

# Abstract

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Title of diploma thesis: Matrix computations for mixtures and solutions

In this work, we determined drug concentrations from mixtures using multicomponent analysis without separating them. The condition was the knowledge of the molar absorption coefficients of individual drugs for certain wavelengths. To do this, we used tools from matrix calculations, especially the Moore-Penrose inverse, and we were interested in whether we would achieve more accurate results using standard, square systems or overdetermined systems of linear equations.

Based on the results, we came to the conclusion that there is no dependence between the accuracy of the results and the number of wavelengths used. Only in some cases did the results appear to be more accurate when using overdetermined systems with a higher number of wavelengths.

Keywords: mixtures, solutions, linear systems, least squares problems, Moore-Penrose pseudoinverses