**« SAR out of the box »: insights into the relations between molecular structure, membrane interaction and activity of biomolecules using complementary biophysical tools**

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**Abstract**

Classically, structure-Activity Relationship (SAR) is an approach designed to find relationships between chemical structure (or structural-related properties), 3D structure and biological activity of compounds of interest, 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 to pharmacological drug design and 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, notably at the level of the cellular membrane.

In this talk, I propose to overview some complementary “*in vitro*” and “*in silico*” biophysical approaches (Deleu et al, 2014) that can give information about the relation between chemical structure (or structural-related properties), 3D structure and membrane activity of bioactive molecules.

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**References**

Deleu,M, Crowet, JM, Nasir, MN, Lins, L. Complementary biophysical tools to investigate lipid specificity in the interaction between bioactive molecules and the plasma membrane, 2014, BBA, 1838, 3171-3190