Jorge Galvez et al., J Pharm Drug Deliv 2019, Volume 8
DOI: 10.4172/2325-9604-C1-039

Novel antifungal drugs design by molecular topology

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Some species of fungi act as pathogens against both mammals and plants. The search for new effective antifungals against these pathogenic strains constitutes one of the priority objectives of the pharmaceutical and phyto sanitary industry, since deadly diseases may arise. However, the problems of the antifungals and fungicides currently available are basically two: On the one hand they are not exempt from toxicity to the host and on the other they generate resistance in more or less long terms. The objective of the present work is the search for new antifungals that follow new, more effective mechanisms of action with lower toxicity. This search is done by molecular topology, a method that has shown extraordinary efficacy in the design of new drugs. In this sense, the MOAs related to the inhibition of chitin formation of fungi are very attractive, among other reasons because some of them stimulate the immune system of the host, which is thus able to defend the host against the fungus. In addition, said MOAs are less susceptible to the development of resistance by fungi. As a result, a set of compounds potentially effective in the inhibition of chitin formation and of possible future utility as drugs and/or phyto sanitary products is proposed.

Figure : The main paradigm of Molecular Topology. Transform chemical objects (molecules) in numbers

Recent Publications:

1. Zanni R, Galvez-Llompart M, Morell C, Rodríguez-Henche N, Díaz-Laviada I, Recio-Iglesias M C, Garcia-Domenech R and Galvez J (2015) Novel cancer chemotherapy hits by molecular topology: dual Akt and Beta-catenin inhibitors. PLoS One. 10(4):e0124244.

2. Vincent Blay, Jesús Gullón-Soleto, María Gálvez-Llompart, Jorge Gálvez, and Ramón García-Domenech (2016) Biodegradability prediction of fragrant molecules by molecular topology. ACS Sustainable Chem. Eng. 4(8):4224-4231.

3. Zanni R, Galvez-Llompart M, Machuca J, Garcia-Domenech R, Recacha E, Pascual A, Rodriguez-Martinez J M and Galvez J (2017) Molecular topology: a new strategy for antimicrobial resistance control. European Journal of Medicinal Chemistry 137:233-246.

4. Jorge Galvez, María Galvez-Llompart, Riccardo Zanni and Ramón García-Domenech (2017) Molecular topology as a powerful tool for searching for new repellents and novel drugs against diseases transmitted by mosquitoes. Computational Design of Chemicals for the Control of Mosquitoes and Their Diseases 107-138.

5. R Zanni, M Galvez-Llompart, I Garcia-Pereira, J Galvez and R Garcia-Domenech (2018) Molecular topology and QSAR multi-target analysis to boost the in silico research for fungicides in agricultural chemistry. Molecular Diversity 1-9.

Biography

Jorge Galvez is Full Professor in Physical Chemistry and Director of the Molecular Topology and Drug Design Research Unit at the University of Valencia (Spain). He authored over 200 articles, 100 communications and 6 patents of new drugs designed or selected by molecular topology. He is member of the Spanish Royal Society of Chemistry, the Academy of Medicine of Valencia, the International Academy of Mathematical Chemistry (Founder Member), the European Academy of Mathematical Chemistry (Founder Member) and the Spanish Society of Green Chemistry. He has leaded the discovery of some 200 new hit-lead compounds in cancer, Alzheimer, malaria, etc.

Notes: