Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

A coarse-grained xDLVO model for colloidal protein-protein interactions

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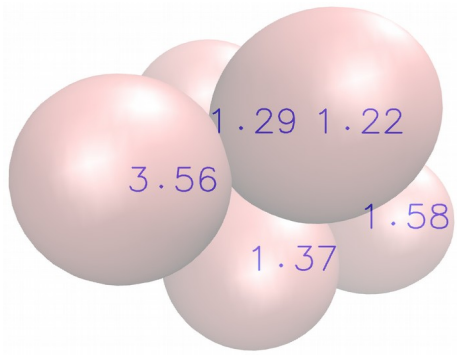
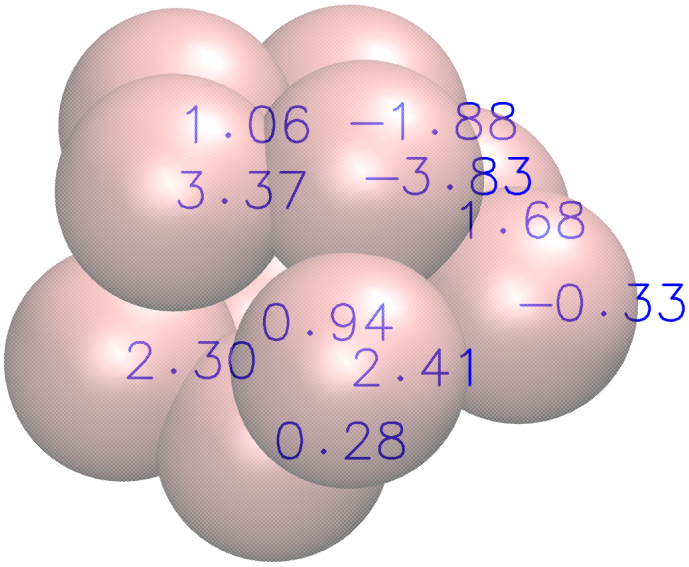
Table S1. Charges of proteins at different pH obtained by protonation protocol (PROPKA/H++) in comparison with experimental values and values calculated in xDLVO.[1]

LYZ			
pH	**PROPKA**	**Experiment**	**xDLVO charge**
3	+14	+9	+16.18
4.5	+11	+10	+10.03
5	+11	+9 (1M KCl, pH 5.5)	+8.77
7	+9	+8	+7.73
8	+8	+7.50	+5.39
BSA			
pH	**PROPKA/H++**	**Experiment**	**xDLVO charge**
6.2	-5	-13.50/-9	-9.85
6.2 (H++)	-8	-13.50/-9	-9.85
7.4	-16	-20.30	-20.06
Subs			
pH	**PROPKA**	**Experiment**	**xDLVO charge**
5.5	+6	n/a	+4.13
7	+4	n/a	+3.09
IgG1			
pH	**PROPKA**	**Experiment**	**xDLVO charge**
5	+68	+10.20/12/24	+38.05
5.75	+46	+5.10/6	+25.83
6.5	+27.38	+5/10.60/18.90/22.80	+18.88

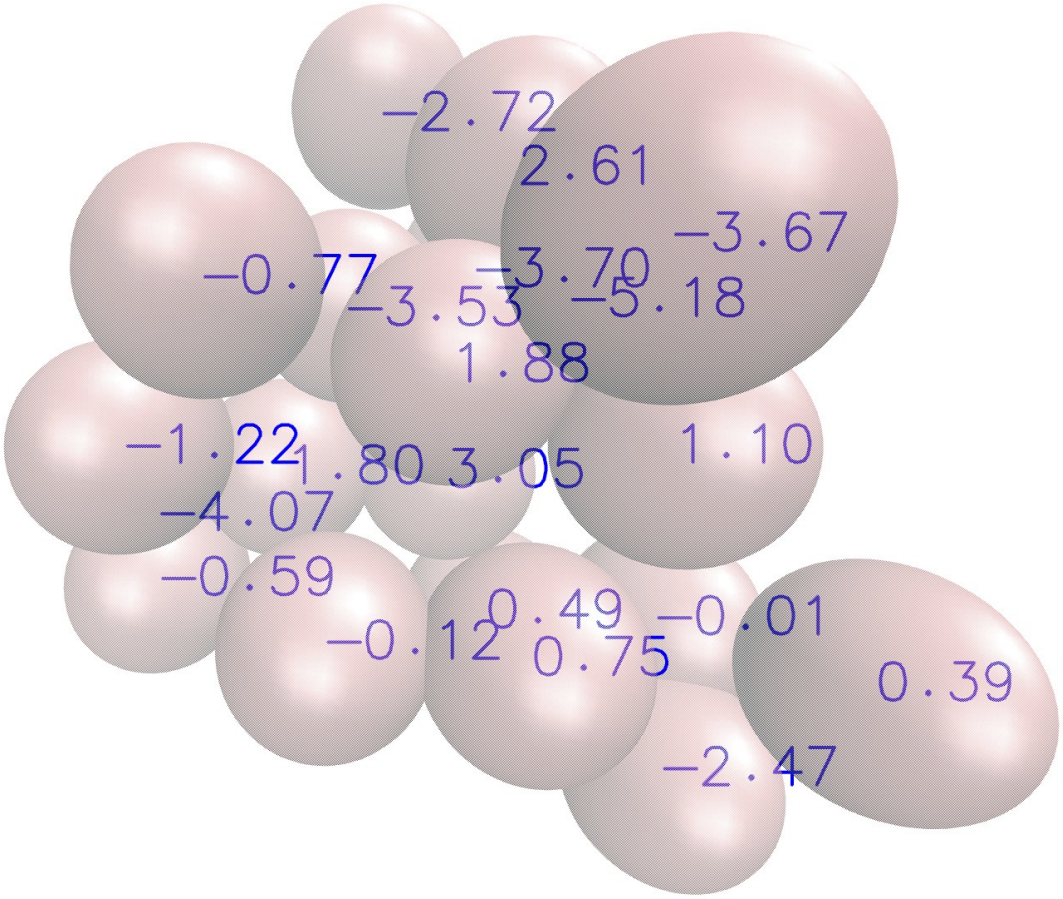
a) LYZ, pH 7



b) Subs, pH 5.5



c) BSA, pH 7.4



d) IgG1 pH 6.5

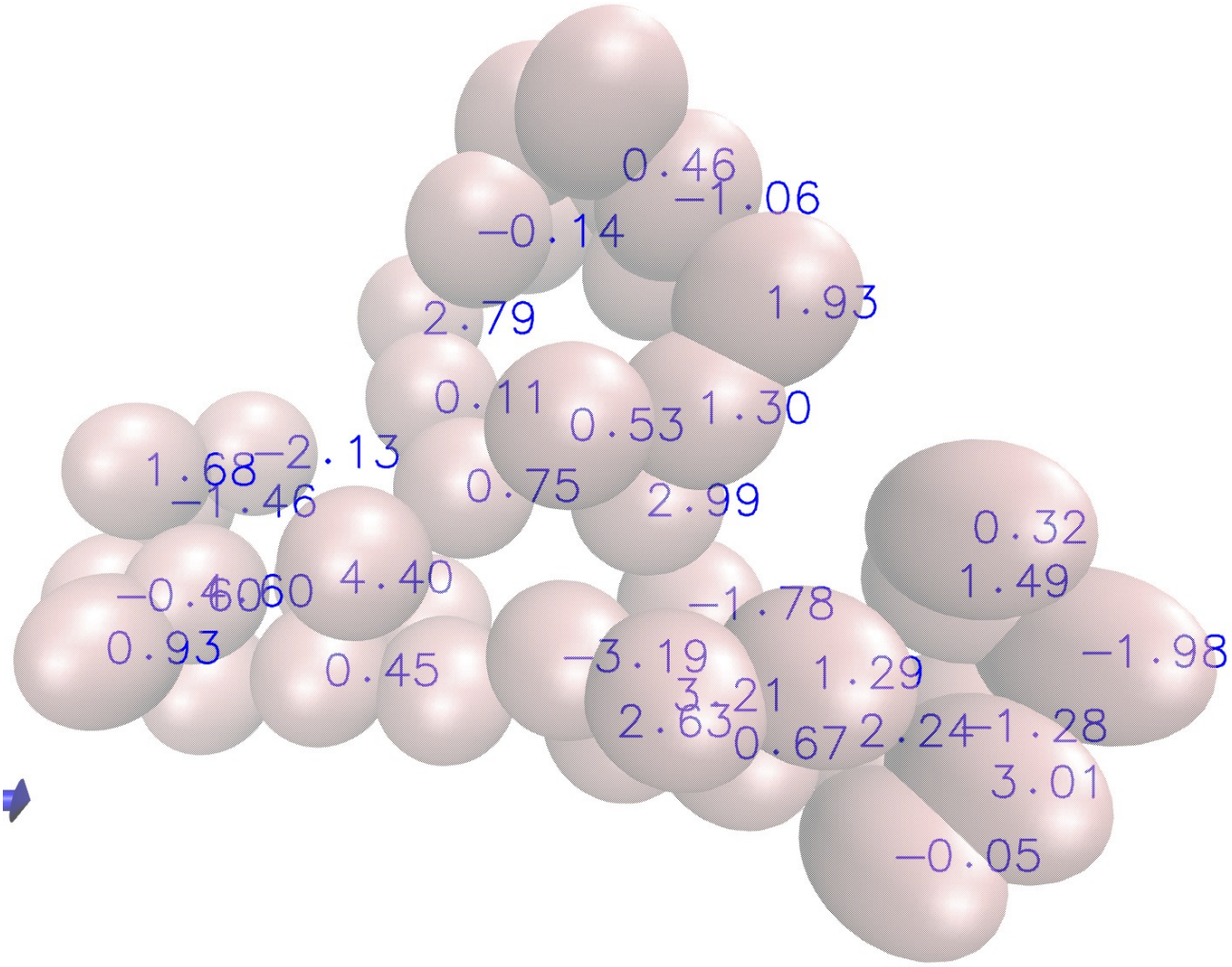


Figure S1. Charge distribution over coarse grained beads of four studied proteins. Partial charges of atoms included in the CG beads were obtained by using PROPKA protonation protocol.[2,3]

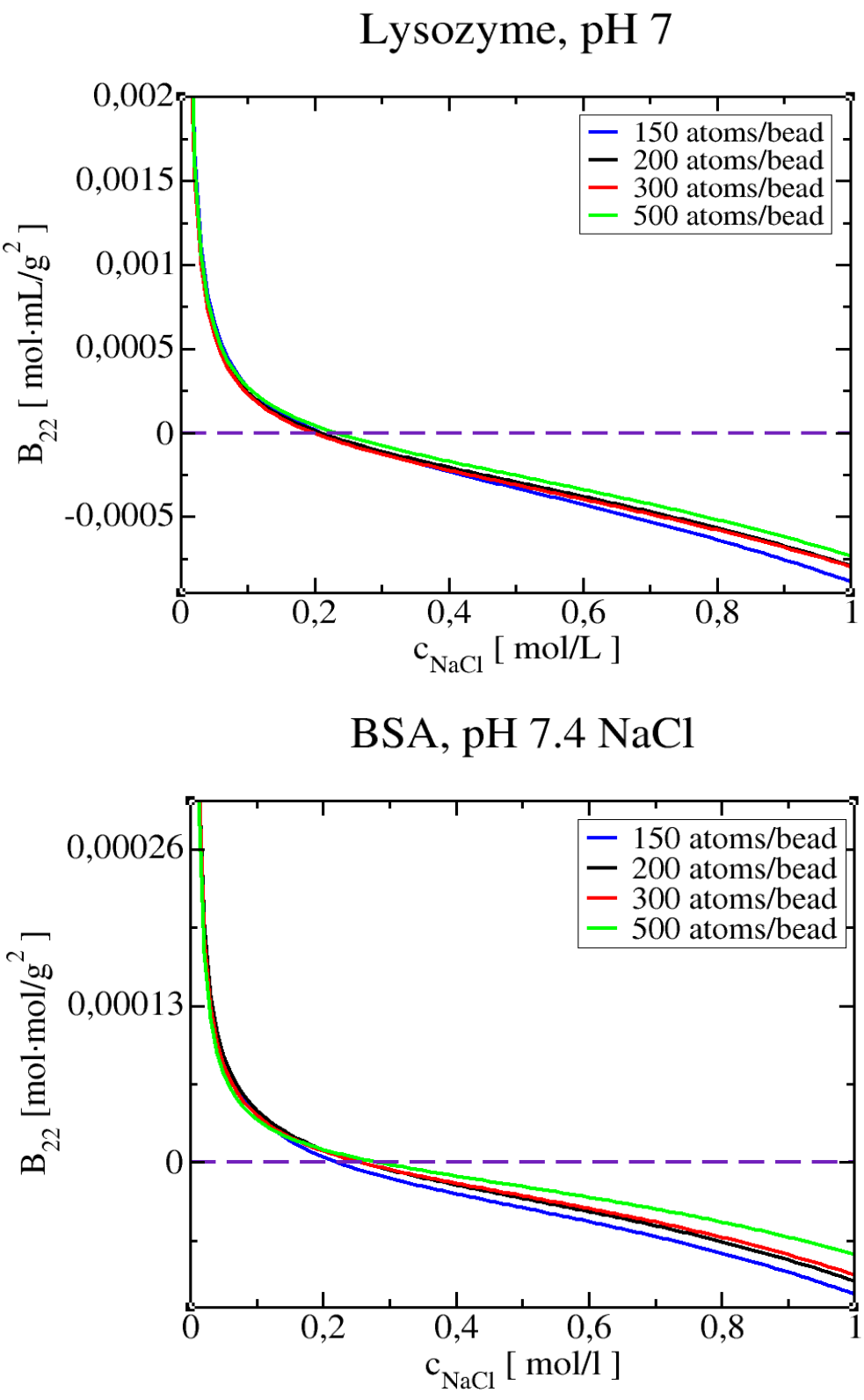


Figure S2. Influence of size of coarse-graining: number of atoms per CG bead, on the calculated B_{22} values for lysozyme at pH 7 and BSA at pH 7.4 in NaCl solution.

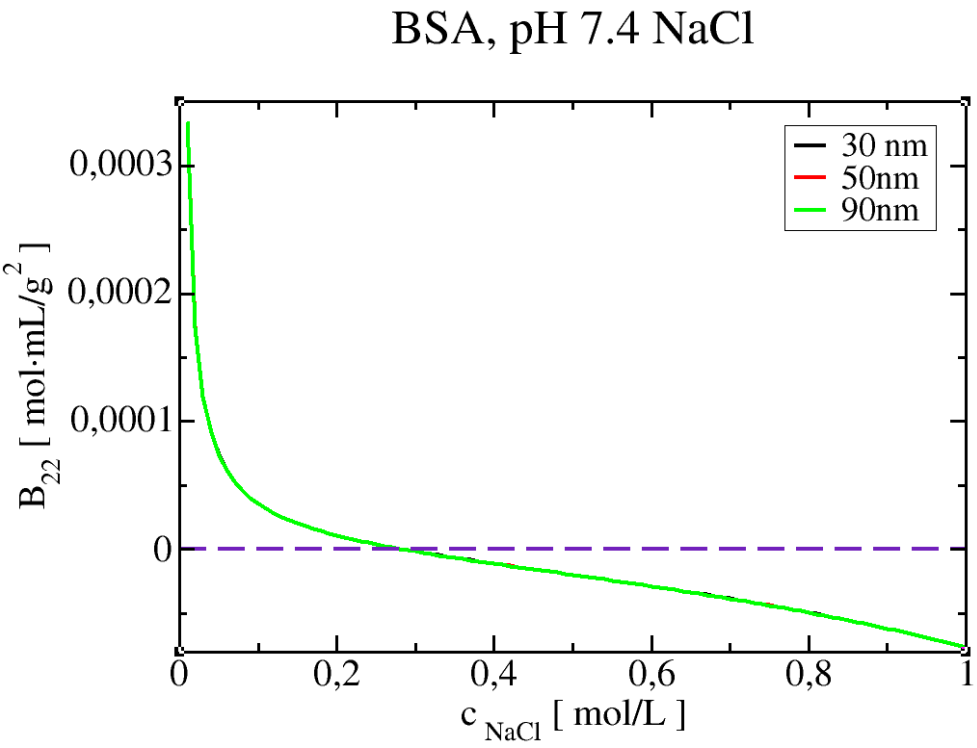


Figure S3. Influence of pulling distance between proteins used to calculate PMF for calculating B_{22} values of BSA at pH 7.4 in NaCl.

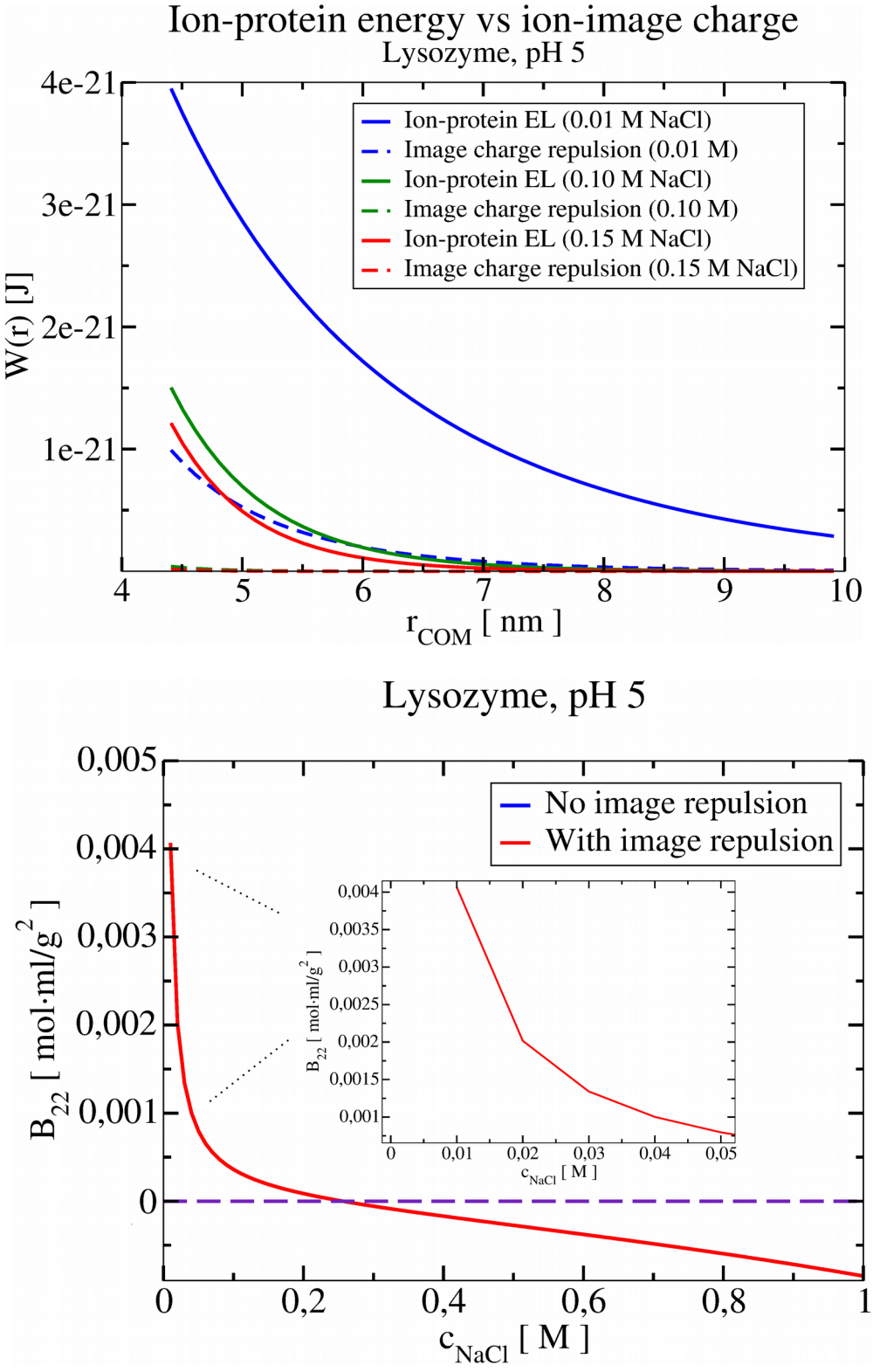


Figure S4. The influence of the image-based repulsion interactions between salt ions (NaCl) and proteins (LYZ at pH 5) in xDLVO-CG model (upper panel). Equations for electrostatic shielding were implemented according to Ref. 4. B_{22} of LYZ at pH 5 from PMF including image-based ion-protein repulsion interactions (lower panel). No difference is noticed after the inclusion of the image-charge-based repulsion in the protein-ion electrostatic interactions.

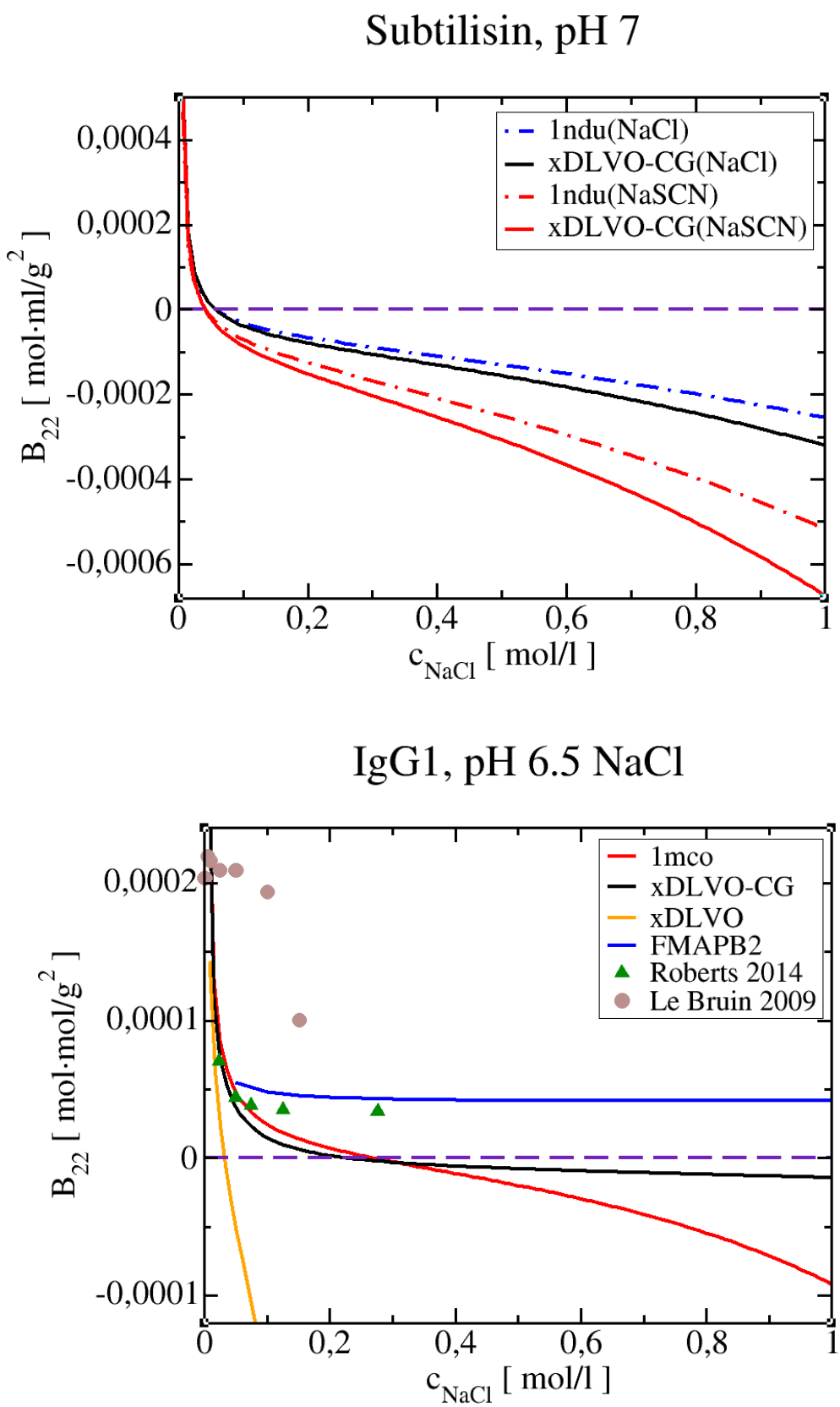


Figure S5. Change of the B_{22} coefficients with the change of salt concentration for Subs at pH 7 and b) IgG1 at pH 6.5 in NaCl.

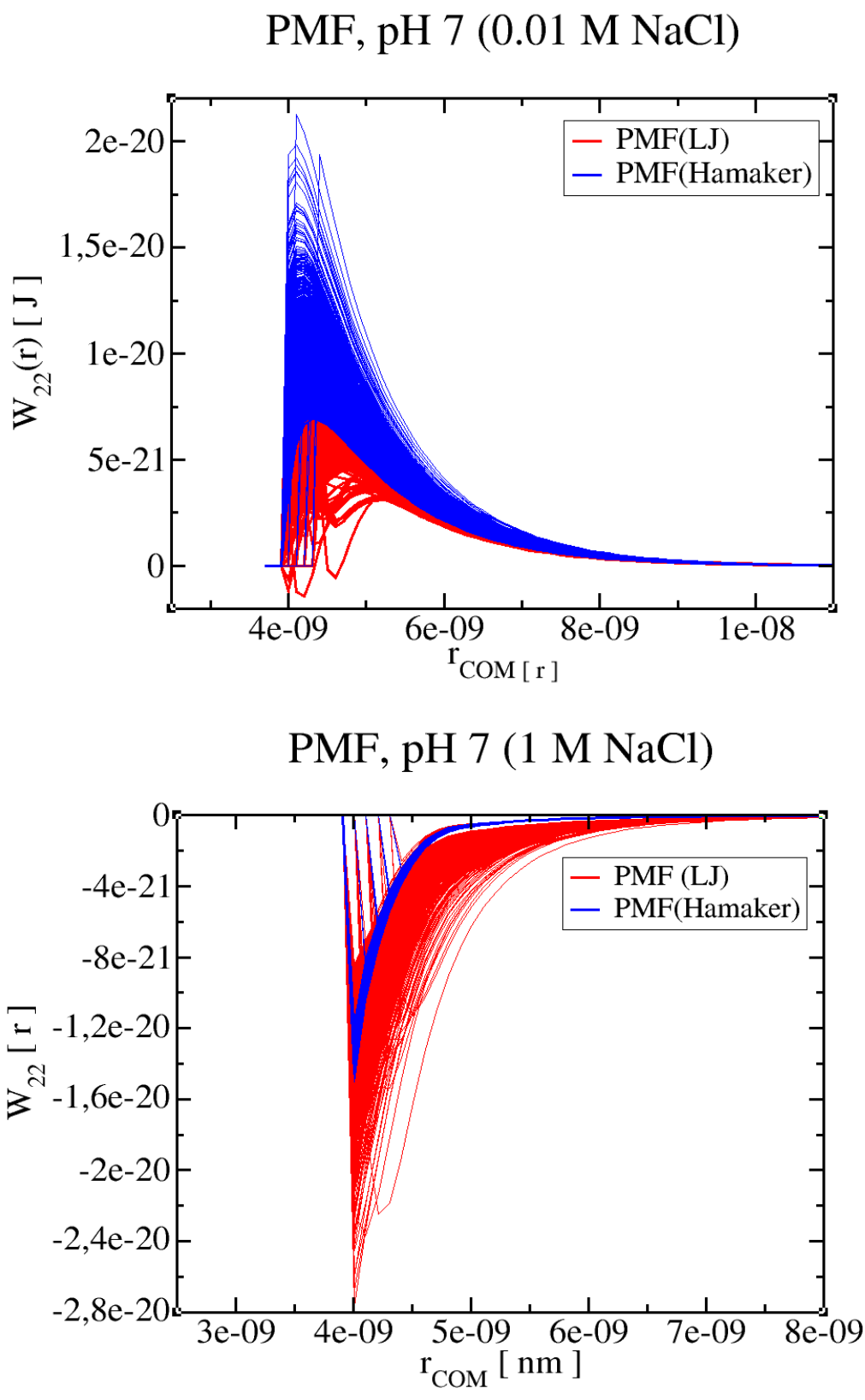


Figure S6. Comparison of PMF obtained from 1328 starting structures during PPI sampling protocol for LYZ at pH 7 at 0.01 M and 1 M NaCl.

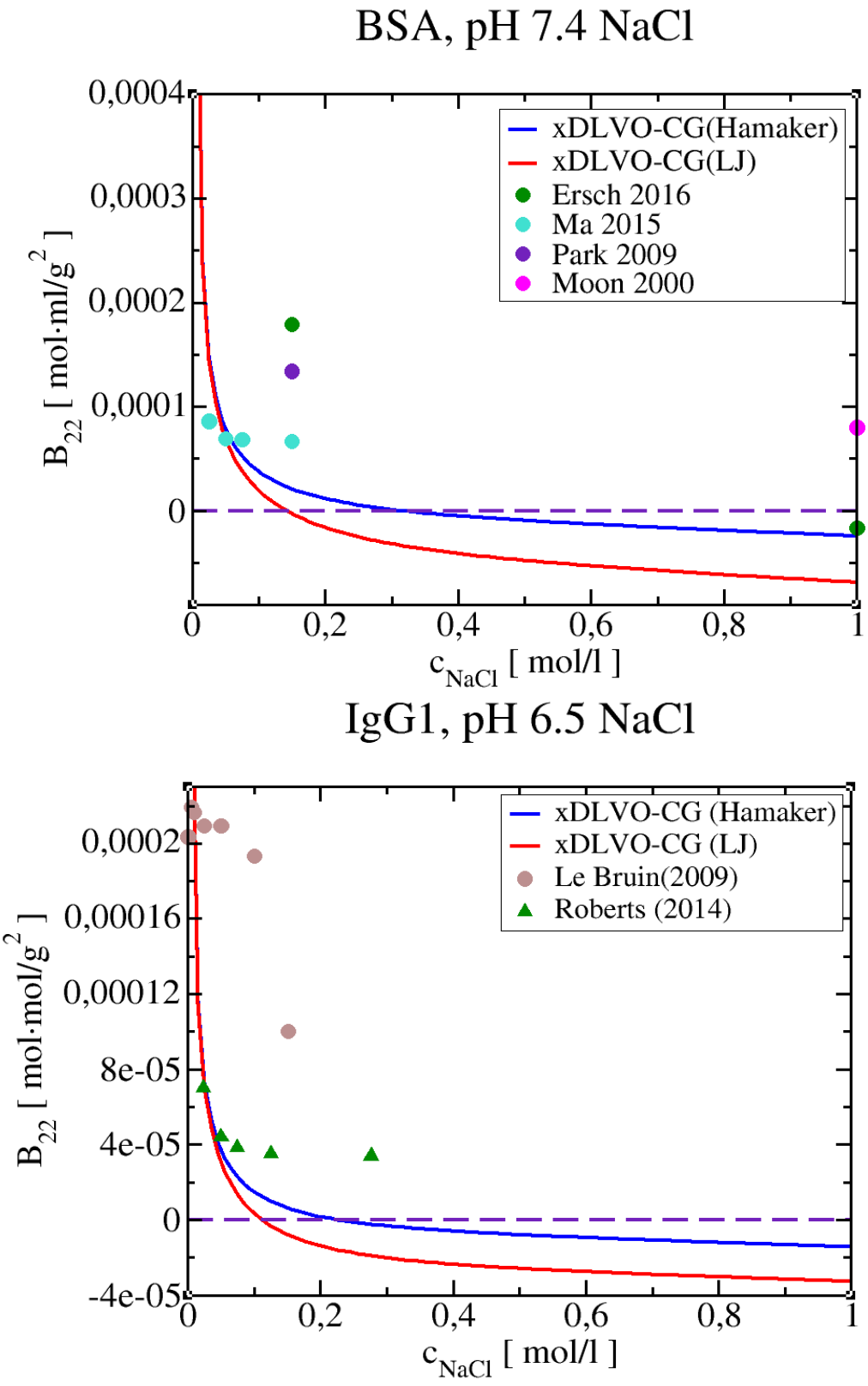


Figure S7. Comparison of the calculated B_{22} coefficients with Hamaker and Lennard-Jones dispersion potential type for a) BSA at pH 7.4 and b) IgG1 at pH 6.5 in NaCl.

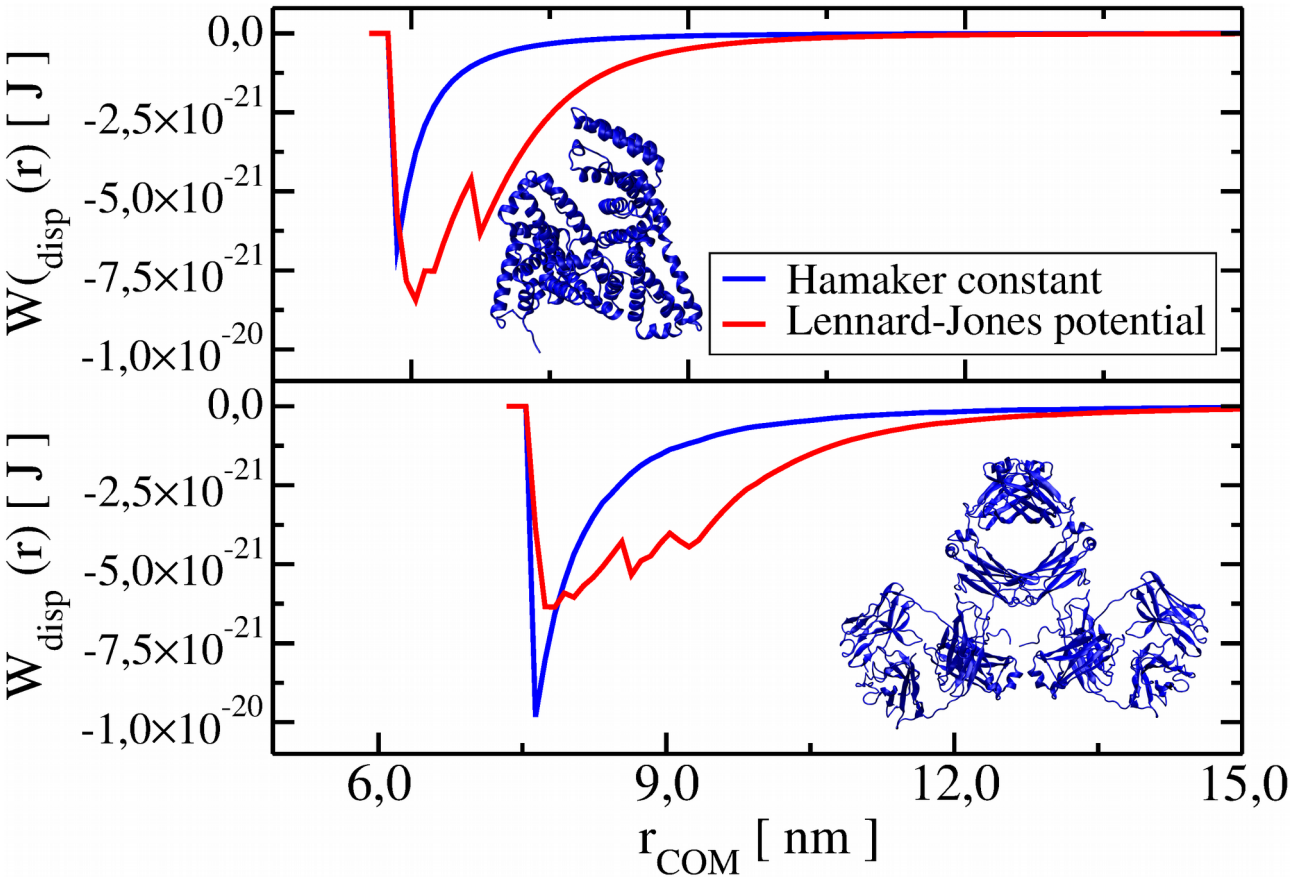


Figure S8. Comparison of the dispersion potential using Hamaker constant and Lennard-Jones potential for BSA (upper panel) and IgG1 (lower panel).

References

1. Herhut, M., Brandenbusch, C. & Sadowski, G. Modeling and prediction of protein solubility using the second osmotic virial coefficient. *Fluid Phase Equilibria* **422**, 32–42 (2016).
2. Li, H., Robertson, A. D. & Jensen, J. H. Very fast empirical prediction and rationalization of protein pKa values. *Proteins Struct. Funct. Bioinforma.* **61**, 704–721 (2005).
3. Søndergaard, C. R., Olsson, M. H. M., Rostkowski, M. & Jensen, J. H. Improved Treatment of Ligands and Coupling Effects in Empirical Calculation and Rationalization of p K_a Values. *J. Chem. Theory Comput.* **7**, 2284–2295 (2011).
4. Cherstvy, A. G. & Winkler, R. G., Polyelectrolyte Adsorption onto Oppositely Charged Interfaces: Image-Charge Repulsion and Surface Curvature. *J. Phys. Chem. B* **116**, 9838−9845 (2012).