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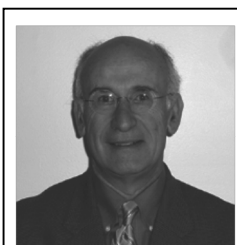
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EDITORIAL

New Experimental and Computational Tools for Drug Discovery: From Chemistry to Biology. Metabolomics, Pharmacokinetics, and Medicinal Chemistry. Part - IV

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Enabling technologies like Computational Chemistry, Bioinformatics, Combinatorial Chemistry, Metabolomics, Proteomics (OMICS in general), *etc.*, are expected to speed up the discovery of more efficient and safer drugs in Medicinal Chemistry. Recently, this journal has launched a series of special issues focused on this topic. The title of this series of special issues is: New experimental and computational tools for drug discovery: From chemistry to biology. Four (1-4) special issues are currently available. In these issues, experts from around the world discuss the state-of-art and/or report new methodologies. The methodologies focus on organic synthesis of new lead compounds, the *in silico* screening of new lead compounds, computational discovery of drugs from natural compounds isolated from plants, the repurposing of known drugs, re-engineering of cost-effective medicines, nano-systems for drug release, *etc.* The present issue is entitled: New experimental and computational tools for drug discovery: From chemistry to biology. Part 4. Metabolomics, Pharmacokinetics, and Medicinal Chemistry. Part 4 is the continuation of the series and provides six papers focused on new technologies used in drug discovery, but this time with emphasis on Metabolomics, Pharmacokinetics, and Medicinal Chemistry. The papers included in Part 4 can be summarized as follows:

Gross *et al.* point out that metabolomics experiments generate a rich array of complex high-dimensional data. They suggest that this may, in part, account for past and more recent incomplete replications of previously specified biomarker panels, especially if not adequately considered. Herein, they identify common impediments challenging the analysis of raw, targeted Metabolomic abundance data and review methods that may remedy these issues, based on personal experiences and those of others. In doing so, they propose an analytical pipeline suitable for the pre-processing of data prior to downstream biomarker discovery.

González-Domínguez *et al.*, present work focused on intervention and observational trials as complementary tools in Metabolomics. The authors provide a review of the literature regarding the application of metabolomics in assessing metabolic alterations with diabetes, diabetic insulin resistance, and provide an oral glucose tolerance test case study to demonstrate the complementarity of observational and interventional study designs.

Kataria *et al.*, presented a work on the role of morin in Neurodegenerative Diseases (NDDs). NDDs are known to cause profound effects on families and patients, and a tremendous financial burden on the healthcare system of most populations worldwide. Morin, being a super antioxidant compound, may help prevent and mitigate such disorders by suppression of reactive oxygen species (ROS) and through the inhibition of multiple additional targets. In this review, the authors discuss various neuropathological conditions and their specific target sites that may be relevant to morin's neurobiological mechanisms.

Bueso-Bordils *et al.*, focused on obtaining microbiological and pharmacokinetic predictive equations. They reviewed the state-of-art in the area and also reported a new study. Multi-linear regression (MLR) analysis was carried out in order to accurately predict physicochemical properties and biological activities on a group of antibacterial quinolones by means of a set of structural descriptors called topological indices. The aim of this work included developing prediction equations for such properties, after reviewing the relevant literature on antibacterial quinolones.

De Sousa Eduardo *et al.*, focus on the requirement of research related to new antimicrobial agents, as increasing numbers of microorganisms expressing antibiotic-resistance are emerging. In this paper, the authors review the topic and also provide veri-

fication for the activity of a phytoconstituent against *Escherichia coli* strains ATCC 25922 and *Staphylococcus aureus* ATCC 25923. The authors recommend further investigations, utilizing different methodologies assessing whether (+) - α -pinene may provide an effective compound in future antimicrobial therapy.

Srivastava *et al.*, focused on the inhibition of biofilm and virulence factors associated with *Candida albicans* by the partially purified secondary metabolites of *Streptomyces chrestomyceticus* strain ADP4. Despite several advancements in antifungal drug discovery, fungal diseases, such as Invasive Candidiasis (IC), remain associated with inordinately high rates of morbidity and mortality worldwide. In this paper, chemical profiling indicates that ADP4 secondary metabolites contained potentially beneficial alkaloids, flavonoids, polyphenols, terpenoids and triterpenes. The authors also report other experimental and computational findings.

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(Guest Editor)

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