

CHIRAL SEPARATIONS

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Chirality has been one of the main interests of the pharmaceutical industry over the last two decades. The reason is that many drug molecules possess at least one asymmetric center, producing different enantiomers that often are distinguished by biological systems, where receptors, enzyme systems have chiral properties themselves. As a consequence, the enantiomers of chiral pharmaceuticals can behave very differently in the human body. One enantiomer, the eutomer, expresses the therapeutic effect while the other, the distomer, either is inactive, has a different effect, is responsible for unwanted side effects, or even can be toxic for human beings. Over the last years, the development of chiral separation technologies to either resolve racemic mixtures or to test the purity of synthesized enantiomers has been of particular interest to the pharmaceutical industry. The lecture will give an overview of chiral separations of pharmaceutical compounds, mainly by means of HPLC. Capillary electrophoresis, which is besides HPLC the most popular technique to perform chiral separations at the analytical level, will also be discussed.

HERBAL FINGERPRINTS: DEVELOPMENT AND DATA ANALYSIS

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Worldwide, herbs are used for preventive and therapeutic goals. Therefore, identification and quality control of these products of natural origin is required. Determination of some of the active compounds does not always allow assessing their total intrinsic quality. Since 1991 the World Health Organization accepts fingerprint chromatography as identification and quality evaluation technique for medicinal herbs. In fingerprint development, the goal is to create general conditions to maximize the peak capacity within an acceptable analysis time.

A fingerprint can be developed for a number of reasons: identification, classification or calibration purposes. Identification is to confirm that a sample is originating from the herb expected and to exclude that it is another, i.e. to attain a better quality control of the herbs. Classification can be performed to classify samples according to, for instance, their origin. This can be either a geographic origin or to distinguish between natural and synthetic compounds, e.g. vanillin from herbal, synthetic or microbiologic origin. Such evaluation is most often done by a principal component analysis, occasionally by a cluster analysis. A multivariate calibration can be performed when the herb or its extract also can be characterized by an activity, e.g. an antioxidant or a cytotoxic activity. The activity then can be modeled as a function of the complete chromatogram. The most commonly used modeling techniques are stepwise multivariate regression, principal component regression and partial least squares. The goal of the modeling can be either to build models that are able to predict the activity for future samples based on the chromatogram (e.g. the antioxidant activity from green tea) or to identify the main compounds/peaks responsible for a given activity.