

## Application News

SSI-LCMS-045

Liquid Chromatography Mass Spectrometry

# Quantitative Analysis of Cannabinoids using the LCMS-2020 Single Quad MS



LCMS-2020



### Summary

Evaluation and quantitation of a variety of cannabinoids on an LCMS-2020 single quadrupole mass spectrometer.

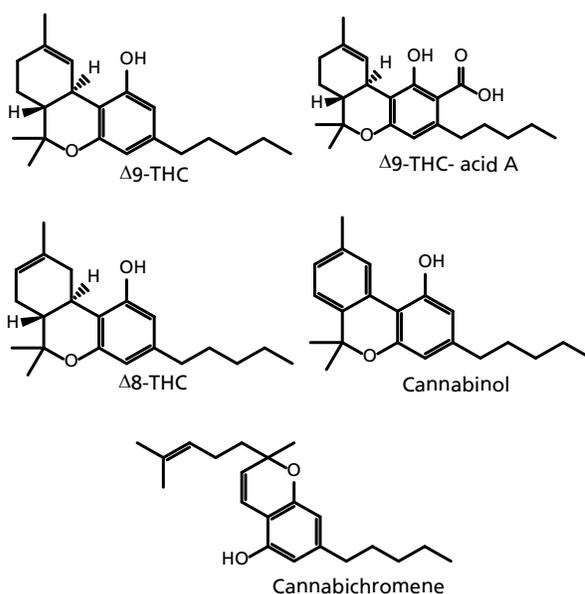
### Method

Cannabichromene (CBC) and  $\Delta^9$ -THC Acid A (THCA) standards were purchased from Restek (Bellefonte, PA). Cannabinol (CBN),  $\Delta^8$ -THC (d8-THC),  $\Delta^9$ -THC (d9-THC) and Cannabidiol (CBD) were purchased from Cerilliant (Round Rock, TX). A stock concentration of 1  $\mu\text{g}/\text{mL}$  for each standard was used for SIM optimization. The standards were combined into one solution and then serially diluted with 70/30 (%) methanol/water using 2-fold dilutions yielding concentrations ranging from 8192 ng/mL to 1 ng/mL. The standards (**Figure 1**) were transferred to autosampler vials and injected into a Nexera-LCMS-2020 system for analysis.

A Thermo Hypersil Gold (1.9  $\mu\text{m}$  x 2.1 mm x 100 mm) was used with a binary gradient of 5 mM ammonium acetate in water and acetonitrile. The gradient conditions are shown in **Figure 2**. The flow rate was 0.5 mL/min with a run time of 6.8 min. The column temperature was 45° C and the injection volume was 5  $\mu\text{L}$ .

### LCMS-2020 Analysis

Dual ion electrospray ionization (DUIS) in both positive and negative modes was used for ionization of the analytes on the LCMS-2020. A positive and negative scan and selected ion monitoring (SIM) modes were used simultaneously for analysis. Details of the MS parameters are shown in **Table 1**.

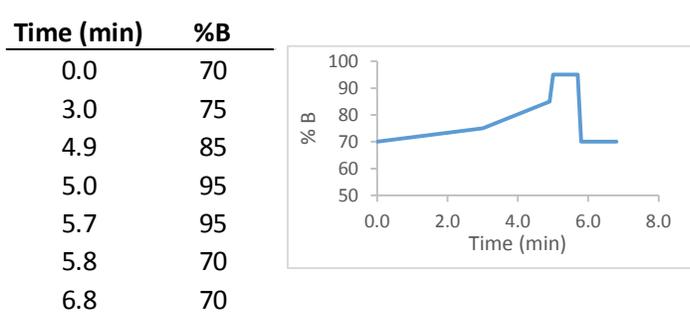


**Figure 1.** Chemical structures for cannabinoids.

**Results and Discussion**

Peaks were smoothed using the standard method set to 2 counts and 2 sec for width. The auto integration setting was used with a setting of 1 max peak and 6 sec width. d8-THC was integrated by turning off peak integration from 4.8-5.0 minutes. Linearity was achieved from 0.5-1024ng/mL for CBN and d9-THC, 1-1024ng/mL for d8-THC, 2-128ng/mL for

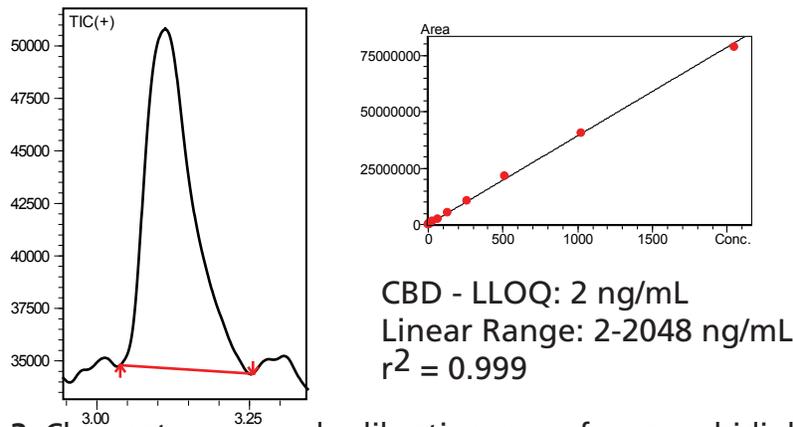
THCA, 2-2048ng/mL for CBD and 4-2048ng/mL for CBC. The calibration curve was weighted using 1/C and not forced through zero. No standards were excluded over the included range and  $r^2$  values ranged from 0.998-0.999. A representative chromatogram and calibration curve for each analyte are shown in **Figures 3-8**.



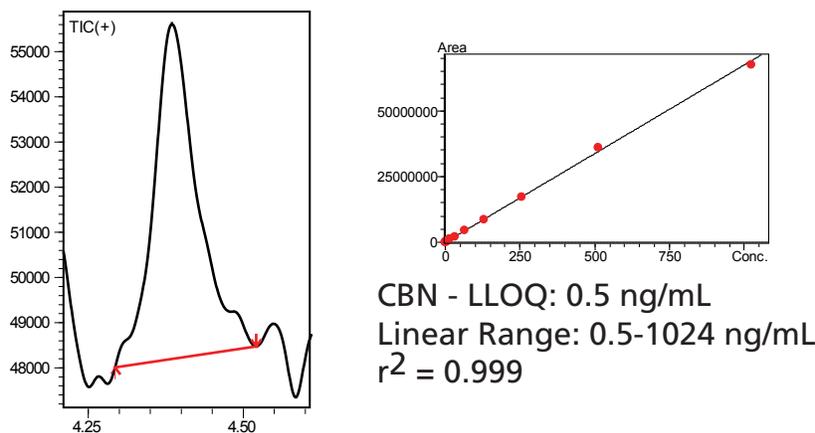
**Figure 2.** Gradient conditions.

<b>MS Interface Parameters</b>	
Interface	DUIS
Nebulizing gas flow	2 L/min
Drying gas flow	15 L/min
DL Temperature	300 °C
Heat Block Temperature	500 °C
Polarity	(+) CBD, CBN, d8-THC, d9-THC, CBC (-) THCA

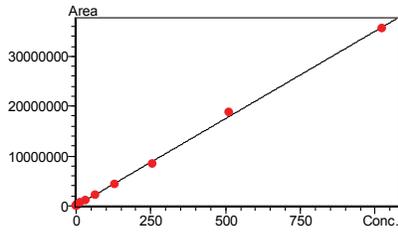
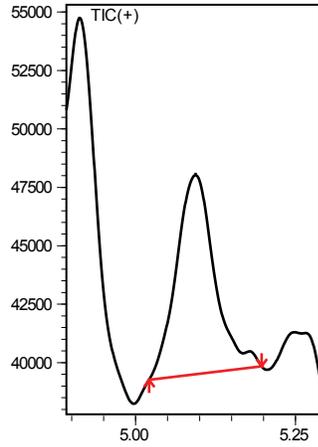
**Table 1.** MS Interface parameters.



**Figure 3.** Chromatogram and calibration curve for cannabidiol (CBD).

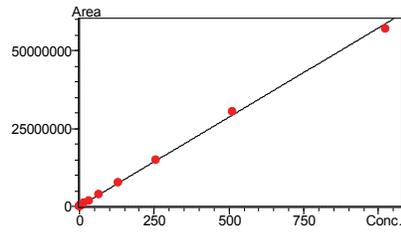
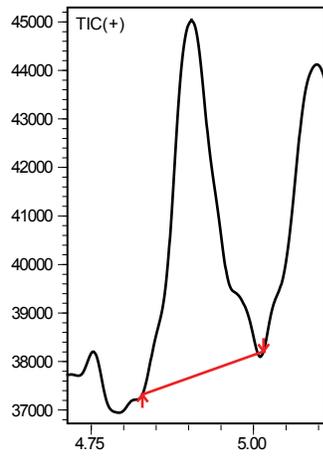


**Figure 4.** Chromatogram and calibration curve for cannabinol (CBN).



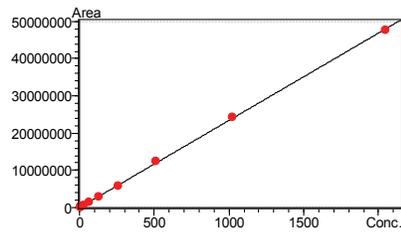
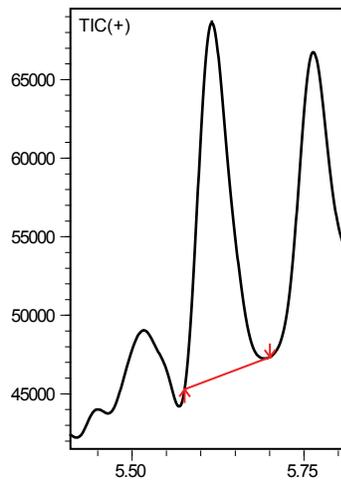
d8-THC- LLOQ: 1 ng/mL  
 Linear Range: 1-1024 ng/mL  
 $r^2 = 0.999$

Figure 5. Chromatogram and calibration curve for d8-THC.



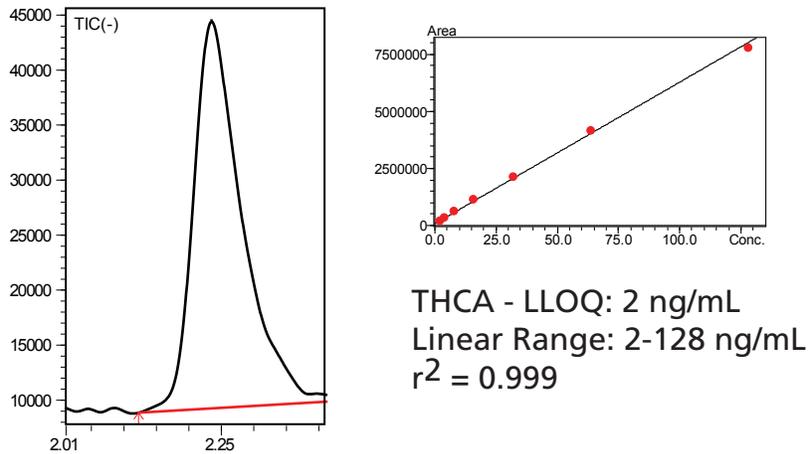
d9-THC- LLOQ: 0.5 ng/mL  
 Linear Range: 0.5-1024 ng/mL  
 $r^2 = 0.999$

Figure 6. Chromatogram and calibration curve for d9-THC.



CBC - LLOQ: 4 ng/mL  
 Linear Range: 4-2048 ng/mL  
 $r^2 = 0.999$

Figure 7. Chromatogram and calibration curve for cannabichromene (CBC).



**Figure 8.** Chromatogram and calibration curve for d9-THC Acid A (THCA).

### Conclusion

A method for rapid quantitation of various cannabinoids was requested utilizing UHPLC equipment and LCMS to increase the speed and sensitivity of analysis. A 7 minute method was developed, with the main limiting factor being the separation of d8-THC and d9-THC. If d8-THC and d9-THC do not need to be individually quantified then the method could be shortened further.

It is important to note that these results were achieved using standards without matrix, but the ability of the Nexera X2 system and LCMS-2020 mass spectrometer to enable rapid, sensitive quantitative analysis of cannabinoids is highlighted by this method.

# UPLC-MS

ULTRA FAST MASS SPECTROMETRY



LCMS-8030



LCMS-8040



LCMS-8050



LCMS-2020



LCMS-IT-TOF

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