

# AI-POWERED MOLECULAR MODELING FOR NEXT-GENERATION BIOTHERAPEUTICS

**Biologics are expanding at a faster rate** than small molecule drugs, but they come with a different set of challenges

## Higher R&D costs

**\$1.5B-\$2.5B**, twice the cost of small molecule R&D

## Administration challenges

**>80%** injected or infused, requiring optimal solubility

## Formulation challenges

**Up to 20%** of batches fail due to poor stability or yield

## Safety and immunogenicity

**20-30%** of patients develop adverse reactions

## The Solution

BIOVIA Discovery Studio Simulation

### Market-leading algorithms

leveraged by scientists worldwide

### AI- and physics-based methods

integrated seamlessly for complete workflows



### SaaS application

access high-cloud computing and latest functionality 24/7

### Collaborative science

on a unified platform for maximized productivity

**Address the challenges** in design and optimization upfront, streamlining the path to successful biotherapeutic development

### Predict and model 3D structures

- Structure prediction with AlphaFold2/OpenFold
- Market-leading homology modeling with MODELER

### Simulate biological systems in various conditions

- Best-in-class MD engines NAMD and CHARMM
- GaMD for conformational sampling

### Explore binding affinity and molecular interactions

Protein-protein docking with ZDOCK

### Enhance binding and stability with mutagenesis

Mutation energy prediction (pH-/temperature-dependent)

### Reduce immunogenicity and adverse reactions

Humanization with ML or through germline sequence optimization

### Optimize formulation properties

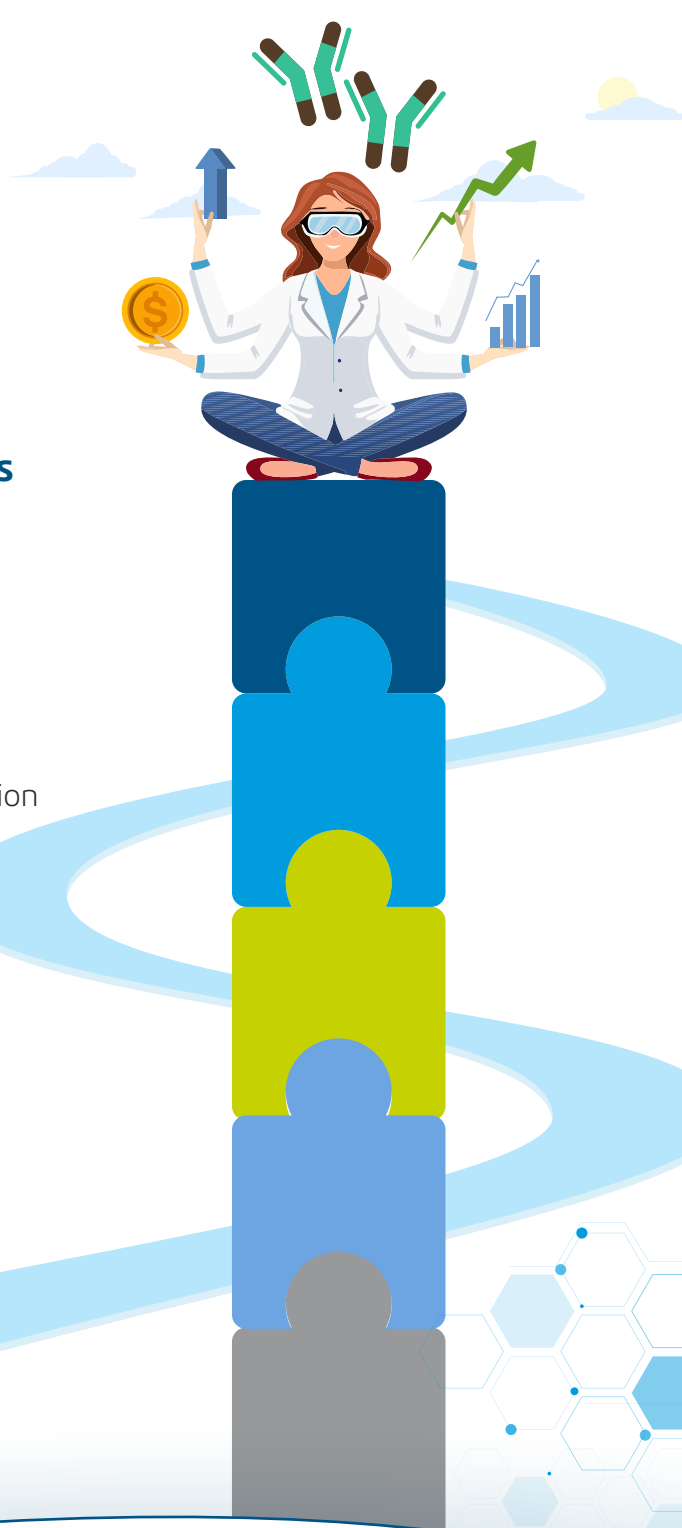
Prediction of viscosity, aggregation, stability, and solubility

### Predict excipient interactions

Validated ML methods to guide formulation design

### Design novel biotherapeutics with AI

RFDiffusion and ProteinMPNN family of models for generative biologics design



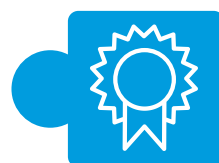
## Value



Reduce costs by **40-60%**



Shorten the discovery phase by **50-60%**



Improve candidates with up to **75%** success rates in lab



Screen **1000s** of candidates *in silico*

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