

YOUNGFACE

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Problem statement

- (1) **Cosmetical products are not effective and not personalized**
- (2) **The process of new compounds discovery in skincare is slow and expensive**
- (3) **Most products provide only supportive care**

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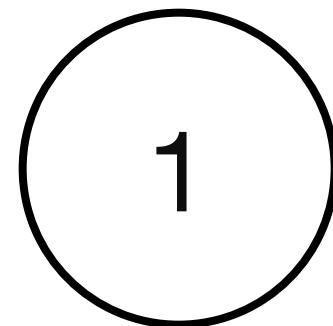
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Problem statement & Solution

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A platform for fast and effective development of small molecule anti-aging drugs in skin care industry

Values

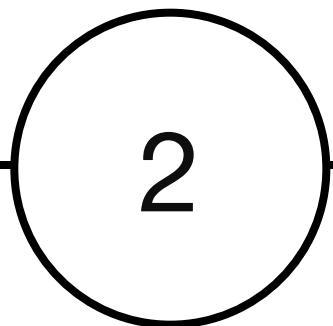


**Strong scientific
validations**

(1)

Our goal is to create innovative cosmetics aimed at the primary causes of skin aging, not its consequences

We set ambitious goals, so our internal scientific standards need to be high



Acceleration

(2)

The drug development process takes an embarrassing amount of time

The main business value of our project is an acceleration of cosmetic products development with the use of data analysis and AI. That is why our drug discovery process will be efficient



Inclusivity

(3)

Differences in pigmentation, signs of aging, and stratum corneum function could reflect the versatility of epidermal functions among different skin types and different genders

We see YoungFace as smart cosmetics suitable for everyone, that is why we take into account skin ethnicity and genders in the development of our models

Team

Diverse areas of expertise in our team help us to cover all of the processes, happening in the field of AI-accelerated drug discovery, starting from target generation ending up with a computational assessment of lead properties

Long experience of intra-team interactions and collective problem-solving bring our team together and highlight our potential

**Kirill Denisov**

ML Engineer with experience in aging biology, data science and deep learning

**Daniel Igumnov**

Bioengineer with experience in work with laboratory animal models and neurointerface applications

**Bohdan Didenko**

Deep learning engineer with experience of designing neural architectures in the NLP domain

**Georgiy Andreev**

Structural biologist with experience in molecular modeling, computational pharmacology and AI applications

**Ciara Makievskaya**

Bioengineer with experience in eukaryotic cell biology and epigenetics

**Ruslan Gumerov**

OMICS-bioinformatician with experience in transcriptomics, metabolomics and single-cell sequencing data analysis

Market opportunity

\$511B Beauty &
Personal Care industry

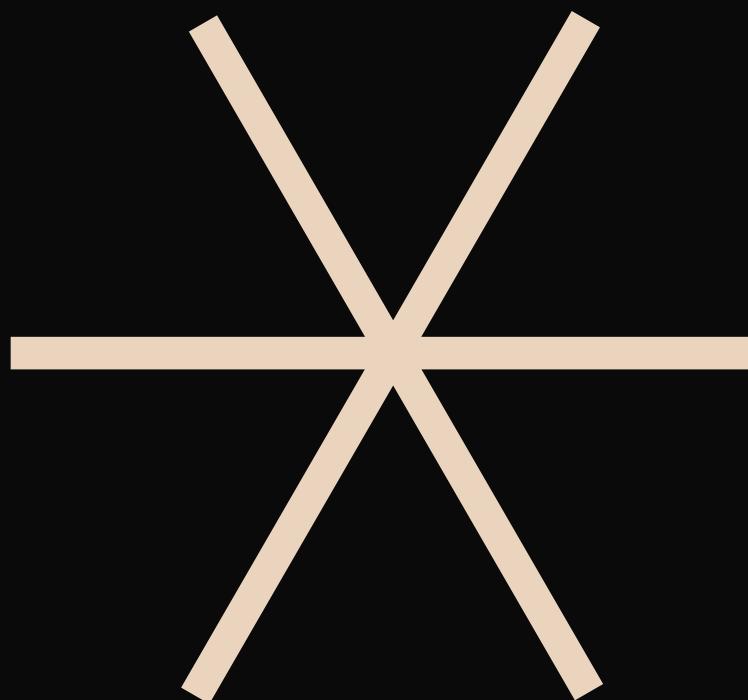
\$112B Skincare
industry

\$21B Anti-aging
market

Business model



Proprietary products



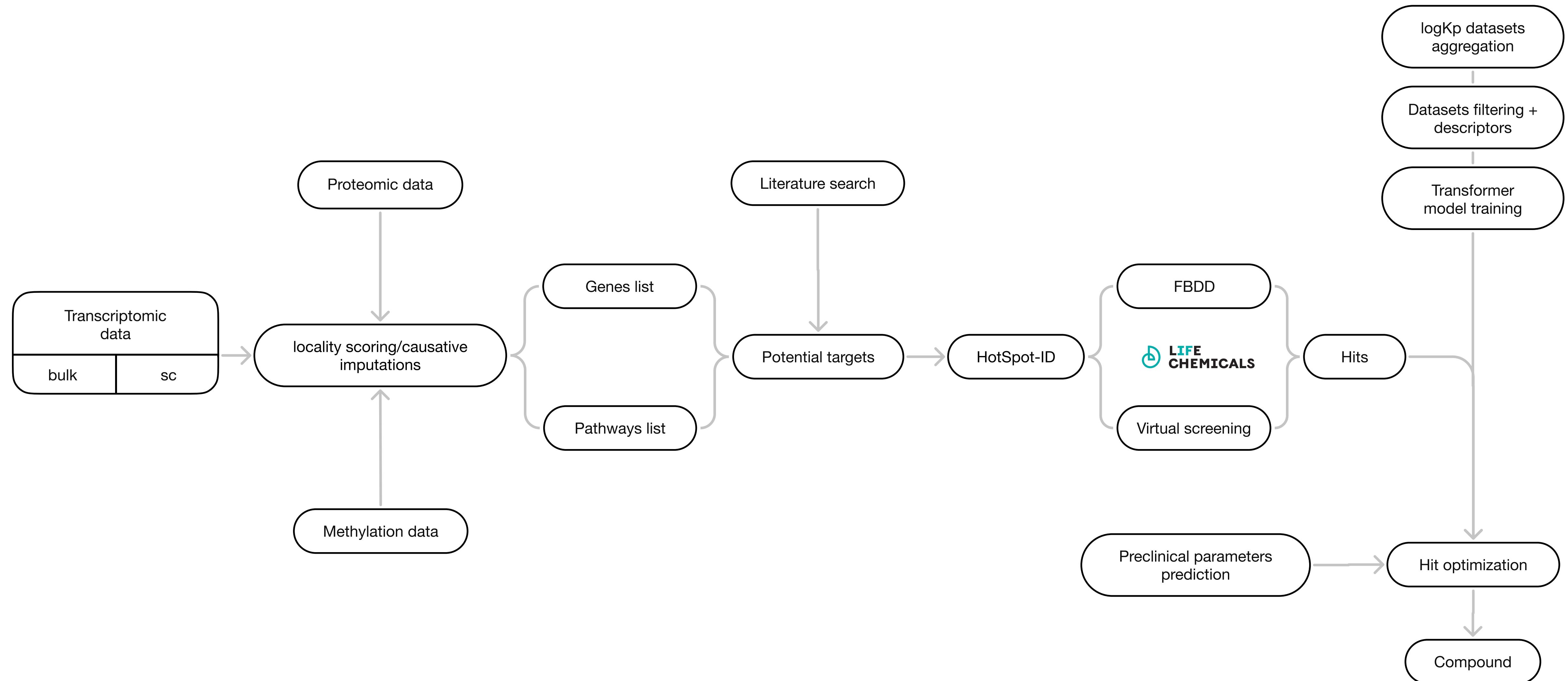
Models for prediction of preclinical parameters for skin care compounds

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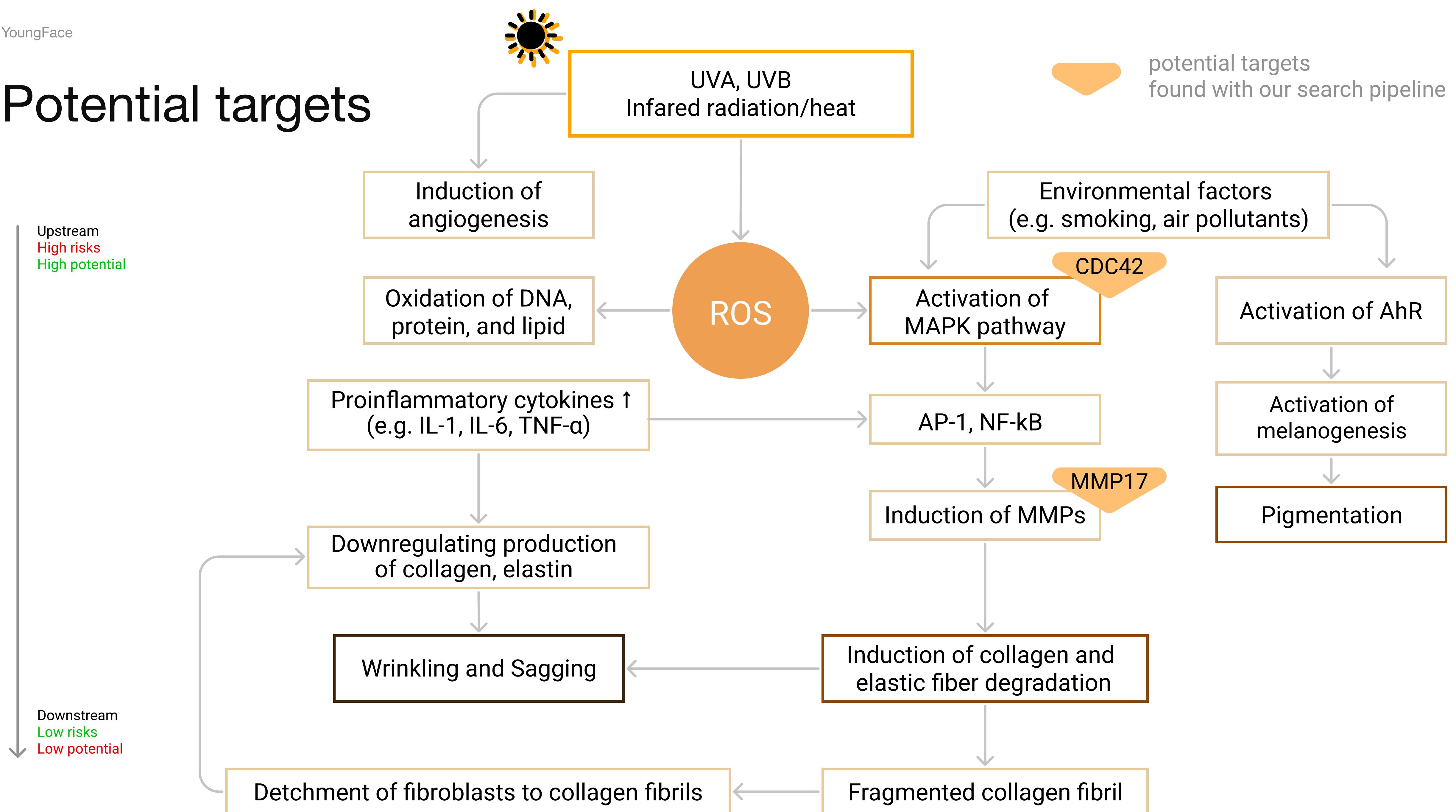


Service for investigation of targets for personalized skin care and skin diseases

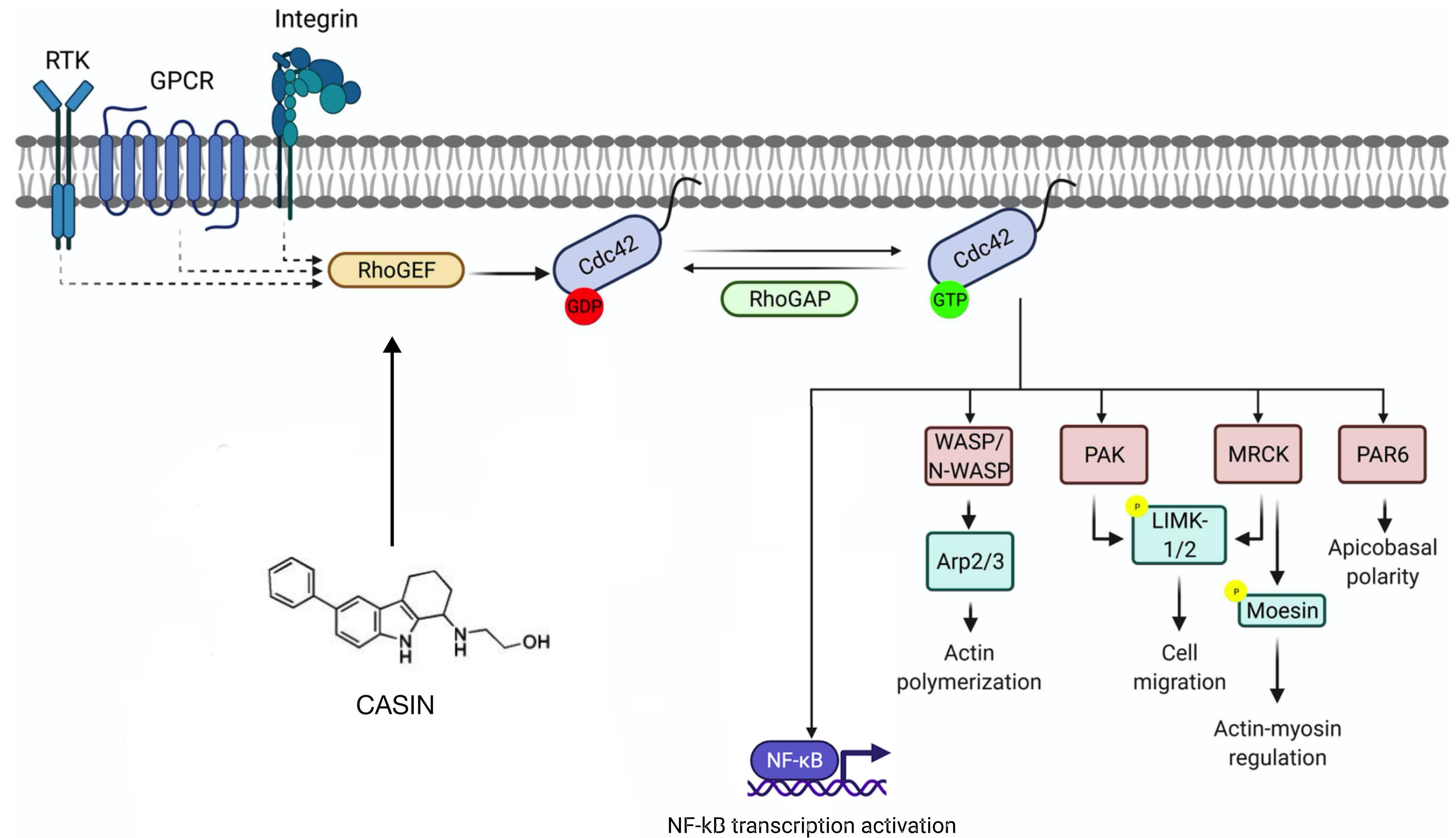
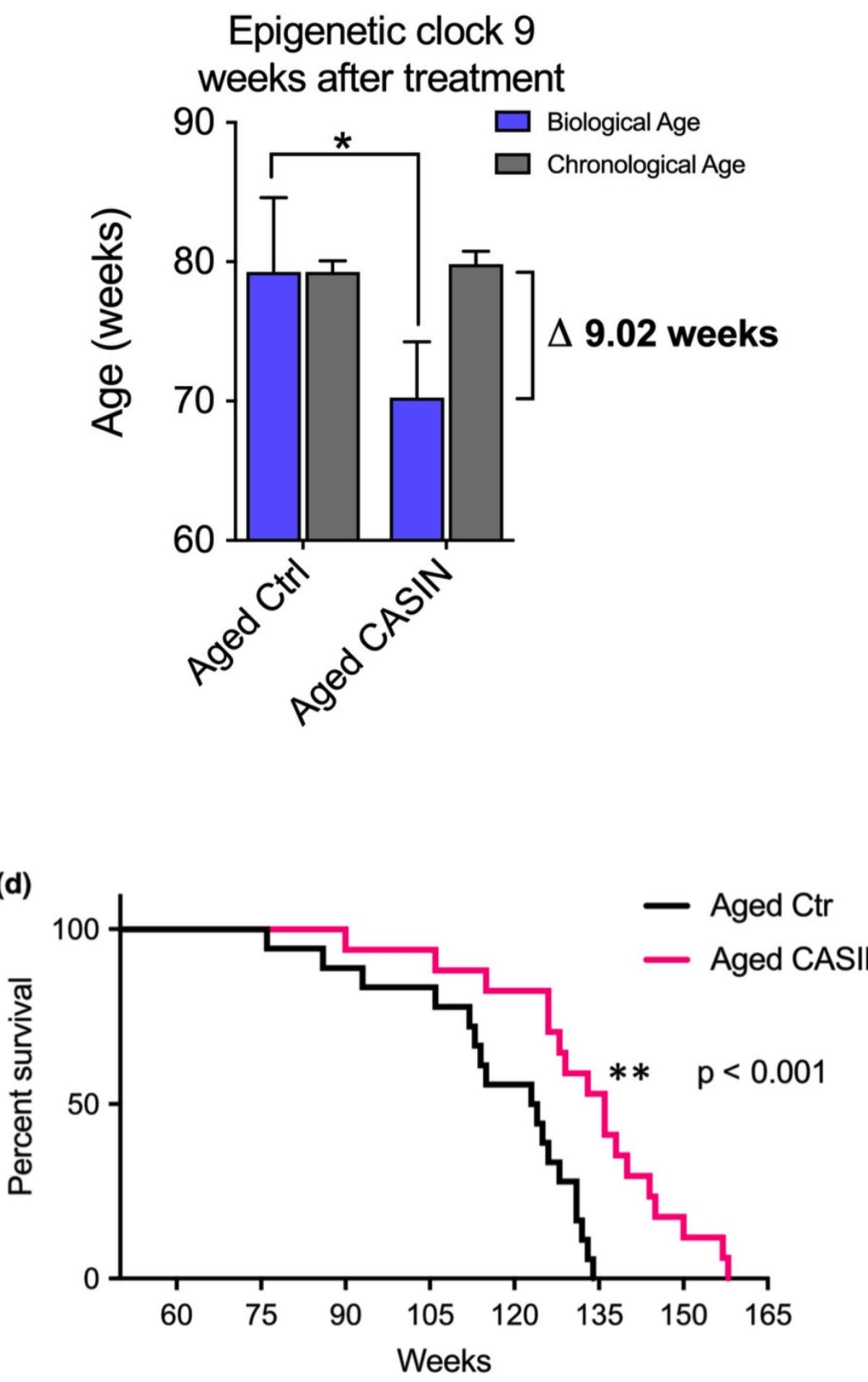
Technology



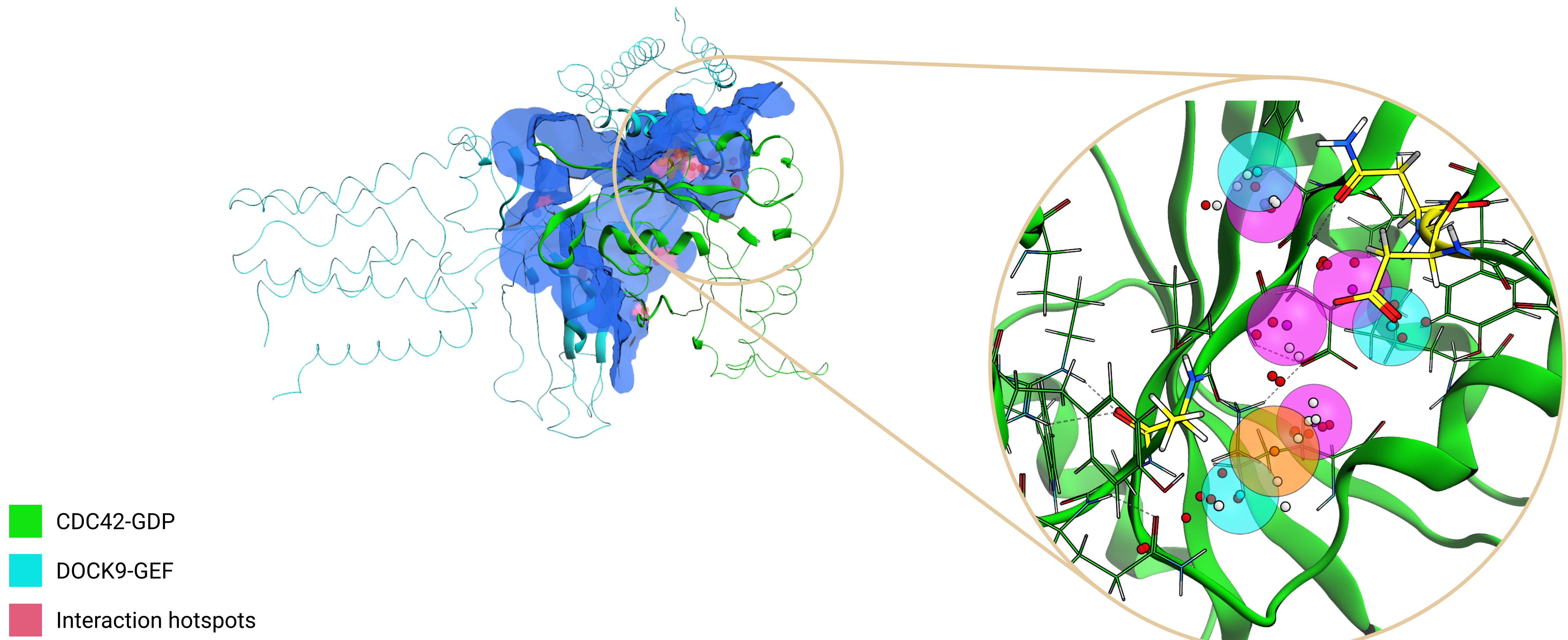
Potential targets



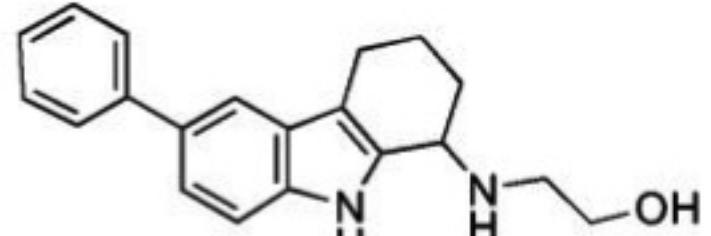
Potential target: CDC42



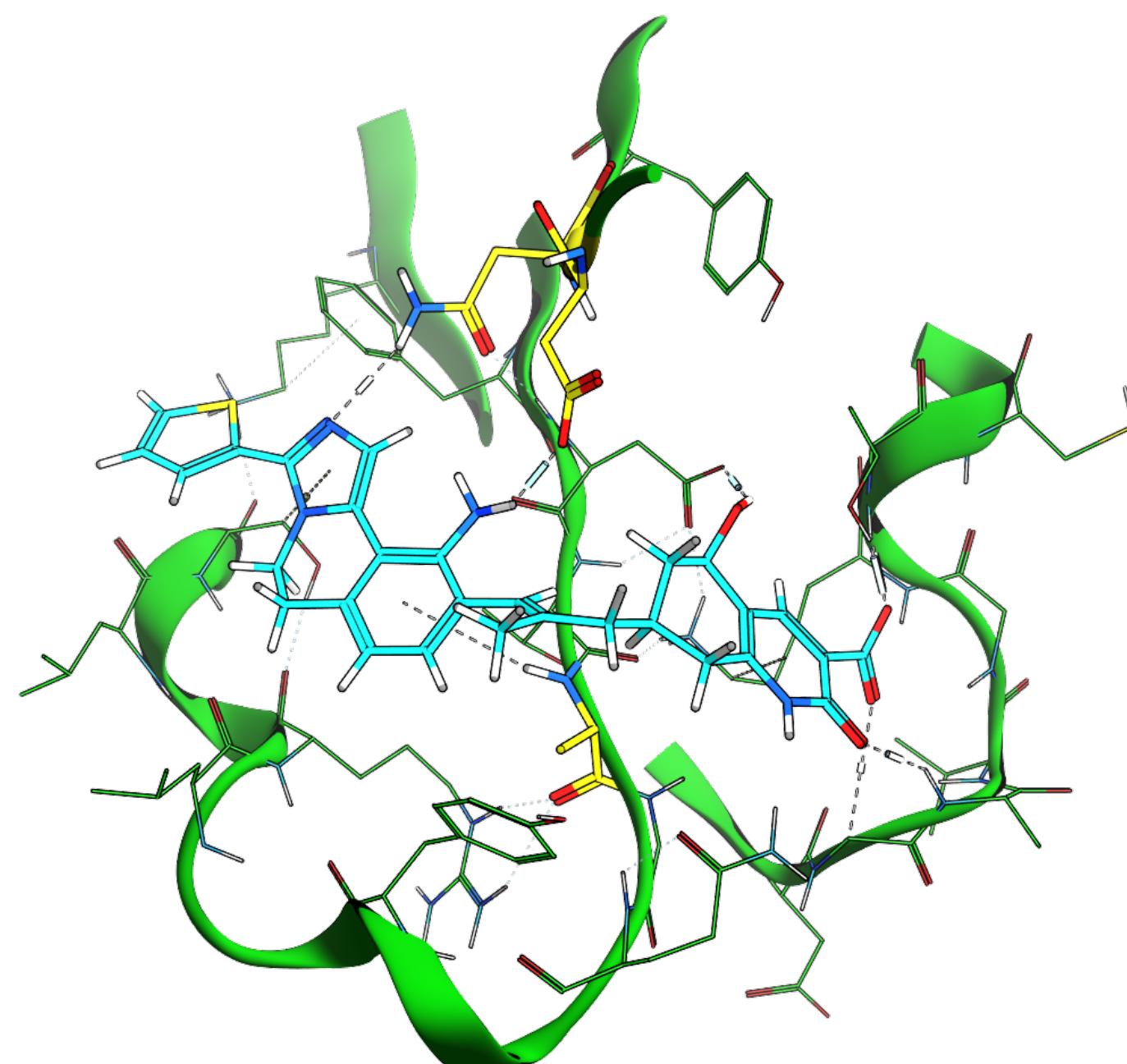
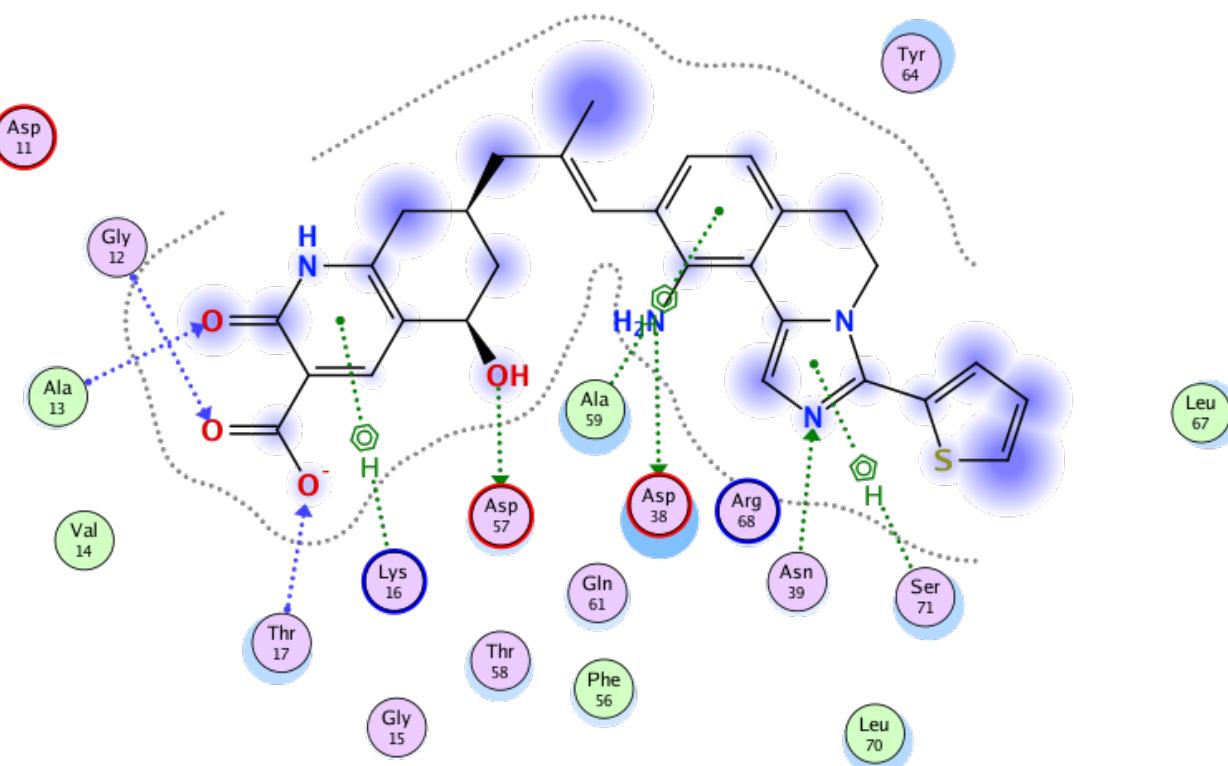
Target interface



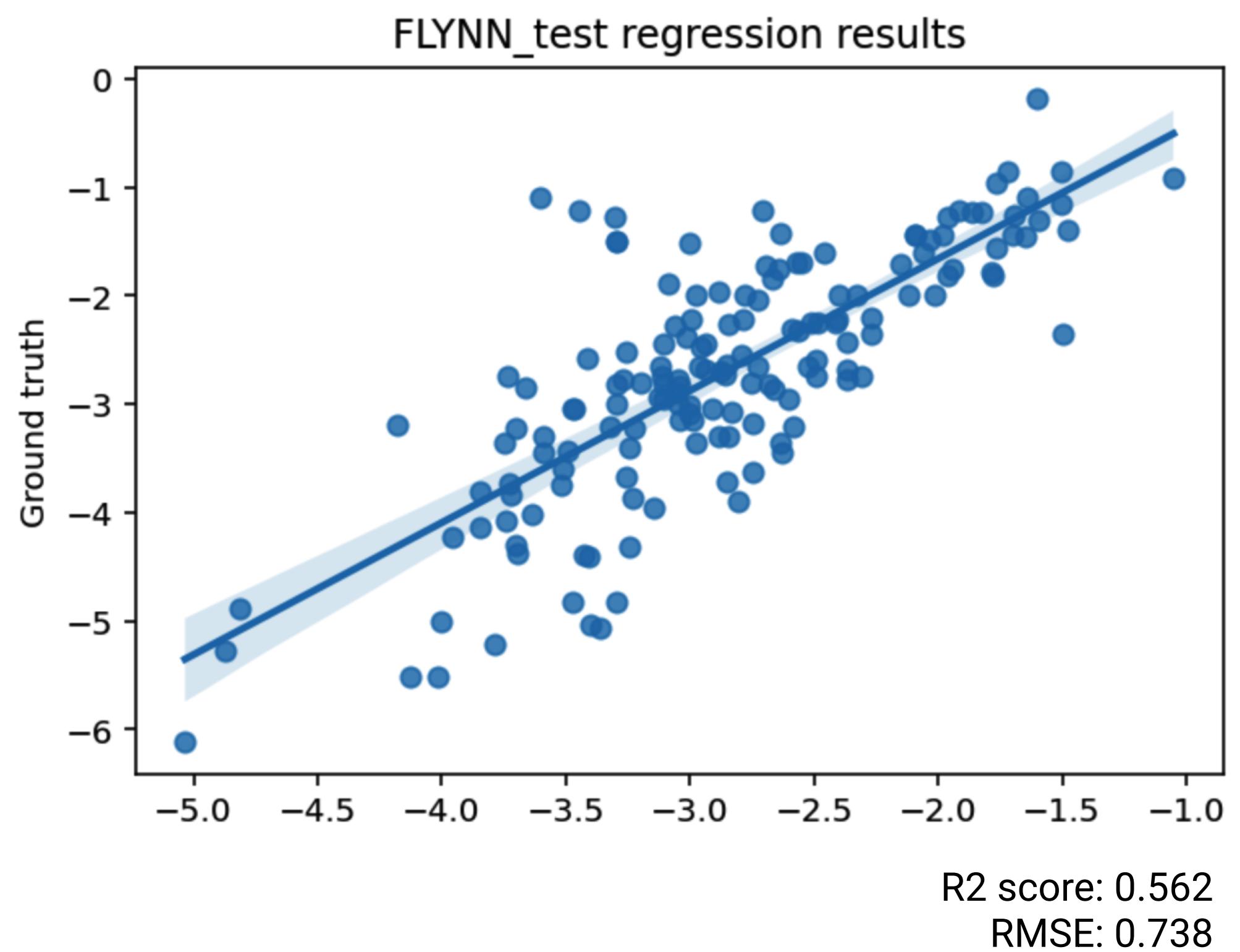
Hit optimization



CASIN logK_p = -4.32



New molecule logK_p = -3.66



Results

In a span of a week we have:

1. Successfully identified a viable skin-aging target based on OMICS data and literature review
2. Located and characterized a novel small molecule binding cryptic pocket in CDC42-GDP using in silico FBDD approach
3. Performed HTVS on a library of 400k compounds and 8k fragments and obtained moderate fragment hits for FBDD
4. Applied our novel in-house skin permeation model for hit optimization and reached a promising CDC42-GDP inhibitor

Our plans:

1. assemble a more complex penetration model from a combination of finetuned ChemBERTa and a fully connected NN trained on descriptors
2. collect more skin penetration datasets and bring them to a single standard in terms of solvent, donor types, etc.
3. perform skin permeation and ligand binding assessment using SOTA alchemical MD simulations to further optimize our hit