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Search & Optimization of Novel Proteins by 3D Point-Cloud Catalophores

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PURPOSE OF THE ABSTRACT

Biocatalysis is increasingly becoming a key technology for developing a more environmentally friendly and efficient chemical industry. Some natural enzymes do not have the required activity, stability, selectivity, or specificity for many desired chemical transformations. Recent advances in computational technology offer a potential roadmap for the search, identification, and development of new biocatalysts.

Innophore, a TechBio company, is using AI-powered point cloud technology to identify and optimize drugs and proteins. Point clouds provide a structurally independent approach to representing the properties of voids or surfaces. Each point in the cloud corresponds to a property at a specific location, making it a valuable tool for separating structural information from function. In addition, these point clouds serve as search templates for identifying proteins with similar binding features. We focus on volumetric voids and surface volumes to predict function, properties, and reactivity. Using our Catalophores™ point cloud, we are accelerating the discovery of new and better enzymes by translating biomolecules into machine-readable datasets.

This talk will review the strategies and opportunities for applying point clouds to enzyme and drug discovery.

FIGURES

FIGURE 1

FIGURE 2

KEYWORDS

BIBLIOGRAPHY