Supplementary Material

Comprehensive analysis of 19 cannabinoids in commercial CBD oils: concentrations, profiles, and safety implications

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Table S1 Selected product information displayed on the packaging

Sample	CBD declaration	THC declaration	Carrier oil	Spectrum	Origin
1	2.5 %	none	tincture	full	AT
2	5.0 %	none	hemp seed	isolate	DE
3	5.0 %	none	MCT, hemp seed, sunflower	probably full	AT
4	5.0 %	Δ^9-THC < 0.2% Δ^8-THC < 0.01%	hemp seed	full	CZ
5	5.0 %	none	sunflower	full	CH
6	5.0 %	2 x 4 drops < 60 µg THC	olive, hemp seed	mono	AT
7	5.0 %	2 x 4 drops < 60 µg THC	hemp seed, MCT	full	AT
8	5.0 %	"from low-THC industrial hemp (THC < 0.2%)"	MCT, hemp seed	probably full	DE
9	5.0 %	<0.2 %	sunflower	full	CH
10	5.0 %	none	sesame	full	unknown
11	6.0 %	none	NA	full	AT
12	5.0 %	<0.3 %	hemp seed	full	FR
13	5.0 %	none	olive	full	DE

14	5.0 %	2x4 drops < 60 µg THC	sunflower, hemp seed	broad	AT
15	5.0 %	none	MCT	broad	US
16	5.35 %	none	sesame	full	CH
17	5.0 %	0.13 %	hemp seed	full	AT
18	10.0 %	none	hemp seed	full	DE
19	12.0 %	none	hemp seed, sunflower	full or broad	IT
20	15.0 %	'THC FREE'	hemp seed	full	DE
21	20.0 %	none	hemp seed	full	unknown
22	20.0 %	'THC FREE'	hemp seed	full	DE
23*	5.0 %	0.0 %	hemp seed, mint	full	AT
24*	5.0 %	<0.3 %	hemp seed	full	FR
25†	2.5 %	2x4 drops < 60 µg THC	hemp seed	broad	AT
26†	5.0 %	<0.3 %	hemp seed	full	FR

* CBG oil
† CBN oil

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16 **Table S2a** Overview of the quality control parameters

Analyte	**limit of quantification (LOQ)** [a]		**Recovery in %** [b]	**Precision in %**
	ng mL^{-1}	**mg kg^{-1}**		
CBC	0.5	0.025	91 ± 11	12
CBCA	0.5	0.025	106 ± 6	6
CBD	0.25	0.013	112 ± 3	3
CBDA	0.25	0.013	127 ± 4	3
CBDV	0.25	0.013	117 ± 2	2
CBDVA	0.5	0.025	120 ± 4	3
CBG	0.25	0.013	118 ± 9	8
CBGA	0.25	0.013	125 ± 2	2
CBL	0.1	0.003	90 ± 4	5
CBLA	0.5	0.025	122 ± 4	3
CBN	0.25	0.013	105 ± 3	3
CBNA	0.25	0.013	120 ± 9	8
Δ^9-THC	0.1	0.003	96 ± 2	3
Δ^8-THC	0.25	0.013	96 ± 3	3
THCA	0.5	0.025	117 ± 2	2
THCV	0.1	0.003	109 ± 2	2
THCVA	0.25	0.013	121 ± 4	3

(*R*)-HHC	0.25	0.013	96 ± 1	4
(*S*)-HHC	0.25	0.013	100 ± 1	4

[a)] The determination of the limit of quantification was carried out via the signal-to-noise ratio according to DIN32645. The conversion to mg kg^{-1} has been made taking into account the dilution and solvation of 100 mg of oil sample to a total volume of 10 mL with acetone.

[b)] To investigate the recovery, 200 mg of blank matrix sunflower seed oil were spiked with 200 µL cannabinoid standard mix (c = 1 µg mL^{-1}), corresponding to an absolute level of 200 ng. The spiked sample was dissolved and prepared as described in Lindekamp et al. (2024).

Table S2b Recovery and precision of CBD and CBDV upon considerable dilution of a certified reference material (CRM) for CBD oil. According to the CRM manufacturer's data sheet, the CRM was an oil (not further specified) with assigned values for CBD and CBDV of 0.463 % w/w and 7.51 mg kg^{-1}, respectively

	CBD		**CBDV**	
Dilution Factor	**Recovery [%]**	**Precision [%]**	**Recovery [%]**	**Precision [%]**
100	n. d.	8	102	10
250*	n. d.		95	
500	91		88	
1000*	109		112	
2500	103		n. d.	
5000	98		n. d.	
10 000	114		n. d.	
25 000*	102		n. d.	
50 000*	95		n. d.	

n. d. = not determined; applies when the cannabinoids were outside of the calibration range due to dilution

*These are the dilution levels used for the sample preparation described in the manuscript

Table S3 UHPLC-MS/MS parameters for each cannabinoid. Quantifier ions are indicated by '*', other ions are qualifiers. Dwell time is 30 ms for all masses

Analyte	Precursor ion $[M+H]^+$	Transition	Declustering potential [V]	Collision energy [V]	Retention time [min]
CBC	315.2	315.2/193.1*	60	35	10.0
		315.2/259.1		25	
		315.2/123.1		43	
CBCA	359.2	341.1/219.1*	100	42	11.2
		341.2/261.1		25	
		341.1/285.1		37	
		359.2/261.2	56	30	
		359.2/219.1		42	
		359.2/341.1		25	
CBD	315.2	315.2/193.1*	60	35	6.1
		315.2/259.1		25	
		315.2/123.1		43	
CBDA	359.2	341.2/219.1*	100	42	5.9
		341.2/261.1		25	
		341.2/285.1		37	
		359.2/219.1	56	42	
		359.2/341.1		25	
		359.2/261.2		30	
CBDV	287.2	287.2/165.1*	76	28	5.0
		287.2/231.1		27	
		287.2/135.1		31	
CBDVA	331.2	313.2/191.1*	80	25	4.8
		313.2/233.1		34	
		313.2/257.1		37	
		331.2/313.1	61	17	
		331.2/233.1		34	
		331.2/191.1		37	
CBG	317.2	317.2/193.1*	46	22	6.3
		317.2/123.1		43	
		317.2/233.1		20	
CBGA	361.2	343.2/219.1*	51	37	6.3
		343.2/343.1		11	
CBL	315.2	315.2/235.1*	60	25	9.7
		315.2/165.1		37	
		315.2/123.1		43	
CBLA	359.2	359.2/341.1*	56	25	11.3
		359.2/219.1		42	

		359.2/261.2	100	30	
		341.2/219.1		42	
		341.2/261.1		25	
		341.2/285.1		37	
CBN	311.2	311.2/223.2	76	35	7.9
		311.2/195.2		35	
		311.2/293.2		37	
CBNA	355.2	355.2/337.1*	56	25	9.3
		355.2/235.1		43	
		355.2/253.1		43	
		337.2/281.2	120	30	
		337.2/235.1		35	
		337.2/253.1		35	
Δ^9-THC	315.2	315.2/193.1*	60	35	8.9
		315.2/123.1		43	
		315.2/259.1		25	
Δ^8-THC	315.2	315.2/193.1*	60	35	9.0
		315.2/123.1		43	
		315.2/259.1		25	
THCA	359.2	341.2/219.1*	100	42	10.4
		341.2/285.1		37	
		341.2/261.1		25	
		359.2/341.1	56	25	
		359.2/219.1		42	
		359.2/261.2		30	
THCV	387.2	287.2/165.1*	76	28	6.7
		287.2/231.1		27	
		287.2/135.1		31	
THCVA	331.2	313.2/191.1*	80	25	7.9
		313.2/233.1		34	
		313.2/257.1		37	
		331.2/191.1		17	
		331.2/233.1		34	
		331.2/313.1		37	
(*R*)-HHC	316.5	317.2/193.0*	76	35	9.8
		317.2/122.9		49	
		317.2/137.2		29	
(*S*)-HHC	316.5	317.2/193.1*	61	33	9.7
		317.2/123.1		49	
		317.2/136.9		29	

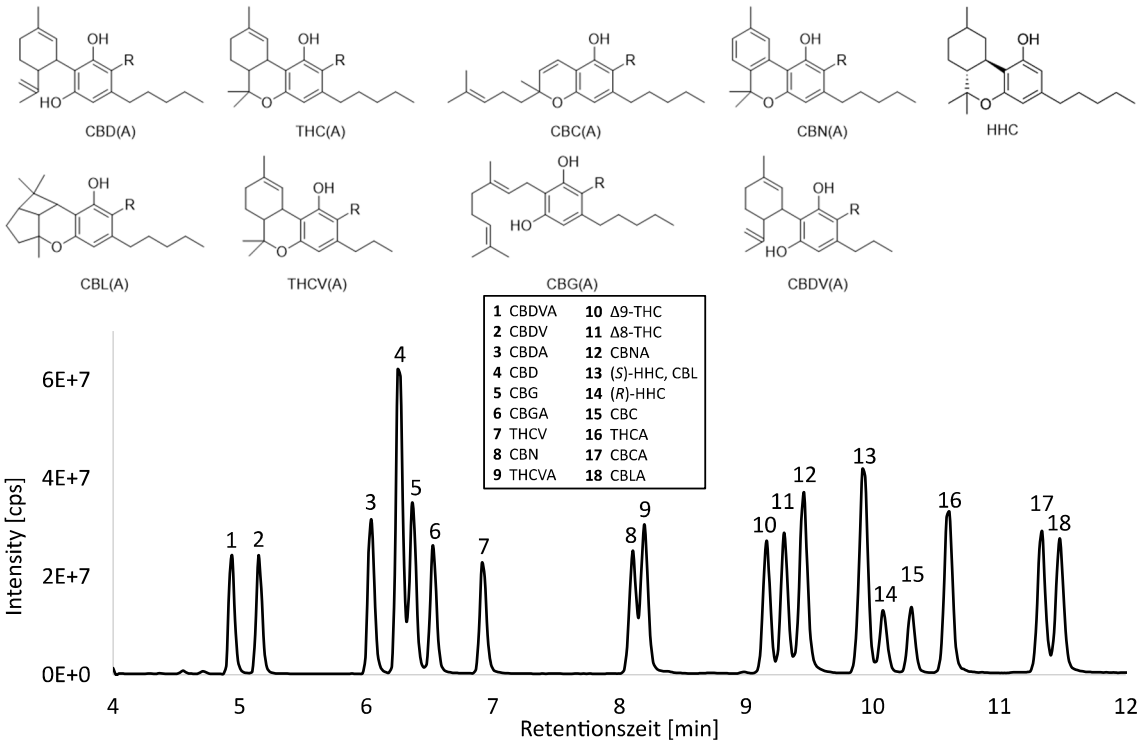

Figure S1 Structures of the cannabinoids analysed in this study. R = COOH are the cannabinoid acids, R = H the corresponding neutral forms

Figure S2 Total Ion Count (TIC) of a standard working solution with a concentration of c = 100 ng mL^{-1} for each analyte

Table S4 Overview of declared and measured major cannabinoid concentrations

Sample	major cannabinoid‡ declared	major cannabinoid‡ measured	measured deviation from declaration	major cannabinoid‡ certificate	certificate deviation from declaration
1	2.5 %	3.9 %	156 %	NA	NA
2	5.0 %	5.8 %	116 %	NA	NA
3	5.0 %	5.8 %	116 %	NA	NA
4	5.0 %	5.8 %	115 %	5.22 %	104 %
5	5.0 %	5.5 %	111 %	5.30 %	106 %
6	5.0 %	6.3 %	126 %	5.69 %	114 %
7	5.0 %	5.8 %	115 %	5.55 %	111 %
8	5.0 %	6.4 %	128 %	5.80 %	116 %
9	5.0 %	4.0 %	81 %	3.80 %	76 %
10	5.0 %	6.2 %	124 %	NA	NA
11	6.0 %	5.0 %	83 %	4.38 %	73 %
12	5.0 %	5.4 %	107 %	9.43 %	189 %
13	5.0 %	6.2 %	125 %	5.74 %	115 %
14	5.0 %	6.5 %	130 %	5.47 %	109 %
15	5.0 %	6.8 %	135 %	5.21 %	104 %
16	5.4 %	6.6 %	124 %	NA	NA
17	5.0 %	11.3 %	226 %	4.73 %	95 %
18	10.0 %	11.3 %	113 %	13.70 %	137 %
19	12.0 %	16.5 %	138 %	NA	NA
20	15.0 %	18.0 %	120 %	16.37 %	109 %
21	20.0 %	23.5 %	118 %	NA	NA
22	20.0 %	24.2 %	121 %	22.15 %	111 %
23*	5.0 %	5.3 %	106 %	6.77 %	135 %
24*	5.0 %	4.4 %	88 %	NA	NA
25†	2.5 %	3.1 %	124 %	3.11 %	124 %
26†	5.0 %	4.6 %	92 %	NA	NA

‡ CBD, CBG or CBD, whatever applicable
* CBG oil
† CBN oil

Table S5 Number of drops needed to exceed the ARfD for Δ^9-THC and provisional ADI for CBD for a 70 kg person. The estimation has only been calculated for samples in which Δ^9-THC or CBD could be quantified. The calculation of the number of drops is described in **Equation 1**

Sample	Δ^9-THC [mg kg^{-1}]	Δ^9-THC [µg $drop^{-1}$]	number of drops to exceed ARfD[§]	CBD [mg kg^{-1}]	CBD [mg $drop^{-1}$]	number of drops to exceed ADI[§]
1	–	–	–	39 026	1.45	7
2	25	0.93	76	58 231	2.16	5
3	–	–	–	58 047	2.15	5
4	283	10.49	7	57 619	2.14	5
5	1576	58.45	2	55 295	2.05	5
6	–	–	–	63 248	2.35	5
7	8	0.29	245	57 550	2.13	5
8	100	3.70	19	63 768	2.36	5
9	1031	38.24	2	40 498	1.50	7
10	1136	42.11	2	61 970	2.30	5
11	596	22.12	4	49 643	1.84	6
12	1347	49.94	2	53 626	1.99	6
13	57	2.13	33	62 472	2.32	5
14	–	–	–	65 019	2.41	5
15	38	1.40	51	67 651	2.51	4
16	1216	45.09	2	66 304	2.46	5
17	70	2.60	27	113 094	4.19	3
18	12	0.45	155	113 437	4.21	3
19	–	–	–	165 434	6.13	2
20	182	6.75	11	180 438	6.69	2
21	611	22.67	4	235 093	8.72	2
22	150	5.56	13	241 683	8.96	2
23*	5	0.17	414	2138	0.08	127
24*	1208	44.78	2	52 629	1.95	6
25†	–	–	–	15 987	0.59	17
26†	1071	39.70	2	52 711	1.95	6

§ assuming 70 kg body weight; results are rounded up to the full drop
* CBG oil
† CBN oil