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Editorial

Nuclear Receptors: From Drugs to Food, and from *In Silico* to *In Vitro*

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In silico techniques are an emerging field in Food Science. *In silico* means done using computer, also defined as dry experiments while traditional lab experiments are commonly defined as wet experiments. These techniques come from Medicinal Chemistry and Computational Chemistry where they have been known for many decades.

Common applications of informatics techniques in Food Science are traditionally statistics and QSAR (Quantitative Structure Activity Relationship) approaches. However, massive screening of databases of chemicals, docking and scoring of most promising chemicals into known receptors are not common applications in food science, i.e. food safety, food security, food toxicology, predictive toxicology, etc. One of the most important questions we would like to answer is: could we merge *in silico* and *in vitro* tests for a better food safety?

Because we live in a world of chemicals where more than 110 million chemical compounds are known to exist to date (source: CAS, Chemical abstract Service), we are exposed to many of these chemicals during our lifetime. Unfortunately, it is not realistic to think we can check the safety of such huge number of compounds.

If indeed it is true that humans produce about 500~1000 chemicals every year, we have to be conscious about the potential of some of them to negatively affect our metabolic and physiological pathways, and about the possibility to encounter potential disruptors in our daily life. Unfortunately, this huge number of chemicals is too big to be investigated by means of standard experimental approaches, as *in vitro* and *in vivo* test, in particular if we consider the number of possible associated metabolites. Computational methods could represent a valuable alternative to dramatically reduce the number of potential disruptors to be experimentally tested.

Nuclear Receptors represent an important class of potential targets for medicinal chemistry and food safety; thus, computational techniques, widely applied in medicinal chemistry field, can represent valuable tools also in food science. Food additives, food contact materials, mycotoxins, plasticizers and their metabolites can interact with this class of receptors acting as endocrine disruptors. *In silico* methods can predict these potential interactions between a ligand (food additive, mycotoxins, food contact material, etc.) and a receptor of known 3D structure, representing a unique way to test the effect of a huge amount of chemicals without *in vitro* tests. *In vitro* tests must be applied only for molecules predicted as good possible interactors. It should be stated, however, that *in silico* interaction prediction is not an absolute certainty of the real activation of the receptor made by the ligand, where binding of a ligand within a cavity of a receptor is not always synonymous with a receptor activation, it is necessary to understand the whole complex biochemical pathway.

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This thematic issue of Nuclear Receptor Research is an excellent opportunity to define the state of the art of the application of computational techniques in the nuclear receptor field and to investigate the potentiality of computational methodologies in predicting nuclear receptor interaction not just with drugs but, most of all, with nutritional agents, mycotoxins, food contact chemicals, plasticizers, etc. We asked the authors to be critical, to state pros and cons of different methodologies, as well as success and limits of the current research. We are confident that the contributing authors have expressed their opinion and supplied the readers an exhaustive and "real" overview of nuclear neceptors *in silico/in vitro* investigations.

This thematic issue contains papers about, but not limited to, the following areas: the interaction of nuclear receptor with possible endocrine disruptors, and the development and application of computational approaches for predicting these interactions and eventually reducing or even eliminating the use of *in vivo* tests. The main subtopics covered in this issue are: a general overview on NR family, NR signaling maps, NR as target for diseases, NR and mycotoxins, NR and pollutants (xenobiotics), virtual screening and docking/re-scoring techniques, QSAR and read across methods, NR and natural compounds, and *In silico/in vitro* tests.

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