

Supplementary material

Metabolomic Signature Discriminates Normal Human Cornea from Keratoconus—A Pilot GC/MS Study

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Table S1. Metabolites identified and quantified by GC/MS in keratoconus (KC) and healthy cornea (HC) samples.

No	Metabolite name	Class	Mol. mass	Rt	KC		HC	
					mean abundance	S.D.	mean abundance	S.D.
1	Lactic acid	α -hydroxy acids	88	06.19	1.70E-04	1.73E-04	1.38E-04	1.64E-04
2	Glycolic acid	α -hydroxy acids	88	06.34	2.65E-05	4.10E-05	6.18E-05	5.39E-05
3	Oxalic acid	Carboxylic acids	189	07.20	2.56E-04	3.039E-04	2.53E-04	2.01E-04
4	Urea	Others	189	08.56	1.22E-03	9.00E-04	1.48E-03	4.71E-04
5	Phosphoric acid	Others	299	09.21	6.77E-01	9.24E-02	5.69E-01	3.75E-02
6	Glycerol	Sugar alcohols	218	09.23	6.94E-04	4.70E-04	7.06E-04	4.99E-04
7	3-Indoleacetic acid	Others	130	09.39	3.21E-03	1.15E-03	3.41E-03	1.30E-03
8	Glycine	Amino acids	174	09.51	3.48E-03	2.14E-03	5.33E-03	7.32E-03
9	Succinic acid	Carboxylic acids	147	09.58	5.36E-03	1.21E-03	7.71E-03	1.41E-03

10	Serine	Amino acids	204	10.34	1.95E-03	2.38E-03	1.22E-03	3.95E-04
11	Benzoic acid	Carboxylic acids	215	10.37	1.19E-03	4.38E-04	1.80E-03	4.05E-04
12	Lactic acid dimer	α -hydroxy acids	88	10.54	7.54E-05	7.56E-05	1.64E-04	8.12E-05
13	L-Aspartic acid	Amino acids	232	12.38	3.45E-04	4.07E-04	1.90E-04	5.52E-05
14	L-5-Oxoproline	Amino acids	156	12.39	6.29E-03	9.94E-03	2.61E-03	8.44E-04
16	Octanoic acid 2-ethylhexyl ester	Fatty acid esters	84	14.53	3.62E-04	2.25E-04	4.63E-04	9.15E-05
17	Azelaic acid	Carboxylic acids	317	15.51	9.17E-05	3.76E-05	1.38E-04	6.83E-05
18	Citric acid	Carboxylic acids	273	16.03	2.51E-04	1.83E-04	4.47E-04	5.07E-04
19	Myristic acid	Fatty acids	285	16.25	1.12E-03	3.94E-04	1.75E-03	3.06E-04
20	D-Fructose	Saccharides	217	16.36	1.41E-03	1.12E-03	1.34E-03	4.90E-04
21	D-Psicose	Saccharides	307	16.42	3.10E-04	1.92E-04	2.85E-04	9.51E-05
22	D-Glucose	Saccharides	319	16.52	2.10E-03	2.18E-03	2.88E-03	7.89E-04
23	Decanoic acid, 2-ethylhexyl ester	Carboxylic acid esters	84	16.59	5.39E-04	2.58E-04	7.25E-04	1.85E-04
24	Palmitic acid methyl ester	Fatty acid esters	87	17.14	2.32E-03	1.04E-03	3.04E-03	6.91E-04
25	Sorbitol	Sugar alcohols	319	17.16	6.15E-04	7.34E-04	5.68E-05	4.93E-05
26	Pentadecanoic acid	Fatty acids	117	17.26	7.43E-04	2.62E-04	1.22E-03	3.31E-04
27	Hexadecanol	Alcohols	299	17.34	7.63E-04	1.88E-04	1.09E-03	1.80E-04
28	Talose	Saccharides	204	17.40	4.83E-04	4.25E-04	8.26E-04	5.60E-04
29	Gluconic acid	Carboxylic acids	435	17.54	5.62E-06	7.30E-06	N.D.	N.D.
30	Palmitoleic acid	Fatty acids	311	18.11	2.93E-04	1.45E-04	3.81E-04	2.08E-04
31	Palmitic acid	Fatty acids	313	18.24	4.25E-02	1.57E-02	7.24E-02	1.26E-02
32	Myo-Inositol	Sugar alcohols	305	18.47	9.41E-05	5.87E-05	1.49E-04	6.52E-05
33	Stearic acid, methyl ester	Fatty acid esters	87	19.11	1.16E-03	5.16E-04	1.50E-03	3.68E-04
34	Linoleic acid	Fatty acids	337	19.55	3.88E-04	3.79E-04	1.03E-03	4.99E-04
35	trans-9-Octadecenoic acid	Fatty acids	84	19.59	1.35E-03	7.10E-04	9.30E-04	1.26E-03
36	Petroselinic acid	Fatty acids	339	19.59	N.D.	N.D.	2.56E-03	3.24E-03
37	trans-13-Octadecenoic acid	Fatty acids	357	20.00	8.33E-04	1.71E-04	1.49E-03	2.11E-04
38	Stearic acid	Fatty acids	341	20.13	4.81E-02	1.77E-02	7.44E-02	1.68E-02
39	3-Chloropropionic acid, heptadecyl ester	Others	84	20.42	2.97E-04	1.39E-04	6.56E-04	1.31E-04
40	Myo-Inositol phosphate	Others	318	21.37	4.49E-03	4.41E-03	1.92E-03	5.32E-04
41	Arachidic acid	Fatty acids	369	21.53	4.78E-04	1.96E-04	6.28E-04	1.35E-04
42	Sucrose	Saccharides	361	23.22	2.34E-03	8.76E-04	3.63E-03	1.27E-03
43	Cholesterol chloroformate	Sterol esters	368	24.31	8.70E-05	8.29E-05	4.96E-04	2.35E-04
44	Cholesta-3,5-diene – isomer 1	Sterols	368	25.11	1.76E-04	1.63E-04	8.36E-04	4.03E-04
45	Cholesta-3,5-diene – isomer 2	Sterols	368	25.27	8.55E-04	7.59E-04	4.21E-03	2.01E-03

46	Cholesterol propionate	Sterol esters	351	25.27	1.20E-06	1.85E-06	N.D.	N.D.
47	Cholesterol	Sterols	133	27.34	1.96E-02	1.51E-02	5.68E-02	1.52E-02

N.D. – not detected, Rt – retention time (min), S.D. – standard deviation.