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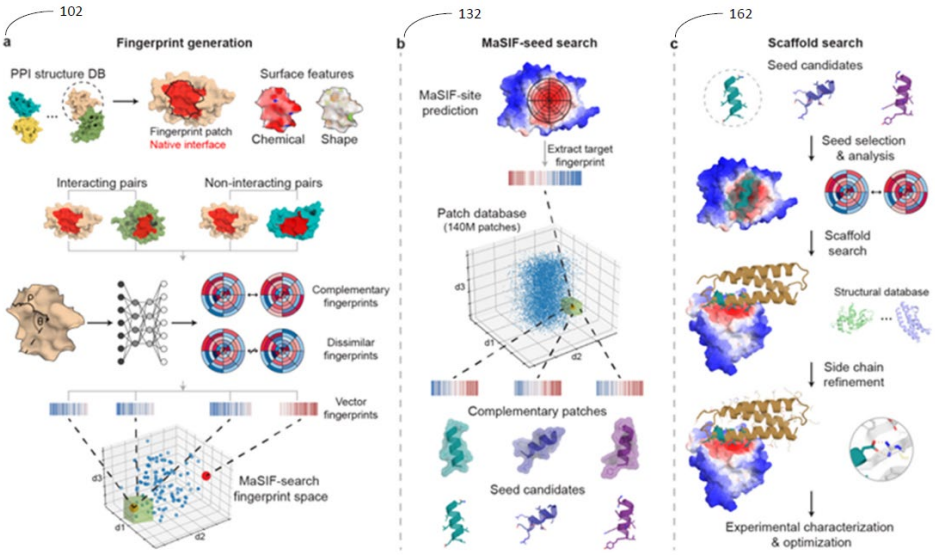
Licensing Opportunity

TTO – Technology Transfer Office

De novo design of protein interactions with learned surface fingerprints



example surface-centric design of protein interactions and related systems and methods

Ref. Nr

6.2337

Keywords

Protein-surface
Protein-protein interaction
Fingerprint
SARS-CoV-2 spike
PD-1
PD-L1
CTLA-4

Intellectual Property

US 18/206,873
Priority 07.06.2022

Publications

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09/10/2024

Description

Deep learning framework to generate surface fingerprints from protein structures, which are learned from protein interfaces to describe geometric and chemical features critical to drive protein-protein interactions (PPIs).

Surface-centric approach to describe structure and capture molecular recognition determinants enabling a novel approach for the de novo design of protein interactions and, more broadly, of artificial proteins with function.

A general method using surface centric approach to describe structure, capture molecular recognition determinants and further build de novo design of protein interactions and, more broadly, of artificial proteins with function.

As a proof-of-principle, computationally design of four de novo protein binders to engage three protein targets: SARS-CoV-2 spike, PD-1, and PD-L1. The designs bound the target sites with high affinity upon experimental optimization, structural and mutational characterization showed highly accurate predictions.

Advantages

Geometric deep learning framework to generate surface fingerprints from protein structures, which are learned from protein interfaces to describe geometric and chemical features critical to drive PPIs

Modularity and predictability of helical structures

Applications

- binding seeds with helical structure
- de novo design of protein binders that are crucial for synthetic biology and and chemical features critical to drive PPIs