18TH ANNUAL WORKSHOP ON EMERGING HIGH-RESOLUTION MASS SPECTROMETRY (HRMS) AND LC-MS/MS APPLICATIONS IN ENVIRONMENTAL ANALYSIS AND FOOD SAFETY

BARCELONA,
10-11 OCTOBER 2022

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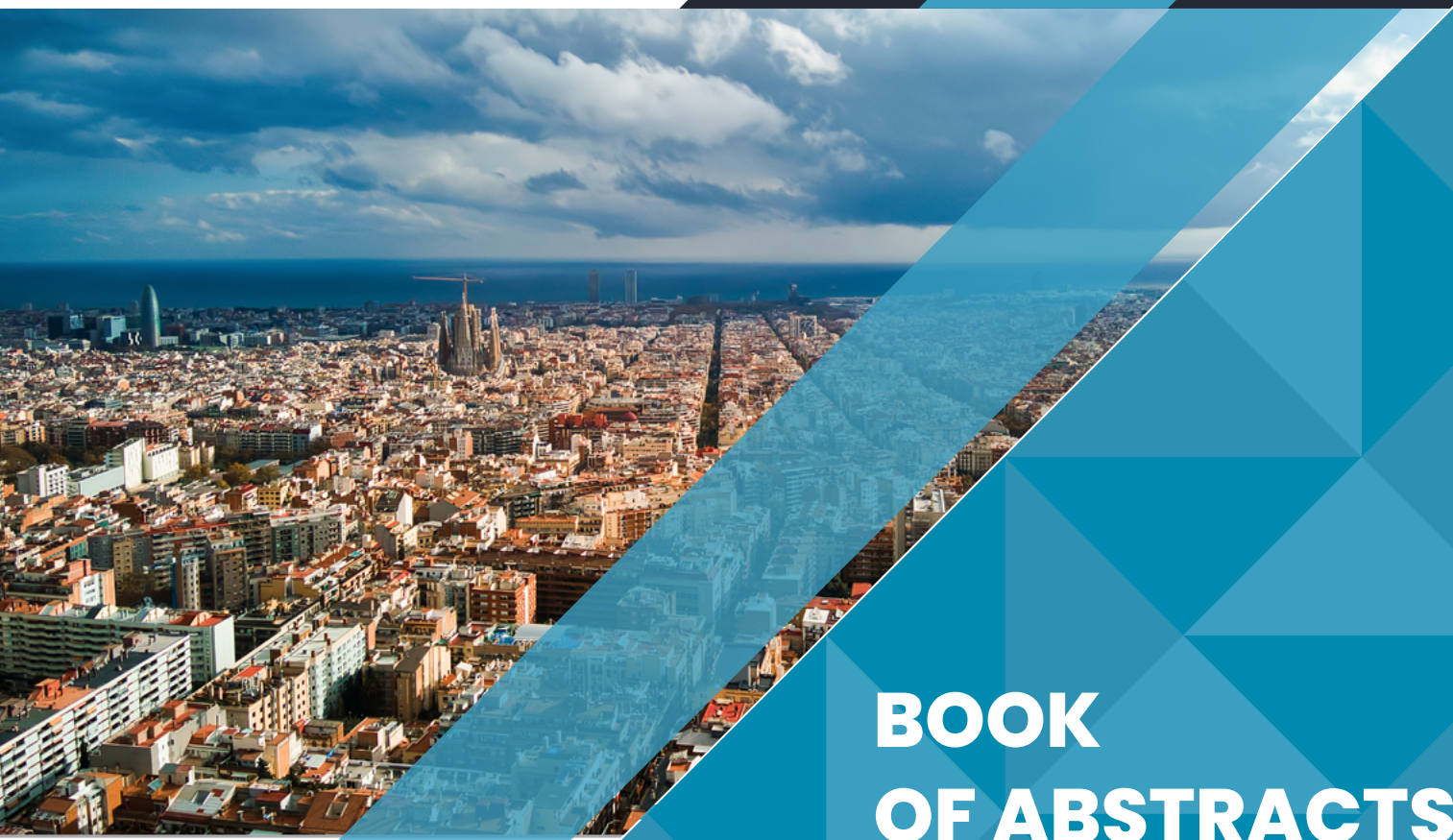

BOOK OF ABSTRACTS

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CERTIFICATE

I HEREBY CERTIFY THE ATTENDANCE OF:

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Damià Barcelò
Chair of the Scientific Committee

BARCELONA, 11 OCTOBER 2020

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Have given the ORAL presentation entitled: *Combination of analytical platforms for the comprehensive study of myclobutanil-based plant protection product degradation in tomato and grape*

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Combination of analytical platforms for the comprehensive study of myclobutanil-based plant protection product degradation in tomato and grape

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Myclobutanil is a pesticide widely used for fungus pest treatment, especially in some important crops in Spain as tomatoes and grapes. However, its use can affect both human and environment. Although this compound has been widely studied its degradation products have been scarcely elucidated.1 Besides, together with the active substance, plant protection products (PPPs) contain other compounds which improve their performance, the additives, being the most important one the co-formulant family. But, despite the beneficial properties of these compounds, they can cause also serious adverse health and environmental effects.2
Here, dissipation of a myclobutanil PPP (Mitrus®) was performed in tomato and grape samples at different storage conditions (3°C and dark or 22°C and light) employing solid-liquid extraction (SLE) and ultra-high performance liquid chromatography coupled to high resolution mass spectrometry (UHPLC-Q-Orbitrap-HRMS). Dissipation was fit to a biphasic kinetic model with a suitable adjustment (R2>0.95) and with residual levels lower than 24 days in all cases. Myclobutanil metabolites were elucidated, identifying six myclobutanil metabolites, four out of them described for the first time. One of them was confirmed using 1H, 13C, (1H-1H)-COSY, (1H-13C)-HMQC and (1H-13C)-HMBC nuclear magnetic resonance (NMR). Their degradation curves were also evaluated, increasing their concentrations when myclobutanil concentration decreases. Additionally, headspace solid-phase microextraction method (HS-SPME)-gas chromatography coupled to HRMS (GC-Q-Orbitrap-HRMS) was used to search co-formulants present in the PPP. Seven co-formulants were identified and quantified after the internal standard acquisition. Their dissipation curves were studied, observing that all of them degraded 12 days after application.
Acknowledgements
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References

(1) European Food Safety Authority. Conclusion on the Peer Review of the Pesticide Risk Assessment of the Active Substance Myclobutanil. EFSA Journal 2010, 8 (10), 1-83.
(2) European Commission. Regulation (EC) No 1107/2009. Official Journal of the European Union 2009, 24 (8), 1–50

Topic: 2-Non Target Analysis (NTA) and Bioinformatics applied to environmental and food samples

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