Tentative Outline

Special Issue for Current Medicinal Chemistry

Guest Editor: Dr. Jelena Popović-Djordjević

Hot natural products for the prevention and treatment of diabetes mellitus (DM)

Aims & Scope:

Diabetes mellitus is a complex and heterogeneous metabolic disorder caused millions of deaths all over the world yearly. The estimations indicated that the subtypes of this disease (especially type 2 diabetes) is the main factor for patients' morbidity and mortality by 2050, and unfortunately, the currently available commercial anti-diabetic drugs could not prevent the pathogenesis of this disease entirely. With the reinvigorated interest on drug design programs for diabetes therapy, searching new methods, compounds and strategies for declining the financial burden of diabetes received the tremendous amount of attention from eligible researchers to attend the current scientific movement for fighting against diabetes.
An accumulating number of studies suggested that flavonoids, alkaloids, and their essential metabolites are deserving compounds for developing anti-diabetic drugs or decreasing diabetes risk factors among susceptible individuals. These naturally occurring secondary metabolites can regulate (or modulate) various types of signaling pathways involved in diabetes. On the other hand, recent advancements in computational methods for producing high-throughput outcomes enabled researchers to combine their experimental results with high-quality computational methods (especially molecular dynamics simulation and chemical quantum analysis) for removing, reducing or managing all unexpected errors with their results. This thematic issue aims to identify and review the latest achievements with the above-discussed secondary metabolites and new computational perspectives that can decline the risk factors of all types of diabetes mellitus from class 1 to gestational diabetes.

Subtopics:

- Pancreatic β-cell failure .
- Insulin secretion or sensitivity.
- Neuropathic diabetes.
- Insulin resistant in Alzheimer's disease.
- Hyperlipidemia.
- Hyperglycemia.
- Mitochondrial dysfunction.
- Immunological responses and inflammatory responses.
- Fatty liver and obesity.
- Diabetic-based cardiovascular dysfunctions.
- Engineered natural metabolites for diabetes.

- Formulating discussed metabolites for improving gestational diabetes.
- Quantum-based calculations for engineering enzymes involved in diabetes mellitus.
- Q-SAR analysis for drug-receptor interactions in diabetes mellitus.
- Prodrug synthesis and development by focusing on the main backbone of flavonoids or alkaloids
- Molecular dynamics simulation-based methods for screening anti-diabetic drug-like compounds
- High-throughput docking simulation strategies (both blind and fixed docking criteria) for diabetes therapy (Note that the editorial team will never publish papers with simple docking protocols. The docking outcomes should be validated by MD or quantum-based methods for at least 65ns of time. For special cases, the authors should give a powerful discussion for simple docking protocols).
- Green synthesis of novel anti-diabetic drug like compounds (For in vitro assays, the authors should provide enzymatic assays regarding the interaction of synthesized compounds with alpha-glucosidase, alpha-amylase enzymes. The mode of action of the studied compound should be validated with both docking and MD-simulation methods. For in vivo assays, the effect of synthesized compounds should be evaluated through measuring the expression of genes associated with diabetes. All in vivo-based papers should also provide information about the effect of compounds on diabetic inflammation).
- Characterization and pharmacological analysis of new flavonoid or alkaloid metabolites for diabetes therapy.
- Meta-analysis and systematic reviews regarding the effect of flavonoid/alkaloid metabolites on diabetes.
- Machine-learning methods for prediction the interaction of flavonoid/alkaloid metabolites with gene/protein networks involved in diabetes.

Keywords:

Diabetes mellitus, natural products, flavonoids, alkaloids, oxidative stress, signaling pathways, gene expression, in silico analysis.

Schedule:

April 2020