Creating the Calibration Curve and Generating Method 8261 Quantitation Reports through SMCReporter V4.0

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# Demonstration. Install SMCREPORTER

- This slide show is in addition to documentation provided with method 8261 software.
- The reader can reproduce the processing to be presented by installing Smcreporter 4.0 http://www.epa.gov/nerlesd1/chemistry/vacuu m/methods/software.htm
- Download the zip file as per Installation Guide at the site.
- You will have created a folder "SMCREPORTER" on the C drive as the default.



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# Load Demonstration Files for this Exercise

 The reader can reproduce the processing to be presented by installing data files used. They can be downloaded in a zip file (example.zip) from http://www.epa.gov/nerlesd1/chemistry/vacuum/methods/software.

htm When the software and data files are installed, a ne

- When the software and data files are installed, a new folder, SMCREPORTER, is created. Under this folder a sub-folder, Example, contains the example data files including the method 8261 library (CLPLibrary.txt), internal standard file (CLP
- istds.ini), blank (t4050601.txt), and five standards (t4050604.txt, t4050605.txt, t4050606.txt, t4050607.txt, t4050609.txt).
- This presentation assumes an understanding of the method 8261 calculations using surrogates. See <a href="http://www.epa.gov/nerlesd1/chemistry/vacuum/reference/analysis">http://www.epa.gov/nerlesd1/chemistry/vacuum/reference/analysis</a>

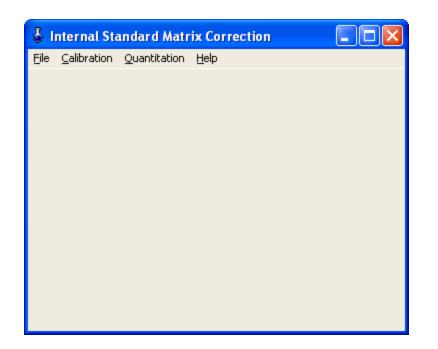
/anal.htm .



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# **Run SmcReporter**

 Go to Windows->Programs->and click on SmcReporter. The following is displayed

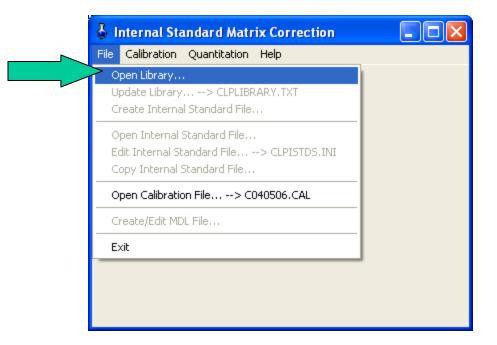




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### Load Library "CLPLibrary.txt"

• Go to File then "Open Library"



 Open File window is displayed. Navigate to the Example folder and highlight CLPLibrary.txt and Open. CLPLibrary is now activated.



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# Load Internal Standard File "CLPistds.ini"

• Go to File then "Open Internal Standard File"

File		on 🔄 🗖 🕑
	Calibration Quantitation Help	
U	pen Library pdate Library> CLPLIBRARY.TXT reate Internal Standard File	
0	pen Internal Standard File	
	dit Internal Standard File opy Internal Standard File	
0	pen Calibration File	
C	reate/Edit MDL File	
E:	xit	

 Open File window is displayed. Navigate to the Example folder and highlight CLPistds.ini and Open. The internal standard file is activated.

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## GC/MS data set

- The raw data must be in ASCII format and readable in Notepad (e.g. t4050601.txt)
- These text files are generated by software available on this site and convert instrument data files to the required format.
- These data files contain the GC/MS response (area) and retention time for each compound.
- Each compound in the "CLPlibrary.txt" library is present in the data file.
- The first line of the data file contains the label "DATA FILE" followed by version of software



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# Data File Example

- Open the blank data file in notepad (t4050601.txt)
- Note each compound is identified with a GC/MS response tab delimited

		601.txt				J
File	Edit	F <u>o</u> rmat	⊻iew	<u>H</u> elp		
		E – Ver		4.0		
		06 13:1 bur∖dat		soco	11 12 204	
1. V	carr	Dui (dai	La(14)	5080	11.1 aw	
GC ∕N						
	POUND		41.0		1107500 F 11000777777777	
	one-				1197589 5.44688333333333 5.72995	
		ie_chlor			1184756 6.14635	
		hane-13			1486225 7.11223333333333	
hexa	ifluo Jahvo	robenze	ene		4011500 6.829166666666667 934259 7.661716666666667	
		tate-13			5623404 7.312233333333333	
		iorobenz				
	zene-				8.3612	
		lloroetk nzene			1446947 8.3112 8.6609333333333	
			izene	520	8268919 8.71093333333333	
1,2-	dich	loropro	opane-	-d6	8268919 8.71093333333333 1881452 9.260416666666667 9.71015	
1,4-	·diox	ane-d8	7759	935	9.71015	
	lene- dine	-d8 :-d5			10.9591166666667 11.05885	
		ichloro				
		omoetha		ł	11118745 12.97396666666667	
		nzene-o -d10		E GA	3626277 13.88985 14.9888	
		luorobe			3648841 16.7375	
					17.1039	
1,2-	dich	lorober	izene-	-d4	4455462 19.96796666666667	
ueca nitr	oben	robiphe Izene-de	enyi Si 6109	975	2012995 19.96796666666667 21.217183333333 20.70105	
acet	:ophe	none-ds	5 1409	388	20.70105	
1,2,	4-tr	richloro	obenze	ene-c	i3 4932303 22.0997333333333	
		ene-d8			22.3828166666667 12829688 23.8981833333333	
T-UIE	; cny i	napricha	arene-	010	12027000 23.0701033333333	
<						>

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## **Calibration**

- The library and internal standard files represent the compounds in the internal standards and standards (see slide presentation "Running Samples")
- Standards are prepared as in "Running Samples" slide presentation (<u>http://www.epa.gov/nerlesd1/chemistry/vacuum/training/pdf/run\_samples.pdf</u>).
- The standard amounts are expressed as dilutions of conc1 in the CLPlibrary.txt library (the mass is by compound and not global)
- All runs contain 5 uL of the working surrogate solution and standards are as follows:
  - A. 10uL 1:1 working standard, dilution 2; t4050607
  - B. 3uL 1:1 working standard, dilution 0.6 ; t4050606
  - C. 5uL 1:10 working standard, dilution 0.1 ; t4050605
  - D. 1uL 1:10 working standard, dilution 0.02 ; t4050604
  - E. 3uL 1:100 working standard, dilution 0.006 ; t4050609

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### Creating the Calibration Curve for Data Processing

• Go to Calibration and select "Create/New"

ا 🕹 ا	nternal Sta	andard Matr	ix Correction	
File	Calibration	Quantitation	Help	
	Create/N	lew		
T	Review			
	Print Cali	bration		
	Check Ca	alibration		
			1	

 A display indicates library and surrogate files that are going to be used for calibration.
 Verify "CLPistds.ini" and select "OK"

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#### **Create Calibration File**

• The next window, "Create Calibration File" is then displayed. The "Add Reference File" button will be discussed next.

\$ Create Calibrati	ion File	
Compound Library:	C:\SMCREPORTER\EXAMPLE\CLPLIBRARY.TXT	
Surrogate Library:	C:\SMCREPORTER\EXAMPLE\CLPISTDS.INI	
Data Directory	Concentration	
Surrogate Refe	۳	
Add Standard	Add Reference File Delete	
Print	Save Review Exit Help	

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### **Reference File**

- The reference file used in calibration is the initial condition of internal standards that the standard are compared. The response of internal standard compounds in the reference file is taken to be the 100 % response. The internal standards in the standard runs are compared to their response in the reference file and deviations from 100% are determined as functions of their boiling points (BP's) and relative volatilities (α's).
- An internal standard reference file can be any of the runs used to generate a calibration but typically, the blank run (t4050601.txt) run prior to the calibration standards is used.
- Select "Add Reference File" and using the "Open" window that is displayed navigate to the Example folder and select the t4050601.txt file.
- Internal standards have been called 'surrogates" in the past (and you will still see some use of 'surrogates' in place of internal standards.

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#### Create Calibration File with Reference Added

• Click on "Add Standard."

🕹 Create Calibration File	
Compound Library: C:\SMCREPORTER\EXAMPLE\CLPLIBRARY.TXT	
Surrogate Library: C:\SMCREPORTER\EXAMPLE\CLPISTDS.INI	
Data Directory Concentration	
pgate Reference: C:\SMCREPORTER\Example\t4050601.txt	
Add Standard Add Reference File Delete	
Print     Save     Review     Exit     Help       D0 N0T print Surrogate report	

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#### **Add the First Standard**

• Using the "Open" window navigate to the Example folder and select the file t4050607.txt then open. This file is the standard "A" listed in slide #9. Click

Open					? 🛛
Look jn:	🗁 Example		•	← 🗈 💣 📰•	
My Recent Documents Desktop My Documents My Computer	<ul> <li>CLPLibrary.txt</li> <li>t4050601.txt</li> <li>t4050604.txt</li> <li>t4050605.txt</li> <li>t4050606.txt</li> <li>t4050607.txt</li> <li>t4050607.txt</li> <li>t4050609.txt</li> </ul>				
My Network Places	File <u>n</u> ame:			•	<u>O</u> pen
	Files of <u>type</u> :	Quantitated data file (*.txt)		-	Cancel

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"Open."

# **Adding Standards**

- The Identify Standard Level window is displayed
- Enter 2 in the Dilution factor field
- If a dilution factor is entered the Concentration as Dilution of Conc1 is automatically toggled.
- Select Exit to enter

Identify Standard Level	X
Standard file path C:\SMCREPORTER\E	xample\t4050607.txt
C Conc1 C Conc2 C Conc3 C Conc4	
C Conc5 C Concentration as Dilution of Conc1	Dilution Factor
Exit	

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#### **Create Calibration File with Standard A Added**

 If there was an error in entry, highlight the standard file in the Data Directory and press "Delete" and repeat the Add Standard routine

🕹 Create Calibrati	on File	
Compound Library:	C:\SMCREPORTER\EXAMPLE\CLPLIBRARY.TXT	
Surrogate Library:	C:\SMCREPORTER\EXAMPLE\CLPISTDS.INI	
Data Directory	Concentration	
C:\SMCREPORTE	R\Example\t4050607.txt	
Surrogate Referenc	e: C:\SMCREPORTER\Example\t4050601.txt	
Add Standard Print DO NOT print S	Add Reference File     Delete       Save     Review       urrogate report	

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#### **Add Standards B-E**

- Repeat the "Add Standard" routine for standards B-E. The dilutions for these standards are (0.6, 0.1, 0.02, and 0.006 respectively.
- The Create Calibration File should appear as

🕹 Create Calibration File	
Compound Library: C:\SMCREPORTER\EXAMPLE\CLPLIBRARY.TXT	
Surrogate Library: C:\SMCREPORTER\EXAMPLE\CLPISTDS.INI	
Data Directory Concentrat	ion
C:\SMCREPORTER\Example\t4050607.txt         2           C:\SMCREPORTER\Example\t4050606.txt         0.6           C:\SMCREPORTER\Example\t4050605.txt         0.1           C:\SMCREPORTER\Example\t4050604.txt         0.02           C:\SMCREPORTER\Example\t4050609.txt         0.006	
Surrogate Reference: C:\SMCREPORTER\Example\t4050601.txt	_
Add Standard     Add Reference File     Delete       Print     Save     Review     Exit     Help       D0 N0T print Surrogate report	

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## **Review calibration curve**

- If all entries are correct the next step is to review the data.
- Press the "Review" tab on the "Create Calibration File" form.
- The following slide presents the "Review Calibration" form, starting at the first library entry (the default).
- Note that no sample sizes are entered. Only the total ngs are being displayed. This is an important feature of method 8261 as calibration is by mass and not by matrix or sample size.

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#### Review Calibration Form

The Previous' and 'Next' buttons move the review stepwise through all compounds

Move through the scroll box and highlight a compound jumps the review to the selected compound

Review Calibration					
Compound Number: 1	Compound	d:diethyleth	er-d10	diethyl_ethe acetone-130	
<- <u>P</u> revious <u>N</u> ext->				meNylene_c	hloride-d2
				het afluorobe tetrahydrofur ethylacetate	an-d8
				pentafluorob	enzene
Library File: C:\SMCREP(	)RTER\Example	\CLPLibrary.txt		benzene-d6 1,2-dichloroe fluorobenzer	
Surrogate File: C:\SMCREP(	RTER\EXAMPL	E\CLPISTDS.IN	I	1,4-difluorob 1,2-dichlorop	propane-d6
Reference file t4050601.txt				1,4-dioxane- toluene-d8	d8
				pyridine-d5 1,1,2-trichlor	oethane-d3
Calibration File:					
Standard File Name	Std1	Std2	Std3	Std4	Std5
Concentrations	t4050607.txt	t4050606.txt	t4050605.txt	t4050604.txt	t4050609.txt
Loncentrations	250	250	250	250	250
Recoveries (%)	95.864	80.118	76.947	102.720	93.423
Recovery (Dev.)	0.072	0.024	0.056	0.074	0.038
Area	1072358	939866	920424	1202804	1089734
Response Factors	4474.495	4692.435	4784.729	4683.798	4665.792
Response Factor(Dev.)	335.573	143.012	350.778	335.495	191.488
Standard Included	$\overline{\mathbf{v}}$	V	V		V
Curve response factors	Standard Leve	ls	Average	e Deviatio	n %Deviation
Average	(250, 250, 250	), 250, 250)	4660.2	50 113.60	1 2.438
	1.		,	,	,
Print	Save A	As 🗌	Exit	Help	
🔲 DO NOT Include Surrogate i	nformation on Ca	libration report			
🔲 DO NOT Print Surrogate Re	port				

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# Reviewing Calibration by Compound

- By selecting the "Next" tab (upper left corner) each compound is displayed.
- Scroll or jump the review to chloroethane. If you scroll you will see the % Deviation box (toward lower left) of all compounds have been <25 % until we get to chloroethane.
- The results for chloroethane show that the lowest standard (1.5ng) response factor is not equivalent to the others.

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#### Eliminating a Data Point

Std5 response factor is twice the average (red arrow) resulting in elevated %Deviation (green arrow)

Click of check box (yellow arrow) to remove the 1.5 ng standard for chloroethane. This only removes the data point for chloroethane and no other compounds are changed.

Review Calibration					
Compound Number: 34	Compound	t: chloroetha	ne	1,2-dibromoe chlorobenze	
<- <u>P</u> revious <u>N</u> ext->				o-xylene-d10 4-bromofluor	
				bromobenzer 1,2-dichlorob	ne-d5 📃
				decafluorobi nitrobenzene	-d5
Library File: C:\SMCREP0	) RTER\Example	CLPLibrary.txt			obenzene-d3
Surrogate File: C:\SMCBEP0	) RTER\EXAMPL			naphthalene 1-methylnaph	hthalene-d10
		EXCEPTSTD 5.IN		dichlorodifluc chloromethat	ne
Reference file t4050601.txt				vinylchloride bromomethat chloroethane	ne 🔄
Calibration File:	C1.11	0.40	0.12		
Standard File Name	Std1 t4050607.txt	Std2 t4050606.txt	Std3 t4050605.txt	Std4 t4050604.txt	Std5 t4050609.txt
Concentrations	500	150	25	5	1.5
Recoveries (%)	96.757	94.121	97.950	105.936	96.655
Recovery (Dev.)	0.013	0.013	0.028	0.028	0.011
Area	1588625	657955	82227	23356	12978
Response Factors	3283.744	4660.351	3357.915	4409.468	8951.406
Response Factor(Dev.)	42.473	64.571	96.195	114.621	105.851
Standard Included					
Curve response factors	Standard Level	s	Average	e Deviatio	n %Deviation
Average	(500, 150, 25,	5, 1.5)	4932.57	77 2328.99	47.217
Print	Save A	.s	Exit	Help	
🔲 DO NOT Include Surrogate i	nformation on Cal	ibration report			$\checkmark$
🔲 DO NOT Print Surrogate Rej	port				

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## Std5 Chloroethane Removed

- Removing Std5 improved the linearity dramatically.
- This action also eliminated the calibration point from the standard levels (green arrow).
- The lower limit of quantitation has now been raised from 1.5 to 5 ng for this calibration curve.

🅉 Review Calibration					_		
Compound Number: 34	1,2-dibromo chlorobenze o-xylene-d1i 4-bromofluo bromobenze 1,2-dichloro decafluorob nitrobenzen acetophenc	ene-d5 ) robenzene ene-d5 benzene-d4 iphenyl e-d5					
Library File: C:\SMCRE	PORTER\Exampl	e\CLPLibrary.txt			robenzene-d3		
Surrogate File: C:\SMCRE	PORTER\EXAMP	LE\CLPISTDS.IN	I	1-methylnap	hthalene-d10 oromethane		
Reference file t4050601.	txt			chlorometha vinylchloride bromometha	•		
Calibration File:				chloroethan		~	
Standard File Name	Std1 t4050607.txt	Std2 t4050606.txt	Std3 t4050605.txt	Std4 t4050604.txt	Std5 t4050609.txt		
Concentrations	500	150	25	5	1.5		
Recoveries (%)	96.757	94.121	97.950	105.936	96.655		
Recovery (Dev.)	0.013	0.013	0.028	0.028	0.011		
Area	1588625	657955	82227	23356	12978		
Response Factors	3283.744	4660.351	3357.915	4409.468	8951.406		
Response Factor(Dev.)	42.473	64.571	96.195	114.621	105.851		
Standard Included		$\overline{\mathbf{v}}$			Γ		
Curve response factors	Standard Lev	els	Average	e Deviatio	on %Devi	iation	
Average	(500, 150, 25	5, 5)	3927.8	70 709.04	0 18.052	2	
Print Save As Exit Help							
DO NOT Include Surrogate information on Calibration report							
DO NOT Print Surrogate	Report						
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# **Editing the Calibration Curve**

- The large deviation for chloroethane indicated there was a problem with the compound at the lowest concentration.
- Evaluating the chromatogram for chloroethane we found that low level interference was causing the bias.
- Removing a calibration point for a compound changes the calibration range. Such changes may be necessary to ensure the response factor is consistent and we are working a justifiable calibration range.
- When compounds are also consistently in the system blanks their low calibration points could be compromised and these should also be 'unchecked'. This action puts background below LOQ and also mitigates background bias from their response factor.
- By removing a data point, the linearity will be recalculated and the LOQ changed.



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## **More Changes!**

- Stepping through the calibration review we find diethyl ether (compound #36) is the next compound that requires the low-level calibration point to be removed.
- The next compound that has a large linearity deviation is a common laboratory contaminant, Acetone (#38). This compound is a very persistent compound in the laboratory that generated the data as the laboratory is not isolated as most volatile analyses laboratories. Removing all data points except the largest raises the LOQ to the highest standard. This means any detection of acetone in a sample will be flagged as below LOQ or exceeds the upper limit of quantitation.
- Methylene chloride (#45) and 2-butanone are additional laboratory contaminants and their two lowest calibration points are unchecked.
- If a compound is not detected in a standard, the standard included checkbox is unchecked and the calibration point is not used in the calibration range.
- Additional compounds that are to be unchecked from the lowest standard are 39, 43, 54, 61, 69, 73, 112, 114, and 115.



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## Save calibration curve

- After the review, save the calibration curve. Click on the "Save as" button on the lower right hand corner of the review and save the file as "Calibration.cal".
- The calibration file is a standalone file containing all information necessary to process sample data. If the SMCReporter program is closed test.cal can be reloaded for sample processing. "CLPlibrary.txt" and "CLPistds.ini" do not have to be recalled.

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## **Quantitate samples**

- The newly created calibration file can now be used to process data.
- Load the calibration file by File->Open Calibration File

🌡 Internal Standard Matrix Correction	
File Calibration Quantitation Help	
Open Library Update Library> CLPLIBRARY.TXT Create Internal Standard File	
Open Internal Standard File Edit Internal Standard File> CLPISTDS.INI Copy Internal Standard File	
Open Calibration File	
Create/Edit MDL File	
Exit	

• Select the newly created Calibration.cal



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# **Calibration Loaded**

- Notice that after loading the calibration file that library CLPlibrary.txt and CLPistds.ini are disabled (under File).
- The main window (see slide 4) now has Calibration and Quantitation menu options enabled.
- In the Calibration menu options for review, printing, and check standard reporting are now enabled.

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- With calibration file test.cal loaded the next step is to start the quantitation process.
- Select Quantitation->Process Sample Files

δ.	nternal Sta	andard Matr	ix Correction	
File	Calibration	Quantitation	Help	
		Process sa	mple files	

• The Process Files window for entering samples appears (next slide).



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#### **Enter File for Quantitation**

Process Files	
Calibration File: C:\SMCREPORTER\EXAMPLE\CALIBRATION.CAL Data Directory	
Add File Delete File Process Review Exit Help	

- Select "Add File" and navigate to the low-level standard we used in calibration, t4050604.
- Upon selection of file a window for inputting sample information appears (next slide).

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#### Input Window for File Processing

When the file is called, SMCReporter extracts file information (green arrows).

Note we can include the calibration error (the % Deviation) in results (red arrow). This error will be propagated with the analytical results.

Fi	le Processing Inp	ut
	Current Sample File:	C:\SMCREPORTER\EXAMPLE\T4050604.TXT
	Analyzed Date	04/05/2006 17:11 Sample ID
	Lab Sample ID	Std D 0.02 dilution Instrument ID GC/MS
	Lab File ID	t4050604.raw
	Method Detection I Limits C MDL C CRQL I None	Limits
	Reporting Units Sample Size Matrix	ng/mL
	DO NOT Print Comment 1:	Surrogate Report 🔽 Quantitation report
	Er	Help

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# **Sample Information**

- Leave the "List MDL" "no" checked.
- Leave the reporting units as ng/mL.
- Enter 5 for the sample size (5 mL).
- Enter "Water" for matrix.
- The fields Sample ID and comment 1 are for entering sample specific information at this time.
- Check the "DO NOT print surrogate report" box. We will address that report later.
- Click "Enter". The next window should look like the following slide.



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# **Sample Ready to Process**

🕹 Process Files
Calibration File: C:\SMCREPORTER\EXAMPLE\CALIBRATION.CAL
Data Directory
C:\SMCREPORTER\Example\t4050604.txt
Add File Delete File Process Review Exit Help

- For this exercise we will only process the one standard run but a sample batch can be entered at this point.
- Now click "Process" and a quantitation report (both paper and electronic) will be generated for the sample. You can select a pdf writer as default printer and the output will be a pdf format.



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## **Electronic Data Report**

	📑 t4050604_Calibration.prn - Notepad	
	<u>File E</u> dit F <u>o</u> rmat <u>V</u> iew <u>H</u> elp	
	Quantitation Report - Linear: BP - Ln: RVW - Version 4.0	~
The file name of the report is t4050604_Calibratio n.prn and resides in the folder, Example.	File Identification: C:\SMCREPORTER\Example\t4050604.txt Calibration File:C:\SMCREPORTER\Example\Calibration.cal Process Date: 05/05/2006 10:47 Acquisition Date: 04/05/2006 17:11 Lab File ID: t4050604.raw; Sample ID: Std D 0.02 dilution; Instrument ID: GC/MS Compound Library:C:\SMCREPORTER\EXAMPLE\CLPLIBRARY.TXT Sample Size: 5.00 Surrogate Groups: C:\SMCREPORTER\EXAMPLE\CLPISTDS.INI Sample Type: waterNone - No limits indicated for reporting Comment 1: Client Sample ID: Std D 0.02 dilution Sample ID: X - Compound detected at less than LOQ Y - Compound exceeds F	100
The .prn file combines the data and the calibration file names.	Compound#;Compound;ng/mL;PM;Error;Qualifier;Recovery;PM;Deviation;Area;Retention Time; 30;dichlorodifluoromethane;0.83;±;0.007;;106.23;±;0.83;29220.00;2.67;75-71-8 31;chloromethane;0.89;±;0.007;;105.18;±;0.83;110845.00;3.62;74-87-3 32;vinylchloride;0.81;±;0.006;;106.23;±;0.83;36974.00;3.95;75-01-4 33;bromomethane;0.82;±;0.007;;104.54;±;0.83;16536.00;4.73;74-83-9 34;chloroethane;1.12;±;0.009;;105.87;±;0.83;23356.00;4.86;75-00-3 35;trichlorofluoromethane;0.91;±;0.007;;106.23;±;0.83;243492.00;5.13;75-69-4	
The information is semicolon delimited for inputting into other programs.	<pre>36;diethyl_ether;2.56;±;0.194;;102.90;±;7.79;79582.00;5.51;60-29-7 37;1,1,2-trichloro-1,2,2-trifluoroethane;0.99;±;0.008;;106.23;±;0.83;41746.00;5.56;76- 38;acetone;34.22;±;3.627;X;130.82;±;13.86;780713.00;5.75;67-64-1 39;1,1-dichloroethane;0.87;±;0.007;X;106.23;±;0.83;27735.00;5.71;75-35-4 40;iodomethane;2.03;±;0.016;;104.03;±;0.83;37721.00;6.00;74-88-4 41;allylchloride;1.17;±;0.009;;105.23;±;0.83;23006.00;6.06;107-05-1 42;acetonitrile;3.82;±;0.427;;124.11;±;13.86;67506.00;5.98;75-05-8 43;methyl_acetate;1.22;±;0.086;;109.58;±;7.79;138637.00;6.08;79-20-9 44;carbon_disulfide;0.89;±;0.007;;106.23;±;0.83;124724.00;6.15;75-15-0 45;methylene_chloride;1.64;±;0.012;X;102.50;±;0.76;73456.00;6.16;75-09-2</pre>	-13-1
Surrogate data is at the bottom of this	46;MTBE;0.99;±;0.075;;102.77;±;7.79;109230.00;6.30;1634-04-4 47;acrylonitrile;1.77;±;0.127;;108.42;±;7.79;71686.00;6.33;107-13-1 <	<b>∨</b> ≥ .::

ট t4050604_Calibration.prn - Notepad	
<u>F</u> ile <u>E</u> dit F <u>o</u> rmat <u>V</u> iew <u>H</u> elp	
114;2-methylnaphthalene;1.99;±;0.152;;113.74;±;8.67;151175.00;23.67;91-57-6 115;1-methylnaphthalene;2.02;±;0.154;;113.74;±;8.67;140942.00;24.00;90-12-0	-
Surrogate Determinations	
Volatile Compound Surrogates(boiling point<159) 3;methylene_chloride-d2;85.4;±;0.6;102.5;±;0.8;1065506.00;6.15;1665-00-5 9;benzene-d6;103.0;±;1.1;103.4;±;1.1;9830983.00;8.36;1076-43-3 13;1,2-dichloropropane-d6;97.2;±;1.6;103.5;±;1.7;1959368.00;9.28;93952-08-0 17;1,1,2-trichloroethane-d3;100.1;±;1.6;103.2;±;1.7;2348351.00;11.63;171086-93-4 21;4-bromofluorobenzene;100.6;±;1.7;101.0;±;1.7;3753607.00;16.75;460-00-4	
	> .



file.

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**RESEARCH & DEVELOPMENT** 

#### Quantitation

Surrogate Groups:

Report Printout

File Identification: C1/SMCREPORTER/Example/t4050604.txt Process Date: 05/05/2006 10:47 Acquisition Date: 04/05/2006 17:11 Sample Size: 5 Sample Type: water Comment: Sample ID: Lab Sample ID: Std D 0.02 dilution Instrument ID: GC/MS Lab File ID: t4050604.raw

#### Qualifier: X - Compound detected at less than LOQ\_Y - Compound exceeds HOQ

	Compound	ng/mL	Error	Q	Recovery±D	eviation	Com	pound	ng/mL	Error	Q	Recovery±De	viation
30:	dichlorodifluoromethane	0.833	± 0.007		106.23	± 0.83	77:	1,3-dichloropropane	0.956	± 0.016		102.86	± 1.70
31:	chloromethane	0.892	± 0.007		105.18	± 0.83	78:	tetrachloroethene	1.03	± 0.017		104.99	± 1.76
32:	vinytchloride	0.807	± 0.006		106.23	± 0.83	79:	dibromochloromethane	0.980	± 0.016		102.74	± 1.70
33:	bromomethane	0.825	± 0.007		104.54	± 0.83	80:	1,2-dibromoethane	0.960	± 0.016		102.40	± 1.70
34:	chloroethane	1.12	± 0.009		105.87	± 0.83	81:	chlorobenzene	0.947	± 0.017		101.82	± 1.85
35:	trichlorofluoromethane	0.912	± 0.007		106.23	± 0.83	82:	1,1,1,2-tetrachioroethane	0.842	± 0.014		102.08	± 1.69
36:	diethyl ether	2.56	± 0.194		102.90	± 7.79	83:	ethylbenzene	0.987	± 0.017		102.30	± 1.73
37:	1,1,2-trichloro-1,2,2-trifluoroethane	0.986	± 0.008		106.23	± 0.83	84:	m, p-xylenes	0.993	± 0.018		102.56	± 1.86
38:	acetone	34.2	± 3.63	х	130.82	± 13.86	85:	o-xylene	0.969	± 0.018		101.54	± 1.85
39:	1,1-dichloroethene	0,869	± 0.007	х	106.23	± 0.83	86:	styrene	0.984	± 0.016		101.25	± 1.69
40:	iodomethane	2.03	± 0.016		104.03	± 0.83	87:	isopropylbenzene	1.01	± 0.017		102.24	± 1.74
41:	allyichioride	1.17	± 0.009		105.23	± 0.83	88:	bromoform	0.845	± 0.014		101.61	± 1.69
42:	acetonitrile	3,82	± 0.427		124.11		89:	cis-1,4-dichloro-2-bulene	3.64	± 0.281		101.37	± 7.84
43:	methyl_acetate	1.22	± 0.086		109.58	± 7.79	90:	1,1,2,2-tetrachloroethane	1.05	± 0.081		101.28	± 7.85
44:	carbon disulfide	0.892	± 0.007		106.23	± 0.83	91:	1,2,3-trichloropropane	0.913	± 0.069		100.78	± 7.65
45:	methylene_chloride	1.64	± 0.012	х	102.50	± 0.76	92:	propylbenzene	0.995	± 0.009		102.00	± 0.90
46:	MTBE	0.989	± 0.075		102.77	± 7.79	93:	bromobenzene	1.02	± 0.008		100.35	± 0.83
47:	acrytonitrile	1.77	± 0.127		108.42	± 7.79	94:	trans-1,4-dichloro-2-bulene	3.84	± 0.292		100.74	± 7.64
48:	trans-1,2-dichloroethene	0.839	± 0.007		104.02	± 0.83	95:	1,3,5-trimethylbenzene	1.01	± 0.009		101.39	± 0.90
49:	1,1-dichloroethane	0.944	± 0.010		103.24	± 1.07	96:	2-chlorotoluene	1.03	± 0.011		101.41	± 1.11
50:	2,2-dichloropropane	0.864	± 0.007		105.18	± 0.83	97:	4-chiorotoluene	1.01	± 0.011		101.21	± 1.11
51:	propionitrile	1.41	± 0.105		192.59			tert-butylbenzene	0.985	± 0.009		102.34	± 0.90
52:	2-butanone	6.02	± 0.563	х	148.24		99:	sec-butylbenzene	1.01	± 0.009		103.36	± 0.90
53:	cis-1,2-dichloroethene	0.968	± 0.010		102.65	± 1.07	100:		0.996	± 0.008		100.93	± 0.83
54:	methacrylonitrile	1.97	± 0.146		108.02	± 8.04		1,2,4-trimethylbenzene	0.991	± 0.011		101.75	± 1.11
55:	chloroform	1.03	± 0.008		102.29	± 0.76		p-isopropyltoluene	0.991	± 0.009		103.35	± 0.91
56:	bromochloromethane	0.896	± 0.007		102.70	± 0.76		1,3-dichlorobenzene	1.02	± 0.011		101.44	± 1.11
57:	cy clohexane	0.831	± 0.007		106.23	± 0.83		1,4-dichlorobenzene	1.04	± 0.011		101.34	± 1.11
58:	1,1,1-trichloroethane	0.898	± 0.007		105.28	± 0.83		n-butylbenzene	0.941	± 0.008		103.98	± 0.91
59:	1,1-dichloropropene	0.983	± 0.016		106.79	± 1.78		1,2-dichlorobenzene	0.791	± 0.006		101.74	± 0.84
50:	carbon_letrachloride	0.839	± 0.007		106.23	± 0.83		acelophenone	2.44	± 0.175		109.14	± 7.85
51:	1,2-dichloroethane	0.838	± 0.006	х	102.79	± 0.76		1,2-dibromo-3-chioropropane	0.962	± 0.073		103.57	± 7.82
52:	benzene	0.962	± 0.008		103.04	± 0.83		nitrobenzene	1.90	± 0.140		107.40	± 7.89
53:	trichloroethene	0.954	± 0.016		105.28	± 1.75		1,2,4-trichlorobenzene	0.932	± 0.019		105.43	± 2.18
54:	methyl_cyclohexane	0.754	± 0.013		106.97	± 1.78		hexachlorobutadiene	0.974	± 0.020		107.70	± 2.24
85:	1,2-dichloropropane	0.857	± 0.014		103.45	± 1.70		naphthalene	1.05	± 0.021		107.19	± 2.19
56:	methylmethacrylate	1.82	± 0.137		106.22	± 8.00		1,2,3-trichlorobenzene	0.952	± 0.019		107.00	± 2.18
57:	dibromomethane	0.943	± 0.015		103.78	± 1.70		2-methylnaphthalene	1.99	± 0.152		113.74	± 8.67
58:	bromodichloromethane	0.828	± 0.014		103.75	± 1.70	115:	1-methylnaphthalene	2.02	± 0.154		113.74	± 8.67
59:	1,4-dioxane	10.4	± 0.522		290.60	± 14.60							
70:	4-methyl-2-pentanone	3.56	± 0.263		107.43	± 7.95							
71:	trans-1,3-dichloropropene	4.77	± 0.079		102.92	± 1.70							
72:	toluene	0.958	± 0.017		103.69	± 1.86							
73:	pyridine	16.3	± 3.59		281.04	± 61.94							
74:	cis-1,3-dichloropropene	4.75	± 0.078		103.40	± 1.70							
75:	2-hexanone	2.04	± 0.151		107.28	± 7.92							
76:	1,1,2-trichloroethane	0.912	± 0.015		103.13	± 1.70							

**RESEARCH & DEVELOPMENT** 



Building a scientific foundation for sound environmental decisions

Page: 1

C:\SMCREPORTER\EXAMPLE\CALIBRATION.CAL

C:\SMCREPORTER\EXAMPLE\CLPISTDS.INI

Compound Library File: C1SMCREPORTER/EXAMPLE/CLPLIBRARY.TXT

# **Quantitation Report**

- Note the header contains a description of all components that were used to generate the report and the file path.
- Each compound is listed with its calculated concentration, method error, predicted recovery and deviation.
- The paper copy of the report contains the same information as the electronic version but in different formats.
- Note the compounds that are marked with an 'X' qualifier. These compounds we remember from reviewing the curve were below the calibration LOQ.



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# **Reporting Limits**

- File Processing Input window is the means to limit results to only those above a threshold. The MDL selection allows using this threshold on a compound by compound basis.
- Similar to the MDL option is the CRQL selection. This selection provides both a limit and use of qualifiers consistent with the Superfund CLP contract SOM1.01. With this option values can be reported below the limit (as a percentage) with another qualifier indicating it below the limit.
- A limit file was created for this presentation as the the concentration of the lower calibration point in 5 mL water (5ml\_low.mdl).
- The adventurous can create their own limit file. This requires reloading the library, CLPlibrary.txt, and the internal standard file, CLPistds.ini. Then Menu->File->Create/Edit MDL File. Type of limit file (matrix and sample size) are entered and compound limits be entered individually or modify an existing MDL file. See the SMCReporter operating manual for greater detail.
- The next slide presents the format of the file (5ml\_low.mdl).



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# 5ml\_low.mdl

- The limit file is a ";" delimited \*.mdl file.
- The header contains information to identify what sample size, matrix, library and surrogate are related to the limit.
- Labeling limit files should include pertinent information such as "5mLwatermdl\_inst1.mdl" or "5mLreportlimit.mdl" for ease of locating.

📮 5ml_low.mdl - Notepad	
<u>File E</u> dit F <u>o</u> rmat <u>V</u> iew <u>H</u> elp	
<pre>% Treation Date;05/05/2006 13:46 Compound Library File:C:\SMCREPORTER\EXAMPLE\CLPLIBRARY.TXT Surrogate File;C:\SMCREPORTER\CLP\clpistds.ini 5.00;water;ng/mL Other; dichlorodifluoromethane;1.00 chloromethane;1.00 bromomethane;1.00 chloroethane;1.00 trichlorofluoromethane;1.00 diethyl_ether;1.00 1,1,2-trichloro-1,2,2-trifluoroethane;1.00 acetone;1.00 1,1-dichloroethene;1.00 iodomethane;1.00</pre>	
allylchloride;1.00 acetonitrile;1.00 methyl_acetate;1.00 carbon_disulfide;1.00 MTBE;1.00 acrylonitrile;1.00 trans-1,2-dichloroethene;1.00 1,1-dichloroethane;1.00 2,2-dichloropropane;1.00 propionitrile;5.00 cis-1,2-dichloroethene;1.00 methacrylonitrile;5.00 chloroform;1.00 bromochloromethane;1.00 1,1,1-trichloroethane;1.00 1,1,1-trichloroethane;1.00 1,2-dichloropropene;1.00 1,2-dichloroethane;1.00	
<	





# Process Files with a Reporting Limit

- To observe the use of limits return Quantitation->Process Files and enter the blank file t4050601.txt.
- When the "File Processing Input" window is displayed check the "MDL" option.
- Note that the window retains the previous inputs as new defaults.



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## Input with Limit Option

- After the MDL option is checked, use browse to locate the MDL file 5ml\_low.mdl and load. (green arrow)
- Uncheck the Surrogate Report. (red arrow)
- For now the "Reporting Limits" box remains "0". (yellow arrow)
- Click "Enter".
- Then click "Process" on the returned Process Files window.

File Processing Inpu	ut		
Current Sample File:	C:\SMCREPORTER\EXAMPLE\T4	050608.TXT	
Analyzed Date	04/05/2006 20:05	Sample ID	
Lab Sample ID	5mL blank	Instrument ID GC/MS	
Lab File ID	t4050608.raw		
Method Detection I Limits MDU C CRQL None Browse for MDL fi C:\SMCREPORTE Reporting Units Sample Size Matrix	Reporting Limits (Numb		
DO NOT Print 🦵	Surroga, Report 🔲 Quanti	tation report	
Comment 1:			
Er	nter Help		

RESEARCH & DEVELOPMENT



Page: 1



The Error term includes propagated calibartion error

The MDL limits are identified in the header, and the analytical results are identified as ND followed by the limit in the results column

		The Erici term nondes propagated care												
		Compound	ng/mL	Error(1s)	Q	Recov	ery±Deviation	Com		ng/mL	Error(1s)	Q	Recove	ry±Deviation
	30:	dichlorodiluoromethane	ND 1.00		х	99.46	± 0.77	74:	cis-1,3-dichloropropene	ND 1.00		х	77.08	± 1.38
	31:	chloromethane	ND 1.00		х	97.05	± 0.77	75:	2-hexanone	ND 2.00		х	73.17	± 5.60
	32:	vinylchloride	ND 1.00		х	99.46	± 0.77	76:	1, 1, 2 trichloroethane	ND 1.00		х	74.58	± 1.37
	33:	bromomethane	ND 1.00		х	95.58	± 0.77	77:	1,3 dichloropropane	ND 1.00		х	75.15	± 1.37
	34:	chloroethane	ND 1.00		х	98.63	± 0.77	78:	tetrachioroethene	ND 1.00		х	98.56	± 1.19
	35:	trichlorofluoromethane	ND 1.00		х	99.46	± 0.77	79:	dibromochloromethane	ND 1.00		х	77.56	± 1.38
	36:	diethyl ether	ND 1.00		х	71.84	± 5.46	80:	1,2-dipromoethane	ND 1.00		х	74.72	± 1.37
, 	37:	1, 1, 2 trichloro 1, 2, 2 trilluoroethane	ND 1.00		х	99.46	± 0.77	81:	chlorobenzene	ND 1.00		х	88.63	± 1.01
	38:	acetone	36.1	± 4.42	х	84.54	± 10.36		1, 1, 1, 2 tetrachloroethane	ND 1.00		х	82.43	± 1.41
	39:	1, 1-dichloroethene	ND 1.00		х	99.46	± 0.77	83:	othy bonzone	ND 1.00		х	94.02	± 1.16
	40:	iodomethane	ND 1.00		х	94.39	± 0.77	84:	m,p-xylenes	ND 1.00		х	94.01	± 1.05
	41:	allylchloride	ND 1.00		х	97.17	± 0.77	85:	o-xylene	ND 1.00		х	89.97	± 1.02
	42:	acetonirie	1.67	± 0.272		79.92	± 10.36		styrene	ND 1.00		х	87.59	± 1.43
	43:	methyl acetate	ND 1.00		х	71.74	± 5.46	87:	isopropylbenzene	ND 1.00		х	95.79	± 1.17
	44:	carbon disulfide	ND 1.00		х	99. <b>4</b> 6	± 0.77	88:	bromoform	ND 1.00		х	76.26	± 1.38
	45:	methylene_chloride	1.15	± 0.119	х	82.OV	± 1.17	89:	cis 1,4-dichloro 2 butene	ND 1.00		х	73.65	± 5.63
	46:	MTBE	ND 1.00		х	71.84	± 5.46	90:	1, 1, 2, 2 tetrachloroethane	ND 1.00		х	73.55	± 5.63
	47:	acry lonitrile	ND 1.00		x	71.76	± 5.46	91:	1,2,3 trichloropropane	ND 1.00		x	74.29	± 6.03
	48:	trans-1,2-dichloroethene	ND 1.00		х	94.37	± 0.77	82:	propybenzene	ND 1.00		x	97.09	± 2.88
	49:	1, 1-dichloroethane	ND 1.00		x	91.39	± 0.61	83:	bromobenzene	ND 1.00		x	87.29	± 2.76
	50:	2,2 dichloropropane	ND 1.00		x	97.05	± 0.77	94:	trans 1,4-dichloro-2-butene	ND 1.00		x	74.37	± 6.03
	51:	propionitrile	ND 5.00		x	127.45	± 10.55		1,3,5 trimethylbenzene	ND 1.00		x	94.16	± 2.82
	52:	2-butanone	ND 5.00		x	96.52	± 10.36		2-chlorotoluene	ND 1.00		x	84.54	± 2.77
	53:	cis 1,2-dichloroethene	ND 1.00		x	88.35	± 0.61	97:	4-chlorotoluene	ND 1.00		x	82.21	± 2.71
	54: 55:	methacry lonitrile chloroform	ND 5.00 ND 1.00		ŵ	72.54 86.24	± 5.56 ± 1.17	98:	tert-butylbenzene sec-butylbenzene	ND 1.00 ND 1.00		ŵ	95.45 96.89	± 2.87 ± 2.82
	56:	bromochloromethane	ND 1.00		ŵ	78.23	± 1.17 ± 1.17	99: 100:		ND 1.00		ŵ	81.91	± 2.62 ± 2.64
	57:	cyclohexane	ND 1.00		ŵ	99.46	± 0.77		1,2,4 trimethylbenzene	ND 1.00		ŵ	92.23	± 2.64 ± 2.73
	58:	1, 1, 1-trichloroethane	ND 1.00		â	97.28	± 0.77	102		ND 1.00		â	94.43	± 2.73 ± 2.87
	59:	1, 1-dichloropropene	ND 1.00		â	100.72	± 1.20	103		NO 1.00		â	88.98	± 2.65
	60:	carbon tetrachloride	ND 1.00		â	99.46	± 0.77	104:		ND 1.00		â	88.04	± 2.63
	61:	1.2 dichloroethane	ND 1.00		â	76.46	± 1.17	105:		ND 1.00		â	95.92	± 2.82
	62:	benzene	ND 1.00		â	92.12	± 0.77	106		NO 1.00		â	85.08	± 2.75
	63:	trichloroethene	ND 1.00		â	95.20	± 1.17	107:		ND 5.00		~	70.54	± 5.77
	64:	methyl cyclohexane	ND 1.00		â	100.77	± 1.20		1.2 dibromo-3-chloropropane	ND 1.00		х	71.17	± 5.81
	65:	1.2 dichloropropane	ND 1.00		x	82.34	± 1.40		nitrobenzene	ND 5.00			69,94	± 5.72
	66:	methylmethacrylate	ND 5.00		x	72,74	± 5.57	110:	1,2,4 trichlorobenzene	ND 1.00		х	79,75	± 1.78
	67:	dibromomethane	ND 1.00		х	75.13	± 1.37			ND 1.00		х	88.92	± 1.72
	68:	bromodichloromethane	ND 1.00		х	81.12	± 1.39	112	naphthalene	ND 1.00		х	71.04	± 1.67
	69:	1,4-dioxane	ND 5.00		х	195.63	± 10.64	113;	1,2,3 trichlorobenzene	ND 1.00		х	74.30	± 1.71
	70:	4-methyl-2-pentanone	ND 5.00		х	72.99	± 5.59	114:	2-methylnaphthalene	2.61	± 0.212	х	60.50	± 4.75
	71:	trans 1,3-dichloropropene	ND 1.00		х	80.27	± 1.39	115:	1-methylnaphthalene	2.98	± 0.244	х	60.50	± 4.75
	72:	toluene	ND 1.00		х	93.51	± 1.05							
	73:	pyridine	ND 10.0		х	162.51	± 67.86							

#### **RESEARCH & DEVELOPMENT**



# **Quantitation Report with Limits**

- The report limit file is identified in the header when used.
- Results are 'ND' followed by the limit value when results are below the limit
- The number of standard deviations if greater than '0' is used to increase the confidence that the value is below the reporting limit. For instance if 3 sigma deviation were selected, only if an analytical result plus 3 times the analytical error are greater than the limit will 'ND' be reported.
- Example: If benzene is 0.7 ± 0.2 and a limit is 1.0 then if 0, or 1 sigma is identified the result for benzene will be ND 1. If 2 sigma was selected the reported value for benzene would be 0.7 ± 0.2.



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- The QC report contains the equations used to generate the results (paper copy presents a graphic presentation of effects observed).
- The QC report contains the method 8261 calculations on the monitoring surrogates as individual compounds and as volatile, non-purgeable volatile, and semivolatile groupings.
- With the exception of graphics the electronic version of the QC report contains the same data as the printed report.



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# **QC** Report

- The QC Report is 2 pages when printed. An electronic version is also created.
- An Internal standard report presenting the relationships of recovery to boiling point and relative volatility are presented as a single page.
- The surrogates data are presented on the second page.
- The electronic QC report is included in a \*.SQL file. To read the file use notepad and open t4050608.SQC.

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**QC** Report Page 1

> This page presents the internal standard data used to generate results

	ess Date: pound Library File:		05/05/2006	15:43	aport- Version 4		– Ln: RW	N Page:1
Sum Data	ogate Groupings Fi File: rration File:		C1/SMCRE C1/SMCRE	PORTERIEX	AMPLE/CLPISTI AMPLE/CLPISTI AMPLE/CALIBR	DB.INI IB.TXT		
First Pass relative V (Used to Estimate Compound	olatility (Log) vs. R Rel vol effects on BP		al Standards Meas. Re		Siope	176	Brr%	100 1 31 1 1
hexafuorobenzene fluorobenzene	81.5 85	0.86	99.50 92.48	99.50	-4.9969-02	0.9874	0.00	
luoroberzene 1,2-dichioroethane-	85 54 84	3.5 20	92.48 75.07	92.48 75.07	-9.9929-02	1.0500	0.00	*
Recovery vs. Boiling	Point - (First Pase	Bal Vol C	omections) -	. Bolina sola	ti rangel 85.00.	229.001		30 08
, ,				0.				70
Compound pentatiuorobenzene toluene-d8 bromobenz ene-d5	8P 85 111 155	RVW 1.51 4.28 7.93	Meas.,Re 97.14 92.54 86.25	00000(%) 100.47 102.29 102.31	Siope 2.365e-04	int. 0.9992	Brr% 0.92	0 1 2 3 Relative Volatility (log scale)
bromoberz ene-d5 1,2-dichloroberz ene 1,2,4-trichloroberze		7.93 8.03 7.88	86.25 86.84 81.10	, 102.31 , 103.15 , 95.12	-1.1109-03	1.2085	2.95	
1,2,4 trichlorobertze naphthalene-d8 1-methylnaphthalen	217	7.88 18 20*	81.10 69.36 57.30	95.12 91.11 75.33	-6.751e-03	2.3986	1.64	100
								**
Recovery(bp correct	ted) vs. Relative Vo	slatility (Lr)	- Relative	Volatiliy rang	ge( 0.86 - 14999	.00)		30 + + + + + 0e
Compound hexafuorobenzene fluorobenzene 1,4-difluorobenzene	BP 81.5 85 88.5	RVW 0.86 3.5 3.83	Meas.,Re 99.50 92.48 93.19	000000(%) 99.50 91.63 92.26	Slope -5.178e-02	int. 0.9968	Brr% 0.77	70 90 120 160 200 240 280 Bolling Point
1,4-difluorobenzene o-xylene-d10 chlorobenzene-d5	88.5 143 131	3.83 6.14 6.27	93.19 98.26 98.65	92.26 95.29 95.89	-1.170-01	1.0795	0.61	boung Point
o-xylene-d10 chiorobertzene-d5 1,2-dibromoeinane- diethyl_ether-d10	143 131 14 131 35	6.14 6.27 26 32.5	88.26 88.65 73.75 72.44	95.28 95.89 72.29 72.44	-9.109e-02	1.0312	1.17	200
1,2-dibromoeihane- diothyl_ether-d10 totrahydrofuran-d8 acetone-13C	14 131 35 66 57	26 32.5 355 600	73.75 72.44 65.70 76.58	72.20 72.44 65.70 76.58	-5.1169-04	0.7202	5.46	190
tetrahydrofuran-d8 acetone-13C	66 57 101	355 600 5800	65.79 76.58 197.57	65.79 76.58 195.01	0.4803	-2.227@+00	10.36	
1,4-diaxane-d8	57	600	76.58 197.57	, 76.58 , 195.01	0.2193	-4.803e-01	66.73	0 1 2 3 4 5 6 Relative Volatility (log scale)

\* The relative volatility is outside the range of first pass internal Standards. Value displayed is default.

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**QC** Report page 2

> This page presents the surrogate results data

Compound Library File: Sumgate Groupings File: Data File: Calibration File:		05/05/2006 15:43 Page: 2 C3SMCREPORTERIEXAMPLE/CLPLIBRARY.TXT C3SMCREPORTERIEXAMPLE/CLPISTDS.INI C3SMCREPORTERIEXAMPLE/T4050608.TXT C3SMCREPORTERIEXAMPLE/CALIBRATION.CAL								
		Su	mogate De	eterm instions						
Volatile Compound Surrogate	es(boiling point	k 150)								
Compound nethylene_chloride-d2 serzene-d5 (.1.2-trichloroptopane-d6 (.1.2-trichloroptopane-d3 4-bromofluoroberz ene	8P 40 79 06 112 152	RVW 11.10 3.92 11.00 25.60 8.05	Maas. 76.6 93.6 82.5 75.3 95.7	E.P.Predict/em 100.0 0.0 100.0 0.0 101.2 0.9 101.6 0.9 102.5 0.9	81.2 92.0 81.3 73.3	diciverr 1.2 0.6 1.2 1.2 1.2	Total Pre 81.2 92.0 82.2 74.4 86.3	adict/err 1.2 0.5 1.4 1.4 1.4	Recover 94.4 101.8 100.4 101.3 99.4	y/err 1.4 0.7 1.7 1.9 1.6
Group Averages									99.4	1.4
Von-Purgeable Volatile Com, Compound titomethane-19C strylasotate-19C syridine-d5	pound Burroga BP 101 77 115	tes(nws 100) RVW 510.00 150.00 15000.00	Meas. 70.3 66.1 127.5	B.P.Prodict/err 101.3 0.0 100.0 0.0 101.6 0.0	76.7 71.8	dict/err 10.4 5.5 66.7	Total Pre 77.7 71.8 165.5	adic#err 10.5 5.5 67.8	Racover 90.5 92.2 77.0	12.2 7.0 31.6
Compound hitomethane-13C atrylacetate-13C	8P 101 77	RVW 510.00 150.00	70.3 66.1	101.3 0.9 100.0 0.0	76.7 71.8	10.4 5.5	77.7 71.8	10.5 5.5	90.5 92.2	12.2 7.0
Compound httpmsthane-19C ethylacelate-19C syridine-d5 Group Averages Semi-Volatile Compound Sur	BP 101 77 115	RVW 510.00 150.00 15000.00	70.3 66.1 127.5	101.3 0.0 100.0 0.0 101.6 0.0	76.7 71.8 162.8	10.4 5.5 66.7	77.7 71.8 165.5	10.5 5.5 67.8	90.5 92.2 77.0 95.6	12.2 7.0 31.6 16.9
Compound attornethane-19C ethylacotate-19C yridine-d5 Group Averages	80 101 77 115	RVW 510.00 150.00 15000.00	70.3 66.1	101.3 0.9 100.0 0.0	76.7 71.8 162.9 92.9 71.8 71.8	10.4 5.5 66.7	77.7 71.8	10.5 5.5 67.8	90.5 92.2 77.0	12.2 7.0 31.6 16.9

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- The process of calibration and sample quantitation for method 8261 is presented. All data is generated in paper and electronic format.
- QC is generated for each sample.
- There are options for limits to report data.
- Data generated can be read into other programs for customizing reports.



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