Summary

The genus Scleranthus L. (Caryophyllaceae, carnation family) encompasses perennial herbaceous plants encountered mainly in dry and sandy habitats of the temperate climate zone. A comprehensive analysis of two selected species was carried out in response to the scarcity of reports on the chemical composition and biological activity of these plants. The species of interest included Perennial knawel (S. perennis L.) and Annual knawel (S. annuus L.). The first stage of the study was dedicated to the spectrophotometric determination of total polyphenolic compounds as well as phenolic acids and tannins. Qualitative assessment of the content of polyphenolic compounds was performed in extracts and fractions collected from examined species. The results show that acetate fractions were the richest source of flavonoids in all the test samples of both test species. In-depth chromatographic analysis using LC-PDA-MSⁿ facilitated the identification of twenty-four compounds, predominantly C-glycosidic flavone derivatives and phenolic acid derivatives. As a result of attempts at isolation and structural identification of components of the aerial parts of S. perennis, a total of nine chromatographically homogeneous substances were obtained. Compounds were subjected to structural characterization by means of spectral and spectrophotometric studies (UV, IR, MS, ¹H, ¹³C NMR, DEPT, COSY, HSQC, HMBC). Four of these compounds were found to be novel, first-reported floral flavonoids; these included 5,7,3'trihydroksy-4'-acetoxyflavone 8-C-β-D-xylopyranoside-2"-O-glucopyranoside (scleranthoside 5,7,3'-trihydroxy-4'-methoxyflavone 8-*C*-β-D-xylopyranoside-2"-*O*-glucopyranoside A), (scleranthoside B), 5,7-dihydroxy-3'-methoxy-4'-acetoxyflavone 8-C-β-D-xylopyranoside-2"-O-(4"'-acetoxy)-glucopyranoside (scleranthoside C), and 5,7-dihydroxy-3'-methoxy-4'acetoxyflavone 8-C-β-D-arabinopyranoside-2"-O-(4"-acetoxy)-glucopyranoside (scleranthoside D). Moreover, the presence of an isolated phenolic derivative, apiopaeonoside, was first described for the family Caryophyllaceae. The novel analytical method of HPLC-PDA facilitated simultaneous quantitative evaluation of nine isolated compounds within the extracts and fractions from the knawel species. 5,7-dihydroxy-3'-methoxy-4'-acetoxyflavone 8-C-β-D-xylopyranoside-2"-O-glucopyranoside was found to be the most predominant component. The next stage of the study concerned the evaluation of the biological activity of extracts, fractions and pure compounds with regard to their antioxidative properties (DPPH, FRAP, CUPRAC, ABTS) and their potential collagenase inhibition activity. In the in vitro test model, methanolic extracts and acetate fractions obtained from both species of interest were found to have the highest percentage inhibition of collagenase activity at test concentrations. The final stage of the study on compounds isolated from Knawel species involved the comparison of their structure and tyrosinase inhibition activities with those of the other forty flavonoids selected for research purposes. The comparison of IC₅₀ values, molecular docking (in silico), and statistical analysis outcomes facilitated the identification of characteristic flavonoid structures that affect tyrosinase inhibition activity. Kinetic studies of the most active compounds have led to the first determination of a noncompetitive type of inhibition exerted by two rare floral flavonoids – isookanin and robinetin.