

Supplementary Information

Currently Used Pesticides in Water Matrices in Central-Western Brazil

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Limits of detection (LOD) and quantification (LOQ) of the employed method were determined according to the criteria proposed by Thier and Zeumer¹ using recovery experiments.

LOQ was determined as the lowest concentration of the compounds that gives a response that could be quantified with an RSD (relative standard deviation) of less than 20%, sensitivity (recovery) of at least 0.70. It is greater than or equal to the limit of detection. LOD was determined from recovery experiments at the smallest fortification level using equations 1 to 5 as follow:

$$\text{LOD} = \frac{2 t_{f,95} \hat{\sigma}_{\text{com}}}{S} \quad (1)$$

The standard deviation ($\hat{\sigma}_{\text{com}}$) (equation 2) is computed from the standard deviation of the blank signal ($\hat{\sigma}_{\text{B}}$) (equation 3) and from the standard deviation $\hat{\sigma}_{\text{A}}$ (equation 4), estimated during the experiment with the lowest fortification level.

$$\hat{\sigma}_{\text{com}} = \sqrt{\frac{(m-1) \hat{\sigma}_{\text{A}} + (n-1) \hat{\sigma}_{\text{B}}}{m+n-2}} \quad (2)$$

$$\hat{\sigma}_{\text{B}} = \sqrt{\frac{\sum_{i=1}^n (B_i - \bar{B})^2}{n-1}} \quad (3)$$

Where m is the number of analytical values (A_i) and n is the number of blank values (B_i). Degree of freedom (f) = $m + n - 2$.

$$\hat{\sigma}_{\text{A}} = \sqrt{\frac{\sum_{i=1}^m (A_i - \bar{A})^2}{m-1}} \quad (4)$$

Where \bar{B} and \bar{A} are the mean blank and mean analytical value, respectively.

The sensitivity of the analytical method (S), which means the change in signal value *per* change of concentration, can be estimated from the mean analytical value and from the lowest fortification level (q) (equation 5):

$$S = \frac{\bar{A}}{q} \quad (5)$$

Reference

1. Thier, H. P.; Zeumer, H.; *Manual of Pesticides Analysis*; Verlag Chemie: New York, 1987, p. 37-41.

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