

Naturally Occurring Chemicals in Biopesticides' Resistance Control through Molecular Topology

Authors : Riccardo Zanni, Maria Galvez-Llompart, Ramon Garcia-Domenech, Jorge Galvez

Abstract : Biopesticides, such as naturally occurring chemicals, pheromones, fungi, bacteria and insect predators are often a winning choice in crop protection because of their environmental friendly profile. They are considered to have lower toxicity than traditional pesticides. After almost a century of pesticides use, resistances to traditional insecticides are wide spread, while those to bioinsecticides have raised less attention, and resistance management is frequently neglected. This seems to be a crucial mistake since resistances have already occurred for many marketed biopesticides. With an eye to the future, we present here a selection of new natural occurring chemicals as potential bioinsecticides. The molecules were selected using a consolidated mathematical paradigm called molecular topology. Several QSAR equations were depicted and subsequently applied for the virtual screening of hundred thousands molecules of natural origin, which resulted in the selection of new potential bioinsecticides. The most innovative aspect of this work does not only reside in the importance of the identification of new molecules overcoming biopesticides' resistances, but on the possibility to promote shared knowledge in the field of green chemistry through this unique in silico discipline named molecular topology.

Keywords : green chemistry, QSAR, molecular topology, biopesticide

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