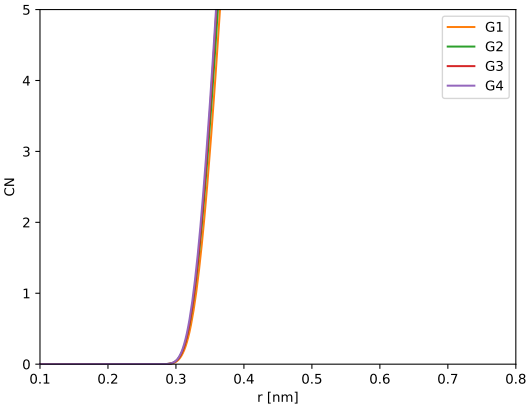
I^- – H-solvent 200mM 20,000 ppm



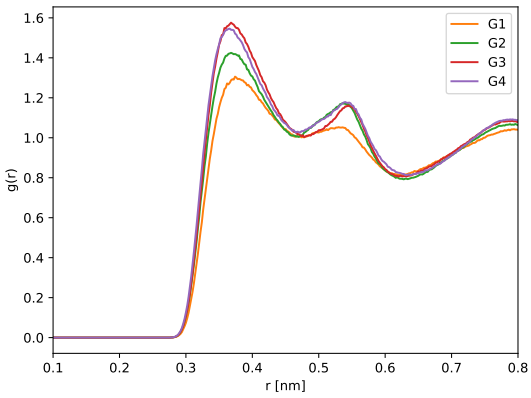


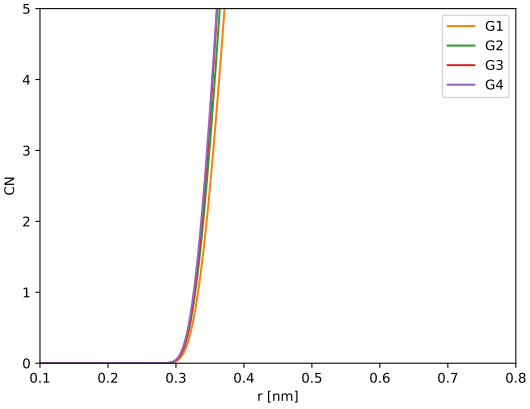
I^- – H-solvent 300mM neat



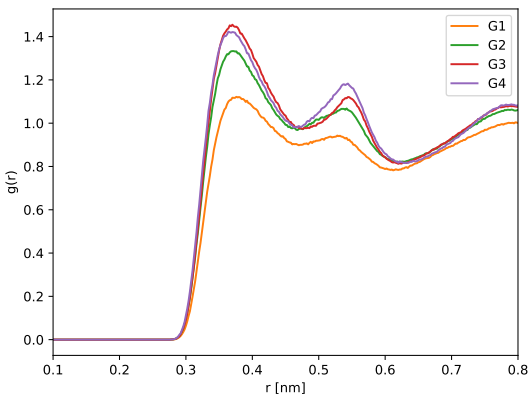


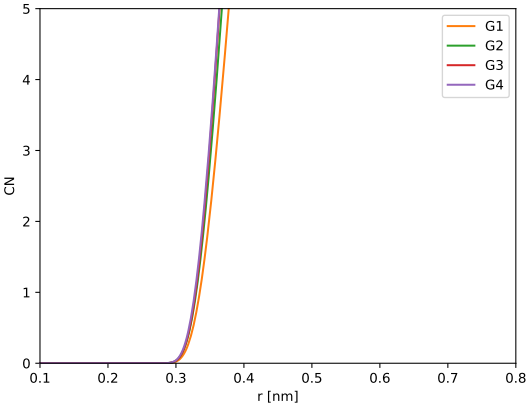
I^- – H-solvent 300mM 1,000 ppm



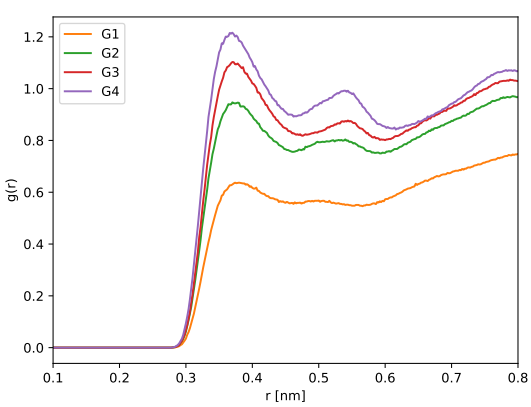


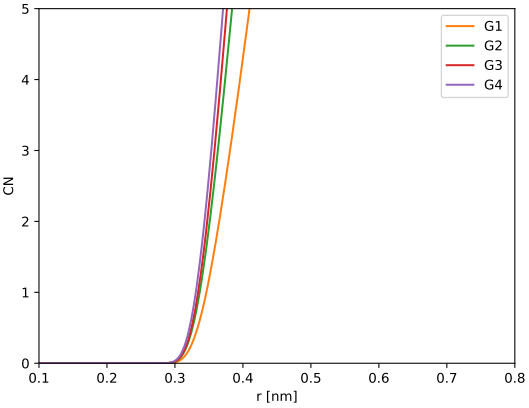
I^- – H-solvent 300mM 5,000 ppm



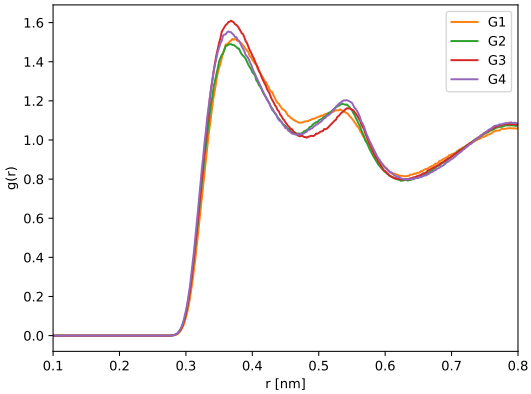


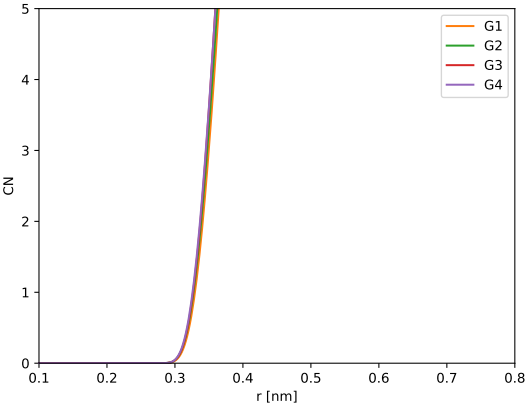
I^- – H-solvent 300mM 20,000 ppm



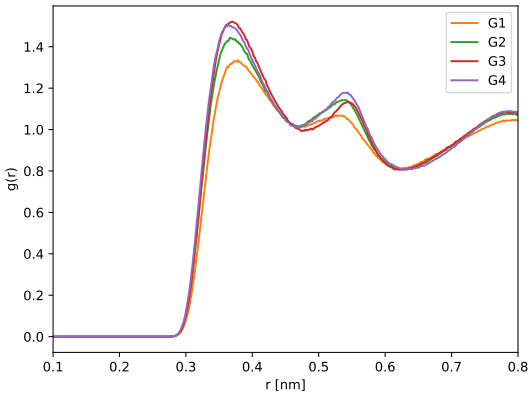


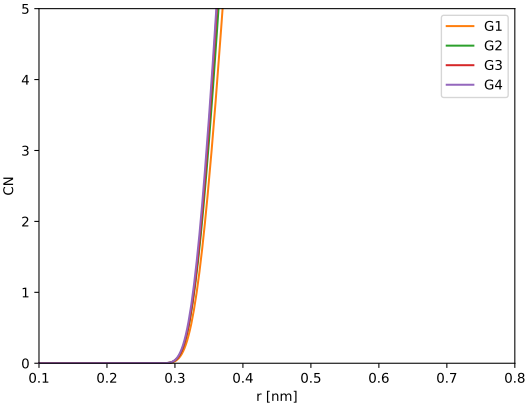
I^- – H-solvent 400mM neat



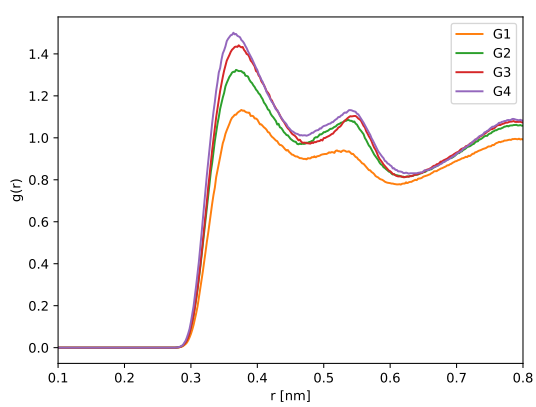


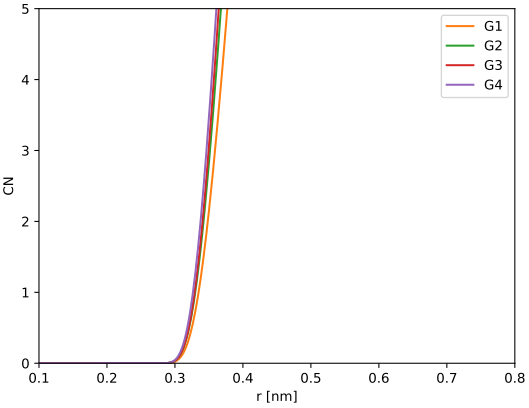
I^- – H-solvent 400mM 1,000 ppm



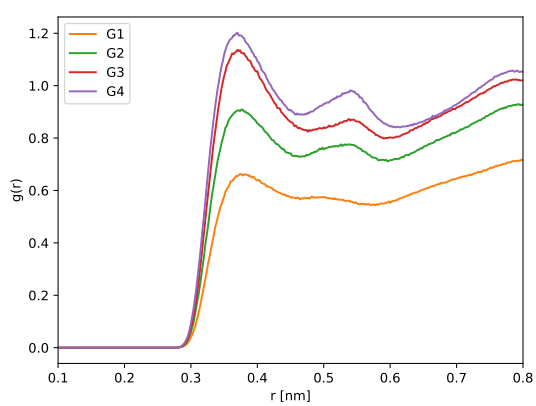


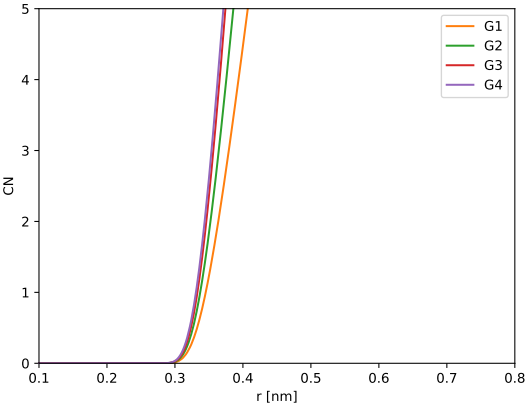
I^- – H-solvent 400mM 5,000 ppm





I^- – H-solvent 400mM 20,000 ppm





2.3 $I^- - I^-$

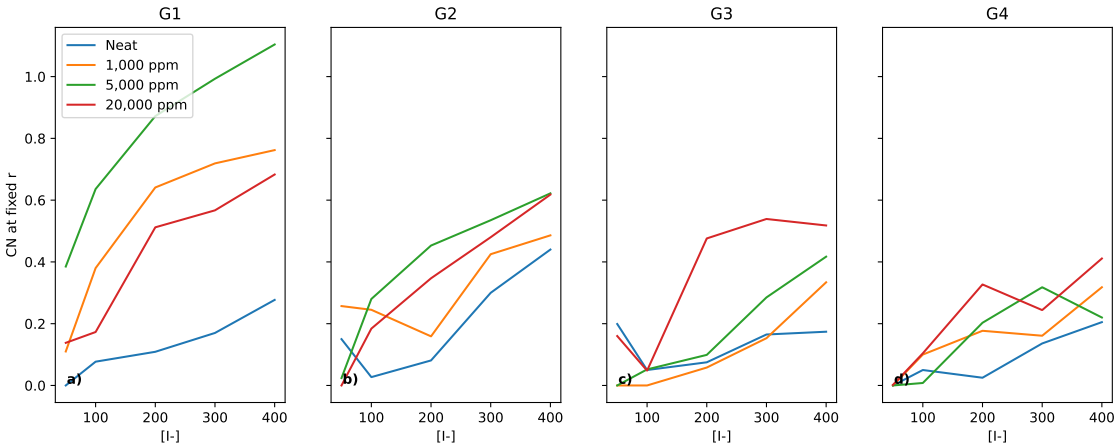


Figure 5: Coordination number of I^- to I^- at a fixed distance of 5Å, for the four different water containing systems (neat = blue, 1,000 ppm = yellow, 5,000 ppm = green and 20,000 ppm = red) studied here, across the four different solvents (with a): G1, b): G2, c): G3 and d): G4).

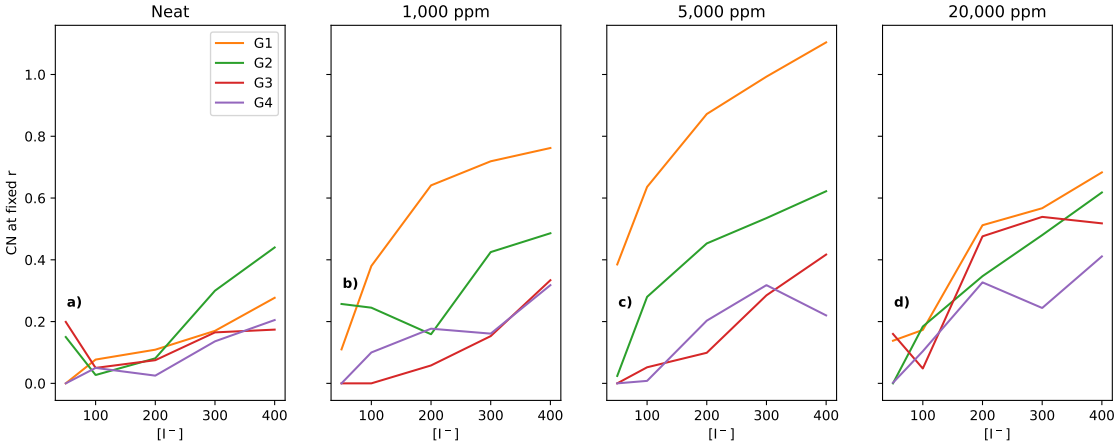
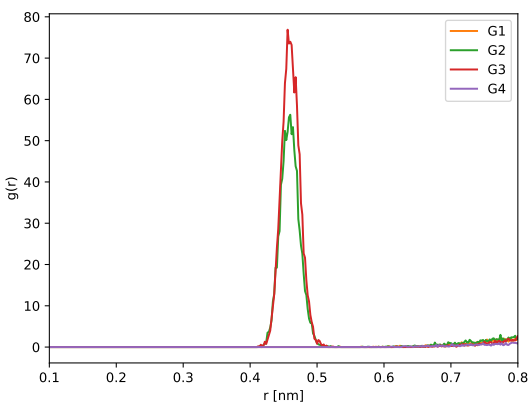
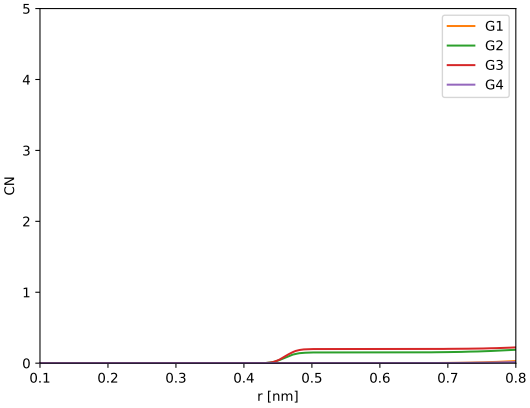


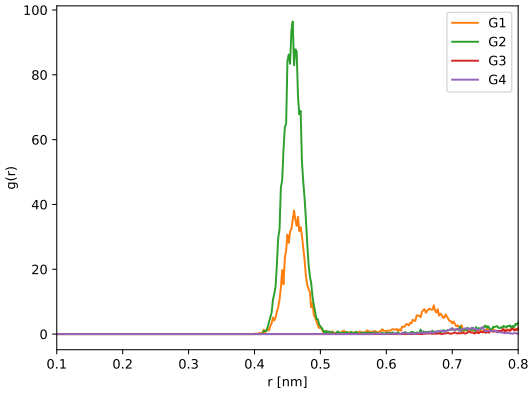
Figure 6: Coordination number of I^- to I^- at a fixed distance of 5 Å, for the four different glymes (G1 = yellow, G2 = green, G3 = red, G4 = purple) studied here, across the four different water concentrations (with a): neat, b): 1,000, c): 5,000, d): 20,000 ppm of water).

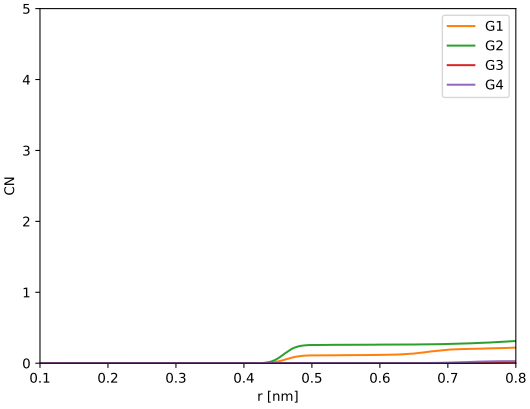
I^- – I^- 50mM neat



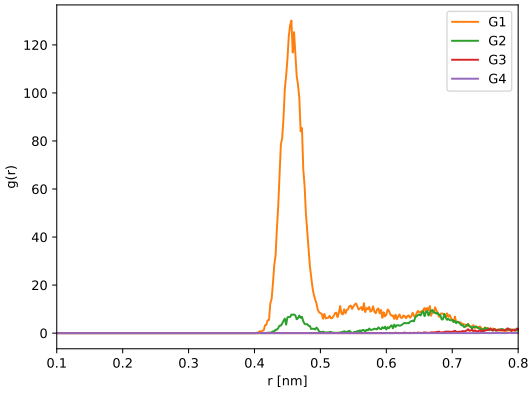


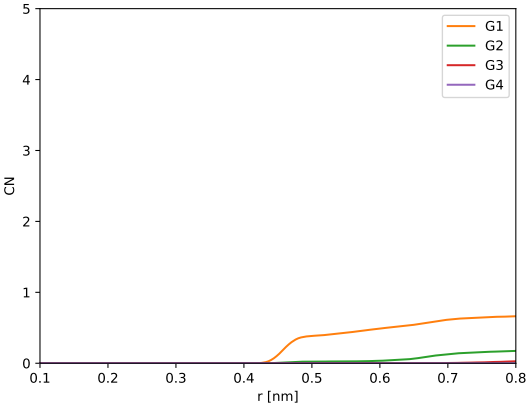
I^- – I^- 50mM 1,000 ppm



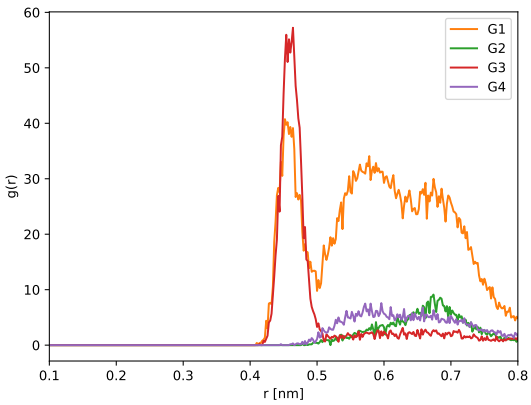


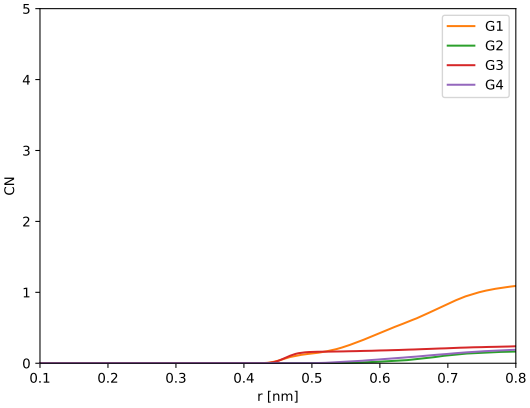
I^- – I^- 50mM 5,000 ppm



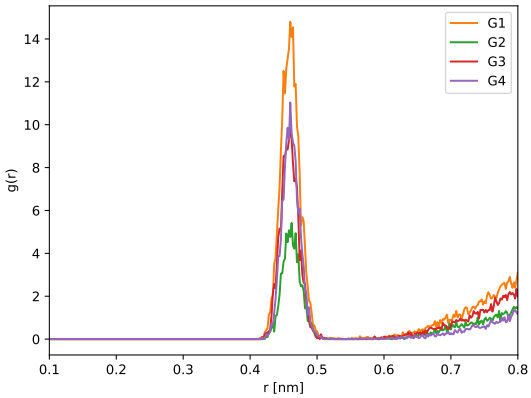


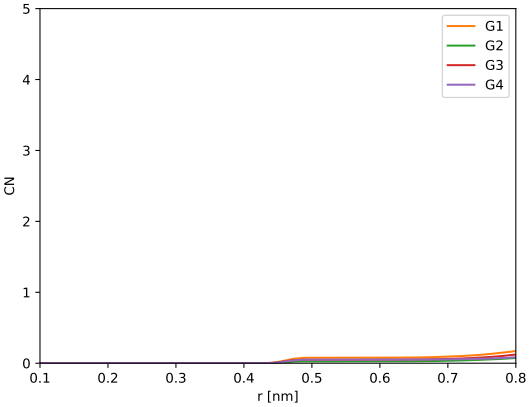
I^- – I^- 50mM 20,000 ppm



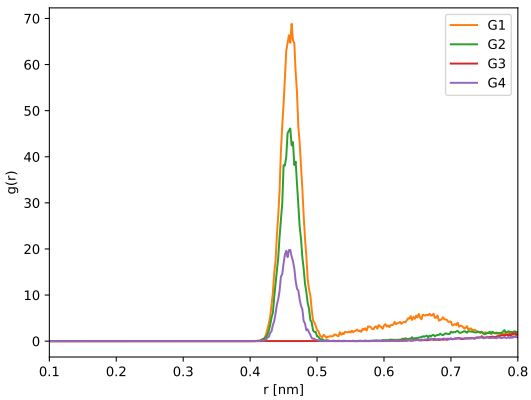


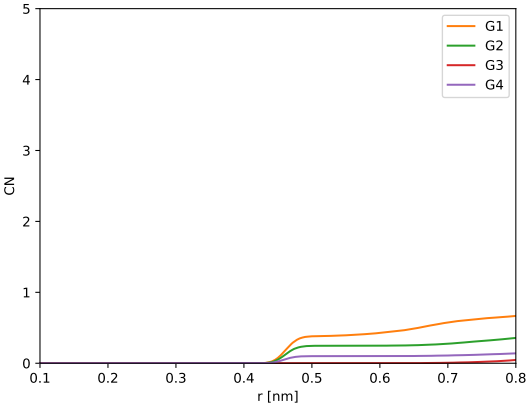
I^- – I^- 100mM neat



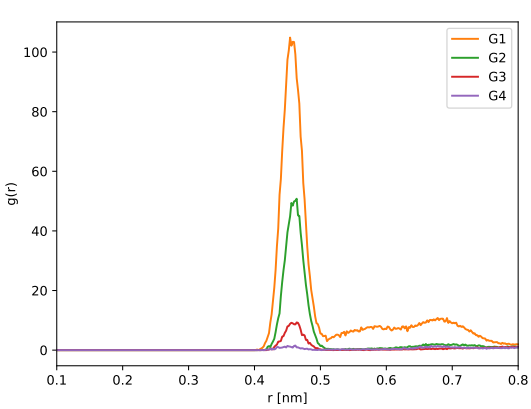


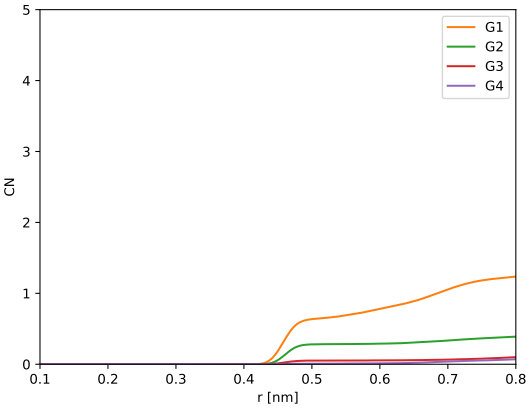
I^- – I^- 100mM 1,000 ppm



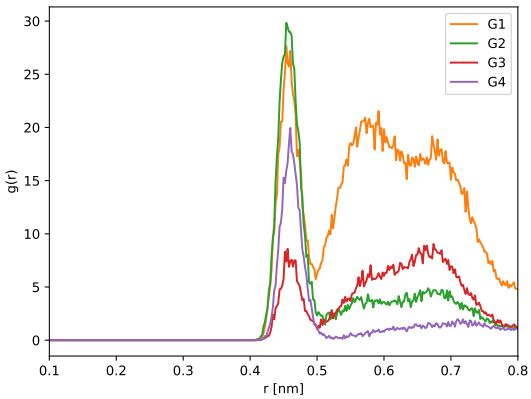


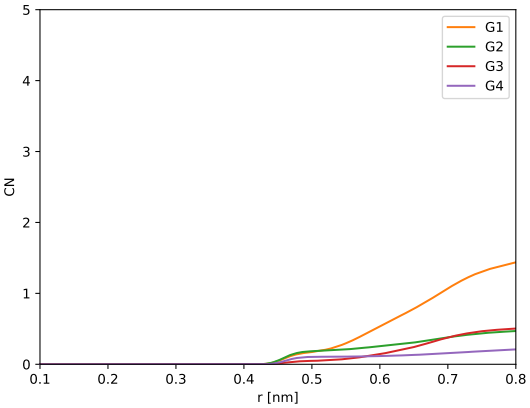
I^- – I^- 100mM 5,000 ppm



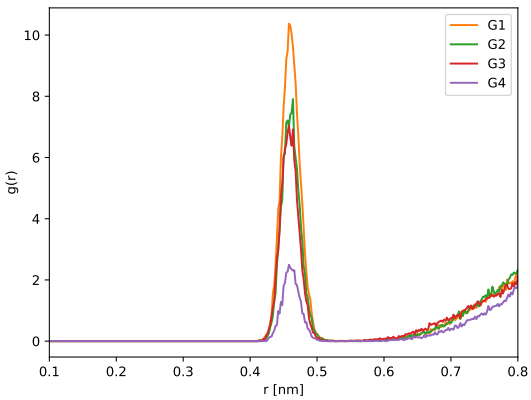


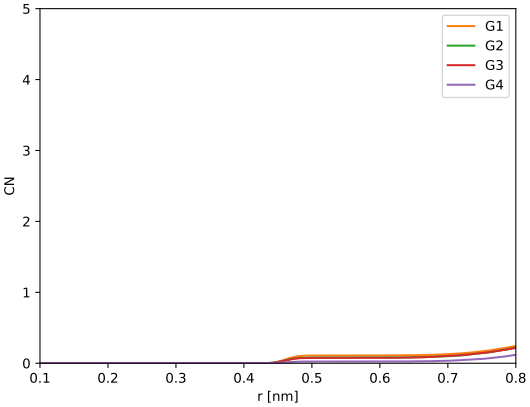
I^- – I^- 100mM 20,000 ppm



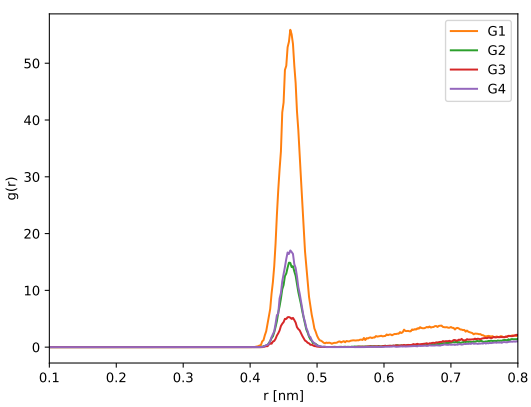


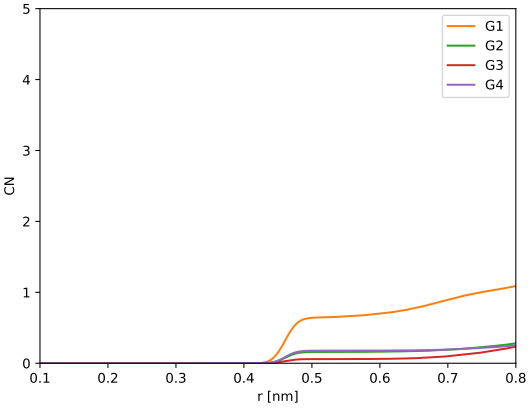
I^- – I^- 200mM neat



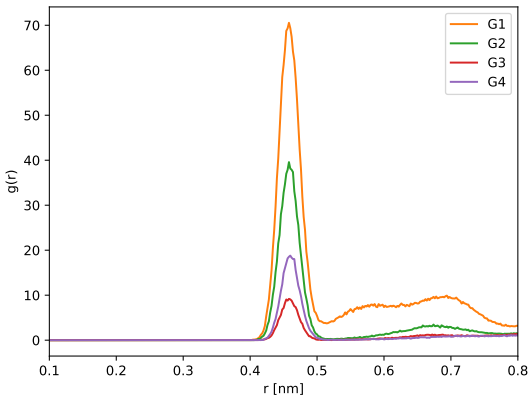


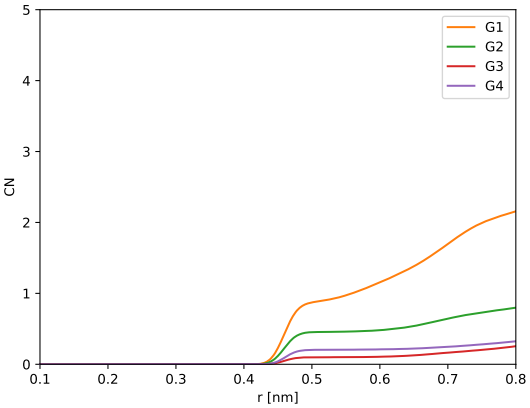
I^- – I^- 200mM 1,000 ppm



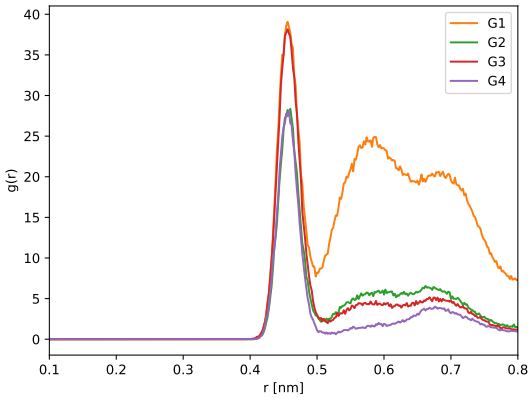


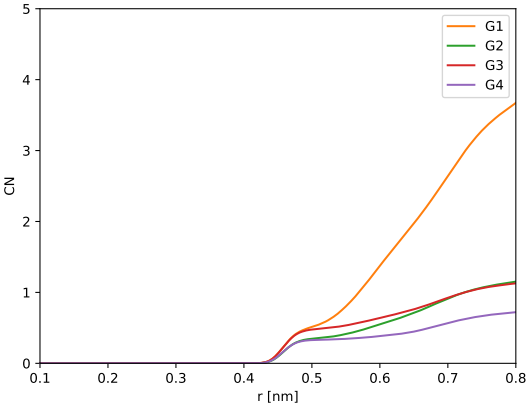
I^- – I^- 200mM 5,000 ppm



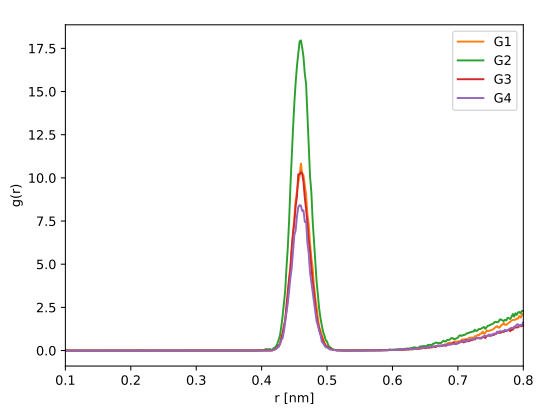


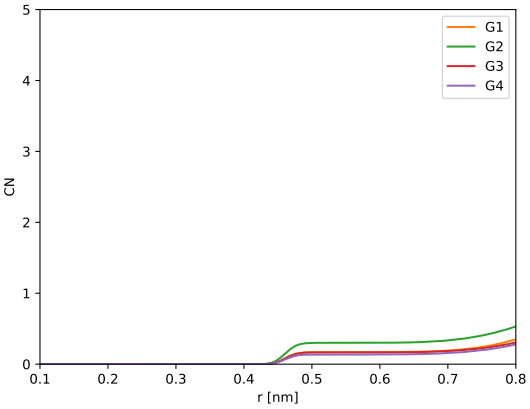
I^- – I^- 200mM 20,000 ppm



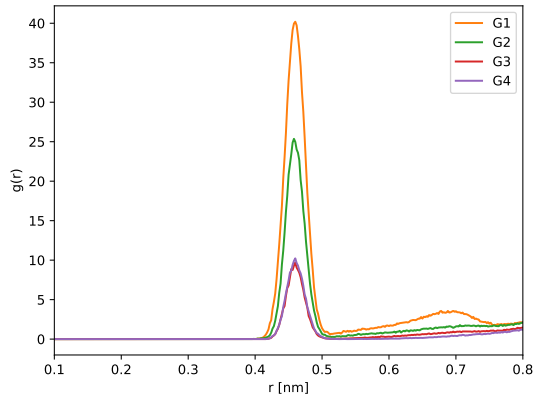


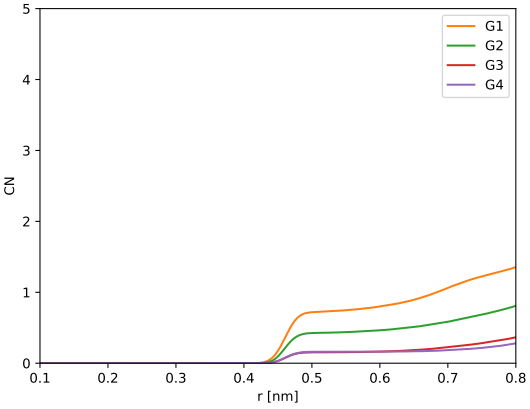
I^- – I^- 300mM neat



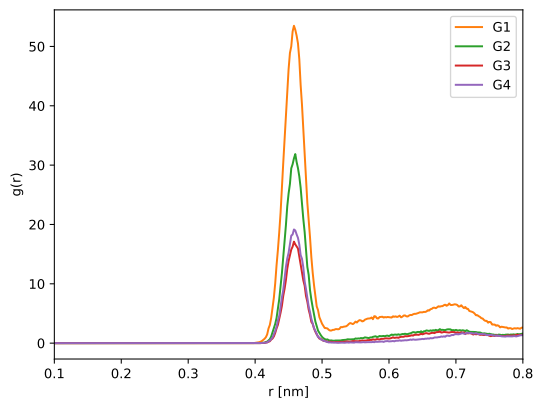


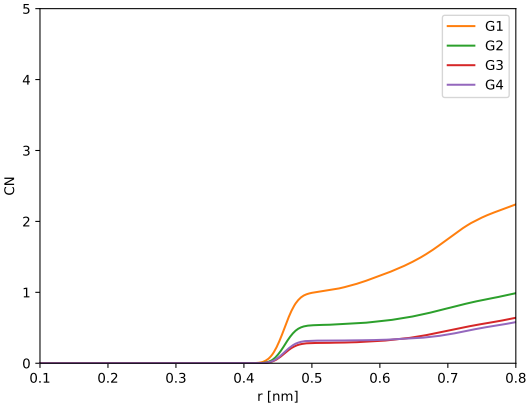
I^- – I^- 300mM 1,000 ppm



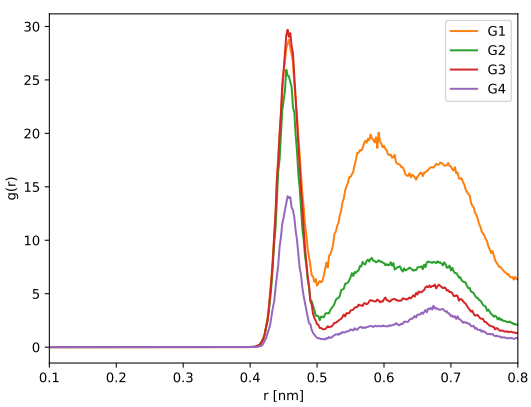


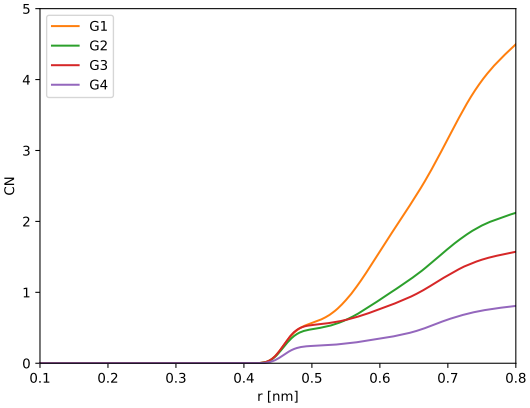
I^- – I^- 300mM 5,000 ppm



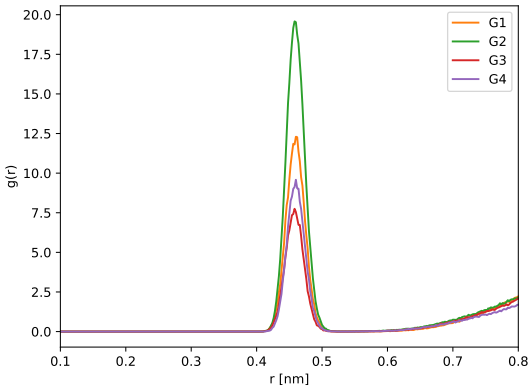


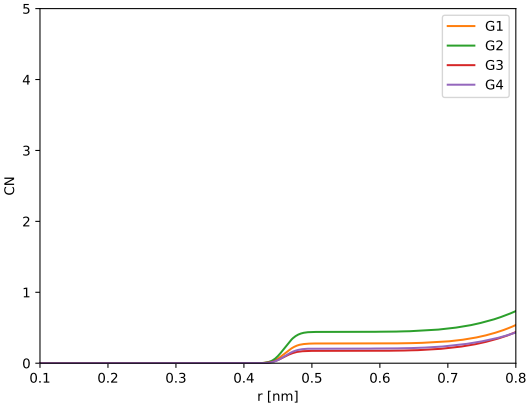
I^- – I^- 300mM 20,000 ppm



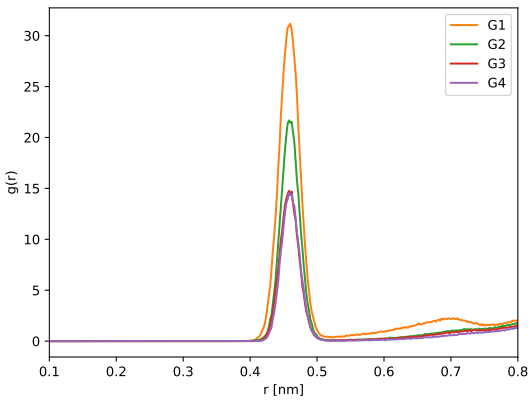


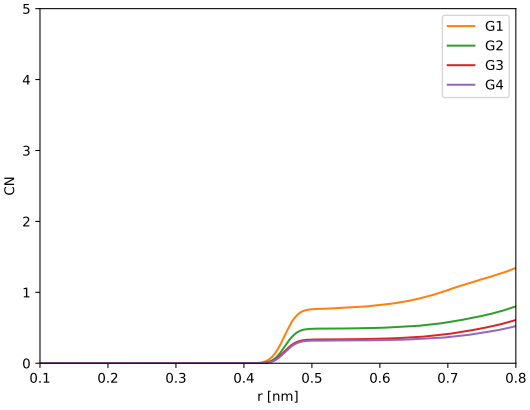
I^- – I^- 400mM neat



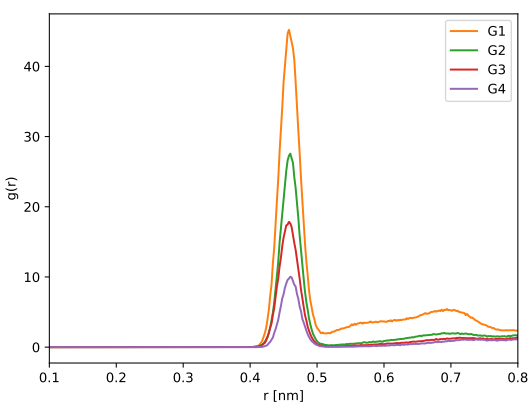


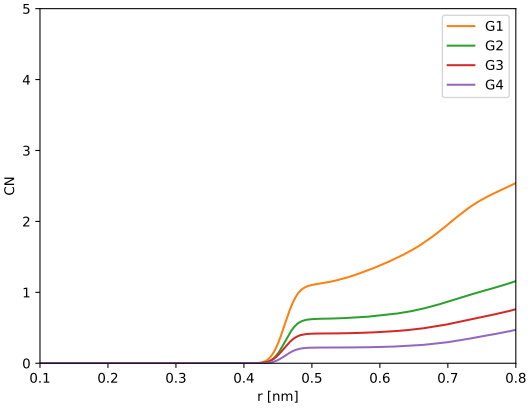
I^- – I^- 400mM 1,000 ppm



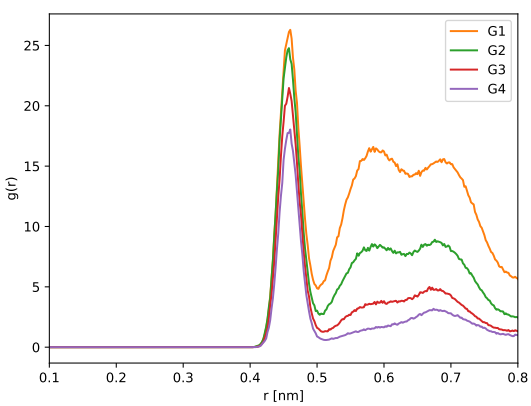


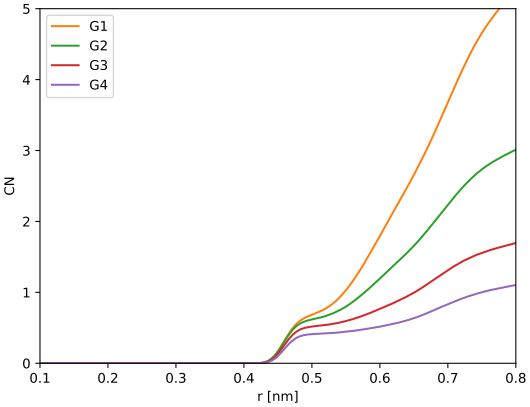
I^- – I^- 400mM 5,000 ppm





I^- – I^- 400mM 20,000 ppm





2.4 I^- – O-solvent

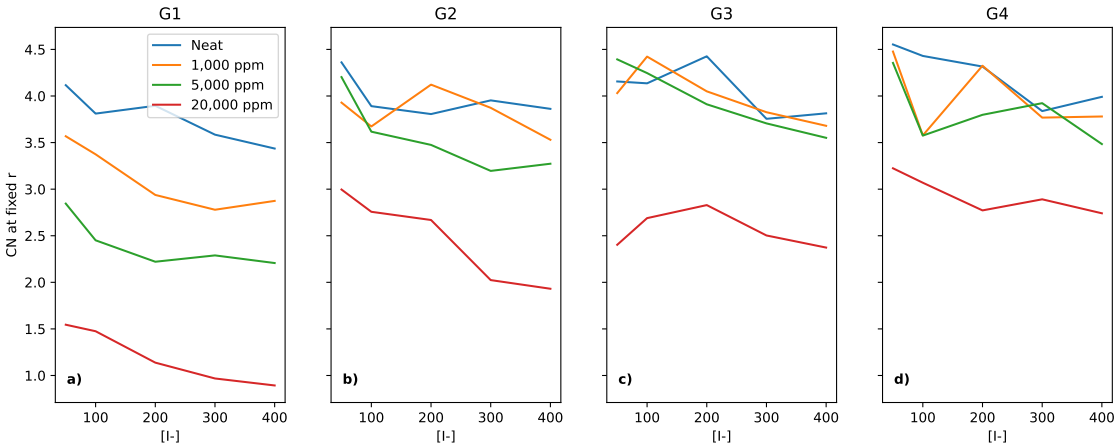


Figure 7: Coordination number of I^- to O (of the glyme solvent) at a fixed distance of 5 Å, for the four different water containing systems (neat = blue, 1,000 ppm = yellow, 5,000 ppm = green and 20,000 ppm = red) studied here, across the four different solvents (with a): G1, b): G2, c): G3 and d): G4).

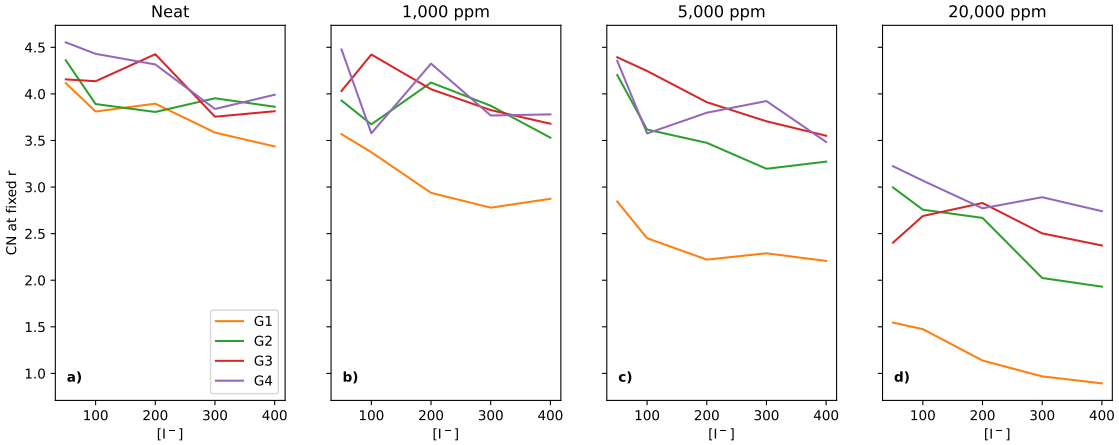
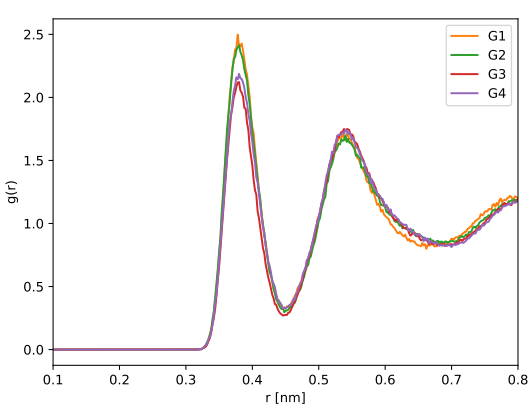
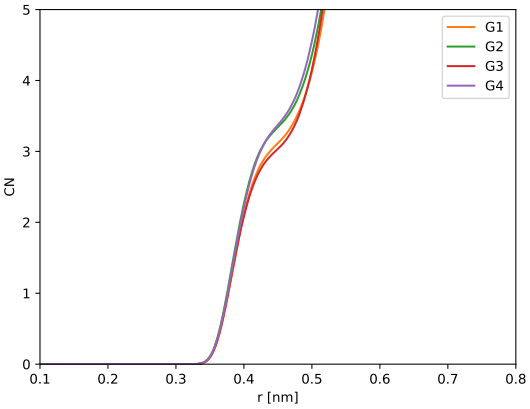


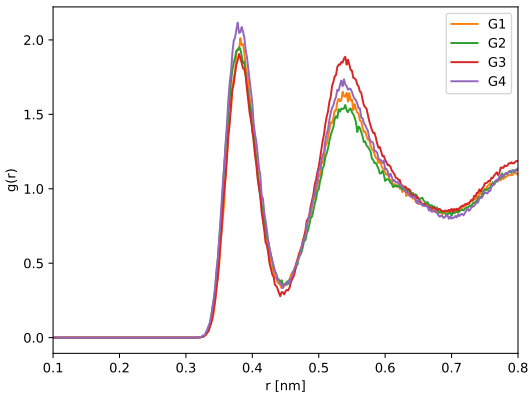
Figure 8: Coordination number of I^- to O (of the glyme solvent) at a fixed distance of 5 Å, for the four different glymes (G1 = yellow, G2 = green, G3 = red, G4 = purple) studied here, across the four different water concentrations (with a): neat, b): 1,000, c): 5,000, d): 20,000 ppm of water).

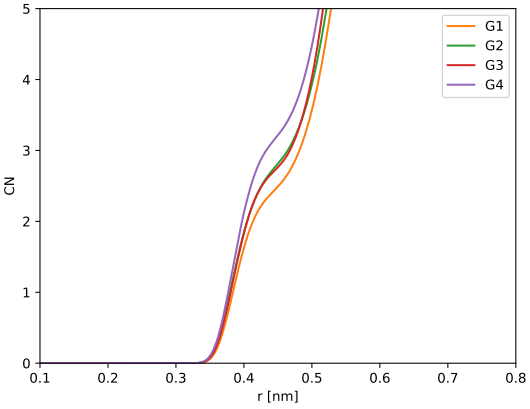
I^- – O-solvent 50mM neat



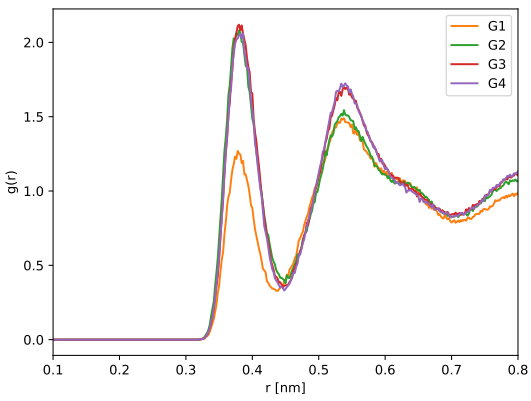


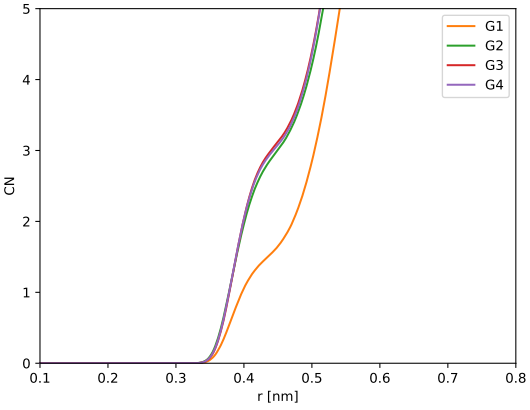
I^- – O-solvent 50mM 1,000 ppm



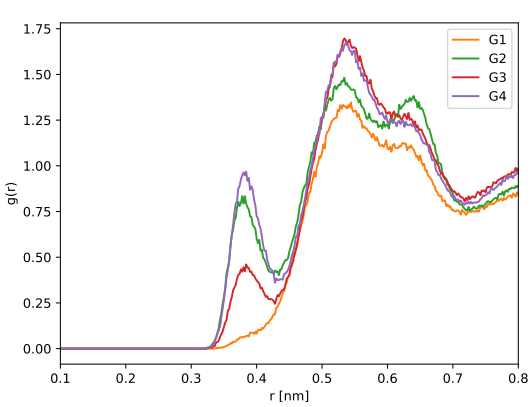


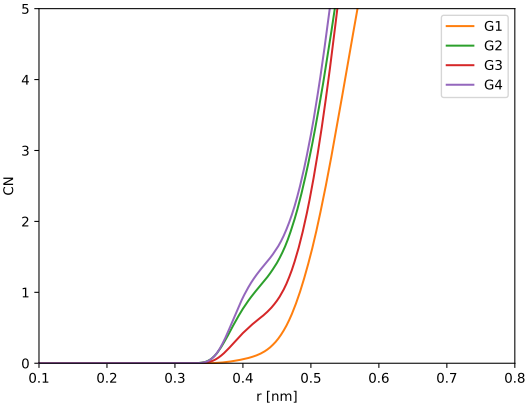
I^- – O-solvent 50mM 5,000 ppm



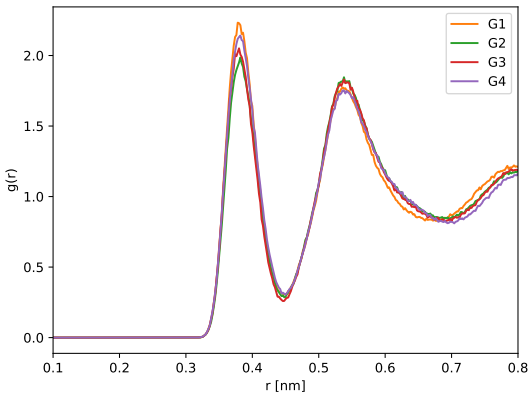


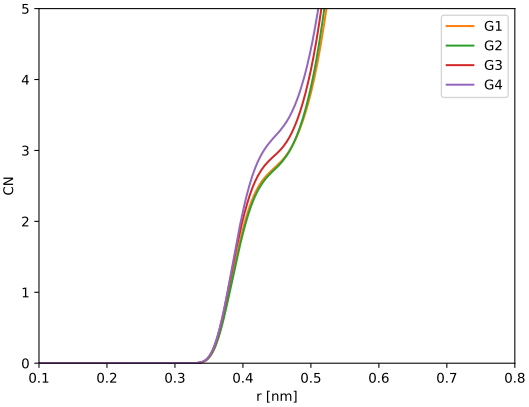
I^- – O-solvent 50mM 20,000 ppm



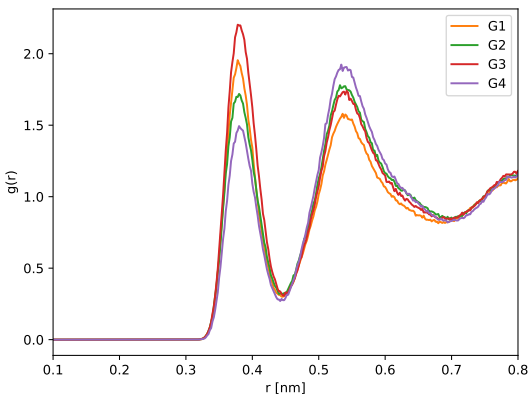


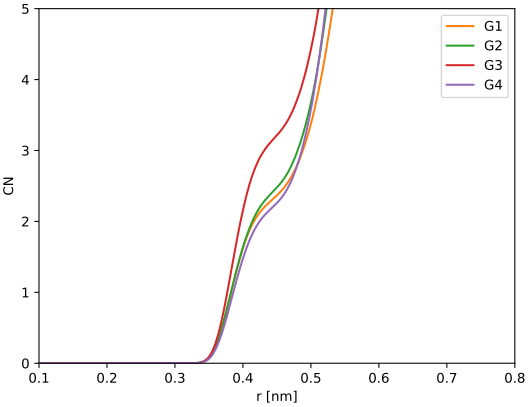
I^- – O-solvent 100mM neat



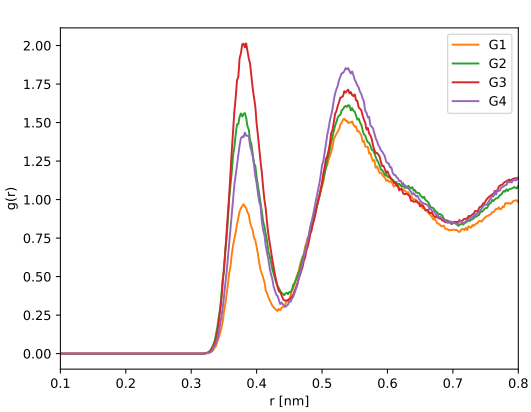


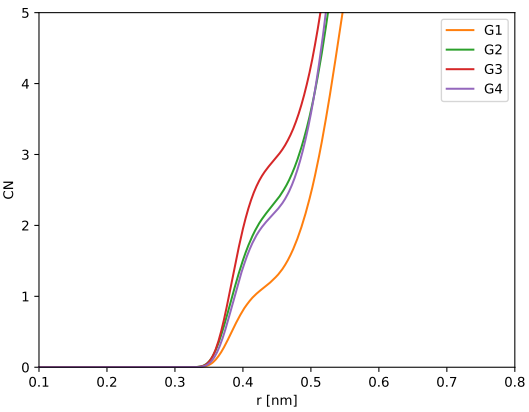
I^- – O-solvent 100mM 1,000 ppm



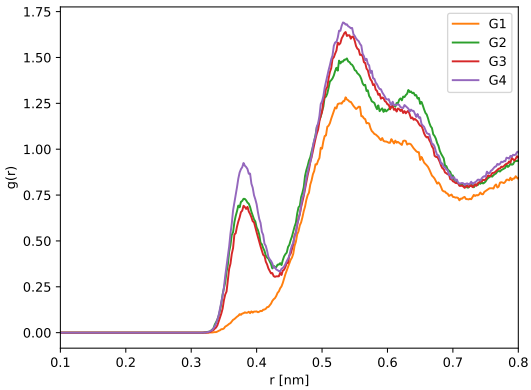


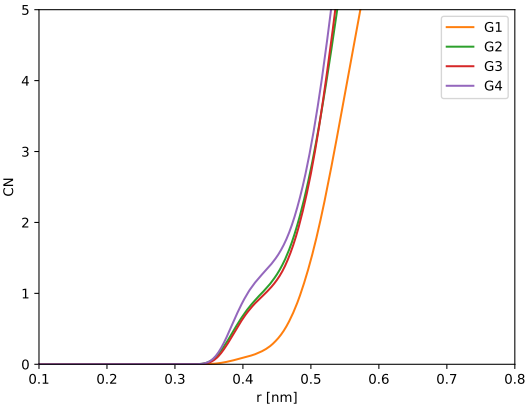
I^- – O-solvent 100mM 5,000 ppm



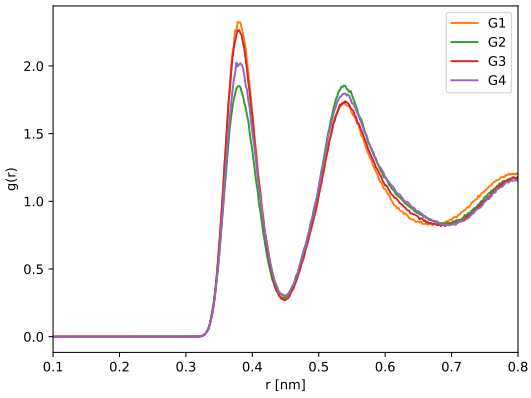


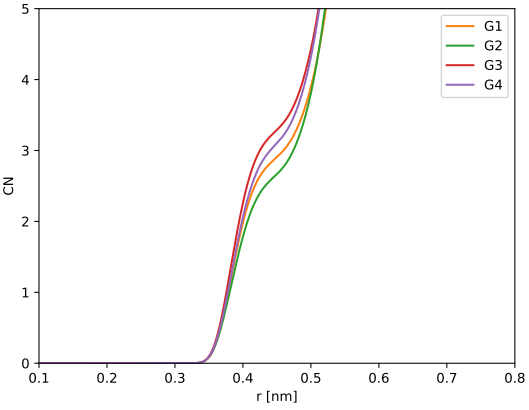
I^- – O-solvent 100mM 20,000 ppm



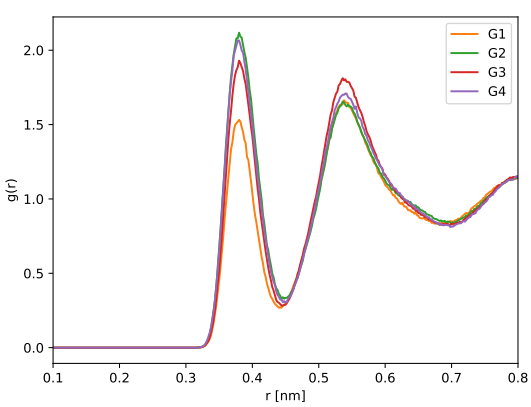


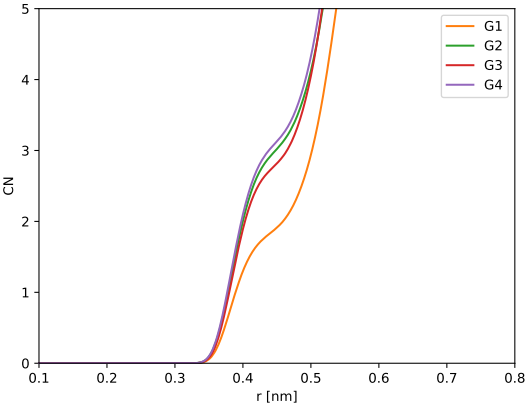
I^- – O-solvent 200mM neat



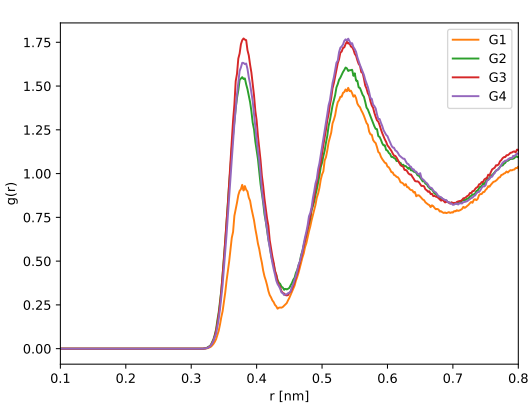


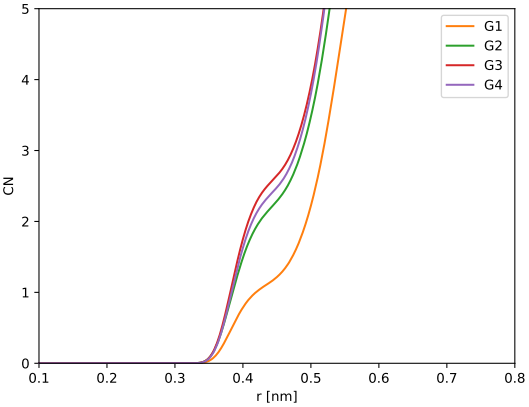
I^- – O-solvent 200mM 1,000 ppm



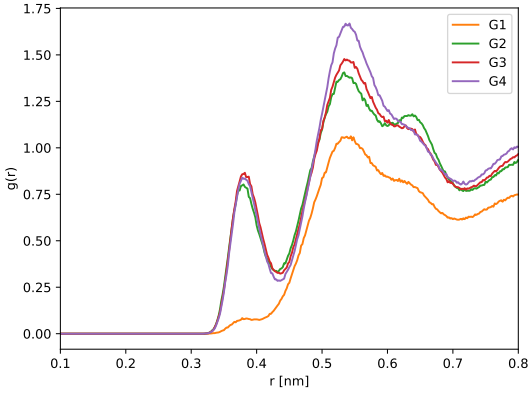


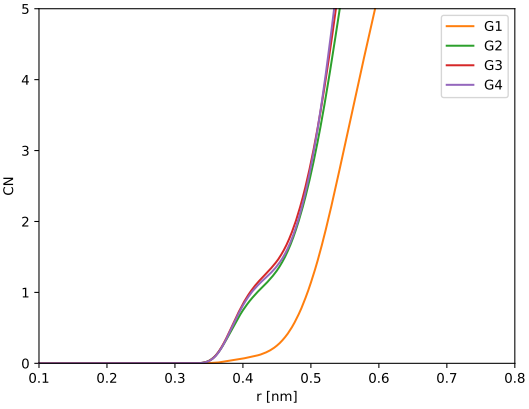
I^- – O-solvent 200mM 5,000 ppm



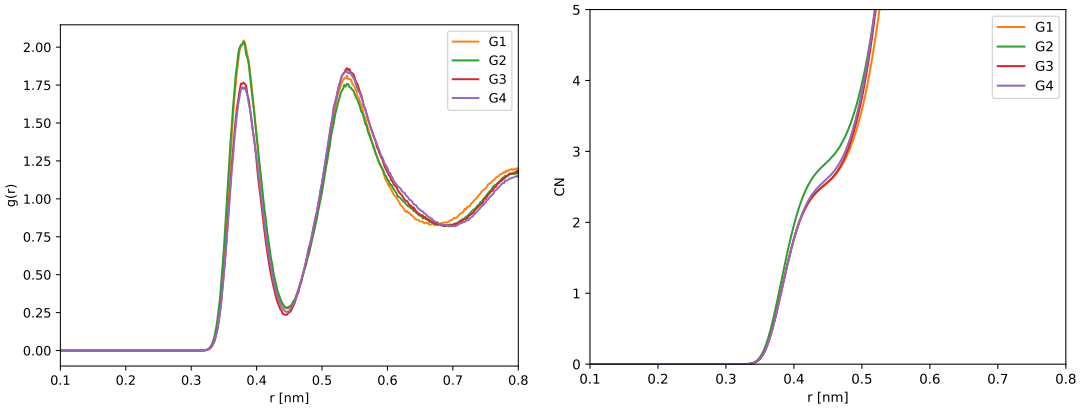


I^- – O-solvent 200mM 20,000 ppm

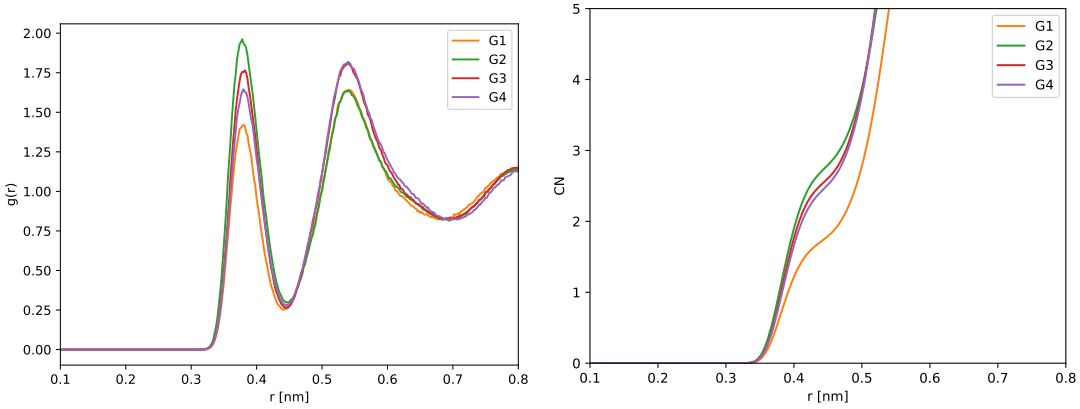




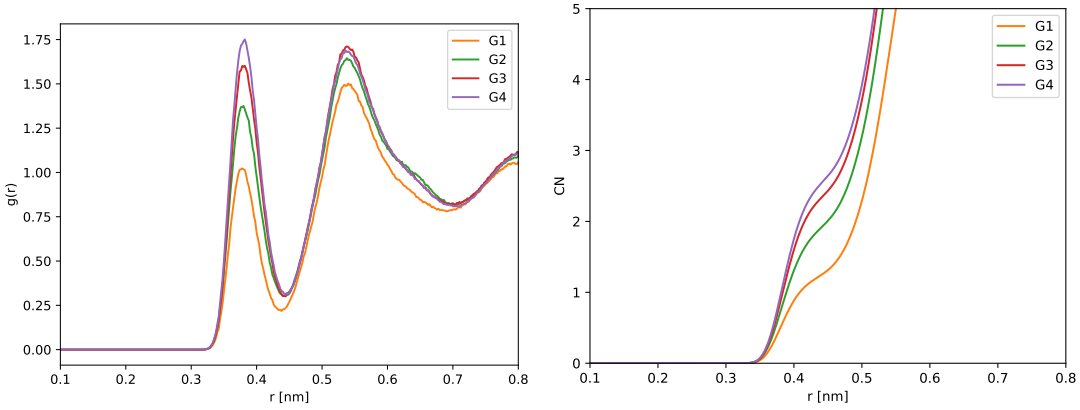
I^- – O-solvent 300mM neat



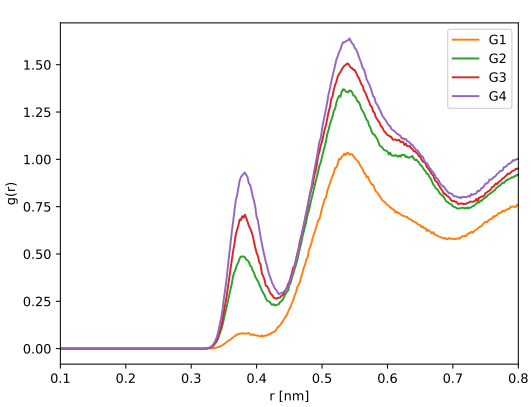
I^- – O-solvent 300mM 1,000 ppm

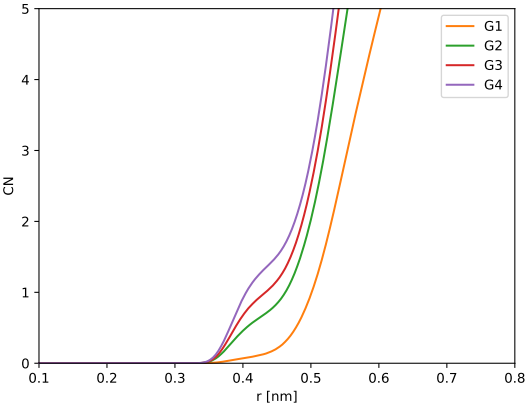


I^- – O-solvent 300mM 5,000 ppm

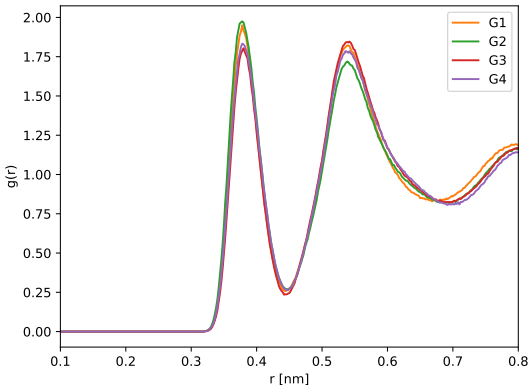


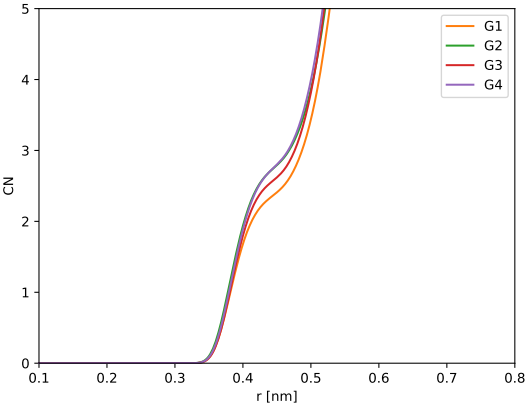
I^- – O-solvent 300mM 20,000 ppm



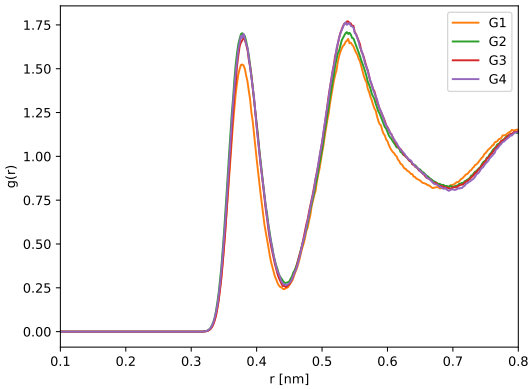


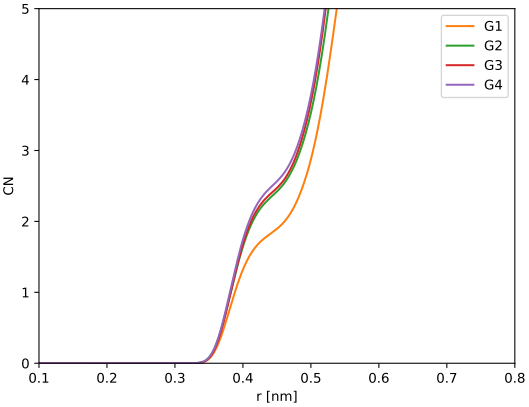
I^- – O-solvent 400mM neat



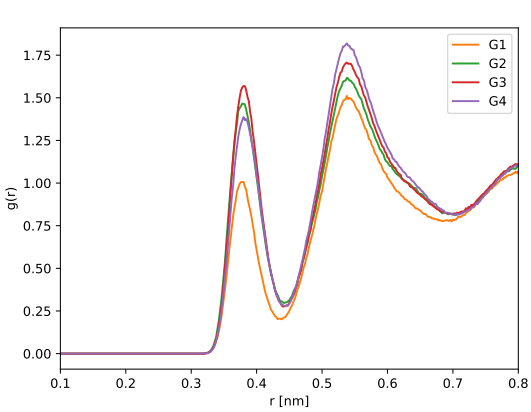


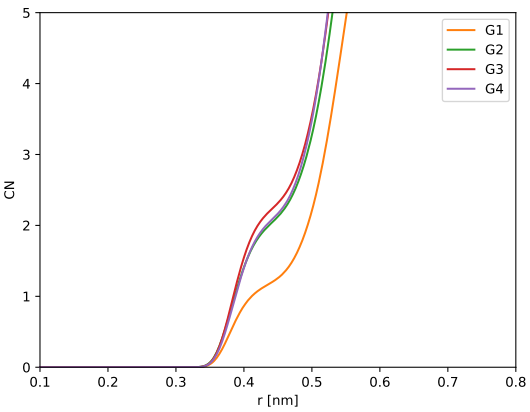
I^- – O-solvent 400mM 1,000 ppm



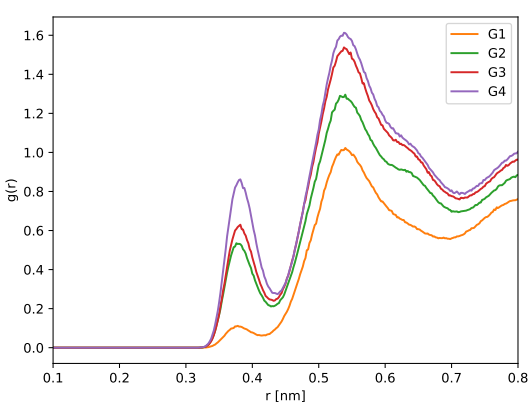


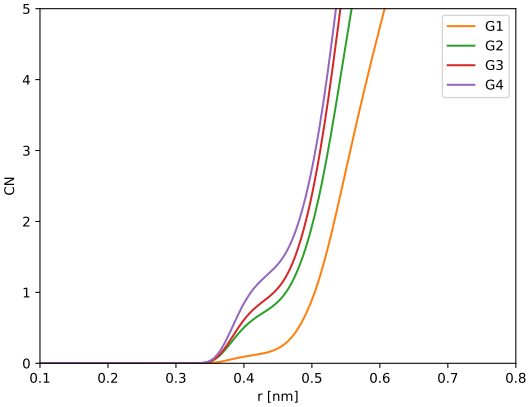
I^- – O-solvent 400mM 5,000 ppm





I^- – O-solvent 400mM 20,000 ppm





2.5 I^- – N-TFSI

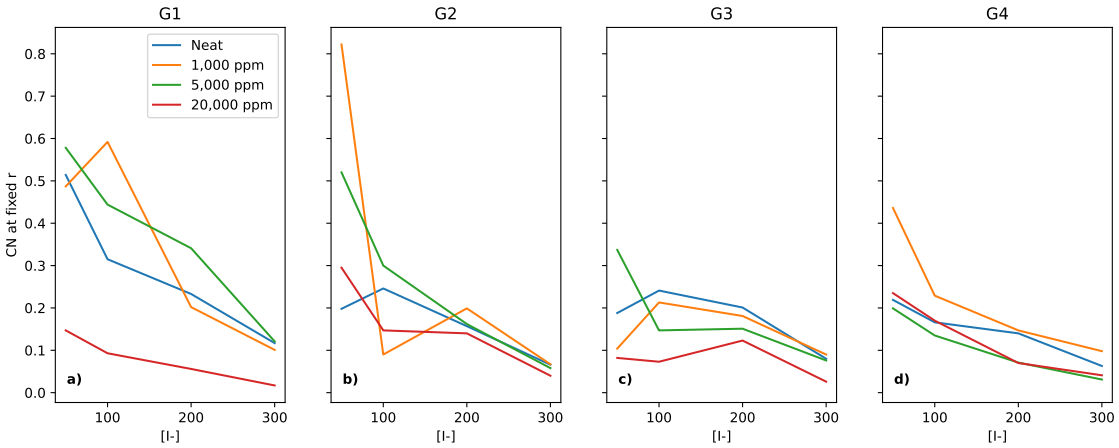


Figure 9: Coordination number of I^- to N (of the TFSI) at a fixed distance of 4.5 Å, for the four different water containing systems (neat = blue, 1,000 ppm = yellow, 5,000 ppm = green and 20,000 ppm = red) studied here, across the four different solvents (with a): G1, b): G2, c): G3 and d): G4).

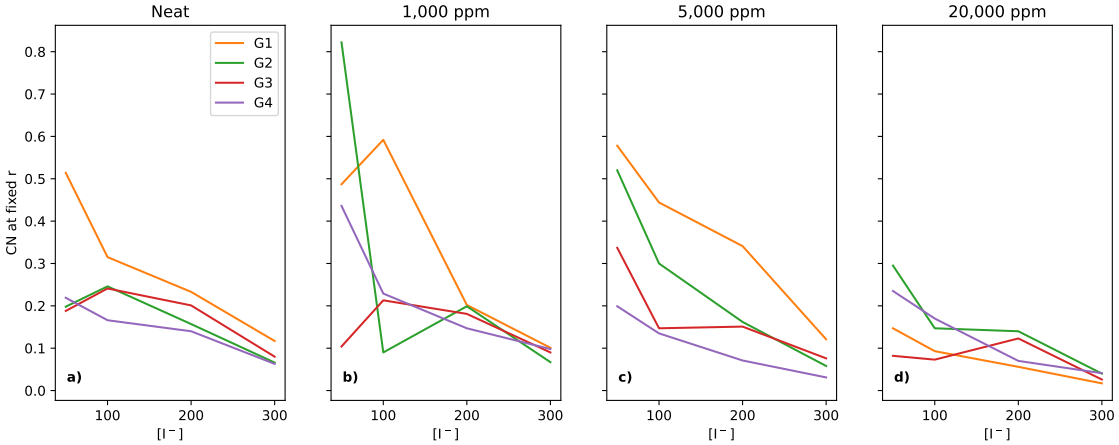
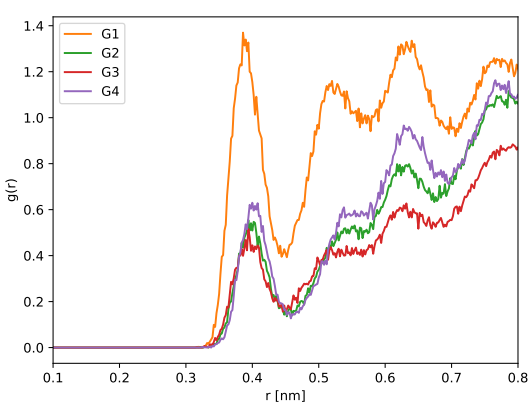
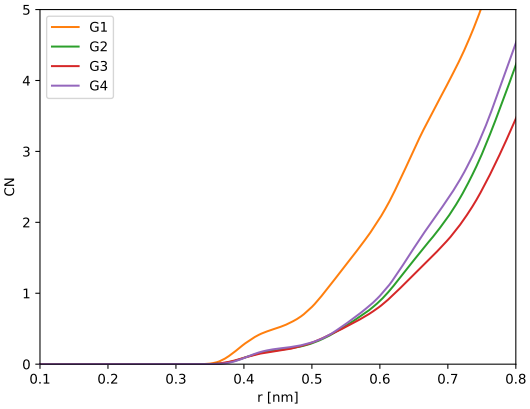


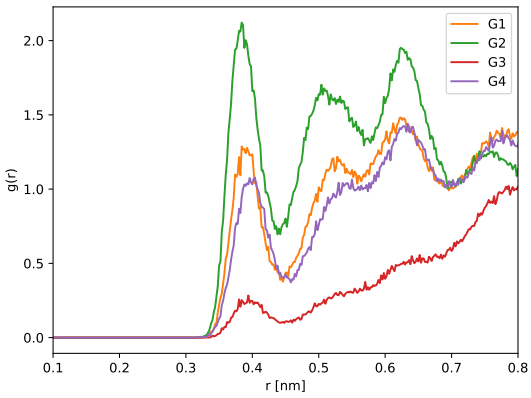
Figure 10: Coordination number of I^- to N (of the TFSI) at a fixed distance of 4.5 Å, for the four different glymes (G1 = yellow, G2 = green, G3 = red, G4 = purple) studied here, across the four different water concentrations (with a): neat, b): 1,000, c): 5,000, d): 20,000 ppm of water).

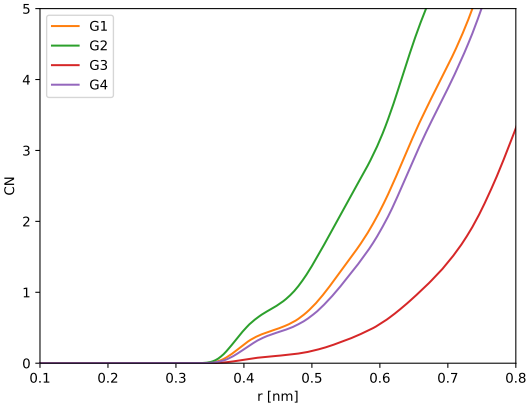
I^- – N-TFSI 50mM neat



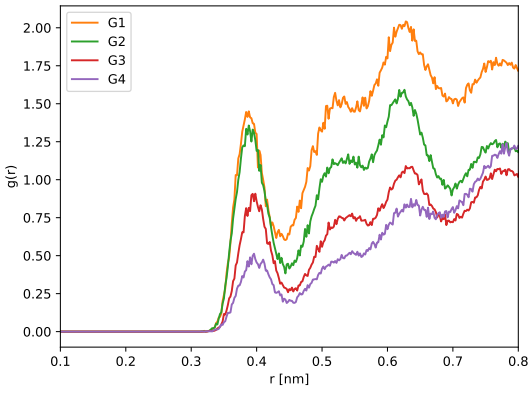


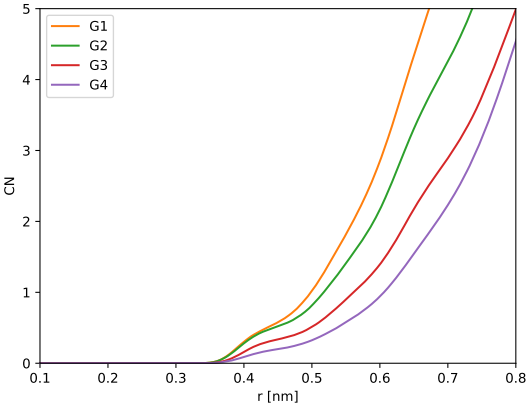
I^- – N-TFSI 50mM 1,000 ppm



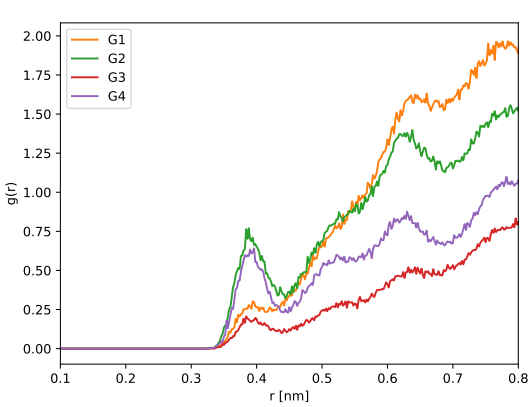


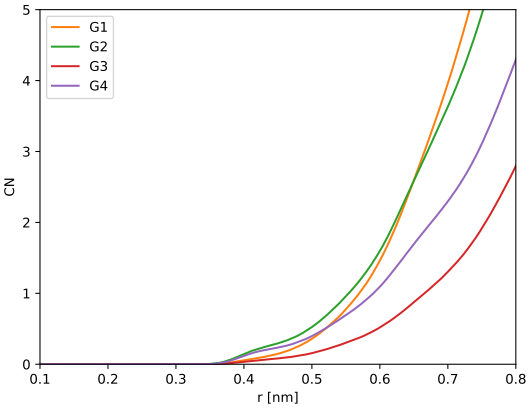
I^- – N-TFSI 50mM 5,000 ppm



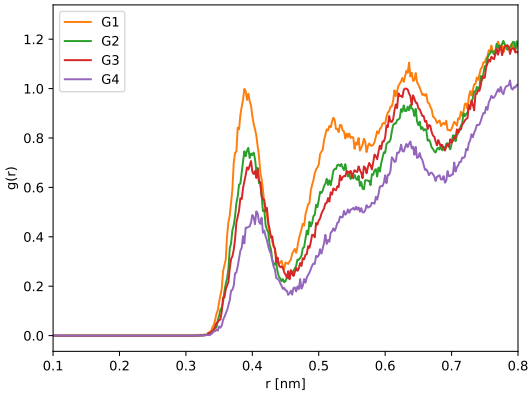


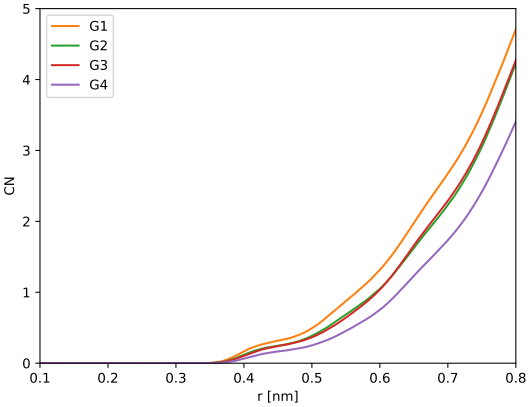
I^- – N-TFSI 50mM 20,000 ppm



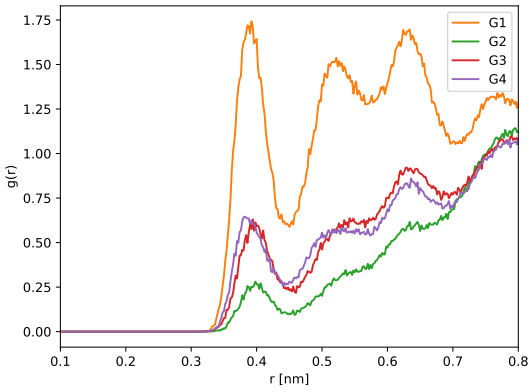


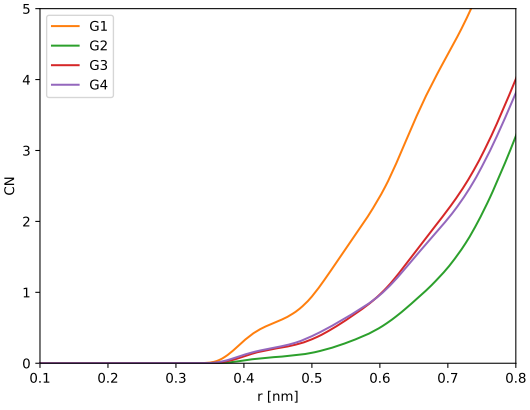
I^- – N-TFSI 100mM neat



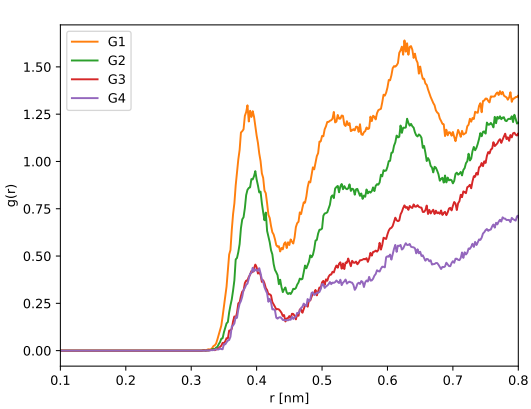


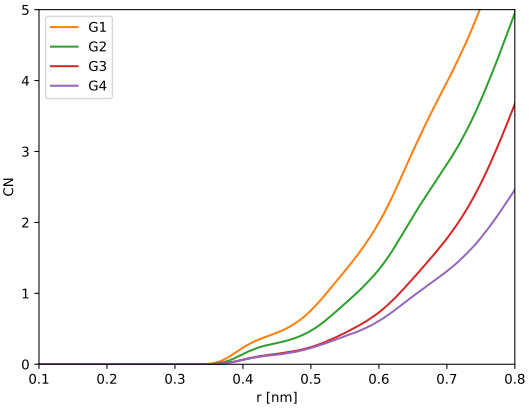
I^- – N-TFSI 100mM 1,000 ppm



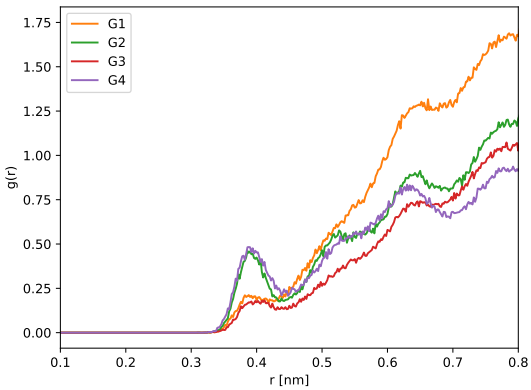


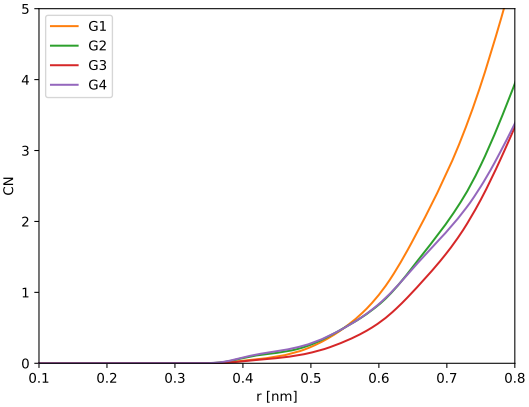
I^- – N-TFSI 100mM 5,000 ppm



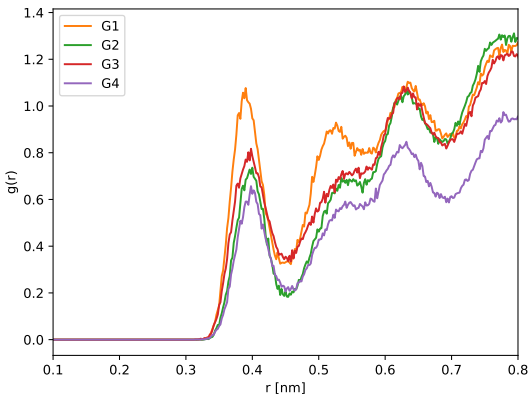


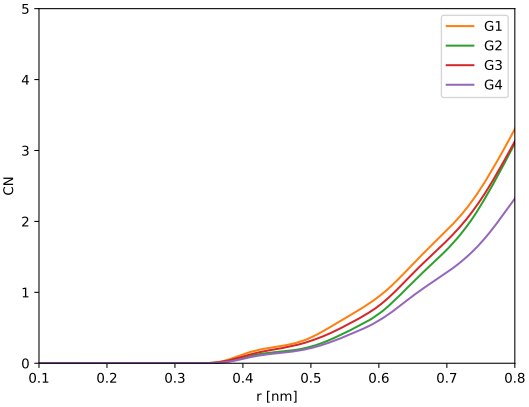
I^- – N-TFSI 100mM 20,000 ppm



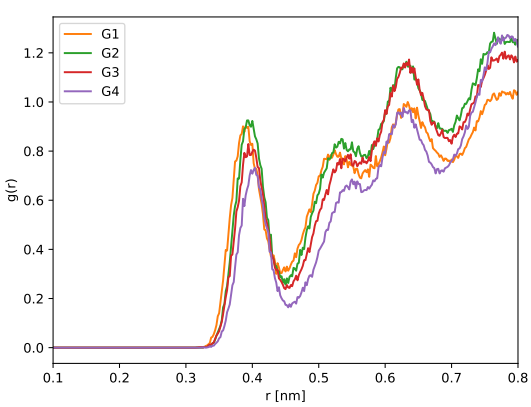


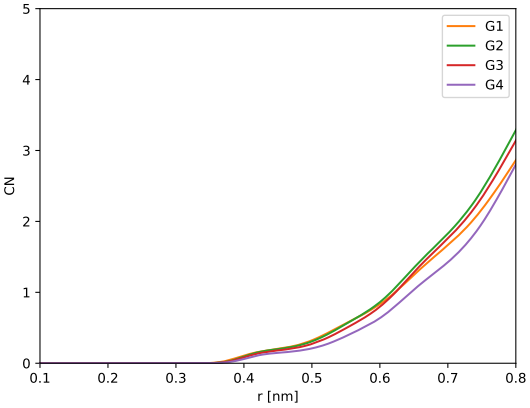
I^- – N-TFSI 200mM neat



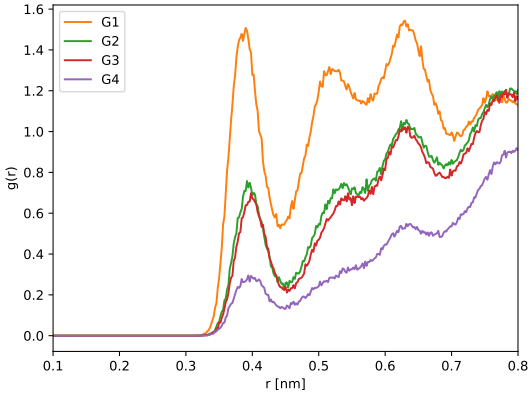


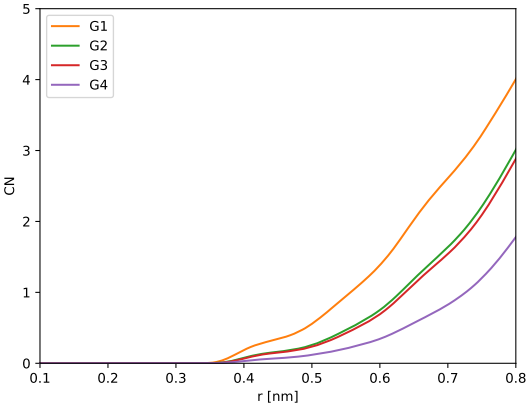
I^- – N-TFSI 200mM 1,000 ppm



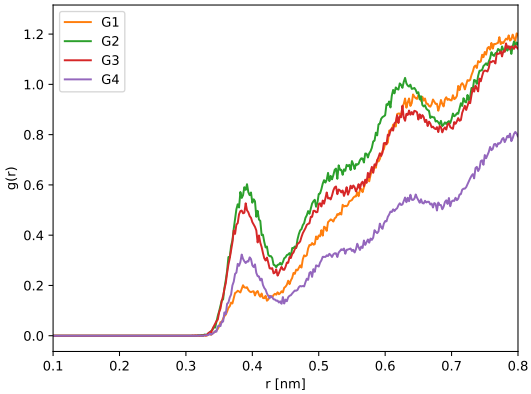


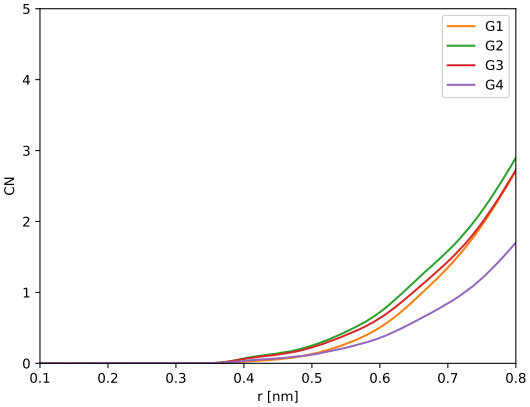
I^- – N-TFSI 200mM 5,000 ppm



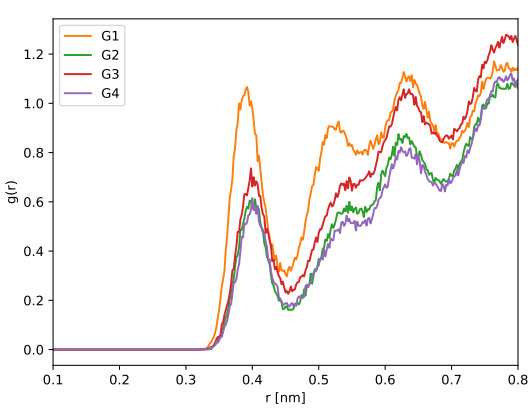


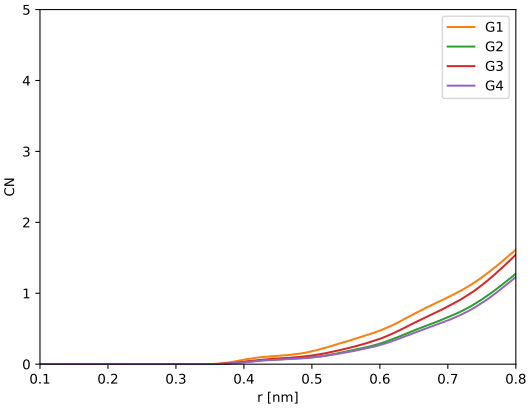
I^- – N-TFSI 200mM 20,000 ppm



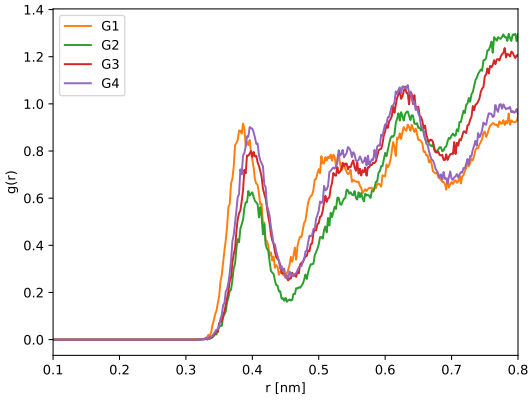


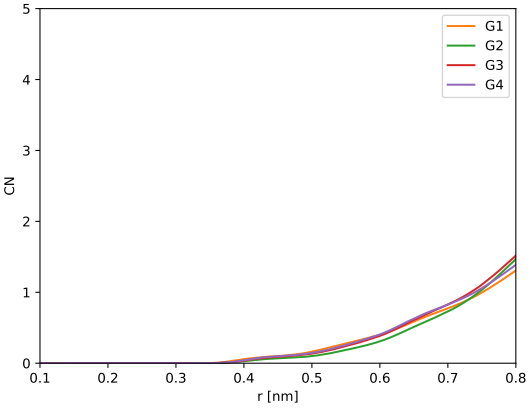
I^- – N-TFSI 300mM neat



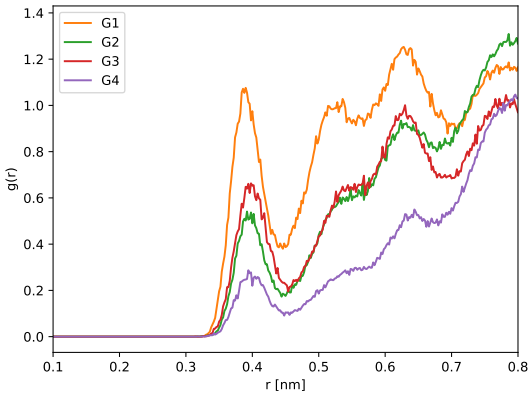


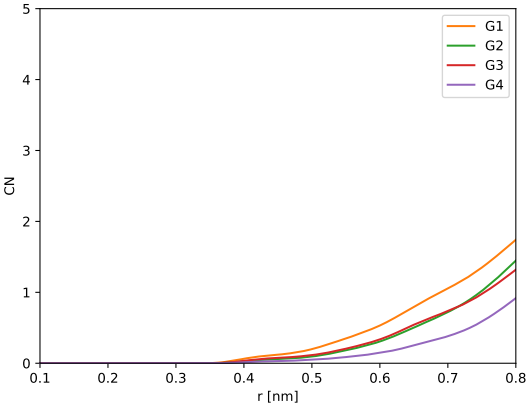
I^- – N-TFSI 300mM 1,000 ppm



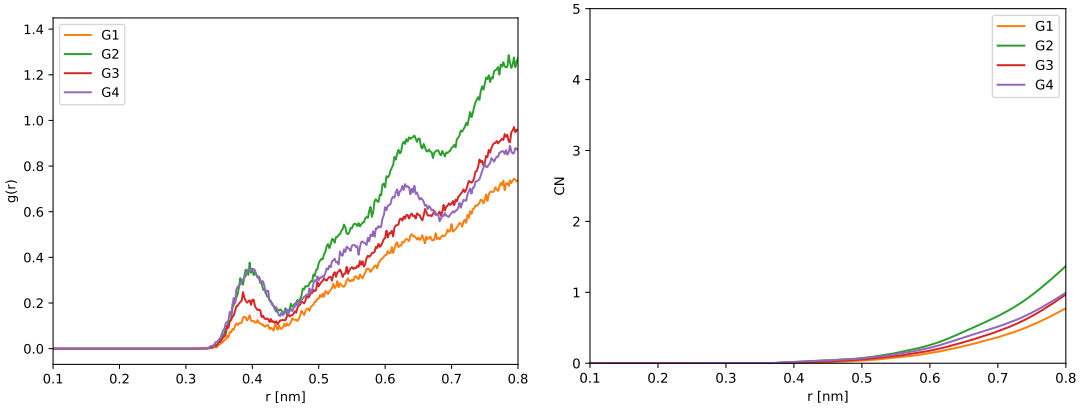


I^- – N-TFSI 300mM 5,000 ppm





I^- – N-TFSI 300mM 20,000 ppm



2.6 $I^- - Li^+$

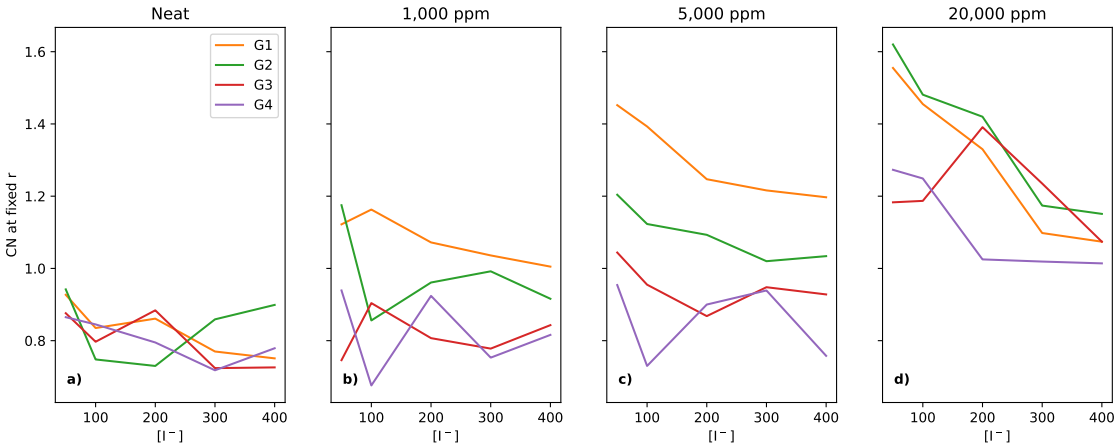


Figure 11: Coordination number of I^- to Li^+ at a fixed distance of 3 Å, for the four different glymes (G1 = yellow, G2 = green, G3 = red, G4 = purple) studied here, across the four different water concentrations (with a): neat, b): 1,000, c): 5,000, d): 20,000 ppm of water).

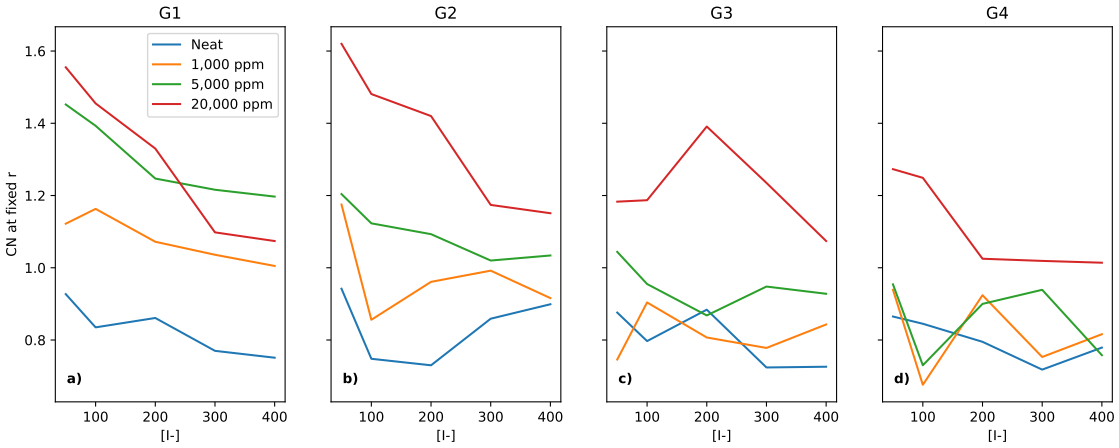
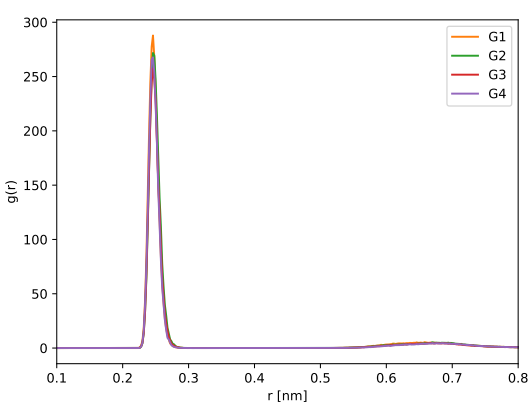
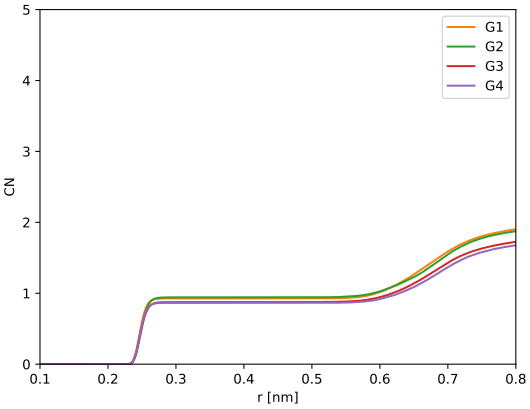


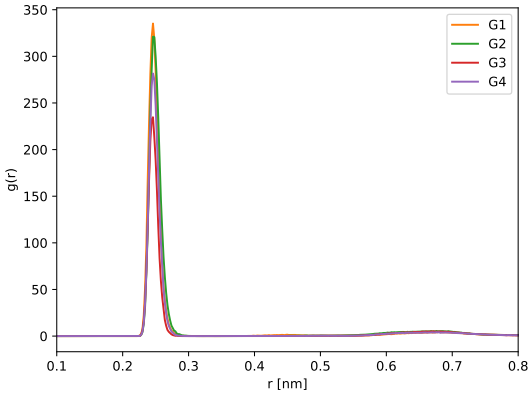
Figure 12: Coordination number of I^- to Li^+ at a fixed distance of 3 Å, for the four different water containing systems (neat = blue, 1,000 ppm = yellow, 5,000 ppm = green and 20,000 ppm = red) studied here, across the four different solvents (with a): G1, b): G2, c): G3 and d): G4).

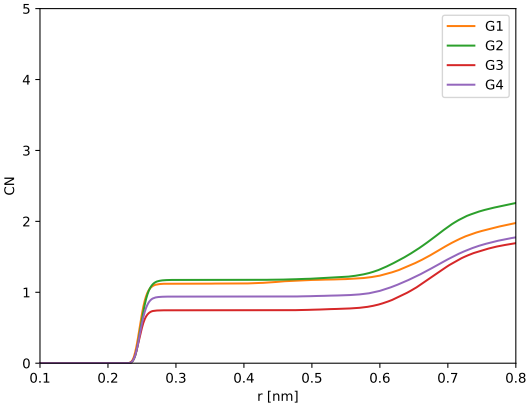
I^- – Li^+ 50mM neat



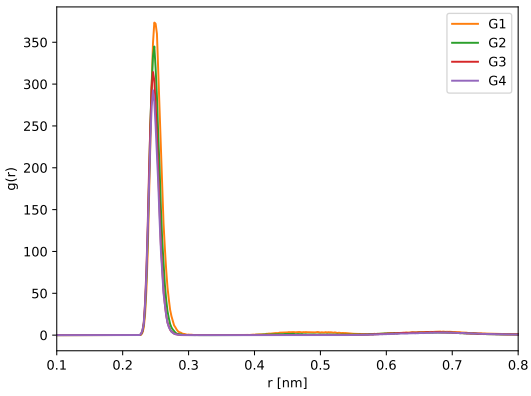


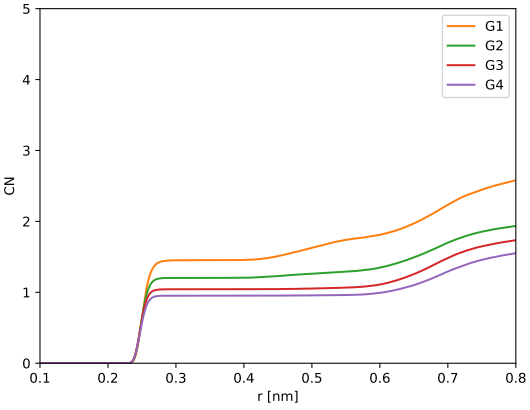
I^- – Li^+ 50mM 1,000 ppm



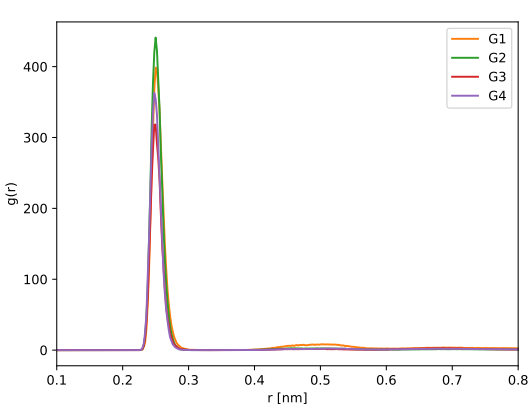


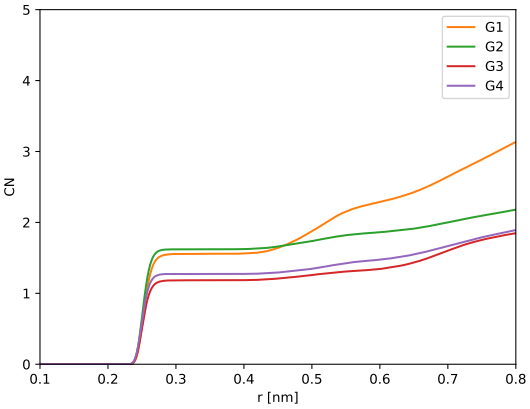
I^- – Li^+ 50mM 5,000 ppm



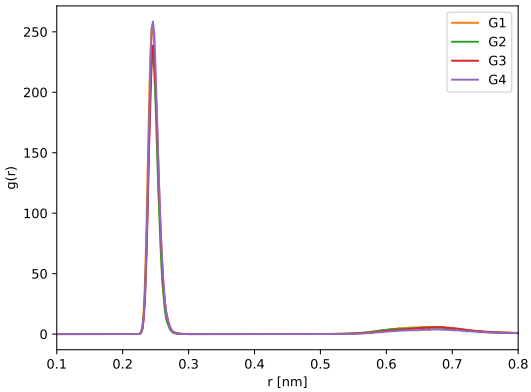


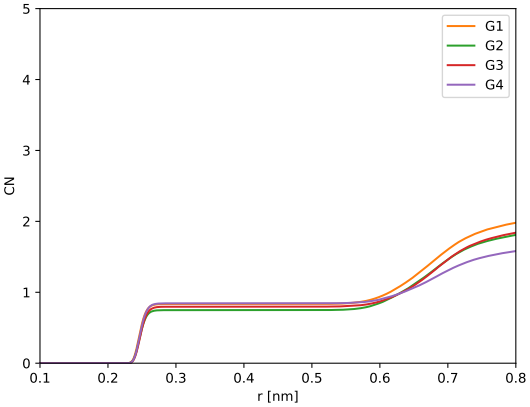
I^- – Li^+ 50mM 20,000 ppm



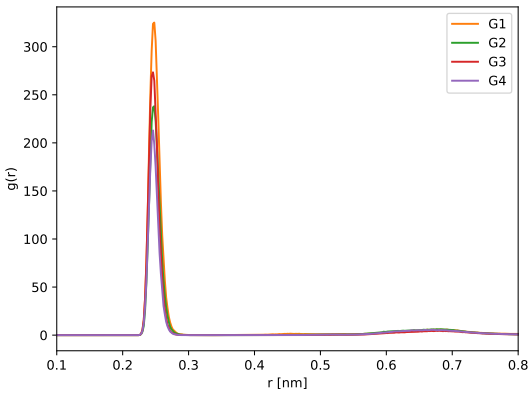


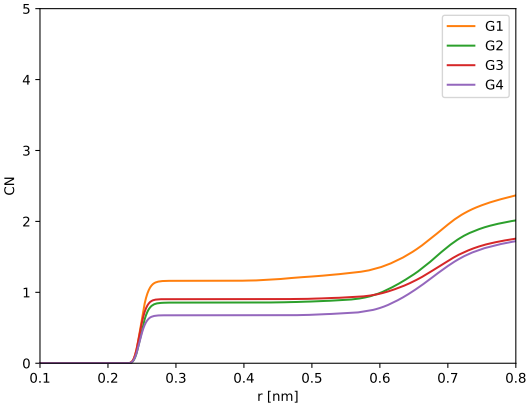
I^- – Li^+ 100mM neat



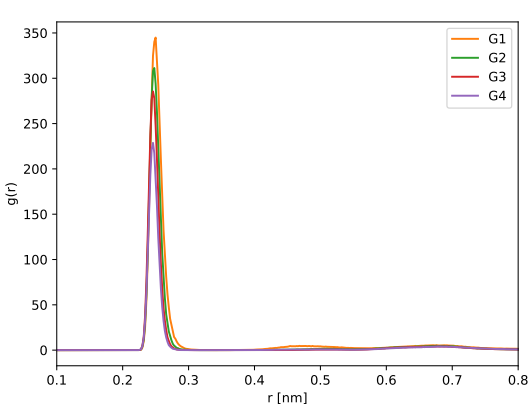


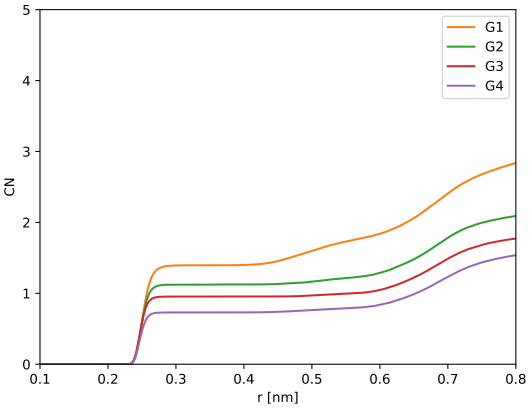
I^- – Li^+ 100mM 1,000 ppm



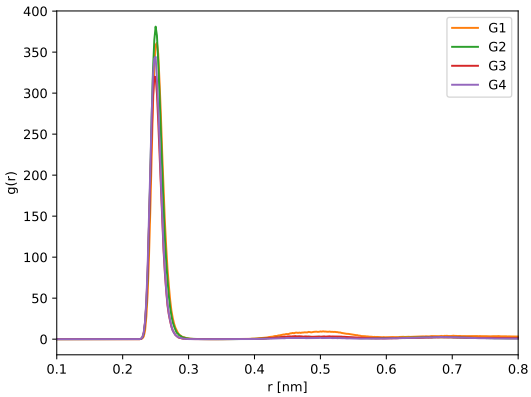


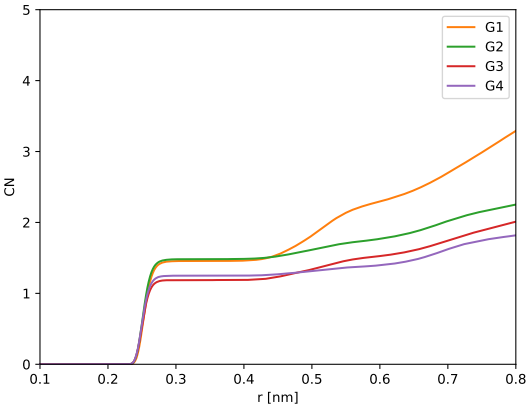
I^- – Li^+ 100mM 5,000 ppm



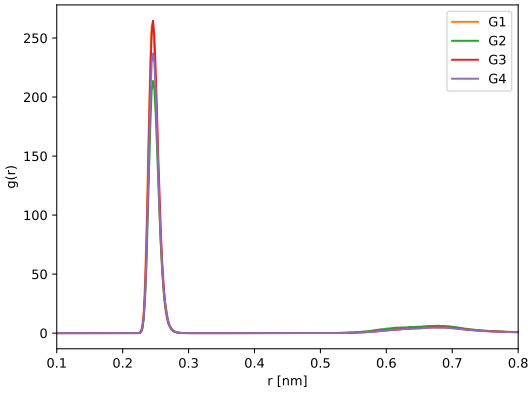


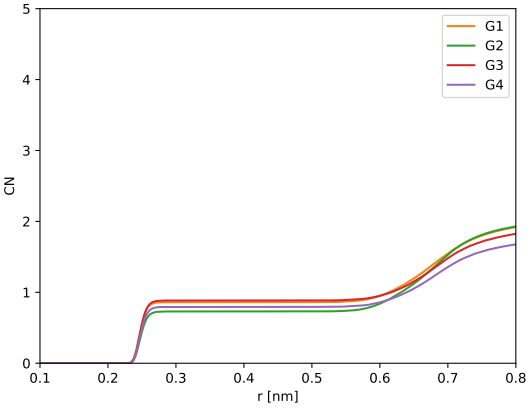
I^- – Li^+ 100mM 20,000 ppm



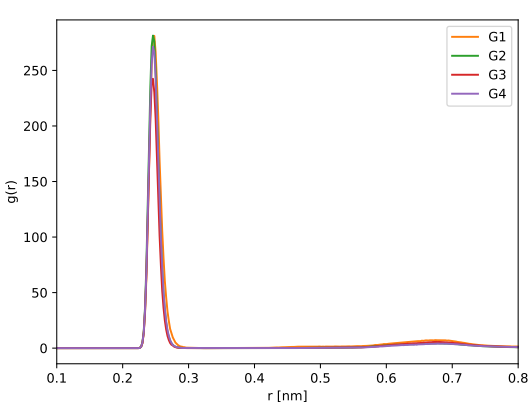


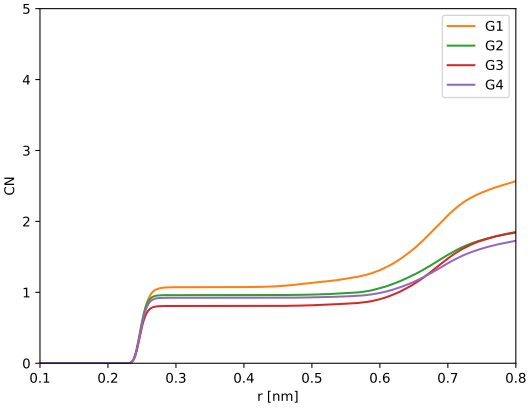
I^- – Li^+ 200mM neat



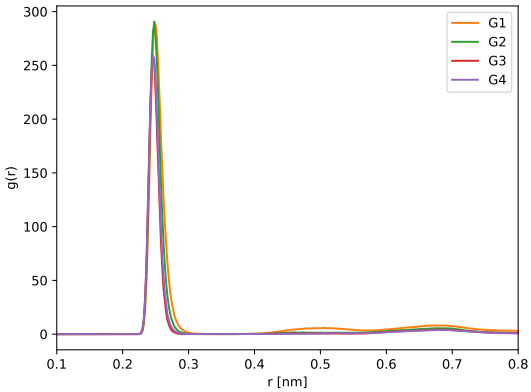


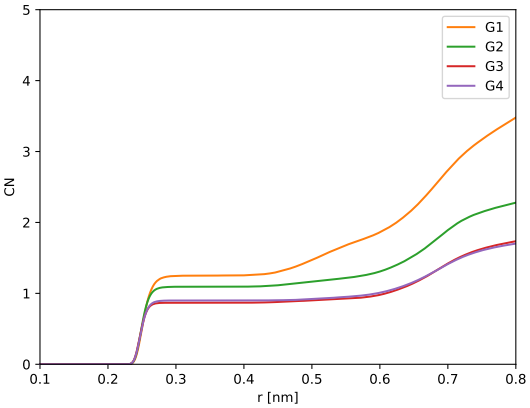
I^- – Li^+ 200mM 1,000 ppm



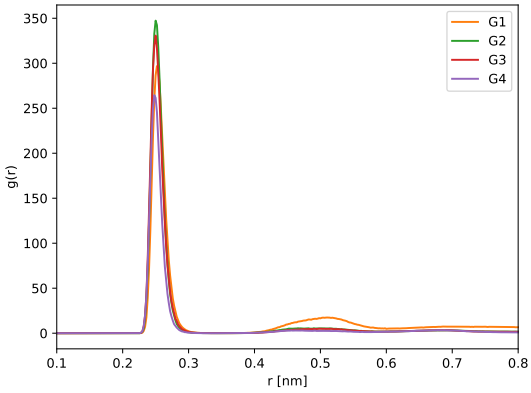


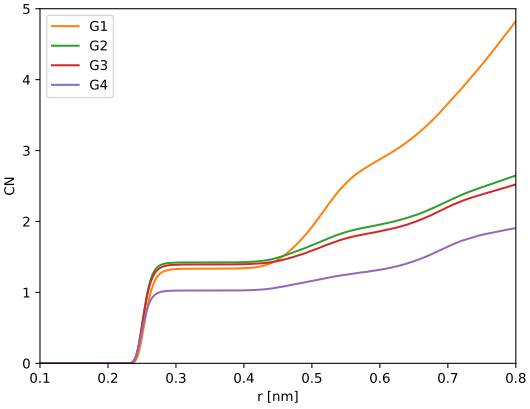
I^- – Li^+ 200mM 5,000 ppm



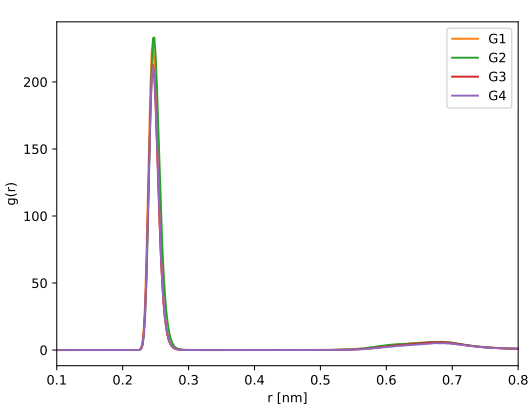


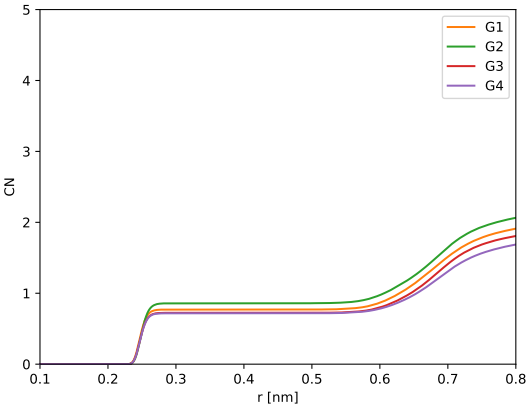
I^- – Li^+ 200mM 20,000 ppm



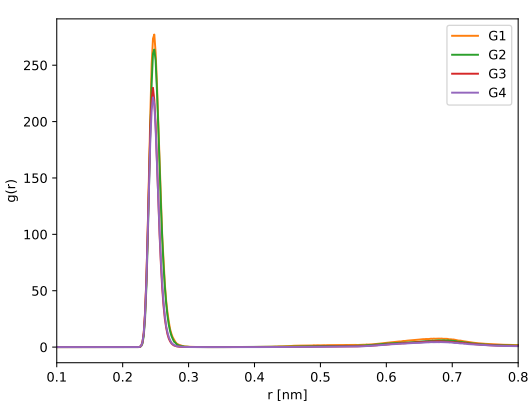


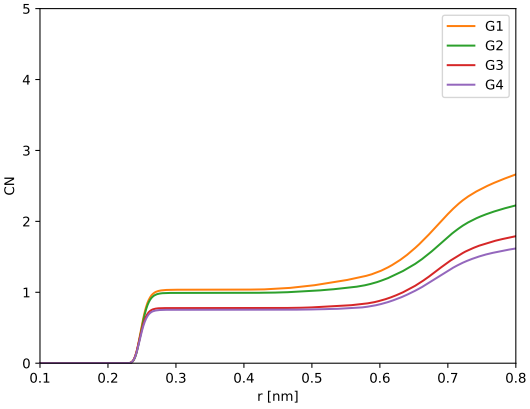
I^- – Li^+ 300mM neat



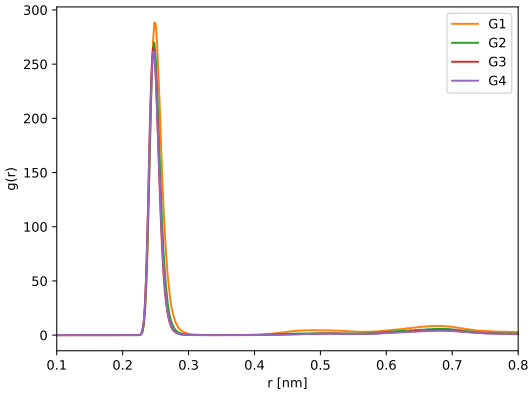


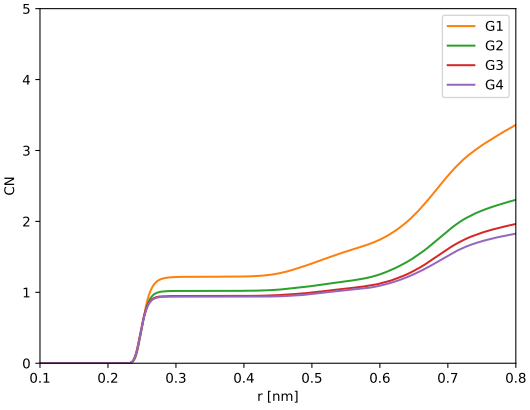
I^- – Li^+ 300mM 1,000 ppm



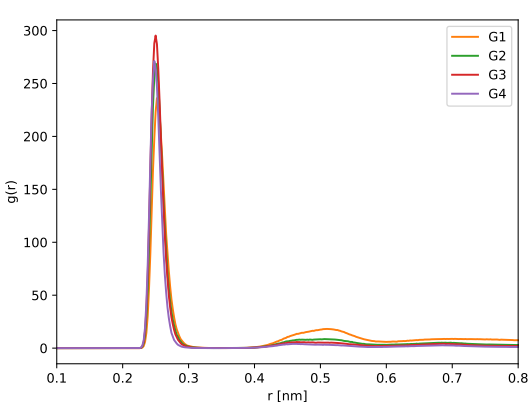


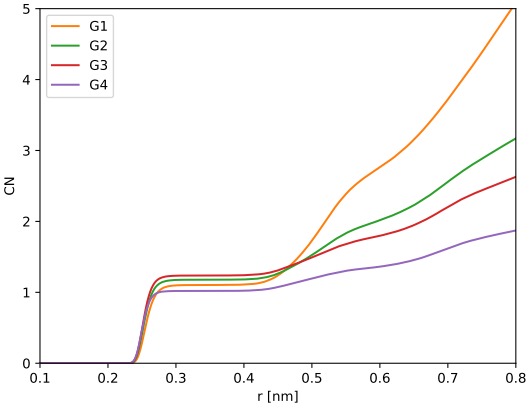
I^- – Li^+ 300mM 5,000 ppm



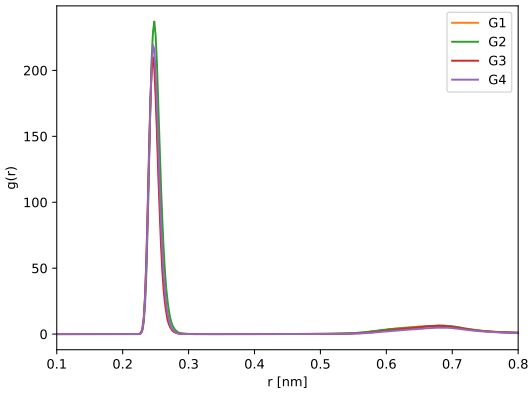


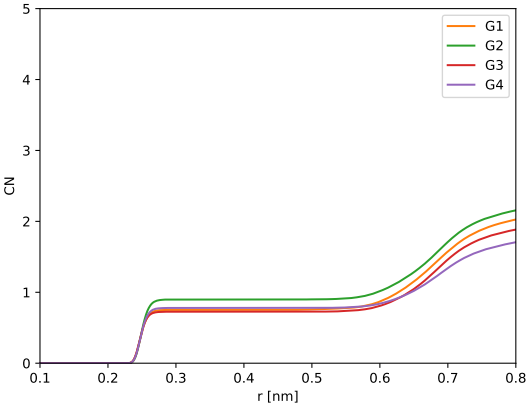
I^- – Li^+ 300mM 20,000 ppm



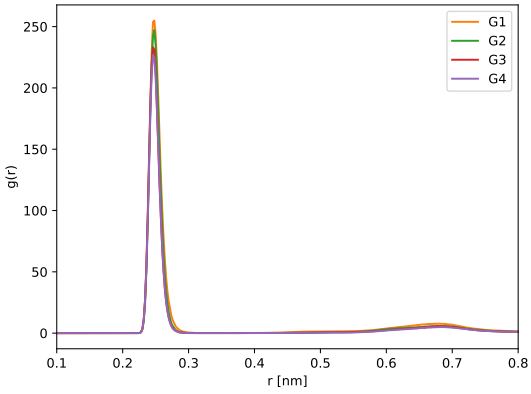


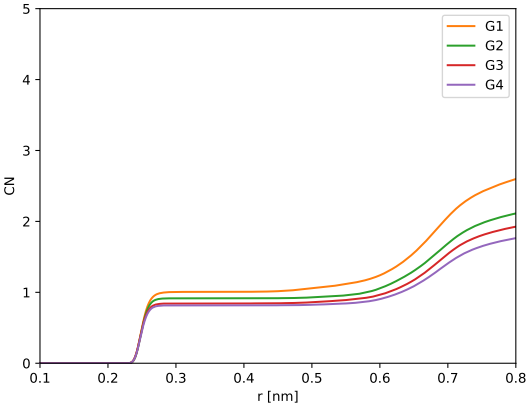
I^- – Li^+ 400mM neat



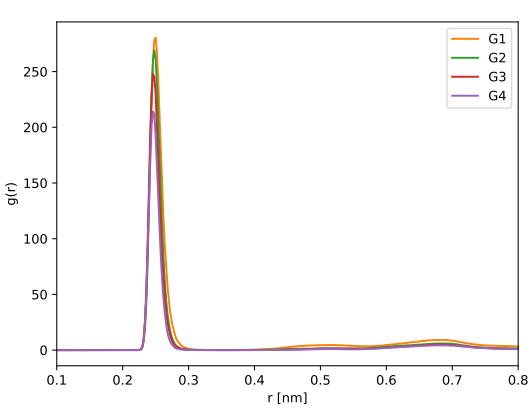


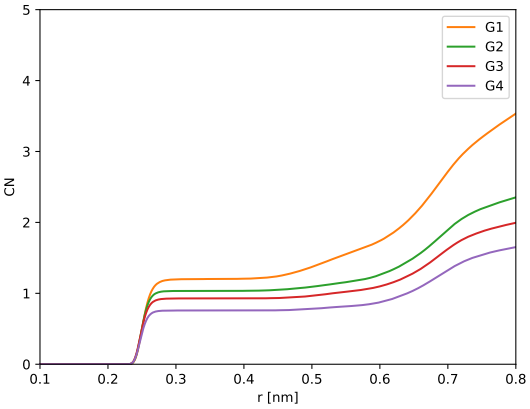
I^- – Li^+ 400mM 1,000 ppm



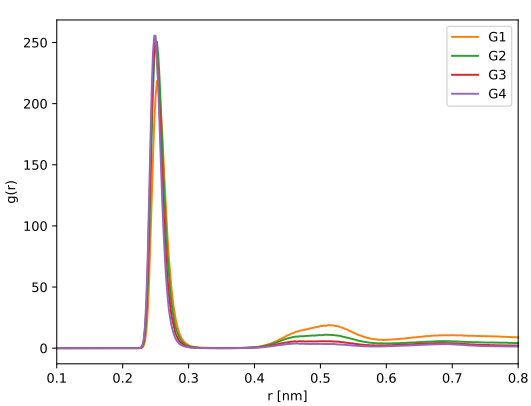


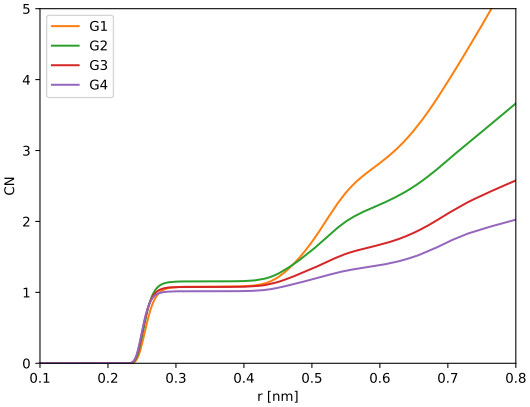
I^- – Li^+ 400mM 5,000 ppm





I^- – Li^+ 400mM 20,000 ppm





2.7 $Li^+ - I^-$

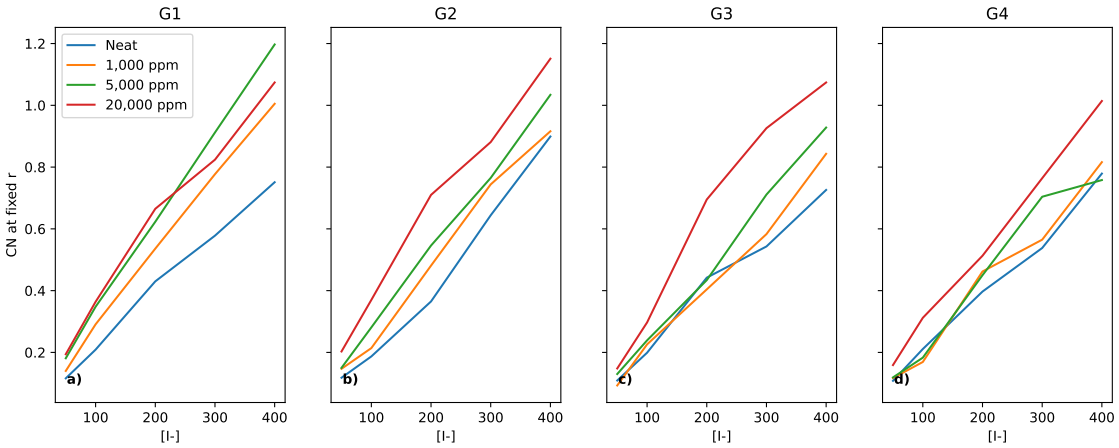


Figure 13: Coordination number of Li^+ to I^- at a fixed distance of 3 Å, for the four different glymes (G1 = yellow, G2 = green, G3 = red, G4 = purple) studied here, across the four different water concentrations (with a): neat, b): 1,000, c): 5,000, d): 20,000 ppm of water).

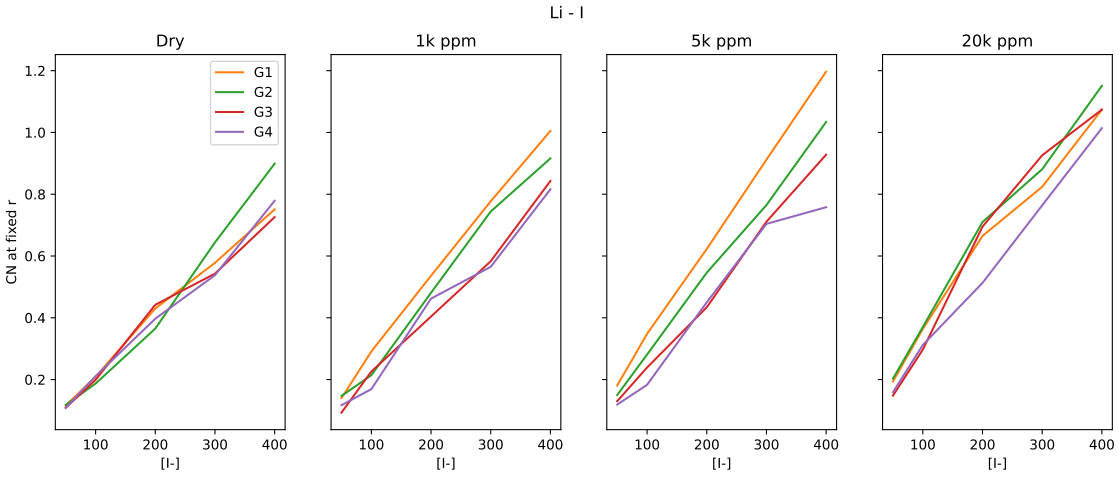
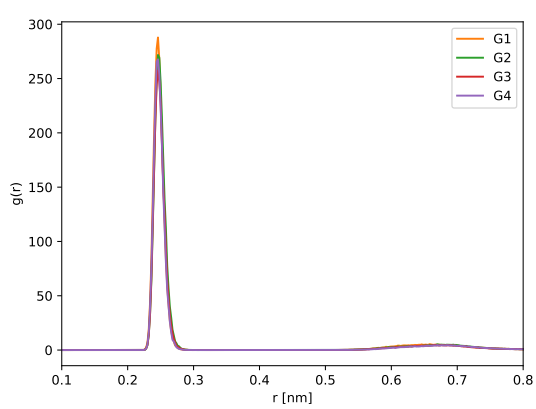
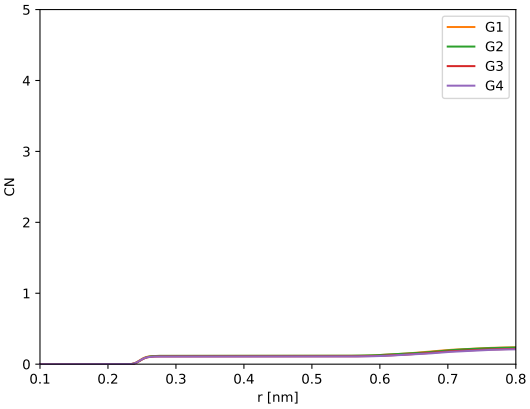


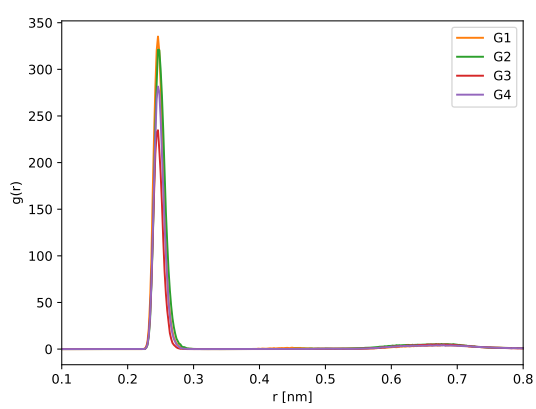
Figure 14: Coordination number of Li^+ to I^- at a fixed distance of 3 Å, for the four different glymes (G1 = yellow, G2 = green, G3 = red, G4 = purple) studied here, across the four different water concentrations (with a): neat, b): 1,000, c): 5,000, d): 20,000 ppm of water).

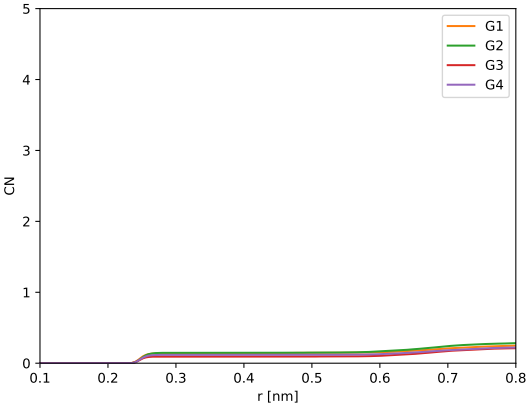
Li^+ – I^- 50mM neat



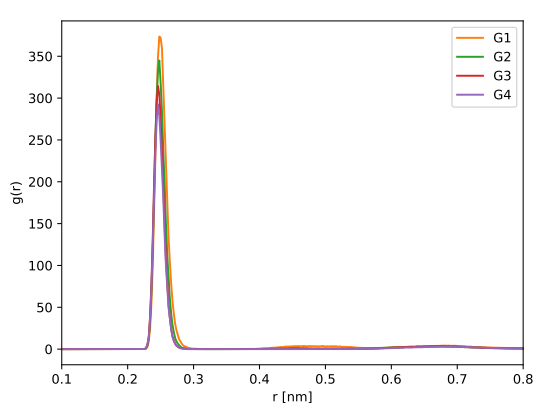


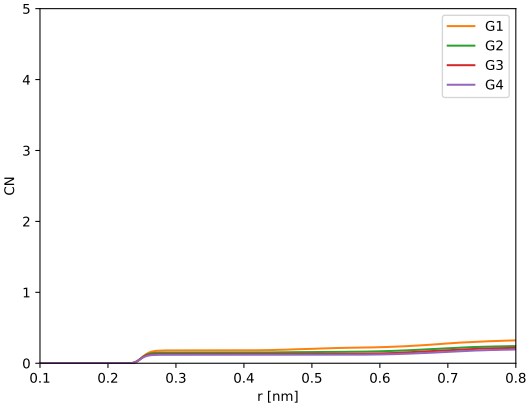
Li^+ – I^- 50mM 1,000 ppm



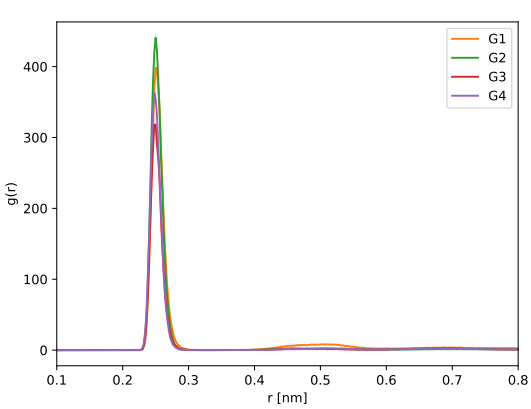


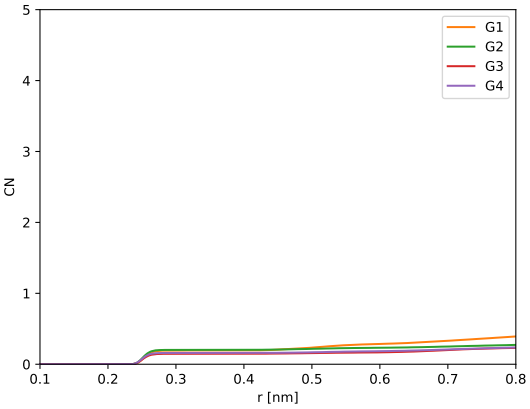
Li^+ – I^- 50mM 5,000 ppm



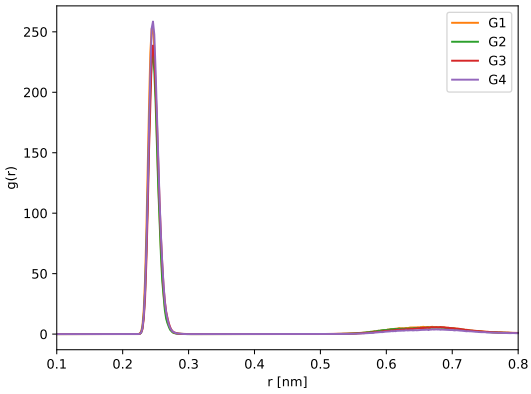


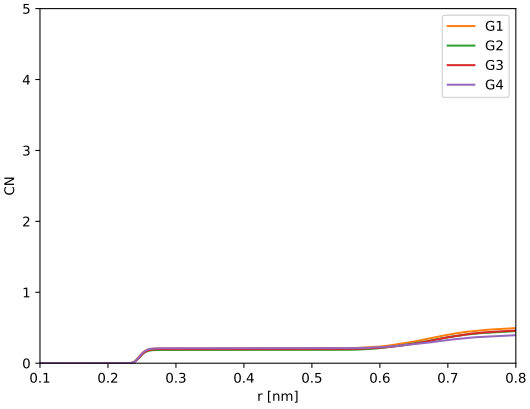
Li^+ – I^- 50mM 20,000 ppm



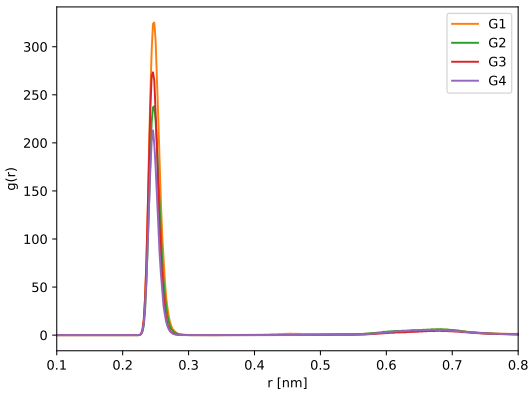


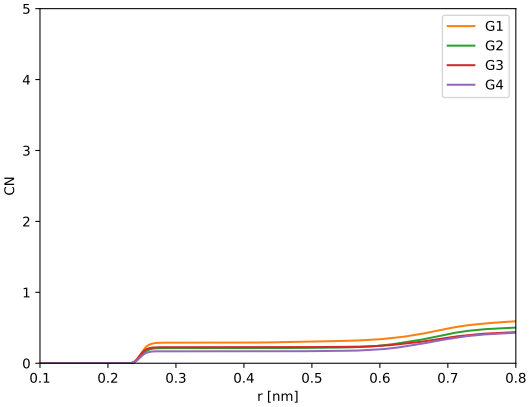
Li^+ – I^- 100mM neat



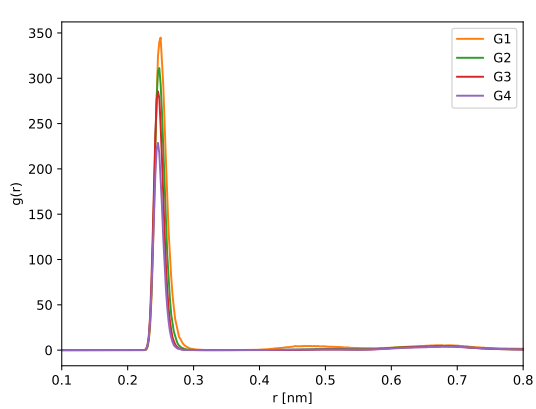


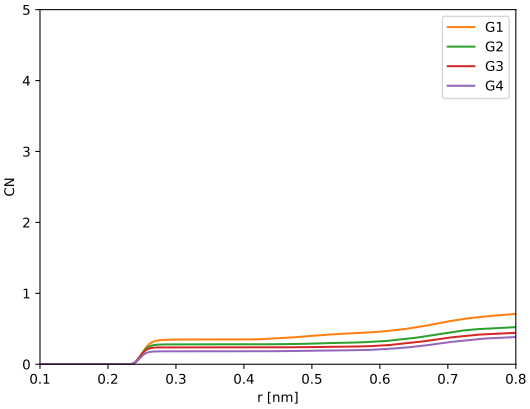
Li^+ – I^- 100mM 1,000 ppm



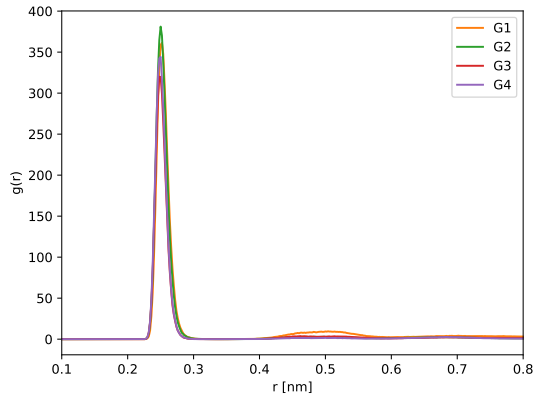


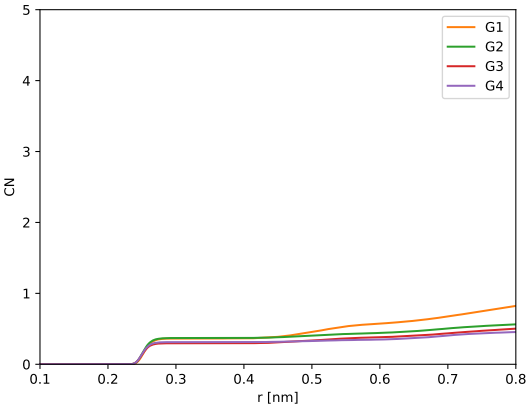
Li^+ – I^- 100mM 5,000 ppm



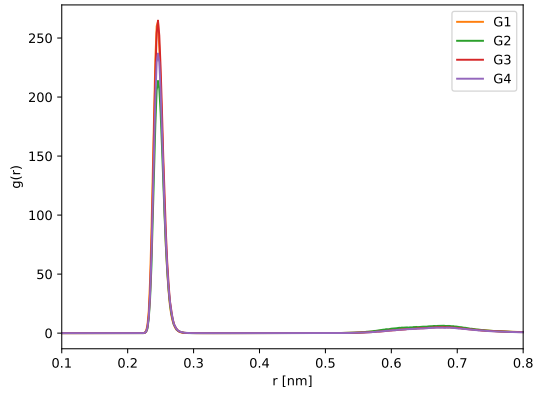


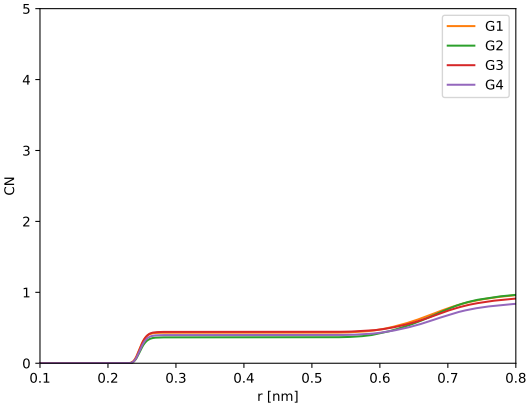
Li^+ – I^- 100mM 20,000 ppm



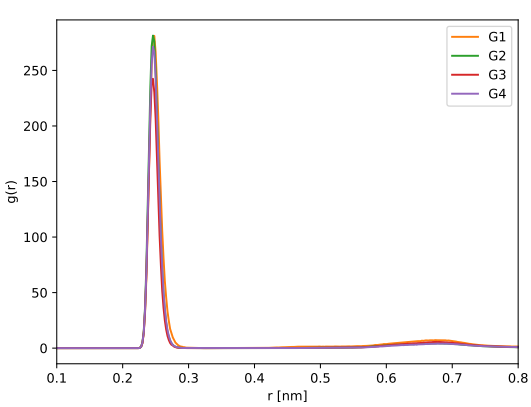


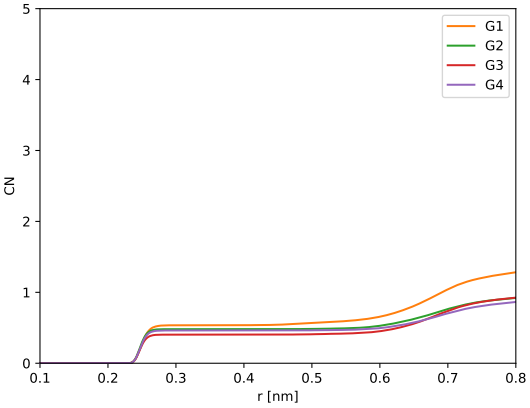
Li^+ – I^- 200mM neat



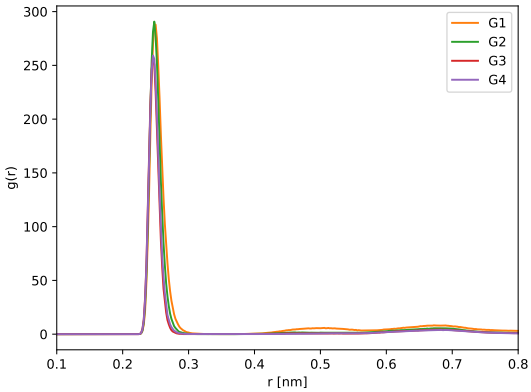


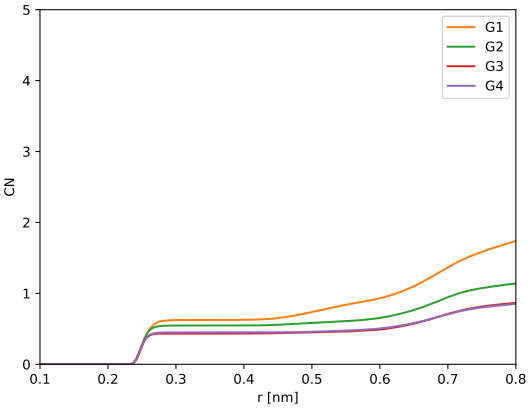
Li^+ – I^- 200mM 1,000 ppm



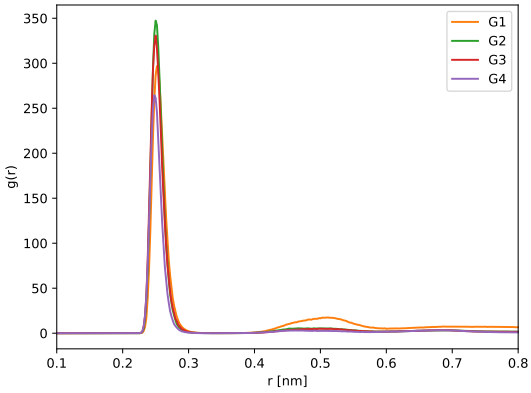


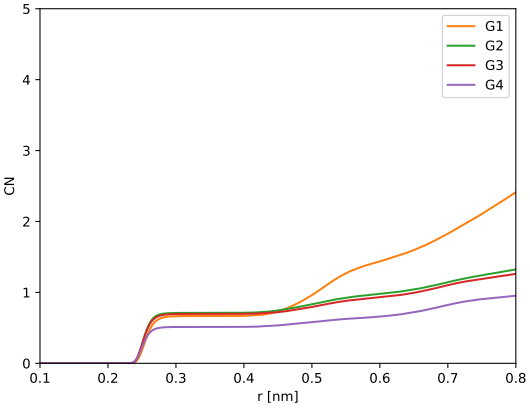
Li^+ – I^- 200mM 5,000 ppm



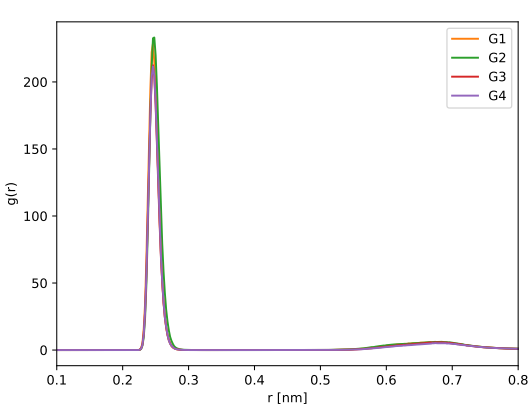


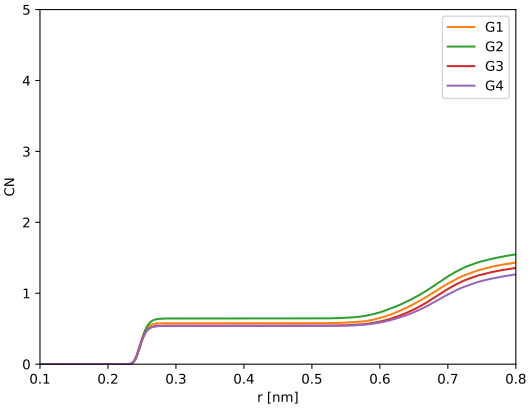
Li^+ – I^- 200mM 20,000 ppm



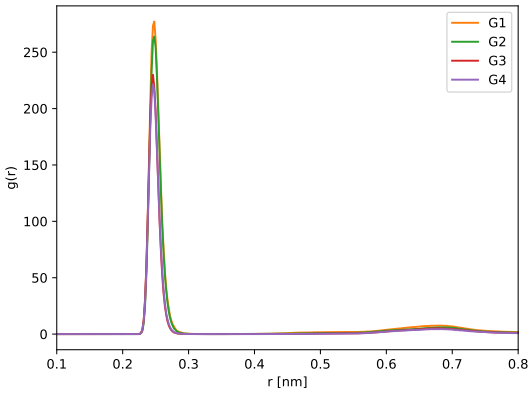


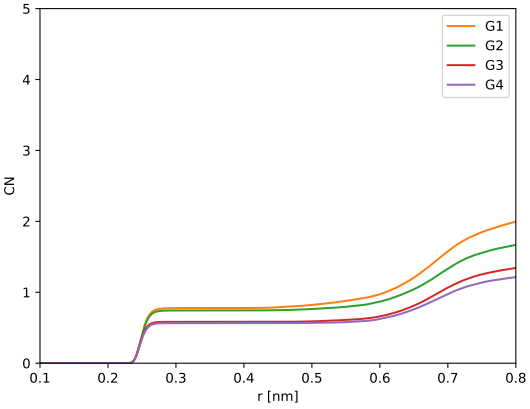
$Li^+ – I^-$ 300mM neat



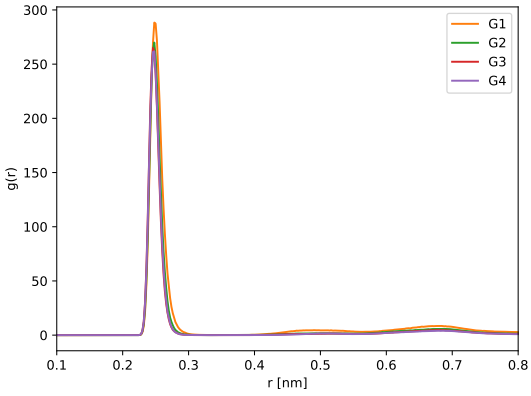


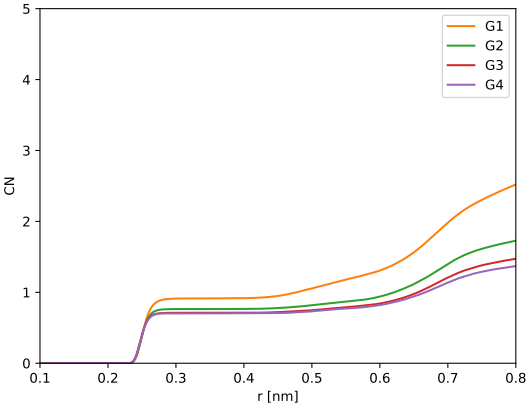
$Li^+ – I^-$ 300mM 1,000 ppm



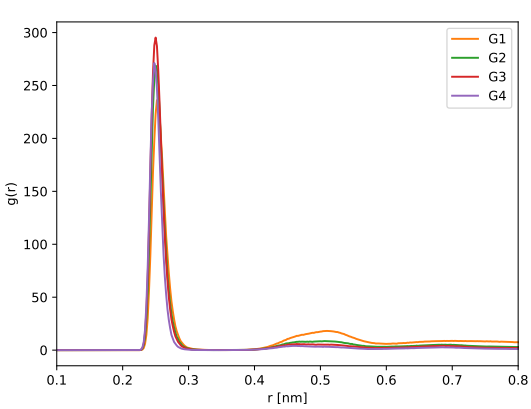


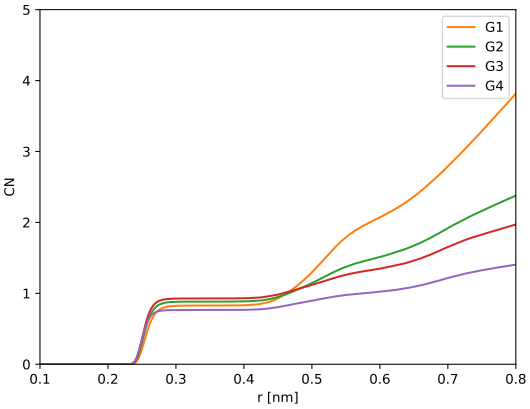
$Li^+ – I^-$ 300mM 5,000 ppm



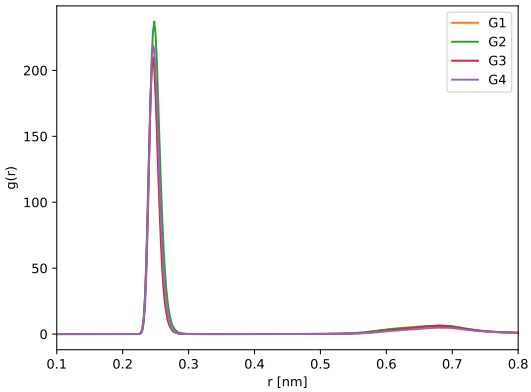


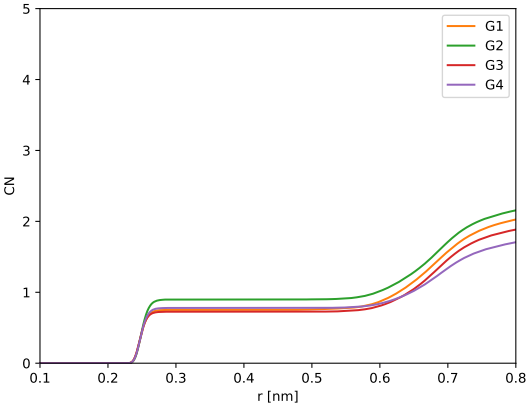
Li^+ – I^- 300mM 20,000 ppm



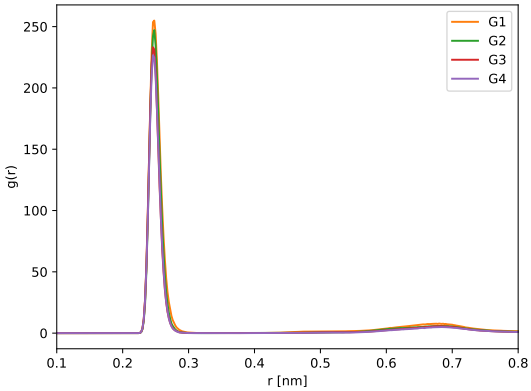


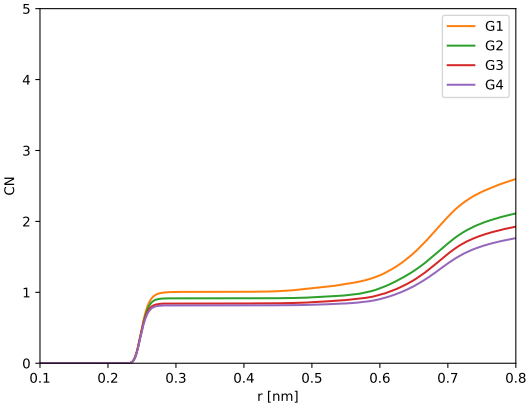
Li^+ – I^- 400mM neat



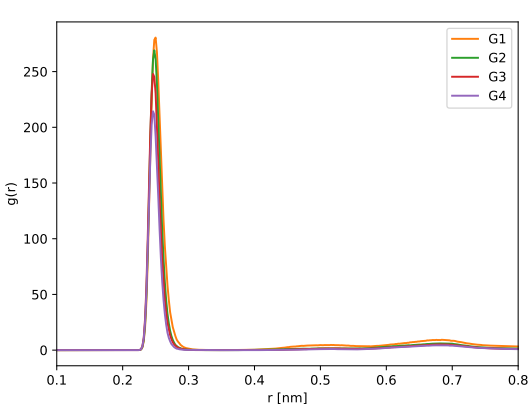


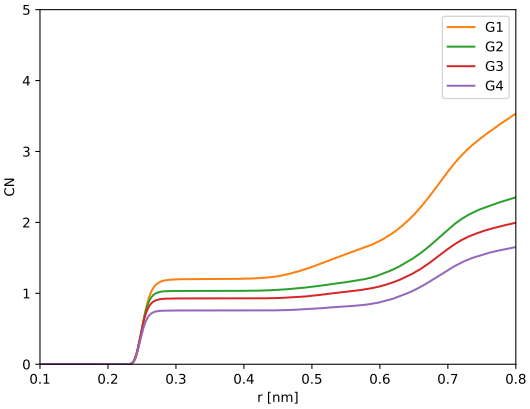
Li^+ – I^- 400mM 1,000 ppm



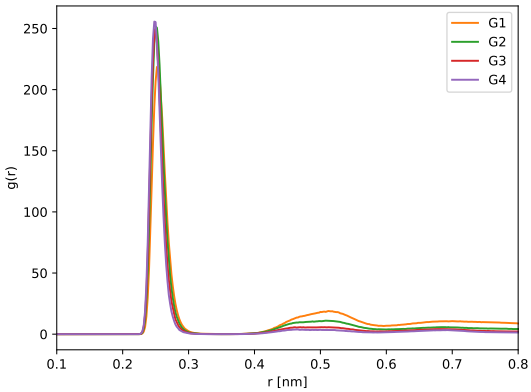


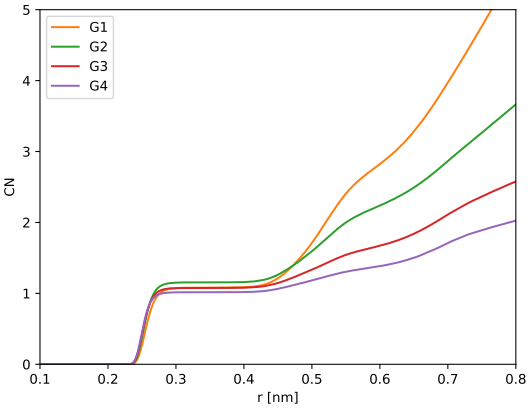
$Li^+ – I^-$ 400mM 5,000 ppm





$Li^+ – I^-$ 400mM 20,000 ppm





2.8 $Li^+ - Li^+$

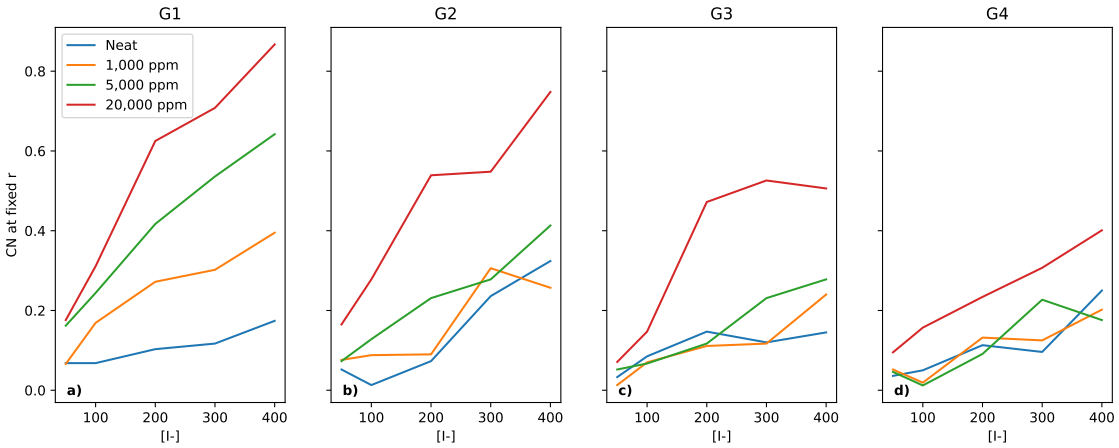


Figure 15: Coordination number of Li^+ to Li^+ at a fixed distance of 5.5 Å, for the four different glymes (G1 = yellow, G2 = green, G3 = red, G4 = purple) studied here, across the four different water concentrations (with a): neat, b): 1,000, c): 5,000, d): 20,000 ppm of water).

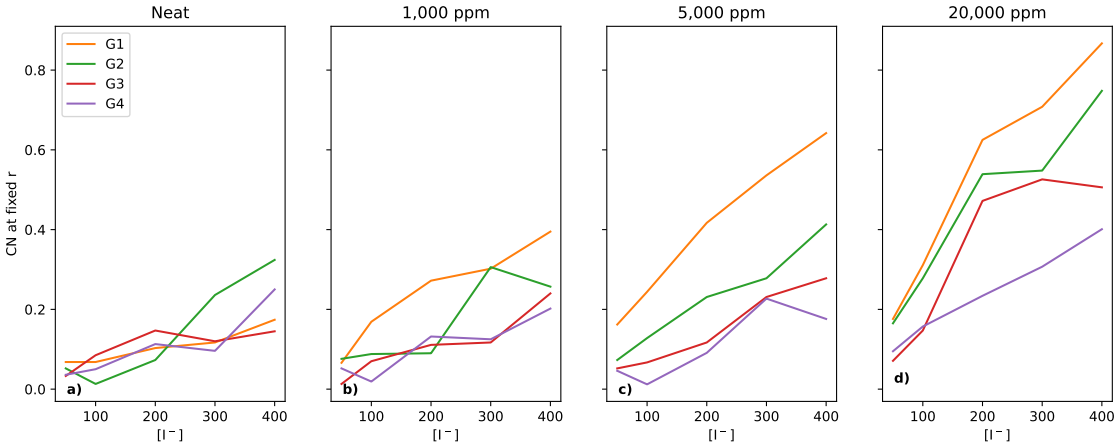
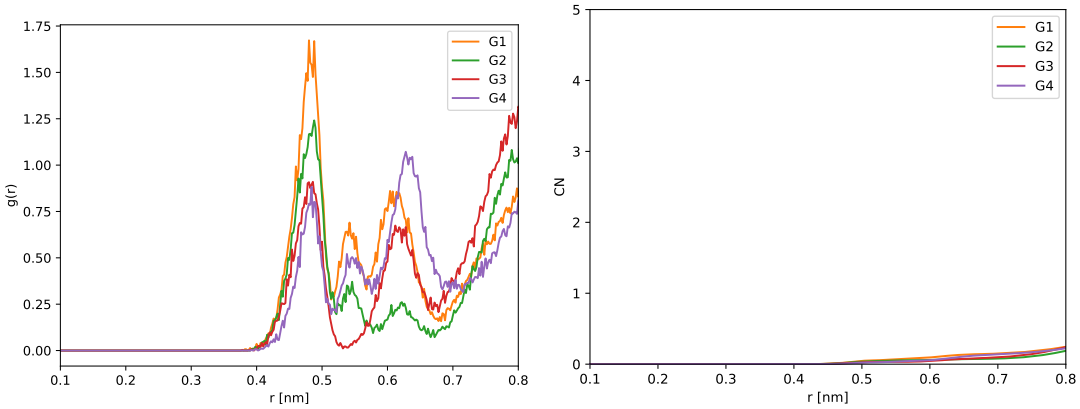
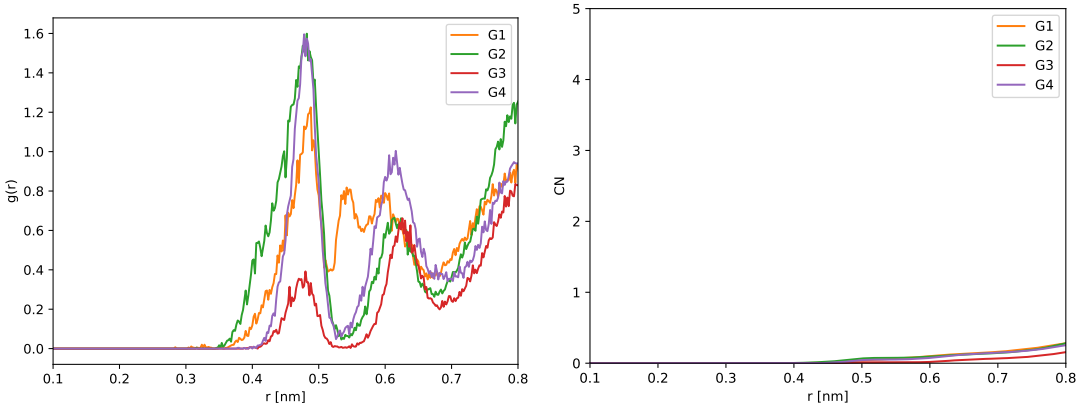


Figure 16: Coordination number of Li^+ to Li^+ at a fixed distance of 5.5 Å, for the four different glymes (G1 = yellow, G2 = green, G3 = red, G4 = purple) studied here, across the four different water concentrations (with a): neat, b): 1,000, c): 5,000, d): 20,000 ppm of water).

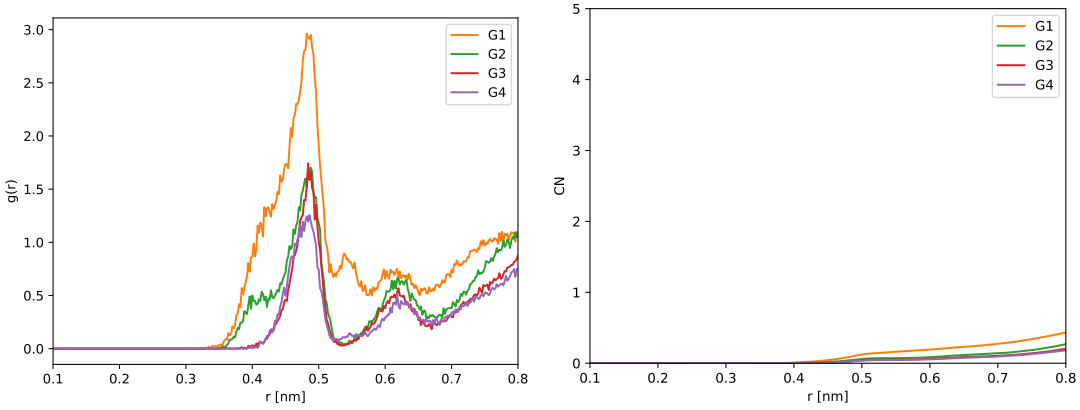
Li^+ – Li^+ 50mM neat



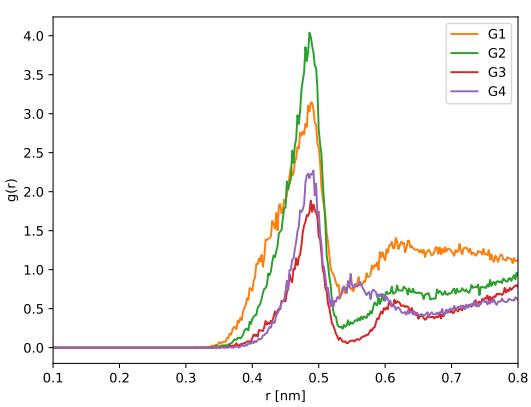
Li^+ – Li^+ 50mM 1,000 ppm

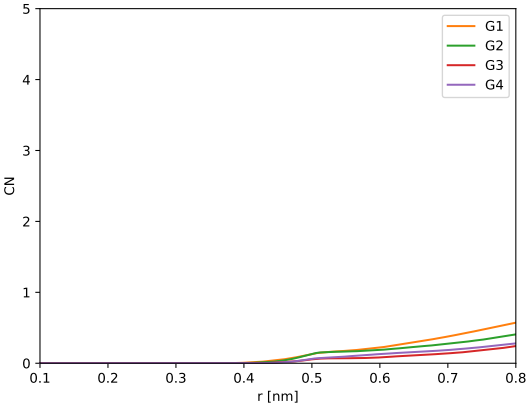


Li^+ – Li^+ 50mM 5,000 ppm

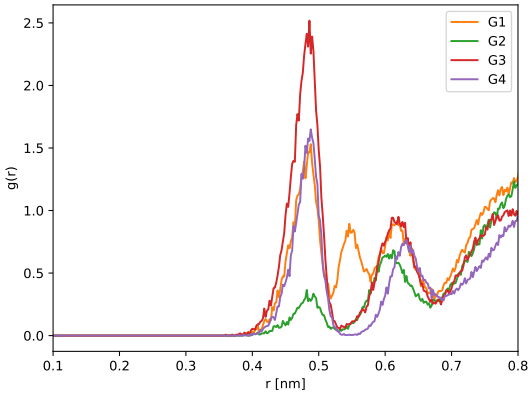


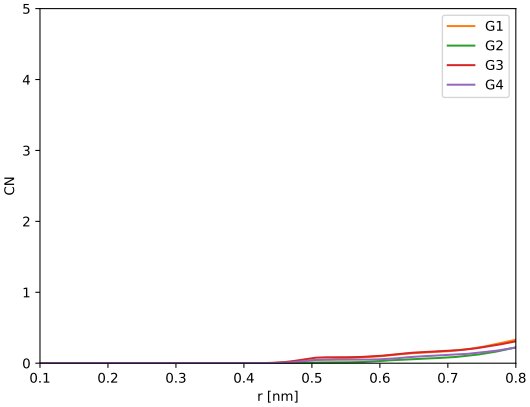
Li^+ – Li^+ 50mM 20,000 ppm



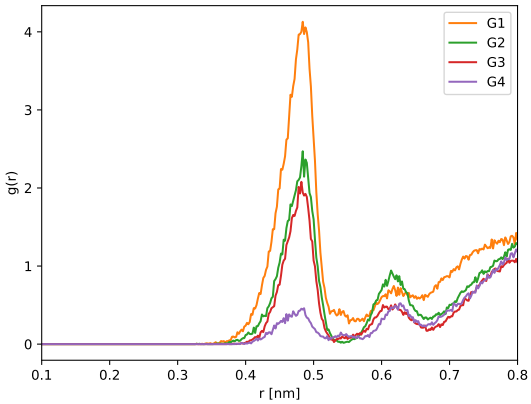


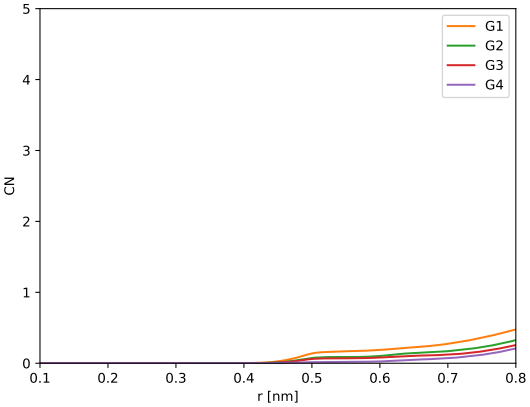
Li^+ – Li^+ 100mM neat



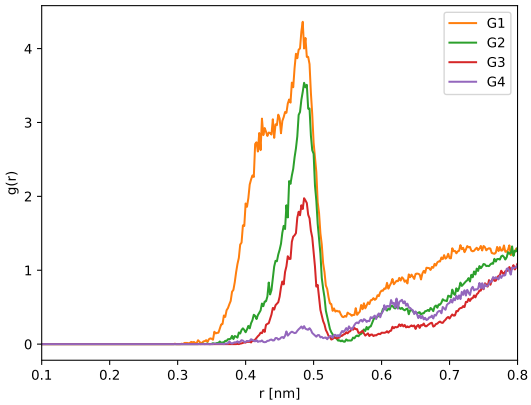


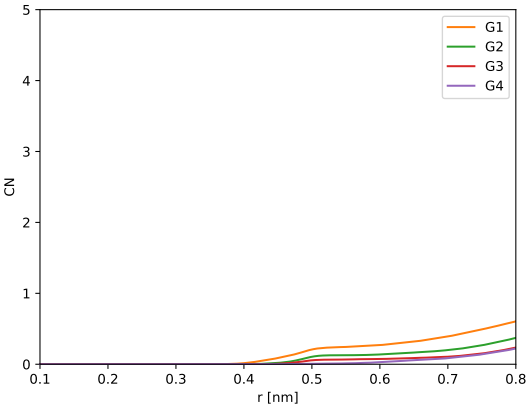
Li^+ – Li^+ 100mM 1,000 ppm



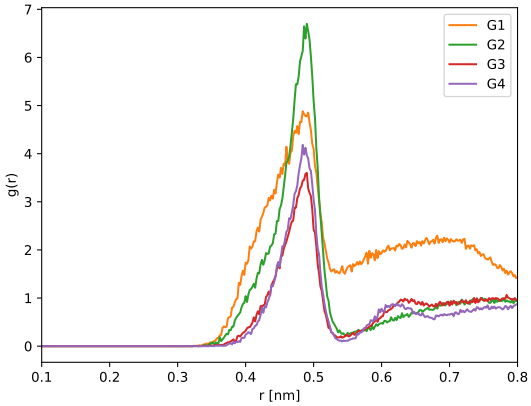


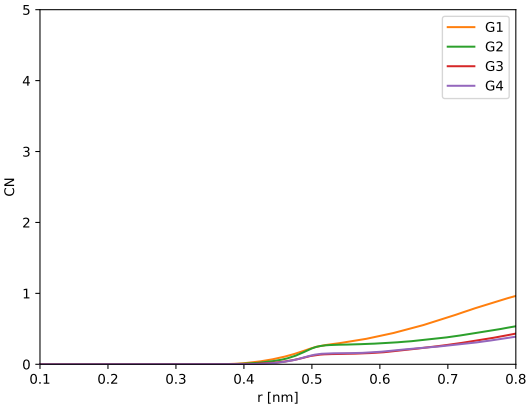
Li^+ – Li^+ 100mM 5,000 ppm



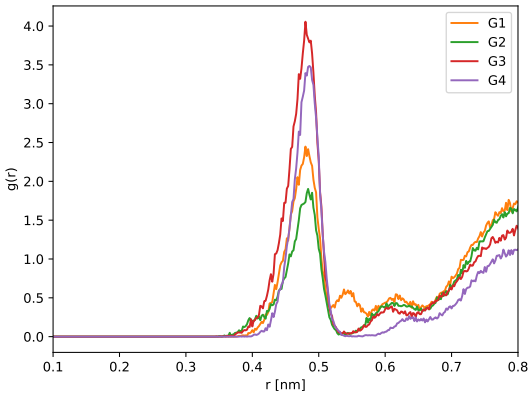


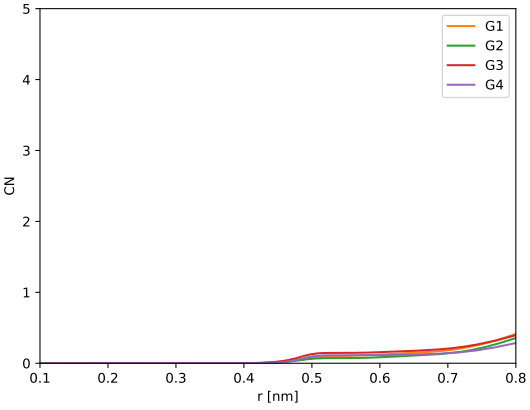
Li^+ – Li^+ 100mM 20,000 ppm



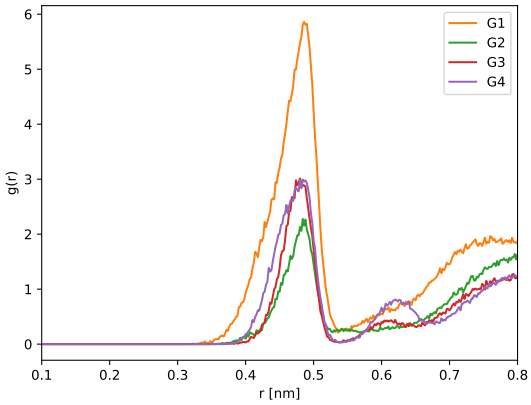


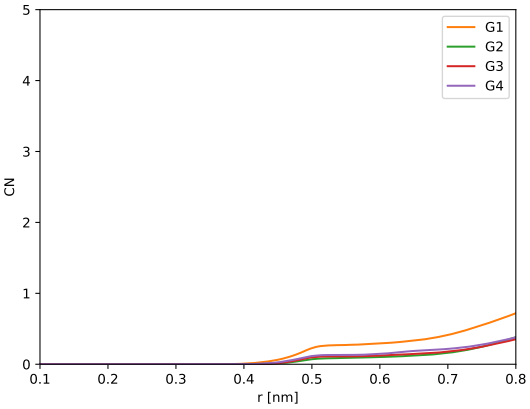
Li^+ – Li^+ 200mM neat



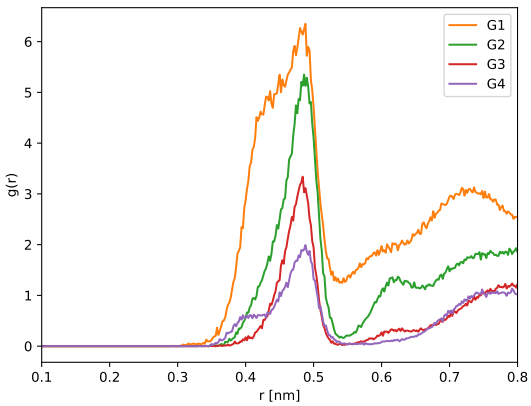


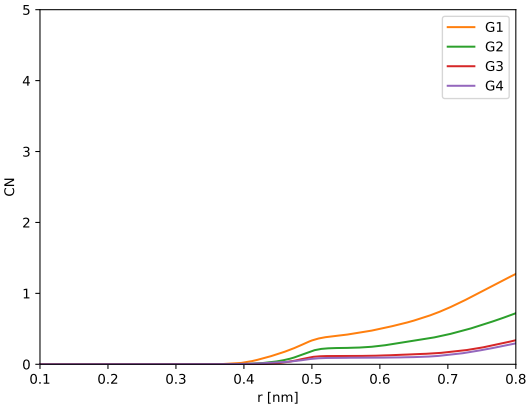
Li^+ – Li^+ 200mM 1,000 ppm



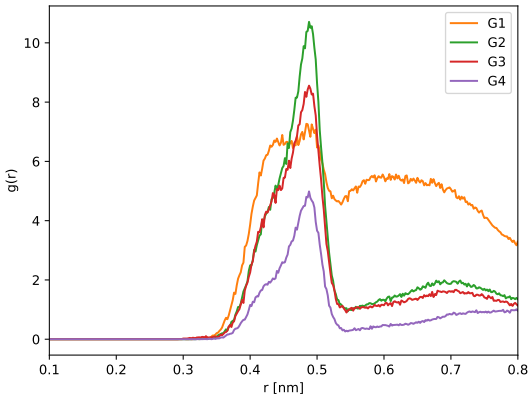


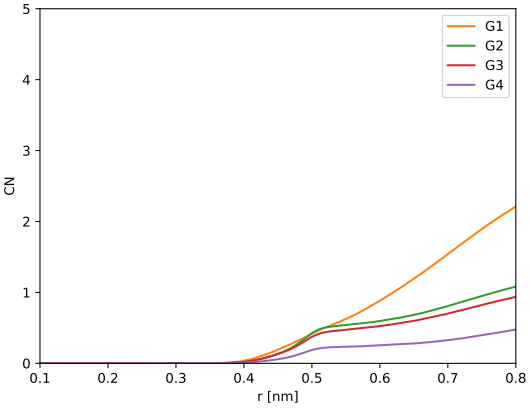
Li^+ – Li^+ 200mM 5,000 ppm



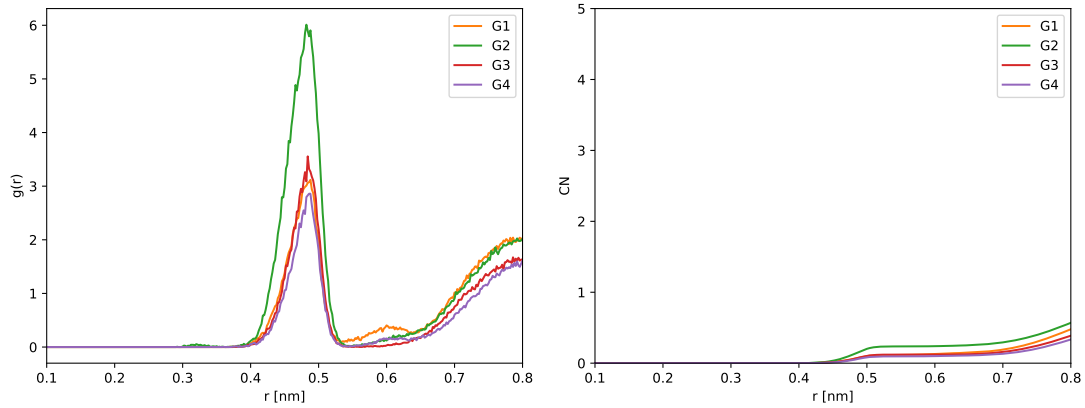


Li^+ – Li^+ 200mM 20,000 ppm

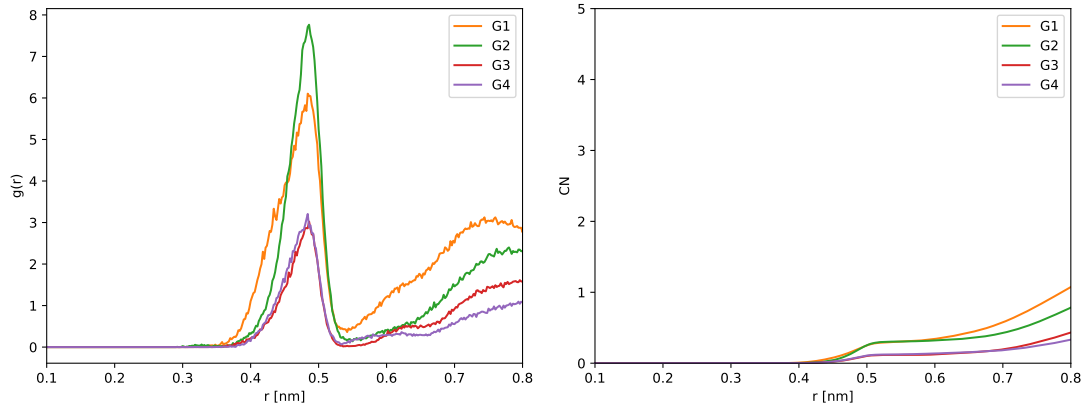




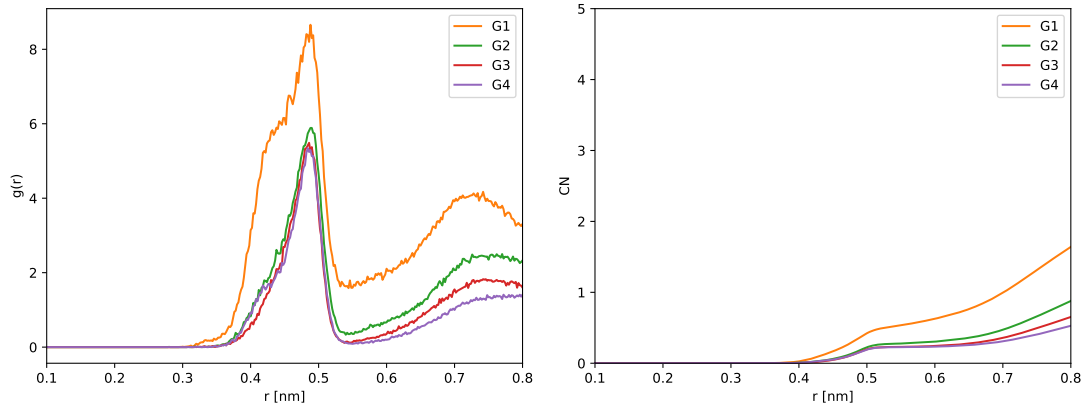
Li^+ – Li^+ 300mM neat



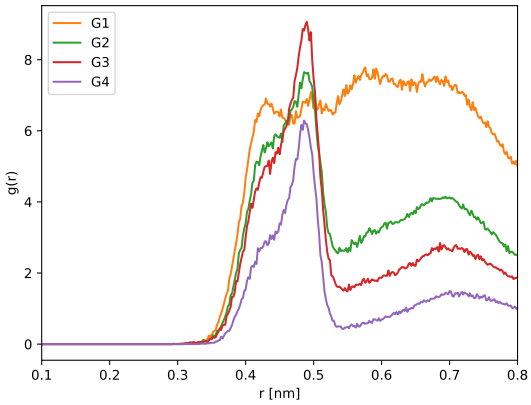
Li^+ – Li^+ 300mM 1,000 ppm

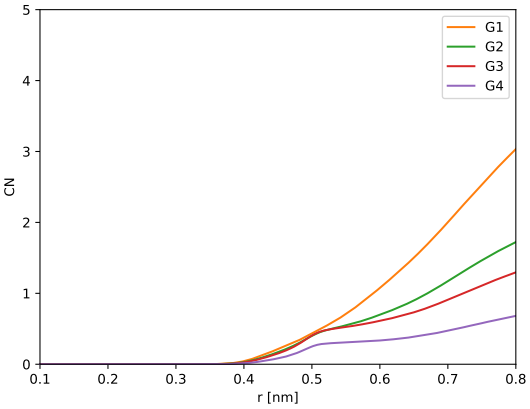


Li^+ – Li^+ 300mM 5,000 ppm

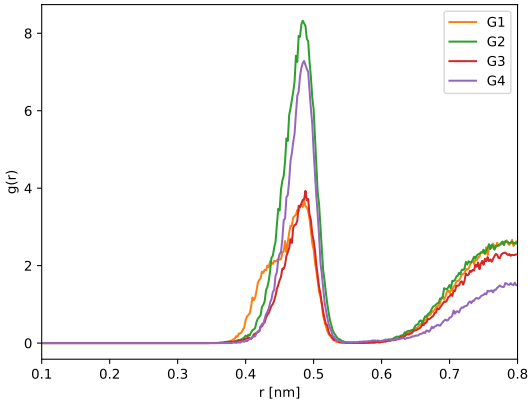


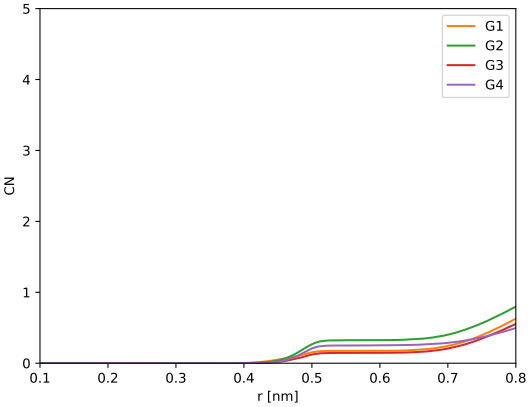
Li^+ – Li^+ 300mM 20,000 ppm



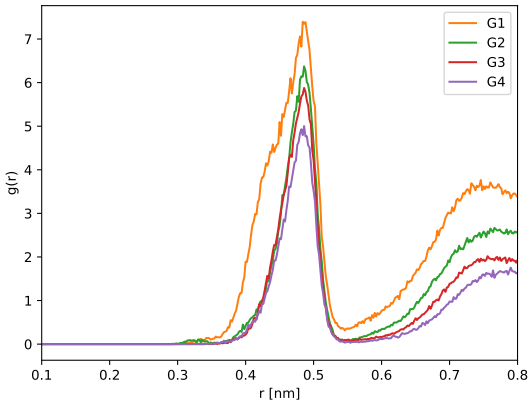


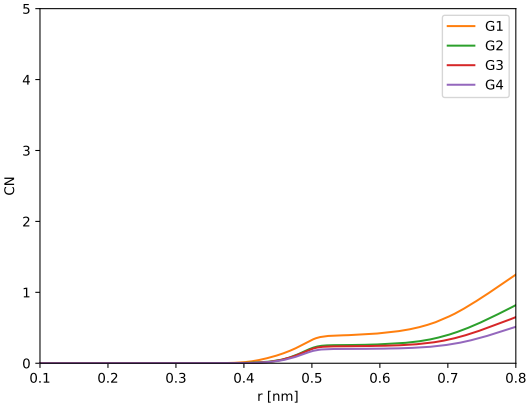
Li^+ – Li^+ 400mM neat



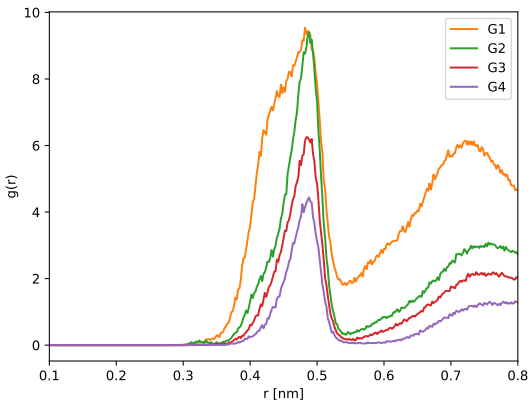


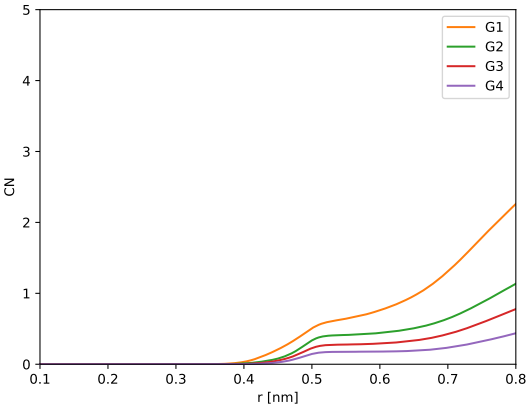
Li^+ – Li^+ 400mM 1,000 ppm



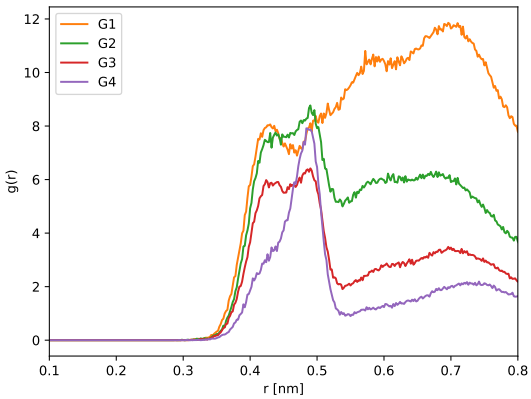


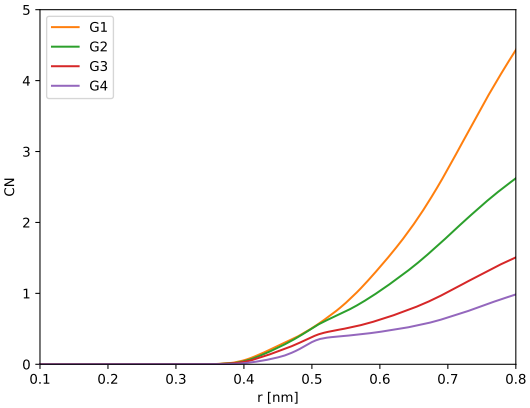
Li^+ – Li^+ 400mM 5,000 ppm





Li^+ – Li^+ 400mM 20,000 ppm





2.9 Li^+ – TFSI

Note that here the analysis uses the full TFSI molecule, hence the larger CN values.

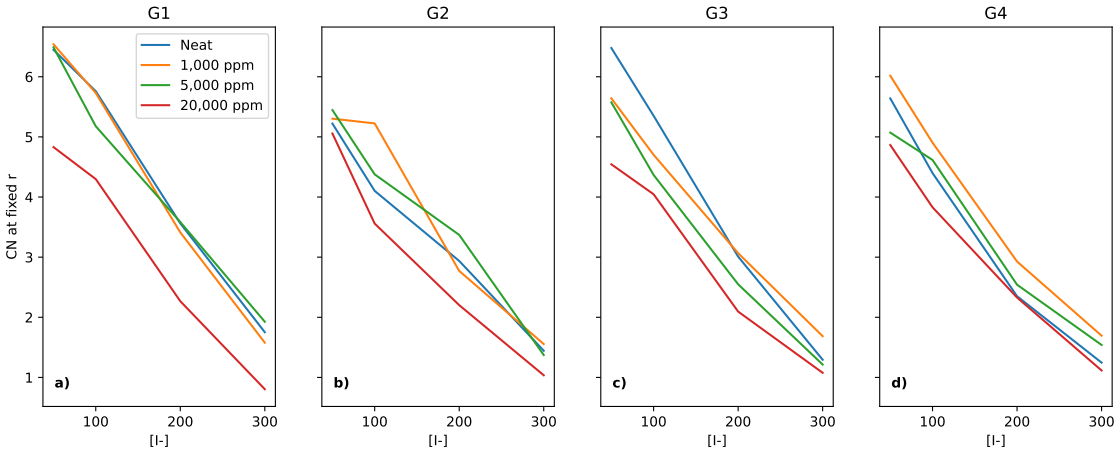


Figure 17: Coordination number of Li^+ to TFSI (the full molecule) at a fixed distance of 5 Å, for the four different glymes (G1 = yellow, G2 = green, G3 = red, G4 = purple) studied here, across the four different water concentrations (with a): neat, b): 1,000, c): 5,000, d): 20,000 ppm of water).

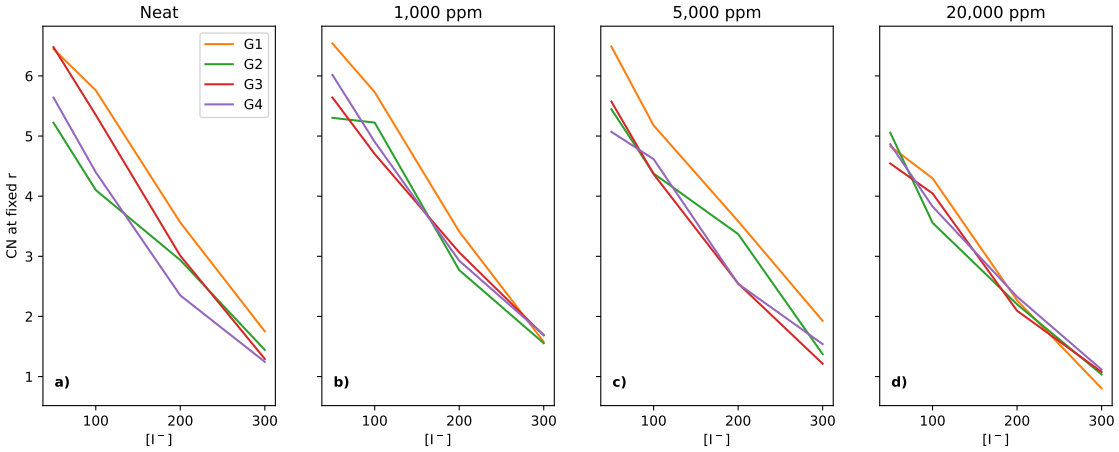
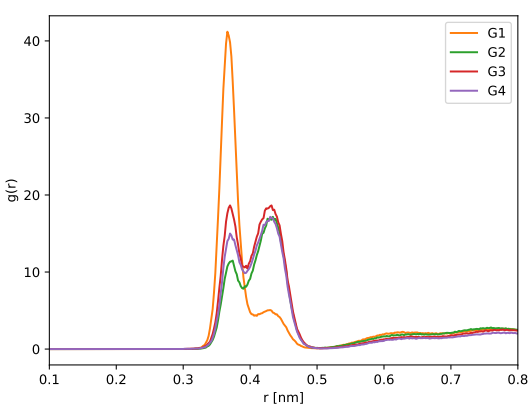
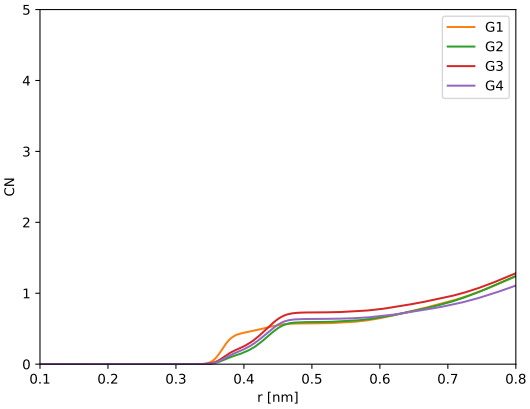


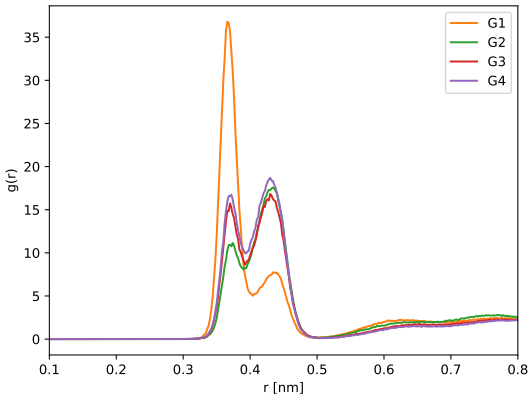
Figure 18: Coordination number of Li^+ to TFSI (the full molecule) at a fixed distance of 5 Å, for the four different glymes (G1 = yellow, G2 = green, G3 = red, G4 = purple) studied here, across the four different water concentrations (with a): neat, b): 1,000, c): 5,000, d): 20,000 ppm of water).

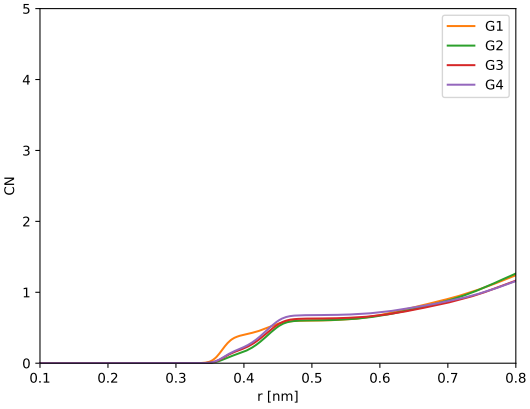
Li^+ – TFSI 50mM neat



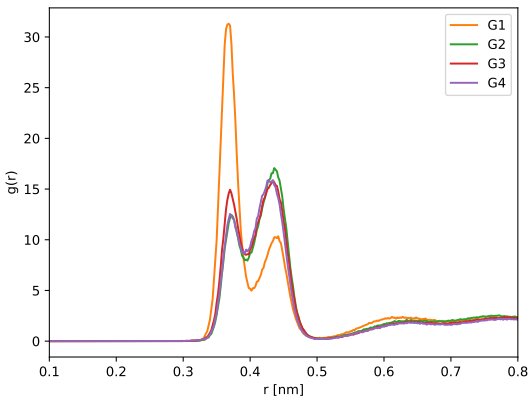


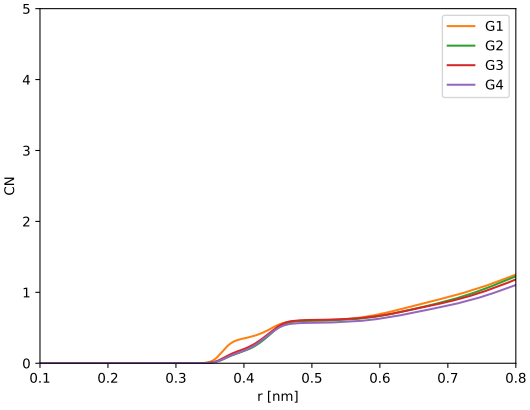
Li^+ – TFSI 50mM 1,000 ppm



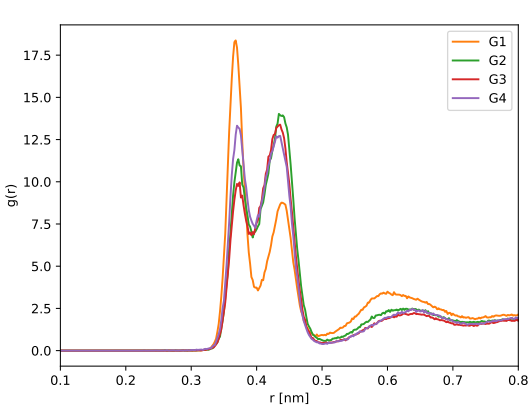


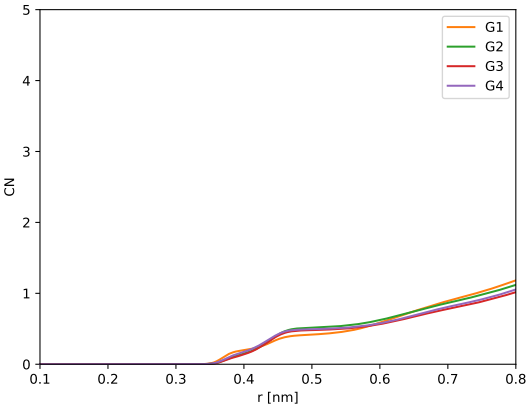
Li^+ – TFSI 50mM 5,000 ppm



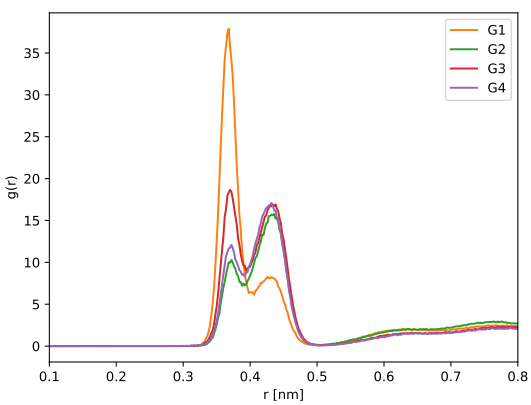


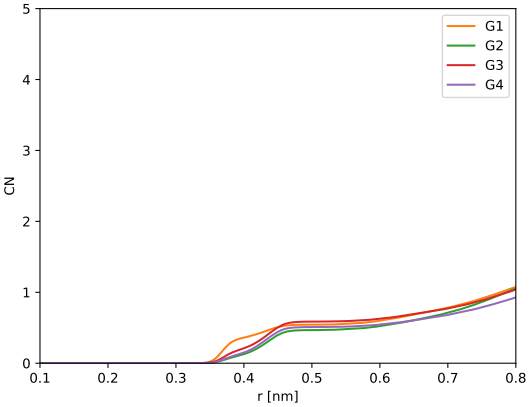
Li^+ – TFSI 50mM 20,000 ppm



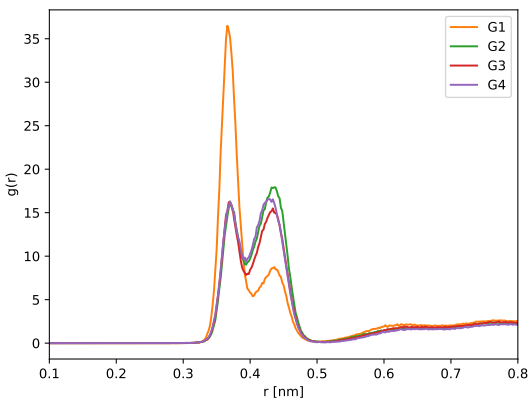


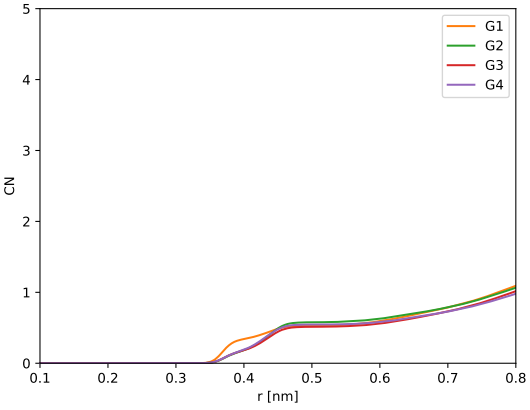
Li^+ – TFSI 100mM neat



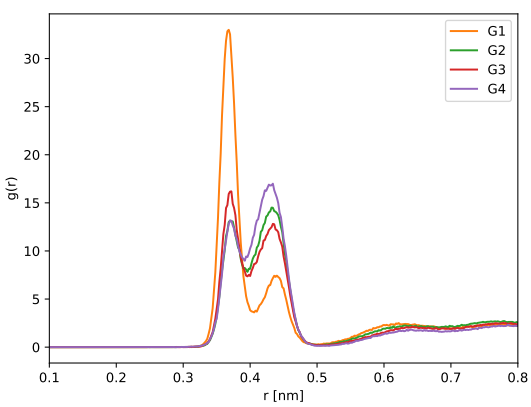


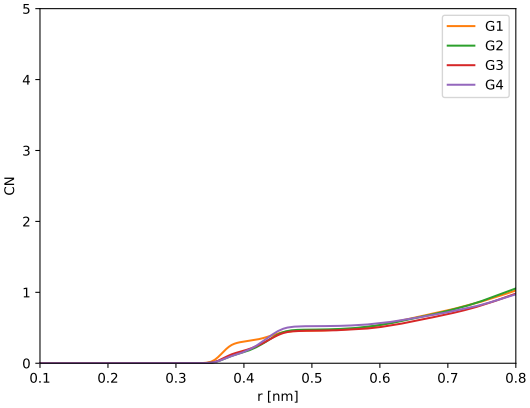
Li^+ – TFSI 100mM 1,000 ppm



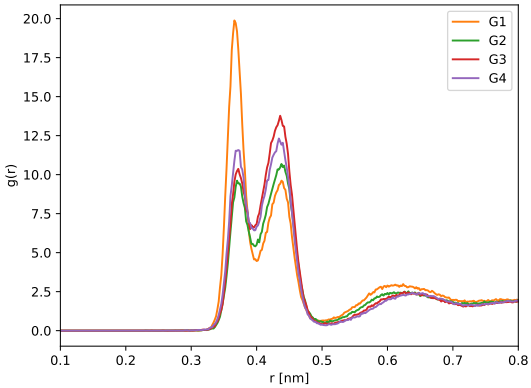


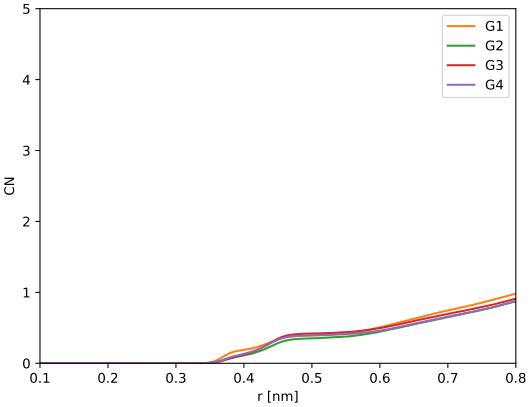
Li^+ – TFSI 100mM 5,000 ppm



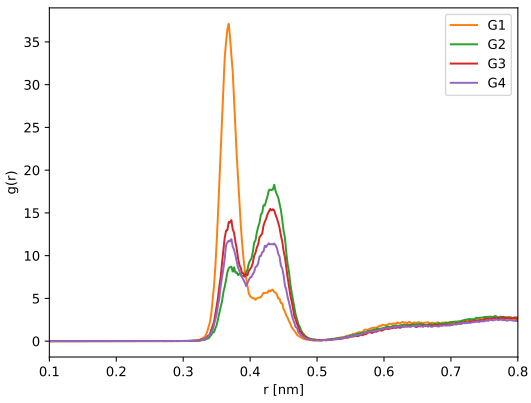


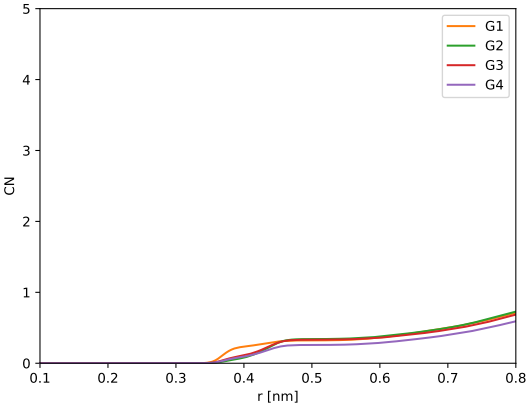
Li^+ – TFSI 100mM 20,000 ppm



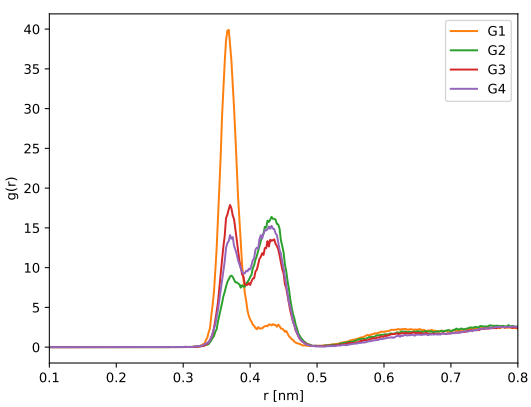


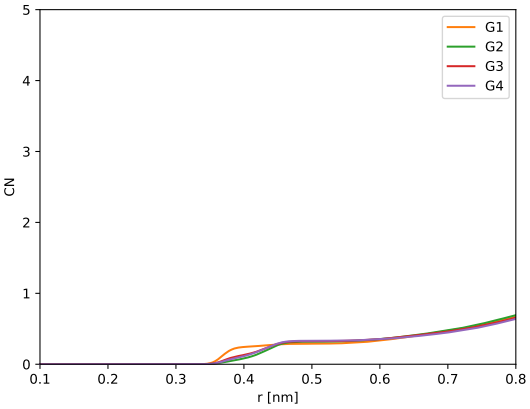
Li^+ – TFSI 200mM neat



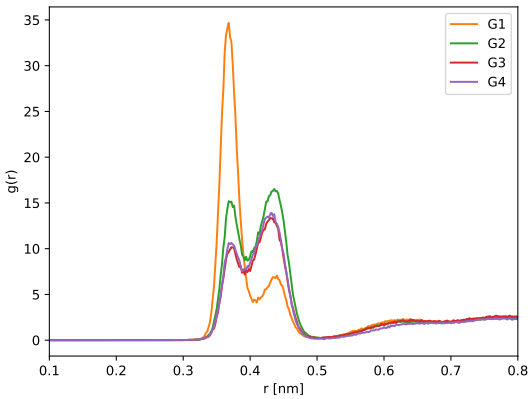


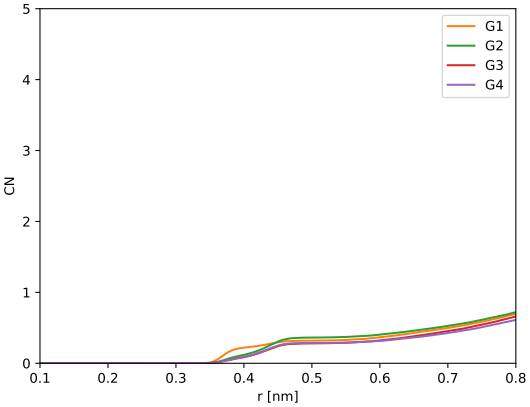
Li^+ – TFSI 200mM 1,000 ppm



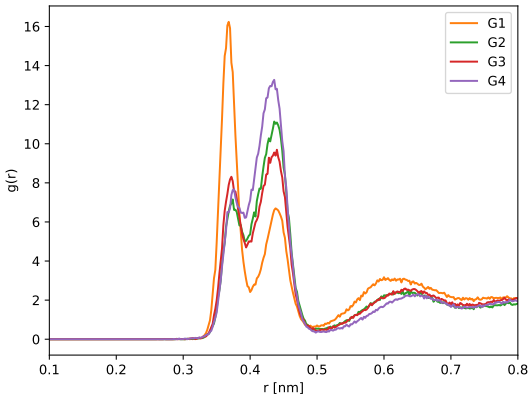


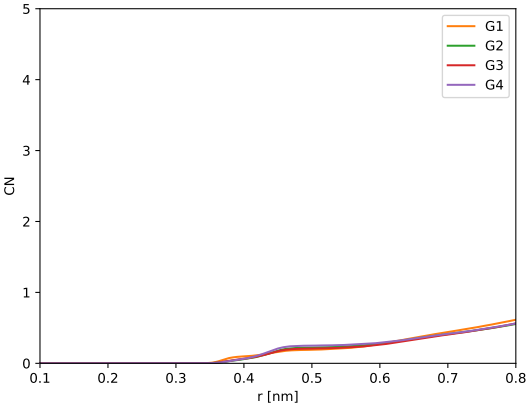
Li^+ – TFSI 200mM 5,000 ppm



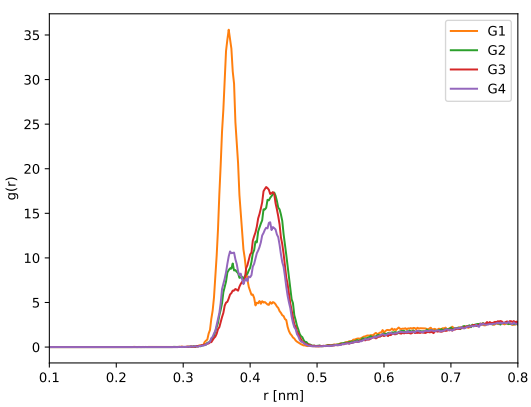


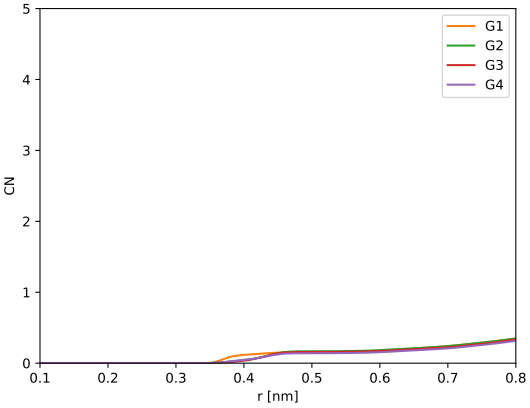
Li^+ – TFSI 200mM 20,000 ppm



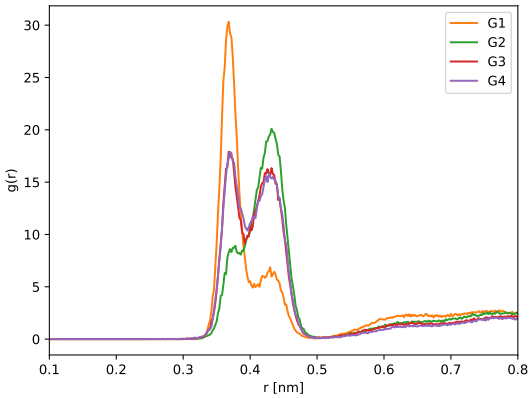


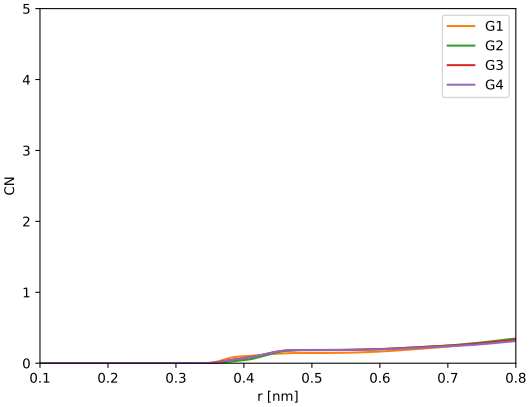
Li^+ – TFSI 300mM neat



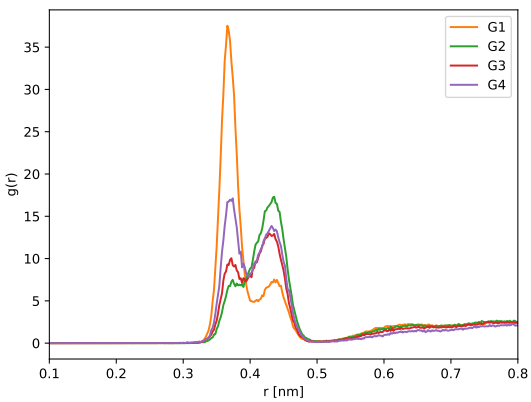


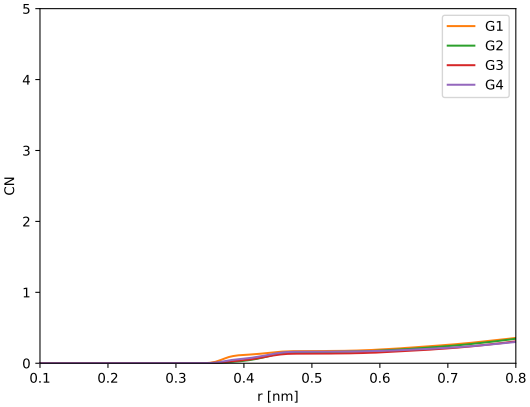
Li^+ – TFSI 300mM 1,000 ppm



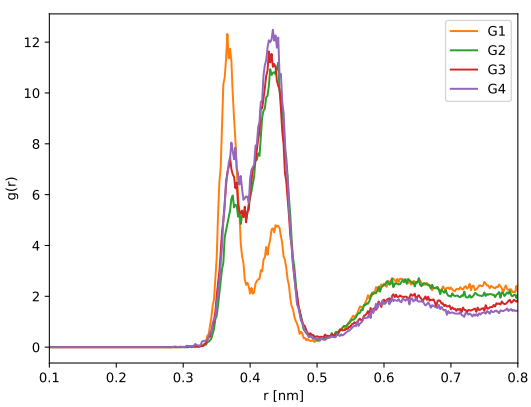


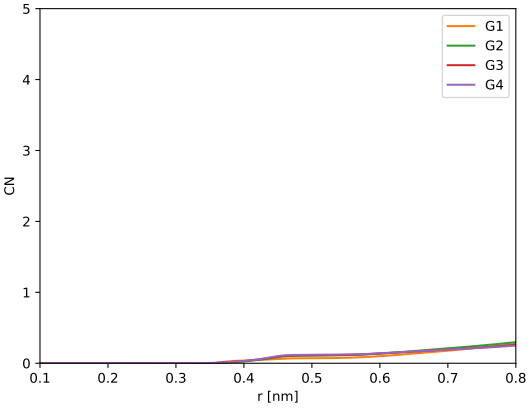
Li^+ – TFSI 300mM 5,000 ppm





Li^+ – TFSI 300mM 20,000 ppm





2.10 Li^+ – O-H_2O

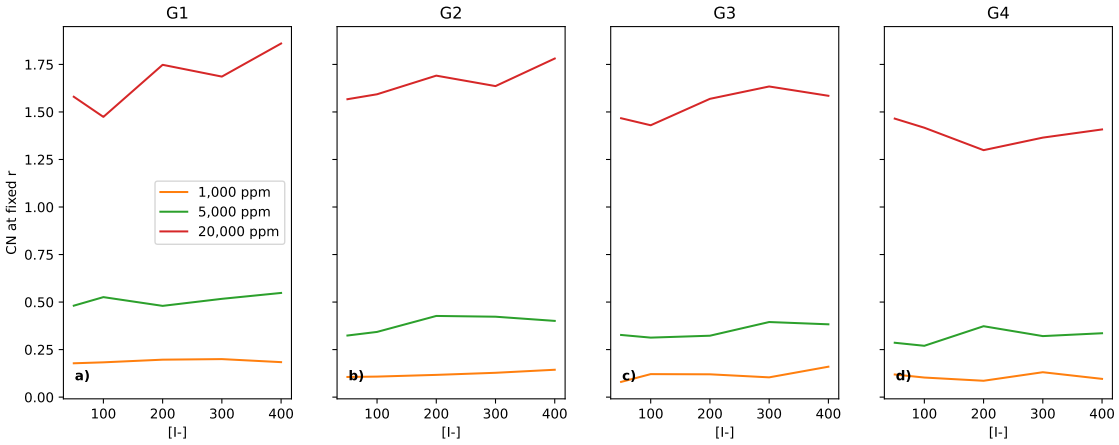


Figure 19: Coordination number of Li^+ to Li+ at a fixed distance of 3 Å, for the four different glymes (G1 = yellow, G2 = green, G3 = red, G4 = purple) studied here, across the four different water concentrations (with a): neat, b): 1,000, c): 5,000, d): 20,000 ppm of water).

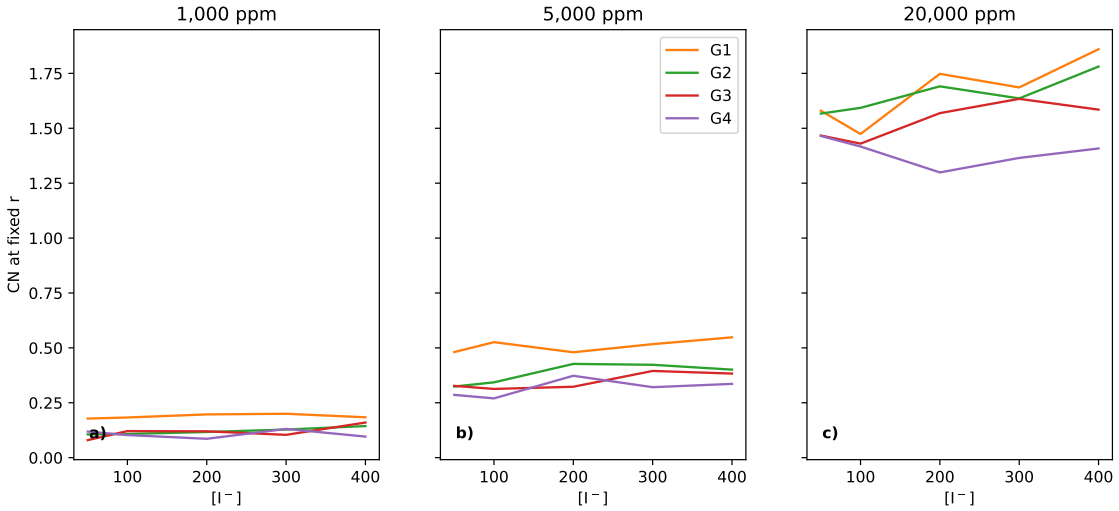
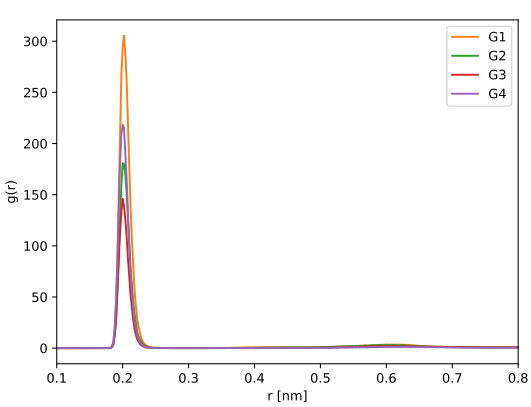
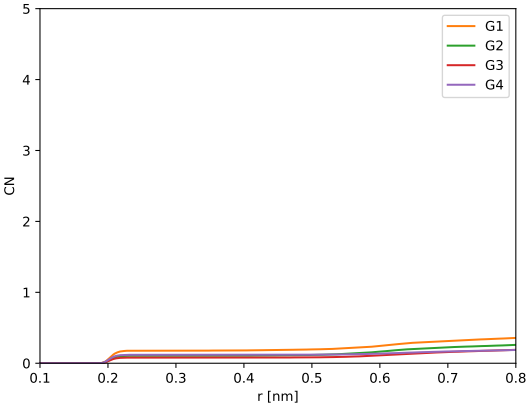


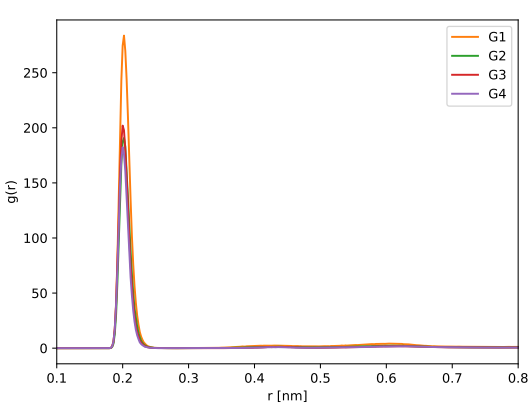
Figure 20: Coordination number of Li^+ to O (of H_2O) at a fixed distance of 3 Å, for the four different glymes (G1 = yellow, G2 = green, G3 = red, G4 = purple) studied here, across the four different water concentrations (with a): neat, b): 1,000, c): 5,000, d): 20,000 ppm of water).

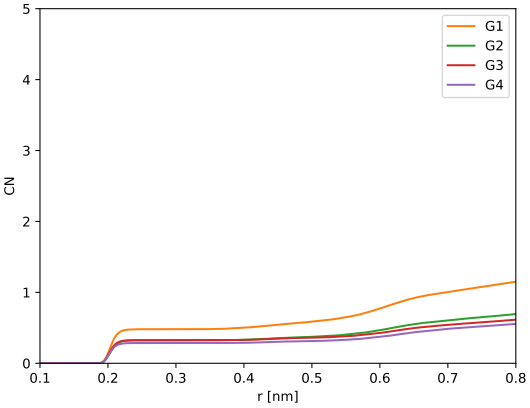
Li^+ – O-H_2O 50mM 1,000 ppm



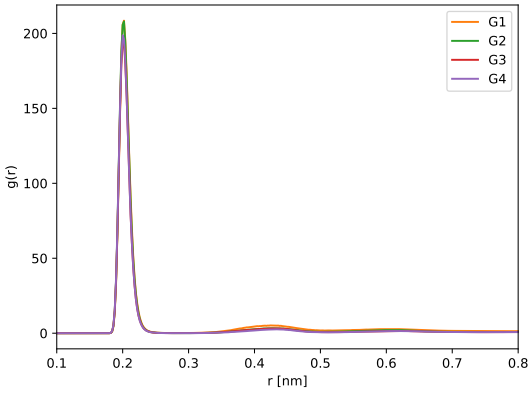


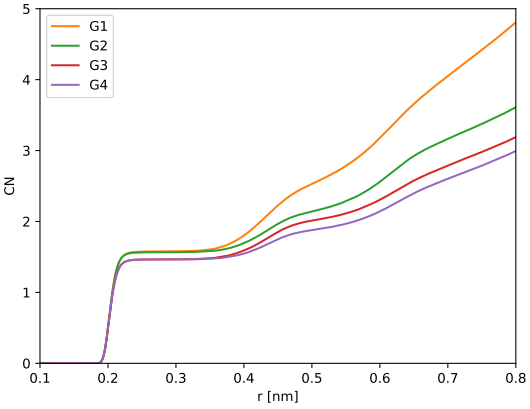
Li^+ – O-H_2O 50mM 5,000 ppm



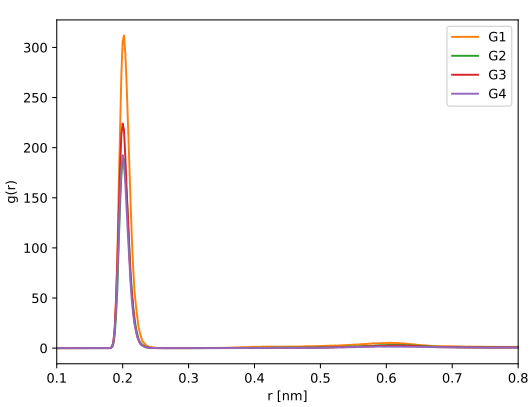


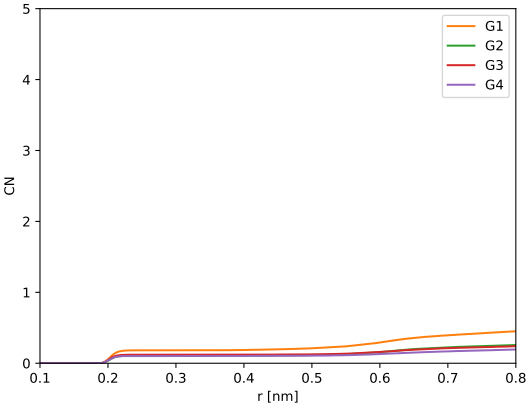
Li^+ – O-H_2O 50mM 20,000 ppm



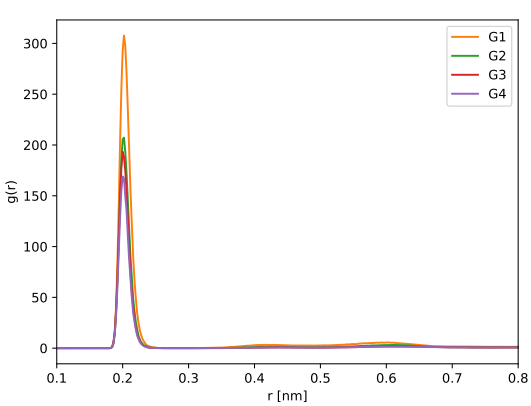


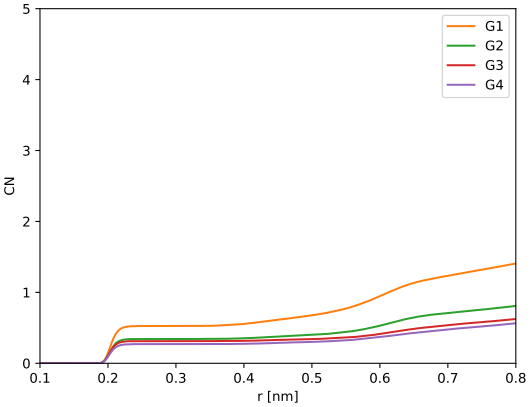
Li^+ – O-H_2O 100mM 1,000 ppm



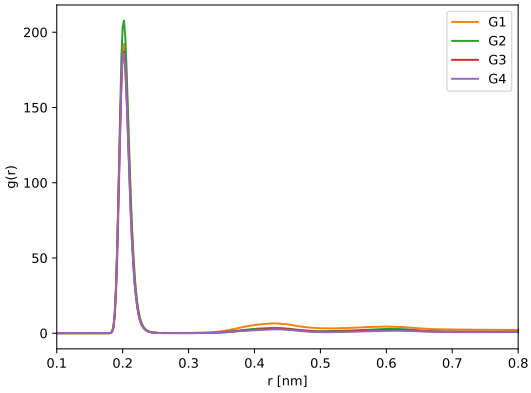


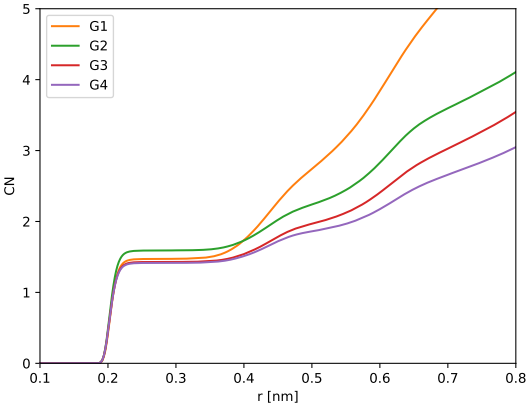
Li^+ – O-H_2O 100mM 5,000 ppm



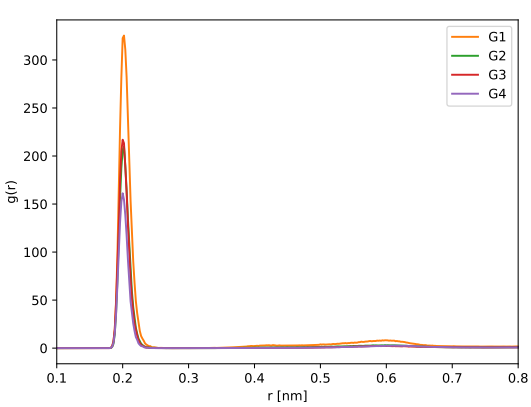


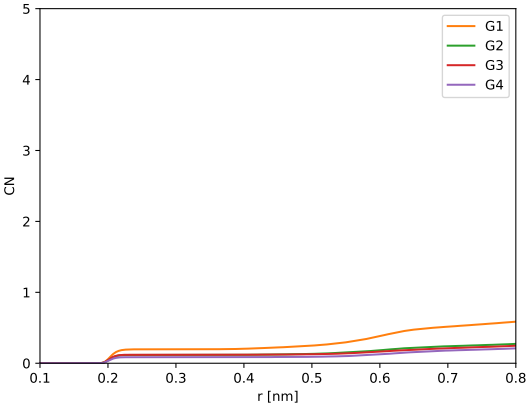
Li^+ – O-H_2O 100mM 20,000 ppm



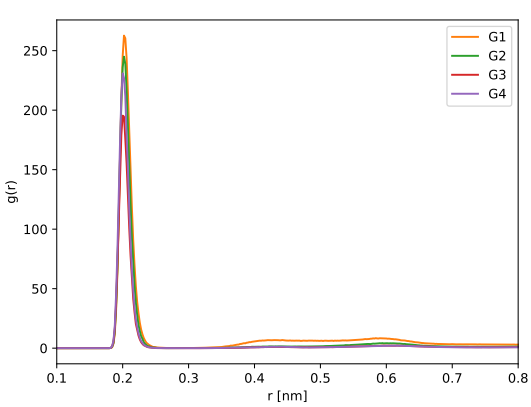


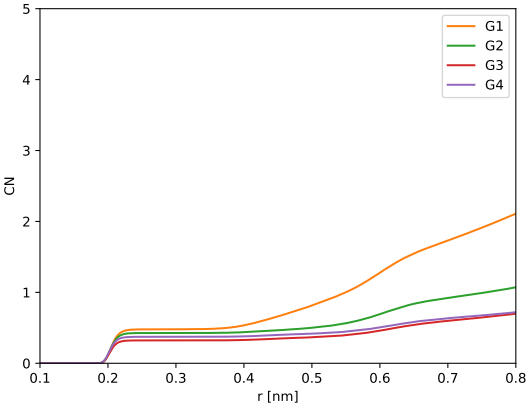
Li^+ – O-H_2O 200mM 1,000 ppm



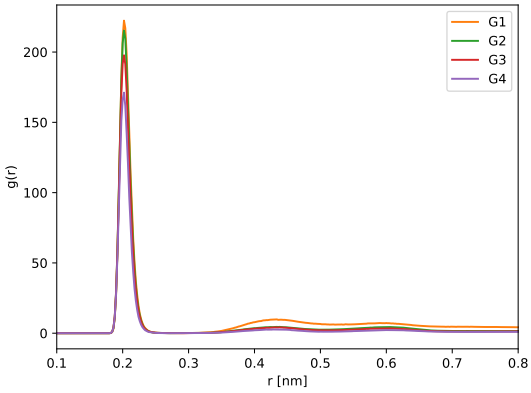


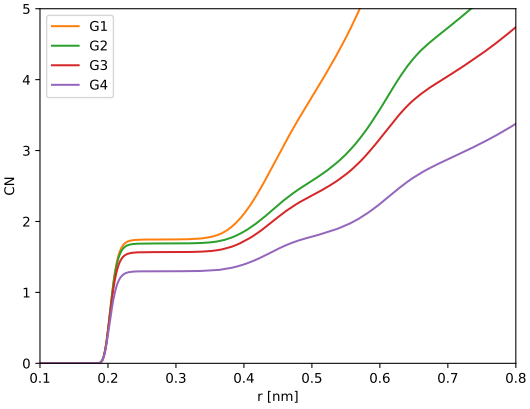
Li^+ – O-H_2O 200mM 5,000 ppm



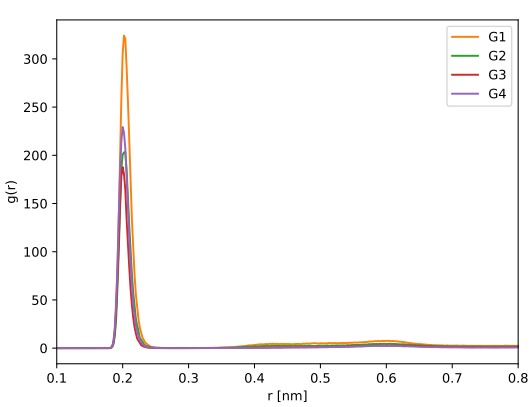


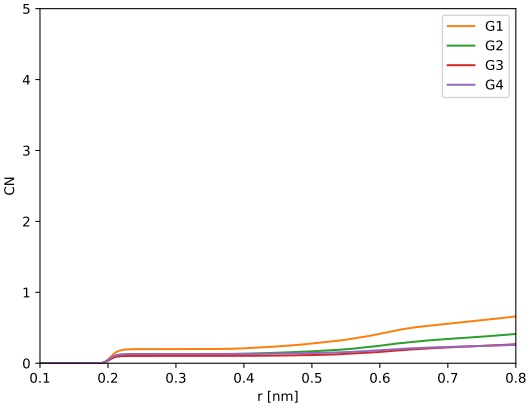
Li^+ – O-H_2O 200mM 20,000 ppm



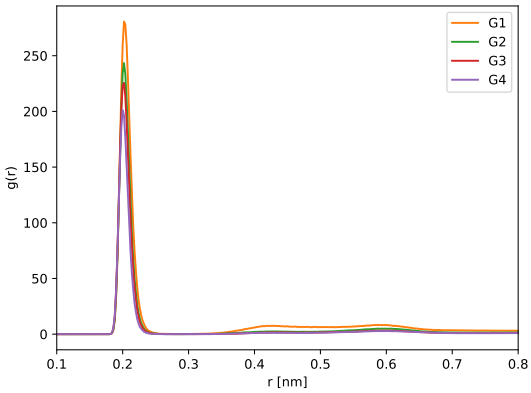


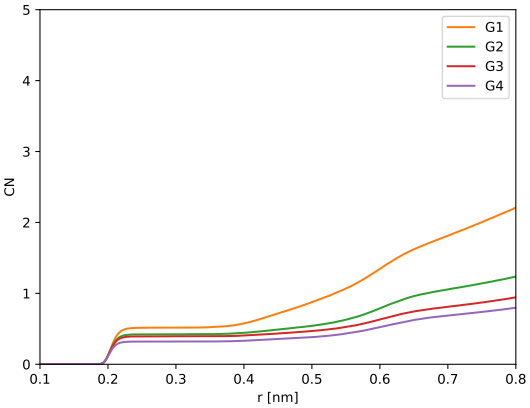
Li^+ – O-H_2O 300mM 1,000 ppm



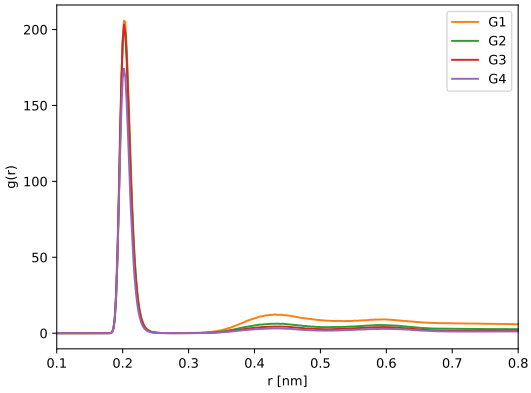


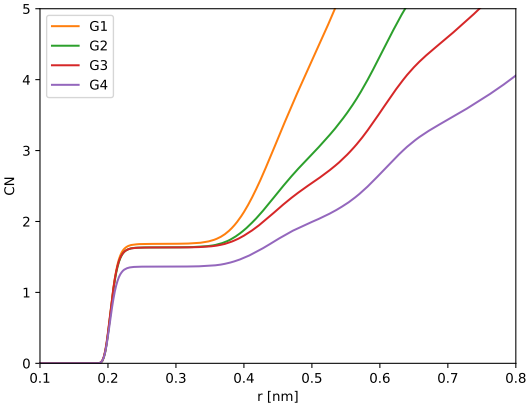
Li^+ – O-H_2O 300mM 5,000 ppm



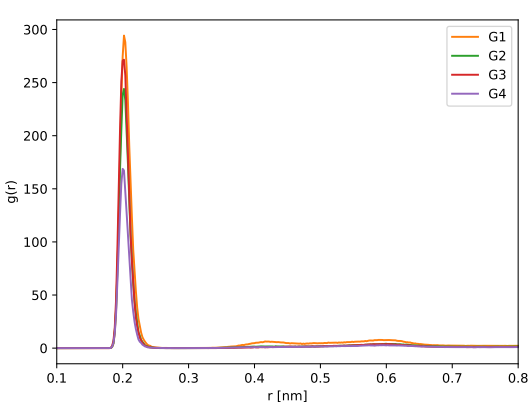


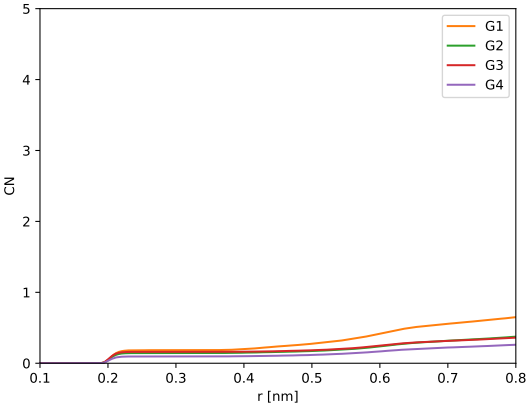
Li^+ – O-H_2O 300mM 20,000 ppm



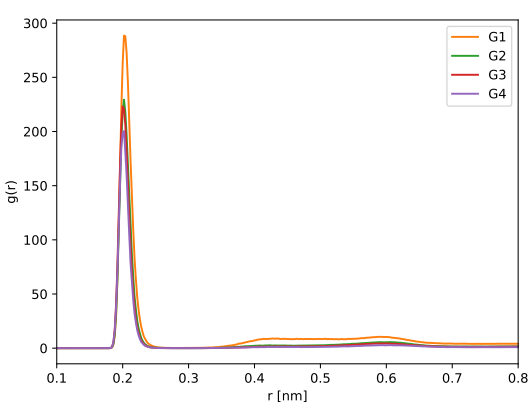


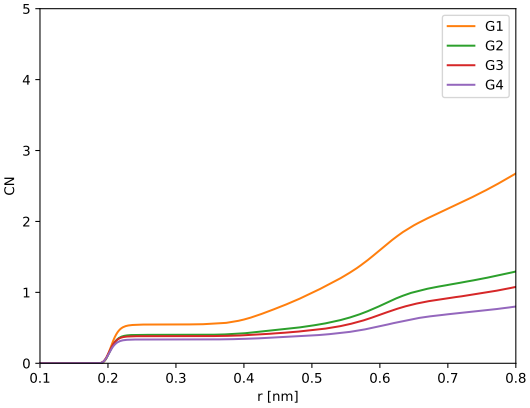
Li^+ – O-H_2O 400mM 1,000 ppm



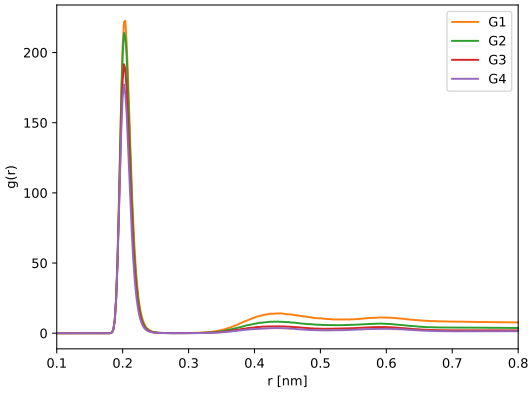


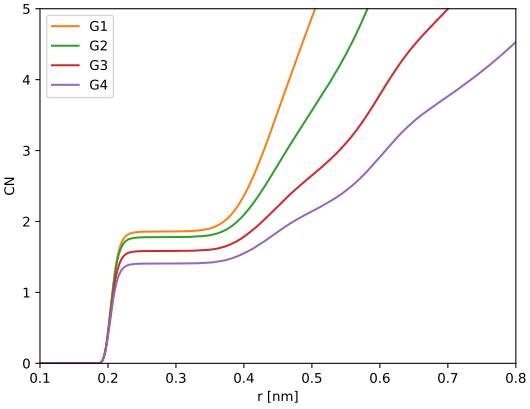
Li^+ – O-H_2O 400mM 5,000 ppm





Li^+ – O-H_2O 400mM 20,000 ppm





2.11 Li^+ – O-solvent

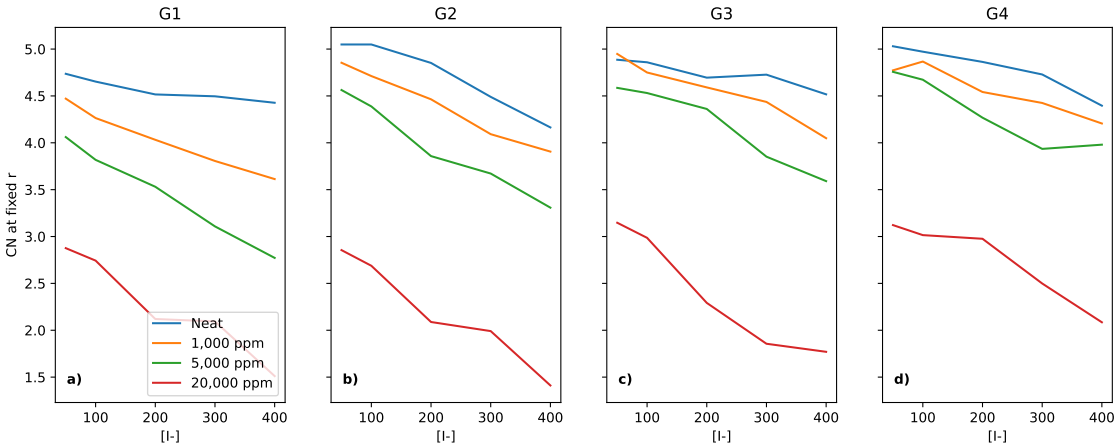


Figure 21: Coordination number of Li^+ to Li+ at a fixed distance of 3 Å, for the four different glymes (G1 = yellow, G2 = green, G3 = red, G4 = purple) studied here, across the four different water concentrations (with a): neat, b): 1,000, c): 5,000, d): 20,000 ppm of water).

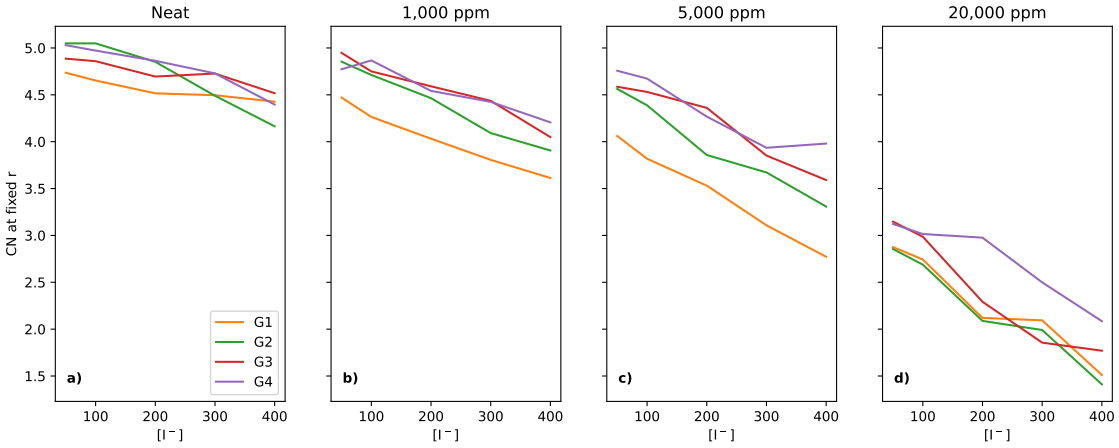
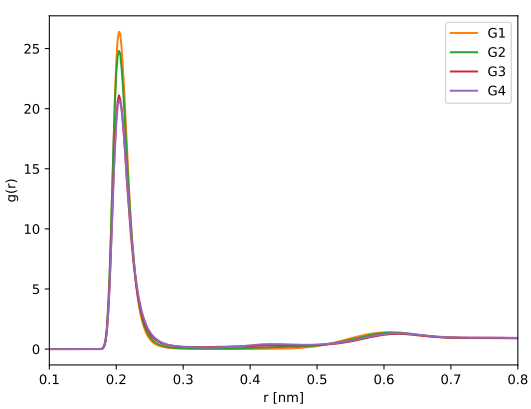
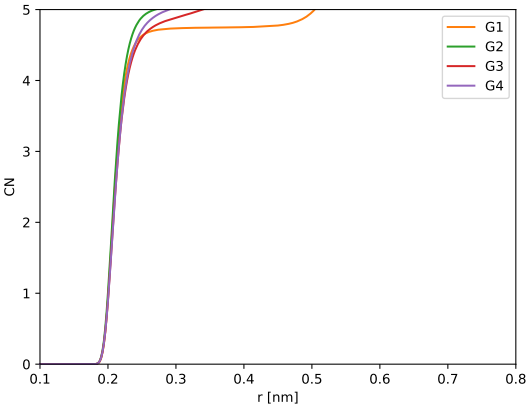


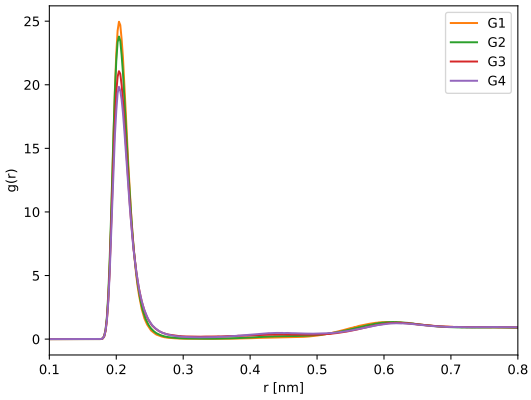
Figure 22: Coordination number of Li^+ to O (of the solvent) at a fixed distance of 3 Å, for the four different glymes (G1 = yellow, G2 = green, G3 = red, G4 = purple) studied here, across the four different water concentrations (with a): neat, b): 1,000, c): 5,000, d): 20,000 ppm of water).

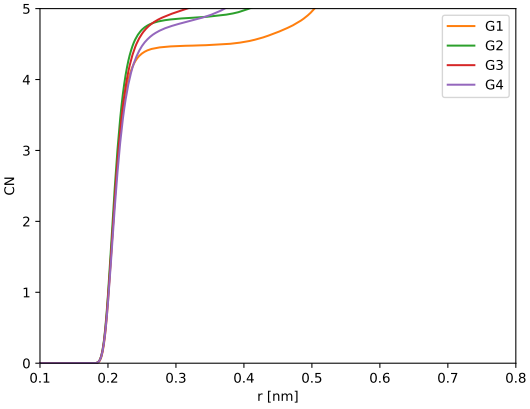
Li^+ – O-solvent 50mM neat



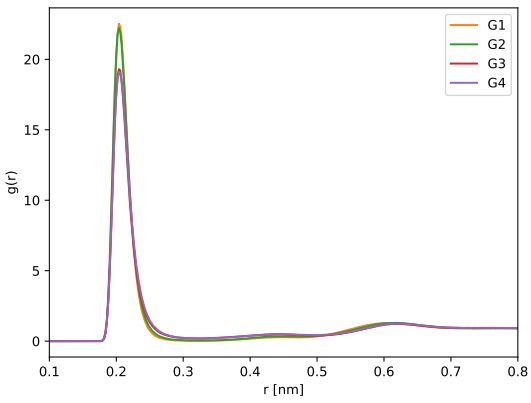


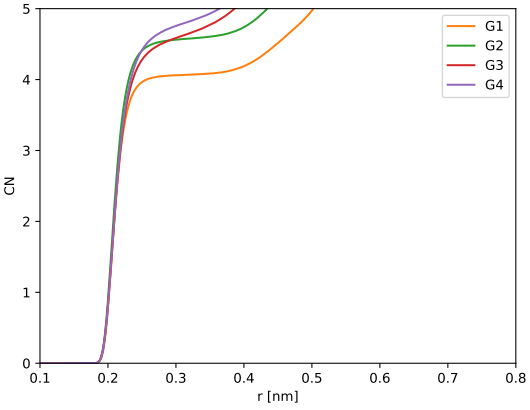
Li^+ – O-solvent 50mM 1,000 ppm



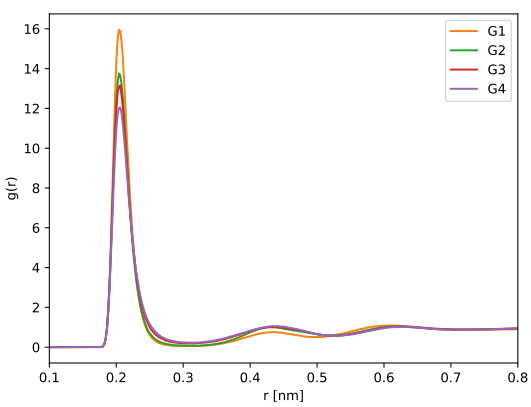


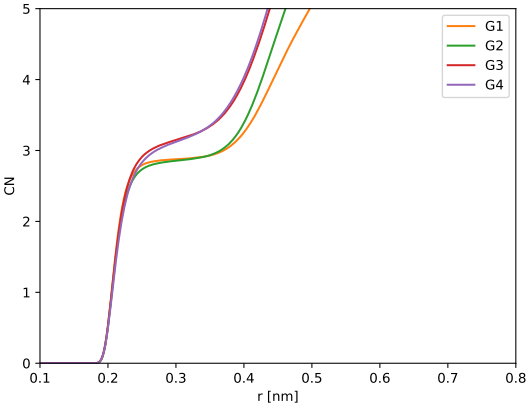
Li^+ – O-solvent 50mM 5,000 ppm



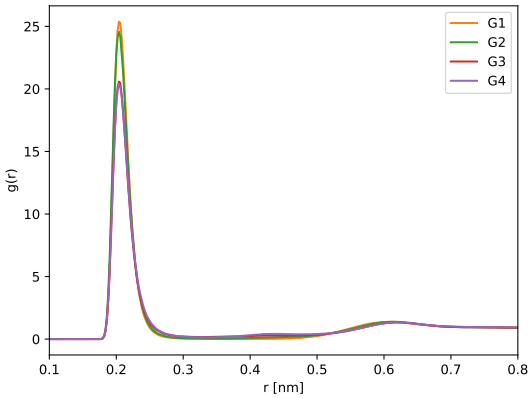


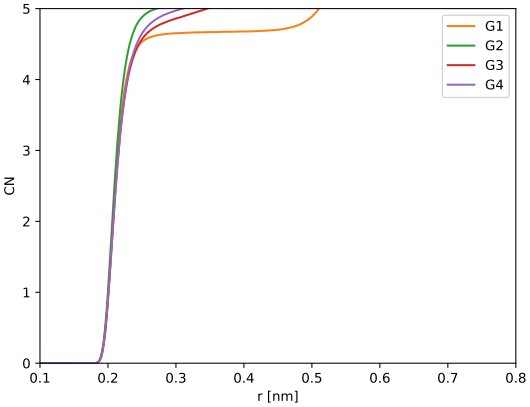
Li^+ – O-solvent 50mM 20,000 ppm



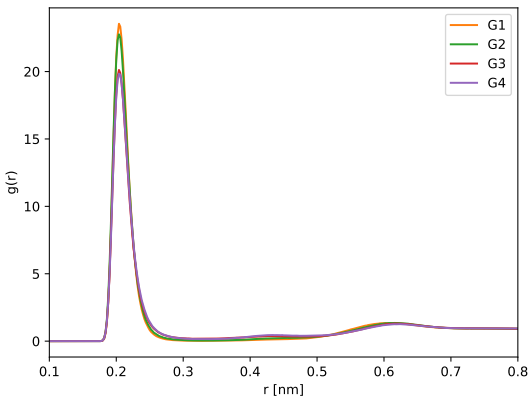


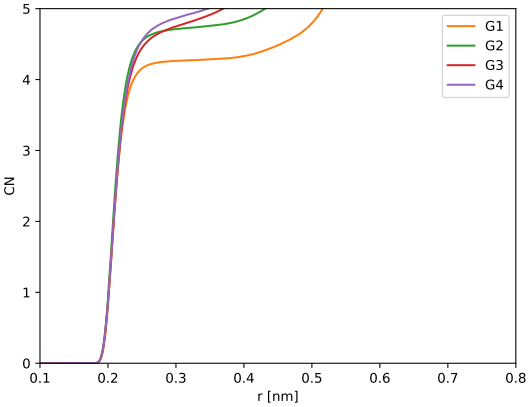
Li^+ – O-solvent 100mM neat



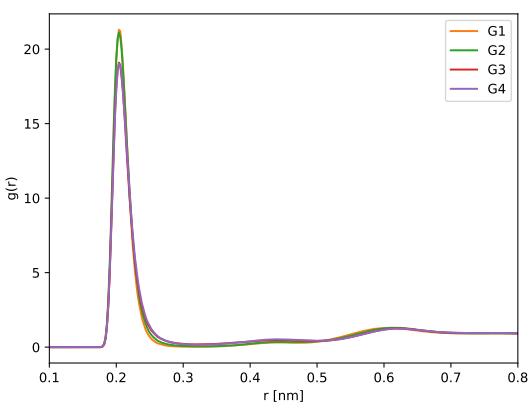


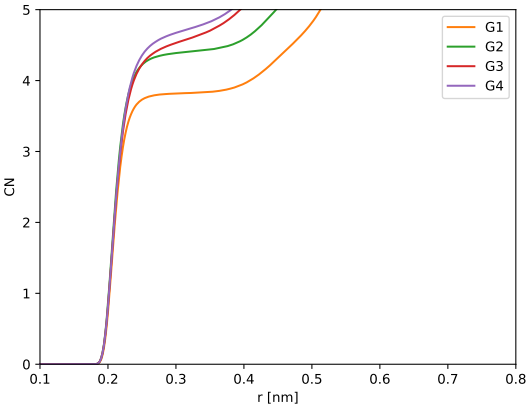
Li^+ – O-solvent 100mM 1,000 ppm



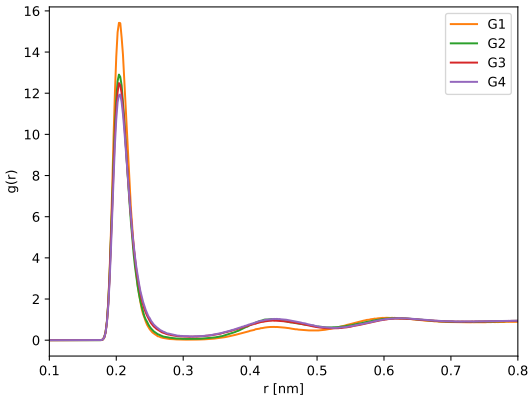


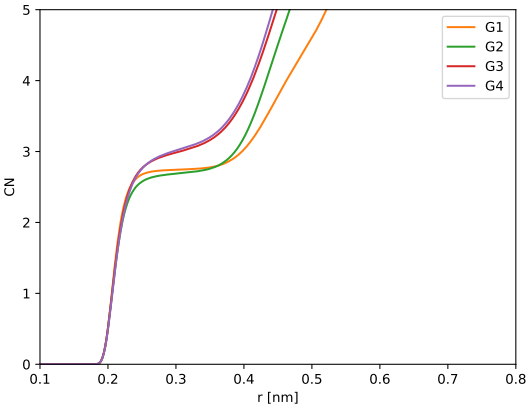
Li^+ – O-solvent 100mM 5,000 ppm



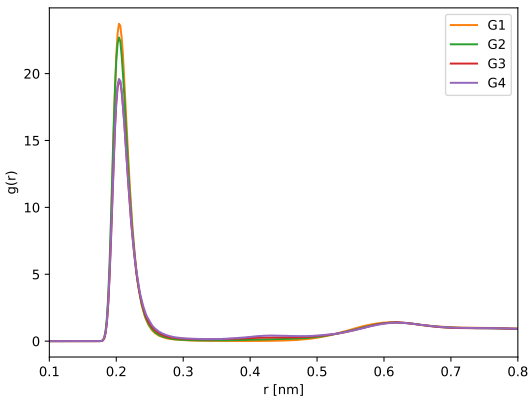


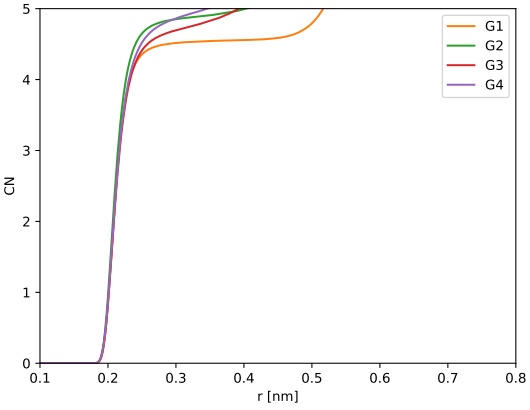
Li^+ – O-solvent 100mM 20,000 ppm



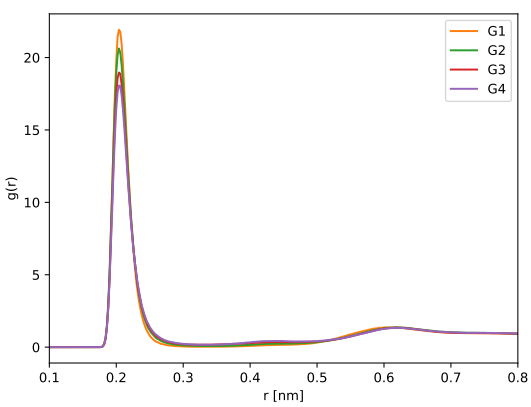


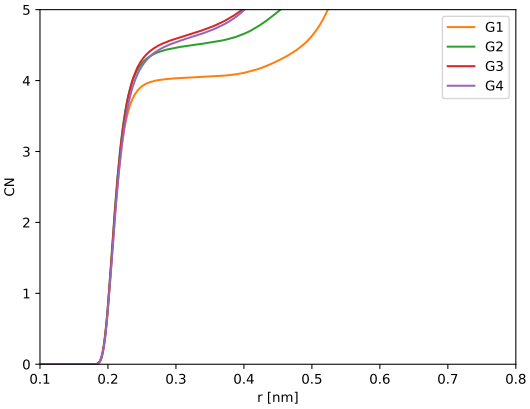
Li^+ – O-solvent 200mM neat



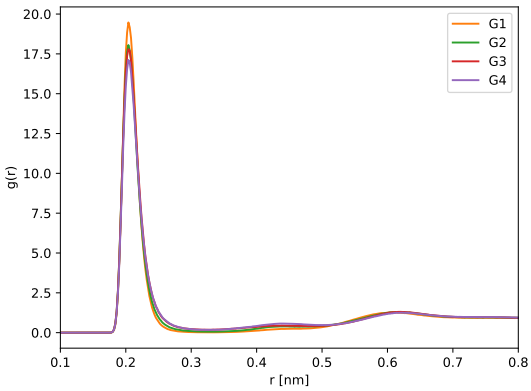


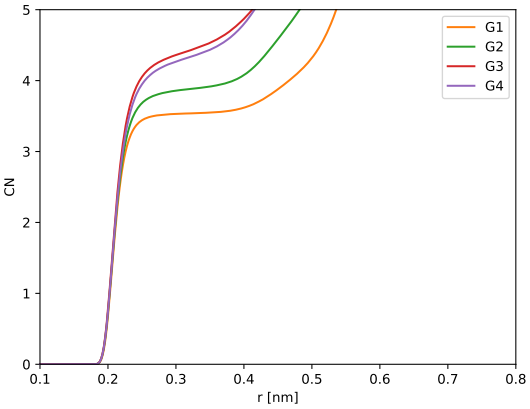
Li^+ – O-solvent 200mM 1,000 ppm



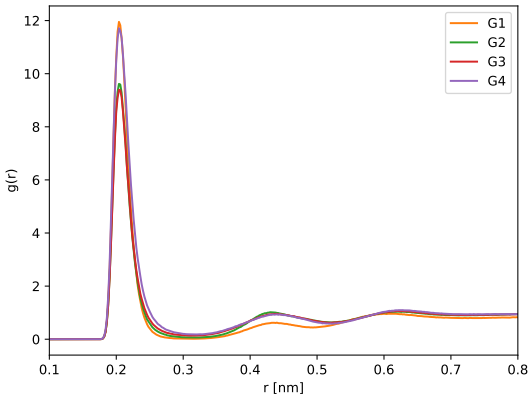


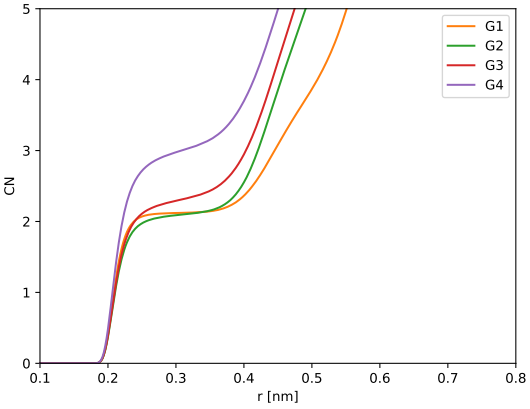
Li^+ – O-solvent 200mM 5,000 ppm



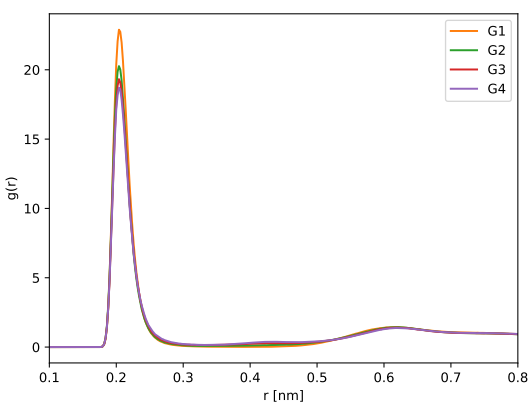


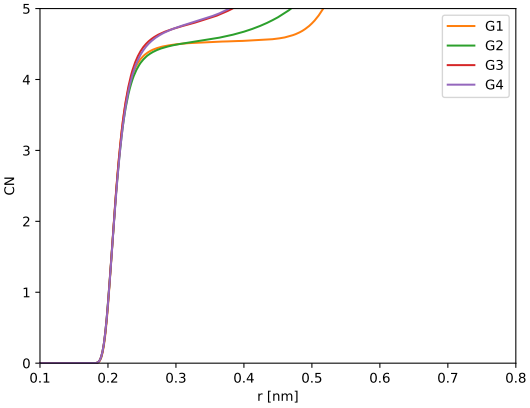
Li^+ – O-solvent 200mM 20,000 ppm



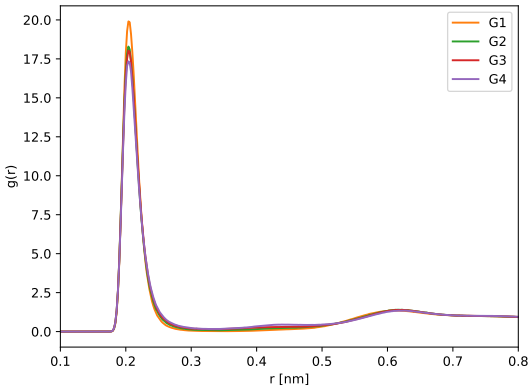


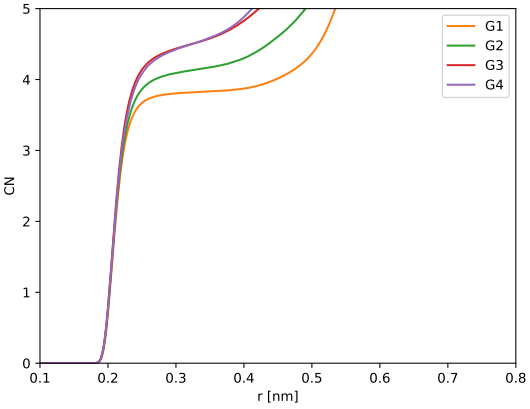
Li^+ – O-solvent 300mM neat



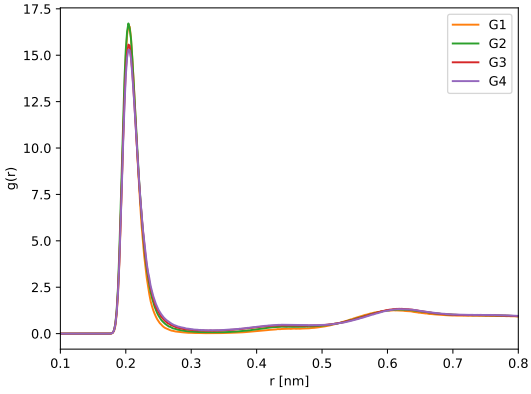


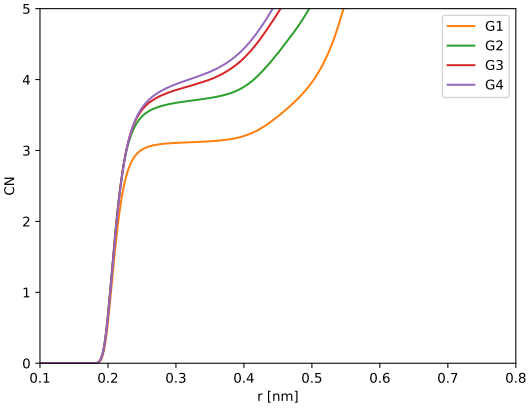
Li^+ – O-solvent 300mM 1,000 ppm



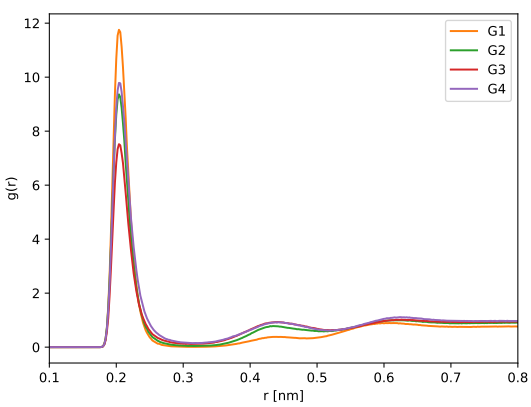


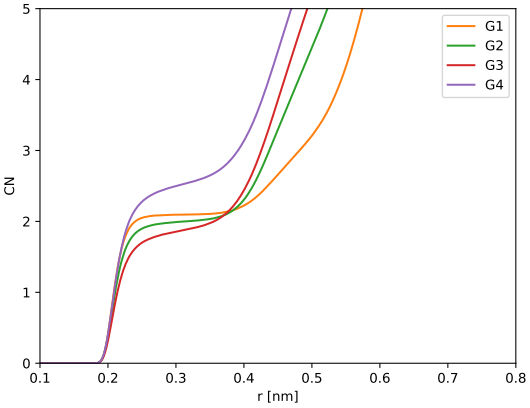
Li^+ – O-solvent 300mM 5,000 ppm



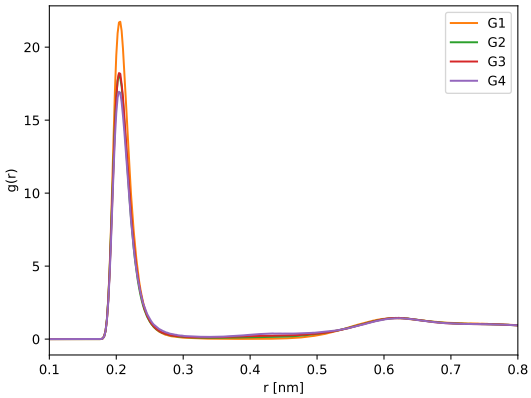


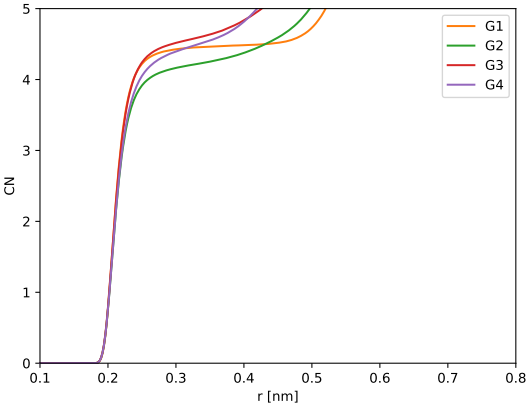
Li^+ – O-solvent 300mM 20,000 ppm



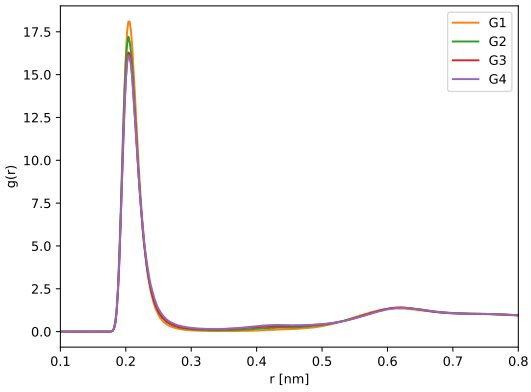


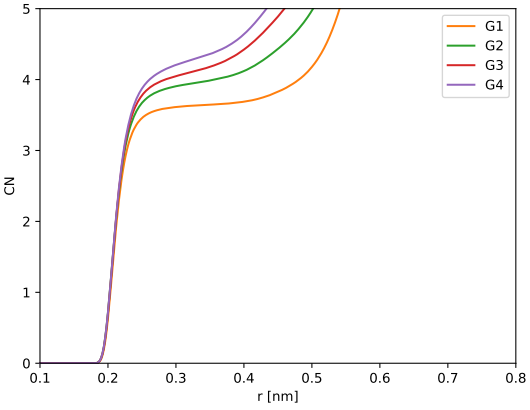
Li^+ – O-solvent 400mM neat



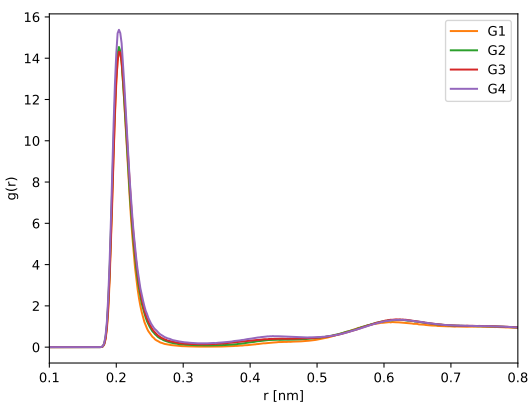


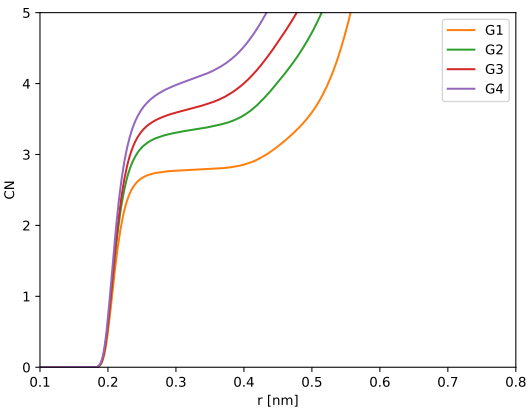
Li^+ – O-solvent 400mM 1,000 ppm





Li^+ – O-solvent 400mM 5,000 ppm





Li^+ – O-solvent 400mM 20,000 ppm