Towards a Simple Model for Understanding Peptide Aggregation Based on the Thermodynamics of Binary Solutions

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Peptide aggregation is an important problem related to a variety of diseases. Our understanding of peptide aggregation could be dramatically improved if one could rationalize the differences in aggregation behavior between different peptide sequences. Here, we present our initial efforts in this direction. The pair preferential interaction model (PPIM) attempts to decompose the preferential interaction between pairs of peptide molecules at infinite dilution in water into contributions arising from the different functional groups present in the peptide. The preferential interactions are obtained from activity data on a variety of amino acids and small peptides using the Kirkwood-Buff (KB) theory of solutions as a guide. It is observed that, for the albeit limited number of systems studied so far, the decomposition into groups provides consistent results across a series of solutes that appear to make physical sense.