Supporting information

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The establishment of metrological characteristics of the method "Ethanol as Internal Standard" for the direct determination of volatile compounds in alcoholic products

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Table S. 1. The results of GC measurements of standard solution "WES-A" in LAR.

Compound	Ethanol as IS					Traditional Internal Standard					External Standard				
	Concentration, mg/L AA			RSD, %	Bias, %	Concentration, mg/L AA			RSD, %	Bias, %	Concentration, mg/L AA			RSD, %	Bias, %
	1	2	3			1	2	3			1	2	3		
acetaldehyde	4467	4449	4437	0.3	2.7	4627	4586	4678	0.8	6.8	5298	5206	5200	0.9	20.7
methyl acetate	5548	5558	5545	0.1	0.3	5747	5728	5847	0.9	4.4	6580	6502	6499	0.6	18.0
ethyl acetate	6805	6831	6823	0.2	0.1	7048	7040	7194	1.0	4.1	8070	7992	7997	0.4	17.7
methanol	5733	5732	5746	0.1	-0.1	5938	5908	6058	1.1	3.9	6800	6707	6735	0.6	17.5
2-propanol	5757	5759	5750	0.1	-0.3	5962	5936	6063	0.9	3.7	6827	6739	6740	0.6	17.2
ethanol	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—
1-propanol	5995	6002	6002	0.1	-0.2	6209	6186	6328	1.0	3.8	7110	7022	7035	0.5	17.4
isobutyl alc.	6171	6196	6196	0.2	-0.4	6392	6386	6533	1.1	3.6	7319	7249	7262	0.4	17.1
2-pentanol	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—
1-butanol	5985	5985	5983	0.0	-0.2	6199	6168	6308	1.0	3.8	7098	7002	7013	0.6	17.4
isoamyl alc.	6227	6226	6226	0.0	-0.3	6450	6417	6564	1.0	3.7	7385	7285	7298	0.6	17.3

Table S. 2. The results of GC measurements of standard solution "WES-B" in LAR.

Compound	Ethanol as IS					Traditional Internal Standard					External Standard				
	Concentration, mg/L AA			RSD, %	Bias, %	Concentration, mg/L AA			RSD, %	Bias, %	Concentration, mg/L AA			RSD, %	Bias, %
	1	2	3			1	2	3			1	2	3		
acetaldehyde	434	444	433	1.1	0.3	433	446	433	1.4	0.2	428	504	400	9.9	1.9
methyl acetate	489	479	496	1.4	0.2	487	481	496	1.2	0.2	482	544	458	7.3	1.6
ethyl acetate	478	470	484	1.2	0.2	476	472	483	1.0	0.2	471	534	447	7.6	1.6
methanol	528	526	528	0.2	0.2	527	528	527	0.1	0.2	521	597	488	8.6	1.7
2-propanol	514	509	514	0.4	0.0	512	511	513	0.2	0.0	506	578	475	8.3	1.5
ethanol	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—
1-propanol	532	532	533	0.0	0.0	531	534	532	0.3	0.0	525	604	492	8.7	1.5
isobutyl alc.	553	552	554	0.2	0.0	551	554	554	0.2	0.0	545	626	512	8.6	1.5
2-pentanol	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—
1-butanol	531	532	531	0.1	-0.1	529	534	531	0.4	-0.1	523	604	491	8.8	1.4
isoamyl alc.	555	556	555	0.1	-0.1	553	558	554	0.4	-0.1	547	631	512	8.8	1.4

Table S. 3. The results of GC measurements of standard solution "WES-1" in LAR.

Compound	Ethanol as IS					Traditional Internal Standard					External Standard				
	Concentration, mg/L AA			RSD, %	Bias, %	Concentration, mg/L AA			RSD, %	Bias, %	Concentration, mg/L AA			RSD, %	Bias, %
	1	2	3			1	2	3			1	2	3		
acetaldehyde	49.9	48.8	49.0	1.0	1.3	50.2	49.0	49.2	1.1	1.8	61.2	48.2	49.9	10.9	9.2
methyl acetate	52.1	52.0	51.6	0.4	1.0	52.4	52.3	51.8	0.5	1.5	63.8	51.4	52.5	10.0	8.9
ethyl acetate	50.0	50.6	49.9	0.6	0.8	50.3	50.8	50.1	0.6	1.3	61.3	50.0	50.8	9.5	8.6
methanol	71.4	72.0	71.4	0.4	-0.1	71.9	72.4	71.7	0.4	0.4	87.6	71.2	72.8	9.6	7.7
2-propanol	52.5	55.7	55.7	2.7	-1.7	52.8	56.0	55.9	2.7	-1.2	64.4	55.1	56.7	6.9	5.6
ethanol	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—
1-propanol	56.4	56.4	56.1	0.2	-0.4	56.8	56.7	56.3	0.3	0.1	69.2	55.8	57.1	9.9	7.4
isobutyl alc.	59.2	59.1	59.0	0.2	0.3	59.6	59.3	59.3	0.3	0.8	72.6	58.4	60.1	10.0	8.2
2-pentanol	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—
1-butanol	56.6	56.7	56.9	0.2	0.2	57.0	57.0	57.1	0.1	0.7	69.4	56.1	57.9	9.6	8.0
isoamyl alc.	59.3	59.2	59.3	0.1	0.1	59.7	59.5	59.5	0.2	0.6	72.7	58.5	60.4	9.9	7.9

Table S. 4. The results of GC measurements of standard solution "WES-2" in LAR.

Compound	Ethanol as IS					Traditional Internal Standard					External Standard				
	Concentration, mg/L AA			RSD, %	Bias, %	Concentration, mg/L AA			RSD, %	Bias, %	Concentration, mg/L AA			RSD, %	Bias, %
	1	2	3			1	2	3			1	2	3		
acetaldehyde	11.2	11.2	11.2	0.2	1.7	11.3	11.2	11.3	0.2	2.2	13.5	13.7	13.7	0.8	23.7
methyl acetate	9.7	9.7	9.7	0.4	-0.4	9.7	9.8	9.7	0.4	0.1	11.6	12.0	11.8	1.2	21.2
ethyl acetate	9.5	9.6	9.6	0.4	0.9	9.6	9.7	9.6	0.4	1.4	11.5	11.8	11.7	1.3	22.7
methanol	27.5	27.8	27.6	0.4	-0.1	27.6	27.9	27.7	0.5	0.4	33.0	34.1	33.7	1.4	21.6
2-propanol	11.9	11.9	12.0	0.4	0.0	12.0	11.9	12.0	0.4	0.5	14.3	14.6	14.6	0.9	21.7
ethanol	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—
1-propanol	10.9	10.9	10.8	0.6	1.4	11.0	10.9	10.8	0.6	1.9	13.1	13.4	13.1	0.9	23.3
isobutyl alc.	11.3	11.1	11.2	0.5	-0.5	11.3	11.2	11.3	0.4	0.0	13.5	13.7	13.7	0.7	21.1
2-pentanol	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—
1-butanol	11.3	11.1	10.9	1.6	1.2	11.4	11.2	10.9	1.6	1.7	13.6	13.6	13.3	1.2	23.1
isoamyl alc.	12.2	11.7	11.7	2.0	2.1	12.3	11.8	11.7	2.0	2.6	14.6	14.4	14.2	1.1	24.2

Table S. 5. The results of GC measurements of standard solution "WES-3" in LAR.

Compound	Ethanol as IS					Traditional Internal Standard					External Standard				
	Concentration, mg/L AA			RSD, %	Bias, %	Concentration, mg/L AA			RSD, %	Bias, %	Concentration, mg/L AA			RSD, %	Bias, %
	1	2	3			1	2	3			1	2	3		
acetaldehyde	3.98	4.02	3.87	1.6	0.8	4.0	4.1	3.9	2.0	1.0	3.6	3.7	3.6	1.4	-6.7
methyl acetate	1.09	1.06	1.02	2.7	2.4	1.1	1.1	1.0	3.0	2.6	1.0	1.0	1.0	1.5	-5.2
ethyl acetate	1.11	1.10	1.19	3.5	1.7	1.1	1.1	1.2	3.1	1.9	1.0	1.0	1.1	4.5	-5.8
methanol	18.75	18.61	18.53	0.5	0.7	18.8	18.8	18.5	0.7	1.0	17.1	17.3	17.4	0.9	-6.7
2-propanol	2.92	2.65	2.59	5.3	-1.2	2.9	2.7	2.6	5.4	-1.0	2.7	2.5	2.4	3.9	-8.5
ethanol	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—
1-propanol	1.27	1.31	1.12	6.6	-3.0	1.3	1.3	1.1	7.0	-2.7	1.2	1.2	1.1	5.9	-10.1
isobutyl alc.	1.41	1.47	1.32	4.4	-3.2	1.4	1.5	1.3	4.8	-3.0	1.3	1.4	1.2	4.0	-10.4
2-pentanol	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—
1-butanol	1.61	1.72	1.59	3.5	-4.6	1.6	1.7	1.6	3.9	-4.4	1.5	1.6	1.5	3.7	-11.6
isoamyl alc.	1.75	1.78	1.67	2.6	-11.1	1.8	1.8	1.7	3.0	-10.9	1.6	1.6	1.6	2.1	-17.6

Table S. 6. The results of GC measurements of standard solution "WES-A" in RCH.

Compound	Ethanol as IS					Traditional Internal Standard					External Standard				
	Concentration, mg/L AA			RSD, %	Bias, %	Concentration, mg/L AA			RSD, %	Bias, %	Concentration, mg/L AA			RSD, %	Bias, %
	1	2	3			1	2	3			1	2	3		
acetaldehyde	4603	4644	4708	0.9	7.3	4785	4764	4851	0.8	10.7	4661	5000	5088	3.7	13.4
methyl acetate	5843	5927	5956	0.8	6.8	6074	6080	6137	0.5	10.2	5917	6381	6436	3.7	12.9
ethyl acetate	6792	6801	7146	2.4	1.5	7061	6976	7363	2.3	4.7	6879	7321	7722	4.7	7.3
methanol	5935	5921	5935	0.1	3.3	6170	6073	6116	0.6	6.6	6011	6375	6415	2.9	9.2
2-propanol	5889	5906	5934	0.3	2.3	6122	6058	6114	0.5	5.6	5964	6359	6413	3.2	8.2
ethanol	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—
1-propanol	6257	6284	6274	0.2	4.3	6505	6446	6465	0.4	7.7	6337	6766	6781	3.1	10.3
isobutyl alc.	6533	6587	6585	0.4	5.7	6791	6757	6786	0.2	9.1	6617	7092	7117	3.3	11.7
2-pentanol	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—
1-butanol	6225	6293	6294	0.5	4.6	6472	6455	6485	0.2	7.9	6305	6775	6802	3.4	10.5
isoamyl alc.	6549	6601	6601	0.4	5.4	6808	6771	6801	0.2	8.8	6633	7107	7134	3.3	11.4

Table S. 7. The results of GC measurements of standard solution "WES-B" in RCH.

Compound	Ethanol as IS					Traditional Internal Standard					External Standard				
	Concentration, mg/L AA			RSD, %	Bias, %	Concentration, mg/L AA			RSD, %	Bias, %	Concentration, mg/L AA			RSD, %	Bias, %
	1	2	3			1	2	3			1	2	3		
acetaldehyde	406	425	439	3.2	-2.9	417	428	439	2.1	-1.8	337	386	430	9.9	-11.8
methyl acetate	462	484	503	3.5	-0.8	475	488	503	2.3	0.3	384	440	493	10.1	-9.9
ethyl acetate	465	488	506	3.5	2.1	478	492	506	2.3	3.3	386	443	496	10.1	-7.2
methanol	533	531	529	0.3	0.9	548	535	529	1.5	2.1	443	483	518	6.4	-8.5
2-propanol	494	496	502	0.7	-2.8	508	500	502	0.7	-1.7	411	451	492	7.3	-11.9
ethanol	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—
1-propanol	533	535	537	0.3	0.5	548	540	536	0.9	1.6	443	486	526	7.0	-8.9
isobutyl alc.	546	554	559	1.0	0.0	561	559	559	0.2	1.2	453	503	548	7.7	-9.3
2-pentanol	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—
1-butanol	531	533	536	0.4	0.3	545	538	535	0.8	1.4	441	485	525	7.1	-9.1
isoamyl alc.	553	558	559	0.5	0.1	568	562	558	0.7	1.3	459	507	548	7.2	-9.2

Table S. 8. The results of GC measurements of standard solution "WES-1" in RCH.

Compound	Ethanol as IS					Traditional Internal Standard					External Standard				
	Concentration, mg/L AA			RSD, %	Bias, %	Concentration, mg/L AA			RSD, %	Bias, %	Concentration, mg/L AA			RSD, %	Bias, %
	1	2	3			1	2	3			1	2	3		
acetaldehyde	48.0	48.4	48.4	0.4	-0.8	47.9	48.1	48.2	0.3	-1.1	45.7	46.6	52.2	6.0	-0.8
methyl acetate	52.6	53.0	53.3	0.5	3.2	52.6	52.7	53.1	0.5	2.8	50.2	51.0	57.6	6.3	3.1
ethyl acetate	49.8	50.2	50.8	0.8	1.0	49.7	50.0	50.5	0.7	0.7	47.4	48.4	54.8	6.5	1.0
methanol	70.2	71.2	70.9	0.6	-1.3	70.1	70.8	70.6	0.4	-1.7	67.0	68.6	76.6	5.9	-1.4
2-propanol	55.1	56.3	56.4	1.0	0.7	55.0	56.0	56.1	0.9	0.3	52.6	54.2	60.9	6.4	0.6
ethanol	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—
1-propanol	56.4	56.4	56.2	0.1	-0.4	56.3	56.1	56.0	0.2	-0.7	53.7	54.3	60.7	5.6	-0.5
isobutyl alc.	58.5	58.8	58.9	0.2	-0.3	58.4	58.5	58.6	0.1	-0.7	55.8	56.6	63.6	5.9	-0.4
2-pentanol	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—
1-butanol	55.5	55.8	56.4	0.7	-1.3	55.4	55.5	56.2	0.6	-1.7	52.9	53.7	60.9	6.4	-1.4
isoamyl alc.	58.1	58.4	58.5	0.3	-1.4	58.0	58.1	58.2	0.1	-1.8	55.4	56.3	63.1	5.9	-1.5

Table S. 9. The results of GC measurements of standard solution "WES-2" in RCH.

Compound	Ethanol as IS					Traditional Internal Standard					External Standard				
	Concentration, mg/L AA			RSD, %	Bias, %	Concentration, mg/L AA			RSD, %	Bias, %	Concentration, mg/L AA			RSD, %	Bias, %
	1	2	3			1	2	3			1	2	3		
acetaldehyde	9.8	9.9	10.2	1.5	-9.5	9.7	9.9	10.1	1.5	-10.3	10.5	9.7	10.2	3.5	-8.0
methyl acetate	10.1	10.0	10.1	0.6	3.2	9.9	10.0	10.0	0.4	2.3	10.8	9.8	10.2	4.0	5.0
ethyl acetate	9.8	10.1	9.7	1.5	4.3	9.7	10.1	9.6	2.0	3.4	10.5	9.9	9.8	3.3	6.1
methanol	27.8	27.6	27.7	0.3	0.1	27.4	27.5	27.4	0.3	-0.8	29.7	27.0	27.8	4.1	1.9
2-propanol	12.3	11.9	12.0	1.5	1.4	12.2	11.9	11.8	1.2	0.5	13.2	11.7	12.0	5.3	3.2
ethanol	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—
1-propanol	10.5	10.5	10.7	0.9	-1.0	10.4	10.5	10.6	1.0	-1.8	11.3	10.3	10.8	3.6	0.8
isobutyl alc.	11.5	11.2	11.3	1.0	0.8	11.4	11.2	11.2	0.6	-0.1	12.3	11.0	11.4	4.8	2.6
2-pentanol	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—
1-butanol	10.9	10.8	10.8	0.5	-1.4	10.7	10.8	10.6	0.6	-2.2	11.6	10.6	10.8	4.2	0.4
isoamyl alc.	11.1	11.3	11.2	0.8	-3.6	10.9	11.3	11.1	1.2	-4.5	11.9	11.0	11.3	3.1	-1.9

Table S. 10. The results of GC measurements of standard solution "WES-3" in RCH.

Compound	Ethanol as IS					Traditional Internal Standard					External Standard				
	Concentration, mg/L AA			RSD, %	Bias, %	Concentration, mg/L AA			RSD, %	Bias, %	Concentration, mg/L AA			RSD, %	Bias, %
	1	2	3			1	2	3			1	2	3		
acetaldehyde	4.0	3.6	3.5	5.5	-6.2	3.8	3.5	3.4	4.7	-8.2	5.0	4.1	3.4	15.6	5.7
methyl acetate	1.0	1.1	1.1	6.7	3.4	0.9	1.1	1.1	7.5	1.3	1.2	1.2	1.1	4.3	15.1
ethyl acetate	1.1	1.0	1.0	4.4	-6.9	1.1	1.0	1.0	3.6	-8.8	1.4	1.2	1.0	14.5	4.8
methanol	18.3	18.1	18.6	1.1	-0.7	17.8	17.7	18.5	2.0	-2.7	23.1	20.5	18.2	9.6	11.3
2-propanol	2.7	2.6	2.7	1.6	-3.4	2.6	2.5	2.7	1.9	-5.3	3.4	2.9	2.6	10.9	8.4
ethanol	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—
1-propanol	1.2	1.2	1.1	3.0	-7.9	1.2	1.1	1.1	2.1	-9.8	1.5	1.3	1.1	13.0	3.6
isobutyl alc.	1.3	1.4	1.4	4.6	-6.2	1.2	1.3	1.4	5.5	-8.1	1.6	1.5	1.4	5.7	4.6
2-pentanol	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—
1-butanol	1.7	1.5	1.7	5.8	-4.9	1.7	1.5	1.6	5.8	-6.8	2.2	1.7	1.6	13.7	6.9
isoamyl alc.	2.0	2.0	1.9	3.6	0.8	2.0	2.0	1.9	2.7	-1.3	2.5	2.3	1.8	13.2	13.4

Table S. 11. The results of GC measurements of standard solution "WES-B" in CU.

Compound	Ethanol as IS					Traditional Internal Standard					External Standard				
	Concentration, mg/L AA			RSD, %	Bias, %	Concentration, mg/L AA			RSD, %	Bias, %	Concentration, mg/L AA			RSD, %	Bias, %
	1	2	3			1	2	3			1	2	3		
acetaldehyde	427	428	425	0.3	-2.2	412	421	417	0.9	-4.5	424	428	425	0.3	-2.4
methyl acetate	503	502	502	0.1	3.1	485	494	492	0.8	0.7	500	502	502	0.2	2.9
ethyl acetate	477	476	477	0.1	0.1	460	469	468	0.8	-2.2	474	476	476	0.2	-0.1
methanol	533	538	537	0.4	1.9	514	530	527	1.3	-0.5	530	538	537	0.7	1.7
2-propanol	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—
ethanol	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—
1-propanol	546	549	542	0.5	2.5	527	540	532	1.0	0.1	543	548	542	0.5	2.2
isobutyl alc.	569	570	568	0.2	2.9	549	561	557	0.9	0.5	566	570	567	0.3	2.6
2-pentanol	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—
1-butanol	543	544	538	0.4	1.9	524	535	528	0.9	-0.5	540	543	538	0.4	1.6
isoamyl alc.	572	572	568	0.3	2.7	552	563	557	0.8	0.3	569	572	568	0.3	2.5

Table S. 12. The results of GC measurements of standard solution "WES-1" in CU.

Compound	Ethanol as IS					Traditional Internal Standard					External Standard				
	Concentration, mg/L AA			RSD, %	Bias, %	Concentration, mg/L AA			RSD, %	Bias, %	Concentration, mg/L AA			RSD, %	Bias, %
	1	2	3			1	2	3			1	2	3		
acetaldehyde	48.8	46.8	49.8	2.6	-0.2	48.4	47.0	49.1	1.8	-1.0	49.0	47.0	50.0	2.6	0.1
methyl acetate	51.1	51.0	50.7	0.4	-0.9	50.6	51.2	49.9	1.1	-1.5	51.3	51.2	50.9	0.4	-0.5
ethyl acetate	48.9	49.0	49.0	0.1	-1.5	48.4	49.3	48.3	0.9	-2.2	49.1	49.2	49.2	0.1	-1.1
methanol	72.9	77.5	72.6	3.0	3.7	72.2	77.9	71.5	3.9	3.0	73.2	77.9	72.9	3.0	4.1
2-propanol	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—
ethanol	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—
1-propanol	52.8	53.4	53.9	0.8	-5.5	52.3	53.7	53.1	1.0	-6.2	53.0	53.6	54.2	0.9	-5.2
isobutyl alc.	57.4	58.5	58.8	1.0	-1.2	56.8	58.7	57.9	1.4	-1.9	57.6	58.7	59.0	1.0	-0.8
2-pentanol	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—
1-butanol	55.7	56.7	56.2	0.7	-0.8	55.2	56.9	55.4	1.4	-1.4	55.9	56.9	56.5	0.7	-0.4
isoamyl alc.	57.9	57.0	57.0	0.7	-3.2	57.3	57.2	56.1	1.0	-3.9	58.1	57.2	57.2	0.7	-2.9

Table S. 13. The results of GC measurements of standard solution "WES-2" in CU.

Compound	Ethanol as IS					Traditional Internal Standard					External Standard				
	Concentration, mg/L AA			RSD, %	Bias, %	Concentration, mg/L AA			RSD, %	Bias, %	Concentration, mg/L AA			RSD, %	Bias, %
	1	2	3			1	2	3			1	2	3		
acetaldehyde	12.5	12.2	12.3	1.2	11.8	12.2	12.0	12.1	0.8	9.7	12.6	12.3	12.3	1.0	12.6
methyl acetate	10.0	9.7	9.2	3.3	-0.8	9.8	9.5	9.2	2.6	-2.7	10.1	9.8	9.3	3.4	-0.1
ethyl acetate	10.2	10.1	10.0	0.7	6.3	9.9	9.9	9.9	0.2	4.2	10.2	10.2	10.0	1.0	7.0
methanol	29.2	30.0	26.9	4.6	3.9	28.4	29.4	26.7	4.1	1.9	29.3	30.4	27.0	4.9	4.6
2-propanol	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—
ethanol	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—
1-propanol	10.3	10.5	10.6	1.3	-2.1	10.0	10.3	10.5	2.0	-4.0	10.3	10.7	10.6	1.5	-1.5
isobutyl alc.	11.2	11.4	9.9	6.2	-4.0	10.9	11.2	9.8	5.7	-5.9	11.2	11.5	9.9	6.5	-3.3
2-pentanol	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—
1-butanol	10.0	10.4	10.6	2.5	-5.7	9.7	10.2	10.5	3.1	-7.5	10.1	10.5	10.7	2.5	-5.1
isoamyl alc.	10.9	11.2	11.1	1.4	-4.7	10.6	11.0	11.0	1.9	-6.5	10.9	11.4	11.1	1.7	-4.1

Table S. 14. The results of GC measurements of standard solution "WES-C" in three laboratories.

Compound	Peak area, nA·min								
	LAR			RCH			CU		
	1	2	3	1	2	3	1	2	3
acetaldehyde	2.458	2.378	2.425	6199	6440	6230	5.783	5.806	5.825
methyl acetate	2.360	2.295	2.325	6068	6267	6060	4.954	4.981	4.914
ethyl acetate	3.105	3.013	3.061	7976	8228	7998	6.464	6.530	6.487
methanol	3.107	2.978	3.046	9103	9563	9194	5.356	5.196	5.291
2-propanol	4.606	4.476	4.556	12982	13506	12888	—	—	—
ethanol	11383.312	11018.411	11228.543	41393292	43305261	41734325	39397.264	39574.609	39494.731
1-propanol	5.570	5.386	5.493	15793	16549	15994	11.996	12.030	12.048
isobutyl alc.	6.891	6.671	6.791	18533	19377	18753	14.326	14.115	13.936
2-pentanol	1.706	1.655	1.686	4563	4743	4619	3.475	3.505	3.453
1-butanol	6.123	5.945	6.056	17855	18695	18034	13.664	13.682	13.771
isoamyl alc.	6.934	6.725	6.851	19891	20787	20024	15.362	15.332	15.498

Table S. 15. The average measurement results of standard solution "WES-C" and the calibration coefficients for three analytical methods obtained in RCH and CU.

Compound	Average calibration coefficients							
	RCH				CU			
	Average peak area, nA·min	Ethanol as IS	2-pentanol as IS	External standard, mg/L AA·(nA·min)$^{-1}$·10^{2}	Average peak area, nA·min	Ethanol as IS	2-pentanol as IS	External standard, mg/L AA··(nA·min)$^{-1}$
acetaldehyde	6290	1.893	2.351	3,547	5.804	1.923	1.909	38.43
methyl acetate	6131	2.106	2.615	3,946	4.949	2.445	2.427	48.87
ethyl acetate	8067	1.542	1.914	2,889	6.494	1.795	1.782	35.88
methanol	9287	1.558	1.934	2,919	5.281	2.567	2.549	51.31
2-propanol	13125	1.049	1.303	1,966	—	—	—	—
ethanol	42144293	1.000	1.242	1,874	39488.868	1.000	0.993	19.99
1-propanol	16112	0.878	1.090	1,645	12.025	1.102	1.094	22.03
isobutyl alc.	18888	0.778	0.966	1,458	14.126	0.975	0.968	19.49
2-pentanol	4642	0.805	1.000	1,509	3.478	1.007	1.000	20.13
1-butanol	18195	0.776	0.963	1,453	13.706	0.965	0.958	19.29
isoamyl alc.	20234	0.729	0.905	1,366	15.397	0.898	0.892	17.95

Table S. 16. Inter-laboratory repeatability limits.

Compound	Repeatability limit, %														
	WES-A			WES-B			WES-1			WES-2			WES-3		
	Eth[2]	Trad	Ext	Eth	Trad	Ext	Eth	Trad	Ext	Eth	Trad	Ext	Eth	Trad	Ext
acetaldehyde	2.4	2.7	8.9	8.1	6.3	32.9	6.7	5.0	31.0	4.4	3.8	7.8	13.4	12.0	39.8
methyl acetate	2.0	2.4	8.9	8.7	6.4	28.3	1.8	2.9	28.8	7.9	6.2	12.2	17.5	19.3	11.9
ethyl acetate	5.8	6.1	10.8	8.8	6.3	29.2	2.4	3.1	28.2	4.2	4.9	8.4	13.4	11.4	38.0
methanol	0.4	3.0	6.9	1.3	4.7	25.3	7.5	9.4	28.0	11.2	9.9	14.7	2.8	4.9	25.1
2-propanol	0.8	2.4	7.5	1.9	1.7	26.9	7.0	6.7	22.6	3.7	2.9	12.0	13.4	13.9	29.6
1-propanol	0.4	2.5	7.3	1.4	3.3	26.2	2.0	2.5	28.3	4.1	5.3	8.9	17.7	18.1	36.0
isobutyl alc.	1.0	2.5	7.8	2.5	2.2	26.8	2.5	3.2	28.5	14.5	13.0	17.8	15.3	17.5	17.2
1-butanol	1.2	2.3	8.2	1.4	3.1	26.6	2.3	3.6	28.2	6.9	8.2	11.2	16.2	16.7	36.9
isoamyl alc.	0.9	2.4	7.9	1.4	2.7	26.6	1.8	2.3	28.4	6.2	7.2	8.2	10.9	9.6	37.0

[2] Here and further “Eth”, “Trad” and “Ext” are the short forms of the “Ethanol as Internal Standard”, “Traditional Internal Standard” and “External Standard” methods.

Table S. 17. Inter-laboratory biases.

Compound	Bias, %														
	WES-A			WES-B			WES-1			WES-2			WES-3		
	Eth	Trad	Ext	Eth	Trad	Ext	Eth	Trad	Ext	Eth	Trad	Ext	Eth	Trad	Ext
acetaldehyde	5.0	8.7	17.1	1.6	2.0	4.1	0.1	0.1	2.8	1.3	0.5	9.5	2.7	3.6	0.5
methyl acetate	3.6	7.3	15.4	0.8	0.4	1.8	1.1	0.9	3.8	0.7	0.1	8.7	2.9	2.0	5.0
ethyl acetate	0.8	4.4	12.5	0.8	0.4	1.9	0.1	0.1	2.8	3.8	3.0	11.9	2.6	3.5	0.5
methanol	1.6	5.3	13.3	1.0	0.6	1.7	0.8	0.6	3.5	1.3	0.5	9.4	0.0	0.8	2.3
2-propanol	1.0	4.6	12.7	1.4	0.9	5.2	0.5	0.5	3.1	0.7	0.5	12.5	2.3	3.2	0.1
1-propanol	2.1	5.8	13.8	1.0	0.6	1.7	2.1	2.3	0.6	0.6	1.3	7.5	5.4	6.2	3.3
isobutyl alc.	2.6	6.3	14.4	1.0	0.5	1.7	0.4	0.6	2.3	1.2	2.0	6.8	4.7	5.5	2.9
1-butanol	2.2	5.9	14.0	0.7	0.3	2.0	0.6	0.8	2.1	2.0	2.7	6.1	4.7	5.6	2.4
isoamyl alc.	2.6	6.3	14.4	0.9	0.5	1.8	1.5	1.7	1.2	2.1	2.8	6.1	5.1	6.1	2.1

Table S. 18. Inter-laboratory uncertainties.

Compound	Uncertainty, %														
	WES-A			WES-B			WES-1			WES-2			WES-3		
	Eth	Trad	Ext	Eth	Trad	Ext	Eth	Trad	Ext	Eth	Trad	Ext	Eth	Trad	Ext
acetaldehyde	6.4	5.3	10.3	5.2	5.7	21.7	3.9	4.1	18.6	21.2	20.2	29.6	12.9	15.2	29.3
methyl acetate	8.9	7.8	8.1	5.9	3.2	19.9	4.1	4.7	16.8	5.8	5.9	21.3	12.6	14.0	8.6
ethyl acetate	3.9	3.7	14.6	4.8	6.3	17.2	3.0	4.0	17.0	5.7	3.7	17.2	14.7	17.1	27.0
methanol	4.7	4.0	11.2	1.8	3.5	17.3	6.4	6.6	16.3	7.0	5.5	20.8	2.6	6.0	28.9
2-propanol	3.8	3.0	12.2	4.2	2.6	25.5	5.3	4.5	15.0	2.9	1.7	24.3	9.7	10.0	21.4
1-propanol	6.3	5.3	9.8	2.7	2.4	18.1	6.2	7.1	18.7	4.1	6.6	25.9	12.8	15.1	29.2
isobutyl alc.	8.5	7.5	8.1	3.5	1.6	18.7	2.0	3.2	17.1	8.7	9.4	25.4	11.1	12.6	12.4
1-butanol	6.6	5.6	9.8	2.2	2.5	18.1	1.9	3.1	17.1	7.9	10.3	28.7	11.7	12.1	26.6
isoamyl alc.	7.9	6.9	8.6	3.2	2.0	18.5	3.5	4.7	18.1	8.1	10.5	30.0	7.9	6.9	26.7