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In-silico approach in risk assessment of nutraceutical properties
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Abstract
Dietary supplements, including those containing botanical ingredients and botanical-derived compounds, have been marketed to consumers globally for many decades. However, the legislative framework for such products remains inconsistent across jurisdictions internationally. A common problem, concerning these nutraceutical products, is deficient information and lack of data for assessing the hazards posed to human health. The main objective is to explore the use of in silico tools in a risk assessment context of nutraceutical product, to relate properties of the molecular structure to the toxic effect of the chemical substance, by using principles and methods of computational chemistry. Further consideration of the actual impact of adverse events arising from nutraceutical food supplement usage will be helpful in guiding such issue as a potential for misidentification, and adulteration of botanical supplements by pharmacologically active substances. © 2019 The Authors.

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In silico; Nutraceutical; QSAR; Risk assessment; SAR

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nutraceutical; biological activity, chemical structure, computer model, dietary supplement, drug manufacture, drug safety, Food and Drug Administration, Organisation for Economic Co-operation and Development, pharmacology, quantitative structure activity relation, risk assessment, Short Survey, toxicity testing

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