

Supplementary material

Integrated Strategy for Informative Profiling and Accurate Quantification of Key-Volatiles in Dried Fruits and Nuts: An Industrial Quality Control Perspective

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Supplementary Table S1: List of VOCs putatively identified in analyzed samples together with the CAS Registry Number, experimental I^r determined on a polar stationary phase (i.e., Heavy-Wax from Agilent Technologies – equivalent to Carbowax 20M), odor quality and presence in the specified sample.

Compound Name	CAS	I^r	Odor Quality	Walnut	Almond	Pineapple
Pentane	109-66-0	500		x	x	
Hexane	110-54-3	600		x	x	
Methanethiol	74-93-1	688	Boiled cabbage			x
Heptane	142-82-5	700		x		
2-Methyl-pentane	107-83-5	754		x	x	
Octane	111-65-9	800				x
Acetone	67-64-1	814				x
2-Octene	111-67-1	854		x	x	
Butanal	123-72-8	877	Chocolate, cocoa	x	x	
Ethyl acetate	141-78-6	899	Ethereal, fruity	x	x	x
2-Butanone	78-93-3	903	Ethereal, fruity	x	x	x
2-Methyl-butanal	96-17-3	915	Malty, dark chocolate	x	x	x
Isopropyl alcohol	67-63-0	920		x	x	
3-Methyl-butanal	590-86-3	927	Malty, dark chocolate	x	x	x
Ethanol	64-17-5	937		x	x	x
Propanoic acid, ethyl ester	105-37-3	951	Etherial, fruity, sweet			x
2-Ethyl-furan	3208-16-0	955	Chemical, beany	x		
Pentanal	110-62-3	973	Fermented, winey	x	x	x
Butyl ether	142-96-1	974		x		x
Dibutyl ether	142-96-1	974			x	
2,3-Butanedione	431-03-8	980	Sweet, buttery, creamy			x
2-Propenoic acid, ethyl ester	140-88-5	980				x
2-Pentanone	107-87-9	983	Fruity, banana	x		
Acetic acid, sec-butyl ester	105-46-4	988		x		
Butanoic acid, methyl ester	623-42-7	992	Fruity, banana, pineapple			x
Decane	124-18-5	1000		x	x	x
α -Pinene	80-56-8	1024	Herbal, woody	x	x	
β -Ocimene	13877-91-3	1031	Floral, green			x
Toluene	108-88-3	1034		x	x	x
Isovaleric acid, ethyl ester	108-64-5	1064				x
Dimethyl disulfide	624-92-0	1065	Sulfurous, cabbage, onion			x
Camphene	79-92-5	1068			x	

Butanoic acid, 2-methyl-, ethyl ester	7452-79-1	1073	Fruity, fresh, pineapple			x
Hexanal	66-25-1	1080	Green, cut grass	x	x	x
Pentanoic acid, methyl ester	624-24-8	1081	Apple, pineapple			x
Isobutyl alcohol	78-83-1	1086		x		
Isobutyl isobutyrate	97-85-8	1094		x	x	
2-Methyl-2-butenal	1115-11-3	1097	Cocoa, phenolic	x		
(E)-2-Pentenal	1576-86-9	1103	Green fruity apple	x		
β -Pinene	127-91-3	1113	Herbal, pine	x	x	
Isoamyl acetate	123-92-2	1115	Sweet, banana			x
Ethylbenzene	100-41-4	1116	Phenol, spice	x		
p-Xylene	106-42-3	1129		x	x	x
1-Butanol	71-36-3	1134	Fruity, balsamic	x	x	x
Pentanoic acid, ethyl ester	539-82-2	1134	Sweet, fruity, acidic			x
1-Methoxy-2-propanol	107-98-2	1135			x	
2-Butylfuran	4466-24-4	1138		x		
δ -3-Carene	13466-78-9	1144	Citrus, terpenic	x	x	x
Propanoic acid, 2-methyl-, butyl ester	97-87-0	1154	Fruity, tropical, banana			x
β -Myrcene	123-35-3	1161	Spicy, peppery		x	x
2-Methyl-2-pentenal	623-36-9	1177	Green, pungent	x		
Hexanoic acid, methyl ester	106-70-7	1184	Fruity, apricot			x
Heptanal	111-71-7	1185	Green, fresh	x	x	x
o-Xylene	95-47-6	1186	Geranium	x	x	
Dodecane	112-40-3	1200		x		x
Limonene	138-86-3	1205	Citrus	x	x	x
1,8-Cineole	470-82-6	1212		x	x	
β -Phellandrene	555-10-2	1215		x	x	
2-Ethyl-2-hexenal	123-05-7	1216		x	x	x
2-Ethyl-hexanal	123-05-7	1216		x	x	
Isoamyl alcohol	123-51-3	1217	Fruity banana	x	x	x
(E)-2-Hexenal	6728-26-3	1220	Green, leaf		x	x
Butanoic acid, butyl ester	109-21-7	1221	Sweet fruity ethereal	x	x	x
2-Hexenal	505-57-7	1225		x		
2-Pentyl-furan	3777-69-3	1230	Fruity, vegetable	x	x	
Hexanoic acid, ethyl ester	123-66-0	1232	Fruity, pineapple			x
1-Pentanol	71-41-0	1252	Fermented, fusel	x	x	
m-Cymene	535-77-3	1267			x	
p-Cymene	99-87-6	1272	Terpenic, wood	x	x	x
Isoamyl-2-methyl butyrate	27625-35-0	1274				x
Acetoin	513-86-0	1280	Buttery, creamy			x
2-Octanone	111-13-7	1287	Dairy, waxy	x		
α -Terpinolene	586-62-9	1288				x
Octanal	124-13-0	1289	Pungent, orange	x	x	x
3-Hexenoic acid, ethyl ester	2396-83-0	1290	Fruity, pineapple			x
1-Octen-3-one	4312-99-6	1305	Mushroom, metal		x	x
(E)-2-Heptenal	18829-55-5	1334	Green, sweet	x	x	x
6-Methyl-5-hepten-2-one	110-93-0	1337	Citrus, lemongrass	x	x	x

4-Hydroxy-4-methyl-2-pentanone	123-42-2	1352				x
1-Hexanol	111-27-3	1363	Herbal, ethereal	x	x	x
Dimethyl trisulfide	3658-80-8	1373				x
Nonanal	124-19-6	1398	Aldehydic, rose	x	x	x
2-Butoxy ethanol	111-76-2	1405		x	x	x
Butanoic acid, hexyl ester	2639-63-6	1406		x	x	
Amilfenol	80-46-6	1417				x
(E)-2-Octenal	2548-87-0	1434	Fatty, cucumber	x	x	x
Octanoic acid, ethyl ester	106-32-1	1440	Fruity, winey			x
Acetic acid	64-19-7	1449	Sour, vinegar	x	x	x
1-Octen-3-ol	3391-86-4	1451	Earthy, mushroom	x	x	
1-Heptanol	111-70-6	1465	Green, leafy	x	x	x
Methional	3268-49-3	1466	Cooked potatoes			x
4-Octenoic acid, ethyl ester	138234-61-4	1470				x
2H-Furan-3-one, 2,5-dimethyl	14400-67-0	1483				x
2-Ethyl-1-hexanol	104-76-7	1484	Citrus, fresh	x	x	
α -Copaene	3856-25-5	1488	Spicy, woody			x
α -Muurolene	10208-80-7	1497	Woody			x
Decanal	112-31-2	1498	Waxy, fatty, sweet	x	x	x
2-Acetylfuran	1192-62-7	1501				x
3-(Methylthio)propanoic acid methyl ester	13532-18-8	1510	Sulfurous, onion			x
Benzaldehyde	100-52-7	1520	Sweet, marzipan, fruity	x	x	x
α -Gurjunene	489-40-7	1520				x
Propanoic acid	79-09-4	1534				x
(E)-2-Nonenal	18829-56-6	1540	Green grass	x	x	x
1-Octanol	111-87-5	1556	Waxy, green	x	x	x
5-Methyl-2-furfural	620-02-0	1570				x
3-(Methylthio)propanoic acid ethyl ester	13327-56-5	1571	Sulfurous, onion			x
3(2H)-Furanone, 4-methoxy-2,5-dimethyl-	4077-47-8	1584	Strawberry			x
4-Terpineol	562-74-3	1598	Cooling, woody, earthy			x
2-Furoic acid, ethyl ester	614-99-3	1611				x
4-Decenoic acid, methyl ester	1191-02-2	1611				x
Butyrolactone	96-48-0	1617	Creamy, milky			x
2-(2-Ethoxyethoxy)-ethanol	111-90-0	1619		x	x	
Hexanoic acid, 3-hydroxy-, methyl ester	21188-58-9	1631	Pineapple, sweet			x
p-Menthan-3-ol	1490-04-6	1631		x		
Butyric acid	107-92-6	1637		x	x	
Decanoic acid, ethyl ester	110-38-3	1638	Sweet, apple			x
Benzeneacetaldehyde	122-78-1	1648	Green floral, hyacinth			x
2-Methylbutanoic acid	116-53-0	1657	Cheesy, pungent			x
4-Decenoic acid, ethyl ester	7367-84-2	1659				x
Furfuryl alcohol	98-00-0	1669	Sweet caramel, bread	x		x
α -Amorphene	20085-19-2	1692				x
γ -Caprolactone	695-06-7	1703	Sweet, creamy, lactonic			x

Germacrene D	23986-74-5	1705	Woody, spice			x
1-Propanol, 3-(methylthio)-	505-10-2	1720	Sulfureous, onion-like			x
β -Selinene	17066-67-0	1729				x
Nicotinic acid, methyl ester	93-60-7	1743				x
Naphthalene	91-20-3	1749		x	x	
3-methyl-2(5H)-furanone	22122-36-7	1750			x	
Methyl 5-acetoxylhexanoate	35234-22-1	1759				x
Benzeneacetic acid, ethyl ester	101-97-3	1779				x
δ -Valerolactone	542-28-9	1780		x		
δ -Pentalactone	542-28-9	1784			x	
2-(2-Butoxyethoxy)-ethanol	112-34-5	1796		x	x	
δ -Caprolactone	823-22-3	1818	Creamy fruity coconut			x
Dodecanoic acid, ethyl ester	106-33-2	1825	Waxy, fruity			x
Hexanoic acid	142-62-1	1839		x	x	x
Benzocic acid, butyl ester	136-60-7	1847		x	x	
Benzyl alcohol	100-51-6	1877	Floral, rose		x	x
2-Phenyl-2-butenal	4411-89-6	1911				x
Phenylethyl alcohol	60-12-8	1920	Sweet, floral, fresh			x
β -Ionone	79-77-6	1947	Violet-like, floral			x
δ -Octalactone	698-76-0	1965	Sweet, coconut, creamy			x
2-Acetylpyrrole	1072-83-9	1971	Pop-corn like			x
Cinnamaldehyde	104-55-2	2007	Pungent, cinnamon-like	x	x	x
Phenol	108-95-2	2008	Phenolic, plastic rubber	x	x	x
1H-Pyrrole-2-carboxaldehyde	1003-29-8	2032				x
Furaneol	3658-77-3	2037	Caramellic, candy			x
Octanoic acid	124-07-2	2046		x	x	x
p-Cresol	106-44-5	2089				x
4-Phenyl-3-buten-2-one	122-57-6	2103			x	x
Ethyl cinnamate	103-36-6	2108				x
2-Phenoxyethanol	122-99-6	2126		x	x	x
Eugenol	97-53-0	2167	Clove			x
Nonanoic acid	112-05-0	2173		x	x	x
Methyl dihydrojasmonate	24851-98-7	2237		x	x	x
4H-Pyran-4-one, 2,3-dihydro-						
3,5-dihydroxy-6-methyl-	28564-83-2	2274				x
Decanoic acid	334-48-5	2281		x	x	
p-Allylphenol	501-92-8	2329				x
Isophthalaldehyde	626-19-7	2341				x
Phthalide	87-41-2	2356			x	x
Furfural	84-66-2	2372	Bready, brown	x	x	
2H-Pyran-2,6(3H)-dione	5926-95-4	2427				x
Benzophenone	119-61-9	2462				x
Dodecanoic acid	143-07-7	2474			x	
Vanillin	121-33-5	2566	Vanilla-like, sweet			x
Tetradecanoic acid	544-63-8	2724		x	x	x
Pentadecanoic acid	1002-84-2	2822	Waxy, fatty	x	x	x
Squalene	111-02-4	2865		x	x	
Hexadecanoic acid	57-10-3	2923			x	x

Heptadecanoic acid	506-12-7	3027	x	x	
Octadecanoic acid	57-11-4	3120	x	x	x
Oleic acid	112-80-1	3173	x	x	x
