Patent Claims

1. Method for the identification of a substance in a sample, comprising the following steps:

a) Providing an NMR spectrum of a sample containing at least one substance having at least one NMR-active nucleus,

b) Converting the NMR spectrum into discrete spectral values, wherein each spectral value has an integral value, specifying the height and/or the area of an individual line of the NMR spectrum or of an individual spectral section of the NMR spectrum, and a position value, specifying the mean position of the line considered or of the considered spectral section in the NMR spectrum,

c) Determining a multitude of integral ratio values, in each case from two integral values of the NMR spectrum, wherein each integral ratio value specifies the ratio of the height and/or of the area of the underlying spectral values,

d) Determining a multitude of distance values, in each case from two position values of the NMR spectrum, wherein each distance value specifies the spectral distance between the underlying spectral values,

e) Comparing the integral ratio values of the NMR spectrum with corresponding integral ratio values of an NMR reference spectrum of at least one reference substance,

f) Selecting a first proper subset from the integral ratio values of the NMR spectrum, wherein the first subset comprises those integral ratio values which correspond to an integral ratio value of the NMR reference spectrum within first tolerance limits that can be given in each case,

g) Comparing the distance values of the NMR spectrum with corresponding distance values of the NMR reference spectrum,

h) Selecting a second proper subset from the distance values of the NMR spectrum, wherein the second subset comprises those distance values which correspond to

a distance value of the NMR reference spectrum within second tolerance limits that can be given in each case,

i) Comparing the first subset with the second subset and selecting those integral ratio values and distance values from both subsets as third proper subset which were formed from the same spectral values,

j) Deciding whether the substance contained in the sample is identified as the reference substance, with the help of a quality criterion of the values of the third subset, said criterion being determined by comparing these values with the integral ratio values and/or the distance values of the NMR reference spectrum.

2. Method according to Claim 1, **characterized** in that the NMR reference spectrum is an NMR spectrum of exactly one reference substance.

3. Method according to Claim 1 or 2, **characterized** in that the quality criterion comprises a measure for the deviation of the integral ratio values of the NMR spectrum from the integral ratio values of the NMR reference spectrum and/or the deviation of the distance values of the NMR spectrum from the distance values of the NMR reference spectrum.

4. Method according to any of the preceding claims, **characterized** in that the quality criterion comprises a measure for the number of values of the third subset in comparison with the number of integral ratio values or of distance values of the NMR reference spectrum.

5. Method according to any of the preceding claims, **characterized** in that the steps e) to j) are repeated with further NMR reference spectra of other reference substances so often until the substance contained in the sample is identified as reference substance or until there are no further NMR reference spectra.

6. Method according to any of the preceding claims, **characterized** in that the distance values are calculated as direct differences of the position values, as standardized differences of the position values or as quotient of the position values.

7. Method according to any of the preceding claims, **characterized** in that the substance contained in the sample is identified quantitatively.

8. Method according to any of the preceding claims, **characterized** in that the method is performed by using a decoupled NMR spectrum and, when the substance is not unequivocally identified, is performed again by using a non-decoupled NMR spectrum of the same sample.

9. Software product having a software which has a program code to perform a method according to any of the preceding claims, when the software is run on a computer.

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Patent Claims

1. Method for the identification of a substance in a sample, comprising the following steps:

   a) Providing an NMR spectrum of a sample containing at least one substance having at least one NMR-active nucleus,

   b) Converting the NMR spectrum into discrete spectral values, wherein each spectral value has an integral value, specifying the height and/or the area of an individual line of the NMR spectrum or of an individual spectral section of the NMR spectrum, and a position value, specifying the mean position of the line considered or of the considered spectral section in the NMR spectrum,

   c) Determining all possible integral ratio values, in each case from two integral values of the NMR spectrum, wherein each integral ratio value specifies the ratio of the height and/or of the area of the underlying spectral values,

   d) Determining all possible distance values, in each case from two position values of the NMR spectrum, wherein each distance value specifies the spectral distance between the underlying spectral values,

   e) Comparing the integral ratio values of the NMR spectrum with corresponding integral ratio values of an NMR reference spectrum of at least one reference substance,

   f) Selecting a first proper subset from the integral ratio values of the NMR spectrum, wherein the first subset comprises those integral ratio values which correspond to an integral ratio value of the NMR reference spectrum within first tolerance limits that can be given in each case,

   g) Comparing the distance values of the NMR spectrum with corresponding distance values of the NMR reference spectrum,

   h) Selecting a second proper subset from the distance values of the NMR spectrum, wherein the second subset comprises those distance values which correspond to a distance value of the NMR reference spectrum within second tolerance limits that can be given in each case,

i) Comparing the first subset with the second subset and selecting those integral ratio values and distance values from both subsets as third proper subset which were formed from the same spectral values,

j) Deciding whether the substance contained in the sample is identified as the reference substance, with the help of a quality criterion of the values of the third subset, said criterion being determined by comparing these values with the integral ratio values and/or the distance values of the NMR reference spectrum,

wherein steps e) to j) are repeated with further NMR reference spectra of other reference substances so often until the substance contained in the sample is identified as reference substance or until there are no further NMR reference spectra.

2. Method according to Claim 1, **characterized** in that the NMR reference spectrum is an NMR spectrum of exactly one reference substance.

3. Method according to Claim 1 or 2, **characterized** in that the quality criterion comprises a measure for the deviation of the integral ratio values of the NMR spectrum from the integral ratio values of the NMR reference spectrum and/or the deviation of the distance values of the NMR spectrum from the distance values of the NMR reference spectrum.

4. Method according to any of the preceding claims, **characterized** in that the quality criterion comprises a measure for the number of values of the third subset in comparison with the number of integral ratio values or of distance values of the NMR reference spectrum.

5. Method according to any of the preceding claims, **characterized** in that the distance values are calculated as direct differences of the position values, as standardized differences of the position values or as quotient of the position values.

6. Method according to any of the preceding claims, **characterized** in that the substance contained in the sample is identified quantitatively.

7. Method according to any of the preceding claims, **characterized** in that the method is performed by using a decoupled NMR spectrum and, when the substance is not unequivocally identified, is performed again by using a non-decoupled NMR spectrum of the same sample.

8. Software product having a software which has a program code to perform a method according to any of the preceding claims, when the software is run on a computer.

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