# Formulas for converting concentration values from one unit of measurement to another

$$C[\mathrm{mg/L}] = C[\mu\mathrm{g/g}] \cdot \rho_{Sample}[\mathrm{g/L}]/1000\ ; \qquad C[\mu\mathrm{g/g}] = C[\mathrm{mg/L}] \cdot 1000/\rho_{Sample}[\mathrm{g/L}]$$

$$C\ [\mathrm{mg/L\ AA}] = \frac{C\ [\mu\mathrm{g/g}] \cdot \rho_{Sample}[\mathrm{g/L}]}{1000 \cdot (ABV_{Sample}\%/100\%)}\ ; \qquad C[\mu\mathrm{g/g}] = \frac{C[\mathrm{mg/L\ AA}] \cdot 1000}{\rho_{Sample}[\mathrm{g/L}]} \cdot \frac{ABV_{Sample}\%}{100\%}$$

$$C^{compound}[\%\mathrm{v/v}] = \frac{C[\mu\mathrm{g/g}] \cdot \rho_{Sample}[\mathrm{g/L}] \cdot 100\%}{10^6 \cdot \rho^{compound}[\mathrm{g/L}^c]} \qquad C[\mu\mathrm{g/g}] = \frac{C^{compound}[\%\mathrm{v/v}] \cdot 10^6}{100\%} \cdot \frac{\rho^{compound}[\mathrm{g/L}^c]}{\rho_{Sample}[\mathrm{g/L}]}$$

$$C^{compound}[\%\mathrm{v/v\ AA}] = \frac{C[\mu\mathrm{g/g}] \cdot \rho_{Sample}[\mathrm{g/L}] \cdot 100\% \cdot 100\%}{10^6 \cdot \rho^{compound}[\mathrm{g/L}^c] \cdot ABV_{sample}\%}$$

$$C[\mu\mathrm{g/g}] = \frac{C^{compound}[\%\mathrm{v/v\ AA}] \cdot 10^6 \cdot \rho^{compound}[\mathrm{g/L}^c] \cdot ABV_{sample}\%}{\rho_{Sample}[\mathrm{g/L}] \cdot 100\% \cdot 100\%}$$

$$C[\mathrm{mg/L\ AA}] = \frac{C[\mathrm{mg/L}]}{(ABV_{sample}\%/100\%)}\ ; \qquad C[\mathrm{mg/L}] = C[\mathrm{mg/L\ AA}] \cdot (ABV_{sample}\%/100\%)$$

$$C^{compound}[\%\mathrm{v/v}] = \frac{C^{compound}[\mathrm{mg/L}] \cdot 100\%}{\rho^{compound}[\mathrm{mg/L}^c]} = \frac{C^{compound}[\mathrm{mg/L}] \cdot 100\%}{\rho^{compound}[\mathrm{g/L}^c] \cdot 1000}$$

$$C^{compound}[\mathrm{mg/L}] = \frac{C^{compound}[\%\mathrm{v/v}] \cdot \rho^{compound}[\mathrm{mg/L}^c]}{100\%} = \frac{C^{compound}[\%\mathrm{v/v}] \cdot \rho^{compound}[\mathrm{g/L}^c] \cdot 1000}{100\%}$$

$$C^{compound}[\%\mathrm{,v/v\ AA}] = \frac{C^{compound}[\mathrm{mg/L}] \cdot 100\%}{\rho^{compound}[\mathrm{g/L}^c] \cdot 1000} \cdot \frac{100\%}{ABV_{sample}\%}$$

$$C^{compound}[\mathrm{mg/L}] = \frac{C^{compound}[\%\mathrm{,v/v\ AA}] \cdot \rho^{compound}[\mathrm{g/L}^c] \cdot 1000}{100\%} \cdot \frac{ABV_{sample}\%}{100\%}$$

$$C^{compound}[\mathrm{mg/L\ AA}] = \frac{C^{compound}[\%\mathrm{,v/v}] \cdot \rho^{compound}[\mathrm{g/L}^c] \cdot 1000}{100\% \cdot (ABV_{sample}\%/100\%)}$$

$$C^{compound}[\%\mathrm{,v/v}] = \frac{C^{compound}[\mathrm{mg/L\ AA}]}{\rho^{compound}[\mathrm{g/L}^c] \cdot 1000} \cdot \frac{ABV_{sample}\%}{100\%} \cdot 100\%$$

$$C^{compound}[\%\mathrm{,v/v\ AA}] = \frac{C^{compound}[\mathrm{mg/L\ AA}]}{\rho^{compound}[\mathrm{g/L}^c] \cdot 1000} \cdot 100\%$$

$$C^{compound}[\mathrm{mg/L\ AA}] = \frac{C^{compound}[\%\mathrm{,v/v\ AA}] \cdot \rho^{compound}[\mathrm{g/L}^c] \cdot 1000}{100\%}$$

$$C[\mathrm{g/100\ L\ AA}] = 0.1 \cdot C[\mathrm{mg/L\ AA}] \qquad C[\mathrm{mg/L\ AA}] = 10 \cdot C[\mathrm{g/100\ L\ AA}]$$

$$C^{measured}_{methanol}[\%\mathrm{,v/v\ AA}] = \tilde{C}^{measured}_{methanol}[\%\mathrm{,v/v}] \cdot 100\% / ABV_{sample}\%$$

## **Internal standard method** (here for ethanol, and for traditional - similarly)

## For calibration level only:

$$RRF_i^{\text{ethanol}} = \frac{\dfrac{C_{i,\text{calibr}}^{certified}}{\rho_{eth}} \cdot \left( \sum_{k=1}^{M_j} \dfrac{A_{i,calibr,k}}{A_{eth,calibr,k}} \right)}{\cdot \sum_{k=1}^{M_j} \left( \dfrac{A_{i,calibr,k}}{A_{eth,calibr,k}} \right)^2} \quad (\textbf{CA}); \quad rRF_i^{\text{ethanol}} = \frac{\dfrac{C_{i,calibr}^{certified}}{\rho_{eth}} \cdot \sum_{k=1}^{M_j} \dfrac{A_{i,calibr,k}}{A_{eth,calibr,k}}}{M_{calibr} \cdot \left( \dfrac{C_{i,calibr}^{certified}}{\rho_{eth}} \right)^2} = \frac{\left( \sum_{k=1}^{M_j} \dfrac{A_{i,calibr,k}}{A_{eth,calibr,k}} \right)}{\left( M_{calibr} \cdot \dfrac{C_{i,calibr}^{certified}}{\rho_{eth}} \right)} \quad (\text{AC}),$$

## FOR ALL levels *j*,

$$\sigma_{i,j},\% = \frac{\tilde{\sigma}_{i,j}}{\langle \tilde{C} \rangle_{i,j}^{measured}} \cdot 100\% = \sqrt{\sum_{k=1}^{M_j} \frac{\left( \dfrac{A_{i,j,k}}{A_{eth,j,k}} - \left( \left( \sum_{k=1}^{M_j} \dfrac{A_{i,j,k}}{A_{eth,j,k}} \right) / M_j \right) \right)^2}{M_j - 1}} \Bigg/ \left( \left( \sum_{k=1}^{M_j} \frac{A_{i,j,k}}{A_{eth,j,k}} \right) / M_j \right) \cdot 100\%$$

$$C_{i,j,k}^{measured} = RRF_i^{\text{ethanol}} \cdot \rho_{\text{eth}} \cdot \frac{A_{i,j,k}}{A_{eth,j,k}} \quad (5\ \textbf{CA}); \qquad C_{i,j,k}^{measured} = \left( 1 / rRF_i^{\text{ethanol}} \right) \cdot \rho_{eth} \cdot \frac{A_{i,j,k}}{A_{eth,j,k}} \quad (5'\ \text{AC})$$

$$\langle C \rangle_{i,j}^{measured} = \left( \sum_{k=1}^{M_j} C_{i,j,k}^{measured} \right) / M_j \ \ (6); \ \ \delta_{i,j},\% = \frac{\left( \langle C \rangle_{i,j}^{изм} - C_{i,j}^{certified} \right)}{C_{i,j}^{certified}} \cdot 100\% \ \ (7). \ \ \sigma_{i,j} = \frac{\sigma_{i,j},\% \cdot \langle C \rangle_{i,j}^{изм}}{100\%} \ \ (2);$$

## Linearity control - for all *j* levels except calibration

$$RRF_i^{\text{ethanol}}\_l = \frac{\sum_{j^*=1}^{N} \left( \dfrac{C_{i,j}^{certified}}{\rho_{eth}} \cdot \sum_{k=1}^{M_j} \dfrac{A_{i,j,k}}{A_{eth,j,k}} \right)}{\sum_{j^*=1}^{N} \sum_{k=1}^{M_j} \left( \dfrac{A_{i,j,k}}{A_{eth,j,k}} \right)^2} \quad (3\ \text{CA}); \quad rRF_i^{\text{ethanol}}\_l = \frac{\sum_{j^*=1}^{N} \left( \dfrac{C_{i,j}^{certified}}{\rho_{eth}} \cdot \sum_{k=1}^{M_j} \dfrac{A_{i,j,k}}{A_{eth,j,k}} \right)}{\sum_{j^*=1}^{N} \left( M_j \cdot \left( \dfrac{C_{i,j}^{certified}}{\rho_{eth}} \right)^2 \right)} \quad (3'\ \textbf{AC}),$$

$$R_i^2 = 1 - \frac{\sum_{j^*=1}^{N} \sum_{k=1}^{M_j} \left( \dfrac{C_{i,j}^{certified}}{\rho_{eth}} - RRF_i^{\text{ethanol}}\_l \cdot \dfrac{A_{i,j,k}}{A_{eth,j,k}} \right)^2}{\sum_{j^*=1}^{N} \left( M_j \cdot \left( \dfrac{C_{i,j}^{certified}}{\rho_{eth}} - \left( \dfrac{1}{N} \sum_{j=1}^{N} \dfrac{C_{i,j}^{certified}}{\rho_{eth}} \right) \right)^2 \right)} \quad (4\ \text{CA});$$

$$R_i^2 = 1 - \frac{\sum_{j^*=1}^{N} \sum_{k=1}^{M_j} \left( \dfrac{A_{i,j,k}}{A_{eth,j,k}} - rRF_i^{\text{ethanol}}\_l \cdot \dfrac{C_{i,j}^{certified}}{\rho_{eth}} \right)^2}{\sum_{j^*=1}^{N} \sum_{k=1}^{M_j} \left( \dfrac{A_{i,j,k}}{A_{eth,j,k}} - \left( \left( \sum_{j=1}^{N} \sum_{k=1}^{M_j} \dfrac{A_{i,j,k}}{A_{eth,j,k}} \right) / \sum_{j=1}^{N} M_j \right) \right)^2} \quad (4'\ \textbf{AC}),$$

$$C_p = \frac{\sum_{j^*=1}^{N} \sum_{k=1}^{M_j} \left( \left( \dfrac{C_{i,j}^{certified}}{\rho_{eth}} - \left( \sum_{j^*=1}^{N} \dfrac{C_{i,j}^{certified}}{\rho_{eth}} / \sum_{j^*=1}^{N} M_j \right) \right) \cdot \left( \dfrac{A_{i,j,k}}{A_{eth,j,k}} - \left( \left( \sum_{j^*=1}^{N} \sum_{k=1}^{M_j} \dfrac{A_{i,j,k}}{A_{eth,j,k}} \right) / \sum_{j^*=1}^{N} M_j \right) \right) \right)}{\sqrt{\left( \sum_{j^*=1}^{N} M_j \cdot \left( \dfrac{C_{i,j}^{certified}}{\rho_{eth}} - \left( \sum_{j^*=1}^{N} \dfrac{C_{i,j}^{certified}}{\rho_{eth}} / \sum_{j^*=1}^{N} M_j \right) \right)^2 \right) \cdot \left( \sum_{j^*=1}^{N} \sum_{k=1}^{M_j} \left( \dfrac{A_{i,j,k}}{A_{eth,j,k}} - \left( \left( \sum_{j^*=1}^{N} \sum_{k=1}^{M_j} \dfrac{A_{i,j,k}}{A_{eth,j,k}} \right) / \sum_{j^*=1}^{N} M_j \right) \right)^2 \right)}}$$

For a traditional internal standard, its concentration is used instead of the density of ethanol $\rho_{eth}$.

## External standard method (absolute calibration)

$$\tilde{\sigma}_{i,j}=\sqrt{\sum_{k=1}^{M_j}\frac{\left(\tilde{C}_{i,j,k}^{measured}-\langle\tilde{C}\rangle_{i,j}^{measured}\right)^2}{M_j-1}}\ (1);\qquad \sigma_{i,j},\%=\frac{\tilde{\sigma}_{i,j}}{\langle\tilde{C}\rangle_{i,j}^{measured}}\cdot 100\%\ (2);$$

$$\tilde{R}_i^2=1-\frac{\sum_{j=1}^{N}\sum_{k=1}^{M_j}\left(\tilde{C}_{i,j}^{certified}-R\tilde{F}_i\cdot A_{i,j,k}\right)^2}{\sum_{j=1}^{N}\left(M_j\cdot\left(\tilde{C}_{i,j}^{certified}-\frac{1}{N}\sum_{j=1}^{N}\tilde{C}_{i,j}^{certified}\right)^2\right)}\ (3\ CA);$$

$$R\tilde{F}_i=\frac{\sum_{j=1}^{N}\left(\tilde{C}_{i,j}^{certified}\cdot\sum_{k=1}^{M_j}A_{i,j,k}\right)}{\sum_{j=1}^{N}\sum_{k=1}^{M_j}\left(A_{i,j,k}{}^2\right)}\ (4\ CA);$$

$$\tilde{C}_{i,j,k}^{measured}=R\tilde{F}_i\cdot A_{i,j,k}\ (5\ CA);$$

$$\sigma_{i,j},\%=\frac{\tilde{\sigma}_{i,j}}{\langle\tilde{C}\rangle_{i,j}^{measured}}\cdot 100\%=\sqrt{\sum_{k=1}^{M_j}\frac{\left(A_{i,j,k}-\left(\left(\sum_{k=1}^{M_j}A_{i,j,k}\right)/M_j\right)\right)^2}{M_j-1}}\Bigg/\left(\left(\sum_{k=1}^{M_j}A_{i,j,k}\right)/M_j\right)\cdot 100\%$$

$$\tilde{R}_i^2=1-\frac{\sum_{j=1}^{N}\sum_{k=1}^{M_j}\left(A_{i,j,k}-R\tilde{F}_i\cdot\tilde{C}_{i,j}^{certified}\right)^2}{\sum_{j=1}^{N}\sum_{k=1}^{M_j}\left(A_{i,j,k}-\left(\sum_{j=1}^{N}\sum_{k=1}^{M_j}A_{i,j,k}\right)/\sum_{j=1}^{N}M_j\right)^2}\ (3'\ AC),$$

$$R\tilde{F}_i=\frac{\sum_{j=1}^{N}\left(\tilde{C}_{i,j}^{certified}\cdot\sum_{k=1}^{M_j}A_{i,j,k}\right)}{\sum_{j=1}^{N}\left(M_j\cdot\left(\tilde{C}_{i,j}^{certified}\right)^2\right)}\ (4'\ AC),$$

$$\tilde{C}_{i,j,k}^{measured}=\left(1/R\tilde{F}_i\right)\cdot A_{i,j,k}\ (5'\ AC),$$

$$\langle\tilde{C}\rangle_{i,j}^{measured}=\left(\sum_{k=1}^{M_j}\tilde{C}_{i,j,k}^{measured}\right)/M_j\ (6);\quad \delta_{i,j},\%=\frac{\left(\langle\tilde{C}\rangle_{i,j}^{measured}-\tilde{C}_{i,j}^{certified}\right)}{\tilde{C}_{i,j}^{certified}}\cdot 100\%\ (7).$$

$$C_p=\frac{\sum_{j=1}^{N}\sum_{k=1}^{M_j}\left(\left(C_{i,j}^{certified}-\left(\sum_{j=1}^{N}C_{i,j}^{certified}/\sum_{j=1}^{N}M_j\right)\right)\cdot\left(A_{i,j,k}-\left(\sum_{j=1}^{N}\sum_{k=1}^{M_j}A_{i,j,k}\right)/\sum_{j=1}^{N}M_j\right)\right)}{\sqrt{\left(\sum_{j=1}^{N}M_j\cdot\left(C_{i,j}^{certified}-\left(\sum_{j=1}^{N}C_{i,j}^{certified}/\sum_{j=1}^{N}M_j\right)\right)^2\right)\cdot\left(\sum_{j=1}^{N}\sum_{k=1}^{M_j}\left(A_{i,j,k}-\left(\sum_{j=1}^{N}\sum_{k=1}^{M_j}A_{i,j,k}\right)/\sum_{j=1}^{N}M_j\right)^2\right)}}$$

All calibration curves are constructed using the least squares method