

Divya Karade

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Professional Summary

- AI researcher in drug discovery with 8+ years of experience in Biological Sciences (Cheminformatics, Comp. Biology & Biotech.)
- National & India International-award-winning innovator for “AIDrugApp: AI-based Web-Application for Drug Discovery”.
- Led a team 'Tesseract Gene' for developing 'AIDrugApp'.
- Presented several invited talks at conferences and universities for development of web app and DL/ML tech. in drug discovery.
- Implemented R/ Python (TensorFlow, Keras, sklearn, RDKit etc) for scientific and real-life data analysis problems.
- Proficient knowledge in Drug Designing, Machine/ Deep Learning, Data Analytics, Algorithms and small molecular datasets.
- Excellent record of inter-disciplinary collaboration with researchers from biology, chemistry & computational science fields.
- Solid publication record with first-author publications in peer-reviewed journals and many more in the pipeline.

Technical Skills

- **Programming Languages:** Python, R/RStudio - Bioconductor, HTML
- **Machine learning:** Building and deploying ML/ DL algorithms, Auto-ML/DL, NLP, Web-app development - Streamlit, Data analysis - TensorFlow, Keras, scikit-learn, NumPy, Pandas, Data visualization - Matplotlib, seaborn, yellowbrick & ggplot2
- **Data Science:** Metabolomics and Chemical Data analysis, Data science pipeline (cleansing, wrangling, optimization, EDA, modeling, interpretation), Feature engineering, Statistics, Hypothesis testing, GitHub, Data curation, Cloud tech. - Heroku, AWS
- **Cheminformatics:** Structure & ligand-based drug design, Text mining, Knowledge graph, Chemical structure analysis, QSAR, virtual screening, virtual libraries, ADME, scaffold analysis, MOE, ChemAxon, ChemDraw, Cytoscape, RDKit, PubChemPy
- **Bioinformatics:** Molecular docking and analysis using computational chemistry tools like Schrodinger, MOE and AutoDock
- **Metabolomics:** Untargeted metabolomics, Mass spectrometric data analysis, Univariate and Multivariate statistical analysis

Innovation Project

AIDrugApp: Artificial Intelligence-based Virtual Screening Web-App for Drug Discovery (v1.2.5)

Sep 2020 - Present

Drug Discovery Hackathon 2020, Govt. of India

(Python3| TensorFlow| Keras| sklearn | RDKit | Streamlit)

- Innovated and founded a user-friendly and novel web application platform called '[AIDrugApp](#)' for drug discovery.
- **Bioactivity prediction:** Built QSAR based DL algorithms for bioactivity prediction of user-defined molecules against SARS-CoV2.
- **DeepDocker:** Originated and Implemented QSAR based DL algorithms for predicting binding affinity of user-defined molecules.
- **Custom ML Tools:** ML tools integrated to AIDrugApp for user-defined model building, calculations and predictions on user data.
 1. **Auto-Multi-ML:** Created for building and comparing user-defined multiple ML models and making predictions on user's data.
 2. **Auto-DL:** Developed to build user-defined deep learning models with neural networks and making predictions on user's data.
 3. **DesCal:** Developed for calculating user-defined 2-D descriptors and fingerprints using molecular SMILES of user's data.
 4. **Mol_Identifier:** Developed to identify molecular information like chemical name, SMILES & similarity scores.

Experience

Post-Doctoral Scientist

Aug 2023 - Present

EMPA, Swiss Federal Laboratories for Materials Science and Technology

St. Gallen, Switzerland

- Developing a cheminformatics toolbox for open data on the uses of chemicals and materials

Senior Research Scientist (QSAR Modeller)

May 2022 – Feb 2023

Syngenta Ltd, Jealott's Hill International Research Centre

Bracknell, England, UK

- Developed python codes to extract and filter approx. 5k molecular data from ChEMBL database to evaluate predictive models
- Presented novel ideas to stakeholders/ clients to implement predictive ML/DL models relevant to agrochemical research. Metrics: Increased the number of predictive models (both classical and deep learning) used for decision making
- Collaborate with QSAR, cheminformatics and ML modelling project teams to develop and promote the use of predictive models by employing metrics, measurement and analysis of results

Senior Research Fellow

Jan 2017 - Dec 2021

CSIR National Chemical Laboratory, Chemical Engineering and Process Development Division

Pune, India

- Discovered and reported the presence of 14 novel small molecules in soybean by mass spectrometry data analysis
- Formulated 4 computational protocols for designing drug-like novel molecules from metabolites of medicinal & food plants
- Investigated 280 allelochemicals from 162 plants for their pesticide properties by cheminformatics and QSAR approaches
- Designed virtual libraries of allelochemicals that were then quantitatively evaluated to screen 169 pesticide-like molecules

Junior Research Fellow

Jan 2015 - Dec 2016

CSIR National Chemical Laboratory, Chemical Engineering and Process Development Division

Pune, India

- Analyzed molecular data (n=3459) by text mining 91206 PubMed literature related to 104 Indian medicinal plants
- Created and Contributed a virtual library of 4147 novel drug-like molecules for building a database of Indian medicinal plants

- Examined current technology and patent updates for constructing a technological patent landscape for 5 life sciences projects
- Interpreted comparative and competitive patent portfolio after novelty, patentability and prior art search

Education

Ph.D. in Science (Cheminformatics, Metabolomics and Comp. Biology) - Cumulative GPA: 7.94 /10.0

Jan 2015 – Dec 2021

Academy of Scientific and Innovative Research (AcSIR)

Pune, Maharashtra, India

- Thesis: Cheminformatics based investigation of plant metabolites for their medicinal and crop protection values

Master of Science (Plant Biotechnology) - Cumulative GPA: 8.14 /10.0

Sep 2008 - Nov 2010

A.N.G.R.A. University, Dept. of Biotechnology

Hyderabad, India

- Thesis: Characterization of genetic variability in cowpea using morphological, biochemical and molecular markers.

Bachelor of Science - Cumulative GPA: 7.68 /10.0

Aug 2004 - Aug 2008

Dr. Panjab Rao Deshmukh Krishi Vidyapeeth

Nagpur, Maharashtra, India

- Relevant Coursework: Statistics, Maths, Plant Biotechnology, Plant Biochemistry, Molecular Biology, Genetics, Microbiology

Honors & Awards

Invited Talks

- **Invited speaker** for a national webinar on “Development of web application for drug discovery” organised by Dept. of Biotechnology of Vignan's Foundation of Science, Technology & Research. May 2022
- **Invited speaker** for an expert talk on “Revolutionising Drug Discovery with AI” as a part of Capacity Building Programmes for NextGen Entrepreneurs organised by Marwadi University Centre for Innovation, Incubation and Research (MUIR) Jan 2022

National & International

- National-level [AWS DeepRacer](#) (Selected in top 100) at Woman's league for community car races driven by reinforcement learning codes in python through AWS cloud-based 3D racing simulator organized by AWS Educate Apr 2021
- National Award ([Consolation](#) - Selected in top 10 out of 377 shortlisted applicants) for “AIDrugApp” at the open-source “Drug Discovery Hackathon-2020” against Covid-19 in phase-1 under moonshot category organized by Govt. of India. Mar 2021
- National Award ([Certificate of Merit](#) - Selected in top 4 out of 31 finalists) for “AIDrugApp” in student engineering model competition under “Digital India” theme held at “India International Science Festival” organized by Govt. of India Dec 2020

Academic

- Awarded Senior Research Fellowship for Ph.D. Life-Science, CSIR-UGC (National Eligibility Test) NET exam, India 2017
- All India rank **90** for Junior Research Fellowship for Ph.D. admission in Life-Science, CSIR-UGC NET exam, India 2013
- All India rank **64** with National Eligibility for Lectureship in Life-Science, CSIR-UGC NET, India 2012
- Awarded National Eligibility for Lectureship in Plant Biotechnology, ASRB NET, India 2011
- All India rank **31** in Plant Biotechnology common entrance exam for P.G. admission, JNU, India 2008
- All India rank **14** in Plant Biotechnology entrance exam for P.G. admission, ICAR, India 2008

Publications

A list of publications can be viewed on my [Google Scholar](#) page. The following are a few recent publications:

- **Divya Karade**, Vikas Karade. AIDrugApp: Artificial Intelligence-based Web-App for Virtual Screening of Inhibitors against SARS-COV-2. *Journal of Experimental and Theoretical Artificial Intelligence* **2022**. (Impact factor: 2.11, [click here](#))
- **Divya Karade**. Custom ML Module of AIDrugApp for Molecular Identification, Descriptor Calculation, and Building ML/DL QSAR Models. *ChemRxiv. Cambridge: Cambridge Open Engage*; **2021**. (Web-App: [click here](#))
- **Divya Karade**. AutoDL: Automated Deep Learning (Machine learning module of AIDrugApp - Artificial Intelligence Based Virtual Screening Web-App for Drug Discovery) (Version 1.0.0). *Zenodo*. **2021**. (Software: [click here](#))
- **Divya Karade**, D. V., N. Kadoo, R. Vyas, P. K. Ingle and M. Karthikeyan. Design of Novel Drug-like Molecules using Informatics Rich Secondary Metabolites Analysis of Indian Medicinal and Aromatic Plants. *Combinatorial Chemistry & High Throughput Screening* **2020**, 23 (10), pp. 1113-1131. (Impact factor: 1.2, [click here](#))

Research Presentations

- **Oral presentation** of ‘AIDrugApp: Artificial Intelligence Based Virtual Screening Web-App for Drug Discovery’ at “Drug Discovery Hackathon-2020” organized by GOI and awarded consolation cash prize (**2021**)
- **Oral presentation** of ‘AIDrugApp: Artificial Intelligence Based Virtual Screening Web-App for Drug Discovery’ at “Indian International Science Festival-2020” organized by GOI and awarded Certificate of Merit with cash prize (**2020**)
- **Poster presentation** on ‘Antidiabetic Drug Designing Based on Organic Metabolites from Fenugreek: A Chemo-and Bioinformatics Approach’ at “International Symposium on Accelerated Biology” conducted by C-DAC, Pune (**2019**)
- **Poster presentation** on ‘Cheminformatics Investigation of Organic Metabolites from Soybean Reveals Common Drug Scaffolds presented at CSIR-National Chemical Laboratory, Pune on the “National Science Day” (**2017**)
- **Poster presentation** on ‘Chemoinfo. approaches for drug designing’ at CSIR-NCL, Pune on the “National Science Day” (**2017**)