Thermodynamics of Ion Pair Formations in Proteins

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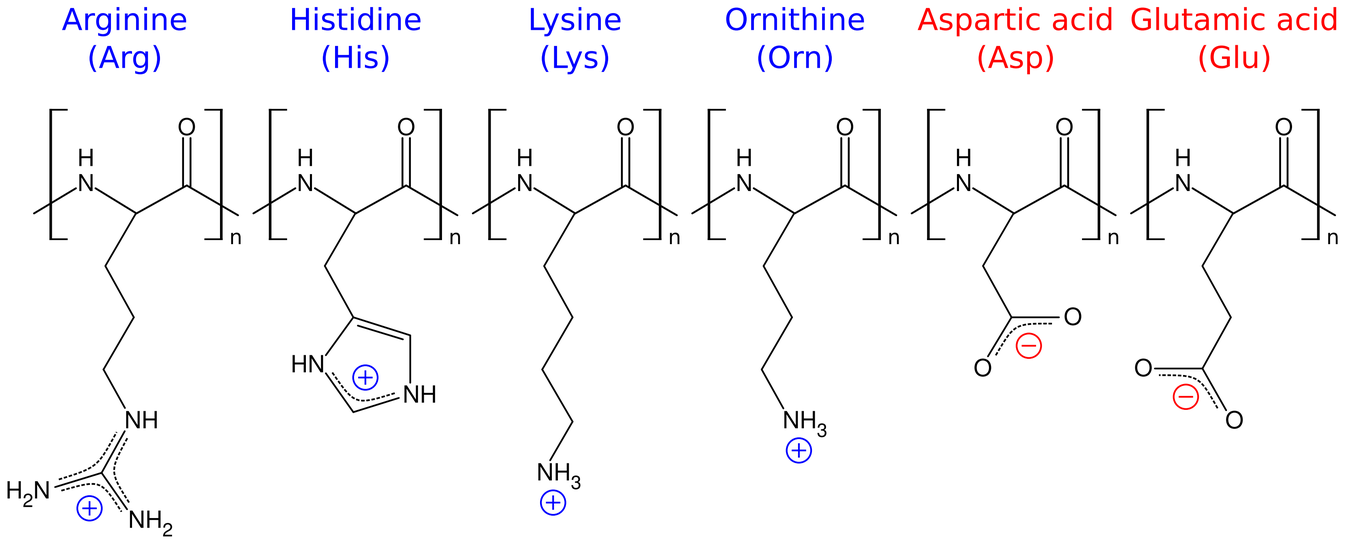
Abstract

Seven of the 20 naturally occurring amino acids in proteins are ionizable and may exist in negatively or positively charged form dependent on *pH* and their pK_as. Interactions between the positively and negatively charged amino acids (electrostatic bonds or salt bridges, sometimes called ionic hydrogen bonds) are among the most important interactions in proteins.

Ionic groups on protein surfaces usually make them soluble (preferentially interact with water), but in some cases the oppositely charged amino acid functional groups preferentially interact with each other rather than water. Thermodynamics of ionic interactions in proteins is not well understood, thus it is important to determine the average standard values of thermodynamic parameters (such as enthalpy, entropy, Gibbs free energy, heat capacity, etc.) of ionic interactions using model ionic compounds.

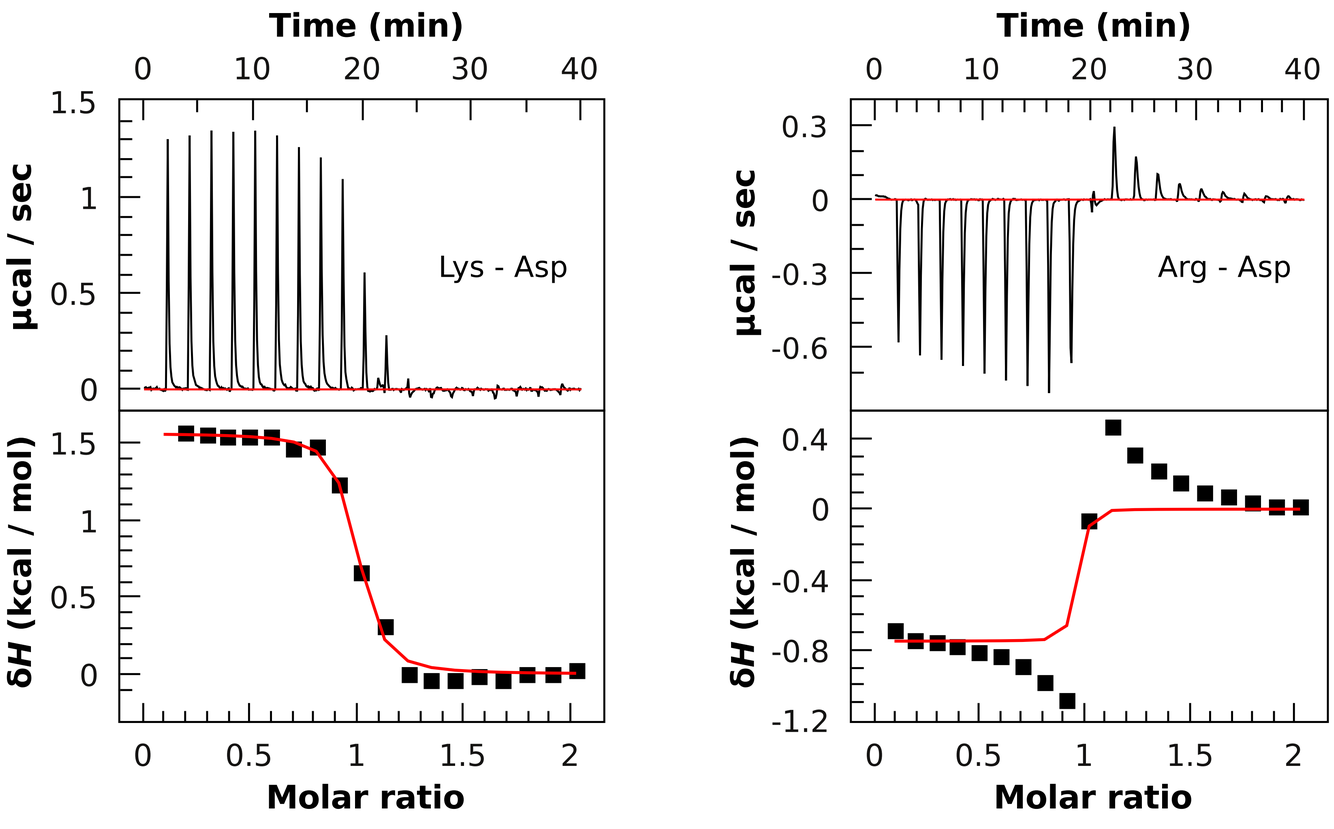
In this work, the isothermal titration calorimetry (ITC) technique is used to measure the thermodynamic properties of interaction between oppositely charged amino acid homopolymers (positive – Arg, His, Lys, Orn and negative – Asp, Glu).

Charged amino acids

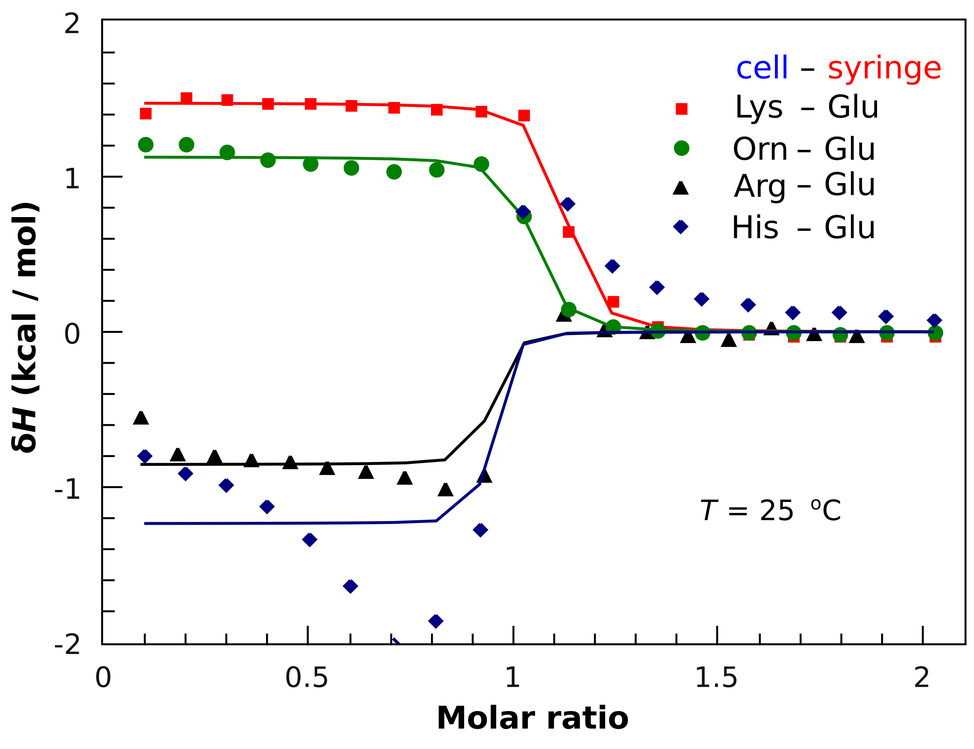


Polyamino acid homopolymers (length ~50-100 a.a.) were used in ITC experiments.

Isothermal titration calorimetry curves

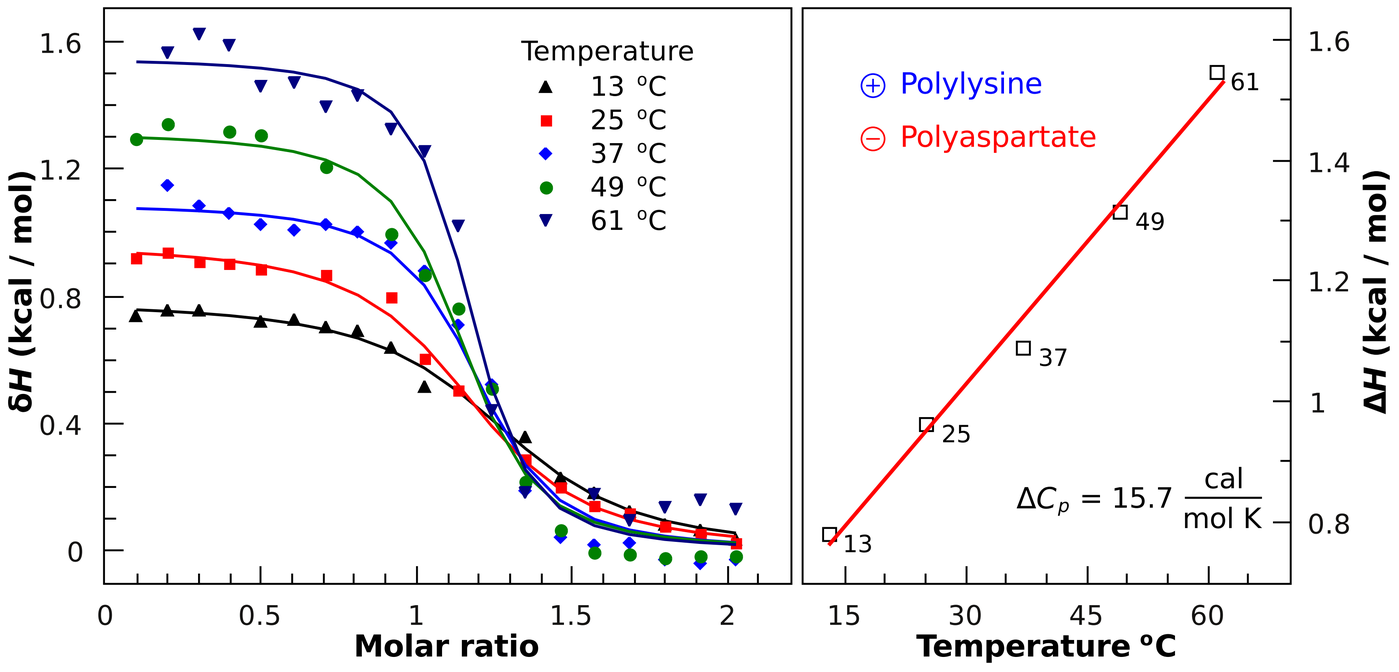


Interaction of polylysine (left) and polyarginine (right) with polyaspartic acid (syringe)



Interaction of polycationic amino acids with polyglutamic acid

Dependence on temperature



T-Dependence of polylysine (cell) interaction with polyaspartate (syringe)

Conclusions

- Isothermal titration calorimetry results showed that oppositively charged amino acid homopolymers interact with each other.
- Stoichiometry of interaction was 1 positive amino acid with 1 negative amino acid.
- Interaction K_b depends on the model (mathematical model is in progress).
- The enthalpies of Arg and His interaction with Asp and Glu were small and exothermic, while Lys and Orn – endothermic.
- The heat capacity was small and positive as determined from the enthalpy dependence on temperature.

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