Divya Karade

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EDUCATION

Ph.D. in Biological Sciences (Chemoinformatics, Metabolomics and Computational Biology) Jan 2015 - Expected July 2021
CSIR National Chemical Laboratory, Chemical Engineering and Process Development Pune, Maharashtra, India

Thesis Title: "Chemoinformatics based investigation of plant metabolites for their medicinal and crop protection values"

- **Developed computational protocols** for designing novel potential drug candidate molecules from Indian medicinal plants.
- **Collected and Analyzed molecular data** by using chemoinformatics tools and techniques like **MOE, Cytoscape, ChemAxon, ChemDraw**, etc. and for creating a **database cum toolkit of Indian medicinal plants**.
- Investigated drug-like and lead-like molecules in Indian medicinal plants and food crops using chemoinformatics methods like **text mining, chemical structure analysis, molecule scaffold network analysis, descriptor generation and interpretation**, etc.
- **Designed and executed laboratory biochemical experiments** for optimizing soybean samples for **LC/MS experiments**.
- **Conceptualized analyzing methods** for mass spectrometric data using **machine learning** tools and techniques.
- Analyzed LC/MS experimental data (quantitative and qualitative) by using **multivariate statistical analysis**, **Supervised and Unsupervised machine learning** techniques in **R** and other online tools.
- **Discovered and reported the presence of 14 novel small molecules in soybean** through mass spectrometry analysis.
- **Designed drug-like molecules** from soybean metabolites through chemoinformatics and mass spectrometry experiments.
- **Investigated designing of pesticide-like molecules** from plants using chemoinformatics tools and QSAR methods.

Publication: - **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)

- **Divya Karade**, S. Mundhe, N. Kadoo, M. Ratnaparkhe, R. Vyas and M. Karthikeyan. Bridging In-Silico and Experimental: Chemoinformatics Analysis for Mass Spectrometry-Based Metabolomics Study of Soybean. *Metabolomics* **2021**. (Under review)

- Awarded Senior Research Fellowship for continuing Ph.D., 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
- Awarded for Graduate Aptitude Test in Engineering (Biotechnology) for Ph.D. admission, MHRD, India 2011, 2012
- All India rank **64** in National Eligibility for Lectureship in Life-Science, CSIR-UGC NET, India. 2011
- Awarded National Eligibility for Lectureship in Plant biotechnology by ASRB NET, India. 2011

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, A.P., India

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

- Studied genetic variability among fifty germplasm accessions of cowpea using RAPD genetic markers.
- Characterized fifty cowpea germplasm using morphological descriptors (Qualitative and Quantitative).
- Examined variations in fifty cowpea varieties using protein gel electrophoresis techniques (SDS - PAGE).
- Performed **data analysis** of morphological, biochemical and molecular experiments.

Publication: - **Divya Karade**, S. Sivaramakrishnan, K. Venkateswaran, R.S. Reddy. Characterization of genetic variability among cowpea (Vigna Unguiculata L. Walp) germplasm using morphological, biochemical and molecular markers. *Jour. Of Med. Sci. & Tech*.2012, 1 (2), pp. 43-61. (click here)

Relevant Coursework: **Statistics**, Plant Biotech, Recombinant DNA tech., Molecular Biology, Plant Biochemistry, Genetics, OMICS

- 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

Bachelor of Science (Agricultural Science) - Cumulative GPA: 7.68 /10.0 Aug 2004 - Aug 2008
Dr. P.D.K.V. University, College of Agriculture Nagpur, Maharashtra, India

Relevant Coursework: **Statistics**, **Maths**, Plant **Biotech**, Plant Biochem., Plant Physiology, Molecular Biology, Genetics, Pathology

Rural Agricultural Work Experience for a period of 6 months in Lonwahi village, Sindewahi district, Maharashtra state, India. 2008

- Awarded State-level debater & elocutionist in Maharashtra state inter-university at Youth Festival, Mumbai University. 2007

INNOVATION PROJECT FOR HACKATHON

AIDrugApp: Artificial Intelligence-based Virtual Screening Web-App for Drug Discovery Sep. 2020 - Present
https://sars-covid-app.herokuapp.com/ **(Python3 | TensorFlow | Keras | scikit-learn | Streamlit | Heroku)**

AIDrugApp is a **National award-winning** ongoing **self-conceived** project to develop an AI-based virtual screening **web-application** platform for drug discovery. The current version 1.2.1 is for bioactivity prediction of user's molecules of interest through **Deep Learning AI models** towards **SARS-CoV-2**. It is also useful for **Exploratory Data Analysis** (EDA) or **data visualization** and **feature engineering** of user-specific data for building **Automated Multiple Machine Learning Models** (AutoMultiML) & **Automated Deep Learning Models** (AutoDL) which can eventually be used for predicting/virtual screening of target data. We also conducted two case studies where large sets of molecules were screened by our app against **SARS-CoV-2**. The future versions will include a collaborative networking platform with advanced features for many other diseases. (*Under development*)

- National Award winner at the open-source "Drug Discovery Hackathon-2020" against Covid-19 in phase-1 under moonshot category organized by Govt. of India. **(Selected in top 10 out of 377 shortlisted applicants)** March 2021
- National Award winner of "Certificate of Merit" in student engineering model competition under "Digital India" theme held at "Indian International Science Festival" organized by Govt. of India. **(Selected in top 4 out of 31 finalists)** Dec 2020

Publication**:** - **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**. (click here)
- **Divya Karade**, Vikas Karade. AIDrugApp: Artificial Intelligence-based Web-App for Virtual Screening of Inhibitors against SARS-COV-2. *ChemRxiv. Preprint* **2020**. (click here)
- **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* **2021**. (Under review)

PROFESSIONAL EXPERIENCE

Patent Analyst, Life Science Division Mar 2013 – Dec 2014
CSIR Unit of Research & Development of Information Products Pune, India

- Examined current technology alerts and patent updates in the field of life sciences for 5 projects.
- Interpreted comparative and competitive patent portfolio after novelty, patentability and prior art search.
- Mapped data for constructing a technological patent landscape.

Reviewed and revised papers for the Journal of Experimental and Theoretical Artificial Intelligence (Taylor & Francis) Feb 2021

CONFERENCE POSTERS AND WORKSHOP

Posters

- **Divya Karade**, N. Kadoo, M. Karthikeyan (**2019**) '**Antidiabetic Drug Designing** Based on Organic Metabolites from Fenugreek: A Chemo-and Bioinformatics Approach' presented at an international symposium on "Accelerating Biology: Towards Thinking Machines" conducted by C-DAC, Pune.
- **Divya Karade**, N. Kadoo, M. Karthikeyan (**2017**) '**Chemoinformatics Investigation** of Organic Metabolites from Soybean Reveals Common Drug Scaffolds' presented at CSIR-National Chemical Laboratory, Pune on the "National Science Day".
- **Divya Karade**, N. Kadoo, M. Karthikeyan (**2017**) '**Drug Design based on Metabolomics** of Indian Medicinal and Aromatic Plants: A Chemoinformatics Approach' presented at CSIR-National Chemical Laboratory, Pune on the "National Science Day".

Workshop

- Trained (**10** people) and self-participated for "**Chemoinformatics-2018**" for skill development program by CSIR-NCL, Pune

TECHNICAL SKILLS

- **Programming Languages:** Python, R, MySQL
- **Data Science & Miscellaneous Technologies:** Biological and Chemical Data analysis, Data science pipeline (cleansing, wrangling, EDA, visualization, modeling, interpretation) Statistics, Experimental design, Hypothesis testing, Excel, GitHub
- **Big Data and Machine learning:** Python (eg. TensorFlow, Keras, scikit-learn, streamlit, NumPy, pandas, matplotlib, seaborn, etc.), Building and deploying ML, Auto-ML and deep learning applications, Web-app development, cloud platform - Heroku
- **Bioinformatics:** Molecular docking and analysis using computational chemistry tools like Schrodinger, MOE, AutoDock, etc.
- **Patinformatics:** Prior art search, Freedom to operate analysis, Landscaping, Novelty check
- **Chemoinformatics:** Drug designing, data mining, text mining, Network analysis, Chemical structure analysis, QSAR, virtual screening, building virtual libraries, scaffold analysis using chemoinformatics tools like MOE, ChemAxon, ChemDraw, Cytoscape.
- **Genomics:** DNA and RNA extraction, PCR analysis, Phylogenetic statistical analysis
- **Proteomics:** Protein extraction from plant tissues, Electrophoresis techniques – PAGE
- **Metabolomics:** Untargeted metabolomics, Mass- spectrometric data analysis, Univariate and Multivariate statistical analysis