

Supplementary information of

Secondary Metabolites Profiled in Cannabis Inflorescences, Leaves, Stem Barks, and Roots for Medicinal Purposes

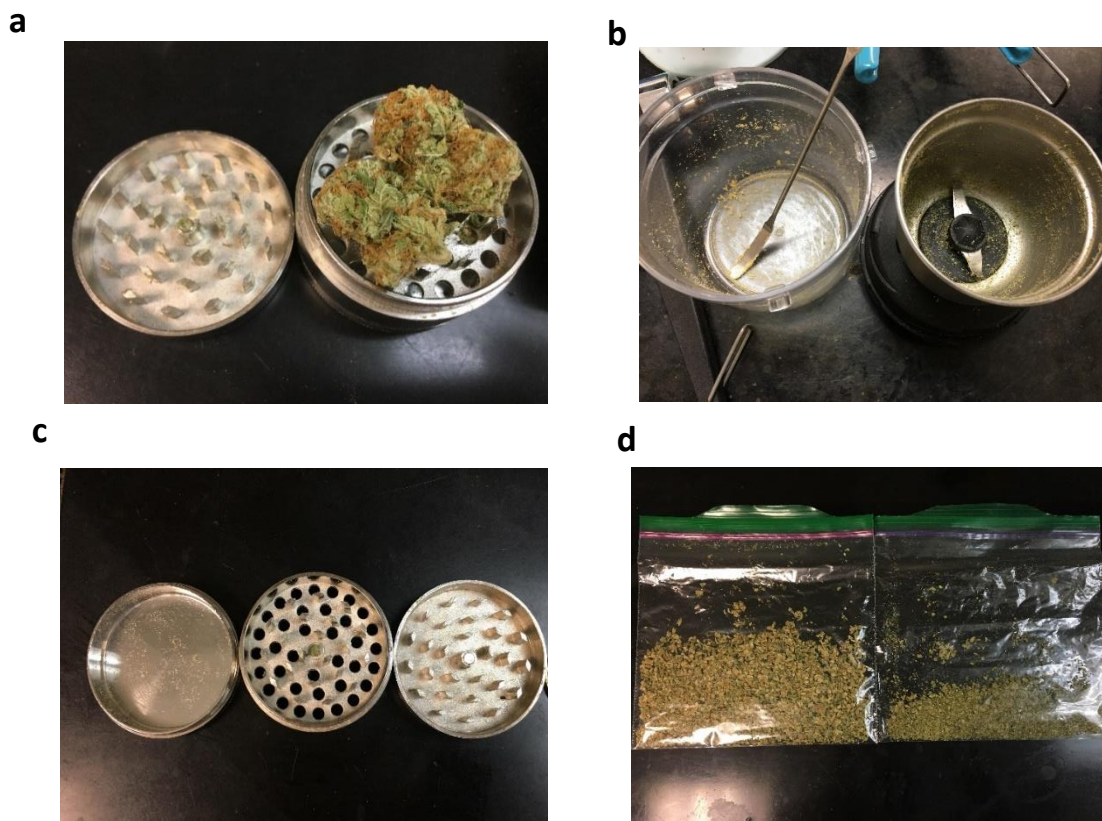
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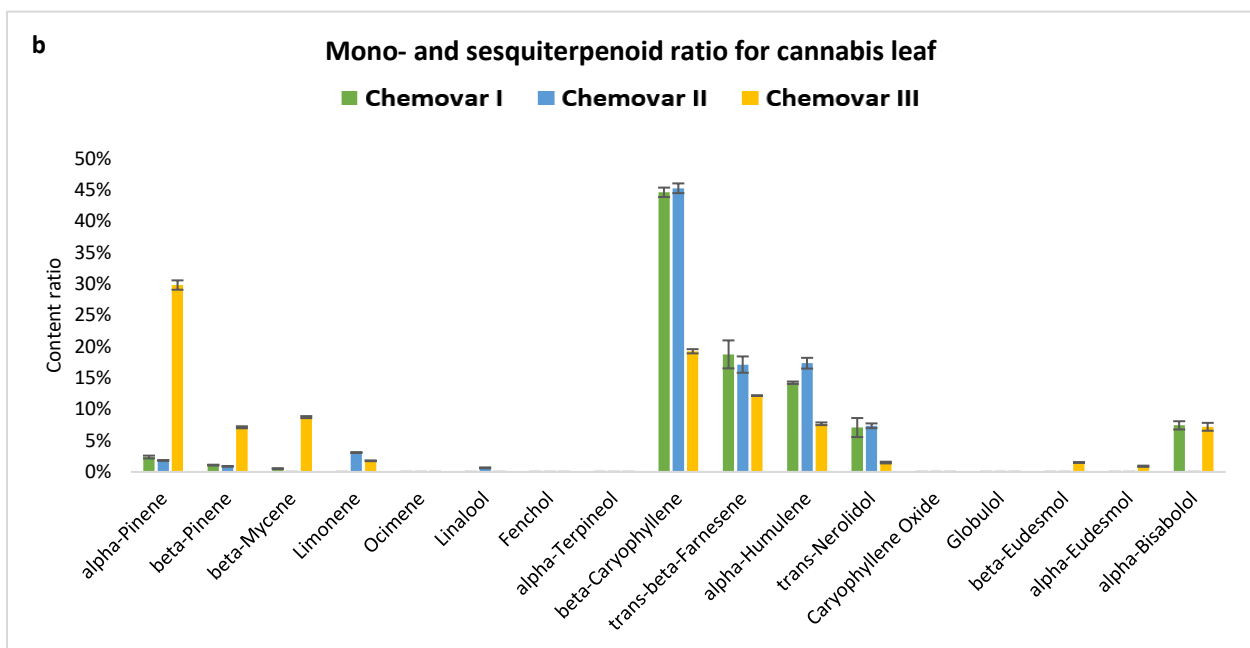
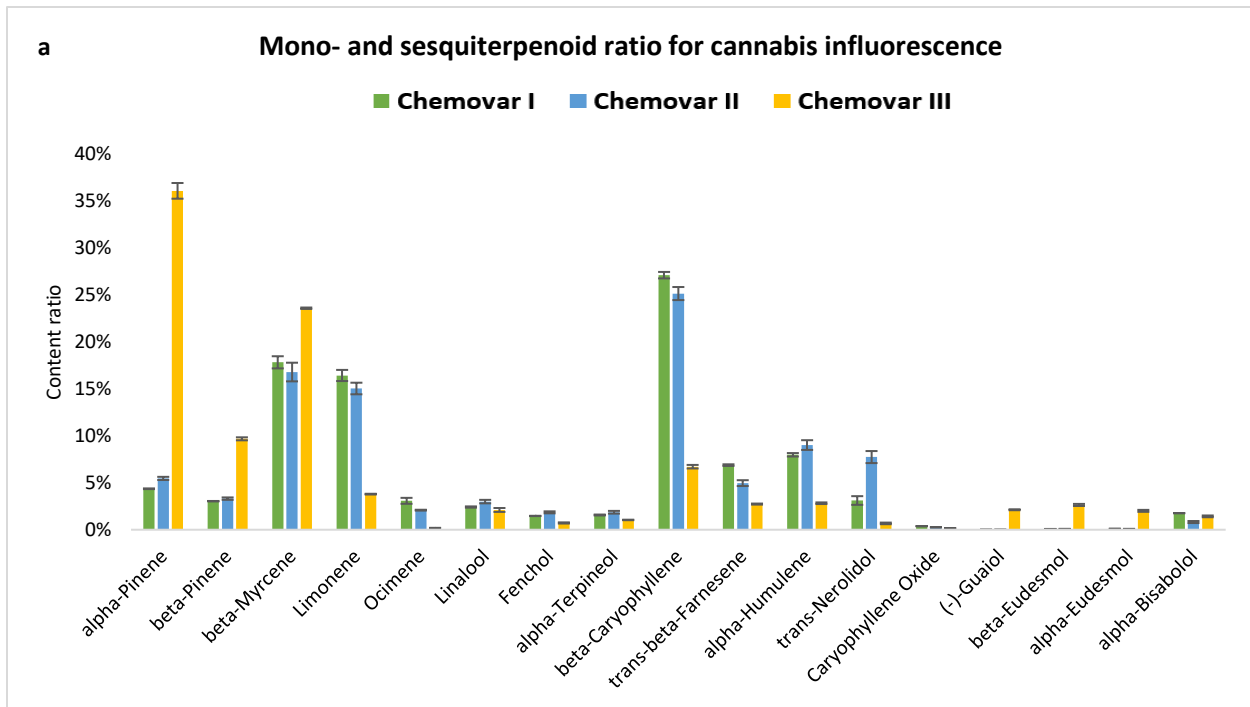
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Supplementary Figure 1. Pulverization of cannabis raw samples using **a.** manual grinder and **b.** electric blender. **c.** The inside of manual grinder is relatively clean without much resin left behind whereas there is a layer of resin stuck to the inside of the cup of the electric blender. **d.** The resultant particle size is larger using the manual grinder (left) than the electric blender (right).



Supplementary Figure 2. Mono- and sesquiterpenoid ratios in inflorescences and leaves in three strains. a. Mono- and sesquiterpenoid ratios in inflorescence. **b.** Mono- and sesquiterpenoid ratios in leaves. The absolute values and ratios of individual terpenoids were consistent when compared among three strains, although total terpenoid content was significantly different.

Supplementary Table 1. ANOVA regression statistics for cannabinoids.

	Quantification Range ($\mu\text{g/mL}$)	Correlation Coefficient R^2	Slope \pm SD	LOD ($\mu\text{g/mL}$)	LOQ ($\mu\text{g/mL}$)
1. CBDV	0.01-1.00	1.0000	1.3246 \pm 0.0031	0.001	0.003
2. CBDVA	0.01-1.00	1.0000	0.7432 \pm 0.0008	0.002	0.005
3. CBG	0.01-1.00	0.9998	0.8367 \pm 0.0053	0.002	0.005
4. CBD	0.01-1.00	1.0000	1.3841 \pm 0.0040	0.0005	0.001
5. CBDA	0.01-1.00	1.0000	0.7174 \pm 0.0004	0.001	0.003
6. THCV	0.01-1.00	1.0000	1.8763 \pm 0.0022	0.0004	0.001
7. CBGA	0.01-1.00	1.0000	0.6690 \pm 0.0015	0.003	0.008
8. CBN	0.01-1.00	0.9999	2.9331 \pm 0.0127	0.001	0.002
9. Δ^9 -THC	0.01-1.00	1.0000	1.8042 \pm 0.0024	0.001	0.003
10. Δ^8 -THC	0.01-1.00	1.0000	0.9145 \pm 0.0009	0.002	0.005
11. THCVA	0.01-1.00	0.9999	0.5474 \pm 0.0028	0.003	0.010
12. CBC	0.01-1.00	1.0000	0.6329 \pm 0.0018	0.002	0.007
13. THCA	0.01-1.00	1.0000	0.5700 \pm 0.0012	0.003	0.009
14. CBCA	0.01-1.00	0.9998	0.2333 \pm 0.0017	0.004	0.012

Supplementary Table 2. Trueness, precision, and accuracy for cannabinoids

Analyte	Spike 0.1 µg/mL				Spike 0.5 µg/mL				Spike 1.0 µg/mL			
	Repeatability	Intermediate precision	Trueness	Accuracy	Repeatability	Intermediate precision	Trueness	Accuracy	Repeatability	Intermediate precision	Trueness	Accuracy
	-	-	-	-	-	-	-	-	-	-	-	-
	Pooled RSD%	RSD%	Relative bias%	Uncertainty of measurement%	Pooled RSD%	RSD%	Relative bias%	Uncertainty of measurement%	Pooled RSD%	RSD%	Relative bias%	Uncertainty of measurement%
(n=3)	(n=9)	(n=9)	(n=9)	(n=3)	(n=9)	(n=9)	(n=9)	(n=3)	(n=9)	(n=9)	(n=9)	
1. CBDV	1.0	1.7	-4.0	4.3	1.0	4.8	-0.1	4.8	0.9	3.6	-2.6	4.4
2. CBDVA	1.7	1.5	0.2	1.5	0.8	4.6	-0.3	4.6	1.2	3.8	-2.7	4.7
3. CBG	3.0	12.3	0.9	12.3	6.5	6.1	2.1	6.4	4.0	7.7	-5.2	9.3
4. CBD	1.7	2.0	-4.8	5.2	0.7	4.9	-1.1	5.1	1.0	3.9	-3.1	5.0
5. CBDA	1.7	3.7	-4.2	5.6	1.3	4.7	-1.2	4.9	1.3	4.2	-3.4	5.4
6. THCV	1.5	2.3	-4.1	4.7	0.6	4.8	-1.0	4.9	1.0	4.0	-3.0	5.0
7. CBGA	3.8	3.5	-1.8	3.9	0.9	4.7	-1.2	4.9	0.9	3.7	-3.5	5.1
8. CBN	0.9	2.6	-6.4	6.9	0.6	5.5	-2.5	6.1	1.1	4.6	-4.2	6.2
9. Δ ⁹ -THC	1.9	2.6	-3.9	4.7	0.5	5.3	-1.3	5.5	1.3	4.2	-3.3	5.3
10. Δ ⁸ -THC	1.7	3.7	-4.8	6.0	0.4	5.4	-1.4	5.6	1.0	4.4	-3.9	5.9
11. THCVA	3.2	4.0	-4.8	6.2	0.7	4.7	-1.4	4.9	1.4	4.4	-4.0	5.9
12. CBC	1.9	3.7	-6.3	7.3	0.7	5.0	-1.2	5.2	1.1	4.7	-3.5	5.9
13. THCA	9.2	12.0	0.1	12.0	6.4	5.5	-1.2	5.6	1.2	5.0	-4.2	6.6
14. CBCA	8.5	8.8	6.9	11.2	1.8	4.7	0.0	4.7	0.9	3.7	-3.2	4.8

Supplementary Table 3. Matrix effect and extraction efficiency (recovery).

Analyte	Spike 0.1µg/mL		Spike 0.5µg/mL		Spike 1.0 µg/mL	
	Matrix effect ± SD	Extraction efficiency (recovery± SD)	Matrix effect ± SD	Extraction efficiency (recovery± SD)	Matrix effect ± SD	Extraction efficiency (recovery± SD)
1. CBDV	97.96 ± 0.38	94.41 ± 1.36	96.63 ± 1.40	94.52 ± 0.79	96.78 ± 0.45	99.62 ± 4.23
2. CBDVA	101.65 ± 0.18	87.96 ± 5.07	97.63 ± 1.32	87.29 ± 1.09	97.76 ± 0.32	90.05 ± 3.30
3. CBG	86.39 ± 0.73	98.97 ± 1.07	97.98 ± 0.66	94.42 ± 3.89	94.49 ± 0.10	80.04 ± 2.19
4. CBD	96.72 ± 1.88	95.68 ± 1.20	96.11 ± 0.23	94.04 ± 0.50	96.07 ± 0.51	94.26 ± 5.40
5. CBDA	98.47 ± 0.84	85.05 ± 3.56	96.40 ± 0.82	87.91 ± 1.20	96.58 ± 0.16	89.70 ± 3.26
6. THCV	96.89 ± 0.74	96.55 ± 1.14	96.07 ± 0.63	94.45 ± 0.17	96.04 ± 0.41	80.73 ± 2.19
7. CBGA	94.14 ± 5.08	83.96 ± 3.02	96.45 ± 0.74	86.44 ± 1.17	96.30 ± 0.34	89.99 ± 2.99
8. CBN	94.82 ± 1.78	95.71 ± 1.19	93.24 ± 0.42	93.73 ± 0.51	93.90 ± 0.39	77.21 ± 2.18
9. Δ ⁹ -THC	97.11 ± 1.19	100.44 ± 1.13	95.43 ± 0.57	95.45 ± 0.53	94.60 ± 0.58	89.28 ± 2.29
10. Δ ⁸ -THC	98.13 ± 0.66	97.50 ± 1.00	95.16 ± 0.31	94.73 ± 0.58	94.97 ± 0.65	89.17 ± 2.61
11. THCVA	98.55 ± 1.22	82.83 ± 3.95	96.75 ± 1.05	86.49 ± 0.79	95.28 ± 0.57	89.15 ± 3.04
12. CBC	96.94 ± 1.54	98.26 ± 1.32	95.42 ± 0.65	94.46 ± 0.80	94.73 ± 0.19	79.03 ± 1.54
13. THCA	100.02 ± 16.37	98.28 ± 9.88	96.53 ± 2.21	90.27 ± 1.27	93.03 ± 3.22	88.17 ± 3.00
14. CBCA	99.53 ± 0.33	94.30 ± 0.81	96.63 ± 1.40	89.41 ± 0.72	93.72 ± 0.60	82.94 ± 1.41

Supplementary Table 4. ANOVA regression statistics and LOD and LOQ for mono- and sesquiterpenoids.

		Quantification Range ($\mu\text{g/mL}$)	R ²	Slope \pm SD	LOD ($\mu\text{g/mL}$)	LOQ ($\mu\text{g/mL}$)
1.	α -Pinene	1 - 250	0.9993	0.0043 \pm 0.0001	0.022	0.065
2.	Camphene	1 - 250	0.9999	0.0093 \pm 0.0000	0.020	0.059
3.	Sabinene	1 - 250	0.9996	0.0154 \pm 0.0001	0.015	0.045
4.	β -Pinene	1 - 250	0.9994	0.0172 \pm 0.0002	0.018	0.054
5.	β -Myrcene	1 - 250	0.9998	0.0080 \pm 0.0000	0.014	0.042
6.	α -Phellandrene	1 - 250	0.9998	0.0161 \pm 0.0001	0.014	0.043
7.	Δ^3 -Carene	1 - 250	0.9996	0.0038 \pm 0.0000	0.015	0.044
8.	α -Terpinene	1 - 250	0.9997	0.0094 \pm 0.0001	0.013	0.038
9.	P-Cymene	1 - 250	0.9997	0.0249 \pm 0.0002	0.012	0.037
10.	Limonene	1 - 250	0.9999	0.0069 \pm 0.0000	0.029	0.088
11.	1,8-Cineole (Eucalyptol)	1 - 250	0.9991	0.0020 \pm 0.0000	0.009	0.026
12.	Ocimene	1 - 250	0.9998	0.0073 \pm 0.0000	0.015	0.044
13.	γ -Terpinene	1 - 250	1.0000	0.0146 \pm 0.0000	0.012	0.035
14.	Sabinene Hydrate	1 - 250	0.9997	0.0054 \pm 0.0000	0.016	0.049
15.	Terpinolene	1 - 250	0.9996	0.0081 \pm 0.0001	0.011	0.033
16.	Fenchone	1 - 250	0.9995	0.0194 \pm 0.0002	0.012	0.035
17.	Linalool	1 - 250	0.9996	0.0062 \pm 0.0001	0.046	0.137
18.	Fenchol	1 - 250	0.9999	0.0015 \pm 0.0000	0.012	0.035
19.	(-)-Isopulegol	1 - 250	1.0000	0.0023 \pm 0.0000	0.012	0.037
20.	Camphor	1 - 250	0.9996	0.0116 \pm 0.0001	0.010	0.029
21.	Borneol	1 - 250	0.9998	0.0036 \pm 0.0000	0.026	0.077
22.	Terpinen-4-ol	1 - 250	0.9994	0.0112 \pm 0.0001	0.016	0.047
23.	α -Terpineol	1 - 250	1.0000	0.0038 \pm 0.0000	0.012	0.035
24.	(+)-Dihydrocarvone	1 - 250	0.9999	0.0033 \pm 0.0000	0.012	0.037
25.	Nerol	1 - 250	0.9995	0.0111 \pm 0.0001	0.167	0.500
26.	Pulegone	1 - 250	0.9998	0.0037 \pm 0.0000	0.014	0.041
27.	(+)-Carvone	1 - 250	0.9999	0.0106 \pm 0.0000	0.024	0.072
28.	Geraniol	1 - 250	0.9991	0.0145 \pm 0.0002	0.125	0.375
29.	Geranyl Acetate	1 - 250	0.9996	0.0094 \pm 0.0001	0.022	0.065
30.	(-)- β -Elemene	1 - 250	0.9999	0.0016 \pm 0.0000	0.017	0.051
31.	β -Caryophyllene	1 - 250	0.9997	0.0021 \pm 0.0000	0.015	0.045
32.	Aromadendrene	1 - 250	0.9996	0.0020 \pm 0.0000	0.011	0.033
33.	trans- β -Farnesene	1 - 250	0.9992	0.0105 \pm 0.0001	0.019	0.056
34.	α -Humulene	1 - 250	0.9995	0.0104 \pm 0.0001	0.013	0.040
35.	Valencene	1 - 250	0.9996	0.0034 \pm 0.0000	0.014	0.041
36.	Ledene	1 - 250	0.9997	0.0014 \pm 0.0000	0.010	0.029
37.	Trans-Nerolidol	1 - 250	0.9995	0.0024 \pm 0.0000	0.017	0.051
38.	Caryophyllene Oxide	1 - 250	0.9997	0.0034 \pm 0.0000	0.031	0.093
39.	Globulol	1 - 250	0.9989	0.0017 \pm 0.0000	0.019	0.057
40.	Viridiflorol	1 - 250	0.9996	0.0020 \pm 0.0000	0.020	0.060
41.	(-)-Guaiol	1 - 250	0.9998	0.0043 \pm 0.0000	0.018	0.054
42.	(+)-Cedrol	1 - 250	0.9997	0.0029 \pm 0.0000	0.017	0.051
43.	β -Eudesmol	1 - 250	0.9997	0.0033 \pm 0.0000	0.028	0.083
44.	α -Bisabolol	1 - 250	0.9995	0.0007 \pm 0.0000	0.011	0.033

Supplementary Table 5. Trueness, precision, and accuracy for mono- and sesquiterpenoids.

Analyte	Spike 10 µg/mL				Spike 20 µg/mL				Spike 50 µg/mL			
	Repeatability	Intermediate	Trueness	Accuracy	Repeatability	Intermediate	Trueness	Accuracy	Repeatability	Intermediate	Trueness	Accuracy
	-	precision	-	-	-	precision	-	-	-	precision	-	-
	Pooled RSD%	RSD%	Relative	Uncertainty of	Pooled RSD%	RSD%	Relative	Uncertainty of	Pooled RSD%	RSD%	Relative	Uncertainty of
(n=3)	(n=9)	bias%	measurement%	(n=3)	(n=9)	bias%	measurement%	(n=3)	(n=9)	bias%	measurement%	
		(n=9)	(n=9)			(n=9)	(n=9)			(n=9)	(n=9)	
1. α-Pinene	1.5	4.1	-3.9	5.7	1.6	2.8	0.9	2.9	1.8	4.4	1.3	4.6
2. Camphene	1.3	2.0	-0.3	2.0	1.5	2.4	3.1	3.9	1.2	4.0	2.8	4.9
3. Sabinene	0.8	8.8	2.4	9.1	1.4	3.8	4.2	5.7	0.7	4.0	4.0	5.6
4. β-Pinene	0.9	7.2	0.7	7.2	1.4	3.0	4.0	5.0	1.0	4.2	3.8	5.7
5. β-Myrcene	0.7	6.5	4.2	7.7	1.2	3.3	6.9	7.6	0.8	2.8	5.7	6.3
6. α-Phellandrene	0.7	5.1	0.5	5.1	1.4	2.8	3.4	4.4	1.1	3.5	4.0	5.4
7. Δ ³ -Carene	0.8	3.4	-0.2	3.4	1.5	3.2	4.6	5.6	1.2	3.6	5.2	6.3
8. α-Terpinene	0.7	6.2	0.9	6.3	1.4	2.4	3.3	4.1	1.2	3.3	4.5	5.5
9. P-Cymene	0.7	2.0	-1.8	2.7	1.6	2.1	4.4	4.8	0.6	2.1	6.7	7.0
10. Limonene	3.7	4.1	-2.4	4.7	4.5	4.0	1.8	4.4	1.9	4.2	2.3	4.8
11. 1,8-Cineole(Eucalyptol)	1.2	7.7	-1.8	7.9	1.2	2.3	3.4	4.1	0.7	1.3	6.0	6.1
12. Ocimene	0.5	2.4	2.0	3.1	1.3	1.3	2.8	3.1	0.5	2.1	3.0	3.6
13. γ-Terpinene	0.5	3.4	1.0	3.6	1.2	2.3	2.5	3.4	0.7	4.2	2.4	4.9
14. Sabinene Hydrate	1.9	4.4	-0.1	4.4	3.0	2.7	6.1	6.7	4.8	5.9	3.8	7.0
15. Terpinolene	0.5	5.0	0.3	5.1	1.3	2.0	3.7	4.2	0.6	1.3	5.1	5.2
16. Fenchone	1.9	2.8	-3.9	4.8	1.6	2.3	4.6	5.2	0.6	0.6	7.9	7.9
17. Linalool	4.9	6.2	3.0	6.9	3.7	3.4	4.2	5.4	1.6	3.3	5.7	6.6
18. Fenchol	1.9	2.8	4.7	5.4	1.2	1.1	7.2	7.3	0.8	1.0	8.7	8.8
19. (-)-Isopulegol	3.8	3.7	1.5	4.0	1.3	1.8	6.6	6.8	1.2	1.2	7.9	8.0
20. Camphor	0.8	4.1	1.7	4.5	1.2	2.1	5.7	6.1	1.3	3.8	6.2	7.2
21. Borneol	1.3	2.7	1.2	3.0	1.7	2.3	2.2	3.2	1.3	3.4	4.5	5.6
22. Terpinen-4-ol	3.9	5.8	2.9	6.5	1.2	4.1	5.8	7.2	1.5	2.9	4.7	5.5
23. α-Terpineol	0.7	3.2	0.5	3.2	1.1	4.1	5.3	6.7	1.7	2.4	6.3	6.7
24. (+)-Dihydrocarvone	1.3	3.8	0.1	3.8	1.1	2.7	3.8	4.7	1.1	2.2	6.0	6.4
25. Nerol	2.6	3.6	-1.5	3.9	6.4	6.0	-1.3	6.2	3.6	3.6	4.5	5.7
26. Pulegone	3.6	5.2	3.8	6.4	3.2	3.4	5.9	6.9	1.6	2.7	5.0	5.7
27. (+)-Carvone	3.2	4.9	0.2	4.9	2.9	3.0	2.3	3.8	1.9	2.4	5.7	6.1
28. Geraniol	2.0	5.9	2.3	6.4	3.5	5.3	3.1	6.2	1.2	2.0	6.2	6.5
29. Geranyl Acetate	2.7	3.3	3.6	4.9	1.5	2.6	6.8	7.3	1.0	1.9	6.3	6.5
30. (-)-β-Elemene	0.4	1.5	-0.2	1.5	1.0	1.1	3.9	4.0	1.3	3.5	6.7	7.5
31. β-Caryophyllene	0.6	3.1	-4.9	5.8	0.9	3.4	3.3	4.7	0.9	1.1	6.9	7.0
32. Aromadendrene	1.4	1.7	-6.3	6.6	1.1	5.1	1.0	5.2	1.2	1.3	5.9	6.0
33. trans-β-Farnesene	0.8	5.5	4.9	7.4	1.1	1.4	6.4	6.6	0.7	1.2	7.7	7.8
34. α-Humulene	2.2	3.8	-4.6	5.9	3.1	3.0	1.5	3.3	1.2	2.2	5.6	6.1
35. Valencene	1.2	4.0	2.3	4.6	2.4	2.4	5.0	5.5	1.5	1.4	6.2	6.4
36. Ledene	3.9	5.4	-1.2	5.5	2.6	2.5	1.0	2.7	2.7	3.2	4.2	5.3
37. trans-Nerolidol	2.3	3.9	-1.3	4.1	3.5	5.5	1.6	5.7	2.4	2.4	5.1	5.7
38. Caryophyllene Oxide	2.9	2.9	2.7	4.0	2.6	2.8	2.9	4.0	1.4	2.0	4.8	5.2
39. Globulol	2.9	5.8	1.3	5.9	3.0	4.1	2.1	4.6	2.0	2.0	4.6	5.0

40. Viridiflorol	2.9	2.7	5.8	6.4	2.4	2.8	5.9	6.6	2.2	3.3	5.0	5.9
41. (-)-Guaialol	4.0	4.4	1.8	4.7	3.4	3.6	1.9	4.0	3.5	3.5	4.2	5.4
42. (+)-Cedrol	2.9	4.0	-0.2	4.0	2.2	2.9	3.2	4.3	2.2	2.0	6.6	6.9
43. β -Eudesmol	2.5	3.0	4.4	5.3	2.6	4.0	4.1	5.7	1.7	1.7	6.5	6.7
44. α -Bisabolol	1.3	2.3	6.6	7.0	2.8	3.6	4.4	5.7	1.7	1.8	6.2	6.5

Supplementary Table 6. ANOVA regression statistics for flavonoids.

	Quantification Range ($\mu\text{g/mL}$)	Correlation Coefficient R^2	Slope \pm SD	LOD ($\mu\text{g/mL}$)	LOQ ($\mu\text{g/mL}$)
1. Orientin	1-25	1.0000	21.73 \pm 0.06	0.04	0.12
2. Vitexin	1-25	1.0000	12.40 \pm 0.03	0.04	0.11
3. Isovitexin	1-25	1.0000	14.99 \pm 0.02	0.04	0.13
4. Quercetin	1-25	1.0000	14.02 \pm 0.31	0.08	0.23
5. Luteolin	1-25	1.0000	15.76 \pm 0.09	0.04	0.13
6. Kaempferol	1-25	0.9997	15.84 \pm 0.21	0.07	0.20
7. Apigenin	1-25	1.0000	19.48 \pm 0.07	0.06	0.17

Supplementary Table 7 Accuracy (recovery) and repeatability for flavonoids in cannabis leaf over three spiked levels

Spike level	Compound	Nominal spiked mass (µg)	Mass in sample (µg) (n=3) (mean±SD)	Measured spiked mass (µg) (n=3) (mean±SD)	Recovery% (n=3) (mean±SD)	RSD% (n=3)
Level 1	1. Orientin	20	34.27±0.04	17.77±0.52	88.8±2.6%	2.9%
	2. Vitexin	20	75.24±0.08	21.33±0.80	106.6±4.0%	3.8%
	3. Isovitexin	20	6.23±0.01	15.87±0.36	79.3±1.8%	2.3%
	4. Quercetin	50	ND	35.73±0.67	71.5±1.3%	1.9%
	5. Luteolin	50	58.10±0.07	42.03±1.74	84.1±3.5%	4.1%
	6. Kaempferol	50	ND	36.23±0.86	72.5±1.7%	2.4%
	7. Apigenin	50	29.50±0.03	40.23±0.46	80.5±0.9%	1.2%
Level 2	1. Orientin	50	34.27±0.04	46.39±1.49	92.8±3.0%	3.2%
	2. Vitexin	30	79.05±0.27	28.75±0.25	95.8±0.8%	0.9%
	3. Isovitexin	50	6.23±0.01	36.25±0.76	72.5±1.5%	2.1%
	4. Quercetin	100	ND	72.07±0.64	72.1±0.6%	0.9%
	5. Luteolin	100	58.10±0.07	80.02±2.57	80.0±2.6%	3.2%
	6. Kaempferol	100	ND	70.50±0.87	70.5±0.9%	1.2%
	7. Apigenin	100	29.50±0.03	78.74±1.85	78.7±1.9%	2.4%
Level 3	1. Orientin	80	34.27±0.04	75.78±1.34	94.7±1.7%	1.8%
	2. Vitexin	80	75.24±0.08	75.60±1.64	94.5±2.0%	2.2%
	3. Isovitexin	80	6.23±0.01	63.52±1.05	79.4±1.3%	1.7%
	4. Quercetin	150	ND	115.07±3.51	76.7±2.3%	3.0%
	5. Luteolin	150	58.10±0.07	121.22±2.28	80.8±1.5%	1.9%
	6. Kaempferol	150	ND	112.67±1.10	75.1±0.7%	1.0%
	7. Apigenin	150	29.50±0.03	121.69±0.85	81.1±0.6%	0.7%

Supplementary Table 8. ANOVA regression statistics for sterols and triterpenoids.

	Quantification Range (µg/mL)	Correlation Coefficient R ²	Slope ± SD	LOD (µg/mL)	LOQ (µg/mL)
1. Campesterol	1.00-100	0.9996	0.0134±0.0001	0.20	0.61
2. Stigmasterol	1.00-100	0.9999	0.0129±0.0001	0.21	0.63
3. β-Sitosterol	1.00-100	0.9989	0.0123±0.0002	0.26	0.79
4. β-Amyrin	1.00-100	0.9992	0.0559±0.0007	0.17	0.50
5. Epifriedelanol	1.00-100	0.9989	0.0280±0.0004	0.25	0.74
6. Friedelin	1.00-100	0.9998	0.0284±0.0002	0.26	0.78

Supplementary Table 9. Trueness, precision, and accuracy for compounds for sterols and triterpenoids.

Analyte	Spike 5 µg/mL				Spike 10 µg/mL				Spike 25 µg/mL			
	Repeatability	Intermediate	Trueness	Accuracy	Repeatability	Intermediate	Trueness	Accuracy	Repeatability	Intermediate	Trueness	Accuracy
	-	precision	-	-	-	precision	-	-	-	precision	-	-
	Pooled RSD%	RSD%	Relative	Uncertainty of	Pooled RSD%	RSD%	Relative	Uncertainty of	Pooled RSD%	RSD%	Relative	Uncertainty of
(n=3)	(n=9)	bias%	measurement%	(n=3)	(n=9)	(n=9)	measurement%	(n=3)	(n=9)	(n=9)	measurement%	(n=9)
1. Campesterol	4.9%	4.7%	-2.6%	5.5%	2.3%	2.1%	-1.1%	2.5%	2.3%	2.1%	0.5%	2.3%
2. Stigmasterol	4.2%	4.7%	-4.0%	5.8%	4.0%	3.9%	0.2%	4.0%	1.6%	1.4%	0.8%	1.8%
3. β-Sitosterol	2.5%	2.9%	0.1%	2.5%	2.7%	3.4%	0.7%	2.8%	1.5%	1.3%	0.8%	1.7%
4. β-Amyrin	4.7%	4.3%	-2.8%	5.5%	1.8%	2.8%	-0.8%	2.0%	2.4%	2.2%	0.1%	2.4%
5. Epifriedelanol	3.1%	4.5%	-2.9%	4.3%	1.5%	2.2%	0.0%	1.5%	1.1%	1.1%	0.8%	1.4%
6. Friedelin	3.2%	3.0%	0.4%	3.3%	2.2%	2.9%	1.4%	2.7%	3.84%	3.6%	0.1%	3.8%

Supplementary Table 10. Cannabinoid profile in root and stem bark for three strains.

Compound	Strain I root	Strain I stem bark	Strain II root	Strain II stem bark	Strain III root	Strain III stem bark
1. CBDV	ND	ND	ND	ND	ND	ND
2. CBDVA	ND	ND	ND	ND	ND	ND
3. CBG	0.0007±0.00003%	0.0002±0.00001%	ND	ND	0.0001±0.00002%	0.0001±0.00009%
4. CBD	ND	ND	ND	ND	ND	ND
5. CBDA	ND	ND	ND	ND	ND	ND
6. THCVA	ND	ND	ND	ND	ND	ND
7. CBGA	ND	0.0001±0.00003%	ND	0.0001±0.00001%	0.0002±0.00001%	0.0001±0.00001%
8. CBN	ND	0.0001±0.00001%	ND	ND	ND	0.0001±0.00001%
9. Δ ⁹ -THC	0.0001±0.00008%	0.0006±0.00008%	ND	0.0003±0.00001%	0.0001±0.00001%	0.0010±0.0002%
10. Δ ⁸ -THC	0.0001±0.00016%	0.0001±0.00005%	0.0001±0.00001%	ND	ND	0.0001±0.00004%
11. THCVA	0.0001±0.00004%	0.0002±0.00002%	0.0001±0.00001%	0.0001±0.00002%	0.0001±0.00001%	0.0002±0.00004%
12. CBC	ND	0.0001±0.00001%	ND	ND	ND	0.0001±0.00009%
13. THCA	0.0016±0.0004%	0.0058±0.0005%	0.0008±0.00001%	0.0040±0.0003%	0.0037±0.0002%	0.0062±0.0008%
14. CBCA	0.0001±0.00005%	0.0003±0.00005%	ND	0.0003±0.00005%	0.0001±0.00001%	0.0004±0.00009%
Total THC**	0.0015±0.0005%	0.0056±0.0005%	0.0007±0.00002%	0.0038±0.0003%	0.0034±0.00004%	0.0064±0.00082%
Total CBD**	0.0001±0.00001%	0.0001±0.00001%	ND	ND	ND	0.0001±0.00001%
Total cannabinoids	0.0027±0.0006%	0.0074±0.0008%	0.0011±0.00005%	0.0050±0.00007%	0.0043±0.00007%	0.0083±0.001%

* Content expressed in mean ± SD% (n=3). ND=Not detected.

Supplementary Table 11. Cannabinoid profile in leaves and inflorescences for three strains.

Compound	Strain I leaf	Strain I inflorescence	Strain II leaf	Strain II inflorescence	Strain III leaf	Strain III inflorescence
1. CBDV	ND	ND	ND	ND	ND	ND
2. CBDVA	ND	ND	ND	ND	ND	0.05 ± 0.003%
3. CBG	ND	0.08 ± 0.004%	ND	0.18 ± 0.01%	ND	0.03 ± 0.001%
4. CBD	ND	ND	ND	ND	0.02 ± 0.001%	0.33 ± 0.02%
5. CBDA	ND	0.04 ± 0.001%	ND	0.04 ± 0.002%	1.16 ± 0.02%	12.06 ± 0.84%
6. THCVA	ND	ND	ND	ND	ND	ND
7. CBGA	0.02 ± 0.001%*	0.26 ± 0.01%	0.02 ± 0.001%	0.37 ± 0.04%	0.02 ± 0.001%	0.35 ± 0.03%
8. CBN	ND	ND	ND	ND	ND	ND
9. Δ ⁹ -THC	0.05 ± 0.002%	0.24 ± 0.003%	0.06 ± 0.003%	0.30 ± 0.02%	0.03 ± 0.001%	0.47 ± 0.02%
10. Δ ⁸ -THC	ND	ND	ND	ND	ND	ND
11. THCVA	0.02 ± 0.001%	0.09 ± 0.004%	0.01 ± 0.001%	0.13 ± 0.007%	ND	0.02 ± 0.001%
12. CBC	ND	ND	ND	ND	ND	0.04 ± 0.002%
13. THCA	1.01 ± 0.02%	14.68 ± 0.07%	0.68 ± 0.02%	18.55 ± 0.70%	0.62 ± 0.01%	6.32 ± 0.44%
14. CBCA	0.29 ± 0.005%	0.39 ± 0.002%	0.34 ± 0.01%	0.79 ± 0.05%	0.25 ± 0.01%	0.24 ± 0.02%
Total THC**	0.93 ± 0.01%	13.11 ± 0.06%	0.65 ± 0.02%	16.57 ± 0.63%	0.57 ± 0.01%	6.02 ± 0.40%
Total CBD**	ND	0.03 ± 0.001%	ND	0.04 ± 0.002%	1.04 ± 0.02%	10.91 ± 0.75%
Total cannabinoids	1.42 ± 0.023%	15.77 ± 0.81%	1.10 ± 0.04%	20.37 ± 0.80%	2.10 ± 0.04%	19.93 ± 1.36%

* Content expressed in mean (n=3) ± SD%. ND=Not detected.

** ¹ Total THC = THC + 0.877× THCA, Total CBD = CBD + 0.877× CBDA

Supplementary Table 12 Mono- and sesquiterpenoid profile in cannabis leaf and inflorescence for three cannabis strains

Compound	LRI	LRI	Strain I	Strain I	Strain II	Strain II	Strain III	Strain III
	Calc.	Lit. ^a	Leaf	inflorescence	Leaf	inflorescence	Leaf	inflorescence
1. α-Pinene	934	932	0.004±0.0002%*	0.067±0.002%	0.002±0.0001%	0.117±0.006%	0.083±0.003%	0.463±0.006%
2. Camphene	948	952	ND	0.008±0.0001%	ND	0.011±0.0006%	ND	ND
3. Sabinene	974	976	0.001±0.0001%	ND	0.001±0.0001%	ND	ND	ND
4. β-Pinene	978	980	0.002±0.0001%	0.047±0.001%	0.001±0.000%	0.071±0.005%	0.020±0.0007%	0.124±0.007%
5. β-Myrcene	992	992	0.001±0.0001%	0.274±0.013%	ND	0.359±0.016%	0.024±0.0007%	0.302±0.011%
6. α-Phellandrene	1006	1006	ND	ND	ND	ND	ND	ND
7. Δ ³ -Carene	1011	1011	ND	ND	ND	ND	ND	ND
8. α-Terpinene	1017	1017	ND	ND	ND	ND	ND	ND
9. P-Cymene	1025	1026	ND	ND	ND	ND	ND	ND
10. Limonene	1029	1031	ND	0.252±0.004%	0.004±0.0001%	0.322±0.015%	0.005±0.0002%	0.049±0.002%
11. 1,8-Cineole (Eucalyptol)	1031	1032	0.006±0.0016%	ND	0.006±0.001%	0.006±0.0003%	ND	ND
12. Ocimene	1047	1050	ND	0.047±0.006%	ND	0.045±0.003%	ND	0.002±0.0001%
13. γ-Terpinene	1058	1059	ND	ND	ND	ND	ND	ND
14. Sabinene Hydrate	1069	1068	ND	0.003±0.0001%	0.001±0.0002%	0.004±0.0005%	ND	0.003±0.0003%
15. Terpinolene	1089	1088	ND	0.003±0.0001%	ND	0.003±0.0001%	ND	0.001±0.0001%
16. Fenchone	1088	1088	ND	0.003±0.0001%	ND	0.003±0.0001%	ND	0.002±0.0002%
17. Linalool	1103	1100	ND	0.037±0.005%	0.001±0.0001%	0.064±0.006%	ND	0.027±0.002%
18. Fenchol	1117	1112	ND	0.023±0.001%	ND	0.040±0.004%	ND	0.009±0.0009%
19. (-)-Isopulegol	1146	1146	ND	0.002±0.0001%	ND	0.004±0.0005%	ND	0.002±0.0002%
20. Camphor	1143	1143	ND	ND	ND	ND	ND	ND
21. Borneol	1168	1168	ND	0.004±0.0002%	ND	0.007±0.0007%	ND	0.005±0.0004%
22. Terpinen-4-ol	1179	1179	ND	0.001±0.0001%	ND	0.001±0.0001%	ND	0.001±0.0001%
23. α-Terpineol	1194	1190	ND	0.024±0.001%	ND	0.040±0.004%	ND	0.013±0.0005%
24. (+)-Dihydrocarvone	1197	1200	ND	ND	ND	ND	ND	ND
25. Nerol	1232	1228	ND	ND	ND	ND	ND	ND
26. Pulegone	1239	1244	ND	ND	ND	ND	ND	ND
27. (+)-Carvone	1245	1243	ND	ND	ND	ND	ND	ND
28. Geraniol	1258	1256	ND	0.001±0.001%	ND	0.001±0.0002%	ND	ND
29. Geranyl Acetate	1385	-	ND	ND	ND	ND	ND	ND
Total monoterpeneoids	-	-	0.014±0.002%	0.796±0.008%	0.016±0.002%	1.097±0.045%	0.132±0.005%	1.004±0.043%
30. (-)-β-Elementene	1394	1392	ND	ND	ND	ND	ND	ND
31. β-Caryophyllene	1420	1420	0.077±0.003%	0.416±0.030%	0.057±0.002%	0.538±0.034%	0.053±0.0024%	0.086±0.002%
32. Aromadendrene	1440	1440	ND	ND	ND	ND	ND	ND
33. trans-β-Farnesene	1459	1446	0.032±0.003%	0.106±0.002%	0.021±0.002%	0.106±0.008%	0.034±0.002%	0.035±0.001%
34. α-Humulene	1455	1455	0.025±0.001%	0.123±0.006%	0.022±0.0007%	0.193±0.019%	0.021±0.001%	0.036±0.002%
β - selinene	1485	1485	ND	0.043±0.001%	ND	0.046±0.001%	ND	0.034±0.001%
α - selinene	1494	1496	ND	0.037±0.001%	ND	0.036±0.001%	ND	0.026±0.001%
35. Valencene	1494	1491	ND	ND	ND	ND	ND	0.001±0.001%
36. Ledene	1497	1493	ND	0.011±0.0004%	ND	0.013±0.0009%	ND	0.005±0.0004%
α - Farnesene	1508	1508	ND	0.017±0.001%	ND	0.025±0.001%	ND	0.024±0.001%
37. trans-Nerolidol	1568	1565	0.012±0.003%	0.048±0.014%	0.009±0.0005%	0.166±0.014%	0.004±0.0004%	0.009±0.001%
38. Caryophyllene Oxide	1584	1583	ND	0.006±0.0003%	ND	0.005±0.0008%	ND	0.002±0.0001%
39. Globulol	1588	1584	ND	0.002±0.0001%	ND	0.001±0.0001%	ND	ND
40. Viridiflorol	1595	1588	ND	ND	ND	ND	ND	ND
41. (-)-Guaiol	1602	1602	ND	ND	ND	ND	0.007±0.0003%	0.027±0.0009%
42. (+)-Cedrol	1605	1601	ND	ND	ND	ND	ND	ND
43. β-Eudesmol	1651	1650	ND	0.001±0.0002%	ND	0.002±0.0001%	0.004±0.0002%	0.034±0.001%
α -Eudesmol	1653	1657	ND	0.002±0.0001%	ND	0.002±0.0002%	0.003±0.0002%	0.026±0.001%
44. α-Bisabolol	1685	1684	0.013±0.002%	0.027±0.005%	ND	0.002±0.0006%	0.020±0.002%	0.018±0.0006%
Total sesquiterpenoids	-	-	0.159±0.005%	0.741±0.035%	0.109±0.004%	1.044±0.043%	0.146±0.008%	0.279±0.011%
Total mono- and sesquiterpenoids	-	-	0.173±0.007%	1.537±0.043%	0.125±0.005%	2.141±0.102%	0.278±0.011%	1.283±0.018%

* Terpenoid content expressed in mean ± SD% (n=3). Bolded terpenoid was semi-quantified by GC-FID. ND=Not detected

^a LRI from the literature²⁻⁴.

Supplementary Table 13. Mono- and sesquiterpenoid ratios relative to total terpenoids in leaves and inflorescences

Compound	LRI		Strain I		Strain II		Strain III	
	Calc.	Lit. ^a	Leaf	inflorescence	Leaf	inflorescence	Leaf	inflorescence
1. α-Pinene	934	932	2.37±0.22%*	4.36±0.04%	1.82±0.07%	5.46±0.17%	29.81±0.75%	36.07±0.84%
2. Camphene	948	952	0.18±0.015%	0.51±0.01%	0.17±0.01%	0.51±0.02%	ND	ND
3. Sabinene	974	976	0.30±0.05%	ND	0.56±0.05%	ND	ND	ND
4. β-Pinene	978	980	1.08±0.06%	3.04±0.02%	0.89±0.02%	3.31±0.13%	7.12±0.16%	9.67±0.16%
5. β-Myrcene	992	992	0.52±0.07%	17.82±0.65%	ND	16.78±0.99%	8.74±0.16%	23.57±0.08%
6. α-Phellandrene	1006	1006	ND	ND	ND	ND	ND	ND
7. Δ ³ -Carene	1011	1011	ND	ND	0.21±0.05%	ND	ND	ND
8. α-Terpinene	1017	1017	0.11±0.02%	ND	ND	ND	ND	ND
9. P-Cymene	1025	1026	ND	ND	0.23±0.03%	ND	ND	ND
10. Limonene	1029	1031	ND	16.42±0.59%	0.74±0.14%	15.03±0.62%	1.77±0.06%	3.79±0.04%
11. 1,8-Cineole (Eucalyptol)	1031	1032	3.19±0.80%	ND	4.56±0.73%	0.28±0.04%	ND	0.03±0.01%
12. Ocimene	1047	1050	ND	3.07±0.32%	ND	2.08±0.04%	ND	0.19±0.01%
13. γ-Terpinene	1058	1059	0.14±0.01%	ND	0.23±0.03%	ND	ND	ND
14. Sabinene Hydrate	1069	1068	ND	0.22±0.01%	0.74±0.14%	0.02±10.57%	ND	0.27±0.02%
15. Terpinolene	1089	1088	ND	0.16±0.01%	ND	0.15±0.01%	ND	0.07±0.001%
16. Fenchone	1088	1088	ND	0.22±0.001%	ND	0.16±0.001%	ND	0.13±0.01%
17. Linalool	1103	1100	ND	2.41±0.07%	ND	2.99±0.19%	ND	2.10±0.21%
18. Fenchol	1117	1112	ND	1.46±0.01%	ND	1.85±0.11%	ND	0.72±0.06%
19. (-)-Isopulegol	1146	1146	ND	0.15±0.001%	ND	0.17±0.01%	ND	0.12±0.01%
20. Camphor	1143	1143	ND	ND	ND	ND	ND	ND
21. Borneol	1168	1168	ND	0.29±0.01%	ND	0.32±0.02%	ND	0.40±0.02%
22. Terpinen-4-ol	1179	1179	ND	0.06±0.001%	ND	0.05±0.001%	ND	0.06±0.01%
23. α-Terpineol	1194	1190	ND	1.56±0.05%	ND	1.86±0.15%	ND	1.04±0.03%
24. (+)-Dihydrocarvone	1197	1200	ND	ND	ND	ND	ND	ND
25. Nerol	1232	1228	ND	ND	ND	ND	ND	ND
26. Pulegone	1239	1244	ND	ND	ND	ND	ND	ND
27. (+)-Carvone	1245	1243	ND	ND	ND	ND	ND	0.02±0.001%
28. Geraniol	1258	1256	ND	0.04±0.001%	ND	0.05±0.001%	ND	ND
29. Geranyl Acetate	1385	-	ND	ND	ND	ND	ND	ND
Total monoterpenoids	-	-	7.91±0.72%	51.8±0.94%	12.93±0.82%	51.25±1.55%	47.45±1.12%	78.25±0.65%
30. (-)-β-Elementene	1394	1392	ND	ND	ND	ND	ND	ND
31. β-Caryophyllene	1420	1420	44.61±0.74%	27.09±0.35%	45.25±0.78%	25.14±0.70%	19.25±0.34%	6.71±0.19%
32. Aromadendrene	1440	1440	ND	ND	ND	ND	ND	ND
33. trans-β-Farnesene	1459	1446	18.75±2.23%	6.87±0.09%	17.12±1.3%	4.96±0.31%	12.17±0.06%	2.73±0.05%
34. α-Humulene	1455	1455	14.22±0.19%	7.97±0.18%	17.34±0.85%	9.01±0.52%	7.68±0.22%	2.82±0.09%
β - selinene	1485	1485	ND	0.04±0.001%	ND	0.05±0.001%	ND	0.03±0.001%
α - selinene	1494	1496	ND	0.04±0.001%	ND	0.04±0.001%	ND	0.03±0.001%
35. Valencene	1494	1491	ND	ND	ND	ND	ND	0.06±0.001%
36. Ledene	1497	1493	ND	0.74±0.01%	ND	0.63±0.03%	ND	0.39±0.03%
α - Farnesene	1508	1508	ND	0.02±0.01%	ND	0.03±0.001%	ND	0.02±0.001%
37. trans-Nerolidol	1568	1565	7.07±1.51%	3.11±0.46%	7.35±0.38%	7.73±0.64%	1.49±0.14%	0.67±0.09%
38. Caryophyllene Oxide	1584	1583	ND	0.38±0.01%	ND	0.25±0.02%	ND	0.16±0.01%
39. Globulol	1588	1584	ND	0.10±0.001%	ND	0.06±0.001%	ND	ND
40. Viridiflorol	1595	1588	ND	ND	ND	ND	ND	ND
41. (-)-Guaïol	1602	1602	ND	ND	ND	ND	2.36±0.05%	2.12±0.05%
42. (+)-Cedrol	1605	1601	ND	ND	ND	ND	ND	0.02±0.001%
43. β-Eudesmol	1651	1650	ND	0.07±0.01%	ND	0.07±0.02%	1.50±0.04%	2.64±0.11%
α -Eudesmol	1653	1657	ND	0.10±0.02%	ND	0.08±0.01%	0.90±0.09%	2.01±0.10%
44. α-Bisabolol	1685	1684	7.42±0.65%	1.76±0.01%	ND	0.82±0.11%	7.20±0.63%	1.42±0.09%
Total sesquiterpenoids	-	-	92.08±0.72%	48.20±0.94%	87.07±0.82%	48.75±1.55%	52.55±1.12%	21.75±0.65%
Total mono- and sesquiterpenoids	-	-	100%	100%	100%	100%	100%	100%

* Terpenoid ratio (relative to total terpenoid) is expressed as mean value ± SD% (n=3). ND= Not detected. Bolded entries were semi-quantified by relative area by GC-FID.

^a LRI from the literature²⁻⁴.

Supplementary Table 14 Flavonoid profile in cannabis

Compound	Orientin	Vitexin	Isovitexin	Quercetin	Luteolin	Kaempferol	Apigenin	Total flavonoids
Strain I leaf	0.08± 0.003%	0.12± 0.008%	0.01± 0.004%	ND	0.09± 0.008%	ND	0.05± 0.004%	0.34± 0.02%
Strain II leaf	0.07± 0.002%	0.17± 0.005%	0.02± 0.002%	ND	0.10± 0.01%	ND	0.07± 0.006%	0.44± 0.02%
Strain III leaf	0.07± 0.002%	0.13± 0.004%	0.05± 0.001%	ND	0.05± 0.002%	ND	0.03± 0.001%	0.40± 0.009%
Strain I inflorescence	0.01± 0.0003%	0.02± 0.0006%	0.002± 0.00005%	0.01± 0.0003%	0.01± 0.0004%	0.01± 0.0002%	0.004± 0.0002%	0.07± 0.001%
Strain II inflorescence	0.02± 0.001%	0.03± 0.002%	0.002± 0.0001%	0.01± 0.0004%	0.02± 0.001%	0.01± 0.0002%	0.01± 0.0004%	0.10± 0.005%
Strain III inflorescence	0.03± 0.0001%	0.06± 0.0008%	0.01± 0.0001%	0.01± 0.0008%	0.02± 0.0001%	0.005± 0.0003%	0.01± 0.0003%	0.14± 0.002%

* Content expressed in mean ± SD% (n=3). ND = Not detected.

Supplementary Table 15 Sterol profile in cannabis

Compound	Campesterol	Stigmasterol	β-sitosterol	Total sterols
Strain I root	0.016 ± 0.001%	0.010 ± 0.001%	0.051 ± 0.004%	0.077 ± 0.005%
Strain II root	0.020 ± 0.001%	0.009 ± 0.0005%	0.058 ± 0.003%	0.088 ± 0.004%
Strain III root	0.010 ± 0.0004%	0.013 ± 0.001%	0.040 ± 0.001%	0.063 ± 0.002%
Strain I stem bark	0.016 ± 0.001%	0.011 ± 0.0003%	0.044 ± 0.002%	0.071 ± 0.003%
Strain II stem bark	0.016 ± 0.001%	0.008 ± 0.0004%	0.044 ± 0.003%	0.069 ± 0.004%
Strain III stem bark	0.017 ± 0.0005%	0.010 ± 0.001%	0.050 ± 0.007%	0.076 ± 0.006%
Strain I leaf	ND	0.026 ± 0.003%	0.027 ± 0.001%	0.053 ± 0.003%
Strain II leaf	ND	0.030 ± 0.002%	0.022 ± 0.0004%	0.052 ± 0.002%
Strain III leaf	ND	0.030 ± 0.001%	0.024 ± 0.0002%	0.053 ± 0.001%

* Content expressed in mean ± SD% (n=3). ND = Not detected.

Supplementary Table 16 Triterpenoid profile in cannabis

Compound	β-Amyrin	Epifriedelanol	Friedelin	Total triterpenoids
Strain I root	0.006 ± 0.0003%	0.043 ± 0.004%	0.083 ± 0.007%	0.132 ± 0.011%
Strain II root	0.005 ± 0.0001%	0.033 ± 0.001%	0.091 ± 0.004%	0.128 ± 0.005%
Strain III root	0.013 ± 0.001%	0.092 ± 0.003%	0.135 ± 0.003%	0.239 ± 0.006%
Strain I stem bark	0.006 ± 0.001%	0.013 ± 0.001%	0.033 ± 0.004%	0.052 ± 0.006%
Strain II stem bark	0.006 ± 0.001%	0.021 ± 0.002%	0.065 ± 0.007%	0.092 ± 0.010%
Strain III stem bark	0.007 ± 0.0004%	0.041 ± 0.002%	0.100 ± 0.004%	0.149 ± 0.007%
Strain I leaf	0.026 ± 0.002%	ND	ND	0.026 ± 0.002%
Strain II leaf	0.024 ± 0.001%	ND	ND	0.024 ± 0.001%
Strain III leaf	0.012 ± 0.001%	ND	ND	0.012 ± 0.001%

* Content expressed in mean ± SD% (n=3). ND = Not detected.

Supplementary Table 17. Chemical profile of cannabis plant parts

	Root	Stem bark	Leaf	Inflorescence
Total cannabinoids	-*	-	1.10% - 2.10%	15.77% - 20.37%
Total mono- and sesquiterpenoids	-	-	0.13% - 0.28%	1.28% - 2.14%
Total triterpenoids	0.13% - 0.24%	0.05% - 0.15%	-	-
Total sterols	0.06% - 0.09%	0.07 - 0.08%	0.05% - 0.05%	-
Total flavonoids	-	-	0.34% - 0.44%	0.07% - 0.14%

* Less than 0.05%.

Supplementary Table 18. SIM method parameters for cannabinoids

Name	Retention Time (min)	POS/NEG	Quantifier
IS: Δ^9 -THC- d_3	16.059	POS	318.3
1. CBDV	8.102	POS	287.2
2. CBDVA	9.256	POS	331.2
3. CBG	11.263	POS	317.3
4. CBD	11.410	POS	315.3
5. CBDA	12.181	POS	359.2
6. THCV	12.393	POS	287.2
7. CBGA	13.539	POS	343.3
8. CBN	15.048	POS	311.2
9. Δ^9 -THC	16.471	POS	315.3
10. Δ^9 -THC	17.156	POS	315.3
11. THCVA	17.282	POS	331.2
12. CBC	18.398	POS	315.2
13. THCA	22.350	POS	359.3
14. CBCA	23.722	POS	359.3

Supplementary Table 19. SIM method parameters for flavonoids

Name	Retention Time (min)	POS/NEG	Quantifier
1. Orientin	15.393	NEG	447
2. Vitexin	19.444	NEG	431
3. Isovitexin	21.643	NEG	431
4. Quercetin	36.288	NEG	301
5. Luteolin	40.932	NEG	285
6. Kaempferol	44.875	NEG	285
7. Apigenin	48.708	NEG	269

Supplementary Table 20. SIM method parameters for monoterpenoids and sesquiterpenoids

	Retention Time (min)	Quantifier	Qualifier 1	Qualifier 2	Qualifier 3
IS: tridecane	11.497	71	85	57	
1. α -Pinene	5.597	77	91	121	
2. Camphene	5.787	93	121	136	
3. Sabinene	6.073	93	77	79	136
4. β -Pinene	6.132	93	69	77	136
5. β -Myrcene	6.242	69	79	136	
6. α -Phellandrene	6.462	93	77	91	136
7. Δ^3 -Carene	6.542	77	91	121	
8. α -Terpinene	6.621	121	91	93	136
9. <i>p</i> -Cymene	6.732	119	91	134	
10. Limonene	6.790	93	121	136	
11. 1,8-Cineole (Eucalyptol)	6.835	154	93	139	
12. Ocimene	7.004	93	79	121	
13. γ -Terpinene	7.207	93	77	121	136
14. Sabinene Hydrate	7.373	71	93	121	154
15. Terpinolene	7.662	93	121	136	
16. Fenchone	7.685	81	69	152	
17. Linalool	7.816	93	69	121	
18. Fenchol	8.145	93	111	121	
19. (-)-Isopulegol	8.656	121	136	154	
20. Camphor	8.646	95	108	152	
21. Borneol	9.064	110	67	139	
22. Terpinen-4-ol	9.238	71	93	111	154
23. α -Terpineol	9.492	121	59	136	
24. (+)-Dihydrocarvone	9.569	95	109	137	152
25. Nerol	10.120	69	93	121	
26. Pulegone	10.398	109	67	152	
27. (+)-Carvone	10.485	82	93	108	
28. Geraniol	10.613	69	93	123	
29. Geranyl Acetate	13.309	69	93	121	
30. (-)- β -Elemene	13.665	147	161	189	
31. β -Caryophyllene	14.339	105	91	79	
32. Aromadendrene	14.775	161	189	204	
33. trans- β -Farnesene	14.988	69	93	133	
34. α -Humulene	15.100	93	79	91	
35. Valencene	15.974	161	189	204	
36. Ledene	16.000	161	189	204	
37. trans-Nerolidol	17.406	93	107	136	
38. Caryophyllene Oxide	17.851	95	105	107	
39. Globulol	17.889	161	189	204	
40. Viridiflorol	18.021	161	189	204	
41. (-)-Guaial	18.067	161	105	107	
42. (+)-Cedrol	18.192	150	95	151	
43. β -Eudesmol	18.810	59	149	164	
44. α -Bisabolol	19.135	204	189	161	

Supplementary Table 21. SIM method parameters for triterpenoids and sterols

Name	Retention Time (min)	Quantifier	Qualifier 1	Qualifier 2
IS: Cholesterol	16.093	105	133	386
1. Campesterol	17.044	105	133	400
2. Stigmasterol	17.350	105	133	412
3. β -Sitosterol	17.955	105	133	414
4. β -Amyrin	18.466	218	189	203
5. Epifriedelanol	20.519	109	123	413
6. Friedelin	20.900	109	123	426

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