

Predicting the behaviour of proteins in hydrophobic interaction chromatography:

2. Using a statistical description of their surface amino acid distribution

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This paper focuses on the prediction of the dimensionless retention time (DRT) of proteins in hydrophobic interaction chromatography (HIC) by means of mathematical models based on the statistical description of the amino acid surface distribution. Previous models characterise the protein surface as a whole. However, most of the time it is not the whole protein but some of its specific regions that interact with the environment. It seems much more natural to use local measurements of the characteristics of the surface. Therefore, the statistical characterisation of the distribution of an amino acid property on the protein surface was carried out from the systematic calculation of the local average of this property in a neighbourhood placed sequentially on each of the amino acids on the protein surface. This process allowed us to characterise the distribution of this property quantitatively using three main statistics: average, standard deviation and maximum. In particular, if the prope