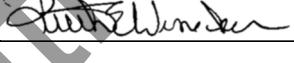


# **SOP 056 - Sequence Setup and Data Processing – Thermo ToxLab Forms**

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<b>SOP Name:</b>  <b>Sequence Setup and Data Processing – Thermo ToxLab Forms</b>		<b>SOP #:</b>  <b>056</b>
	<b>Revision:</b>	<b>Revision Date/Initials:</b>
North Carolina Office of the Chief Medical Examiner Toxicology Laboratory		
<b>Approving Authority Name</b>	<b>Approving Authority Signature</b>	<b>Approval Date</b>
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. ToxLab Forms

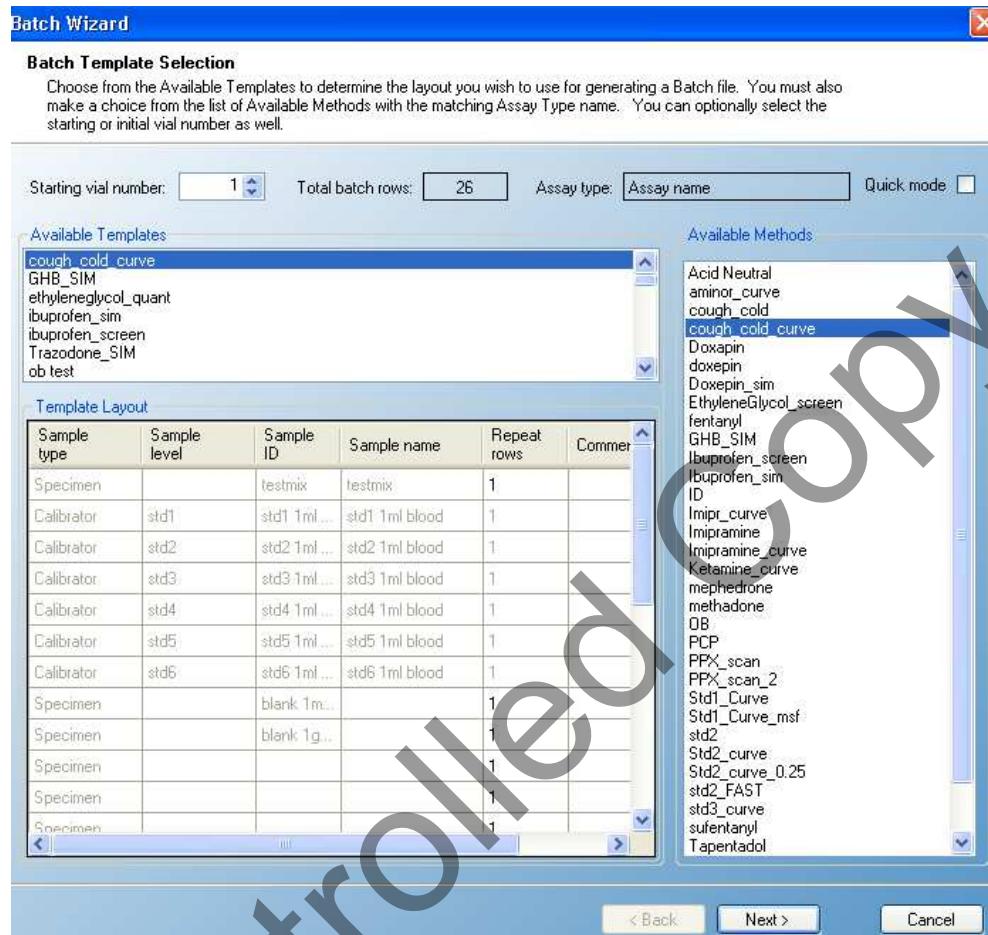
5.1.2. Close the welcome screen (click “Close”) and select the “Batch Wizard” icon.



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).

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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

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**Batch Wizard**

**Batch Specification**

Use this screen to lay out the final specification for generating your batch file. You may use the buttons below to remove or add samples to customize the batch to your specific needs.

*Note: Samples without Sample ID or Sample Name will be discarded upon batch creation*

Batch Template: C:\Xcalibur\TLF\Templates\BatchTemplates\cough\_cold\_curve.btmp  
Master Method: C:\Xcalibur\TLF\Methods\cough\_cold\_curve.mmx  
Batch File: C:\Xcalibur\TLF\Batches\cough\_cold\_curve\_462015\_a\cough\_cold\_curve\_462015\_a.btx  
Calibration File: C:\Xcalibur\TLF\Batches\cough\_cold\_curve\_462015\_a\Methods\cough\_cold\_curve\_462015\_a.calx

Quick mode

Filename	Sample type	Sample level	Sample ID	Sam name	Vial position	Injection volume	Dilution	Comment
Data_001	Specimen	▼	▼ testmix		1	1.0	1.0	
Data_002	Calibrator	▼	std1	▼ std1 1ml blood	2	1.0	1.0	SOP 202 extracted 9/12/14 MSF
Data_003	Calibrator	▼	std2	▼ std2 1ml blood	3	1.0	1.0	
Data_004	Calibrator	▼	std3	▼ std3 1ml blood	4	1.0	1.0	
Data_005	Calibrator	▼	std4	▼ std4 1ml blood	5	1.0	1.0	
Data_006	Calibrator	▼	std5	▼ std5 1ml blood	6	1.0	1.0	
Data_007	Calibrator	▼	std6	▼ std6 1ml blood	7	1.0	1.0	
Data_008	Negative	▼		▼ blank 1ml blood	8	1.0	1.0	
Data_009	Negative	▼		▼ blank 1g liver	9	1.0	1.0	
Data_010	Specimen	▼		▼ S# T# 1mL Blood	10	1.0	1.0	
Data_011	Specimen	▼		▼ S# T# 0.2mL Blood	11	1.0	5.0	
Data_012	QC	▼	BqcL	▼ qc low 1ml blood	12	1.0	1.0	
Data_013	QC	▼	LqcL	▼ qc low 1g liver	13	1.0	1.0	
Data_014	QC	▼	BqcH	▼ qc high 1ml blood	14	1.0	1.0	
Data_015	QC	▼	LqcH	▼ qc high 1g liver	15	1.0	1.0	

< Back    Next >    Cancel

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.

Please make sure the Batch name you want is typed into the box below.

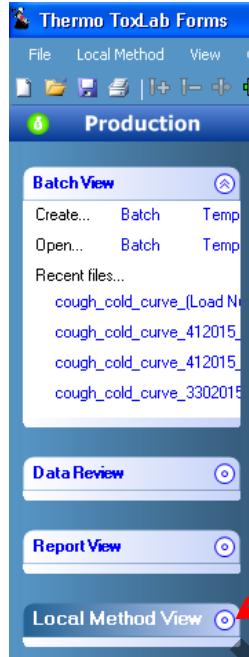
Batch name:

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.

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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.

The screenshot shows the "Local Method View" window for the file "cough\_cold\_curve\_(Load Number)\_cough\_cold\_curve\*". The window has tabs for General, Compounds, QA/QC, Groups, and Reports. The Compounds tab is selected. Under Identification, there is a table with columns: RT, Compound, Compound type, Active, CAS No, LIMS ID, and Use as RT Reference. The "Active" column contains checkboxes for each compound. A red circle highlights the row for compound 9.53 (Doxylamine), which has an unselected checkbox in the Active column. Other compounds listed include Alphaprodine, Diphenhydramine, Orphenadrine, Chlorpheniramine, Brompheniramine, and Dextromethorphan, all with selected checkboxes in the Active column.

RT	Compound	Compound type	Active	CAS No	LIMS ID	Use as RT Reference
8.73	Alphaprodine	Internal Standard	<input checked="" type="checkbox"/>			<input checked="" type="checkbox"/>
9.22	Diphenhydramine	Target Compound	<input checked="" type="checkbox"/>			<input checked="" type="checkbox"/>
9.53	Doxylamine	Target Compound	<input type="checkbox"/>			<input checked="" type="checkbox"/>
9.69	Orphenadrine	Target Compound	<input type="checkbox"/>			<input checked="" type="checkbox"/>
10.16	Chlorpheniramine	Target Compound	<input type="checkbox"/>			<input checked="" type="checkbox"/>
10.81	Brompheniramine	Target Compound	<input type="checkbox"/>			<input checked="" type="checkbox"/>
11.01	Dextromethorphan	Target Compound	<input checked="" type="checkbox"/>			<input checked="" type="checkbox"/>

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

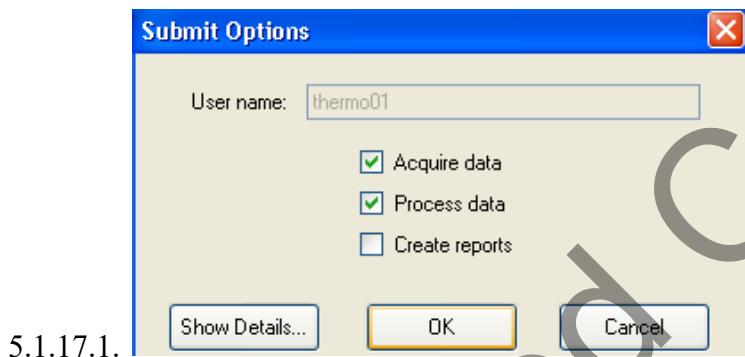
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5.1.15. Have another analyst check the sequence for errors.

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”.



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

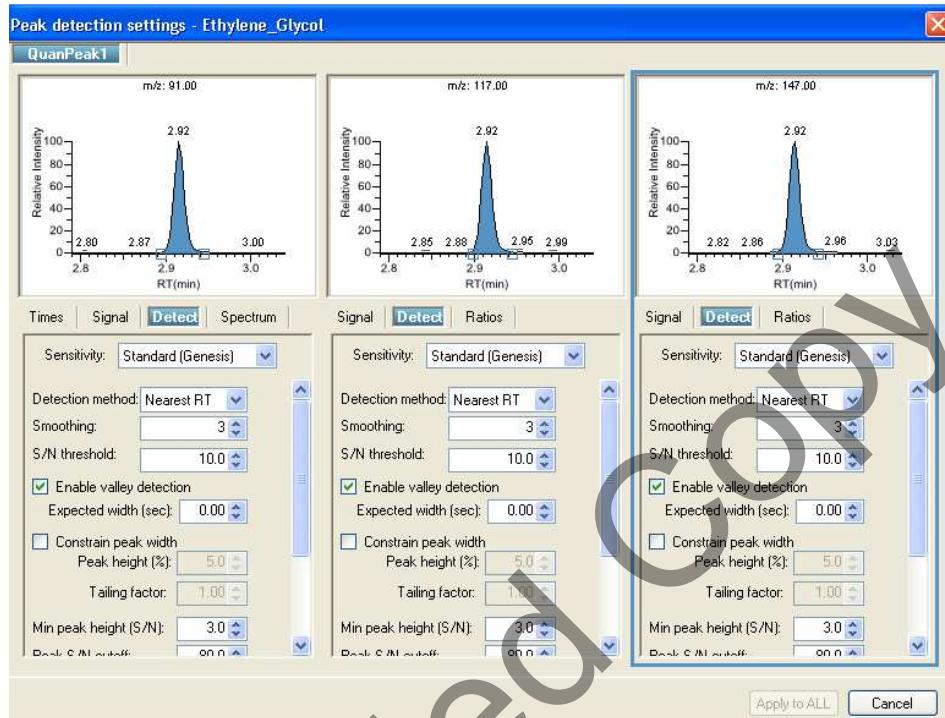
## 5.2. Data Processing

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.

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## 5.2.2.4.3.1.

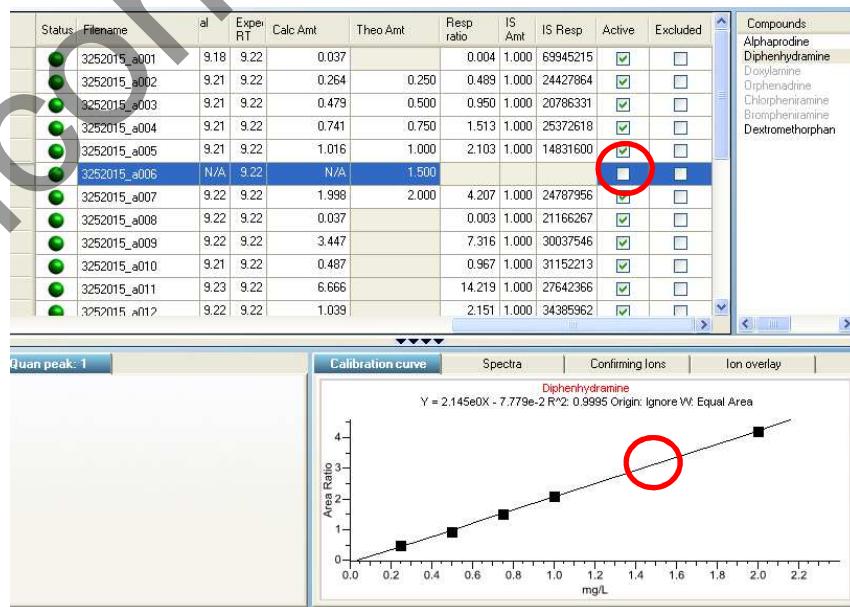
## 5.2.2.5. Save the workbook.

### 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.

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## **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.