Journal of Chemistry

Hindawi

Special Issue on

Amino Acids and Peptides: Study of Conformational, Electrostatic, and Dynamic Behaviors Using Computations

CALL FOR PAPERS

Amino acids and peptides are fundamental biomolecules that play important functions in living systems. Unlike its complicated successor proteins, amino acids and peptides have the reasonable size that can be well controlled and thoroughly studied while maintaining similar chemical functional groups that play crucial roles in various interactions occurring along biological pathways. Thus, amino acids and peptides are good model systems for studying many fundamental chemistry problems that are highly related to life sciences. Using computational chemistry methods including both quantum mechanics (QM) and molecular mechanics (MM) state-of-the-art techniques, various aspects related to amino acids and peptides such as conformational preferences, spectrum characteristics, interaction energetic profiles, and dynamic behaviors have been and are being effectively studied since last decades and have accumulated much valuable knowledge that can help people to more precisely and fundamentally understand the behavior of proteins and other larger biomolecular systems.

In this special issue, we invite the submission of original research articles as well as review articles that cover broadly defined researches on amino acids and peptides using advanced computational approaches.

Potential topics include, but are not limited to:

- Conformational behavior of amino acids in gas phase and bulk phase including determination of protonation states, zwitterion forms, and isomerism
- Energetic properties of amino acids and peptides
- Secondary structure preference and conformational changes of peptides in gas phase and bulk phase
- Interactions of amino acids and peptides with biology environmental species such as water, metal ions, and larger biomolecules
- Spectra characteristics of amino acids and peptides
- Inter- and intramolecular hydrogen bonding properties of amino acids and peptides
- Dynamics behavior of amino acids and peptides in bulk phase
- Aggregation of peptides
- Amino acids and peptides on the interface, such as solid surface
- Use of amino acids and peptide models to optimize molecular mechanics force fields
- Amino acids and peptides involved in chemical reactions
- Peptide based drug discovery and development

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