Electronic Supplementary Material (ESI) for Molecular Systems Design & Engineering.

Supporting Information

Accurate Calculation of Second Osmotic Virial Coefficients of Proteins using Mixed Poisson-Boltzmann and Extended DLVO Theory

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Table S1. Values of the Hamaker constant, A_H, used to calculate the dispersion potential according to Equation (11), explained in the main body. Scaling factors, which were necessary to scale all-atom LJ potentials to have the same depth like Hamaker potentials, are listed for clarity. Values of A_H for BPTI, RbnA, BSA and IgG1 were taken from literature.[1–4]

Protein	A_H [k_BT]	LJ scaling factor
BPTI	4.5	0.202
RbNA	3.5	0.145
ChmT	5	0.163
ConcA	8	0.223
BSA	3	0.062
IgG1	3	0.082

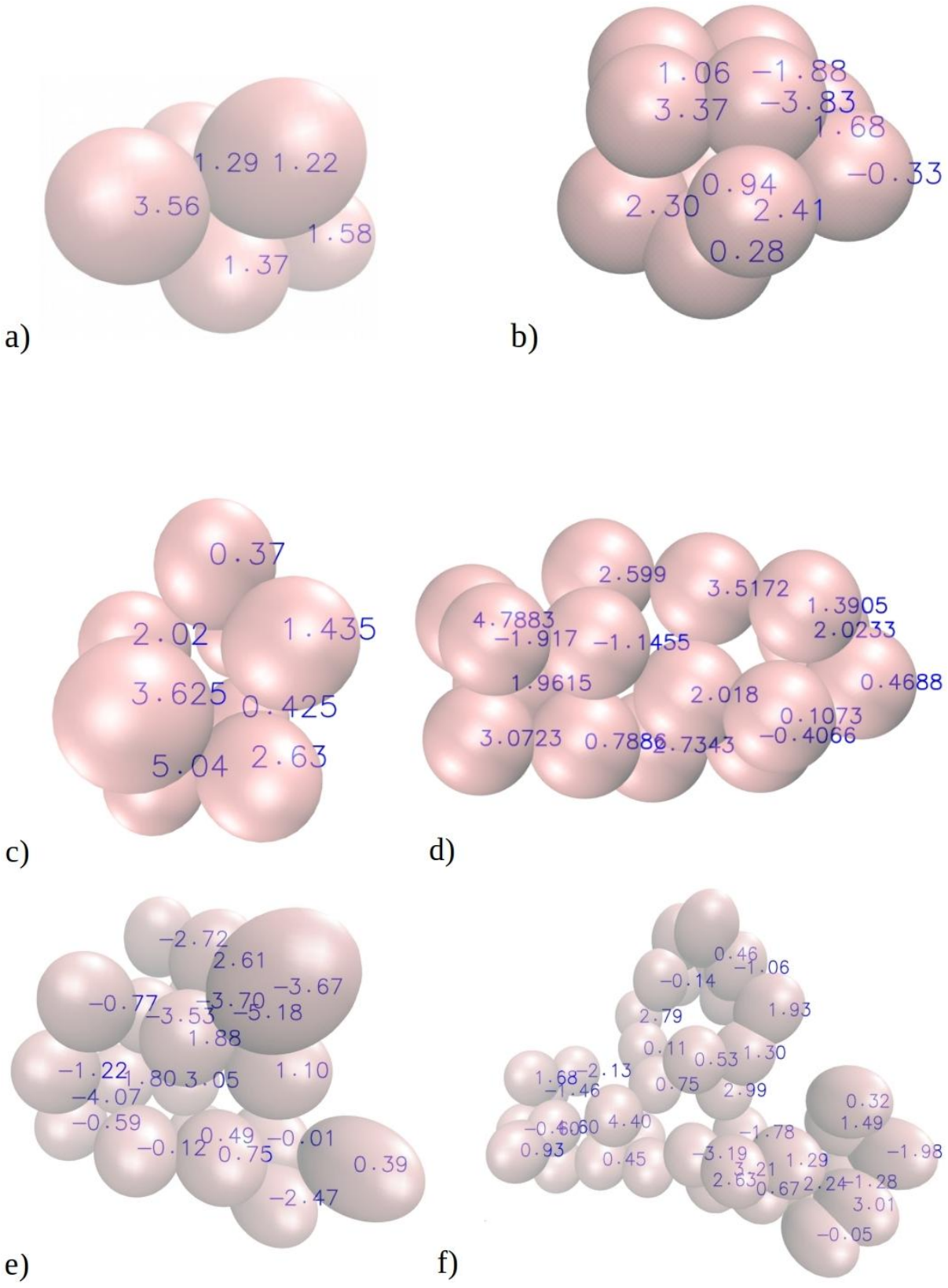


Figure S1. Charge distribution over coarse grained beads of six studied proteins: a) BPTI at pH 4.9, b) RbnA at pH 3, c) ChmT at pH 3, d) ConcA at pH 4, e) BSA at pH 7.4 and f) IgG1 at pH 6.5. Partial charges of atoms included in the CG beads were obtained by using PROPKA protonation protocol.

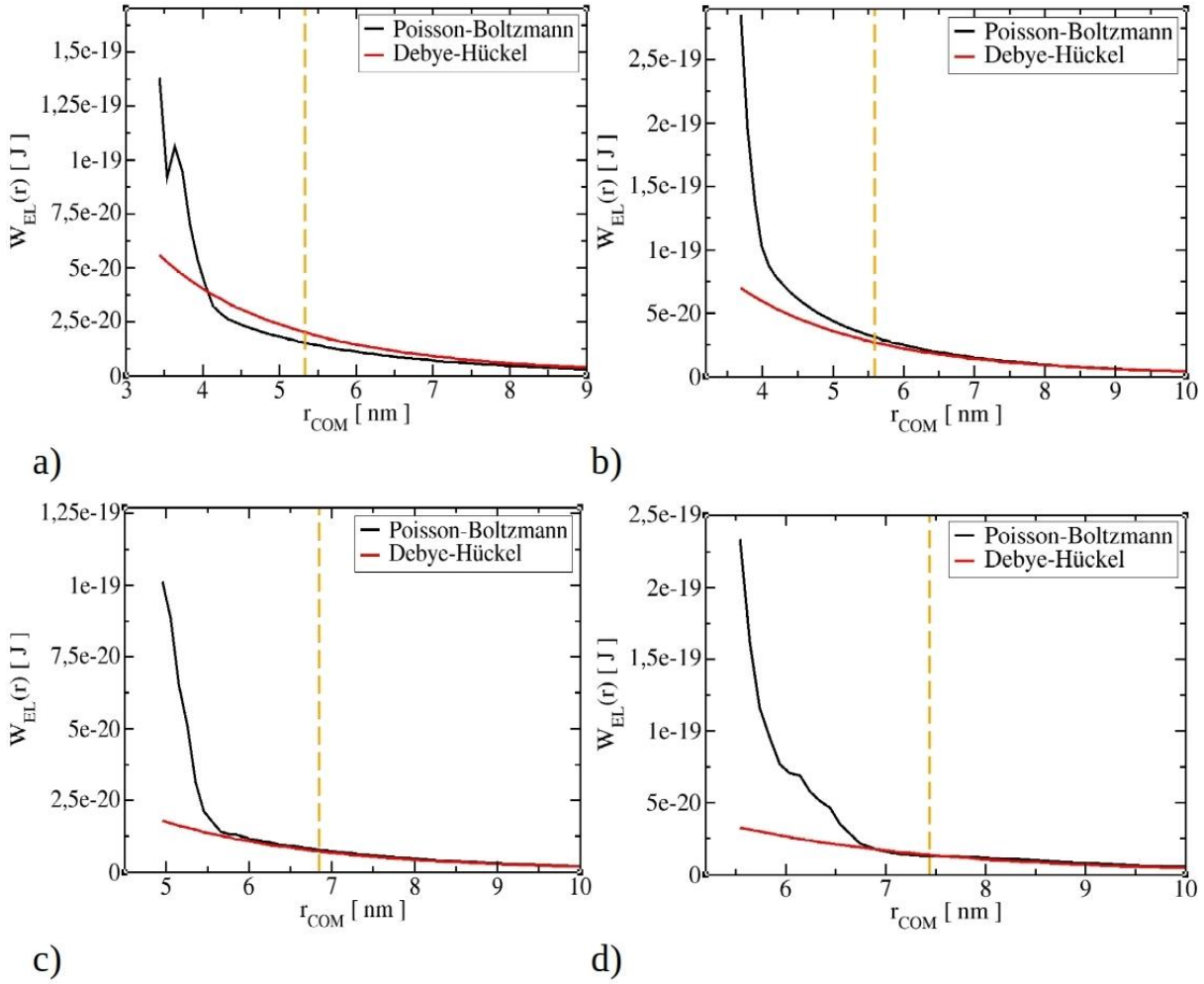
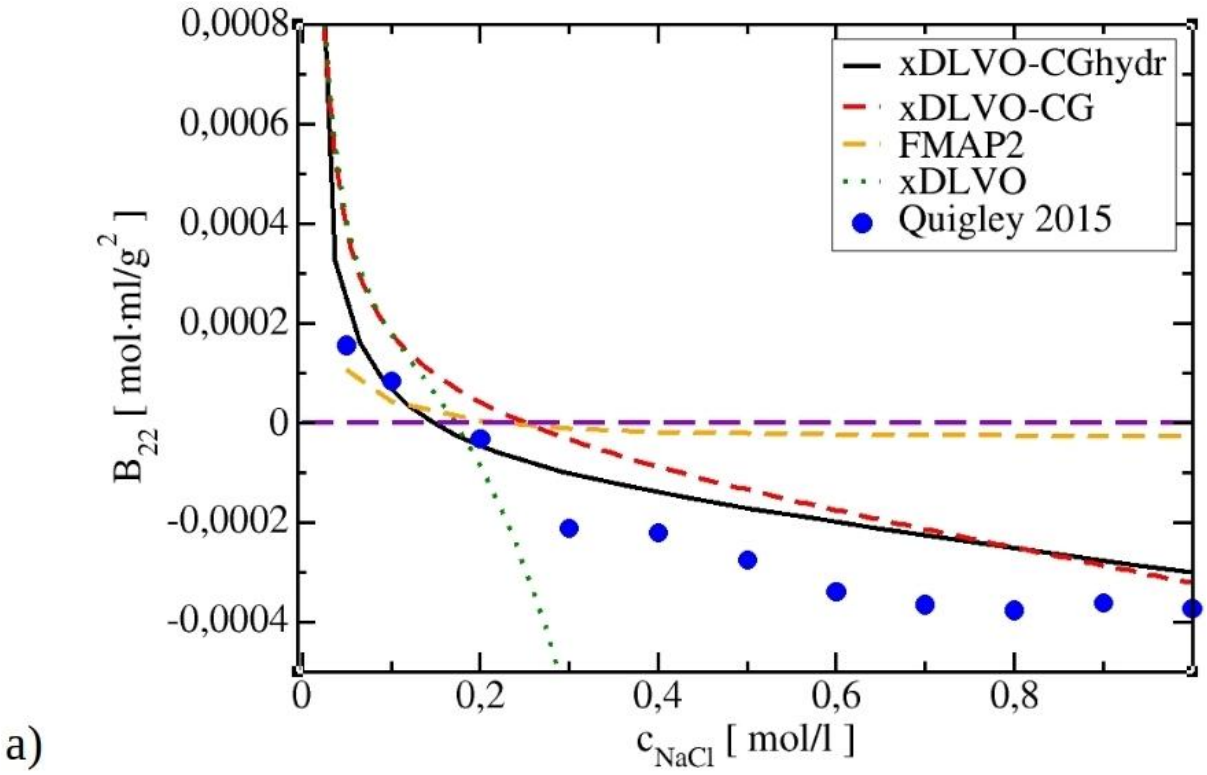


Figure S2. Comparison of calculated energy of electrostatic interactions between two a) RbnA, b) ChmT, c) ConcA and d) BSA proteins by solving Poisson-Boltzmann equations (applied to the full all-atom structure of proteins) and by using Debye-Hückel theory (applied to the coarse-grained model of proteins). The vertical dashed orange line indicates the COM distance (at R_0 + *2nm*), i.e. where electrostatic potential in xDLVO-CGhybr is switched from Poisson-Boltzmann to Debye-Hückel model.



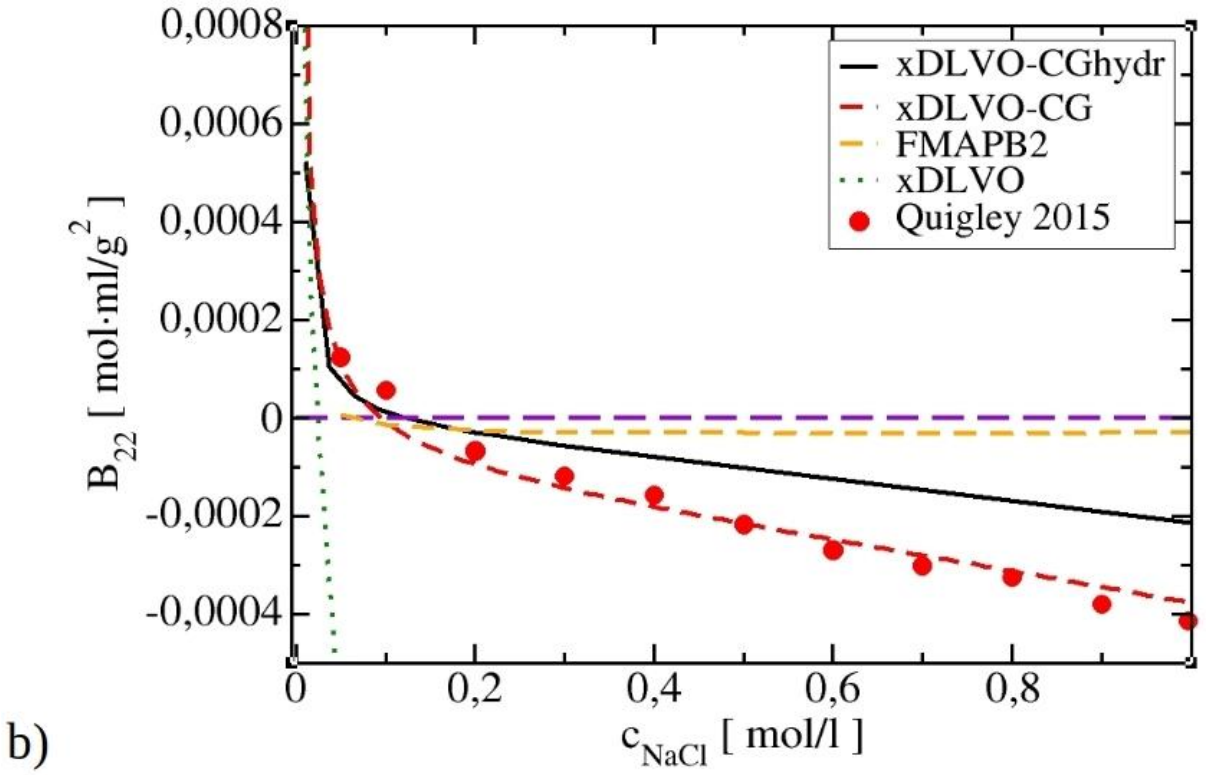


Figure S3. Calculated B_{22} coefficients for ConcA at pH 4 (b) and at pH 5 (b) as a function of NaCl concentration. B_{22} values are compared with the values obtained with xDLVO-CG (dashed red), FMAPB2 (dashed orange) and xDLVO (green dots) models and experimental results (blue and red circles).

References

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2. M. Farnum and C. Zukoski, *Biophys. J.*, 1999, **76**, 2716–2726.
3. S. Pusara, P. Yamin, W. Wenzel, M. Krstić and M. Kozlowska, *Phys. Chem. Chem. Phys.*, 2021, **23**, 12780–12794.
4. M. Andersen and S. Nir, *Polymer*, 1977, **18**, 867–870.