[L9] Molecular Modeling: Not Just Drug Design

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Over the last decades, the field of molecular modeling has evolved to contribute to many aspects of chemical, physical, biological and materials related research. In fact, any discipline which is engaged with molecular properties in the broadest possible sense can benefit from the insight provided by the plethora of molecular simulation techniques developed over the years (quantum mechanical calculations, docking and scoring, molecular dynamics simulations, machine learning, and cheminformatics approaches to name just a few). Yet despite the diversity of topics amenable to molecular modeling, medicinal chemistry and drug design are by far the main beneficiaries.

This seminar will focus on the application of molecular modeling approaches to topics other than medicinal chemistry / drug design. In particular, the following projects will be discussed: (1) The design of compact biomimetic peptides capable of binding cellulose. These peptides could be regarded as the first component of a modular machinery for the degradation of cellulose en route to developing biological fuels. (2) The study of phenolic compounds produced by plants in order to ward off bacteria attacks by interfering with the bacterium quorum sensing machinery. This could be regarded as the first step towards the development of new compounds for crop protection. (3) The development of QSAR models for the design of solar cells with improved photovoltaic properties.

We demonstrate that all three projects, performed in close collaboration with experimentalists, greatly benefitted from the application of various molecular modeling approaches.