

## SUPPLEMENTARY MATERIAL

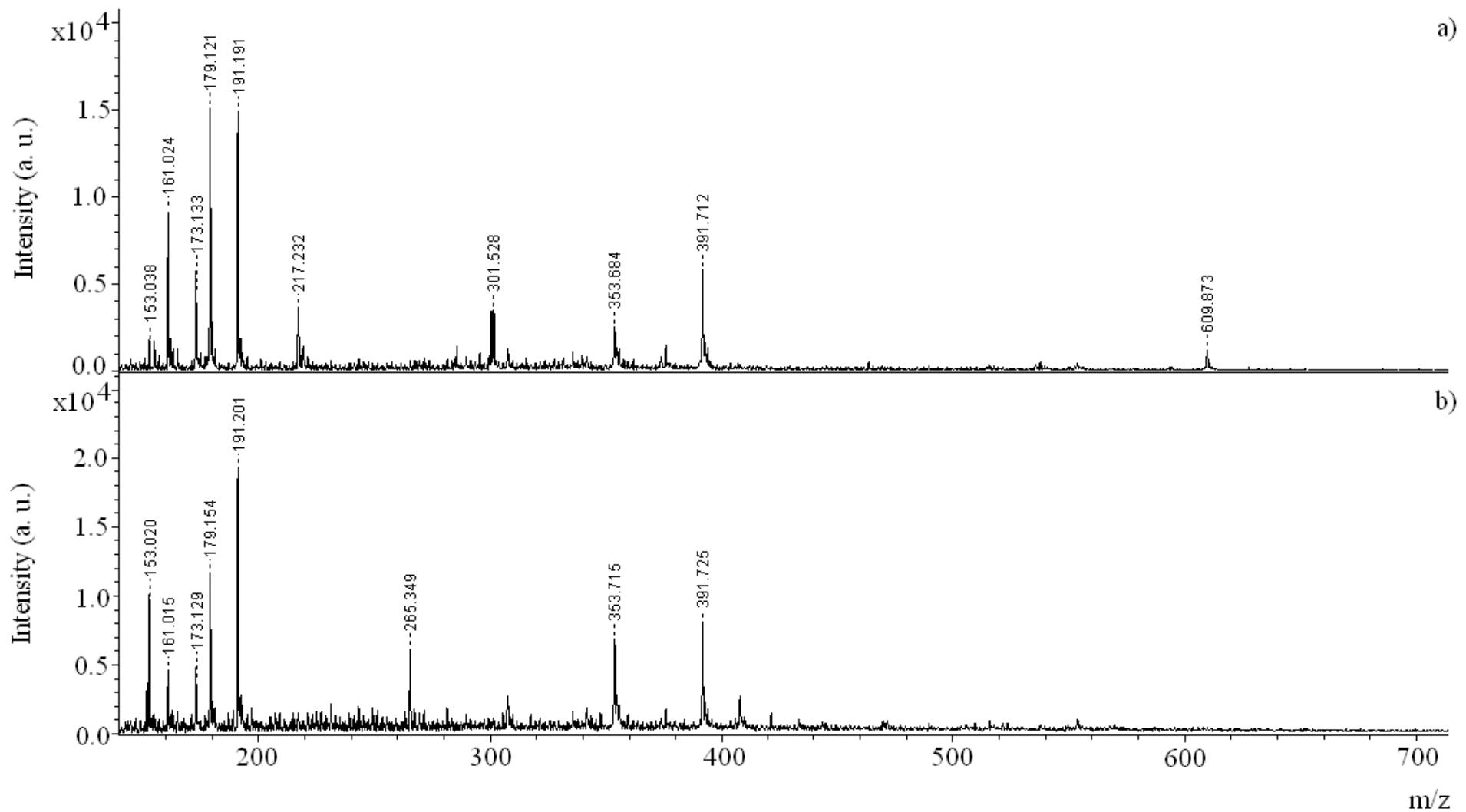
### Biospectroscopy, biospectrometry and imaging of *Ilex paraguariensis*. Basis for non-destructive quality evaluation using artificial vision

Tamara L. Parapugna<sup>1</sup>, Gabriela Petroselli<sup>2</sup>, Rosa Erra-Basells<sup>2</sup> and M. Gabriela Lagorio\*<sup>1</sup>

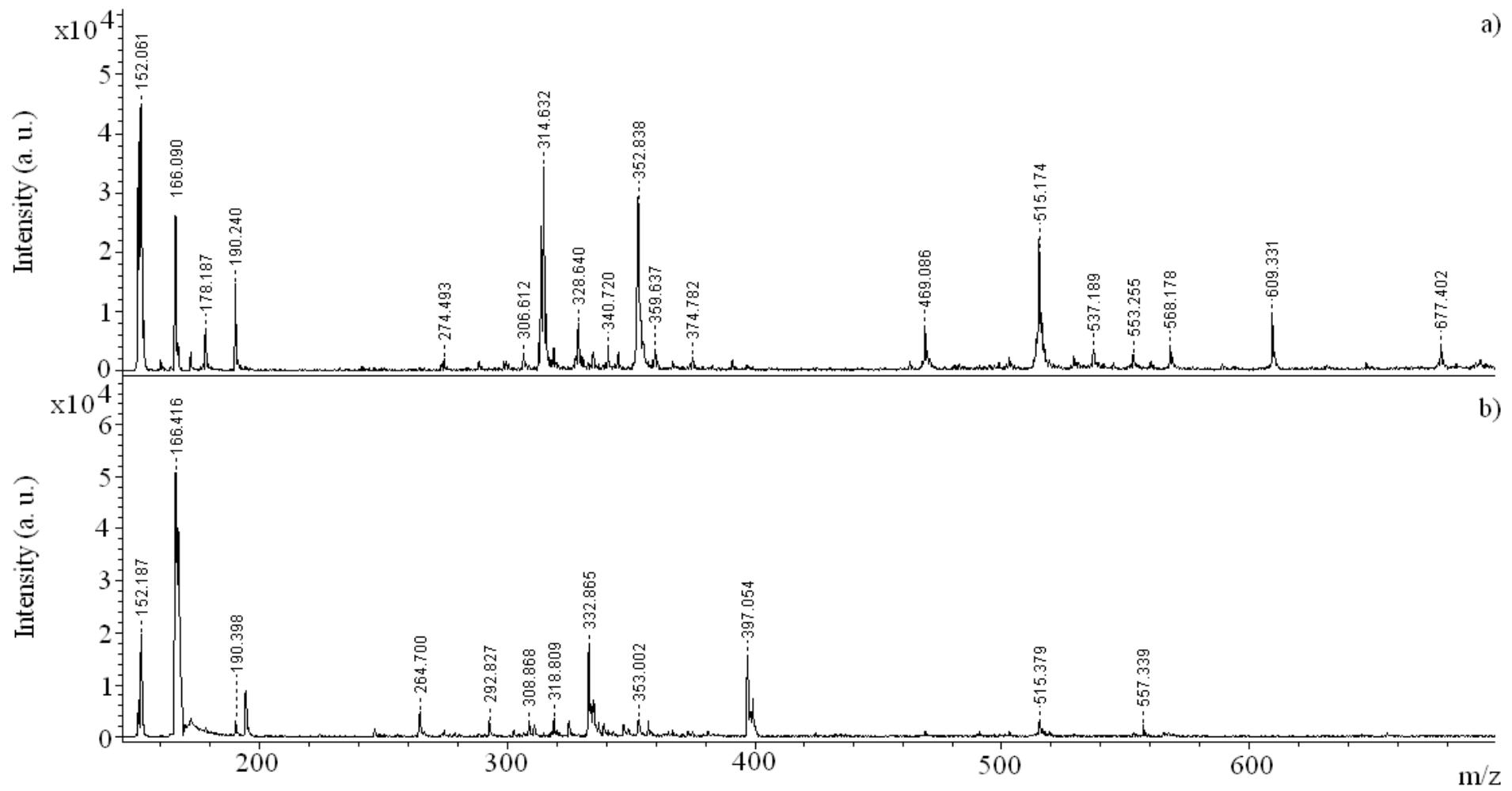
<sup>1</sup>INQUIMAE/ Dpto. de Química Inorgánica, Analítica y Química Física, Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires, Pabellón II, 1er piso, C1428EHA, Buenos Aires, Argentina.

<sup>2</sup>CIHIDECAR-CONICET/ Dpto. de Química Orgánica, Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires, Pabellón II, 3er piso, C1428EHA, Buenos Aires, Argentina.

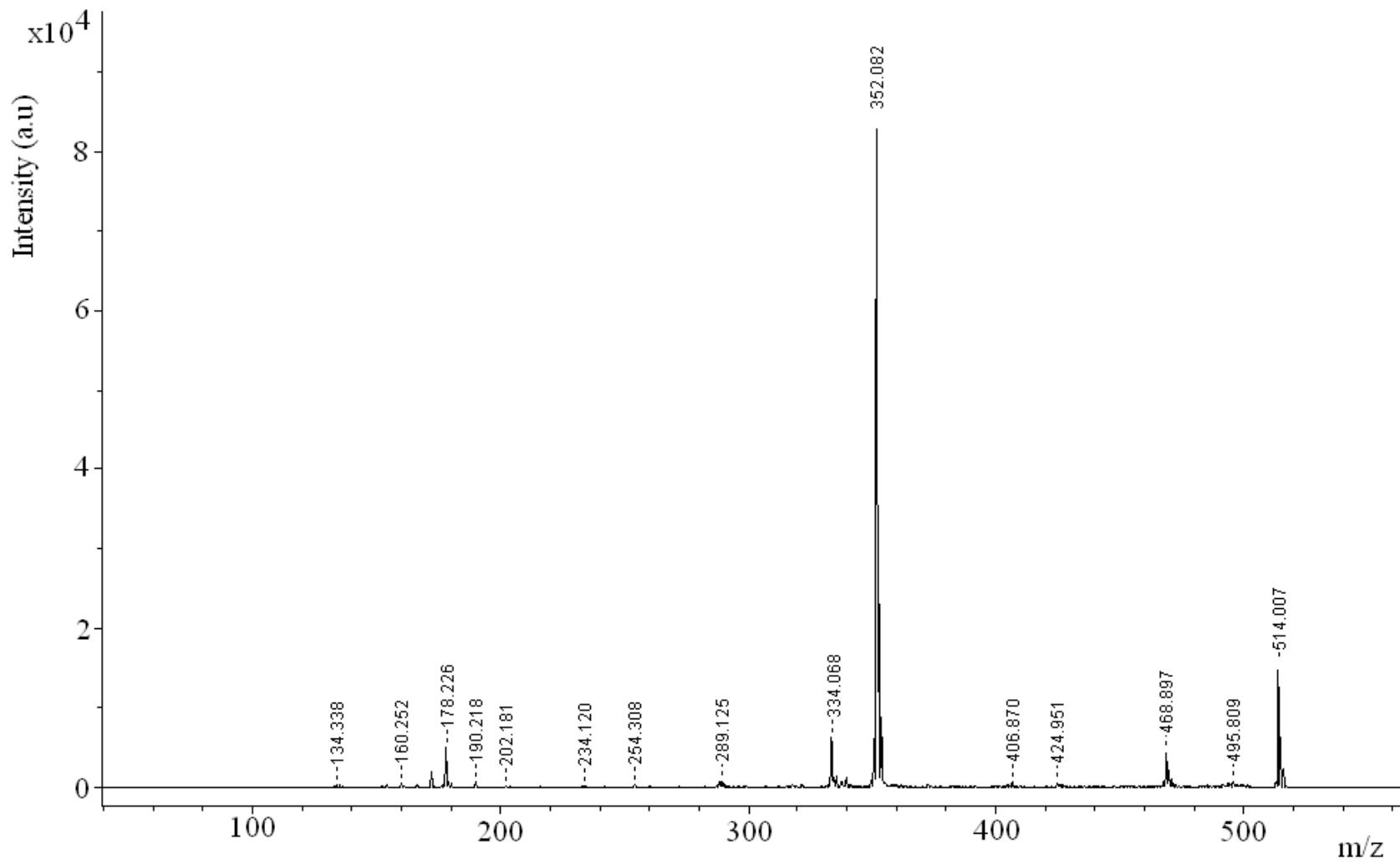
\* Corresponding author. E-mail: mgl@qi.fcen.uba.ar; Fax: +5411 4576 3341; Tel: +5411 4576 3378 ext. 106



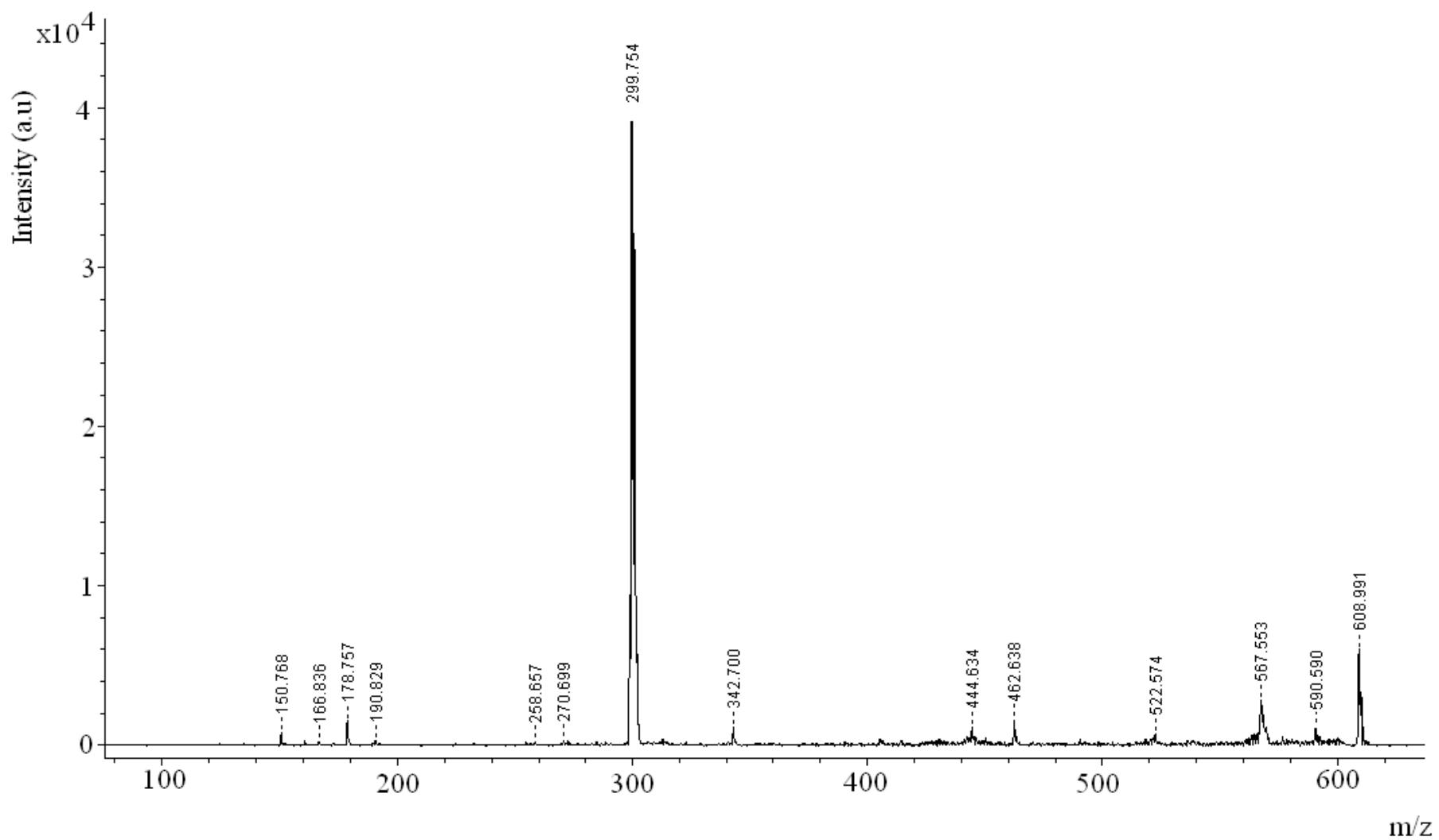
**Figure S1.** UV-LDI mass spectra of a) leaves and b) sticks pulverized (smashed) in a mortar. Negative ion mode.



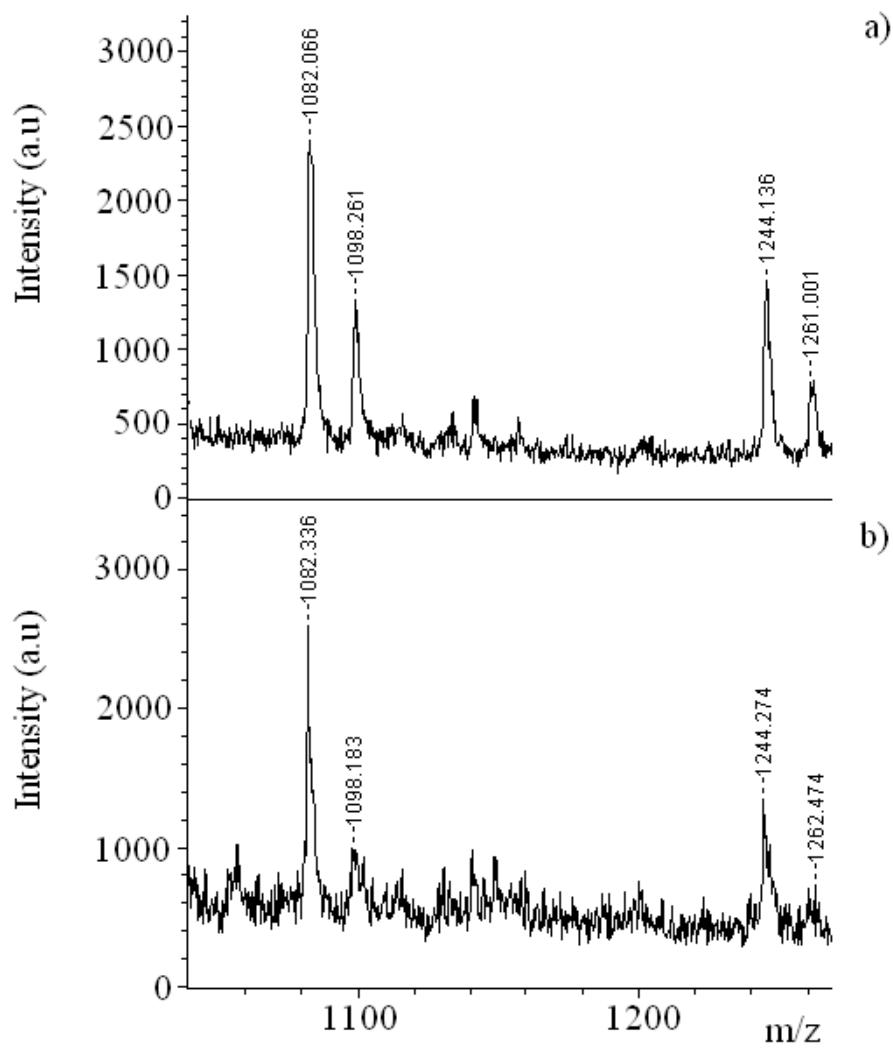
**Figure S2.** UV-MALDI mass spectra of hot water infusions from a) leaves and b) sticks. Matrix: nHo. Negative ion mode.



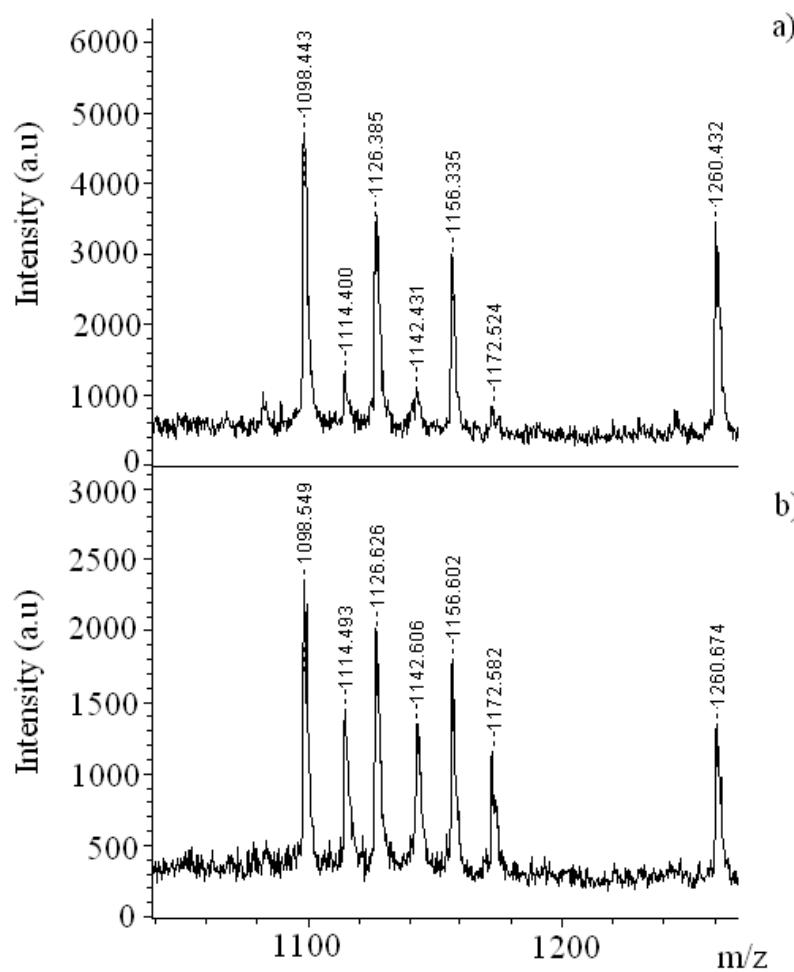
**Figure S3.** UV-MALDI MS/MS spectrum of precursor ion m/z 514.007 ([3,4-dicaffeoylquinic acid-H]<sup>-</sup>) from leaves sample (smashed in a mortar). Matrix: nHo. Negative ion mode.



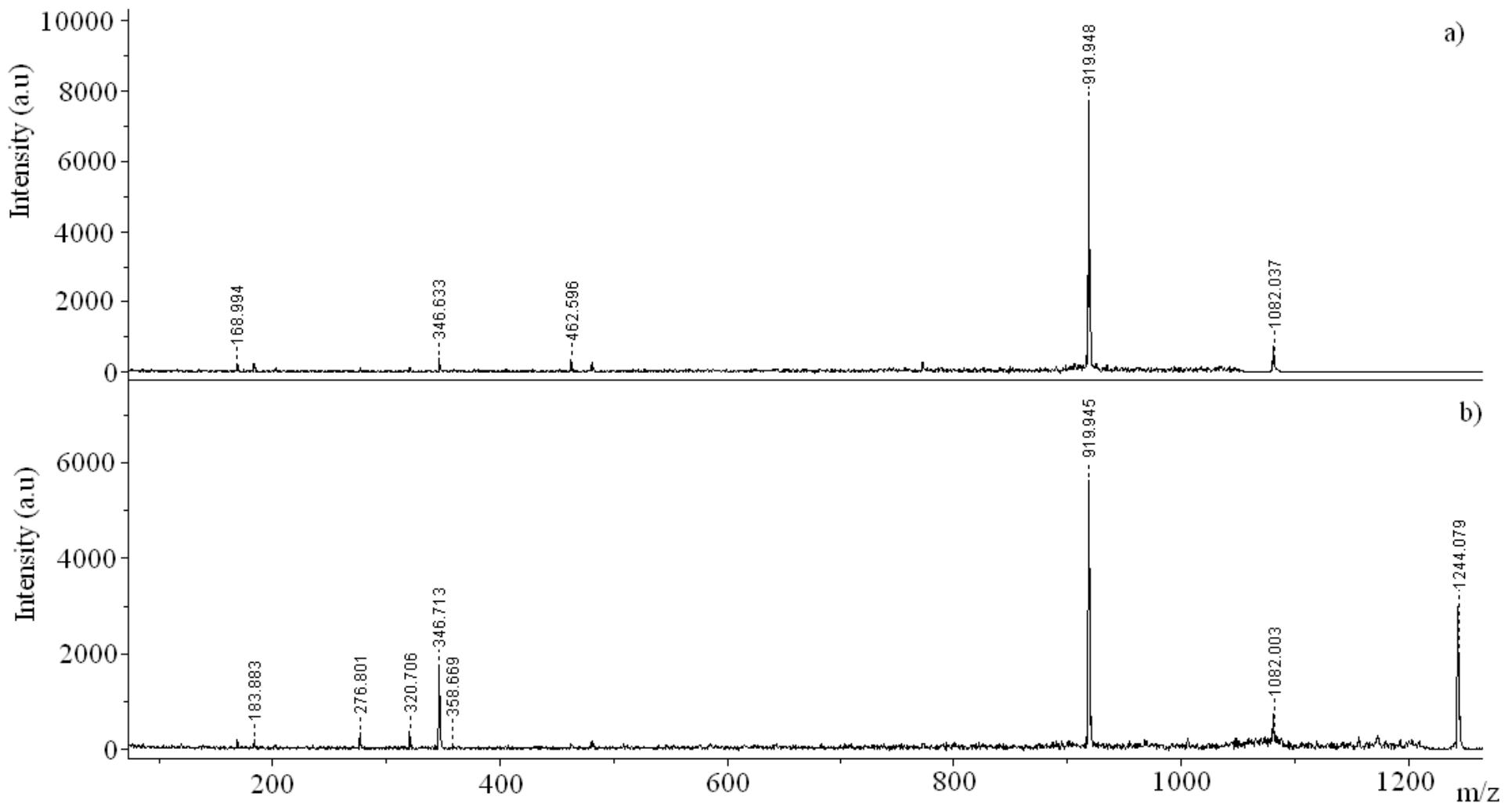
**Figure S4.** UV-MALDI MS/MS spectrum of precursor ion m/z 608.991 ([rutin-H]<sup>-</sup>) from leaves sample (smashed in a mortar). Matrix: nHo. Negative ion mode.



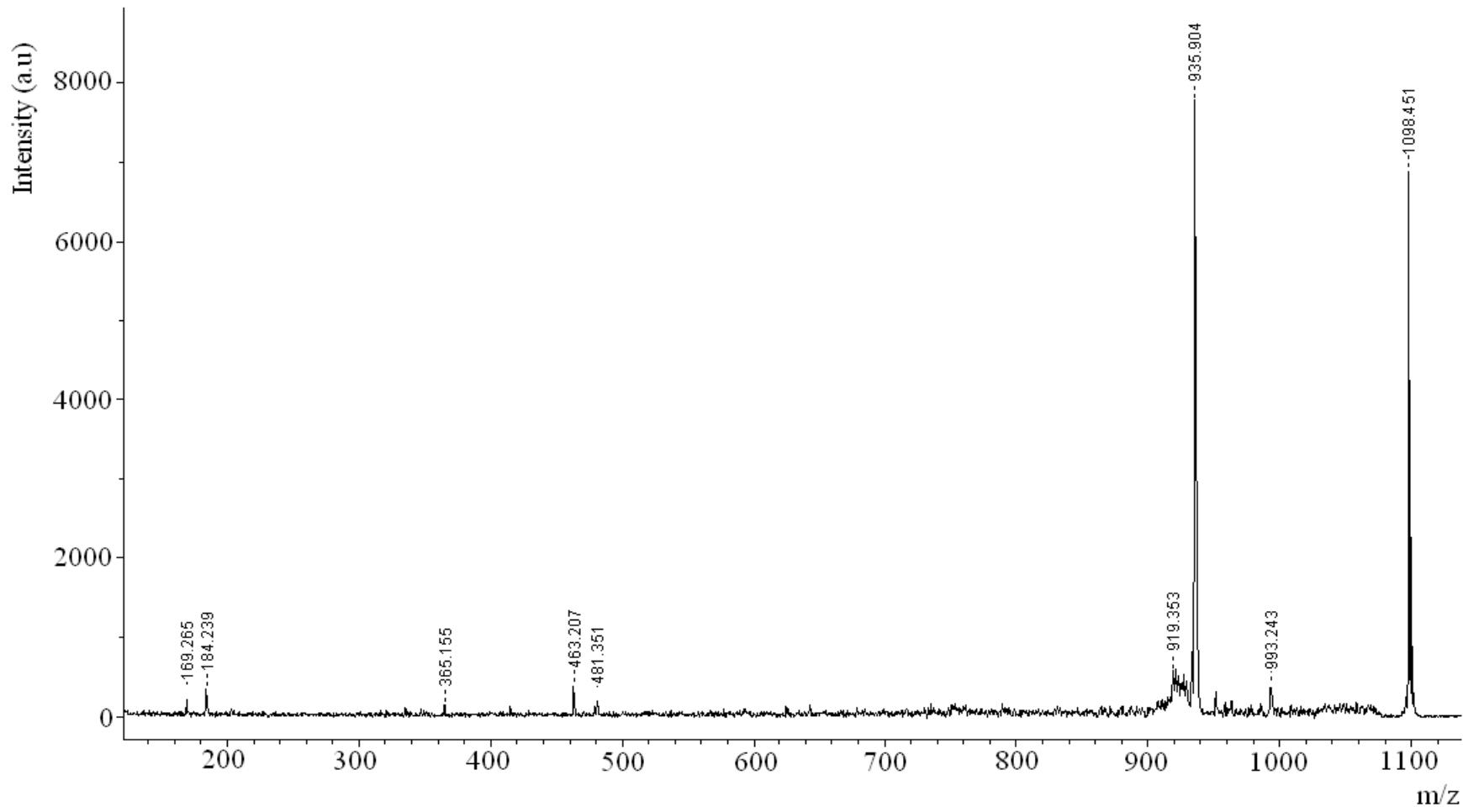
**Figure S5.** UV-MALDI mass spectra of leaves a) smashed in a mortar; b) hot water infusion. Matrix: nHo. Positive ion mode.



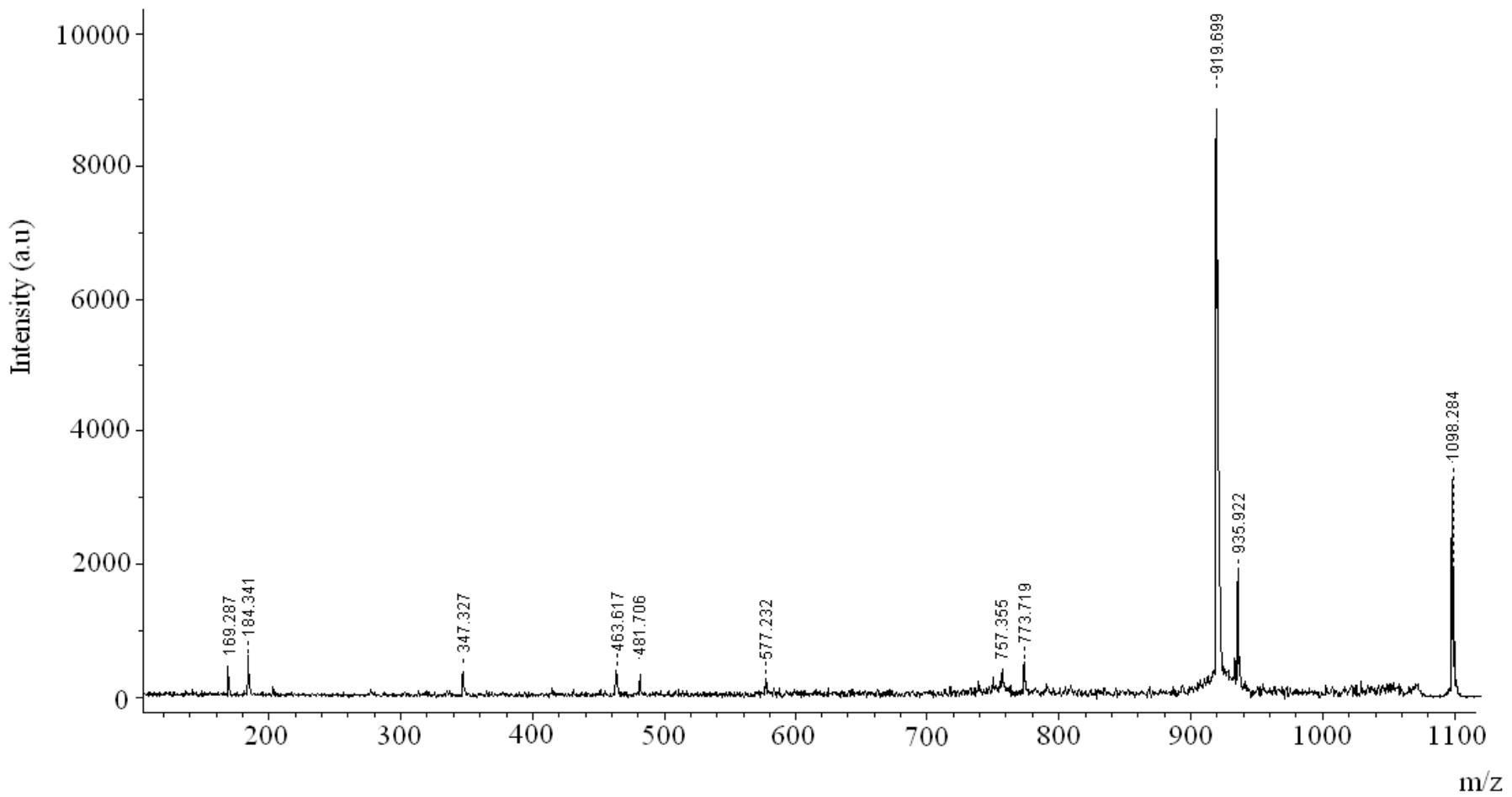
**Figure S6.** UV-MALDI mass spectra of sticks a) smashed in a mortar; b) hot water infusion. Matrix: nHo. Positive ion mode.



**Figure S7.** UV-MALDI MS/MS spectra of precursor ions a)  $m/z$  1082.037 ([metasaponine 2 + Na] $^+$ ) and b)  $m/z$  1244.079 ([metasaponine 4 + Na] $^+$ ) from leaves sample (smashed in a mortar). Matrix: nHo. Positive ion mode.



**Figure S8.** UV-MALDI MS/MS spectrum of precursor ion  $m/z$  1098.451 ([metasaponine 3 + Na] $^+$ ) from sticks sample (smashed in a mortar). Matrix: nHo. Positive ion mode.



**Figure S9.** UV-MALDI MS/MS spectrum of precursor ion  $m/z$  1098.284 ([metasaponine 3\* + Na] $^+$ ) from leaves sample (smashed in a mortar). Matrix: nHo. Positive ion mode.