Supporting Information

Stoffel et al. 10.1073/pnas.1506076112

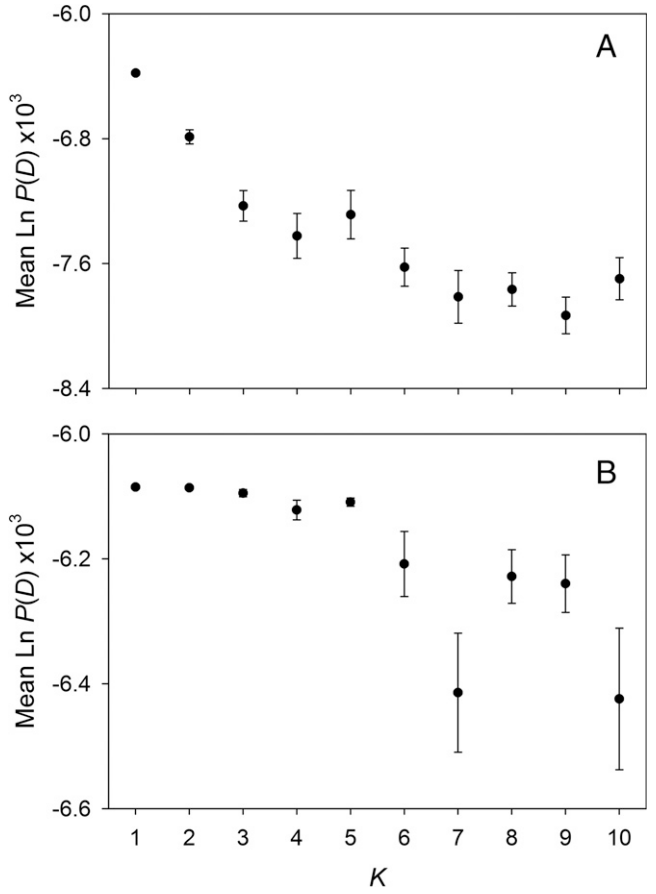

Fig. S1. Results of Bayesian analyses of population structure. Mean ± SE Ln *P*(*D*) values are shown based on five replicates for each value of *K*, the hypothesized number of genetic clusters represented in the data, for (*A*) mothers and (*B*) pups.

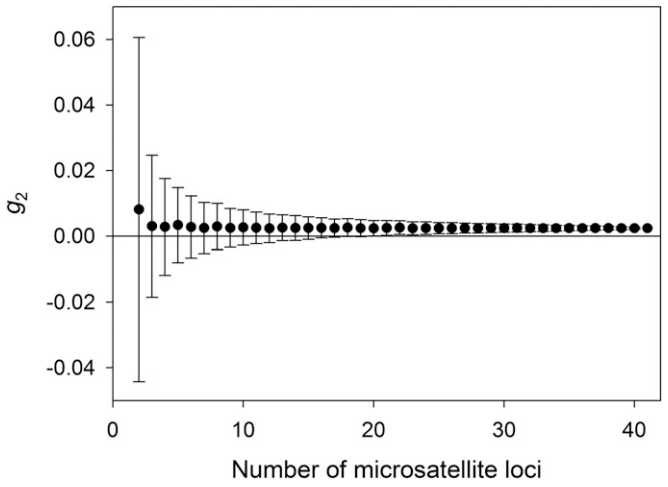

Fig. S2. Sensitivity of g_2 to the number of microsatellite loci deployed. Different-sized subsets of loci were each resampled 1,000 times and the mean ± SD calculated.

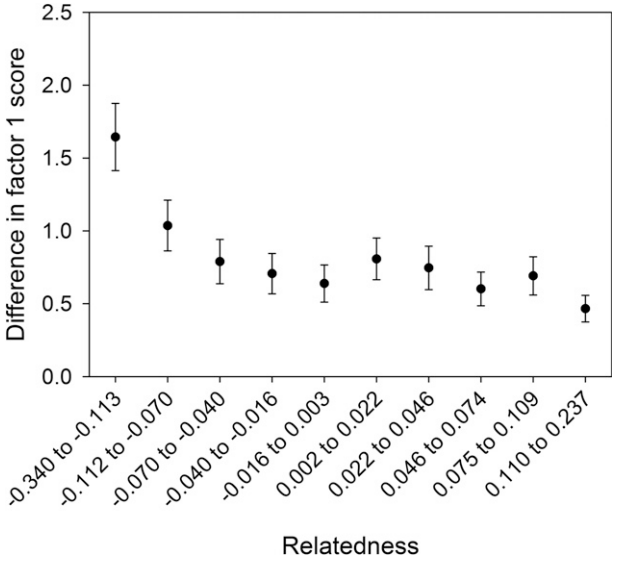

Fig. S3. Relationship between pairwise relatedness among mothers and the difference between individuals in their factor 1 scores. Mean and SEs are shown for the data partitioned into roughly equal-sized groups.

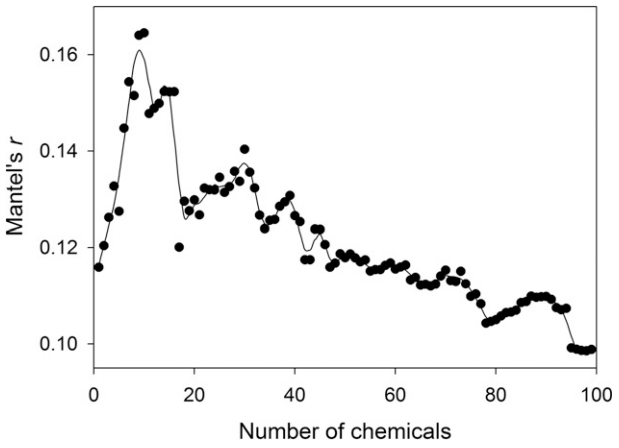

Fig. S4. Results of the BIO-ENV bootstrapping procedure. See *Methods* for details. The *y* axis shows the strength of correlation between genetic relatedness and pairwise Bray–Curtis similarity. On the *x* axis, the chemicals are shown in decreasing order of importance, given by the number of subsamples in which the chemical was retained in the "best" subset. Each chemical was progressively added to the calculation of Bray–Curtis similarity. The relationship between chemical similarity and relatedness is maximized for a subset of the 10 most important chemicals.

Table S1. Details of the 43 microsatellite loci used in this study together with their polymorphism characteristics in 41 mother–offspring pairs

						HWE *P* value	
Locus	Sources	Mix	T_a	Number of alleles	Observed heterozygosity	Mothers	Offspring
Pv9	(61)	1	53	10	0.691	**0.037**	0.129
Hg6.1	(61)	7	60	13	0.888	0.691	0.991
Hg6.3	(61)	1	53	12	0.901	0.942	0.074
Hg8.10	(61)	1	53	2	0.407	0.399	1.000
PvcA	(62)	1	53	7	0.802	0.998	0.412
PvcE	(62)	2	60	13	0.926	0.836	0.755
Aa4	(63)	4	60	6	0.720	0.685	0.419
Hg1.3	(63)	1	53	11	0.815	0.136	0.443
Pv11	(64)	8	60	11	0.329	0.399	**0.000**
OrrFCB2	(65)	2	60	11	0.888	0.394	0.234
OrrFCB7	(65)	2	60	10	0.813	0.391	0.649
M11a	(66)	4	60	17	0.867	0.331	0.654
Lc28	(67)	4	60	9	0.875	0.988	0.542
Lw10	(67)	2	60	15	0.938	0.605	0.525
Zcc7t	(68)	7	60	13	0.896	0.568	0.492
ZcwCgDh1.8	(68)	3	60	9	0.744	0.608	**0.020**
ZcwDh3.6	(68)	4	60	4	0.234	0.590	0.392
ZcwCgDh4.7	(68)	3	60	13	0.924	0.842	0.336
ZcwCgDh5.16	(68)	2	60	7	0.500	**0.000**	**0.000**
ZcCgDh5.8	(68)	6	60	11	0.850	0.489	0.748
ZcwCgDh7tg	(68)	3	60	12	0.742	0.347	**0.026**
ZcwCgDhB.14	(68)	2	60	6	0.747	0.287	0.587
Zcwb09	(69)	6	60	12	0.864	0.652	0.933
Zcwc03	(69)	6	60	11	0.813	0.124	0.544
Zcwc11	(69)	6	60	14	0.875	0.100	0.678
Zcwd02	(69)	3	60	13	0.878	0.346	0.596
Zcwe03	(69)	7	60	9	0.838	0.602	0.919
Ssl301	(70)	3	60	14	0.901	0.473	0.910
Zcwa05	(71)	5	60	14	0.896	0.645	0.999
Zcwb07	(71)	1	53	11	0.914	0.465	0.093
Zcwc01	(71)	2	60	11	0.823	0.345	0.511
Zcwe04	(71)	8	60	12	0.864	0.132	0.362
Zcwe12	(71)	8	60	8	0.768	0.595	0.881
Zcwf07	(71)	4	60	9	0.802	0.194	0.834
Ag1	(72)	3	60	10	0.813	0.706	0.733
Ag2	(72)	2	60	7	0.854	0.847	0.428
Ag3	(72)	2	60	2	0.420	0.454	0.311
Agaz2	(73)	1	53	8	0.802	0.215	0.394
Agaz3	(73)	2	60	5	0.629	0.896	0.288
Agaz5	(73)	2	60	3	0.469	0.641	0.174
Agaz6	(73)	2	60	4	0.765	0.750	0.156
Agaz10	(73)	2	60	11	0.767	0.572	0.493
Zcwe05		3	60	9	0.866	0.999	0.564

HWE *P* values are shown separately for mothers and offspring, with significant values highlighted in bold. Values that remained significant following table-wide correction for the FDR are underlined. Loci Pv11 and ZcwCgDh5.16 were excluded from further analyses because they deviated significantly from HWE after FDR correction in either or both mothers or offspring. "Mix" denotes the PCR mastermix into which each locus was multiplexed and "T_a" denotes the annealing temperature used. Locus Zcwe05 is unpublished.

Table S2. Details of the mother-offspring pairs and their match probabilities calculated based on 41 microsatellite loci within Colony (46)

Colony	Mother ID	Offspring ID	Probability (%)
Special study beach	AGF11002	AGP11014	100
Special study beach	AGF11003	AGP11022	100
Special study beach	AGF11004	AGP11026	100
Special study beach	AGF11005	AGP11018	100
Special study beach	AGF11006	AGP11032	100
Special study beach	AGF11007	AGP11051	100
Special study beach	AGF11008	AGP11041	100
Special study beach	AGF11009	AGP11078	100
Special study beach	AGF11010	AGP11065	100
Special study beach	AGF11011	AGP11063	100
Special study beach	AGF11012	AGP11079	100
Special study beach	AGF11014	AGP11125	100
Special study beach	AGF11015	AGP11144	100
Special study beach	AGF11016	AGP11145	100
Special study beach	AGF11018	AGP11174	100
Special study beach	AGF11019	AGP11151	100
Special study beach	AGF11020	AGP11192	100
Special study beach	AGF11021	AGP11185	100
Special study beach	AGF11022	AGP11211	100
Special study beach	AGF11023	AGP11200	100
Freshwater beach	W8913mum	W8913pup	100
Freshwater beach	W8914mum	W8914pup	100
Freshwater beach	W8915mum	W8915pup	100
Freshwater beach	W8916mum	W8916pup	100
Freshwater beach	W8918mum	W8918pup	100
Freshwater beach	W8920mum	W8920pup	100
Freshwater beach	W8921mum	W8921pup	100
Freshwater beach	W8922mum	W8922pup	100
Freshwater beach	W8923mum	W8923pup	100
Freshwater beach	W8924mum	W8924pup	100
Freshwater beach	W8925mum	W8925pup	100
Freshwater beach	W8927mum	W8927pup	100
Freshwater beach	W8928mum	W8928pup	100
Freshwater beach	W8552/8258mum	W8552/8258pup	100
Freshwater beach	W8930mum	W8930pup	100
Freshwater beach	W8931mum	W8931pup	100
Freshwater beach	W8933mum	W8933pup	100
Freshwater beach	W8935mum	W8935pup	100
Freshwater beach	W8936mum	W8936pup	100
Freshwater beach	W8937mum	W8937pup	100
Freshwater beach	W8939mum	W8939pup	100

Table S3. Mean and SD of pairwise Queller and Goodnight (48) relatedness values

Sample	All individuals	Mothers	Offspring
Entire sample	0.009 ± 0.1	0.0008 ± 0.09	0.004 ± 0.09
Special study beach	0.016 ± 0.1	−0.005 ± 0.09	0.012 ± 0.09
Freshwater beach	0.011 ± 0.1	−0.004 ± 0.09	0.008 ± 0.10

Table S4. List of putative substances identified as being important for chemical similarity within mother–offspring pairs, chemical dissimilarity between the colonies, and genetic relatedness

Retention time (min)	Mean similarity explained (mother/offspring); Similarity contribution (colony); Occurrences in best subsets (relatedness)	Chemical name	Probability	Empirical Kovats Index	Kovats Index
Mother-offspring similarity					
19.723	15.54	Ethyl hexadecanoate (hexadecanoic acid ethyl ester)	58.3	1,992	1,993
15.458	12.25	1-Hexadecene	20	1,591	1,593
26.789	11.97	Squalene	46	2,815	2,790
16.397	11.30	8-Pentadecanone	94	1,673	1,648
19.525	10.87	Ethyl 9-hexadecenoate	87	1,972	1,977
21.405	8.49	Ethyl oleate	66	2,175	2,171
37.564	6.48	Not identified	—	—	—
15.623	6.48	Not identified	—	1,606	—
33.637	6.28	Campesterol	71	—	—
30.804	6.03	Cholestanol	67	—	—
20.362	5.34	Heptadecanoic acid	69	2,086	2,067
17.409	4.79	Not identified	—	1,766	—
Colony dissimilarity					
15.458	3.01	1-Hexadecene	20	1,591	1,593
16.397	2.42	8-Pentadecanone	94	1,673	1,648
26.789	2.07	Squalene	46	2,815	2,790
19.525	1.97	Ethyl 9-hexadecenoate	87	1,972	1,977
21.405	1.89	Ethyl oleate	66	2,175	2,171
21.348	1.67	Not identified	—	—	—
19.723	1.67	Ethyl hexadecanoate (hexadecanoic acid ethyl ester)	58.3	1,992	1,993
30.804	1.48	Cholestanol	67	—	—
38.518	1.44	Not identified	—	—	—
17.409	1.33	Not identified	—	1,766	—
20.511	1.29	Not identified	—	—	—
33.637	1.27	Campesterol	71	—	—
21.575	1.21	Octadecanoic acid ethyl ester	85	2,194	2,194
15.742	1.18	Not identified	—	—	—
19.665	1.13	Not identified	—	—	—
Relatedness					
36.941	315,926	Not identified	—	—	—
19.525	250,140	Ethyl 9-hexadecenoate	87	1,972	1,977
13.124	245,569	Not identified	—	—	—
20.362	214,830	Heptadecanoic acid	69	2,086	2,067
14.699	207,155	Not identified	—	—	—
21.090	203,683	Not identified	—	—	—
21.575	198,366	Octadecanoic acid ethyl ester	85	2,194	2,194
37.049	192,000	Not identified	—	—	—
19.620	189,049	Not identified	—	—	—
37.074	185,017	Not identified	—	—	—

Substances are listed in decreasing order of importance, as measured by the mean proportion of mother-pup similarity explained in the SIMPER analysis, the percentage contribution toward dissimilarity between beaches, and the number of occurrences within the best subsets identified by the BIO-ENV bootstrap procedure (see *Methods* for details). The chemical name and assignment probability are derived by a comparison of the empirical mass spectra with the most similar substance in the NIST library. The Kovats Index (*Methods*) was calculated for all substances with a retention time less than 28 min. For comparison, we provide the Kovats indices (60) of the substances to which our compounds show the closest resemblance.

Other Supporting Information Files

Dataset S1 (PDF)
Dataset S2 (XLSX)