

Supporting Information

Understanding the molecular signatures in leaves and flowers by
desorption electrospray ionization mass spectrometry (DESI MS)
imaging

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Table S1. Tandem mass spectral data of surface-bound co-existing metabolites in Madagascar periwinkle - *Catharanthus roseus* (L.) G. Don.

S.No.	Molecular Weight	KEGG (Kyoto Encyclopedia of Genes and Genomes) Structure and ID*	<i>m/z</i>	MS/MS data matching with literature ¹⁷⁻²¹	PubChem ID**
1.	336.4275	 C09107	337	Catharanthine	197771
2.	348.3951	 C09241	349	Serpentine	73391
3.	382.4528	 C11812	383	Lochnerinine	443417

4.	396.4794	<p>C11784</p>	397	Echitovenine	443402
5.	398.4953	<p>C02673</p>	399	Deacetoxy vindoline	439783
6.	456.5314	<p>C01626</p>	457	Vindoline	16596
7.	530.5669	<p>C03470</p>	531	Strictosidine	161336
8.	792.9588	<p>C11641</p>	793	Anhydro vinblastine	443324
9.	810.9741	<p>C07201</p>	811	Vinblastine	241903

Additional data (namely compound information including chemical and physical properties, 2D and 3D structures, reactions and pathways of formation, similar compounds, related synthetic substances, pharmacology, biomedical effects and toxicity data, etc.) of the compounds investigated in this study can be had using * KEGG ID and ** PubChem ID. ^{21,22} The references are quoted in the main text.

Figure S1

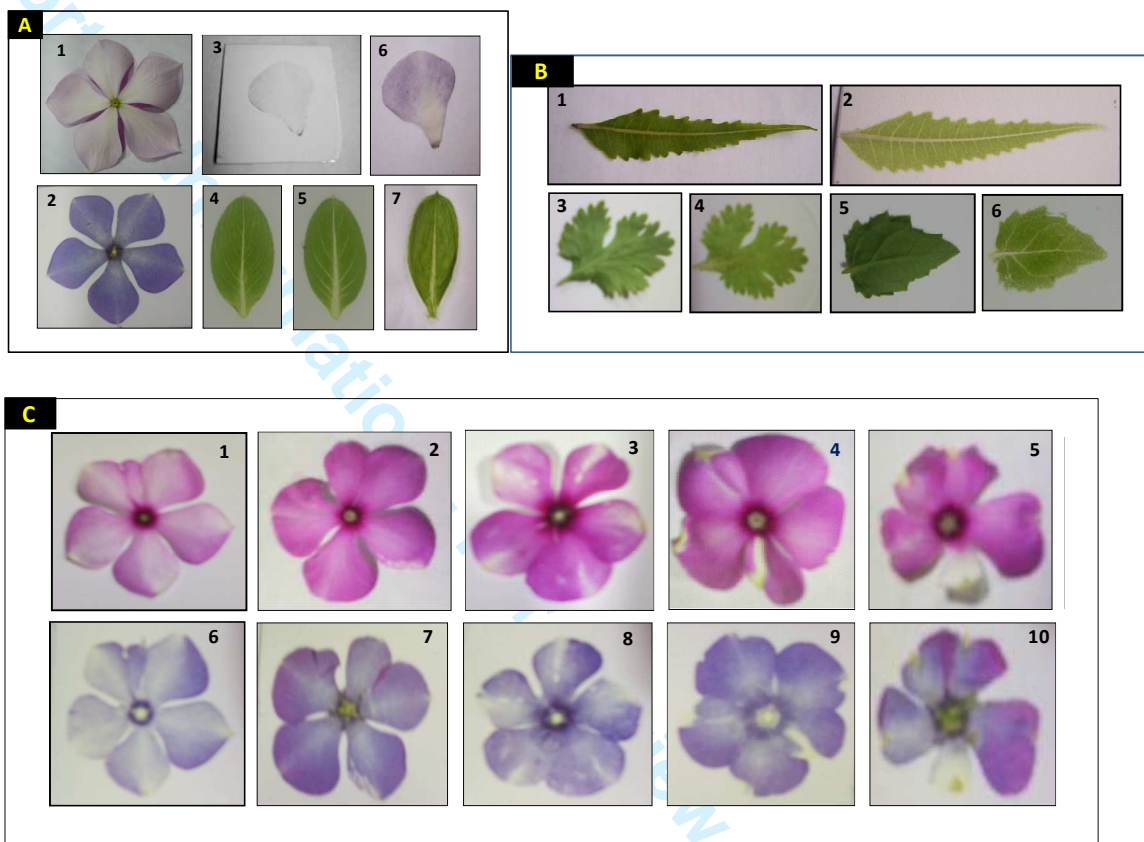


Figure S1A. Madagascar periwinkle-(*Catharanthus roseus* (L.) G. Don). (1) Photograph of lower surface of flower, TLC-imprint of (2) upper surface of flower. (3) lower surface of flower petal, (4) upper surface of leaf (5) lower surface of leaf, Thin membrane after imprinting in (6) flower petal (7) leaf

Figure S1B. (1) Photograph of leaf of neem (*Azadirachta indica* A. Juss.), (2) TLC-imprint of upper surface of neem leaf, (3) Photograph of leaf of Coriander (*Coriandrum sativum* L.), (4) TLC-imprint of coriander leaf, (5) Photograph of leaf of Patchouli (*Pogostemon cablin* (Blanco) Benth.), (6) TLC-imprint of patchouli leaf.

Figure S1C. (a) Photographs showing five different conditions (changes in size and shape) of the atrophied flowers in *C.roseus* during environmental stress.

Figure S2

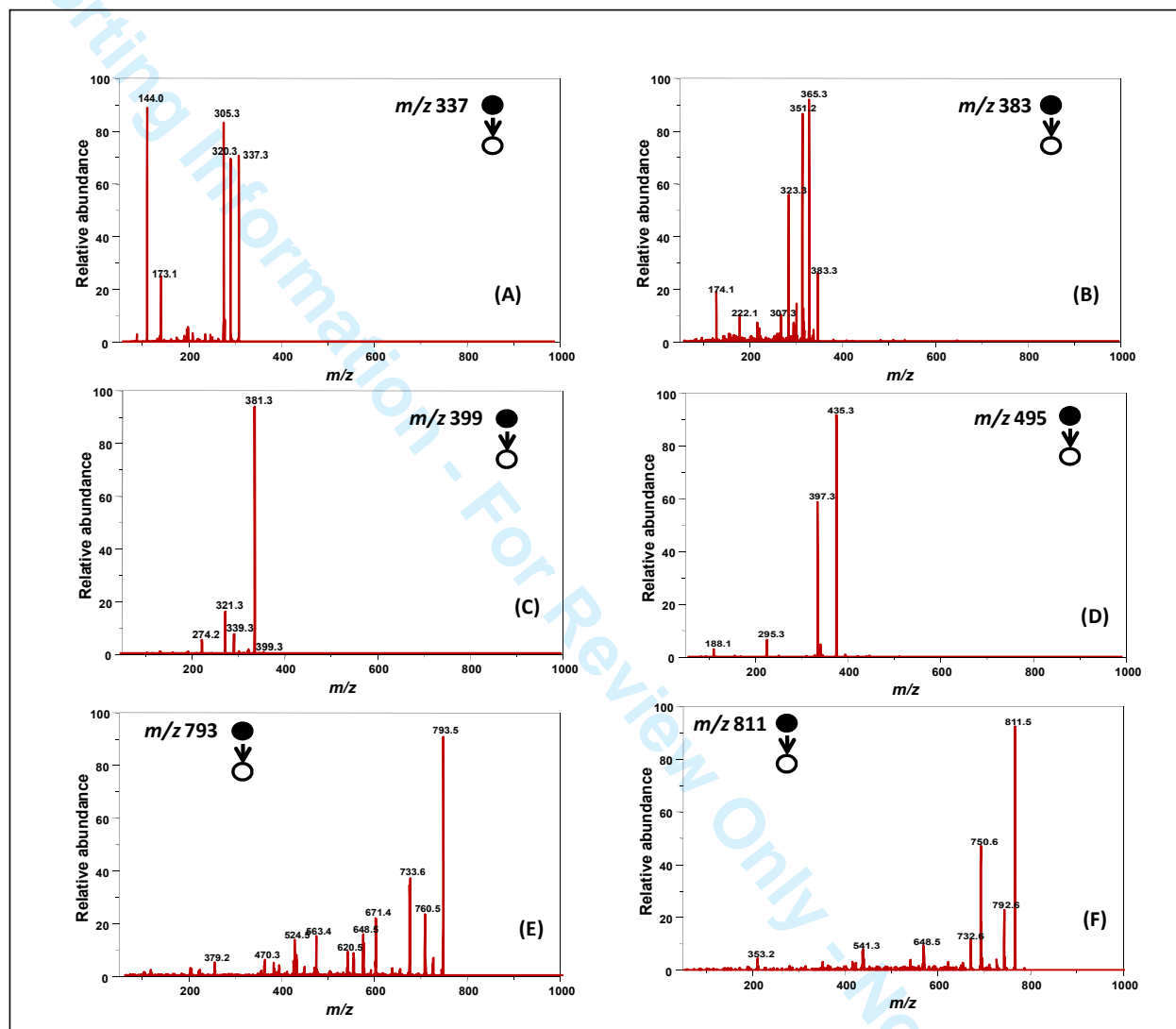


Figure S2. ESI MS tandem mass spectra for (A) m/z 337 (B) m/z 383 (C) m/z 399 (D) m/z 495 (E) m/z 793 (F) m/z 811.

Figure S3

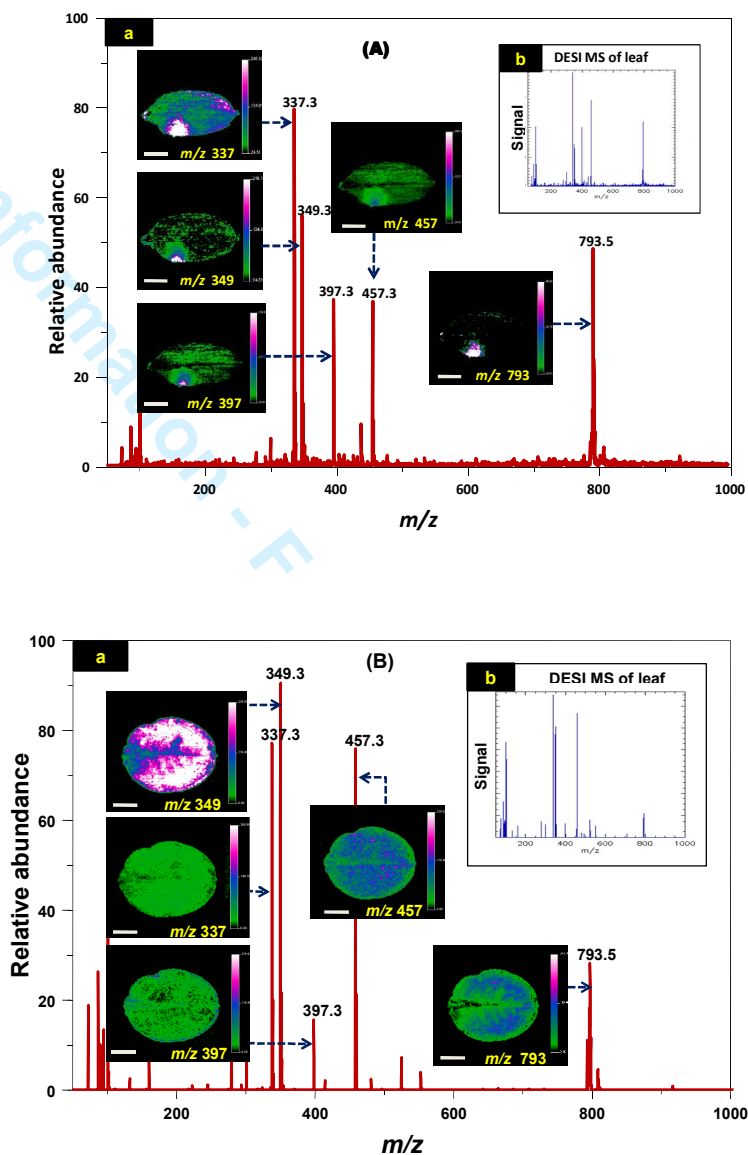
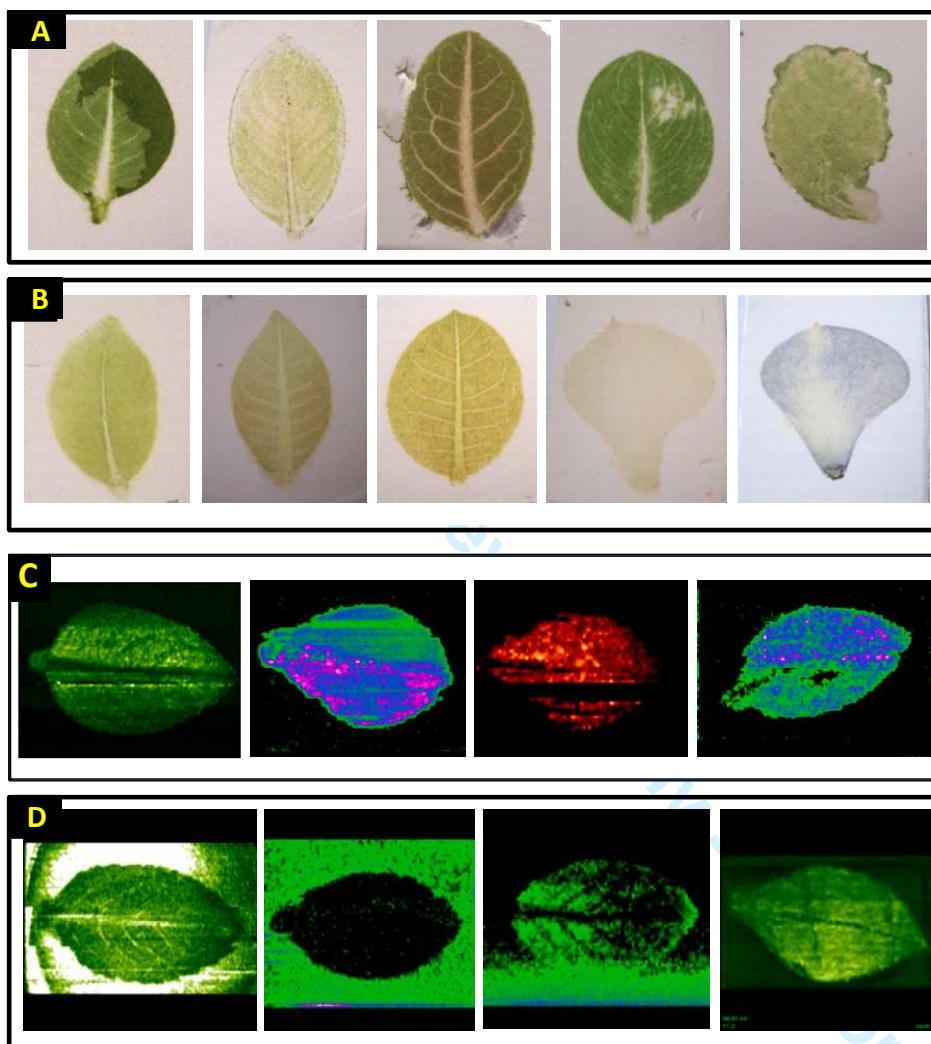


Figure S3. ESI MS spectrum and DESI MS images showing the distribution of selected alkaloids during (A) Leaf spot disease on leaf and (B) Aphid attack on leaf of *C.roseus*. A(a) ESI MS spectrum, (b) One of the DESI MS spectra collected from the infected leaf during imaging

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corresponding to one pixel ($400\mu\text{m}^2$) of the image. Similar data for aphid attacked leaf is shown in B. Images corresponding to various peaks are shown. The scale is uniform in all the images (5mm).

Figure S4



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Figure S4. Photographs showing (A) defective TLC- imprints due to possible manual errors in pressing and (B) loss of color in TLC- imprints on storage. DESI MS images showing the defects due to (C) instrument setup error and (D) interfering impurity peaks.