



GRASEQA 2022

LIBRO DE RESÚMENES



Grupo Regional Andaluz
Sociedad Española de Química Analítica



Sociedad Española de Química Analítica

XVII Reunión del Grupo Regional Andaluz de la Sociedad Española de Química Analítica



Libro de resúmenes



Sevilla, 6 y 7 de octubre de 2022



El Comité Organizador de la XVII Reunión del Grupo Regional Andaluz de la Sociedad Española de Química Analítica (GRASEQA 2022) CERTIFICA que:

D/D^a Rosalía López Ruiz

Ha asistido a esta reunión, celebrada los días 6 y 7 de octubre de 2022 en Sevilla (España).

En Sevilla a 7 de octubre de 2022.

Profesor Dr. Fernando de Pablos Pons
Coordinador del GRASEQA 2022



GRUPO REGIONAL ANDALUZ
SOCIEDAD ESPAÑOLA DE QUÍMICA ANALÍTICA



El Comité Organizador de la XVII Reunión del Grupo Regional Andaluz de la Sociedad Española de Química Analítica (GRASEQA 2022) CERTIFICA que el trabajo:

DETERMINATION OF TRANSFORMATION PRODUCTS OF CHLORANTRANILIPROLE IN FIELD AND LABORATORY TOMATOES BY LC-Q-ORBITRAP AND A NON-TARGETED APPROACH

Antonio Jesús Maldonado-Reina, Rosalía López-Ruiz, Roberto Romero-González, José Luis Martínez-Vidal,
Antonia Garrido-Frenich.

Ha sido presentado a esta reunión en modalidad de **PÓSTER**.

En Sevilla a 7 de octubre de 2022

Profesor Dr. Fernando de Pablos Pons
Coordinador del GRASEQA 2022

P-006

DETERMINATION OF TRANSFORMATION PRODUCTS OF CHLORANTRANILIPROLE IN FIELD AND LABORATORY TOMATOES BY LC-Q-ORBITRAP AND A NON-TARGETED APPROACH

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Chlorantraniliprole, a man-made anthranilic diamide insecticide first synthesised by DuPont, was approved as an active substance in Spain, and therefore, it is routinely monitored in commercialised agricultural products. Despite this, the monitoring of its transformation products (TPs) currently remains disregarded, even though it is certainly possible that they be present in foodstuff treated with chlorantraniliprole plant protection products (PPPs). Therefore, elucidating possible TPs stemming from its degradation and monitor them is a key task, either those previously addressed in literature,¹ or those not listed, using a non-targeted approach (suspect screening and unknown analysis).

To this end, field (greenhouse) and laboratory studies were performed in tomato samples hoping to monitor the degradation of chlorantraniliprole into TPs. Altacor® was diluted and applied to tomato samples at different concentrations. Field studies were carried out at the single recommended dose (7.53 g chlorantraniliprole/L) for 53 days. Moreover, laboratory studies were done at single and twofold (15.05 g chlorantraniliprole/L) dose, for 30 days at room temperature. A solid-liquid extraction method (SLE) was applied, with acetonitrile (MeCN) as extracting solvent (5 g tomato per 5 mL MeCN). Data acquisition was performed by ultra-high performance liquid chromatography coupled to Q-Orbitrap high resolution mass accuracy spectrometry (LC-Q-Orbitrap-HRMAS), in Full Scan MS and data independent acquisition (DIA) modes. Data processing was carried out by a non-target approach combining suspect screening, through a home-made database from literature review, and unknown analysis, through MassChemSite, which predicts possible TPs generated from a parent compound.

In all, 2 TPs of chlorantraniliprole were tentatively identified and semiquantified by an analytical standard of chlorantraniliprole, on account of to their structural similitude. TP IN-F6L99 was present in both studies, and was detected from day 0 (laboratory) and day 2 (greenhouse), with a peak concentration of 20.35 µg/kg, in laboratory studies at day 5. TP C20 was only detected in laboratory studies at day 21, at a concentration of 0.22 µg/kg (likely intermediary TP). Toxicity of identified TPs was determined by ToxTree, in line with Cramer rules, which showed that IN-F6L99 could be classified as a highly toxic compound (Class III), along with chlorantraniliprole. This leads to the conclusion that the toxicity of TPs can be similar to that of the active substance, and hence, their monitoring should not be underestimated.

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