Manas Mahale

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Experience

July 2023–Present

Group Member
The Bender Group, University of Cambridge, UK & BBU, RO

Developing Ligand-Target Prediction models for phenotypic screening. Researching Foundational Models for Single Cell Perturbation data.

Aug 2022–June 2023

AI & ML Intern
Pangea Botanica, Berlin, DE

Created Ligand-Target Prediction suite, and deployed computational metabolomics modules on AWS. Optimized MS2DeepScore for Natural Product similarity. Developed computational Pharmacokinetic models.

Feb 2022–June 2023

Affiliate Undergraduate Researcher
Center for Molecular Informatics, University of Cambridge, UK

Investigated methods to predict structural similarity given MS/MS data using Positional Embeddings and Attention. Explored Masked Language Models (BERT) for constrained small molecule library generation.

June 2022–July 2022

Computational Chemistry Consultant
ChemBio Discovery, Boston, USA

Automated Schrödinger workflows for the computational validation of Covalent Docking Pipelines, reducing processing time by 75%. Streamlined protein alignment and homology modeling processes, enhancing accuracy and efficiency.

Aug 2021–Aug 2022

Undergraduate Researcher
The Coutinho Lab, Mumbai, IN

Developed Chemical Language Models for Fragment Based Drug Design and Analogue Split as a chemically biased parametric data splitting method for model validation against IID activity cliff data.

Open Source Software

`pip install dilipred`

DILIPredictor
github.com/Manas02/dili-pip

Developed a package for in-silico prediction of drug-induced liver injury (DILI). Achieved an AUC-PR of 0.79 enabling improved detection of hepatotoxic compounds in humans.

`pip install analoguesplit`

Analogue Split
github.com/Manas02/analogue-split

Validates QSAR model robustness in handling activity cliffs. Introduced $\gamma-$plot visualization for model diagnostics across test set cases.

pip install fbdd

FragmentBERT

github.com/Manas02/fbdd

BERT-based Masked Language Model trained on tokens of drug-like compound's substructures. Retrospectively validated fragment linking, merging and growth modalities using virtual screening.

pip install molecularnetwork

MolecularNetwork

github.com/Manas02/molecularnetwork

A tool to create molecular similarity networks using RDKit and NetworkX, with customizable descriptors for graph-based SAR exploration.

pip install pksmart

PKSmart

github.com/Manas02/pksmart-web

Developed a package and webapp that models human PK parameters (VD_{ss}, Cl, f_u) using structural fingerprints, physicochemical descriptors and predicted animal data. Achieved prediction accuracies comparable to industry-standard models for key PK parameters.

Publications

2025 **Mahale, Manas**, Ricardo Scheufen Tieghi, Dea Gogishvili, Dinh Long Huynh, Renan Augusto Gomes, Shagun Krishna, Deidre Dalmas, Andreas Bender, and Srijit Seal. *The Medicinal Chemist's Map to Deep Learning: Concepts, Applications, and Case Studies*. In Reference Module in Chemistry, Molecular Sciences and Chemical Engineering. Elsevier. https://doi.org/10.1016/B978-0-443-29808-0.00066-2.

2025 Seal, Srijit, Maria-Anna Trapotsi, **Manas Mahale**, Vigneshwari Subramanian, Nigel Greene, Ola Spjuth, and Andreas Bender. *PKSmart: An Open-Source Computational Model to Predict Intravenous Pharmacokinetics of Small Molecules*. Journal of Cheminformatics. https://doi.org/10.1186/s13321-025-01066-5.

2025 Seal, Srijit, **Manas Mahale**, Miguel García-Ortegón, Chaitanya K. Joshi, Layla Hosseini-Gerami, Alex Beatson, Matthew Greenig, et al. *Machine Learning for Toxicity Prediction Using Chemical Structures: Pillars for Success in the Real World*. Chemical Research in Toxicology. https://doi.org/10.1021/acs.chemrestox.5c00033.

2024 Seal, Srijit, Dominic Williams, Layla Hosseini-Gerami, **Manas Mahale**, Anne E. Carpenter, Ola Spjuth, and Andreas Bender. *Improved Detection of Drug-Induced Liver Injury by Integrating Predicted in Vivo and in Vitro Data*. Chemical Research in Toxicology. https://doi.org/10.1021/acs.chemrestox.4c00015.

2023 Gupta, et al. *CXCR4 Expression Is Elevated in TNBC Patient Derived Samples and Z-Guggulsterone Abrogates Tumor Progression by Targeting CXCL12/CXCR4 Signaling Axis in Preclinical Breast Cancer Model*. Environmental Research. https://doi.org/10.1016/j.envres.2023.116335.

2023 Martis, Elvis A.F., **Manas Mahale**, Aishwarya Choudhary, and Evans C. Coutinho. *Understanding Protein-Ligand Interactions Using State-of-the-Art Computer Simulation Methods*. In Cheminformatics, QSAR and Machine Learning Applications for Novel Drug Development. Elsevier. https://doi.org/10.1016/B978-0-443-18638-7.00015-3.

Education

2025–2027

Master in Chemoinformatics for Organic Chemistry
Universidade Nova de Lisboa, PT & Université de Strasbourg, FR

Current focus: Developing Cheminformatics tools for Supramolecular Chemistry, Synthetic Organic Electrochemistry and Multi-omics

2021–2025

Bachelor of Pharmacy
Bombay College of Pharmacy, Mumbai, IN

Key courses: Medicinal Chemistry, Pharmacokinetics, Pharmacology, Novel Drug Delivery Systems, Organic Chemistry, Pharmacognosy and Phytochemistry.
Thesis on *Foundational Methodologies for Initiating Caenorhabditis elegans Research: A Report on Laboratory Setup, Protocol Validation and Preliminary Longevity Assay*

Honours

2025

Erasmus Mundus Joint Master - ChEMoinformatics+
The European Commission

Full Scholarship for Masters program in Chemoinformatics for Organic Chemistry.

2024

Gold Medal & Fellowship
Anveshan, Association of Indian Universities

National Winner in Health Sciences with a $1000 Fellowship.

2023

Silver Medal & Fellowship
Avishkar Research Convention, Governor of Maharashtra

Fellowship of $350 for the work on *FragmentBERT: Masked Language Models are Fragment Based Drug Designers*

Volunteering

2023–2024

Teaching Volunteer
U&I, Our Lady's Home, Mumbai, IN