Increasing Productivity with LC/MS Easy Access Software

Technical Note

Wayne Duncan and Douglas McIntyre
Agilent Technologies

Introduction

With the explosive growth of synthetic organic chemistry over the past several years, there is corresponding demand for easy to use, robust, rapid turnaround systems to analyze and confirm the molecular weight of the tremendous numbers of new compounds. Synthetic chemists typically want to concentrate on organic synthesis issues and want to minimize the time spent on the analysis of their compounds. The Agilent LC/MS Easy Access software described here allows users to simply "walk up" with their samples, input simple sample information, choose from a list of methods, position the samples as directed by the system, and then return to their labs and wait for an e-mail of the results.

Key Features of LC/MS Easy Access Software

- Very simple and easy sample submission and status checking

- Rapid confirmation of molecular weight and target ion presence

- Supports Agilent 1100 Series well plate sampler and automatic liquid sampler

- Automatic pre-equilibration on change of method

- Supports automated e-mailing of data and reports

- Flexible administrator tools to set user access, queue tracking and project management

- Multiple Instrument Networking so instruments can share databases, eliminating the need to manage redundant configurations for each instrument and reducing administrative tasks

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Experimental

The data shown here were generated using an Agilent 1100 Series LC/MSD SL quadrupole mass spectrometer system (G2708DA). In addition to the ChemStation software (G2710AA Rev. A.09.01), the system included LC/MS Easy Access software (G2725AA Rev. A.02.00).

Discussion

After the user has logged in by supplying a password (optional security), described the samples, and assigned methods from a list, the system shows the locations in the sampler where the samples should be placed (Figure 1). Figure 2 shows the status screen which displays the overall status of the system and contains the following key information:

- Current samples and approximate time remaining in the queue

- The method currently running and name of last submitter

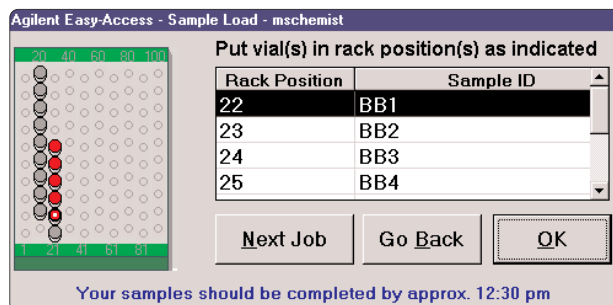- Status of ChemStation, autosampler and UV/Vis lamp

Figure 1. System directs user where to place samples and provides an approximate completion time

System administration

The system administrator is responsible for overall management of the Easy Access system. Key capabilities include:

- User and group administration including optional passwords, method access and ChemStation availability

- Sample queue management including moving priority samples to the front of the queue

- Method management which defines the methods available to the users
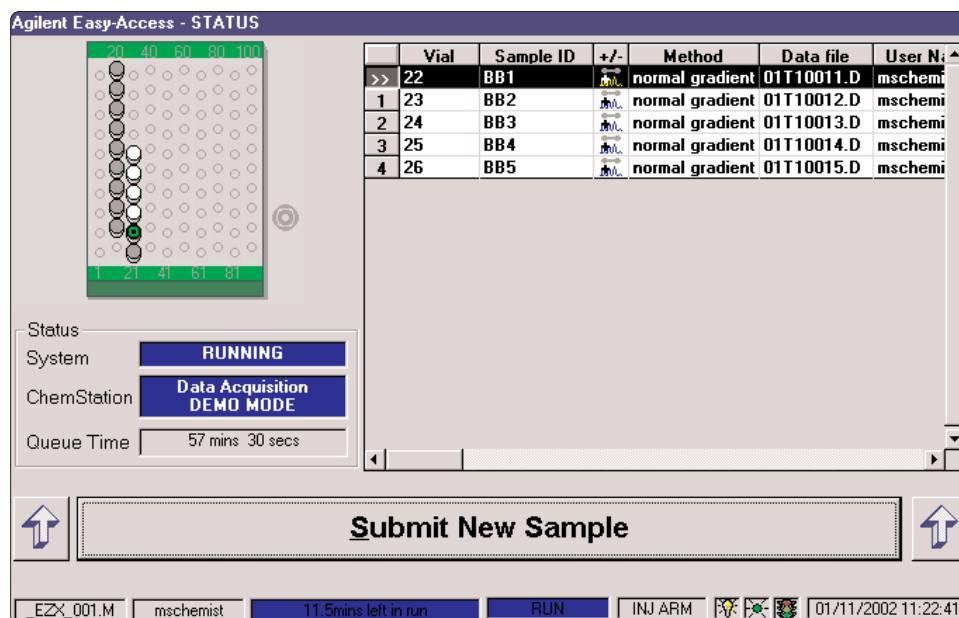

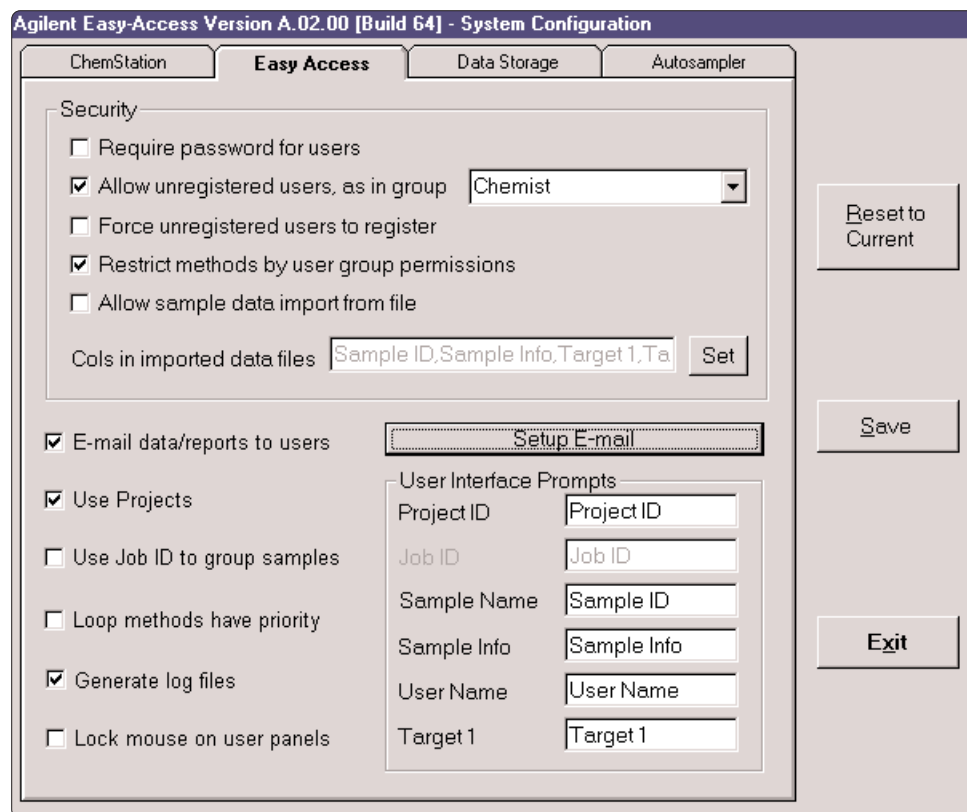Figure 2. Status screen provides key information at a glance

Figure 3. Easy Access configuration screen sets user access and establishes e-mail capabilities

Figure 3 shows the main configuration screen for Easy Access. Some key security related choices here for the system administrator are to require a password for specific users or groups and to limit access to specific methods. Note also that the mouse can be locked on the user panels, preventing access to anything but Easy Access. Finally, this screen is also where e-mailing of results to users is set up.

Results sent by e-mail

The system can be directed to send the results of the analysis to selected users by e-mail. At right is an example of the information received and Figure 4 shows one of the pages from an e-mail report.

```
Your sample run has been completed.
Sample: ESdemo05'
Info: Sulfa Drugs'
Target masses: 270 278 284 310
Method: Loop2
Info: Loop SIM ES, multi signal
Data file: E00009-3.D


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A message generated by the Agilent
Easy-Access system
```

```
Data File C:\MSDNE1\testlab\01-02\E00009-3.D                    Sample Name: ESdemo05

    DataPath  : C:\MSDNE1\TESTLAB\01-02\E00009-3.D
    DateTime: 17 Jan 02   4:18 pm
    Operator  : testlab                          Vial  : 5
    Sample    : ESdemo05
    Retention : 1.613 minutes

    MW      : 270:Yes   MW+(-H)-:Yes   MW+OAc-  :No
                        MW+TFA-  :No   MW+-     :No
                        2MW+(-H)-:No   2MW+OAc- :No
                        2MW+TFA- :No   2MW+-    :No
    MW      : 278:No    MW+(-H)-:No    MW+OAc-  :No
                        MW+TFA-  :No   MW+-     :No
                        2MW+(-H)-:No   2MW+OAc- :No
                        2MW+TFA- :No   2MW+-    :No
    MW      : 284:No    MW+(-H)-:No    MW+OAc-  :No
                        MW+TFA-  :No   MW+-     :No
                        2MW+(-H)-:No   2MW+OAc- :No
                        2MW+TFA- :No   2MW+-    :No
    MW      : 310:No    MW+(-H)-:No    MW+OAc-  :No
                        MW+TFA-  :No   MW+-     :No
                        2MW+(-H)-:No   2MW+OAc- :No
                        2MW+TFA- :No   2MW+-    :No
```

NILE 1/17/2002 4:22:11 PM testlab   Page 2 of 7
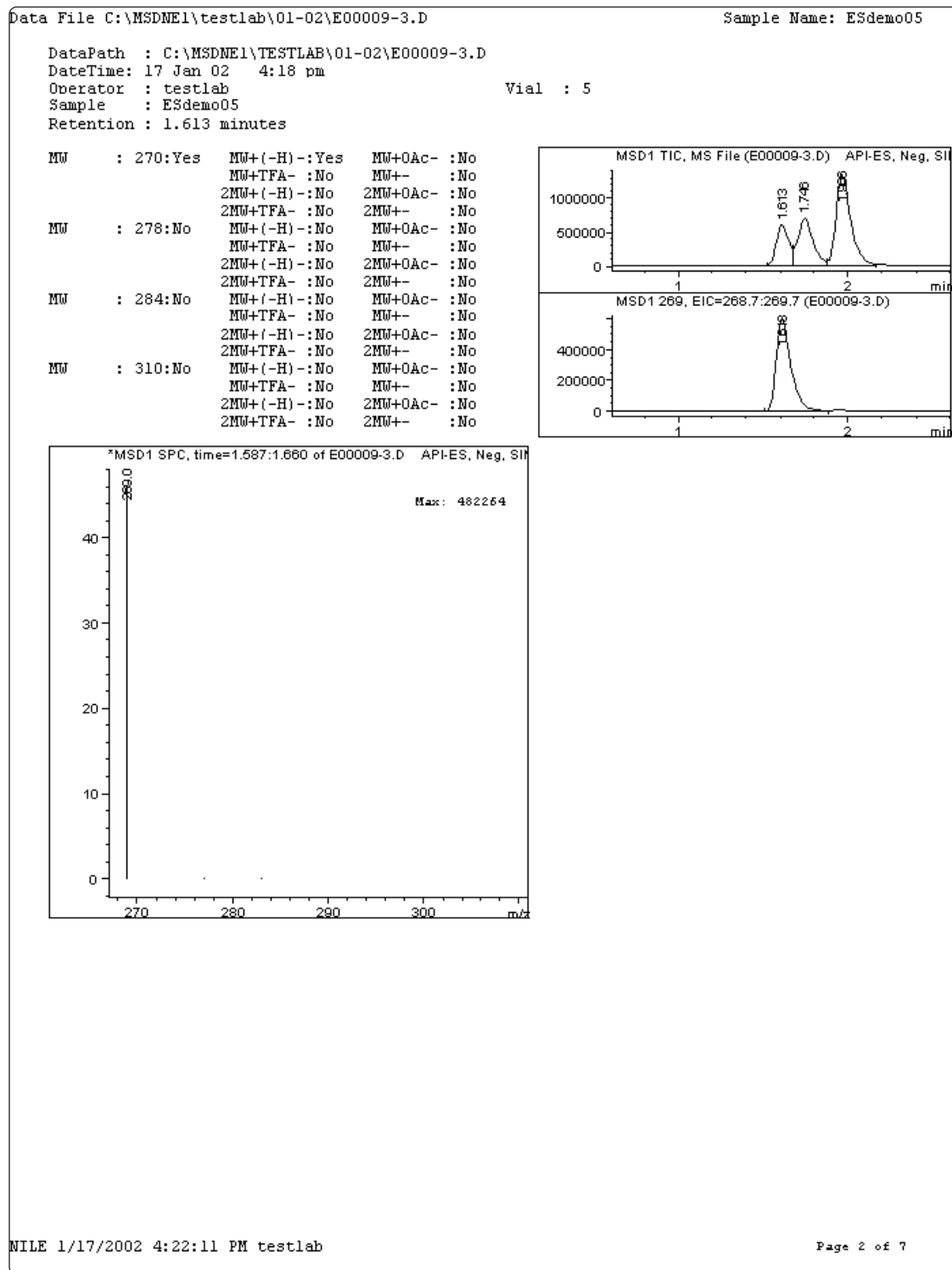
Figure 4. One page of a multipage report confirming the presence of a target mass at *m/z* 270

Conclusions

LC/MS Easy Access is a very effective tool, helping synthetic organic chemists be more productive by confirming the identity of their compounds in a shorter period of time while requiring less analytical expertise.

Authors

Wayne Duncan is a product marketing manager and *Douglas McIntyre* is an applications chemist at Agilent Technologies.

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