Marie Charpentier, Nicolas Barthes, Magali Proffit, Marie Bessière, Claude Grison, et al.. Critical thinking in the chemical ecology of mammalian communication: roadmap for future studies. Functional Ecology, Wiley, 2012, 26 (4), pp.769-774. 10.1111/j.1365-2435.2012.01998.x

### 1 SUPPLEMENTARY INFORMATION

2 3 4

### Table S1

5 Species studied in the 41 selected original papers. For each study, the odorant sources, the number of molecules analyzed and the study type are

6 indicated. We distinguished four different types of studies: those based on chemical identifications only (a), on chemical identifications coupled

7 with behavioral bioassays (b), on the analysis of the odor bouquet or individual compounds as signals of individual or population parameters (c)

8 and on the analysis of the odor bouquet or individual compounds as signals of individual or population parameters coupled with behavioral

9 bioassays (d).

Species	Odorant source	References	Molecules found /Molecules used in analyses	Study type
House mouse ( <i>Mus musculus</i> )	Preputial gland, urine	(Lin, Zhang, Block <i>et al.</i> , 2005) (Rock, Mueller, Weimar <i>et al.</i> , 2006) (Novotny, Soini, Koyama <i>et al.</i> , 2007) (Zhang, Rao, Sun <i>et al.</i> , 2007) (Osada, Tashiro, Mori <i>et al.</i> ,	5/5 67/39 18/17 51/37 38/20	b a c c d

		2008)		
		(Zhang, Sun, Zhang et al.,		
Grey rat	Preputial gland, urine	2008)	35/24	с
(Rattus norvegicus)		(Osada, Kashiwayanagi &	47/31	d
		Izumi, 2009)		
Black rat	Urine	(Selvaraj & Archunan, 2002)	unknown/5	b
(Rattus rattus)				
Dwarf hamster		(Burger, Smit, Spies et al.,	38/35	а
(Phodopus sungorus sungorus)	Buccal or ventral secretions	2001)	64/50	2
(I nouopus sungorus sungorus)		(Burger et al., 2001)	01/00	u
Hamster <sup>1</sup> (Phodopus campbelli: P. roborowsky: P. sungorus)	Urine	(Soini, Wiesler, Apfelbach et	Unknown <sup>2</sup> /45	c
		al., 2005)		
Svrian golden hamster (Mesocricetus auratus)	Vaginal secretions	(Briand, Blon, Trotier et al.,	5/5	а
	, uginar socretions	2004)	5,5	u
Eurasian beaver ( <i>Castor fiber</i> )	Snow mark, anal gland, castoreum	(Rosell & Sundsdal, 2001)	207/75	с
		(Hayes, Richardson & Wyllie,		
European rabbit	Scent marks or chin gland	2002)	16/12	с
(Oryctolagus cuniculus)	Seent marks of chini grand	(Hayes, Richardson, Claus et	34/14	с
		al., 2002)		
				1

White-lipped peccary (Tayassu pecari)	Dorsal gland	(Waterhouse, Hudson, Pickett et al., 2001)	50/31	a
Ox (Bos indicus)	Sweat	(Gikonyo, Hassanali, Njagi <i>et</i> <i>al.</i> , 2002) <sup>2</sup>	17/14	b
Buffalo (Syncerus caffer)	Sweat	(Gikonyo <i>et al.</i> , 2002) <sup>2</sup>	17/15	b
Suni (Neotragus moschatus)	Preorbital secretions	(Stander, Burger & Le Roux, 2002)	98/83	a
Waterbuck (Kobus defassa)	Sweat	(Gikonyo <i>et al.</i> , 2002) <sup>2</sup>	30/28	b
Red hartebeest (Alcelaphus buselaphus caama)	Interdigital secretions	(Reiter, Burger & Dry, 2003)	70/52	а
Sika deer (Cervus nippon)	Metatarsal gland	(Wood, 2003)	35/33	a
Moose (Alces alces)	Urine	(Whittle, Bowyer, Clausen <i>et al.</i> , 2000)	9/6	с
African elephant (Loxodonta africana)	Temporal gland	(Goodwin, Brown, Counts <i>et</i> <i>al.</i> , 2002)	3/3	a
Asian elephant ( <i>Elephas maximus</i> )	Urine	(Dehnhard, Heistermann, Goritz <i>et al.</i> , 2001)	2/2	с
European badger (Meles meles)	Subcaudal gland	(Buesching, Waterhouse & Macdonald, 2002)	110/5	с
Hooded skunk (Mephitis macroura)	Anal sac	(Wood, Sollers, Dragoo et al.,	14/14	а

		2002)		
Ferret (Mustela furo)	Anal gland, urine	(Zhang, Soini, Bruce <i>et al.</i> , 2005)	47/38	с
Siberian weasel ( <i>Mustela sibirica</i> ) Steppe polecat ( <i>M. eversmanni</i> )	Anal gland	(Zhang, Sun, Zhang <i>et al.</i> , 2002) (Zhang, Ni, Ren <i>et al.</i> , 2003)	9/8 17/15	c c
Wolverine (Gulo gulo)	Anal gland	(Wood, Terwilliger & Copeland, 2005)	123/59	a
Bengal tiger (Panthera tigris)	Marking fluids	(Burger, Viviers, Bekker <i>et al.</i> , 2008)	118/110	a
Giant panda	Ano-genital gland, vaginal secretions,	(Hagey & Macdonald, 2003)	111/65	с
(Ailuropoda melanoleuca)	scent marks, urine	(Zhang, Liu, Sun et al., 2008)	39/23	с
Coquerel's sifaka (Propithecus verreauxi coquereli)	Ano-genital gland	(Hayes, Morelli & Wright, 2004) <sup>2</sup>	22/8	с
		(Hayes <i>et al.</i> , 2004) <sup>2</sup> (Knapp, Robson &	44/18	с
Ring-tailed lemur	Ano-genital, brachial, antebrachial	Waterhouse, 2006)	16/11	c
(Lemur catta)	glands, tail odorants	(Scordato, Dubay & Drea, 2007)	122/30	с

Marmoset (Callithrix jacchus)	Circumgenital scent marks	(Smith, Tomlinson, Mlotkiewicz <i>et al.</i> , 2001)	162/76	c
Mandrill ( <i>Mandrillus sphinx</i> )	Sternal gland, hairs of the sternal gland	(Setchell, Vaglio, Moggi- Cecchi <i>et al.</i> , 2010)	97/90	с
Human (Homo sapiens sapiens)	Sweat, whole-body volatiles	(Meijerink, Braks, Brack <i>et al.</i> , 2000) (Curran, Rabin, Prada <i>et al.</i> , 2005) (Logan, Birkett, Clark <i>et al.</i> , 2008) (Vaglio, Minicozzi, Bonometti <i>et al.</i> , 2009)	81/74 47/47 33/23 unknown/5	b c b c

11 <sup>1</sup>Compounds of the three species of hamsters studied by Soini et al 2005 are considered together.

12 <sup>2</sup>Chemical analyses were performed on a subset of 17 compounds.

13 <sup>3</sup>A subset of the total number of compounds found in the different species was possibly identical across species.

#### Data S1

15 16

17

### Nine chemical rules and representative figures

18 The nine following rules were designed following two outstanding reference books 19 (Mann, 1994, Mann, Davidson, Hobbs et al., 1994) and a review (Rodríguez-Concepción, 20 2006) that document the occurrence, or the absence, of molecules from the five major 21 pathways of secondary metabolism in the various major groups of organisms, supplementing 22 these with other references as needed. The following nine rules we provide should, however, 23 only be considered as a first helping step. Indeed, the same compound may sometimes be 24 produced by different biosynthetic pathways in different organisms; this is especially true, for 25 example, for plants (Mann, 1994, Mann et al., 1994).

26

27 1. The shikimate pathway is a prerogative of micro-organisms, fungi, algae and plants 28 The shikimate pathway leads to the synthesis of the aromatic cores of three aromatic amino acids: phenylalanine, tyrosine and tryptophan (Figure 2a). These three aromatic amino acids 29 30 are not produced by mammals and are therefore "essential" to such organisms which acquire 31 them through food. These three aromatic amino acids are themselves the precursors of 32 numerous acids and alcohols (e.g., cinnamic acid, 4-coumaric acid, caffeic acid, coniferyl 33 alcohol, sinapyl alcohol; Figure 2b) and their cyclic derivatives such as coumarins, flavonoids 34 and anthraquinones (Figure 2c). To summarize, the shikimate pathway produces aromatic 35 hydrocarbons which are always oxidized in the 4-position (e.g., 4-coumaric acid). Further 36 oxidations may occur in adjacent positions to give 3,4-dihydroxy (e.g., caffeic acid) or 3,4,5trihydroxy (e.g., sinapyl alcohol) patterns. The shikimate biosynthetic pathway is only found 37 38 in micro-organisms, fungi, algae and plants (Pichersky, Noel & Dudareva, 2006). Finding 39 derivatives of the shikimate pathway in mammalian secretions leads inevitably to questions 40 about their origin and, more importantly, about their biological relevance as chemical 41 mediators.

42

43 *Examples of molecules illustrating rule 1; a. three amino acids that are the precursors of the* 44 *acids and alcohols illustrated on b. and their cyclic derivatives illustrated on c.* 

45 a.



46 47 b.



57

# 2. Aromatic hydrocarbon compounds derived from the acetate pathway are a prerogative of micro-organisms, fungi, algae and plants

- Like the shikimate pathway, the acetate pathway may also produce aromatic derivatives.
  However, by contrast with the shikimate pathway, the acetate pathway produces aromatic
- 59 However, by contrast with the shikimate pathway, the acetate pathway produces 60 hydrocarbon compounds oxidized in the 1,3,5-positions (e.g., methyl salicylate,
- 61 phloroglucinol; Figure 3). Note that one or more of these hydroxyl groups may disappear
- 62 during acetate biosynthesis. Conversely, albeit rarely, complex biosynthesis involving both
- 63 the shikimate and the acetate pathways can lead to the 1,3,4,5-tetrahydroxy pattern. The
- 64 acetate pathway requires the intervention of polyketide synthases of types I and II, found in
- 65 bacteria and fungi, or of polyketide synthases of type III, found in plants. Aromatic molecules
- 66 derived from this pathway are therefore very unlikely to be directly produced by mammals.
- 67
- 68 *Two examples of aromatic hydrocarbon compounds that illustrate rule 2.*



- 70
- 3. Non-oxidized aromatic derivatives are not of natural origin

As shown above, the shikimate and acetate pathways both lead to the production of oxidized

aromatic compounds (rules 1 and 2). In the absence of evidence to the contrary, non-oxidized

aromatic hydrocarbons, such as mesitylene or naphthalene (Figure 4a) are not natural

75 compounds because they are not derived from one of these two biosynthetic pathways. Exotic

- chemical structures such as pentachloro aromatic compounds (even algae are not known for
   their ability to introduce such a large number of halogen atoms) are also not natural. Records
- 78 of these types of non-natural molecules in mammalian secretions should be discarded. The
- 79 unique exception to this rule concerns phenylpropanoids (Figure 4b), which are the only class
- 80 of aromatic molecules naturally not oxidized (deriving from cinnamic acid).
- 81 Phenylpropanoids are, however, only produced by micro-organisms, fungi, algae and plants.
- 82
- 82 Examples of molecules illustrating rule 3; a. two non-oxidized aromatic hydrocarbons; b. the
- 84 general pattern of a phenylpropanoid, an aromatic molecule that is naturally not oxidized.
- 85 a.



### phenylpropanoid

88 89

86 87

b.

90

91 4. Whether mammals can produce heterocyclic aromatic molecules is not established 92 Most heterocyclic aromatic molecules are nitrogenous compounds and come from the amino 93 acid and mevalonate pathways. Mammals are able to metabolize nitrogenous heterocyclic 94 aromatic molecules acquired from exogenous sources, such as food. In a small number of 95 cases, some of these molecules may also act as mammalian chemical mediators. Examples 96 include castoramine (Svendsen & Jollick, 1978) and muscopyridine (Hagiwara, Katsumi, 97 Kamat et al., 2000) (both shown in Figure 5). Castoramine has even been proposed as being 98 directly produced by beaver because of the absence of bacterial flora in the animal's gland 99 responsible for its secretion (Svendsen et al., 1978). The examples of castoramine and 100 muscopyridine suggest that similar molecules could be found. Whether mammals directly 101 produce these compounds or acquire them through exogenous sources remains, in our opinion, to be established. The origin of these compounds could affect whether or not they 102 103 could play a role as chemical mediators, for example by affecting the constancy (or not) of 104 their presence in secretions.

105

106 *Two examples of nitrogenous heterocyclic aromatic molecules that illustrate rule 4.* 



109 5. Trans mono-unsaturated fatty acids are extremely rare in the living world 110 Mono-unsaturated fatty acids are derived from the acetate pathway. Most naturally produced molecules of this class have the double bond in cis configuration (Figure 6a). Trans 111 112 configurations of mono-unsaturated fatty acids (e.g., methyl-(E)-9-octadecenoate; Figure 6b) 113 are extremely rare in the living world, except for a few reports in insects (e.g., Bosa, Cotes 114 Prado, Fukumoto et al., 2005). Another possible exception occurs in ruminants, however, 115 where trans fat is endogenously produced in tissues from natural cis isomers via oxidative 116 stress generation under pathological conditions (Tsuzuki, 2010). The production of trans 117 mono-unsaturated fatty acids is therefore exceptional and results from very particular 118 physiological conditions. In addition, studies have shown that microflora from the digestive 119 system of ruminants are apparently able to produce a few percent (2-5%) of trans mono-120 unsaturated fatty acids (Booyens, 1986). It is important to keep in mind, however, that it is 121 possible to obtain trans configuration when molecules in cis configuration are heated 122 (Tsuzuki, 2010). In other words, trans molecules may easily appears during analyses if 123 heated, like for GCMS analyses. Consequently, when trans mono-unsaturated fatty acids are 124 found in mammalian secretions, both their natural origin and their relevance as chemical 125 mediators are suppositions that need to be carefully examined.

126

127 Examples of molecules illustrating rule 5; a. general pattern of mono-unsaturated fatty acids
128 in cis configuration; b. a mono-unsaturated fatty acid in trans configuration.

129

a.



# 134 6. The position of the oxidative desaturation in mono-unsaturated fatty acids indicates 135 their biological origin

136 In the case of vertebrates such as mammals, the oxidative desaturation process occurs

137 exclusively between C-9 and C-10 carbons (e.g., in oleic and palmitoleic acids; Figure 7a).

- 138 Oxidative desaturation at other positions occurs only in micro-organisms, algae and plants
- 139 (e.g., angelic acid; Figure 7b) and finding them in mammalian secretions should therefore
- 140 lead to questions about the accuracy of their identification.
- 141

Examples of molecules illustrating rule 6; a. two mono-unsaturated fatty acids with an
oxidative desaturation between C9 and C10; b. a mono-unsaturated fatty acid with an
oxidative desaturation in position C2.



# The position of a double bond in poly-unsaturated fatty acids indicates their plant or animal origin

156 Poly-unsaturated fatty acids are also derived from the acetate pathway. Animal enzymes can introduce a new double bond only between an existing double bond and the acid group 157 158 (Figure 8a). On the other hand, plant enzymes can introduce a new double bond only between 159 an existing double bond and the terminal position, resulting in poly-unsaturated fatty acids. Such compounds are therefore highly unlikely to have been directly produced by a mammal. 160 Thereby, omega-3 (e.g., α-linolenic acid; Figure 8b) and omega-6 (e.g., arachidonic acid and 161 162 linoleic acid; Figure 8b) fatty acids found in mammalian secretions are likely derived from the animal's food. It is important to note that mammalian enzymes may also modify a poly-163 164 unsaturated fatty acid originating from plants by introducing a new double bond between an existing double bond and the acid group. For example, mammals convert linoleic acid, an 165 omega 6, to γ-linolenic acid, which is an important constituent of the phospholipids found in 166 167 cell membranes.

168



171 a.



174

α-linolenic acid



179 8. Saturated fatty acids are ubiquitous in all living organisms

180 The acetate pathway is also responsible for the production of saturated fatty acids, such as 181 decanoic acid, eicosanoic acid, heptadecanoic acid (Figure 9). All saturated fatty acids are

possibly directly produced by mammals and could therefore have a role in mammalian

- 183 chemical communication (see below).
- 184





#### 190 191 192

## 9. Steroids and terpenoids

The mevalonate pathway leads to the production of steroids, such as cholesterol (Figure 10a), which are probably produced by all living species, including mammals. This pathway is also responsible for the production of terpenoids. Only micro-organisms, fungi, algae, plants and insects have developed various secondary pathways to produce and store numerous complex terpenes. Mammals only produce the parent molecules of each series:

- 198 IsopentenylPyroPhosphate for hemiterpenes, GeranylPyroPhosphate for monoterpenes,
- 199 FarnesylPyroPhosphate for sesquiterpenes. These three terpenoids (IPP, GPP and FPP; Figure
- 10b) are not stored in mammals, which directly use them as intermediate metabolites toproduce farnesene and squalene (Figure 10c). Squalene is the linear precursor of lanosterol
- 202 (Figure 10d), the starting point of all steroids (see Table 4).

A second metabolic pathway has also been recently identified as an alternate or supplementary way to produce terpenoids: the 'MEP pathway' (for methylerythritol 4phosphate pathway; (Rodríguez-Concepción, 2006). Both the MEP and the mevalonate

206 pathways act in different cell compartments but the MEP pathway can also produce IPP as for

the former pathway. While the MEP pathway is only known in plants and bacteria, suchorganisms may present both pathways.

We suggest that if terpenoids other than farnesene or squalene are characterized in mammals, they likely come from exogenous sources (food, bacteria). Examples of terpenoids not directly produced by mammals, but reported in their secretions, include limonene and nerolidol, for example.

- 213
- 214 *Examples of molecules illustrating rule 9; a. a steroid; b. the three parent molecules that are*
- 215 the precursors of each terpenoid series; c. squalene and  $\alpha$ -farnesene; d. lanosterol, the 216 starting point of all steroids.
- 217 a.





- 227 228 229 230 231
- - Names of molecules reported that are incorrect or insufficiently precise to identify the molecule.

Compounds	Notes	No. of studies involved
1-1'-oxybis octane	Incomplete	1
cholest-5-ene-3-ol	Incomplete $(3-\alpha \text{ or } 3-\beta)$	1
2-methoxy-1,1-biphenyl	Incomplete (main structure is missing)	1
methoxymethylphenol	Incomplete (positions of the functional groups are missing)	1
butanol	Incomplete (alcohol position is missing)	1
cyclohexandiol	Incomplete (alcohol position is missing)	1
hexanol	Incomplete (alcohol position is missing)	1
1-octenol	Incomplete (alcohol position or the position of the double bond is missing)	1
cyclopentanetridecanoic acid-methyl ester	Incomplete (cyclopentane position is missing)	1
ethylphenol	Incomplete (ethyl position is missing)	1
6-methyl-6-heptenone	Incomplete (ketone position is missing)	1
heptanone	Incomplete (ketone position is missing)	1
propylphenol	Incomplete (propyl position is missing)	1
dimethoxyacetophenone	Incomplete (methoxy positions are missing)	1
methylaniline	Incomplete (methyl position is missing)	1
methyl-butyric acid	Incomplete (methyl position is missing)	1
methylpyrrolidinone	Incomplete (methyl position is missing)	1
methylsuccimimide	Incomplete (methyl position is missing)	1
dimethylbenzene	Incomplete (methyl positions are missing)	2
trimethylbenzene	Incomplete (methyl positions are missing)	1
xylene	Incomplete (methyl positions are missing)	1
hexamethyl-	Incomplete (positions of methyl and the double bond are	
tetracosatetraene	missing)	1
phenylethanol	Incomplete (phenyl position is missing)	1
6,10-dimethyl-5,9- undecadien-2-one	Incomplete (Z/E stereochemistry is missing)	1
7-hexadecenoic acid- methyl-ester	Incomplete (Z/E stereochemistry is missing)	1
9,12-octadienyl acetate	Incomplete (Z/E stereochemistry is missing)	1
4-(heptadecadien-1-yl)-	Incomplete (position and Z/E stereochemistry of double bonds in	1
butanolide	heptadecadiene are missing)	1
4-(hexadecadien-1-yl)-	Incomplete (position and Z/E stereochemistry of double bonds in	1
butanolide	heptadecadiene are missing)	1
heptadecene	Incomplete (position of the double bond and stereochemistry Z/E are missing)	1
heptadecenoic acid	Incomplete (position of the double bond and stereochemistry Z/E are missing)	1
hexadecene	Incomplete (position of the double bond and stereochemistry Z/E are missing)	1
hexadecen-1-ol decanoate	Incomplete (position of the double bond and the stereochemistry Z/E are missing) and misspelled	1
undecadienone	Incomplete (positions and Z/E stereochemistries of the double bonds are missing; ketone position is missing)	1
octen-2-ol	Incomplete (position of the double bond is missing)	1
pentadecene	Incomplete (position of the double bond is missing)	2
tetradecen-1-ol decanoate	Incomplete (position of the double bond is missing)	1
tetradecen-1-ol nonanoate	Incomplete (position of the double bond is missing)	1
heptadecadiene	Incomplete (positions of the double bond are missing)	1

hexadecadiene	Incomplete (positions of the double bond are missing)	1
phenylethylamine	Incomplete (several molecules are possible with this name)	1
1-hexadecanal, acetate	Incorrect	2
4-methyl-5-thiazole ethanol	Incorrect	1
9-(Z)-Octadecanoic acid	Incorrect	1
benzenemethanol	Incorrect	1
benzenepropanoic acid or	Incorrect	3
butylated hydroxytoluene	Incorrect	1
dodecanoic acid, 1-	Incorrect	1
tridecanol		-
ethyl butyric acid	Incorrect	1
hexamethyl 8-	Incorrect	1
methylnonanoate	Incorroct	1
avime methovy phonyl	Incorrect	1
phonol 4.4' (1	Incorrect	1
methylethylidene)bis-	Incorrect	1
6-methyl-1-hepten-2-one	Incorrect (a pentavalent carbon is impossible)	1
E-2.3-dimethylthietane	Incorrect (E is a nonsensical prefix)	3
E-2.4-dimethylthietane	Incorrect (E is a nonsensical prefix)	1
E-2-ethyl-3-methylthietane	Incorrect (E is a nonsensical prefix)	3
E-3,4-dimethyl-1,2-	Incorrect (E is a nonsensical prefix)	1
E-3,4-dimethyl-1,2-	Incorrect (E is a nonsensical prefix, and incorrect nomenclature:	1
dithiacyclopentane	dithiacyclopentane should be dithiolane)	1
4-hydroxy-3-	Incorrect (only 1 carbon: substituents in positions 3 and 4 are	1
methoxymethanoic acid	1mpossible)	
4-hydroxy-4-methyl-penten- 2-one	Incorrect (the double bond is impossible here)	1
4-methyl-1-undecane	Incorrect (why 1-?)	1
Z-2-ethyl-3-methylthietane	Incorrect (Z is a nonsensical prefix)	3
Z-3,4-dimethyl-1,2-	Incompati (7 is a nonconsist matix)	2
dithiacyclopentane	Incorrect (Z is a nonsensical prefix)	Z
Z-3,4-dimethyl-1,2-	Incorrect (Z is a nonsensical prefix)	1
dithiolane		1
2-methoxy-4-propylfenol	Misspelled	1
3,4-dihydro-2h-1-	Misspelled	1
benzophyrane-2-one		
4-hydroxy-3-	Misspelled	1
dimethyl digylphide	Misspalled	1
dimethyl aulphone	Misspelled	1
have deavel extense	Misspelled	1
mexadecyl octaliat	Misspelled	1
disulphide	Misspelled	1
methyl hexadecanate	Misspelled	1
nitromethame	Misspelled	1
octodecanoic acid	Misspelled	1
p-methoxybenzaldvhvde	Misspelled	1
s-3-methylbutanyl	Misspelled	-
thioacetate	<sup>E</sup>	1
Z9,Z12-octadecenoic acid	Misspelled	1
No. of the second s		

Molecules of non-natural origin found in the 41 studies. When possible, we provide references to support the non-natural origin of the molecules.

~	)2	5
4	5	J

Compounds	Notes	No. of studies involved	References supporting non-natural origin
1,1'-biphenyl, 2,3',4,4',5-pentachloro-	Non oxidized aromatic hydrocarbon (rule 3)	1	(Ghiasuddin, Menzer & Nelson, 1976)
1,1'-biphenyl, 2,3,4,4',6-pentachloro-	Non oxidized aromatic hydrocarbon (rule 3)	1	(Ghiasuddin et al., 1976)
1,2,4-trimethylbenzene	Non oxidized aromatic hydrocarbon (rule 3)	2	http://www.epa.gov/chemfact/s_trimet.txt
1,2-benzenedicarboxylic acid, diisooctyl ester	Non oxidized aromatic hydrocarbon (rule 3)	1	http://www.npi.gov.au/substances/dibutyl-phthalate/index.html
1,3-dimethylbenzene or m-xylene	Non oxidized aromatic hydrocarbon (rule 3)	3	http://hc-sc.gc.ca/ewh-semt/pubs/contaminants/psl1-lsp1/xylenes/xylenes_2-eng.php
1,4-dichlorobenzene	Non oxidized aromatic hydrocarbon (rule 3)	1	http://www.epa.gov/ttnatw01/hlthef/dich-ben.html
ethylbenzene	Non oxidized aromatic hydrocarbon (rule 3)	1	http://www.npi.gov.au/substances/ethylbenzene/index.html
naphthalene	Non oxidized aromatic hydrocarbon (rule 3)	3	http://ces.iisc.ernet.in/energy/HC270799/HDL/ENV/enven/vol350.htm
naphthalene, 1,2,3,4-tetrahydro-6-methyl-	Non oxidized aromatic hydrocarbon (rule 3)	1	http://ces.iisc.ernet.in/energy/HC270799/HDL/ENV/enven/vol350.htm
naphthalene, 1,4-dimethyl-	Non oxidized aromatic hydrocarbon (rule 3)	1	http://ces.iisc.ernet.in/energy/HC270799/HDL/ENV/enven/vol350.htm
naphthalene, 1,5-dimethyl-	Non oxidized	1	http://ces.iisc.ernet.in/energy/HC270799/HDL/ENV/enven/vol350.htm

	aromatic		
	Non oxidized		
naphthalene, 2-ethyl-	aromatic hydrocarbon (rule 3)	1	http://ces.iisc.ernet.in/energy/HC270799/HDL/ENV/enven/vol350.htm
	Non oxidized		
naphthalene, 2-methyl-	aromatic	1	http://ces.iisc.ernet.in/energy/HC270799/HDL/ENV/enven/vol350.htm
	hydrocarbon (rule 3)		
o-toluidine	aromatic	1	http://msds.chem.ox.ac.uk/TO/o-toluidine.html
o totalanie	hydrocarbon (rule 3)	1	http://msds.enenii.ok.ue.uk/10/0 totulane.html
	Non oxidized		
o-xylene	aromatic	1	http://msds.chem.ox.ac.uk/XY/o-xylene.html
	hydrocarbon (rule 3)		
	Non oxidized	2	
p-xylene	aromatic	3	http://msds.chem.ox.ac.uk/XY/p-xylene.html
	Non oxidized		
toluene	aromatic	4	http://ces.jisc.ernet.jn/energy/HC270799/HDL/ENV/enven/vol364.htm#toluene
	hvdrocarbon (rule 3)	•	
1,13-tetradecadiene	, , , , , , , , , , , , , , , , , , ,	1	http://www.chemicaldictionary.org/dic/T/Tetradeca-113-diene_2426.html
1-chlorodecane		1	
1-hexanol, 2-ethyl-		1	
1-nitropentane		1	
2,3,4,5,6-pentafluorobenzylalcohol		1	(Harrison & Wells, 2009)
2,6-di-tert-butyl-phenol		1	http://msds.chem.ox.ac.uk/DI/2,6-di-tert-butylphenol.html
2-ethylhexanoic acid		2	(Juberga, Davida, Katza et al., 1998)
2-ethylhexanol		3	http://www.ec.gc.ca/ese-ees/default.asp?lang=En&n=1D5253CB-1
2-methyl-2-propenal		1	(Smith, Perfetti, Morton et al., 2002)
2-methyl-2-propenoic acid		1	http://www.osha.gov/SLTC/healthguidelines/methacrylicacid/recognition.html
2-phenoxyethanol		2	http://www.inrs.fr/inrs- pub/inrs01.nsf/inrs01_collec_view/4E44A7A01BD02508C125748200239ED8/\$File/ft269.pdf
3,5-di-tert-butyl-4-hydroxybenzaldehyde		1	(Inagaki, Matsumoto & Tsuri, 2003)
carbon disulfide		1	http://www.npi.gov.au/substances/carbon-disulfide/index.html
chloroform		1	http://www.ineris.fr/rsde/fiches/fiche_Chloroforme_VF.pdf
fluoren-9-ol, 3,6-dimethoxy-9-(2- phenylethynyl)-		1	

hydrazoic acid	1	
n-(methylthio)methylaniline	1	
nitromethane	1	http://www.ec.gc.ca/ese-ees/default.asp?lang=En&n=111EA8E9-1#a5
nonane, 1-chloro	1	
propenoic acid	1	http://www.inrs.fr/inrs- pub/inrs01.nsf/inrs01_search_view/9AABEEAE872022B7C1256CE8005A3BB7/\$File/ft233.pdf
siloxanes	1	http://en.wikipedia.org/wiki/Siloxane

Molecules of natural, but non-mammalian, origin. We indicate the main biosynthetic pathway from which each molecule is derived and which of our nine rules would be violated if the molecule were considered to have been directly produced by a mammal. SP: shikimate pathway; AAP: Amino acid pathway; AP: acetate pathway; MP: mevalonate pathway; MEP: methylerythritol 4-phosphate pathway.

Compounds	Notes	Rule	No. of studies involved
2-(4-hydroxybenzene)-ethanol	(SP)	1	1
4-(4-hydroxy-3-methoxyphenyl)-2-butanol	(SP)	1	1
4-(4-hydroxy-3-methoxyphenyl)-2-butanone	(SP)	1	1
4-(4-hydroxyphenyl)-2-butanol	(SP)	1	1
4-methylphenol or p-cresol or phenol, 4-methyl	(SP)	1	9
α-hexyl-cinnamic aldehyde	(SP)	1	1
albicanol	(SP)	1	1
benzyl methyl ketone	(SP)	1	2
ethylcinnamate	(SP)	1	1
methyl salicylate	(SP)	1	2
phenylmethanethiol	(SP)	1	1
vitamine E	(SP)	1	1
vitamine K	(SP)	1	1
3-phenyl-2-propenoic acid	Cinnamic acid (SP)	1	1
3-methyl-4-hydroxyphenyl 2-methylbutanoate	Cinnamic acid derivative (SP)	1	1
3-methyl-4-hydroxyphenyl 2-methylpropanoate	Cinnamic acid derivative (SP)	1	1
3-phenylpropanoic acid	Cinnamic acid derivative (SP)	1	4
3-phenylpropanol	Cinnamic acid derivative (SP)	1	1
4-(4-hydroxyphenyl)-2-butanone	Cinnamic acid derivative (SP)	1	1
4-ethyl phenol	Cinnamic acid derivative (SP)	1	2
4-methoxyphenylacetic acid	Cinnamic acid derivative (SP)	1	1
4-phenyl-3-buten-2-one	Cinnamic acid derivative (SP)	1	1
benzenepropanoic acid, methyl ester	Cinnamic acid derivative (SP)	1	1
2-methoxyhydroquinone	Conyferilic acid derivative (SP)	1	1
3,4-dimethoxyphenylmethyl propanoate	Conyferilic acid derivative (SP)	1	1
eugenol	Conyferilic alcohol derivative (SP)	1	1

2,3-dihydro-3,5-dihydroxy-6-methylpyrane-4-one	Flavone derivative (SP)	1	1
2-hydroxy-5-methylacetophenone	Flavone derivative (SP)	1	1
styrene	Monomere of polystyrene (petroleum industry) and little present in a natural state (SP)	1	1
2-methoxyphenol	Or anisole (SP)	1	3
2-hydroxybenzoic acid	Or salicylic acid (SP)	1	1
1,4-benzenediol or hydroquinone	Oxydation in position 4 (SP)	1	3
2-methyl-4-hydroxyphenyl 2-methylbutanoate	Phenol in position 4 (SP)	1	1
2-methyl-4-hydroxyphenyl 2-methylpropanoate	Phenol in position 4 (SP)	1	1
1,2-benzenediol or 2-hydroxybenzyl alcohol	Salicylic acid derivative (SP)	1	2
4-ethyl-2-methoxyphenol	Shikimic acid derivative (SP)	1	1
4-hydroxy-3-methoxy acetophenone	Shikimic acid derivative (SP)	1	1
4-hydroxy-3-methoxy-benzoacetic acid	Shikimic acid derivative (SP)	1	1
4-hydroxy-3-methoxybenzoic acid, methylester	Shikimic acid derivative (SP)	1	1
4-hydroxyacetophenone	Shikimic acid derivative (SP)	1	1
4-methoxybenzoic acid	Shikimic acid derivative (SP)	1	2
α-tocopherol	Degradation from vitamine E (SP)	1	1
menadione	vitamine K precursor (SP)	1	1
2-phenylethanol	Phenylalanine derivative (SP+AAP)	1	3
2-phenylethylamine	Phenylalanine derivative (SP+AAP)	1	1
phenyl acetaldehyde	Phenylalanine derivative (SP+AAP)	1	1
phenylacetamide	Phenylalanine derivative (SP+AAP)	1	1
phenylacetic acid	Phenylalanine derivative (SP+AAP)	1	5
indole	(SP+AAP)	1	12
3-hydroxy benzoic acid	Oxydation in meta (AP)	2	1
3-n-propylphenol	Oxydation in meta (AP)	2	1
m-hydroxyacetophenone	Oxydation in meta (AP)	2	1
5-methyl-1,3-benzenediol	Oxydation in positions 1 and 3 (AP)	2	1
nicotine	(AAP)	4	1
lupanine	Alcaloid (AAP)	4	1
1-methylpiperidine	Alcaloid involved in tropane metabolism (AAP)	4	1
2-pyrrolidinone	Lactame of $\beta$ -alanine (produced by vegetals to synthesize vitamine B5; AAP)	4	2
skatole	Or 3-methylindole (AAP)	4	1
(E)-9-henicosene	Trans mono-unsaturated fatty acid (AP)	5	1
(E)-9-octadecenoic acid	Trans mono-unsaturated fatty acid (AP)	5	2
9-octadecenoic acid, methyl ester, (E)-	Trans mono-unsaturated fatty acid (AP)	5	1
E-9-octadecen-1-ol	Trans mono-unsaturated fatty acid (AP)	5	1

Z-5-tetradecenol acetate	(AP)	6	1
icosanoic acid	Or arachidonic acid (AP)	6	2
(all-Z)5,8,11,14-eicosatetraenoic acid	Positions of double bond are not mammalian (AP)	6	1
(all-Z)8,11,14-eicosatrienoic acid	Positions of double bond are not mammalian (AP)	6	1
(Z)-8-tetradecen-1-yl formate	Positions of double bond are not mammalian (AP)	6	1
(Z,Z)-9,12-octadecadien-1-ol	Positions of double bond are not mammalian (AP)	6	1
11-octadecenoic acid, methyl ester, (Z)	Positions of double bond are not mammalian (AP)	6	1
linoleic acid	Or omega 6; positions of double bond are not mammalian (AP)	6	2
erucic acid	Or omega 9; positions of double bond are not mammalian (AP)	6	1
9,12-octadecadienoic acid (Z,Z), methyl ester	Poly-unsaturations in position 9 and 12 (AP)	7	1
Z11,Z14-eicosadienoic acid	Poly-unsaturation in terminal positions (AP)	7	1
(E)-2,3-dihydrofarnesol	(MP or MEP)	9	1
(E)-6,10-dimethyl-5,9-undecadien-2-one or		0	(
geranylacetone	(MP of MEP)	9	0
(E,E)-farnesyl decanoate	(MP or MEP)	9	1
(E,Z)-farnesyl decanoate	(MP or MEP)	9	1
3,7-dimethyl-2,6-octadienal	(MP or MEP)	9	1
hexahydrofarnesylacetone	(MP or MEP)	9	1
α-isomethylionone	Carotenoid (MP or MEP)	9	1
1,8-cineole	Or eucalyptol monoterpene (MP or MEP)	9	1
α-pinene	Monoterpene (MP or MEP)	9	4
α-terpinene	Monoterpene (MP or MEP)	9	1
α-terpineol	Monoterpene (MP or MEP)	9	2
borneol	Camphre derivative, monoterpene (MP or MEP)	9	1
β-pinene	Monoterpene (MP or MEP)	9	2
cis-furanoid linalool oxide	Monoterpene (MP or MEP)	9	1
cis-linaloloxide	Monoterpene (MP or MEP)	9	1
dihydromyrcenol	Monoterpene (MP or MEP)	9	1
D-limonene	Monoterpene (MP or MEP)	9	1
geraniol	Monoterpene (MP or MEP)	9	1
limonene	Monoterpene (MP or MEP)	9	3
linalool	Monoterpene (MP or MEP)	9	2
linalool oxide trans	Monoterpene (MP or MEP)	9	1
menthol	Monoterpene (MP or MEP)	9	2
myrthanol	Monoterpene (MP or MEP)	9	1
myrthenol	Monoterpene (MP or MEP)	9	1

p-cymene	Monoterpene (MP or MEP)	9	1
trans-furanoid linalool oxide	Monoterpene (MP or MEP)	9	1
verbenone	$\alpha$ -pinene derivative, monoterpene (MP or MEP)	9	1
(3E,6E,10E)-α-springene	Diterpene (MP or MEP)	9	1
(3Z,6E,10E)-α-springene	Diterpene (MP or MEP)	9	1
(6E,10E)-β-springene	Diterpene (MP or MEP)	9	1
(E)-nerolidol	Sesquiterpene (MP or MEP)	9	1
(Z,E)-farnesyl decanoate	Sesquiterpene (MP or MEP)	9	1
(Z,Z)-farnesyl decanoate	Sesquiterpene (MP or MEP)	9	1
1,6,10-dodecatriene,7,11-dimethyl-3-methylene, (E)-	Sesquiterpene (MP or MEP)	9	1
isocurcumenol	Sesquiterpene (MP or MEP)	9	1
nerolidol	Sesquiterpene (MP or MEP)	9	1

Molecules of mammalian origin. We indicate the main biosynthetic pathway from which each molecule is derived as well as its family. When possible, we also indicate the possible role in mammalian communication as reported in the studied references (if different roles have been reported, we separated them with semicolons).

AAP: Amino-acid pathway; AP: acetate pathway; MP: mevalonate pathway.

Compounds	Notes	Main result	No. of studies involved	Molecule family
2-octenoic acid	AP	-	1	acid
acetic acid or ethanoic acid	AP	-	6	acid
decanoic acid	AP	-	5	acid
docosanoic acid	AP	-	2	acid
dodecanoic acid	AP	only present in males (two species)	9	acid
eicosanoic acid	AP	-	2	acid
heneicosanoic acid	AP	-	1	acid
heptadecanoic acid	AP	-	1	acid
hexadecanoic acid or n-hexadecanoic acid	AP	-	15	acid
isopentanoic acid	AP	-	1	acid
nonadecanoic acid	AP	-	2	acid
nonanoic acid	AP	only present in males	6	acid
octanoic acid	AP	-	9	acid
oleic acid	AP	-	2	acid
pentadecanoic acid	AP	only present in males	8	acid
stearic acid or octadecanoic acid	AP	-	10	acid
tetradecanoic acid	AP	only present in males	13	acid
undecanoic acid	AP	-	3	acid
(Z)-9-dodecenoic acid	AP	-	1	unsaturated acid
(Z)-9-hexadecenoic acid	AP	-	2	unsaturated acid
(Z)-9-octadecenoic acid	AP	-	4	unsaturated acid
9-hexadecenoic acid	AP	-	1	unsaturated acid
heptane	AP	-	1	alkane
(Z)-9-henicosene	AP	-	1	alkene

1,4,8-dodecatriene, (E,E,E)-	AP	-	1	alkene
1,9-cyclohexadecadiene	AP	-	1	alkene
10-docosene	AP	-	1	alkene
10-henicosene	AP	_	1	alkene
10-tricosene	AP	-	1	alkene
1-octene	AP	-	2	alkene
1-tetradecene	AP	only present in males	1	alkene
1-tridecene	AP	only present in males	2	alkene
7-heptadecene	AP	-	1	alkene
9-docosene	AP	-	1	alkene
9-nonadecene	AP	-	1	alkene
9-tricosene	AP	-	1	alkene
1,2-hexadecanediol	AP	-	1	alcohol
1-decanol	AP	-	1	alcohol
1-dodecanol	AP	signal of pregnancy	4	alcohol
1-heptadecanol	AP	-	1	alcohol
1-hexadecanol	AP	molecule bound to sexual pheromone; more present in males and relative abundance differs among genetic strains; only found in males	8	alcohol
1-hexanol	AP	-	4	alcohol
1-nonanol	AP	-	3	alcohol
1-octadecanol	AP	molecule bound to sexual pheromone; relative abundance differs among genetic strains	4	alcohol
1-octanol	AP	-	3	alcohol
1-pentadecanol	AP	-	2	alcohol
1-tetradecanol	AP	more present in males	4	alcohol
1-tridecanol	AP	-	1	alcohol
1-undecanol	AP	-	1	alcohol
2-nonadecanol	AP	-	1	alcohol
2-nonanol	AP	-	1	alcohol
tridecanol	AP	-	1	alcohol
6-methyl-1-heptanol	MP	-	1	alcohol
6-methyl-5-hepten-2-ol	MP	-	1	unsaturated alcohol
(Z)-9-hexadecen-1-ol	AP	-	2	unsaturated alcohol
(Z)-9-octadecen-1-ol	AP	molecule bound to sexual pheromone	2	unsaturated alcohol
11-hexadecen-1-ol, (Z)-	AP	-	1	unsaturated alcohol
1-octen-3-ol	AP	-	1	unsaturated alcohol
pentadecanal	AP	-	1	aldehyde

1-dodecyl formate	AP	-	1	ester
1-henicosyl formate	AP	-	1	ester
1-heptadecanol, acetate	AP	-	1	ester
1-hexadecanol, acetate	AP	more present in males	1	ester
1-hexadecyl formate	AP	- -	1	ester
1-hydroxyheptadec-2-yl pentanoate	AP	-	1	ester
1-hydroxyhexadec-2-yl pentanoate	AP	-	1	ester
1-icosyl formate	AP	-	1	ester
1-nonadecyl formate	AP	-	1	ester
1-octadecyl formate	AP	-	1	ester
1-octyl acetate	AP	-	1	ester
1-pentadecanol acetate	AP	more present in males	1	ester
1-pentadecanol decanoate	AP	more present in females	1	ester
1-pentadecyl formate	AP	-	1	ester
1-tetracosyl formate	AP	-	1	ester
1-tetradecanol, acetate	AP	more present in males	1	ester
1-tetradecyl formate	AP	-	1	ester
1-tricosyl formate	AP	-	1	ester
1-tridecyl formate	AP	-	1	ester
1-undecyl formate	AP	-	1	ester
2-hydroxyheptadec-1-yl pentanoate	AP	-	1	ester
2-hydroxyhexadec-1-yl pentanoate	AP	-	1	ester
2-hydroxyicos-1-yl acetate	AP	-	2	ester
2-hydroxyoctadec-1-yl acetate	AP	-	1	ester
dec-9-enoic acid, ethyl ester	AP	-	1	ester
decanoic acid, decyl ester	AP	-	1	ester
decanoic acid, ethyl ester	AP	-	1	ester
decanoic acid, methyl ester	AP	-	2	ester
docosanoic acid, methyl ester	AP	only present in males	1	ester
dodecanoic acid, methyl ester	AP	-	2	ester
dodecyl octanoate	AP	more present in males and relative abundance differs among genetic strains	1	ester
ethyl decanoate	AP	-	2	ester
ethyl dodecanoate	AP	-	1	ester
ethyl heptanoate	AP	-	1	ester
ethyl hexanoate	AP	-	1	ester
ethyl isododecanoate	AP	-	1	ester

ethyl isohexanoate	AP	-	1	ester
ethyl isotetradecanoate	AP	-	1	ester
ethyl isotridecanoate	AP	-	1	ester
ethyl nonanoate	AP	present only in females	2	ester
ethyl octanoate or octanoic acid, ethyl ester	AP	-	2	ester
ethyl pentadecanoate	AP	-	1	ester
ethyl tetradecanoate	AP	-	1	ester
ethyl undecanoate	AP	-	1	ester
heptadecanoic acid, pentadecyl ester	AP	only present in males	1	ester
hexadecanoic acid, butyl ester	AP	-	1	ester
hexadecanoic acid, hexadecyl ester	AP	only present in males	2	ester
hexadecanoic acid, methyl ester	AP	only present in males	3	ester
hexadecyl decanoate	AP	present only in females; relative abundance differs among genetic strains	2	ester
hexadecyl dodecanoate	AP	more present in males	1	ester
hexadecyl undecanoate	AP	more present in females	1	ester
hexanoic acid or capronic acid or caproic acid	AP	possibly reflects genetic variation	14	ester
hexanoic acid, ethyl ester	AP	-	1	ester
hexanoic acid, methyl ester	AP	-	2	ester
hexyl acetate	AP	-	1	ester
isoamyl laurate	AP	-	1	ester
isopropyl myristate	AP	signal of pregnancy	1	ester
methyl 9-methyl tetradecanoate	AP	-	2	ester
methyl tetradecanoate or tetradecanoic acid, methyl ester	AP	only present in males	3	ester
nonanoic acid, methyl ester	AP	-	2	ester
octadecanoic acid, hexadecylester	AP	only present in males	1	ester
octadecanoic acid, methyl ester	AP	-	2	ester
octadecyl acetate	AP	more present in males	1	ester
octanoic acid, heptadecyl ester	AP	-	1	ester
octanoic acid, hexadecyl ester	AP	-	2	ester
octanoic acid, methyl ester	AP	-	2	ester
octanoic acid, pentadecyl ester	AP	-	1	ester
octanoic acid, tetradecyl ester	AP	-	1	ester
octanoic acid, tridecyl ester	AP	-	1	ester

pentadecanoic acid, 14-methyl-, methyl ester	AP	-	1	ester
pentadecanoic acid, methyl ester	AP	only present in males	3	ester
tetradecanoic acid, dodecyl ester	AP	-	1	ester
tetradecanoic acid, hexadecyl ester	AP	-	1	ester
tetradecanoic acid, tetradecyl ester or tetradecyl-tetradecanoate	AP	-	2	ester
tetradecanol decanoate	AP	-	1	ester
tetradecanol dodecanoate	AP	-	1	ester
undecanoic acid, methyl ester	AP	-	2	ester
benzeneacetic acid, ethyl ester	AAP	-	1	ester
benzeneacetic acid, methyl ester	AAP	-	1	ester
10-heptadecen-1-yl formate	AP	-	1	unsaturated ester
10-nonadecen-1-yl formate	AP	-	1	unsaturated ester
11-hexadecen-1-ol, acetate (Z)-	AP	more present in males	1	unsaturated ester
1-docosyl formate	AP	-	1	unsaturated ester
2-penten-1-ol acetate	AP	-	1	unsaturated ester
5-tetradecen-1-ol, octanoate, (Z)-	AP	more present in males and relative abundance differs among genetic strains	1	unsaturated ester
9-hexadecenoic acid, methyl ester (Z)	AP	-	1	unsaturated ester
9-octadecenoic acid (Z), methyl ester	AP	-	1	unsaturated ester
9-octadecenoic acid, hexadecyl ester	AP	only present in males	1	unsaturated ester
9-octadecenoic acid, methyl ester	AP	-	1	unsaturated ester
ethyl 9-hexadecenoate	AP	-	1	unsaturated ester
ethyl 9-tetradecenoate	AP	-	1	unsaturated ester
Z-9-hexadecen-1-ol acetate	AP	more present in males and relative abundance differs among genetic strains	1	unsaturated ester
pyrazole	AAP	-	1	heterocyclic aromatic compound
pyridine	AAP	-	2	heterocyclic aromatic compound
quinoline	AAP	more present in males	2	heterocyclic aromatic compound
2-nonadecanone	AP	-	1	ketone
2-nonanone	AP	tsetse fly attractant	5	ketone
2-octadecanone	AP		1	ketone
2-octanone	AP	tsetse fly attractant	4	ketone
2-pentadecanone	AP	-	2	ketone

2-pentanone	AP	-	2	ketone
2-tricosanone	AP	-	1	ketone
2-tridecanone	AP	-	2	ketone
2-undecanone	AP	-	2	ketone
6-hydroxy-6-methyl-3-heptanone	MP	relative abundance differs among genetic strains	3	ketone
6-methyl-2-heptanone	MP	-	1	ketone
6-methyl-3-heptanone	MP	-	1	ketone
6-methyl-3,5-heptadiene-2-one	MP	-	1	unsaturated ketone
6-methyl-5-hepten-2-one	MP	increased attractiveness from mosquitoes (Aedes and Anopheles)	7	unsaturated ketone
6-methyl-5-hepten-3-one	MP	linked to MHC variation	2	unsaturated ketone
6-methyl-6-hepten-3-one	MP	-	1	unsaturated ketone
phenylacetonitrile	AAP	more present in males and age-specific	2	nitrile
1-acetylimidazole	AAP		1	nitrogen compound
n-benzylidene-2-phenylethylamine	AAP	-	1	nitrogen compound
n-benzylidenepentylamine	AAP	-	1	nitrogen compound
sparteine	AAP	only present in females	1	nitrogen compound
1 1 dimethylymaa	AAP +		2	nitro con compound
1,1-dimentylurea	AP	-	2	introgen compound
n pontuluroo	AAP +		1	nitrogen compound
n pentylulea	AP		1	muogen compound
urea	AAP +	<u>-</u>	1	nitrogen compound
	AP		-	introgen compound
$4-\alpha$ -methylcholest-8 (14)-ene-3- $\beta$	MP	-	1	steroid
4-β-methyl-24(R)-methylcholest-8 (14)-ene-3-β	MP	only present in females	1	steroid
4-methylcholest-7-ene-3-one	MP	only present in females	1	steroid
5α-androst-2-en-17β-ol	MP	reflect ovarian cycle	1	steroid
5α-androst-2-en-17-one	MP	reflect ovarian cycle	1	steroid
cholest-3-ene (5-α)	MP	only present in females	1	steroid
cholest-4-ene-3-one	MP	- · · ·	1	steroid
cholest-7-ene-3-ol (3-β,5-α)	MP	only present in females	1	steroid
cholestan-3-ol-(3-β,5-α)	MP	- · · ·	1	steroid
cholestanol or 5-α cholestanol	MP	-	1	steroid
cholesterol	MP	-	6	steroid
desmosterol	MP	-	2	steroid
dihydrocholesterol	MP	only present in males	1	steroid

dihydrolanosterol	MP	only present in females	1	steroid
lanosta-8,24-diene-3-ol (3-β)	MP	only present in females	1	steroid
lanosterol	MP	-	3	steroid
(E)- $\beta$ -farnesene or $\beta$ -farnesene	MP	more present in males in one species, and more present in females in another species	6	terpenoid
(E,E)-α-farnesene	MP	more present in males in one species, and more present in females in another species	3	terpenoid
α-farnesene	MP	-	1	terpenoid
squalene	MP	only present in males in one species and more present in males in two other species	6	terpenoid

Non-classified molecules.

Compounds	No. of studies involved
(1H)-pyrrole-2-carboxaldehyde	1
(E)-2-butene-1-thiol	1
(E)-2-butenyl 3-methylbutyl disulfide	1
(E)-2-decenal	2
(E)-2-heptenal	2
(E)-2-nonenal	5
(E)-2-octenal	3
(E)-2-undecenal	2
(E)-4-heptadecene	1
(E)-4-octene	1
(E)-6-heptadecene	1
(E)-7-methyl-2-octenal	1
(E)-7-nonadecene	1
(E)-8-methyl-2-nonenal	1
(E)-9-methyl-2-decenal	1
(methylthio) methanethiol (MTMT)	1
(s)-2-sec-butyl-4,5-dihydrothiazole or 2-sec-butyl-4, 5-dihydrothiazole	3
(Z)-10-heptadecen-2-one	1
(Z)-11-octadecen-2-one	1
(Z)-12-nonadecen-2-one	1
(Z)-14-henicosen-2-one	1
(Z)-2-decene	1
(Z)-2-octenal	1
(Z)-2-undecenal	1
(Z)-4-heptadecene	1
(Z)-6-dodecen-4-olide	1
(Z)-6-heptadecene	1
(Z)-6-tridecen-1-yl formate	1
(Z)-7-hexadecene	2
(Z)-7-nonadecene	1
(Z)-8-henicosen-2-one	1
(Z)-8-heptadecen-2-one	1
(Z)-8-hexadecen-2-one	1
(Z)-8-methyl-2-nonenal	1
(Z)-8-nonadecen-2-one	1
(Z)-8-octadecen-2-one	1
(Z)-9-methyl-2-decenal	1
1,2-bis(p-methoxyphenyl)ethane	1
1,2-dimethyl-4-ethenylbenzene	1
1,3,5 triazone-2,4-diamine	1

1,3-diphenylpropane-2-one	1
11-methyltridecanoic acid	1
11-tricosene	1
12-henicosen-1-yl formate	1
12-methyl-oxa-cyclododec-6-en-2-one	1
12-methyltridecanoic acid	1
12-nonadecen-1-yl formate	1
13-icosen-1-yl formate	1
13-methyltetradecanoic acid	1
13-octadecenoic acid, methyl ester	1
14-henicosen-1-yl formate	1
14-methylhexadecanoic acid	1
14-methylpentadecanoic acid	2
14-tricosen-1-yl formate	1
15-docosen-1-yl formate	1
15-methylhexadecanoic acid	1
16-henicosen-1-yl formate	1
16-methylheptadecanoic acid	1
16-pentacosen-1-yl formate	1
16-tricosen-1-yl formate	1
17-methyloctadecanoic acid	1
17-tetracosen-1-yl formate	1
18-methylnonadecanoic acid	1
18-pentacosen-1-yl formate	1
18-tricosen-1-yl formate	1
19-methylicosanoic acid	1
1-butanol	2
1-butyl-1-methyl-2-propyl-cyclopropane	2
1-furfuryl pyrrole	1
1-heptadecene	1
1-heptadecyl formate	1
1-heptanol	3
1-methoxy-2-propanol	2
1-methoxy-2-propyl acetate	1
1-methyl,4-isopropylbenzene	1
1-methyl-2-pyrrolidine	1
1-methyl-2-pyrrolidone	1
1-methyl-4-isopropylbenzene	1
1-methylhydantoin	1
1-pentanol	2
1-propanol	1
1s,4r,7r,11r-1,3,4,7-tetramethyltricyclo[5.3.1.0(4,11)] undec-2-en-8-one	1
2(3H)-furanone, 5-ethyldihydro-	1
2(5H)-furanone	1
2,2-dimethyloctane	1

2,2-dimethylthietane	3
2,3-dehydro-exo-brevicomin	1
2,3-dimethylcyclohexanol	1
2,3-dimethylpyrazine	1
2,4 dimethylcyclopentanone	1
2,4,6-trimethyloctane	2
2,5-dimethylpyrazine	3
2,5-dimethyltetrahydrofurane	1
2,5-pyrrolidindione	1
2,6-dimethylpyridine	1
2-acetylpyrrol	1
2-butanol	1
2-cyanopyridine	1
2-decanone	3
2-decenoic acid	1
2-dodecanone	1
2-ethyl-2-pentenal	1
2-ethyl-5-methyl-5,6-dihydro-(4H)pyran	1
2-ethylquinoline	1
2-ethylthietane	3
2-furancarboxaldehyde	1
2-furanmethanol	2
2-henicosanol	1
2-henicosanone	1
2-heptadecanol	1
2-heptadecanone	2
2-heptanone	9
2-hexadecanone	1
2-hexanone	1
2h-pyran-2-one, tetrahydro-6-methyl-	1
2-icosanone	1
2-isopropyl-4,5-dihydrothiazole	2
2-isopropylthietane	2
2-methyl butyric acid	1
2-methyl-1-butanol	2
2-methyl-1-propanol	1
2-methyl-2,3-epoxypentane	1
2-methyl-2-hexanol	1
2-methyl-3-buten-2-ol	2
2-methyl-5-phenyl-pyridine	1
2-methylbenzoxazol	1
2-methylbutanoic acid	4
2-methyldecanoic acid	3
2-methyldocosane	1
2-methylhenicosane	1

2-methylheptadecane	1
2-methylheptane	1
2-methylhexadecane	1
2-methylhexane	1
2-methylhexanoic acid	2
2-methylicosane	1
2-methylnonanoic acid	1
2-methyloctadecane	1
2-methyloctane	1
2-methyloctanoic acid	1
2-methylpentanoic acid	1
2-methylphenol	1
2-methylpropanamide	1
2-Methylpropanoic acid	2
2-methylpyrrol	1
2-methylquinoline	2
2-methyltetracosane	1
2-methyltetradecane	1
2-methyltricosane	1
2-methylundecane	1
2-methylundecanoic acid	1
2-pentylfuran	1
2-pentylthietane	2
2-phenylethanethiol	1
2-phenylphenol	1
2-piperidinone	1
2-piperidone	4
2-propanol	1
2-propylthietane	3
2-pyperidinone	1
2-quinolinemethanethiol	1
2-sec-butyl-4,5-dihydrothioazole	1
3,3-dimethyl-1,2-dithiacyclopentane or 3,3-dimethyl-1,2-dithiolane	3
3,3-Dimethyl-1,2-dithiolane	1
3,4-dehydro-exo-brevicomin	2
3,4-dimethylheptane	1
3,5,5-trimethyl-1-hexanol	1
3-aminopyridine	1
3-ethyl-1,2-dithiacyclopentane or 3-ethyl-1,2-dithiolane	2
3-Ethyl-1,2-dithiolane	1
3-ethyl-2,2-dimethyloxirane	1
3-ethyl-2-methyl-1-heptene	1
3-ethylcyclopentanone	1
3-heptanone	1
3-hepten-2-one	5

3-hexanone	1
3-hydroxy-2-butanone	2
3-hydroxy-2-methyl-4-pyrone	1
3-isopropyl-6-methylphenol	1
3-methyl butanoic acid	4
3-methyl-1-butanethiol	1
3-methyl-1-butanol	4
3-methyl-2-butanone	1
3-methyl-2-buten-1-ol	2
3-methyl-2-decanone	1
3-methyl-2-hexanone	1
3-methyl-2-nonanone	1
3-methyl-2-octanone	1
3-methyl-3-buten-1-ol	1
3-methyl-3-butenal	1
3-methyl-6-octen-1-ol	1
3-methylbutanal	1
3-methylbutanamide	1
3-methylbutanoic acid	4
3-methyl-cyclopentanone	1
3-methyl-dihydro-2(3H) furanone	1
3-methylnonane	1
3-methylquinoline	1
3-nonen-2-one	1
3-nonenoic acid, methyl ester	1
3-octanone	2
3-pentanone	1
3-penten-2-one	1
3-phenylpyridine	1
3-propyl-1,2-dithiolane	1
3-pyridinole	1
3-tetradecene	1
3-tridecanone	1
4,9-dimethylnaptho[2,3-b]thiophene	1
4-azidoheptane	1
4-decene	2
4-ethyl-1,3-benzenediol	1
4-heptanone	4
4-hepten-2-one	1
4-hydroxybenzaldehyde	1
4-methyl-3-penten-2-one	2
4-methyl-4-penten-2-ol	1
4-methyl-6-hepten-3-one	1
4-methyl-dihydro-2(3H) furanone	1
4-methyloctanoic acid	1

4-methylpentanal	1
4-methylpentanoic acid	1
4-methylquinazoline	1
4-nonadecene	1
4-nonanone	1
4-oxo-2-pyrrolidinone	1
4-undecanone	1
5,6,7,7-tetrahydro-2(4H)benzofuranone	1
5-heptadecene	1
5-hepten-2-one	4
5-icosene	1
5-methyl-1-hexanol	1
5-methyl-2-hexenal	1
5-methylfurfural	1
5-methylhexanal	1
5-methylhydantoin or 5-methyl-2.4-imidazolidinedione	2
5-nonadecene	1
6-henicosene	1
6-methyl-2-octanol	1
6-methylbeptanal	1
6-methylheptanoic acid	1
6-nonadecene	1
6-tridecene	1
7-henicosene	1
7-methyloctanal	1
7-methyloctanoic acid	1
7-octenoic acid	1
7-tetradecen-1-vl formate	1
8-henicosene	1
8-heptadecen-1-vl formate	1
8-methylnonal	1
8-pentadecen-1-vl formate	1
acetamide	2
acetic acid-phenylmethyl ester	1
acetone	4
acetophenone	6
α-lactone	1
benzaldehyde	14
benzaldehyde, 3.4-dimethyl-	1
benzamide	1
benzoic acid	3
benzoic acid, 4-ethoxy-, ethyl ester	1
benzoic acid, ethyl ester	1
benzoic acid, methyl ester	1
benzonitrile	1

benzothiazole	3
benzyl alcohol	3
bis(3-methylbutyl) disulfide	1
bis(methylthio)methane	2
bis[(e)-2-butenyl] disulfide	1
but-2-enolide	1
butanal	1
butanoic acid	5
butanoic acid, 3-methyl-	1
butanoic acid, 3-methyl-, ethyl ester	1
butanoic acid, 3-methyl-, methyl ester	1
butanoic acid, methyl ester	1
butanone	2
butylbenzoate	1
butyric acid	1
butyrolactone	1
carbon dioxide	1
cyclododecane	2
cycloheptadecanone	1
cyclohexane-carboxylic acid	1
cyclohexanecarboxylic acid, methyl ester	1
cyclohexanone	2
cyclooctane	1
cyclopent-2-en-1,4-dione	1
cyclopentanone	1
cyclotetradecene	1
decan-4-olide	1
decan-5-olide	1
decanal	12
decane	2
decanoicacid, methylester	1
dehydro-exo-brevicomin	1
dimethyl adipate	1
dimethyl disulfide	3
dimethyl glutarate	1
dimethyl succinate	1
dimethyl sulfone	7
dimethyl trisulfide	2
dodecan-4-olide	1
dodecan-5-olide	1
dodecanal	3
dodecane	2
dodecane, 4,6-dimethyl-	1
dodecane, 4-methyl-	1
dodecane, 6-methyl-	1

dodecanoic acid, 10-methyl-, methyl ester	1
E2,E4-decadienal	1
e-5,5-dimethyl-2-ethylidenetetrahydrofuran	1
elemental sulfur (s8)	1
ethanol	1
ethanol,2-(octylthio)	1
ethyl 2-methylbutanoate	1
ethyl 3-methylbutanoate	1
ethyl 4-methyldecanoate	1
ethyl 4-methyldodecanoate	1
ethyl 4-methylheptanoate	1
ethyl 4-methylhexanoate	1
ethyl 4-methyloctanoate	1
ethyl 4-methylundecanoate	1
ethyl butanoate	1
formamide	1
formanilide	1
furancarboxylic acid-methyl ester	2
furanone	1
furfural	2
furfuryl alcohol	2
g-octalactone	1
henicosane	1
heptadecane	3
heptadecane-1,2-diol	1
heptanal	11
heptanoic acid, methyl ester	1
hexadecan-4-olide	1
hexadecan-5-olide	1
hexadecanal	2
hexadecane	5
hexadecane-1,2-diol	1
hexan-4-olide	1
hexanal	12
hexyl aldehyde	1
hydrogen sulfide	1
isobutyric acid	1
maleimide	1
m-cresol	1
methyl (methylthio)methyl disulfide	1
methyl butyrate	1
methyl mercaptan	1
methyl-cyclodecane	1
n-butane	1
n-cyclopentylidene methylamine	1

n-decane	1
n-decanol	1
n-decyl aldehyde	1
n-dodecane	1
n-heptane	1
nicotinamide	1
n-octane or octane	2
nonadecane	1
nonadecane, 9-methyl-	1
nonadecanoic acid, methyl ester	1
nonan-4-olide	1
nonan-5-olide	1
nonane	2
nonanedioic acid, dimethyl ester	1
nonvl aldebyde or nonanal	1/
n pentencie acid or pentencie acid	10
n-pentanoic acid of pentanoic acid	10
	/
n-undecanoi	1
n-valeraldenyde or pentanal	3
o-aminoacetophenone	2
o-cresol	I
octacosane	1
octadecane	2
octan-4-olide	1
octan-5-olide	1
octanal	12
octanedioic acid, dimethyl ester	1
octyl aldehyde	1
o-tolualdehyde	1
oxacycloheptadec-8-en-2-one	1
oxindole (1,3-dihydro-2h-indol-2-one)	1
pentadecane	5
pentan-4-olide	1
pentan-5-olide	1
pentanedinitrile, 2-methylene-	1
pentanoic acid, ethyl ester	1
pentanoic acid, methyl ester	1
pentanone	10
phenol	10
phenyl metnyl ketone	1
propanamide	1
propanedioic acid-dimethyl ester	1
propanoic acid, 2-methyl-	3
propanoic acid, 2-methyl-, ethyl ester	1
propanoic acid, 2-methyl-, methyl ester	1

propionic acid or propanoic acid	6
pyrrol	
PJIIOI	1
s-(e)-2-butenyl thioacetate	1
s-2-phenylethyl thioacetate	1
s-2-quinolinemethyl thioacetate	1
sebacic acid monomethyl ester	1
s-phenylmethyl thioacetate	1
succimimide	1
tetracosanoic acid	2
tetradecan-4-olide	1
tetradecan-5-olide	1
tetradecanal	3
tetradecane	2
tetradecanoic acid, 12-methyl-, methyl ester	1
tricosane	1
tricosanoic acid	1
tridecan-4-olide	1
tridecan-5-olide	1
tridecanal	2
tridecane	1
tridecane-2,4-dione	1
tridecanoic acid	3
tridecanoic acid-methyl ester	1
trimethylamine	3
trimethylpyrazine	1
undecan-4-olide	1
undecan-5-olide	1
undecanal	4
undecane,3,6-dimethyl-	1
Z-2-pentenyl acetate	1
Z-5,5-dimethyl-2-ethylidenetetrahydrofuran	1
Z-7-octadecen-1-ol acetate	1
Z-7-tetradecen-1-ol	1

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