

Towards multimodal and context-aware representations of the tumor microenvironment

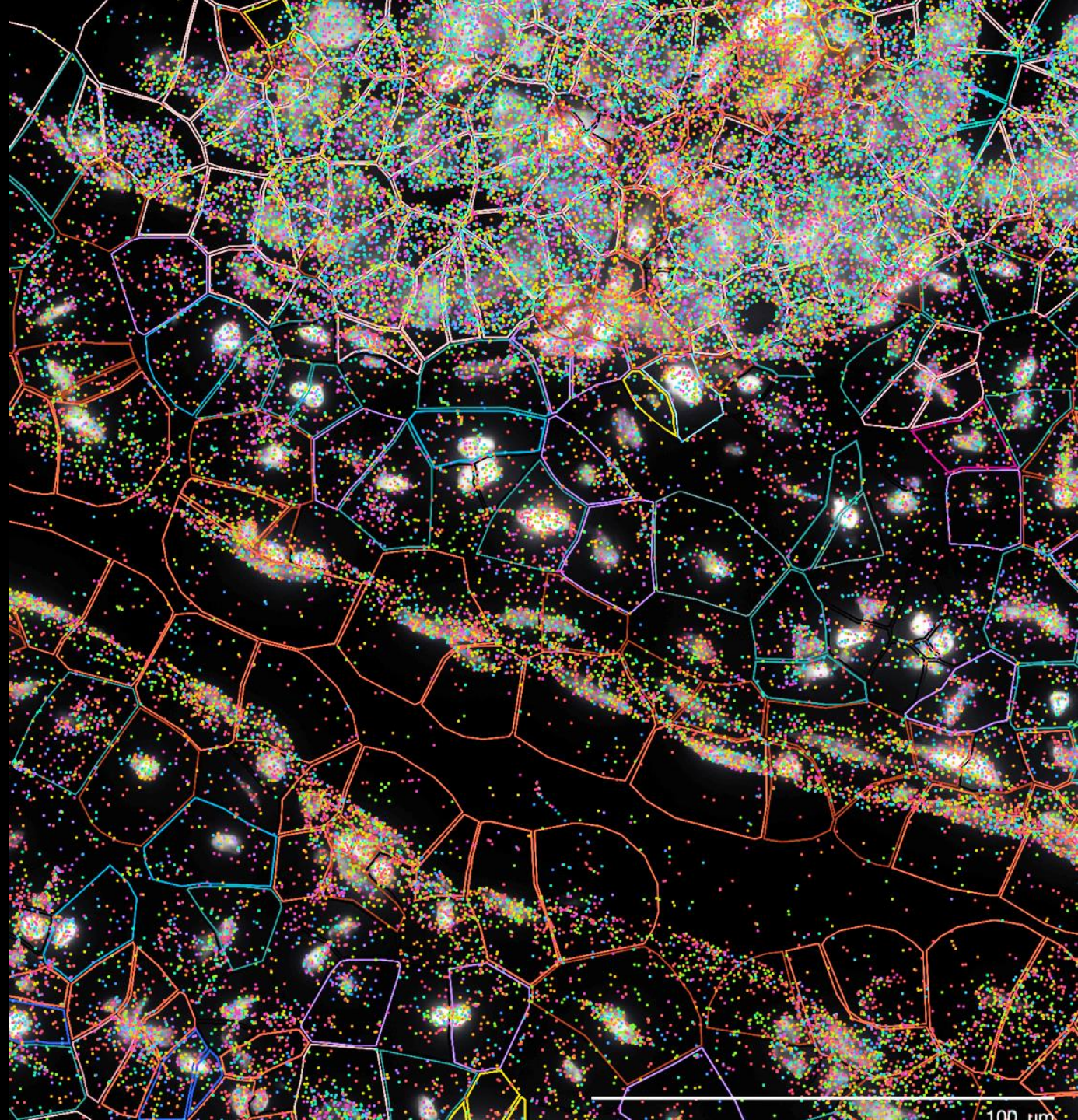
Marianna Rapsomaniki
Assistant Professor
Biomedical Data Science Center



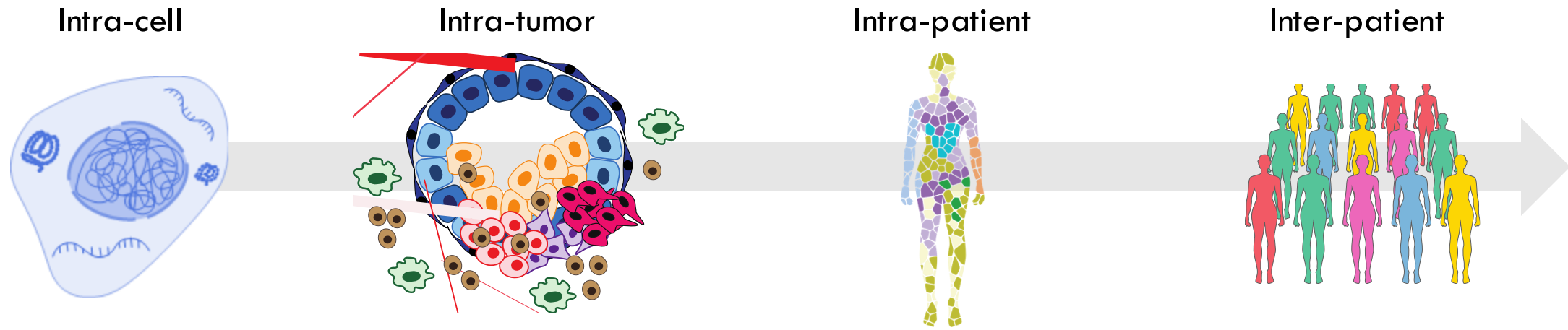
Unil.



Lyon AI/ML sc-spatial omics workshop
Oct. 16th, 2025

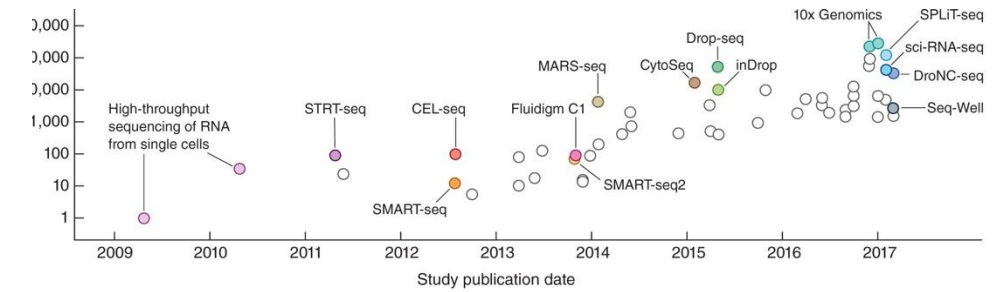


From biological stochasticity to tumor heterogeneity



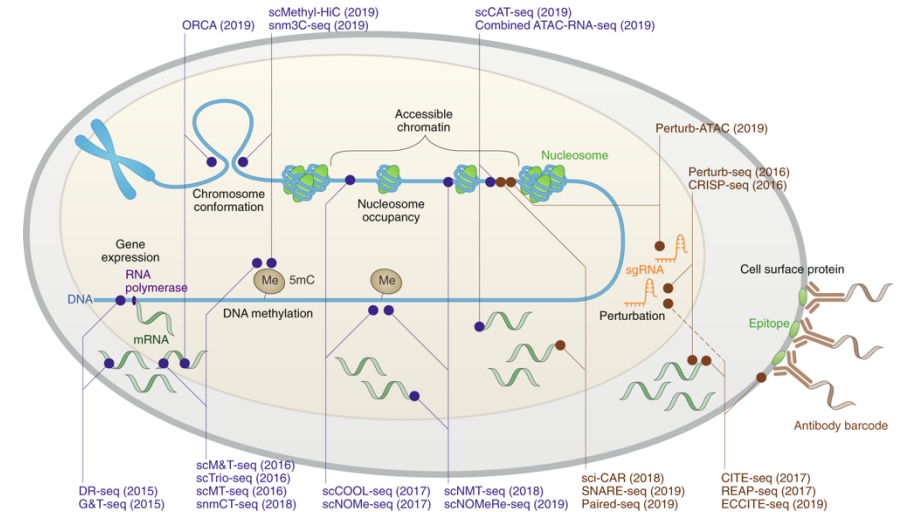
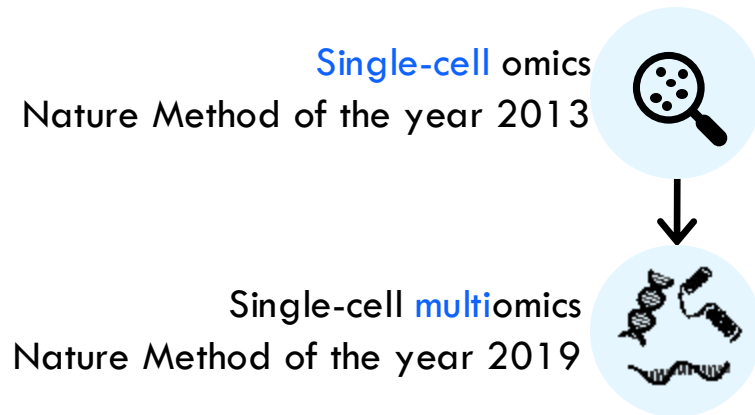
From single-cell biology...

Single-cell omics
Nature Method of the year 2013



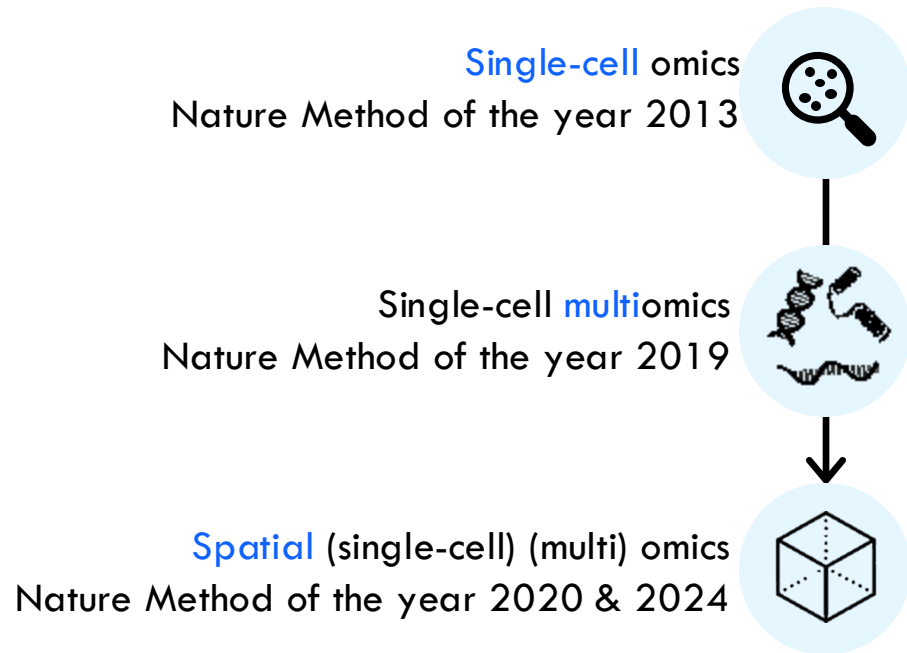
Svensson et al., Nat Protocols, (2018)

... to multi-modal single-cell biology

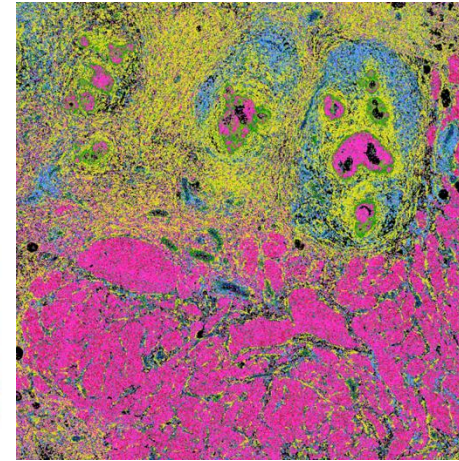


Zhu et al., *Nat Methods*, (2020)

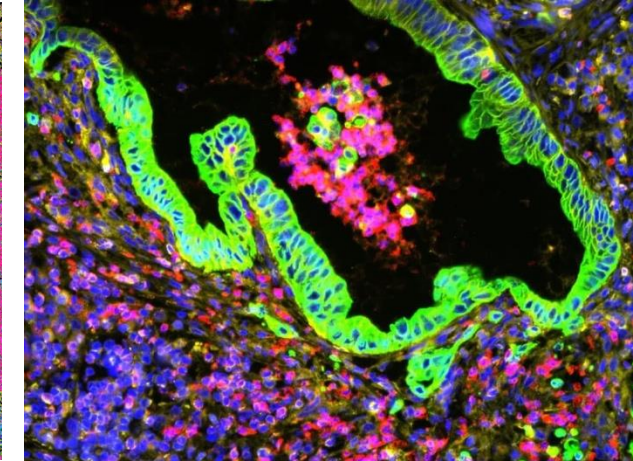
... to **spatial** single-cell biology



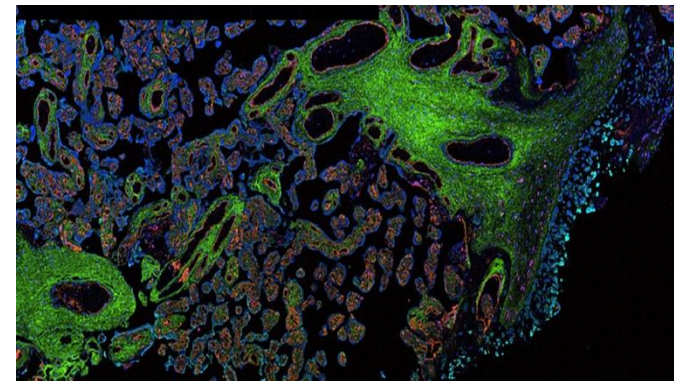
10X Xenium - Breast Cancer



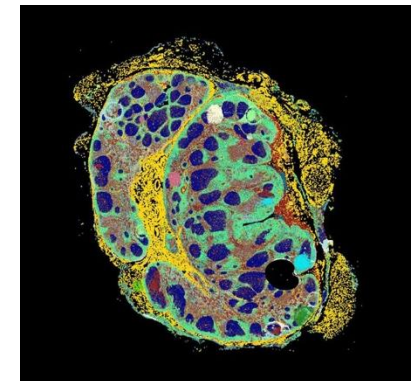
Nanostring CosMx - Human Lung



Imaging Mass Cytometry - Human Placenta

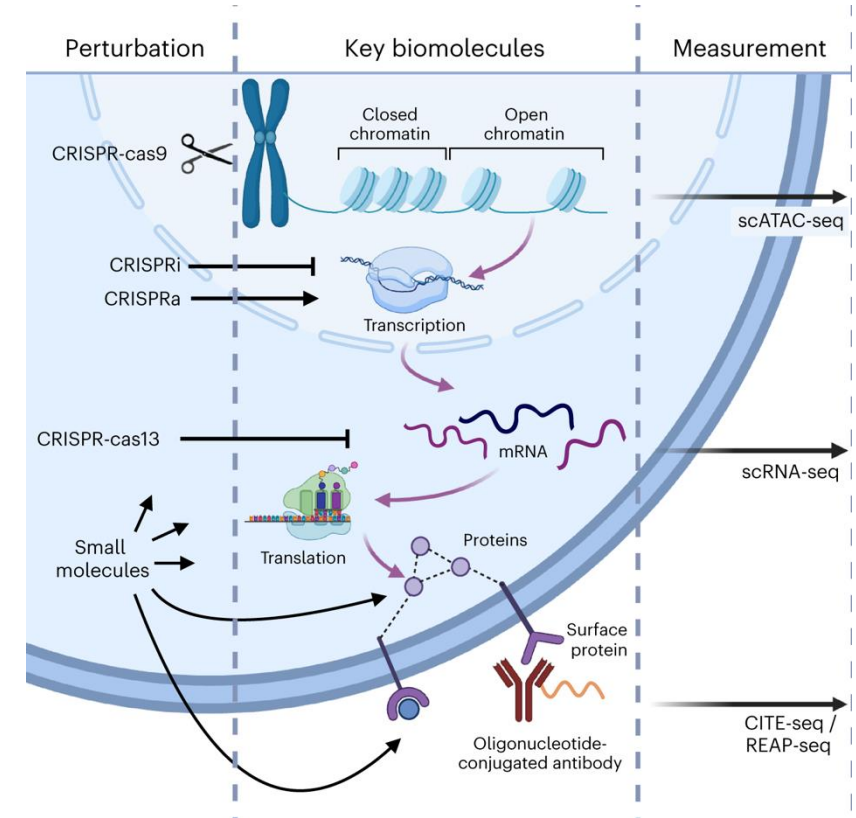
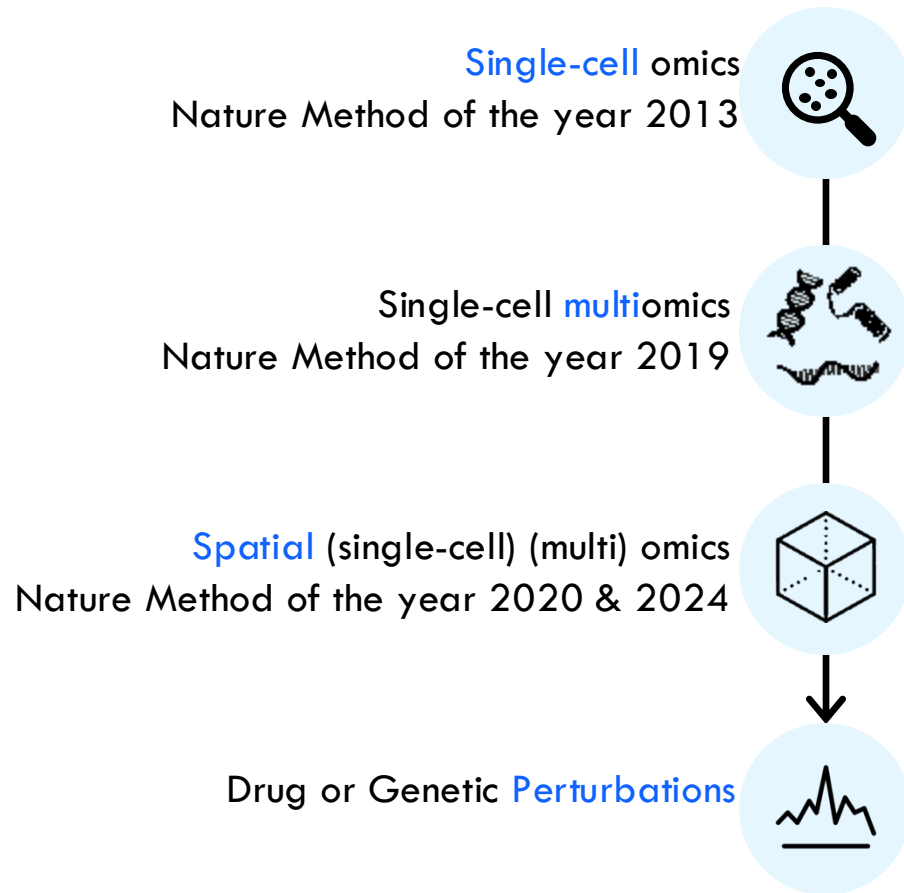


CODEX - Lymph node

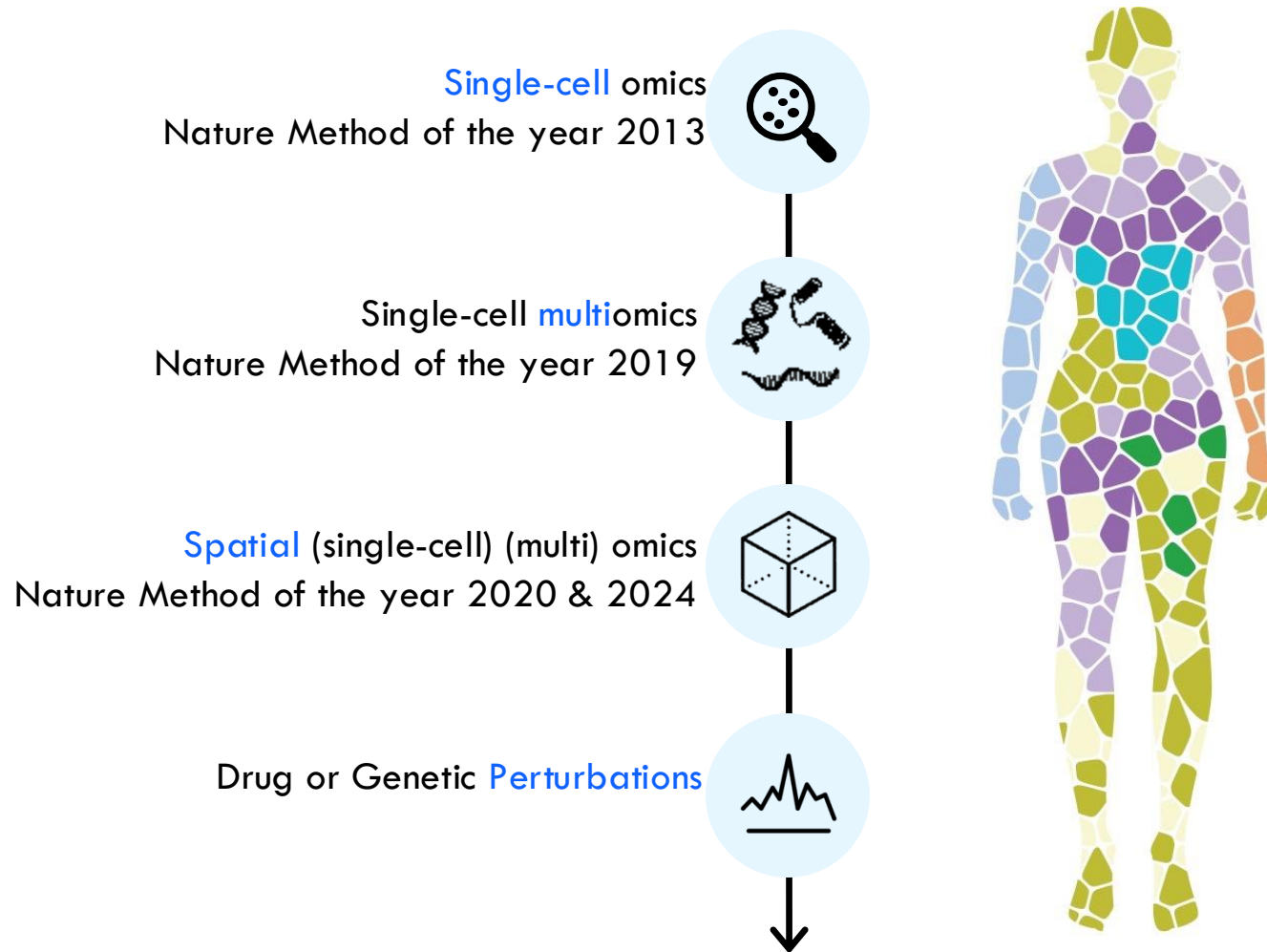


Images from <https://hubmapconsortium.org>, [10Xgenomics.com](https://10xgenomics.com) and [Nanostring.com](https://nanosttring.com)

... and **perturbation** biology

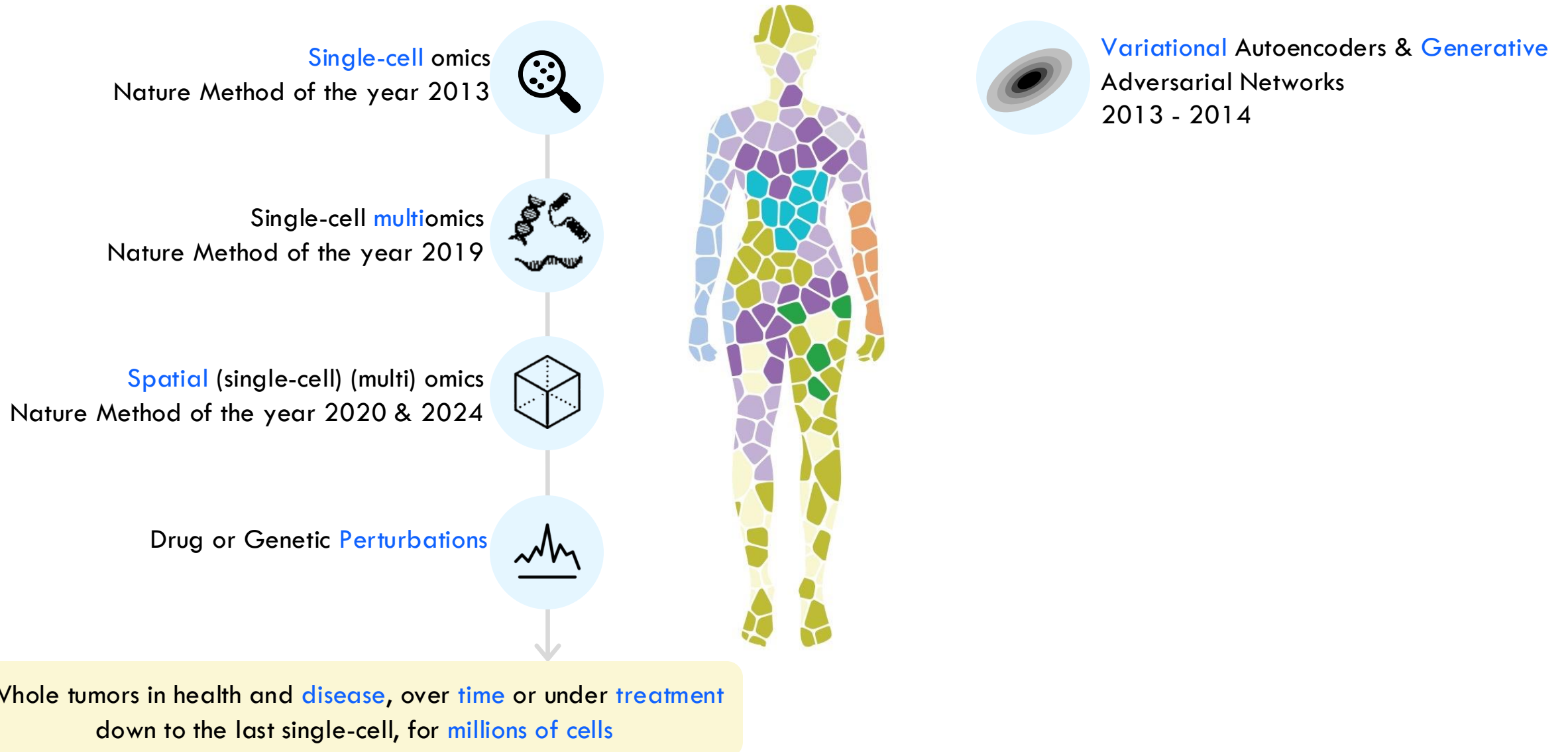


Peidl et al, Nature Methods, 2024

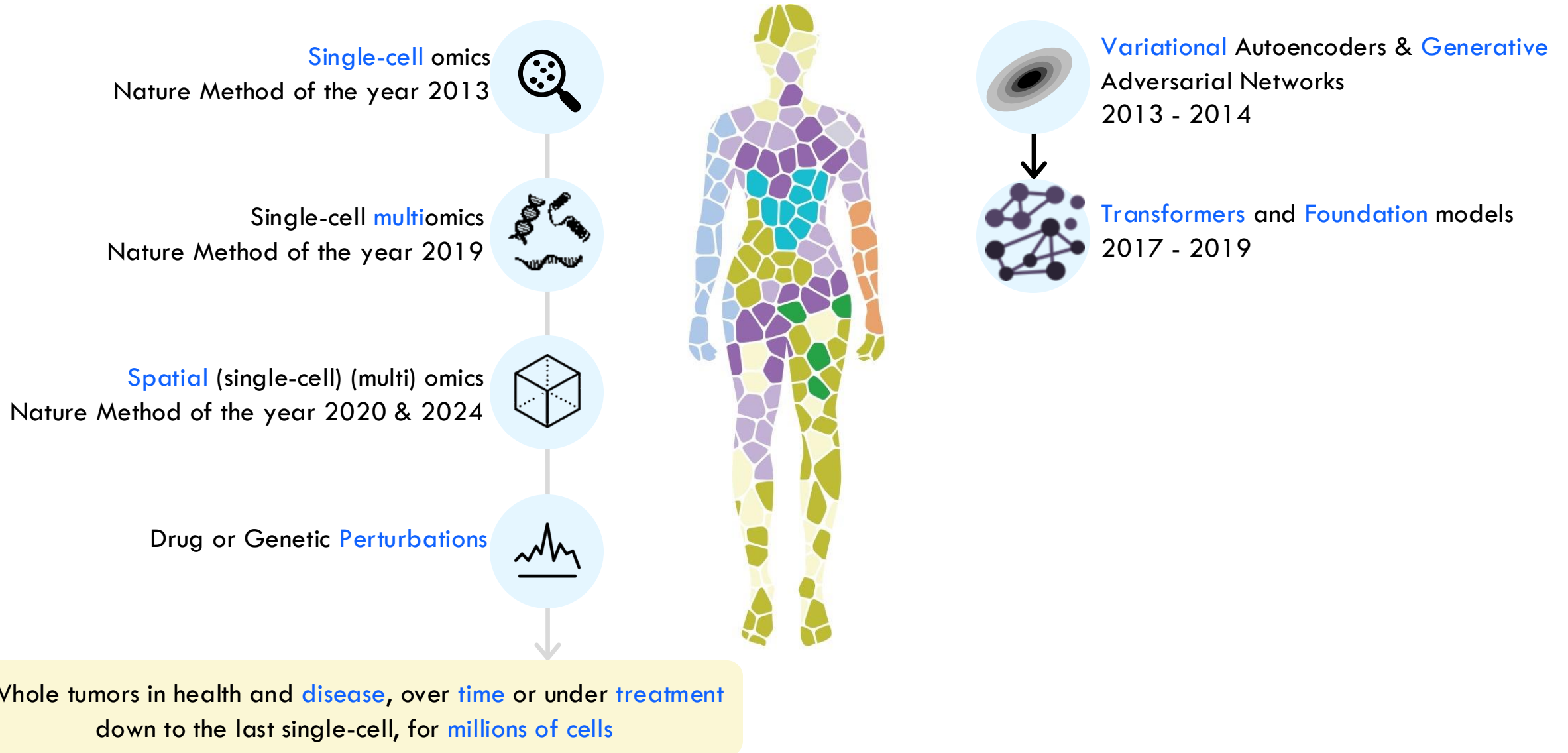


Whole tumors in health and disease, over time or under treatment
down to the last single-cell, for millions of cells

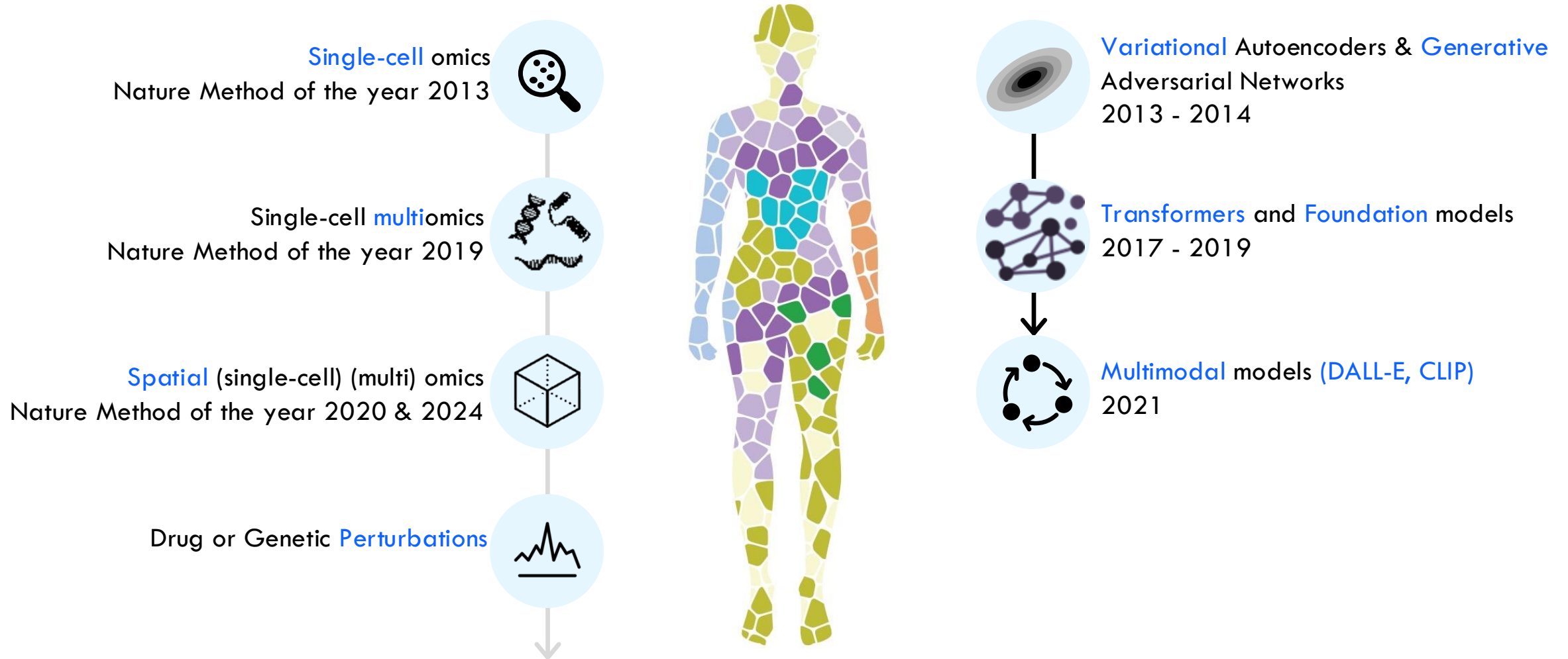
... to new paradigms in AI



... to new paradigms in AI

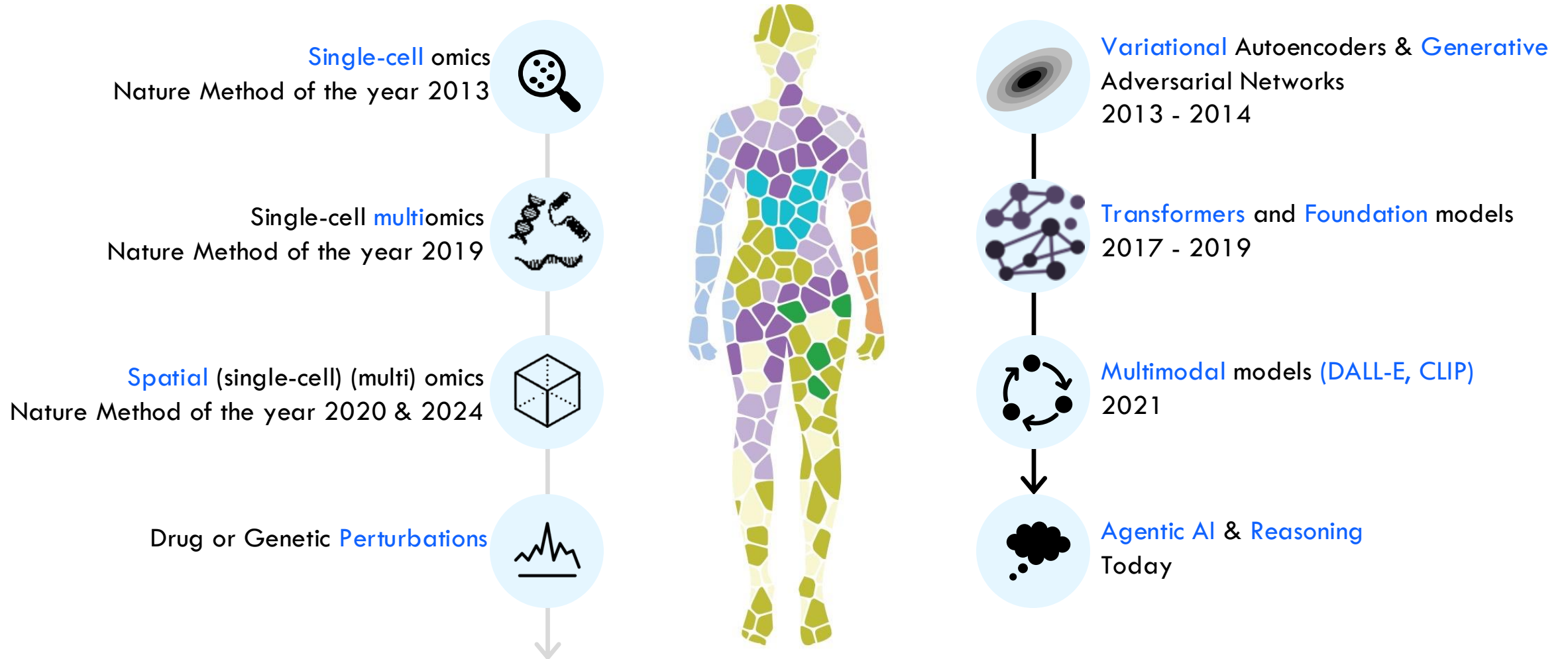


... to new paradigms in AI



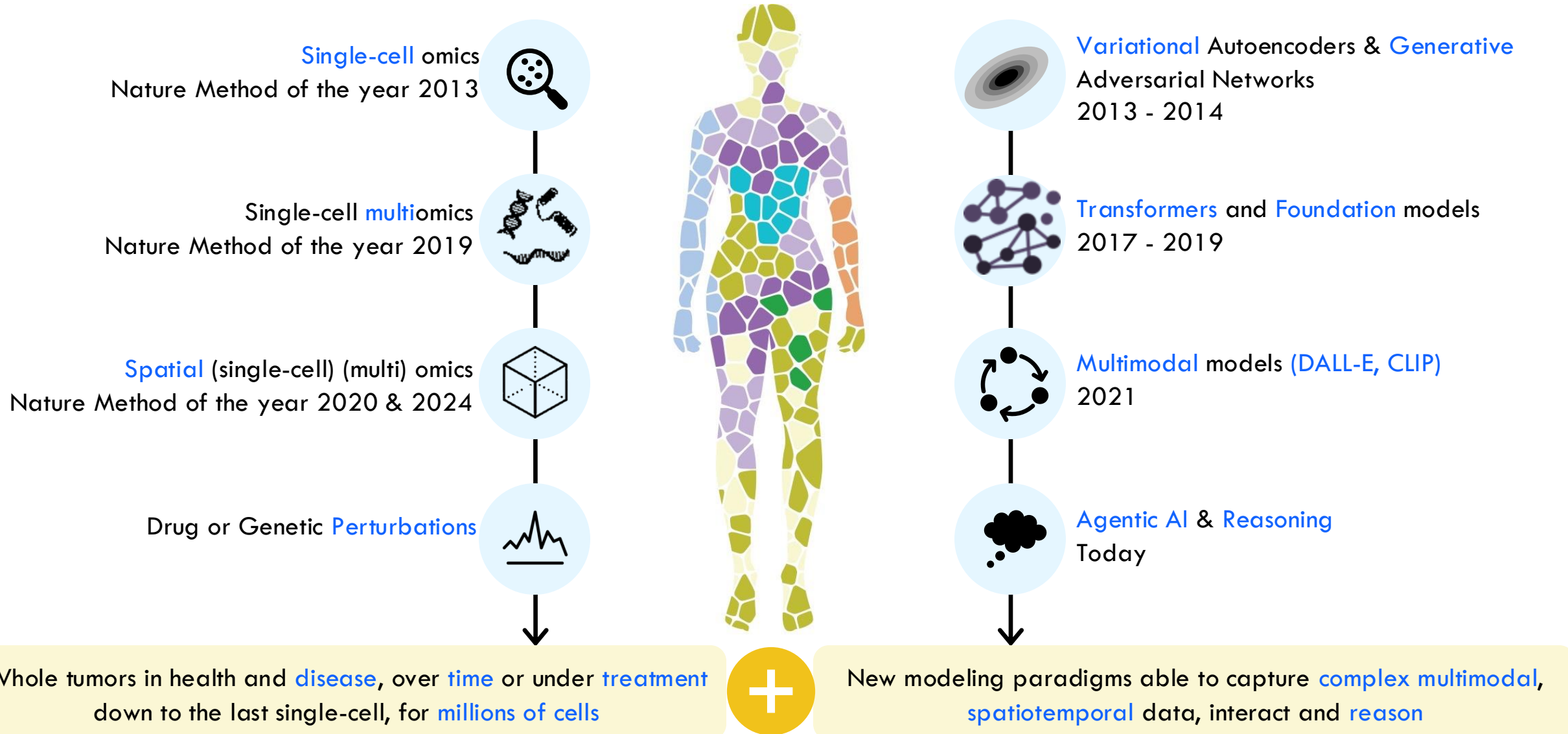
Whole tumors in health and **disease**, over **time** or under **treatment**
down to the last single-cell, for **millions of cells**

... to new paradigms in AI



Whole tumors in health and **disease**, over **time** or under **treatment**
down to the last single-cell, for **millions of cells**

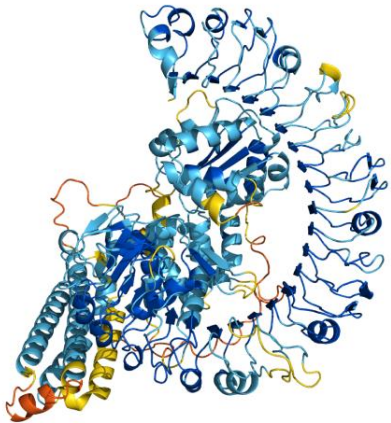
... to new paradigms in AI



From molecules to whole tissues

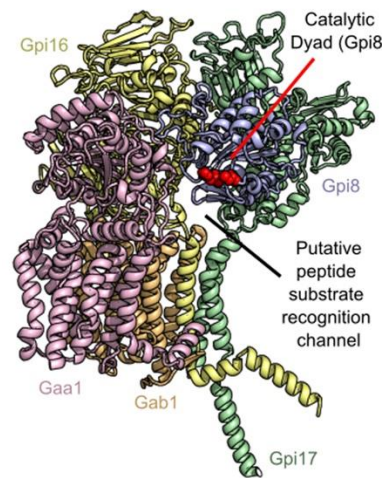
Prediction of protein structure

(Jumper *et al.*, *Nature*, 2021)



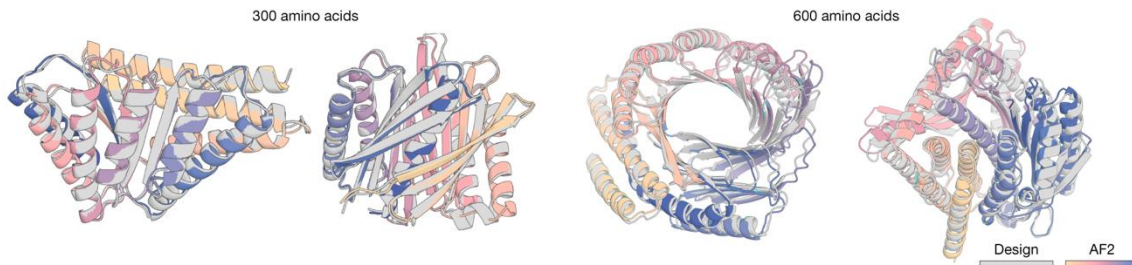
Structure of protein complexes

(Humphreys *et al.*, *Science*, 2021)



De novo protein or enzyme design

(Watson *et al.*, *Nature*, 2023)

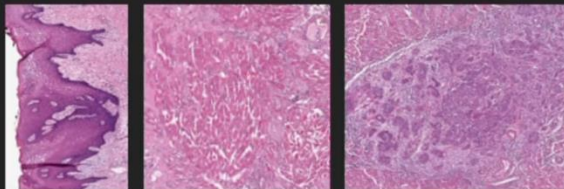


A Multimodal Generative AI Copilot for Human Pathology

(Lu *et al.*, *Nature*, 2024)

PathChat 2 WSI demo

You
describe what you see in these images. what organ am i looking at?



PathChat

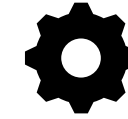
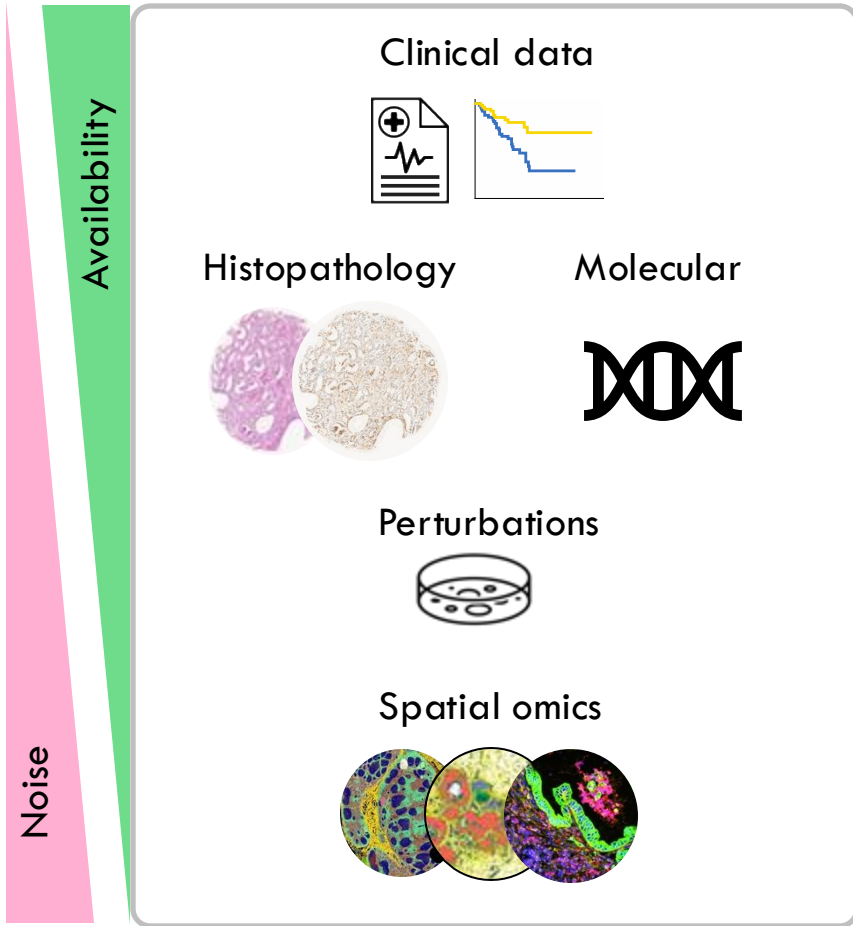
You are looking at the tongue. The first image shows normal squamous mucosa, which is the typical lining of the oral cavity, including the tongue. The second image shows skeletal muscle fibers, which are a normal component of the tongue's structure. The third image shows a squamous cell carcinoma, which is a malignant tumor arising from the squamous epithelium of the tongue.

Towards a general-purpose foundation model for computational pathology

(Chen *et al.*, *Nature Medicine*, 2024)

A visual-language foundation model for computational pathology (Lu *et al.*, *Nature Medicine*, 2024)

A reality check



Modeling limitations

Models are not directly transferrable

Model selection/tuning

Validation and assessment

Generalizability



Reliable and Safe



Explainability



Avoiding Bias

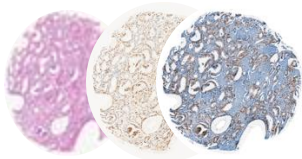


Privacy and Security

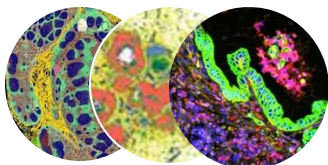


Represent

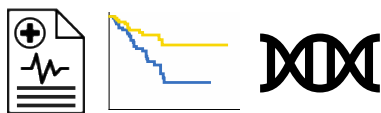
Histopathology



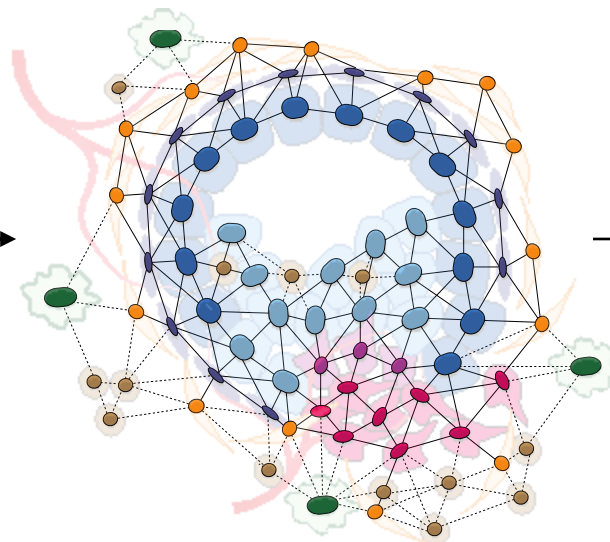
Spatial omics



Clinical data



Interpret

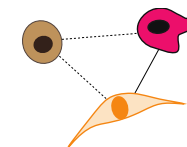


Perturb

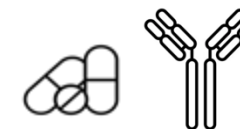
Perturbations



Biological discovery

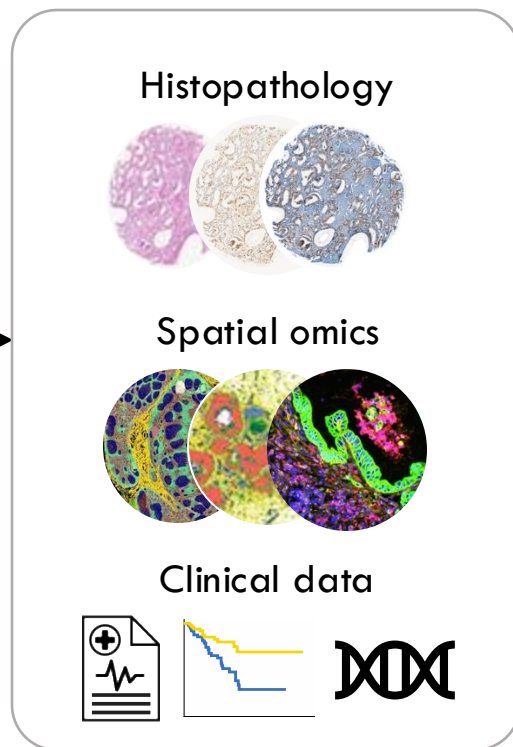


Treatment selection



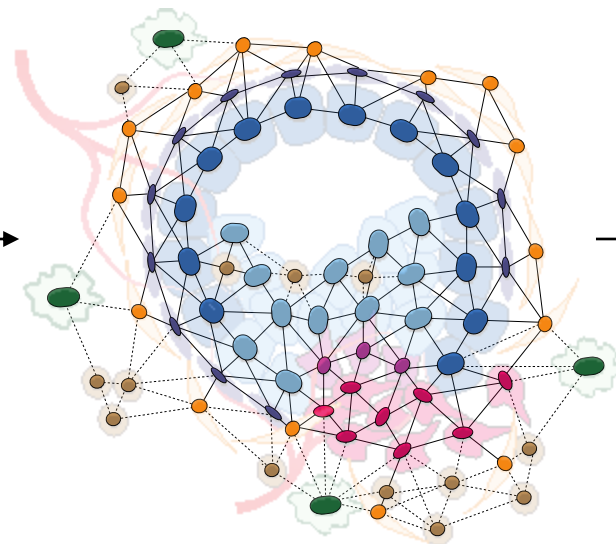


Represent



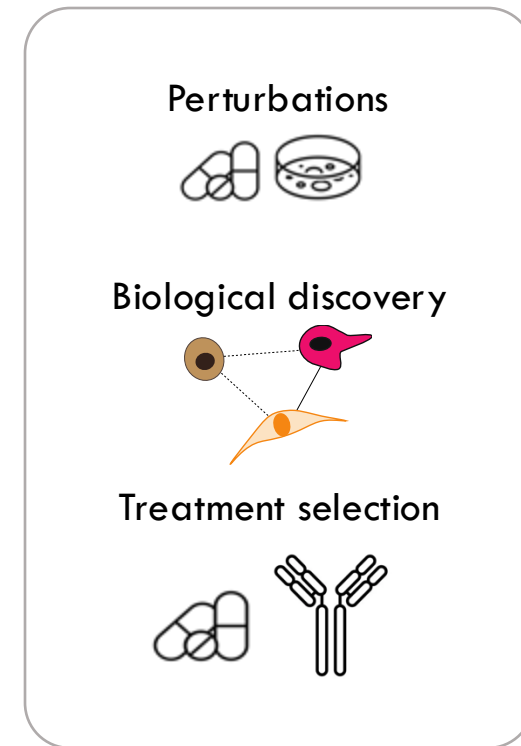
How can we learn multimodal **representations** from spatial omics?

Interpret



How can we **interpret** these representations of the TME?

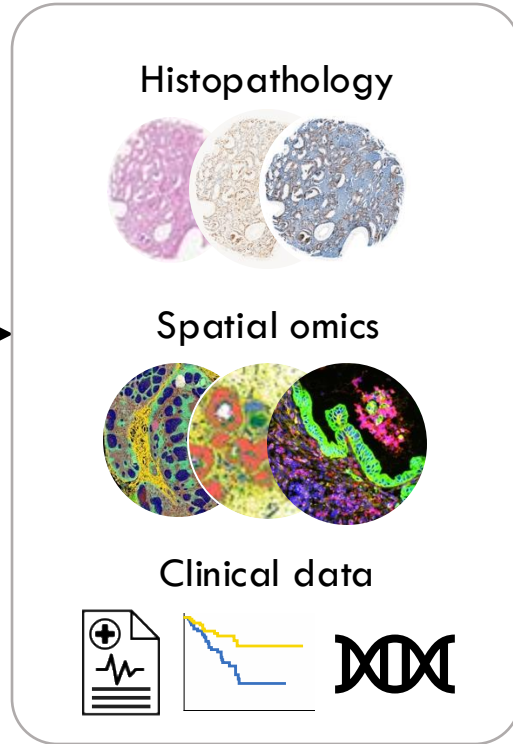
Perturb



How can we predict the effects of drug **perturbations**?

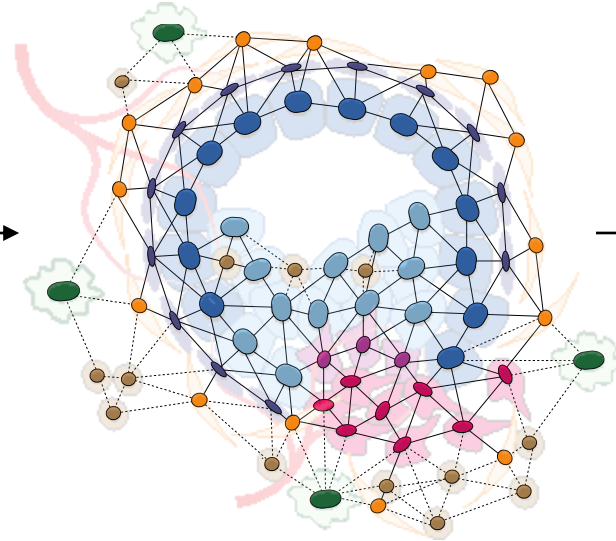


Represent



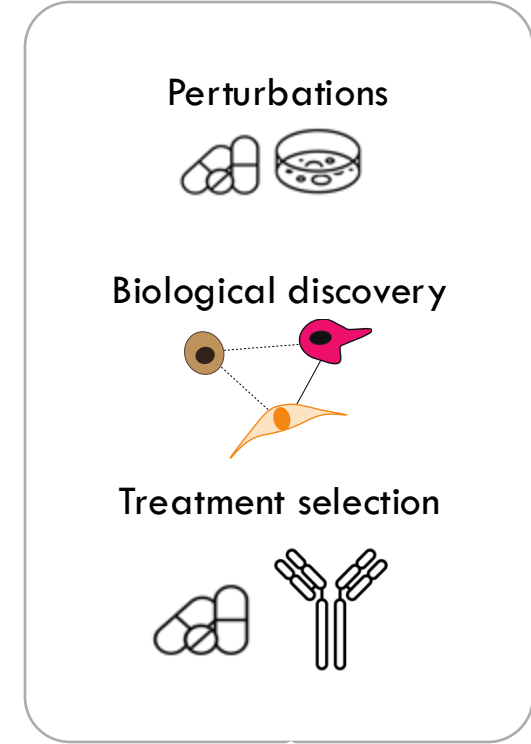
How can we learn multimodal **representations** from spatial omics?

Interpret



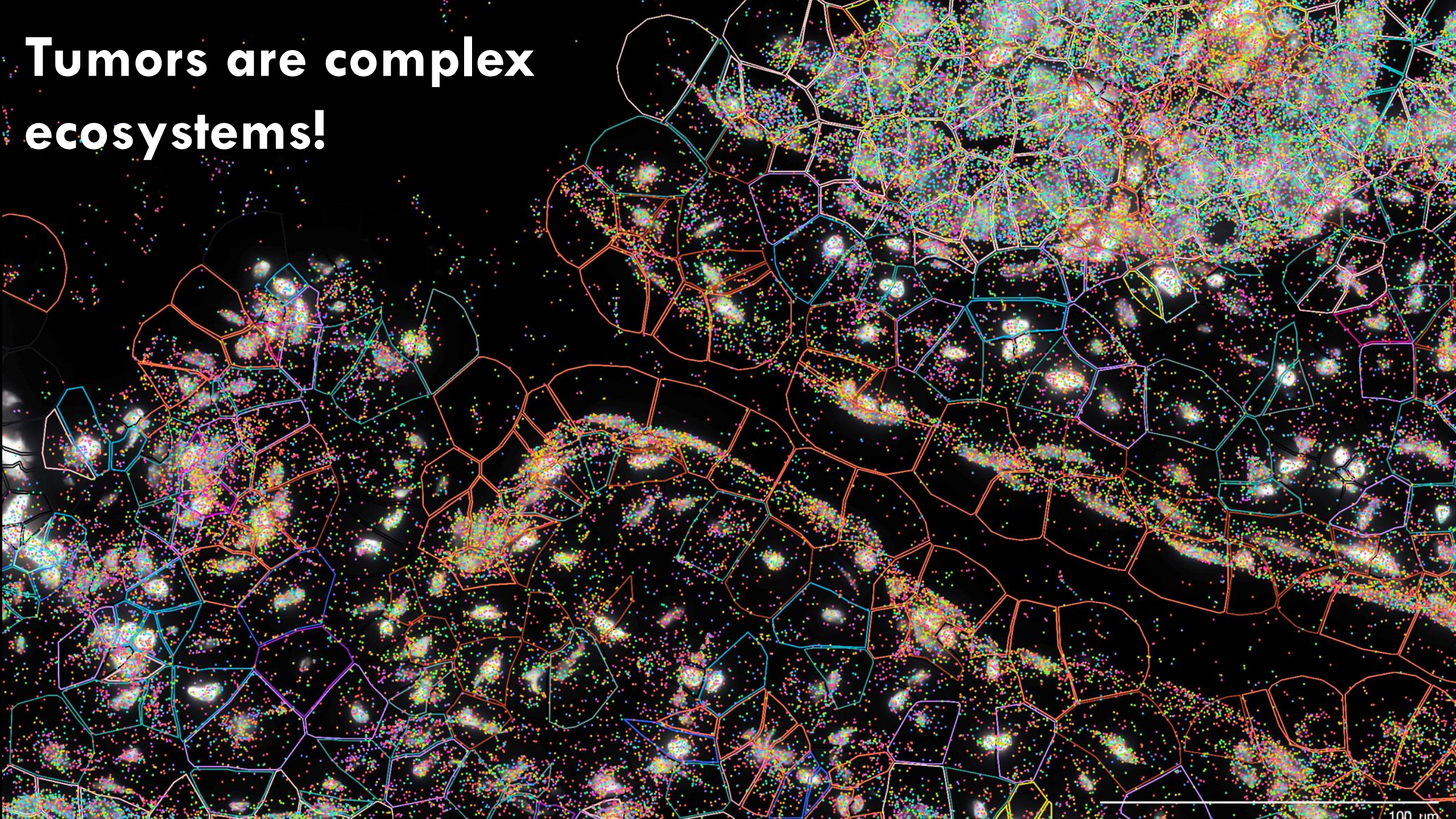
How can we **interpret** these representations of the TME?

Perturb



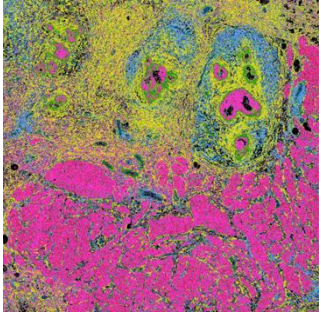
How can we predict the effects of drug **perturbations**?

**Tumors are complex
ecosystems!**

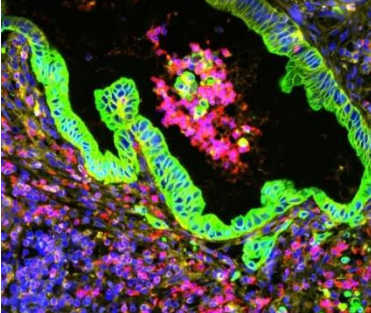


The Bottleneck: Scale, Cost, and Complexity

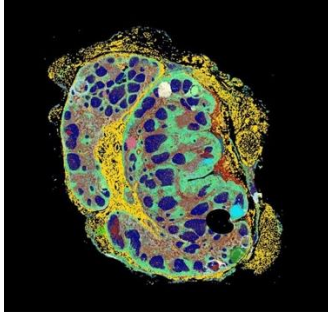
10X Xenium-Breast Cancer



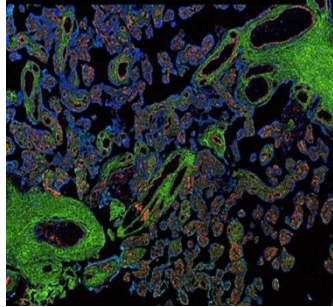
Nanostring CosMx -Lung



CODEX - Lymph node



IMC - Human Placenta

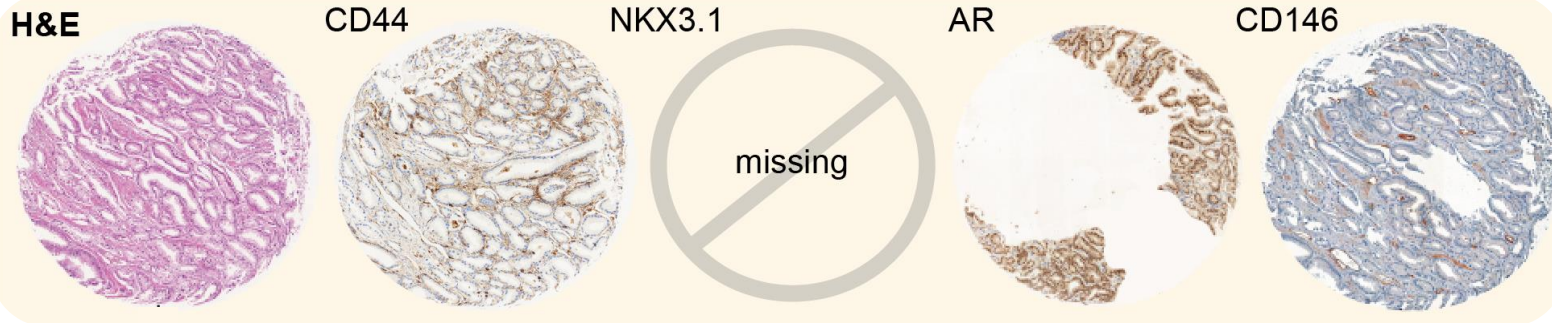


Images from <https://hubmapconsortium.org>, 10Xgenomics.com and Nanostring.com

Spatial omics – multiplexed imaging:

- ✓ Many genes/proteins simultaneously
- x High cost and long turnaround
- x Specialized equipment
- x Tissue-destructive
- x Small capture area

Immunohistochemistry (IHC)



Traditional histopathology:

- ✓ Fast & cheap
- ✓ Standardized protocols
- x Unaligned images (no multiplexing)

Virtual staining

Source domain



Photograph



Target domain



Monet



Van Gogh

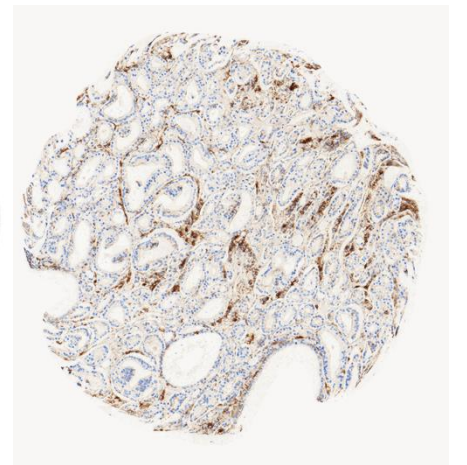
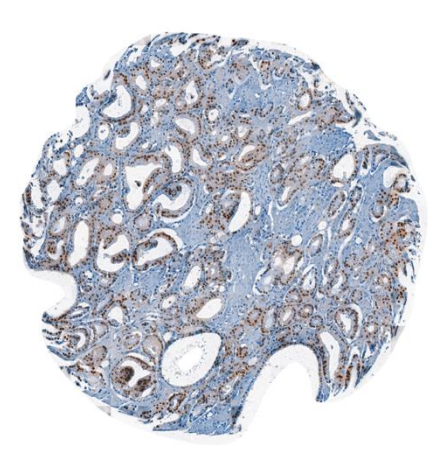
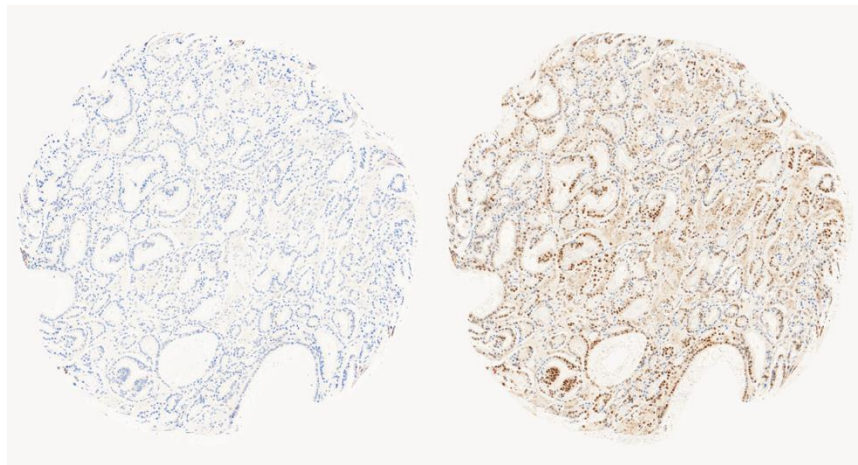
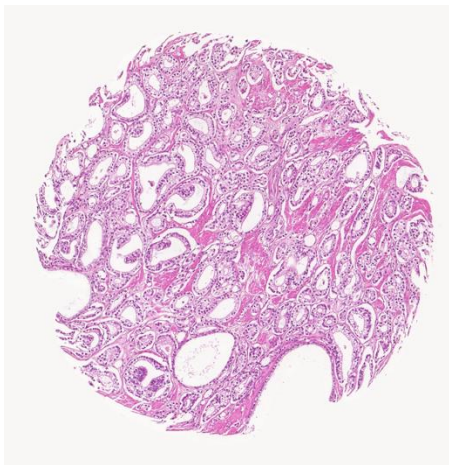


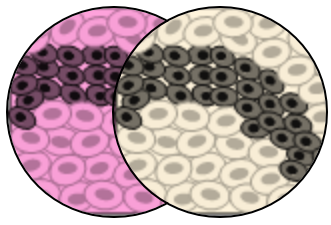
Cezanne



Ukiyo-e

Zhu et al., ICCV, 2017.



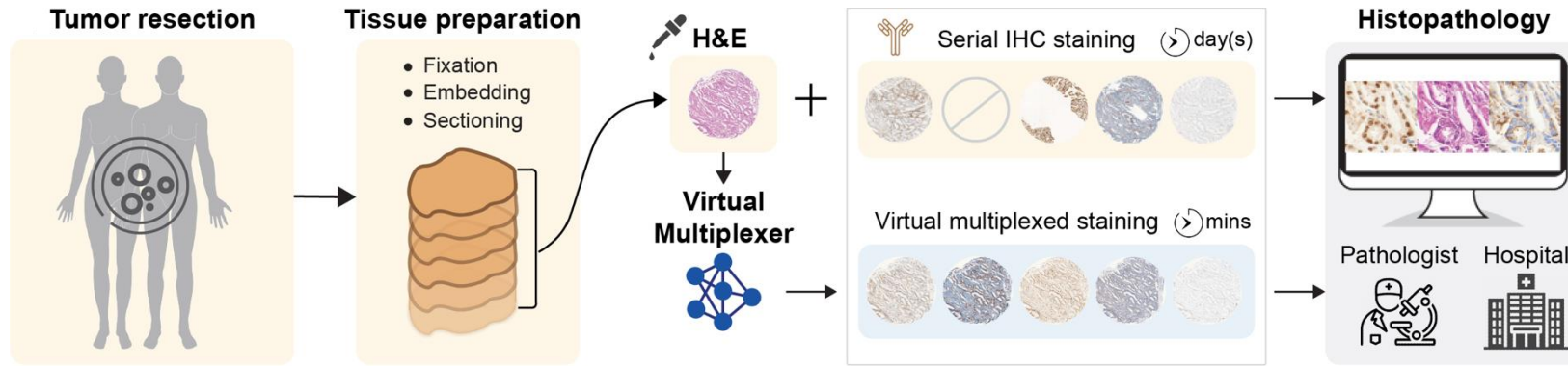


Virtual Multiplexer

Multiplexed tumor profiling with generative AI

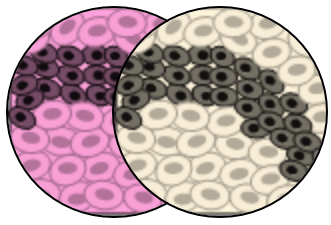


Pushpak Pati



Virtual staining:

- ✓ Fast & cheap
- ✓ Standardized protocols

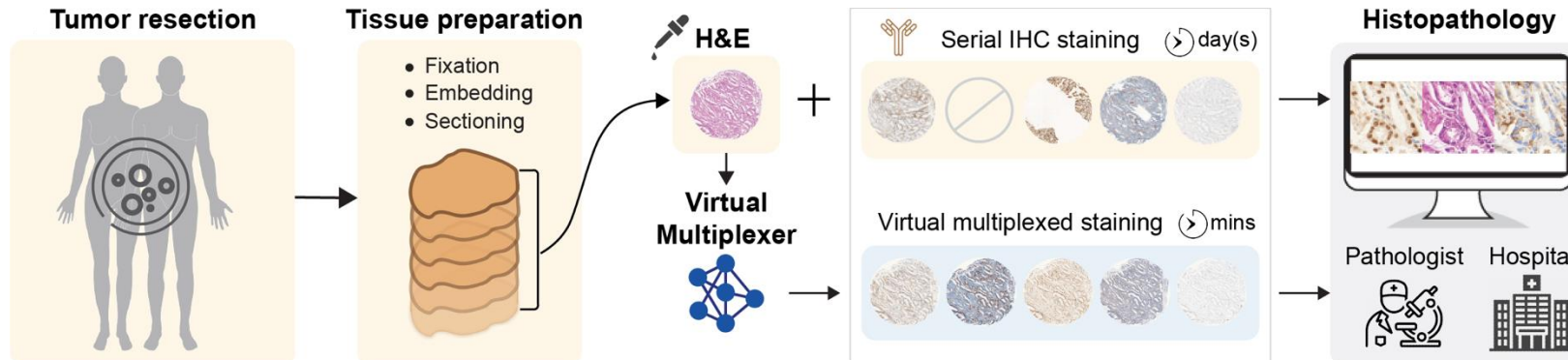


Virtual Multiplexer

Multiplexed tumor profiling with generative AI

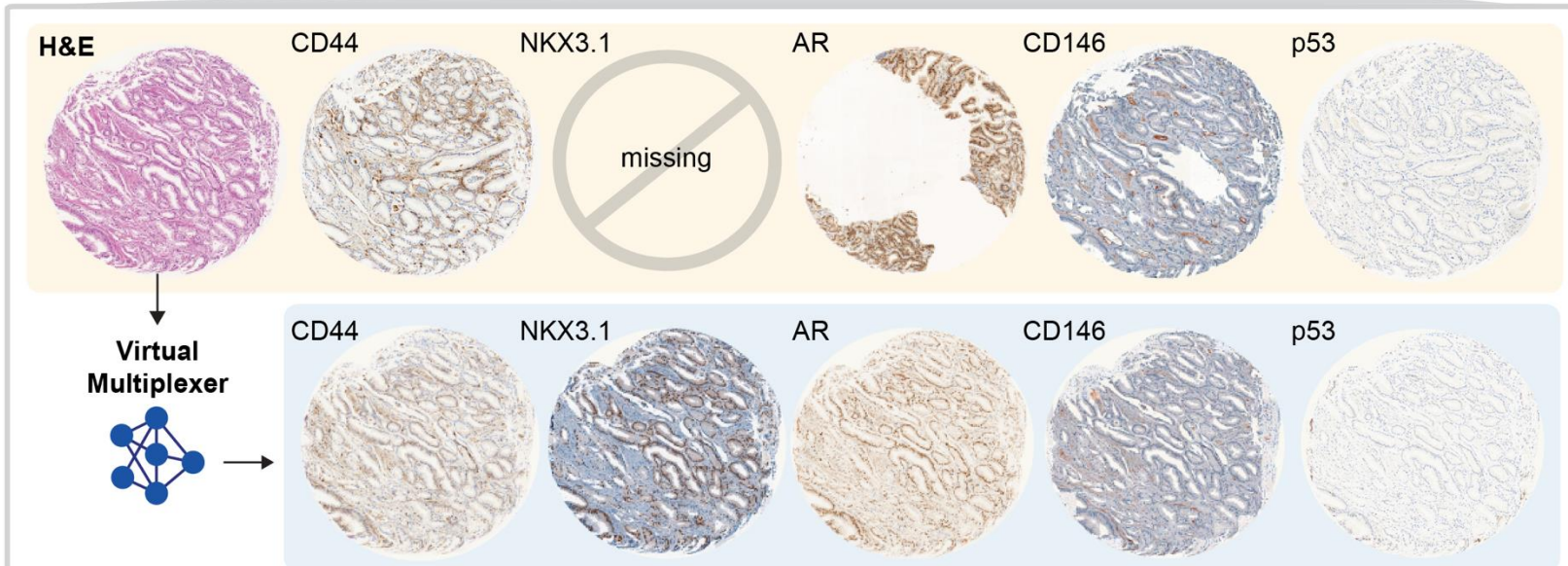


Pushpak Pati



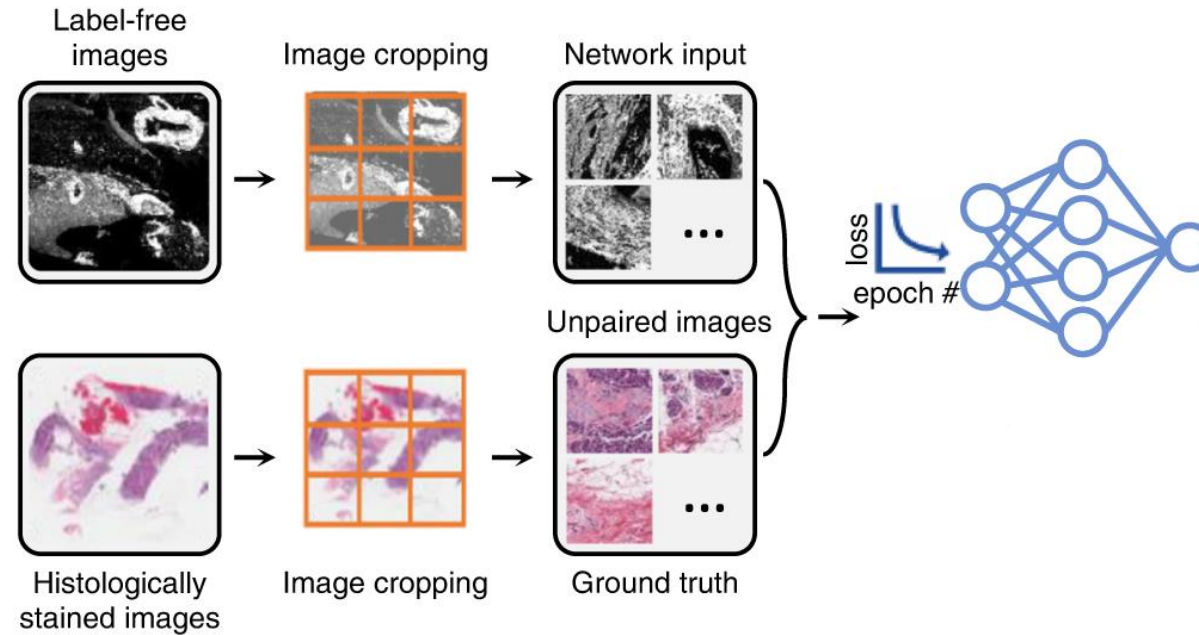
Virtual staining:

- ✓ Fast & cheap
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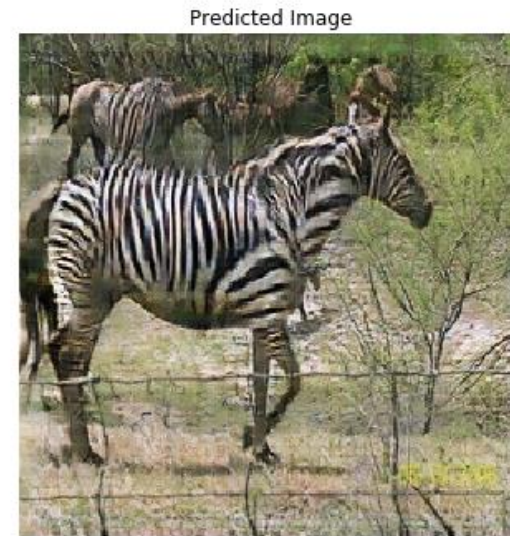
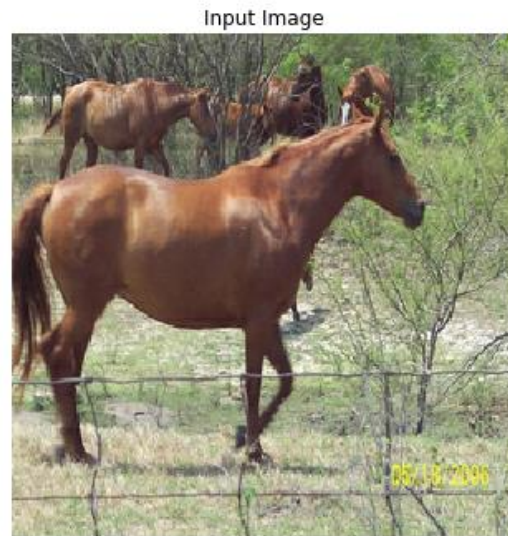
- ✓ Generates realistic virtual stains for several markers
- ✓ Unpaired data → paired, virtually multiplexed data

Unpaired image-to-image translation

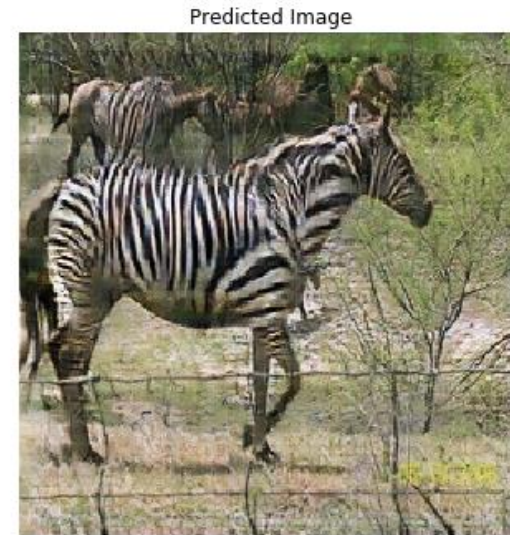
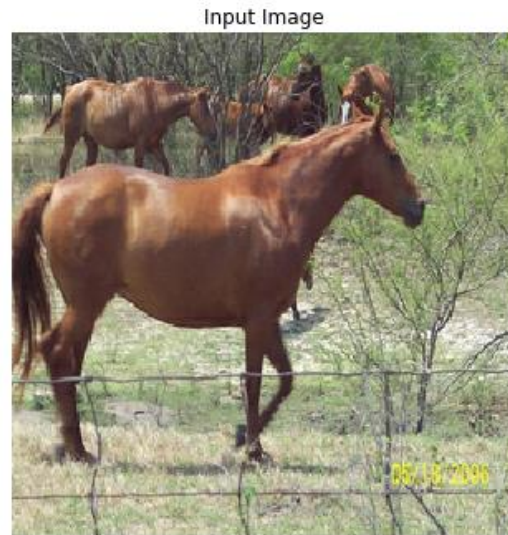


Bai *et al.*, 2023.

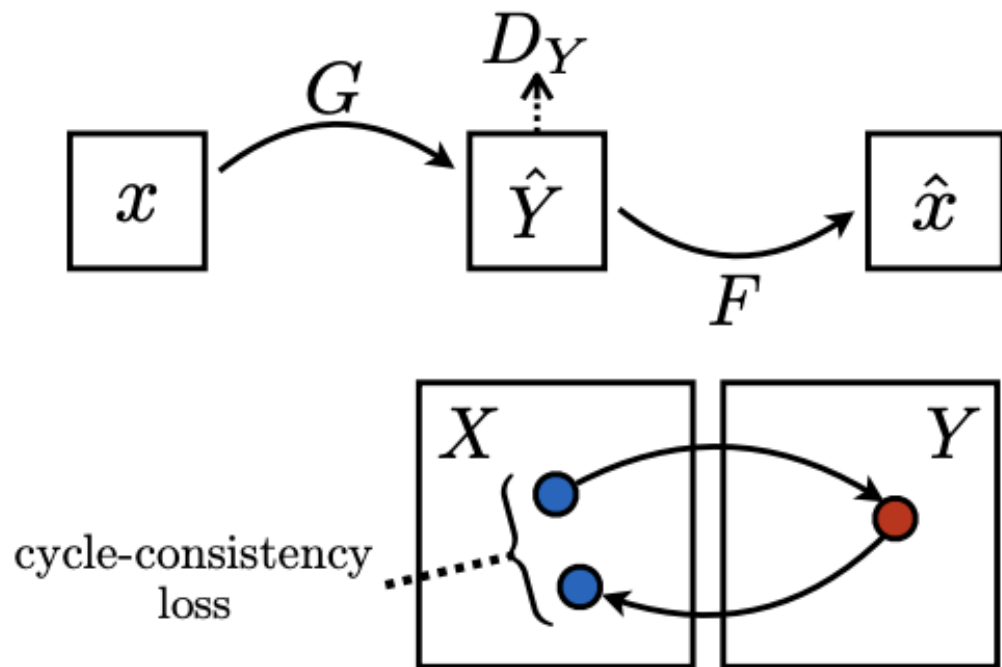
Unpaired image-to-image translation



Unpaired image-to-image translation

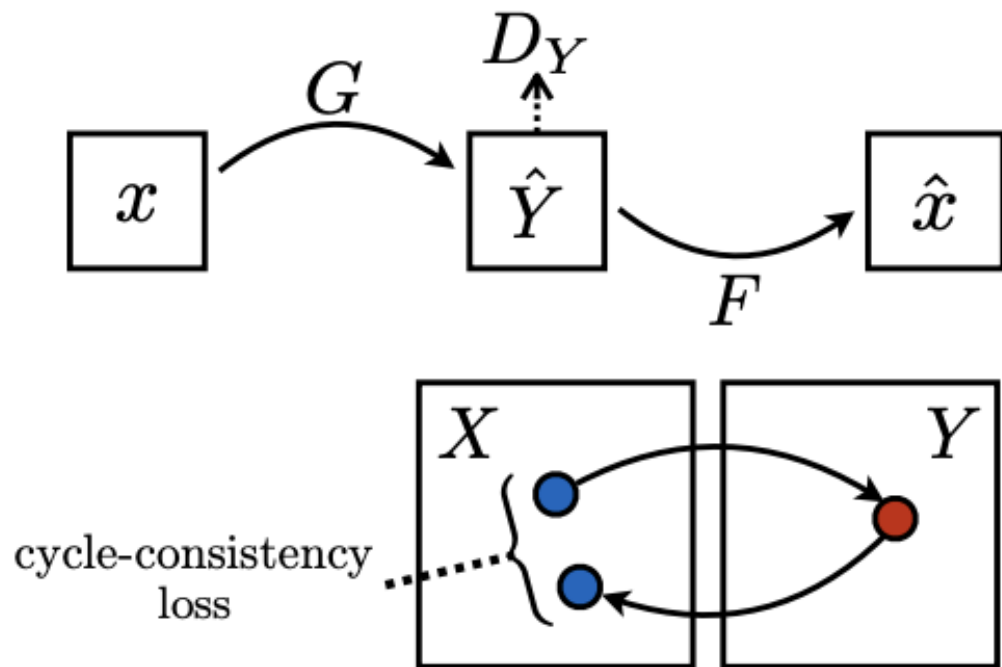


Cycle consistency loss



Zhu *et al.*, ICCV 2017

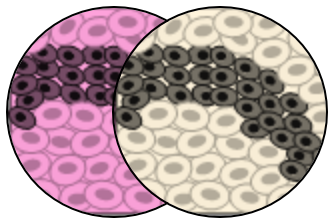
Cycle consistency loss



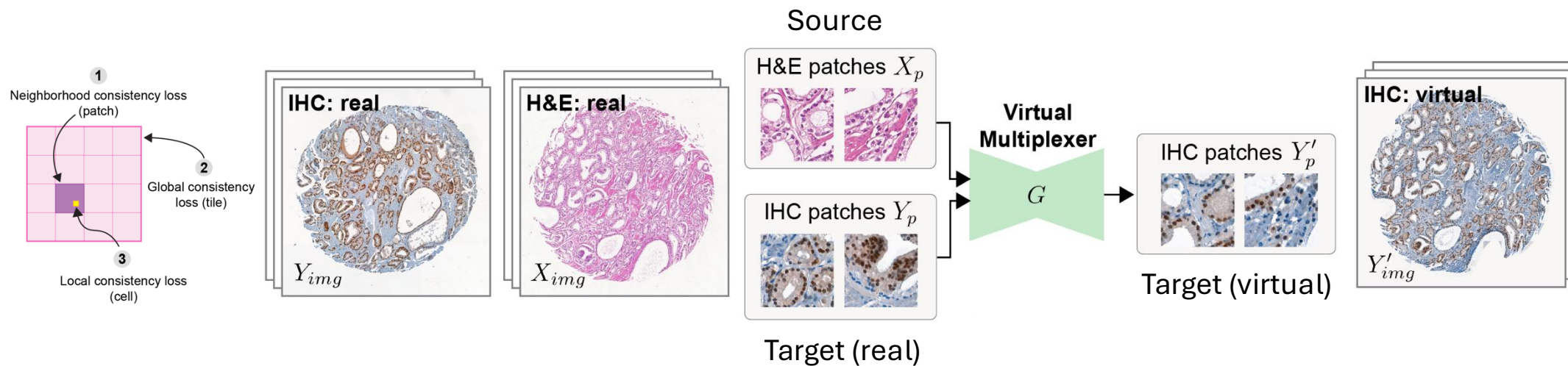
Zhu et al., ICCV 2017

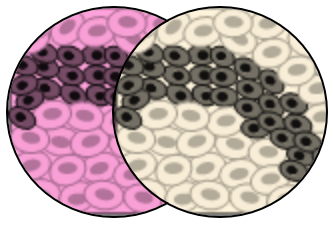


<https://github.com/junyanz/CycleGAN>

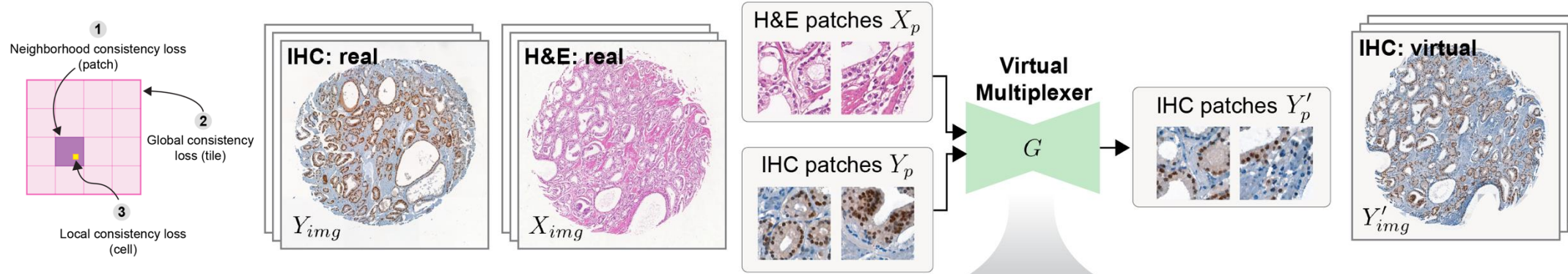


VirtualMultiplexer: model architecture

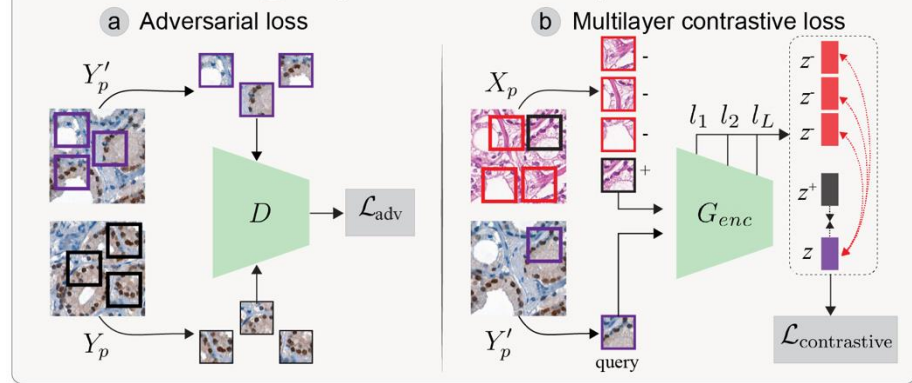




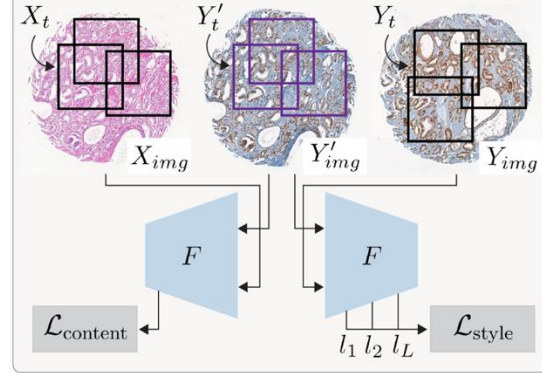
VirtualMultiplexer: model architecture



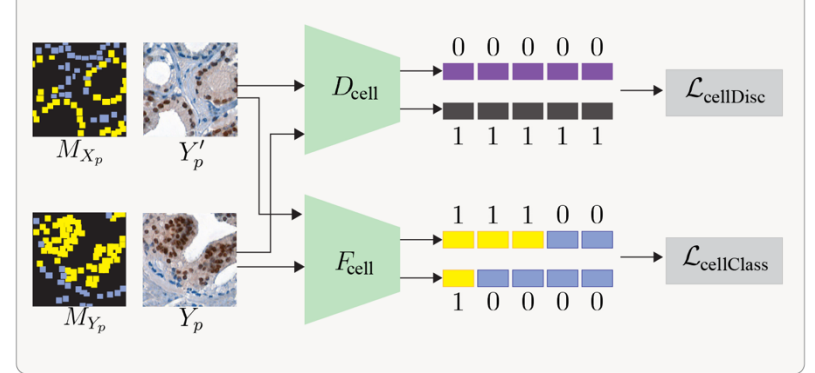
1 Neighborhood consistency loss



2 Global consistency loss



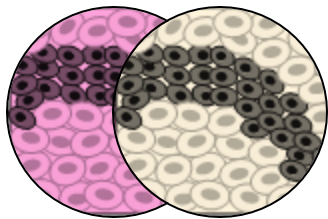
3 Local consistency loss



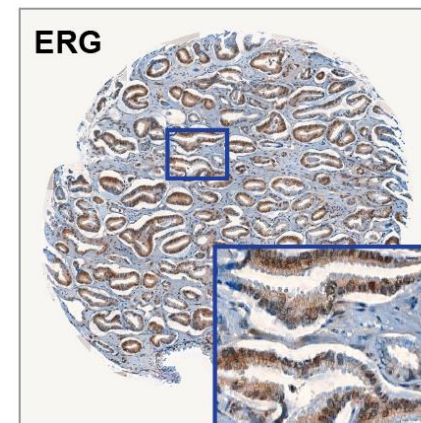
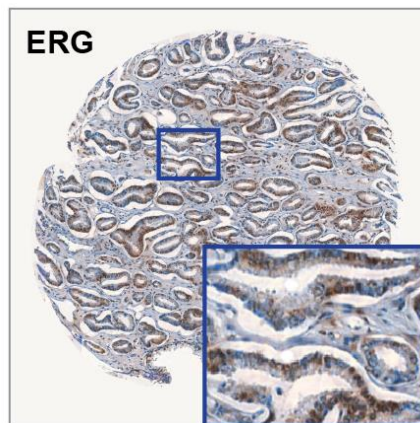
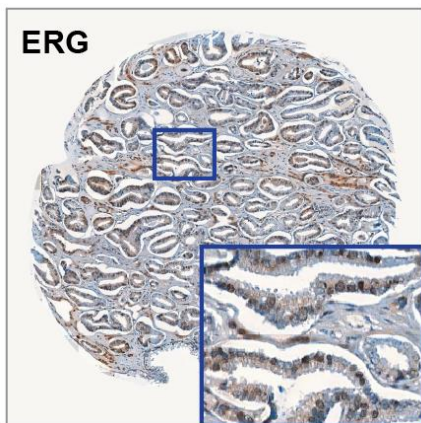
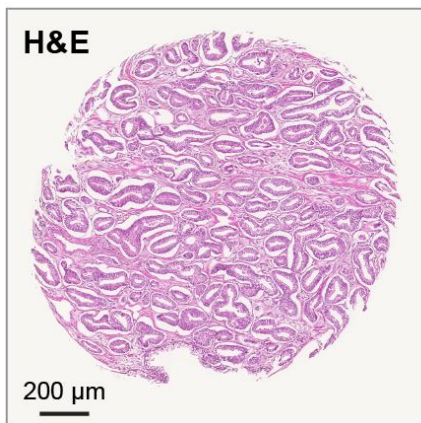
Notations: ■ Frozen model | ■ Trainable model | ■ ■ Real/Virtual | ■ ■ Positive/Negative cells

G : Encoder | D : Patch discriminator | D_{cell} : Cell discriminator | F : Feature extractor | F_{cell} : Cell classifier | $l_1 l_2 l_L$: Layers

X_p : Real H&E patches | Y_p, Y'_p : Real/Virtual IHC patches | $X_{\text{img}}, Y_{\text{img}}, Y'_{\text{img}}$: Images | X_t, Y_t, Y'_t : Tiles

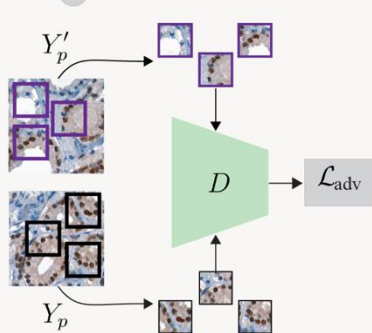


Effect of different losses

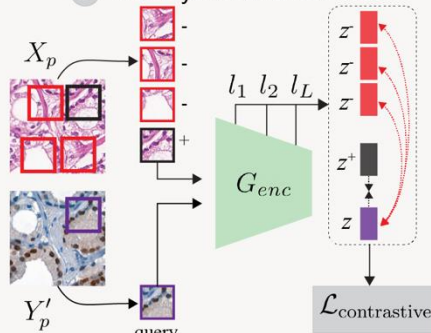


1 Neighborhood consistency loss

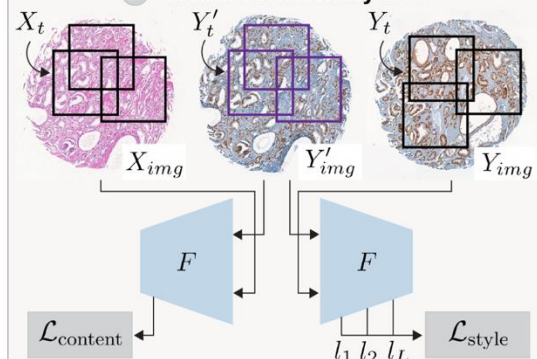
a Adversarial loss



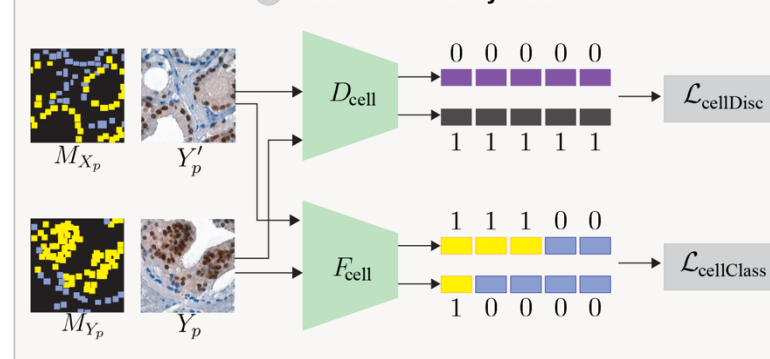
b Multilayer contrastive loss

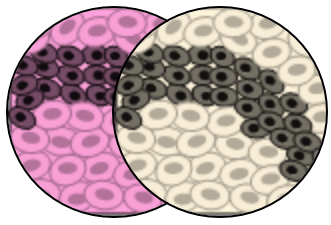


2 Global consistency loss



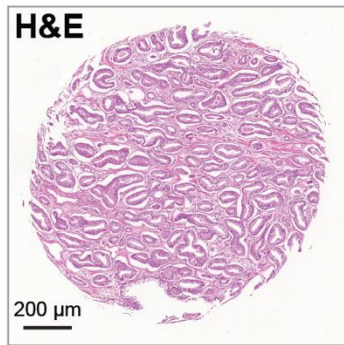
3 Local consistency loss



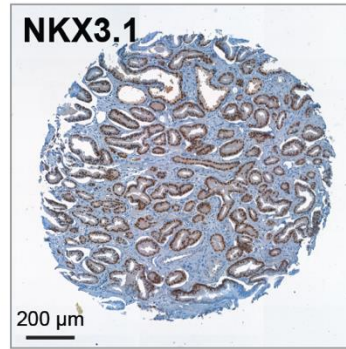


Performance assessment

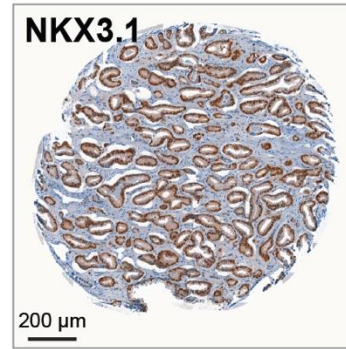
Real H&E



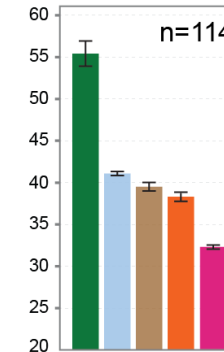
Real IHC



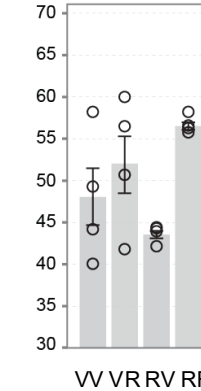
Virtual IHC



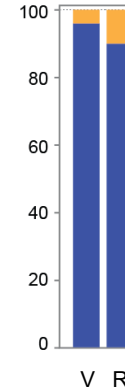
Fréchet Inception Distance



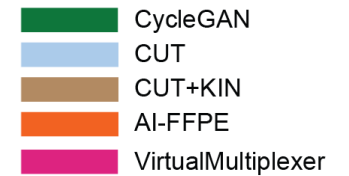
Visual Turing Test



Staining quality



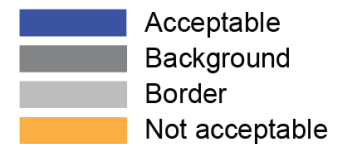
Unpaired S2S translation methods



Visual Turing test

VV: Virtual as Virtual
VR: Virtual as Real
RV: Real as Virtual
RR: Real as Real

Staining quality



EMPaCT prostate cancer TMA*:

- 210 patients (4 cores / patient)
- 6 markers (NKX3.1, AR, CD44, CD146, p53, ERG)
- The VirtualMultiplexer **outperformed all other methods** in all 6 IHC markers in terms of FID score.
- Visual Turing test **close to random guess**: average sensitivity/ specificity of 52.1% / 54.1% across all six markers
- Virtual staining quality was **on par or higher than real** staining quality for 4/6 markers

Picasso

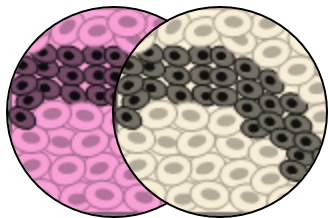


Van Gogh

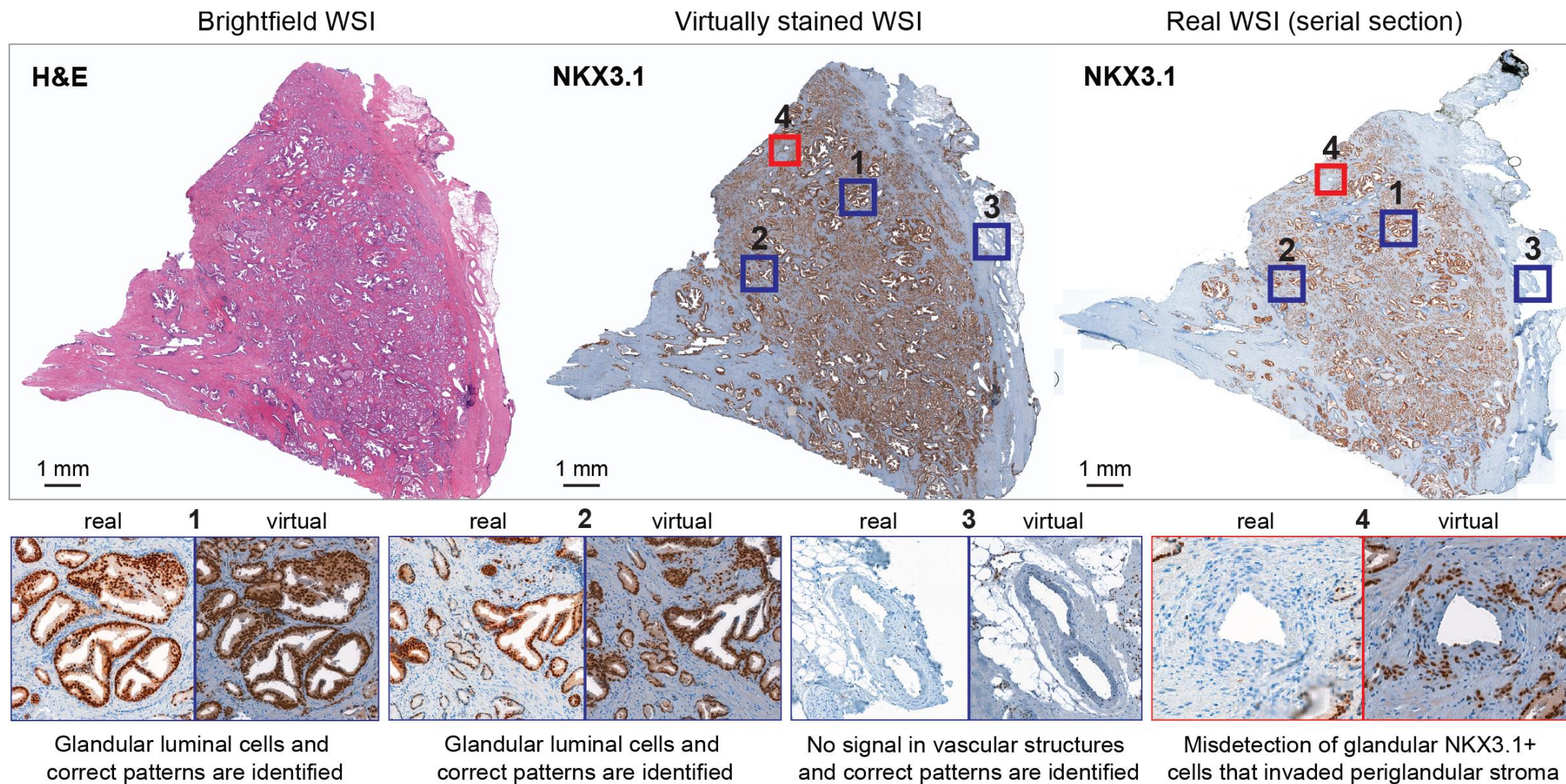


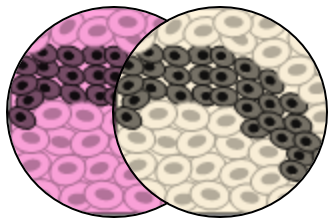
Monet



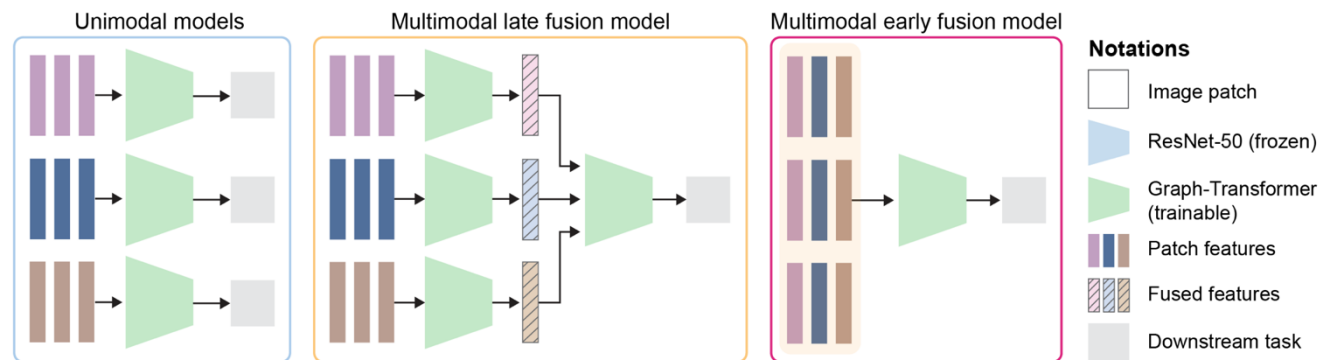
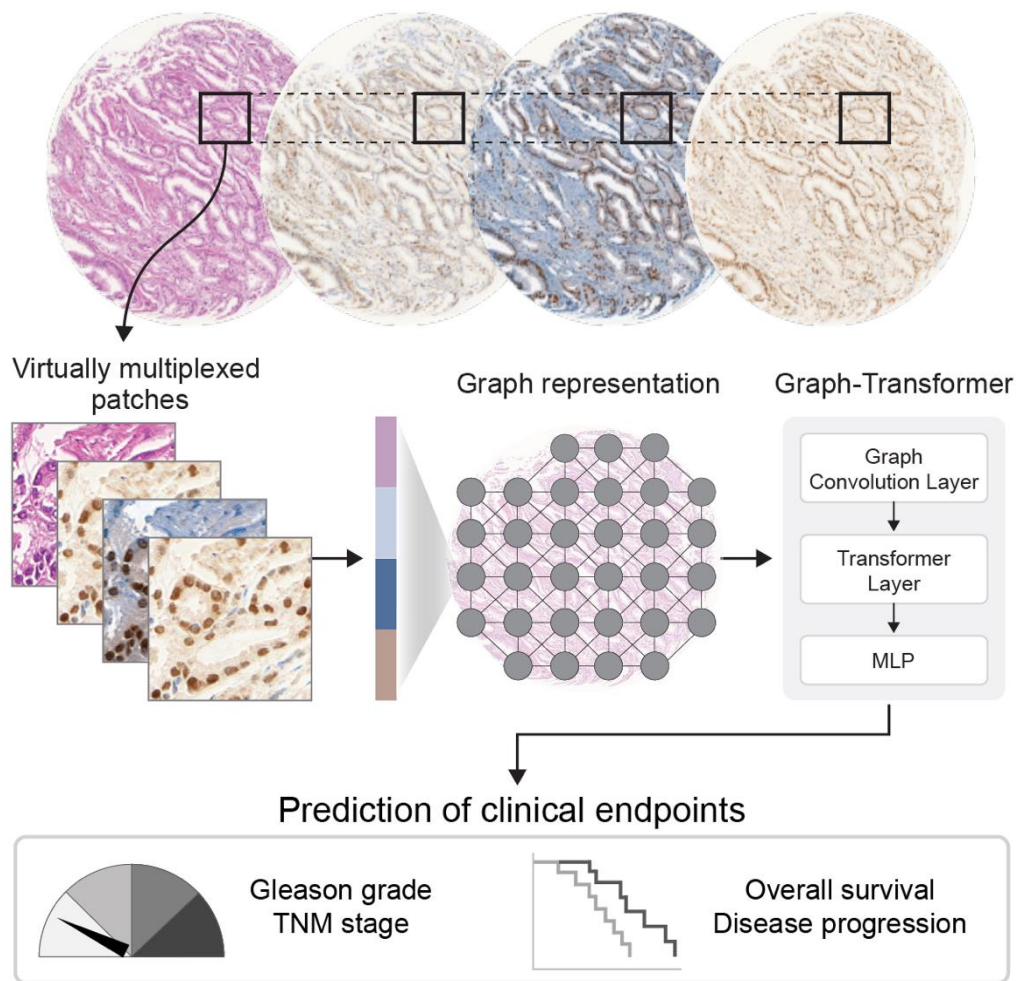


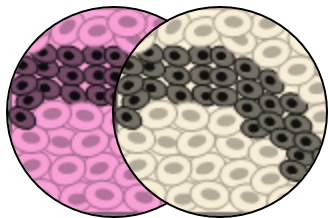
Generalization on OOD WSIs



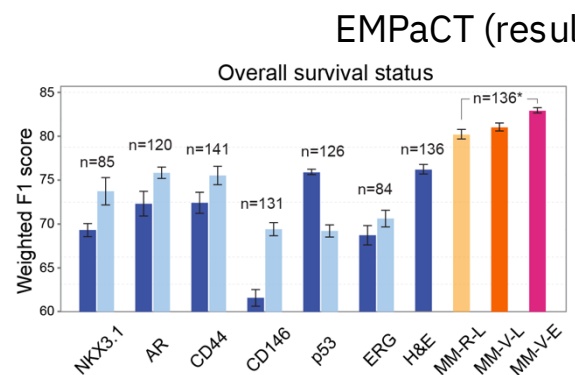
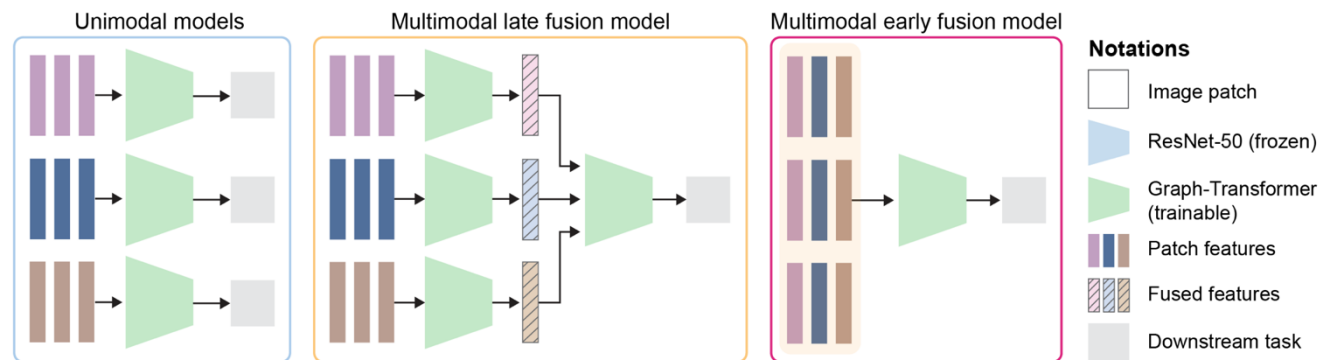
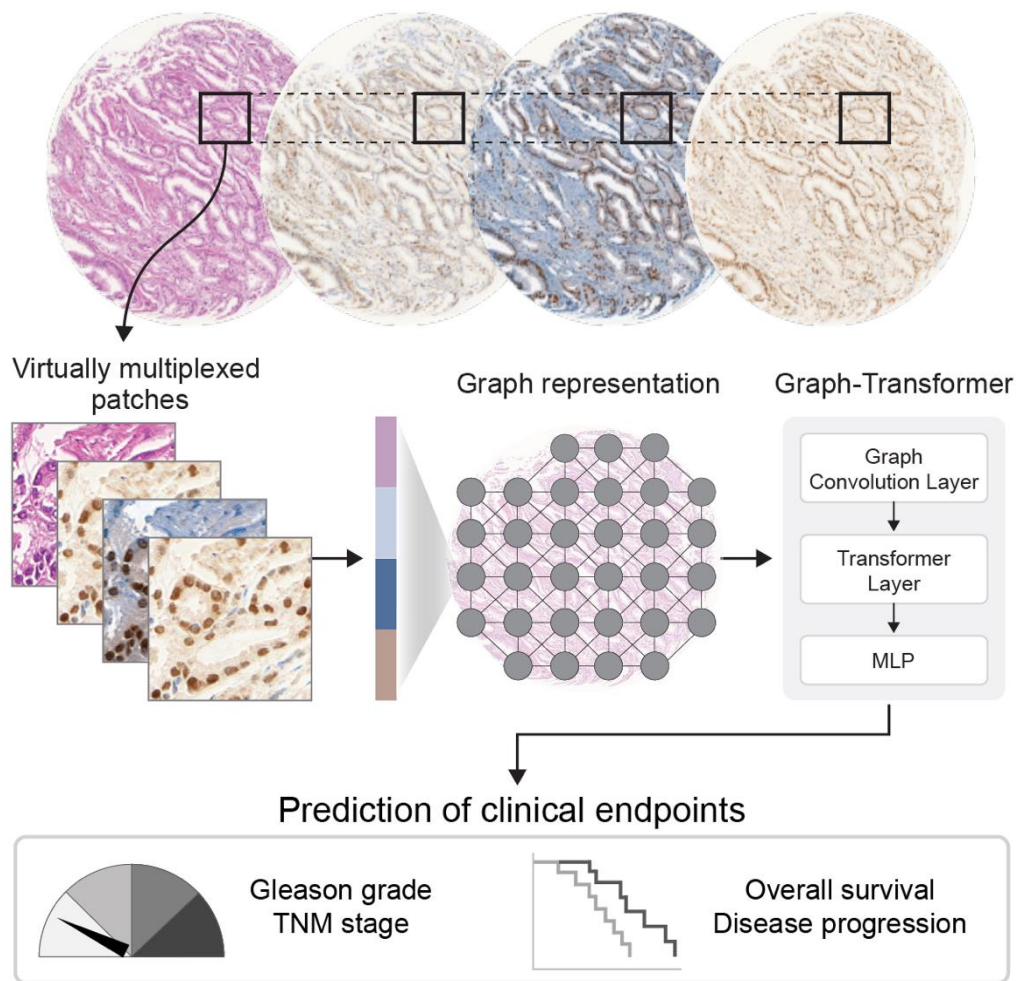


Improved clinical predictions



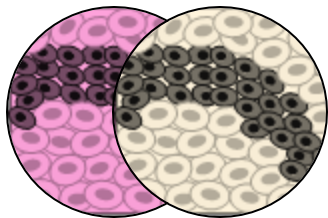


Improved clinical predictions



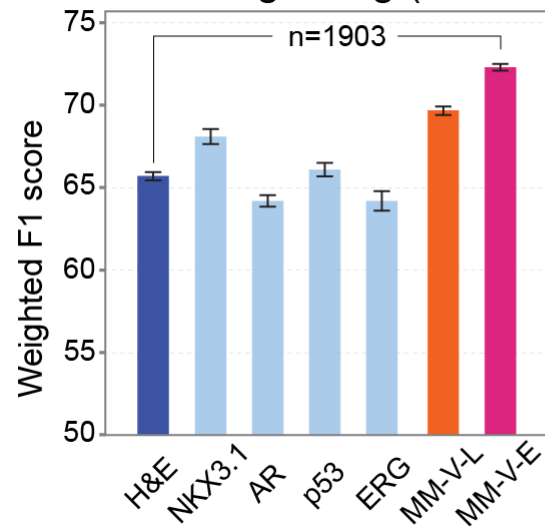
Training settings

- Unimodal - Real
- Unimodal - Virtual
- MM-R-L: Multimodal - Real - Late fusion
- MM-V-L: Multimodal - Virtual - Late fusion
- MM-V-E: Multimodal - Virtual - Early fusion



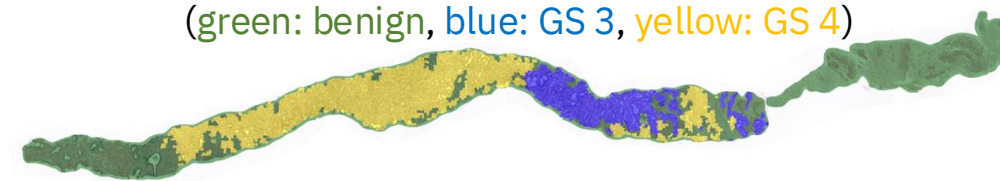
Transfer to other datasets - PANDA

Gleason grading (PANDA)

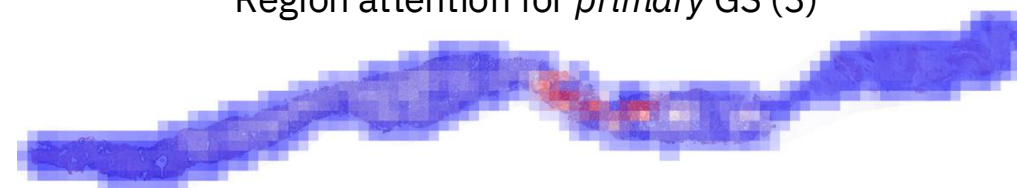


True label	Predicted label					
	Benign	Grade6	Grade7	Grade8	Grade9	Grade10
Benign	466	35	7	5	0	2
Grade6	80	353	43	3	0	0
Grade7	15	95	282	53	21	0
Grade8	4	8	41	127	34	2
Grade9	8	2	23	29	135	11
Grade10	0	0	2	1	5	11

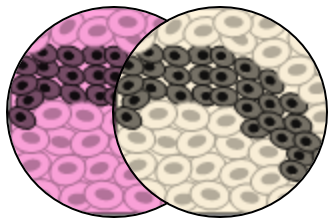
Ground-Truth Gleason Score (GS): 3 + 4
(green: benign, blue: GS 3, yellow: GS 4)



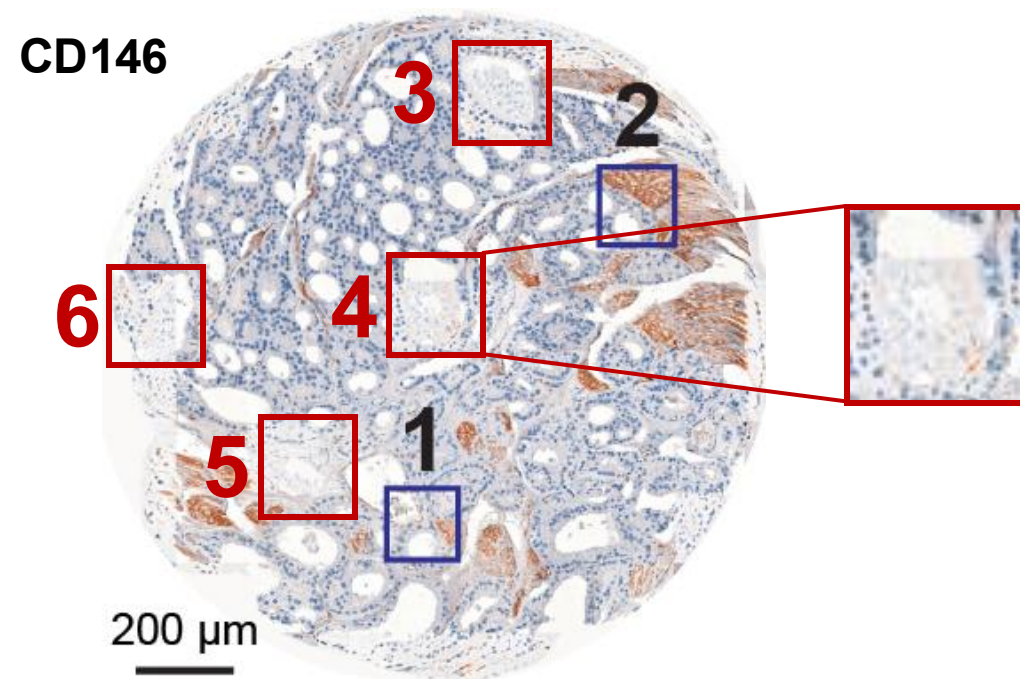
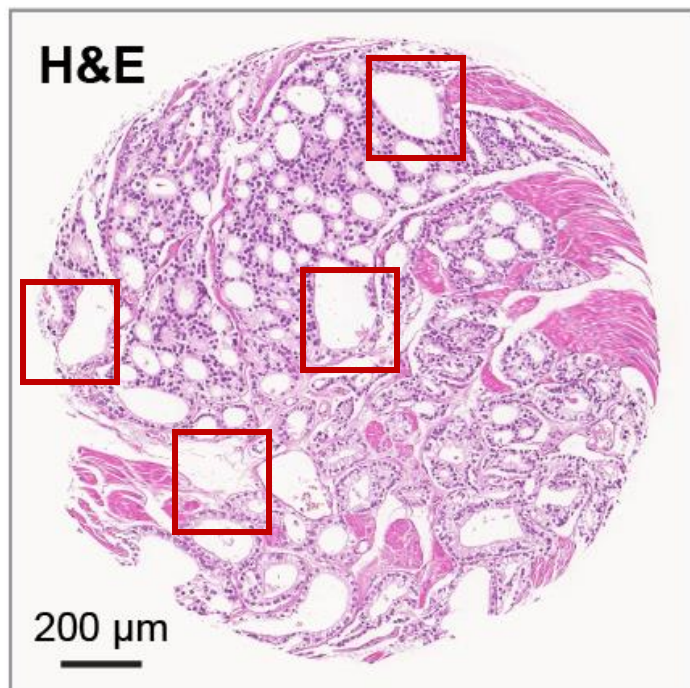
Region attention for *primary* GS (3)

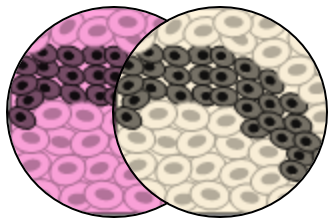


Region attention for *secondary* GS (4)

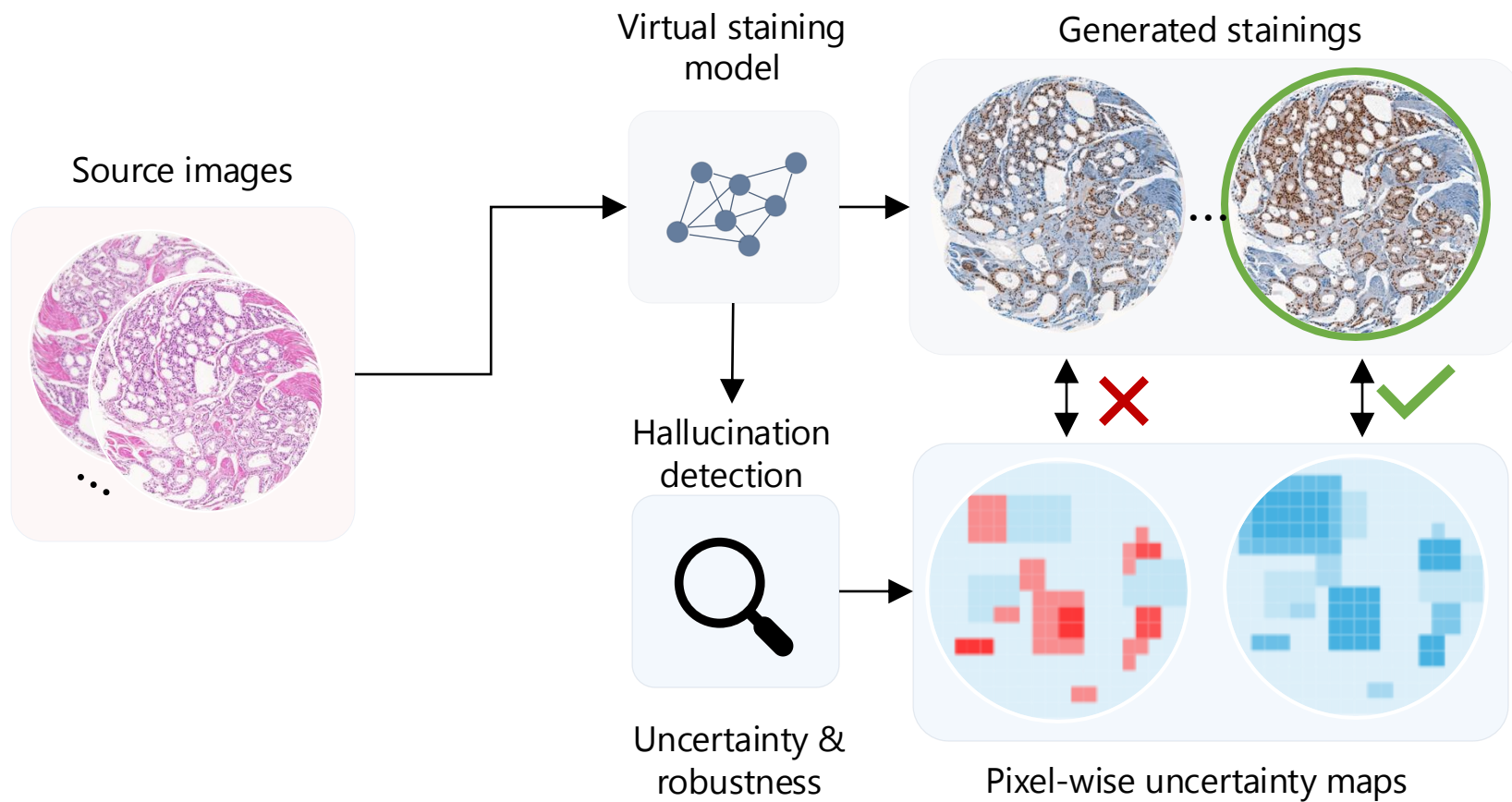


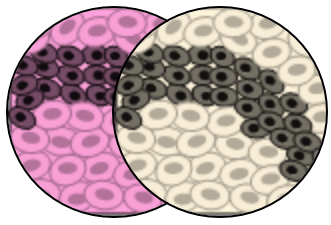
Draw me a cell?





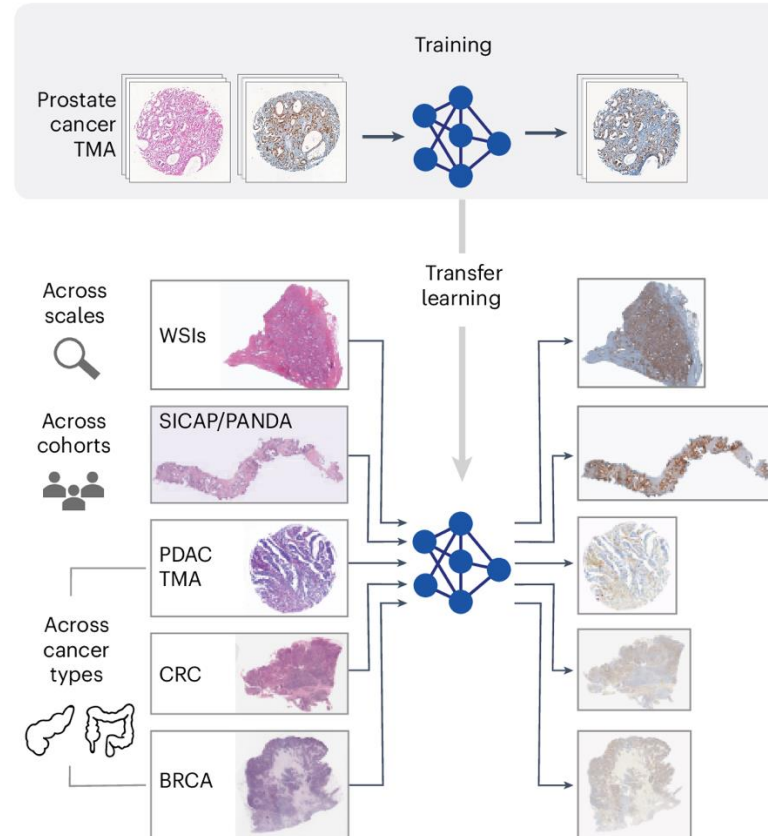
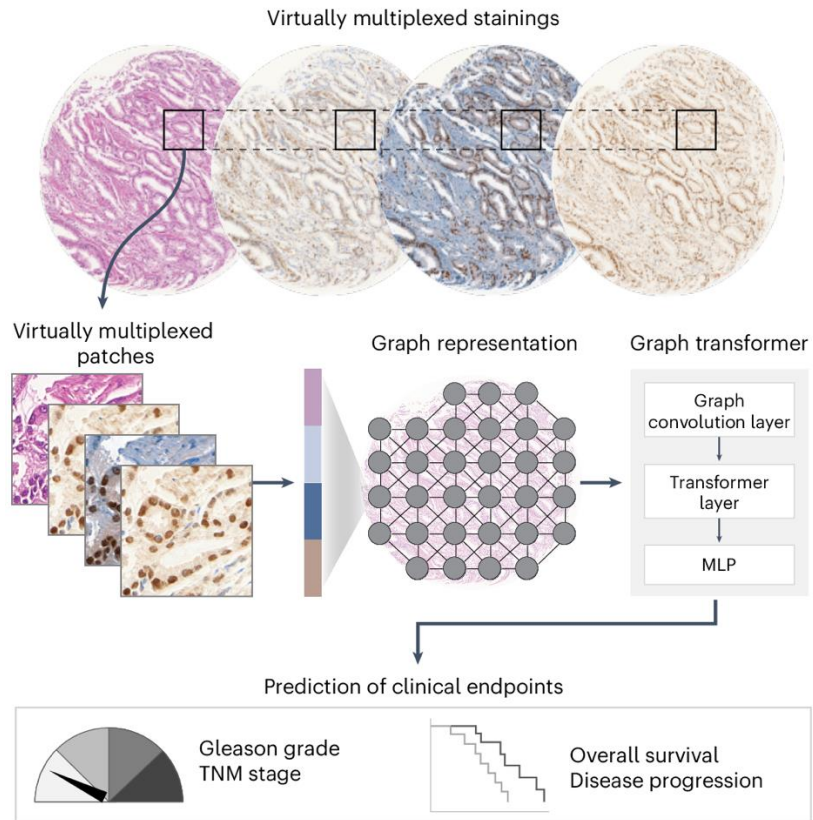
Hallucination detection





Virtual Multiplexer

Multiplexed tumor profiling with generative AI



✓ Consistently **improved the prediction** of clinically relevant endpoints

✓ Able to **generalize** to unseen cohorts and cancer types

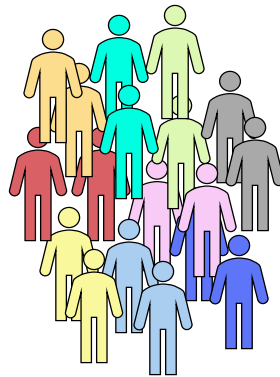
Towards **AI-assisted histopathology**:

- Data inpainting, sample imputation, harmonizing datasets, **experimental design**
- Translation to cutting-edge **spatial omics** technologies (e.g., spatial transcriptomics)

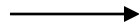
An end-to-end AI framework for Inflammatory Skin Diseases

- Atopic Dermatitis (AD)
- Psoriasis (PsO)
- Lichen Planus (LP)
- Lupus Erythematosus (CLE)
- Bullous Pemphigoid (BP)
- Neutrophilic Diseases (NeuD)
- Drug Hypersensitivity Reaction (DHR)
- Healthy Skin
- Wells Syndrome

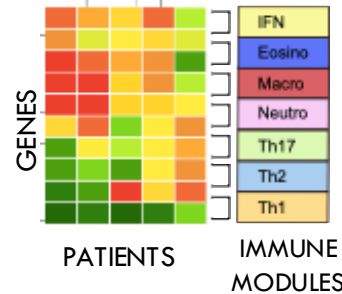
ISD Patients
(n=126)



Histology



Bulk
Transcriptomic
Profiles



Can we extract H&E representations that capture tissue heterogeneity?



Can we use them to train AI models to predict molecular characteristics or diagnostic labels?



How interpretable and clinically understandable are the representations learned by these models?

30

①



Melissa Ensmenger

Collaboration with Prof. Raphael Gottardo (BDSC) and Prof. Michel Gilliet (Department of Dermatology, CHUV)

Team members: Antoine Girardin, Jeremy Di Domizio, Hugo Cometto

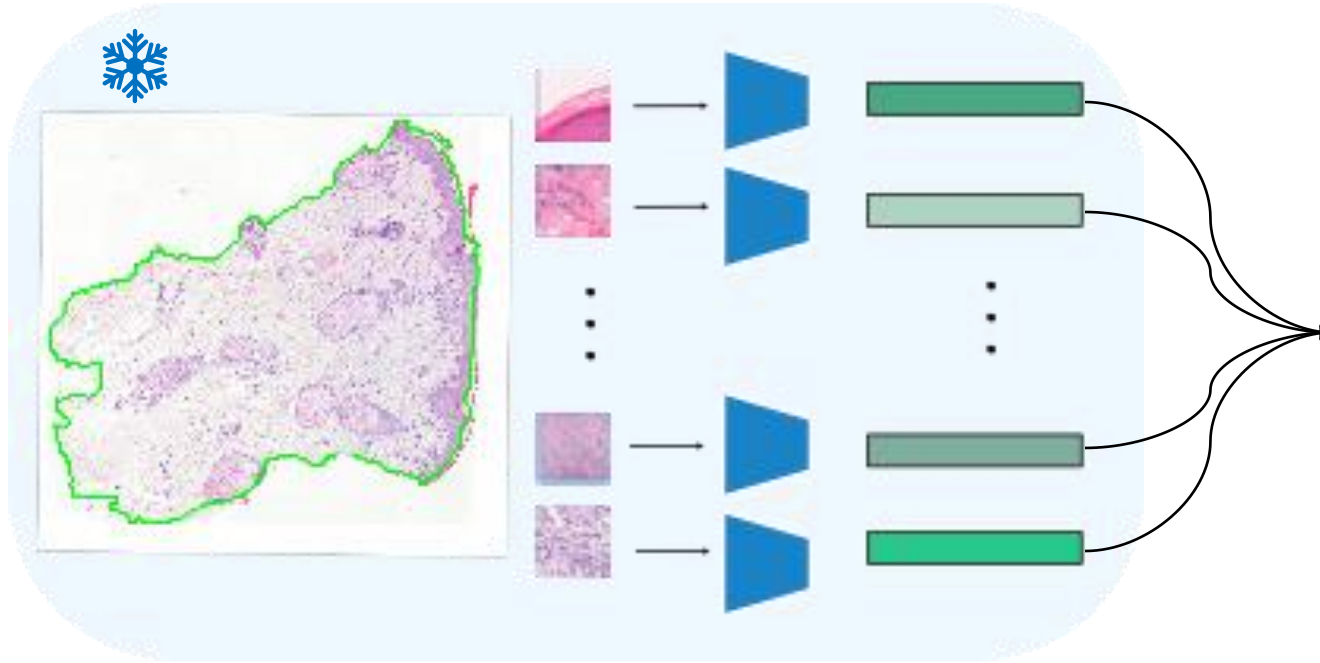
An end-to-end AI framework for Inflammatory Skin Diseases

① Segment and patch WSI H&E

② Extract patch embeddings with pre-trained foundation models

③ Train MIL aggregator + head for prediction tasks

④ Explain prediction by visualizing patch attention scores



Patch-level Foundation Model

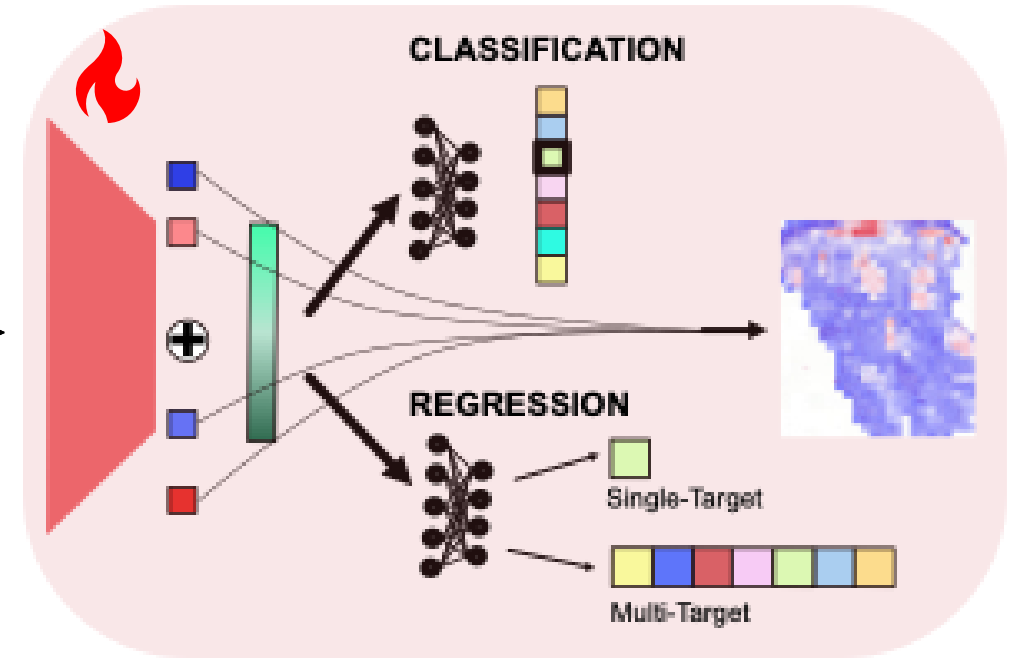
Hopitimus-0⁶ – UNI-v2⁴ – Virchow-2⁸ –
CONCH-v1.5⁵ – Hibou-L⁷



Patch embeddings



Frozen weights



MIL Aggregator

Attention-based MIL
module (ABMIL)



Prediction Head

2-layer MLP



Trainable parameters



Patient
embedding



Attention Scores

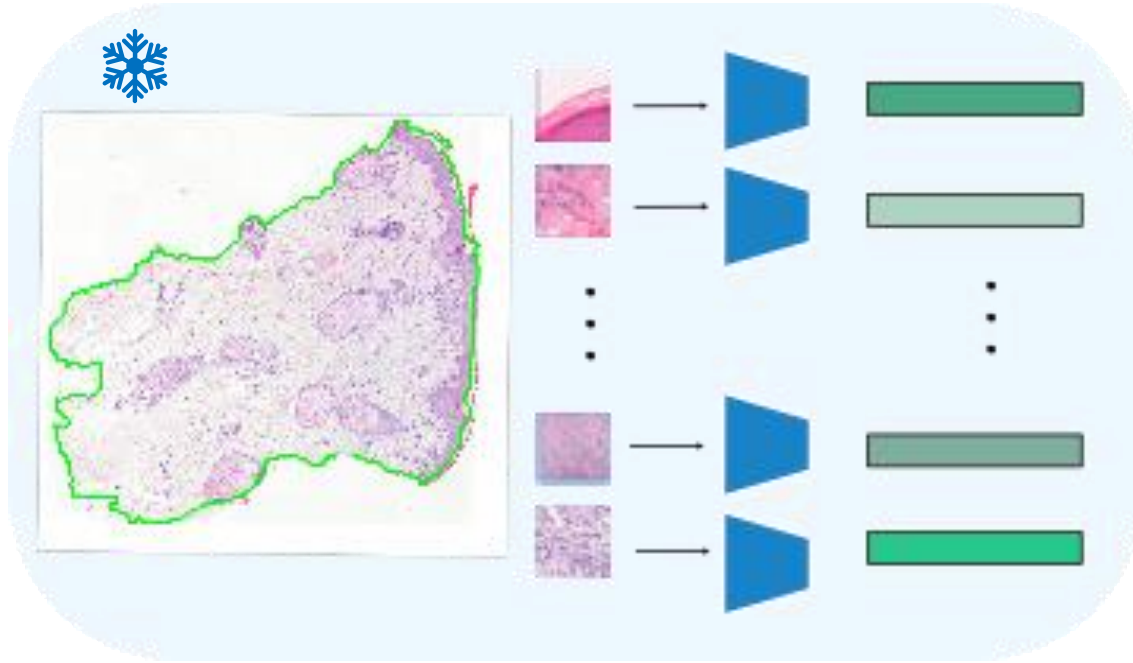


= weights for patch aggregation

An end-to-end AI framework for Inflammatory Skin Diseases

① Segment and patch WSI H&E

② Extract patch embeddings with pre-trained foundation models



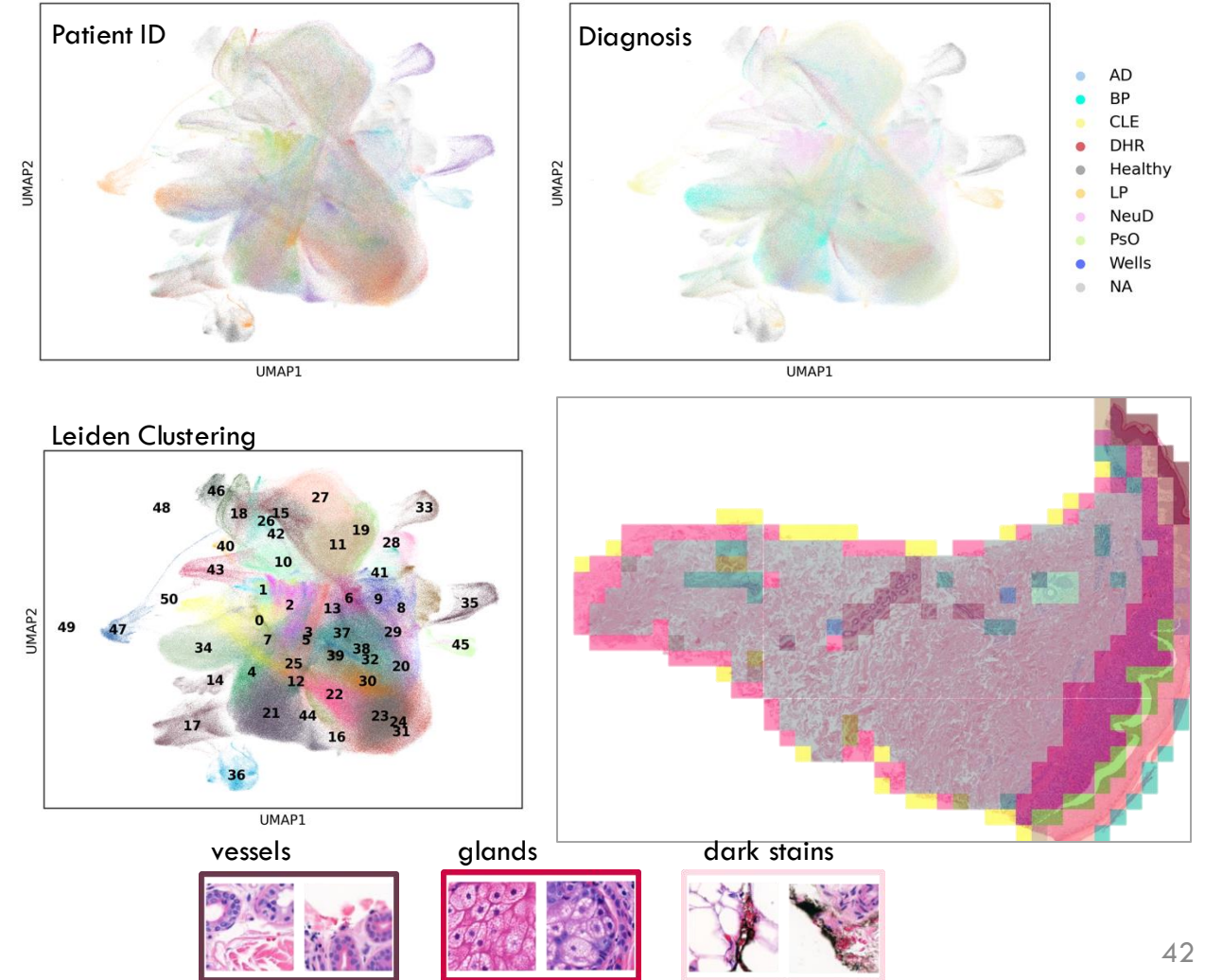
Patch-level Foundation Model

Hoptimus-0⁶ – UNI-v2⁴ – Virchow-2⁸ –
CONCH-v1.5⁵ – Hibou-L⁷

Patch embeddings

Frozen weights

FM representations capture different layers of the skin as well as specialized morphological structures and technical artifacts.



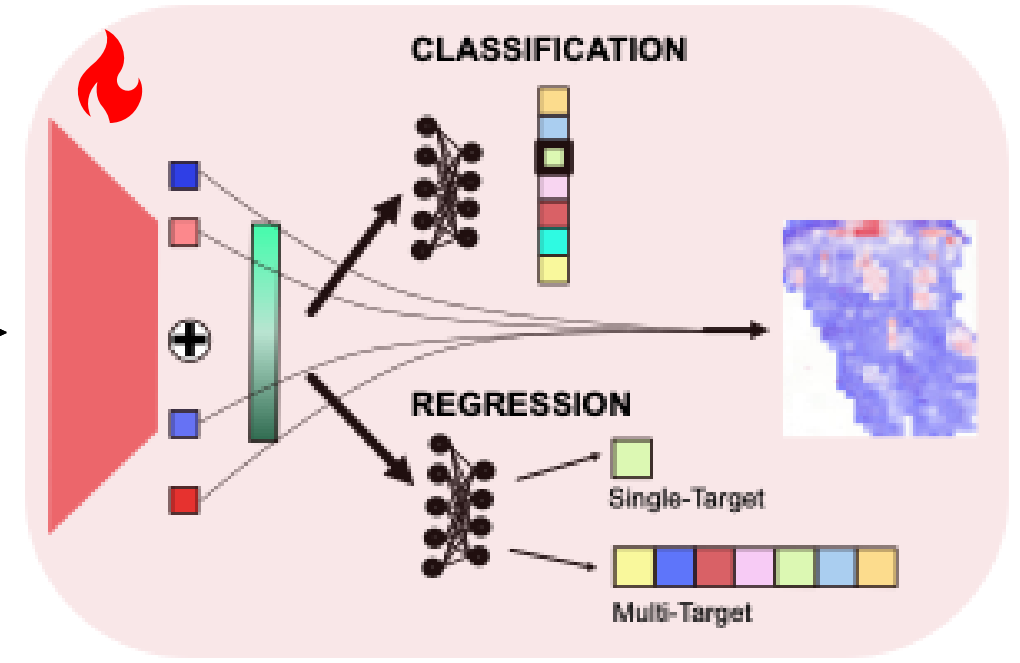
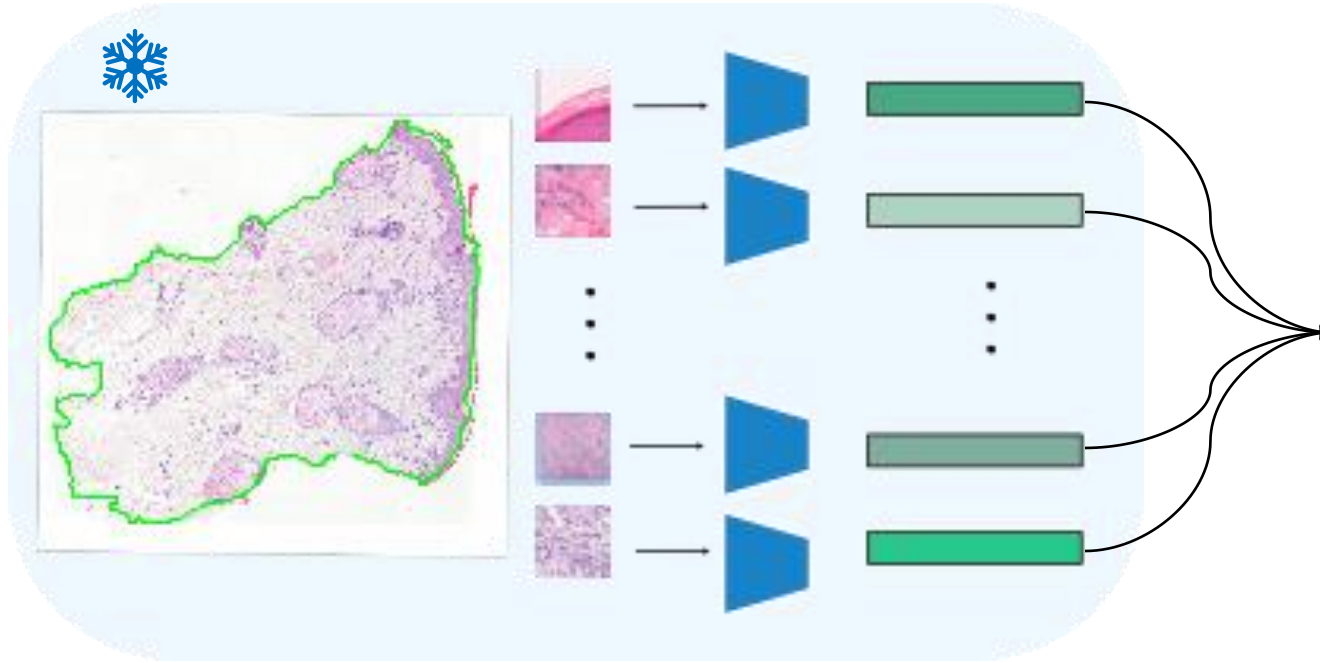
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Patch embeddings



Frozen weights



MIL Aggregator

Attention-based MIL
module (ABMIL)



Prediction Head

2-layer MLP



Trainable parameters



Patient
embedding



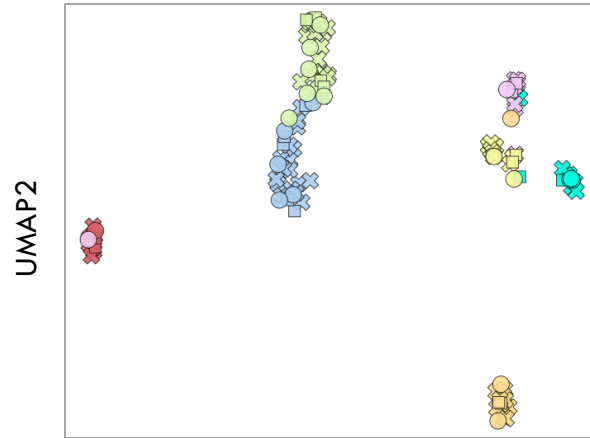
Attention Scores



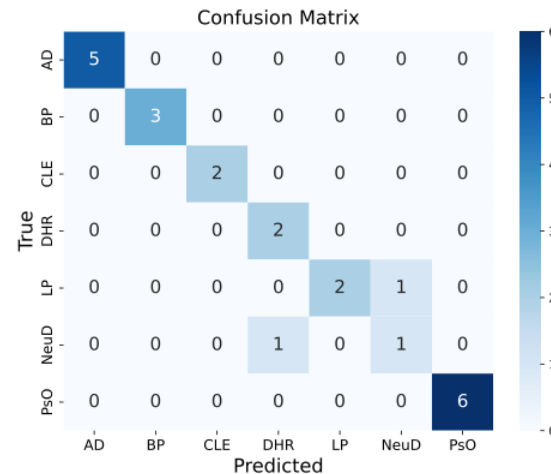
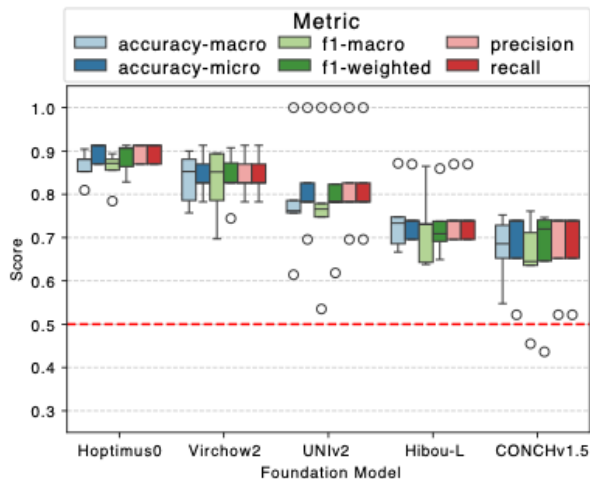
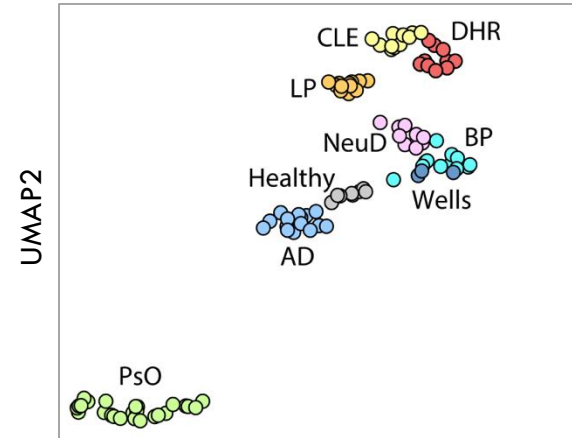
= weights for patch aggregation

An end-to-end AI framework for Inflammatory Skin Diseases

H&E patient embeddings

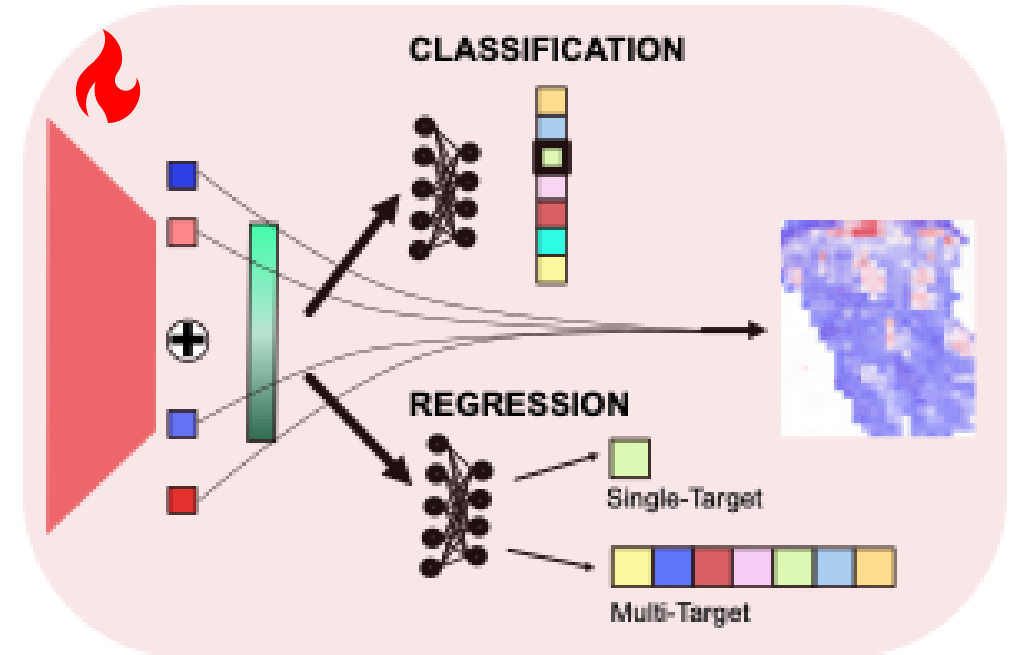


Gene expression patient embeddings



3 Train MIL aggregator + head for prediction tasks

4 Explain prediction by visualizing patch attention scores



MIL Aggregator
Attention-based MIL module (ABMIL)



Prediction Head
2-layer MLP



Trainable parameters



Patient embedding



Attention Scores



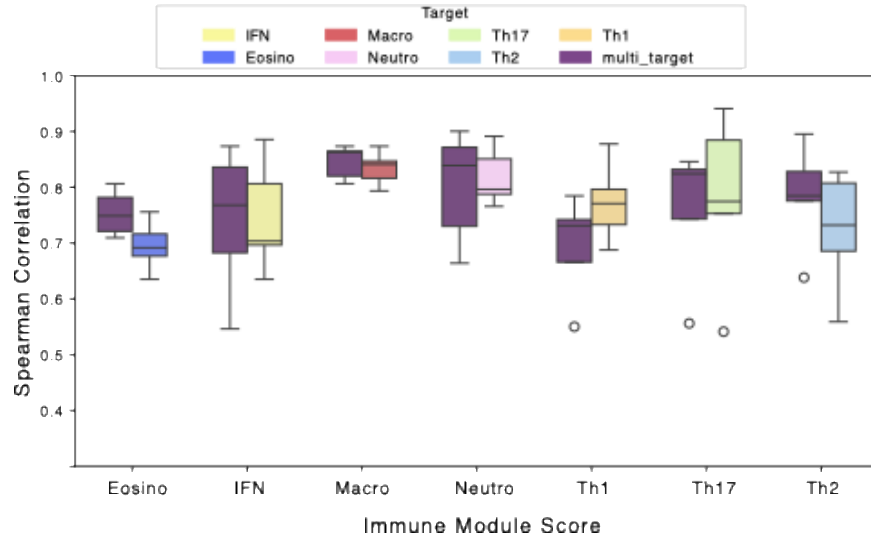
= weights for patch aggregation

An end-to-end AI framework for Inflammatory Skin Diseases

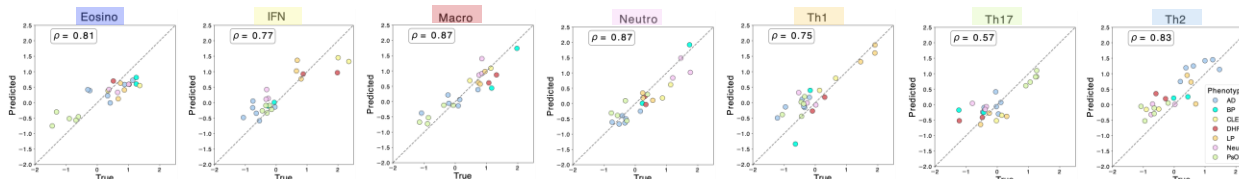
Our framework can predict joint immune pathway activity from tissue morphology (H&E)...

Comparison of **5-fold cross-validation Spearman correlations** for pathway activity prediction between **multi-target** and **single-target models***

*trained on Hoptimus0 patch embeddings

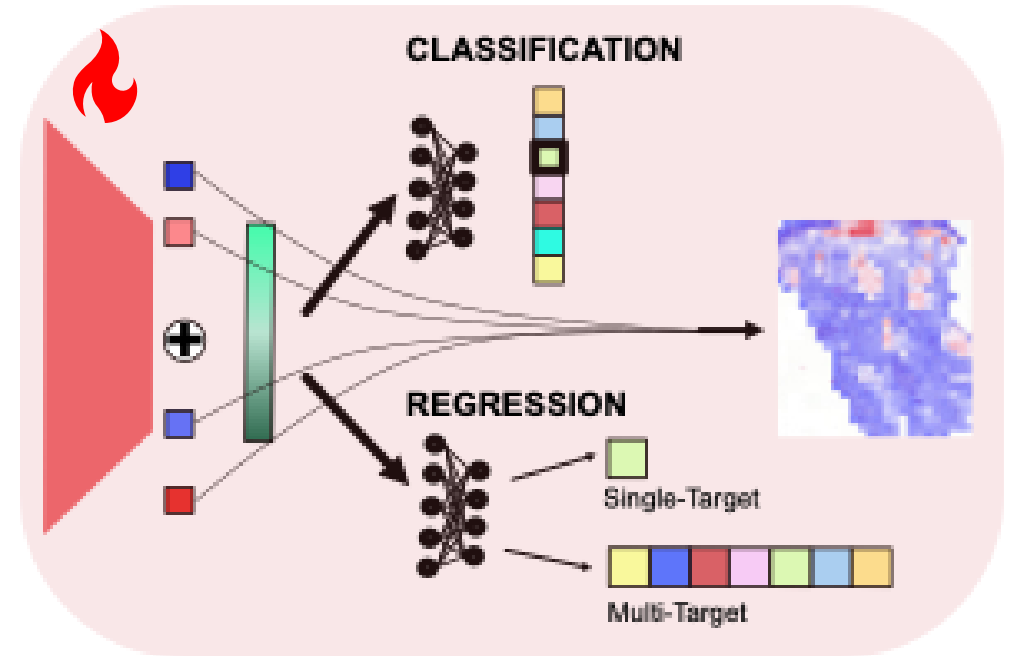


Predicted (y-axis) vs. reference (x-axis) pathway activity for the multi-objective model
(example test set of specific split)



3 Train MIL aggregator + head for prediction tasks

4 Explain prediction by visualizing patch attention scores



MIL Aggregator
Attention-based MIL module (ABMIL)

Prediction Head
2-layer MLP

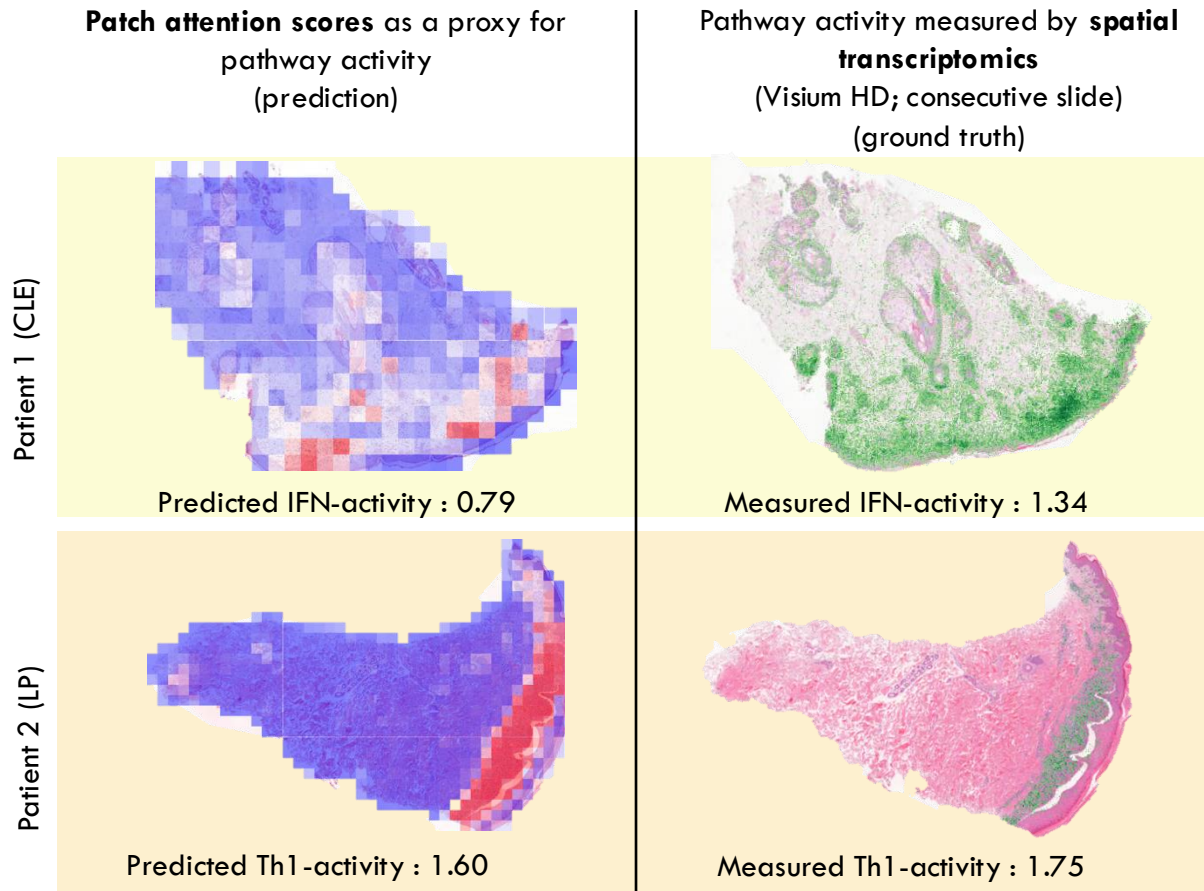
Trainable parameters

Patient embedding

Attention Scores
= weights for patch aggregation

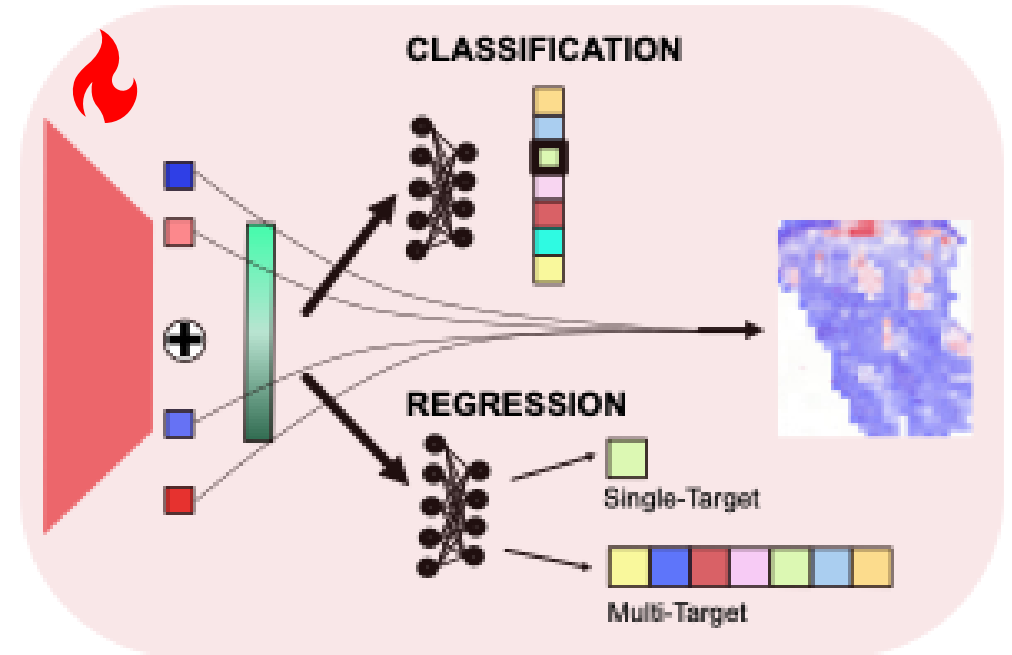
An end-to-end AI framework for Inflammatory Skin Diseases

... and map it back to specific tissue regions using attention scores.



3 Train MIL aggregator + head for prediction tasks

4 Explain prediction by visualizing patch attention scores



MIL Aggregator
Attention-based MIL module (ABMIL)

Prediction Head
2-layer MLP

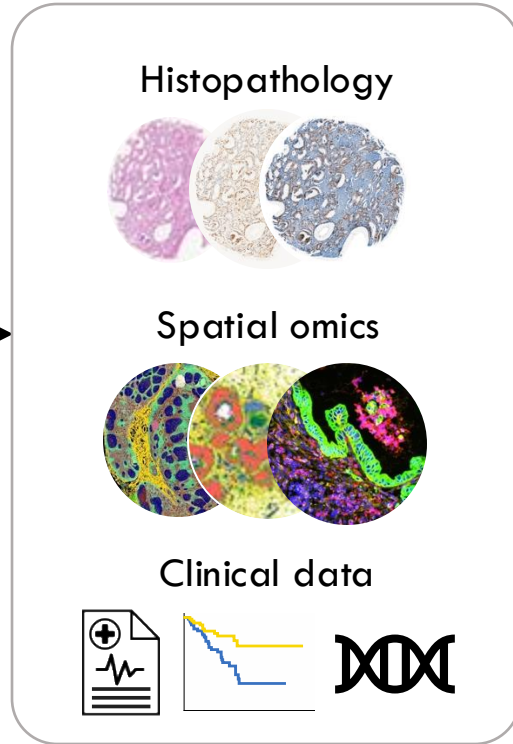
Trainable parameters

Patient embedding

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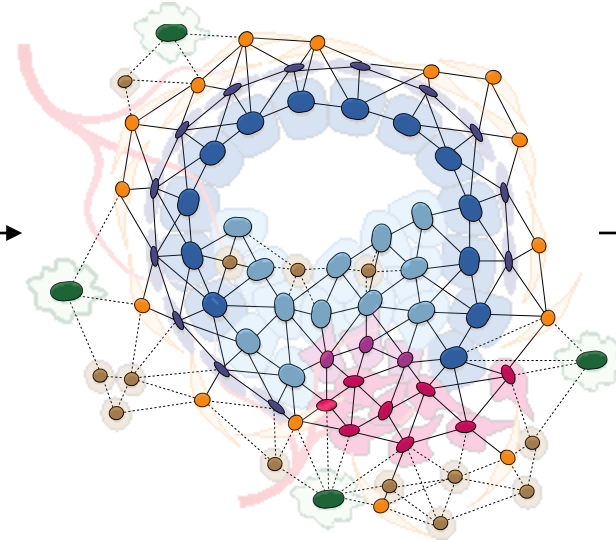


Represent



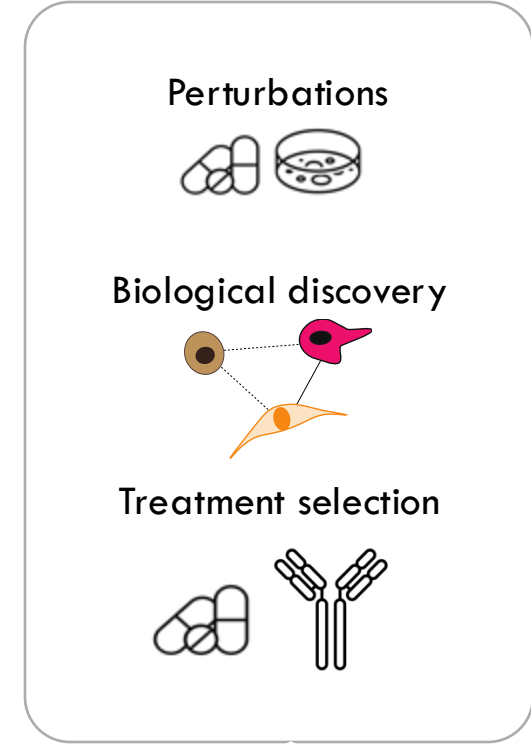
How can we learn multimodal **representations** from spatial omics?

Interpret



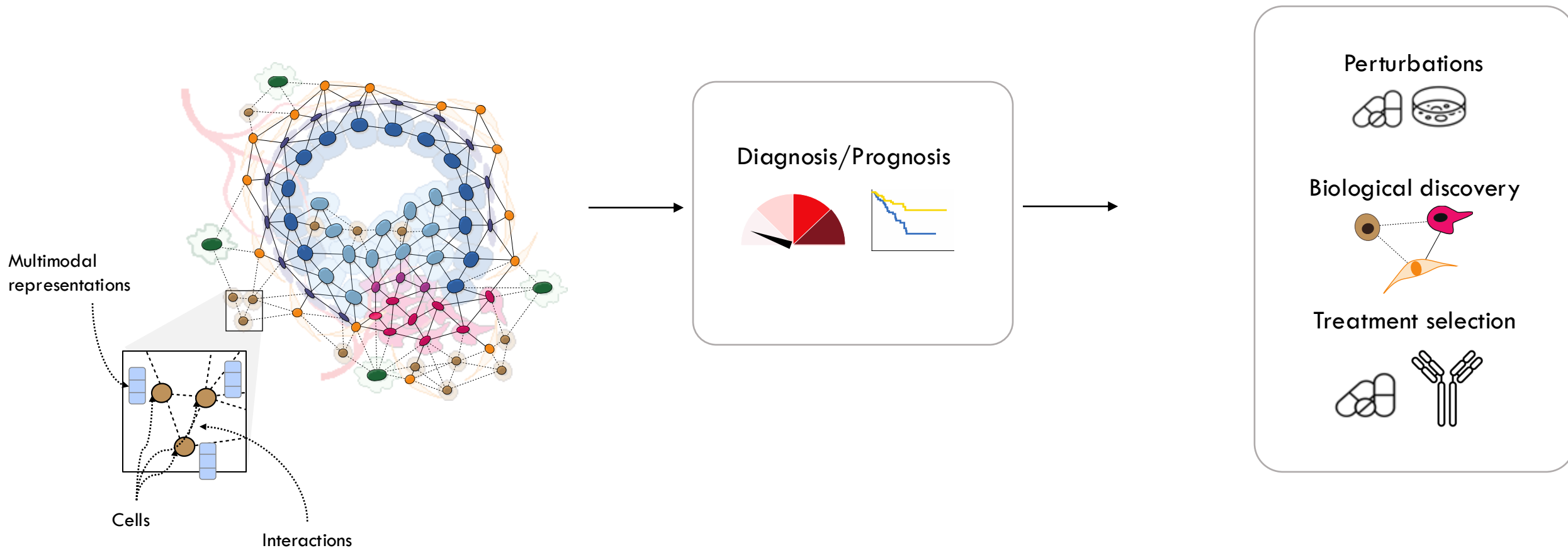
How can we **interpret** these representations of the TME?

Perturb

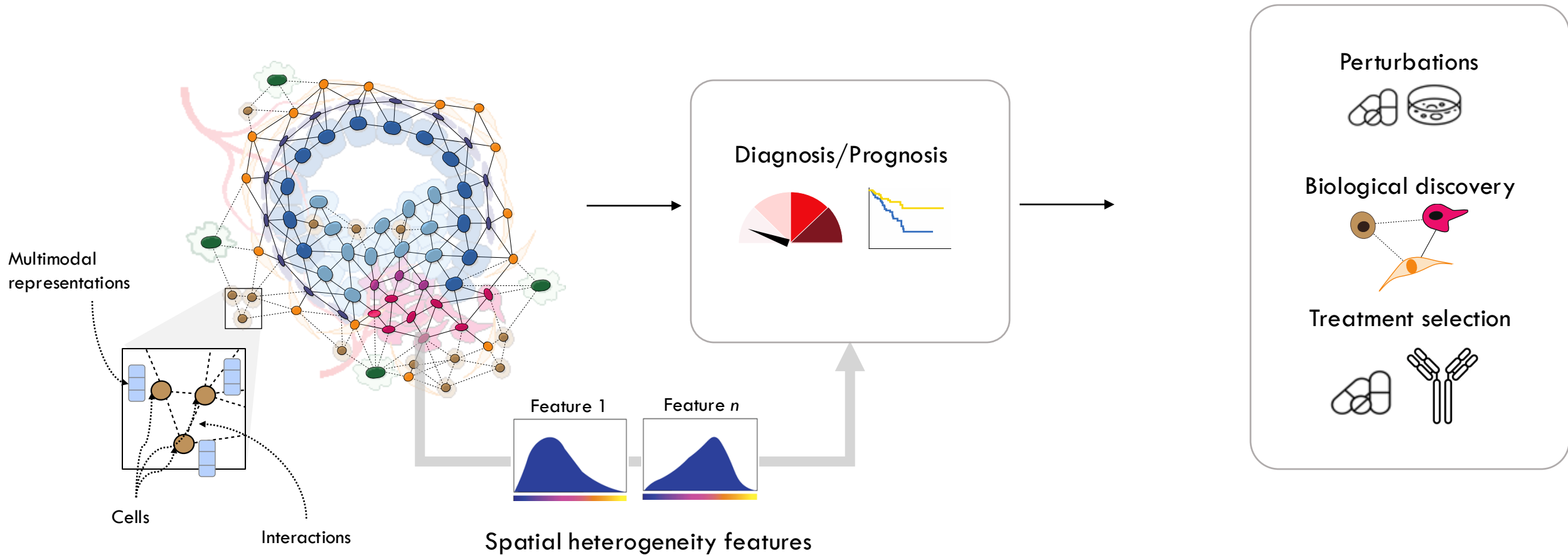


How can we predict the effects of drug **perturbations**?

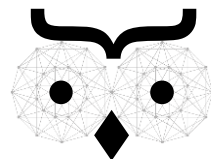
Modeling the TME with Graph Representation Learning



Modeling the TME with Graph Representation Learning



Adriano Martinelli



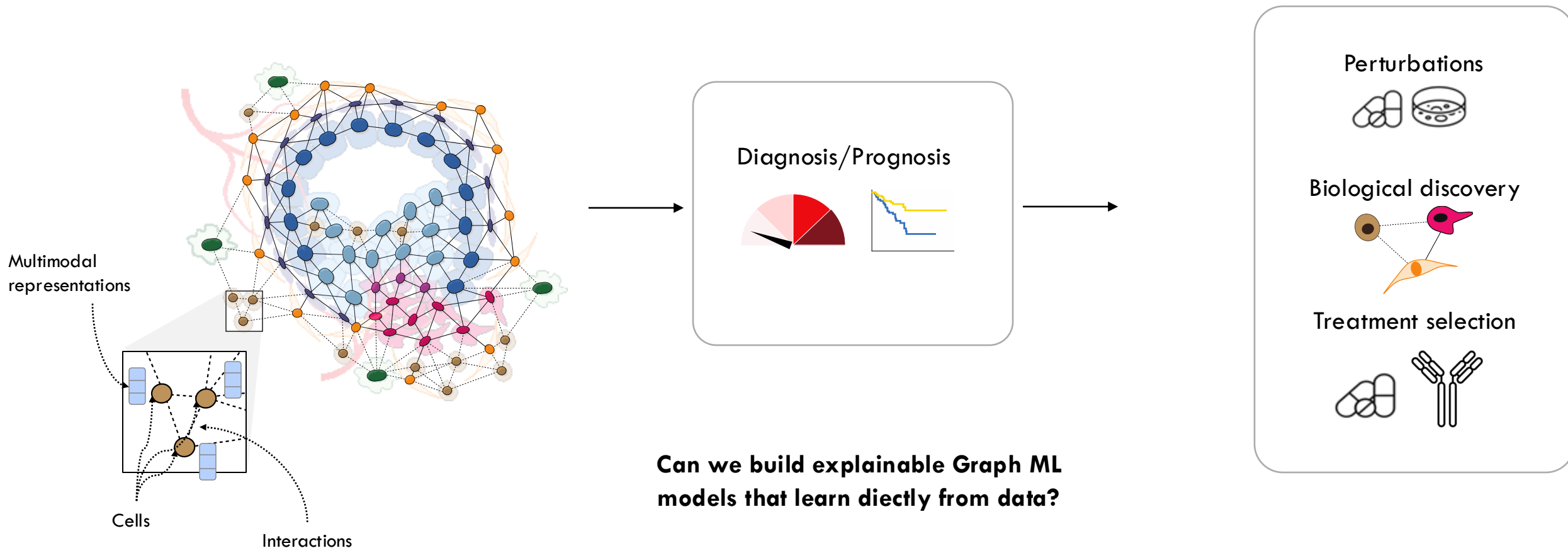
ATHENA

Martinelli and Rapsomaniki, *Bioinformatics* (2022)



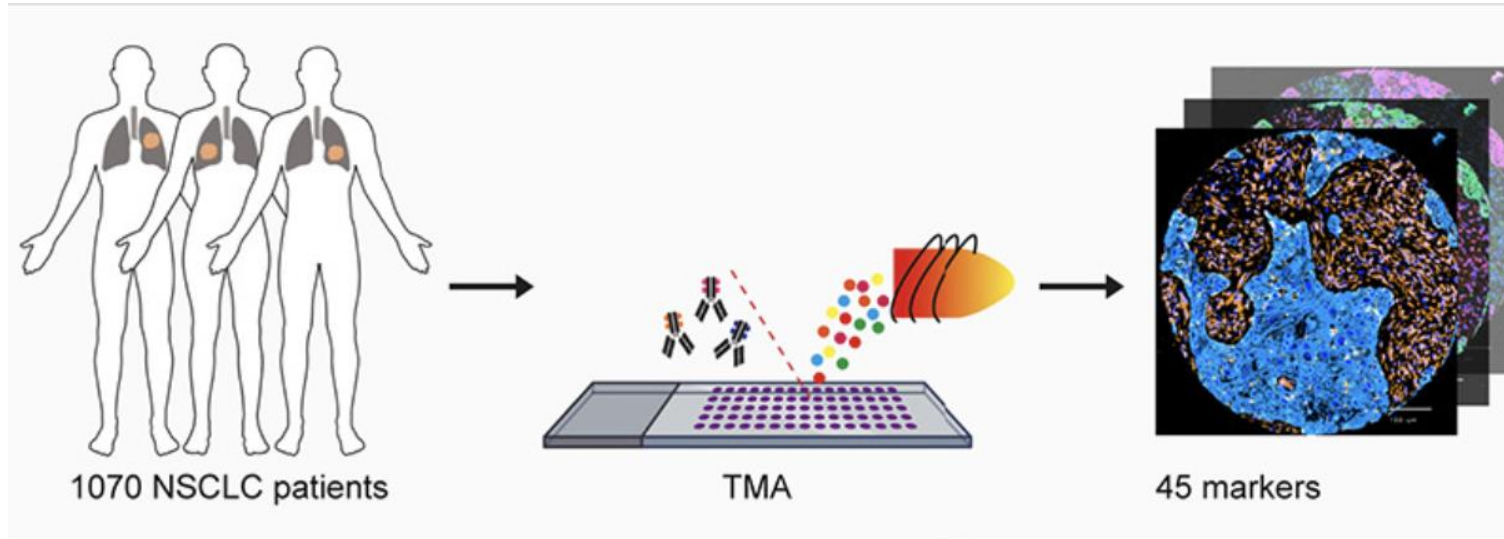
<https://github.com/AI4SCR/ATHENA>

Modeling the TME with **Graph Representation Learning**



Post-hoc explainers are not consistent

Publicly available NSCLC IMC dataset (Cords et al., 2024).



58% LUAD, 36% LUSC

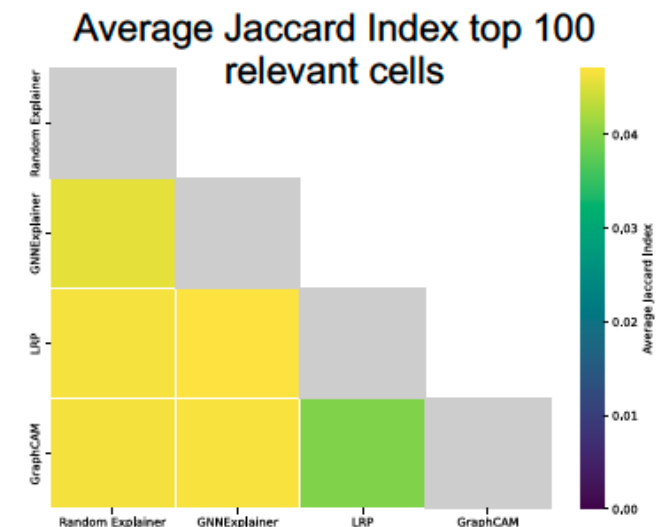
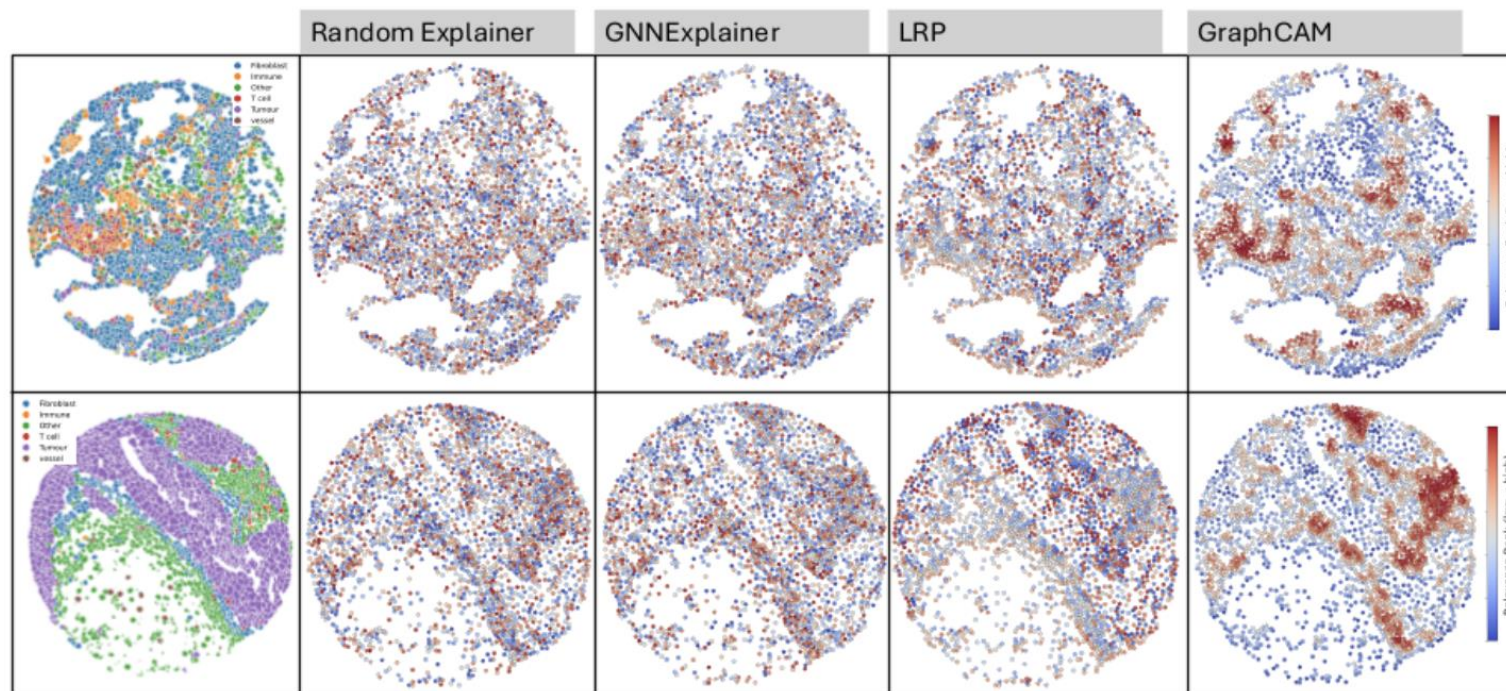


Theo Maffei

Predict LUAD vs. LUSC

Model	metric	
	F1 weighted	F1 macro
MLP	0.641 ± 0.005	0.635 ± 0.013
GCN	0.715 ± 0.007	0.704 ± 0.004
GAT	0.760 ± 0.016	0.752 ± 0.015
GIN	0.723 ± 0.013	0.710 ± 0.029

Post-hoc explainers are not consistent



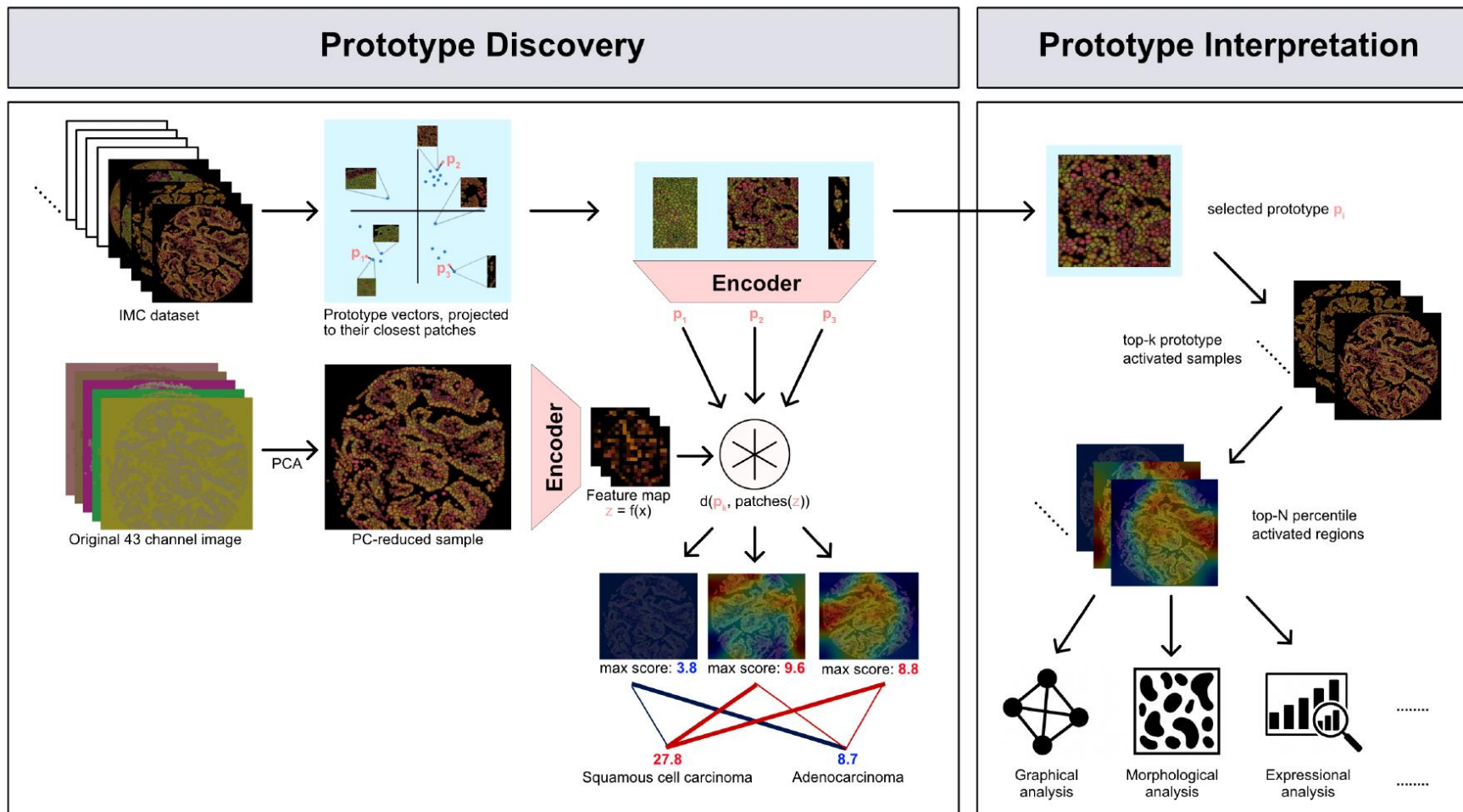
Theo Maffei

Although GNN-based models achieves an F1-weighted score of 0.76, post hoc explainers exhibit limited agreement

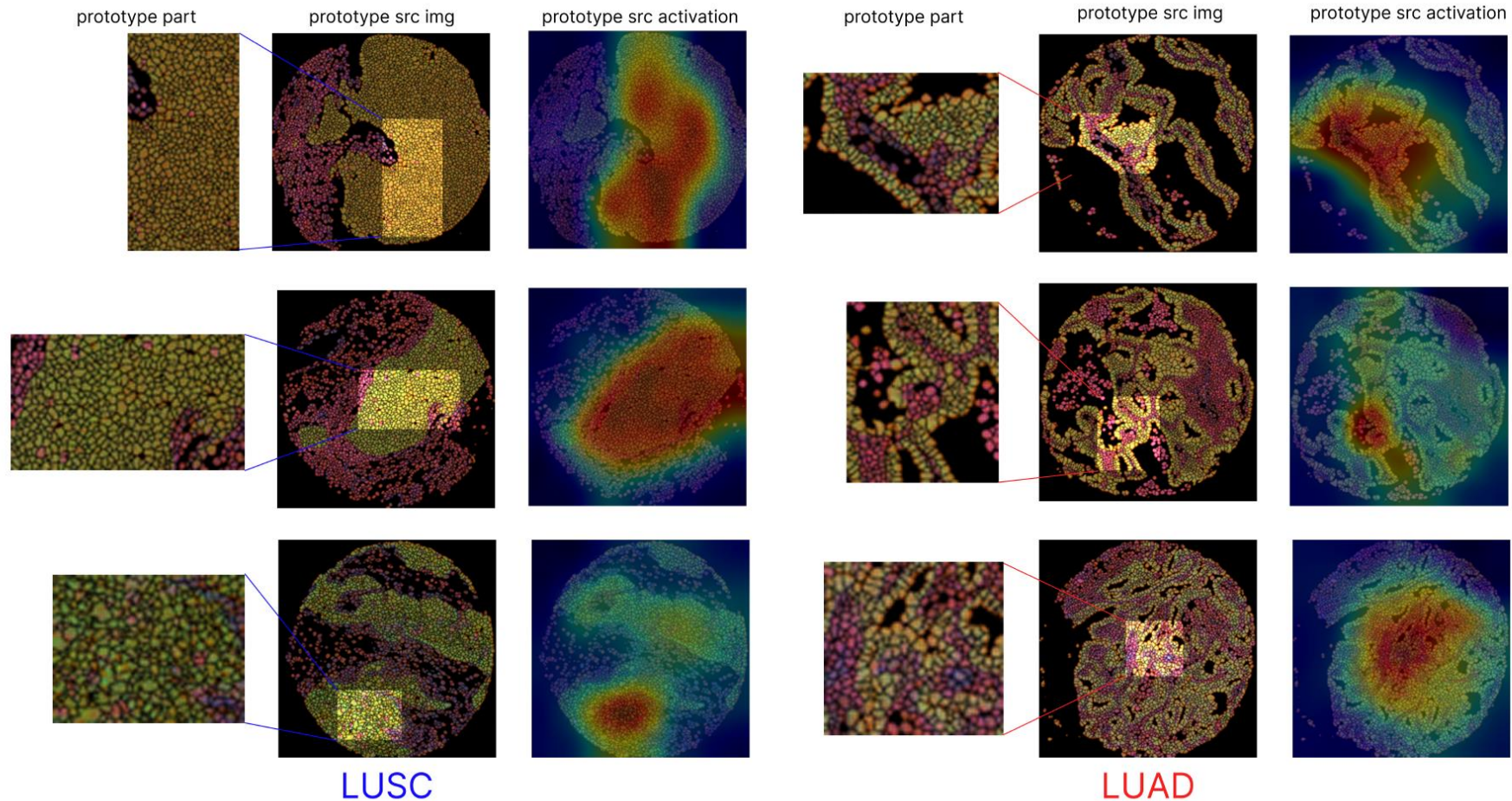
ProteinPNet: Prototypical Part Networks for Concept Learning in Spatial Proteomics



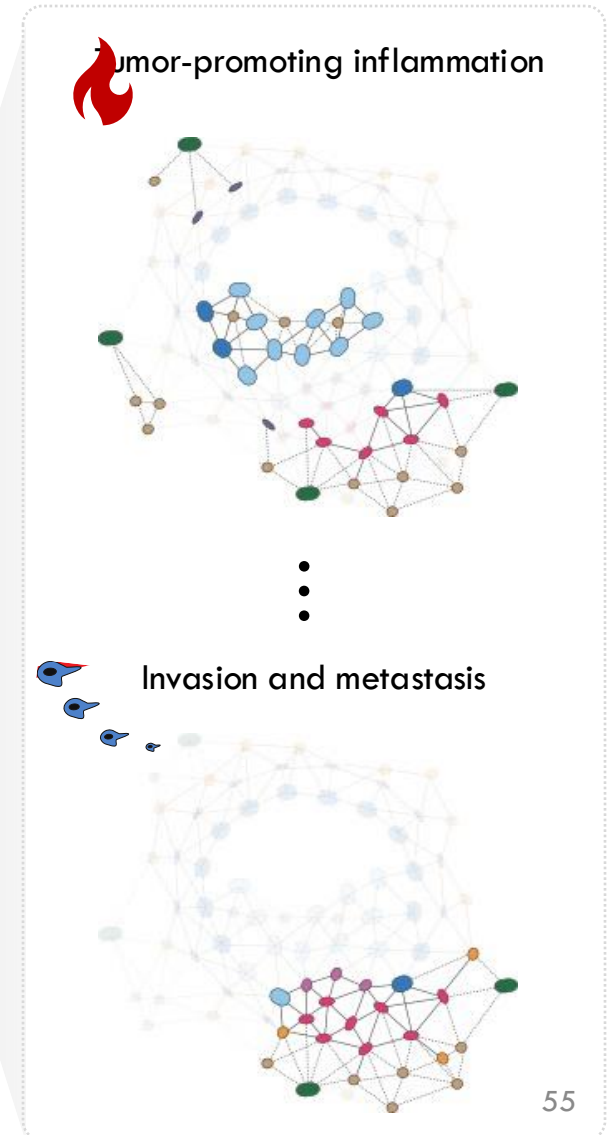
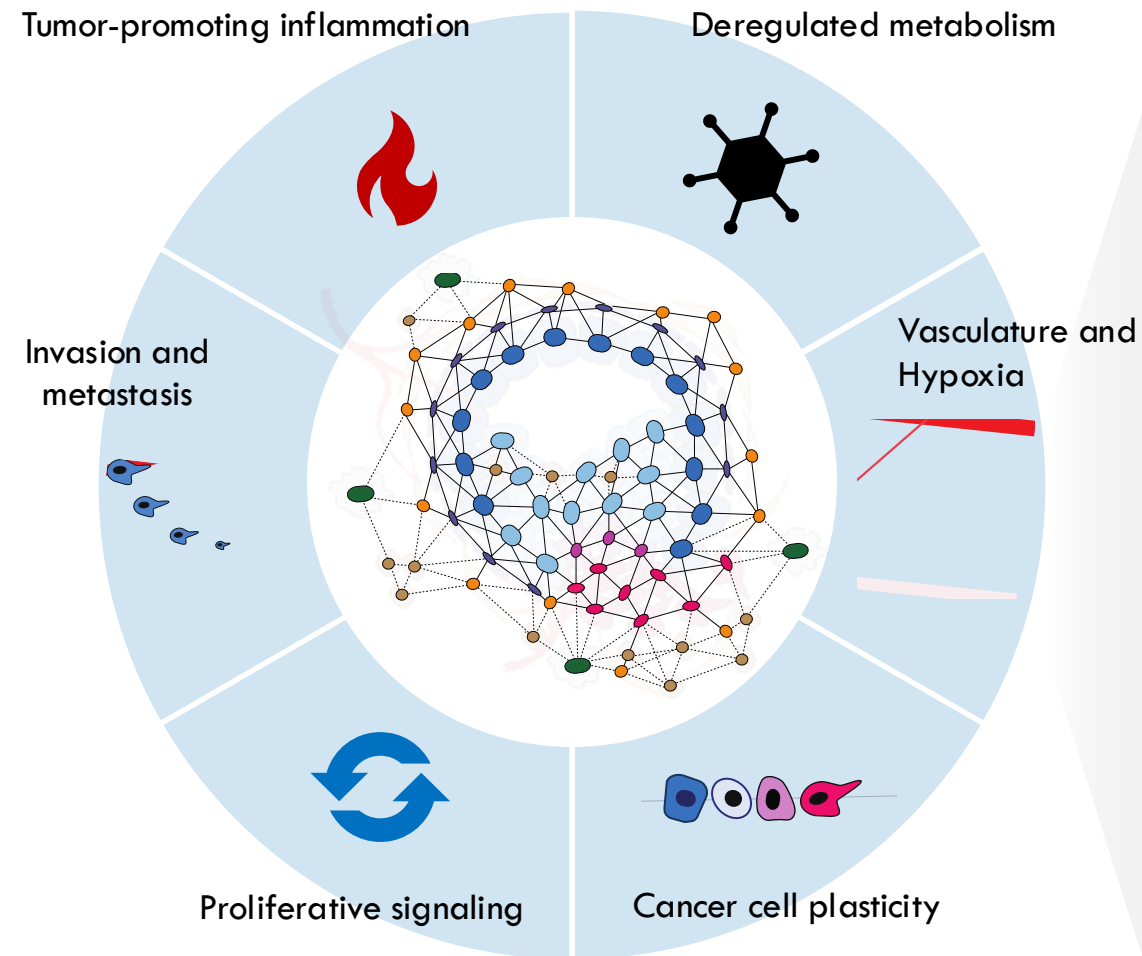
Louis McConnell



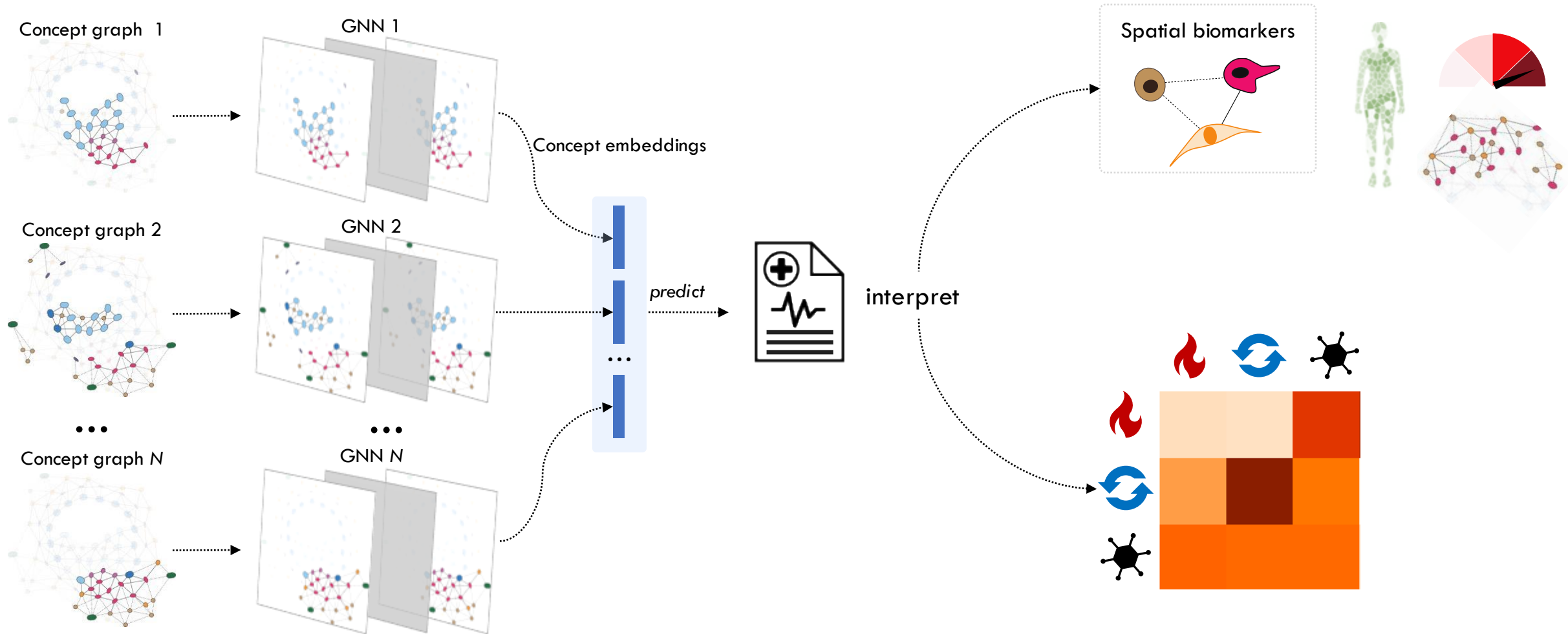
ProteinPNet: Prototypical Part Networks for Concept Learning in Spatial Proteomics



From TME complexity to interpretable concepts



From TME complexity to interpretable concepts



MOSAIC: the world's largest spatial multiomic dataset in oncology

**mosaic**
an owkin initiative

Spatial transcriptomics

Single-cell RNA-Seq

Bulk RNA-Seq

Whole Exome Sequencing

Digitized H&E

Clinical data

9	Cancer indications	2,055	Total patients included
6	Data modalities	1,833	Spatial omics data generated
100	Clinical variables per patient	1,449	Single-cell omics generated

OWKIN
Owkin uses artificial intelligence (AI) to find the right treatment for every patient.

Uniklinikum Erlangen
Since 1815, Erlangen University hospital has operated at the frontier of healthcare innovation.

CHUV
Centre hospitalier universitaire vaudois
The CHUV, since 2019 ranked among the best 15 hospitals worldwide by Newsweek, is one of the five Swiss universities.

GUSTAVE ROUSSY
CANCER CAMPUS GRAND PARIS
Leading Cancer Center in Europe, ranked third best oncology hospital in the world, according to Newsweek in 2023.

CHARITÉ
UNIVERSITÄTSMEDIZIN BERLIN
The Charité is the medical faculty of the Humboldt University and the Free University of Berlin.

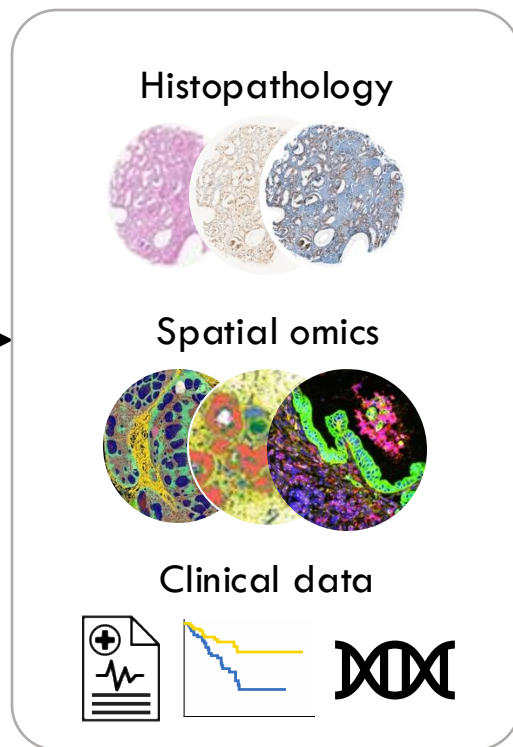
University of Pittsburgh
A top-ranked, public institution in the U.S.

Collaboration with Prof. Raphael Gottardo (BDSC), Dr. Krisztian Homicsko (Dept. of Oncology, CHUV), Prof. Laurence de Laval (Dept. Pathology, CHUV)

Team members: Sari Issa, Theo Maffei, Spencer Watson, Jonathan Bac

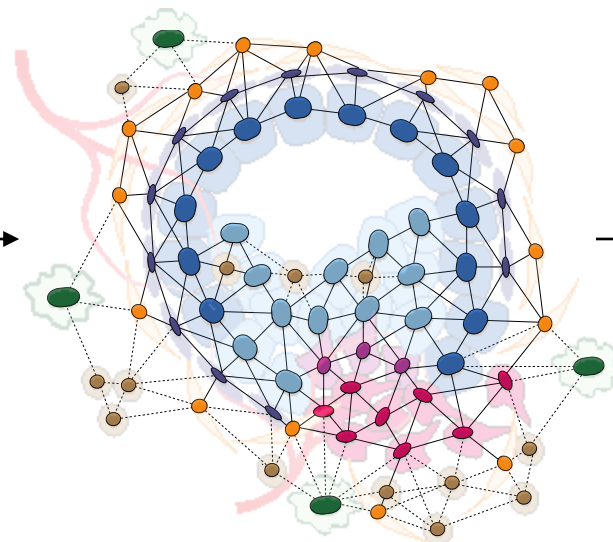


Represent



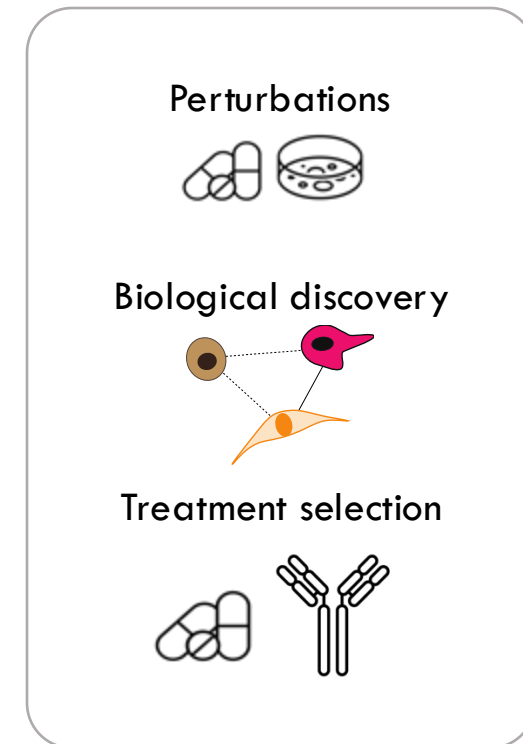
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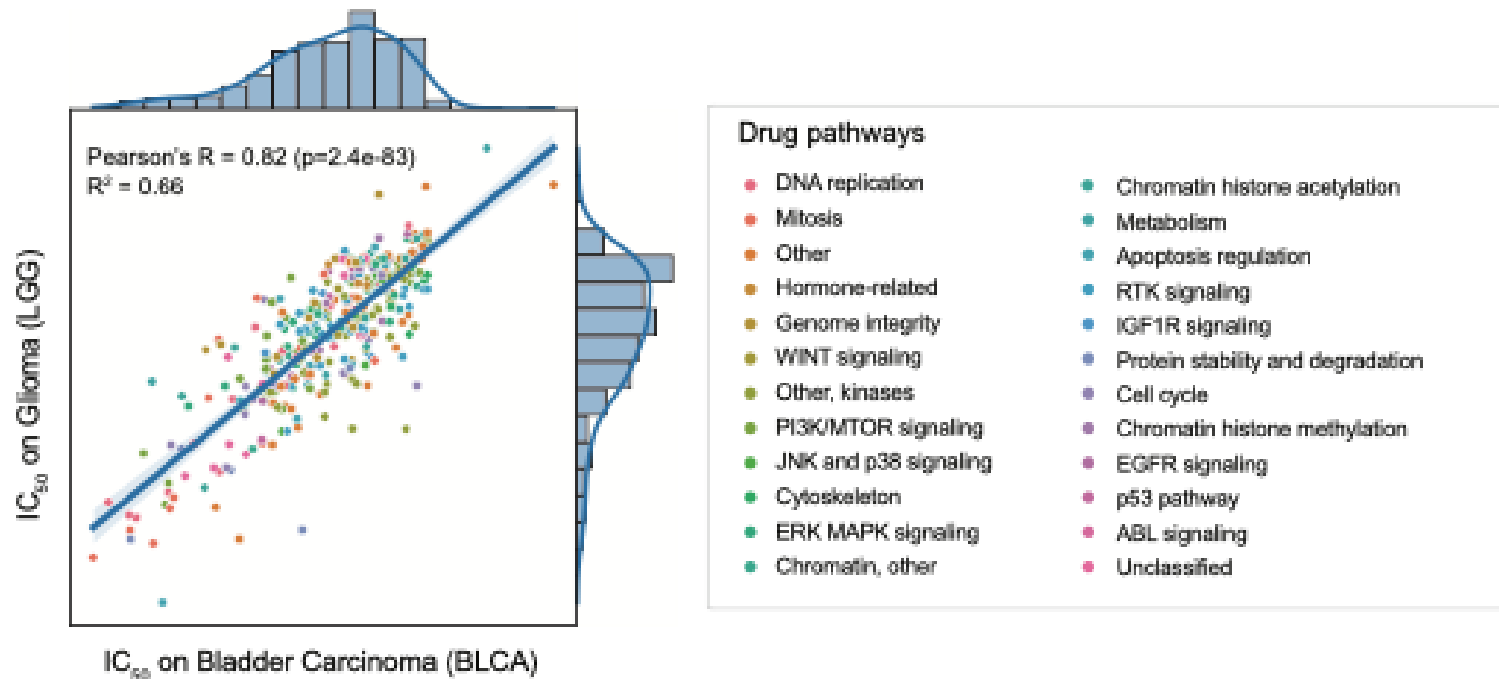
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Perturb



How can we predict the effects of drug **perturbations**?

High correlations of drug response metrics between cell lines of distinct origins

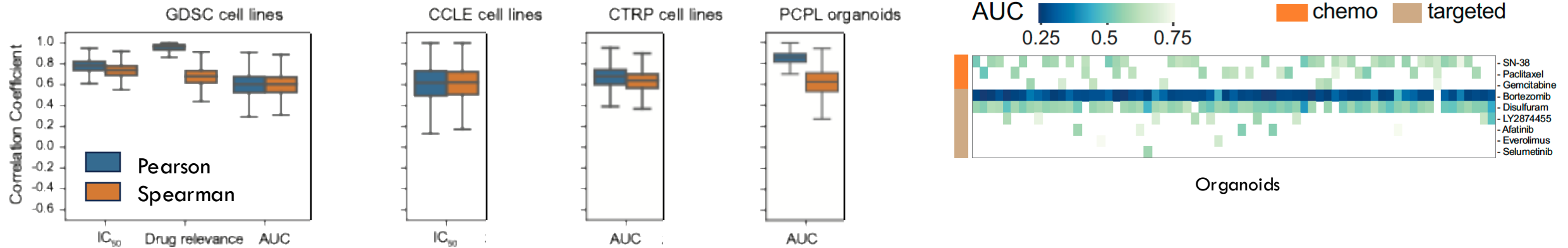


**u^b UNIVERSITÄT
BERN**

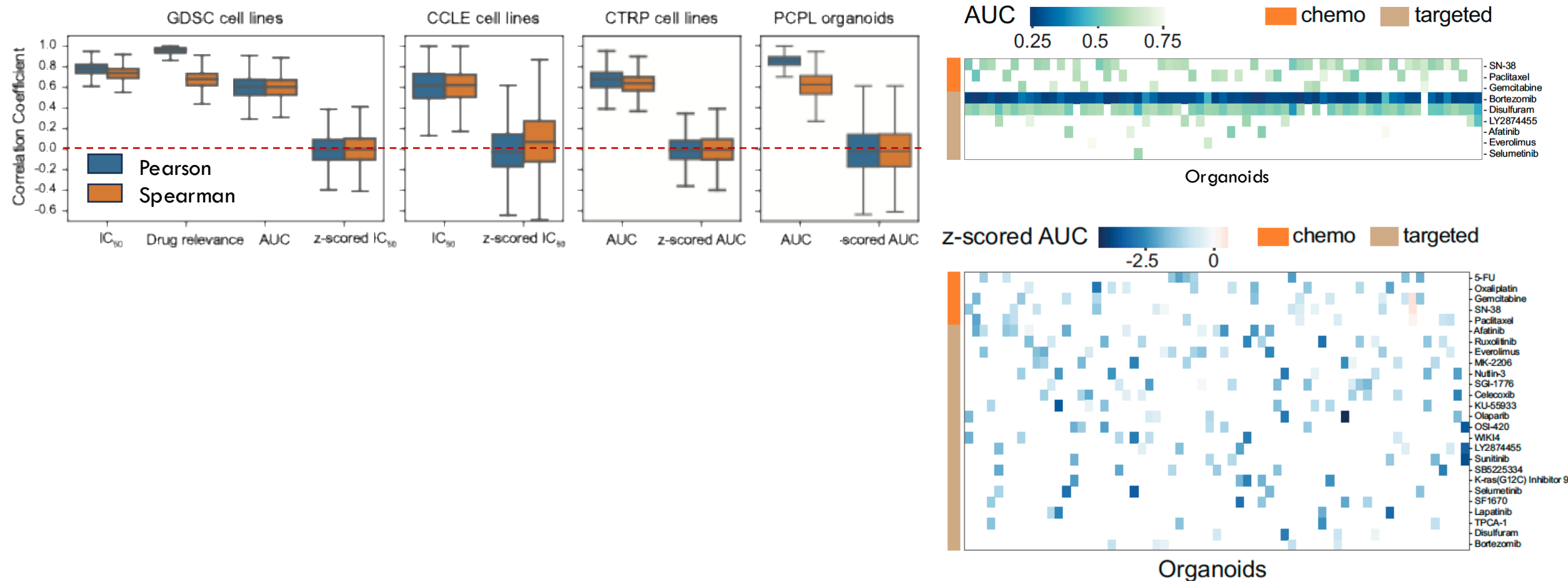
Katia Ovchinnikova
Marianna Kruithof-de Julio

IBM Research Zurich
Jannis Born

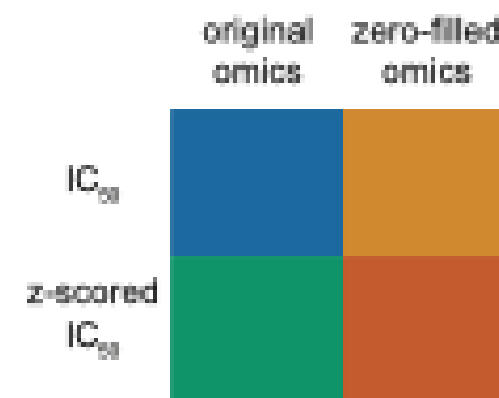
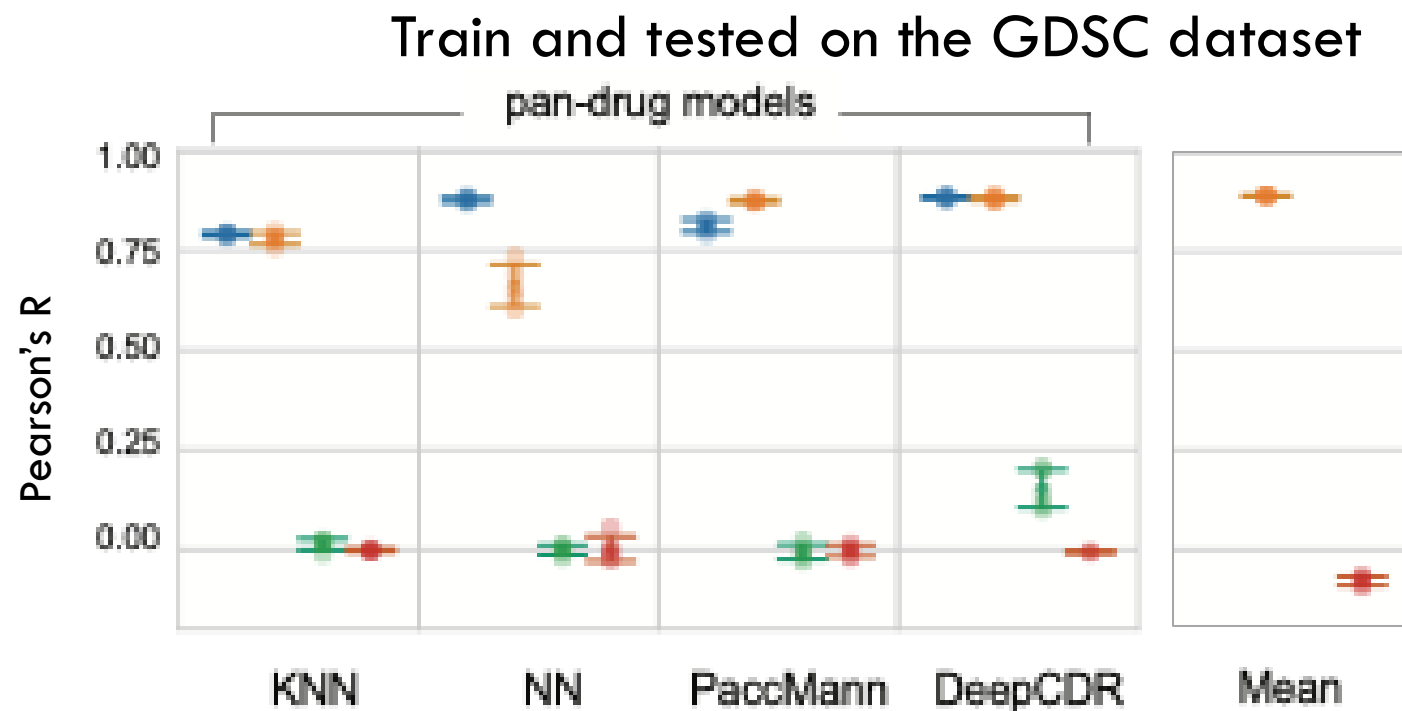
Drug response is heavily affected by the inherent **potency** or **toxicity** of each drug **independently** of the cell line/organoid it was tested on



Z-score normalization for all values separately for each drug removes the drug-specific bias

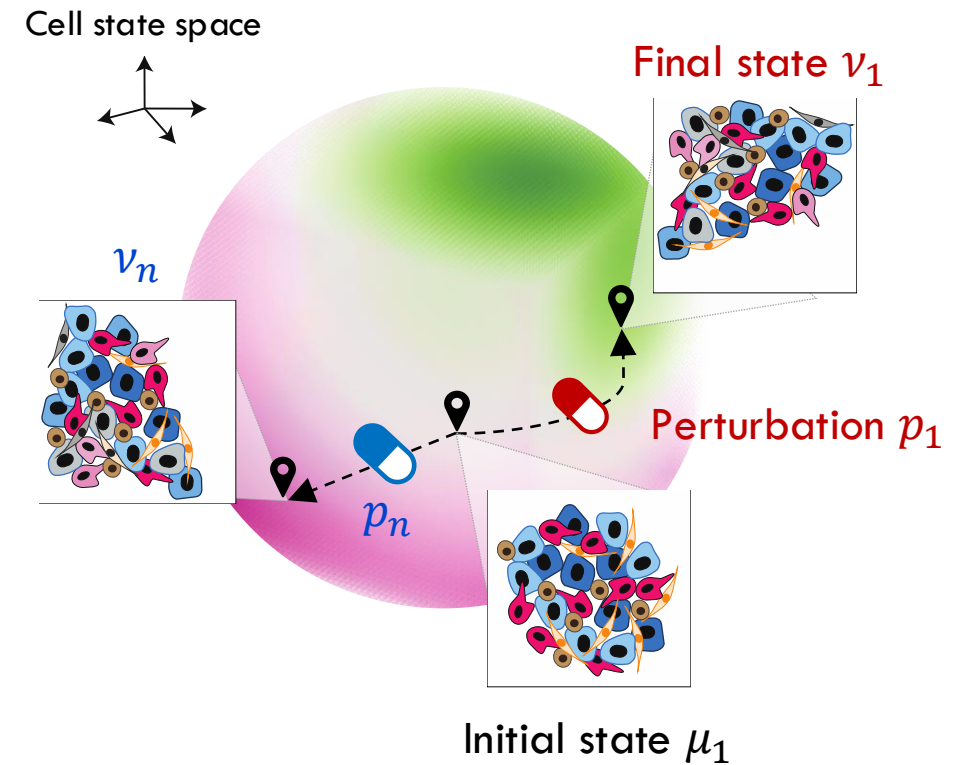


AI models are heavily affected by these issues!



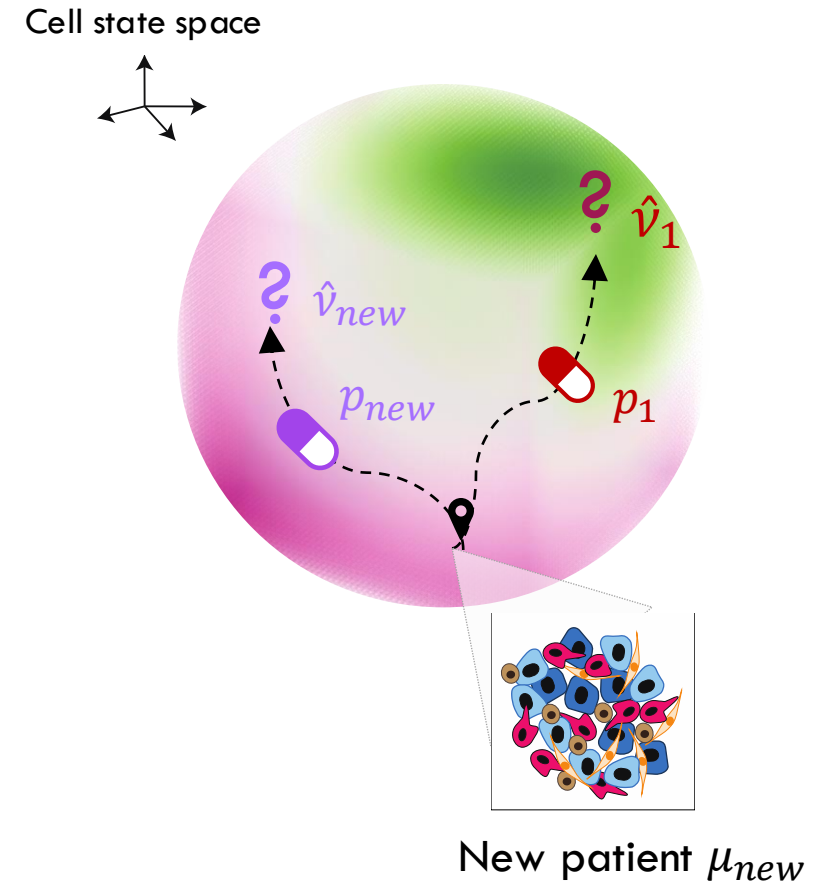
Predicting perturbation effects at the single-cell level

- **Challenge:** scRNA-seq measurements are destructive, no direct pairing between cells
- **Input:** a dataset of *before* & *after* cell states coupled to perturbations $(p_i(\mu_i, v_i))$



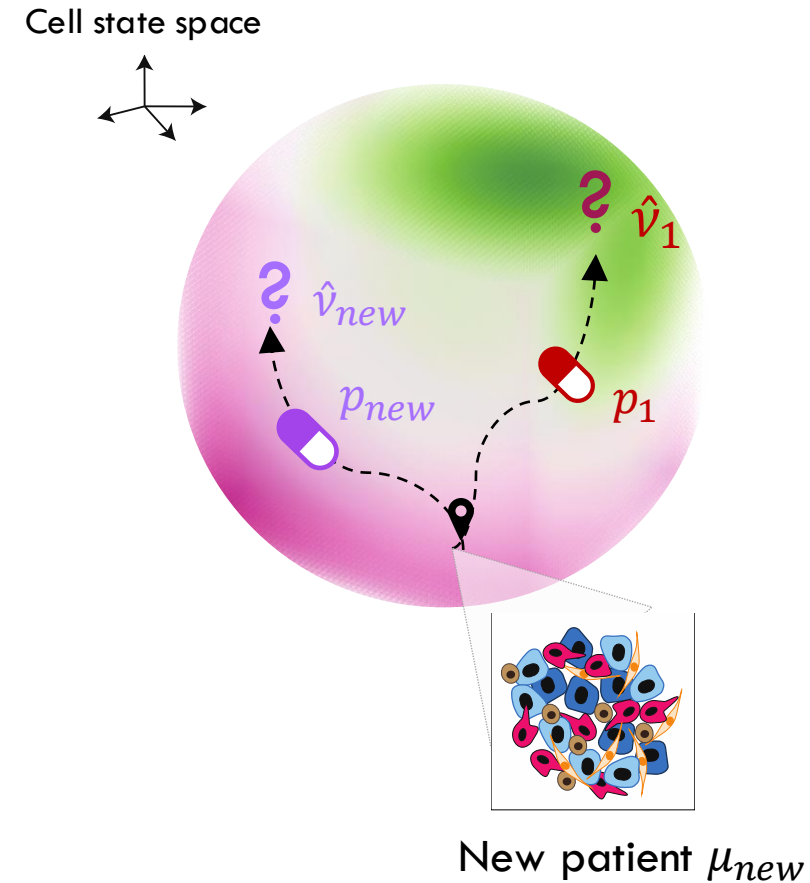
Predicting perturbation effects at the single-cell level

- **Challenge:** scRNA-seq measurements are destructive, no direct pairing between cells
- **Input:** a dataset of *before* & *after* cell states coupled to perturbations $(p_i(\mu_i, v_i))$
- **The problem:** Given an unseen initial state μ_{new} , predict the final state $\hat{v}_1$ after known perturbation p_1 or predict the final state $\hat{v}_{new}$ after unseen perturbation p_{new}



Predicting perturbation effects at the single-cell level

- **CMonge***: Use conditional Optimal Transport (OT) to learn transportation maps M_k conditioned on covariates (e.g., dosage, drug, or cell type)



Jannis Born



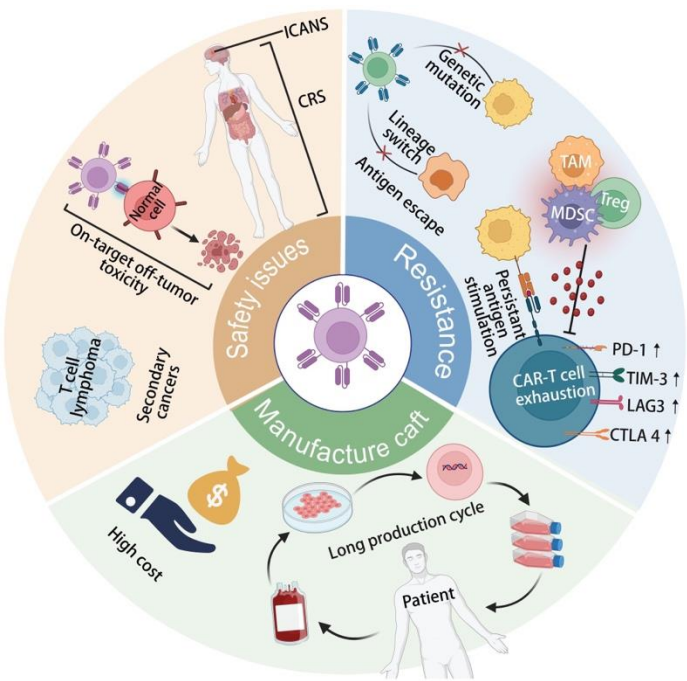
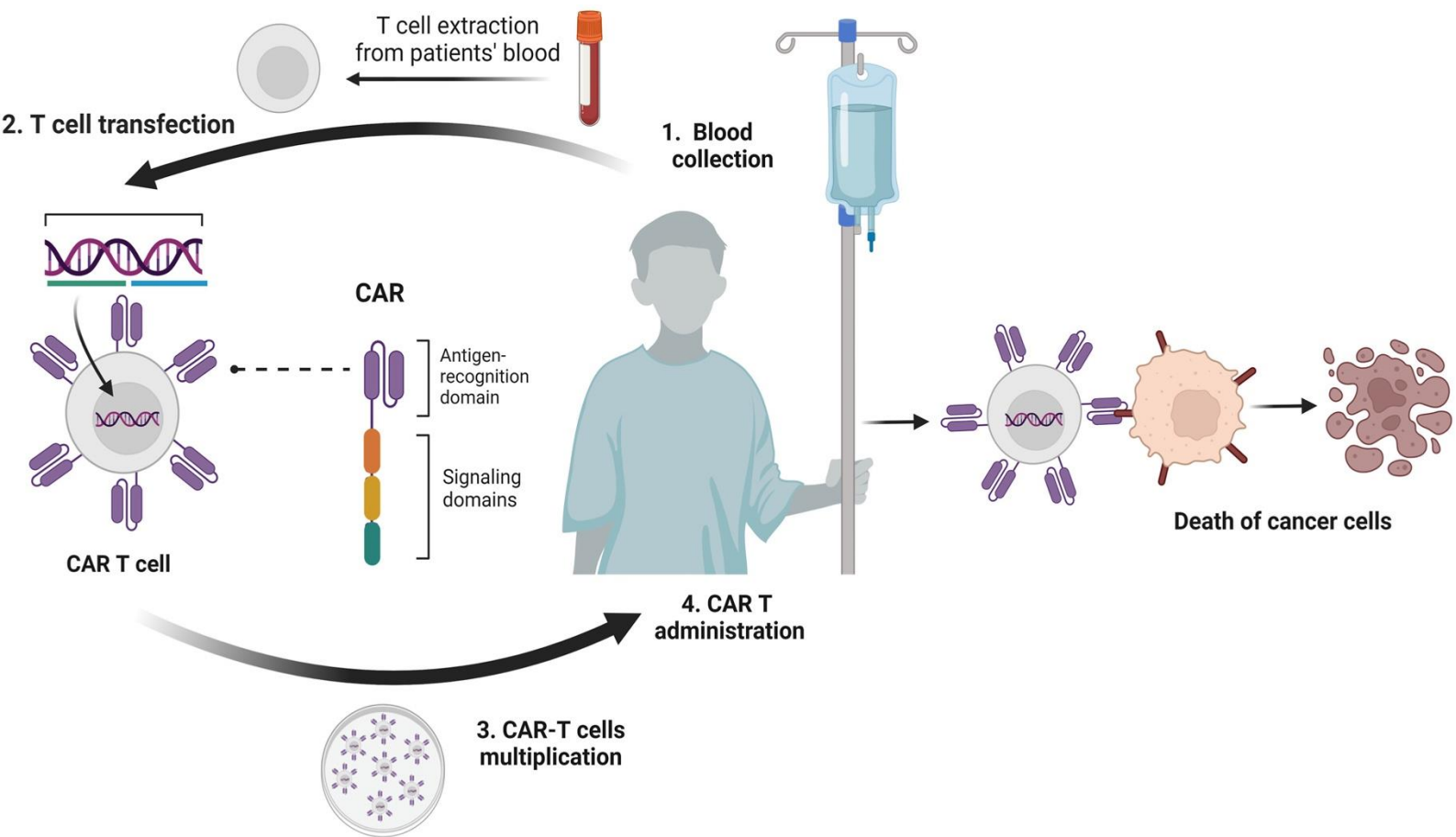
Benedek Harsanyi



Alice Driessen

*Driessen *et al.* (under review) arXiv:2504.08328

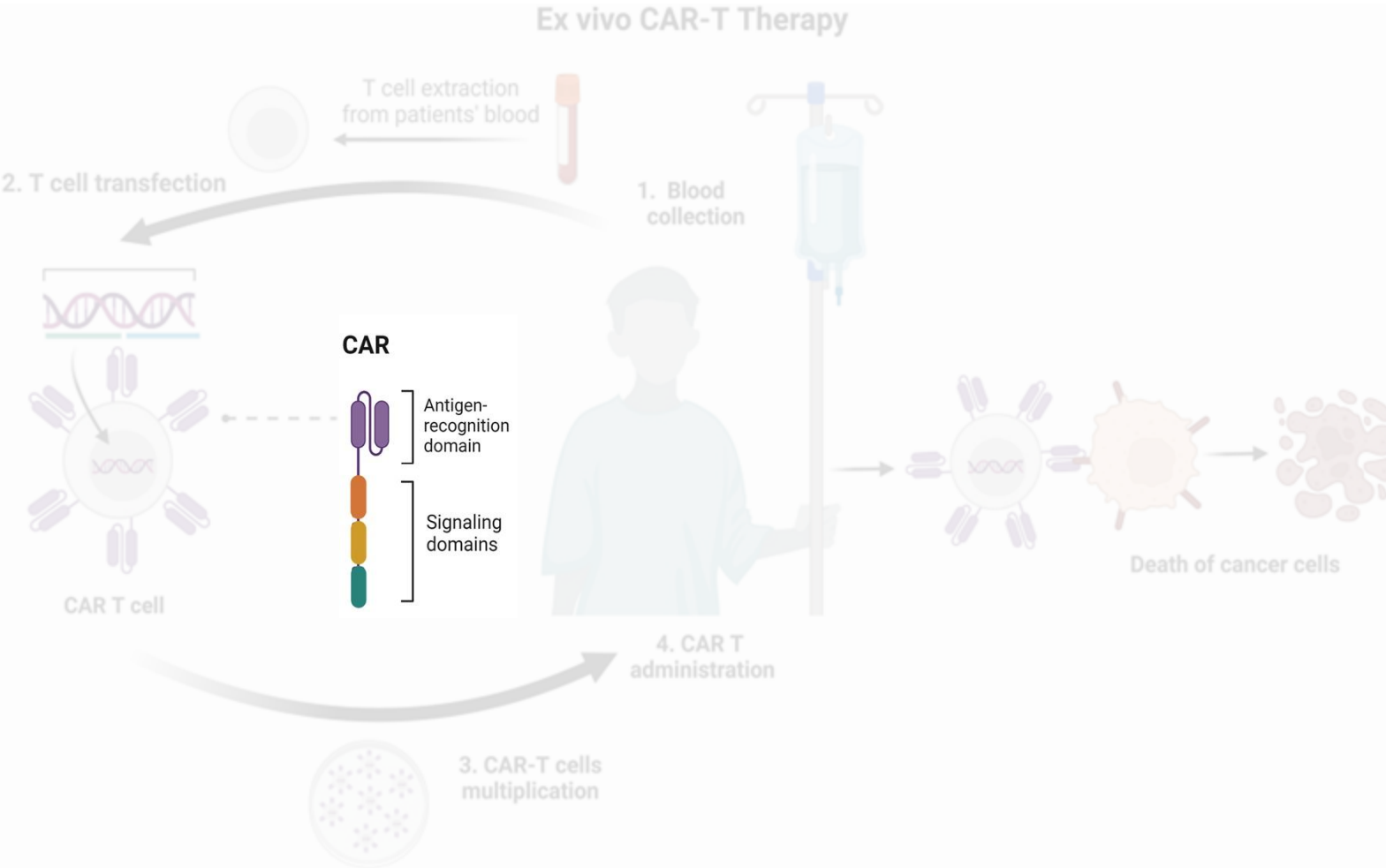
Modeling responses to CAR T cell therapy

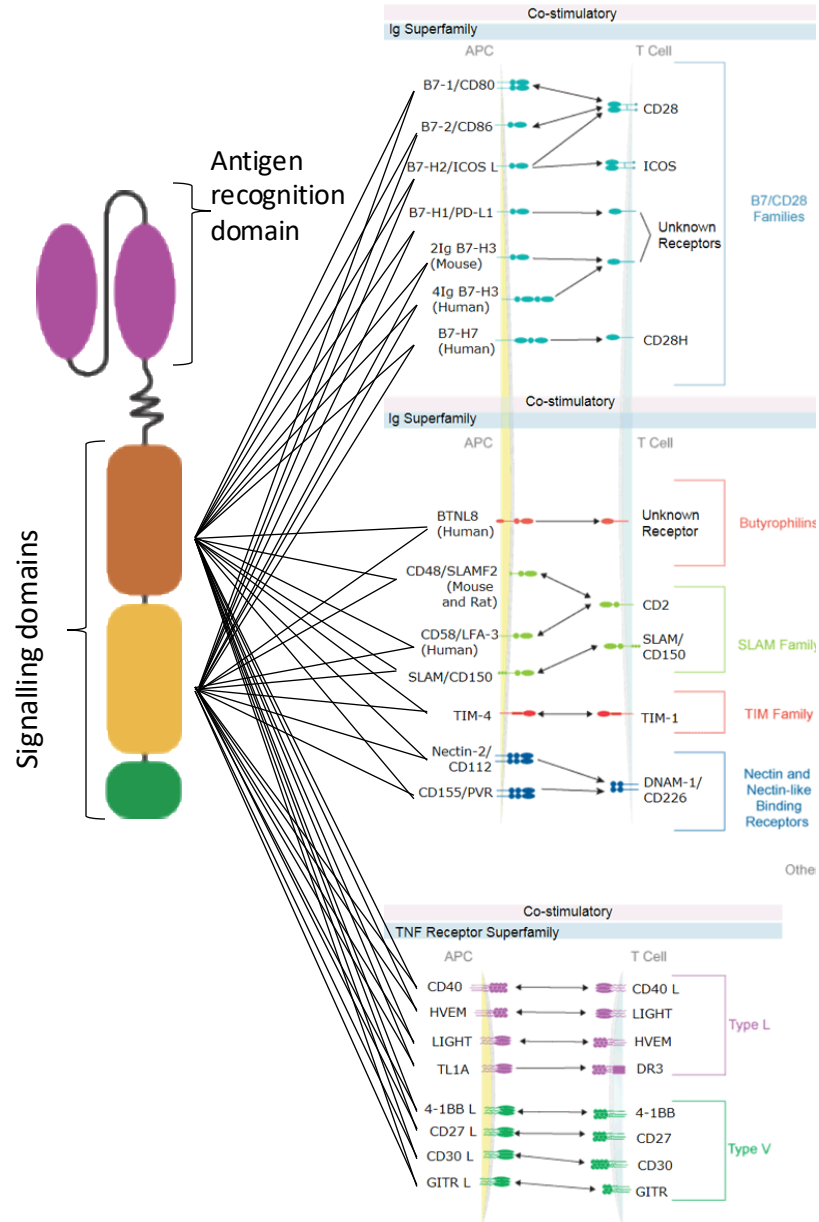


Li Ying et al. Frontiers in Immunology 2024

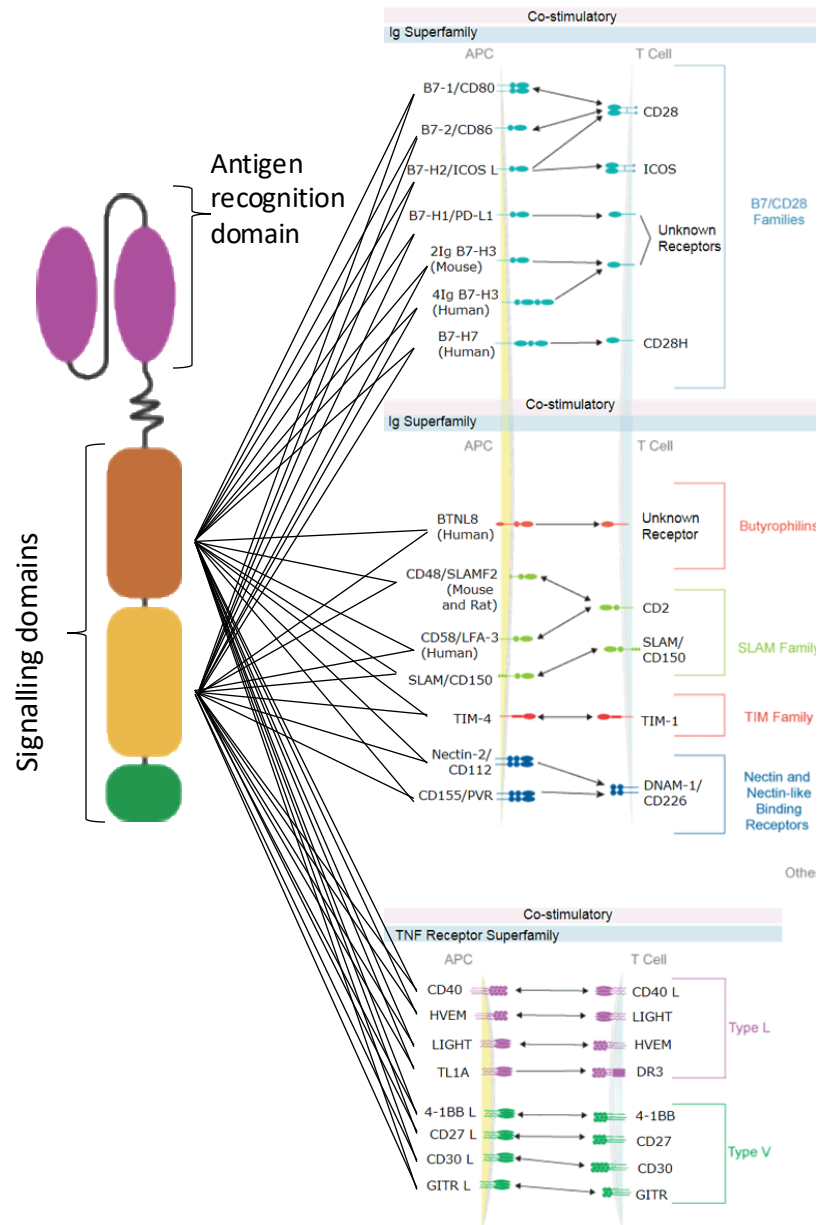
Bui, Thuy Anh et al. eBioMedicine 2024

Modeling responses to CAR T cell therapy

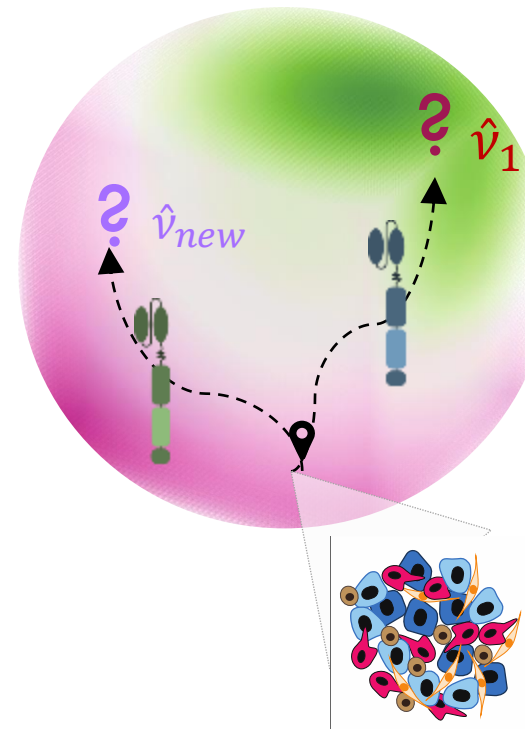




>100'000 possible CARs



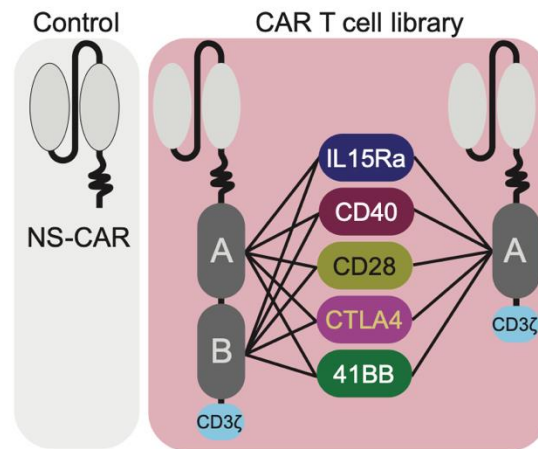
>100'000 possible CARs



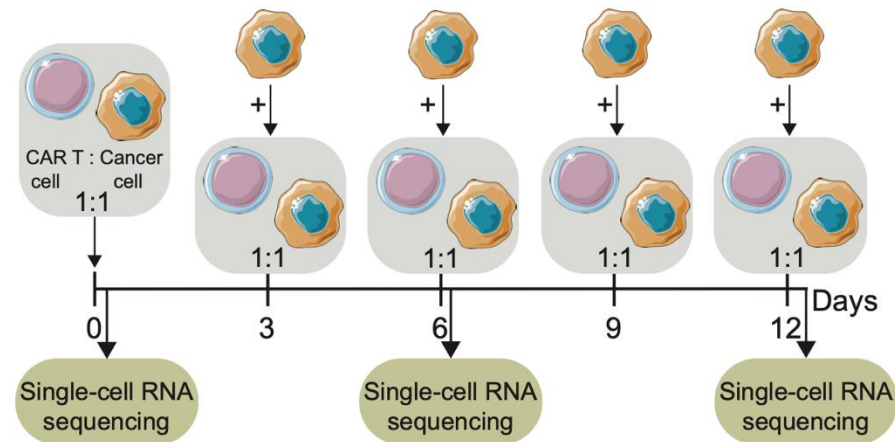
Modeling responses to CAR T cell therapy



Alice Driessen

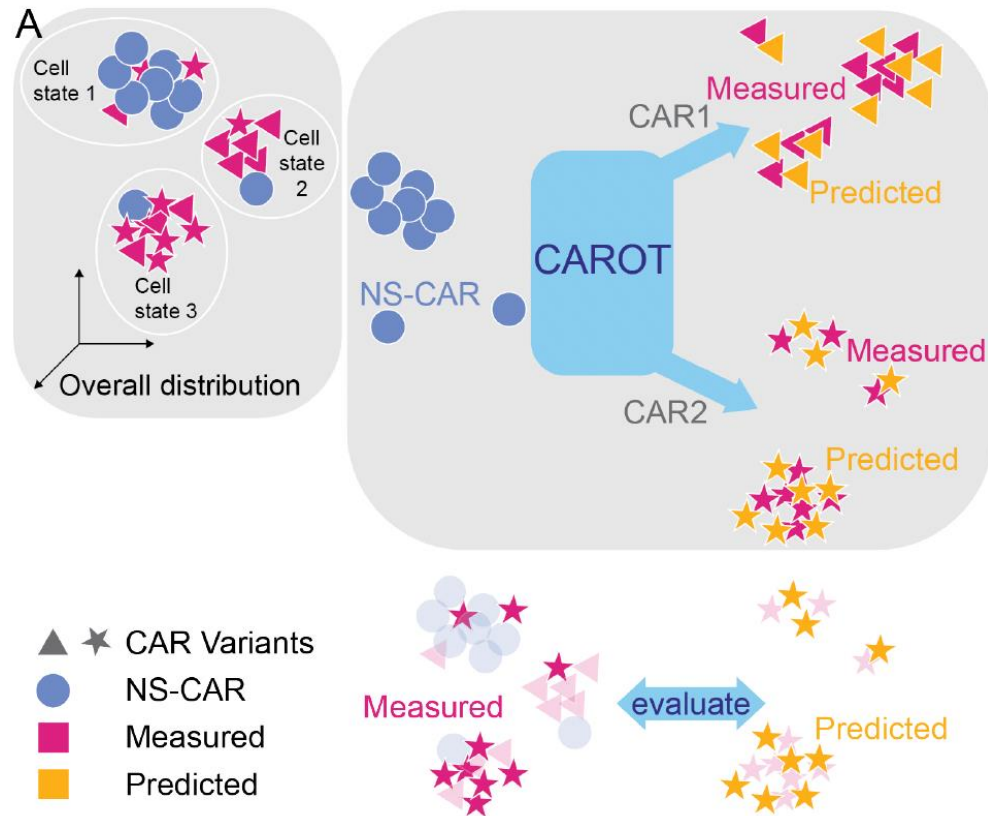


30 different CAR designs

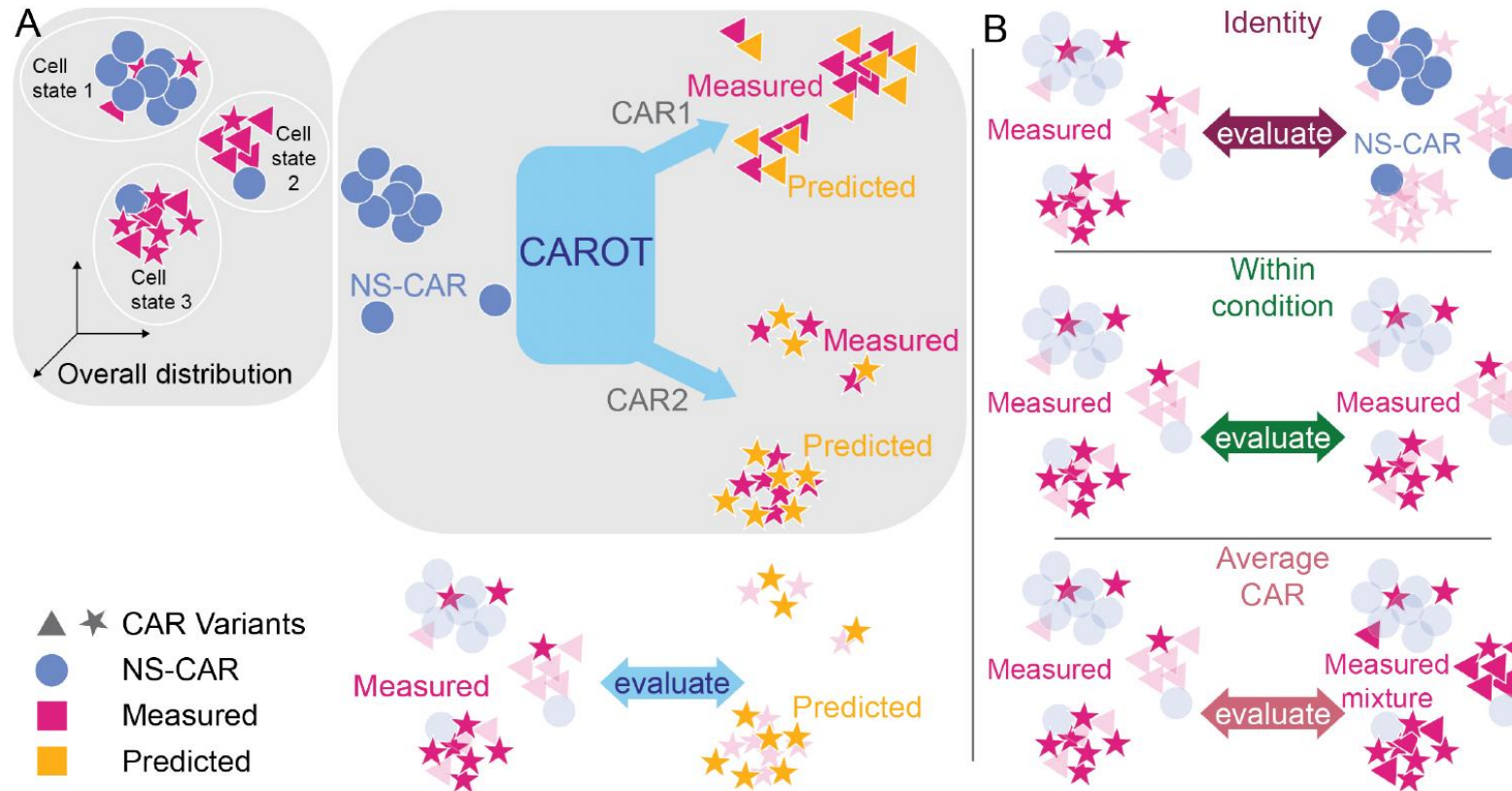


Collaboration with Prof. Sai Reddy, ETHZ BSSE

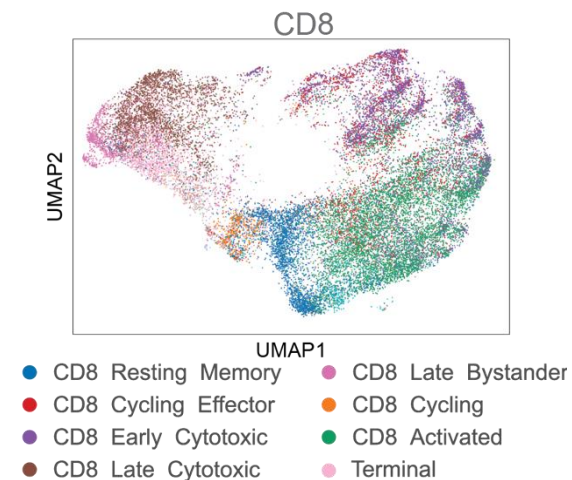
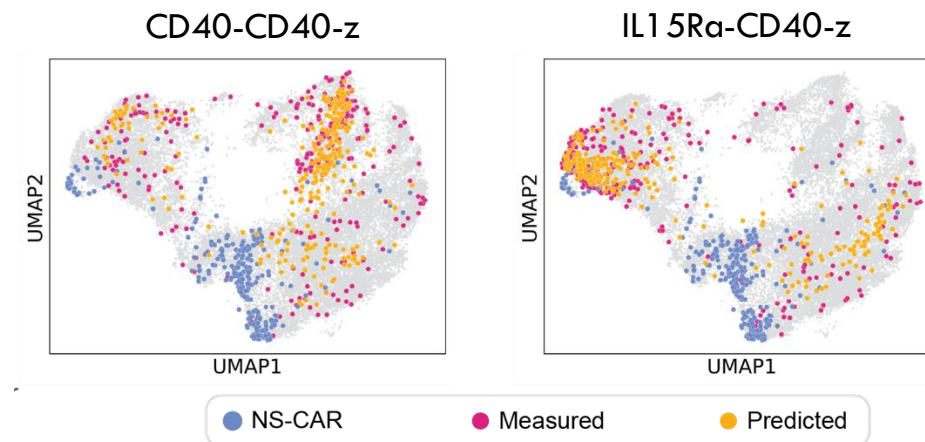
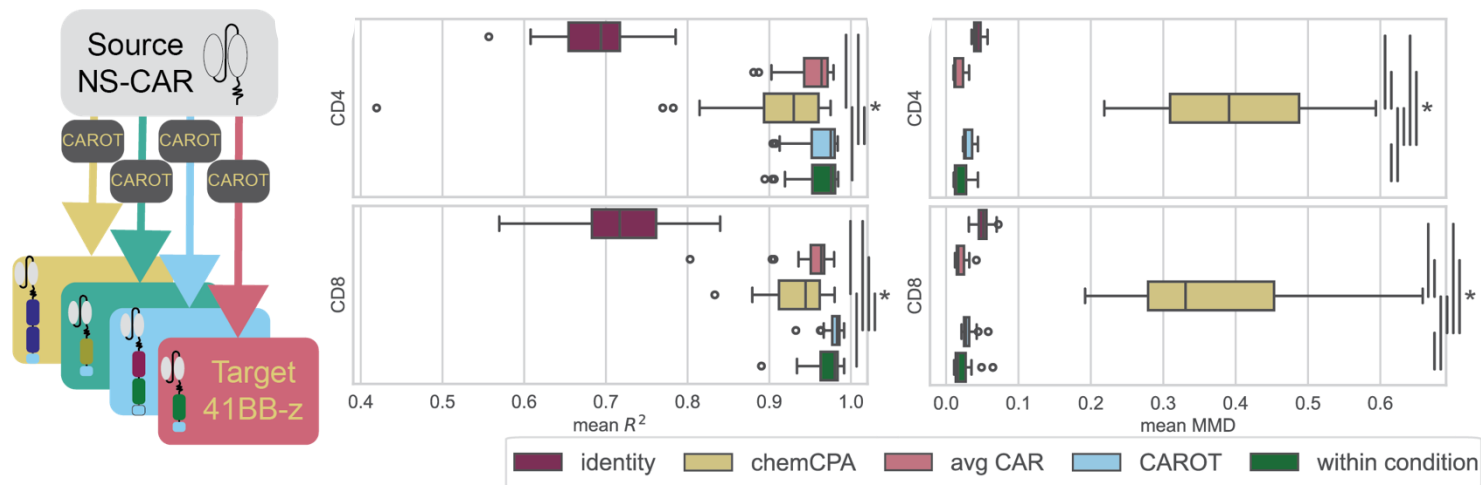
Modeling responses to CAR T cell therapy



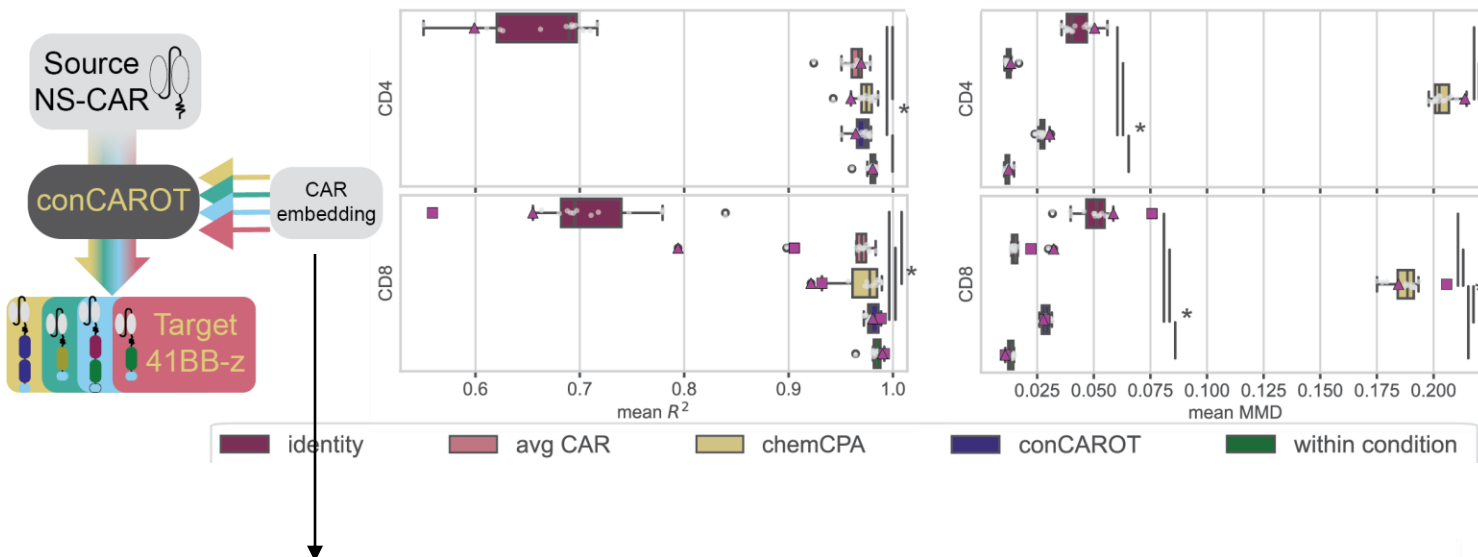
Modeling responses to CAR T cell therapy



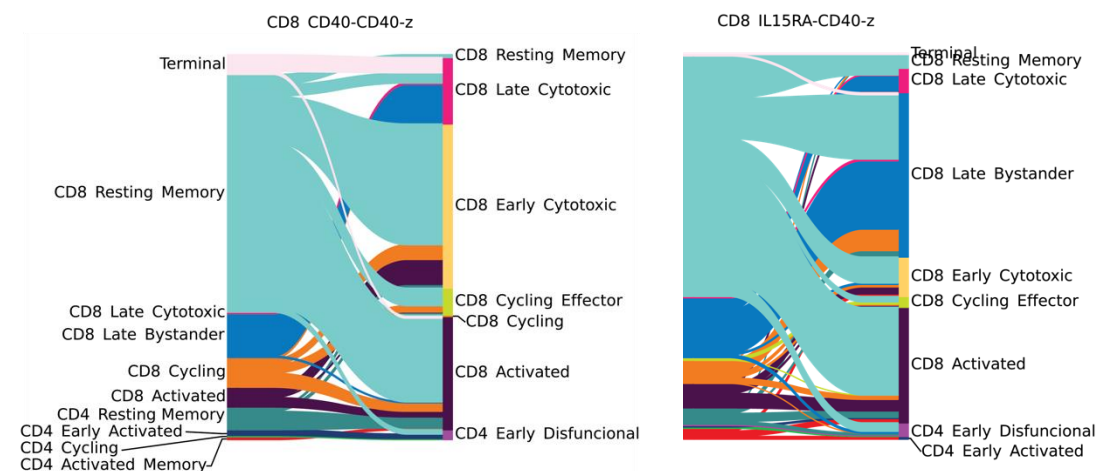
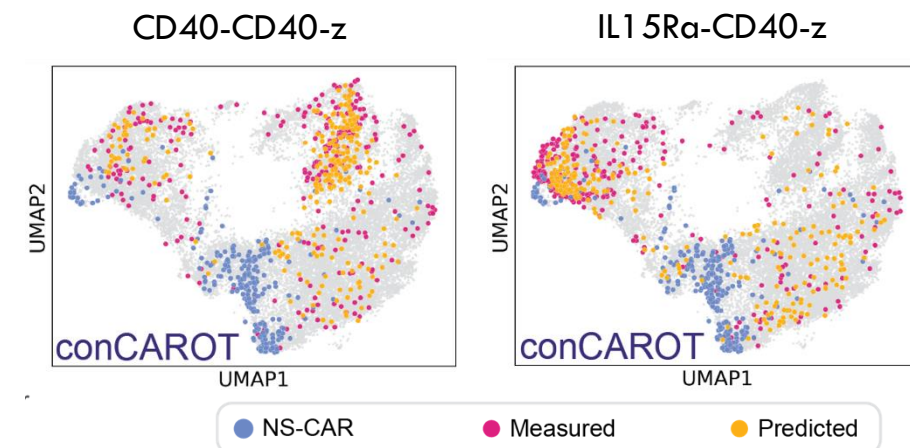
One CAROT model *per* CAR



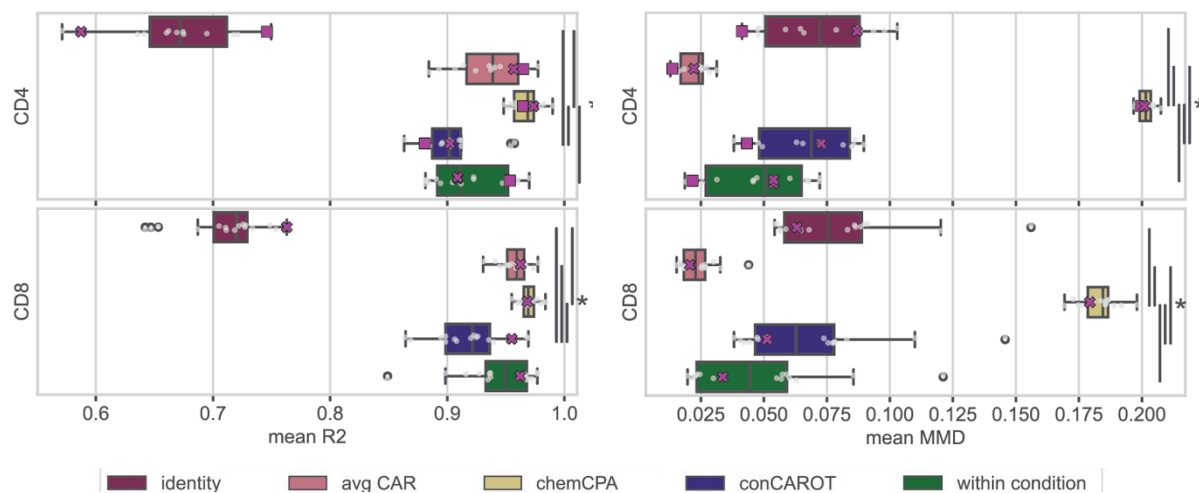
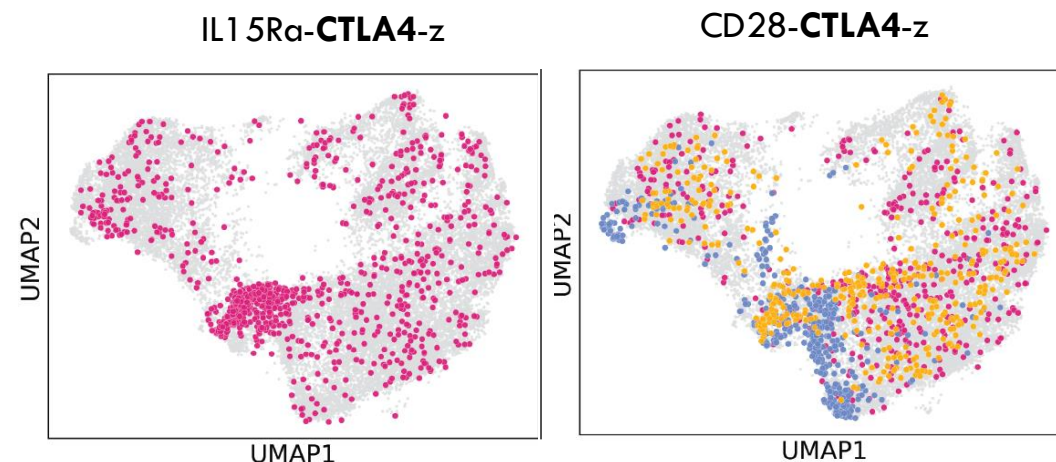
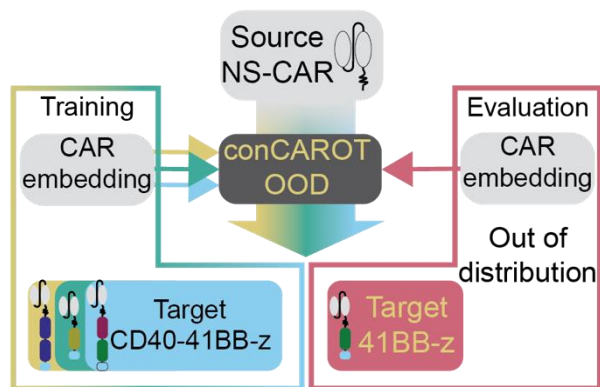
One CAROT model across all CARs



- 🥕 ESM2 CAR embedding
- 🥕 Predict novel CAR designs

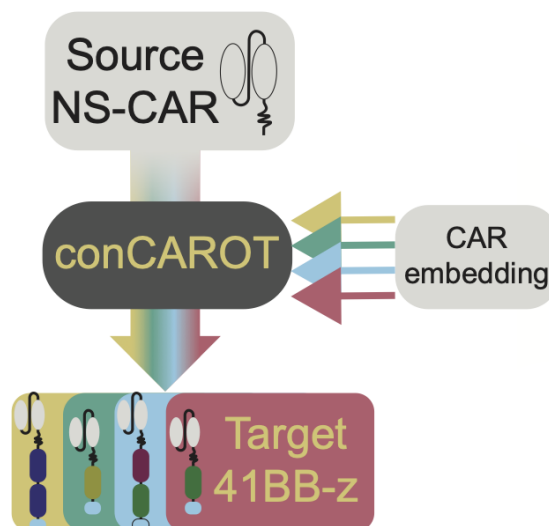


One CAROT model on *unseen* CARs





CAROT: modeling response to CAR T cell therapy with conditional OT



First single-cell generative AI CAR T cell model



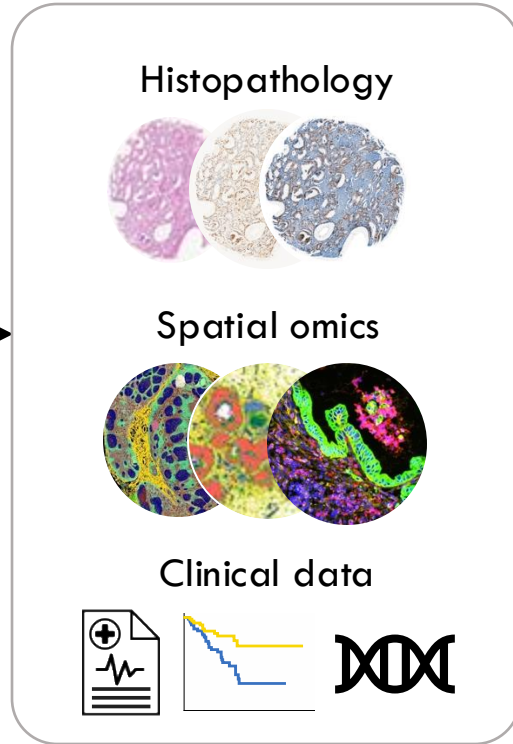
Conditional model on par with 1-1 model



ESM2 CAR embedding: Predict novel CAR designs

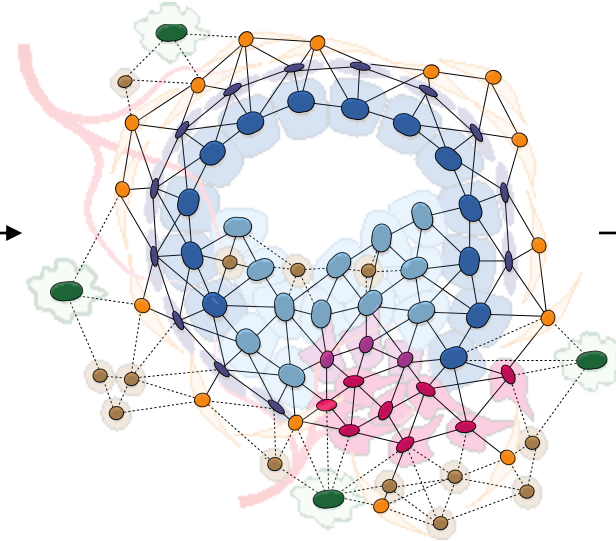


Represent



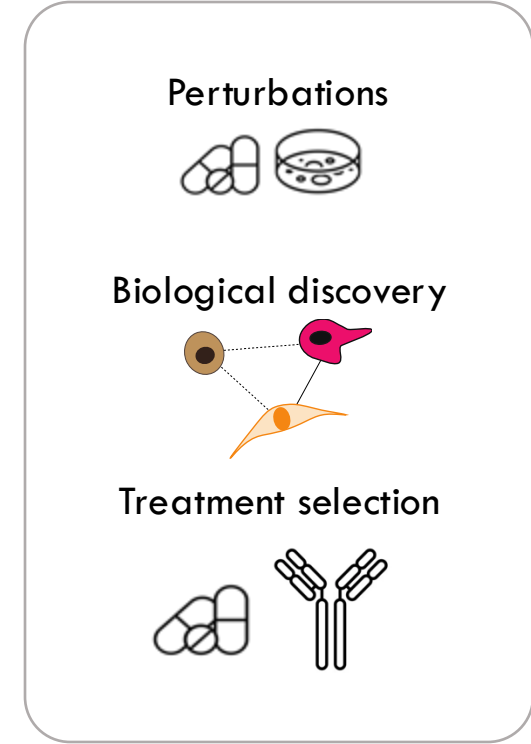
- **MatchCLOT:** Gossi et al., *Briefings in Bioinformatics*, 2023
- Precision Dermatology: Predicting molecular signatures from H&E (in prep)
- Upcoming: Multimodal Foundation models for oncology (in prep)

Interpret



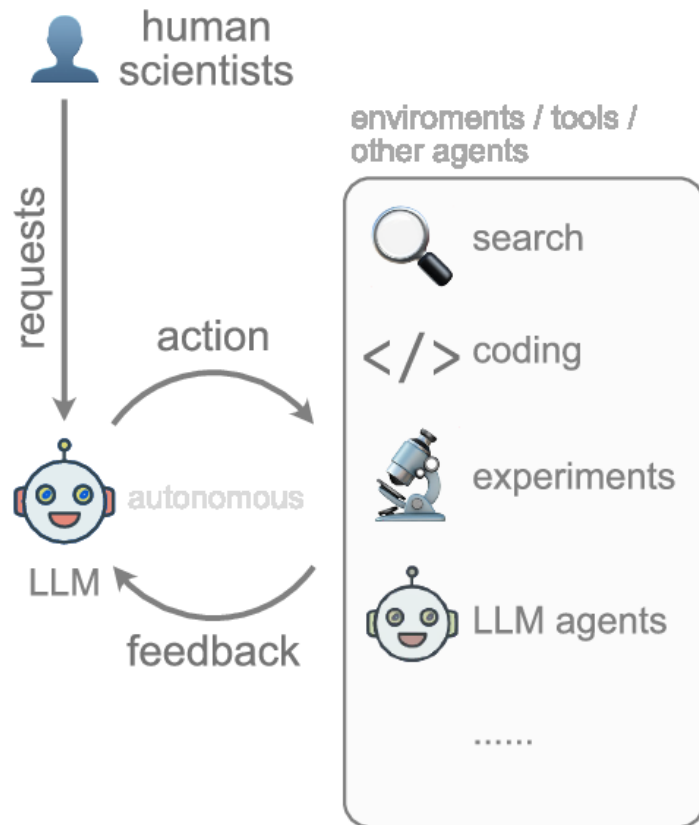
- **ATHENA:** Martinelli & Rapsomaniki, *Bioinformatics*, 2022
- ProteinPNet (McConnel, Imageomics NeurIPS, to appear)
- Concept learning and discovery (in prep)

Perturb



- **Ovchinnikova et al.,** *npj Precision Oncology*, 2024
- **CMonge:** Driessen et al., *ICML MLXGen Workshop*, arxiv, 2024
- **CAROT:** Driessen et al., *bioRxiv* 2024.11.11.622906

Agentic AI: the new frontier?



Automating scientific discovery.

We're a non-profit building AI agents to automate research in biology and other complex sciences.

Business Wire

Owkin Launches K Navigator, a Ground-breaking Agentic Co-pilot to Speed up Breakthroughs in Biomedical Research by 20x



Sam Rodriques ✓
@SGRodriques



Today, we're announcing the first major discovery made by our AI Scientist with the lab in the loop: a promising new treatment for dry AMD, a major cause of blindness.

Our agents generated the hypotheses, designed the experiments, analyzed the data, iterated, even made figures for the paper. The resulting manuscript is a first-of-a-kind in the natural sciences, in which everything that needed to be done to write the paper was done by AI agents, apart from actually conducting the physical experiments in the lab and writing the final manuscript. We are also introducing Robin, the first multi-agent system that fully automates the in-silico components of scientific discovery, which made this discovery. This is the first time that we are aware of that hypothesis generation, experimentation, and data analysis have been joined up in closed loop, and is the beginning of a massive acceleration in the pace of scientific discovery that will be driven by these agents. We will be open-sourcing the code and data next week.



AI/ML for Biomedicine



 <https://github.com/AI4SCR/> marianna.rapsomaniki@unil.ch

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Robert Berke, Fei Tang



Sai Reddy & team

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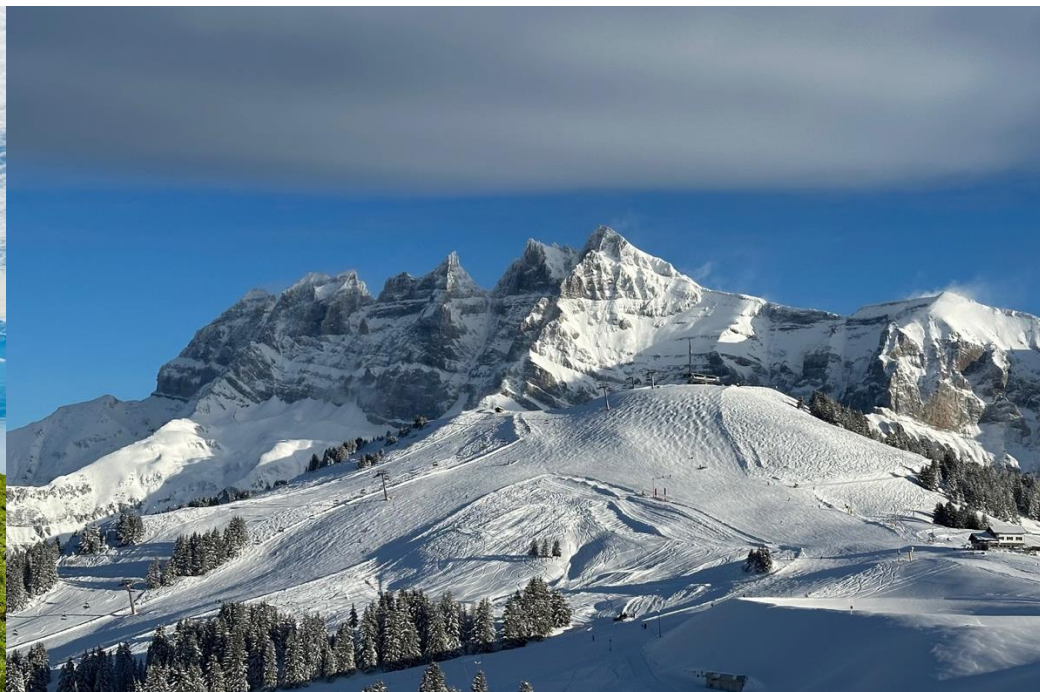
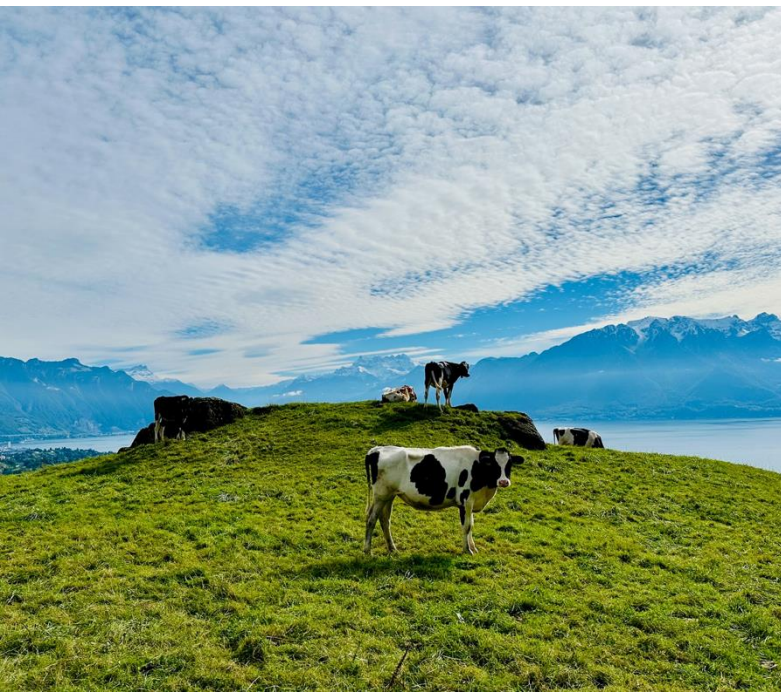
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Martin Wartenberg

University of Vienna

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