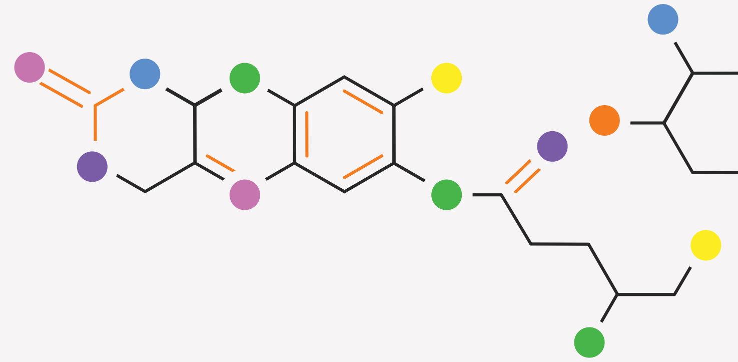

USE CASE

Sequence Design of Advanced Biopolymers for Bioactive Delivery

Elevate sustainable materials for bioactive delivery using Science-Based AI on the VIP Platform

Target

Peptides and polysaccharides are unique classes of polymers that provide precise control over their chemical sequences. This precision enables the design of novel, environmentally friendly, water-soluble, and biodegradable polymers specifically tailored for the effective delivery of bioactive compounds, such as those used in personal care, drug delivery, and other advanced biomedical applications.

Challenge

Controlling the monomer sequences within peptides and polysaccharides generates an extremely large and complex design space, far exceeding the scale of random copolymer design. Exploring this vast sequence space to identify polymers with optimized performance characteristics requires evaluating countless possibilities, which is both time-consuming and costly. Without computational guidance, navigating these high-dimensional sequence variations to efficiently predict and optimize bioactive compatibility, stability, and delivery performance becomes an overwhelming task.

Solution

Leverage advanced natural language processing (NLP) machine-learning architectures to encode polymer sequences into meaningful, chemically relevant feature spaces. These novel language-based features are integrated within the VIP Platform to guide an efficient and targeted exploration of sequence diversity. This approach enables more strategic experimental design to identify polymers that effectively complex with bioactive molecules and form self-assembled structures such as micelles or coacervates for delivery.

Further, the language-based featurization supports the development of machine-learned models that accurately predict key performance metrics, including compatibility with specific bioactives and the stability of micelle or coacervate structures.

By deploying these Science-Based AI models on the VIP Platform, users gain access to powerful inverse design and optimization algorithms, enabling the suggestion of new polymer sequences with enhanced performance for bioactive delivery.