



SSR

COLLEGE OF PHARMACY

NEWSLETTER

June–July 2026 Edition



EDITOR-IN-CHIEF

Dr. Chandrakant Bonde



EDITOR

Ms. Hemangi Rathod



From the Editorial Desk



It gives us immense pleasure to present this edition of the SSR College of Pharmacy newsletter – a reflection of the vibrant academic, research, and co-curricular activities that continue to shape our institution.



At SSR College of Pharmacy, we are committed to fostering innovation, critical thinking, and ethical responsibility in the field of pharmaceutical sciences. This issue highlights some of the recent achievements of our students and faculty, academic collaborations, seminars, workshops, and community outreach initiatives that continue to inspire growth and excellence.



Our college remains dedicated to nurturing future pharmacists who are not only skilled and knowledgeable but also socially responsible contributors to healthcare. We applaud the consistent efforts of our students, faculty members, and alumni who make SSR College of Pharmacy a hub of academic brilliance.



We hope this edition serves as a source of pride, motivation, and information for our readers. We look forward to your continued support and contributions in making each edition more engaging and impactful.

Warm regards,

EDITORIAL BOARD

EDITORIAL BOARD

- **Dr. Smita Bonde**



- **Dr. Sonal Desai**



- **Dr. Himanshu Solanki**



- **Dr. Parixit Prajapati**



- **Mr. Vipul Prajapati**



- **Dr. Lata Manani**



- **Ms. Priya Shukla**





WORLD ENVIRONMENT DAY CELEBRATION

Let's nurture nature for a sustainable future

To commemorate **World Environment Day**, SSR College of Pharmacy organized a **Tree Plantation Drive on 5th June 2026** within the college premises. The initiative aimed to promote environmental sustainability, ecological awareness, and a sense of responsibility toward nature among students and staff.



As part of the program, saplings of **Asopalav** (*Polyalthia longifolia*), **Neem** (*Azadirachta indica*), and **Banyan** (*Ficus benghalensis*) were planted in the open spaces surrounding the hostel area to enhance the campus green cover and contribute to ecological balance.

The plantation drive was inaugurated by the **Principal of SSR College of Pharmacy** in the presence of faculty members, non-teaching staff, and enthusiastic student volunteers. The participants actively engaged in the activity, demonstrating their commitment to environmental conservation and sustainable development.



The event concluded with an inspiring message from the Principal, highlighting the importance of collective efforts in protecting and preserving the environment for future generations. The program successfully fostered environmental consciousness and encouraged everyone to contribute towards a **greener and healthier planet**.

"Clinical Workshop on 'EMERGENCY FIRST AID KIT'"

Conducted by Department of Pharmacology



The Department of Pharmacology, SSR College of Pharmacy, successfully organized a Clinical Workshop on "Emergency First Aid Kit" to enhance students' knowledge and practical skills in managing emergency situations through appropriate first-aid measures. The workshop was conducted by the First Year M. Pharm (Pharmacology) students under the guidance of the department faculty members and was divided into two interactive sessions.



The informative sessions. The first session featured a PowerPoint presentation highlighting the importance of emergency first aid, essential components of a well-equipped first-aid kit, and the management of common medical emergencies. The presenters explained the uses of first-aid supplies and the precautions to be followed during emergencies.



The second session focused on practical demonstrations of emergency case scenarios, including burns, bleeding, fractures, injuries, fainting, and other common situations. Audience members actively participated in scenario-based activities, gaining valuable hands-on experience in applying first-aid principles. The workshop witnessed enthusiastic participation and served as an excellent platform for promoting awareness and preparedness during emergencies. The programme concluded with a Vote of Thanks delivered by Ms. Jenifer Ferreir, who expressed gratitude to the Principal, faculty members, presenters, and participants for their contributions. The workshop was a great success and provided all participants with valuable knowledge and practical skills in emergency first-aid management.



Final Year B.Pharm Students Successfully Complete Research Project Presentations

The Final Year B.Pharm students of SSR College of Pharmacy, Silvassa, successfully completed the final presentation of their research and review projects on 21st and 22nd May 2026. The presentations marked the culmination of extensive research work carried out under the guidance of faculty mentors from the Departments of **Pharmaceutics, Pharmacology, Pharmacognosy, Pharmaceutical Chemistry, and Quality Assurance.**



Be Prepared.
Be Safe.



Hands-on Learning.
Lifelong Impact.



Research Today,
Better Tomorrow.



Knowledge
Saves Lives.



During the presentations, students showcased their research methodology, experimental findings, data analysis, and conclusions before faculty members and project guides. The activity provided an excellent platform for enhancing scientific temperament, critical thinking, teamwork, research aptitude, and presentation skills.



A total of **22 project groups** comprising **75 students** presented innovative research and review projects addressing contemporary pharmaceutical and healthcare challenges.

The projects covered diverse areas such as herbal formulations, nutraceuticals, analytical method development, antioxidant studies, molecular docking, antimicrobial evaluation, probiotic formulations, cosmetic preparations, wound healing systems, and healthcare technologies.



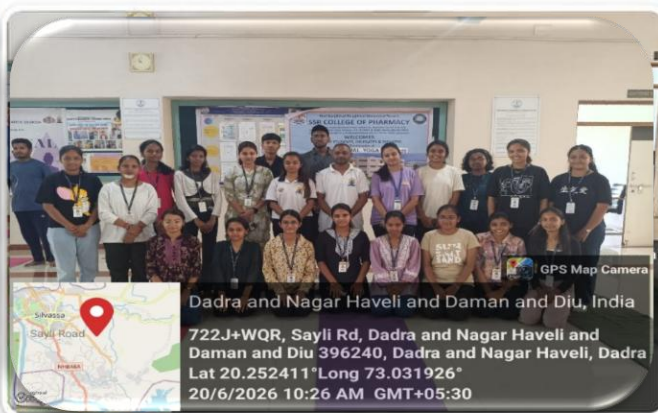
CELEBRATING RESEARCH. INSPIRING INNOVATION.
SHAPING THE FUTURE OF HEALTHCARE.





The management and faculty members appreciated the sincere efforts of the students and acknowledged the valuable guidance provided by the project mentors. The successful completion of these projects reflects SSR College of Pharmacy's commitment to promoting research culture, experiential learning, and academic excellence among undergraduate students.

The institution congratulates all the final-year B.Pharm students and their faculty guides for their dedication, hard work, and successful completion of the research project presentations during the academic year 2025–26.



The programme was graced by **Dr. Chandrakant Bonde, Principal**, SSR College of Pharmacy, and **Dr. Rakesh Patil, Director**, SSR College of IMR. The yoga session was led by renowned Yoga Trainer **Mr. Kiran Patel** and Yoga enthusiast **Ms. Ushma Patel**, who guided participants through a series of yoga asanas, pranayama, stretching exercises, and meditation techniques.

SSR College of Pharmacy celebrated **International Yoga Day 2026** on **20 June 2026** with great enthusiasm under the theme **"Yoga for Self and Society."** The event aimed to promote the significance of yoga in achieving physical fitness, mental well-being, and social harmony while encouraging a balanced and healthy lifestyle.

Held on the **Ground Floor of SSR College of IMR**, the event commenced with a welcome address followed by an insightful introduction by **Mr. Kiran Patel**, highlighting the role of yoga in reducing stress, improving overall health, and fostering inner peace. The trainers explained the benefits of each practice and motivated participants to incorporate yoga into their daily lives.



Learn.
Lead.
Excel.



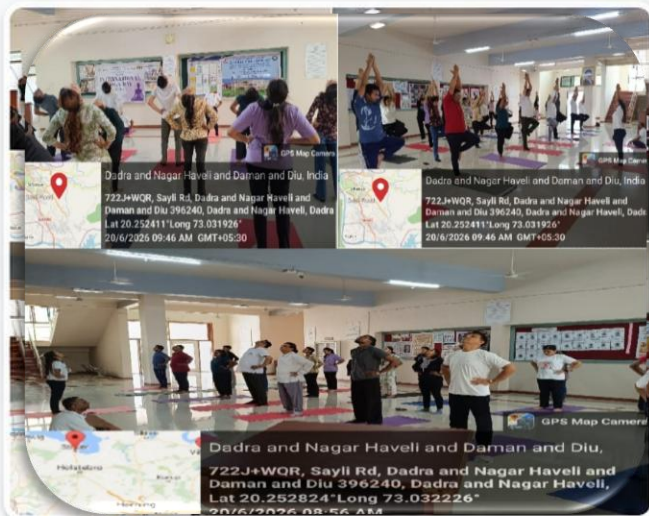
Knowledge
Empowers.



Research Today,
Better Tomorrow.



Care.
Commit.
Contribute.



The programme was graced by **Dr. Chandrakant Bonde**, Principal, SSR College of Pharmacy, and **Dr. Rakesh Patil**, Director, SSR College of IMR.

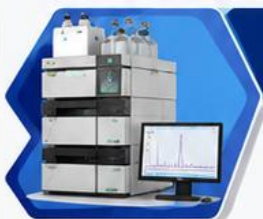
The yoga session was led by renowned Yoga Trainer **Mr. Kiran Patel** and Yoga enthusiast **Ms. Ushma Patel**, who guided participants through a series of yoga asanas, pranayama, stretching exercises, and meditation techniques.



*Yoga is not just
an exercise,
it is a way of life.*



The celebration concluded successfully with heartfelt appreciation to the dignitaries, trainers, participants, and volunteers whose enthusiastic support contributed to the success of **International Yoga Day 2026** at SSR College of Pharmacy.



A hands-on training session on the operation of JASCO HPLC Systems was organized for M.Pharm. students of the Department of Quality Assurance at SSR College of Pharmacy, Silvassa, on 25th June 2026.



The training was conducted by **Mr. Pranay Jadhav**, Engineer, Anatek Services Pvt. Ltd., Mumbai, who provided comprehensive practical training on the operation, handling, and maintenance of the JASCO HPLC system.



The session covered instrument start-up and shutdown procedures, preparation of the HPLC system, software operation, method setup, sample injection, data acquisition, troubleshooting, and routine maintenance practices.



Students were given the opportunity to operate the instrument under expert guidance, enabling them to gain valuable practical exposure and confidence in handling sophisticated analytical equipment.

REPORT ON HANDS-ON TRAINING ON OPERATION OF JASCO HPLC SYSTEMS

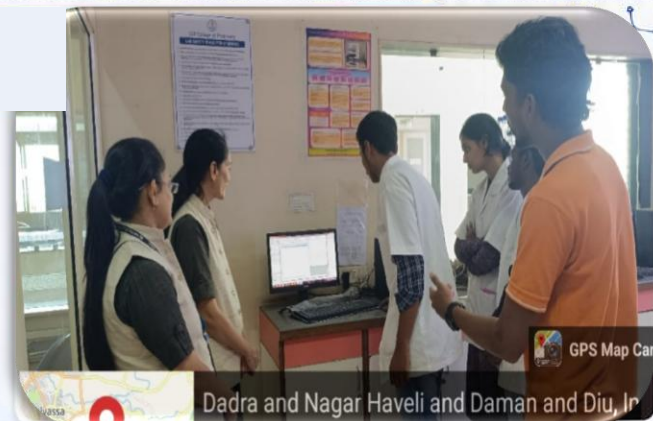
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Students, faculty members, and staff enthusiastically participated in the session, making the celebration a vibrant and memorable experience. The programme fostered unity, discipline, and wellness while reinforcing the message that yoga is not merely a form of exercise but a holistic way of life.



The programme was coordinated by **Dr. Sonal Desai**, Head, Department of Quality Assurance, SSR College of Pharmacy, Silvassa. The training proved to be highly beneficial in enhancing the technical skills of the M.Pharm. students and bridging the gap between theoretical knowledge and practical application in pharmaceutical analysis. The Department of Quality Assurance expressed its sincere gratitude to **Mr. Pranay Jadhav** and **Anatek Services Pvt. Ltd.**, Mumbai, for their valuable contribution towards strengthening the practical competencies of the students.



Nasha Mukti Bharat Abhiyan

A STEP TOWARDS A DRUG-FREE INDIA

“Say No to Drugs, Say Yes to Life”

SSR College of Pharmacy, Sayli, Silvassa, in collaboration with Savitribai Phule Pune University (SPPU), successfully organized **Nasha Mukti Bharat Abhiyan** on **25 June 2026**. The campaign aimed to create awareness among students about the harmful effects of substance abuse and to promote a healthy, drug-free lifestyle.

Objectives

- ✓ To create awareness about the ill effects of substance abuse.
- ✓ To encourage youth to adopt a healthy and responsible lifestyle.
- ✓ To build a drug-free and stronger India.

Key Activities

Online Mass Pledge Against Drug Abuse

Students and faculty members took an Online Mass Pledge, vowing to stay away from drugs and to contribute towards a drug-free society.



Educational Film Screening

Short films on drug abuse prevention were screened, highlighting the physical, psychological, social and economic consequences of substance abuse, motivating students to make informed and responsible life choices.



Date : 17–26 June 2026



Venue : SSR College of Pharmacy, Sayli, Silvassa



Organized by : SSR College of Pharmacy in collaboration with Savitribai Phule Pune University (SPPU)



Nasha Mukti Mitr Registration Drive

Students actively participated in the Nasha Mukti Mitr Registration Drive, demonstrating their commitment to become ambassadors of awareness and contribute to the nationwide mission of eradicating substance abuse.



Competitions by Savitribai Phule Pune University

Students enthusiastically participated in various competitions.



Poster Making
Competition

Slogan Writing
Competition

Essay Writing
Competition

The competitions provided a platform for students to express their creativity, knowledge and social responsibility with impactful messages promoting a drug-free lifestyle.



Coordinators

The programme was coordinated by Ms. Parthika Patel and Dr. Lata M. Manani, with active support from faculty members. Students from both B.Pharm and M-Pharm programmes participated enthusiastically in all activities.



Outcomes

- ✓ Raised awareness among youth about the dangers of drug abuse.
- ✓ Encouraged collective commitment for a healthier and safer future.
- ✓ Strengthened the message of a greener, healthier and addiction-free India.

The event witnessed active participation from students and faculty and successfully conveyed the importance of preventing drug abuse. SSR College of Pharmacy remains dedicated to conducting such awareness initiatives for the overall well-being of students and society.

Say No to Drugs, Say Yes to Life



Healthy Youth
Healthy India



Drug Free India
Our Responsibility



DTE INTAKE APPROVAL MEETING

A meeting regarding the **DTE Intake Approval Form** was successfully conducted with **Ms. Priya Shukla (Admission Head)**, the admission committee members, and the Principal. During the meeting, all required documents, intake details, and compliance requirements were thoroughly reviewed in accordance with the Directorate of Technical Education (DTE) guidelines.



- ❖ Key aspects of the intake approval process were discussed, and the necessary actions were finalized to ensure the **timely and accurate submission** of the DTE intake approval form. The meeting concluded successfully with a shared commitment to maintaining regulatory compliance and facilitating a smooth admission approval process.



SCRUTINY CENTRE (SC) REGISTRATION MEETING

A meeting on the **Scrutiny Centre (SC) Registration and Scrutiny Form Filling Process** for CAP 2026–27 was successfully conducted by **Ms. Priya Shukla, Admission Head** and admission committee members. The meeting was organized following the commencement of the **registration process** for institutes to apply as **Scrutiny Centres (SC)** for the CAP Process 2026–27.



The meeting included a detailed discussion on the **registration procedure, required documentation, Scrutiny Form filling, eligibility norms**, and important timelines. The team ensured that all procedures are followed as per the DTE and CET Cell guidelines for a hassle-free CAP process.



During the session, detailed instructions regarding the **SC registration process, scrutiny form filling, document verification, eligibility criteria, and compliance** with the prescribed admission guidelines were discussed. All queries were addressed to ensure accurate and timely completion of the registration and scrutiny process. The meeting concluded with clear action points and a coordinated approach to facilitate a smooth and efficient **CAP admission process** for the academic year 2026–27.



MEMORANDUM OF UNDERSTANDING (MoU) SIGNED BETWEEN SSR COLLEGE OF PHARMACY AND S KANT HEALTHCARE LTD.



SSR College of Pharmacy proudly signed a Memorandum of Understanding (MoU) with S Kant Healthcare Ltd. This partnership aims to promote collaboration in areas of **academics, training, research, and industry exposure**, benefiting students and faculty through knowledge sharing and hands-on learning opportunities.





OBJECTIVES OF THIS PARTNERSHIP

- Bridge the gap between theoretical knowledge and practical industry exposure.
- Offer internships, industrial visits, expert lectures, and skill development programs.
- Promote research collaborations and training initiatives.
- Enable faculty and students to gain insights into current pharmaceutical industry practices.
- Foster innovation, professional growth, and career readiness.



SSR COLLEGE OF PHARMACY, SILVASSA



Congratulations!

Heartly Congratulations to
Mr. Vipul D. Prajapati
for being recognized among the
WORLD'S TOP 5% SCIENTISTS
in the 2025 SciRank Global Registry

A proud moment for SSR College of Pharmacy, Silvassa.
Your achievement inspires us all!



Global Recognition
Ranked among the
World's Top 5% Scientists
in 2025 by SciRank Global Registry



Research Excellence
A testament to exceptional
research impact and
academic excellence



Inspiration to All
Your success motivates
students, faculty and the
entire SSR family



PRIDE OF SSR | INSPIRATION FOR GENERATIONS

NPTEL MENTOR RECOGNITION -



NPTEL



CERTIFICATE

OF APPRECIATION

is awarded to

HEMANGI HARSHESH RATHOD

SSR COLLEGE OF PHARMACY
SILVASSA, DADRA AND NAGAR HAVELI

in recognition of his/her role as a mentor for the
NPTEL Online Certification course

HUMAN PHYSIOLOGY

JAN - APR 2026



Prof. Andrew Thangaraj
NPTEL Coordinator
IIT Madras

Mentors Enrolled	Mentors Present	Score (in %) <40	Score (in %) 40-59	Score (in %) 60-74	Score (in %) 75-89	Score (in %) >>90	Toppers
54	48	34	11	3	0	0	0

Human Physiology (Jan–Apr 2026) +

Mrs. Hemangi Harshesh Rathod, SSR College of Pharmacy, Silvassa, received a Certificate of Appreciation from NPTEL-SWAYAM, IIT Madras, in recognition of her role as a mentor for the NPTEL Online Certification Course on “Human Physiology” (January–April 2026).



Under her mentorship, **54 students** enrolled for the course, out of which **48 students** appeared for the examination.



The initiative encouraged students to enhance their understanding of human physiology through an online learning platform and promoted self-directed learning beyond the regular curriculum.



This achievement reflects the institution's commitment to fostering academic excellence and encouraging participation in national-level online certification programmes.

SSR College of Pharmacy congratulates **Mrs. Hemangi Harshesh Rathod** for her valuable contribution and continued efforts in guiding students towards quality education and skill development.



COLLABORATE.
INNOVATE.
TRANSFORM.



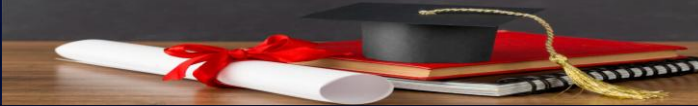
LEARN TODAY.
LEAD TOMORROW.



KNOWLEDGE EMPOWERS.
RESEARCH INSPIRES.



TOGETHER FOR
A HEALTHIER FUTURE.



NPTEL

CERTIFICATE OF APPRECIATION
is awarded to

VIPULKUMAR PRAJAPATI
SSR COLLEGE OF PHARMACY
SILVASSA, DADRA AND NAGAR HAVELI

in recognition of his/her role as mentor for the
NPTEL Online Certification course

HERBAL PRODUCT TECHNOLOGY AND REGULATORY SCIENCE
JAN - APR 2026

QR Code

Metrics Invited	Metrics Active	Score (in %) 0-59	Certified (Score in %)				
			60-74	75-89	>=90	In 5% Toppers	
58	30	3	1	6	18	2	0

PROF. ANDREW THANGARAJ
NPTEL Coordinator
IIT Madras

NPTEL

CERTIFICATE OF APPRECIATION
is awarded to

VIPULKUMAR PRAJAPATI
SSR COLLEGE OF PHARMACY
SILVASSA, DADRA AND NAGAR HAVELI

in recognition of his/her role as mentor for the
NPTEL Online Certification course

GENERAL PHARMACOLOGY
JAN - APR 2026

QR Code

Metrics Invited	Metrics Active	Score (in %) 0-59	Certified (Score in %)				
			60-74	75-89	>=90	In 5% Toppers	
34	27	2	5	10	9	0	0

PROF. ANDREW THANGARAJ
NPTEL Coordinator
IIT Madras

OUTSTANDING ACADEMIC ACHIEVEMENTS



Under his guidance, **58 students** enrolled in the **Herbal Product Technology and Regulatory Science** course, of which **30 students** appeared for the examination. The students achieved excellent results, with **18 students** securing scores between **75–89%**, **2 students** scoring above **90%**, and **6 students** scoring between **60–74%**.



Similarly, in the **General Pharmacology** course, **34 students** enrolled, and **27 students** appeared for the examination. The students demonstrated commendable performance, with **19 students** securing scores between **60–74%** and **1 student** scoring between **75–89%**.



These achievements reflect the effectiveness of **Mr. Vipulkumar Prajapati's** mentorship, his continuous academic support, and his commitment to promoting self-directed learning among students. This recognition also highlights **SSR College of Pharmacy's** dedication to fostering online learning, skill enhancement, and academic excellence through national-level certification programmes. The institution congratulates **Mr. Vipulkumar Prajapati** on this remarkable achievement and appreciates his valuable contribution towards motivating students to excel in interdisciplinary learning and professional development.

TOP PERFORMING MENTOR RECOGNITION



Mr. Vipulkumar Prajapati, faculty member of **SSR College of Pharmacy, Silvassa**, was honoured with the “**Top Performing Mentor – Certificate of Appreciation**” by **NPTEL–SWAYAM, IIT Madras** for his outstanding mentorship in two NPTEL Online Certification Courses, “**Herbal Product Technology and Regulatory Science**” and “**General Pharmacology**” conducted during **January–April 2026**.



This recognition is a testament to his dedication, mentorship excellence, and commitment towards academic growth and student success.

CAMPUS PLACEMENT HIGHLIGHTS 2026

SSR College of Pharmacy proudly celebrates the outstanding placement achievements of its students during **May and June 2026**. A total of **24 students** from **B.Pharm and M.Pharm** programmes secured placements in leading pharmaceutical industries, research organizations, and academic institutions across India. The placement drive witnessed an overwhelming response from reputed recruiters, with the **highest salary package of ₹4.20 LPA** offered to our students. This achievement reflects the institute's unwavering commitment to academic excellence, industry-oriented training, and holistic career development.





SSR College of Pharmacy Newsletter

Excellence in Education, Research & Innovation

June-July-2026

Edition



B.Pharm Students – Placement & Internship Details

B.Pharm			
Student Name	Organization	Location	Month
 Bibek Rajendra Behera	IPCA Laboratories Ltd.	Silvassa, Dadra & Nagar Haveli	May
 Vimla Kumari Singh	IPCA Laboratories Ltd.	Silvassa, Dadra & Nagar Haveli	May
 Kiran Kale	IPCA Laboratories Ltd.	Silvassa, Dadra & Nagar Haveli	May
 Survi Sathvarajsingh	IPCA Laboratories Ltd.	Silvassa, Dadra & Nagar Haveli	May
 Lokesh Manohar Khaimar	IPCA Laboratories Ltd.	Silvassa, Dadra & Nagar Haveli	May
 Satyam Kumar	Alkem Laboratories Ltd.	Silvassa, Dadra & Nagar Haveli	May
 Reema Elia Biju	Alkem Laboratories Ltd.	Daman	May
 Yash Mishra	Alkem Laboratories Ltd.	Daman	May
 Meetali Mukesh Bhatia	Alkem Laboratories Ltd.	Daman	May
 Aarya Chandra Bhushan	Alkem Laboratories Ltd.	Daman	May
 Ahire Rohan Naradev	Alkem Laboratories Ltd.	Daman	May
 Shubham Patil	Alkem Laboratories Ltd.	Daman	May
 Dipesh Shinde	Exemed. Pharmaceuticals	Vapi, Gujarat	June

M.Pharm (Pharmaceutical Chemistry)			
Student Name	Organization	Location	Month
 Maithil V. Dabhi	Pharmaco Research Laboratories Pvt Ltd.	Ahmedabad, Gujarat	May
 Himani Dange	Nuvi AI Pvt. Ltd.	Ahmedabad, Gujarat	May
 Patil Harshal Mohan	UKA Tarsadia University	Bardoli, Gujarat	June
 Sandeep Bokara	IPCA Laboratories Ltd.	Silvassa, Dadra & Nagar Haveli	June
 Jaiswal Priya Jaydeep	IPCA Laboratories Ltd.	Silvassa, Dadra & Nagar Haveli	June

M.Pharm (Quality Assurance)			
Student Name	Organization	Location	Month
 Alkesh Mourya	Veeda Lifesciences	Ahmedabad, Gujarat	May
 Anandha Krishnan	Ensami Ltd.	Vapi, Gujarat	June
 Hiral Vadgama	Universal Twin Laboratories	Ahmedabad, Gujarat	June
 Shivang Kahar	Universal Twin Laboratories	Ahmedabad, Gujarat	June
 Varad Gore	Universal Twin Laboratories	Ahmedabad, Gujarat	June

M.Pharm (Pharmacology)			
Student Name	Organization	Location	Month
 Wagh Bharati Govindlal	UKA Tarsadia University	Bardoli, Gujarat	June



Opportunities

We create pathways to your future.



Industry Connect

Strong collaborations for real-world exposure.



Growth

Nurturing talent, building leaders.



Success

Celebrating your achievements.



Future Ready

Equipped with skills to excel globally.



Publications and Award

11

Mitochondrial targeting in cancer therapeutics

Dhara Patel¹, Payal Kholiya², Grishma Patel¹, Vivek Patel³, Hely Patel⁴, * and Jayvadan K. Patel⁵

¹ PIONEER PHARMACY COLLEGE, VADODARA, GUJARAT, INDIA; ² SSR COLLEGE OF PHARMACY, SILVASSA, DADRA AND NAGAR HAVELI, INDIA; ³ SUN PHARMACEUTICAL INDUSTRIES LTD., VADODARA, GUJARAT, INDIA; ⁴ SARVAJANK UNIVERSITY, SURAT, GUJARAT, INDIA; ⁵ VIESIAI PHARMA, LLC, COLUMBUS, GA, UNITED STATES

Introduction

Mitochondria, often referred to as the “powerhouses of the cell,” are highly dynamic and multifunctional organelles that serve as critical hubs in cellular metabolism, signaling, and death regulation. They are double-membraned organelles primarily responsible for producing adenosine triphosphate (ATP) through oxidative phosphorylation (OXPHOS). While classically known for generating ATP through OXPHOS, mitochondria also participate in biosynthetic reactions, reactive oxygen species (ROS) generation and detoxification, calcium buffering, and initiation of apoptosis. Their double-membrane structure, encompassing an outer membrane and a highly folded inner membrane (forming cristae), provides distinct compartments for biochemical reactions and regulatory mechanisms. The mitochondrial matrix houses its own DNA (mtDNA), which encodes a subset of components necessary for respiratory chain function, reflecting their endosymbiotic origin [1].



SSR College of Pharmacy proudly congratulates Mrs. Payal Kholiya on the publication of her book chapter, “Mitochondrial Targeting in Cancer Therapeutics,” in the book *Emerging Trends in Cancer Research*. This remarkable achievement reflects her dedication to research and contributes significantly to advancing knowledge in the field of cancer therapeutics.



SSR COLLEGE OF PHARMACY, SILVASSA

Permanently Affiliated to Savitribai Phule Pune University; Approved by AICTE & PCI
(NBA Accredited for B.Pharm Program 2019-2025)



Congratulations

Mr. Shreehari Thombare (PG Student)
For publication of research article entitled



“Comparative evaluation and selection of optimal QSAR-based machine learning model for liver toxicity prediction” in “**Molecular Biodiversity**” journal

Molecular Diversity
<https://doi.org/10.1007/s11000-026-11615-1>

RESEARCH

Comparative evaluation and selection of optimal QSAR-based machine learning model for liver toxicity prediction

Shreehari Thombare¹, Chandrakant Bonde^{2*}, Prashant Khatkar¹, Janeekumar Garwad³

Received: 8 April 2025 / Accepted: 27 May 2025
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Abstract

Drug-induced liver toxicity remains the most common cause of acute liver failure. Conventional toxicity detection relies on resource-intensive in vivo and in vitro assays that are costly, time-consuming, and poorly scalable to the volumes of candidate compounds typical of modern drug discovery. Robust, interpretable computational tools capable of early stage toxicity prioritization are therefore indispensable. We systematically compared seven widely used molecular descriptor sets (PaDEL, ATC, ADR, MHFP, maccs, CDK, and E-state indices), five machine learning algorithms (random-forest, logistic regression, support vector machine, k-Nearest Neighbors, and naive Bayes), and performance metrics (Q^2 , RMSE, AUC, and MAE). Our findings show: (i) Random-forest with RDKit descriptors consistently delivered the best cross-validation performance (highest Q^2 and AUC, lowest RMSE and MAE); (ii) feature-based models outperformed all fingerprint-based variants; and (iii) the final model achieved 86% external test set accuracy, 89% sensitivity, and 82% specificity. These results establish a reproducible, interpretable QSAR workflow that can streamline early-stage hepatotoxicity assessment and reduce late-stage attrition.



Research
Excellence



Recognition



Innovation



Impact