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ISSN: 2167-7956
Journal of
Biomolecular Research
& Therapeutics

Commentary

Biomolecular Electrostatic Characteristics Using Novel Multi-Resolution Techniques

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DESCRIPTION

A technique for comparing biomolecular electrostatic potentials, at many resolutions without the necessity for biomolecules to be structurally aligned globally. Multi-resolution Attributed Contour Trees (MACTs) are employed by the underlying computational geometry algorithm to compare the topological characteristics of volumetric scalar fields. For a sizable collection of protein chains with varied levels of sequence, structural and function similarity and MACTs to compute electrostatic similarity metrics. In addition, using a more conventional method based on 3D structural alignment and study of Carbo similarity indices, it generates similarity metrics for these chains for calibration. The MACT technique also promises to perform well in future large-scale classification attempts across groups of structurally varied proteins because it does not rely on structural alignment. The MACT method accurately clusters proteins into functionally relevant groups that show a substantial dependence on ligand binding sites, discriminating across protein chains at a level comparable to the Carbo similarity index method.

Biomolecular 3D structure determination has dramatically increased as a result of structural genomics, but there are still relatively few techniques available for analyzing and interpreting all of this structural information in terms of potential physiological functions and biochemical characteristics. Effective approaches for biomolecular comparison and classification are crucial for comprehending their structural and functional characteristics. Methods for comparing proteins typically rely on similarities in their sequences in biomolecular chains' three-dimensional structures. Although these techniques have shown to be very effective for geometric comparison of protein structures, they do not provide an atomistic description of the chemical features because some functions might result from the chemical heterogeneity that gives a specific protein structure its particular molecular function. Comparing biomolecules by quantitatively calculating the volumetric functions of key attributes and matching those 3D functions is an alternate approach. Although other characteristics have also been employed, molecule shape and electrostatic potential are the two most frequently used functions. An essential aspect of biomolecules, the electrostatic potential is crucial for interactions both and between biological structures. Through the numerical solutions of partial differential equations like the Poisson-Boltzmann (PB) equation, the electrostatic potential of a biomolecule is typically calculated given the atomic charges, radii and dielectric properties of the biomolecule and solvent. Wide-ranging applications of electrostatic properties particularly those derived by solving the PB equation have been identified in the interpretation of the structure and functions of biomolecular systems.

Additionally, some effort has been put towards pursuing more "informatics-based" methods of interpreting electrostatic characteristics. A significant portion of this study involves finding functionally important residues in biomolecules by examining structural traits including protein membrane contacts, electrostatic destabilization of conserved residues, dramatically shifted pKa values clusters of charged residues and others. Other studies have compared electrostatic potentials and included global evaluations of the biomolecular structure both in two and three-dimensional space over the entire biomolecular structure as well as at specific locations like active sites. Previous applications concentrated solely on a few quantitative measurements of electrostatic properties and with a few exceptions. While the characterization of electrostatic properties of biomolecules has provided insight into a variety of biomolecular features, restricted their research to just a few biomolecules. Tools to facilitate the analysis of electrostatic properties across thousands of biomolecular structures will however become more crucial due to the proliferation of protein structures revealed by structural genomics efforts and the growing interest in understanding biomolecular interactions in a proteomics context. The new "MACT" method that uses local topological feature matching rather than global structural alignment to align local areas of similar electrostatic potential and molecular structure. Even though chemical specificity is not solely determined by electrostatics and molecular shape, we

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Received: 02-Aug-2022, Manuscript No. BOM-22-18006; **Editor assigned:** 05-Aug-2022, Pre QC No. BOM-22-18006(PQ); **Reviewed:** 19-Aug-2022, QC No. BOM-22-18006; **Revised:** 26-Aug-2022, Manuscript No. BOM-22-18006 (R); **Published:** 02-Sep-2022, DOI: 10.35248/2167-7956.22.11.226.

Citation: Oliver A (2022) Biomolecular Electrostatic Characteristics Using Novel Multi-Resolution Techniques. J Biol Res Ther. 11:226.

think the current approaches have promise for locating areas of similar electrostatic potential between structurally different biomolecules.