



HPC/Exascale
Centre of
Excellence in
Personalised
Medicine

PROJECT OVERVIEW



The PerMedCoE project has received funding from the European Union's Horizon 2020 research and innovation programme under the grant agreement N°951773

OVERVIEW

PerMedCoE

Grant agreement ID: 951773

Status

Ongoing project

Start date

1 October 2020

End date

30 September 2023

Funded under

H2020-EU.1.4.1.3.

Overall budget

€ 4 999 567,50

EU contribution

€ 4 999 567,50

Coordinated by

BARCELONA SUPERCOMPUTING CENTER -

CENTRO NACIONAL DE SUPERCOMPUTACION

 Spain



Barcelona
Supercomputing
Center

Centro Nacional de Supercomputación



A donut chart with a blue outer ring and a white center, representing 100% completion.



A map of Europe showing the locations of project partners. Green pins are located in Ireland, United Kingdom, Netherlands, Belgium, Luxembourg, Germany, Czechia, Austria, Slovenia, Croatia, Serbia, Montenegro, Albania, Greece, Italy, Monaco, San Marino, Andorra, Portugal, Spain, France, Liechtenstein, Switzerland, Slovakia, Hungary, Romania, Bulgaria, North Macedonia, Turkey, Cyprus, Syria, Lebanon, Georgia, Armenia, Azerbaijan, Ukraine, Moldova, Belarus, Lithuania, Latvia, Estonia, Denmark, Finland, Sweden, Norway, Iceland, Malta, Tunisia, Algeria, Morocco, Egypt, Libya, Sudan, Ethiopia, Kenya, Tanzania, Uganda, Rwanda, Burundi, DRC, Congo, Angola, Namibia, Botswana, Zimbabwe, Mozambique, Swaziland, Lesotho, South Africa, Madagascar, Mauritius, Reunion, Mayotte, Guadeloupe, Martinique, French Guiana, Guernsey, Jersey, Gibraltar, Madeira, Azores, Canary Islands, Iceland, Faroe Islands, Greenland, and the Azores. A red pin is located in Spain.

HPC/Exascale Centre of Excellence for Personalised Medicine



Per
Med
CoE

PARTNERS



MISSION

PerMedCoE is the HPC/Exascale Centre of Excellence for Personalised Medicine in Europe

Our motivation

The performance of current simulation software is still insufficient to tackle medical problems such as tumour evolution or patient-specific treatments.

Simulation of cellular mechanistic models are essential for the translation of omic data to medical relevant actions and these should be accessible to the end-users in the appropriate environment of the PerMed-specific big confidential data.

Our vision

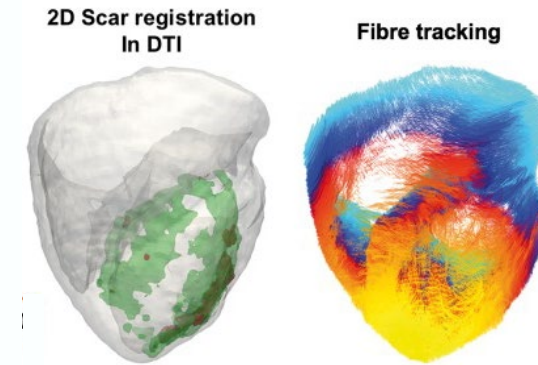
The challenge is to develop a sustainable roadmap to scale-up the essential software for the cell-level simulation to the new European HPC/Exascale systems.

Our goal is **to provide an efficient and sustainable entry point to the HPC/Exascale-upgraded methodology** to translate omics analysis into actionable models of cellular functions of medical relevance.

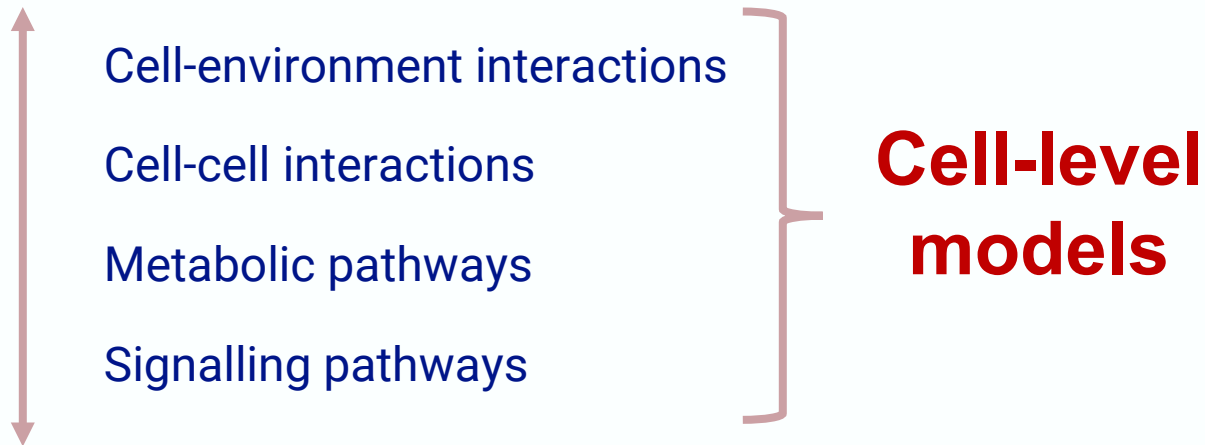
www.permedcoe.eu

PerMedCoE aims to integrate PerMed into the new European HPC/Exascale ecosystem

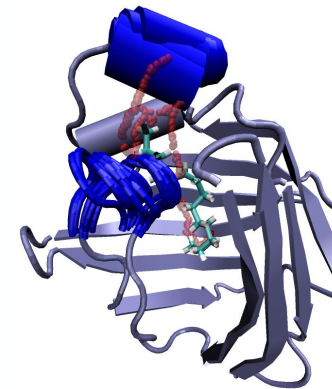
- Physiological-level models (Fluid dynamics – **CompBioMed**)



*Europace. 2019 May,
21(5): 822–832.*



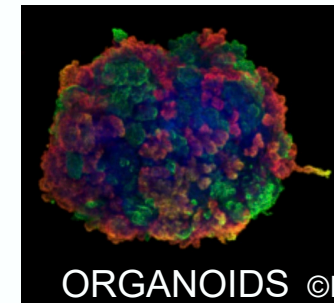
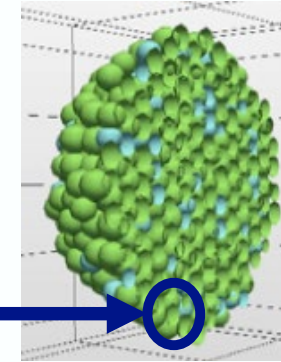
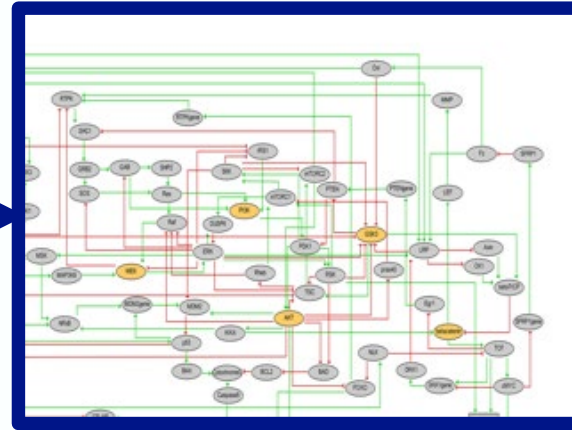
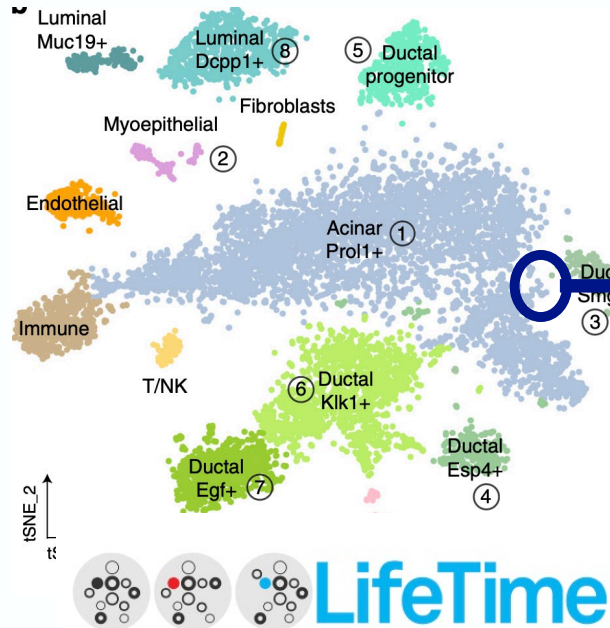
- Atomic-level models (Molecular dynamics – **BioExcel**)



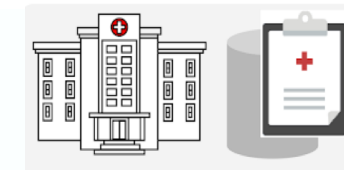
*J. Chem. Theo. Comp.
2005, 6, 1304-1311*



From Single Cell Data to Models

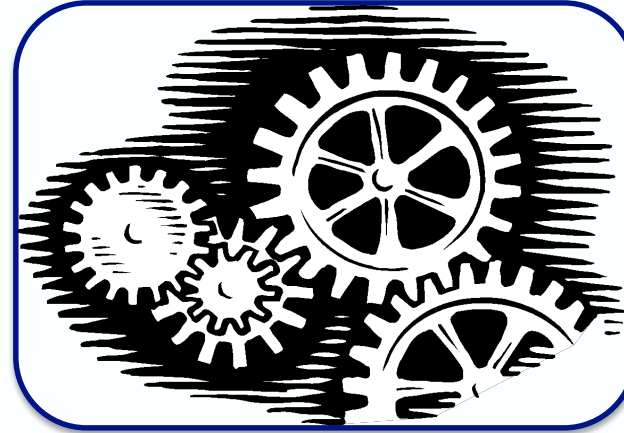
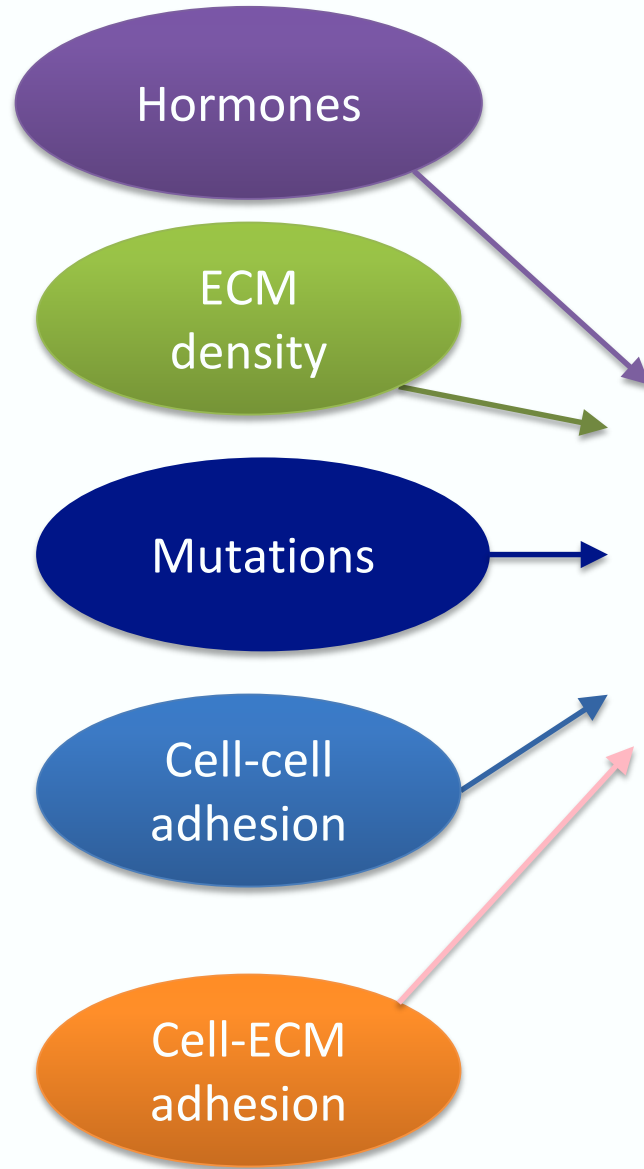


End Users Communities



*"Replace the current generation of bioinformatics methods with **cellular models, providing mechanistic descriptions and testable hypotheses**, instead of current statistical approximations and intuitive descriptions"*

The motivation: Genotype-to-phenotype modelling



Multiscale modelling

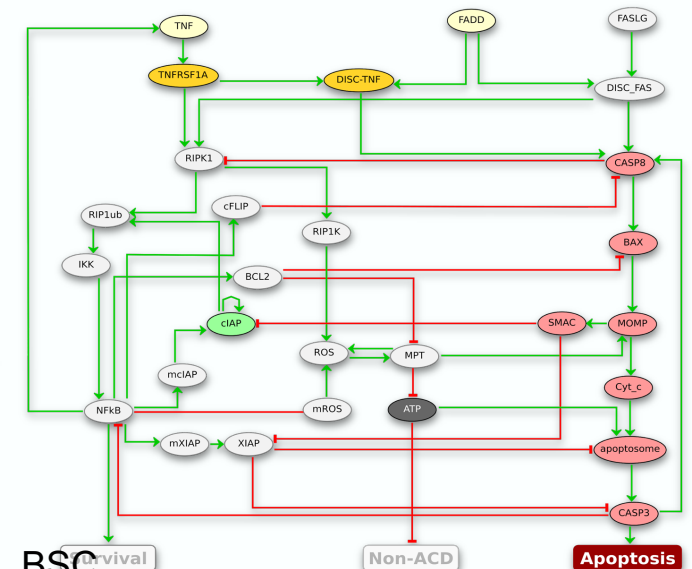
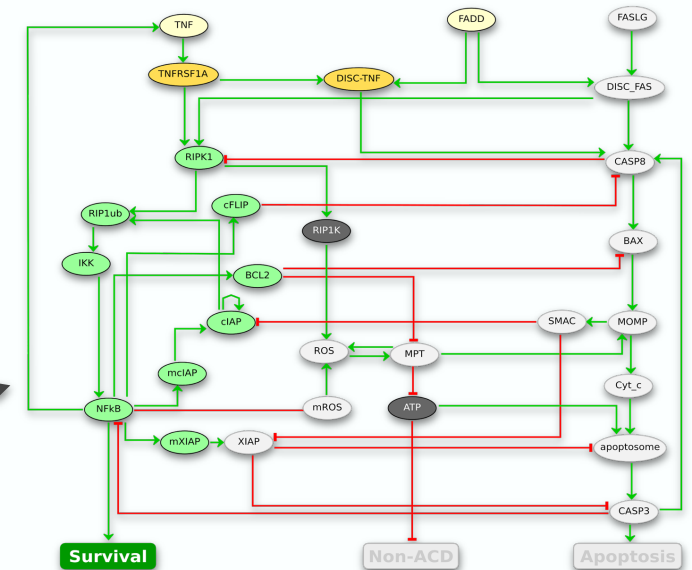
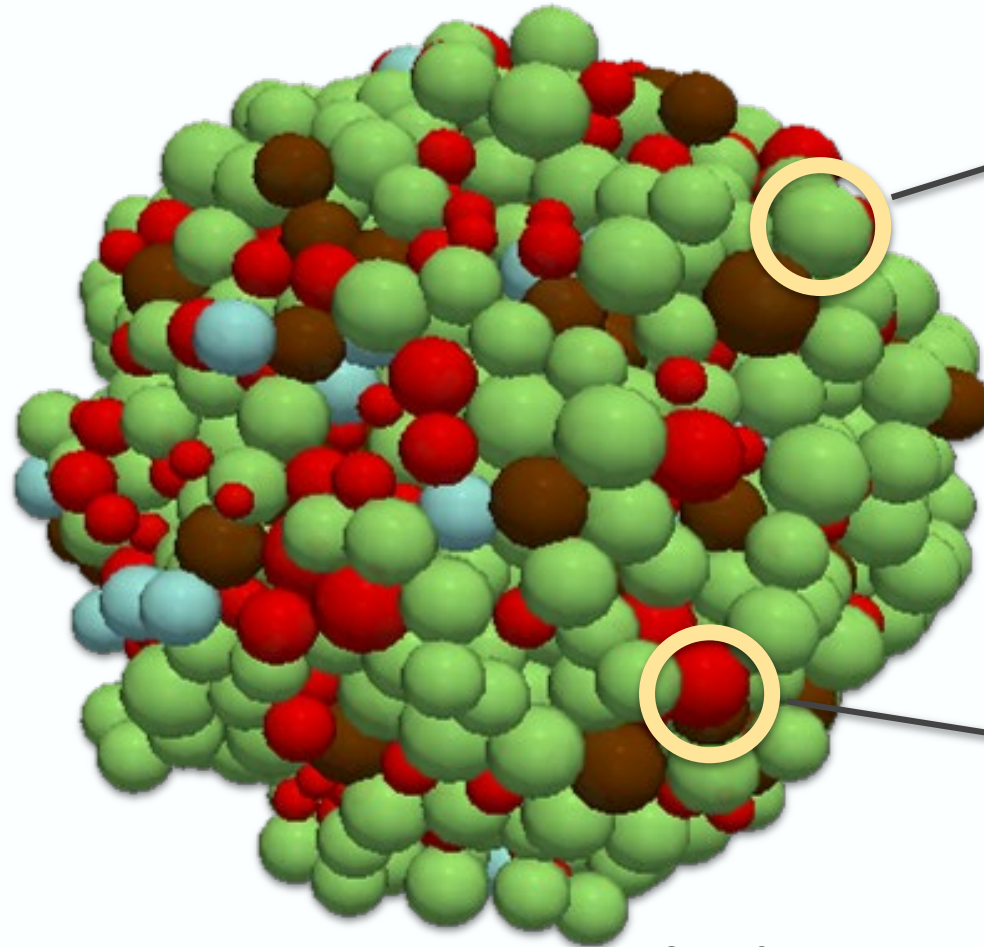
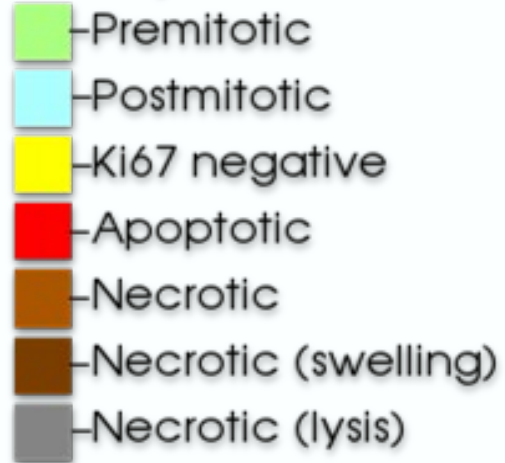
Gene mutations
Signalling pathways
Cell - environment
ECM modification

			Cell-cell junctions	Tumor type
Individual-cell migration	Single-cell migration	Amoeboid	-	Leukemia, lymphoma cell subsets (all tumors)
		Mesenchymal	-	Stromal tumors, epithelial tumors after EMT
	Multicellular streaming	Amoeboid (multicellular)	?	All tumors developing amoeboid single-cell dissemination
		Mesenchymal (multicellular)	(+)	Tumors with mesenchymal invasion; fibroblasts leading tumor cells
Multicellular migration	Collective cell migration	Cluster	++	Moderately differentiated epithelial tumors
		Solid strand	++	Moderately differentiated epithelial tumors with subregions after EMT; basal and squamous cell carcinoma
		Strand (with lumen)	++	Differentiated epithelial tumors; vascular neoplasia
	Expansive growth	Strand (protrusive)	++	Moderately differentiated epithelial tumors lacking EMT
		Outward pushing tumor	++	All solid tumors

Friedl and Alexander, *Cell*, 2011

Cells have different phenotypes depending on their genes' activation

Different cells have different signalling states

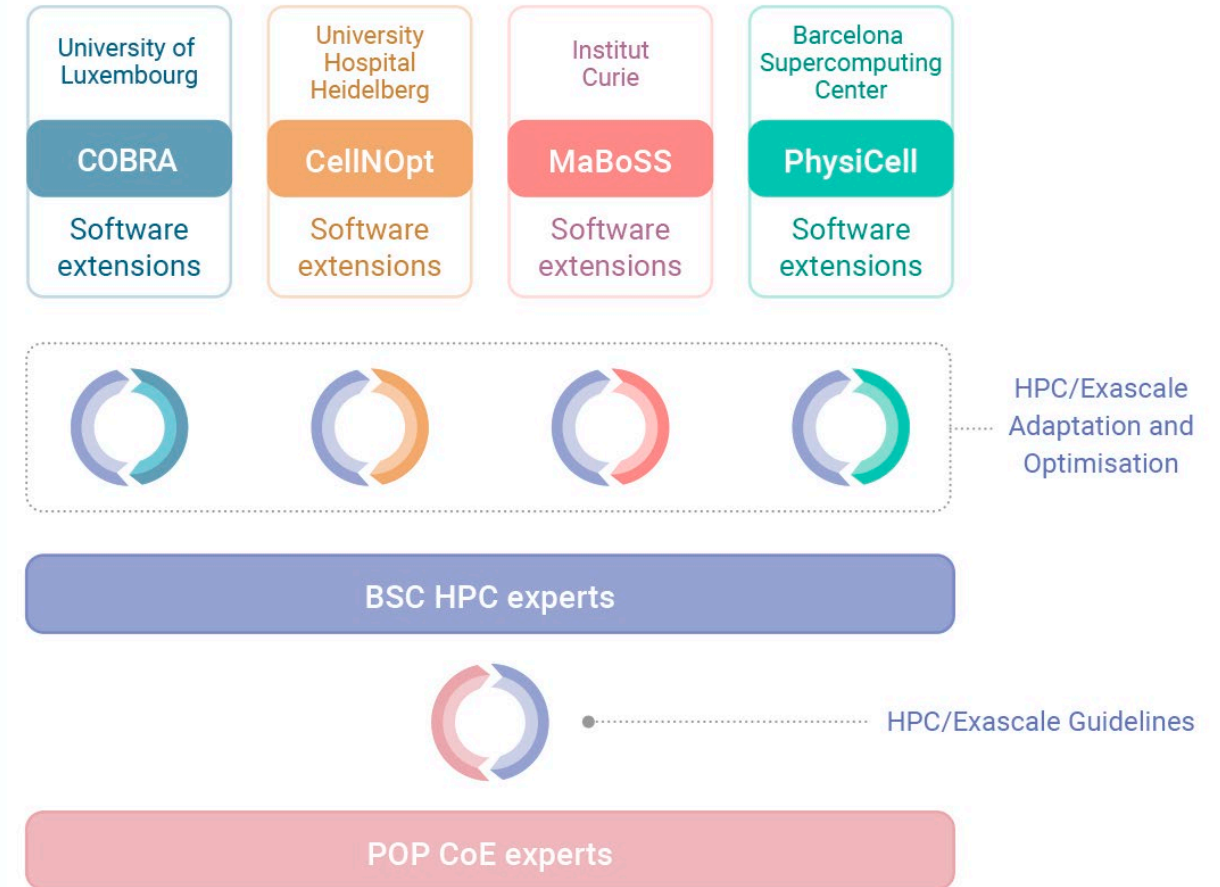


CORE APPLICATIONS

PerMedCoE optimises key software for cell-level simulations to the new preexascale platforms

The PerMedCoE four core applications are:

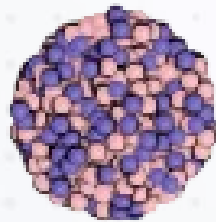
- **COBRA** for the simulation of cellular metabolism at genome-scale
- **CellNOpt** for modelling signal transduction networks
- **MaBoSS** for stochastic simulations of Boolean models
- **PhysiCell** an agent-based modelling framework for simulating cell-cell interactions



For more information, visit <https://permedcoe.eu/core-applications/>

USE CASES

PerMedCoE works on five use cases to drive the development of cell-level simulations



Tumour Evolution
Based on Single-Cell
Omic and Imaging

USE CASES

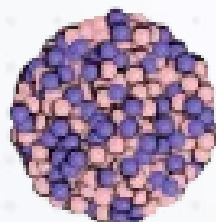
PerMedCoE works on five use cases to drive the development of cell-level simulations



COVID-19
Multiscale
Modelling of
the Virus and
Patients' Tissue



Cancer Diagnosis
Based on Omics
Information



Tumour Evolution
Based on Single-Cell
Omic and Imaging



Drug Synergies for
Cancer Treatment



Personalised
Modelling of Groups
of Rare-Disease
Related Patients

USE CASES

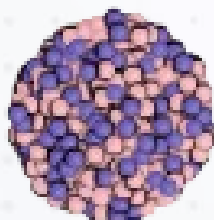
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COVID-19
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Cancer Diagnosis
Based on Omics
Information



Tumour Evolution
Based on Single-Cell
Omic and Imaging

**Standard Cancer
Practice
/
Hospitals / Health
Software Providers**

**Cancer Research
/
Biotech & Omic to
Organois based**



Drug Synergies for
Cancer Treatment



Personalised
Modelling of Groups
of Rare-Disease
Related Patients

**Clinical Trials
/
Pharma**

**Rare Diseases
/
EU Health Systems &
Patient Organisation**

THANK YOU



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