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Quantitative Structure Activity Relationship (QSAR):

Fundamentals, Methodologies and its Practical Utilizations

Edtitor

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Preface

Quantitative Structure-Activity Relationship (QSAR) represents an intriguing domain that integrates chemistry, biology, and computer science. This book serves as an extensive resource for comprehending the principles, methodologies, and applications of QSAR in areas such as drug development, environmental science, and other relevant fields.

In a time when drug discovery and environmental protection are critically significant, QSAR emerges as an invaluable instrument that assists researchers in forecasting the biological activity and characteristics of chemical compounds based on their structural attributes. By establishing a quantitative correlation between the chemical structure of compounds and their biological effects, QSAR facilitates the systematic design of novel and effective drugs, as well as the assessment of the toxicity and environmental behavior of various chemicals.

This publication aims to be a significant resource for students, researchers, and professionals eager to explore QSAR and its various applications. It encompasses an extensive array of subjects, such as molecular descriptors, mathematical modeling, validation methods, and case studies that demonstrate the effective use of QSAR across different scientific fields.

With straightforward explanations and illustrative examples, readers will acquire a comprehensive understanding of the processes involved in the development, evaluation, and practical application of QSAR models.

This book further underscores the necessity of stringent validation protocols in QSAR studies to guarantee the dependability and predictive accuracy of the models developed. Adhering to the best practices presented in this text will enable researchers to improve the quality and trustworthiness of their QSAR predictions, thereby facilitating more informed decision-making in the realms of drug discovery and chemical risk assessment.

As the QSAR field progresses with innovations in computational chemistry and machine learning, it is essential for researchers to remain informed about the latest developments and methodologies. This book seeks to connect theoretical concepts with practical applications in QSAR, providing readers with the essential knowledge and skills to effectively utilize this influential approach in their research activities.

The book addresses a wide range of subjects, including the historical development of QSAR, the molecular descriptors utilized in QSAR modeling, the processes for selecting training and test datasets, various approaches to model development, as well as validation and evaluation techniques. It also explores Hansch analysis, free Wilson analysis, and advanced QSAR methodologies. Additionally, the text discusses the application of QSAR in drug design and discovery, toxicology, environmental chemistry, materials science, agrochemicals, and industrial uses. Specific topics include COX II inhibitors,

carboxylesterase inhibitors analyzed through multiple linear regression, substituted N,N-diphenyl urea derivatives functioning as CCR5 receptor antagonists, an external validation study of carboxylesterase inhibitors, the challenges and future prospects in QSAR modeling, software and tools relevant to QSAR, and the examination of Isatin derivatives as selective inhibitors of carboxylesterases using partial least square regression (PLSR).

I extend my sincere appreciation to Dr. M. Prakash of Excellent Publishers for their steadfast support and generous collaboration in facilitating the prompt release of this edition. Additionally, I wish to convey my heartfelt thanks to my wife, Mrs. Nidhi, whose constant support and encouragement have served as a beacon throughout the writing process. Her faith in my vision and her unwavering patience have rendered this undertaking not only achievable but also profoundly rewarding.

I cordially invite you to join us on this enlightening journey, where scientific exploration meets practical implementation, and the quest for improved pharmaceuticals fuels innovation and discovery. We hope this experience will spark your interest in the molecules that influence our environment and motivate you to imagine the potential advancements in the quest for a healthier future. Any suggestions for enhancing the book's value will be sincerely considered for inclusion in future editions.

In summary, the Quantitative Structure-Activity Relationship (QSAR) represents a crucial advancement in the methodologies employed for the design, testing, and regulation of chemicals. This book acts as an extensive resource for understanding the complex domain of QSAR, equipping readers with the knowledge to leverage its capabilities in tackling significant issues in drug discovery, environmental science, and other fields. It is my aspiration that readers will consider this book to be enlightening, motivating, and essential in their quest for scientific achievement.

Dr.Sanmati Kumar Jain

About the Editor

Dr. Sanmati Kumar Jain holds the distinguished position of Professor of Pharmaceutical Chemistry at Guru Ghasidas Vishwavidyalaya, a Central University located in Bilaspur, Chhattisgarh, India. With an impressive teaching career that spans over twenty-three years at both the postgraduate and undergraduate levels, he has garnered a reputation as a highly skilled educator. Dr. Jain's significant contributions to pharmaceutical chemistry are reflected in his authorship of more than hundred research and review articles published in esteemed national and international scientific journals. Additionally, his mentorship has played a crucial role in the successful attainment of 30 M. Pharm. and 3 Ph.D. degrees.

Dr. Jain has been distinguished for his exceptional contributions to research, receiving accolades such as the Best Research Paper Award, the Best Researcher Award, and the International Outstanding Academician Award. His proficiency is further evidenced by his authorship of over 100 scientific articles published in esteemed journals, along with his contributions to 55 book chapters. Additionally, he has presented more than 30 research works at various national and international conferences and seminars.
His research initiatives have been bolstered by a project funded by AICTE (AICTE-RPS). In addition, he has authored two books and holds a total of 39 patents, of which 35 have been granted and 4 are published. Dr. Jain's primary research interests focus on Drug Design and Medicinal Chemistry.

Dr. Jain, a committed professional, holds active life membership in prestigious organizations including the Indian Pharmaceutical Association (IPA), the Association of Pharmaceutical Teachers of India (APTI), and the Society of Pharmaceutical Education and Research (SPER). Furthermore, he serves as a reviewer for various peer-reviewed international journals, contributing to the advancement of scientific knowledge in his field.