

Continuous Symmetry and Chirality Measures – Algorithms and Applications

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Many molecules are naturally symmetric at their equilibrium state, but due to conformational flexibility, substitution, changing physical conditions, or during chemical processes, it is more likely to find them with different levels of distortion. Continuous symmetry and chirality measures quantify the level of distortion by estimating the distance between the input structure and the nearest symmetric (or achiral) structure with the same atoms and connectivity. Recently we developed algorithms for calculating these measures that utilize the connectivity map of the input molecule to reduce the number of possible permutations by scanning only structure-preserving permutations. This strategy resulted with significantly increased accuracy and dramatic reduction of the running time, by up to tens orders of magnitude. Consequently, a wide variety of molecules can now be analyzed, turning the measures into powerful and robust molecular descriptors. The methodology will be discussed along with various applications of measuring symmetry and chirality to explore structural effects of organic and inorganic systems as well as protein structure.