

Antimycotic and antioxidant effects of water extract from inflorescences of industrial hemp: results from *in silico*, *in vitro* and *ex vivo* studies

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Abstract: Industrial hemp (*Cannabis sativa*) is traditionally cultivated as a valuable source of fibers and nutrients. Multiple studies also demonstrated antimicrobial, anti-proliferative, phytotoxic and insecticide effects of the essential oil from hemp female inflorescences. On the other side, only a few studies explored the potential pharmacological application of polar extracts from inflorescences. In the present study, we investigated the water extract from inflorescences of industrial hemp Futura 75 variety, from phytochemical and pharmacological point of view. The water extract was assayed for phenolic compound content, radical scavenger/reducing, chelating and anti-tyrosinase effects. Through an *ex vivo* model of toxicity induced by lipopolysaccharide (LPS) on isolated rat colon and liver, we explored the extract effects on serotonin, dopamine and kynurenine pathways and the production of prostaglandin (PGE)₂. Anti-proliferative effects were also evaluated against human colon cancer HCT116 cell line. Additionally, antimycotic effects were investigated against *Trichophyton rubrum*, *Trichophyton interdigitale*, *Microsporum gypseum*. Finally, *in silico* studies, including bioinformatics, network pharmacology and docking approaches were conducted in order to predict the putative targets underlying the observed pharmacological and microbiological effects. Futura 75 water extract was able to blunt LPS-induced reduction of serotonin and increase of dopamine and kynurenine turnover, in rat colon. Additionally, the reduction of PGE₂ levels was observed in both colon and liver specimens, as well. The extract inhibited the HCT116 cell viability, the growth of *T. rubrum* and *T. interdigitale* and the activity of tyrosinase, *in vitro*, whereas *in silico* studies highlighting the inhibitions of cyclooxygenase-1 (induced by carvacrol), carbonic anhydrase IX (induced by chlorogenic acid and gallic acid) and lanosterol 14- α -demethylase (induced by rutin) further support the observed pharmacological and antimycotic effects. The present findings suggest female inflorescences from industrial hemp as high quality by-products, thus representing promising sources of nutraceuticals and cosmeceuticals against inflammatory and infectious diseases.

Keywords: Industrial hemp; Dermatophytes; Oxidative Stress; PGE₂;

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