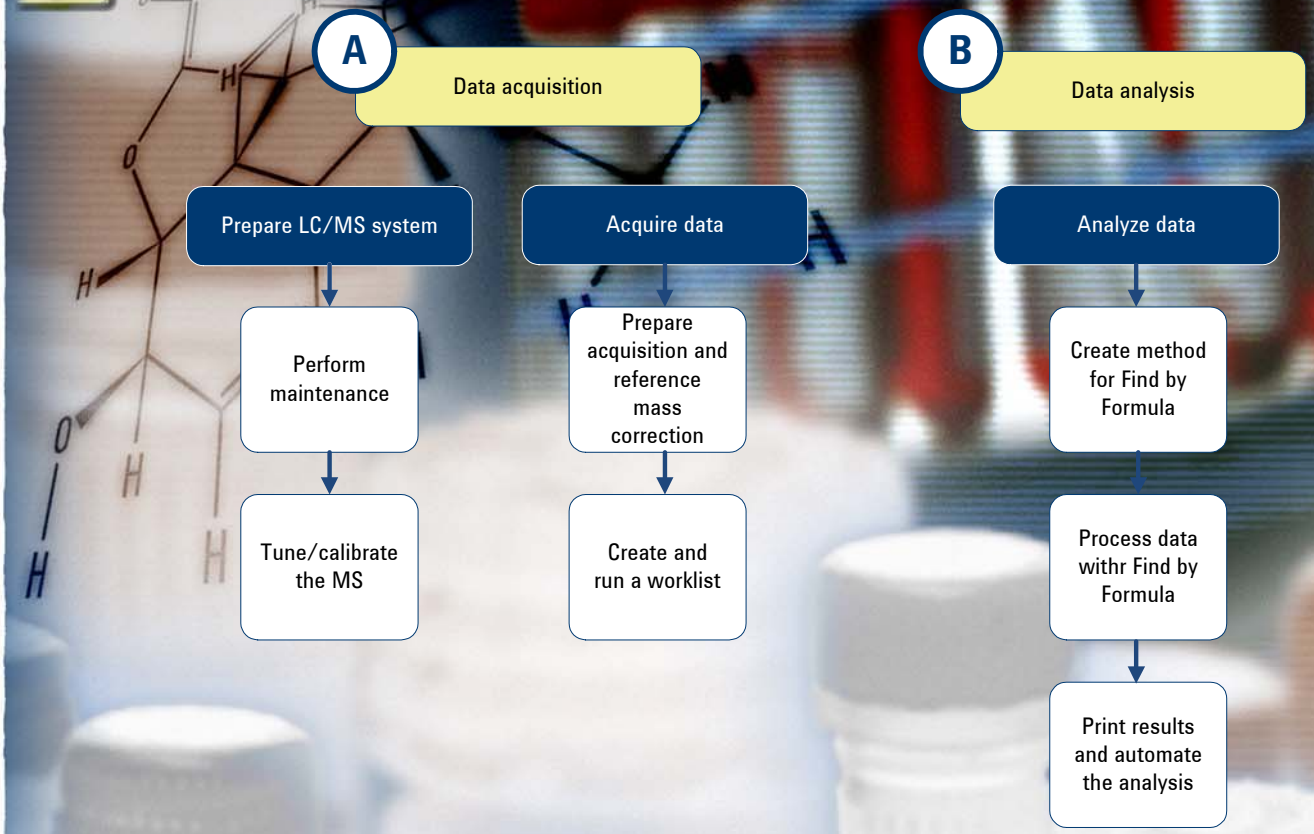
Agilent TOF LC/MS Drug Screening

Workflow Overview



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Prepare the LC/MS System

Perform maintenance

1. Do daily MS maintenance.

   a Rinse source chamber and door.

   b Clean the spray shield.

   c Clean the nozzle.

   d Latch the source chamber.

   e Verify calibrant bottles.

2. Do weekly MS maintenance.

   a Remove the source chamber door.

   b Clean the insulators.

3. Do daily LC maintenance.

   a Confirm mobile phase volumes.

   b Update the solvent levels in MassHunter.

   c Prepare the autosampler.

Tune/calibrate the MS

1. Equilibrate the system.

   a In MassHunter Acquisition, load the method to be used for the batch.

   b Start the pump with the ON button and verify pump ripple < 1%.

   c Go to Tune context.

   d Wait at least 20 minutes.

2. Do the Tune.

   a Turn on calibrant.

   b Perform a Check Tune.

   c Verify that mass errors and resolution are acceptable.

   d Save the tune file.

   e Go back to Acquisition context.

Acquire Data

The workflow includes both data acquisition and data analysis. See the *Agilent TOF LC/MS Drug Screening Workflow Guide* (Agilent publication 5991-1109EN) for details about the steps in this *Workflow Overview*.

Prepare Acquisition and reference mass correction

1. Prepare Acquisition.

   a Load first method of the batch.

   b Confirm that the correct method is loaded.

2. Prepare reference mass correction.

   a Verify the reference masses.

   b Verify parameters for reference mass correction.

   c Turn on reference mass flow and confirm proper abundances of reference masses.

Create and run a worklist

1. Create the worklist.

   a Save the current worklist.

   b Load a template worklist or create a new worklist.

   c Set up the Worklist Run Parameters *before* you edit the worklist. To prevent long path names in the worklist itself, do this step *before* you add samples to the worklist.

   d Edit the worklist to include all the blanks, controls, and samples for the batch.

   e Save the new worklist with a new name.

2. Run the worklist.

   a Confirm that all the system modules are in the Ready state.

   b Start the worklist.

Analyze Data

Create method for Find by Formula

1. Configure MassHunter Qualitative Analysis.

   a Configure the workflow to MS Target Compound Screening.

   b Load or create a Window Layout.

2. Load or create the method.

   a Set the Extraction Data Format.

   b Set options for Chromatograms.

   c Set options for Mass Spectra.

   d Set options for Find by Formula.

   e Save your data analysis method.

Process data with Find by Formula

1. Find compounds.

   a Confirm that MassHunter Qualitative Analysis is properly set up.

   b Set File Open Actions to do **Find Compounds by Formula**.

   c Open files.

   d Sort the Compound Table.

2. If necessary, update retention times in the PCDL database.

   If you have a single data file you wish to use for the update, follow this procedure:

   a Choose the analysis of a standard and export the compound table for one data file to a csv file.

   b Open the database for editing.

   c Open the csv file.

   d Verify appropriate retention times and mass tolerances.

   e Find the compounds.

   f Update retention times in the Personal Compound Database and Library (PCDL).

If you have multiple data files you wish to use for the update, follow this procedure:

a Process with Find by Formula all the files of standards (QCs, etc.) that contain all the compounds for which you wish to update retention times.

b Verify that all compounds have been found correctly.

c Sort the compound table alphabetically by compound name.

d Export the compound table to a single csv file.

e In PCDL Manager, import that csv file and do Find Compounds.

f Review and verify the results. Make any manual compound assignments as necessary and ensure that isobaric compound are assigned correctly.

3. If necessary, update the report template with Peak Filter area thresholds.

a Process all quality control (QC) samples.

b Sort and export the Compound Table.

c Display the data in Microsoft® Excel and copy to Clipboard.

d Open the report template for editing.

e Paste parts of the csv file into the template.

f Save the template.

Print results and automate the analysis

1. Print paper and/or electronic copies.

a Set options for the Compound Report.

b Print the report to paper and/or an Excel file.

2. Automate screening and reporting.

a Set options for the Compound Report.

b Set options for Automation.

c Test the method and save the Qualitative Analysis method into the Acquisition method.

d Set parameters in Worklist Run Parameters to run MassHunter Qualitative Analysis immediately after Acquisition.

e Save the updated Acquisition method.

f Reprocess the data if necessary.

For More Information

For details about these procedures, see the *Agilent TOF LC/MS Drug Screening Workflow Guide,* Agilent publication 5991-1109EN.

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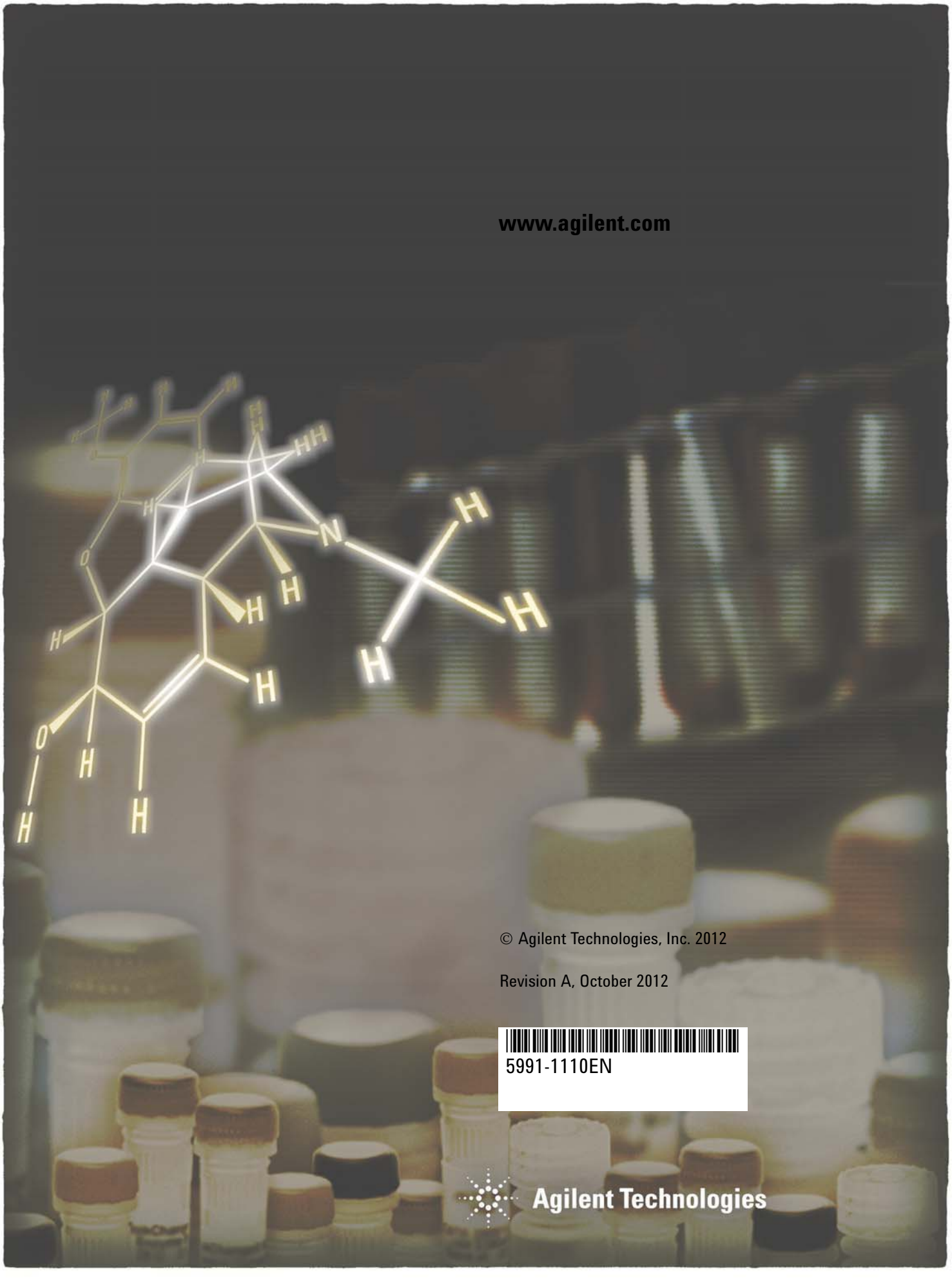

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