Abstract:

Morphinan alkaloids belong to important class of compounds acting as painkillers. Understanding of the mechanism of their action is important for improved therapy using these alkaloids, for example, through the synthesis of new analogues with improved effect. The goal of this work is to summarize existing knowledge of these compounds including information about their biosynthesis in the plants and overall effect on the organism. The goal of the practical part of the work is a determination of the relative configuration of morphinan *N*-oxides produced by *in situ* oxidation of parent alkaloids using NMR spectroscopy and molecular modelling.

Relative configurations of both oxidized and non-oxidized forms of morphine, codeine and thebaine were analyzed using NMR spectroscopy. NMR spectra were analyzed to detect ratio of different N-oxide products *in situ*. These values were compared with results of DFT quantum chemical computation. Using correlation analysis, reliability of computational method was verified.

(in Czech)

Key words: NMR spectroscopy, morphine, codeine, thebaine, *N*-oxides, metabolism of alkaloids