Metabolomics integrative analysis with genome-scale metabolic networks

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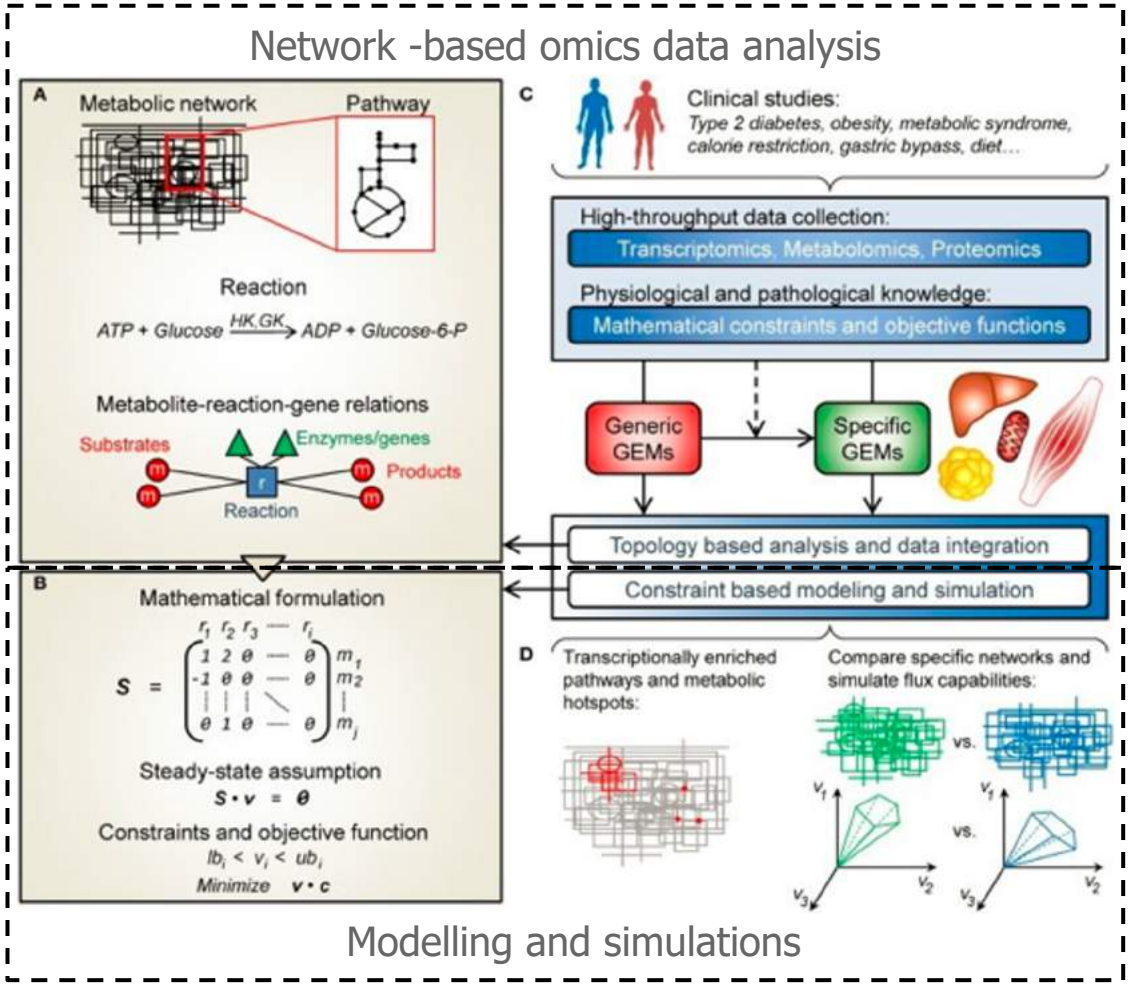
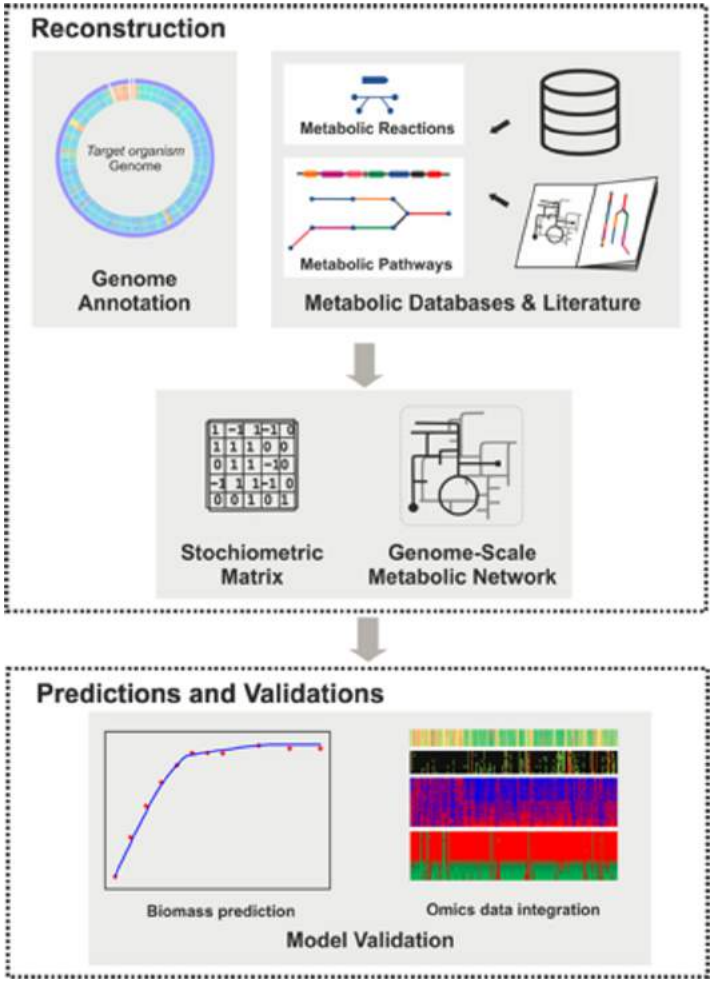
World Health Organization

Genome-scale metabolic networks

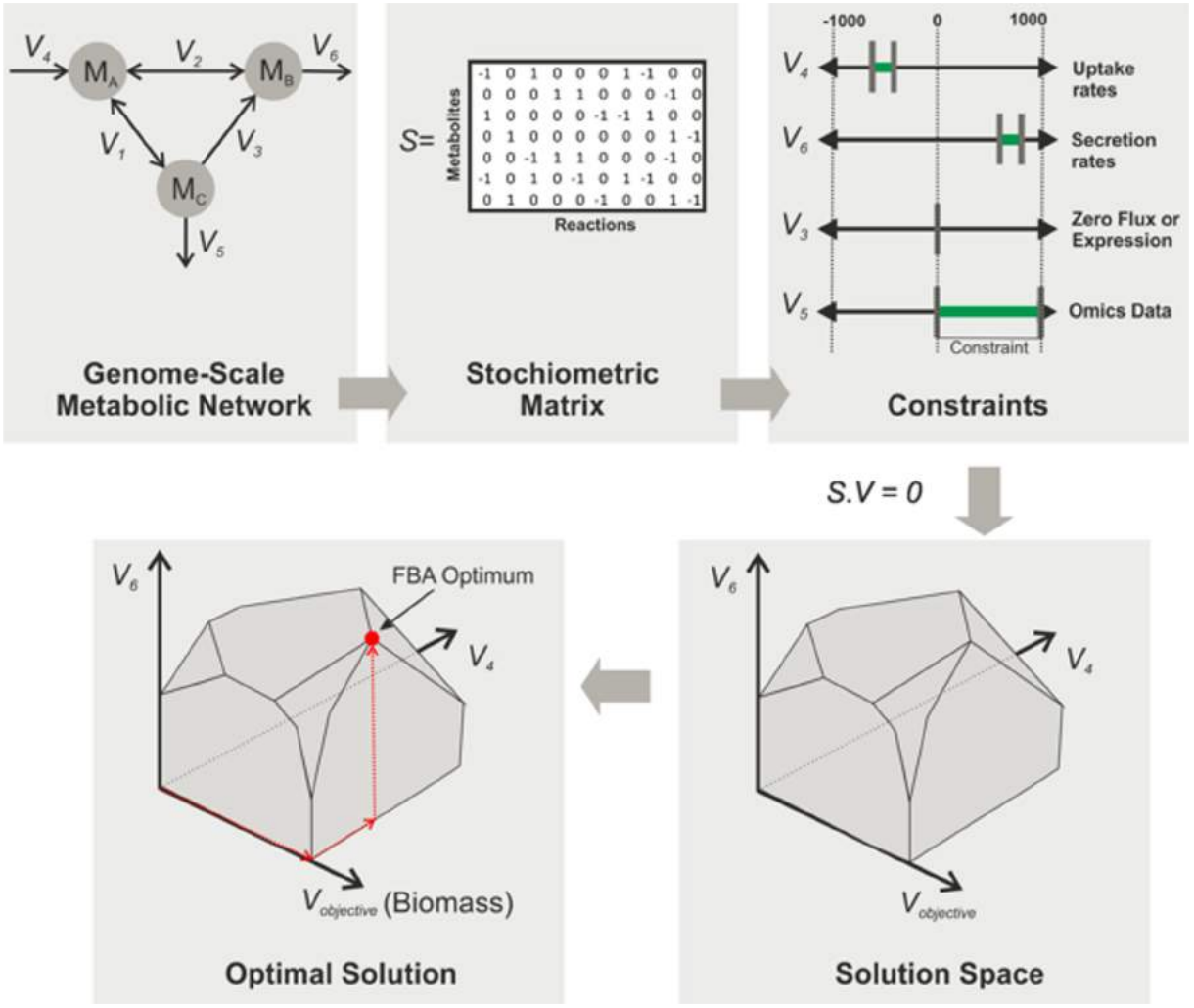
How does it work?

How to build one?

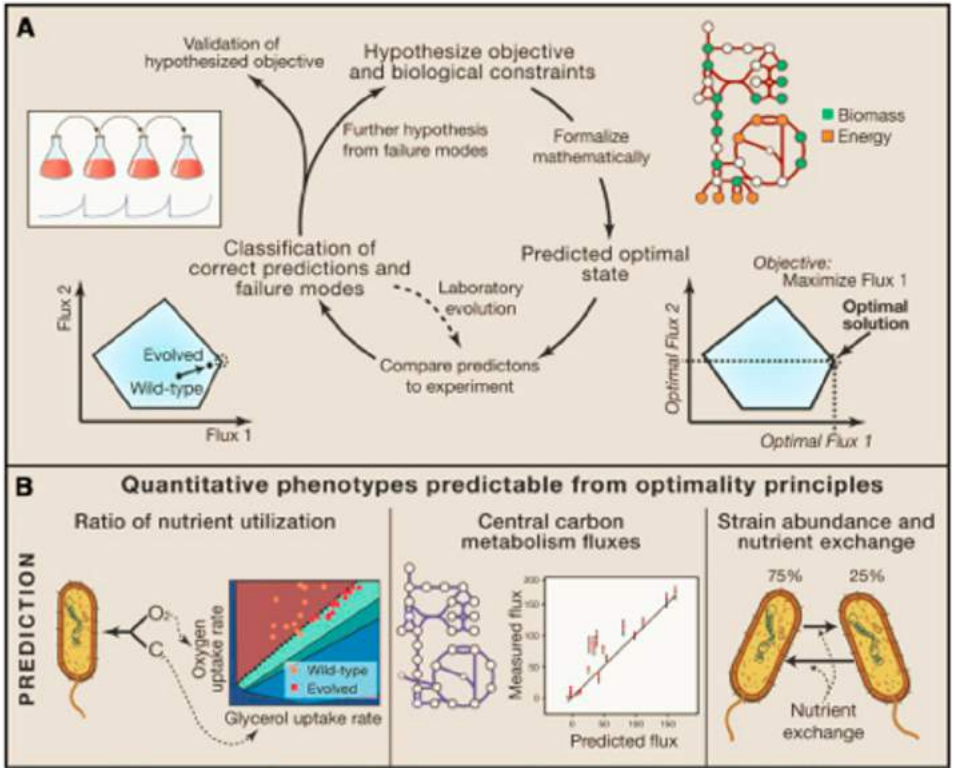


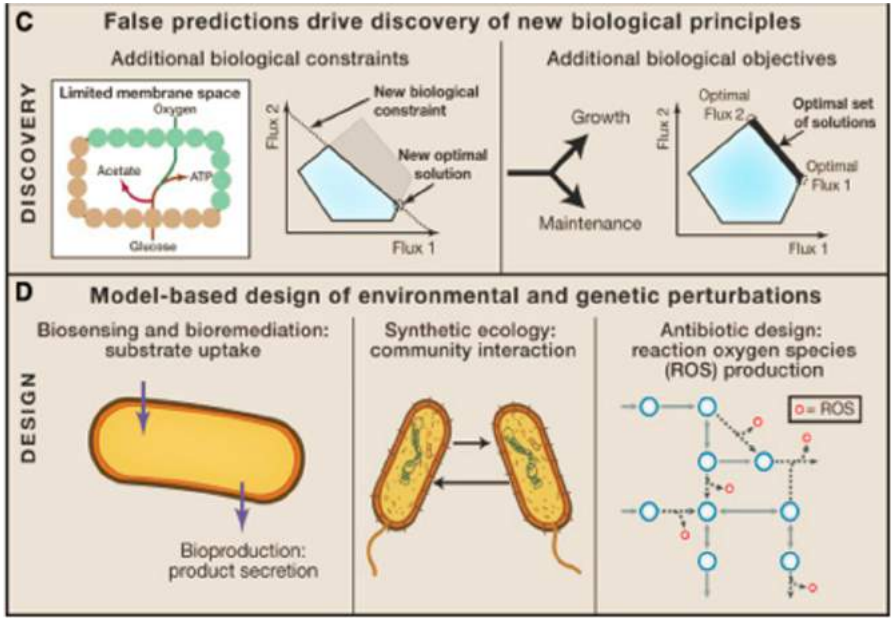


Constraint-based modelling



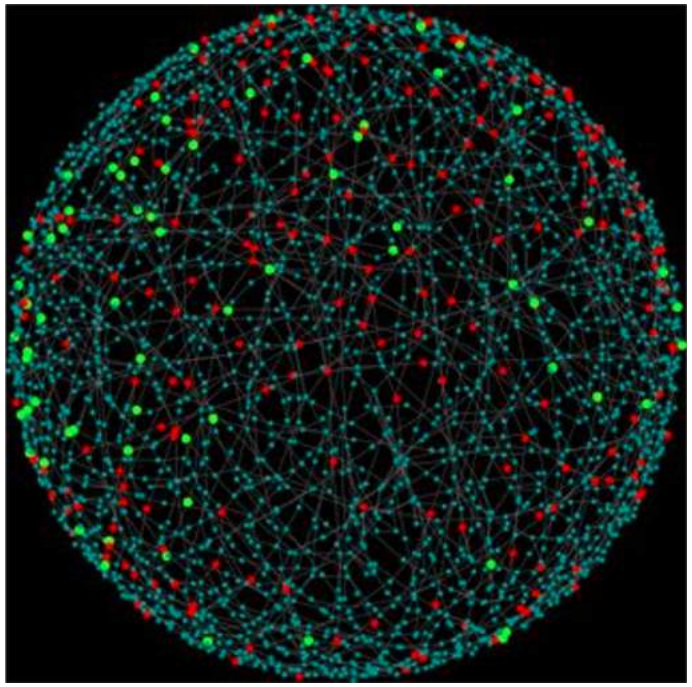
Models-based simulations





Metabolomics and metabolic networks

MANCHESTER 1824
The University of Manchester
Manchester Institute of Biotechnology



Automated untargeted metabolomics data processing/analysis/integration in the *Streptomyces coelicolor* network:
Green: Level 1 annotated metabolites
Red: Level 2 annotated metabolites
Blue: organism metabolites

Identification of metabolic pathways changing due to antibiotics production:
Pinpoint key metabolites changing between two conditions (producer/non-producer).
Quantitative metabolomics data integrated as metabolic fluxes values.

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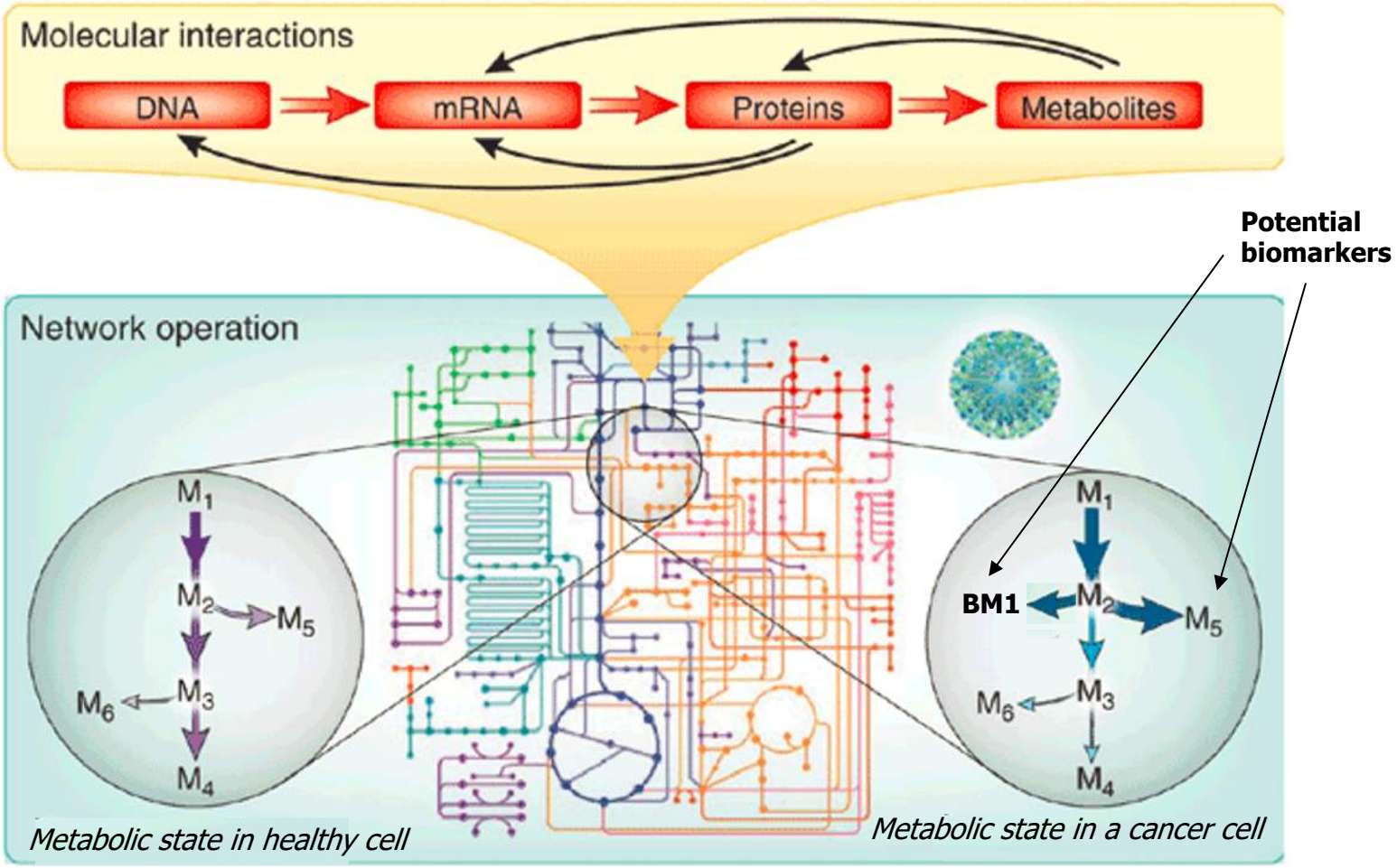
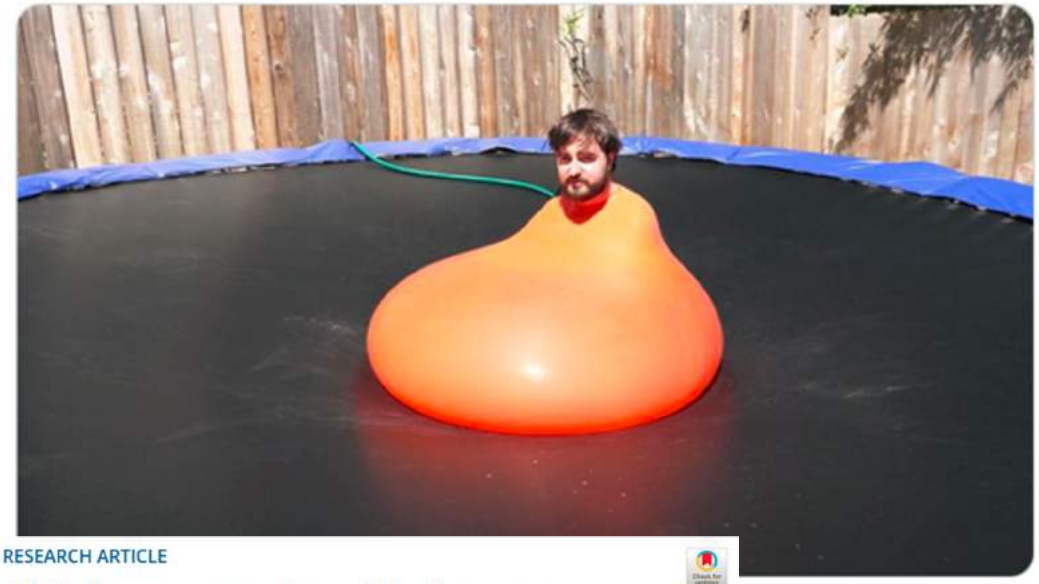
Example


Molecular interactions
DNA
mRNA
Proteins
Metabolites
Potential biomarkers
Network operation
M1
M2
M5
M6
M3
M4
BM1
Metabolic state in healthy cell
Metabolic state in a cancer cell

Evolution of human metabolic networks



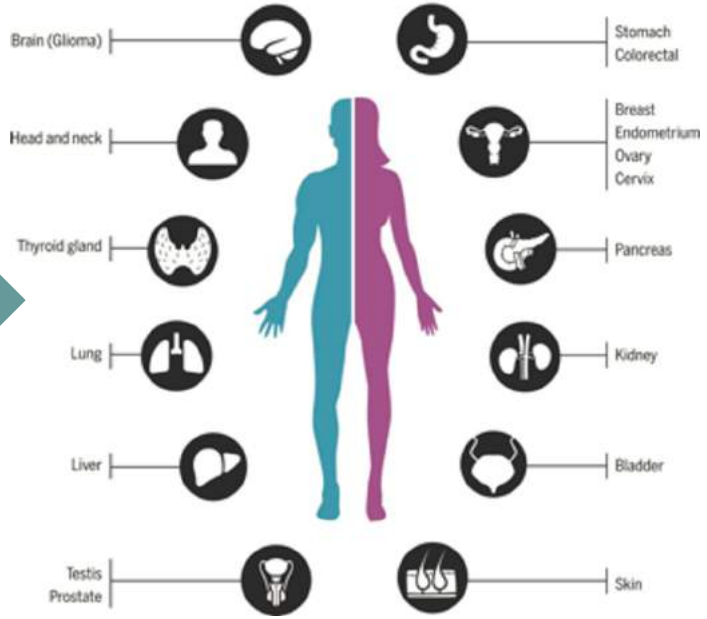
RESEARCH ARTICLE

Global reconstruction of the human metabolic network based on genomic and bibliomic data

Natalie C. Duarte, Scott A. Becker, Neema Jamshidi, Ines Thiele, Monica L. Mo, Thuy D. Vo, Rohith Srivas, and Bernhard Ø. Palsson

PNAS February 6, 2007 104 (6) 1777-1782; https://doi.org/10.1073/pnas.0610772104

Recon1
2007



Human1
2020

RESEARCH ARTICLE | METABOLISM

An atlas of human metabolism

Jonathan L. Robinson[1,2,*], Pınar Kocabaş[1,2,*], Hao Wang[1,3,4,*], Pierre-Etienne Cholley[4,*], Daniel Cook[1], Avlan...
+ See all authors and affiliations

Science Signaling 24 Mar 2020:
Vol. 13, Issue 624, eaaz1482
DOI: 10.1126/scisignal.aaz1482

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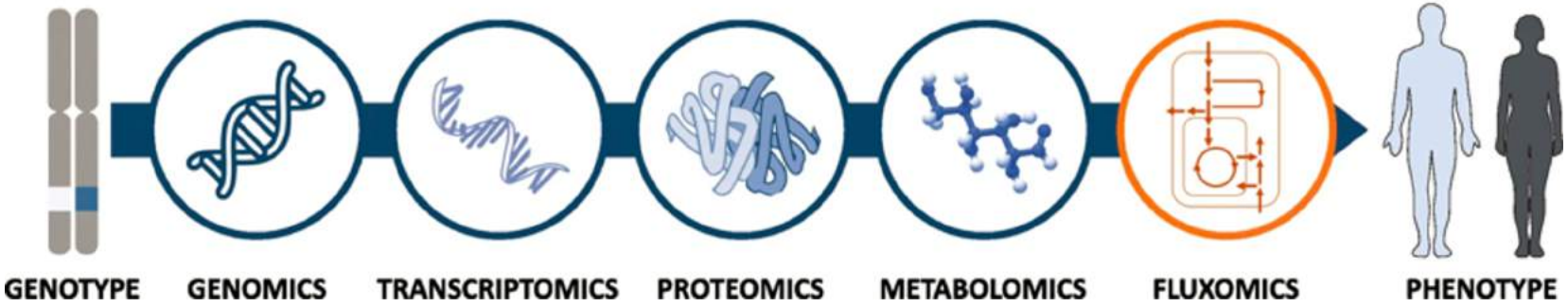
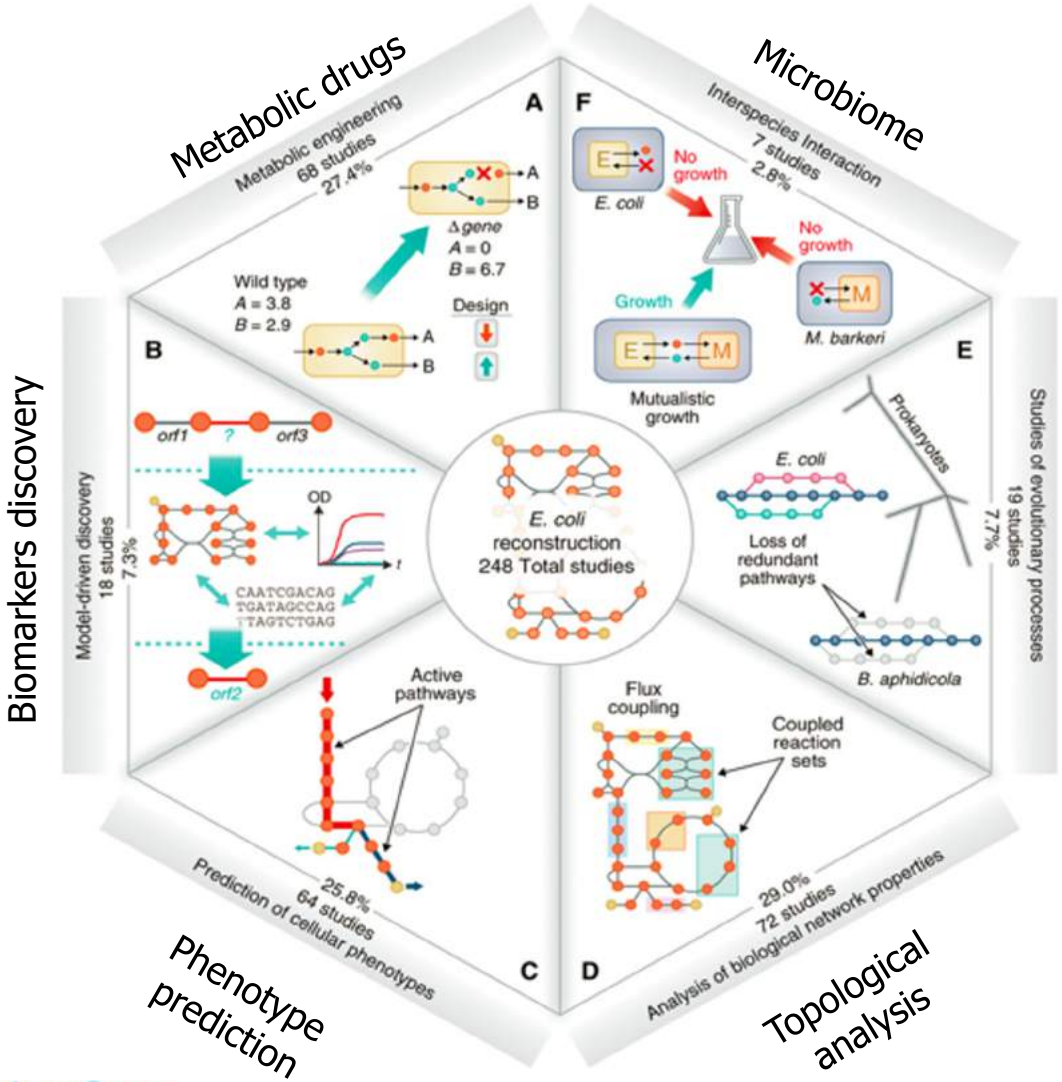
Applications for cancer research

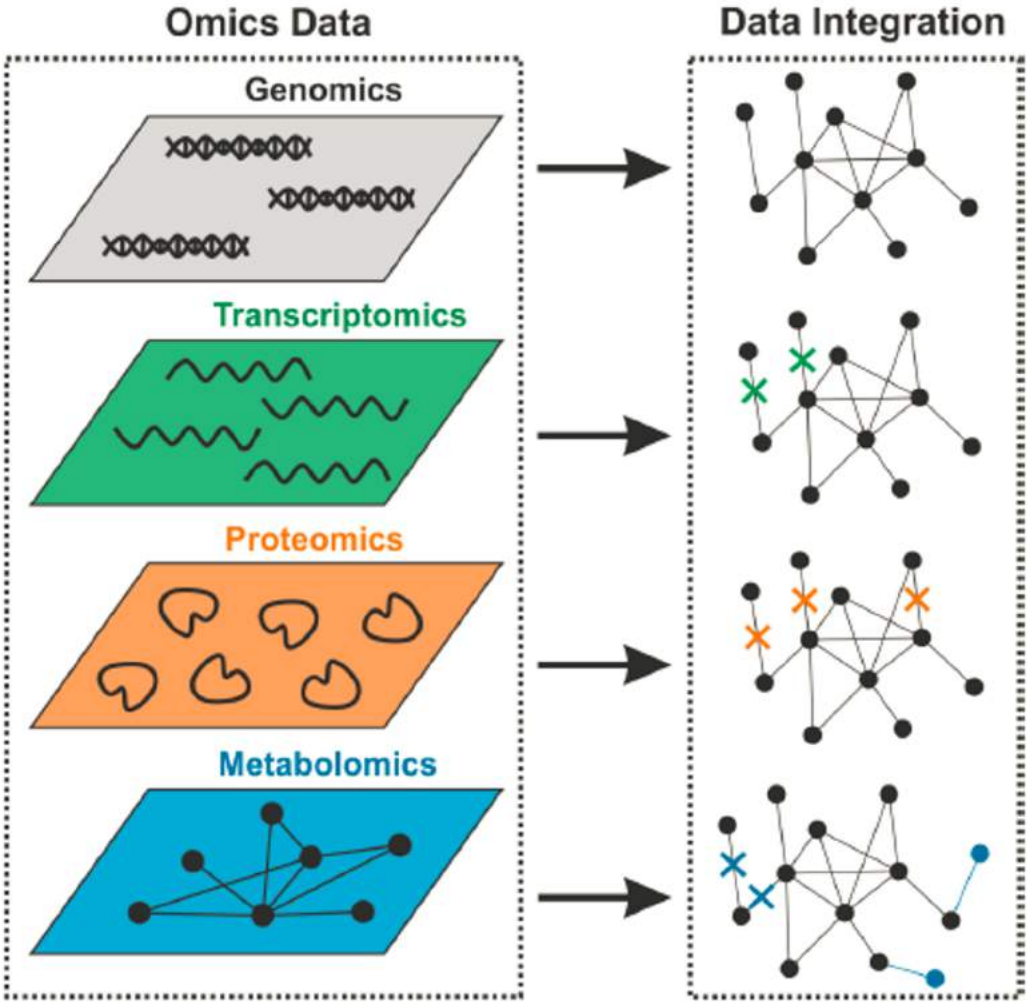
- Improve metabolites annotation (MetClassNet)
- Biomarkers discovery
- Studying metabolic adaptation changes
- Comparative metabolic analysis of cancers
- Multi-omics analysis from genotype to phenotype



Applications



Using omics to constrain the metabolic models



Part 2

What we do at IARC

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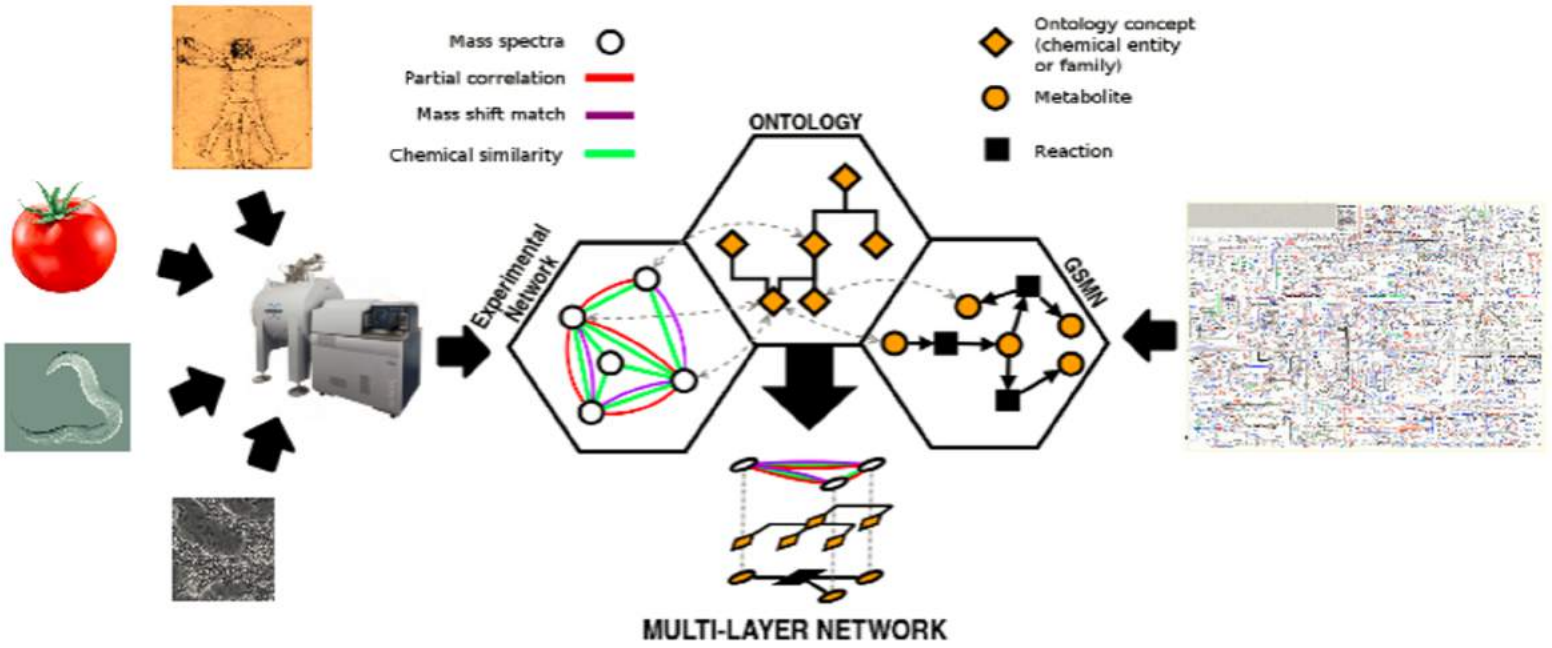
MetClassNet



MetClassNet overall objectives:

1. Develop a novel computational framework to build multilayer networks
2. Develop state of art computational solutions exploiting the multilayer topology to improve the power of metabolism analysis
3. Generate new biological insight by using combined power of the above approaches.
4. Liberate the new software solutions and data toward the community.

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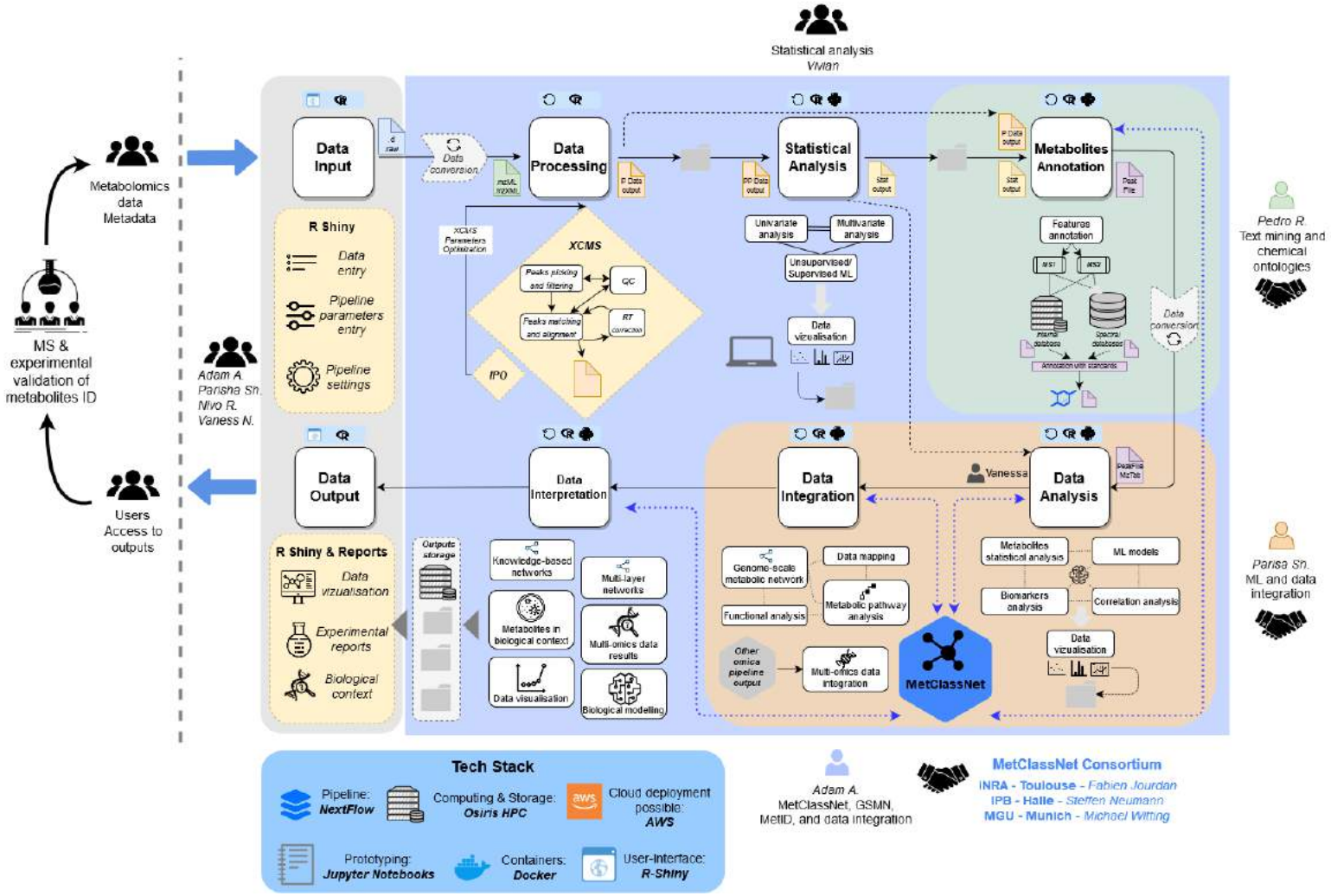
A reproducible and modular metabolomics integrative analysis pipeline



Thanks - MetClassNet

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