GAS CHROMATOGRAPHY EXACT MASS TIME-OF-FLIGHT Mass Spectrometry: Quantitation and Screening of Pesticide Residues in Food

INTRODUCTION

A GC-exact mass TOF-MS based method has been developed for the quantification of approximately 100 pesticides in baby food, pear, and lettuce samples. Extracts spiked with pesticides at 0.10 and 0.01 mg kg⁻¹ yielded average recoveries in the range of 70 - 100% with RSDs less than 26%, with good linearity.

CONCLUSIONS

A GC-exact mass TOF-MS method has been developed for the quantification of approximately one hundred pesticides and transformation products at 0.01 and 0.1 mg kg⁻¹ in fruit-based baby food, pear and lettuce samples. Good linearity and satisfactory recoveries were obtained for the majority of pesticides in fruit-based baby food, pear and lettuce.

The mass accuracy improved with the concentration of the analytes of interest and was more critical for analyses with low m/z values (m/z < 200).

The TOF instrument provided an improvement in selectivity for the pesticides by narrowing the m/z window, giving better separation of the target compounds from co-eluting compounds, which is very important when analyzing complex matrices.

A targeted approach (using TargetLynx) and an untargeted approach (using ChromaLynx and a library search to detect and identify incurred residues) were used for screening, successfully identifying incurred pesticides in pear and lettuce samples at concentrations above 0.01 mg kg⁻¹, and with a good agreement with previous results obtained from GC-single quadrupole analysis. The targeted approach with TargetLynx is essential for successful identification and confirmation of the analytes and ChromaLynx is a valuable tool for additional analysis, enabling untargeted analytes to be recognised.

A targeted approach and an untargeted approach were used for screening, successfully identifying incurred pesticides in pear and lettuce samples at concentrations above 0.01 mg kg⁻¹. The untargeted approach with library search and elemental composition information detected and identified an incurred residue (chlordimeform) in lettuce at 0.07 mg kg⁻¹.

RESULTS AND DISCUSSION

The improvement in selectivity results in enhanced S/N, thereby improving LODs.

Reducing the mass window results in elimination of the background interferences of any origin (e.g. matrix co-extractives).

Satisfactory method recoveries were obtained for the majority of the pesticides spiked at concentrations of 0.10 and 0.01 mg kg⁻¹ in fruit-based baby food (70 – 100%, RSD < 22%), pear (72 – 108%, RSD < 25%) and lettuce (70 – 109%, RSD < 26%).

CONCLUSIONS

A targeted approach (using TargetLynx) and an untargeted approach (using ChromaLynx and a library search to detect and identify incurred residues) were used for screening, successfully identifying incurred pesticides in pear and lettuce samples at concentrations above 0.01 mg kg⁻¹, and with a good agreement with previous results obtained from GC-single quadrupole analysis. The targeted approach with TargetLynx is essential for successful identification and confirmation of the analytes and ChromaLynx is a valuable tool for additional analysis, enabling untargeted analytes to be recognised.

A targeted approach and an untargeted approach were used for screening, successfully identifying incurred pesticides in pear and lettuce samples at concentrations above 0.01 mg kg⁻¹. The untargeted approach with library search and elemental composition information detected and identified an incurred residue (chlordimeform) in lettuce at 0.07 mg kg⁻¹.

REGOLARITY AND SELECTIVITY

Satisfactory method recoveries were obtained for the majority of the pesticides spiked at concentrations of 0.10 and 0.01 mg kg⁻¹ in fruit-based baby food (70 – 100%, RSD < 22%), pear (72 – 108%, RSD < 25%) and lettuce (70 – 109%, RSD < 26%).

Screening of samples

Chlordimeform (DCPA), a non-targeted pesticide in the MS screen method, was detected and identified by ChromaLynx.

Re-extraction of the lettuce sample, where it was detected DCPA, and its analysis using the GC-single quadrupole MS method confirmed the presence of this pesticide at 0.07 mg kg⁻¹.