

# **Aroma Investigation of Chios Mastic Gum (*Pistacia lentiscus* var. *Chia*) using Headspace Gas Chromatography Combined with Olfactory Detection and Chiral Analysis**

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### Supporting Information

Table S1. Key aroma compounds, flavor dilution factors (FD  $\geq$  8), and *m/z* fragments for quantification.

<b>compound</b>	<b>FD factor</b>	<b>quantifier ion (<i>m/z</i>)</b>	<b>qualifier ions (<i>m/z</i>)</b>
$\alpha$ -pinene	256 <sup>a</sup>	93	91 & 77
$\beta$ -pinene	128 <sup>a</sup>	93	41 & 69
camphene	64 <sup>a</sup>	93	79 & 107
$\beta$ -myrcene	128 <sup>b</sup>	93	69 & 41
limonene	8 <sup>a</sup>	93	93 & 95
2-nonalone	128 <sup>a</sup>	58	43 & 71
perillene	128 <sup>b</sup>	69	81 & 150
$\beta$ -linalool	256 <sup>a</sup>	93	71 & 121
terpinen-4-ol	16 <sup>b</sup>	71	93 & 111
Z-verbenol	8 <sup>a</sup>	94	109 & 119

<sup>a</sup>by means of a HS-SPME-GC-MS/MS-O system. <sup>b</sup> by means of HS-SBSE-GC-MS-O with TDU system.

Table S2. Preparation of aqueous standard solutions for external calibration by means of MHS-SPME.

<b>compound</b>	<b>mass (mg)</b>	<b>purity (%)</b>	<b>methanol (mL)</b>	<b>concentration (mg/L)</b>
$\alpha$ -pinene	89.0	98		3488.8
$\beta$ -pinene	33.1	99		1310.8
camphene	20.4	98		799.7
$\beta$ -myrcene	63.8	90		2268.0
limonene	31.6	97	25	1226.1
2-nonalone	20.0	99		792.0
perillene	29.7	98		1163.5
$\beta$ -linalool	19.4	97		752.7
terpinen-4-ol	3.5	97		137.0
Z-verbenol	39.6	97		1536.5

Table S3. Odor-active compounds of Chios mastic gum perceived at the ODP after HS-SPME-GC-MS/MS-O utilizing CAR/PDMS and CAR/PDMS/DVB fibers.

No.	RI (VF-WAXms)	compound	odor impression	CAR/PDMS	CAR/PDMS/DVB
1	< 900	acetone	fresh, solvent	-	+
2	935	ethanol	ethanoic, forest-like	-	+
3	1026	$\alpha$ -pinene	forest-like, resinous	+	+
4	1091	<i>trans,trans</i> -5-caranol	green, forest-like, vanilla	+	+
5	1093	<i>cis</i> -2,6-dimethyl-2,6-octadiene	green, forest-like	-	+
6	1126	$\beta$ -pinene	resinous, fresh, terpene-like	+	+
7	1138	camphene	harsh, spicy, buttery	+	+
8	1199	limonene	sugary, fruity, citrus-like	+	+
9 <sup>a</sup>	1300	oct-1-en-3-one	mushroom-like	+	+
10	1389	2-nonenone	fresh, green, resinous	+	+
11	1408	2-methoxytoluene	woody, fresh	+	+
12	1427	perillene	green, pea-like, citrus-like	+	+
13	1433	$\gamma$ -campholenale	woody, green	+	+
14	1446	acetic acid	sourish, vinegar-like	+	+
15	1546	$\beta$ -linalool	floral, fresh, fruity	+	+
16	1593	isothymol methylether	green, fruity	-	+
17	1627	myrtenal	pungent, sweaty	+	+
18	1642	terpinen-4-ol	earthy	+	+
19	1675	Z-verbénol	pine-like, sweetish	+	+
20	1866	carveol	fresh, citrus-like	-	+
21	2035	humulene-1,2-epoxide	sweetish, earthy, buttery	-	+
22	2130	<i>unknown</i>	sweetish, marzipan-like	-	+
23	2226	<i>unknown</i>	earthy	-	+
Total				15	23

<sup>a</sup> MS spectrum was ambiguous. The compound was tentatively identified on basis of RI, odor and literature data. + perceived. - not perceived.

Table S4. Calibration parameters obtained for aqueous solutions of key aroma compounds of Chios mastic gum quantified by means of MHS-SPME.

<b>compound</b>	<b><i>m</i></b>	<b><i>b</i></b>	<b><i>R</i><sup>2</sup></b>	<b><i>K</i> (<math>\mu</math>g)</b>
$\alpha$ -pinene	16214808	-12477523	0.994	0.7 – 34.9
$\beta$ -pinene	15168438	-6206950	0.997	0.3 – 13.1
camphene	4393041	1013534	0.978	0.2 – 8.0
$\beta$ -myrcene	42433758	-59070248	0.972	0.5 – 22.9
limonene	11774347	-4544071	0.980	0.3 – 12.3
2-nonanone	26976855	-12939301	0.973	0.2 – 7.9
perillene	2880409	-499424	0.996	0.2 – 11.6
$\beta$ -linalool	12405851	-3731277	0.970	0.2 – 7.5
terpinen-4-ol	15688568	-603086	0.996	0.02 – 1.3
Z-verbenol	1204161	-1133026	0.965	0.3 – 15.4

*m* slope. *b* axis section. *R*<sup>2</sup> linear regression coefficient. *K* linear calibration range, absolute amount of analyte in HS-vials.

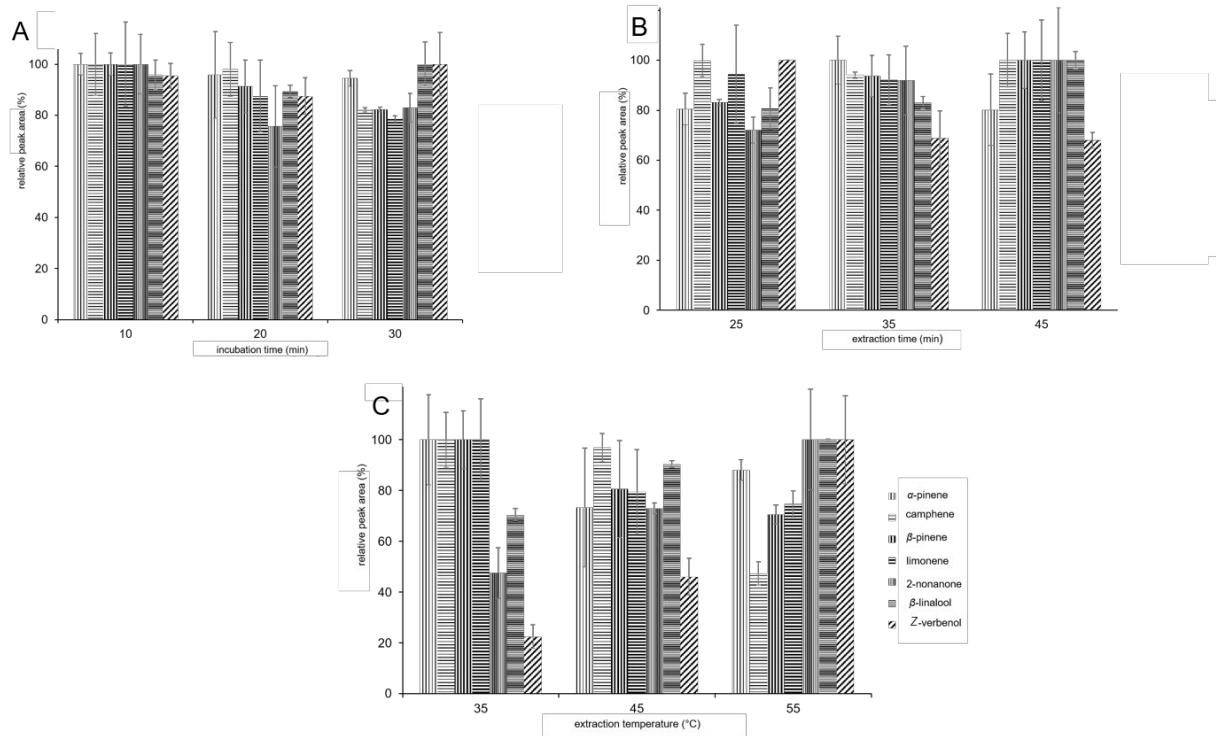


Figure S1. Influence of incubation time, extraction time, and extraction temperature on the extraction efficiency of selected odorants expressed in percent of maximum peak area.