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Data Article

Original GC/EI/MS total ion chromatograms of *Lemna* (*Lemna minor* L.) treated or not with metribuzin, glyphosate, and their binary mixtures



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ABSTRACT

The GC/EI/MS metabolite profiles of *Lemna minor* L. plants were recorded following treatments with sub-lethal concentrations of the herbicidal active ingredients (a.i.) metribuzin and glyphosate, and various of their binary mixtures. The raw GC/EI/MS total ion chromatograms (*.cdf format) of the *Lemna*'s endo-metabolomes were recorded, which are included in this article. Since *Lemna* is a model organism in ecotoxicological studies, the dataset could serve as a reference for *Lemna* metabolomics studies related to the investigation of the effects of phytotoxic compounds and their mixtures on its metabolism. Also, the dataset could be a valuable resource for the discovery of validated biomarkers of the toxicity of mixtures. The dataset support the research article "Kostopoulou et al., Assessment of the effects of metribuzin, glyphosate, and their

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mixtures on the metabolism of the model plant Lemna minor L. applying metabolomics. "Chemosphere 239, 2020, 124582."

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Specifications Table

Subject	Agricultural and Biological Sciences (General)
Specific subject area	Ecotoxicology, ecotoxicogenomics
Type of data	Raw GC/EI/MS total ion chromatograms (*.cdf format)
How data were acquired	Untargeted GC/EI/MS metabolomics analysis Instrument: Agilent 6890 MS platform (Agilent Technologies Inc.), equipped with a 5973 series mass selective detector (MSD) and a 7683 autosampler Acquisition of data using the MSD Chemstation (Agilent)
Data format	Raw (*.cdf)
Parameters for data collection	Column: HP-5MS, length; 30 m, i.d.; 0.25 mm, film thickness 0.25 µm, Agilent Technologies Inc. Split ratio: 5:1 Injector temperature: 230°C Oven temperature: 70°C, stable for 5 min, 5°C min ⁻¹ increase to 295°C, stable for 2 min. Carrier gas: Helium at a flow rate of 1 mL min ⁻¹ Ionization: Positive electron ionization, 70eV Full scan 50–800 Da (4 scans s ⁻¹) Temperature of the MS source, 230°C, quadrupole 230°C
Description of data collection	TIC of the <i>Lemna</i> metabolomes performing full scanning over the mass range between 50 and 800 Da
Data source location	Institution: Agricultural University of Athens City/Town/Region: Athens Country: Greece
Data accessibility	Repository name: Pesticide Metabolomics Group database Data identification number: <i>Lemna minor</i> L. (PMG-04-19) Direct URL to data: https://www.aua.gr/pesticide-metabolomicsgroup/Resources/default.html
Related research article	Author's name; <i>Sofia Kostopoulou, Georgia Ntatsi, Gerasimos Arapis, Konstantinos A. Aliferis</i> Title; <i>Assessment of the effects of metribuzin, glyphosate, and their mixtures on the metabolism of the model plant Lemna minor L. applying metabolomics</i> Journal; <i>Chemosphere 239, 2020, 124582.</i> DOI; https://doi.org/10.1016/j.chemosphere.2019.124582 .

Value of the Data

- The data provide an overview of the effects of the herbicides metribuzin, glyphosate, and their mixtures on the metabolism of *Lemna minor* L.
- The dataset could be used by researchers working on the investigation of the combined effects of mixtures on the metabolism of model biological systems
- To the best of our knowledge, no similar data exist on the combine effect of phytotoxic compounds on the metabolism of *Lemna*

1. Data

TIC of *Lemna minor* L. endo-metabolomes in *.cdf format corresponding to profiles of untreated (control) plants and plants treated with metribuzin (M), glyphosate (G), and binary mixtures [glyphosate-metribuzin 50%–50%, 25%–75%, 75%–25% (% of their corresponding EC₅₀ values)].

2. Experimental design, materials, and methods

The aquatic microphyte *Lemna minor* L. was used for the monitoring of the effects of metribuzin, glyphosate, and binary mixtures on its metabolism and the discovery of the corresponding biomarkers of toxicity [1]. The experimental design and sample preparation was based on previously described protocols following optimization [2–4].

For the extraction of the *Lemna* endo-metabolomes a mixture (50-50, v/v) of ethyl acetate and methanol (MeOH) (GC/MS grade, 99.9% purity) (Carlo Erba Reagents, val de Reuil, France) was used. In sample preparation for GC/EI/MS metabolomics analyses, pyridine (99.8%, v/v), methoxylamine hydrochloride (98%, w/w), ribitol, and analytical standards of selected *Lemna* metabolites, were used (Sigma-Aldrich Ltd., Darmstadt, Germany). N- Trimethylsilyl-N-methyl trifluoroacetamide (MSTFA, Macherey and Nagel, Düren, Germany) was used for the silylation of the samples.

The derivatized *Lemna* extracts (1 μ L) were injected on column. An HP-5MS column (Agilent Technologies Inc.) was used; length; 30 m, i.d.; 0.25 mm, film thickness 0.25 μ m. Samples were injected applying a 5:1 split. The injector's temperature was set at 230°C. The temperature of the oven was set initially at 70°C, kept stable for 5 min, followed by a 5°C min⁻¹ increase to 295°C, stable for 2 min. Positive electron ionization at 70eV was used and full scan mass spectra were acquired in the mass range 50–800 Da (4 scans s⁻¹), with a 10 min solvent delay. The temperature of the MS source was set at 230°C and that of the quadrupole at 230°C. Helium was used as the carrier gas at a 1 mL min⁻¹ flow rate.

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Conflict of Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

References

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