Richard P. Feynman Center for Innovation

Technology Snapshot

Technology Licensing Opportunity

Los Alamos NATIONAL LABORATORY

SurfGraphPro

Mapping protein surfaces at the speed of AI

Value Proposition

SurfGraphPro, an AI tool from Los Alamos National Laboratory, transforms complex protein structures into an easy-to-analyze format that helps researchers quickly identify binding sites, predict molecular interactions and understand protein behavior with greater speed and scalability than traditional approaches.

Technology Readiness Level 3

IP Information for S-196061

U.S. Patent pending

Contact Information

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Overview

By combining 3D surface graph representations with advanced machine learning, this technology from Los Alamos National Laboratory reduces the computational burden of protein analysis while preserving the structural detail needed for high-value applications in drug discovery, antibody design, pathogen detection and custom protein engineering.

Advantages

- Helps turn complex protein structures into information computers can use more easily
- Speeds up protein analysis compared with older approaches
- Reduces the amount of manual feature engineering needed
- Preserves important details about both protein shape and chemical properties
- Supports multiple uses, including drug discovery, antibody design and pathogen detection
- Offers a flexible platform that can be adapted to different protein-related tasks

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Technology Description

Protein surfaces are extremely complex, three-dimensional structures, and that complexity makes them difficult to analyze using traditional computational approaches. In practice, many existing methods rely on hand-selected biochemical features, expensive calculations or narrow task-specific models that do not generalize well to new questions. As a result, researchers can face slow runtimes, limited scalability and incomplete insight when trying to identify binding sites, predict molecular interactions or understand broader protein behavior across large sets of proteins. These limitations can make it difficult to move quickly from protein structure data to useful predictions in areas such as drug discovery, antibody design, pathogen detection and protein engineering.

SurfGraphPro solves these problems by converting protein surfaces into a graph-based representation that preserves both the physical shape of the surface and the biochemical information carried by surface-exposed amino acids. This tool gives machine learning models a more efficient and flexible way to process protein structures without requiring repeated manual feature engineering or highly specialized analysis pipelines for each new use case. By reducing computational burden while keeping the key structural details needed for prediction, SurfGraphPro makes it possible to analyze proteins more quickly, at larger scale and across a wider range of applications.

Continued on reverse

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NNSA National Nuclear Security Administration

Technology Description continued

This approach includes identifying likely binding sites, estimating molecular compatibility, supporting drug screening efforts, improving antibody and protein design workflows, and enabling other protein-focused prediction tasks where speed, scalability and adaptability matter.

Market Applications

- **Pharmaceuticals and Biotechnology** (drug discovery, target screening, protein optimization)
- **Biologics and Antibody Development** (antibody engineering, binding analysis, therapeutic design)
- **Diagnostics and Infectious Disease** (pathogen detection, biomarker analysis, assay development)
- **Agricultural Biotechnology** (protein analysis, crop trait research, bio-based product development)
- **Materials and Industrial Science** (protein-mineral interaction studies, polymer compatibility, bio-inspired materials)
- **Research Tools and Software** (protein modeling, computational biology, prediction platforms)