From spectroscopic signatures to 3-D structure of protein building blocks

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A comprehensive analysis of the properties of amino acids oligomers and the detailed characterization of their supra-molecular structure, orientation and dynamics is the basic requirement for understanding the structure-function relationships. Molecular structures can be "directly" obtained from microwave (MW) spectroscopy (amino acids and small peptides) or X-ray crystallography and cryo-EM (proteins). On the other hand, structure and properties can be monitored by different spectroscopic measurements such as infrared (IR), Raman, Resonance Raman, UV-vis absorption or fluorescence or circular dichroism (CD), electron spin resonance (ESR). However, it is seldom straightforward to link directly the experimental data to the desired information on the specific structure and properties of complex molecular systems. Moreover, traditionally, these experimental results are analysed separately. Quantum chemistry computations provides a missing link between different experimental techniques, which could not be integrated and fully explored otherwise.
I will discuss status and perspective of the project aimed at spectroscopy studies for systems of increasing size and complexity, from small prebiotic molecules to large bio-molecules, complexes and oligomers. We devise effective theoretical schemes through step-by-step strategy, starting from comparison with highly accurate theoretical models and/or state-of-the art experimental data for isolated amino acids and small peptides, gradually moving towards larger and more complex molecular systems featuring dispersion interactions, hydrogen bonding, variable local stereochemistry-conformation, and chirality.

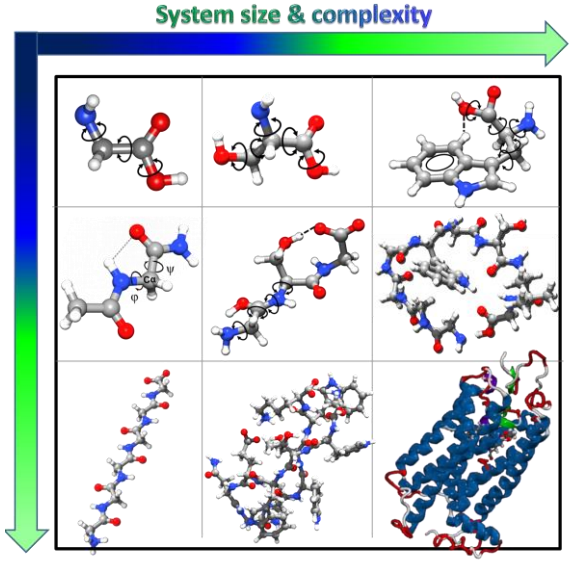

Figure 1: Step-by-step derivation and validation of computational models, from small prebiotic molecules to larger bio-molecules, complexes and oligomers.

References

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