Supporting Information

Minor, Non-Terpenoid Volatile Compounds Drive the Aroma Differences of Exotic *Cannabis*

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Table S1. Calibration curve data of analytes used to quantify aroma compounds in samples.

Compound name	^1t_R	^2t_R	slope	intercept	R^2	LOD* (µg/mL)	LOQ* (µg/mL)
Isobutyl n-butyrate	7.36	3.409	104843.3	-21892.8	0.9992	0.0116	0.0353
Isopropyl isobutyrate	8.55	3.602	94355.96	645183.8	0.9996	0.1803	0.5463
Ethyl n-butyrate	8.6	3.682	98561.92	12737.43	0.9990	0.0458	0.1387
Hexanal	8.9	4.067	116431.3	-72409.3	0.9996	0.0097	0.0294
Prenylthiol	9.4	4.11	30133.63	-7477.28	0.9993	0.0339	0.1026
Ethyl 2-methylbutyrate	10.4	3.868	68955.37	-4962.76	0.9989	0.0407	0.1232
Methyl senecioate	10.612	4.603	109911.6	-108898	0.9979	0.0047	0.0143
Ethyl isovalerate	10.75	3.772	136376	-72457.6	0.9988	0.0142	0.0431
2-Heptanone	12.55	4.404	136393.7	-161264	0.9963	0.0021	0.0063
n-Propyl n-butyrate	12.675	3.715	148470.2	-51831.5	0.9994	0.0069	0.0208
Isobutyl isobutyrate	13.45	3.326	184242.7	-15825	0.9996	0.0093	0.0281
Methyl hexanoate	14	3.949	50196.87	-33436.4	0.9980	0.0137	0.0415
Ethyl senecioate	14.136	4.417	69009.72	-32693.6	0.9982	0.0082	0.0249
α-Pinene	14.3	3.368	155145.7	53187.64	0.9997	0.0098	0.0298
Camphene	15.1	3.476	183041.7	26154.73	0.9990	0.0113	0.0342
Ethyl isobutyrate	15.4	3.602	77149.87	-6612.37	0.9980	0.0659	0.1997
Isopropyl senecioate	15.84	4.024	202562.4	-298181	0.9970	0.0021	0.0065
Sabinene	16.2	3.549	154734.7	-18785.4	0.9999	0.0326	0.0986
β-Pinene	16.567	3.352	193682.3	92735.92	0.9995	0.0165	0.0500
β-Myrcene	17.044	3.435	161938.9	-61971.4	0.9999	0.007	0.0211
Sulcatone	17.16	4.941	255317.9	-173685	0.9956	0.0017	0.0053
Ethyl hexanoate	17.667	3.88	138166.3	-168236	0.9954	0.0022	0.0067
n-Octanal	18.017	4.564	69162.42	-55293.9	0.9994	0.0165	0.0500
3-Carene	18.1	3.325	148849.7	-4798.95	0.9993	0.0109	0.0331
n-Hexyl acetate	18.313	4.01	86359.44	-100823	0.9986	0.0079	0.0239
α-Terpinene	18.52	3.369	174888.7	-28847.7	0.9999	0.0093	0.0282
n-Propyl senecioate	18.9	4.259	206547.8	-411672	0.9897	0.0068	0.0206
p-Cymene	18.975	3.799	219554.5	-31212.5	0.9995	0.0054	0.0165
D-Limonene	19.271	3.406	200640.9	-38806.3	0.9998	0.0072	0.0219
trans-β-Ocimene	19.9	3.52	105861.6	-24901	0.9997	0.0077	0.0233
Melonal	20.433	4.289	273418.5	-69506.5	0.9994	0.0058	0.0177
γ-Terpinene	20.65	3.486	188307.3	-1861.87	0.9999	0.0037	0.0113
trans-Sabinene hydrate	21.356	4.987	152614.1	-34807.7	0.9999	0.004	0.0121
1-Octanol	21.55	0.667	154888.7	-249689	0.9965	0.0031	0.0095
Terpinolene	22	3.428	168142.1	15111.61	0.9997	0.0033	0.0099
n-Propyl hexanoate	22.25	3.578	82633.57	-46907.6	0.9986	0.0042	0.0127
Linalool	22.646	5.34	146094.5	-83241.3	0.9999	0.0039	0.0119
Nonanal	22.95	3.816	86767.59	-93041.5	0.9954	0.0118	0.0358
n-Heptyl acetate	23.05	3.534	110676.3	-23921.2	0.9986	0.0156	0.0472
n-Butyl senecioate	23.533	3.774	213179.1	-430589	0.9869	0.0026	0.0078
Methyl octanoate	23.56	3.456	110129.9	5982.239	0.9979	0.0059	0.0178
endo-Fenchol	23.625	5.139	162685.9	23694.49	0.9997	0.0044	0.0135

3-mercaptohexanol	24.2	4.053	63567.39	-136215	0.9949	0.0088	0.0266
n-Hexyl isobutyrate	24.35	3.11	89162.5	-59901.3	0.9959	0.03	0.0908
Isobutyl hexanoate	24.56	3.285	181094.8	105988.1	0.9977	0.0033	0.0100
Isopulegol	24.758	4.512	150051.1	-162444	0.9993	0.0034	0.0103
cis-3-Hexenyl n-butyrate	25.667	3.381	109224.4	-47179.6	0.9986	0.0088	0.0268
endo-Borneol	25.7	5.278	182279	-26768.9	0.9999	0.0012	0.0037
Isoamyl senecioate	25.8	3.529	264590.5	-376932	0.9947	0.0052	0.0158
n-Hexyl n-butyrate	26	3.175	226713	-85640.3	0.9994	0.0126	0.0383
Cherry propanol	26.336	1.203	160735.2	-91441.7	0.9986	0.0047	0.0142
α-Terpineol	26.463	5.034	207902.6	-43400.1	0.9999	0.0017	0.0051
n-Octyl acetate	26.633	3.341	129286.2	-34566.5	0.9997	0.0033	0.0100
Citronellol	27.243	4.987	253917.3	-158442	0.9961	0.0039	0.0117
Hexyl 2-methylbutyrate	27.35	3.116	157438.2	-29225.6	0.9994	0.01	0.0304
α-Citral	27.767	4.103	48631.74	-31298.2	0.9999	0.0195	0.0590
(+)-Pulegone	27.85	3.829	170940.9	-126487	0.9997	0.0076	0.0231
Isoamyl hexanoate	27.88	3.059	141237.9	64502.48	0.9992	0.0066	0.0199
Geraniol	27.985	5.469	173983.4	-189535	0.9991	0.0043	0.0129
3-mercaptohexyl acetate	28.033	4.297	131254.4	-107211	0.9940	0.0116	0.0350
1-Decanol	28.55	4.321	308496.8	-200553	0.9961	0.0024	0.0072
n-Heptyl n-butyrate	28.967	3.018	158113.7	-42012.5	0.9995	0.0057	0.0172
n-hexyl senecioate	29.7	3.068	225563.3	-321843	0.9883	0.0052	0.0157
Indole	29.814	4.272	80542.46	-134212	0.9962	0.0074	0.0225
Citronellol acetate	30.3	3.093	170720.1	-11643.9	0.9979	0.0066	0.0199
Phenylethyl propionate	30.586	4.006	157760.6	-76222.9	0.9995	0.0076	0.0232
Methyl anthranilate	30.744	1.601	45264.29	-32786	0.9964	0.012	0.0364
n-Hexyl hexanoate	31	2.813	283314.2	-3193.27	0.9997	0.0133	0.0402
Phenylethyl isobutyrate	31.54	3.698	174042.4	2821.69	0.9994	0.0033	0.0099
n-Decyl acetate	31.6	2.988	175028.2	-35228.2	0.9994	0.0106	0.0320
Skatole	31.982	0.702	169433.9	-109860	0.9974	0.0015	0.0045
Methyl N-methylanthranilate	32.129	5.005	136819.2	-42788	0.9990	0.0028	0.0084
Caryophyllene	32.175	2.951	255406.7	-6229.36	0.9997	0.0116	0.0353
3-mercaptohexyl butyrate	32.2	3.624	156754.5	-94576	0.9967	0.0087	0.0264
Ethyl anthranilate	32.308	1.195	214174.9	-180086	0.9962	0.0018	0.0055
Phenylethyl n-butyrate	32.5	4.027	172406	-50376.5	0.9998	0.0042	0.0129
Humulene	32.933	3.016	212837.4	-3795.57	0.9997	0.0147	0.0445
6-amyl-α-pyrone	33.15	5.61	276587.9	-175985	0.9972	0.0022	0.0065
cis-Nerolidol	34.34	4.035	182571.4	-32215	0.9998	0.0035	0.0105
trans-Nerolidol	35.1	3.884	207804.5	-110737	0.9998	0.0074	0.0224
(-)-Guaiol	36.35	4.333	255159	-15171.8	.9999	0.0259	0.0784
α-Bisabolol	38.8	4.903	255480.8	-39859	0.9997	0.0023	0.007

*LOD and LOQ are defined by the equations: $LOD = \frac{3.3 \cdot \sigma}{S}$; $LOQ = \frac{10 \cdot \sigma}{S}$ where σ is the standard deviation of the region in the chromatogram for each analyte from seven hexane blanks and S is the slope of the curve.

Table S2. Summary of Sensory Panel Exotic Score data.

Variety name	Panelist 1	Panelist 2	Panelist 3	Panelist 4	Panelist 5	Panelist 6	Panelist 7	exotic score
Grape Pie x Do-Si-Do	98	90	80	95	70	80	99	87.4(11)
Juice Man	89	95	70	95	85	80	96	87.1(9.6)
Papaya Peach	94	95	80	100	50	90	95	86.3(17.2)
Cake Crasher	77	70	90	85	95	70	99	83.7(11.7)
Starburst 36 #1	60	85	85	90	80	80	92	81.7(10.6)
Upsidedown frown #5	85	85	80	75	70	75	95	80.7(8.4)
Motor Nana	91	85	50	80	75	85	96	80.3(15)
Garlic Cocktail #7	70	75	75	75	90	80	96	80.1(9.4)
Zkittlez 710	83	65	80	80	86	75	92	80.1(8.6)
Banana Scream	90	90	75	75	50	85	93	79.7(15)
Bubblegum Zkittlez	91	70	85	95	30	85	83	77(22.1)
TK x Butterscotch	88	80	90	70	50	60	96	76.3(16.9)
Purple Churro	96	80	60	70	40	80	94	74.3(19.7)
Pure Guava	68	75	70	95	90	60	60	74(13.8)
Rainbow 2.0	92	70	40	70	40	90	99	71.6(24.2)
Fruity Pebbles	65	80	80	50	90	35	100	71.4(22.9)
OPP x Smarties	89	60	50	75	70	80	72	70.9(12.8)
Gorilla Glue	75	60	75	40	75	60	71	65.1(13)
Bubba Kush	43	60	70	75	80	30	77	62.1(19)
Bacio Gelato	42	40	25	50	55	50	40	43.1(9.9)
MAC 1	15	10	45	30	65	65	45	39.3(22.1)
Gelato 33	37	25	15	45	25	40	55	34.6(13.7)
Kimbo Kush	15	35	55	45	40	30	18	34(14.3)
Lucky Charms	15	15	30	65	50	35	5	30.7(21.3)
Pie Hoe	22	15	35	20	30	35	20	25.3(8)
Cookies and Cream	1	20	35	0	25	25	2	15.4(14.2)
GMO Cookies	3	10	0	10	0	5	12	5.7(5)
OG	10	0	5	5	1	0	0	3(3.8)
710 chem	0	2	5	0	1	0	5	1.9(2.3)
GMO	0	10	0	0	0	0	2	1.7(3.7)

Table S3. Sensory Descriptors obtained from sensory panel for all samples.

Descriptor	Classification
fuel	Prototypical
gas	Prototypical
burnt	Prototypical
lemon	Prototypical
lime	Prototypical
earth	Prototypical
musky	Prototypical
wood	Prototypical
bright	Prototypical
ethereal	Prototypical
citrus	Prototypical
camphoric	Prototypical
mentholic	Prototypical
floral	Prototypical
grass	Prototypical
green	Prototypical
herbal	Prototypical
pine	Prototypical
plant	Prototypical
vegetables	Prototypical
pungent	Prototypical
sulfuric	Prototypical
anisic	Prototypical
pepper	Prototypical
rosemary	Prototypical
spicy	Prototypical
bitter	Prototypical
fatty	Prototypical
fresh	Prototypical
sharp	Prototypical
sour	Prototypical
terpenic	Prototypical

waxy	Prototypical
banana	sweet exotic
berry	sweet exotic
blueberry	sweet exotic
grape	sweet exotic
grapefruit	sweet exotic
guava	sweet exotic
jam	sweet exotic
lychee	sweet exotic
mango	sweet exotic
papaya	sweet exotic
peach	sweet exotic
pineapple	sweet exotic
raspberry	sweet exotic
red fruit	sweet exotic
ripe	sweet exotic
stone fruit	sweet exotic
strawberry	sweet exotic
tangerine	sweet exotic
tropical	sweet exotic
yellow fruit	sweet exotic
cherry	sweet exotic
coconut	sweet exotic
dark berry	sweet exotic
fruit	sweet exotic
melon	sweet exotic
sweet	sweet exotic
tart	sweet exotic
bready	sweet exotic
cereal	sweet exotic
butterscotch	sweet exotic
honey	sweet exotic
bubblegum	sweet exotic
candy	sweet exotic
chocolate	sweet exotic
cream	sweet exotic
alliaceous	savory exotic
astringent	savory exotic
cheese	savory exotic
chemical	savory exotic
moth balls	savory exotic
savory	savory exotic

Table S4. Sensory intensity descriptors.

Intensity descriptor	**Multiplier**
negligible	0.5
somewhat	0.75
more	1.25
Strong	1.5
overwhelmingly	2

Table S5. Tabulated sensory panel results (1/5).

Variety	fuel	gas	lemon	lime	earth	musky	wood	bright	ethereal	citrus	camphoric	mentholic	floral	grass	green
grape pie x do-si-do	0	3	0	0	3	0	2	0	0	0	0	0	0	0	0
juice man	0	2	0	0	1.5	0	2	0	0	2	0	2	3	0	0
papaya peach	0	1	1	0	0	0	1	1	0	3	0	0	1	0	0
cake crasher	0	1	0	0	0	1	0	0	0	1	0	0	0	0	0
starburst 36 #1	0	1	0	0	0	2	0	0	0	3	0	0	0	0	0
upsidedown frown #5	0	0	0	0	1	1	0	0	0	4	0	0	0	0	1
motor nana	0	6	0	0	3.5	0	1	0	0	2	0	0	1	0	0.75
garlic cocktail #7	0	1	0	2	1	1	0	0	0	6.75	0	0	0	0	0
zkittlez 710	0	4.5	1	1	0	0	0	0	0	2	0	0	1	0	0
banana scream	0	2	0	0	3	0	4	0	1	3	0	1	0	0	1
bubblegum zkittlez	0	2	0	0	0	0	0	0	0	3	0.75	0	4	0	1
tk x butterscotch	0	1	0	0	1	1	0	0	0	0	0	0	1	2	1
purple churro	1	6	0	0	7	1	3	0	0	1	0	0	2	0	0
pure guava	0	0	0	0	0	0	1	1	0	3.5	0	0	0	0	0.75
rainbow 2.0	0	5	1	1	1.5	0	1	0	0	0	0	0	2	0	0
fruity pebbles	0	0	0	0	1	1	0	0	0	0	0	0	0	0	0
opp x smarties	0	3	0	0	1	0	1	0	0	3	0	1	0	0	1
gorilla glue	0	2	2	1	1	0	0	0	0	5.75	0	0	0	0	0
bubba kush	0	0.75	0	0	0	1	0	0	0	0	0	0	0	0	0
trainwreck	0	0	6	1	0	0	4	1	0	4	1	0	1	0	1
bacio gelato	0	10	0	0	3.5	2	1	1	1	1	5	0	1	0	0
mac 1	0	2	0	0	0	1	0	0	1	2	1	0	0	0	0
gelato 33	2	5	1	1	1	0	0	1	0	3.75	3	1	0	0	0
kimbo kush	0	5	0	0	0	2	1	0	0	0.75	0	0	0	1	0
lucky charms	0	0	0	0	2	0	0	0	0	2	2	0	0	1	0
pie hoe	0	2.75	0	0	2.5	1	1	0	0	1	0	0	0	3	2
cookies and cream	0	0	0	0	0	0	0.75	0	0	1.75	1	0	1.5	1	2
gmo cookies	0	4	0	0	1	0	0	0	0	0	3	1	0	0	0
og	0	3	3	0	4	2	0	0	0	2	1	1	0	0	0
710 chem	0	9.5	0	0	4.5	0	2	0	0	2	0	0	0	0	0
gmo	0	2.5	0	0	1	1	0	0	0	0	0	0	0	0	0

Table S6. Tabulated sensory panel results (2/5).

Variety	herbal	pine	plant	vegetables	sulfuric	pepper	rosemary	spicy	bitter	fatty	fresh	sharp	sour
grape pie x do-si-do	0	0	0	0	1	0	0	0	0	0	0	0	0
juice man	1	0	0	0	0	0	0	0.75	0	1	0	0	0
papaya peach	0	1	0	0	0	0	0	1	0	1	0	0	1
cake crasher	1	0	0	0	0	0	0	0	0	0	0	0	0
starburst 36 #1	0	1	0	0	0	0	0	0.75	0	0	0	0	0
upsidedown frown #5	0	1	0	0	0	0	0	0	0	0	0	0	0
motor nana	1	0	0	0	0	0	0	1	0	0	0	0	0
garlic cocktail #7	0	0	0	0	1	0	0	1	0	2	0	0	0
zkittlez 710	0	0	0	0	0	0	0	0	0	0	0	0	0
banana scream	1	1	0	0	0	0	0	1	0	0	0	0	0
bubblegum zkittlez	0	0	0	0	0	0	0	0	0	0	0	0	0
tk x butterscotch	2	0	0	0	0	0	0	0	0	0	0	0	0
purple churro	2	0	0	0.75	1	0	0	0	0	0	0	0	0
pure guava	2	0	0	0.75	0	0	1	0.75	0	0	0	0	0
rainbow 2.0	1	0	0	0	0	0	0	0	0	0	0	0	0
fruity pebbles	0	0	0	0	0	0	0	1	0	0	0	1	0
opp x smarties	2	0	1	1	0	0	0	0	0	0	0	0	0
gorilla glue	0	0	1	0	0	2	0	1	0	1	0	0	0
bubba kush	2	1	0	0	0	0	0	0	0	0	0	0	0
trainwreck	0	4	0	0	0	0	1	3	0	0	0	1	3
bacio gelato	0	0	0	0	0	0	0	1	0	0	0	2	0
mac 1	0	0	0	0	0	1	0	1	0	0	0	0	0
gelato 33	1	1	0	0	0	0	0	0	0	0	0	0	0
kimbo kush	0	0	0	0	0	0.75	0	0	0	1	0	0	0
lucky charms	1	0	1.75	0	0	0	0	0	0	0	0	1	0
pie hoe	2	0	0	1	0	0	0	0	0	0	0	0	0
cookies and cream	3	0	2	0	0.75	0	0	0	0	0	1	0	0
gmo cookies	0	2	0	0	0	0	0	0	0	0	0	0	0
og	4	1	0	0	1	0	0	0	0	0	0	0	0
710 chem	1	0	0	0	0	0	0	2	1	0	0	0	0
gmo	1	0	0	0	0	0	0	0	0	0	0	0	0

Table S7. Tabulated sensory panel results (3/5).

Variety	terpenic	waxy	banana	berry	blueberry	grape	grape fruit	guava	lychee	papaya	peach	pineapple	red fruit
grape pie x do-si-do	0	0	0	4	0	5	0	0	0	0	1	0	0
juice man	0	0	0	0	0	0	0	0	0	1	0	0	0
papaya peach	0	0	0	1	0	0	0	0	1	1	5	0	1
cake crasher	0	0	0	2	0	1	0	0	0	0	0	0	0
starburst 36 #1	0	0	0	1	0	1	0	1	0	1	0	1	0
upsidedown frown #5	0	0	0	3	1	0	0	1	0	0	0	1	0
motor nana	0	0	3.75	2	0	0	0	0	0	0	0	0	0
garlic cocktail #7	0	1	0	0	0	1	1	0	0	0	0	0	0
zkittlez 710	0	0	0	1	0	0	0	0	0	0	0	0	0
banana scream	0	0	3	0	0	0	0	0	0	0	0	0	0
bubblegum zkittlez	0	0	0	2	0	0	0	0	0	0	0	0	0
tk x butterscotch	0	0	0	0	0	0.5	0	0	0	0	0	0	0
purple churro	0	0	0	3	0	1	0	0	0	0	0	0	0
pure guava	0	0	0	0	0	1	1	0	0	0	0	0	0
rainbow 2.0	0	0	1	2	0	0	0	0	0	0	0	0	0
fruity pebbles	0	0	0	1	0	0	0	0	0	0	0	0	0
opp x smarties	0	0	0	0	0	1	0	0	0	0	0	0	0
gorilla glue	1	1	0	0	0	0	0	0	0	0	0	0	0
bubba kush	0	0	0	1.75	0	0	0	0	0	0	0	1	0
trainwreck	2	0	0	0	0	0	0	0	0	0	0	0	0
bacio gelato	0	0	0	4	1	0	0	0	0	0	0	0	0
mac 1	0	0	0	1.5	0	0	0	0	0	0	0	0	0
gelato 33	0	1	0	2	0	0	0	0	0	0	2	0	0
kimbo kush	0	0	0	1	0	1	0	0	0	0	0	0	0
lucky charms	2	0	0	2	0	0	0	0	0	0	0	0	0
pie hoe	1	0	0	0	0	0	0	0	0	0	0	0	0
cookies and cream	0	0	0	0	0	0	0	0	0	0	0	0	0
gmo cookies	1	0	0	1	0	0	0	0	0	0	0	0	0
og	0	0	0	0	0	0	0	0	0	0	0	0	0
710 chem	0	0	0	0	0	0	0	0	0	0	0	0	0
gmo	0	0	0	0	0	0	0	0	0	0	0	0	0

Table S8. Tabulated sensory panel results (4/5).

Variety	ripe	strawberry	tangerine	tropical	cherry	coconut	dark berry	fruit	melon	sweet	tart	bready	cereal
grape pie x do-si-do	0	1	0	0	0	1	0	1	0	3	0	0	1
juice man	1	0	1	3	0	0	0	4.5	0	4	0	0	0
papaya peach	1	0	0	2	0	1	0	2.5	0	4	0	0	0
cake crasher	0	0	0	2	0	1	0	5	0	6	0	0	0
starburst 36 #1	0	0	1.75	2	0	0	0	2.5	0	1	0	0	0
upsidedown frown #5	0	1	0.75	2	0	0	0	0	0	5.5	0	0	0
motor nana	1	0	0	2	0	0	0	2	0	3	0	0	0
garlic cocktail #7	0	0	4.5	1	0	0	0	1	0	3	0	0	0
zkittlez 710	0	1	0	1	0	0	0	5.5	0	4	0	0	0
banana scream	1	0	2	2	0	0	0	3	0	3	0	0	0
bubblegum zkittlez	0	0	0	1	1	0	0	1	0.75	4.75	0	0	0
tk x butterscotch	0	0	0	0	0	0	0	0	0	6.75	0	0	0
purple churro	0	0	0	1	0	0	1	1	0	4	0	0	0
pure guava	0	0	1	2	0	0	0	2	0	2	0	0	0
rainbow 2.0	1	0	1	0	0	1	0	2	0	7	0	0	0
fruity pebbles	0	0	0	1	0	0	0	0	0	5	0	0	1
opp x smarties	0	0	0	0	0	0	0	2	0	2.75	0	0	0
gorilla glue	0	0	3.5	0	0	0	0	2	0	2	0	0	0
bubba kush	0	0	0	0	0	0	0	0	0	5.75	0	0	0
trainwreck	0	0	0	2	0	0	0	0	0	1	0	0	0
bacio gelato	0	0	0	0	1	0	0	1	0	4	1	0	0
mac 1	0	0	1.75	1	0	0	0	1	0	2.5	0	0	0
gelato 33	0	0	1.5	1	0	0	0	3	0	4	0	0	0
kimbo kush	1	0	0	3	0	0	1	3	0	1.75	0	0	0
lucky charms	0	0	1	1	0	0	0	0	0	1.75	0	0	0
pie hoe	0	0	0	0	0	0	0	0.75	0	3.5	0	0	0
cookies and cream	0	0	0	0	0	0	0	0.5	0	2.75	0	0	0
gmo cookies	0	0	0	0	0	0	0	0	0	0	0	0	0
og	0	0	0	0	0	0	0	0	0	0.75	0	1	0
710 chem	0	0	0	0	0	0	0	0.75	0	0	0	0	0
gmo	0	0	0	0	0	0	0	0	0	1	0	0	0

Table S9. Tabulated sensory panel results (5/5).

Variety	butterscotch	bubblegum	candy	chocolate	cream	alliaceous	astringent	chemical	moth balls	savory
grape pie x do-si-do	0	0	0	0	1	0	0	0	0	0
juice man	0	0	0	0	0	0	0	0	0	0
papaya peach	0	0	1	0	2	0	0	0	0	0
cake crasher	0	0	1	0	2	0	0	0	0	0
starburst 36 #1	1	0	0	0	0.75	0	0	0	0	0
upsidedown frown #5	0	0	0	0	1	0	0	0	0	0
motor nana	0	0	2	0	0	0	0	0	0	0
garlic cocktail #7	0	0	0	0	0	0	0	0	0	1
zkittlez 710	0	0	1	0	1	0	0	0	0	0
banana scream	0	0	0	1	3	0	0	0	0	0
bubblegum zkittlez	0	1	2	0	0	0	0	0	0	0
tk x butterscotch	2	0	1	0	2	0	0	0	0	1
purple churro	0	0	0	0	1	0	0	0	0	0
pure guava	0	0	0	0	0	0	0	0	0	0
rainbow 2.0	0	0	1	1	3	0	0	0	0	0
fruity pebbles	0	0	2	0	0	1	0	1.5	0	1
opp x smarties	0	0	0	0	0	0	0	0	0	0
gorilla glue	0	0	0	0	0	0	0	0	0	0
bubba kush	0	0	2	0	0.75	0	0	0	0	0
trainwreck	0	0	0	0	0	0	0	0	0	0
bacio gelato	2	0	0	0	2	0	0	2	0	0
mac 1	0	0	0	0	0	0	0	1	0	0
gelato 33	0	0	0	0	0	0	0	2	0	0
kimbo kush	1	0	0	0	0	0	0	0	0	0
lucky charms	0	0	0	0	0	0	0	0	0	0
pie hoe	0	0	0	0	0	0	0	0	0	0
cookies and cream	0	0	0	0	0	0	0	0	0	0
gmo cookies	0	0	0	0	0	2	0	1.75	0	4
og	0	0	0	0	1	0	0	0	0	0
710 chem	0	0	0	0	0	0	1	3	0	0
gmo	0	0	0	0	0	5	0	3	1	4

Table S10. Analyte concentrations (µg/mg) (1/5).

Compound name	type	subtype	Grape Pie x Do-Si-Do	Juice Man	Papaya Peach	Cake Crasher	Starburst 36 #1	Upsidedown frown #5
Exotic score	**NA**	**NA**	**87.4**	**87.1**	**86.3**	**83.7**	**81.7**	**80.7**
d-limonene	terpene	monoterpene	27.4856	27.3671	25.394	31.1784	13.4118	9.314
caryophyllene	terpene	sesquiterpene	14.4908	7.2246	9.1608	28.4825	12.4374	7.3378
α-pinene	terpene	monoterpene	3.3254	3.2823	3.1695	5.7667	0.972	0.4858
trans-β-ocimene	terpene	monoterpene	0.1933	0.1885	0.2244	7.469	0.1357	0.1226
humulene	terpene	sesquiterpene	5.0325	3.28	3.2626	6.0714	6.3386	2.7254
β-myrcene	terpene	monoterpene	8.4562	11.5103	26.9216	2.7682	8.3258	5.7506
linalool	terpene	monoterpenoid	8.071	10.7348	10.6784	10.3456	12.1843	13.2357
endo-fenchol	terpene	monoterpenoid	2.6743	3.5406	2.7459	2.1907	1.7568	2.087
α-terpineol	terpene	monoterpenoid	1.7571	2.2204	1.6647	1.8809	1.598	1.8398
β-pinene	terpene	monoterpene	1.1978	0.7743	1.0717	6.0899	1.9764	1.0672
(-)-guaiol	terpene	sesquiterpenoid	2.2616	3.0298	2.9779	2.5023	4.4824	0.0164
camphene	terpene	monoterpene	0.9	0.9077	0.8632	0.792	0.3164	0.1916
endo-borneol	terpene	monoterpenoid	0.7082	1.0366	0.8795	0.473	0.4902	0.4583
α-bisabolol	terpene	sesquiterpenoid	2.41	1.7787	2.2111	1.0052	2.3823	1.3026
terpinolene	terpene	monoterpene	0.4237	0.419	0.3954	0.4109	0.1938	0.1716
n-hexyl hexanoate	flavorant	ester	0.1249	0.3954	0.238	0.2203	0.1352	0.1231
trans-nerolidol	terpene	sesquiterpenoid	0.0767	0.7445	0.5893	0.0386	1.1993	0.7392

ethyl hexanoate	flavorant	ester	0.1837	0.0405	0	1.6701	0.1899	0.0938
γ-terpinene	terpene	monoterpene	0.1033	0.1318	0.1512	0.1133	0.0551	0.0548
n-hexyl acetate	flavorant	ester	0.0246	0.033	0.0261	0	0.041	0
isopulegol	terpene	monoterpenoid	0.085	0.0504	0.0489	0.3113	0.1937	0.1616
α-terpinene	terpene	monoterpene	0.0832	0.0884	0.1159	0.044	0.0521	0.0521
n-propyl hexanoate	flavorant	ester	0.0347	0.0424	0.0286	0.0961	0.0405	0.0214
1-octanol	flavorant	alcohol	0.0361	0.0592	0.0353	0.1534	0.4848	0.0407
geraniol	terpene	monoterpenoid	0.1047	0.1157	0.0453	0.1315	0.1622	0.0743
ethyl senecioate	flavorant	ester	0.1687	0.1576	0.1243	0.1039	0.4156	0.0102
n-butyl senecioate	flavorant	ester	0	0	0	0.0449	0.0404	0
indole	flavorant	heterocycle	0.0333	0.0341	0.038	0.0373	0	0.048
n-propyl senecioate	flavorant	ester	0	0.0398	0.0386	0.0396	0.0474	0
trans-sabinene hydrate	terpene	monoterpenoid	0.0187	0.0119	0.0146	0.0863	0.0464	0.0411
2-heptanone	flavorant	ketone	0.0268	0.0306	0.0311	0.1086	0.0762	0.0474
α-citral	terpene	monoterpenoid	0	0	0.0232	0.0235	0.0169	0.0202
isoamyl senecioate	flavorant	ester	0.0286	0	0.0392	0	0.03	0
nonanal	flavorant	aldehyde	0.0268	0.0238	0.023	0.0236	0.0233	0
isoamyl hexanoate	flavorant	ester	0.0187	0.1084	0.016	0.0113	0.0366	0.0431
prenylthiol	flavorant	vsc	0.0779	0.0582	0.0364	0.3614	0.0107	0.3156
3-carene	terpene	monoterpene	0.0256	0.0361	0.0609	0.0139	0.0246	0.0265
methyl anthranilate	flavorant	ester	0.0188	0.0279	0.0369	0.0277	0.0205	0.0213
n-octyl acetate	flavorant	ester	0.007	0.0316	0.0261	0.0278	0.0377	0.0187
n-octanal	flavorant	aldehyde	0	0	0	0	0	0
n-hexyl n-butyrate	flavorant	ester	0.0125	0.5765	0.9892	0.0255	0.0184	0.0096
ethyl anthranilate	flavorant	ester	0	0	0.0191	0	0	0.018
citronellol	terpene	monoterpenoid	0.0376	0.04	0.0153	0.0408	0.0308	0.0286
3-mercaptohexyl acetate	flavorant	vsc	0	0	0.0203	0	0.038	0.0172
cherry propanol	flavorant	alcohol	0.0131	0.0178	0.0141	0.0138	0.0146	0.0129
1-decanol	flavorant	alcohol	0.0128	0.017	0.0134	0.024	0.1183	0
sulcatone	flavorant	ketone	0.0136	0.0146	0.0132	0	0.015	0
sabinene	terpene	monoterpene	0.0106	0.0098	0.0123	0.0177	0.0129	0.0143
methyl hexanoate	flavorant	ester	0	0.0142	0.0145	0.0263	0.0369	0.0215
ethyl isovalerate	flavorant	ester	0.0158	0.012	0.0111	0.0181	0.0179	0
methyl octanoate	flavorant	ester	0	0	0	0	0	0.0652
ethyl 2-methylbutyrate	flavorant	ester	0.0056	0.0037	0.0027	0.024	0.0101	0.0024
n-propyl n-butyrate	flavorant	ester	0	0	0	0.0084	0	0
n-heptyl acetate	flavorant	ester	0	0	0	0.0056	0.0057	0.0047
ethyl isobutyrate	flavorant	ester	0.007	0.0087	0.0024	0	0.0174	0.0057
p-cymene	terpene	monoterpene	0.0073	0.006	0.0061	0.006	0.0068	0.0063
cis-nerolidol	terpene	sesquiterpenoid	0	0.0039	0	0.0081	0.0086	0.0046
hexyl 2-methylbutyrate	flavorant	ester	0	0.0111	0.0184	0.0049	0.0049	0
ethyl n-butyrate	flavorant	ester	0.0011	0	0	0	0	0
isobutyl hexanoate	flavorant	ester	0	0.0031	0	0	0.0087	0
cis-3-hexenyl n-butyrate	flavorant	ester	0	0.0341	0.0091	0	0	0
n-hexyl isobutyrate	flavorant	ester	0	0.0294	0.0474	0	0.0906	0.014
n-heptyl n-butyrate	flavorant	ester	0.0083	0.0104	0.0306	0	0	0.0139
methyl n-methylanthranilate	flavorant	ester	0	0.0086	0.0108	0	0	0
phenylethyl n-butyrate	flavorant	ester	0	0.0075	0.0505	0	0	0
isobutyl n-butyrate	flavorant	ester	0	0.0071	0.0058	0	0.0054	0
citronellol acetate	flavorant	ester	0.004	0.0067	0.002	0.0027	0.0021	0.0042
phenylethyl isobutyrate	flavorant	ester	0	0.0006	0.0045	0	0.0013	0
isopropyl isobutyrate	flavorant	ester	0	0	0	0	0	0
n-hexyl senecioate	flavorant	ester	0.027	0	0	0	0.0309	0.0631
isopropyl senecioate	flavorant	ester	0.0319	0	0.0299	0.035	0.0458	0
hexanal	flavorant	aldehyde	0	0	0	0.0176	0.0148	0.0156
phenylethyl propionate	flavorant	ester	0	0	0.0107	0	0	0
isobutyl isobutyrate	flavorant	ester	0	0	0	0	0	0
melonal	flavorant	aldehyde	0	0	0	0	0	0.0055
3-mercaptohexanol	flavorant	vsc	0	0	0	0	0.0748	0
6-amyl-α-pyrone	flavorant	lactone	0	0	0	0.0038	0.0063	0.0038
3-mercaptohexyl butyrate	flavorant	vsc	0	0	0	0	0	0.0158
methyl senecioate	flavorant	ester	0	0	0	0	0	0

skatole	flavorant	heterocycle	0	0	0	0	0	0
n-decyl acetate	flavorant	ester	0	0	0	0	0	0

Table S11. Analyte concentrations (µg/mg) (2/5).

Compound name	type	subtype	Motor Nana	Garlic Cocktail #7	Zkittlez 710	Banana Scream	Bubblegum Zkittlez	TK x Butterscotch
Exotic score	**NA**	**NA**	**80.3**	**80.1**	**80.1**	**79.7**	**77**	**76.3**
d-limonene	terpene	monoterpene	30.1899	20.6988	22.9777	33.8001	8.6232	31.8435
caryophyllene	terpene	sesquiterpene	12.559	17.0237	49.8183	14.7668	8.9827	16.9542
α-pinene	terpene	monoterpene	4.1389	8.3863	2.3211	8.5825	9.1326	3.2845
trans-β-ocimene	terpene	monoterpene	3.0344	2.7158	0.1538	6.338	0.9326	0.2379
humulene	terpene	sesquiterpene	4.8495	6.333	19.5995	5.7279	3.4366	7.1073
β-myrcene	terpene	monoterpene	10.039	13.8353	1.6187	4.6416	32.6996	13.9165
linalool	terpene	monoterpenoid	2.5033	3.6134	23.7398	3.8049	2.9639	8.5705
endo-fenchol	terpene	monoterpenoid	3.3026	1.5068	2.4911	3.6034	1.4796	2.9572
α-terpineol	terpene	monoterpenoid	2.0005	1.3968	1.8638	2.1845	0.9133	1.7879
β-pinene	terpene	monoterpene	1.6709	5.5737	4.4285	2.0087	1.5536	2.1156
(-)-guaiol	terpene	sesquiterpenoid	3.056	0.0065	0.061	1.6661	0.0523	0.3958
camphene	terpene	monoterpene	1.0281	0.5598	0.707	1.246	0.7128	0.8798
endo-borneol	terpene	monoterpenoid	0.9106	0.4445	0.5514	1.1941	0.7032	0.7826
α-bisabolol	terpene	sesquiterpenoid	1.3724	0.9904	2.6348	1.0114	1.1927	1.5535
terpinolene	terpene	monoterpene	0.4412	0.3011	0.3112	0.4972	0.1799	0.4574
n-hexyl hexanoate	flavorant	ester	0.5816	1.2356	0.9347	0.3317	0.493	1.0694
trans-nerolidol	terpene	sesquiterpenoid	0.4332	0.4918	2.4942	0.2549	0.7181	1.2905
ethyl hexanoate	flavorant	ester	0.2415	0	0.0315	0.219	0	0
γ-terpinene	terpene	monoterpene	0.1361	0.0919	0.0614	0.1783	0.1106	0.1358
n-hexyl acetate	flavorant	ester	0.2117	0.59	0.1014	0.1367	0.0508	0.0266
isopulegol	terpene	monoterpenoid	0.0901	0.2046	0.2986	0.1138	0.0604	0.1358
α-terpinene	terpene	monoterpene	0.0948	0.0734	0.0409	0.1083	0.1437	0.0857
n-propyl hexanoate	flavorant	ester	0.0701	0.0289	0.0251	0.0676	0.0214	0.0357
1-octanol	flavorant	alcohol	0.0778	0.7446	1.8385	0.0503	0.1198	0.0392
geraniol	terpene	monoterpenoid	0.0276	0.035	1.0345	0.042	0.0318	0.0726
ethyl senecioate	flavorant	ester	0.2353	0.0118	0.015	0.0408	0.0117	0.0396
n-butyl senecioate	flavorant	ester	0	0.0466	0.04	0.0393	0	0
indole	flavorant	heterocycle	0.0324	0.334	0.0439	0.0393	0.0592	0.0504
n-propyl senecioate	flavorant	ester	0.05	0	0	0.0392	0	0
trans-sabinene hydrate	terpene	monoterpenoid	0.0197	0.0703	0.0579	0.0382	0.016	0.0275
2-heptanone	flavorant	ketone	0.0334	0.3413	0.0359	0.0335	0.0334	0.0285
α-citral	terpene	monoterpenoid	0	0.0173	0.02	0.0282	0.018	0
isoamyl senecioate	flavorant	ester	0.0284	0.0313	0.0281	0.0275	0.0283	0
nonanal	flavorant	aldehyde	0.0234	0.0262	0.0223	0.0258	0.0241	0
isoamyl hexanoate	flavorant	ester	0.0447	0.0098	0.0123	0.0252	0.0094	0.0793
prenylthiol	flavorant	vsc	0.0772	0.029	0.0932	0.0241	0.0764	0.05
3-carene	terpene	monoterpene	0.0286	0.0342	0.0159	0.0226	0.0732	0.0395
methyl anthranilate	flavorant	ester	0.0196	0.0707	0.0189	0.019	0.0283	0
n-octyl acetate	flavorant	ester	0.0604	0.4245	0.2983	0.019	0.0448	0.0271
n-octanal	flavorant	aldehyde	0.0212	0	0	0.0179	0	0
n-hexyl n-butyrate	flavorant	ester	0.0432	0.0892	0.0971	0.0178	0.0785	1.0008
ethyl anthranilate	flavorant	ester	0	0	0	0.0174	0.0176	0
citronellol	terpene	monoterpenoid	0.015	0.0202	0.5933	0.0169	0.1898	0.042
3-mercaptohexyl acetate	flavorant	vsc	0	0.0323	0	0.0161	0	0.0173
cherry propanol	flavorant	alcohol	0.013	0.0136	0.0127	0.0152	0.0144	0.0168
1-decanol	flavorant	alcohol	0.0178	0.1227	0.2093	0.0144	0.0238	0.014
sulcatone	flavorant	ketone	0	0	0.0137	0.0144	0	0
sabinene	terpene	monoterpene	0.0112	0.0138	0.0142	0.0143	0.0177	0.0167
methyl hexanoate	flavorant	ester	0.014	0.0179	0.0154	0.014	0.0151	0
ethyl isovalerate	flavorant	ester	0.0154	0.0166	0	0.0134	0.0154	0
methyl octanoate	flavorant	ester	0	0	0.0016	0.013	0	0
ethyl 2-methylbutyrate	flavorant	ester	0.0095	0.0107	0.0025	0.0122	0	0
n-propyl n-butyrate	flavorant	ester	0.0081	0	0	0.0095	0	0
n-heptyl acetate	flavorant	ester	0.0092	0.0139	0.0169	0.0068	0.0057	0.0051
ethyl isobutyrate	flavorant	ester	0.01	0	0	0.0066	0.0024	0.013
p-cymene	terpene	monoterpene	0.0071	0	0.0046	0.0061	0.0141	0.0063

cis-nerolidol	terpene	sesquiterpenoid	0	0.0076	0.0094	0.0045	0.0065	0.0047
hexyl 2-methylbutyrate	flavorant	ester	0.0084	0.0067	0.0086	0.0042	0.0074	0.0315
ethyl n-butyrate	flavorant	ester	0.0002	0.0105	0	0.0038	0	0
isobutyl hexanoate	flavorant	ester	0	0	0	0	0	0
cis-3-hexenyl n-butyrate	flavorant	ester	0.0089	0	0	0	0.0097	0.0674
n-hexyl isobutyrate	flavorant	ester	0.0145	0.0276	0.0236	0	0.0212	0.0415
n-heptyl n-butyrate	flavorant	ester	0.0114	0	0	0	0.0058	0.0156
methyl n-methylanthranilate	flavorant	ester	0	0	0	0	0.0074	0
phenylethyl n-butyrate	flavorant	ester	0	0	0	0	0	0
isobutyl n-butyrate	flavorant	ester	0	0	0	0	0	0
citronellol acetate	flavorant	ester	0.0021	0	0.0226	0	0.0349	0.009
phenylethyl isobutyrate	flavorant	ester	0	0	0	0	0	0.0013
isopropyl isobutyrate	flavorant	ester	0	0	0	0	0	0
n-hexyl senecioate	flavorant	ester	0.0291	0	0.0297	0	0.0289	0.0389
isopropyl senecioate	flavorant	ester	0.0307	0	0	0	0	0.0323
hexanal	flavorant	aldehyde	0	0	0.0144	0	0	0
phenylethyl propionate	flavorant	ester	0	0.0126	0.0563	0	0	0
isobutyl isobutyrate	flavorant	ester	0.0018	0	0	0	0	0
melonal	flavorant	aldehyde	0	0	0.005	0	0	0
3-mercaptohexanol	flavorant	vsc	0	0.057	0	0	0	0
6-amyl-α-pyrone	flavorant	lactone	0	0	0.0065	0	0	0
3-mercaptohexyl butyrate	flavorant	vsc	0	0	0	0	0	0
methyl senecioate	flavorant	ester	0	0	0	0	0	0
skatole	flavorant	heterocycle	0	0.0227	0	0	0	0
n-decyl acetate	flavorant	ester	0	0	0	0	0	0

Table S12. Analyte concentrations (μg/mg) (3/5).

Compound name	type	subtype	Purple Churro	Pure Guava	Rainbow 2.0	Fruity Pebbles	OPP x Smarties	Gorilla Glue
Exotic score	**NA**	**NA**	**74.3**	**74**	**71.6**	**71.4**	**70.9**	**65.1**
d-limonene	terpene	monoterpene	28.0271	10.5413	29.5132	13.5712	27.8193	2.3165
caryophyllene	terpene	sesquiterpene	16.5482	25.7297	9.1492	20.2296	6.9884	27.5644
α-pinene	terpene	monoterpene	5.3067	0.7374	4.4826	0.5774	6.7141	0.2849
trans-β-ocimene	terpene	monoterpene	2.2323	0.9149	3.222	0.047	1.5933	0.081
humulene	terpene	sesquiterpene	4.1935	10.9186	3.052	5.7167	2.3988	9.4912
β-myrcene	terpene	monoterpene	3.3628	12.1224	8.4449	0.9231	10.4521	2.7247
linalool	terpene	monoterpenoid	12.4994	5.5128	9.4179	13.1933	5.2782	7.0479
endo-fenchol	terpene	monoterpenoid	4.0565	1.3085	3.2957	1.7389	3.3224	0.5528
α-terpineol	terpene	monoterpenoid	2.6993	0.9476	2.1758	1.3756	2.0837	0.4967
β-pinene	terpene	monoterpene	4.4967	1.3538	2.7691	1.4349	2.5859	0.5975
(-)-guaiol	terpene	sesquiterpenoid	0.0439	0.0183	2.3959	1.0144	0.5916	3.2394
camphene	terpene	monoterpene	1.1106	0.22	0.9643	0.1956	1.3501	0.0988
endo-borneol	terpene	monoterpenoid	0.8454	0.3738	0.9154	0.3928	1.0352	0.1631
α-bisabolol	terpene	sesquiterpenoid	0.7636	1.2108	0.9282	1.6121	0.2734	2.9936
terpinolene	terpene	monoterpene	0.3909	0.0456	0.4184	0.2006	0.4048	0.0397
n-hexyl hexanoate	flavorant	ester	4.5421	0.2073	2.2578	0.2917	0.9549	0.4845
trans-nerolidol	terpene	sesquiterpenoid	0.7855	1.3576	0.8958	1.0882	0.1357	0.6998
ethyl hexanoate	flavorant	ester	0.0243	0	0.0275	0.0238	0	0.0352
γ-terpinene	terpene	monoterpene	0.1245	0.0578	0.1465	0.0427	0.1561	0.0462
n-hexyl acetate	flavorant	ester	0.0736	0.0295	0.0786	0.0369	0	0.0541
isopulegol	terpene	monoterpenoid	0.1738	0.1099	0.1101	0.178	0.0645	0.066
α-terpinene	terpene	monoterpene	0.0811	0.0582	0.0895	0.0336	0.1133	0.0216
n-propyl hexanoate	flavorant	ester	0.0286	0.0155	0.0311	0.021	0.0293	0.0158
1-octanol	flavorant	alcohol	0.361	0.0333	0.1158	0.1105	0.0389	0.1342
geraniol	terpene	monoterpenoid	0.065	0.0847	0.089	0.3171	0.0466	0.0382
ethyl senecioate	flavorant	ester	0.0104	0.054	0.0513	0.0641	0.0248	0.0119
n-butyl senecioate	flavorant	ester	0.0385	0.0419	0	0	0	0
indole	flavorant	heterocycle	0.05	0.0339	0	0.0332	0.0345	0
n-propyl senecioate	flavorant	ester	0	0	0	0.0377	0	0

trans-sabinene hydrate	terpene	monoterpenoid	0.0429	0.0511	0.0318	0.0451	0.028	0.0182
2-heptanone	flavorant	ketone	0.037	0.0402	0.0549	0.044	0.0307	0.0399
α-citral	terpene	monoterpenoid	0.0166	0.0232	0	0	0.0234	0.0195
isoamyl senecioate	flavorant	ester	0.0273	0.0337	0.0287	0.0267	0.0279	0
nonanal	flavorant	aldehyde	0.0215	0.0215	0.0252	0	0.0288	0.0361
isoamyl hexanoate	flavorant	ester	0.1958	0	0.0884	0.009	0.1198	0.0084
prenylthiol	flavorant	vsc	0.2307	0.1059	0.1009	0.4876	0.066	0.0199
3-carene	terpene	monoterpene	0.0222	0.0307	0.0309	0.0117	0.0385	0.0184
methyl anthranilate	flavorant	ester	0.0218	0.0184	0.0182	0.0189	0.0228	0.0273
n-octyl acetate	flavorant	ester	0.1597	0.0062	0.0405	0.0314	0.0132	0.0471
n-octanal	flavorant	aldehyde	0	0	0	0	0	0
n-hexyl n-butyrate	flavorant	ester	0.1802	0.0091	0.1027	0.0138	0.0369	4.2155
ethyl anthranilate	flavorant	ester	0.0168	0	0	0.0164	0	0
citronellol	terpene	monoterpenoid	0.0266	0.016	0.0464	0.0962	0.0952	0.0167
3-mercaptohexyl acetate	flavorant	vsc	0.0161	0.063	0.0169	0	0	0.0172
cherry propanol	flavorant	alcohol	0.0138	0.0264	0.0143	0.0116	0.0159	0.0124
1-decanol	flavorant	alcohol	0.0546	0.0154	0.0208	0.021	0.0148	0.0619
sulcatone	flavorant	ketone	0.0159	0	0.0157	0.0142	0.0135	0.0164
sabinene	terpene	monoterpene	0.0172	0.0155	0.016	0.0124	0.0072	0.0172
methyl hexanoate	flavorant	ester	0.0146	0	0.0157	0.016	0.0141	0.0182
ethyl isovalerate	flavorant	ester	0	0	0	0.0103	0	0
methyl octanoate	flavorant	ester	0	0	0	0.0003	0	0.0006
ethyl 2-methylbutyrate	flavorant	ester	0	0	0.0032	0	0	0
n-propyl n-butyrate	flavorant	ester	0	0	0	0	0	0
n-heptyl acetate	flavorant	ester	0.0069	0	0.0053	0.0047	0	0.0103
ethyl isobutyrate	flavorant	ester	0.0026	0	0.0071	0.0045	0.0095	0
p-cymene	terpene	monoterpene	0.0057	0.0273	0.0053	0.0047	0.0073	0.0054
cis-nerolidol	terpene	sesquiterpenoid	0.0043	0	0.004	0.0043	0.004	0.0059
hexyl 2-methylbutyrate	flavorant	ester	0.0051	0	0.0048	0	0.0047	0.045
ethyl n-butyrate	flavorant	ester	0	0	0	0	0	0
isobutyl hexanoate	flavorant	ester	0	0	0	0	0	0
cis-3-hexenyl n-butyrate	flavorant	ester	0.0107	0	0.0096	0	0.0147	0.0901
n-hexyl isobutyrate	flavorant	ester	0.0196	0	0.0167	0.0133	0.0146	0.1081
n-heptyl n-butyrate	flavorant	ester	0.0099	0	0.0088	0	0.0082	0.0903
methyl n-methylanthranilate	flavorant	ester	0	0	0	0	0	0
phenylethyl n-butyrate	flavorant	ester	0	0	0	0	0	0
isobutyl n-butyrate	flavorant	ester	0	0.0058	0	0	0	0.0064
citronellol acetate	flavorant	ester	0.0057	0.002	0.0047	0.0106	0.0154	0
phenylethyl isobutyrate	flavorant	ester	0	0	0	0	0	0.0005
isopropyl isobutyrate	flavorant	ester	0	0	0	0	0	0
n-hexyl senecioate	flavorant	ester	0	0.0306	0.0286	0.0276	0.0293	0.0292
isopropyl senecioate	flavorant	ester	0	0.0315	0.0301	0.0331	0.0292	0
hexanal	flavorant	aldehyde	0	0.0138	0.0131	0	0	0.0143
phenylethyl propionate	flavorant	ester	0	0.0101	0	0	0	0.0123
isobutyl isobutyrate	flavorant	ester	0	0	0	0	0	0
melonal	flavorant	aldehyde	0.0051	0	0	0	0	0
3-mercaptohexanol	flavorant	vsc	0	0	0	0	0	0.0435
6-amyl-α-pyrone	flavorant	lactone	0	0.0050	0	0.0065	0	0.0033
3-mercaptohexyl butyrate	flavorant	vsc	0	0	0	0	0	0.032
methyl senecioate	flavorant	ester	0	0.0334	0	0	0	0
skatole	flavorant	heterocycle	0	0	0	0.0132	0	0
n-decyl acetate	flavorant	ester	0	0	0	0	0	0

Table S13. Analyte concentrations (μg/mg) (4/5).

Compound name	type	subtype	Bubba Kush	Trainwreck	Bacio Gelato	MAC 1	Gelato 33	Kimbo Kush	Lucky Charms
Exotic score	**NA**	**NA**	62.1	43.7	43.1	39.3	34.6	34	30.7
d-limonene	terpene	monoterpene	19.5705	6.9983	34.3947	11.6332	28.9228	29.4287	26.2159
caryophyllene	terpene	sesquiterpene	14.2841	7.4599	10.7122	11.5929	14.0053	9.1111	20.0846
α-pinene	terpene	monoterpene	2.6567	1.807	6.5956	2.6069	5.2179	2.7139	1.5105
trans-β-ocimene	terpene	monoterpene	0.1919	2.7805	1.5016	0.488	0.862	0.1711	0.0346

humulene	terpene	sesquiterpene	4.7684	1.9742	1.6138	3.6209	2.6116	2.4851	7.7092
β-myrcene	terpene	monoterpene	16.1311	3.7173	2.0578	1.4605	4.4012	1.5987	10.4934
linalool	terpene	monoterpenoid	11.5074	2.5926	4.066	5.0844	5.1709	8.159	3.3316
endo-fenchol	terpene	monoterpenoid	3.1162	0.8612	3.291	2.9018	2.5978	2.184	2.7065
α-terpineol	terpene	monoterpenoid	2.0882	0.9597	2.0833	2.2016	1.7069	1.8632	2.1238
β-pinene	terpene	monoterpene	0.4141	2.9235	7.2345	3.5418	5.9615	4.7961	2.827
(-)-guaiol	terpene	sesquiterpenoid	4.2564	0.0023	0.0078	0.0087	0.0059	0.0103	0.0106
camphene	terpene	monoterpene	0.8593	0.5725	0.991	0.5596	0.822	0.8335	0.4577
endo-borneol	terpene	monoterpenoid	0.8734	0.2863	0.4913	0.5536	0.4101	0.4776	0.7657
α-bisabolol	terpene	sesquiterpenoid	1.8241	0.8199	1.2141	5.1759	1.2977	1.5762	1.8005
terpinolene	terpene	monoterpene	0.3716	14.351	0.3507	0.1787	0.3028	0.3802	0.2444
n-hexyl hexanoate	flavorant	ester	0.1336	0.1076	0.0227	0.2127	0.1509	0.1448	1.2487
trans-nerolidol	terpene	sesquiterpenoid	0.3966	0.6463	0.1835	0.9418	0.1426	0.435	1.4892
ethyl hexanoate	flavorant	ester	0	0	0	0.0251	0	0.0354	0
γ-terpinene	terpene	monoterpene	0.1313	0.6888	0.2045	0.0815	0.186	0.097	0.0414
n-hexyl acetate	flavorant	ester	0.0341	0	0	0	0	0	0.0468
isopulegol	terpene	monoterpenoid	0.027	0.3333	0.4178	0.2395	0.3463	0.149	0.2007
α-terpinene	terpene	monoterpene	0.1399	0.8861	0.056	0.0586	0.0511	0.0752	0.0568
n-propyl hexanoate	flavorant	ester	0	0	0.0316	0	0.031	0	0
1-octanol	flavorant	alcohol	0.0497	0.0245	0.0353	0.0342	0.0348	0.0321	0.4394
geraniol	terpene	monoterpenoid	0.3395	0.1064	0.3839	0.0261	0.2652	0.2077	1.1484
ethyl senecioate	flavorant	ester	0.0349	0.0146	0.2033	0.0167	0.1454	0.0101	0.0098
n-butyl senecioate	flavorant	ester	0.0379	0	0	0.0401	0	0.0404	0.0381
indole	flavorant	heterocycle	0.0323	0.0161	0	0.0352	0	0.0407	0.0354
n-propyl senecioate	flavorant	ester	0	0	0	0	0	0	0
trans-sabinene hydrate	terpene	monoterpenoid	0.0097	0.113	0.0941	0.0785	0.0751	0.056	0.0543
2-heptanone	flavorant	ketone	0.052	0.0288	0.0353	0.0251	0.0499	0.0406	0.0367
α-citral	terpene	monoterpenoid	0	0	0	0	0.0383	0.0259	0
isoamyl senecioate	flavorant	ester	0.0272	0	0	0.0286	0	0	0.0271
nonanal	flavorant	aldehyde	0.0238	0	0.0234	0.0497	0.026	0.0252	0.0218
isoamyl hexanoate	flavorant	ester	0	0.0074	0	0.0192	0	0	0.0153
prenylthiol	flavorant	vsc	0.074	0.0061	0.2939	0.0249	0.2141	0.0515	0.0925
3-carene	terpene	monoterpene	0.047	4.2249	0.0249	0.0213	0.0314	0.0268	0.0313
methyl anthranilate	flavorant	ester	0.0345	0.0284	0.0207	0.0241	0.0214	0.0247	0.0146
n-octyl acetate	flavorant	ester	0.0195	0.0058	0.0068	0.0071	0.0058	0.0073	0.1539
n-octanal	flavorant	aldehyde	0	0	0	0	0	0	0
n-hexyl n-butyrate	flavorant	ester	0.0148	0.3566	0.014	0.016	0.0146	0.019	0.0741
ethyl anthranilate	flavorant	ester	0	0	0	0	0	0	0
citronellol	terpene	monoterpenoid	0.1239	0	0.0905	0.0591	0.0784	0.1377	0.027
3-mercaptohexyl acetate	flavorant	vsc	0	0	0.0265	0	0	0	0.0206
cherry propanol	flavorant	alcohol	0.0135	0.7394	0.0168	0.0159	0.0137	0.0157	0.0259
1-decanol	flavorant	alcohol	0.0145	0.0204	0.0143	0.014	0.014	0	0.0569
sulcatone	flavorant	ketone	0.0172	0.0355	0.0152	0.0193	0.0139	0.0229	0
sabinene	terpene	monoterpene	0.009	0.2946	0.0153	0.026	0.0153	0.016	0.0111
methyl hexanoate	flavorant	ester	0.0172	0.0125	0.0148	0.0163	0.0171	0.0159	0.0155
ethyl isovalerate	flavorant	ester	0.0122	0	0.0111	0	0	0.0146	0
methyl octanoate	flavorant	ester	0	0	0	0	0	0	0
ethyl 2-methylbutyrate	flavorant	ester	0	0	0.0029	0	0	0.0169	0
n-propyl n-butyrate	flavorant	ester	0	0	0	0	0	0.0086	0
n-heptyl acetate	flavorant	ester	0.0048	0	0.0048	0	0	0	0.0061
ethyl isobutyrate	flavorant	ester	0	0	0	0	0	0	0
p-cymene	terpene	monoterpene	0.0149	0.4663	0.0085	0.0082	0	0.008	0.0219
cis-nerolidol	terpene	sesquiterpenoid	0.0038	0	0	0.0075	0	0.0038	0
hexyl 2-methylbutyrate	flavorant	ester	0.0039	0.0112	0.0047	0.0042	0	0	0.0067
ethyl n-butyrate	flavorant	ester	0	0	0	0	0	0.036	0
isobutyl hexanoate	flavorant	ester	0	0	0	0	0	0	0
cis-3-hexenyl n-butyrate	flavorant	ester	0	0.0145	0	0	0	0	0
n-hexyl isobutyrate	flavorant	ester	0	0	0	0	0	0	0
n-heptyl n-butyrate	flavorant	ester	0.0051	0.0202	0	0	0	0	0
methyl n-methylanthranilate	flavorant	ester	0.0073	0	0	0	0	0	0
phenylethyl n-butyrate	flavorant	ester	0	0	0	0.0062	0	0	0
isobutyl n-butyrate	flavorant	ester	0	0	0	0	0	0	0
citronellol acetate	flavorant	ester	0.0196	0	0.004	0.0124	0.0034	0.0089	0.004

phenylethyl isobutyrate	flavorant	ester	0	0	0	0	0	0	0
isopropyl isobutyrate	flavorant	ester	0.0065	0	0	0	0	0	0
n-hexyl senecioate	flavorant	ester	0.0329	0	0.0278	0	0.0277	0	0
isopropyl senecioate	flavorant	ester	0.0481	0	0.0312	0	0.0301	0	0
hexanal	flavorant	aldehyde	0.015	0	0	0.0133	0	0.0147	0
phenylethyl propionate	flavorant	ester	0	0	0	0.01	0	0	0.0118
isobutyl isobutyrate	flavorant	ester	0	0	0	0	0	0	0
melonal	flavorant	aldehyde	0.005	0	0	0.0054	0	0.0054	0.005
3-mercaptohexanol	flavorant	vsc	0	0	0	0	0	0	0
6-amyl-α-pyrone	flavorant	lactone	0.0050	0	0	0	0	0	0
3-mercaptohexyl butyrate	flavorant	vsc	0	0	0	0	0	0	0
methyl senecioate	flavorant	ester	0.0235	0	0.0366	0	0.0302	0	0
skatole	flavorant	heterocycle	0	0	0	0	0	0	0
n-decyl acetate	flavorant	ester	0	0	0	0	0	0	0

Table S14. Analyte concentrations (μg/mg) (5/5).

Compound name	**type**	**subtype**	**Pie Hoe**	**Cookies and Cream**	**GMO Cookies**	**OG**	**710 chem**	**GMO**
Exotic score	**NA**	**NA**	**25.3**	**15.4**	**5.7**	**3**	**1.9**	**1.7**
d-limonene	terpene	monoterpene	15.8407	17.6323	25.2498	25.7865	16.4857	24.5405
caryophyllene	terpene	sesquiterpene	17.7841	34.0783	29.9326	20.6312	35.1996	15.0594
α-pinene	terpene	monoterpene	1.601	1.8241	3.0744	2.1525	1.2337	1.8156
trans-β-ocimene	terpene	monoterpene	0.0281	0.0472	0.0469	0.0594	0.046	0.0528
humulene	terpene	sesquiterpene	6.139	10.9633	13.7882	6.8673	9.1274	7.0209
β-myrcene	terpene	monoterpene	15.9356	4.7757	11.5495	19.0079	7.9803	18.7704
linalool	terpene	monoterpenoid	10.6298	3.2682	3.286	12.3449	0.0343	3.2623
endo-fenchol	terpene	monoterpenoid	1.7666	1.3177	2.6743	3.8153	2.1029	2.1722
α-terpineol	terpene	monoterpenoid	1.3884	0.9837	1.4604	3.4542	1.4519	1.669
β-pinene	terpene	monoterpene	2.6247	3.3774	1.6553	4.5607	2.446	3.1151
(-)-guaiol	terpene	sesquiterpenoid	0.0091	0.0143	0.0283	0.0139	0.0162	0.011
camphene	terpene	monoterpene	0.4548	0.5457	0.7009	0.6728	0.3704	0.51
endo-borneol	terpene	monoterpenoid	0.4991	0.3685	0.6457	1.0104	0.4798	0.5736
α-bisabolol	terpene	sesquiterpenoid	1.5905	0.7495	4.9999	1.4106	1.5455	2.1558
terpinolene	terpene	monoterpene	0.1106	0.1885	0.4581	0.3244	0.225	0.2675
n-hexyl hexanoate	flavorant	ester	0.4436	0.0963	0.3373	1.1202	0.5615	0.8012
trans-nerolidol	terpene	sesquiterpenoid	0.0284	0.5606	0.6585	0	1.1922	0.7709
ethyl hexanoate	flavorant	ester	0	0	0	0.0258	0	0
γ-terpinene	terpene	monoterpene	0.0462	0.0475	0.1612	0.0597	0.0356	0.141
n-hexyl acetate	flavorant	ester	0.0252	0	0.0307	0.0266	0	0.0254
isopulegol	terpene	monoterpenoid	0.1573	0.1722	0.0355	0.5873	0.2854	0.1849
α-terpinene	terpene	monoterpene	0.0611	0.0466	0.1452	0.0658	0.0501	0.0941
n-propyl hexanoate	flavorant	ester	0.0178	0	0.0296	0	0.0236	0.0248
1-octanol	flavorant	alcohol	0.1047	0.0336	0.0361	0.0446	0.0342	0.0316
geraniol	terpene	monoterpenoid	0.3287	0.0344	0.0506	0.3603	0.1365	0.0339
ethyl senecioate	flavorant	ester	0.0376	0.2098	0.0975	0	0.027	0.0172
n-butyl senecioate	flavorant	ester	0.0382	0	0	0	0.0431	0.0395
indole	flavorant	heterocycle	0.0354	0.0315	0.0316	0.033	0.0414	0
n-propyl senecioate	flavorant	ester	0	0.0393	0	0	0	0
trans-sabinene hydrate	terpene	monoterpenoid	0.0507	0.0748	0.0157	0.1027	0.0495	0.0438
2-heptanone	flavorant	ketone	0.0332	0.0264	0.0284	0.0286	0.0338	0.0338
α-citral	terpene	monoterpenoid	0.0152	0.0267	0	0	0	0
isoamyl senecioate	flavorant	ester	0.0273	0.0271	0.0284	0	0.0293	0.028
nonanal	flavorant	aldehyde	0	0.0431	0	0	0.0243	0
isoamyl hexanoate	flavorant	ester	0	0	0	0.0466	0.1424	0.0095
prenylthiol	flavorant	vsc	0.1175	0.0516	0.0946	0.0724	0.1541	0.1535
3-carene	terpene	monoterpene	0.0371	0.0215	0.037	0.0368	0.0259	0.0396
methyl anthranilate	flavorant	ester	0.0159	0.0197	0.0173	0	0	0.015
n-octyl acetate	flavorant	ester	0.039	0.0082	0.0079	0.0105	0.0104	0
n-octanal	flavorant	aldehyde	0	0.0163	0	0	0	0
n-hexyl n-butyrate	flavorant	ester	0.0153	0.0117	0.0096	0.0208	0.0222	0.0362
ethyl anthranilate	flavorant	ester	0	0	0	0	0	0
citronellol	terpene	monoterpenoid	0.1081	0.0296	0.0522	0.3528	0.0249	0.0243

3-mercaptohexyl acetate	flavorant	vsc	0	0	0	0	0	0
cherry propanol	flavorant	alcohol	0.0254	0.0158	0.0154	0.0183	0.0126	0.0184
1-decanol	flavorant	alcohol	0.0206	0.0124	0.013	0.0161	0	0
sulcatone	flavorant	ketone	0	0.0222	0.014	0.0133	0	0
sabinene	terpene	monoterpene	0.0139	0.0147	0.0115	0.0216	0.0136	0.0121
methyl hexanoate	flavorant	ester	0.0149	0.0154	0	0.0147	0.0185	0.0136
ethyl isovalerate	flavorant	ester	0.0105	0.0108	0	0	0.0108	0
methyl octanoate	flavorant	ester	0	0.0016	0.0032	0	0	0
ethyl 2-methylbutyrate	flavorant	ester	0	0.0026	0	0	0	0
n-propyl n-butyrate	flavorant	ester	0	0	0	0	0	0
n-heptyl acetate	flavorant	ester	0.0043	0	0	0.0045	0	0
ethyl isobutyrate	flavorant	ester	0.004	0	0	0	0	0.0024
p-cymene	terpene	monoterpene	0.0235	0.0067	0.1023	0.0051	0.0045	0.0172
cis-nerolidol	terpene	sesquiterpenoid	0	0.011	0.0081	0.004	0	0
hexyl 2-methylbutyrate	flavorant	ester	0	0.004	0.0046	0.006	0.0052	0.0044
ethyl n-butyrate	flavorant	ester	0	0	0	0	0	0
isobutyl hexanoate	flavorant	ester	0	0	0	0	0	0
cis-3-hexenyl n-butyrate	flavorant	ester	0	0	0	0	0	0
n-hexyl isobutyrate	flavorant	ester	0	0	0	0.0156	0	0.017
n-heptyl n-butyrate	flavorant	ester	0	0	0	0	0	0
methyl n-methylanthranilate	flavorant	ester	0	0	0	0	0	0
phenylethyl n-butyrate	flavorant	ester	0	0	0	0	0	0
isobutyl n-butyrate	flavorant	ester	0	0	0	0	0	0
citronellol acetate	flavorant	ester	0.0165	0.005	0.0076	0.0487	0.0017	0.0073
phenylethyl isobutyrate	flavorant	ester	0	0	0	0	0	0
isopropyl isobutyrate	flavorant	ester	0	0	0	0	0	0
n-hexyl senecioate	flavorant	ester	0.029	0.0266	0.0374	0	0	0.0293
isopropyl senecioate	flavorant	ester	0.0309	0.0291	0	0	0	0.0305
hexanal	flavorant	aldehyde	0	0.015	0	0.0163	0	0
phenylethyl propionate	flavorant	ester	0	0	0	0	0	0
isobutyl isobutyrate	flavorant	ester	0	0	0	0	0	0
melonal	flavorant	aldehyde	0	0.0055	0	0	0.0053	0.0051
3-mercaptohexanol	flavorant	vsc	0	0	0	0	0	0
6-amyl-α-pyrone	flavorant	lactone	0.0025	0	0	0	0	0
3-mercaptohexyl butyrate	flavorant	vsc	0	0	0	0	0	0
methyl senecioate	flavorant	ester	0.0236	0.0228	0.0257	0	0	0.0335
skatole	flavorant	heterocycle	0	0	0.0139	0	0.0145	0.0187
n-decyl acetate	flavorant	ester	0	0	0	0	0	0

Table S15. Analyte Relative-% of volatile fraction (1/5).

Compound name	type	subtype	Grape Pie x Do-Si-Do	Juice Man	Papaya Peach	Cake Crasher	Starburst 36 #1	Upsidedown frown #5
Exotic score	**NA**	**NA**	**87.4**	**87.1**	**86.3**	**83.7**	**81.7**	**80.7**
d-limonene	terpene	monoterpene	33.9681	34.0391	26.7979	27.9894	18.8864	19.238
caryophyllene	terpene	sesquiterpene	17.9084	8.986	9.6673	25.5693	17.5143	15.1561
α-pinene	terpene	monoterpene	4.1097	4.0825	3.3447	5.1768	1.3688	1.0034
trans-β-ocimene	terpene	monoterpene	0.2389	0.2345	0.2368	6.7051	0.1912	0.2532
humulene	terpene	sesquiterpene	6.2194	4.0797	3.443	5.4505	8.926	5.6294
β-myrcene	terpene	monoterpene	10.4505	14.3164	28.41	2.485	11.7244	11.8777
linalool	terpene	monoterpenoid	9.9745	13.3519	11.2688	9.2874	17.1579	27.3382
endo-fenchol	terpene	monoterpenoid	3.305	4.4038	2.8977	1.9666	2.4739	4.3107
α-terpineol	terpene	monoterpenoid	2.1715	2.7618	1.7568	1.6885	2.2503	3.8001
β-pinene	terpene	monoterpene	1.4803	0.9631	1.1309	5.467	2.7832	2.2043
(-)-guaiol	terpene	sesquiterpenoid	2.795	3.7684	3.1426	2.2464	6.3121	0.0338
camphene	terpene	monoterpene	1.1123	1.129	0.9109	0.711	0.4456	0.3958
endo-borneol	terpene	monoterpenoid	0.8753	1.2894	0.9281	0.4246	0.6903	0.9466
α-bisabolol	terpene	sesquiterpenoid	2.9783	2.2124	2.3334	0.9024	3.3547	2.6906
terpinolene	terpene	monoterpene	0.5237	0.5211	0.4172	0.3688	0.2729	0.3545

n-hexyl hexanoate	flavorant	ester	0.1544	0.4918	0.2511	0.1978	0.1904	0.2542
trans-nerolidol	terpene	sesquiterpenoid	0.0948	0.9261	0.6219	0.0346	1.6889	1.5269
ethyl hexanoate	flavorant	ester	0.2271	0.0503	0	1.4993	0.2674	0.1938
γ-terpinene	terpene	monoterpene	0.1276	0.1639	0.1595	0.1017	0.0776	0.1133
n-hexyl acetate	flavorant	ester	0.0304	0.041	0.0276	0	0.0577	0
isopulegol	terpene	monoterpenoid	0.1051	0.0626	0.0516	0.2795	0.2728	0.3338
α-terpinene	terpene	monoterpene	0.1028	0.11	0.1223	0.0395	0.0734	0.1077
n-propyl hexanoate	flavorant	ester	0.0429	0.0527	0.0302	0.0863	0.057	0.0442
1-octanol	flavorant	alcohol	0.0446	0.0736	0.0372	0.1377	0.6827	0.0841
geraniol	terpene	monoterpenoid	0.1294	0.1439	0.0478	0.118	0.2285	0.1535
ethyl senecioate	flavorant	ester	0.2084	0.196	0.1312	0.0933	0.5852	0.0211
n-butyl senecioate	flavorant	ester	0	0	0	0.0403	0.0569	0
indole	flavorant	heterocycle	0.0412	0.0424	0.0401	0.0335	0	0.0991
n-propyl senecioate	flavorant	ester	0	0.0495	0.0407	0.0355	0.0667	0
trans-sabinene hydrate	terpene	monoterpenoid	0.0231	0.0147	0.0154	0.0775	0.0653	0.0849
2-heptanone	flavorant	ketone	0.0332	0.038	0.0328	0.0975	0.1074	0.0978
α-citral	terpene	monoterpenoid	0	0	0.0245	0.0211	0.0238	0.0418
isoamyl senecioate	flavorant	ester	0.0354	0	0.0414	0	0.0423	0
nonanal	flavorant	aldehyde	0.0331	0.0296	0.0243	0.0212	0.0328	0
isoamyl hexanoate	flavorant	ester	0.0231	0.1348	0.0169	0.0102	0.0515	0.0891
prenylthiol	flavorant	vsc	0.0963	0.0724	0.0384	0.3245	0.015	0.6518
3-carene	terpene	monoterpene	0.0317	0.0449	0.0643	0.0124	0.0346	0.0548
methyl anthranilate	flavorant	ester	0.0233	0.0347	0.0389	0.0249	0.0289	0.044
n-octyl acetate	flavorant	ester	0.0087	0.0393	0.0275	0.0249	0.0531	0.0386
n-octanal	flavorant	aldehyde	0	0	0	0	0	0
n-hexyl n-butyrate	flavorant	ester	0.0155	0.717	1.0439	0.0229	0.0259	0.0198
ethyl anthranilate	flavorant	ester	0	0	0.0202	0	0	0.0373
citronellol	terpene	monoterpenoid	0.0465	0.0497	0.0161	0.0366	0.0433	0.0591
3-mercaptohexyl acetate	flavorant	vsc	0	0	0.0214	0	0.0535	0.0356
cherry propanol	flavorant	alcohol	0.0162	0.0222	0.0149	0.0124	0.0206	0.0266
1-decanol	flavorant	alcohol	0.0159	0.0211	0.0141	0.0215	0.1665	0
sulcatone	flavorant	ketone	0.0168	0.0181	0.0139	0	0.0212	0
sabinene	terpene	monoterpene	0.0131	0.0122	0.0129	0.0159	0.0181	0.0296
methyl hexanoate	flavorant	ester	0	0.0177	0.0153	0.0236	0.052	0.0445
ethyl isovalerate	flavorant	ester	0.0196	0.0149	0.0117	0.0162	0.0253	0
methyl octanoate	flavorant	ester	0	0	0	0	0	0.1347
ethyl 2-methylbutyrate	flavorant	ester	0.0069	0.0046	0.0028	0.0215	0.0142	0.0049
n-propyl n-butyrate	flavorant	ester	0	0	0	0.0076	0	0
n-heptyl acetate	flavorant	ester	0	0	0	0.0051	0.0081	0.0096
ethyl isobutyrate	flavorant	ester	0.0086	0.0108	0.0026	0	0.0245	0.0117
p-cymene	terpene	monoterpene	0.009	0.0075	0.0065	0.0054	0.0096	0.013
cis-nerolidol	terpene	sesquiterpenoid	0	0.0048	0	0.0073	0.0122	0.0095
hexyl 2-methylbutyrate	flavorant	ester	0	0.0137	0.0194	0.0044	0.0069	0
ethyl n-butyrate	flavorant	ester	0.0014	0	0	0	0	0
isobutyl hexanoate	flavorant	ester	0	0.0039	0	0	0.0123	0
cis-3-hexenyl n-butyrate	flavorant	ester	0	0.0425	0.0096	0	0	0
n-hexyl isobutyrate	flavorant	ester	0	0.0365	0.05	0	0.1276	0.029
n-heptyl n-butyrate	flavorant	ester	0.0102	0.0129	0.0323	0	0	0.0287
methyl n-methylanthranilate	flavorant	ester	0	0.0108	0.0114	0	0	0
phenylethyl n-butyrate	flavorant	ester	0	0.0094	0.0533	0	0	0
isobutyl n-butyrate	flavorant	ester	0	0.0088	0.0061	0	0.0077	0
citronellol acetate	flavorant	ester	0.0049	0.0084	0.0022	0.0025	0.003	0.0087
phenylethyl isobutyrate	flavorant	ester	0	0.0007	0.0047	0	0.0019	0
isopropyl isobutyrate	flavorant	ester	0	0	0	0	0	0
n-hexyl senecioate	flavorant	ester	0.0334	0	0	0	0.0434	0.1304
isopropyl senecioate	flavorant	ester	0.0394	0	0.0315	0.0314	0.0645	0
hexanal	flavorant	aldehyde	0	0	0	0.0158	0.0208	0.0322
phenylethyl propionate	flavorant	ester	0	0	0.0112	0	0	0
isobutyl isobutyrate	flavorant	ester	0	0	0	0	0	0
melonal	flavorant	aldehyde	0	0	0	0	0	0.0113
3-mercaptohexanol	flavorant	vsc	0	0	0	0	0.1053	0
6-amyl-α-pyrone	flavorant	lactone	0	0	0	0.0057	0.0095	0.0057

3-mercaptohexyl butyrate	flavorant	vsc	0	0	0	0	0	0.0326
methyl senecioate	flavorant	ester	0	0	0	0	0	0
skatole	flavorant	heterocycle	0	0	0	0	0	0
n-decyl acetate	flavorant	ester	0	0	0	0	0	0

Table S16. Analyte Relative-% of volatile fraction (2/5).

Compound name	type	subtype	Zkittlez 710	Banana Scream	Bubblegum Zkittlez	TK x Butterscotch	Purple Churro	Pure Guava
Exotic score	**NA**	**NA**	**80.1**	**79.7**	**77**	**76.3**	**74.3**	**74**
d-limonene	terpene	monoterpene	16.1753	36.2481	11.3096	32.6762	29.7709	14.1172
caryophyllene	terpene	sesquiterpene	35.0699	15.8363	11.781	17.3976	17.5779	34.4578
α-pinene	terpene	monoterpene	1.6339	9.2041	11.9776	3.3704	5.6369	0.9875
trans-β-ocimene	terpene	monoterpene	0.1083	6.797	1.2231	0.2441	2.3712	1.2253
humulene	terpene	sesquiterpene	13.7972	6.1428	4.5072	7.2931	4.4544	14.6224
β-myrcene	terpene	monoterpene	1.1395	4.9778	42.8863	14.2805	3.572	16.2345
linalool	terpene	monoterpenoid	16.7118	4.0804	3.8872	8.7946	13.2772	7.3829
endo-fenchol	terpene	monoterpenoid	1.7536	3.8643	1.9405	3.0345	4.3089	1.7524
α-terpineol	terpene	monoterpenoid	1.312	2.3427	1.1978	1.8347	2.8673	1.2691
β-pinene	terpene	monoterpene	3.1175	2.1542	2.0376	2.171	4.7765	1.8131
(-)-guaiol	terpene	sesquiterpenoid	0.0429	1.7868	0.0686	0.4061	0.0466	0.0246
camphene	terpene	monoterpene	0.4977	1.3363	0.9348	0.9028	1.1797	0.2946
endo-borneol	terpene	monoterpenoid	0.3882	1.2805	0.9222	0.8031	0.898	0.5005
α-bisabolol	terpene	sesquiterpenoid	1.8548	1.0847	1.5642	1.5941	0.8111	1.6215
terpinolene	terpene	monoterpene	0.2191	0.5332	0.2359	0.4694	0.4152	0.0611
n-hexyl hexanoate	flavorant	ester	0.658	0.3557	0.6466	1.0974	4.8248	0.2776
trans-nerolidol	terpene	sesquiterpenoid	1.7558	0.2733	0.9418	1.3242	0.8343	1.8181
ethyl hexanoate	flavorant	ester	0.0222	0.2348	0	0	0.0259	0
γ-terpinene	terpene	monoterpene	0.0432	0.1912	0.1451	0.1393	0.1323	0.0775
n-hexyl acetate	flavorant	ester	0.0714	0.1466	0.0666	0.0273	0.0782	0.0395
isopulegol	terpene	monoterpenoid	0.2102	0.122	0.0793	0.1394	0.1846	0.1471
α-terpinene	terpene	monoterpene	0.0288	0.1161	0.1884	0.0879	0.0862	0.078
n-propyl hexanoate	flavorant	ester	0.0177	0.0725	0.028	0.0366	0.0304	0.0207
1-octanol	flavorant	alcohol	1.2942	0.054	0.1571	0.0402	0.3835	0.0446
geraniol	terpene	monoterpenoid	0.7283	0.045	0.0418	0.0745	0.0691	0.1134
ethyl senecioate	flavorant	ester	0.0105	0.0437	0.0153	0.0406	0.011	0.0723
n-butyl senecioate	flavorant	ester	0.0281	0.0421	0	0	0.0409	0.0561
indole	flavorant	heterocycle	0.0309	0.0421	0.0777	0.0517	0.0531	0.0454
n-propyl senecioate	flavorant	ester	0	0.042	0	0	0	0
trans-sabinene hydrate	terpene	monoterpenoid	0.0408	0.0409	0.0209	0.0283	0.0455	0.0685
2-heptanone	flavorant	ketone	0.0253	0.0359	0.0438	0.0292	0.0393	0.0539
α-citral	terpene	monoterpenoid	0.0141	0.0302	0.0236	0	0.0176	0.031
isoamyl senecioate	flavorant	ester	0.0198	0.0295	0.0371	0	0.029	0.0452
nonanal	flavorant	aldehyde	0.0157	0.0277	0.0316	0	0.0228	0.0289
isoamyl hexanoate	flavorant	ester	0.0087	0.027	0.0123	0.0813	0.208	0
prenylthiol	flavorant	vsc	0.0656	0.0258	0.1003	0.0514	0.2451	0.1418
3-carene	terpene	monoterpene	0.0112	0.0242	0.096	0.0405	0.0236	0.0411
methyl anthranilate	flavorant	ester	0.0133	0.0204	0.0371	0	0.0231	0.0247
n-octyl acetate	flavorant	ester	0.21	0.0204	0.0588	0.0278	0.1697	0.0084
n-octanal	flavorant	aldehyde	0	0.0192	0	0	0	0
n-hexyl n-butyrate	flavorant	ester	0.0683	0.0191	0.103	1.027	0.1914	0.0122
ethyl anthranilate	flavorant	ester	0	0.0186	0.0231	0	0.0179	0
citronellol	terpene	monoterpenoid	0.4176	0.0181	0.249	0.0431	0.0282	0.0214
3-mercaptohexyl acetate	flavorant	vsc	0	0.0173	0	0.0177	0.0171	0.0844
cherry propanol	flavorant	alcohol	0.009	0.0163	0.0189	0.0172	0.0147	0.0353
1-decanol	flavorant	alcohol	0.1474	0.0154	0.0313	0.0144	0.058	0.0207
sulcatone	flavorant	ketone	0.0096	0.0154	0	0	0.0169	0
sabinene	terpene	monoterpene	0.01	0.0153	0.0232	0.0171	0.0182	0.0207
methyl hexanoate	flavorant	ester	0.0108	0.015	0.0198	0	0.0155	0
ethyl isovalerate	flavorant	ester	0	0.0143	0.0201	0	0	0
methyl octanoate	flavorant	ester	0.0011	0.014	0	0	0	0
ethyl 2-methylbutyrate	flavorant	ester	0.0017	0.0131	0	0	0	0
n-propyl n-butyrate	flavorant	ester	0	0.0102	0	0	0	0
n-heptyl acetate	flavorant	ester	0.0119	0.0073	0.0074	0.0052	0.0074	0

ethyl isobutyrate	flavorant	ester	0	0.0071	0.0032	0.0134	0.0028	0
p-cymene	terpene	monoterpene	0.0032	0.0065	0.0185	0.0064	0.006	0.0366
cis-nerolidol	terpene	sesquiterpenoid	0.0066	0.0049	0.0086	0.0049	0.0045	0
hexyl 2-methylbutyrate	flavorant	ester	0.006	0.0045	0.0096	0.0323	0.0054	0
ethyl n-butyrate	flavorant	ester	0	0.004	0	0	0	0
isobutyl hexanoate	flavorant	ester	0	0	0	0	0	0
cis-3-hexenyl n-butyrate	flavorant	ester	0	0	0.0127	0.0692	0.0113	0
n-hexyl isobutyrate	flavorant	ester	0.0166	0	0.0278	0.0426	0.0209	0
n-heptyl n-butyrate	flavorant	ester	0	0	0.0076	0.016	0.0105	0
methyl n-methylanthranilate	flavorant	ester	0	0	0.0096	0	0	0
phenylethyl n-butyrate	flavorant	ester	0	0	0	0	0	0
isobutyl n-butyrate	flavorant	ester	0	0	0	0	0	0.0078
citronellol acetate	flavorant	ester	0.0159	0	0.0457	0.0092	0.0061	0.0027
phenylethyl isobutyrate	flavorant	ester	0	0	0	0.0014	0	0
isopropyl isobutyrate	flavorant	ester	0	0	0	0	0	0
n-hexyl senecioate	flavorant	ester	0.0209	0	0.0378	0.0399	0	0.041
isopropyl senecioate	flavorant	ester	0	0	0	0.0331	0	0.0421
hexanal	flavorant	aldehyde	0.0102	0	0	0	0	0.0185
phenylethyl propionate	flavorant	ester	0.0396	0	0	0	0	0.0136
isobutyl isobutyrate	flavorant	ester	0	0	0	0	0	0
melonal	flavorant	aldehyde	0.0035	0	0	0	0.0055	0
3-mercaptohexanol	flavorant	vsc	0	0	0	0	0	0
6-amyl-α-pyrone	flavorant	lactone	0	0	0.0098	0	0	0
3-mercaptohexyl butyrate	flavorant	vsc	0	0	0	0	0	0
methyl senecioate	flavorant	ester	0	0	0	0	0	0.0448
skatole	flavorant	heterocycle	0	0	0	0	0	0
n-decyl acetate	flavorant	ester	0	0	0	0	0	0

Table S17. Analyte Relative-% of volatile fraction (3/5).

Compound name	**type**	**subtype**	**Rainbow 2.0**	**Fruity Pebbles**	**OPP x Smarties**	**Gorilla Glue**	**Bubba Kush**	**Trainwreck**	**Bacio Gelato**
Exotic score	**NA**	**NA**	**71.6**	**71.4**	**70.9**	**65.1**	**62.1**	43.7	**43.1**
d-limonene	terpene	monoterpene	34.3789	20.718	36.9823	3.5968	23.0339	12.2101	43.5127
caryophyllene	terpene	sesquiterpene	10.6575	30.8829	9.2902	42.7991	16.812	13.0155	13.552
α-pinene	terpene	monoterpene	5.2216	0.8815	8.9255	0.4424	3.1268	3.1527	8.3441
trans-β-ocimene	terpene	monoterpene	3.7532	0.0718	2.118	0.1258	0.2258	4.8512	1.8997
humulene	terpene	sesquiterpene	3.5552	8.7273	3.1889	14.7369	5.6122	3.4444	2.0416
β-myrcene	terpene	monoterpene	9.8372	1.4092	13.8948	4.2307	18.9858	6.4857	2.6034
linalool	terpene	monoterpenoid	10.9706	20.1411	7.0167	10.9433	13.5439	4.5234	5.1439
endo-fenchol	terpene	monoterpenoid	3.839	2.6546	4.4167	0.8583	3.6677	1.5026	4.1635
α-terpineol	terpene	monoterpenoid	2.5345	2.1	2.77	0.7712	2.4577	1.6744	2.6356
β-pinene	terpene	monoterpene	3.2256	2.1906	3.4377	0.9278	0.4873	5.1007	9.1523
(-)-guaiol	terpene	sesquiterpenoid	2.791	1.5485	0.7865	5.0298	5.0096	0.004	0.0099
camphene	terpene	monoterpene	1.1233	0.2987	1.7948	0.1533	1.0114	0.1877	1.2537
endo-borneol	terpene	monoterpenoid	1.0664	0.5997	1.3762	0.2533	1.0279	0.9989	0.6216
α-bisabolol	terpene	sesquiterpenoid	1.0812	2.461	0.3634	4.6481	2.147	0.4995	1.536
terpinolene	terpene	monoterpene	0.4874	0.3062	0.5381	0.0617	0.4374	1.4305	0.4436
n-hexyl hexanoate	flavorant	ester	2.63	0.4454	1.2694	0.7523	0.1572	25.0386	0.0287
trans-nerolidol	terpene	sesquiterpenoid	1.0435	1.6612	0.1804	1.0865	0.4668	1.1276	0.2321
ethyl hexanoate	flavorant	ester	0.0321	0.0363	0	0.0546	0	0	0
γ-terpinene	terpene	monoterpene	0.1706	0.0653	0.2075	0.0718	0.1545	1.2018	0.2587
n-hexyl acetate	flavorant	ester	0.0916	0.0563	0	0.0839	0.0402	0	0
isopulegol	terpene	monoterpenoid	0.1283	0.2718	0.0858	0.1025	0.0318	0.5815	0.5285
α-terpinene	terpene	monoterpene	0.1042	0.0513	0.1506	0.0335	0.1646	1.546	0.0708
n-propyl hexanoate	flavorant	ester	0.0363	0.032	0.0389	0.0246	0	0	0.04
1-octanol	flavorant	alcohol	0.1349	0.1688	0.0517	0.2084	0.0585	0.0427	0.0447
geraniol	terpene	monoterpenoid	0.1036	0.4841	0.0619	0.0594	0.3996	0.1856	0.4856
ethyl senecioate	flavorant	ester	0.0597	0.0978	0.0329	0.0185	0.0411	0.0255	0.2572
n-butyl senecioate	flavorant	ester	0	0	0	0	0.0446	0	0
indole	flavorant	heterocycle	0	0.0507	0.0458	0	0.038	0.0281	0
n-propyl senecioate	flavorant	ester	0	0.0576	0	0	0	0	0
trans-sabinene hydrate	terpene	monoterpenoid	0.037	0.0689	0.0372	0.0282	0.0114	0.1972	0.119

2-heptanone	flavorant	ketone	0.064	0.0672	0.0408	0.062	0.0612	0.0502	0.0447
α-citral	terpene	monoterpenoid	0	0	0.0311	0.0303	0	0	0
isoamyl senecioate	flavorant	ester	0.0334	0.0408	0.0371	0	0.032	0	0
nonanal	flavorant	aldehyde	0.0294	0	0.0383	0.056	0.028	0	0.0296
isoamyl hexanoate	flavorant	ester	0.103	0.0137	0.1593	0.0131	0	0.0129	0
prenylthiol	flavorant	vsc	0.1175	0.7444	0.0877	0.0309	0.0871	0.0106	0.3718
3-carene	terpene	monoterpene	0.036	0.0178	0.0512	0.0286	0.0553	7.3713	0.0315
methyl anthranilate	flavorant	ester	0.0212	0.0289	0.0303	0.0425	0.0406	0.0496	0.0262
n-octyl acetate	flavorant	ester	0.0472	0.0479	0.0175	0.0732	0.0229	0.0101	0.0087
n-octanal	flavorant	aldehyde	0	0	0	0	0	0	0
n-hexyl n-butyrate	flavorant	ester	0.1196	0.021	0.049	6.5454	0.0174	0.6222	0.0177
ethyl anthranilate	flavorant	ester	0	0.025	0	0	0	0	0
citronellol	terpene	monoterpenoid	0.054	0.1468	0.1265	0.0259	0.1458	0	0.1145
3-mercaptohexyl acetate	flavorant	vsc	0.0197	0	0	0.0267	0	0	0.0335
cherry propanol	flavorant	alcohol	0.0166	0.0178	0.0211	0.0192	0.0159	1.2901	0.0212
1-decanol	flavorant	alcohol	0.0243	0.0321	0.0197	0.0962	0.0171	0.0356	0.0181
sulcatone	flavorant	ketone	0.0183	0.0217	0.018	0.0255	0.0203	0.0619	0.0192
sabinene	terpene	monoterpene	0.0186	0.019	0.0096	0.0266	0.0106	0.514	0.0194
methyl hexanoate	flavorant	ester	0.0183	0.0244	0.0187	0.0283	0.0203	0.0218	0.0187
ethyl isovalerate	flavorant	ester	0	0.0157	0	0	0.0143	0	0.0141
methyl octanoate	flavorant	ester	0	0.0004	0	0.001	0	0	0
ethyl 2-methylbutyrate	flavorant	ester	0.0038	0	0	0	0	0	0.0037
n-propyl n-butyrate	flavorant	ester	0	0	0	0	0	0	0
n-heptyl acetate	flavorant	ester	0.0062	0.0071	0	0.0161	0.0056	0	0.0061
ethyl isobutyrate	flavorant	ester	0.0082	0.0069	0.0126	0	0	0	0
p-cymene	terpene	monoterpene	0.0062	0.0072	0.0097	0.0083	0.0175	0.8136	0.0108
cis-nerolidol	terpene	sesquiterpenoid	0.0046	0.0066	0.0054	0.0092	0.0045	0	0
hexyl 2-methylbutyrate	flavorant	ester	0.0056	0	0.0062	0.0699	0.0046	0.0195	0.0059
ethyl n-butyrate	flavorant	ester	0	0	0	0	0	0	0
isobutyl hexanoate	flavorant	ester	0	0	0	0	0	0	0
cis-3-hexenyl n-butyrate	flavorant	ester	0.0111	0	0.0196	0.1399	0	0.0253	0
n-hexyl isobutyrate	flavorant	ester	0.0195	0.0203	0.0194	0.1678	0	0	0
n-heptyl n-butyrate	flavorant	ester	0.0102	0	0.0108	0.1402	0.006	0.0352	0
methyl n-methylanthranilate	flavorant	ester	0	0	0	0	0.0086	0	0
phenylethyl n-butyrate	flavorant	ester	0	0	0	0	0	0	0
isobutyl n-butyrate	flavorant	ester	0	0	0	0.01	0	0	0
citronellol acetate	flavorant	ester	0.0054	0.0162	0.0204	0	0.0231	0	0.0051
phenylethyl isobutyrate	flavorant	ester	0	0	0	0.0008	0	0	0
isopropyl isobutyrate	flavorant	ester	0	0	0	0	0.0085	0	0
n-hexyl senecioate	flavorant	ester	0.0333	0.0421	0.0389	0.0453	0.0387	0	0.0351
isopropyl senecioate	flavorant	ester	0.035	0.0506	0.0389	0	0.0566	0	0.0394
hexanal	flavorant	aldehyde	0.0153	0	0	0.0221	0.0177	0	0
phenylethyl propionate	flavorant	ester	0	0	0	0.0191	0	0	0
isobutyl isobutyrate	flavorant	ester	0	0	0	0	0	0	0
melonal	flavorant	aldehyde	0	0	0	0	0.0059	0	0
3-mercaptohexanol	flavorant	vsc	0	0	0	0.0676	0	0	0
6-amyl-α-pyrone	flavorant	lactone	0	0.0075	0	0.0098	0	0.0050	
3-mercaptohexyl butyrate	flavorant	vsc	0	0	0	0.0496	0	0	0
methyl senecioate	flavorant	ester	0	0	0	0	0.0277	0	0.0463
skatole	flavorant	heterocycle	0	0.0201	0	0	0	0	0
n-decyl acetate	flavorant	ester	0	0	0	0	0	0	0

Table S18. Analyte Relative-% of volatile fraction (4/5).

Compound name	type	subtype	MAC 1	Gelato 33	Kimbo Kush	Lucky Charms	Pie Hoe	MAC 1
Exotic score			39.3	34.6	34	30.7	25.3	39.3
d-limonene	terpene	monoterpene	21.61	37.865	43.487	30.5529	20.2043	21.61
caryophyllene	terpene	sesquiterpene	21.5352	18.3354	13.4636	23.4073	22.683	21.5352
α-pinene	terpene	monoterpene	4.8425	6.8311	4.0104	1.7604	2.0421	4.8425
trans-β-ocimene	terpene	monoterpene	0.9066	1.1285	0.2528	0.0403	0.0358	0.9066
humulene	terpene	sesquiterpene	6.7262	3.419	3.6722	8.9846	7.8301	6.7262

β-myrcene	terpene	monoterpene	2.713	5.762	2.3623	12.2294	20.3253	2.713
linalool	terpene	monoterpenoid	9.4449	6.7697	12.0566	3.8827	13.558	9.4449
endo-fenchol	terpene	monoterpenoid	5.3905	3.4009	3.2274	3.1542	2.2533	5.3905
α-terpineol	terpene	monoterpenoid	4.0897	2.2347	2.7533	2.4752	1.7709	4.0897
β-pinene	terpene	monoterpene	6.5793	7.8047	7.0872	3.2947	3.3477	6.5793
(-)-guaiol	terpene	sesquiterpenoid	0.0162	0.0078	0.0152	0.0124	0.0116	0.0162
camphene	terpene	monoterpene	1.0395	1.0761	1.2317	0.5334	0.5801	1.0395
endo-borneol	terpene	monoterpenoid	1.0285	0.5368	0.7057	0.8924	0.6365	1.0285
α-bisabolol	terpene	sesquiterpenoid	9.6149	1.6989	2.3292	2.0984	2.0287	9.6149
terpinolene	terpene	monoterpene	0.332	0.3964	0.5618	0.2849	0.1411	0.332
n-hexyl hexanoate	flavorant	ester	0.3951	0.1976	0.214	1.4552	0.5657	0.3951
trans-nerolidol	terpene	sesquiterpenoid	1.7494	0.1867	0.6428	1.7355	0.0362	1.7494
ethyl hexanoate	flavorant	ester	0.0466	0	0.0522	0	0	0.0466
γ-terpinene	terpene	monoterpene	0.1513	0.2434	0.1433	0.0483	0.059	0.1513
n-hexyl acetate	flavorant	ester	0	0	0	0.0546	0.0322	0
isopulegol	terpene	monoterpenoid	0.4448	0.4534	0.2201	0.2338	0.2006	0.4448
α-terpinene	terpene	monoterpene	0.1089	0.0669	0.1111	0.0662	0.0779	0.1089
n-propyl hexanoate	flavorant	ester	0	0.0406	0	0	0.0227	0
1-octanol	flavorant	alcohol	0.0635	0.0455	0.0474	0.5121	0.1335	0.0635
geraniol	terpene	monoterpenoid	0.0485	0.3472	0.307	1.3384	0.4192	0.0485
ethyl senecioate	flavorant	ester	0.031	0.1903	0.015	0.0114	0.0479	0.031
n-butyl senecioate	flavorant	ester	0.0744	0	0.0598	0.0444	0.0487	0.0744
indole	flavorant	heterocycle	0.0654	0	0.0601	0.0413	0.0451	0.0654
n-propyl senecioate	flavorant	ester	0	0	0	0	0	0
trans-sabinene hydrate	terpene	monoterpenoid	0.1459	0.0983	0.0828	0.0632	0.0646	0.1459
2-heptanone	flavorant	ketone	0.0466	0.0654	0.0601	0.0427	0.0424	0.0466
α-citral	terpene	monoterpenoid	0	0.0501	0.0383	0	0.0193	0
isoamyl senecioate	flavorant	ester	0.0531	0	0	0.0316	0.0348	0.0531
nonanal	flavorant	aldehyde	0.0924	0.034	0.0373	0.0254	0	0.0924
isoamyl hexanoate	flavorant	ester	0.0357	0	0	0.0178	0	0.0357
prenylthiol	flavorant	vsc	0.0463	0.2803	0.076	0.1078	0.1499	0.0463
3-carene	terpene	monoterpene	0.0396	0.0411	0.0396	0.0365	0.0474	0.0396
methyl anthranilate	flavorant	ester	0.0447	0.028	0.0366	0.017	0.0203	0.0447
n-octyl acetate	flavorant	ester	0.0133	0.0076	0.0107	0.1794	0.0497	0.0133
n-octanal	flavorant	aldehyde	0	0	0	0	0	0
n-hexyl n-butyrate	flavorant	ester	0.0298	0.0191	0.028	0.0864	0.0195	0.0298
ethyl anthranilate	flavorant	ester	0	0	0	0	0	0
citronellol	terpene	monoterpenoid	0.1098	0.1027	0.2035	0.0315	0.1379	0.1098
3-mercaptohexyl acetate	flavorant	vsc	0	0	0	0.024	0	0
cherry propanol	flavorant	alcohol	0.0296	0.018	0.0232	0.0301	0.0324	0.0296
1-decanol	flavorant	alcohol	0.026	0.0183	0	0.0663	0.0263	0.026
sulcatone	flavorant	ketone	0.0359	0.0182	0.0339	0	0	0.0359
sabinene	terpene	monoterpene	0.0482	0.02	0.0237	0.013	0.0177	0.0482
methyl hexanoate	flavorant	ester	0.0303	0.0224	0.0235	0.018	0.019	0.0303
ethyl isovalerate	flavorant	ester	0	0	0.0216	0	0.0134	0
methyl octanoate	flavorant	ester	0	0	0	0	0	0
ethyl 2-methylbutyrate	flavorant	ester	0	0	0.025	0	0	0
n-propyl n-butyrate	flavorant	ester	0	0	0.0128	0	0	0
n-heptyl acetate	flavorant	ester	0	0	0	0.0071	0.0054	0
ethyl isobutyrate	flavorant	ester	0	0	0	0	0.0051	0
p-cymene	terpene	monoterpene	0.0152	0	0.0118	0.0256	0.03	0.0152
cis-nerolidol	terpene	sesquiterpenoid	0.0139	0	0.0057	0	0	0.0139
hexyl 2-methylbutyrate	flavorant	ester	0.0078	0	0	0.0079	0	0.0078
ethyl n-butyrate	flavorant	ester	0	0	0.0531	0	0	0
isobutyl hexanoate	flavorant	ester	0	0	0	0	0	0
cis-3-hexenyl n-butyrate	flavorant	ester	0	0	0	0	0	0
n-hexyl isobutyrate	flavorant	ester	0	0	0	0	0	0
n-heptyl n-butyrate	flavorant	ester	0	0	0	0	0	0
methyl n-methylanthranilate	flavorant	ester	0	0	0	0	0	0
phenylethyl n-butyrate	flavorant	ester	0.0115	0	0	0	0	0.0115
isobutyl n-butyrate	flavorant	ester	0	0	0	0	0	0
citronellol acetate	flavorant	ester	0.023	0.0045	0.0131	0.0047	0.021	0.023
phenylethyl isobutyrate	flavorant	ester	0	0	0	0	0	0

isopropyl isobutyrate	flavorant	ester	0	0	0	0	0	0
n-hexyl senecioate	flavorant	ester	0	0.0362	0	0	0.0369	0
isopropyl senecioate	flavorant	ester	0	0.0394	0	0	0.0394	0
hexanal	flavorant	aldehyde	0.0248	0	0.0218	0	0	0.0248
phenylethyl propionate	flavorant	ester	0.0186	0	0	0.0138	0	0.0186
isobutyl isobutyrate	flavorant	ester	0	0	0	0	0	0
melonal	flavorant	aldehyde	0.0101	0	0.008	0.0058	0	0.0101
3-mercaptohexanol	flavorant	vsc	0	0	0	0	0	0
6-amyl-α-pyrone	flavorant	lactone	0.0075	0	0	0	0	0
3-mercaptohexyl butyrate	flavorant	vsc	0	0	0	0	0	0
methyl senecioate	flavorant	ester	0	0.0396	0	0	0.0301	0
skatole	flavorant	heterocycle	0	0	0	0	0	0
n-decyl acetate	flavorant	ester	0	0	0	0	0	0

Table S19. Analyte Relative-% of volatile fraction (5/5).

Compound name	type	subtype	Cookies and Cream	GMO Cookies	OG	710 chem	GMO	Cookies and Cream
Exotic score			15.4	5.7	3	1.9	1.7	15.4
d-limonene	terpene	monoterpene	21.5036	24.8209	24.4908	20.1589	29.3007	21.5036
caryophyllene	terpene	sesquiterpene	41.5605	29.424	19.5946	43.0426	17.9806	41.5605
α-pinene	terpene	monoterpene	2.2246	3.0221	2.0443	1.5085	2.1678	2.2246
trans-β-ocimene	terpene	monoterpene	0.0576	0.0462	0.0564	0.0562	0.0631	0.0576
humulene	terpene	sesquiterpene	13.3704	13.554	6.5222	11.1611	8.3828	13.3704
β-myrcene	terpene	monoterpene	5.8242	11.3533	18.0528	9.7584	22.4114	5.8242
linalool	terpene	monoterpenoid	3.9858	3.2301	11.7246	0.042	3.8951	3.9858
endo-fenchol	terpene	monoterpenoid	1.6071	2.6289	3.6236	2.5714	2.5936	1.6071
α-terpineol	terpene	monoterpenoid	1.1996	1.4356	3.2807	1.7754	1.9927	1.1996
β-pinene	terpene	monoterpene	4.119	1.6272	4.3316	2.991	3.7193	4.119
(-)-guaiol	terpene	sesquiterpenoid	0.0174	0.0278	0.0132	0.0198	0.0132	0.0174
camphene	terpene	monoterpene	0.6655	0.689	0.639	0.4529	0.6089	0.6655
endo-borneol	terpene	monoterpenoid	0.4494	0.6347	0.9596	0.5867	0.6849	0.4494
α-bisabolol	terpene	sesquiterpenoid	0.914	4.915	1.3397	1.8899	2.574	0.914
terpinolene	terpene	monoterpene	0.2299	0.4503	0.3081	0.2752	0.3194	0.2299
n-hexyl hexanoate	flavorant	ester	0.1174	0.3316	1.0639	0.6866	0.9566	0.1174
trans-nerolidol	terpene	sesquiterpenoid	0.6837	0.6473	0	1.4578	0.9205	0.6837
ethyl hexanoate	flavorant	ester	0	0	0.0245	0	0	0
γ-terpinene	terpene	monoterpene	0.058	0.1585	0.0567	0.0435	0.1683	0.058
n-hexyl acetate	flavorant	ester	0	0.0301	0.0253	0	0.0303	0
isopulegol	terpene	monoterpenoid	0.2099	0.0349	0.5578	0.349	0.2207	0.2099
α-terpinene	terpene	monoterpene	0.0568	0.1428	0.0625	0.0613	0.1124	0.0568
n-propyl hexanoate	flavorant	ester	0	0.0291	0	0.0288	0.0296	0
1-octanol	flavorant	alcohol	0.041	0.0355	0.0424	0.0418	0.0377	0.041
geraniol	terpene	monoterpenoid	0.042	0.0497	0.3422	0.1669	0.0405	0.042
ethyl senecioate	flavorant	ester	0.2558	0.0958	0	0.0331	0.0205	0.2558
n-butyl senecioate	flavorant	ester	0	0	0	0.0527	0.0471	0
indole	flavorant	heterocycle	0.0384	0.031	0.0314	0.0507	0	0.0384
n-propyl senecioate	flavorant	ester	0.048	0	0	0	0	0.048
trans-sabinene hydrate	terpene	monoterpenoid	0.0913	0.0154	0.0975	0.0606	0.0523	0.0913
2-heptanone	flavorant	ketone	0.0323	0.0279	0.0271	0.0413	0.0404	0.0323
α-citral	terpene	monoterpenoid	0.0326	0	0	0	0	0.0326
isoamyl senecioate	flavorant	ester	0.033	0.0279	0	0.0359	0.0335	0.033
nonanal	flavorant	aldehyde	0.0526	0	0	0.0297	0	0.0526
isoamyl hexanoate	flavorant	ester	0	0	0.0443	0.1741	0.0113	0
prenylthiol	flavorant	vsc	0.0629	0.093	0.0688	0.1884	0.1832	0.0629
3-carene	terpene	monoterpene	0.0262	0.0364	0.0349	0.0317	0.0473	0.0262
methyl anthranilate	flavorant	ester	0.024	0.017	0	0	0.0179	0.024
n-octyl acetate	flavorant	ester	0.01	0.0077	0.0099	0.0127	0	0.01
n-octanal	flavorant	aldehyde	0.0199	0	0	0	0	0.0199
n-hexyl n-butyrate	flavorant	ester	0.0142	0.0095	0.0198	0.0271	0.0432	0.0142
ethyl anthranilate	flavorant	ester	0	0	0	0	0	0
citronellol	flavorant	alcohol	0.0361	0.0513	0.3351	0.0305	0.029	0.0361
3-mercaptohexyl acetate	flavorant	vsc	0	0	0	0	0	0
cherry propanol	flavorant	alcohol	0.0193	0.0152	0.0173	0.0154	0.022	0.0193

1-decanol	flavorant	alcohol	0.0152	0.0128	0.0153	0	0	0.0152
sulcatone	flavorant	ketone	0.0271	0.0137	0.0126	0	0	0.0271
sabinene	terpene	monoterpene	0.0179	0.0113	0.0205	0.0166	0.0145	0.0179
methyl hexanoate	flavorant	ester	0.0188	0	0.0139	0.0227	0.0163	0.0188
ethyl isovalerate	flavorant	ester	0.0132	0	0	0.0132	0	0.0132
methyl octanoate	flavorant	ester	0.002	0.0032	0	0	0	0.002
ethyl 2-methylbutyrate	flavorant	ester	0.0031	0	0	0	0	0.0031
n-propyl n-butyrate	flavorant	ester	0	0	0	0	0	0
n-heptyl acetate	flavorant	ester	0	0	0.0042	0	0	0
ethyl isobutyrate	flavorant	ester	0	0	0	0	0.0028	0
p-cymene	terpene	monoterpene	0.0081	0.1005	0.0048	0.0056	0.0205	0.0081
cis-nerolidol	terpene	sesquiterpenoid	0.0134	0.008	0.0038	0	0	0.0134
hexyl 2-methylbutyrate	flavorant	ester	0.0049	0.0046	0.0057	0.0064	0.0052	0.0049
ethyl n-butyrate	flavorant	ester	0	0	0	0	0	0
isobutyl hexanoate	flavorant	ester	0	0	0	0	0	0
cis-3-hexenyl n-butyrate	flavorant	ester	0	0	0	0	0	0
n-hexyl isobutyrate	flavorant	ester	0	0	0.0148	0	0.0203	0
n-heptyl n-butyrate	flavorant	ester	0	0	0	0	0	0
methyl n-methylanthranilate	flavorant	ester	0	0	0	0	0	0
phenylethyl n-butyrate	flavorant	ester	0	0	0	0	0	0
isobutyl n-butyrate	flavorant	ester	0	0	0	0	0	0
citronellol acetate	flavorant	ester	0.0061	0.0075	0.0463	0.002	0.0088	0.0061
phenylethyl isobutyrate	flavorant	ester	0	0	0	0	0	0
isopropyl isobutyrate	flavorant	ester	0	0	0	0	0	0
n-hexyl senecioate	flavorant	ester	0.0325	0.0368	0	0	0.035	0.0325
isopropyl senecioate	flavorant	ester	0.0355	0	0	0	0.0364	0.0355
hexanal	flavorant	aldehyde	0.0182	0	0.0155	0	0	0.0182
phenylethyl propionate	flavorant	ester	0	0	0	0	0	0
isobutyl isobutyrate	flavorant	ester	0	0	0	0	0	0
melonal	flavorant	aldehyde	0.0067	0	0	0.0065	0.0061	0.0067
3-mercaptohexanol	flavorant	vsc	0	0	0	0	0	0
6-amyl-α-pyrone	flavorant	lactone	0.0038	0	0	0	0	0
3-mercaptohexyl butyrate	flavorant	vsc	0	0	0	0	0	0
methyl senecioate	flavorant	ester	0.0278	0.0253	0	0	0.04	0.0278
skatole	flavorant	heterocycle	0	0.0136	0	0.0178	0.0223	0
n-decyl acetate	flavorant	ester	0	0.0044	0	0	0	0

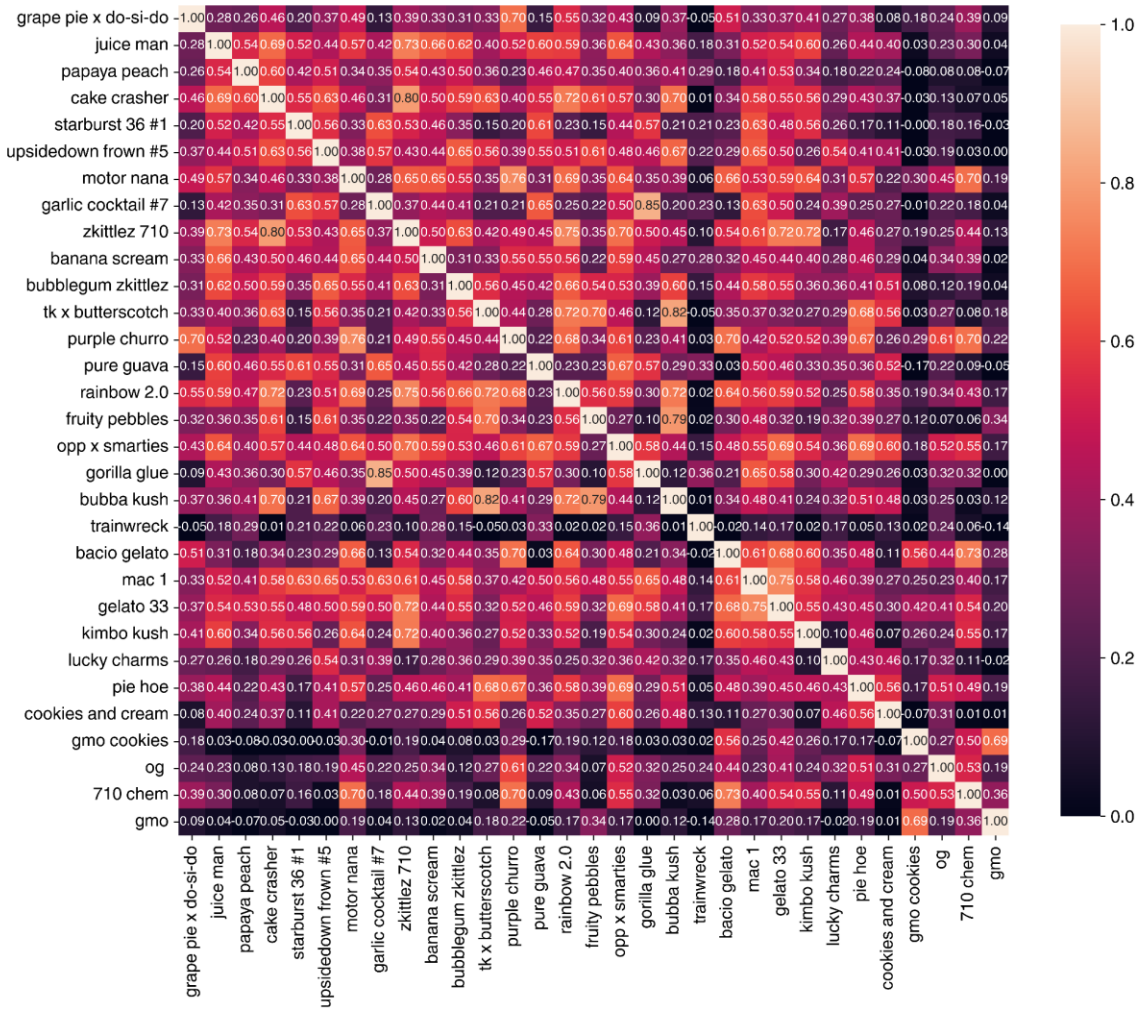

Figure S1. Pearson Correlation matrix showing relationship between sensory results of each variety measured. Higher values indicate greater aromatic similarity between varieties.

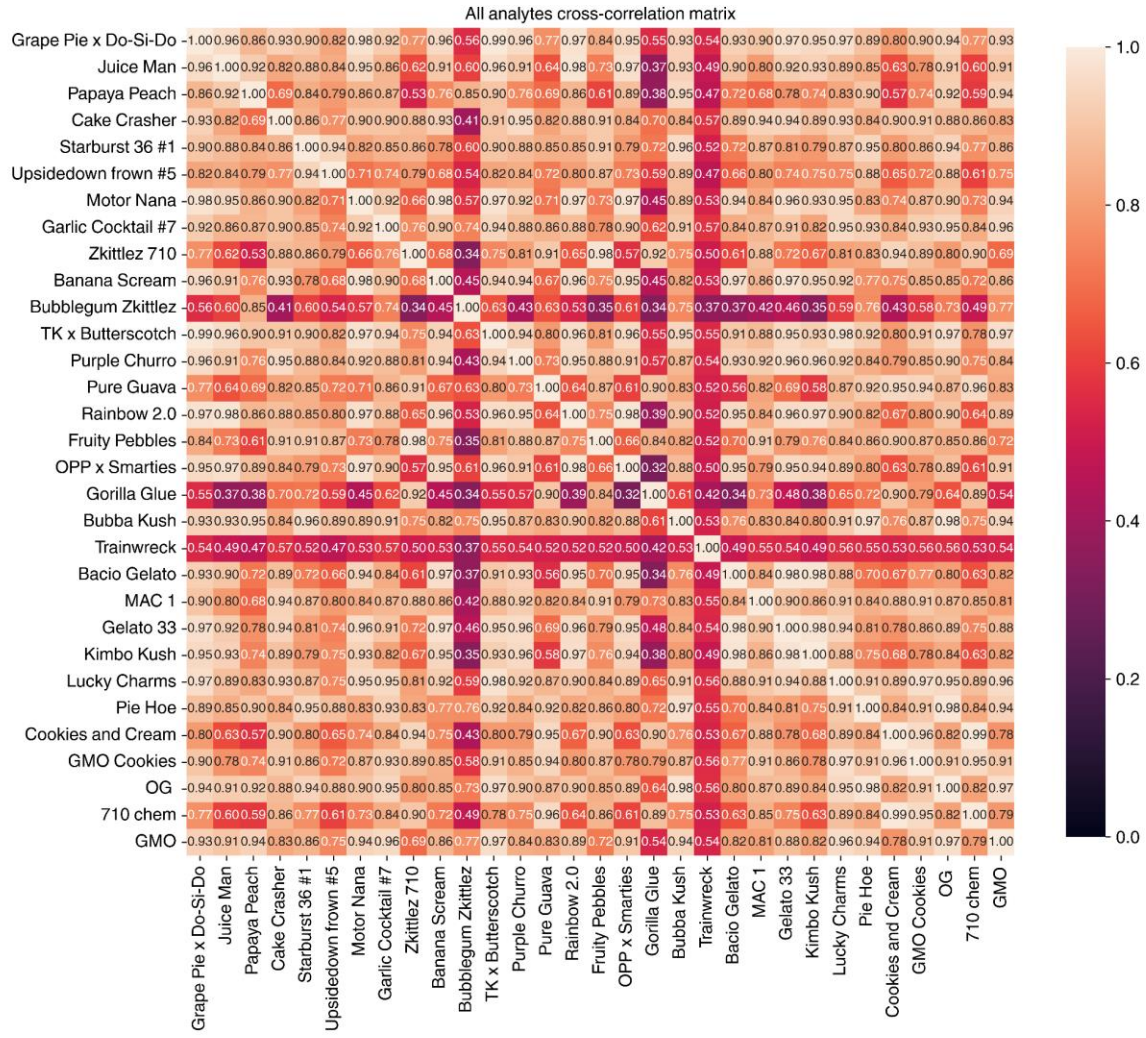

Figure S2. Pearson Correlation matrix showing relationship between each variety measured for all analytes. Higher values indicate greater chemical similarity between varieties.

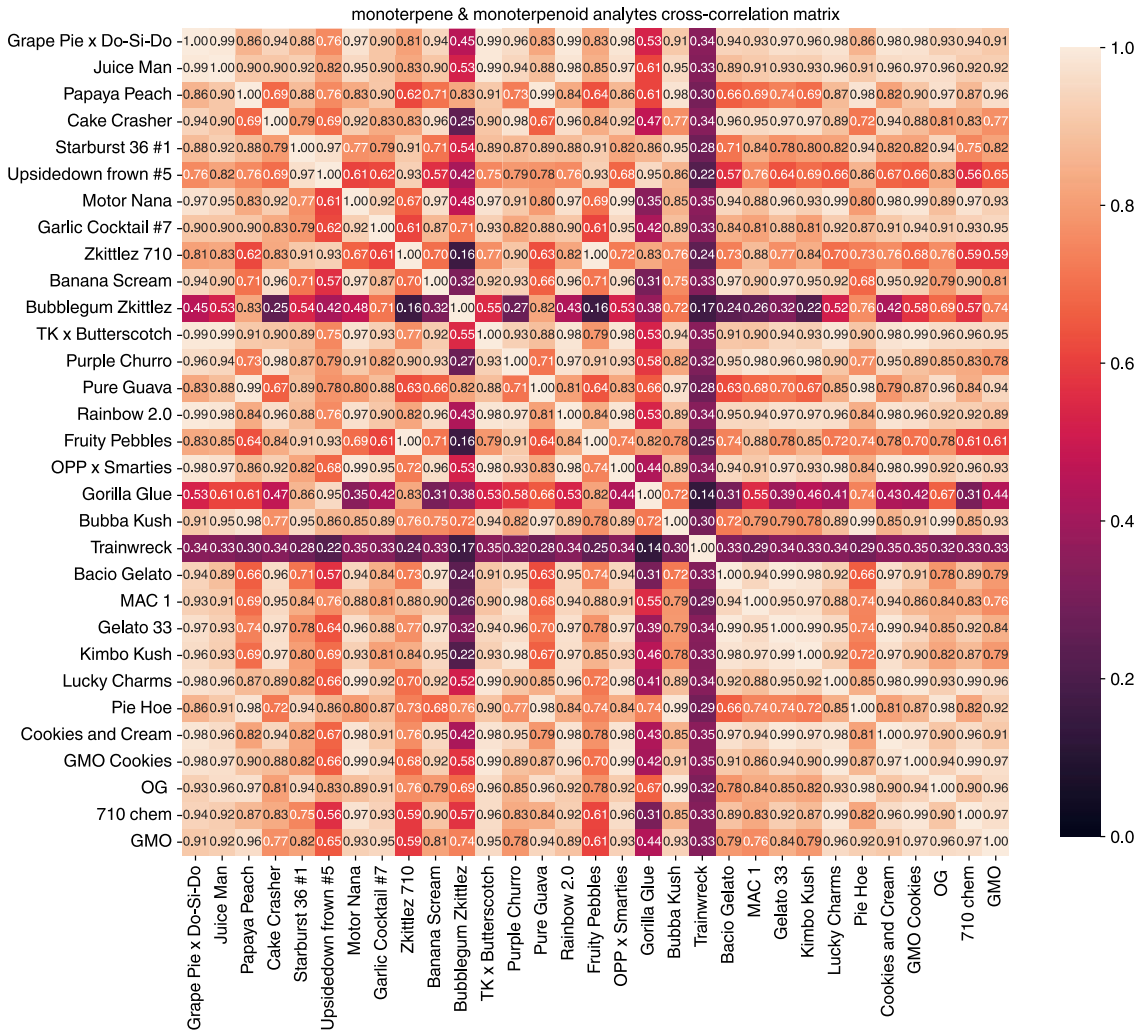

Figure S3. Pearson Correlation matrix showing relationship between each variety measured for monoterpene and monoterpenoids. Higher values indicate greater chemical similarity between varieties.

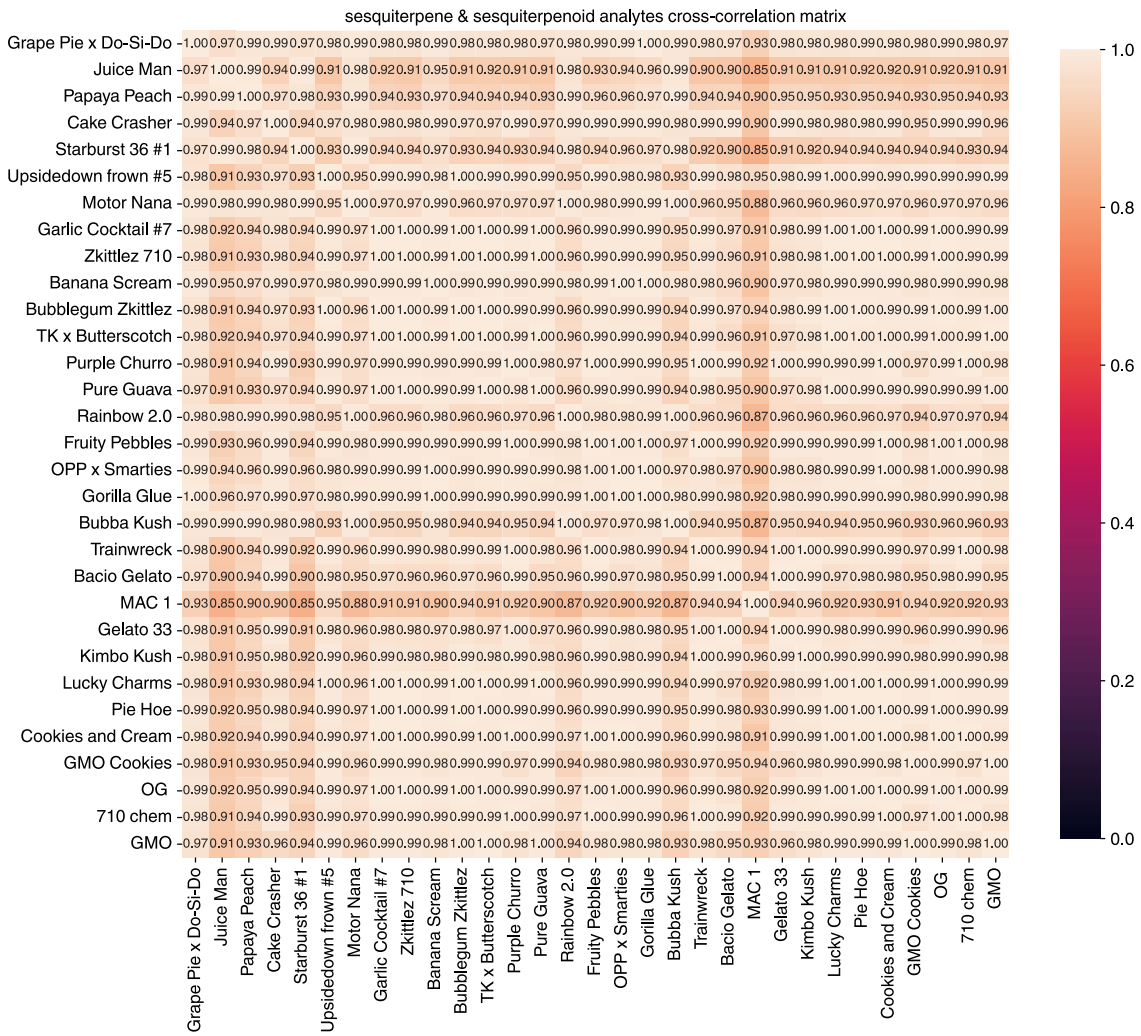

Figure S4. Pearson Correlation matrix showing relationship between each variety measured for sesquiterpene and sesquiterpenoids. Higher values indicate greater chemical similarity between varieties.

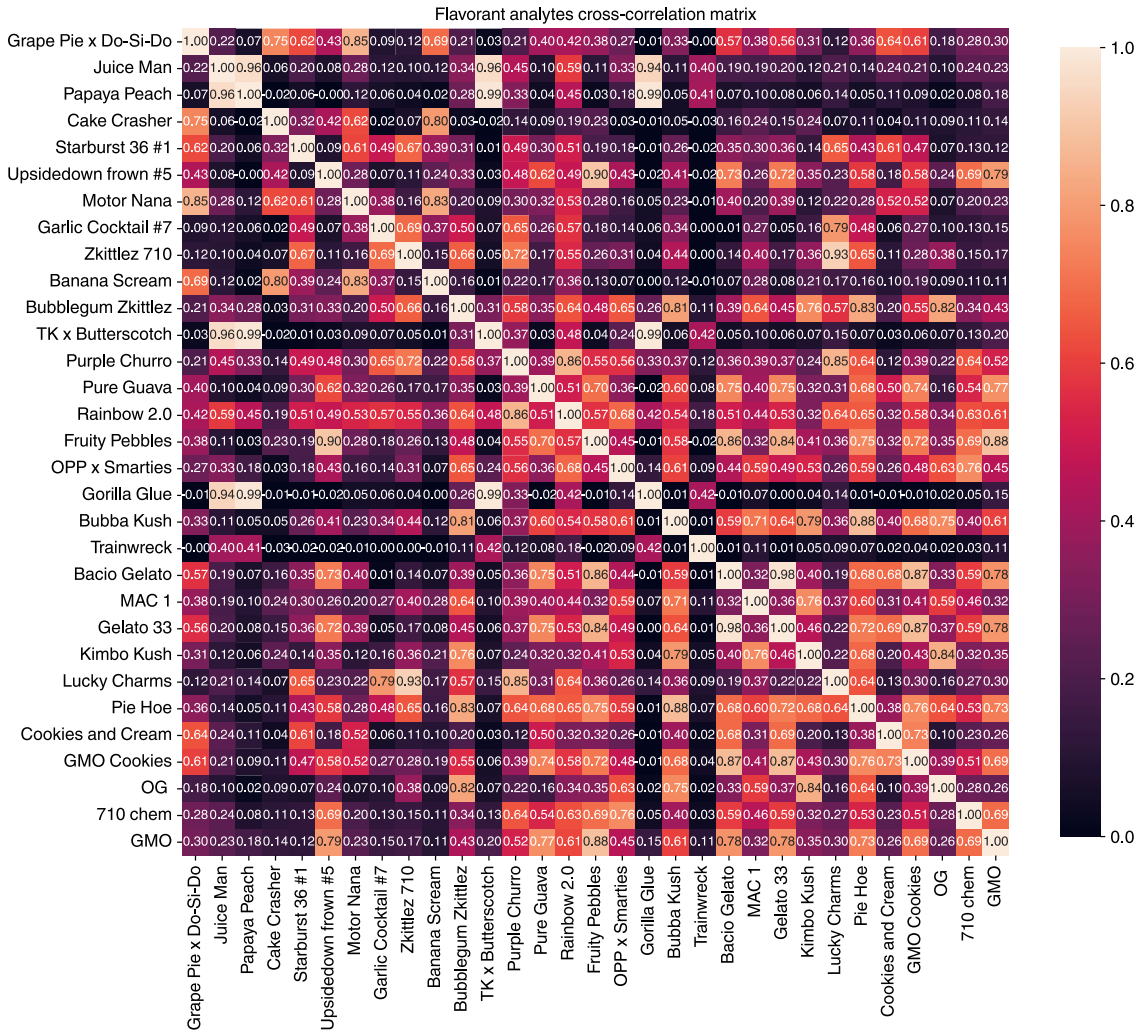

Figure S5. Pearson Correlation matrix showing relationship between each variety measured for flavorants excluding *n*-hexyl hexanoate. Higher values indicate greater chemical similarity between varieties.

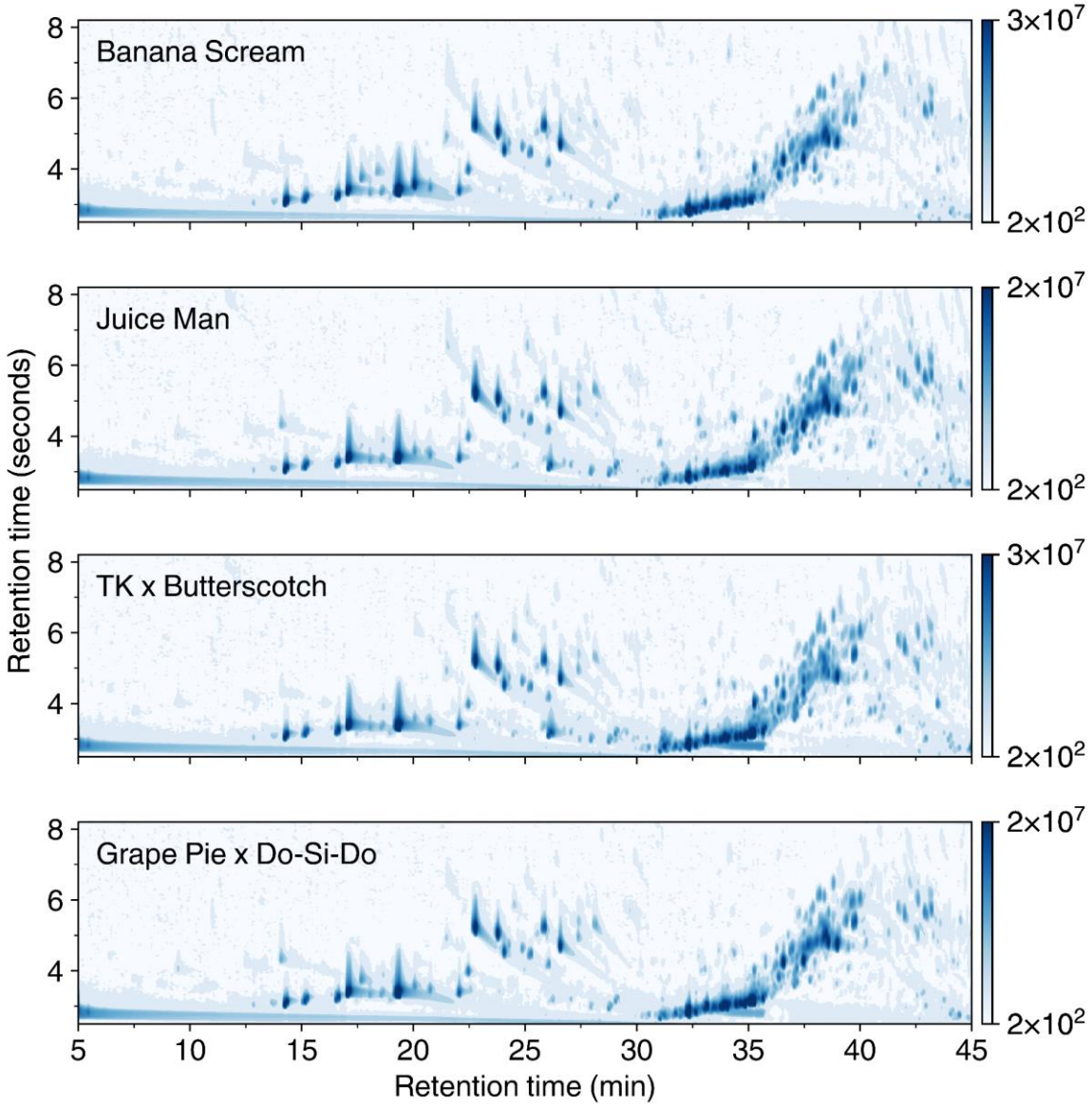

Figure S6. GC×GC–FID 2-Dimensional chromatograms for Banana Scream, Juice Man, TK x Butterscotch, and Grape Pie x Do-Si-Do.

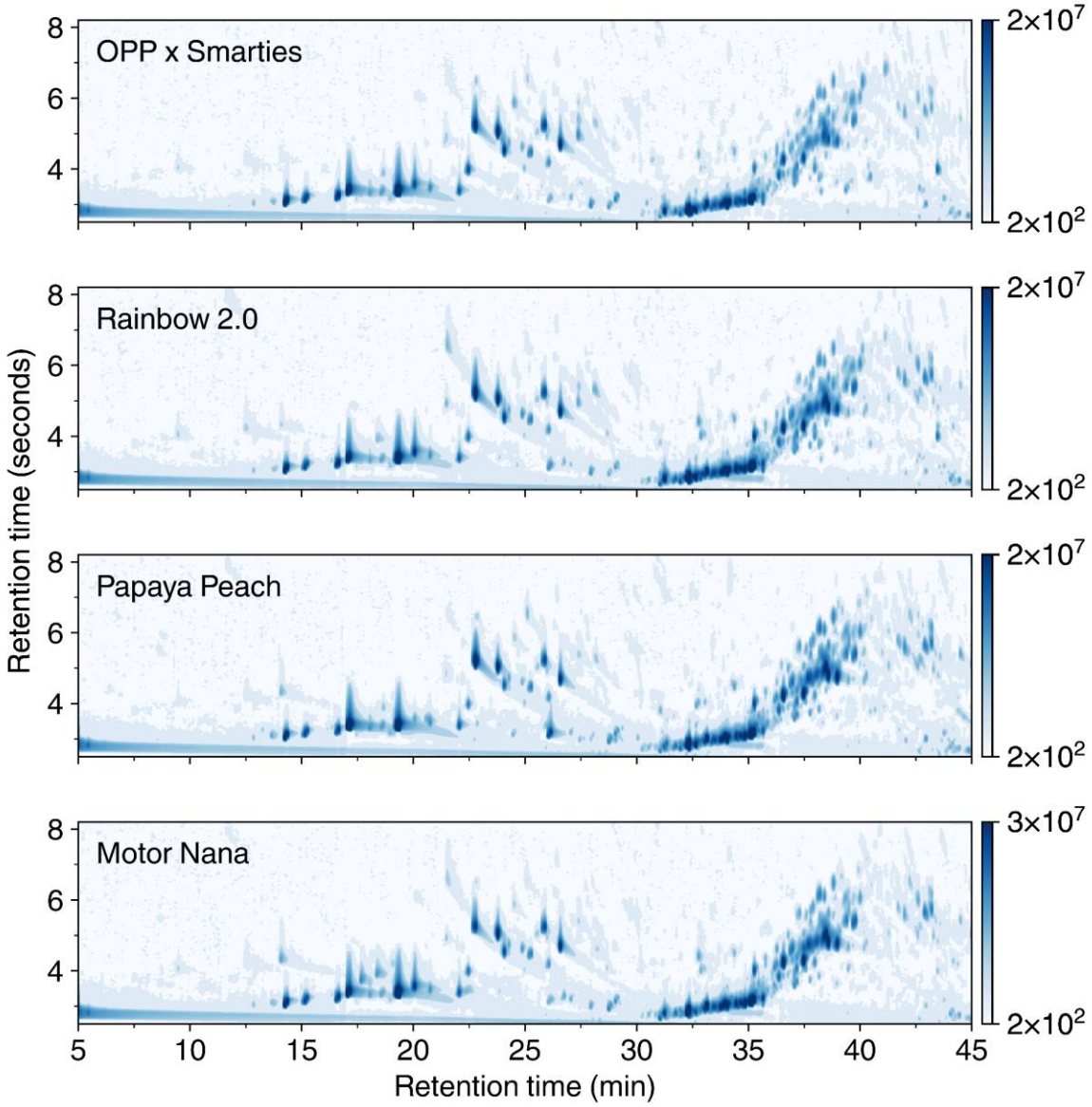

Figure S7. GC×GC–FID 2-Dimensional chromatograms for OPP x Smarties, Rainbow 2.0, Papaya Peach, and Motor Nana.

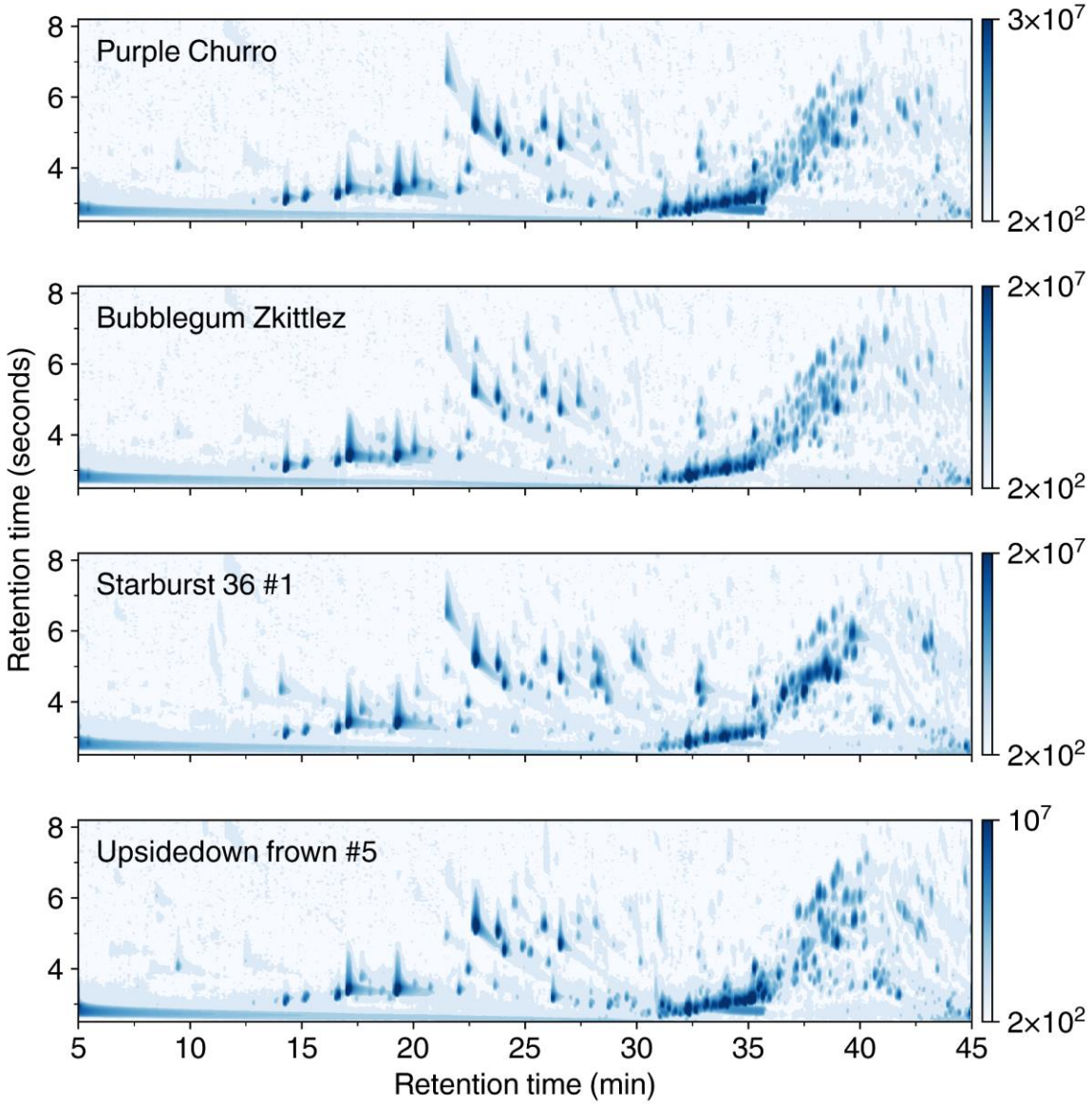

Figure S8. GC×GC–FID 2-Dimensional chromatograms for Purple Churro, Bubblegum Zkittlez, Starburst 36 #1, and Upsidedown frown #5.

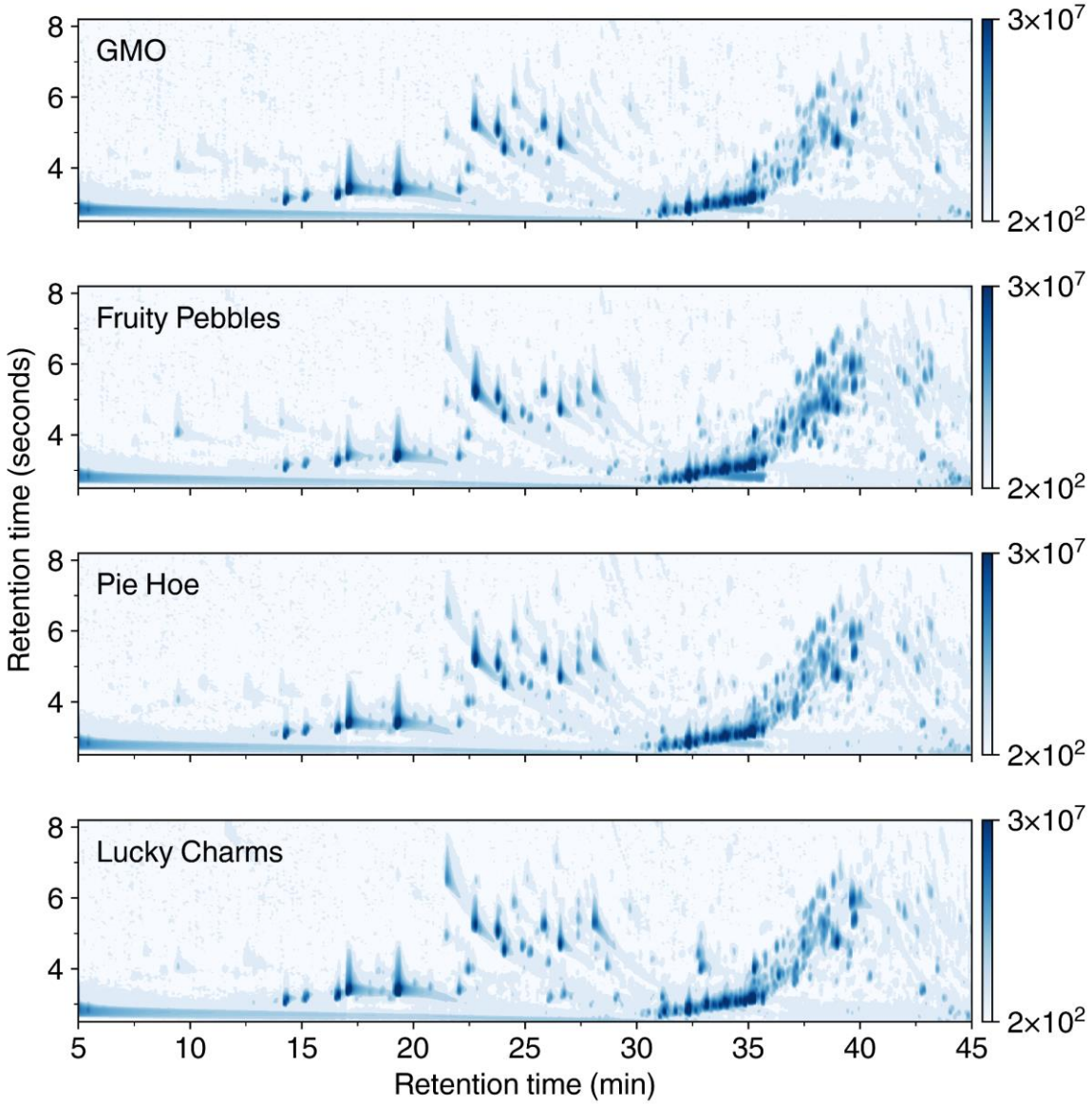

Figure S9. GC×GC–FID 2-Dimensional chromatograms for GMO, Fruity Pebbles, Pie Hoe, and Lucky Charms.

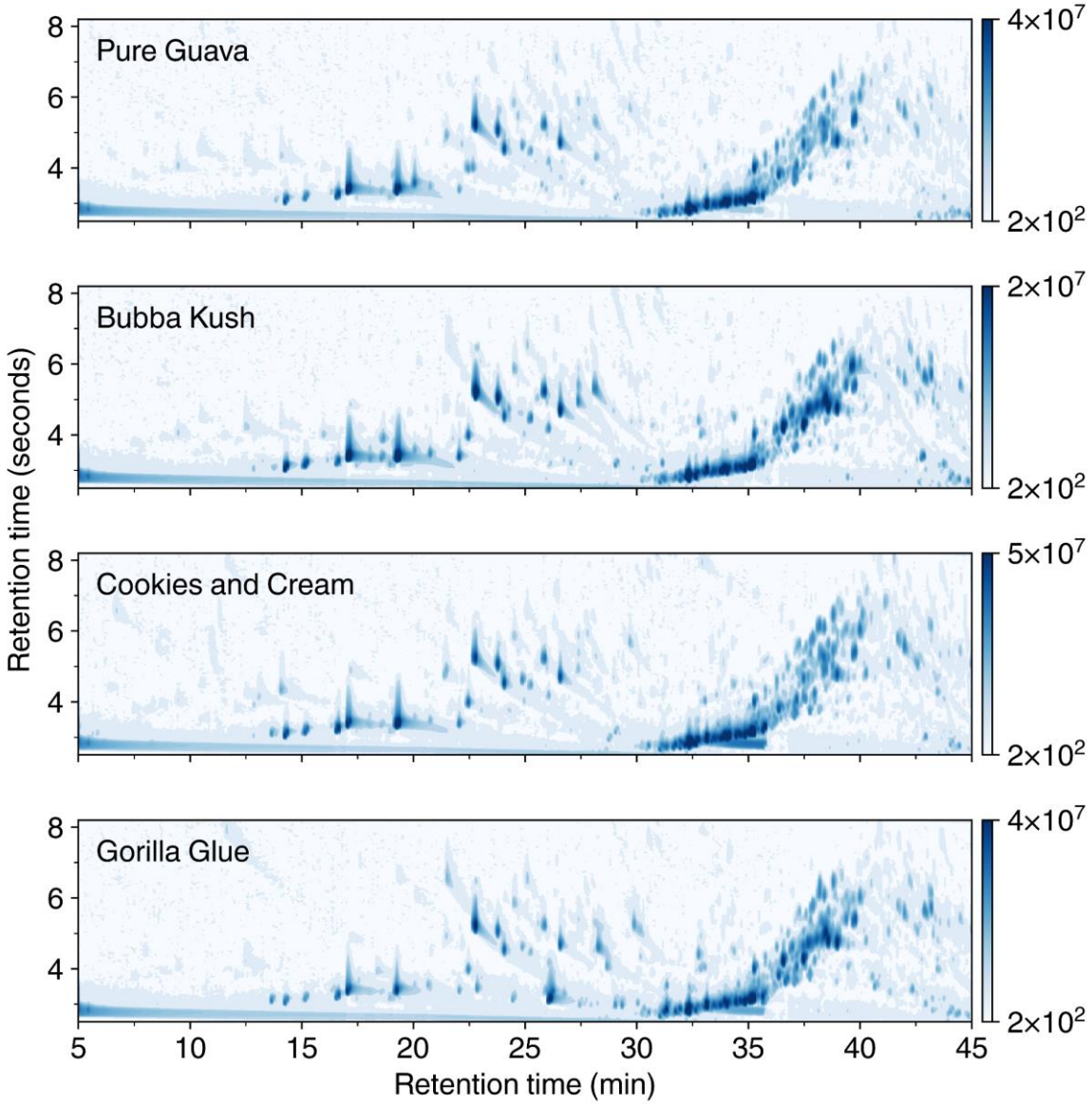

Figure S10. GC×GC–FID 2-Dimensional chromatograms for Pure Guava, Bubba Kush, Cookies and Cream, and Gorilla Glue.

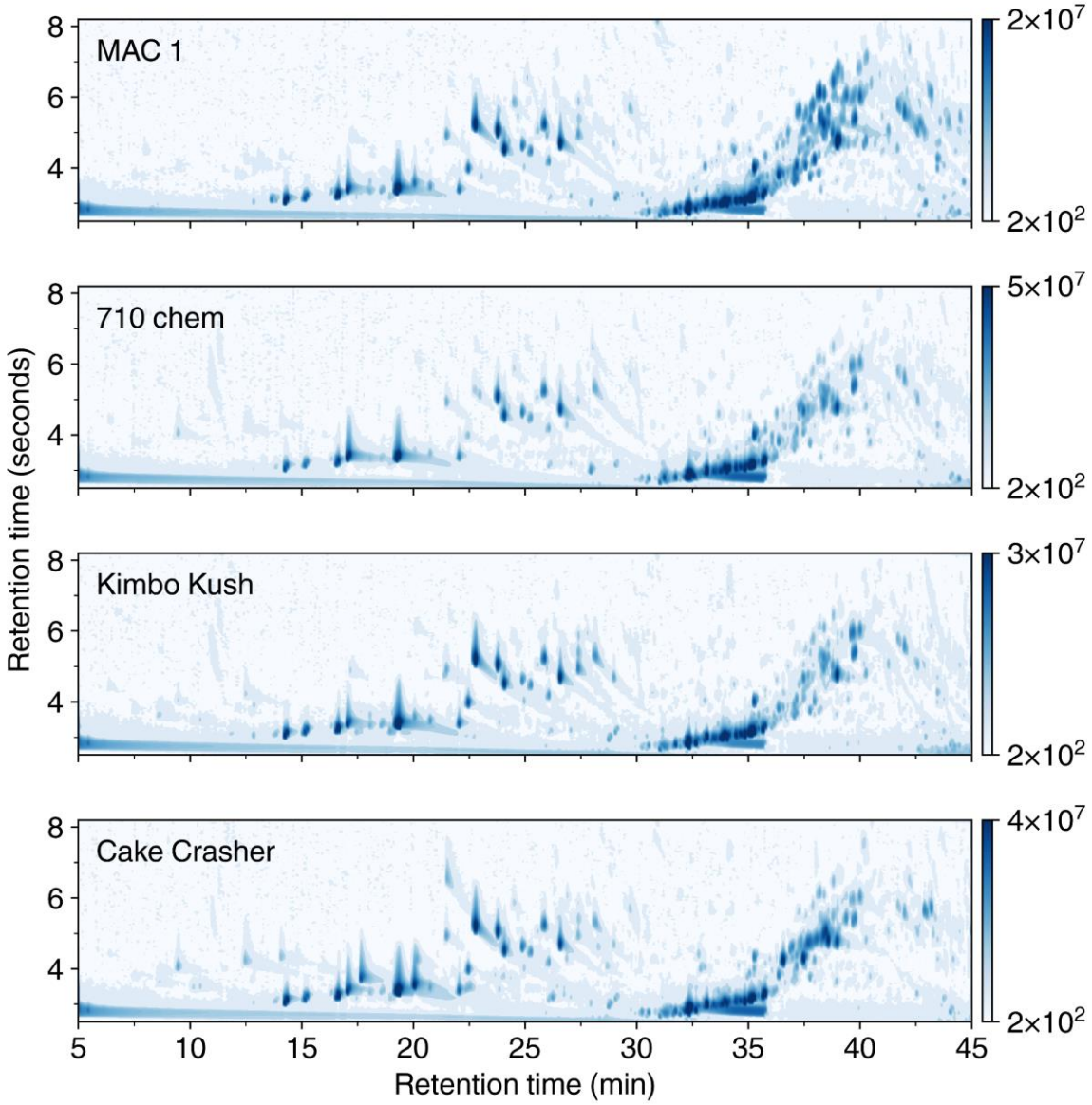

Figure S11. GC×GC–FID 2-Dimensional chromatograms for MAC 1, 710 Chem, Kimbo Kush, and Cake Crasher.

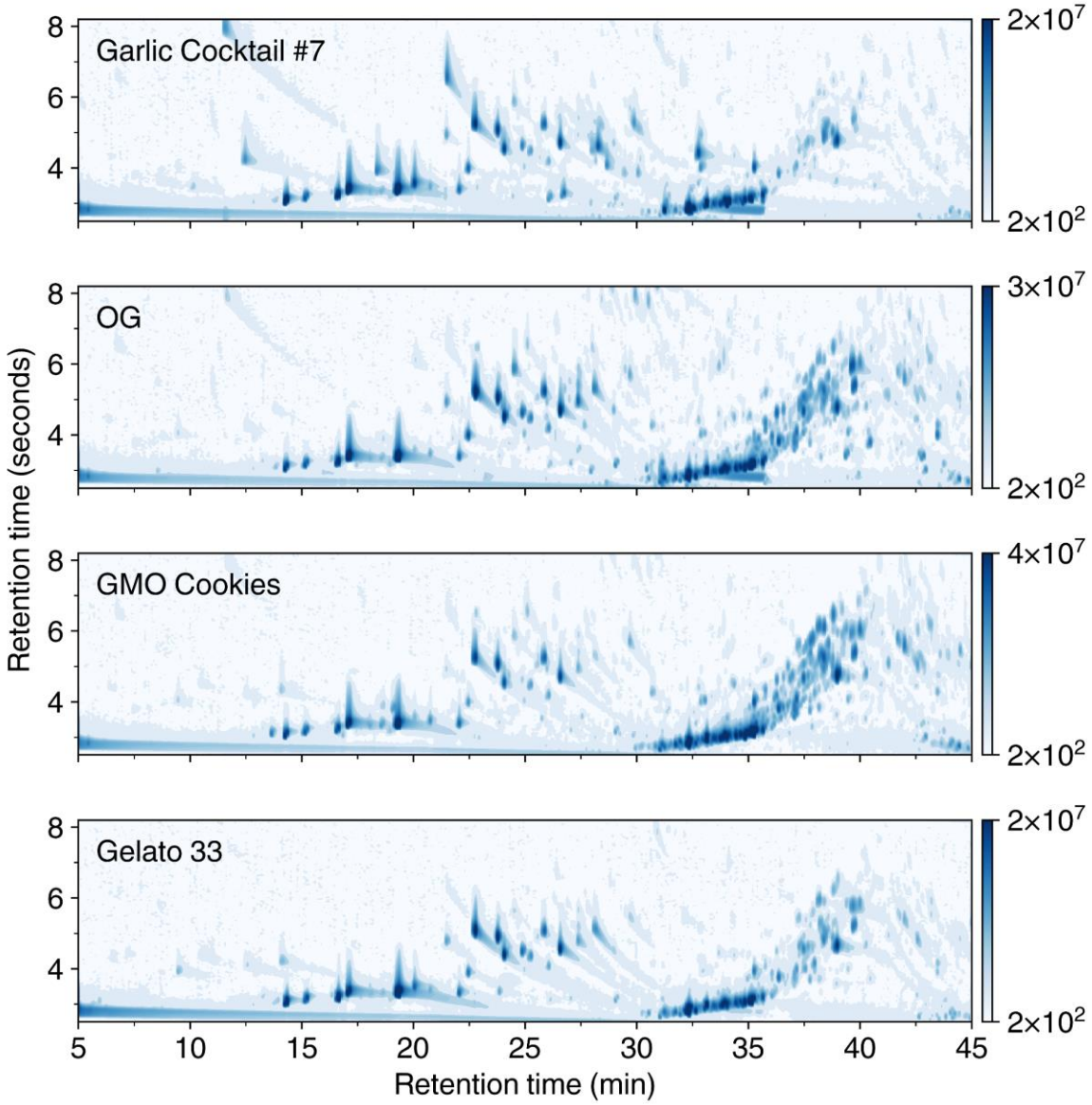

Figure S12. GC×GC–FID 2-Dimensional chromatograms for Garlic Cocktail #7, OG, GMO Cookies, and Gelato 33.

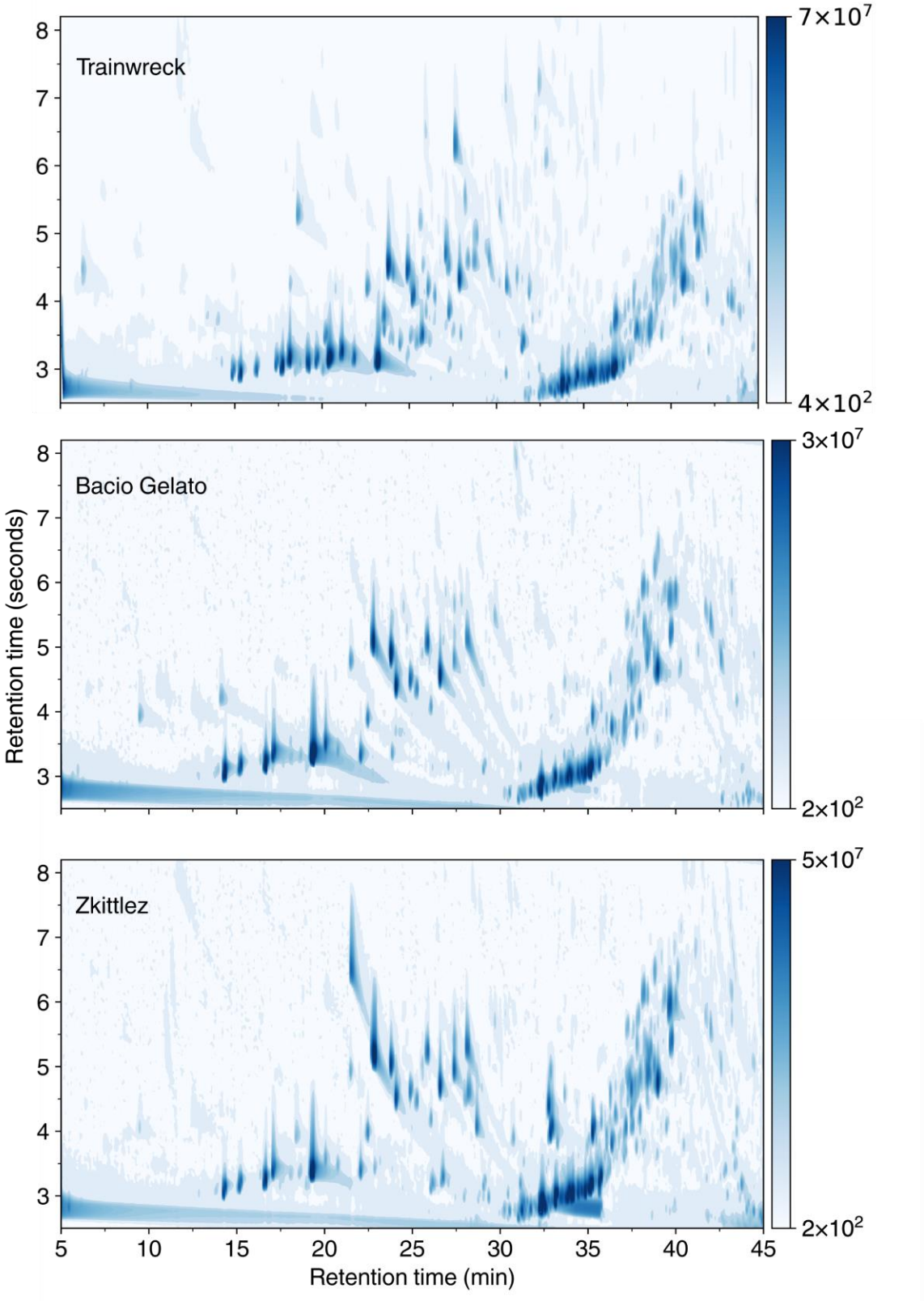

Figure S13. GC×GC–FID 2-Dimensional chromatograms for Trainwreck, Bacio Gelato, and Zkittlez 710.

Mass spectra of analytes. All analytes used were indexed using the NIST17 mass structural database. Standards were then used to confirm retention times and mass spectral data for all analytes.

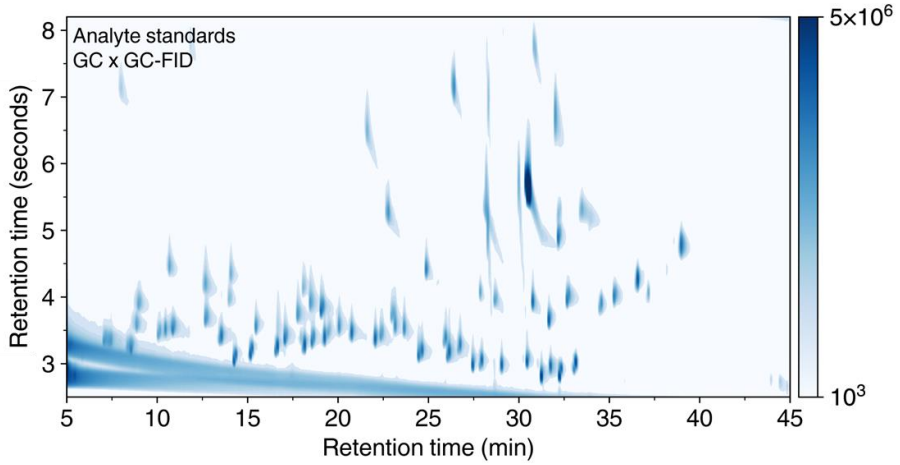

Figure S14. GC × GC–FID chromatogram of analyte standards. Independent standards were combined graphically. Two bands exist in the analyte standard chromatogram as ethanol was used as the solvent for the FLV-1 standard versus hexanes for the remaining samples. The dark peak near $^{1}t_{r}$ ~31 min $^{2}t_{r}$ ~5.8 is triacetin, the solvent FLV-1 was prepared in.

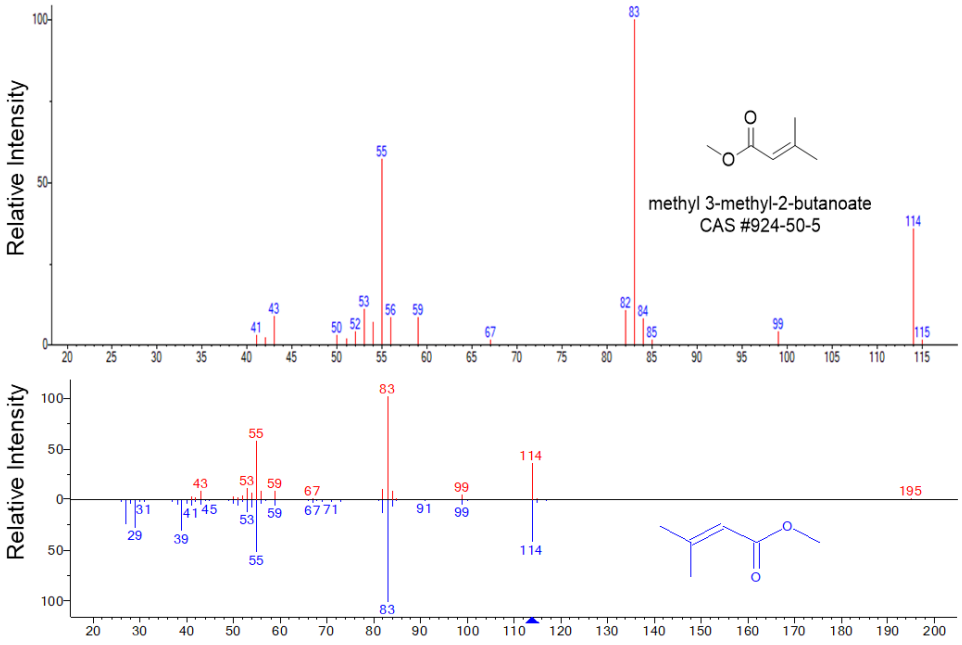

Figure S15. Comparison of mass spectra of methyl senecioate found in Bubba Kush (top) and the NIST Spectral Library v17 (2017) (bottom).

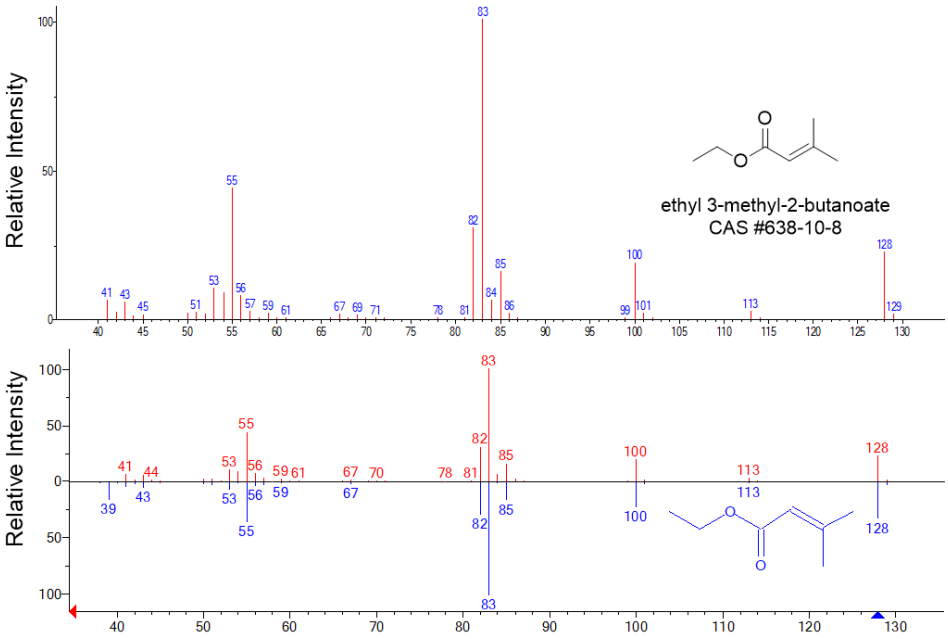

Figure S16. Comparison of mass spectra of ethyl senecioate found in Bubba Kush (top) and the NIST Spectral Library v17 (2017) (bottom).

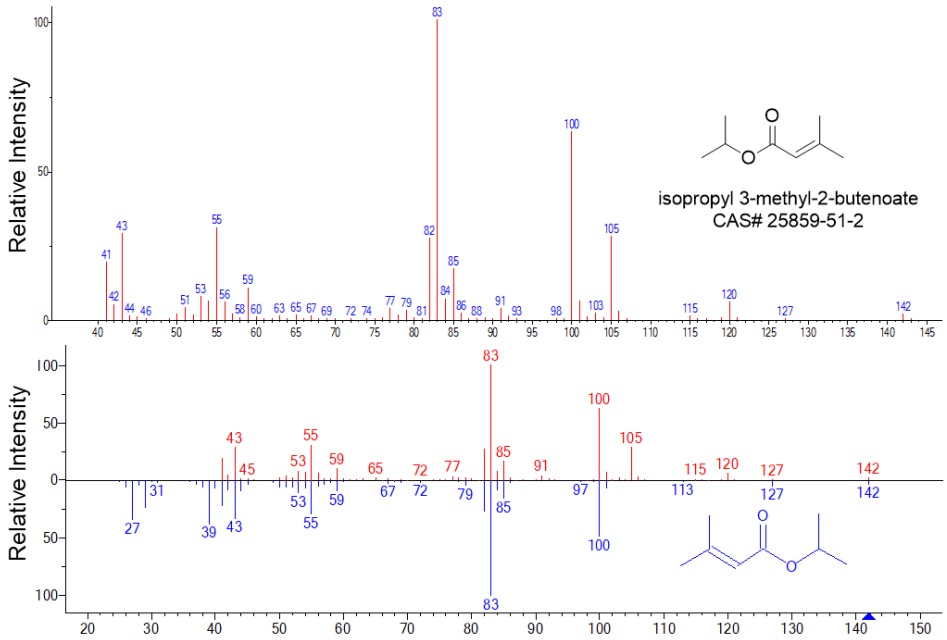

Figure S17. Comparison of mass spectra of isopropyl senecioate found in Bubba Kush (top) and the NIST Spectral Library v17 (2017) (bottom).

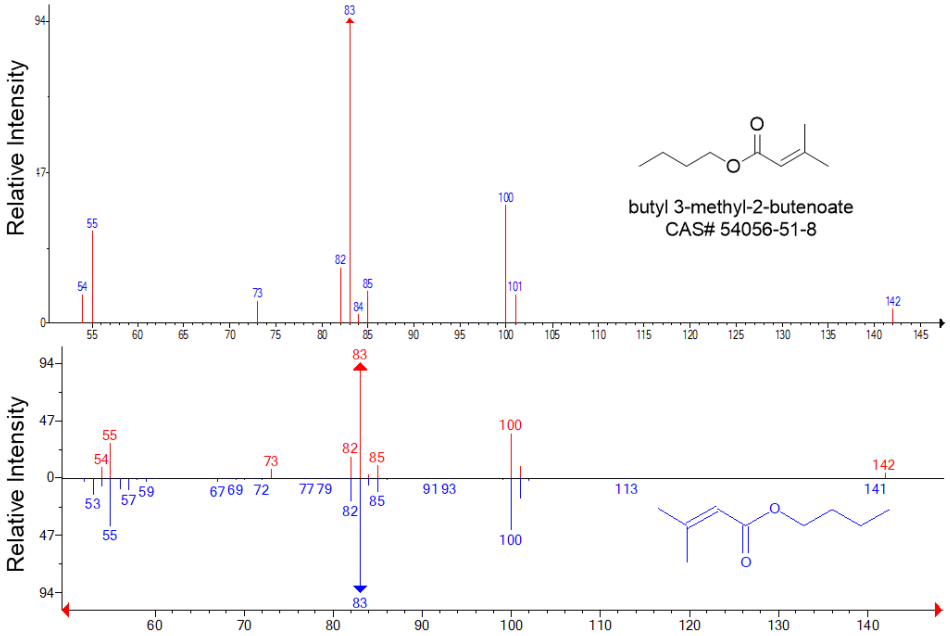

Figure S18. Comparison of mass spectra of *n*-butyl senecioate found in Bubba Kush (top) and the NIST Spectral Library v17 (2017) (bottom).

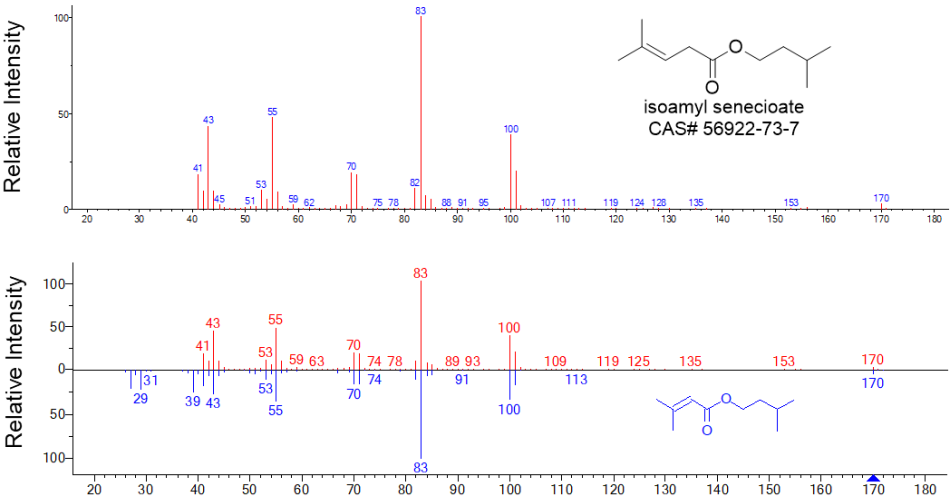

Figure S19. Comparison of mass spectra of isoamyl senecioate found in Grape Pie x Do-Si-Do (top) and the NIST Spectral Library v17 (2017) (bottom).

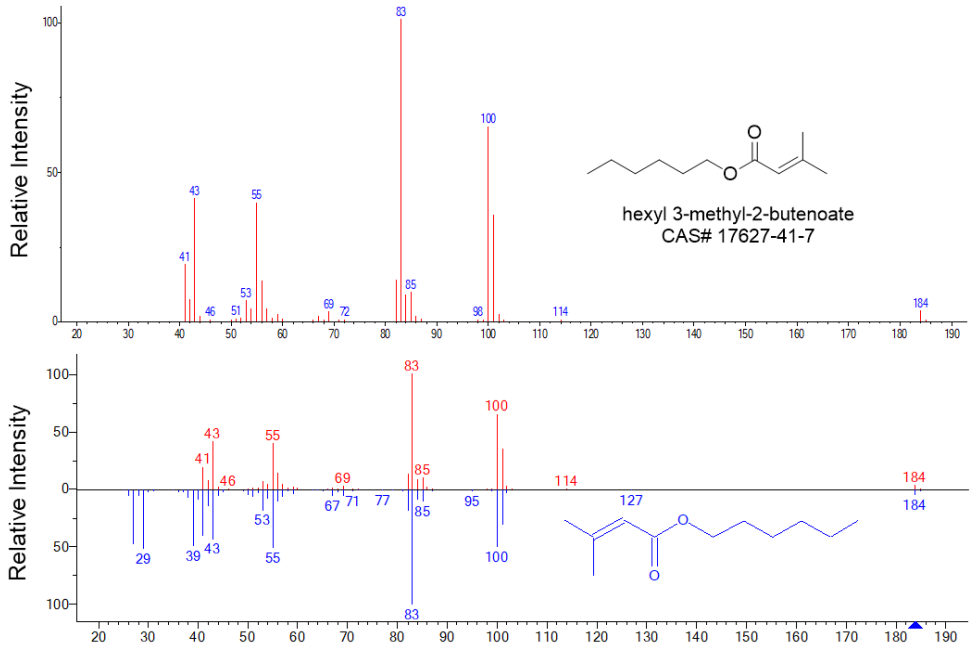

Figure S20. Comparison of mass spectra of n-hexyl senecioate found in Bubba Kush (top) and the NIST Spectral Library v17 (2017) (bottom).

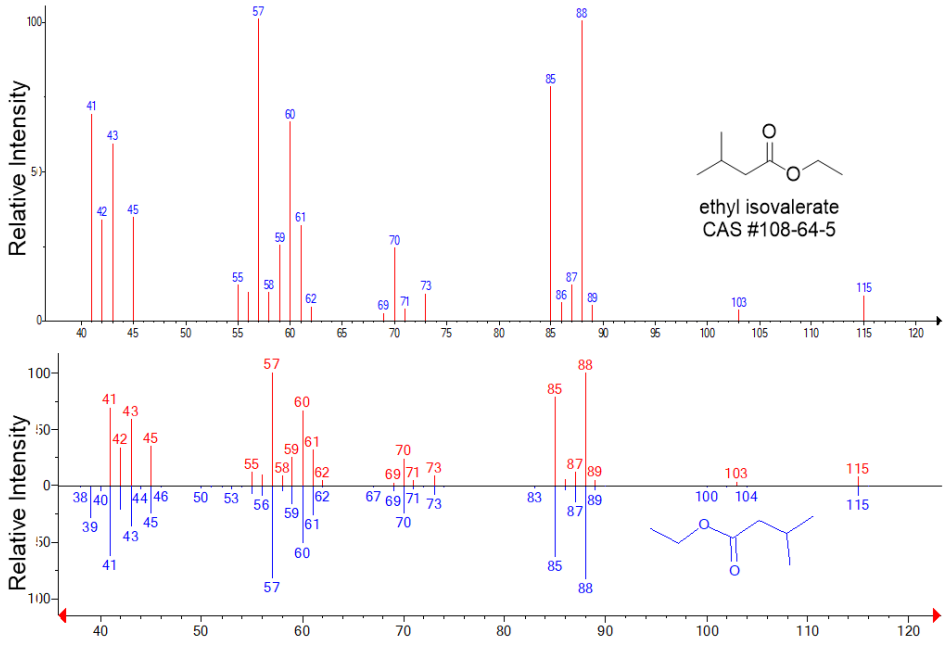

Figure S21. Comparison of mass spectra of ethyl isovalerate found in Bubba Kush (top) and the NIST Spectral Library v17 (2017) (bottom).

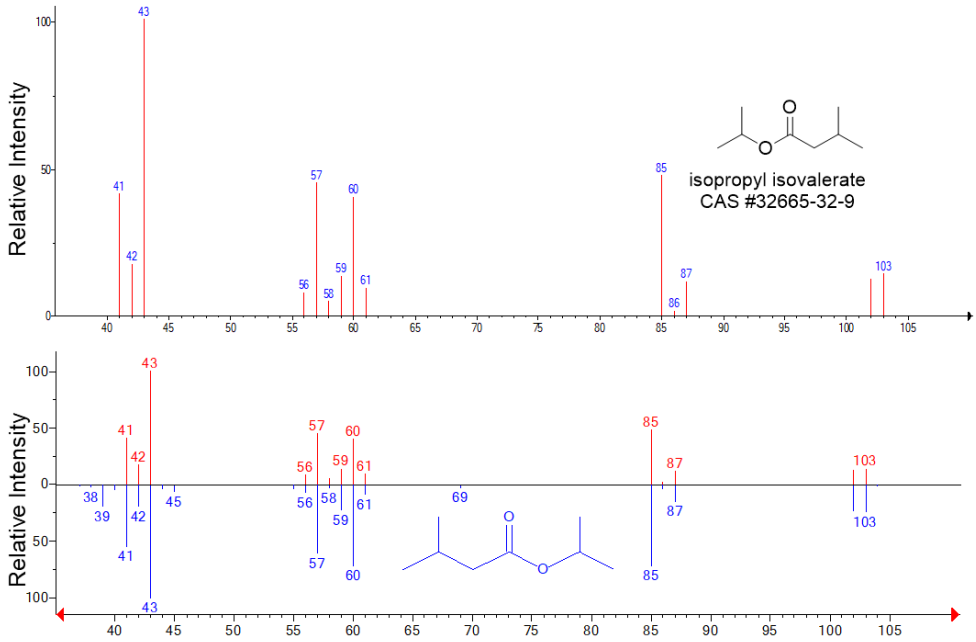

Figure S22. Comparison of mass spectra of isopropyl isovalerate (isopropyl isobutyrate) found in Bubba Kush (top) and the NIST Spectral Library v17 (2017) (bottom).

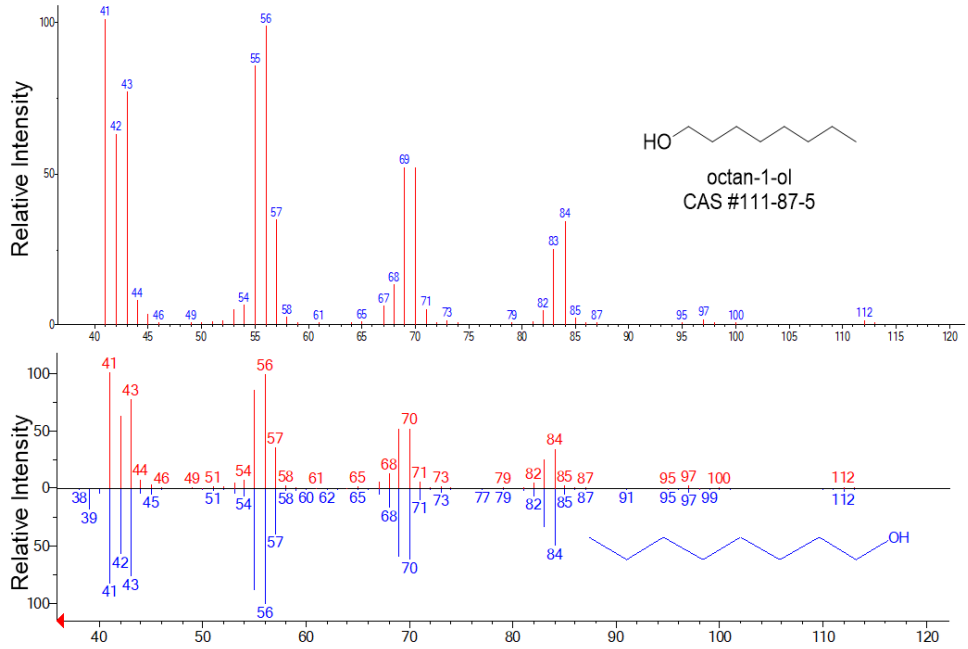

Figure S23. Comparison of mass spectra of 1-octanol found in Bubba Kush (top) and the NIST Spectral Library v17 (2017) (bottom).

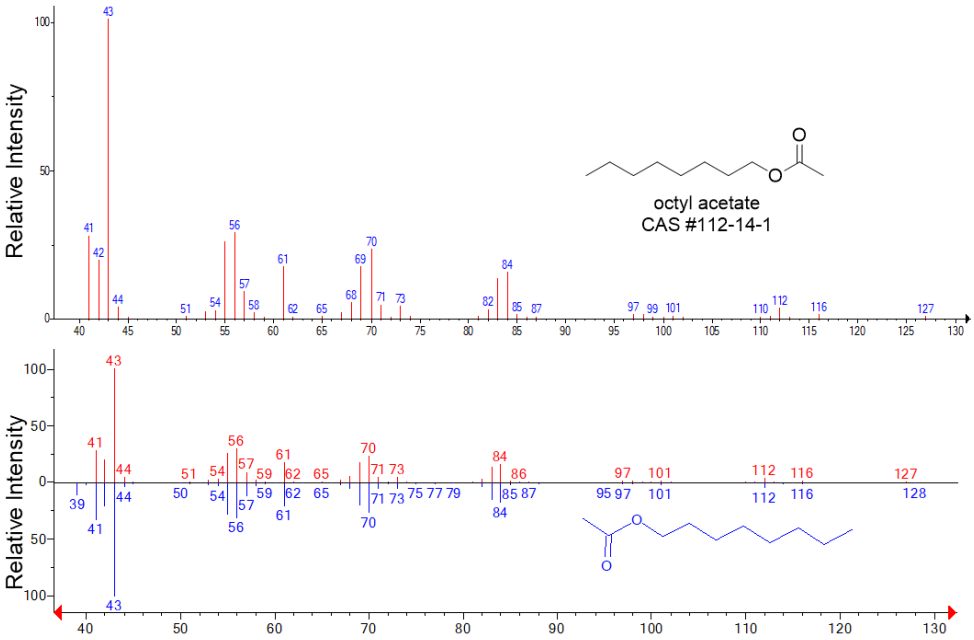

Figure S24. Comparison of mass spectra of *n*-octyl acetate found in Bubba Kush (top) and the NIST Spectral Library v17 (2017) (bottom).

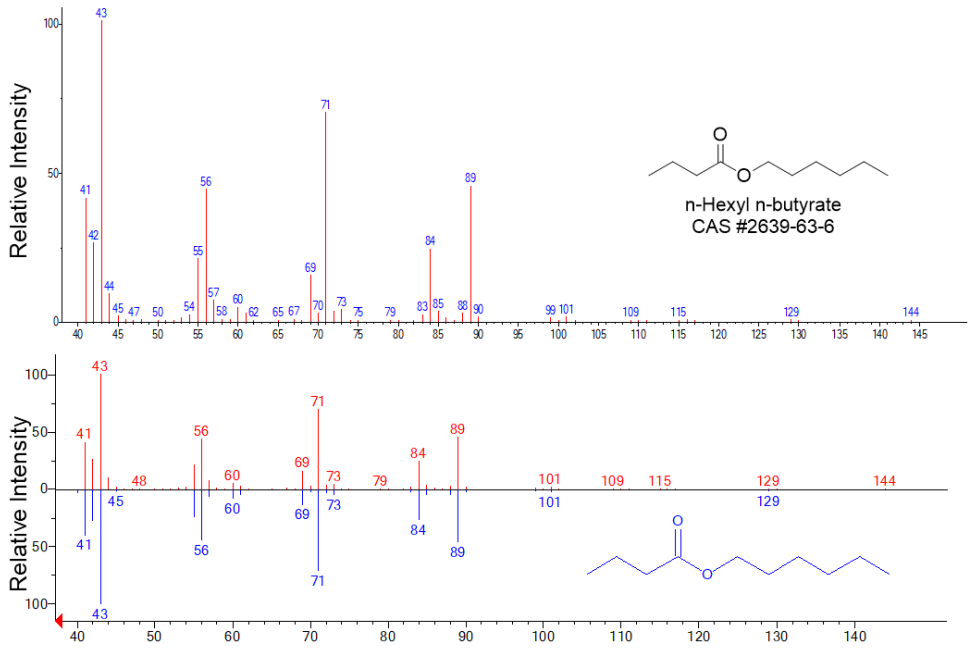

Figure S25. Comparison of mass spectra of *n*-hexyl *n*-butyrate found in Bubba Kush (top) and the NIST Spectral Library v17 (2017) (bottom).

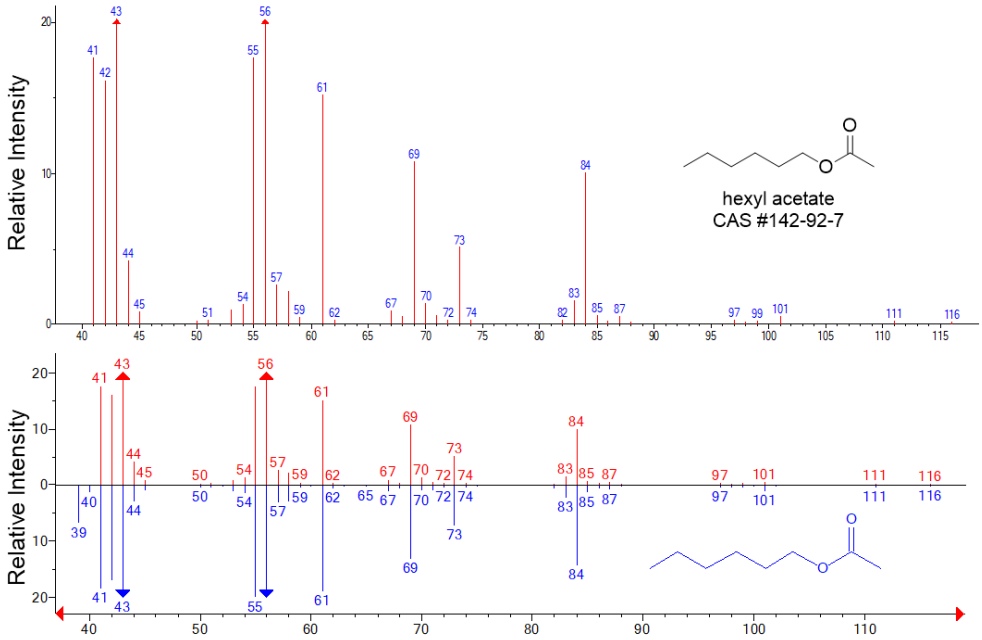

Figure S26. Comparison of mass spectra of *n*-hexyl acetate found in Bubba Kush (top) and the NIST Spectral Library v17 (2017) (bottom).

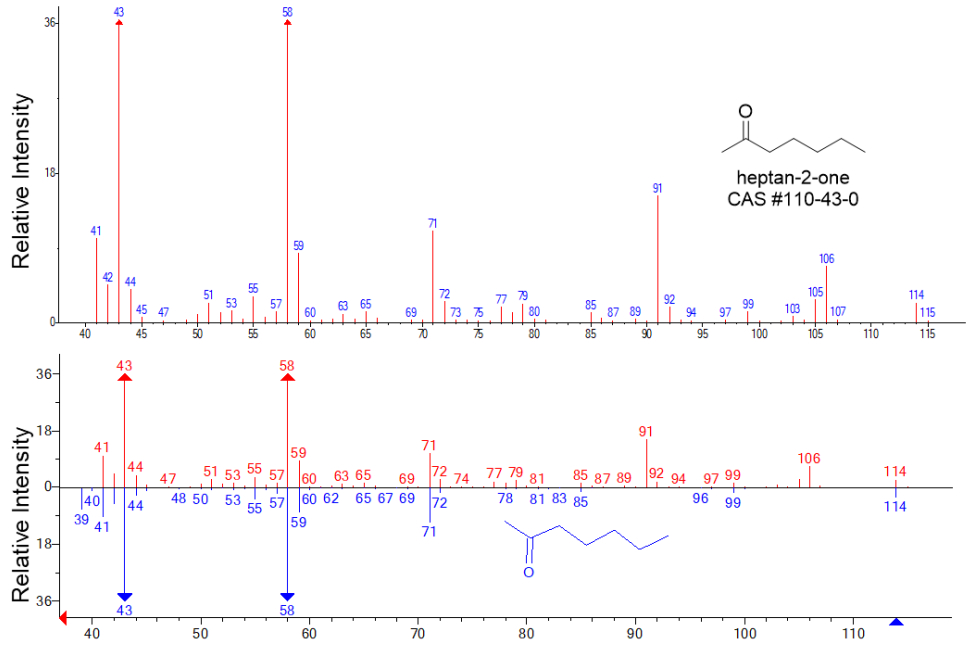

Figure S27. Comparison of mass spectra of 2-heptanone found in Bubba Kush (top) and the NIST Spectral Library v17 (2017) (bottom).

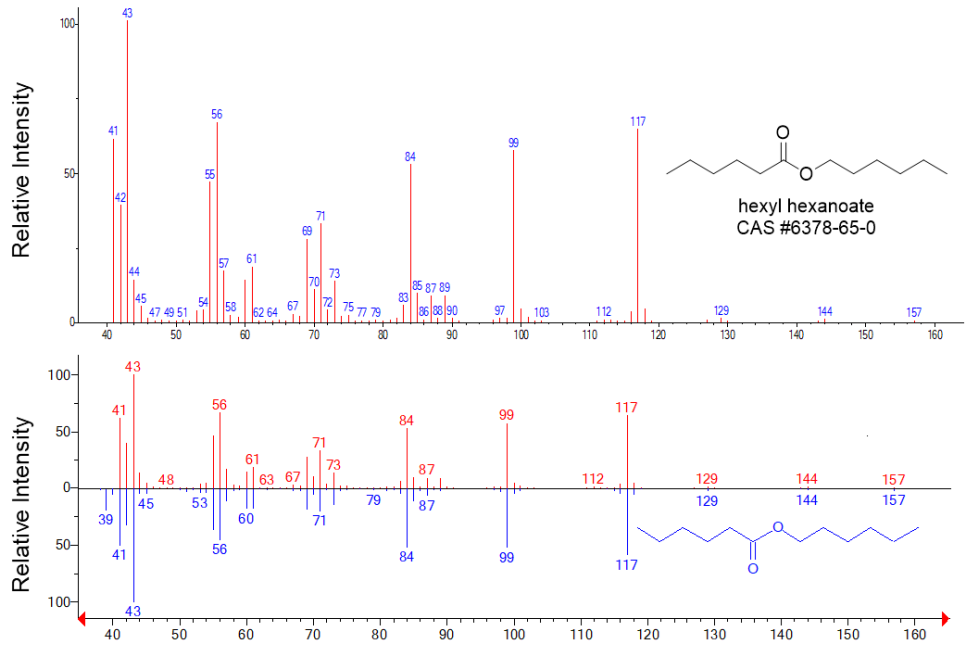

Figure S28. Comparison of mass spectra of *n*-hexyl hexanoate found in Juiceman (top) and the NIST Spectral Library v17 (2017) (bottom).

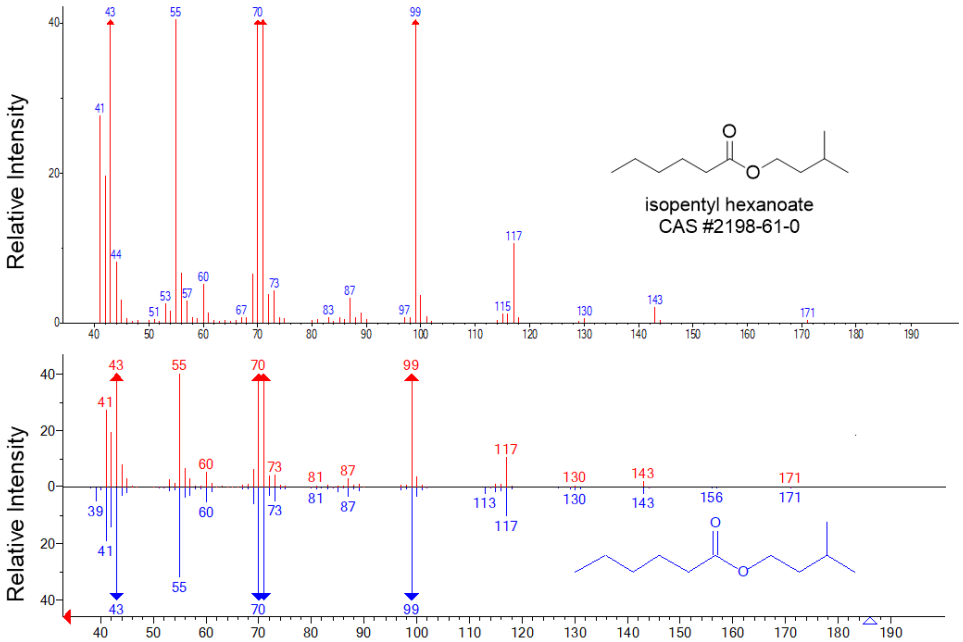

Figure S29. Comparison of mass spectra of isopentyl hexanoate (i.e., isoamyl hexanoate) found in Juiceman (top) and the NIST Spectral Library v17 (2017) (bottom).

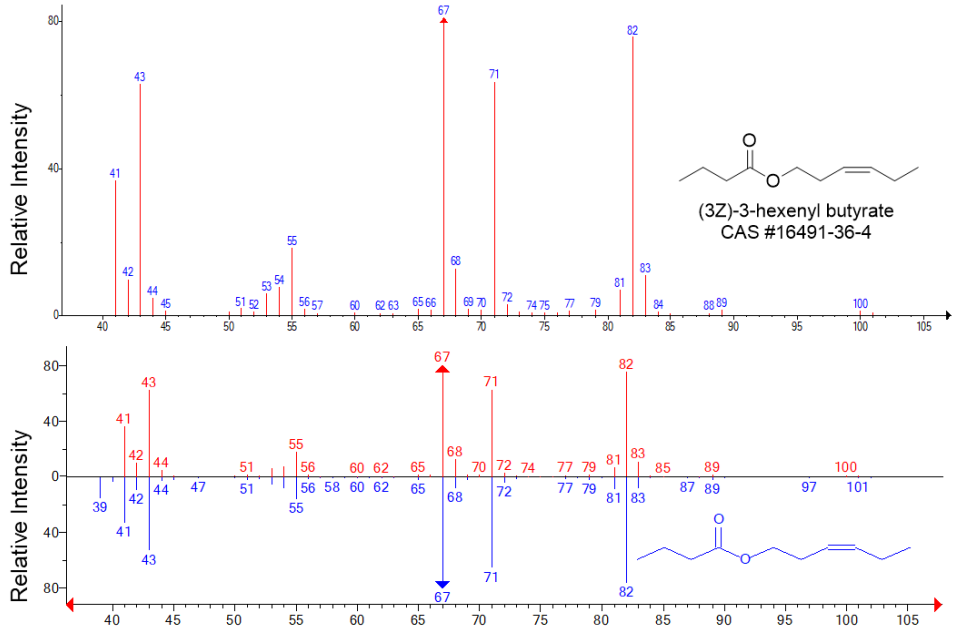

Figure S30. Comparison of mass spectra of cis-3-hexenyl *n*-butyrate found in Juiceman (top) and the NIST Spectral Library v17 (2017) (bottom).

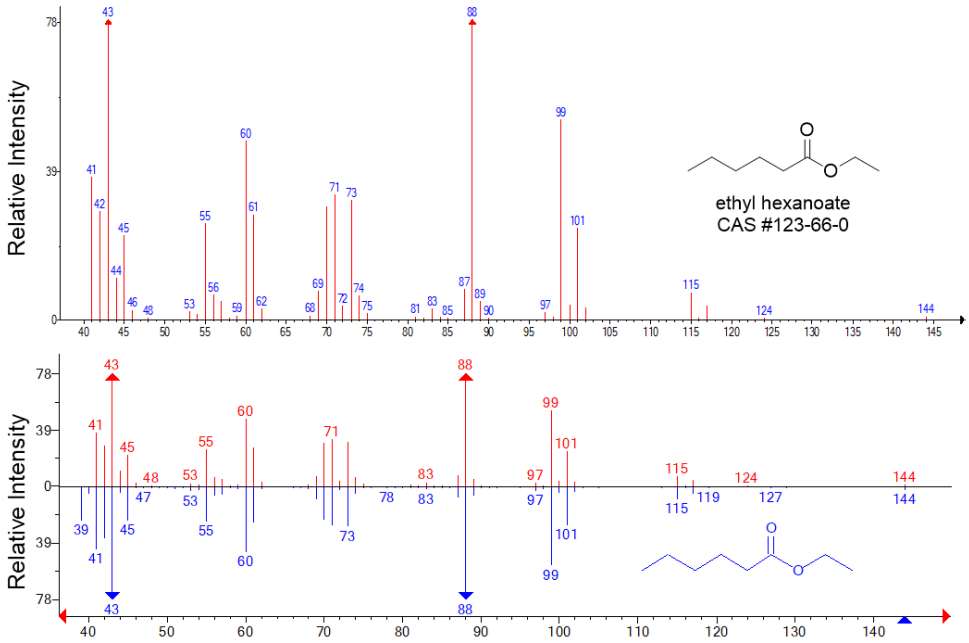

Figure S31. Comparison of mass spectra of ethyl hexanoate found in Juiceman (top) and the NIST Spectral Library v17 (2017) (bottom).

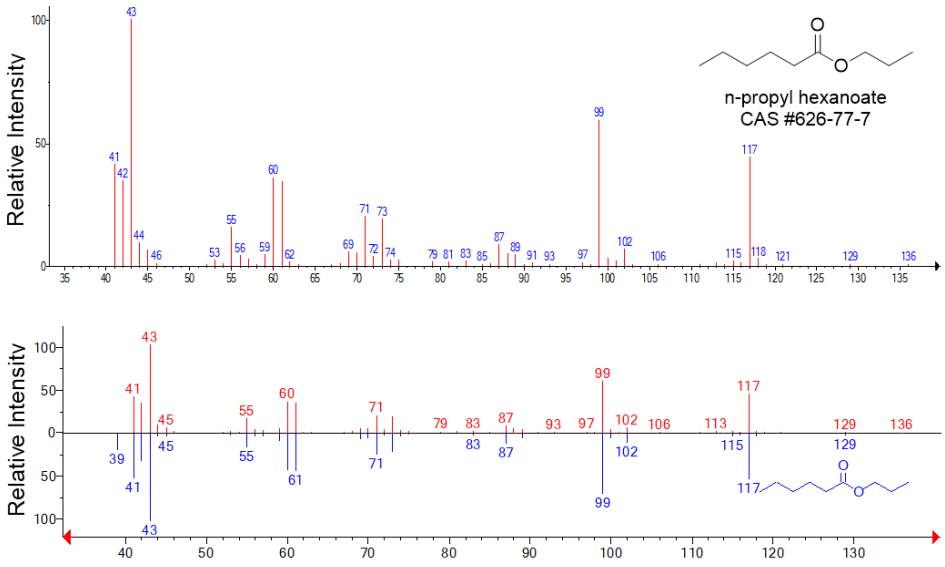

Figure S32. Comparison of mass spectra of n-propyl hexanoate found in Juiceman (top) and the NIST Spectral Library v17 (2017) (bottom).

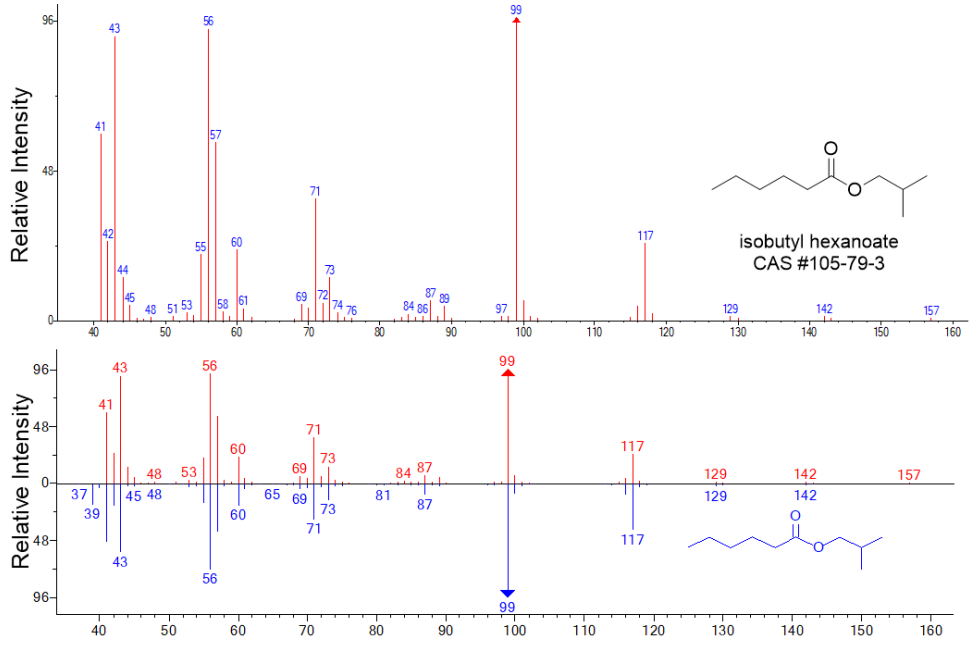

Figure S33. Comparison of mass spectra of isobutyl hexanoate found in Juiceman (top) and the NIST Spectral Library v17 (2017) (bottom).

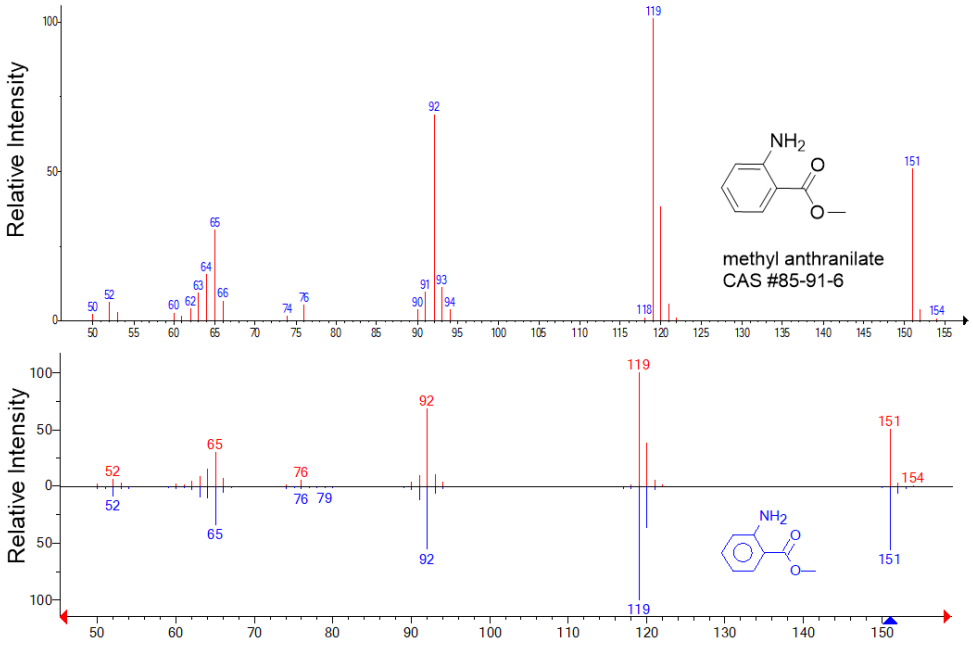

Figure S34. Comparison of mass spectra of methyl anthranilate found in Juiceman (top) and the NIST Spectral Library v17 (2017) (bottom).

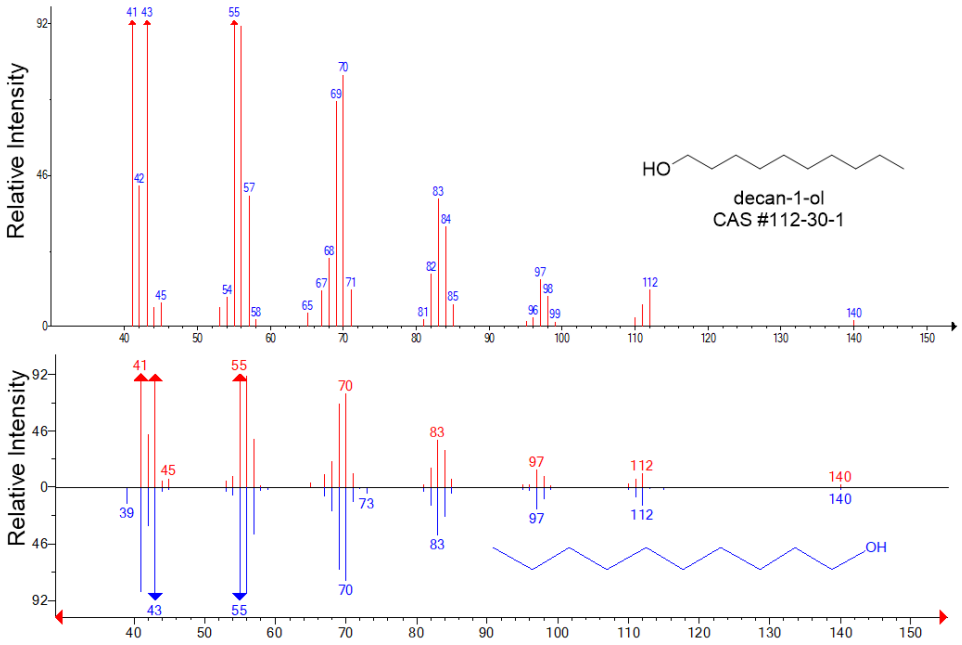

Figure S35. Comparison of mass spectra of 1-decanol found in Juiceman (top) and the NIST Spectral Library v17 (2017) (bottom).

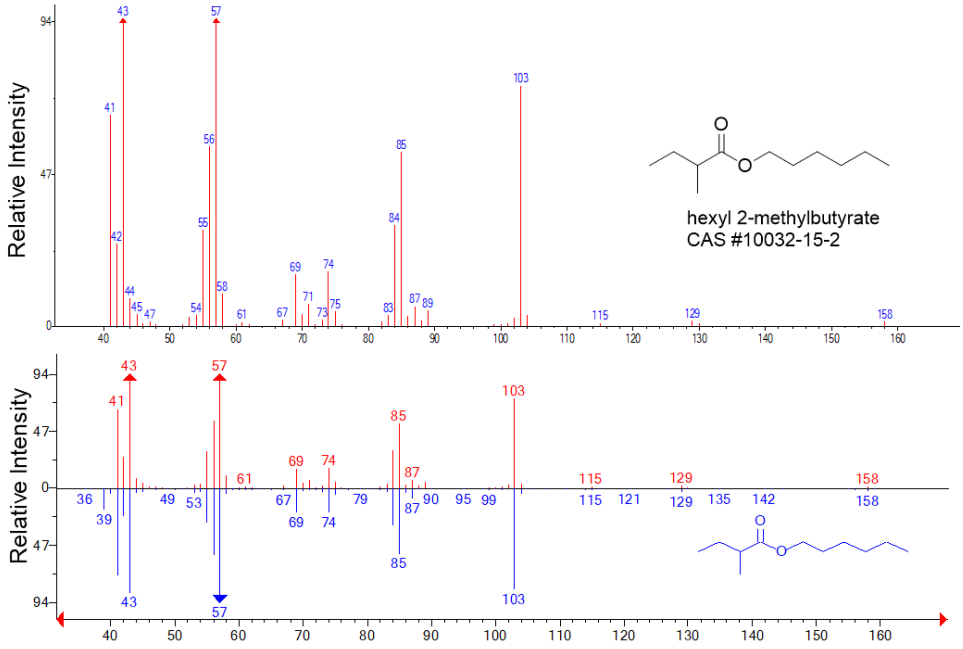

Figure S36. Comparison of mass spectra of hexyl 2-methylbutyrate found in Juiceman (top) and the NIST Spectral Library v17 (2017) (bottom).

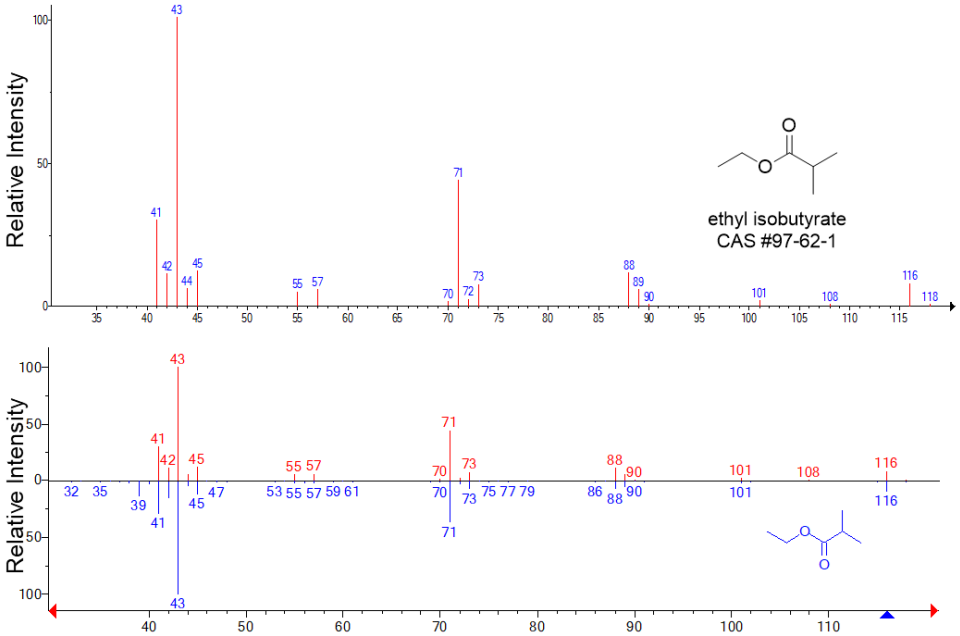

Figure S37. Comparison of mass spectra of ethyl isobutyrate found in Juiceman (top) and the NIST Spectral Library v17 (2017) (bottom).

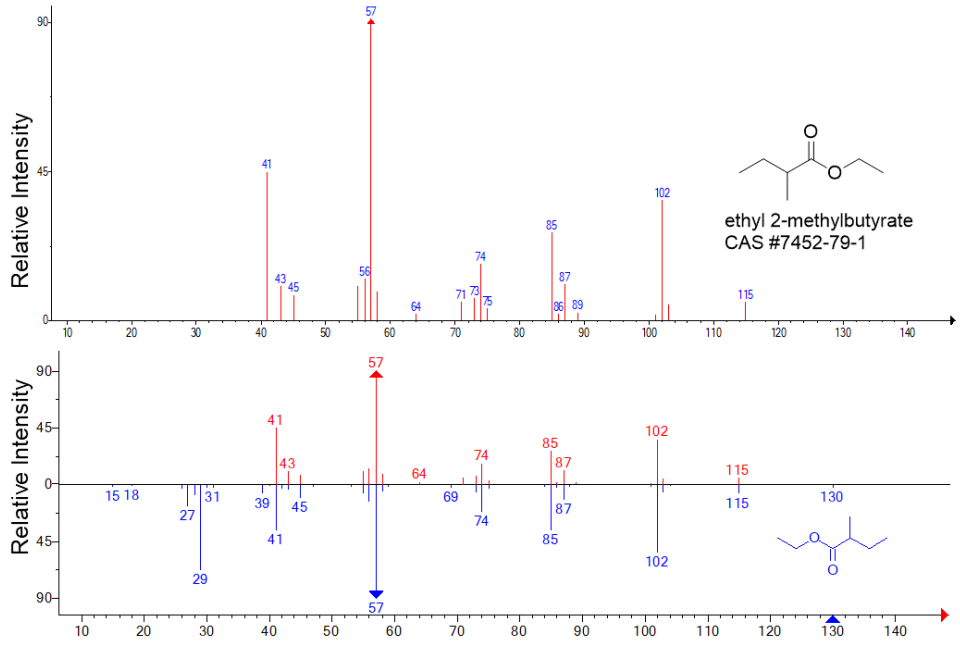

Figure S38. Comparison of mass spectra of ethyl 2-methylbutyrate found in Juiceman (top) and the NIST Spectral Library v17 (2017) (bottom).

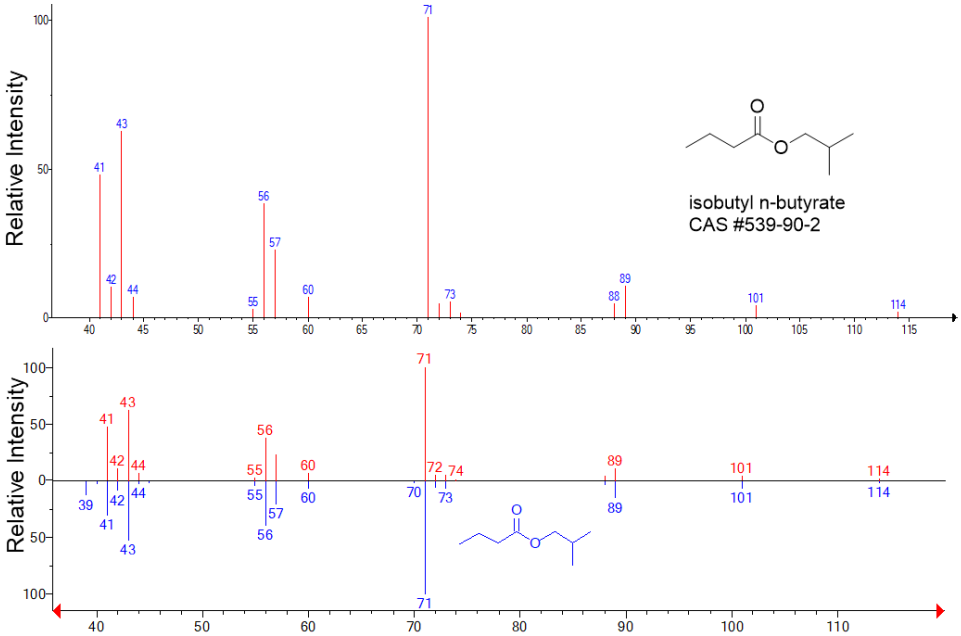

Figure S39. Comparison of mass spectra of isobutyl n-butyrate found in Juiceman (top) and the NIST Spectral Library v17 (2017) (bottom).

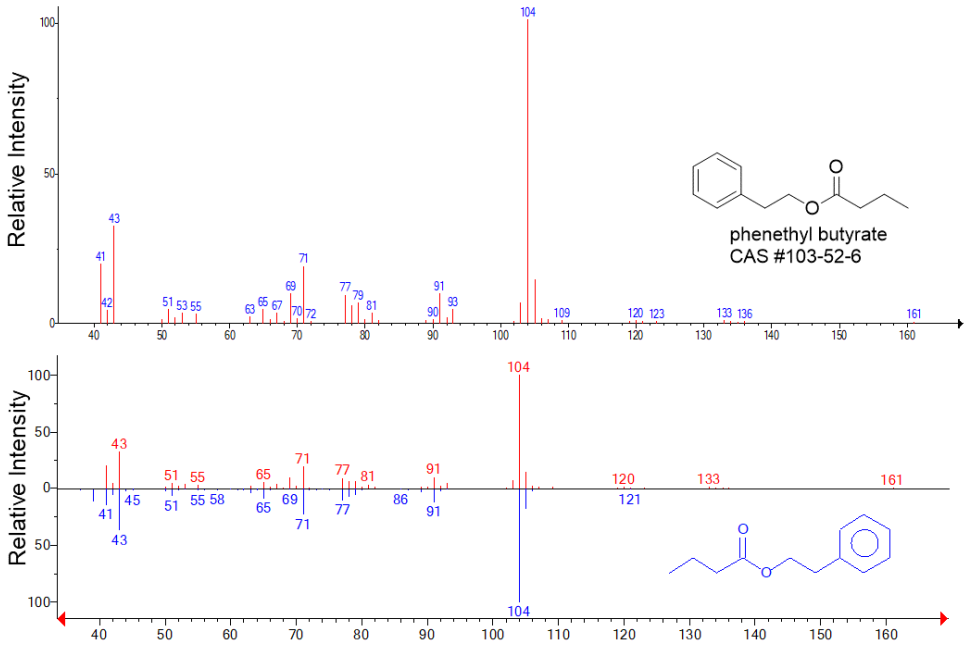

Figure S40. Comparison of mass spectra of phenethyl *n*-butyrate found in Juiceman (top) and the NIST Spectral Library v17 (2017) (bottom).

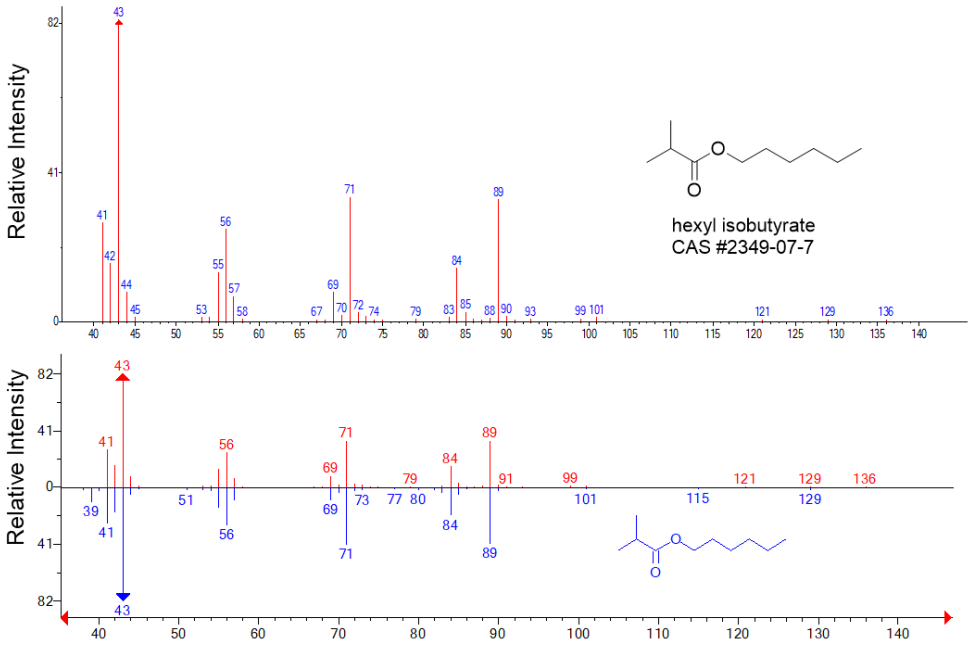

Figure S41. Comparison of mass spectra of *n*-hexyl isobutyrate found in Juiceman (top) and the NIST Spectral Library v17 (2017) (bottom).

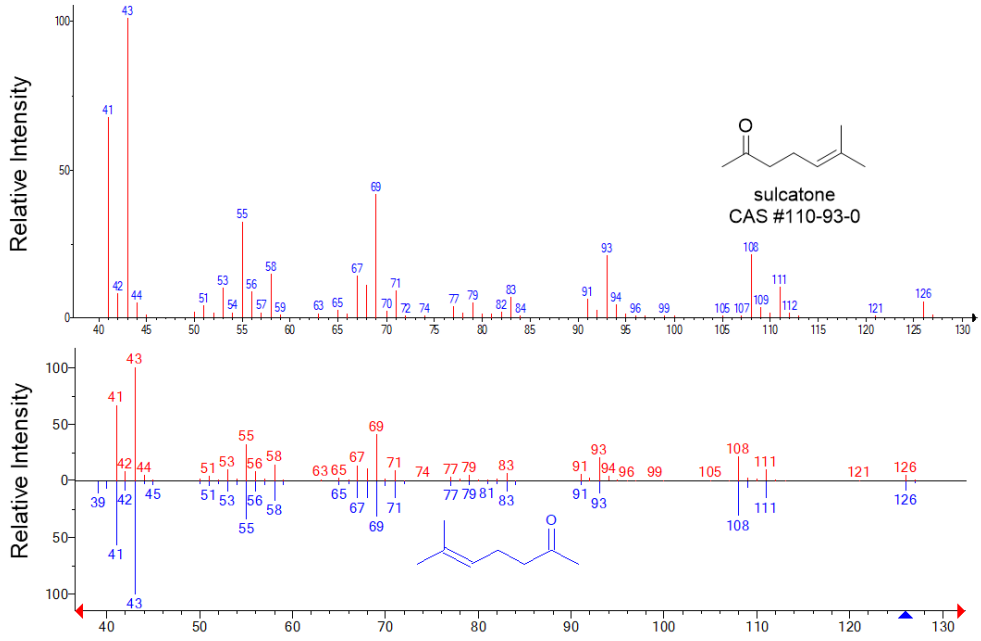

Figure S42. Comparison of mass spectra of sulcatone found in Juiceman (top) and the NIST Spectral Library v17 (2017) (bottom).

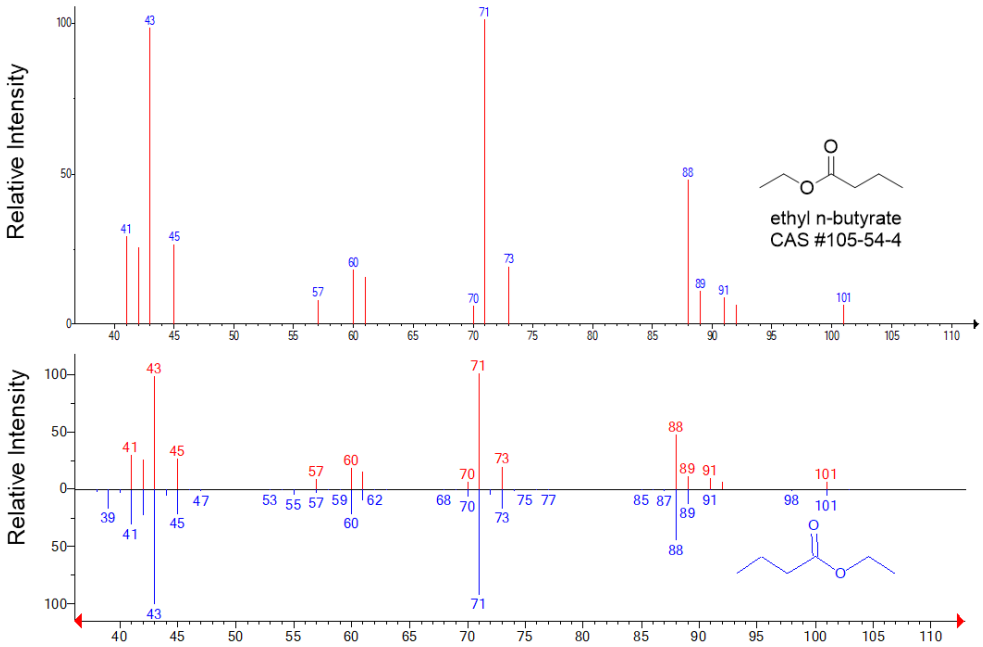

Figure S43. Comparison of mass spectra of ethyl *n*-butyrate found in Motor Nana (top) and the NIST Spectral Library v17 (2017) (bottom).

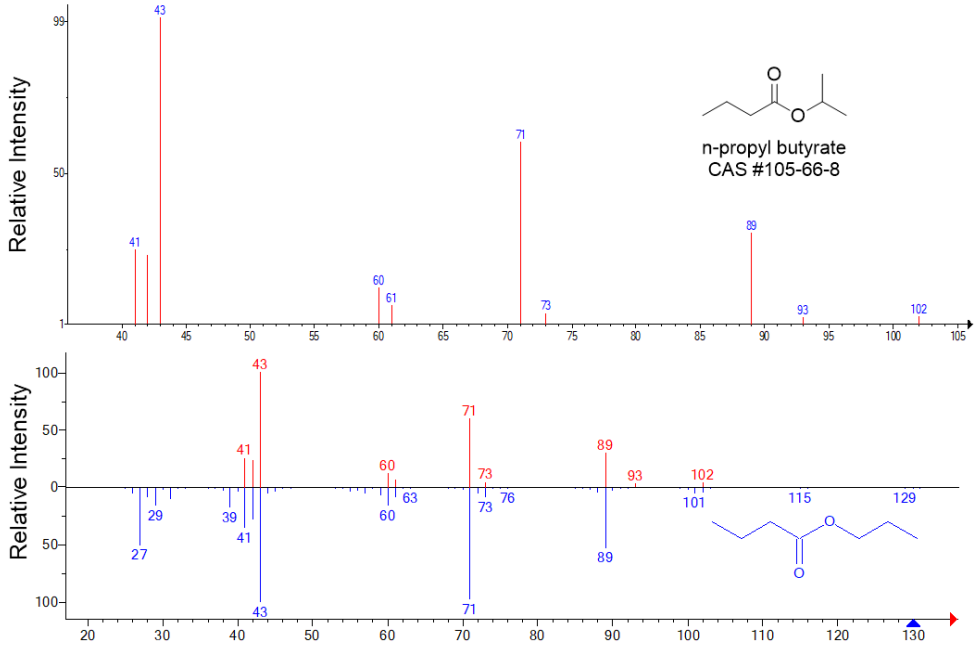

Figure S44. Comparison of mass spectra of *n*-propyl *n*-butyrate found in Juiceman (top) and the NIST Spectral Library v17 (2017) (bottom).

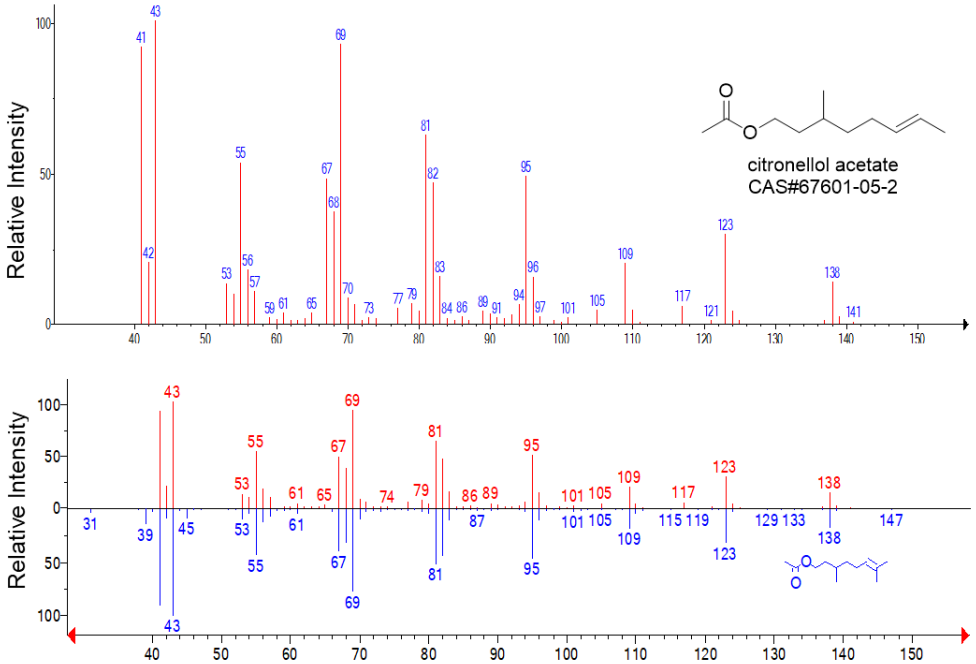

Figure S45. Comparison of mass spectra of citronellol acetate found in Juiceman (top) and the NIST Spectral Library v17 (2017) (bottom).

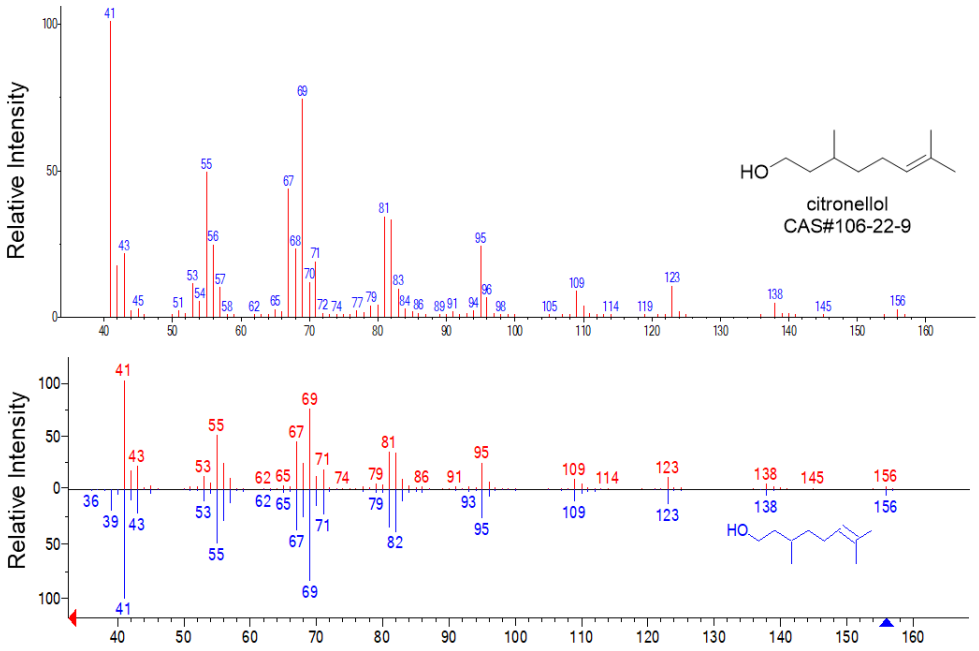

Figure S46. Comparison of mass spectra of citronellol found in Juiceman (top) and the NIST Spectral Library v17 (2017) (bottom).

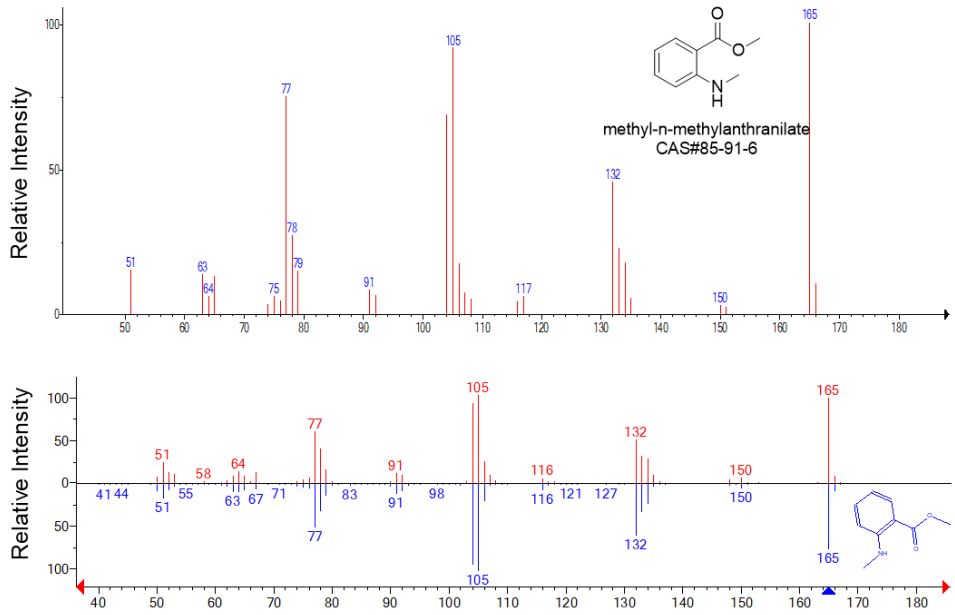

Figure S47. Comparison of mass spectra of methyl *n*-methylanthranilate found in Juiceman (top) and the NIST Spectral Library v17 (2017) (bottom).

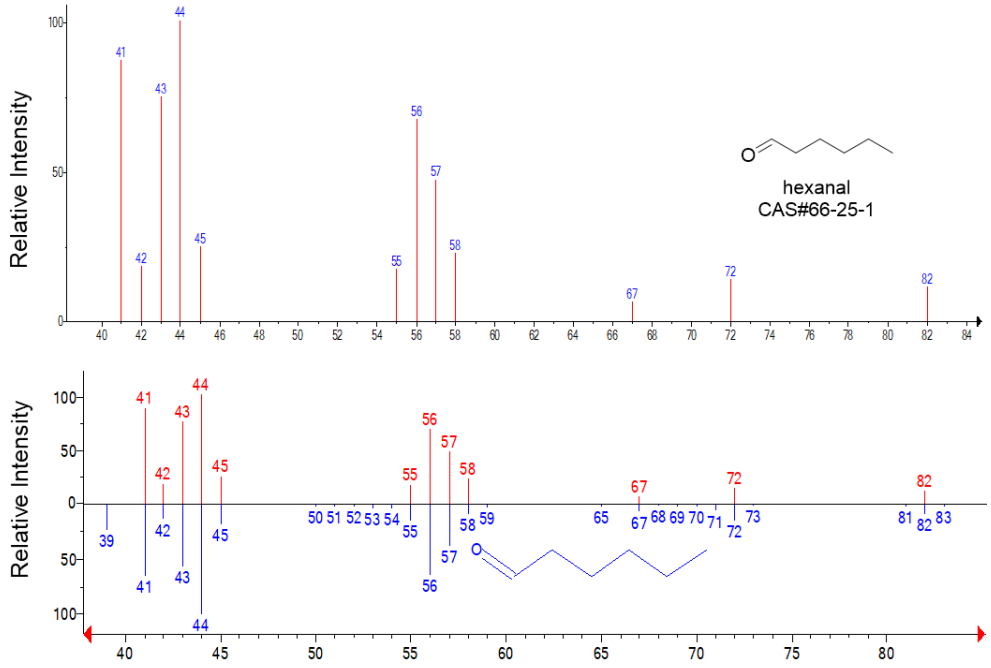

Figure S48. Comparison of mass spectra of hexanal found in rainbow 2.0 (top) and the NIST Spectral Library v17 (2017) (bottom).

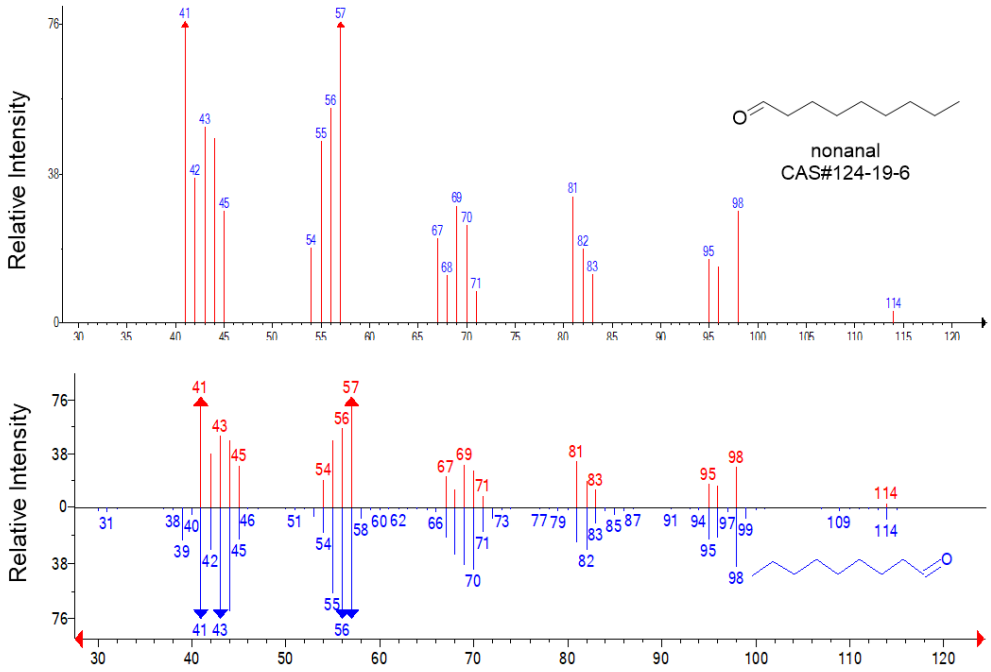

Figure S49. Comparison of mass spectra of nonanal found in rainbow 2.0 (top) and the NIST Spectral Library v17 (2017) (bottom).

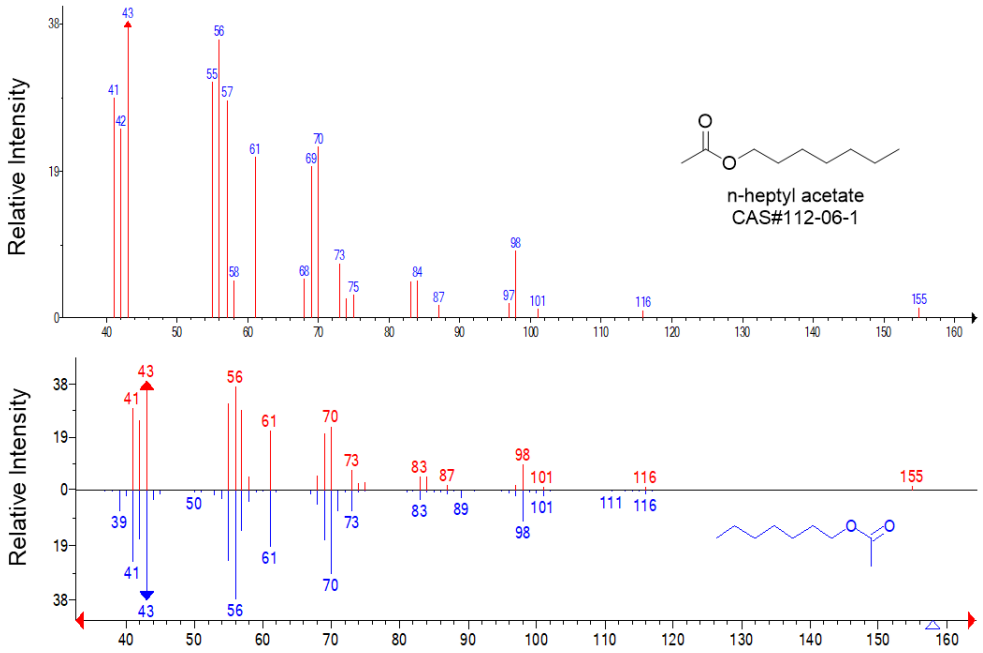

Figure S50. Comparison of mass spectra of heptyl acetate found in rainbow 2.0 (top) and the NIST Spectral Library v17 (2017) (bottom).

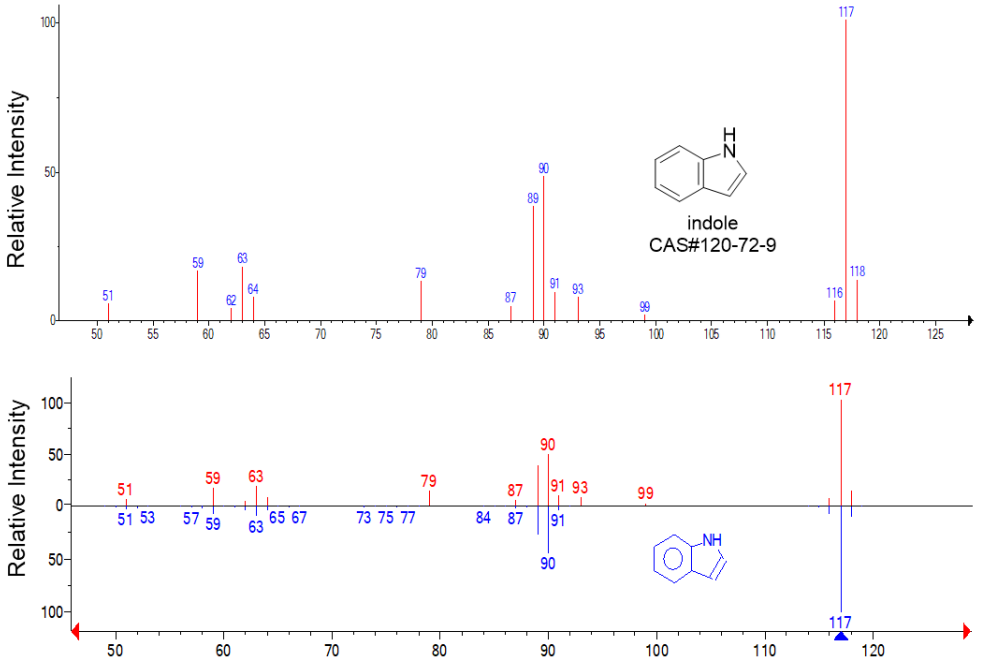

Figure S51. Comparison of mass spectra of indole found in fruity pebble (top) and the NIST Spectral Library v17 (2017) (bottom).

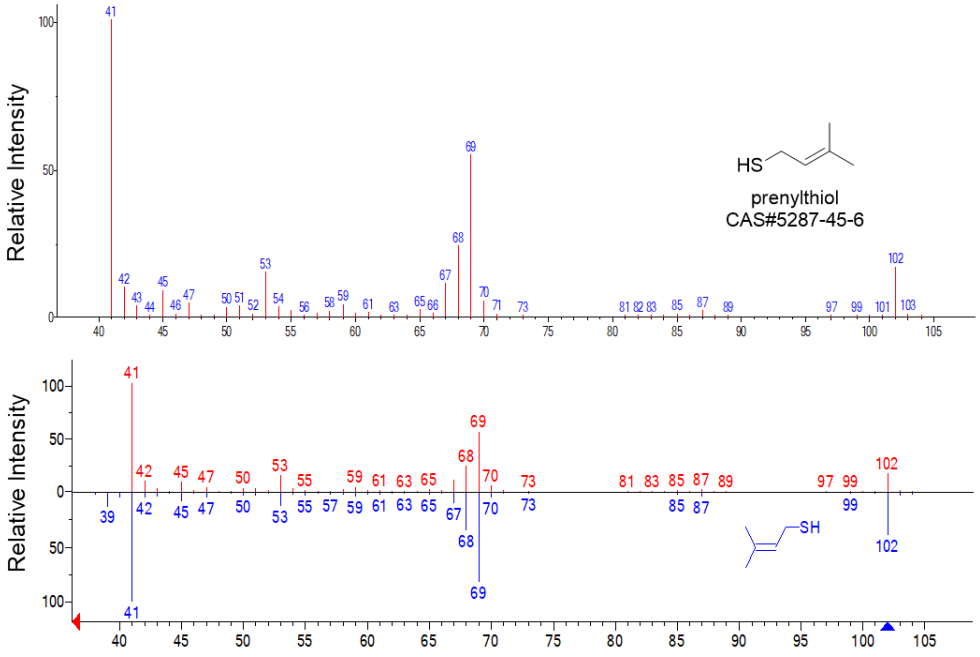

Figure S52. Comparison of mass spectra of prenylthiol found in fruity pebblez (top) and the NIST Spectral Library v17 (2017) (bottom).

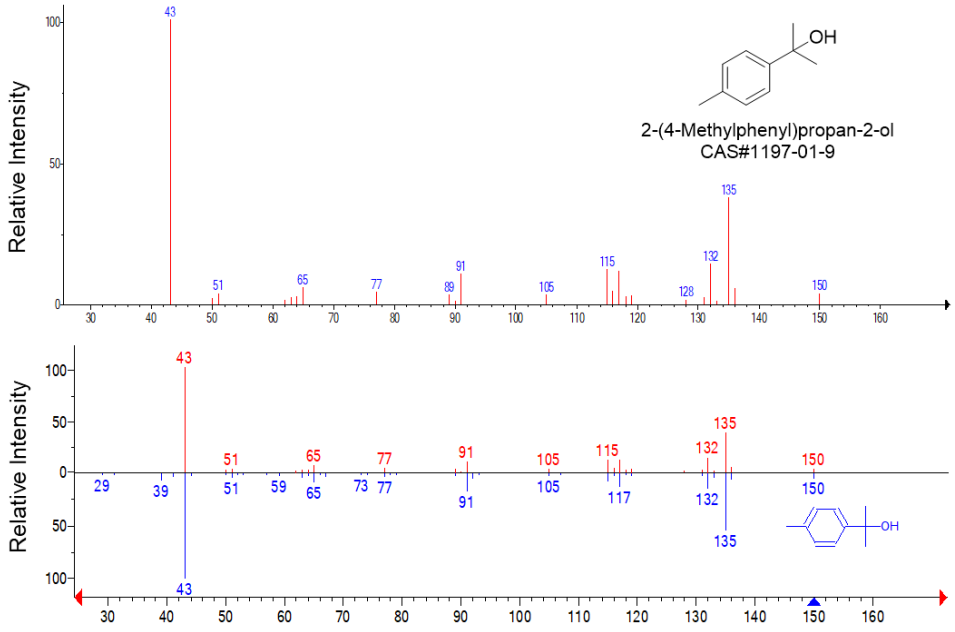

Figure S53. Comparison of mass spectra of cherry propanol in starburst 36-1 (top) and the NIST Spectral Library v17 (2017) (bottom).

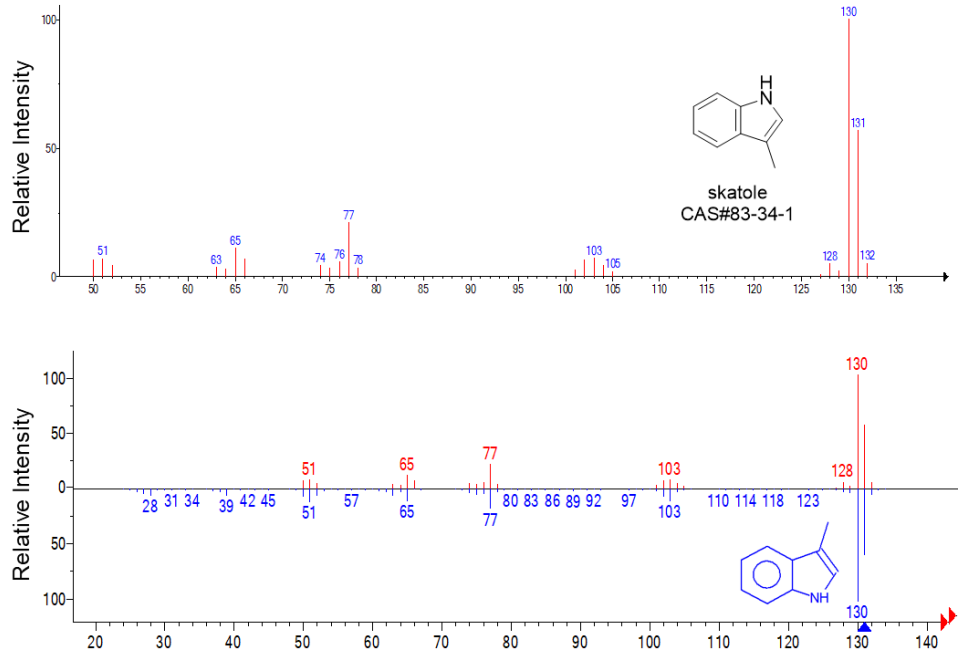

Figure S54. Comparison of mass spectra of skatole in fruity pebbles (top) and the NIST Spectral Library v17 (2017) (bottom).

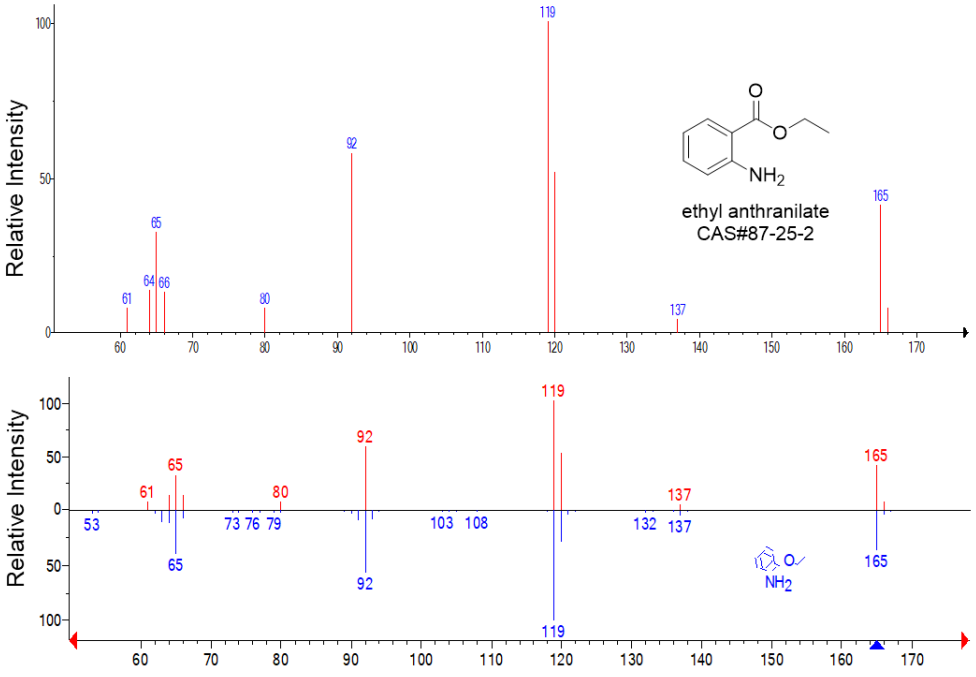

Figure S55. Comparison of mass spectra of ethyl anthranilate in fruity pebbles (top) and the NIST Spectral Library v17 (2017) (bottom).

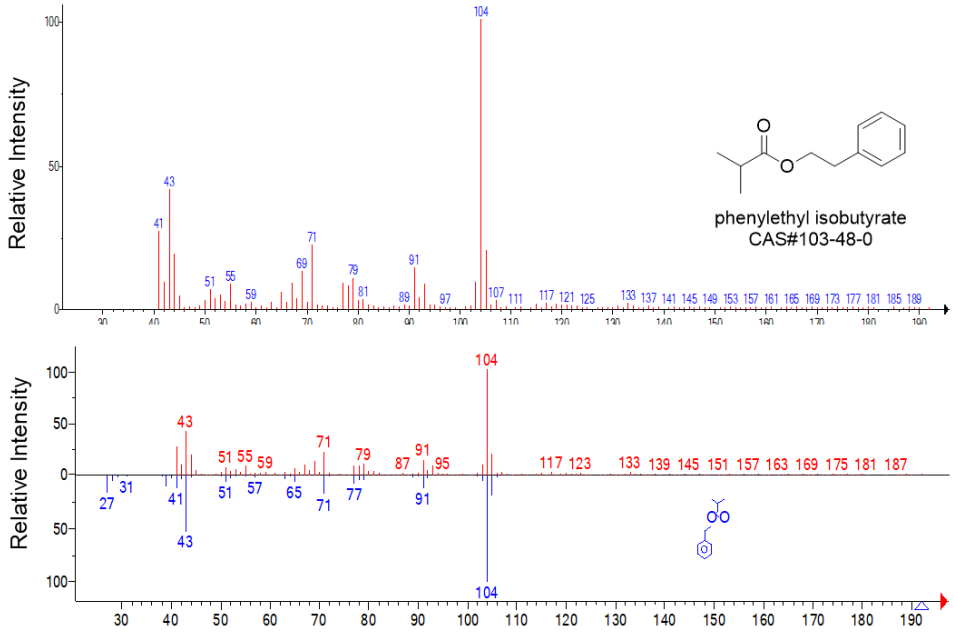

Figure S56. Comparison of mass spectra of phenylethyl isobutyrate in Juiceman (top) and the NIST Spectral Library v17 (2017) (bottom).

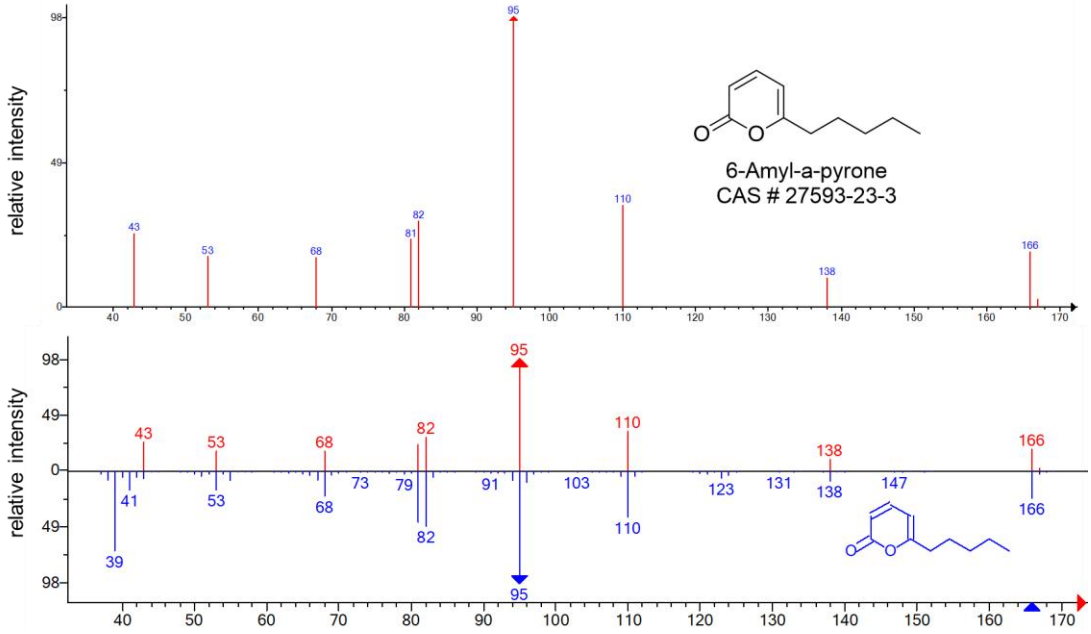

Figure S57. Comparison of mass spectra of 6-Amyl-α-pyrone in Zkittlez 710 (top) and the NIST Spectral Library v17 (2017) (bottom).

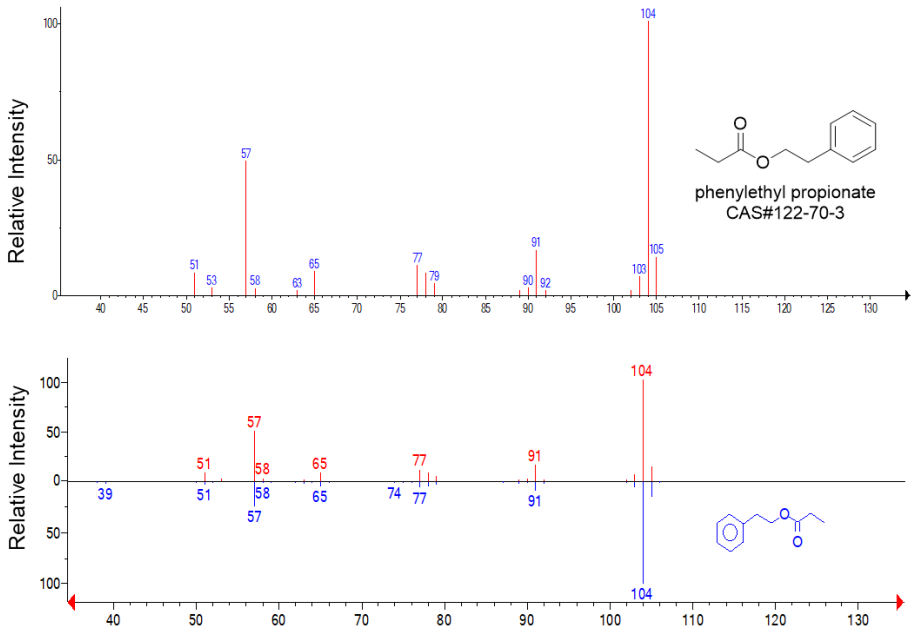

Figure S58. Comparison of mass spectra of phenylethyl propionate in juiceman (top) and the NIST Spectral Library v17 (2017) (bottom).

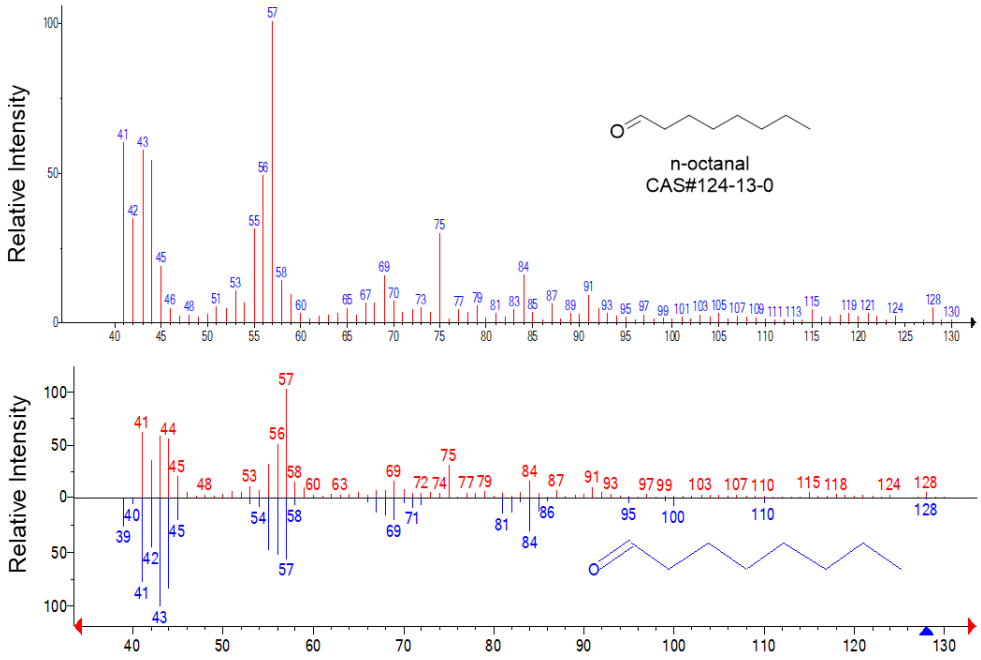

Figure S59. Comparison of mass spectra of octanal in gorilla glue (top) and the NIST Spectral Library v17 (2017) (bottom).

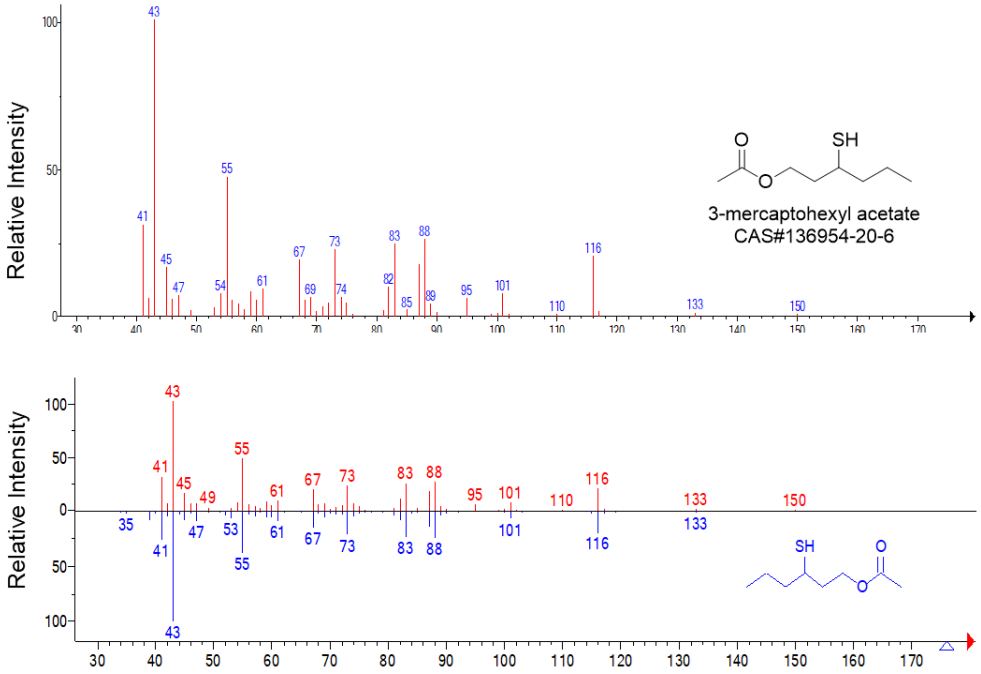

Figure S60. Comparison of mass spectra of 3-mercaptohexyl acetate in papaya peach (top) and the NIST Spectral Library v17 (2017) (bottom).

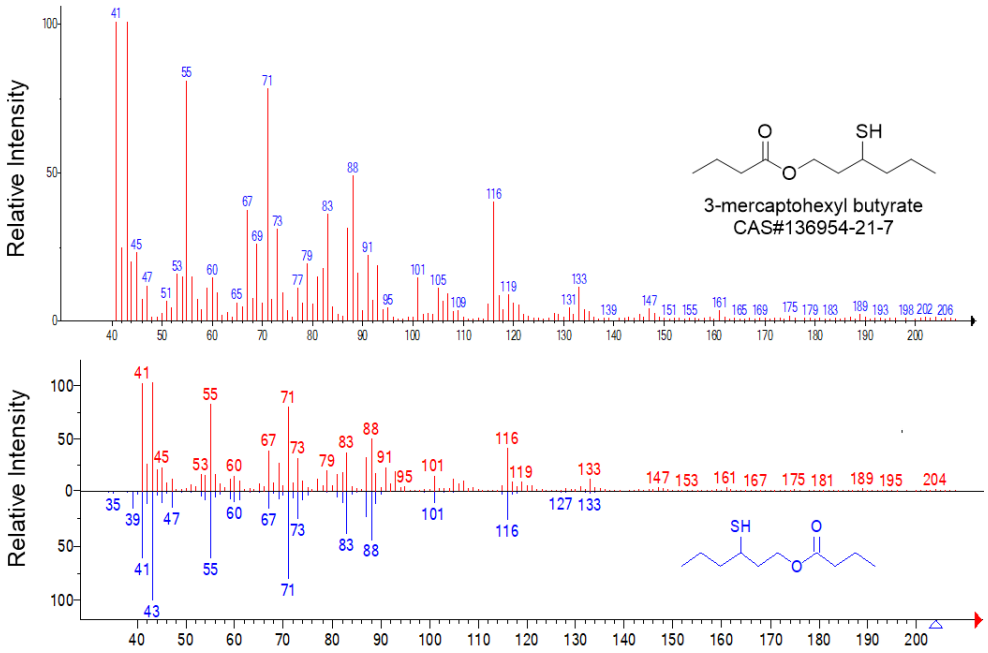

Figure S61. Comparison of mass spectra of 3-mercaptohexyl butyrate in gorilla glue (top) and the NIST Spectral Library v17 (2017) (bottom).

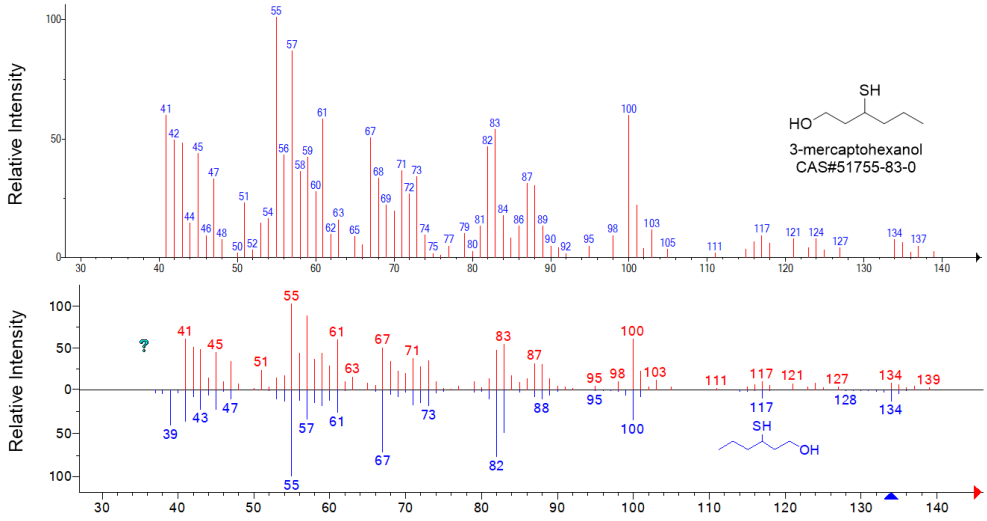

Figure S62. Comparison of mass spectra of 3-mercaptohexanol in Gorilla Glue (top) and the NIST Spectral Library v17 (2017) (bottom).

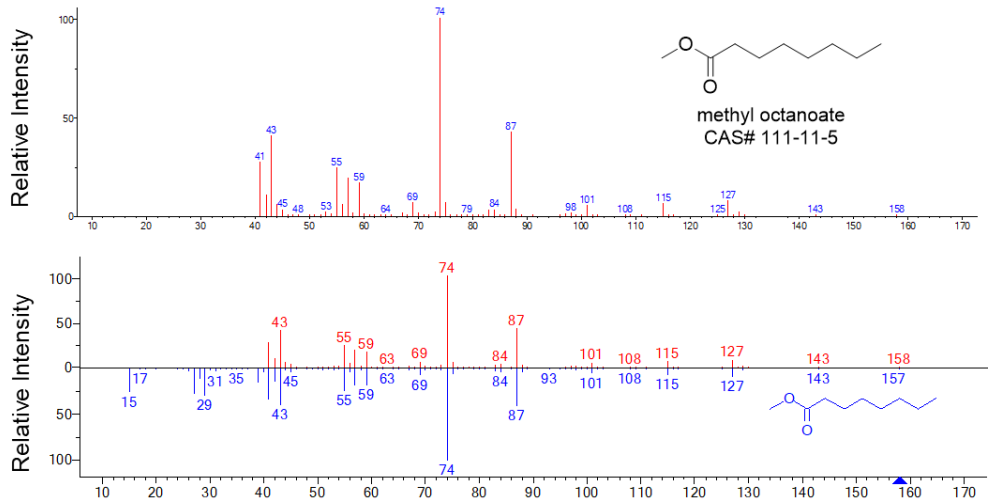

Figure S63. Comparison of mass spectra of methyl octanoate in Banana Scream (top) and the NIST Spectral Library v17 (2017) (bottom).

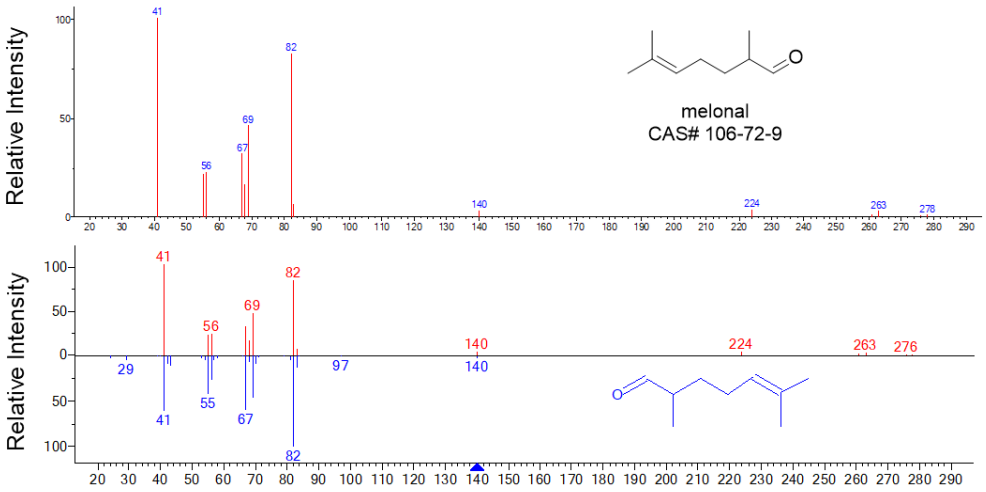

Figure S64. Comparison of mass spectra of melonal in Purple Churro (top) and the NIST Spectral Library v17 (2017) (bottom).

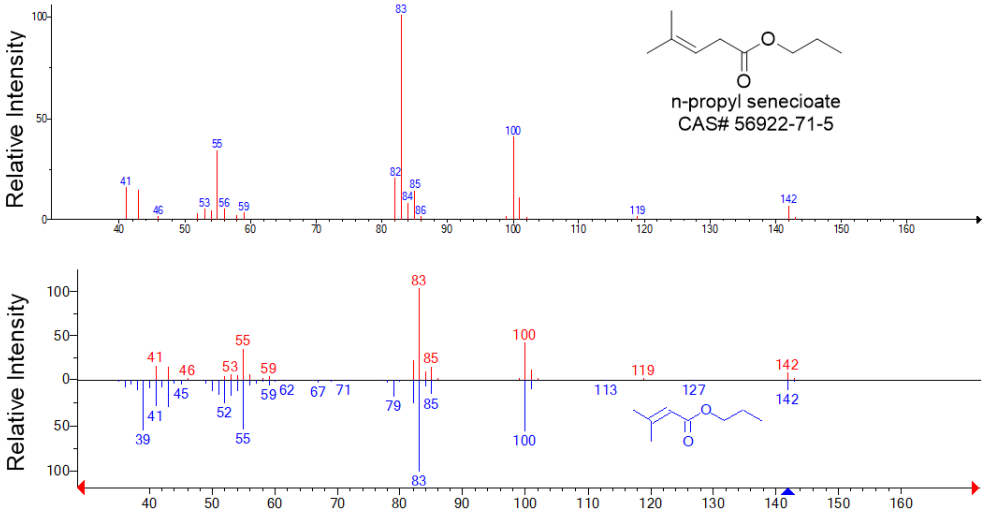

Figure S65. Comparison of mass spectra of *n*-propyl senecioate in Juiceman (top) and the NIST Spectral Library v17 (2017) (bottom).

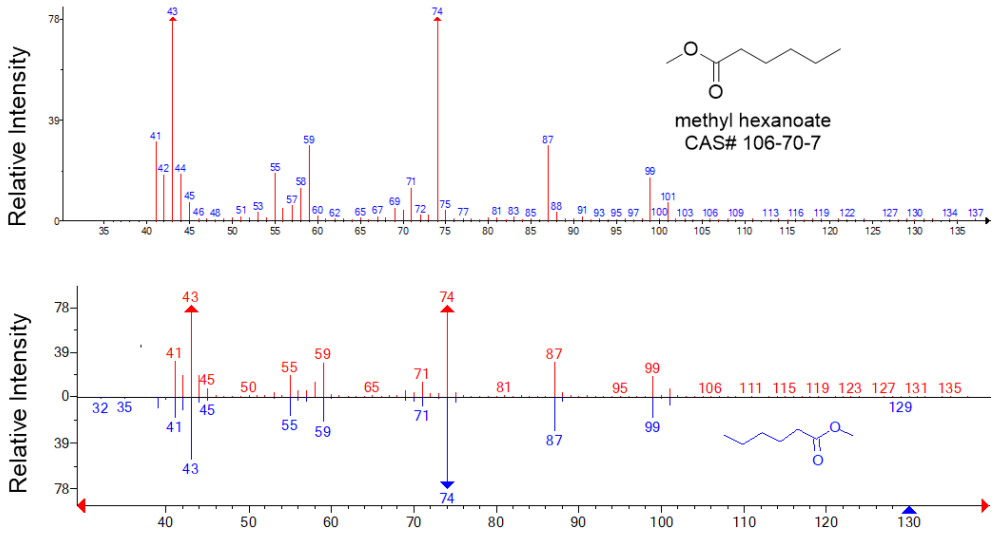

Figure S66. Comparison of mass spectra of methyl hexanoate in Starburst 36 #1 (top) and the NIST Spectral Library v17 (2017) (bottom).

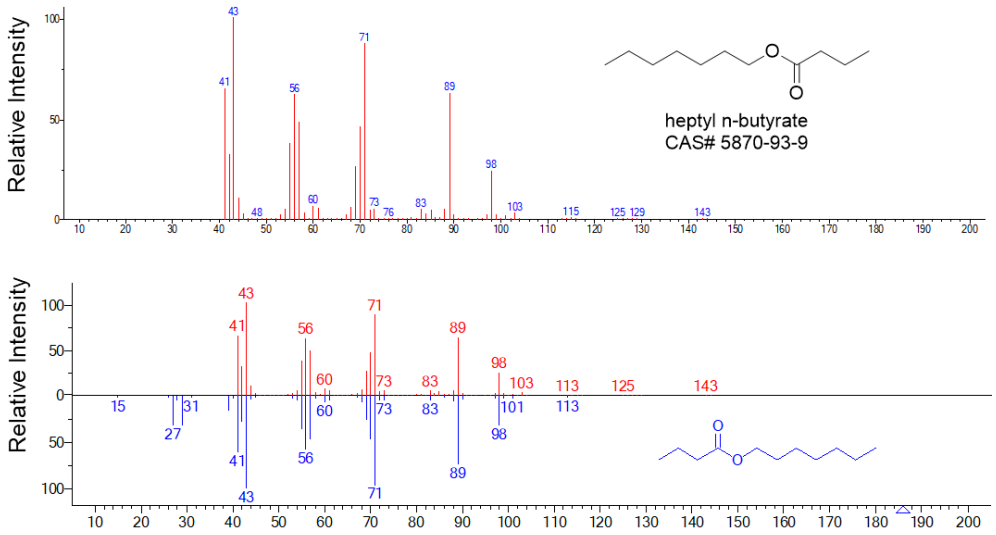

Figure S67. Comparison of mass spectra of heptyl *n*-butyrate in Gorilla Glue (top) and the NIST Spectral Library v17 (2017) (bottom).

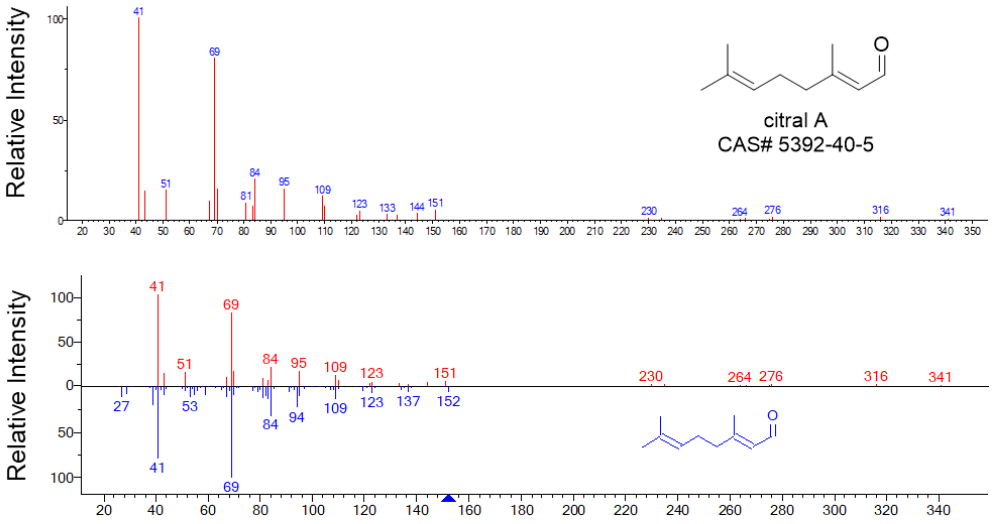

Figure S68. Comparison of mass spectra of citral A in Cookies n' Cream (top) and the NIST Spectral Library v17 (2017) (bottom).

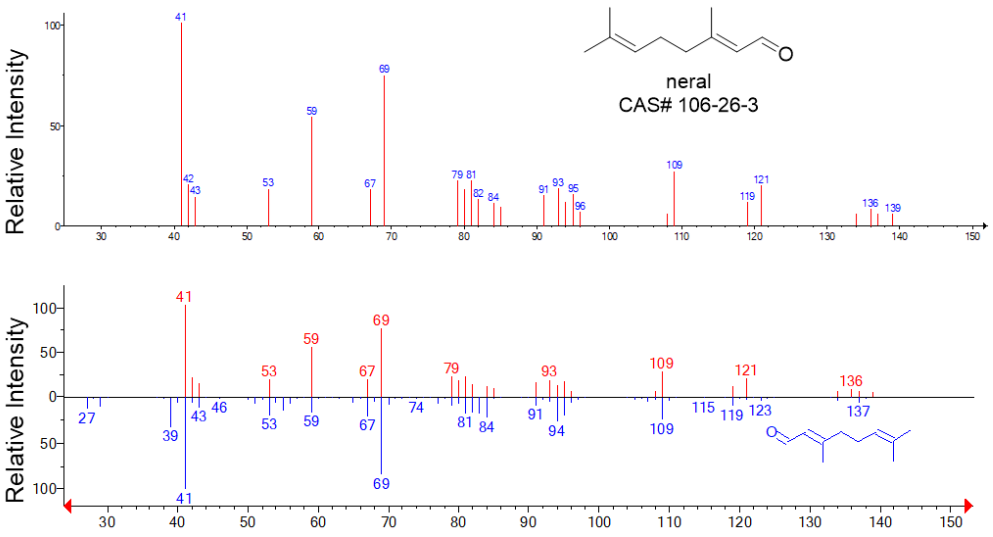

Figure S69. Comparison of mass spectra of neral (citral B) in Cookies n' Cream (top) and the NIST Spectral Library v17 (2017) (bottom).

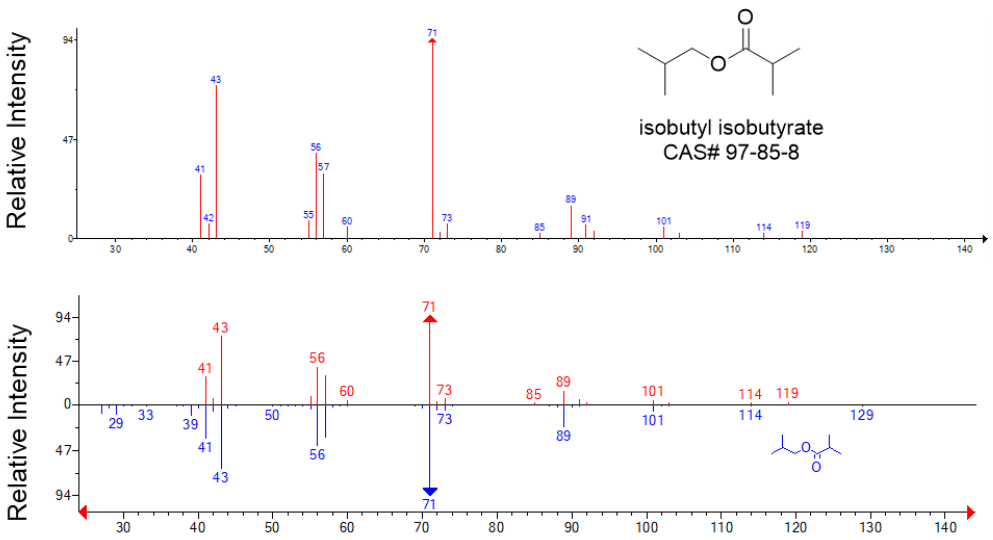

Figure S70. Comparison of mass spectra of heptyl *n*-butyrate in Gorilla Glue (top) and the NIST Spectral Library v17 (2017) (bottom).

Chemical synthesis of senecioates.

propan-2-yl 3-methylbut-2-enoate (isopropyl senecioate)

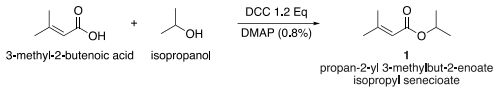

Figure S71. Scheme 1 Synthetic pathway to **1.**

This procedure was carried out open to air. In a 500 mL oven dried round bottom flask (RBF) equipped with a stir bar, 3-methyl-2-butenoic acid (28.87g, 100 mmol, 1 equiv.) was dissolved in 100 mL dichloromethane (DCM) at room temperature. 4-Dimethylaminopyridine (DMAP) (1.01 g, 8.5 mmols, 0.085 equiv.) was added with isopropanol (31.0 mL, 400 mmols, 4 equiv.). The RBF was placed into an ice bath for five minutes before adding, N, N′-Dicyclohexylcarbodiimide (DCC) (24.70 g,120 mmols, 1.2 equiv) into the reaction flask. The reaction stirred in an ice bath for another five minutes. During this time, the reaction mixture changed color rapidly from orange to off-white as precipitate forms. The mixture is removed from of the ice bath and continued stirring for 24 hours. The reaction mixture was filtered using a Buchner funnel. Any remaining solids were suspended in DCM and added to the filter. If precipitate passed through the Büchner funnel it was run again until no precipitate was in the resulting solution. The supernatant was partially concentrated using rotary evaporator. The organic solution was transferred to a separation flask and washed twice with aqueous 0.5 N HCl and twice with saturated sodium bicarbonate. Anhydrous magnesium sulfate was added to the organic layer in small increments while stirring. Once the anhydrous magnesium sulfate starts to clump, the solution was filtered. The crude material was analyzed by TLC, using several different non-polar systems. The TLC plate was eluted using 90:10, Hexane: Diethyl Ether, in a glass chamber. Column chromatography was carried out to purify the crude product. Silica gel was used as the stationary phase and packed with 90:10 Hexane: Diethyl Ether. Normal phase TLC was used again to identify product in the collection test tubes having a R_f value of 0.75. The appropriate samples were concentrated using the roto evaporator and isopropyl senecioate was analyzed using in-house gas chromatography-FID with an internal standard (isoamyl butyrate) to test for purity**.** The sample was analyzed by mixing 5uL of the internal standard and 5uL of compound **1** in 1 mL with hexanes (yield = 50-55%). ^{1}H NMR (400 MHz, DMSO-d_6): δ 11.29 (s, 1H), 7.24 (d, 1H, J = 8.7 Hz), 7.13 (s, 1H), 7.05 (1H, s), 6.71 (d, 1H, J = 8.7 Hz), 3.75 (s, 3H), 3.45–3.36 (m, 2H), 3.25–3.16 (m, 2H), 3.12 (s, 6H); ^{13}C NMR (101 MHz, DMSO-d_6): δ 153.0, 131.5, 127.4, 123.6, 112.1, 111.1, 109.9, 100.2, 69.9, 58.5, 55.4, 19.1.

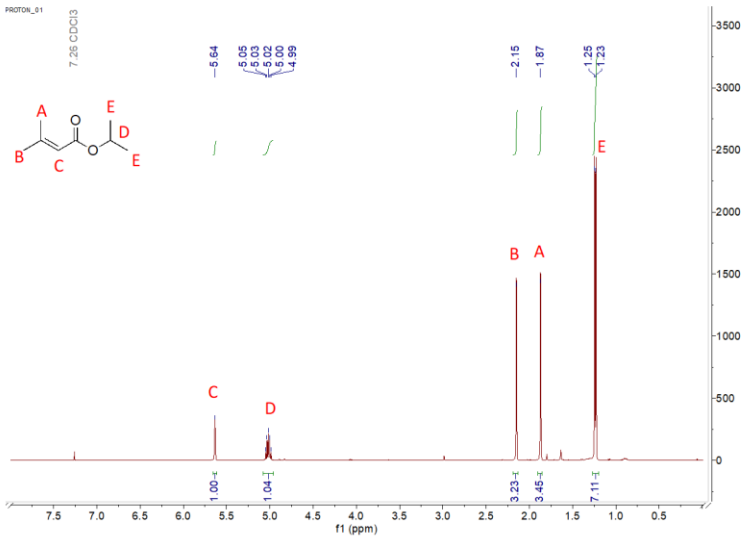

Figure S72. H1 NMR spectrum of 1.

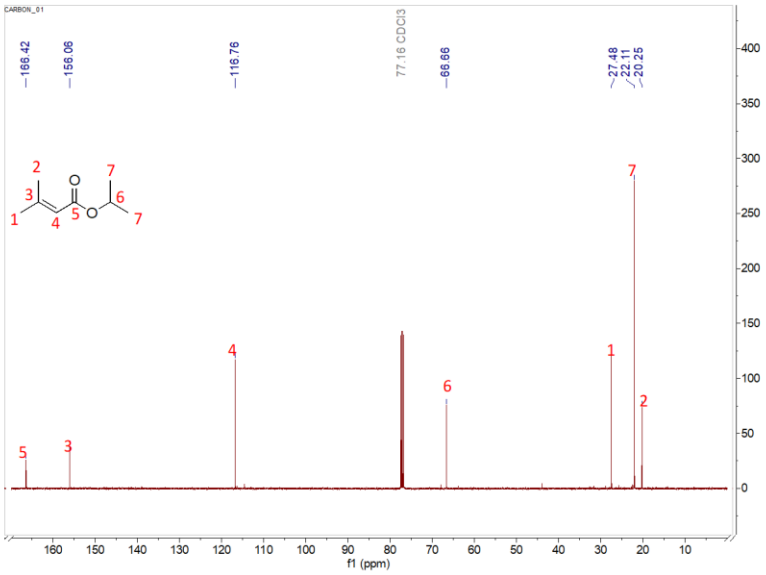

Figure S73. carbon NMR spectrum of 1.

propyl 3-methylbut-2-enoate (propyl senecioate)

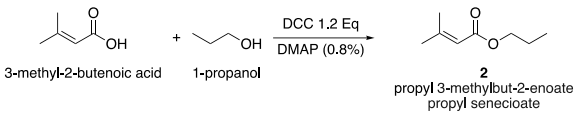

Figure S74. Synthetic pathway to **2.**

This procedure was carried out open to air. In a 500 mL oven dried round bottom flask (RBF) equipped with a stir bar, 3-methyl-2-butenoic acid (28.9g, 100 mmol, 1 equiv.) was dissolved in 100 mL dichloromethane (DCM) at room temperature. 4-Dimethylaminopyridine (DMAP) (1.1 g, 8.5 mmols, 0.085 equiv.) was added with 1-propanol (32.0 mL, 400 mmols, 4 equiv.). The RBF was placed into an ice bath for five minutes before adding, N, N′-Dicyclohexylcarbodiimide (DCC) (24.9 g, 120 mmols, 1.2 equiv) into the reaction flask. The reaction stirred in an ice bath for another five minutes. During this time, the reaction mixture changed color rapidly from orange to off-white as precipitate forms. The mixture is removed from of the ice bath and continued stirring for 24 hours. The reaction mixture was filtered using a Buchner funnel. Any remaining solids were suspended in DCM and added to the filter. If precipitate passed through the Büchner funnel it was run again until no precipitate was in the resulting solution. The supernatant was partially concentrated using rotary evaporator. The organic solution was transferred to a separation flask and washed twice with aqueous 0.5 N HCl and twice with saturated sodium bicarbonate. Anhydrous magnesium sulfate was added to the organic layer in small increments while stirring. Once the anhydrous magnesium sulfate starts to clump, the solution was filtered. The crude material was analyzed by TLC, using several different non-polar systems. The TLC plate was eluted using 90:10, Hexane: Diethyl Ether, in a glass chamber. Column chromatography was carried out to purify the crude product. Silica gel was used as the stationary phase and packed with 90:10 Hexane: Diethyl Ether. Normal phase TLC was used again to identify product in the collection test tubes having a Rf value of 0.75. The appropriate samples were concentrated using the roto evaporator and propyl senecioate was analyzed using in-house gas chromatography-FID with an internal standard (isoamyl butyrate) to test for purity (Yield = 55%). ^{1}H NMR (400MHz, Chloroform-d): A= 2.16ppm, s, 3H, B= 1.88ppm, s, 3H; C=5.68ppm, s, 1H; D=4.1-4.0ppm, s, 2H; E=1.69-1.60ppm, q, 2H; F=0.97-0.93, t, 2H. ^{13}C NMR (400MHz, Chloroform-d): 1=20.29ppm, s,1C; 2=27.50ppm, s,1C; 3=156.43ppm, s,1C; 4=116.28ppm, s, 1C; 5=167.00ppm, s, 1C; 6=65.30ppm, s, 1C; 7=22.23ppm, s, 1C.

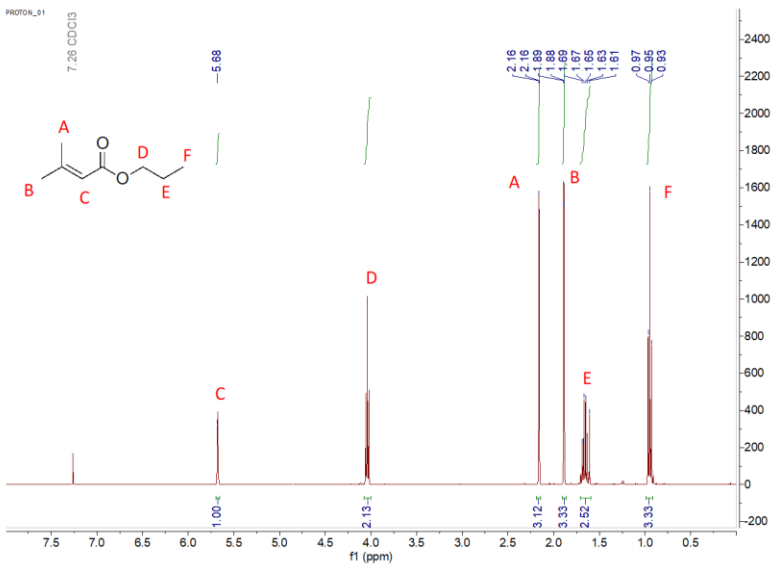

Figure S75. H1 NMR spectrum of 2.

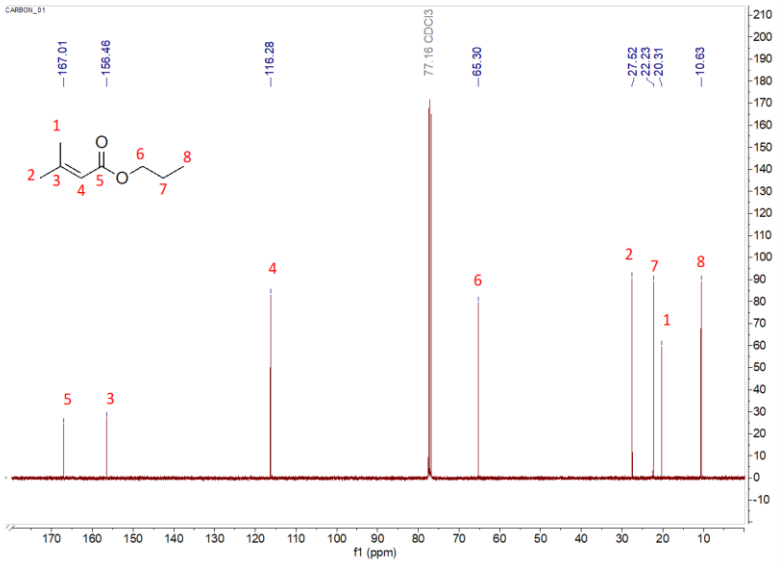

Figure S76. Carbon NMR spectrum of 2.

butyl 3-methylbut-2-enoate (butyl senecioate)

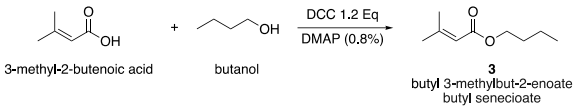

Figure S77. Synthetic pathway to **3.**

This procedure was carried out open to air. In a 500 mL oven dried round bottom flask (RBF) equipped with a stir bar, 3-methyl-2-butenoic acid (27.8g, 100 mmol, 1 equiv.) was dissolved in 100 mL dichloromethane (DCM) at room temperature. 4-Dimethylaminopyridine (DMAP) (1.0 g, 8.5 mmols, 0.085 equiv.) was added with butanol (32.0 mL, 400 mmols, 4 equiv.). The RBF was placed into an ice bath for five minutes before adding, N, N′-Dicyclohexylcarbodiimide (DCC) (24.8 g, 120 mmols, 1.2 equiv) into the reaction flask. The reaction stirred in an ice bath for another five minutes. During this time, the reaction mixture changed color rapidly from orange to off-white as precipitate forms. The mixture is removed from of the ice bath and continued stirring for 24 hours. The reaction mixture was filtered using a Buchner funnel. Any remaining solids were suspended in DCM and added to the filter. If precipitate passed through the Büchner funnel it was run again until no precipitate was in the resulting solution. The supernatant was partially concentrated using rotary evaporator. The organic solution was transferred to a separation flask and washed twice with aqueous 0.5 N HCl and twice with saturated sodium bicarbonate. Anhydrous magnesium sulfate was added to the organic layer in small increments while stirring. Once the anhydrous magnesium sulfate starts to clump, the solution was filtered. The crude material was analyzed by TLC, using several different non-polar systems. The TLC plate was eluted using 90:10, Hexane: Diethyl Ether, in a glass chamber. Column chromatography was carried out to purify the crude product. Silica gel was used as the stationary phase and packed with 90:10 Hexane: Diethyl Ether. Normal phase TLC was used again to identify product in the collection test tubes having a Rf value of 0.45. The appropriate samples were concentrated using the roto evaporator and butyl senecioate was analyzed using in-house gas chromatography-FID with an internal standard (isoamyl butyrate) to test for purity (Yield = 55%). ^{1}H NMR (400MHz, Chloroform-d): A= 2.15ppm, s, 3H, B= 1.88ppm, s, 3H; C=5.67ppm, s, 1H; D=4.09-4.06ppm, s, 2H; E=1.64-1.60ppm, q, 2H; F=1.58-1.34ppm, q, 2H; G=0.94-.91ppm, t, 3H; ^{13}C NMR (400MHz, Chloroform-d): 1=20.31ppm, s,1C; 2=27.52ppm, s,1C; 3=156.46ppm, s,1C; 4=116.28ppm, s, 1C; 5=167.00ppm, s, 1C; 6=65.53ppm, s, 1C; 7=30.93ppm, s, 1C; 8=19.36, s, 1C; 9=13.87ppm, s,1C.

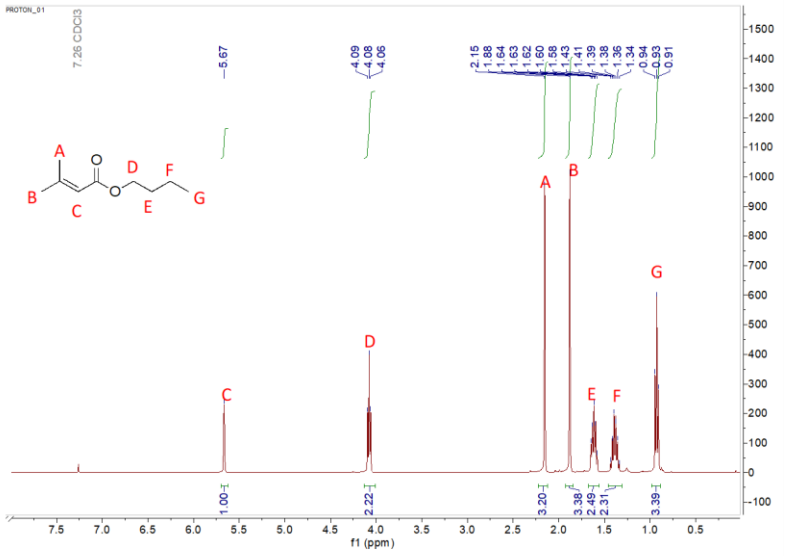

Figure S78. H1 NMR spectrum of 3.

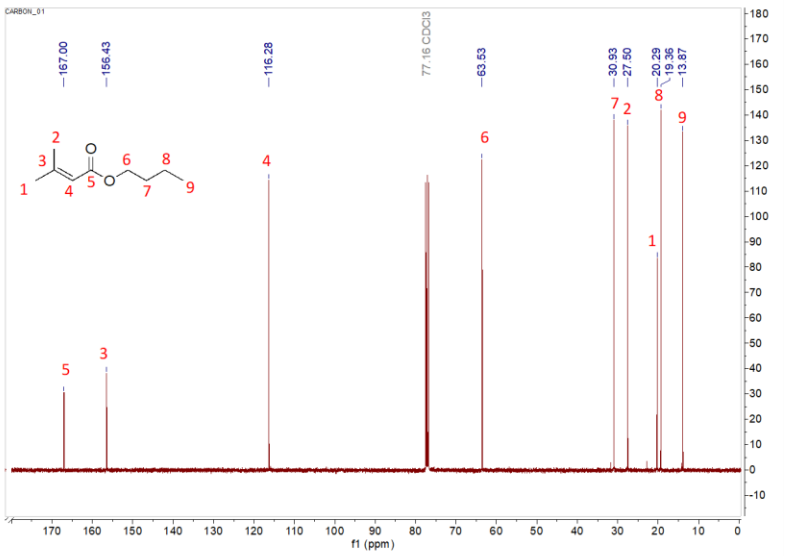

Figure S79. Carbon NMR spectrum of 3.

isopentyl 3-methylbut-2-enoate (isoamyl senecioate)

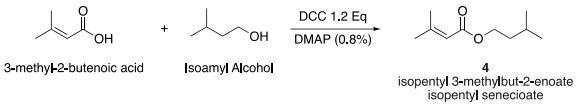

Figure S80. Synthetic pathway to **4.**

This procedure was carried out open to air. In a 500 mL oven dried round bottom flask (RBF) equipped with a stir bar, 3-methyl-2-butenoic acid (27.9g, 100 mmol, 1 equiv.) was dissolved in 100 mL dichloromethane (DCM) at room temperature. 4-Dimethylaminopyridine (DMAP) (1.1 g, 8.5 mmols, 0.085 equiv.) was added with butanol (32.0 mL, 400 mmols, 4 equiv.). The RBF was placed into an ice bath for five minutes before adding, N, N′-Dicyclohexylcarbodiimide (DCC) (25.5 g, 120 mmols, 1.2 equiv) into the reaction flask. The reaction stirred in an ice bath for another five minutes. During this time, the reaction mixture changed color rapidly from orange to off-white as precipitate forms. The mixture is removed from of the ice bath and continued stirring for 24 hours. The reaction mixture was filtered using a Buchner funnel. Any remaining solids were suspended in DCM and added to the filter. If precipitate passed through the Büchner funnel it was run again until no precipitate was in the resulting solution. The supernatant was partially concentrated using rotary evaporator. The organic solution was transferred to a separation flask and washed twice with aqueous 0.5 N HCl and twice with saturated sodium bicarbonate. Anhydrous magnesium sulfate was added to the organic layer in small increments while stirring. Once the anhydrous magnesium sulfate starts to clump, the solution was filtered. The crude material was analyzed by TLC, using several different non-polar systems. The TLC plate was eluted using 90:10, Hexane: Diethyl Ether, in a glass chamber. Column chromatography was carried out to purify the crude product. Silica gel was used as the stationary phase and packed with 90:10 Hexane: Diethyl Ether. Normal phase TLC was used again to identify product in the collection test tubes having a Rf value of 0.75. The appropriate samples were concentrated using the roto evaporator and isoamyl senecioate was analyzed using in-house gas chromatography-FID with an internal standard (isoamyl butyrate) to test for purity (Yield = 65%).^{1}H NMR (400MHz, Chloroform-d): A= 2.15ppm, s, 3H, B= 1.88ppm, s, 3H; C=5.67ppm, s, 1H; D=4.09-4.06ppm, s, 2H; E=1.64-1.60ppm, q, 2H; F=1.88-1.68ppm, q, 1H; G=0.92-.91ppm, d, 3H. ^{13}C NMR (400MHz, Chloroform-d) See **Figure 38,** for exact numbering: 1=20.29ppm, s,1C; 2=27.52ppm, s,1C; 3=156.47ppm, s,1C; 4=116.28ppm, s, 1C; 5=167.00ppm, s, 1C; 6=62.31ppm, s, 1C; 7=37.60ppm, s, 1C; 8=25.25, s, 2C; 9=22.62ppm, s,1C.

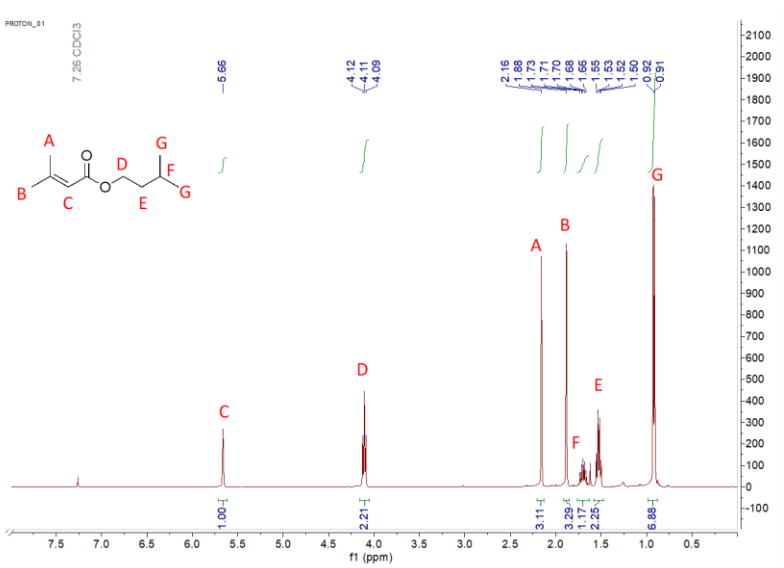

Figure S81. H1 NMR spectrum of 4.

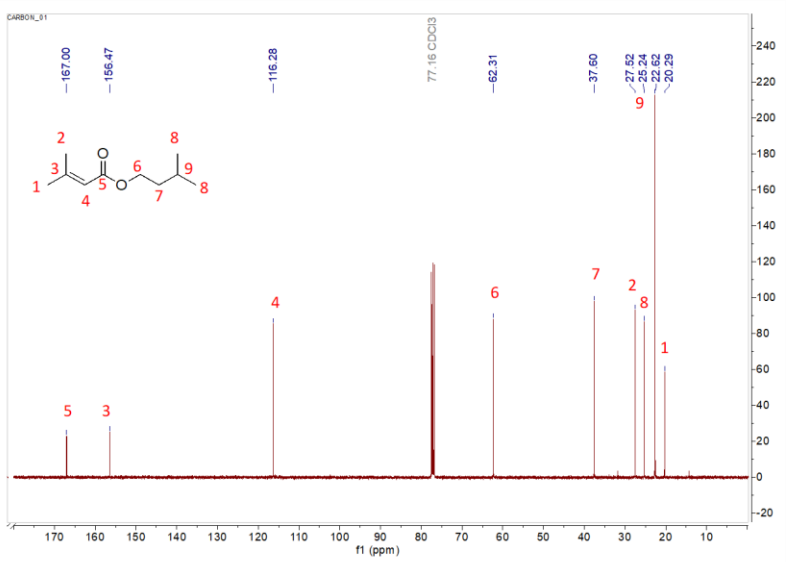

Figure S82. Carbon NMR spectrum of 4.

hexyl 3-methylbut-2-enoate (hexyl senecioate)

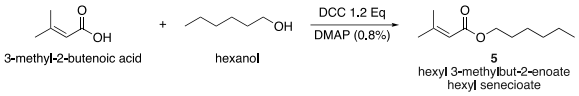

Figure S83. Synthetic pathway to **5.**

This procedure was carried out open to air. In a 500 mL oven dried round bottom flask (RBF) equipped with a stir bar, 3-methyl-2-butenoic acid (27.9g, 100 mmol, 1 equiv.) was dissolved in 100 mL dichloromethane (DCM) at room temperature. 4-Dimethylaminopyridine (DMAP) (1.1 g, 8.5 mmols, 0.085 equiv.) was added with butanol (32.0 mL, 400 mmols, 4 equiv.). The RBF was placed into an ice bath for five minutes before adding, N, N′-Dicyclohexylcarbodiimide (DCC) (25.5 g, 120 mmols, 1.2 equiv) into the reaction flask. The reaction stirred in an ice bath for another five minutes. During this time, the reaction mixture changed color rapidly from orange to off-white as precipitate forms. The mixture is removed from of the ice bath and continued stirring for 24 hours. The reaction mixture was filtered using a Buchner funnel. Any remaining solids were suspended in DCM and added to the filter. If precipitate passed through the Büchner funnel it was run again until no precipitate was in the resulting solution. The supernatant was partially concentrated using rotary evaporator. The organic solution was transferred to a separation flask and washed twice with aqueous 0.5 N HCl and twice with saturated sodium bicarbonate. Anhydrous magnesium sulfate was added to the organic layer in small increments while stirring. Once the anhydrous magnesium sulfate starts to clump, the solution was filtered. The crude material was analyzed by TLC, using several different non-polar systems. The TLC plate was eluted using 90:10, Hexane: Diethyl Ether, in a glass chamber. Column chromatography was carried out to purify the crude product. Silica gel was used as the stationary phase and packed with 90:10 Hexane: Diethyl Ether. Normal phase TLC was used again to identify product in the collection test tubes having a Rf value of 0.62. The appropriate samples were concentrated using the roto evaporator and hexyl senecioate was analyzed using in-house gas chromatography-FID with an internal standard (isoamyl butyrate) to test for purity (yield = 75%). ^{1}H NMR (400MHz, Chloroform-d): A= 2.16ppm, s, 3H, B= 1.88ppm, s, 3H; C=5.67ppm, s, 1H; D=4.09-4.05ppm, s, 2H; E=1.65-1.59ppm, q, 2H; F=1.30ppm, t, 2H; G=1.301ppm, t, 2H; H=1.30ppm, t,2H; I=0.88ppm, s, 3H; ^{13}C NMR (400MHz, Chloroform-d): 1=20.29ppm, s,1C; 2=27.52ppm, s,1C; 3=156.46ppm, s,1C; 4=116.30ppm, s, 1C; 5=167.02ppm, s, 1C; 6=63.86ppm, s, 1C; 7=37.60ppm, s, 1C; 8=27.53ppm, s, 2C; 9=31.62ppm, s,1C; 10=20.31ppm, s, 1C, 11=14.15ppm, s, 1C.

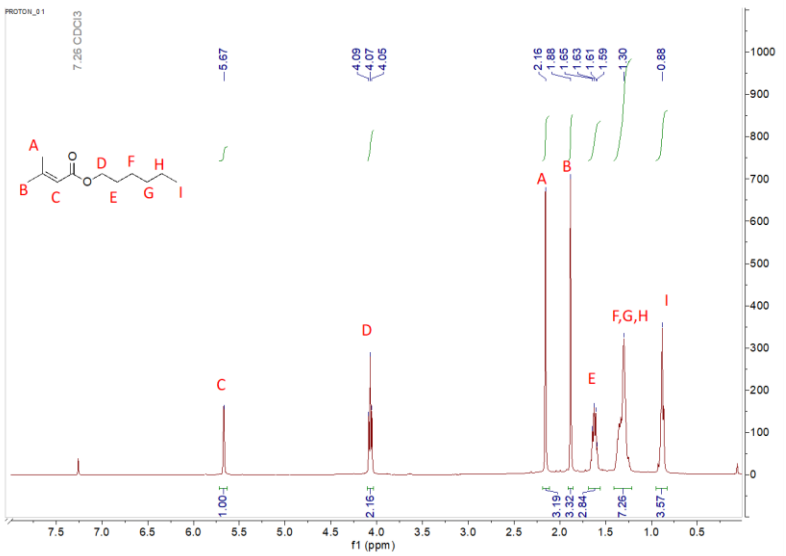

Figure S84. H1 NMR spectrum of 5.

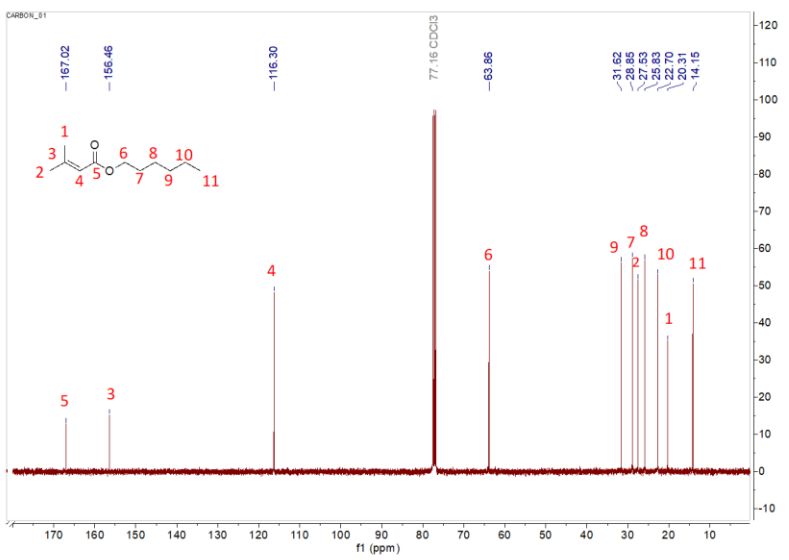

Figure S85. Carbon NMR spectrum of 5.