

## Raman spectroscopy as a potential tool for label free therapeutic drug monitoring from human serum: the case of Busulfan and Methotrexate

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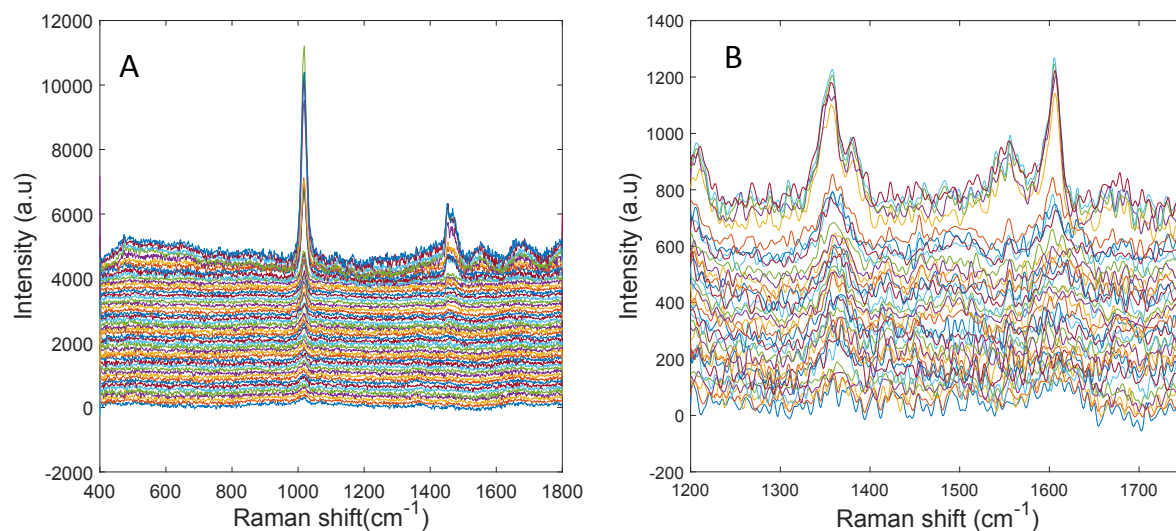
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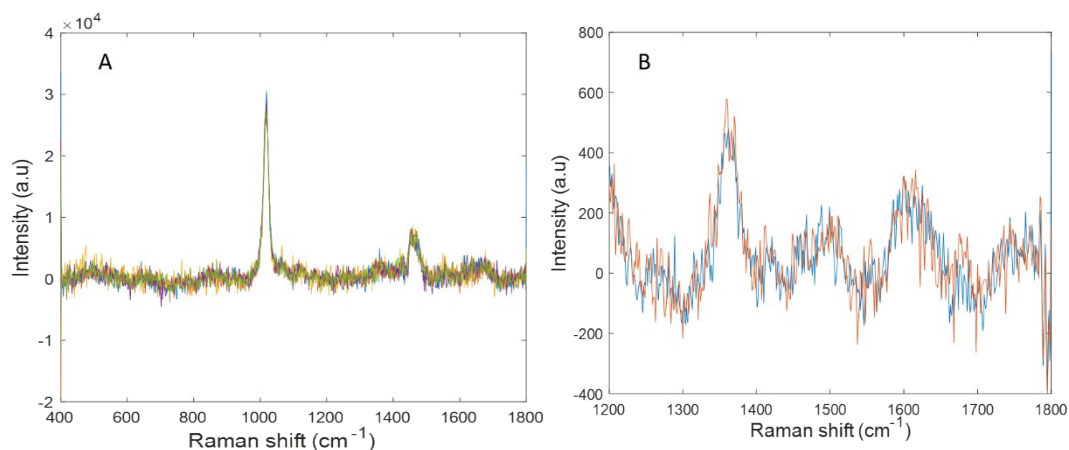
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### 1. EMSC corrected dataset of Busulfan and Methotrexate



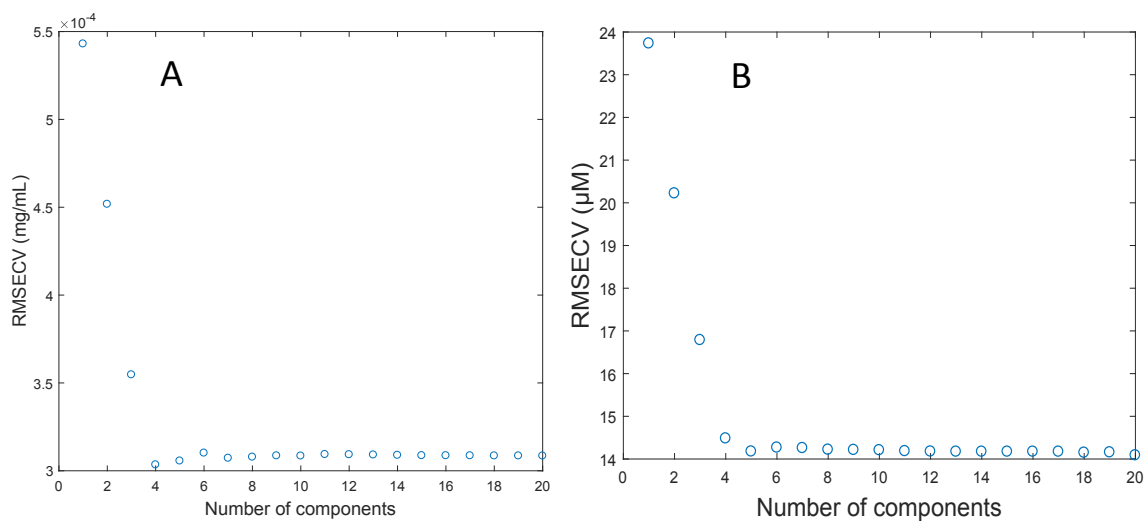
**Figure S1:** EMSC corrected and smoothed dataset of **A** Busulfan from 0mg/mL to 0.05mg/mL in the fingerprint region. **B:** Methotrexate from 0 $\mu$ M to 500 $\mu$ M from 1200 $\text{cm}^{-1}$  to 1800 $\text{cm}^{-1}$ . The spectra are offset for clarity.

## 2. EMSC corrected data of Busulfan and Methotrexate at the LOD



**Figure S2:** EMSC corrected and smoothed dataset of **A** Busulfan at 0.0002mg/mL in the fingerprint region. **B:** Methotrexate at 10μM from 1200cm<sup>-1</sup> to 1800cm<sup>-1</sup>. The spectra are offset for clarity.

## 3. Root Mean Square Error Cross Validation (RMSECV) plots for Busulfan and Methotrexate



**Figure S3.** Evolution of RMSECV for **(A)** Busulfan and **(B)** Methotrexate. The RMSECV values are calculated to be 0.0003mg/mL for Bu and 4.02μM for MTX