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Global optimization analysis of viral capsids and amide planes

A scheme of Combinatorial Optimization (CO) is introduced in order to describe the geometrical pattern of the macromolecular structures like A-DNA and molecular aggregates like Tobacco Mosaic Virus (TMV). Backbone sequences of internal atom sites are seen to be associated to sequences of Steiner points of an Euclidean Steiner Tree Problem. The agreement with experimental data is 94.6% and 98.2% for A-DNA and TMV, respectively.
Another CO scheme in which the Steiner points have a fundamental role, is the introduction of an objective function which minimum will lead to the confirmation of the existence of Amide planes in protein structure. This is a Mathematical Programming approach such that the variables are small perturbations of bond and dihedral angles. Objective function and constraints are derived only from knowledge of the 3-dimensional molecular structure.
These results provide excellent examples of robust methods of optimization as applied to the study of geometrical modeling of biopolymers and molecular aggregates.

References

[1] R. P. Mondaini, *Steiner Ratio of Biomolecular Structures* - in Encyclopedia of Optimization, 2nd ed., Springer Verlag, 2007, **6** 3718–3723.
[2] R. P. Mondaini, *The Steiner Tree problem and its application to the Modelling of Biomolecular Structures* - in Mathematical Modelling of Biosystems, Applied Optimization Series, Springer Verlag, 2008, **102** 199–220.
[3] R. P. Mondaini, *An Analytical Method for derivation of the Steiner Ratio of 3D Euclidean Steiner Trees* - J. Global Optimization, 2009, **43** 459–470.
[4] R. P. Mondaini, *A Correlation between Atom Sites and Amide Planes in Protein Structures* - in BIOMAT 2009 International Symposium on Mathematical and Computational Biology, BIOMAT Series, World Scientific, 2010, 136–151.
[5] R. P. Mondaini, S. P. Vilela, *A Proposal for modelling the Structure of Biomacromolecules* - in BIOMAT 2010 International Symposium on Mathematical and Computational Biology, BIOMAT Series, World Scientific, 2011, 61–72.