Non-proteogenic amino acids database

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Abstract

Proteins represent a key tool for many biomedical and material engineering works. Since protein amino acid sequence has influence over the 3-D structure and protein function, developing new methods to control protein 3-D structure soars as a crucial point for future protein uses. Among those methods, the use of new non-proteogenic amino acids, many time called "synthetic amino acids", is the most important way to control such protein properties. Information about non-proteogenic amino acids is usually scattered among several publications concerning aspects like theoretical studies, synthetic studies, physical and chemical characterization, applications, patents and a long etcetera. This scattered information requires new tools that can put the information together and offer it in user-friendly way to anyone interested in any of the above mentioned aspects. Our non-proteogenic amino acids database compiles information from both theoretical and experimental background. Our database is mainly based on theoretical quantum mechanics calculations already performed and published in referenced and consolidated publications, nevertheless it does not overlook the experimental information, dealing with synthesis, crystallographic studies on the amino acid, physical features, and a special focus on biomedical applications and registered patents. In this work, for instance we investigated a targeted substitution of $C^{\alpha,\alpha}$-dialkylated amino acids obtained from a database search in the Methionine-Enkephalin peptide.