SUPPORTING INFORMATION for

The Chemical Composition of Commercial Cannabis

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Material and Methods:

Table S1. Detailed chemical and vendor information for metabolites in the common plant metabolite assay.

Chemical subclass and chemicals	Vendors
Acids: α-or ɣ-keto, α-or β-hydroxy, mono, di or tricarboxylic citric acid, fumaric acid, glutaric acid, β-hydroxybutyric acid, 5-hydroxyindoleacetic acid, indole-3-acetic acid, α-ketoglutaric acid, lactic acid, malic acid, methylmalonic acid, nitro-tyrosine, oxalic acid, oxaloacetic acid, propionic acid, pyruvic acid, succinic acid, trans-aconitic acid	Sigma-Aldrich (Oakville, CA)
Amines or aminoxide or phenethylamine (7) histamine, phenylethylamine, putrescine, spermidine, spermine, trimethylamine N-oxide (TMAO), tyramine	
Amino acids, peptides and analogues (3) alanine, arginine, asparagine, aspartic acid, asymmetric dimethylarginine (ADMA), betaine, citrulline, creatine, creatinine, glutamine, glutamic acid, glycine, histidine, homoserine, levodopa (DOPA), leucine, isoleucine, kynurenine, lysine, methionine, 3-methylhistidine, ornithine, phenylalanine, proline, sarcosine, serine, threonine, trans-hydroxyproline, tyrosine, tryptophan, valine	
Alcohols and polyols (1) shikimic acid	
Benzoic acids and derivatives; phenylpropanionic acid; benzenoids; benzenediols, **methoxyphenol (4)** benzoic acid, dopamine, hippuric acid, *p*-hydroxyphenylacetic acid	
Carbohydrate and carbohydrate conjugates (3) glyceric acid, glucose, $^{13}C_6$-glucose	
Carnitines (10) acetyl-L-carnitine hydrochloride, propionyl-L-carnitine, butyryl-L-carnitine, hexanoyl-L-carnitine, octanoyl-L-carnitine, decanoyl-L-carnitine, dodecanoyl-L-carnitine, tetradecanoyl-L-carnitine, hexadecanoyl-L-carnitine, octadecanoyl-L-carnitine	
Fatty acid and conjugates (2) butyric acid, valeric acid	
Organosulfonic acids and derivatives (1) taurine	
Phosphatidylcholines (8)	

N-stearoyl-D-erythro-sphingosylphosphorylcholine,1,2-dilinolenoyl-sn-glycero-3-phosphocholine, 1,2-dioctadecanoyl-sn-glycero-3-phosphocholine, 1-oleoyl-2-hydroxy-sn-glycero-3-phosphocholine, 1,2-dimyristoyl-sn-glycero-3-phosphocholine, 1,2-diarachidoyl-sn-glycero-3-phosphocholine, 1-nonanoyl-2-hydroxy-sn-glycero-3-phosphocholine, N-hexanoyl-D-erythro-sphingosylphosphorylcholine	
Plant hormones (4) abscisic acid, jasmonic acid, salicylic acid, zeatin	
Quaternary ammonium salts (2) L-carnitine inner salt, choline	Sigma-Aldrich (Oakville, CA)
Tryptamines and derivatives (1): serotonin	
Carboximidic acids: N^1, N^{12}-diacetylspermine hydrochloride **Amino acids, peptides and analoques:** proline-betaine	Cayman Chemical (Ann Arbor, MI)
(D, ^{13}C, ^{15}N)-labelled internal standards (ISTD) D_2-ornithine, ^{15}N-histidine, D_3-creatinine, D_3-DOPA, D_4-dopamine, ^{13}C-tyrosine, ^{13}C-D_3-methionine, D_3-proline, D_4-serotonin, D_4-putrescine, D_3-sarcosine, $^{13}C_2$-taurine, D_4-tyramine, ^{15}N-alanine, $^{13}C_6$-arginine, ^{15}N-asparagine, D_3-aspartic acid, D_7-citrulline, D_3-glutamic acid, D_5-glutamine, $^{13}C_2$-glycine, ^{13}C-leucine, ^{15}N-phenylalanine, ^{13}C-serine, D_2-threonine, $^{15}N_2$-tryptophan, D_8-valine, D_9-TMAO and $^{15}N_2$-uric acid	Cambridge Isotope Laboratories Inc. (Tewksbury, MA)
ISTDs Labelled carnitine standard set	Cambridge Isotope Laboratories Inc. (Tewksbury, MA)
ISTDs D_8-spermine tetrahydrochloride, D_8-spermidine trihydrochloride	IsoSciences (Ambler, PA)
ISTDs D_6-N^1, N^{12}-diacetylspermine dihydrochloride and D_6-ADMA	Toronto Research Chemicals (North York, CA)
ISTDs D_3-creatinine, D_9-choline chloride, D_9-betaine hydrochloride, 2-D_1-sodium L-lactate, D_4-sodium beta-hydroxybutyrate, 1-^{13}C-alpha-ketoglutaric acid, D_4-citric acid, 1-^{13}C-butyric acid, 1-^{13}C-propionic acid, D_4-succinic acid, $^{13}C_2$-D_2-fumaric acid, ^{13}C-pyruvic acid, D_2-hippuric acid, methyl-D_3-malonic acid, and D_2-indole-3-acetic acid	C/D/N Isotopes Inc. (Pointe-Claire, CA)

Abbreviations; D_6-ADMA - asymmetric-dimethyl-d_6-arginine; ISTDs - internal standards

Table S2. List of vendors and/or concentrations of cannabinoid certified reference material standards, their peak-picking standards, terpene mixtures and polyphenols used in the cannabinoid, terpenoid, pesticide and polyphenol assays.

Compound	Vendor	Concentration
Cannabinoid certified reference material standards		
Δ9-tetrahydrocannabinol (THC)	Cerilliant Corp.	1.000 mg/mL methanol
Δ9-tetrahydrocannabinolic acid A (THCA)	Cerilliant Corp.	1.000 mg/mL acetonitrile
tetrahydrocannabivarin (THCV)	Cerilliant Corp.	1.000 mg/mL methanol
cannabidiol (CBD)	Cerilliant Corp.	1.000 mg/mL methanol
cannabidiolic acid (CBDA)	Cerilliant Corp.	1.000 mg/mL acetonitrile
cannabichromene (CBC)	Cerilliant Corp.	1.000 mg/mL methanol
cannabigerol (CBG)	Cerilliant Corp.	1.000 mg/mL methanol
cannabinol (CBN)	Cerilliant Corp.	1.000 mg/mL methanol
Terpene mixtures		
Terpene Mixture 1 (21 compounds) 3-carene, camphene, fenchone, camphor, menthol, geranyl acetate, cis-nerolidol, cedrol, α-bisabolol, linalool, trans-caryophyllene, farneses (mix of isomers), β-myrcene, caryophyllene oxide, ocimene (mix of isomers), α-phellandrene, eucalyptol, valencene, isopulegol, nerol, isoborneol	Cayman Chemical (Ann Arbor, MI).	1000 µg/mL methanol
Terpene Mixture 2 (16 compounds) α-pinene, β-pinene, α-terpinene, R-(+)-limonene, ɣ-terpinene, fenchyl alcohol, α-humulene, trans-nerolidol, terpinolene, borneol, terpineol (mix of isomers), geraniol, guaiol, sabinene hydrate, sabinene, and pulegone	Cayman Chemical (Ann Arbor, MI).	1000 µg/mL methanol
Peak-picking standards		
Δ8 -tetrahydrocannabinol (Δ8-THC)	Cerilliant Corp.	1.000 mg/mL

		methanol
cannabigerolic acid (CBGA)	Cerilliant Corp.	1.000 mg/mL acetonitrile
cannabicyclol (CBL)	Cerilliant Corp.	1.000 mg/mL acetonitrile
cannabidivarin (CBDV)	Cerilliant Corp.	1.000 mg/mL methanol
cannabidivarinic acid (CBDVA)	Cerilliant Corp.	1.000 mg/mL acetonitrile
beta-eudesmol	Sigma-Aldrich (St Louis, MO).	
bulnesol	Sigma-Aldrich (St Louis, MO).	
Polyphenols		
3,4-dihydroxybenzoic acid, caffeic acid, catechin hydrate, p-coumaric acid, ferulic acid, gallic acid monohydrate, gallocatechin, piceol, protocatechuic aldehyde, pungenol, vanillic acid	Sigma-Aldrich (St Louis, MO).	
Vanillin	Fluka (Mexico City, MX)	
Quercetin	Cayman Chemical (Ann Arbor, MI)	
Apigenin	AK Scientific (Union City, CA)	
Polyphenol ISTDs		
^{13}C3-ferulic acid	Sigma (Oakville, Canada)	
d_5-apigenin, ^{13}C3-caffeic acid, d_3-quercetin	Toronto Research Chemicals (North York, Canada)	
^{13}C3-catechin	Cambridge Isotope Laboratories Inc. (Tewksbury, U.S.A	
d_6-coumaric acid, d_2-gallic acid, d_3-vanillic acid, and d_3-vanillin	C/D/N Isotopes Inc. (Pointe-Claire, Canada).	
Pesticides Acephate, acetomiprid, aldicarb, allethrin, azoxystrobin, benzovindiflupyr, bifenazate, boscalid, buprofezin, carbaryl, carbofuran, chlorantraniliprole, chlorpyrifos, clofentezine, clothianidin, coumaphos, cyantraniliprole, cyprodinil, diazinon, dichlorvos, dimethoate, dinotefuran, dodemorph, ethoprophos, etofenprox, etoxazole, fenoxycarb, fenpyroximate, fensulfothion, fenthion,	SPEX CertiPrep (Metuchen, NJ)	100 µg/mL in acetonitrile

flonicamid, fluopyram, hexythiazox, imazalil, imidacloprid, iasmolin, kresoxim-methyl, malathion, metalaxyl, methiocarb, methoprene, mevinphos, MGK-264, myclobutanil, naled, novaluron, oxamyl, paclobutrazol, phenothrin, phosmet, pirimicarb, prallethrin, propoxur, pyraclostrobin, pyrethrins, pyridaben, spinetoram, spinosad A, spinosad B, spiridiclofen, spiromesifin, spiroxamine, tebuconazole, tebufenozide, teflubenzuron, tetrachlorvinphos, tetramethrin, thiacloprid, thiametoxam, thiophanate-methyl, trifloxystrobin		

Methods for the separation, identification and quantification of cannabinoids by LC–MS/MS

Preparation of stock solutions, Internal Standard (ISTD) mixture, and calibration curve standards. All chemicals were received as 1 mg/mL stock solutions in methanol. Isotope-labeled ISTD mixture was prepared by mixing and diluting individual stock solutions to a final concentration of 5 µg/mL for each ISTD using methanol. Ten-point calibration curves of analytes from 0.0625 to 12.5 µg/mL were prepared by mixing and diluting the stock solutions using methanol.

LC-MS/MS Instrumentation and conditions. An Agilent 1290 series UHPLC system (Palo Alto, CA, USA) coupled with an AB Sciex QTRAP® 5500 mass spectrometer (Concord, ON, USA) was used for all online LC-MS/MS analyses. The column used was a Waters ACQUITY UPLC BEH C18 column (2.1 mm x 75 mm, 1.7 µm particle size, 130 Å pore size). The controlling software for the sample analysis was Analyst® 1.7.2. The data analysis software was Analyst ® 1.6.3.

The UHPLC parameters used to separate cannabinoids were as follows: solvent A was 0.2% (v/v) formic acid (FA) in water, and solvent B was 0.2% (v/v) FA in acetonitrile. The gradient profile for this UHPLC elution was as follows: t = 0.0 min, 50% A; t = 1.0 min, 50% A; t = 3.0 min, 95% A; t = 3.51 min, 50% A; and maintained at 50% A for another 5.0 min until the column pressure was stable for the next injection. The flow rate was set to 0.6 mL/min, and 10 µL of the final sample solution was injected for analysis. The column oven was set at 40 °C. The QTRAP® 5500 mass spectrometer was set to a positive electrospray ionization (ESI) mode with a scheduled multiple reaction monitoring (sMRM) scan for the quantification of THC, CBD, CBN, CBG, CBDV, CBC, THCV, and CBL (see Table S2 for definitions of abbreviations); and to a negative ESI mode with sMRM to quantify THC-COOH, THCA, CBNA, CBLA+CBCA, CBDVA, CBDA, and CBGA (see Table S2 for definitions of abbreviations). The IonSpray voltage was set at 5500 volts for positive mode and -4500 volts for negative mode; and the ion source temperature was set at 500 °C. The curtain gas (CUR), ion source gas 1 (GAS1), ion source gas 2 (GAS2) and collision gas (CAD) were set at 20, 40, 50 and medium, separately. The entrance potential (EP) was set to 15 volts, whereas the declustering potential (DP), collision energy (CE), collision cell exit potential (CXP), MRM precursor ion (Q1) and fragment ion (Q3) were optimized and set specifically for each analyte and isotope-labeled standard (ISTD).

Methods for separation and quantification of polyphenols by UHPLC-MS.

Preparation of stock solutions, Internal Standard (ISTD) mixture, and calibration curve standards. All chemicals were weighed carefully on a Sartorius CPA225D semi-micro electronic balance (Mississauga, ON, CA) with a precision of 0.0001 g. Stock solutions were prepared by dissolving the accurately weighed chemicals in 80 % methanol (MeOH) with 0.1% FA (gallic acid monohydrate, 3-5-dihydroxybenzoic acid, vanillic acid, caffeic acid, p-coumaric acid, ferulic acid, piceol, pungenol), in 80% MeOH (protocatechuic aldehyde), in 100% MeOH (vanillin), in DMSO (apigenin), 100% ethanol (EtOH; ((+)-catechin hydrate, gallocatechin) and 100% EtOH with 0.1% FA (quercetin). Eight-point calibration curves of analytes (Calibrant (Cal) 1 to Cal 8) were devised from concentration ranges that are expected for plants (from 0.01-70 µM for apigenin, caffeic acid, p-coumaric acid, gallic acid, protocatechuic aldehyde and quercetin; from 1.13-250 µM for ferulic acid, gallocatechin, piceol, vanillic acid and vanillin; from 3.13-900 µM for catechin, 3,4-dihydroxybenzoic acid and pungenol).

LC-MS/MS Instrumentation and conditions. A Thermo Scientific Vanquish UHPLC system (Waltham, MA, U.S.A.) and an Agilent (Santa Clara, CA, U.S.A.) reversed-phase Zorbax Eclipse XDB C18 column (3.0 mm × 100 mm, 3.5 µm particle size, 80 Å pore size) with an ACQUITY UPLC CSH C18 VanGuard Pre-column (2.1 mm × 5 mm, 1.7 µm particle size, 130 Å pore size) were used for all online UHPLC-HRMS analyses with a Thermo Scientific Q-Exactive HF Hybrid Quadrupole-Orbitrap Mass Spectrometer (Waltham, MA, U.S.A.). The controlling software for the sample analysis was Thermo Xcalibur 4.1.31.9.

The UHPLC parameters used for analysis were as follows: solvent A- 0.1% (v/v) FA in the water, and solvent B- 0.1% (v/v) FA in methanol. The gradient profile for this HPLC solvent run was as follows: t = 0 min, 1% B; t = 0.5 min, 1% B; t = 3.5 min, 60% B; t = 4.5 min 99% B; t = 5.7 min, 99% B; t = 5.71 min, 1% B; and finally maintained at 1% B for 2.3 min before the next injection. The column oven was set at 30 °C. The flow rate was 500 µL/min, and

the sample injection volume was 5 µL. For HRMS analysis, both solvents A and B were introduced to a heated electrospray ionization (HESI-II) probe at 370 °C auxiliary gas heater temperature, 320 °C capillary temperature, and 2.70 kV spray voltage. Nitrogen gas was used as both auxiliary and sheath gas at a flow rate of 50 and 12 mL/min, respectively. Mass scan range was set to m/z 70 to 1000 and resolution was set at 30,000 Full Width at Half Maximum (FWHM). Data acquisition was done using parallel reaction monitoring (PRM) in a negative ionization mode and analyte peak identification and integration were done by TraceFinder 4.1.

Results

Table S3. Targeted GC-MS analysis of terpenoids in six cannabis cultivars.

Terpenoid (mg per g)	Cultivar					
	Alien Dawg	**Tangerine Dream**	**Sensi Star**	**Quadra**	**Gabriola**	**Island Honey**
Camphene	0.03±0.003	0.02±0.002	0.01±0.001	0.06±0.006	0.10±0.001	ND
β-Myrcene	1.17±0.02	1.71±0.01	0.75±0.008	0.38±0.004	0.42±0.004	0.44±0.004
α-Phellandrene	ND	ND	0.10±0.001	ND	ND	ND
3-Carene	ND	ND	0.10±0.001	ND	ND	ND
Eucalyptol	ND	ND	0.04±0.004	ND	ND	ND
Ocimene	ND	ND	0.30±0.01	0.10±0.001	0.06±0.006	ND
(+)-Fenchone	ND	ND	ND	0.02±0.002	0.10±0.001	ND
Linalool	0.11±0.01	0.29±0.003	ND	0.89±0.01	0.70±0.01	0.19±0.002
trans-Caryophyllene	1.86±0.01	0.85±0.009	0.78±0.008	1.02±0.01	2.37±0.02	1.32±0.009
E- β-Farnesene	1.54±0.18	2.21±0.05	ND	1.01±0.01	3.10±0.02	ND
(-)-Caryophyllene Oxide	0.14±0.001	0.15±0.001	0.13±0.001	0.15±0.001	0.18±0.001	0.15±0.001
(-)-α-Bisabolol	0.26±0.003	0.50±0.01	0.40±0.004	0.46±0.005	0.45±0.004	0.39±0.004
α-Pinene	0.13±0.001	0.75±0.008	0.25±0.003	0.25±0.003	0.58±0.01	0.02±0.002
Sabinene	ND	ND	0.05±0.006	ND	ND	ND
β-Pinene	0.12±0.00	0.27±0.003	0.16±0.001	0.25±0.003	0.55±0.01	0.04±0.004
α-Terpinene	ND	ND	0.12±0.001	ND	ND	ND
R-(+)-Limonene	0.86±0.01	0.26±0.003	0.18±0.002	1.38±0.01	2.48±0.01	0.12±0.001
ɣ-Terpinene	ND	ND	0.10±0.001	ND	ND	ND
Sabinene hydrate	ND	ND	0.05±0.006	0.02±0.002	0.03±0.003	ND
Terpinolene	ND	ND	1.89±0.03	ND	ND	ND
Fenchyl Alcohol	0.13±0.001	0.06±0.007	0.06±0.007	0.59±0.01	0.45±0.01	0.03±0.003
Borneol	0.09±0.01	0.07±0.007	0.08±0.008	0.27±0.01	0.13±0.001	0.07±0.007
α-Terpineol	0.25±0.02	0.22±0.002	0.37±0.004	0.69±0.007	0.62±0.006	0.19±0.002
α-Humulene	0.62±0.01	0.24±0.01	0.23±0.002	0.29±0.003	0.60±0.01	0.34±0.003
trans-Nerolidol	ND	1.09±0.009	ND	ND	ND	1.10±0.009

Guaiol	ND	0.56±0.01	0.37±0.003	ND	ND	ND
Bulnesol	ND	0.57±0.006	0.31±0.01	ND	ND	ND
β-Eudesmol	ND	0.35±0.01	0.21±0.01	ND	ND	ND
cis-2-pinanol*	0.08±0.002	0.04±0.002	0.04±0.001	0.39±0.009	0.44±0.004	0.02±0.001
trans-2-Pinanol*	ND	ND	ND	0.03±0.001	0.06±0.001	ND
Camphene hydrate*	ND	ND	ND	0.02±0.002	0.01±0.001	ND
A-Ylangene*	0.07±0.009	0.05±0.001	ND	0.06±0.001	0.06±0.001	ND
α-Copaene*	0.05±0.009	ND	ND	ND	ND	ND
Selina-5,11-diene*	0.09±0.002	ND	0.06±0.001	0.08±0.001	0.13±0.001	0.07±0.001
ɣ-Elemene*	ND	ND	ND	ND	0.18±0.001	0.05±0.001
trans α-Bergamotene*	0.28±0.001	0.29±0.001	0.16±0.001	0.19±0.001	0.32±0.001	0.14±0.001
α-Guaiene*	ND	ND	0.13±0.002	0.18±0.001	ND	ND
ɣ-Muurolene*	0.11±0.006	ND	0.06±0.001	0.08±0.001	0.15±0.001	0.07±0.0001
β-Selinene*	0.23±0.001	0.08±0.001	0.11±0.003	0.21±0.001	0.34±0.006	0.19±0.001
α-Selinene*	0.27±0.004	ND	0.12±0.001	0.24±0.001	0.35±0.004	0.18±0.001
Δ -Cadinene*	0.10±0.005	ND	ND	ND	ND	ND
β-Bisabolene*	ND	0.18±0.001	ND	ND	ND	ND
Eudesma-3,7(11)-diene*	1.32±0.002	ND	0.39±0.003	0.77±0.007	1.58±0.007	0.59±0.011
α-Eudesmol*	ND	0.40±0.023	0.24±0.003	ND	ND	ND
Juniper camphor*	0.13±0.007	0.07±0.005	ND	0.09±0.001	0.14±0.001	0.06±0.006

Abbreviations: ND – not detected.

Table S4. Untargeted GC-MS analysis of terpenoids and volatile compounds.

RT (min)	Cultivar	Compound name	RI (experimental)	RI (Theoretical)	RI Relative variance
5.322	**Alkane standard**	**n-Nonane**	**NA**	**NA**	**NA**
5.424	Island Honey	3-Methylcyclopentyl acetate	902	988	-8.66
5.793	Sensi Star	Dimethylaminoethanol acetate	911	834	9.27
6.149	Sensi Star	Ethyl dimethylacrylate	920	869	5.85
6.245	Sensi Star	beta-Thujene	922	873	5.63
6.480	Alien Dawg	alpha-Pinene	928	948	-2.14
6.480	Tangerine Dream	alpha-Pinene	928	948	-2.14
6.480	Sensi Star	alpha-Pinene	928	948	-2.14
6.480	Quadra	alpha-Pinene	928	948	-2.14
6.480	Gabriola	alpha-Pinene	928	948	-2.14
6.486	Island Honey	alpha-Pinene	928	948	-2.12
7.034	Gabriola	Camphene	941	943	-0.21
7.040	Alien Dawg	Camphene	941	943	-0.20
7.040	Tangerine Dream	Camphene	941	943	-0.20
7.040	Sensi Star	Camphene	941	943	-0.20
7.040	Quadra	Camphene	941	943	-0.20
7.040	Island Honey	Camphene	941	943	-0.20
8.147	Sensi Star	Sabinene	968	897	7.88
8.255	Alien Dawg	beta-Pinene	970	943	2.89
8.255	Tangerine Dream	beta-Pinene	970	943	2.89
8.255	Sensi Star	beta-Pinene	970	943	2.89
8.255	Quadra	beta-Pinene	970	943	2.89
8.261	Gabriola	beta-Pinene	970	943	2.91
8.261	Island Honey	beta-Pinene	970	943	2.91
8.790	Sensi Star	3-Methyl-3-cyclohexen-1-one	983	962	2.19
9.044	Sensi Star	beta-Myrcene	989	958	3.25
9.050	Alien Dawg	beta-Myrcene	989	958	3.27
9.050	Tangerine Dream	beta-Myrcene	989	958	3.27
9.050	Quadra	beta-Myrcene	989	958	3.27
9.050	Gabriola	beta-Myrcene	989	958	3.27
9.050	Island Honey	beta-Myrcene	989	958	3.27
9.496	**Alkane standard**	**n-Decane**	**NA**	**NA**	**NA**
9.757	Sensi Star	alpha-Phellandrene	1003	969	3.56
10.094	Sensi Star	3-Carene	1008	948	6.32
10.539	Sensi Star	alpha-Terpinene	1014	998	1.59
11.074	Sensi Star	o-Cymene	1021	1042	-2.02
11.334	Tangerine Dream	Limonene	1024	1018	0.62

Table S4. Continued

RT (min)	Cultivar	Compound name	RI (experimental)	RI (Theoretical)	RI Relative variance
11.334	Island Honey	Limonene	1024	1018	0.62
11.341	Sensi Star	Limonene	1024	1018	0.63
11.347	Alien Dawg	Limonene	1025	1018	0.64
11.366	Quadra	Limonene	1025	1018	0.67
11.404	Gabriola	Limonene	1025	1018	0.72
11.500	Sensi Star	Eucalyptol	1027	1059	-3.06
11.519	Gabriola	Eucalyptol	1027	1059	-3.04
12.957	Sensi Star	beta-Ocimene	1046	976	7.16
12.957	Quadra	beta-Ocimene	1046	976	7.16
12.957	Gabriola	beta-Ocimene	1046	976	7.16
13.650	Sensi Star	gamma-Terpinene	1055	998	5.72
14.254	Gabriola	trans-Sabinene hydrate	1063	1041	2.12
14.255	Sensi Star	trans-Sabinene hydrate	1063	1041	2.12
15.832	Gabriola	Fenchone	1084	1121	-3.30
15.845	Quadra	Fenchone	1084	1121	-3.29
15.947	Sensi Star	Terpinolene	1086	1052	3.18
16.685	Sensi Star	cis-beta-Terpineol	1095	1158	-5.42
17.041	**Alkane standard**	**n-Undecane**	**NA**	**NA**	**NA**
17.041	Alien Dawg	Linalool	1100	1082	1.66
17.041	Tangerine Dream	Linalool	1100	1082	1.66
17.041	Island Honey	Linalool	1100	1082	1.66
17.060	Sensi Star	Linalool	1100	1082	1.68
17.066	Gabriola	Linalool	1100	1082	1.69
17.073	Quadra	Linalool	1100	1082	1.70
17.811	Alien Dawg	Fenchyl Alcohol	1109	1138	-2.51
17.824	Tangerine Dream	Fenchyl Alcohol	1110	1138	-2.49
17.824	Sensi Star	Fenchyl Alcohol	1110	1138	-2.49
17.830	Island Honey	Fenchyl Alcohol	1110	1138	-2.49
17.836	Gabriola	Fenchyl Alcohol	1110	1138	-2.48
17.843	Quadra	Fenchyl Alcohol	1110	1138	-2.47
18.390	Alien Dawg	Bicyclo[3.1.1]heptan-2-ol, 2,6,6-trimethyl-	1117	1088	2.63
18.396	Tangerine Dream	Bicyclo[3.1.1]heptan-2-ol, 2,6,6-trimethyl-	1117	1088	2.64
18.396	Sensi Star	Bicyclo[3.1.1]heptan-2-ol, 2,6,6-trimethyl-	1117	1088	2.64
18.396	Island Honey	Bicyclo[3.1.1]heptan-2-ol, 2,6,6-trimethyl-	1117	1088	2.64

Table S4. Continued

RT (min)	Cultivar	Compound name	RI (experimental)	RI (Theoretical)	RI Relative variance
18.403	Quadra	Bicyclo[3.1.1]heptan-2-ol, 2,6,6-trimethyl-	1117	1088	2.65
18.415	Gabriola	Bicyclo[3.1.1]heptan-2-ol, 2,6,6-trimethyl-	1117	1088	2.66
19.987	Quadra	trans-2-Pinanol	1136	1088	4.44
19.987	Gabriola	trans-2-Pinanol	1136	1088	4.44
19.993	Alien Dawg	trans-2-Pinanol	1136	1088	4.44
20.012	Sensi Star	cis-2-Menthenol	1137	1109	2.49
20.451	Quadra	Camphene hydrate	1142	1088	4.96
20.451	Gabriola	Camphene hydrate	1142	1088	4.96
20.458	Alien Dawg	Camphene hydrate	1142	1088	4.97
20.534	Sensi Star	3-Oxabicyclo[4.3.0]non-8-en-2-one, cis-	1143	1189	-3.87
20.814	Alien Dawg	Tetrahydrofuran	1146	1108	3.47
21.946	Alien Dawg	Borneol	1160	1138	1.97
21.953	Quadra	Borneol	1161	1138	1.98
21.953	Gabriola	Borneol	1161	1138	1.98
21.972	Tangerine Dream	Borneol	1161	1138	2.00
21.972	Sensi Star	Borneol	1161	1138	2.00
21.984	Island Honey	Borneol	1161	1138	2.01
22.952	Quadra	Terpinen-4-ol	1173	1137	3.15
22.958	Sensi Star	2-Isopropenyl-5-methylhex-4-enal	1173	1092	7.41
23.760	Sensi Star	p-Cymene-8-ol	1183	1197	-1.19
24.084	Alien Dawg	alpha-Terpineol	1187	1143	3.83
24.084	Tangerine Dream	alpha-Terpineol	1187	1143	3.83
24.084	Sensi Star	alpha-Terpineol	1187	1143	3.83
24.103	Quadra	alpha-Terpineol	1187	1143	3.85
24.103	Gabriola	alpha-Terpineol	1187	1143	3.85
24.109	Island Honey	alpha-Terpineol	1187	1143	3.86
24.682	Tangerine Dream	Hexyl butyrate	1194	1183	0.94
24.707	Alien Dawg	Hexyl butyrate	1194	1183	0.97
25.159	**Alkane standard**	**n-Dodecane**	**NA**	**NA**	**NA**
26.591	Sensi Star	(+)-cis-Verbenol, acetate	1231	1276	-3.54
28.983	Quadra	2,6-Dimethyl-1,7-octadien-3,6-diol	1282	1227	4.52
29.174	Sensi Star	5-Isopropenyl-2-methyl-7-oxabicyclo[4.1.0]heptan-2-ol	1287	1169	10.06
29.269	Alien Dawg	Bornyl acetate	1289	1277	0.91

Table S4. Continued

RT (min)	Cultivar	Compound name	RI (experimental)	RI (Theoretical)	RI Relative variance
29.269	Quadra	(-)-Bornyl acetate	1289	1277	0.91
29.269	Gabriola	(-)-Bornyl acetate	1289	1277	0.91
29.797	**Alkane standard**	**n-Tridecane**	**NA**	**NA**	**NA**
30.847	Quadra	Limonene glycol	1344	1346	-0.18
31.559	Tangerine Dream	alpha-Ylangene	1373	1221	12.46
31.559	Gabriola	alpha-Ylangene	1373	1221	12.46
31.559	Island Honey	alpha-Ylangene	1373	1221	12.46
31.566	Alien Dawg	alpha-Ylangene	1373	1221	12.48
31.661	Island Honey	Germacrene D	1377	1515	-9.09
31.667	Alien Dawg	alpha-Copaene	1378	1221	12.82
31.909	Alien Dawg	beta-Cubebene	1388	1339	3.63
31.954	Gabriola	Hexyl hexanoate	1389	1381	0.61
31.960	Tangerine Dream	Hexyl hexanoate	1390	1381	0.63
32.017	Tangerine Dream	cis-sesquisabinene hydrate	1392	1523	-8.60
32.030	Quadra	Selina-5,11-diene	1393	1474	-5.52
32.030	Gabriola	Selina-5,11-diene	1393	1474	-5.52
32.030	Island Honey	Selina-5,11-diene	1393	1474	-5.52
32.036	Alien Dawg	Selina-5,11-diene	1393	1474	-5.50
32.037	Sensi Star	Selina-5,11-diene	1393	1474	-5.50
32.208	**Alkane standard**	**n-Tetradecane**	**NA**	**NA**	**NA**
32.335	Tangerine Dream	trans-alpha-Bergamotene	1407	1430	-1.60
32.336	Quadra	trans-alpha-Bergamotene	1407	1430	-1.60
32.342	Alien Dawg	trans-alpha-Bergamotene	1407	1430	-1.58
32.342	Gabriola	trans-alpha-Bergamotene	1407	1430	-1.58
32.52	Alien Dawg	alpha-Bergamotene	1417	1430	-0.89
32.52	Tangerine Dream	alpha-Bergamotene	1417	1430	-0.89
32.52	Quadra	alpha-Bergamotene	1417	1430	-0.89
32.52	Gabriola	alpha-Bergamotene	1417	1430	-0.89
32.596	Tangerine Dream	trans-Caryophyllene	1422	1494	-4.85
32.596	Sensi Star	trans-Caryophyllene	1422	1494	-4.85
32.603	Quadra	trans-Caryophyllene	1422	1494	-4.82
32.609	Alien Dawg	trans-Caryophyllene	1422	1494	-4.80
32.609	Island Honey	trans-Caryophyllene	1422	1494	-4.80
32.615	Gabriola	trans-Caryophyllene	1423	1494	-4.78
32.692	Alien Dawg	1H-Cycloprop[e]azulene	1427	1386	2.95
32.876	Gabriola	gamma-Elemene	1437	1431	0.43
32.876	Island Honey	gamma-Elemene	1437	1431	0.43
32.914	Tangerine Dream	alpha-Bergamotene	1437	1430	0.64

Table S4. Continued

RT (min)	Cultivar	Compound name	RI (experimental)	RI (Theoretical)	RI Relative variance
32.915	Sensi Star	alpha-Bergamotene	1439	1430	0.65
32.921	Alien Dawg	alpha-Bergamotene	1440	1430	0.67
32.921	Quadra	alpha-Bergamotene	1440	1430	0.67
32.921	Gabriola	alpha-Bergamotene	1440	1430	0.67
32.921	Island Honey	alpha-Bergamotene	1440	1430	0.67
32.972	Sensi Star	alpha-Guaiene	1442	1490	-3.19
32.972	Quadra	alpha-Guaiene	1442	1490	-3.19
33.252	Tangerine Dream	alpha-Humulene	1458	1579	-7.67
33.252	Sensi Star	alpha-Humulene	1458	1579	-7.67
33.258	Quadra	alpha-Humulene	1458	1579	-7.64
33.258	Island Honey	alpha-Humulene	1458	1579	-7.64
33.264	Alien Dawg	alpha-Humulene	1459	1579	-7.62
33.264	Gabriola	alpha-Humulene	1459	1579	-7.62
33.296	Tangerine Dream	cis-beta-Farnesene	1460	1440	1.42
33.296	Quadra	cis-beta-Farnesene	1460	1440	1.42
33.302	Gabriola	cis-beta-Farnesene	1461	1440	1.44
33.303	Alien Dawg	cis-beta-Farnesene	1461	1440	1.44
33.665	Sensi Star	gamma-Muurolene	1481	1435	3.20
33.671	Gabriola	gamma-Muurolene	1481	1435	3.22
33.672	Alien Dawg	gamma-Muurolene	1481	1435	3.23
33.672	Island Honey	gamma-Muurolene	1481	1435	3.23
33.799	Alien Dawg	2-Isopropenyl-4a,8-dimethyl-1,2,3,4,4a,5,6,7-octahydronaphthalene	1488	1502	-0.91
33.799	Tangerine Dream	2-Isopropenyl-4a,8-dimethyl-1,2,3,4,4a,5,6,7-octahydronaphthalene	1488	1502	-0.91
33.799	Quadra	2-Isopropenyl-4a,8-dimethyl-1,2,3,4,4a,5,6,7-octahydronaphthalene	1488	1502	-0.91
33.799	Island Honey	2-Isopropenyl-4a,8-dimethyl-1,2,3,4,4a,5,6,7-octahydronaphthalene	1488	1502	-0.91
33.805	Gabriola	2-Isopropenyl-4a,8-dimethyl-1,2,3,4,4a,5,6,7-octahydronaphthalene	1489	1502	-0.89
33.843	Tangerine Dream	beta-Selinene	1491	1474	1.14
33.85	Alien Dawg	beta-Selinene	1491	1474	1.16
33.85	Sensi Star	beta-Selinene	1491	1474	1.16
33.85	Quadra	beta-Selinene	1491	1474	1.16

Table S4. Continued

RT (min)	Cultivar	Compound name	RI (experimental)	RI (Theoretical)	RI Relative variance
33.85	Gabriola	beta-Selinene	1491	1474	1.16
33.85	Island Honey	beta-Selinene	1491	1474	1.16
34.002	Alien Dawg	alpha-Selinene	1500	1474	1.74
34.002	Sensi Star	alpha-Selinene	1500	1474	1.74
34.002	Quadra	alpha-Selinene	1500	1474	1.74
34.002	Gabriola	alpha-Selinene	1500	1474	1.74
34.002	Island Honey	alpha-Selinene	1500	1474	1.74
34.009	**Alkane standard**	**n-Pentadecane**	**NA**	**NA**	**NA**
34.098	Tangerine Dream	Dihydroagarofuran	1505	1514	-0.60
34.174	Sensi Star	alpha-Bulnesene	1511	1490	1.40
34.18	Island Honey	alpha-trans-Farnesene	1511	1458	3.66
34.181	Quadra	alpha-Bulnesene	1511	1490	1.43
34.187	Gabriola	alpha-trans-Farnesene	1512	1458	3.69
34.2	Alien Dawg	delta-Cadinene	1513	1469	2.97
34.2	Tangerine Dream	beta-Bisabolene	1513	1500	0.84
34.378	Alien Dawg	gamma-Gurjunene	1524	1461	4.34
34.378	Tangerine Dream	gamma-Gurjunene	1524	1461	4.34
34.378	Sensi Star	gamma-Gurjunene	1524	1461	4.34
34.378	Island Honey	gamma-Gurjunene	1524	1461	4.34
34.422	Sensi Star	alpha-Gurjunene	1527	1419	7.63
34.429	Alien Dawg	alpha-Gurjunene	1528	1419	7.66
34.429	Island Honey	alpha-Gurjunene	1528	1419	7.66
34.499	Alien Dawg	alpha-Gurjunene	1532	1419	7.99
34.499	Sensi Star	alpha-Gurjunene	1532	1419	7.99
34.499	Island Honey	alpha-Gurjunene	1532	1419	7.99
34.658	Sensi Star	(4aR,8aS)-4a-Methyl-1-methylene-7-(propan-2-ylidene)decahydronaphthalene	1543	1502	2.72
34.664	Quadra	(4aR,8aS)-4a-Methyl-1-methylene-7-(propan-2-ylidene)decahydronaphthalene	1543	1502	2.75
34.67	Alien Dawg	(4aR,8aS)-4a-Methyl-1-methylene-7-(propan-2-ylidene)decahydronaphthalene	1544	1502	2.77
34.67	Island Honey	(4aR,8aS)-4a-Methyl-1-methylene-7-(propan-2-ylidene)decahydronaphthalene	1544	1502	2.77
34.689	Tangerine Dream	beta-Maaliene	1545	1432	7.89

Table S4. Continued

RT (min)	Cultivar	Compound name	RI (experimental)	RI (Theoretical)	RI Relative variance
34.702	Alien Dawg	beta-Maaliene	1546	1432	7.95
34.734	Tangerine Dream	cis-alpha-Bisabolene	1548	1518	1.97
34.735	Gabriola	Eudesma-3,7(11)-diene	1548	1507	2.72
34.766	Sensi Star	Eudesma-3,7(11)-diene	1550	1507	2.85
34.772	Quadra	Eudesma-3,7(11)-diene	1550	1507	2.88
34.772	Island Honey	Eudesma-3,7(11)-diene	1550	1507	2.88
34.785	Alien Dawg	Eudesma-3,7(11)-diene	1551	1507	2.94
35.02	Gabriola	Germacrene B	1567	1603	-2.26
35.046	Tangerine Dream	trans-Nerolidol	1568	1564	0.29
35.046	Sensi Star	trans-Nerolidol	1568	1564	0.29
35.09	Alien Dawg	beta-Maaliene	1571	1432	9.73
35.421	Alien Dawg	Caryophyllene oxide	1593	1507	5.72
35.421	Tangerine Dream	Caryophyllene oxide	1593	1507	5.72
35.421	Sensi Star	Caryophyllene oxide	1593	1507	5.72
35.421	Quadra	Caryophyllene oxide	1593	1507	5.72
35.421	Gabriola	Caryophyllene oxide	1593	1507	5.72
35.421	Island Honey	Caryophyllene oxide	1593	1507	5.72
35.523	**Alkane standard**	**n-Hexadecane**	**NA**	**NA**	**NA**
35.606	Sensi Star	Guaiol	1606	1614	-0.49
35.612	Tangerine Dream	Guaiol	1607	1614	-0.46
35.733	Tangerine Dream	alpha-Eudesmol	1616	1598	1.10
35.803	Tangerine Dream	Humulene-1,2-epoxide	1621	1592	1.81
35.936	Alien Dawg	Selina-6-en-4-ol	1631	1593	2.36
35.956	Sensi Star	gamma-Eudesmol	1632	1626	0.38
35.962	Tangerine Dream	gamma-Eudesmol	1633	1626	0.40
36.102	Tangerine Dream	gamma-Eudesmol	1643	1626	1.04
36.382	Tangerine Dream	beta-Eudesmol	1664	1593	4.44
36.382	Sensi Star	beta-Eudesmol	1664	1593	4.44
36.401	Alien Dawg	Isovalencenol	1665	1745	-4.58
36.407	Gabriola	Isovalencenol	1666	1750	-4.83
36.414	Quadra	beta-Guaiene	1666	1523	9.39
36.42	Tangerine Dream	alpha-Eudesmol	1666	1598	4.29
36.42	Sensi Star	alpha-Eudesmol	1666	1598	4.29
36.592	Tangerine Dream	Bulnesol	1679	1614	4.04
36.598	Sensi Star	Bulnesol	1680	1614	4.07
36.766	Tangerine Dream	alpha-Bisabolol	1692	1625	4.13
36.77	Quadra	alpha-Bisabolol	1692	1625	4.15
36.77	Gabriola	alpha-Bisabolol	1692	1625	4.15

Table S4. Continued

RT (min)	Cultivar	Compound name	RI (experimental)	RI (Theoretical)	RI Relative variance
36.77	Island Honey	alpha-Bisabolol	1692	1625	4.15
36.776	Sensi Star	alpha-Bisabolol	1693	1625	4.18
36.872	**Alkane standard**	**n-Heptadecane**	**NA**	**NA**	**NA**
36.999	Quadra	Juniper camphor	1710	1647	3.84
36.999	Gabriola	Juniper camphor	1710	1647	3.84
37.005	Alien Dawg	Juniper camphor	1711	1647	3.87
37.005	Tangerine Dream	Juniper camphor	1711	1647	3.87
37.005	Sensi Star	Juniper camphor	1711	1647	3.87
37.005	Island Honey	Juniper camphor	1711	1647	3.87
37.164	Gabriola	Pentanoic acid, 4-methyl-, 3,7-dimethyl-6-octenyl ester	1724	1636	5.35
37.253	Gabriola	Isoaromadendrene epoxide	1731	1281	35.11
37.26	Island Honey	Isospathulenol	1731	1569	10.34
37.59	Gabriola	Geranyl caproate	1758	1749	0.51
38.112	**Alkane standard**	**n-Octadecane**	**NA**	**NA**	**NA**
38.316	Sensi Star	Selina-4,7-diol	1818	1738	4.57
38.59	Quadra	3,7,11,15-Tetramethyl-2-hexadecen-1-ol	1841	2045	-9.97
38.596	Sensi Star	3,7,11,15-Tetramethyl-2-hexadecen-1-ol	1842	2045	-9.95
38.596	Gabriola	3,7,11,15-Tetramethyl-2-hexadecen-1-ol	1842	2045	-9.95
38.596	Island Honey	3,7,11,15-Tetramethyl-2-hexadecen-1-ol	1842	2045	-9.95
38.602	Alien Dawg	3,7,11,15-Tetramethyl-2-hexadecen-1-ol	1842	2045	-9.92
38.672	Quadra	Hexahydrofarnesyl acetone	1848	1754	5.36
38.678	Gabriola	Hexahydrofarnesyl acetone	1849	1754	5.39
38.678	Island Honey	Hexahydrofarnesyl acetone	1849	1754	5.39
38.679	Sensi Star	Hexahydrofarnesyl acetone	1849	1754	5.40
38.685	Alien Dawg	Hexahydrofarnesyl acetone	1849	1754	5.43
38.774	Gabriola	8-Hydroxyageraphorone	1857	1789	3.79
39.098	Alien Dawg	3,7,11,15-Tetramethyl-2-hexadecen-1-ol	1885	2045	-7.84
39.098	Island Honey	3,7,11,15-Tetramethyl-2-hexadecen-1-ol	1885	2045	-7.84
39.277	**Alkane standard**	**n-Nonadecane**	**NA**	**NA**	**NA**
39.576	Quadra	Methyl hexadecanoate	1927	1814	6.23
39.582	Sensi Star	Methyl hexadecanoate	1928	1814	6.26
39.582	Gabriola	Methyl hexadecanoate	1928	1814	6.26

Table S4. Continued

RT (min)	Cultivar	Compound name	RI (experimental)	RI (Theoretical)	RI Relative variance
39.582	Island Honey	Methyl hexadecanoate	1928	1814	6.26
39.588	Alien Dawg	Methyl hexadecanoate	1928	1814	6.29
39.588	Tangerine Dream	Methyl hexadecanoate	1928	1878	2.67
39.976	Island Honey	Palmitic acid	1963	1968	-0.25
39.983	Tangerine Dream	Palmitic acid	1964	1968	-0.21
39.983	Sensi Star	Palmitic acid	1964	1968	-0.21
39.983	Quadra	Palmitic acid	1964	1968	-0.21
40.384	**Alkane standard**	**n-Icosane**	**NA**	**NA**	**NA**
41.401	Island Honey	Methyl linoleate	2098	2093	0.22
41.402	Sensi Star	Methyl linolelaidate	2098	2093	0.22
41.402	Quadra	Methyl linoleate	2098	2093	0.22
41.408	Alien Dawg	Methyl linoleate	2098	2093	0.25
41.408	Tangerine Dream	Methyl linolelaidate	2098	2093	0.25
41.427	**Alkane standard**	**n-Heneicosane**	**NA**	**NA**	**NA**
41.471	Island Honey	Methyl linolenate	2104	2101	0.16
41.478	Alien Dawg	Methyl linolenate	2105	2101	0.20
41.478	Sensi Star	Methyl linolenate	2105	2101	0.20
41.478	Quadra	Methyl linolenate	2105	2101	0.20
41.516	Island Honey	10-Octadecenoic acid, methyl ester	2109	2085	1.15
41.643	Island Honey	Phytol	2122	2045	3.75
41.649	Gabriola	Phytol	2122	2045	3.78
41.847	Alien Dawg	Phytol	2142	2045	4.75
42.018	Gabriola	Murralongin	2159	2225	-2.96
42.038	Alien Dawg	Furo[2,3-H]coumarine, 2-(1-hydroxyethyl)-1,6-dimethyl-	2161	2242	-3.61
42.426	**Alkane standard**	**n-Docosane**	**NA**	**NA**	**NA**
43.514	Alien Dawg	DELTA.8-Tetrahydrocannabinol	2298	2475	-7.14
43.514	Tangerine Dream	DELTA.8-Tetrahydrocannabinol	2298	2475	-7.14
43.514	Sensi Star	DELTA.8-Tetrahydrocannabinol	2298	2475	-7.14
43.514	Quadra	DELTA.8-Tetrahydrocannabinol	2298	2475	-7.14
43.514	Gabriola	DELTA.8-Tetrahydrocannabinol	2298	2475	-7.14
43.514	Island Honey	DELTA.8-Tetrahydrocannabinol	2298	2475	-7.14
43.533	**Alkane standard**	**n-Tricosane**	**NA**	**NA**	**NA**
43.953	Sensi Star	DELTA 9-Tetrahydrocannabivarin	2331	2276	2.44
43.953	Island Honey	DELTA 9-Tetrahydrocannabivarin	2331	2276	2.44
43.959	Quadra	DELTA 9-Tetrahydrocannabivarin	2332	2276	2.46
43.959	Gabriola	DELTA 9-Tetrahydrocannabivarin	2332	2276	2.46

Table S4. Continued

RT (min)	Cultivar	Compound name	RI (experimental)	RI (Theoretical)	RI Relative variance
43.965	Tangerine Dream	DELTA 9-Tetrahydrocannabivarin	2332	2276	2.48
43.972	Alien Dawg	DELTA 9-Tetrahydrocannabivarin	2333	2276	2.50
44.042	Alien Dawg	Oxymetazoline	2338	2361	-0.97
44.042	Island Honey	Oxymetazoline	2338	2361	-0.97
44.048	Gabriola	Oxymetazoline	2339	2361	-0.95
44.194	Quadra	Cannabidiol	2349	2605	-9.81
44.194	Island Honey	Cannabidiol	2349	2605	-9.81
44.201	Sensi Star	Cannabidiol	2350	2605	-9.79
44.201	Gabriola	Cannabidiol	2350	2605	-9.79
44.869	**Alkane standard**	**n-Tetracosane**	**NA**	**NA**	**NA**
44.888	Alien Dawg	DELTA 1-Tetrahydrocannabinol	2401	2552	-5.91
45.123	Alien Dawg	DELTA 9-tetrahydrocannabinol methyl ether	2415	2443	-1.14
45.123	Sensi Star	DELTA 9-tetrahydrocannabinol methyl ether	2415	2443	-1.14
45.123	Quadra	DELTA 9-tetrahydrocannabinol methyl ether	2415	2443	-1.14
45.123	Gabriola	DELTA 9-tetrahydrocannabinol methyl ether	2415	2443	-1.14
45.123	Island Honey	DELTA 9-tetrahydrocannabinol methyl ether	2415	2443	-1.14
45.454	Tangerine Dream	Cannabidiol	2435	2605	-6.52
45.454	Sensi Star	Cannabidiol	2435	2605	-6.52
45.454	Quadra	Cannabidiol	2435	2605	-6.52
45.454	Island Honey	Cannabidiol	2435	2605	-6.52
45.46	Gabriola	Cannabidiol	2435	2605	-6.51
45.467	Alien Dawg	DELTA 9-Tetrahydrocannabinol	2436	2475	-1.58
45.549	Tangerine Dream	Cannabichrome	2441	2486	-1.82
45.562	Sensi Star	Cannabichrome	2442	2486	-1.79
45.575	Alien Dawg	Cannabichrome	2442	2486	-1.76
45.588	Gabriola	Cannabichrome	2443	2486	-1.72
45.607	Quadra	Cannabichrome	2444	2486	-1.68
45.607	Island Honey	Cannabichrome	2444	2486	-1.68
46.345	Tangerine Dream	DELTA 9-Tetrahydrocannabinol	2489	2475	0.55
46.351	Sensi Star	exo-THC, acetate	2489	2629	-5.33
46.357	Alien Dawg	DELTA 9-Tetrahydrocannabinol	2489	2475	0.58
46.357	Island Honey	exo-THC, acetate	2489	2629	-5.32
46.358	Quadra	exo-THC, acetate	2489	2629	-5.31
46.364	Gabriola	exo-THC, acetate	2490	2629	-5.30

Table S4. Continued

RT (min)	Cultivar	Compound name	RI (experimental)	RI (Theoretical)	RI Relative variance
46.485	Island Honey	3-Methoxy-5-pentyl-2-prenylphenyl, acetate	2497	2256	10.68
46.491	Gabriola	3-Methoxy-5-pentyl-2-prenylphenyl, acetate	2497	2256	10.70
46.536	**Alkane standard**	**n-Pentacosane**	**NA**	**NA**	**NA**
47.445	Sensi Star	(-)-.DELTA.9-THC	2561	2475	3.47
47.47	Tangerine Dream	(-)-.DELTA.9-THC	2562	2475	3.53
47.541	Alien Dawg	(-)-.DELTA.9-THC	2567	2475	3.73
47.566	Quadra	(-)-.DELTA.9-THC	2569	2475	3.79
47.566	Gabriola	(-)-.DELTA.9-THC	2569	2475	3.79
47.566	Island Honey	(-)-.DELTA.9-THC	2569	2475	3.79
47.955	Island Honey	Cannabigerol	2595	2610	-0.58
48.024	**Alkane standard**	**n-Hexacosane**	**NA**	**NA**	**NA**
48.056	Island Honey	Cannabinol	2603	2582	0.83
48.075	Quadra	Cannabinol	2606	2582	0.93
48.075	Gabriola	Cannabinol	2606	2582	0.93
48.094	Sensi Star	Cannabigerol	2609	2610	-0.05
48.756	**Alkane standard**	**n-Heptacosane**	**NA**	**NA**	**NA**
48.75	Tangerine Dream	Heptacosane	2699	2705	-0.22
48.756	Alien Dawg	Heptacosane	2700	2705	-0.18
48.756	Sensi Star	Heptacosane	2700	2705	-0.18
48.756	Gabriola	Heptacosane	2700	2705	-0.18
48.756	Island Honey	Heptacosane	2700	2705	-0.18
48.762	Quadra	Heptacosane	2701	2705	-0.15
48.826	Quadra	8-alpha-Hydroxy-delta-9-tetrahydrocannabinol	2711	2663	1.81
48.826	Island Honey	8-alpha-Hydroxy-delta-9-tetrahydrocannabinol	2711	2663	1.81
48.832	Gabriola	8-alpha-Hydroxy-delta-9-tetrahydrocannabinol	2712	2663	1.84
49.38	**Alkane standard**	**n-Octacosane**	**NA**	**NA**	**NA**
50.022	Alien Dawg	Nonacosane	2899	2904	-0.175
50.022	Tangerine Dream	Nonacosane	2899	2904	-0.175
50.022	Sensi Star	Nonacosane	2899	2904	-0.175
50.022	Quadra	Nonacosane	2899	2904	-0.175
50.022	Gabriola	Nonacosane	2899	2904	-0.175
50.022	Island Honey	Nonacosane	2899	2904	-0.175
50.028	**Alkane standard**	**n-Nonacosane**	**NA**	**NA**	**NA**
50.722	**Alkane standard**	**n-Triacontane**	**NA**	**NA**	**NA**

Table S5. Cannabinoids quantified using a targeted LC-MS/MS metabolomics assay.

Cannabinoid (mg per g)	Cultivar					
	Alien Dawg	**Tangerine Dream**	**Sensi Star**	**Quadra**	**Gabriola**	**Island Honey**
Cannabichromene (CBC)	0.235 ± 0.0131	0.778 ± 0.0069	0.703 ± 0.0221	1.28 ± 0.0588	0.373 ± 0.0197	0.258 ± 0.0002
Cannabidiol (CBD)	0.850 ± 0.0387	0.245 ± 0.0195	0.459 ± 0.0433	0.230 ± 0.0056	0.331 ± 0.0020	0.197 ± 0.0031
Cannabidiolic acid (CBDA)	0.239 ± 0.0244	0.179 ± 0.0022	0.220 ± 0.0028	0.290± 0.0045	0.237 ± 0.0086	0.195 ± 0.0005
Cannabidivarin (CBDV)	0.000312 ± 0.0001	0.00276 ± 0.0001	0.00293 ± 0.0001	0.00158 ± 0.0001	0.000644 ± 0.0001	0.00096 ± 0.0001
Cannabidivarinic acid (CBDVA)	0.0476 ± 0.0015	0.0844 ± 0.0023	0.045 ± 0.0005	0.0994 ± 0.0002	0.0752 ± 0.0009	0.0238 ± 0.0001
Cannabigerol (CBG)	0.774 ± 0.0024	0.813 ± 0.0441	1.5 ± 0.035	0.273 ± 0.0030	0.256 ± 0.0014	0.811 ± 0.0115
Cannabigerolic acid (CBGA)	0.244 ± 0.0141	0.258 ± 0.0101	0.541 ± 0.002	0.304 ± 0.0008	0.261 ± 0.0045	0.294 ± 0.0064
Cannabicyclol (CBL)	0.206 ± 0.0024	0.794 ± 0.0133	0.882 ± 0.010	1.78 ± 0.0522	0.813 ± 0.0143	0.193 ± 0.0081
Cannabicyclolic acid (CBLA) + cannabichromenic acid (CBCA)	0.109 ± 0.0012	0.0858 ± 0.0063	0.0946 ± 0.004	0.127 ± 0.0004	0.0814 ± 0.0004	0.096 ± 0.0079
Cannabinol (CBN)	0.647 ± 0.0145	0.67 ± 0.0464	0.318 ± 0.033	0.498 ± 0.0029	0.198 ± 0.0079	0.143 ± 0.0021
Cannabinolic acid (CBNA)	0.177 ± 0.0053	0.159 ± 0.0046	0.198 ± 0.014	0.218 ± 0.0004	0.147 ± 0.0042	0.158 ± 0.0021
Δ9-Tetrahydrocannabinol (THC)	5.81 ± 0.142	2.88 ± 0.170	8.14 ± 0.344	3.55 ± 0.126	4.07 ± 0.0153	4.3 ± 0.109
Tetrahydrocannabinolic acid (THCA)	162 ± 6.53	133 ± 3.99	162 ± 7.13	174 ± 2.96	133 ± 1.68	129 ± 5.41
11-Nor-9-carboxy-Tetrahydrocannabinol (THC-COOH)	0.0937 ± 0.0015	0.05751 ± 0.0016	0.0603 ± 0.001	0.109 ± 0.003	0.186 ± 0.0097	0.0141 ± 0.0084
Tetrahydrocannabivarin (THCV)	0.228 ± 0.0067	0.353 ± 0.011	0.248 ± 0.001	0.246 ± 0.005	0.17 ± 0.0061	0.117 ± 0.0013

Table S6. Targeted LC-MS/MS analysis of phenolic compounds found in cannabis.

Polyphenol (mg/g dry weight)	Cultivars					
	Alien Dawg	Tangerine Dream	Sensi Star	Quadra	Gabriola	Island Honey
Apigenin	0.000680 ± 0.0000299	0.000420 ± 0.0000133	0.00270 ± 0.0000286	0.000610 ± 0.0000132	0.000820 ± 0.0000204	0.000420 ± 0.0000282
Caffeic acid	0.00200 ± 0.0000188	0.00292 ± 0.0000118	0.00119 ± 0.0000421	0.000960 ± 0.0000426	0.00112 ± 0.0000244	0.00138 ± 0.0000175
Catechin	0.149 ± 0.00792	0.151 ± 0.00290	0.136 ± 0.000728	0.171 ± 0.00345	0.128 ± 0.000745	0.138 ± 0.00356
p-coumaric acid	0.0168 ± 0.000618	0.0367 ± 0.000668	0.0184 ± 0.00157	0.00965 ± 0.000483	0.00253 ± 0.0000509	0.00608 ± 0.000166
3,4-Dihydroxybenzoic acid	0.0451 ± 0.00205	0.0336 ± 0.000931	0.0213 ± 0.0000313	0.0426 ± 0.000502	0.0253 ± 0.000196	0.0224 ± 0.000717
Ferulic acid	0.0213 ± 0.000874	0.0132 ± 0.000125	0.0114 ± 0.000356	0.00985 ± 0.000324	0.0108 ± 0.000258	0.0135 ± 0.000696
Gallic acid	0.000800 ± 0.000000848	0.00132 ± 0.00000275	0.000990 ± 0.0000199	0.000790 ± 0.00000782	0.00104 ± 0.0000224	0.000830 ± 0.0000470
Gallocatechin	<LOD	ND	ND	<LOD	ND	ND
Kaempferol	0.0140 ± 0.000405	0.00735 ± 0.000225	0.00459 ± 0.000230	0.00446 ± 0.000109	0.00443 ± 0.000218	0.00364 ± 0.000287
Isorhamnetin	0.00174 ± 0.0000188	0.00117 ± 0.00000559	0.000580 ± 0.0000244	0.000750 ± 0.0000368	0.00103 ± 0.00000534	0.000390 ± 0.0000143
Myricetin	0.0214 ± 0.000551	0.0207 ± 0.000426	0.0182 ± 0.000520	0.0199 ± 0.000450	0.0190 ± 0.000765	0.0191 ± 0.0000426
Naringenin	<LOD	<LOD	0.000840 ± 0.0000146	0.000620 ± 0.0000125	<LOD	<LOD
Piceol	ND	0.00679 ± 0.0000645	0.00603 ± 0.000198	ND	ND	0.00643 ± 0.0000139
Protocatecuic aldehyde	0.00458 ± 0.0000330	0.00181 ± 0.0000217	0.00149 ± 0.000145	0.00170 ± 0.00000707	0.00208 ± 0.00000532	0.00295 ± 0.0000287
Pungenol	<LOD	ND	ND	<LOD	ND	ND
Quercetin	0.0203 ± 0.000988	0.0224 ± 0.000539	0.00385 ± 0.000229	0.00387 ± 0.000338	0.00604 ± 0.000312	0.00340 ± 0.000198
Taxifolin	0.0167 ± 0.000571	0.0175 ± 0.00131	0.0163 ± 0.0000899	0.0166 ± 0.0000311	0.0166 ± 0.000184	0.0170 ± 0.000182
Vanillic acid	0.00630 ± 0.000199	0.00742 ± 0.000400	<LOD	0.00965 ± 0.000875	0.0184 ± 0.000847	0.00485 ± 0.000415
Vanillin	0.0294 ± 0.00151	0.0277 ± 0.00173	0.0252 ± 0.000297	0.0279 ± 0.00224	0.0281 ± 0.00200	0.0290 ± 0.000519

Abbreviations: ND – not detected; <LOD – below limit of detection.

Table S7. Pesticides quantified in select cannabis cultivars.

Pesticide (ppm)	Cultivar					
	Alien Dawg	Tangerine Dream	Sensi Star	Quadra	Gabriola	Island Honey
Acephate	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Acetomiprid	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Aldicarb	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Allethrin	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	0.0285 (± 0.0055)
Azoxystrobin	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Benzovindiflupyr	0.0349 (± 0.0078)	0.0059 (± 0.0001)	< LOQ	0.0099 (± 0.0003)	< LOQ	0.0057 (± 0.0019)
Bifenazate	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Boscalid	0.0033 (± 0.0023)	< LOQ	0.0166 (± 0.0011)	0.0058 (± 0.0005)	< LOQ	< LOQ
Buprofezin	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Carbaryl	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Carbofuran	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Chlorantraniliprole	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Chlorpyrifos	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Clofentezine	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Clothianidin	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Coumaphos	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Cyantraniliprole	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Cyprodinil	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Diazinon	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Dichlorvos	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Dimethoate	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Dinotefuran	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Dodemorph	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Ethoprophos	< LOQ	< LOQ	0.0032 (± 0.0002)	< LOQ	< LOQ	< LOQ
Etofenprox	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Etoxazole	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Fenoxycarb	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Fenpyroximate	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Fensulfothion	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	0.1365 (± 0.0109)
Fenthion	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Flonicamid	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Fluopyram	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Hexythiazox	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Imazalil	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Imidacloprid	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Jasmolin	0.0359 (± 0.0146)	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Kresoxim-Methyl	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Malathion	< LOQ	< LOQ	< LOQ	< LOQ	0.002	< LOQ

Metalaxyl	0.025 (± 0.0064)	0.0047 (± 0.0016)	< LOQ	< LOQ	< LOQ	0.0112 (± 0.003)
Methiocarb	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Methoprene	2.9 (± 0.2263)	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Mevinphos	0.0027 (± 0.00004)	< LOQ	0.0126 (± 0.0031)	< LOQ	0.0045 (± 0.0014)	< LOQ
MGK-264	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Myclobutanil	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Naled	< LOQ	0.0039 (± 0.0015)	< LOQ	< LOQ	< LOQ	< LOQ
Novaluron	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Oxamyl	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Paclobutrazol	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Phenothrin	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Phosmet	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Pirimicarb	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Prallethrin	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Propoxur	< LOQ	< LOQ	< LOQ	< LOQ	0.0126 (± 0.0014)	0.0061 (± 0.0016)
Pyraclostrobin	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Pyrethrins	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Pyridaben	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Spinetoram	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Spinosad A	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Spinosad B	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Spiridiclofen	< LOQ	< LOQ	< LOQ	0.261 (± 0.0495)	< LOQ	< LOQ
Spiromesifen	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Spiroxamine	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Tebuconazole	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Tebufenozide	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Teflubenzuron	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Tetrachlorvinphos	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	0.021 (± 0.0127)
Tetramethrin	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Thiacloprid	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Thiametoxam	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Thiophanate-methyl	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ
Trifloxystrobin	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ	< LOQ

Table S8. Common plant metabolites detected in cannabis cultivars using TMIC Plant Prime assay.

Metabolites	Cannabis Cultivars (mg/g dry weight)					
	Alien Dawg	**Tangerine Dream**	**Sensi Star**	**Quadra**	**Gabriola**	**Island Honey**
Glycine	0.137 ± 0.00300	0.0849 ± 0.00367	0.104 ± 0.00482	0.177 ± 0.000290	0.0932 ± 0.00178	0.0520 ± 0.00116
Alanine	0.284 ± 0.0160	0.432 ± 0.0135	0.452 ± 0.00113	0.315 ± 0.00555	0.337 ± 0.00387	0.462 ± 0.00916
Serine	0.637 ± 0.0152	0.588 ± 0.00552	0.386 ± 0.00957	0.404 ± 0.0116	0.372 ± 0.00558	0.511 ± 0.00202
Histamine	0.000600 ± 0.0000618	0.000300 ± 0.0000183	0.000200 ± 0.0000101	0.000006 ± 0.00000756	0.000300 ± 0.00000083	0.000900 ± 0.00000429
Proline	1.13 ± 0.00510	1.04 ± 0.0283	0.604 ± 0.0370	0.316 ± 0.00167	0.345 ± 0.000272	2.73 ± 0.104
Valine	0.537 ± 0.00197	0.172 ± 0.00684	0.198 ± 0.00368	0.439 ± 0.0105	0.334 ± 0.00661	0.422 ± 0.0184
Threonine	0.281 ± 0.00987	0.175 ± 0.00207	0.129 ± 0.000501	0.240 ± 0.0115	0.241 ± 0.0190	0.201 ± 0.00235
Phenylethylamine	0.000100 ± 0.00000169	0.000100 ± 0.00000175	0	0.000200 ± 0.00000868	0.000700 ± 0.0000153	0.000100 ± 0.000000142
Taurine	0.00290 ± 0.0000508	0.000500 ± 0.00000221	0.00370 ± 0.000163	0.00470 ± 0.0000103	0.00120 ± 0.0000671	0.00200 ± 0.000117
Putrescine	0.00170 ± 0.00000466	0.00120 ± 0.0000223	0.00100 ± 0.0000113	0.000900 ± 0.0000201	0.000900 ± 0.0000272	0.000900 ± 0.0000428
trans-Hydroxyproline	0.00220 ± 0.0000378	0.00380 ± 0.000153	0.00300 ± 0.000203	0.00330 ± 0.000171	0.00340 ± 0.000181	0.00440 ± 0.0000385
Leucine	0.303 ± 0.000171	0.165 ± 0.000203	0.0575 ± 0.00233	0.184 ± 0.000271	0.159 ± 0.000148	0.207 ± 0.00343
Isoleucine	0.416 ± 0.00936	0.120 ± 0.00545	0.0613 ± 0.00154	0.331 ± 0.00168	0.191 ± 0.00332	0.429 ± 0.00274
Asparagine	36.3 ± 0.694	13.2 ± 0.747	27.0 ± 0.926	13.5 ± 0.317	16.4 ± 0.280	16.9 ± 0.0541
Aspartic acid	1.45 ± 0.00487	0.675 ± 0.0756	1.61 ± 0.114	0.391 ± 0.0166	1.28 ± 0.0432	0.827 ± 0.0102
Glutamine	2.16 ± 0.00358	5.35 ± 0.0326	2.24 ± 0.0296	0.631 ± 0.0172	4.87 ± 0.140	4.31 ± 0.00927
Glutamic acid	0.516 ± 0.00816	0.259 ± 0.0124	0.223 ± 0.00127	0.552 ± 0.00783	0.521 ± 0.0157	0.225 ± 0.00897
Methionine	0.00740 ± 0.000470	0.0138 ± 0.000654	0.00800 ± 0.000503	0.0117 ± 0.000716	0.00960 ± 0.000283	0.0124 ± 0.000588
Histidine	0.673 ± 0.0321	0.299 ± 0.00572	0.526 ± 0.00831	0.382 ± 0.00916	0.875 ± 0.0220	1.02 ± 0.00393
alpha-Aminoadipic acid	0.103 ± 0.00190	0.0377 ± 0.000550	0.111 ± 0.00277	0.0301 ± 0.00153	0.0522 ± 0.00118	0.0933 ± 0.000190
Phenylalanine	0.307 ± 0.0164	0.0507 ± 0.000458	0.143 ± 0.00894	0.208 ± 0.00570	0.335 ± 0.00108	0.150 ± 0.00214
Methionine-sulfoxide	0.00630 ± 0.000454	0.0175 ± 0.000814	0.00750 ± 0.0000149	0.0296 ± 0.00320	0.0540 ± 0.00399	0.0172 ± 0.000330
Arginine	7.91 ± 0.0564	4.65 ± 0.00977	3.47 ± 0.101	4.58 ± 0.0182	4.77 ± 0.00468	6.11 ± 0.0801
Acetyl-ornithine	0.0230 ± 0.00155	0.0109 ± 0.000775	0.0119 ± 0.000105	0.0174 ± 0.000572	0.0148 ± 0.000277	0.0222 ± 0.000668
Citrulline	0.0731 ± 0.00222	0.0583 ± 0.00126	0.0237 ± 0.00118	0.0297 ± 0.00171	0.0657 ± 0.00606	0.0557 ± 0.000735
Tyrosine	0.108 ± 0.00129	0.0532 ± 0.00107	0.0678 ± 0.000303	0.0756 ± 0.00166	0.0587 ± 0.00313	0.0544 ± 0.00259

Asymmetric dimethylarginine	0.00690 ± 0.000218	0.000300 ± 0.00000957	0.00370 ± 0.000217	0.00220 ± 0.0000926	0.00250 ± 0.000153	0.00370 ± 0.0000944
Total dimethylarginine	0.0105 ± 0.000267	0.00540 ± 0.0000880	0.00770 ± 0.000144	0.00680 ± 0.000177	0.00600 ± 0.0000461	0.00630 ± 0.00017
Tryptophan	0.396 ± 0.0166	0.166 ± 0.00452	0.210 ± 0.00347	0.245 ± 0.00165	0.846 ± 0.0402	0.400 ± 0.0177
Kynurenine	0.00170 ± 0.0000320	0.000500 ± 0.0000141	0.000400 ± 0.00000306	0.000400 ± 0.0000168	0.000500 ± 0.00000164	0.00160 ± 0.0000872
Ornithine	0.0936 ± 0.00174	0.0374 ± 0.000278	0.00590 ± 0.000251	0.0155 ± 0.000377	0.0107 ± 0.000159	0.0351 ± 0.00240
Lysine	0.413 ± 0.00896	0.203 ± 0.00401	0.0993 ± 0.00233	0.157 ± 0.0132	0.247 ± 0.0102	0.304 ± 0.00371
Spermidine	0.00150 ± 0.0000393	0.00210 ± 0.0000823	0.00140 ± 0.0000540	0.00460 ± 0.000238	0.00120 ± 0.0000544	0.00810 ± 0.000647
Spermine	0.000900 ± 0.0000266	0.000800 ± 0.0000209	0.00100 ± 0.0000226	0.000200 ± 0.000000704	0.000300 ± 0.00000543	0.00150 ± 0.0000513
Tyramine	0.0124 ± 0.000401	0.0407 ± 0.00158	0.00790 ± 0.000172	0.00880 ± 0.000994	0.00360 ± 0.000414	0.00730 ± 0.000476
Creatine	0.00350 ± 0.000117	0.00430 ± 0.0000628	0.00300 ± 0.000225	0.00190 ± 0.0000709	0.00200 ± 0.0000466	0.00190 ± 0.0000975
Betaine	0.0168 ± 0.000349	0.0104 ± 0.00000731	0.00950 ± 0.000494	0.00900 ± 0.000677	0.00750 ± 0.000509	0.0165 ± 0.000695
Choline	1.42 ± 0.0710	1.08 ± 0.000802	0.931 ± 0.0424	1.01 ± 0.0256	0.853 ± 0.0137	1.13 ± 0.0511
Trimethylamine N-oxide	0.00320 ± 0.0000474	0.00370 ± 0.0000681	0.00300 ± 0.00000244	0.00280 ± 0.0000459	0.00280 ± 0.000128	0.00290 ± 0.000151
Methylhistidine	0.00430 ± 0.0000856	0.00220 ± 0.0000422	0.00460 ± 0.0000414	0.00410 ± 0.000171	0.00400 ± 0.000106	0.00760 ± 0.000420
Shikimic acid	0.00170 ± 0.0000590	0.00170 ± 0.00000597	0.00210 ± 0.0000355	0.00100 ± 0.0000483	0.00140 ± 0.0000114	0.00140 ± 0.0000846
Glyceric acid	0.158 ± 0.00370	0.243 ± 0.0168	0.314 ± 0.0377	0.246 ± 0.00270	0.0624 ± 0.00172	0.199 ± 0.00261
beta-Hydroxybutyric acid	0.00520 ± 0.000145	0.00900 ± 0.000344	0.00820 ± 0.000287	0.00920 ± 0.000480	0.00680 ± 0.000313	0.00470 ± 0.000275
Lactic acid	0.0221 ± 0.00120	0.0443 ± 0.000735	0.0132 ± 0.00106	0.0182 ± 0.00151	0.00990 ± 0.000691	0.0400 ± 0.00326
HPHPA	0.000100 ± 0.00000225	0.000100 ± 0.00000542	0.000100 ± 0.00000747	0.000100 ± 0.00000864	0.000100 ± 0.00000938	0.000100 ± 0.0000197
Homovanillic acid	0.000100 ± 0.00000276	0.000200 ± 0.00000390	0.000300 ± 0.00000227	0.000100 ± 0.00000752	0.000700 ± 0.0000462	0.00130 ± 0.0000767
Propionic acid	0.00930 ± 0.000365	0.00250 ± 0.0000160	0.0238 ± 0.00197	0.0182 ± 0.00166	0.0188 ± 0.00297	0.0195 ± 0.000645
p-Hydroxyphenylacetic acid	0.00180 ± 0.0000763	0.00130 ± 0.0000189	0.00130 ± 0.0000404	0.00200 ± 0.000178	0.00240 ± 0.0000581	0.00280 ± 0.000168
Malic acid	0.716 ± 0.00656	0.475 ± 0.00309	0.921 ± 0.00254	0.216 ± 0.0108	0.288 ± 0.032	0.583 ± 0.0391
Butyric acid	0.0211 ± 0.00172	0.0362 ± 0.00409	0.0263 ± 0.000618	0.00560 ± 0.000218	0.0121 ± 0.0000626	0.0160 ± 0.000558
Hippuric acid	0.00320 ± 0.000105	0.000500 ± 0.0000215	0.00100 ± 0.0000142	0.00120 ± 0.0000940	0.00110 ± 0.000128	0.00100 ± 0.0000481

Succinic acid	0.0337 ± 0.000775	0.0289 ± 0.0000902	0.0616 ± 0.00312	0.0291 ± 0.00160	0.0383 ± 0.00131	0.0379 ± 0.00265
Glutaric acid	0.0314 ± 0.000681	0.0279 ± 0.000274	0.0655 ± 0.00282	0.0346 ± 0.00526	0.0190 ± 0.00145	0.0785 ± 0.00539
Methylmalonic acid	0.000300 ± 0.00000816	0.000200 ± 0.00000182	0.000300 ± 0.00000690	0.000300 ± 0.0000240	0.000300 ± 0.0000306	0.000200 ± 0.00000292
Fumaric acid	0.0222 ± 0.00109	0.0142 ± 0.000285	0.0745 ± 0.000122	0.00700 ± 0.000938	0.0121 ± 0.000869	0.0209 ± 0.000978
Benzoic acid	0.0456 ± 0.000362	0.0225 ± 0.000783	0.0943 ± 0.00280	0.0718 ± 0.00147	0.0861 ± 0.00334	0.0436 ± 0.000872
Oxalic acid	0.196 ± 0.000122	0.0242 ± 0.000109	1.43 ± 0.0366	0.0181 ± 0.000847	0.0162 ± 0.000930	0.0332 ± 0.000677
Salicylic acid	0.0231 ± 0.00107	0.00850 ± 0.000239	0.0104 ± 0.0000591	0.0214 ± 0.000749	0.0236 ± 0.000913	0.0103 ± 0.000375
Citric acid	6.76 ± 0.183	4.05 ± 0.0286	11.4 ± 0.0886	1.98 ± 0.0613	4.42 ± 0.0247	6.28 ± 0.151
Abscisic acid	0.00270 ± 0.0000286	0.000600 ± 0.00000768	0.00260 ± 0.0000426	0.000700 ± 0.0000167	0.00180 ± 0.0000178	0.000700 ± 0.0000347
Aconitic acid	0.919 ± 0.0234	0.289 ± 0.0151	1.14 ± 0.0971	0.121 ± 0.00180	0.257 ± 0.00694	0.508 ± 0.00452
Jasmonic acid	0.0112 ± 0.0000738	0.00990 ± 0.000148	0.0202 ± 0.000158	0.00940 ± 0.000151	0.00880 ± 0.000305	0.0266 ± 0.00140
Pyruvic acid	0.00180 ± 0.0000229	0.00270 ± 0.0000135	0.00340 ± 0.000140	0.00240 ± 0.0000694	0.00240 ± 0.0000576	0.00260 ± 0.0000666
alpha-Ketoglutaric acid	0.00130 ± 0.0000176	0.00360 ± 0.0000418	0.00250 ± 0.0000227	0.000500 ± 0.000000750	0.00130 ± 0.000117	0.00190 ± 0.0000608
Uric acid	0.0218 ± 0.000286	0.0149 ± 0.000794	0.0110 ± 0.000395	0.0195 ± 0.00137	0.0240 ± 0.000547	0.0299 ± 0.00127
Glucose	0.973 ± 0.0445	22.6 ± 0.0659	4.03 ± 0.0146	2.57 ± 0.0459	4.39 ± 0.122	15.1 ± 1.33
LysoPC a C16:0	0.00390 ± 0.000154	0.00600 ± 0.000332	0.00520 ± 0.0000441	0.00560 ± 0.000578	0.00940 ± 0.00114	0.00640 ± 0.000746
LysoPC a C18:2	0.00470 ± 0.000129	0.00600 ± 0.000112	0.0136 ± 0.000680	0.00470 ± 0.000205	0.0112 ± 0.000314	0.00550 ± 0.000308
LysoPC a C18:1	0.00120 ± 0.0000316	0.00190 ± 0.00000694	0.00220 ± 0.000187	0.00240 ± 0.000175	0.00160 ± 0.0000877	0.00110 ± 0.0000578
PC aa C36:6	0.000900 ± 0.0000457	0.00150 ± 0.0000347	0.00170 ± 0.0000311	0.00160 ± 0.0000442	0.00140 ± 0.0000336	0.00170 ± 0.0000916
PC aa C36:0	0.000400 ± 0.0000209	0.000600 ± 0.0000144	0.000300 ± 0.00000501	0.000400 ± 0.0000366	0.000600 ± 0.0000262	0.000400 ± 0.00000476
Carnitine	0.00560 ± 0.000108	0.00370 ± 0.0000111	0.00210 ± 0.0000146	0.00590 ± 0.0000561	0.00370 ± 0.0000466	0.00550 ± 0.0000583

Table S9. Trace elemental analysis using ICP-MS.

Metal ion (mg/g)	Cultivar					
	Alien Dawg	**Tangerine Dream**	**Sensi Star**	**Quadra**	**Gabriola**	**Island Honey**
Boron (B)	0.040 ± 0.003	0.031 ± 0.004	0.027 ± 0.003	0.028 ± 0.004	0.032 ± 0.003	0.032 ± 0.004
Magnesium (Mg)	5.44 ± 0.03	4.01 ± 0.02	3.84 ± 0.05	4.16 ± 0.05	4.05 ± 0.02	6.62 ± 0.03
Phosphorous (P)	11.4 ± 0.9	7.69 ± 0.15	7.95 ± 0.34	9.88 ± 0.24	10.4 ± 0.2	10.6 ± 0.3
Potassium (K)	46.9 ± 0.4	29.9 ± 0.5	44.7 ± 0.3	36.9 ± 0.6	44.4 ± 0.3	41.7 ± 0.4
Calcium (Ca)	15.6 ± 0.3	9.24 ± 0.16	2.80 ± 0.25	6.74 ± 0.34	8.60 ± 0.26	14.9 ± 0.3
Titanium (Ti)	0.0016 ± 0.0005	0.0011 ± 0.0004	0.0011 ± 0.0003	0.0011 ± 0.0004	0.0013 ± 0.0003	0.0011 ± 0.0004
Manganese (Mn)	0.160 ± 0.002	0.160 ± 0.005	0.080 ± 0.004	0.089 ± 0.005	0.135 ± 0.003	0.124 ± 0.007
Iron (Fe)	0.195 ± 0.005	0.087 ± 0.006	0.098 ± 0.007	0.216 ± 0.003	0.297 ± 0.006	0.198 ± 0.004
Copper (Cu)	0.0025 ± 0.0004	0.0019 ± 0.0005	0.0061 ± 0.0004	0.0139 ± 0.0031	0.0146 ± 0.0023	0.0085 ± 0.0007
Zinc (Zn)	0.0329 ± 0.0012	0.0478 ± 0.0009	0.0369 ± 0.0010	0.077 ± 0.005	0.132 ± 0.007	0.093 ± 0.005
Rubidium (Rb)	0.0108 ± 0.0021	0.0085 ± 0.0009	0.0071 ± 0.0005	0.0119 ± 0.0006	0.0064 ± 0.0009	0.0149 ± 0.0010
Strontium (Sr)	0.087 ± 0.011	0.059 ± 0.009	0.014 ± 0.002	0.064 ± 0.005	0.139 ± 0.012	0.207 ± 0.015
Molybdenum (Mo)	0.00088 ± 0.005	0.0066 ± 0.0007	0.0064 ± 0.0005	0.0012 ± 0.0008	0.0019 ± 0.0007	0.0030 ± 0.0006
Cesium (Cs)	<LOQ	<LOQ	<LOQ	<LOQ	ND	0.00004 ± 0.00001
Barium (Ba)	0.0048 ± 0.0009	<LOQ	0.0010 ± 0.0002	0.0016 ± 0.0002	0.0039 ± 0.0002	0.0066 ± 0.0005
Thallium (Tl)	0.00001 ± 0.000009	0.000003 ± 0.000001	0.000002 ± 0.000001	0.000004 ± 0.000001	0.000003 ± 0.000001	0.000009 ±0.000001

Table S10. Validation data for the targeted GC-MS assay for selected terpenoids.

Terpenoid	Validation Parameter			
	LOD (µg/mL)	LOQ (µg/mL)	Accuracy (%)	Precision (%)
Camphene	0.26	0.78	104	2.49
beta-Myrcene	0.68	2.05	98	0.99
alpha-Phellandrene	0.28	0.84	82	1.34
3-Carene	0.25	0.75	97	1.05
Eucalyptol	0.39	1.18	101	2.84
E-beta-Ocimene	0.78	2.37	92	1.05
cis-beta-Ocimene	1.58	4.78	88	11.62
Fenchone	0.26	0.8	107	1.72
Linalool	3.9	11.81	88	8.5
Camphor	0.47	1.42	97	1.02
(-)-Isopulegol	4.09	12.39	90	1.97
Camphene	0.26	0.78	104	2.49
beta-Myrcene	0.68	2.05	98	0.99
alpha-Phellandrene	0.28	0.84	82	1.34
3-Carene	0.25	0.75	97	1.05
Eucalyptol	0.39	1.18	101	2.84

Table S11. Validation data for the LC-MS/MS assay for cannabinoids.

Cannabinoid	Validation Parameter			
	LOD (ng/mL)	LOQ (ng/mL)	Accuracy (%)	Precision (%)
CBC	0.00278	0.00927	105	0.891
CBD	0.00125	0.00417	102	7.97
CBDA	0.00213	0.00710	92.9	1.26
CBDV	0.00176	0.00587	96.0	3.45
CBDVA	0.00115	0.00383	94.8	2.74
CBG	0.00100	0.00333	92.6	5.43
CBGA	0.00223	0.00743	94.3	3.91
CBL	0.00100	0.00333	94.7	1.68
CBLA+CBCA	0.00426	0.0142	102	7.37
CBN	0.00134	0.00447	93.2	6.93
CBNA	0.00357	0.0119	96.6	2.95
THC	0.00144	0.00480	91.3	5.89
THCA	0.00208	0.00693	93.4	3.00
THC-COOH	0.00100	0.00333	95.0	2.92
THCV	0.00283	0.00943	96.0	2.97

Table S12. Validation data for the LC-MS/MS assay for polyphenols and phenolic acids.

Polyphenol	Validation Parameter			
	LOD (µM)	LOQ (µM)	Accuracy (%)	Precision (%)
Apigenin	0.00142	0.00473	107	4.44
Gallic acid	0.0866	0.28867	98.4	3.12
p-Coumaric acid	0.599	1.99667	122	1.78
Protocatechuic aldehyde	0.119	0.39667	109	4.93
Caffeic acid	0.108	0.36	109	3.31
Quercetin	0.684	2.28	111	1.40
Piceol	0.198	0.66	108	3.24
Vanillic acid	0.81	2.7	118	12.6
Gallocatechin	1.11	3.7	120	2.09
Pungenol	1.54	5.13333	99.8	7.44
Ferulic acid	0.512	1.70667	113	0.797
3,4-Dihydrobenzoic acid	3.17	10.5667	87.8	5.10
Vanillin	1.14	3.8	110	3.29
Catechin	4.86	16.2	89.0	3.29

Table S13. Validation data for the LC-MS/MS assay for pesticides.

Pesticide	Validation Parameter			
	Mandatory Testing Limits LOQ (ppm)	Method LOQ (ppm)	Accuracy (%)	Precision (%)
Acephate	0.02	0.01	95.1139	9.8793
Acetomiprid	0.1	0.01	100.3861	10.0521
Aldicarb	1.0	0.01	87.4785	3.7203
Allethrin	0.2	0.02	96.9399	9.6752
Azoxystrobin	0.02	0.01	90.3565	11.4346
Benzovindiflupyr	0.02	0.002	112.0645	12.3517
Bifenazate	0.02	0.01	109.9349	7.7376
Boscalid	0.02	0.002	89.5125	12.8118
Buprofezin	0.02	0.002	94.3475	11.3523
Carbaryl	0.05	0.002	89.1919	1.9271
Carbofuran	0.02	0.01	99.1317	0.6727
Chlorantraniliprole	0.02	0.002	106.7826	12.0125
Chlorpyrifos	0.04	0.01	105.4168	0.7387
Clofentezine	0.02	0.002	110.7223	11.5656
Clothianidin	0.05	0.01	105.8724	4.2674
Coumaphos	0.02	0.002	106.0628	13.7407
Cyantraniliprole	0.02	0.002	94.6362	5.0202
Cyprodinil	0.25	0.002	111.0254	2.3069
Diazinon	0.02	0.01	89.5809	11.4693
Dichlorvos	0.1	0.05	86.4422	10.7398
Dimethoate	0.02	0.01	95.3876	7.8982
Dinotefuran	0.1	0.02	111.3919	9.3833
Dodemorph	0.05	0.02	99.4976	3.5727
Ethoprophos	0.02	0.002	86.3213	4.8031
Etofenprox	0.05	0.002	89.2605	13.3854
Etoxazole	0.02	0.002	101.1975	11.8025

Fenoxycarb	0.02	0.002	96.6048	6.6407
Fenpyroximate	0.02	0.01	108.7202	2.6309
Fensulfothion	0.02	0.02	99.0175	11.5267
Fenthion	0.02	0.05	90.0848	13.9963
Flonicamid	0.05	0.002	92.3141	11.7838
Fluopyram	0.02	0.002	96.1215	2.9432
Hexythiazox	0.01	0.002	99.9175	8.9576
Imazalil	0.05	0.01	109.4439	3.3203
Imidacloprid	0.02	0.01	88.5515	8.0378
Jasmolin	-	0.002	87.2922	6.2919
Kresoxim-Methyl	0.02	0.02	112.0663	6.1074
Malathion	0.02	0.002	106.4088	12.8404
Metalaxyl	0.02	0.002	92.2817	4.3747
Methiocarb	0.02	0.002	101.9312	10.3135
Methoprene	2.000	0.1	86.8098	7.5552
Mevinphos	0.05	0.002	97.8242	14.4839
MGK-264	0.05	0.002	105.4348	6.0173
Myclobutanil	0.02	0.002	102.5578	10.8688
Naled	0.1	0.002	114.0733	11.9469
Novaluron	0.05	0.002	91.8589	7.0305
Oxamyl	3.0	0.01	97.4211	12.2655
Paclobutrazol	0.02	0.002	105.9366	12.3163
Phenothrin	0.05	0.05	104.4569	4.0355
Phosmet	0.02	0.002	91.3291	10.2884
Pirimicarb	0.02	0.002	104.8624	5.6584
Prallethrin	0.05	0.02	114.9826	1.6488
Propoxur	0.02	0.002	114.4835	4.6464
Pyraclostrobin	0.02	0.002	97.3278	4.0725
Pyrethrins	0.05	0.01	86.8619	1.6585
Pyridaben	0.05	0.01	107.3032	12.3557

Spinetoram	0.02	0.002	96.2958	7.9388
Spinosad A	0.1	0.002	107.8561	3.5409
Spinosad B	0.1	0.002	107.4508	6.6883
Spiridiclofen	0.25	0.2	107.0463	7.2558
Spiromesifin	3.0	0.02	99.6787	12.2009
Spiroxamine	0.1	0.002	108.2498	6.5045
Tebuconazole	0.05	0.01	87.0511	12.1581
Tebufenozide	0.02	0.002	113.6216	12.4449
Teflubenzuron	0.05	0.002	94.6232	6.2443
Tetrachlorvinphos	0.02	0.002	90.0878	7.1086
Tetramethrin	0.1	0.01	98.7663	0.2898
Thiacloprid	0.02	0.01	91.0345	12.7631
Thiametoxam	0.02	0.002	106.7528	2.6952
Thiophanate-methyl	0.05	0.01	109.6889	1.1942
Trifloxystrobin	0.02	0.002	102.4385	4.3888

Table S14. Validation data for the LC-MS/MS assay for metal ions.

Element	Validation Parameter			
	LOD (µM)	LOQ (µM)	Accuracy (%)	Precision (%)
Boron (B)	0.636	2.27	98	2.5
Magnesium (Mg)	0.104	0.417	102	2.1
Phosphorous (P)	4.84	16.1	97	3.2
Potassium (K)	2.56	10.3	101	3.5
Calcium (Ca)	0.568	1.14	98	2.8
Titanium (Ti)	0.0213	0.0532	99	4.1
Manganese (Mn)	0.00455	0.00909	102	2.7
Iron (Fe)	0.0358	0.179	97	3.7
Copper (Cu)	0.00315	0.0126	96	3.8
Zinc (Zn)	0.0153	0.0612	98	2.6
Rubidium (Rb)	0.000353	0.00118	101	3.9
Strontium (Sr)	0.000568	0.00284	98	4.2
Molybdenum (Mo)	0.00258	0.0103	97	2.7
Cesium (Cs)	0.000117	0.000376	96	3.2
Barium (Ba)	0.000365	0.00182	99	3.6

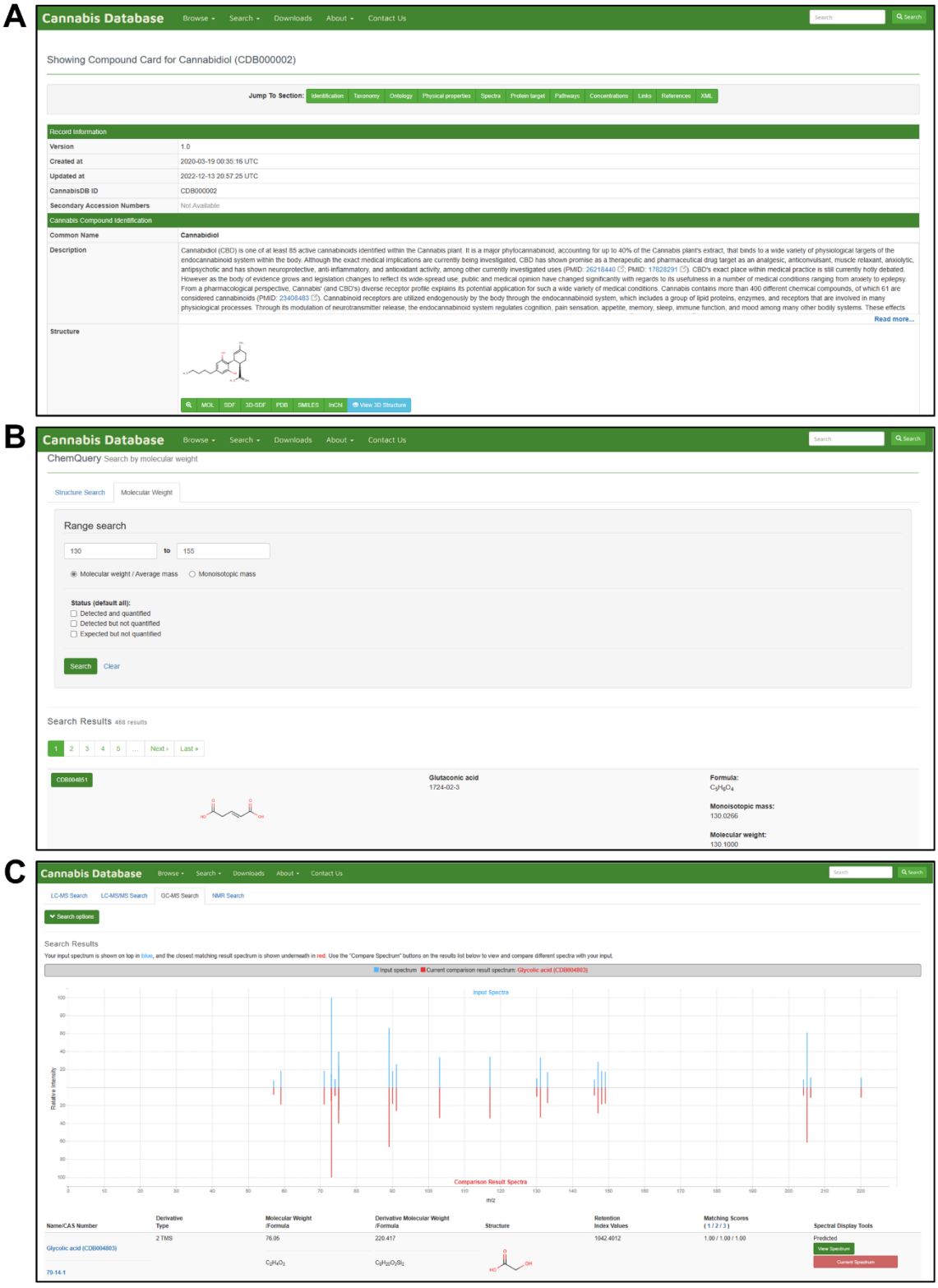

Figure S1. A screenshot montage showing A) the CCD MetaboCard for cannabidiol (CBD000002), B) the Search by molecular weight option with one of the results shown and C) the GC-MS Search option for glycolic acid (CDB004803).