

Title: **Evaluation of several equations for the deconvolution of overlapped chromatographic peaks, as user-defined functions in the MS Excel™ spreadsheet.**

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Date: September 2020

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When a multicomponent chromatography is carried out there is a high probability of overlapping or superposition between peaks, causing problems in the definition of their shape and therefore in the quantification of the different species to be determined. One of the factors responsible for this overlap is the asymmetry of the peaks, the most common being that observed at the tail of the peak.

In several fields of analytical chemistry, the problem of peak adjustment and resolution is very important. For this reason, there are currently many studies that try to adjust mathematical functions to UV-Vis absorption spectra or to chromatograms, for example; this type of mathematical application is known as peak deconvolution. From the deconvolutions, the information of the individual peaks can be obtained, even if they are overlapped. There are several functions that have been and continue to be studied to perform deconvolutions, the most used is the Exponentially Modified Gaussian (EMG) function, since it has demonstrated good efficiency in many cases.

In this work, the adjustment is studied and compared through mathematical functions such as EMG or derived from it, also developing a new variant (EMG_POLI) to be used under the MS-Excel™ spreadsheet. The peak parameters are optimised by means of an iterative non-linear regression algorithm.

The equation developed has been applied to chromatograms obtained by reverse phase chromatography (RP-HPLC) of mixtures of B vitamins (nicotinic acid, thiamine, and pyridoxine), as well as to their calibration.

Keywords: Liquid chromatography, deconvolution, function adjustment, EMG