

# STANDARD SUBSTANCE FREE QUANTIFICATION IN LC/ESI/MS IN EXAMPLE OF PESTICIDES IN CEREALS

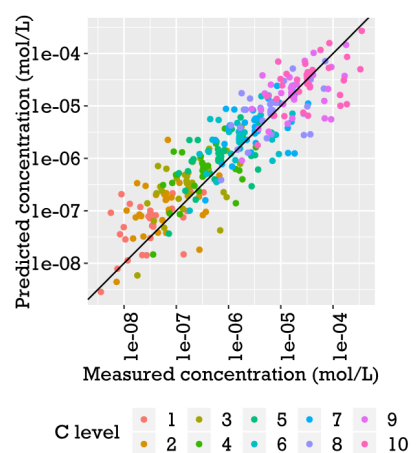
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Hundreds of different pesticides are used to enhance the yield of crops and make the agriculture more profitable thus sustainable. Unfortunately, most of pesticides are harmful to humans and thus monitoring of trace amounts of used pesticides is needed to ensure food safety. This is nowadays mainly done with LC/ESI/MS thanks to specificity and sensitivity it is offering. For quantitation, standard substances are needed because the electrospray ionization differs between different compounds over 6 orders of magnitude. As the number of screened contaminants in food are rapidly growing the analysis cost using standard substances is rocketing. Standard substance free quantitation using ionization efficiency prediction models can help to prioritize compounds for targeted analysis thus helping to lower the cost of analysis. Additionally, it allows to quantify the identified new contaminants and/or transformation products.



*Fig.1 Comparison of predicted concentrations and measured concentrations in example of barley. Colors denote different concentration levels*

We studied the application of standard substance free quantitation with the example of pesticides in cereal matrix. 152 different pesticides were spiked on different concentration levels into 6 different cereal matrices – barley, wheat, rye, maize, rice and oats. Ionization efficiencies of these pesticides were predicted using previously developed ionization efficiency prediction model. Concentration estimates were calculated from the recorded peak areas using predicted ionization efficiencies.

On average predicted concentrations were 5.6 times off. For 88.5% of compounds, the error was less than 10 times, for 77% of compounds the error was less than 5 times and for 25% of compounds the error was less than 25%. These results show that standard substance free quantitation in LC/ESI/MS is feasible.