Divya Karade

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Professional Summary

- AI researcher in drug discovery with 7+ 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 'Tesseractal 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, Auto-DL, 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, Network analysis, 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 users data.
  2. *Auto-DL***:** Developed to build user-defined deep learning models with neural networks and making predictions on users data.
  3. *DesCal***:** Developed for calculating user-defined 2-D descriptors and fingerprints using molecular SMILES of users data.
  4. *Mol_Identifier***:** Developed to identify molecular information like chemical name, SMILES & similarity scores.

Experience

Senior Research Scientist *(QSAR Modeller)* *May 2022 - Present*

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.
- Developed a novel deep learning approach to improve the prediction of various physicochemical, biological and environmental endpoints for agrochemicals.
- 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*

- Bridging In-Silico and Experimental: Cheminformatics Analysis of Mass Spectrometry-Based Metabolomics Study of Soybean
  - 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.
- Chemoinformatics Investigation on Chemical Defense in 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*

- Design of Novel Drug-like Molecules using Informatics Rich Secondary Metabolites Analysis of Indian Medicinal Plants
  - 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

Patent Analyst (Life Science) *Mar 2013 - Dec 2014*
CSIR Unit of Research & Development of Information Products, Life Science Division *Pune, India*
- 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 (MUIIR) *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**)