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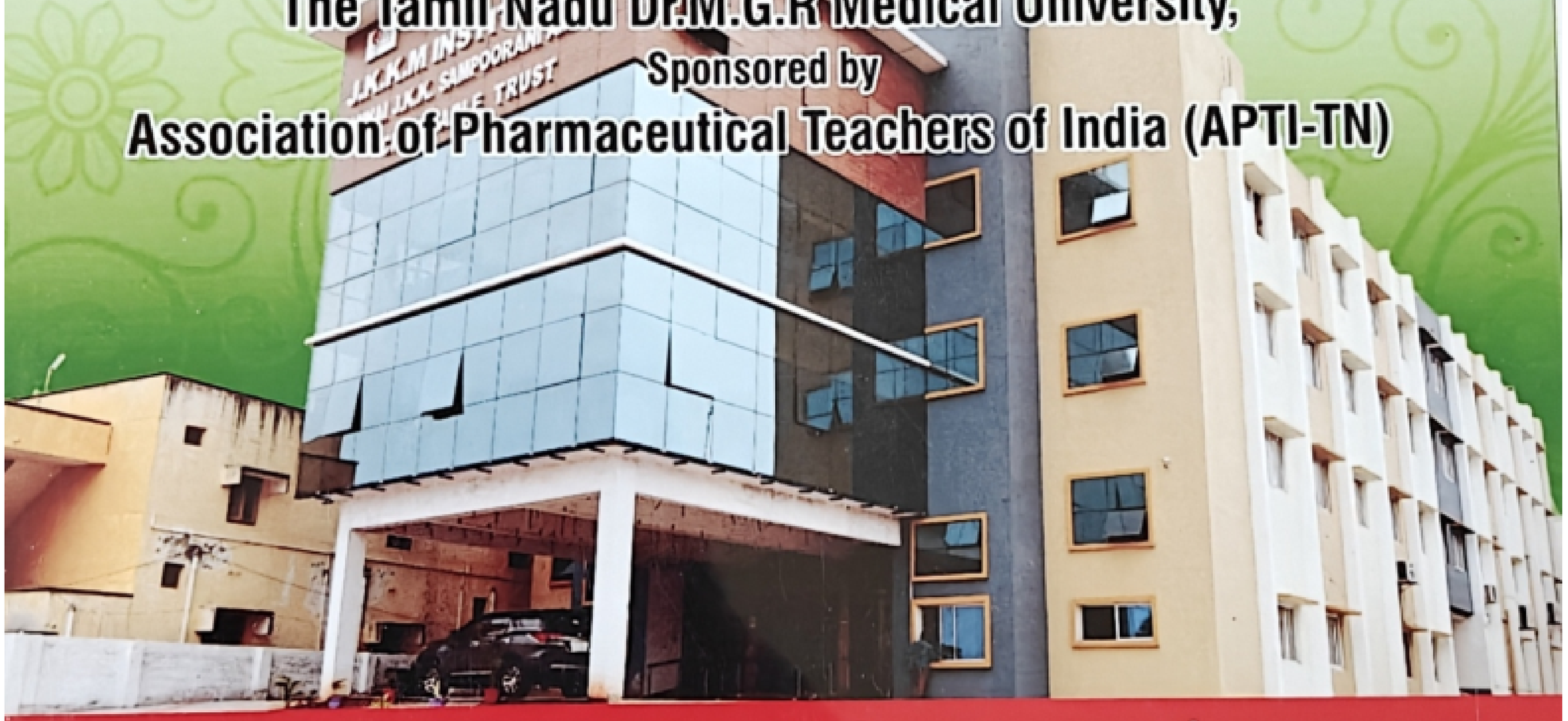

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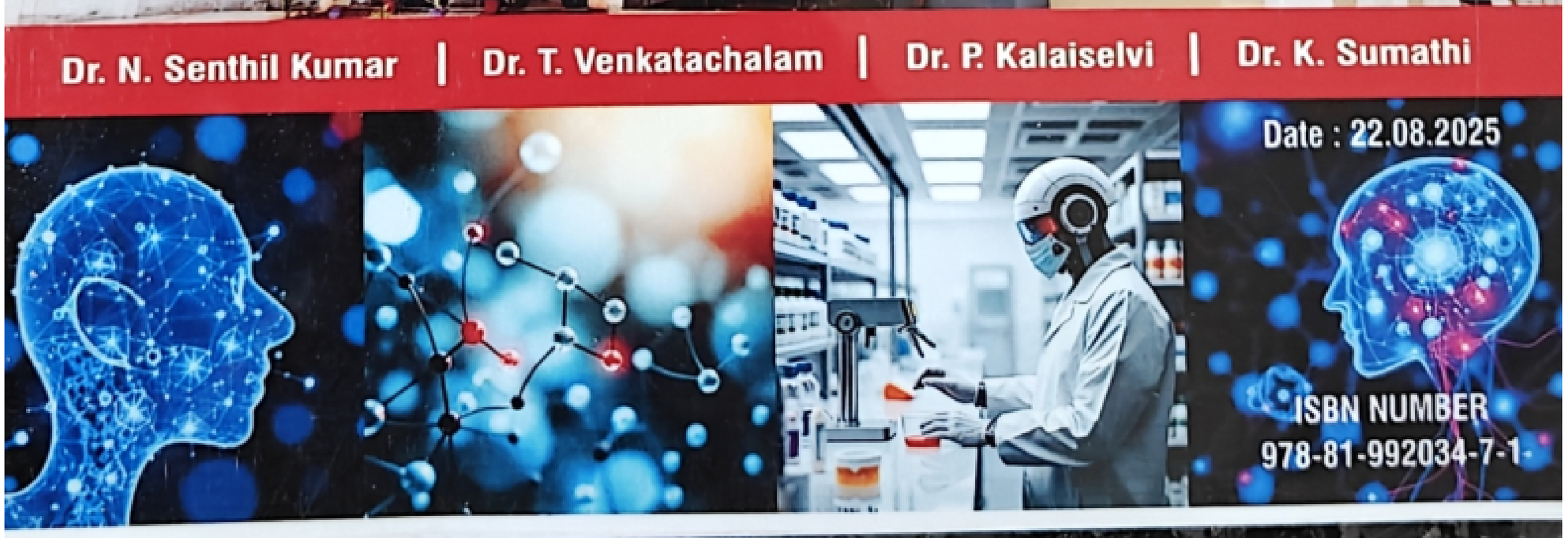

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Green Analytical Chemistry in Pharmaceuticals: Tools, Metrics, and Sustainable Practices.

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ABSTRACT: JKKM- EP 039

Every stage of the pharmaceutical lifecycle (from raw materials to the end product), requires analytical chemistry for evaluation of safety, quality, and stability. Although, some of solvents used for analysis have a environmental impact. Formulated by Paul Anastas in the 1990s, Green Chemistry, which focused on more sustainable synthesis pathways, renewable resources, and developing safer solvents, more environmentally friendly practices broadened the area of chemistry. In turns it gave rise to Green Analytical Chemistry (GAC), which focuses on incorporating sustainability into the classical analytical techniques of chromatography and spectroscopy, and stability studies (now including the use of water, supercritical CO_2, ionic liquids, and bio-based solvents in place of the toxic solvents). In relation to the 12 principles of GAC, NEMI, GSST, The Analytical Eco-Scale, HPLC-EAT, AMVI, GAPI, AMGS, PMI-LCA, RGB Colour Model, AGREE, Complex GAPI, AGREEprep, iGAL, NQS Index, HEXAGON, RGB 12 Algorithm, BAGI and RAPI are just a few of the numerous green metric tools created are based on the principles of "Green" thinking and to measure and enhance greenness. They include qualitative, semi-quantitative, or quantitative methodologies with some parameters and limitations. The toxicity of the solvents involved, waste production, the amount of energy consumed, the practicality of the analytical method used, the carbon footprint, and the cost. The methods used to represent the outputs are pictogram, colour coding, and scoring etc. These ensure methods optimization and validation of the pharmaceutical processes, enable resource conservation and regulatory compliance, and advocate sustainable innovation in the pharmaceutical sector. These parameters are always evolving to keep pace with global environmental concerns and innovations in the field of science.

KEYWORDS: Green analytical chemistry, Green metric tools, Greenness, Sustainability, Eco-friendly.

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Phytochemicals in Action: Targeting Cancer and Viruses with "*Solanum xanthocarpum*",

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ABSTRACT: JKKM- EP 040

Solanum xanthocarpum (commonly known as Kantakari or Yellow-berried Nightshade) is a traditional medicinal plant belonging to the Solanaceae family, widely recognized for its rich phytochemical profile and diverse pharmacological activities. Its bioactive constituents, including alkaloids (solanine, solamargine, solasodine), flavonoids, saponins, tannins, and phenolic compounds, have been extensively studied for therapeutic potential. Among these, glycoalkaloids such as solamargine and solanine exhibit potent anticancer activity by inducing apoptosis, inhibiting tumour cell proliferation, and arresting the cell cycle at specific phases. Similarly, flavonoids and phenolics contribute to antioxidative and immunomodulatory effects, which enhance cancer prevention strategies. In addition to anticancer properties, phytochemicals of *S. xanthocarpum* demonstrate antiviral activity by interfering with viral replication, blocking entry pathways, and modulating host immune responses, making them promising candidates for antiviral drug development. Analytical techniques such as GC-MS, LC-MS, and NMR spectroscopy have been utilized to identify and characterize these phytoconstituents, thereby aiding in standardization and quality assurance. This poster highlights the dual role of *S. xanthocarpum* phytochemicals in combating cancer and viral infections, while emphasizing the importance of modern analytical approaches in validating traditional knowledge. Harnessing these bioactive molecules may pave the way for novel plant-based therapeutics in modern medicine. Future research on *Solanum xanthocarpum* phytochemicals may focus on exploring their potential anti-HIV activity. Advanced molecular docking, in vitro assays, and clinical evaluations will help to validate their efficacy against HIV. If proven, effective, low-cost, and safer therapeutic agents for HIV management are developed in the future.

KEYWORDS: Botanical profile, phytoconstituent profile,anti-cancer activity,anti-viral activity (HIV), Analytical Tools, Modern Significance, Future Perspectives on Anti-HIV research

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Comprehensive Review of QbD-Driven Analytical Procedures for Analyzing Marketed CVS Drug.

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ABSTRACT: JKKM- EP 042

Quality by Design (QbD) has transformed analytical method development by ensuring robustness, reliability, and regulatory flexibility. Its application to analytical procedures, known as Analytical Quality by Design (AQbD), is increasingly adopted for marketed cardiovascular (CVS) drugs, including statins, β-blockers, ACE inhibitors, ARBs, calcium channel blockers, and antiplatelet agents. AQbD begins with defining an Analytical Target Profile (ATP) aligned with product Critical Quality Attributes, followed by risk assessment to identify Critical Method Attributes (CMAs) and Parameters (CMPs). Design of Experiments (DoE) supports optimization by linking method variables, such as mobile-phase pH, gradient slope, stationary phase selection, and detector settings, to performance indicators like accuracy, precision, and robustness, establishing a Method Operable Design Region (MODR). Case studies highlight AQbD in UHPLC and LC–MS/MS for impurity profiling, dissolution testing, and stability indicating assays, reducing Out of Specification (OOS) events and improving method transfer. Regulatory guidance (ICH Q8–Q14) emphasizes lifecycle management, continual verification, and risk-based post-approval changes. Challenges include matrix effects in complex formulations and co-elution of impurities, while opportunities lie in digital method twins, machine learning for peak resolution, and real time control strategies. AQbD ultimately delivers greener, resilient methods with enhanced compliance and adaptability for CVS drug analysis.

KEYWORDS: Analytical Quality by Design (AQbD), Cardiovascular drugs, Analytical Target Profile (ATP), Critical Method Attributes (CMA),

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"Green Solvent Selection for HPLC: A Focus on Solvmate and the GSK Solvent Guide"

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BSTRACT: JKKM- EP 047

In High-Performance Liquid Chromatography (HPLC), solvent choice plays a decisive role in determining both analytical performance and environmental sustainability. Conventional solvents such as methanol and acetonitrile are widely used, yet they raise significant health, safety, and environmental (HSE) concerns. To address these issues, the application of green chemistry principles has encouraged the development of solvent selection tools that provide guidance on safer, sustainable alternatives. Among these, **Solvmate** and the **GSK Solvent Sustainability Guide** stand out as highly effective approaches. Solvmate, a computational web-based tool, integrates machine learning and solubility prediction algorithms to rank solvents according to compatibility with specific analytes, offering precise recommendations for method development in research and quality control laboratories. On the other hand, the GSK Solvent Sustainability Guide applies a structured, color-coded scoring system that categorizes solvents based on their health, safety, and environmental profiles, thereby facilitating informed decision-making in academic and industrial settings. While Solvmate enhances analytical efficiency through predictive modeling, the GSK guide ensures compliance with sustainability standards and regulatory requirements. When combined, these tools provide a comprehensive strategy for achieving both performance optimization and eco-friendly practices in HPLC.

KEYWORDS: HPLC, Green Chemistry, Solvent Selection, Sustainability, Solvmate, GSK Solvent Sustainability Guide

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APPLICATIONS OF QUALITY BY DESIGN IN ANTI-EPILEPTIC DRUGS.

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ABSTRACT:- JKKM- EP 057

This review explores current developments in the use of Analytical Quality by Design (AQbD) ideas to create clonazepam High-Performance Liquid Chromatography (HPLC) methods. Because of its small therapeutic index, poor aqueous solubility, and sensitivity to light, pH changes, and oxidative stress, clonazepam—a widely prescribed benzodiazepine for the management of epilepsy and anxiety disorders—presents several analytical problems. Although HPLC is the preferred analytical method because of its accuracy and flexibility, a systematic, science-based approach like AQbD is required for the long-term dependability of processes.

Defining the Analytical Target Profile (ATP) marks the first stage in the AQbD approach, followed by the identification of Critical Quality Attributes (CQAs) and Critical Method Parameters (CMPs). Two risk assessment techniques, the Failure Mode and Effects Analysis (FMEA) and Ishikawa diagrams help one to identify the most significant variables. The next step is to methodically improve the conditions using Design of Experiments (DoE) techniques, such Plackett–Burman, Box–Behnken, and Central Composite Designs. Additionally, the incorporation of green analytical chemistry concepts guarantees that environmentally friendly practices are followed without sacrificing performance.

Published studies show clonazepam often is better examined by HPLC methods based on AQbD, with enhanced sensitivity, increased resolution, fewer peak tailing, and reduced analysis times. Introducing a Method Operable Design Region (MODR) helps to ensure excellent performance under many of conditions. Finally, AQbD provides a systematic approach to producing dependable HPLC methods that can be used for therapeutic monitoring, stability testing, and impurity profiling throughout the course of clonazepam's existence; these techniques are environmentally friendly and regulatory-compliant.

KEYWORDS

Design of Experiments (DoE); High-Performance Liquid Chromatography (HPLC); Analytical Quality by Design (AQbD); Stability-Indicating Techniques; Critical Method Parameters (CMPs); Clonazepam; Green Analytical Chemistry.

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Decoding drugs with Data: AI innovations in Pharmaceutical analysis

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Abstract: JKKM-ORAL 023

Artificial Intelligence (AI) is transforming the way we study and understand medicines. In modern pharmaceutical labs, techniques like high-performance liquid chromatography (HPLC), liquid chromatography mass spectrometry (LC–MS), nuclear magnetic resonance (NMR) spectroscopy, Raman spectroscopy, and infrared spectroscopy produce huge amounts of complex data. In the past, analysing this information took hours of skilled work and could still leave room for errors. Today, AI can act like a tireless digital assistant, processing data in minutes, spotting patterns that the human eye might miss, and even fine-tuning experiments for better results. These capabilities are making a big difference. AI speeds up the process of finding promising new drugs, ensures manufacturing quality in real time, and uses spectral fingerprints to identify counterfeit or poor-quality medicines before they reach patients. It can also combine results from multiple scientific areas like genomics, proteomics, and metabolomics to design treatments that are tailored to an individuals unique biology. By turning raw data into clear, actionable insights, AI is helping scientists work faster, smarter, and more accurately. Its not just making pharmaceutical analysis more efficient its shaping a future where new medicines can be discovered, tested, and delivered with greater precision and safety than ever before.

Keywords: Artificial Intelligence, Drug Discovery, HPLC, LC–MS, Personalized medicine, Analytical methods.

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Goal-Oriented Molecule Discovery Through Human-AI Collaboration

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ABSTRACT: JKKM-ORAL 024

By enabling the rapid creation, screening, and optimization of possible molecules, artificial intelligence (AI) is transforming the way new drugs are found. On the other hand, AI alone can find difficulty with things like disregarding little components that affect the safety and efficacy of medications or producing synthetic chemicals that are physically impossible. Human-AI interaction, particularly through human-in-the-loop active learning, which enables expert knowledge to guide computational power, makes possible a balanced approach to goal-oriented molecule discovery. With this approach, human experts constantly improve the results of artificial intelligence models, therefore suggesting possible molecules based on certain objectives including pharmacokinetics, safety profiles, and target binding affinity. Real-world restrictions, structural insights, and feasibility studies by medicinal chemists and analysts guarantee that the chosen compounds may be manufactured and tested rather than only intellectually promising. This collaborative circle quickens hit-to-lead timelines, strengthens analytic methods including method development and stability prediction, and increases multi-parameter optimization. Actual case studies show that combining the speed of AI with human judgement produces better decision-making than using either alone. Emphasized in the presentation, this hybrid approach tackles typical drug design problems, fosters more efficient research and development, and prepares the way for a future wherein artificial intelligence helps researchers create safer and more effective therapies more quickly.

Key words: Human-in-the-loop, Artificial Intelligence, Drug Discovery, Molecule Generation, Active Learning.

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AI in Ophthamology – The Current State, Challenges and Future Prospects.

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ABSTRACT:- JKKM-ORAL 053

AI has been significantly playing a major role in enhancing and improving many sectors and fields. Especially in the medical and clinical sector of ophthalmology there are many application of AI algorithm, such as from diagnosing ocular diseases to creating a 3D printed cornea and also for effective ocular drug delivering system. AI in ophthalmology clinical practice enhances the productivity of workplace. AI platforms are being explored with future prospects of Detection, Surveillance and Treatment.AI algorithms are implemented in several fields like Glaucoma, diabetic retinopathy, age-related mucular degeneration, cataract etc… In AI there are six subset. In which two subsets are widely used for prediction and diagnosing of diseases. They are Machine learning (ML) and Deep learning algorithm (DLA). In clinical diagnosis of ophthalmology Deep learning algorithm (DLA) is widely used due to its Artificial Neural Network (ANN) technology. As they say "Every invention has its own limitation". AI in ophthalmology also has its own area of limitation and challenges.

KEYWORDS: Artificial Intelligence in Ophthalmology, Machine Learning & Deep Learning for Eye Disease Detection,AI-Driven Diagnostics & Clinical Workflow, Explainability, Bias, and Ethical Challenges

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A Comparitive Review of Hydrophilic Interaction Chromatography (Hilic) with Reversed Phase, Ion Exchange, and Normal Phase Chromatography in the Analysis of Aminoglycoside Antibiotics

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ABSTRACT: -JKKM-ORAL 056

BACKGROUND: Gram-negative bacteria-related severe infections are treated in human and veterinary medicine with aminoglycoside antibiotics. Due to their quite polar and hydrophilic nature, aminoglycosides are difficult for standard chromatographic techniques to properly retain and separate. Traditional methods, including normal phase (NP), ion exchange (IEX), and reversed phase (RP) chromatography, usually need a lot of sample preparation, derivatization, or usage of ion-pairing reagents, which can make them less efficient and less compatible with mass spectrometry (MS) detection. **TARGET:** To critically contrast Hydrophilic Interaction Chromatography (HILIC) with RP, IEX, and NP chromatography, highlighting their ability to separate and examine aminoglycoside medicines across several matrices. **OBJECTIVES:** To highlight the physicochemical issues found in the chromatographic study of aminoglycosides. I evaluated HILIC's performance against RP, IEX, and NP methods. To sum up latest advancements in MS-coupled detection techniques and HILIC column chemistry. To highlight the advantages of HILIC in food safety, clinical, and pharmaceutical uses. To suggest future ways for enhancing chromatographic techniques for polar antibiotic chemicals. **RESULTS:** The review shows that HILIC, especially when used with MS detection and zwitterionic stationary phases, makes aminoglycoside analysis more sensitive, retentive, and repeatable. On the other hand, because of derivatization requirements or buffer incompatibilities, RP and IEX techniques are still helpful but have restrictions. In summary, HILIC seems to be the best chromatographic method for aminoglycoside analysis since it strikes a mix of simplicity, selectivity, and MS compatibility. Its growing application in research, medical, and regulatory contexts emphasizes its benefits above more conventional approaches.

KEYWORDS: Aminoglycosides; Zwitterionic Columns; Ion Exchange Chromatography (IEX); LC-MS/MS, Hydrophilic Interaction Chromatography (HILIC); Reversed Phase Chromatography (RP-HPLC); Normal Phase Chromatography (NP)

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Trends and Evolution from Analytical Chemistry to Green Analytical Chemistry Guide

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Abstract: JKKM-ORAL 092

From traditional analytical chemistry to Green Analytical Chemistry (GAC), there is a clear move toward making scientific methods more environmentally friendly and sustainable. Conventional analytical techniques, particularly in pharmaceutical analysis of lipid lowering drugs like atorvastatin,lovastatin have long depended on hazardous solvents acetonitrile, methanol, and tetrahydrofuran as well as long run times and gear using a lot of energy. Though they are sensitive and abide the regulations, these approaches generate a great deal of hazardous waste and raise safety issues for lab employees.GAC aims to reduce or remove hazardous solvents, minimize waste, and reduce environmental effect without compromising analytical correctness by following the twelve fundamental concepts of green chemistry and enhanced by the ten principles of green sample preparation.Ethanol-based reversed-phase HPLC, micellar liquid chromatography, and microextraction techniques are among the most recent developments offering safer, quicker, more environmentally friendly substitutes for traditional approaches. Importantly, including greenness evaluation tools like GAPI, AGREE, Eco-scale, and life-cycle analysis ensures that more environmentally friendly techniques are validated for both performance and sustainability in addition to performance. Beyond pharmaceutical uses, GAC is now more and more used in environmental monitoring, food safety therefore emphasizing its adaptability and importance in many fields and highlighting trade-offs between solvent use, energy efficiency, and analytical robustness. This review argues that utilizing more environmentally friendly methods is not only a moral responsibility but also a sensible approach to lower costs, produce safer labs, and fulfill shifting rules. GAC finally enables the twin aims of offering great analytical results while simultaneously safeguarding the environment and human health.

KEYWORDS: Green Analytical Chemistry,Sustainable HPLC, Eco-friendly solvents, Greenness metrics, lipid lowering drugs, Environmental sustainability