

# Divya Karade

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## Education

**Ph.D. in Biological Science (Chemoinformatics, Metabolomics and Computational Biology)**

Academy of Scientific and Innovative Research (AcSIR)

*Jan 2015 - Thesis submitted*

*Pune, Maharashtra, India*

- Thesis: Chemoinformatics 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 (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 Biotechnology, Plant Biochemistry, Molecular Biology, Genetics, Microbiology

## Innovation Project

**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 | Matplotlib | Streamlit | Heroku)

- Innovated and founded a user-friendly web application platform called 'AIDrugApp' for drug discovery.
- Created and Implemented 8 DL algorithms to AIDrugApp for the virtual screening of inhibitor molecules against SARS-CoV-2.
- Originated and integrated machine learning tools like Auto-Multi-ML, Auto-DL, etc to AIDrugApp.

## Experience

**Senior Research Fellow (Ph.D. Candidate)**

*Jan 2017 - Present*

CSIR National Chemical Laboratory, Chemical Engineering and Process Development

*Pune, India*

- Designed and executed laboratory biochemical experiments to optimize 4 Indian varieties of soybean samples for LC/MS studies.
- Conceptualized analyzing methods for mass spectrometric data (7185 mass features) using machine learning tools and techniques.
- Discovered and reported the presence of 14 novel small molecules in soybean through tandem mass spectrometry analysis.
- Generated virtual library of 815 novel drug-like molecules from soybean small molecules through chemoinformatics techniques.
- Investigated and designed 169 pesticide-like molecules from 162 plants using chemoinformatics tools and QSAR approaches.

**Junior Research Fellow (Ph.D. Candidate)**

*Jan 2015 - Dec 2016*

CSIR National Chemical Laboratory, Chemical Engineering and Process Development

*Pune, India*

- Analyzed molecular data (n=3459) by text mining 91206 PubMed literature related to 104 Indian medicinal plants.
- Developed 4 computational protocols for designing novel molecules from small molecules of medicinal plants & food crops.
- Created virtual library of 4147 novel drug-like molecules for building a database cum toolkit of Indian medicinal plants.

**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.

**Reviewer** for the "Journal of Experimental and Theoretical Artificial Intelligence" (Taylor & Francis)

*Feb 2021- Present*

## Skills

- **Programming Languages:** Python, R, MySQL, HTML
- **Data Science & Miscellaneous Technologies:** Biological and Chemical Data analysis, Data science pipeline (cleansing, wrangling, EDA, visualization, modeling, interpretation) Statistics, Hypothesis testing, Excel, GitHub
- **Big Data and Machine learning:** TensorFlow, Keras, scikit-learn, streamlit, NumPy, pandas, Matplotlib, seaborn, Building and deploying ML/ DL algorithms, Feature engineering, Auto-ML, Auto-DL, Web-app development, cloud platform – Heroku, AWS
- **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:** Structure- & ligand based drug design, data/ text mining, Network analysis, Chemical structure analysis, SAR/ QSAR, virtual screening, building virtual libraries, ADME, scaffold analysis, 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

## Honors & Awards

### National & International

- National-level AWS DeepRacer at Woman's league for community car races driven by reinforcement learning codes in python through AWS cloud-based 3D racing simulator. **(Selected in top 100)** Apr 2021
- National Award for "AIDrugApp" 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)** Mar 2021
- Certificate of Merit for "AIDrugApp" 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

### Academic

- 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
- 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

**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**, Vikas Karade. AIDrugApp: Artificial Intelligence-based Web-App for Virtual Screening of Inhibitors against SARS-COV-2. *ChemRxiv. Preprint* **2020**. (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**, S. Sivaramkrishnan, 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](#))

**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**. (Impact factor: 2.111, Under review)

**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**. (Impact factor: 3.167, Under review)

## Research Presentations

### 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

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