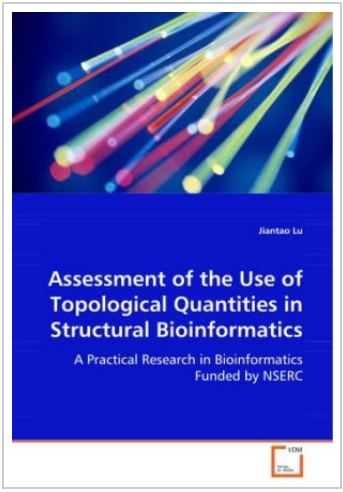

Assessment of the Use of Topological Quantities in Structural Bioinformatics

By Jiantao Lu

VDM Verlag Aug 2008, 2008. Taschenbuch. Book Condition: Neu. 220x150x6 mm. Neuware - Protein structure is complex trajectory in 3D space and it can be abstracted into a polygonal curve. Capturing structural properties from the Cartesian coordinates of thousands of atoms is an important step in performing structural analysis such as similarity detection and defining patterns. The objective of this research is to investigate the potential use of some knot theoretic quantities such as self-linking, R30 invariants and HEO vector for structural Bioinformatics applications. The work presented suggests that self-linking (writhing) can be used to identify a-helices. A revised sliding window approach together with 2 curve simplification methods were employed in the optimal window analysis to capture regions that maximize or minimize self-linking properties in a protein s backbone trajectory. The accuracy of this method is significant although insufficient to be used for domain boundary identification. Most interestingly, the topological properties of adjacent protein domains are significantly larger than for domain that are not adjacent within a gene. This experimental result suggests that proteins tend to evolve contiguous domains with polarized topological properties. 108 pp. Englisch.

Reviews

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