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POSTER SESSION 580-2P

## **Reconstruction of Out-of-range Peaks Using Exponentially Modified Gaussian Peak Shape**

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Exponentially Modified Gaussian (EMG) peak shape [1] is widely used for peak approximation in chromatography. We constructed EMG peak deconvolution routine for chromatography, using combination of two EMG formulas [1,2] and linear optimization methods. This routine accounts for maximum linear range of the detector and can work with out-of range peaks.

Optimization routine is applied to reconstruction of out-of-range peaks, so that analyst can get an idea about area/height and concentration of such peaks. We found, that in many cases such reconstruction provides reasonable prediction error. This information helps in reducing number of chromatographic runs while method development and routine work. A possibility of reconstructing out-of-range peaks using pre-defined peak shape, obtained while calibration, is also discussed.

[1] McWilliam, I. G.; Bolton, H. C. Anal. Chem. 1969, 41, 1755-1762.

[2] Delley, R. Anal. Chem. 1985, 57, 388

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