FastCompChem

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UNLOCKING QUANTUM POTENTIAL

GET STARTED →

www.quantum-tox.eu

FastCompChem

Pedro Lopes, PhD
Founder & CSO

Founder

Quantum Chemist

Post-Doc Researcher
University of Manchester

Research
Fellow CDC, USA

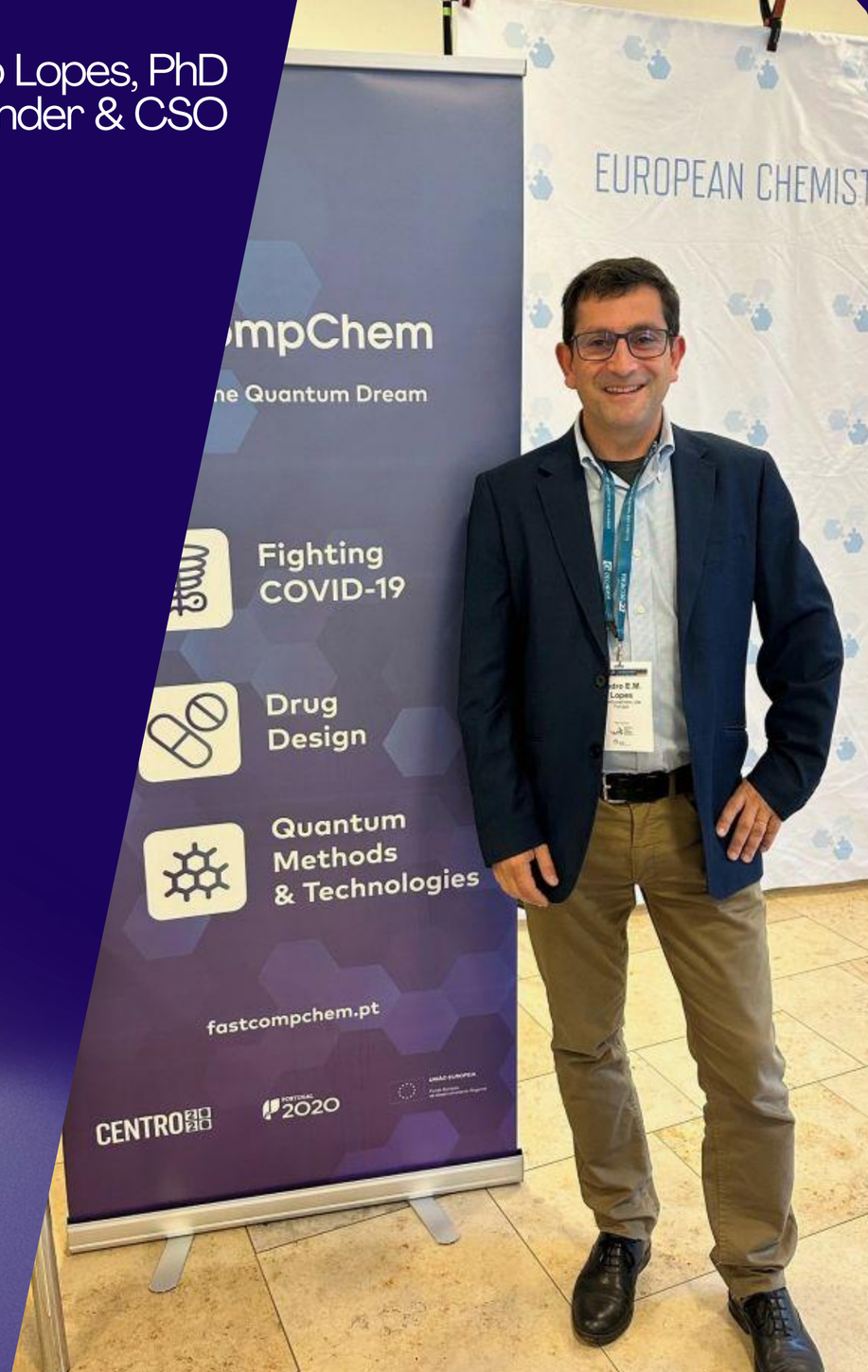
Faculty position
School of Pharmacy
University of Maryland
Baltimore, USA

Relevant publications

SPRINGER NATURE

arXiv

> 15.000 citations on Google Scholar



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Current Focus

BRINGING QUANTUM MECHANICS TO DRUG-DISCOVERY

Quantum Chemistry

Artificial Intelligence

Computational Toxicology

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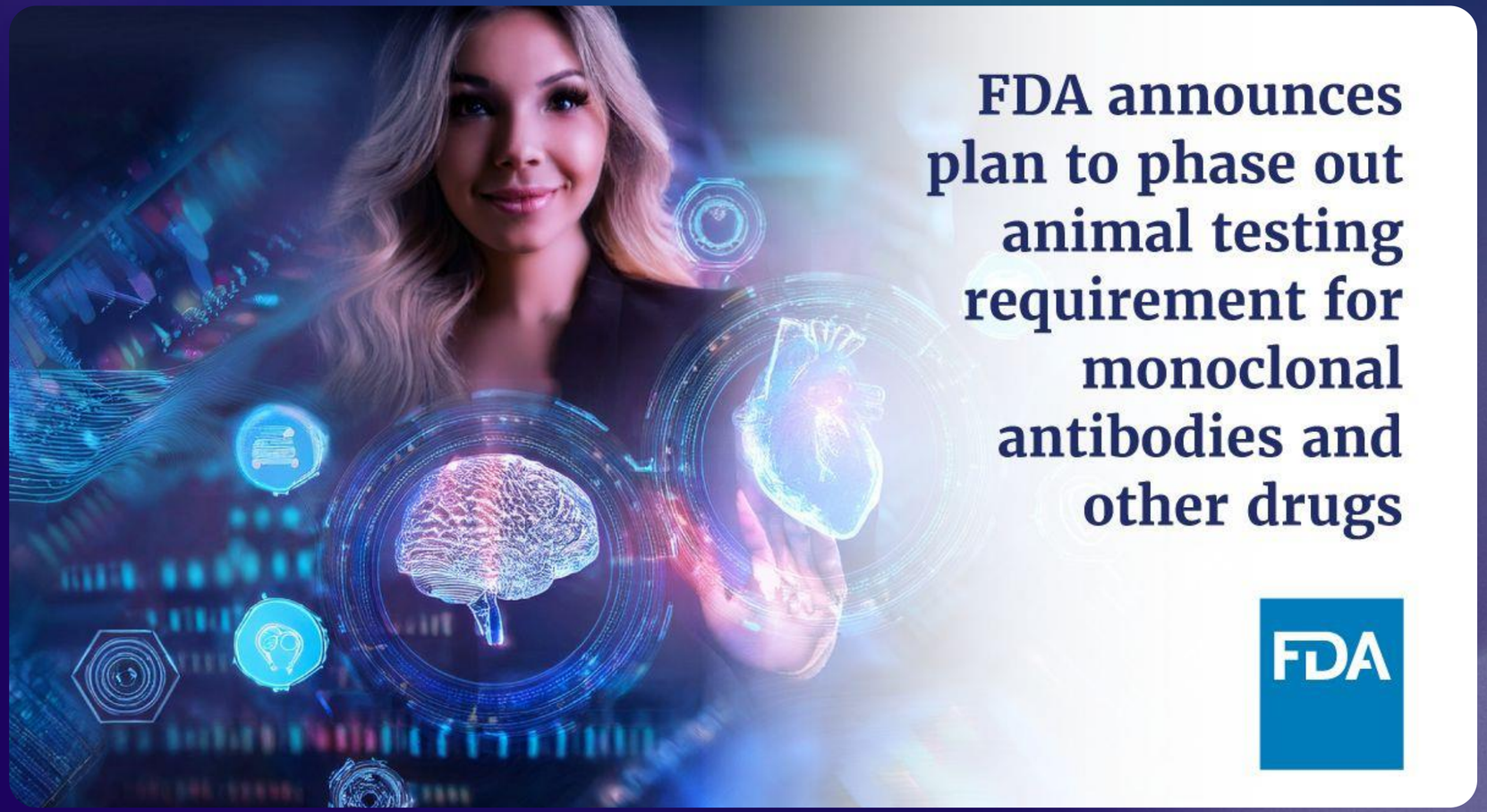
Momentous Change

April 10, 2025



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Toxicology Screening

Addressing current shortcomings

Disruptive Innovation

E-Signs
(Electronic Fingerprints)

- A new type of descriptor, totally based on **quantum mechanics;**
- Uses **Artificial Intelligence** to relate the ESigns to toxicity;
- Can cover the whole chemical space;
- Relies on a small number of parameters that are easily interpretable.

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Toxicology Screening

ROADMAP for Collaborative Development

APPROVED EC GRANT

EIC Pathfinder

European Innovation Council

One of the 57 projects selected, out of 858 applicants

FastCompChem retains **commercial rights**

Renowned **Academic Partners**

LIVERPOOL JOHN MOORES UNIVERSITY

ISTITUTO DI RICERCHE FARMACOLOGICHE MARIO NEGRI · IRCCS

MANCHESTER 1824

The University of Manchester

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Maximize Use of HPC

Reactivity studies of well-defined organic reactions (ex. Michael additions)

Perturbation studies of intermomecular forces

Ingenuity in the theoretical approaches: avoidance of costly and hard to define chemical structures (ex. transition states)

Application to thousands of compounds

Reliance on common QM software: Gaussian, PySCF and MOPAC

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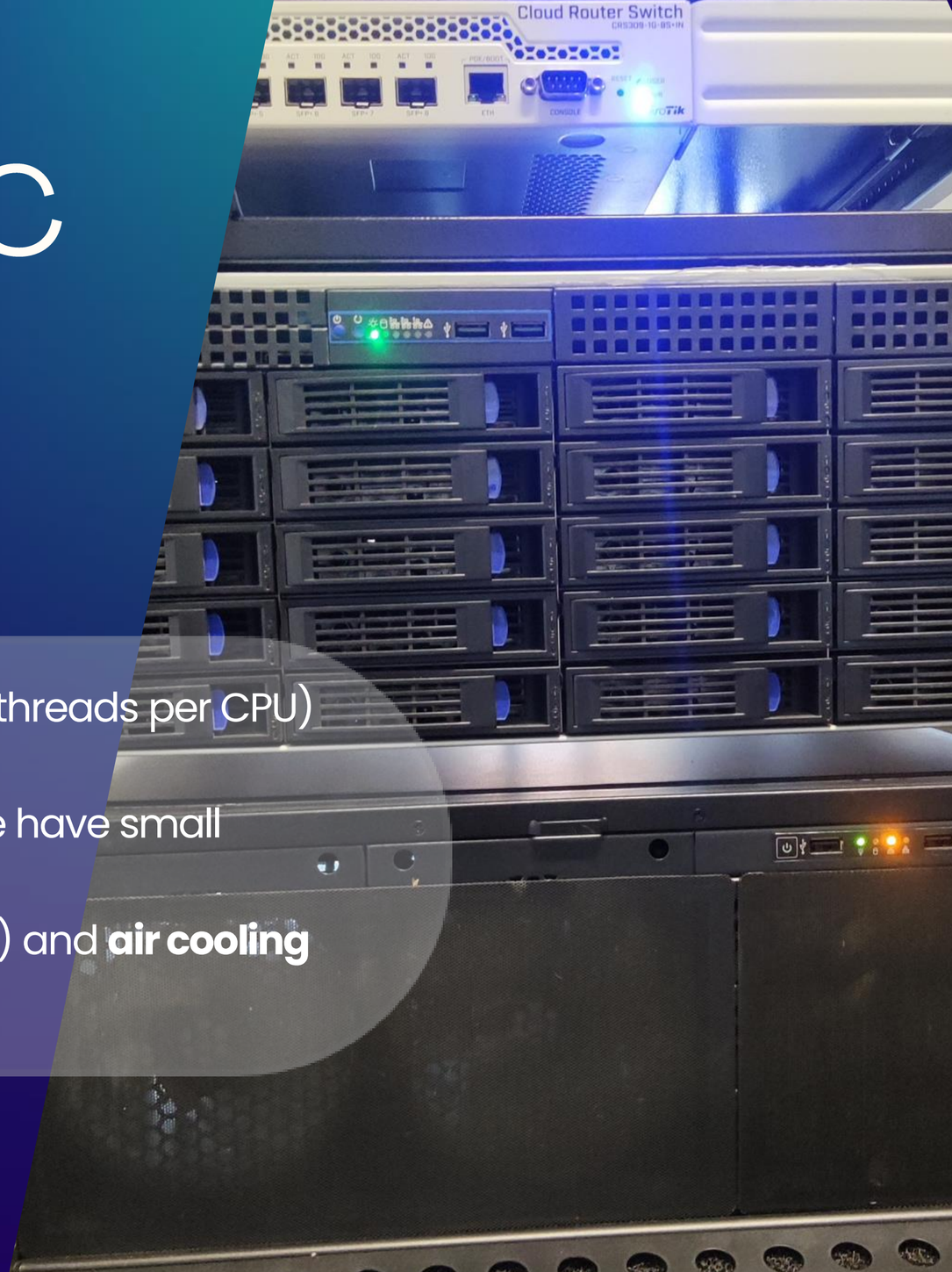
FastCompChem's HPC

SIMPLICITY AND COST EFFECTIVENESS

- Compute nodes with **AMD Zen4 Epyc 9754** (128 cores / 256 threads per CPU) – Currently Zen5 cores
- Small **258 GB memory per node** (QM calculations as we use have small memory requirements)
- **4U nodes** to maximize use of commodity hardware (ex. PSU) and **air cooling**
- Future **scalability, SLURM, Ubuntu Server**



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Difficulties

LACK OF QUALIFIED PERSONNEL IN QUANTUM CHEMISTRY

- No active research in Quantum Chemistry in Portugal
- **Low attractiveness** for northern European scientists
- Difficulty in processing immigration VISAs

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Core Team

PEDRO LOPES, PhD

Founder & CSO

QUANTUM CHEMIST

VÍTOR CRESPO

CEO

MANAGEMENT & VENTURE BUILDING

BEATRIZ COSTA, MSc

CTO

COMPUTER SCIENCE AND AI ENGINEER

SOFIA ALMEIDA, MSc

Intern

CHEMIOINFORMATICS ANALYST