**Possibilities of hybride quadrupole-orbital trap mass spectrometer for screening and identification of pharmaceuticals and their transformation products in soils and sediments**

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Pharmaceuticals are recognized as emerging pollutants in aquatic environment. However, aplication of treated waste water or sediments for soil fertilization can pose significant risk for soil or undergroung water. Due to high variability of physico-chemical properties both soils and pharmaceuticals, mobility of this compounds vary too [[1](#_ENREF_1)]. Simirarly to pesticides, parent compounds with relatively high sorption to soil can be transformed by bacterias to more polar compounds with unpredictable ecotoxicological efect and better mobility in the matrix.

We studied stability and transformation of selected pharmaceuticals in different soil types. While the degradation rate is possible to determine as decrease of target compounds, investigation of transformation product and their further stability or degradation is almost impossible with conventional methods.

We present several approaches to reveal possible metabolites. Simple methods based on liquid chromatography with high resolution mass spectrometry in full scan were succesfull only for few transformation products. Using softwares for automated screen of possible transformation products (TPs) led to increase of detected TP but identity must be confirmed with high resolution product scan (HRPS) of MS/MS experiment. Besides of degradation experiment, possibilities of the screening method for high range of pharmaceuticals in soils and sediment extract were tested. High resolution full scan method (70000 FWHM) was combined with data dependent HRPS.

Compare to pesticides there is just a limited availability of standards or HRPS spectra for transformation products of pharmaceuticals. We would like to present possibilities of proper software for interpretation of HRPS spectra and compound identity confirmation.

References:

[1] R. Kodešová, R. Grabic, M. Kočárek, A. Klement, O. Golovko, M. Fér, A. Nikodem, O. Jakšík, Science of The Total Environment, 511 (2015) 435-443.

Acknowledgment:

The authors acknowledge the financial support of the Czech Science Foundation (Project No. 13-12477S, Transport of pharmaceuticals in soils). Pharmaceutical concentrations were measured using devices financially

supported by the Ministry of Education, Youth and Sports of the Czech Republic, projects CENAKVA (No. CZ.1.05/2.1.00/01.0024) and CENAKVA II (No. LO1205 under the NPU I program).