

PSO Europe Trap Data Browser Concept: Making Remote Ion Trap Data Review Easy and Efficient

Technical Note

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Introduction

In the modern drug discovery laboratory there is a tremendous growth in the number of new drug compounds to be analyzed and purified. Analysis is often accomplished by the synthetic organic and medicinal chemists "walking up" to a central LC Trap system to submit the samples and then returning to their labs to generate more syntheses. This has greatly increased the need for chemists to be able to review the data from their own PCs in their own labs without returning to the central LC Trap lab. The PSO Europe Trap Data Browser concept is based on the standard Agilent Data Browser A.02.00. This is accomplished by generating an LC MSD Data File out of the Trap Data File. This LC MSD Data file regenerates by an automated process the data browser file, which can then be made available to remote PCs through a server.

Global Process Overview

The Agilent PSO Trap Data Browser Add-on enables use of the Agilent ChemStation Data Browser to efficiently review LC Ion Trap data and to generate reports by an easy simple process. There are two steps achieved within the Agilent PSO Trap Data Browser Add-On product:

- Conversion of Ion trap Files into MS data files
- Automatic reprocessing of the data files to create the AEV files

Step 1: Converting Agilent Ion Trap Data

The Standard Data Browser cannot convert the Agilent Ion Trap data files directly into AEV files. Therefore we first need to convert the Ion trap data file (analysis.yep) into a MSD data file (msd1.ms). This is done with the use of a Visual Basic Script, which is delivered with the PSO Trap Data Browser Add-on product.

Step 2: Creating AEV files out of converted trap data files

The AEV files are created automatically after each run or sequence within a LC MSD ChemStation Session.



However the LC MSD ChemStation and the LC Ion Trap ChemStation are not co executable, which means that both ChemStations need to be installed on a different PC. As second PC, we a use a Virtual PC running from the Ion Trap PC .



Figure 2: Virtual PC - Trap PC

What is needed at customer site?

As the LCMSD ChemStation and the LC – Ion Trap ChemStation are not co executable, a Virtual Machine License will be needed (VMWare Workstation 4 or higher , VMWare, Inc http://www.vmware.com/).

Features

- Central data storage
- Notification options
- - Automatic or manually generating AEV files
- Automatic Transfer of AEV files to a central storage location.

What is included?

- Latest LC MSD G2710 BA version
- Latest Data Browser G2727AA up to 10 licenses
- PSO Trap Data Browser Add-on
- Installation and familiarization

Ordering Process

This customized solution is covered in a PSO proposal, which describes the deliverables and addresses individual customer expectations and needs. Therefore, the following order process should be followed.

- Fill in the FAX sheet on the last page of this document.
- Fax the completed form to PSO in Waldbronn.
- PSO will respond with a "customized proposal".
- The proposal delivered will describe the customized solution in detail.

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Please prepare a Proposal	
for the following Customer:	

Customer Contact:	
Phone:	
Customer Address:	
E-Mail Address:	
FE Name / E-mail:	

Description	Include in Proposal	Quantity
PSO Trap Data Browser Add-ons	~	
Other Requests		