Modeling Biological Systems with Semi-Empirical Methods of Quantum Chemistry

4-hour theoretical/practical mini-course

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In chemistry, one of the great challenges in the area of molecular modeling is the complete chemical-quantum treatment of highly complex systems, such as: biomolecules, materials, surfaces, polymers, solutions, etc. [1]. When linear scaling techniques are used in today's computers, it is already possible to model large molecules with about 1 million atoms using DFT[2] and 2 million using semiempirical methods[3]. These techniques also reduce the computation time of specific properties in systematic studies of large sets of medium-sized molecules[4,5,6]. Still from this perspective, linearly scaling electron structure methods can be combined with molecular dynamics[7] producing highly efficient computational strategies for simulation of complex molecular systems. These facts create the real possibility of studying and presenting new understandings of important phenomena in biochemistry, biophysics, biotechnology and nanotechnology. Something along these lines has been done in our research group [8,9,10,11] using the PRIMoRDiA[12] software, which is in the public domain (https://github.com/igorChem/PRIMoRDiA1.0v). In this theoretical/practical mini-course, theoretical aspects of semiempirical methods of quantum chemistry will be addressed and computational activities will be carried out involving: (i) protein folding, (ii) thermodynamics of enzyme-ligand complexes, (iii) intermolecular interactions of enzyme-ligand complexes and (iv) reactivity in enzymatic catalysis.

The requirements to follow this mini-course are to have a Google account and understand Python at least. We will use the Google Colab platform (https://colab.research.google.com/) for our modeling and simulations. We have a public repository where various materials can be consulted: https://github.com/RochaGerd/Chemistry_with_Python.

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