(b) separating, by mass spectrometry, each diacylglycerol thus detected in step (a) into corresponding fatty acid fragments.

SUMMARY

[0004] However, the method disclosed in Patent Literature 1 takes many man-hours, and, therefore, an easier and simpler analysis method is demanded. Moreover, there are numerous combinations of fatty acids in a TAG (at least 3000 combinations), so it is not an easy task to prepare reference standards for all the possible combinations prior to TAG analysis. For this reason, there is a need for a method capable of estimating TAG-constituting fatty acids without requiring reference standards for possible combinations of fatty acids.

[0005] The present disclosure has been devised in light of the above-described circumstances, and an object thereof is to provide a method for easy and simple estimation for a target compound containing an acyl group, in terms of the total number of carbon atoms in the acyl group as well as the total number of carbon-carbon double bond(s) in the acyl group.

[0006] The inventors of the present disclosure have conducted intensive research, and, as a result, have found that the retention time in chromatograph analysis correlates with the total number of carbon atoms in the acyl group and the total number of carbon-carbon double bond(s) in the acyl group in the target compound. Thus, the present disclosure has now been completed.

[0007] A first aspect of the present disclosure relates to a method of estimating a structure of a target compound containing a linear acyl group, the method comprising:

analyzing a sample containing the target compound on a chromatograph to determine a retention time; and

estimating a combination of a total number of carbon atoms and a total number of carbon-carbon double bond(s) in the acyl group in the target compound from the retention time, based on the following equations 1 and 2:

$$N=f(T) \quad \text{... (Equation 1)}$$

$$T=t/D^m \quad \text{... (Equation 2)}$$

in the equation 1, N represents the total number of carbon atoms in the acyl group, and f(T) represents a function that is derived from a homologue of a saturated compound corresponding to the target compound and that expresses a correlation between the total number of carbon atoms and the retention time; and in the equation 2, t represents the retention time, D represents a coefficient based on carbon-carbon double bond(s), and m represents the total number of carbon-carbon double bond(s).

[0008] A second aspect of the present disclosure relates to a computer-readable storage medium storing a database that is to be used for causing a computer to implement the method of estimating a structure as disclosed herein, wherein

the database stores:

analysis conditions for the chromatograph; and

the function f(T) derived at the time of analysis of the homologue under the analysis conditions, and the coefficient D based on carbon-carbon double bond(s),

in association with one another.

[0009] According to the present disclosure, it is possible to provide a method for easy and simple estimation for a target compound containing an acyl group, in terms of the total number of carbon atoms in the acyl group as well as the total number of carbon-carbon double bond(s) in the acyl group.

BRIEF DESCRIPTION OF THE DRAWINGS

[0010] Fig. 1 shows a graph that presents results of analysis of fully saturated triacylglycerols carried out on a supercritical fluid chromatograph (left), and a graph that presents the correlation between the total number of carbon atoms in the acyl groups in the triacylglycerols (on the horizontal axis) and the retention time (on the vertical axis) based on the analysis results (right). On the left graph, the horizontal axis indicates the retention time (minutes), and the vertical axis indicates the detection intensity.

Fig. 2 shows a graph that presents results of analysis of triacylglycerols carried out on a supercritical fluid chromatograph (left), and a table that presents the correlation between the total number of carbon-carbon double bond(s) in the acyl