Supplementary information

Electrospun Nanofiber Mats as "Smart Surfaces" for Desorption Electrospray Ionization Mass Spectrometry (DESI MS) based Analysis and Imprint imaging

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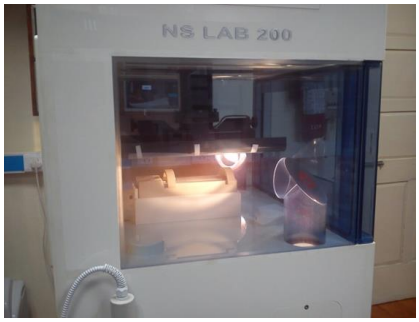


NF - VideoS1.avi (Command Line)

Video S1- Preparation of nanofiber mat by needleless electrospinning as observed using the instrument, Nanospider (NS LAB 200).

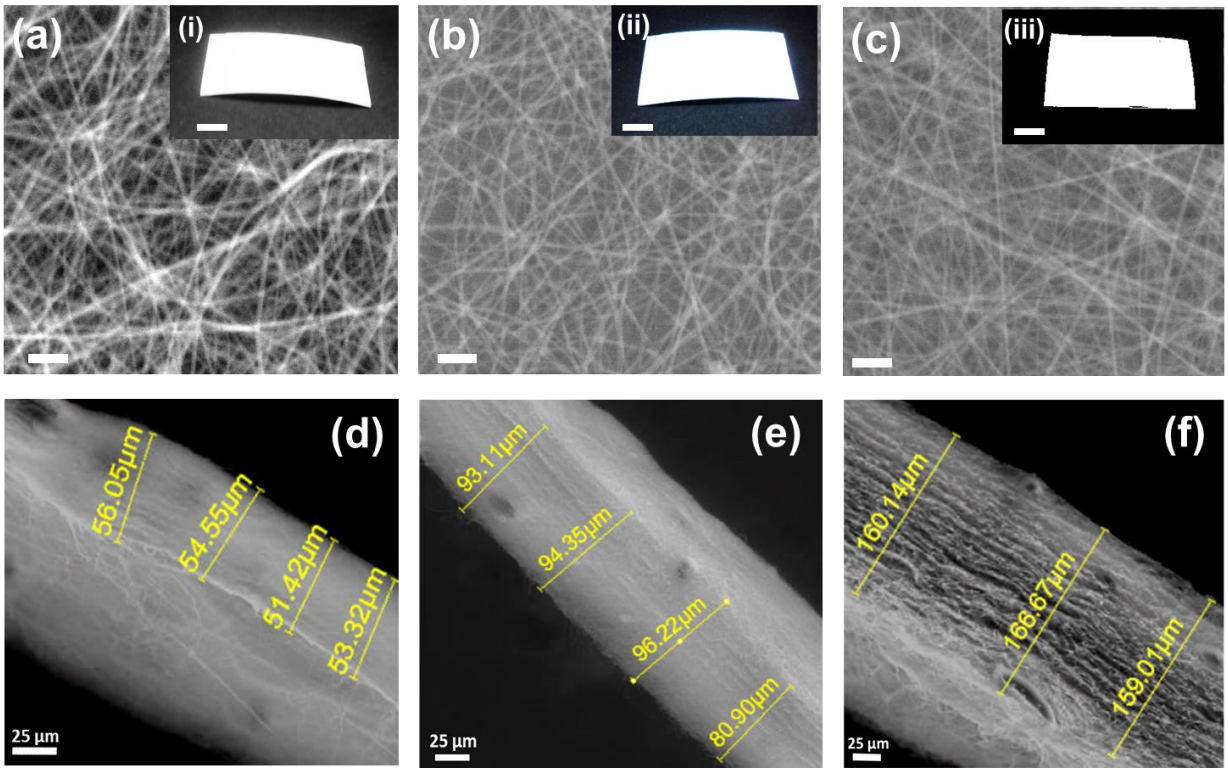


Figure S1. (a, b and c). SEM images and corresponding photographs (i, ii, iii) of electrospun nanofibers using three different concentrations (18, 16 and 12% (w/w) of nylon-6. The scale in SEM images (a-c) is 5 µm and in the insets is 5 mm.

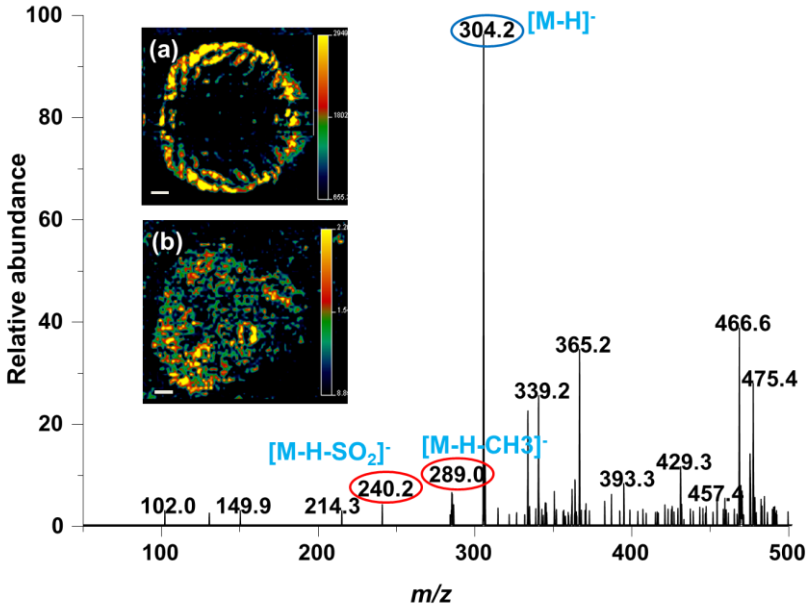


Figure S2. DESI MS spectrum showing discoloration/degradation of methyl orange (MO) spot on TLC-plate during storage under ambient conditions. (a,b) DESI MS image showing the spatial distribution of halo and the interior regions during degradation of spot of methyl orange. Encircled peaks are the degradation products corresponding to the peak at *m/z* 304. The scale in all DESI MS images is 5 mm.

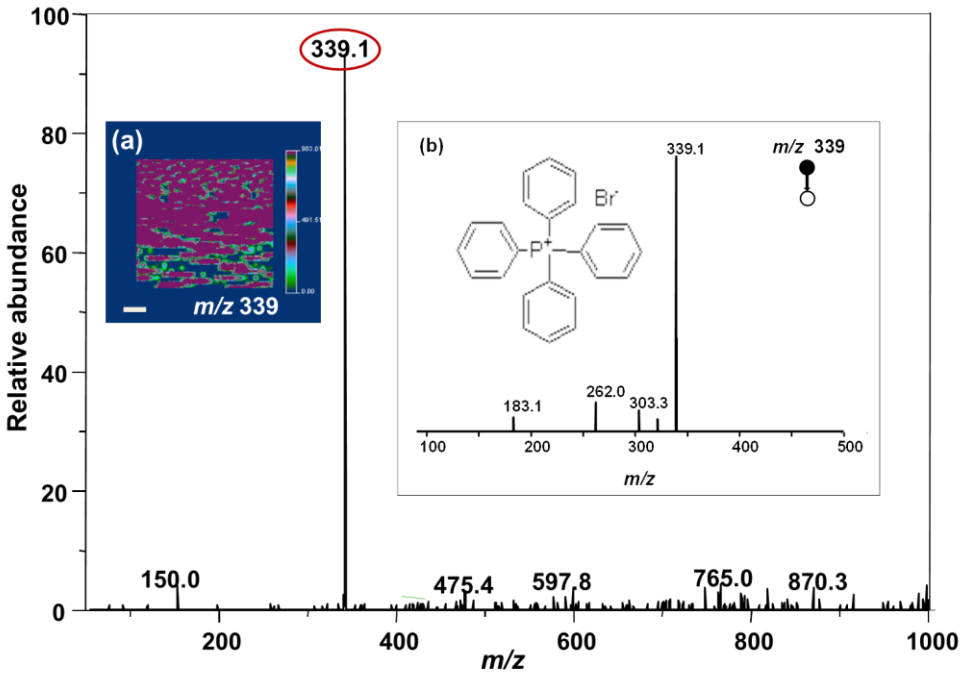
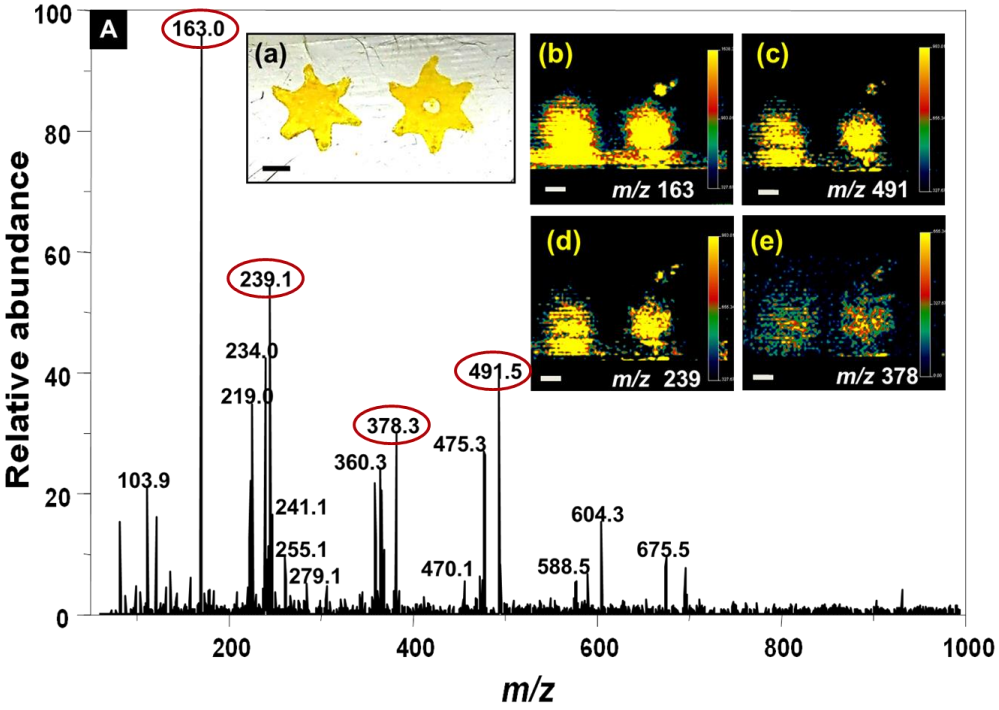
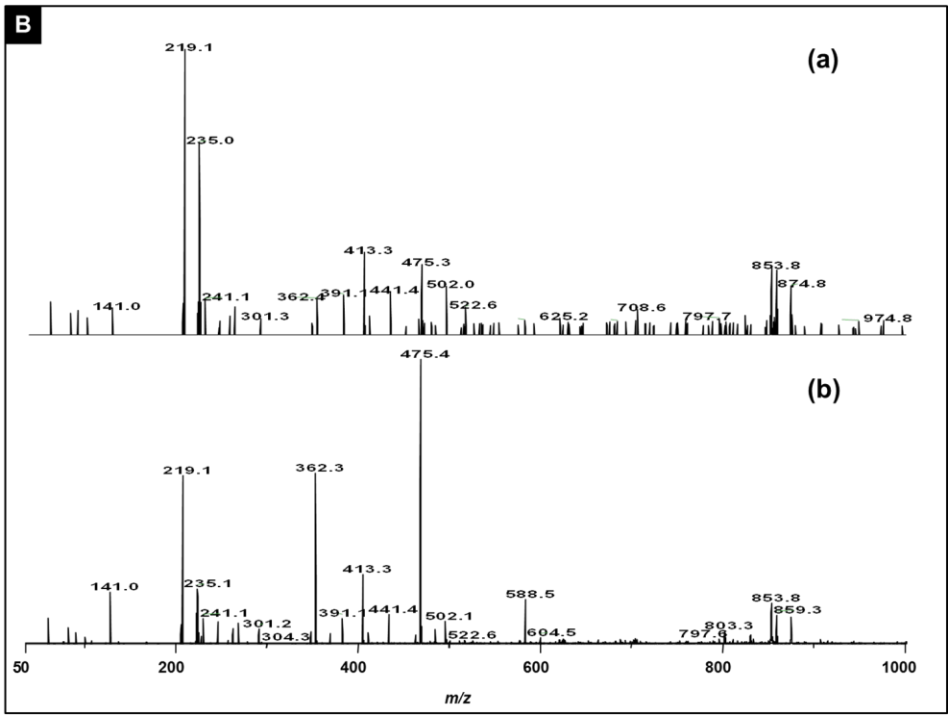


Figure S3. DESI MS spectrum corresponding to tetraphenylphosphoniumbromide (TPPB) incorporated nylon nanofiber mat. Inset (a) shows the DESI MS image and (b) tandem mass spectrum corresponding to the peak at *m/z* 339. Scale in DESI MS image is 5 mm.


A
163.0
(a)
(b)
m/z 163
(c)
m/z 491
(d)
m/z 239
(e)
m/z 378
239.1
234.0
219.0
491.5
378.3
475.3
360.3
103.9
241.1
255.1
279.1
470.1
588.5
604.3
675.5
Relative abundance
m/z


B
(a)
219.1
235.0
413.3
475.3
853.8
874.8
141.0
241.1
362.4
391.1
441.4
502.0
522.6
301.3
625.2
708.6
797.7
974.8
(b)
475.4
219.1
362.3
141.0
235.1
413.3
588.5
853.8
859.3
241.1
301.2
304.3
391.1
441.4
502.1
522.6
604.5
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803.3
50
200
400
600
800
1000
m/z

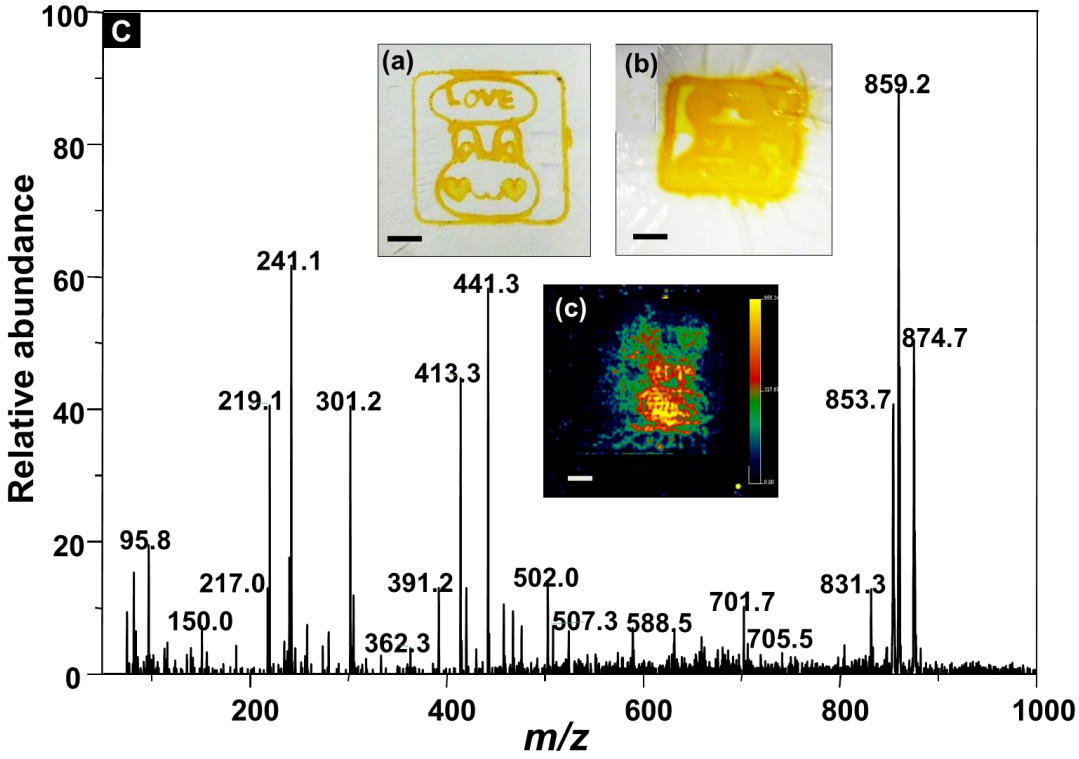


Figure S4. (A). DESI MS spectrum showing peaks eluted while using methanol as spray solvent for water exposed turmeric extract imprinted pattern on nylon nanofiber mat. (a) Optical image of the turmeric extract imprinted pattern on nylon nanofiber mat. (b-e) DESI images of encircled peaks showing changes in intensities and distortions from the imprinted pattern. (B). DESI MS spectra showing differences in peaks eluted due to spray solvents (a) methanol:water (50:50) and (b) acetonitrile. (C). DESI MS spectrum from turmeric extract imprinted pattern on printing paper using methanol:water as the spray solvent. (a) Optical image of the turmeric extract imprinted pattern on paper and (b) corresponding distortions in the printed pattern after the solvent (methanol: water (50:50)) spray. (c) DESI MS showing the distortions of the imprinted pattern. The scale in all images is 5 mm.

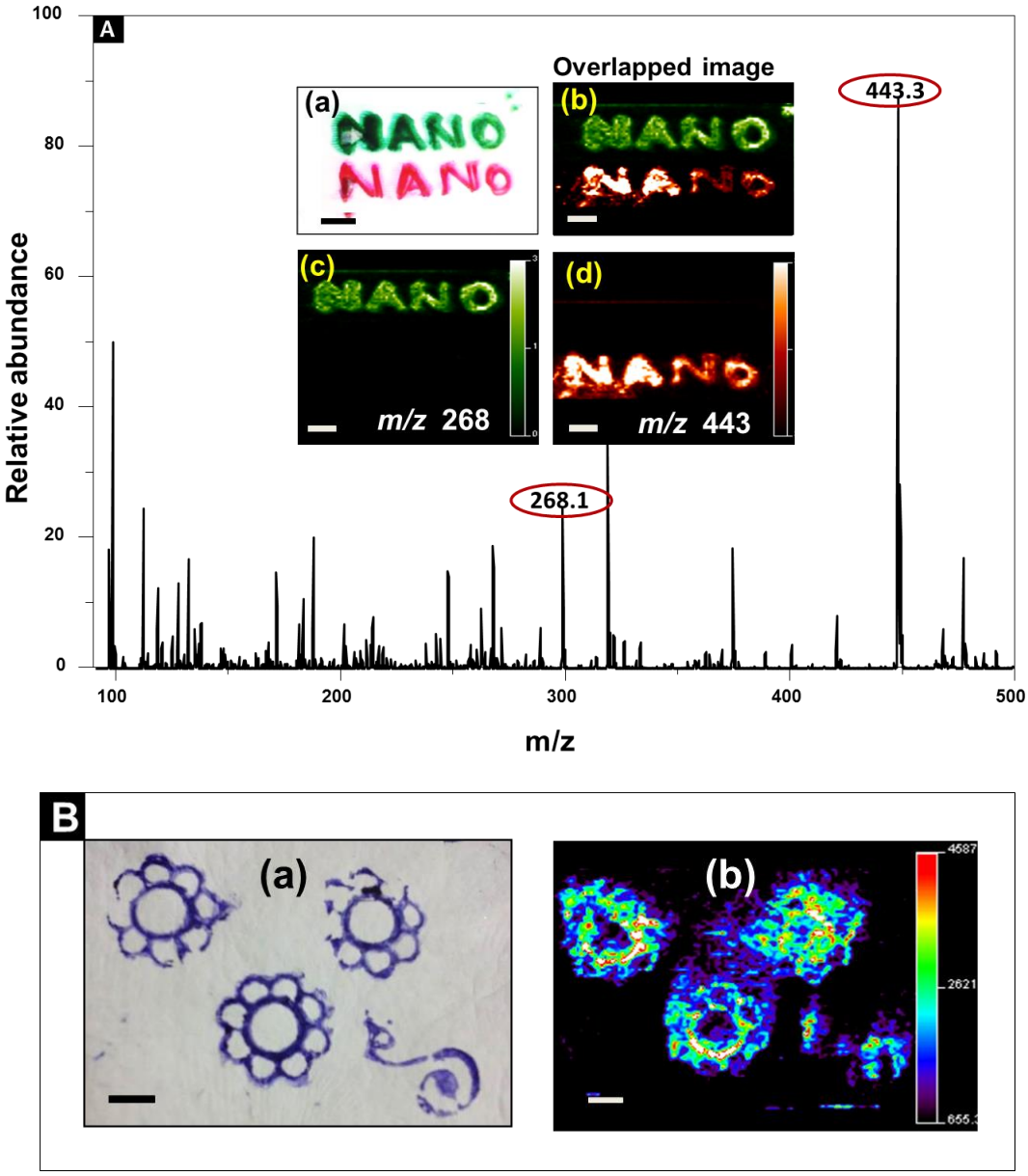


Figure S5. (A). DESI MS spectrum corresponding to a label written on a printing paper using green and red marker pens. The characteristic mass features due to the marker pens are encircled. A photograph of the paper is shown in inset (a). (b-d). DESI MS images corresponding to the green (*m/z* 268) and red (*m/z* 443) colored marker pen features.
(B).(a) Optical image of the imprinted pictorial pattern on printing paper and corresponding (b) DESI MS image showing the distortions in pictorial pattern. The scale in all images is 5 mm.

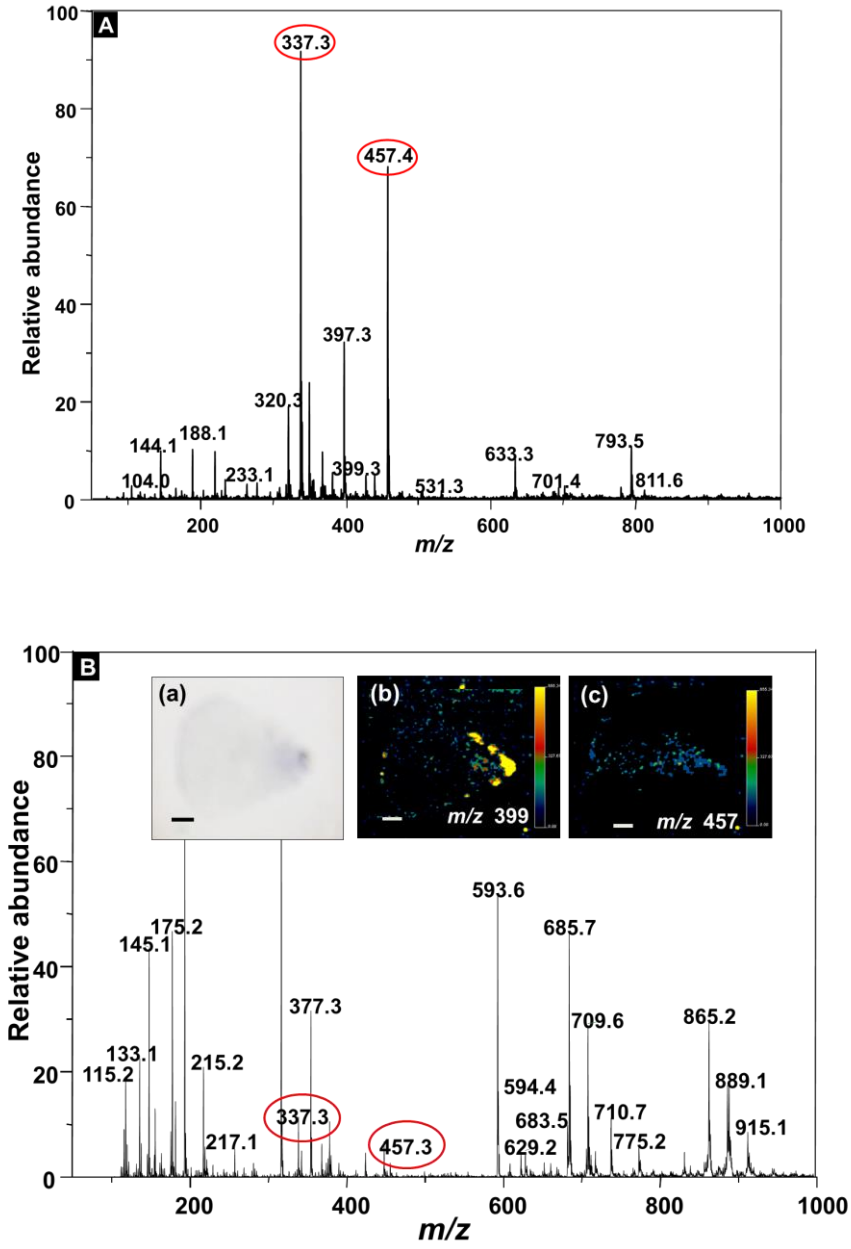
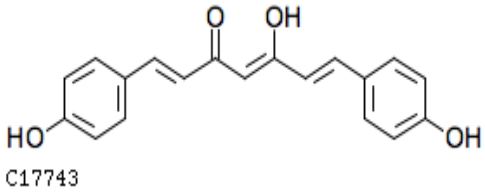
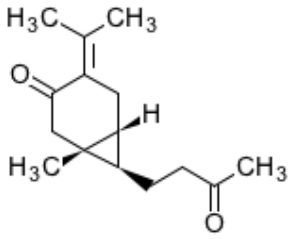
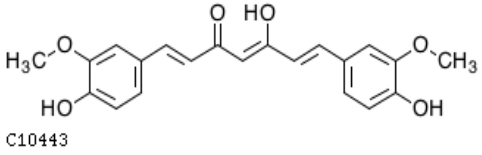
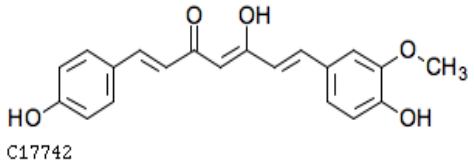
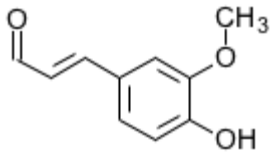
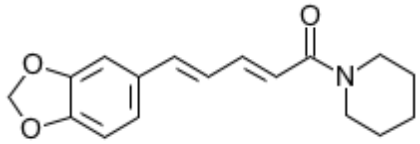
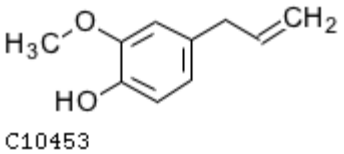
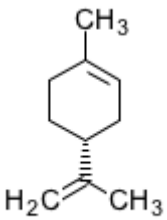
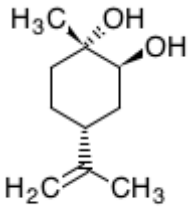


Figure S6. (A). DESI MS spectrum from TLC-imprint of petal of Madagascar periwinkle. Encircled peaks correspond to predominant metabolites- catharanthine (*m/z* 337) and vindoline (*m/z* 457). (B). Corresponding DESI MS spectrum from TLC-imprint after storage under ambient conditions for ten days. (a) Optical image showing discoloration of the TLC-imprint after storage. (b,c) Corresponding DESI MS images for encircled (catharanthine, vindoline) peaks showing very low (relative abundance <20%) ion intensities. The scale in all images is 5 mm.

Table S1: Identification of plant metabolite peaks using database search.

S. No	Name	Structure	Mol.wt	Database ID
1.	Bisdemethoxycurcumin	 C17743	308.3279	C17743 MID 58097
2.	Curcumenone	 C17492	234.334	C17492 MID 53443
3.	Curcumin	 C10443	368.3799	C10443 MID 44447
4.	Demethoxycurcumin	 C17742	338.3539	C17742 MID 45207
5.	Coniferaldehyde	 C02666	178.1846	C02666
6.	Piperine	 C03882	285.3377	C03882 MID 43568
7.	Eugenol	 C10453	164.2011	C10453 MID 4022

8.	Limonene		136.234	C06099 MID 41087
9.	Limonene-1,2-diol		170.2487	C07276 MID 41093

Identification of metabolite ion peaks using spectrum search tools of databases. [1,2]
* C numbers for KEGG database (http://www.kegg.jp/kegg/compound) to get additional information on the metabolite(s) including chemical and physical properties, structures, reactions and associated biosynthetic pathways of formation, etc.
**MID numbers for METLIN –Metabolite and Tandem MS database (http://metlin.scripps.edu/metabo_advanced.php) to get additional information on the metabolite(s) including data on tandem mass spectra and structures for fragments.

References:

1. Kanehisa, M.; Goto, S., *Nucleic Acids Res.*, **2000**, *28*, 27-30.

2. Smith, C. A.; O'Maille, G.; Want, E. J.; Qin, C.; Trauger, S. A.; Brandon, T. R.; Custodio, D. E.; Abagyan, R.; Siuzdak, G. *Ther. Drug Monit.*, **2005**, *27*, 747-751.