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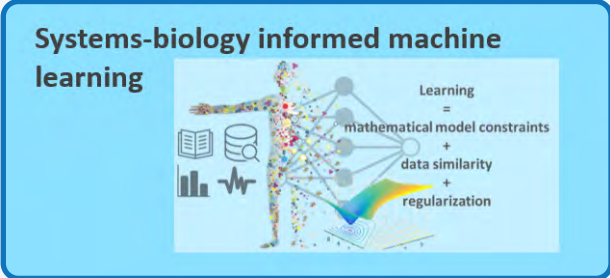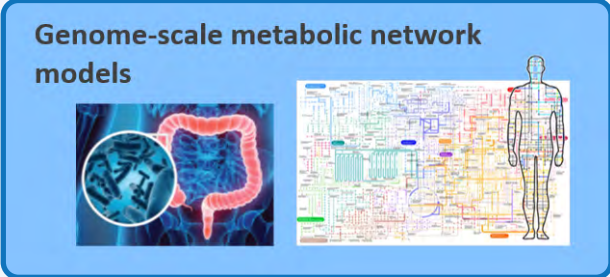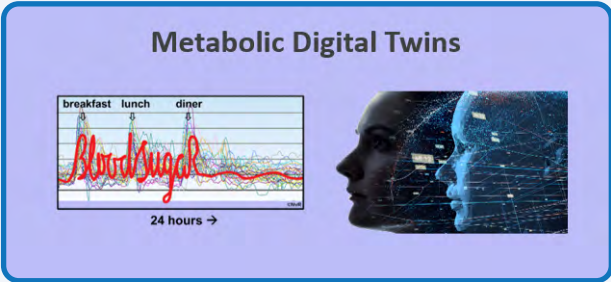CE 1.44c, tel. 8109
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Natal van Riel, Roy van Mierlo, Freek Relouw, Ryan de Vries

In our Systems Biology and Metabolic Disease program we reconstruct human metabolism in computer models. Metabolism is studied and modeled at different levels: intracellular pathways, interactions between organs and tissues, and the processes that control metabolism. In particular, we study the interaction of glucose and lipids in energy metabolism of liver, intestine, adipose tissue and skeletal muscle to discover disease mechanisms underlying chronic, cardio-metabolic diseases associated with obesity and an unhealthy lifestyle, such as Metabolic Syndrome and Type 2 Diabetes. Techniques from machine learning and computational statistics are combined with dynamic models of human metabolism and its multi-level regulation. Experimental and/or patient-derived data combined with nonlinear differential equation models are used for discovery of disease mechanisms and development of personalized approaches for treatment. Network models provide a powerful approach to analyze large and complex datasets, combining data from genetics, transcriptomics, proteomics and meta-bolomics with clinical outcome.

Clinical applications

Metabolic Digital Twins

breakfast lunch diner

BloodSugar

24 hours →

Genome-scale metabolic network models

Systems-biology informed machine learning

Learning
=
mathematical model constraints
+
data similarity
+
regularization

Your Metabolic Digital Twin

Eindhoven Diabetes Education Simulator

For students in the BME and ME master program, and open for both the BMT and MWT major

Federica Eduati, Maaruthy Yellewarapu, Hao Cao, Mike van Santvoort, Esther Visser, Glenn Weber

Tumors are complex ecosystems composed of tumor cells and non-malignant cells (e.g. stroma, immune cells). Tumor development and response to therapy is determined by how molecules and cells interact in the tumor microenvironment. Anticancer treatments aim to either directly target tumor cells (e.g. chemotherapy, small-molecule inhibitors) or boost the body's own immune system to fight cancer (e.g. immune checkpoint blockers). Response to treatment is mediated by dynamic intra- and intercellular networks, where the overall behavior cannot be predicted from individual component. Rather than focusing on individual cellular mechanisms, we use systems biology to have a holistic view of how cells and molecules interact in the tumor and define tumor behavior.

We use machine learning approaches to:

Biomarker-based diagnostic and prognostic machine learning

Healthy

Cancer

Non-responder

Responder
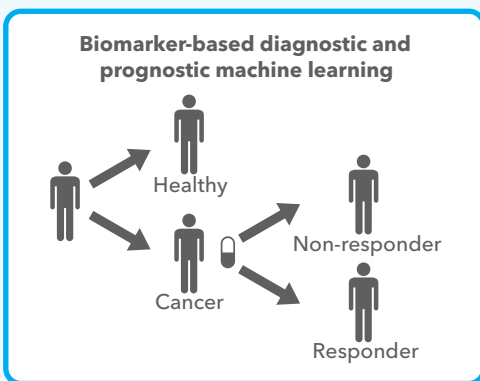
- Support cancer diagnosis and treatment follow-up based on biomarkers measured in blood samples (with Catharina Hospital, Eindhoven).
- Derive mechanistic system-based signatures of the tumor microenvironment from genomic data to predict patients' response to immune checkpoint blockers (with Institute of Molecular Biology (IMB), Innsbruck).

We develop network-based models to:
- Study intracellular pathways deregulations in tumor cells (with Heidelberg University).
- Understand mechanisms underlying T cells plasticity (with IMB, Innsbruck).
- Derive multicellular models of tumor development (with Netherlands Cancer Institute).

Mathematical modeling of inter- and intra-cellular communication

Tumor cells   Immune cells   Fibroblasts

- Build probabilistic cell-cell interaction models to study inter-patient differences (with Mathematics department, TU/e).

Microfluidics Perturbation Screening (MPS) platform

cells+drugs

functional measure
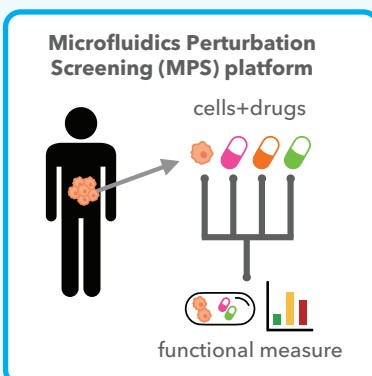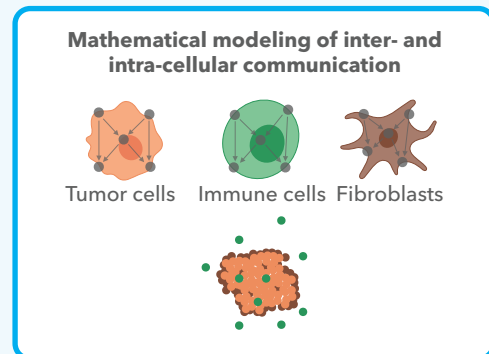
We work on a new microfluidics-based technology to perform high-throughput drug screening directly on live cells from cancer patients' biopsies. This data uniquely allows to study intracellular signaling in individual patients and build predictive models of treatment response to guide personalized therapy.

Shauna O'Donovan, Max de Rooij

The innate immune system forms our first line of defense against infection. Impairments in immune function in aging and obesity can give rise to chronic low-grade inflammation, contributing to the development of cardiometabolic diseases. We use mathematical models and machine learning to untangle the complex processes that underly immune responses to acute infection and sepsis.

Personalised models reveal sub-populations in immune health
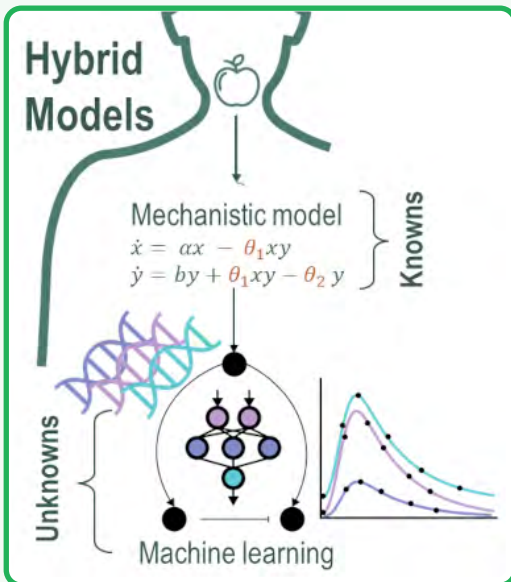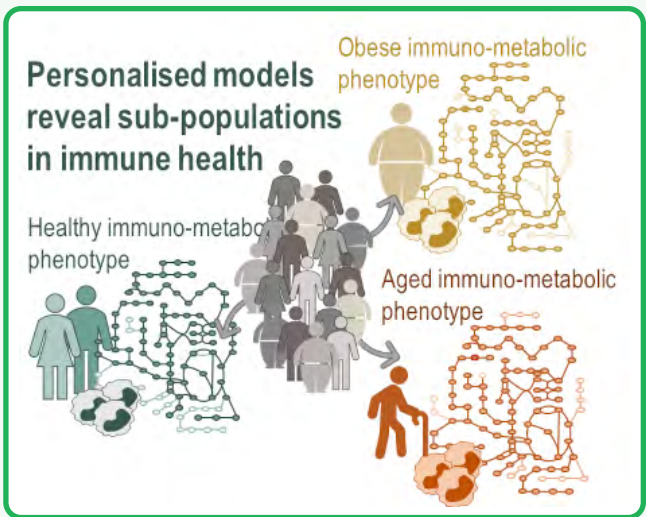
We also develop hybrid modelling approaches; combining machine learning with mechanistic models to integrate data from sensors and clinical/omics measurements in blood to create personalised models of immunometabolism. These models are used to reveal differences in immune metabolism and function between individuals that lead to disease states. Our aim is to build a Digital Twin of immunometabolism, helping us to identify those at risk of disease development earlier, allow continuous monitoring of patients, and provide decision support to clinicians by predicting targeted personalised treatment plans to restore health.
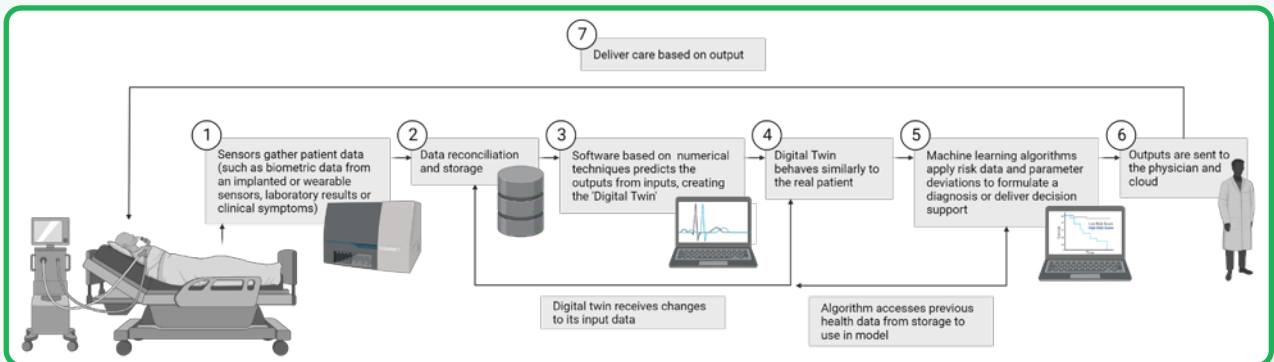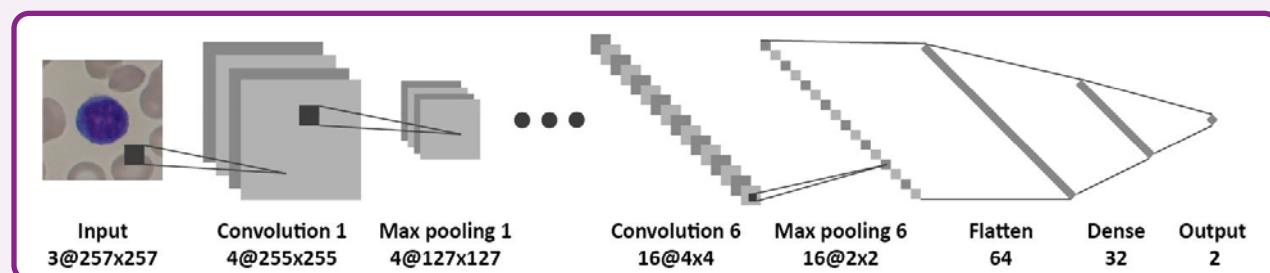
Dragan Bošnački, **Peter Hilbers**, **Natal van Riel**, Ruben Deneer, Jonna van der Stam, Boris Breuer

Next to approaches from systems and computational biology, we use data analysis techniques, including machine learning and artificial intelligence, and methods of algorithmic nature for modelling diseases and disease progression. Formalisms like graphs, formal grammars, and automata are used to develop cutting-edge scalable solutions to meet big data challenges. To this end we capitalize on the capabilities of the state-of-the art parallel technology, like GPUs, multi-core processors, and computer clusters.

In close collaboration with hospitals we develop and apply algorithms and models to analyze data of patients and make predictions about treatment. For example, to identify genetic variants in the DNA of patients with inherited metabolic diseases, to develop predictive models to quantify metabolic health in Metabolic Syndrome patients undergoing bariatric surgery, or to extract diagnostic and predictive information from continuous glucose measurements in diabetes patients. Based on molecular data of the patient the models will assist in establishing more accurate diagnosis and more targeted and personalized medication or other therapy. Recent examples in this context include developing diagnostics methods for COVID-19.
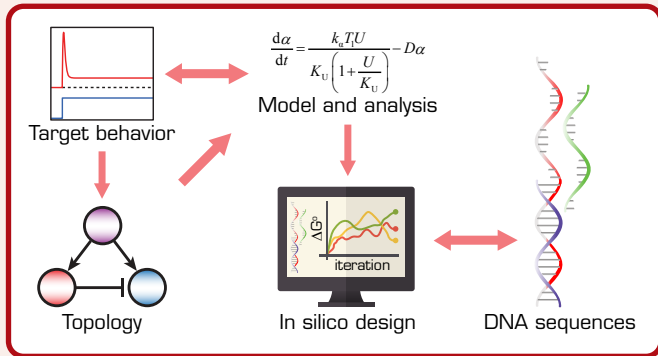
We have extensive collaboration with other research groups at BME: BioInterface Science, Biomedical Materials and Chemistry, Molecular Biosensing for Medical Diagnostics, Nanoscopy for Nanomedicine, and Chemical Biology, as well as research groups abroad, like the Institute for Computational Biology (Helmholtz Centre, Munich). We apply advanced data analysis techniques, e.g., deep learning and convolutional neural networks, on a broad range of topics. The examples include influence of topography features of surfaces on cell proliferation, developing of polymer arrays for high throughput screening, topics in digital pathology, like image analysis for automated diagnostic of leukaemia and non-alcoholic fat liver disease.

Input	Convolution 1	Max pooling 1	Convolution 6	Max pooling 6	Flatten	Dense	Output
3@257x257	4@255x255	4@127x127	16@4x4	16@2x2	64	32	2

DATA SCIENCE AND BIOINFORMATICS

For students in the BME and ME master program, and open for both the BMT and MWT major

Tom de Greef, Tom Meuleman, Indra Van Zundert, Mart Bartelds, Bas Bögels, Jesse Lentjes, Ardjan van der Linden, Anna Makri Pistikou, Bryan Nathalia, Gökçe Özkul, Robin Vermathen, Angelina Yurchenko

SYNTHETIC BIOLOGY

In 1988, the famous physicist Richard Feynman wrote on a Caltech chalkboard: "What I cannot create I do not understand". This phrase captures the central goal of the emerging field of synthetic biology in which scientists challenge the bewildering complexity of nature by building new biological systems using

$$\frac{\mathrm{d}\alpha}{\mathrm{d}t} = \frac{k_a T_i U}{K_U\left(1+\dfrac{U}{K_U}\right)} - D\alpha$$

Model and analysis

Target behavior

Topology

In silico design

DNA sequences

forward engineering principles. Typically, synthetic biology is 'top down' in the sense that it uses cellular platforms and then re-engineers the cellular circuitry for some desired purpose. Another approach to engineering novel biological systems works strictly from the 'bottom up' in the sense that it attempts to construct complex biochemical networks under cell-free conditions. The analysis, modeling, and experimental study of such minimal biological systems is a promising route for understanding the fundamental design principles and molecular logic of regulatory networks in living cells. Currently, we are using enzymatic and cell-free genetic circuits to design complex biochemical networks using computational methods and employing micro-engineering tools to control biochemical reactions in space and time.

DNA NANOTECHNOLOGY

DNA nanotechnology is a branch of nanotechnology concerned with the design, study and application of synthetic structures based on DNA. DNA nanotechnology takes advantage of the physical and chemical properties of DNA rather than the genetic information it carries. We use DNA nanotechnology to understand how the spatial organization of enzymatic reactions influence signaling transduction and use DNA nanotechnology to understand and enhance immune cells.
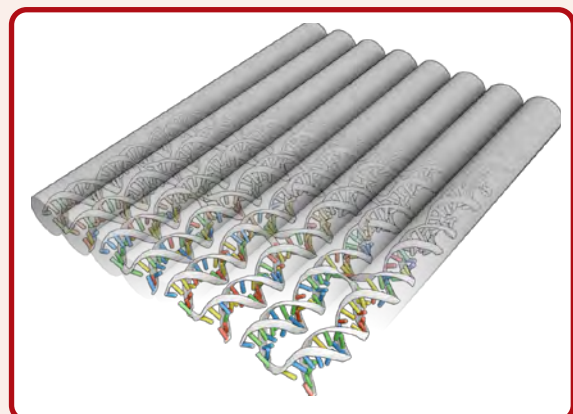
Bart Markvoort, Peter Hilbers

Self-assembly is the autonomous organization of molecules into patterns or structures as a result of weak non-covalent interactions. Examples of interest include the binding of a ligand to a protein, the fibrillization of proteins into amyloidal plaques and the formation of lipid bilayer membranes. In collaboration with several experimental groups, we study these self-assembly processes from a mixed experimental/theoretical point of view. Given the enormous range and complexity of the temporal and spatial dimensions involved in self-assembly of molecular matter, a comprehensive physical understanding is needed on all levels of modeling, i.e., from (quantum-classical) all-atom to coarse-grained representations.

COMPUTATIONAL PROTEIN DESIGN
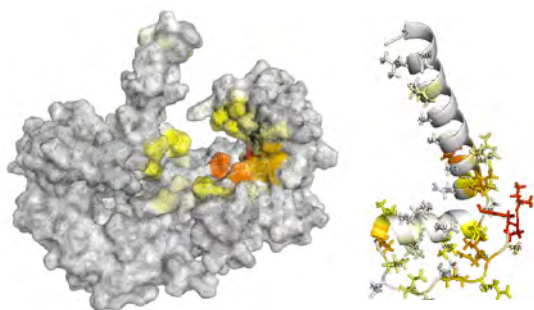
Apart from the exact folding of individual proteins and protein-ligand interactions, also protein–protein interactions (PPIs) are vital in many cellular processes. These are studied using the Rosetta package. Ultimate goal is to understand PPIs and to design customized cell signaling circuits (see Synthetic Biology, cooperation with Chemical Biology group).

## SIMULATION OF MEMBRANES AND MEMBRANE PROCESSES
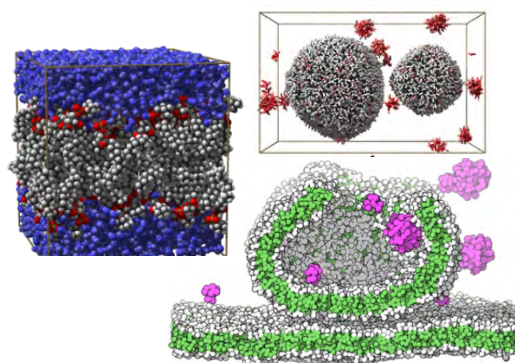
Single membrane proteins can be studied at the atomistic scale using molecular dynamics (MD) simulations. To study larger membranes as well as membrane processes such as vesicle formation, membrane fusion and fission, so called coarse grained MD simulations can be used.

MULTI SCALE SIMULATION OF DNA-ORIGAMI
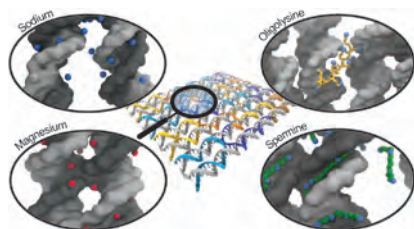
The DNA origami technique has tremendous potential for therapeutic and diagnostic applications, but DNA origamis easily destabilize and degrade *in vivo*. We use both atomistic and coarse-grained simulations to optimize such DNA structures.

FILAMENT FORMATION
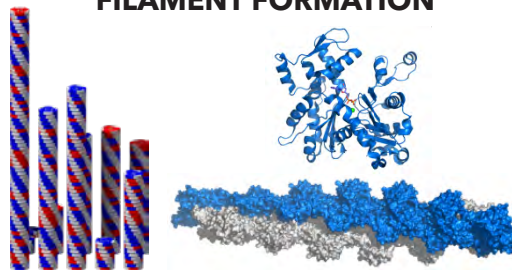
Filament, i.e. long 1D aggregate, formation occurs both for proteins and synthetic molecules. (Un)desirable examples in cells include actin, microtubuli, and amyloid. The aggregation is studied, next to experimentally, using mass-balance models as well as Gillespie simulations.

For students in the BME master program and open for both the BMT and MWT major

Francesca Grisoni, Emanuele Criscuolo, Helena Brinkmann, Yves Nana Teukam, Rıza Özçelik, Derek van Tilborg

Discovering innovative molecules with the desired bioactivity is an essential step to develop new drugs and gather a greater understanding of biological systems. Machine learning bears promise to accelerate the molecule discovery pipeline, by allowing for a time- and cost-efficient navigation of the vast chemical universe.
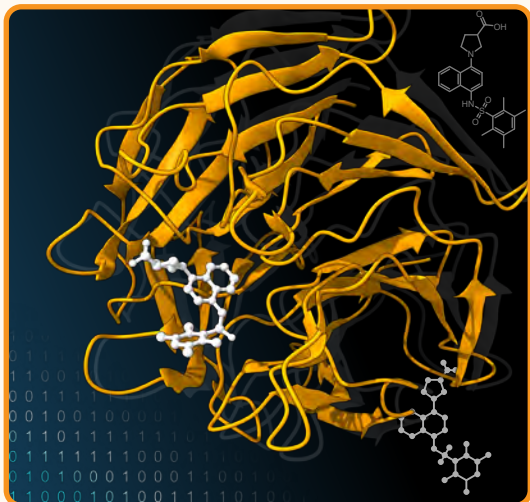
The Molecular Machine Learning team develops and applies data-driven methods to design novel molecules and unveil structure-activity relationships of small molecules and peptides. With research located at the interface between chemistry, biology, and AI, our mission is to develop cutting-edge computational tools to augment human intelligence in drug discovery.

Students can do research on one of the following topics:
- *De novo* design of bioactive molecules with generative deep learning.
- Graph neural networks for bioactivity prediction.
- Explainable artificial intelligence and data-efficient approaches for medicinal chemistry.

If successful, the results of your project will be validated *in vitro*, *e.g.*, in collaboration with the group of prof. Luc Brunsveld. Projects with both machine learning and wet-lab experience are also possible for those of you who want to challenge themselves!
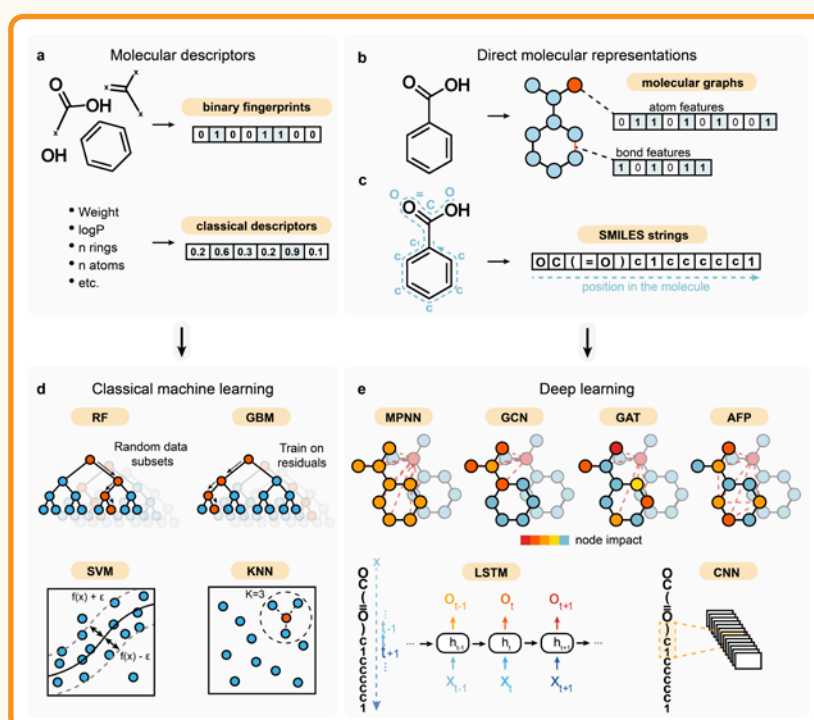
Collaborations within our department

- **BioInterface Science** – genome-scale metabolic models of stem cell growth and differentiation
- **Chemical Biology** – clinical chemistry and clinical data science, Expert Center Clinical Chemistry Eindhoven (ECCCE)
- **Molecular Biosensing for Medical Diagnostics** – mathematical modelling for continuous patient monitoring (sepsis in neonates)
- **BioInterface Science** – differentially expressed gene analysis on macrophages after *in vitro* exposure to flat and textured breast silicone implant surfaces
- **Biomedical Materials and Chemistry** – developing of polymer arrays for high throuput screening
- **Chemical Biology** – identifying epigenetics characteristics of tumour cells using machine learning
- **Molecular Biosensing for Medical Diagnostics** – optical barcoding of nanoparticles
- **Bio-Organic Chemistry** – DPD simulation of polymersome formation and fusion
- **Chemical Biology** – modeling protein-protein interactions
- **Chemical Biology** – *de novo* design and virtual screening with machine learning
- **Nanoscopy for Nanomedicine** – data analysis for nanomaterials

Collaborations within our university

- **EAISI** and **e/MTIC** – advancing cardiac care through interpretable AI (ACACIA)
- **Information Systems (IE&IS)** – wearables and data science for continuous monitoring and digital twinning
- **Institute for Complex Molecular Systems** – immunoengineering program
- **Probability (M&CS)** – probabilistic modelling of cell-cell interaction networks
- **Macro-Organic Chemistry** and **Supramolecular Chemistry & Catalysis (CE&C)** – mass balance models of supramolecular polymers
- **Macro-Organic Chemistry (CE&C)** – machine learning for liquid crystals
- **Supramolecular Chemistry & Catalysis (CE&C)** – machine learning for polymers

Collaborations outside our university

- **Amsterdam UMC (location AMC)** – machine learning and personalized modelling of metabolic disease
- **Catharina Ziekenhuis** – clinical data science for cardiometabolic disease and ICU
- **Maastricht University (Maastricht Centre for Systems Biology)** – systems biology of obesity and metabolic syndrome
- **Máxima Medisch Centrum** – digital twinning and serious gaming for patients with diabetes
- **Philips** – advancing cardiac care through interpretable AI (ACACIA)
- **UMC Utrecht** – genome-scale metabolic models of inborn errors of metabolism
- **Catharina Ziekenhuis** – biomarkers from liquid biopsies for lung cancer diagnosis and follow-up
- **EPFL, Switzerland** – microfluidics perturbation screening platform
- **Heidelberg University, Germany** – mechanising modeling of intracellular signaling pathways
- **University of Innsbruck (Institute of Molecular Biology), Austria** – characterization of the tumor microenvironment and immunotherapy prediction

- **Netherlands Cancer Institute** – multicellular modeling of prostate cancer tumor microenvironment
- **Wageningen University (Human Nutrition)** – precision nutrition, digital twinning, immunometabolism
- **Amsterdam UMC (location AMC)** – effectiveness prediction of fecal microbiota transplants in metabolic syndrome obese patients using machine learning
- **Helmholtz Center (Institute of Computational Biology), Germany** – image analysis with convolutional neural networks for automated diagnostics of leukaemia
- **IBM Zurich, Switzerland** – enzyme design with machine learning
- **Ludwig Maximilian University of Munich, Germany** – computer-assisted medicinal chemistry
- **Novartis, Switzerland** – generative AI for drug discovery
- **Sanofi** – explainable AI for *de novo* design

Key publications

- N.A.W. van Riel, C.A. Tiemann, P.A.J. Hilbers, A.K. Groen, *"Metabolic modeling combined with machine learning integrates longitudinal data and identifies the origin of LXR-induced hepatic steatosis"*, Frontiers in Bioengineering and Biotechnology 2021, *8*, 536957. DOI: 10.3389/fbioe.2020.536957

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- E. Visser, S.A.A.M. Genet, R.P.P.A. de Kock, B.E.E.M. van den Borne, M. Youssef-El Soud, H.N.A. Belderbos, G. Stege, M.E.A. de Saegher, S.C. van 't Westeinde, L. Brunsveld, M.A.C. Broeren, D. van de Kerkhof, B.A.L.M. Deiman, F. Eduati, V. Scharnhorst, *"Liquid biopsy-based decision support algorithms for diagnosis and subtyping of lung cancer"*, Lung Cancer 2023, *178*, 28–36. DOI: 10.1016/j.lungcan.2023.01.014

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- B. Erdős, B. van Sloun, M.E. Adriaens., S.D. O'Donovan, D. Langin, A. Astrup, E.E. Blaak, I.C.W. Arts, N.A.W. van Riel, *"Personalized computational model quantifies heterogeneity in postprandial responses to oral glucose challenge"*, PLoS Computational Biology 2021, *17*(3), e1008852. DOI: 10.1371/journal.pcbi.1008852

- J.P.E. Schouten, C. Matek, L.F.P. Jacobs, M.C. Buck, D. Bošnački, C. Marr, *"Tens of images*

can suffice to train neural networks for malignant leukocyte detection", Scientific Reports 2021, *11*(1), 7995. DOI: 10.1038/s41598-021-86995-5

- S.L.M. van Loon, R. Deneer, S.W. Nienhuijs, A. Wilbik, U. Kaymak, N.A.W. van Riel, V. Scharnhorst, A.-K. Boer, *"Metabolic health index (MHI): Assessment of comorbidity in bariatric patients based on biomarkers"*, Obesity Surgery 2020, *30*, 714–724. DOI: 10.1007/s11695-019-04244-1

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