User manual (calc 106)

Introduction

This manual describes the interface of the **calc 106** program and describes the key points of using this software.

The program is designed for the analysis of chromatograms obtained using **Chromos4**. When analyzing chromatograms, the composition of LPG (liquefied petroleum gases) and the concentration of components are determined according to GOST R 54484-2011, GOST 33012-2014 or GOST 10679-76 (optional). Based on the concentrations and composition obtained, the pressure and density of LPG are calculated according to GOST 28656-90, and the octane number is calculated according to STB EN 589-2014.

To get started, you need to read the following documents:

- GOST R 54484-2011, GOST 33012-2014, GOST 10679-76

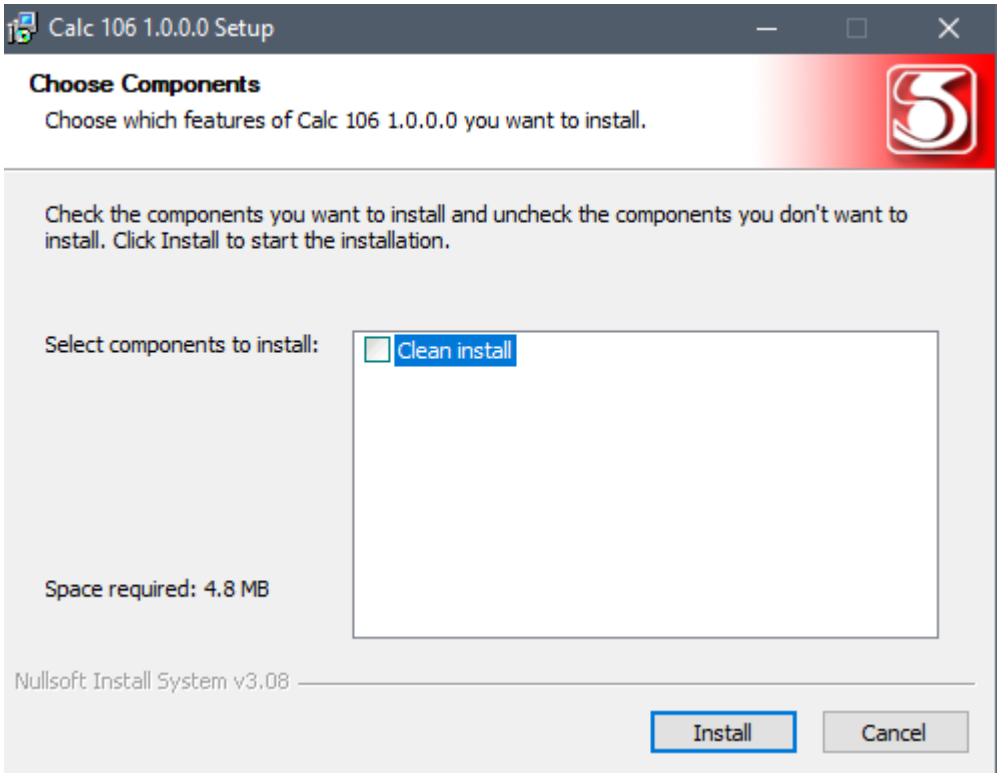
- GOST 28656-90

- STB EN 589-2014.

Install

The installation file can be downloaded at: http://kb.has.ru/soft:dop_raschjot_106

After launching the installation file, it is enough to follow the instructions of the installation wizard (Picture 1).

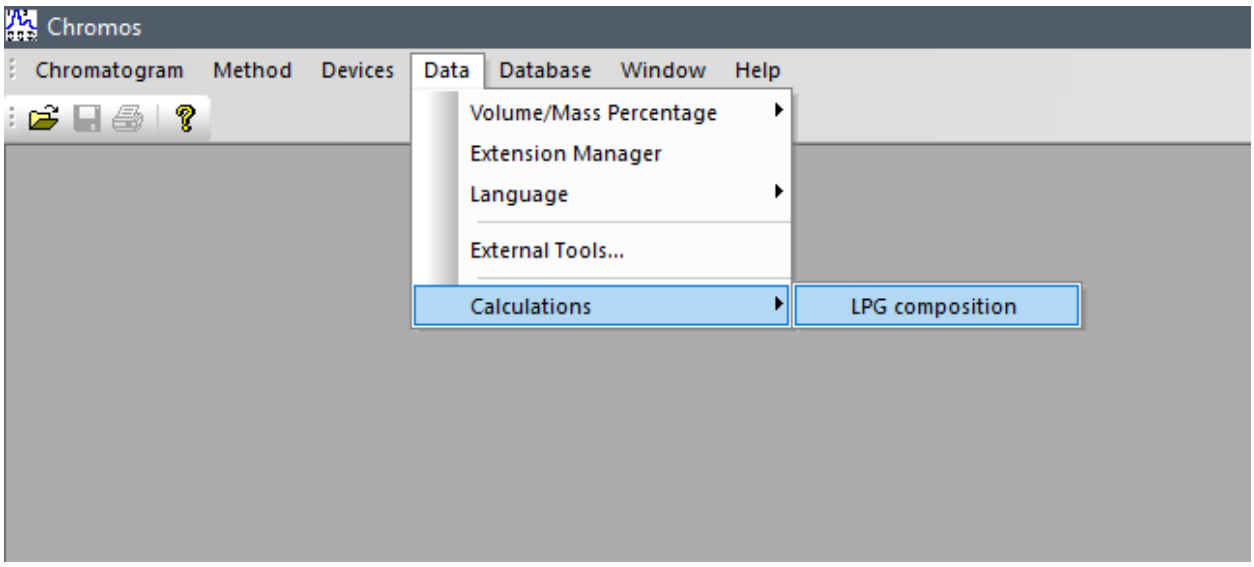


(picture 1)

The “Clean install” mark will clear all user data set by them in the previous version of the program (coefficients, aliases, settings) and set them to default values.

Upon completion of the installation, to start the calculation, open the main **Chromos4** application. The calculation will be available in the tab:

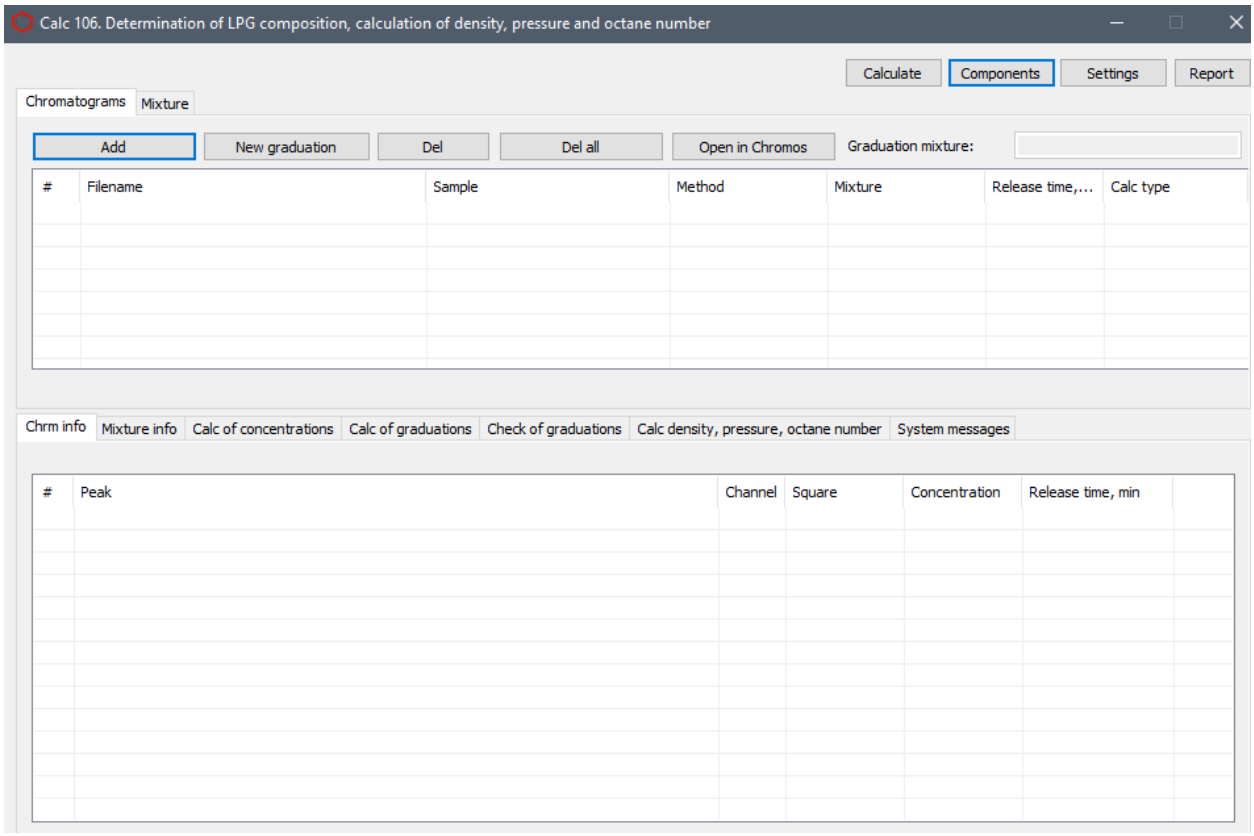
Menu->Data->Calculations->Calculation name (picture 2)



(picture 2)

Common interface

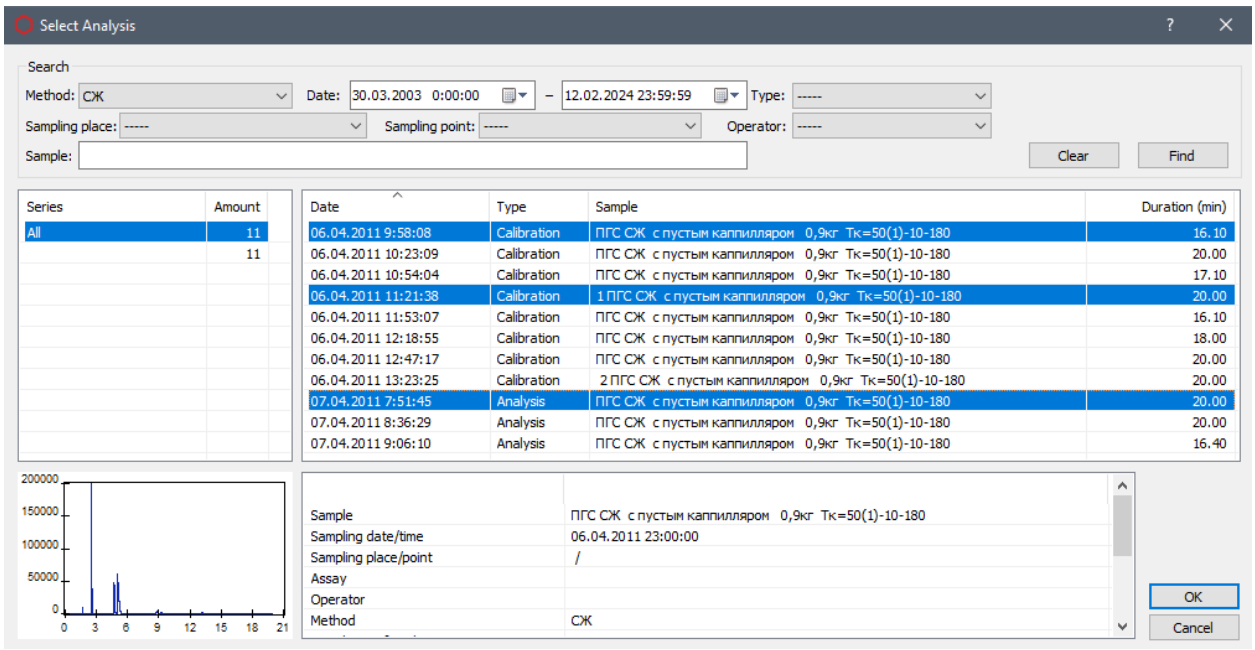
The common interface of the program is shown in picture 3.



(picture 3)

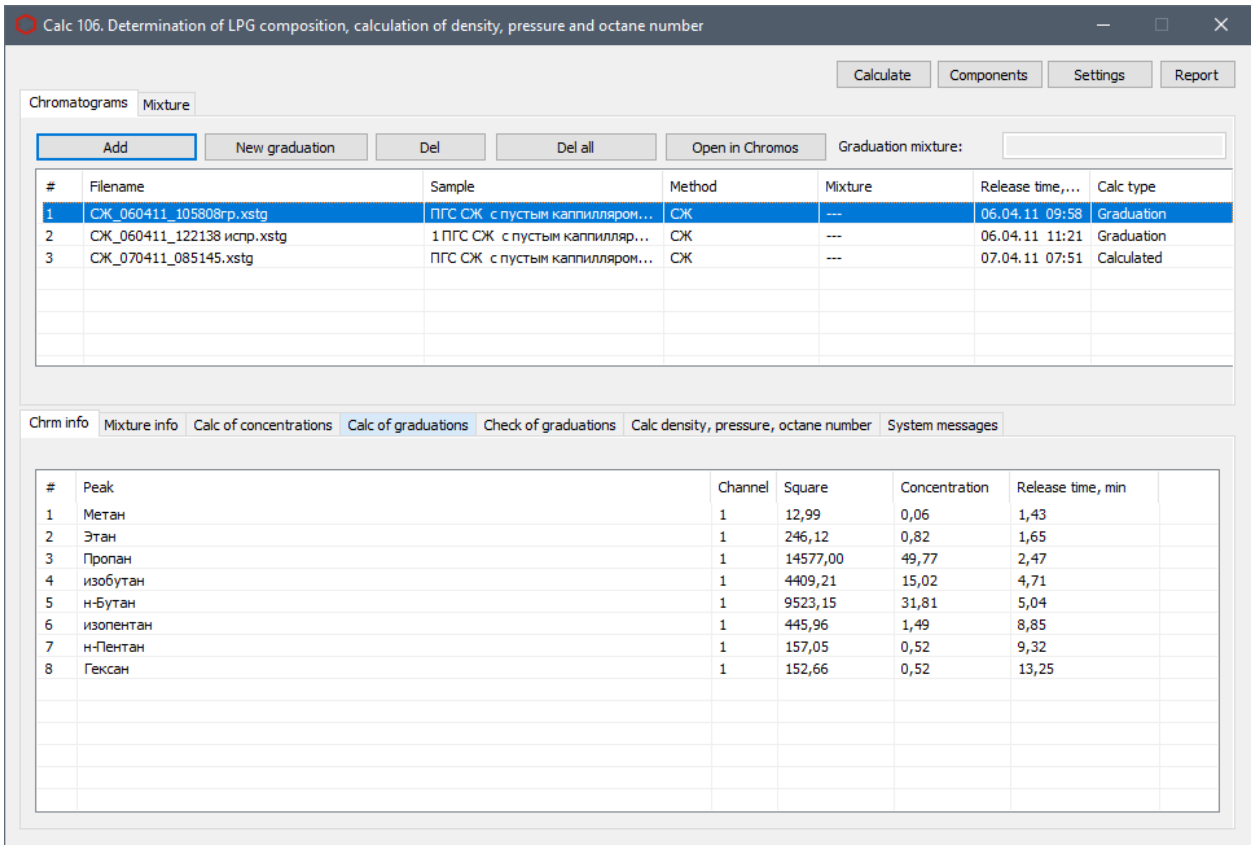
To add chromatogram files, 2 buttons are used (picture 3) **Add** and **New Calibration**. Using the "Add" button, files are opened for calculations, and the "New calibration" button adds chromatograms to check the graduations (see GOST R 54484-2011).

Pressing these buttons opens the chromatogram window (picture 4). To work, 2 types of chromatograms are needed: "Calibration" and "Analyses" (Calculated). Using the **ctrl** and **shift** keyboard buttons, you can select multiple files at the same time. Click **OK** after selecting the desired chromatograms.



(picture 4).

The selected chromatograms will be displayed in the main window (picture 5).



(picture 5)

Detailed information is available for each chromatogram (**Chrm info**), as well as information on available mixtures (**Mixture, Mixture Info**).

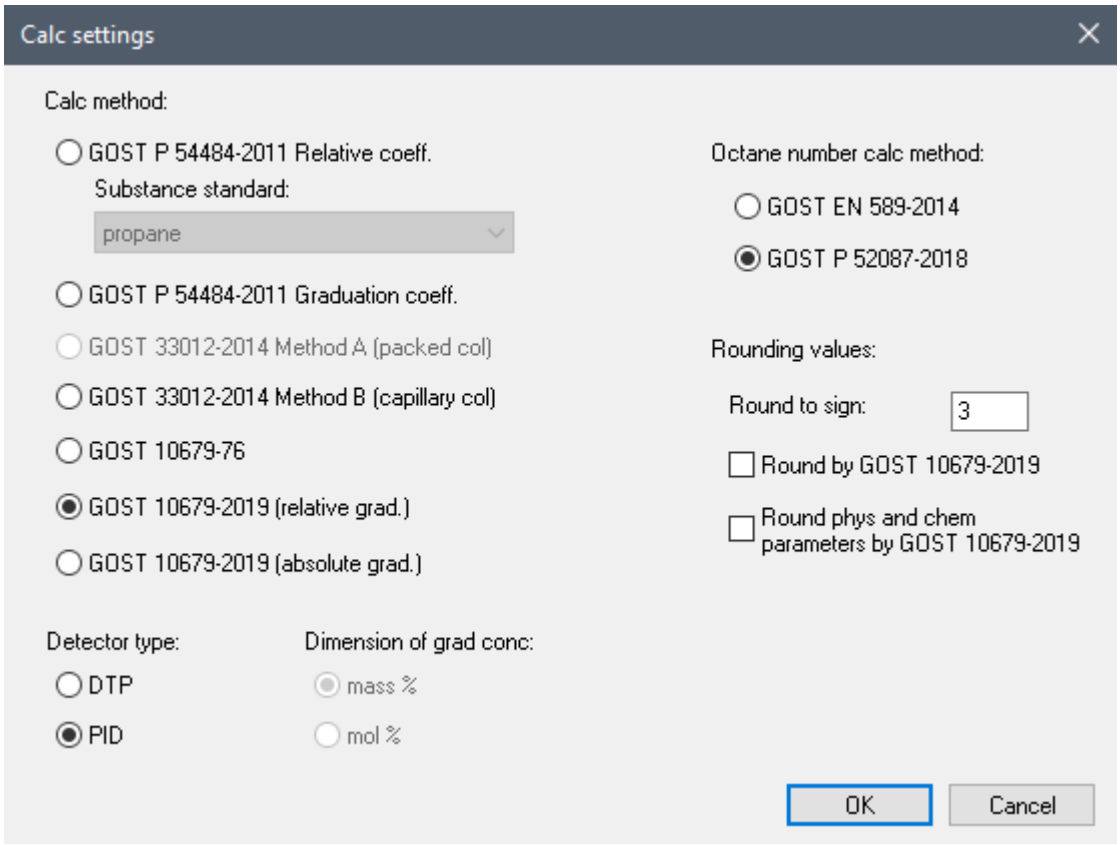
If suitable chromatograms are selected, a full calculation will be performed immediately, otherwise error and warning messages will be displayed in the **System Messages** window. For calculation, it is enough to add, depending on the chosen method, 1 chromatogram of the "Calibration" type and 1 chromatogram of the "Analysis" type, but in order to comply with GOST R 54484-2011, at least 3 chromatograms of the calibration type must be added (GOST R 54484-2011 paragraph 9.5.3).

The **Del** button excludes the selected chromatograms from the calculation.

The **Del all** button excludes all chromatograms from the calculation.

Calc settings

Calc 106 has a settings window (picture 6).



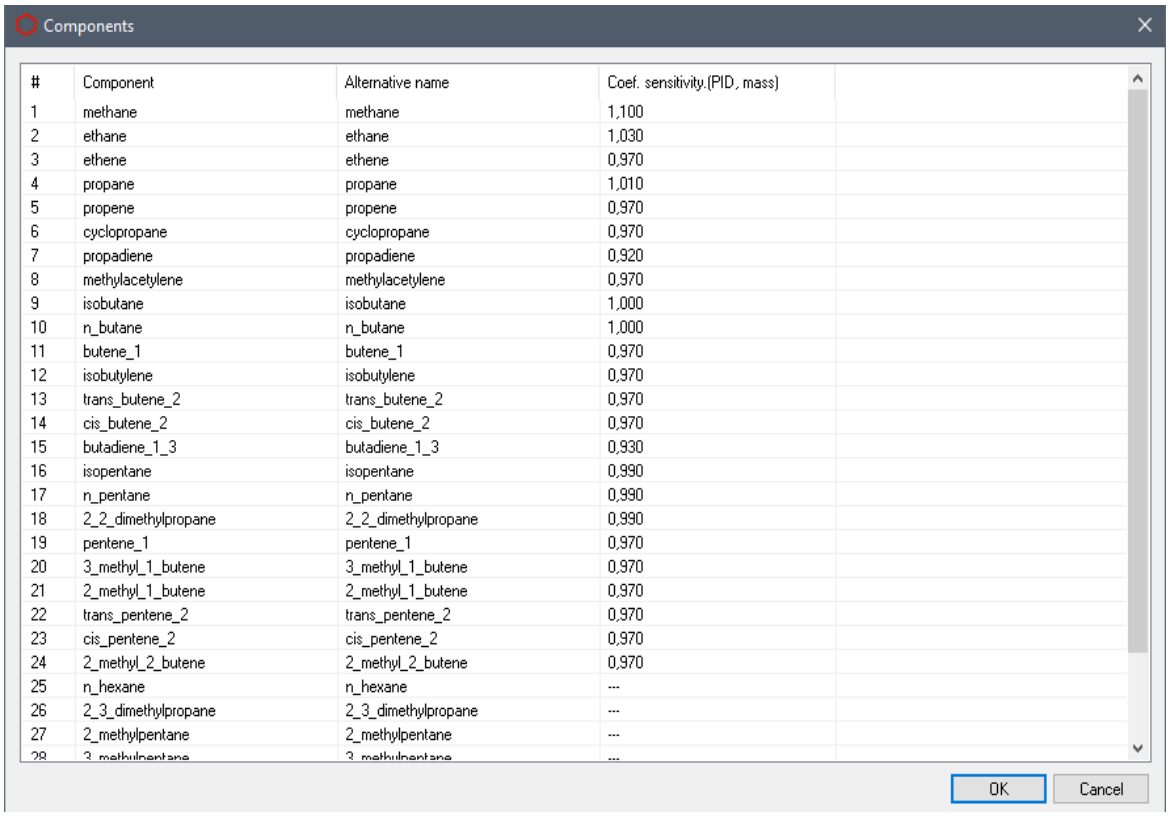
(picture 6)

Depending on the selected calculation method, certain settings become available.

When changing the configuration of the settings, they must be saved with the **OK** button. To get up-to-date results corresponding to the current settings, it is necessary to recalculate by clicking the **Calculate** button (main program window, picture 5).

During recalculations, the **System Messages** tab is updated and provides detailed information about the current calculation status (warnings, errors, etc.).

The Components window (picture 7) is called by clicking the **Components** button (the main program window, picture 5). In this window, you can set alternative component names and corresponding sensitivity coefficients. To edit the alternative name or sensitivity coefficient of a component, double-click in the field opposite the desired component and enter the desired value. If there is a dash in the sensitivity coefficient field, it means that the component was not explicitly specified in the selected guest. Components with a dash instead of a sensitivity coefficient will be skipped during calculations, if the component needs to be taken into account, then the corresponding coefficient should be entered instead of a dash.

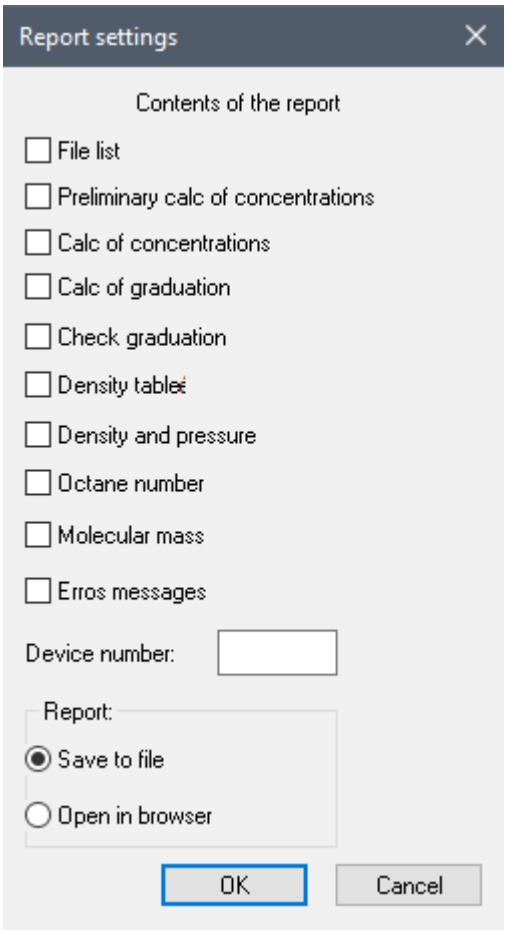


#	Component	Alternative name	Coef. sensitivity.(PID, mass)
1	methane	methane	1,100
2	ethane	ethane	1,030
3	ethene	ethene	0,970
4	propane	propane	1,010
5	propene	propene	0,970
6	cyclopropane	cyclopropane	0,970
7	propadiene	propadiene	0,920
8	methylacetylene	methylacetylene	0,970
9	isobutane	isobutane	1,000
10	n_butane	n_butane	1,000
11	butene_1	butene_1	0,970
12	isobutylene	isobutylene	0,970
13	trans_butene_2	trans_butene_2	0,970
14	cis_butene_2	cis_butene_2	0,970
15	butadiene_1_3	butadiene_1_3	0,930
16	isopentane	isopentane	0,990
17	n_pentane	n_pentane	0,990
18	2_2_dimethylpropane	2_2_dimethylpropane	0,990
19	pentene_1	pentene_1	0,970
20	3_methyl_1_butene	3_methyl_1_butene	0,970
21	2_methyl_1_butene	2_methyl_1_butene	0,970
22	trans_pentene_2	trans_pentene_2	0,970
23	cis_pentene_2	cis_pentene_2	0,970
24	2_methyl_2_butene	2_methyl_2_butene	0,970
25	n_hexane	n_hexane	---
26	2_3_dimethylpropane	2_3_dimethylpropane	---
27	2_methylpentane	2_methylpentane	---
28	3_methylpentane	3_methylpentane	---

(picture 7)

Generating a report

To generate a report, you must specify what content it will be filled with, as well as specify how it will be saved (picture 8).



(picture 8)

The file report is generated in the format **.html**