

Spices volatilomic fingerprinting – a comprehensive approach to explore its authentication and bioactive properties

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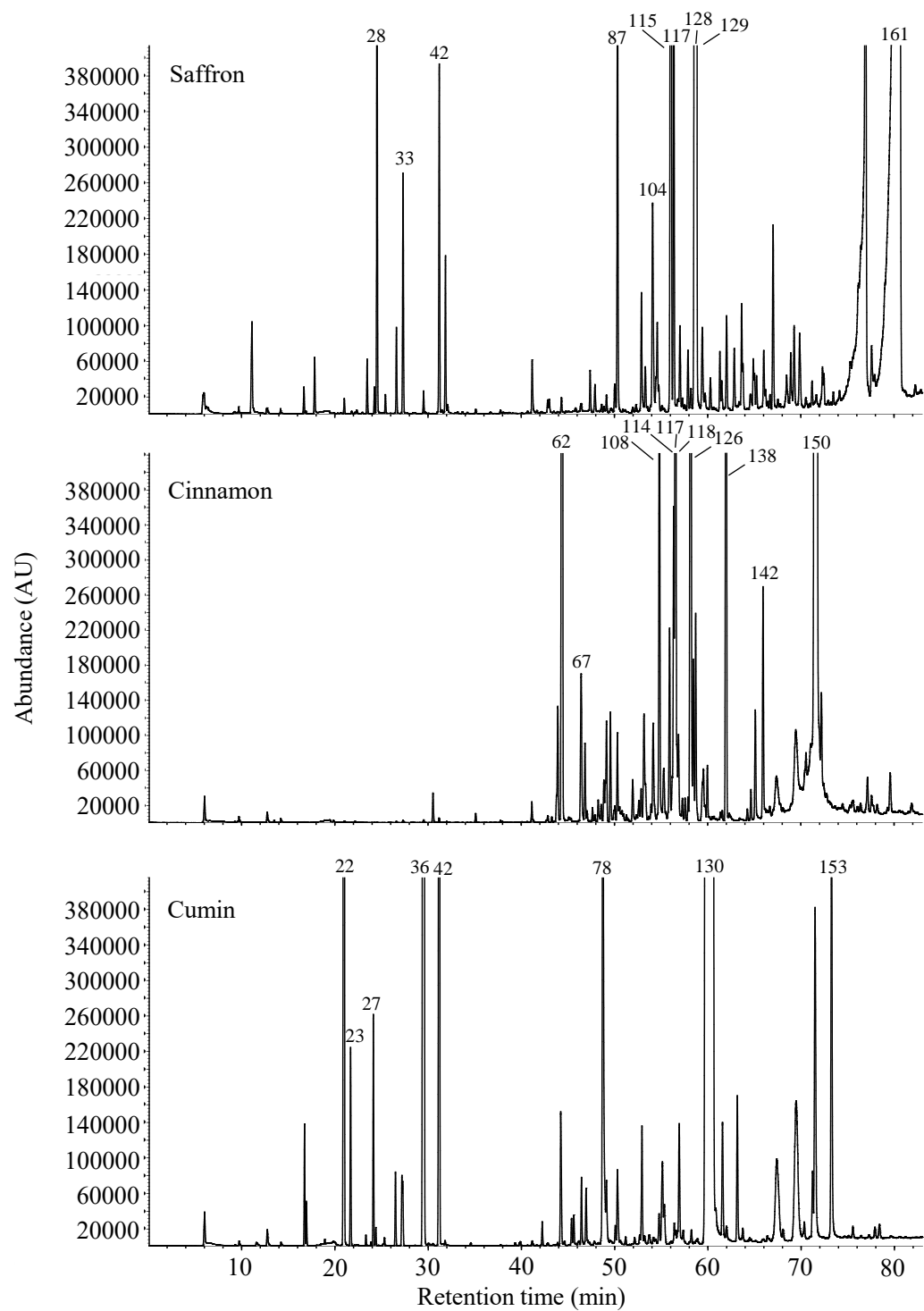
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SUPPLEMENTARY MATERIAL

Table S1. Volatile organic metabolites (VOMs) identified only in a determined spice using HS-SPME_{DVB/CAR/PDMS}/GC-qMS.

Saffron	Cinnamon	Cumin	Curry	Black pepper	Sweet paprika
Ethyl acetate	3-Ethyl-o-xylene	2-Heptenal	2-Methyl-2-butenal	α -Fenchene	4-Methylheptane
Octanal	β -Ionone	Pinocamphone	2-Hexenal	β -Phellandrene	2,4-Dimethylheptane
3-Methyl styrene	TMB ^a	Isobornyl acetate	Allyl isothiocyanate	α -Ocymene	Acetone
β -Bourbonene	Isolodene	<i>p</i> -2-Menthen-1-ol	Pulegone	Fenchone	4-Methyloctane
calarene,	α -Bergamotene	Myrtenal	Citronellol	α -Cububene	2-Methylfuran
α -Cedrene	α -Santalene	Pinocarveol	4-Methyl-guaiacol	α -Patchoulene	DMH ^b
Aristolene	Longifolene	β -Patchoulene		β -cubebene	2-Methyl butanal
2-Undecanone	Aromadendrene	α -Guaiene		Estragole	3-Methyl butanal
Farnesene,	α -Cedrene	Nerolidol		β -Cadinene	1-Methyl pyrrole
β -Panasinsene	γ -Gurjunene	D-Germacrene		Valencene	2-Pentyl furan
cis-Carveol	β -Humulene			α -Selinene	TMCH ^c
Geraniol	γ -Muurolene			β -Selinene	Linalyl acetate
Cadinol	γ -Himachelene			Germacrene B	β -Cyclocitral
Carvacrol	Bicyclogermacrene			Neryl isobutyrate	Citral
	α -Panasinsense			Thymol acetate	Jasmone
	α -Bisabolol			Safrol	
	t-Muurolol			<i>o</i> -Cresol	
	Cadalene			Spathulenol	

^a 1,2,3,4-Tetramethyl benzene; ^b 2,4-Dimethyl-1-heptene; ^c 2,6,6-teimethyl cyclohexanone



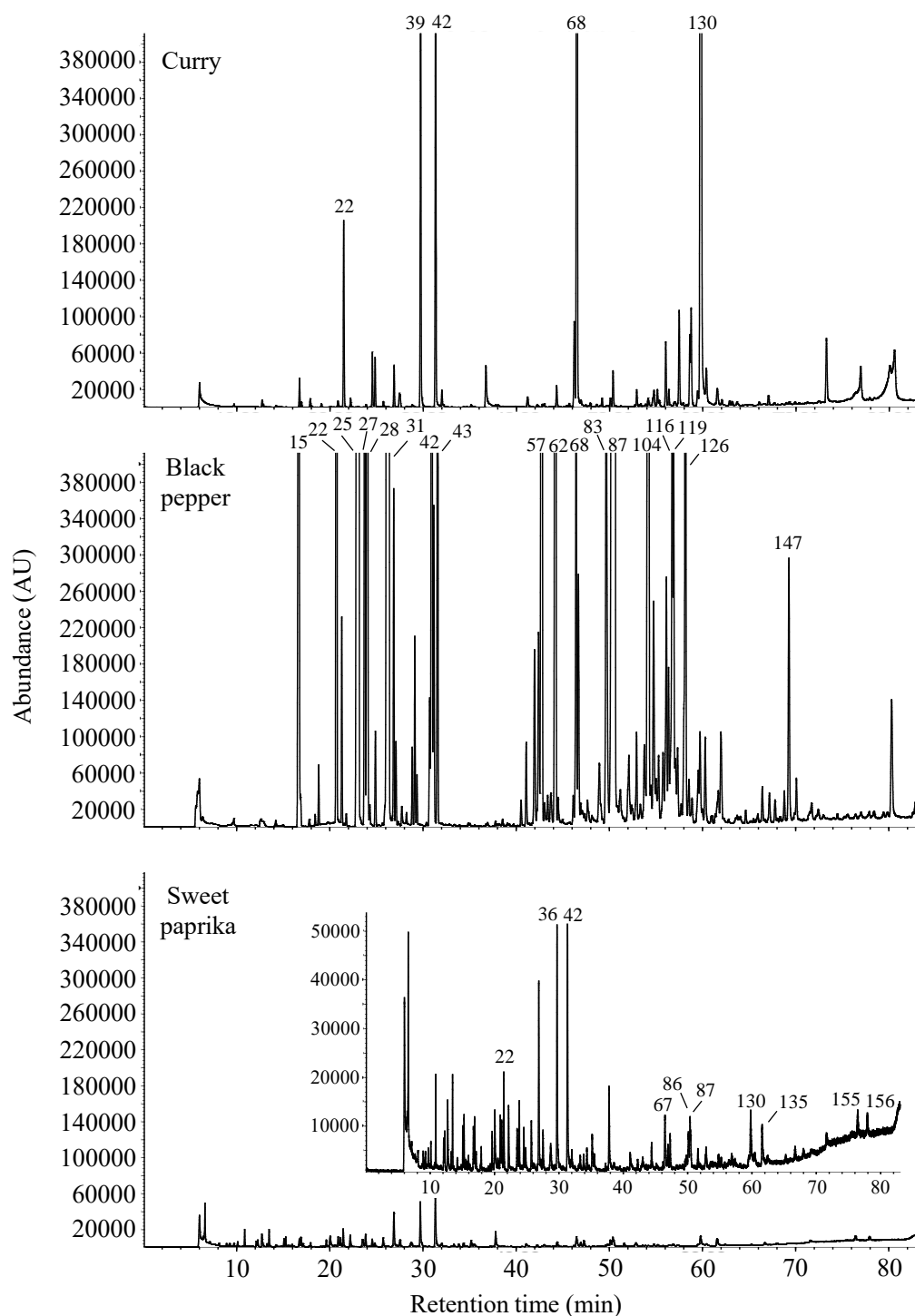


Figure S1. Chromatogram of the volatile fraction of the spice samples obtained by HS-SPME-GC-qMS. Numbers above the peaks indicate the volatile organic metabolites (VOMs) identified in Table 1. Peak number identification: 15 – α -pinene, 22 – β -pinene, 23 – sabinene, 25 – 3-carene, 27 – β -myrcene, 28 – α -phellandrene, 31 – limonene, 33 – eucalyptol, 36 – terpinene isomer, 39 – terpinene isomer, 42 – p-cymene, 43 – terpinolene, 57 – δ -elemene, 62 – copaene, 67 – benzaldehyde, 68 – linalool, 78 – pinocamphone, 83 – β -elemene, 86 – terpinen-4-ol, 87 – caryophyllene isomer, 104 – epizonarene, 108 – γ -muurolene, 114 – bicyclogermacrene, 115 – (-)- δ -cadinene, 116 – selinene isomer, 117 – β -bisabolene, 118 – α -muurolene, 119 – selinene isomer, 126 – δ -cadinene, 128 – β -sesquiphellandrene, 129 – α -curcumene, 130 – cuminaldehyde, 135 – geraniol, 138 – calamenene, 142 – α -calacorene, 147 – caryophyllene oxide, 150 – cinnamaldehyde, 153 – γ -eudesmol, 155 – eugenol, 156 – thymol, 161 – dihydrojuneol.