

SmartTune wizard and easy, vent-free column replacement - two innovations in low-resolution GC-MS technology

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ABSTRACT

Unit resolution gas chromatography-mass spectrometry (GC-MS) is one of the most popular analytical techniques for analyzing compounds of interest in a variety of matrices. GC-MS is traditionally regarded as a complex analytical instrument requiring high level of user expertise to run. The two major pain points for the end user are tuning the MS and venting the system in order to change the GC column.

In this presentation we highlight two recent innovations that improve the usability of the GC-MS system with respect to the above mentioned points. Tuning of the mass spectrometer is a critical aspect of running the instrument that ensures the system is in the right working state and is ready to run samples. Mass calibration and resolution tuning are two of the most important steps that are performed to ensure that the system is in good working state. Most modern instruments have an Auto Tune function that is fairly easy to use, but unnecessary tuning of the system is not recommended since it could result in shortening the lifetime of the detector. We present here the concept of the SmartTune wizard which, with minimal clicks, checks the current tune state of the system and tunes it only when necessary. In case of tune/diagnostic failures, it gives specific recommendations to bring the system back into its recommended usable state. With the help of this wizard, a novice user would be able to start running their samples with minimal training.

The second innovation that we describe here is the vent-free column replacement. Mass spectrometers are maintained under high vacuum, thus changing the GC column requires the user to shut down the system, vent it, and bring the system back to steady state equilibrium, which often requires a day of down time. Current vent-free systems are prone to leaks and require high level of user training, however, we present here an innovative vent-free column replacement technology that makes use of the vacuum probe interlock and is easy to use.

INTRODUCTION

GC-MS is a mature analytical technique with a commercial history of over 50 years. Major innovations have taken place over the years, both in terms of hardware and software to make the modern instrument smaller and easier to use and operate. Tuning of the MS is an important procedure that must be performed in order to ensure that the results that are generated are valid. Perfluorotributylamine (PFTBA) is a common reagent that is used for tuning of the quadrupole mass spectrometer. Most modern GC-MS instruments have an Auto Tune software routine that performs a series of itemized steps in order to tune the system. Mass calibration and resolution tuning are the essential functions that are carried out during this Auto Tune procedure. Mass calibration assures that the m/z scale is accurate and resolution tune makes certain that the masses are unit resolved. Most novice and untrained users are unfamiliar with the tuning procedure and can't troubleshoot when the Auto Tune procedure fails. The introduction of SmartTune on the Thermo Scientific™ ISQ™ 7000 single quadrupole GC-MS system and the Thermo Scientific™ TSQ™ 9000 triple quadrupole GC-MS/MS system represent a major step forward in improving the usability of the instrument especially for new users. SmartTune is designed to have minimal user input while ensuring it meets the minimum criteria for mass calibration and resolution. It is also designed to provide troubleshooting feedback in case of issues.

The vent-free column replacement is another major hardware innovation for the ISQ 7000 GC-MS and TSQ 9000 GC-MS/MS systems. It is a part of the Thermo Scientific™ NeverVent™ technology which includes the Vacuum Probe Interlock (VPI) and the V-Lock source plug. The picture below shows an analyst using the VPI tool. NeverVent technology is designed to maintain the mass spectrometer under high vacuum during routine column changes. In theory, one would never have to vent the mass spectrometer; thus maintaining the internal components like the source block, quadrupole assemblies and the detector system in equilibrium.



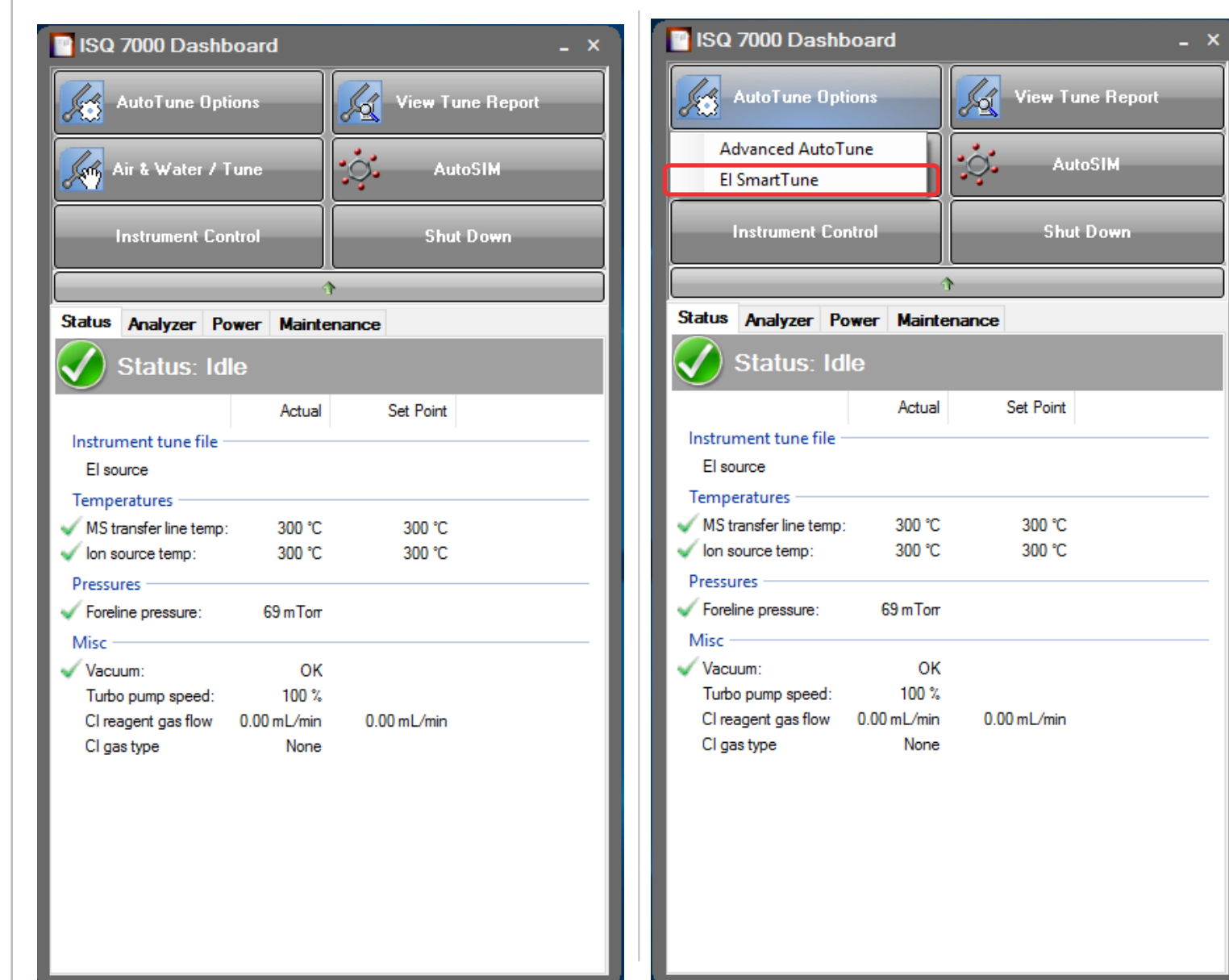
MATERIALS AND METHODS

The ISQ 7000 GC-MS and TSQ 9000 GC-MS/MS systems are designed with SmartTune and NeverVent technologies and are used here. SmartTune is part of the Thermo Scientific ISQ and TSQ 4.0 Instrument Control Software (ICS) and is compatible with both the ExtractaBrite ion source and Advanced Electron Ionization (AEI) source. NeverVent technology is only compatible with the ExtractaBrite ion source.

SmartTune

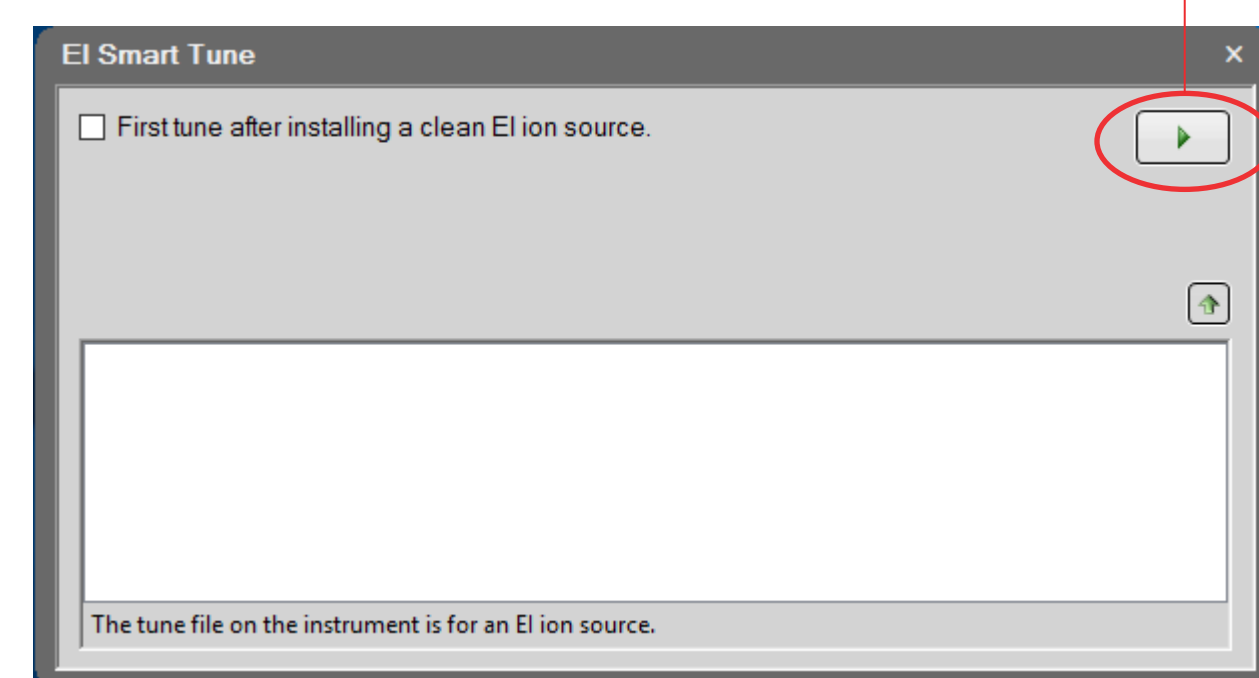
The SmartTune functionality is part of the Dashboard (Figure 1). The Dashboard is the primary control interface for the mass spectrometer with various options for controlling and monitoring the instrument.

Figure 1. The Dashboard for the ISQ 7000 GC-MS system.



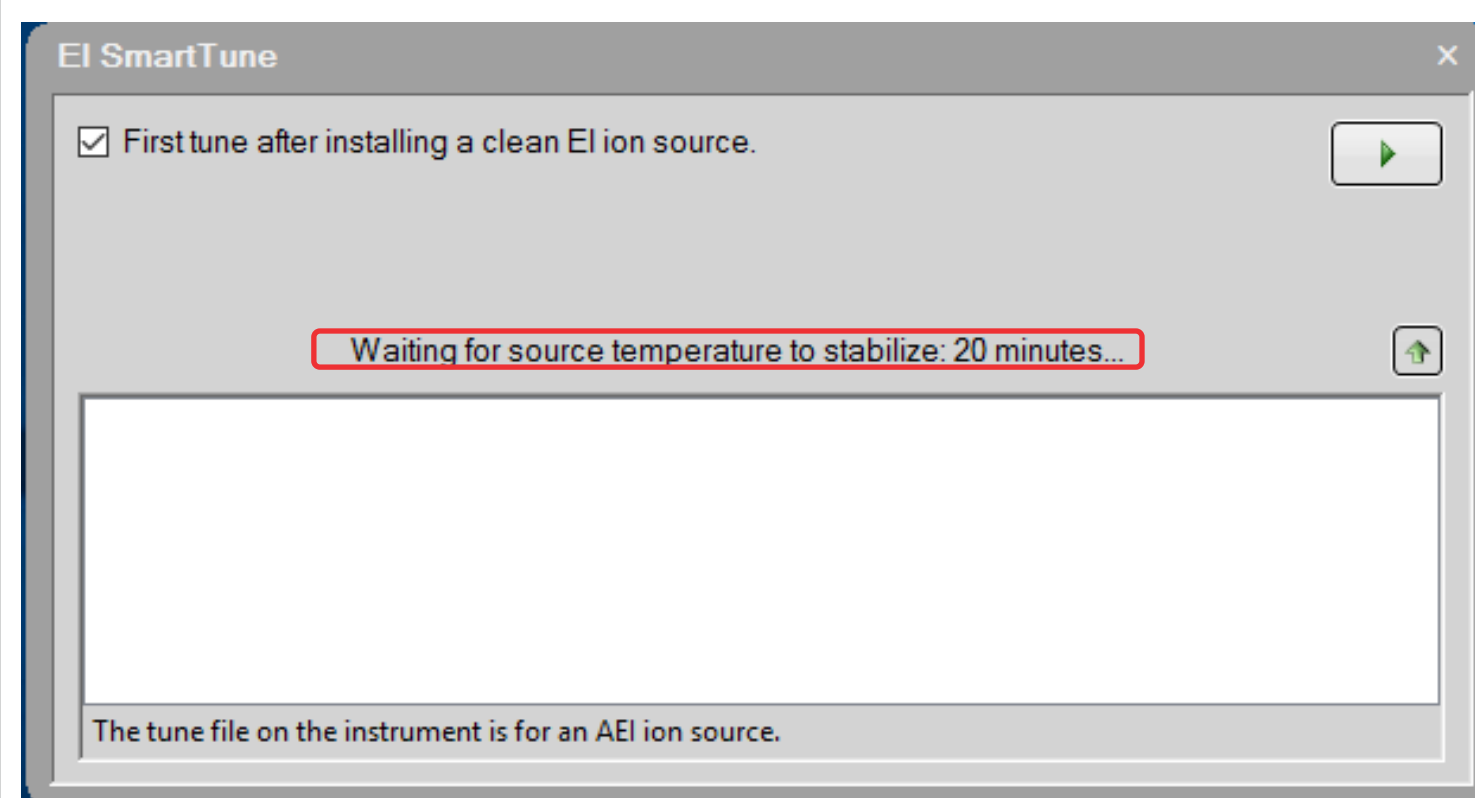
The tuning of the MS can be performed manually (by clicking the "Air & Water/Tune" or more commonly by AutoTuning by clicking the "AutoTune Options" button). The AutoTune options menu features Advanced AutoTune, designed for creating and editing tune and EI/AEI SmartTune, the new easy-to-use intelligent tune wizard. The SmartTune interface is shown in Figure 2.

Figure 2. SmartTune Interface showing the one-click "Start" button.



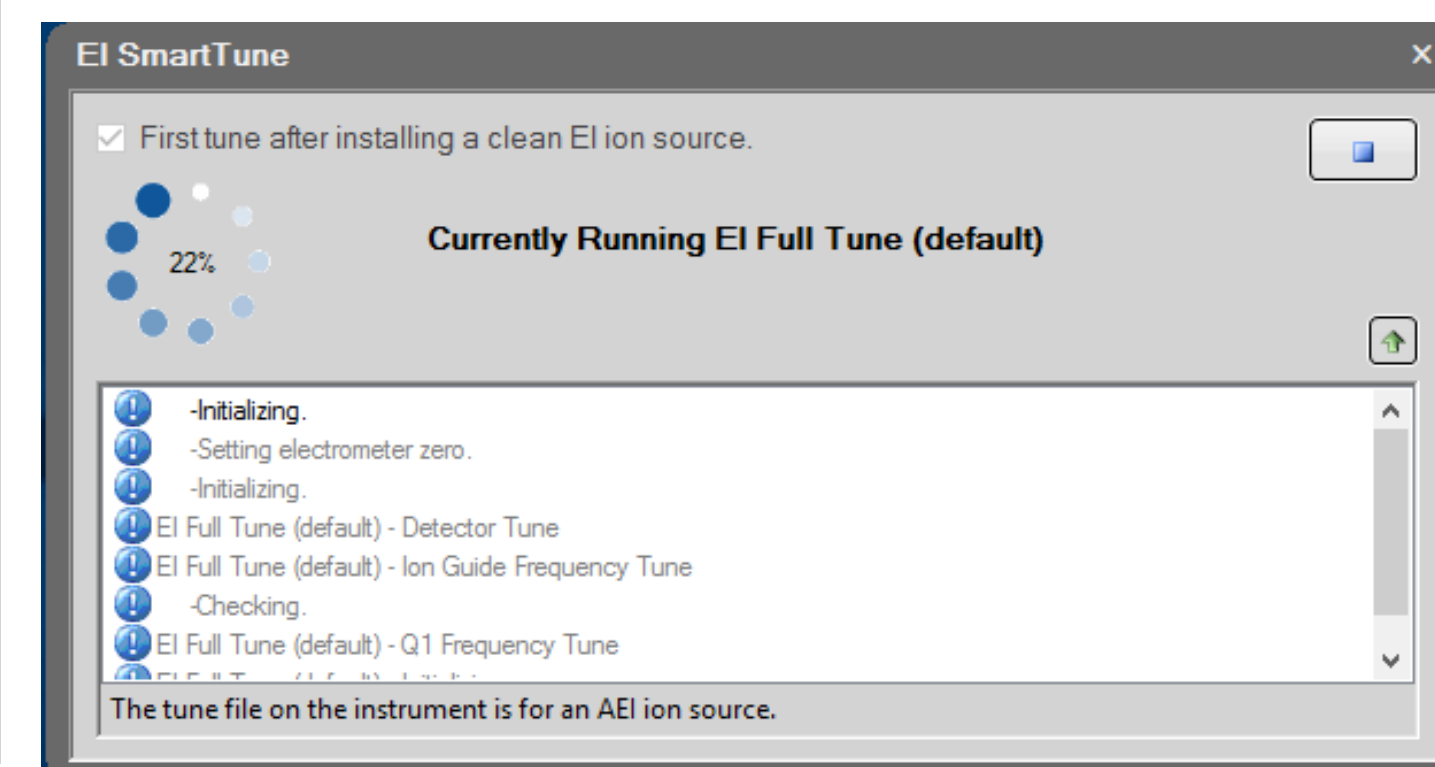
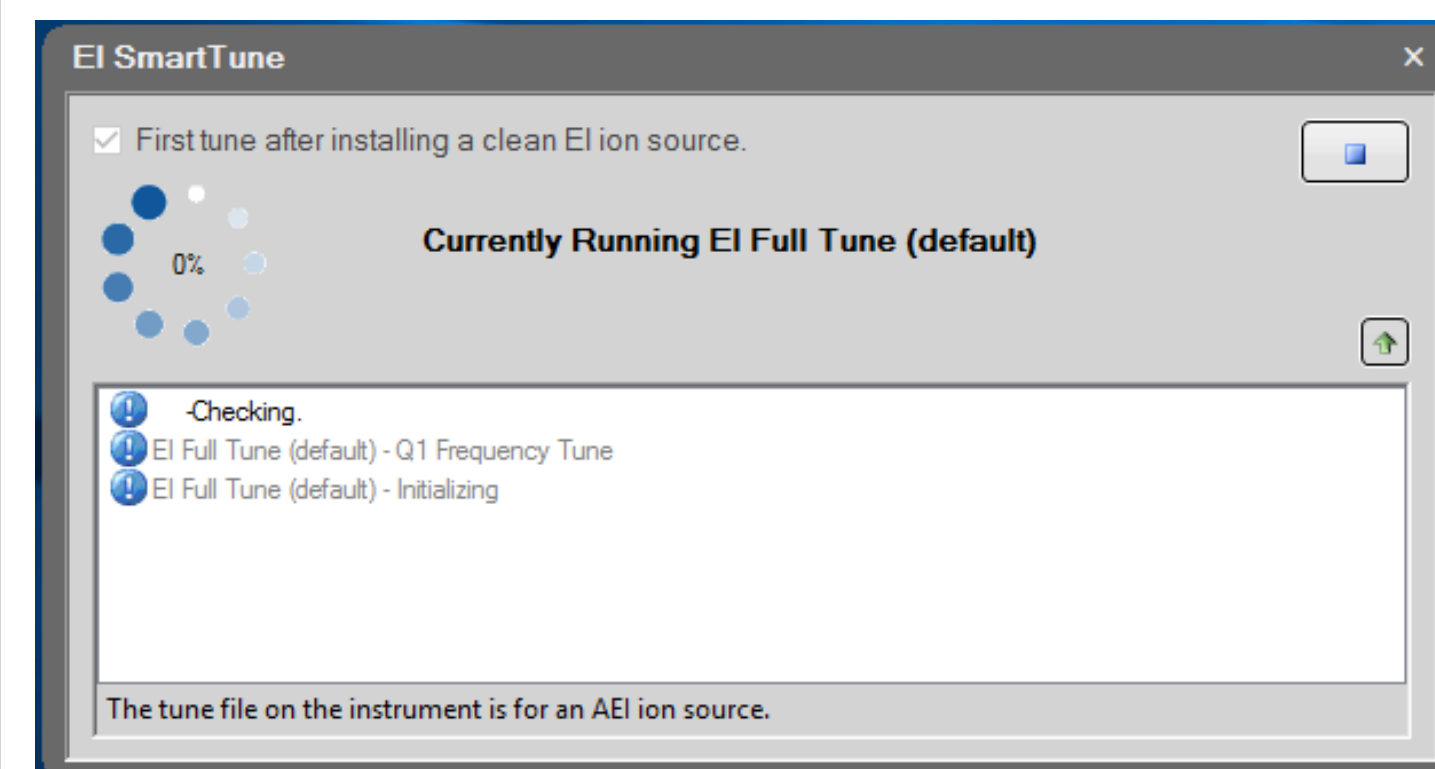
Intelligent software features- Figure 3 shows the ability of SmartTune to know that the source temperature is not yet stable (and thus not advisable to start the tuning process).

Figure 3. SmartTune advising that source temperature is not yet stable.



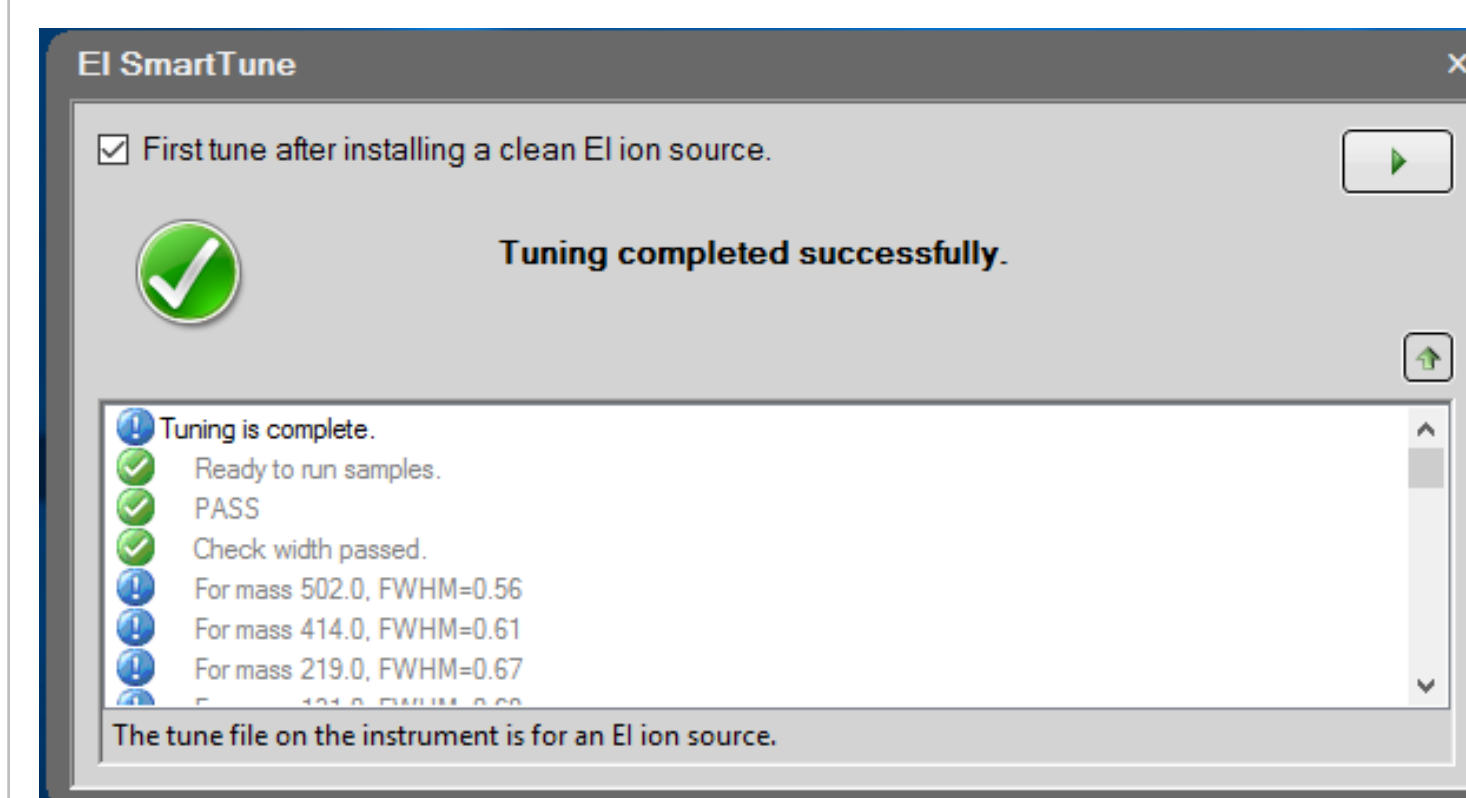
It gives a detailed step-by-step account of the tuning processing being carried out (Figure 4)

Figure 4. Start of the SmartTune showing processes that are carried out. (a) Start of the tune; (b) detector tuning in progress.



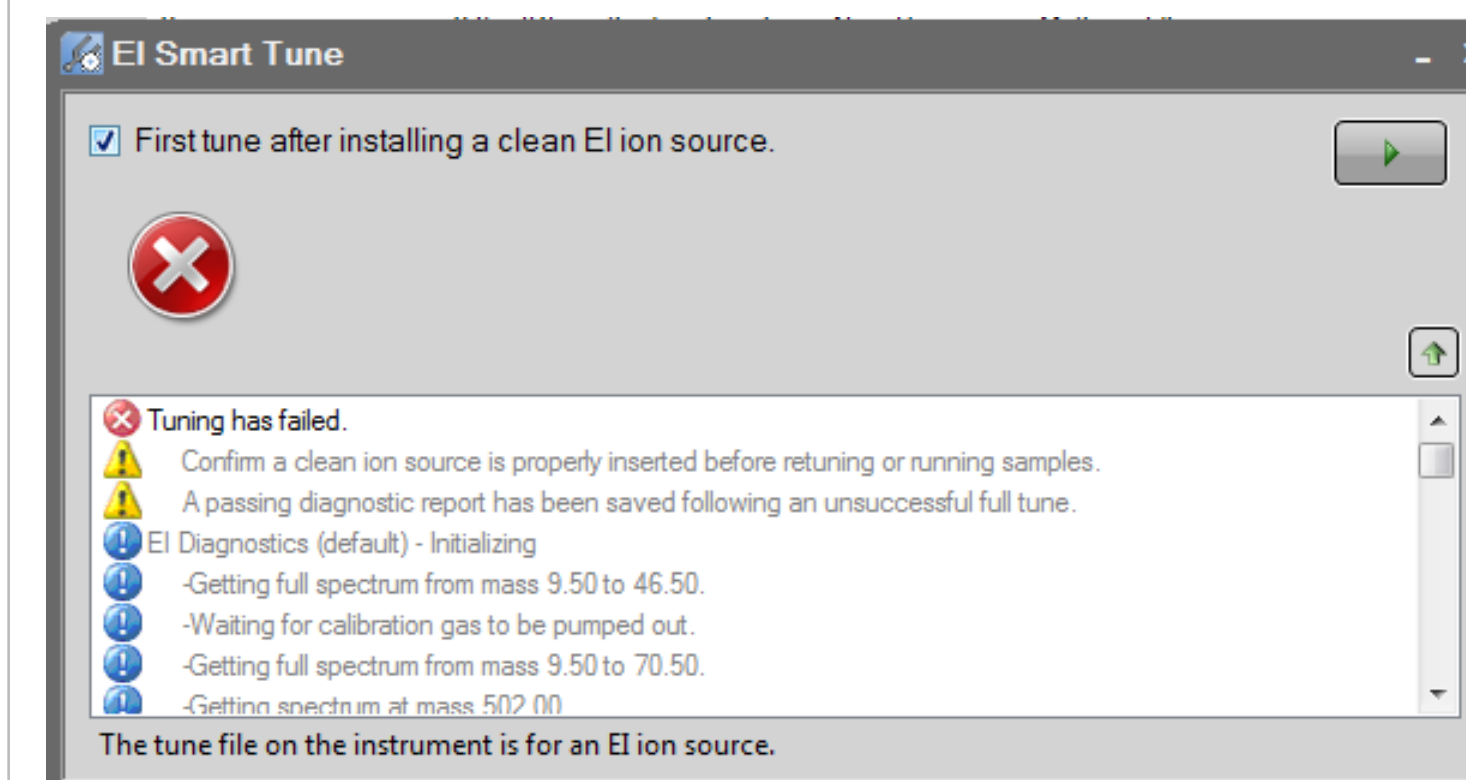
Once the tuning is successfully completed it gives a "Green Check" with message that one is ready to run samples (Figure 5).

Figure 5. Completion of a successful tune.



In case of issues, the SmartTune provides recommendations on what might be wrong, and runs a full diagnostics for further investigation of the issue (Figure 6).

Figure 6. Unsuccessful tune with recommendation to "Confirm a clean source is properly inserted."



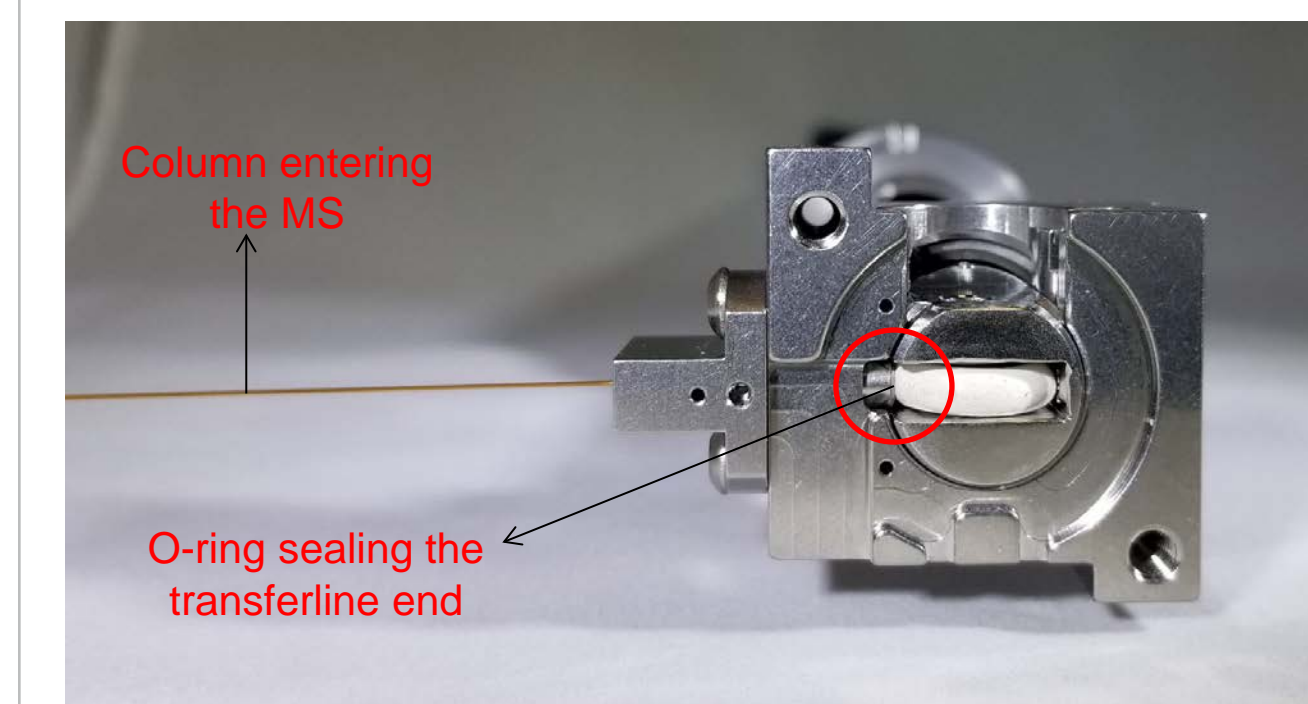
NeverVent technology

Significant productivity and instrument up-time gains can be realized with the NeverVent technology. Table 1 shows the estimated time savings achievable with the NeverVent technology.

System	Column Change	Source Change
Standard GC-MS	~4.5 hours	~4.0 hours
ISQ/TSQ with NeverVent	~35 minutes	~5 minutes
NeverVent Time Savings	87%	98%

Figure 7 shows the hardware involved with the NeverVent technology for vent-free column replacement. The source plug is attached to the vacuum probe interlock (VPI) tool. The source plug consists of a teflon-based O-ring which seals the transferline end and allows users to change the column without breaking the vacuum.

Figure 7. NeverVent technology hardware and mechanism of vent-free column replacement.



CONCLUSIONS

This poster presents two major software and hardware innovations in the field of GC-MS.

- SmartTune: an intuitive easy-to-use tuning software with troubleshooting feedback capability.
- NeverVent technology: vent-free column replacement is now possible allowing for minimal downtime during column changes.

TRADEMARKS/LICENSING

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