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Information-based measure of chirality for biomolecules KAROL BACA LOPEZ, Faculty of Sciences, Autonomous University of the State of Mexico, B. ROY FRIEDEN, College of Optical Sciences, The University of Arizona, ROBERTO LOPEZ, MIGUEL MAYORGA, Faculty of Sciences, Autonomous University of the State of Mexico, ENRIQUE HENANDEZ LEMUS, Computational Genomics Department, National Institute of Genomic Medicine — Homochirality is a common property of biomolecules such as DNA, RNA and proteins. In particular, D-ribose and D-deoxyribose enantiomers are found within living cells, while their mirror images, the L-enantiomers, are not known to occur naturally even though the configurations are highly stable. On the other hand, proteins are formed by L-amino acids, not by their mirror images. Why? In this work, we propose the use of Fisher Information (FI) I as a measure of chirality or dissimilarity between enantiomers. We performed Hartree-Fock (HF) and Density Functional Theory (DFT) calculations to obtain the electronic wave function $\Psi(x, y, z)$ and corresponding density function $\rho(x, y, z)$ for each of the natural and synthetic forms of oligoribonucleotides and alanine amino acid. The four wave functions $\Psi(x, y, z)$ are used to compute the FI evaluated from two different view points: a coherent viewpoint, which includes the phase part of each $\Psi(x, y, z)$, and an incoherent or classical viewpoint, which ignores the phase. Our goal is to describe the extent to which the information content in chiral molecules (D- and L-) plays a role in selecting one or the other isomer in nature.

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