



Supplementary material: Composition of antifungal volatile organic compounds in *Sextonia rubra* fruit by molecular networks

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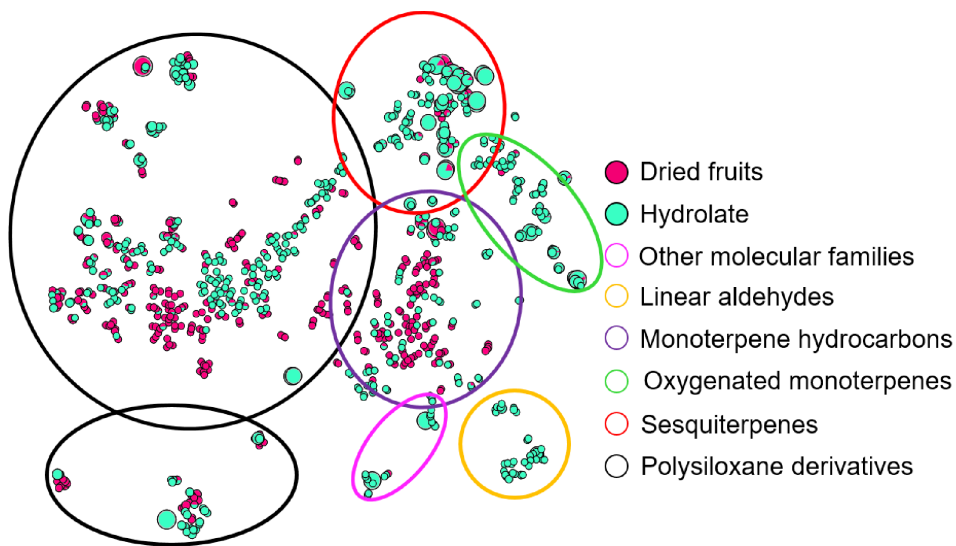
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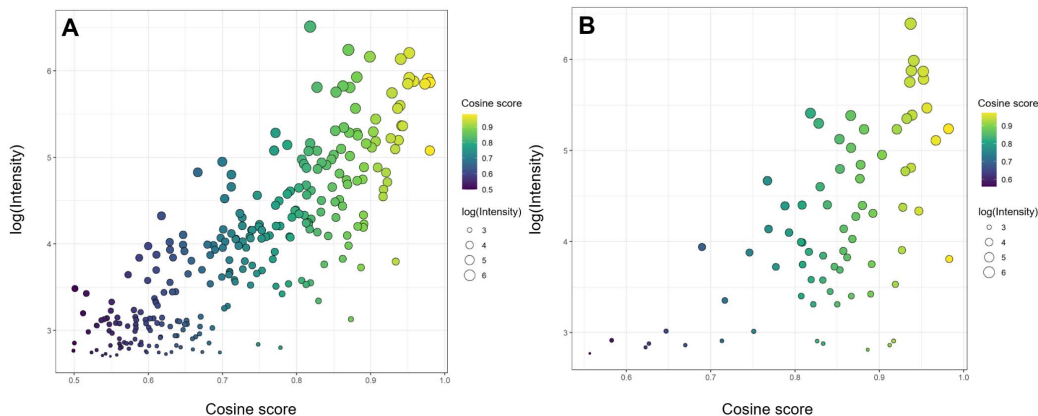
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Supplementary Figure S1. Total t-SNE representation obtained by using MetGem software. The azure nodes are the ions detected in the hydrolate and the magenta node correspond to the ions detected in the dried fruits. The total molecular network contains 1088 nodes, 482 of which are shown in this figure. 199 nodes are singletons and 407 correspond to polysiloxane derivatives. Pie-charts correspond to the peak areas of each detected ion. Node size is defined by the maximum area for a peak corresponding to an ion detected in both samples.



Supplementary Figure S2. **A**, Correlations between the intensity of compounds detected in *S. rubra* fruit hydrolate and their cosine score assigned by MetGem. **B**, Correlations between the intensity of compounds detected in *S. rubra* dried fruits and their cosine score assigned. The cosine score scale tends towards green when the assigned score is significant and conversely tends towards purple.

Supplementary Table S1. Summary table of the main compounds detected in fruit (this study), branch and leaf (Alcântara *et al.*, 2013) samples of *S. rubra* and relative compositions of the molecular families detected

	Dried fruit	Fruit Hydrolate	Branches	Leaves
Main compounds (5 most abundant)	α -pinene (26.8%—MH)	eucalyptol (13.5%—MH)	α -copaene (22.9%—SH)	α -pinene (21.7%—MH)
	α -copaene (14.4%—SH)	α -calamenene (7.4%—SH)	β -selinene (7.9%—SH)	β -pinene (15.4%—MH)
	β -sabinene (10.3%—MH)	β -caryophyllene (7.4%—SH)	β -elemene (7.2%—SH)	α -copaene (12.5%—SH)
	(-)-germacrene D (8.4%—SH)	α -copaene (7.3%—SH)	δ -cadinene (6.2%—SH)	germacrene D (12.1%—SH)
	β -caryophyllene (6.3%—SH)	δ -cadinene (5.8%—SH)	epi- α -cadinol (6.1%—OS)	β -caryophyllene (7.1%—SH)
Other molecular families	3.8%	17.2%	-	-
Monoterpene hydrocarbons (MH)	15.4%	6.9%	1.2%	44.6%
Oxygenated monoterpenes (OM)	7.7%	24.1%	-	3.2%
Sesquiterpene hydrocarbons (SH)	69.2%	43.1%	66.8%	47.7%
Oxygenated sesquiterpenes (OS)	3.8%	8.6%	26.7%	-

All percentages correspond to the peak area of a compound or to the sum of the peak areas of compounds annotated in one of the 5 categories listed below (highly, volatile molecular families).

Supplementary Table S2. Relatives MIC of the hydrolate against M.R.S.A., *C. albicans* and *T. rubrum*

Strains	Relative MIC values (% or $\mu\text{g}\cdot\text{mL}^{-1}$)			
	Hydrolate	Water	Vancomycin	Fluconazole
M.R.S.A. (ATCC33591)	-	-	6.8% (4 $\mu\text{g}\cdot\text{mL}^{-1}$)	ND
<i>C. albicans</i> (ATCC10231)	-	-	ND	1.7% (2 $\mu\text{g}\cdot\text{mL}^{-1}$)
<i>T. rubrum</i> (SNB-TR1)	5%	-	ND	3.4% (4 $\mu\text{g}\cdot\text{mL}^{-1}$)

ND: Not determined, - : No growth inhibition.

Supplementary Table S3. Summary table of cytotoxicity tests

Relative concentrations of hydrolate (%)	10	5	1	0 (Negative control)
MRC-5 IC ₅₀ (μM)	95 \pm 1	97 \pm 2	97 \pm 4	97 \pm 2



Supplementary Figure S3. Photography of a longitudinal section of *S. rubra* fruits.