Luisa Di Paola et al., Mod Chem Appl 2017, 5:3(Suppl)
DOI: 10.4172/2329-6798-C1-005

5th Global Chemistry Congress

The structural formula of proteins

Luisa Di Paola[1] and Alessandro Giuliani[2]
[1]Università Campus Bio-Medico di Roma, Italy
[2]Istituto Superiore di Sanità, Italy

The identification of computational tools to analyze the relationship between protein function and structure is a hot research field since 1960s. Despite the advancement of both experimental methods and computational tools, it is still lacking a benchmark methodology identifying clearly and without biases the relationship between structural properties and recognized protein functions. Inspired by the classical theory of Debye-Huckel, we propose a new interpretation of protein contact networks so to define the structural formula of proteins as the network of non-covalent intramolecular bonds. In this way, the peptide bonds would embody the role of nuclear bonds in organic molecules, too strong to determine the adaptation of the molecule to environment. On the other hand, non-covalent intramolecular bonds, which rearrange during protein adaptation of proteins to environment stimuli, represent the right level of analysis to define protein functionality. As for the organic molecules, through chemical graph theory, it is possible to identify key topological parameters fitting with protein properties (protein stability, allostery). The predictive potentiality of the methodology is stunning: once the structural data are available (from X-ray crystallography on NMR), the protein contact network formalism may allow quantifying protein functionality (such as allosteric sites in enzymes or hot spot residues in protein-protein interactions).

Biography

Luisa Di Paola completed her Doctorate in Chemical Industrial Processes at University Roma "La Sapienza". She collaborated, during her doctorate, with prof. J M Prausnitz and H Blanch at University of California at Berkeley. Currently, she is an Assistant Professor at University Campus Biomedico in Rome. Her research interests span from bioinformatics to biotechnological processes. She is author of 45 papers published in international journals and books. She is an Editor-in-chief of the *International Journal of Biochemistry Research & Review*, Associate Editor of *Journal of Physical Chemistry & Biophysics; Advances in Systems Biology and; International Journal of Medical Biotechnology & Genetics (IJMBG)*.

l.dipaola@unicampus.it

Notes: