Malaya Ranjan Patra
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Education	Institute	%	Year
MSc Chemistry	IIT Bombay	92.2	2021

RELEVANT COURSES / CERTIFICATIONS

- **Structured Query Language (SQL) – HackerRank, HTML & CSS - OpenClassrooms**
- **Python – HackerRank, Java Script – OpenClassrooms, Git & Github - OpenClassrooms**
- **Machine Learning for Drug Discovery – Uresearcher, PyTorch - Guvi**

RELEVANT CURRENT WORK EXPERIENCE

AI RESEARCH SCIENTIST | THE MAMA AI | PRAGUE, CZECH REPUBLIC | AUGUST 2022 – PRESENT

- Highly proficient in writing python codes and implementing various scientific libraries like **Numpy, Pandas, Matplotlib, Seaborn, RDKit, Scikit, PyTorch, Keras (TensorFlow) etc.**
- **Developed UI for molecule optimization and property prediction.**
- **Software Development: GitHub, Git, Docker, Jenkins, Streamlit, Fast API.**
- **Molecule Generation, Property Optimization, Docking, Reinforcement Learning, Genetic Algorithm.**

RELEVANT PAST WORK EXPERIENCE

RESEARCH ASSOCIATE 1 – COMPUTATIONAL CHEMISTRY | AURIGENE DISCOVERY TECHNOLOGIES LTD | BENGALURU | FEB 2022 – AUGUST 2022

- **Supported 5 projects simultaneously in computational drug discovery**.
- **Developed insilico models** for predicting potency & physico-chemical properties of compounds.
- **Homology modelling, Reversible docking, Covalent docking, Ensemble docking, PROTACs.**
- Supporting **AI platform development and new software evaluations**.
- ChemAxon's Chemcurator: Analysis of patents and journals from drug discovery domain, extractions of chemical structures and activity (IC50, EC50, GI50 etc) in a systematic manner.
- **Data Science software: Tibco Statistica and DataWarrior.**
- **RDKit: Tanimoto similarity analysis, Descriptor generation, Butina and Murcko Scaffold Clustering.**
- **Artificial Intelligence: Developed models to predict solubility, Caco2 permeability, Mouse / Human Liver Microsomal stability, hERG Toxicity.**
- Extraction of information from UniProt, RCSB, PubChem, ChemSpider, ChEMBL .
- Chemical/biological Information hunting using SciFinder, PubMed, WIPO Patent, Google Scholar.
- **Supervised and mentored an intern student of computer science on his AI project**

RESEARCH INTERN | BOLTZMANN LABS PVT LTD | BENGALURU | JAN 2022 – FEB 2022

- **Literature analysis, data curation, reported bugs and improved Boltchem platform.**
- **Worked in a highly interdisciplinary environment involving people from computer science, biotechnology, bio-informatics, and chemistry.**

RELEVANT ACADEMIC PROJECT EXPERIENCE

INSILICO DESIGN OF INHIBITORS TARGETING POLIV OF *E. COLI* BACTERIA | DEPARTMENT OF CHEMISTRY | IIT BOMBAY | JULY 2020 – JUNE 2021

- Completed the whole work under the **supervision of Prof. Dr. Pradeepkumar P.I.**
- Discovered potential hit compounds for the target enzyme.
- Skills: **Gaussian**, **Schrodinger's Maestro**, **Amber, SwissADME, Linux (HPC, SLURM)**.
- Analysis of **pharmacokinetic (PK), druglike nature and medicinal chemistry friendliness.**
- **Geometry optimization, docking, cluster analysis and Molecular Dynamics simulation on HPC system.**

COMPUTATIONAL CHEMISTRY SKILLS AT A GLANCE

- **DATAWARRIOR**
- **CRESSET'S SPARK**
- **CHEMAXON'S JCHEM**
- **PYMOL (VISUALIZATION)**
- **GAUSSIAN** (GEOMETRY OPTIMIZATION)
- WINCOOT
- **SLURM**
- **SCHRÖDINGER** (MAESTRO)
- **AMBER** (MOLECULAR DYNAMICS SIMULATION)
- **AUTODOCK**
- KNIME
- **CHEMAXON'S CHEMCURATOR**
- **TIBCO STATISTICA**
- AVOGADRO
- BIOVIA DISCOVERY STUDIO
- **CHEMDRAW, CHEMOFFICE**
- **CCDC GOLD**
- **MOLDEN**
- **VMD** (VIDEO RENDERING)
- **MOLSOFT ICM PRO**