EDITORIAL

Current Trends in Enzyme Inhibition and Docking Analysis in Drug Design-Part-IV

This is the fourth part of issue which related to current trends in enzyme inhibition and docking analysis in drug design and consists of three papers.

The topics which are presented deal with the review on docking methods, advances in the development of 1,2,3-triazole-containing derivatives as potential antifungal agents, and extensive review on tuberculosis.

The first manuscript is an extensive review on antifungal activity of 1,2,3-triazole-containing derivatives underlying the period during 2015-2020. Hybridization of 1,2,3-triazole with other antimicrobial pharmacophores appears to be a judicious strategy to develop new efficacious anti-fungal candidates aiming at combating the emergence of drug-sensitive and drug-resistant infection disease. In this review hybrids of 1,2,3-triazole scaffold with fluconazole, coumarines, benzimidazole/imidazoles, pyrazoles, oxindole/indoles, chromene/pyranes, quinazoline, sugar, hetero/benzotriazoles are discussed. Accordingly, a number of 1,2,3-triazole-incorporating hybrids such as cefatrizine, tazobactam and radezolid have already been demonstrated efficacy and are already adopted as marketed antimicrobial drugs for the treatment of antibacterial infections. Hybrid triazoles appeared to possess the holding potential to overwhelm drug cross resistance and subsequently serve as promising candidates for the development of new antifungals. This review embraces the latest advances of the development of 1,2,3-triazole hybrids as potential fungicidal agents. Number of them revealed exceptional efficacy in most instances equivalent or superior to the corresponding reference marketed drug against both drug-sensitive and drug-resistant pathogens, corroborating the potential of 1,2,3-triazole hybrids as antifungal drug candidates [1].

The second paper is a review dealing with different types of docking programs. They include docking of non-covalent small ligands, protein-protein docking, supercomputer docking, quantum docking, the new generation of the docking programs and the application of docking for covalent inhibitors discovery. Taking into account the threat of COVID-19 authors present here a short review of docking applications to discovery of inhibitors of SARS-CoV and SARS-CoV-2 target proteins including their own original result of the search for inhibitors of SARS-CoV-2 main protease using docking and quantum chemical post-processing. The conclusion is made that docking is extremely demanded in the fighting against COVID-19 at the process of development of antivirus drugs of the direct action on SARS-CoV-2 target proteins [2].

The last paper of this issue is an extensive review on tuberculosis (TB) were pathogenesis of TB, current global and emergence of drug resistant, several molecular mechanisms of drug resistance, acquired resistant mechanisms, newly approved drugs, advancements in the clinical development of newer anti-TB drugs, novel compounds, repurposed drugs, search for new drug regimens against DS-TB and DR-TB, tyrosine kinase and many other aspects are discussed. The DR-TB exhibits the greatest threat to derail the insubstantial TB control programmes across the globe [3].

Finally I would like to thank all authors who contributed to this issue “Trends in enzyme inhibition and docking analysis in drug design”.

REFERENCES


Prof. Athina Geronikaki
(Guest Editor)
Member of Mediterranean And European Academies of Science and Arts
School of Pharmacy, Aristotle University of Thessaloniki, Thessaloniki 54124, Greece
Tel: +302310997616
Fax: +302310997612
E-mail: geronik@pharm.auth.gr