Abstract

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Title of Diploma thesis: HPLC-high resolution mass spectrometry analysis of *in vitro* and *in vivo* metabolism of scoparone

Scoparone is an active ingredient of *Artemisia scoparia*, a medicinal plant used in traditional Chinese medicine. It has been studied for various pharmacological effects such as upregulation of conjugation enzymes included in excretion of bilirubin, reduction of proinflammatory cytokines, lowering of plasma lipids levels and inhibition of platelet aggregation. In this thesis, metabolism of scoparone was studied by LC-MS method using Q-ToF device. Scoparone was incubated with liver microsomes obtained from 6 different mammal species to study *in vitro* oxidation. In total, six metabolites were detected in the incubation samples. Scopoletin and isoscopoletin were identified as major metabolites in every species, however, the rates of scoparone oxidation as well as a ratio of formed isoscopoletin and scopoletin varied. Furthermore, *in vivo* metabolites in human were studied in urine samples obtained from two healthy volunteers after oral administration of scoparone. Nine metabolites were detected in the urine samples in total, major metabolites being glucuronide and sulphate conjugates. The highest levels of metabolites were detected in the urine samples taken three hours after scoparone administration suggesting rapid elimination. Unfortunately, conjugation metabolites could not have been fully identified during this study, however, it has been proved that this LC-MS method is suitable for further research of scoparone metabolism both *in vivo* and *in vitro*.