About the Simulation

Purpose

The software consists of two apps that provide a simulation of an inductively coupled plasma – mass spectrometer (ICP-MS). The apps were developed via a collaboration between Loughborough University and Reid-IT, in order to complement a lecture course on mass spectrometry. We are now making the apps freely available for teaching at other institutions. If you find them helpful, please get in touch to let us know!

Installation

The apps do not require any special installer or uninstaller. Simply unzip the archive you've downloaded and place the "ICP-MS TuneSim" and "ICP-MS InstrumentSim" folders onto your desktop. The apps use associated text and HTML files to control their behaviour. These files must remain in the folder alongside the app itself (*.exe). Do not rename the folders or the files within them.

Note that both Mac and Windows users may be asked to give permission to run the apps for the first time. This is because we haven't gone through the processes to register the apps with Apple and Microsoft - it's not worth the effort for limited distribution apps. If you are unhappy about this or unsure that you trust our apps, then don't use them! Otherwise, see "Can't Open Mac App.pdf " or " Can't Open Windows App.pdf " for guidance.

ICP-MS TuneSim

This app aims to increase student understanding of the factors involved in tuning, through interaction with a simulated tuning window. Parameters, such as sample gas flow rates, torch position and RF power can be adjusted and their impact on the signal monitored on the screen. The objective of the exercise is to achieve the highest possible sensitivity for indium, whilst keeping oxide ratio as low as possible. The results of the tuning can be saved and used to personalise the output of subsequent experiments using the InstrumentSim.

Note that you will be asked for a student ID when you open the app. Non-Loughborough users can use A123456 to access the app. You will need to press Enter after entering a name and ID. Step by step instructions on how to use the app are available in the User Guide. You can find a copy within the Support Files folder or alternatively via the Help menu within the app.

ICP-MS InstrumentSim

This app enables students to perform analysis of a range of samples. Applications include quantitative analysis of selenium in a nutritional supplement, analysis of gadolinium-based contrast agents in cell populations and determination of common metals in fabric samples. A qualitative study of gunshot residue is also available. Sample details and step by step instructions on how to use the app are available in the User Guide, which can be found within the Support Files folder and via the Help menu within the app.

The app is intended to work with tune files produced by TuneSim, which will influence the signal intensity and reproducibility of the results generated. However, an example tune file has been provided for those who prefer to use the InstrumentSim as a standalone exercise.

Further Support

A 10 minute introductory video, demonstrating the use of both apps is available [here](). Additional documentation, including student worksheets and instructions on how to customise the app, are available on request. Please contact Amy (A.J.Managh@lboro.ac.uk) for details.