

**Supplementary Table.** <sup>1</sup>H NMR chemical shift assignments of the metabolites detected in saliva.

	Metabolites	ppm	a		Metabolites	ppm	a		Metabolites	ppm	a
1	acetic acid	1.92	s	19	choline	3.20	s	37	sarcosine	2.74 3.61	s s
2	lactic acid	1.33 4.12	d q	20	phosphocholine	3.22	s	38	threonine	1.33 4.26 3.59	d
3	propanoic acid	1.06 2.19	t q	21	taurine	3.26 3.43	t t	39	alanine	1.48 3.79	d q
4	butanoic acid	0.90 1.56 2.16	t sx t	22	β-galactose	4.59 3.50 3.66 3.94	d t d d d	40	proline	2.02 2.07; 2.36 3.34; 3.42 4.13	m m  dt dd
5	2-methylbutanoic acid	0.86 1.39, 1.49 1.05 2.20	t m d	23	α-galactose	5.27 3.81 3.86 4.00	d d d d d d	41	valine	0.99 1.05 2.27 3.62	d d m d
6	2-methylpropionic (isobutyric acid)	2.39 1.07	sp d	24	β-glucose	4.65 3.25 3.49 3.42	d t	42	leucine	0.96 0.97 1.72 3.73	d d  d
7	4-methylpentanoic (isocaproic acid)	0.88 1.52 1.45 2.19	d  q t	25	α-glucose	5.24 3.54	d	43	isoleucine	0.94 1.01 1.48 1.98 3.67	t d
8	3-methylbutanoic acid (isovaleric acid)	0.91 1.96 2.05	d m d	26	β-fucose	4.56 3.45 3.65 3.76 3.81 1.25	d t d d d q d	44	lysine	3.76 1.90 1.45 1.73 3.03	
9	5-aminopentanoic acid	2.24 1.64 1.68 3.02	t m m t	27	α-fucose	5.21 3.77 3.86 3.82 4.20 1,21	d d d d d q d	45	ornithine?	3.78 1.94 3.06	
10	pyruvic acid	2.38	s	28	maltose?	5.42 5.23? 4.66	d d d	46	tyrosine	3.06, 3.21 3.95 6.90	

										7.20	
11	succinic acid	2.41	s	29	glycine	3.56	s	47	phenylalanine	3.13, 3.29 4.00 7.33 7.39 7.42	
12	3-phenylpropionic acid	2.50 2.92 7.30	m m m	30	ethanol	1.19 3.66	t q	48	histidine	7.09 7.87	
13	3-(4-hydroxyphenyl)propionic acid (phloretic acid)	2.45 2.82 6.85 7.18	t t m m	31	glycerol	3.66 3.56 3.79	m m m	49	N-acetyl groups	2.06	s
14	phenylacetic acid	3.54 7.30 7.37	s m m	32	propylene glycol	1.15 3.88 3.55 3.45	d	50	unknown	1.15 3.63	d
15	4-hydroxyphenyl acetic acid	3.45 6.87 7.17	s m m	33	trimethylamine	2.90	s	51	unknown	1.15 3.73	d
16	$\delta$ valerolactam	2.33 1.78 1.74 3.30	t m m t	34	dimethylamine	2.73	s	52	unknown (acetoin?)	1.38 4.43	d
17	formate	8.46	s	35	monomethylamine	2.61	s	53	unknown	3.16	s
18	ethanolamine	3.15 3.83	m m	36	putrescine	1.77 3.06	m t				

a: <sup>1</sup>H multiplicity (s, singlet; d, doublet; dd, doublet of doublets; t, triplet; q, quartet; m, multiplet; sx, sextet)