

Sample extracts were prepped separately for positive and negative ions in LC/MS and LC/MS² analysis. Injection standards were used to ensure injection and chromatographic consistency. The LC/MS platform was based on Waters ACQUITY UPLC and Thermo-Finnigan LTQ MS, consisting of electrospray ionization (ESI) source and linear ion-trap (LIT) mass analyzer front end and a Fourier transform ion cyclotron resonance (FT-ICR) MS back end. Ions with counts >2 million, could be measured with mass error of <5 ppm. GC/MS analysis was performed using Thermo-Finnigan Trace DSQ fast-scanning single-quadrupole MS using electron impact ionization.

Stringent QC practices were employed with addition of QC compounds, monitoring of process variation and data output quality. All experimental samples were randomly distributed throughout each day's run. Data was extracted, examined, and appropriate QC limits were imposed. Compounds were identified based on a metabolomic library of more than 1,000 purified standards. Curation procedures ensured a high quality dataset for statistical analysis and data interpretation. Confirmation of consistency in peak identification was also performed manually.

Adapted from: Mrinalini et al. 2015. Parasitoid venom induces metabolic cascades in fly hosts. *Metabolomics* 11(2) 350-366.