

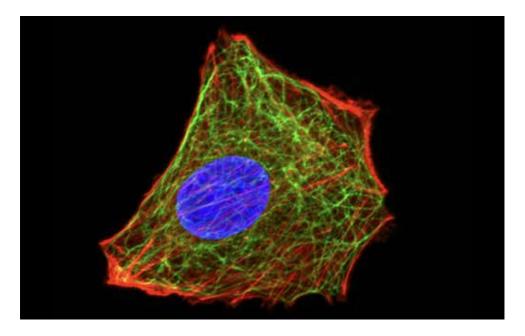


# CBIO CENTRE FOR COMPUTATIONAL BIOLOGY

### CBIO: RESEARCH DRIVING INNOVATIVE HEALTHCARE

The Centre for Computational Biology (CBIO), *Centre de Bio-informatique*, at Mines Paris – PSL develops machine learning methods to analyze biological data, from the molecular scale to that of populations. In addition to its

contributions to fundamental biology, the center engages in numerous partnerships focused on drug discovery and personalized medicine, including a close collaboration with the Institut Curie.



Mines Paris – PSL offers training from the engineering curriculum through to the PhD level, supported by its 18 research centers organized into five departments aligned with major themes and future societal challenges.

As part of Université PSL, recognized for its international excellence, the School provides CBIO with an ideal environment to combine theoretical knowledge with practical applications.

In line with a double-impact approach, CBIO forges strong connections between academic research and industry, guiding strategic thinking among economic players and strengthening innovative collaborations to address today's key challenges.

### **KEY FIGURES OF CBIO**



### OVERVIEW

CBIO stands out for its high-level publications, the result of the work conducted by our researchers, helping shape the future of economic and industrial challenges.

35+ scientific		50+ collaborations
publications	10 PhD projects	in France
each year	underway, including 2	and abroad
	with industry partners	
4 postdocs		50+ alumni

#### Thomas Walter - Director of CBIO, Professor

Develops artificial intelligence and computer vision methods for the analysis of biomedical images, with applications such as high-content screening and computational pathology.

#### Chloé-Agathe Azencott - Associate Professor

Focuses on developing and applying machine learning techniques for therapeutic research, with a particular interest in feature selection in high-dimensional multi-omics data.

#### Véronique Stoven - Professor

Specializes in computational biology approaches, combining docking and machine learning to study protein-ligand interactions and understand molecular recognition mechanisms, particularly in drug design.

#### Florian Massip - Research Scientist

Investigates the causes of genomic alterations and their impact on human health, exploring their connections with diseases and underlying biological mechanisms.

#### Vincent Mallet - Research Scientist

Works on machine learning for protein and RNA structure, using geometric deep learning with applications in structural bioinformatics and drug design.

#### Éloïse Berson - Junior Professor (Chair)

Develops multimodal deep learning methods applied to genomic and clinical data, with applications in neuroscience and Alzheimer's disease research.

#### **Key Publications**

• Komet is a predictive algorithm for drug-target interactions. Trained on the extensive LCldb dataset, it outperforms current state-of-the-art methods.

G. Guichaoua, P. Pinel, B. Hoffmann, C.-A. Azencott, and V. Stoven. Drug-Target Interactions Prediction at scale: The Komet algorithm with the LCIdb dataset. J. Chem. Inf. Model, 64(18):6938-6956, 2024. doi: 10.1021/acs.jcim.4c00422.

# ComSeg is a cell segmentation algorithm based on the spatial distribution of RNA. Tailored for complex tissues, it enhances cell type analysis and opens new avenues in spatial biology.

T. Defard, H. Laporte, M. Ayan, S. Juliette, S. Curras-Alonso, C. Weber, F. Massip, J.-A. Londoño-Vallejo, C. Fouillade, F. Mueller, and T. Walter. A point cloud segmentation framework for image-based spatial transcriptomics, *Communications Biology*, 2024. doi: 10.1038/s42003-024-06480-3

# This method models bacterial evolution by integrating mutations and horizontal gene transfers, enabling the estimation of divergence times between species and the construction of calibrated phylogenetic trees.

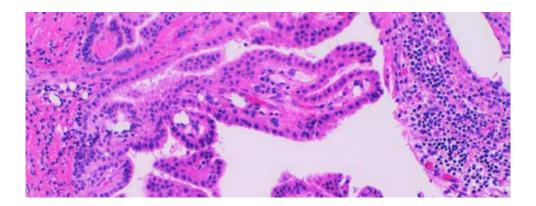
M. Sheinman, P.F. Arndt, F. Massip, Modeling the mosaic structure of bacterial genomes to infer their evolutionary history, *Proceedings of the National Academy of Science*, 2024, doi: https://doi.org/10.1073/pnas.2313367121

# This deep learning algorithm predicts homologous recombination deficiency (HRD) in cancer and uncovers novel morphological features associated with this phenotype.

T. Lazard, G. Bataillon, P. Naylor, T. Popova, F.-C. Bidard, D. Stoppa-Lyonnet, M.-H. Stern, E. Decencière, T. Walter, and A. Vincent-Salomon; Deep learning identifies morphological patterns of homologous recombination deficiency in luminal breast cancers from whole slide images. Cell Reports Medicine, Dec. 2022, doi: 10.1016/j.xcrm.2022.100872



## CBIO RESEARCH AREAS: INNOVATION IN BIOLOGY, MEDICINE, AND DRUG DESIGN



#### Fundamental and systemic in silico biology

CBIO develops methods in statistics and machine learning to model biological systems and address various questions in fundamental biology. This includes molecular biology (cell cycle, replication, RNA distribution within cells), evolutionary biology (molecular evolution, phylogeny), and the study of biological mechanisms involved in disease emergence, particularly cancer. These projects require the integration of complex data such as high-throughput sequencing, spatial transcriptomics, and imaging data.

#### **Predictive and precision medicine**

CBIO creates tools for classifying tumors and identifying biomarkers for diagnosis, prognosis, and treatment response. These tools analyze clinical, genomic, and imaging data using statistical learning and artificial intelligence techniques.

#### **Drug design**

The fundamental approaches at CBIO contribute to identifying new therapeutic targets. When no known drugs exist for these targets, CBIO develops virtual screening methods to identify new molecules that may modulate these targets, serving as drug precursors. This includes the joint analysis of the chemical space of small molecules and the biological space of proteins, aiming to understand the mechanisms behind drug action to optimize their efficacy and minimize side effects.

## FUNDED RESEARCH: INSTITUTIONAL SUPPORT AND INNOVATIVE PROJECTS

#### **Partnering institutions**

European	National Agency for	Cancéropôle
Commission	Research (ANR)	Île-de-France
Institut Pasteur	Institut Curie	INSERM

#### Our key collaborative funded projects

# ANR (PRCI): "STEVE" – considering transposable elements and their epigenetic variation in genotype-phenotype relationship studies

In this collaboration with biologists from ENS – PSL, CBIO investigates the role of transposable elements and their methylation in the relationship between the genome and phenotype, aiming to integrate them into genotype-phenotype studies. This interdisciplinary project aims to better understand the genetic basis of complex traits and the impact of transposable elements, with applications in human health and agriculture.

# Carnot M.I.N.E.S: biomarkers/data extraction for prediction. Image analysis and machine learning for health diagnostics

This international collaboration with researchers and clinicians from the University of Cambridge aims to develop an early and non-invasive diagnostic tool for lung cancer, often detected at an advanced stage. Our work focuses on statistical methods applied to high-throughput sequencing data (RNAseq) to identify biomarkers and identify patients at risk.

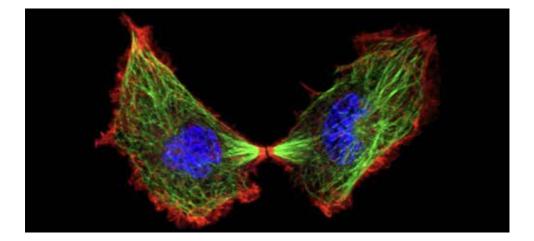
# PRTK – SELECT: prediction of survival in bladder cancer patients treated with neoadjuvant chemotherapy before cystectomy

Muscle-invasive bladder cancer (MIBC) is a common and aggressive disease. Identifying and validating criteria to identify patients who could benefit from neoadjuvant chemotherapy (NAC) is a major need. Our project aims to optimize the prediction of survival in MIBC patients treated with NAC using predictive models for histopathological slides.

## A COLLABORATIVE NETWORK DRIVING INNOVATION

CBIO develops strategic partnerships with academic, industrial, and institutional stakeholders to foster innovation and address technological challenges. These collaborations bridge fundamental research and practical applications, supporting the emergence of new solutions and the implementation of cutting-edge technologies in fields such as bioinformatics and precision medicine.





#### Academic-industry collaborations

Direct partnerships Service agreements Sponsorship chairs

Publicly funded research projects

Research consortia Industrial PhD contracts Joint laboratories

## SUPPORT FOR INNOVATIVE PROJECTS

## Mines Paris – PSL mobilizes the expertise of its research teams and specialists to establish collaborations:

- accelerated development of products and services
- exploring new markets
- access to funding and grants for collaborative projects
- trengthening teams through the integration of specialized skills (industrial PhD contracts, etc.)
- expanding professional networks and increasing visibility
- activities with high societal impact

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