Supporting Information

Identification of New Family of Prenylated Volatile Sulfur Compounds in *Cannabis* Revealed by Comprehensive Two-Dimensional Gas Chromatography

Iain W. H. Oswald[1*], Marcos A. Ojeda[1], Ryan J. Pobanz[1], Kevin A. Koby[1], Anthony J. Buchanan[2], Josh Del Rosso[3], Mario A. Guzman[4], Thomas J. Martin[1]

[1]*Department of Research and Development, Abstrax Tech, 2661 Dow Avenue, Tustin, CA 92618, United States*

[2]*SepSolve Analytical Ltd., 4 Swan Court, Forder Way, Peterborough, Cambridgeshire, PE7 8GX, United Kingdom*

[3]*Josh D, 325 18th Street, Huntington Beach, CA 92648, United States*

[4]*Elysian Group Inc., 1650 Westwood Blvd. suite #200, Los Angeles, CA 90024, United States*

[*]correspondence to: iain.oswald@abstraxtech.com

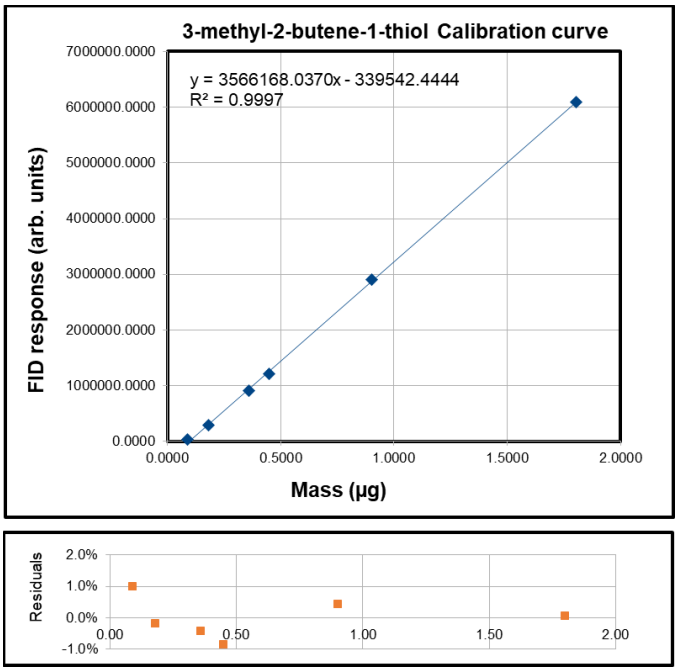

Figure S1. Calibration curve obtained for 3-methyl-2-butene-1-thiol (**VSC3**).

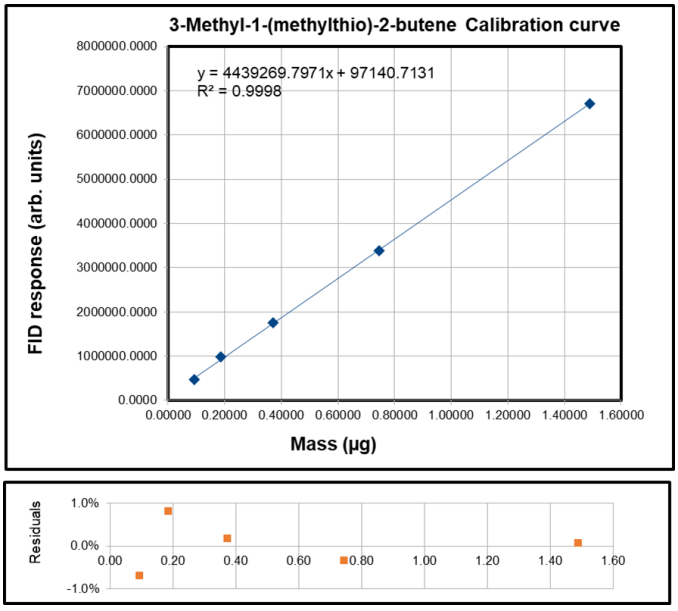

Figure S2. Calibration curve obtained for 3-Methyl-1-(methylthio)-2-butene (**VSC4**).

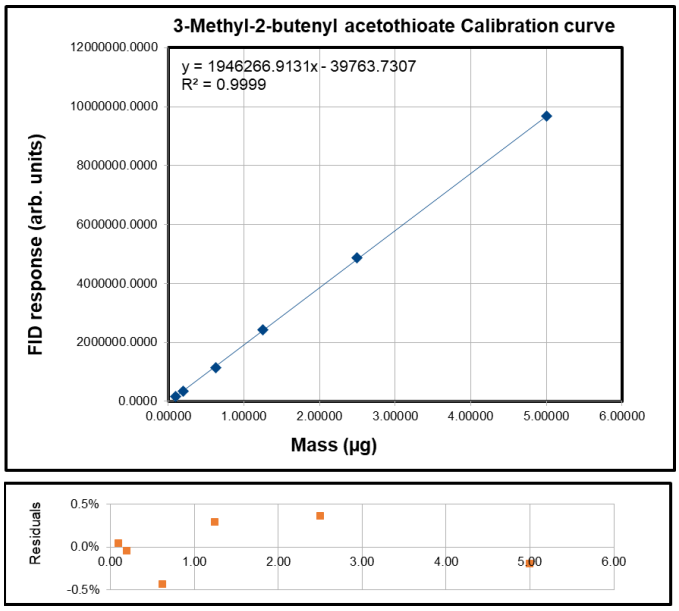

Figure S3. Calibration curve obtained for 3-Methyl-2-butenyl acetothioate (**VSC5**).

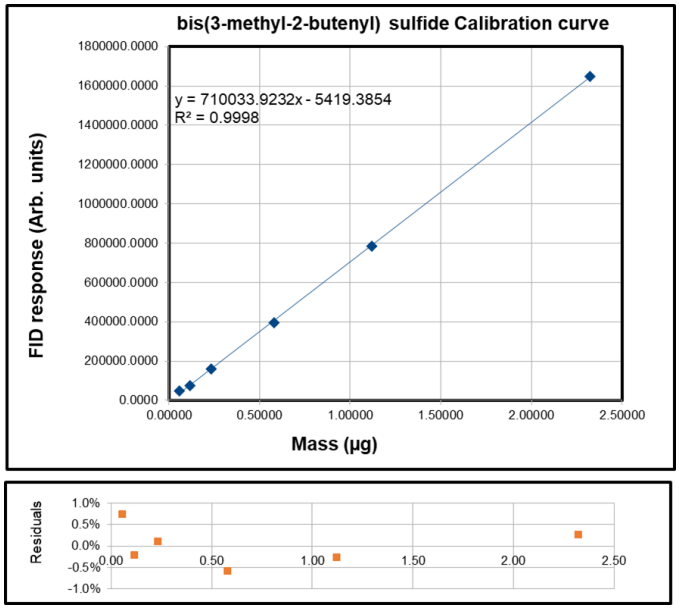

Figure S4. Calibration curve obtained for bis(3-methyl-2-butenyl) sulfide (**VSC6**).

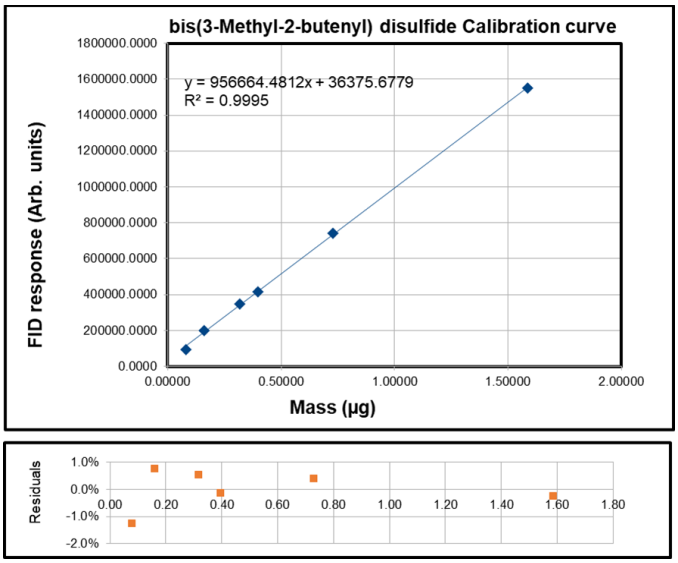

Figure S5. Calibration curve obtained for bis(3-Methyl-2-butenyl) disulfide (**VSC7**).

Table S1. Calibration curve data for VSC standards.

Compound name	slope	intercept	R^2	LOD*	LOQ*
3-methyl-2-butene-1-thiol	3566168.037	-339542.444	0.9997	0.0413	0.1250
3-Methyl-1-(methylthio)-2-butene	4439269.797	97140.713	0.9998	0.0327	0.0991
3-Methyl-2-butenyl acetothioate	1946266.913	-39763.730	0.9999	0.0551	0.1669
bis(3-methyl-2-butenyl) sulfide	710033.923	-5419.385	0.9998	0.0254	0.0769
bis(3-Methyl-2-butenyl) disulfide	956664.481	36375.677	0.9995	0.0437	0.0133

*LOD and LOQ are defined by the equations: $LOD = 3.3 \cdot \frac{\sigma}{S}$; $LOQ = 10 \cdot \frac{\sigma}{S}$ where σ is the standard deviation of the y-intercept and S is the slope of the curve.

Table S2. Calibration curve data of cannabis terpene standard used to quantify major aroma compounds in cultivars.

Compound name	slope	intercept	R^2	LOD*	LOQ*	STD
(+)-Cedrol	950929.1	-10838	0.999107	0.024	0.074	7017.150
(-)-Isopulegol	2490659	-80494	0.999481	0.019	0.056	14010.908
3-Carene	1815333	10688	0.999799	0.012	0.035	6354.137
Camphene	5035385	5230	0.999954	0.006	0.017	8430.713
Camphor	3202872	-27610	0.999831	0.011	0.032	10271.194
Caryophyllene	2393393	11151	0.999738	0.013	0.040	9566.680
Caryophyllene oxide	684208.4	-24100	0.99072	0.079	0.239	16346.295
Fenchone	3697566	-85718	0.99169	0.075	0.226	83553.655
Geranyl acetate	1050417	-41580	0.994326	0.062	0.186	19587.701
Isoborneol	2958475	-58697	0.991953	0.073	0.222	65776.919
Linalool	2945207	-43159	0.999952	0.006	0.017	5051.017
Menthol	2300718	-25902	0.99834	0.033	0.101	23159.093
Nerol**	631185.8	-9784	0.925232	0.232	0.702	44292.747
Valencene	2051537	-25307	0.999939	0.006	0.019	3942.882
cis-Nerolidol	863783.1	-25351	0.999673	0.015	0.045	3858.102
α-Bisabolol	460421.2	-6677	0.996178	0.050	0.153	7040.231

α-Phellandrene	6299806	-61298	0.999916	0.007	0.023	14238.957
β-Myrcene	3983419	16289	0.999963	0.005	0.015	6022.747
β-Ocimene	3247385	-57569	0.999826	0.011	0.033	10567.730
(+)-Pulegone**	512474.7	-18102	0.973636	0.246464	0.746861	22000
Camphor	6878673	-162308	0.995964	0.095347	0.28893	284000
Geraniol	2503981	-150385	0.987835	0.166209	0.503664	58437
Guaiol**	717502.1	11145	0.935813	0.392262	1.188672	28907
Humulene	2857654	-90132	0.991378	0.139682	0.423278	121000
Limonene	5194645	-74418	0.995282	0.103122	0.312492	267000
Sabinene	3792703	-97700	0.996617	0.087259	0.26442	143000
Terpinolene	4514111	-137420	0.992288	0.132045	0.400137	176000
endo-Borneol	5176182	-137987	0.999568	0.031155	0.094409	164000
endo-Fenchol	3081473	-47145	0.998957	0.048408	0.146692	124000
trans-Nerolidol	641674.3	-14424	0.986496	0.175242	0.531036	18036
trans-Sabinene hydrate	1792484	-56566	0.996241	0.092004	0.2788	57265
α-Pinene	5038302	-10371	0.997008	0.082054	0.248647	294000
α-Terpinene	4634677	-121630	0.995327	0.102627	0.31099	183000
α-Terpineol	1746898	-50997	0.99532	0.102709	0.31124	45772
β-Pinene	5857299	-82800	0.996525	0.088445	0.268015	285000
γ-Terpinene	5302039	-126354	0.995006	0.106109	0.321541	227000

*LOD and LOQ are defined by the equations: $LOD = 3.3 \cdot \frac{\sigma}{S}$; $LOQ = 10 \cdot \frac{\sigma}{S}$ where σ is the standard deviation of the *y*-intercept and *S* is the slope of the curve. **Analytes with R^2 less than 0.98 were excluded from analysis.

Table S3. Unidentified Volatile sulfur compounds (VSCs) detected in certain cultivars and their respective retention times.

Compound ID	Samples detected in	^1t_R, ^2t_R (min, s)
U1	All samples	4.079, 1.768
U2	C1, C2, C3	9.009, 1.985
U3	C1 – C7	25.441, 2.851
U4	C7, Acai Berry Gelato BHO	17.409, 4.045
U5	C7	23.291, 3.881

Table S4. Cultivars, cultivators, sample ages, individual olfactory scores, and average olfactory scores.

Sample ID	Cultivar	Cultivator	Sample Age (days)[2]	Score 1	Score 2	Score 3	Score 4	Olfactory score
C1	Bacio Gelato	Sherbinskis	13	10	10	10	10	10.0(0)
C2	Clone Guy OG	This work[1]	1	9	8.5	8.2	8.8	8.6(4)
C3	Gelato[3]	Clone Guy	4	8	7.5	8.5	7.6	7.9(5)
C4	Area 41	Alien Labs	24	7.7	8.5	8.2	8	8.1(3)
C5	Jetlag OG	Andretti	28	8	7.5	7.5	7	7.5(4)
C6	Gushers	Connected	109	6	7.5	7.4	7	7.0(7)
C7	WiFi Cake	Jungle Boys	15	6	6.5	7	6.6	6.5(4)
C8	Apple Fritter	Fresh Baked	41	6	5	4.5	5.5	5.3(6)
C9	Chem 91	Jungle Boys	50	1.5	2	2	1	1.6(5)
C10	Gelato[3]	Clone Guy	46	2.5	4	2	2	2.6(9)
C11	Cali Berry	Lumpy's	35	1	1	1.5	1	1.1(3)
C12	Gouda Berry	Exotic Genetix	46	0	0	0	0	0.0(0)
C13	Black Jack	Hyperwolf	10	0	0	0	0	0.0(0)
-	Bacio Gelato BHO	Sherbinskis	-	9.5	9.8	10	9.8	9.8(2)
-	Gello Gelato BHO	Sherbinskis	-	9.4	9.8	9.7	9.8	9.7(2)
-	Acai Berry Gelato BHO	Sherbinskis	-	9.4	9.7	9.9	9.5	9.6(2)

[1]Clone Guy OG data was obtained from samples from indoor greenhouse trial. [2]Sample age is defined as the time between packaging date and data collection date. [3]C3 and C10 were same product lot measured at different sample ages.

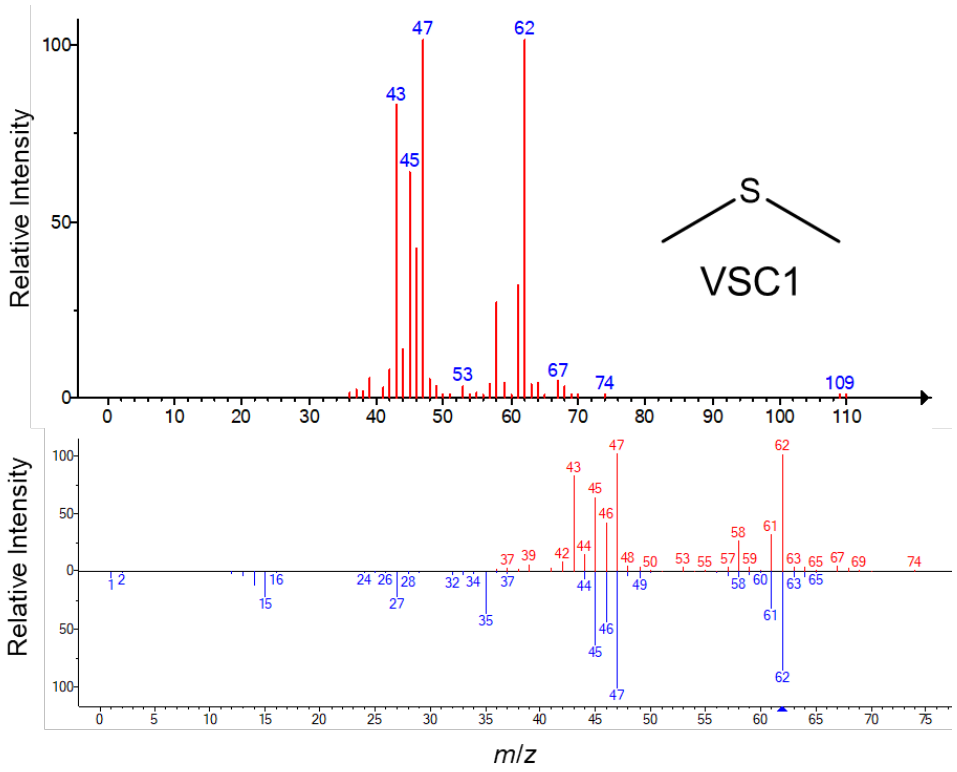

Figure S6. Top: Mass spectrum of **VSC1** in **C1**. Bottom: Mass spectrum of **VSC1** compared with Dimethyl disulfide from NIST Spectral Library v17 (2017) (CAS # 75-18-3).

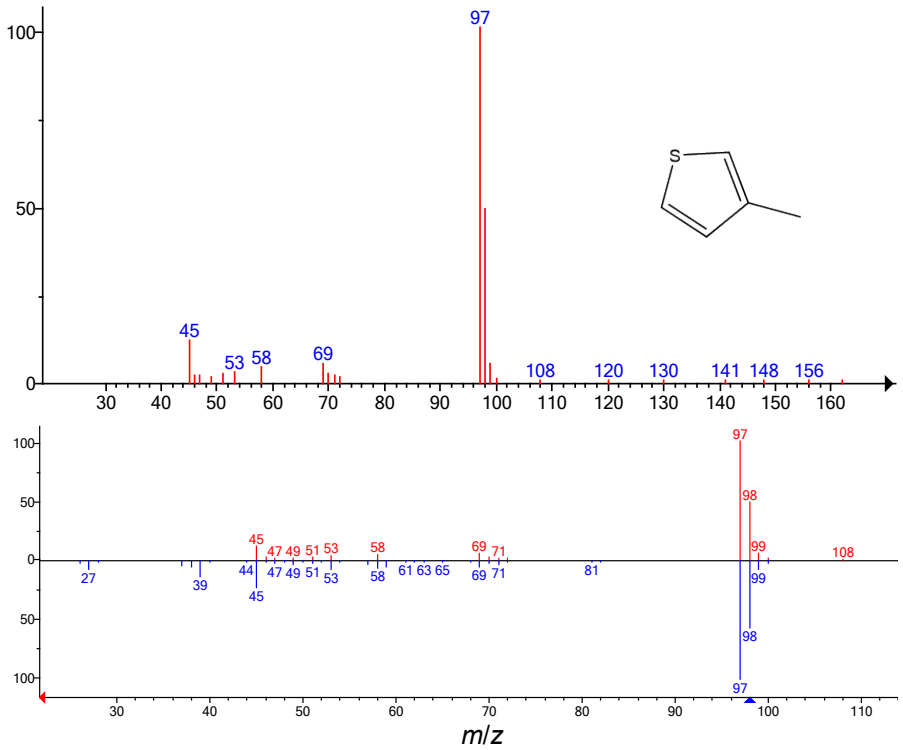

Figure S7. Mass spectrum of compound **VSC2** in **C1**. Bottom: Mass spectrum of **VSC2** compared with 3-Methylthiophene from the NIST Spectral Library v17 (2017) (CAS # 616-44-4).

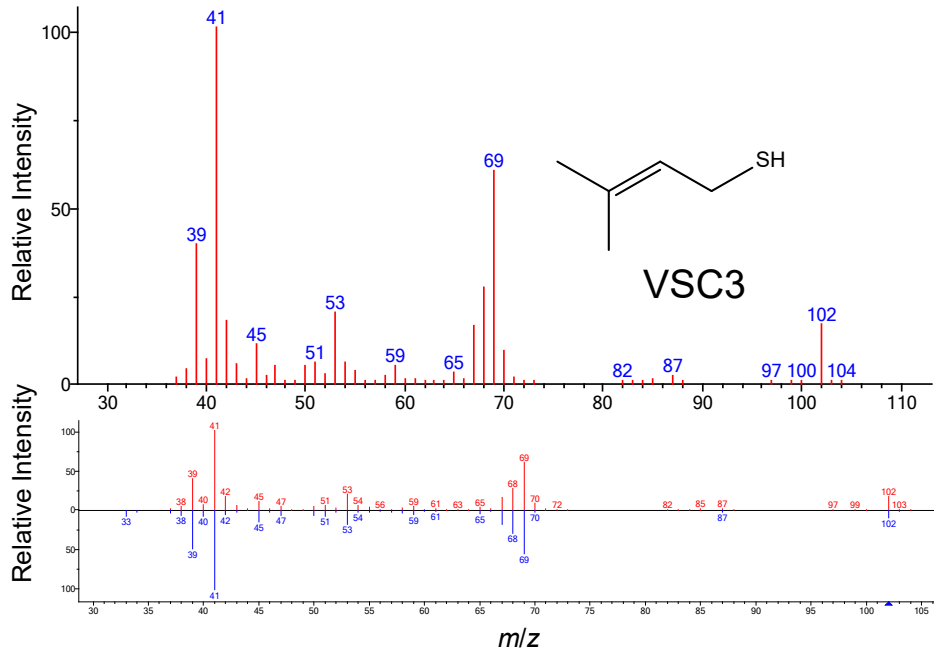

Figure S8. Top: Mass spectrum of compound **VSC3** in **C1**. Bottom: Mass spectrum of **VSC3** compared with 3-methylbut-2-ene-1-thiol from the NIST Spectral Library v17 (2017) (CAS # 5287-45-6).

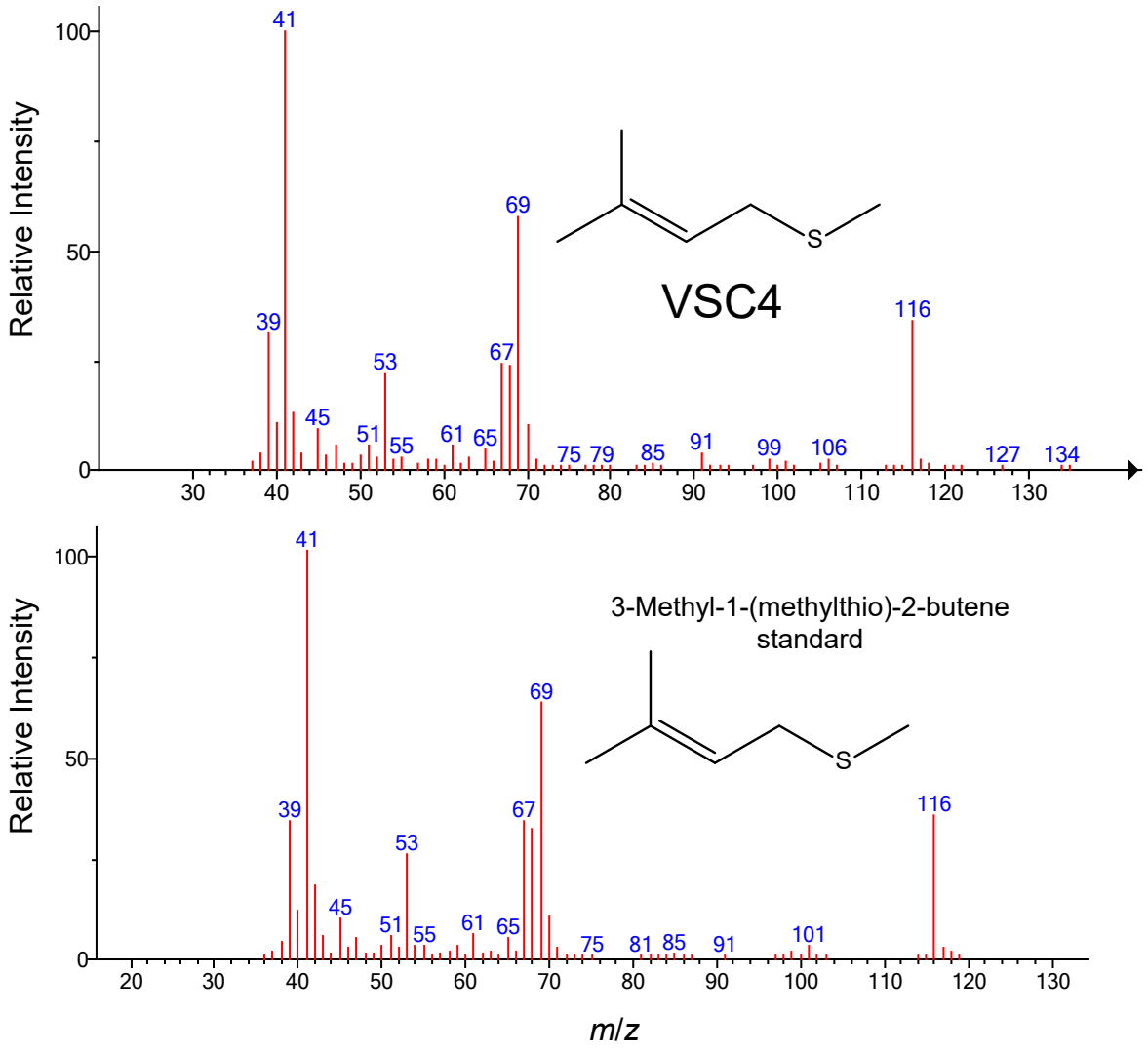

Figure S9. Top: Mass spectrum of compound **VSC4** in **C1**. Bottom: Mass spectrum of 3-Methyl-1-(methylthio)-2-butene standard.

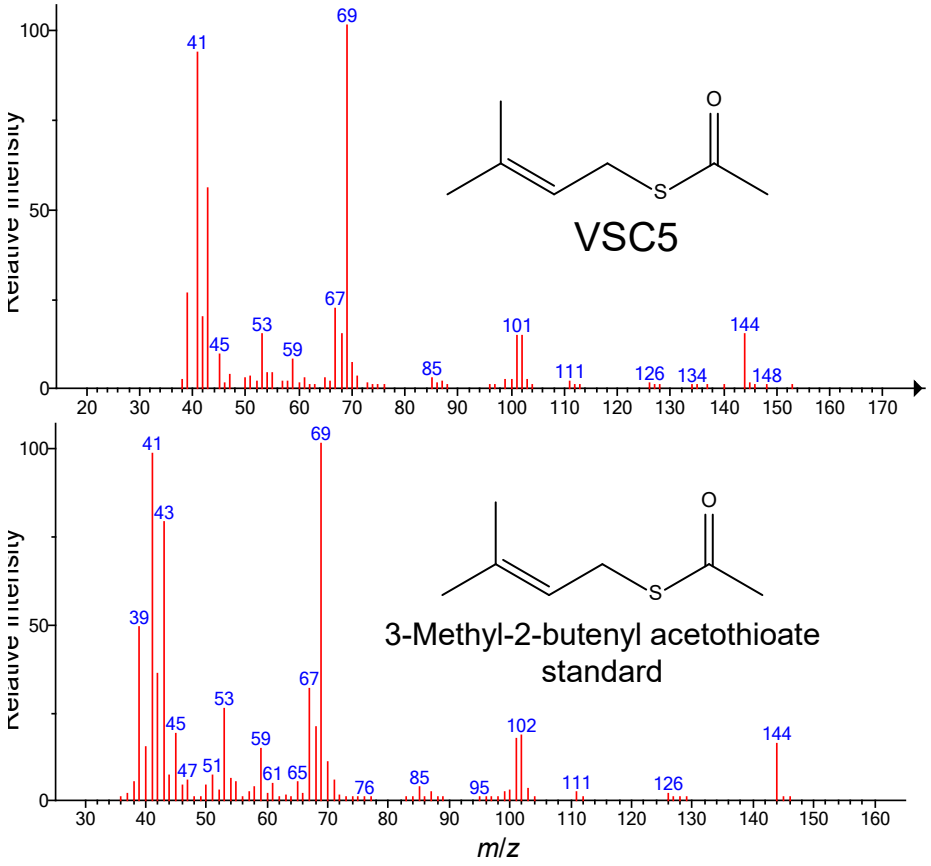

Figure S10. Top: Mass spectrum of compound **VSC5** in **C1**. Bottom: Mass spectrum of 3-Methyl-2-butenyl acetothioate standard (CAS # 33049-93-3).

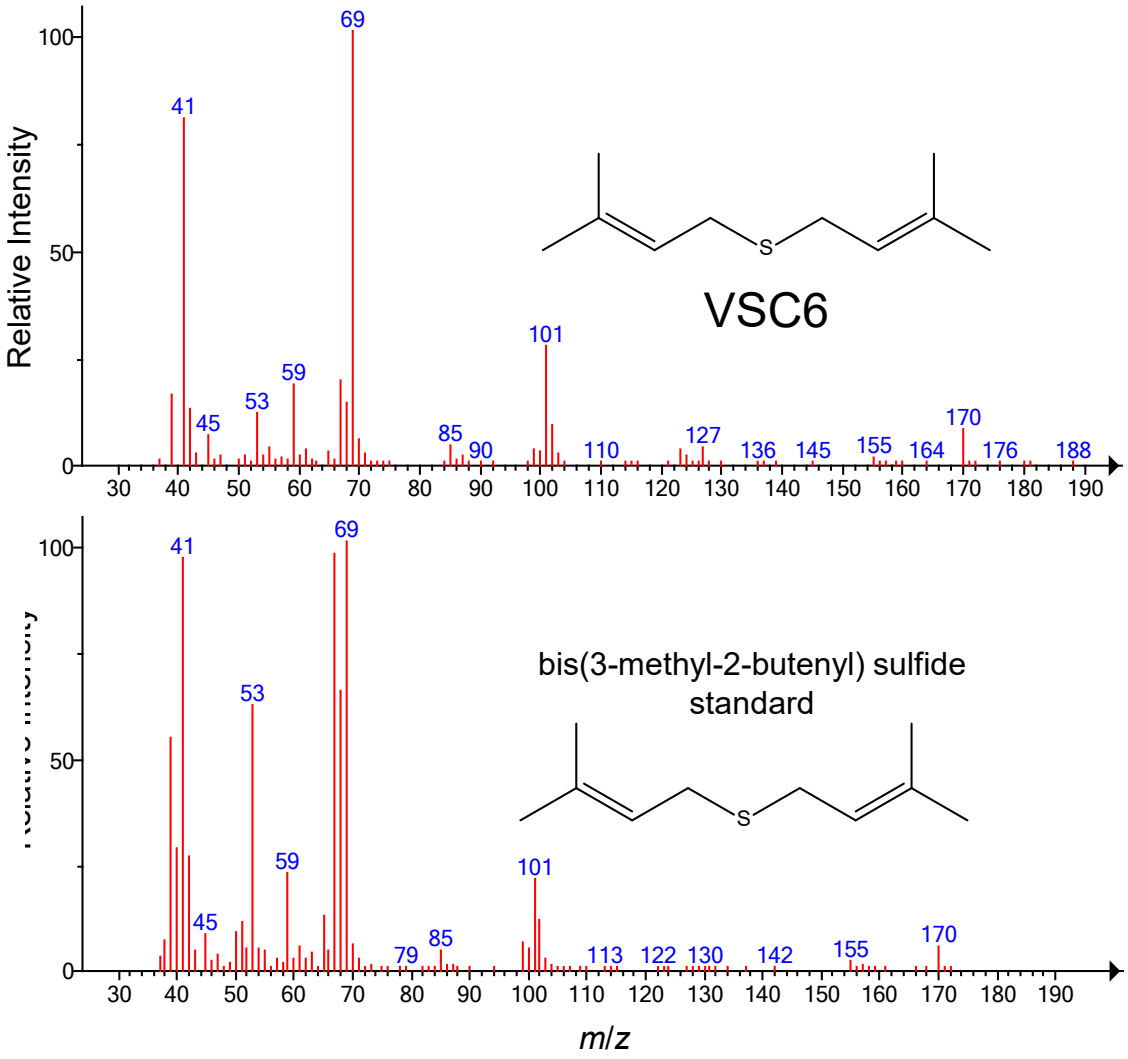

Figure S11. Top: Mass spectrum of compound of **VSC6** in **C1**. Bottom: Mass spectrum of bis(3-methyl-2-butenyl) sulfide standard.

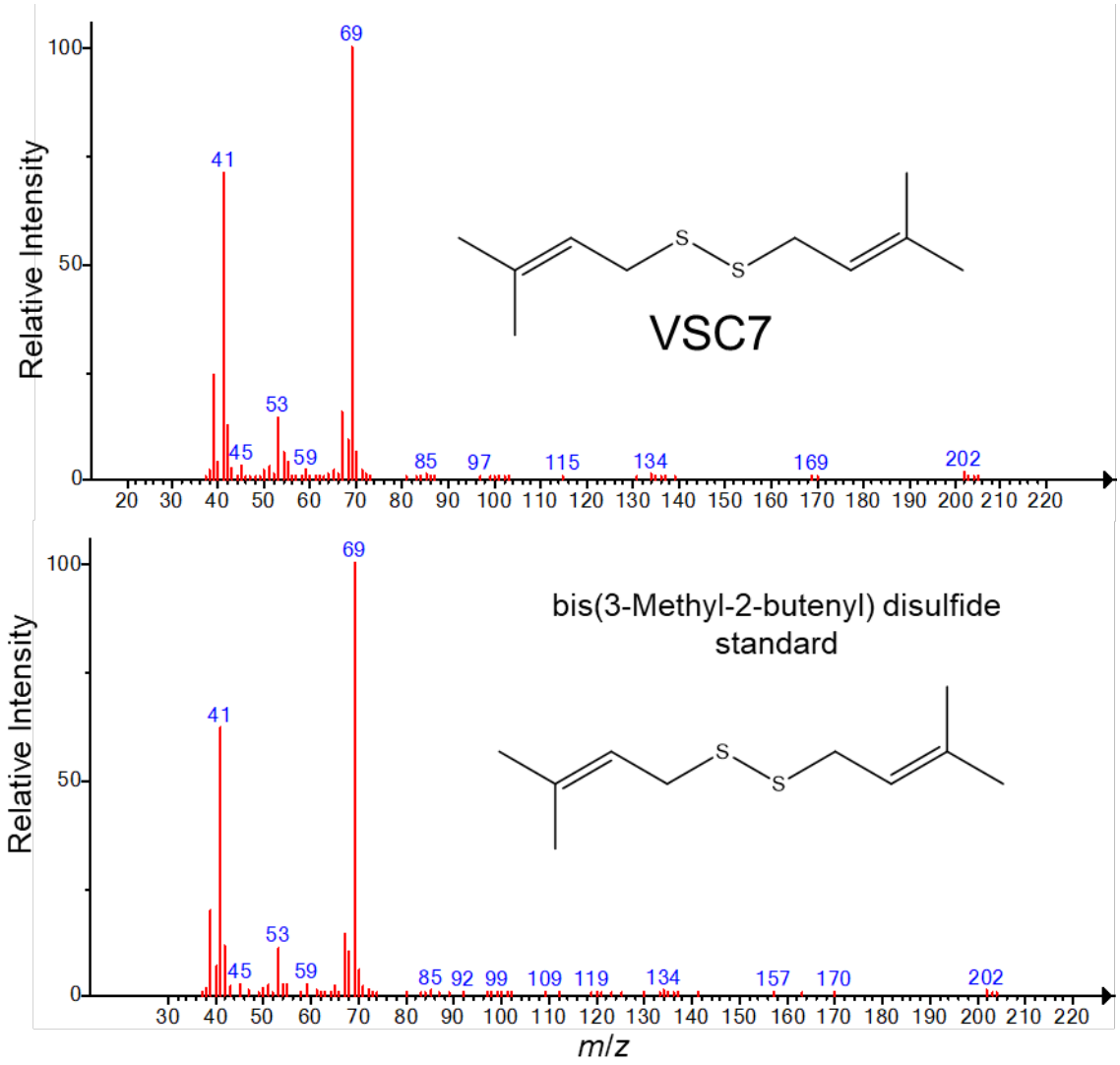

Figure S12. Top: Mass spectrum of compound **VSC7** in **C1**. Bottom: Mass spectrum of bis(3-Methyl-2-butenyl) disulfide standard.

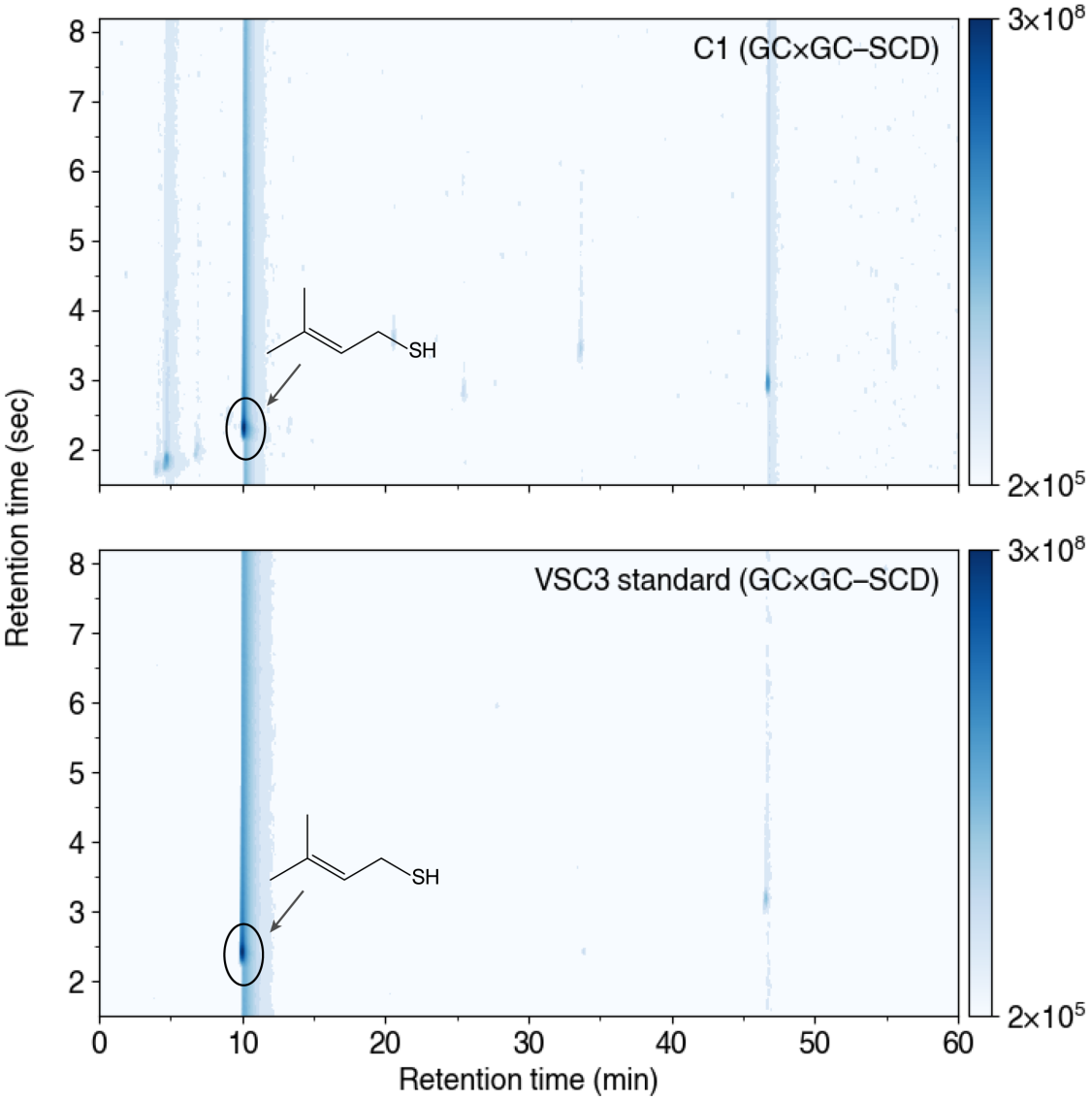

Figure S13. GC×GC–SCD 2-Dimensional chromatograms comparing **VSC3** elution in Bacio Gelato versus 3-methyl-2-butene-1-thiol (**VSC3**) standard.

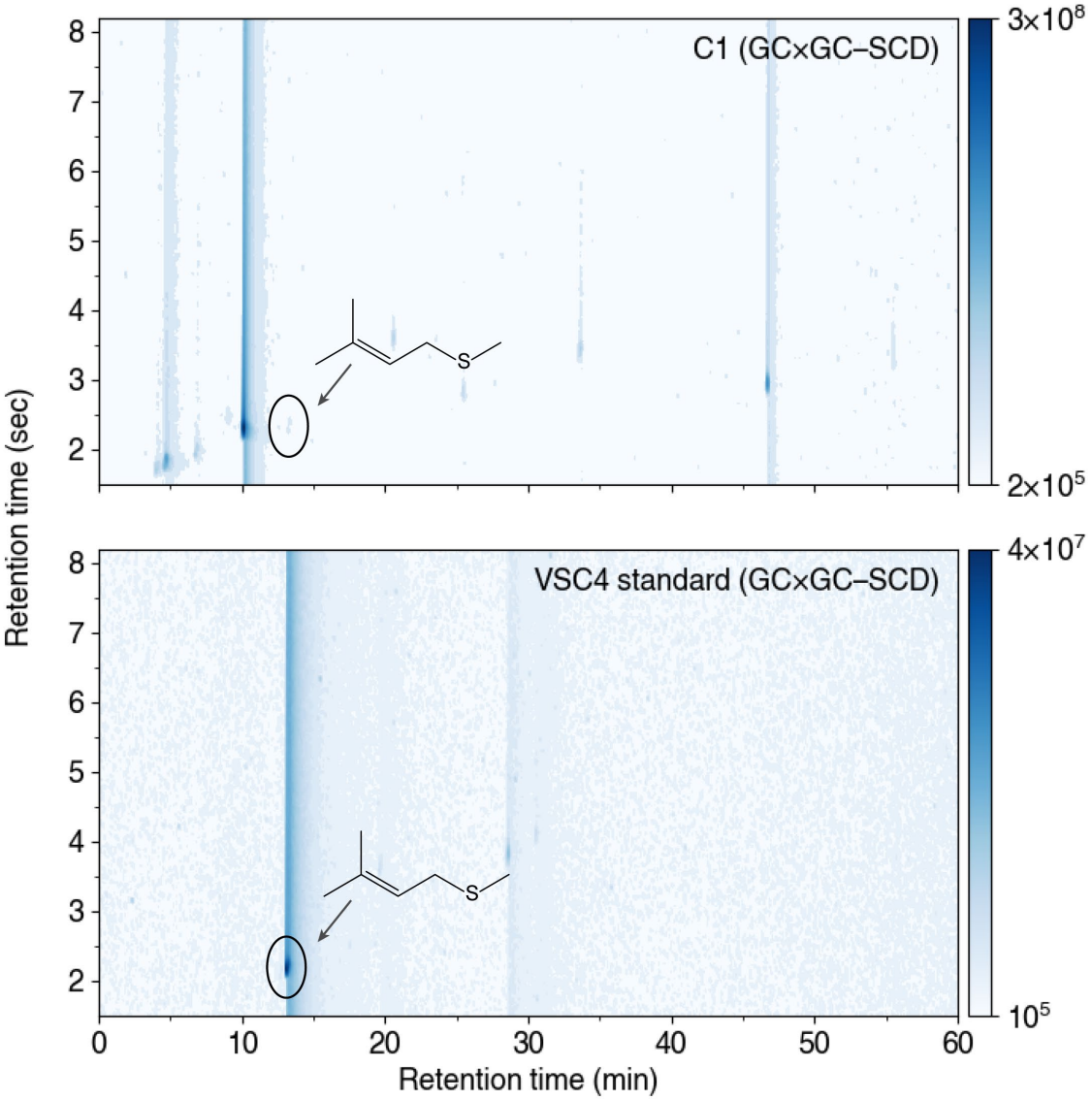

Figure S14. GC×GC–SCD 2-Dimensional chromatograms comparing **VSC4** elution in Bacio Gelato versus 3-Methyl-1-(methylthio)-2-butene (**VSC4**) standard.

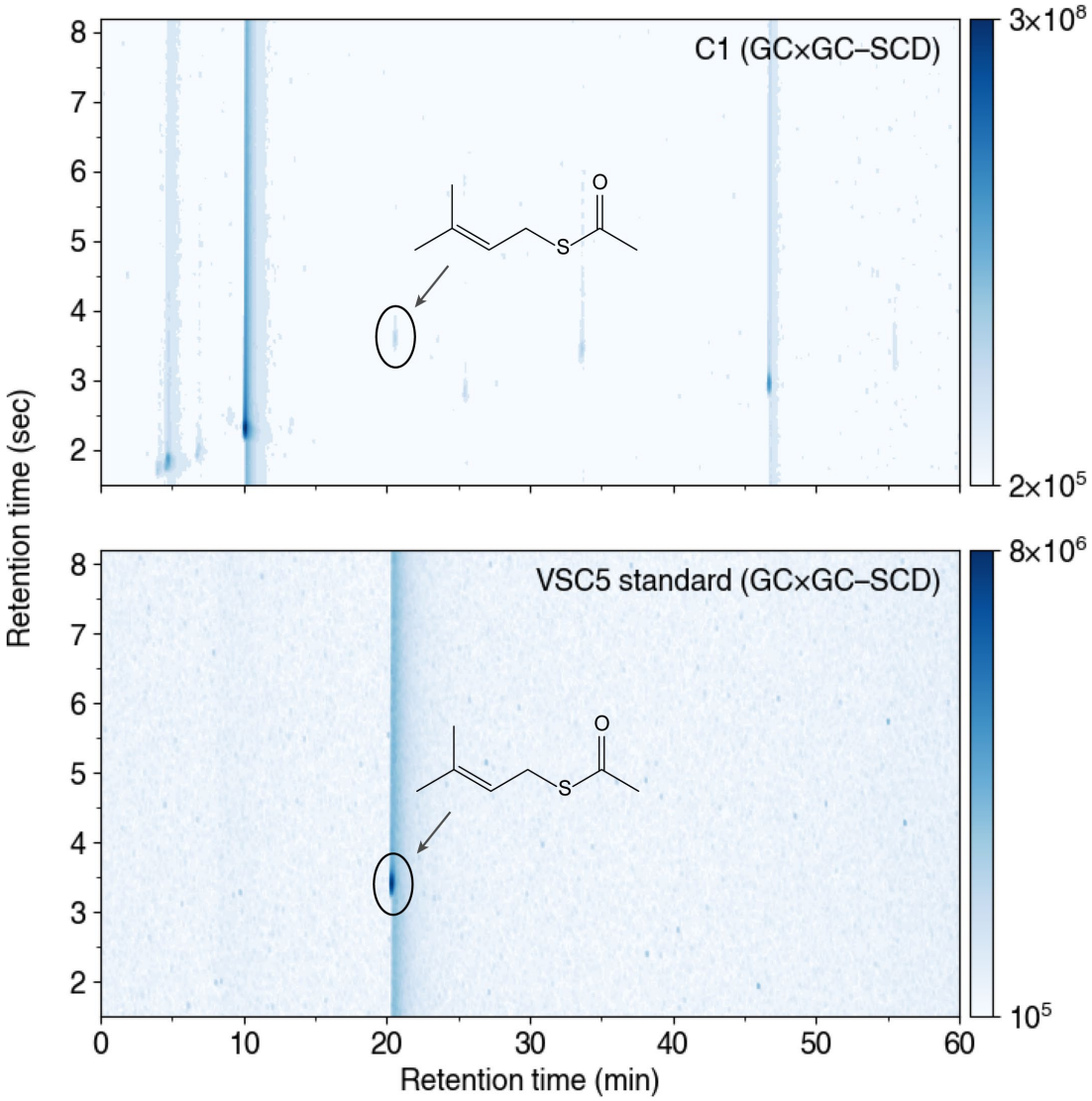

Figure S15. GC×GC–SCD 2-Dimensional chromatograms comparing **VSC5** elution in Bacio Gelato versus 3-Methyl-2-butenyl acetothioate (**VSC5**) standard.

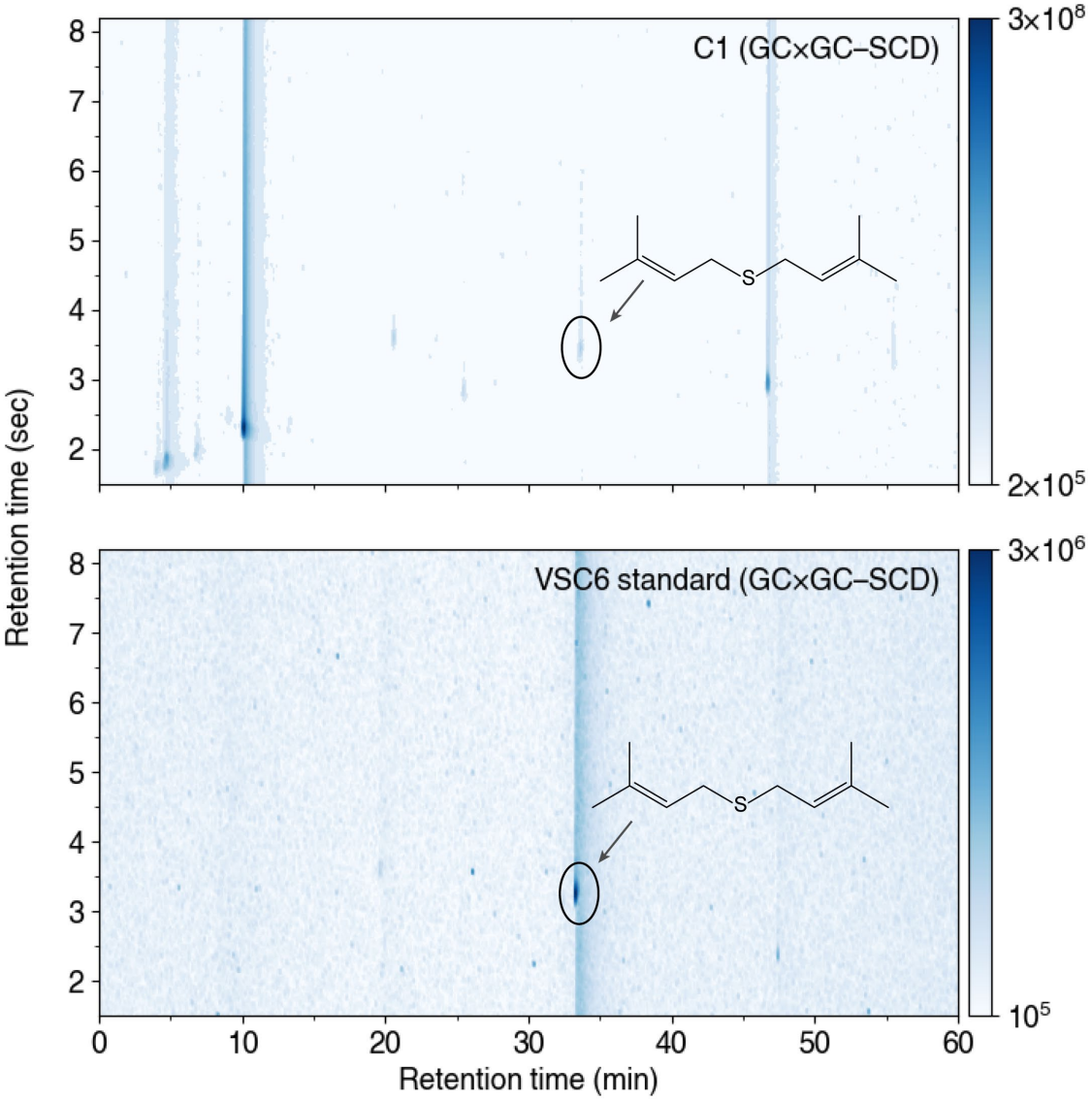

Figure S16. GC×GC–SCD 2-Dimensional chromatograms comparing **VSC6** elution in Bacio Gelato versus bis(3-methyl-2-butenyl) sulfide (**VSC6**) standard.

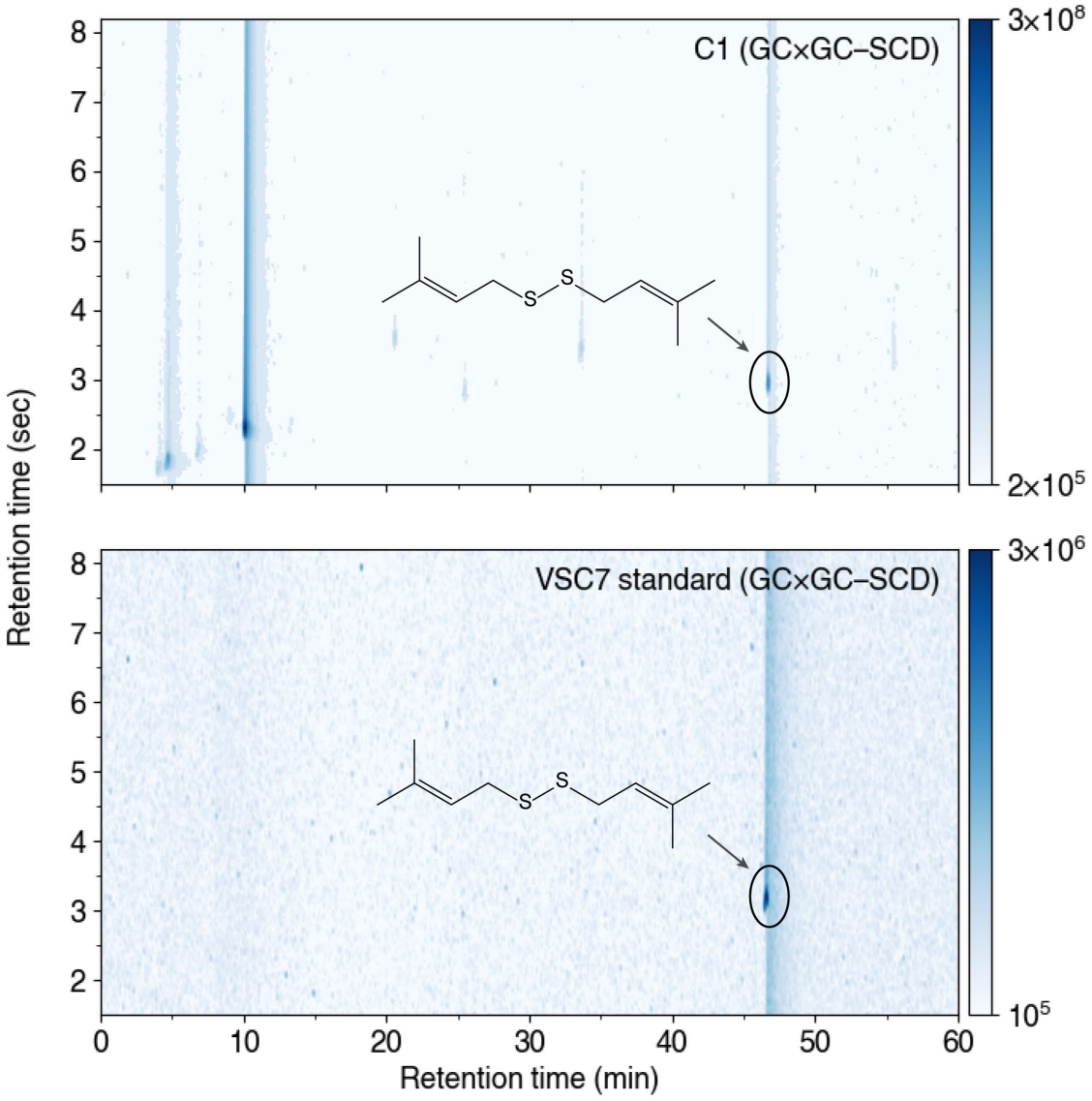

Figure S17. GC×GC–SCD 2-Dimensional chromatograms comparing **VSC7** elution in Bacio Gelato versus bis(3-methyl-2-butenyl) disulfide (**VSC7**) standard.

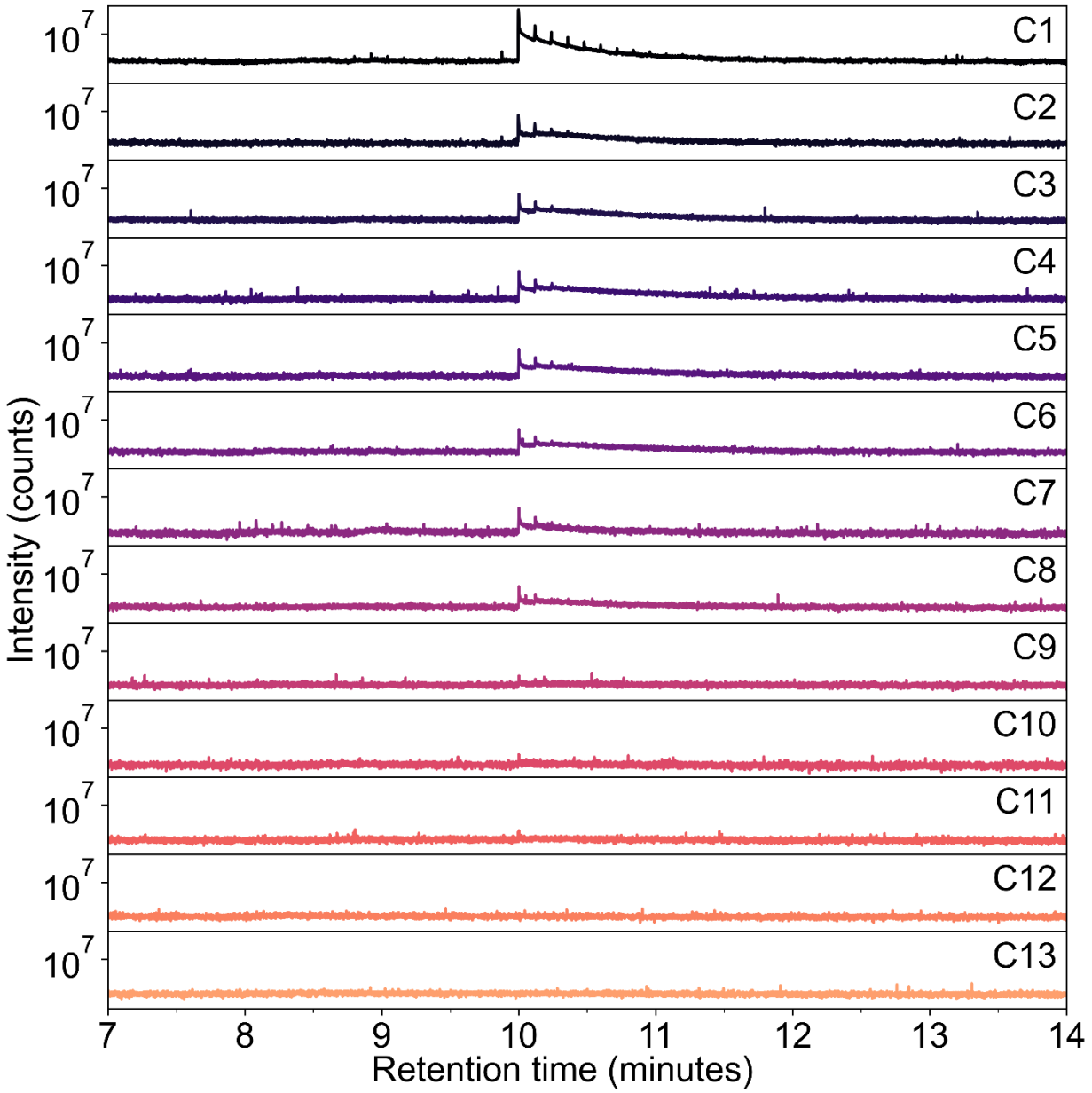

Figure S18. 1-Dimensional plots of 2-Dimensional GC × GC–SCD chromatograms showing **VSC3** peak located at $^{1}t_R$ = 10.082 min drop in intensity as a function of cultivar number, closely matching the change in olfactory scores.

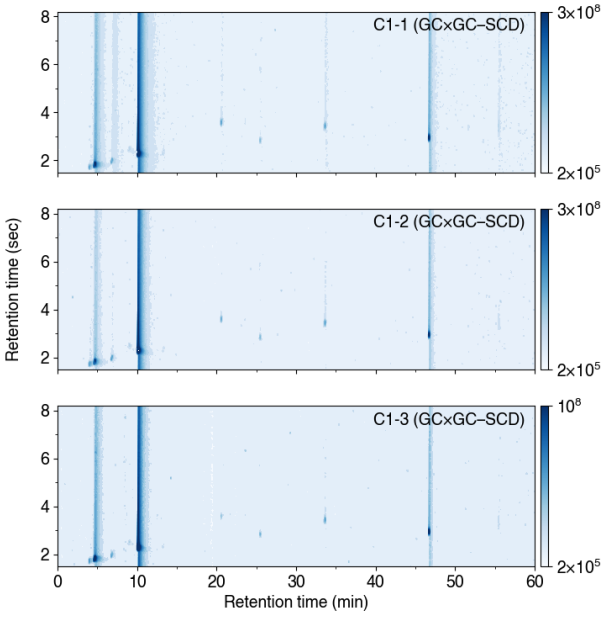

Figure S19. Triplicate of GC×GC–SCD 2-Dimensional chromatograms for sample **C1**.

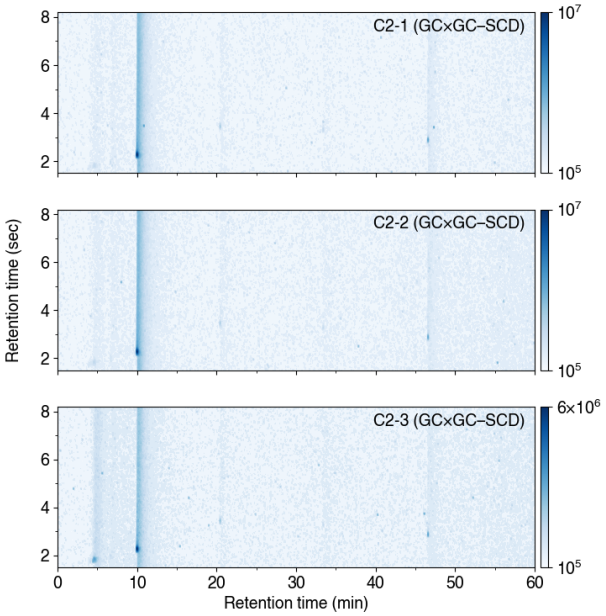

Figure S20. Triplicate of GC×GC–SCD 2-Dimensional chromatograms for sample **C2**.

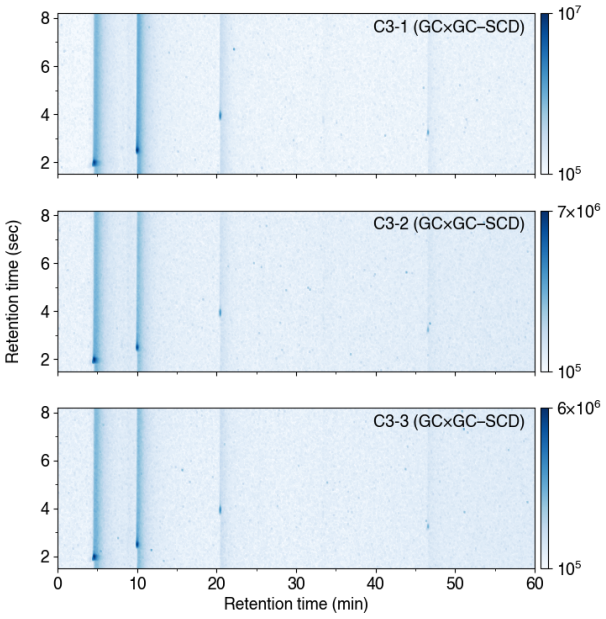

Figure S21. Triplicate of GC×GC–SCD 2-Dimensional chromatograms for sample **C3**.

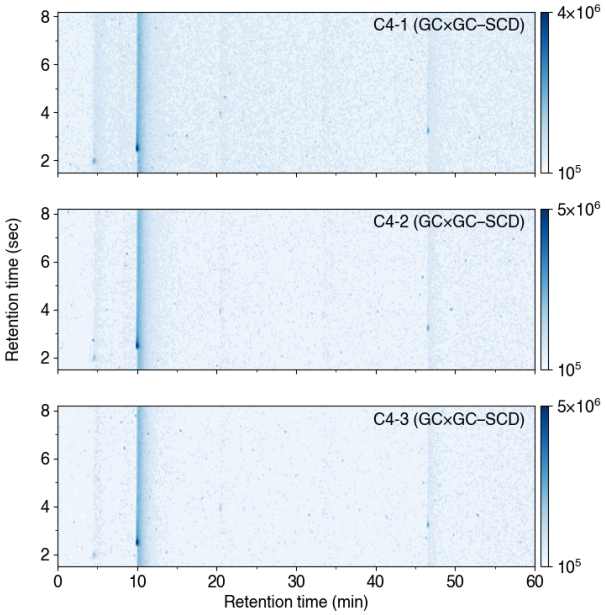

Figure S22. Triplicate of GC×GC–SCD 2-Dimensional chromatograms for sample **C4**.

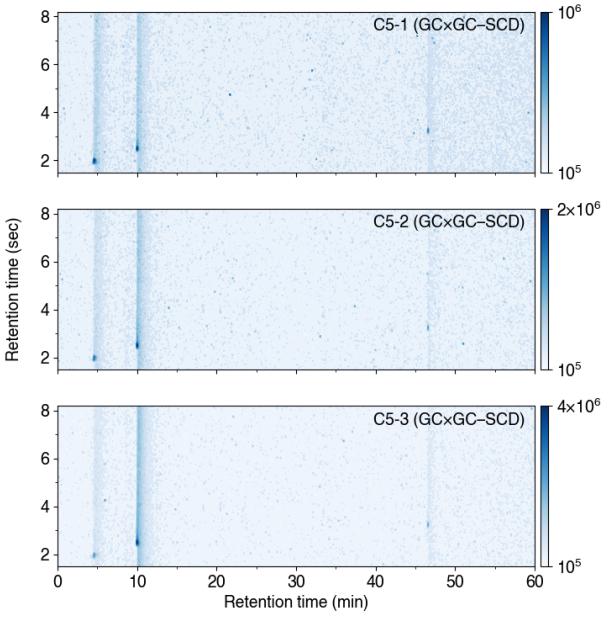

Figure S23. Triplicate of GC×GC–SCD 2-Dimensional chromatograms for sample **C5**.

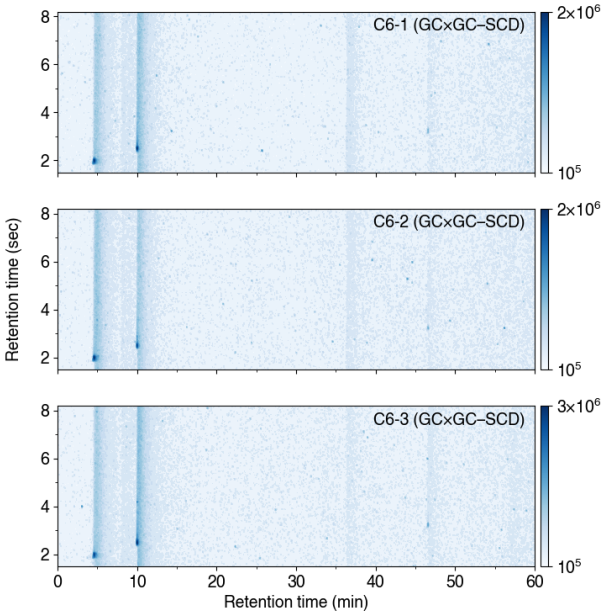

Figure S24. Triplicate of GC×GC–SCD 2-Dimensional chromatograms for sample **C6**.

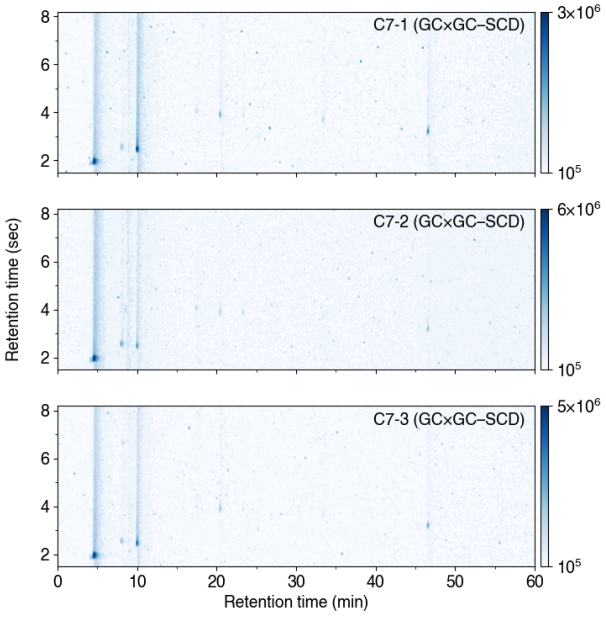

Figure S25. Triplicate of GC×GC–SCD 2-Dimensional chromatograms for sample **C7**.

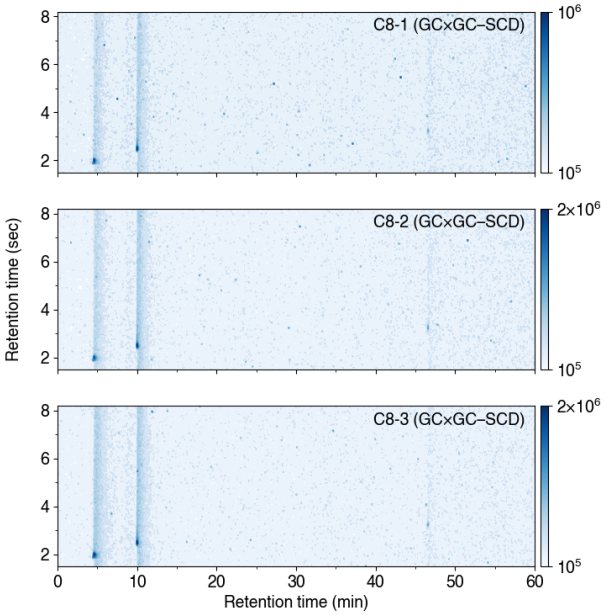

Figure S26. Triplicate of GC×GC–SCD 2-Dimensional chromatograms for sample **C8**.

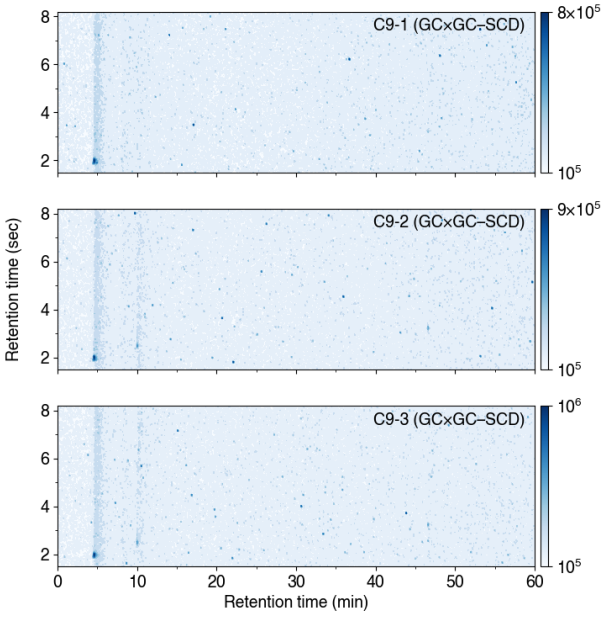

Figure S27. Triplicate of GC×GC–SCD 2-Dimensional chromatograms for sample **C9**.

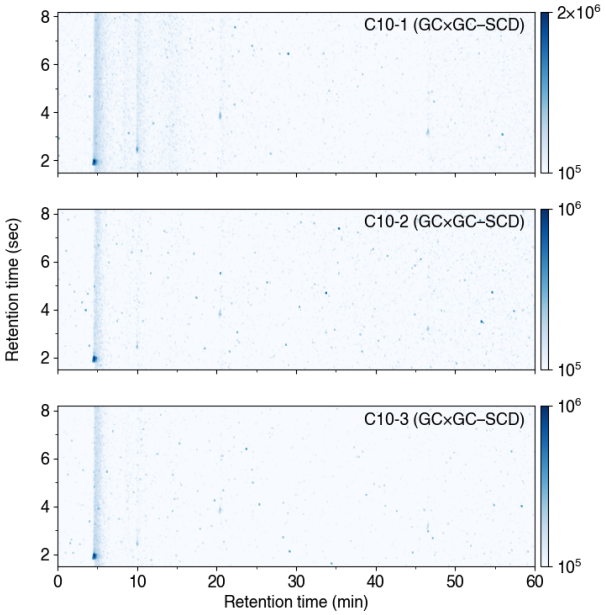

Figure S28. Triplicate of GC×GC–SCD 2-Dimensional chromatograms for sample **C10**.

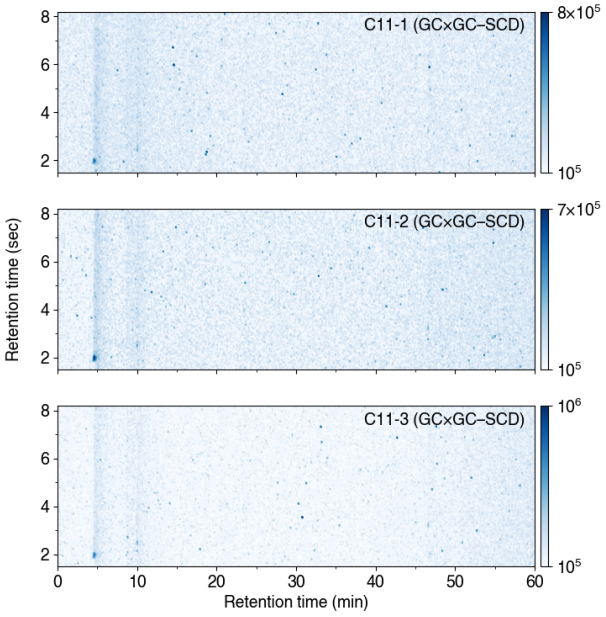

Figure S29. Triplicate of GC×GC–SCD 2-Dimensional chromatograms for sample **C11**.

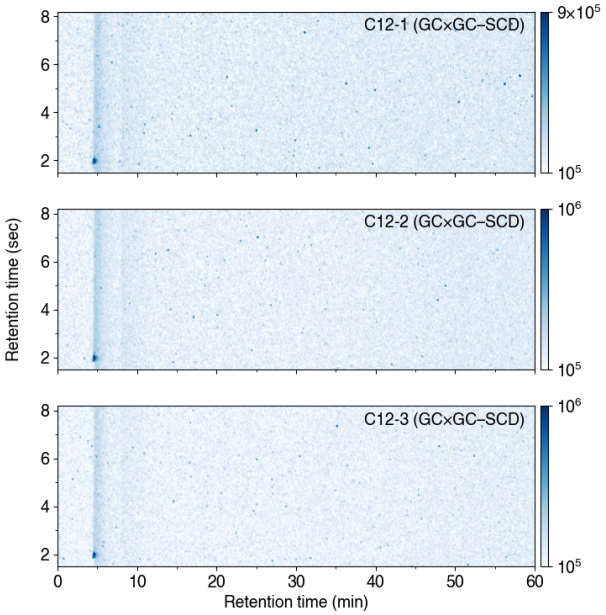

Figure S30. Triplicate of GC×GC–SCD 2-Dimensional chromatograms for sample **C12**.

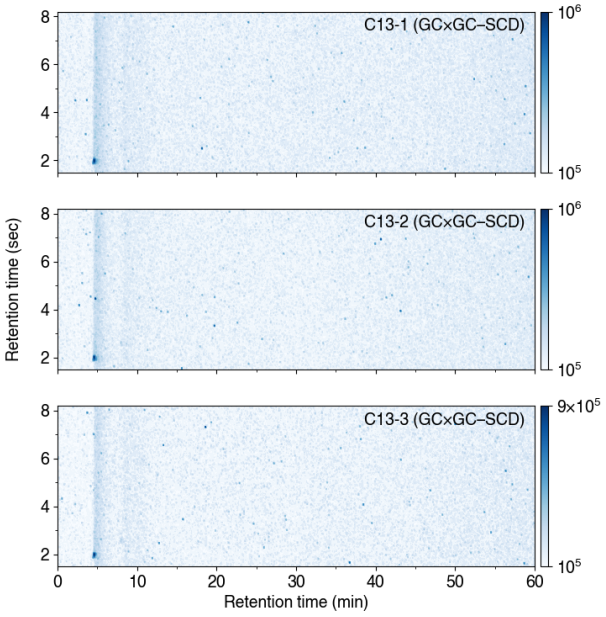

Figure S31. Triplicate of GC×GC–SCD 2-Dimensional chromatograms for sample **C13**.

Table S5. Highest concentration VOCs identified in cultivar Bacio Gelato (**C1**).

Compound name	RT (min)	Relative-%	Calculated amount (µg/mg)	CAS #
D-Limonene	17.68	25.771	5.61003	5989-27-5
Caryophyllene	42.76	9.945	2.164922	87-44-5
β-Myrcene	15.76	7.01	1.525976	123-35-3
Linalool	21.37	4.465	0.971973	78-70-6
β-Pinene	15.4	4.112	0.895155	127-91-3
α-Terpineol	27.85	3.894	0.847753	98-55-5
Humulene	44.66	3.215	0.699931	6753-98-6
α-Pinene	13.74	2.65	0.576887	80-56-8
endo-Fenchol	22.94	2.301	0.500912	14575-74-7
α-Bisabolol	52.44	1.43	0.31132	515-69-5
Caryophyllene oxide	49.64	1.104	0.240257	1139-30-6
Terpinolene	20.62	1.099	0.239275	586-62-9
Fenchone	21.15	0.991	0.215771	1195-79-5
Camphene	14.41	0.898	0.19554	79-92-5
cis-β-Farnesene	44.24	0.885	0.192691	28973-97-9
trans-Sabinene hydrate	20.02	0.806	0.175399	546-79-2
(-)-Isopulegol	24.68	0.744	0.161906	232-102-8
α-Terpinene	17.16	0.651	0.14175	99-86-5
endo-Borneol	26.48	0.645	0.140398	507-70-0
γ-Terpinene	19.17	0.605	0.131641	99-85-4
α-Phellandrene	16.72	0.249	0.054212	99-83-2
3-Carene	16.84	0.02	0.004412	13466-78-9

Table S6. Highest concentration VOCs identified in cultivar Clone Guy OG (**C2**).

Compound name	**RT (min)**	**Relative-%**	**Calculated amount (µg/mg)**	**CAS #**
D-Limonene	17.5575	38.321%	1.57393	5989-27-5
β-Myrcene	15.7281	30.334%	1.24590	123-35-3
β-Pinene	15.3942	10.314%	0.42362	127-91-3
α-Pinene	13.6808	9.361%	0.38448	80-56-8
Linalool	21.3357	3.425%	0.14067	78-70-6
Camphene	14.3813	3.097%	0.12718	79-92-5
Caryophyllene	42.9613	1.609%	0.06609	87-44-5
endo-Fenchol	22.902	0.793%	0.03258	14575-74-7
Terpinolene	20.5929	0.506%	0.02078	586-62-9
α-Terpineol	27.8425	0.495%	0.02032	98-55-5
Fenchone	21.1963	0.441%	0.01811	1195-79-5
Humulene	44.5605	0.432%	0.01773	6753-98-6
α-Phellandrene	16.5972	0.215%	0.00881	99-83-2
α-Terpinene	17.1547	0.133%	0.00545	99-86-5
cis-β-Farnesene	44.0802	0.129%	0.00530	28973-97-9
γ-Terpinene	19.1467	0.104%	0.00427	99-85-4
3-Carene	16.8375	0.041%	0.00168	13466-78-9
endo-Borneol	26.4575	0.037%	0.00151	507-70-0
α-Bisabolol	52.4622	0.027%	0.00112	515-69-5
trans-Sabinene hydrate	19.9609	0.025%	0.00102	546-79-2
Caryophyllene oxide	49.5767	0.018%	0.00075	1139-30-6

Table S7. Highest concentration VOCs identified in cultivar Gelato (4 days old) (**C3**).

Compound name	**RT (min)**	**Relative-%**	**Calculated amount (µg/mg)**	**CAS #**
D-Limonene	17.68	34.848	5.945506	5989-27-5
Linalool	21.34	9.916	1.691778	78-70-6
β-Myrcene	15.76	9.817	1.674884	123-35-3
Caryophyllene	42.76	9.519	1.623994	87-44-5
β-Pinene	15.4	5.956	1.016239	127-91-3
α-Terpineol	27.69	4.961	0.846426	98-55-5
α-Pinene	13.74	4.873	0.831383	80-56-8
endo-Fenchol	22.95	4.259	0.726583	14575-74-7
Humulene	44.71	3.431	0.585419	6753-98-6
cis-β-Farnesene	44.24	2.056	0.350849	28973-97-9
Camphene	14.41	1.503	0.256444	79-92-5
Fenchone	21.2	1.073	0.18308	1195-79-5
Terpinolene	20.63	0.931	0.158791	586-62-9
Caryophyllene oxide	49.64	0.811	0.138387	1139-30-6
endo-Borneol	26.45	0.69	0.117674	507-70-0
trans-Nerolidol	48.47	0.605	0.103145	40716-66-3
α-Bisabolol	52.52	0.551	0.093927	515-69-5
trans-Sabinene hydrate	19.99	0.522	0.089034	546-79-2
α-Terpinene	17.18	0.516	0.088042	99-86-5
γ-Terpinene	19.15	0.465	0.079253	99-85-4
α-Phellandrene	16.72	0.19	0.032431	99-83-2
3-Carene	16.84	0.02	0.003328	13466-78-9

Table S8. Highest concentration VOCs identified in cultivar Area 41 (**C4**).

Compound name	RT (min)	Relative-%	Calculated amount (µg/mg)	CAS #
β-Myrcene	15.76	26.279	7.526606	123-35-3
D-Limonene	17.68	24.772	7.094881	5989-27-5
Caryophyllene	42.76	13.081	3.746509	87-44-5
Linalool	21.35	7.231	2.071128	78-70-6
β-Pinene	15.4	5.064	1.450266	127-91-3
α-Terpineol	27.85	3.449	0.987877	98-55-5
Humulene	44.71	3.233	0.925917	6753-98-6
endo-Fenchol	22.95	3.045	0.872065	14575-74-7
α-Pinene	13.75	2.894	0.828783	80-56-8
Camphene	14.41	0.972	0.2785	79-92-5
Fenchone	21.2	0.692	0.198056	1195-79-5
Terpinolene	20.64	0.671	0.192181	586-62-9
α-Bisabolol	52.47	0.483	0.13836	515-69-5
endo-Borneol	26.45	0.462	0.132228	507-70-0
Caryophyllene oxide	49.58	0.451	0.129105	1139-30-6
trans-Sabinene hydrate	20.02	0.349	0.099959	546-79-2
α-Terpinene	17.18	0.324	0.092733	99-86-5
γ-Terpinene	19.18	0.286	0.081822	99-85-4
Sabinene	15.28	0.245	0.070123	3387-41-5
cis-β-Farnesene	44.25	0.24	0.068733	28973-97-9
α-Phellandrene	16.72	0.133	0.038063	99-83-2
3-Carene	16.84	0.058	0.016744	13466-78-9

Table S9. Highest concentration VOCs identified in cultivar Jetlag OG (**C5**).

Compound name	RT (min)	Relative-%	Calculated amount (µg/mg)	CAS #
D-Limonene	17.68	25.938	4.840071	5989-27-5
Linalool	21.34	14.848	2.770769	78-70-6
Caryophyllene	42.76	12.984	2.422941	87-44-5
α-Terpineol	27.85	5.153	0.961588	98-55-5
endo-Fenchol	22.95	4.914	0.916925	14575-74-7
α-Pinene	13.75	4.821	0.899695	80-56-8
β-Pinene	15.4	4.364	0.814424	127-91-3
Humulene	44.71	3.576	0.667236	6753-98-6
β-Myrcene	15.76	3.059	0.570735	123-35-3
cis-β-Farnesene	44.26	2.194	0.409429	28973-97-9
Camphene	14.41	1.252	0.233701	79-92-5
Terpinolene	20.64	0.849	0.158463	586-62-9
trans-Nerolidol	48.51	0.819	0.152883	40716-66-3
Caryophyllene oxide	49.59	0.77	0.143775	1139-30-6
endo-Borneol	26.44	0.66	0.123237	507-70-0
trans-Sabinene hydrate	20.02	0.52	0.096952	546-79-2
Fenchone	21.15	0.516	0.09637	1195-79-5
α-Bisabolol	52.53	0.492	0.091772	515-69-5
α-Terpinene	17.18	0.491	0.091567	99-86-5
γ-Terpinene	19.15	0.438	0.081754	99-85-4
α-Phellandrene	16.72	0.166	0.030916	99-83-2
3-Carene	16.84	0.011	0.002047	13466-78-9

Table S10. Highest concentration VOCs identified in cultivar Gushers (**C6**).

Compound name	RT (min)	Relative-%	Calculated amount (µg/mg)	CAS #
D-Limonene	17.56	25.672	3.799173	5989-27-5
Caryophyllene	42.76	15.815	2.34043	87-44-5
Linalool	21.34	7.761	1.148611	78-70-6
β-Myrcene	15.76	6.593	0.975758	123-35-3
α-Terpineol	27.85	4.961	0.734154	98-55-5
β-Pinene	15.4	4.416	0.653584	127-91-3
endo-Fenchol	22.95	4.101	0.60697	14575-74-7
Humulene	44.71	4.074	0.602883	6753-98-6
α-Pinene	13.74	3.589	0.531117	80-56-8
Camphene	14.41	1.583	0.234227	79-92-5
Terpinolene	20.64	1.304	0.192962	586-62-9
Fenchone	21.18	1.004	0.148556	1195-79-5
Caryophyllene oxide	49.59	0.813	0.120347	1139-30-6
cis-β-Farnesene	44.24	0.768	0.113697	28973-97-9
α-Terpinene	17.23	0.724	0.107091	99-86-5
α-Bisabolol	52.52	0.667	0.098774	515-69-5
(-)-Isopulegol	24.71	0.597	0.088406	232-102-8
endo-Borneol	26.48	0.584	0.086367	507-70-0
γ-Terpinene	19.18	0.516	0.076292	99-85-4
α-Phellandrene	16.72	0.232	0.034364	99-83-2

Table S11. Highest concentration VOCs identified in cultivar WiFi Cake (**C7**).

Compound name	RT (min)	Relative-%	Calculated amount (µg/mg)	CAS #
D-Limonene	17.68	35.648	5.58046	5989-27-5
β-Myrcene	15.76	17.643	2.761949	123-35-3
Linalool	21.34	9.61	1.504312	78-70-6
Caryophyllene	42.76	6.655	1.041734	87-44-5
β-Pinene	15.4	6.648	1.040715	127-91-3
α-Pinene	13.74	4.257	0.666448	80-56-8
α-Terpineol	27.86	3.097	0.484825	98-55-5
endo-Fenchol	22.95	2.923	0.457649	14575-74-7
Humulene	44.71	1.975	0.309148	6753-98-6
Camphene	14.41	1.549	0.242438	79-92-5
cis-β-Farnesene	44.24	1.446	0.2264	28973-97-9
Terpinolene	20.64	0.871	0.136381	586-62-9
Caryophyllene oxide	49.64	0.824	0.128921	1139-30-6
trans-Nerolidol	48.56	0.797	0.124795	40716-66-3
endo-Borneol	26.45	0.644	0.100813	507-70-0
Fenchone	21.21	0.594	0.092952	1195-79-5
α-Terpinene	17.17	0.585	0.091522	99-86-5
γ-Terpinene	19.17	0.494	0.077338	99-85-4
Sabinene	15.28	0.462	0.072334	3387-41-5
α-Phellandrene	16.72	0.211	0.033055	99-83-2
3-Carene	16.84	0.041	0.006401	13466-78-9

Table S12. Highest concentration VOCs identified in cultivar Apple Fritter (**C8**).

Compound name	RT (min)	Relative-%	Calculated amount (µg/mg)	CAS #
Caryophyllene	42.76	33.549	5.172868	87-44-5
D-Limonene	17.68	21.796	3.36059	5989-27-5
Humulene	44.71	7.49	1.154909	6753-98-6
Linalool	21.38	5.567	0.858309	78-70-6
α-Pinene	13.74	5.44	0.83876	80-56-8
β-Pinene	15.4	4.057	0.625533	127-91-3
α-Terpineol	27.85	3.221	0.49659	98-55-5
endo-Fenchol	22.95	2.816	0.434163	14575-74-7
β-Myrcene	15.76	2.699	0.416114	123-35-3
cis-β-Farnesene	44.24	2.384	0.367521	28973-97-9
Caryophyllene oxide	49.64	1.181	0.182021	1139-30-6
α-Bisabolol	52.46	1.071	0.165104	515-69-5
Camphene	14.41	0.985	0.151811	79-92-5
trans-Nerolidol	48.51	0.812	0.125227	40716-66-3
Terpinolene	20.64	0.809	0.124726	586-62-9
Fenchone	21.21	0.759	0.116986	1195-79-5
endo-Borneol	26.46	0.653	0.100694	507-70-0
trans-Sabinene hydrate	19.96	0.586	0.090316	546-79-2
α-Terpinene	17.18	0.516	0.079579	99-86-5
γ-Terpinene	19.16	0.507	0.078208	99-85-4
α-Phellandrene	16.72	0.187	0.028841	99-83-2

Table S13. Highest concentration VOCs identified in cultivar Chem 91 (**C9**).

Compound name	**RT (min)**	**Relative-%**	**Calculated amount (µg/mg)**	**CAS #**
β-Myrcene	15.76	19.476	2.751967863	123-35-3
Caryophyllene	42.76	18.177	2.568458669	87-44-5
D-Limonene	17.68	11.423	1.61407907	5989-27-5
Humulene	44.71	5.673	0.801625339	6753-98-6
β-Pinene	15.4	5.087	0.718858184	127-91-3
Linalool	21.38	4.293	0.606552937	78-70-6
endo-Fenchol	22.95	4.154	0.586954043	14575-74-7
α-Pinene	13.74	3.062	0.432730689	80-56-8
α-Terpineol	27.86	2.894	0.408880382	98-55-5
α-Bisabolol	52.46	2.007	0.283581572	515-69-5
Caryophyllene oxide	49.64	1.579	0.223146286	1139-30-6
Fenchone	21.2	1.356	0.191606487	1195-79-5
endo-Borneol	26.45	1.269	0.179269785	507-70-0
Terpinolene	20.64	1.25	0.176676161	586-62-9
Camphene	14.41	1.059	0.149628579	79-92-5
trans-Sabinene hydrate	20.1	1.052	0.14867136	546-79-2
α-Terpinene	17.22	0.956	0.13511981	99-86-5
γ-Terpinene	19.16	0.851	0.120242656	99-85-4
α-Phellandrene	16.72	0.354	0.049984536	99-83-2
cis-β-Farnesene	44.26	0.341	0.048183245	28973-97-9

Table S14. Highest concentration VOCs identified in cultivar Gelato (46 days old) (**C10**).

Compound name	**RT (min)**	**Relative-%**	**Calculated amount (µg/mg)**	**CAS #**
D-Limonene	17.56	26.73	1.665898	5989-27-5
Linalool	21.36	12.101	0.754195	78-70-6
Caryophyllene	42.76	10.066	0.627324	87-44-5
α-Terpineol	27.85	6.889	0.429328	98-55-5
endo-Fenchol	22.94	6.511	0.405764	14575-74-7
β-Pinene	15.4	5.838	0.36382	127-91-3
α-Pinene	13.74	4.888	0.304643	80-56-8
Humulene	44.66	4.796	0.298909	6753-98-6
β-Myrcene	15.76	4.693	0.292464	123-35-3
Terpinolene	20.63	2.782	0.173361	586-62-9
cis-β-Farnesene	44.23	2.227	0.138781	28973-97-9
Camphene	14.41	2.001	0.124734	79-92-5
Fenchone	21.2	1.623	0.101128	1195-79-5
α-Terpinene	17.17	1.497	0.093316	99-86-5
endo-Borneol	26.46	1.404	0.087481	507-70-0
γ-Terpinene	19.17	1.207	0.075244	99-85-4
α-Phellandrene	16.72	0.486	0.030283	99-83-2
3-Carene	16.84	0.173	0.010759	13466-78-9

Table S15. Highest concentration VOCs identified in cultivar Caliberry (C11).

Compound name	RT (min)	Relative-%	Calculated amount (µg/mg)	CAS #
β-Myrcene	15.76	53.906	8.308325	123-35-3
α-Pinene	13.75	9.118	1.405261	80-56-8
Linalool	21.38	6.234	0.960748	78-70-6
D-Limonene	17.68	6.093	0.939039	5989-27-5
β-Pinene	15.4	5.286	0.814685	127-91-3
Caryophyllene	42.76	4.726	0.728443	87-44-5
Humulene	44.71	1.732	0.266898	6753-98-6
α-Terpineol	27.86	1.175	0.181157	98-55-5
trans-Nerolidol	48.51	1.033	0.159233	40716-66-3
α-Bisabolol	52.46	0.931	0.143551	515-69-5
Caryophyllene oxide	49.64	0.881	0.135753	1139-30-6
endo-Fenchol	22.97	0.798	0.123016	14575-74-7
Terpinolene	20.65	0.664	0.102323	586-62-9
Camphene	14.41	0.596	0.091811	79-92-5
γ-Terpinene	19.08	0.555	0.085577	99-85-4
Fenchone	21.21	0.546	0.084095	1195-79-5
endo-Borneol	26.38	0.532	0.082004	507-70-0
α-Terpinene	17.24	0.505	0.077793	99-86-5
Sabinene	15.33	0.482	0.074319	3387-41-5
cis-β-Farnesene	44.25	0.282	0.043422	28973-97-9
α-Phellandrene	16.72	0.225	0.034732	99-83-2
3-Carene	16.84	0.082	0.012613	13466-78-9

Table S16. Highest concentration VOCs identified in cultivar Gouda Berry (**C12**).

Compound name	RT (min)	Relative-%	Calculated amount (µg/mg)	CAS #
Caryophyllene	42.76	18.097	2.719838	87-44-5
β-Myrcene	15.76	16.917	2.542454	123-35-3
D-Limonene	17.68	14.813	2.226217	5989-27-5
Linalool	21.35	6.584	0.989467	78-70-6
Humulene	44.71	4.411	0.662926	6753-98-6
β-Pinene	15.4	3.961	0.59525	127-91-3
α-Terpineol	27.85	2.814	0.422983	98-55-5
endo-Fenchol	22.95	2.575	0.386982	14575-74-7
α-Pinene	13.74	2.265	0.340432	80-56-8
cis-β-Farnesene	44.3	1.06	0.159356	28973-97-9
α-Bisabolol	52.46	0.906	0.136179	515-69-5
Caryophyllene oxide	49.64	0.895	0.134566	1139-30-6
Camphene	14.41	0.862	0.129512	79-92-5
Terpinolene	20.64	0.786	0.118152	586-62-9
endo-Borneol	26.45	0.719	0.107992	507-70-0
trans-Nerolidol	48.56	0.685	0.102986	40716-66-3
α-Terpinene	17.16	0.52	0.078164	99-86-5
Fenchone	21.2	0.512	0.076945	1195-79-5
γ-Terpinene	19.18	0.487	0.073204	99-85-4
Sabinene	15.16	0.475	0.071392	3387-41-5
α-Phellandrene	16.72	0.198	0.029806	99-83-2

Table S17. Highest concentration VOCs identified in cultivar Black Jack (**C13**).

Compound name	RT (min)	Relative-%	Calculated amount (µg/mg)	CAS #
Terpinolene	20.62	26.152	2.318045	586-62-9
Caryophyllene	42.76	22.125	1.961073	87-44-5
β-Myrcene	15.76	7.355	0.651928	123-35-3
Humulene	44.71	7.213	0.639356	6753-98-6
β-Pinene	15.4	5.856	0.519053	127-91-3
α-Pinene	13.75	4.979	0.441357	80-56-8
D-Limonene	17.56	2.834	0.251219	5989-27-5
α-Terpineol	27.86	2.622	0.232374	98-55-5
cis-β-Farnesene	44.24	2.507	0.222197	28973-97-9
3-Carene	16.84	2.482	0.219965	13466-78-9
Linalool	21.39	2.154	0.190912	78-70-6
α-Phellandrene	16.72	1.983	0.175747	99-83-2
α-Terpinene	17.16	1.823	0.161626	99-86-5
Caryophyllene oxide	49.64	1.701	0.150752	1139-30-6
γ-Terpinene	19.14	1.513	0.134151	99-85-4
trans-Sabinene hydrate	20.02	1.279	0.113336	546-79-2
trans-Nerolidol	48.56	1.052	0.093243	40716-66-3
Sabinene	15.16	0.916	0.081167	3387-41-5
endo-Borneol	26.43	0.832	0.073781	507-70-0
endo-Fenchol	22.97	0.806	0.07145	14575-74-7
Camphene	14.41	0.559	0.049536	79-92-5

Table S18. Details of Clone Guy OG indoor greenhouse trial.

Week	Organ measured	Stage of growth
1	N/A	Flowering
2	Flower (4 samples)	Flowering
3	Flower (4 samples)	Flowering
4	Flower (4 samples)	Flowering
5	Flower (4 samples)	Flowering
6	Flower (4 samples)	Flowering
7	Flower (4 samples)	Flowering
8	Flower (4 samples)	Flowering
9	Flower (4 samples)	Flowering
10	Flower (4 samples)	End of flowering
11	Cured Flower (4 samples)	End of curing & drying
12	Cured Flower(4 samples)	10 days post cure