Prediction of Retention Volumes and UV Spectra of Peptides in Reversed Phase HPLC

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Abstract—A method for calculating retention volumes of linear peptides with known primary structures and the values of their UV absorption at chosen wavelengths in reversed phase HPLC are described. These parameters are calculated for every peptide on the basis of the contributions of its amino acid residues determining its degree of retention and its UV spectrum. The contribution values are experimentally found from chromatograms of the free amino acids obtained by multiwavelength photometric detection under the conditions of the peptide chromatography. Thirty peptides have been chromatographed for the evaluation of the proposed method, and the correlation coefficients between the calculated and the experimental retention volumes have been found to be 0.95.

Key words: peptides, reversed phase high performance liquid chromatography, UV spectroscopy