Interlaboratory study of ethanol usage as an internal standard in direct determination of volatile compounds in alcoholic products

Supplementary Materials

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\[ u(C_i (B)) = \rho_{Eth} \cdot \sqrt{\left( \frac{\partial C_i (B)}{\partial m_i^B} \right)^2 + \left( \frac{\partial C_i (B)}{\partial C_i} \right)^2 + \left( \frac{\partial C_i (B)}{\partial m_{HS}^B} \right)^2 + \left( \frac{\partial C_i (B)}{\partial C_{Eth} (HS)} \right)^2}, \]  
\text{(S.1)}

\[ u(C_i (HS)) = \frac{\rho_{Eth}}{\rho_{HS}} \sqrt{\frac{\partial C_i (HS)}{\partial A_i^{HS}} + \frac{\partial C_i (HS)}{\partial RRF_i^{Eth}} + \frac{\partial C_i (HS)}{\partial C_{Eth} (HS)} + \frac{\partial C_i (HS)}{\partial A_{Eth}^{HS}}}, \]  
\text{(S.2)}

\[ u(RRF_i^{Eth}) = \sqrt{\left( \frac{\partial RRF_i^{Eth}}{\partial A_i^{HS}} \right)^2 + \left( \frac{\partial RRF_i^{Eth}}{\partial m_i (C)} \right)^2 + \left( \frac{\partial RRF_i^{Eth}}{\partial A_i^{st}} \right)^2 + \left( \frac{\partial RRF_i^{Eth}}{\partial m_{Eth} (C)} \right)^2}, \]  
\text{(S.3)}

\[ u(C_i (C, D, 1, 2)) = \rho_{Eth} \cdot \sqrt{\left( \frac{\partial C_i (C, D, 1, 2)}{\partial m_b^{C, D, 1, 2}} \right)^2 + \left( \frac{\partial C_i (C, D, 1, 2)}{\partial C_i (B)} \right)^2 + \left( \frac{\partial C_i (C, D, 1, 2)}{\partial C_{Eth} (B)} \right)^2 + \left( \frac{\partial C_i (C, D, 1, 2)}{\partial C_{Eth} (HS)} \right)^2 + \left( \frac{\partial C_i (C, D, 1, 2)}{\partial m_{Eth} (HS)} \right)^2}, \]  
\text{(S.4)}
**Table S.1. Results of z-score determination for SS-B**

|      | acetaldehyde | methyl acetate | ethyl acetate |
|------|--------------|----------------|--------------|
| **Lab** | Mean, mg/L AA | Standard deviation, mg/L AA | z-score | Outlier | Mean, mg/L AA | Standard deviation, mg/L AA | z-score | Outlier | Mean, mg/L AA | Standard deviation, mg/L AA | z-score | Outlier |
| 1    | 412          | 0.90           | -0.38       |         | 416      | 0.33           | -0.67       |         | 417      | 0.36           | -0.35       |         |
| 2    | 416          | 10.77          | 0.48        |         | 424      | 6.25           | -0.17       |         | 442      | 10.65          | 1.34        |         |
| 3    | 411          | 0.38           | -0.67       |         | 415      | 0.28           | -0.78       |         | 422      | 0.64           | -0.01       |         |
| 4    | 422          | 1.31           | 1.70        |         | 444      | 2.41           | 1.02        |         | 421      | 2.82           | -0.12       |         |
| 5    | 412          | 2.69           | -0.53       |         | 459      | 0.28           | 1.99        |         | 441      | 1.64           | 1.26        |         |
| 6    | 408          | 6.81           | -1.19       |         | 420      | 9.66           | -0.47       |         | 415      | 8.44           | -0.52       |         |
| 7    | 413          | 1.96           | -0.22       |         | 421      | 3.33           | -0.36       |         | 417      | 3.51           | -0.37       |         |
| 8    | 408          | 6.81           | -1.19       |         | 420      | 9.66           | -0.47       |         | 415      | 8.44           | -0.52       |         |
| 9    | 406          | 1.52           | -1.60       |         | 447      | 1.10           | 1.23        |         | 393      | 1.36           | -1.99       |         |

|      | methanol     | 2-propanol     | 1-propanol |
|------|--------------|----------------|------------|
| **Lab** | Mean, mg/L AA | Standard deviation, mg/L AA | z-score | Outlier | Mean, mg/L AA | Standard deviation, mg/L AA | z-score | Outlier | Mean, mg/L AA | Standard deviation, mg/L AA | z-score | Outlier |
| 1    | 425          | 0.72           | 0.99        |         | 405      | 0.34           | -0.46       |         | 418      | 0.01           | -0.28       |         |
| 2    | 425          | 6.69           | 1.29        |         | 407      | 1.03           | 0.73        |         | 423      | 2.06           | 1.72        |         |
| 3    | 425          | 0.23           | 0.84        |         | 406      | 0.90           | -0.90       |         | 417      | 0.28           | -0.64       |         |
| 4    | 422          | 1.07           | -1.07       |         | 406      | 1.14           | 0.18        |         | 417      | 0.56           | -0.36       |         |
| 5    | 425          | 1.32           | 0.98        |         | 420      | 0.79           | 9.33        |         | 422      | -0.50          | 1.35        |         |
| 6    | 423          | 1.68           | -0.67       |         | 405      | 1.69           | -0.57       |         | 416      | 0.70           | -0.81       |         |
| 7    | 425          | 0.67           | 1.34        |         | 409      | 1.92           | 1.95        |         | 419      | 0.32           | 0.14        |         |
| 8    | 423          | 1.68           | -0.67       |         | 405      | 1.69           | -0.57       |         | 416      | 0.70           | -0.81       |         |
| 9    | 425          | 0.96           | -9.44       | Grubbs** | 423      | 0.67           | 1.34        |         | 415      | 2.21           | -1.15       |         |

|      | 2-methyl-1-propanol | 1-butanol | 3-methyl-1-butanol |
|------|---------------------|---------|---------------------|
| **Lab** | Mean, mg/L AA | Standard deviation, mg/L AA | z-score | Outlier | Mean, mg/L AA | Standard deviation, mg/L AA | z-score | Outlier | Mean, mg/L AA | Standard deviation, mg/L AA | z-score | Outlier |
| 1    | 430          | 0.35           | -0.13       |         | 417      | 0.57           | -0.15       |         | 412      | 0.18           | -0.23       |         |
| 2    | 436          | 2.86           | 1.72        |         | 428      | 0.75           | 8.55        |         | 421      | 3.37           | 5.58        |         |
| 3    | 429          | 0.18           | -0.57       |         | 417      | 0.19           | 0.40        |         | 412      | 0.58           | -0.42       |         |
| 4    | 429          | 1.10           | -0.49       |         | 415      | 0.88           | -1.37       |         | 410      | 0.86           | -1.31       |         |
| 5    | 432          | 0.59           | 0.55        |         | 416      | 0.47           | -0.64       |         | 413      | 0.96           | 0.22        |         |
| 6    | 428          | 0.10           | -0.86       |         | 417      | 0.69           | 0.02        |         | 411      | 1.11           | -0.84       |         |
| 7    | 431          | 1.07           | 0.03        |         | 419      | 0.42           | 1.97        |         | 414      | 0.63           | 1.40        |         |
| 8    | 428          | 0.10           | -0.86       |         | 417      | 0.69           | 0.02        |         | 411      | 1.11           | -0.84       |         |
| 9    | 425          | 2.71           | -1.83       |         | 416      | 0.49           | -0.82       |         | 410      | 5.82           | -1.88       |         |

* Straggler, ** Statistical outlier
### Table S.2. Results of z-score determination for SS-D

| Lab | Mean, mg/L AA | Standard deviation, mg/L AA | z-score | Outlier |
|-----|---------------|-----------------------------|---------|---------|
| 1   | 182           | 0.38                        | 1.46    |         |
| 2   | 179           | 6.14                        | -1.45   |         |
| 3   | 182           | 0.38                        | -0.57   |         |
| 4   | 184           | 0.94                        | 0.55    |         |
| 5   | 179           | 1.57                        | -1.79   |         |
| 6   | 182           | 6.85                        | -0.25   |         |
| 7   | 182           | 2.25                        | -0.24   |         |
| 8   | 182           | 6.85                        | -0.25   |         |
| 9   | 184           | 0.58                        | 0.48    |         |
|     |               | mg/L AA                     |         |         |
| 1   | 179           | 0.89                        | -1.92   |         |
| 2   | 179           | 8.16                        | 1.76    |         |
| 3   | 181           | 0.96                        | -0.37   |         |
| 4   | 182           | 1.32                        | -0.14   |         |
| 5   | 181           | 1.75                        | -0.67   |         |
| 6   | 181           | 6.85                        | -0.39   |         |
| 7   | 181           | 2.50                        | -0.40   |         |
| 8   | 181           | 6.85                        | -0.39   |         |
| 9   | 183           | 0.79                        | 0.71    |         |

**Acetaldehyde**

| Lab | Mean, mg/L AA | Standard deviation, mg/L AA | z-score | Outlier |
|-----|---------------|-----------------------------|---------|---------|
| 1   | 199           | 0.60                        | 1.57    |         |
| 2   | 186           | 0.26                        | -17.60  | Grubbs**|
| 3   | 197           | 0.45                        | -0.47   |         |
| 4   | 199           | 0.84                        | 1.99    |         |
| 5   | 198           | 0.62                        | 0.18    |         |
| 6   | 197           | 0.85                        | -0.55   |         |
| 7   | 197           | 0.54                        | -0.28   |         |
| 8   | 197           | 0.85                        | -0.55   |         |
| 9   | 197           | 0.15                        | -0.13   |         |

**Methanol**

| Lab | Mean, mg/L AA | Standard deviation, mg/L AA | z-score | Outlier |
|-----|---------------|-----------------------------|---------|---------|
| 1   | 192           | 0.28                        | 1.79    |         |
| 2   | 189           | 7.48                        | -1.83   |         |
| 3   | 191           | 0.24                        | 0.93    |         |
| 4   | 191           | 0.41                        | 0.31    |         |
| 5   | 191           | 0.36                        | 0.51    |         |
| 6   | 190           | 1.30                        | 0.11    |         |
| 7   | 191           | 0.80                        | 0.26    |         |
| 8   | 190           | 1.30                        | 0.11    |         |
| 9   | 190           | 0.96                        | -0.62   |         |

**2-Methyl-1-Propanol**

| Lab | Mean, mg/L AA | Standard deviation, mg/L AA | z-score | Outlier |
|-----|---------------|-----------------------------|---------|---------|
| 1   | 185           | 0.40                        | 0.27    |         |
| 2   | 183           | 9.12                        | -1.79   |         |
| 3   | 185           | 0.17                        | 0.85    |         |
| 4   | 185           | 0.95                        | -0.35   |         |
| 5   | 186           | 1.28                        | 1.46    |         |
| 6   | 185           | 0.58                        | -0.11   |         |
| 7   | 185           | 0.12                        | 0.60    |         |
| 8   | 184           | 3.09                        | -1.17   |         |

**Ethyl Acetate**

| Lab | Mean, mg/L AA | Standard deviation, mg/L AA | z-score | Outlier |
|-----|---------------|-----------------------------|---------|---------|
| 1   | 190           | 0.60                        | 0.48    |         |
| 2   | 192           | 5.26                        | 1.99    |         |
| 3   | 187           | 0.88                        | -1.41   |         |
| 4   | 189           | 0.52                        | 0.36    |         |
| 5   | 188           | 1.30                        | -0.26   |         |
| 6   | 189           | 7.61                        | 0.25    |         |
| 7   | 188           | 2.48                        | -0.58   |         |
| 8   | 189           | 7.61                        | 0.25    |         |
| 9   | 191           | 0.46                        | 1.33    |         |

**2-Propanol**

| Lab | Mean, mg/L AA | Standard deviation, mg/L AA | z-score | Outlier |
|-----|---------------|-----------------------------|---------|---------|
| 1   | 186           | 0.26                        | 1.68    |         |
| 2   | 190           | 1.49                        | 11.28   | Grubbs**|
| 3   | 186           | 0.14                        | -0.23   |         |
| 4   | 186           | 1.01                        | -0.32   |         |
| 5   | 186           | 0.46                        | 0.12    |         |
| 6   | 186           | 0.24                        | -0.36   |         |
| 7   | 185           | 0.32                        | -0.67   |         |
| 8   | 186           | 0.24                        | -0.36   |         |
| 9   | 185           | 0.47                        | -1.96   |         |

**1-Propanol**

| Lab | Mean, mg/L AA | Standard deviation, mg/L AA | z-score | Outlier |
|-----|---------------|-----------------------------|---------|---------|
| 1   | 183           | 0.19                        | 0.30    |         |
| 2   | 188           | 0.02                        | 2.54    |         |
| 3   | 183           | 0.09                        | 0.34    |         |
| 4   | 182           | 0.84                        | -0.34   |         |
| 5   | 184           | 0.40                        | 0.37    |         |
| 6   | 183           | 0.68                        | 0.02    |         |
| 7   | 183           | 0.36                        | 0.07    |         |
| 8   | 183           | 0.68                        | 0.02    |         |
| 9   | 180           | 3.48                        | -1.25   |         |

* Straggler, ** Statistical outlier
Table S.3. Results of z-score determination for SS-1

| Lab | Mean, mg/L AA | Standard deviation, mg/L AA | z-score | Outlier |
|-----|---------------|----------------------------|---------|---------|
| 1   | 48.3          | 0.05                       | 0.44    |         |
| 2   | 49.4          | 1.49                       | 1.34    |         |
| 3   | 47.4          | 0.09                       | -0.28   |         |
| 4   | 48.1          | 0.70                       | 0.28    |         |
| 5   | 47.1          | 0.69                       | -0.57   |         |
| 6   | 47.0          | 0.53                       | -0.61   |         |
| 7   | 45.7          | 0.66                       | -1.72   |         |
| 8   | 47.0          | 0.53                       | -0.61   |         |
| 9   | 49.4          | 1.20                       | 1.36    |         |

| Lab | Mean, mg/L AA | Standard deviation, mg/L AA | z-score | Outlier |
|-----|---------------|----------------------------|---------|---------|
| 1   | 61.4          | 0.09                       | 0.80    |         |
| 2   | 57.1          | 3.15                       | -1.38   |         |
| 3   | 59.9          | 0.07                       | 0.03    |         |
| 4   | 56.6          | 0.59                       | -1.62   |         |
| 5   | 59.0          | 1.58                       | -0.43   |         |
| 6   | 60.8          | 0.18                       | 0.51    |         |
| 7   | 59.1          | 0.30                       | -0.38   |         |
| 8   | 60.8          | 0.18                       | 0.51    |         |
| 9   | 62.6          | 1.42                       |         |         |

| Lab | Mean, mg/L AA | Standard deviation, mg/L AA | z-score | Outlier |
|-----|---------------|----------------------------|---------|---------|
| 1   | 49.2          | 0.06                       | 0.68    |         |
| 2   | 49.7          | 1.54                       | 1.96    |         |
| 3   | 48.9          | 0.18                       | 0.18    |         |
| 4   | 48.4          | 0.42                       | -1.05   |         |
| 5   | 49.1          | 0.19                       | 0.55    |         |
| 6   | 48.7          | 0.16                       | -0.33   |         |
| 7   | 48.3          | 0.14                       | -1.18   |         |
| 8   | 48.7          | 0.16                       | -0.33   |         |
| 9   | 49.3          | 0.32                       | 0.93    |         |

* Straggler, ** Statistical outlier
| Lab | Mean, mg/L AA | Standard deviation, mg/L AA | z-score | Outlier |
|-----|---------------|-----------------------------|---------|---------|
| 1   | 9.7           | 0.17                        | -1.02   |         |
| 2   | 10.5          | 0.21                        | -0.15   |         |
| 3   | 10.8          | 0.10                        | 0.22    |         |
| 4   | 11.5          | 0.66                        | 0.97    |         |
| 5   | 11.8          | 0.06                        | 1.26    |         |
| 6   | 9.5           | 0.18                        | -1.26   |         |
| 7   | 9.6           | 0.06                        | -1.17   |         |
| 8   | 9.5           | 0.18                        | -1.26   |         |
| 9   | 11.1          | 0.32                        | 0.46    |         |

| Lab | Mean, mg/L AA | Standard deviation, mg/L AA | z-score | Outlier |
|-----|---------------|-----------------------------|---------|---------|
| 1   | 22.7          | 0.12                        | 0.11    |         |
| 2   | 24.7          | 0.64                        | 1.65    |         |
| 3   | 22.4          | 0.14                        | -0.12   |         |
| 4   | 21.7          | 0.50                        | -0.71   |         |
| 5   | 20.8          | 0.42                        | -1.40   |         |
| 6   | 22.4          | 0.30                        | -0.16   |         |
| 7   | 22.2          | 0.03                        | -0.33   |         |
| 8   | 22.4          | 0.30                        | -0.16   |         |
| 9   | 24.7          | 1.24                        | 1.62    |         |

| Lab | Mean, mg/L AA | Standard deviation, mg/L AA | z-score | Outlier |
|-----|---------------|-----------------------------|---------|---------|
| 1   | 9.9           | 0.08                        | 0.52    |         |
| 2   | 9.1           | 0.16                        | -1.36   |         |
| 3   | 9.8           | 0.05                        | 0.17    |         |
| 4   | 9.4           | 0.14                        | -0.57   |         |
| 5   | 9.9           | 0.08                        | 0.58    |         |
| 6   | 9.2           | 0.06                        | -1.06   |         |
| 7   | 9.7           | 0.13                        | -0.06   |         |
| 8   | 9.2           | 0.06                        | -1.06   |         |
| 9   | 10.4          | 0.35                        | 1.76    |         |

Table S.4. Results of z-score determination for SS-2

* Straggler, ** Statistical outlier
| Statistical parameter     | acetaldehyde | methyl acetate | ethyl acetate | methanol | Compound | 2-propanol | 1-propanol | isobutanol | 1-butanol | isoamylol |
|---------------------------|-------------|--------------|--------------|----------|----------|------------|------------|------------|-----------|-----------|
| Assigned value, mg/L AA   | 414         | 427          | 423          | 424      | 405      | 418        | 431        | 417        | 412       |
| Mean, mg/L AA             | 412         | 429          | 421          | 424      | 406      | 418        | 430        | 417        | 412       |
| n                         | 9           | 9            | 9            | 9        | 8        | 9          | 9          | 9          | 8         |
| Outliers                  | 0           | 0            | 0            | 1        | 1        | 0          | 0          | 1          | 1         |
| n<sup>1</sup>             | 9           | 9            | 9            | 8        | 7        | 9          | 9          | 8          | 8         |
| r, %                      | 3.4         | 3.4          | 3.7          | 1.6      | 0.8      | 0.7        | 0.9        | 0.4        | 1.4       |
| s<sub>r</sub>, mg/L AA    | 5.0         | 5.2          | 5.6          | 2.4      | 1.2      | 1.1        | 1.5        | 0.5        | 2.0       |
| RSD<sub>r</sub>, %        | 1.2         | 1.2          | 1.3          | 0.6      | 0.3      | 0.3        | 0.3        | 0.1        | 0.5       |
| Ho<sub>r</sub>            | 0.3         | 0.3          | 0.3          | 0.1      | 0.1      | 0.1        | 0.1        | 0.03       | 0.1       |
| R, %                      | 4.5         | 4.5          | 4.9          | 2.2      | 1.1      | 1.0        | 1.3        | 0.5        | 1.9       |
| s<sub>R</sub>, mg/L AA    | 6.7         | 7.0          | 7.5          | 3.3      | 1.6      | 1.5        | 1.9        | 0.7        | 2.8       |
| RSD<sub>R</sub>, %        | 1.6         | 1.6          | 1.8          | 0.8      | 0.4      | 0.4        | 0.5        | 0.2        | 0.7       |
| Ho<sub>R</sub>            | 0.5         | 0.5          | 0.6          | 0.3      | 0.1      | 0.1        | 0.1        | 0.1        | 0.2       |
| δ<sup>†</sup>, mg/L AA    | -2.0        | 2.4          | -2.1         | 0.5      | 0.1      | -0.2       | -0.9       | -0.1       | -0.7      |
| S<sub>δ</sub>, mg/L AA    | 1.8         | 1.8          | 2.0          | 0.9      | 0.5      | 0.4        | 0.5        | 0.2        | 0.8       |
| δ<sup>†</sup>, %          | -0.5        | 0.5          | -0.5         | 0.1      | 0.0      | -0.1       | 0.0        | -0.2       | 0.0       |
| Interval for the bias,    | -5.4        | -1.3         | 1.5          | 6.0      | -6.0     | -1.3       | -1.3       | -0.9       | -1.0      |
| mg/L AA                   | 14.2        | 14.7         | 14.9         | 13.2     | 12.3     | 12.6       | 13.1       | 12.5       | 12.7      |
| u, mg/L AA                | 3.4         | 3.4          | 3.5          | 3.1      | 3.0      | 3.0        | 3.0        | 3.0        | 3.1       |
| U, % (P=0.95 k=2)          | 6.9         | 6.9          | 7.0          | 6.2      | 6.1      | 6.0        | 6.1        | 6.0        | 6.2       |
Table S.6. Summary of calculated statistical parameters for SS-D⁻

| Statistical parameter | acetaldehyde | methyl acetate | ethyl acetate | methanol | 2-propanol | 1-propanol | isobutanol | 1-butanol | isoamylol |
|-----------------------|--------------|----------------|---------------|---------|-----------|-----------|------------|-----------|-----------|
| Assigned value, mg/L AA | 183          | 182            | 189           | 198     | 180       | 186       | 190        | 185       | 183       |
| Mean, mg/L AA         | 182          | 182            | 189           | 198     | 180       | 186       | 191        | 185       | 183       |
| n                     | 9            | 9              | 9             | 9       | 8         | 9         | 9          | 9         | 9         |
| Outliers              | 0            | 0              | 0             | 0       | 0         | 0         | 0          | 0         | 0         |
| n_i                   | 9            | 9              | 9             | 9       | 8         | 8         | 8          | 9         | 9         |
| r, %                  | 6.0          | 6.7            | 6.0           | 0.9     | 2.0       | 0.7       | 3.8        | 4.9       | 1.9       |
| s_r, mg/L AA          | 4.0          | 4.4            | 4.1           | 0.6     | 1.3       | 0.4       | 2.6        | 3.3       | 1.3       |
| RSD_r, %              | 2.2          | 2.4            | 2.2           | 0.3     | 0.7       | 0.2       | 1.4        | 1.8       | 0.7       |
| Ho_r                  | 0.4          | 0.5            | 0.4           | 0.1     | 0.1       | 0.04      | 0.3        | 0.3       | 0.1       |
| R                      | 8.0          | 9.0            | 8.1           | 1.2     | 2.7       | 0.9       | 5.1        | 6.6       | 2.6       |
| s_R, mg/L AA          | 5.3          | 5.9            | 5.5           | 0.8     | 1.7       | 0.6       | 3.5        | 4.4       | 1.7       |
| RSD_R, %              | 2.9          | 3.2            | 2.9           | 0.4     | 1.0       | 0.3       | 1.8        | 2.4       | 0.9       |
| Ho_R                  | 0.8          | 0.9            | 0.8           | 0.1     | 0.3       | 0.1       | 0.5        | 0.7       | 0.3       |
| ̂δ , mg/L AA           | -0.5         | -0.3           | 0.4           | 0.1     | 0.2       | -0.1      | 0.1        | 0.0       | 0.4       |
| ̂S_δ , mg/L AA         | 1.4          | 1.6            | 1.5           | 0.2     | 0.5       | 0.2       | 0.9        | 1.2       | 0.5       |
| ̂δ , %                 | -0.3         | -0.2           | 0.2           | 0.1     | 0.1       | -0.1      | 0.1        | 0.0       | 0.2       |
| Interval for the bias, mg/L AA | -3.3      | -2.2          | -3.4          | -2.4    | -3.3      | -0.3      | -0.7       | -0.4      | -0.2      |
| u, mg/L AA            | 7.7          | 8.2            | 8.0           | 6.0     | 5.7       | 5.6       | 6.8        | 7.2       | 5.8       |
| u, %                  | 4.2          | 4.5            | 4.3           | 3.0     | 3.2       | 3.0       | 3.5        | 3.9       | 3.2       |
| U, % (P=0.95 k=2)      | 8.5          | 9.0            | 8.5           | 6.1     | 6.3       | 6.0       | 7.1        | 7.7       | 6.3       |
Table S.7. Summary of calculated statistical parameters for SS-1°

| Statistical parameter | acetaldehyde | methyl acetate | ethyl acetate | methanol | Compound 2-propanol | 1-propanol | isobutanol | 1-butanol | isoamylol |
|-----------------------|--------------|---------------|--------------|----------|---------------------|------------|------------|-----------|-----------|
| Assigned value, mg/L AA | 48           | 45            | 48           | 60       | 46                  | 48         | 49         | 47        | 47        |
| Mean, mg/L AA         | 48           | 45            | 48           | 60       | 46                  | 48         | 49         | 47        | 47        |
| n                     | 9            | 9             | 9            | 9        | 8                   | 9          | 9          | 9         | 9         |
| Outliers              | 0            | 0             | 1            | 0        | 0                   | 0          | 0          | 0         | 0         |
| n_i                   | 9            | 9             | 8            | 9        | 8                   | 9          | 9          | 9         | 9         |
| r, %                  | 4.6          | 2.8           | 5.6          | 5.7      | 3.9                 | 2.8        | 3.2        | 4.5       | 3.5       |
| s, mg/L AA            | 0.8          | 0.5           | 1.0          | 1.2      | 0.6                 | 0.5        | 0.6        | 0.8       | 0.6       |
| RSD_r, %              | 1.7          | 1.0           | 2.0          | 2.0      | 1.4                 | 1.0        | 1.1        | 1.6       | 1.2       |
| Ho_r                  | 0.3          | 0.2           | 0.3          | 0.3      | 0.2                 | 0.2        | 0.2        | 0.2       | 0.2       |
| R, %                  | 6.2          | 3.8           | 7.8          | 7.6      | 5.2                 | 3.9        | 4.2        | 6.0       | 4.6       |
| s_R, mg/L AA          | 1.1          | 0.6           | 1.3          | 1.6      | 0.9                 | 0.7        | 0.7        | 1.0       | 0.8       |
| RSD_R, %              | 2.2          | 1.4           | 2.8          | 2.7      | 1.9                 | 1.4        | 1.5        | 2.2       | 1.7       |
| Ho_R                  | 0.5          | 0.3           | 0.6          | 0.7      | 0.4                 | 0.3        | 0.4        | 0.5       | 0.4       |
| 作δ, mg/L AA          | 0.0          | -0.3          | 0.2          | -0.1     | 0.2                 | -0.2       | 0.1        | -0.1      | -0.1      |
| s_δ, mg/L AA          | 0.3          | 0.2           | 0.4          | 0.4      | 0.2                 | 0.2        | 0.2        | 0.3       | 0.2       |
| 作δ, %                | -0.1         | -0.7          | 0.5          | -0.2     | 0.4                 | -0.5       | 0.1        | -0.2      | -0.1      |
| Interval for the bias, mg/L AA | -0.6 | -0.6 | -0.5 | -0.5 | 1.0 | -1.0 | -0.3 | -0.3 | 0.7 | -0.7 | -0.6 | -0.6 | -0.3 | -0.3 | 0.4 | -0.5 | -0.5 | -0.4 | 0.4 |
| u, mg/L AA            | 1.8          | 1.5           | 2.0          | 2.5      | 1.7                 | 1.6        | 1.7        | 1.8       | 1.6       |
| u, %                  | 3.8          | 3.3           | 4.2          | 4.1      | 3.6                 | 3.3        | 3.4        | 3.7       | 3.5       |
| U, % (P=0.95 k=2)     | 7.6          | 6.6           | 8.4          | 8.2      | 7.2                 | 6.7        | 6.8        | 7.5       | 6.9       |
**Table S.8. Summary of calculated statistical parameters for SS-2°**

| Statistical parameter | acetaldehyde | methyl acetate | ethyl acetate | methanol | Compound               | 2-propanol | 1-propanol | isobutanol | 1-butanol | isoamylol |
|-----------------------|--------------|----------------|---------------|----------|------------------------|------------|------------|------------|-----------|-----------|
| Assigned value, mg/L AA | 10.7         | 8.7            | 9.4           | 22.6     | 10.1                   | 9.7        | 9.7        | 9.2        | 9.3       |           |
| Mean, mg/L AA          | 10.5         | 8.6            | 9.3           | 22.7     | 10.1                   | 9.7        | 9.7        | 9.6        | 9.2       | 9.2       |
| n                     | 9            | 9              | 9             | 9        | 7                      | 9          | 9          | 9          | 9         | 9         |
| Outliers              | 0            | 1              | 1             | 0        | 1                      | 0          | 0          | 0          | 0         | 1         |
| n_1                   | 9            | 8              | 8             | 9        | 7                      | 9          | 9          | 9          | 8         |           |
| r, %                  | 7.5          | 4.6            | 4.6           | 6.7      | 4.8                    | 6.5        | 4.4        | 4.8        | 6.1       |           |
| s_r, mg/L AA          | 0.3          | 0.1            | 0.2           | 0.6      | 0.2                    | 0.1        | 0.2        | 0.2        | 0.2       | 0.2       |
| RSD_r, %              | 2.7          | 1.7            | 1.7           | 2.4      | 1.7                    | 2.3        | 1.6        | 1.7        | 2.2       |           |
| H_0_r                 | **0.3**      | **0.2**        | **0.2**       | **0.3**  | **0.2**                | **0.3**    | **0.2**    | **0.2**    | **0.3**   |           |
| R, %                  | 10.0         | 6.3            | 6.3           | 8.9      | 6.4                    | 8.5        | 5.9        | 6.3        | 8.3       |           |
| s_r, mg/L AA          | 0.4          | 0.2            | 0.2           | 0.7      | 0.2                    | 0.3        | 0.2        | 0.2        | 0.3       |           |
| RSD_r, %              | 3.6          | 2.3            | 2.3           | 3.2      | 2.3                    | 3.1        | 2.1        | 2.3        | 3.0       |           |
| H_0_r                 | **0.7**      | **0.4**        | **0.4**       | **0.7**  | **0.4**                | **0.6**    | **0.4**    | **0.4**    | **0.5**   |           |
| δ_0, mg/L AA          | -0.2         | -0.1           | -0.1          | 0.1      | 0.0                    | 0.0        | -0.1       | 0.0        | 0.0       |           |
| s_δ_0, mg/L AA        | 0.1          | 0.1            | 0.1           | 0.2      | 0.1                    | 0.1        | 0.1        | 0.1        | 0.1       |           |
| δ_0, %                | -1.8         | -0.6           | -1.2          | 0.3      | -0.3                   | 0.4        | -0.5       | -0.3       | -0.5      |           |
| Interval for the bias, mg/L AA | -0.4 < δ < 0.002 | -0.2 < δ < 0.1 | -0.2 < δ < 0.0 | -0.3 < δ < 0.5 | -0.2 < δ < 0.1 | -0.1 < δ < 0.2 | -0.2 < δ < 0.1 | -0.1 < δ < 0.1 | -0.2 < δ < 0.1 | -0.1 < δ < 0.1 |
| u, mg/L AA            | 0.5          | 0.3            | 0.4           | 1.0      | 0.4                    | 0.4        | 0.4        | 0.4        | 0.4       |           |
| u, %                  | 4.7          | 3.8            | 3.8           | 4.5      | 3.8                    | 4.4        | 3.7        | 3.8        | 4.3       |           |
| U, % (P=0.95 k=2)      | 9.5          | 7.6            | 7.6           | 9.0      | 7.7                    | 8.8        | 7.4        | 7.6        | 8.6       |           |
Figure S.1. Z-scores SS-B
Figure S.2. Z-scores SS-D
Figure S.3. Z-scores SS-1
Figure S.4. Z-scores SS-2
Figure S5. The linearity of the method in laboratory 1
Figure S6. The linearity of the method in laboratory 2
Figure S7. The linearity of the method in laboratory 3
**Figure S8.** The linearity of the method in laboratory 4
Figure S9. The linearity of the method in laboratory 5
Figure S10. The linearity of the method in laboratory 6
Figure S11. The linearity of the method in laboratory 7
Figure S12. The linearity of the method in laboratory 8
Figure S13. The linearity of the method in laboratory 9