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Electronic Supplementary Information

Does the inclusion of electronic polarisability lead to a better modelling of peptide aggregation?

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Table S1: List of simulations performed in this work.[a]

System	#Aβ_{16-22}	#water	#Na^+	#Cl^-	Runs
CHARMM-Drude					
monomer [150 mM NaCl] [1–3]	1	4,299 SWM4-NDP	12	12	3×1 μs
monomer [no salt] [4–6]	1	4,369 SWM4-NDP	0	0	3×1 μs
dimer [150 mM NaCl] [7–9]	2	10,564 SWM4-NDP	30	30	3×900 ns
dimer [no salt] [10–12]	2	10,725 SWM4-NDP	0	0	3×1 μs
CHARMM36m					
dimer [150 mM NaCl] [13–15]	2	10,564 TIP3P	29	29	3×1 μs

a The monomer simulations with CHARMM36m were taken from ref. 16.

Table S2: The number of sodium ions obtained by integration of the radial distributions of Na^+ around the carbonly-oxygen atoms of the Aβ_{16-22} till a distance of 0.35 nm.

	K16	L17	V18	F19	F20	A21	E22
C-Drude	0.127	0.266	0.396	0.058	0.672	0.143	0.193
C36m	0.002	0.000	0.002	0.002	0.002	0.003	0.003

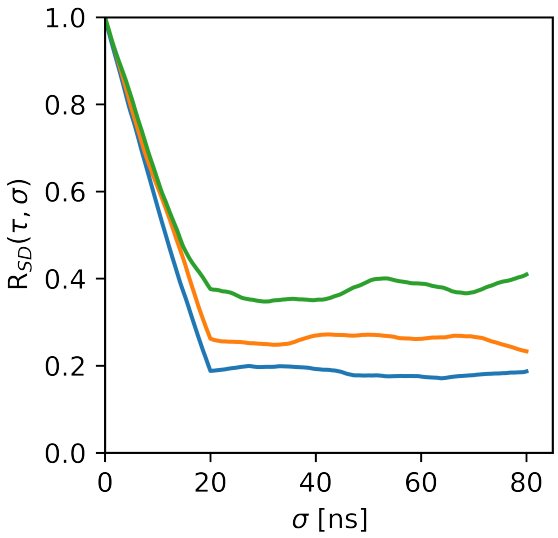

Figure S1: The normalized autocorrelation function of the squared displacements calculated from the Aβ_{16-22} monomer simulations with the CHARMM-Drude force field at 150 mM NaCl concentration. Results are shown as averages over 20 ns time windows with increasing lag time between them retrieved from the three MD runs performed for this Aβ_{16-22} monomer system.

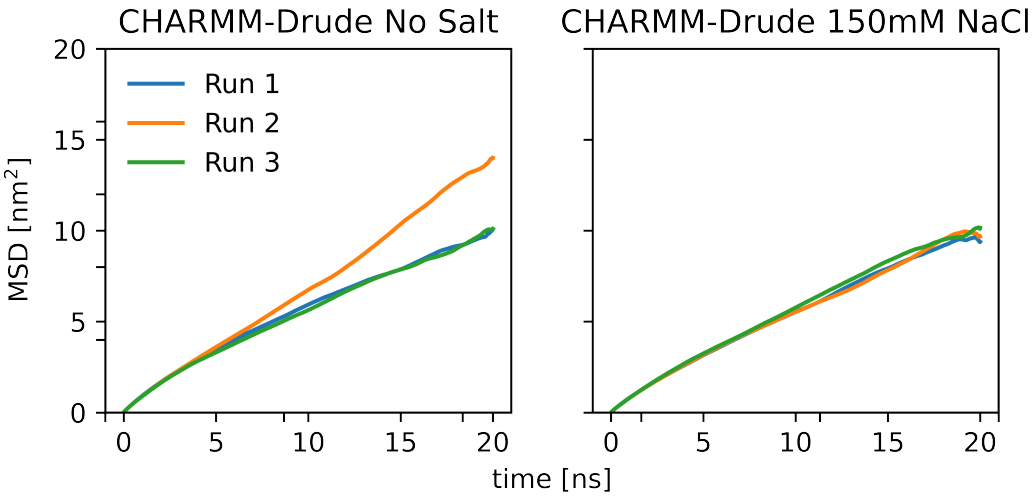

Figure S2: The MSD vs. time calculated with τ=20 ns and σ=20 ns for the Aβ_{16-22} monomers using the CHARMM-Drude force field.

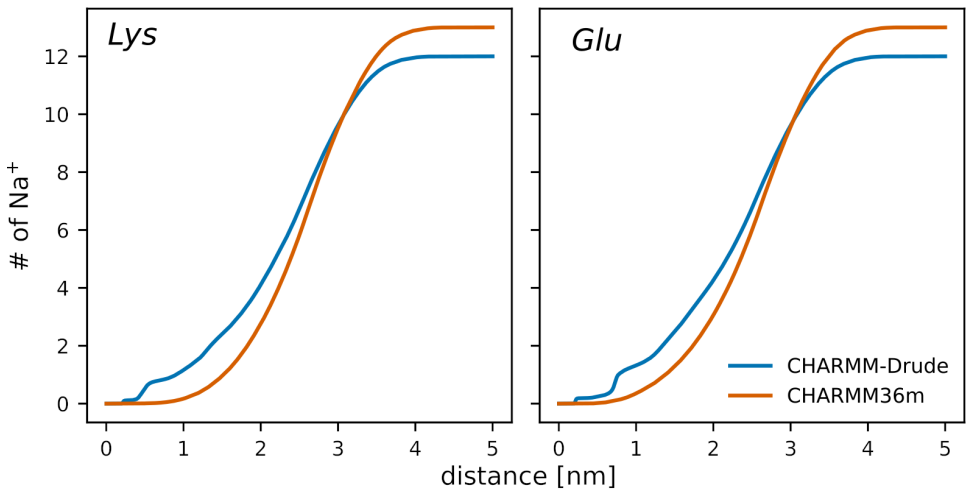

Figure S3: The number of sodium ions obtained by integration of the radial distributions of Na+ around the carbonly-oxygen atoms of K16 and E22.

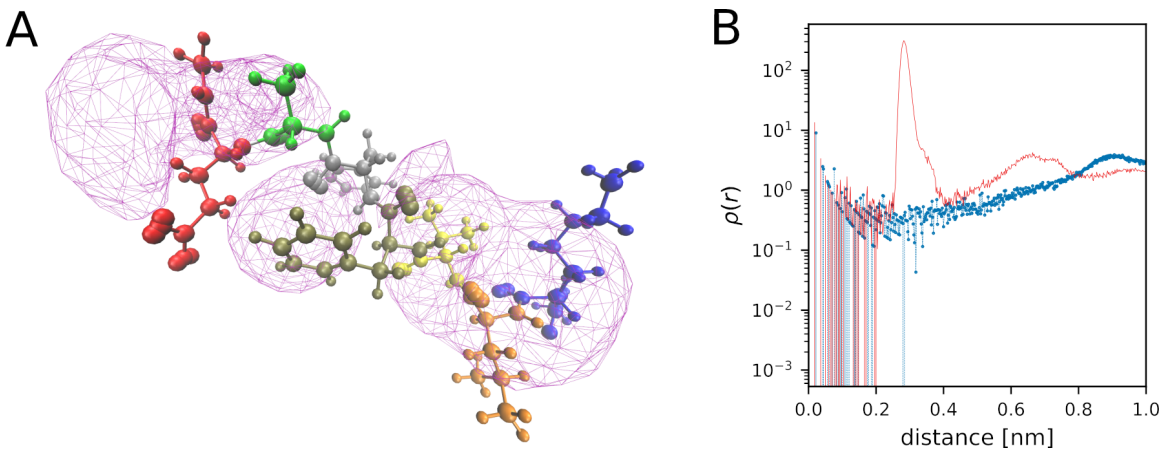

Figure S4: (A) The volumetric isosurface of the sodium ions around the Aβ_{16-22} peptide for the C-Drude force field. K16 and E22 are shown in blue and red, respectively. For clarity, only the results from the most populated structural cluster of the Aβ_{16-22} peptide is shown. (B) The radial distribution of Na^+ around the side-chain terminals of K16 (blue) and E22 (red).

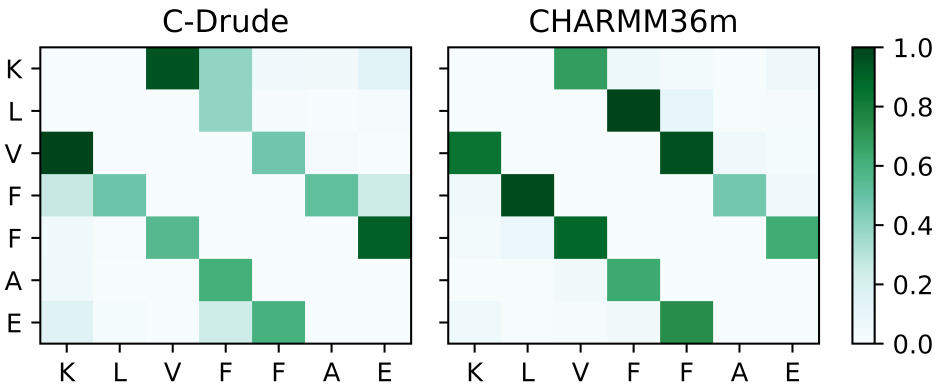

Figure S5: The time-averaged contact probabilities between residues of Aβ_{16-22} obtained from the monomer simulations including NaCl with C-Drude (left) and C36m (right). Self-contacts and direct-neighbor contacts are not shown for clarity (as they are 1.0). A contact between two residues is assumed to be present if the minimum distance between the two residues in question was within 0.5 nm.

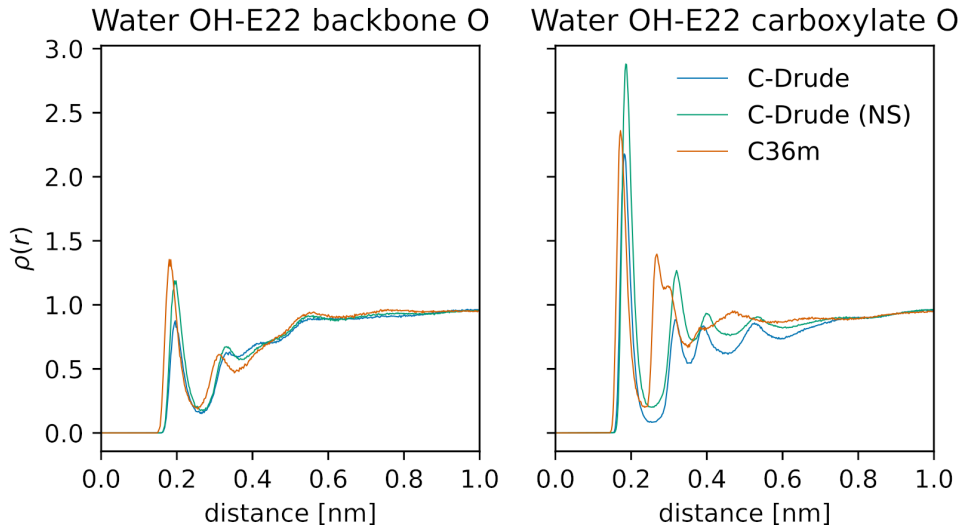

Figure S6: Radial distributions between the water H atoms around the O atom of the backbone (left) and the O atoms of the carboxylate group of the side chain (right) of E22. These distributions are the basis for H-bonds between the peptide and water with E22 being the acceptor.

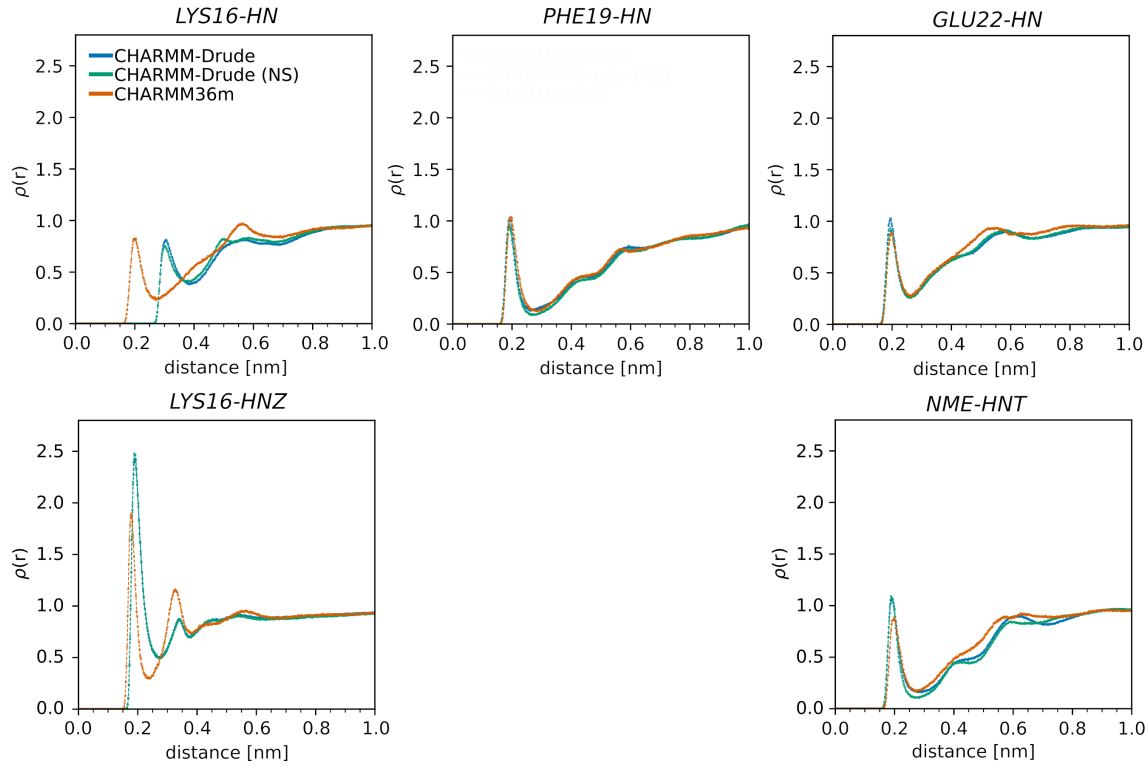

Figure S7: Radial distributions of the water O atoms relative to the H atoms bound to nitrogen atoms: backbone HN of K16 (top left) and side-chain HNZ of K16 (bottom left), backbone HN of F19 (middle), backbone HN of E22 (top right) and HNT of the C-terminal NME capping group (bottom right). These distributions are the basis for H-bonds between the peptide and water with the shown peptide residues being the donor. Please note that NME capping group is not available in CHARMM force fields as a separate residue but as an extension of the C-terminal residue, yet we keep this notation for clarity.

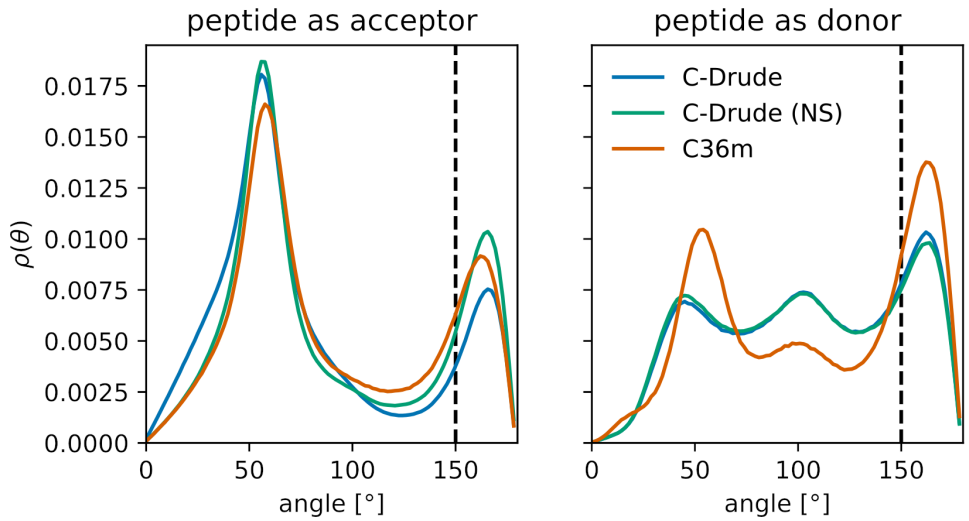

Figure S8: Water density as a function of the D–H–A angles at a D–A distance of 0.35 nm for the cases that the peptide groups act as acceptor (left) and as donor (right). Only the results between 0 and 180° are shown. The cutoff distance of 150° used for calculating the number of H-bonds is indicated by vertical dashed lines.

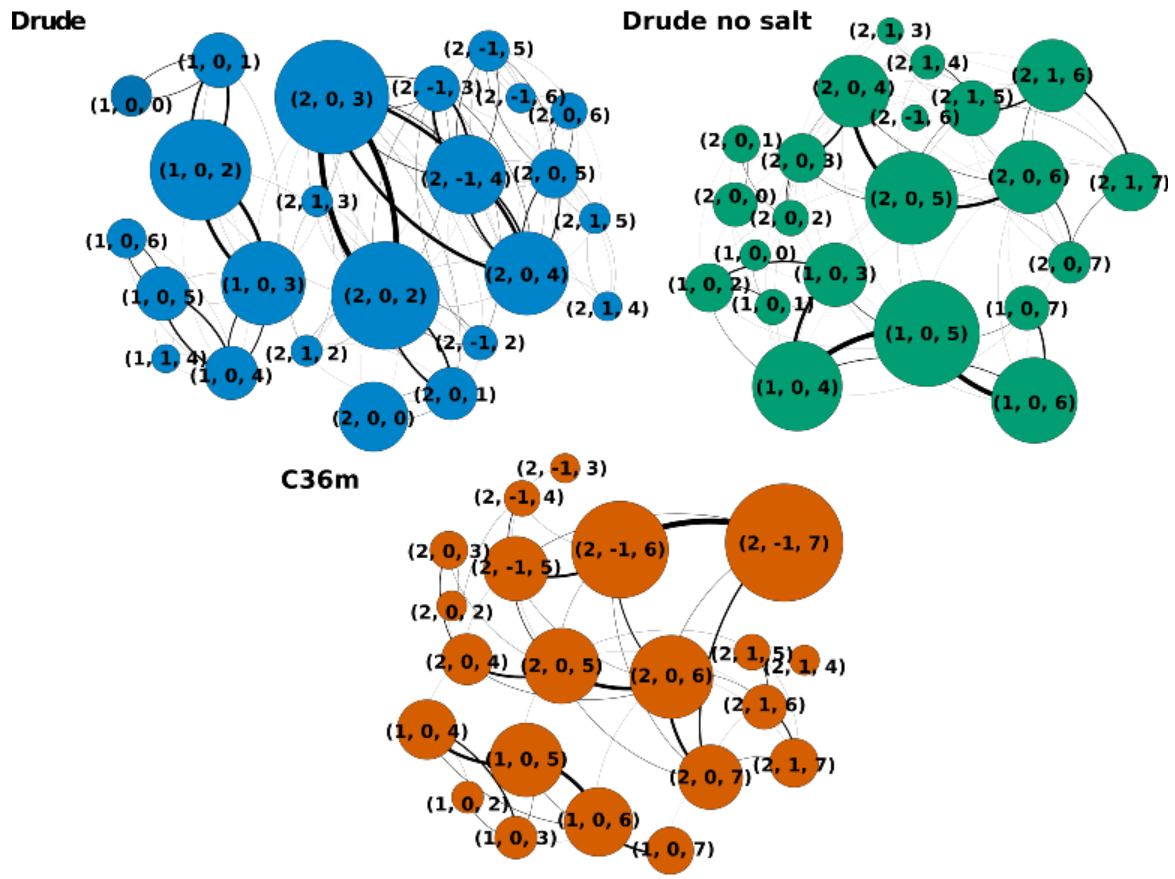

Figure S9: Transition networks of Aβ_{16-22} dimerisation obtained with (top) C-Drude with and without NaCl and (bottom) C36m. The states are defined by the oligomer size (1 or 2), the nematic order parameter (-1, 0, or 1) and the peptide-averaged amount of residues in β-strand conformation (from 0 to 7). The size of the nodes reflects the population of the corresponding state and the thickness of the lines corresponds to the transition probability. Only nodes with at least 1% of the total population are shown.

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