SOP 056 - Sequence Setup and Data Processing – Thermo ToxLab Forms

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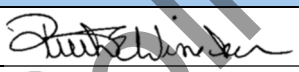
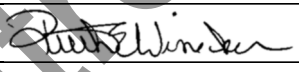
SOP Name: Sequence Setup and Data Processing – Thermo ToxLab Forms		SOP #: 056
North Carolina Office of the Chief Medical Examiner Toxicology Laboratory	**Revision:**	**Revision Date/Initials:**

Approving Authority Name	Approving Authority Signature	Approval Date
Ruth E. Winecker, Ph.D.		04/07/2015
Ruth E. Winecker, Ph.D.		06/10/2016
Ruth E. Winecker, Ph.D.		08/29/2017

SOP 056 - Sequence Setup and Data Processing – Thermo ToxLab Forms

1. **Principle**
   1.1. This method is designed to allow the user to create a sequence, acquire, and process GC/MS data using Thermo ToxLab Forms software.

2. **Specimens**
   2.1. N/A

3. **Reagents and Materials**
   3.1. N/A

4. **Instrumentation and Equipment**
   4.1. Thermo GC/MS
   4.2. ToxLab Forms software
   4.3. Data reporting system (PC)

5. **Procedure**

   5.1. Create Sequence and Acquire Data

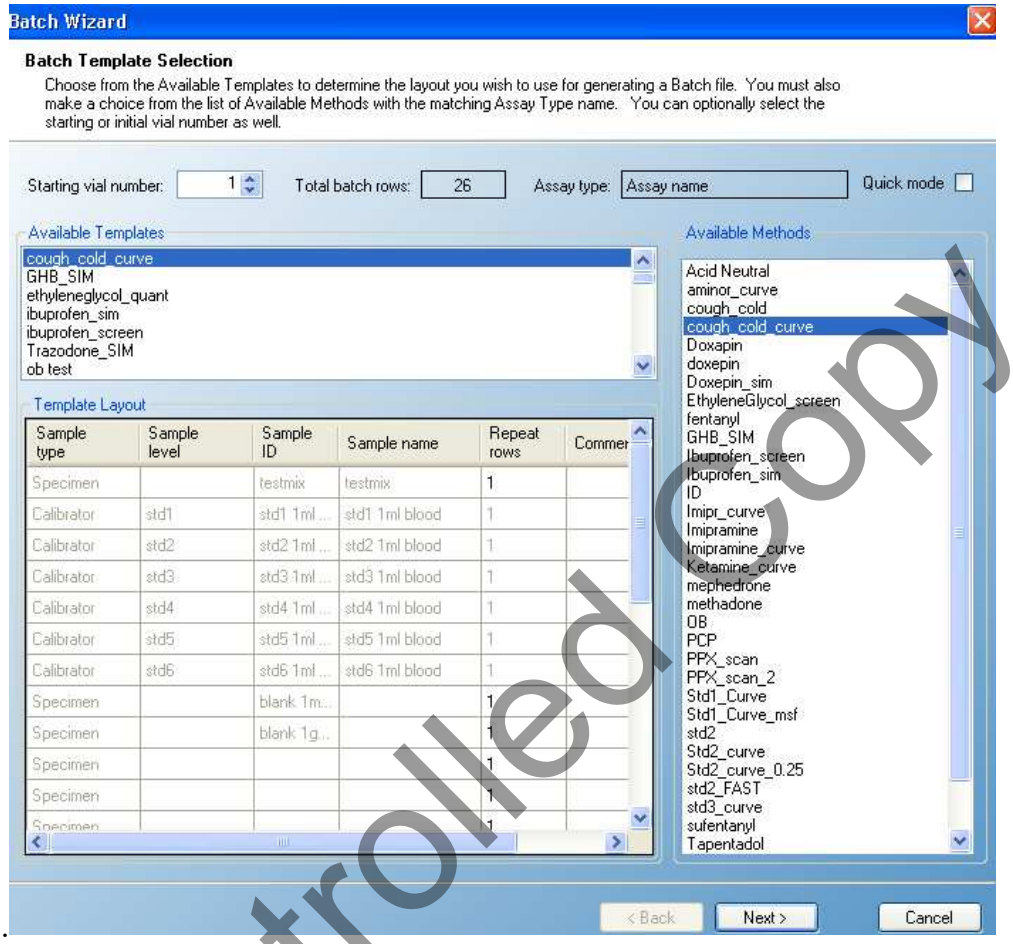
   5.1.1. On a networked PC with Thermo ToxLab Forms software installed, open the ToxLab Forms software by double-clicking the ICON.

   5.1.1.1. 

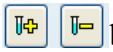
   5.1.2. Close the welcome screen (click “Close”) and select the “Batch Wizard” icon.

   5.1.3. In the Batch Wizard Window, choose a sequence template in the drop-down menu labeled “Available Templates” (see 5.1.4.1).

   5.1.4. Select the Instrument/processing method from the drop-down menu labeled “Available Methods” (see 5.1.4.1).

5.1.4.1. 

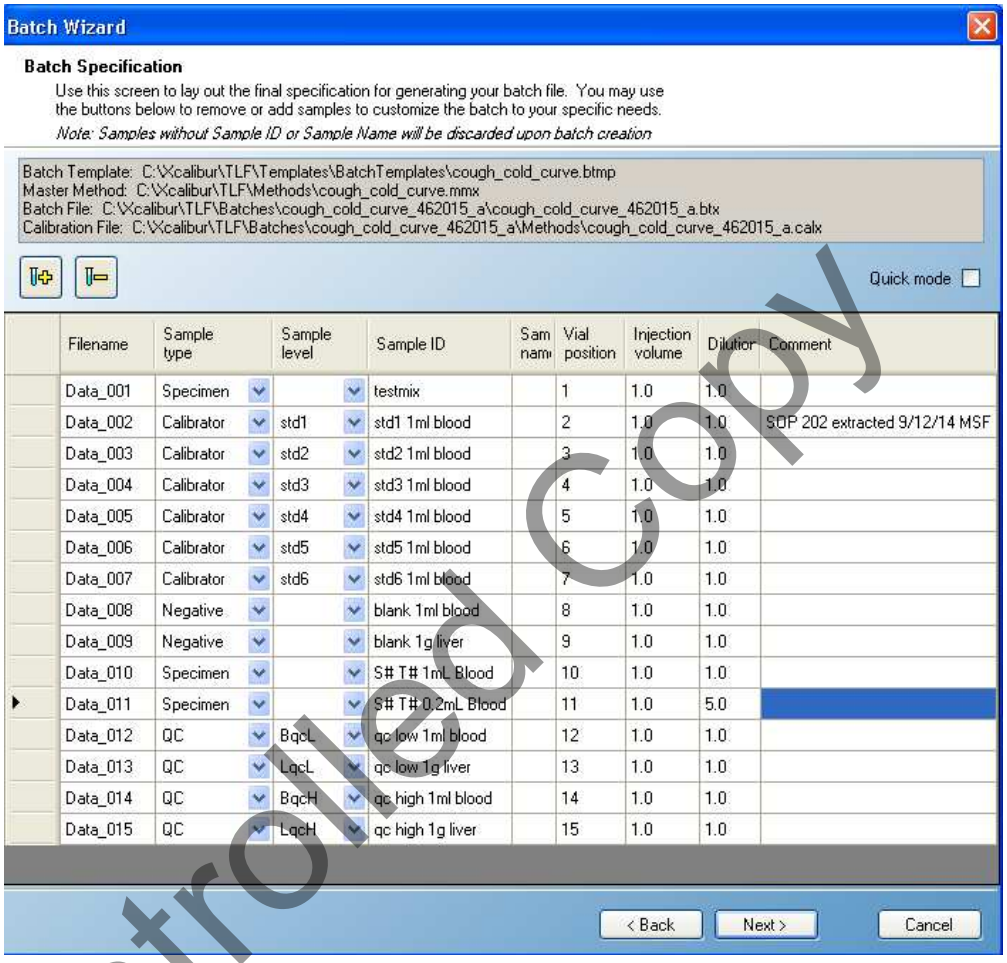
5.1.5. Click “Next >”.

5.1.6. In the “Batch Specification” screen (see 5.1.8.1), use the  buttons to add or remove rows as appropriate.

5.1.7. Use drop-down menu in each row to select appropriate “Sample type” and “Sample level”.

5.1.8. Enter each “Sample ID”, “Vial position”, “Dilution”, and Sample “Comment” in corresponding columns

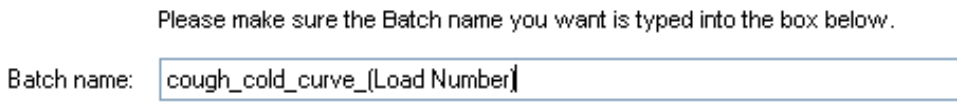
5.1.8.1.



5.1.9. Click “Next >”.

5.1.10. Finally, name the Batch: (Method Name)_(Load Number). Click “Finish”.

5.1.10.1.

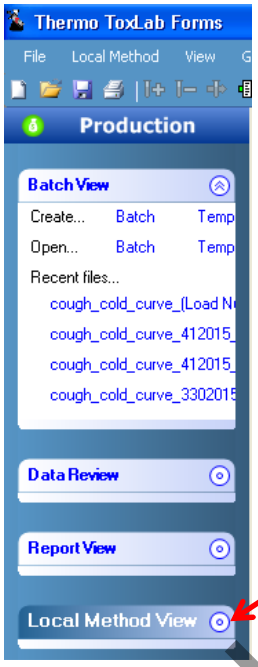


5.1.11. The screen has now changed to “Batch View”. Double check that the sequence table is correct and make changes as needed.

5.1.12. If the method is set up for multiple target analytes, not all of which are to be confirmed in the current load, see 5.1.12.1, if not skip to 5.1.16.

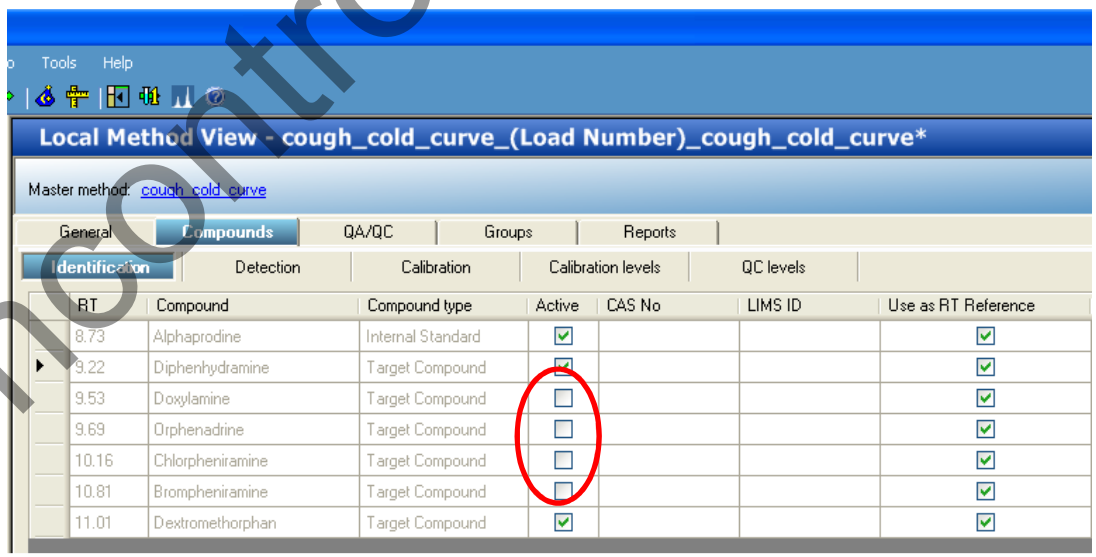
5.1.12.1. In the "Production" Menu (left side of screen), choose "Local Method View".

5.1.12.1.1.



5.1.12.2. In the "Compounds" Tab under "Identification", de-select the non-targeted compounds in the "Active" column.

5.1.12.2.1.



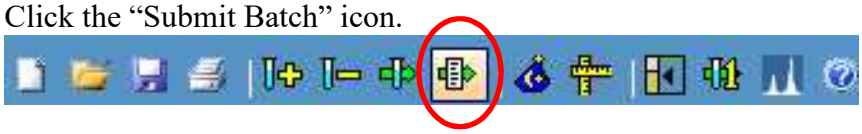
5.1.12.3. Return to "Batch View" by selecting it in the "Production" menu.

5.1.13. Save batch by clicking "Save" icon.

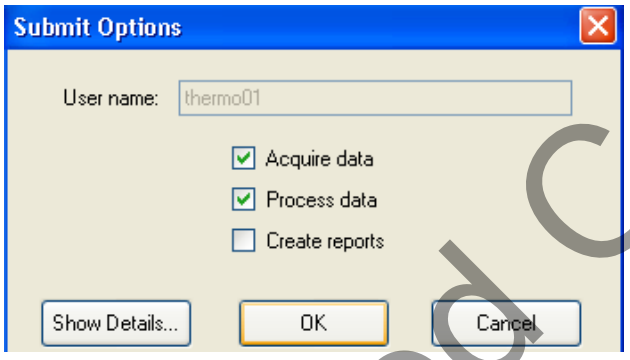
5.1.14. Print sequence by clicking the printer icon

5.1.15. Have another analyst check the sequence for errors.

5.1.16. Click the "Submit Batch" icon.



5.1.17. In the "Submit Options:" window, de-select the "Create Reports" option and click "OK".

5.1.17.1. 

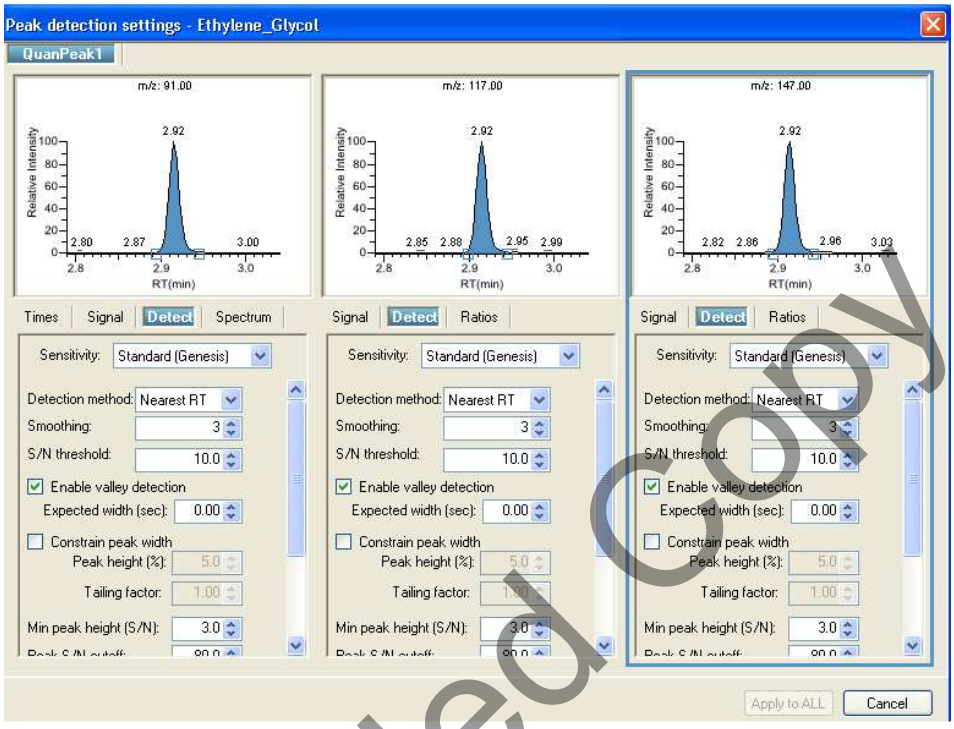
5.1.18. The instrument will now start injecting specimens and acquiring data.

5.2. Data Processing

5.2.1. After data acquisition has completed, select "Data Review" in the "Production" menu.

5.2.2. Review the chromatography for all target analytes in each data file.

5.2.2.1. Choose the analyte name in the "Compounds" window (right).
5.2.2.2. Select the "Confirming Ions" Tab (Bottom Right).
5.2.2.3. Choose a data file to view by clicking on the corresponding row.
5.2.2.4. In the "Quan peak: 1" window, check that the peak is integrated properly. If not, right click on the peak and choose "Peak detection settings".
5.2.2.4.1. Adjust the expected retention time (if needed) in the "Times" tab.
5.2.2.4.2. In the "Detect" tab, integration parameters can be adjusted as needed to achieve desired chromatography.
5.2.2.4.3. Select "Apply to ALL" when finished.

5.2.2.4.3.1. 

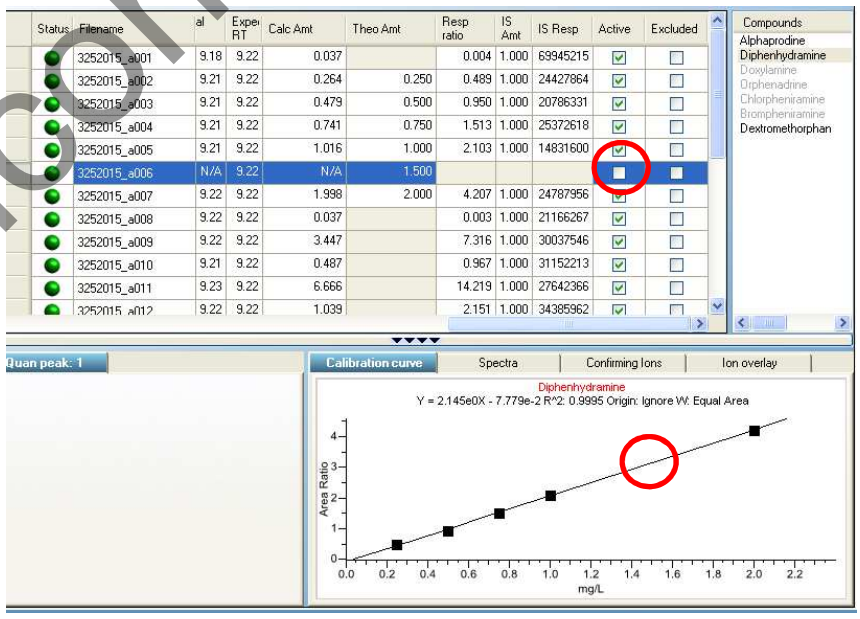
5.2.2.5. Save the workbook.

5.2.3. Review the calibration curve for each target analyte.

5.2.3.1. Choose the "Calibration curve" tab in the bottom right window.

5.2.3.2. Evaluate the curve as described in the assay specific SOP.

5.2.3.3. To remove a calibration level, de-select the corresponding level in the "Active" column.

5.2.3.3.1. 

5.3. Print Reports

5.3.1. Select “Report View” from the “Production” menu.
5.3.2. Select the following reports to print from the “Select a report” drop-down menu” Note – some of the reports require “All” to be selected in an additional drop-down menu.
5.3.2.1. Method Report.
5.3.2.2. Batch Summary Report.
5.3.2.3. Compound Calibration report (Select “All Compounds”).
5.3.2.4. Sample Report (Select “All”).

6. References

6.1. *ToxLab Forms Data Review Quick Reference Guide*. USA: Thermo Fisher Scientific, Inc, 2010. PDF.