The APD-RMSD descriptor for molecules' and ligands' conformation

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Abstract

There exists a deep need for computational methods that accurately represent the spatial relationships between different biological structures, such as molecules and ligands. To cater this demand, the APD-RMSD descriptor was proposed. This approach incorporates two different types of descriptors: the angle-plane deviation (APD) and root-mean-square deviation (RMSD). Due to, the synergic description of angles (APD) and distance (RMSD) conformational changes of the molecules could be described more precisely. The method was validated and successfully applied to parameterize the model of the glucokinase (GCK) and its regulatory protein (GCKR). The analysis was implemented in dedicated computational environment called Grow_4 being a molecular modeling platform available free of charge at www.grow4.eu. The project was founded by Rafal Urniaz and subsequently it is developed at Medical University of Lublin (Poland).

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