

Supplementary Information

Investigating the abundance, stability and activity of specialized metabolites in the roots vs leaves of a medicinal tree *Oroxylum indicum*

Supriya K. Acharya^{1#}, Natasha Kelkar^{1, 2}, Advait Agashe¹, Sagar S. Datir^{1, 3}, Charvi Mahuli¹,
Yashwant Kumar⁴ and Vaijayanti A. Tamhane^{1*}

Affiliations

¹ Department of Biotechnology, Savitribai Phule Pune University, Ganeshkhind Road, Pune 411007, Maharashtra, India.

² Present affiliation - Department of Microbiology and Immunology, Geisel School of Medicine at Dartmouth, Dartmouth College, Hanover, NH, USA

³ The Naoroji Godrej Centre for Plant Research, Shirwal, Maharashtra, India

⁴ Plant Molecular Biology Unit, National Chemical Laboratory, Pune, India. Present affiliation - Translational Health Science and Technology Institute, NCR biotech cluster, Faridabad-121001, Haryana

***Corresponding author:**

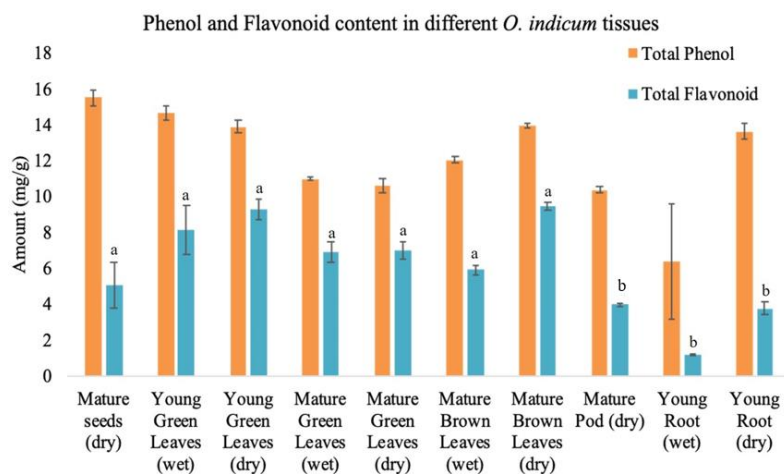
Vaijayanti A. Tamhane

E-mail: vatamhane@unipune.ac.in, vatamhane@gmail.com

Department of Biotechnology, Savitribai Phule Pune University, Ganeshkhind Road, Pune 411007, Maharashtra, India

Supplementary Figures

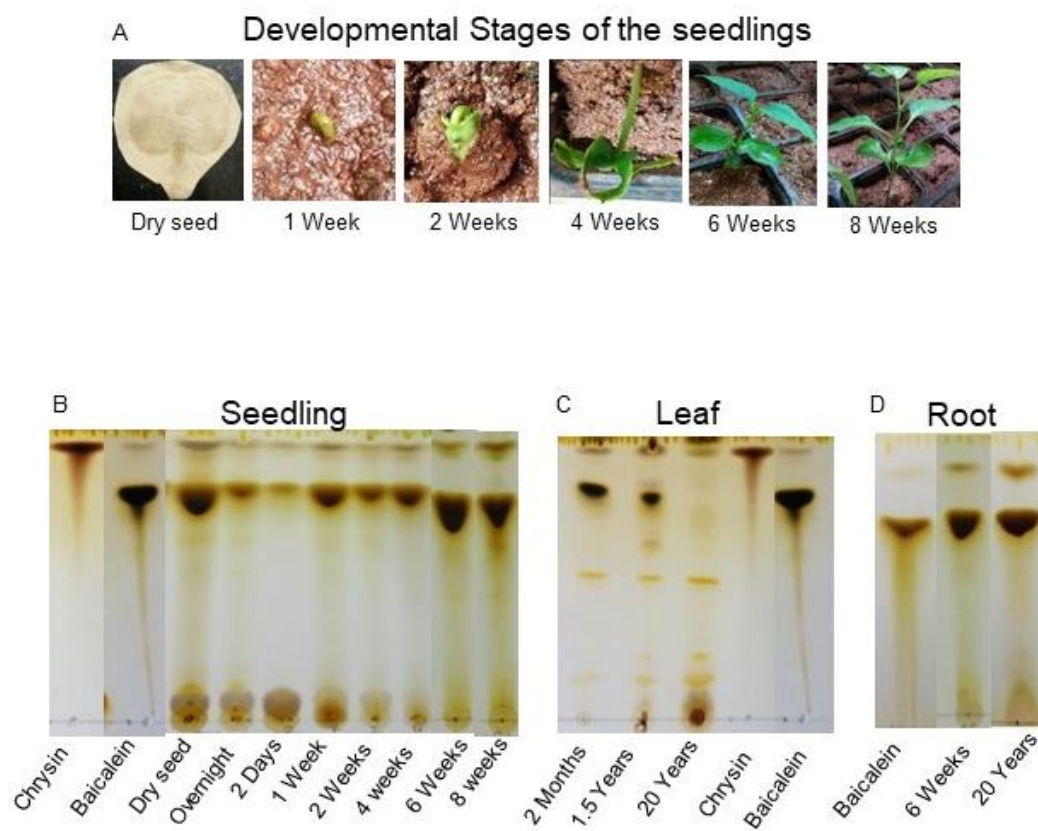
Fig. S1



Analysis of total phenol and flavonoid contents from different tissues of *O. indicum*

The total phenol (gallic acid equivalent) and flavonoid (quercetin equivalent) content from different tissues of *O. indicum* was estimated. Statistical analysis was performed by ANOVA followed by Tukey's post hoc analysis ($n=3$, $\alpha=0.05$). No significant difference was seen in the total phenol content in the different *O. indicum* tissues. In case of total flavonoid content, the root tissues displayed a significantly lower abundance of flavonoids.

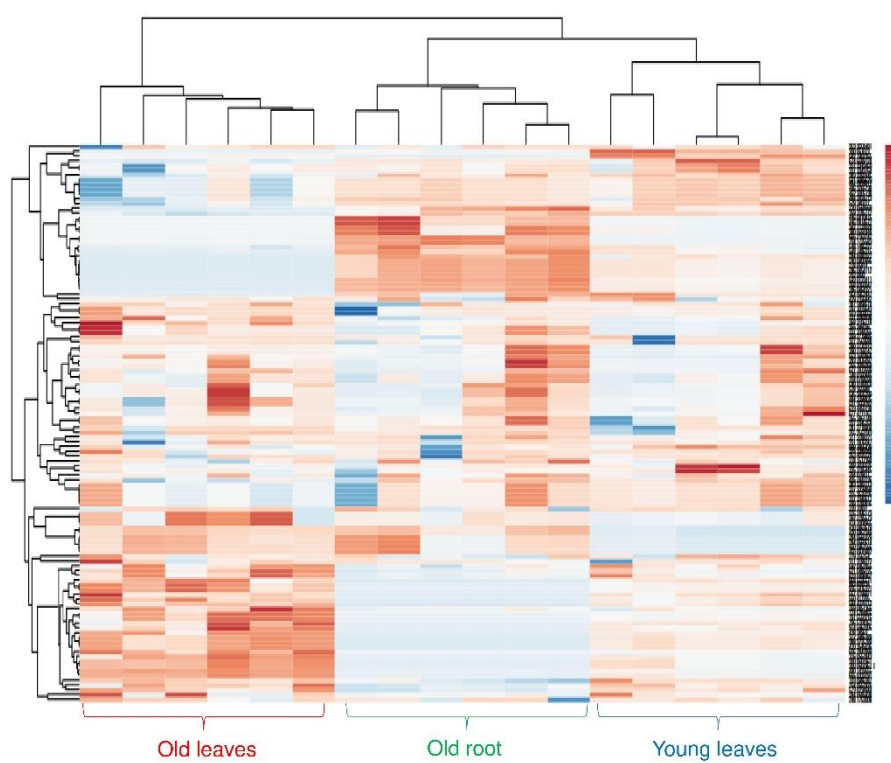
Fig. S2



**Variation in number of specialized metabolites depending upon the developmental stage and age
of *O. indicum* tree**

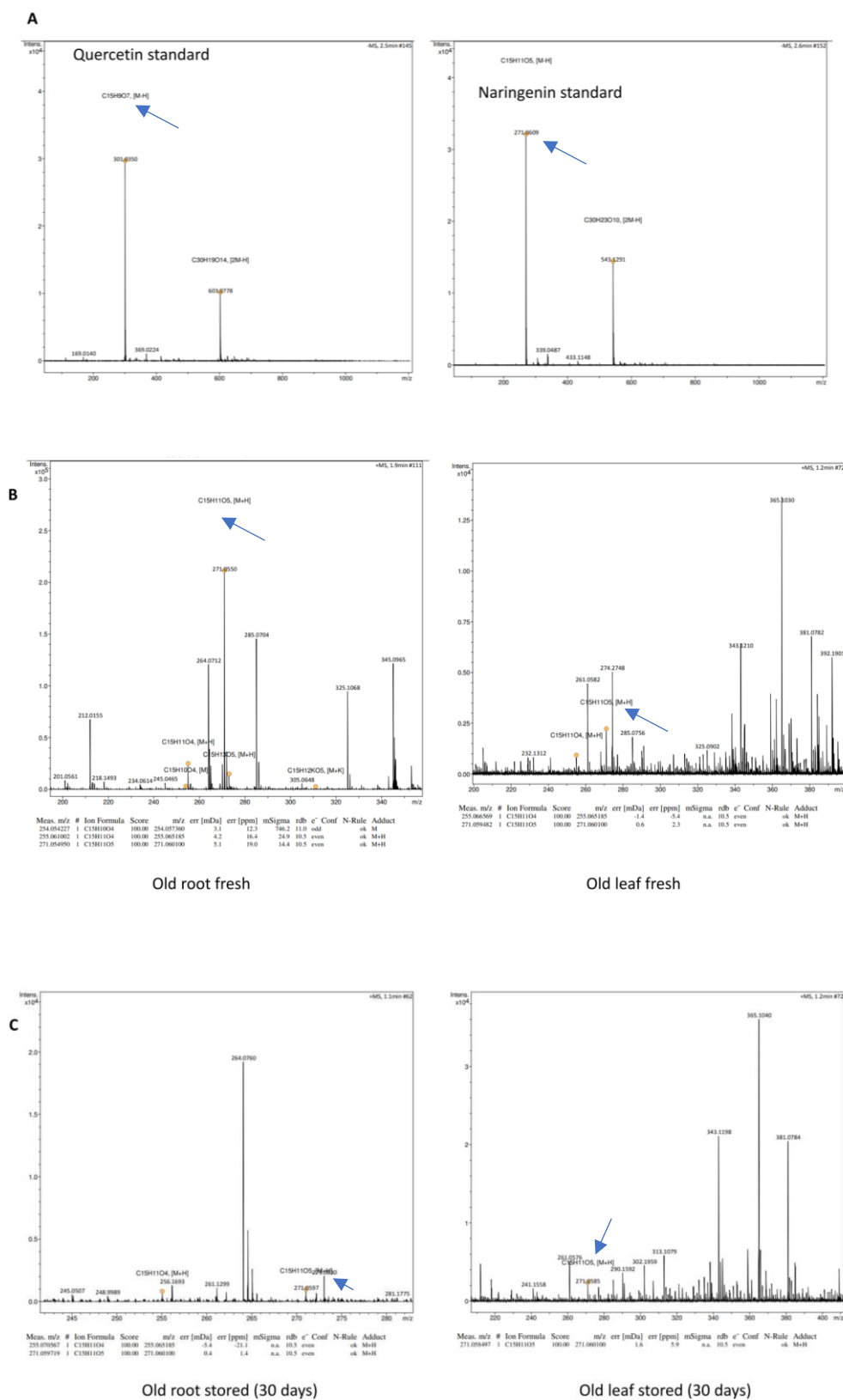
A: The different developmental stages at which samples were collected from *O. indicum*. B: The thin layer chromatography (TLC) analysis of the flavonoids extracted from *O. indicum* seedlings at different stages. Chrysin and baicalein were used as standards in the analysis. C: TLC analysis of the flavonoids extracted from leaves of *O. indicum* of different ages- 2 months, 1.5 years and 20 years. D: TLC analysis of the flavonoids extracted from roots of *O. indicum* trees of at different ages- 6 weeks and 20 years.

Fig. S3

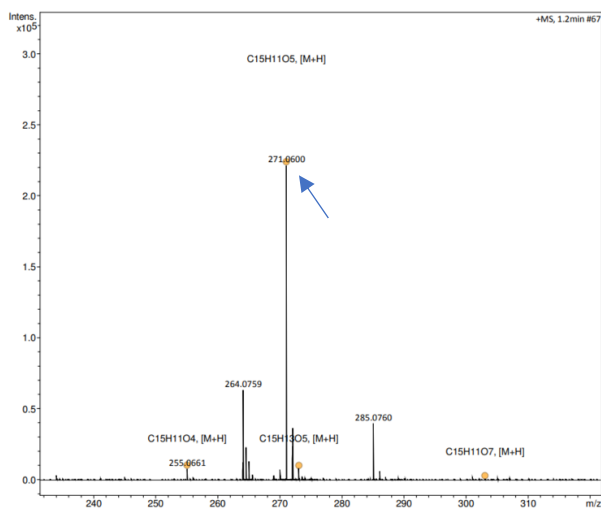


Heatmap displaying comparative distribution of metabolites in old leaves, old root and young leaves

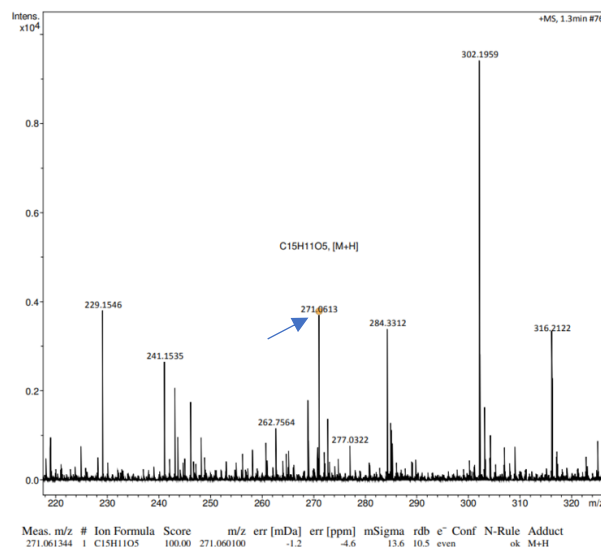
Fig. S4



D

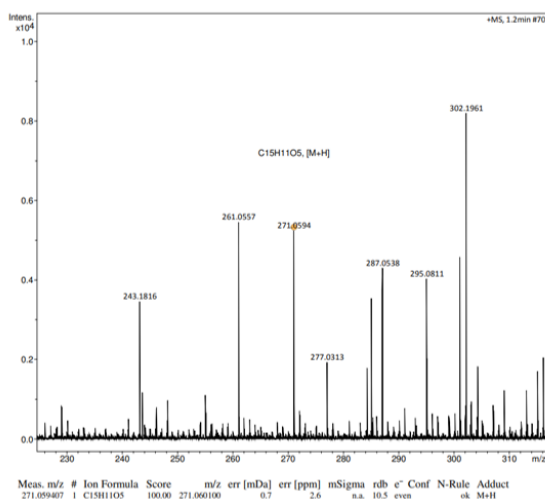


young root (fresh)

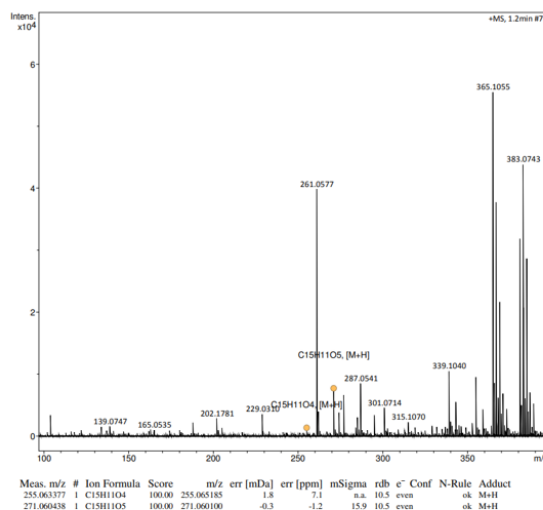


young root stored (30 days)

E



young leaf (fresh)



young leaf stored (30 days)

A. Intensity peak of standard quercetin and naringenin. Naringenin detection in **B.** old root and leaf (fresh) displaying peaks, **C.** old root and leaf (stored for 30 days) **D.** young root (fresh and stored) **E.** young leaf (fresh and stored)

Table S1	Identification of metabolites from tissues of <i>O. indicum</i> HR-LC/MS analysis was carried out to determine the different metabolites in young leaf, old leaf and old root of <i>O. indicum</i>. (separately attached file)
Table S2	Loading and scoring plots of PCA analysis (separately attached file)
Table S3	List of HRMS data analysis of fresh extracts of young leaves, young roots, old leaves and old roots and stored extracts (30 days stored) (separately attached file)
Table S4	<i>In-silico</i> docking of <i>O. indicum</i> metabolites with enzymes of inflammatory pathway <i>In silico</i> docking of <i>O. indicum</i> metabolites with enzymes of inflammatory pathway was performed by using software Patch dock. (separately attached file)