Online calculator for calculating the mass concentration of volatile compounds in alcohol-containing products

MANUAL

Content

1 Use

The program is designed to perform calculations during chromatographic analysis to determine the quantitative content of volatile compounds in ethanol-containing products.

2 Scope

The program was developed for use in testing laboratories for the quality and safety control of alcoholic and alcohol-containing products to calculate the values of mass concentrations of volatile compounds in alcohol-containing products.

3 Functionality

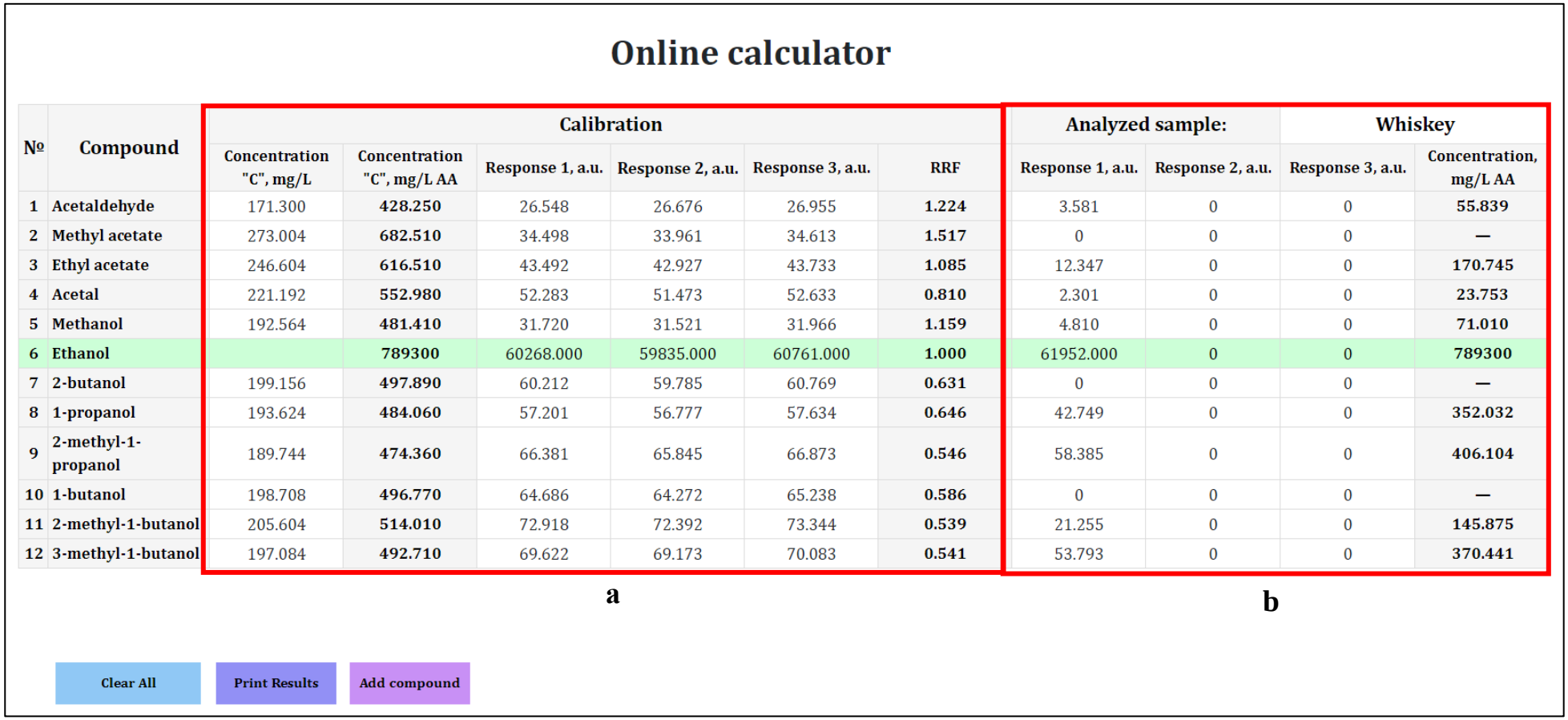
The program allows you to calculate the values of mass concentrations of volatile compounds in alcohol-containing products online using a browser.

The program allows you to set the conditions according to which a table will be generated that meets the user's needs: it provides a choice of the calibration mixture, the number of measurements of the calibration mixture and the test sample.

The program allows you to print and save the received report.

4 Workspace

The workspace of the program consists of two blocks: a calibration block and a sample test block (Fig. 1).



Online calculator

№	Compound	Calibration						Analyzed sample:		Whiskey	
		Concentration "C", mg/L	Concentration "C", mg/L AA	Response 1, a.u.	Response 2, a.u.	Response 3, a.u.	RRF	Response 1, a.u.	Response 2, a.u.	Response 3, a.u.	Concentration, mg/L AA
1	Acetaldehyde	171.300	**428.250**	26.548	26.676	26.955	**1.224**	3.581	0	0	**55.839**
2	Methyl acetate	273.004	**682.510**	34.498	33.961	34.613	**1.517**	0	0	0	—
3	Ethyl acetate	246.604	**616.510**	43.492	42.927	43.733	**1.085**	12.347	0	0	**170.745**
4	Acetal	221.192	**552.980**	52.283	51.473	52.633	**0.810**	2.301	0	0	**23.753**
5	Methanol	192.564	**481.410**	31.720	31.521	31.966	**1.159**	4.810	0	0	**71.010**
6	Ethanol		**789300**	60268.000	59835.000	60761.000	**1.000**	61952.000	0	0	**789300**
7	2-butanol	199.156	**497.890**	60.212	59.785	60.769	**0.631**	0	0	0	—
8	1-propanol	193.624	**484.060**	57.201	56.777	57.634	**0.646**	42.749	0	0	**352.032**
9	2-methyl-1-propanol	189.744	**474.360**	66.381	65.845	66.873	**0.546**	58.385	0	0	**406.104**
10	1-butanol	198.708	**496.770**	64.686	64.272	65.238	**0.586**	0	0	0	—
11	2-methyl-1-butanol	205.604	**514.010**	72.918	72.392	73.344	**0.539**	21.255	0	0	**145.875**
12	3-methyl-1-butanol	197.084	**492.710**	69.622	69.173	70.083	**0.541**	53.793	0	0	**370.441**

a

b

Clear All

Print Results

Add compound

Fig. 1. Workspace of the program: a) a calibration block, b) a sample test block.

A more detailed description of the program is presented in paragraphs 4.1-4.5 of this user manual.

4.1 Button “Clear All”

The "Clear All" button is designed to clear the contents of the table. When you click on this button, the table contents are completely cleared, as a result of which all cells are cleared.

a)

№	Compound	Calibration						Analyzed sample:		Whiskey	
		Concentration "C", mg/L	Concentration "C", mg/L AA	Response 1, a.u.	Response 2, a.u.	Response 3, a.u.	RRF	Response 1, a.u.	Response 2, a.u.	Response 3, a.u.	Concentration, mg/L AA
1	Acetaldehyde	171.300	**428.250**	26.548	26.676	26.955	**1.224**	3.581	0	0	**55.839**
2	Methyl acetate	273.004	**682.510**	34.498	33.961	34.613	**1.517**	0	0	0	**—**
3	Ethyl acetate	246.604	**616.510**	43.492	42.927	43.733	**1.085**	12.347	0	0	**170.745**
4	Acetal	221.192	**552.980**	52.283	51.473	52.633	**0.810**	2.301	0	0	**23.753**
5	Methanol	192.564	**481.410**	31.720	31.521	31.966	**1.159**	4.810	0	0	**71.010**
6	Ethanol		**789300**	60268.000	59835.000	60761.000	**1.000**	61952.000	0	0	**789300**
7	2-butanol	199.156	**497.890**	60.212	59.785	60.769	**0.631**	0	0	0	**—**
8	1-propanol	193.624	**484.060**	57.201	56.777	57.634	**0.646**	42.749	0	0	**352.032**
9	2-methyl-1-propanol	189.744	**474.360**	66.381	65.845	66.873	**0.546**	58.385	0	0	**406.104**
10	1-butanol	198.708	**496.770**	64.686	64.272	65.238	**0.586**	0	0	0	**—**
11	2-methyl-1-butanol	205.604	**514.010**	72.918	72.392	73.344	**0.539**	21.255	0	0	**145.875**
12	3-methyl-1-butanol	197.084	**492.710**	69.622	69.173	70.083	**0.541**	53.793	0	0	**370.441**

Clearing

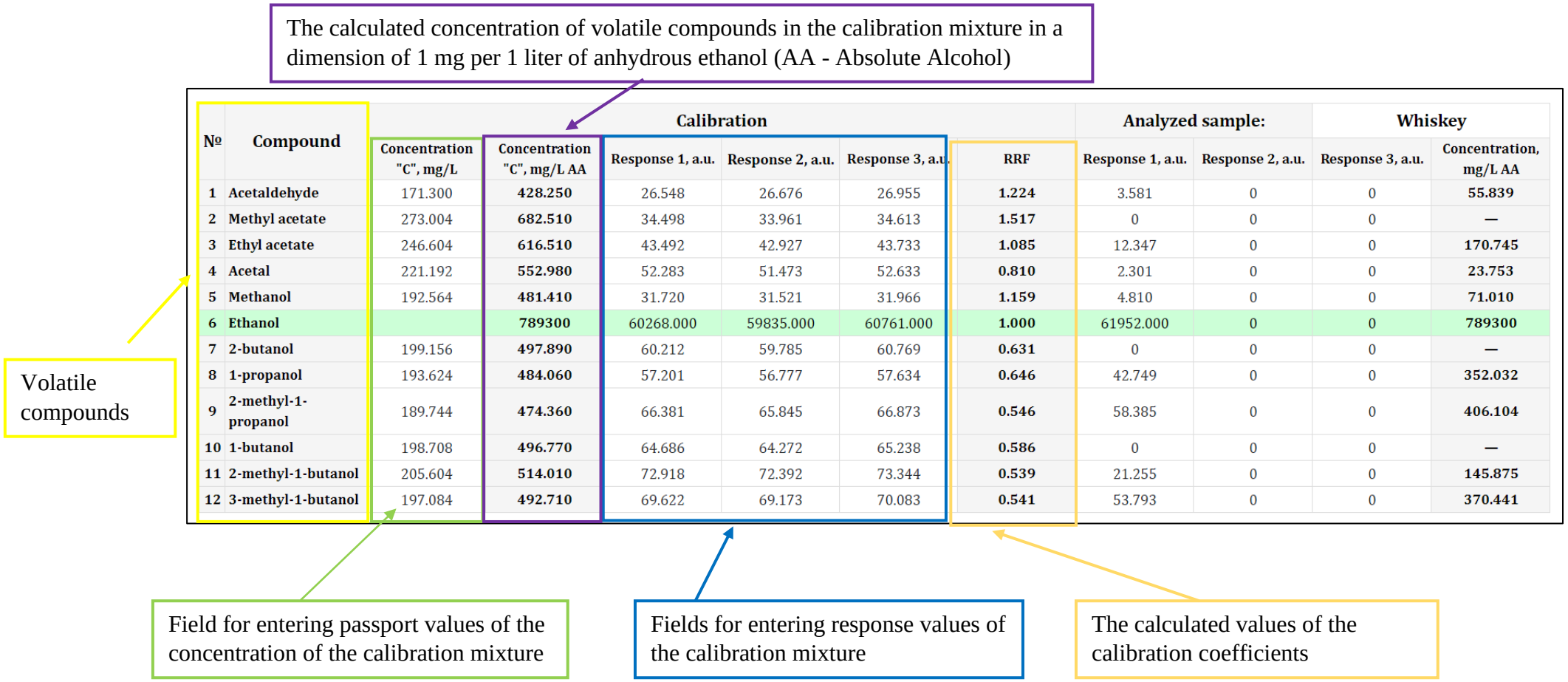
b)

№	Compound	Calibration						Analyzed sample:			
		Concentration "C", mg/L	Concentration "C", mg/L AA	Response 1, a.u.	Response 2, a.u.	Response 3, a.u.	RRF	Response 1, a.u.	Response 2, a.u.	Response 3, a.u.	Concentration, mg/L AA
1	Acetaldehyde	0	**0**	0	0	0	**—**	0	0	0	**—**
2	Methyl acetate	0	**0**	0	0	0	**—**	0	0	0	**—**
3	Ethyl acetate	0	**0**	0	0	0	**—**	0	0	0	**—**
4	Acetal	0	**0**	0	0	0	**—**	0	0	0	**—**
5	Methanol	0	**0**	0	0	0	**—**	0	0	0	**—**
6	Ethanol		**789300**	0	0	0	**—**	0	0	0	**—**
7	2-butanol	0	**0**	0	0	0	**—**	0	0	0	**—**
8	1-propanol	0	**0**	0	0	0	**—**	0	0	0	**—**
9	2-methyl-1-propanol	0	**0**	0	0	0	**—**	0	0	0	**—**
10	1-butanol	0	**0**	0	0	0	**—**	0	0	0	**—**
11	2-methyl-1-butanol	0	**0**	0	0	0	**—**	0	0	0	**—**
12	3-methyl-1-butanol	0	**0**	0	0	0	**—**	0	0	0	**—**

Fig. 2. Form of the table: a) before cleaning, b) after cleaning.

4.2 Calibration block

The program calibration block is intended for entering data on the used calibration mixtures (concentration, response values) and calculation of the calibration coefficients RRF (Fig. 3).

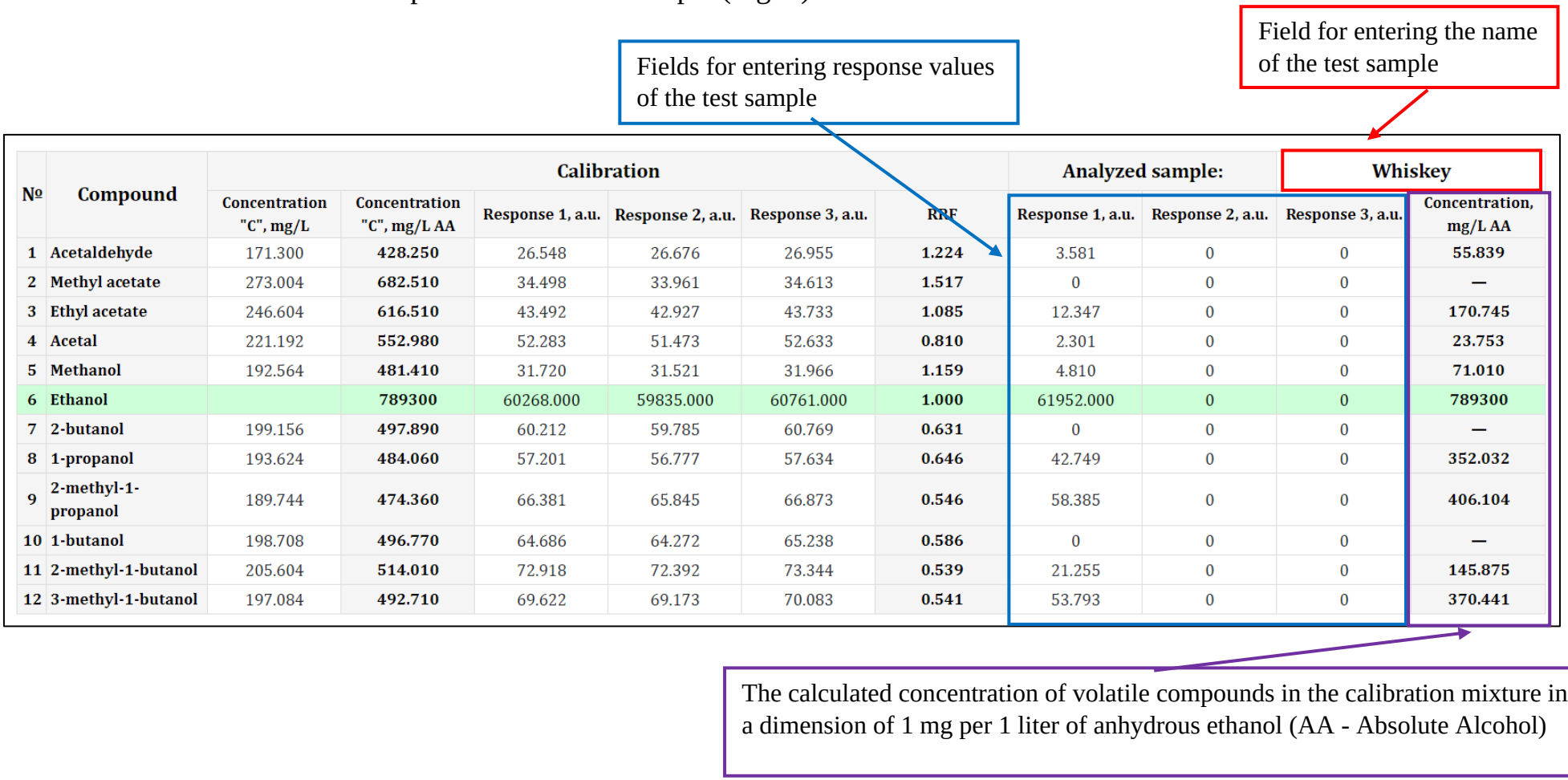


№	Compound	Calibration						Analyzed sample:		Whiskey	
		Concentration "C", mg/L	Concentration "C", mg/L AA	Response 1, a.u.	Response 2, a.u.	Response 3, a.u.	RRF	Response 1, a.u.	Response 2, a.u.	Response 3, a.u.	Concentration, mg/L AA
1	Acetaldehyde	171.300	**428.250**	26.548	26.676	26.955	**1.224**	3.581	0	0	**55.839**
2	Methyl acetate	273.004	**682.510**	34.498	33.961	34.613	**1.517**	0	0	0	**—**
3	Ethyl acetate	246.604	**616.510**	43.492	42.927	43.733	**1.085**	12.347	0	0	**170.745**
4	Acetal	221.192	**552.980**	52.283	51.473	52.633	**0.810**	2.301	0	0	**23.753**
5	Methanol	192.564	**481.410**	31.720	31.521	31.966	**1.159**	4.810	0	0	**71.010**
6	Ethanol		**789300**	60268.000	59835.000	60761.000	**1.000**	61952.000	0	0	**789300**
7	2-butanol	199.156	**497.890**	60.212	59.785	60.769	**0.631**	0	0	0	**—**
8	1-propanol	193.624	**484.060**	57.201	56.777	57.634	**0.646**	42.749	0	0	**352.032**
9	2-methyl-1-propanol	189.744	**474.360**	66.381	65.845	66.873	**0.546**	58.385	0	0	**406.104**
10	1-butanol	198.708	**496.770**	64.686	64.272	65.238	**0.586**	0	0	0	**—**
11	2-methyl-1-butanol	205.604	**514.010**	72.918	72.392	73.344	**0.539**	21.255	0	0	**145.875**
12	3-methyl-1-butanol	197.084	**492.710**	69.622	69.173	70.083	**0.541**	53.793	0	0	**370.441**

Fig. 3. Calibration block.

4.3 Test sample block

The unit for testing the sample is intended for entering data obtained during measurements of the test sample and calculating the concentrations of volatile compounds in the test sample (Fig. 4).



№	Compound	Calibration						Analyzed sample:			Whiskey
		Concentration "C", mg/L	Concentration "C", mg/L AA	Response 1, a.u.	Response 2, a.u.	Response 3, a.u.	RRF	Response 1, a.u.	Response 2, a.u.	Response 3, a.u.	Concentration, mg/L AA
1	Acetaldehyde	171.300	**428.250**	26.548	26.676	26.955	**1.224**	3.581	0	0	**55.839**
2	Methyl acetate	273.004	**682.510**	34.498	33.961	34.613	**1.517**	0	0	0	**—**
3	Ethyl acetate	246.604	**616.510**	43.492	42.927	43.733	**1.085**	12.347	0	0	**170.745**
4	Acetal	221.192	**552.980**	52.283	51.473	52.633	**0.810**	2.301	0	0	**23.753**
5	Methanol	192.564	**481.410**	31.720	31.521	31.966	**1.159**	4.810	0	0	**71.010**
6	Ethanol		**789300**	60268.000	59835.000	60761.000	**1.000**	61952.000	0	0	**789300**
7	2-butanol	199.156	**497.890**	60.212	59.785	60.769	**0.631**	0	0	0	**—**
8	1-propanol	193.624	**484.060**	57.201	56.777	57.634	**0.646**	42.749	0	0	**352.032**
9	2-methyl-1-propanol	189.744	**474.360**	66.381	65.845	66.873	**0.546**	58.385	0	0	**406.104**
10	1-butanol	198.708	**496.770**	64.686	64.272	65.238	**0.586**	0	0	0	**—**
11	2-methyl-1-butanol	205.604	**514.010**	72.918	72.392	73.344	**0.539**	21.255	0	0	**145.875**
12	3-methyl-1-butanol	197.084	**492.710**	69.622	69.173	70.083	**0.541**	53.793	0	0	**370.441**

Fig. 4. Test sample block.

4.4 Button “Print”

The “Print” button is intended for printing the contents of the table. When you click on this button, the contents of the table are printed.

4.5 Button “Add compound”

The “Add compound” button is used to add a substance to the table. By clicking on this button, you can add from 1 to 3 compounds to the table (Fig. 5).

Online calculator

№	Compound	Calibration						Analyzed sample:		Whiskey	
		Concentration "C", mg/L	Concentration "C", mg/L AA	Response 1, a.u.	Response 2, a.u.	Response 3, a.u.	RRF	Response 1, a.u.	Response 2, a.u.	Response 3, a.u.	Concentration, mg/L AA
1	Acetaldehyde	171.300	**428.250**	26.548	26.676	26.955	**1.224**	3.581	0	0	**55.839**
2	Methyl acetate	273.004	**682.510**	34.498	33.961	34.613	**1.517**	0	0	0	**—**
3	Ethyl acetate	246.604	**616.510**	43.492	42.927	43.733	**1.085**	12.347	0	0	**170.745**
4	Acetal	221.192	**552.980**	52.283	51.473	52.633	**0.810**	2.301	0	0	**23.753**
5	Methanol	192.564	**481.410**	31.720	31.521	31.966	**1.159**	4.810	0	0	**71.010**
6	Ethanol		**789300**	60268.000	59835.000	60761.000	**1.000**	61952.000	0	0	**789300**
7	2-butanol	199.156	**497.890**	60.212	59.785	60.769	**0.631**	0	0	0	**—**
8	1-propanol	193.624	**484.060**	57.201	56.777	57.634	**0.646**	42.749	0	0	**352.032**
9	2-methyl-1-propanol	189.744	**474.360**	66.381	65.845	66.873	**0.546**	58.385	0	0	**406.104**
10	1-butanol	198.708	**496.770**	64.686	64.272	65.238	**0.586**	0	0	0	**—**
11	2-methyl-1-butanol	205.604	**514.010**	72.918	72.392	73.344	**0.539**	21.255	0	0	**145.875**
12	3-methyl-1-butanol	197.084	**492.710**	69.622	69.173	70.083	**0.541**	53.793	0	0	**370.441**
13				0	0	0	**—**	0	0	0	**—**
14				0	0	0	**—**	0	0	0	**—**
15				0	0	0	**—**	0	0	0	**—**

Clear All Print Results Remove

Fig. 5. Appearance of the calculator after adding compounds.

5 Error messages

When using the program, error messages may appear. Examples of such messages are shown in the table 1.

Table 1. Error messages

Error	The cause of the error	Solution
Ethanol!	The response values for ethanol are not entered.	Enter response values for ethanol.

6 Calculations

The principle of calculating the mass concentrations of volatile compounds in alcohol-containing products is based on the use of ethanol as an internal standard. http://www.inp.bsu.by/ethanol/en/Method_theory.html.

7 Example

7.1 Establishment of calibration characteristics

Concentration values, obtained during preparation of standard solutions, are entered in the field “Concentration “C”, mg/L” (Fig. 6, a). After that, the program recalculates the concentrations of volatile compounds in CO from 1 mg per 1 liter of the mixture to 1 mg per 1 liter of anhydrous ethanol in the "Concentration “C”, mg/L AA" field (Fig. 6, b).

№	Compound	a)	b)	Calibration			
		Concentration "C", mg/L	Concentration "C", mg/L AA	Response 1, a.u.	Response 2, a.u.	Response 3, a.u.	RRF
1	Acetaldehyde	171.300	**428.250**	26.548	26.676	26.955	**1.224**
2	Methyl acetate	273.004	**682.510**	34.498	33.961	34.613	**1.517**
3	Ethyl acetate	246.604	**616.510**	43.492	42.927	43.733	**1.085**
4	Acetal	221.192	**552.980**	52.283	51.473	52.633	**0.810**
5	Methanol	192.564	**481.410**	31.720	31.521	31.966	**1.159**
6	Ethanol		**789300**	60268.000	59835.000	60761.000	**1.000**
7	2-butanol	199.156	**497.890**	60.212	59.785	60.769	**0.631**
8	1-propanol	193.624	**484.060**	57.201	56.777	57.634	**0.646**
9	2-methyl-1-propanol	189.744	**474.360**	66.381	65.845	66.873	**0.546**
10	1-butanol	198.708	**496.770**	64.686	64.272	65.238	**0.586**
11	2-methyl-1-butanol	205.604	**514.010**	72.918	72.392	73.344	**0.539**
12	3-methyl-1-butanol	197.084	**492.710**	69.622	69.173	70.083	**0.541**

Fig. 6. Fields: a) “Concentration “C”, mg/L”, b) “Concentration “C”, mg/L AA”

The Fig. 7 shows the measured chromatogram of calibration solution in a logarithmic scale.

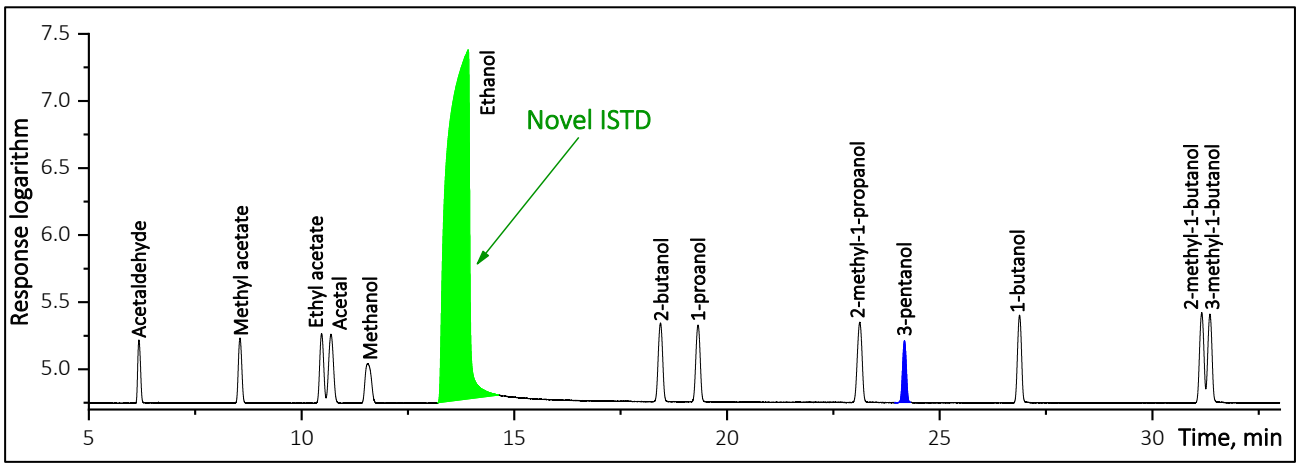


Fig. 7. Chromatogram of calibration solution on a logarithmic scale.

The data of the response values obtained during the measurements are entered in the field “Response, a.u.” (Fig 8).

№	Compound	Calibration					
		Concentration "C", mg/L	Concentration "C", mg/L AA	Response 1, a.u.	Response 2, a.u.	Response 3, a.u.	RRF
1	Acetaldehyde	171.300	428.250	26.548	26.676	26.955	1.224
2	Methyl acetate	273.004	682.510	34.498	33.961	34.613	1.517
3	Ethyl acetate	246.604	616.510	43.492	42.927	43.733	1.085
4	Acetal	221.192	552.980	52.283	51.473	52.633	0.810
5	Methanol	192.564	481.410	31.720	31.521	31.966	1.159
6	Ethanol		789300	60268.000	59835.000	60761.000	1.000
7	2-butanol	199.156	497.890	60.212	59.785	60.769	0.631
8	1-propanol	193.624	484.060	57.201	56.777	57.634	0.646
9	2-methyl-1-propanol	189.744	474.360	66.381	65.845	66.873	0.546
10	1-butanol	198.708	496.770	64.686	64.272	65.238	0.586
11	2-methyl-1-butanol	205.604	514.010	72.918	72.392	73.344	0.539
12	3-methyl-1-butanol	197.084	492.710	69.622	69.173	70.083	0.541

Fig. 8. Entering data on the response values of the compounds of the calibration solution.

After that, the program calculates the RRF values that are displayed in the “RRF” field (Fig. 9).

№	Compound	Calibration					
		Concentration "C", mg/L	Concentration "C", mg/L AA	Response 1, a.u.	Response 2, a.u.	Response 3, a.u.	RRF
1	Acetaldehyde	171.300	428.250	26.548	26.676	26.955	1.224
2	Methyl acetate	273.004	682.510	34.498	33.961	34.613	1.517
3	Ethyl acetate	246.604	616.510	43.492	42.927	43.733	1.085
4	Acetal	221.192	552.980	52.283	51.473	52.633	0.810
5	Methanol	192.564	481.410	31.720	31.521	31.966	1.159
6	Ethanol		789300	60268.000	59835.000	60761.000	1.000
7	2-butanol	199.156	497.890	60.212	59.785	60.769	0.631
8	1-propanol	193.624	484.060	57.201	56.777	57.634	0.646
9	2-methyl-1-propanol	189.744	474.360	66.381	65.845	66.873	0.546
10	1-butanol	198.708	496.770	64.686	64.272	65.238	0.586
11	2-methyl-1-butanol	205.604	514.010	72.918	72.392	73.344	0.539
12	3-methyl-1-butanol	197.084	492.710	69.622	69.173	70.083	0.541

Fig. 9. Form of the filled calibration block.

7.2 Test sample

A gas chromatographic measurement of a Whiskey sample is performed. In the field “Analyzed sample” the name of the sample “Whiskey” is indicated (Fig. 10)

Analyzed sample:	Whiskey

Fig. 10. Entering of initial parameters: name of the test sample.

The Fig. 11 shows the measured chromatogram of whiskey sample in a logarithmic scale.

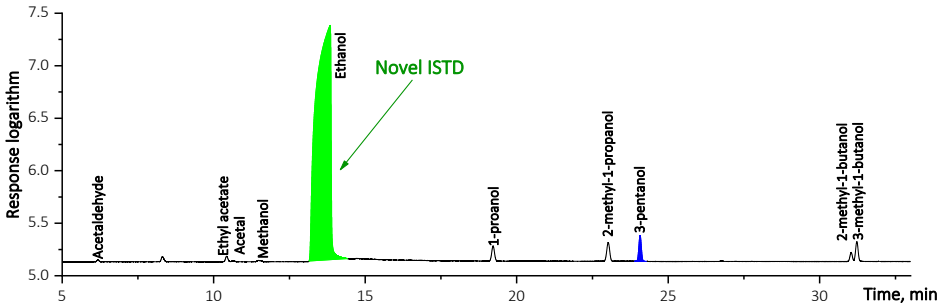


Fig. 11. Chromatogram of whiskey sample.

The data of the response values obtained during the measurements are entered in the field “Response, a.u.” (Fig 12).

Analyzed sample:		Whiskey	
Response 1, a.u.	Response 2, a.u.	Response 3, a.u.	Concentration, mg/L AA
3.581	0	0	55.839
0	0	0	—
12.347	0	0	170.745
2.301	0	0	23.753
4.810	0	0	71.010
61952.000	0	0	789300
0	0	0	—
42.749	0	0	352.032
58.385	0	0	406.104
0	0	0	—
21.255	0	0	145.875
53.793	0	0	370.441

Fig. 12. Entering data on the response values of the compounds of the calibration solution.

After that, the program calculates the concentrations of volatile compounds in the test sample in a dimension of 1 mg per 1 liter of anhydrous ethanol (Fig. 13).

Online calculator

№	Compound	Calibration						Analyzed sample:		Whiskey	
		Concentration "C", mg/L	Concentration "C", mg/L AA	Response 1, a.u.	Response 2, a.u.	Response 3, a.u.	RRF	Response 1, a.u.	Response 2, a.u.	Response 3, a.u.	Concentration, mg/L AA
1	Acetaldehyde	171.300	**428.250**	26.548	26.676	26.955	**1.224**	3.581	0	0	**55.839**
2	Methyl acetate	273.004	**682.510**	34.498	33.961	34.613	**1.517**	0	0	0	**—**
3	Ethyl acetate	246.604	**616.510**	43.492	42.927	43.733	**1.085**	12.347	0	0	**170.745**
4	Acetal	221.192	**552.980**	52.283	51.473	52.633	**0.810**	2.301	0	0	**23.753**
5	Methanol	192.564	**481.410**	31.720	31.521	31.966	**1.159**	4.810	0	0	**71.010**
6	Ethanol		**789300**	60268.000	59835.000	60761.000	**1.000**	61952.000	0	0	**789300**
7	2-butanol	199.156	**497.890**	60.212	59.785	60.769	**0.631**	0	0	0	**—**
8	1-propanol	193.624	**484.060**	57.201	56.777	57.634	**0.646**	42.749	0	0	**352.032**
9	2-methyl-1-propanol	189.744	**474.360**	66.381	65.845	66.873	**0.546**	58.385	0	0	**406.104**
10	1-butanol	198.708	**496.770**	64.686	64.272	65.238	**0.586**	0	0	0	**—**
11	2-methyl-1-butanol	205.604	**514.010**	72.918	72.392	73.344	**0.539**	21.255	0	0	**145.875**
12	3-methyl-1-butanol	197.084	**492.710**	69.622	69.173	70.083	**0.541**	53.793	0	0	**370.441**

Clear All | Print Results | Add compound

Fig. 13. Appearance of the filled table.