

Abstract

Nguyen, T. P.: Isolation, Structural Analysis and *In Silico* Prediction of Selected ADMET Parameters of Alkaloids Isolated from *Croton linearis* Jacq. (Euphorbiaceae); Diploma Thesis, Charles University, Faculty of Pharmacy in Hradec Králové, Department of Pharmacognosy and Pharmaceutical Botany, Hradec Králové 2025, 93 pages.

The subject of this diploma thesis was the isolation and identification of alkaloids from the dichloromethane extract of *Croton linearis* Jacq. (Euphorbiaceae) and the subsequent *in silico* prediction of selected ADMET parameters. The alkaloids (+)-cularine, (+)-glaucine and (–)-laudanine were isolated from selected fractions (i.e. CL-CH₂Cl₂-7, CL-CH₂Cl₂-8 a CL-CH₂Cl₂-13) using chromatographic methods. The structure of the individual compounds was confirmed using GC-MS, LC-MS, NMR analyses and measurements of specific optical rotation. In the *in silico* evaluation, physicochemical properties (number of hydrogen bond acceptors and donors, total polar surface area, consensus logarithm of octanol/water partition coefficient), pharmacokinetic properties (gastrointestinal absorption, permeability across the blood-brain barrier, cytochrome inhibition and interaction with P-glycoprotein) and toxicological characteristics (oral LD₅₀, toxicity class) were predicted using the SwissADME and ProTox-3.0 software. All compounds met Lipinski's rule of five and Veber's rule. Based on the predicted data, the investigated alkaloids show a favorable pharmacokinetic and toxicological profile and may represent promising candidates for further research in the field of drugs targeting the central nervous system.

Key words: *Croton linearis*, alkaloids, isolation, structural analysis, ADMET *in silico* prediction