**Effects of amino acid side chain length and chemical structure on anionic poly glutamic and poly aspartic acid cellulose-based polyelectrolyte brushes.**

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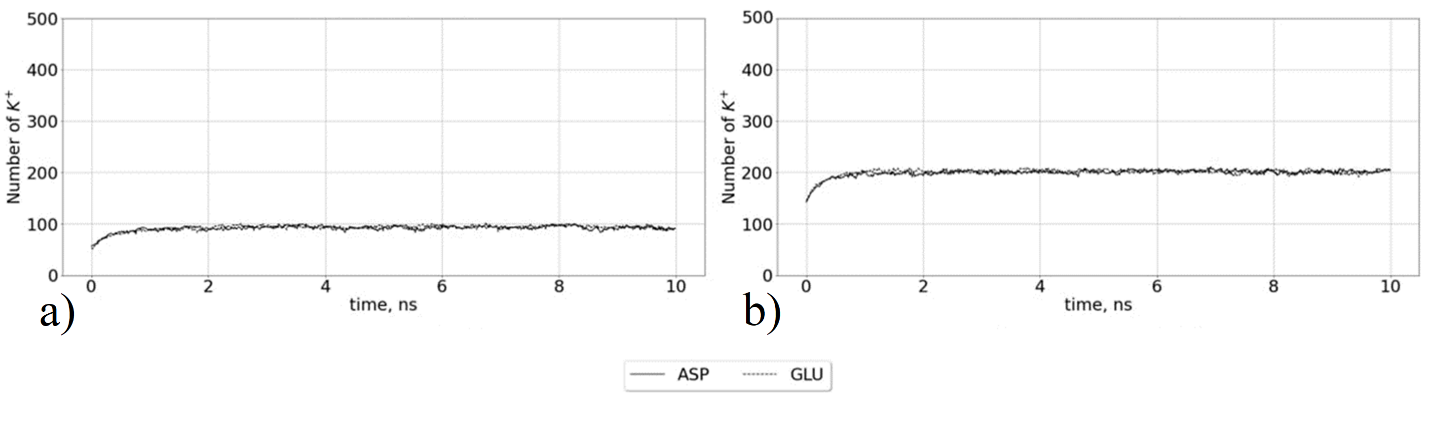
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Figure S1. The number of K+ ions in the brush during the first 10 ns in the simulations without CaCl2 salt. a) systems with 12% degree surface modification, b) systems with 25% degree surface modification

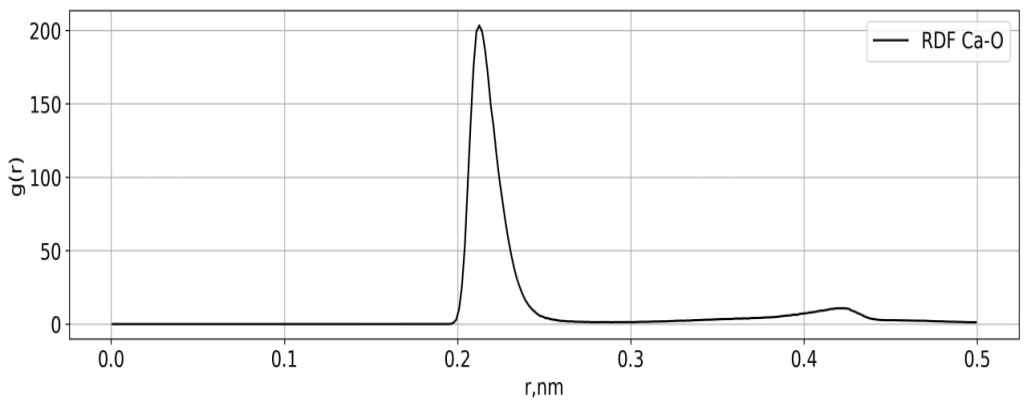


Figure S2. Radial distribution function of Ca2+ ions around oxygens of amino acid carboxyl groups.

Radial distribution function was calculated as:

, (1)

where ρB is the average density of type B atoms around atoms A, NA and NB are the number of A and B atoms, respectively, rij is the distance between two atoms A and B, and δ is the Kronecker delta function.

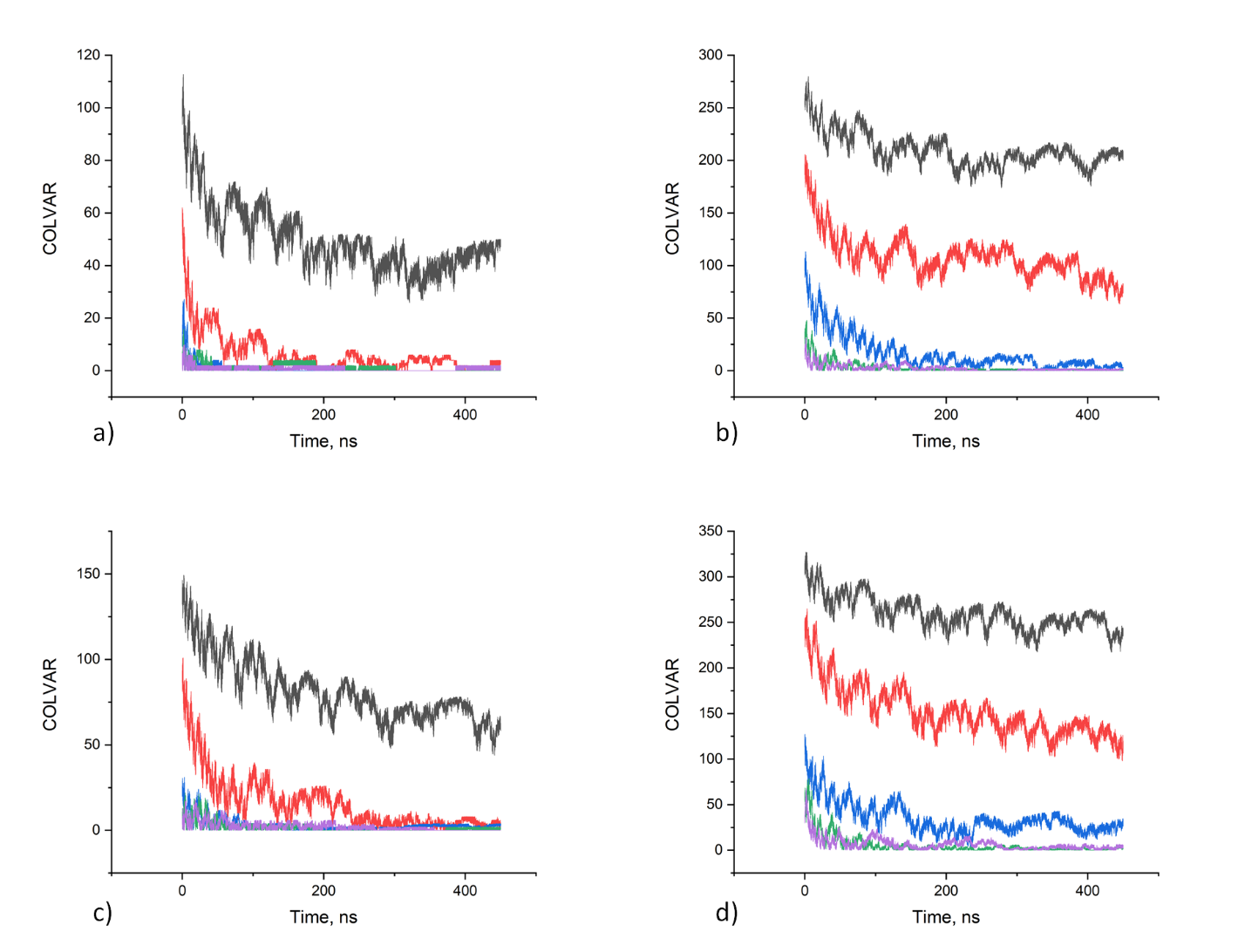


Figure S3. Time dependence of the collective variables (carboxyl group free from adsorbed calcium ions). The collective variable was calculated using differentiable switching function (1) in the text. The results of the simulation in different CaCl2 concentration 0.07 mol/kg, 0.15 mol/kg, 0.30 mol/kg, 0.62 mol/kg, 0.94 mol/kg are presented by black, red, blue, green and purple colors correspondingly. a) Aspartic acid brush with 12% surface modification, b) aspartic acid brush with 25% degree surface modification, c) glutamic acid brush with 12% degree surface modification d) glutamic acid brush with 25% degree surface modification.

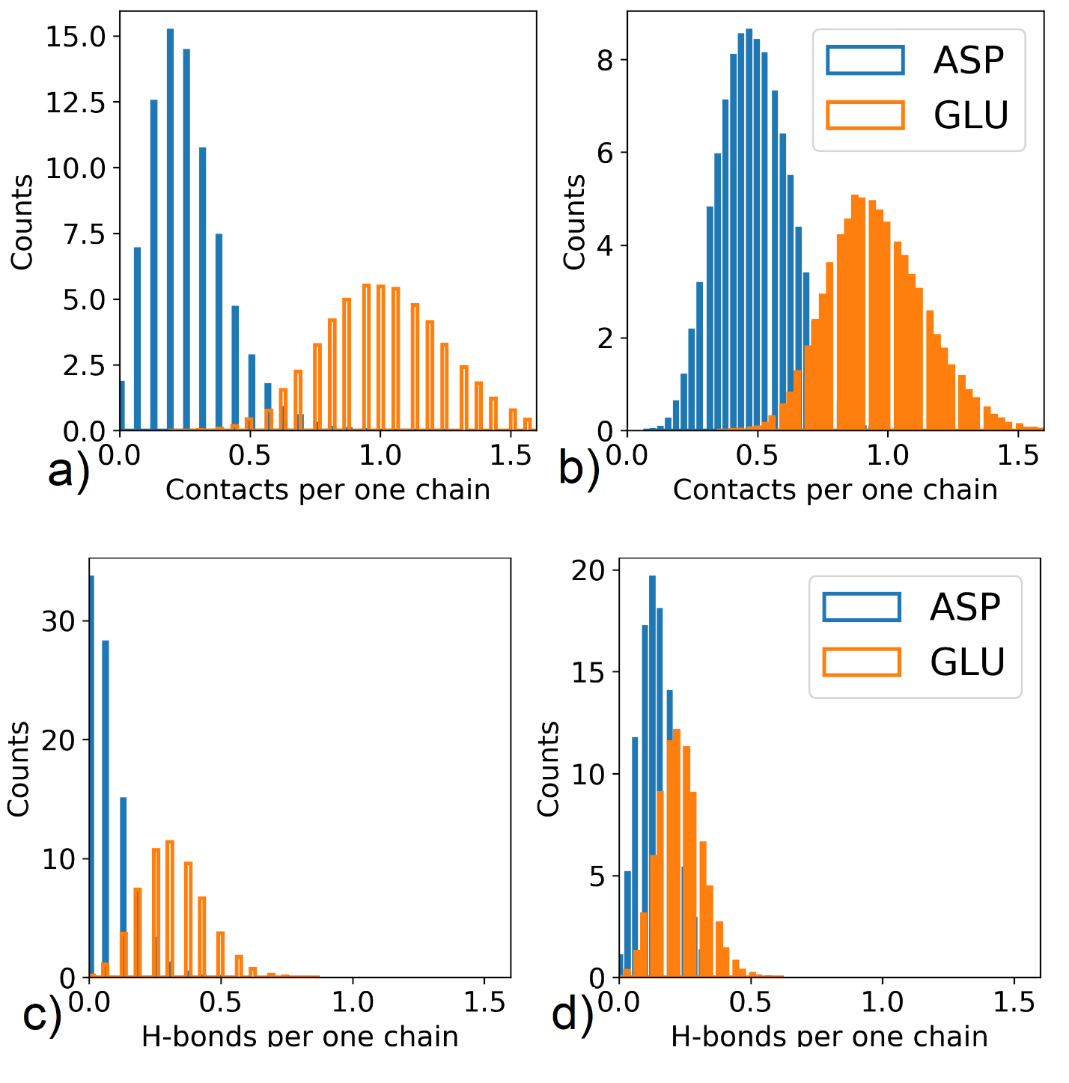
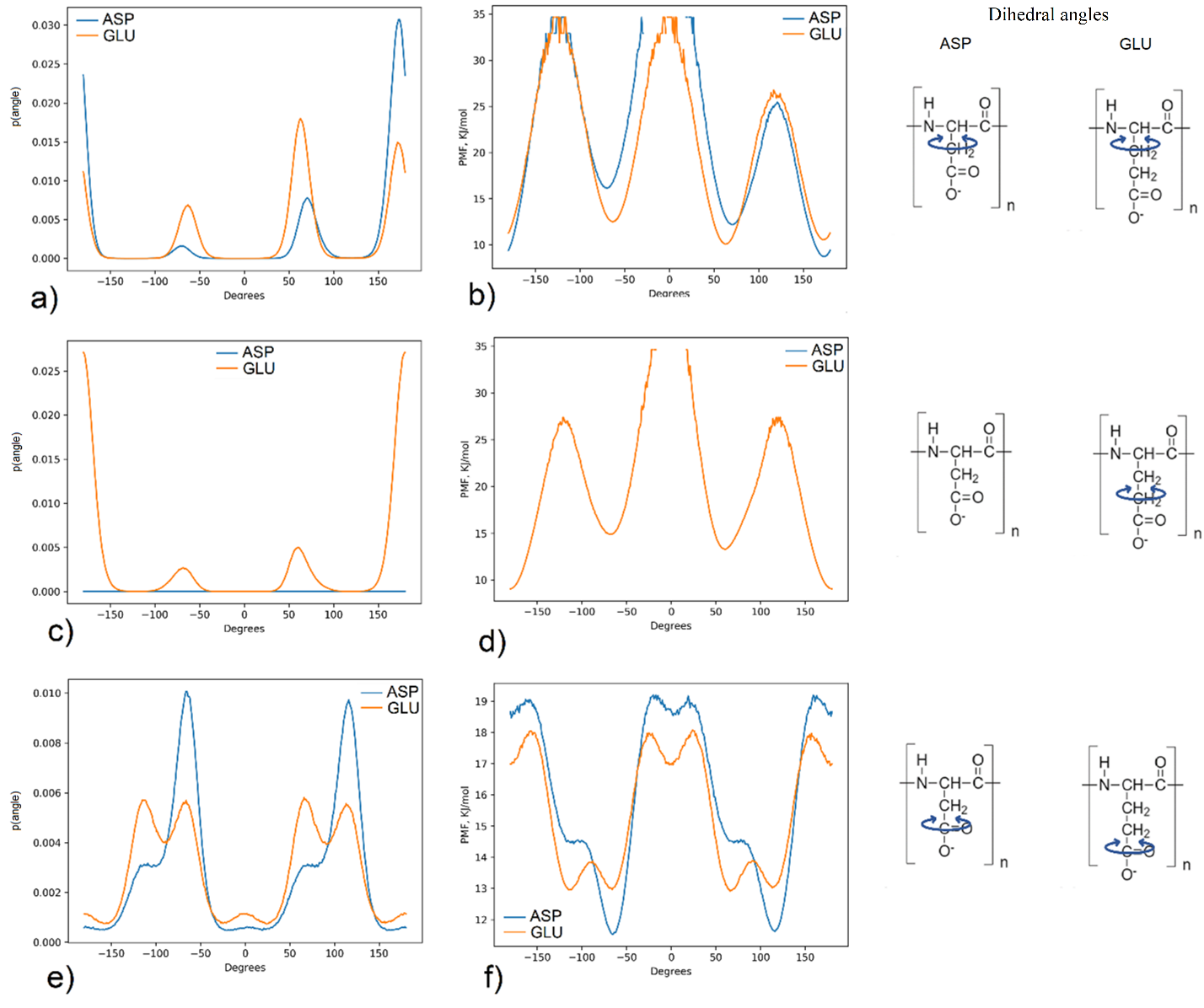


Figure S4. Distributions of the number of a, b) close contacts between hydrogens of surface hydroxyl groups and oxygens of amide groups and (the distance between atoms less then 0.35 nm) c,d) H-bonds between them (the distance between atoms less then 0.35 nm and the angle formed by acceptor, hydrogen and donor less than 35°). a,c) systems with 12% degree surface modification, b,d) systems with 25% degree surface modification

Figure S5. Dihedral angle distributions of the side chain (a,c,e) and potential mean force (b,d,f) obtained from the distributions with the schemes illustrating considering angles.

The distributions was obtained using 1 μs trajectory of the poly(amino acids) in water with degree polymerization 32. The potential mean force was obtained from the distributions using the following dependence:

(2)

where α – is dihedral angle, g(α) – distribution of α, k- the Boltzmann constant, T- temperature,

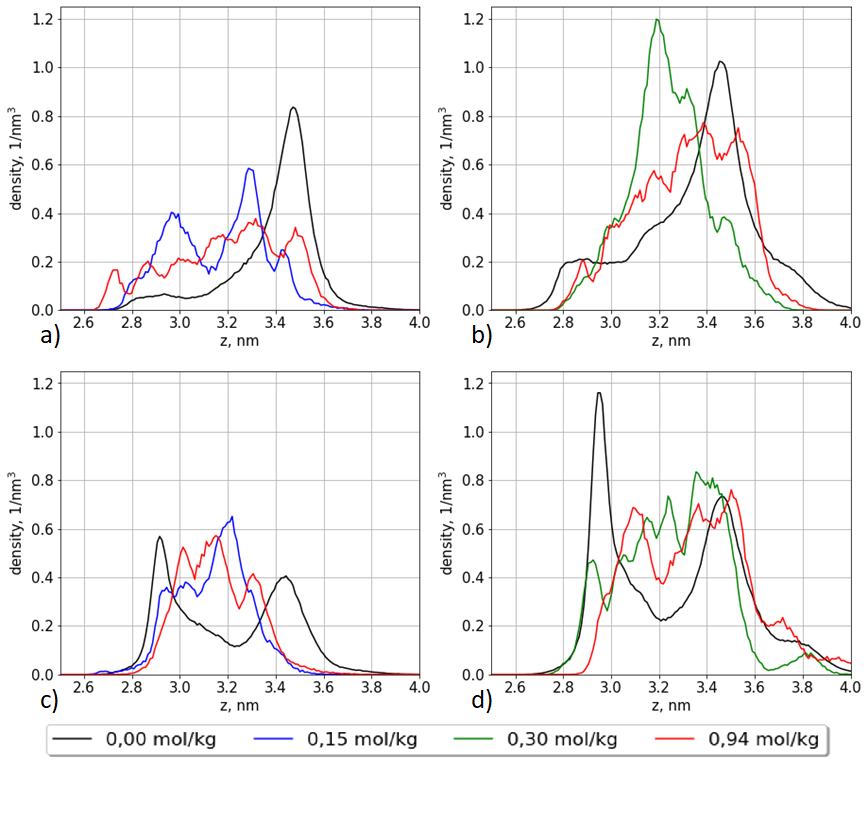


Figure S6. Density profiles of the ends of the grafted oligomers of aspartic and glutamic acids in at different CaCl2 concentrations. a) Aspartic acid brush with 12% surface modification, b) aspartic acid brush with 25% degree surface modification, c) glutamic acid brush with 12% degree surface modification d) glutamic acid brush with 25% degree surface modification.