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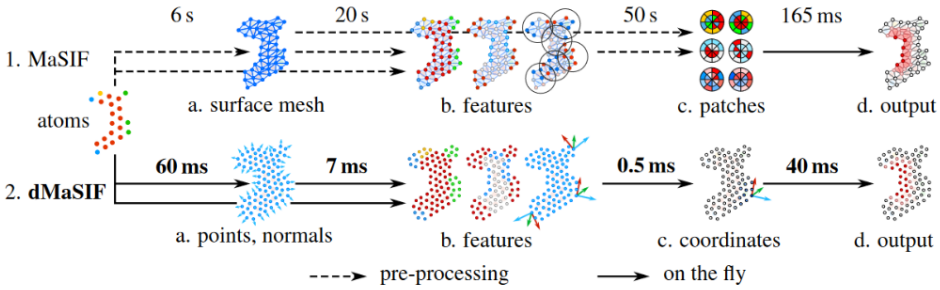
Licensing Opportunity

TTO – Technology Transfer Office

A method and system for fast end-to-end learning on protein surfaces



Both MaSIF and dMaSIF go through the same steps for interface prediction on protein surfaces. Starting from a raw atomic point cloud, we compute (a) a representation of the protein molecular surface, (b) geometric and chemical features, and (c) local coordinate systems; (d) a binding site is then predicted by a geometric convolutional neural network operating on (quasi-)geodesic patches on the protein surface

Ref. Nr

6.2275

Keywords

Structural biology
Protein protein interactions
Functional sites
Deep learning
Protein surface

Intellectual Property

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Description

Computer-system-implemented method for predicting properties of a protein molecule. Tested to identify interaction sites and predict protein-protein interactions.

Computation and sampling of the molecular surface on the fly from the underlying atomic point cloud, geometric deep learning.

Novel efficient convolutional layer.

Advantages

Order of magnitude faster and more memory efficient method

Large collections of proteins are processed in an and to end fashion from raw 3D coordinates and atom

Eliminating hand crafted -precomputed figures

Applications

- Structural biology
- Protein science
- Large protein number and size (>10kD) analysis
- Analysis of entire protein-protein interactions networks in living organisms