

Supporting Information

Age-Related Changes to Human Stratum Corneum Lipids Detected Using Time-of-Flight Secondary Ion Mass Spectrometry Following in Vivo Sampling

Nichola J. Starr[§], Daniel J. Johnson[†], Judata Wibawa[‡], Ian Marlow[‡], Mike Bell[‡], David A. Barrett[§], David J. Scurr^{*§}

[§] School of Pharmacy, University of Nottingham, Nottingham, NG7 2RD, U.K

[†] College of Engineering, Swansea University, Swansea, SA1 8EN, U.K

[‡] Walgreens Boots Alliance, Thane Road, Nottingham, NG90 1BS, U.K

*E-mail: David.Scurr@nottingham.ac.uk

Contents:

Figure S1: Individual strip AFM data.....	Page S-2
Figure S2: PCA score plots of ToF-SIMS data.....	Page S-2
Figure S3: ToF-SIMS OPLSDA S-plot data.....	Page S-2
Figure S4: ToF-SIMS peak intensities for lignoceric and hexacosanoic acid.....	Page S-3

Strip No.	Young Arm			Young Hand			Old Arm			Old Hand		
	Mean (nm)	Std. Error (nm)	Variation (%)	Mean (nm)	Std. Error (nm)	Variation (%)	Mean (nm)	Std. Error (nm)	Variation (%)	Mean (nm)	Std. Error (nm)	Variation (%)
2	963.16	200.23	20.79	647.11	167.89	25.94	627.19	82.87	13.21	465.84	57.41	12.32
4	442.95	62.20	14.04	649.49	141.01	21.71	519.13	56.36	10.86	699.94	134.19	19.17
6	720.36	94.14	13.07	565.63	82.59	14.60	622.88	95.77	15.38	927.48	131.95	14.23
8	461.16	61.99	13.44	775.54	100.77	12.99	523.16	50.23	9.60	449.12	55.02	12.25
10	428.10	77.01	17.99	566.07	46.07	8.14	823.49	59.90	7.27	545.73	73.10	13.39
12	430.17	89.24	20.75	461.62	102.55	22.21	612.59	147.36	24.06	446.47	75.39	16.88
14	351.79	40.67	11.56	552.34	101.25	18.33	736.45	156.63	21.27	546.15	75.46	13.82

Figure S1. Tabulated AFM data showing the measured SC layer depth for each tape strip number for each sample group. The data is from one volunteer per sample group and the table presents the mean, standard error and hence percentage variation across the strip calculated from 3 lines profiles taken per 3 different areas across the strip ($n = 9$).

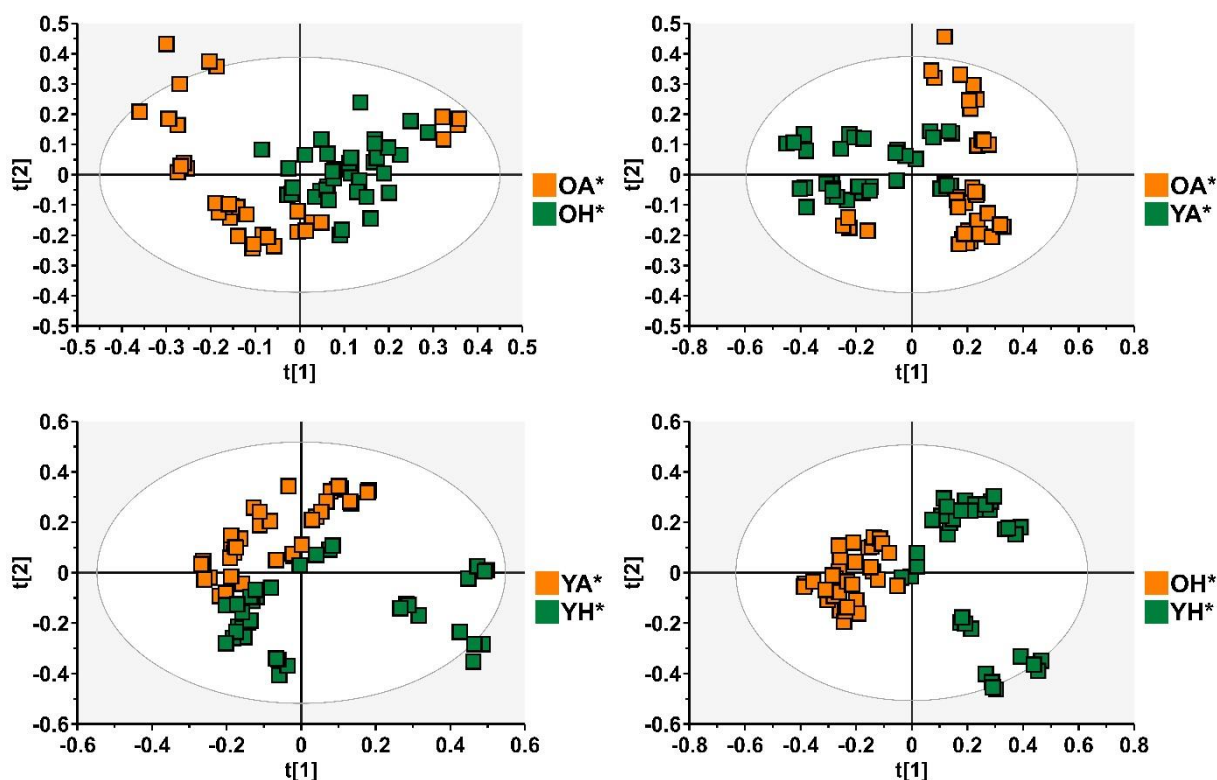


Figure S2. The PCA score plots for the negative polarity ToF-SIMS data for the four aging comparisons. Data was taken from tape strip number 7 for $n = 9$ volunteers per sample type and $n = 4$ measurements per sample.

m/z	OA vs OH		YA vs YH		OA vs YA		OH vs YH	
	$p[1]$	$p(\text{corr})[1]$	$p[1]$	$p(\text{corr})[1]$	$p[1]$	$p(\text{corr})[1]$	$p[1]$	$p(\text{corr})[1]$
367	-0.087	-0.285	-0.166	-0.824	0.175	0.907	0.154	0.636
395	-0.131	-0.499	-0.131	-0.827	0.118	0.868	0.123	0.624
465	0.282	0.691	0.104	0.403	0.13	0.546	0.11	0.518

Figure S3. Tabulated $p[1]$ and $p(\text{corr})[1]$ values for three ions with m/z 367, 395 and 465 from the ToF-SIMS OPLSDA loadings S-plots produced for the four comparisons.

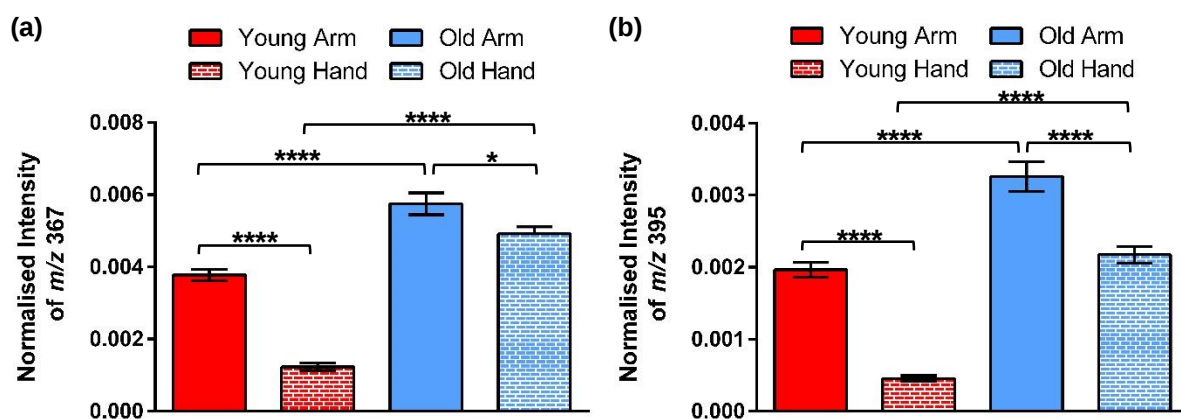


Figure S4. ToF-SIMS secondary ion intensities, normalised to total ion counts, for (a) lignoceric acid and (b) hexacosanoic acid for the four sample types. The data is shown as the mean and standard error values calculated from tape strip number 7 for $n = 9$ volunteers per sample type and $n = 4$ measurements per sample. An unpaired, two-tailed t test with Welch's correction was conducted on each sample pair (**** p value < 0.0001 , *** p value < 0.001 , ** p value < 0.01 , * p value < 0.05).