

<b>Title: Updating the VOC Calibration Database</b>		Copy No: ##
SOP No.: 7.05/4.1/S	Effective Date: September 11, 2013	Location: ###

QSM Approval: \_\_\_\_\_

## Updating the VOC Calibration Database

### 1. Introduction

This Standard Operating Procedure provides instructions for updating “Initial” VOC calibrations using the Agilent ChemStation software in the EnviroQuant mode.

### 2. Procedure

- 2.1 From the Windows program menu, select and open the standalone “**Data Analysis**” module of the Agilent ChemStation software.
- 2.2 From the “**File**” menu, select and load an appropriate method.
- 2.3 From the “**File**” menu, select and load an appropriate data file.
- 2.4 From the “**Quant**” menu, select “**Calculate/Generate Report**”. In the window which then appears, select “**Detailed, text only**” as the “**Style**” of report, click the “**File**” box under “**Destination**”, and click “**OK**”. The generated report will be saved as a file named “**detail.xls**”.
- 2.5 Select “**QEdit Quant Results**” option in the “**Quant**” menu. Ensure that there is an “**x**” next to each compound name in the “**Quick QEdit**” box. If there a missing “**x**”, it is almost always due to the assignment of an incorrect retention time. Double click on the compound name to view the expected location of the peak. Manually integrate it by clicking on the right mouse button and dragging the baseline. Note the retention time generated. Exit the “**Quick QEdit**” box. From the “**InitCal**” menu, select “**Edit Compounds**”, select “**View**” for the required compound in the list. On “**Page 1**” enter the new retention time. Repeat step 2.4 and ensure that there is now an “**x**” beside all compounds.
- 2.6 **The integration of all standard compounds must be examined CLOSELY for ALL levels.** This is done via the “**QEdit Quant Results**” option in the “**Quant**” menu. Manually integrate as required. When all required corrections for a given level have been made, “**EXIT**” the Quick QEdit box and save changes by selecting “**YES**”. Repeat steps 2.4 and 2.6 for all calibration levels.

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- 2.7 From the “InitCal” menu, select “Clear All Calibration Responses”. From the “InitCal” menu, select “Edit Compounds”, highlight any compound and select “View”. Go to “Page 3” and confirm that there are no entries under “Response” in the table.
- 2.8 **Before proceeding further, save the selected method under a new name which incorporates the current date.**
- 2.9 Select and load the 500 mL CANMIX run. From the “InitCal” menu, select “Update Levels”. “Delete” any unnecessary “Level”.
- 2.10 From the “InitCal” menu, select “Update Levels” again. Select “Recalibrate”. Select the “Level” represented by the CANMIX data file. Select “No Update” under “Responses”. Select “Replace” under “Retention Times”. Click “Do Update”. “Exit” the “Edit Compounds” window which pops up.
- 2.11 Repeat step 2.10, this time selecting “No Update” for “Retention Times”, selecting “Replace” for “Responses”, and marking the “Replace Qualifier Ions Relative Responses” box. Click “Do Update” once more. Step 2.10 and 2.11 are separate to ensure that all updates are processed by ChemStation. In some versions of the software, this will not occur if updates to Responses, Retention Times and Qualifier Ion Relative Responses are done simultaneously. This completes the update for one level.
- 2.12 Load a CANMIX data file representing another “Level”. Repeat step 2.11, **but first UNMARK the “Replace Qualifier Ion Relative Responses” box. Repeat until all calibration levels are updated.**
- 2.13 From the “InitCal” menu, select “Edit Compounds”, select “View” for the first compound in the list, then click on “Page 3”. Check that a response value is entered beside each calibration level which was just updated. Click on “Next”, and check that a response value is entered for **EVERY** compound in the database
- 2.14 To evaluate the results of the calibration update versus VOC method acceptance criteria, re-load the CANMIX file representing the 300 mL calibration level. Repeat step 2.4. Check the integration of each peak and manually integrate as required. Go to the “CustRpt” menu and select “Custom Report”. If necessary, click on “Change Method Report Template”, and click “OK”. A list of available templates will appear. Select the current calibration check template and click “OK”. Click on “Edit Template” option and click “OK”. A template described as “VOC CALIBRATION CHECK” will appear.

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2.15 In order to ensure that the analytical system remains in control, a daily calibration check is done by inserting at least one 300mL CANMIX run into the sequence. Repeat step **2.14** to determine if any corrective actions are required.

### 3. Revisions

Sep 2011: Changed "HP" to "Agilent" and corrected typographical errors  
 Section 2.14 Eliminated the specific template name to make the SOP more generic  
 Section 2.6 Removed note about 5973 MSD as there are now several 5975 MSDs in service  
 Reordered steps as required to reflect current practice and make them clearer  
 Deleted previous revisions  
 Aug 2013: Section 2.11 Added note to give reason for separate steps in 2.10 & 2.11  
 Swapped Sections 2.12 & 2.13 to ensure that there would be a check on the presence of responses for each level in all compounds once the calibration update was complete

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