DIVYA KARADE

Cheminformatics & AI Drug Discovery Scientist | Scientific Software Innovator

divya.karade@gmail.com | +91-8830379882 | India (Open to Relocation) | LinkedIn | Portfolio | GitHub | YouTube | Blog

PROFESSIONAL SUMMARY

- **AI-Driven Cheminformatics Scientist:** 9+ years of experience across academia, industry, Govt. R&D labs in international settings.
- **Founder of AIDrugApp:** National & international award-winning AI virtual screening drug discovery platform for global research.
- **Expert in QSAR, docking, and SBDD/LBDD**, delivering scalable automation pipelines for hit discovery and lead optimisation.
- **Built predictive and generative ML models** using Python, RDKit, TensorFlow, and Scikit-learn for drug design.
- **Led cross-functional teams and mentored PhDs**, driving collaboration across Syngenta, EMPA, and CSIR-NCL projects.
- **Published author and invited speaker**, recognised for advancing AI-based drug discovery tools and methods.

PROFESSIONAL EXPERIENCE

Postdoctoral Scientist - Cheminformatics **Aug 2023 - Jan 2024**
EMPA, Swiss Federal Lab for Materials Science *Switzerland*

- Engineered ML+NLP-driven cheminformatics toolkit, boosting chemical data extraction accuracy by 35% over baseline tools.
- Automated classification and curation workflows using Scikit-learn and Pandas, reducing data processing time by 25%.
- Mentored 2 PhD researchers in AI-based cheminformatics tools.

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

- Streamlined QSAR models analysing 5,000+ ChEMBL compounds using RDKit & Scikit-learn for bioactivity predictions.
- Improved environmental & reproductive early risk assessment regulatory decisions by 30% using predictive models (e.g., DT50).
- Created deep ensemble models (TensorFlow, Scikit-learn), achieving a 25% accuracy boost in chemical predictions.
- Collaborated with 20+ global scientists to integrate cheminformatics into early-phase toxicology pipelines.

Senior Research Fellow - Comp. Drug Design **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.
- Developed QSAR models for aquatic toxicity (LC50, EC50) & screened 169 pesticide leads.
- Discovered 14 new soybean drug candidates with in vitro (UHPLC-MS/MS) and Bayesian optimised ML model validation.
- Co-developed SQL chemical database with 10,000+ compounds.

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

- Constructed disease-target-drug knowledge graphs by text mining 5,361 molecules from 91K PubMed records.
- Standardised 4 cheminformatics workflows for Ro5-compliant drug design, boosting lead identification efficiency.
- Implemented SBDD workflows using Schrödinger and MOE.

Patent Analyst (Life Sciences) **Mar 2013 - Dec 2014**
CSIR Unit for Research & Dev. of Info. Products *Pune, India*

- Delivered IP landscape reports for 5 drug discovery projects.

SKILLS

- **Cheminformatics Tools:** RDKit, OpenBabel, Schrödinger, ChemAxon, MOE, ChemDraw, CytoScape.
- **Drug Discovery Techniques:** QSAR, Molecular Docking, Virtual Screening, ADMET, SBDD, LBDD, Fragment-Based Drug Design, Knowledge Graphs, Bioactivity Prediction, Property Modeling.
- **Programming & ML Frameworks:** Python, R, TensorFlow, Keras, PyTorch, Transformer, Scikit-Learn, Deep Learning & Generative algorithms (GANs, GNNs, DNNs), NLP (SpaCy), Predictive Modeling (Regression, Classification), MLOps, ETL pipelines.
- **Data Engineering & Visualisation:** NumPy, Pandas, SciPy, Matplotlib, Seaborn, EDA, FAIR data principles, Data curation.
- **Cloud:** AWS, Google, Heroku, Streamlit, Docker, GitHub, CI/CD.
- **Collaboration & Comm.:** Cross-functional, Mentoring, Agile, Presentation, Project Management, Stakeholder Engagement.

PROJECTS & INNOVATIONS

Founder & Product Owner, AIDrugApp **Sep 2021 - Present**
National & International Award Winner, Govt of India.

- Led team of 3 and built cloud-based AI drug discovery platform.
- Virtually screened 50K+ molecules against SARS-CoV-2 using bioactivity DL models; validated hits via docking and ADMET.
- Key Products of AIDrugApp Platform:

1. **Bioactivity Prediction (COVID-19):** DL models + UI for SARS-CoV-2 bioactivity classification & pIC_{50} regression prediction.
2. **DeepDocker (COVID-19):** DNN-based docking score predictor.
3. **Auto-Multi-ML:** Automated ML pipeline to develop and benchmark multiple models with EDA tools. *(GitHub)*
4. **AutoDL:** No-code DL model builder for chemical data. *(GitHub)*
5. **DesCal:** Descriptor/fingerprint calculator with DL-based solubility (logS) predictor. *(Preprint)*
6. **ChemInsight:** Tools for chemical name/SMILES conversion, similarity search, and 2D structure visualisation. *(Blog)*
7. **ChemDesigner:** Molecule generator using GANs and GNNs under user-defined atomic constraints. *(Blog)*

OTHER AI COMPETITIONS & CHALLENGES

- **DREAM Target 2035 Challenge** **Apr - June 2025**
  Top 20/212. Predicted binding hits from 4.4M DEL compounds using DL & transformer models on ECFP4 + SMILES. *(GitHub)*
- **Global AI Kaggle Hackathon 2025, Elucidata** **Mar- May 2025**
  Top 204 globally for CNN model predicting spatial cell-type composition from histology images. *(GitHub)*
- **AWS DeepRacing Simulator** **Mar- Apr 2021**
  Top 100 nationally in AWS DeepRacer competition; Generated RL models with optimised reward functions. *(GitHub)*

EDUCATION

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

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

M.Sc. in Biotechnology **Sep 2008 - Nov 2010**
ANGRAU, Institute of Biotechnology *Hyderabad, India*

- **Thesis:** Genetic variability analysis in cowpea using morphological, protein and DNA markers.

AWARDS & HONORS

- **National Award, AIDrugApp**, DDH, Govt India (**Top 10**, 2021).
- **International Innovation Award,** IISF, India (**Top 4**, 2021)
- **AWS DeepRacer**, AWS Educate (**Top 100** Rank, 2021).
- **Senior Research Fellowship**, CSIR-UGC (**Top 90** Rank, 2017).
- **Lectureship, Life Sciences**, UGC-NET (**Top 64** Rank, 2012).

SELECTED PUBLICATIONS & TALKS

- **Karade, D.** & Karade, V. *AIDrugApp: AI Web-App for Virtual screening of Inhibitors against SARS-CoV-2*. JETAI, 2022 (link).
- **Invited Speaker:** *AI-based Drug Discovery Web App*, Vignan's Foundation of Science & Technology, 2022 (link).
- **Invited Speaker:** AI Drug Design, Marwari Univ., 2022 (link).
- **Karade D.** et al., *Design of Drug-like Molecules from Indian Medicinal Plant Metabolites.* CCHTS, 2020 (link).