De Novo Engineered Living Materials Expand the Design Space for Functional Biomaterials

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Engineered living materials (ELMs) are systems that integrate living cells and functional materials such that they are capable of growth, self-organization, adaptation, and programmable biological functions. Prospective ELM applications range from biomedicine and environmental remediation to biomanufacturing. Autogenic ELMs are particularly attractive because they continually remodel their own extracellular matrix. A major challenge has been the limited diversity of extracellular matrix proteins available for constructing autogenic ELMs.

Researchers at Virginia Tech developed SECRETE, a platform that combines protein database mining, artificial intelligence-based structure prediction, molecular dynamics simulations, and synthetic biology to discover and manufacture new extracellular protein nanofibers. By engineering *E. coli* to produce protein building blocks identified from diverse bacterial species, the team created programmable living materials with tunable mechanical properties, ultraviolet-protection capabilities, 3D printability, and customizable binding functions. The resulting extracellular matrices expand the design toolkit for ELMs and provide a foundation for future biomimetic matrices that more closely replicate the complexity and functionality of natural extracellular environments.

GlycoMIP contributed specialized computational modeling capabilities and expertise to this study through all-atom molecular dynamics simulations of newly identified β-solenoid proteins. GlycoMIP researchers evaluated the structural stability, hydrogen-bonding networks, and intermolecular interactions of candidate protein building blocks identified through protein mining and AlphaFold2 structure prediction. These simulations provided molecular-level evidence that the proteins could assemble into stable extracellular nanofibers, establishing a new class of extracellular matrix building blocks for biomimetic ELM design.

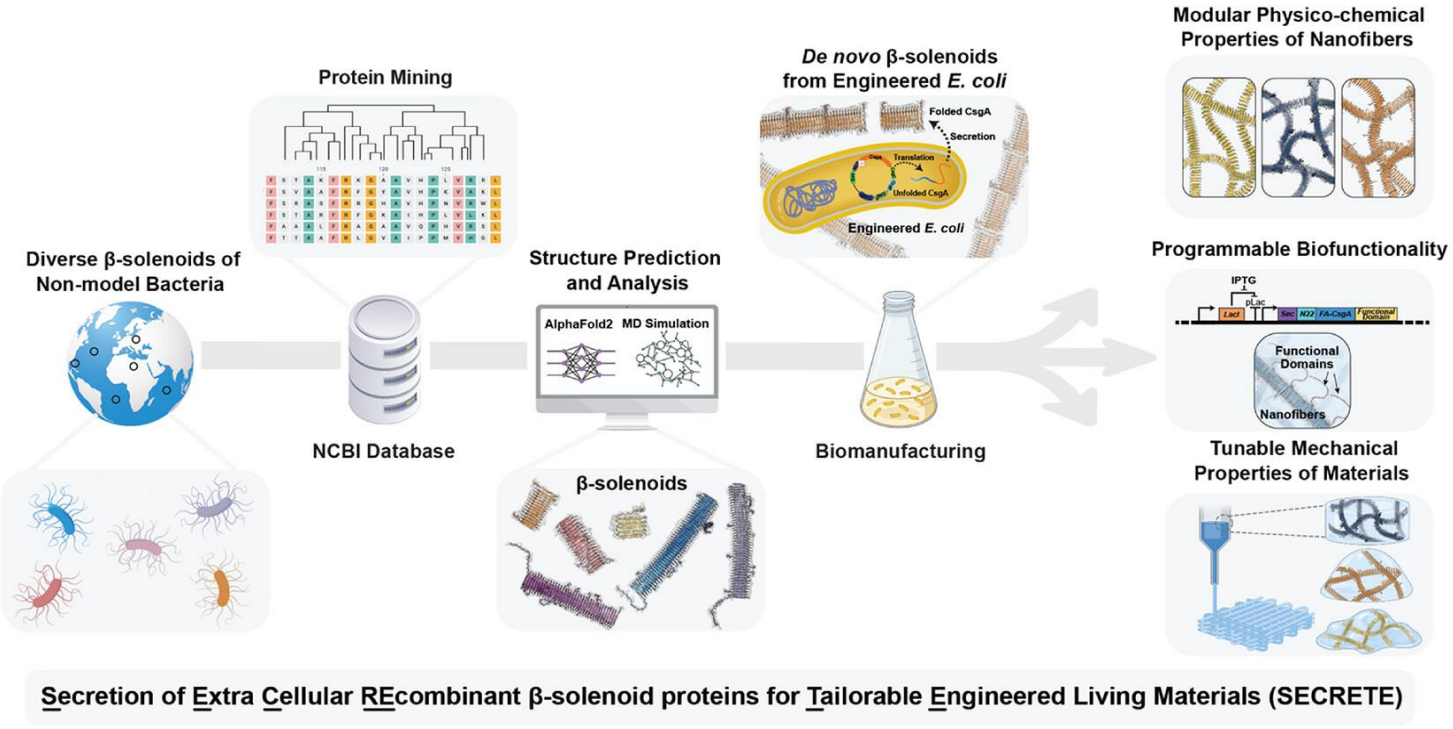

Figure. Overview of the SECRETE platform for discovering, modeling, and manufacturing extracellular matrix protein nanofibers that serve as building blocks for engineered living materials.