Molecular Modeling of 11β-hydroxysteroid dehydrogenase type 2 inhibition, glucocorticoid antagonism, and mineralocorticoid agonism for predicting chronic toxic effects of phytochemicals

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A large number of people around the globe is using plant constituents as food and/or as medicine in their daily life [1, 2]. Most of them are unaware of potentially harmful effects of used plant constituents. 11β-hydroxysteroid dehydrogenase is the enzyme which catalyzes the interconversion of cortisone and cortisol in humans [3]. Our objective is to predict the chronic immunologic and cardiovascular toxicity of commonly used plant constituents, inhibiting11β-hydroxysteroid dehydrogenase type 2, mineralocorticoid activation and glucocorticoid blockade. Pharmacophore based virtual screening will be used for selection of putatively active compounds. Widely used phytochemicals will be evaluated by *in vitro* methods after filtering by *in silico* models. Therefore we propose to identify the toxicological effects of commonly consumed plant constituents.

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