

Computational assessment of the toxicological profiles of various chemicals to which humans are exposed. A review

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Abstract. This study contains a brief description of the common computational methods used in the prediction of the toxicological effects of chemical substances, and a synthetic review of the literature on the results of computational studies on the prediction of the toxicological effects of substances to which humans are frequently exposed: food additives, food contaminants, cosmetic ingredients, drug-related compounds and pesticides. The advantages and limitations of using current computational toxicology in assessing the toxicity of chemicals are also discussed.

Keywords: pharmacokinetics; ADMET profile; food additives; pesticides; drug-related compounds.

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