Alexandre (Alex) Borrel, PhD.

ORCID: 0000-0001-6499-4540 | https://www.alexborrel.com/ | h-index 16 (Google Scholar) | 28 peer review publications

Profile

A friendly, detail-oriented, and engaging team player and leader, adept at inspiring teams to achieve their best. A multi-tasking PhD-level Cheminformatician specializing in the application of modern AI, including deep learning and generative models, for toxicology. Possesses extensive expertise in QSAR modeling, analysis of high-throughput screening data, and the development of scientific software and web applications, complemented by strong project and team management capabilities.

Experience

CHEMINFORMATICIAN | SCIOME LLC | NC, USA | AUGUST 2024 – PRESENT

- Support NTP Interagency Center for the Evaluation of Alternative Toxicological Methods (NICEATM).
- Develop modeling for carcinogenicity, mutagenicity using modern AI such as muti-task deep learning.
- Support development of generative chemistry AI, work on selecting oracles, analysis output and improve fine tuning, benchmarking datasets.
- Support development of software such as OrbiTox and the NIH Integrated Chemical Environment (https://www.sciome.com/), providing scientific content support and technical support.
- Develop agentic tools with LLM orchestration.
- Actively mentor junior researchers, and continuously present research and education courses at national conferences (e.g., SOT Annual Meeting).

PRINCIPAL CHEMINFORMATICIAN | INOTIV | NC, USA | JULY 2022 – AUGUST 2024

- Support NICEATM – part of the PFAS group and scientific lead of the NIH Integrated Chemical Environment (https://ice.ntp.niehs.nih.gov/).
- Development of class based read across on organophosphate flame retardant.
- Developer and Scientific Advisor to ensure high standards of computational reproducibility for https://biobricks.ai/ a bioinformatic repository.
- Analysis of high throughput screening data from the ToxCast/Tox21 US program.
- KNIME workflows development for regulatory purposes, PBTK/IVIVE modeling and data formatting in international standards (OHT 201).
- Management of the cheminformatic teams. Mentored team members, chaired scientific symposiums, and instructed continuing education courses (e.g., ASCCT Annual Meeting).

BIOINFORMATICS LEAD | SILENT SPRING INSTITUTE | MA, USA | JUNE 2021 – JULY 2022

- Development of QSAR models using deep learning for predicting chemicals disrupting steroidogenesis.
- Work on advanced mixture risk assessment models to evaluate combined chemical exposures.
- Collaborated with IT to enhance the PFAS-exchange platform (https://pfas-exchange.org) using Ruby.
- Support of bioinformatics though the institute is participating in various projects such as non-targeted analysis, population modeling, differentiate gene expression analysis.

INDEPENDENT CONSULTANT | FREELANCE | JANUARY 2020 – JUNE 2021

- Build a consulting company in France, develop accounting and administration expertise.

- Design QSAR models for carcinogenicity.
- Analyze chemical space using chemmaps.com for environmental chemicals.
- Support development of population specific anti-diabetic drug.

POST-DOC | NIH/NIEHS | JANUARY 2018-JANUARY 2020

- Supervisor: Dr. Kleinstreuer (currently office of director NIH).
- Develop interference QSAR models part of the US Tox21 program.
- Work on mapping in vitro assays on human organ systems.
- Lead web development of chemmaps.com (https://apps.sciome.com/chemmaps/), Interpred (https://apps.sciome.com/interferences/) and Tox21BodyMap (https://apps.sciome.com/bodymap/).
- Facilitate literature review project with sysrev (https://www.sysrev.com/p/3588).
- Work on expending the use of the key characteristic of cancer for invitro assays (https://keycharacteristics.org/).

POST-DOC | NORTH CAROLINA STATE UNIVERSITY | JANUARY 2017 – JANUARY 2018

- Supervisor: Dr. Fourches (currently director at Sciome, LLC).
- Develop Molecular Dynamic based QSAR models on brc-abl kinases.
- Work on developing new antibiotics specific for bacterial strains.
- Ran multiple Molecular Dynamics on GPU server.
- Create augmented reality application for chemists.

PHD STUDENT | UNIVERSITIES OF HELSINKI AND PARIS CITE (PARIS DIDEROT) | SEPTEMBER 2012 – MAY 2016

- Supervisors: Dr. Xhaard and Prof. Camproux.
- Develop druggability model, PockDrug, based on 3D protein pockets (https://pockdrug.rpbs.univ-paris-diderot.fr/cgi-bin/index.py?page=home).
- Characterize salt-bridge molecular environments to help docking and 3D modeling.
- Develop pipelines to retrieve 3D phosphate structural isosteres.

Education

- PhD, Bioinformatics, Biostatistics and Computational Pharmaceutical Chemistry | University Paris Cité in joint program with University of Helsinki | May 2016 | Paris, France – Helsinki, Finland
- Master, Bioinformatics | University Paris Cité | June 2012 | Paris, France
- Bachelor, Biochemistry | University Paris Cité | June 2010 | Paris, France

Award and Honors

- Ed Carney Predictive Toxicology Award, ASCCT 2023 – development of novel AI to predict chemical carcinogenicity. Seminar: https://www.youtube.com/watch?v=64zXzc-0oYA (2023).
- SOT 2022 – Top5 poster at computational toxicology specialty section (2022).
- Article “High-Throughput Screening to Predict Chemical-Assay Interference.” in Top 100 chemistry publication 2020 in Scientific report (2020).
- NIEHS, 2020 article of the year “Tox21BodyMap: a webtool to map chemical effects on the human body” (2020).
- NIH Summer Research Mentor Award (2019).

- Travel grant of French bioinformatics society (SFBI) (2018).
- PhD student fellowship from Magnus Ehrnrooth's foundation (2016).
- Mobility fellowship from France-Finland KAKSIN program (2015-2016).

Skills

DATA SCIENCE & AI/ML

- Supervised and non-supervised modeling
- Imputation modeling
- Data visualization
- Agentic development
- Deep learning
- Feature engineering
- Machine learning

PROGRAMMING AND WEB DEVELOPMENT

- Python (NumPy, Scikit-learn, TensorFlow, ...)
- R
- Ruby / JAVA
- Full-stack web development
- Database management (SQL, PostgreSQL)
- Django / Ruby on Rails

MANAGEMENT

- Conflict Resolution
- Leadership
- Problem Solving
- Strategic Planning
- Time Management

CHEMINFORMATICS / SCIENTIFIC EXPERTISES

- Molecular Dynamics (GROMACS, SCHRODINGER)
- Docking (Glide, Autodock Vina)
- Read-across
- PBTK/PBPK
- Chemical space modeling
- QSAR modeling