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Supplementary Material

Characterisation of volatile organic compounds in dingo scat and a comparison with those of the domestic dog

Tyler J. Lepan[A], *Thy T. Truong*[B], *Sonu Yadav*[C,D], *and J. William O. Ballard*[A,E,*]

[A]Department of Environment and Genetics, SABE, La Trobe University, Melbourne, Vic. 3086, Australia.

[B]Proteomics and Metabolomics Platform, School of Agriculture, Biomedicine and Environment, La Trobe University, Melbourne, Vic. 3086, Australia.

[C]Biosecurity and Animal Welfare, Department of Industry, Trade and Tourism, Northern Territory Government, Darwin, NT, Australia.

[D]School of Biotechnology and Biomolecular Sciences, University of New South Wales, Sydney, NSW, Australia.

[E]School of Biosciences, University of Melbourne, Royal Parade, Parkville, Vic. 3052, Australia.

[*]Correspondence to: J. William O. Ballard Department of BioSciences, University of Melbourne, Melbourne, Vic. 3052, Australia Email: jwoballard@gmail.com

Supplementary Table S1.

List of dingoes and German Shepherd Dogs (GSD) included in this study.

Name	Canid	Sex	Age (years)	Name	Canid	Sex	Age (years)
Allira	Dingo	Female	3	Apari	Dingo	Male	4
Cooinda	Dingo	Female	8	Gubbah	Dingo	Male	3
Gili	Dingo	Female	3	Gunyah	Dingo	Male	8
Guyra	Dingo	Female	4	Kinta	Dingo	Male	3
Kareela	Dingo	Female	1.5	Mungka	Dingo	Male	5
Kora	Dingo	Female	4	Nooka	Dingo	Male	1
Pinchi	Dingo	Female	3	Typia	Dingo	Male	8
Adele	GSD	Female	1.8	Arrow	GSD	Male	5.9
Bea	GSD	Female	1.8	Rundo	GSD	Male	2.2
Destiny	GSD	Female	3.6	Cruz	GSD	Male	5.6
Gina	GSD	Female	5.6				
Mischa	GSD	Female	5.9				
Ruza	GSD	Female	2.1				
Topla	GSD	Female	2.3				
Dana	GSD	Female	4.1				

Supplementary Table S2.

List of all the VOCs (159) detected and identified in the scats of dingo and GSD samples. MSI ID levels indicate the confidence of identification, where 1. confirmed identification with standard, NIST library mass spectra and Kovats non-isothermal retention index (RI), 2: putative identification with NIST reference mass spectra and Kovats RI, or 3: NIST reference spectra match score (≥ 70% confidence).

No.	Compound	Chemical Classification	RT (min)	Reference m/z	CAS No.	NIST SI	NIST RSI	Total Score	Calculated RI	NIST RI	PubChem RI	PubChem CID	MSI ID level
1	2-Butanone	Aliphatic ketones	4.29	43	78-93-3	871	895	90	645	598	622	6569	1
2	Acetic acid	Aliphatic acids	4.852	43	64-19-7	957	964	97	661	610	661	176	1
3	Isovaleral	Aliphatic aldehydes	5.268	44	590-86-3	935	942	94	672	652	671	11552	2
4	2-Pentanone	Aliphatic ketones	5.979	43	107-87-9	915	927	93	692	685	695	7895	2
5	Heptane	Hydrocarbons	6.252	43	142-82-5	901	902	90	700	700	700	8900	1
6	Propanoic acid	Aliphatic acids	7.771	74	79-09-4	936	936	94	748	706	748	1032	2
7	Methyl butanoate	Aliphatic esters	7.061	74	623-42-7	903	918	92	729	723	730	12180	2
8	Isopentanol	Aliphatic alcohols	7.624	55	123-51-3	888	893	89	744	736	744	31260	2
9	Dimethyldisulfide	Sulfur-containing volatiles	7.80	94	624-92-0	962	962	96	748	746	748	12232	2
10	Methyl isopentanoate	Aliphatic esters	9.04	74	556-24-1	868	891	89	780	776	793	11160	2
11	Isobutyric acid	Aliphatic acids	9.081	43	79-31-2	843	846	85	781	765	785	6590	2
12	Octane	Hydrocarbons	9.824	43	111-65-9	936	950	95	800	800	800	356	1
13	Hexanal	Aliphatic aldehydes	9.958	44	66-25-1	834	842	84	803	801	803	6184	1
14	Butyric Acid	Aliphatic acids	10.81	60	107-92-6	824	878	88	825	802	825	264	1
15	Methyl pentanoate	Aliphatic esters	10.87	74	624-24-8	859	863	86	827	823	829	12206	2
16	Furfural	Other volatiles	11.30	96	98-01-1	974	990	99	838	833	838	7362	2
17	1-Hexanol	Aliphatic alcohols	12.70	56	111-27-3	968	969	97	874	868	874	8103	2
18	Isovaleric acid	Aliphatic acids	12.85	60	503-74-2	806	808	81	878	850	878	10430	1
19	Methyl butyric acid	Aliphatic acids	13.27	74	116-53-0	914	914	92	888	861	888	8314	2
20	2-Heptanone	Aliphatic ketones	13.43	43	110-43-0	824	874	88	892	891	892	8051	1
21	Nonane	Hydrocarbons	13.73	43	111-84-2	944	944	95	900	900	900	8141	1
22	Heptanal	Aliphatic aldehydes	13.90	70	111-71-7	908	909	91	905	901	905	8130	2
23	Valeric acid	Aliphatic acids	13.96	60	109-52-4	806	808	81	906	901	906	7991	1

24	Methyl caproate	Aliphatic esters	14.70	74	106-70-7	865	882	88	927	925	927	7824	2
25	alpha-Pinene	Terpenes	15.01	93	80-56-8	926	926	93	935	937	935	6654	2
26	Methanethiol isovalerate	Sulfur-containing volatiles	15.29	57	23747-45-7	833	924	93	943	939	938	90246	2
27	Propyl 2-methylbutanoate	Aliphatic esters	15.47	57	37064-20-3	849	858	86	947	946	947	162239	2
28	Propyl isopentanoate	Aliphatic esters	15.65	85	557-00-6	918	923	92	952	946	952	11176	2
29	2-Isooctanone	Aliphatic ketones	15.82	43	928-68-7	856	901	90	957	956	957	13572	2
30	2-Heptenal	Aliphatic aldehydes	15.99	41	18829-55-5	831	840	84	962	958	962	5283316	2
31	Isocaproic acid	Aliphatic acids	16.02	57	646-07-1	877	923	92	962	949	955	12587	2
32	5-Methyl-2-heptanone	Aliphatic ketones	16.15	43	18217-12-4	910	926	93	966	971	965	28965	2
33	Benzaldehyde	Benzenoids	16.19	77	100-52-7	965	966	97	967	962	967	240	1
34	Dimethyl trisulfide	Sulfur-containing volatiles	16.40	126	3658-80-8	907	913	91	973	971	973	19310	2
35	1-Heptanol	Aliphatic alcohols	16.46	70	111-70-6	910	910	91	974	970	974	8129	2
36	1-Octen-3-ol	Aliphatic alcohols	16.76	57	3391-86-4	934	934	94	983	980	983	18827	1
37	Phenol	Volatile phenols	16.87	94	108-95-2	949	966	97	986	981	986	996	2
38	2-Octanone	Aliphatic ketones	17.14	43	111-13-7	896	910	91	993	991	993	8093	2
39	Butyl butanoate	Aliphatic esters	17.30	71	109-21-7	824	860	86	997	995	997	7983	2
40	Decane	Hydrocarbons	17.38	57	124-18-5	946	950	95	1000	1000	900	15600	1
41	Octanal	Aliphatic aldehydes	17.59	43	124-13-0	945	962	96	1006	1003	1006	454	1
42	2-Thienaldehyde	Sulfur-containing volatiles	17.62	111	98-03-3	847	876	88	1007	1008	1006	7364	2
43	alpha-Phellandrene	Terpenes	17.66	93	99-83-2	915	936	94	1008	1005	1008	7460	2
44	2,4-Heptadienal	Aliphatic aldehydes	17.95	81	5/03/4313	902	906	91	1017	1012	1017	5283321	2
45	Isovalerylacetone	Aliphatic ketones	18.20	85	3002-23-1	861	941	94	1024	1033	1029	76354	2
46	Methyl heptanoate	Aliphatic esters	18.24	74	106-73-0	871	875	88	1025	1023	1025	7826	2
47	p-Cymene	Terpenes	18.31	119	99-87-6	888	890	89	1027	1025	1027	7463	2
48	2-Ethylhexanol	Aliphatic alcohols	18.45	57	104-76-7	935	942	94	1032	1030	1032	7720	2
49	Eucalyptol	Terpenes	18.61	43	470-82-6	919	923	92	1036	1032	1036	2758	2
50	Benzyl alcohol	Benzenoids	18.78	79	100-51-6	895	895	90	1041	1036	1041	244	1
51	3-Octen-2-one	Aliphatic ketones	18.80	55	1669-44-9	888	893	89	1042	1040	1042	5363229	2
52	Butyl 2-methylbutanoate	Aliphatic esters	18.82	57	15706-73-7	826	858	86	1043	1043	1043	61812	2
53	Butyl isopentanoate	Aliphatic esters	19.02	85	109-19-3	818	821	82	1049	1045	1048	7981	2
54	Benzeneacetaldehyde	Benzenoids	19.05	91	122-78-1	948	948	95	1050	1045	1050	998	1

55	2-Octenal	Aliphatic aldehydes	19.48	41	2548-87-0	939	943	94	1062	1060	1062	5283324	2
56	Acetophenone	Benzenoids	19.80	105	98-86-2	967	968	97	1072	1066	1072	7410	1
57	1-Octanol	Aliphatic alcohols	19.87	56	111-87-5	817	843	84	1074	1070	1074	957	2
58	p-Cresol	Volatile phenols	20.11	107	106-44-5	950	953	95	1081	1077	1081	2879	2
59	Octanenitrile	Nitrogen-containing volatiles	20.20	82	124-12-9	809	809	81	1084	1081	1085	31286	2
60	2-Nonanone	Aliphatic ketones	20.50	58	821-55-6	931	934	94	1093	1092	1093	13187	1
61	Nitrobenzene	Benzenoids	20.52	77	98-95-3	942	965	97	1094	1080	1100	7416	1
62	Undecane	Hydrocarbons	20.73	57	1120-21-4	915	944	95	1100	1100	1100	14257	1
63	Linalool	Terpenes	20.79	71	78-70-6	915	916	92	1102	1099	1102	6549	2
64	2-Nonanol	Aliphatic alcohols	20.85	45	628-99-9	904	907	91	1104	1102	1106	12367	2
65	Nonanal	Aliphatic aldehydes	20.95	57	124-19-6	938	939	94	1107	1104	1107	31289	1
66	Phenylethyl alcohol	Benzenoids	21.34	91	60-12-8	954	959	96	1120	1116	1120	6054	1
67	Methyl octanoate	Aliphatic esters	21.50	74	111-11-5	905	921	92	1125	1126	1125	8091	2
68	3-Nonen-2-one	Aliphatic ketones	22.04	55	14309-57-0	813	835	84	1142	1142	1142	5317045	2
69	2-Methylhexadecanal	Aliphatic aldehydes	22.53	58	55019-46-0	748	769	77	1158	N/A	N/A	546976	3
70	Benzenepropanal	Benzenoids	22.90	91	104-53-0	934	936	94	1170	1163	1178	7707	2
71	1-Nonanol	Aliphatic alcohols	23.04	56	143-08-8	909	911	91	1175	1173	1175	8914	2
72	Methyl benzeneethanoate	Benzenoids	23.23	91	101-41-7	857	857	86	1181	1178	1183	7559	2
73	4-Terpineol	Terpenes	23.43	71	562-74-3	907	909	91	1187	1177	1187	11230	2
74	2-Decanone	Aliphatic ketones	23.63	58	693-54-9	890	928	93	1194	1193	1194	12741	2
75	Dodecane	Hydrocarbons	23.81	57	112-40-3	953	955	96	1199	1200	1200	8182	1
76	Methyl salicylate	Volatile phenols	23.82	120	119-36-8	822	940	94	1200	1192	1200	4133	1
77	alpha-Terpineol	Terpenes	23.87	59	98-55-5	919	921	92	1201	1189	1201	17100	2
78	2-Decanol	Aliphatic alcohols	23.94	45	1120-06-5	913	947	95	1204	1200	1204	14254	2
79	N-(2-Hydroxyethyl)-N-methyl-perfluorobutane-1-sulfonamide	Sulfur-containing volatiles	24.11	69		904	904	91	1210	N/A	N/A	N/A	3
80	2-Piperidinone	Nitrogen-containing volatiles	24.33	99	675-20-7	902	927	93	1217	1174	1174	12665	1
81	Methyl nonanoate	Aliphatic esters	24.53	74	1731-84-6	915	915	92	1225	1223	1225	15606	2
82	3,4-Dimethylbenzaldehyde	Benzenoids	24.58	133	5973-71-7	924	946	95	1226	1236	N/A	22278	2

83	Mequinol	Volatile phenols	25.12	109	150-76-5	872	927	93	1244	1240	1210	9015	2
84	3-Phenylpropanol	Aliphatic alcohols	25.11	117	122-97-4	935	942	94	1245	1233	1252	31234	2
85	Ethylmethylmaleimide	Nitrogen-containing volatiles	25.22	139	20189-42-8	779	779	78	1248	1239	1265	29995	2
86	Quinoline	Nitrogen-containing volatiles	25.41	129	91-22-5	960	960	96	1255	1238	1255	7047	2
87	Benzeneacetic acid	Benzenoids	25.80	91	103-82-2	864	902	90	1269	1262	1269	999	2
88	Methylvinylmaleimide	Nitrogen-containing volatiles	26.12	66	21494-57-5	887	896	90	1279	1261	1261	152426	2
89	Methyl 3-phenylpropanoate	Aliphatic esters	26.16	104	103-25-3	944	958	96	1281	1279	1293	7643	2
90	3-Undecanone	Aliphatic ketones	26.48	57	2216-87-7	920	923	92	1292	1283	1298	75189	2
91	Indole	Nitrogen-containing volatiles	27.10	117	120-72-9	865	865	87	1314	1295	1328	798	1
92	2-Aminoacetophenone	Nitrogen-containing volatiles	27.26	120	551-93-9	848	854	86	1320	1308	1325	11086	2
93	Tridecane	Hydrocarbons	26.71	57	629-50-5	948	949	95	1300	1300	1300	12388	1
94	Mesitaldehyde	Benzenoids	27.23	147	487-68-3	879	885	89	1319	1339	1323	10254	2
95	2-Methoxy-4-vinylphenol	Volatile phenols	27.35	135	7786-61-0	928	936	94	1324	1316	1324	332	2
96	Khinaldin	Nitrogen-containing volatiles	27.38	143	91-63-4	906	906	91	1325	1311	1313	7060	1
97	2,4-Decadienal	Aliphatic aldehydes	27.45	81	2363-88-4	827	849	85	1327	1317	1327	5283349	2
98	Tetrahydroquinoline	Nitrogen-containing volatiles	27.96	132	635-46-1	852	915	92	1346	1326	1339	69460	2
99	Hydrocinnamic acid	Benzenoids	28.16	91	501-52-0	931	951	95	1353	1356	1347	107	2
100	2-Methylundecanal	Aliphatic aldehydes	28.35	58	110-41-8	738	841	79	1360	1365	1363	61031	2
101	gamma-Nonanolactone	Other volatiles	28.59	85	104-61-0	778	852	85	1369	1365	1369	7710	2
102	2,4-Tridecanedione	Aliphatic ketones	28.92	43	25276-80-6	768	803	80	1381	N/A	N/A	529776	3
103	2-Dodecanone	Aliphatic ketones	29.33	58	6175-49-1	811	904	91	1396	1395	1396	22556	2
104	Tetradecane	Hydrocarbons	29.41	57	629-59-4	955	962	96	1399	1400	1400	12389	1
105	4-tert-Amylphenol	Volatile phenols	29.54	135	80-46-6	857	871	87	1404	1400	1404	6643	2
106	Butyl phenylacetate	Benzenoids	30.51	91	122-43-0	953	967	97	1439	1440	1446	31210	2

107	Geranylacetone	Terpenes	30.92	43	3796-70-1	857	891	89	1454	1453	1454	1549778	2
108	2,6-Di-tert-butylbenzoquinone	Aliphatic ketones	31.44	177	719-22-2	921	935	94	1473	1472	1473	12867	2
109	Hexahydrofarnesol	Aliphatic alcohols	31.67	57	6750-34-1	803	862	86	1482	1571	1576	138824	2
110	3-tert-Butyl-4-methoxyphenol	Volatile phenols	31.81	165	88-32-4	860	906	91	1486	1490	1490	6932	2
111	trans-beta-Ionone	Terpenes	31.89	177	79-77-6	877	913	91	1489	1486	1489	638014	2
112	5,6-beta-Ionone epoxide	Terpenes	31.97	123	23267-57-4	814	820	82	1492	1473	1492	90899	2
113	2-tert-Butyl-4-methoxyphenol	Volatile phenols	32.06	165	121-00-6	932	948	95	1496	1496	1496	8456	2
114	2-Tridecanone	Aliphatic ketones	32.12	58	593-08-8	812	852	85	1498	1496	1498	11622	2
115	Pentadecane	Hydrocarbons	32.16	57	629-62-9	939	939	94	1499	1500	1500	12391	1
116	2-Tridecanol	Aliphatic alcohols	32.29	45	1653-31-2	804	828	83	1506	1510	1510	15449	2
117	2,6-Di-tert-butyl-p-cresol	Volatile phenols	32.33	205	128-37-0	939	939	94	1509	1513	1509	31404	2
118	2,4-Di-tert-butylphenol	Volatile phenols	32.39	191	96-76-4	889	897	90	1513	1514	1513	7311	2
119	Methyl dodecanoate	Aliphatic esters	32.63	74	111-82-0	819	829	83	1528	1526	1528	8139	2
120	Dihydroactinidolide	Other volatiles	33.02	111	17092-92-1	911	912	91	1552	1532	1568	6432173	2
121	2-[(2-Ethoxy-3,4-dimethyl-2-cyclohexen-1-ylidene)methyl]furan	Other volatiles	33.28	232	55162-49-7	723	747	75	1569	N/A	N/A	5376746	3
122	2-Tetradecanone	Aliphatic ketones	33.34	58	2345-27-9	814	857	86	1573	1597	1595	75364	2
123	2-Nonylthiophene	Sulfur-containing volatiles	33.55	97	57754-07-1	801	803	80	1586	N/A	N/A	566346	3
124	Diethyltoluamide	Benzenoids	33.57	119	134-62-3	889	911	91	1552	1582	1571	4284	2
125	Spathulenol	Terpenes	33.67	119	6750-60-3	916	920	918	1555	N/A	N/A	92231	3
126	Hexadecane	Hydrocarbons	33.75	57	544-76-3	911	911	91	1599	1600	1600	11006	1
127	Methyl tridecanoate	Aliphatic esters	34.06	74	1731-88-0	773	819	82	1627	1624	1631	15608	2
128	gamma-Eudesmol	Terpenes	34.34	189	1209-71-8	913	922	92	1652	1631	1654	6432005	2
129	beta-Selinenol	Terpenes	34.62	59	473-15-4	899	921	92	1678	1649	1677	6432456	2
130	Methyl 12-methyltridecanoate	Aliphatic esters	34.75	74	5129-58-8	868	871	87	1690	1686	1689	21204	2
131	Heptadecane	Hydrocarbons	34.86	57	629-78-7	895	939	94	1700	1700	1700	12398	1
132	2-Pentadecanone	Aliphatic ketones	34.87	58	2345-28-0	815	921	92	1701	1698	1702	61303	2
133	2-Hexadecanol	Aliphatic alcohols	34.94	55	14852-31-4	866	888	89	1709	1702	1702	85779	2
134	2-Pentadecanol	Aliphatic alcohols	34.94	45	1653-34-5	864	864	87	1710	1710	1710	96687	2
135	Methyl cis-9-tetradecenoate	Aliphatic esters	34.99	55	56219-06-8	890	892	89	1715	1715	1715	5352674	2

136	Trifluoroacetic acid pentadecyl ester	Other volatiles	34.94	57	959010-23-2	818	898	90	1709	1722	1717	536403	2
137	Methyl tetradecanoate	Aliphatic esters	35.10	74	124-10-7	913	913	91	1727	1725	1727	31284	2
138	3,5-ditert-butyl-4-hydroxycyclohexa-2,4-dien-1-one	Other volatiles	35.14	207	54965-43-4	742	920	92	1733	N/A	N/A	610030	3
139	4-Formyl-2,6-di-tert-butylphenol	Volatile phenols	35.52	219	1620-98-0	892	897	90	1777	1772	1774	73219	2
140	Methyl 12-methyltetradecanoate	Aliphatic esters	35.70	74	5129-66-8	783	859	86	1798	1788	1786	21206	2
141	Octadecane	Hydrocarbons	35.70	57	593-45-3	939	939	94	1799	1800	1800	11635	1
142	Methyl pentadecanoate	Aliphatic esters	35.91	74	7132-64-1	888	889	89	1828	1824	1826	23518	2
143	Methyl 2-oxohexadecanoate	Aliphatic esters	36.14	57	55836-30-1	819	857	86	1859	N/A	N/A	545549	3
144	1-Nonadecene	Hydrocarbons	36.34	57	18435-45-5	844	904	91	1887	1893	1885	29075	2
145	1-Hexadecanol	Aliphatic alcohols	36.34	55	36653-82-4	925	929	93	1887	1880	1886	2682	2
146	Nonadecane	Hydrocarbons	36.42	57	629-92-5	914	940	94	1899	1900	1900	12401	1
147	Methyl hexadecanoate	Aliphatic esters	36.60	74	112-39-0	903	931	93	1928	1926	1928	8181	2
148	Palmitic acid	Aliphatic acids	36.84	73	57-10-3	887	891	89	1967	1968	1967	985	2
149	Ethenyl hexadecanoate	Aliphatic esters	36.96	57	693-38-9	892	892	89	1987	1977	1986	69658	2
150	Eicosane	Hydrocarbons	37.03	57	112-95-8	935	938	94	1999	2000	2000	8222	1
151	Heneicosane	Hydrocarbons	37.59	57	629-94-7	943	943	94	2099	2000	2000	12403	1
152	Methyl trans-11-octadecenoate	Aliphatic esters	37.61	55	52380-33-3	852	852	85	2105	2115	2105	5364432	2
153	Methyl octadecanoate	Aliphatic esters	37.73	74	112-61-8	882	893	89	2129	2128	2129	8201	2
154	Docosane	Hydrocarbons	38.08	57	629-97-0	903	903	90	2199	2200	2200	12405	1
155	Tricosane	Hydrocarbons	38.55	57	638-67-5	845	847	85	2299	2300	2300	12534	1
156	Tetracosane	Hydrocarbons	38.99	57	646-31-1	863	881	88	2399	2400	2400	12592	1
157	2-Phenyl-3-benzylidenepyrrolidine	Nitrogen-containing volatiles	39.03	235	122949-15-9	779	780	78	2408	N/A	N/A	5376823	3
158	Pentacosane	Hydrocarbons	39.41	57	629-99-2	861	869	87	2499	2500	2500	12406	1
159	3,3-Methylenebis-1H-indole	Nitrogen-containing volatiles	41.39	245	4/05/1968	907	946	95	2625	2879	2700	3071	2

Supplementary Table S3.

List of all the relative concentrations (ng/g ± rsd) for the 154 VOCs detected and identified in the scats of male and female dingo and GSD samples, including the QC samples (Pooled and All Pooled).

No.	Metabolite	Mean All Pooled (ng/g, n=8)	%RSD	Mean Pooled (ng/g, n=8)	%RSD	Mean GSD (ng/g, n=11)	%RSD	Mean Dingo (ng/g, n=14)	%RSD
1	2-Butanone	465.24	24.01			79.41	70.08	103.98	53.49
2	Acetic acid	393.13	29.33	813.57	36.14	75.92	40.55	85.44	56.45
3	Isovaleral	42.55	30.31	56.13	35.93	8.29	53.70	9.00	39.93
4	2-Pentanone	77.68	29.33	103.48	31.63	20.26	61.32	16.72	97.64
5	Heptane			46.81	31.59	11.67	47.83		
6	Propanoic acid	189.46	39.29	475.38	30.46	63.64	53.75	74.11	78.48
7	Methyl butanoate	276.50	21.19	188.10	28.97	39.49	60.67	38.14	86.64
8	Isopentanol	65.76	33.03	86.73	30.15	19.33	104.78	7.21	68.62
9	Dimethyldisulfide	25.55	8.29	24.10	33.83	12.20	117.95	8.71	125.57
10	Methyl isopentanoate	51.53	27.24	59.23	37.09	12.39	56.06	8.41	56.97
11	Isobutyric acid	236.91	28.37	220.28	20.04	56.54	51.46	44.56	73.87
12	Hexanal	63.86	27.04	87.02	29.06	17.64	39.80	19.86	28.99
13	Methyl pentanoate	115.83	33.52	80.69	38.48	13.74	57.05	15.76	86.40
14	Butyric Acid	2793.46	19.42	1586.57	17.66	537.58	55.07	592.21	72.55
15	Furfural	6.09	27.87	4.64	30.68	1.72	74.93	1.35	65.57
16	Isovaleric acid	2235.92	26.59	1426.39	25.39	435.08	70.51	379.69	67.82
17	1-Hexanol	323.64	27.70	436.51	21.57	77.36	46.18	54.71	53.47
18	Methyl butyric acid	1409.89	21.21	1004.99	27.22	230.55	56.84	227.94	55.43
19	2-Heptanone	130.40	32.34	140.05	30.04	25.52	39.93	23.74	37.11
20	Nonane			280.55	17.64	3.47	144.60	15.44	163.06
21	Heptanal	25.44	21.32	18.99	24.06	7.81	20.38	5.63	21.74
22	Valeric acid	380.30	22.44	383.21	37.92	63.31	39.67	64.39	80.94
23	Methyl caproate	27.62	23.58	14.82	26.04	3.89	66.76	4.88	42.37
24	alpha-Pinene	11.68	1.18			3.14	87.72		
25	Methanethiol isovalerate	44.14	37.57	56.68	37.49	23.14	103.31	14.89	114.88
26	Propyl 2-methylbutanoate	1.45	22.54	4.26	38.27	2.35	104.63	1.44	71.60

27	Propyl isopentanoate	9.51	38.74	23.49	30.56	6.41	112.86	3.35	96.54
28	2-Isooctanone	68.28	28.53	98.29	31.56	14.98	49.50	16.09	51.43
29	2-Heptenal	35.77	21.45	17.84	29.64	7.16	50.60	3.85	39.93
30	Isocaproic acid	120.29	24.35	167.14	12.81				
31	5-Methyl-2-heptanone	152.24	27.37	186.19	19.87	37.60	56.55	37.70	74.86
32	Benzaldehyde	395.17	23.66	462.69	27.11	104.26	36.23	87.56	23.17
33	Dimethyl trisulfide	55.37	3.40	47.02	18.47	14.97	69.85	19.45	143.89
34	1-Heptanol	69.30	25.48	72.75	24.66	23.02	46.67	12.91	34.06
35	1-Octen-3-ol	361.81	30.26	318.33	22.18	63.51	41.92	98.71	74.70
36	Phenol	7576.43	22.66	9272.42	26.09	2166.57	82.75	1059.74	148.78
37	2-Octanone	98.44	25.51	119.42	22.99	23.71	29.88	21.65	41.75
38	Butyl butanoate	7.31	37.69			5.05	131.35	11.46	222.08
39	Octanal	19.90	19.70	17.78	38.58	6.11	29.30	5.40	20.45
40	2-Thienaldehyde	2.97	22.82	2.79	34.51	0.80	16.03	0.56	23.35
41	alpha-Phellandrene	4.56	25.17						
42	2,4-Heptadienal	162.13	22.40	120.30	31.95	34.97	25.74	38.51	26.01
43	Isovalerylacetone	199.80	29.37	189.62	26.42	37.48	24.54	56.32	36.99
44	Methyl heptanoate	27.85	19.67	19.85	37.90	3.98	62.56	5.79	72.10
45	p-Cymene	48.42	35.77			10.04	239.60	66.66	215.16
46	2-Ethylhexanol	159.70	28.28	145.95	37.75	49.88	27.97	29.22	42.49
47	Eucalyptol	18.83	20.96					41.21	198.83
48	Benzyl Alcohol	36.76	22.98	31.40	27.06	7.50	27.96	7.18	33.03
49	3-Octen-2-one	46.87	26.39	45.18	34.31	8.01	63.44	12.47	31.94
50	Butyl 2-methylbutanoate	6.71	26.41			2.73	76.25	3.68	122.58
51	Butyl isopentanoate	11.87	25.25	17.54	28.69	4.14	101.63	4.70	126.56
52	Benzeneacetaldehyde	240.10	32.91	342.60	34.09	21.52	49.61	58.36	39.30
53	2-Octenal	118.36	22.44	113.29	24.39	26.84	19.45	27.19	26.60
54	Acetophenone	456.61	23.01	593.34	33.66	213.57	48.47	15.96	61.83
55	1-Octanol	84.18	22.24	88.43	28.55	23.89	48.43	17.66	49.29
56	p-Cresol	152.96	24.31	139.45	33.96	35.44	93.63	29.72	60.78
57	Octanenitrile	6.34	26.56	6.10	20.18	1.32	32.89	1.49	38.62
58	2-Nonanone	189.45	27.65	255.03	20.00	36.33	27.41	47.37	30.48
59	Linalool	14.98	30.52			6.16	143.86	3.26	191.83
60	2-Nonanol	91.91	26.56	87.49	29.55	21.99	39.24	19.75	43.73
61	Nonanal	65.59	17.83	43.88	33.76	18.49	35.50	13.23	36.98

62	Phenylethyl Alcohol	2338.00	31.62	1075.59	35.17	193.96	114.01	453.93	49.64
63	Methyl octanoate	127.90	23.05	115.01	40.04	19.02	49.77	24.62	53.82
64	3-Nonen-2-one	39.05	22.93	36.89	22.91	8.30	58.64	9.07	36.75
65	2-Methylhexadecanal	130.22	27.41	148.01	21.08	23.17	49.79	29.54	64.41
66	Benzenepropanal	36.38	18.38	62.91	36.95	17.49	97.77	3.14	40.81
67	1-Nonanol	259.27	20.99	278.99	27.69	78.30	55.63	44.06	33.14
68	Methyl benzeneethanoate	49.85	38.61	38.49	38.95	6.20	53.91	12.53	100.23
69	2-Decanone	253.36	27.40	314.41	26.72	51.07	28.26	53.67	76.64
70	Dodecane	6.90	34.64	1389.69	34.58				
71	Methyl salicylate	35.19	29.92	44.93	23.27	8.70	65.15	8.75	170.43
72	alpha-Terpineol	15.68	29.01			7.58	138.84	109.96	261.78
73	2-Decanol	78.95	24.48	128.18	29.59	21.97	62.28	11.55	112.86
74	N-(2-Hydroxyethyl)-N-methyl-perfluorobutane-1-sulfonamide	148.95	31.49	139.45	34.74	13.29	126.12	16.92	50.88
75	2-Piperidinone	7219.96	28.24	7136.88	36.40	1843.31	52.74	998.88	57.74
76	Methyl nonanoate	482.17	26.88	439.29	39.54	57.35	48.68	72.08	92.68
77	3,4-Dimethylbenzaldehyde	20.87	36.50			7.59	97.04		
78	Mequinol	19.06	17.15					5.23	72.11
79	3-Phenylpropanol	279.05	26.44	169.82	29.73	128.26	110.06	7.41	107.11
80	Ethylmethylmaleimide	26.84	11.43	297.16	32.76	91.23	69.11	44.52	51.01
81	Quinoline	32277.99	24.04	49303.86	39.52	7323.61	64.78	3904.24	77.45
82	Benzeneacetic acid	239.86	31.75	321.56	29.29	20.71	71.66	42.00	78.30
83	Methylvinylmaleimide	108.16	24.29	118.79	33.64	17.32	53.32	23.24	71.80
84	Methyl 3-phenylpropanoate	3632.88	23.84	2977.64	27.62	1048.73	60.21	159.88	125.73
85	3-Undecanone	105.54	23.14	137.90	38.66			26.95	81.71
86	Indole	90922.33	22.72	147260.63	37.31	22957.11	41.64	13155.10	65.31
87	2-Aminoacetophenone	27.53	25.96	31.92	20.85	6.04	31.64	6.92	91.27
88	Tridecane	38.70	42.09	865.70	34.41	11.76	141.62	3.08	57.88
89	Mesitaldehyde	2.50	32.90					2.92	62.70
90	Khinaldin	4353.94	32.55	6255.34	30.84	1400.92	38.51	305.79	63.93
91	2-Methoxy-4-vinylphenol	367.83	29.01	521.97	28.95	83.10	28.83	31.73	37.48
92	2,4-Decadienal	290.13	25.42	498.93	27.75	56.75	37.06	44.16	37.93
93	Tetrahydroquinoline	1334.62	25.74	2001.39	25.78	348.25	89.54	220.48	126.73
94	Hydrocinnamic acid	2165.48	31.52	1527.06	33.59	583.41	69.61	55.23	76.29
95	2-Methylundecanal	109.46	23.50	169.81	32.77	17.00	48.29	23.78	75.85

96	gamma-Nonanolactone	203.64	26.25	275.34	29.49	38.03	41.57	36.36	40.68
97	2,4-Tridecanedione	125.65	21.51	168.87	38.28			27.39	40.62
98	2-Dodecanone	147.94	24.19	214.11	24.10	31.61	48.90	26.39	112.78
99	Tetradecane	7.99	35.99	489.85	35.46	4.50	140.73	0.80	71.57
100	4-tert-Amylphenol	72.63	21.63	122.59	26.04	17.48	25.44	17.17	25.79
101	Butyl phenylacetate	5.65	35.06	8.16	31.29				
102	Geranylacetone	215.71	26.11	312.46	31.03	42.45	62.76	27.05	26.26
103	2,6-Di-tert-butylbenzoquinone	286.98	27.20	215.01	24.25	140.40	94.65		
104	Hexahydrofarnesol	10.08	29.02	9.70	10.86	1.29	88.40	3.02	164.26
105	3-tert-Butyl-4-methoxyphenol	61.35	29.95	95.24	35.59	35.60	115.94		
106	trans-beta-Ionone	78.92	26.45	163.45	36.36	25.80	63.29	9.08	27.34
107	5,6-beta-Ionone epoxide	102.92	27.27	195.84	39.07	35.33	48.19	10.58	32.71
108	2-tert-Butyl-4-methoxyphenol	5502.37	29.80	5669.41	39.76	2155.96	117.40	31.83	68.54
109	2-Tridecanone	156.80	24.17			29.16	33.72	26.60	46.29
110	Pentadecane	64.43	27.65	599.30	35.44	16.61	53.49	5.08	68.01
111	2-Tridecanol	78.98	23.79	134.32	39.06	16.24	62.07	12.09	63.38
112	2,6-Di-tert-butyl-p-cresol	365.74	25.89	891.36	37.23	191.70	112.08	5.17	24.57
113	2,4-Di-tert-butylphenol	58.35	22.30	118.62	23.85	13.65	15.37	12.34	20.21
114	Methyl dodecanoate	37.85	15.17	79.14	34.38	10.35	67.60	6.74	82.29
115	Dihydroactinidolide	36.51	30.33	60.40	36.97	11.39	61.73	3.49	30.20
116	2-[(2-Ethoxy-3,4-dimethyl-2-cyclohexen-1-ylidene)methyl]furan	10.54	26.24	11.89	26.77	4.50	95.63		
117	2-Tetradecanone	55.27	24.58	98.80	39.67	11.19	38.09	8.68	56.29
118	2-Nonylthiophene***	27.48	31.34	38.62	32.77			6.14	91.93
119	Diethyltoluamide	16.83	18.75	26.19	26.52	1.65	53.72	5.23	82.35
120	Spathulenol	7.94	36.94	9.53	38.91				
121	Hexadecane	32.09	21.15	377.37	21.03	6.94	63.85	4.31	60.75
122	Methyl tridecanoate	9.82	26.11	15.53	23.38	2.45	38.59	1.96	72.74
123	gamma-Eudesmol	8.16	36.00					3.72	316.08
124	beta-Selinenol	66.44	38.95			8.62	271.70	14.45	281.85
125	Methyl 12-methyltridecanoate	14.88	17.94	23.33	26.64				
126	Heptadecane	80.57	23.38	335.21	32.62	16.27	57.44	9.04	42.55
127	2-Pentadecanone	110.22	26.18	174.66	24.96	27.88	87.17	11.09	53.25
128	2-Hexadecanol	43.14	29.08	53.20	21.85	7.84	77.58	4.65	80.68
129	2-Pentadecanol	43.35	28.06	54.11	22.42	8.58	68.85	4.63	81.50

130	Methyl cis-9-tetradecenoate	10.89	27.97	15.43	19.44				
131	Trifluoroacetic acid, pentadecyl ester	15.41	33.77	22.38	17.77	3.26	62.80	2.16	72.58
132	Methyl tetradecanoate	152.12	23.90	229.20	36.69	24.26	74.16	15.68	85.21
133	3,5-ditert-butyl-4-hydroxycyclohexa-2,4-dien-1-one	99.85	33.80	38.77	33.90	13.94	53.57		
134	4-Formyl-2,6-di-tert-butylphenol	39.60	30.02	64.75	27.78	15.36	95.84		
135	Methyl 12-methyltetradecanoate	107.65	24.64	161.01	32.54	16.69	85.45	8.28	65.91
136	Octadecane	33.97	20.51	446.26	31.40	5.39	68.90	2.77	67.66
137	Methyl pentadecanoate	44.99	26.49	63.73	29.28	7.09	68.81	3.71	81.03
138	Methyl 2-oxohexadecanoate	15.04	31.96	7.99	36.19			2.36	66.62
139	1-Nonadecene	38.59	31.51	37.97	38.85	9.79	73.14	3.40	37.98
140	1-Hexadecanol	45.14	38.76	50.04	37.95	7.90	114.22	3.00	46.05
141	Nonadecane	4.84	17.91	52.57	21.77	1.98	191.95	0.76	97.76
142	Methyl hexadecanoate	347.66	27.72	436.99	18.72	45.25	67.41	21.82	56.89
143	Palmitic acid	46.16	34.52	17.55	35.67	3.02	104.73	2.27	62.09
144	Ethenyl hexadecanoate	20.03	37.15	20.60	36.48	2.09	104.88	1.62	50.98
145	Eicosane	4.46	30.94	27.49	15.67	0.78	64.00	0.76	90.71
146	Heneicosane	6.17	14.24	22.86	28.28	1.29	52.05	1.66	146.23
147	Methyl trans-11-octadecenoate	120.31	40.00	131.56	35.44	16.71	88.79	6.95	54.81
148	Methyl octadecanoate	27.72	31.33	28.10	35.75	3.18	52.38	2.00	50.42
149	Docosane	2.05	13.78	11.67	15.26	1.16	56.53	0.78	95.06
150	Tricosane	4.94	26.22	15.44	25.85	1.67	41.50	1.34	69.64
151	Tetracosane	4.21	17.52	10.42	21.18	1.26	47.03	0.99	67.21
152	2-Phenyl-3-benzylidenepyrrolidine	58.28	33.95	26.23	39.49	7.46	108.52	9.07	123.59
153	Pentacosane	2.61	21.15	5.61	39.42	0.72	43.72	0.58	64.51
154	3,3-Methylenebis-1H-indole	162.04	35.58	334.13	29.40	33.33	64.58	11.63	71.04

No.	**Metabolite**	**Mean GSD Female (ng/g, n=8)**	**%RSD**	**Mean GSD Male (ng/g, n=3)**	**%RSD**	**Mean Dingo Female (ng/g, n=7)**	**%RSD**	**Mean Dingo Male (ng/g, n=7)**	**%RSD**
1	2-Butanone	61.27	63.63	133.83	58.77	123.12	44.37	80.06	67.21
2	Acetic acid	72.48	20.32	85.10	72.49	95.55	65.35	75.33	39.87
3	Isovaleral	8.61	57.27	7.44	47.61	9.58	35.04	8.43	47.41
4	2-Pentanone	19.60	61.43	22.93	82.44	25.27	85.78	9.59	49.91

5	Heptane	11.30	59.36	12.58	16.77				
6	Propanoic acid	81.69	23.99	21.51	81.77	102.28	72.67	49.96	52.50
7	Methyl butanoate	42.14	39.16	32.43	131.34	40.78	84.98	35.51	95.47
8	Isopentanol	21.40	103.00	13.83	123.03	7.70	81.57	6.79	58.28
9	Dimethyldisulfide	14.48	113.19	6.12	70.87	15.94	99.15	4.57	96.72
10	Methyl isopentanoate	12.34	44.53	12.58	118.61	11.22	41.53	5.60	56.00
11	Isobutyric acid	60.49	35.35	46.02	106.54	59.96	60.59	29.15	74.62
12	Hexanal	16.31	42.62	21.19	33.82	22.30	29.32	17.43	22.95
13	Methyl pentanoate	14.74	57.48	11.07	58.05	23.97	63.04	7.56	56.34
14	Butyric Acid	559.16	23.98	480.06	126.45	641.84	63.25	542.59	88.28
15	Furfural	1.56	91.34	2.14	42.16	1.83	56.98	0.87	32.42
16	Isovaleric acid	439.16	50.21	424.19	129.15	478.87	63.02	280.51	61.39
17	1-Hexanol	85.89	43.97	54.63	33.04	53.91	71.75	55.51	35.34
18	Methyl butyric acid	250.83	36.97	176.48	126.38	280.75	46.57	175.13	59.86
19	2-Heptanone	26.03	45.29	24.17	22.34	26.68	30.51	20.79	43.45
20	Nonane	3.75	150.80	2.50	109.43	26.10	130.64	6.90	199.78
21	Heptanal	7.80	21.59	7.81	21.12	6.31	12.81	4.95	25.04
22	Valeric acid	63.59	35.63	62.55	58.88	92.76	62.86	36.02	68.42
23	Methyl caproate	4.30	65.09	2.80	70.19	5.30	34.53	4.51	51.56
24	alpha-Pinene	3.71	82.35	1.72	93.63				
25	Methanethiol isovalerate	24.49	105.13	19.54	115.67	19.15	124.33	11.49	98.36
26	Propyl 2-methylbutanoate	2.29	117.35			1.54	70.35	1.31	81.42
27	Propyl isopentanoate	6.67	120.10	5.37	81.27	4.23	88.30	2.48	108.88
28	2-Isooctanone	13.94	47.74	17.74	57.51	18.57	51.92	13.61	47.06
29	2-Heptenal	8.18	40.95	4.45	75.25	4.13	40.07	3.58	41.64
30	Isocaproic acid	29.40	37.62						
31	5-Methyl-2-heptanone	40.33	59.61	30.33	37.39	45.73	69.39	29.66	80.32
32	Benzaldehyde	98.54	40.32	119.52	28.12	89.31	17.05	85.82	30.07
33	Dimethyl trisulfide	15.76	71.50	12.85	74.89	28.26	136.03	10.64	58.20
34	1-Heptanol	24.86	47.88	18.12	31.04	12.73	40.66	13.08	30.23
35	1-Octen-3-ol	64.26	42.03	61.50	50.98	114.76	76.95	82.67	72.02
36	Phenol	2162.31	86.71	2177.94	89.11	1660.39	123.84	459.08	122.49
37	2-Octanone	23.98	33.92	23.00	18.58	23.51	34.89	19.79	50.95
38	Butyl butanoate	4.72	142.70	6.37	135.13	5.83	113.47	17.09	211.42
39	Octanal	5.97	32.13	6.48	26.09	5.87	9.06	4.94	27.76

40	2-Thienaldehyde	0.82	15.26	0.73	17.20	0.61	21.48	0.52	24.67
41	alpha-Phellandrene			3.36	119.17				
42	2,4-Heptadienal	33.47	29.90	38.98	11.93	39.77	30.88	37.25	21.29
43	Isovalerylacetone	38.62	25.57	32.90	15.46	56.94	42.36	49.30	33.68
44	Methyl heptanoate	4.48	60.56	2.64	46.98	7.43	68.95	3.82	35.54
45	p-Cymene	0.99	147.17	32.65	138.04	62.10	205.67	71.22	238.67
46	2-Ethylhexanol	51.79	27.06	44.79	34.04	28.78	37.22	29.66	49.87
47	Eucalyptol					48.77	202.27		
48	Benzyl Alcohol	7.73	24.72	6.88	42.17	7.61	37.19	6.74	28.62
49	3-Octen-2-one	7.19	56.93	10.18	76.43	12.04	42.69	12.91	21.26
50	Butyl 2-methylbutanoate	2.25	85.20			2.29	124.31	5.41	111.22
51	Butyl isopentanoate	3.97	82.82	4.60	154.40	3.94	122.69	5.46	132.00
52	Benzeneacetaldehyde	24.63	43.46	13.22	39.14	63.05	21.26	53.67	56.67
53	2-Octenal	26.62	19.29	27.44	23.97	29.29	24.83	25.09	28.22
54	Acetophenone	201.40	53.79	246.03	41.32	19.72	63.18	12.20	41.01
55	1-Octanol	26.16	48.36	17.82	32.20	19.04	59.97	16.28	33.23
56	p-Cresol	26.85	47.83	58.36	106.25	25.05	78.93	34.39	47.34
57	Octanenitrile	1.24	18.30	1.51	54.71	1.37	42.26	1.60	36.69
58	2-Nonanone	36.34	31.11	36.28	19.12	47.46	35.52	47.28	27.93
59	Linalool	7.52	129.43	1.38	3.46	4.47	183.47	1.57	50.58
60	2-Nonanol	23.91	33.63	16.85	56.74	18.67	50.14	20.84	40.52
61	Nonanal	19.30	36.94	16.33	32.37	14.39	28.13	12.06	47.62
62	Phenylethyl Alcohol	243.08	99.77	62.99	90.79	352.02	38.32	555.83	47.12
63	Methyl octanoate	21.56	42.70	12.27	61.92	26.99	50.91	22.26	60.97
64	3-Nonen-2-one	6.78	21.71	12.34	71.17	8.86	52.36	9.29	16.93
65	2-Methylhexadecanal	20.77	32.31	29.55	69.65	33.44	66.07	25.65	63.00
66	Benzenepropanal	20.73	92.57	8.88	51.64	3.48	46.72	2.80	28.59
67	1-Nonanol	87.65	54.08	53.35	34.53	44.63	34.69	43.49	34.23
68	Methyl benzeneethanoate	6.59	48.82	5.16	80.81	16.96	94.94	8.10	74.76
69	2-Decanone	51.83	33.04	49.05	5.25	56.81	53.90	50.52	102.94
70	Dodecane	4.79	91.00						
71	Methyl salicylate	9.56	66.95	6.42	40.35	12.96	162.14	4.54	48.64
72	alpha-Terpineol	0.97	61.73	20.79	25.63	191.49	198.88		
73	2-Decanol	25.61	56.06	12.27	36.93	9.50	61.00	13.61	132.51
74	N-(2-Hydroxyethyl)-N-methyl-perfluorobutane-	8.80	64.11	29.01	129.96	14.55	65.65	19.76	36.74

	1-sulfonamide								
75	2-Piperidinone	1872.01	38.42	1766.77	96.43	1055.70	71.07	942.06	41.16
76	Methyl nonanoate	63.12	40.24	41.96	80.81	77.11	96.73	67.05	94.86
77	3,4-Dimethylbenzaldehyde	6.25	104.98	10.94	100.92				
78	Mequinol					5.87	90.08	4.60	44.58
79	3-Phenylpropanol	149.89	106.73	70.57	79.99	8.65	124.05	6.17	68.50
80	Ethylmethylmaleimide	91.88	76.66	89.52	55.91	50.80	53.77	38.24	43.72
81	Quinoline	6727.41	65.93	8913.46	69.60	4582.44	85.59	3226.04	59.05
82	Benzeneacetic acid	21.64	74.06			34.93	70.74	49.07	81.93
83	Methylvinylmaleimide	16.80	60.87			27.26	77.36	19.23	59.17
84	Methyl 3-phenylpropanoate	1171.46	56.82	721.46	65.27	261.86	90.36	57.91	147.60
85	3-Undecanone					34.45	78.43	17.94	59.37
86	Indole	23281.79	43.76	22091.31	43.45	16425.04	52.06	9885.16	80.68
87	2-Aminoacetophenone	5.48	27.02			6.32	92.46	6.50	113.02
88	Tridecane	15.01	128.83	4.16	33.55	2.94	41.04	3.19	71.64
89	Mesitaldehyde	3.26	103.04			2.74	82.10	3.10	48.22
90	Khinaldin	1376.26	37.27	1466.66	49.43	359.88	67.64	251.70	53.02
91	2-Methoxy-4-vinylphenol	87.52	19.02	71.33	56.34	35.40	38.25	28.07	34.15
92	2,4-Decadienal	58.27	40.53	52.69	28.49	47.60	32.41	40.71	45.42
93	Tetrahydroquinoline	315.03	82.63	436.85	110.45	227.61	123.30	213.36	142.85
94	Hydrocinnamic acid	639.41	61.85	434.07	110.79	60.44	80.39	49.16	74.63
95	2-Methylundecanal	16.02	41.76	19.62	65.72	28.78	78.63	18.78	61.74
96	gamma-Nonanolactone	42.68	29.29	25.64	76.64	37.30	49.11	35.41	32.97
97	2,4-Tridecanedione					28.15	46.80	26.63	36.26
98	2-Dodecanone	33.94	51.16	25.40	30.39	27.50	53.70	25.27	163.06
99	Tetradecane	5.26	135.03	1.84	20.33	1.06	46.39		
100	4-tert-Amylphenol	17.56	29.13	17.24	15.46	19.17	24.76	15.17	21.45
101	Butyl phenylacetate							2.99	58.27
102	Geranylacetone	48.90	59.21	25.24	7.51	30.08	22.26	24.02	27.31
103	2,6-Di-tert-butylbenzoquinone	148.29	98.30	119.36	95.57				
104	Hexahydrofarnesol	1.48	83.63	0.62	42.81	2.88	138.10	3.13	192.80
105	3-tert-Butyl-4-methoxyphenol	33.47	120.68	43.05	141.23				
106	trans-beta-Ionone	29.12	62.01	16.95	32.55	9.94	30.19	8.21	19.61
107	5,6-beta-Ionone epoxide	36.43	49.97	31.45	54.18			9.67	23.04
108	2-tert-Butyl-4-methoxyphenol	2465.77	114.01	1329.80	129.37	31.78	73.58	31.88	69.04

109	2-Tridecanone	30.43	34.27			29.33	46.32	23.87	47.14
110	Pentadecane	17.95	53.07	13.03	54.60	6.09	72.78	4.08	50.23
111	2-Tridecanol	18.96	54.93	8.98	49.35	11.66	61.25	12.52	69.54
112	2,6-Di-tert-butyl-p-cresol	202.82	107.67	162.04	153.78	5.86	17.28	4.47	26.04
113	2,4-Di-tert-butylphenol	13.71	15.38	13.50	18.73	13.13	16.70	11.55	23.27
114	Methyl dodecanoate	12.22	53.17	5.34	125.75	8.24	78.15	5.24	85.12
115	Dihydroactinidolide	13.16	55.02	6.66	62.64	3.85	35.29	3.13	16.44
116	2-[(2-Ethoxy-3,4-dimethyl-2-cyclohexen-1-ylidene)methyl]furan	4.85	92.80	3.56	125.07				
117	2-Tetradecanone	12.54	33.94	7.58	10.46	10.14	51.82	7.21	60.51
118	2-Nonylthiophene***	19.02	92.90					3.90	83.97
119	Diethyltoluamide	1.71	51.19	1.47	73.18	4.01	70.36	6.45	83.21
120	Spathulenol			1.25	57.02				
121	Hexadecane	7.90	61.26	4.40	38.87	6.01	39.23	2.28	38.55
122	Methyl tridecanoate	2.45	38.59					1.10	58.31
123	gamma-Eudesmol			4.04	137.50	0.64	107.25	7.31	237.85
124	beta-Selinenol	1.26	44.29	25.80	166.13	6.19	176.00	22.71	253.52
125	Methyl 12-methyltridecanoate	6.15	39.98						
126	Heptadecane	17.39	60.58	13.27	40.98	10.21	32.10	7.87	54.70
127	2-Pentadecanone	32.20	84.79	16.35	51.03	12.19	48.47	9.99	62.45
128	2-Hexadecanol	8.75	75.62	5.42	81.88	4.38	70.72	4.93	92.53
129	2-Pentadecanol	8.80	74.64	7.69	41.12	4.23	72.43	4.98	90.72
130	Methyl cis-9-tetradecenoate	4.98	78.52						
131	Trifluoroacetic acid, pentadecyl ester	3.52	66.05	2.49	34.91	1.98	52.28	2.34	89.45
132	Methyl tetradecanoate	29.08	60.86	11.38	117.78	17.35	86.37	14.02	89.11
133	3,5-ditert-butyl-4-hydroxycyclohexa-2,4-dien-1-one	15.39	52.73	10.09	41.96				
134	4-Formyl-2,6-di-tert-butylphenol	12.43	116.50	23.18	64.55				
135	Methyl 12-methyltetradecanoate	20.99	69.28	5.20	40.21	8.46	75.71	8.06	58.27
136	Octadecane	6.41	60.34	2.65	38.40	3.32	68.39	2.23	61.35
137	Methyl pentadecanoate	8.69	54.13	2.83	71.80	4.93	72.85	2.66	80.03
138	Methyl 2-oxohexadecanoate					2.46	63.72	2.26	76.09
139	1-Nonadecene	7.50	66.55			3.88	34.21	3.01	40.93
140	1-Hexadecanol	6.56	107.92	11.47	124.91	3.16	28.49	2.84	63.64
141	Nonadecane	2.28	197.07	1.17	31.58	1.03	97.14	0.49	33.32

142	Methyl hexadecanoate	53.85	55.82	22.32	90.15	23.79	57.75	19.85	58.74
143	Palmitic acid	3.83	88.79	0.87	30.11	2.91	50.37	1.63	67.30
144	Ethenyl hexadecanoate	2.53	96.68	0.91	51.43	1.69	56.03	1.54	48.55
145	Eicosane	0.70	77.07	1.01	36.55	0.88	74.74	0.65	117.24
146	Heneicosane	1.26	60.70	1.35	42.87	2.76	113.84	0.56	44.74
147	Methyl trans-11-octadecenoate	20.43	76.44	6.78	97.41	8.94	36.60	5.24	68.03
148	Methyl octadecanoate	3.51	45.90	2.29	77.23	2.19	51.21	1.80	51.16
149	Docosane	1.02	63.69	1.44	48.42	1.05	87.45	0.51	85.22
150	Tricosane	1.60	44.02	1.88	41.13	1.80	62.80	0.88	39.15
151	Tetracosane	1.21	49.16	1.39	49.86	1.28	64.66	0.70	38.10
152	2-Phenyl-3-benzylidenepyrrolidine	7.03	119.40	9.20	102.99	13.44	106.49	4.71	102.37
153	Pentacosane	0.73	43.96	0.67	52.14	0.76	60.70	0.41	38.81
154	3,3-Methylenebis-1H-indole	34.88	50.06	29.18	119.37	16.61	59.43	7.36	41.38

Supplementary Table S4. Statistically significant metabolic VOCs (58) in the scats of the dingoes and German Shepherd dogs (GSD) broken down by sex

Relative concentrations (ng/g) with relative standard deviations (%) are shown for only the 58 statistically significant VOCs . QC samples (All Pooled and Pooled) show percent relative standard deviation (RSD) < 40%. Asterisks denotes VOCs significantly higher in dingoes.

Metabolite	GSD Female (ng/g, n=8)	%RSD	GSD Male (ng/g, n=3)	%RSD	Dingo Female (ng/g, n=7)	%RSD	Dingo Male (ng/g, n=7)	%RSD	All Pooled (ng/g, n=8)	%RSD	Pooled (ng/g, n=8)	%RSD
Methyl 2-oxohexadecanoate*					2.46	63.72	2.26	76.09	15.04	31.96	7.99	36.19
2,4-Tridecanedione*					28.15	46.8	26.63	36.26	125.65	21.51	168.87	38.28
Benzeneacetic acid*	21.64	74.06			34.93	70.74	49.07	81.93	239.86	31.75	321.56	29.29
Mequinol*					5.87	90.08	4.6	44.58	19.06	17.15		
gamma-Eudesmol*			4.04	137.5	0.64	107.25	7.31	237.85	8.16	36.00		
3-Octen-2-one*	7.19	56.93	10.18	76.43	12.04	42.69	12.91	21.26	46.87	26.39	45.18	34.31
3-Undecanone*					34.45	78.43	17.94	59.37	105.54	23.14	137.90	38.66
Eucalyptol*					48.77	202.27			18.83	20.96		
Mesitaldehyde*	3.26	103.04			2.74	82.1	3.1	48.22	2.5	32.90		
Phenylethyl Alcohol*	243.08	99.77	62.99	90.79	352.02	38.32	555.83	47.12	2338.0	31.62	1075.59	35.17
Benzeneacetaldehyde*	24.63	43.46	13.22	39.14	63.05	21.26	53.67	56.67	240.1	32.91	342.60	34.09
Butyl phenylacetate*							2.99	58.27	5.65	35.06	8.16	31.29
2,6-Di-tert-butylbenzoquinone	148.29	98.30	119.36	95.57					286.98	27.20	215.01	24.25
2-[(2-Ethoxy-3,4-dimethyl-2-cyclohexen-1-ylidene)methyl]furan	4.85	92.80	3.56	125.07					10.54	26.24	11.89	26.77

Acetophenone	201.40	53.79	246.03	41.32	19.72	63.18	12.20	41.01	456.61	23.01	593.34	33.66
3,5-ditert-butyl-4-hydroxycyclohexa-2,4-dien-1-one	15.39	52.73	10.09	41.96					99.85	33.80	38.77	33.90
3-Phenylpropanol	149.89	106.73	70.57	79.99	8.65	124.05	6.17	68.5	279.05	26.44	169.82	29.73
4-Formyl-2,6-di-tert-butylphenol	12.43	116.5	23.18	64.55					39.6	30.02	64.75	27.78
2-Methoxy-4-vinylphenol	87.52	19.02	71.33	56.34	35.4	38.25	28.07	34.15	367.83	29.01	521.97	28.95
2-tert-Butyl-4-methoxyphenol	2465.77	114.01	1329.8	129.37	31.78	73.58	31.88	69.04	5502.37	29.80	5669.41	39.76
Benzenepropanal	20.73	92.57	8.88	51.64	3.48	46.72	2.8	28.59	36.38	18.38	62.91	36.95
Khinaldin	1376.26	37.27	1466.66	49.43	359.88	67.64	251.7	53.02	4353.94	32.55	6255.34	30.84
Hydrocinnamic acid	639.41	61.85	434.07	110.79	60.44	80.39	49.16	74.63	2165.48	31.52	1527.06	33.59
Methyl 3-phenylpropanoate	1171.46	56.82	721.46	65.27	261.86	90.36	57.91	147.6	3632.88	23.84	2977.64	27.62
2,6-Di-tert-butyl-p-cresol	202.82	107.67	162.04	153.78	5.86	17.28	4.47	26.04	365.74	25.89	891.36	37.23
trans-beta-Ionone	29.12	62.01	16.95	32.55	9.94	30.19	8.21	19.61	78.92	26.45	163.45	36.36
3-tert-Butyl-4-methoxyphenol	33.47	120.68	43.05	141.23					61.35	29.95	95.24	35.59
Dihydroactinidolide	13.16	55.02	6.66	62.64	3.85	35.29	3.13	16.44	36.51	30.33	60.40	36.97
Pentadecane	17.95	53.07	13.03	54.60	6.09	72.78	4.08	50.23	64.43	27.65	599.30	35.44
2-Ethylhexanol	51.79	27.06	44.79	34.04	28.78	37.22	29.66	49.87	159.70	28.28	145.95	37.75
1-Nonanol	87.65	54.08	53.35	34.53	44.63	34.69	43.49	34.23	259.27	20.99	278.99	27.69
1-Heptanol	24.86	47.88	18.12	31.04	12.73	40.66	13.08	30.23	69.30	25.48	72.75	24.66
3,3-Methylenebis-1H-indole	34.88	50.06	29.18	119.37	16.61	59.43	7.36	41.38	162.04	35.58	334.13	29.40
2-Pentadecanone	32.20	84.79	16.35	51.03	12.19	48.47	9.99		110.22	26.18	174.66	24.96
2-Thienaldehyde	0.82	15.26	0.73	17.2	0.61	21.48	0.52	24.67	2.97	22.82	2.79	34.51
Heptadecane	17.39	60.58	13.27	40.98	10.21	32.1	7.87	54.7	80.57	23.38	335.21	32.62
Indole	23281.79	43.76	22091.31	43.45	16425.04	52.06	9885.16	80.68	90922.33	22.72	147260.63	37.31
Isocaproic acid	29.4	37.62							120.29	24.35	167.14	12.81
Octadecane	6.41	60.34	2.65	38.40	3.32	68.39	2.23	61.35	33.97	20.51	446.26	31.40
2-Heptenal	8.18	40.95	4.45	75.25	4.13	40.07	3.58	41.64	35.77	21.45	17.84	29.64
2-Nonylthiophene	19.02	92.90					3.9	83.97	27.48	31.34	38.62	32.77

Tridecane	15.01	128.83	4.16	33.55	2.94	41.04	3.19	71.64	38.7	42.09	865.70	34.41
Hexadecane	7.9	61.26	4.4	38.87	6.01	39.23	2.28	38.55	32.09	21.15	377.37	21.03
2-Tridecanone	30.43	34.27			29.33	46.32	23.87	47.14	156.8	24.17		
2-Piperidinone	1872.01	38.42	1766.77	96.43	1055.7	71.07	942.06	41.16	7219.96	28.24	7136.88	36.40
Methanethiol isovalerate	24.49	105.13	19.54	115.67	19.15	124.33	11.49	98.36	44.14	37.57	56.68	37.49
Heptanal	7.80	21.59	7.81	21.12	6.31	12.81	4.95	25.04	25.44	21.32	18.99	24.06
Methyl cis-9-tetradecenoate	4.98	78.52							10.89	27.97	15.43	19.44
Diethyltoluamide	1.71	51.19	1.47	73.18	4.01	70.36	6.45	83.21	16.83	18.75	26.19	26.52
5,6-beta-Ionone epoxide	36.43	49.97	31.45	54.18			9.67	23.04	102.92	27.27	195.84	39.07
Phenol	2162.31	86.71	2177.94	89.11	1660.39	123.84	459.08	122.49	7576.43	22.66	9272.42	26.09
Tetradecane	5.26	135.03	1.84	20.33	1.06	46.39			7.99	35.99	489.85	35.46
Ethylmethylmaleimide	91.88	76.66	89.52	55.91	50.80	53.77	38.24	43.72	26.84	11.43	297.16	32.76
1-Hexanol	85.89	43.97	54.63	33.04	53.91	71.75	55.51	35.34	323.64	27.70	436.51	21.57
Geranylacetone	48.9	59.21	25.24	7.51	30.08	22.26	24.02	27.31	215.71	26.11	312.46	31.03
2-Decanol	25.61	56.06	12.27	36.93	9.5	61.0	13.61	132.51	78.95	24.48	128.18	29.59
Nonanal	19.3	36.94	16.33	32.37	14.39	28.13	12.06	47.62	65.59	17.83	43.88	33.76
p-Cymene	0.99	147.17	32.65	138.04	62.1	205.67	71.22	238.67	48.42	35.77		

Supplementary Table S5

HS-SPME-GC/MS analysis of all the samples (Samples, QC blanks, QC Pooled and All-Pooled samples, QC standard spiked samples and QC standards) was completed over six consecutive days of batch runs

Example: Day 1			
#	SPME-GC/MS batch sequence		
1	Blank_1		Empty 20 mL HS vial
2	Standard_1		20 mL vial with 10 µl of each nitrobenzene, alkanes, VOC mix (20 mg/L)
3	Scat_NaCl_Spiked_Std_1	Cooinda (50mg)	50 mg scat in 20 mL vial with 10 µl of each nitrobenzene, alkanes, VOC mix (20 mg/L)
4	NaCl_Blank_1		20 mL HS vial with 2 mL NaCl solution
5	Pooled_1		20 mL HS vial, added each of 50 mg of Cooinda, Kinta, Rundo, Gina, Typia, Kora; add 2 ml NaCl solution, 10 µl of each nitrobenzene and alkanes (20 mg/L)
6	Cooinda	300 mg	20 mL HS vial with 2 mL NaCl solution and 10 µl of each nitrobenzene (20 mg/L)
7	Kinta	300 mg	
8	Rundo	300 mg	
9	Gina	300 mg	
10	Kora	300 mg	
11	Typia	300 mg	
12	Pooled_2		20 mL HS vial, added each of 50 mg of Cooinda, Kinta, Rundo, Gina, Typia, Kora; add 2 ml NaCl solution, 10 µl of each nitrobenzene and alkanes (20 mg/L)
13	Standard_2		20 mL vial with 10 µl of each nitrobenzene, alkanes, VOC mix (20 mg/L)
14	Scat_NaCl_Spiked_Std_2	Gina (50mg)	50 mg scat in 20 mL vial with 10 µl of each nitrobenzene, alkanes, VOC mix (20 mg/L)
15	NaCl_Blank_2		20 mL HS vial with 2 mL NaCl solution
16	Blank_2		Empty 20 mL HS vial
All Pooled sample_1	20 mL vial add each of 50 mg of Cooinda, Kinta, Rundo, Gina, Typia, Kora; add 2 mL NaCl solution, store in -20^{o}C freezer. Each day, new samples were added to this QC All Pooled sample vial which was analysed on day 5.		
All Pooled sample_2	20 mL vial add each of 50 mg of Cooinda, Kinta, Rundo, Gina, Typia, Kora; add 2 mL NaCl solution, store in -20^{o}C freezer. Each day, new samples were added to this QC All Pooled sample vial which was analysed on day 5.		
Example: Day 5			
SPME-GC/MS batch sequence			
Blank_1			Empty 20 mL HS vial
Standard_1			20 mL vial with 10 µl of each nitrobenzene, alkanes, VOC mix (20 mg/L)
Scat_NaCl_Spiked_Std_1	Mungka (50mg)		50 mg scat in 20 mL vial with 10 µl of each nitrobenzene, alkanes, VOC mix (20 mg/L)
NaCl_Blank_1			20 mL HS vial with 2 mL NaCl solution
All Pooled_1a			All Pooled sample_1 vial homogenized, divided into 2 mL in 20 mL HS vials (n=4) and spiked with nitrobenzene with 10 µl of each nitrobenzene (20 mg/L)
All Pooled_1b			
All Pooled_1c			
All Pooled_1d			
All Pooled_2a			All Pooled sample_2 vial homogenized, divided into 2 mL in 20 mL HS vials (n=4) and spiked with
All Pooled_2b			

All Pooled_2c		nitrobenzene with 10 µl of each nitrobenzene (20 mg/L)
All Pooled_2d		
Standard_2		20 mL vial with 10 µl of each nitrobenzene, alkanes, VOC mix (20 mg/L)
Scat_NaCl_Spiked_Std_2	Bea (50mg)	50 mg scat in 20 mL vial with 10 µl of each nitrobenzene, alkanes, VOC mix (20 mg/L)
NaCl_Blank_2		20 mL HS vial with 2 mL NaCl solution
Blank_2		Empty 20 mL HS vial