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Artificial Intelligence and Emerging Technologies in Drug Discovery and Smart Therapeutics

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The pharmaceutical and healthcare sectors are being transformed by the convergence of artificial intelligence (AI), machine learning, deep learning, big data analytics, bioinformatics, nanotechnology, quantum computing, and digital health. Conventional drug discovery is lengthy, expensive, and associated with high failure rates due to inadequate efficacy, toxicity, poor pharmacokinetics, and unpredictable clinical outcomes. AI and emerging technologies offer new opportunities to accelerate drug discovery and develop safer, more effective, and personalized therapies.

AI-Driven Target Identification and Molecular Design

AI and machine learning are increasingly used in computer-aided drug discovery to analyse chemical, genomic, proteomic, and clinical datasets. These approaches can predict biological activity, toxicity, physicochemical properties, drug–target interactions, and pharmacokinetic behaviour, reducing the need for extensive experimental screening. AI-based integration of genomic, transcriptomic, proteomic, and metabolomic data can identify novel therapeutic targets, biomarkers, and disease pathways. Generative AI and deep-learning models can also design or prioritize new molecules with desirable potency, selectivity, solubility, and safety profiles. Combined with molecular docking, molecular dynamics, QSAR, and virtual screening, these approaches can accelerate lead identification and optimization [1].

Multi-Omics and Precision Medicine

The integration of genomics, transcriptomics, proteomics, metabolomics, and epigenomics enables comprehensive understanding of complex diseases. AI can analyse these datasets to identify disease signatures, biomarkers, therapeutic targets, and patient subgroups. Such approaches support precision medicine, allowing treatments to be increasingly tailored to individual molecular and genetic characteristics [2-3].

AI in Clinical Trials and Pharmacovigilance

AI is improving clinical development by supporting patient selection, trial design, patient stratification, outcome prediction, and adverse-event monitoring. Analysis of electronic health records and clinical data can improve recruitment and help identify patients most likely to respond to specific therapies. AI also strengthens pharmacovigilance by analysing adverse-event reports, medical records, and scientific literature. Natural language processing can extract safety information from unstructured data, enabling earlier detection of potential drug-related risks [4].

Smart Therapeutics, Nanotechnology, and Digital Health

Emerging technologies are enabling smart and targeted drug-delivery systems that respond to biological stimuli such as pH, enzymes, temperature, glucose, or disease-specific biomarkers. Nanotechnology-based carriers, including lipid and polymeric nanoparticles, can improve drug solubility, bioavailability, targeted delivery, and therapeutic efficacy. Wearable devices, smartphones, and connected healthcare technologies generate continuous patient-specific data. AI can analyse these data to monitor treatment response, detect

physiological changes, predict disease progression, and support personalized healthcare and digital therapeutics [5].

Quantum Computing in Drug Discovery

Quantum computing offers a promising future for molecular simulation and computational chemistry. As molecular systems become increasingly complex, quantum technologies may provide new approaches for modelling molecular interactions and accelerating drug discovery. Although large-scale pharmaceutical applications are still developing, this technology has considerable long-term potential [6].

Challenges and Future Perspectives

Despite its potential, AI-driven pharmaceutical research faces challenges involving data quality, standardization, algorithmic bias, model interpretability, privacy, cybersecurity, and regulatory acceptance. AI predictions must be supported by rigorous laboratory and clinical validation, while ethical and regulatory frameworks must evolve with technological advances. The future will require collaboration among pharmacists, medicinal chemists, biologists, clinicians, AI specialists, data scientists, engineers, and regulatory experts. AI should complement rather than replace scientific expertise, supporting more efficient and evidence-based decision-making [2-3].

Conclusion

AI and emerging technologies are reshaping the pharmaceutical landscape, from target identification and molecular design to clinical trials, pharmacovigilance, smart drug delivery, and precision medicine. Their integration can make drug development faster, more accurate, and increasingly patient-centered. However, successful implementation requires scientific validation, responsible data use, ethical governance, regulatory preparedness, and interdisciplinary collaboration. This thematic issue invites original research, reviews, short communications, and innovative perspectives addressing the application of AI and emerging technologies in drug discovery, development, smart therapeutics, and precision healthcare.

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