



**User Manual: Calculation №101
«Detailed Hydrocarbon Analysis of Gasoline»**

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1. Introduction

1. Introduction

The “Detailed Hydrocarbon Analysis of Gasoline” program is designed to analyze chromatograms obtained using Chromos SW to determine the hydrocarbon composition of gasoline in accordance with GOST R 52714-2007. For analysis, the database can be used either from GOST R 52714-2007 or ASTM 9730.

Before getting started, it is recommended to study GOST R 52714-2007.

This software works as an extension and can only be launched on a registered copy of Chromos SW. To run the program you need a key.

The plug-in installation file and documentation are available on the Internet at: kb.has.ru/soft:dop_raschjot_101.

E-mail your suggestions and comments on the software to: soft@has.ru

2. Installing the Software

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You need 4 Mb of free space on your local drive. To install the software, do the following:

1. Run the installation file.
2. Specify the installation path and click **Install**.
3. When installed, click **Finish**.

After the software is successfully installed you can run it from Chromos SW.

3. Running the Plug-in

3. Running the Plug-in

This software works as an extension for Chromos SW. To run the extension, do the following:

1. Connect the key to a USB port.
2. Run Chromos SW.
3. In the *Data* menu, navigate to **Calculations** > **Detailed Hydrocarbon Analysis of Gasoline** (Fig. 1). The main program window opens (Fig. 2).

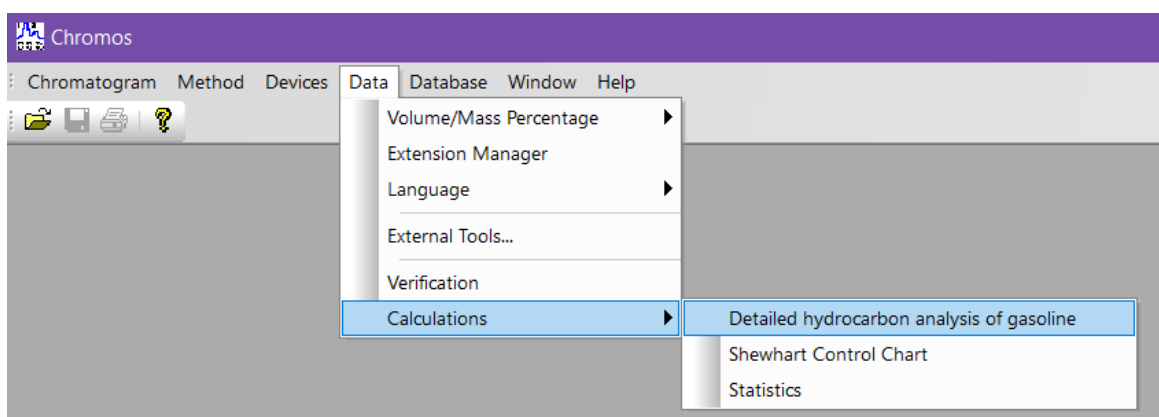


Fig. 1. Running the plug-in from Chromos SW

4. Program Overview

The main program window (Fig. 2) contains the following elements:

1. Chromatogram controls;
2. Device number field;
3. Program settings;
4. Report controls;
5. List of opened chromatograms;
6. Operation tabs.

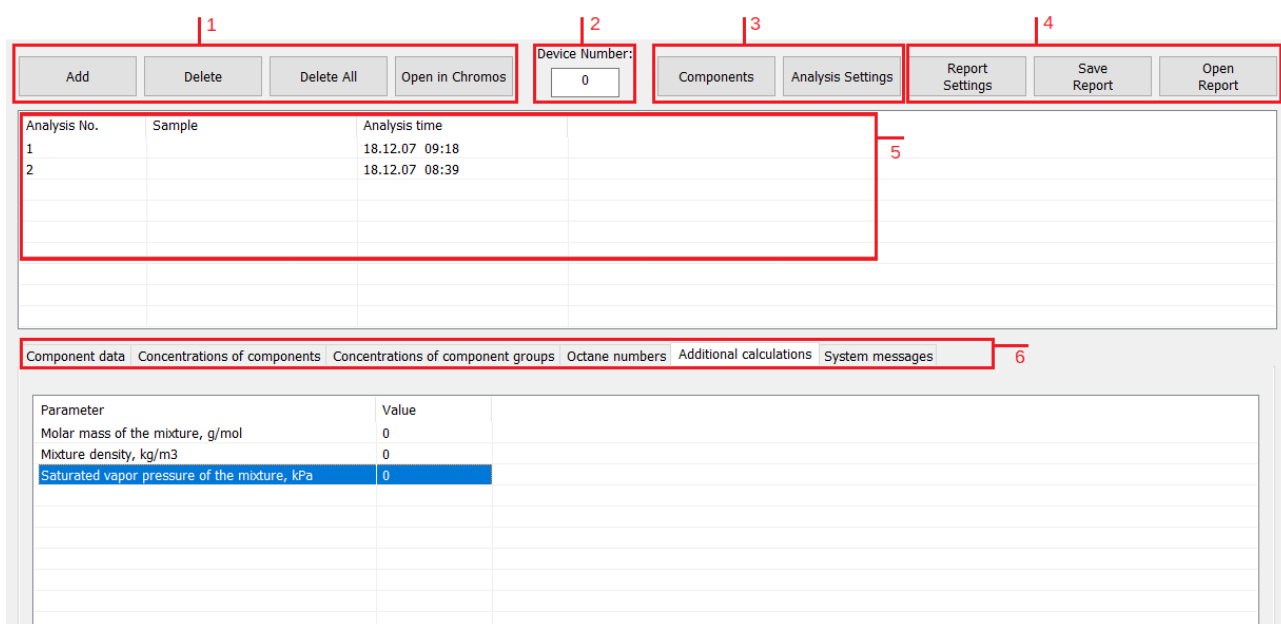


Fig. 2. Main program window

The main program window contains the following operation tabs:

- *Component data* — the tab displays information about sample components (you can select the analysis by number):
 - *No.* — string number;
 - *Component* — sample component name;
 - *Group* — group of organic compounds;
 - *Cn* — number of carbon atoms;
 - *Exit time (min)* — peak exit time (in minutes);
 - *Peak area* — peak area;
 - *Mass%* — mass fraction;
- *Concentrations of components*:
 - *No.* — string number;
 - *Component* — sample component name;
 - *Molar%* — molar fraction;
 - *Vol%* — volume fraction;
 - *Mass%* — mass fraction;

4. Program Overview

- *Difference, mass%* — difference between successive measurements (in mass fraction);
- *Diff tolerance, mass%* — permissible difference (in mass fraction);
- *Compliance* — compliance with the standard;
- *Concentrations of component groups* (you can select calculations of mole, volume, or mass fractions):
 - *C_n* — number of carbon atoms;
 - *Paraffins, Isoparaffins, Aromatics, Naphthenes, Olefins, Oxygenates* — component groups;
 - *Sum* — sum of values for all groups with a certain number of carbon atoms;
- *Octane numbers*:
 - *Component* — sample component name;
 - *Research method* — octane number calculated by the research method;
 - *Motor method* — octane number calculated by the motor method;
- *Additional calculations* — the tab displays data on additional calculation parameters;
- *System messages* — the tab displays errors and warning messages about any inconsistency or the impossibility of performing calculations due to missing data.

5. Adding Data

5. Adding Data

- To carry out the calculation, you need to add chromatograms. To add data, do the following:
 - Click **Add**. The *Select Analysis* window opens (Fig. 3).
 - In the *Select Analysis* window, select the chromatograms and click **OK**. The added files are displayed in the list of chromatograms in the main program window.

To select chromatograms, you can use filters by method, date, type, sampling place and sampling point, operator and sample. You can also select multiple files at once using combinations Ctrl + Mouse and Shift + ←↑↓→

- To delete the chromatogram, select it and click **Delete**.
- To clear the list of chromatograms, click **Delete All**.
- To open the chromatogram in Chromos SW, double-click it or select it and click **Open in Chromos**.

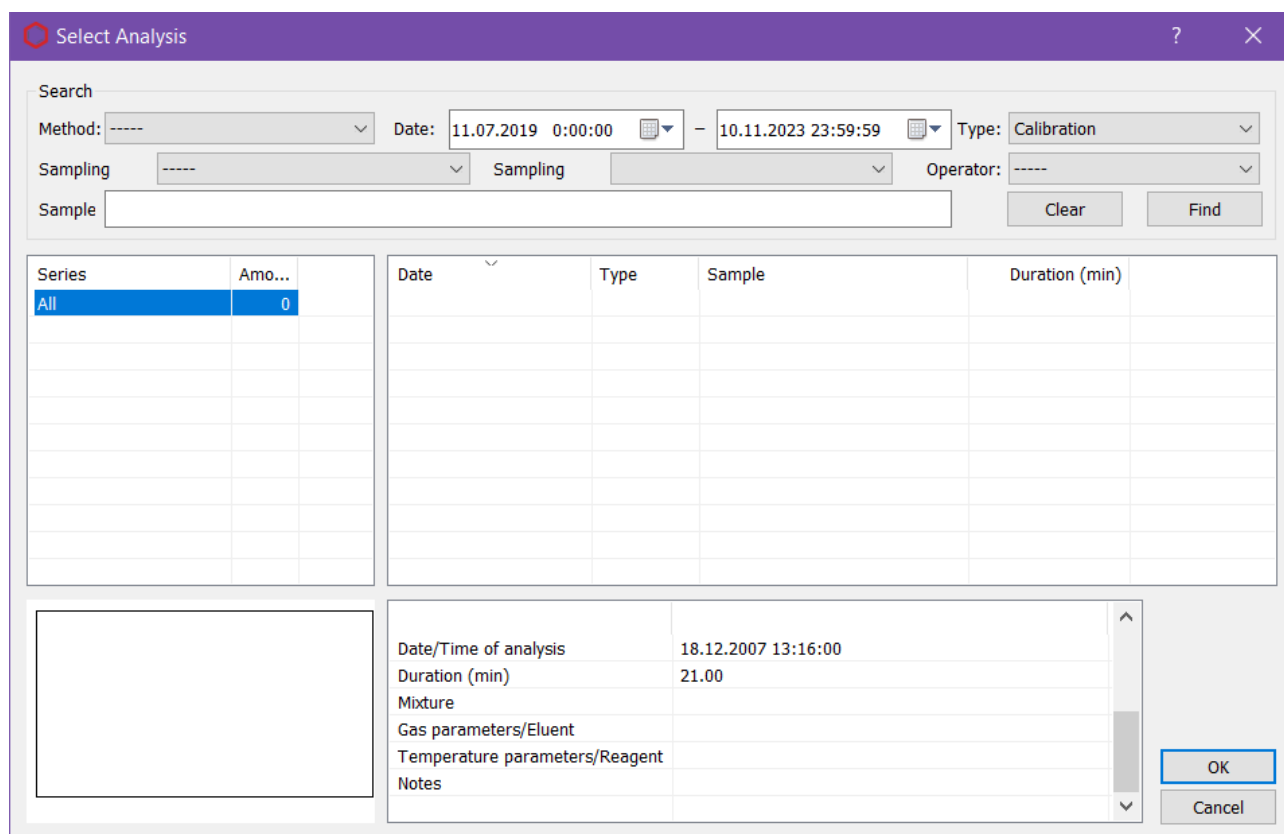


Fig. 3. Select Analysis

- In the main program window, in the *Device number* field, enter the device number.
- (Optional) Set additional components (see 7.1).

6. Reporting

You can write the calculated data to a report. In the report settings (7.3), you can select the data to add to the report.

- To generate and view the report, click **Open Report**. The report is written to an html file and automatically opened in your browser.
- To save the report, click **Save Report**. In the dialog window, specify the path and click **Save**.

By default the report is named like **Report101_17102023_114811.html**, with:

- *Report101* – program name;
- *17102023* — date in DDMMYYYY format;
- *114811* — time in HHMMSS format;
- *html* – file extension.

7. Configuring the Program Settings

Setting up the program includes managing the components, configuring the analysis parameters, and configuring the report parameters.

7.1. Managing the Components

The component list contains predefined component entries. Additional components also can be added. To manage the components, do the following:

1. In the main program window, click **Components**. The *Components* window opens (Fig. 4).
2. To add a component, click **Add Component**. A new entry is displayed in the list.
3. To edit component parameters, double-click the corresponding field. When edited, new entries are highlighted in yellow, existing ones are highlighted in green.

- In the *Component* field, enter the component name.

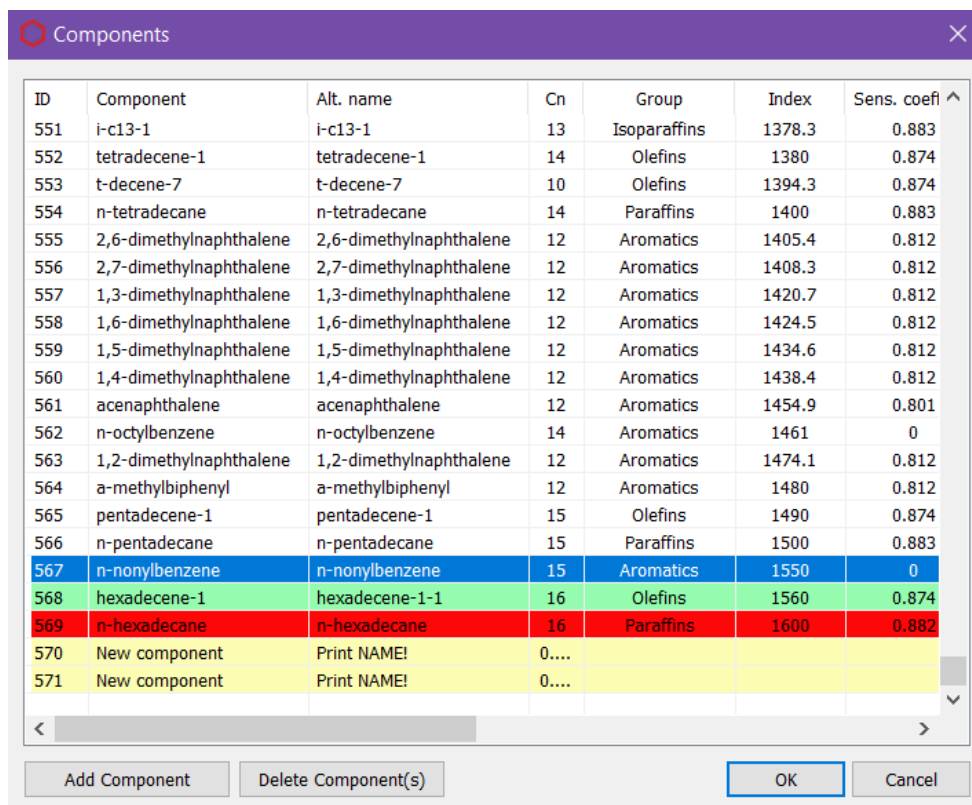
Components should have unique names.

- In the *Sens. coefficient* field, enter the column sensitivity coefficient.

To exclude any peak from the calculation, add the appropriate component and set the sensitivity coefficient to zero.

- In the *Alt. name* enter the additional component name (can match the main name).
 - In the *Cn* field, enter the number of carbon atoms.
 - In the *Group* field, enter the name of a component group.
 - In the *Index* field, enter the retention index value.
 - In the *Density* field, enter the component density (in g/cm³).
 - In the *Boiling temp, °C* field, enter the boiling temperature value (in °C).
 - In the *Molar mass* field, enter the component molar mass (in g/mol).
 - In the *Octane number (RON)* field, enter the octane number calculated using the research method.
 - In the *Octane number (MON)* field, enter the octane number calculated using the motor method.
 - In the *Pressure* field, enter the saturated vapor pressure (in kPa).
4. To delete the component, select it and click **Delete Component(s)**. New components (yellow entries) are removed immediately, existing ones are highlighted in red.
 5. To save the changes, click **OK**. The color coding of entries disappears.

7.1. Managing the Components



ID	Component	Alt. name	Cn	Group	Index	Sens. coef
551	i-c13-1	i-c13-1	13	Isoparaffins	1378.3	0.883
552	tetradecene-1	tetradecene-1	14	Olefins	1380	0.874
553	t-decene-7	t-decene-7	10	Olefins	1394.3	0.874
554	n-tetradecane	n-tetradecane	14	Paraffins	1400	0.883
555	2,6-dimethylnaphthalene	2,6-dimethylnaphthalene	12	Aromatics	1405.4	0.812
556	2,7-dimethylnaphthalene	2,7-dimethylnaphthalene	12	Aromatics	1408.3	0.812
557	1,3-dimethylnaphthalene	1,3-dimethylnaphthalene	12	Aromatics	1420.7	0.812
558	1,6-dimethylnaphthalene	1,6-dimethylnaphthalene	12	Aromatics	1424.5	0.812
559	1,5-dimethylnaphthalene	1,5-dimethylnaphthalene	12	Aromatics	1434.6	0.812
560	1,4-dimethylnaphthalene	1,4-dimethylnaphthalene	12	Aromatics	1438.4	0.812
561	acenaphthalene	acenaphthalene	12	Aromatics	1454.9	0.801
562	n-octylbenzene	n-octylbenzene	14	Aromatics	1461	0
563	1,2-dimethylnaphthalene	1,2-dimethylnaphthalene	12	Aromatics	1474.1	0.812
564	a-methylbiphenyl	a-methylbiphenyl	12	Aromatics	1480	0.812
565	pentadecene-1	pentadecene-1	15	Olefins	1490	0.874
566	n-pentadecane	n-pentadecane	15	Paraffins	1500	0.883
567	n-nonylbenzene	n-nonylbenzene	15	Aromatics	1550	0
568	hexadecene-1	hexadecene-1-1	16	Olefins	1560	0.874
569	n-hexadecane	n-hexadecane	16	Paraffins	1600	0.882
570	New component	Print NAME!	0....			
571	New component	Print NAME!	0....			

Fig. 4. Components

7.2. Configuring the Analysis Settings

The components base standard is selected in the analysis settings:

1. In the main program window, click **Analysis Settings**. The *Analysis Settings* window opens (Fig. 5).
2. In the *Analysis Settings* window, select the components base standard:
 - GOST 52714-2007
 - ASTM D6730
3. To save the changes, click **OK**.

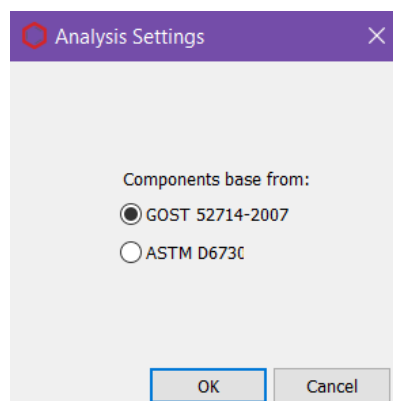


Fig. 5. Analysis Settings

7.3. Configuring the Report Setting

7.3. Configuring the Report Setting

To set the report contents, do the following:

1. In the main program window, click **Report Settings**. The *Report Settings* window opens (Fig. 6).
2. In the *Report Settings* window, check the boxes of the elements that you need to add to a report.
3. Click **OK**.

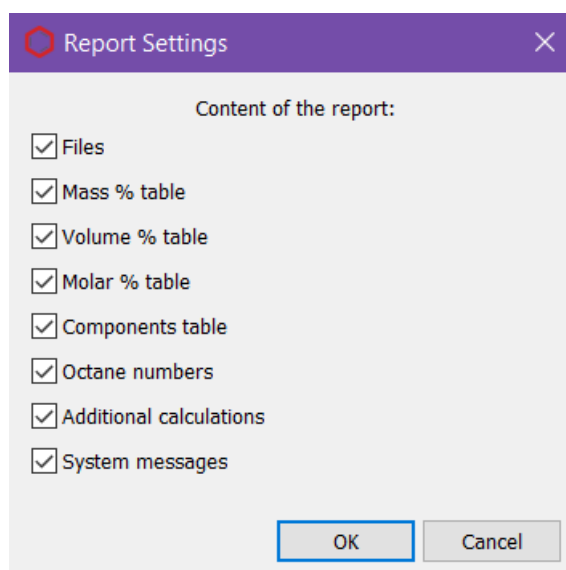


Fig. 6. Report Settings

8. Program Identification

To view the program details, in the top left corner click on the icon, then in the context menu select **Plug-in details...** The *About...* window opens (Fig. 7).

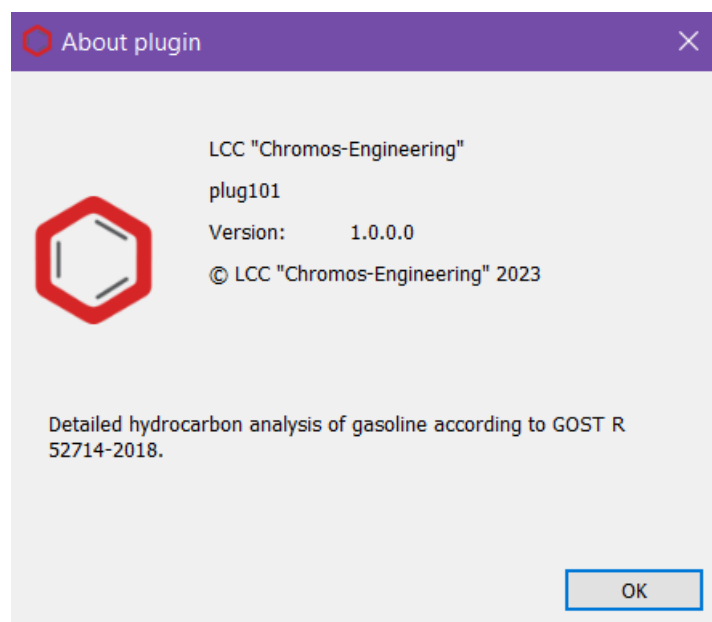


Fig. 7. About...