DISCLOSURE ON MOLECULAR INFORMATICS

In this Review we will look back some basic aspects of stereochemical conformation of Bio-Oganic rmolecule as an application of informatics aspects of C++ coding . The Bio-Informatics software Modelling is conservatively based on Visual C++ including C coding . The graphic interface (GUI)of this Visual tool - Integrated Developement Environment can be correlated to Character Interface (CUI) . The Bio-Organic molecule includes mainly Protein , Genetic Structural Properties , Medicinal Organic Molecule ie Proteomix , Genomix & SAR studies .

The Basics of Methodogy incude the Linear Application of Free Energy Relationship like Hammett -Taft Equation . The Gibbs Free Energy [del G = f (Keq)] is a linear function of Equlilibrium Constant . The Thermodynamic functions can be directly related to molecular descriptor depending on STRUCTURE - ACTIVITY - BIOLOGICAL relationship . The Quantum Mechanical Descriptors depends on LCAO - Linear Combination Atomic Orbitals ie interms of wavefunctions . From Informatics part along with Visual C++ platform some database support like Front End as well as back End informatics support can be added advantage .The application of statistical software like STATA / Best fit analysis will be more helpful for Correlation analysis where molecular descriptors can be signified with the value of Correlation Coefficiant (R^2) .The application molecule may be of two types 1. Bio-Polymers mainly Proteins , DNA , RNA . 2. Synthetic Medicinal Compounds . In a brief the main aspects of Molecular Design depends on Quantitative Approaches of Structural Descrptors / Ligands . **Several in Built software** for QSAR / QSTR (Activity / Toxicity Relationship) depends on Pharmaco-Kinetic properties along with Thermodynamic Properties of Bio-Organic molecule and the pricipals as stated above .

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