
Supplementary Materials

Evaluation of an Oral Fluid Collection Device and a Solid-Phase Extraction Method for the Determination of Coca Leaf Alkaloids by Gas Chromatography–Mass Spectrometry

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Table S1. Matrix effect equations.

| | |
|---|---|
| Matrix Effect equation | $ME(\%) = \left(\frac{B}{A} - 1 \right) \times 100$ |
| Matrix Effect equation with normalized areas (deuterated internal standard) | $ME_{(n)}(\%) = \left(\frac{B}{A} - 1 \right) \times 100$ |
| Matrix Effect equation using Quantisal® device | $ME_Q(\%) = \left(\frac{B_Q}{A} - 1 \right) \times 100$ |
| Matrix Effect equation with normalized areas using Quantisal® device | $ME_{Q(n)}(\%) = \left(\frac{B_Q}{A} - 1 \right) \times 100$ |

Table S2. Recovery equations.

| $R_{(x)}$ | $[x \text{ areac}/x \text{ areab}] \times 100^{(.)}$ |
|--------------------------|---|
| $R_{(n)}(x/x\text{-d3})$ | $[x \text{ areac}/x\text{-d3}]/[x \text{ areab}/x\text{-d3}] \times 100^{(.,)}$ |

x: EME, CUS, TRO, COC, t-CIN.; x-d3: EME-d3, COC-d3; ^(.) Compound area obtained from Study Design C and B (absolute areas); ^(.,) Compound area obtained from Study Design C and B (normalized areas with deuterated).

Table S3. Process Efficiency and Extraction Recovery equations.

| Process Efficiency or Apparent Recovery (R_A and $R_{A(Q)}$) | | Extraction Recovery or Extraction Efficiency (R_E and $R_{E(Q)}$) | |
|--|--|---|--|
| $R_A (\%) = (\text{absolute area C}/\text{absolute area A}) \times 100$ | | $R_E (\%) = (\text{absolute area C}/\text{absolute area B}) \times 100$ | |
| $R_{A(Q)} (\%) = (\text{absolute area } C_Q/\text{absolute area A}) \times 100$ | | $R_{E(Q)} (\%) = (\text{absolute area } C_Q/\text{absolute area } B_Q) \times 100$ | |
| Normalized areas (IS) | | | |
| $R_{A(n)} (\%) = \text{area (C/IS-d3)}/\text{area (A/IS-d3)} \times 100$ | | $R_{E(n)} (\%) = \text{area (C/IS-d3)}/\text{area (B/IS-d3)} \times 100$ | |
| $R_{A(Q)(n)} (\%) = \text{area (C}_Q/\text{IS-d3)}/\text{area (A/IS-d3)} \times 100$ | | $R_{E(Q)(n)} (\%) = \text{area (C}_Q/\text{IS-d3)}/\text{area (B}_Q/\text{IS-d3)} \times 100$ | |