EXPLORATION OF THE PEPTIDE-DRUG SPACE

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(O.Ref/2014-135b)

The chemical properties of peptide drugs, known as the 'peptide-drug space' is considered a multi-dimensional subset of the global peptide space. Each dimension represents a chemical descriptor which is a numeric variable obtained by *in silico* calculations or by experiments, hiding fundamental physicochemical properties which can be correlated, to varying degrees, with biofunctional medicinal properties. Knowledge of this space can increase the efficiency of the peptide-drug discovery and development process.

Using more than 250 peptide drugs already on the market as well as in clinical development and starting with more than 3000 physicochemical descriptors for each peptide as well as the specific peptide-drug target and clinical use, multivariate data-exploration (e.g. PCA and HCA) was performed. Our retrospective analysis indicate that clusters in the peptide-drug space are located in a relatively narrow range of the physiochemical space: dense and empty regions were found and can be used as guidelines in peptide drug discovery.

Key words: Peptide therapeutics, Chemical space, Drug discovery