

Identification of a Biomarker Panel for Diagnosis of Early Childhood Caries Using Salivary Metabolic Profile

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Supplementary Data

Snyder's caries activity test Approximately 0.2 µL of the saliva was pipetted into melted Snyder's medium at 50 °C. After the addition of saliva to the medium, the tube was rotated for proper mixing of saliva and the medium and incubated at 37 °C for up to 72 h. Color changes were observed every 24 h. The rate of color change of Snyder's medium from green to yellow is indicative of caries activity. Snyder's test results were evaluated as follows: Score 1: no color change up to 72 h (negative caries activity); score 2: color change at 48–72 h (slight caries activity); score 3: color change at 24–48 h (moderate caries activity); and score 4: color change within 24 h (severe caries activity).

Table S1. Identified and quantified salivary metabolites from ¹H-NMR spectra.

Metabolites	Control (n=29)				ECC (n=25)			
	Mean (mM)	SD	Mean (mM)	SD	ECC0 (n=6)		ECC2 (n=19)	
					Mean (mM)	SD	Mean (mM)	SD
3-Hydroxybutyrate	0.0037	0.0014	0.0043	0.0016	0.0038	0.0012	0.0045	0.0017
3-Hydroxyisovalerate	0.0052	0.0017	0.0073	0.0025	0.0064	0.0037	0.0076	0.002
5-Aminopentanoate	0.0135	0.0044	0.0122	0.0041	0.0133	0.0023	0.0118	0.0046
Acetate	0.8554	0.2712	0.6242	0.1463	0.6216	0.1736	0.625	0.1419
Acetoin	0.0063	0.0043	0.0049	0.0042	0.0073	0.0077	0.0041	0.0021
Acetone	0.0034	0.0018	0.0041	0.0019	0.0037	0.0014	0.0043	0.002
Alanine	0.0157	0.0077	0.0094	0.0045	0.0124	0.0055	0.0085	0.0039
Aspartate	0.0167	0.0047	0.0121	0.0034	0.0127	0.0042	0.0119	0.0032
Betaine	0.002	0.0011	0.002	0.0011	0.0022	0.001	0.0019	0.0012
Butyrate	0.0116	0.0048	0.0151	0.0053	0.0122	0.0041	0.016	0.0054
Choline	0.0021	0.0013	0.0019	0.0008	0.0026	0.0009	0.0017	0.0007
Citrate	0.0048	0.0018	0.0045	0.0017	0.0051	0.0027	0.0043	0.0014
Creatine	0.006	0.0013	0.0058	0.0014	0.0063	0.0009	0.0056	0.0015
Dimethyl sulfone	0.0021	0.0011	0.0035	0.0019	0.0029	0.0015	0.0037	0.002
Ethanol	0.012	0.0085	0.0201	0.0095	0.0153	0.009	0.0217	0.0094
Ethanolamine	0.0116	0.0081	0.0136	0.0053	0.0113	0.0055	0.0144	0.0051
Formate	0.2164	0.2457	0.7101	0.3461	0.6104	0.4358	0.7416	0.3203
Fucose	0.0164	0.0079	0.0101	0.0029	0.0101	0.0034	0.0101	0.0029
Glucose	0.0272	0.0091	0.0406	0.0112	0.0409	0.0087	0.0406	0.0121
Glutamine	0.0356	0.0253	0.0158	0.0083	0.0216	0.0094	0.014	0.0072
Glycerol	0.0238	0.0185	0.0321	0.0095	0.0325	0.0112	0.032	0.0092
Glycerophosphocholine	0.0024	0.001	0.0037	0.0009	0.003	0.0009	0.0039	0.0008
Glycine	0.1152	0.0636	0.0375	0.025	0.0619	0.0387	0.0298	0.0126
Glycolate	0.0273	0.0117	0.0373	0.0116	0.0368	0.0148	0.0374	0.0109
Isoleucine	0.0044	0.0021	0.0021	0.0009	0.0025	0.0013	0.002	0.0008
Isovalerate	0.0019	0.0006	0.002	0.0007	0.0019	0.0007	0.002	0.0007
Lactate	0.0382	0.0416	0.0967	0.0939	0.116	0.1367	0.0906	0.0801
Leucine	0.0056	0.0021	0.0038	0.0013	0.0045	0.0011	0.0035	0.0013
Lysine	0.0187	0.0087	0.0098	0.004	0.0115	0.0048	0.0093	0.0037
Malonate	0.0048	0.0018	0.0042	0.0019	0.0045	0.0023	0.0041	0.0018
Methanol	0.0265	0.0133	0.0419	0.0183	0.0282	0.0091	0.0462	0.0185
Ornithine	0.0104	0.006	0.0053	0.0032	0.0072	0.0039	0.0048	0.0029
Phenylacetate	0.0038	0.0018	0.004	0.0018	0.0032	0.0015	0.0043	0.0018
Phenylalanine	0.009	0.0035	0.0059	0.0019	0.0055	0.002	0.006	0.0018
Phosphocholine	0.0027	0.0013	0.0034	0.0016	0.0024	0.0012	0.0037	0.0016
Proline	0.1275	0.1135	0.0323	0.0273	0.0539	0.0497	0.0254	0.0101
Propionate	0.0642	0.0304	0.0624	0.02	0.0595	0.0246	0.0633	0.019
Pyruvate	0.0133	0.0113	0.0201	0.0154	0.0272	0.0225	0.0179	0.0124
Succinate	0.0069	0.0052	0.0106	0.0049	0.0089	0.0031	0.0111	0.0053
Taurine	0.0227	0.0065	0.0247	0.0076	0.0224	0.0071	0.0254	0.0078
Tyrosine	0.0205	0.0092	0.0107	0.0041	0.0121	0.0038	0.0102	0.0041
Urea	0.1919	0.1732	0.4093	0.2733	0.2749	0.2271	0.4517	0.2781
Valerate	0.0076	0.0047	0.0121	0.0063	0.0102	0.0037	0.0127	0.0068
Valine	0.0042	0.0024	0.0022	0.001	0.0026	0.0012	0.0021	0.0009

Figure S1. ROC curves for 17 important metabolites identified via multivariate and univariate statistical analyses.

