P-004: Step-by-step filter: quantitative characterization of *Arnicae flos* by NIR spectroscopy

Daniela Ivanova[1], Vera Deneva[1], Dimitrina Zheleva-Dimitrova[2], Vesela Balabanova-Bozushka[2], Daniela Nedeltcheva-Antonova[1], Reneta Gevrenova[2], Liudmil Antonov[1]

[1]*Institute of Organic Chemistry with Centre of Phytochemistry, Bulgarian Academy of Sciences, Sofia, Bulgaria*
[2]*Faculty of Pharmacy, Medical University of Sofia, Sofia, Bulgaria*
E-mail: lantonov@orgchm.abs.bg

The tremendous importance of the mountain arnica for the pharmaceutical market and the variations in composition and respectively pharmacological activity require the use of reliable analytical techniques for qualitative and quantitative characterization as well as for fast monitoring of the raw material. In the present study, we aim to investigate the prospect of applying a non-destructive NIRS method for the rapid quantification of pharmacologically relevant components (phenolic acids, flavonoids and sesquiterpene lactones) of *Arnicae flos* using HPLC as a reference method. In the chemometric processing of the spectral data, along with the traditionally used Golay-Savitzky differentiation procedure [1] we use a newly developed "step by step" filter [2], where the spectral distortion is substantially reduced. To our best knowledge, this is the first comparative study of these two pre-processing approaches in the investigation of dried medicinal plants.

The obtained results have shown that the Step-by-step filter derivatives provide better signal-to-noise ratio at lower convolution window. As a result, better calibration for the content of protocatechuic acid, chlorogenic acid, caffeic acid, p-cumaric acid, ferulic acid, isoquercitrin and quercetin was obtained by step-by-step filter derivatives comparing to the direct raw spectra processing and the Golay-Savitzky approach.

References

[1] SAVITZKY, A., and M. J. E. GOLAY, 1964: Analytical Chemistry, **36**, 1627–1639.
[2] ANTONOV, L., 2017: Journal of Near Infrared Spectroscopy, **25**, 145–148.