

Supplemental Information

Table S1. Annotated metabolites detected from GC-MS and HS-GC-MS analysis

Chemical Class	Chemical Subclass	Metabolite Name	Chemical Formula	Detection Method	RT (sec)	Average MW	Reported Sensory
Organooxygen	Alcohol and polyols	2,3-Butanediol	C ₄ H ₁₀ O ₂	GC-MS	213.38	90.121	butter, cream, fruity
Keto acid	Alpha-keto acid	Pyruvic acid	C ₃ H ₄ O ₃	GC-MS	220.62	88.0621	na
Hydroxy acid	Alpha hydroxy acid	Lactic acid	C ₃ H ₆ O ₃	GC-MS	226.7	90.0779	sour
Carboxylic acid	Amino acid	Alanine	C ₃ H ₇ NO ₂	GC-MS	248.32	89.0932	na
Carboxylic acid	Dicarboxylic acid	Oxalic acid	C ₂ H ₂ O ₄	GC-MS	268.31	90.0349	tart
Carboxylic acid	Amino acid	Isoleucine	C ₆ H ₁₃ NO ₂	GC-MS	275.56	131.1729	bitter
Carboxylic acid	Amino acid	Valine	C ₅ H ₁₁ NO ₂	GC-MS	308.31	117.1463	mildly bitter
Benzene	na	Phenylethyl alcohol	C ₈ H ₁₀ O	GC-MS	314.67	122.1644	rose, honey
Organic carbonic acid	Ureas	Urea	CH ₄ N ₂ O	GC-MS	316.13	60.0553	na
Organonitrogen	Amines	Ethanolamine	C ₂ H ₇ NO	GC-MS	335.79	61.0831	na
Organooxygen	Carbohydrate	Glycerol	C ₃ H ₈ O ₃	GC-MS	338.64	92.0938	sweet
Carboxylic acid	Amino acid	Leucine	C ₆ H ₁₃ NO ₂	GC-MS	349.56	131.1729	bitter
Carboxylic acid	Amino acid	Proline	C ₅ H ₉ NO ₂	GC-MS	352.35	115.1305	na
Carboxylic acid	Dicarboxylic acid	Succinic acid	C ₄ H ₆ O ₄	GC-MS	356.68	118.088	sour, umami

Carboxylic acid	Amino acid	Glycine	C2H5NO2	GC-MS	356.96	75.0666	sweet
Organooxygen	Carbohydrate	Glyceric acid	C3H6O4	GC-MS	368.01	106.0773	Na
Diazines	Pyrimidines	Uracil	C4H4N2O2	GC-MS	372.29	112.0868	na
Diazines	Pyrimidines	Thymine	C5H6N2O2	GC-MS	404.34	126.1133	na
Hydroxy acid	Beta hydroxy acid	Malic acid	C4H6O5	GC-MS	446.17	134.0874	tart, sour
Carboxylic acid	Amino acid	Pyroglutamic acid	C5H7NO3	GC-MS	464.1	129.114	umami
Carboxylic acid	Amino acid	4-amino-Butanoic acid	C4H9NO2	GC-MS	467.2	103.1198	na
Phenol	Tyrosols	Tyrosol	C8H10O2	GC-MS	485.22	138.1638	mild, sweet, floral
Hydroxy acid	Short-chain hydroxy acid	L-2-Hydroxyglutaric acid	C5H8O5	GC-MS	486.02	148.114	na
Carboxylic acid	Amino acid	Glutamic acid	C5H9NO4	GC-MS	505.87	147.1293	sour, mild umami
Carboxylic acid	Amino acid	Phenylalanine	C9H11NO2	GC-MS	513.14	165.1891	na
Carboxylic acid	Amino acid	Asparagine	C4H8N2O3	GC-MS	531.13	132.1179	na
Organooxygen	Carbohydrate	Unknown sugar 1	na	GC-MS	537.98	na	na
Organooxygen	Carbohydrate	Xylitol	C5H12O5	GC-MS	551.75	152.1458	sweet
Organooxygen	Carbohydrate	Arabitol	C5H12O5	GC-MS	556.91	152.1458	sweet
Organonitrogen	Amines	Putrescine	C4H12N2	GC-MS	562.21	88.1515	foul odor, rotting
Glycerophospholipid	Glycerophosphate	Glycerol-3-phosphate	C3H9O6P	GC-MS	571.95	172.0737	na
na	na	Known unknown 3	na	GC-MS	575.86	na	na

na	na	Sugar acid 1	na	GC-MS	584.18	na	na
Carboxylic acid	Tricarboxylic acid	Citric acid	C6H8O7	GC-MS	595.87	192.1235	tart, sour
na	na	Known unknown 5	na	GC-MS	614.17	na	na
Organooxygen	Carbohydrate	Fructose	C6H12O6	GC-MS	621.28	180.1559	sweet, fruity aroma
Organooxygen	Carbohydrate	Unknown sugar 2	na	GC-MS	625.24	na	na
Organooxygen	Carbohydrate	Glucose	C6H12O6	GC-MS	632.28	180.1559	sweet
Organooxygen	Carbohydrate	Unknown sugar 3	na	GC-MS	639.83	na	na
Carboxylic acid	Amino acid	Tyrosine	C9H11NO3	GC-MS	642.55	181.1885	bitter
Organooxygen	Carbohydrate	Mannitol	C6H14O6	GC-MS	645.49	182.1718	sweet
Organooxygen	Alcohol	myo-Inositol	C6H12O6	GC-MS	706.02	180.1559	neutral
Organooxygen	Carbohydrate	Sucrose	C12H22O11	GC-MS	917.23	342.1162	sweet
Organooxygen	Carbohydrate	Maltose	C12H22O11	GC-MS	925.45	342.2965	sweet
Organooxygen	Carbohydrate	Unknown sugar 4	na	GC-MS	936.9	na	na
Organooxygen	Carbohydrate	Maltotriose	C18H32O16	GC-MS	1138.5	504.4371	sweet
Carboxylic acid	Carboxylic acid ester	Ethyl Acetate	C4H8O2	HS-GC-MS	462.74	88.1051	nail polish remover, solvent, fruity, sweet
Organooxygen	Alcohol	Isobutanol	C4H10O	HS-GC-MS	559.57	74.1216	malty, solvent
Carboxylic acid	Carboxylic acid derivative	Ethyl Propanoate	C5H10O2	HS-GC-MS	675.42	102.1317	fruity, estery
Organooxygen	Alcohol and polyols	Isoamyl Alcohol	C5H12O	HS-GC-MS	710.43	88.1482	alcohol, banana, sweet, fusel

Organoxygen	Alcohol	Pentanol	C5H12O	HS-GC-MS	797.43	88.1482	sweet, balsamic, fusel
Lipid	Fatty acid ester	Ethyl Butyrate	C6H12O2	HS-GC-MS	869.63	116.1583	pineapple, mango, papaya, butter, sweet
Carboxylic acid	Carboxylic acid derivative	2-Pentyl Acetate	C7H14O2	HS-GC-MS	999.81	130.1849	citrus, spicy, ripe fruit, apple
Carboxylic acid	Carboxylic acid derivative	Isoamyl Acetate	C7H14O2	HS-GC-MS	1027.46	130.1849	banana
Benzene	Styene	Styrene	C8H8	HS-GC-MS	1066.59	104.1491	plastic, sweet, floral, balsamic
Carboxylic acid	Carboxylic acid ester	Isobutyl Isobutyrate	C8H16O2	HS-GC-MS	1098.6	144.2114	grape skin, pineapple, tropical
Lipid	Monoterpenoid	β -pinene	C10H16	HS-GC-MS	1196.12	136.234	woody, green, resinous, dry
Lipid	Monoterpenoid	β -myrcene	C10H16	HS-GC-MS	1208.84	136.238	peppery, spicy, citrus, resinous, piney, lemon, woody
Lipid	Fatty acid ester	Ethyl Hexanoate	C8H16O2	HS-GC-MS	1237.21	144.2114	apple, anise seed, citrus, solvent
Lipid	Fatty acid ester	Ethyl 5-methylhexanoate	C9H18O2	HS-GC-MS	1245.62	158.238	na
Lipid	Fatty acid ester	Isoamyl Butyrate	C9H18O2	HS-GC-MS	1270.74	158.238	fruity, green, apricot, pear, banana
Lipid	Fatty acid ester	2-Methylbutyl butyrate	C9H18O2	HS-GC-MS	1282.7	158.238	fruity, pear, apricot, tropical, spicy, apple
Lipid	Monoterpenoid	Pinocarvone	C10H14O	HS-GC-MS	1423.59	150.2176	minty
Lipid	Monoterpenoid	Linalool	C10H18O	HS-GC-MS	1447.21	154.253	citrus, floral, rose, woody
Benzene	na	2-Phenylethanol	C8H10O	HS-GC-MS	1522.74	122.1644	alcohol, floral, honey, sweet rose
Lipid	Fatty acid ester	Ethyl Octanoate	C10H20O2	HS-GC-MS	1570.01	172.2646	apple, sweet, fruity, sour apple
Benzene	na	Phenethyl Acetate	C10H12O2	HS-GC-MS	1707.9	164.2011	honey, floral, cabbage, fruity, rose, apply, sweet

Organooxygen	Carbonyl	2-Undecanone	C ₁₁ H ₂₂ O	HS-GC-MS	1743.71	170.2918	varnish, bitter, green plants, geranium, fruity, citrus
Lipid	Monoterpenoid	Methyl Geranate	C ₁₁ H ₁₈ O ₂	HS-GC-MS	1765.54	182.263	waxy, green, fruity, floral, citrus
Lipid	Fatty acid ester	Ethyl Decanoate	C ₁₂ H ₂₄ O ₂	HS-GC-MS	1849.09	200.3178	caprylic, soapy, estery
Lipid	Sesquiterpenoid	Humulene	C ₁₅ H ₂₄	HS-GC-MS	1961.06	204.357	spicy, herbal, grassy, woody, clove
Lipid	Sesquiterpenoid	α -calacorene	C ₁₅ H ₂₀	HS-GC-MS	2068.97	200.3196	citrus, spicy, woody
Lipid	Fatty acid ester	Ethyl Dodecanoate	C ₁₄ H ₂₈ O ₂	HS-GC-MS	2102.07	228.3709	caprylic, soapy, estery

Table S2. Linear models of metabolite abundance over aging time.

Metabolite	R ² _a	IPA			AA		
		Baseline _b	OT _c Bottle	OT Can	Baseline	OT Bottle	OT Can
Glycine	0.950	0.58	No	No	<0.001	No	No
Tyrosine	0.990	0.24	No	No	<0.001	No	Yes
Asparagine	0.940	0.74	No	No	<0.001	No	No
Ethyl acetate	0.428 _d	0.56	No	No	0.21	No	Yes
Isobutyl isobutyrate	0.998	0.96	No	No	<0.001	No	No
Ethyl decanoate	0.977	0.88	No	No	<0.001	Yes	Yes
Ethyl octanoate	0.170	0.04	Yes	No	0.06	No	Yes
Ethyl hexanoate	0.687	0.20	Yes	No	0.74	No	Yes
2-Methylbutyl butyrate	0.997	0.62	No	No	<0.001	No	Yes
Pinocarvone	0.994	0.001	No	Yes	0.33	No	No
β-myrcene	0.994	0.05	Yes	Yes	0.76	Yes	Yes
β-pinene	0.966	0.06	No	No	0.41	No	No
Humulene	0.980	<0.001	Yes	Yes	<0.001	Yes	Yes
α-calacorene	0.964	0.02	Yes	Yes	0.47	Yes	Yes
Isobutanol	0.794	0.02	No	No	0.43	No	No
myo-Inositol	0.954	0.14	No	No	<0.001	No	Yes
2-Undecanone	0.991	0.16	Yes	Yes	0.50	No	No

(a) Demonstrates fitness of a linear model after necessary transformations to meet assumptions of normality

(b) *P*-values produced from the *emmeans()* function in R Programming to determine significance in relative abundance in week 0 samples between cans and bottles within each style

(c) Over Time (OT) demonstrates if a linear model is significantly changing over the 24-week aging period with a 95% confidence interval in each style and package type, where YES indicates statistical significance and NO indicates no statistical significance.

Analysis performed by the *emtrends()* function in R Programming.

(d) Metabolites with R² values < 0.900 are highlighted in red and considered as an unacceptable model fit.