

Supplementary information

Cheating on forensic hair testing? Detection of potential biomarkers for cosmetically altered hair samples using untargeted hair metabolomics

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Table S1 Listed are compounds with an identification level 3 (according to the Metabolomics Standard Initiative guidelines ¹) found as significantly altered between untreated and bleached hair samples (arranged in compound classes).

Feature name	Analytics	Adduct	Measured m/z	RT [min]	FDR adjusted p-value	Fold change	Conc. change	Formula	Tentative Identification	Compound Class
0.94_276.1544m/z	HSSTpos	M+H	276.1544	0.9	2.1E ⁻⁰⁶	3.7	↓	C ₁₁ H ₂₁ N ₃ O ₅	Glu Lys	Amino acids, peptides and analogues
1.24_146.0921m/z	HSSTpos	M+H	146.0921	1.2	3.4E ⁻⁰⁹	2.4	↑	C ₅ H ₁₁ N ₃ O ₂	Guanidinobutanoic acid	Amino acids, peptides and analogues
3.59_288.2020m/z	HSSTpos	M+H	288.2020	3.6	3.5E ⁻⁰⁵	2.3	↓	C ₁₂ H ₂₅ N ₅ O ₃	Arg-Ile	Amino acids, peptides and analogues
3.97_247.1280m/z	HSSTpos	M+H	247.1280	4.0	2.1E ⁻⁰⁶	6.0	↓			Amino acids, peptides and analogues
4.09_429.2201m/z	HSSTpos	M+H	429.2201	4.1	2.1E ⁻⁰⁶	12.0	↑			Amino acids, peptides and analogues
4.24_279.1329m/z	HSSTpos	M+H	279.1329	4.2	2.1E ⁻⁰⁶	2.9	↓			Amino acids, peptides and analogues
4.24_346.1700m/z	HSSTpos	M+H	346.1700	4.2	2.1E ⁻⁰⁶	2.3	↑			Amino acids, peptides and analogues
4.36_414.1854n	HSSTpos		415.1926	4.4	2.1E ⁻⁰⁶	11.2	↑			Amino acids, peptides and analogues
4.77_405.1750m/z	HSSTpos		405.1750	4.8	2.1E ⁻⁰⁶	10.8	↑			Amino acids, peptides and analogues
4.85_521.2426m/z	HSSTpos		521.2426	4.9	2.1E ⁻⁰⁶	19.5	↑			Amino acids, peptides and analogues
4.87_229.1532m/z	HSSTpos		229.1532	4.9	2.1E ⁻⁰⁶	4.5	↓			Amino acids, peptides and analogues
4.87_356.1264m/z	HSSTpos		356.1264	4.9	2.1E ⁻⁰⁶	6.6	↑			Amino acids, peptides and analogues
4.98_305.1033n	HSSTpos		328.0935	5.0	2.1E ⁻⁰⁶	13.4	↓			Amino acids, peptides and analogues
5.09_333.1546m/z	HSSTpos	M+H	333.1546	5.1	4.7E ⁻⁰³	2.6	↓	C ₁₆ H ₂₀ N ₄ O ₄	Trp Gln	Amino acids, peptides and analogues
5.46_433.2070m/z	HSSTpos		433.2070	5.5	2.1E ⁻⁰⁶	6.0	↓			Amino acids, peptides and analogues
5.65_481.2394m/z	HSSTpos		481.2394	5.7	2.1E ⁻⁰⁶	2.9	↑			Amino acids, peptides and analogues

Feature name	Analytics	Adduct	Measured m/z	RT [min]	FDR adjusted p-value	Fold change	Conc. change	Formula	Tentative Identification	Compound Class
5.86_229.1534m/z	HSSTpos	M+H	229.1534	5.9	2.1E ⁻⁰⁶	2.9	↓	C ₁₁ H ₂₀ N ₂ O ₃	Ile Pro	Amino acids, peptides and analogues
6.05_261.1433m/z	HSSTpos	M+H	261.1433	6.1	2.1E ⁻⁰⁶	3.1	↓	C ₁₁ H ₂₀ N ₂ O ₅	gamma-Glu-Leu	Amino acids, peptides and analogues
6.13_231.1692m/z	HSSTpos	M+H	231.1692	6.1	3.7E ⁻⁰⁷	2.4	↓	C ₁₁ H ₂₂ N ₂ O ₃	Val Ile	Amino acids, peptides and analogues
6.52_302.1497m/z	HSSTpos		302.1497	6.5	2.1E ⁻⁰⁶	3.2	↓			Amino acids, peptides and analogues
7.15_263.1373m/z	HSSTpos	M+H	263.1373	7.2	2.1E ⁻⁰⁶	2.8	↓	C ₁₄ H ₁₈ N ₂ O ₃	Phe Pro	Amino acids, peptides and analogues
12.33_311.1691n	HILICpos	M+H, M+2H	312.1765	12.3	5.0E ⁻⁰⁶	26.5	↑			Amino acids, peptides and analogues
8.39_288.2009m/z	HILICpos		288.2009	8.4	2.9E ⁻⁰⁶	11.8	↓			Amino acids, peptides and analogues
8.50_338.1799m/z	HILICpos		338.1799	8.5	2.9E ⁻⁰⁶	11.8	↓			Amino acids, peptides and analogues
9.06_290.1443m/z	HILICpos	M+H	290.1443	9.1	2.9E ⁻⁰⁶	9.0	↓	C ₁₀ H ₁₉ N ₅ O ₅	Asp Arg	Amino acids, peptides and analogues
9.10_274.1855m/z	HILICpos		274.1855	9.1	5.0E ⁻⁰⁶	8.6	↓			Amino acids, peptides and analogues
9.36_246.1789m/z	HILICpos		246.1789	9.4	2.9E ⁻⁰⁶	16.0	↓			Amino acids, peptides and analogues
9.52_276.1656m/z	HILICpos	M+H	276.1656	9.5	1.1E ⁻⁰⁵	4.4	↓	C ₁₀ H ₂₁ N ₅ O ₄	Arg Thr	Amino acids, peptides and analogues
9.96_232.1394m/z	HILICpos		232.1394	10.0	5.0E ⁻⁰⁶	4.4	↓			Amino acids, peptides and analogues
8.35_275.1476n	HILICneg		274.1403	8.4	5.1E ⁻⁰⁶	10.0	↓			Amino acids, peptides and analogues
0.79_650.6389m/z	HILICpos		650.6389	0.8	7.0E ⁻⁰⁴	1107.3	↑			Ceramides
5.72_181.0713m/z	HILICneg		181.0713	5.7	1.5E ⁻⁰⁴	46.0	↓			Sugars
0.90_195.0512m/z	HSSTneg		195.0512	0.9	1.8E ⁻⁰⁶	15.2	↓			Sugar acid

Feature name	Analytics	Adduct	Measured m/z	RT [min]	FDR adjusted p-value	Fold change	Conc. change	Formula	Tentative Identification	Compound Class
1.06_134.0212n	HSSNeg		133.0143	1.1	4.8E ⁻⁰⁶	6.9	↓			Dicarboxylic acids
7.08_145.0132m/z	HILICneg	M-H	145.0132	7.1	3.1E ⁻⁰⁶	23.4	↓	C ₅ H ₆ O ₅	Oxoglutaric acid	Dicarboxylic acids
2.23_118.0263n	HSSNeg		117.0194	2.2	4.8E ⁻⁰⁶	7.8	↓			Dicarboxylic acids
14.74_269.2121m/z	HSSNeg		269.2121	14.7	7.7E ⁻⁰⁴	2.1	↑			Hydroxylated fatty acids
14.87_293.2110m/z	HSSNeg		293.2110	14.9	1.8E ⁻⁰⁶	4.3	↑			Hydroxylated fatty acids
14.89_295.2271m/z	HSSNeg		295.2271	14.9	1.8E ⁻⁰⁶	4.2	↑			Hydroxylated fatty acids
15.14_296.2344n	HSSNeg		295.2271	15.1	1.8E ⁻⁰⁶	4.8	↑			Hydroxylated fatty acids
15.39_324.2657n	HSSNeg		323.2584	15.4	1.8E ⁻⁰⁶	6.5	↑			Hydroxylated fatty acids
15.99_279.2323m/z	HSSNeg	M-H	279.2323	16.0	6.9E ⁻⁰⁴	2.8	↑	C ₁₈ H ₃₂ O ₂	Linoleic acid	Fatty acids
1.22_295.2267m/z	HILICneg		295.2267	1.2	5.1E ⁻⁰⁶	7.1	↑			Fatty acids
0.82_339.2507m/z	HILICneg		339.2507	0.8	3.7E ⁻⁰⁵	3.8	↓			Prostanoids

↑: increase after bleaching; ↓ decrease after bleaching.

References

1. L. W. Sumner, A. Amberg, D. Barrett, M. H. Beale, R. Beger, C. A. Daykin, T. W. Fan, O. Fiehn, R. Goodacre, J. L. Griffin, T. Hankemeier, N. Hardy, J. Harnly, R. Higashi, J. Kopka, A. N. Lane, J. C. Lindon, P. Marriott, A. W. Nicholls, M. D. Reily, J. J. Thaden and M. R. Viant, *Metabolomics*, 2007, **3**, 211-221.