

Формулы для перевода значений концентраций из одних единиц измерения в другие

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Только для калибровочного уровня:

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

ДЛЯ ВСЕХ уровней j,

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

$$C_{i,j,k}^{\text{изм}} = RRF_i^{\text{ethanol}} \cdot \rho_{\text{этанол}} \cdot \frac{A_{i,j,k}}{A_{\text{этанол},j,k}} \quad (5 \text{ CA}); \quad C_{i,j,k}^{\text{изм}} = (1 / rRF_i^{\text{ethanol}}) \cdot \rho_{\text{этанол}} \cdot \frac{A_{i,j,k}}{A_{\text{этанол},j,k}} \quad (5' \text{ AC})$$

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

Контроль линейности - для всех уровней j, кроме калибровочного

$$RRF_i^{\text{ethanol}} - l = \frac{\sum_{j^*=1}^N \left(\frac{C_{\text{аттест}}}{\rho_{\text{этанол}}} \cdot \sum_{k=1}^{M_j} \frac{A_{i,j,k}}{A_{\text{этанол},j,k}} \right)}{\sum_{j^*=1}^N \sum_{k=1}^{M_j} \left(\frac{A_{i,j,k}}{A_{\text{этанол},j,k}} \right)^2} \quad (3 \text{ CA}); \quad rRF_i^{\text{ethanol}} - l = \frac{\sum_{j^*=1}^N \left(\frac{C_{\text{аттест}}}{\rho_{\text{этанол}}} \cdot \sum_{k=1}^{M_j} \frac{A_{i,j,k}}{A_{\text{этанол},j,k}} \right)}{\sum_{j^*=1}^N \left(M_j \cdot \left(\frac{C_{\text{аттест}}}{\rho_{\text{этанол}}} \right)^2 \right)} \quad (3' \text{ AC}),$$

$$R_l^2 = 1 - \frac{\sum_{j^*=1}^N \sum_{k=1}^{M_j} \left(\frac{C_{\text{аттест}}}{\rho_{\text{этанол}}} - RRF_i^{\text{ethanol}} - l \cdot \frac{A_{i,j,k}}{A_{\text{этанол},j,k}} \right)^2}{\sum_{j^*=1}^N \left(M_j \cdot \left(\frac{C_{\text{аттест}}}{\rho_{\text{этанол}}} - \left(\frac{1}{N} \sum_{j^*=1}^N \frac{C_{\text{аттест}}}{\rho_{\text{этанол}}} \right) \right)^2 \right)} \quad (4 \text{ CA});$$

$$R_l^2 = 1 - \frac{\sum_{j^*=1}^N \sum_{k=1}^{M_j} \left(\frac{A_{i,j,k}}{A_{\text{этанол},j,k}} - rRF_i^{\text{ethanol}} - l \cdot \frac{C_{\text{аттест}}}{\rho_{\text{этанол}}} \right)^2}{\sum_{j^*=1}^N \sum_{k=1}^{M_j} \left(\frac{A_{i,j,k}}{A_{\text{этанол},j,k}} - \left(\left(\sum_{j^*=1}^N \sum_{k=1}^{M_j} \frac{A_{i,j,k}}{A_{\text{этанол},j,k}} \right) / \sum_{j^*=1}^N M_j \right) \right)^2} \quad (4' \text{ AC}),$$

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

Для традиционного внутреннего стандарта используется его концентрация вместо плотности этанола.

Метод внешнего стандарта (абсолютная градуировка)

$$\tilde{\sigma}_{i,j} = \sqrt{\sum_{k=1}^{M_j} \frac{(\tilde{C}_{i,j,k}^{u3M} - \langle \tilde{C} \rangle_{i,j}^{u3M})^2}{M_j - 1}} \quad (1); \quad \sigma_{i,j}, \% = \frac{\tilde{\sigma}_{i,j}}{\langle \tilde{C} \rangle_{i,j}^{u3M}} \cdot 100\% \quad (2);$$

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

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

$$\tilde{C}_{i,j,k}^{u3M} = R\tilde{F}_i \cdot A_{i,j,k} \quad (5 \text{ CA});$$

$$\sigma_{i,j}, \% = \frac{\tilde{\sigma}_{i,j}}{\langle \tilde{C} \rangle_{i,j}^{u3M}} \cdot 100\% = \sqrt{\sum_{k=1}^{M_j} \frac{\left(A_{i,j,k} - \left(\left(\sum_{k=1}^{M_j} A_{i,j,k} \right) / M_j \right) \right)^2}{M_j - 1}} / \left(\left(\sum_{k=1}^{M_j} A_{i,j,k} \right) / M_j \right) \cdot 100\%$$

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

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

$$\tilde{C}_{i,j,k}^{u3M} = (1 / R\tilde{F}_i) \cdot A_{i,j,k} \quad (5' \text{ AC}),$$

$$\langle \tilde{C} \rangle_{i,j}^{u3M} = \left(\sum_{k=1}^{M_j} \tilde{C}_{i,j,k}^{u3M} \right) / M_j \quad (6); \quad \delta_{i,j}, \% = \frac{(\langle \tilde{C} \rangle_{i,j}^{u3M} - \tilde{C}_{i,j}^{ammecm})}{\tilde{C}_{i,j}^{ammecm}} \cdot 100\% \quad (7).$$

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

Все градуировочные зависимости строятся по методу наименьших квадратов