Advancements at the Nexus of Mathematics, Artificial Intelligence, and IoT in Medicinal Chemistry and Healthcare

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Introduction:

The field of medicinal chemistry and healthcare is experiencing a transformative phase with the convergence of mathematics, artificial intelligence (AI), and the Internet of Things (IoT). The integration of these disciplines has the potential to revolutionize drug discovery, personalized medicine, and healthcare delivery, offering unprecedented opportunities for improved patient outcomes and efficient healthcare systems.

Mathematics serves as the foundational language for understanding complex systems and modeling biological processes. It provides quantitative tools and analytical frameworks to study drug interactions, pharmacokinetics, and pharmacodynamics. By utilizing mathematical models and simulations, researchers can gain valuable insights into the behavior and efficacy of pharmaceutical compounds, leading to more efficient drug design and discovery processes. Artificial intelligence and machine learning algorithms have emerged as powerful tools in medicinal chemistry and healthcare. These technologies can analyze vast amounts of data, identify patterns, and generate predictive models. In drug development, AI algorithms can assist in virtual screening, predicting drug-target interactions, and designing novel compounds with desired properties. Moreover, AI-driven precision medicine enables the customization of treatments based on individual patient characteristics, optimizing therapeutic outcomes. The Internet of Things (IoT) complements the advancements in medicinal chemistry and healthcare by enabling seamless connectivity and data exchange among various healthcare devices and systems. IoT-enabled technologies, such as wearable devices, remote patient monitoring systems, and smart healthcare devices, facilitate real-time data collection, remote patient management, and preventive care. These interconnected devices provide healthcare professionals with valuable insights into patient health status, enabling proactive interventions and personalized healthcare delivery.

This special issue aims to explore the cutting-edge research, methodologies, and applications at the intersection of mathematics, artificial intelligence, and IoT in medicinal chemistry and healthcare. It provides a platform for researchers, scientists, and practitioners to share their findings and advancements in this rapidly evolving field. The contributions in this special issue will encompass a wide range of topics,

including mathematical modeling and simulations in drug discovery, AI-driven approaches for personalized medicine, IoT-enabled healthcare devices and systems, and data analytics for healthcare management. By bringing together experts from diverse disciplines, this special issue will foster interdisciplinary collaborations and stimulate further advancements in medicinal chemistry and healthcare. It will provide a comprehensive overview of the latest research and developments, addressing both the scientific and practical implications of harnessing mathematics, artificial intelligence, and IoT in improving patient care, optimizing drug development processes, and shaping the future of healthcare systems. Hence, the integration of mathematics, artificial intelligence, and IoT has the potential to revolutionize medicinal chemistry and healthcare. This special issue will serve as a platform for disseminating novel research, fostering collaborations, and inspiring further innovations in this exciting and rapidly evolving field.

List of topics included:

- Mathematical modeling and simulations for drug discovery and optimization
- Machine learning algorithms for drug repurposing and virtual screening
- Predictive modeling for drug-target interactions and pharmacokinetics
- IoT-enabled biosensors for real-time monitoring of biomarkers
- AI-driven analysis of medical imaging data in drug development
- Computational approaches and modeling for predicting adverse drug reactions and drug safety using (or without using) IoT data
- Graph theoretical analysis to discover hidden relations between drugs and disease
- Graph theoretical analysis of complex networks in brain

Important Dates

Call for papers: September 2023
Submission Deadline: 30 June 2024
Publication: All accepted papers will be published in volume 22 (2024)

How to submit

The authors are kindly invited to register at our paper processing system and submit their contribution (both original papers or reviews are welcome) using a special track established for this special issue: Section/Category – "SI Advancements at the Nexus of Mathematics, Artificial Intelligence, and IoT in Medicinal Chemistry and Healthcare". We offer a 20 % discount on publication on this special issue. All manuscripts will undergo the standard peer-review process (single-blind, at least two independent

reviewers) and will be treated in the same way as other regular articles (indexing, abstracting, immediate publication, etc.). Instructions for authors are available here.

In case of any questions please contact Open Chemistry Managing Editor:

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