

## Supporting Information

### **Sustainable biotransformation of microalgae *via* probiotic fermentation for enhanced functional, nutritional, and sensory properties**

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62

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67 precursor amino acids during *L. plantarum*-mediated fermentation of microalgae (MA) over  
68 96 hours.

69 Figure S3. Olfactory evaluation of microalgae fermented with *L. plantarum*.

70

## 71 **Appendix**

### 72 **Supporting Methods**

73 Unless specified otherwise, chemicals and reagents are purchased from Sigma-Aldrich (St.  
74 Louis, MO, USA).

75

#### 76 ***Bacterial strains cultivation***

77 Non-lactic acid bacteria (non-LAB) strains—including *Bacillus* spp., *Cupriavidus necator*,  
78 *Microbacterium imperiale*, *Weizmannia coagulans*, and *Priestia megaterium*—were cultured  
79 in Luria-Bertani (LB) broth at 37 °C with agitation at 200 rpm until mid-logarithmic phase  
80 ( $OD_{600} \approx 0.4$ ). Lactic acid bacteria (LAB) strains were cultivated in De Man, Rogosa, and  
81 Sharpe (MRS) broth under identical conditions (37 °C, 200 rpm) until  $OD_{600} \approx 0.4$ .  
82 *Streptococcus thermophilus* was cultured separately in M17 broth (Difco™, Becton, Dickinson  
83 and Company, Sparks, MD, USA) at 42 °C, 200 rpm till a similar growth phase.

84

#### 85 ***Protease assay***

86 The proteolytic activity of the bacterial strains was qualitatively evaluated using the skim milk  
87 agar assay method. Skim milk agar was prepared with the following composition: 28 g/L skim  
88 milk powder, 5 g/L casein, 2.5 g/L yeast extract, 1 g/L dextrose, and 15 g/L agar in 1 L of  
89 distilled water, adjusted to a final pH of  $7.0 \pm 0.2$  at 25 °C. 10  $\mu$ L aliquot of the bacteria culture

90 supernatant was aseptically spotted onto the surface of the agar and incubated at 37 °C.  
91 Proteolytic activity, as indicated by a zone of clearance around the inoculation site, was  
92 monitored across 96 hours.

93

#### 94 *Lipase assay*

95 The lipolytic activity of the bacterial strains was qualitatively assessed using the tributyrin agar  
96 assay method. Tributyrin agar was prepared by dissolving 20 g of tributyrin agar powder in 1  
97 L of distilled water, followed by adding 10 mL of glyceryl tributyrate upon cooling to 80 °C  
98 after autoclaving. 10 µL of the bacterial culture supernatant was spotted on the tributyrin agar  
99 and incubated at 37 °C. Lipolytic activity, as indicated by a zone of clearance around the  
100 inoculation site, was monitored across 96 hours.

101

#### 102 *β-glucosidase assay*

103 β-glucosidase activity of the bacterial strains was assessed by quantifying the hydrolysis of *p*-  
104 nitrophenyl-β-D-glucopyranoside (pNPG). Bacterial culture supernatants were obtained by  
105 centrifugation at 4,000 × *g* for 20 minutes at 4 °C. For each sample, 0.5 mL of the culture  
106 supernatant was mixed with 2 mL of 1 mM pNPG solution and incubated at 45 °C for 30  
107 minutes. The reaction was terminated by the addition of 2.5 mL of 1 M sodium carbonate. The  
108 release of *p*-nitrophenol was quantified by measuring absorbance at 400 nm using a  
109 spectrophotometer. β-glucosidase activity was calculated based on a standard calibration curve  
110 constructed using a commercial β-glucosidase enzyme, and all reactions were performed in  
111 triplicates.

## 112 ***Cellulase assay***

113 Cellulolytic activity of the bacterial strains was qualitatively determined using the  
114 carboxymethyl cellulose (CMC) agar assay method. 0.2% CMC agar was prepared based on  
115 the following composition: CMC 2 g, sodium nitrate (NaNO<sub>3</sub>) 20 mL, dipotassium hydrogen  
116 phosphate (K<sub>2</sub>HPO<sub>4</sub>) 1 g, potassium chloride (KCl) 1 g, magnesium sulfate (MgSO<sub>4</sub>) 0.5 g,  
117 yeast extract 0.5 g, agar 15 g, 1 L distilled water. 10 µL of the culture supernatant was spotted  
118 on the 0.2% CMC agar and incubated at 37 °C. Cellulolytic activity, as indicated by a zone of  
119 clearance around the inoculation site, was monitored across 96 hours.

120

## 121 ***Submerged fermentation of microalgae***

122 Lyophilized *C. vulgaris* powder was reconstituted in 50 mL of sterile deionized water to a final  
123 solids content of 5 % (w/v). The suspension was autoclaved at 121 °C for 15 min, cooled to  
124 room temperature, and inoculated with *Lactiplantibacillus plantarum* at an initial density of  
125 10<sup>6</sup> CFU/g. Fermentation was carried out in 250 mL baffled Erlenmeyer flasks containing 50  
126 mL working volume, leaving adequate headspace for gas exchange. Submerged fermentation  
127 was conducted at 37 °C in a thermostatically controlled shaker incubator at 200 rpm for 96 h  
128 under dark, aerobic conditions. No external aeration or gas flushing was applied. As the  
129 microalgae biomass was non-viable, illumination was omitted, and no photosynthetic activity  
130 was expected. Uninoculated *C. vulgaris* biomass flasks served as controls and were processed  
131 identically. Samples were collected at 0, 24, 48, 72 h and 96 h for subsequent biochemical and  
132 sensory analyses. Harvested samples were immediately frozen at -80 °C and freeze-dried for 7  
133 days. The dried fermentates were then ground into a fine powder using a sterile blender and  
134 stored at -20 °C until further analysis.

135 ***Biomass yield and percentage change over time***

136 To determine the percentage dry yield of the biomass (% weight/volume), 0.5 mL of each  
137 sample of unfermented and fermented microalgae suspensions were pipetted into pre-weighed  
138 5 mL tubes for each sample. The samples were frozen overnight in -80 °C freezer, followed by  
139 freeze-drying until fully dried. After drying, the tubes were weighed again to obtain the weight  
140 of the dry biomass. Data were analysed using GraphPad Prism version 8.0, and the percentage  
141 dry yield of the biomass (% weight/volume) and the percentage change in biomass (%) were  
142 calculated using the following formulae:

143  $\text{Dry Yield (\%w/v)} = (\text{Weight of dry biomass (g)} / \text{Volume of wet sample (mL)}) \times 100$

144  $\text{Percentage Change in Biomass (\%)} = [(\text{Fermented biomass} - \text{Unfermented biomass}) /$   
145  $(\text{Unfermented biomass})] \times 100$

146

147 ***In-house olfactory evaluations***

148 An in-house, untrained olfactory panel (n = 10) was recruited to perform time-course olfactory  
149 evaluations on microalgae fermentates inoculated with selected bacterial strains. Panelists  
150 assessed samples at various fermentation timepoints under blinded conditions, with all samples  
151 coded to eliminate bias. Aroma profiling focused on four key sensory attributes: grassy, sour,  
152 fishy, and earthy. Perceived odour intensity was rated using a structured 3-point scale, where  
153 1 = *very weak*, 2 = *moderate*, and 3 = *very strong*. All evaluations were conducted  
154 anonymously. Panellists also completed a demographic and lifestyle questionnaire, which  
155 captured data on age, gender, ethnicity, dietary habits, smoking status, and self-rated smell  
156 sensitivity (on a 5-point scale, where 1 = *very poor* and 5 = *very strong*) (**Table S7**). Prior to

157 participation, all individuals were briefed on the study objectives and procedures and provided  
158 written informed consent.

159

#### 160 *Electronic tongue (E-tongue) analysis*

161 The taste and flavour evolution of the fermented microalgae samples was analysed using the  
162 ASTREE E-tongue system (Alpha MOS, Toulouse, France), a sensor-based technology  
163 designed to mimic human taste perception. The system employs seven potentiometric sensors  
164 (AHS, ANS, CPS, CTS, NMS, PKS, SCS) alongside an Ag/AgCl reference electrode, enabling  
165 the detection of key taste modalities such as bitterness, sweetness, umami, sourness, and  
166 saltiness, thereby generating a comprehensive taste fingerprint of each sample. E-tongue  
167 analysis was conducted following this protocol<sup>1</sup>. Briefly, 300 mg of freeze-dried fermentate  
168 was weighed into a 50 mL Falcon tube and reconstituted with 30 mL of sterile water. The  
169 mixture was vortexed and shaken on a rotary shaker for 30 minutes at room temperature,  
170 followed by centrifugation at  $4000 \times g$  for 30 minutes to obtain the supernatant. Between each  
171 sample run, the sensors and reference electrode were rinsed with water for 10 seconds to  
172 prevent cross-sample interference. Each sample was analysed for 120 seconds, with  
173 measurements repeated nine times to ensure system stability. The sensor signal at the 120th  
174 second was extracted from the last six measurements and averaged to generate the final raw  
175 data. Principal component analysis (PCA) was conducted using R software, and biplots were  
176 generated to visualize sample clustering and taste profile evolution during fermentation.

177

#### 178 *Headspace Solid Phase Micro Extraction (HS-SPME) GC-MS Analysis*

179 Headspace solid-phase microextraction (HS-SPME) was conducted using a 23-gauge, 50/30  
180  $\mu\text{m}$  DVB/CAR/PDMS fibre (Supelco, USA). A volume of 500  $\mu\text{L}$  of the wet sample was  
181 transferred into a 20 mL headspace vial and spiked with 100  $\mu\text{L}$  of an internal standard solution  
182 (2,3-dimethoxytoluene at 10 ppm). The sample was incubated at 80 °C for 10 minutes, after  
183 which the SPME fibre was exposed to the headspace for 30 minutes while agitated at 250 rpm.  
184 Volatile compounds were then thermally desorbed from the fibre in the gas chromatograph  
185 (GC) injector at 250 °C for 600 seconds. Subsequent GC-MS analysis was performed using an  
186 Agilent 7890B GC system coupled with a 5977B mass spectrometer and equipped with a  
187 multimode inlet (Agilent Technologies, USA). Separation was achieved on a polar J&W DB-  
188 Wax Ultra Inert capillary column (30 m  $\times$  0.25 mm I.D., 0.25  $\mu\text{m}$  film thickness; Agilent  
189 Technologies). The injection was operated in split/splitless mode, with split ratios of 1:10. The  
190 oven temperature was initially set to 35 °C, then ramped at 100 °C/min to 60 °C, followed by  
191 8 °C/min to 190 °C, and finally increased at 20 °C/min to 250 °C, where it was held for 6.5  
192 minutes. Helium was used as the carrier gas at a constant flow of 1.0 mL/min. The mass  
193 spectrometer operated in electron ionization mode at 70 eV, with source and transfer line  
194 temperatures of 230 °C and 250 °C, respectively, and data was collected in full scan mode over  
195 the  $m/z$  range 35–450.

196

#### 197 **Untargeted metabolite analysis by LC-MS**

198 Freeze-dried biomass (100 mg) was extracted with 20 mL of 50% aqueous MeOH. The mixture  
199 was vortexed briefly and sonicated for 10 min at room temperature. After sonication, the  
200 samples were centrifuged at 14,000 rpm for 5 min to separate the supernatant and solid  
201 biomass. The supernatant was transferred into LCMS glass vial for LCMS analysis (injection

202 volume: 5 uL). Supernatant which exhibited turbidity were further filtered using 0.45 µm  
203 Claristep hydrophilic filter (Sartorius, Goettingen, Germany) prior to LCMS analysis.

204 HPLC-MS analyses were conducted using Agilent UHPLC 1290 Infinity coupled to Agilent  
205 6540 accurate-mass quadrupole time-of-flight (QTOF) mass spectrometer and an ESI source.  
206 Gradient elution that starts from 98% water with 0.1% formic acid to 100% acetonitrile in 0.1%  
207 formic acid over 8.6 min along with an Acquity UPLC BEH C18 (2.1 × 50 mm, 1.7 µm) column  
208 at a flow rate of 0.5 mL/min was used. The operating parameters for QTOF were the same as  
209 previously reported<sup>2</sup>.

210 The HRMS data were processed and analyzed using Agilent MassHunter Qualitative Analysis  
211 version 10.0 software; The untargeted metabolites analysis and annotation was performed  
212 using MZmine 3.9.0<sup>3</sup>; Compounds annotation in MZmine was performed by matching  
213 experimental MS/MS spectra against library MS/MS spectra. The actual identity of indole  
214 lactic acid, phenyl lactic acid, and hydroxyphenyl lactic acid was validated by comparing  
215 MS/MS spectra and retention time with analytical standards. Metaboanalyst 6.0 was used for  
216 heatmap data visualization<sup>4</sup>.

217

## 218 **Statistical analysis**

219 Olfactory evaluation data were analysed using GraphPad Prism version 8.0. For each aroma  
220 attribute, mean intensity scores were subjected to two-way repeated measures ANOVA, with  
221 treatment (unfermented vs. *Lactiplantibacillus plantarum*-fermented) and fermentation time-  
222 point (0, 24, 48, 72 and 96 hours) specified as within-subject factors. Panellist variation was  
223 included as a blocking factor to account for individual differences. The assumption of

sphericity was not made, and Geisser-Greenhouse correction was applied where necessary.

Statistical significance was determined at an alpha level of 0.05.

## Figures preparation

BioRender (BioRender.com) was used to generate schematic figures for visualising experimental workflows and processes.

## Supporting Data

## Supporting Tables

**Table S1. Enzymatic Activity Profiles of 22 Selected Bacterial Strains**

Strains	Protease Activity	Lipase Activity	Cellulase Activity	β-Glucosidase Activity (mU/mL)
<i>Cupriavidus necator</i>	-	+	+	0.05
<i>Microbacterium imperiale</i>	-	-	+	0
<i>Bacillus pumilus</i>	+++	++	-	0
<i>Bacillus subtilis</i>	++	++	+++	0.07
<i>Bacillus amyloliquefaciens</i>	++	+++	++	0.73
<i>Bacillus licheniformis</i>	+	++	++	0.14
<i>Weizmannia coagulans</i>	-	+++	-	0.14
<i>Priestia megaterium</i>	+++	++	+	0

<i>Lacticaseibacillus paracasei</i>	+++	-	-	0.40
<i>Lacticaseibacillus paracasei</i> ATCC 11578	++	-	-	0
<i>Lactiplantibacillus plantarum</i>	-	-	-	0
<i>Lactiplantibacillus plantarum</i>	-	+	+	0.48
<i>Lactiplantibacillus plantarum</i> ATCC 14917	+++	-	-	0
<i>Lacticaseibacillus rhamnosus</i>	++	-	-	0.54
<i>Limosilacobacillus fermentum</i>	++	-	-	0
<i>Streptococcus thermophilus</i>	++	-	-	0
<i>Liquorilactobacillus nagelii</i>	++	-	-	0
<i>Ligilactobacillus salivarius</i>	++	-	-	0
<i>Pediococcus pentosaceus</i>	++	-	-	0.22
<i>Pediococcus pentosaceus</i>	++	-	-	0
<i>Leuconostoc mesenteroides</i>	++	-	-	0
<i>Leuconostoc citreum</i>	++	-	-	0

233 Agar assays were used to assess protease, lipase, and cellulase activity and are scored  
234 qualitatively. Symbols represent relative activity levels: – (no activity), + (low), ++ (moderate),  
235 +++ (high).  $\beta$ -glucosidase activity was quantified from culture supernatants and expressed in

236 milliunits per milliliter (mU/mL). Strains exhibiting  $\geq$  **0.20mU/mL** of  $\beta$ -glucosidase activity  
237 are classified as positive (values highlighted in red).

238 **Table S2: Dry biomass yield (%w/v) and percentage change (%) of unfermented and fermented microalgae biomass over 72 hours**

Sample	Dry Yield (% w/v)			Mean (n =3)	Standard deviation	Percentage change in fermented biomass (relative to unfermented controls)			Mean (n=3)	Standard deviation
	Replicate 1	Replicate 2	Replicate 3			Replicate 1	Replicate 2	Replicate 3		
Microalgae_0h (unfermented)	9.18	9.22	8.7	9.03	0.29	-	-	-	-	-
Microalgae_24h (unfermented)	8.92	9.16	9.24	9.11	0.17	-	-	-	-	-
Microalgae_48h (unfermented)	9.14	8.94	9.26	9.11	0.16	-	-	-	-	-
Microalgae_72h (unfermented)	9.4	9.1	9.08	9.19	0.18	-	-	-	-	-
<i>B. amyloliquefaciens</i> _MA_0h	9.2	9.26	8.72	9.06	0.30	0.22	0.43	0.23	0.29	0.12
<i>B. amyloliquefaciens</i> _MA_24h	7.94	8.16	8.16	8.09	0.13	-10.99	-10.92	-11.69	-11.20	0.43
<i>B. amyloliquefaciens</i> _MA_48h	8.38	7.72	8.26	8.12	0.35	-8.32	-13.65	-10.80	-10.92	2.67
<i>B. amyloliquefaciens</i> _MA_72h	6.22	5.46	6.04	5.91	0.40	-33.83	-40.00	-33.48	-35.77	3.67
<i>B. subtilis</i> _MA_0h	9.2	9.24	8.7	9.05	0.30	0.22	0.22	0.00	0.14	0.13
<i>B. subtilis</i> _MA_24h	8.18	8.32	8.14	8.21	0.09	-8.30	-9.17	-11.90	-9.79	1.88
<i>B. subtilis</i> _MA_48h	7.94	7.68	7.76	7.79	0.13	-13.13	-14.09	-16.20	-14.47	1.57
<i>B. subtilis</i> _MA_72h	7.7	7.42	7.14	7.42	0.28	-18.09	-18.46	-21.37	-19.30	1.80
<i>L. plantarum</i> _MA_0h	9.18	9.26	8.8	9.08	0.25	0.00	0.43	1.15	0.53	0.58

<i>L. plantarum</i> _MA_24h	9.2	9.46	8.98	9.21	0.24	3.14	3.28	3.22	3.21	0.07
<i>L. plantarum</i> _MA_48h	9.46	9.28	9.6	9.45	0.16	3.50	3.80	3.90	3.73	0.21
<i>L. plantarum</i> _MA_72h	9.82	9.5	9.68	9.67	0.16	4.47	4.40	4.54	4.47	0.07

239 Dry biomass yield (% w/v) and percentage change in microalgae biomass (%) during 72-hour fermentation with selected microbial strains. *B.*  
240 *amyloliquefaciens*, *B. subtilis*, *L. plantarum* are labelled as “*B. amyloliquefaciens*\_MA”, “*B. subtilis*\_MA” and “*L. plantarum*\_MA” respectively;  
241 unfermented samples are labelled as Microalgae. Fermentation timepoints are expressed as 0h, 24h, 48h, and 72h, corresponding to 0, 24, 48, and  
242 72 hours of fermentation, respectively. Dry biomass yield was quantified as dry weight (% w/v) and percentage change was calculated relative to  
243 unfermented controls at corresponding time points. Data represent mean  $\pm$  standard deviation (n = 3 biological replicates). Notably, biomass  
244 decreased progressively during *Bacillus spp.* fermentations, with *B. amyloliquefaciens* showing the highest reduction (~36% at 72 h), while *L.*  
245 *plantarum* showed a modest increase in biomass over time (~+5%).

246 **Table S3: List of volatiles detected in unfermented microalgae and *L. plantarum*-fermented microalgae throughout fermentation**

								Microalgae only (unfermented)					<i>L. plantarum</i> -fermented microalgae				
No	Name	CAS No	Formula	Retention Time (min)	Retention Index (RI)	Compound class	Odour Description	0h	24h	48h	72h	96h	0h	24h	48h	72h	96h
1	Acetic acid	64-19-7	C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	11.2	1462	Acid	Sharp, sour, vinegar	0.000373829	5.59499E-05	0.000102105	7.71635E-05	0.000117517	8.44834E-05	0.000230327	2.85498E-05	1.42339E-05	0
2	Butanoic acid	107-92-6	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	13.9	1640	Acid	Sharp, acetic, cheese, dairy	0.000224656	7.06529E-05	8.0395E-05	0.000100432	9.52012E-05	7.0737E-05	0.0002923	0	0	0
3	Hexanoic acid	142-62-1	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	17.0	1860	Acid	Sour, fatty, sweaty, cheesy	1.72991E-05	1.32659E-05	2.2313E-05	1.95154E-05	2.3045E-05	2.02186E-05	2.65836E-05	4.02418E-06	5.36998E-06	0
4	Octanoic acid	124-07-2	C <sub>8</sub> H <sub>16</sub> O <sub>2</sub>	19.5	2077	Acid	Fatty, waxy, rancid, cheesy	1.73104E-05	4.65514E-05	3.47141E-05	2.71749E-05	5.11016E-05	4.19597E-05	2.47645E-05	0	0	0
5	Propanoic acid	79-09-4	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	12.6	1549	Acid	Pungent, acidic, cheesy, vinegar	0	0	0	1.44669E-05	1.71544E-05	0	1.33469E-05	0	0	0

														05			
6	1-Hexanol	111-27-3	C6H14O	9.6	1358	Alcohol	Green, fruity, sweet	1.1306 1E-05	7.48597 E-06	6.23502 E-06	6.79656 E-06	5.62038 E-06	7.581 96E-06	8.148 62E-05	0	0	0
7	1-Octanol	111-87-5	C8H18O	12.6	1548	Alcohol	Mushroom, green, waxy	0	0	0	0	0	0	0	0	0	4.317 49E-06
8	1-Octen-3-ol	3391-86-4	C8H16O	11.1	1453	Alcohol	Mushroom	0.0001 08602	7.89387 E-05	0.00011 246	0.000122 192	0.00012 6945	0.000 1171 02	0.000 1129 86	5.945 33E-05	4.576 77E-05	4.489 33E-05
9	1-Pentanol	71-41-0	C5H12O	8.0	1256	Alcohol	Fresh, bready, winey	3.4081 5E-05	0.00010 8101	0.00011 1004	0.000106 372	0.00011 0896	6.817 37E-05	0.000 1628 8	5.756 53E-06	9.027 69E-06	9.838 97E-06
10	1-Penten-3-ol	616-25-1	C5H10O	6.6	1163	Alcohol	Pungent, green, horseradish, green vegetable, tropical, fruity	0.0001 30451	0.00013 3269	8.80199 E-05	0.000114 489	0.00013 0628	9.508 3E-05	7.846 61E-05	0	0	0
11	Isobutanol	78-83-1	C4H10O	5.7	1098	Alcohol	Ethereal, winey	0	0	0	0	0	0	0	6.837 8E-	0	0

															06		
12	Isopentyl alcohol	123-51-3	C5H12O	7.4	1215	Alcohol	Fusel, alcoholic, fruity, banana	3.8701 3E-06	1.64211 E-05	3.58926 E-06	4.64628 E-06	5.24433 E-07	2.801 9E-06	1.336 8E-05	6.884 74E-05	7.679 48E-05	4.841 16E-05
13	Isophytol	505-32-8	C20H40 O	21.1	2290	Alcohol	Floral, herbal, green	0.0002 83568	0.00024 7227	0.00030 138	0.000257 763	0.00021 8515	0.000 2522 64	0.000 2987 84	0.000 3068 44	0.000 2925 7	0.000 3684 16
14	2-Heptenal, (Z)-	57266-86-	C7H12O	9.2	1334	Aldehyde	Green, fatty, sweet	3.5713 3E-05	4.22325 E-05	2.06006 E-05	3.77043 E-05	3.64459 E-05	6.316 58E-05	3.863 03E-05	5.355 39E-06	1.195 44E-05	1.841 86E-05
15	2-Hexenal, (E)-	6728-26-3	C6H10O	7.6	1229	Aldehyde	Green, banana, aldehydic, fresh, herbal	4.1539 9E-05	2.95631 E-05	4.40041 E-05	3.84183 E-05	4.39E-05	4.755 77E-05	3.496 7E-05	1.343 8E-05	1.367 17E-05	7.358 64E-06
16	2-Nonenal, (E)-	18829-56-6	C9H16O	12.6	1550	Aldehyde	Cucumber, fatty, green	1.3641 E-05	1.93503 E-05	6.58394 E-06	1.08327 E-05	1.23925 E-05	7.660 58E-06	4.314 69E-06	5.837 61E-06	2.550 98E-06	0
17	Heptanal	111-71-7	C7H14O	7.0	1191	Aldehyde	Fatty, green	8.1421 8E-06	5.3004E-06	1.77838 E-05	1.34867 E-05	1.59664 E-05	1.346 07E-05	0	0	0	3.113 4E-06

18	Hexanal	66-25-1	C <sub>6</sub> H <sub>12</sub> O	5.6	1085	Aldehyde	Green, grassy	2.9506 9E-05	4.9805E -05	7.3148 E-05	3.17118 E-06	4.81524 E-05	8.812 79E-05	2.973 48E-06	2.182 73E-05	2.396 16E-05	1.652 79E-05
19	Nonanal	124-19-6	C <sub>9</sub> H <sub>18</sub> O	10.3	1400	Aldehyde	Green, cucumber	3.6746 1E-05	3.55442 E-05	3.17581 E-05	3.06157 E-05	2.04399 E-05	2.305 36E-05	9.418 31E-06	8.651 51E-06	1.492 92E-05	1.392 31E-05
20	2-Octenal, (E)-	2548-87-0	C <sub>8</sub> H <sub>14</sub> O	10.9	1441	Aldehyde	Fresh, cucumber, fatty, green, citrus	3.0478 E-05	3.47488 E-05	2.22665 E-05	3.24509 E-05	3.86952 E-05	2.441 24E-05	0	9.478 91E-06	1.051 35E-05	9.661 93E-06
21	2-Pentenal, (E)-	1576-87-0	C <sub>5</sub> H <sub>8</sub> O	6.3	1138	Aldehyde	Pungent, green, fruity, apple orange, tomato	1.5116 4E-05	4.7341E -05	4.86063 E-05	4.22268 E-05	4.86639 E-05	4.970 87E-05	2.668 13E-05	6.983 78E-06	9.204 E-06	2.390 77E-05
22	3- methylbutanal	590-86-3	C <sub>5</sub> H <sub>10</sub> O	3.9	921	Aldehyde	Ethereal, aldehydic, chocolate, peach, fatty	2.5536 3E-05	1.69893 E-05	1.53889 E-05	9.52913 E-06	1.05045 E-05	2.140 92E-05	5.196 1E-06	0	0	0
23	4-Heptenal, (Z)-	6728-31-0	C <sub>7</sub> H <sub>12</sub> O	7.9	1247	Aldehyde	Green, oily, fatty, dairy	3.6757 5E-06	5.52971 E-06	4.70133 E-06	5.25069 E-06	5.82723 E-06	5.472 14E-06	3.674 06E-06	4.420 02E-06	0	2.936 83E-06
24	beta-	432-	C <sub>10</sub> H <sub>16</sub>	14.0	1643	Aldehyde	Tropical, saffron,	9.1109	7.51192	3.68818	9.54359	6.1081	3.993	0.000	9.155	2.874	4.798

	Cyclocitral	25-7	O				herbal, clean, rose, sweet, tobacco, green, fruity	8E-05	E-05	E-05	E-05	E-05	24E-05	107971	99E-05	44E-05	27E-05
25	cis-2-Butenal	590-18-1	C <sub>4</sub> H <sub>6</sub> O	5.1	1047	Aldehyde	Pungent, suffocating, irritating	4.05156E-05	4.18626E-05	4.11305E-05	4.13284E-05	4.00872E-05	3.88505E-05	2.45241E-05	4.86375E-06	4.81032E-06	1.94214E-06
26	Dodecanal	112-54-9	C <sub>12</sub> H <sub>24</sub> O	15.3	1732	Aldehyde	Soapy, waxy, aldehydic, citrus, green, floral	0.000104569	4.85737E-06	1.72808E-05	0	1.15631E-05	5.45698E-06	4.29987E-06	4.93151E-06	0	2.65449E-06
27	Octanal	124-13-0	C <sub>8</sub> H <sub>16</sub> O	8.6	1296	Aldehyde	Orange peel, green	0	3.71881E-06	3.18694E-06	6.57751E-06	3.00568E-06	3.68664E-06	0	0	0	0
28	Pentanal	110-62-3	C <sub>5</sub> H <sub>10</sub> O	4.5	984	Aldehyde	Fermented, bready, cocoa	0.000164836	0.000127786	0.000128118	0.000111268	0.000125985	0.000137583	3.51212E-05	0	1.45685E-05	3.46825E-05
29	Undecanal	112-44-7	C <sub>11</sub> H <sub>22</sub> O	13.6	1614	Aldehyde	Waxy, soapy, floral, aldehydic, citrus, green, fatty, laundered cloth	0	3.1398E-06	2.86654E-06	0	0	0	0	0	0	0

30	4-ethylbenzaldehyde	4748-78-1	C <sub>9</sub> H <sub>10</sub> O	15.2	1729	Aromatic	Almond, bitter, sweet, anise cherry	1.90247E-05	6.79073E-05	8.25158E-05	8.93263E-05	0.000107134	3.87547E-05	0	0	0	0
31	Benzaldehyde	100-52-7	C <sub>7</sub> H <sub>6</sub> O	12.4	1540	Aromatic	Almond, cherry, sharp, sweet	0.000686077	0.000670456	0.000738445	0.000639122	0.000723182	0.000667591	0.000174753	0.000287285	0.000264358	0.000245761
32	Benzaldehyde, 2,4-dimethyl-	613-45-6	C <sub>9</sub> H <sub>10</sub> O	15.5	1751	Aromatic	Naphthyl, cherry, almond, spicy, vanilla	0.00014304	0.00020615	0.000191227	0.00017273	0.000183541	0.000185366	6.22234E-05	3.82608E-05	1.39722E-05	3.62033E-05
33	Benzaldehyde, 3-methyl-	620-23-5	C <sub>8</sub> H <sub>8</sub> O	13.9	1641	Aromatic	Sweet, fruity, cherry, almond	3.63298E-05	0	0	0	0	0	0	0	0	0
34	Benzene, 1,3-bis(1,1-dimethylethyl)-	1014-60-4	C <sub>14</sub> H <sub>22</sub>	10.8	1433	Aromatic	-	4.89165E-05	5.79204E-05	6.22572E-05	5.59074E-05	4.92305E-05	7.00738E-05	0	3.06168E-05	4.80208E-05	3.11789E-05
35	Benzyl alcohol	100-51-6	C <sub>7</sub> H <sub>8</sub> O	17.5	1892	Aromatic	Floral, rose, phenolic, balsamic	0	0	0	0	0	0	3.24128E-05	2.45013E-05	0	0
36	Naphthalene,	447-	C <sub>13</sub> H <sub>16</sub>	15.8	1768	Aromatic	Licorice	0.0001	8.07668	0.00019	0.000154	0.00016	8.171	0.000	0.000	0.000	0.000

	1,2-dihydro- 1,1,6- trimethyl-	53-0						71255	E-05	4913	746	5185	33E- 05	1792 82	1286 24	2094 27	2138 28
37	Phenylacetaldehyde	122- 78-1	C8H8O	14.2	1659	Aromatic	Rose, sweet, floral	0	1.34409 E-05	2.36096 E-05	0	7.33735 E-06	2.182 27E- 05	0	0	0	0
38	Phenylethyl alcohol	60-12- 8	C8H10O	17.9	1933	Aromatic	Floral, rose, sweet	0.0002 91961	0.00025 571	0.00027 5207	0.000254 718	0.00027 4726	0.000 1778 31	0.000 3015 47	0.001 5459 77	0.002 3880 9	0.002 4782 73
39	p-Xylene	106- 42-3	C8H10	6.4	1147	Aromatic	Sweet	1.1166 8E-05	0	0	0	0	8.238 51E- 06	0	0	0	0
40	2,4- Decadienal, (E,E)-	25152 -84-5	C10H16 O	16.6	1827	Enal	Satty, chicken	0	0	0	0	1.28238 E-05	0	0	0	0	0
41	2,4- Heptadienal, (E,E)-	4313- 03-5	C7H10O	11.9	1507	Enal	Fatty, green, oily, aldehydic, vegetable, cinnamon	0.0005 76431	0.00070 9327	0.00077 8931	0.000728 95	0.00092 8734	0.000 7242 94	0.000 3731 58	0	5.456 77E- 05	0.000 1060 13

42	2,4-Hexadienal, (E,E)-	142-83-6	C <sub>6</sub> H <sub>8</sub> O	10.5	1415	Enal	Sweet, green, spicy, floral, citrus	2.6175 3E-05	4.4413E -05	3.19583 E-05	1.63111 E-05	1.95492 E-05	5.348 76E-05	0	4.864 28E-06	3.272 38E-06	8.944 91E-06
43	2,4-Nonadienal, (E,E)-	5910-87-2	C <sub>9</sub> H <sub>14</sub> O	15.0	1717	Enal	Fatty, melon, cucumber, chicken fat	1.7184 7E-05	7.44766 E-05	7.43974 E-05	5.47693 E-05	9.9412 E-05	8.661 24E-05	1.738 4E-05	0	0	9.033 27E-06
44	2,6-Nonadienal, (E,Z)-	557-48-2	C <sub>9</sub> H <sub>14</sub> O	13.3	1599	Enal	Green, fatty, dry, cucumber, violet leaf	4.2153 2E-05	2.43174 E-05	2.53043 E-05	3.00407 E-05	2.21378 E-05	1.305 E-05	2.798 58E-05	1.365 66E-05	1.382 85E-05	4.886 94E-06
45	Methyl palmitate	112-39-0	C <sub>17</sub> H <sub>34</sub> O <sub>2</sub>	20.7	2228	Ester	Fatty, waxy	6.4327 E-05	1.85663 E-05	3.67519 E-05	5.34491 E-05	2.14683 E-05	3.953 51E-05	2.320 69E-05	4.145 7E-05	4.105 57E-05	1.847 66E-05
46	Methyl salicylate	119-36-8	C <sub>8</sub> H <sub>8</sub> O <sub>3</sub>	16.2	1799	Ester	Wintergreen, minty	0.0007 48143	0.00064 7308	0.00058 2888	0.000574 573	0.00052 8463	0.000 5890 75	0.000 6150 54	0.000 1730 08	0.000 5354 53	0.000 5405 67
47	2-Acetyl-5-methylfuran	1193-79-9	C <sub>7</sub> H <sub>8</sub> O <sub>2</sub>	13.4	1607	Furan	Sweet, musty, nutty, caramellic	0	0	0	0	0	0	0	0	8.277 36E-05	0
48	2-ethylfuran	3208-	C <sub>6</sub> H <sub>8</sub> O	4.2	955	Furan	Chemical, beany,	2.9886	2.66821	2.75321	2.68418	3.24093	3.115	2.309	2.124	1.554	2.426

		16-0					ethereal, cocoa, bready, malty, coffee, nutty	7E-05	E-05	E-05	E-05	E-05	1E-05	77E-05	33E-05	44E-05	48E-05
49	2-Pentylfuran	3777-69-3	C9H14O	7.6	1234	Furan	Fruity, beany, vegetable	0.000262495	0.000170152	0.000153915	0.000109902	8.60189E-05	0.000304494	8.22013E-05	7.5605E-05	6.40852E-05	0.000113595
50	3-Furanmethanol	4412-91-3	C5H6O2	14.3	1669	Furan	Sweet, nutty, herbal	0	0	0	0	0	0	1.66561E-05	0	0	0
51	5-methylfurfural	620-02-0	C6H6O2	12.9	1568	Furan	Sweet, caramel, maple	1.64153E-05	1.40762E-05	1.45381E-05	1.31659E-05	1.43611E-05	1.52432E-05	0	0	0	0
52	Furan, 2-methyl-	534-22-5	C5H6O2	3.6	874	Furan	Chocolate, ethereal, acetone	3.37885E-06	1.99509E-06	1.92152E-06	1.74903E-06	0	3.19082E-06	5.8813E-07	1.14447E-06	0	1.37179E-06
53	Furfural	98-01-1	C5H4O2	11.4	1473	Furan	Sweet, woody, almond, bread, baked	0.000192257	0.000176687	0.000234249	0.000142119	9.04195E-05	0.000169261	2.00106E-05	2.41157E-06	0	0
54	trans-2-(2-	70424	C9H12O	8.8	1306	Furan	Bean, grassy	5.5219	1.06584	1.05849	9.12875	1.08564	9.220	0	1.834	3.566	0

	Pentenyl)furan	-14-5						5E-06	E-05	E-05	E-06	E-05	86E-06		51E-06	62E-07	
55	1,3,5,7-Cyclooctatetraene	629-20-9	C8H8	8.1	1265	Hydrocarbon	-	0	0	0	0	0	0	0	0	0	1.98204E-06
56	3-Heptadecene, (Z)-	68155-00-0	C9H18O	15.1	1723	Hydrocarbon	-	0.000283823	0.000362702	0.00058726	0.000529519	0.00050902	0.000171216	0.000183636	0.000484612	0.000403239	0.000484425
57	Heptadecane	629-78-7	C17H36	14.8	1698	Hydrocarbon	Waxy	0.000700864	0.000731208	0.001215075	0.001006742	0.001170633	0442546	0.000442546	0.00047186	0.000493414	0.000950684
58	Pentadecane	629-62-9	C15H32	11.8	1498	Hydrocarbon	-	4.04429E-05	9.63707E-05	0.000130275	9.38504E-05	0.000123106	6.7386E-05	6.13493E-05	4.87533E-05	5.03987E-05	5.40487E-05
59	Undecane	1120-21-4	C10H22	4.6	999	Hydrocarbon	-	0	4.80151E-06	5.10924E-06	4.5991E-06	0	3.23377E-06	0	2.66008E-06	0	6.42428E-06
60	(E,E)-3,5-Octadiene-2-	30086-02-3	C8H12O	13.1	1584	Ketone	Fruity, green, grassy	0.001027837	0.000853237	0.00081154	0.00071048	0.000752466	0.0009705	0.0008568	0.0002118	0.0001063	7.81424E-

	one												66	94	37	35	05
61	1-Octen-3-one	4312-99-6	C <sub>8</sub> H <sub>14</sub> O	8.8	1309	Ketone	Herbal, mushroom, earthy, must,y dirty	1.3969E-05	1.60312E-05	1.79359E-05	0	1.32361E-05	1.37119E-05	1.8517E-05	1.60293E-05	5.74918E-06	1.69357E-05
62	1-Penten-3-one	1629-58-9	C <sub>5</sub> H <sub>8</sub> O	4.9	1026	Ketone	Spicy, pungent, peppery, mustard, garlic, onion	0	0	1.80323E-05	0	0	0	1.4325E-05	0	0	0
63	1-Propanone, 1-(2-furanyl)-	3194-15-8	C <sub>7</sub> H <sub>8</sub> O <sub>2</sub>	13.2	1590	Ketone	Fruity	0	0	0	0	0	0	0	0	3.11861E-06	4.629E-06
64	2,3-Butanedione	431-03-8	C <sub>4</sub> H <sub>6</sub> O <sub>2</sub>	4.4	976	Ketone	Buttery, sweet, creamy, pungent, caramellic	0	0	0	1.55107E-05	0	0	0	2.16852E-05	0	0
65	2,3-Pentanedione	600-14-6	C <sub>5</sub> H <sub>8</sub> O <sub>2</sub>	5.2	1056	Ketone	Sweet, buttery, creamy	7.004E-06	2.19717E-05	2.35508E-05	2.08714E-05	2.55922E-05	2.23478E-05	1.63437E-05	1.83899E-05	1.67855E-05	5.24942E-06
66	2-Butanone	78-93-3	C <sub>4</sub> H <sub>8</sub> O	3.8	908	Ketone	Acetone, ethereal, fruity, camphoraceous	0.00024514	0.000221226	0.000348183	0.000155413	0.000153143	0.000223449	0.000126828	0.000274341	0.000202228	0.000144416

67	2-Heptanone	110-43-0	C7H14O	7.0	1187	Ketone	Cheesy, fruity, ketogenic, green, banana, creamy	3.4466 9E-05	1.6017E-05	1.51541 E-05	0	0	0	0	0	0	0
68	2-Nonanone	821-55-6	C9H18O	10.2	1397	Ketone	Fruity, sweet, waxy, soapy, cheesy, green, herbal, coconut	1.3666 9E-05	2.43512 E-05	3.91895 E-05	0	0	4.486 29E-05	1.563 26E-05	0	0	0
69	2-Pentadecanone, 6,10,14-trimethyl-	502-69-2	C18H36O	20.0	2137	Ketone	Oily, herbal, jasmine, celery, woody	0.0003 21032	0.00029 6771	0.00032 2788	0.000317 161	0.00039 4462	0.000 2991 94	0.000 2071 34	0.000 1879 17	0.000 2342 06	0.000 2122 84
70	2-Tridecanone	593-08-8	C13H26O	16.5	1820	Ketone	Fatty, waxy, dairy, milky	2.1947 6E-05	2.93369 E-05	1.91158 E-05	2.79608 E-05	3.16983 E-05	2.987 41E-05	2.029 39E-05	0	0	0
71	3,5-Octadien-2-one	38284-27-4	C8H12O	12.3	1532	Ketone	Fruity, fatty, mushroom	0.0001 41213	0.00015 384	0.00016 6226	9.56053 E-05	0.00012 918	0.000 1088 19	9.728 88E-05	0	0	0
72	3-Nonen-2-one	14309-57-0	C9H16O	12.2	1524	Ketone	Fruity, berry, fatty, oily	0	1.54487 E-05	1.45496 E-05	2.19196 E-05	2.7222 E-05	2.130 97E-05	1.197 24E-05	5.082 51E-06	0	0

73	3-Octanone	106-68-3	C8H16O	8.1	1260	Ketone	Lavender, mushroom, sweet	1.0029 4E-05	7.74798 E-06	3.31775 E-06	0	0	9.172 42E-06	2.680 99E-05	0	0	1.463 66E-06
74	3-Octanone, 2-methyl-	923-28-4	C9H18O	9.0	1323	Ketone	-	0.0001 0475	7.37462 E-05	0.00010 4964	0	3.45306 E-05	0.000 1234 55	1.749 83E-05	0	0	0
75	5-Hepten-2-one, 6-methyl-	110-93-0	C8H14O	9.4	1345	Ketone	Citrus, green, musty, lemongrass, apple	2.8076 4E-05	2.42381 E-05	2.37667 E-05	2.75072 E-05	3.0203 E-05	2.553 02E-05	1.943 99E-05	0	0	0
76	6-Methyl-3,5-heptadiene-2-one	1604-28-0	C8H12O	13.5	1608	Ketone	Spicy, cinnamon, coconut, spicy, woody, sweet, weedy	0.0001 8724	0.00024 5117	0.00024 3097	0.000150 534	0.00023 5556	0.000 2630 96	0.000 1792 41	0	0	0
77	Acetoin	513-86-0	C4H8O2	8.7	1299	Ketone	Buttery, creamy, dairy, milky, fatty	0	0	0	0	1.11621 E-05	0	0	0	0	0
78	Acetone	67-64-1	C3H6O	3.2	818	Ketone	Solvent, ethereal, apple, pear	0	0	0	0	1.89788 E-05	0	1.275 31E-05	1.878 63E-05	9.595 86E-05	9.938 38E-05
79	Acetophenone	98-86-	C8H8O	14.4	1670	Ketone	Sweet, hawthorn	1.4756	0	0	0	0	0	1.450	0	0	0

		2						9E-05						63E-05			
80	Cyclohexanon e, 2,2,6- trimethyl-	2408- 37-9	C9H16O	9.2	1335	Ketone	Thujonic, pungent, labdanum, honey	2.4851 9E-05	5.27998 E-05	4.69297 E-05	2.01988 E-05	3.13161 E-05	4.283 09E- 05	2.552 85E- 05	2.175 41E- 05	0	5.135 E-06
81	Isophorone	78-59- 1	C9H14O	13.6	1621	Ketone	Cooling, woody, sweet, green, camphoraceous, fruity, musty	8.9816 5E-05	0.00012 6727	4.45773 E-05	0	4.33334 E-05	3.967 4E- 05	8.854 49E- 05	4.153 23E- 05	7.954 99E- 05	0.000 1170 45
82	m- Methylacetop henone	585- 74-0	C9H10O	16.2	1795	Ketone	Hawthorn, sweet, mimosa, coumarinic, cherry, acacia	0.0002 03678	0.00021 3941	0.00021 4632	0.000199 17	0.00020 2363	0.000 2366 24	0.000 1757 38	0.000 1643 06	0.000 1879 12	0.000 1846 4
83	alpha-Ionone	127- 41-3	C13H20 O	17.2	1874	Terpene	Sweet, woody, floral, violet, orris, tropical, fruity	0.0021 00297	0.00127 0786	0.00192 1168	0.001877 712	0.00126 9374	0.002 0122 84	0.001 8867 74	0.001 8128 74	0.001 8023 84	0.001 9332 68
84	beta-Ionone epoxide	23267 -57-4	C13H20 O2	18.9	2019	Terpene	Fruity, sweet, berry, woody, violet, orris, powdery	0.0014 56673	0.00133 0894	0.00131 4103	0.001370 537	0.00149 5476	0.001 3948 85	0.001 3816 75	0.001 1931 37	0.001 3258 55	0.001 4819 14

85	Neophytadiene	504-96-1	C <sub>20</sub> H <sub>38</sub>	17.9	1929	Terpene	-	0.000179889	0.000251886	0.000341725	0.000260144	0.000364417	0.000273054	0.000324966	0.00032797	0.000322565	0.000437689
86	trans-beta-Ionone	79-77-6	C <sub>13</sub> H <sub>20</sub> O	18.3	1966	Terpene	dry powdery floral woody orris berry seedy	0.001467838	0	0.004007879	0.001349576	0	0.004001712	0.003838057	0.003551018	0.003691388	0.003880322
87	trans-Geranylacetone	3796-70-1	C <sub>13</sub> H <sub>22</sub> O	17.1	1865	Terpene	Floral, fresh, green, rose	0.000366719	0.000322123	0.000318789	0.000209751	0.000342013	0.000337794	0.000332665	0	0	0
88	2-Acetylthiazole	24295-03-2	C <sub>5</sub> H <sub>5</sub> NO <sub>2</sub> S	14.3	1665	Others	Pandan, popcorn, hazelnut, peanut	4.19906E-05	5.78992E-05	6.20847E-05	3.29585E-05	7.25037E-05	6.0368E-05	1.98643E-05	1.23594E-06	0	0
89	2,3,5-Trimethylpyrazine	14667-55-1	C <sub>7</sub> H <sub>10</sub> N <sub>2</sub>	10.6	1421	Pyrazine	Nutty	5.56146E-06	6.45521E-06	1.25676E-05	0	0	0	4.92684E-06	1.19941E-05	1.3142E-05	1.35664E-05
90	2,5-Dimethylpyrazine	123-32-0	C <sub>6</sub> H <sub>8</sub> N <sub>2</sub>	9.3	1340	Pyrazine	Cocoa, roasted, beefy, nutty	2.83319E-05	0	0	2.30964E-05	1.68021E-05	0	1.85597E-05	0	4.28933E-05	1.95621E-05
91	2,6-	108-	C <sub>6</sub> H <sub>8</sub> N <sub>2</sub>	9.3	1338	Pyrazine	Cocoa, roasted,	0	0	0	0	0	0	0	1.703	0	1.017

	dimethylpyrazine	50-9					nutty, meaty								75E-05		84E-05
92	2-ethyl-3,6-dimethylpyrazine	13360-65-1	C8H12N2	11.2	1460	Pyrazine	Roasted, potato	2.4717E-05	2.25479E-05	2.13461E-05	1.89756E-05	2.06317E-05	2.2107E-05	5.59949E-06	2.93993E-05	1.99367E-05	1.892E-05
93	2-Ethyl-5-methylpyrazine	13360-64-0	C7H10N2	10.4	1408	Pyrazine	Coffee, nut	8.4125E-06	1.40265E-05	1.44929E-05	1.0381E-05	1.704E-05	1.73075E-05	1.08178E-05	8.73359E-06	1.25065E-05	1.31454E-05
94	2-Ethylpyrazine	13925-00-3	C6H8N2	9.5	1350	Pyrazine	Nutty, fermented coffee, meaty	0	1.4925E-06	0	0	0	0	0	0	0	0
95	2-Methylpyrazine	109-08-0	C5H6N2	8.4	1281	Pyrazine	Nutty, cocoa, chocolate	5.64735E-06	1.56795E-05	1.67164E-05	1.50864E-05	1.66667E-05	1.35332E-05	0	1.45025E-05	1.58873E-05	1.60826E-05
96	2,4,6-trimethylpyridine	108-75-8	C8H11N	10.0	1388	Pyridine	-	5.35797E-06	6.96537E-06	8.23105E-06	6.81916E-06	7.76736E-06	8.21101E-06	4.28681E-06	7.05771E-06	4.94132E-06	5.82558E-06
97	3-methylpyridine	108-99-6	C6H7N	8.9	1316	Pyridine	Green, earthy, hazelnut, nutty	4.72888E-06	3.89947E-06	0	7.09646E-06	0	3.85177E-06	0	0	8.36633E-06	4.07514E-06

98	Pyridine	110-86-1	C <sub>5</sub> H <sub>5</sub> N	7.2	1204	Pyridine	Sour, fishy	1.0131 6E-05	9.70381 E-06	1.02752 E-05	7.86009 E-06	6.04669 E-06	1.053 57E-05	1.152 31E-05	1.073 48E-05	9.524 69E-06	9.122 24E-06
99	1H-Pyrrole-2,5-dione, 3-ethyl-4-methyl-	21494-57-5	C <sub>7</sub> H <sub>9</sub> NO	21.2	2298	Pyrrole	-	0.0001 92216	0.00016 3596	0.00018 2589	0.000195 079	0.00021 8631	0.000 1708 95	0.000 1886 6	0.000 1682 9	0.000 1784 33	0.000 1967 25
101	Dimethyl trisulfide	3658-80-8	C <sub>2</sub> H <sub>6</sub> S <sub>3</sub>	10.2	1399	Sulphurous	Sulphurous, onion, meaty, rotten eggs	0	0	0	2.53319 E-06	0	0	0	0	0	0

247 Summary of all the volatile compounds detected by GC-MS in unfermented microalgae samples and *L. plantarum*-fermented microalgae samples  
248 across different time points (0h, 24h, 48h, 72h, and 96h). Each compound entry includes its chemical name, CAS number, molecular formula,  
249 retention time (min), retention index (RI), compound class, and odour description and abundances at different time points.

250

251 **Table S4: ASTREE E-tongue sensor summary with food applications**

	Sensor	Taste Modality	Sensitivity and typical detected compounds	Common applications
1	AHS	Sour	Organic acids, H <sup>+</sup> ions	<ul style="list-style-type: none"> <li>· Fermented foods (e.g., yogurt, kimchi, sauerkraut).</li> <li>· Vinegar/acidity profiling in sauces.</li> <li>· Spoilage detection (e.g., acid build-up).</li> </ul>
2	CTS	Salty	Na <sup>+</sup> , K <sup>+</sup> , Cl <sup>-</sup> , mineral salts	<ul style="list-style-type: none"> <li>· Salt reduction in soups and snacks.</li> <li>· Mineral water profiling.</li> <li>· Electrolyte beverage development.</li> </ul>
3	NMS	Umami	Glutamate, IMP, GMP, amino acids	<ul style="list-style-type: none"> <li>· Umami enhancement in broth/stock.</li> <li>· Fermented soy (miso, soy sauce).</li> <li>· Meat analogues or plant-based meat optimization.</li> </ul>
4	ANS	Sweet	Glucose, fructose, sucrose, and artificial sweeteners	<ul style="list-style-type: none"> <li>· Sweetener formulation in beverages</li> <li>· Sugar content consistency in fruit juices</li> <li>· Sugar-free product comparisons</li> </ul>
5	SCS	Bitter	Caffeine, polyphenols, quinine, alkaloids	<ul style="list-style-type: none"> <li>· Coffee and tea bitterness profiling.</li> <li>· Cocoa/chocolate evaluation.</li> <li>· Bitterness masking in functional foods/supplements.</li> </ul>
6	PKS	General/Reference	Detects overall ionic strength or changes in general chemical environment	<ul style="list-style-type: none"> <li>· Acts as a reference to help differentiate complex mixtures and stabilize the signal</li> </ul>
7	CPS	General/Reference		

252 Description of electronic tongue (E-tongue) sensors used for taste modality detection in food  
253 samples. The table summarizes the target analytes for each sensor and their common  
254 applications in food quality evaluation, flavour profiling, and product development <sup>5-13</sup>.

255

256 **Table S5. Metabolite profile of umami-related compounds detected during *L. plantarum*-**  
257 **mediated biotransformation of microalgae**

Compound name	Mass to charge ratio (m/z)	Peak Area				
		<i>L. plantarum</i> _MA_0h	<i>L. plantarum</i> _MA_24h	<i>L. plantarum</i> _MA_48h	<i>L. plantarum</i> _MA_72h	<i>L. plantarum</i> _MA_96h
Glutamic acid	148.0605	26077.91	25747.33	7396.46	6104.25	4747.83

3'-AMP	346.0547	15341.44	15621.17	64523.82	71823.88	56305.31
Adenosine 2',3'-cyclic monophosphate (cAMP)	330.059	10029.51	8643.28	14599.89	8634.29	4084.71
Adenosine 5'-monophosphate (AMP)	348.07	1293.7	13687.83	57535.56	68646.83	57002.32
Cyclic GMP (cGMP)	344.0396	4024.884766	4647.526367	7276.584961	3959.945313	774.7654419
Guanosine 5'-monophosphate	362.0501	40930.2	48802.02	61079.58	32945.93	15488.41

258 Umami-related compounds were detected using LC-MS and identified based on their mass-to-  
259 charge ratio (m/z) Peak area values represent relative abundances at each fermentation time  
260 point (0h, 24h, 48h, 72h, 96h).

261

262 **Table S6. Metabolite profile of amino acids and their bioconversion products during *L.***  
263 ***plantarum*-mediated biotransformation of microalgae**

Compound name	Mass to charge ratio (m/z)	Peak Area				
		<i>L. plantarum</i> _MA_0h	<i>L. plantarum</i> _MA_24h	<i>L. plantarum</i> _MA_48h	<i>L. plantarum</i> _MA_72h	<i>L. plantarum</i> _MA_96h
L-Tyrosine	182.0787	37898	34893	7181	0	0
Phenylalanine	166.0866	89252	89795	8013	6714	4542
4-Hydroxyphenyllactic acid	181.0503	7257	5588	87693	127266	145663
D-Tryptophan	205.0973	58778	57684	8754	16172	13113
D-3-phenyllactic acid	165.0557	28351	20197	136790	327943	389709
DL-Indole-3-lactic acid	204.0666	0	0	24333.55	53092.48	60450.36

264 Amino acids and their relevant metabolites were detected using LC-MS and identified based  
 265 on their mass-to-charge ratio (m/z). Peak area values represent relative abundances at each  
 266 fermentation time point (0h, 24h, 48h, 72h, 96h).

267

268 **Table S7. Demographic and lifestyle information of the sniff test panellists (n = 10).**

<b>Participant (n=10)</b>	<b>Gender</b>	<b>Age range</b>	<b>Race</b>	<b>Diet</b>	<b>Smoker?</b>	<b>Self-rated smell sensitivity</b>
1	Male	31-40	Chinese	Omnivore	No	5
2	Male	41-50	Chinese	Omnivore	No	2
3	Male	31-40	Chinese	Omnivore	No	3
4	Male	21-30	Chinese	Omnivore	No	3
5	Male	31-40	Chinese	Omnivore	No	3
6	Female	31-40	Chinese	Omnivore	No	5
7	Female	41-50	Indian	Omnivore	No	3
8	Female	31-40	Malay	Omnivore	No	5
9	Female	21-30	Chinese	Omnivore	No	3
10	Female	31-40	Chinese	Omnivore	No	3

269 Demographic details and lifestyle factors of the untrained olfactory evaluation panel (n = 10).  
 270 All panellists were non-smokers and followed an omnivorous diet. Self-rated olfactory  
 271 sensitivity was collected using a 5-point scale (1 = very poor, 5 = very strong).

272

273 **Table S8. Two-way ANOVA statistics for grassy odour intensity.**

ANOVA table	SS	DF	MS	F (DFn, DFd)	P value	Significance and Interpretation
Interaction (Time × Treatment)	3.400	4	0.8500	F (4, 72) = 3.161	P=0.0188	The change in grassy odour over time depends on treatment.
Time (Row Factor)	2.440	4	0.6100	F (3.282, 59.07) = 2.269	P=0.0845	No significant change in grassy odour intensity over time alone.
Treatment (Column Factor)	0.2500	1	0.2500	F (1, 18) = 0.2089	P=0.6531	No overall difference between fermented and unfermented samples.
Subject (Panellist variation)	21.54	18	1.197	F (18, 72) = 4.450	P<0.0001	Panellists varied significantly in how they rated the grassy odour.

274 A two-way repeated measures ANOVA was used to assess the effects of fermentation  
 275 treatment, time, and their interaction on grassy odour intensity. A significant interaction  
 276 between time and treatment (p = 0.0188) indicates that the change in grassy odour perception  
 277 over time differed depending on fermentation condition. A significant subject effect indicates  
 278 variability among panellist ratings (P<0.0001). No significant main effects of time or treatment  
 279 were observed. Geisser-Greenhouse correction was applied to the time effect ( $\epsilon$  = 0.8204).  
 280 Note: *F* = F-ratio; DF = degrees of freedom; SS = sum of squares; MS = mean square.

281

282 **Table S9. Statistical summary of pairwise comparison for grassy odour intensity between**  
 283 **unfermented and *L. plantarum*-fermented microalgae.**

<b>Difference between column means</b>	
Mean of Microalgae only	2.060
Mean of <i>L. plantarum</i> _MA	1.960
Difference between means	0.1000
SE of difference	0.2188
95% CI of difference	-0.3596 to 0.5596

284 Reported values include mean difference, standard error (SE), and 95% confidence interval  
285 (CI).

286

287 **Table S10. Two-way ANOVA statistics for sour odour intensity.**

<b>ANOVA table</b>	<b>SS</b>	<b>DF</b>	<b>MS</b>	<b>F (DFn, DFd)</b>	<b>P value</b>	<b>Significance and Interpretation</b>
Interaction (Time × Treatment)	1.840	4	0.4600	F (4, 72) = 2.875	P=0.0287	The change in sour odour over time depends on treatment.
Time (Row Factor)	1.840	4	0.4600	F (2.301, 41.41) = 2.875	P=0.0607	No significant change in sour odour intensity over time alone.
Treatment (Column Factor)	0.8100	1	0.8100	F (1, 18) = 0.9480	P=0.3431	No overall difference in sour odour between the fermented and unfermented groups.
Subject (Panellist variation)	15.38	18	0.8544	F (18, 72) = 5.340	P<0.0001	Panellists varied significantly in how they rated sour odour.

288 A two-way repeated measures ANOVA was used to assess the effects of fermentation  
 289 treatment, time, and their interaction on sour odour intensity. A significant interaction between  
 290 time and treatment ( $p = 0.0287$ ) indicates that the change in grassy odour perception over time  
 291 differed depending on fermentation condition. A significant subject effect indicates variability  
 292 among panellist ratings ( $P < 0.0001$ ). No significant main effects of time or treatment were  
 293 observed. Geisser-Greenhouse correction was applied to the time effect ( $\varepsilon = 0.5751$ ). Note:  $F$   
 294 = F-ratio; DF = degrees of freedom; SS = sum of squares; MS = mean square.

295

296 **Table S11. Statistical summary of pairwise comparison for sour odour intensity between**  
 297 **unfermented and *L. plantarum*-fermented microalgae.**

Difference between column means	
Mean of Microalgae only	1.220
Mean of <i>L. plantarum</i> _MA	1.400
Difference between means	-0.1800
SE of difference	0.1849
95% CI of difference	-0.5684 to 0.2084

298 Reported values include mean difference, standard error (SE), and 95% confidence interval  
 299 (CI).

300

301 **Table S12. Two-way ANOVA statistics for fishy odour intensity.**

ANOVA table	SS	DF	MS	F (DFn, DFd)	P value	Significance and Interpretation
Interaction (Time $\times$ Treatment)	0.1000	4	0.02500	F (4, 72) = 0.06329	P=0.9925	No difference in changes between fermented and unfermented samples over time.
Time (Row)	1.460	4	0.3650	F (2.627, 47.29) = 0.9241	P=0.4262	No significant change in fishy odour intensity

Factor)						over time alone.
Treatment (Column Factor)	0.000	1	0.000	F (1, 18) = 0.000	P>0.9999	No overall difference in fishy odour between the fermented and unfermented groups.
Subject (Panelist variation)	24.96	18	1.387	F (18, 72) = 3.511	P<0.0001	Panellists varied significantly in how they rated fishy odour.

302 A two-way repeated measures ANOVA was used to assess the effects of fermentation  
303 treatment, time, and their interaction on fishy odour intensity. A significant subject effect  
304 indicates variability among panellist ratings ( $P<0.0001$ ). No significant main effects of  
305 interaction, time or treatment were observed. Geisser-Greenhouse correction was applied to the  
306 time effect ( $\epsilon = 0.6569$ ). Note:  $F$  = F-ratio; DF = degrees of freedom; SS = sum of squares; MS  
307 = mean square.

308

309 **Table S13. Statistical summary of pairwise comparison for fishy odour intensity between**  
310 **unfermented and *L. plantarum*-fermented microalgae.**

<b>Difference between column means</b>	
Mean of Microalgae only	1.520
Mean of <i>L. plantarum</i> _MA	1.520
Difference between means	0.000
SE of difference	0.2355
95% CI of difference	1.520

311 Reported values include mean difference, standard error (SE), and 95% confidence interval  
312 (CI).

313

314 **Table S14. Two-way ANOVA statistics for earthy odour intensity.**

ANOVA table	SS	DF	MS	F (DFn, DFd)	P value	Significance and Interpretation
Interaction (Time × Treatment)	0.9400	4	0.2350	F (4, 72) = 0.7719	0.9400	No difference in changes between fermented and unfermented samples over time.
Time (Row Factor)	1.140	4	0.2850	F (3.299, 59.38) = 0.9361	1.140	No significant change in earthy odour intensity over time alone.
Treatment (Column Factor)	0.3600	1	0.3600	F (1, 18) = 0.1617	0.3600	No overall difference in earthy odour between the fermented and unfermented groups.
Subject (Panellist variation)	40.08	18	2.227	F (18, 72) = 7.314	40.08	Panellists varied significantly in how they rated earthy odour.

315 A two-way repeated measures ANOVA was used to assess the effects of fermentation  
316 treatment, time, and their interaction on earthy odour intensity. A significant subject effect  
317 indicates variability among panellist ratings ( $P < 0.0001$ ). No significant main effects of  
318 interaction, time or treatment were observed. Geisser-Greenhouse correction was applied to the  
319 time effect ( $\epsilon = 0.5470$ ). Note:  $F$  = F-ratio; DF = degrees of freedom; SS = sum of squares; MS  
320 = mean square.

321

322 **Table S15. Statistical summary of pairwise comparison for earthy odour intensity**  
323 **between unfermented and *L. plantarum*-fermented microalgae.**

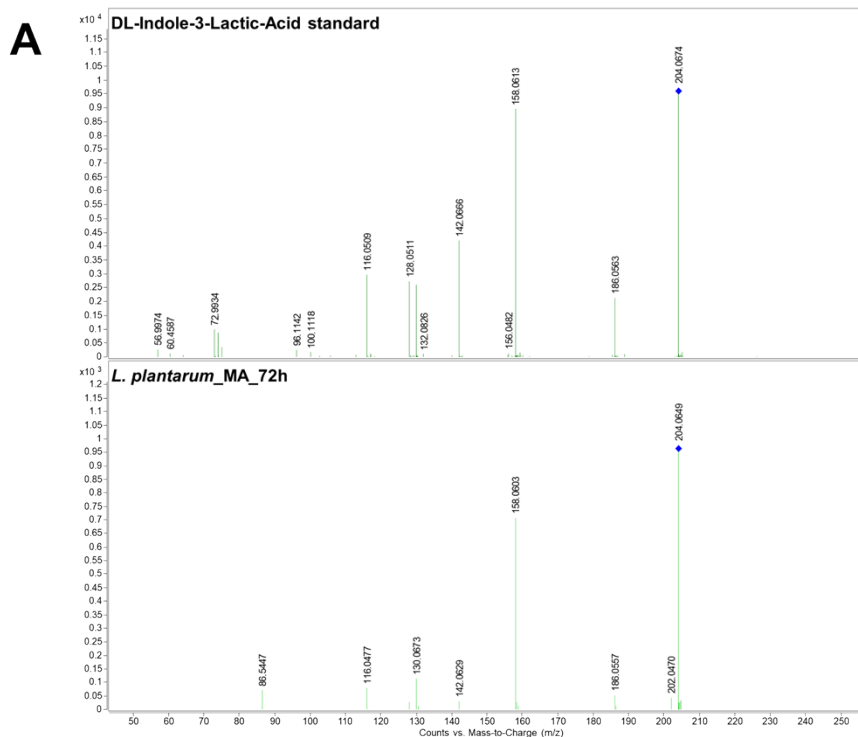
Difference between column means	
Mean of Microalgae only	1.720

Mean of <i>L. plantarum</i> _MA	1.600
Difference between means	0.1200
SE of difference	0.2984
95% CI of difference	-0.5070 to 0.7470

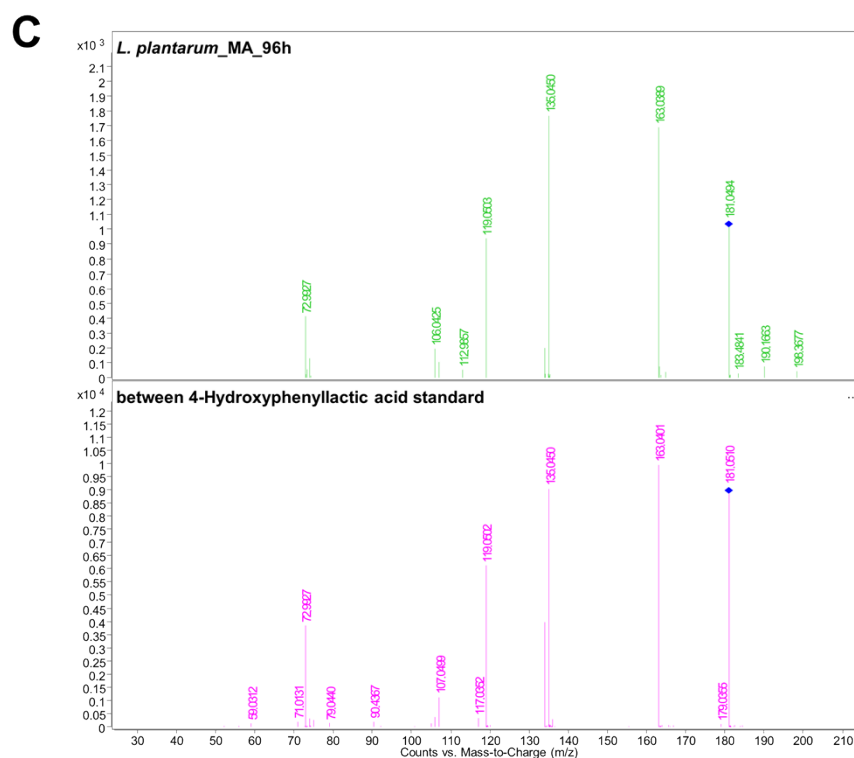
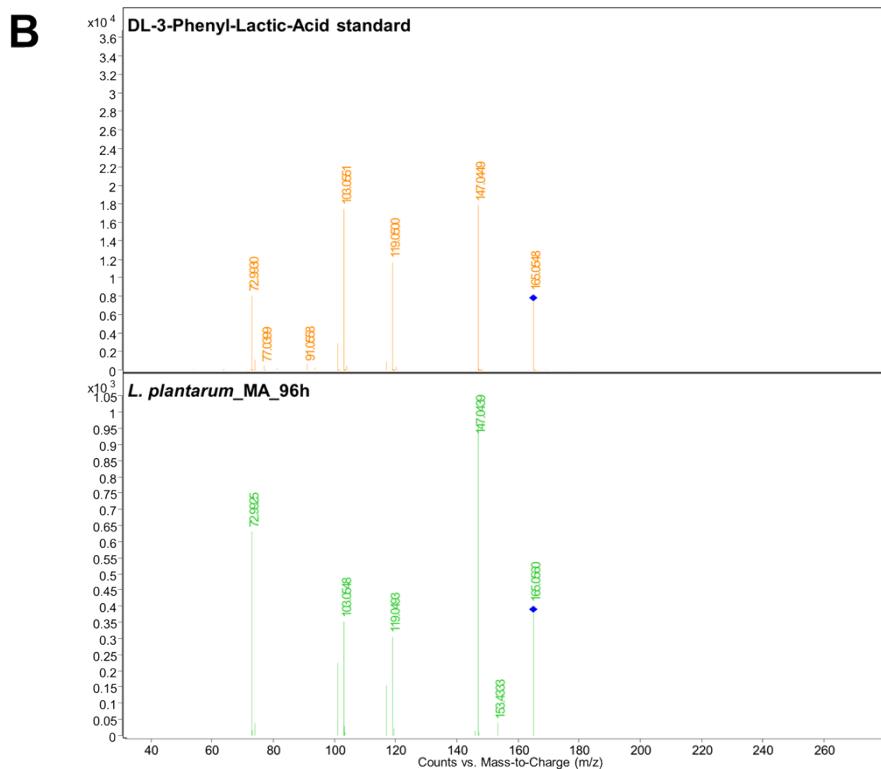
324 Reported values include mean difference, standard error (SE), and 95% confidence interval  
325 (CI).

326

## 327 Supporting Figures

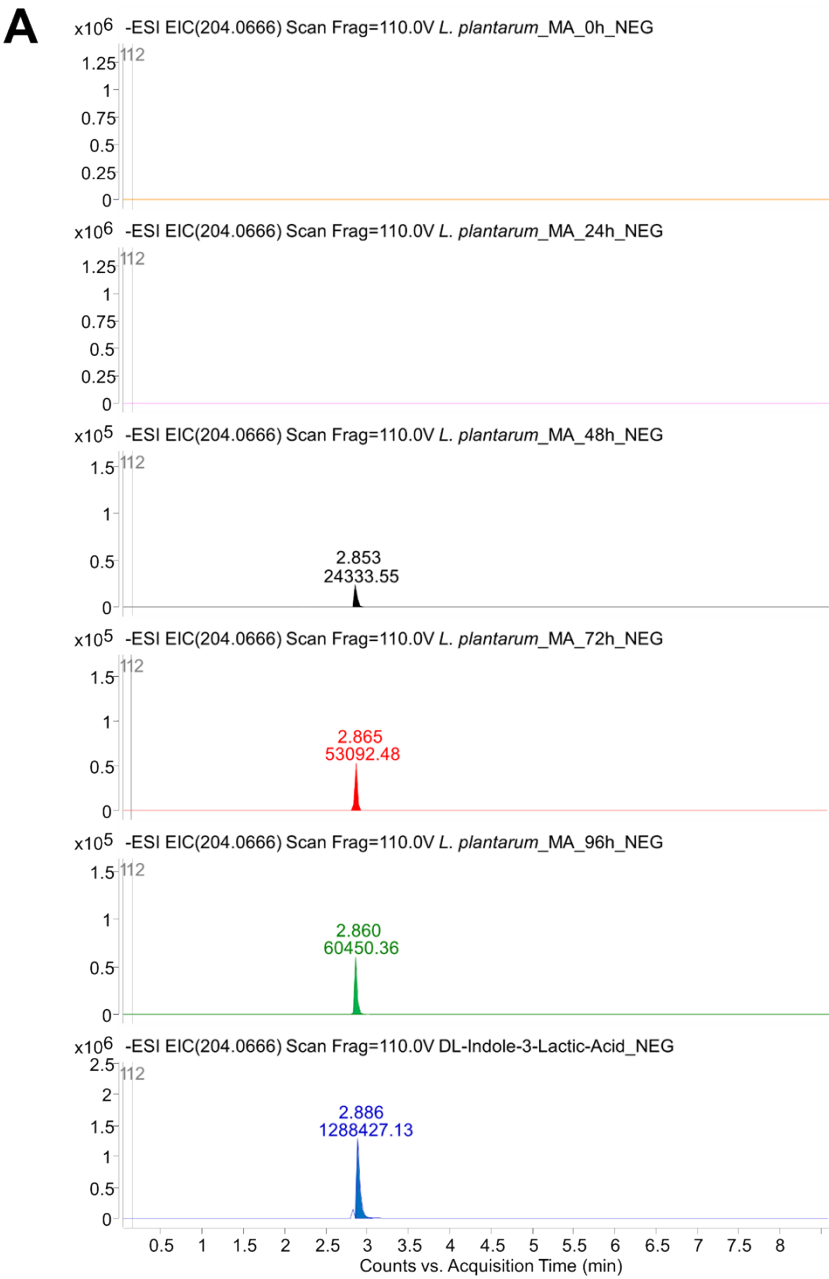


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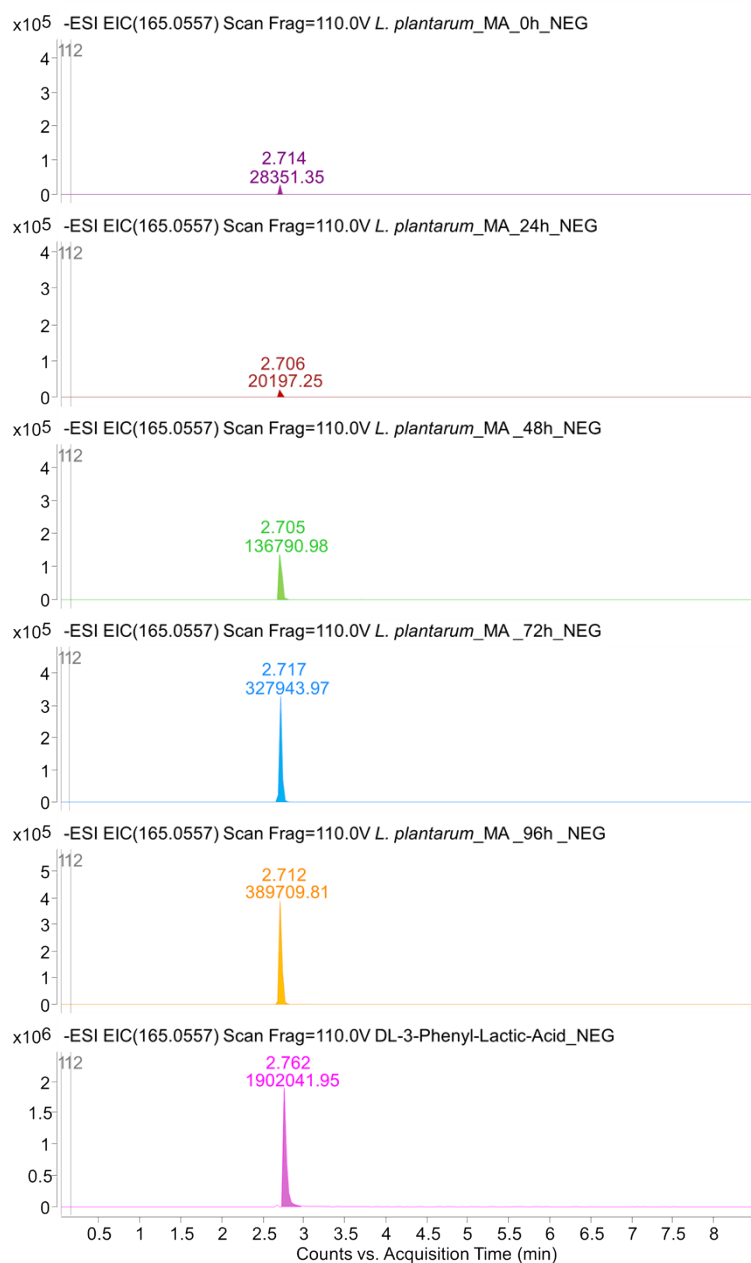


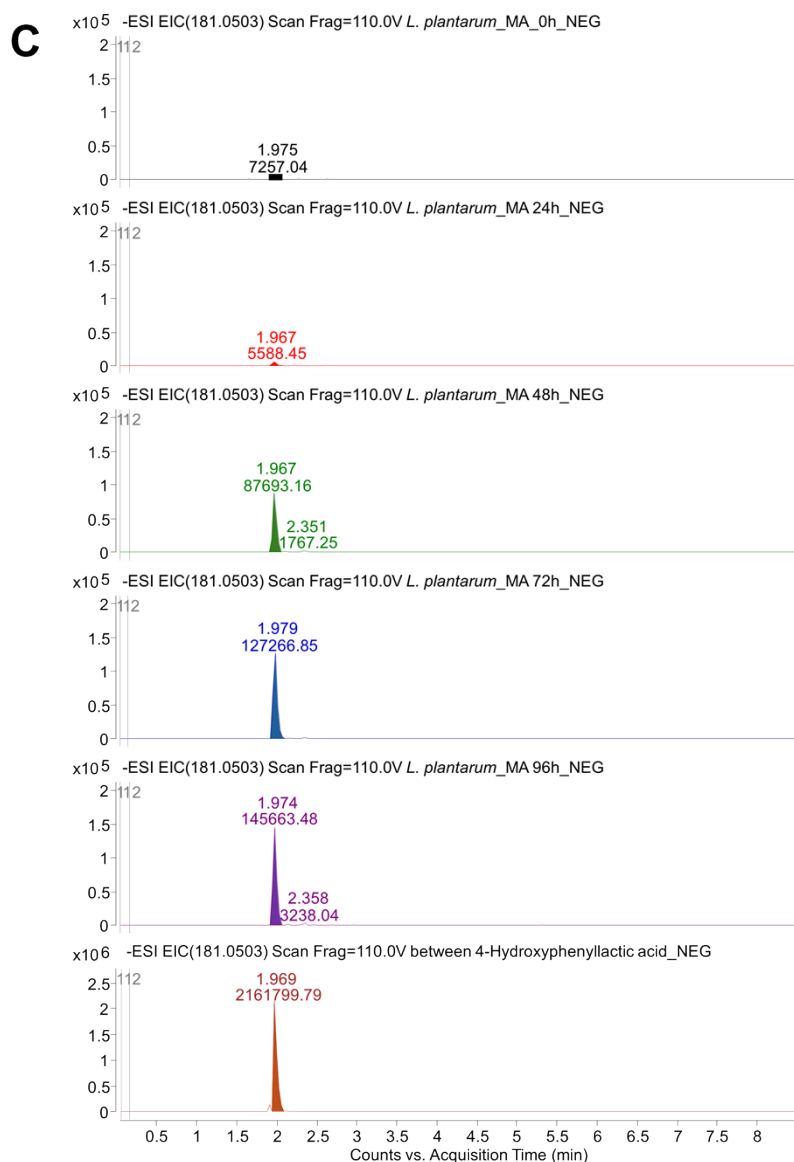
333 **Figure S1. LC-MS/MS fragmentation spectra at collision-induced dissociation (CID)10V**  
 334 **of aromatic lactic acid derivatives in *L. plantarum*-fermented microalgae. (A)** MS/MS  
 335 spectra of key fragment ions matched between DL-Indole-3-lactic acid reference standard and  
 336 *L. plantarum*-fermented microalgae at 72h of fermentation. **(B)** MS/MS spectra of key  
 337 fragment ions matched between DL-3-phenyllactic acid reference standard and *L. plantarum*-  
 338 fermented microalgae at 96 h of fermentation. **(C)** MS/MS spectra of key fragment ions  
 339 matched between 4-Hydroxyphenyllactic acid reference standard and *L. plantarum*-fermented  
 340 microalgae at 96h of fermentation.

341



342

**B**

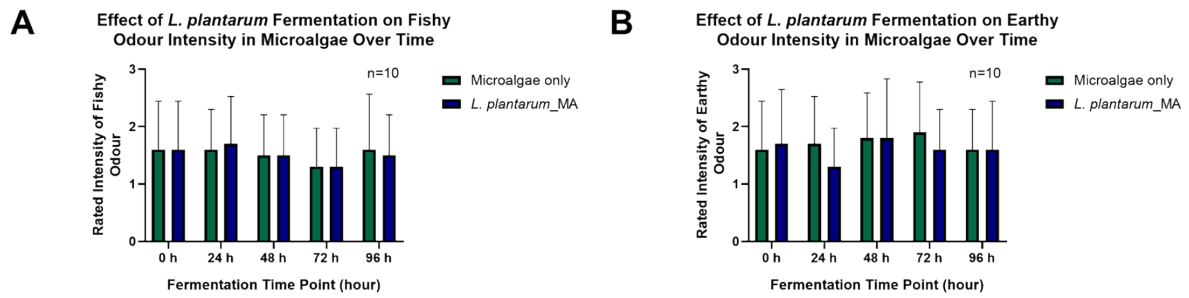


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345

346 **Figure S2. Extracted ion chromatograms (EICs) from LC-MS showing the bioconversion**  
 347 **of precursor amino acids during *L. plantarum*-mediated fermentation of microalgae (MA)**  
 348 **over 96 hours. (A–C) LC-MS EICs showing the time-dependent increase in signal intensity**  
 349 **of (A) DL-indole-3-lactic acid (m/z 204.0666), (B) D-3-phenyllactic acid (m/z 165.0557), and**  
 350 **(C) 4-Hydroxyphenyllactic acid (m/z 181.0503), across fermentation time points (0h, 24h, 48h,**  
 351 **72h, 96h) compared to reference standards.**

352



353

354 **Figure S3. Olfactory evaluation of microalgae fermented with *L. plantarum*. (A-B)**  
 355 Sensory intensities of (A) fishy and (B) earthy odour attributes in unfermented microalgae  
 356 (Microalgae only) and *L. plantarum*-fermented microalgae (*L. plantarum*\_MA) over 96 hours.  
 357 Olfactory evaluation was performed by an untrained in-house olfactory panel (n = 10), with  
 358 intensities ranked on a structured 3-point scale (1 = weak, 2 = moderate, 3 = strong). Bars  
 359 represent mean  $\pm$  standard deviation.

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