BIOTECHNOLOGY AND BIOSCIENCES SEMINARS

Dipartimento di Biotecnologie e Bioscienze – UNIMIB

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Modeling studies in organic chemistry: from the conformations of biomolecules to the investigation of reaction mechanisms

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Abstract: The most accessible way to represent the unobservable world is to make a model. Chemical properties and behaviors of molecules can be predicted manipulating their 3D structures. Molecular modeling represents compounds through models on scale that allow to visualize molecules. Nowadays, the computer is the standard tool for generating these models.

Molecules are not rigid and all atoms permanently move. The low-energy conformers give major contribution to the overall population. To convert one geometry to another, the torsional angle values are changed, favoring complete conformational studies. The exploration of the potential energy surface allows also the localization of the lowest energy barriers connecting minima. This opens the way to study organic reaction mechanisms.

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