

Vanilla beyond *Vanilla planifolia* and *Vanilla x tahitensis*: taxonomy and historical notes, reproductive biology and metabolites

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Supplementary Table S1. Metabolites identified from vanilla crop wild relatives and/or non-commercial vanilla species, following the alphabetical order of direct parent classes.

Metabolite	Species	Methods	Flavor DB descriptors	CID (PubChem)	Direct parent
2,3-butanediol	10c	GC-MS	onion, fruit, creamy, fruity, buttery	262	1,2-diols
phenol	8h, 15h, 10c	GC-MS, GC-O	phenol, plastic, rubber, phenolic	996	1-hydroxy-4-unsubstituted benzenoids
2,3-dihydroxypropyl acetate	8h	DTD-GC-MS		33510	1-monoacylglycerols
homoeriodictyol	1a, 2a	UHPLC-MS/MS	bitter	73635	3'-O-methylated flavonoids
viridiflorol	10c	GC-MS		11996452	5,10-cycloaromadendrane sesquiterpenoids
alpinumisoflavone	1a, 2a	UHPLC-MS/MS		5490139	6-prenylated isoflavanones
bletilol A	1a, 2a	UHPLC-MS/MS		102121477	7-O-methylated isoflavanoids
nevadensin	1a, 2a	UHPLC-MS/MS	if glucoside can be sweet-like	160921	8-O-methylated flavonoids
3-hydroxypropyl prop-2-enoate	15h	DTD-GC-MS		33101	Acrylic acid esters
methyl acrylate	8h, 10c, 15h	DTD-GC-MS, GC-MS		7294	Acrylic acid esters
cis-beta-ocimene	16i	GC-MS		5320250	Acyclic monoterpenoids
geranylacetone	10c	GC-O	magnolia, rose, fresh, floral, aldehydic, fruity, leaf, green	1549778	Acyclic monoterpenoids
linalool	16i	GC-MS		6549	Acyclic monoterpenoids
myrcene	16i	GC-MS		31253	Acyclic monoterpenoids

3-hydroxy-2-pentanone	10c	GC-MS	truffle, herbal, herb	62484	Acyloins
3-hydroxybutan-2-one	15h	DTD-GC-MS	butter, cream, milky, fatty, creamy, sweet, dairy, buttery	179	Acyloins
alanine	5d, 11d, 13d	NMR		5950	Alanine and derivatives
docosane	8h, 15h, 10c	GC-MS	alkane, waxy	12405	Alkanes
dodecane	10c	GC-MS	alkane	8182	Alkanes
eicosane	10c	GC-MS	alkane, waxy	8222	Alkanes
hentriacontane	15h	DTD-GC-MS		12410	Alkanes
heptacosane	8h, 15h, 10c	GC-MS		11636	Alkanes
heptadecane	10c	GC-MS	alkane	12398	Alkanes
heptane	10c	GC-MS	alkane, ethereal, sweet	8900	Alkanes
hexacosane	8h, 15h	DTD-GC-MS		12407	Alkanes
hexadecane	10c	GC-MS	alkane	11006	Alkanes
nonacosane	8h, 15h	DTD-GC-MS		12409	Alkanes
pentacosane	8h, 15h, 10c	GC-MS		12406	Alkanes
pentadecane	10c	GC-MS	alkane, waxy	12391	Alkanes
tetracosane	8h, 15h, 10c	GC-MS		12592	Alkanes
tetradecane	10c	GC-MS	alkane, waxy, mild	12389	Alkanes
tricosane	8h, 15h, 10c	GC-MS	alkane, waxy	12534	Alkanes
tridecane	10c	GC-MS	alkane	12388	Alkanes
undecane	10c	GC-MS	alkane	14257	Alkanes
2,4-dihydroxy-acetophenone	15h	DTD-GC-MS		6990	Alkyl-phenylketones

acetovanillone	1a, 2a, 15h, 10c	GC-MS, UHPLC-MS/MS, GC-O	vanilla, sweet, vanillin, faint	2214	Alkyl-phenylketones
o-acetyl-p-cresol	15h	DTD-GC-MS	floral, heavy, sweet, herbal	15068	Alkyl-phenylketones
propiophenone	10c	GC-MS	lilac, hawthorn	7148	Alkyl-phenylketones
threonine	5d, 11d, 13d	NMR		6288	Alpha amino acids
lactic acid	5d, 11d, 13d, 10c	GC-MS, NMR	acidic (if D or L)	612	Alpha hydroxy acids and derivatives
2,3-octanedione	10c	GC-MS	dill, buttery, broccoli, cooked	11449	Alpha-diketones
butane-2,3-dione	15h	DTD-GC-MS	butter, caramel, oily, creamy, sweet, pungent, strong	650	Alpha-diketones
hexane-2,3-dione	15h	DTD-GC-MS	butter, caramel, oily, fatty, sweet, creamy, fruity, phenolic, dry	19707	Alpha-diketones
pentane-2,3-dione	15h	DTD-GC-MS	butter, cream, caramel, sweet, pungent, creamy, nutty, cheese	11747	Alpha-diketones
3-methylpentanal	15h	DTD-GC-MS		27523	Alpha-hydrogen aldehydes
pyruvic alcohol	8h, 15h	DTD-GC-MS	caramellic, sweet, pungent, ethereal	8299	Alpha-hydroxy ketones
methyl pyruvate	10c	GC-MS		11748	Alpha-keto acids and derivatives
p-methylanisole	10c	GC-MS	powdery, cresol, naphthyl, camphoraceous, nutty, ylang, cedar	7731	Anisoles
arginine	1a, 2a, 5d, 11d, 13d	NMR, UHPLC-MS/MS	faint	6322	Arginine and derivatives
2-acetyl-5-methylthiophene	10c	GC-MS		83655	Aryl alkyl ketones
2-acetylpyrrole	10c	GC-MS, GC-O	nut, licorice, coumarin, bread, musty, nutty, walnut	14079	Aryl alkyl ketones

acetyl furan	8h	DTD-GC-MS	caramel, tobacco, balsamic, potato, coffee, sweet, cocoa, peanut, balsam, almond, beef	14505	Aryl alkyl ketones
2,5-furandicarboxaldehyde	10c	GC-MS		69980	Aryl-aldehydes
5-ethylfurfural	8h	DTD-GC-MS		89989	Aryl-aldehydes
5-hydroxymethylfurfural	1a, 2a, 8h, 10c, 15h	GC-MS, DTD-GC-MS, UHPLC-MS/MS	caramel, waxy, fatty, musty, cardboard	237332	Aryl-aldehydes
5-methylfurfural	8h, 15h, 10c	GC-MS	caramel, spice, burnt sugar, maple, almond	12097	Aryl-aldehydes
furfural	8h, 10c, 15h	DTD-GC-MS, GC-MS	fragrant, bread, woody, sweet, baked, almond	7362	Aryl-aldehydes
asparagine	5d, 11d, 13d	NMR		6267	Asparagine and derivatives
phenethanol	10c	GC-MS, GC-O	lilac, rose, rose water, honey, rose flower, floral, spice, bitter, rose dried	6054	Benzene and substituted derivatives
piperonal	9h, 10b	HPLC, DTD-GC-MS	coconut, heliotrope, powdery, sweet, vanilla, flower, violet, bitter	8438	Benzodioxoles
dihydroactinidiolide	10c	GC-MS	red fruit, coumarin, woody, musk, ripe apricot	27209	Benzofurans
dibutyl phthalate	10c	GC-MS	faint	3026	Benzoic acid esters
methyl benzoate	1a, 2a	UHPLC-MS/MS	prune, cananga, floral, wintergreen, lettuce, sweet, almond, herb, phenolic	7150	Benzoic acid esters
benzoic acid	10c	GC-MS	balsam, urine, faint	243	Benzoic acids
benzophenone	10c	GC-MS	peach, powdery, apricot, rose, balsam, geranium, metallic	3102	Benzophenones
benzaldehyde	15h, 10c	GC-MS	cherry, almond, sweet, burnt sugar, sharp, strong, bitter	240	Benzoyl derivatives

m-anisaldehyde	10b	HPLC	anise	11569	Benzoyl derivatives
p-anisaldehyde	10bc, 15h	GC-MS, HPLC, HPLC-DAD, DTD-GC-MS, GC-O	mimosa, hawthorn, cherry, powdery, bitter, vanilla, anise, hawthorne, chocolate, balsam, creamy, minty, berry, sweet, floral, mint, almond, cinnamon	31244	Benzoyl derivatives
p-anisyl alcohol	1g, 6g, 7g, 8h, 9h, 10bc, 11eg, 12g, 14g, 15h	GC-MS, HPLC, HPLC-DAD, DTD-GC-MS, GC-O	caramel, chocolate, powdery, vanilla, rose, lilac, floral, sweet, honey, hawthorn, hyacinth, flower	7738	Benzyl alcohols
p-hydroxybenzyl alcohol	1g, 4g, 5d, 6g, 7g, 9h, 11deg, 12g, 13d, 14g, 10c	GC-MS, HPLC, HPLC-DAD, DTD-GC-MS	coconut, bitter, sweet, fruity, almond	125	Benzyl alcohols
benzaldehyde dimethyl acetal	10c	GC-MS	wine, sharp, floral, hummus, fruity, almond, green	62375	Benzylethers
(4-methoxyphenyl) methyl tetradecanoate	15h	DTD-GC-MS		18004148	Benzyloxycarbonyls
(4-methoxyphenyl)methyl hexadecanoate	8h, 15h	DTD-GC-MS		10809570	Benzyloxycarbonyls
(4-methoxyphenyl)methyl octadec-9-enoate	15h	DTD-GC-MS		10739892	Benzyloxycarbonyls
(4-methoxyphenyl)methyl octadecanoate	15h	DTD-GC-MS		23119703	Benzyloxycarbonyls
anisyl acetate	15h, 10c	GC-MS, GC-O	powdery, coumarin, vanilla, creamy, plum, sweet, balsam, fruity, cherry, almond, tonka	7695	Benzyloxycarbonyls
anisyl formate	15h, 10c	GC-MS, GC-O	vanilla, anise, floral, fruity, seaweed	61054	Benzyloxycarbonyls
benzyl formate	10c	GC-MS	pineapple, apricot, floral, fruity, cranberry, almond, black tea, spicy	7708	Benzyloxycarbonyls

malic acid	5d, 11d, 13d	NMR		525	Beta hydroxy acids and derivatives
4-cyclopentene-1,3-dione	8h, 10c	GC-MS, DTD-GC-MS		70258	Beta-diketones
hentriacontene-2,4-dione	15h	DTD-GC-MS		56636502	Beta-diketones
heptacosene-2,4-dione	8h, 15h	DTD-GC-MS		53966535	Beta-diketones
nonacosene-2,4-dione	8h, 15h, 10c	GC-MS, DTD-GC-MS		16064344	Beta-diketones
nonadecane-2,4-dione	10c	GC-MS		567637	Beta-diketones
alpha-pinene oxide	16i	GC-MS		91508	Bicyclic monoterpenoids
I-R-alpha-pinene	16i	GC-MS		6654	Bicyclic monoterpenoids
(-)-beta-pinene	16i	GC-MS		440967	Bicyclic monoterpenoids
3,4-dimethyl-2,5-furandione	8h, 10c	GC-MS, DTD-GC-MS		13010	Butenolides
gibberellin A3	1a, 2a	UHPLC-MS/MS		6466	C19-gibberellin 6-carboxylic acids
butyl formate	10c	GC-MS	brandy, plum, fruity, rum	11614	Carboxylic acid esters
ethyl acetate	8h	DTD-GC-MS	pineapple, ethereal, sweet, anise, fruity, balsam, weedy, green	8857	Carboxylic acid esters
isopropyl acetate	8h	DTD-GC-MS	ethereal, chemical, banana, sweet, fruity	7915	Carboxylic acid esters
n-amyl formate	10c	GC-MS	ethereal, powerful, earthy, unripe banana, fruity, green	12529	Carboxylic acid esters
acetic acid	5d, 8h, 11d, 13d, 15h, 10c	GC-MS, NMR	sour, pungent, sharp, vinegar	176	Carboxylic acids
formic acid	8h, 15h, 10c	GC-MS	pungent, vinegar, formyl	284	Carboxylic acids
isobutyric acid	10c	GC-MS	rancid, butter, strawberry, cheese	6590	Carboxylic acids

propionic acid	10c	GC-MS	cheesy, soy, acidic, vinegar, rancid, pungent	1032	Carboxylic acids
catechin	1a, 2a	UHPLC-MS/MS	bitter	9064	Catechins
cinchonain 1a	1a, 2a	UHPLC-MS/MS		442675	Catechins
catechol	8h, 10c	GC-MS		289	Catechols
7-hydroxy-2-methyl-4-oxo-4H-1-benzopyran-5-acetic acid	1a, 2a	UHPLC-MS/MS		14429402	Chromones
cinnamaldehyde	1a, 2a	UHPLC-MS/MS	spice, warm, red hots, paint, clove, sweet, candy, cinnamon	637511	Cinnamaldehydes
methyl-3-phenylprop-2-enoate	8h, 10c, 15h	DTD-GC-MS, GC-MS	balsam, sweet, cherry, strawberry	637520	Cinnamic acid esters
coumaran	8h	DTD-GC-MS		10329	Coumarans
sibiricose A1	1a, 2a	UHPLC-MS/MS		6326016	Coumaric acids and derivatives
coumarin	10b	HPLC	sweet, new mown hay, green, tonka, bitter	323	Coumarins and derivatives
2-ethylcyclobutanol	8h	DTD-GC-MS		37109	Cyclic alcohols and derivatives
2-hydroxy-2-cyclopenten-1-one	10c	GC-MS		82674	Cyclic ketones
cyclohexanone	8h, 15h	DTD-GC-MS	minty, acetone	7967	Cyclic ketones
1,3,5-trimethyl-cyclohexane	8h	DTD-GC-MS		35364	Cycloalkanes
bromocyclohexane	10c	GC-MS		7960	Cyclohexyl halides
methyl hexyl ether	8h	DTD-GC-MS	painty, herbal, sweet, fruity, lavender	78484	Dialkyl ethers
diisopropyl disulfide	10c	GC-O	cabbage, sulfurous, onion, alliaceous, meaty	77932	Dialkyldisulfides

fumaric acid	5d, 11d, 13d	NMR		444972	Dicarboxylic acids and derivatives
2,3-dihydro-2,5-dimethylfuran	8h	DTD-GC-MS		86510	Dihydrofurans
3H-pyran-2,6-dione	8h, 15h	DTD-GC-MS		574367	Dihydropyranones
5,6-dihydromaltol	10c	GC-MS		6429306	Dihydropyranones
5-hydroxy-5,6-dihydromaltol	10c	GC-MS		119838	Dihydropyranones
1,4-dimethoxybenzene	10c	GC-MS	sweet, fennel, bitter, green, new mown hay	9016	Dimethoxybenzenes
veratraldehyde	10c	GC-MS	caramel, vanilla, creamy, sweet, woody, cherry, minty	8419	Dimethoxybenzenes
veratryl alcohol	15h, 10c	GC-MS, DTD-GC-MS		7118	Dimethoxybenzenes
2-butenal	10c	GC-MS		447466	Enals
4,5-epoxydec-2(trans)-enal	10c	GC-O		15825667	Enals
(5Z)-octa-1,5-dien-3-one	10c	GC-O		6429343	Enones
1-octen-3-one	10c	GC-O	herbal, earthy, metal, musty, mushroom, dirty	61346	Enones
3-octen-2-one	10c	GC-MS, GC-O	crushed bug, nut, herbal, earthy, hay, sweet, blueberry, mushroom, spicy	5363229	Enones
4-hexen-3-one	10c	GC-MS	ethereal, pungent, tropical, metallic, spicy, green	5365811	Enones
ethyl caprate	10c	GC-MS	apple, brandy, waxy, grape, oily, sweet, fruity, pear	8048	Fatty acid esters
ethyl caprylate	10c	GC-MS	apricot, fat, wine, waxy, banana, brandy, fruit, sweet, fruity, pear	7799	Fatty acid esters
ethyl oleate	10c	GC-MS		5363269	Fatty acid esters

ethyl palmitate	8h, 10c	GC-MS	mild, wax, milky, waxy, creamy, fruity, balsam	12366	Fatty acid esters
isopropyl myristate	10c	GC-MS	oily, fatty, faint, cinnamon	8042	Fatty acid esters
methyl cis- 12-octadecenoate	10c	GC-MS		5370350	Fatty acid esters
methyl palmitate	15h, 10c	GC-MS	oily, fatty, waxy	8181	Fatty acid methyl esters
1-dodecanol	10c	GC-MS	coconut, wax, fat, waxy, fatty, earthy, honey, soapy	8193	Fatty alcohols
1-hexanol	10c	GC-MS	oil, alcoholic, ethereal, resin, fusel, sweet, fruity, flower, green	8103	Fatty alcohols
1-octen-3-ol	10c	GC-MS	raw, fishy, oily, earthy, fungal, chicken, mushroom, green	18827	Fatty alcohols
heptacosan-1-ol	8h, 15h	DTD-GC-MS		74822	Fatty alcohols
hexacosan-1-ol	8h, 15h	DTD-GC-MS		68171	Fatty alcohols
octacosan-1-ol	15h	DTD-GC-MS		68406	Fatty alcohols
cis-9-octadecenal	10c	GC-MS		5364492	Fatty aldehydes
hexacosanal	8h	DTD-GC-MS		3084462	Fatty aldehydes
luteolin 7-glucoside-4'-(Z-2-methyl-2-butenate)	1a, 2a	UHPLC-MS/MS	sweet-like	44258141	Flavonoid-7-O-glycosides
wyerol	1a, 2a	UHPLC-MS/MS		131752561	Furanoid fatty acids
2-hydroxyfuraneol	10c	GC-MS		538757	Furanones
furaneol	8h, 15h	DTD-GC-MS	caramel, strawberry, grape, cotton, sweet, sugar, candy, almond	19309	Furanones
methyl furan-2-carboxylate	8h	DTD-GC-MS	tobacco, fungal, sweet, fruity, mushroom	11902	Furoic acid esters

3-pentyl-5-methyldihydro-2(3H)-furanone	10c	GC-MS		12393246	Gamma butyrolactones
a,d-dimethyltetronic acid	8h	DTD-GC-MS		228435	Gamma butyrolactones
γ -butyrolactone	8h, 15h	DTD-GC-MS	caramel, oily, fatty, sweet, creamy	7302	Gamma butyrolactones
γ -nonalactone	10c	GC-O	peach, coconut, waxy, oily, creamy, sweet, buttery	7710	Gamma butyrolactones
4-oxopentanoic acid	8h	DTD-GC-MS	caramel, acetoin, acidic, sweet, buttery	11579	Gamma-keto acids and derivatives
galactosylglycerol	1a, 2a	UHPLC-MS/MS	sweet	16048618	Glycosylglycerols
2-methyl-3-furanthiol	10c	GC-O	coconut, meat, sulfury, fishy, metallic, meaty	34286	Heteroaromatic compounds
2-pentylfuran	10c	GC-MS	butter, green bean, vegetable, earthy, beany, fruity, metallic, green	19602	Heteroaromatic compounds
3-furfurol	10c	GC-MS		20449	Heteroaromatic compounds
furfuryl alcohol	8h, 15h	DTD-GC-MS	coffee, alcoholic, bitter, musty, chemical, caramel, sweet, burnt, bread	7361	Heteroaromatic compounds
glucose (D-glucose, α -glucose, β -glucose)	1a, 2a, 5d, 11d, 13d	NMR, UHPLC-MS/MS	sweet	5793	Hexoses
L-histidine	1a, 2a	UHPLC-MS/MS	bitter	6274	Histidine and derivatives
glucosyringic acid	1a, 2a	UHPLC-MS/MS		10383888	Hydrolyzable tannins
newbouldioside A	1a, 2a	UHPLC-MS/MS		102180527	Hydrolyzable tannins
vanillic acid 4-beta-D-glucoside	1a, 2a	UHPLC-MS/MS		14132336	Hydrolyzable tannins
citramalic acid	1a, 2a	UHPLC-MS/MS		1081	Hydroxy fatty acids
ethyl vanillin	10b	HPLC	vanilla, caramel, sweet, creamy	8467	Hydroxybenzaldehydes

p-hydroxybenzaldehyde	1ag, 2a, 6g, 7g, 8h, 10bc, 11eg, 12g, 14g, 15h	GC-MS, HPLC, HPLC-DAD, DTD-GC-MS, UHPLC-MS/MS	woody, sweet, balsam, nutty, almond	126	Hydroxybenzaldehydes
p-hydroxybenzoic acid	1ag, 2a, 3g, 4g, 6g, 7g, 9h, 10b, 11eg, 12g, 14g, 15h	HPLC, HPLC-DAD, DTD-GC-MS, UHPLC-MS/MS	nutty, phenolic	135	Hydroxybenzoic acid derivatives
protocatechuic acid	1a, 2a	UHPLC-MS/MS	phenolic, balsamic, mild	72	Hydroxybenzoic acid derivatives
1-O-sinapoylglucose	1a, 2a	UHPLC-MS/MS		6168296	Hydroxycinnamic acid glycosides
p-hydroxycinnamic acid	1a, 2a	UHPLC-MS/MS	balsam, balsamic	637542	Hydroxycinnamic acids
plumieride	1a, 2a	UHPLC-MS/MS		72319	Iridoid O-glycosides
tectoridin	1a, 2a	UHPLC-MS/MS	sweet-like	5281810	Isoflavonoid O-glycosides
isoleucine	5d, 11d, 13d	NMR		6306	Isoleucine and derivatives
acetoin propyleneglycol acetal	10c	GC-MS		11971259	Ketals
2-heptanone	10c	GC-MS	coconut, soap, herbal, sweet, woody, fruity, spicy, cinnamon	8051	Ketones
2-nonanone	10c	GC-MS	soap, herbal, fresh, fishy, hot milk, earthy, sweet, soapy, weedy, green	13187	Ketones
3-methylpentan-2-one	15h	DTD-GC-MS		11262	Ketones
3-octanone	10c	GC-MS	butter, herbal, resin, fresh, mushroom, sweet, lavender, herb	246728	Ketones
pentan-2-one	15h	DTD-GC-MS	potato, alcohol, ether, ethereal, wine, banana, fishy, fruit, sweet, woody, fruity	7895	Ketones
leucine	5d, 11d, 13d	NMR		6106	Leucine and derivatives
9,12-octadecadienoic acid	8h, 15h	DTD-GC-MS		3931	Lineolic acids and derivatives

ethyl linoleate	10c	GC-MS		5282184	Lineolic acids and derivatives
ethyl linolenate	10c	GC-MS		5367460	Lineolic acids and derivatives
linoleic acid	10c	GC-MS	fatty, faint	5280450	Lineolic acids and derivatives
heptadecanoic acid	8h, 15h	DTD-GC-MS		10465	Long-chain fatty acids
hexadecanoic acid	8h, 15h, 10c	GC-MS	fatty, slightly waxy	985	Long-chain fatty acids
octadecanoic acid	8h, 15h	DTD-GC-MS	fatty, odorless, mild	5281	Long-chain fatty acids
oleic acid	1a, 2a, 8h, 15h	DTD-GC-MS, UHPLC-MS/MS	lard, fat, waxy, fatty, fried, faint	445639	Long-chain fatty acids
palmitoleic acid	15h	DTD-GC-MS		445638	Long-chain fatty acids
pentadecanoic acid	8h, 15h, 10c	GC-MS	waxy	13849	Long-chain fatty acids
tetradecanoic acid	8h, 15h, 10c	GC-MS	fatty, soapy, waxy, coconut	11005	Long-chain fatty acids
1-hexadecanol	10c	GC-MS	wax, floral, waxy, flower	2682	Long-chain fatty alcohols
1-octadecanol	10c	GC-MS	oil, bland	8221	Long-chain fatty alcohols
(2E,4E)-deca-2,4-dienal	10c	GC-MS, GC-O	citrus, orange, nut, wax, meat, fat, fresh, fatty, oily, cucumber, sweet, melon, pumpkin, fried, green	5283349	Medium-chain aldehydes
(2E,4Z)-deca-2,4-dienal	10c	GC-MS, GC-O	fat, waxy, fatty, geranium, fried, green	6427087	Medium-chain aldehydes
(2E,6E)-nona-2,6-dienal	10c	GC-O	citrus, fresh, green, melon, cucumber	636687	Medium-chain aldehydes
10-undecenal	10c	GC-O	citrus, rose, waxy, mandarin, fatty, aldehydic, soapy	8187	Medium-chain aldehydes
2,4-nonadienal	10c	GC-O		5283339	Medium-chain aldehydes
2-undecenal	10c	GC-O	citrus, soap, orange peel, fat, fresh, sweet, fruity, green	5283356	Medium-chain aldehydes

3,3-dimethylhexanal	8h	DTD-GC-MS		558458	Medium-chain aldehydes
cis-3-hexenal	10c	GC-O	apple, fatty, fruity, leaf, grassy, weedy, green	643941	Medium-chain aldehydes
cis-3-nonenal	10c	GC-MS, GC-O	cucumber	6431042	Medium-chain aldehydes
decanal	8h, 15h	DTD-GC-MS	citrus, soap, orange peel, tallow, waxy, floral, sweet, aldehydic	8175	Medium-chain aldehydes
heptanal	10c	GC-MS	citrus, ozone, fat, herbal, fresh, wine-lee, rancid, fatty, aldehydic, green	8130	Medium-chain aldehydes
hexanal	10c	GC-O	leafy, grass, sweaty, tallow, fat, fresh, fatty, fruity, aldehydic, green	6184	Medium-chain aldehydes
nonanal	8h, 15h, 10c	GC-MS, GC-O	citrus, lime, orange peel, rose, fat, green, fishy, waxy, fresh, fatty, peely, aldehydic, orris, grapefruit	31289	Medium-chain aldehydes
octanal	10c	GC-O	lemon, citrus, soap, orange peel, fat, waxy, fatty, aldehydic, green	454	Medium-chain aldehydes
trans-2-heptenal	10c	GC-MS, GC-O	soap, vegetable, fat, fresh, fatty, pungent, almond, green	5283316	Medium-chain aldehydes
trans-2-nonenal	10c	GC-MS	waxy, green, fatty, paper, melon, cucumber	5283335	Medium-chain aldehydes
trans-2-octenal	10c	GC-MS	nut, fat, herbal, fresh, green, fatty, banana, waxy, leaf, cucumber	5283324	Medium-chain aldehydes
decanoic acid	10c	GC-MS	sour, citrus, fat, rancid, fatty, unpleasant	2969	Medium-chain fatty acids
heptanoic acid	10c	GC-MS	sour, cheesy, sweat, rancid, cheese	8094	Medium-chain fatty acids
nonanoic acid	10c	GC-MS	cultured dairy, fat, waxy, green, dirty, cheese	8158	Medium-chain fatty acids

carvone	16i	GC-MS		7439	Menthane monoterpenoids
cis-beta-terpineol	16i	GC-MS		8748	Menthane monoterpenoids
cis-carveol	16i	GC-MS		330573	Menthane monoterpenoids
L-h-terpineol	16i	GC-MS		17100	Menthane monoterpenoids
limonene	10c	GC-MS	lemon, citrus, orange, herbal, woody, terpene, citric, camphor	22311	Menthane monoterpenoids
S-(-)-limonene	16i	GC-MS		439250	Menthane monoterpenoids
terpinolene	16i	GC-MS		11463	Menthane monoterpenoids
trans-dihydrocarvone	16i	GC-MS		6432474	Menthane monoterpenoids
α -terpineol	9h	DTD-GC-MS	oil, mint, citrus, lilac, floral, woody, anise, terpene, pine	442501	Menthane monoterpenoids
4-hydroxy-3- methoxyphenylacetone	10c	GC-MS		17262	Methoxyphenols
4-vinylguaiaicol	1a, 2a, 8h, 10c	GC-MS, UHPLC-MS/MS, GC-O	curry, smoky, clove, peanut, spicy	332	Methoxyphenols
creosol	8h, 10c, 15h	DTD-GC-MS, GC-MS, GC- O	phenolic, clove, leather, smoky, bacon, medical, mesquite, carnation, medicinal, bitter, vanilla, spice	7144	Methoxyphenols
guaiaicol	8h, 15h, 10c	GC-MS	spice, vanilla, smoky, sweet, woody, phenolic, medicine, medicinal, smoke	460	Methoxyphenols
homovanillic acid	10c	GC-MS		1738	Methoxyphenols
syringic aldehyde	15h	DTD-GC-MS	mild, sweet, woody, tonka, plastic	8655	Methoxyphenols
vanillin	1a, 2a, 6g, 7g, 8h, 9h, 10bc, 11eg, 14g, 15h	GC-MS, HPLC, HPLC- DAD, UHPLC-MS/MS, GC-O	vanilla, chocolate, sweet, creamy	1183	Methoxyphenols

vanillin 1,2-glyceryl acetal I	10c	GC-MS		82115125	Methoxyphenols
vanillyl acetone	15h	DTD-GC-MS	vanilla, clove, animal, sweet, ginger, woody, spicy, phenolic	31211	Methoxyphenols
vanillyl alcohol	1ag, 2a, 3g, 6g, 7g, 9h, 11eg, 12g, 14g, 15h	HPLC, HPLC-DAD, DTD-GC-MS, UHPLC-MS/MS	vanilla, sweet, anise, creamy, balsam, tonka, phenolic	62348	Methoxyphenols
methyl acetate	10c	GC-MS	sweet, bitter, ether, fruity	6584	Methyl esters
2-methylbutyric acid	10c	GC-MS	sour, sweat, acid, strawberry, roquefort cheese, pungent, cheese	8314	Methyl-branched fatty acids
isovaleric acid	10c	GC-MS, GC-O	sour, sweat, acid, stinky, sweaty, animal, rancid, tropical, feet, cheese	10430	Methyl-branched fatty acids
methyl vanillate	8h, 15h, 10c	GC-MS	butterscotch, caramel, warm, vanilla, spicy	19844	M-methoxybenzoic acids and derivatives
vanillic acid	1ag, 2a, 6g, 7g, 8h, 9h, 10b, 11eg, 12g, 15h	HPLC, HPLC-DAD, DTD-GC-MS, NMR, UHPLC-MS/MS	powdery, vanilla, bean, milky, sweet, creamy, dairy	8468	M-methoxybenzoic acids and derivatives
1-hydroxy-2-pentanone	10c	GC-MS		522131	Monosaccharides
fructose (α -fructose, β -fructose)	5d, 11d, 13d	NMR		5984	Monosaccharides
1,4-dimethylpiperazine	15h	DTD-GC-MS		7818	N-methylpiperazines
6-O-alpha-L-rhamnopyranosylcatalpol	1a, 2a	UHPLC-MS/MS		102252680	O-glycosyl compounds
rhodioloside	1a, 2a	UHPLC-MS/MS		159278	O-glycosyl compounds
sucrose	5d, 11d, 13d	NMR		5988	O-glycosyl compounds
verbasoside	1a, 2a	UHPLC-MS/MS		11754080	O-glycosyl compounds
anisyl salicylate	10c	GC-MS		3085862	O-Hydroxybenzoic acid esters
trans-carvone oxide	16i	GC-MS		11829800	Oxepanes

cis-carvone oxide	16i	GC-MS		11030188	Oxepanes
limonene oxide	16i	GC-MS		91496	Oxepanes
limonene oxide, cis	16i	GC-MS		6432449	Oxepanes
limonene oxide, trans	16i	GC-MS		8029780	Oxepanes
D-arabinose	1a, 2a	UHPLC-MS/MS	sweet	439195	Pentoses
methyl creosol	10c	GC-MS		75715	Phenol ethers
apiopaeonoside	1a, 2a	UHPLC-MS/MS		127509	Phenolic glycosides
arbutin	1a, 2a	UHPLC-MS/MS	bitter	440936	Phenolic glycosides
coelovirin A or B	1a, 2a	UHPLC-MS/MS		132472119	Phenolic glycosides
glucovanillin	1a, 2a	UHPLC-MS/MS	bitter	6452133	Phenolic glycosides
icariside D2	1a, 2a	UHPLC-MS/MS		10614148	Phenolic glycosides
paeonoside	1a, 2a	UHPLC-MS/MS		442924	Phenolic glycosides
pseudolaroside A	1a, 2a	UHPLC-MS/MS			Phenolic glycosides
phenylacetaldehyde	1a, 2a	UHPLC-MS/MS	hyacinth, honey, clover, sweet, hawthorne, cocoa, grapefruit, green, peanut, floral, bitter	998	Phenylacetaldehydes
phenylalanine	1a, 2a, 5d, 11d, 13d	NMR, UHPLC-MS/MS	bitter (L), sweet (D)	6140	Phenylalanine and derivatives
1-(4-methoxyphenyl)- 2-methyl-3-buten-1-ol	15h	DTD-GC-MS		586295	Phenylpropanes
propyl 4-hydroxybenzoate	8h	DTD-GC-MS	burnt, smoky, sweet, woody, hawthorn	7175	<i>p</i> -Hydroxybenzoic acid alkyl esters
isovanillic acid	10c	GC-MS		12575	<i>p</i> -methoxybenzoic acids and derivatives
p-anisic acid	8h, 10bc, 15h	GC-MS, HPLC, HPLC-DAD, DTD-GC-MS	putrid, sweet, faint, cadaverous	7478	<i>p</i> -methoxybenzoic acids and derivatives

1-butanol	10c	GC-MS	oil, vanilla, fruit, fusel, sweet, balsam, medicine, medicinal	263	Primary alcohols
1-pentanol	10c	GC-MS	oil, balsamic, vanilla, fusel, sweet, balsam	6276	Primary alcohols
ethanol	5d, 11d, 13d	NMR		702	Primary alcohols
neoheptanol	8h	DTD-GC-MS		16911	Primary alcohols
maltol	8h, 15h, 10c	GC-MS, GC-O	caramel, jam, bread, cotton, sweet, fruity, baked, candy	8369	Pyranones and derivatives
2-ethylpyrazine	10c	GC-MS	butter, peanut, musty, cocoa, nutty, wood, roasted, woody, bitter, peanut butter	26331	Pyrazines
2-acetyl-1-pyrroline	10c	GC-O	roast, nut, roasted, ham, sweet, nutty	522834	Pyrrolines
quinic acid	1a, 2a	UHPLC-MS/MS		6508	Quinic acids and derivatives
hexan-2-ol	15h	DTD-GC-MS	chemical, winey	12297	Secondary alcohols
trans-3-penten-2-ol	10c	GC-MS	vinyl, green	5366239	Secondary alcohols
alpha-cadinol	10c	GC-MS		10398656	Sesquiterpenoids
alpha-calacorene	10c	GC-MS		12302243	Sesquiterpenoids
alpha-d-curcumene	10c	GC-MS	herb	92139	Sesquiterpenoids
cadalene	10c	GC-MS		10225	Sesquiterpenoids
calamenene	10c	GC-MS		6429077	Sesquiterpenoids
delta-cadinene	10c	GC-MS	herbal, woody, thyme, wood, medicine, dry	441005	Sesquiterpenoids
epi-alpha-cadinol	10c	GC-MS	earthy, odorless, balsam	160799	Sesquiterpenoids
epi-alpha-muurolol	10c	GC-MS	spicy, herbal, weak spice, herb	3084331	Sesquiterpenoids

gamma-muurolene	10c	GC-MS		12313020	Sesquiterpenoids
hexahydrofarnesyl acetone	10c	GC-MS	jasmin, herbal, fat, oily, woody, celery	10408	Sesquiterpenoids
acetaldehyde	15h	DTD-GC-MS	ethereal, ether, whiskey, pungent, fruity, aldehydic	177	Short-chain aldehydes
4-methyl-2 oxovaleric acid	15h	DTD-GC-MS	fruity	70	Short-chain keto acids and derivatives
butanoic acid	10c	GC-MS	butter, sweat, acetic, sharp, rancid, fruit, cheese	264	Straight chain fatty acids
4-vinylphenol	1a, 2a, 10c	GC-MS, UHPLC-MS/MS	medical, chemical, almond shell, sweet, phenolic	62453	Styrenes
styrene	10c	GC-MS	balsamic, gasoline, floral, sweet, balsam, plastic	7501	Styrenes
2-methyl-3-buten-2-ol	10c	GC-MS	oily, earthy, herbal, herb	8257	Tertiary alcohols
tert-amyl alcohol	10c	GC-MS	pungent	6405	Tertiary alcohols
homocitric acid (in its lactone form)	5d, 13d	NMR		28371	Tricarboxylic acids and derivatives
squalene	8h, 15h, 10c	GC-MS,		638072	Triterpenoids
tyrosine	5d, 13d	NMR	sweet (D)	6057	Tyrosine and derivatives
tyrosol	1a, 2a	UHPLC-MS/MS	floral, sweet, fruity, mild	10393	Tyrosols
1-eicosene	10c	GC-MS		18936	Unsaturated aliphatic hydrocarbons
1-tricosene	8h, 15h	DTD-GC-MS		181154	Unsaturated aliphatic hydrocarbons
cis-9-tricosene	10c	GC-MS		5365075	Unsaturated aliphatic hydrocarbons

docosene	15h	DTD-GC-MS	74138	Unsaturated aliphatic hydrocarbons
hexacosene	15h	DTD-GC-MS	29303	Unsaturated aliphatic hydrocarbons
nonacos-1-ene	8h, 15h	DTD-GC-MS	156989	Unsaturated aliphatic hydrocarbons
pentacos-1-ene	15h	DTD-GC-MS	528972	Unsaturated aliphatic hydrocarbons
valine	5d, 11d, 13d	NMR	6287	Valine and derivatives
5,7-dihydroxy-2-(3-hydroxy-4-methoxy-phenyl)-3-methoxy-chromone	1a, 2a	UHPLC-MS/MS		
5-vinyl-guaiacol	10c	GC-O		
anisyl palmitate	8h, 15h, 10c	GC-MS		
dracunculifoside J	1a, 2a	UHPLC-MS/MS		
glucoside A	11d	NMR		
glucoside B	5d, 11d, 13d	NMR		
hydroxydi-hydromaltol	8h, 15h	DTD-GC-MS		
methyl-2-(4-hydroxyphenoxy) benzoate	15h	DTD-GC-MS		
p-hydroxybenzyl alcohol glucoside	5d, 11d, 13d	NMR		
γ -aminobutyric acid	5d, 11d, 13d	NMR		

1 = *V. bahiana*, 2 = *V. chamissonis*, 3 = *V. crenulata*, 4 = *V. imperialis*, 5 = *V. palmarum*, 6 = *V. planifolia* x *V. phaeantha*, 7 = *V. planifolia* x *V. pompona*, 8 = *V. pompona* (from Madagascar), 9 = *V. pompona* (origin unknown), 10 = *V. pompona* Shiede (cured), 11 = *V. pompona* subsp *grandiflora*, 12 = *V. pompona* subsp *pittieri*, 13 = *V. ribeiroi*, 14 = *V. sotoarenasii*, 15 = Wild Type (from Peru), 16 = *V. pompona* (flowers); a = [1], b = [2], c = [3], d = [4] *, e = [5], f = [6] *, g = [7], h = [8], i = [9] **. * Study based on leaves. ** Study based on flowers.

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