

Degradation of limonene and cinnamaldehyde in soil, and detection of their metabolites by UHPLC and GC-HRMS

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Table S1. Physicochemical characteristics of soils

Type of soil	Code	pH	Carbon Monoxide (%)	Organic matter (%)	% Grit	% Sand	% Silt	% Clay
Sandy clay loam	SCL1	8.4	2.4	4.1	74.2	51.9	24.3	23.9
	SCL2	8.4	0.9	1.5	23.0	58.6	14.2	27.2
Clay loam	CL1	8.4	0.8	1.4	46.0	29.6	33.1	37.2
	CL2	8.6	0.6	1.4	12.1	26.1	44.4	29.5

Table S2. Characteristic chromatographic-MS parameters of limonene and *trans*-cinnamaldehyde

Compound	Molecular formula	Retention time (min)	Precursor ion			Fragment ions			Method
			Adduct	Theoretical mass (<i>m/z</i>)	Error mass (ppm)	Molecular formula	Theoretical mass (<i>m/z</i>)	Error mass (ppm)	
<i>trans</i> -Cinnamaldehyde	C ₉ H ₈ O	14.54	[M+H] ⁺	133.0648	-3.393	C ₈ H ₉	105.0699	0.220	UHPLC
						C ₇ H ₇	91.0542	2.012	

Compound	Kovats retention index (RI)	Retention time (min)	Characteristic ions						Method
			Molecular formula	Theoretical mass (<i>m/z</i>)	Error mass (ppm)	Molecular formula	Theoretical mass (<i>m/z</i>)	Error mass (ppm)	
Limonene	1030	8.10	C ₇ H ₉	93.0699	0.249	C ₆ H ₇	79.0542	0.293	GC

Table S3. Recoveries and RSD of limonene and *trans*-cinnamaldehyde in different extraction methods^a

Method extraction	Compound	Recovery (%)	RSD (%)
Rotatory extraction 30 min	Limonene	56.7	5.6
	<i>trans</i> -Cinnamaldehyde	50.9	2.2
Rotatory extraction 60 min	Limonene	98.5	4.7
	<i>trans</i> -Cinnamaldehyde	101.4	1.0
UAE 20 min	Limonene	111.6	4.6
	<i>trans</i> -Cinnamaldehyde	111.4	2.7

^aAbbreviation: RSD: relative standard deviation; UAE: ultrasound-assisted extraction

Table S4. UHPLC-Q-Orbitrap parameters of *trans*-cinnamaldehyde metabolites found with MassChemSite

Code	Retention time (min)	Molecular formula	Adduct	<i>m/z</i>
CM1	3.12	C ₉ H ₁₂ O ₃	[M+H] ⁺	169.0859
CM2	13.97	C ₉ H ₆ O ₃	[M+H] ⁺	163.0390
CM3	14.96	C ₉ H ₁₀	[M+H] ⁺	119.0855
CM4	16.05	C ₉ H ₁₀ O	[M+H] ⁺	135.0804