Hur AI hjälper forskaren

Design av nya biomaterial inom timmar istället för år

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26.3.2026

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Article | Open access | Published: 14 August 2024

Material engineering and application of hybrid biomimetic-de novo designed elastin-like polypeptides

Zhuoran Geng, Timo Laakko, Ari Hokkanen, Caj Södergård, Ilari Maasilta & Pezhman Mohammadi

Communications Materials 5, Article number: 152 (2024) | Cite this article

6293 Accesses | 7 Citations

Google Patents

A structural protein, a medical product, an electrospun filament, photonic crystals, metamaterial, thermoresponsive glass and a method for preparing a product

Classifications

C07K17/14 Peptides being immobilised on, or in, an inorganic carrier

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Landscapes

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FI131721B1

Finland

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Other languages: Finnish, Swedish

Inventor: Pezhman Mohammadi, Caj Södergård, Timo Laakko, Anssi Laukkanen, Merja Penttilä

Worldwide applications

2023 · FI · 2024 · WO

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2025-03-21 • Publication of FI20236041A1

2025-10-16 • Application granted

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ADVANCED MATERIALS

Research Article | Open Access

Accelerated Engineering of ELP-Based Materials through Hybrid Biomimetic-De Novo Predictive Molecular Design

Timo Laakko, Antti Korkealaakso, Burcu Firatligil Yildirir, Piotr Batys, Ville Liljeström, Ari Hokkanen, Nonappa, Merja Penttilä, Anssi Laukkanen, Ali Miserez, Caj Södergård, Pezhman Mohammadi

First published: 06 May 2024 | https://doi.org/10.1002/adma.202312299 | VIEW METRICS

SECTIONS

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A61K 9/70 2006.1 · A61K 38/00 2006.1 · B82Y 5/00 2011.1 · C07K 14/00 2006.1 · C07K 14/47 2006.1 · D01F 4/00 2006.1

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CPC

A61K 38/00 · A61K 9/5169 · A61L 27/50 · B33Y 70/00 · B82Y 30/00 · B82Y 5/00

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SÖDERGÅRD, Caj
LAAKKO, Timo
LAUKKANEN, Anssi
PENTTILÄ, Merja

[EN] A STRUCTURAL PROTEIN, A MEDICAL PRODUCT, AN ELECTROSPUN FILAMENT, PHOTONIC CRYSTALS, METAMATERIAL, THERMORESPONSIVE GLASS, A METHOD FOR PREPARING A PRODUCT AND USE OF THE STRUCTURAL PROTEIN
[FR] PROTÉINE STRUCTURALE, PRODUIT MÉDICAL, FILAMENT ÉLECTROFILÉ, CRISTAUX PHOTONIQUES, MÉTAMATÉRIAU, VERRE THERMOSENSIBLE, PROCÉDÉ DE PRÉPARATION D'UN PRODUIT ET UTILISATION DE LA PROTÉINE STRUCTURALE

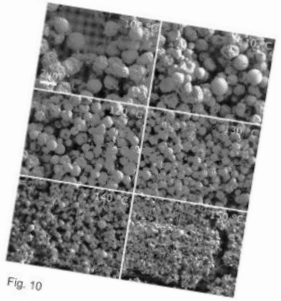

Fig. 10

Abstract

[EN] The present disclosure provides a structural protein comprising an amino acid sequence unit comprising a motif [VPGVG]n, wherein n is 2 or more, and an amino acid sequence selected from SEQ ID NO:1-10. The present disclosure also provides a polynucleotide, an expression vector and a host cell, as well as a method for producing the structural protein. The present disclosure also provides a medical product, an electrospun filament comprising one or more of the structural proteins. The present disclosure also provides a metamaterial and thermoresponsive glass comprising one or more of the structural proteins for preparing a method for preparing a product. The present disclosure also provides use of one or more of the structural proteins for preparing a product.

[FR] La présente divulgation concerne une protéine structurale comprenant une unité de séquence d'acides aminés comprenant un motif [VPGVG]n, n étant supérieur ou égal à 2, et une séquence d'acides aminés choisie parmi SEQ ID NO : 1-10. La présente divu

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ems†

on, Jill K. Meldrum,
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s, Mark S. Searle Prof.

emie International Edition

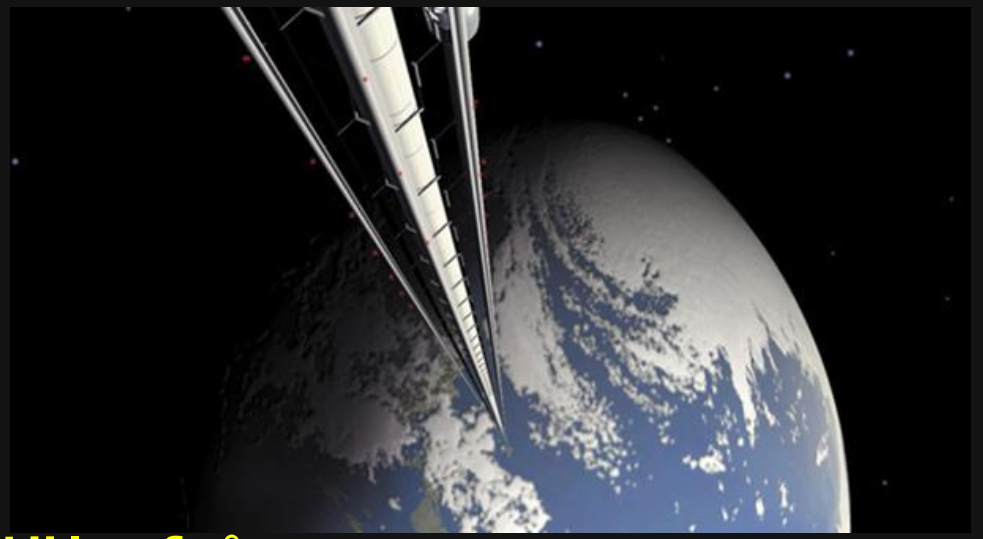
of a ββα Motif†

ao Chen Dr.,
g Wei Dr.,
angwen Jin Prof.,

Innehåll

- **Problem**
- **Hur accelererar vi utvecklandet av nya material?**
- **Vårt biomaterial**
- **Hur hjälper AI oss att uppfinna nya biomaterial ?**
- **Validering av biomaterialen i laboratoriet**

Problemet



Hjälp från Naturen

Ohållbara fossil-baserade material

Undermåliga material

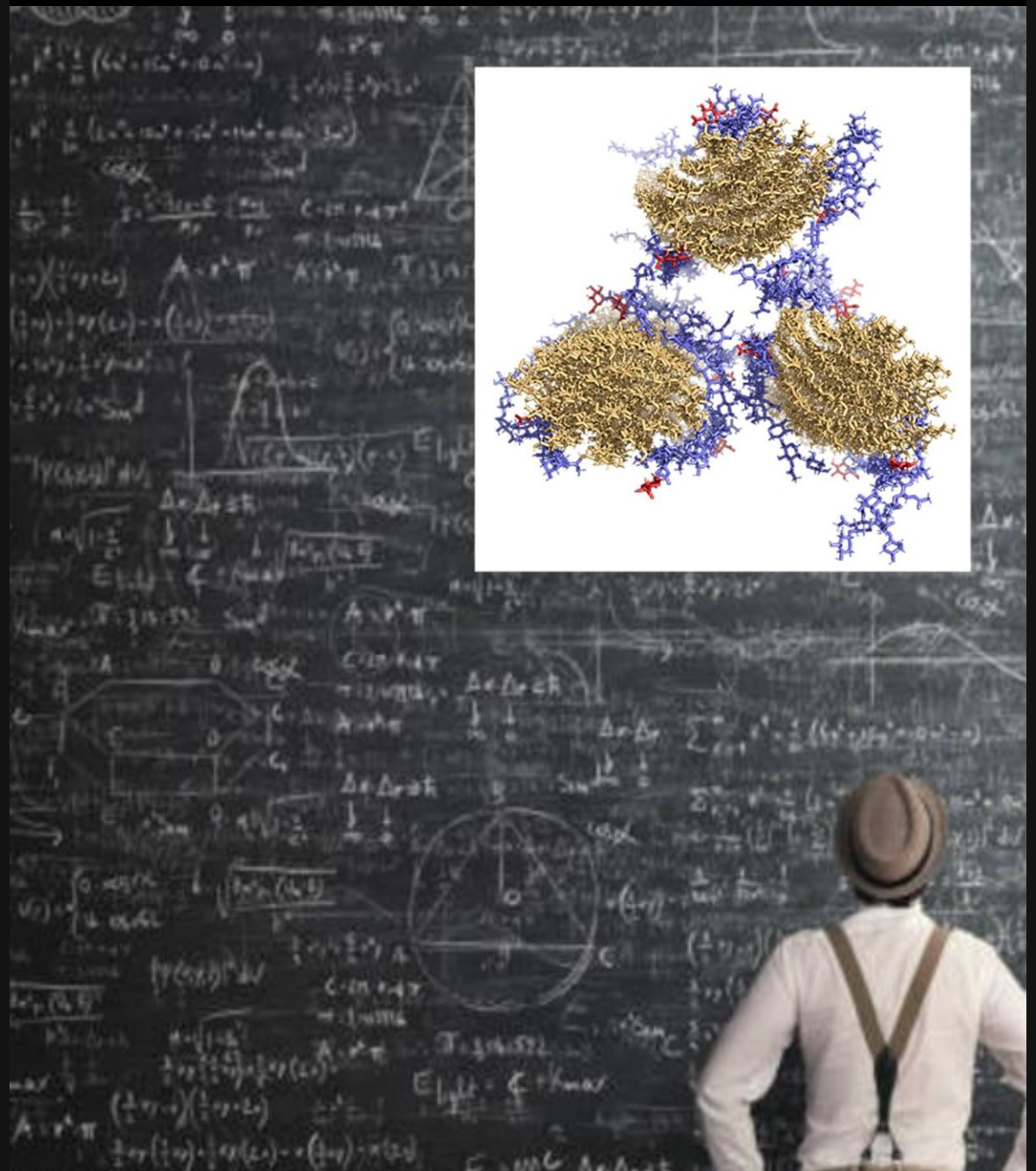
→

Behov av förnybara material

Behov av extrema prestanda

Utmaningar

- ✓ Försök och misstag
  - ✓ Tar år att utveckla
  - ✓ Massiva kostnader
- ✓ Komplexitet
  - ✓ överskrider mänsklig förmåga



Vår ansats

AIMS VTT

AIMS gruppen

Prof Caj Södergård, AI (ledning)

Prof Merja Penttilä, Synbio

Prof Anssi Laukkanen, Material

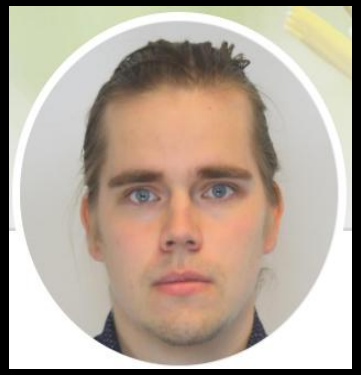
Initiatorer

Dr Pezhman Mohammadi, Synbio

Dr Timo Laakko, AI

Forskare

Antti Korkealaakso,
AI & Simulering



Praktikant

Dr Ville Kotovirta,
AI & kvantdatorer

Expert

Hur accelererar vi utvecklandet av nya material?

AIMS

Synbio labb

Expert

Design av material-varianter

DNA

Celler

Nya proteiner & material

Försök & misstag

Data om egenskaper

AI-stöd snabbar upp utvecklandet

AIMS

Synbio labb

Expert

Design av material-varianter

DNA

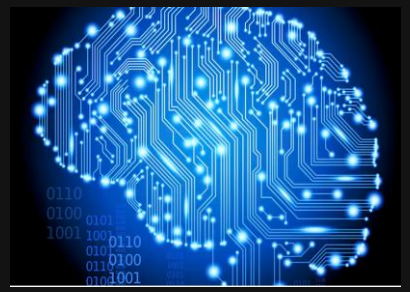
Celler

Nya proteiner & material

Finalister

AI-stöd

Protein databaser



Djupinlärning,

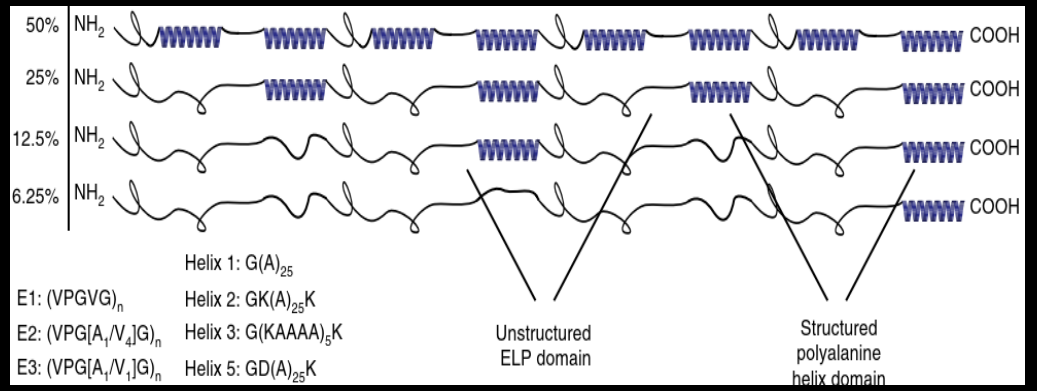
Generera nya kandidater

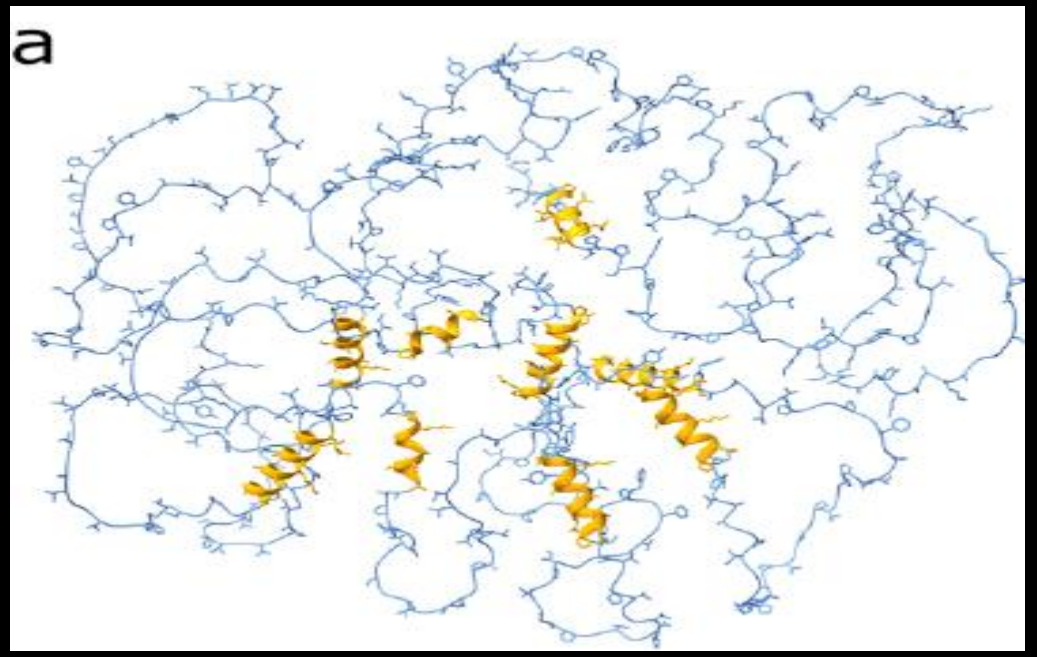
Förutspå egenskaper hos kandidater

Vårt biomaterial

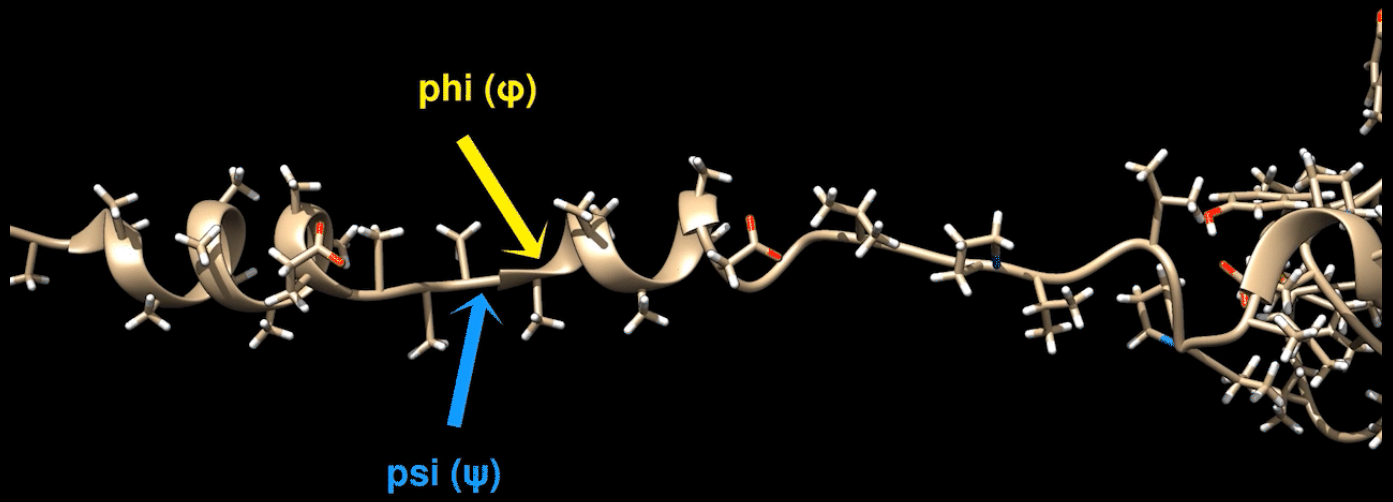
Vårt material: ELP - Elastin-like polypeptides

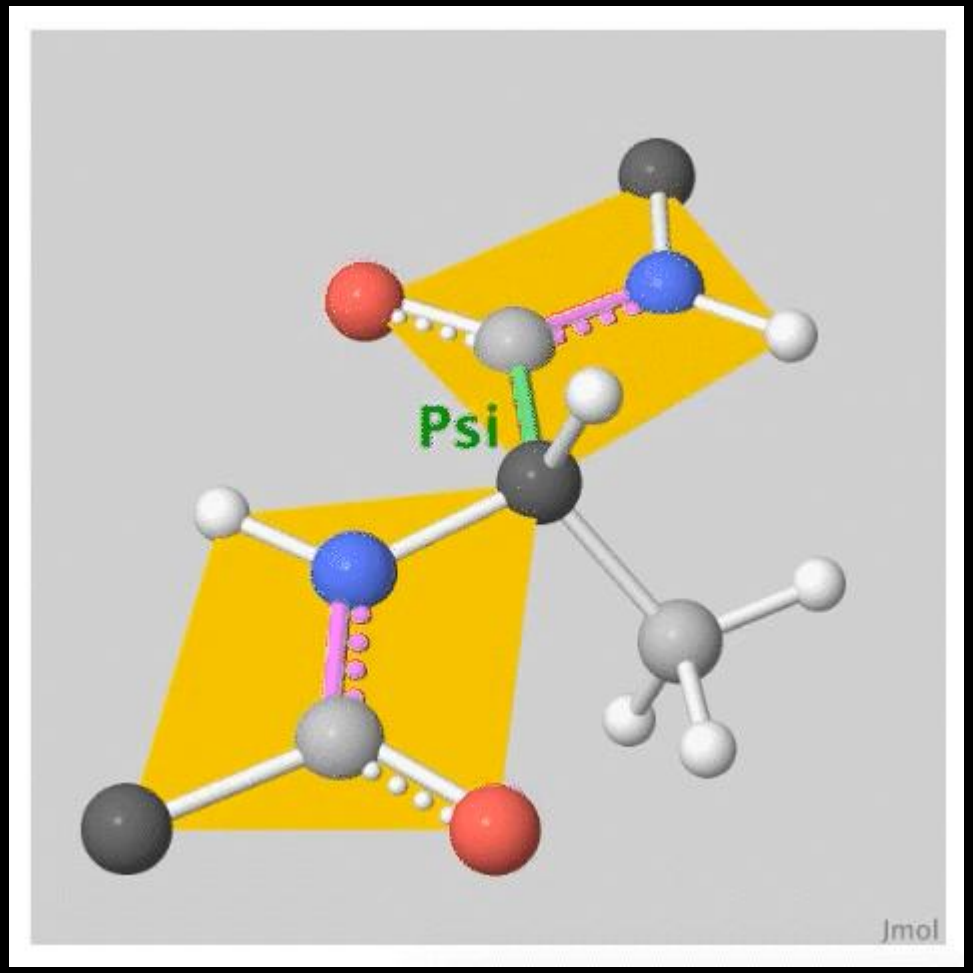
- Elastin är ett s.k. strukturprotein (bl.a. i vår hud)
- ELP produceras med genmanipulation
- Är ett *smart material* som reagerar på temperatur och pH värde
- Är biodegraderande & biokompatibelt
- Tillämpningar: medicin, fibermaterial, bioplaster





Proteinets form styrs av bindningsvinklarna Phi och Psi — och formen avgör egenskaperna



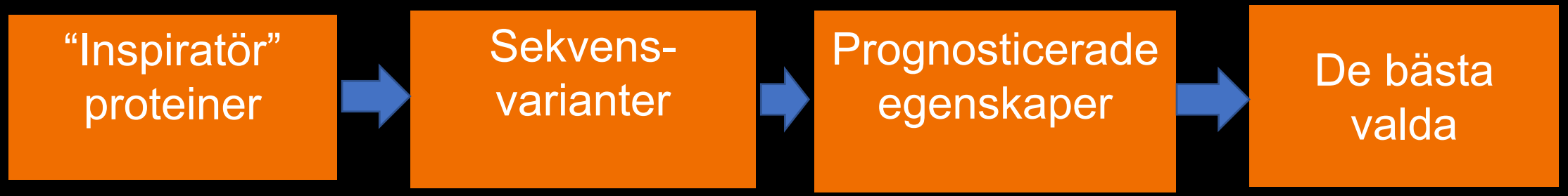


Källa: Ramachandran Principle: Protein Atomic Clashes vs. Phi & Psi

Hur hjälper AI oss att uppfinna nya biomaterial ?

Nobelpris i kemi 2024 för prediktion proteinstruktur

AI hjälper oss att utforma *helt nya* protein



Komplexitet:

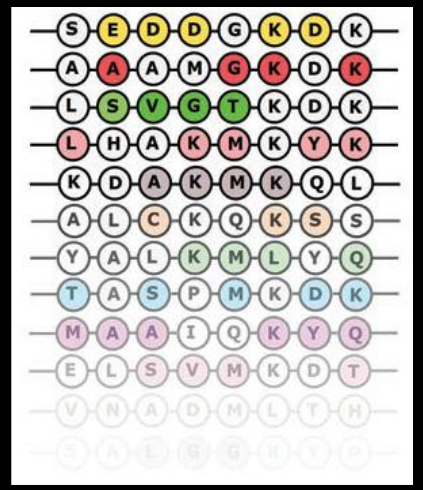
En aminosyras sekvens med längden 10:

20^{10} =10 240 000 000 000 kombinationer

Maskininlärning

VTT

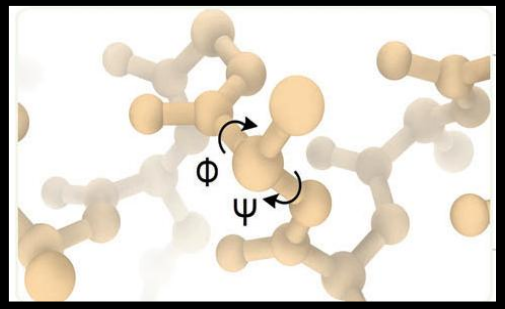
Aminosyra-sekvenser ~ 95 000



Protein databaser

Sekundär struktur parametrar

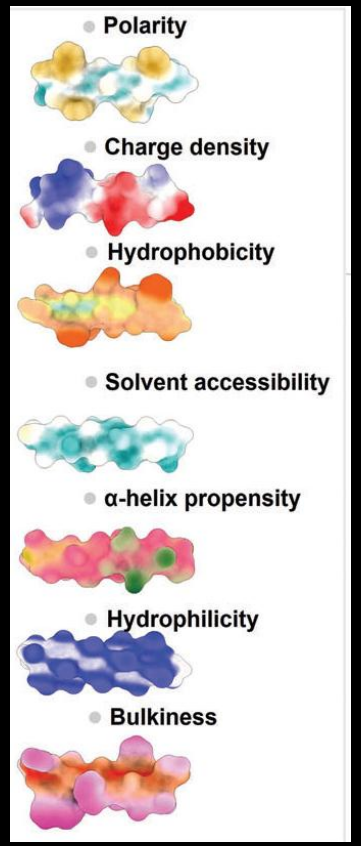
a.a.	Φ	Ψ
D	180	131.5
A	-66.90	-40.61
A	-91.02	2.37
A	-63.69	-41.67
A	-70.11	-30.75
A	-66.37	-40.24
A	-64.24	-41.73
A	-62.35	-40.82
A	-64.42	-40.74



Global-lokal CNN modell

- **13 miljoner parametrar**

Material-egenskaper-skalor

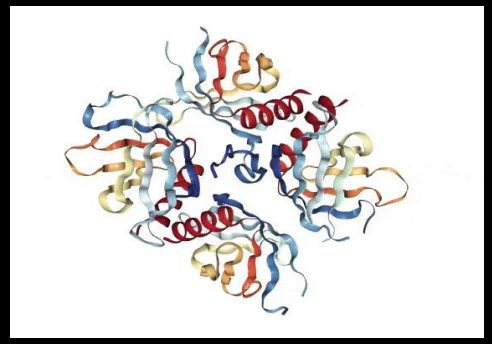


Transformer & Diffusion metoder under utveckling

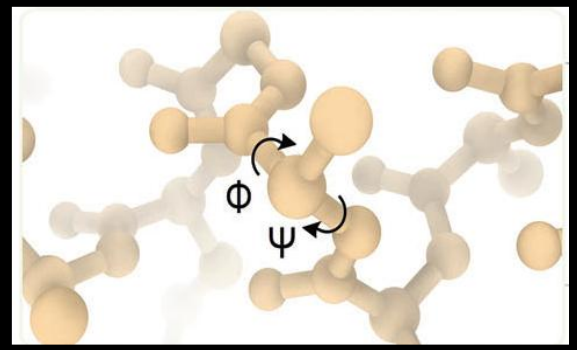
Generera nya sekvenser & förutspå deras egenskaper

VTT

Nya aminosyra-sekvenser & egenskaper



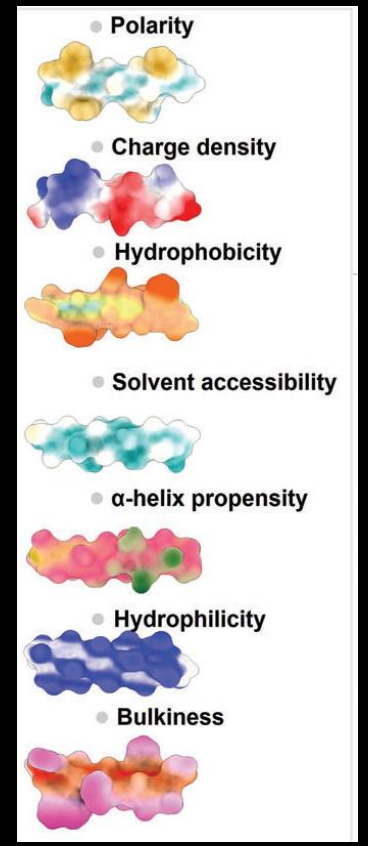
Sekundär struktur



Global-lokal CNN modell

- 13 milj. parametrar

Variera ”inspiratör” proteinernas egenskaper



Resultat: 10 nya validerade proteinmaterial

VTT

AI

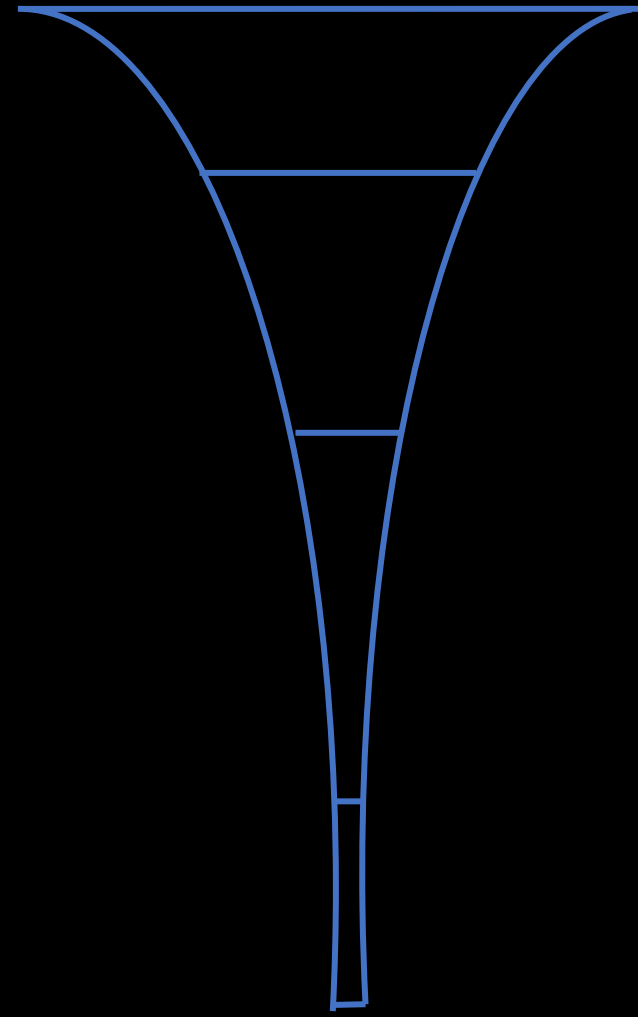
- 1800 digitala protein föreslagna av AIMS AI

- **144** nya & stabila protein filtrerade av AI & Molekulär Dynamik

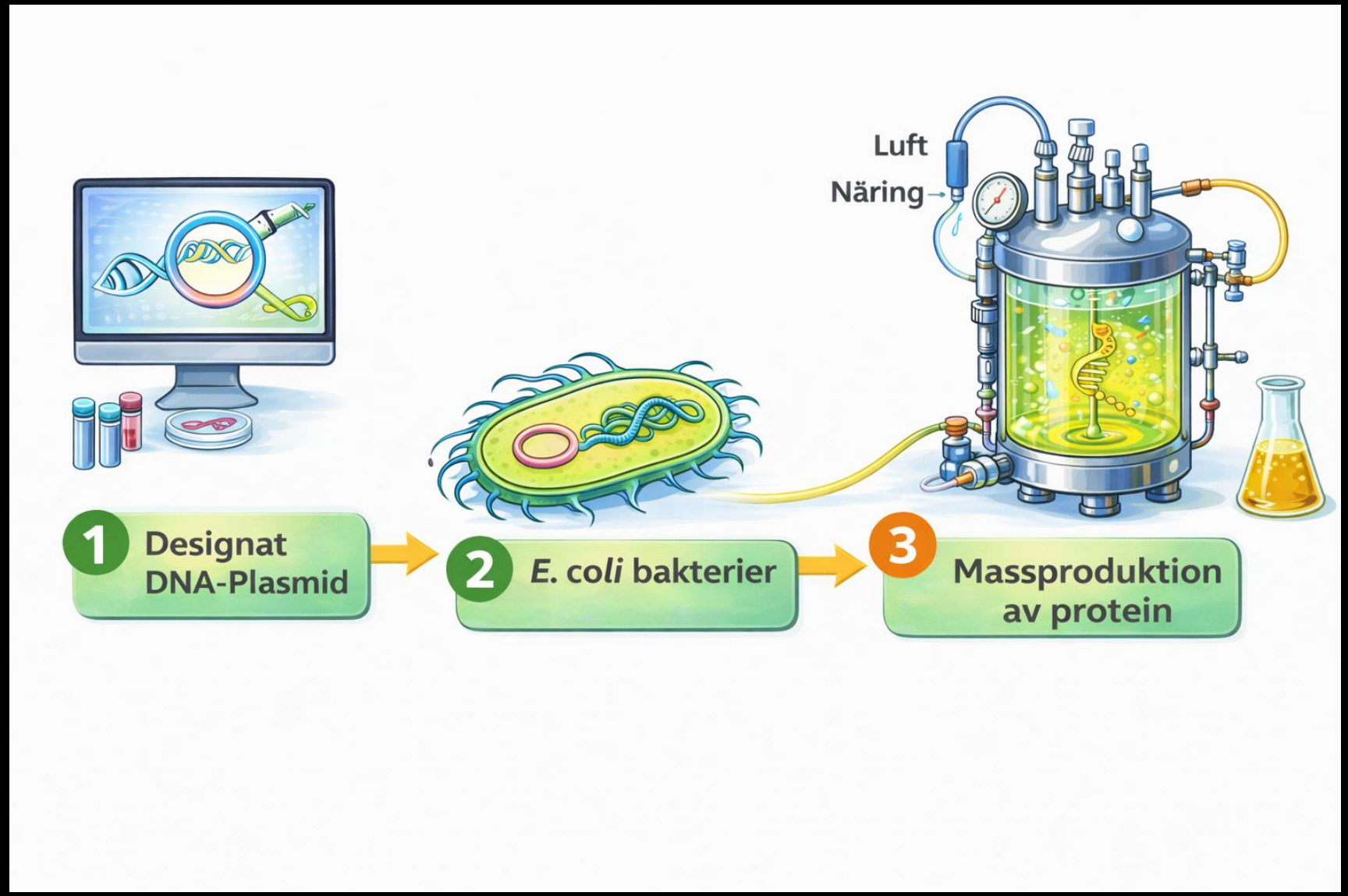
Män-niska

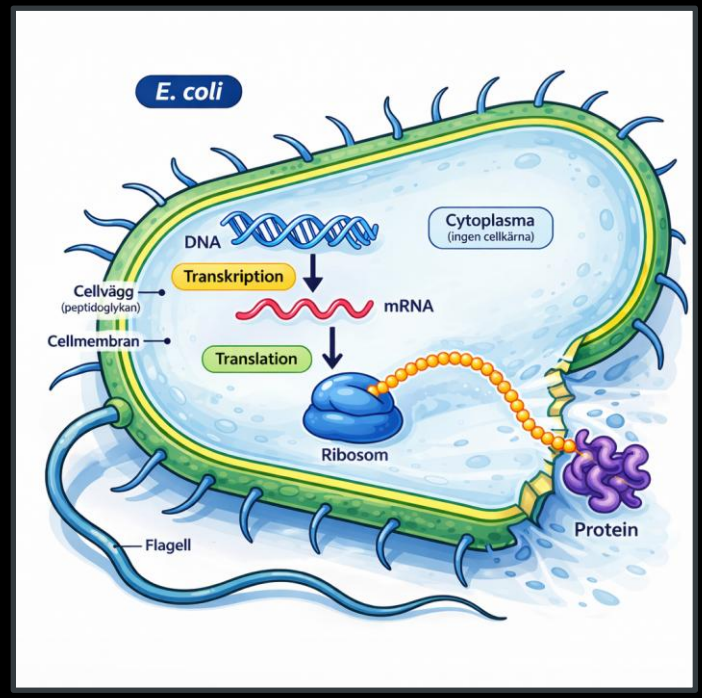
- **25** protein sekvenser handplockade av Synbio expert & syntetiserade till ELP

- **10** nya protein material validerade i labb med goda resultat



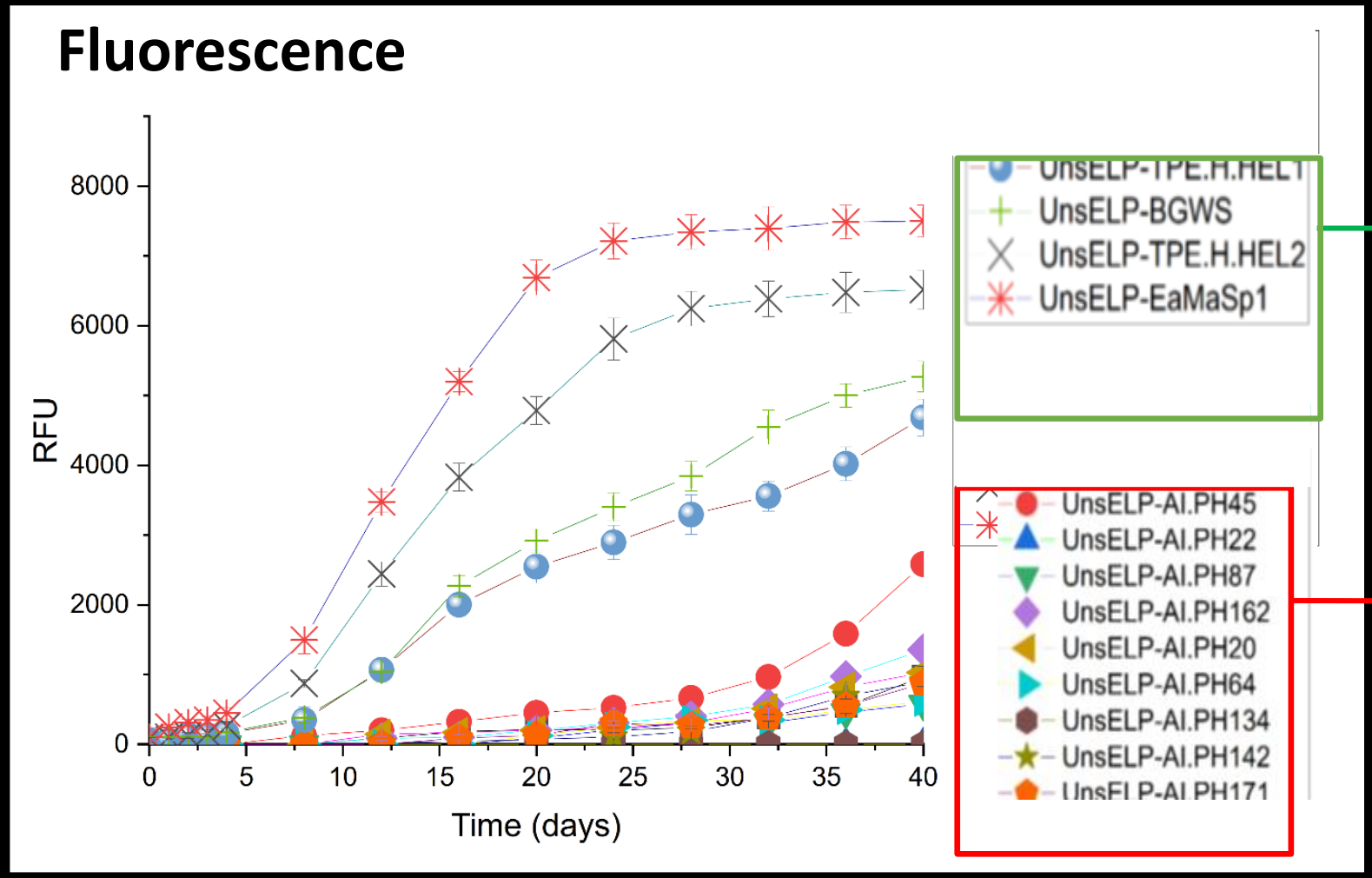
Proteinen syntetiseras i en bioreaktor





Resultat – validering av AI uppfunna biomaterial i laboratoriet

Våra AI-designade protein är överlägsna i stabilitet



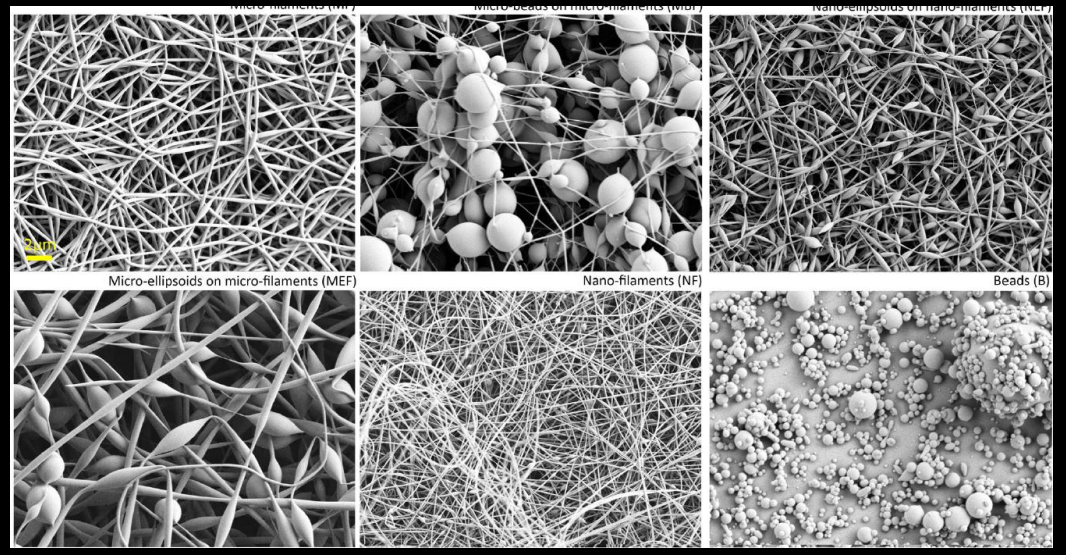
Naturliga och mänskligt designade ELP

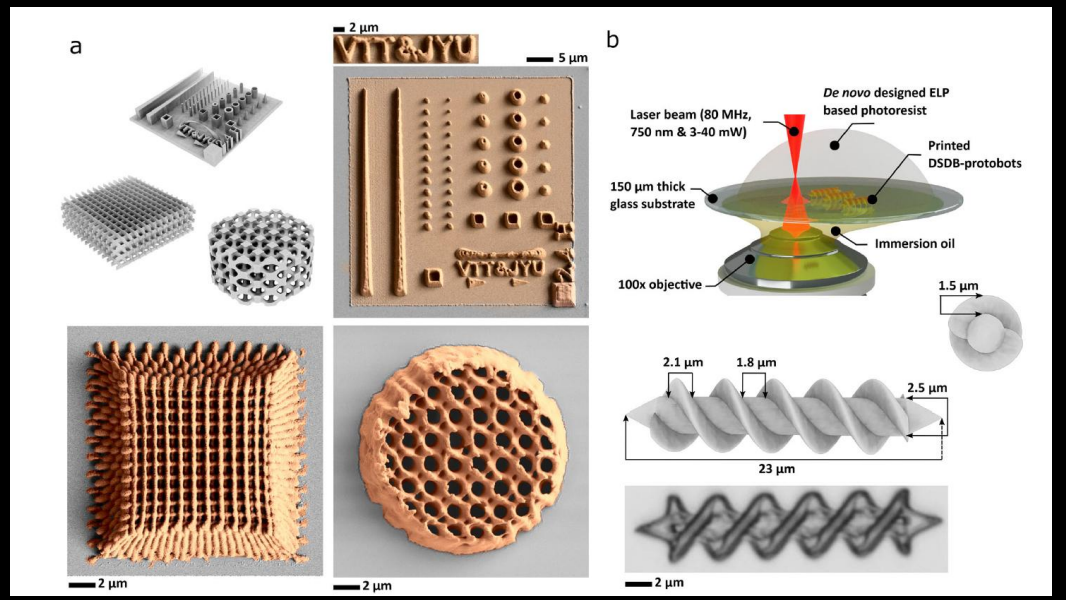
AI-designade ELP

ELP = Elastine-Like Polypeptides

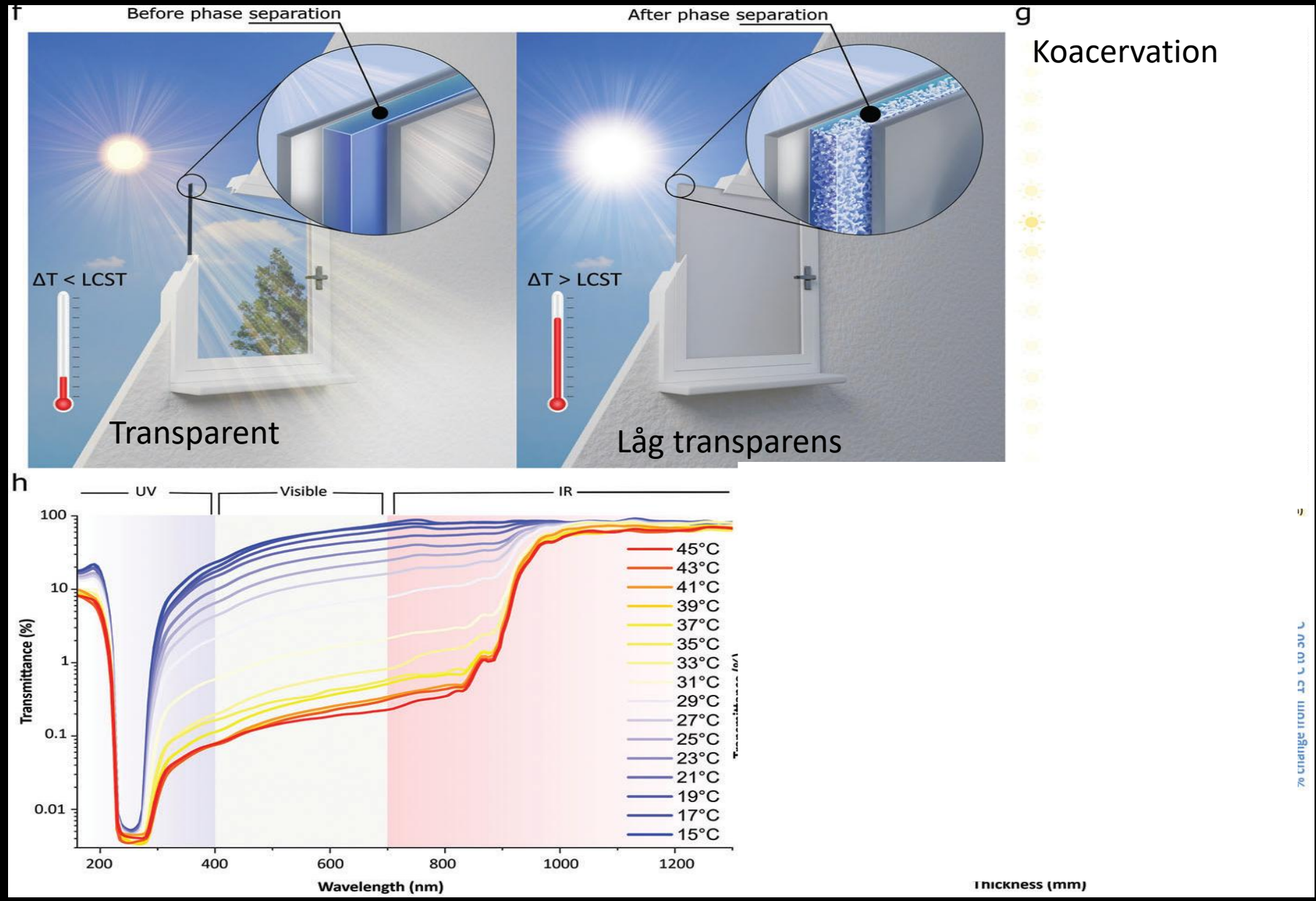
Valideringar och experiment

- Fasseparation (1170 fall)
- Morfologisk struktur, mekaniska egenskaper
- Elektrospinning av fibrer
- Viskositet
- Molekylära interaktioner
- Cytokompatibilitet
- Solstrålning, transmission
- Frisättning av läkemedel i kroppen
- Fotoresister med 3D-utskrift
- Mikrorobotar





Smarta fönster



Sammandrag

- Vi utvecklade ***kollaborativa*** AI modeller för att förutspå egenskaper hos biomaterial & ***snabba upp*** utvecklandet
- Vi uppfann med AI ***nya*** omställbara ELP protein material & ***patenterade*** dem
- Vi validerade de materialen experimentellt och fann ***överlägsen stabilitet*** och ***robusta*** funktioner
- Senaste AIMS resultat: de uppfunna materialen hade ***oplanerade*** anti-mikrobiella egenskaper (*serendipity*)
- ***Kvantdatorer*** kan ytterligare snabba upp utvecklandet av helt nya material