

Computational Systems Medicine for Drug Response Modelling, Network Biology, and Precision Therapeutics



Challenges

Modern healthcare and drug development increasingly rely on the ability to **predict cellular responses**, understand **mechanistic pathways**, and tailor interventions to individual patients. Major challenges include:

- Integrating **multi-omics datasets** into coherent, mechanistic models of disease.
- Predicting **drug responses**, drug combinations, and resistance mechanisms.
- Modelling cellular signalling networks with sufficient biological realism for clinical use.
- Bridging the gap between **computational modelling** and **clinical decision-making**.
- Understanding how perturbations affect cellular networks at the molecular level.

Technology

Prof. Saez-Rodriguez develops robust, scalable technologies for **mechanistic modelling** of biological systems, integrating large-scale biological data with network-based computational frameworks:

- **Mechanistic Signalling Network Models** - Detailed, executable models of signalling pathways to quantify and predict: drug sensitivity, drug synergy, cellular response to genetic or chemical perturbations, disease-specific alterations in pathway activity.
- **Multi-Omics Data Integration Frameworks** - Technologies integrating data across Transcriptional (RNA-seq) (Phospho)Proteomic Metabolomics Single-cell/spatial and bulk to generate mechanistic insights linked to phenotype and clinical outcomes.
- **AI and Machine-Learning Approaches** - Algorithms for predicting responses to targeted therapies, Identifying biomarkers, Prioritising combination therapies, Reverse-engineering biological networks
- **Open-Source Computational Tools/Resources** - The Saez Lab maintains widely used software tools/resources with respect to Systems biology modelling, Causal network inference, Molecular Interaction databases, Benchmarking of computational methods and resources

Internal EMBLEM Reference

2026-039

Key Inventors

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Applications

- Drug response prediction for targeted therapies
- Mechanistic pathway modelling for cancer, inflammation, and other diseases
- Identification of therapeutic combinations
- Multi-omics-driven patient stratification
- Network-based biomarker discovery
- Pharmaceutical screening and target validation
- Clinical decision-support based on pathway activity

Seeking

- Industry partners in pharma, biotech, and diagnostic development
- Collaborations on predictive modelling for complex diseases
- Joint development of decision-support tools
- Licensing opportunities for computational platforms
- Partnerships for large-scale multi-omics studies

Benefits

- **Mechanistic and interpretable:** not black-box models; biologically grounded outputs.
- **Highly scalable:** usable for large patient cohorts or screening datasets.
- **Predictive:** identifies drug responses and potential synergies.
- **Translational:** bridges experimental data with clinical applications.
- **Open-source and community-driven:** accessible, extendable tools and workflows.
- **Transparency:** clear and reliable metrics to benchmark methods performances

Keywords

Systems biology
Mechanistic modelling
Drug response prediction
Multi-omics
Network biology
Precision medicine
Pathway modelling
Machine learning
Systems pharmacology
Computational biology

Commercial Opportunity

- **Pharmaceutical R&D:** predicting drug response, resistance, and combination efficacy.
- **Precision Medicine Providers:** patient-specific modelling of pathway activation and treatment response.
- **Clinical Diagnostics:** mechanistic biomarkers for disease subtype classification.
- **AI-Driven Drug Development:** integration of mechanistic models with machine learning systems.

Further Reading

<https://saezlab.org/publications/>

Intellectual Property

Potential for future IP around predictive models, decision-support algorithms, or diagnostic pipelines.

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