

16. A method according to claim 13, wherein said point-assessment is obtained by sequentially deriving data for each partial structure, by calculating membership function $\phi(t)_i$ for every spectral data of each partial structure encompassed in the unknown substance according to the following formulas:

$$t_i = \frac{|P_0 - P_k|}{\sigma}$$

$$\phi(t)_i = \exp(-\frac{1}{2}t_i^2)$$

wherein P_0 is the central frequency, P_k is the frequency of each spectral data, and σ is the standard deviation, and by calculating the weighted average ϕ_T of the membership functions of said spectral data of said partial structure according to the following formula:

$$\phi_T = \frac{W_1\phi(t)_1 + W_2\phi(t)_2 + \dots}{W_1 + W_2 + \dots}$$

wherein W_1, W_2, \dots are weights of said spectral data, said weighted average ϕ_T being used as said point-assessment.

17. A method according to claim 16, wherein said membership function is calculated only for every input spectral data whose number of splitting patterns coincides with the number of splitting patterns of the spectral data of the partial structure.

18. A method according to claim 13, wherein said prememorized chemical shift values include at least the central position and the standard deviation of each spectral signal for every partial structure.

19. A method according to claim 18, wherein said prememorized chemical shift values further include weight data for every spectral signal.

20. A method according to claim 18, wherein said prememorized chemical shift values further include splitting pattern data for every spectral signal.

21. A method according to claim 13, wherein said prememorized chemical shift values include those cor-

responding to a plurality of aromatic ring partial structures of known substances.

22. A method according to claim 21, wherein said prememorized chemical shift values include data of highest and lowest positions of the shift range of the spectral signal of every partial structure.

23. A method according to claim 21, wherein said point-assessment is obtained by sequentially deriving data for each aromatic ring partial structure, by calculating membership function $\phi(t)_i$ for every spectral data of each aromatic ring partial structure encompassed in the unknown substance according to the following formulas:

$$t_i = \frac{|P_0 - P_k|}{\sigma}$$

$$\phi(t)_i = \exp(-\frac{1}{2}t_i^2)$$

wherein P_0 is the central frequency, P_k is the frequency of each spectral data, and σ is the standard deviation, by combining aromatic ring partial structures each having membership function equal to or larger than a predetermined threshold value so as to form a ring structure, and by calculating the weighted average ϕ_T of the membership functions of said spectral data of said partial structures according to the following formula:

$$\phi_T = \frac{W_1\phi(t)_1 + W_2\phi(t)_2 + \dots}{W_1 + W_2 + \dots}$$

wherein W_1, W_2, \dots are weights of said spectral data, said weighted average ϕ_T being used as said point-assessment.

24. A method according to claim 23, wherein said membership function is calculated only for every input spectral data whose number of splitting patterns coincides with the number of splitting patterns of the spectral data of the aromatic ring partial structure.

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