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SPATIAL DISTRIBUTION AND COMPARTMENTALIZATION OF CYCLOPEPTIDES AND 4-QUINOLONE ALKALOIDS IN WALTHERIA INDICA REVEALED BY MALDI-MSI

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Waltheria indica L. (Malvaceae) is a pantropical shrub ("broom") distributed throughout the Americas (Mexico-Brazil), West Africa, Southeast Asia, and Australia, frequently cited as an invasive species. In this study, we investigated the spatial distribution of 4-quinolone and cyclopeptide alkaloids in stems, leaves, and roots using MALDI–Mass Spectrometry Imaging (MALDI-MSI), a technique that enables direct metabolite mapping within tissues while requiring minimal biomass. Plant sections (50 µm) were prepared, coated with 2,5-dihydroxybenzoic acid (DHB), and analyzed in positive mode (MALDI-TOF/TOF, Bruker). In stems, 4-quinolones predominated in the xylem, including 2-hydroxymethyl-waltherione C or 10-hydroxy-waltherione C (*m/z* 364.1544), 8-hydroxy-waltherione M + Na^+ or waltherione O + Na^+ (*m/z* 378.204), 11-hydroxy-waltherione F + Na^+ (*m/z* 370.1989), waltherione P + Na^+ (*m/z* 376.1883), waltherione V or 11-dehydroxy-waltherione A (*m/z* 378.1700), walindicaone E (*m/z* 380.186), waltherione A or waltherione B (*m/z* 394.1577), melovinone (*m/z* 396.499), waltherione A + Na^+ (*m/z* 416.1468), waltherione H + Na^+ (*m/z* 422.2302), and waltherione D (*m/z* 512.1921). Most showed higher intensity in the xylem, with additional signals in the phloem and cortex. In leaves, no alkaloids were detected in the blade, but lateral sections revealed waltherione P + Na^+ throughout the lamina but absent from the central region. Cyclopeptides, including adouetine Y' or waltherine A (*m/z* 535.3200), appeared in scattered foci. In roots, alkaloids concentrated mainly in the cortex and endodermis: 10-hydroxy-waltherione C or 2-hydroxymethyl-waltherione C, waltherione V or 11-dehydroxy-waltherione A, 8-hydroxy-waltherione M + Na^+ or waltherione O + Na^+, and waltherione A or waltherione B. Waltherione P + Na^+ was also detected across vascular tissues, while waltherione U + Na^+ (*m/z* 414.1676) was distributed throughout the root, with highest abundance in the cortex. Overall, MALDI-MSI revealed tissue-specific localization and compartmentalization of alkaloids in *W. indica*, highlighting differences among organs and metabolite classes. These findings provide insights into the biosynthesis and ecological functions of these compounds, particularly their potential roles in chemical defense, intercellular signaling, and storage. This study contributes to sustainable use and understanding of plant chemical diversity, supporting Sustainable Development Goals(SDG) 3 (Good Health and Well-Being) and 15 (Life on Land).

Keywords: *Waltheria indica; MALDI-MSI; 4-quinolone alkaloids; cyclopeptide alkaloids; SDG 15*