# E-SYMPOSIUM PROCEEDINGS

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## ARTIFICIAL INTELLIGENCE DRIVEN STRATEGIES IN *DENOVO* DRUG DESIGN

Mr. Aarav Kumar

*UG Scholar, Department of Pharmacy, Yelamarty B. Pharmacy College, Vishakhapatnam, AP, India*

*aarav.kumar99@outlook.com*

**Abstract:** The integration of Artificial Intelligence (AI) and Machine Learning (ML) has catalyzed a paradigm shift in pharmaceutical R&D, moving from trial-and-error methods to predictive, data-driven frameworks. Modern AI algorithms facilitate *de novo* drug design by analyzing vast chemical libraries to identify lead compounds with high binding affinity and minimal toxicity. These computational models, including deep learning and neural networks, are now capable of predicting protein structures and drug-target interactions with unprecedented accuracy. AI significantly reduces the timelines and astronomical costs traditionally associated with drug discovery by streamlining the hit-to-lead optimization phase. Moreover, AI-driven automation is being applied to clinical trial design, enabling more precise patient stratification and real-time monitoring of therapeutic efficacy. This technological synergy not only accelerates the arrival of life-saving medications to the market but also enhances the safety profile of experimental candidates. As the industry moves toward 2026, the convergence of AI with high-throughput screening remains the cornerstone of next-generation pharmaceutical innovation.

**Keywords:** Artificial Intelligence, Machine Learning, De Novo Design, Drug Discovery, Predictive Modelling.

## ADVANCEMENTS IN LIPID NANOPARTICLE SYSTEMS FOR mRNA VACCINE DELIVERY

Miss Ananya Rasi

*UG Scholar, Department of Pharmacy, Green Royal Academy of Pharmaceutical Education and Sciences, Koyyalagudem, Warangal, Andhra Pradesh, India*

*ananya.rasi@yahoo.com*

**Abstract:** The global success of mRNA-based therapeutics has highlighted the critical role of Lipid Nanoparticles (LNPs) as a revolutionary delivery platform. mRNA molecules are inherently unstable and susceptible to enzymatic degradation; therefore, the development of sophisticated LNP formulations is essential for protecting the genetic payload and ensuring efficient intracellular uptake. Recent trends focus on the engineering of ionizable lipids that remain neutral at physiological pH but become positively charged within acidic endosomes, facilitating endosomal escape and subsequent protein translation. Beyond infectious diseases, LNP technology is being adapted for cancer immunotherapy and rare genetic disorders by tailoring the lipid composition for organ-specific targeting. Innovations in manufacturing, such as microfluidic mixing, have improved the scalability and uniformity of these complex formulations. The optimization of LNP stability and the reduction of potential immunogenicity remain primary research objectives. These advancements represent a significant leap in the ability to utilize the body's own cellular machinery for therapeutic protein production.

**Keywords:** Lipid Nanoparticles, mRNA Therapeutics, Endosomal Escape, Vaccine Delivery, Ionizable Lipids.

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## 3D PRINTING TECHNOLOGY IN THE FABRICATION OF PERSONALIZED POLYPILLS

Mr. Rohan Deshmukh

*UG Scholar, Department of Pharmacy, Manipal College of Pharmaceutical Sciences, Udupi, India*

*orohan.d.pharm@gmail.com*

**Abstract:** The transition from a "one-size-fits-all" approach to personalized medicine has been significantly accelerated by the advent of 3D printing in pharmaceutical manufacturing. This technology allows for the precise fabrication of "polypills" single dosage forms containing multiple active pharmaceutical ingredients (APIs) with customized release profiles. Techniques such as Fused Deposition Modeling (FDM) and Stereolithography enable the creation of complex internal geometries that dictate drug release kinetics, such as immediate, sustained, or pulsatile release. This is particularly beneficial for geriatric populations and patients with chronic comorbidities who often struggle with complex dosing regimens and polypharmacy. 3D printing improves patient adherence and reduces the risk of medication errors by consolidating several medications into a single, daily tablet. Current research is also exploring "Printlets" tailored to individual genetic profiles and metabolic rates, ensuring optimal therapeutic concentration while minimizing adverse reactions. As regulatory frameworks adapt to decentralized manufacturing, 3D printing stands to redefine the role of the pharmacist in the digital age.

**Keywords:** 3D Printing, Polypills, Personalized Medicine, Fused Deposition Modeling, Patient Compliance.

## GREEN CHEMISTRY PRINCIPLES IN SUSTAINABLE API SYNTHESIS

Miss Ishita Kapoor

*Assistant Professor, Department of Pharmaceutical Chemistry, Dr. B. C. Roy College of Pharmacy and AHS, Durgapur, West Bengal, India*

*ishita.kapoor.edu@rediffmail.com*

**Abstract:** Environmental sustainability has become a top priority in the pharmaceutical industry, leading to the widespread adoption of Green Chemistry principles in the synthesis of Active Pharmaceutical Ingredients (APIs). Traditional chemical manufacturing often involves hazardous solvents and generates significant waste, measured by high E-factors. Recent trends emphasize the use of biocatalysis, microwave-assisted organic synthesis (MAOS), and continuous flow chemistry to minimize ecological footprints. Biocatalysts, such as engineered enzymes, allow for highly stereoselective reactions under mild conditions, reducing the need for toxic reagents. The shift from batch processing to continuous flow manufacturing enhances energy efficiency and safety through better heat and mass transfer. Solvent selection has also evolved, with a focus on bio-based and recyclable alternatives like supercritical fluids. These "green" methodologies not only align with global carbon-reduction goals but also offer economic advantages by improving atom economy and reducing purification steps. The integration of sustainable practices ensures that the development of new drugs does not come at the expense of environmental health.

**Keywords:** Green Chemistry, Biocatalysis, Sustainable Synthesis, Atom Economy, Continuous Flow.

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# PROTAC TECHNOLOGY AS A NEW FRONTIER IN TARGETED PROTEIN DEGRADATION

Mr. Kabir Verma

*Assistant Professor, Department of Biotechnology, Jyothishmathi Institute of Pharmaceutical Sciences, Karimnagar, Telangana, India*

*kabir.verma@gmail.com*

**Abstract:** Proteolysis-Targeting Chimeras (PROTACs) represent a breakthrough in pharmaceutical drug development, offering a strategy to target "undruggable" proteins that lack traditional binding pockets for inhibitors. Unlike conventional small-molecule inhibitors that require high occupancy to block a protein's function, PROTACs act catalytically to hijack the cell's endogenous ubiquitin-proteasome system. These heterobifunctional molecules consist of a ligand for the target protein, a ligand for an E3 ubiquitin ligase, and a specialized linker.The PROTAC induces ubiquitination and subsequent degradation of the disease-causing protein by bringing the target protein into proximity with the E3 ligase. This approach has shown immense potential in oncology, particularly in overcoming drug resistance associated with kinase mutations. Current formulation research focuses on improving the oral bioavailability and cell permeability of these relatively large molecules. As PROTACs progress through clinical trials, they open new avenues for treating complex conditions, including neurodegenerative diseases and autoimmune disorders, by eliminating pathogenic proteins rather than simply inhibiting them.

**Keywords:** PROTACs, Protein Degradation, E3 Ubiquitin Ligase, Targeted Therapy, Undruggable Targets.

# SMART HYDROGELS AND STIMULI-RESPONSIVE SYSTEMS FOR SITE-SPECIFIC RELEASE

Miss Meera Nair

*UG Scholar, Department of Pharmacy, Malla Reddy Institute of Pharmaceutical Sciences, Mechal, Telangana, India*

*meera.nair.pharm@gmail.com*

**Abstract:** Stimuli-responsive drug delivery systems, often referred to as "smart" systems, are designed to release their therapeutic payload in response to specific internal or external triggers. Among these, smart hydrogels have gained prominence due to their biocompatibility and tunable physical properties. These polymeric networks can undergo reversible structural changes such as swelling or shrinking when exposed to variations in pH, temperature, light, or enzyme concentration. In cancer therapy, pH-responsive hydrogels exploit the acidic microenvironment of tumors to trigger localized drug release, thereby protecting healthy tissues from systemic toxicity. Similarly, thermo-responsive systems can be engineered to remain liquid at room temperature for easy injection and form a stable gel depot at body temperature for sustained release. Recent advancements also include "dual-stimuli" systems that require two distinct triggers for activation, providing an extra layer of precision. These intelligent formulations represent the future of site-specific drug delivery, ensuring that medications are released only when and where they are most needed, thereby maximizing efficacy and minimizing patient discomfort.

**Keywords:** Smart Hydrogels, Stimuli-Responsive, Controlled Release, Site-Specific Delivery, Polymeric Networks

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## EXTRASOMAL DELIVERY SYSTEMS AS DERIVED VESICLES FOR TARGETED THERAPY


Mr. Vikram Mehta

*PG Scholar, Department of Pharmaceutics, Manipal College of Pharmaceutical Sciences, Karnataka, India*

*vikram.m.pharm@outlook.com*



**Abstract:** Exosomes, a sub-population of extracellular vesicles, have emerged as a sophisticated "nature-made" delivery platform in modern pharmaceutics. These nano-sized vesicles are naturally secreted by cells and possess innate biocompatibility, low immunogenicity, and the unique ability to cross biological barriers, including the blood-brain barrier (BBB). Recent research focuses on loading exosomes with diverse payloads, ranging from small-molecule chemotherapeutics to large genetic sequences like siRNA. Unlike synthetic nanoparticles, exosomes retain the surface proteins of their parent cells, which can be bio-engineered to display specific ligands for highly precise tissue targeting. This trend is particularly transformative in the treatment of neurodegenerative diseases and metastatic cancers, where traditional drug entry is severely restricted. Furthermore, "designer exosomes" are being developed to facilitate personalized immunotherapy by modulating the immune response directly at the cellular level. As isolation and purification techniques like tangential flow filtration become more standardized, exosome-based therapy is poised to bridge the gap between biological and synthetic drug delivery systems, offering a highly efficient and safe alternative for complex clinical applications.



**Keywords:** Exosomes, Extracellular Vesicles, Targeted Delivery, Biocompatibility, siRNA.


## ENHANCING THE SOLUBILITY OF BCS CLASS II DRUGS WITH CRYSTAL ENGINEERING AND CO-CRYSTALS


Miss Sneha Reddy

*Research Scholar, Department of Pharmaceutics, JSS College of Pharmacy, Ooty, India*

*sneha.reddy.jss@gmail.com*



**Abstract:** A significant hurdle in contemporary drug development is the poor aqueous solubility of nearly 40% of newly discovered chemical entities, often categorized as BCS Class II drugs. Crystal engineering has surfaced as a powerful trend to overcome these limitations without altering the pharmacological properties of the active pharmaceutical ingredient (API). The formation of pharmaceutical co-crystals multicomponent crystalline solids allows for the modification of physical properties such as dissolution rate, stability, and bioavailability. By pairing an API with a non-toxic co-former through non-covalent interactions like hydrogen bonding, researchers can tailor the solid-state behavior of the drug. This approach is particularly advantageous for drugs that are non-ionizable and cannot form salts. Recent advancements in "solvent-drop grinding" and "hot-melt extrusion" have made the industrial scale-up of co-crystals more viable. These engineered crystals not only improve therapeutic efficacy but also extend the patent life of existing drugs through the development of novel crystalline forms. This strategic manipulation of the molecular arrangement represents a cornerstone in formulation science for improving the performance of poorly soluble medicines.



**Keywords:** Crystal Engineering, Co-crystals, BCS Class II, Solubility Enhancement, Bioavailability.

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# NANO-EMULSIONS AS VECTORS FOR ENHANCED PERMEATION IN TRANSDERMAL DELIVERY

Mr. Aditya Kulkarni

*UG Scholar, Department of Pharmacy, Poona College of Pharmacy, Pune, India*

*aditya.k.pharm@yahoo.co.in*

**Abstract:** Transdermal drug delivery offers a non-invasive alternative to oral and parenteral administration, yet it is often limited by the skin's primary barrier, the stratum corneum. Nano-emulsions kinetically stable dispersions of oil and water with droplet sizes in the range of 10 to 200 nm have emerged as a leading solution to this challenge. Due to their small droplet size and high surface area, nano-emulsions provide a significant increase in drug loading and skin permeation. They act as penetration enhancers by disrupting the lipid bilayer of the skin, allowing for the systemic absorption of both lipophilic and hydrophilic drugs. Recent trends include the development of "self-nanoemulsifying drug delivery systems" (SNEDDS) which spontaneously emulsify upon contact with physiological fluids. This technology is being extensively researched for the delivery of anti-inflammatory drugs, hormones, and even vaccines. By providing a sustained release profile and bypassing first-pass metabolism, nano-emulsions reduce dosing frequency and minimize gastrointestinal side effects. As the demand for patient-friendly delivery routes increases, nano-emulsion technology continues to redefine the boundaries of topical and systemic therapy.

**Keywords:** Nano-emulsion, Transdermal Delivery, Stratum Corneum, SNEDDS, Permeation Enhancement.

# THE ROLE OF MICROFLUIDICS IN THE PRECISION MANUFACTURING OF NANOMEDICINES

Miss Tanvi Iyer

*UG Scholar, Department of Pharmacy, Aadya College of Pharmacy, Chitradurga, Karnataka, India*

*tanvi.iyer@gmail.com*

**Abstract:** Traditional "top-down" methods for nanoparticle synthesis, such as homogenization and sonication, often suffer from high polydispersity and poor batch-to-batch reproducibility. To address these challenges, the pharmaceutical industry is increasingly adopting microfluidic technology for the "bottom-up" assembly of nanomedicines. Microfluidics allows for the precise control of fluid flow at the sub-millimeter scale, enabling rapid and uniform mixing of reactants. This precision ensures the production of nanoparticles such as liposomes, polymeric micelles, and lipid nanoparticles with highly controlled sizes and narrow distribution. The laminar flow conditions within microfluidic chips facilitate the encapsulation of sensitive biological payloads, including DNA, RNA, and proteins, with minimal degradation. Furthermore, this technology supports the rapid screening of formulation parameters, significantly accelerating the early-stage development process. As the industry moves toward continuous manufacturing and "lab-on-a-chip" concepts, microfluidics provides a scalable and robust platform for the production of next-generation personalized therapeutics. The ability to produce uniform nanocarriers is essential for ensuring consistent pharmacokinetic profiles and therapeutic safety in clinical settings.

**Keywords:** Microfluidics, Nanomedicine, Continuous Manufacturing, Lab-on-a-chip, Liposomes.

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## *IN SILICO* MODELING AND PHARMACOKINETIC PREDICTION IN EARLY DRUG DEVELOPMENT


Mr. Sameer Azad

*Assistant Professor, Department of Pharmaceutics, Sujana College of Pharmacy, Vishakhapatnam, Andhra Pradesh, India*

*sameerazad99@gmail.com*



**Abstract:** The high failure rate of drug candidates in clinical trials is often attributed to poor pharmacokinetic profiles that were not identified during the pre-clinical phase. *In silico* modeling computer-based simulation is now being utilized as a proactive tool to predict Absorption, Distribution, Metabolism, Excretion, and Toxicity (ADMET) properties before physical synthesis. Physiologically Based Pharmacokinetic (PBPK) models integrate physiological data with chemical properties to simulate how a drug behaves within a virtual human body. This "virtual clinical trial" approach allows researchers to identify potential safety issues and optimize dosage regimens for specific populations, such as pediatric or geriatric patients. Recent trends involve the use of Quantitative Structure-Activity Relationship (QSAR) models to link molecular structure to biological activity, further refining the selection of lead compounds. By reducing the reliance on extensive animal testing and minimizing the risk of late-stage failures, *in silico* tools provide a cost-effective and ethically sound framework for modern drug discovery. The convergence of computational biology and pharmaceutical science is essential for the rapid development of safer, more effective medicines in the 2026 landscape.



**Keywords:** *In Silico*, PBPK Modeling, ADMET, QSAR, Drug Discovery.


## OXYGEN-SENSITIVE AND HYPOXIA-TARGETED PRODRUGS IN ONCOLOGY


Miss Riya Chawla

*UG Scholar, Department of Pharmacy, Unity College of Pharmacy, Bhuvanagiri, Telangana, India*

*riya4chawla@yahoo.com*



**Abstract:** Hypoxia, or low oxygen tension, is a hallmark of solid tumors and is frequently associated with resistance to conventional radiotherapy and chemotherapy. To exploit this physiological anomaly, recent pharmaceutical trends have shifted toward the development of hypoxia-activated prodrugs (HAPs). These are pharmacologically inactive compounds that undergo selective chemical reduction only in the oxygen-deficient environment of a tumor, releasing a highly cytotoxic active agent. This mechanism ensures that the potent drug is delivered specifically to the malignant core while sparing the well-oxygenated healthy tissues. Modern HAPs are being combined with specialized nanocarriers to improve their solubility and prolong their circulation time. Researchers are exploring the use of hypoxia-responsive polymers that undergo a phase transition triggered by low oxygen levels, facilitating a "burst release" of medication directly within the tumor microenvironment. Oxygen-sensitive systems represent a significant advancement in the precision of cancer treatment, by addressing the challenges of tumor heterogeneity and drug resistance moving closer to the goal of high-efficacy therapy with minimal systemic toxicity.



**Keywords:** Hypoxia, Prodrugs, Oncology, Targeted Therapy, Tumor Microenvironment.

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## NOVEL DRUG DELIVERY SYSTEMS

Mr. Shivansh Singh

*UG Scholar, Department of Pharmacy, Delhi College of Pharmacy, DIRD, Holambi Khurd, India*

*shivansh010104@gmail.com*

**Abstract:** Novel drug delivery systems (NDDS) include advanced formulations such as nanoparticles, polymers, and 3D printing to achieve precise, controlled release of therapeutic agents. These systems protect medicinal compounds from degradation, enhance their stability, and significantly improve bioavailability by utilizing specialized carriers including liposomes and dendrimers. Unlike traditional administration methods, NDDS facilitates targeted delivery by guiding drugs to specific cells or tissues. Release is often triggered by localized physiological conditions, such as pH fluctuations within a tumor microenvironment, which ensures optimal dosing at the exact site of action. This precision minimizes the systemic exposure of healthy cells, thereby reducing adverse side effects. The clinical importance of these technologies is particularly evident in the treatment of complex diseases like cancer, where they maximize the efficacy of high-cost pharmaceuticals while making regimens safer. These systems improve patient compliance and overall therapeutic outcomes by reducing dosing frequency and simplifying administration

**Keywords:** Nanoparticles, Liposomes, Dendrimers, Bioavailability, 3D printing, Targeted delivery.

## DEVELOPMENT OF INHALABLE NANOPARTICLES FOR PULMONARY DRUG DELIVERY

Mr. Arun Paul

*UG Scholar, Department of Pharmacy, Balaji College of Pharmacy, Anantapuram, Andhra Pradesh, India*

*arunpaul143@gmail.com*

**Abstract:** Pulmonary drug delivery is increasingly favored for both local lung diseases and systemic conditions due to the lungs' large surface area, thin alveolar epithelium, and extensive vascularization. Recent trends focus on the engineering of inhalable nanoparticles designed to overcome the natural clearance mechanisms of the respiratory tract, such as mucociliary clearance and macrophage uptake. Researchers can achieve sustained release and targeted deposition within the deep lung tissues by encapsulating drugs within biodegradable polymers or lipid-based carriers,. These "nano-in-micro" formulations where nanoparticles are spray-dried into micro-sized clusters ensure optimal aerodynamic properties for inhalation while maintaining the benefits of nanotechnology. This approach is particularly promising for the delivery of antibiotics in cystic fibrosis, insulin for diabetes, and even gene therapies for lung cancer. Advancements in dry powder inhaler (DPI) technology have further improved the stability and ease of administration of these complex formulations. As the burden of respiratory diseases grows globally, inhalable nanomedicines offer a direct, high-concentration therapeutic route that minimizes systemic side effects and improves patient quality of life.

**Keywords:** Pulmonary Delivery, Inhalable Nanoparticles, Dry Powder Inhaler, Sustained Release, Alveolar Targeting.