

### The specific calculation process of $f_{\text{ar}}^{\text{H}}$ , H/C, CH<sub>3</sub>/CH<sub>2</sub> and $f_{\text{ar}}$ .

#### (1) Aromatic hydrogen rate

$f_{\text{ar}}^{\text{H}}$  is the ratio of the number of aromatic hydrogen atoms to the total hydrogen atoms of the FA. Generally speaking, the hydrogen atoms in FA include only aliphatic hydrogen and aromatic hydrogen. The relative contents of aromatic hydrogen and aliphatic hydrogen can be calculated from the total area of characteristic peaks in the wave interval of 700~850 cm<sup>-1</sup> and 2800~3050 cm<sup>-1</sup>.

$$\begin{aligned} f_{\text{ar}}^{\text{H}} &= \frac{H_{\text{ar}}}{H_{\text{total}}} = \frac{A_{\text{ar}}}{A_{\text{ar}}+A_{\text{al}}} = \frac{A_{(700-850 \text{ cm}^{-1})}}{A_{(700-850 \text{ cm}^{-1})}+A_{(2800-3050 \text{ cm}^{-1})}} \\ &= \frac{0.5125}{0.5125+1.0399} \\ &= 0.3314 \end{aligned}$$

Therefore, the calculated aromatic hydrogen rate of FA is 0.3314.

#### (2) Hydrogen to carbon atomic ratio

The hydrogen to carbon atom ratio refers to the ratio of the number of hydrogen atoms in the FA to the number of carbon atoms, which can be calculated according to the elemental analysis result as follows:

$$\begin{aligned} \frac{\text{H}}{\text{C}} &= \frac{H_{\text{ad}}/1}{C_{\text{ad}}/12} \\ &= 1.09 \end{aligned}$$

Thus, the hydrogen to carbon atomic ratio of FA was calculated to be 1.09.

#### (3) Aliphatic chain length

The length of the aliphatic chain refers to the ratio of the number of carbon atoms of the methyl group and the methylene group in the fatty structure of the FA, which can be obtained from the area ratio ratio of the methyl group to the methylene

group:

$$\frac{\text{CH}_3}{\text{CH}_2} = \frac{A_{(2872 \text{ cm}^{-1})} + A_{(2999 \text{ cm}^{-1})}}{A_{(2927 \text{ cm}^{-1})} + A_{(2963 \text{ cm}^{-1})}}$$
$$= 0.4717$$

Thus, the aliphatic chain length of FA can be calculated to be 0.4717

(4) Aromatic carbon rate

The aromatic carbon ratio is based on the ratio of all  $\text{sp}^2$  carbon atoms in the FA to the total number of carbon atoms. The calculation results<sup>21,22</sup> are as follows:

$$f_{\text{ar}} = 1 - \frac{C_{\text{al}}}{C} = 1 - \left( \frac{H_{\text{al}}}{H} \times \frac{H}{C} \right) \div \frac{H_{\text{al}}}{C_{\text{al}}}$$
$$= 1 - \frac{1 - 0.3314}{1.8} \times 1.09$$
$$= 0.5951$$

In the formula,  $\frac{C_{\text{al}}}{C}$  —The ratio of aliphatic carbon to the total carbon number;

$\frac{H_{\text{al}}}{C_{\text{al}}}$  —The ratio of the number of hydrogen carbon atoms of the aliphatic

hydrocarbon is generally 1.8;

$\frac{H}{C}$  —The ratio of the number of hydrogen atoms to carbon atoms in the

elemental analysis;

$\frac{H_{\text{al}}}{H}$  —The ratio of the number of aliphatic hydrogens to the total

hydrogen.

Therefore, the aromatic carbon rate of FA can be calculated to be 0.5951.