# Topological fingerprints for revealing the topology-function relationship of biomolecules

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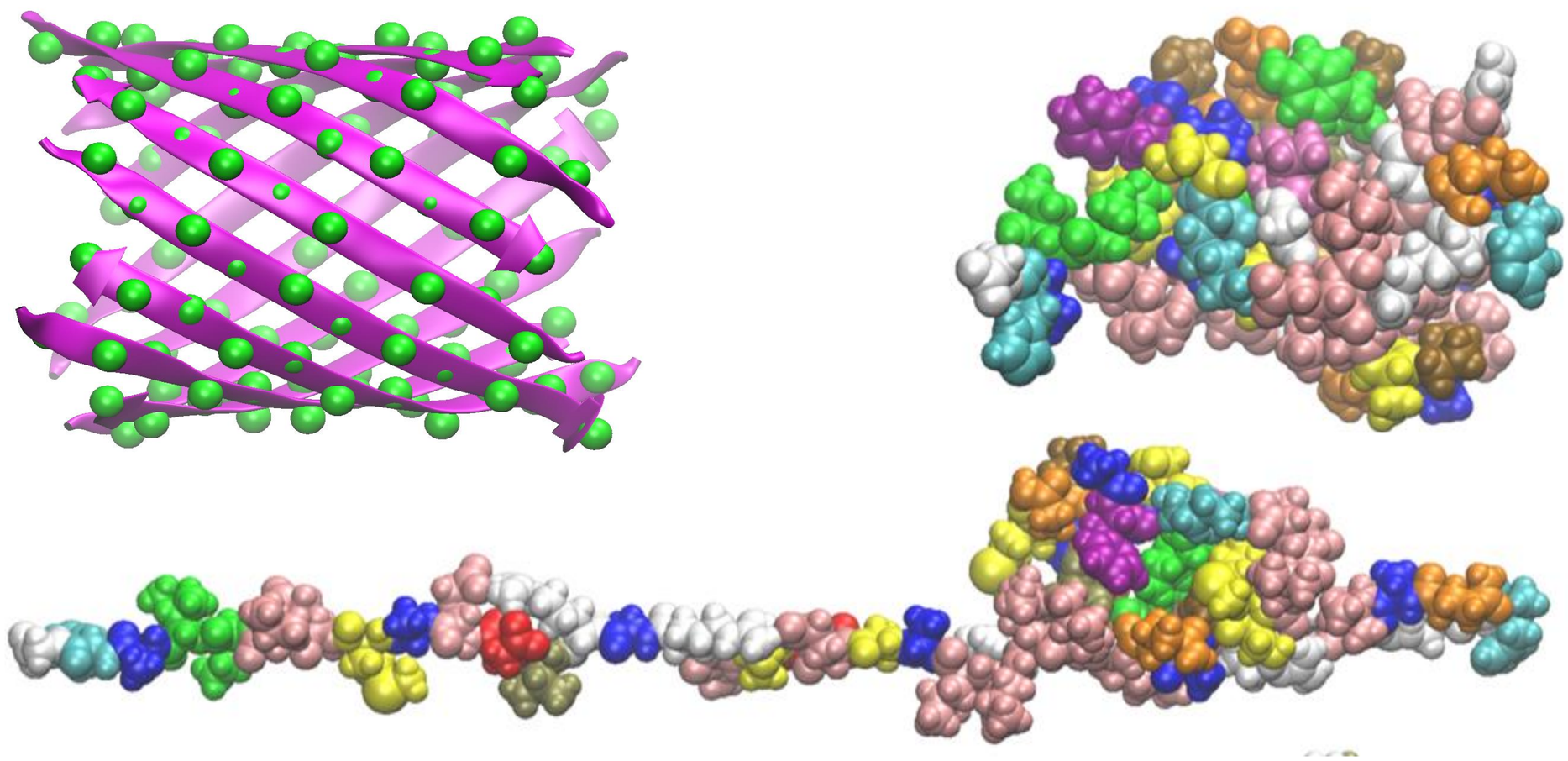
Topological tools often incur too much reduction of the original geometric information, while geometric tools are frequently inundated with too much structural detail and can be computationally too expensive to be practical. Persistent homology bridges between geometry and topology, and offers an effective strategy for biomolecular analysis. This work introduces molecular topological fingerprints (MTFs) based on persistent homology analysis of topological invariants to reveal the topology-function relationship of macromolecules as shown in the illustration, where the MTFs of a beta barrel (top left), a protein (top right) and its unfolded conformation (middle) are depicted in the bottom from the left to the right, respectively.




**Reference :**
Kelin Xia and G. W. Wei, Persistent homology analysis of protein structure, flexibility, and folding, International Journal for Numerical Methods in Biomedical Engineering, 30, 814-844 (2014).