Metabolite profiling of the hop flower (*Humulus Lupulus* L.) – focus on metabolites of medical interest

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The economic importance of hop is predominantly derived from its use in the brewing industry. As one of the four key ingredients of beer, the female flowers contribute significantly to its aroma. However, hop has also been acknowledged as medicinal plant for centuries. Phytotherapeutic hop preparations have long been used to treat nervous conditions, insomnia or indigestion. Hop contains several medicinally active components, with the focus of scientific attention primarily on prenylflavonoids. Numerous studies have already confirmed anti-inflammatory, antimicrobial and chemoprotective properties of xanthohumol (XN), and 8-prenylnaringinin (8-PN) has been shown to be a potent phytoestrogen.

Currently, the non-volatile metabolome of hop cones of different varieties, origins and harvest years is analyzed, and the contents of selected active ingredients and numerous other known and unknown metabolites will be determined. For this purpose, an LC-MS method was developed that allows quantification of these substances and simultaneous profiling.

Though the contents of the targets differ by orders of magnitude, the combination of reversed-phase liquid chromatography (RP-UHPLC) with mass spectrometry and UV-detection resulted in reproducible measurements of XN, 6- and 8-PN and multifidol glucoside on a single analysis platform. In addition, more than 4000 putative polar metabolites were detected in both positive and negative ionization mode of the mass spectrometer, allowing a comparative analysis of metabolite profiles.

Five sets of samples consisting of 995 specimens in total, including populations with high genetic and phenotypic variance as well as a F1-generation segregating with respect to XN-content are measured.

All profiled accessions were genotyped by sequencing in order to perform a genome wide association (GWAS) and to identify genetic markers related to metabolites or traits of interest in a future step.

The results of the study, genetic and metabolic markers for high value traits, should be used in marker assisted breeding programs for the development of high-quality hop products.