



USE CASE

Sequence Design of Advanced Biopolymers for Delivery of Bioactives

Elevate sustainable materials for bioactive delivery with NobleAI's sequence design.

Target

Peptide and polysaccharides are unique polymer classes that offer unprecedented control over their chemical sequence properties, offering potential for the design of new, unique polymers with tailored performance profiles. This opens the opportunity for environmentally friendly, water-soluble, biodegradable materials for applications in the delivery of bioactive materials (e.g. in personal care, drug delivery).

Challenge

Control over the sequence of monomers within a peptide or polysaccharide opens up a combinatorially large design space that is significantly larger than the design space accessible to random copolymers.

Solution

Leverage natural language processing machine-learned architectures that excel in encoding sequences into meaningful feature spaces. Definition of novel language-based feature spaces can be combined with NobleAI Reactor to design a tailored traversal of sequence design space for breadth and chemical diversity, enabling more efficient experimental design and exploration of polymers that efficiently complex with bioactive molecules and form self assembled micelle or coacervate structures for delivery.

Subsequently, the language-based featurization of polymer sequence space will be used to build machine-learned models predicting performance, e.g. compatibility with specific bioactive molecules and micelle or coacervate stability.

Deployment of the machine-learned models on NobleAI Reactor allows access to inverse design optimization algorithms to suggest new polymer sequences to explore.