Analytical and Bioanalytical Chemistry

Electronic Supplementary Material

Quantitative determination and validation of 17 cannabinoids in cannabis and hemp using liquid chromatography–mass spectrometry

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### Table S1 Calibration standard and QC sample concentrations (prepared in methanol, concentrations for each of 17 cannabinoids for each standard level)

| Standard / QC Sample ID | Cannabinoid Concentration (ng/mL) |
|-------------------------|-----------------------------------|
| STD-10                  | 10 000                            |
| STD-9                   | 9 000                             |
| STD-8                   | 6 000                             |
| STD-7                   | 2 000                             |
| STD-6                   | 1 000                             |
| STD-5                   | 400                               |
| STD-4                   | 100                               |
| STD-3                   | 40                                |
| STD-2                   | 20                                |
| STD-1                   | 10                                |
| STD-0                   | 0                                 |
| QC-3                    | 8 000                             |
| QC-2                    | 1 500                             |
| QC-1                    | 30                                |
| QC-LLOQ                 | 10                                |

### Table S2 Chromatographic peak resolution of key cannabinoids within 2 m/z of each other

| Cannabinoid-1 | Cannabinoid-2 | Δ m/z | Resolution |
|---------------|---------------|-------|------------|
| CBDV          | THCV          | 0     | 5.8        |
| CBD           | Δ9-THC        | 0     | 7.2        |
| Δ9-THC        | Δ8-THC        | 0     | 1.9        |
| Δ8-THC        | CBC           | 0     | 1.9        |
| CBC           | CBL           | 0     | 2.4        |
| CBD           | CBG           | 2     | 4.7        |
| CBG           | Δ9-THC        | 2     | 2.1        |
| CBDVA         | THCVA         | 0     | 7.4        |
| CBDA          | Δ9-THCA       | 0     | 8.5        |
| Δ9-THCA       | CBCA          | 0     | 3.6        |
| CBCA          | CBLA          | 0     | 2.1        |
| CBDA          | CBGA          | 2     | 9.5        |
| Δ9-THCA       | CBGA          | 2     | 1.0        |
Fig. S1 Δ9-THC Linear regression, weighted 1/x² (duplicate injection of a calibration curve, beginning and end of batch)

THC-1

$Y = -0.00133272 + 0.00233073 \times X$  $R^2 = 0.9982$  W: 1/X²

Fig. S2 Δ9-THCA Linear regression, weighted 1/x² (duplicate injection of a calibration curve, beginning and end of batch)

THCA-1

$Y = -0.00352983 + 0.00467283 \times X$  $R^2 = 0.9986$  W: 1/X²
Fig. S3 CBD Linear regression, weighted $1/x^2$ (duplicate injection of a calibration curve, beginning and end of batch)

Fig. S4 CBDA Linear regression, weighted $1/x^2$ (duplicate injection of a calibration curve, beginning and end of batch)
**Fig. S5** CBG Linear regression, weighted 1/x^2 (duplicate injection of a calibration curve, beginning and end of batch)

**Fig. S6** CBGA Linear regression, weighted 1/x^2 (duplicate injection of a calibration curve, beginning and end of batch)
**Fig. S7** CBN Linear regression, weighted 1/x² (duplicate injection of a calibration curve, beginning and end of batch)

Y = -0.00214749 + 0.00254246 * X  \( R^2 = 0.9991 \)  W: 1/X²

![CBN Linear regression graph](image1)

**Fig. S8** CBNA Linear regression, weighted 1/x² (duplicate injection of a calibration curve, beginning and end of batch)

Y = -0.000645604 + 0.000788326 * X  \( R^2 = 0.9985 \)  W: 1/X²

![CBNA Linear regression graph](image2)
**Fig. S9** CBC Linear regression, weighted $1/x^2$ (duplicate injection of a calibration curve, beginning and end of batch)

**Fig. S10** CBCA Linear regression, weighted $1/x^2$ (duplicate injection of a calibration curve, beginning and end of batch)
**Fig. S11** THCV Linear regression, weighted $1/x^2$ (duplicate injection of a calibration curve, beginning and end of batch)

**Fig. S12** THCV-1 Linear regression, weighted $1/x^2$ (duplicate injection of a calibration curve, beginning and end of batch)
**Fig. S13** CBDV Linear regression, weighted 1/x^2 (duplicate injection of a calibration curve, beginning and end of batch)

**CBDV-1**

\[ Y = -0.00196683 + 0.00249242 \times X \]

\[ R^2 = 0.9991 \]

W: 1/X^2

**Fig. S14** CBDVA Linear regression, weighted 1/x^2 (duplicate injection of a calibration curve, beginning and end of batch)

**CBDVA-1**

\[ Y = -0.00962057 + 0.00918429 \times X \]

\[ R^2 = 0.9988 \]

W: 1/X^2
Fig. S15 CBL Linear regression, weighted $1/x^2$ (duplicate injection of a calibration curve, beginning and end of batch)

Fig. S16 CBLA Linear regression, weighted $1/x^2$ (duplicate injection of a calibration curve, beginning and end of batch)
Fig. S17 Δ8-THC Linear regression, weighted 1/x² (duplicate injection of a calibration curve, beginning and end of batch)