

Special Issue

SAR "Out of the Box": From Pharmacological Drug Design to Cellular Activity of Biomolecules from Plants and Bacteria to Animals

Message from the Guest Editors

Dear colleagues, Classically, the structure–activity relationship (SAR) is an approach designed to find relationships between the chemical structure (or structural-related properties), 3D structure, and biological activity of studied compounds, as defined by Crum-Brown and Fraser in 1865. This is because similar compounds should have similar physico-chemical and biological properties. If this notion is almost always associated with pharmacological drug design and the assessment of side effects of existing compounds in the human health field, it can actually be extended to a large number of bioactive molecules exerting a number of cellular activities. For instance, interactions between plant or bacterial secondary metabolites as well as proteins belonging to the same structural family could have differential activities at the level of the cellular membrane. This Special Issue is dedicated to widening the notion of SAR to a more general concept concerning the relationships between structure and activity of bioactive molecules belonging to all living organisms, whether they have pharmacological effects or not.

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