Nmr Spectroscopy In Pharmaceutical Analysis

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Chiral derivatizing agent

resolution, the actual physical separation of the enantiomers. Since NMR spectroscopy has been available to chemists, there have been numerous studies on

In analytical chemistry, a chiral derivatizing agent (CDA), also known as a chiral resolving reagent, is a derivatization reagent that is a chiral auxiliary used to convert a mixture of enantiomers into diastereomers in order to analyze the quantities of each enantiomer present and determine the optical purity of a sample. Analysis can be conducted by spectroscopy or by chromatography. Some analytical techniques such as HPLC and NMR, in their most commons forms, cannot distinguish enantiomers within a sample, but can distinguish diastereomers. Therefore, converting a mixture of enantiomers to a corresponding mixture of diastereomers can allow analysis. The use of chiral derivatizing agents has declined with the popularization of chiral HPLC. Besides analysis, chiral derivatization is also...

Operando spectroscopy

an in situ reaction involves the real-time measurement of a catalytic process using techniques such as mass spectrometry, NMR, infrared spectroscopy, and

Operando spectroscopy is an analytical methodology wherein the spectroscopic characterization of materials undergoing reaction is coupled simultaneously with measurement of catalytic activity and selectivity. The primary concern of this methodology is to establish structure-reactivity/selectivity relationships of catalysts and thereby yield information about mechanisms. Other uses include those in engineering improvements to existing catalytic materials and processes and in developing new ones.

Desmethoxycurcumin

Solid-State Measurements of Drugs and Drug Formulations", NMR Spectroscopy in Pharmaceutical Analysis, Amsterdam: Elsevier, pp. 201–231, doi:10.1016/b978-0-444-53173-5

Desmethoxycurcumin is a curcuminoid found in turmeric. Commercial grade curcumin contains a mixture of curcuminoids (desmethoxycurcumin 10–20%, bisdesmethoxycurcumin 5% or less).

Analytical chemistry

chromatography-infrared spectroscopy, liquid chromatography-mass spectrometry, liquid chromatography-NMR spectroscopy, liquid chromatography-infrared spectroscopy, and capillary

Analytical chemistry studies and uses instruments and methods to separate, identify, and quantify matter. In practice, separation, identification or quantification may constitute the entire analysis or be combined with another method. Separation isolates analytes. Qualitative analysis identifies analytes, while quantitative analysis determines the numerical amount or concentration.

Analytical chemistry consists of classical, wet chemical methods and modern analytical techniques. Classical qualitative methods use separations such as precipitation, extraction, and distillation. Identification may be based on differences in color, odor, melting point, boiling point,

solubility, radioactivity or reactivity. Classical quantitative analysis uses mass or volume changes to quantify amount. Instrumental...

In a mixture of enantiomers, these methods can help quantify the optical purity by integrating the area under the NMR peak corresponding to each stereoisomer. Accuracy of integration can be improved by inserting a chiral derivatizing agent with a nucleus other than hydrogen or carbon, then reading the heteronuclear NMR spectrum: for example fluorine-19 NMR or phosphorus-31 NMR. Mosher's acid contains a -CF3 group, so if the adduct has no other fluorine atoms, the 19F NMR of a...

Solid-state nuclear magnetic resonance

magnetic resonance (ssNMR) is a spectroscopy technique used to characterize atomic-level structure and dynamics in solid materials. ssNMR spectra are broader

Solid-state nuclear magnetic resonance (ssNMR) is a spectroscopy technique used to characterize atomic-level structure and dynamics in solid materials. ssNMR spectra are broader due to nuclear spin interactions which can be categorized as dipolar coupling, chemical shielding, quadrupolar interactions, and j-coupling. These interactions directly affect the lines shapes of experimental ssNMR spectra which can be seen in powder and dipolar patterns. There are many essential solid-state techniques alongside advanced ssNMR techniques that may be applied to elucidate the fundamental aspects of solid materials. ssNMR is often combined with magic angle spinning (MAS) to remove anisotropic interactions and improve the sensitivity of the technique. The applications of ssNMR further extend to biology...

NMR involves the quantum-mechanical properties of the central core ("nucleus...

Nuclear magnetic resonance spectroscopy of stereoisomers

resonance spectroscopy of stereoisomers most commonly known as NMR spectroscopy of stereoisomers is a chemical analysis method that uses NMR spectroscopy to

Nuclear magnetic resonance spectroscopy of stereoisomers most commonly known as NMR spectroscopy of stereoisomers is a chemical analysis method that uses NMR spectroscopy to determine the absolute configuration of stereoisomers. For example, the cis or trans alkenes, R or S enantiomers, and R,R or R,S diastereomers.

Nuclear magnetic resonance spectroscopy of proteins

magnetic resonance spectroscopy of proteins (usually abbreviated protein NMR) is a field of structural biology in which NMR spectroscopy is used to obtain

Nuclear magnetic resonance spectroscopy of proteins (usually abbreviated protein NMR) is a field of structural biology in which NMR spectroscopy is used to obtain information about the structure and dynamics of proteins, and also nucleic acids, and their complexes. The field was pioneered by Richard R. Ernst and Kurt Wüthrich at the ETH, and by Ad Bax, Marius Clore, Angela Gronenborn at the NIH, and Gerhard Wagner at Harvard University, among others. Structure determination by NMR spectroscopy usually consists of several phases, each using a separate set of highly specialized techniques. The sample is prepared, measurements are made, interpretive approaches are applied, and a structure is calculated and validated.

Fluorine-19 nuclear magnetic resonance spectroscopy

Fluorine-19 nuclear magnetic resonance spectroscopy (fluorine NMR or 19F NMR) is an analytical technique used to detect and identify fluorine-containing

Fluorine-19 nuclear magnetic resonance spectroscopy (fluorine NMR or 19F NMR) is an analytical technique used to detect and identify fluorine-containing compounds. 19F is an important nucleus for NMR spectroscopy because of its receptivity and large chemical shift dispersion, which is greater than that for proton nuclear magnetic resonance spectroscopy.

Benchtop nuclear magnetic resonance spectrometer

quantum mechanical spectral analysis, for 1H-1D NMR spectra also known as HiFSA. NMR spectroscopy can be used for chemical analysis, reaction monitoring, and

A Benchtop nuclear magnetic resonance spectrometer (Benchtop NMR spectrometer) refers to a Fourier transform nuclear magnetic resonance (FT-NMR) spectrometer that is significantly more compact and portable than the conventional equivalents, such that it is portable and can reside on a laboratory benchtop. This convenience comes from using permanent magnets, which have a lower magnetic field and decreased sensitivity compared to the much larger and more expensive cryogen cooled superconducting NMR magnets. Instead of requiring dedicated infrastructure, rooms and extensive installations these benchtop instruments can be placed directly on the bench in a lab and moved as necessary (e.g., to the fumehood). These spectrometers offer improved workflow, even for novice users, as they are simpler...