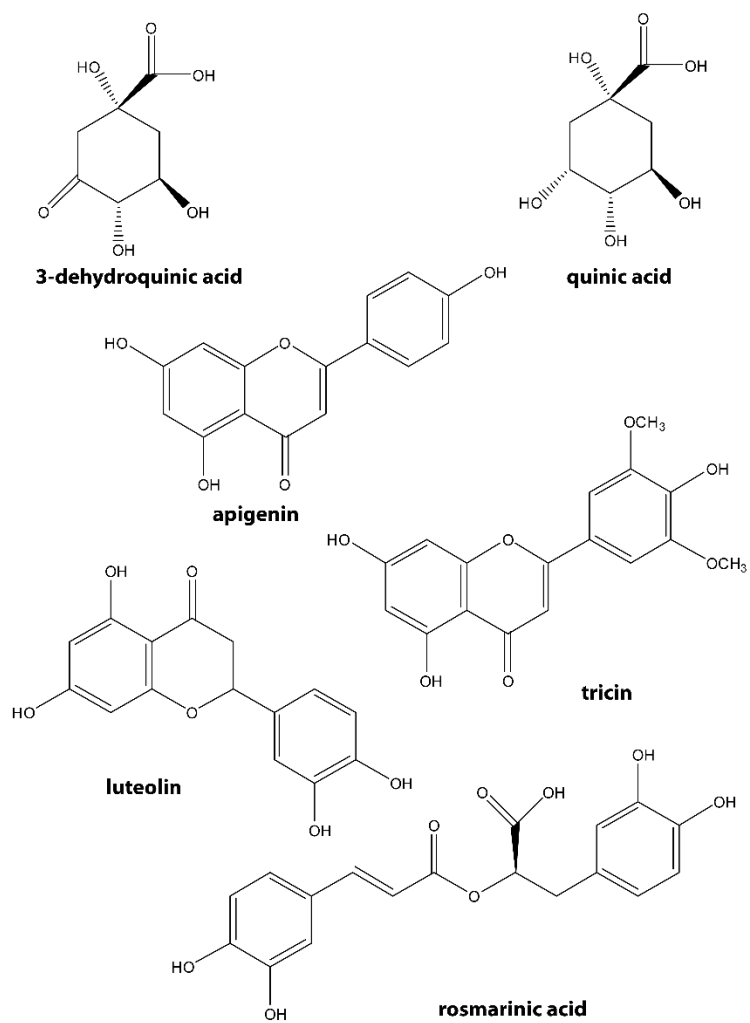


## **Analytical and Bioanalytical Chemistry**

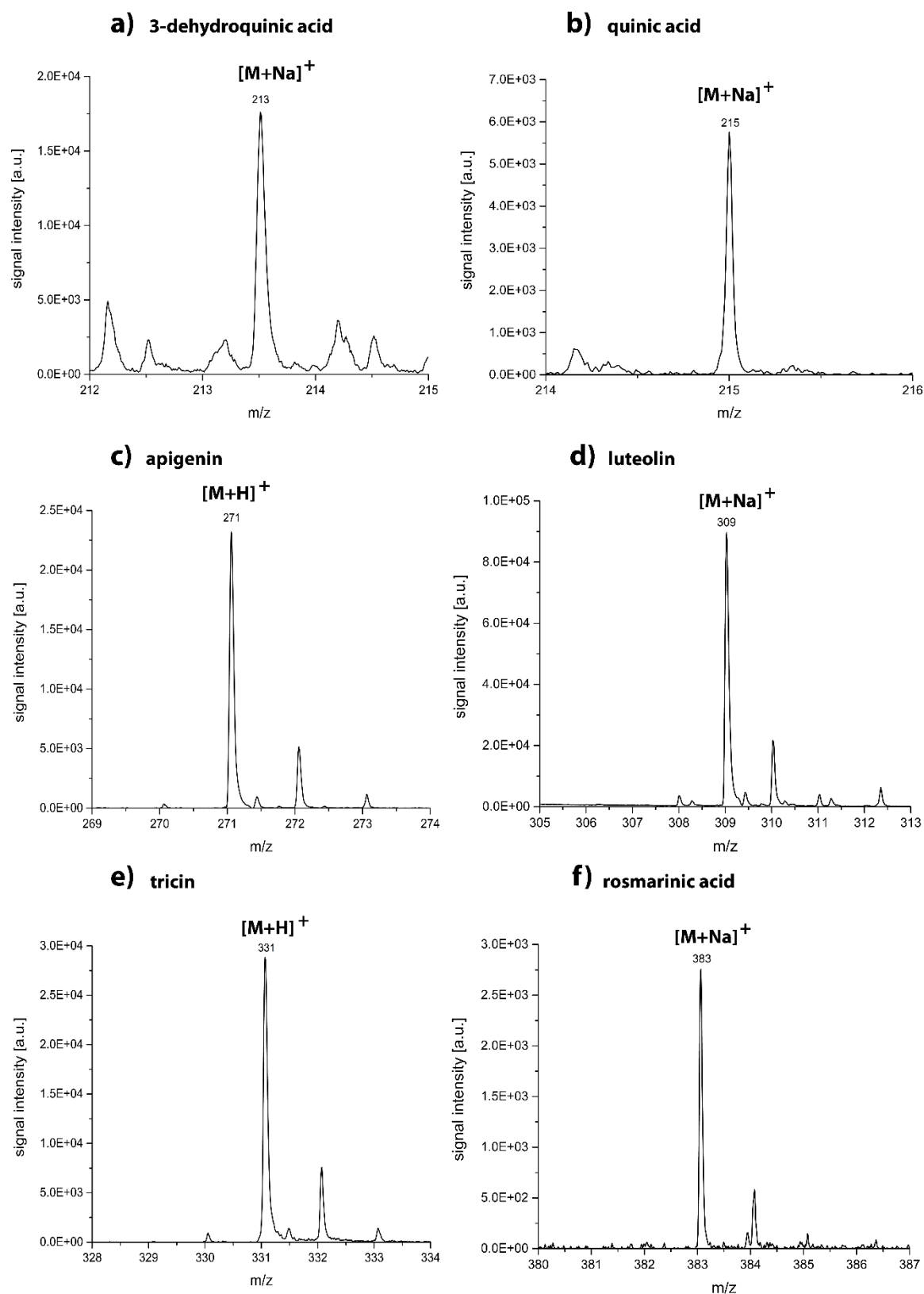
### **Electronic Supplementary Material**

#### **Tracing the fate and transport of secondary plant metabolites in a laboratory mesocosm experiment by employing mass spectrometric imaging**

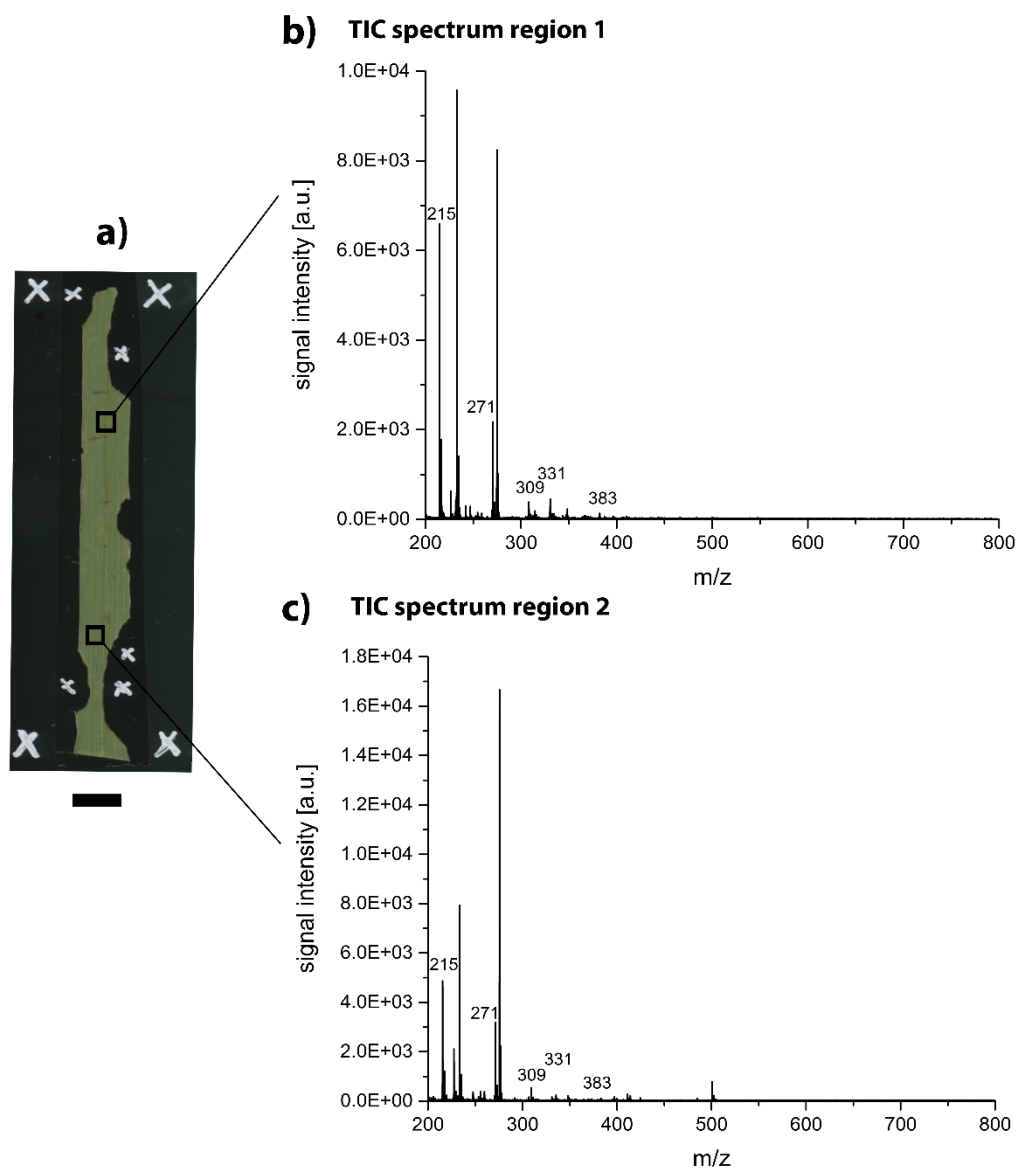
Anna C. Crecelius, Beate Michalzik, Karin Potthast, Stefanie Meyer, Ulrich S. Schubert



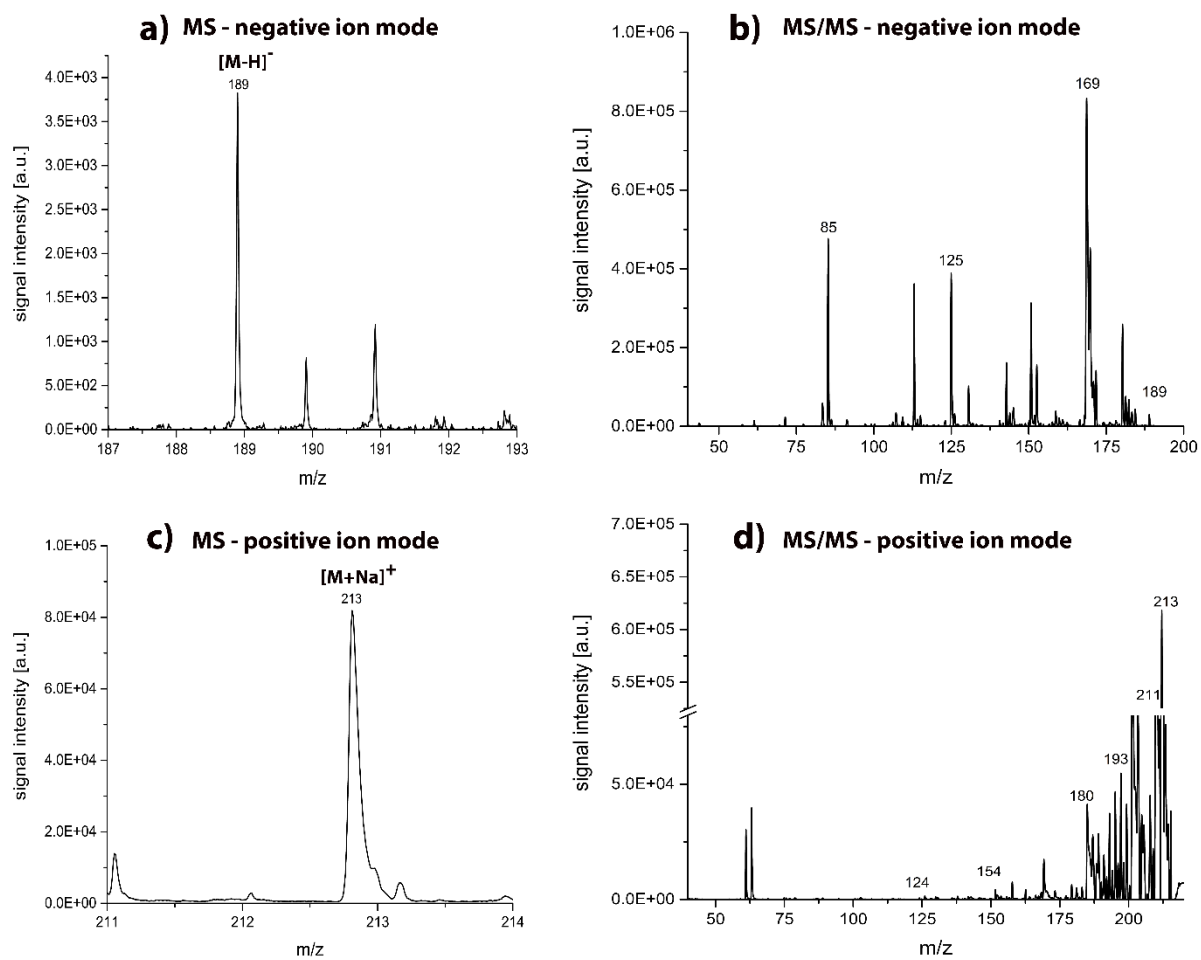
**Fig. S1** Structures of secondary metabolites identified in *Dactylis glomerata* leaves



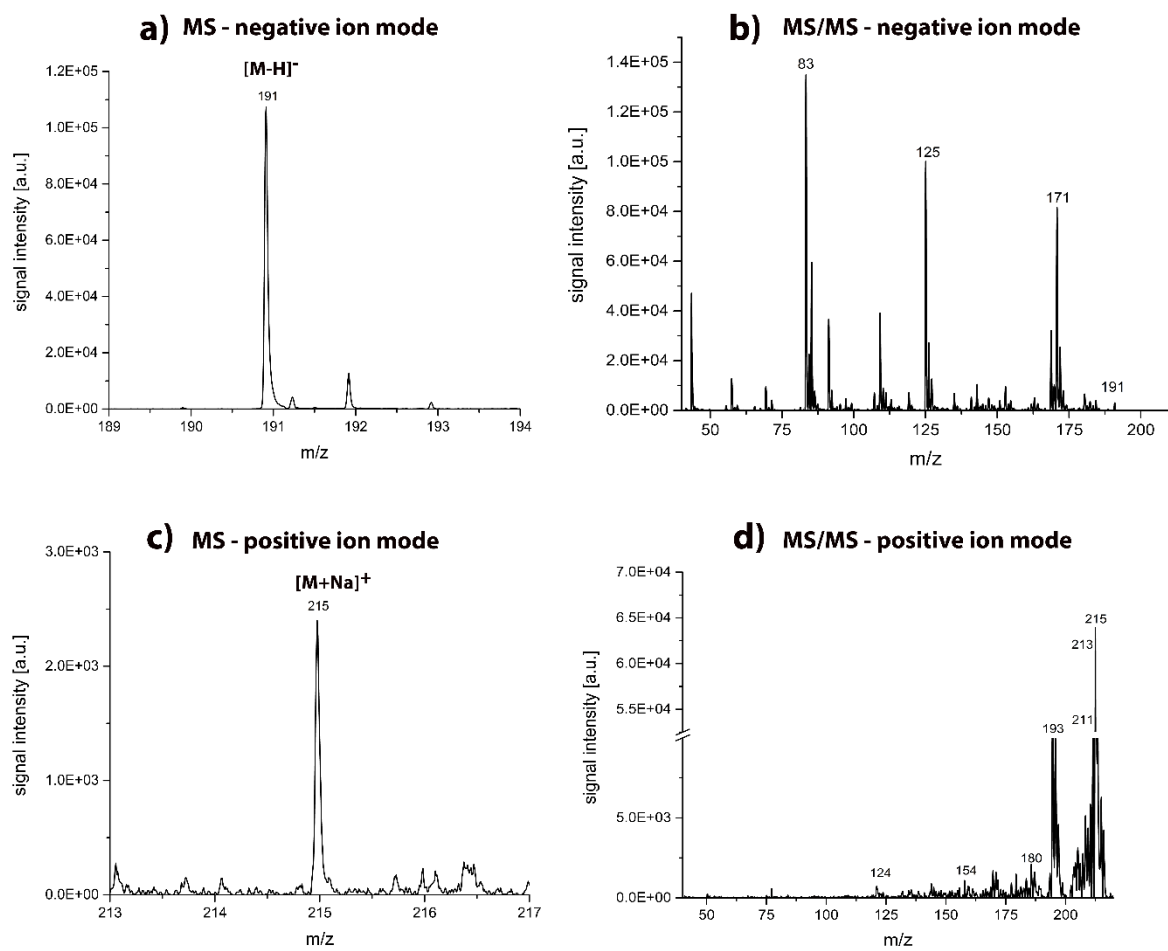
**Fig. S2** MALDI-TOF MS spectra of the reference standards **a)** 3-dehydroquinic acid, **b)** quinic acid, **c)** apigenin, **d)** luteolin, **e)** tricrin (generated as in-source decay product from the reference standard tricrin-5-glycoside), and **f)** rosmarinic acid in positive ion mode using DHB as matrix



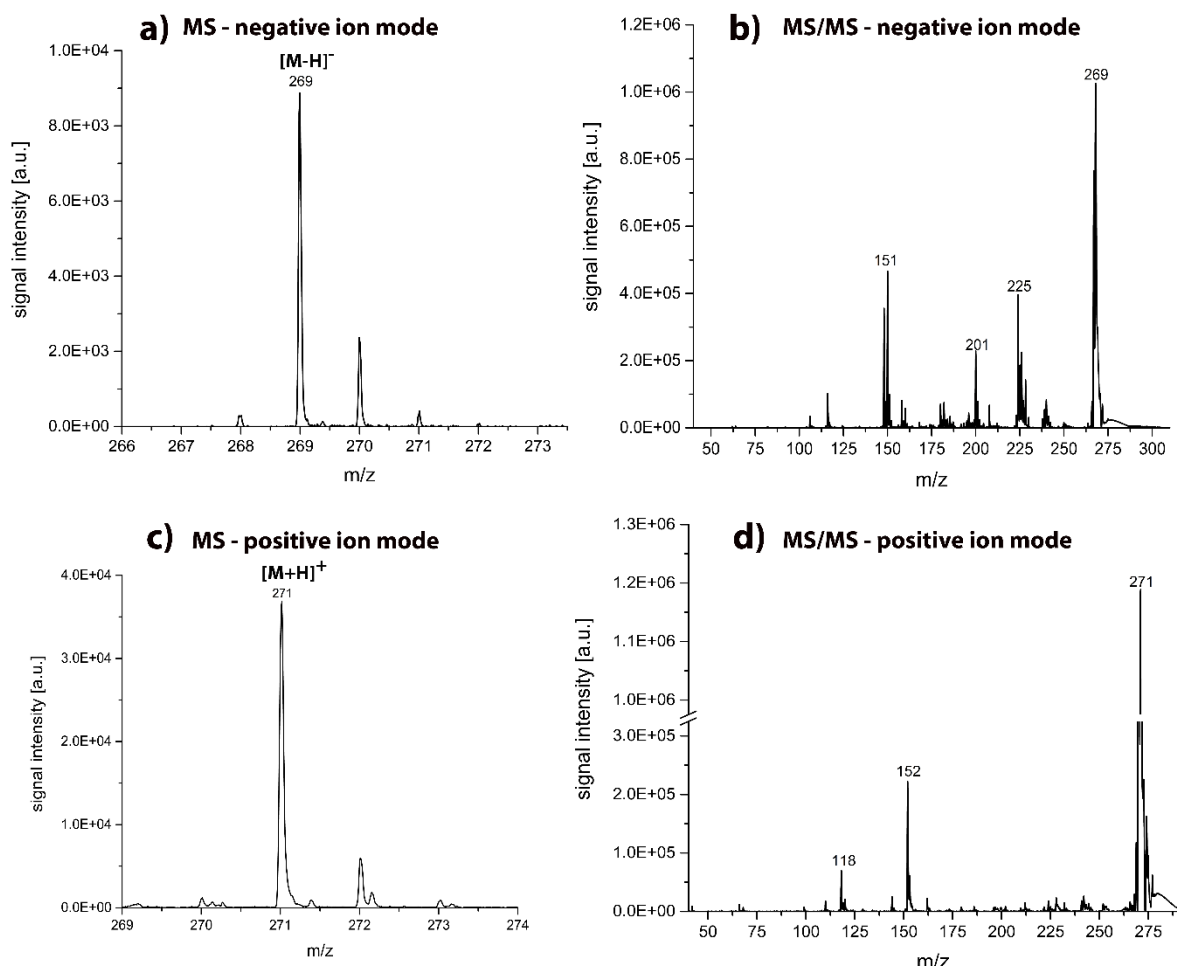
**Fig. S3** MALDI-TOF MSI dataset of a *Dactylis glomerata* leaf. **a)** Optical image taken before the matrix application, indicating two areas, from which TIC spectra were constructed, **b)** TIC spectrum from region 1, **c)** TIC spectrum from region 2. Scale bar 5 mm **a)**



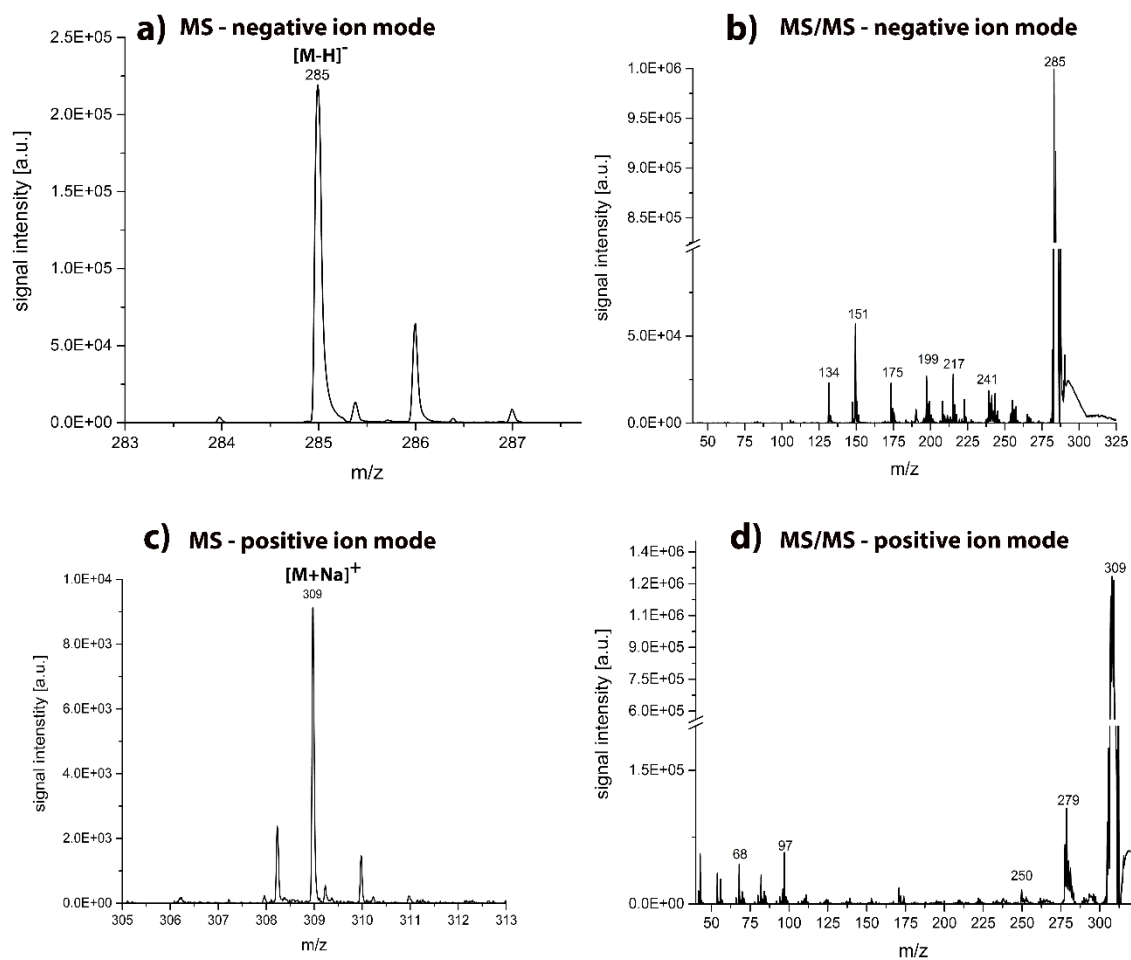
**Fig. S4** LDI-TOF MS and MS/MS spectra of the reference standard 3-dehydroquinic acid in the negative and positive ion mode, respectively



**Fig. S5** LDI-TOF MS and MS/MS spectra of the reference standard quinic acid in the negative and positive ion mode, respectively

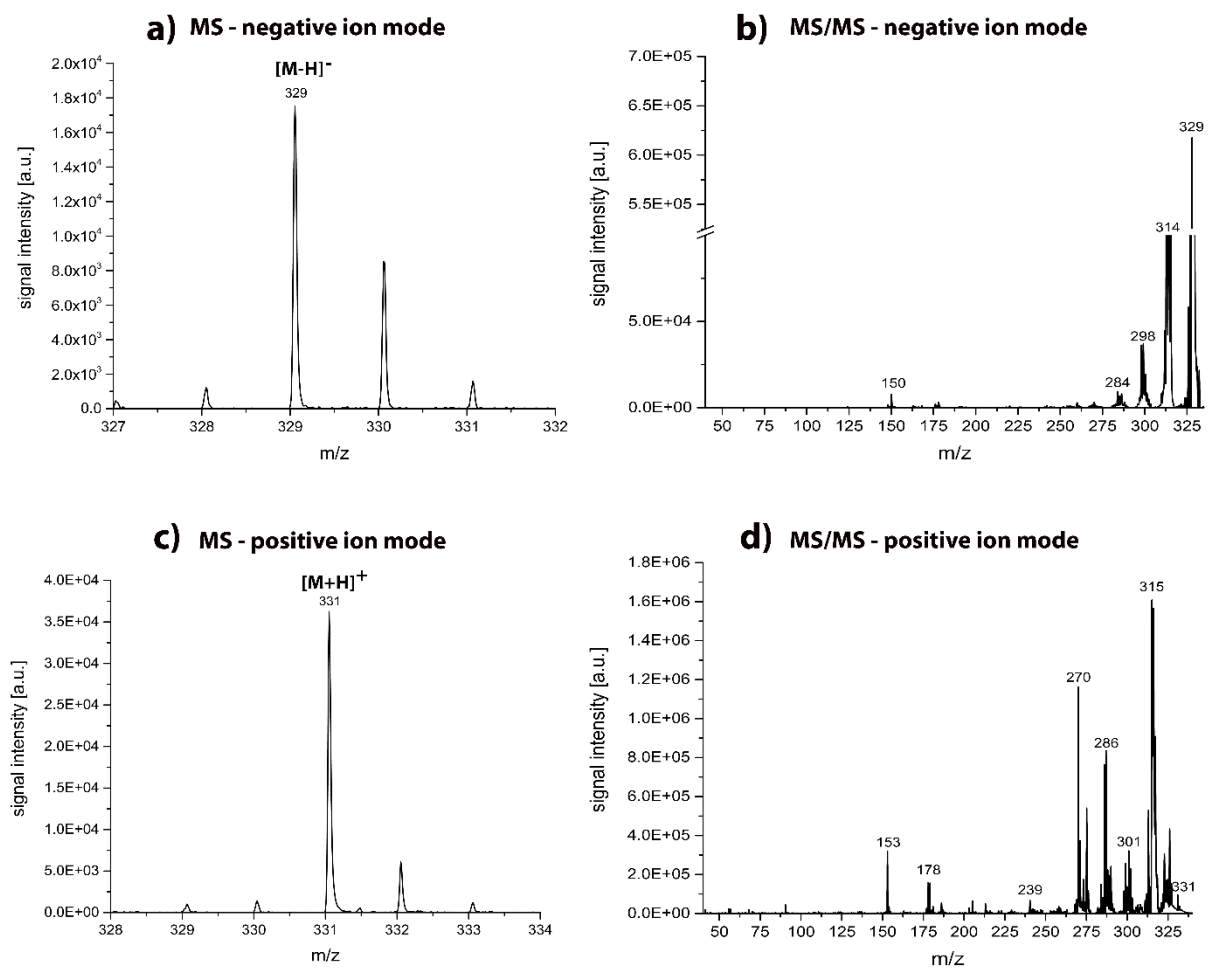


**Fig. S6** LDI-TOF MS and MS/MS spectra of the reference standard apigenin in the negative and positive ion mode, respectively

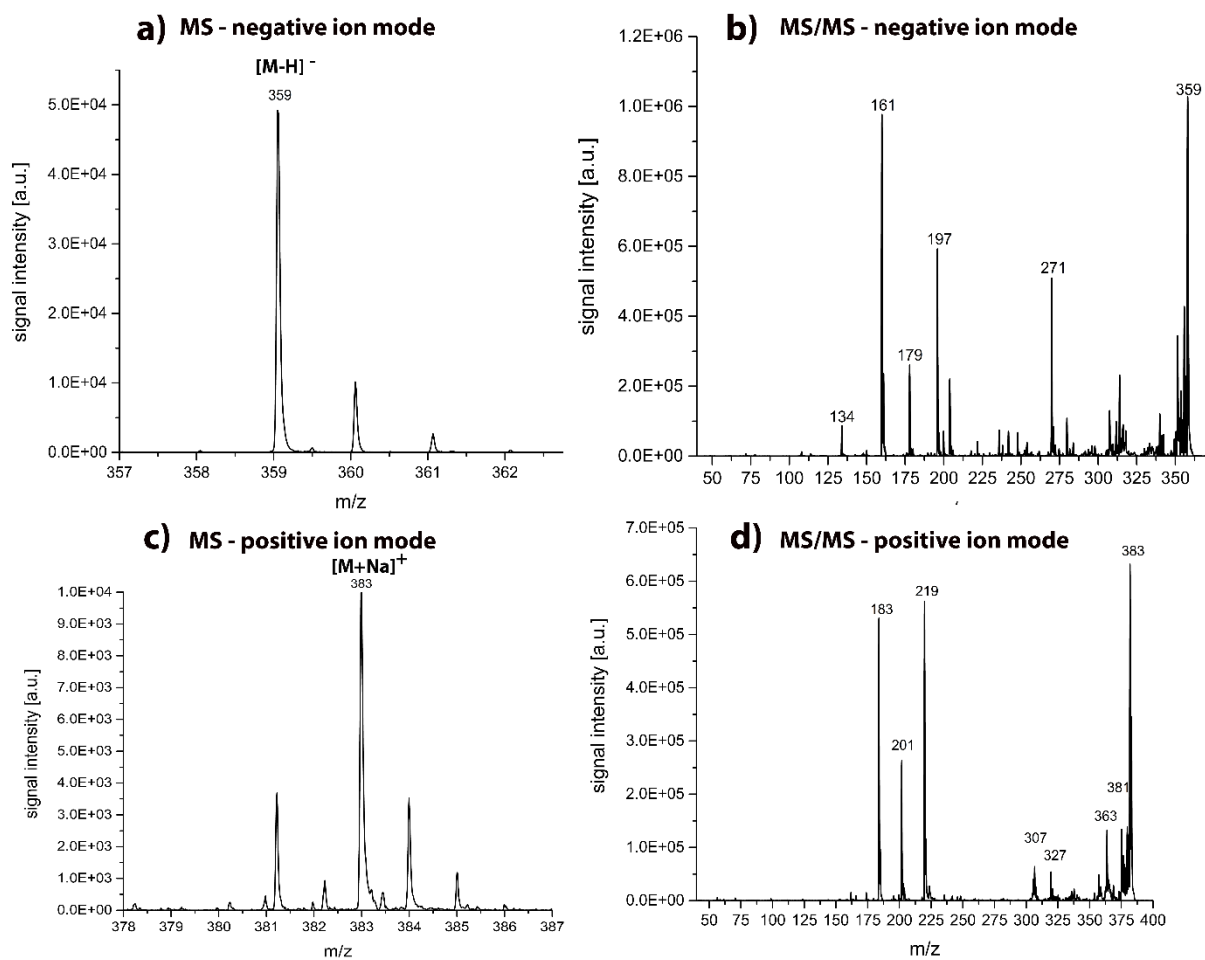


**Fig. S7** LDI-TOF MS and MS/MS spectra of the reference standard luteolin in the negative and positive ion mode, respectively

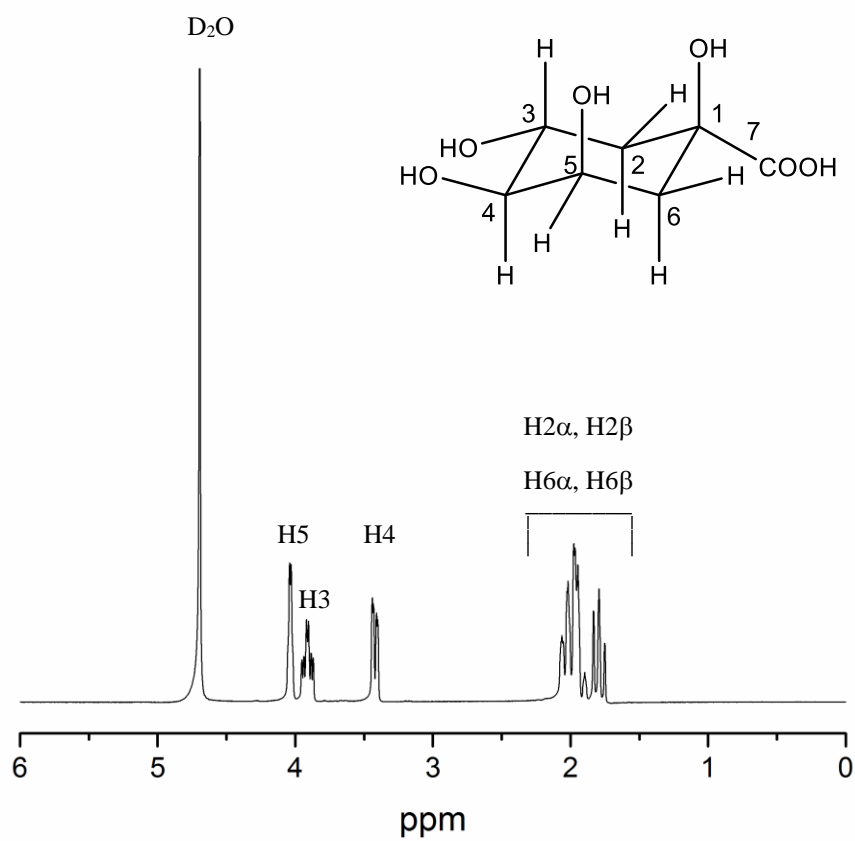




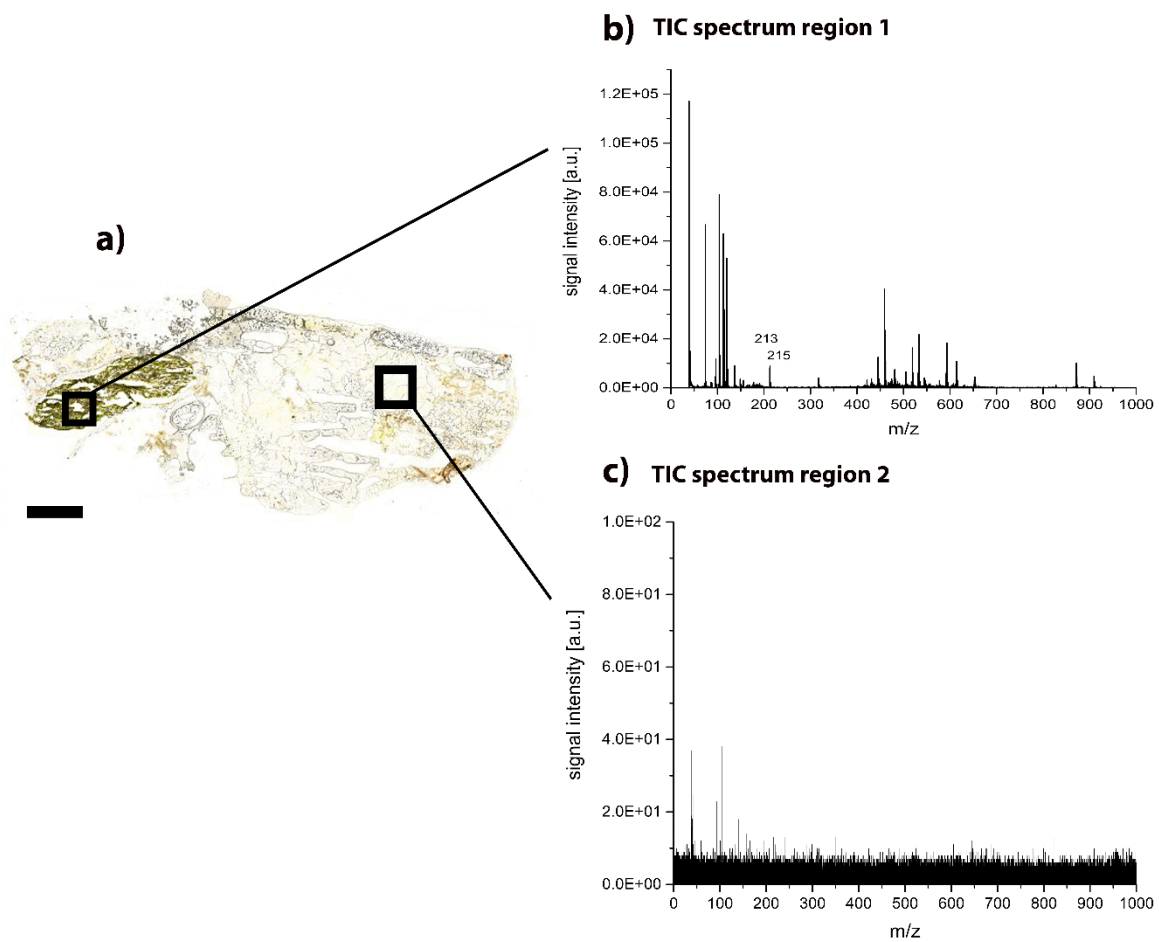
**Fig. S8** LDI-TOF MS and MS/MS spectra of tricin, generated as in-source decay product from the reference standard tricin-5-glycoside, in the negative and positive ion mode, respectively



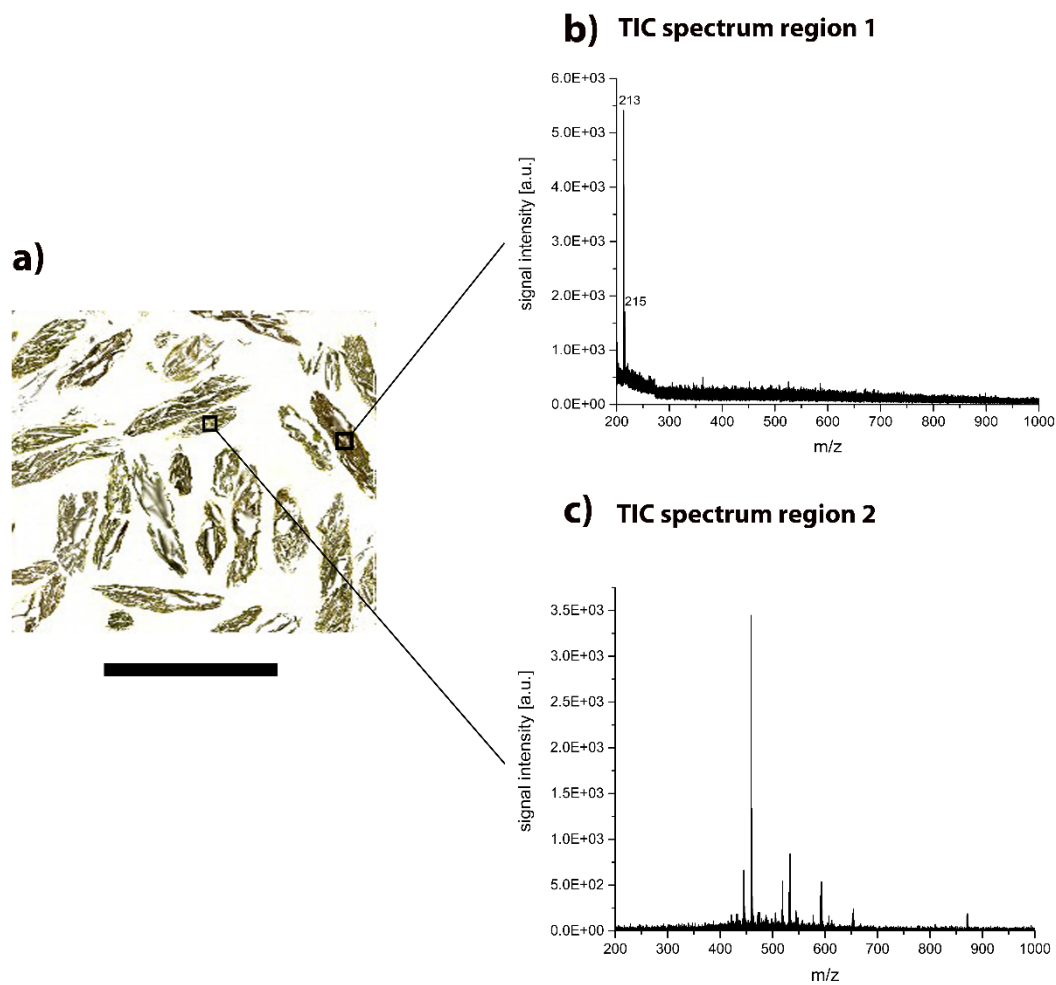
**Fig. S9** LDI-TOF MS and MS/MS spectra of the reference standard rosmarinic acid in the negative and positive ion mode, respectively



**Fig. S10**  $^1\text{H}$  NMR spectrum of the reference standard quinic acid



**Fig. S11** LDI-TOF MSI dataset of the gastrointestinal tract of a female *Chorthippus dorsatus*. **a)** Optical image indicating two areas, from which TIC spectra were constructed, **b)** TIC spectrum from region 1, **c)** TIC spectrum from region 2. Scale bar 1 mm **a)**



**Fig. S12** LDI-TOF MSI dataset of excrements of *Chorthippus dorsatus*. **a)** Optical image indicating two areas, from which TIC spectra were constructed, **b)** TIC spectrum from region 1, **c)** TIC spectrum from region 2. Scale bar 5 mm **a)**