

Supplemental Information

Table 1. Distribution of marker compounds characteristic of individuals

Individual compounds	% subjects in which compound occurred in no (0) to all 5 samples						% subjects found in \geq 1 sample*
	0	1	2	3	4	5	
Alcohols and Phenols							
2-phenylethanol *	73	16	8	2	0	1	27
α -terpineol *	92	6	1	1	1	0	8
geraniol *	86	10	2	2	1	1	14
eugenol *	82	11	3	3	1	1	18
isoeugenol *	68	21	8	3	1	0	32
1-tridecanol *	78	9	7	2	3	1	22
Aldehydes							
geranial *	58	18	18	4	1	1	42
undecanal *	9	24	30	25	11	1	91
tridecanal *	30	35	23	10	2	0	70
lilial	3	14	13	14	26	30	97
Ketones							
jasmone	94	4	1	0	0	1	6
α -ionone *	74	14	6	4	2	1	26
benzophenone *	6	18	24	26	18	9	94
2-acetyl-3,5,5,6,8,8-hexa-methyl- 5,6,7,8-tetrahydronaphthalene	63	20	10	3	3	1	37
7-acetyl-6-ethyl-1,1,4,4- tetramethyltetrahydro (Musk 36A)	91	5	3	2	0	0	9
Esters							
α -terpineyl acetate *	86	10	2	3	1	0	14
methyl N-methylantranilate	87	8	3	1	1	1	13
2-hexyl 2-pentenoate	84	10	3	3	1	1	16
E-cinnamyl acetate	84	10	3	3	1	1	16

α -trichloromethyl-benzyl acetate	94	4	1	0	1	1	6
isoeugenol acetate	77	14	4	4	1	1	23
methylcis-dihydrojasmonate	10	18	21	15	24	13	90
3Z-1-hexenyl salicylate	84	11	4	2	1	0	16
ethyl tetradecanoate *	73	14	7	3	2	2	27
2-ethylhexyl salicylate	77	11	6	5	1	1	23
ethyl pentadecanoate	81	10	5	3	1	1	19
2-phenylethyl phenylacetate	72	14	6	3	4	1	28
decyl octanoate	97	2	1	0	1	1	3
dodecyl hexanoate	98	0	1	0	1	0	2
ethyl heptadecanoate	84	12	4	1	1	0	16
a branched dodecyl benzoate	93	4	1	2	0	0	7
dodecyl octanoate	69	15	7	2	3	6	31
dodecyl benzoate	36	20	19	12	11	1	64
tridecyl benzoate	69	19	6	4	2	1	31
tetradecyl octanoate	96	2	1	1	1	0	4
tetradecyl benzoate	95	4	0	0	2	0	5
Hydrocarbons							
a propyl substituted dodecane	71	15	10	3	2	1	29
4-phenyltridecane	88	8	2	2	1	0	12
3-methyloctadecane	98	1	1	1	0	0	2
3-methyl nonadecane	98	1	0	1	0	0	2
Other							
4-sec-butylaniline	93	6	1	0	1	0	7
diphenyl ether	94	5	0	0	1	0	6
an unknown bicyclic compound	74	14	7	2	2	1	26
a diethyl acetal	48	14	16	10	8	4	52

* Percent of subjects the compound was found in at least one sample. The average number of subjects these compounds were detected in at least once is 43, the maximum number of subjects is 192, and the minimum 3.

Table 2. 118 Additional compounds identified from axillary samples

RT (min)	Identification
Alcohols	
12.47	γ -terpineol
12.90	2-phenoxyethanol
13.34	citronellol
26.83	pentadecanol
27.75	a hexadecadienol
29.51	hexadecanol
Aldehydes	
12.74	decanal
13.93	p-anisaldehyde
15.46	undecanal
18.10	dodecanal
23.00	tetradecanal
23.58	pentylcinnamaldehyde
26.04	E-2-hexylcinnamaldehyde
28.09	hexadecanal
Ketones	
8.98	acetophenone
9.49	2-nonanone
14.99	2-undecanone
15.42	an isopropylacetophenone
17.69	2-dodecanone
19.45	γ -irone
19.66	β -ionone
20.22	2-tridecanone
20.54	Z- α -irone
22.52	2-tetradecanone
24.08	1-ethyl-3-methyl- β -ionone

24.92 2-pentadecanone

27.54 2-hexadecanone

Amines

12.65 2-pentylpyrrole

13.28 2-phenoxyethylmethylamine

15.19 an aliphatic amine

16.34 nicotine

16.81 4-sec-butylaniline

20.37 N,N-dimethyl-1-dodecylamine

30.24 N,N-dimethyl-1-hexadecylamine

35.88 N,N-dimethyl-1-octadecylamine

Amides

17.18 methyl N,N-diethylthiocarbamate

18.04 a hydroxy acetanilide

21.98 n-propylbenzamide

Carboxylic acids

12.24 octanoic acid

14.76 nonanoic acid

21.03 8-methylundecanoic acid

21.90 dodecanoic acid

22.80 a methyl dodecanoic acid

23.18 9-methyldodecanoic acid

25.74 10-methyltridecanoic acid

26.80 myristic acid (tetradecanoic acid)

28.36 a methyltetradecanoic acid

28.65 a methyltetradecanoic acid

28.84 9-pentadecenoic acid

29.31 pentadecanoic acid

30.76 a methylpentadecanoic acid

31.70 9-hexadecenoic acid

32.49-33.00 palmitic acid (hexadecanoic acid)

34.37	9-heptadecenoic acid
37.31	oleic acid
38.03	stearic acid (octadecanoic acid)

Lactones

12.27	γ -heptanolactone
16.70	γ -nonanolactone
18.60	coumarin

Esters

11.40	benzyl acetate
12.07	2-phenylethyl acetate
12.73	dihydromyrcenol acetate
14.82	cis-2-tert-butylcyclohexyl acetate
16.43	citronellol acetate
16.62	neryl acetate
17.16	geranyl acetate
21.95	pentyl salicylate
22.21	isooctanedioldibutyrate
23.30	isopropyl dodecanoate
24.46	1-hexyl salicylate
25.01	methyl trans-jasmonate
25.73	a hexenyl salicylate
26.65	benzyl benzoate
28.23	a branched isopropyl hexadecanoate
30.93	methyl palmitate
32.40	hexyl dodecanoate
32.99	ethyl hexadecanoate
33.70	isopropyl hexadecanoate
37.35	2-ethyl-hexyl 4-methoxycinnamate

Hydrocarbons

7.67	p-cymene
12.26	1-dodecene
12.50	dodecane
15.15	tridecane
17.55	1-tetradecene
17.77	tetradecane
18.22	β -caryophyllene
19.72	trans-muurolo-4(14),5-diene
19.96	a methyl biphenyl
20.02	a methyl biphenyl
20.36	α -farnesene
20.38	pentadecane
21.77	4-methylpentadecane
22.56	hexadecane
23.28	5-phenylundecane
23.53	4-phenylundecane
23.99	3-phenylundecane
24.94	2-phenylundecane
25.04	heptadecane
25.49	6-phenyldodecane
25.66	a sesquiterpene
25.77	5-phenyldodecane
27.48	octadecane
27.57	2-phenyldodecane
28.09	6-phenyltridecane
29.40	3-phenyltridecane
30.13	1-nonadecene
30.22	nonadecane
30.38	2-phenyltridecane

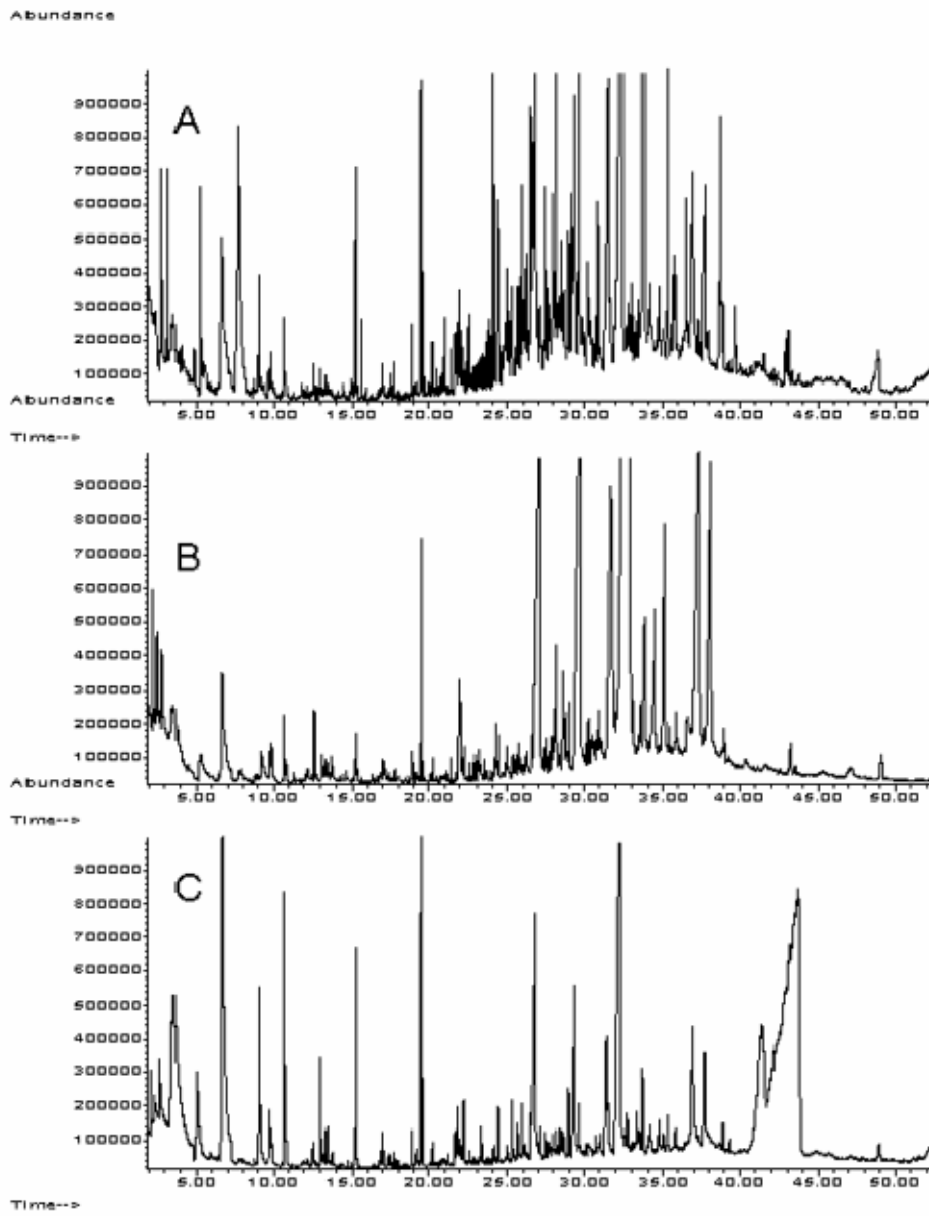
32.93	eicosane (C-20 linear hydrocarbon)
35.79	heneicosane (C-21 linear hydrocarbon)
38.79	docosane (C-22 linear hydrocarbon)
41.49	tricosane (C-23 linear hydrocarbon)
43.44	tetracosane (C-24 linear hydrocarbon)

Esters and steroids

24.43	dioctylether
29.26	bis(benzyloxy)methane
31.75	an androgen steroid
37.39	an androgen steroid
42.01	an androgen steroid

Figure 1

GC-MS profiles of skin volatile compounds



A: D90 female, B: P219 male, C: B57 male