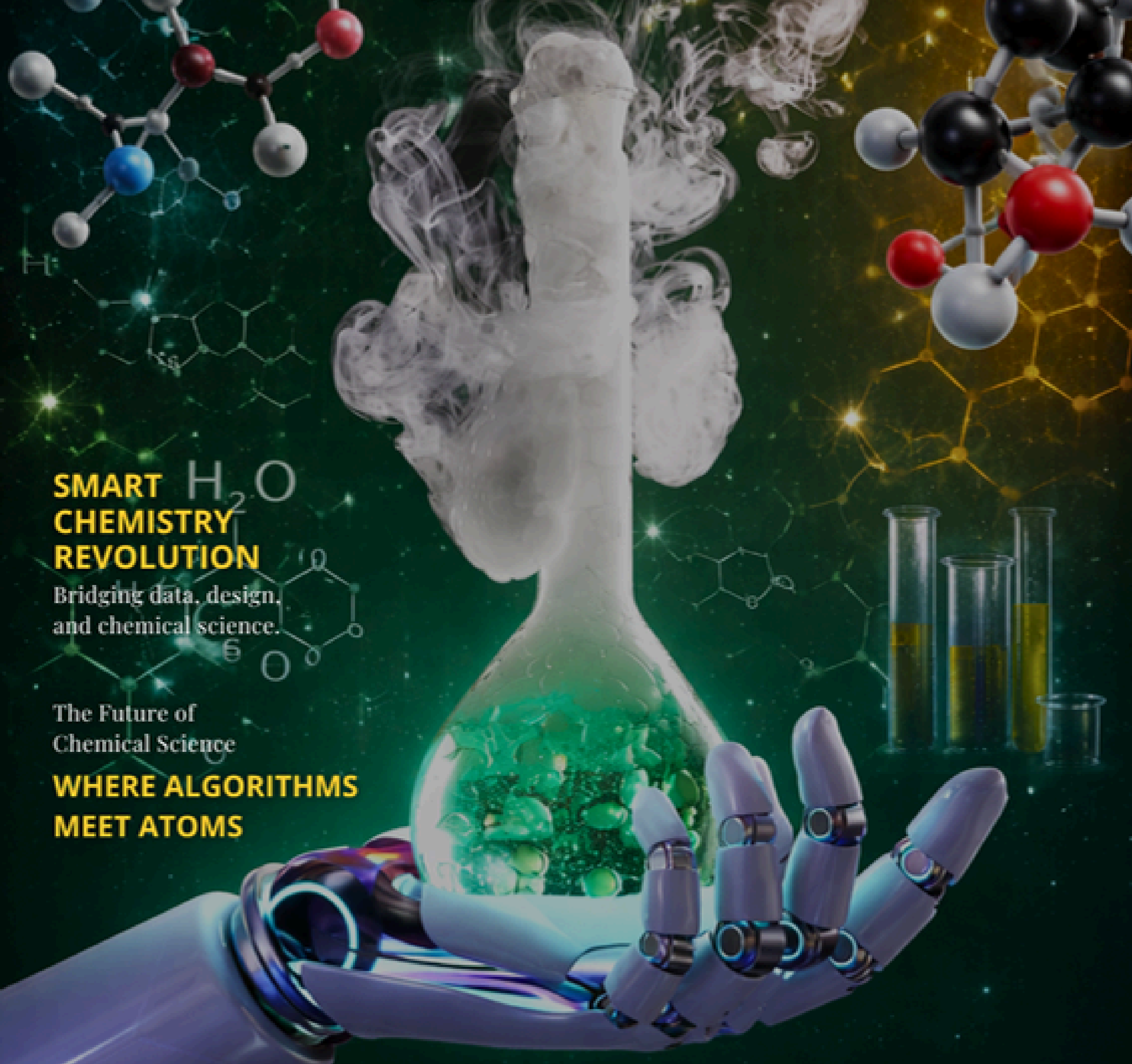
DEPARTMENT OF CHEMISTRY

SRI VENKATESWARA COLLEGE
DELHI UNIVERSITY



SMART CHEMISTRY REVOLUTION

Bridging data, design, and chemical science.

The Future of Chemical Science

WHERE ALGORITHMS MEET ATOMS

ABHIGYA

MAGAZINE 2025-26

ABOUT THE THEME

Artificial Intelligence in Chemistry is revolutionizing the way we explore, understand, and apply chemical knowledge. It enables scientists to analyze vast datasets, predict chemical reactions, and design complex molecules with remarkable speed and accuracy. By integrating machine learning with traditional chemical principles, AI is helping bridge the gap between theoretical research and real-world applications.

One of the most impactful contributions of AI in chemistry is in drug discovery and healthcare. AI-driven models can identify potential drug candidates, predict their behavior, and optimize their effectiveness, significantly reducing the time and cost involved in pharmaceutical development. This not only accelerates innovation but also opens new possibilities for personalized medicine and treatment strategies.

AI is also transforming laboratory practices through automation and smart experimentation. From robotic synthesis to real-time data analysis, AI enhances precision, reduces human error, and allows researchers to focus more on creativity and problem-solving. It supports sustainable chemistry by optimizing processes, minimizing waste, and promoting environmentally friendly solutions.

Through ABHIGYA, we aim to explore and celebrate this powerful intersection of technology and chemistry. This magazine serves as a platform to highlight innovations, inspire curiosity, and encourage young minds to delve into the evolving world of AI in chemistry, shaping a smarter and more sustainable future.

ABOUT
SRI VENKATESWARA COLLEGE

The desire to share knowledge and the dream to make education accessible to all brought together three visionaries, Smt Durgabai Deshmukh, Shri K. L. Rao and Shri C. Anna Rao in the early decades of India’s independence. The aim was to craft a dynamic space for knowledge sharing that would seamlessly blend traditional values, learning with modern outlook and rationale in the heart of our country, Delhi. The dream blossomed into reality with the aid and encouragement rendered by Tirumala Tirupati Devasthanams (TTD) and Sri Venkateswara College made its modest beginnings in Andhra Education Society 1961.

The foundation stone of the present day campus in Dhaula Kuan was laid in the same year by eminent Indian philosopher and statesman Dr. Sarvepalli Radhakrishnan. Since then, the Upanishadic principle “Truth through self-education” has been the guiding principle in all our endeavors. Thus, began our journey in shaping sensitive, balanced global citizens of tomorrow whose heart is cultured in indigenous values and mind is sharpened in critical thinking.

The College relentlessly pursued the ideals set by founders and took pride in creating a holistic learning atmosphere for students from diverse backgrounds at a minimum cost in the national capital for more than six decades. Sri Venkateswara College offers a platform for students from diverse backgrounds to excel in academics, research, cultural as well as social activities and sports. We take pride in the fact that “Venkyites” in today’s world are known for their penchant to excel in all walks of life.

PRINCIPAL'S DESK

Prof. Vajala Ravi
Principal SVC

Om Namo Venkatesaya!

I am delighted to note the publication of this issue of the chemistry magazine based on the theme "Role of Artificial Intelligence in Chemistry." The choice of such a contemporary and interdisciplinary theme reflects an innovative academic outlook and a commitment to keeping pace with the rapidly advancing frontiers of science.

The convergence of artificial intelligence with chemistry is opening new pathways in research, industry, and education. It is particularly encouraging to see our students engaging with such emerging areas, as it not only broadens their perspective but also equips them with the skills required for the future.

Over the years, ABHIGYA has grown into a valuable platform for students to showcase their scientific curiosity, creativity, and passion. This magazine not only reflects their dedication but also highlights the Department's commitment to nurturing young minds.

I warmly congratulate the Convener and the faculty members for their guidance and encouragement throughout this initiative. I also commend the students for their sincere efforts, creativity, and intellectual curiosity in contributing to this magazine. Their work is a reflection of the vibrant academic culture of our institution.

Good Luck!

Prof. Vajala Ravi

MESSAGE FROM EMINENT SCIENTIST AND ACADEMICIAN

Prof. (Dr.) A. K. Bakhshi
Eminent Chemist And Academician

It is a privilege and a matter of deep satisfaction for me to share my thoughts with the students and faculty of Sri Venkateswara College, University of Delhi, through your esteemed annual chemistry magazine. I sincerely thank you for inviting me in this capacity.

We are witnessing a transformative phase in science, where Artificial Intelligence (AI) is redefining the way chemistry is studied and practised. From predicting molecular structures and accelerating drug discovery to designing advanced materials and addressing environmental challenges, AI is enabling chemists to move beyond traditional boundaries with remarkable speed and precision.

While AI significantly enhances our capabilities, it remains a tool guided by human intellect. Curiosity, creativity, and critical thinking continue to be the foundation of meaningful scientific inquiry. The true strength of chemistry lies in the harmonious integration of human insight with technological advancement.

I urge students to embrace this interdisciplinary era by cultivating not only a strong foundation in chemistry but also an openness to emerging technologies such as AI and data science. Teachers, as mentors and guides, have a vital role in nurturing this spirit of inquiry and innovation.
Let us strive to ensure that the synergy between chemistry and AI contributes to the advancement of science for the greater good of society.

Prof. (Dr.) A. K. Bakhshi, FNASc is an eminent chemist and distinguished academician. He served as Head and Sir Shankar Lal Chair Professor of Chemistry at the University of Delhi and has held several prestigious positions, including Vice-Chancellor of PDM University, Haryana; Vice-Chancellor of UP Rajarshi Tandon Open University, Allahabad; and Executive Director of the Tertiary Education Commission, Mauritius. He also served as Chairman of the National Resource Centre of Chemistry, Government of India. A Double Gold Medallist and recipient of numerous awards and academic honours, he was felicitated twice by the former President of India, Dr. A. P. J. Abdul Kalam, for his outstanding contributions to education. Sir has delivered lectures in our college on popular Science themes and topics from Chemistry on several occasions in the past.

Prof. (Dr.) A. K. Bakhshi

MESSAGE FROM CONVENOR

Dr. Vinita Kapoor
Convenor

It gives me immense pleasure to present this issue of our department magazine, on the theme "Role of Artificial Intelligence in Chemistry." In today's rapidly evolving scientific landscape, artificial intelligence is transforming the way we explore, understand, and apply chemistry—enabling faster discoveries, smarter laboratories, and innovative solutions to global challenges.

"Artificial intelligence is not a substitute for human intelligence; it is a tool to amplify human creativity and ingenuity."

This quote by Chinese-American computer scientist, Fei-Fei Li, called the "Godmother of AI," beautifully captures the essence of our theme, where AI serves as a powerful partner in advancing chemical science. This issue aims to introduce readers to the dynamic role of artificial intelligence in chemistry—from accelerating drug discovery and designing advanced materials to enabling sustainable technologies and automated laboratories. I hope this magazine not only enhances your understanding but also inspires you to explore this exciting interdisciplinary frontier.

I would like to express my heartfelt gratitude to our respected Principal for his constant encouragement and unwavering support, which has been instrumental in bringing out this magazine. I also extend my sincere thanks to my fellow faculty members for mentoring the students and providing valuable insights throughout this journey.

A special word of appreciation goes to our dedicated student team. Their enthusiasm, creativity, and commitment have been the driving force behind this publication. Their efforts in exploring emerging topics and presenting them in an engaging and accessible manner are truly commendable.

As you turn these pages, we invite you to reflect on how the synergy between chemistry and AI is shaping the future of science and innovation.

Wishing you an insightful and enriching reading experience.

Dr. Vinita Kapoor

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EDITOR'S MESSAGE

Bhumika Singh
B.Sc.(H) Chemistry
Third Year(III)

Pratha Dhingra
B.Sc.(H) Chemistry
Third Year(III)

To achieve anything meaningful, we need a mission, a vision, and a goal. Our vision—to explore the transformative role of Artificial Intelligence in Chemistry and present it through an engaging and insightful medium—led to the creation of this year's departmental magazine. Blending the precision of science with the innovation of technology, we aim to showcase how AI is reshaping the future of chemistry.

The foundation of any remarkable creation lies in a well-structured plan. Our journey began with designing a thoughtful layout that could effectively integrate scientific knowledge with technological advancements. Once the framework was established, we invited contributions that reflected creativity, research, and curiosity at the intersection of AI and chemistry. With the content in place, our editorial team refined each piece, while the design team brought these ideas to life with their creativity and technical expertise.

The collective dedication of our contributors, combined with the unwavering support and guidance of our respected teachers, has helped us turn this vision into reality. This magazine stands as a testament to teamwork, innovation, and a shared passion for learning.

As it is rightly said, coming together is a beginning, staying together is progress, and working together is success. This magazine is the outcome of a harmonious collaboration, reflecting our enthusiasm, sincerity, and admiration for both chemistry and emerging technologies.

We proudly present to you the annual departmental magazine ABHIGYA, centered around the theme "AI in Chemistry"—a glimpse into the future where intelligence meets molecules, and innovation drives discovery.

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TABLE OF CONTENTS

1. Role of Artificial Intelligence in Medicinal Chemistry

2. Role of Artificial Intelligence in Publications Survey

3. Harnessing Artificial Intelligence for Next-Generation Chemical Education and Mechanistic Insights

4. AI Unleashes a New Era in Material Chemistry: From Sci-Fi Dreams to Real-World Wonders

5. Beyond the Black Box: Demystifying AI's "Chemical Intuition"

6. The Prediction of Reaction outcomes in Molecular Designing

7. Integrating Blockchain and AI for Secure and Efficient Chemical Supply Chains

8. How AI is Designing the Future of Nanoparticles

9. Noble Prizes in Chemistry 2025

10. Chemistry Crossword

11. Rasagya:The Chemical Society

12. Teachers' Achievement

13. Students' Achievement

14. 4th year Highlights

15. Teachers' Day

16. Fresher's Event (Batch 2025)

17. Scribble Day (Batch 2023-2026)

18. Farewell Day (Batch 2023-2026)

Role of Artificial Intelligence in Medicinal Chemistry

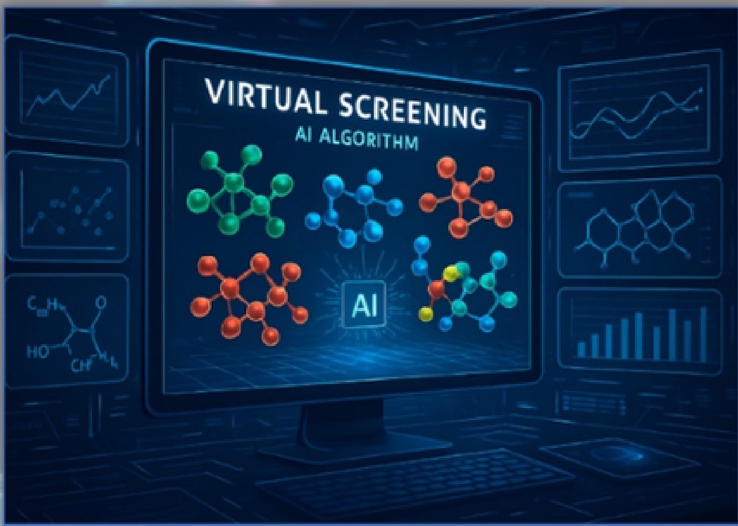
ABSTRACT

Artificial Intelligence (AI) has emerged as a transformative force in medicinal chemistry, offering solutions to challenges in drug discovery, molecular design, lead optimization, and drug repurposing. Traditionally, drug development has been expensive, time-consuming, and burdened by high failure rates in clinical trials. AI, through machine learning, deep learning, and laboratory automation, now accelerates nearly every stage of the drug development pipeline while simultaneously enhancing efficiency and reducing costs. This article explores the numbered applications of AI in medicinal chemistry, highlights real-world examples, introduces widely applied tools such as AlphaFold, ArgusLab, AutoDock, and DeepChem, and discusses current challenges and future prospects.

INTRODUCTION

Medicinal chemistry, the discipline that integrates chemistry and pharmacology to design and develop therapeutic agents, has been historically constrained by lengthy trial-and-error approaches. Bringing a single drug to market typically requires over a decade of research and billions of dollars in investment. High attrition rates in clinical trials, particularly late-stage failures, highlight the inefficiencies of traditional drug discovery pipelines. In recent years, AI technologies have been introduced as a powerful solution to these bottlenecks. By integrating computational power, predictive algorithms, structural biology insights, and automated experimentation, AI enables faster, more accurate, and cost-effective drug development. Its synergy with computational chemistry, bioinformatics, and lab automation has revolutionized the landscape of pharmaceutical sciences.

APPLICATIONS OF ARTIFICIAL INTELLIGENCE IN MEDICAL CHEMISTRY



1. ACCELERATING DRUG DISCOVERY

AI significantly shortens the traditional drug discovery timeline by virtually screening millions of compounds to identify potential therapeutic candidates. Machine learning models can predict drug–target interactions without requiring exhaustive laboratory testing and suggest novel scaffolds, broadening the available chemical space for exploration. A prime example is Insilico Medicine, which designed a novel candidate for idiopathic pulmonary fibrosis in less than eighteen months—an achievement that would have taken several years using conventional approaches.

2. STRUCTURE AND PROPERTY PREDICTION

Understanding drug–target interactions is fundamental in medicinal chemistry. AI has revolutionized this process by accurately predicting protein structures, binding affinities, and docking interactions. DeepMind's AlphaFold is a landmark achievement in this area, producing highly accurate three-dimensional protein models to guide drug design. Complementary docking tools such as ArgusLab, AutoDock Vina, and Schrödinger Glide allow chemists to virtually test thousands of molecules in silico, vastly reducing the experimental workload.

3. OPTIMISATION OF LEAD COMPOUNDS

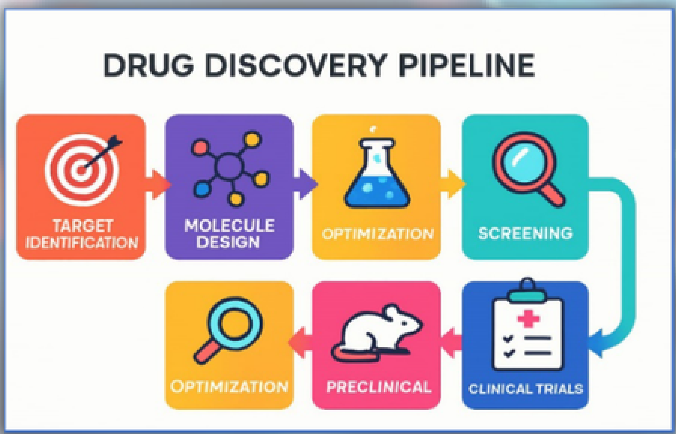
Once potential candidates are identified, AI assists in optimizing their pharmacological and safety profiles. Machine learning algorithms refine molecular structures for improved pharmacokinetics, pharmacodynamics, and drug-likeness. Tools including DeepChem, Chemprop, and ADMETlab predict absorption, distribution, metabolism, excretion, and toxicity (ADMET) properties. This predictive ability reduces the risk of late-stage failures and ensures that only promising molecules advance further in the pipeline. An example of this approach is BenevolentAI, which applied predictive modeling to optimize molecules targeting pathways relevant to amyotrophic lateral sclerosis (ALS).

4. HIGH-THROUGHPUT EXPERIMENTATION AND AUTOMATION

AI-driven laboratory automation and robotics, often called "robot chemists," have transformed experimental workflows. These systems can conduct thousands of reactions simultaneously and learn adaptively from outcomes to refine subsequent experiments. Pharmaceutical companies such as AstraZeneca have successfully combined AI with robotic labs for oncology drug discovery, enabling rapid iteration between computational predictions and real-world experimental testing.

5. DRUG REPURPOSING

AI has proven particularly valuable in drug repurposing, which involves identifying new therapeutic uses for existing approved drugs. By analyzing biomedical big data, literature, and molecular databases, AI reveals hidden connections between drugs and new targets. BenevolentAI identified baricitinib, an anti-rheumatoid arthritis agent, as a potential treatment for COVID-19—a finding that was granted emergency approval during the global pandemic. This example underscores how AI can respond swiftly to urgent medical needs.



CHALLENGES AND FUTURE PROSPECTS

Despite successes, challenges persist that limit the full potential of AI in medicinal chemistry. Data quality is paramount, as biased or incomplete datasets compromise the reliability of predictions. Furthermore, many AI models function as "black boxes," offering results without interpretable reasoning, which complicates their acceptance among chemists and regulators. Ethical, legal, and regulatory considerations also present obstacles to large-scale adoption in healthcare.

Looking forward, the integration of AI with quantum computing, personalized medicine, and synthetic biology promises even greater transformation. Quantum computing may enhance accuracy in simulating molecular interactions, while personalized medicine approaches, empowered by AI, will tailor treatments based on an individual patient's genetic and clinical profile. Combined, these advances point to a future where AI acts not as a supportive tool but as a core partner in therapeutic discovery and design.

CONCLUSION

AI is revolutionizing medicinal chemistry by accelerating drug discovery, enabling accurate structural predictions, optimizing lead compounds, streamlining high-throughput experimentation, and facilitating drug repurposing. Real-world examples, including Insilico Medicine's fibrosis drug, BenevolentAI's COVID-19 therapy, and AlphaFold's structural biology breakthroughs, demonstrate AI's tangible impact. Widely adopted tools such as AlphaFold, AutoDock, DeepChem, SwissADME, and IBM Watson are now indispensable resources. While challenges such as data quality and regulatory acceptance remain, the future of drug discovery lies in a synergistic partnership between human expertise and AI-driven innovation, delivering faster, safer, and more effective therapeutics.

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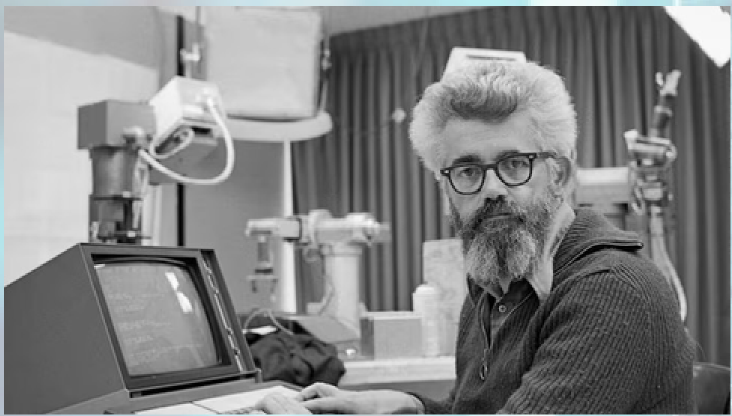
- Dhanjot, B.Sc. (H) Chemistry, III Year

Role of Artificial Intelligence in Publications survey

Introduction

John Mc Carthy was the first to coin the term artificial intelligence in 1956. Artificial intelligence is the branch of computer science that deals with the machine learning process, which can perform different tasks that typically require human intelligence. Artificial Intelligence (AI) has transformed many scientific disciplines, and chemistry is no exception. It refers to the ability of machines to act in seemingly intelligent ways, making decisions in response to new inputs without being explicitly programmed to do so. Over the past two decades, the integration of machine learning (ML), deep learning (DL), and data-driven approaches has enabled chemists to solve problems previously considered intractable. From predicting molecular properties to accelerating drug discovery.



The growth and distribution of AI-related chemistry publications in the last two decades using the CAS (Chemical Abstracts Service) Content Collection with which the volume of both journal and patent publications have increased dramatically, especially since 2015. The CAS Content Collection covers publications in 50 000 scientific journals from around the world in a wide range of disciplines, 62 patent authorities, and 2 defensive publications. There are more than 1000 global scientists specialized in various scientific domains curating, analysing, and connecting data from published sources at CAS.

Growth and Distribution of Publications

We have seen with the rapid growth in global research activity; scientific publication volume has steadily increased over the past 20 years. Using a variety of AI terms in the titles, keywords, abstracts, and CAS expert-curated content, the CAS Content Collection was searched to find publications from 2000 to 2020 that dealt with AI. To reduce false positives caused by polysemy, the search query required screening of every term. Additionally, matches on terms like "brain" and "nerve," which are particularly problematic, were not taken into accounts. The Supporting Information contains the resultant search string, and we found about 70,000 journal articles and 17,500 patents from the CAS Content Collection were found to be connected to AI because of this search. In fact, both journal and patent publication counts rose over time, exhibiting comparable sharply rising patterns after 2015.

This expansion originates in partly due to the well-publicized achievements of deep learning initiatives in open data competitions, like the Merck Molecular Activity Challenge and the ImageNet competition, which began to attract more scientific attention. Further applications of AI to chemistry were made possible by the advent of opensource machine learning frameworks like TensorFlow (2015) and PyTorch (2016), as well as the availability of ever-more-powerful computing hardware, which spurred a global explosion in AI research. As of 2020, more than half of the chemistry papers on AI had been released in the previous four years.

A

Country/Region	%
Peop. Rep. China	26.52
USA	17.20
India	5.79
Iran	5.46
UK	3.94
Germany	3.77
Japan	3.21
S. Korea	2.59
Spain	2.25
Italy	2.03
Canada	2.02
Turkey	1.68
Brazil	1.65
France	1.58
Australia	1.46
Poland	1.21
Taiwan	1.15
Malaysia	0.95
Switzerland	0.90

B

Country/Region	%
Peop. Rep. China	39.03
USA	21.09
S. Korea	10.03
Japan	7.54
India	2.50
Germany	2.30
Canada	1.24
UK	1.01
Israel	0.84
Netherland	0.81
Taiwan	0.78
France	0.64
Switzerland	0.45
Russia	0.41
Ireland	0.34
Australia	0.32
Saudi Arabia	0.23
Sweden	0.23
Finland	0.22

C

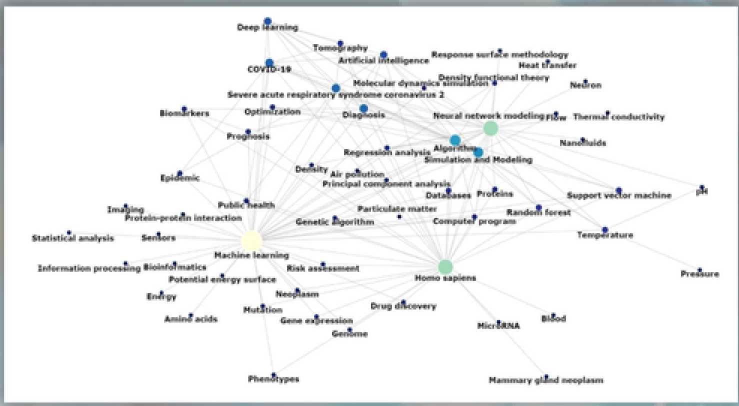
Organization	No. of Patents
LG	263
IBM	222
Fanuc	151
Siemens	115
Ping An Technology	95
Koninklijke Philips	94
Samsung	86
Baidu	71
Toyota	59
Microsoft	56
General Electric	47
Bosch	47
Tata Consultancy Services	46
Tencent	44
Mitsubishi Electric Corporation	42
Google	41
Accenture	40
ChemEssen	38
Fujifilm	32
Ford	31

China and the United States contributed the largest numbers of publications for both journal articles and patents. Beyond growth patterns, it is also important to examine how these publications are distributed across research areas.

Trends Across Research Areas

The approximately 70 000 journal and 17,500 patent publications were further divided into the following 12 categories to provide a more thorough understanding of the ways AI is used in various chemistry-related research areas. Analytical Chemistry, Biochemistry, Energy Technology and Environmental Chemistry, Food and Agriculture, Industrial Chemistry and Chemical Engineering, Inorganic Chemistry, Materials Science, Natural Products, Organic Chemistry, Physical Chemistry, Synthetic Polymers, Pharmacology, Toxicology, and Pharmaceuticals are the categories determined by CAS experts. Among all these specific chemistry-related areas, documents in Analytical Chemistry have the highest normalized volume in the most recent 10 years as it has also risen steeply in the last 5 years. It's interesting to note that although biochemistry is one of the disciplines with the highest representation in AI-related patent publications, its share of journal publications is only moderate in comparison to other fields of study. This suggests that biochemistry has a strong incentive or desire to patent AI technologies, perhaps because of their application in drug development and research.

Topic Analysis In Journal Articles



One can determine when a research topic became potentially useful by examining the relationships between CAS-indexed concepts over time which able to be addressed with AI methods. For the years 2000–2004, we see only a few concepts connected to the concepts Neural network modelling and Algorithms. Several biochemistry-related concepts that appear in conjunction with AI concepts are proteins, protein sequences, and protein conformation. In the years 2005–2009, Homo sapiens become a more popular topic because of the increasing AI related effort in disease diagnosis and prognosis, and related concepts, such as biomarkers, tumour markers, prognosis, and diagnosis start to appear during this period. Genome-related concepts, including genome and single nucleotide polymorphism, were more frequently studied using AI techniques in the years 2010–2014. As the ideas of drug discovery, drug design, blood analysis, neoplasm, and microRNA were widely employed, the use of AI in pharmaceutical and biomedical domains increased. To address issues in research areas like DNA methylation, mutation, nanofluids, heat transfer, and biodiesel fuel, artificial intelligence (AI) has become increasingly prevalent in the years 2015–2019. AI was also commonly mentioned in articles about Alzheimer's and cancer. AI has been widely utilised in the fields of drug discovery, disease diagnosis, and disease prevention since the start of 2020, when the urgent need for COVID-19 research became clear. Examining the development of the concept diagnosis with different AI concepts is instructive. After 2015, there was a sharp rise in the number of documents linking diagnosis to different AI concepts, with support vector machines, random forests, and deep learning seeing the most used. This trend holds true for several chemistry topics, where the rise in AI use since 2015 is widespread rather than specific to one AI approach.

Conclusion

Chemical research has changed dramatically because of the incorporation of artificial intelligence, opening the door to previously unthinkable discoveries. The past 20 years have seen an unparalleled expansion, from the consistent increase in publications about artificial intelligence to the wide range of applications in analytical chemistry, biochemistry, drug discovery, and materials science. The increase in publications since 2015 demonstrates how deep learning, open-source frameworks, and powerful computers can spur innovation. AI's contribution to chemistry will only grow as it develops further, leading to more precise forecasts, effective experimentation, and ground-breaking answers to pressing global issues. In the end, chemistry and AI working together not only advances scientific knowledge but also opens the door to quicker discoveries that will benefit society as a whole.

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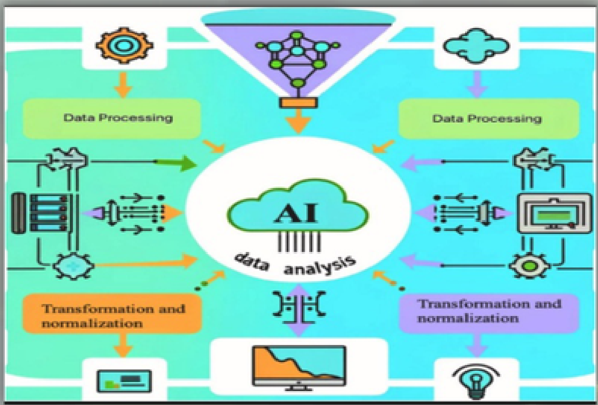
DID YOU KNOW?

AI can predict chemical reactions and design new drugs in seconds—tasks that once took scientists years! Tools like AlphaFold can even predict protein structures with remarkable accuracy, speeding up research like never before.

- Dikhov Pegu, B.Sc. (H) Chemistry, III Year

Harnessing Artificial Intelligence for Next-Generation Chemical Education and Mechanistic Insights

Artificial Intelligence (AI) is rapidly transforming every field of science, and chemistry is no exception. With its ability to analyze vast datasets, recognize patterns, and simulate complex processes, AI is emerging as a game-changer in both chemical education and research. The fusion of AI with chemistry promises not only to accelerate discoveries but also to reimagine how students and researchers learn, practice, and innovate.



AI in Chemical Education: Redefining Learning

Traditional chemical education has relied heavily on lectures, textbooks, and laboratory Experiments. While these methods remain foundational, they often struggle to keep pace with The rapidly evolving scientific landscape. Here, AI-driven tools are opening new possibilities: Personalized Learning: Adaptive learning platforms, powered by AI, can tailor content to Individual student needs. For example, algorithms can identify gaps in a student's understanding Of organic mechanisms and provide targeted practice problems or simulations.

Virtual Laboratories: AI-enabled simulations allow students to conduct virtual experiments with Real-world accuracy, reducing dependency on costly laboratory infrastructure and minimizing Safety risks.

Interactive Mechanistic Learning: Mechanism prediction tools help students visualize electron Movement and intermediate states, deepening their understanding of reaction pathways beyond Static textbook diagrams. Through these innovations, AI democratizes access to advanced learning tools, enabling Students worldwide to engage with chemistry at a higher level, regardless of resource Constraints.

Mechanistic Insights through AI: A Research Revolution

Beyond education, AI is revolutionizing how chemists approach reaction mechanisms. Mechanistic studies—once painstakingly slow and reliant on manual interpretation—are being accelerated with AI models capable of predicting outcomes, intermediates, and reaction Conditions with remarkable accuracy.

Reaction Prediction: AI-driven platforms like deep learning models can forecast products and Plausible pathways, guiding chemists in synthetic planning.

Big Data Analysis: Vast reaction databases are now being mined by AI to uncover hidden Patterns, enabling the discovery of new catalysts, reagents, and green chemistry solutions.

Quantum Chemistry and Simulation: AI accelerates quantum mechanical calculations, making it Feasible to model highly complex systems in drug discovery, materials design, and energy Research.

Automated Hypothesis Testing: AI algorithms generate mechanistic hypotheses and validate Them against experimental or simulated data, significantly reducing the trial-and-error burden on Researchers.

These capabilities free chemists to focus on creativity, interpretation, and real-world Applications, while AI handles the computationally intensive groundwork.

The Synergy: Education Meets Research

The intersection of AI-driven education and research creates a powerful feedback loop. Students trained with AI tools not only understand chemical concepts faster but also enter the Research world equipped with computational literacy. In turn, research innovations powered by AI feed back into education, providing fresh insights and examples for teaching. This synergy Ensures that the next generation of chemists will not only learn the subject but actively shape its Future.

Challenges and Ethical Considerations

Despite its promise, AI integration in chemistry brings challenges:

- Data Quality: AI models are only as good as the data they are trained on, and biases or errors Can mislead predictions.
- Accessibility: Advanced AI tools must remain accessible to institutions with limited resources to Avoid widening the educational gap.
- Ethics in Automation: As AI takes on more tasks, questions about academic integrity and Responsible use must be addressed.

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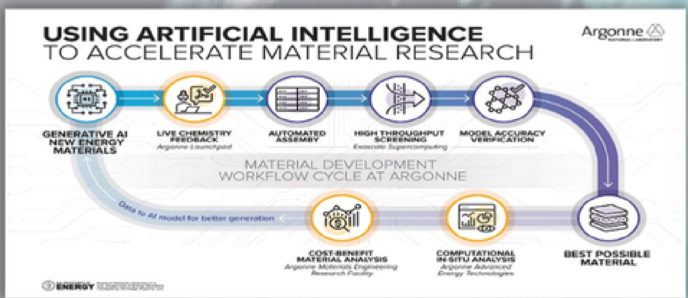
- Aaditya Kumar and Pahi Talukdar, B.Sc. (H) Chemistry, III Year

AI Unleashes a New Era in Material Chemistry: From Sci-Fi Dreams to Real-World Wonders

Introduction:
The notion of machines creating new materials seemed like pure science fiction not so long ago. However, this vision is already becoming a reality thanks to artificial intelligence (AI). AI is transforming material chemistry in a number of ways, from predicting chemical structures to speeding up the development of smart materials. AI is revolutionizing modern science since it can now accomplish tasks that formerly required years of investigation in a fraction of the time.

AI Meets Material Chemistry:
Material chemistry has consistently been crucial to innovation, whether in the formulation of robust alloys, the synthesis of life-saving pharmaceuticals, or the production of environmentally sustainable polymers. Traditional experimental procedures are laborious, expensive, and frequently dependent on trial-and-error method. Artificial intelligence is integral to contemporary scientific research, facilitating the analysis of extensive datasets and the simulation of molecular interactions. It can anticipate the properties of materials even before they are produced, recommend the most efficient reaction paths, and find patterns that could be missed by human researchers. Additionally, AI helps limit laboratory waste and energy utilization, making the research process more sustainable and cost-effective.



Real-World Applications

1. Healthcare and Biomedical Materials: AI is enabling the design of advanced materials for personalized medicine, such as custom implants, drug delivery systems, and tissue scaffolds. These materials can adapt to the human body, improving performance, biocompatibility, and healing outcomes.

Real-World Applications

1. Healthcare and Biomedical Materials: AI is enabling the design of advanced materials for personalized medicine, such as custom implants, drug delivery systems, and tissue scaffolds. These materials can adapt to the human body, improving performance, biocompatibility, and healing outcomes.

2.Clean Energy Solutions: From high-efficiency solar cells to durable battery components and hydrogen storage materials, AI accelerates the discovery of energy materials that are both efficient and environmentally friendly—supporting the global shift toward sustainable energy.

3.Sustainable Industrial Materials: From self-healing polymers to recyclable plastics, AI is driving the creation of materials that reduce waste, lower emissions, and promote a circular economy across industries like construction, electronics, and packaging.

From science to reality:
Technologies once confined to the realm of science fiction—like self-healing plastics, smart fabrics, and shape-shifting alloys—are rapidly becoming part of our reality. Thanks to AI-assisted material design, researchers are now developing self-repairing concrete, shape-shifting polymers, and ultra-lightweight alloys for aerospace and beyond. Inspired by futuristic visions such as Star Trek's replicators and Iron Man's advanced tech, AI-driven material chemistry is turning imaginative concepts into tangible innovations once thought impossible.

Advantages :
1. Optimizes reaction pathways, improving efficiency and reducing waste.
2. Supports greener, more sustainable chemical processes.
3.Detects hidden patterns in complex data for innovative materials.

Limitations of AI in Material Chemistry:

Artificial Intelligence (AI) is revolutionizing material chemistry, but it is not without its challenges. While AI accelerates discovery, it also faces several key limitations:

1. Data Dependency: AI thrives on large, high-quality datasets. In material chemistry, however, experimental data are often scarce, costly, or inconsistent, limiting AI's predictive power.

2. The "Black Box" Problem: Many AI models, especially deep learning, operate as black boxes. They can predict outcomes but often fail to explain the reasoning, making it difficult for chemists to trust or verify results.

3. Need for Human Expertise: AI cannot replace human creativity, intuition, and critical thinking. Instead, it must work in collaboration with chemists to make meaningful progress.

Future Outlook:

1. Accelerated Discovery of Advanced Materials: AI is dramatically speeding up the search for "miracle materials" that can revolutionize industries. From next-generation medical implants to materials for clean energy and space exploration, AI enables scientists to predict and test material properties virtually—saving time, cost, and resources.

2.Sustainable and Greener Chemistry: As the world demands more eco-friendly solutions, AI is helping design chemical processes that produce less waste, use fewer hazardous materials, and consume less energy. This paves the way for a cleaner, more sustainable chemical industry that aligns with global environmental goals.

3. Responsible Innovation at Speed: Beyond just creating new materials, AI is reshaping how we innovate. By combining speed with responsible practices, the future of material chemistry lies in smart, sustainable solutions that move from concept to reality faster than ever before—turning science fiction into everyday experience.

Conclusion:

In material chemistry, artificial intelligence has genuinely ushered in a new era where creativity and imagination coexist. Our daily lives are being shaped by things that were previously only found in science fiction. With the help of AI and human curiosity, the wonders of tomorrow's materials are being written today.

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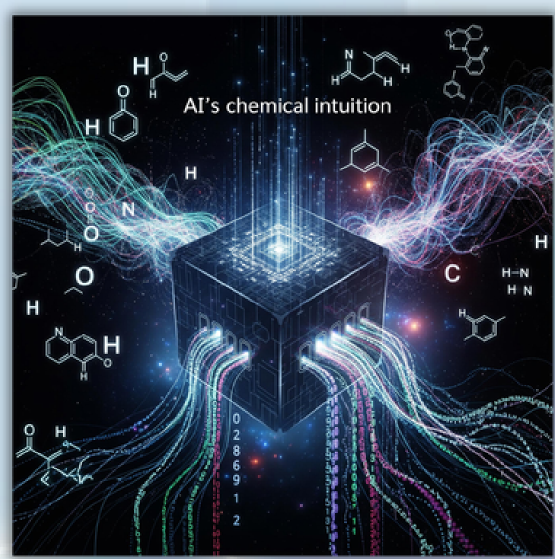
- Priya Bharti, B.Sc.(H) Chemistry, III Year

DID YOU KNOW?

- 🔥 Hot Water Can Freeze Faster Than Cold
- This strange phenomenon is known as the Mpemba effect, and scientists are still exploring why it happens.
- Bubbles Freeze in Winter
- In extremely cold temperatures, soap bubbles can freeze mid-air and form beautiful crystal patterns.
- Oxygen Is Magnetic!
- Liquid oxygen is actually attracted to magnets due to its unpaired electrons.

Beyond the Black Box: Demystifying AI's "Chemical Intuition"



Picture this: a skilled chemist sees a solution change color and just knows what's happening inside the complex dance of atoms and molecules. Meanwhile, a powerful AI crunches tons of data to predict the same final result, and it's usually right. But here's the catch: ask the AI to explain how it got there , the step-by-step process, or mechanism , and it's pretty much clueless.

This gap between getting the right answer and explaining the journey is one of the coolest challenges in chemistry right now. It shows us what AI is great at, but also what it just can't do... yet.

For a chemist, figuring out a reaction mechanism is like being a detective. You have to piece together clues from different lab techniques and experiments, all while using your gut feeling , a feeling that's really just built on years of understanding the basic rules of chemistry.

This is tough enough for simple reactions, but it gets way harder with inorganic chemistry, especially when you're working with certain metals. This kind of chemistry is known for being super unpredictable. The metal atoms can act in many different ways, connect with all sorts of other molecules, and the reaction can go down several different paths at once. A human chemist uses a mix of book-smarts and hands-on experience to figure it out. It's an art that computers struggle to copy

.

The Machine's Best Guess

AI looks at chemistry in a completely different way. Instead of thinking from the ground up like a person, AI tools like IBM's RXN just learn from huge online databases of past reactions. They don't understand the "why," they just get really good at finding patterns.

Think of it like this: a chemist's intuition is like muscle memory from years of practice. For an AI, it's like a giant spreadsheet that finds connections between what you start with and what you end up with. This has worked amazingly well for organic chemistry, where we have tons of data. It's a lot like AlphaFold, the AI that learned to predict how proteins fold by studying thousands of them.

Where AI Gets Stuck:

So why does AI struggle so much with the step-by-step process in inorganic chemistry? There are two big reasons:

Not Enough Data: Compared to organic chemistry, we just don't have as much organized data for these more complex reactions. AI needs lots of examples to learn from, and for many areas of inorganic chemistry, the examples just aren't there.

The "Black Box" Problem: Most of these AIs are a "black box." Data goes in, an answer comes out, but we can't see how it made its decision. It doesn't actually "get" the chemistry rules we learn in class. So, when a reaction doesn't work, the AI can't tell you why. It gives you the destination but has no idea how to read the map.

So, instead of being a magic 8-ball that gives all the answers, AI is becoming more like a lab partner. The future is all about chemists and AI working together.

AI can be a great tool for brainstorming. It can quickly look through thousands of possibilities and suggest ideas a chemist might not have thought of. The chemist then uses their expertise to decide which of the AI's ideas are smart and which are nonsense, and then tests them in the lab. This teamwork uses the best of both worlds: the machine's power to crunch data and the chemist's smart, creative thinking.

Conclusion

Figuring out how these complex reactions work is still one of the biggest puzzles in chemistry. AI isn't going to replace a chemist's gut feeling anytime soon. For a machine, a reaction is just a data point; for a chemist, it's a story.

The real power of AI isn't just giving us answers, but helping us ask smarter questions. It pushes us to think differently and might just help us make our own skills even better, not make them useless.

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- Anmol Raman, B.Sc. (H) Chemistry, I Year

FUN FACTS

Onions Make You Cry for a Reason

When you cut onions, they release sulfur compounds that react with your eyes to form a mild acid—causing tears!

Liquid Nitrogen Is Extremely Cold

At around –196°C, it can instantly freeze objects, even making flowers shatter like glass!

You Are Made of Stardust

The elements in your body were formed in stars billions of years ago—making you literally cosmic!

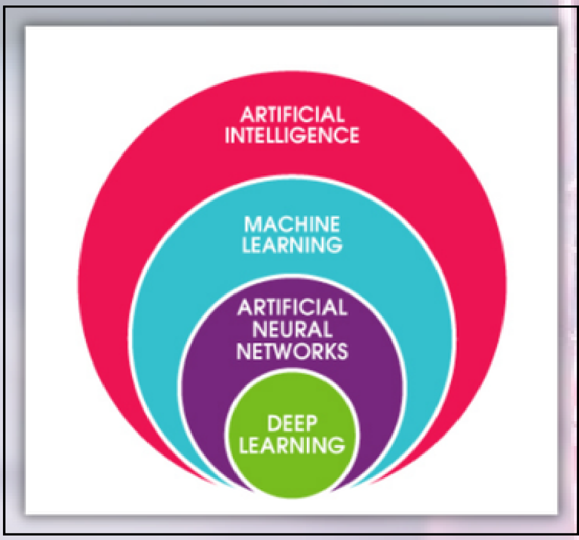
The Prediction of Reaction outcomes in Molecular Designing

Introduction

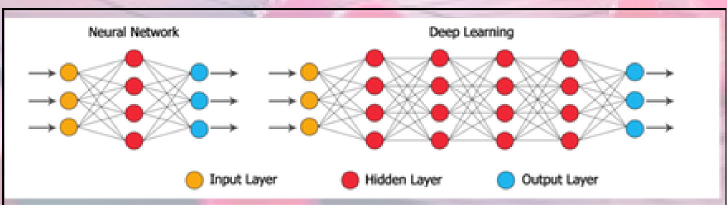
Artificial intelligence (AI) is fundamentally transforming molecular design. It enables rapid simulation, screening, and creation of new molecules. This is achieved through machine learning and genetic programming algorithms. The evolution of AI in this field promises dramatic advances in: Pharmaceuticals, Catalysts, Nanomachine engineering. Benefits include: High efficiency, Novel solutions, a pathway beyond the limitations of human creativity in chemistry.

1. Machine learning for chemistry

Machine learning can be understood as a set of algorithms designed to identify patterns in large datasets by minimizing errors through different optimization approaches. These algorithms underpin technologies such as Google's search engine, Apple's voice assistant, and Facebook's personalized content feeds. Beyond industry, machine learning has also become a powerful tool in academic research, with applications spanning nearly every scientific discipline.



Artificial intelligence (AI) describes software that simulates human intelligence. Machine learning (ML), a branch of AI, improves its accuracy by learning from data with minimal human intervention. Neural networks are ML models inspired by the brain, and when they contain multiple hidden layers, they are referred to as deep learning. These hidden layers enable the system to process information in stages-for example, in facial recognition, detecting lines, then features like eyes or mouth, and finally identifying the person.



The application of machine learning (ML) in chemistry is still in its early stages, but rapid progress is expected to impact a wide range of chemical challenges in the near future.

Current research explores ML for tasks such as predicting reaction mechanisms, approximating density functional theory (DFT) functionals, molecular dynamics simulations, reaction and condition prediction, chemical optimization, protein structure prediction, catalysis improvement, analytical tools, and quantum sensing. For this essay, four areas are of particular interest: quantum molecular simulations, molecular property prediction, compound screening and synthesis development, and molecular design through genetic programming. Together, these approaches aim to generate stable molecular structures with tailored properties.

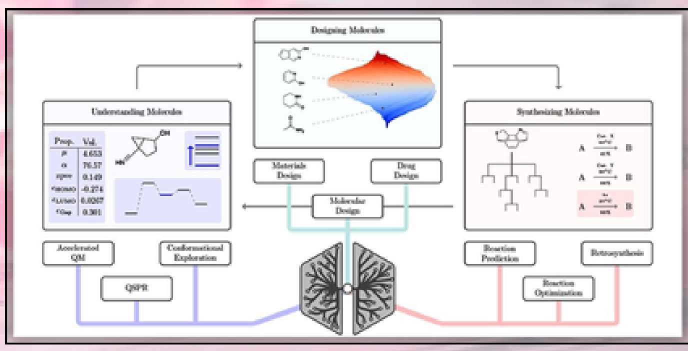
2. Molecular Property Prediction

A molecule's properties are determined by its nuclear and electronic structure. Stable structures correspond to local or global minima on the potential energy surface (PES), allowing structural information to be derived from calculated PES data. Using this structural information, artificial intelligence can predict the properties of hypothetical molecules without the need for experiments. ML enables the screening of millions of compounds, identifying the most promising candidates for the discovery of new drugs and materials.

3. Genetic programming

The most promising application of AI in chemistry lies in integrating molecular property prediction, quantum chemical simulations, and genetic programming. Genetic programming, inspired by evolutionary processes, enables the design of novel molecules tailored for specific tasks. Genetic programming (GP) is already being applied to fields such as optics and electronics, where it has produced human-competitive and even patentable designs (Duettmann and Lewis 2018). Its strength lies in generating valuable solutions with minimal human input, making it especially effective for problems that are not well understood by humans.

4. AI for Molecular Design



Integrating ML-based quantum-chemical simulations with molecular property prediction enables the development of AI-driven molecular design (Figure 4). The proposed approach is a general, efficient, and modular AI framework aimed at generating molecular designs for nanotechnology research. Combining these individual AI platforms into a unified system could lead to novel, unexpected discoveries with wide-ranging applications.

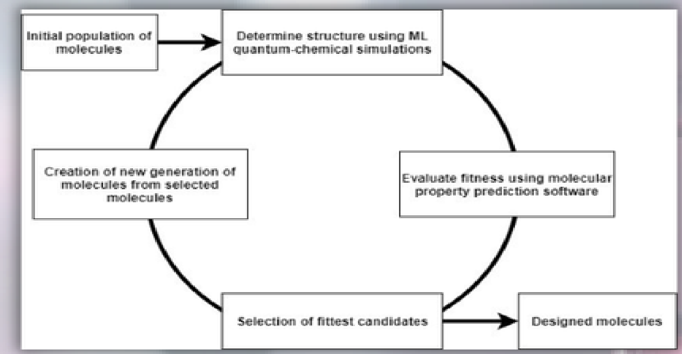


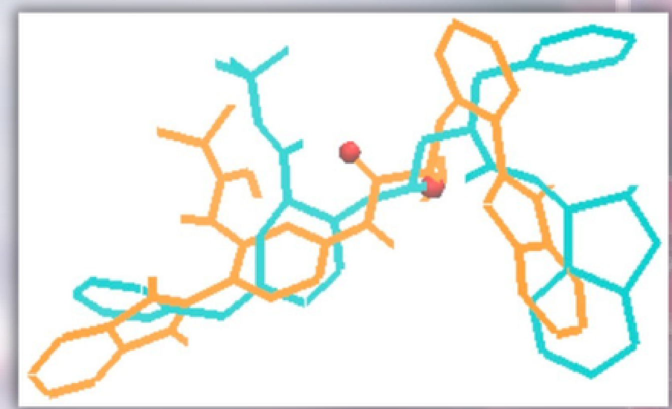
Figure 5: Diagram of steps for one generation done by AI for molecular design.

Enhancing AI Molecular Design

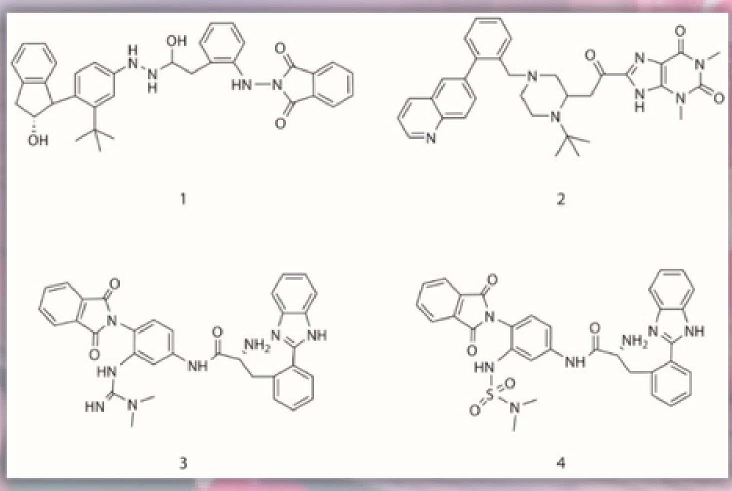
Pre-screening Tools: Use cheaper methods to assess design quality before running expensive quantum-mechanical simulations (Duettmann & Lewis 2018).

Confirm physical viability

Check for novelty to avoid redundant simulations.



Superposition of Molegear created design (orange) using genetic programming and indinavir (cyan) (Chu and He 2019).



Candidate HIV-1 inhibitor molecules designed by Molegear by genetic programming (Chu and He 2019).

AI for Catalyst Design

Genetic programming (GP) has been used to design new catalysts by screening compounds with inexpensive ML algorithms (Freeze, Kelly, & Batista, 2019).

AI enables targeted catalyst design, reducing time and cost compared to traditional trial-and-error methods. These programs are still in early development and will require further improvements for future applications.

AI for Molecular Design: Applications

Researchers are developing ML systems optimized for specific chemical problems. Integrating these approaches- molecular property prediction, quantum simulations, and genetic programming-into a unified AI for molecular design could unlock vast new possibilities. By applying evolutionary strategies, the AI can design molecules inspired by biological processes yet not limited by human chemical knowledge. This approach promises a new generation of complex, effective molecular designs. All components of this AI have already been successfully applied to drug and catalyst development. An advanced AI for molecular design could iteratively identify molecules with complex motions, leading to a new generation of designs with potentially unpredictable applications. The AI could automatically select nanomachine candidates that exploit these movements or be guided to develop dynamic molecules. This shift from human-driven hypotheses to AI-generated techniques represents a potentially transformative change in the field of che
mistry.

The Prediction of Reaction Outcomes Using AI

Chemistry has always been about discovery- synthesizing new molecules, exploring reactions, and understanding how atoms and molecules behave. Predicting exactly what will happen when two compounds react has historically required a mix of intuition, literature knowledge, and experimental trial-and-error. Today, Artificial Intelligence (AI) is revolutionizing reaction prediction, making it faster, more accurate, and opening new doors for molecular design.

AI Enters the Laboratory

Artificial Intelligence is a branch of computer science focused on designing machines that can mimic human intelligence. In chemistry, one of the most exciting applications of AI is predicting reaction outcomes: identifying the most likely products when reactants are combined under specific conditions. Traditionally, chemists relied on reaction rules, heuristics, and databases. While effective, these methods are slow and often fail for complex molecules. AI, particularly machine learning (ML) and deep learning (DL), changes the game by learning patterns from thousands - or even millions - of reactions.

How AI Predicts Reactions

AI-based reaction prediction usually involves training models on historical reaction data. Two main approaches are common. Template-based models: These models learn general reaction patterns (templates) from large reaction datasets. They predict products by matching reactants to these learned templates. Template-free models: Modern deep learning approaches, like Molecular Transformers, treat reactions like a language translation problem, translating reactants and reagents into products.

Example: Suzuki–Miyaura Cross-Coupling

Input: Reactants and reagents (chemical structures represented as SMILES strings). AI model processes this input using neural networks. Output: Predicted products ranked by probability. This allows chemists to screen hundreds of reactions virtually before performing them in the lab, saving time and resources.

Example: A classic example of reaction prediction is the Suzuki–Miyaura cross-coupling, a widely used method for forming carbon–carbon
bonds.

- Mahenoor Bee, B.Sc. (H) Chemistry, II Year

Integrating Blockchain and AI for Secure and Efficient Chemical Supply Chains

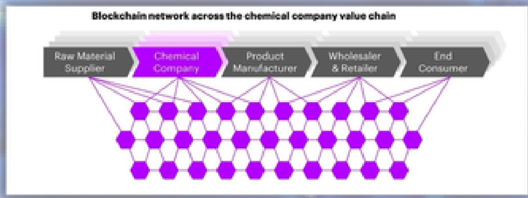
The chemical supply chain is one of the most complex and sensitive industrial systems in the world. It involves the sourcing of raw materials, chemical manufacturing, storage, transportation, regulatory compliance, and delivery to end users. Due to the hazardous nature of chemicals and the strict regulatory environment, ensuring transparency, security, and efficiency across the supply chain is critically important. In recent years, the integration of Blockchain technology and Artificial Intelligence (AI) has emerged as a powerful solution to address long-standing challenges in chemical supply chains.

Blockchain is a decentralized digital ledger that records transactions in a secure, transparent, and tamper-proof manner. In the context of chemical supply chains, blockchain can be used to record every stage of a product's journey, from raw material procurement to final delivery. Each transaction or movement is stored as a block and linked chronologically, ensuring traceability and accountability. This is particularly valuable in preventing counterfeit chemicals, unauthorized substitutions, and data manipulation, which can pose serious safety and economic risks.

Artificial Intelligence, on the other hand, brings advanced data analysis, prediction, and automation capabilities to supply chain management. AI systems can process vast amounts of data generated across the chemical supply chain, including production metrics, transportation conditions, demand forecasts, and regulatory data. Machine learning algorithms can identify patterns, predict potential disruptions, optimize inventory levels, and improve decision-making processes in real time.

When blockchain and AI are integrated, their combined impact significantly enhances supply chain performance. Blockchain ensures the reliability and integrity of data, while AI utilizes this trustworthy data to generate actionable insights. For example, sensor data related to temperature, pressure, or humidity during chemical transportation can be securely recorded on a blockchain. AI algorithms can then analyze this data to detect anomalies, predict spoilage or safety hazards, and trigger automated alerts or corrective actions.

Security is another major advantage of this integration. Chemical supply chains are increasingly vulnerable to cyberattacks, data breaches, and fraud. Blockchain's cryptographic structure makes it extremely difficult for unauthorized parties to alter records. At the same time, AI-driven cybersecurity systems can continuously monitor network activity, identify suspicious behavior, and respond to threats proactively. .



This dual-layer protection strengthens trust among manufacturers, distributors, regulators, and consumers.

Regulatory compliance is a critical requirement in the chemical industry, as organizations must adhere to strict national and international safety and environmental standards. Blockchain-based records provide regulators with real-time access to verified data, simplifying audits and compliance reporting. AI can further assist by automatically checking compliance requirements, generating reports, and predicting regulatory risks before violations occur.

Efficiency and cost reduction are also key benefits. AI-powered demand forecasting helps chemical companies avoid overproduction or shortages, while blockchain-enabled smart contracts can automate payments, approvals, and logistics processes. These smart contracts execute predefined conditions automatically, reducing paperwork, delays, and human errors. As a result, operational costs decrease and overall supply chain responsiveness improves.

Despite its advantages, the integration of blockchain and AI in chemical supply chains also faces challenges. High implementation costs, lack of technical expertise, data standardization issues, and scalability concerns can slow adoption. However, with ongoing technological advancements and increasing digital transformation initiatives, these challenges are gradually being addressed.

In conclusion, integrating blockchain and artificial intelligence offers a transformative approach to building secure, transparent, and efficient chemical supply chains. By combining blockchain's data integrity with AI's analytical intelligence, the chemical industry can enhance safety, improve compliance, reduce costs, and gain a competitive edge. As digital technologies continue to evolve, their adoption will play a crucial role in shaping the future of chemical supply chain management.

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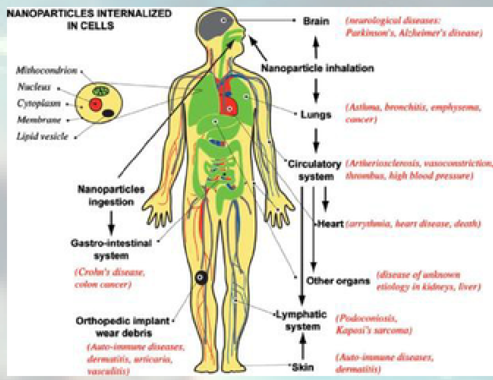
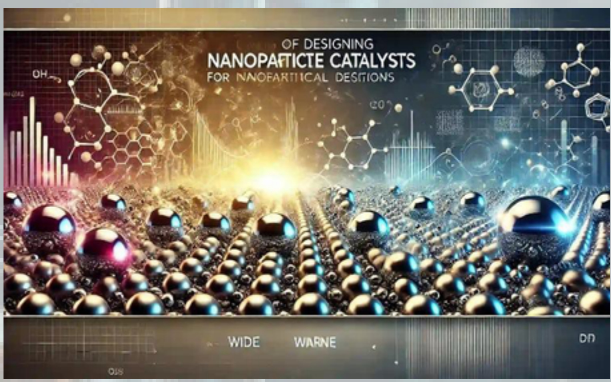
- Dia and Piyush, B.Sc. (H) Chemistry, III Year

How AI is Designing the Future of Nanoparticles

In recent years, artificial intelligence (AI) has begun to redefine the landscape of scientific research—and chemistry is no exception. At the intersection of cutting edge technology and molecular science, AI is proving to be a game-changer in the design and development of nanoparticles. These tiny particles, often less than 100 nanometers in size, are key components in medicine, energy, electronics, and
environmental science. Now, AI is accelerating our ability to engineer them with unprecedented precision and efficiency.





The Role of Nanoparticles in Modern Science Nanoparticles possess unique physical and chemical properties due to their size and high surface-area-to-volume ratio. These properties make them ideal for targeted drug delivery, cancer therapy, clean energy solutions, and even advanced electronics. However, designing nanoparticles with specific characteristics—such as shape, size, surface charge, and functionality—requires complex experimentation and vast amounts of data. Traditional methods can be time-consuming and expensive.

Some examples of nanoparticle use in science include: Nanoparticles are revolutionizing healthcare by enabling targeted drug delivery. For example, lipid nanoparticles (LNPs) are used to deliver mRNA vaccines, including the COVID-19 vaccines developed by Pfizer BioNTech and Moderna. These nanoparticles protect the mRNA and help it enter human cells effectively.

Safety concerns and challenges:
Neuroinvasion and Brain Damage: Some parasites, like Toxoplasma gondii or Naegleria fowleri, can cross the blood-brain barrier, causing inflammation, brain tissue destruction, and potentially fatal conditions like encephalitis or meningoencephalitis.

Immune System Response:
Nanoparticles can trigger unintended immune responses. Some may be recognized as foreign substances, leading to inflammation, allergic reactions, or autoimmune-like effects.

Difficulty in Detection and Monitoring:
Due to their ultra-small size, it's difficult to detect, track, and measure nanoparticles inside the body using standard medical imaging or testing techniques.

Designing the Future: Challenges Ahead
Designing the future of AI in nanoparticle research faces several hurdles. Incomplete or biased data can limit AI accuracy, while the complex behavior of nanoparticles in real world
environments makes prediction difficult. Standardization, data transparency, and ethical concerns also need attention. Without addressing these issues, the full potential of AI-driven nanotechnology may remain unrealized.

The Smarter Future
As artificial intelligence merges with nanotechnology, science is entering a smarter, faster, and more efficient era. AI is transforming how nanoparticles are designed—making the process predictive rather than experimental. This leads to quicker discoveries, reduced waste, and highly customized materials for medicine, energy, and environmental solutions. The future of chemistry is not just more advanced—it is intelligently driven, sustainable, and deeply innovative.

AI-powered nanoparticle design supports sustainability by reducing toxic chemicals, minimizing material waste, and enabling cleaner manufacturing. These smart materials can purify water, capture pollutants, and improve renewable energy technologies. With AI guiding innovation, nanotechnology becomes a powerful tool for solving environmental challenges—building a cleaner, greener future through intelligent, efficient, and ecofriendly science.

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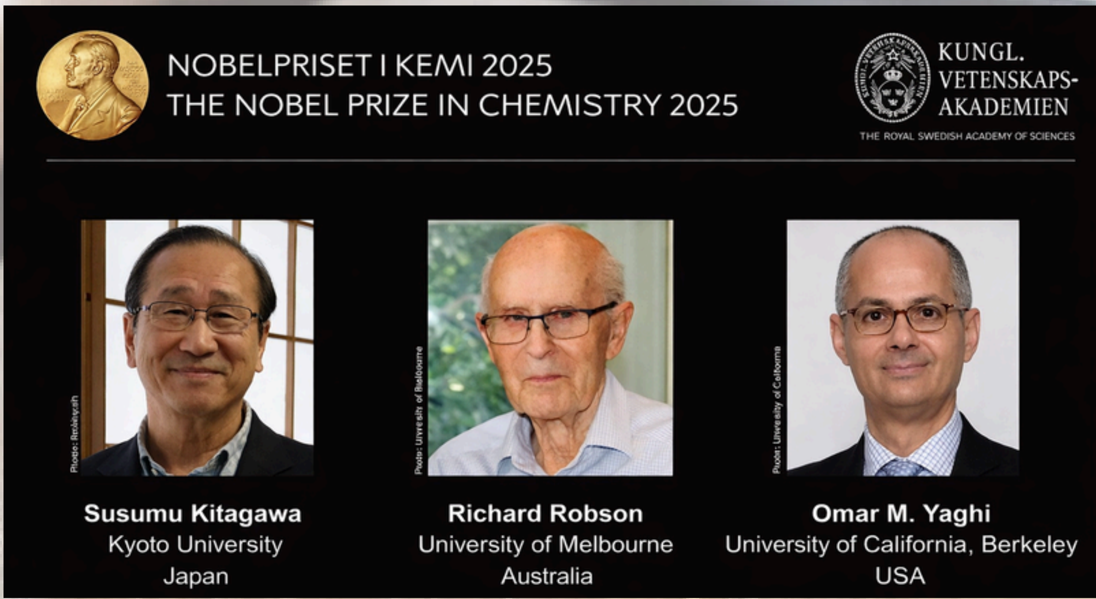
- Ankit, B.Sc. (H) Chemistry, III Year

NOBEL PRIZE IN CHEMISTRY 2025: METAL-ORGANIC FRAMEWORKS AND THE FUTURE OF POROUS MATERIALS

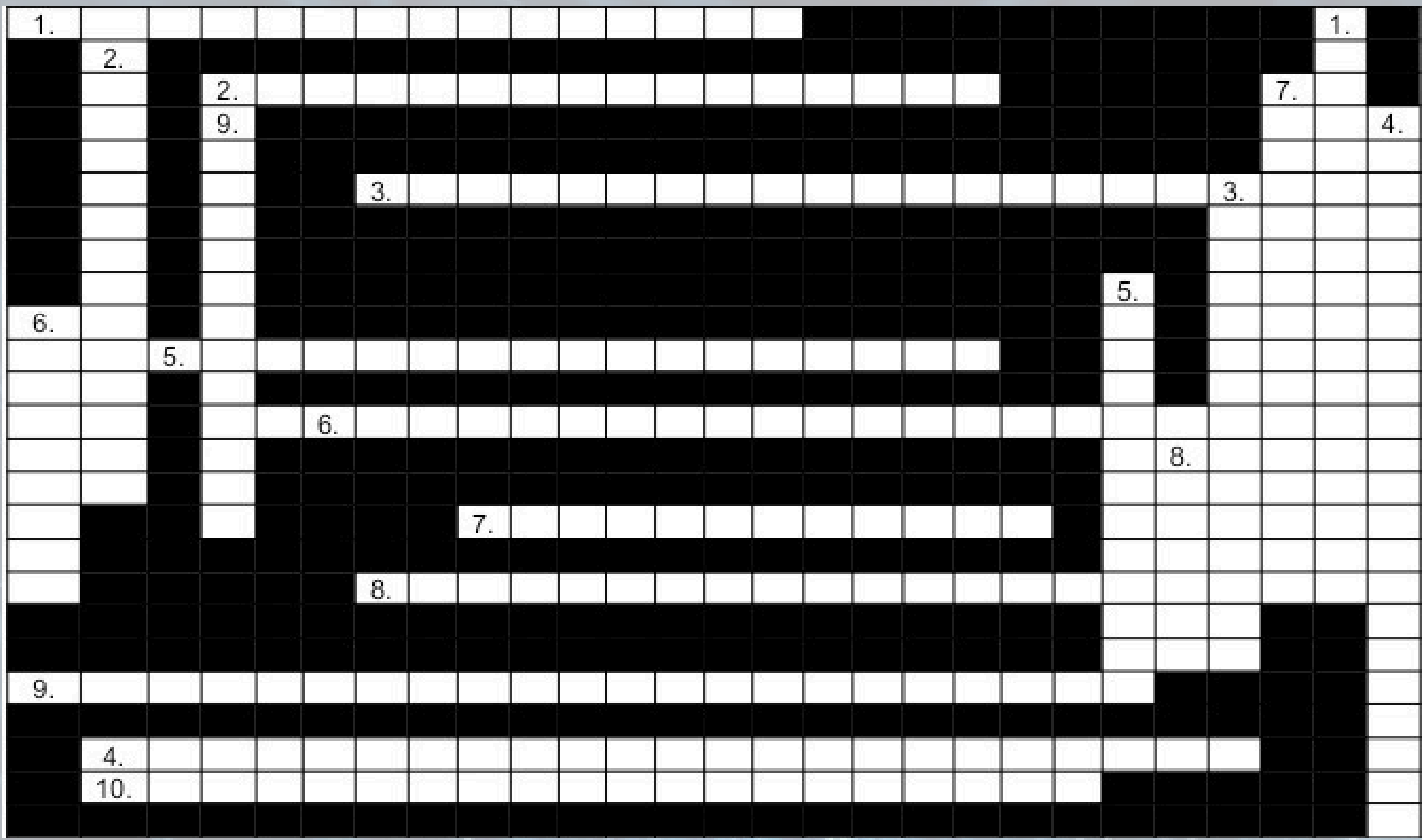
On October 9, 2025, the Nobel Prize in Chemistry was awarded to Susumu Kitagawa, Richard Robson, and Omar M. Yaghi by Royal Swedish Academy of Sciences for the development of metal-organic frameworks and for elucidating their vast potential in a wide range of chemical applications. To appreciate the significance of this achievement, it is essential to examine what metal-organic frameworks are and why they have become so important in modern chemistry.



WHAT ARE METAL-ORGANIC FRAMEWORKS?

Metal-organic frameworks, commonly abbreviated as MOFs, are a class of crystalline porous materials composed of metal ions or metal clusters coordinated to organic ligands to form extended network structures. In these frameworks, the metal ions or clusters act as connecting nodes, while the organic molecules serve as linkers that bridge these nodes together. The resulting architecture can extend in one, two, or three dimensions, most commonly forming highly ordered three-dimensional lattices with permanent porosity. The linkages in MOFs are typically coordination bonds formed between metal centers and functional groups on organic ligands such as carboxylates, azolates, or phosphonates. What sets MOFs apart from conventional coordination polymers is the deliberate design of their structures, which allows precise control over pore size, shape, and internal chemical environment. This structural regularity and tunability enable MOFs to exhibit exceptionally high surface areas and highly selective interactions with guest molecules, essentially turning empty space into a functional chemical asset.

CROSSWORD



Across:

1. AI approach used to predict reaction mechanisms from large datasets (2 words)
2. Mathematical representation of molecular structures as nodes and edges (3 words)
3. Deep learning architecture widely used for chemical property prediction (3 words)
4. Quantum chemistry method often accelerated using AI (abbreviation)
5. Technique used to extract features from spectroscopic data using AI (2 words)
6. Process of optimizing molecular structures using computational methods (2 words)
7. Type of chemical bond involving orbital overlap
8. AI-driven method to design novel molecules with desired properties (2 words)
9. Branch of chemistry that uses computer simulations extensively (2 words)
10. Algorithm used for nonlinear regression and classification in chemical data

Down

2. AI learning method trained on labeled chemical datasets (2 words)
3. Study of energy and heat changes in chemical systems
4. Field combining chemistry, data science, and informatics
5. Technique to group similar molecules without prior labels (2 words)
6. Instrumental method generating spectra for structure elucidation
7. Type of bond formed by electron transfer between atoms
8. Study of the rate and mechanism of chemical reactions
9. Public database of chemical compounds (abbreviation)
10. AI model inspired by biological neural systems (2 words)

RASAGYA:THE CHEMICAL SOCIETY

RASAGYA, the Chemical Society of the Department of Chemistry, is a vibrant platform dedicated to fostering academic excellence and overall student development. The society actively organizes seminars, workshops, guest lectures, industrial visits, and alumni interactions, helping students stay connected with advancements in science and industry.

Beyond academics, RASAGYA promotes leadership, teamwork, and interpersonal skills through various co-curricular and extracurricular activities. Its strong alumni network further inspires and guides students by sharing valuable experiences and career insights, making it an integral part of the department's dynamic learning environment.

It is with great pride and enthusiasm that I present RASAGYA, the Chemical Society of our department. RASAGYA serves as a dynamic platform that nurtures curiosity, encourages innovation, and brings together students who share a passion for chemistry. The society regularly organizes seminars, workshops, industrial visits, and interactive sessions with esteemed scientists and researchers, providing students with valuable exposure beyond the classroom. These initiatives help bridge the gap between theoretical knowledge and real-world applications.

Beyond academics, RASAGYA is committed to holistic development.
Through various extracurricular activities, we aim to build leadership qualities, teamwork, and interpersonal skills, while fostering a strong sense of unity within the department. I extend my heartfelt gratitude to our faculty members and student coordinators for their constant support and dedication. I also encourage every student to actively participate, explore new ideas, and make the most of the opportunities provided.
Let us continue to learn, innovate, and grow together.

Pratha Dhingra
President, RASAGYA

ORIENTATION AND ICE BREAKER

The Department of Chemistry warmly welcomed the new batch with an engaging Orientation Program, marking the beginning of their academic journey. The session introduced students to the curriculum, covering core subjects—Physical, Inorganic, and Organic Chemistry—along with GE, AEC, SEC, and VAC courses designed for holistic development.
Faculty members highlighted the importance of laboratory work, giving students a glimpse into the practical aspects of chemistry through experiments and modern techniques. They also encouraged active participation in seminars, fests, and extracurricular activities for overall growth.

To give more knowledge about RASAGYA, there was a fun ice-breaker session, helping freshers interact, connect, and feel at ease in their new environment.
The program concluded on a positive and enthusiastic note, setting the stage for a journey filled with learning, exploration, and memorable experiences.

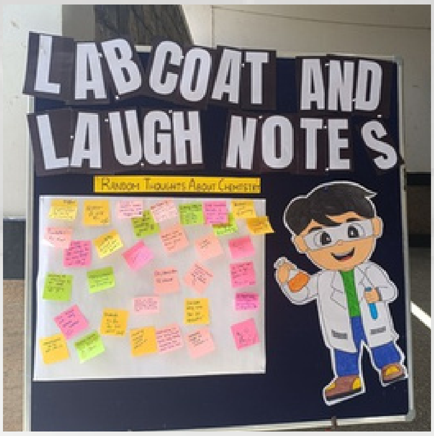
Inaugural and International seminar on Innovation and Education
The Department of Chemistry successfully organized an engaging international seminar titled "From the Bench to Beyond: Chemistry as a Bridge to Innovation and Education" on 4th November. The event commenced with the traditional lighting of the lamp and Saraswati Vandana, followed by a warm welcome and introduction of the speaker, Dr. Abhishek K. Singh. In his insightful session, Dr. Singh highlighted advancements in antibacterial research, including reducing testing time from 48 hours to just 4 hours, and introduced concepts such as supramolecules, in vivo testing, and cryo-TEM through interactive explanations. He also emphasized the importance of higher education and research opportunities, particularly abroad. The seminar concluded with an engaging Q&A session, leaving students inspired and curious. Overall, the event marked a promising beginning for Rasagya, fostering a spirit of innovation and scientific inquiry among students

Seminar on How basic Chemistry Contributes to Research:
A seminar titled "From Textbook to Test Tube: How Basic Chemistry Contributes to Useful Research" was organized by Rasagya. The talk was delivered by Dr. Sudipta Raha Roy, Department of Chemistry, IIT Delhi. The session provided valuable insight into how every great scientific discovery begins with a simple concept rooted in basic chemistry. The speaker explained how fundamental ideas, such as the use of sunlight as an alternative to heat and other energy sources in chemical reactions, can lead to sustainable and innovative research outcomes.The talk highlighted how core concepts of chemistry including atomic structure, molecular interactions, chemical bonding, and reaction mechanisms form the backbone of impactful and application-oriented research.

SCIENCE DAY

Rasagya, the Chemical Society of Sri Venkateswara College, celebrated National Science Day with the event "Lab Coats and Laughter Notes" on 27th February 2026. The foyer came alive with engaging live experiments that attracted enthusiastic participation from students.

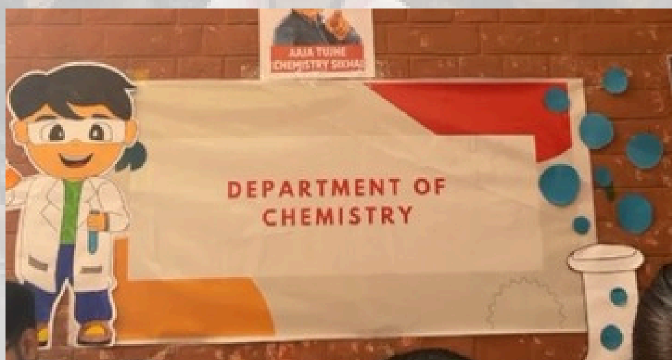
A key highlight was the Experimentation Competition, where participants showcased innovative experiments and explained the underlying concepts, with a special emphasis on sustainability in their reactions. The event successfully blended learning with creativity, promoting scientific curiosity and awareness about responsible practices in chemistry.



OPEN DAY

The Department of Chemistry of Sri Venkateswara College actively participated in the Open Day (under SVC-SPARK conference) by setting up an engaging stall that attracted students from classes 9 to 12. The stall featured a variety of live experiments demonstrating fundamental concepts along with their real-life applications, making chemistry both interactive and relatable.

Alongside the demonstrations, visitors were also introduced to the diverse career opportunities in the field of chemistry. The initiative successfully sparked curiosity among young students and provided valuable insight into the academic and professional pathways in chemistry



JASHN-E-RASAYAN'26

(ANNUAL DEPARTMENTAL FEST OF CHEMISTRY)

Rasagya-The Chemical Society, hosted its annual fest Jashn-e-Rasayan over two dynamic days, from 01 to 02 April, 2026. The event was a vibrant display of the passion and innovation of its members. Featuring seven exciting events, the fest celebrated the diverse and fascinating world of chemistry in all its forms.The festival began with a thought-provoking “Inaugural Lecture on What makes nano better”, delivered by Prof. Rakesh Kumar Sharma. His insights into chemistry's role in securing our future inspired students to think beyond academics and embrace environmental responsibility through scientific innovation. The session marked a powerful start to the celebration.

THE SCIENCE SPRINT

With minds racing and buzzers blazing , "The Science Sprint” (Quiz) tested speed, logic, and chemistry knowledge. Participants battled across multiple rounds, solving puzzles and answering concept-driven questions. The event was a great success, fostering excitement for science in a competitive yet fun atmosphere. The air buzzed with anticipation as teams vied for the prestigious title of quiz champions.

MAD SCIENTIST

In the exciting “Mad Scientist” event, students turned ordinary lab equipment into tools of discovery. Live experiments, chemical reactions, and creative demonstrations wowed the audience. It was a successful platform where science was seen, heard, and felt in its most exciting form.

CHEMOVATE

Chemovate showcased student innovations focusing on sustainable and futuristic chemical solutions. From alternative energy models to eco-friendly materials, the event celebrated creativity backed by scientific thinking.

AD MAD

Creativity and wit came alive in “Ad Mad”, where students presented quirky, humorous ads for fictional chemical products. The event blended advertising with chemistry, resulting in laughter and applause. It was a fresh, engaging experience that highlighted both imagination and understanding.

RASAYAN KI RAJNEETI

The most intellectually stimulating Debate Competition – "Rasayan ki Rajneeti". This high-level debate witnessed active participation from students across the college. The competition saw an impressive footfall, with participants presenting strong arguments and critical perspectives on contemporary issues. The event was conducted smoothly, judged fairly, and concluded successfully with great appreciation from both judges and audience.

TREASURE HUNT

As the dawn of the second day illuminated the horizon, minds converged once again, Clues, riddles and a race against time defined the thrilling "Treasure Hunt". Teams explored, decoded, and competed using their problem-solving skills and chemistry knowledge. Successfully conducted, the event was a fun-filled, intellectually stimulating challenge that energized the entire crowd.

INTEDEPARTMENTAL CRICKET MATCH

The "Interdepartmental Cricket" Match delivered thrilling overs, strong teamwork, and unmatched energy. Teachers and students gave their best in this friendly face-off, creating an unforgettable sporting memory. The event was a resounding success, adding excitement to the academic fest

BADMINTON MATCH

The intense "Badminton Match" was played among the teachers and students in a lively, competitive atmosphere. With smashing rallies and roaring cheers, the game strengthened student-teacher bonds. Conducted exclusively for the department, it was a spirited success full of teamwork and sportsmanship.

TEACHERS' ACHIEVEMENTS

TOTAL NUMBER OF ARTICLES PUBLISHED IN LAST ONE YEAR

- Seela Ramanaiah (2)
- Harshvardhan Meena (1)
- Y.V. Reddy (2)
- Shikha Gulati (5)
- Vinita Kapoor (1)
- Meena Bisht (1)
- Sharda Pasricha (5)
- Rangarajan T.M. (5)
- Saya Devi (4)
- Ravindra Kumar Upadhyay (3)
- R.J. Naik (2)
- Shefali Shukla (1)
- Murali Mohan Achari Kamsali (6)

AWARDS:

Saya Devi- Award for Excellence in Academic collaboration and research given by International Association of Educators for World Peace (affiliated to ECOSOC-United Nations) in the 46th World Management Congress

Vinita Kapoor- National Skilling Award in 2025, received jointly from Indian Institute of Ecology and Environment (IIEE), New Delhi, World Academy of Higher Education and Development(W-AHEAD), National Institute of Skilling (NIS) and Bureau of Revived Ancient Soft Skilling (BRASS)

Murali Mohan Achari Kamsali- Innovative Pedagogy And Curriculum Advancement Award, 2025, Confederation Of Indian Universities, New Delhi.

Thoti Vasantha- Best College For Holistic Student Development Award at the 46th world management Congress, International Association of Educators for World Peace.

OTHER ACHIEVEMENTS:

Book Chapters in Last one Year:

- Murli Mohan Achari Kamsali (2)
- Thoti Vasantha (1)
- Sheela Ramanaiah (1)
- Chandra Sekhar Tekuri (1)
- Saya Devi (5)
- Shefali Shukla (1)
- Shikha Gulati (4)

Books Edited:

- Shikha Gulati(2)

Research projects:

- Shefali Shukla
- Ravindra Kumar Upadhyay

Oral paper presentation:

- Vinita Kapoor(1)

Manuscripts reviewed in last one year

- Thoti Vasantha-8
- Murali Mohan Achari Kamsali-1

STUDENTS' ACHIEVEMENTS

IIT JAM ACHIEVERS 2026

NIKETA-135 (3RD YEAR)
VISHESH - 222 (3RD YEAR)
ARCHIT - 588 (3RD YEAR)
DIYA - 778 (3RD YEAR)
SOMYA - 489 (3RD YEAR)
ALOK - 984 (3RD YEAR)
AMAN MAURYA-186 (4TH YEAR)
DEEPVIJAY SHAKYA - 470 (4TH YEAR)
HARSH PAHUJA-547 (4TH YEAR)
NITESH KUSHWAHA -584 (4TH YEAR)
ASHISH JHA-1262 (4TH YEAR)

OTHER ACHIEVEMENTS

Ayushi Mishra (2nd Year)

- 1st Prize – Policy Hackathon (SVC)
- 1st Prize – Research Paper Presentation (MUN Society)
- Best Speaker – AI Summit Debate (IP College)
- 2nd Prize – Extempore (Biosciences Dept.)
- 3rd Prize – Annual Debate (SSPMC)
- Special Mention – Newsroom Debate (SBSC)
- 2nd Prize – Debate & Paper Presentation (Chemistry & Mathematics Dept.)
- Participated in 15+ debates & 5+ presentations

Pranjal Sharma (2nd Year)

MUN Achievements:

- Verbal Mention (SBSC, KNC)
- Special Mention (DTU)
- Best Delegate (USIMUN)
- Rapporteur – SVC MUN

Debate:

- Special Mention (SVC)
- 1st Position – Presentation Competition (SVC)
- Joint Secretary – Rasagya (SVC)
- Social Media Head – Effulgence (Photography Society)

Prashant Badgujar (2nd Year)

- Member – College Cricket Team
- Played at district level
- 1st Position – BITS Goa (2025)
- Runner-up – UPES Dehradun (2026)
- Winner – BPL tournament

Nikita (3rd Year)

- 3rd Prize – Extempore (NEXUS'24)
- Attended 1-week training on Analytical Tools & Techniques (Shivaji College)

Pratha Dhingra (3rd Year)

- Vice President – The Sankalp Organisation
- President – Rasagya (Chemical Society, SVC)
- Content writer for Sankalp (website & orientation video)
- Scored 92 percentile in XAT

Gaurav Gupta (3rd Year)

- Internship – Grant Thornton Bharat (June–July 2025)
- Completed Praxeum Foundations Leadership Program

Bhumika Singh (3rd year):

- Selected for SHE for STEM Accelerator Program among 600+ participants (Vigyanshala)
- Serving as General Secretary, Rasagya (Chemical Society, SVC) – led events & workshops
- Working as Organic Marketing Executive – managing social media growth & strategy at Leadicious
- Earned Letter of Recommendation from Aarambh Organisation for impactful social work
- Completed Internship at Grant Thornton Bharat / Mastork Technologies with hands-on corporate experience

4th YEAR HIGHLIGHTS

This academic year marks a proud milestone for the Department of Chemistry with the introduction of the fourth year in the undergraduate programme. This batch is the first-ever cohort of Chemistry students to undertake this initiative, setting a new benchmark in academic and research excellence.

Students have actively engaged in both research and review-based projects, exploring diverse areas such as green chemistry, medicinal chemistry, organic synthesis, heterocyclic compounds, conducting polymers, metal–organic frameworks (MOFs), nanomaterials, energy storage systems, ionic liquids, and catalytic/environmental applications.

As pioneers of this new academic structure, their work reflects innovation, scientific curiosity, and a strong commitment towards advancing modern chemistry, marking the beginning of a transformative era for the department.

Student Research & Review Contributions

Green Chemistry:
- Harsh Pahuja
- Deepvijay Shakya
- Gitika Nigam

Nanomaterials:
- Gitika Nigam
- Parikshit Panwar
- Ashish Kumar Jha

Medicinal Chemistry:
- Aman Maurya
- Sneha Prajapati
- Shrinidhi Singh
- Chanchal Kumari

Organic Synthesis / Reactions:
- Harsh Pahuja
- Chanchal Kumari
- Sneha Prajapati
- Shrinidhi Singh

MOFs (Metal-Organic Frameworks):
- Nitesh Kushwaha
- Mohit Yadav

Heterocyclic Chemistry:
- Sneha Prajapati
- Shrinidhi Singh
- Aman Maurya

Energy & Environmental Applications:
- Parikshit Panwar
- Deepvijay Shakya
- Gitika Nigam

Polymer & Conducting Materials:
- Nitesh Kushwaha
- Kanchan
- Akriti Kumari

TEACHERS' DAY

The Chemistry Department celebrated Teachers’ Day with great enthusiasm and heartfelt gratitude, honoring the invaluable contributions of its faculty members. The event was thoughtfully organized by the students to express their appreciation for the dedication, guidance, and unwavering support of their teachers. The celebration reflected a perfect blend of gratitude and festivity, making it a memorable occasion for everyone present.

The program commenced with a heartfelt welcome, followed by speeches from students who expressed their sincere gratitude towards their mentors. They highlighted the pivotal role teachers play not only in imparting knowledge but also in shaping character and inspiring future aspirations. The words of appreciation created an emotional and respectful environment, strengthening the bond between students and faculty.

One of the most special moments of the celebration was when students presented tokens of appreciation and small gifts to their teachers as a mark of respect and love. This gesture symbolized the deep admiration students hold for their mentors and acknowledged their continuous efforts both inside and outside the classroom. The smiles and warmth shared during this moment made it truly meaningful.

The highlight of the event was the series of cultural performances organized by the students, including lively dances, melodious singing, and entertaining skits dedicated to their teachers. These performances not only showcased the creative talents of the students but also brought joy and laughter to the audience, making the celebration vibrant and engaging.

The event concluded on a heartfelt note, leaving everyone with a sense of appreciation and togetherness. The Teachers’ Day celebration was not just a tribute but a reminder of the lasting impact educators have on their students’ lives, making it a truly special and memorable occasion for the Chemistry family.

FRESHERS PARTY

The Chemistry Department extended a warm and enthusiastic welcome to its newest batch of students through a vibrant and memorable Fresher's Party. The event was thoughtfully organized to ensure that the freshers felt comfortable, valued, and excited about the journey ahead. The venue was beautifully decorated, creating a lively atmosphere filled with energy, laughter, and anticipation. From the very beginning, the celebration reflected a perfect blend of tradition and youthful spirit, setting the tone for an unforgettable day.

The कार्यक्रम commenced with inspiring and heartfelt words from the faculty members, who encouraged the freshers to embrace new opportunities, explore their potential, and actively participate in academic and co-curricular activities. Their motivating speeches not only provided guidance but also reassured the newcomers that they were now an integral part of a supportive and nurturing academic community. This warm introduction helped bridge the gap between students and faculty, making the freshers feel welcomed and at ease.

One of the most special moments of the event was the cake-cutting ceremony, which symbolized new beginnings and the start of a promising chapter in the students' lives. The cheerful applause and shared smiles during this moment created a sense of unity among everyone present. It was a simple yet meaningful gesture that highlighted the importance of togetherness and collective celebration within the department.

The highlight of the day was undoubtedly the cultural showcase, where both seniors and freshers took to the stage to display their talents. The audience was captivated by a series of lively dance performances, soulful singing, engaging skits, and other creative acts. The enthusiasm and confidence of the participants made the event truly dynamic, while also giving freshers an opportunity to express themselves and interact with their seniors in a fun and relaxed environment.

The celebration reached its peak with the much-awaited announcement of Mr. and Ms. Freshers, adding excitement and a touch of friendly competition to the event. The Fresher's Party was not just about entertainment—it played a crucial role in fostering strong bonds, building friendships, and creating lasting memories. Overall, the event marked a cheerful and promising beginning for the freshers as they stepped into their new journey as part of the Chemistry family.

SCRIBBLE DAY' 26

The Chemistry Department marked Scribble Day with warmth, laughter, and a touch of nostalgia. Students gathered to fill each other's lab coats and notebooks with heartfelt messages, inside jokes, and memories that captured their shared journey. Every scribble became a small reminder of the bonds formed through lectures, experiments, and countless moments spent together.

As the day went on, the department came alive with energy and excitement. Laughter echoed through the labs and corridors as students revisited memories of practicals, last-minute studies, and fun-filled chaos. Each message written carried emotions that words often fail to express, making the day deeply special for everyone present.

BATCH OF 2023-2026

Scribble Day became a beautiful blend of joy and emotion—a moment to celebrate friendships while also acknowledging the bittersweet feeling of moving forward. The Chemistry Department truly turned the day into a collection of unforgettable memories, filled with love, unity, and togetherness.

FAREWELL' 26

The Department of Chemistry bid a heartfelt farewell to the graduating batch on 24th April 2026 with a warm and memorable celebration. The event brought together students and faculty to reflect on their shared journey, achievements, and countless memories created over the years.

The program featured heartfelt speeches, lively cultural performances, and engaging activities that filled the atmosphere with joy and nostalgia. Seniors expressed their deep gratitude towards the department for its constant support, mentorship, and guidance, while juniors conveyed their admiration and extended their best wishes for the journey ahead.

The event was marked by moments of laughter, appreciation, and a touch of emotion, as everyone reminisced about the experiences that shaped their college life. The farewell concluded on a heartfelt yet hopeful note, leaving behind cherished memories and celebrating the enduring bond of the Chemistry family that will continue to grow beyond the campus.

RELEASE OF LAST YEAR'S MAGAZINE

SRI VENKATESWARA COLLEGE


ABHIGYA
2026
SRI VENKATESWARA COLLEGE