Electronic Supplementary Material (ESI) for Analytical Methods.


# Detection of Organic and Inorganic Gunshot Residues from Hands using Complexing Agents and LC-MS/MS

## Supplemental Figures and Tables

**Table S1:** Detailed description of the mobile phase composition and times for the LC.

| Time (min) | Water w/ 0.1% FA (A%) | Acetonitrile w/ 0.1% FA (B%) |
|---|---|---|
| 0.00 | 80 | 20 |
| 1.30 | 55 | 45 |
| 2.00 | 50 | 50 |
| 2.40 | 45 | 55 |
| 3.30 | 35 | 65 |
| 4.20 | 32 | 68 |
| 4.50 | 30 | 70 |
| 5.30 | 28 | 72 |
| 6.50 | 25 | 75 |
| 8.00 | 5 | 95 |
| 9.00 | 90 | 10 |

**Table S2:** Detailed description of the source parameters for the MS/MS.

| Source Parameters | | |
|---|---|---|
| **Gas Temperature** | 300 °C | |
| **Gas Flow** | 10 l/min | |
| **Nebulizer** | 20 psi | |
| **Sheath Gas Temperature** | 250 °C | |
| **Sheath Gas Flow** | 7 l/min | |
| **Capillary** | **Positive** | **Negative** |
| | 4500 V | 2500 V |
| **Nozzle** | **Positive** | **Negative** |
| | 2000 V | 2000 V |

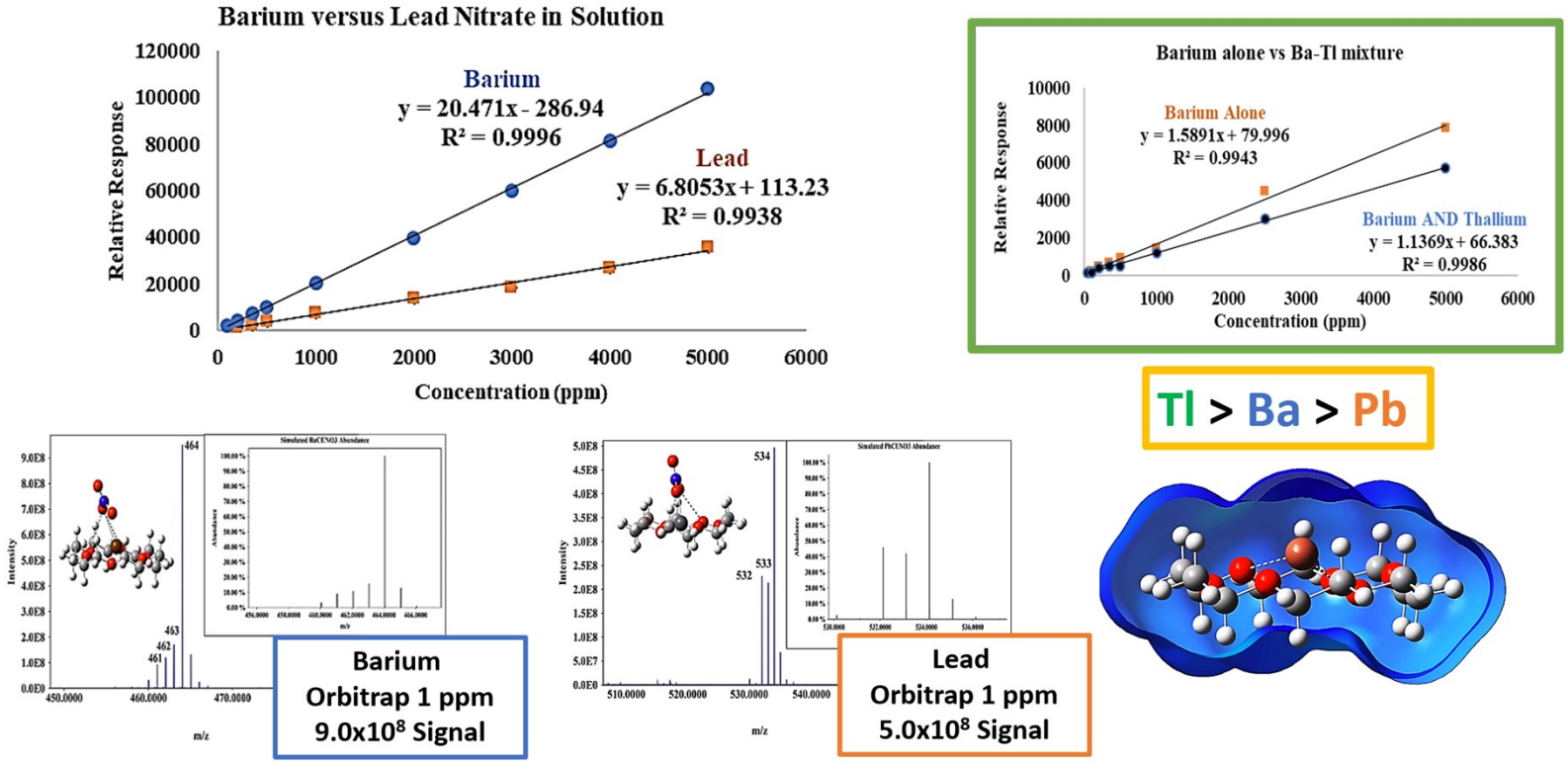


**Figure S1:** Comparison of responses of barium and lead within one solution using 18C6 complexing agent. Additionally, the measured response and proposed theoretical structure of thallium and 18C6.

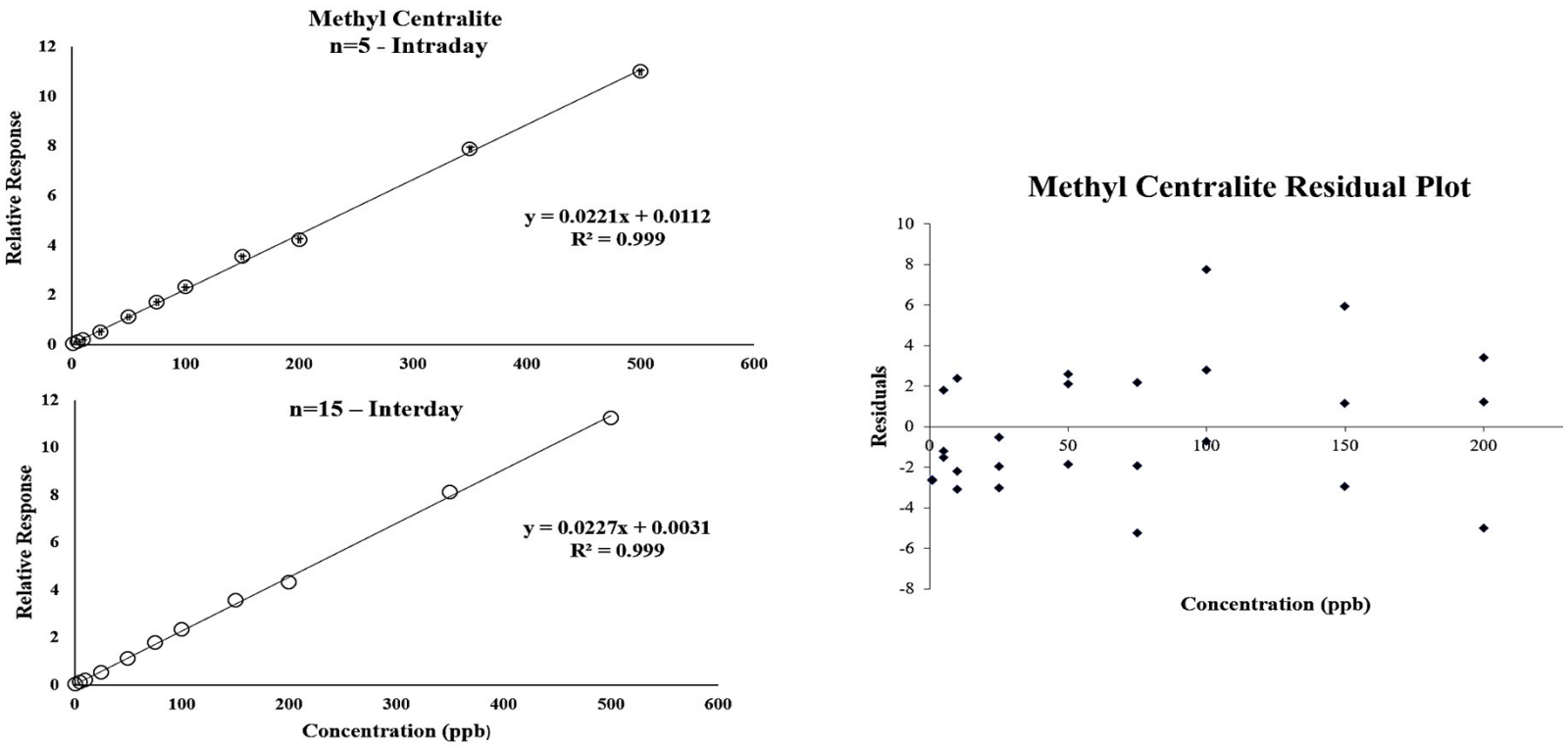


**Figure S2:** Example of intra- and interday variability of methyl centralite along with the residual plot of the working range. These figures demonstrate the linearity and response of this OGSR compound and the randomness and homoscedasticity of the points across all concentration levels.

**Table S3:** Detailed definitions of the Figures of Merit outlined by the Eurachem guidelines. Included are the equations associated with the corresponding validation parameter.

| Figure of Merit | Definition | Equation |
|---|---|---|
| **Selectivity** | The ability of a method to distinguish analytes without interferences. Techniques such as liquid chromatography and mass spectrometric data are helpful to distinguish both elution and fragmentation patterns. Selectivity testing measures standards against other independent methods and test the samples against possible interferences. | **N/A** |
| **Limit of Detection** | The lowest concentration of an analyte detectable at a specified confidence level. Ten blank measurements typically determine it without analytes or 10 replicates of low concentrations. Equation 1 refers to the lowest value at which an accurate detection of an analyte is present or absent qualitatively. | $LOD = 3 * \frac{S}{N}$ |
| **Limit of Quantitation** | The lowest concentration of an analyte performance is deemed acceptable for a specified application. Ten blank measurements typically determine it without analytes or 10 replicates of low concentrations. The lowest value at which the analyte concentration can accurately quantitatively. | $LOD = 10 * \frac{S}{N}$ |
| **Sensitivity** | A change in instrument response, which corresponds to a change in the measured quantity. | **N/A** |
| **Working Range** | Interval over which the method provides results with an acceptable uncertainty. The lower end of a working range is restricted to the LOQ, while significant anomalies in concentrations affecting the analytical sensitivity define the upper end. In this case, residual plots allow for more refined explanations and limitations of calibration curves as they must fall below ± 20% of expected concentrations. | **N/A** |
| **Bias** | Comparing the mean of the results ($\bar{x}$) from the candidate method with a suitable reference value ($x_{ref}$) and calculated. Bias typically describes the percent recovery of a particular extraction procedure, such as collection substrates. | $R\,(\%) = \frac{\bar{x}}{x_{ref}} * 100$ |