

Supporting Information

Accurate quantification of selenoproteins in human plasma/serum by isotope dilution ICP-MS: Focus on Selenoprotein P

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Equation S-1. Model equation for species-specific IDA-ICP-MS for SEPP1

Equation S-2. Model equation for species-unspecific IDA-ICP-MS

Equation S-1. Model equation for species-specific IDA-ICP-MS for SEPP1

The equation used for the determination of SEPP1 mass fraction (expressed as Se) in human plasma/serum by species-specific IDA-ICP-MS is shown below:

$$w_s = w_{sp} \cdot \frac{m_{sp}}{m_s} \cdot \frac{W_s}{W_{sp}} \cdot \frac{(R_{A/B} \cdot k \cdot B_{sp} - A_{sp})}{(A_s - R_{A/B} \cdot k \cdot B_s)} \quad \text{Equation 1}$$

w_s , mass fraction of SEPP1 in the sample blend (ng g⁻¹ Se)

w_{sp} , mass fraction of SEPP1 in the spike (ng g⁻¹ Se): (47.2 ± 1.0) ng g⁻¹ Se, $k=2$

m_s , mass of the sample in the sample blend (g): (0.10487 ± 0.00051) g, $k=2$

m_{sp} , mass of the spike in the sample blend (g): (0.02567 ± 0.00051) g, $k=2$

W_s , atomic weight of the sample (g mol⁻¹): (78.96 ± 0.03) g mol⁻¹, IUPAC value, $k=2$

W_{sp} , atomic weight of the spike (g mol⁻¹): (75.92 ± 0.13) g mol⁻¹, $k=2$

$R_{A/B}$, isotope ratio measured in the mixture: $R_{77/76}$

k , mass bias correction factor: (0.8407 ± 0.0088), $k=2$

A_s , abundance of isotope A in the sample: (7.635 ± 0.010) %, IUPAC value

B_s , abundance of isotope B in the sample: (9.366 ± 0.018) %, IUPAC value

A_{sp} , abundance of isotope A in the spike: (0.03 ± 0.02) %, $k=2$

B_{sp} , abundance of isotope B in the spike: (99.85 ± 0.05) %, $k=2$

Equation S-2. Model equation for species-unspecific IDA-ICP-MS

The on-line equation used for the determination of the Se mass fraction bound to intact selenoproteins (GPx3, SEPP1 and Se-Albumin) in human serum by post-column IDA-AF-HPLC-ICP-MS is shown below:

$$MF_{sample} = w_{sp} \cdot f_{sp} \cdot \frac{W_s}{W_{sp}} \cdot \frac{(R_{A/B} \cdot k \cdot B_{sp} - A_{sp})}{(A_s - R_{A/B} \cdot k \cdot B_s)} \quad \text{Equation 2}$$

MF_{sample} , mass flow of the Se (ng Se)

w_{sp} , mass fraction of the Se in the spike solution (ng g⁻¹ Se): (0.504 ± 0.017) ng g⁻¹ Se, $k=2$

f_{sp} , flow of the spike solution (g min⁻¹): (0.11005 ± 0.00091) g min⁻¹, $k=1$

W_s , atomic weight of the sample (g mol⁻¹): (78.96 ± 0.03) g mol⁻¹, IUPAC value, $k=2$

W_{sp} , atomic weight of the spike (g mol⁻¹): (76.92 ± 0.03) g mol⁻¹, $k=2$

$R_{A/B}$, isotope ratio measured in the mixture: $R_{76/77}$

k , mass bias correction factor: (1.0431 ± 0.0078), $k=1$

A_s , abundance of isotope A in the sample: (9.366 ± 0.018) %, IUPAC value

B_s , abundance of isotope B in the sample: (7.635 ± 0.010) %, IUPAC value

A_{sp} , abundance of isotope A in the spike: (0.051 ± 0.004) %, $k=2$

B_{sp} , abundance of isotope B in the spike: (99.80 ± 0.25) %, $k=2$

The mass fraction of Se (w_{sample} , ng g⁻¹ Se) in the sample was obtained by the integration of the peak area divided by the mass injected (g). The resulted mass fraction can be multiplied by the density of the serum (g mL⁻¹) to get the Se concentration (ng mL⁻¹) in each chromatographic peak.

$$w_{sample} = \frac{Area}{m_{injected}} \quad \text{or} \quad C_{sample} = \frac{Area}{m_{injected}} \cdot \rho_{sample} \quad \text{Equation 3}$$

C_{sample} , concentration of Se in the sample (ng mL⁻¹ Se)

$m_{injected}$, mass injected (g): (0.0495 ± 0.0096) g, $k=2$

ρ_{sample} , density of BCR-637 RM (g mL⁻¹): (1.0237 ± 0.0044) g mL⁻¹, $k=2$