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Sent: Monday, June 10, 2019 2:49 PM
To: Leung, Lam-Wing H
Subject: ⚠ Performance of Selected Table 3+ Analytes
Attachments: ATT00001.txt

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Lam,

As we have discussed several times over the last several weeks, there are 4 compounds within the list of Table 3+ analytes that have proven to be very problematic for analysis under the conditions of the Table 3+ method. Those 4 compounds are;

- a. DFSA - CAS #422-67-3
- b. MMF – CAS #1514-85-8
- c. MTP – CAS #93449-21-9
- d. PPF Acid – CAS #422-64-0

The challenges that are presented by these 4 compounds under the analysis conditions of the Table 3+ are several.

- a. Chromatographically, DFSA and MMF are not retained well and in fact elute essentially in the void volume of the column and column introduction system. MTP and PPF acid elute a little past the void volume but not by very much. The reason this is important is that due to the short carbon chain length of the compounds, the range of options for product ion masses and transition ion masses to monitor for detection is limited. Therefore, without good chromatographic separation, the mass spectrometer struggles to differentiate these compounds from background. This then has a direct impact on the sensitivity that one is able to achieve and has as a direct impact on the ruggedness of the analysis.
- b. In attempts to improve the chromatography to improve detection of these compounds, we have adjusted the mobile phase composition so that upon injection of sample, the mobile phase is essentially 100% water. This has the effect of causing chromatography columns with a C18 functionality to collapse which negatively impacts the chromatography of all of the other Table 3+ compounds, while only marginally improving the performance of these 4 compounds. If and when we have tried to change to a column chemistry that might be more accommodating of high aqueous content, then the performance of the other Table 3+ compounds is significantly impacted.

In summary, it would be our suggestion to develop a technique that uses a completely separate separation and analysis for these 4 compounds so that more reliable detection and analysis can be performed.

Regards,
Chuck

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