DIVYA KARADE

Cheminformatician, AI Drug Discovery Innovator, Data Scientist & Web App Developer

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PROFESSIONAL SUMMARY

- **AI-Powered Drug Discovery Expert:** 9+ years of experience in cheminformatics, computational chemistry, and AI/ML applications.
- **Founder of AIDrugApp:** National & international award-winning AI-based virtual screening platform for small molecule drug discovery.
- **Applied Machine Learning:** Proficient in designing predictive and generative models using Python, TensorFlow, Keras, and Scikit-Learn.
- **Computational Chemistry Expertise:** Specialized in QSAR modeling, molecular docking, ADMET predictions, and virtual screening.
- **Collaborative Problem Solver:** Effectively collaborated with interdisciplinary teams across academic and industrial settings.
- **Leadership & Mentorship:** Led interdisciplinary teams and mentored PhD students in cheminformatics and predictive modeling.
- **Public Speaking & Publications:** Invited speaker and first-author in peer-reviewed journals.

PROFESSIONAL EXPERIENCE

Post-Doctoral Scientist ***Aug 2023 - Jan 2024***
EMPA, Swiss Federal Laboratories **St. Gallen, Switzerland**

- Developed AI-driven cheminformatics tool using ML and NLP, enhancing chemical data extraction by 35%.
- Automated data pipelines using Scikit-learn and Pandas for data classification and curation, reducing analysis time by 25%.
- Mentored 2 PhD students in cheminformatics and AI, guiding interdisciplinary research.

Senior Research Scientist (QSAR Modeller) ***May 2022 - Feb 2023***
Syngenta Ltd. ***Bracknell, England, UK***

- Built and deployed bioactivity predictive QSAR models analysing 5,000+ molecules from ChEMBL using RDKit and Scikit-learn.
- Delivered predictive models for reproductive & environmental risk assessment (e.g. DT50), improving decision-making by 30%.
- Developed ensemble deep learning models (TensorFlow, Scikit-learn), achieving a 25% accuracy boost in chemical predictions.
- Collaborated with 20+ scientists for cross-functional R&D and integrated cheminformatics insights for early risk assessment.

Senior Research Fellow ***Jan 2017 - Dec 2021***
CSIR National Chemical Laboratory **Pune, India**

- Designed a virtual library of 3,382 drug-like molecules using scaffold hopping techniques, accelerating lead optimisation.
- Discovered 14 novel small molecules in soybeans through mass spectrometry for natural product drug discovery.
- Established QSAR models predicting aquatic toxicity (LC-50 & EC-50), identifying 169 pesticide candidates for agrochemicals.
- Built a 10,000+ small molecule database (SQL, cheminformatics tools), enhancing research accessibility.

Junior Research Fellow ***Jan 2015 - Dec 2016***
CSIR National Chemical Laboratory **Pune, India**

- Constructed a structured knowledge graph integrating disease-target-drug associations, leveraging text-mining (PubTator, NLP) to extract 5,361 molecules from 91,206 PubMed articles.
- Streamlined 4 cheminformatics protocols for designing drug-like molecules focused on Ro5, streamlining candidate identification.
- Conducted structure-based drug design using Schrödinger, MOE, ChemAxon & ChemDraw tools & performed molecular docking.

Patent Analyst (Life Science) ***Mar 2013 - Dec 2014***
CSIR Unit of Res. & Dev. of Info. Products (URDIP) **Pune, India**

- Analysed patents and identified emerging drug discovery trends to support R&D strategies.

EDUCATION

PhD in Cheminformatics ***Jan 2015 - Dec 2021***
Academy of Scientific and Innovative Research ***Pune, India***

- **Thesis:** *Cheminformatics-based investigation of plant metabolites for their medicinal & crop protection values* (link).

M.Sc. in Biotechnology
A.N.G.R.A. University, Institute of Biotech. ***Hyderabad, India***

- **Thesis:** *Genetic variability characterisation in cowpeas using morphological, protein, and DNA markers.*

PROJECTS

AIDrugApp: AI-based Drug Discovery Web App Platform
Drug Discovery Hackathon, *Govt. of India* ***Sep 2021 - Present***

- Founded & led AIDrugApp team, awarded National Award by the Government of India and International Award at IISF India.
- Developed an AI-based virtual screening platform using deep learning models (GANs, GNNs, DNNs).
- Implemented cheminformatics ML modules for molecular structure generation, predicting bioactivity & binding affinity.
- Reduced drug discovery time and costs through scalable SaaS solutions & cloud-based integrations.
- Delivered talks & publications on AI-driven drug discovery.

SKILLS

- **Programming & ML Frameworks:** Python, R, TensorFlow, Keras, Scikit-Learn, Deep Learning and Generative algorithms (GAN, GNN, DNN), NLP (SpaCy), Predictive Modeling (Regression, Classification), MLOps.
- **Cheminformatics Tools:** RDKit, OpenBabel, Schrödinger, ChemAxon, MOE, ChemDraw, CytoScape.
- **Drug Discovery Techniques:** QSAR, Molecular Docking, Virtual Screening, ADMET Prediction, SBDD, LBDD, Fragment-Based Drug Design, ADMET Predictions, Knowledge Graphs.
- **Data Analysis & Visualization:** NumPy, Pandas, SciPy, Matplotlib, Seaborn, EDA, FAIR Data management.
- **Cloud:** AWS, SQL, Heroku, Streamlit, Docker, GitHub.
- **Collaboration & Communication:** Cross-functional collaboration, Mentoring, Project Management, Stakeholder Engagement & Scientific Presentations.

AWARDS & ACHIEVEMENTS

National & International

- **National Award** for **AIDrugApp**, Govt. of India (2021, **Top 10**).
- **International Award** for **AIDrugApp**, IISF India (2020, **Top 4**).
- **AWS DeepRacer**, AWS Educate (2021, **Top 100**).
- **Senior Research Fellowship**, CSIR-UGC NET, India (2017).
- **PhD Research Fellowship**, CSIR-UGC, India (2015, **Top 90**).
- **National Eligibility Test Life Science**, CSIR India (2012, **Top 64**).

PUBLICATIONS & PRESENTATIONS

Selected Publications & Talks

- **Karade, D.** *ChemDesigner: Generating and Screening Molecules with GANs & GNNs*. Medium Blog, 2024 (link).
- **Karade, D.** and Karade, V. *AIDrugApp: AI Web-App for Virtual Screening of Inhibitors against SARS-CoV-2*. JETAI, 2022 (link).
- **Karade, D.** *Custom ML Module of AIDrugApp for Molecular Identification, Descriptor Calculation, and Building ML/DL QSAR Models.* ChemRxiv, 2021 (link).
- **Karade, D.**; Kadoo, N.; Vyas, R.; Ingle; Karthikeyan, M. *Design of Novel Drug-like Molecules using Informatics Rich Secondary Metabolites of Indian Medicinal Plants.* CCHTS, 2020 (link).
- **Invited Speaker:** AI in Drug Discovery, Vignan's Foundation of Science & Technology, 2022.
- **Speaker:** Drug Discovery Web App, Marwari University, 2022.