

## ***Abstract***

On the one hand, this study is focused on a phytochemical and biological investigation of *Centaurea involucrata* Desf., an Algerian species that has never been the subject of phytochemical investigation. On the other hand, the chemical composition of the essential oils of *Thymus algeriensis*, *Marrubium vulgare*, and *Senecio massaicus* aerial parts, as well as the assessment of the biological activities of the last specie's essential oil.

The petroleum ether extract of *C. involucrata* was studied using GC-MS, and 13 compounds were identified, the majority of which have a wide range of activities. The HPLC/DAD analysis of phenolic acids and flavonoids of chloroform and *n*-butanol extracts showed the presence of seven phenolic acids and three flavonoids. While, the LC-MS/MS analysis of the ethyl acetate extract showed the presence of 26 phenolic compounds.

Using various chromatographic separation methods, 11 compounds were isolated from the ethyl acetate extract. The structures of these compounds were elucidated by combining the data of UV spectra, NMR (<sup>1</sup>H, <sup>13</sup>C, DEPT, COSY, HSQC, HMBC, and NOESY) and by comparison with data from the literature.

The biological activity tests on the extracts, which included antioxidant, antimicrobial, and anticancer activity, showed that the species has notable antioxidant and anticancer activities.

The chemical analysis of the essential oil of the aerial parts of *T. algeriensis*, *M. vulgare* and *S. massaicus* by GC-MS, showed that the major constituents are: germacrene D (29.6%), β-caryophyllene (11.0%) for *T. algeriensis*, β-bisabolene (36.3%) for *M. vulgare* and *m*-cymene (30.5%), *n*-hexadecanoic acid (14.8%), and docosane-11-decyl (10.43%) for *S. massaicus*.

The essential oil of *S. massaicus* has on one hand moderate antioxidant activity, and the other hand has a higher power of inhibition against butyrylcholinesterase (BChE) compared to acetylcholinesterase (AChE).

The molecular docking study shows that the compounds docosane-11-decyl and octaethylene glycol monododecyl ether exhibited a strong interaction against enzymes linked to Alzheimer's disease and against the main protease Covid-19 and endoribonuclease Nsp15.

Keywords: *Centaurea involucrate* Desf., essential oil, molecular docking, Covid-19, GC/MS, anticancer, anticholinesterase.