

An Insight-Based Computational Approaches to Estimate Molecular Weight Distribution, Allergenicity and Immunological Aspects, Toxicity Profile, Possible Biodegradation, Persistence and Bioaccumulation Factor of Four Phyto-Compounds

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Clinical pharmacology and toxicology are considered nowadays two complementary and indispensable medical disciplines that allowed clinicians to achieve the optimal therapeutic effect of a several substance, but also to characterize their toxicity threshold. The contribution of bioinformatics tools and databases in these two fields has provided key elements, sometimes impossible to explain during early clinical phases. In this context, some computational approaches were used in this work to investigate the molecular weight distribution (MWD), allergenicity, toxicity profile, possible biodegradation, persistence and bioaccumulation factor of four natural compounds. Results revealed that MWD indices of compound 2 and 3 were the best among the tested compounds. However, the route of administration of compound 1 could be considered the safest for rats, especially the oral, intravenous and subcutaneous ways, in which LD₅₀ values were the best, comparing to the other compounds. The two allergenicity tests revealed that the four phyto-compounds could be considered non-allergen agents and may not present any drug toxicity risks. Concerning cytotoxicity, compound 4 exhibited the best cytotoxic effect among these compounds with a corresponding value of Pa = 0.782 against colon carcinoma (HCT-116) cell line. The four bio-compounds could be toxic for avian species but non-toxic for *Daphnia magna*, a key aquatic species. Compound 1 exhibited the lowest bioaccumulation factor value (0.17). All compounds were inactive against Tox21-Stress response pathways, but compound 2 and 3 could potentially be immunotoxic. Finally, all tested compounds may possess a non persistent profile, while only compound 1 and 4 could possibly be

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