

**SCREENING OF CONSTITUENTS OF THE ESSENTIAL OIL OF *SATUREJA MONTANA*
IN THE POTENTIAL TREATMENT OF COVID 19 USING COMPUTATIONAL
METHODS**

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Constituents of essential oil of *Satureja Montana* (SM) were investigated in aim of elucidation of potential activities on viruses that can be transcribed in genetic material, such as *SARS CoV 2* and *HIV*. Chemical structures of constituents (34) of the SM essential oil were built and geometry optimized using *ChemDraw ultra 8.0* and *Chem3D Pro 8.0* programs. Prediction of potential interactions for each constituents with large number of targets was performed by *SwissTargetPrediction* program. Results indicate that constituents, with certain level of probability, can be involved in interactions with some targets significant for antiviral activity, in direct or indirect mode, such are adenosine receptors type 1, UDP-glukuronosyltransferases, receptor-dependent transport channels, peroxisome-proliferator activated receptor alpha, GLI 2, as well as some other targets. Since in this work just constituents of SM essential oil were investigated, further studies should be directed towards investigation of full content of SM, in various solvents, for elucidation of mechanisms of action of this plant in therapy of viremias, presumably for supposed inhibition of transcription of viruses.

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SKRINING KONSTITUENATA ETARSKOG ULJA *SATUREJA MONTANA* U POTENCIJALNOM LEČENJU COVID 19 PRIMENOM KOMPJUTERSKIH METODA

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Konstituenti esencijalnog ulja *Satureja Montana (SM)* ispitivani su u cilju razjašnjenja njihovog potencijalnog delovanja na viruse koji se mogu inkorporirati u genetski materijal, kao što su *SARS CoV 2* i *HIV*. Hemijske strukture konstituenata (34) esencijalnog ulja *SM* su prikazane i optimizovane korišćenjem programa *ChemDraw ultra 8.0* i *Chem3D Pro 8.0*. Predviđanje potencijalnih interakcija za svaki konstituent sa velikim brojem bioloških targeta izvršeno je u programu *SwissTargetPrediction*. Rezultati ukazuju na to da konstituenti, sa odgovarajućom predviđenom verovatnoćom, stupaju u interakcije sa određenim targetima koji mogu biti od značaja za dejstvo na viruse na posredan ili neposredan način, od kojih su najznačajniji adenoziński receptor tipa 1, UDP-glukuronozil transferaza, receptor-zavisni transportni kanali, alfa receptor aktiviran proliferatorom peroksizoma, GLI 2, kao i neki drugi targeti. S obzirom da su u ovom radu ispitivani samo konstituenti esencijalnog ulja *SM*, potrebno je izvršiti dodatne studije konstituenata ukupnog sadržaja *SM*, u različitim rastvaračima, radi sagledavanja potencijala ove lekovite biljke u terapiji viremija, pre svega pretpostavljenoj inhibiciji transkripcije virusa.

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