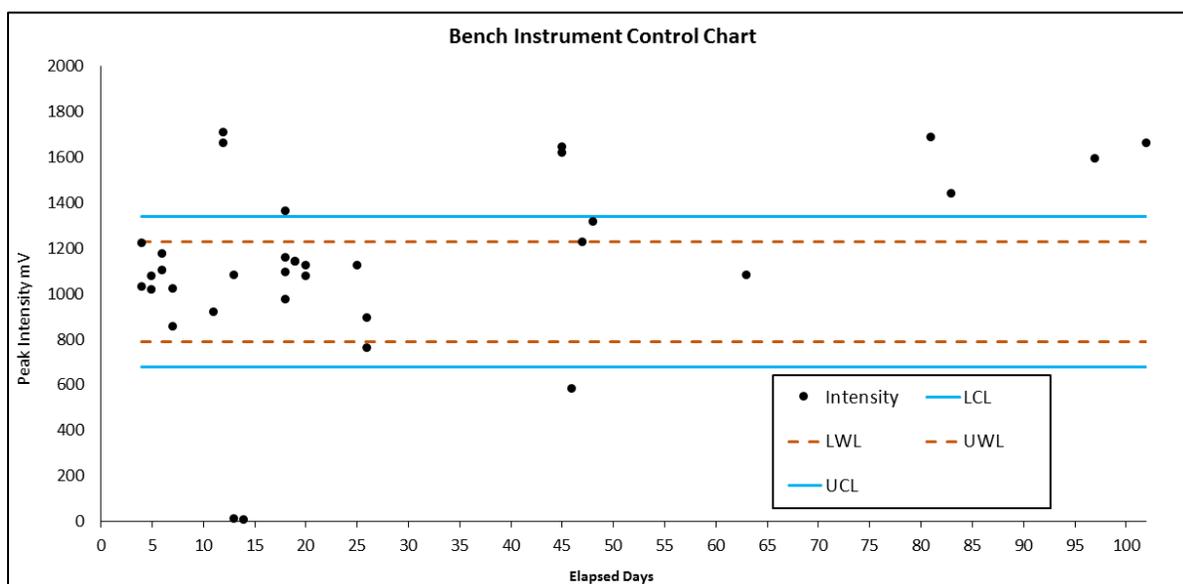


## Evaluation and Validation of Ion Mobility Spectrometry for Presumptive Testing Targeting the Organic Constituents of Firearms Discharge Residue - Supplementary Information

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**Figure S1.** Control chart for the benchtop instrument.

As noted in the article, the performance of this instrument over time indicated a greater variation and degradation compared to the benchtop. Depending on the analysis being done, data was still collected but was flagged for further consideration and scrutiny. Note that on several days, multiple DtBP samples were collected as the instrument was used both morning and afternoon. Intra-day variation was greater with this instrument than with the portable.

It is worth noting that even on days when the warning and control limits were exceeded, the instrument was still operational and would have passed instrument verification challenges. The DtBP was purposely selected to provide additional quality assurance that clearly will be essential if this methodology is to be adapted for screening purposes.

Figures S2-S5. Detection threshold plots, benchtop instrument

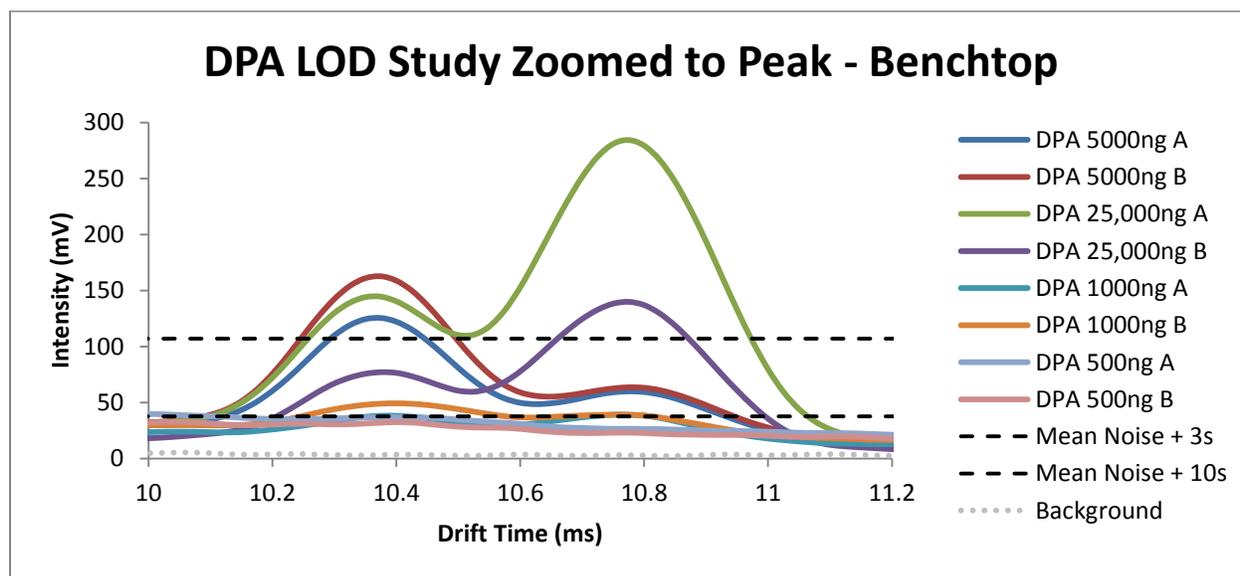


Figure S2. Dimethyl phthalate spectra ranging from 1ng to 25,000ng in which the detection threshold was determined to be 500ng for the benchtop instrument.

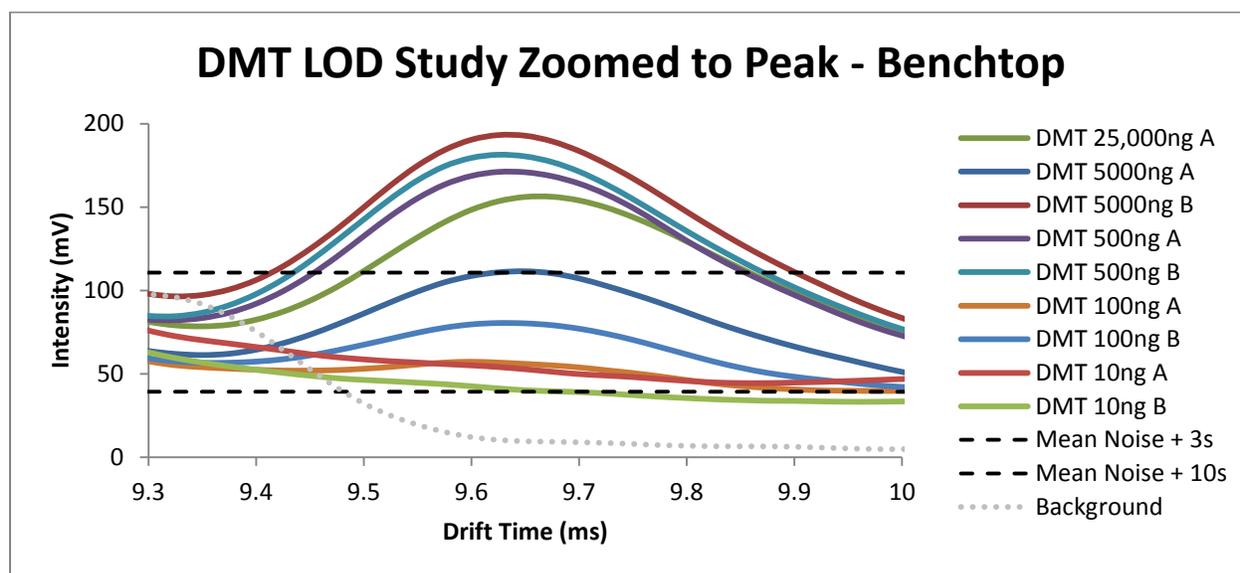
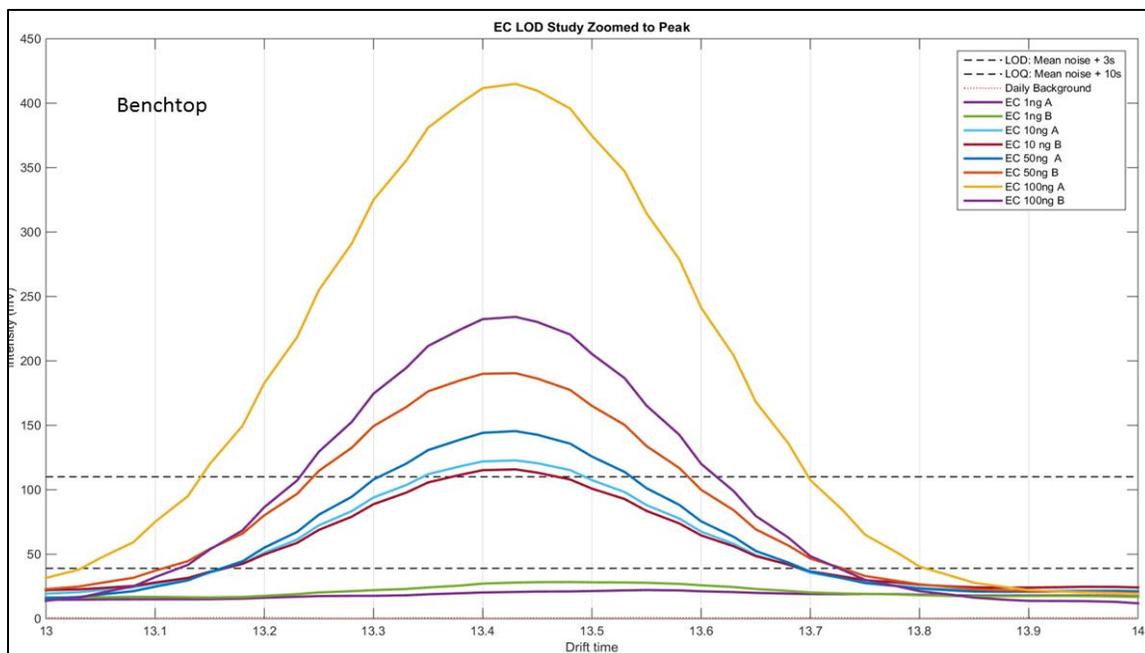
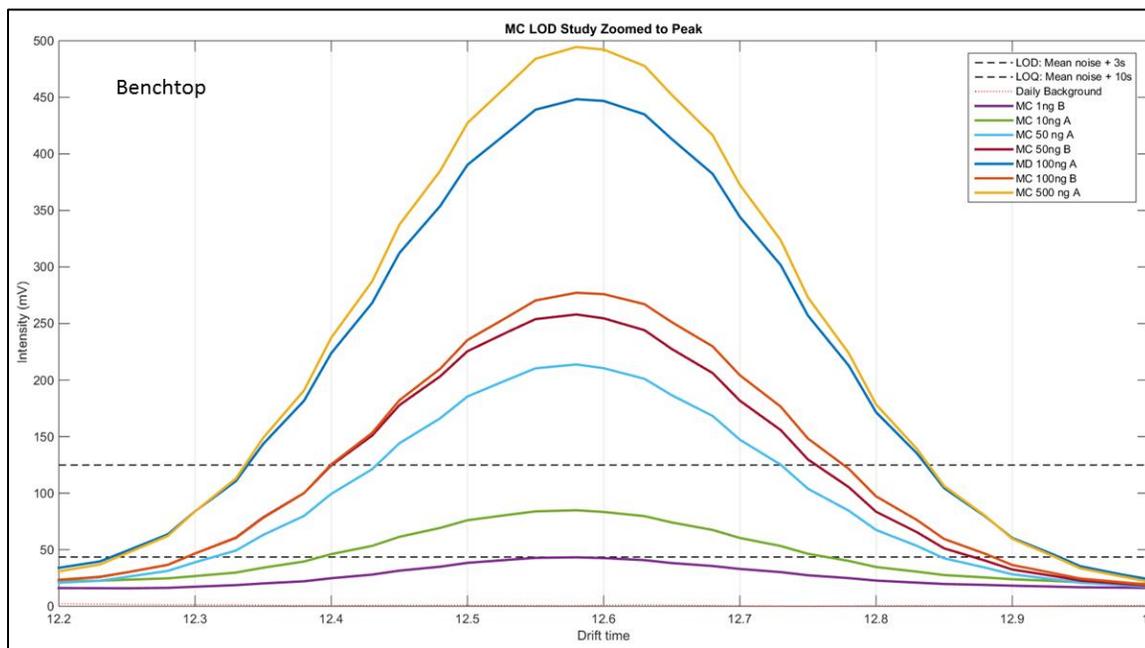


Figure S3. Diphenylamine spectra ranging from 500ng to 25,000ng in which the detection threshold was determined to be 1000ng for the benchtop instrument.

Note that two peaks are associated with DPA (Figure S3). This presumably arises from thermal degradation of DPA although the product(s) is unknown. The benchtop instrument was operated at higher temperatures than the portable (Table 2) for reasons discussed in the text; however for DPA the hotter temperatures appear to be less desirable for peak-based detection. With a pattern-based approach, the higher temperatures may not be a limitation.

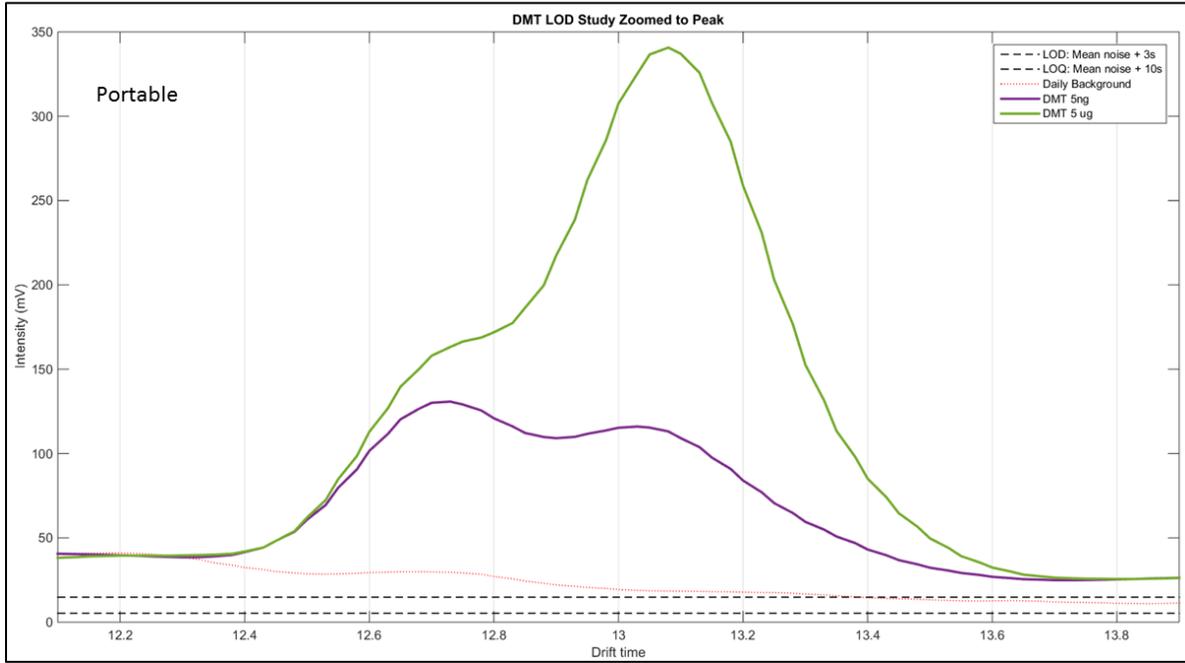


**Figure S4.** Ethyl centralite spectra ranging from 1ng to 100ng in which the detection threshold was determined to be 10ng for the benchtop instrument.

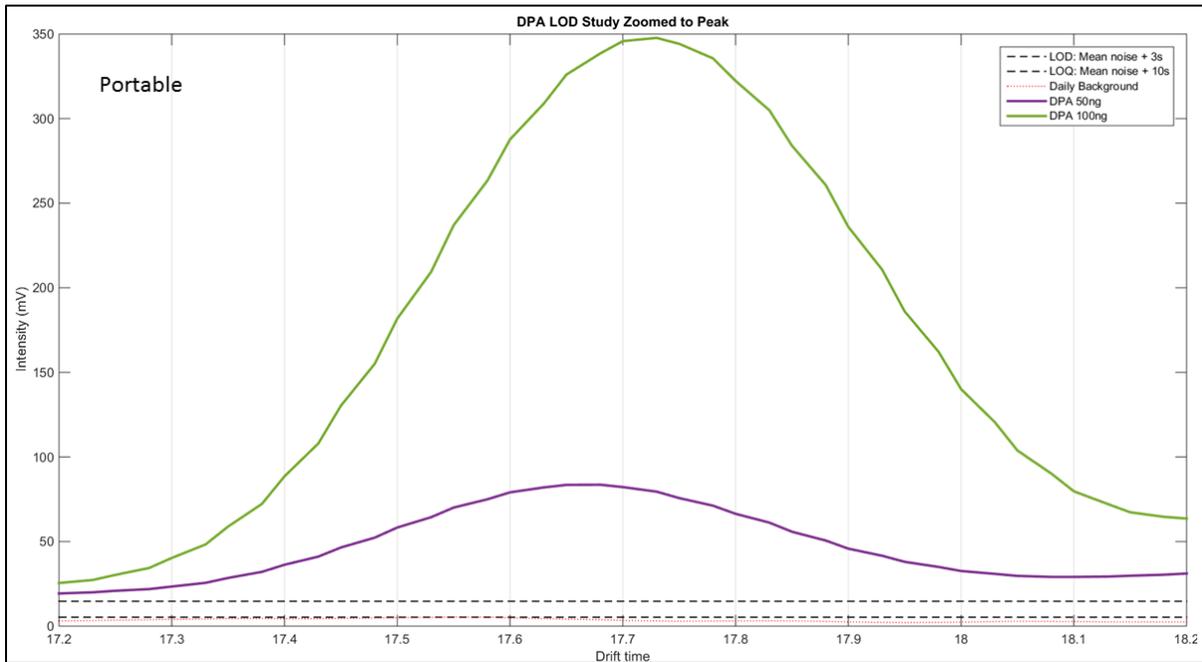


**Figure S5** Methyl centralite spectra ranging from 1ng to 500ng in which the detection threshold was determined to be 10ng for the benchtop instrument.

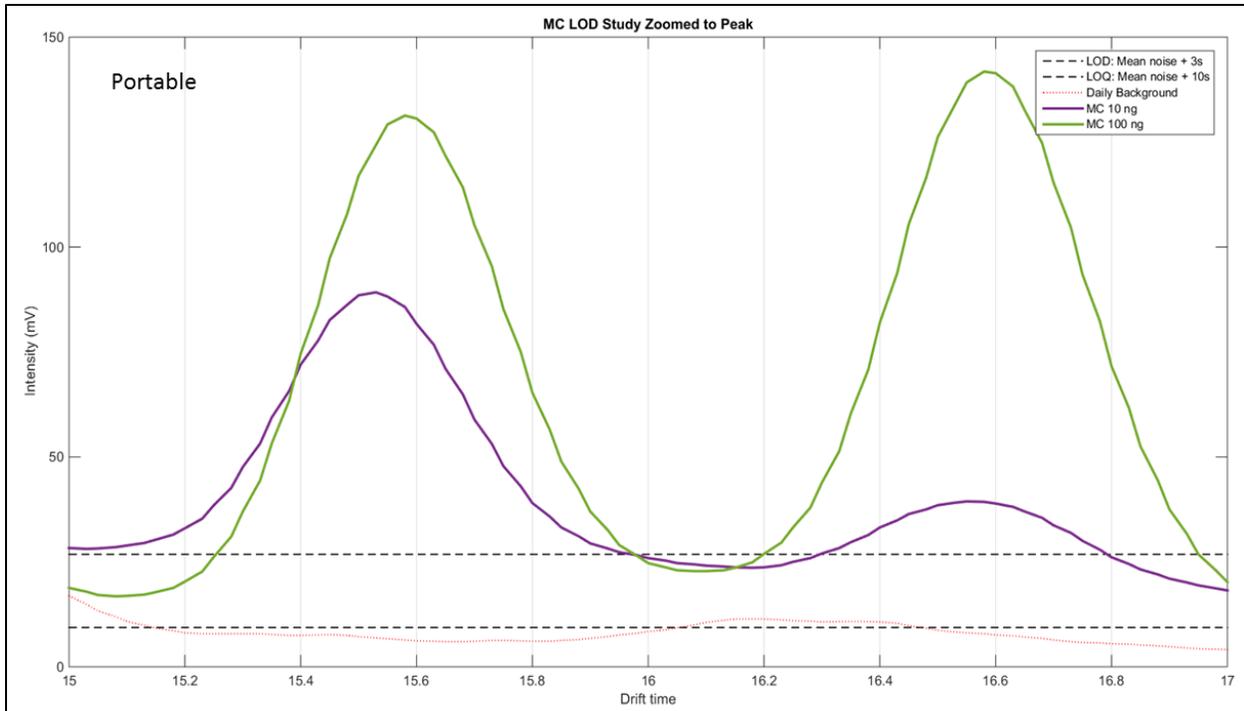
**Figures S6-S9. Detection threshold plots, handheld instrument**



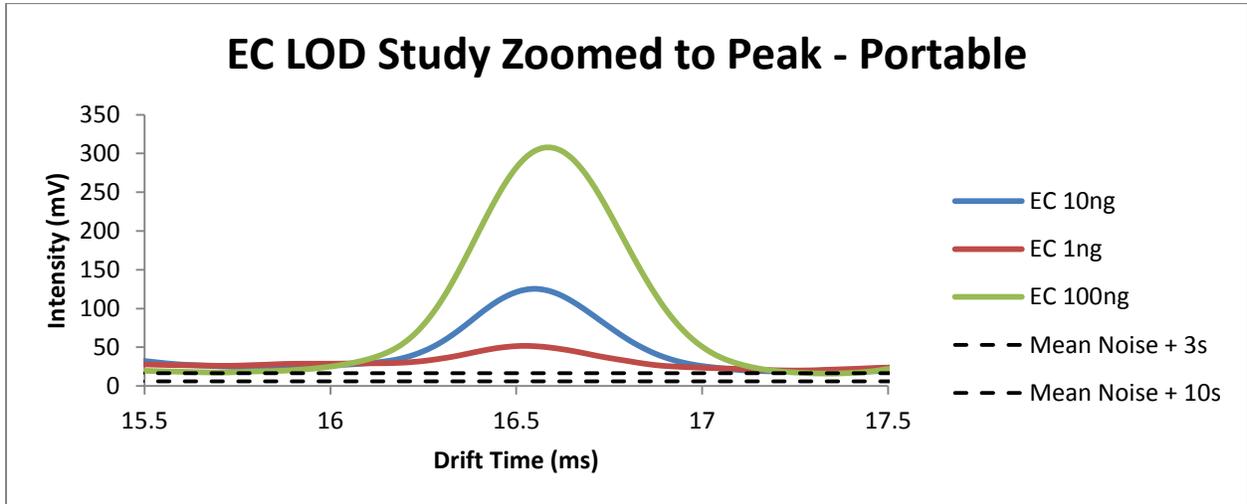
**Figure S6.** Dimethyl phthalate spectra in which the detection threshold was determined to be 5ng for the portable instrument. The width of the peak may be attributable to clustering. For the benchtop instrument (Figure S2, higher temperatures) this pattern was not observed.



**Figure S7.** Diphenylamine spectra in which the detection threshold was determined to be 50ng for the portable instrument.



**Figure S8.** Methyl centralite spectra in which the detection threshold was determined to be 10ng for the portable instrument. The appearance of two mobility peaks was seen in the portable but not with the benchtop (Figure 3 in the text). This could represent a monomer/dimer pair but this is unconfirmed.



**Figure S9.** Ethyl centralite spectra in which the detection threshold was determined to be 1ng for the portable instrument.