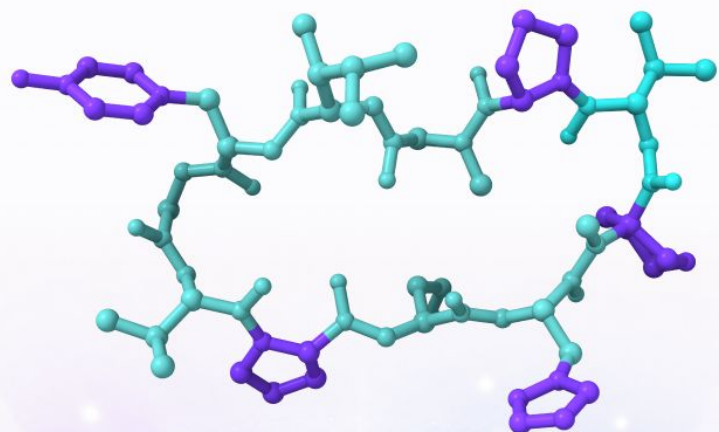




From target to development-ready candidates

across the entire DMTA cycle

Receptor.AI is an integrated peptide discovery platform combining computational and experimental capabilities to drive programs from design through experimental validation and optimization.



**AI-Powered
Design**

Generative models &
physics-based scoring



**Experimental
Validation**

In-house & partner assays
for rapid feedback



**Adaptive
Optimization**

Continuous learning
across the DMTA cycle



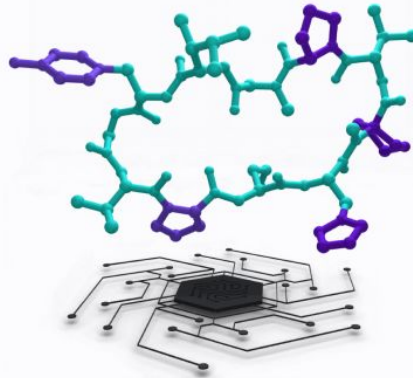
- ▶ **De novo discovery - designing peptides for targets, which lack known peptide binders.**
- ▶ **De novo peptide discovery is much broader than “yet another generative AI model”:**
 - Discovering binding pockets and interfaces suitable for peptide binding.
 - Choosing correct peptide size and topology (linear, cyclic, stapled, etc.).
 - Choosing appropriate chemistry (canonical, non-canonical, peptoid, etc.).
 - Developability - de novo candidate should be suitable for optimization and modification.
 - Turning experimental screening inputs (mRNA/phage display) into design hypotheses.
- ▶ **Decisions during de novo discovery are critical for the whole campaign.**
- ▶ **There is no clear line between de novo design and optimization**
 - De novo hits are already optimized from predicted seed designs.



Oral therapeutic peptides



Cell-permeable peptides



RECEPTOR.AI PEPTIDE PLATFORM

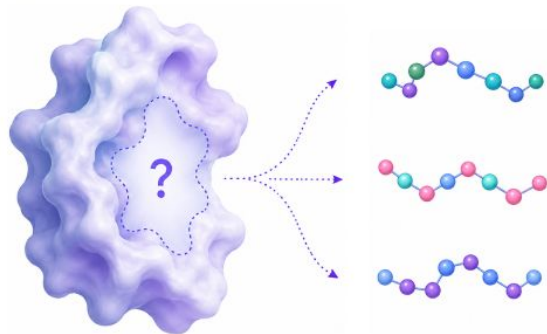


Peptide-drug conjugates



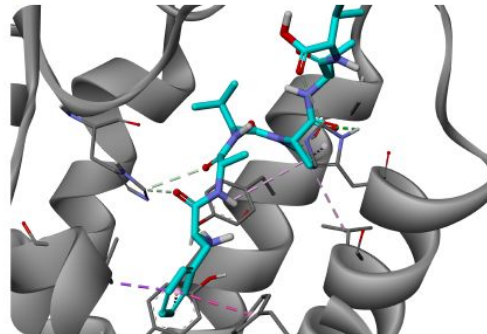
Peptidomimetics

01



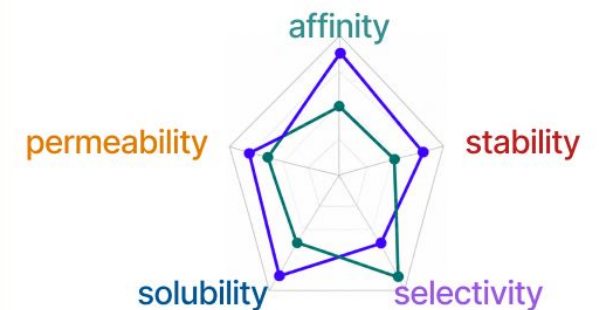
De novo peptide design

02



Peptide-protein 3D complex prediction

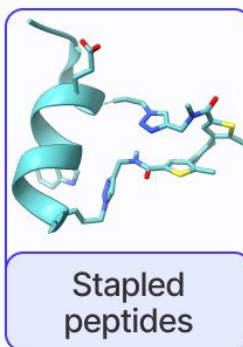
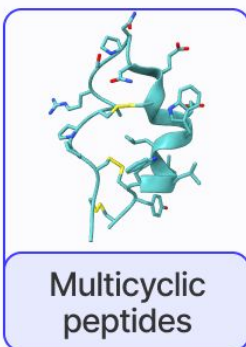
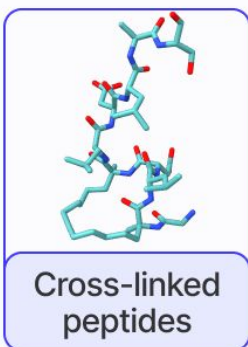
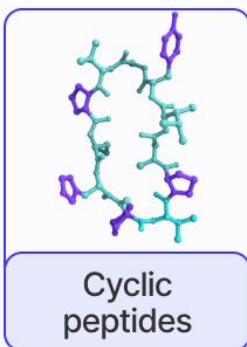
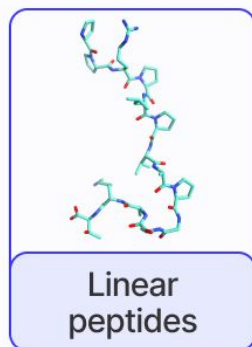
03



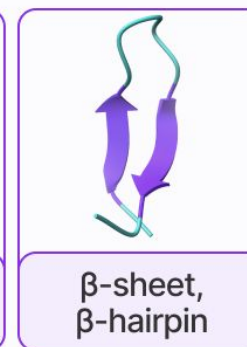
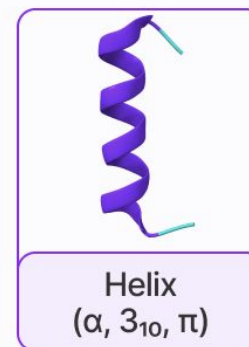
Physics-based + AI optimization

Any structure and non-canonical building blocks, even beyond listed here

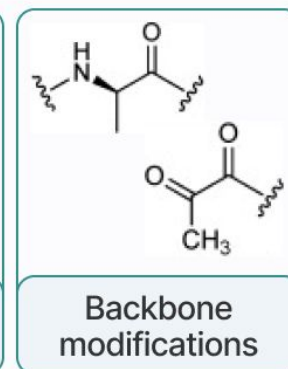
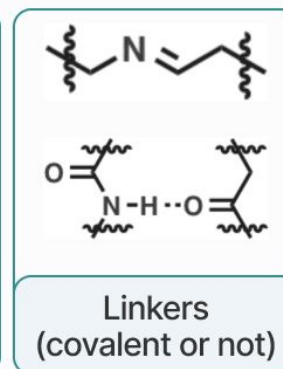
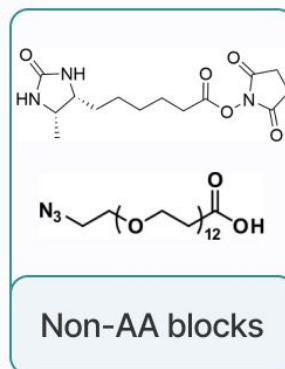
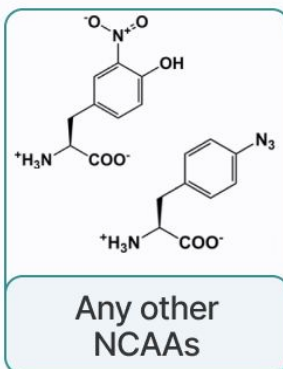
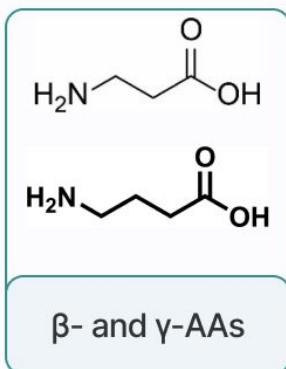
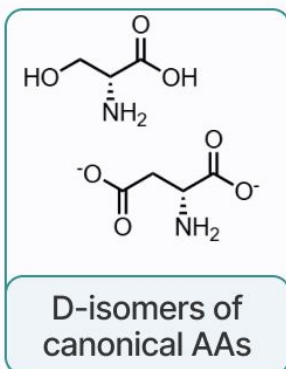
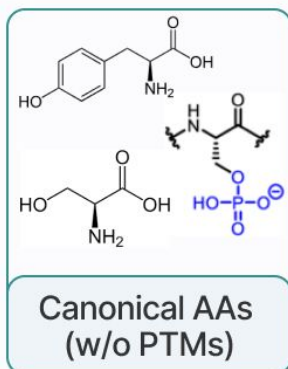
Topologies



Secondary structures



Libraries of non-canonical peptide building blocks (12K+ stock and 10M virtual)



Characterized and clustered by phys-chem class:
hydrophobic · aromatic · polar/uncharged · charged (positive / negative)

DE NOVO PEPTIDE DESIGN

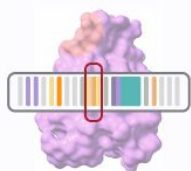


5

Starting chemistry for targets with no known peptide ligand

INPUTS

Target sequence +
design constraints



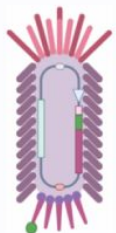
Binding region

Allowed amino acids

Allowed topologies

OPTIONAL

mRNA/ phage display data



5'	Amino acid sequence	3'	Abundance
1	H Y P F V S	1	5
2	A L Y V P S	2	3
3	Q P Q V P P	3	2
4	A L Y V P P	4	2
5	L I L P V P	5	1
6	L Q S T P P	6	1
7	S P I W M H	7	1
8	S P L I S P	8	1
9	Y A P T S P	9	1
10	Q P L L P N	10	1
11	A A Q T S P	11	1
12	F S A H A H	12	1
13	N Q P V P L	13	1
14	T P R L V P	14	1
15	H A I V P P	15	1
16	I P T L P P	16	1
17	A T T P A Y	17	1
18	Y S I P R S	18	1
19	A T P L W L	19	1



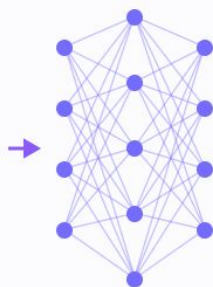
PEPTOR™ Foundation model

INFERENCE

2 generation modes



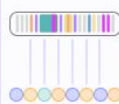
De novo
Generate
from scratch



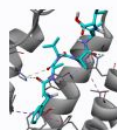
**Conditioned on
display data**
Leverage partner
display signals

TRAINING

Pretrained on large-scale
biochemical and structural data



>10M
peptide-protein
sequence pairs



~50K
experimental
3D complexes

OUTPUTS

Candidate peptides

Sequences + topologies

Linear



S L Y Q R T K L

C-terminal amide

Cyclic



C W G F N K Y C

head-to-tail

Stapled



A E L K Q L A E

i, i+4 staple

Mixed



G R W D P Y N R

non-natural AAs

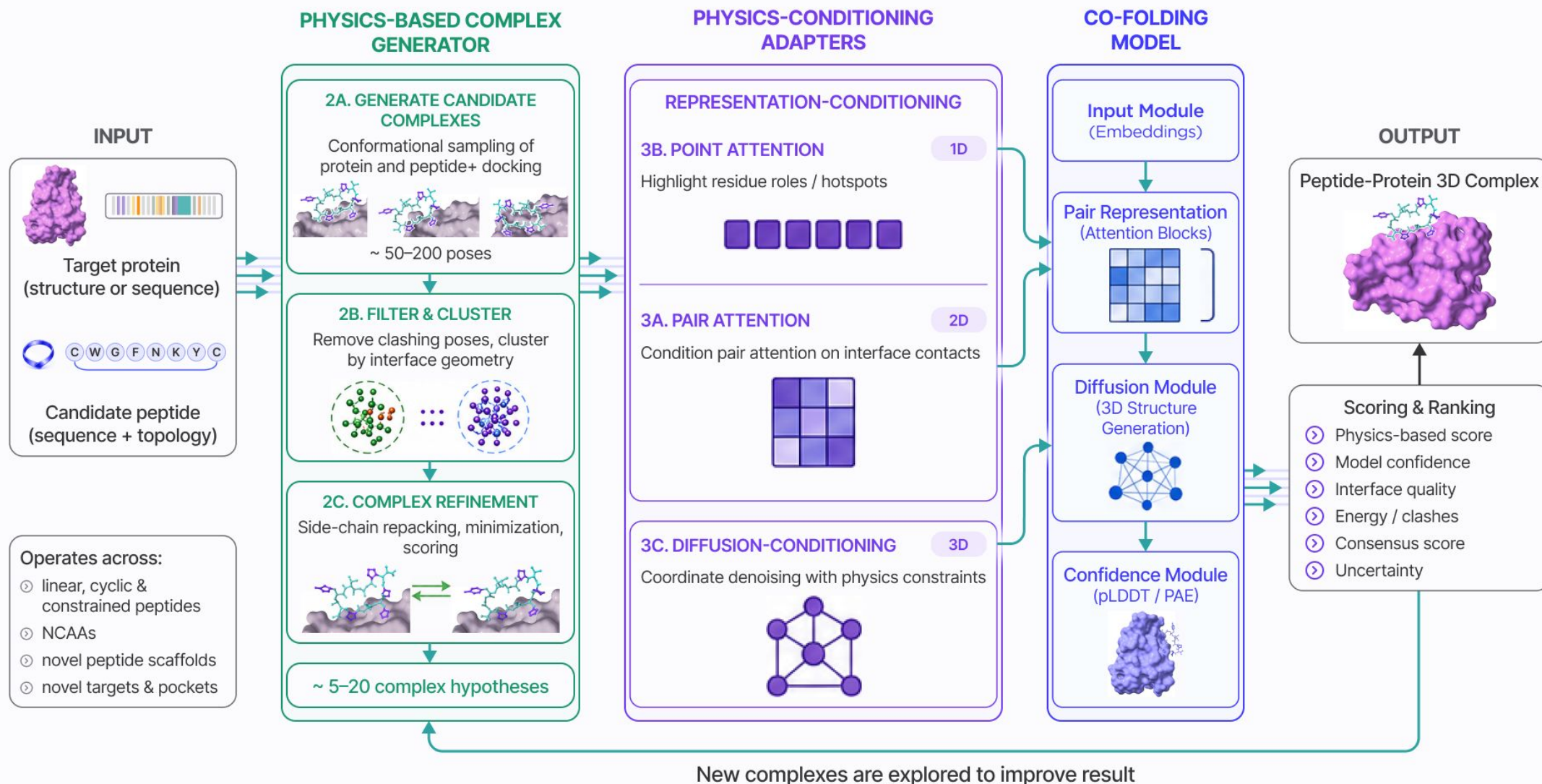
PEPTIDE-PROTEIN 3D COMPLEX PREDICTION



6

ForceFold™ turns sequence hits into a 3D complex to optimize against

ForceFold™ is Receptor.AI's architecture that steers co-folding toward physically valid peptide-protein complexes



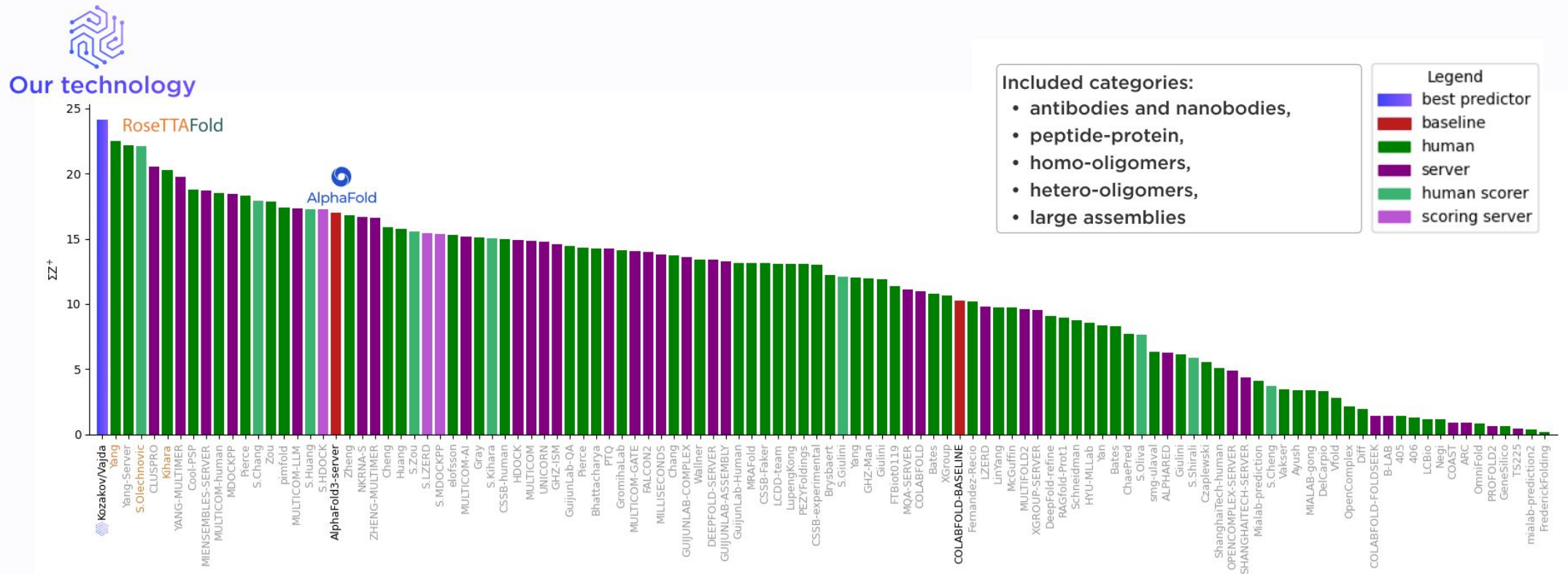
3D COMPLEX PREDICTION - BLIND BENCHMARK



7

Top-ranked among 112 teams in CAPRI-CASP16

CAPRI-CASP16 — the worldwide blind benchmark for protein-complex structure prediction



Participating teams (112)

Receptor.AI was represented by
Dima Kozakov – scientific lead of our
peptide-protein complex prediction track

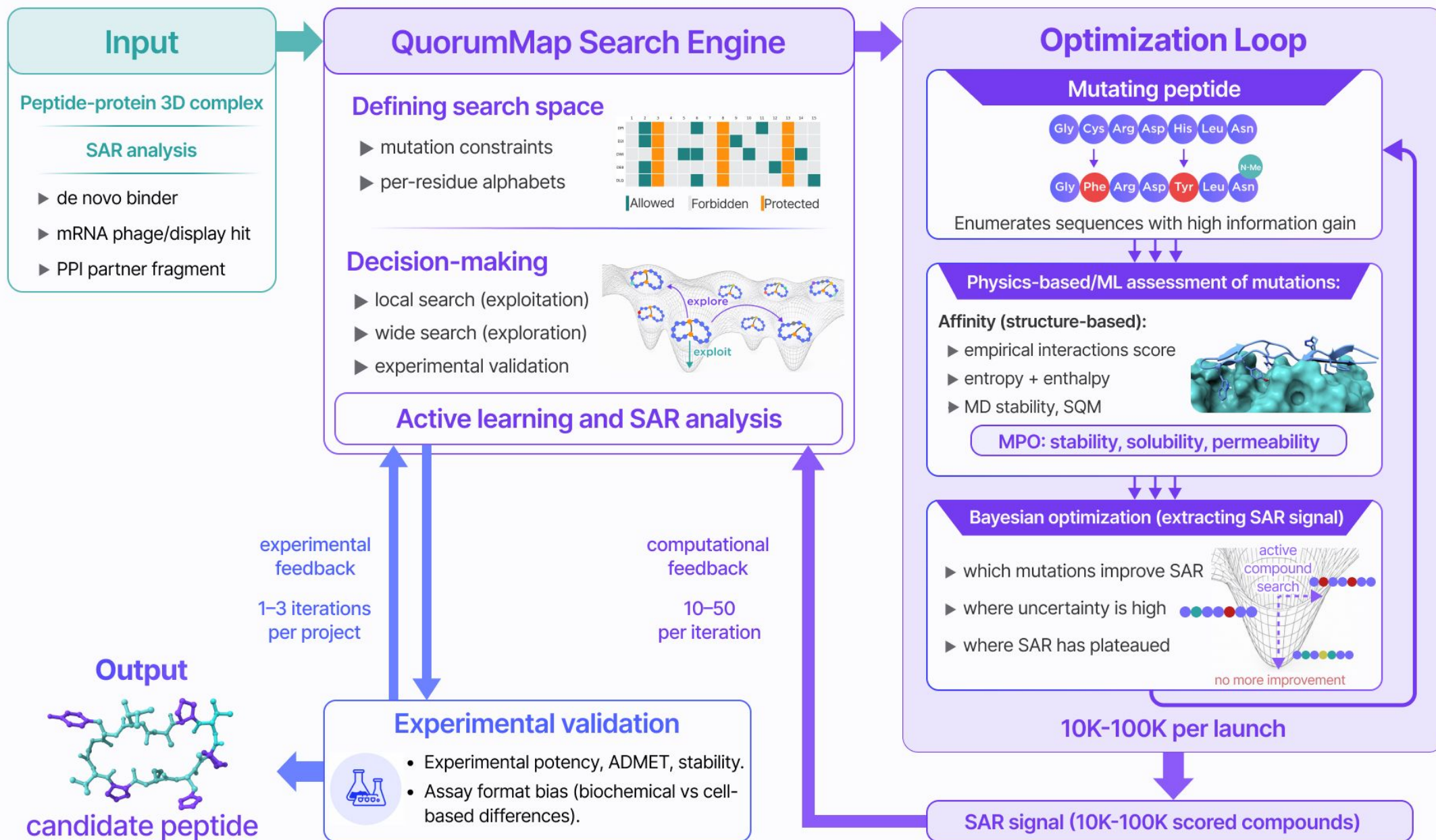
<https://www.capri-docking.org/assessment/>

PHYSICS-BASED + AI OPTIMIZATION



8

Multi-objective search inside large sequence space



DE NOVO SKIN-PERMEABLE GPCR ANTAGONISTS



9

De novo nanomolar, skin-permeable and safe hits

BACKGROUND

Target: dermatology-related GPCR

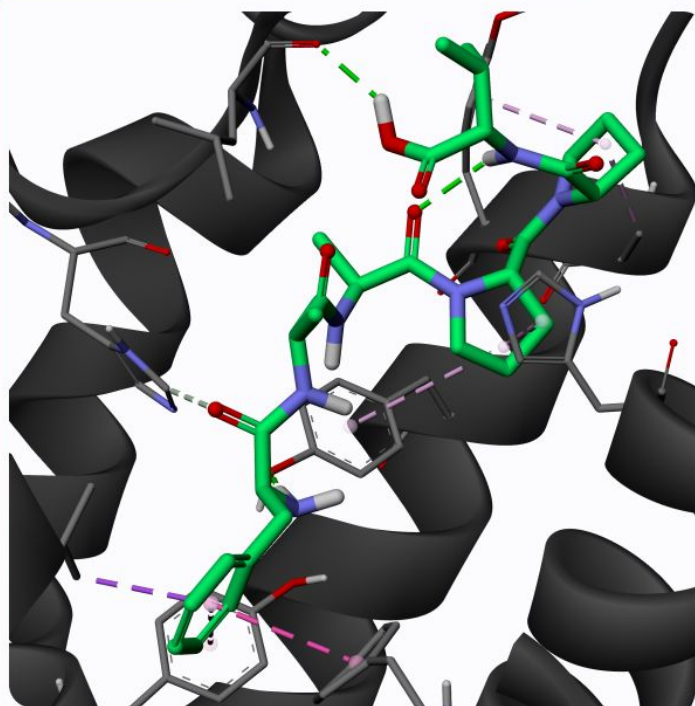
Challenge: no known peptide antagonists

Goal: short, INCI-compliant peptides
— active + skin-permeable + safe

APPROACH

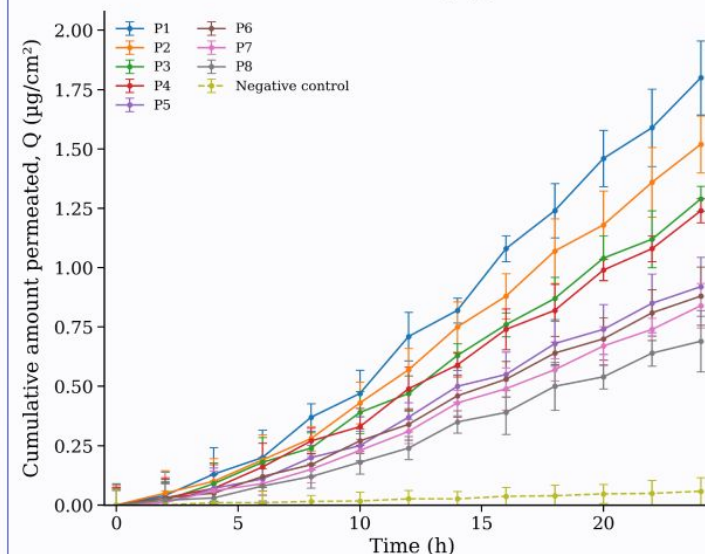
Method: Structure-guided de novo generation + multi-parameter optimization

~10,000 generated →
~2,000 ranked → 100 tested



Binding mode
of the validated peptide

Best peptide (P1):
Q24h = 1.80 $\mu\text{g}/\text{cm}^2$



Skin permeation profile of top hit peptides in a Franz diffusion cell assay using Strat-M membrane

RESULTS

50 / 100
active peptides in vivo

90 nM
best IC_{50}

8
skin-permeable hits

PEPTIDE-siRNA DESIGN FOR BBB PERMEABILITY



10

Developable lead with TfR1-mediated transcytosis in 2 DMTA cycles

BACKGROUND

Indication: Alzheimer's disease

Target: TfR1 on brain endothelium

Goal: compact peptide shuttle conjugated with siRNA

Challenge: avoid competition with TfR1 and preserve transcytosis after conjugation

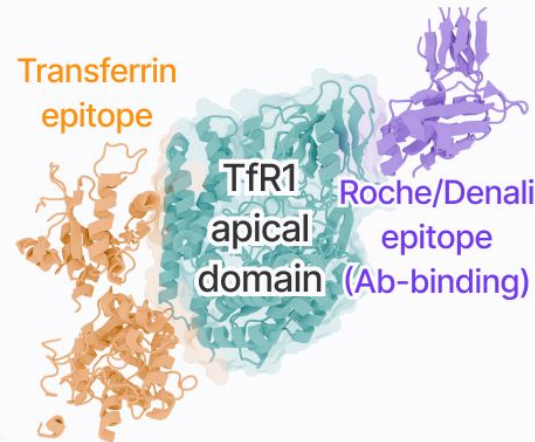
APPROACH

Starting point: anti-TfR1 antibody & its epitope (avoids transferrin competition)

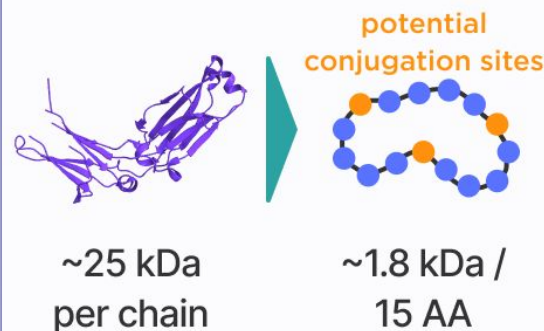
Workflow (2 cycles):

- ▶ **Step 1** - generate compact TfR1 peptide shuttle
- ▶ **Step 2** - conjugate with siRNA

DESIGN RATIONALE

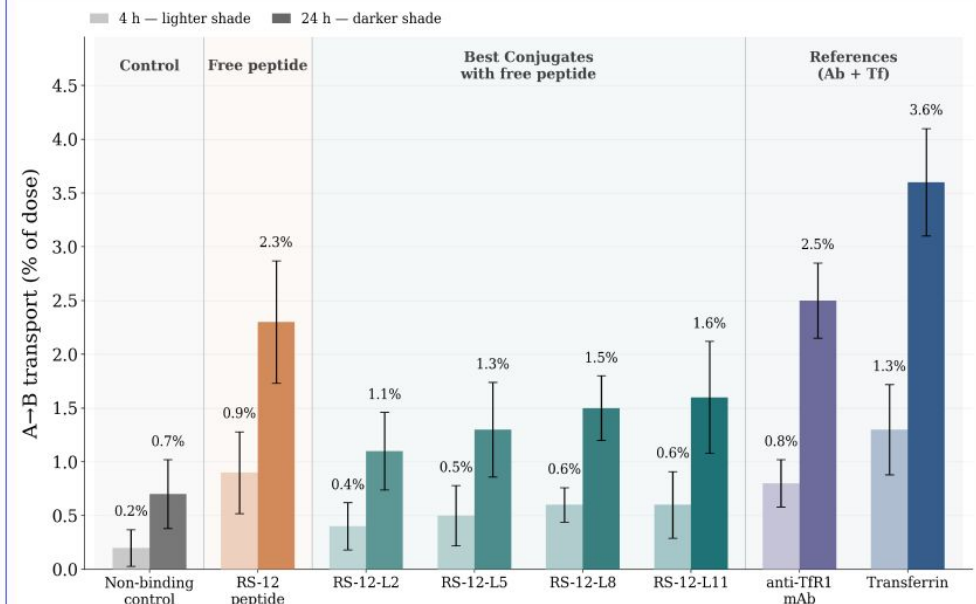


EPITOPE-TO-SHUTTLE



BBB TRANSCYTOSIS OF FINAL CONJUGATES

hCMEC/D3 BBB transcytosis assay,
best free peptide + 4 best conjugates + references



Minor affinity loss
after conjugation



BBB transport
validated

RESULTS

1.6%
best BBB permeability

6-21 h
serum stability $t_{1/2}$

69%
transport retained after conjugation

OUR SOFTWARE FOR PEPTIDE DISCOVERY



RECEPTOR AI

Peptides

New Study

WORKSPACE

Dashboard

SPACES

Chemical Space

Protein Space

ADMIN PANEL

Data Hub

STUDY

TARGET

PROGRAM

PROGRESS

ELAPSED

Complex MD

IL6R-multichain

IL-6R

Inflammati... +2

62%

13m

STUDY

TARGET

PROGRAM

RESULT

Peptide MD

IL6R-multichain

IL-6R

Inflammati... +2

Succeeded

14m ago

Peptide MD

p53-MDM2-stap...

p53-MDM2

Oncology +2

Succeeded

1d ago

Optimizati...

KRAS-linear-scan

KRAS-G12D

Oncology +2

Succeeded

6h ago

Optimizati...

ACE2-turn-seq

ACE2

COVID +2

Succeeded

8h ago

Optimizati...

TNF-interface-o...

TNF-α

Inflammati... +2

Succeeded

3d ago

STUDIES

one optimization study per complex — expand for analytics

8

All studies >

PEP-2024-0038

Metabolic

GLP-1R

TREND

Optimization

Peptide MD

Complex MD

+42%

PEP-2024-0041

Oncology

KRAS G12E

TREND

Optimization

Peptide MD

Complex MD

+33%

PEP-2024-0039

Inflammation

IL-6R

TREND

Optimization

Peptide MD

Complex MD

+31%

PEP-2024-0044

Oncology

p53-MDM2

TREND

Optimization

Peptide MD

Complex MD

+28%

PEP-2024-0037

COVID

ACE2

TREND

Optimization

Peptide MD

Complex MD

+24%

CHEMICAL / PROTEIN SPACE

entities & building blocks

6

Proteins

unique UniProt entries

8

Prepared complexes

protein-peptide

8

Studies

1 per complex

2,302

Candidate peptides

generated

4

Residue databases

standard, uploaded, derived

Ask AI

Ctrl+I

Theme

Light

Dark

VH

Vladyslav Husak

RESIDUE DATABASES

All databases >

TARGETS OVERVIEW

All proteins >



PROF MORTEN P. MELDAL

Scientific Advisor

 Nobel Laureate in Chemistry 2022 for inventing the click chemistry reaction (CuAAC). PhD in chemical engineering with 40+ years of experience in peptide synthesis and combinatorial chemistry. Professor at the University of Copenhagen.
meldal@chem.ku.dk



PROF SCOTT LOKEY

Peptide Drug Discovery Advisor

PhD chemist and Professor of Chemistry at UC Santa Cruz with expertise in constrained peptides, chemical biology, high-throughput screening, and cell permeability. He previously conducted research at Genentech and Harvard Medical School and founded the UCSC Chemical Screening Center.
slokey@ucsc.edu



DR TOMI K. SAWYER

Peptide Drug Discovery Advisor

Leading expert in peptide drug discovery with 40 years of experience in pharma and biotech. He contributed to the development of FDA-approved drugs like Scenesse® and Iclusig®. Recognized for over 600 scientific publications and patents in drug discovery.
tomi.sawyer@maestrotherapeutics.com



PROF ZORAN RANKOVIC

Targeted Protein Degradation Advisor

Expert in targeted protein degradation and medicinal chemistry with 25+ years across pharma and academia. Professor of Chemical Biology and Director of the Centre for Protein Degradation at The Institute of Cancer Research, London. Developed alternative cereblon warheads for PROTAC design and selective degraders of CK1 α and GSPT1.
zoran.rankovic@icr.ac.uk



DR ALDRIN DENNY

Drug Discovery Advisor

Accomplished medicinal chemist with over 20 years of experience in the pharmaceutical industry, including a significant tenure at Pfizer. His work at Pfizer resulted in the successful development of 7 drug candidates.
aldrin.denny@receptor.ai



PROF DIMA KOZAKOV

Induced Proximity Discovery Advisor

Structural biologist specializing in macromolecular complex modeling. Professor of Applied Mathematics at Stony Brook University and Research Professor of Biomedical Engineering at Boston University. Led the team ranked as TOP-1 in CAPRI-CASP16 competition.
dmytro.kozakov@stonybrook.edu

OUR TEAM



13



DR ALAN NAFIIIEV

Chief Executive Officer, Founder

PhD in Data Science with deep expertise in AI-driven drug discovery and computational infrastructure. Led 40+ projects from hit discovery to IND by unifying molecular design, R&D strategy, and integrated in silico and wet lab execution. Brings 15+ years of experience at the intersection of data science, life sciences, and software platforms.



DR SERGII STAROSYLA

Chief Technical Officer, Co-founder

PhD in Molecular Biology with 13 years of experience in drug discovery and scientific software development. Medicinal chemist, expert in development of machine learning models, algorithms for pharmacophore modelling and molecular docking. Author of the number of patented anticancer and anti-microbial biologically active compounds.



DR SEMEN YESYLEVSKYY

Chief Scientific Officer, Co-founder

PhD in biophysics. 25 years of experience in molecular modelling, computational drug discovery and scientific software development. Author of unique techniques and algorithms in simulations of curved and asymmetric lipid membranes and assessment of drug-membrane interactions.



DR DANIELE ANDREOTTI

Medicinal Chemistry

PhD chemist with 30+ years in medicinal chemistry, project leadership, and preclinical drug discovery. Contributed to 15+ preclinical candidates and led programs from hit identification to candidate selection across CNS, anti-infective, and metabolic diseases.



DR ASKAR KUCHUMOV

Head of Business Development

PhD in Biochemistry and Molecular Biology, with 15+ years in biotech business development and venture capital. Co-founded several oncology startups, advancing two first-in-class programs from discovery to Phase II. Co-author of 20+ publications and 2 patents.



DR. VOLODYMYR BDZHOLA

Head of Medicinal Chemistry

PhD in Chemistry with 25 years of research experience, Senior Research Scientist and Deputy Head of the Department of Medicinal Chemistry at the Institute of Molecular Biology and Genetics, National Academy of Sciences of Ukraine. Author of 65+ scientific publications.



DR MARTIN INDARTE

Head of Computational Chemistry

PhD in Pharmaceutical Sciences with 15+ years in computational drug discovery. Specializes in molecular modeling, structure-based drug design, and molecular dynamics. Research spans CNS pharmacology and oncology, with publications and cancer-focused patents.



DR ANDREW GOLUB

Head of Computational Chemistry

PhD in Molecular Biology with 20+ years in industry and Academia, specializing in CADD, computational chemistry, and cheminformatics. Expert in protein structure analysis, drug mechanisms, and therapeutic design. Co-author of scientific papers and patents.



DR YAROSLAV BILOKIN

Head of Chemistry

PhD in Chemistry with 30+ years in medicinal and synthetic organic chemistry. Executive Director at OTAVA Ltd., with numerous patents and publications. Combines expertise and leadership to tackle complex chemistry challenges and lead innovative projects.



Tigran Tsaturyan

Drug Discovery
Project Manager



Sasha Korogodski

Drug Discovery
Project Manager



Roman Stratiichuk

AI Drug Discovery Project
Manager



Ihor Koleiev

Scientist
Medicinal Chemistry



Taras Voitsitskyi

AI Engineer
Computational Chemistry



Vlad Husak

Platform Manager



Daniil Todoryshyn

Product Marketing
Manager



Myroslav Uiazdovskyi

BD Executive,
AI-Enabled Therapeutics

and 20+
other
specialists



Founded in 2021 in Kyiv, relocated R&D to Central Europe and BD to London in 2022, and opened headquarters in Cambridge, MA in 2024

ADDRESS

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