

Simplifying the detection of explosives in a walk-up environment

Peter Luke¹; Richard Sleeman¹; Charles Liddell¹; Scott J. Campbell² and John H. Moncur²

¹Mass Spec Analytical, Bristol, UK. and ²SpectralWorks Limited, Runcorn, UK.



Scan Me

Introduction

Rapid screening and detection of explosives is a critical capability for global security. Here we present an ambient ionisation interface to a triple quadrupole mass spectrometer instrument which allows the comprehensive MS data to be reduced to a simple Yes/No result for non-MS users such as security personnel. The touch screen software interface (Figure 1) is scalable from a single instrument implementation through to an extensive enterprise or cloud-based solution controlling multiple instruments over multiple geographical locations. The instrument agnostic software and ambient ionization hardware allows for the application to be run on any MS vendors' instrument from quadrupole to time of flight. As well as instant feedback to the user, results can be reviewed by expert users, either onsite or remotely, as well as archived and retrieved for data mining purposes and trend analysis.

Method and Workflow

The following hardware and software are used in this workflow:

- Thermal Extraction Ion Source (TEIS) – Mass Spec Analytical, Bristol, UK.
- SCIEX Triple Quadrupole 3500 LC-MS System – SCIEX, Concord, Toronto, Canada.
- RemoteAnalyzer® Open Access Software – SpectralWorks, Runcorn, UK.
- Scintinel™ (powered by RemoteAnalyzer) Software – Mass Spec Analytical/SpectralWorks.

The analytical workflow is as follows:

1. QC check using explosives mixture or simulant.

Prior to sampling, the validity of the instrument needs to be verified by inserting a check solution into the desorber and obtaining a result within predetermined parameters. The results are shown as a Red or Green indication.

2. Blank checks of gloves and swab.

A swab is sampled to ensure its not contaminated. The swab is then used to check the user's gloves and/or working area. Each sample is passed through the desorber in turn and if any positive results should occur the swab and gloves are replaced, work area cleaned if required, and retested. The process is repeated until a clean indication is obtained.

3. Sample collection

A Whatman No. 2 filter paper has been selected as our swab. It is rubbed back and forth by hand across any surface of interest approximately 4 or 5 times to allow transfer from the surface to the swab.

4. Sample acquisition

Touch screen selection or a few mouse clicks is all that is needed to select the sample type and method before initiating the start sample. On-screen directions and audio, if selected, instruct the user when and how long to insert the swab.

5. Results

The analytical run takes 8-10 seconds. The screen updates with a list of all the compounds looked for and positive results, if any, are indicated in red.

6. Confirmation of positive results (an optional advanced step)

Positive indications can be repeated by selecting a confirmation experiment. The confirmation experiment is more specific and only includes the compound of interest. In the case of the Sciex MSMS instrument, we have included more ion pairs in the method to increase specificity. The area where the positive results was obtained is re-swab and resubmitted. As before, the sample result will be shown with either a red or green indicator to show a positive or negative result.

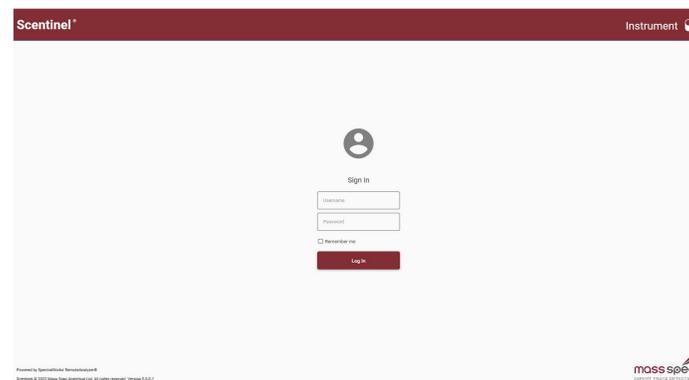
Results

The results, along with the raw data are saved in RemoteAnalyzer. They are available for review either on site or remotely via a web browser. Reports can be automatically generated and emailed to supervisors if requested. Users with Administrative access to the system control other Users access to relevant analyses and data access.

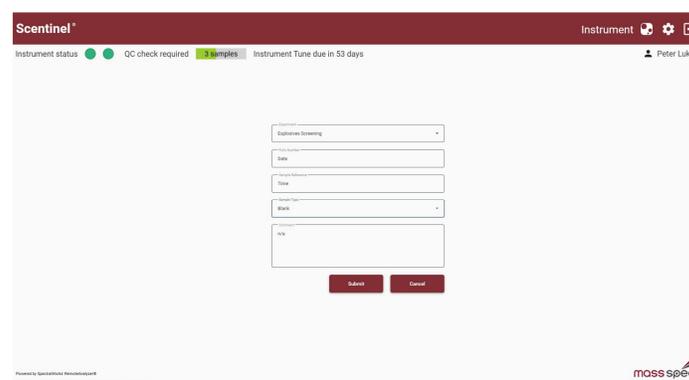
Conclusion

A simple workflow for the detection of explosives has been shown. Each swab takes approximately 8-10 seconds to analyse and indicate near instantaneous results easily understood by a non technical/scientific user.

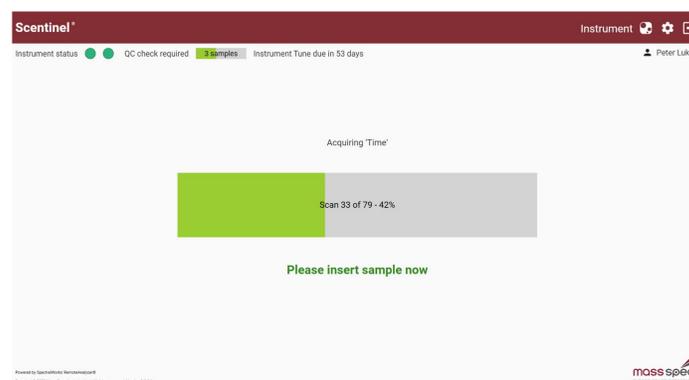
This approach can be extended to other analytes of interest and has been demonstrated with drugs of abuse and pesticides.



User logs into Scintinel to submit a sample.



Sample information is inputted.



Sample is acquired and results displayed.

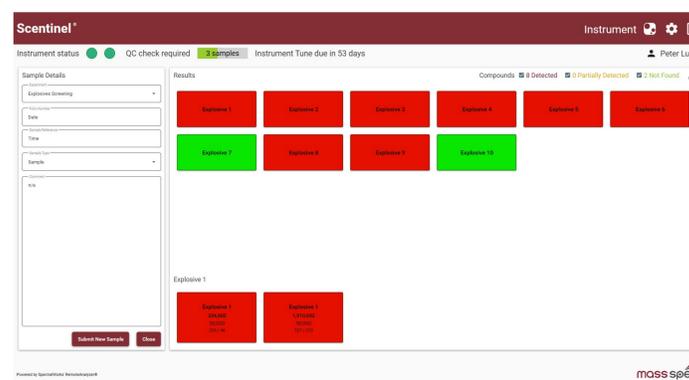


Figure 1. Simplified workflow for the detection of explosives for non-MS user.