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The introduction of artificial intelligence to help in the analysis of the chromatographic big data

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Introduction: For 50 years, the big data of the chromatography of natural and complex products such as essential oils, flavors and fragrance, pharmaceutical, and petroleum products etc. (with 20 to 1000 peaks or more), had to be analysed and compared manually because of the random and non-linear variability of the retention times. Today this problem has been solved with software, based on neuronal algorithms, which automates the analysis of complex chromatograms.

The Problem: In chromatography, the retention times of compounds of the same injected sample will vary from an analysis to the other. Indeed, the ageing of the chemical phase of the columns varies in random and non-linear ways depending on the injected products and their concentrations. The other reasons for these variations are due to the chromatographic technology includes: injection mode; gas control; temperature control; variability of the atmospheric pressure and temperature of the room; chemistry of the injected product; maintenance of the chromatograph; sample impurities; phase oxidation (O^2 in carrier gas); quality of pumps in HPLC; solvent degassing and temperature; etc. Upon repeating analysis, the retention time differences of compounds will vary from fractions of seconds to minutes in a non-linear way on the chromatogram. If the analyzed product has hundreds of compounds, the manual comparison is long, difficult and is subjected to human error or simply impossible. Even if a gas chromatograph has all the new electronic regulation developments of temperature and gas flow rates, it is unable to compensate precisely and efficiently these complex variations.

The Solution: GC-LC Concordance software is based on an original treatment, mixing deductive mathematical theories of polynomial functions and neural network algorithms (recognition and adaptability) and solve these problems of random variations with hundreds millions of calculations per comparison. GC-LC Concordance is a complementary tool to the integration software (CDS) from any brands since it is compatible with all of them in GC, LC and MS and those without changing the settings of the methods used in the laboratories.

Some applications of GC-LC Concordance: Facilitating dramatically the quality control of flavors and fragrances, essential oils and aromas in chromatography in seconds; controlling the composition of a sample following the norms and specifications imposed by your clients in seconds; automatic comparison of one to thousands of complex chromatographic fingerprints within a few seconds (electronic nose, the origin of a product, counterfeiting, etc.); automatic conversion of chromatograms from retention time to retention index molecule identification with some databases of molecules; raw material identification in a mixture and estimation of its concentration; automatic identification of the molecules on each peak of your chromatograms.

Conclusion: The artificial intelligence introduced in chromatographic treatment today, allows solving a problem never solved before: the automatic compensation of random retention times. It solves the problems of laboratories which work in the fields as varied as the quality control or the R&D for the interpretation or classification of complex products by chromatography.