Association between salivary metabolites and gingival bleeding score in healthy subjects. A pilot study

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Table S1. Demographic data of the study participants

Subject	Sex	Age (years)	Height (cm), weight (Kg)	Drugs in the last 12h	Smoke
01	Male	25	176, 79	/	Occasionally
02	Female	25	160, 57	/	/
03	Male	24	175, 68	/	/
04	Male	23	187, 83	/	/
05	Female	25	167, 70	/	/
06	Male	25	175, 68	/	/
07	Female	25	170, 62	/	e-cigarette
08	Female	24	163, 50	Birth-control pill	/
09	Male	25	183, 80	/	/
10	Female	25	170, 65	/	/
11	Male	21	175, 72	/	/
12	Female	24	164, 52	/	Yes (5/die)
13	Female	25	170, 62	Birth-control pill	/
14	Male	23	170, 72	/	/
15	Male	23	170, 63	/	/
16	Male	23	180, 75	/	Occasionally
17	Female	20	177, 64	/	/
18	Female	24	170, 58	Antihistamine	/
19	Female	20	165, 60	/	Yes (5/die)
20	Male	25	175, 65	/	/

Table S2. Dental/periodontal parameters and whole saliva flow of the study participants

Subject	DMFT	PSR	FMBS (%)	FMPS (%)	Whole Saliva Flow (mL/5 min)
01	0	1	5.7%	12.1%	3.0
02	0	1	7.5%	18.4%	1.1
03	1	1	2.9%	16.8%	2.3
04	3	1	0.7%	9.3%	2.0
05	0	1	11.4%	5.0%	2.4
06	2	0	0%	4.3%	1.3
07	0	1	0.7%	8.3%	5.0
08	0	1	3.6%	5.7%	1.9
09	1	1	0.6%	6.8%	2.2
10	5	1	2.9%	19.6%	1.1
11	4	1	2.8%	2.8%	1.0
12	4	1	2.8%	7.7%	4.5
13	2	1	4.5%	24.8%	2.4
14	2	1	3.5%	16.4%	5.0
15	2	1	4.2%	22.4%	2.1
16	3	1	4.5%	23.4%	1.2
17	0	1	1.4%	9.9%	1.8
18	0	1	6.7%	18.8%	1.1
19	2	1	7.1%	22.7%	0.9
20	0	1	1.9%	14.1%	3.0

DFMT: *Decayed, Missing, and Filled Teeth*; PSR: *Periodontal Screening and Recording;* FMBS: *Full Mouth Bleeding Score,* FMPS: *Full Mouth Plaque Score*

Table S3. Eukaryotic and prokaryotic cell counts obtained from whole saliva samples

Subject	Prokaryotic cells (cell/mL)	Eukaryotic cells (cells/mL)
01	1.95E+09	7.75E+05
02	3.71E+09	5.10E+05
03	1.10E+09	1.35E+05
04	2.52E+09	1.50E+04
05	N.d.	7.80E+05
06	1.06E+09	2.85E+05
07	1.16E+09	3.00E+04
08	1.17E+09	2.09E+06
09	2.63E+08	2.40E+05
10	1.11E+09	7.75E+05
11	5.46E+08	5.75E+05
12	9.89E+08	4.40E+05
13	1.02E+08	7.50E+04
14	4.05E+08	8.00E+04
15	7.00E+08	4.70E+05
16	2.85E+09	1.45E+06
17	1.51E+09	4.60E+05
18	3.39E+09	4.95E+05
19	2.08E+09	2.05E+05
20	1.71E+08	3.90E+05
Mean	*1.41E+09*	*5.14E+05*
St dev	*1.07E+09*	*5.04E+05*

N.d. not determined

Amino acids and amino acid derivatives

Y-axis: DOWN-UP, scale from -1.5 to 1.5

Categories: 5-Aminopentanoate, Alanine, Alloisoleucine, Aspartate, Betaine, Carnitine, Creatine, Creatinine, Glutamate, Glutamine, Glycine, Histidine, Isoleucine, Leucine, Lysine, Phenylalanine, Proline, Putrescine, Pyroglutamate, Sarcosine, Taurine, Threonine, Tyrosine, Valine

Organic acids

Y-axis: DOWN-UP, scale from -1.5 to 1

Categories: 2-Aminoadipate, 2-Hydroxy-3-methylvalerate, 2-Hydroxybutyrate, 2-Hydroxyisovalerate, 3-Hydroxybutyrate, 3-Methylglutarate, 3-Phenylpropionate, 4-Hydroxyphenylacetate, 4-Hydroxyphenyllactate, Acetate, Butyrate, Citrate, Formate, Isobutyrate, Isocaproate, Isovalerate, Lactate, Malonate, Phenylacetate, Propionate, Pyruvate, Succinate

Carbohydrates   Pur/Pyr metabolism   Others

Y-axis: DOWN-UP, scale from -1.5 to 1

Categories: Fucose, Galactose, Glucose, Lactose, Maltose, Hypoxanthine, Uracil, Xanthine, Choline, Ethanolamine, Glycerol, N-Acetylglucosamine, O-Phosphoethanolamine, Urea
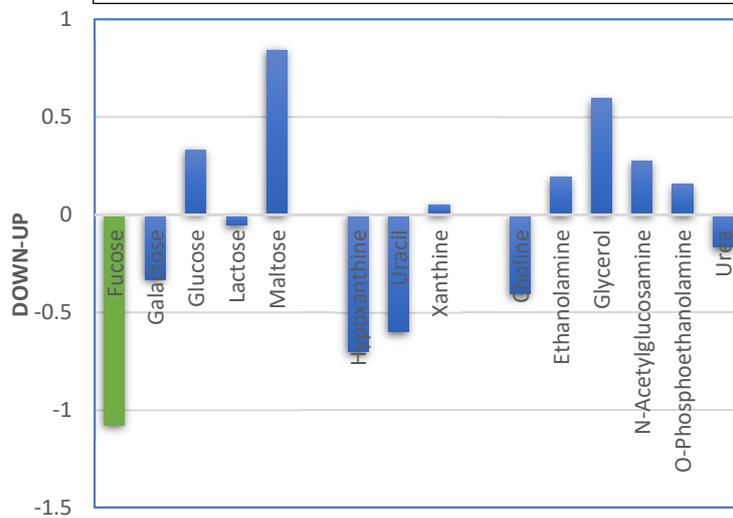
Figure S1. Differences in metabolite concentrations between DOWN and UP groups. Metabolite concentrations have been normalized by the median and autoscaled. The graph displays the difference between the mean values obtained for the UP and DOWN groups (DOWN-UP) for all salivary metabolites. The green bars correspond to the metabolites with a DOWN-UP difference higher than ±1, which coincides with the top five VIP metabolites identified by PLS-DA analysis.
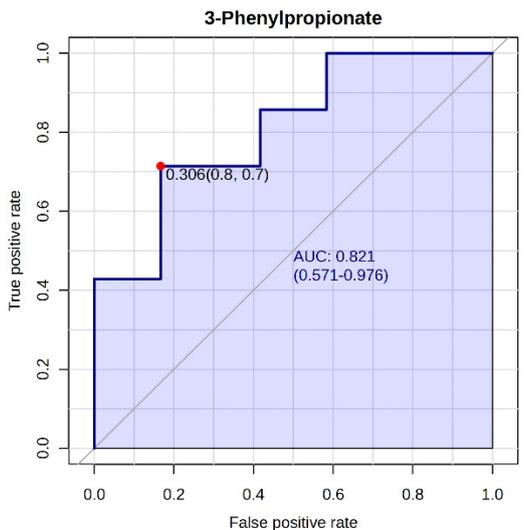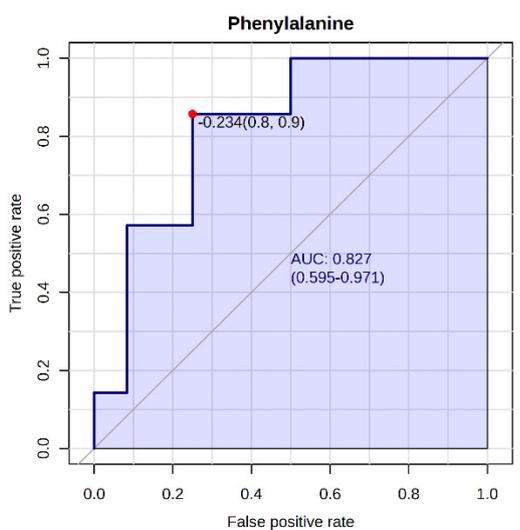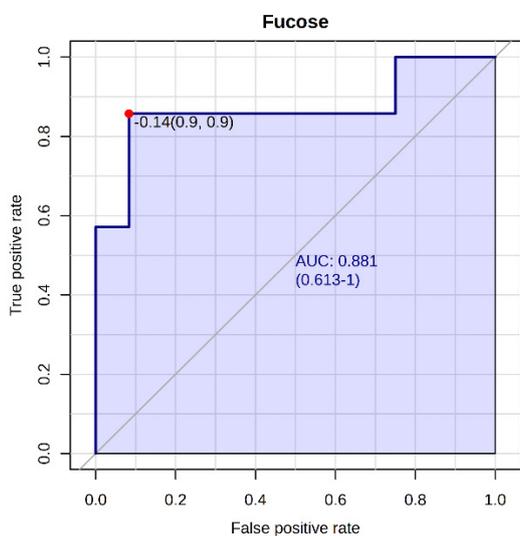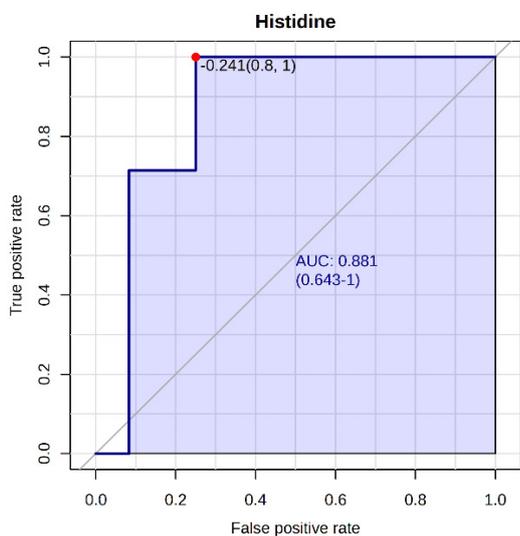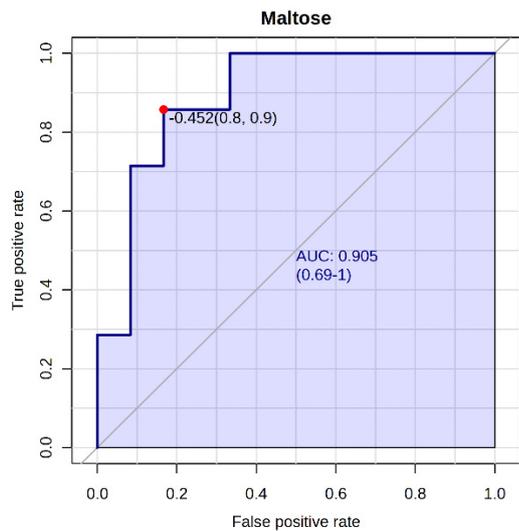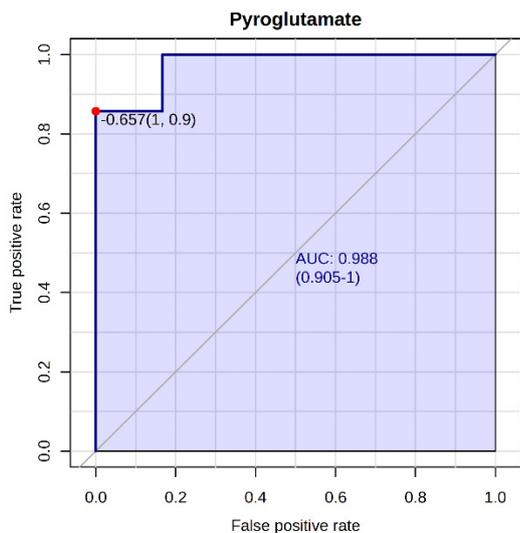
Figure S2. Univariate ROC curve analysis for selected metabolite features. The solid red dot indicates the optimal cutoff with the associated sensitivity and specificity values.