



The Smart Drug Discovery Alliance

Accelerating Decentralized AI-empowered Drug Discovery through Industry-Academia Coalitions



Zhandos Sembay, MS



Swathi Thaker, PhD



Ehsan Saghapour, PhD



Xinxin (Katie) Zhu, MD, PhD

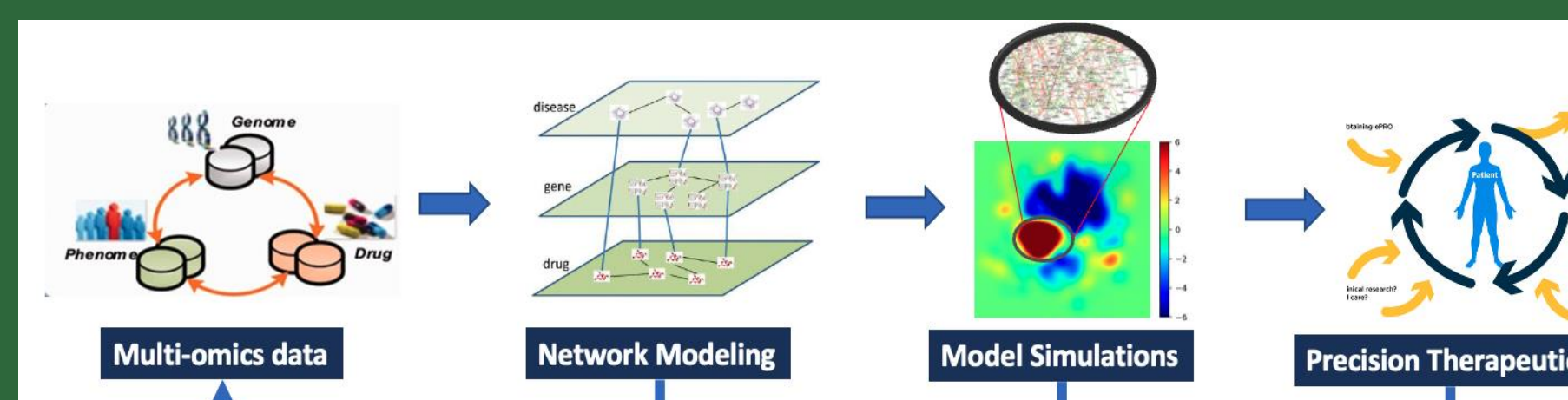


Jake Y. Chen, PhD

smartdrugdiscovery.org

AI + Drug Discovery Manifesto

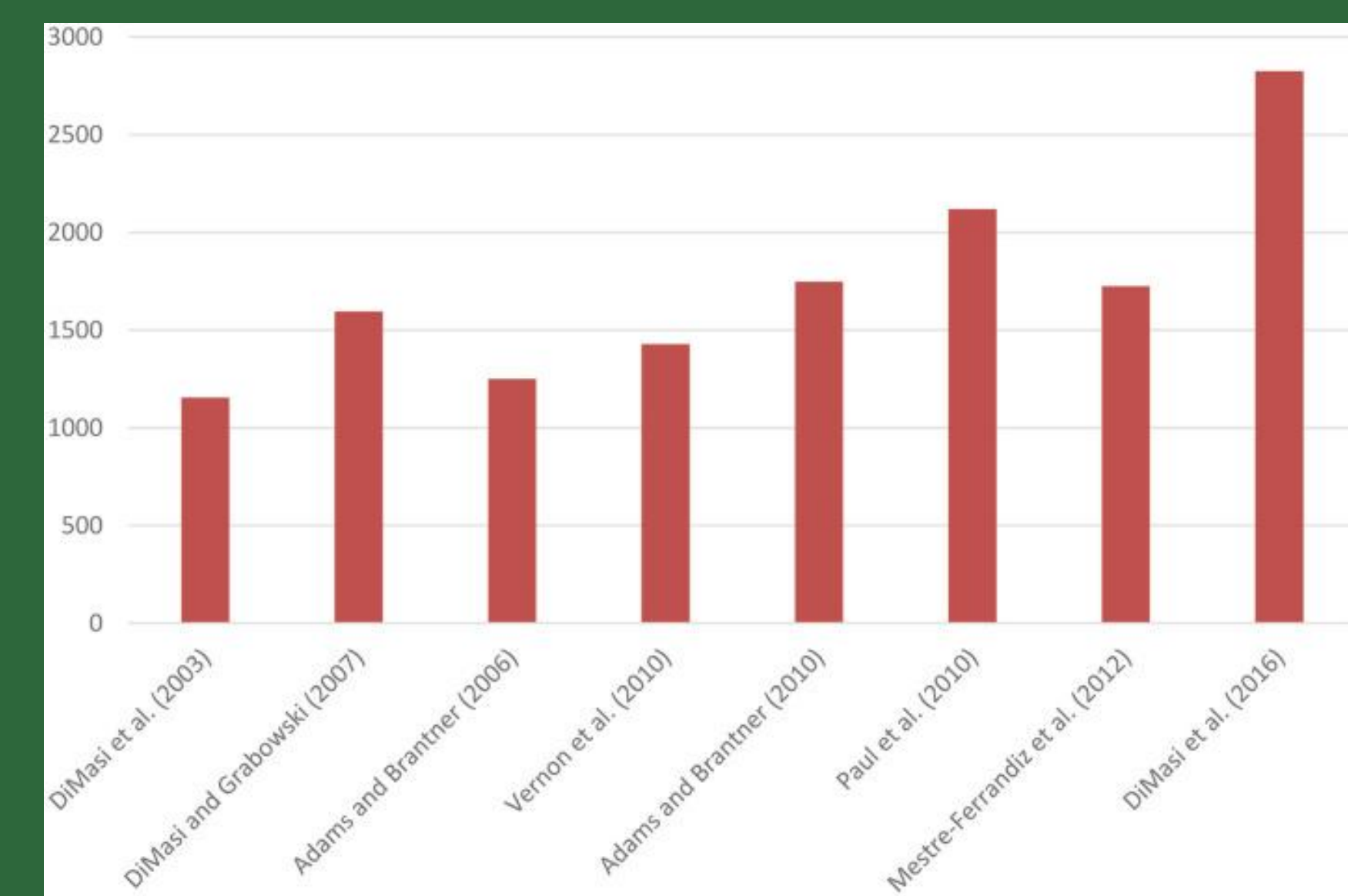
1. Curate AI-ready open **data** sets for drug discovery
2. Develop hierarchical accurate simulation **models** for efficacy/toxicity evaluations.
3. Nurture a decentralized AI drug discovery **ecosystem**
4. Train AI and drug discovery **talents** through expert team
5. Establish **academia-industry collaborations**
 - Platform Licensing
 - Innovation lab with data-driven insights
 - Sponsored research and development projects
 - Industry-academia program (Yale biomedical data science fellowship example)
 - Joint panel, workshop, symposium, report, white papers



Presented at the Intl. Conf. Systems Biology in Human Diseases, Vanderbilt Univ. (07/24)

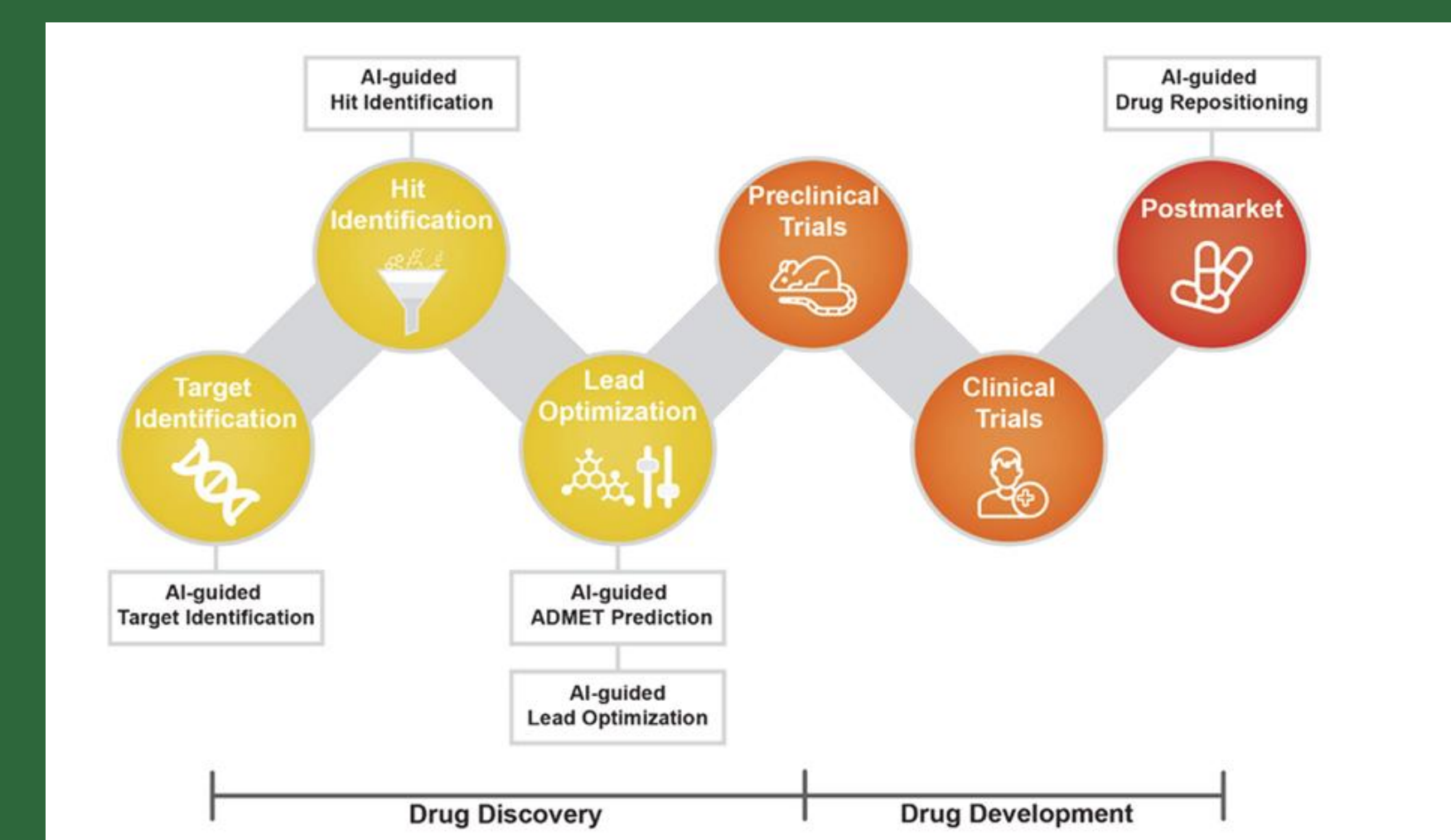
Can AI address drug discovery cost and speed issues?

~3x Drug Development Cost Increase over 20 years (2003-2023)



Simons S, Huys I. R&D Costs of New Medicines: A Landscape Analysis. Front Med. 2021 Oct 26;8:760762. doi: 10.3389/fmed.2021.760762.

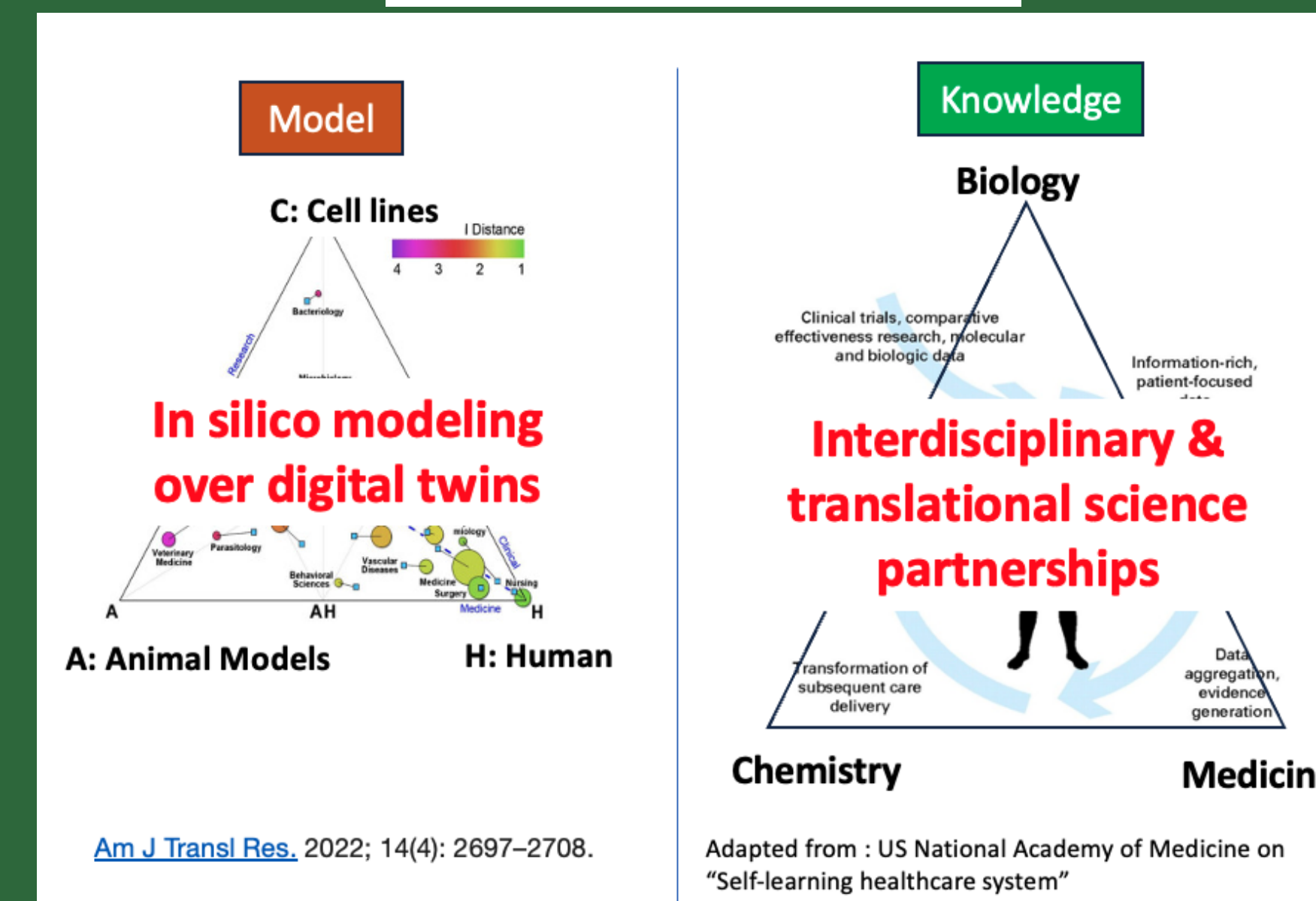
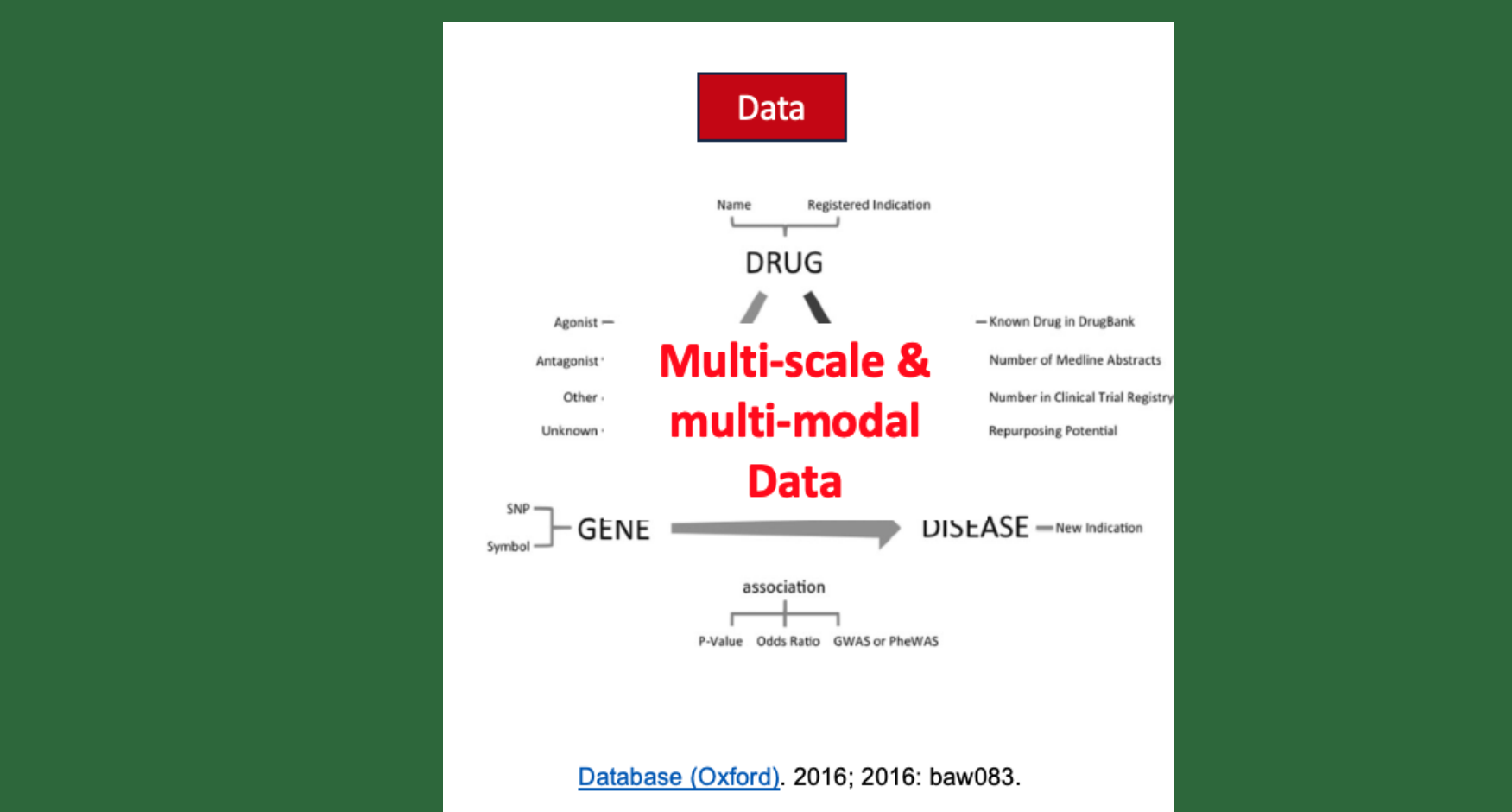
AI has been introduced in all stages of drug discovery today in the industry to optimize processes



In Biotechnology and Bioprocess Engineering 25: 895-930 (2020) DOI 10.1007/s12257-020-0049-y

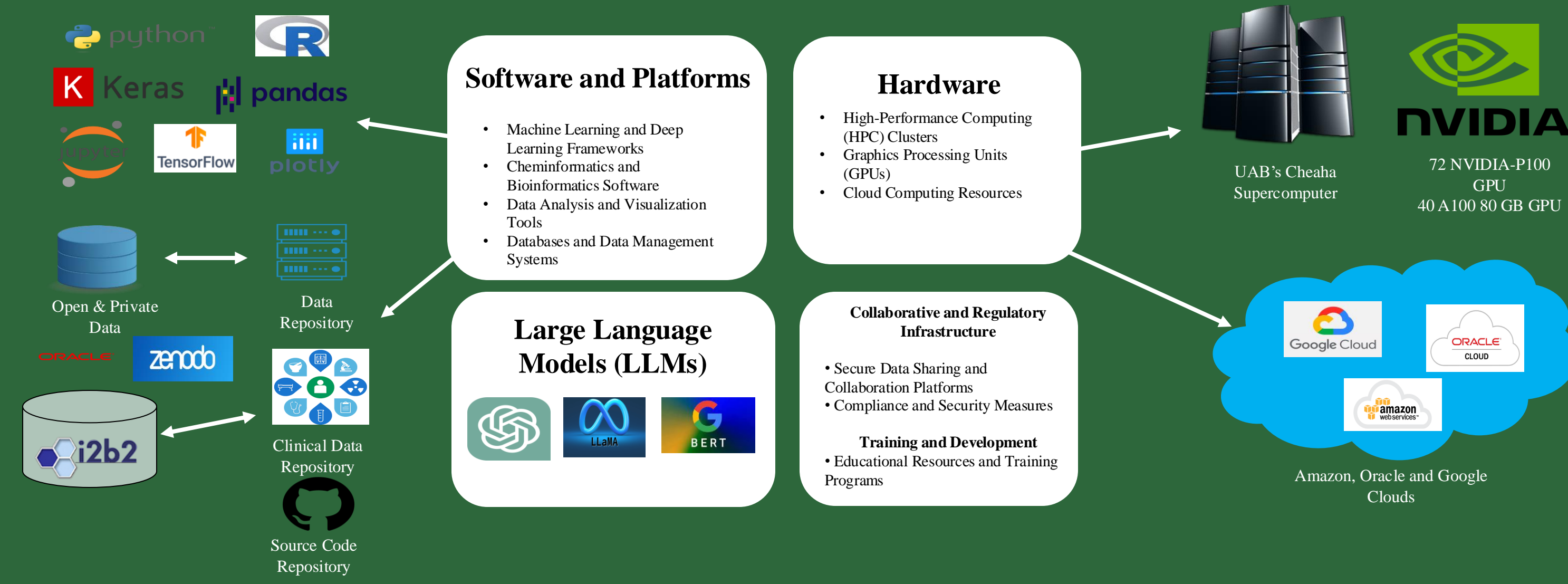
New Disruptive Drug Discovery Pathways Required

Data + Model + Knowledge + Regulatory transformation



Adapted from: US National Academy of Medicine on "Self-learning healthcare system"

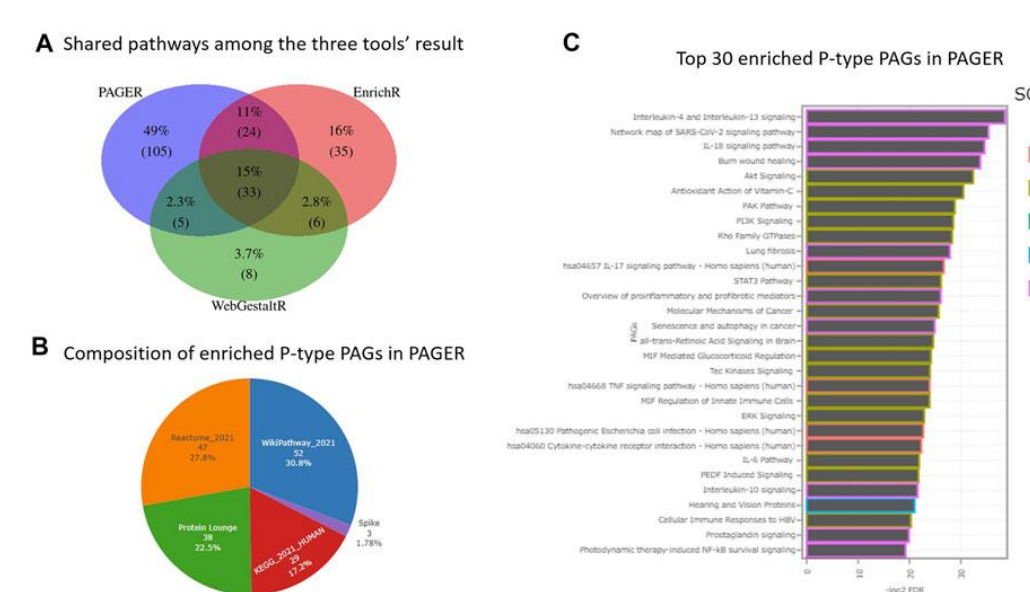
Computing Infrastructure



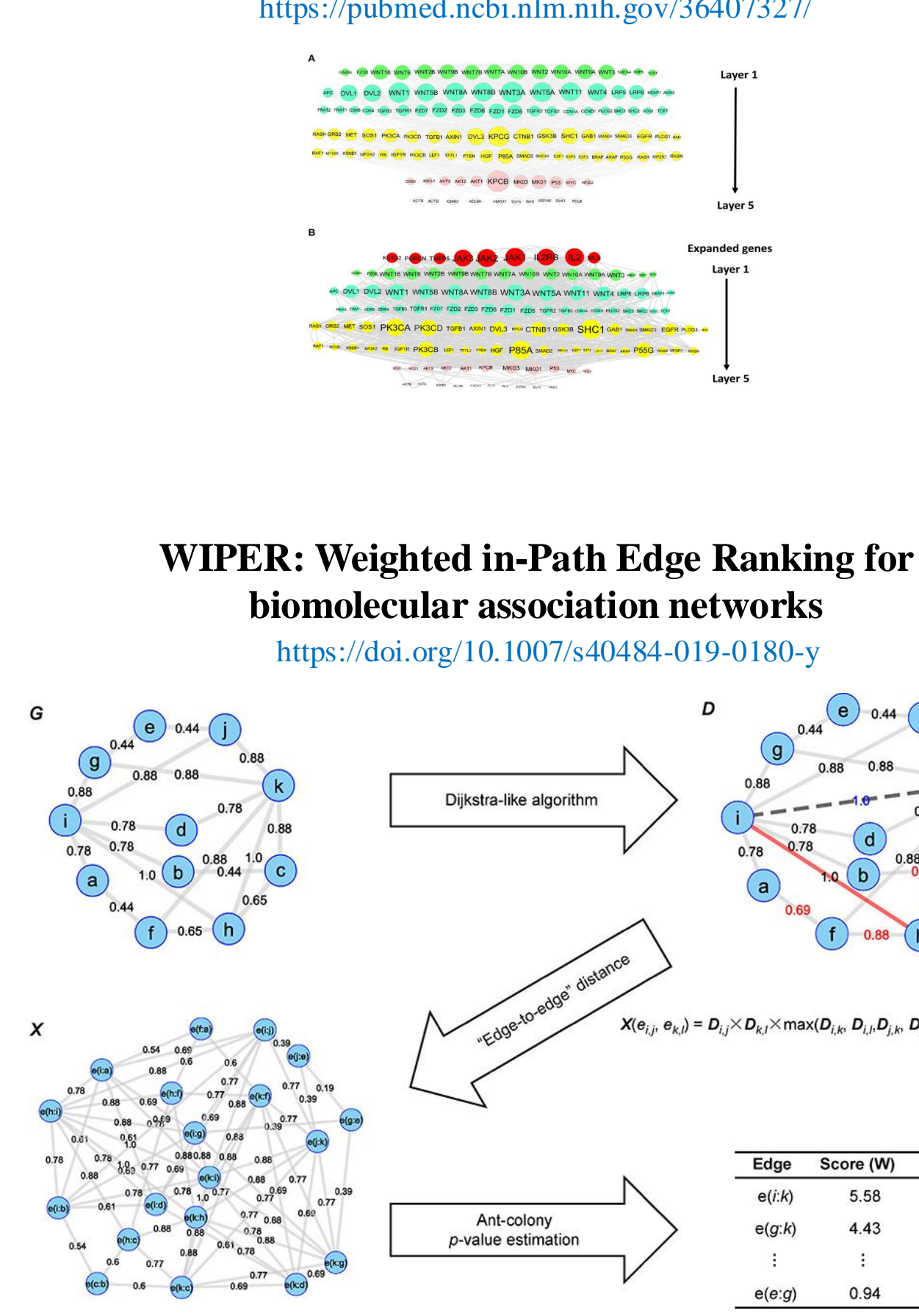
Tools Layer

Network biology tools

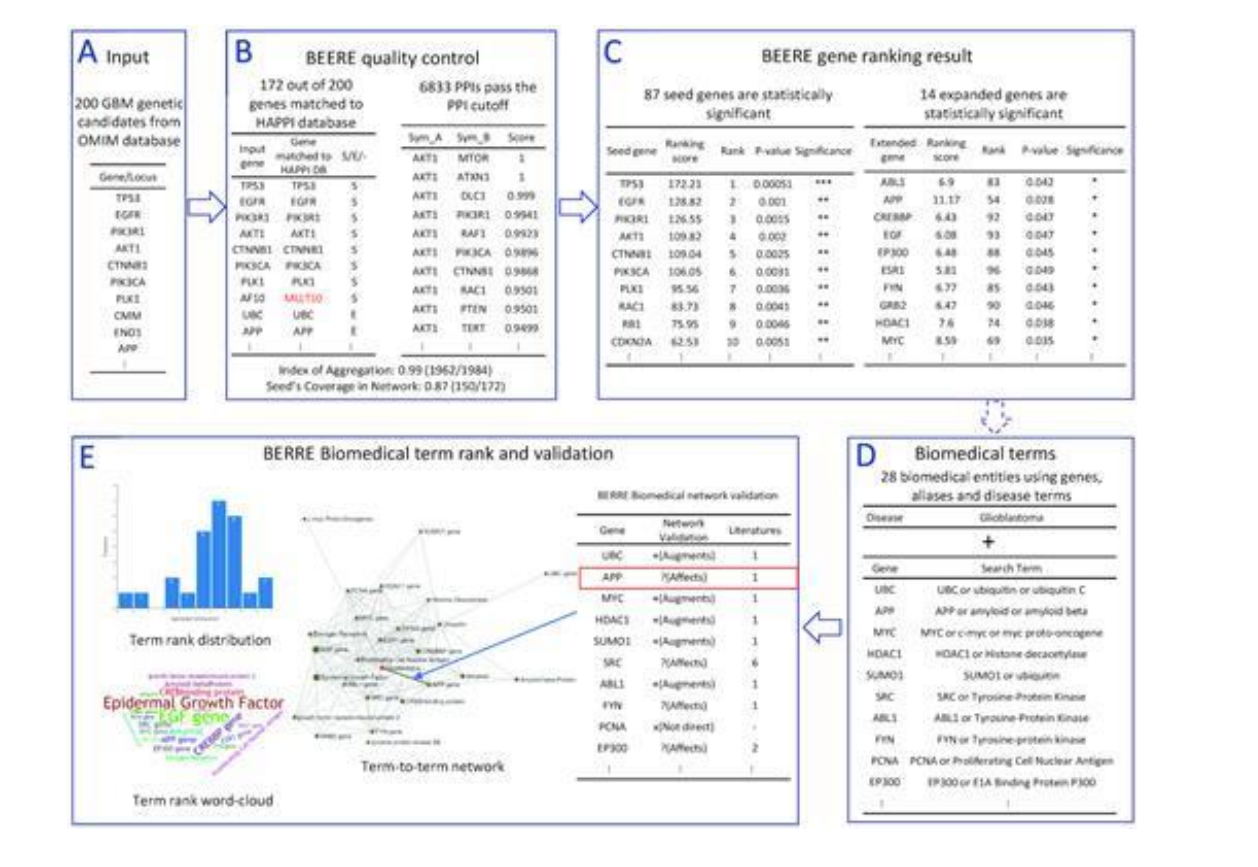
PAGER Web App: An Interactive, Online Gene Set and Network Interpretation Tool for Functional Genomics
<https://doi.org/10.3389/fgene.2022.820361>



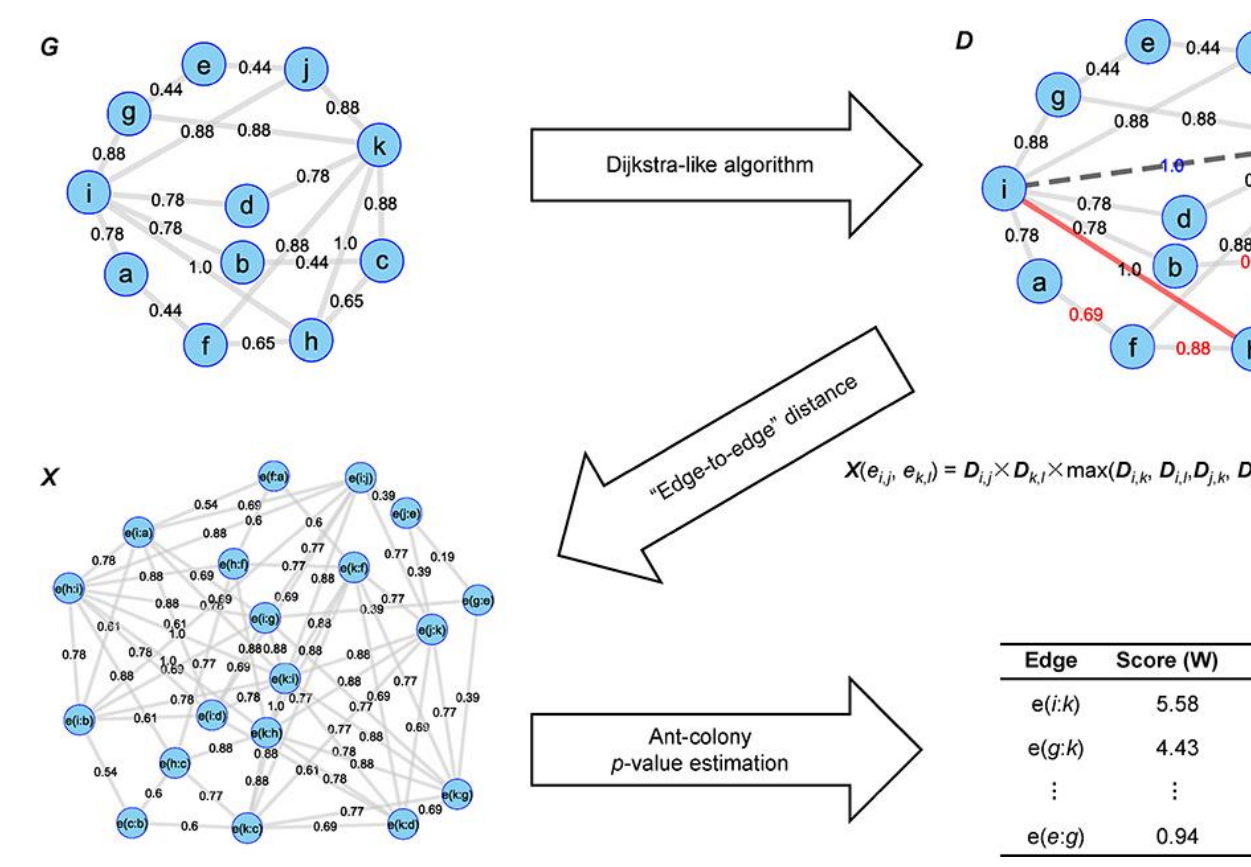
Weighted In-Network Node Expansion and Ranking (WINNER): A network biology tool for biomolecular characterization and prioritization
<https://pubmed.ncbi.nlm.nih.gov/36407327/>



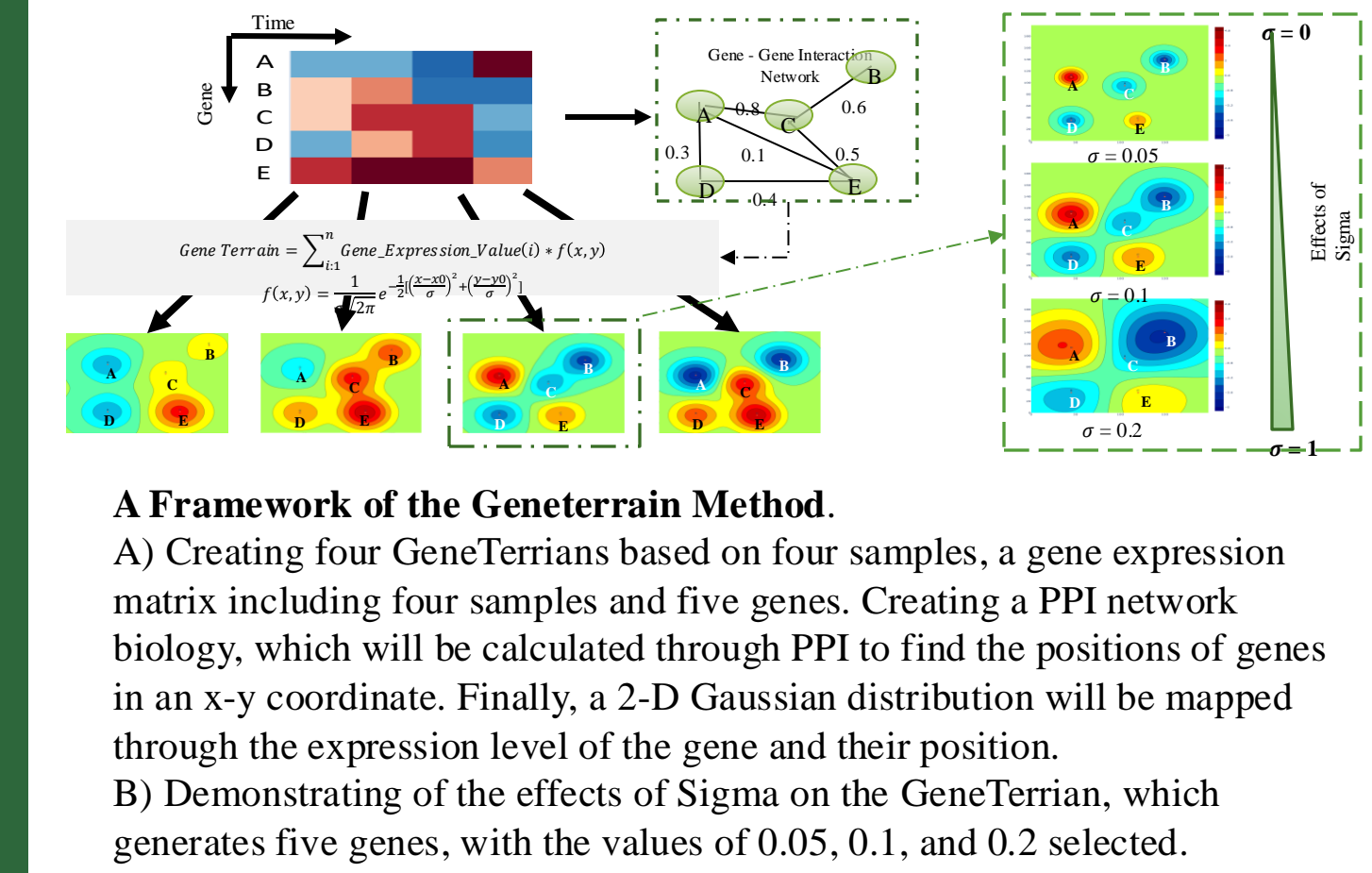
BEERE: a web server for biomedical entity expansion, ranking and explorations
<https://doi.org/10.1093/nar/gkz428>



WIPER: Weighted in-Path Edge Ranking for biomolecular association networks
<https://doi.org/10.1007/s40484-019-0180-y>



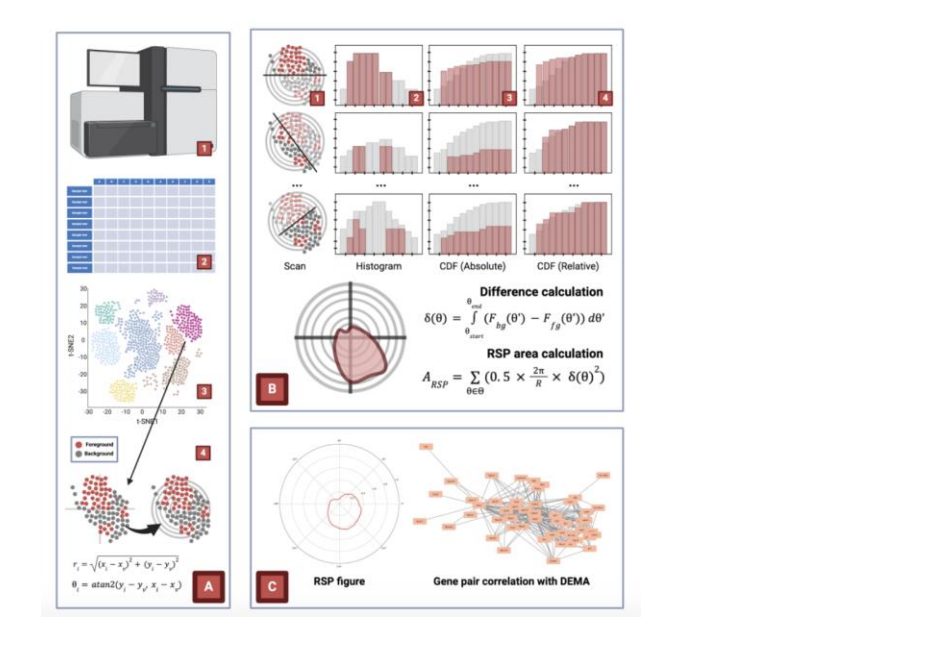
GeneTerrain



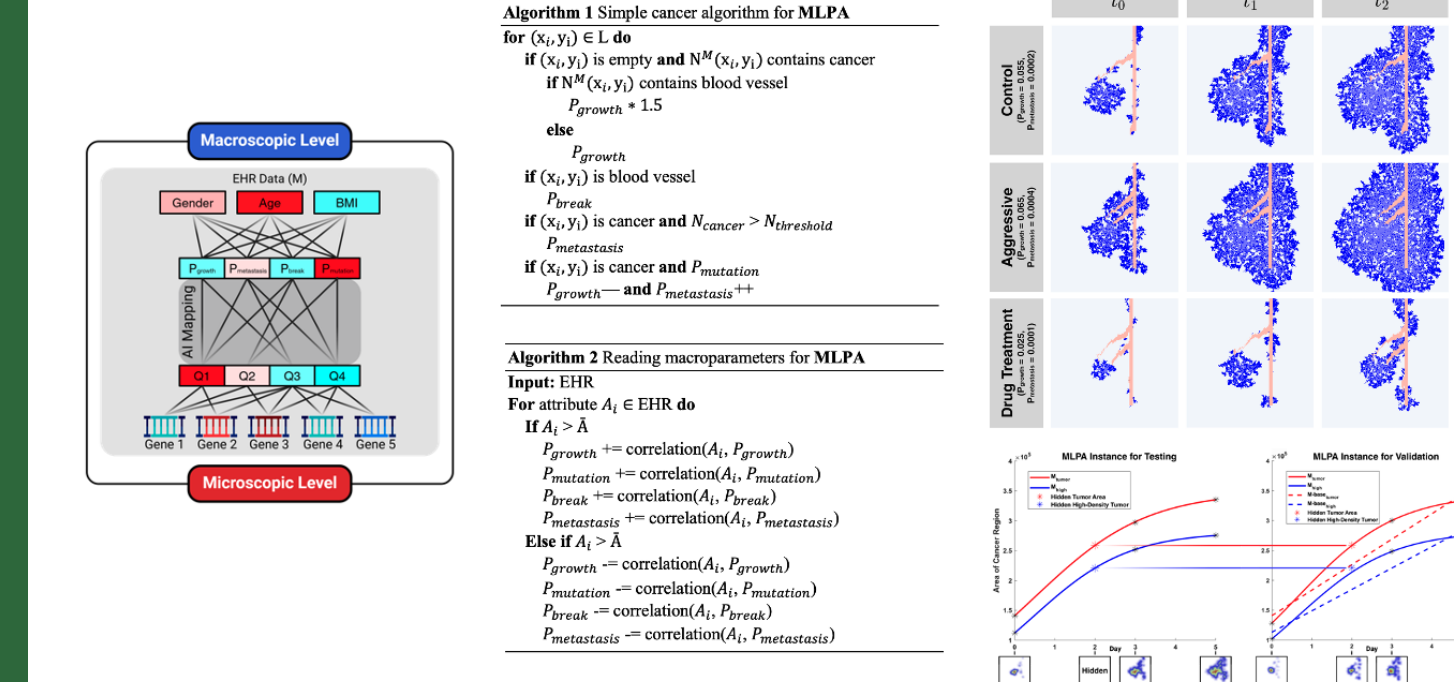
A Framework of the Geneterrain Method.
 A) Creating four GeneTerrains based on four samples, a gene expression matrix including four samples and five genes. Creating a PPI network biology, which will be calculated through PPI to find the positions of genes in an x-y coordinate. Finally, a 2-D Gaussian distribution will be mapped through the expression level of the gene and their position.
 B) Demonstrating the effects of Sigma on the GeneTerrain, which generates five genes, with the values of 0.05, 0.1, and 0.2 selected.

BioRSP: A novel tool for identifying spatial patterns and biomarkers in biological data

Accepted for publication at Patterns (cell press) special issue of ICIBM Oct '24, Houston, TX

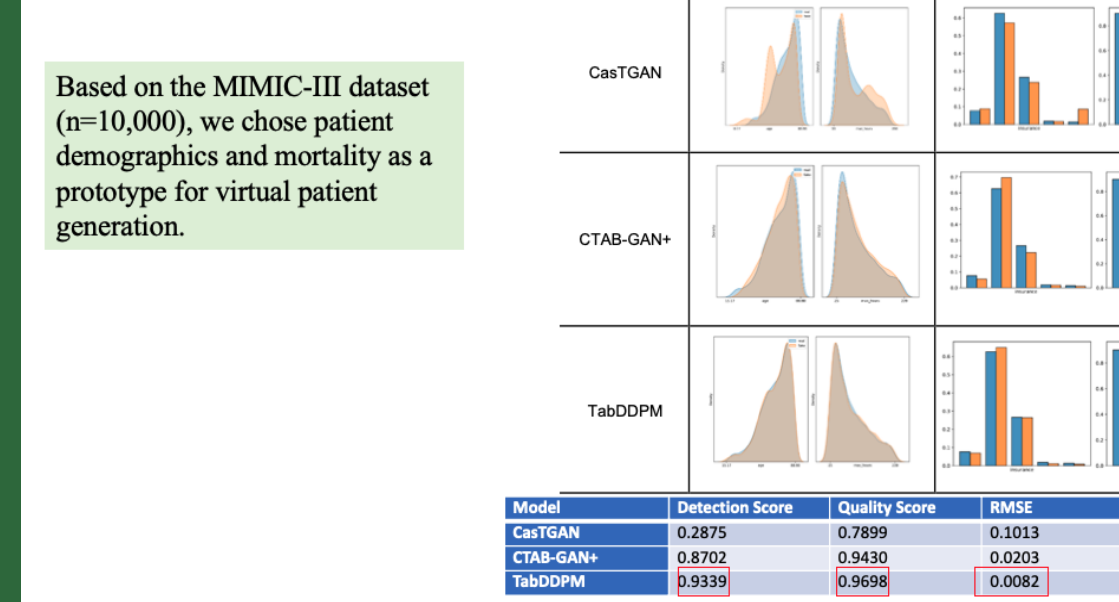


Digital twin simulations of cancer growth and metastasis

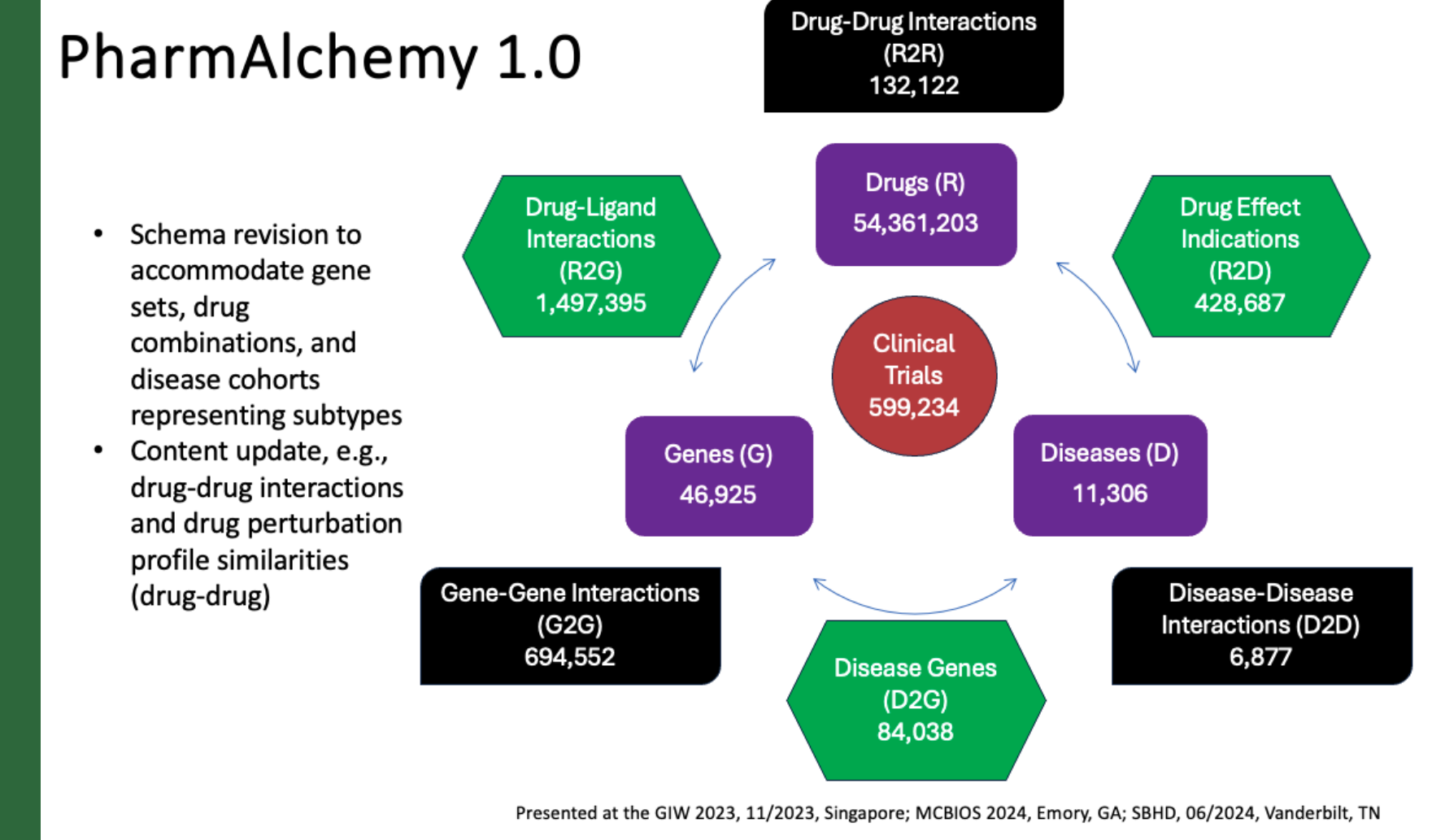


Virtual patients using generative AI

NCI Supplement proposal submitted in Aug '24

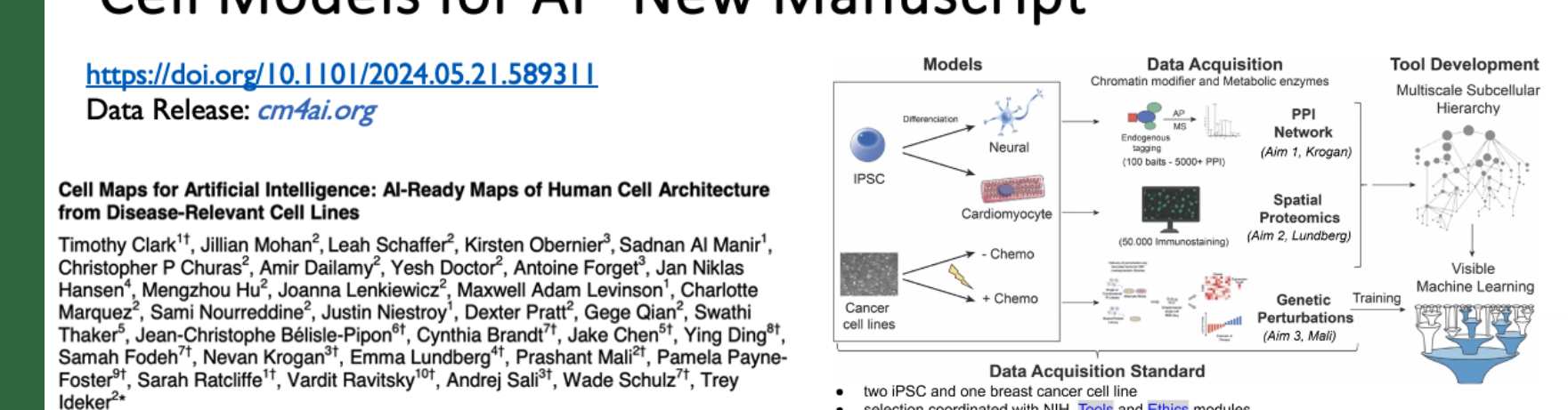


Data Layer

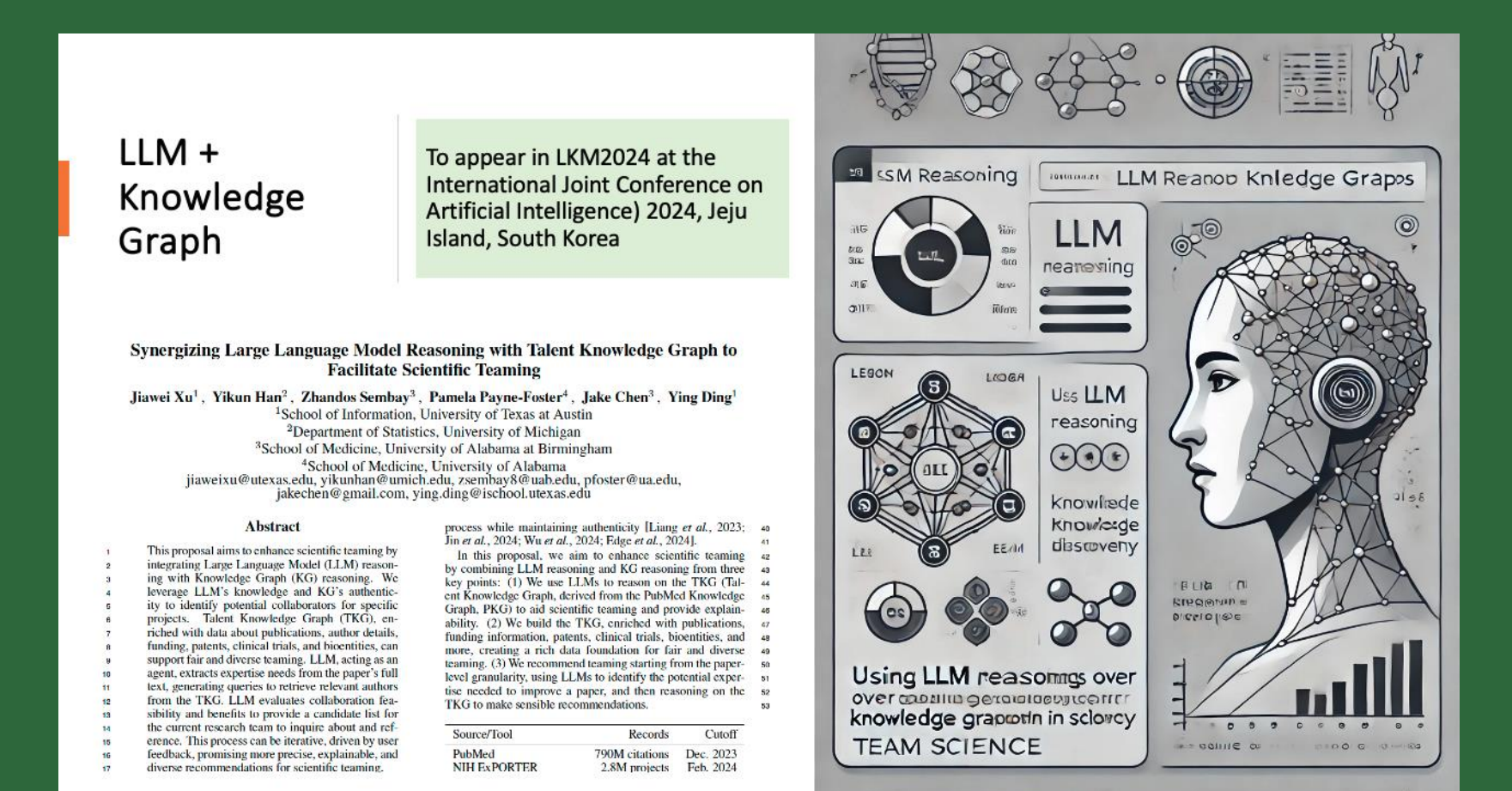
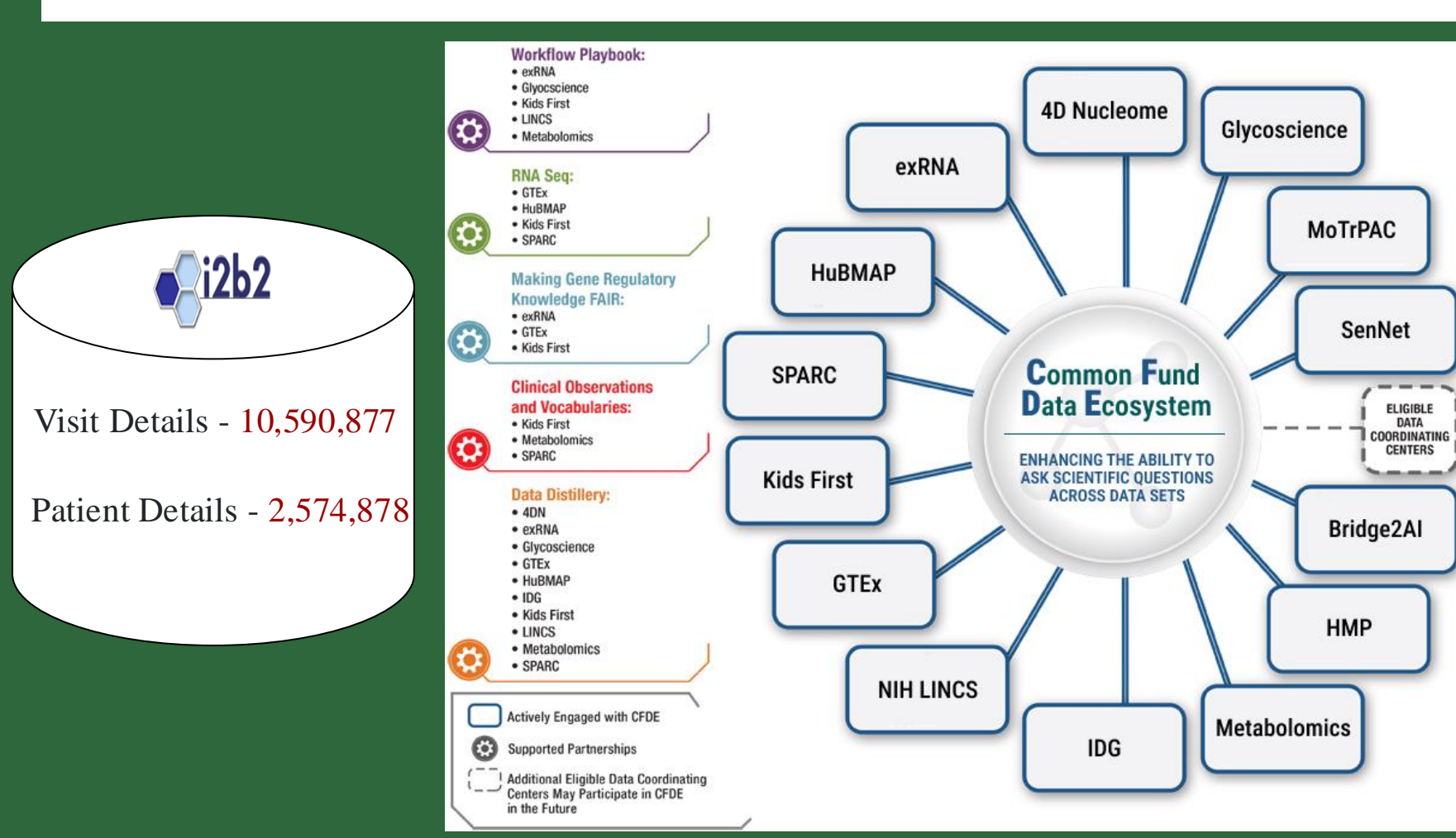


Presented at the GIW 2023, 11/2023, Singapore; MCBOS 2024, Emory, GA; SBHD, 06/2024, Vanderbilt, TN

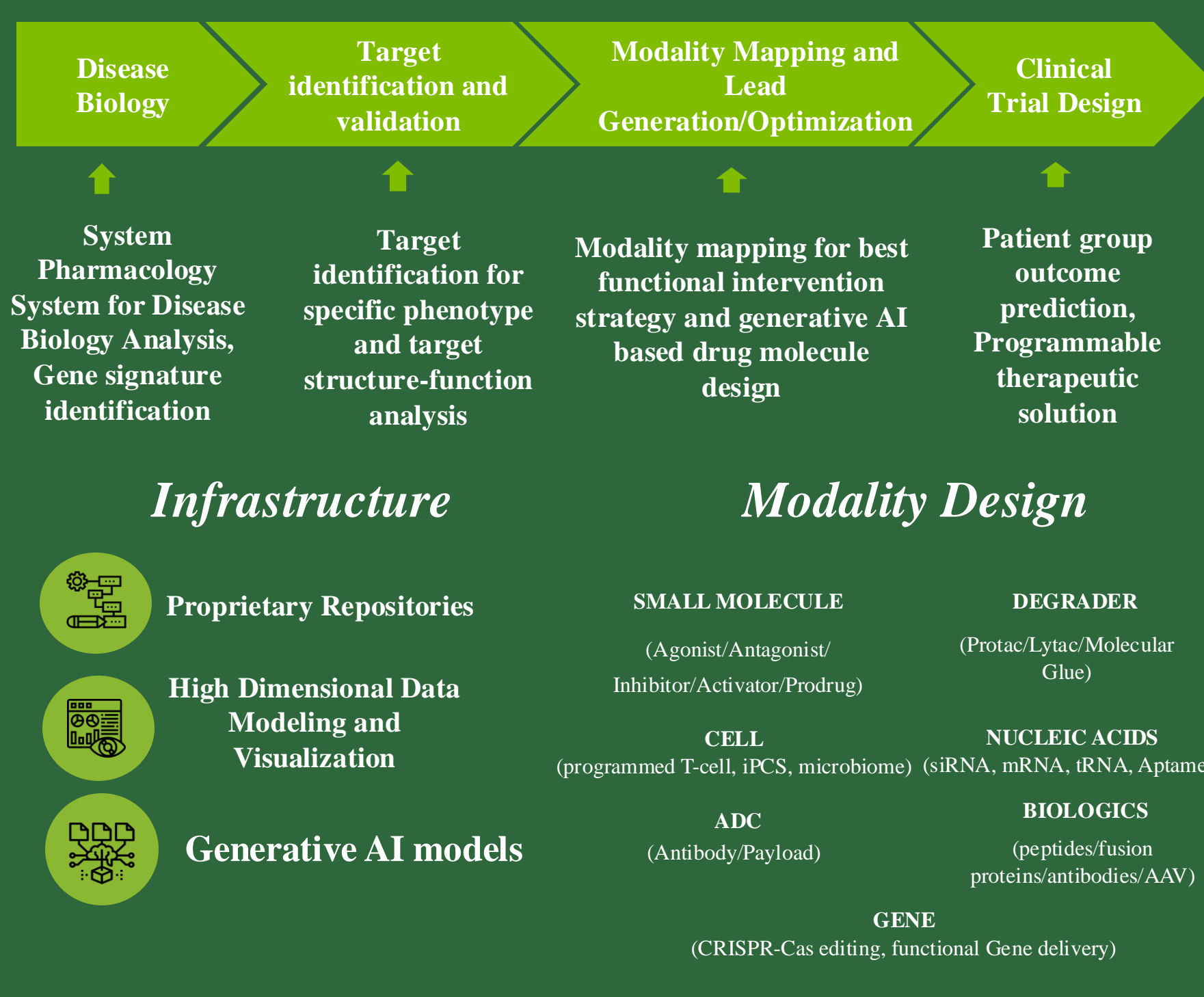
"Cell Models for AI" New Manuscript



Cell Maps for Artificial Intelligence: AI-Ready Maps of Human Cell Architecture from Disease-Relevant Cell Lines
 Timothy Clark¹, Allan Mohr², Leah Schmitt³, Kiran Chatterjee⁴, Stefan St. Maler⁵, Christopher P. Chaturvedi⁶, Aron D. Chaturvedi⁷, Yash Doshi⁸, Andrew Fogarty⁹, Jan Niklas Hansen¹⁰, Mengzhou Hu¹¹, Josefa Lefebvre¹², Maxwell Adams Brantley¹³, Charlotte Marston¹⁴, Sarah Nourmohammadi¹⁵, Justin Neasey¹⁶, Dexter Pratt¹⁷, Caglar Oflar¹⁸, Swathi Thaker¹⁹, Xinxin Zhu²⁰, Xinxin Zhu²¹, Jake Chen²², Qing Ding²³, Samah Fokan²⁴, Naveen Koganti²⁵, Emma Lundberg²⁶, Prashant Malhotra²⁷, Pamela Payne-Poole²⁸, Sarah Ratchin²⁹, Vardit Ravitsky³⁰, Anshu Salil³¹, Wade Schulz³², Trey Sisker³³



Workflow and Core Capabilities



Selected Drug Discovery Meetings Participated/Organized in 2024

SOUTHEAST REGIONAL CLINICAL & TRANSLATIONAL SCIENCE CONFERENCE

Center for Clinical and Translational Science

ATTIS 2024

8th Annual Translational and Transformative Informatics Symposium

UAB 05.03.2024

KDD2024

HEALTHDAY

"Building Health AI Ecosystem: From Data Harmonization to Knowledge Discovery"

Tuesday, August 27th, 2024

International Barcelona Convention Center

Plaça de Willy Brandt, 11-14, Sant Martí, 08019 Barcelona, Spain

INTERNATIONAL CONFERENCE ON SYSTEMS BIOLOGY OF HUMAN DISEASE

SDDS 2024

Stanford Drug Discovery Symposium

April 29-30, 2024

FESTIVAL OF BIOLOGICS

America's Most Exciting Biologics Event

April 15-17, 2024

San Diego Convention Center