

Supplemental Materials

Supplemental Tables

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Table S1. List of full and abbreviated names of phytocannabinoids

1. Cannabigerol (CBG) type	Abbreviated name	Acid Form
Cannabigerol-C5	CBG	CBGA
Cannabigerobutol-C4	CBG-C4 / CBGB	CBGA-C4
Cannabigerovarin-C3	CBGV	CBGVA
Cannabigerorcol-C5	CBGO	CBGOA
Sesquicannabigerol-C5	SesquiCBG	Sesqui-CBGA
Cannabigerol monomethyl ether-C5	CBGM	CBGMA
2. Δ^9-<i>trans</i>-tetrahydrocannabinol (Δ^9-THC) type		
(-)- Δ^9 - <i>trans</i> -Tetrahydrocannabinol-C5	THC	THCA
(-)- Δ^9 - <i>trans</i> -tetrahydrocannabutol-C4	THC-C4 / THCB	THCA-C4
(-)- Δ^9 - <i>trans</i> -Tetrahydrocannabivarin-C3	THCV	THCVA
(-)- Δ^9 - <i>trans</i> -Tetrahydrocannabiorcol-C1	THCO	THCOA
(-)- Δ^9 - <i>trans</i> -Tetrahydrocannabinol monomethyl ether-C5	THCM	THCMA
3. Cannabidiol (CBD) type		
(-)-Cannabidiol-C5	CBD	CBDA
(-)-Cannabidibutol-C4	CBD-C4 / CBDB	CBDA-C4
(-)-Cannabidivarin-C3	CBDV	CBDVA
(-)-Cannabidiorcol-C1	CBDO	CBDOA
Cannabidiol monomethyl ether-C5	CBDM	CBDMA
4. Cannabichromene (CBC) type		
($\pm$)-Cannabichromene-C5	CBC	CBCA
($\pm$)-Cannabibutol-C4	CBC-C4 / CBCB	CBCA-C4
($\pm$)-Cannabichromevarin-C3	CBCV	CBCVA
($\pm$)-Cannabiorchromorcol-C1	CBCO	CBCOA
5. Cannabinol (CBN) type		
Cannabinol-C5	CBN	CBNA
Cannabibutol-C4	CBN-C4 / CBNB	CBNA-C4
Cannabivarin-C3	CBNV	CBNVA
Cannabiorcol-C1	CBNO	CBNOA
Cannabinodivarin-C3	CBNDV	
8-hydroxycannabinol	CBN-8-OH	CBNA-8-OH
Cannabinol monomethyl ether-C5	CBNM	
6. Δ^8-<i>trans</i>-tetrahydrocannabinol (Δ^8-THC) type		
(-)- Δ^8 - <i>trans</i> -(6aR,10aR)-Tetrahydrocannabinol-C5	Δ^8 -THC	
7. Cannabicyclol (CBL) type		
($\pm$)-(1aS,3aR,8bR,8cR)-Cannabicyclol-C5	CBL	
8. Cannabinodiol (CBND) type		
Cannabinodiol-C5	CBND	CBNDA
9. Cannabielsoin (CBE) type		
(5aS,6S,9R,9aR)-Cannabielsoin-C5	CBE	CBEA
Cannabielsoin-C3	CBEV	CBEVA
10. Cannabitrinol (CBT) type		
($\pm$)- <i>cis/trans</i> -Cannabitrinol-C5-1	CBT-1	CBTA-1
($\pm$)- <i>cis/trans</i> -Cannabitrinol-C5-2	CBT-2	
($\pm$)- <i>cis/trans</i> -Cannabitrinol-C5-3	CBT-3	CBTA-3
Cannabitrinol-C3-1	CBTV-1	
Cannabitrinol-C3-3	CBTV-3	

11. Phytocannabinoids without absolute identification. Names prescribed by (Berman et al.,2018)

313-16b	361-17a
327-13a	361-17b
327-13b	371-14a
327-13c	371-14b
329-11a	373-12a
329-11b	373-12b
329-11c	373-12c
329-11d	373-12d
329-11e	373-15b
331-18a	373-15c
331-18b	375-19a
331-18c	375-19b
331-18d	375-19c
357-16a	417-15a

Table S2. Calibration curves used for quantification of terpenoids without commercially available standards

Terpenoid without STD	STDcurve
β -Phellandrene	α -Phellandrene
C ₁₀ H ₁₈ O-154 (93/79/99/121)-1	Linalool
C ₁₀ H ₁₈ O-154 (93/79/99/121)-2	Linalool
α -Cubebene	Isodene
Ylangene	Isodene
α -Copaene	α -Cedrene
7-epi-Sesquithujene	α -Cedrene
C ₁₅ H ₂₄ -204 (105/(120+119)/161)	Isodene
β -Cubebene	Isodene
Sesquithujene	<i>trans</i> - β -Caryophyllene
β -Isocomene	Sativene
α -Santalene	Cyclosativene
cis- α -Bergamotene	α -Cedrene
trans- α -Bergamotene	α -Cedrene
α -Guaiane	Aromadendrene
γ -Elemene	α -Cedrene
β -Santalene	α -Humulene
Guaia-6,9-diene	Aromadendrene
C ₁₅ H ₂₄ -204 (69/91/105/161)	<i>trans</i> - β -Farnesene
C ₁₅ H ₂₄ -204 (91/105/161)	Aromadendrene
C ₁₅ H ₂₄ -204 (161/105/133/91)	Valencene
C ₁₅ H ₂₄ -204 (105/91/133/161/189)	Aromadendrene
Acoradiene	Aromadendrene
C ₁₅ H ₂₄ -204 (105)-1	Aromadendrene
γ -Curcumene	β -Curcumene
C ₁₅ H ₂₄ -204 (133/189)-1	β -Chamigrene
Sesquisabinene	Ledene
γ -Muurelene	Valencene
α -Amorphene	Ledene
Aristolochene	Ledene
Germacrene D	Ledene
C ₁₅ H ₂₄ -204 (133/189)-2	β -Chamigrene
C ₁₅ H ₂₄ -204 (119/93/161)	β -Curcumene
α -Selinene	Ledene
β -Selinene	β -Chamigrene
α -Farnesene	<i>trans</i> - β -Farnesene
β -Bisabolene	<i>trans</i> - β -Farnesene
δ -Guaiane	Ledene
β -Cadinene- C ₁₅ H ₂₄ -204(119/161/105/134)	β -Curcumene
Dihydroagarofuran	β -Curcumene

C₁₅H₂₄-204 (similar to Germacrene B)
Sesquicineole
Eremophilene
β-Sesquiphellandrene
γ-Cadinene
δ-Cadinene
C₁₅H₂₄-204 (105)-2
α-Panasinsene
trans-α-Bisabolene
Selina-3,7(11)-diene
Germacrene B
Guaia-3,9-diene
α-epi-7-epi-5-Eudesmol
C₁₅H₂₆O-222 (similar to γ-Eudesmol)
Humulene oxide II
Selin-6-en-α-ol
Hinesol
γ-Eudesmol
C₁₅H₂₆O-222 (105/161/59)-1
Agarospirene
C₁₅H₂₆O-222 (105/161/59)-2
C₁₅H₂₆O-222 (59/81/107 /149/161)
α-Eudesmol
7-epi-α-Eudesmol
Bulnesol

β-Curcumene
β-Curcumene
Valencene
trans-β-Farnesene
Valencene
β-Curcumene
Ledene
β-Curcumene
α-Humulene
Valencene
β-Curcumene
β-Curcumene
Globulol
β-Eudesmol
Caryophyllene oxide
β-Eudesmol
α-Bisabolol
β-Eudesmol
Globulol
α-Bisabolol
Globulol
β-Eudesmol
β-Eudesmol
α-Bisabolol
α-Bisabolol

Table S3. SRM fragmentation of the terpenoids without commercially available standards

Compound name	RT [min]	Precursor I [m/z]	Product I [m/z]	CE [eV]	Ratio
β -Phellandrene	14.50	93	77	10	Quan
		93	91	6	75
		77	51	14	32
C ₁₀ H ₁₈ O-154 (93/79/99/121)-1	24.10	93	77	12	Quan
		99	43	8	42
		121	93	8	23
C ₁₀ H ₁₈ O-154 (93/79/99/121)-2	26.20	93	77	12	Quan
		99	43	8	40
		121	93	8	25
α -Cubebene	34.61	105	77	18	Quan
		119	91	10	80
		161	105	8	76
Ylangene	36.06	105	77	16	Quan
		119	91	12	96
		161	105	6	59
α -Copaene	36.22	119	91	12	Quan
		105	77	20	80
		91	65	14	44
		161	105	8	85
7-epi-Sesquithujene	36.66	93	77	10	Quan
		69	41	6	32
		119	91	14	55
C ₁₅ H ₂₄ -204 (105/(120+119)/161)	36.84	120	105	8	Quan
		119	91	12	30
		105	77	18	44
		161	105	8	18
β -Cubebene	37.68	105	77	16	Quan
		105	79	12	70
		119	91	12	180
		161	105	10	80
Sesquithujene	37.70	93	77	10	Quan
		69	41	6	35
		91	65	16	30
		119	91	14	55
β -Isocomene	37.80	108	93	5	Quan
		107	91	10	32
		93	77	12	64

<i>cis</i> - α -Bergamotene	38.25	119	91	14	Quan
		69	41	6	70
		93	91	6	140
		107	91	10	60
α -Santalene	38.34	94	79	10	Quan
		41	39	6	20
		95	67	10	18
<i>trans</i> - α -Bergamotene	39.01	119	91	8	Quan
		69	41	6	85
		107	91	10	23
α -Guaiene	39.67	105	77	18	Quan
		133	105	8	73
		147	105	6	100
γ -Elemene	39.88	93	77	12	Quan
		67	41	12	20
		121	93	6	65
		105	77	16	35
β -Santalene	40.10	94	77	20	Quan
		94	79	6	46
		122	94	4	38
Guaia-6,9-diene	40.37	105	77	16	Quan
		91	65	14	45
		119	91	12	65
		161	105	6	55
C ₁₅ H ₂₄ -204 (69/91/105/161)	41.05	69	41	6	Quan
		91	65	16	78
		105	77	16	68
		161	105	8	45
C ₁₅ H ₂₄ -204 (91/105/161)	41.12	91	65	16	Quan
		105	77	16	90
		133	105	8	75
		161	105	6	60
C ₁₅ H ₂₄ -204 (161/105/133/91)	41.22	133	105	8	Quan
		91	65	16	50
		105	77	16	51
		161	105	8	51
C ₁₅ H ₂₄ -204 (105/91/133/161/189)	41.30	133	105	8	Quan
		105	77	16	85
		161	105	8	55
		189	133	8	15
Acoradiene	41.70	119	91	12	Quan
		105	77	16	50

		93	77	12	100
		79	77	10	60
C ₁₅ H ₂₄ -204(105)-1	42.04	105	77	16	Quan
		79	77	10	60
		91	65	16	40
		105	79	10	45
C ₁₅ H ₂₄ -204 (189/133)-1	42.16	133	105	8	Quan
		105	77	18	51
		189	133	18	31
γ-Curcumene	42.16	119	91	12	Quan
		93	77	10	105
		105	77	16	65
		121	93	6	66
Sesquisabinene	42.30	69	41	6	Quan
		41	39	8	24
		69	39	20	31
		93	77	12	73
γ-Muurelene	42.79	161	105	10	Quan
		79	77	10	85
		119	91	12	80
		161	81	10	39
α-Amorphene	42.92	105	77	18	Quan
		119	91	14	72
		161	105	8	65
Aristolochene	42.78	105	77	18	Quan
		91	65	16	48
		189	133	8	23
Germacrene D	43.29	105	77	16	Quan
		120	105	6	20
		161	105	8	80
C ₁₅ H ₂₄ -204 (189/133)-2	43.41	133	105	8	Quan
		105	77	16	30
		189	133	8	64
C ₁₅ H ₂₄ -204 (119/93/161)	43.50	119	91	14	Quan
		133	105	8	53
		161	105	10	42
		204	161	8	50
α-Selinene	43.57	105	77	16	Quan
		67	41	12	54
		81	79	6	86
		133	105	8	90
β-Selinene	43.77	133	105	8	Quan

		81	79	6	65
		189	133	8	72
α -Farnesene	43.86	123	81	10	Quan
		55	29	8	72
		107	91	8	245
β -Bisabolene	45.86	69	41	6	Quan
		41	39	6	91
		69	39	16	33
		93	51	24	34
δ -Guaiene	44.40	108	93	8	Quan
		79	77	10	35
		105	77	18	50
		107	79	6	91
β -Cadinene- C ₁₅ H ₂₄ -204 (119/161/105/134)	44.55	119	91	12	Quan
		105	79	10	32
		134	119	6	50
		161	119	8	28
Dihydroagarofuran	44.76	41	39	8	Quan
		109	67	6	80
		137	94	4	35
		207	105	12	33
C ₁₅ H ₂₄ -204 (similar to Germarcene B)	44.81	121	93	6	Quan
		93	77	12	110
		105	77	16	65
		147	105	10	27
Sesquicineole	44.95	139	43	10	Quan
		43	41	4	15
		95	55	12	35
		139	95	8	55
Eremophilene	45.05	161	119	8	Quan
		105	77	16	110
		147	105	10	70
		161	105	10	98
β -Sesquiphellandrene	45.28	69	41	6	Quan
		41	39	8	36
		93	77	10	70
γ -Cadinene	45.28	161	105	6	Quan
		79	77	10	65
		119	91	8	90
		161	119	6	65
δ -Cadinene	45.45	119	91	10	Quan
		134	119	6	100

		161	105	8	80
C ₁₅ H ₂₄ -204 (105) - 2	45.64	105	77	16	Quan
		107	91	8	75
		119	91	10	55
		147	91	12	55
α -Panasinsene	46.06	122	107	6	Quan
		107	79	8	20
		122	91	18	25
<i>trans</i> - α -Bisabolene	46.55	93	77	12	Quan
		67	41	10	20
		119	91	14	9
		121	93	6	15
Selina-3,7(11)-diene	47.00	107	91	10	Quan
		133	105	8	84
		161	105	10	70
		204	161	5	85
Germacrene B	48.48	121	93	6	Quan
		67	41	12	42
		107	91	10	84
α -epi-7-epi-5-Eudesmol	52.58	109	67	10	Quan
		59	31	12	50
		149	93	8	30
C ₁₅ H ₂₆ O-222 (similar to γ -Eudesmol)	53.58	133	105	8	Quan
		59	31	18	9
		161	105	12	49
		189	133	8	60
Selin-6-en-4 α -ol	54.02	81	79	8	Quan
		43	41	4	15
		105	77	16	70
		161	105	6	82
γ -Eudesmol	54.29	133	105	8	Quan
		59	31	12	16
		161	105	10	55
		189	133	6	68
Hinesol	54.40	161	105	12	Quan
		59	31	10	50
		105	77	18	80
		119	91	10	65
C ₁₅ H ₂₆ O-222 (105/161/59)-1	54.58	105	77	18	Quan
		59	31	10	18
		147	105	6	18
		161	105	6	105

Agarospinol	54.80	119	91	10	Quan
		59	31	10	70
		105	77	16	20
		161	105	12	70
C ₁₅ H ₂₆ O-222 (105/161/59)-2	55.29	105	77	18	Quan
		59	31	10	61
		147	91	8	63
		161	105	6	120
C ₁₅ H ₂₆ O-222 (59/81/107/149/161)	55.42	59	31	12	Quan
		81	79	8	130
		107	91	6	115
		149	93	8	50
α -Eudesmol	56.35	59	31	12	Quan
		149	107	8	83
		161	105	10	140
7-epi- α -Eudesmol	56.64	122	107	6	Quan
		59	31	10	14
		107	91	12	55
		161	105	10	38
Bulnesol	57.00	107	91	10	Quan
		59	41	8	7
		135	107	6	70

RT, retention times; Precursor I, precursor ions mass to charge; Product I, product ions mass to charge; CE, Collision Energy in electron volt; Quan, ratio quantification - the first transition on each row was used for quantification and the rest for qualification.

Table S4. List of identified terpenoids without commercially available standards (based on the NIST library and RIs)

Compound name	Formula	MW [m/z]	RT [min]	NIST		RI _{cal}	RI _{lit}	$\Delta_{RI_{cal}-RI_{lit}}$
				Match	R. Match			
β -Phellandrene	C ₁₀ H ₁₆	136	14.50	896	903	983	1021	38
C ₁₀ H ₁₈ O-154 (93/79/121)-1	C ₁₀ H ₁₈ O	154	24.10	-	-	1104	-	-
C ₁₀ H ₁₈ O-154 (93/79/121)-2	C ₁₀ H ₁₈ O	154	26.20	-	-	1134	-	-
α -Cubebene	C ₁₅ H ₂₄	204	34.62	915	925	1290	1351	61
Isodene *	C ₁₅ H ₂₄	204	35.72	921	928	1311	1375	64
Cyclosativene *	C ₁₅ H ₂₄	204	35.66	936	947	1313	1368	55
Ylangene	C ₁₅ H ₂₄	204	35.91	899	910	1318	1372	54
α -Copaene	C ₁₅ H ₂₄	204	36.22	934	945	1325	1376	51
7-epi-Sesquithujene	C ₁₅ H ₂₄	204	36.83	900	929	1335	1391	56
C ₁₅ H ₂₄ -204 (105/(120+119)/161)	C ₁₅ H ₂₄	204	36.84	-	-	1335	-	-
Sativene*	C ₁₅ H ₂₄	204	37.47	936	925	1348	1396	48
β -Cubebene	C ₁₅ H ₂₄	204	37.60	847	884	1351	1389	38
Sesquithujene	C ₁₅ H ₂₄	204	37.60	914	940	1351	1402	51
β -Isocomene	C ₁₅ H ₂₄	204	37.90	818	843	1358	1412	54
α -Santalene	C ₁₅ H ₂₄	204	38.45	914	923	1365	1420	55
<i>cis</i> - α -Bergamotene	C ₁₅ H ₂₄	204	38.53	925	934	1366	1415	49
<i>trans</i> - α -Bergamotene	C ₁₅ H ₂₄	204	39.10	915	934	1380	1435	55
α -Guaiane	C ₁₅ H ₂₄	204	39.69	922	933	1391	1439	48
γ -Elemene	C ₁₅ H ₂₄	204	39.89	923	926	1395	1433	38
β -Santalene	C ₁₅ H ₂₄	204	40.20	935	946	1407	1448	41
Guaia-6,9-diene	C ₁₅ H ₂₄	204	40.37	936	939	1407	1443	36
C ₁₅ H ₂₄ -204 (69/91/105/161)	C ₁₅ H ₂₄	204	41.05	-	-	1415	-	-
C ₁₅ H ₂₄ -204 (91/105/161)	C ₁₅ H ₂₄	204	41.12	-	-	1417	-	-
C ₁₅ H ₂₄ -204 (161/105/133/91)	C ₁₅ H ₂₄	204	41.22	-	-	1420	-	-
C ₁₅ H ₂₄ -204 (105/91/133/161/189)	C ₁₅ H ₂₄	204	41.30	-	-	1422	-	-
Acoradiene	C ₁₅ H ₂₄	204	41.80	900	905	1436	1471	36
C ₁₅ H ₂₄ -204 (105) - 1	C ₁₅ H ₂₄	204	42.04	-	-	1439	-	-
γ -Curcumene	C ₁₅ H ₂₄	204	42.15	880	904	1443	1480	37
C ₁₅ H ₂₄ -204 (189/133)-1	C ₁₅ H ₂₄	204	42.16	-	-	1443	-	-
Sesquisabinene	C ₁₅ H ₂₄	204	42.27	889	894	1449	1464	17
γ -Muurolene	C ₁₅ H ₂₄	204	42.79	939	944	1449	1477	27
α -Amorphene	C ₁₅ H ₂₄	204	42.93	909	934	1453	1482	29
Aristolochene	C ₁₅ H ₂₄	204	42.78	930	938	1458	1487	29
Germacrene D	C ₁₅ H ₂₄	204	43.29	900	920	1459	1481	21
C ₁₅ H ₂₄ -204 (189/133)-2	C ₁₅ H ₂₄	204	43.41	-	-	1464	-	-
C ₁₅ H ₂₄ -204 (119/93/161)	C ₁₅ H ₂₄	204	43.50	-	-	1465	-	-
α -Selinene	C ₁₅ H ₂₄	204	43.57	950	956	1468	1486	18
β -Selinene	C ₁₅ H ₂₄	204	43.77	900	910	1474	1494	20
α -Farnesene	C ₁₅ H ₂₄	204	43.86	962	967	1476	1508	32
β -Bisabolene	C ₁₅ H ₂₄	204	43.86	948	948	1476	1509	33
δ -Guaiane	C ₁₅ H ₂₄	204	44.40	927	928	1480	1509	29
β -Cadinene- C ₁₅ H ₂₄ - 204(119/161/105/134)	C ₁₅ H ₂₄	204	44.55	912	900	1486	1513	27
Dihydroagarofuran	C ₁₅ H ₂₆ O	222	44.76	935	950	1490	1496	6
C ₁₅ H ₂₄ -204 (similar to Germacrene B)	C ₁₅ H ₂₄	204	44.81	-	-	1491	-	-
Sesquicineole	C ₁₅ H ₂₆ O	222	44.95	924	912	1496	1516	20
Eremophilene	C ₁₅ H ₂₄	204	45.05	842	852	1497	1499	2
β -Sesquiphellandrene	C ₁₅ H ₂₄	204	45.20	942	932	1501	1524	23
γ -Cadinene	C ₁₅ H ₂₄	204	45.28	918	925	1499	1513	14
δ -Cadinene	C ₁₅ H ₂₄	204	45.45	879	897	1502	1524	22
C ₁₅ H ₂₄ -204 (105)-2	C ₁₅ H ₂₄	204	45.64	-	-	1506	-	-
α -Panasinsene	C ₁₅ H ₂₄	204	46.06	848	857	1513	1527	14
<i>trans</i> - α -Bisabolene	C ₁₅ H ₂₄	204	46.55	913	952	1515	1512	-3
Selina-3,7(11)-diene	C ₁₅ H ₂₄	204	47.00	937	941	1520	1542	22

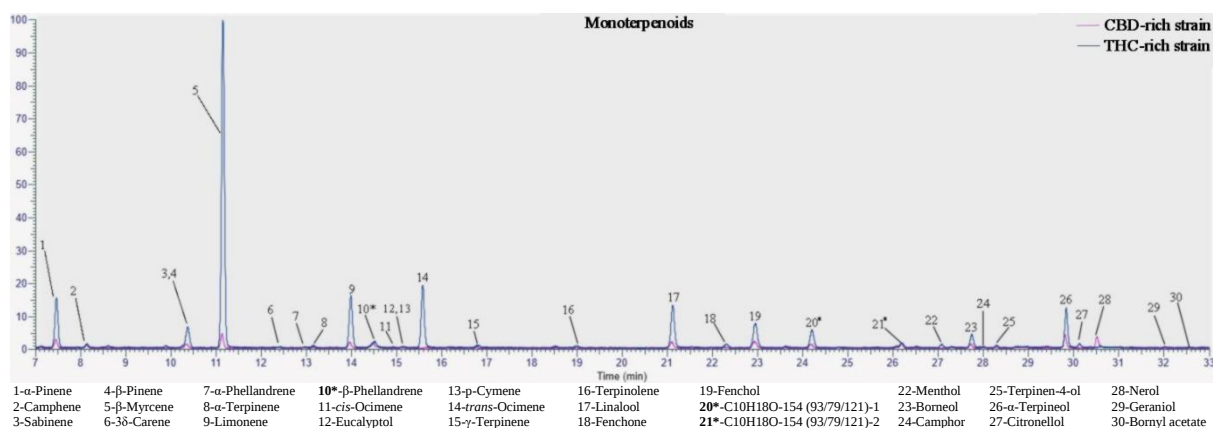
Germacrene B	C ₁₅ H ₂₄	204	48.48	911	913	1548	1557	9
α -epi-7-epi-5-Eudesmol	C ₁₅ H ₂₆ O	222	52.58	896	912	1626	1616	-10
C ₁₅ H ₂₆ O-222 (similar to γ -Eudesmol)	C ₁₅ H ₂₆ O	222	53.58	-	-	1642	-	-
Selin-6-en- α -ol	C ₁₅ H ₂₆ O	222	54.02	870	896	1650	1636	-14
γ -Eudesmol	C ₁₅ H ₂₆ O	222	54.29	933	934	1655	1631	-24
Hinesol	C ₁₅ H ₂₆ O	222	54.40	879	917	1657	1635	-22
C ₁₅ H ₂₆ O-222 (105/161/59)-1	C ₁₅ H ₂₆ O	222	54.58	-	-	1660	-	-
Agarospinol	C ₁₅ H ₂₆ O	222	54.80	864	926	1663	1645	-18
C ₁₅ H ₂₆ O-222 (105/161/59)-2	C ₁₅ H ₂₆ O	222	55.29	-	-	1672	-	-
C ₁₅ H ₂₆ O-222 (59/81/107/149/161)	C ₁₅ H ₂₆ O	222	55.42	-	-	1673	-	-
α -Eudesmol	C ₁₅ H ₂₆ O	222	56.35	900	917	1675	1653	-22
β -Eudesmol*	C ₁₅ H ₂₆ O	222	56.51	932	940	1678	1649	-29
7-epi- α -Eudesmol	C ₁₅ H ₂₆ O	222	56.64	859	879	1687	1658	-29
Bulnesol	C ₁₅ H ₂₆ O	222	57.00	890	907	1692	1667	-25

*STD of the terpenoids used as reference for illustration of the acceptable difference [$\Delta_{RI_{cal}-RI_{lit}}$] between calculated retention time indexes [RI_{cal}] and their literature values [RI_{lit}] in the present chromatographical conditions.

Table S5. Maximum limits of detection (MLOD) of terpenoids

Terpenoid	MLOD [ppm]
Selina-3,7(11)-diene (as Valencene)	1267
Guaiol	2099
Caryophyllene oxide	1890
C ₁₅ H ₂₆ O-222 (similar to γ -Eudesmol) (as Guaiol)	2099
γ -Eudesmol (as β -Eudesmol)	1488
α -Eudesmol (as β -Eudesmol)	1488
β -Eudesmol	1488
α -Bisabolol	3391

A Monoterpenoids



B Sesquiterpenoids

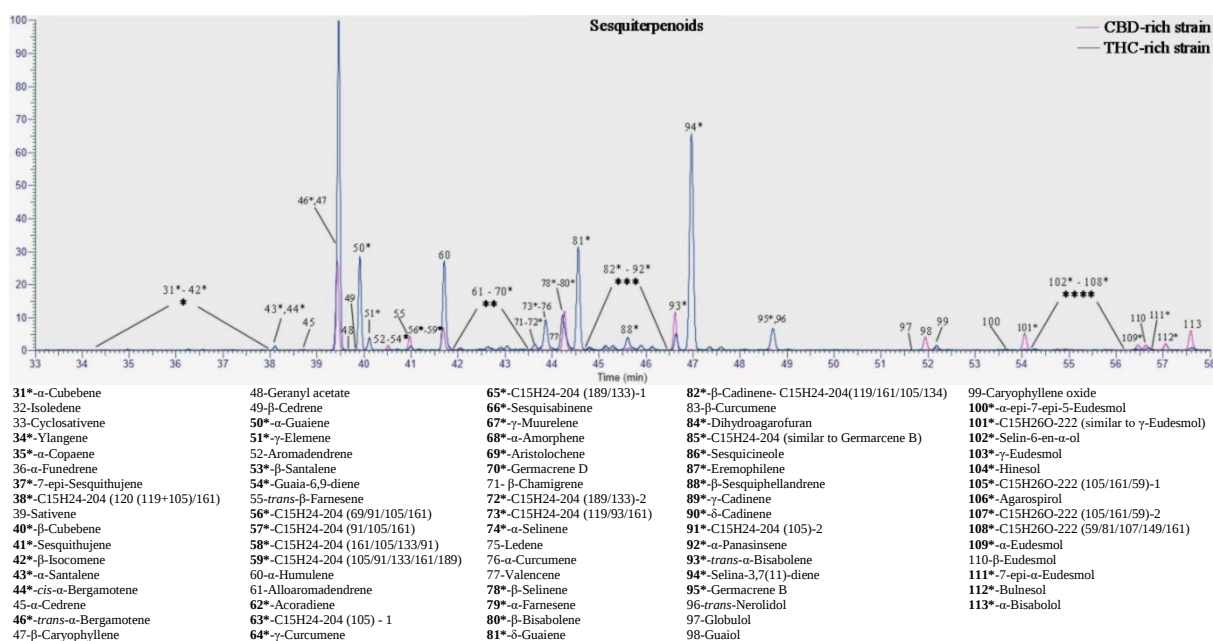
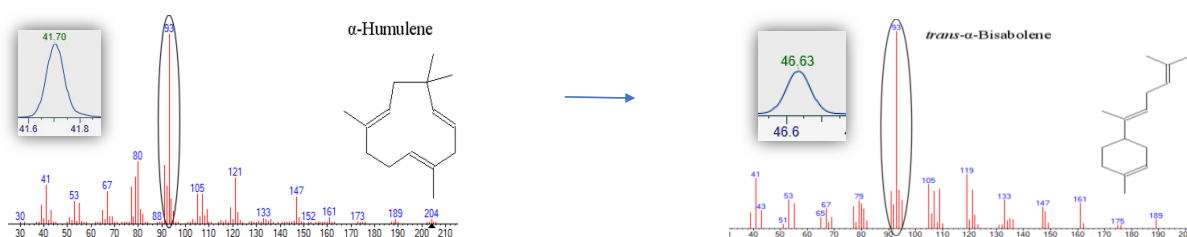


Figure S1. Terpenoid profiles of CBD- and THC-rich unfertilized strains of *Cannabis*. Overlaid chromatograms of unfertilized CBD- and THC-rich female plants divided into (A) monoterpenoids and (B) sesquiterpenoids. Terpenoids are denoted in numbers and the full names appear below the chromatogram. *Terpenoids that were semi-quantified.

a. Similarity of MS spectrums



b. Similarity of MS spectrums and nearness retention times



c. Nearness of retention times

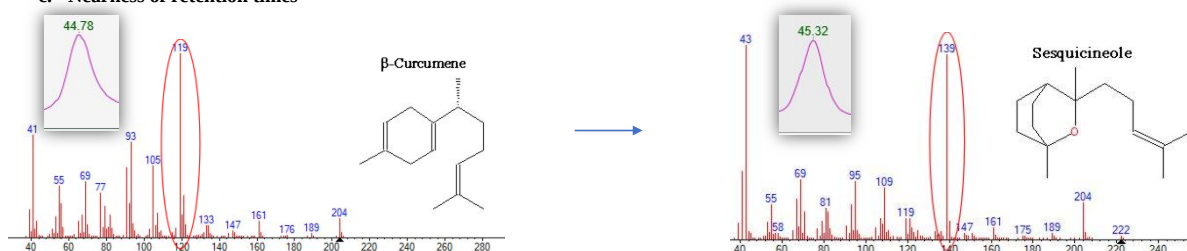


Figure S2. Principles of terpenoid semi-quantification. Terpenoids without commercially available analytical standards are semi-quantified according to three principles from more to less fit: (a) Similarity of MS spectrums, (b) Close similarity of MS spectrums and nearness retention times, and (c) Nearness of retention times only.