

Determining biodiesel composition according to ISO 14103

Calculation of biodiesel composition can be done directly in Clarity

This whitepaper explains how to calculate the content of fatty acid methyl esters (FAME) and the linoleic acid methyl ester in biodiesel fuel according to ISO 14103 in Clarity. As stated in the norm, the content of FAME in biodiesel is greater than 90 % (*m/m*), while the content of the linoleic acid methyl ester is between 1 % and 15 % (*m/m*). The methyl esters in FAME should be between C₁₄ and C₂₄.

Principle

The determination of the content of FAME employs internal calibration (ISTD – methyl heptadecanoate). The ester content in *m/m* percent is calculated as:

$$C = \frac{(\sum A) - A_{\text{ISTD}}}{A_{\text{ISTD}}} \cdot \frac{C_{\text{ISTD}} \cdot V_{\text{ISTD}}}{m} \cdot 100\% = \frac{(\sum A) - A_{\text{ISTD}}}{A_{\text{ISTD}}} \cdot \frac{m_{\text{ISTD}}}{m} \cdot 100\%$$

where *C* is the ester content, $\sum A$ is the total peak area of the methyl esters from C₁₄ to C₂₄, *A*_{ISTD} is the peak area of the ISTD compound, *C*_{ISTD} is the concentration of ISTD (in mg/ml), *V*_{ISTD} is the volume of ISTD (in ml), *m*_{ISTD} is the mass of ISTD (in mg), and *m* is the mass of the sample (including ISTD mass; in mg).

The linoleic acid methyl ester content in *m/m* percent is given as:

$$L = \frac{A_L}{(\sum A) - A_{\text{ISTD}}} \cdot 100\%$$

where *L* is the linoleic acid methyl ester content, $\sum A$ is the total peak area of the methyl esters from C₁₄ to C₂₄, *A*_{ISTD} is the peak area of ISTD, and *A*_L is the peak area corresponding to the linoleic acid methyl ester.

Preparing chromatogram and calibration

After measuring your sample, open your chromatogram in Clarity. Group the FAME peaks using the *Peak Groups...* function (menu *Chromatogram – Peak*). In the *Groups* dialog, set an *ID*, click *Add*, and select the corresponding peaks. In the example chromatogram (download link below), Group A (FAME) does not contain the ISTD peak – this simplifies the subsequent calculations.

Create a new calibration and open the sample chromatogram as a standard. In the *Calibration Options*, change the *Display Mode* to *ISTD* and *Mode* to *Recalibrate*. Use the *Add Peak* function to add the ISTD (methyl heptadecanoate) peak and linoleic acid peak to the calibration. In the *Amount* column, write the known ISTD amount. To add the group of FAME peaks, use the *Add Group* function. Then, on the linoleic acid and FAME compound tabs, set the *Calculate By* option to the ISTD compound name. Save the calibration and link it to the sample chromatogram. To improve clarity, in the *Common for All Signals* pane, select the *All Identified Peaks* option in the *Report in Result Table* section.

Procedure for calculation of FAME content

The desired results can be calculated directly in Clarity using the *User Columns*: right click anywhere in the *Result Table* pane in the *Results* tab of the Chromatogram window and select *User Columns – Add...* in the context menu. In the *Add User Column* dialog, fill in the *Title* and *Units* (e.g. FAME in %) and uncheck the *Calculate Total* checkbox. The following expression can be used to calculate the FAME content, if the ISTD peak was not included in the FAME peak group:

$$\left(\frac{\text{FAME\$Area}}{\text{ISTD\$Area}}\right) \times \left(\frac{\text{ISTD1 Amount}}{\text{[Sample Amount] + [ISTD1 Amount]}}\right) \times 100$$

If the ISTD peak was included in the FAME peak group, its area must be subtracted from the area of the FAME group:

$$\left(\frac{\text{[FAME\$Area] - [ISTD\$Area]}}{\text{ISTD\$Area}}\right) \times \left(\frac{\text{ISTD1 Amount}}{\text{[Sample Amount] + [ISTD1 Amount]}}\right) \times 100$$

Procedure for calculation of the linoleic acid methyl ester content

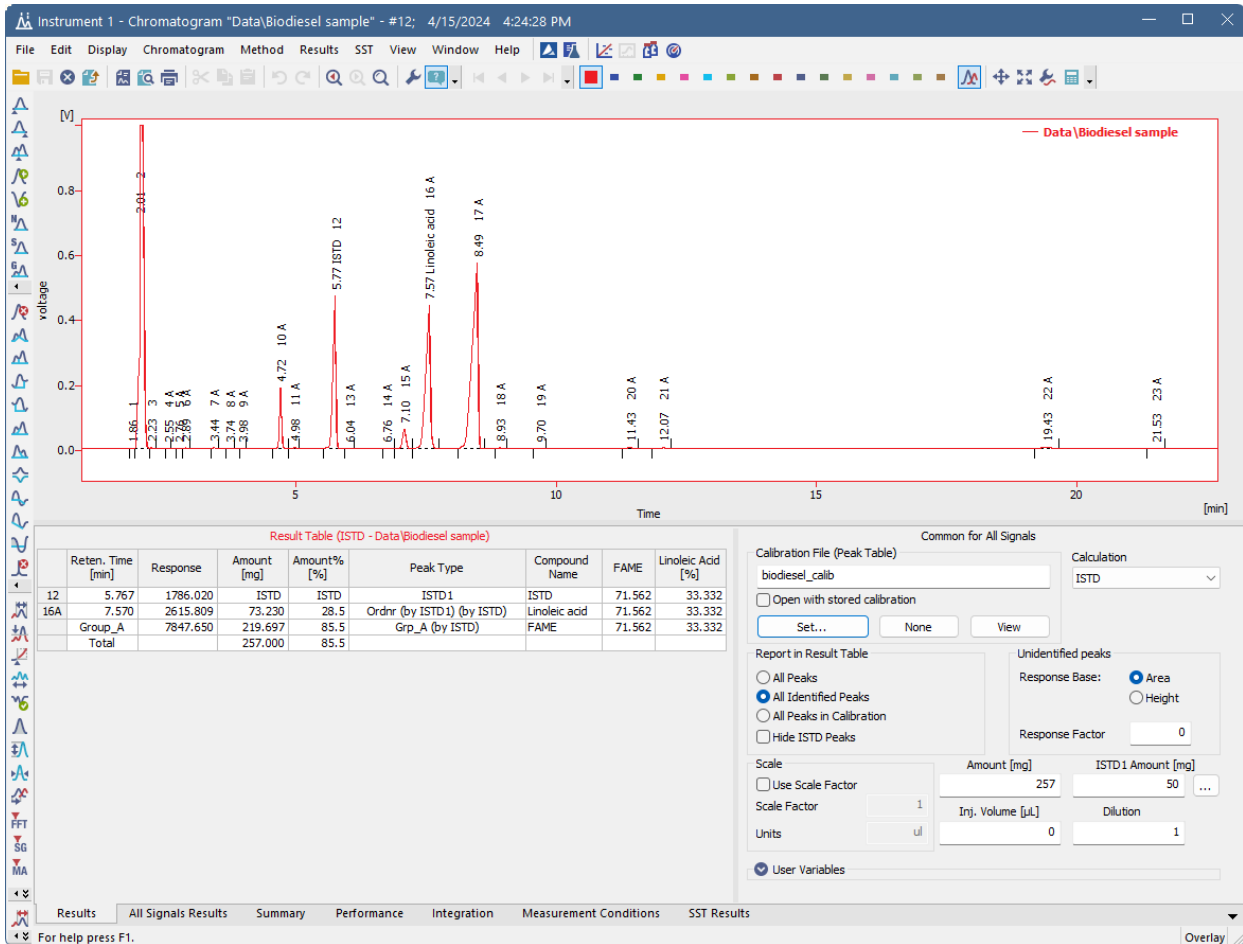
Calculation of linoleic acid methyl ester content is analogous to calculation of the FAME content. Add another user column, fill in the *Title* and *Units* (e.g., Linoleic Acid in %) and uncheck the *Calculate Total* checkbox. If the ISTD peak was not included in the FAME peak group, the following expression can be used:

$$\frac{\text{[Linoleic acid\$Area]}}{\text{[FAME\$Area]}} \times 100$$

Analogously, if the ISTD peak was included in the FAME group, it must be subtracted:

$$\frac{\text{[Linoleic acid\$Area]}}{\text{[FAME\$Area] - [ISTD\$Area]}} \times 100$$

Example of an evaluated chromatogram



Sample data for Clarity

- [Biodiesel.zip](#) – zipped processed chromatogram and calibration.