Supporting Information

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Development of a quality control material for the analysis of volatile compounds in alcoholic beverages

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S.1. Preparation of the QCM

The apparent density of prepared *WES* in air at 20°C $\rho_{WES}^{20°C}$ was measured by pycnometer according to the ISO 758 [1] with following formula

$$\rho_{WES}^{20°C} = \frac{m_{p+water} - m_p}{m_{p+WES} - m_p}\left(\rho_{water}^{(20°C)} - \rho_{air}\right) + \rho_{air}, \quad \text{(S.1)}$$

where m_p is the mass of pycnometer, mg; $m_{p+water}$ is the mass of pycnometer with pure water, mg; m_{p+WES} is the mass of pycnometer with *WES*, mg; $\rho_{water}^{(20°C)}$ is the density of pure water at 20°C, mg/L, $\rho_{water}^{(20°C)}$ = 0.9982 g/mL [1]; ρ_{air} – is the density of air, ρ_{air} = 0.12 g/mL [1].

The exact value of ethanol volume concentration in *WES* $C_{Eth}(WES)_{\%ABV}$ was determined using International alcoholometric tables [2]. Obtained value of ethanol volume concentration $C_{Eth}(WES)_{vol}$ with corresponding uncertainty of method $u(C_{Eth}(WES)_{\%ABV})$ was (40.0±0.1) % ABV.

Ethanol mass concentration $C_{Eth}(WES)_{mg/mg}$ in mg/mg of *WES* was calculated according to the following formula

$$C_{Eth}(WES)_{mg/mg} = \frac{\rho_{Eth}}{\rho_{WES}^{20°C}} \cdot \frac{C_{Eth}(WES)_{\%ABV}}{100\ \%}, \quad \text{(S.2)}$$

where ρ_{Eth} – is the density of pure ethanol, ρ_{Eth} = 0.7893 g/mL [2]; $\rho_{WES}^{20°C}$ – is the density of *WES*, ρ_{WES} = 0.9487 g/mL (calculated value).

The solution A (with approximate concentrations of volatile compounds 5000 mg/L AA (AA – Absolute Alcohol) was prepared by adding of the volatile compounds (acetaldehyde, methyl acetate, ethyl acetate, methanol, propan-2-ol, propan-1-ol, 2-methylpropan-1-ol, butan-1-ol, 3-methylbutan-1-ol) to *WES*.

Since reagent ethanol, depending on its origin, often contains volatile compounds (as rule methanol, acetaldehyde, propan-2-ol, etc.), it necessary to take account volatile compounds, which are present in prepared *WES*. Thus, the mass concentration of the *i*-th volatile compound in solution A, expressed in mg/mg and mg/L AA were calculated according to the following formulas

$$C_i(A)_{mg/mg} = \frac{m_i \cdot P_i + m_{WES} \cdot C_i\ (WES)_{mg/mg}}{\sum_{i=1}^{9} m_i + m_{WES}}, \quad \text{(S.3)}$$

$$C_i(A)_{mg/L\ AA} = \frac{m_i \cdot P_i + m_{WES} \cdot C_i(WES)_{mg/mg}}{m_{WES} \cdot C_{Eth}(WES)_{mg/mg}} \cdot \rho_{Eth}, \quad \text{(S.4)}$$

where m_i is the mass of *i*-th volatile compound, added for preparation of solution A, mg; P_i is the purity of reagent of *i*-th volatile compound, mg/mg; m_{WES} is the mass of *WES*, added for preparation of solution A, mg; $C_i(WES)_{mg/mg}$ is the mass concentration of *i*-th volatile compoundin *WES*, mg/mg.

The solutions B, C, D and E (with approximate concentrations of volatile compounds 500; 250; 200; 25 mg/L AA, correspondingly) were prepared by mixing of solution A and *WES*. The solutions F and G (with approximate concentrations of volatile compounds 10 and 1.2 mg/L AA, correspondingly) were prepared by mixing of solution C and *WES*.

The mass concentration of the *i*-th volatile compound in solutions B, C, D, E, F and G, expressed in mg/mg and mg/L AA were calculated according to the following formulas

$$C_i(B,C,D,E)_{mg/L\ AA} = \frac{m_A \cdot C_i(A)_{mg/mg} + m_{WES} \cdot C_i(WES)_{mg/mg}}{m_A \cdot C_{Eth}(A)_{mg/mg} + m_{WES} \cdot C_{Eth}(WES)_{mg/mg}} \cdot \rho_{Eth}, \quad \text{(S.5)}$$

$$C_i(C)_{mg/mg} = \frac{m_A \cdot C_i(A)_{mg/mg} + m_{WES} \cdot C_i(WES)_{mg/mg}}{m_A + m_{WES}}, \quad \text{(S.6)}$$

$$C_i(F,G)_{mg/L\ AA} = \frac{m_C \cdot C_i(C)_{mg/mg} + m_{WES} \cdot C_i(WES)_{mg/mg}}{m_C \cdot C_{Eth}(C)_{mg/mg} + m_{WES} \cdot C_{Eth}(WES)_{mg/mg}} \cdot \rho_{Eth}, \quad \text{(S.7)}$$

where m_A is the mass of solution A, added for preparation of solutions B, C, D and E, mg; m_C is the mass of solution C, added for preparation of solutions F and G, mg; m_{WES} is the mass of *WES*, added for preparation of solutions B, C, D, E, F and G, mg.

In the zero approximation, it is assumed that the concentration of the analyzed volatile compounds in *WES* $C_i(WES)_{mg/mg}(0)$ = 0 mg/mg. Thus, the mass concentration of the *i*-th volatile compound in solutions A in the zero approximation $C_i(A)_{mg/mg}(0)$ was calculated according to the following formula

$$C_i(A)_{mg/mg}(0) = \frac{m_i \cdot P_i}{\sum_{i=1}^{9} m_i + m_{WES}}. \quad \text{(S.8)}$$

The mass of the *i*-th volatile compound and ethanol in solutions C in the zero approximation $m_i(C)(0)$ and $m_{Eth}(C)(0)$, correspondingly, were calculated according to the following formulas

$$m_i(C)(0) = m_A \cdot C_i(A)_{mg/mg}(0), \quad \text{(S.9)}$$

$$m_{Eth}(C)(0) = m_A \cdot C_{Eth}(A)_{mg/mg} + m_{WES} \cdot C_{Eth}(WES)_{mg/mg}. \quad \text{(S.10)}$$

The relative response factor in the zero approximation $RRF_i^{Eth}(0)$ was calculated according to the following formula

$$RRF_i^{Eth}(0) = \frac{m_i(C)(0)}{m_{Eth}(C)(0)} \cdot \frac{A_{Eth}^C}{A_i^C}, \quad \text{(S.11)}$$

where A_i^C and A_{Eth}^C are the detector responses for the *i*-th volatile and ethanol in solution C, correspondingly, a.u. (arbitrary units).

The mass concentration of *i*-th volatile compound in the first approximation in mg/L AA and mg/mg – $C_i(WES)_{mg/L\ AA}(I)$ and $C_i(WES)_{mg/mg}(I)$, correspondingly, were calculated according to the following formulas

$$C_i(WES)_{mg/L\ AA}(I) = RRF_i^{Eth}(0) \cdot \frac{A_i^{WES}}{A_{Eth}^{WES}} \cdot \rho_{Eth}, \quad \text{(S.12)}$$

$$C_i(WES)_{mg/mg}(I) = \frac{\rho_{Eth}}{\rho_{WES}^{20°C}} \cdot C_i(WES)_{mg/L\ AA}(I), \quad \text{(S.13)}$$

where A_i^{WES} and A_{Eth}^{WES} are the detector responses for the *i*-th volatile and ethanol in *WES*, correspondingly, a.u.

In order to obtain more accurate values of mass concentrations of volatile compounds in *WES*, it is necessary to repeat recalculations (S.11)-(S.13).

The mass concentration of the *i*-th volatile compound in solutions A and C in the first approximation $C_i(A)_{mg/mg}(I)$ was calculated according to the following formula

$$C_i(A)_{mg/mg}(I) = \frac{m_i \cdot P_i + m_{WES} \cdot C_i(WES)_{mg/mg}(I)}{\sum_{i=1}^{9} m_i + m_{WES}}. \quad \text{(S.14)}$$

The mass of the *i*-th volatile compound and ethanol in solution C in the first approximation $m_i(C)(I)$ and $m_{Eth}(C)(I)$, correspondingly, were calculated according to the following formulas

$$m_i(C)(I) = m_A \cdot C_i(A)_{mg/mg}(I) + m_{WES} \cdot C_i(WES)_{mg/mg}(I), \quad \text{(S.15)}$$

$$m_{Eth}(C)(I) = m_A \cdot C_{Eth}(A)_{mg/mg} + m_{WES} \cdot C_{Eth}(WES)_{mg/mg}. \quad \text{(S.16)}$$

The relative response factor in the first approximation $RRF_i^{Eth}(I)$ was calculated according to the following formula

$$RRF_i^{Eth}(I) = \frac{m_i(C)(I)}{m_{Eth}(C)(I)} \cdot \frac{A_{Eth}^C}{A_i^C}, \quad \text{(S.17)}$$

The mass concentration of *i*-th volatile compound in the second approximation in mg/L AA and mg/mg – $C_i(WES)_{mg/L\ AA}(II)$ and $C_i(WES)_{mg/mg}(II)$, correspondingly, were calculated according to the following formulas

$$C_i(WES)_{mg/L\ AA}(II) = RRF_i^{Eth}(I) \cdot \frac{A_i^{WES}}{A_{Eth}^{WES}} \cdot \rho_{Eth}, \quad \text{(S.18)}$$

$$C_i(WES)_{mg/mg}(II) = \frac{\rho_{Eth}}{\rho_{WES}^{20°C}} \cdot C_i(WES)_{mg/L\ AA}(II). \quad \text{(S.19)}$$

The number of approximations was 2 (in final calculation the results of the 2nd approximation was used), because the relative difference between the values of RRF^{Eth} and $C(WES)$, obtained in 3rd and 2nd approximations was less than 0.001 % (Table S.1.1) and there was no need for further recalculations.

The relative difference between the values of RRF^{Eth}, obtained in N-th and (N^{-1})-th approximations was calculated according to the following formula

$$\Delta_{i\ (N-1,\ N)} = \frac{RRF^{Eth}(N) - RRF^{Eth}(N-1)}{RRF^{Eth}(N-1)} \cdot 100\ \%, \qquad (S.20)$$

where $RRF^{Eth}(N)$ and $RRF^{Eth}(N^{-1})$ are calibration coefficients of i-th volatile compound, obtained in N-th and (N^{-1})-th approximations, correspondingly.

Table S.1.1 The mass concentrations of volatile compounds in *WES* and calibration coefficients RRF^{Eth}, obtained in the 1st, 2nd and 3rd approximations

Compound	The zero approximation			The first approximation			$\Delta_{(0,\ I)}$, %
	$C(WES)(0)$		$RRF^{Eth}(0)$	$C(WES)(I)$		RRF^{Eth}	
	mg/L AA	mg/mg		mg/L AA	mg/mg	(I)	
acetaldehyde	0	0	1.2072	0.615	$2.596 \cdot 10^{-7}$	1.2102	0.2
methanol	0	0	1.2762	3.024	$1.276 \cdot 10^{-6}$	1.2912	1.2
propan-2-ol	0	0	0.8040	0.897	$3.783 \cdot 10^{-7}$	0.8068	0.3

Compound	The second approximation			$\Delta_{(I,\ II)}$, %	The third approximation			$\Delta_{(II,\ III)}$, %
	$C(WES)(II)$		RRF^{Eth}		$C(WES)(III)$		RRF^{Eth}	
	mg/L AA	mg/mg	(II)		mg/L AA	mg/mg	(III)	
acetaldehyde	0.617	$2.602 \cdot 10^{-7}$	1.2102	$5.97 \cdot 10^{-4}$	0.617	$2.602 \cdot 10^{-7}$	1.2102	$1.46 \cdot 10^{-6}$
methanol	3.060	$1.291 \cdot 10^{-6}$	1.2914	$1.37 \cdot 10^{-2}$	3.060	$1.291 \cdot 10^{-6}$	1.2914	$1.62 \cdot 10^{-4}$
propan-2-ol	0.900	$3.797 \cdot 10^{-7}$	0.8068	$1.22 \cdot 10^{-3}$	0.900	$3.797 \cdot 10^{-7}$	0.8068	$4.27 \cdot 10^{-6}$

The final values of concentrations were calculated according to the formulas (S.3)-(S.7). There was made two recalculations of $C_i(WES)_{mg/mg}$ and in final calculation $C_i(WES)_{mg/mg}(II)$ was used as $C_i(WES)_{mg/mg}$ in the formulas (S.3)-(S.7). The results of determinations of mass concentrations in the prepared solutions are performed in Table S.1.2.

Table S.1.2 The mass concentrations and corresponding uncertainties of mass concentrations in prepared solutions

Compound	Concentration and uncertainty of concentration $C \pm u(C)$ mg/L AA in solution						
	A	B	C	D	E	F	G
acetaldehyde	4948±20	493±2.0	246±1.0	198±0.7	25.1±0.1	10.7±0.04	1.80±0.009
methyl acetate	5040±18	501±1.7	250±0.9	201±0.6	24.9±0.09	10.3±0.03	1.21±0.004
ethyl acetate	5042±18	502±1.7	250±0.9	201±0.6	24.9±0.09	10.3±0.03	1.21±0.004
methanol	5054±18	505±1.7	253±0.9	204±0.6	28.0±0.09	13.3±0.05	4.27±0.037
propan-2-ol	5043±18	502±1.7	251±0.9	202±0.6	25.8±0.09	11.2±0.03	2.11±0.012
propan-1-ol	5039±18	501±1.7	250±0.9	201±0.6	24.9±0.09	10.3±0.03	1.21±0.004
2-methylpropan-1-ol	5018±19	499±1.9	249±1.0	200±0.7	24.8±0.09	10.2±0.04	1.20±0.005
butan-1-ol	5060±18	503±1.7	251±0.9	202±0.6	25.0±0.09	10.3±0.03	1.21±0.004
3-methylbutan-1-ol	5052±19	502±1.9	250±0.9	201±0.7	25.0±0.09	10.3±0.04	1.21±0.004

S.2. Characterization of the QCM

The characterization of the QCM was carried out by preparation procedure, according to the [3-5].

The uncertainty of apparent density of prepared *WES* in air at 20°C $u\left(\rho_{WES}^{20°C}\right)$ was calculated with following formula

$$u\left(\rho_{WES}^{20°C}\right)=\sqrt{u\left(m_p\right)^2+u\left(m_{p+water}\right)^2+u\left(m_{p+WES}\right)^2+u\left(\rho_{water}^{(20°C)}\right)^2+u\left(\rho_{air}\right)^2}, \quad \text{(S.21)}$$

where $u(m_p)$ is the uncertainty of mass of pycnometer, mg; $m_{p+water}$ is the mass of pycnometer with pure water, mg; m_{p+WES} is the uncertainty of mass of pycnometer with *WES*, mg; $u\left(\rho_{water}^{(20°C)}\right)$ is the uncertainty of density of pure water at 20°C, mg/L; $u(\rho_{air})$ – is the uncertainty of density of air [6].

The uncertainty of ethanol mass concentration $u\left(C_{Eth}(WES)_{mg/mg}\right)$ in mg/mg of *WES* was calculated according to the following formula

$$u\left(C_{Eth}(WES)_{mg/mg}\right)=\sqrt{u\left(\rho_{Eth}\right)^2+u\left(\rho_{WES}^{20°C}\right)^2+u\left(C_{Eth}(WES)_{mL/mL}\right)^2}, \quad \text{(S.22)}$$

where $u\left(\rho_{Eth}\right)$ – is the uncertainty of density of pure ethanol.

The uncertainty of mass concentration of the *i*-th volatile compound in solution A, expressed in mg/mg and mg/L AA were calculated according to the following formulas

$$u\left(C_i(A)_{mg/mg}\right)=\sqrt{u\left(m_i\right)^2+u\left(P_i\right)^2+u\left(m_{WES}\right)^2+u\left(C_i(WES)_{mg/mg}\right)^2+u\left(m_{WES}\right)^2+\sum_{i=1}^{9}u\left(m_i\right)^2}, \quad \text{(S.23)}$$

$$u\left(C_i(A)_{mg/L\ AA}\right)=\sqrt{\begin{matrix}u\left(m_i\right)^2+u\left(P_i\right)^2+u\left(m_{WES}\right)^2+u\left(C_i(WES)_{mg/mg}\right)^2+\\+u\left(m_{WES}\right)^2+u\left(C_{Eth}(WES)_{mg/mg}\right)^2+u\left(\rho_{Eth}\right)^2\end{matrix}}, \quad \text{(S.24)}$$

where $u(m_i)$ is the uncertainty of mass of *i*-th volatile compound, added for preparation of solution A, mg; $u(P_i)$ is the uncertainty of purity of reagent of *i*-th volatile compound, mg/mg; $u\left(m_{WES}\right)$ is the uncertainty of mass of *WES*, added for preparation of solution A, mg; $u\left(C_i(WES)_{mg/mg}\right)$ is the uncertainty of mass concentration of *i*-th volatile compoundin *WES*, mg/mg.

The uncertainty of mass concentration of the *i*-th volatile compound in solutions B, C, D, E, F and G, expressed in mg/mg and mg/L AA were calculated according to the following formulas

$$u\left(C_i(B,C,D,E)_{mg/L\ AA}\right)=\sqrt{\begin{matrix}u\left(m_A\right)^2+u\left(C_i(A)_{mg/mg}\right)^2+u\left(m_{WES}\right)^2+u\left(C_i(WES)_{mg/mg}\right)^2+\\+u\left(C_{Eth}(A)_{mg/mg}\right)^2+u\left(C_{Eth}(WES)_{mg/mg}\right)^2+u\left(\rho_{Eth}\right)^2\end{matrix}}, \quad \text{(S.25)}$$

$$u\left(C_i(C)_{mg/mg}\right)=\sqrt{u\left(m_A\right)^2+u\left(C_i(A)_{mg/mg}\right)^2+u\left(m_{WES}\right)^2+u\left(C_i(WES)_{mg/mg}\right)^2}, \quad \text{(S.26)}$$

$$u\left(C_i(F,G)_{mg/L\ AA}\right)=\sqrt{\begin{matrix}u\left(m_C\right)^2+u\left(C_i(C)_{mg/mg}\right)^2+u\left(m_{WES}\right)^2+u\left(C_i(WES)_{mg/mg}\right)^2+\\+u\left(C_{Eth}(C)_{mg/mg}\right)^2+u\left(C_{Eth}(WES)_{mg/mg}\right)^2+u\left(\rho_{Eth}\right)^2\end{matrix}}, \quad \text{(S.27)}$$

where $u\left(m_A\right)$ is the uncertainty of mass of solution A, added for preparation of solutions B, C, D and E, mg; $u\left(m_C\right)$ is the uncertainty of mass of solution C, added for preparation of solutions F and G, mg; $u\left(m_{WES}\right)$ is the uncertainty of mass of *WES*, added for preparation of solutions B, C, D, E, F and G, mg.

The uncertainty of mass concentration of the *i*-th volatile compound in solutions A and C in the zero approximation $u\left(C_i(A)_{mg/mg}(0)\right)$ and $u\left(C_i(C)_{mg/L\ AA}(0)\right)$ were calculated according to the following formulas

$$u\left(C_i(A)_{mg/mg}(0)\right)=\sqrt{u\left(m_i\right)^2+u\left(P_i\right)^2+\sum_{i=1}^{9}u\left(m_i\right)^2+u\left(m_{WES}\right)^2}, \quad \text{(S.28)}$$

The uncertainty of mass of the *i*-th volatile compound and ethanol in solution C in the zero approximation $m_i(C)(0)$ and $m_{Eth}(C)(0)$, correspondingly, were calculated according to the following formulas

$$u\left(m_i(C)(0)\right)=\sqrt{u\left(m_A\right)^2\cdot u\left(C_i(A)_{mg/mg}(0)\right)^2}, \quad \text{(S.29)}$$

$$u\left(m_{Eth}(C)(0)\right)=\sqrt{u\left(m_A\right)^2+u\left(C_{Eth}(A)_{mg/mg}\right)^2+u\left(m_{WES}\right)^2+u\left(C_{Eth}(WES)_{mg/mg}\right)^2}. \quad \text{(S.30)}$$

The uncertainty of relative response factor in the zero approximation $u\left(RRF_i^{Eth}(0)\right)$ was calculated according to the following formula

$$u\left(RRF_i^{Eth}(0)\right)=\sqrt{u\left(m_i(C)(0)\right)^2+u\left(m_{Eth}(C)(0)\right)^2+u\left(A_i^C\right)^2+u\left(A_{Eth}^C\right)^2+u\left(\rho_{Eth}\right)^2}, \quad \text{(S.31)}$$

where $u\left(A_i^C\right)$ and $u\left(A_{Eth}^C\right)$ are the uncertainties of detector responses for the *i*-th volatile and ethanol in solution C, correspondingly, a.u.

The uncertainty of mass concentration of *i*-th volatile compound in the first approximation in mg/L AA and mg/mg – $u\left(C_i(WES)_{mg/L\ AA}(I)\right)$ and $u\left(C_i(WES)_{mg/mg}(I)\right)$, correspondingly, were calculated according to the following formulas

$$u\left(C_i(WES)_{mg/L\ AA}(I)\right)=\sqrt{u\left(RRF_i^{Eth}(0)\right)^2+u\left(A_i^{WES}\right)^2+u\left(A_{Eth}^{WES}\right)^2+u\left(\rho_{Eth}\right)^2}, \quad \text{(S.32)}$$

$$u\left(C_i(WES)_{mg/mg}(I)\right)=\sqrt{u\left(\rho_{Eth}\right)^2+u\left(\rho_{WES}^{20°C}\right)^2+u\left(C_i(WES)_{mg/L\ AA}(I)\right)^2}. \quad \text{(S.33)}$$

where $u\left(A_i^{WES}\right)$ and $u\left(A_{Eth}^{WES}\right)$ are the uncertainties of detector responses for the *i*-th volatile and ethanol in *WES*, correspondingly, a.u.

The uncertainty of mass concentration of the *i*-th volatile compound in solutions A and C in the first approximation $u\left(C_i(A)_{mg/mg}(I)\right)$ was calculated according to the following formula

$$u\left(C_i(A)_{mg/mg}(I)\right)=\sqrt{u\left(m_i\right)^2+u\left(P_i\right)^2+u\left(m_{WES}\right)^2+u\left(C_i(WES)_{mg/mg}(I)\right)^2+\sum_{i=1}^{9}u\left(m_i\right)^2}. \quad \text{(S.34)}$$

The uncertainty of mass of the *i*-th volatile compound and ethanol in solutions C in the first approximation $u\left(m_i(C)(I)\right)$ and $u\left(m_{Eth}(C)(I)\right)$, correspondingly, were calculated according to the following formulas

$$u\left(m_i(C)(I)\right)=\sqrt{u\left(m_A\right)^2+u\left(C_i(A)_{mg/mg}(I)\right)^2+u\left(m_{WES}\right)^2+u\left(C_i(WES)_{mg/mg}(I)\right)^2}, \quad \text{(S.35)}$$

$$u\left(m_{Eth}(C)(I)\right)=\sqrt{u\left(m_A\right)^2+u\left(C_{Eth}(A)_{mg/mg}\right)^2+u\left(m_{WES}\right)^2+u\left(C_{Eth}(WES)_{mg/mg}\right)^2}. \quad \text{(S.36)}$$

The uncertainty of relative response factor in the first approximation $u\left(RRF_i^{Eth}(I)\right)$ was calculated according to the following formula

$$u\left(RRF_i^{Eth}(I)\right)=\sqrt{u\left(m_i(C)(I)\right)^2+u\left(m_{Eth}(C)(I)\right)^2+u\left(A_i^C\right)^2+u\left(A_{Eth}^C\right)^2+u\left(\rho_{Eth}\right)^2}. \quad \text{(S.37)}$$

The uncertainty of mass concentration of *i*-th volatile compound in the second approximation in mg/L AA and mg/mg – $u\left(C_i(WES)_{mg/L\ AA}(II)\right)$ and $u\left(C_i(WES)_{mg/mg}(II)\right)$, correspondingly, were calculated according to the following formulas

$$u\left(C_i(WES)_{mg/L\ AA}(II)\right)=\sqrt{u\left(RRF_i^{Eth}(I)\right)^2+u\left(A_i^{WES}\right)^2+u\left(A_{Eth}^{WES}\right)^2+u\left(\rho_{Eth}\right)^2}, \quad \text{(S.38)}$$

$$u\left(C_i(WES)_{mg/mg}(II)\right)=\sqrt{u\left(\rho_{Eth}\right)^2+u\left(\rho_{WES}^{20°C}\right)^2+u\left(C_i(WES)_{mg/L\ AA}(II)\right)^2}. \quad \text{(S.39)}$$

The evaluation of standard uncertainties was carried out by type B [3]. Estimates of the standard uncertainty values of each input value and their description are performed in Table S.2.1.

Table S.2.1 Estimating of the standard uncertainty of each input value and their description

Input value	Description of input value	Estimation of uncertainty	Formula for calculation of standard uncertainty
Purity of reagent, ***P***	The value is known from manufacturer's certificate for reagent.	Type B evaluation of uncertainty. Rectangular distribution.	$u(P_i) = \frac{1-P_i}{\sqrt{3}}.$ (S.40)
Mass of solutions' components, ***m***	The value is known from manufacturer's certificate for balances.	Type B evaluation of uncertainty. Rectangular distribution.	$u(m) = \frac{a}{\sqrt{3}},$ where a is error of used analytical balances, a = 1.0 mg. (S.41)
Detector response, ***A***	The value is known from manufacturer's certificate for FID.	Type B evaluation of uncertainty. Rectangular distribution.	$u(A) = \frac{b}{\sqrt{3}} \cdot A,$ where b is relative standard deviation for FID signal, $b \leq 2.0$ %. (S.42)

The final results of calculation of uncertainties of concentrations were calculated according to the formulas (S.22)-(S.27). The results of determinations of uncertainty of mass concentrations in the prepared solutions are performed in Table S.1.2.

References

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S.3. Homogeneity study

Table S.3.1 The obtained results of homogeneity study

Solution G																				
Compound	Mass concentration, obtained for sample, mg/L AA																			
	1		2		3		4		5		6		7		8		9		10	
acetaldehyde	1.78	1.71	1.77	1.68	1.68	1.89	1.68	1.71	1.62	1.72	1.74	1.82	1.65	1.63	1.78	1.64	1.87	1.82	1.83	1.62
methyl acetate	1.21	1.21	1.19	1.21	1.20	1.28	1.22	1.21	1.25	1.21	1.18	1.19	1.21	1.29	1.25	1.19	1.27	1.22	1.27	1.25
ethyl acetate	1.21	1.21	1.20	1.26	1.23	1.27	1.22	1.21	1.23	1.24	1.18	1.16	1.27	1.13	1.26	1.22	1.28	1.22	1.28	1.20
methanol	4.18	4.27	4.17	4.19	4.11	4.32	4.32	4.08	4.21	4.18	4.23	4.25	4.28	4.33	4.30	4.18	4.36	4.31	4.34	4.30
propan-2-ol	2.07	2.06	2.08	2.15	2.07	2.26	2.09	2.09	2.13	2.14	2.11	2.02	1.95	2.13	2.16	1.92	2.14	2.16	2.16	2.13
propan-1-ol	1.18	1.21	1.22	1.15	1.19	1.18	1.24	1.23	1.18	1.21	1.25	1.16	1.21	1.27	1.18	1.19	1.34	1.18	1.28	1.26
2-methylpropan-1-ol	1.21	1.20	1.19	1.23	1.21	1.23	1.23	1.21	1.22	1.23	1.21	1.22	1.17	1.27	1.19	1.14	1.35	1.21	1.24	1.29
butan-1-ol	1.23	1.21	1.20	1.23	1.23	1.22	1.20	1.22	1.23	1.24	1.23	1.22	1.19	1.25	1.25	1.19	1.23	1.27	1.29	1.25
3-methylbutan-1-ol	1.22	1.21	1.18	1.25	1.22	1.25	1.24	1.23	1.25	1.22	1.21	1.24	1.21	1.26	1.26	1.24	1.23	1.28	1.27	1.25
Solution F																				
Compound	Mass concentration, obtained for sample, mg/L AA																			
	1		2		3		4		5		6		7		8		9		10	
acetaldehyde	11.1	10.4	10.7	10.5	10.6	10.0	10.0	10.4	10.7	10.3	11.3	10.0	9.93	10.2	9.42	10.6	10.3	10.3	10.3	11.8
methyl acetate	10.8	10.1	11.1	10.8	11.0	9.46	9.68	10.6	11.1	10.0	10.4	11.0	10.5	10.1	9.75	10.7	9.9	10.2	10.3	11.3
ethyl acetate	11.1	10.2	10.6	10.6	10.6	9.83	9.94	10.9	11.2	10.1	11.1	10.8	10.3	10.6	10.0	10.6	10.4	10.8	10.3	10.7
methanol	13.8	13.0	13.9	13.7	14.1	13.0	13.3	13.9	13.7	13.2	13.5	13.9	13.6	13.4	13.5	13.6	13.3	13.5	12.8	13.4
propan-2-ol	11.6	10.5	11.5	11.2	11.1	10.6	10.4	11.5	11.5	10.7	11.4	11.1	11.2	10.9	10.2	11.0	10.8	10.7	10.9	11.4
propan-1-ol	10.4	10.1	10.4	10.4	10.0	10.3	10.2	10.7	10.4	10.1	10.1	10.3	10.3	10.1	10.7	10.3	10.1	9.82	10.0	10.3
2-methylpropan-1-ol	10.9	10.3	10.9	10.7	10.7	10.0	10.0	11.0	10.7	10.1	10.7	10.6	10.7	10.2	9.93	10.2	10.3	10.2	10.0	11.0
butan-1-ol	11.0	10.2	10.7	10.7	10.8	10.3	10.1	10.7	10.5	10.2	10.4	10.4	10.3	10.3	10.0	10.2	10.2	10.4	10.4	10.6
3-methylbutan-1-ol	10.7	10.4	10.6	10.5	10.5	10.0	10.1	10.5	10.8	10.0	10.6	10.8	11.0	10.3	9.92	10.3	10.1	10.3	10.1	10.7
Solution E																				
Compound	Mass concentration, obtained for sample, mg/L AA																			
	1		2		3		4		5		6		7		8		9		10	
acetaldehyde	24.5	25.7	24.9	25.3	25.2	25.5	25.4	25.2	25.2	25.3	25.0	23.7	25.4	24.6	25.3	24.9	23.7	24.6	24.9	24.2
methyl acetate	25.0	26.3	25.0	26.6	26.5	26.7	26.7	26.7	26.2	26.2	26.2	25.6	26.4	25.2	26.4	26.4	25.6	25.1	25.1	24.4
ethyl acetate	25.3	26.4	25.0	26.6	26.6	27.3	26.8	27.6	26.2	26.3	26.2	24.5	26.5	25.2	26.3	26.8	24.6	25.4	25.5	24.0
methanol	27.7	28.9	27.7	28.7	28.5	29.2	28.8	29.1	28.9	28.9	29.1	28.4	28.8	27.7	28.7	29.3	28.5	27.8	27.9	28.6
propan-2-ol	25.6	26.9	25.9	26.2	26.5	26.4	26.3	26.2	25.8	26.2	26.3	25.9	26.7	26.1	26.4	26.4	25.9	24.9	24.6	26.6
propan-1-ol	25.0	25.2	25.1	25.0	25.0	25.2	25.2	25.2	25.1	25.3	25.1	25.2	25.5	24.5	24.8	24.7	25.1	24.4	24.5	24.8
2-methylpropan-1-ol	24.8	26.2	24.8	25.0	25.1	25.3	24.9	24.9	24.7	24.9	25.1	25.3	25.1	24.1	25.4	25.2	25.2	24.1	23.7	24.8
butan-1-ol	25.6	25.5	24.6	25.3	24.8	25.0	25.4	25.1	25.1	24.9	25.1	25.2	25.2	24.5	25.6	25.0	25.2	24.6	24.7	25.0

Table S.3.1 continuation

3-methylbutan-1-ol	25.0	25.6	24.6	25.0	24.9	25.4	24.9	25.0	24.8	25.0	24.9	25.5	25.0	24.4	25.2	25.1	25.5	24.7	24.3	25.5

Solution D

Compound	Mass concentration, obtained for sample, mg/L AA																			
	1		2		3		4		5		6		7		8		9		10	
acetaldehyde	198.2	190.6	187.7	194.9	184.9	200.5	201.1	204.8	212.6	194.8	208.6	203.3	202.6	212.8	203.8	189.5	196.0	197.5	200.7	202.2
methyl acetate	206.6	203.4	203.4	204.9	207.7	202.7	213.8	213.9	218.2	204.9	218.2	204.2	213.6	218.2	217.2	204.2	189.5	206.5	211.0	215.4
ethyl acetate	211.6	206.7	207.8	200.9	199.9	207.3	214.2	214.7	218.0	201.7	218.3	198.5	214.0	218.9	217.0	207.0	193.8	208.8	204.8	216.0
methanol	206.0	207.4	208.4	205.2	204.8	205.6	213.2	214.2	214.5	206.6	214.1	205.9	214.5	212.3	213.5	207.5	206.3	207.0	206.1	212.8
propan-2-ol	205.0	198.8	198.3	202.5	186.8	204.4	209.9	209.4	210.0	201.6	210.1	200.4	207.8	210.0	209.3	199.0	198.2	207.3	201.9	209.8
propan-1-ol	201.9	201.6	201.4	201.9	202.3	202.3	207.3	206.5	206.8	201.5	206.3	201.4	206.6	206.6	207.0	201.1	201.2	201.1	201.7	207.0
2-methylpropan-1-ol	201.8	198.2	197.0	200.2	199.4	201.7	206.5	205.3	206.3	200.0	206.1	199.0	204.1	205.9	206.8	197.6	198.8	196.9	200.5	206.8
butan-1-ol	202.6	202.7	202.1	203.0	204.8	202.5	205.9	206.1	206.4	202.8	205.4	202.1	205.9	206.4	206.1	203.3	202.7	202.7	203.4	206.6
3-methylbutan-1-ol	202.6	201.3	200.8	202.6	201.8	202.6	205.0	204.3	204.9	200.8	204.8	202.0	204.9	205.1	205.6	201.9	201.4	201.4	203.3	206.3

Solution C

Compound	Mass concentration, obtained for sample, mg/L AA																			
	1		2		3		4		5		6		7		8		9		10	
acetaldehyde	252.8	251.3	251.1	245.6	241.4	252.2	247.2	249.0	242.4	240.4	247.7	238.6	251.6	243.3	240.0	245.5	242.3	241.7	237.0	243.8
methyl acetate	257.6	256.1	256.4	252.8	234.2	256.9	254.7	252.4	238.6	248.4	251.7	253.4	256.7	238.9	254.7	243.4	257.5	255.1	254.0	255.8
ethyl acetate	257.8	255.1	256.3	253.3	234.5	257.1	255.2	263.9	249.6	246.7	251.4	261.1	262.5	249.5	261.1	254.8	262.8	260.5	261.5	260.5
methanol	259.3	258.7	256.9	258.1	258.2	257.0	258.6	257.8	259.0	258.1	257.8	257.5	255.4	256.8	258.2	257.9	257.5	257.9	258.8	256.6
propan-2-ol	255.9	251.4	255.2	254.3	247.1	256.9	255.6	256.9	252.8	251.5	251.6	257.0	257.1	252.4	257.6	253.9	257.1	256.7	258.0	256.2
propan-1-ol	254.0	253.1	253.4	253.0	251.6	253.7	252.8	254.7	253.0	252.9	252.6	254.6	255.0	253.4	254.4	253.1	254.2	254.0	255.2	254.3
2-methylpropan-1-ol	252.2	253.0	253.3	251.1	248.1	253.5	251.4	254.1	249.9	250.5	251.0	254.3	255.8	250.7	253.4	251.6	254.0	253.1	254.0	253.5
butan-1-ol	256.4	254.4	255.3	254.4	254.0	254.8	254.7	255.7	254.3	254.7	253.9	256.0	256.0	255.0	255.0	254.9	255.6	255.6	256.3	256.1
3-methylbutan-1-ol	254.8	254.1	254.7	254.1	252.5	255.2	254.8	255.6	253.7	253.7	253.1	256.7	257.3	253.2	256.0	254.0	256.5	256.0	256.5	256.3

Solution B

Compound	Mass concentration, obtained for sample, mg/L AA																			
	1		2		3		4		5		6		7		8		9		10	
acetaldehyde	473.5	481.4	474.3	474.1	506.1	497.8	498.8	507.3	464.7	473.8	500.3	504.8	501.2	498.3	503.4	477.4	496.8	461.1	466.1	504.0
methyl acetate	509.5	512.3	453.7	511.6	537.0	544.5	503.6	534.6	535.7	453.2	540.7	543.0	546.7	535.3	544.0	458.1	534.6	529.2	502.3	544.0
ethyl acetate	524.5	492.4	487.5	480.9	541.5	544.2	517.0	536.3	510.4	487.3	543.5	544.2	549.0	520.8	542.7	490.6	538.0	504.4	544.4	505.6
methanol	517.0	511.9	532.4	513.1	526.4	528.5	509.6	529.3	529.2	530.3	526.3	528.6	526.1	512.6	530.4	531.1	530.1	528.8	544.1	513.3
propan-2-ol	473.1	501.1	501.1	496.4	521.2	522.7	508.6	521.9	523.4	503.8	523.0	523.5	516.5	522.5	519.6	504.1	513.2	523.0	498.0	519.6
propan-1-ol	516.1	503.0	517.7	502.5	516.8	516.1	503.5	515.9	520.9	520.1	517.3	517.0	516.1	516.4	516.5	521.2	514.8	520.7	514.1	517.4
2-methylpropan-1-ol	482.9	498.2	507.8	494.3	511.2	512.7	503.8	513.0	525.6	509.3	513.3	514.4	507.1	513.6	511.1	512.4	504.6	521.6	491.3	511.9
butan-1-ol	506.1	505.1	513.6	507.1	515.8	514.1	507.3	513.0	520.5	511.3	515.5	514.7	513.1	514.6	514.2	509.4	513.4	518.8	522.8	515.1
3-methylbutan-1-ol	492.2	503.3	497.3	505.1	510.4	509.4	506.8	508.9	520.5	496.2	511.0	510.6	508.0	510.0	509.6	486.9	505.6	520.0	494.2	510.2

Table S.3.1 continuation

Compound	Solution A																			
	Mass concentration, obtained for sample, mg/L AA																			
	1		2		3		4		5		6		7		8		9		10	
acetaldehyde	5180	5146	5126	4729	5140	5149	5105	4755	5170	5162	4725	5092	5149	4732	4843	4806	4844	4724	4482	4806
methyl acetate	5299	5166	5189	4547	5164	5163	5176	4551	5423	5318	4552	5018	5064	4522	4931	4786	5020	4550	5260	5025
ethyl acetate	5518	5389	5413	4881	5374	5377	5385	4898	5214	5133	4876	5194	5235	4874	5116	4970	5205	4870	5182	5172
methanol	5239	5226	5215	5183	5224	5228	5232	5187	5229	5110	5174	5240	5245	5161	5094	5095	5091	5179	5193	5091
propan-2-ol	5245	5236	5227	5045	5231	5237	5233	5052	5226	5227	5017	5228	5240	5029	5057	5018	5088	5016	5227	5018
propan-1-ol	5203	5242	5228	5235	5220	5234	5223	5235	5228	5214	5228	5230	5227	5208	5056	5051	5062	5235	5195	5051
2-methylpropan-1-ol	5236	5242	5227	5108	5217	5231	5222	5107	5212	5210	5104	5217	5223	5080	4988	4973	5038	5104	5227	4990
butan-1-ol	5236	5276	5255	5106	5238	5252	5246	5109	5251	5254	5115	5252	5242	5093	5098	5103	5100	5117	5206	5106
3-methylbutan-1-ol	5218	5257	5230	4973	5210	5226	5215	4947	5211	5223	4969	5223	5219	4944	5069	5066	5073	4971	5186	5068

Table S.3.2 The results of identification of outliers by Cochran's test for the results of homogeneity study

s is the standard deviation between two results, obtained under repeatability conditions, calculated according to formula (5) from the item 7.2.10 of ISO 5725-2, mg/L AA.

s_{max} is the highest standard deviation in the set of data, mg/L AA.

C is the Cochran's test statistic, calculated according to formula (8) from the item 7.3.3.2 of ISO 5725-2.

$C_{crit,\ 1\%}$ and $C_{crit,\ 5\%}$ are 1% and 5% critical values for $p = 10$, $n = 2$ (Table 4from the item 8.1 of ISO 5725-2)

Compound	Solution G					
	s^2_{max}	Σs^2	*C*	$C_{crit,\ 1\%}$	$C_{crit,\ 5\%}$	Result
acetaldehyde	0.0220	0.0731	0.301	0.718	0.602	no outliers
methyl acetate	0.0033	0.0113	0.296	0.718	0.602	no outliers
ethyl acetate	0.0106	0.0198	0.537	0.718	0.602	no outliers
methanol	0.0293	0.0677	0.433	0.718	0.602	no outliers
propan-2-ol	0.0305	0.0717	0.425	0.718	0.602	no outliers
propan-1-ol	0.0128	0.0226	0.566	0.718	0.602	no outliers
2-methylpropan-1-ol	0.0100	0.0183	0.546	0.718	0.602	no outliers
butan-1-ol	0.0018	0.0063	0.285	0.718	0.602	no outliers
3-methylbutan-1-ol	0.0024	0.0067	0.358	0.718	0.602	no outliers
Compound	Solution F					
	$\mathbf{S^2_{max}}$	$\mathbf{\Sigma S_{ij}^2}$	**C**	$C_{crit,\ 1\%}$	$C_{crit,\ 5\%}$	Result
acetaldehyde	1.22	3.33	0.366	0.718	0.602	no outliers
methyl acetate	1.17	3.65	0.321	0.718	0.602	no outliers
ethyl acetate	0.70	2.29	0.304	0.718	0.602	no outliers
methanol	0.60	1.58	0.380	0.718	0.602	no outliers
propan-2-ol	0.59	2.25	0.263	0.718	0.602	no outliers
propan-1-ol	0.13	0.49	0.266	0.718	0.602	no outliers
2-methylpropan-1-ol	0.47	1.78	0.263	0.718	0.602	no outliers
butan-1-ol	0.27	0.67	0.395	0.718	0.602	no outliers
3-methylbutan-1-ol	0.28	1.09	0.253	0.718	0.602	no outliers
Compound	Solution E					
	$\mathbf{S^2_{max}}$	$\mathbf{\Sigma S_{ij}^2}$	**C**	$C_{crit,\ 1\%}$	$C_{crit,\ 5\%}$	Result
acetaldehyde	0.88	2.69	0.328	0.718	0.602	no outliers
methyl acetate	1.22	3.38	0.362	0.718	0.602	no outliers
ethyl acetate	1.56	6.34	0.246	0.718	0.602	no outliers
methanol	0.62	2.88	0.215	0.718	0.602	no outliers
propan-2-ol	1.86	3.77	0.495	0.718	0.602	no outliers
propan-1-ol	0.47	0.83	0.562	0.718	0.602	no outliers
2-methylpropan-1-ol	0.90	2.68	0.338	0.718	0.602	no outliers
butan-1-ol	0.27	0.97	0.274	0.718	0.602	no outliers
3-methylbutan-1-ol	0.65	1.68	0.386	0.718	0.602	no outliers
Compound	Solution D					
	$\mathbf{S^2_{max}}$	$\mathbf{\Sigma S_{ij}^2}$	**C**	$C_{crit,\ 1\%}$	$C_{crit,\ 5\%}$	Result
acetaldehyde	158.60	513.97	0.309	0.718	0.602	no outliers
methyl acetate	143.48	453.74	0.316	0.718	0.602	no outliers
ethyl acetate	195.82	630.70	0.310	0.718	0.602	no outliers
methanol	33.47	114.96	0.291	0.718	0.602	no outliers
propan-2-ol	153.53	393.52	0.390	0.718	0.602	no outliers
propan-1-ol	17.44	57.95	0.301	0.718	0.602	no outliers
2-methylpropan-1-ol	42.26	125.27	0.337	0.718	0.602	no outliers
butan-1-ol	6.42	24.09	0.267	0.718	0.602	no outliers
3-methylbutan-1-ol	8.42	26.78	0.314	0.718	0.602	no outliers

Table S.3.2 continuation

Compound	Solution C					
	S^2_{max}	ΣS_{ij}^2	C	$C_{crit,\ 1\%}$	$C_{crit,\ 5\%}$	Result
acetaldehyde	58.81	193.77	0.303	0.718	0.602	no outliers
methyl acetate	257.31	544.44	0.473	0.718	0.602	no outliers
ethyl acetate	255.95	459.75	0.557	0.718	0.602	no outliers
methanol	2.33	5.77	0.404	0.718	0.602	no outliers
propan-2-ol	47.76	93.78	0.509	0.718	0.602	no outliers
propan-1-ol	2.12	9.00	0.236	0.718	0.602	no outliers
2-methylpropan-1-ol	15.01	42.32	0.355	0.718	0.602	no outliers
butan-1-ol	2.22	6.11	0.362	0.718	0.602	no outliers
3-methylbutan-1-ol	8.34	21.30	0.392	0.718	0.602	no outliers
Compound	Solution B					
	S^2_{max}	ΣS_{ij}^2	C	$C_{crit,\ 1\%}$	$C_{crit,\ 5\%}$	Result
acetaldehyde	717.2	1852.3	0.387	0.718	0.602	no outliers
methyl acetate	3684.3	10233.9	0.360	0.718	0.602	no outliers
ethyl acetate	1356.4	4064.4	0.334	0.718	0.602	no outliers
methanol	474.2	966.2	0.491	0.718	0.602	no outliers
propan-2-ol	391.2	1102.0	0.355	0.718	0.602	no outliers
propan-1-ol	115.0	311.9	0.369	0.718	0.602	no outliers
2-methylpropan-1-ol	211.1	761.5	0.277	0.718	0.602	no outliers
butan-1-ol	42.8	138.9	0.308	0.718	0.602	no outliers
3-methylbutan-1-ol	295.3	881.1	0.335	0.718	0.602	no outliers
Compound	Solution A					
	S^2_{max}	ΣS_{ij}^2	C	$C_{crit,\ 1\%}$	$C_{crit,\ 5\%}$	Result
acetaldehyde	87148	355432	0.245	0.718	0.602	no outliers
methyl acetate	206154	819526	0.252	0.718	0.602	no outliers
ethyl acetate	141482	454174	0.312	0.718	0.602	no outliers
methanol	7088	23589	0.300	0.718	0.602	no outliers
propan-2-ol	22398	102771	0.218	0.718	0.602	no outliers
propan-1-ol	15065	26738	0.563	0.718	0.602	no outliers
2-methylpropan-1-ol	28142	60782	0.463	0.718	0.602	no outliers
butan-1-ol	11111	47074	0.236	0.718	0.602	no outliers
3-methylbutan-1-ol	37680	151865	0.248	0.718	0.602	no outliers

Table S.3.3 The results of the ANOVA test for the homogeneity study

MS_{bb} is between group variance, mg/L AA;
MS_{within} is within group variance, mg/L AA; F_{calc} is the result of Fisher test (F_{crit} = 3.02),
p value is the probability of getting a result at least as extreme as the one that was actually observed, p_{crit}= 0.05

Compound	Solution															
	G				F				E				D			
	MS_{bb}	MS_{within}	F_{calc}	*p value*	MS_{bb}	MS_{within}	F_{calc}	*p value*	MS_{bb}	MS_{within}	F_{calc}	*p value*	MS_{bb}	MS_{within}	F_{calc}	*p value*
acetaldehyde	0.0070	0.0073	0.95	0.52	0.22	0.33	0.65	0.73	0.38	0.27	1.40	0.30	66.16	51.40	1.29	0.35
methyl acetate	0.0011	0.0011	0.98	0.51	0.19	0.36	0.52	0.83	0.69	0.34	2.05	0.14	61.87	45.37	1.36	0.32
ethyl acetate	0.0011	0.0020	0.58	0.79	0.08	0.23	0.37	0.93	1.30	0.63	2.06	0.14	45.86	63.07	0.73	0.68
methanol	0.0064	0.0068	0.95	0.53	0.08	0.16	0.48	0.86	0.24	0.29	0.85	0.59	17.03	11.50	1.48	0.27
propan-2-ol	0.0045	0.0072	0.62	0.76	0.11	0.22	0.48	0.86	0.25	0.38	0.67	0.72	34.18	39.35	0.87	0.58
propan-1-ol	0.0021	0.0023	0.92	0.55	0.05	0.05	1.04	0.47	0.08	0.08	0.95	0.52	7.98	5.80	1.38	0.31
2-methylpropan-1-ol	0.0020	0.0018	1.08	0.45	0.09	0.18	0.49	0.85	0.29	0.27	1.07	0.45	14.00	12.53	1.12	0.43
butan-1-ol	0.0008	0.0006	1.21	0.38	0.06	0.07	0.84	0.60	0.11	0.10	1.13	0.42	3.54	2.41	1.47	0.28
3-methylbutan-1-ol	0.0004	0.0007	0.57	0.79	0.08	0.11	0.76	0.66	0.07	0.17	0.44	0.88	3.70	2.68	1.38	0.31

Compound	Solution											
	C				B				A			
	MS_{bb}	MS_{within}	F_{calc}	*p value*	MS_{bb}	MS_{within}	F_{calc}	*p value*	MS_{bb}	MS_{within}	F_{calc}	*p value*
acetaldehyde	29.16	19.38	1.50	0.27	337.2	185.2	1.82	0.18	59811.6	35543.2	1.68	0.21
methyl acetate	43.71	54.44	0.80	0.62	882.9	1023.4	0.86	0.58	95112.8	81952.6	1.16	0.41
ethyl acetate	53.54	45.97	1.16	0.41	724.3	406.4	1.78	0.19	42020.2	45417.4	0.93	0.54
methanol	1.17	0.58	2.03	0.14	62.3	96.6	0.64	0.74	4051.5	2358.9	1.72	0.21
propan-2-ol	6.50	9.38	0.69	0.70	253.3	110.2	2.30	0.11	10001.8	10277.1	0.97	0.51
propan-1-ol	0.79	0.90	0.87	0.58	31.9	31.2	1.02	0.48	7491.8	2673.8	2.80	0.06
2-methylpropan-1-ol	2.56	4.23	0.60	0.77	128.5	76.2	1.69	0.21	12100.4	6078.2	1.99	0.15
butan-1-ol	0.61	0.61	0.99	0.50	29.6	13.9	2.13	0.13	6100.6	4707.4	1.30	0.34
3-methylbutan-1-ol	1.64	2.13	0.77	0.65	59.4	88.1	0.67	0.72	10854.9	15186.5	0.71	0.69

S.4. Stability study

Table S.4.1 The obtained results of long-term stability study

Compound	Solution G																	
	Mass concentration, obtained in day from start of stability study, mg/L AA																	
	0 day		7 days		14 days		21 days		28 days		35 days		42 days		49 days		56 days	
acetaldehyde	1.84	1.80	1.83	1.91	1.84	1.82	1.69	1.91	1.84	1.75	1.79	1.78	1.74	1.75	1.74	1.68	1.84	1.79
methyl acetate	1.21	1.21	1.21	1.18	1.18	1.26	1.20	1.22	1.18	1.18	1.22	1.15	1.14	1.20	1.18	1.22	1.17	1.17
ethyl acetate	1.21	1.21	1.19	1.20	1.18	1.23	1.20	1.22	1.21	1.19	1.18	1.14	1.20	1.19	1.17	1.19	1.15	1.19
methanol	4.18	4.26	4.20	4.16	4.40	4.20	4.38	4.35	4.21	4.19	4.12	4.08	4.31	4.19	4.09	4.13	4.15	4.19
propan-2-ol	2.10	2.13	2.07	2.09	2.05	2.06	2.10	2.05	2.00	2.10	2.11	2.05	2.04	2.07	2.05	1.92	2.19	2.08
propan-1-ol	1.19	1.20	1.25	1.26	1.23	1.29	1.14	1.21	1.18	1.23	1.21	1.22	1.25	1.25	1.31	1.18	1.28	1.23
2-methylpropan-1-ol	1.21	1.19	1.19	1.24	1.19	1.21	1.21	1.20	1.21	1.29	1.22	1.20	1.19	1.20	1.20	1.25	1.24	1.15
butan-1-ol	1.22	1.20	1.26	1.22	1.21	1.20	1.21	1.18	1.17	1.29	1.22	1.22	1.25	1.23	1.21	1.21	1.21	1.18
3-methylbutan-1-ol	1.22	1.21	1.22	1.22	1.25	1.21	1.12	1.20	1.22	1.18	1.18	1.22	1.21	1.22	1.22	1.22	1.23	1.25
Compound	Mass concentration, obtained in day from start of stability study, mg/L AA																	
	63 days		70 days		77 days		84 days		91 days		98 days		105 days		112 days		119 days	
acetaldehyde	1.84	1.80	1.79	1.80	1.79	1.77	1.76	1.75	1.71	1.86	1.74	1.81	1.75	1.78	1.80	1.77	1.81	1.67
methyl acetate	1.21	1.18	1.19	1.22	1.20	1.17	1.22	1.25	1.24	1.29	1.26	1.19	1.23	1.22	1.23	1.15	1.24	1.15
ethyl acetate	1.24	1.22	1.25	1.28	1.23	1.23	1.23	1.22	1.25	1.29	1.27	1.27	1.28	1.26	1.27	1.15	1.20	1.18
methanol	4.16	4.37	4.39	4.35	4.34	4.36	4.22	4.27	4.36	4.24	4.24	4.26	4.24	4.25	4.34	4.26	4.37	4.20
propan-2-ol	2.30	2.17	2.07	2.09	2.18	2.07	2.14	2.19	2.14	2.16	2.06	2.08	2.10	2.08	2.12	1.98	2.08	2.06
propan-1-ol	1.24	1.23	1.28	1.25	1.22	1.22	1.23	1.16	1.23	1.28	1.25	1.15	1.21	1.15	1.24	1.15	1.24	1.22
2-methylpropan-1-ol	1.25	1.24	1.27	1.22	1.19	1.25	1.21	1.20	1.25	1.20	1.23	1.23	1.24	1.21	1.21	1.19	1.23	1.16
butan-1-ol	1.13	1.19	1.18	1.28	1.18	1.22	1.22	1.22	1.24	1.26	1.26	1.22	1.26	1.23	1.34	1.21	1.28	1.13
3-methylbutan-1-ol	1.26	1.23	1.11	1.23	1.21	1.20	1.24	1.13	1.22	1.29	1.23	1.26	1.21	1.26	1.23	1.25	1.21	1.20
Compound	Mass concentration, obtained in day from start of stability study, mg/L AA																	
	126 days		133 days		140 days		147 days		154 days		161 days		168 days		175 days		182 days	
acetaldehyde	1.80	1.81	1.81	1.76	1.79	1.84	1.77	1.83	1.78	1.76	2.01	1.81	1.76	1.62	1.84	1.74	1.75	1.89
methyl acetate	1.17	1.17	1.22	1.15	1.25	1.21	1.20	1.30	1.24	1.19	1.22	1.23	1.23	1.17	1.19	1.20	1.17	1.25
ethyl acetate	1.14	1.29	1.21	1.21	1.26	1.21	1.20	1.31	1.14	1.21	1.17	1.18	1.25	1.17	1.20	1.19	1.13	1.23
methanol	4.19	4.42	4.25	4.35	4.28	4.30	4.21	4.28	4.21	4.18	4.27	4.16	4.36	4.16	4.30	4.31	4.27	4.42
propan-2-ol	2.10	2.22	2.07	2.06	2.16	2.16	2.14	2.15	2.06	2.06	2.16	2.07	2.07	2.02	2.18	2.05	2.09	2.13
propan-1-ol	1.21	1.17	1.18	1.25	1.25	1.24	1.24	1.24	1.22	1.23	1.19	1.18	1.16	1.21	1.24	1.18	1.16	1.25
2-methylpropan-1-ol	1.27	1.12	1.20	1.17	1.23	1.26	1.21	1.31	1.21	1.25	1.21	1.23	1.20	1.17	1.20	1.22	1.22	1.25
butan-1-ol	1.24	1.22	1.22	1.21	1.24	1.27	1.22	1.26	1.22	1.26	1.19	1.24	1.25	1.18	1.21	1.21	1.19	1.27
3-methylbutan-1-ol	1.14	1.22	1.17	1.24	1.25	1.27	1.26	1.25	1.22	1.21	1.22	1.22	1.20	1.17	1.21	1.21	1.22	1.25

Table S.4.1 continuation

Compound	Solution F													
	Mass concentration, obtained in day from start of stability study, mg/L AA													
	0 day		14 days		28 days		42 days		56 days		70 days		84 days	
acetaldehyde	10.7	10.7	10.8	10.7	10.5	10.5	10.7	10.1	10.6	10.1	11.3	10.0	10.5	10.2
methyl acetate	10.2	10.3	10.4	10.3	9.72	10.2	10.4	9.69	10.5	9.6	10.5	9.9	10.5	10.1
ethyl acetate	10.3	10.3	10.4	10.4	10.1	10.4	10.3	10.2	10.6	9.8	10.4	10.5	10.5	10.2
methanol	13.3	13.3	13.8	13.5	13.2	13.6	13.2	13.7	13.1	13.5	12.9	14.0	13.0	13.0
propan-2-ol	11.1	11.1	10.7	11.0	10.8	11.0	10.8	10.6	11.0	11.1	11.2	11.1	11.0	10.6
propan-1-ol	10.2	10.2	10.3	10.4	10.1	9.9	10.2	10.0	10.2	10.7	10.1	10.3	10.1	10.4
2-methylpropan-1-ol	10.2	10.2	10.3	10.2	10.3	10.2	10.1	9.9	10.2	10.4	10.5	10.2	10.3	10.1
butan-1-ol	10.2	10.2	10.2	10.3	10.2	10.2	10.2	10.3	10.4	10.2	10.7	10.4	10.3	10.3
3-methylbutan-1-ol	10.3	10.3	10.2	10.2	10.5	10.5	10.3	10.0	10.3	9.9	10.4	10.1	10.4	10.0
Compound	Mass concentration, obtained in day from start of stability study, mg/L AA													
	98 days		112 days		126 days		140 days		154 days		168 days		182 days	
acetaldehyde	10.1	11.2	10.6	10.3	10.2	10.7	10.3	10.6	10.8	10.8	10.9	9.76	10.2	11.2
methyl acetate	10.4	10.5	10.3	9.78	10.4	9.74	10.1	10.3	10.6	10.0	10.2	9.71	9.88	10.7
ethyl acetate	10.4	10.6	10.7	10.1	10.7	10.3	10.6	10.2	10.9	10.4	11.0	10.0	10.0	10.4
methanol	13.7	13.2	13.7	13.1	13.5	13.7	13.3	12.8	13.5	13.2	13.8	13.5	13.6	13.7
propan-2-ol	11.1	11.0	11.1	10.8	11.1	11.0	10.8	10.8	10.8	10.8	10.9	10.5	11.3	11.1
propan-1-ol	10.2	10.2	10.3	10.1	10.3	9.90	10.2	10.2	10.2	10.2	10.1	10.1	10.6	10.4
2-methylpropan-1-ol	10.5	10.7	10.5	10.1	10.3	9.90	10.2	10.2	10.2	10.2	10.2	10.5	10.1	10.7
butan-1-ol	10.4	10.3	10.4	10.1	10.4	10.4	10.3	10.4	10.3	10.4	10.3	10.3	10.4	10.7
3-methylbutan-1-ol	10.3	10.1	10.6	10.1	10.3	10.1	10.4	10.5	10.2	10.3	10.5	10.1	10.2	10.6

Table S.4.1 continuation

Compound	Solution E													
	Mass concentration, obtained in day from start of stability study, mg/L AA													
	0 day		14 days		28 days		42 days		56 days		70 days		84 days	
acetaldehyde	25.1	24.9	24.4	25.2	24.0	24.4	25.0	25.1	24.8	25.2	25.6	23.7	25.7	24.6
methyl acetate	25.0	25.0	25.0	25.2	25.1	24.9	24.4	24.4	24.4	24.7	24.8	22.9	25.9	24.8
ethyl acetate	24.9	24.9	25.0	25.2	24.9	24.9	24.3	24.5	24.6	25.3	24.9	25.0	26.7	24.9
methanol	28.1	27.7	27.7	27.9	27.9	28.0	27.9	27.6	27.9	28.2	28.2	27.8	27.9	27.5
propan-2-ol	25.8	26.0	25.5	24.6	24.9	25.6	25.5	25.6	26.1	25.5	26.0	24.4	26.9	24.9
propan-1-ol	25.1	24.9	23.8	24.9	24.3	24.8	24.3	24.5	24.8	24.8	24.5	24.1	25.6	24.4
2-methylpropan-1-ol	24.8	24.7	24.8	24.6	24.9	24.6	24.6	24.8	24.8	25.2	25.2	23.7	25.4	24.4
butan-1-ol	25.0	25.0	24.6	24.6	24.7	24.7	24.6	24.5	25.5	25.2	24.7	24.1	25.2	24.6
3-methylbutan-1-ol	24.9	25.0	24.1	24.3	24.3	24.4	24.6	24.4	24.8	24.9	24.7	23.9	25.1	24.6
Compound	Mass concentration, obtained in day from start of stability study, mg/L AA													
	98 days		112 days		126 days		140 days		154 days		168 days		182 days	
acetaldehyde	25.1	24.0	24.4	25.0	25.2	25.1	24.7	24.9	25.8	25.8	25.0	25.35	25.2	24.6
methyl acetate	24.9	24.9	23.4	25.6	24.8	24.96	25.1	25.0	24.6	24.5	24.8	24.81	24.77	24.1
ethyl acetate	24.5	25.9	24.9	26.0	25.1	25.1	25.1	25.3	24.7	24.9	24.9	24.9	25.8	24.1
methanol	28.8	28.4	28.1	28.7	28.3	27.9	27.6	27.7	27.6	27.7	28.1	28.0	27.9	28.4
propan-2-ol	25.4	25.3	25.0	26.0	25.5	25.3	26.0	24.8	25.0	25.0	24.8	25.2	24.5	26.3
propan-1-ol	24.7	24.6	24.3	24.4	24.1	24.39	24.7	24.9	24.7	24.7	24.5	24.5	25.8	25.0
2-methylpropan-1-ol	24.4	24.3	24.2	25.2	24.1	24.39	24.7	24.9	24.7	24.7	24.7	24.8	24.6	25.7
butan-1-ol	24.5	24.6	24.3	25.2	24.4	24.0	24.2	24.2	24.5	24.7	24.3	24.3	24.7	25.2
3-methylbutan-1-ol	24.6	24.3	24.4	24.7	24.6	24.6	24.8	24.7	24.9	24.7	24.2	24.3	24.7	25.3

Table S.4.1 continuation

Compound	Solution D													
	Mass concentration, obtained in day from start of stability study, mg/L AA													
	0 day		14 days		28 days		42 days		56 days		70 days		84 days	
acetaldehyde	197.7	197.2	200.0	197.1	202.9	201.6	201.9	200.6	199.4	197.4	199.1	201.6	201.2	203.2
methyl acetate	200.5	200.6	203.2	203.2	203.4	203.4	199.4	199.7	205.6	203.4	202.9	202.9	198.9	201.6
ethyl acetate	200.8	198.8	200.7	201.9	202.2	202.3	202.3	201.1	195.2	195.8	204.1	206.1	197.1	200.1
methanol	205.9	205.1	206.8	207.1	207.8	207.6	208.1	209.0	205.5	206.0	208.9	211.3	206.0	206.1
propan-2-ol	201.9	200.1	196.6	195.7	204.7	205.3	201.1	201.6	203.0	203.3	202.7	202.5	207.3	206.6
propan-1-ol	201.3	201.5	200.5	200.2	201.0	200.1	200.3	200.0	202.1	203.7	200.6	200.9	202.7	199.5
2-methylpropan-1-ol	200.6	199.1	196.9	195.7	196.0	196.0	196.7	195.9	204.3	203.6	199.1	199.7	203.3	199.7
butan-1-ol	201.6	201.7	201.5	200.9	201.5	201.9	201.9	202.0	205.2	205.6	200.2	200.6	202.6	199.6
3-methylbutan-1-ol	201.4	200.8	199.4	199.0	199.7	199.7	200.7	200.5	203.0	202.9	199.1	198.9	202.9	200.5
Compound	Mass concentration, obtained in day from start of stability study, mg/L AA													
	98 days		112 days		126 days		140 days		154 days		168 days		182 days	
acetaldehyde	200.6	196.9	205.8	191.9	204.8	195.5	197.8	197.7	197.7	199.1	201.6	193.8	204.3	199.9
methyl acetate	206.8	203.8	202.6	197.1	204.0	203.2	204.2	204.3	195.0	197.5	202.7	205.8	202.0	203.7
ethyl acetate	207.1	200.7	199.7	200.8	201.0	201.0	200.2	201.0	203.5	203.0	199.9	202.0	200.6	205.5
methanol	202.6	207.0	201.3	206.4	204.9	204.3	204.4	205.8	206.7	207.3	204.4	206.3	207.2	210.2
propan-2-ol	202.8	202.5	197.1	198.2	202.0	202.1	202.0	201.1	199.8	199.5	202.2	201.7	203.4	201.3
propan-1-ol	203.6	200.2	203.9	200.1	200.5	200.7	202.4	202.0	202.7	202.0	200.7	202.9	200.4	203.7
2-methylpropan-1-ol	200.9	198.4	202.5	197.1	200.5	200.7	202.4	202.0	202.7	202.0	197.8	200.7	203.9	200.6
butan-1-ol	202.2	199.9	204.3	201.1	198.8	197.4	201.0	201.4	199.7	199.1	199.4	202.7	202.5	205.2
3-methylbutan-1-ol	201.6	198.7	203.8	200.0	200.3	200.6	203.1	203.4	203.5	202.4	197.6	200.1	200.0	202.1

Table S.4.1 continuation

Compound	Solution C													
	Mass concentration, obtained in day from start of stability study, mg/L AA													
	0 day		14 days		28 days		42 days		56 days		70 days		84 days	
acetaldehyde	245.9	246.4	245.7	252.2	247.4	246.8	258.3	248.0	249.7	249.3	251.7	251.7	254.2	248.6
methyl acetate	249.8	249.8	252.4	248.1	253.7	251.6	253.1	233.1	250.6	253.1	251.4	247.3	242.5	254.1
ethyl acetate	250.4	250.2	256.2	240.0	254.6	252.2	251.7	242.5	255.0	257.4	249.8	251.3	242.5	254.3
methanol	253.0	251.3	256.6	257.6	257.4	258.2	258.5	260.9	260.7	257.4	253.6	251.0	251.0	258.9
propan-2-ol	250.9	250.9	254.0	248.9	255.6	255.0	252.4	249.0	249.3	249.9	253.5	255.5	258.0	257.1
propan-1-ol	249.8	249.8	253.4	251.1	253.7	253.5	251.6	252.3	251.9	254.7	252.5	253.6	249.3	248.8
2-methylpropan-1-ol	249.6	248.0	252.5	248.9	252.9	252.1	251.2	248.2	252.3	252.6	252.1	253.8	249.8	252.8
butan-1-ol	251.0	251.9	254.2	253.2	254.7	254.7	252.7	254.1	255.4	255.7	254.7	255.2	250.2	254.4
3-methylbutan-1-ol	250.4	250.7	253.2	251.3	254.5	253.8	252.9	252.4	250.5	251.3	253.6	254.2	250.0	249.5
Compound	Mass concentration, obtained in day from start of stability study, mg/L AA													
	98 days		112 days		126 days		140 days		154 days		168 days		182 days	
acetaldehyde	247.4	247.9	254.8	242.7	252.5	251.2	252.3	248.7	245.9	257.4	246.1	254.7	254.7	247.0
methyl acetate	248.3	248.3	254.7	244.3	254.1	243.3	251.8	254.1	248.7	248.1	250.8	257.0	252.8	235.8
ethyl acetate	250.7	248.6	249.9	247.8	251.8	258.5	251.4	254.3	251.2	259.8	255.5	251.1	249.6	243.5
methanol	250.2	248.8	251.0	258.1	246.9	259.5	256.0	257.2	249.1	259.3	262.8	251.6	258.4	258.3
propan-2-ol	254.8	255.4	250.0	247.4	255.8	252.7	253.6	254.5	250.3	256.9	253.8	255.5	249.1	249.9
propan-1-ol	254.0	253.6	248.9	248.8	252.6	253.8	253.5	253.4	253.7	254.8	252.9	253.0	252.9	252.8
2-methylpropan-1-ol	253.6	253.1	249.0	247.2	252.6	253.8	253.5	253.4	253.7	254.8	251.2	253.7	251.6	249.8
butan-1-ol	253.2	254.2	249.8	250.0	253.6	249.6	253.4	252.4	250.1	254.7	254.8	253.1	253.8	253.9
3-methylbutan-1-ol	254.2	254.6	250.3	249.1	254.1	255.2	254.9	254.5	254.6	255.0	254.7	253.5	252.4	252.3

Table S.4.1 continuation

Compound	Solution B													
	Mass concentration, obtained in day from start of stability study, mg/L AA													
	0 day		14 days		28 days		42 days		56 days		70 days		84 days	
acetaldehyde	492.1	492.9	500.8	485.9	509.4	480.6	489.8	494.9	503.5	500.0	496.8	503.8	503.9	482.5
methyl acetate	501.5	501.9	502.5	513.7	508.4	486.7	494.0	491.9	504.4	504.8	504.2	505.9	493.3	518.2
ethyl acetate	498.2	504.7	507.1	497.0	499.6	509.0	504.9	502.7	511.5	509.7	507.8	515.9	485.5	511.2
methanol	509.6	499.9	541.9	508.0	512.8	505.3	510.7	511.8	518.5	515.0	516.0	521.2	509.8	509.7
propan-2-ol	502.5	509.2	504.2	517.9	504.6	492.6	502.6	501.0	516.1	516.2	505.0	503.4	501.0	514.6
propan-1-ol	503.0	503.7	487.7	506.7	488.6	512.3	500.7	500.7	491.7	490.5	500.4	500.7	519.5	505.2
2-methylpropan-1-ol	499.6	504.6	491.0	510.6	500.7	493.2	501.4	499.4	508.1	506.4	494.3	494.3	505.5	493.3
butan-1-ol	506.0	506.7	510.1	496.0	501.3	498.2	504.1	503.8	497.1	495.1	498.4	499.7	522.6	505.7
3-methylbutan-1-ol	503.5	505.8	501.4	507.0	512.1	499.0	503.5	503.2	497.8	495.9	501.7	502.2	511.0	497.6
Compound	Mass concentration, obtained in day from start of stability study, mg/L AA													
	98 days		112 days		126 days		140 days		154 days		168 days		182 days	
acetaldehyde	493.2	494.6	488.3	501.4	490.1	492.0	486.6	487.9	501.8	503.9	489.0	499.0	506.9	484.3
methyl acetate	510.6	508.1	519.5	487.9	511.4	507.8	510.0	510.6	507.1	509.4	512.0	506.9	481.3	516.4
ethyl acetate	501.4	499.3	512.3	488.3	497.4	501.7	501.1	506.0	509.9	511.5	517.1	500.4	496.1	486.2
methanol	506.1	506.2	528.9	509.8	522.5	526.2	511.3	509.7	513.6	514.1	522.3	505.4	511.4	530.6
propan-2-ol	497.7	500.7	512.7	501.1	504.4	504.7	495.0	499.6	505.1	502.5	494.4	502.7	492.6	504.0
propan-1-ol	500.9	501.7	509.3	495.8	501.0	501.1	503.7	504.3	506.8	507.4	506.4	499.1	514.6	506.4
2-methylpropan-1-ol	500.0	504.6	503.5	496.4	501.0	501.1	503.7	504.3	506.8	507.4	496.7	502.1	503.9	496.5
butan-1-ol	496.3	497.0	505.8	497.6	491.8	494.1	496.8	500.0	507.2	503.8	504.8	497.3	516.9	504.2
3-methylbutan-1-ol	492.2	493.5	502.2	496.1	497.8	499.7	508.7	506.8	507.8	508.7	506.1	501.4	512.3	503.6

Table S.4.1 continuation

Compound	Solution A													
	Mass concentration, obtained in day from start of stability study, mg/L AA													
	0 day		14 days		28 days		42 days		56 days		70 days		84 days	
acetaldehyde	4948	4976	4921	4949	4995	5006	4877	4888	4880	4861	4962	4920	5029	4927
methyl acetate	5054	5055	4939	5102	4877	4961	5045	5026	5016	5016	4992	4867	5067	4892
ethyl acetate	5037	4956	4973	5056	4979	5019	4908	4993	5067	5059	4942	5146	4935	5073
methanol	5083	5092	5234	5075	5001	5065	5137	5123	5051	5051	4954	5172	5140	4986
propan-2-ol	5069	4982	4964	5029	5032	5058	4966	4992	5045	5055	5072	5060	4986	5049
propan-1-ol	5063	5049	5007	5002	4999	4997	5020	5027	5037	5027	5041	5064	4967	5003
2-methylpropan-1-ol	5041	4975	4956	5003	5000	5024	4951	4982	4999	5000	5039	5044	5000	4996
butan-1-ol	5046	5106	4954	5076	4975	5047	5064	5072	5043	5046	5078	5116	4976	5065
3-methylbutan-1-ol	5059	5065	5020	5033	5110	5057	5025	5049	5032	5040	5033	5074	4956	5072
Compound	Mass concentration, obtained in day from start of stability study, mg/L AA													
	98 days		112 days		126 days		140 days		154 days		168 days		182 days	
acetaldehyde	4977	4970	4927	4975	4911	4916	4907	4870	4903	4963	4980	4941	4945	4926
methyl acetate	5065	5014	4935	5057	5044	5043	4964	5009	5040	5007	5042	5006	4969	4916
ethyl acetate	5042	5076	5172	4971	5017	5020	4994	5052	5080	5054	5038	5019	5058	4996
methanol	5069	5058	5070	4980	5056	5059	5080	5072	5049	5054	5134	5107	5041	5040
propan-2-ol	5036	5070	5139	5001	5048	5059	5043	5004	5048	5010	5035	5041	5049	5014
propan-1-ol	5054	5058	4979	4978	5041	5053	5068	5063	5086	5070	5043	5038	5053	5003
2-methylpropan-1-ol	4990	5014	4972	5014	5041	5053	5068	5063	5086	5070	4985	4990	5010	4977
butan-1-ol	5069	5061	5010	4970	5002	5016	5033	5008	5051	5021	5077	5069	5089	5045
3-methylbutan-1-ol	5043	5046	4976	4913	5076	5088	5104	5105	5086	5099	5033	5029	5061	4991

Table S.4.2 The results of identification of outliers by Cochran's and Grubbs' tests for the results of long-term stability study

s is the standard deviation between two results, obtained under repeatability conditions, calculated according to formula (5) from the item 7.2.10 of ISO 5725-2, mg/L AA.
s_{max} is the highest standard deviation in the set of data, mg/L AA.
C is the Cochran's test statistic, calculated according to formula (8) from the item 7.3.3.2 of ISO 5725-2.
$C_{crit,\ 1\%}$ and $C_{crit,\ 5\%}$ are 1% and 5% critical values for $p = 27$ and $n = 2$ – $C_{crit,\ 1\%} = 0.391$; $C_{crit,\ 5\%} = 0.316$; for $p = 14$ and $n = 2$ – $C_{crit,\ 1\%} = 0.599$; $C_{crit,\ 5\%} = 0.492$;
$\bar{\bar{C}}$ is the average mass concentration of volatile compound, obtained during measurements, mg/L AA
S is standard deviation of mass concentrations, calculated according to formula (11) from the item 7.3.4.1 of ISO 5725-2., mg/L AA
$\bar{C}_{max}$ and $\bar{C}_{min}$ are the maximal and minimal value of obtained average mass concentration of volatile in solution, correspondingly, mg/L AA
$G_{max}$and $G_{min}$are the Grubbs' test statistic, calculated according to formulas (9) and (11) from the item 7.3.4.1 of ISO 5725-2, correspondingly
The critical values for Grubbs' test for $p = 27$– $G_{crit,\ 1\%} = 3.178$; $G_{crit,\ 5\%} = 2.859$; for $p = 14$ – $G_{crit,\ 1\%} = 2.755$; $G_{crit,\ 5\%} = 2.507$ (Table 5 from the item 8.3 of ISO 5725-2)

Solution G

Compound	The results of Cochran's test				**The results of Grubbs' test**									
	s^2_{max}	Σs^2	C	Result	$\bar{\bar{C}}$	S	$\bar{C}_{max}$	$\bar{C}_{max} - \bar{\bar{C}}$	G_{max}	Result	$\bar{C}_{min}$	$\bar{\bar{C}} - \bar{C}_{min}$	G_{min}	Result
acetaldehyde	0.0250	0.1106	0.226	no outliers	1.79	0.044	1.91	0.12	2.752	no outliers	1.69	0.10	2.255	no outliers
methyl acetate	0.0049	0.0352	0.138	no outliers	1.21	0.023	1.27	0.06	2.586	no outliers	1.17	0.04	1.654	no outliers
ethyl acetate	0.0115	0.0437	0.263	no outliers	1.21	0.032	1.27	0.06	1.810	no outliers	1.16	0.05	1.663	no outliers
methanol	0.0263	0.1548	0.170	no outliers	4.26	0.070	4.37	0.11	1.604	no outliers	4.10	0.16	2.273	no outliers
propan-2-ol	0.0102	0.0730	0.139	no outliers	2.10	0.051	2.24	0.14	2.707	no outliers	1.99	0.11	2.147	no outliers
propan-1-ol	0.0087	0.0415	0.210	no outliers	1.22	0.028	1.26	0.04	1.544	no outliers	1.17	0.05	1.672	no outliers
2-methylpropan-1-ol	0.0118	0.0388	0.304	no outliers	1.22	0.020	1.26	0.04	2.006	no outliers	1.18	0.03	1.611	no outliers
butan-1-ol	0.0103	0.0468	0.220	no outliers	1.22	0.022	1.27	0.05	2.222	no outliers	1.16	0.06	2.747	no outliers
3-methylbutan-1-ol	0.0070	0.0306	0.229	no outliers	1.22	0.026	1.26	0.04	1.599	no outliers	1.16	0.06	2.148	no outliers

Solution F

Compound	The results of Cochran's test				**The results of Grubbs' test**									
	s^2_{max}	Σs^2	C	Result	$\bar{\bar{C}}$	S	$\bar{C}_{max}$	$\bar{C}_{max} - \bar{\bar{C}}$	G_{max}	Result	$\bar{C}_{min}$	$\bar{\bar{C}} - \bar{C}_{min}$	G_{min}	Result
acetaldehyde	0.911	3.309	0.275	no outliers	10.5	0.162	10.8	0.28	1.726	no outliers	10.3	0.21	1.325	no outliers
methyl acetate	0.337	1.929	0.175	no outliers	10.2	0.158	10.5	0.28	1.776	no outliers	9.95	0.23	1.480	no outliers
ethyl acetate	0.498	1.490	0.334	no outliers	10.4	0.142	10.7	0.30	2.084	no outliers	10.2	0.21	1.449	no outliers
methanol	0.590	1.516	0.389	no outliers	13.4	0.204	13.7	0.25	1.209	no outliers	13.0	0.40	1.946	no outliers
propan-2-ol	0.061	0.286	0.212	no outliers	10.9	0.166	11.2	0.28	1.657	no outliers	10.7	0.24	1.464	no outliers
propan-1-ol	0.126	0.360	0.349	no outliers	10.2	0.135	10.5	0.28	2.043	no outliers	10.0	0.22	1.620	no outliers
2-methylpropan-1-ol	0.186	0.497	0.375	no outliers	10.3	0.134	10.6	0.32	2.379	no outliers	10.0	0.23	1.680	no outliers
butan-1-ol	0.037	0.163	0.228	no outliers	10.3	0.112	10.6	0.23	2.062	no outliers	10.2	0.16	1.399	no outliers
3-methylbutan-1-ol	0.145	0.541	0.268	no outliers	10.3	0.112	10.5	0.23	2.051	no outliers	10.1	0.17	1.521	no outliers

Table S.4.2 continuation

Compound	The results of Cochran's test				The results of Grubbs' test									
	s^2_{max}	Σs^2	C	Result	$\bar{\bar{C}}$	S	$\bar{C}_{max}$	$\bar{C}_{max} - \bar{\bar{C}}$	G_{max}	Result	$\bar{C}_{min}$	$\bar{\bar{C}} - \bar{C}_{min}$	G_{min}	Result
Solution E														
acetaldehyde	1.78	3.88	0.458	no outliers	24.9	0.379	25.8	0.93	2.441	no outliers	24.2	0.70	1.838	no outliers
methyl acetate	2.28	5.14	0.443	no outliers	24.7	0.382	25.4	0.61	1.588	no outliers	23.9	0.88	2.295	no outliers
ethyl acetate	1.51	4.78	0.315	no outliers	25.0	0.322	25.8	0.75	2.314	no outliers	24.4	0.66	2.034	no outliers
methanol	0.21	0.85	0.252	no outliers	28.0	0.283	28.6	0.64	2.251	no outliers	27.7	0.31	1.107	no outliers
propan-2-ol	2.10	7.20	0.291	no outliers	25.4	0.313	25.9	0.51	1.625	no outliers	25.0	0.44	1.398	no outliers
propan-1-ol	0.67	1.93	0.350	no outliers	24.6	0.336	25.4	0.77	2.300	no outliers	24.2	0.40	1.178	no outliers
2-methylpropan-1-ol	1.23	3.02	0.407	no outliers	24.7	0.238	25.1	0.42	1.773	no outliers	24.2	0.46	1.939	no outliers
butan-1-ol	0.45	1.06	0.423	no outliers	24.7	0.317	25.3	0.67	2.117	no outliers	24.2	0.45	1.404	no outliers
3-methylbutan-1-ol	0.32	0.85	0.375	no outliers	24.6	0.263	25.0	0.40	1.515	no outliers	24.2	0.39	1.480	no outliers
Solution D														
acetaldehyde	96.9	201.6	0.481	no outliers	199.6	1.8	202.2	2.6	1.502	no outliers	197.4	2.1	1.211	no outliers
methyl acetate	15.0	35.2	0.425	no outliers	202.2	2.5	205.3	3.1	1.239	no outliers	196.3	5.9	2.346	no outliers
ethyl acetate	20.0	45.1	0.443	no outliers	201.2	2.4	205.1	3.9	1.628	no outliers	195.5	5.7	2.405	no outliers
methanol	12.9	34.0	0.379	no outliers	206.4	1.8	210.1	3.6	2.028	no outliers	203.8	2.6	1.443	no outliers
propan-2-ol	2.3	6.1	0.382	no outliers	201.7	2.7	206.9	5.2	1.933	no outliers	196.1	5.6	2.064	no outliers
propan-1-ol	7.1	28.0	0.252	no outliers	201.4	0.9	202.9	1.5	1.698	no outliers	200.2	1.3	1.484	no outliers
2-methylpropan-1-ol	14.8	36.8	0.403	no outliers	200.0	2.4	203.9	4.0	1.620	no outliers	196.0	3.9	1.611	no outliers
butan-1-ol	5.2	22.7	0.228	no outliers	201.5	1.8	205.4	3.9	2.216	no outliers	198.1	3.4	1.919	no outliers
3-methylbutan-1-ol	7.3	20.6	0.354	no outliers	200.9	1.5	203.2	2.3	1.559	no outliers	198.9	2.1	1.389	no outliers
Solution C														
acetaldehyde	73.3	303.6	0.241	no outliers	250.0	2.0	253.2	3.2	1.573	no outliers	246.2	3.8	1.879	no outliers
methyl acetate	201.2	569.9	0.353	no outliers	249.4	3.0	253.9	4.5	1.482	no outliers	243.1	6.3	2.062	no outliers
ethyl acetate	130.9	346.7	0.377	no outliers	251.1	3.2	256.2	5.0	1.567	no outliers	246.6	4.6	1.417	no outliers
methanol	79.5	266.5	0.298	no outliers	255.5	3.0	259.7	4.2	1.415	no outliers	249.5	6.0	1.995	no outliers
propan-2-ol	21.5	54.0	0.399	no outliers	252.8	2.7	257.6	4.7	1.767	no outliers	248.7	4.2	1.563	no outliers
propan-1-ol	4.0	8.9	0.452	no outliers	252.3	1.8	254.3	2.0	1.099	no outliers	248.8	3.5	1.955	no outliers
2-methylpropan-1-ol	6.3	26.7	0.235	no outliers	251.7	1.9	254.3	2.6	1.374	no outliers	248.1	3.6	1.932	no outliers
butan-1-ol	10.7	31.9	0.334	no outliers	253.2	1.5	255.6	2.4	1.560	no outliers	249.9	3.3	2.135	no outliers
3-methylbutan-1-ol	1.8	5.2	0.348	no outliers	252.8	1.9	254.8	2.0	1.076	no outliers	249.7	3.1	1.629	no outliers

Table S.4.2 continuation

Solution B														
Compound	The results of Cochran's test				**The results of Grubbs' test**									
	s^2_{max}	Σs^2	C	Result	$\bar{\bar{C}}$	S	$\bar{C}_{max}$	$\bar{C}_{max} - \bar{\bar{C}}$	G_{max}	Result	$\bar{C}_{min}$	$\bar{\bar{C}} - \bar{C}_{min}$	G_{min}	Result
acetaldehyde	413.0	1195.3	0.346	no outliers	494.8	4.2	502.9	8.0	1.889	no outliers	487.2	7.6	1.797	no outliers
methyl acetate	616.7	1754.1	0.352	no outliers	504.7	5.3	510.3	5.6	1.071	no outliers	492.9	11.7	2.228	no outliers
ethyl acetate	330.2	984.1	0.336	no outliers	503.3	5.7	511.8	8.5	1.495	no outliers	491.2	12.2	2.141	no outliers
methanol	574.9	1189.6	0.483	no outliers	514.6	6.4	525.0	10.4	1.613	no outliers	504.7	9.8	1.528	no outliers
propan-2-ol	94.6	471.0	0.201	no outliers	503.9	5.5	516.2	12.3	2.248	no outliers	497.3	6.6	1.201	no outliers
propan-1-ol	279.3	715.2	0.391	no outliers	502.5	5.2	512.3	9.8	1.870	no outliers	491.1	11.4	2.173	no outliers
2-methylpropan-1-ol	190.8	388.2	0.492	no outliers	501.1	3.5	507.3	6.2	1.774	no outliers	494.3	6.8	1.954	no outliers
butan-1-ol	142.9	406.6	0.351	no outliers	502.1	5.7	514.1	12.0	2.100	no outliers	493.0	9.1	1.594	no outliers
3-methylbutan-1-ol	89.2	267.2	0.334	no outliers	502.8	4.5	508.3	5.5	1.220	no outliers	492.9	9.9	2.214	no outliers
Solution A														
Compound	The results of Cochran's test				**The results of Grubbs' test**									
	s^2_{max}	Σs^2	C	Result	$\bar{\bar{C}}$	S	$\bar{C}_{max}$	$\bar{C}_{max} - \bar{\bar{C}}$	G_{max}	Result	$\bar{C}_{min}$	$\bar{\bar{C}} - \bar{C}_{min}$	G_{min}	Result
acetaldehyde	5195	11794	0.441	no outliers	4937	38.0	5000	63	1.660	no outliers	4870	67.2	1.771	no outliers
methyl acetate	15431	52630	0.293	no outliers	5001	43.8	5055	54	1.225	no outliers	4919	81.4	1.856	no outliers
ethyl acetate	20771	66321	0.313	no outliers	5026	33.3	5072	45	1.366	no outliers	4951	75.2	2.260	no outliers
methanol	23777	54876	0.433	no outliers	5073	38.1	5155	82	2.158	no outliers	5025	47.7	1.252	no outliers
propan-2-ol	9472	20833	0.455	no outliers	5034	25.4	5070	36	1.413	no outliers	4979	55.1	2.174	no outliers
propan-1-ol	1243	2552	0.487	no outliers	5032	30.6	5078	46	1.513	no outliers	4978	53.4	1.746	no outliers
2-methylpropan-1-ol	2206	6042	0.365	no outliers	5012	33.0	5078	66	1.992	no outliers	4967	45.8	1.386	no outliers
butan-1-ol	7469	19336	0.386	no outliers	5042	32.1	5097	55	1.699	no outliers	4990	52.3	1.627	no outliers
3-methylbutan-1-ol	6779	14007	0.484	no outliers	5046	40.3	5105	59	1.467	no outliers	4945	100.9	2.505	no outliers

Table S.4.3 The results of the long-term stability checking

x_{QCM} is the mass concentration of the *i*-th volatile compound in QCM, mg/L AA;

x_{mon} is the mass concentration of the *i*-th volatile compound in candidate QCM, obtained by measuring monitoring point, mg/L AA;

k is the coverage factor, *k* = 2;

u_{QCM} is the standard uncertainty, associated with the mass concentration of the *i*-th volatile compound in QCM, mg/L AA;

u_{mon} is the standard uncertainty, associated with the mass concentration of the *i*-th volatile compound in QCM, obtained by measuring at monitoring point, mg/L AA.

Solution G															
Compound	The absolute difference between certificated and measured value of mass concentration ($\lvert x_{CRM} - x_{mon} \rvert$) at the monitoring point, mg/L AA														
	0 days	7 days	14 days	21 days	28 days	35 days	42 days	49 days	56 days	63 days	70 days	77 days	84 days	91 days	98 days
acetaldehyde	0.016	0.067	0.027	0.006	0.009	0.015	0.058	0.094	0.010	0.016	0.008	0.025	0.052	0.016	0.030
methyl acetate	0.002	0.011	0.011	0.001	0.030	0.023	0.042	0.009	0.036	0.010	0.002	0.024	0.026	0.057	0.014
ethyl acetate	0.002	0.013	0.008	0.002	0.011	0.051	0.013	0.029	0.043	0.020	0.053	0.020	0.011	0.058	0.059
methanol	0.057	0.095	0.023	0.090	0.075	0.175	0.025	0.166	0.106	0.009	0.095	0.074	0.030	0.026	0.022
propan-2-ol	0.008	0.028	0.058	0.035	0.060	0.027	0.056	0.121	0.024	0.126	0.028	0.014	0.053	0.043	0.039
propan-1-ol	0.013	0.047	0.049	0.036	0.001	0.002	0.040	0.038	0.046	0.024	0.052	0.011	0.014	0.045	0.013
2-methylpropan-1-ol	0.001	0.014	0.000	0.000	0.046	0.007	0.008	0.021	0.008	0.042	0.038	0.016	0.006	0.020	0.026
butan-1-ol	0.005	0.025	0.009	0.015	0.013	0.007	0.023	0.006	0.016	0.053	0.013	0.015	0.006	0.038	0.024
3-methylbutan-1-ol	0.003	0.009	0.017	0.052	0.015	0.012	0.002	0.006	0.028	0.033	0.042	0.010	0.027	0.040	0.033

Compound	The absolute difference between certificated and measured value of mass concentration ($\lvert x_{CRM} - x_{mon} \rvert$) at the monitoring point, mg/L AA												$k \cdot \sqrt{u_{CRM} + u_{mon}}$, mg/L AA
	105 days	112 days	119 days	126 days	133 days	140 days	147 days	154 days	161 days	168 days	175 days	182 days	
acetaldehyde	0.036	0.023	0.064	0.001	0.021	0.008	0.001	0.035	0.109	0.113	0.018	0.015	0.115
methyl acetate	0.014	0.017	0.013	0.035	0.026	0.021	0.037	0.006	0.015	0.008	0.014	0.001	0.077
ethyl acetate	0.059	0.003	0.022	0.008	0.000	0.025	0.043	0.034	0.033	0.001	0.014	0.030	0.077
methanol	0.030	0.026	0.012	0.029	0.027	0.014	0.029	0.082	0.060	0.017	0.033	0.069	0.272
propan-2-ol	0.018	0.056	0.041	0.049	0.046	0.048	0.035	0.051	0.006	0.064	0.008	0.002	0.134
propan-1-ol	0.029	0.015	0.021	0.016	0.005	0.032	0.028	0.018	0.026	0.024	0.001	0.007	0.077
2-methylpropan-1-ol	0.020	0.005	0.008	0.006	0.019	0.041	0.054	0.025	0.017	0.019	0.004	0.034	0.077
butan-1-ol	0.027	0.058	0.009	0.014	0.003	0.041	0.023	0.026	0.0001	0.000	0.004	0.019	0.077
3-methylbutan-1-ol	0.021	0.029	0.006	0.032	0.003	0.046	0.041	0.003	0.012	0.027	0.0001	0.023	0.077

Table S.4.3 continuation

Solution F															
Compound	The absolute difference between certificated and measured value of mass concentration ($\left\|x_{CRM} - x_{mon}\right\|$) at the monitoring point, mg/L AA														$k \cdot \sqrt{u_{CRM} + u_{mon}}$, mg/L AA
	0 days	14 days	28 days	42 days	56 days	70 days	84 days	98 days	112 days	126 days	140 days	154 days	168 days	182 days	
acetaldehyde	0.010	0.079	0.188	0.290	0.332	0.060	0.318	0.050	0.242	0.223	0.243	0.129	0.366	0.019	0.45
methyl acetate	0.009	0.125	0.312	0.193	0.199	0.057	0.034	0.202	0.199	0.195	0.074	0.044	0.299	0.032	0.44
ethyl acetate	0.016	0.141	0.009	0.026	0.079	0.210	0.098	0.262	0.093	0.207	0.139	0.408	0.210	0.093	0.44
methanol	0.048	0.295	0.079	0.147	0.036	0.147	0.324	0.120	0.055	0.248	0.305	0.020	0.314	0.321	0.57
propan-2-ol	0.046	0.315	0.297	0.438	0.123	0.010	0.353	0.101	0.194	0.122	0.326	0.372	0.465	0.053	0.47
propan-1-ol	0.031	0.085	0.259	0.130	0.180	0.056	0.016	0.059	0.068	0.181	0.073	0.054	0.163	0.236	0.44
2-methylpropan-1-ol	0.004	0.065	0.027	0.181	0.052	0.147	0.035	0.363	0.068	0.138	0.030	0.011	0.137	0.149	0.43
butan-1-ol	0.053	0.025	0.126	0.074	0.005	0.254	0.010	0.039	0.052	0.106	0.035	0.039	0.029	0.262	0.44
3-methylbutan-1-ol	0.014	0.095	0.221	0.144	0.177	0.020	0.054	0.075	0.055	0.095	0.126	0.003	0.054	0.113	0.44

Solution E															
Compound	The absolute difference between certificated and measured value of mass concentration ($\left\|x_{CRM} - x_{mon}\right\|$) at the monitoring point, mg/L AA														$k \cdot \sqrt{u_{CRM} + u_{mon}}$, mg/L AA
	0 days	14 days	28 days	42 days	56 days	70 days	84 days	98 days	112 days	126 days	140 days	154 days	168 days	182 days	
acetaldehyde	0.069	0.302	0.847	0.014	0.062	0.430	0.045	0.538	0.373	0.085	0.305	0.777	0.124	0.183	1.06
methyl acetate	0.094	0.193	0.092	0.501	0.334	1.036	0.447	0.023	0.395	0.010	0.147	0.370	0.098	0.489	1.06
ethyl acetate	0.014	0.185	0.026	0.535	0.026	0.040	0.866	0.296	0.532	0.166	0.252	0.118	0.030	0.044	1.06
methanol	0.154	0.254	0.075	0.317	0.013	0.058	0.316	0.587	0.377	0.071	0.362	0.360	0.015	0.145	1.19
propan-2-ol	0.101	0.791	0.598	0.242	0.015	0.593	0.094	0.444	0.343	0.422	0.425	0.844	0.780	0.426	1.10
propan-1-ol	0.073	0.535	0.380	0.538	0.092	0.628	0.115	0.283	0.552	0.660	0.110	0.202	0.409	0.509	1.06
2-methylpropan-1-ol	0.064	0.100	0.029	0.126	0.217	0.339	0.095	0.464	0.107	0.555	0.005	0.097	0.072	0.327	1.05
butan-1-ol	0.003	0.378	0.333	0.434	0.316	0.586	0.101	0.484	0.253	0.800	0.775	0.389	0.695	0.055	1.06
3-methylbutan-1-ol	0.018	0.736	0.604	0.454	0.156	0.633	0.086	0.499	0.428	0.384	0.241	0.174	0.757	0.032	1.06

Solution D															
Compound	The absolute difference between certificated and measured value of mass concentration ($\left\|x_{CRM} - x_{mon}\right\|$) at the monitoring point, mg/L AA														$k \cdot \sqrt{u_{CRM} + u_{mon}}$, mg/L AA
	0 days	14 days	28 days	42 days	56 days	70 days	84 days	98 days	112 days	126 days	140 days	154 days	168 days	182 days	
acetaldehyde	0.250	0.885	4.533	3.554	0.725	2.652	4.475	1.026	1.163	2.483	0.046	0.673	0.009	4.420	8.39
methyl acetate	0.196	2.448	2.634	1.167	3.766	2.143	0.513	4.582	0.922	2.867	3.493	4.486	3.506	2.102	8.52
ethyl acetate	1.028	0.466	1.402	0.836	5.356	4.272	2.241	3.047	0.605	0.139	0.208	2.419	0.083	2.176	8.52
methanol	1.297	2.743	3.476	4.302	1.507	5.833	1.840	0.619	0.377	0.368	0.892	2.763	1.157	4.446	8.66
propan-2-ol	0.730	5.607	3.241	0.350	1.439	0.874	5.216	0.913	4.107	0.329	0.217	2.094	0.211	0.614	8.56
propan-1-ol	0.693	0.384	0.173	0.542	2.179	0.052	0.383	1.187	1.280	0.102	1.520	1.628	1.106	1.343	8.52
2-methylpropan-1-ol	0.060	3.532	3.846	3.579	4.054	0.441	1.624	0.218	0.055	0.742	2.364	2.472	0.635	2.408	8.48
butan-1-ol	0.093	0.368	0.131	0.402	3.823	1.180	0.419	0.476	1.156	3.448	0.353	2.178	0.494	2.281	8.55
3-methylbutan-1-ol	0.084	2.024	1.510	0.595	1.761	2.210	0.491	1.027	0.659	0.754	2.023	1.758	2.348	0.187	8.54

Table S.4.3 continuation

Compound	Solution C: The absolute difference between certificated and measured value of mass concentration ($\lvert x_{CRM} - x_{mon} \rvert$) at the monitoring point, mg/L AA														$k \cdot \sqrt{u_{CRM} + u_{mon}}$, mg/L AA
	0 days	14 days	28 days	42 days	56 days	70 days	84 days	98 days	112 days	126 days	140 days	154 days	168 days	182 days	
acetaldehyde	0.281	3.076	1.195	7.276	3.607	5.793	5.519	1.800	2.877	5.923	4.608	5.757	4.537	4.986	10.4
methyl acetate	0.021	0.368	2.821	6.732	2.048	0.473	1.558	1.523	0.322	1.177	3.106	1.454	4.049	5.568	10.6
ethyl acetate	0.323	1.831	3.422	2.878	6.195	0.579	1.567	0.360	1.100	5.150	2.838	5.501	3.285	3.404	10.6
methanol	1.290	3.665	4.411	6.270	5.597	1.147	1.497	3.915	1.105	0.246	3.168	0.809	3.771	4.913	10.8
propan-2-ol	0.050	0.598	4.436	0.141	1.263	3.660	6.728	4.235	2.185	3.439	3.224	2.766	3.788	1.348	10.6
propan-1-ol	0.010	2.462	3.812	2.143	3.517	3.253	0.754	3.983	0.976	3.393	3.624	4.468	3.158	3.060	10.6
2-methylpropan-1-ol	0.052	1.956	3.740	0.934	3.669	4.196	2.556	4.602	0.660	4.444	4.675	5.518	3.689	1.941	10.6
butan-1-ol	0.612	2.864	3.879	2.568	4.715	4.090	1.473	2.865	0.941	0.762	2.015	1.542	3.086	3.054	10.6
3-methylbutan-1-ol	0.116	1.872	3.740	2.211	0.450	3.510	0.672	3.980	0.738	4.263	4.279	4.406	3.688	1.928	10.6

Compound	Solution B: The absolute difference between certificated and measured value of mass concentration ($\lvert x_{CRM} - x_{mon} \rvert$) at the monitoring point, mg/L AA														$k \cdot \sqrt{u_{CRM} + u_{mon}}$, mg/L AA
	0 days	14 days	28 days	42 days	56 days	70 days	84 days	98 days	112 days	126 days	140 days	154 days	168 days	182 days	
acetaldehyde	0.202	0.612	2.281	0.381	9.081	7.599	0.516	1.216	2.141	1.655	5.470	10.155	1.271	2.892	20.9
methyl acetate	0.428	6.848	3.759	8.334	3.328	3.786	4.494	8.110	2.412	8.328	9.009	6.931	8.170	2.441	21.3
ethyl acetate	0.091	0.519	2.779	2.276	9.069	10.329	3.126	1.147	1.237	1.946	2.059	9.199	7.253	10.34	21.3
methanol	0.637	19.586	3.670	5.885	11.349	13.257	4.344	0.760	13.966	18.951	5.083	8.489	8.502	15.61	21.4
propan-2-ol	3.501	8.685	3.764	0.598	13.785	1.842	5.447	3.171	4.555	2.173	5.077	1.399	3.843	4.055	21.3
propan-1-ol	2.147	3.966	0.764	0.477	10.076	0.622	11.107	0.123	1.349	0.155	2.819	5.917	1.587	9.328	21.3
2-methylpropan-1-ol	3.001	1.721	2.159	1.296	8.165	4.794	0.335	3.215	0.876	1.953	4.927	8.025	0.298	1.133	21.2
butan-1-ol	3.055	0.237	3.488	0.688	7.157	4.216	10.852	6.592	1.550	10.326	4.853	2.178	2.222	7.244	21.4
3-methylbutan-1-ol	2.195	1.792	3.095	0.918	5.602	0.488	1.855	9.564	3.290	3.710	5.304	5.840	1.312	5.480	21.3

Compound	Solution A: The absolute difference between certificated and measured value of mass concentration ($\lvert x_{CRM} - x_{mon} \rvert$) at the monitoring point, mg/L AA														$k \cdot \sqrt{u_{CRM} + u_{mon}}$, mg/L AA
	0 days	14 days	28 days	42 days	56 days	70 days	84 days	98 days	112 days	126 days	140 days	154 days	168 days	182 days	
acetaldehyde	13.55	13.11	52.15	65.92	78.03	7.19	29.70	25.17	2.59	34.87	59.31	15.37	12.00	12.99	209.9
methyl acetate	14.45	19.90	120.64	4.45	23.81	110.67	60.70	0.09	43.88	3.78	53.76	16.50	15.86	97.64	213.8
ethyl acetate	45.68	27.96	43.24	91.56	20.31	1.50	38.25	16.67	29.16	24.26	19.43	24.32	14.12	15.91	213.9
methanol	33.69	101.26	20.67	76.43	2.88	9.05	9.37	9.90	28.68	3.96	22.48	1.87	67.11	12.82	214.4
propan-2-ol	17.20	46.87	2.09	63.92	6.87	22.68	25.35	10.13	27.01	10.31	19.56	13.75	4.68	11.18	214.0
propan-1-ol	16.87	34.60	41.10	15.74	7.04	13.34	53.99	16.63	60.81	7.46	26.33	38.81	1.15	11.52	213.8
2-methylpropan-1-ol	9.89	38.41	5.94	51.54	18.55	23.34	20.22	15.92	24.86	28.65	47.53	60.01	30.43	24.65	212.9
butan-1-ol	15.75	45.16	49.38	8.07	15.79	36.80	39.79	4.96	70.10	50.84	39.73	24.07	13.15	6.78	214.7
3-methylbutan-1-ol	10.16	24.64	32.02	14.74	15.82	1.82	37.88	7.36	106.99	30.19	53.00	40.91	20.58	25.38	214.3

Table S.4.4 The results of the Student's test for the long-term stability study

b_1 is regression parameter (calculated by formula B.14 of ISO Guide 35);
b_0 is regression parameter (calculated by formula B.15 of ISO Guide 35);
$s(b_1)$ is standard error for the estimated slope (calculated by formula B.16 of ISO Guide 35);
t_{b_1} is the critical value for estimation of significance of the slope (calculated by formula B.19 of ISO Guide 35).

Compound	Solution															
	G				F				E				D			
	Slope b_1	b_0	$s(b_1)$	t_{b_1}	Slope b_1	b_0	$s(b_1)$	t_{b_1}	Slope b_1	b_0	$s(b_1)$	t_{b_1}	Slope b_1	b_0	$s(b_1)$	t_{b_1}
acetaldehyde	$-1.1\cdot10^{-4}$	1.80	$1.6\cdot10^{-4}$	0.67	$-2.9\cdot10^{-4}$	10.6	$8.0\cdot10^{-4}$	0.36	$2.5\cdot10^{-3}$	24.7	$1.7\cdot10^{-3}$	1.47	$-1.2\cdot10^{-3}$	200	$8.7\cdot10^{-3}$	0.13
methyl acetate	$8.9\cdot10^{-5}$	1.20	$8.2\cdot10^{-5}$	1.08	$-5.2\cdot10^{-5}$	10.2	$7.8\cdot10^{-4}$	0.07	$-1.1\cdot10^{-3}$	24.9	$1.9\cdot10^{-3}$	0.62	$2.3\cdot10^{-4}$	202	$1.2\cdot10^{-2}$	0.02
ethyl acetate	$3.5\cdot10^{-5}$	1.21	$1.1\cdot10^{-4}$	0.31	$8.6\cdot10^{-4}$	10.3	$6.5\cdot10^{-4}$	1.32	$7.4\cdot10^{-4}$	25.0	$1.6\cdot10^{-3}$	0.47	$9.0\cdot10^{-3}$	200	$1.1\cdot10^{-2}$	0.79
methanol	$3.6\cdot10^{-4}$	4.23	$2.4\cdot10^{-4}$	1.49	$4.6\cdot10^{-4}$	13.4	$1.0\cdot10^{-3}$	0.46	$1.0\cdot10^{-3}$	27.9	$1.4\cdot10^{-3}$	0.75	$-5.1\cdot10^{-3}$	207	$8.7\cdot10^{-3}$	0.58
propan-2-ol	$1.5\cdot10^{-4}$	2.08	$1.8\cdot10^{-4}$	0.81	$-8.7\cdot10^{-5}$	10.9	$8.2\cdot10^{-4}$	0.11	$-1.9\cdot10^{-3}$	25.6	$1.4\cdot10^{-3}$	1.33	$1.5\cdot10^{-3}$	202	$1.3\cdot10^{-2}$	0.11
propan-1-ol	$-1.4\cdot10^{-4}$	1.23	$9.5\cdot10^{-5}$	1.51	$1.7\cdot10^{-4}$	10.2	$6.6\cdot10^{-4}$	0.25	$1.4\cdot10^{-3}$	24.5	$1.6\cdot10^{-3}$	0.84	$7.6\cdot10^{-3}$	201	$3.6\cdot10^{-3}$	2.12
2-methylpropan-1-ol	$2.7\cdot10^{-5}$	1.21	$7.3\cdot10^{-5}$	0.37	$1.0\cdot10^{-3}$	10.2	$5.3\cdot10^{-4}$	1.92	$-4.7\cdot10^{-4}$	24.7	$1.3\cdot10^{-3}$	0.35	$1.5\cdot10^{-2}$	198	$1.0\cdot10^{-2}$	1.48
butan-1-ol	$1.0\cdot10^{-4}$	1.21	$7.8\cdot10^{-5}$	1.34	$8.6\cdot10^{-4}$	10.2	$5.3\cdot10^{-4}$	1.61	$-8.1\cdot10^{-4}$	24.8	$1.3\cdot10^{-3}$	0.64	$4.7\cdot10^{-3}$	202	$6.9\cdot10^{-3}$	0.69
3-methylbutan-1-ol	$8.8\cdot10^{-5}$	1.21	$9.2\cdot10^{-5}$	0.95	$1.3\cdot10^{-3}$	10.2	$6.7\cdot10^{-4}$	1.90	$8.0\cdot10^{-4}$	24.5	$1.5\cdot10^{-3}$	0.54	$1.8\cdot10^{-3}$	200	$6.9\cdot10^{-3}$	0.26

Compound	Solution											
	C				B				A			
	Slope b_1	b_0	$s(b_1)$	t_{b_1}	Slope b_1	b_0	$s(b_1)$	t_{b_1}	Slope b_1	b_0	$s(b_1)$	t_{b_1}
acetaldehyde	$1.5\cdot10^{-2}$	249	$8.9\cdot10^{-3}$	1.74	$2.1\cdot10^{-3}$	495	$2.1\cdot10^{-2}$	0.10	$-6.1\cdot10^{-2}$	4943	$1.9\cdot10^{-1}$	0.33
methyl acetate	$-2.6\cdot10^{-3}$	250	$1.5\cdot10^{-2}$	0.18	$3.4\cdot10^{-2}$	502	$2.4\cdot10^{-2}$	1.44	$-6.6\cdot10^{-2}$	5007	$2.2\cdot10^{-1}$	0.31
ethyl acetate	$9.0\cdot10^{-3}$	250	$1.6\cdot10^{-2}$	0.58	$-1.4\cdot10^{-2}$	505	$2.8\cdot10^{-2}$	0.51	$2.5\cdot10^{-1}$	5004	$1.5\cdot10^{-1}$	1.66
methanol	$-3.3\cdot10^{-5}$	255	$1.5\cdot10^{-2}$	0.002	$2.6\cdot10^{-2}$	512	$3.1\cdot10^{-2}$	0.83	$-2.0\cdot10^{-1}$	5091	$1.8\cdot10^{-1}$	1.11
propan-2-ol	$4.5\cdot10^{-3}$	252	$1.3\cdot10^{-2}$	0.35	$-4.4\cdot10^{-2}$	508	$2.4\cdot10^{-2}$	1.84	$1.2\cdot10^{-1}$	5023	$1.2\cdot10^{-1}$	1.02
propan-1-ol	$8.7\cdot10^{-3}$	252	$8.4\cdot10^{-3}$	1.03	$4.4\cdot10^{-2}$	498	$2.2\cdot10^{-2}$	1.97	$1.5\cdot10^{-1}$	5018	$1.4\cdot10^{-1}$	1.04
2-methylpropan-1-ol	$7.6\cdot10^{-3}$	251	$7.7\cdot10^{-3}$	0.98	$-4.5\cdot10^{-3}$	500	$1.9\cdot10^{-2}$	0.24	$6.2\cdot10^{-2}$	4998	$9.8\cdot10^{-2}$	0.63
butan-1-ol	$4.1\cdot10^{-3}$	253	$7.5\cdot10^{-3}$	0.55	$2.2\cdot10^{-2}$	501	$2.6\cdot10^{-2}$	0.84	$2.2\cdot10^{-1}$	5037	$1.6\cdot10^{-1}$	1.37
3-methylbutan-1-ol	$8.9\cdot10^{-3}$	252	$8.1\cdot10^{-3}$	1.10	$6.0\cdot10^{-3}$	502	$2.4\cdot10^{-2}$	0.25	$-1.0\cdot10^{-1}$	5047	$1.6\cdot10^{-1}$	0.65