

METHOD IMPLEMENTED BY
MEANS OF A COMPUTER FOR
DETERMINING RETENTION TIMES
AND CONCENTRATION VALUES
OF ANALYTES IN A MIXTURE



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PATENT STATUS: PATENT FILED

PRIORITY NUMBER: 102020000028322

PRIORITY DATE: 21/11/2020

PUBLISHED AS: PCT/IB2021/060924

Invention



The present invention relates to the **automation of data interpretation from a chromatography analysis**, such specifically the retention times and concentration values of analytes in a mixture. A high-pressure liquid chromatography (HPLC) with analyte detection by fluorimetric, electrochemical or ultraviolet radiation is taken as an example.

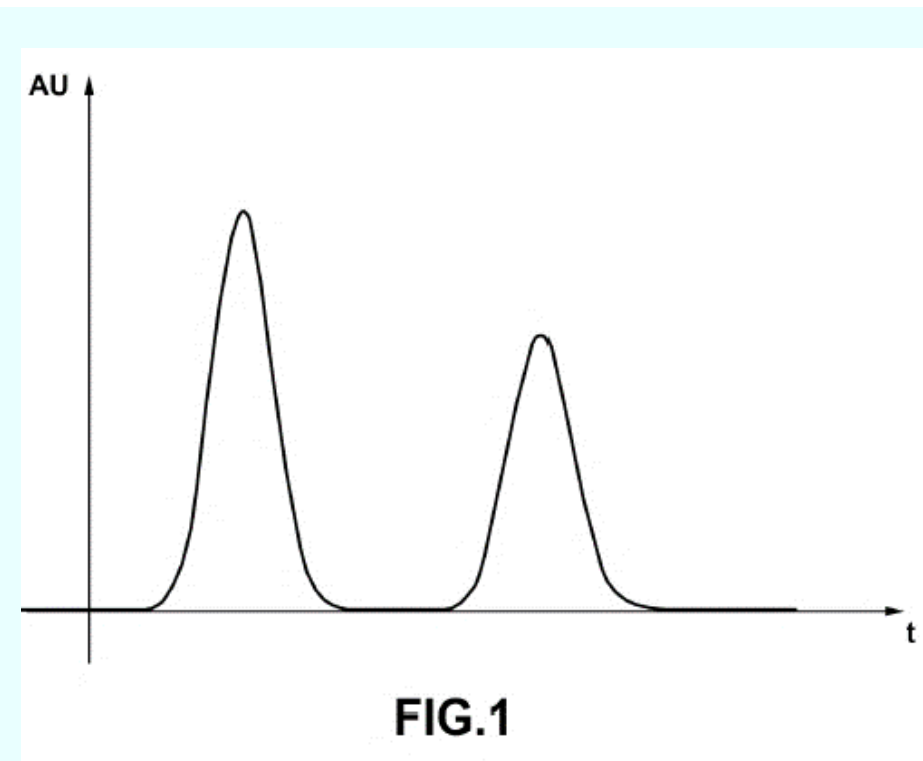
The purpose of the invention is to provide an automated procedure for chromatographic analysis to automatically detect:

- a) the **location of a chromatographic peak curve**, i.e. the automatic determination of retention times, and
- b) the **calculation of the area subtended by a curve**, i.e. the concentration value of the analyte present in the mixture.

A method is proposed that is reproducible and does not require the specification of initial parameters or other intervention by an operator.

In addition, the purpose of the present invention is to provide a procedure for analyzing chromatographic data with an unambiguous and uniform approach, and able to make chromatographic peak curves that are difficult to interpret, due, for example, to the presence of overlapping peaks, easily quantifiable.

Drawings
& pictures

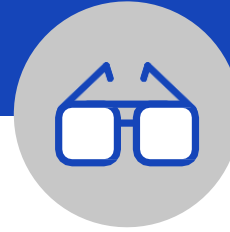


**OBJECTIVE
INTEGRATION
METHOD**

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**HIGH QUALITY
ANALYSIS**

Industrial applications



Liquid chromatography, in the field of biology and medicine, is frequently used to analyze biological and environmental samples for the **presence or absence of known compounds** (e.g., metabolites, drugs, toxins, pesticides) and can aid in the **identification of unknown compounds**.

Chromatographic techniques are also widely used in the pharmaceutical/chemical sector for therapeutic monitoring of drugs and substances of abuse, in the environmental sector for air quality monitoring, and in the food industry for residual toxicological analysis on various foods.

The proposed program can be **combined with current chromatographic software**, sold as part of the instrumentation, to bring an enhancement to the potential of the whole equipment. It can also be associated with any chromatographic kits, in association with specific settings of program variables suitable for performing a predetermined chromatographic method, characterized by specific peaks, specific AUCs and specific retention times.

Possible developments



The present invention enable the realization of a procedure by means of a script on a MATLAB® platform, suitable for automated processing of a predetermined set of collected and digitized measurement data by providing as output the value of the area subtended by the peak curve of an analyte of interest, which is conveniently executed on a computer set up to control the chromatographic analysis process.

The process can be implemented by any MATLAB®-equivalent program appropriate for handling mathematical data processing functions.

The invention may be applied to a **high-pressure liquid chromatography (HPLC) analysis** process and in other **kinds of chromatographic analysis**. In addition, it could also be applied to other analyses or methods, such as **DNA sequencing**, where an output plot is given for analysis that has a peak or peaks with a "valley-peak-valley" pattern.

For more information:



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