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:

\[ \text{LOD} = \frac{2 \times t_{0.95} \hat{\sigma}_{\text{com}}}{S} \]  

(1)

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

\[ \hat{\sigma}_{\text{com}} = \sqrt{\frac{(m-1) \hat{\sigma}_A + (n-1) \hat{\sigma}_B}{m + n - 2}} \]  

(2)

\[ \hat{\sigma}_B = \sqrt{\frac{\sum_{i=1}^{n} (B_i - \bar{B})^2}{n-1}} \]  

(3)

\[ \hat{\sigma}_A = \sqrt{\frac{\sum_{i=1}^{n} (A_i - \bar{A})^2}{m-1}} \]  

(4)

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

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):

\[ S = \frac{\bar{A}}{q} \]  

(5)

Reference


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