Supplementary material
S1 Sigma profiles

Figure S1 correlation may be associated with the Cl^- charge dispersion, which is intensified when short alkyl chains bring the anion closer to the pyridinium positive charge. A nearly complete separation is achieved when alkyl chains are higher than 3 carbons. After that, the addition of less polar methylene groups ($-CH_2-$) only reduces the interaction energies with the solvent, water. Also worth noting that the *in silico* analysis is made on charge density distribution without water molecules, therefore, complex macromolecular interactions containing the solvent were not evaluated.

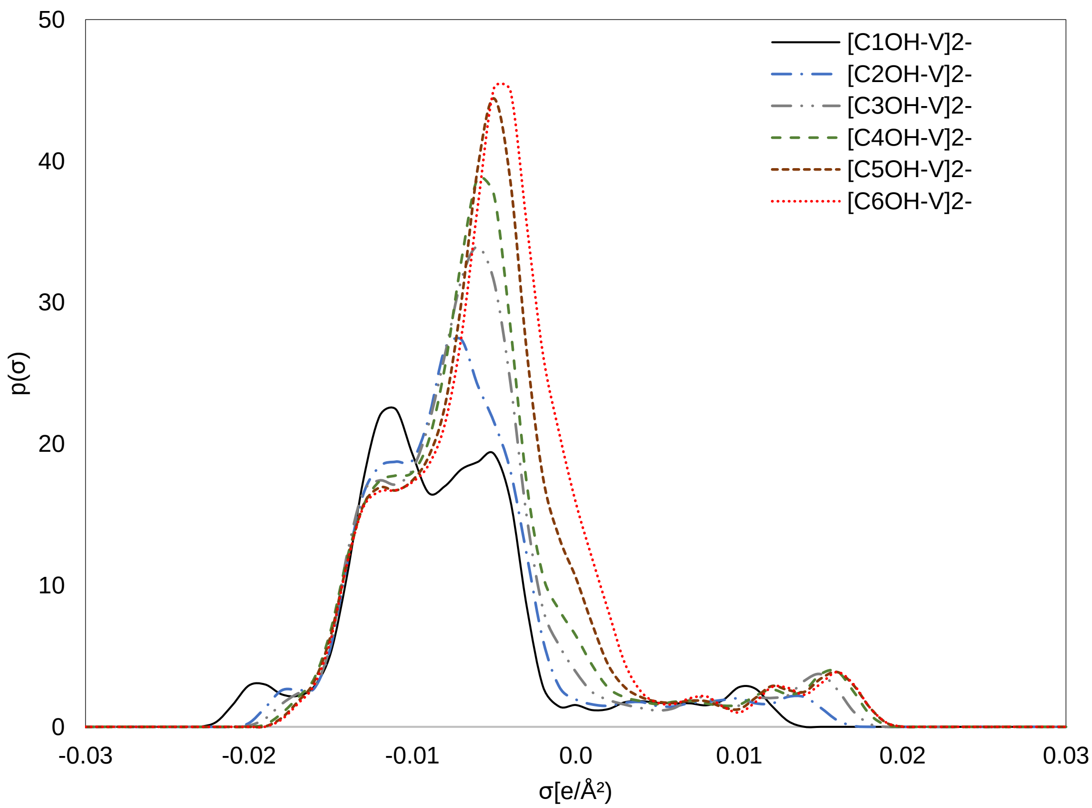

Figure S1. Sigma profile of hydroxyalkyl viologen derivatives

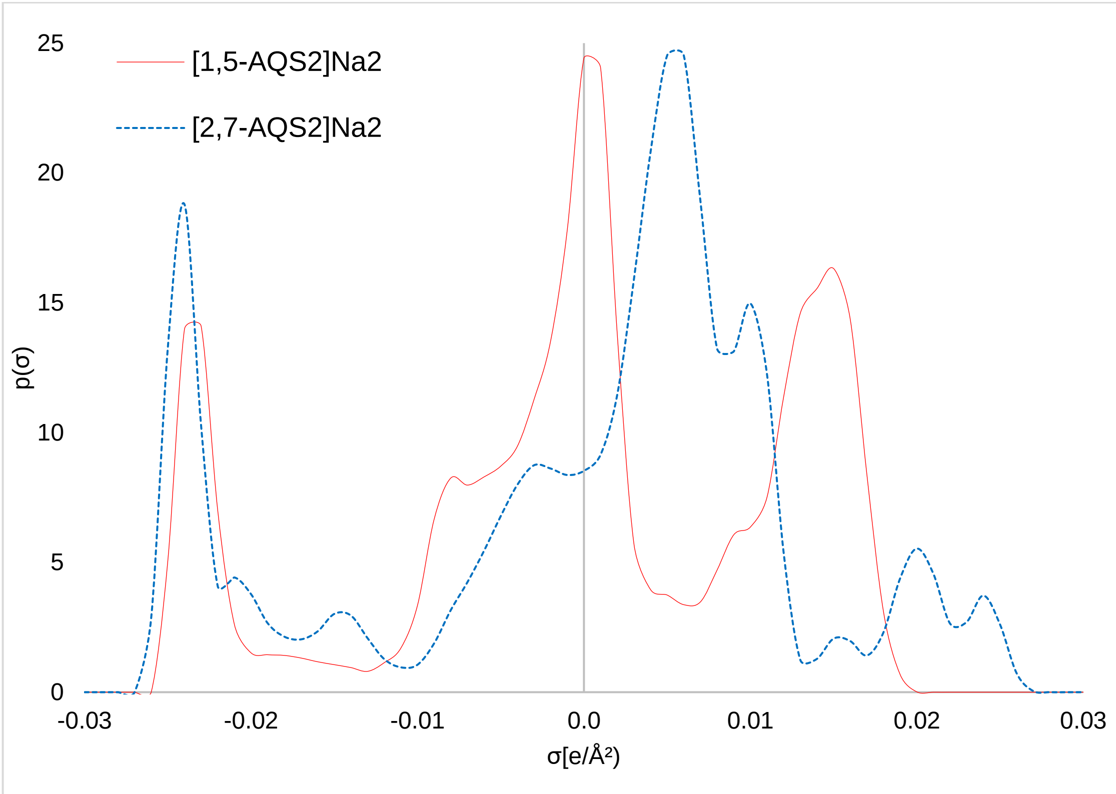

Figure S2. Sigma profile of 1,5 and 1,7 sulfonated anthraquinones

Figure S3. Sigma profiles of $[N_{2222}]^+$(green) and $[N_{2221}]^+$(red)