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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Problem statement & Solution

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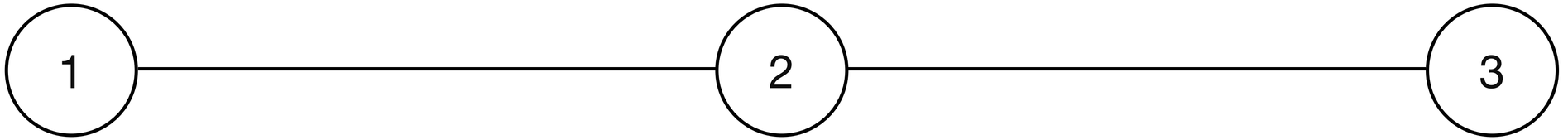
A platform for fast and effective development of small molecule anti-aging drugs in skin care industry

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 applicaitons

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

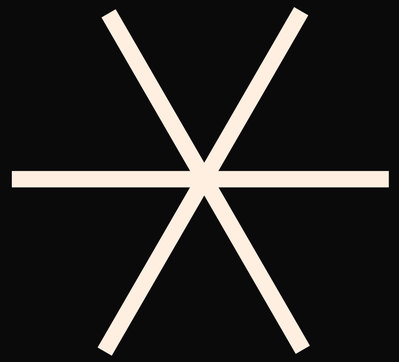
Market opportunity

$511B Beauty & Personal Care industry

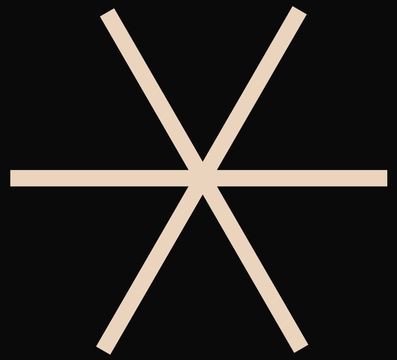
$112B Skincare industry

$21B Anti-aging market

Business model



Proprietary products



Models for prediction of preclinical parameters for skin care compounds

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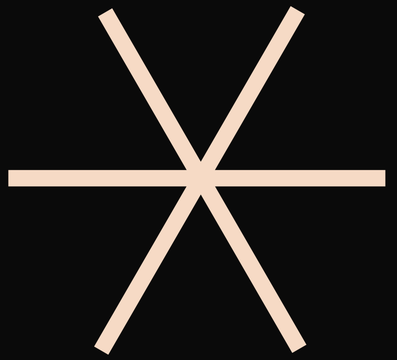
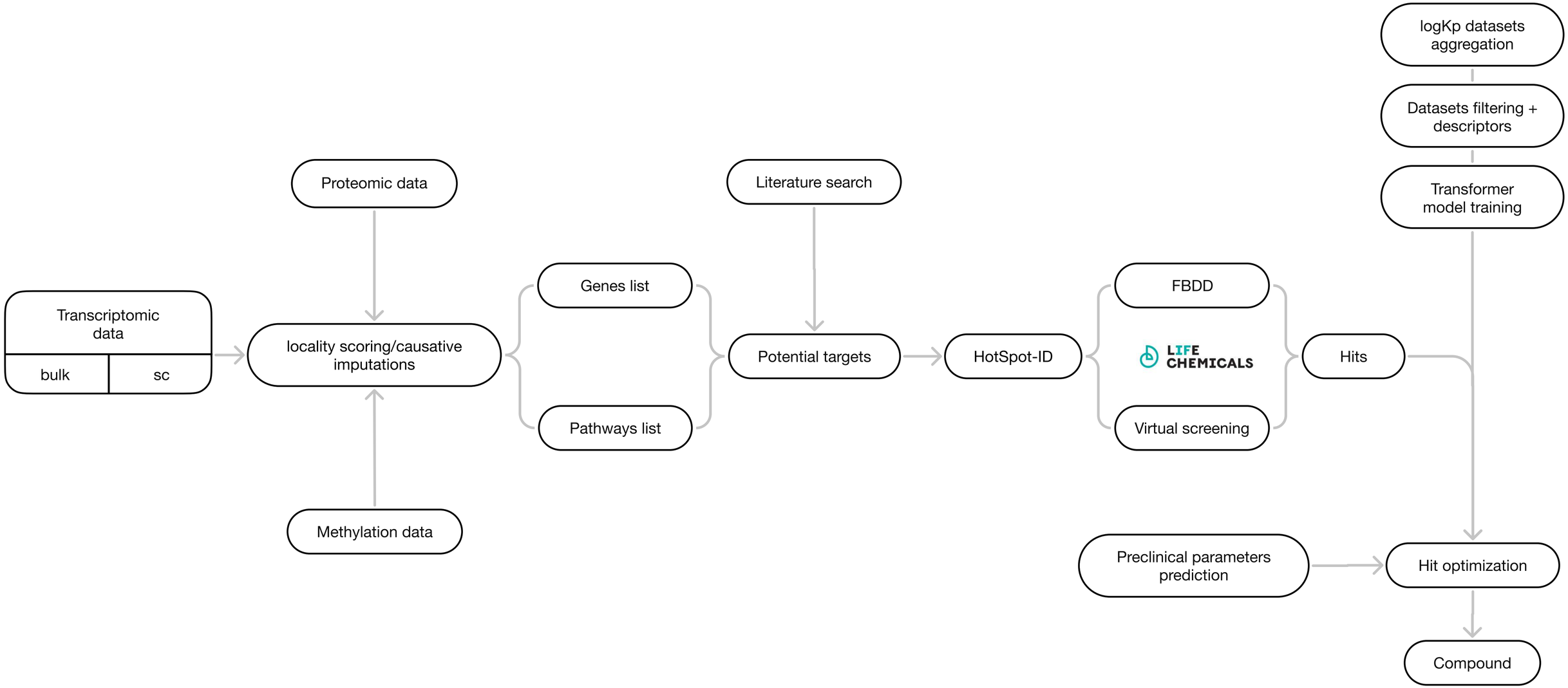
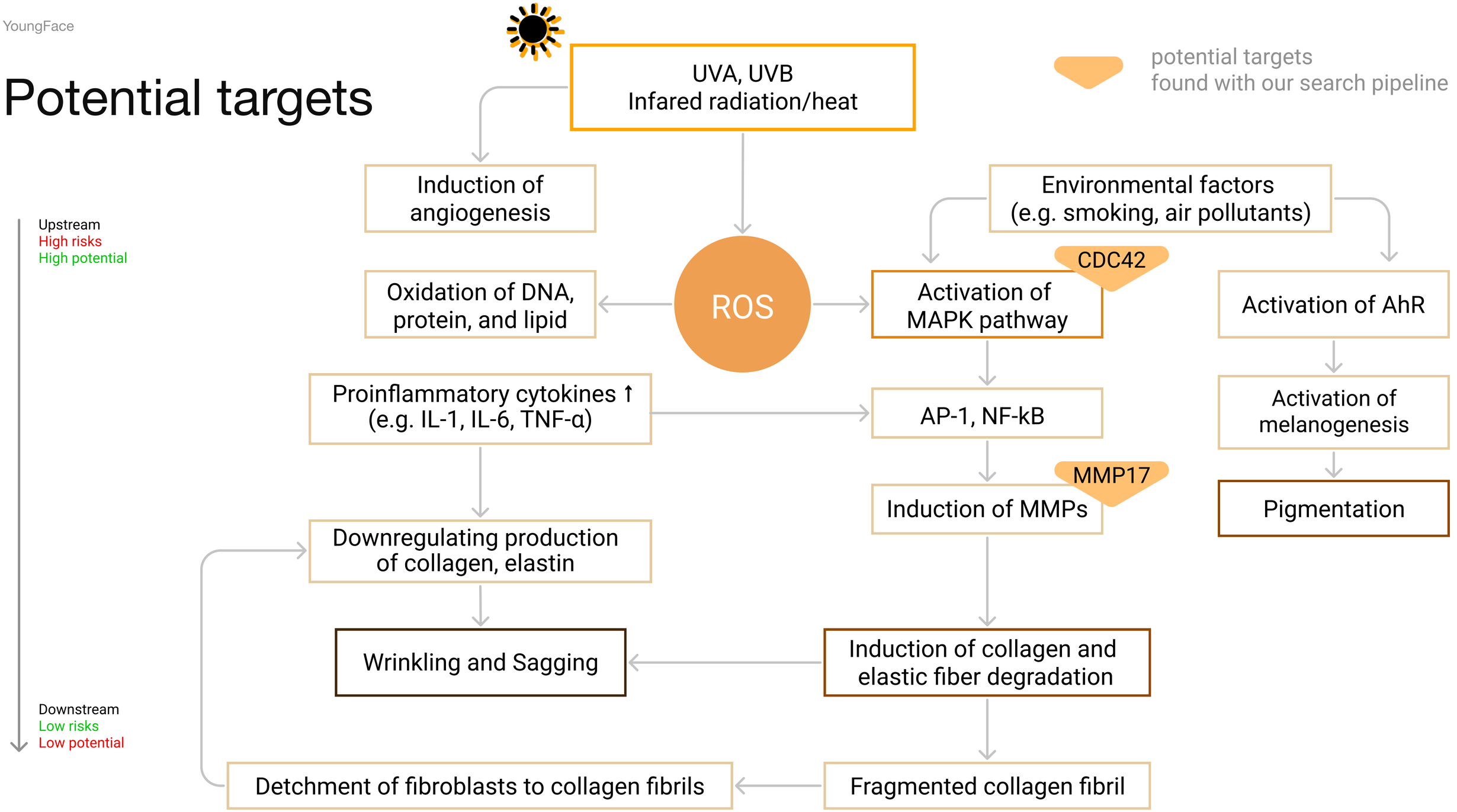


Service for investigation of targets for personalized skin care and skin diseases

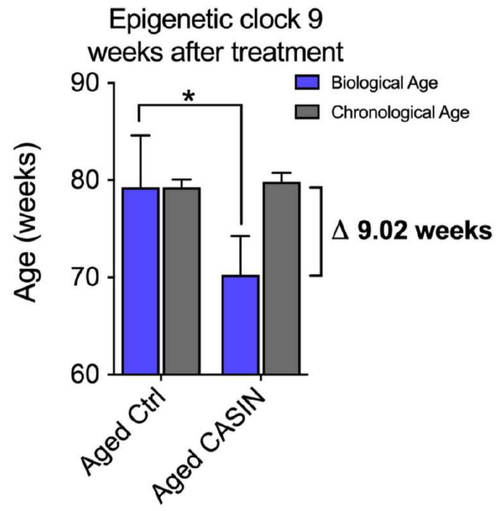
Technology

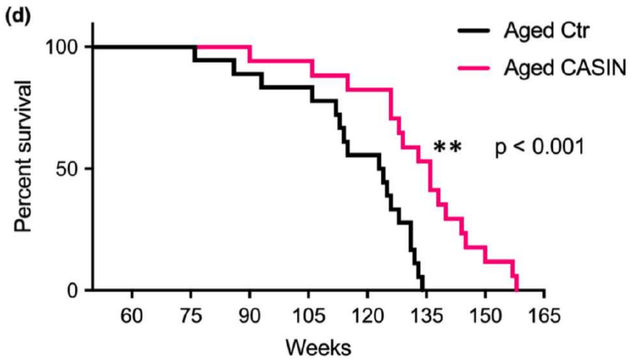

logKp datasets aggregation
Datasets filtering + descriptors
Transformer model training
Proteomic data
Literature search
Transcriptomic data
bulk
sc
locality scoring/causative imputations
Genes list
Pathways list
Potential targets
HotSpot-ID
FBDD
LIFE CHEMICALS
Virtual screening
Hits
Methylation data
Preclinical parameters prediction
Hit optimization
Compound

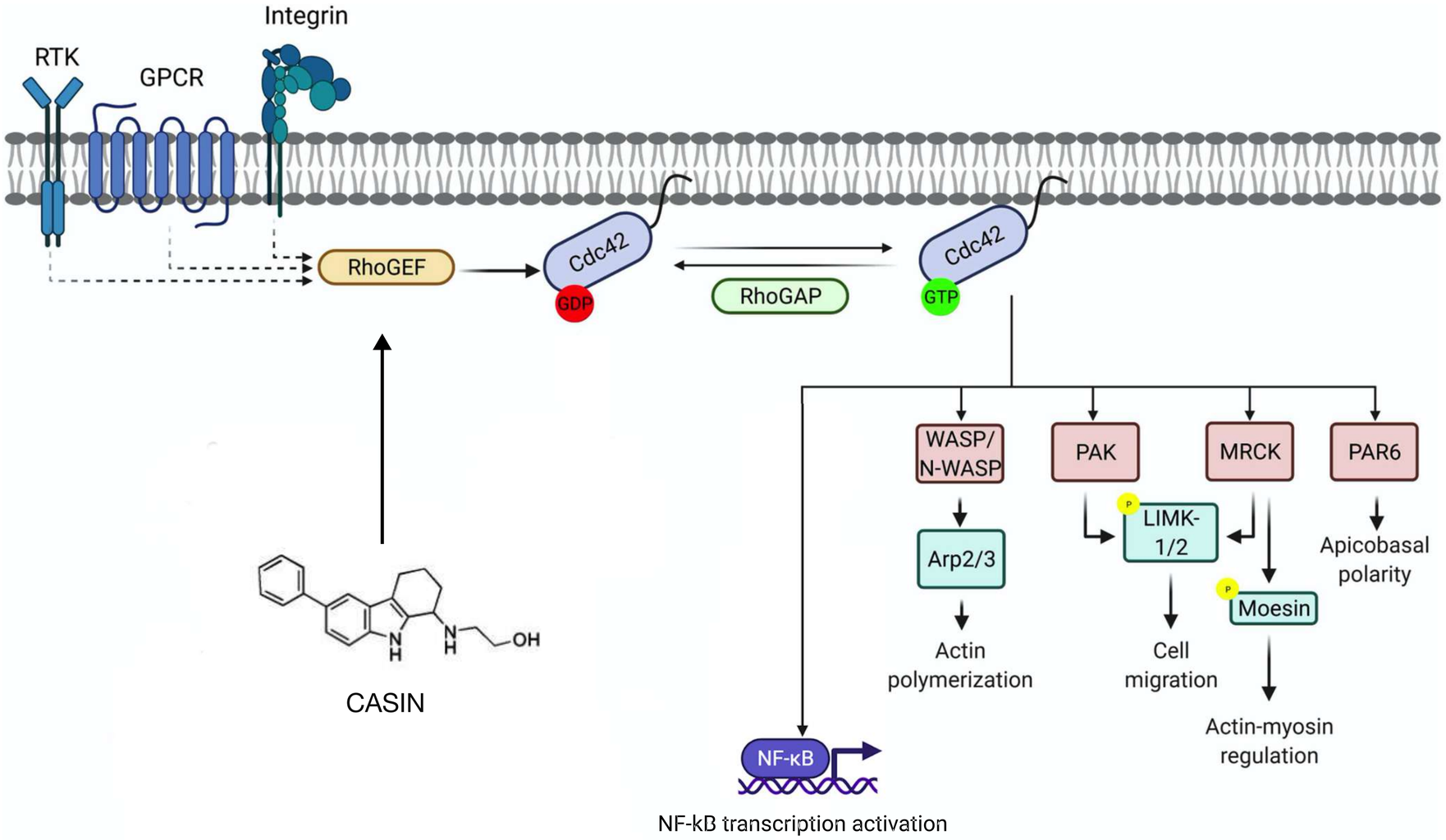
Potential targets



Potential target: CDC42

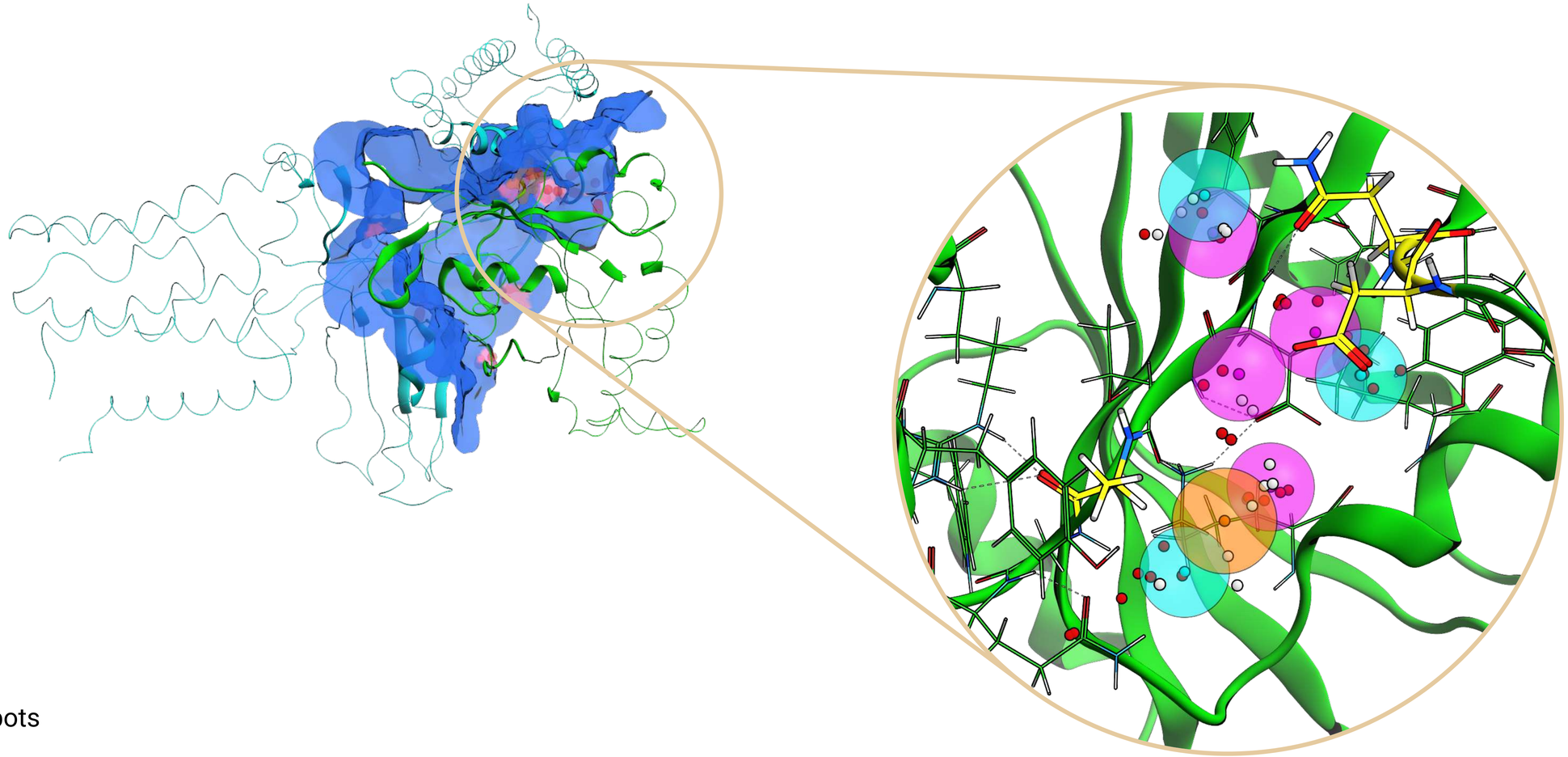






https://doi.org/10.1111/acel.13208
https://doi.org/10.1042/BST20200557

Target interface

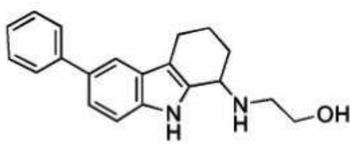


CDC42-GDP

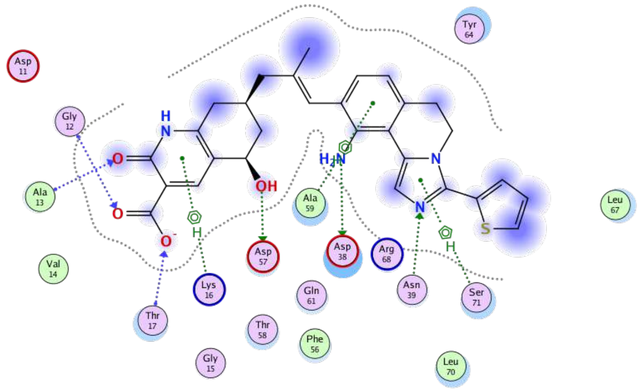
DOCK9-GEF

Interaction hotspots

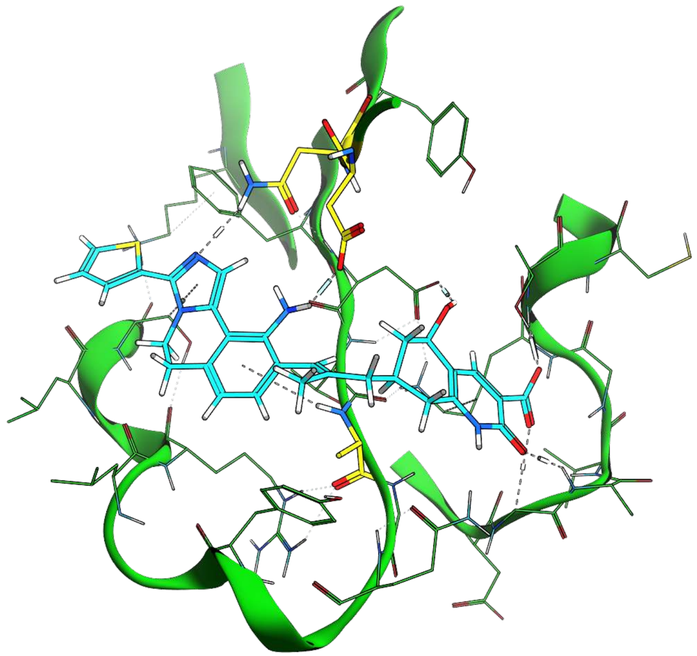
Hit optimization

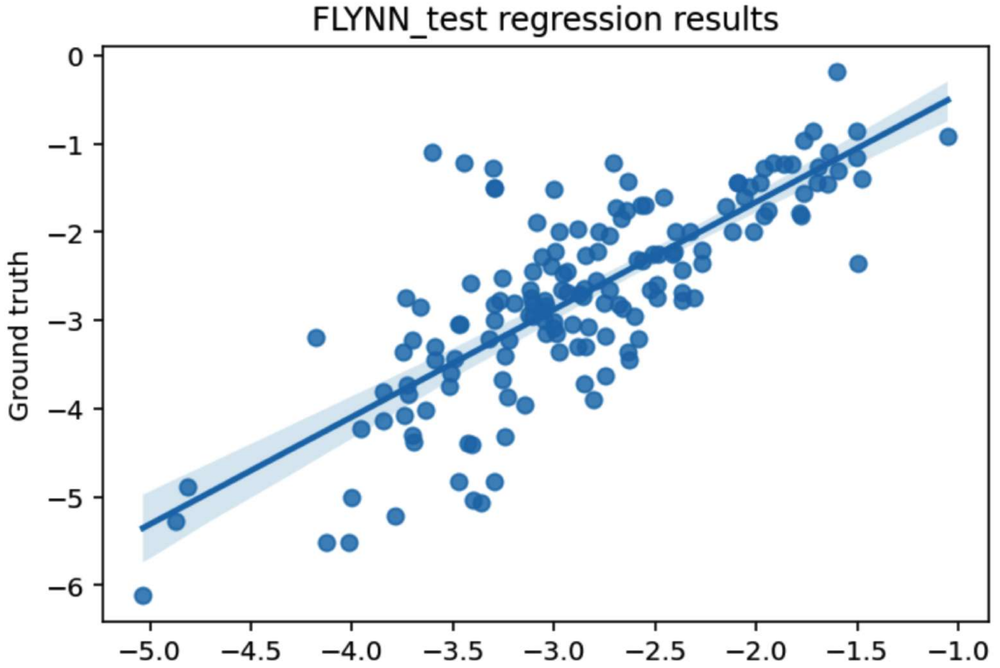


CASIN logKp = -4.32



New molecule logKp = -3.66





R2 score: 0.562
RMSE: 0.738

Results

In a span of a week we have:

1. Successfuly 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 assesment using SOTA alchemical MD simulations to further optimize our hit