Generating CLP Forms from SMCReporter 4.2 Data Files

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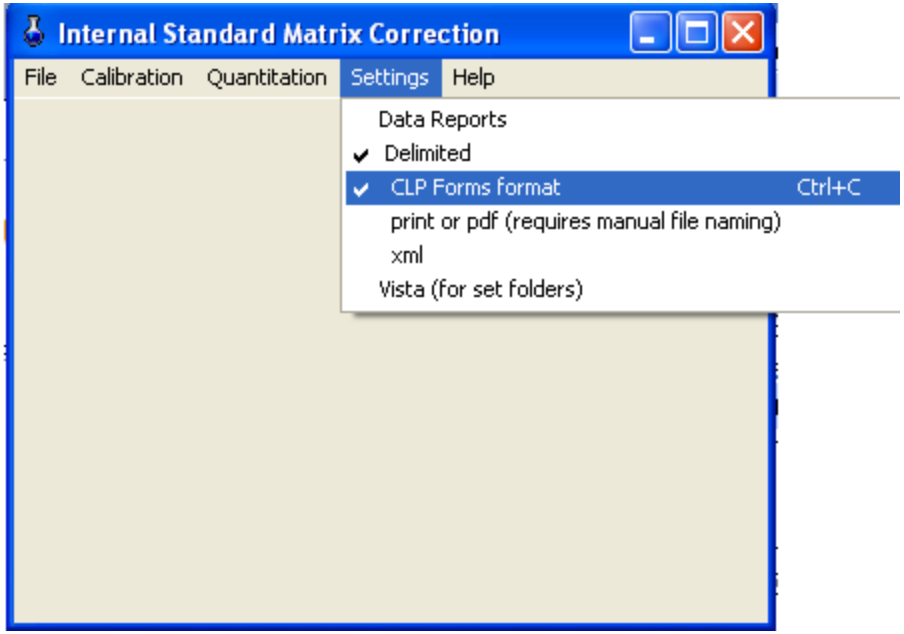
Demonstration Running CLPforms

- This slide show demonstrates creation of CLP forms generated from SMCReporter 4.2 electronic data files.
- CLPForms software download http://www.epa.gov/nerlesd1/chemistry/vacuum/methods/software.htm
- Download the zip file and install CLPForms by running setup.exe contained in the zip file.
- The example files used in this presentation were created by SMCReporter 4.2 with the CLP format option. (next slide) note: to create the CLP format you also need to have a reporting limit file to identify limits for each analyte. This is created by loading library then selecting “Create/Edit MDL File” and entering sample size and each analyte’s limit. Then save MDL file for access during CLP quantitations.

SMCReporter 4.2: Selecting Formatting Required for CLPForms

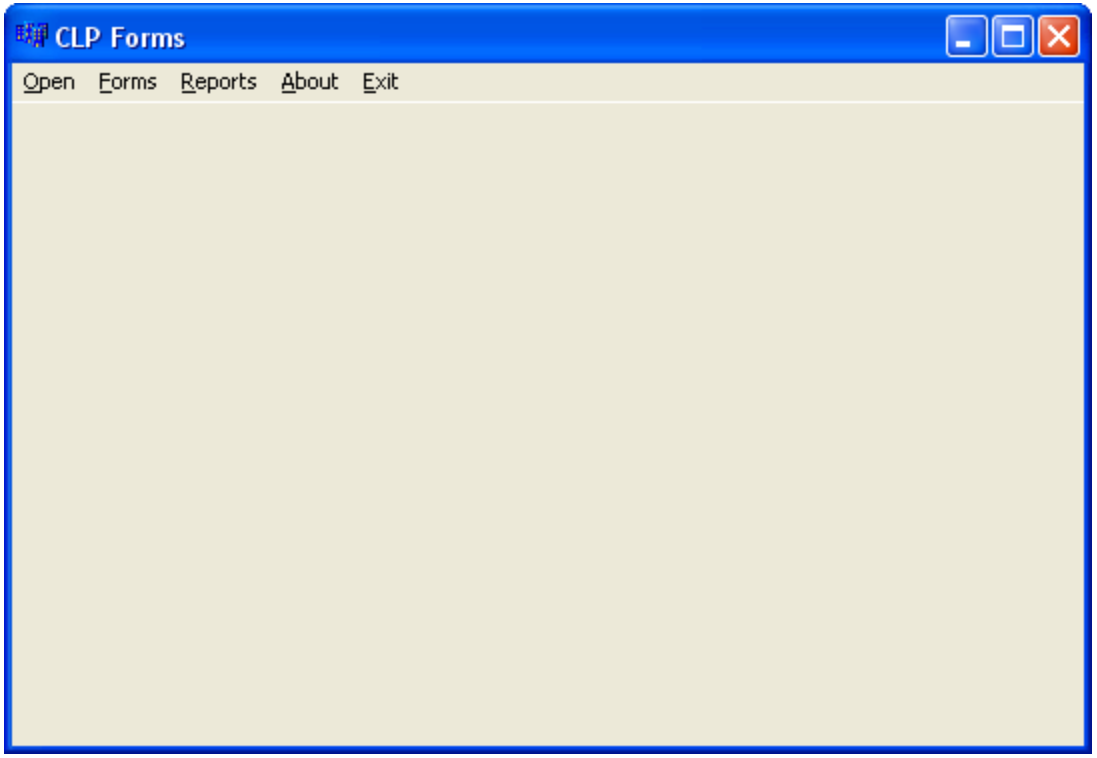


Selecting the CLP Forms format option provides necessary electronic format and information for CLPForms input.

Run CLPForms

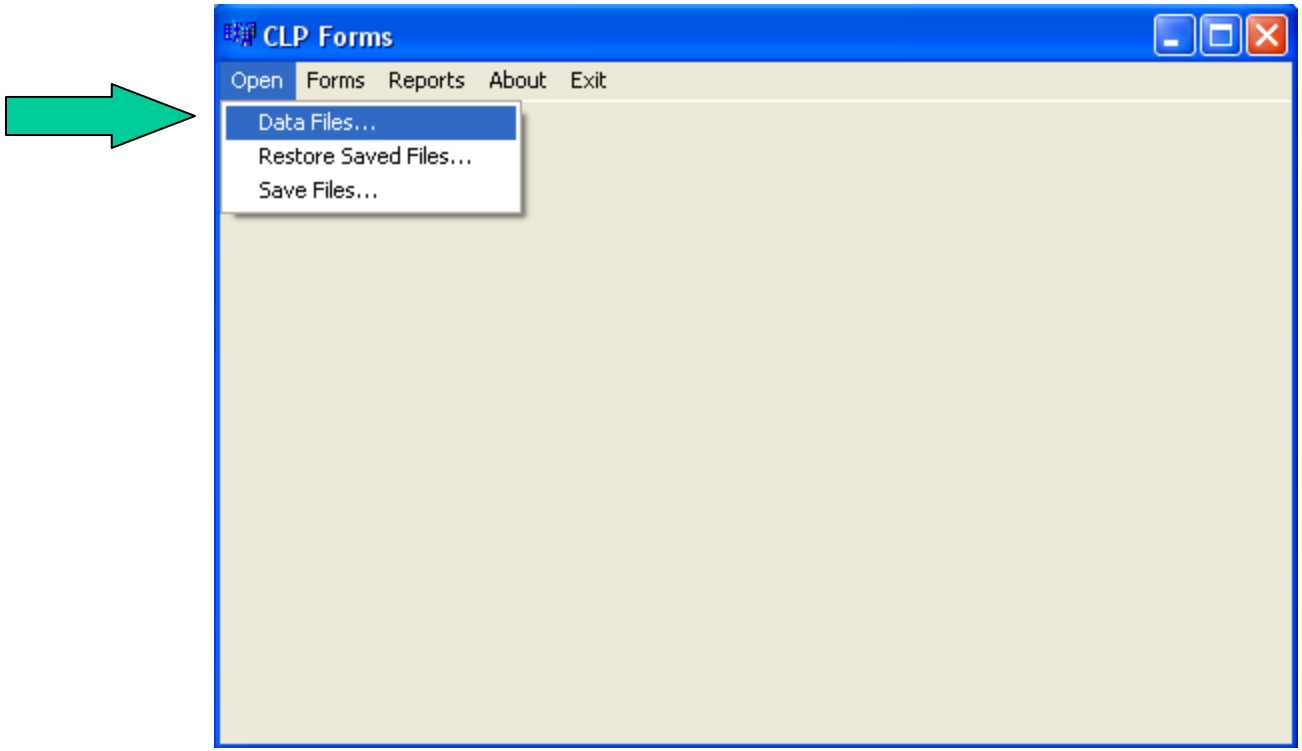
The installation of CLPForms 2.0 created a desktop icon.

The installation of CLPForms 2.0 created a desktop icon. Left click on CLPForms icon and the following is displayed



CLPForms: Inputting Data Files

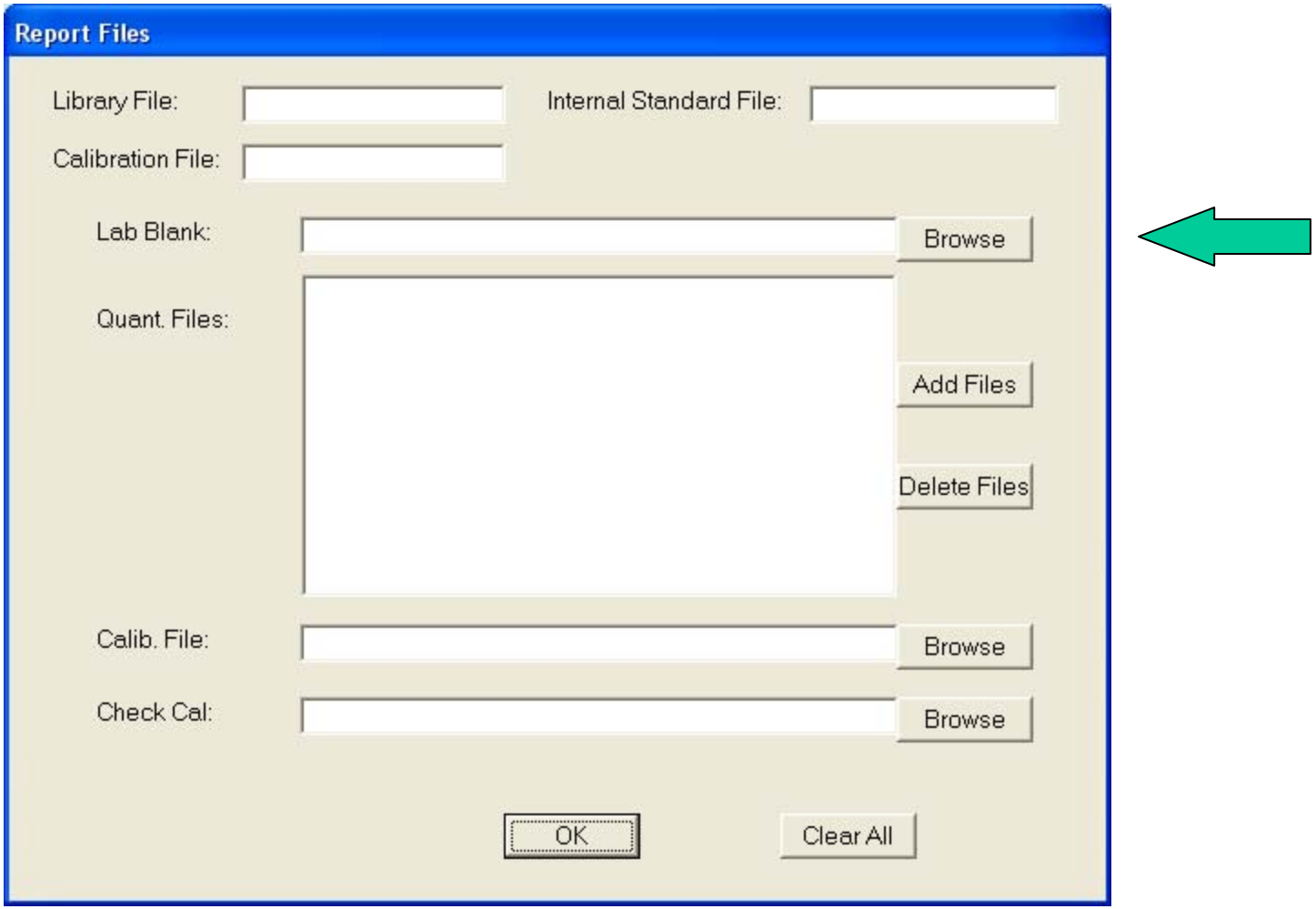
- The data files that are required to generate CLP forms must be identified for processing.
- To load these files go to Open then “Data Files”



Data Files

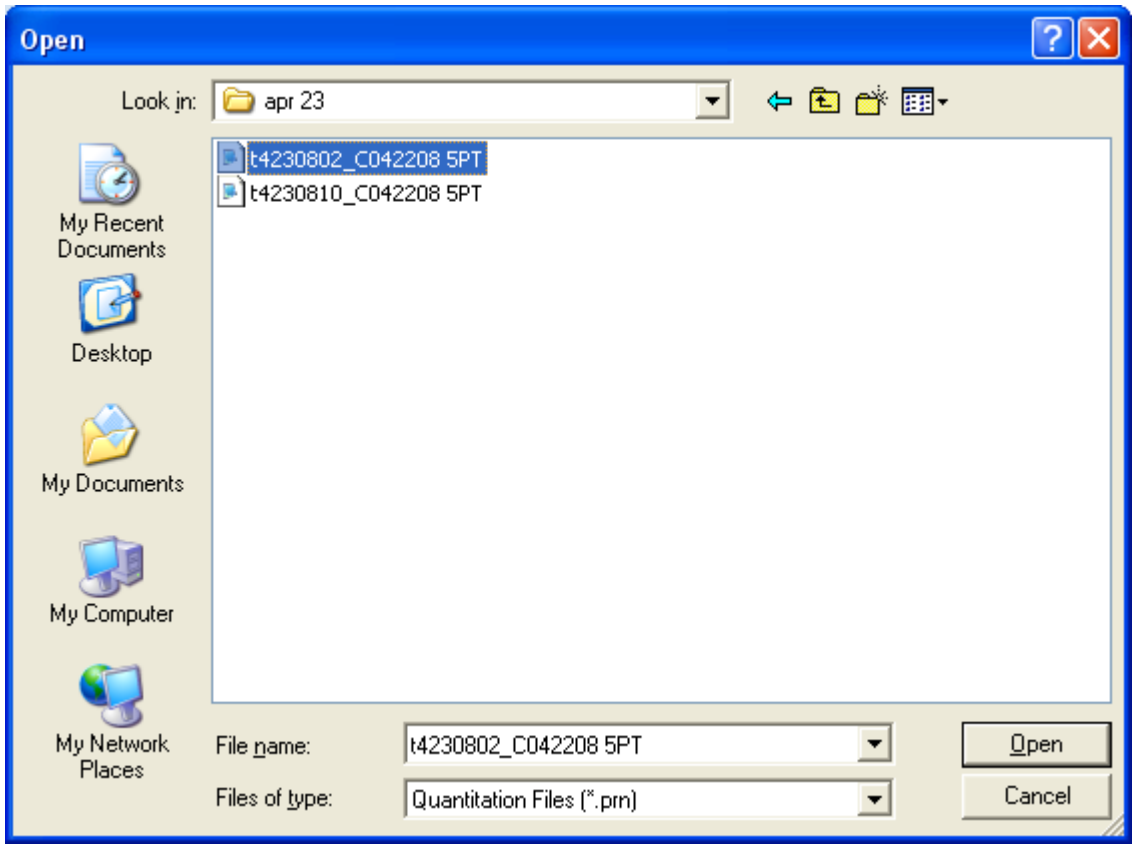
- The data files and their pathways used in the demonstration were created with the CLPForms installation.
- The calibration curve was generated on 4/22/2008 and it was titled C042208 5pt. SMCReporter generated a file containing the calibration information as C042208 5pt.cal. The pathway to this file is c:\SMCReporter\CLP\apr 22\.
- The analysis for which CLP forms are going to be generated is a 5g soil identified as GC01and analyzed on 4/23/2008. the file name for the run is t4230810 and is the GC/MS acquisition file name. When SMCReporter quantitated the file using the calibration curve, a result file t4230810_C042208 5pt.prn was generated.
- The calibration check standard run on 4/23/2008 is t4230801. SMCReporter generated a calibration check report file, t4230801.check.
- The laboratory blank run (labeled blankepa01)after the calibration check standard is t4230802. A quantitation report was generated (as for the sample) as t4230802_C042308 5pt.prn.
- The pathway to the sample, blank, and calibration check files is c:\SMCReporter\CLP\apr 23\.

CLPForms Data Files form



The data files are loaded with this form. The files and their pathway are selected with the buttons “Browse” and “Add Files”. Select the Browse button to the right of the Lab Blank field.

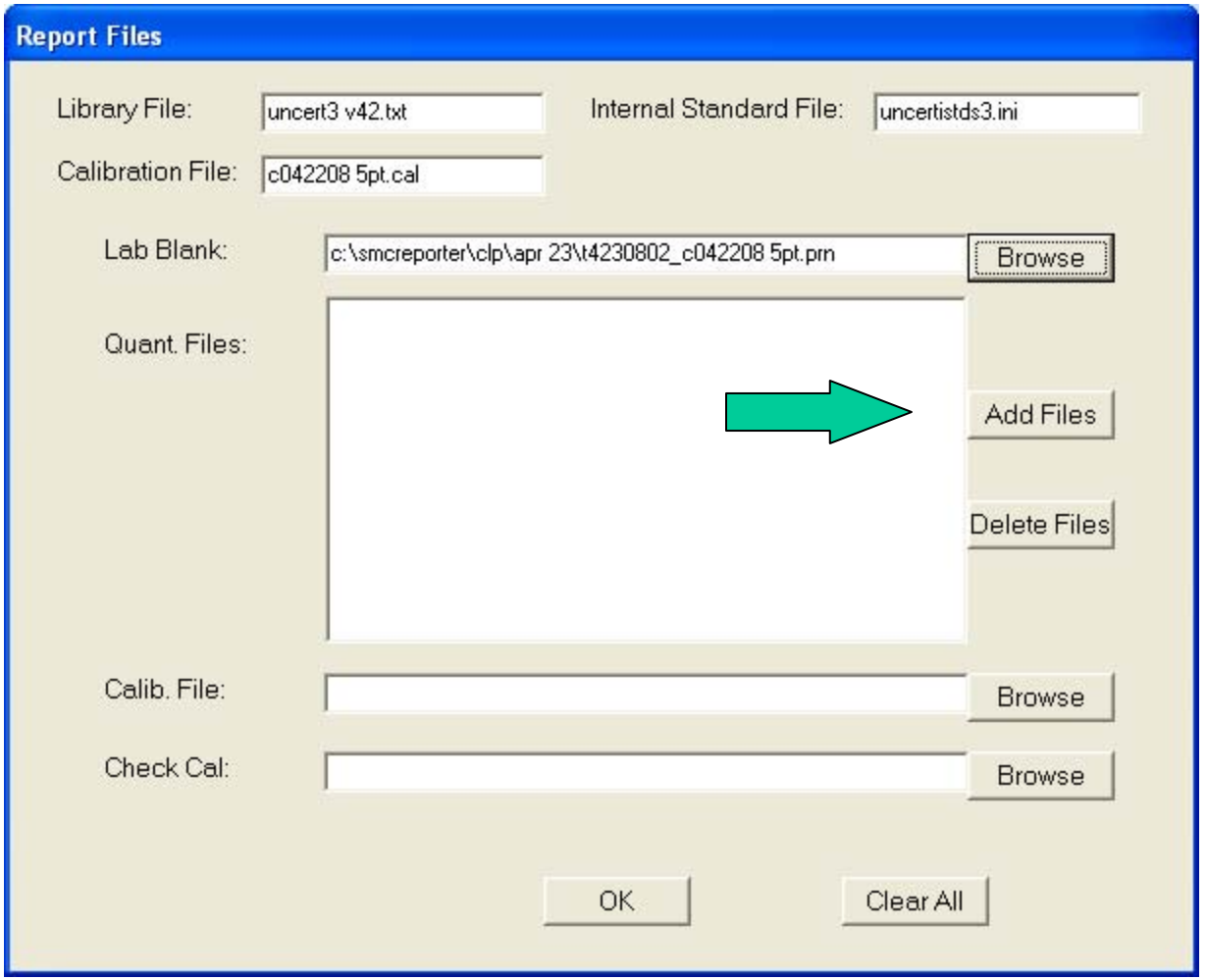
Adding Laboratory Blank file



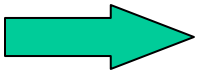
The lab blank quantitation file is t4230802_C042208 5pt.prn. Now browse to the file (c:\SMCReporter\CLP\apr 23\t4230802_C042208 5PT) and select (open) it.

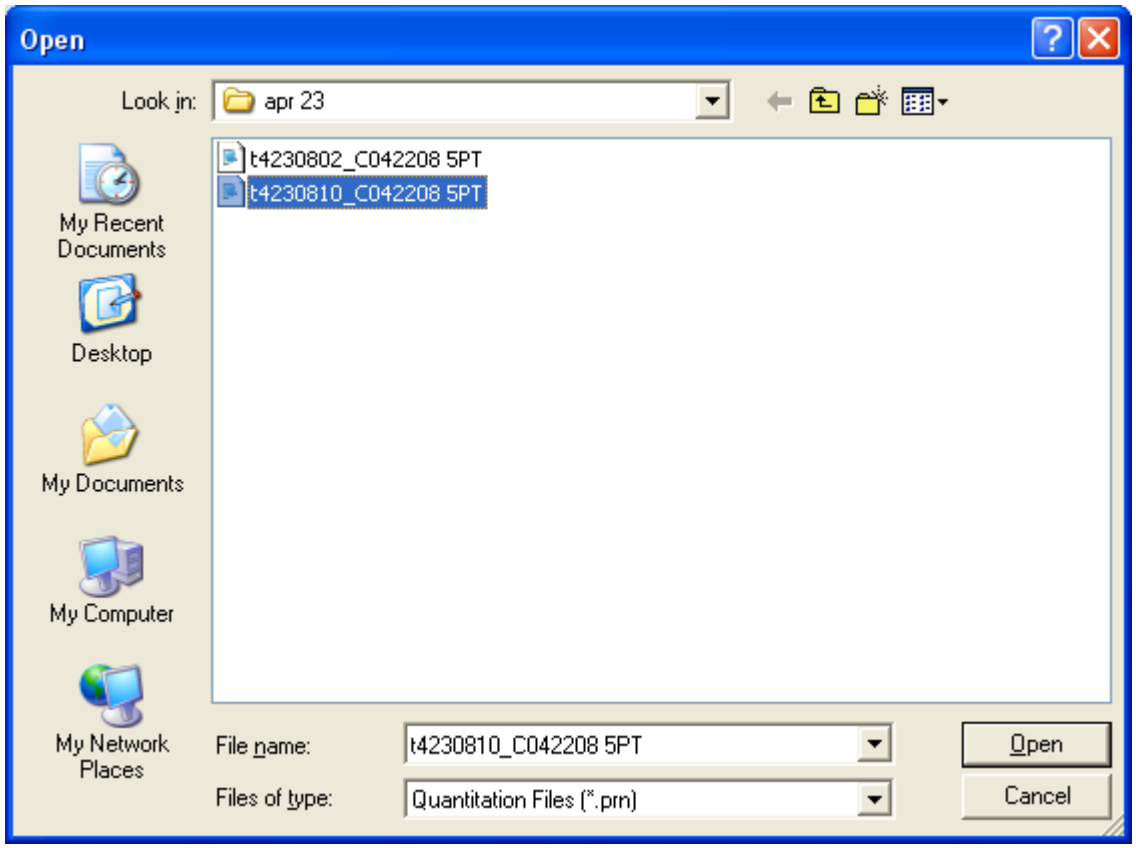
Adding Data Files

- Upon selection of lab blank (or other data file) the library, internal standard, and calibration file names are taken from the lab blank quantitation result file.
- Next add the analysis file. Select “Add Files”.



Adding Data Files (cont.)

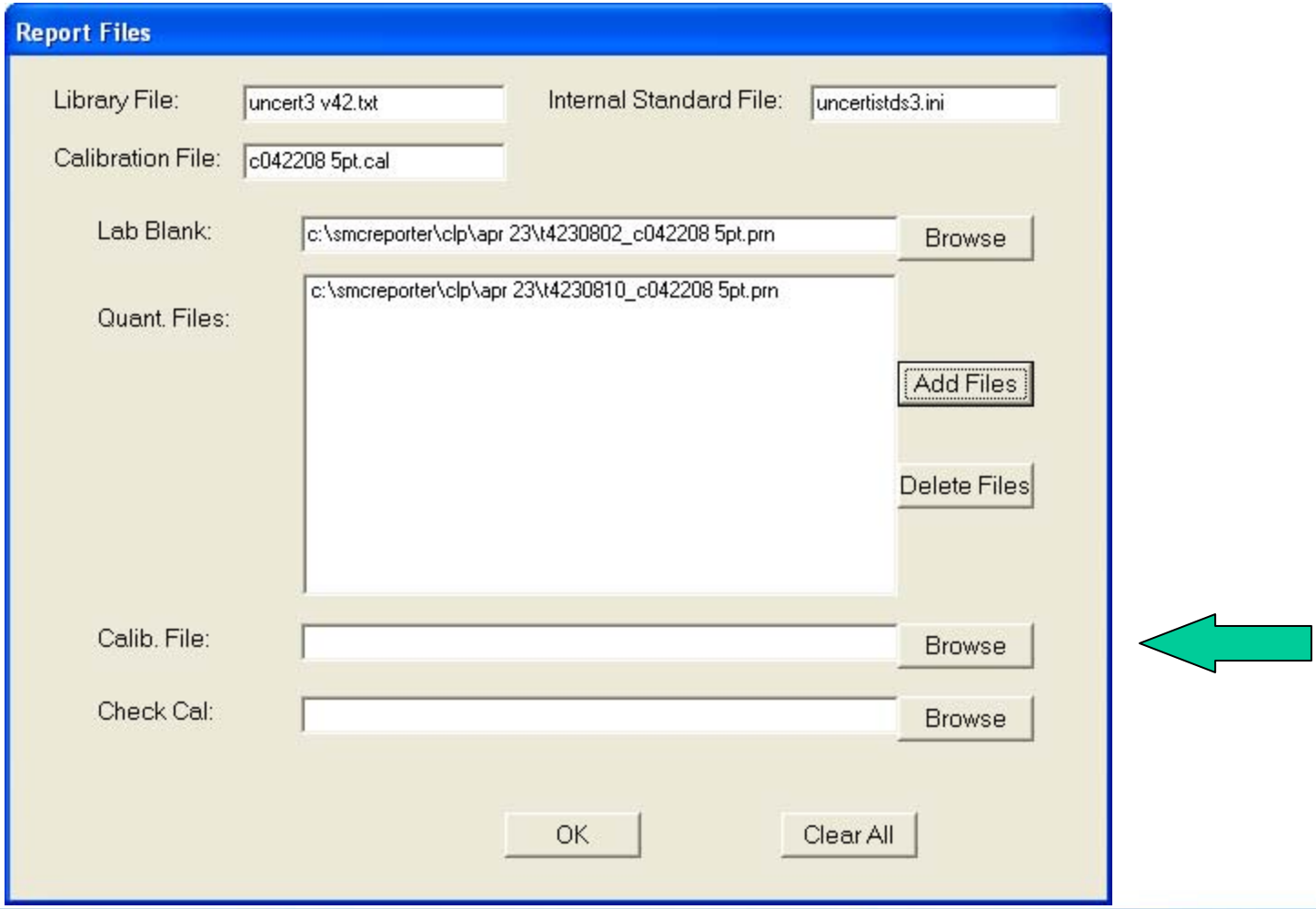




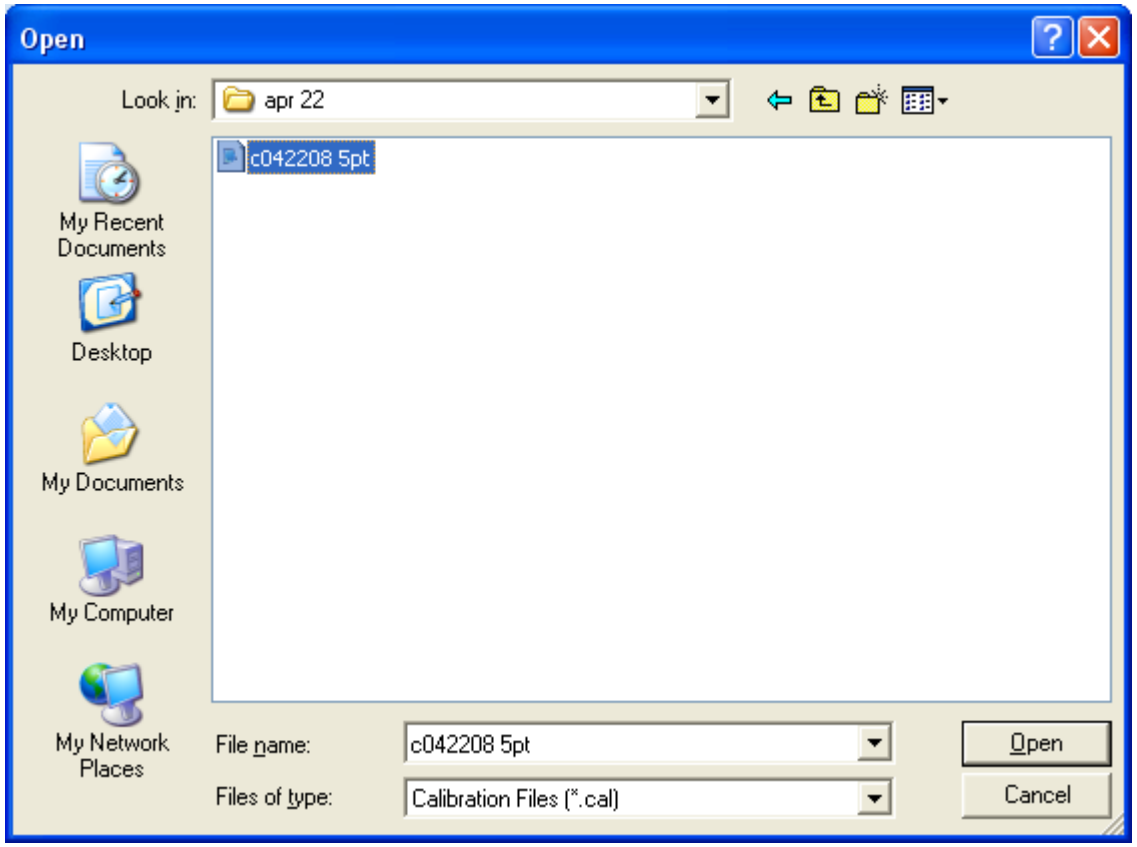
The analysis quantitation result file to be selected is t4230810 23\t4230802_C042208 5PT. As was done for the lab blank, select the quantitation result file c:\SMCReporter\CLP\apr 23\t4230802_C042208 5PT.

Data File added

- Next select the calibration file. While the calibration file has already been identified the pathway to it must be included.



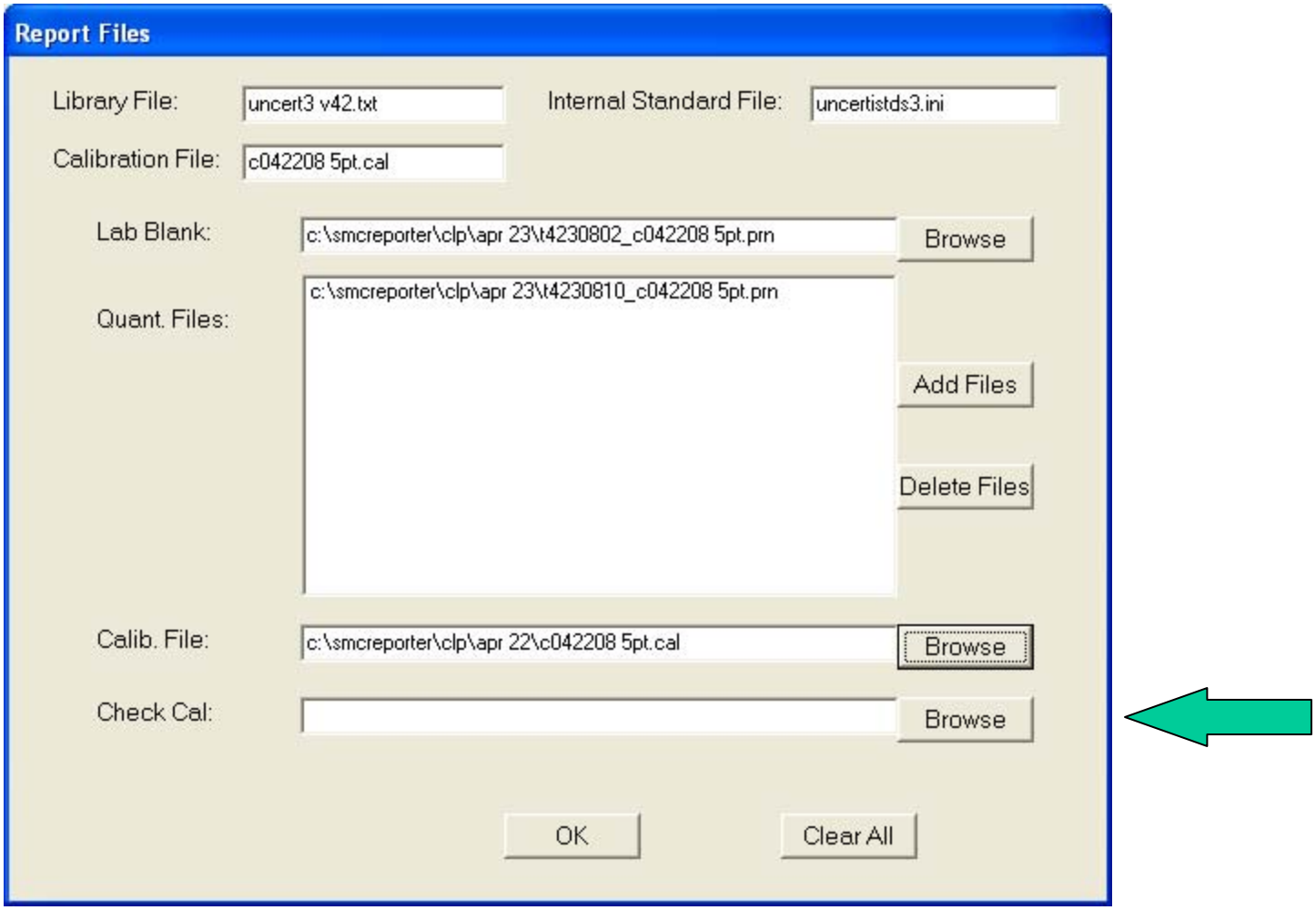
Adding Calibration File data



Select the file c:\SMCReporter\CLP\apr 22\c042208 5PT.

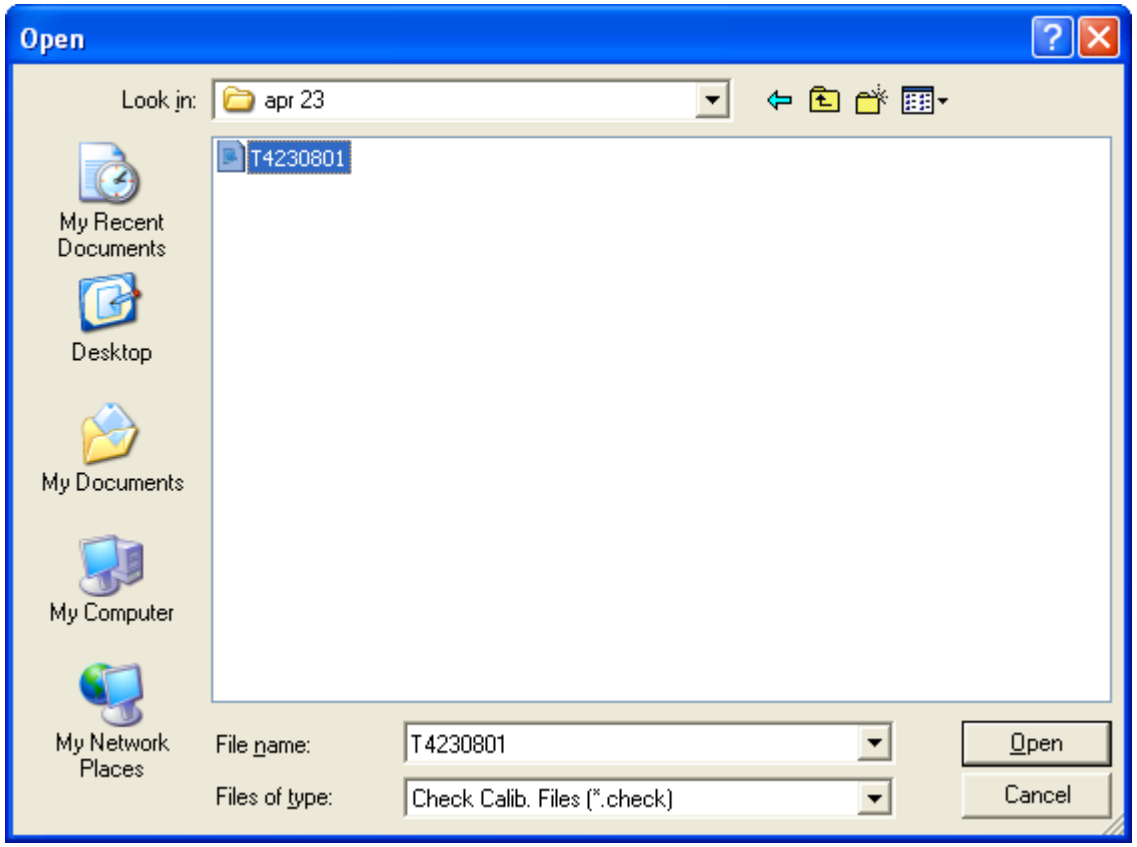
CLPForms will display calibration files identified with a *.cal extension.

Calibration File Added



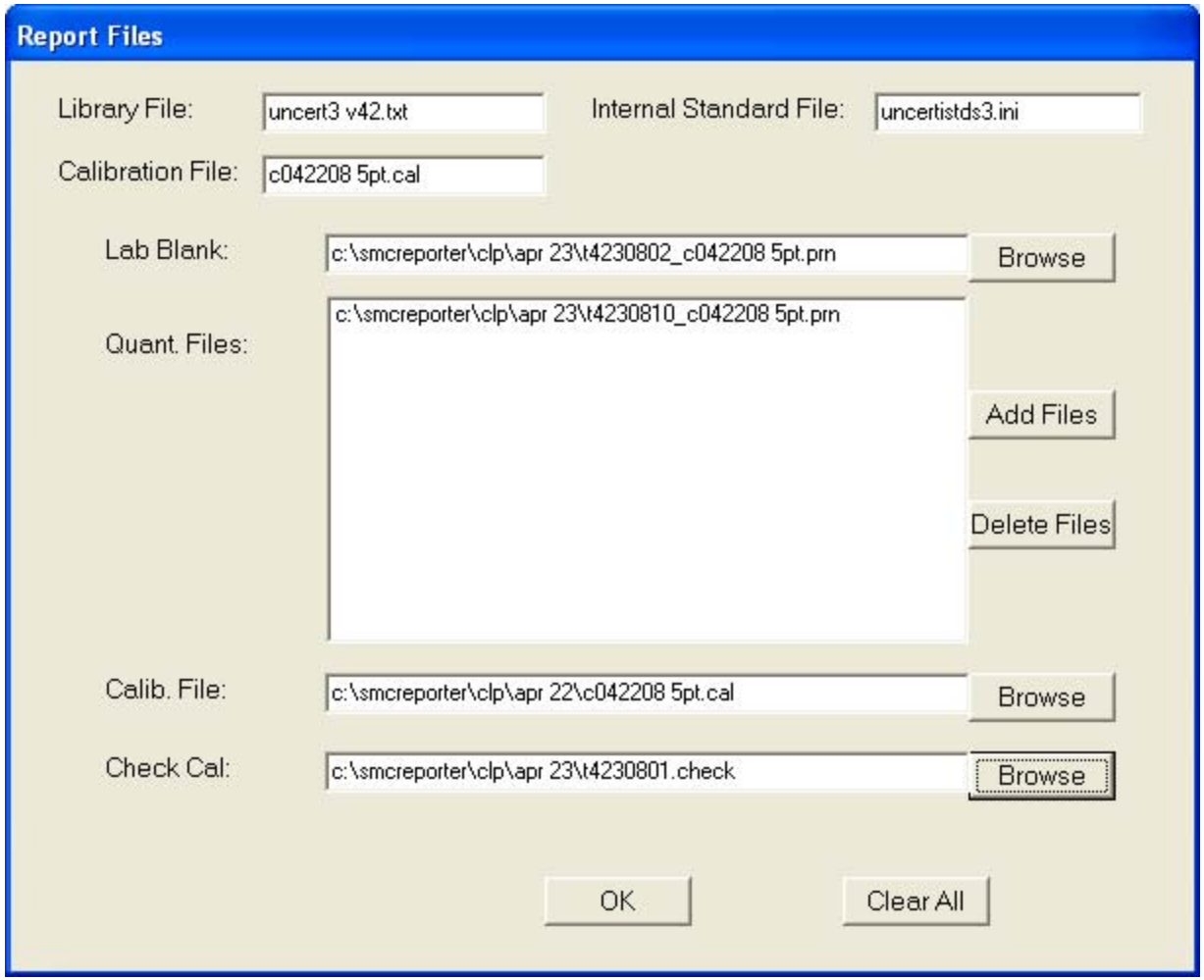
Next add the day's calibration check standard

Adding Check Standard



Select the file c:\SMCReporter\CLP\apr 23\T4230801.check

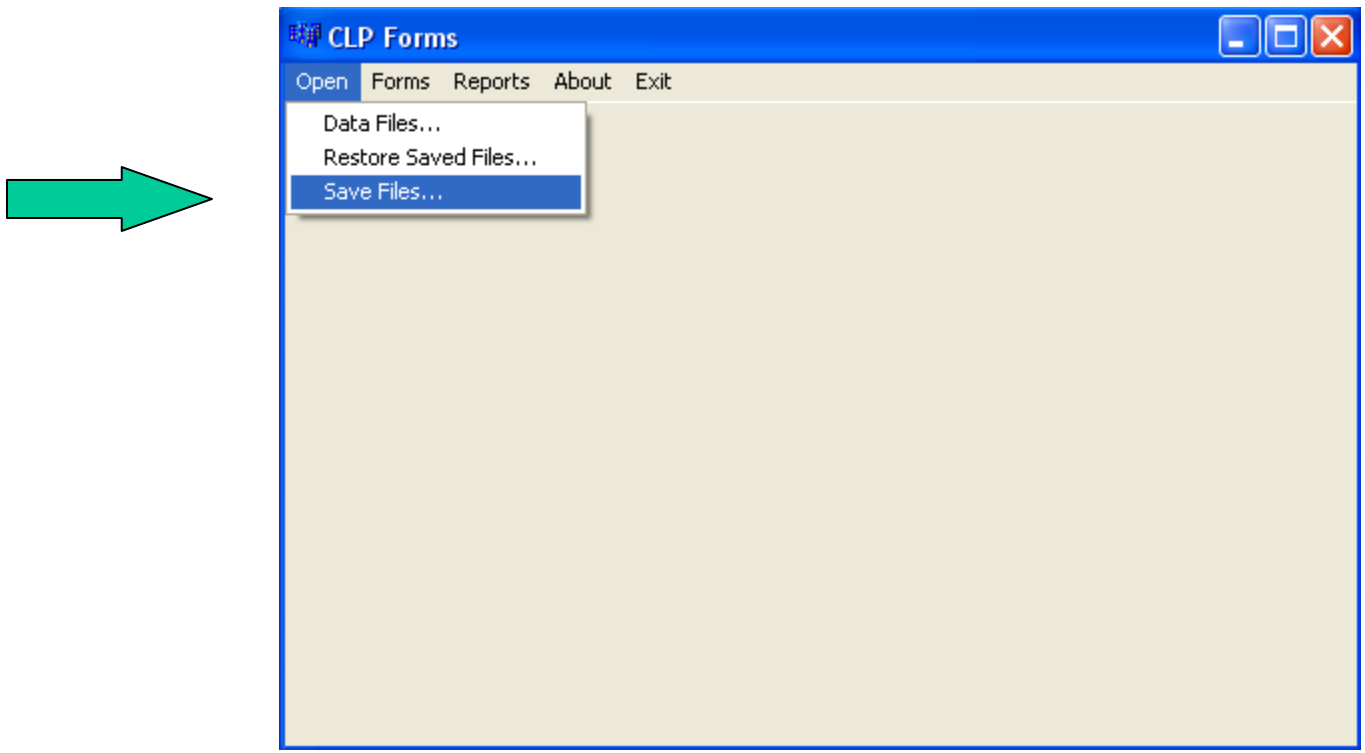
All data files entered to generate reports



All of the data files are now entered. Select “OK”.

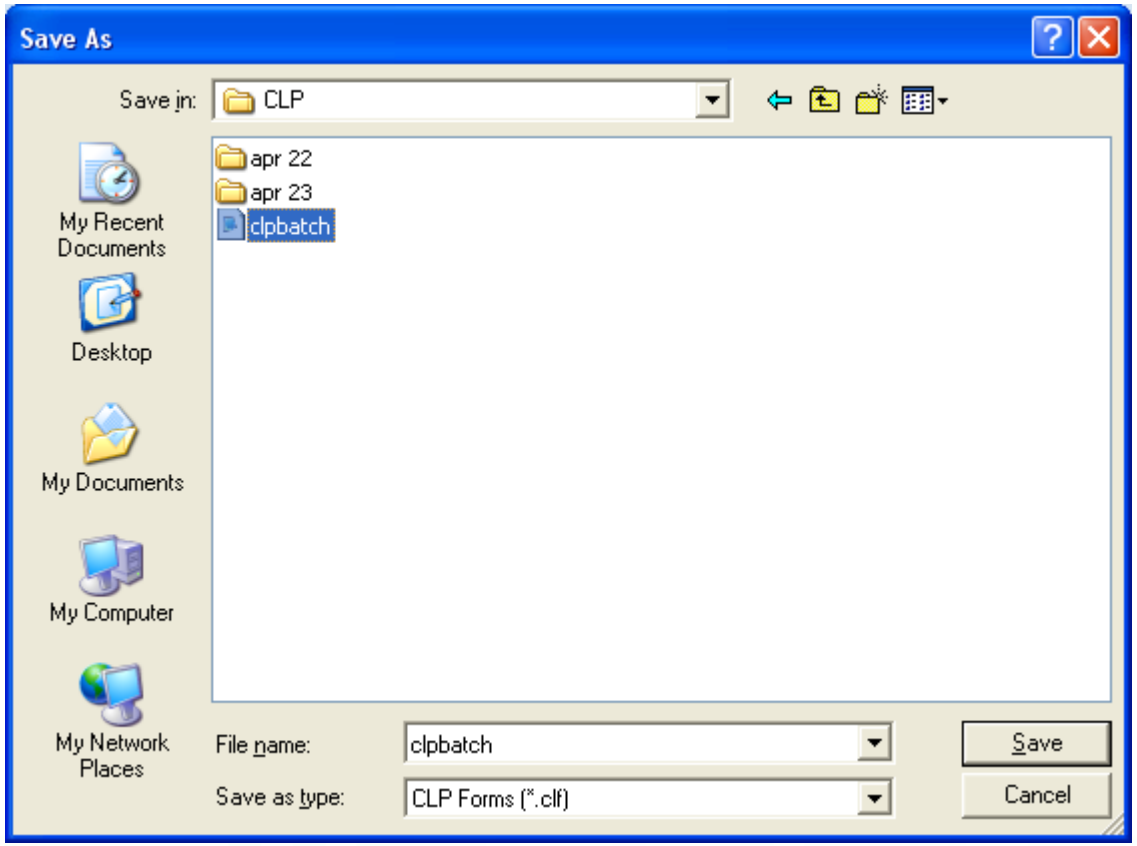
Save the Data files

- The work can be saved as a file for future retrieval.
- Select Save Files.



Saving data

The data can be saved for future retrieval. A batch file containing all of the demonstration data has already been provided (clpbatch 5pt.clf). You can overwrite it or create a new batch file.

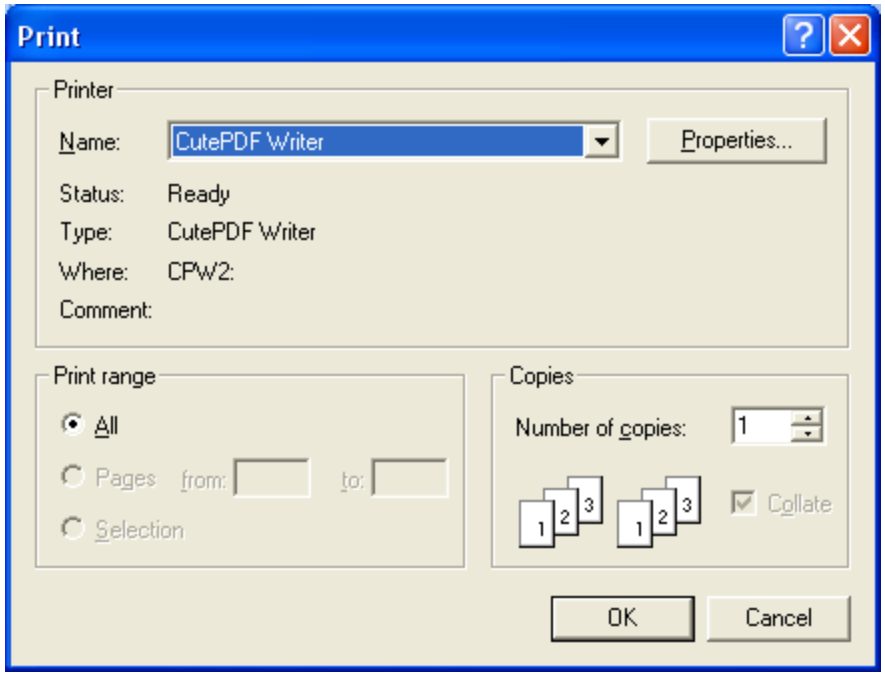


Select mode for reporting

A printer or electronic format printer can be selected for outputting CLP forms

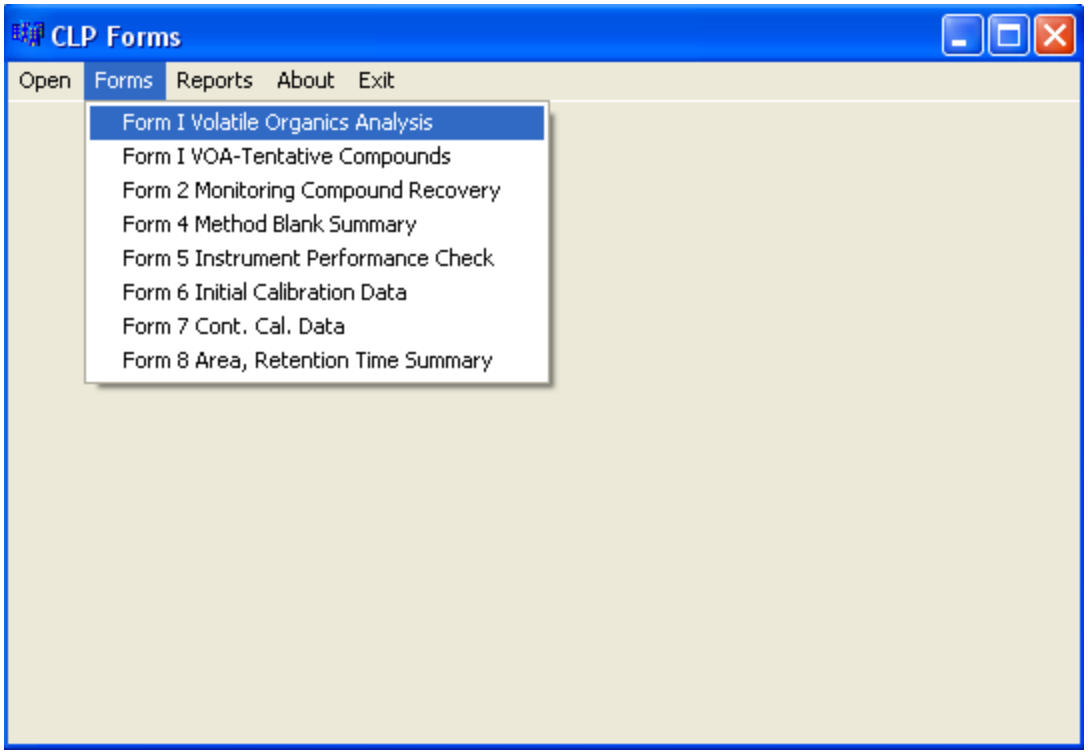
Freeware CutePDF Writer

A pdf writer is selected for demonstration



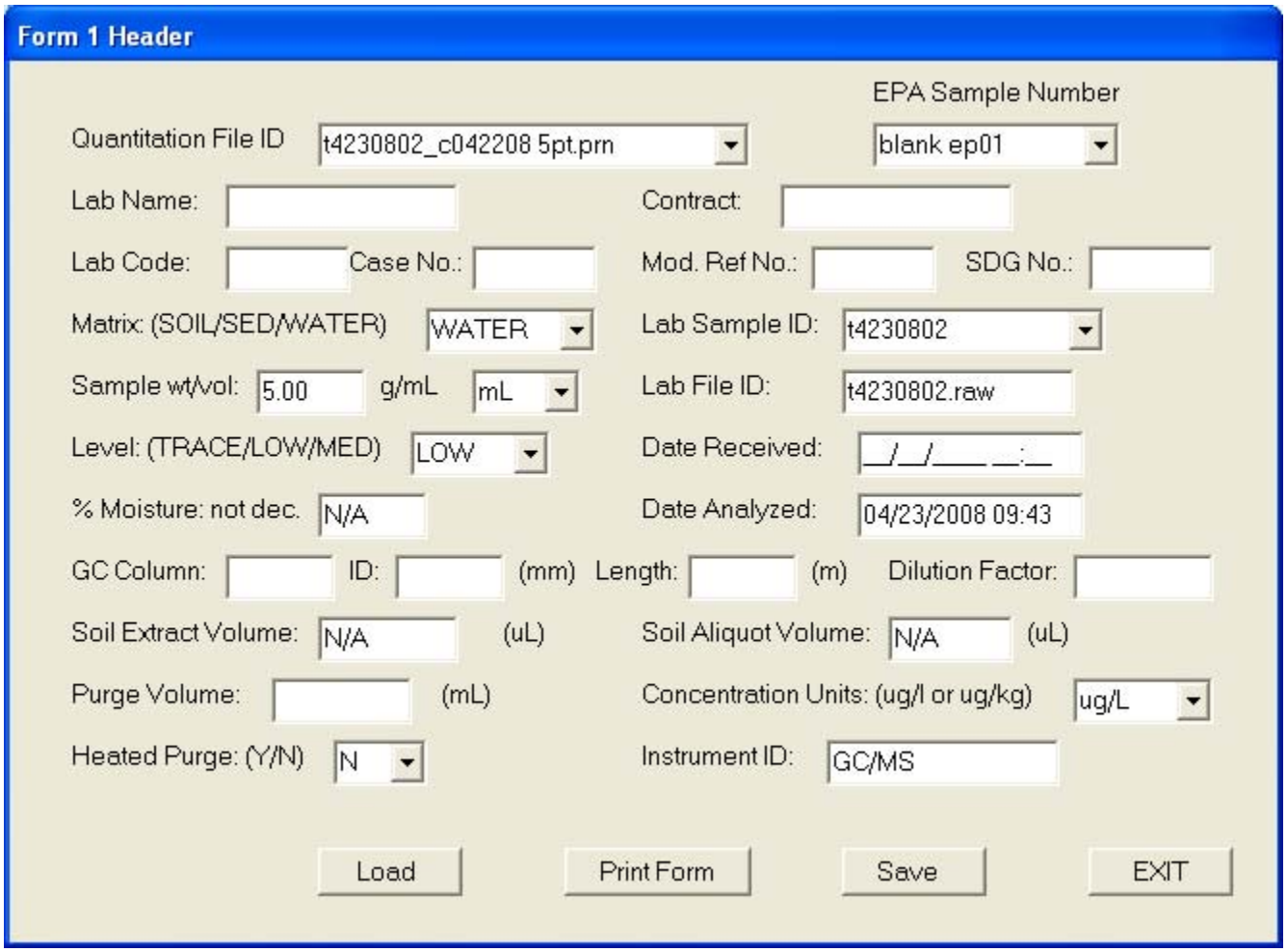
Generating CLP Reports

Select Form 1 to report analyte results



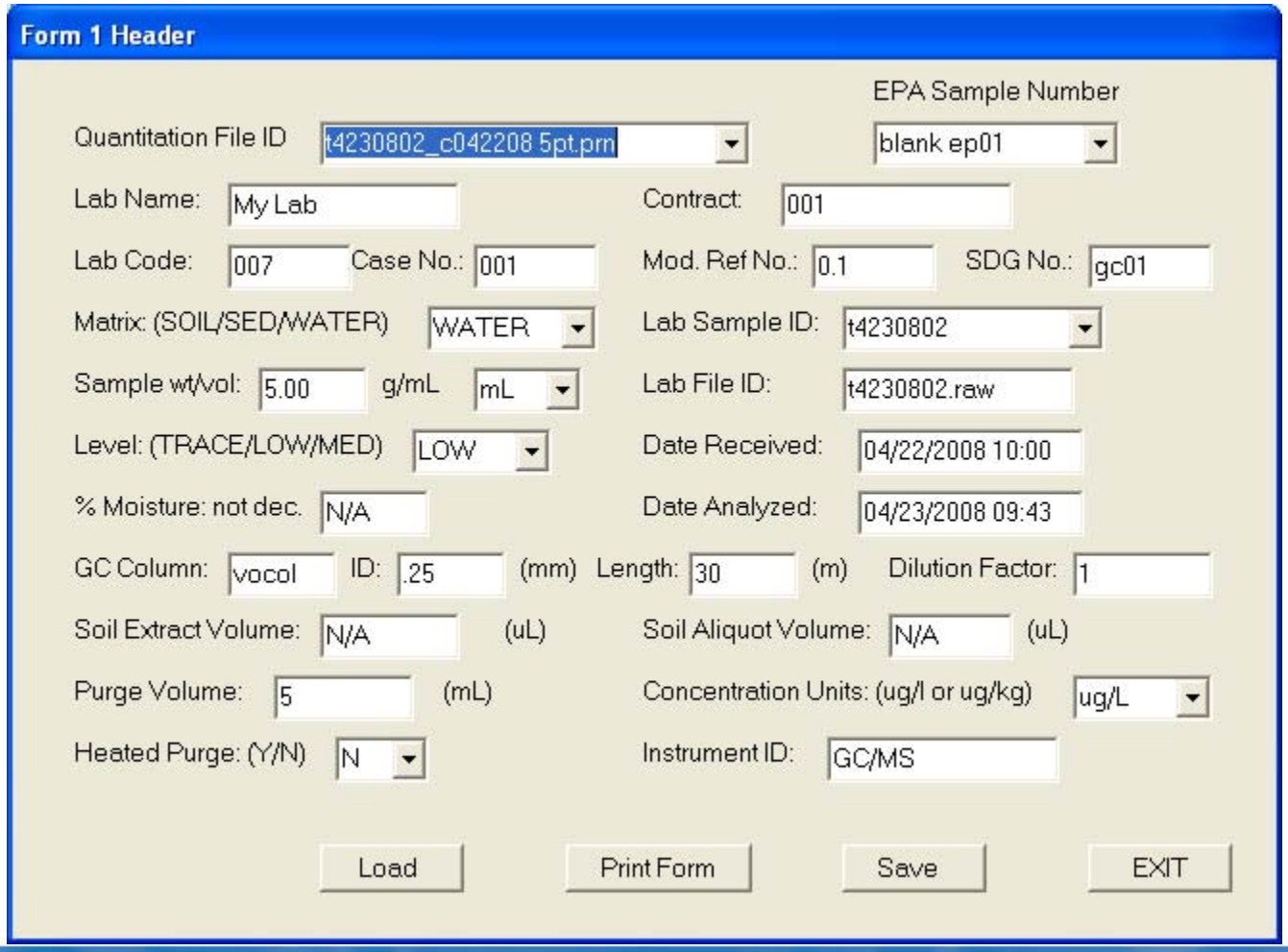
Form 1

The data available from the data files is used to fill in fields. Some fields need be completed manually.



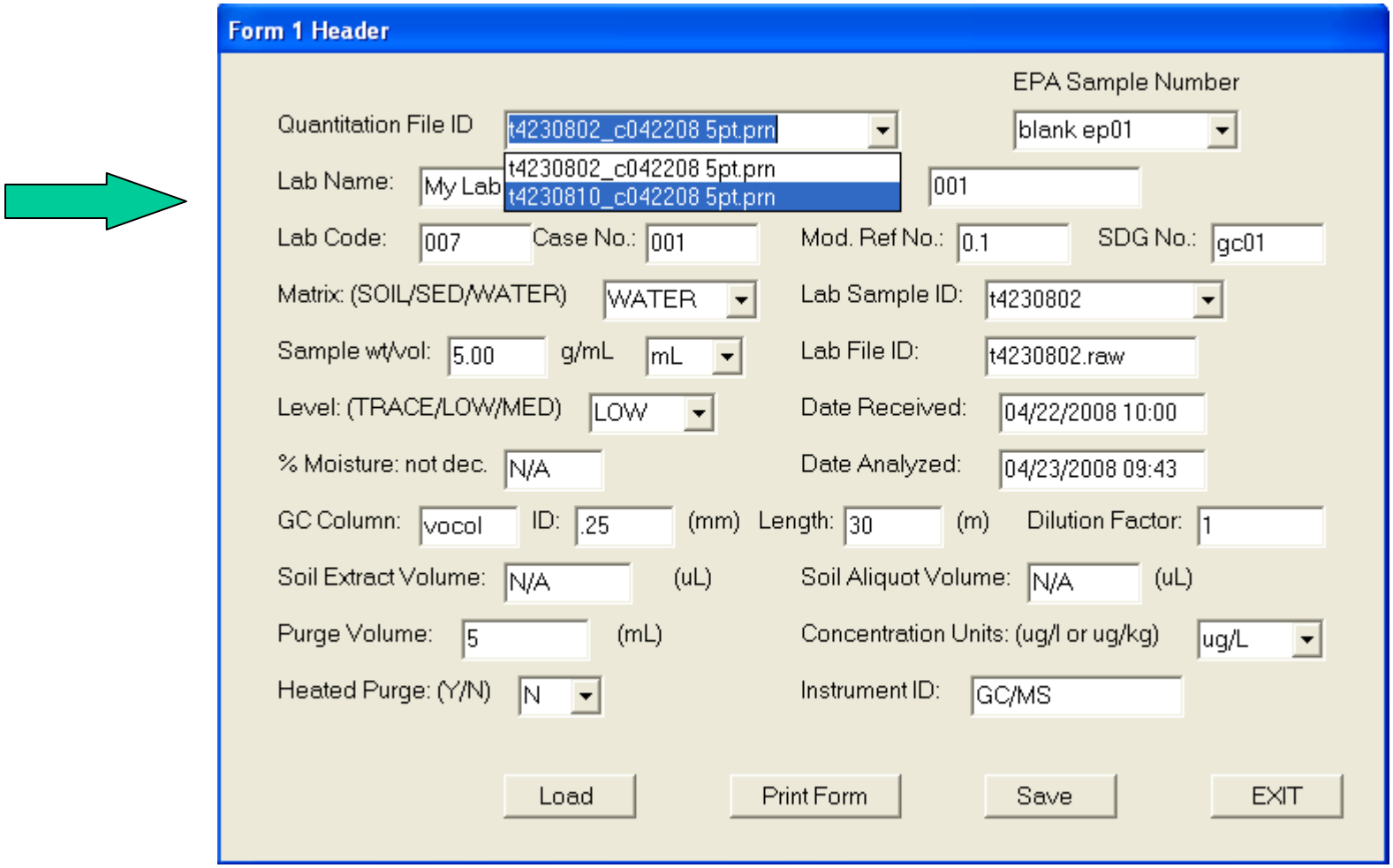
Complete form after including missing data

This previous data was for the lab blank. Now select data file.



Drop-down menu

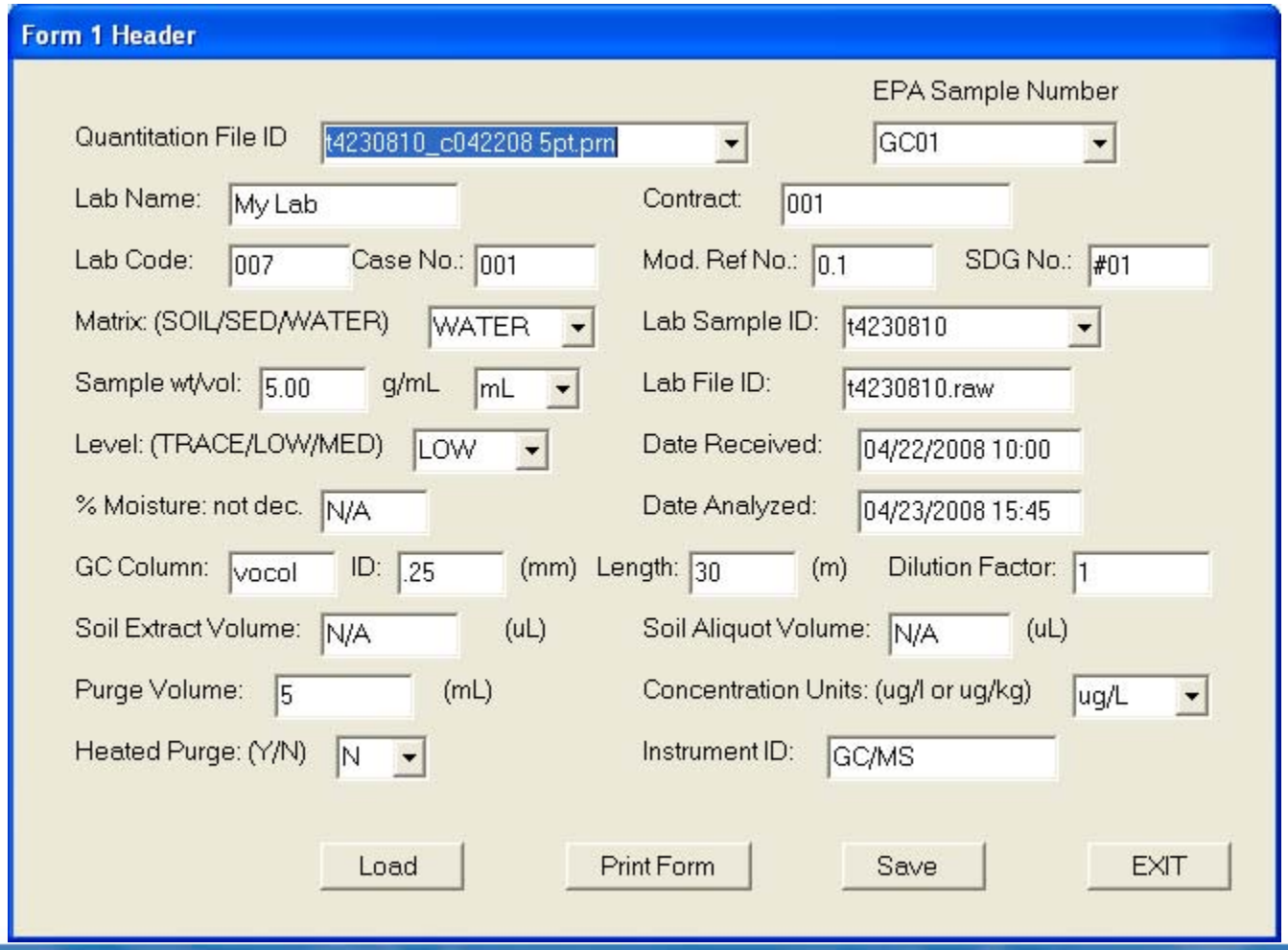
Select t4230810_c042208 5pt.prn from the Quantitation File ID drop-down menu.



Fields are now automatically filled

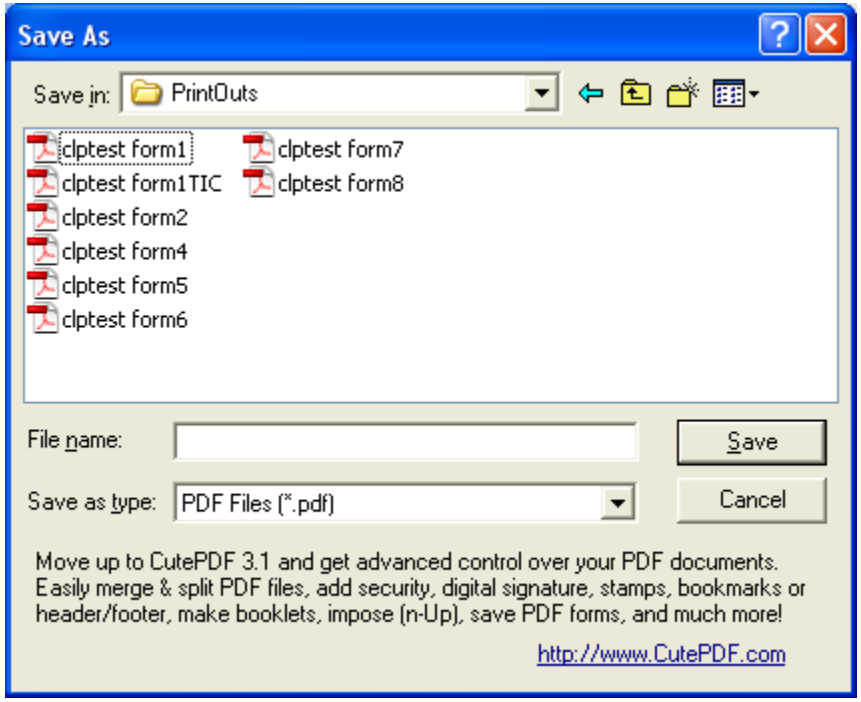
Again, sample specific data is taken from the data file and general data entered for blank is automatically entered for all files.

Select “Print Form”.



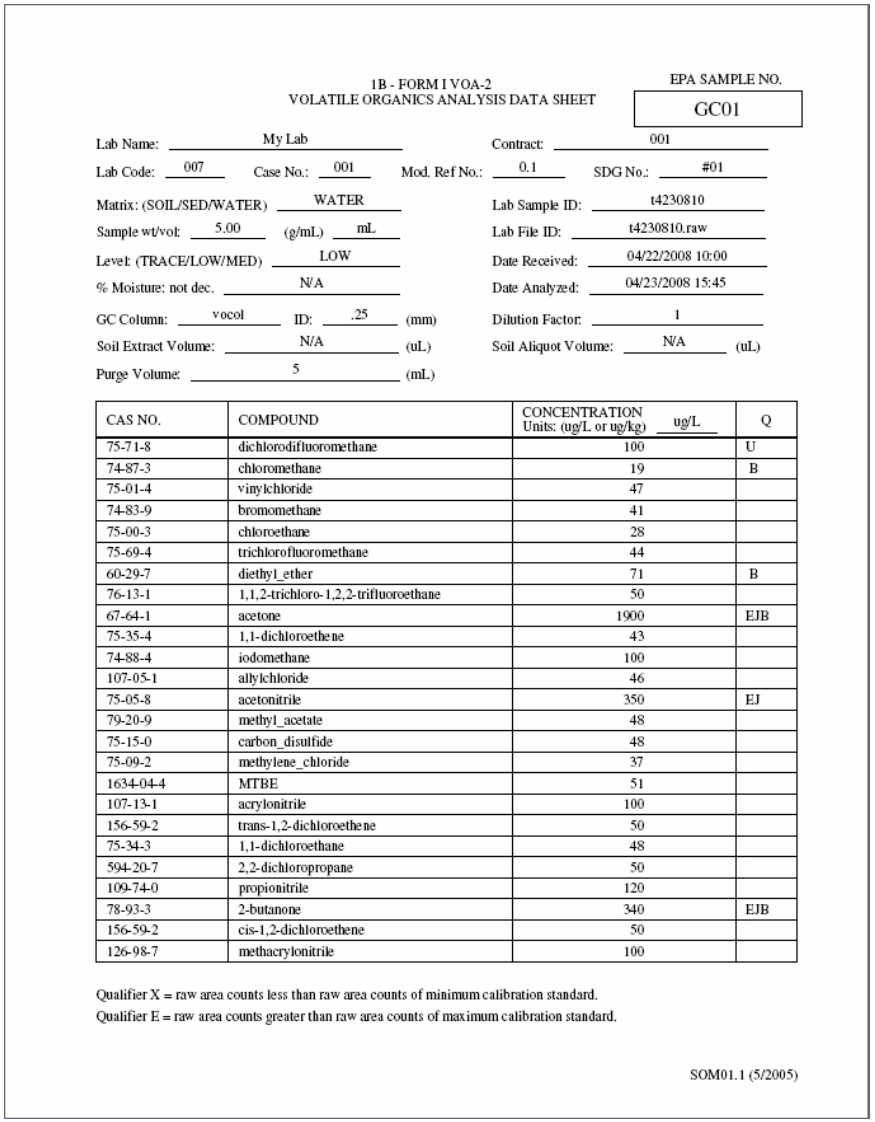
Printing Form 1

The printer that was selected was a pdf writer so there is a prompt for a file name. The CLPForms install created a folder c:\SMCReporter\PrintOuts. The pdf files that are generated with this demonstration are also supplied and are in the PrintOuts folder. You may overwrite the print files or create new files.



Generated Form 1

First Page of Form 1 should look like right.



1B - FORM I VOA-2
VOLATILE ORGANICS ANALYSIS DATA SHEET

EPA SAMPLE NO.
GC01

Lab Name: My Lab
Contract: 001
Lab Code: 007 Case No.: 001 Mod. Ref No.: 0.1 SDG No.: #01
Matrix: (SOIL/SED/WATER) WATER
Lab Sample ID: t4230810
Sample wt/vol: 5.00 (g/mL) mL
Lab File ID: t4230810.raw
Level: (TRACE/LOW/MED) LOW
Date Received: 04/22/2008 10:00
% Moisture: not dec. N/A
Date Analyzed: 04/23/2008 15:45
GC Column: vocol ID: .25 (mm)
Dilution Factor: 1
Soil Extract Volume: N/A (uL)
Soil Aliquot Volume: N/A (uL)
Purge Volume: 5 (mL)

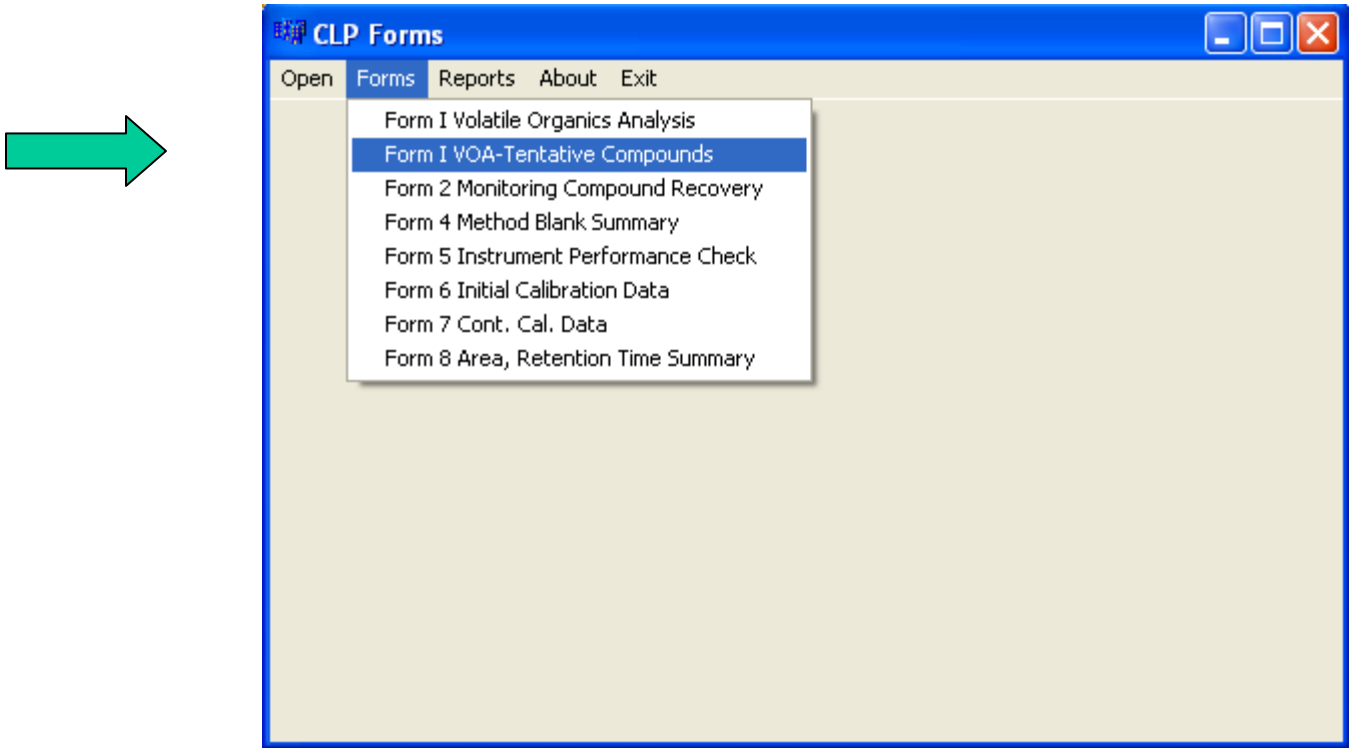
CAS NO.	COMPOUND	CONCENTRATION Units: (ug/L or ug/kg) ug/L	Q
75-71-8	dichlorodifluoromethane	100	U
74-87-3	chloromethane	19	B
75-01-4	vinylchloride	47	
74-83-9	bromomethane	41	
75-00-3	chloroethane	28	
75-69-4	trichlorofluoromethane	44	
60-29-7	diethyl_ether	71	B
76-13-1	1,1,2-trichloro-1,2,2-trifluoroethane	50	
67-64-1	acetone	1900	EJB
75-35-4	1,1-dichloroethene	43	
74-88-4	iodomethane	100	
107-05-1	allylchloride	46	
75-05-8	acetonitrile	350	EJ
79-20-9	methyl_acetate	48	
75-15-0	carbon_disulfide	48	
75-09-2	methylene_chloride	37	
1634-04-4	MTBE	51	
107-13-1	acrylonitrile	100	
156-59-2	trans-1,2-dichloroethene	50	
75-34-3	1,1-dichloroethane	48	
594-20-7	2,2-dichloropropane	50	
109-74-0	propionitrile	120	
78-93-3	2-butanone	340	EJB
156-59-2	cis-1,2-dichloroethene	50	
126-98-7	methacrylonitrile	100	

Qualifier X = raw area counts less than raw area counts of minimum calibration standard.
Qualifier E = raw area counts greater than raw area counts of maximum calibration standard.

SOM01.1 (5/2005)

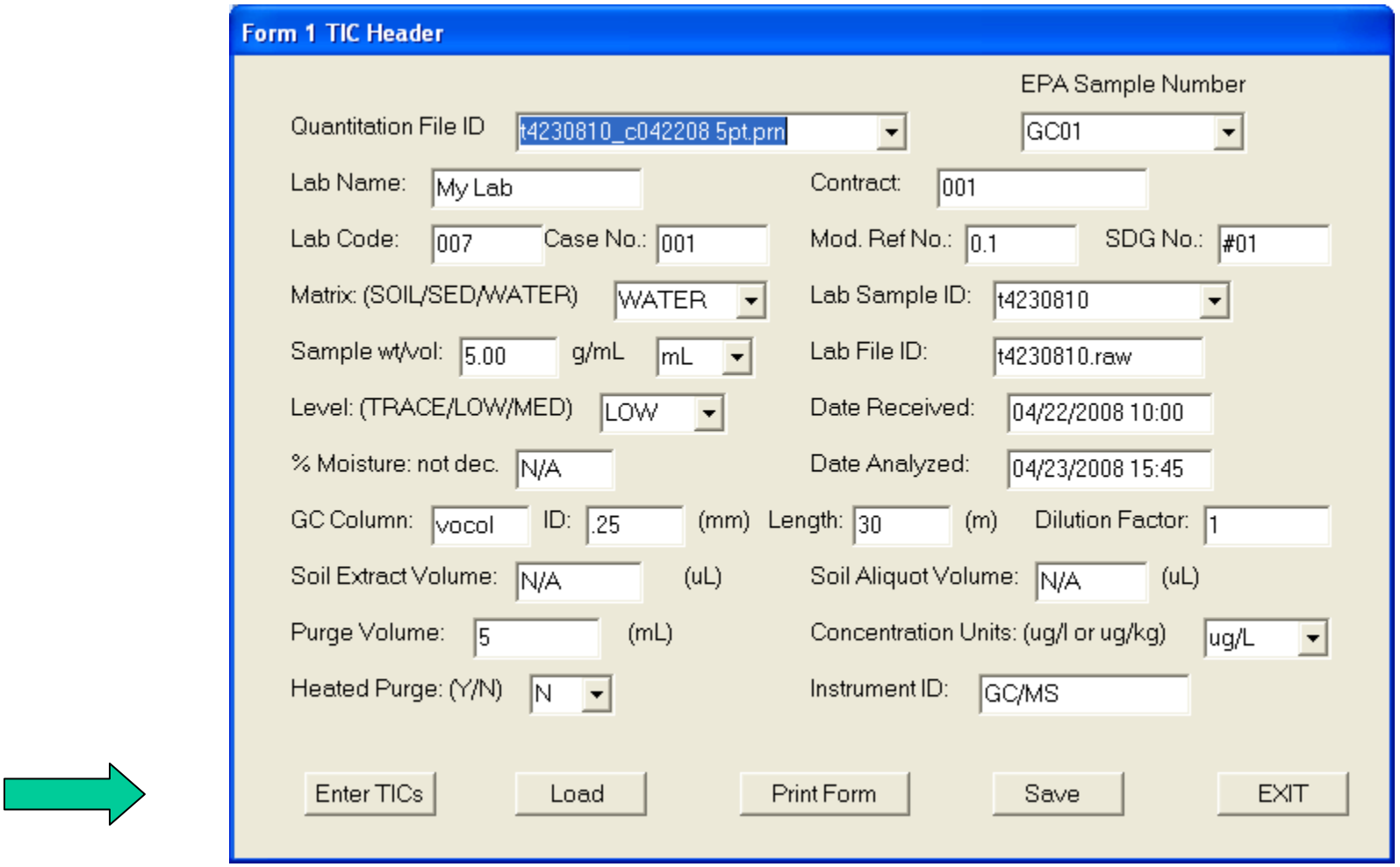
Form 1 TIC

Selecting the Form 1 TIC brings calls the Form1 for a selection of which file to generate TIC form.



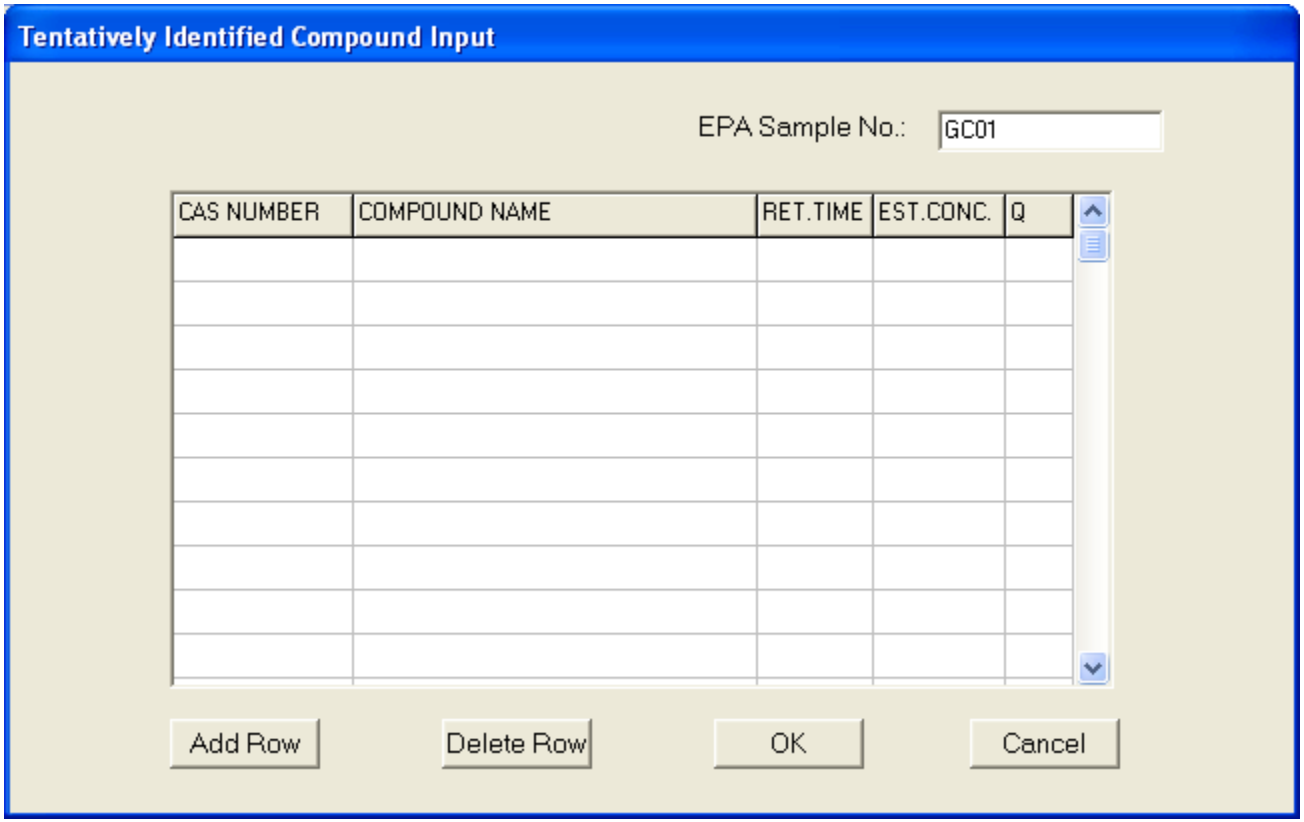
Form 1 TIC select file

Select file ID t423810_c042208 5pt.prn. Note all of the information from Form 1 has been applied to this form as well. Select “Enter TICs”.



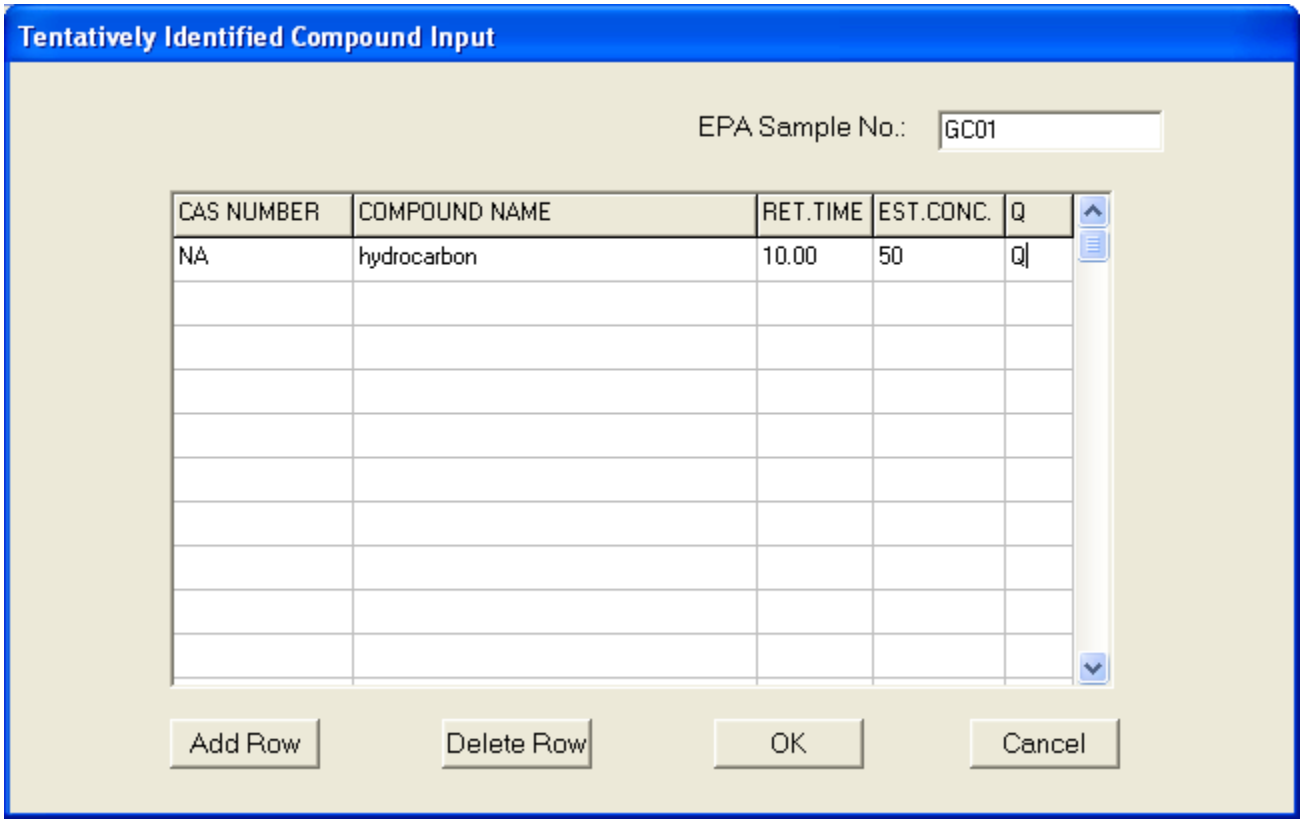
Enter TIC data

- This form takes information manually to complete Form 1 TIC.
- Enter information as presented in following slide.



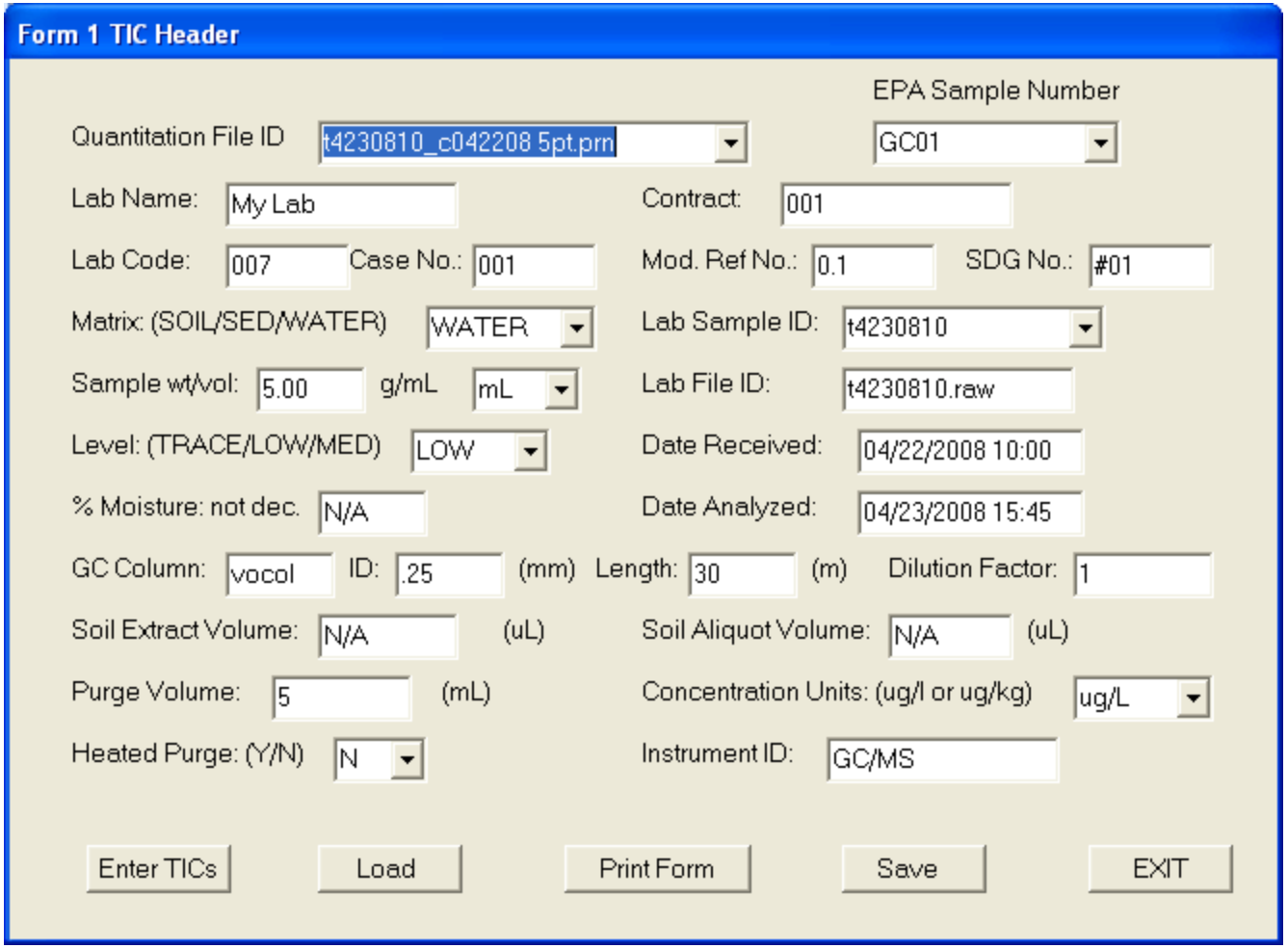
TIC input

Enter the information for a single compound, an unknown hydrocarbon as below.



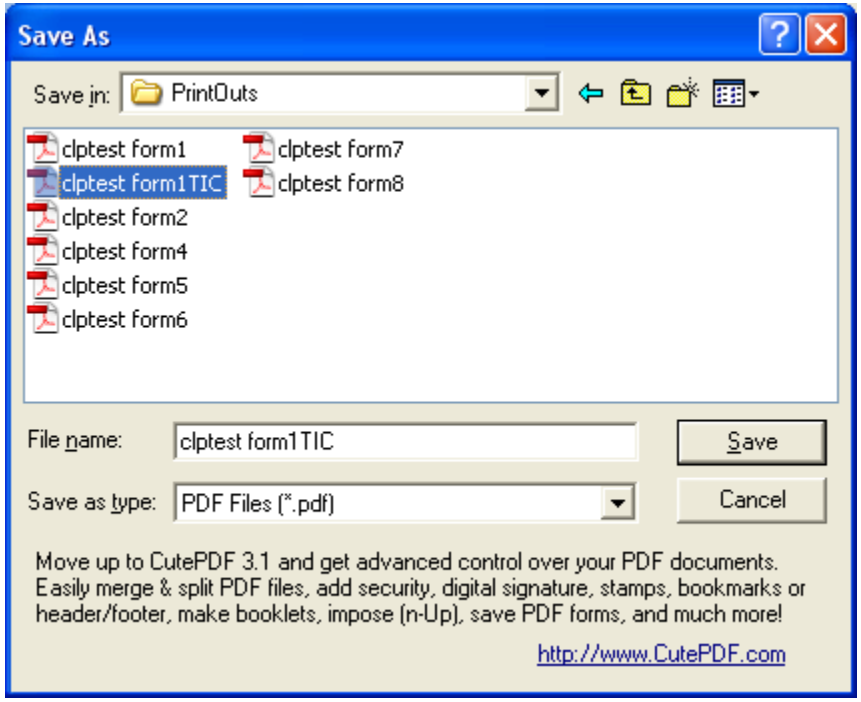
After entering data select “OK”. You will be returned to the previous form.

Printing Form 1 TICs



Now select “Print Form” to print Form 1 TICs.

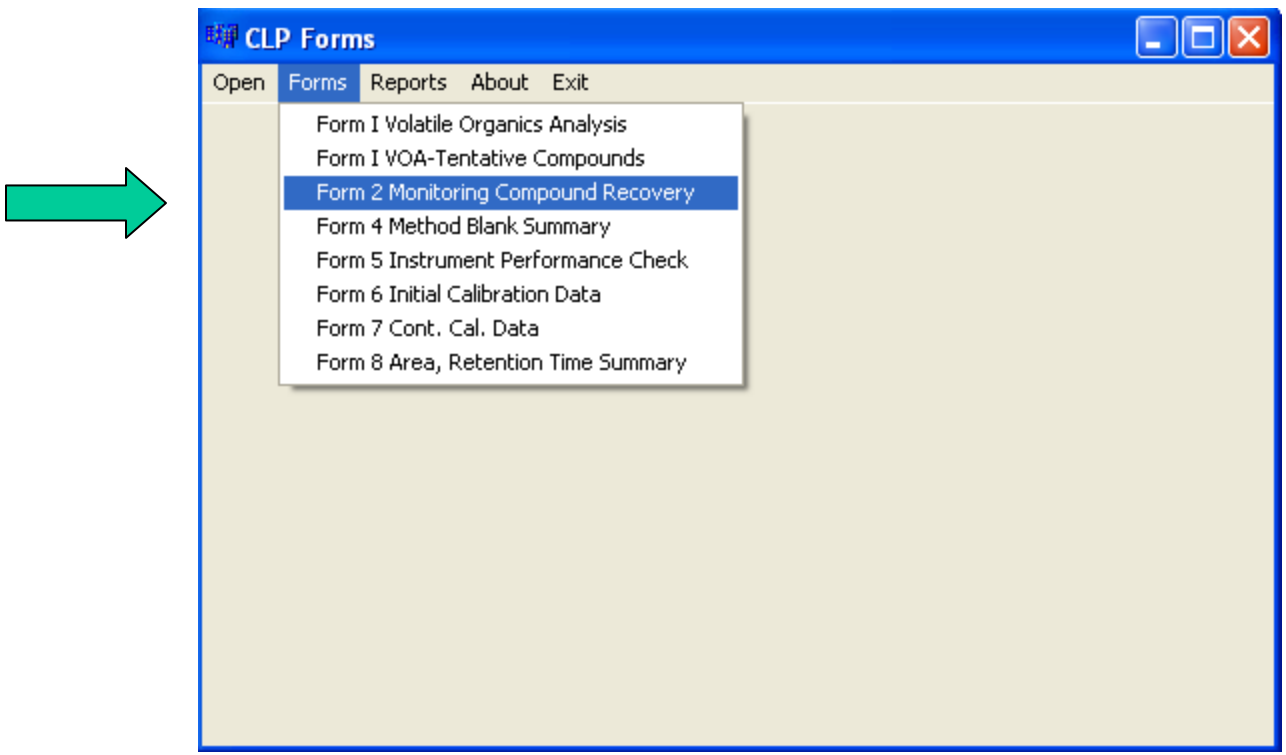
Printing Form 1 TICs



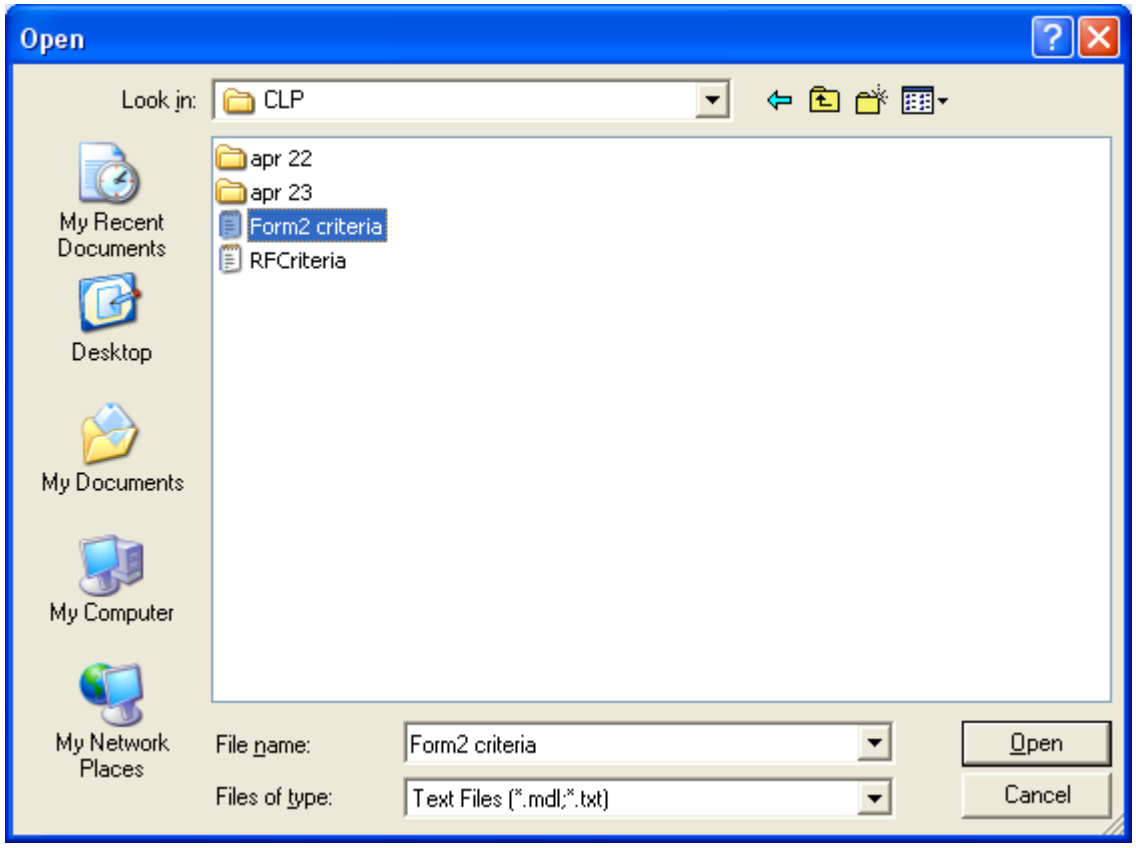
The TIC form is printed. All the forms will be printed as the Form 1 (and TIC) forms.

Form 2

Select Form 2 to print



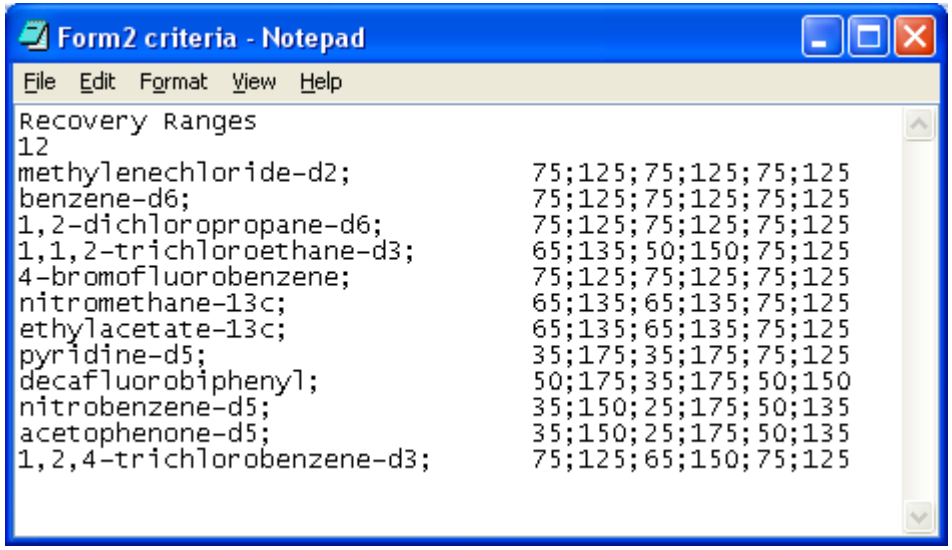
Form 2: Get file containing criteria.



This form requires input of limits for monitoring compound recoveries. This information is contained in a text file, Form2 criteria.txt. Other limits can be generated for use by copying the file and making changes (limits or even the monitoring compounds).

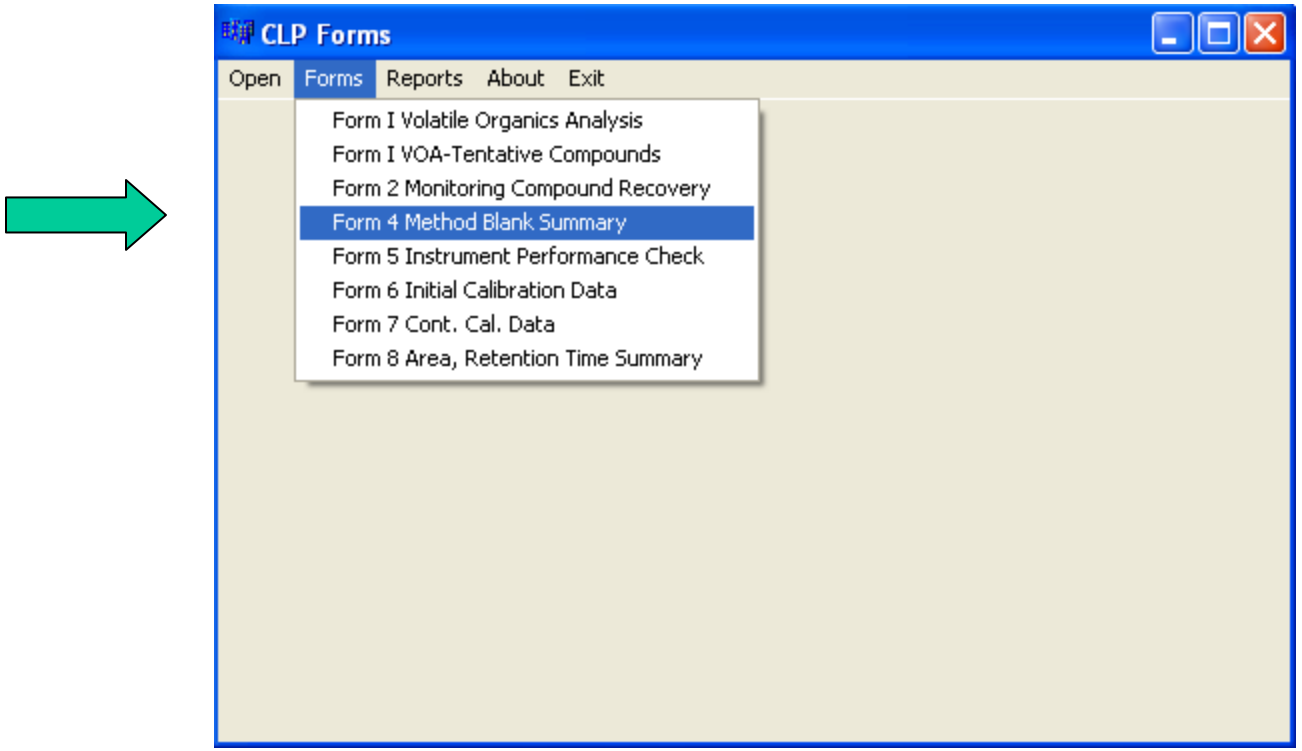
Monitoring Compounds and Limits

- The range file is a text file shown below. The number in upper left is for how many monitoring compounds. All surrogates will be listed in Form 2 but only the surrogates identified in the Range file will have criteria.
- The first two columns of numbers are the low and high range limits for water. The next two columns are for soil. The last two are for oil.
- This file can be changed to match new criteria.



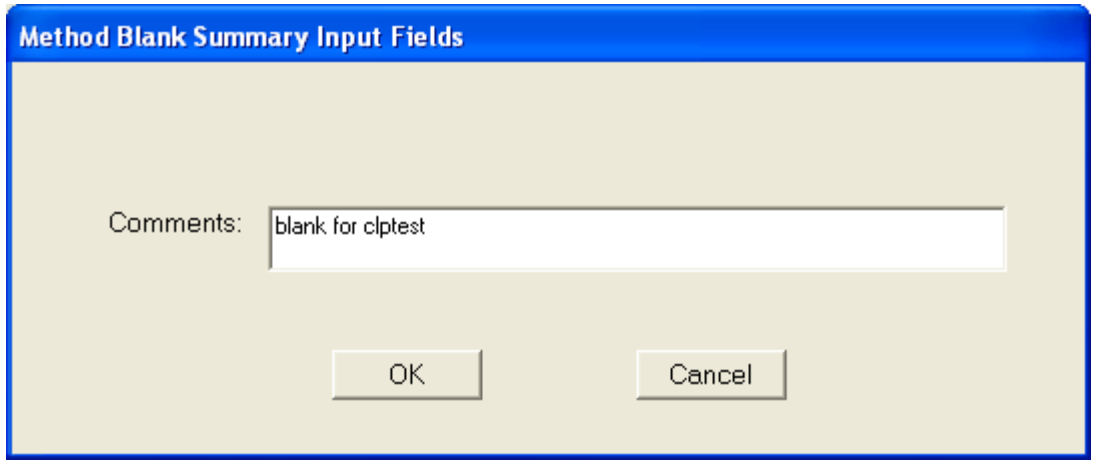
Form 4

Select Form 4 and a form will appear requesting comment information



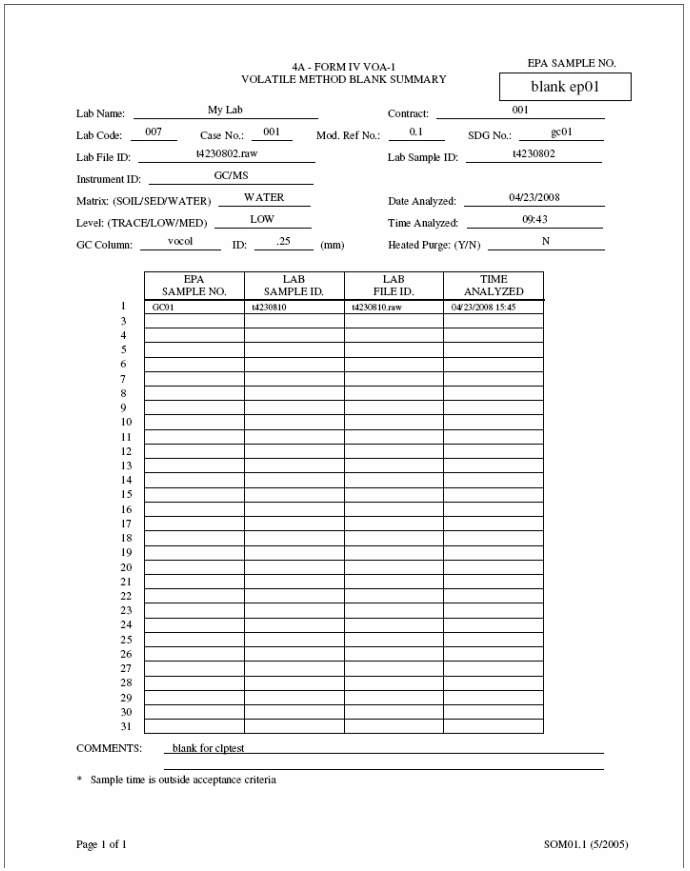
Form 4 comments

Enter comments here when needed



FORM 4

The generated form should look like this



4A - FORM IV VOA-1
VOLATILE METHOD BLANK SUMMARY

EPA SAMPLE NO.
blank ep01

Lab Name: My Lab
Contract: 001
Lab Code: 007 Case No.: 001 Mod. Ref No.: 0.1 SDG No.: gc01
Lab File ID: t4230802.raw
Lab Sample ID: t4230802
Instrument ID: GC/MS
Matrix: (SOIL/SED/WATER) WATER
Date Analyzed: 04/23/2008
Level: (TRACE/LOW/MED) LOW
Time Analyzed: 09:43
GC Column: vocol ID: .25 (mm)
Heated Purge: (Y/N) N

	EPA SAMPLE NO.	LAB SAMPLE ID.	LAB FILE ID.	TIME ANALYZED
1	GC01	t4230810	t4230810.raw	04/23/2008 15:45
3				
4				
5				
6				
7				
8				
9				
10				
11				
12				
13				
14				
15				
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29				
30				
31				

COMMENTS: blank for clptest

* Sample time is outside acceptance criteria

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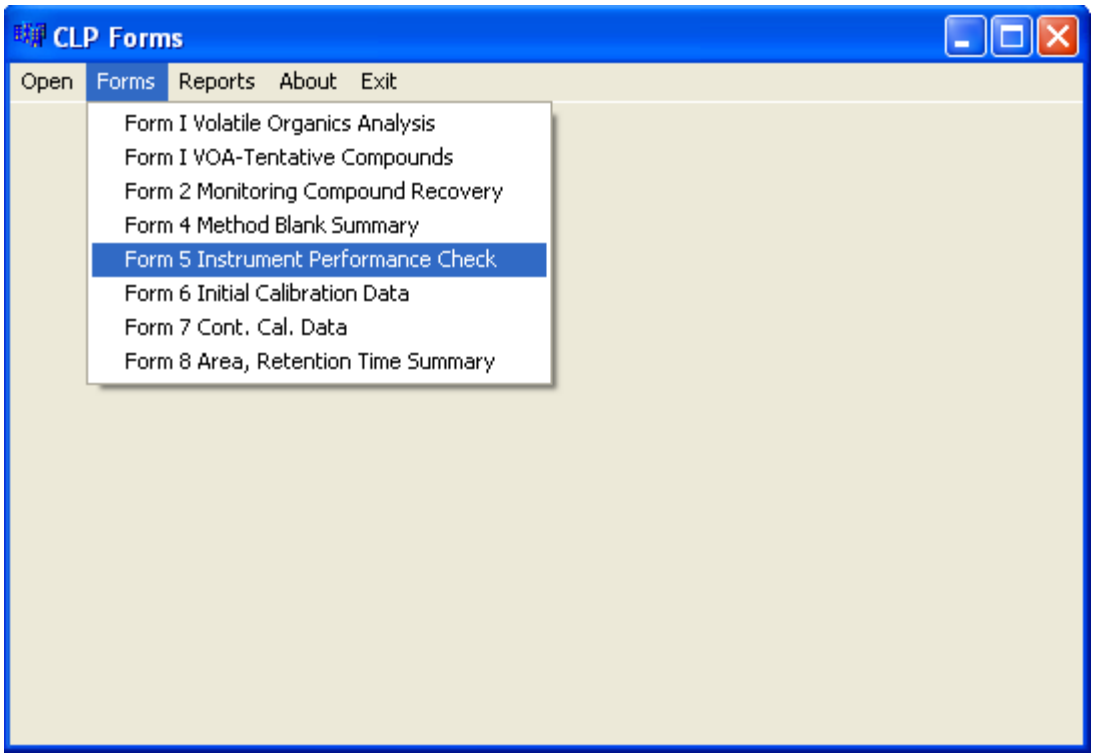
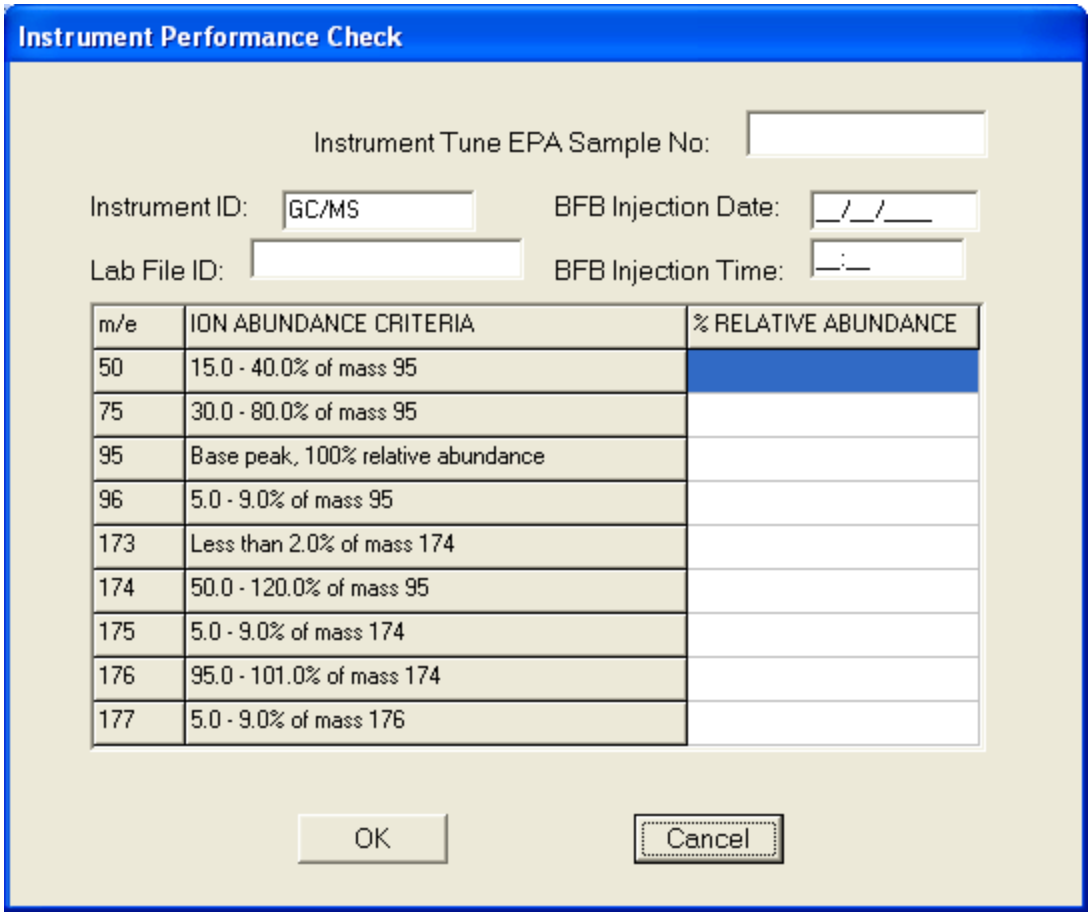
Form 5

Select Form 5 and information will be requested to complete the form.



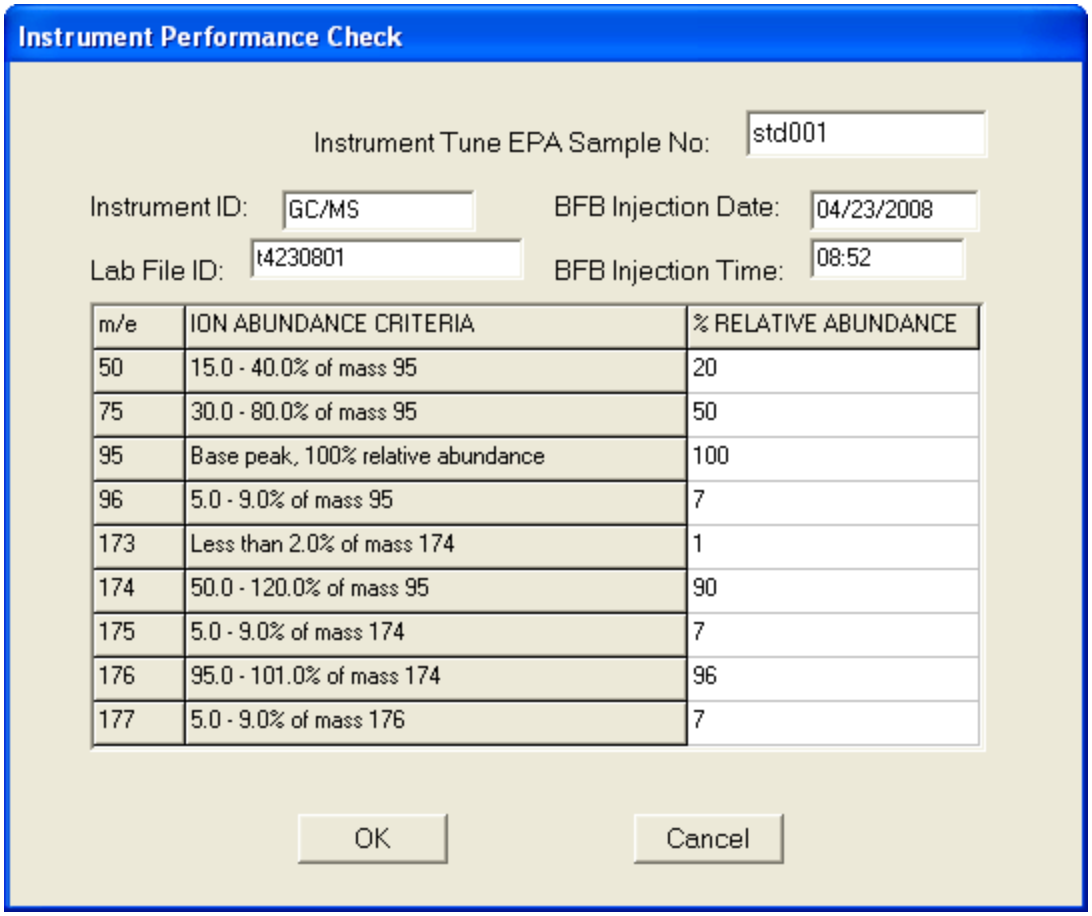
Form 5 data entry

Enter information to complete form as shown in next slide.



Form 5 Printing

After entering data select “OK” to print.



Form 5

Generated form should look like this

5A - FORM V VOA-1
VOLATILE ORGANIC INSTRUMENT PERFORMANCE CHECK
BROMOFLUOROBENZENE (BFB)

EPA SAMPLE NO.: std001

Lab Name: t4230802 Contract: 001

Lab Code: 007 Case No.: 001 Mod. Ref No.: 0.1 SDG No.: gc01

Lab File ID: t4230801 BFB Injection Date: 04/23/2008

Instrument ID: GC/MS BFB Injection Time: 08:52

GC Column: vocol ID: .25 (mm)

m/e	ION ABUNDANCE CRITERIA	%RELATIVE ABUNDANCE
50	15.0 - 40.0% of mass 95	20
75	30.0 - 80.0% of mass 95	50
95	Base peak, 100% relative abundance	100
96	5.0 - 9.0% of mass 95	7
173	Less than 2.0% of mass 174	(1)1
174	50.0 - 120% of mass 95	90
175	5.0 - 9.0% of mass 174	(7)1
176	95 - 101% of mass 174	(96)1
177	5.0 - 9.0% of mass 176	(7)2

1 - Value is %mass 174 2 - Value is %mass 176

	EPA SAMPLE NO.	LAB SAMPLE ID.	LAB FILE ID.	DATE ANALYZED	TIME ANALYZED
1	blank ep01	t4230802	t4230802.raw	04/23/2008	09:43
2	GC01	t4230810	t4230810.raw	04/23/2008	15:45
3					
4					
5					
6					
7					
8					
9					
10					
11					
12					
13					
14					
15					
16					
17					
18					
19					
20					
21					
22					

* Value is outside acceptance criteria

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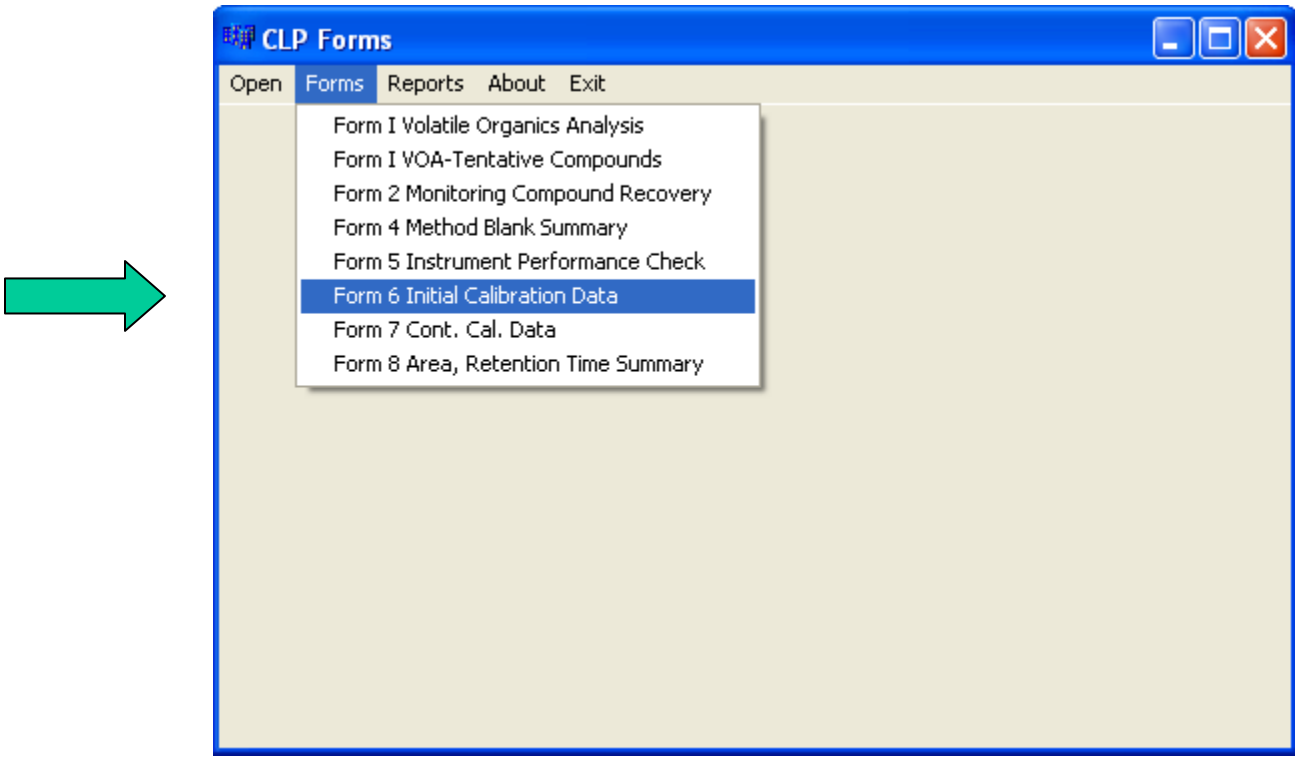
Form 6

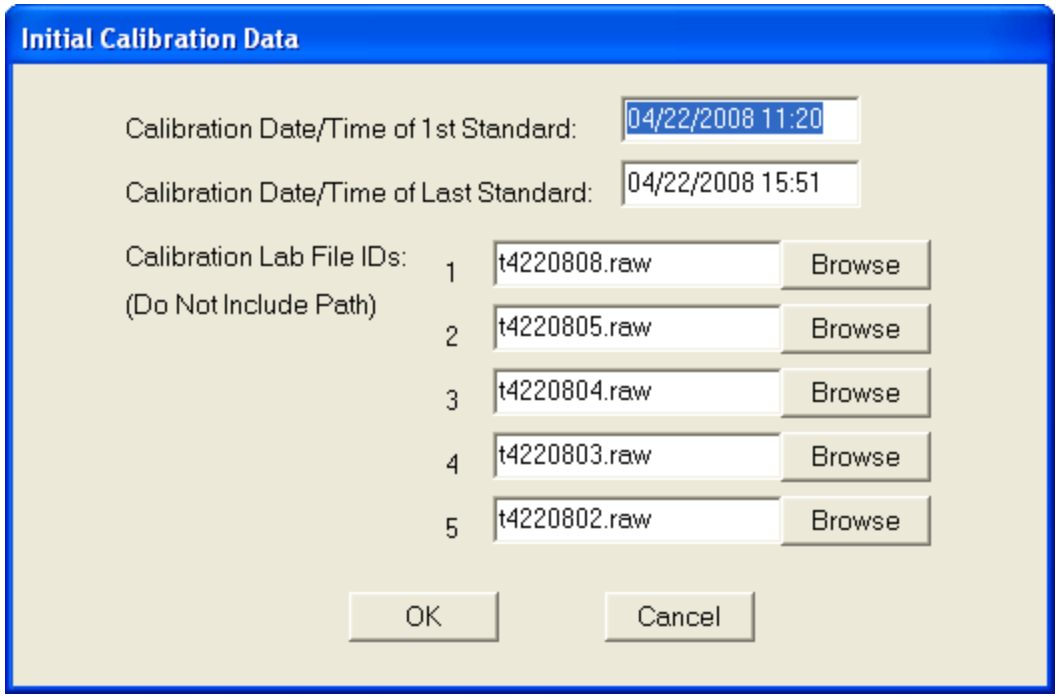
Select Form 6. You will be requested to verify file selection.



Form 6

The fields should be automatically filled but use the browse buttons to locate files if necessary.

Select “OK” to generate form.



Form 6

Generated form should look like this (first page)

6A - FORM VI VOA-1
VOLATILE ORGANICS INITIAL CALIBRATION DATA

Lab Name: My Lab Contract: 001

Lab Code: 007 Case No.: 001 Mod. Ref No.: 0.1 SDG No.: gc01

Instrument ID: GC/MS Calibration Date(s): 04/22/2008 04/22/2008

Heated Purge: (Y/N) N Calibration Time(s): 11:20 15:51

Purge Volume: 5 (ml)

GC Column: vocol ID: .25 (mm) Length: 30 (m)

LAB FILE ID: RF_500 = t4220808.raw RF_50 = t4220805.raw
RF_25 = t4220804.raw RF_15 = t4220803.raw RF_5 = t4220802.raw

COMPOUND	RF_500	RF_50	RF_25	RF_15	RF_5	RF	%RSD
diethyl_ether-d10	1433	1495	1487	1525	1559	1500	2.80
acetone-13c	1067	1121	1066	1072	1102	1086	2.03
methylene_chloride-d2	2786	2440	2315	2362	2312	2443	7.27
nitromethane-13c	1477	1544	1529	1437	1471	1492	2.64
hexafluorobenzene	4091	4317	4224	4184	4158	4195	1.78
tetrahydrofuran-d8	2264	2133	2205	2201	2099	2180	2.67
ethylacetate-13c	1046	1076	1073	1077	1054	1065	1.20
pentafluorobenzene	5622	5834	5768	5859	5724	5761	1.47
benzene-d6	17022	16914	17599	17595	17406	17307	1.66
1,2-dichloroethane-d4	2920	2892	2858	2866	2856	2878	0.85
fluorobenzene	17109	17728	17663	17974	17494	17594	1.63
1,4-difluorobenzene	14951	15652	15341	15365	14941	15250	1.78
1,2-dichloropropane-d6	7929	8300	8005	8023	7978	8047	1.62
1,4-dioxane-d8	781	772	775	776	771	775	0.45
toluene-d8	16684	16475	16704	16418	16481	16552	0.71
pyridine-d5	438	380	382	334	259	359	16.65
1,1,2-trichloroethane-d3	6185	6032	6180	6210	5938	6109	1.74
1,2-dibromoethane-d4	4434	4307	4314	4208	4140	4281	2.35
chlorobenzene-d5	6668	6934	6809	6987	6836	6847	1.61
o-xylene-d10	15467	14831	15136	14753	15154	15068	1.70
4-bromofluorobenzene	3879	3908	3904	3890	3911	3898	0.31
bromobenzene-d5	4085	4185	4153	4227	4043	4139	1.61
1,2-dichlorobenzene-d4	5002	4971	4997	4992	4924	4977	0.57
decafluorobiphenyl	448	443	527	456	577	490	10.82
nitrobenzene-d5	5476	4716	5291	4581	4720	4957	7.20
acetophenone-d5	1421	1214	1492	1250	1308	1337	7.82
1,2,4-trichlorobenzene-d3	5901	5589	5398	5200	5260	5470	4.64

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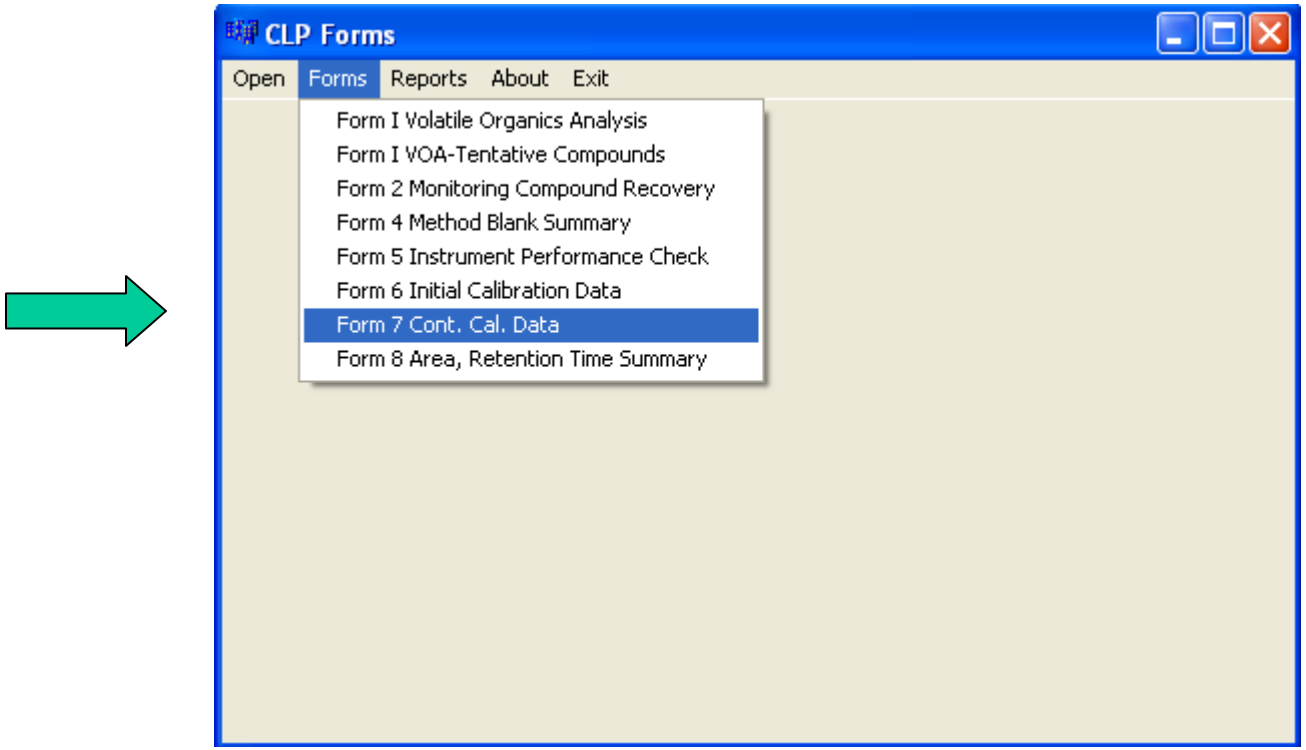
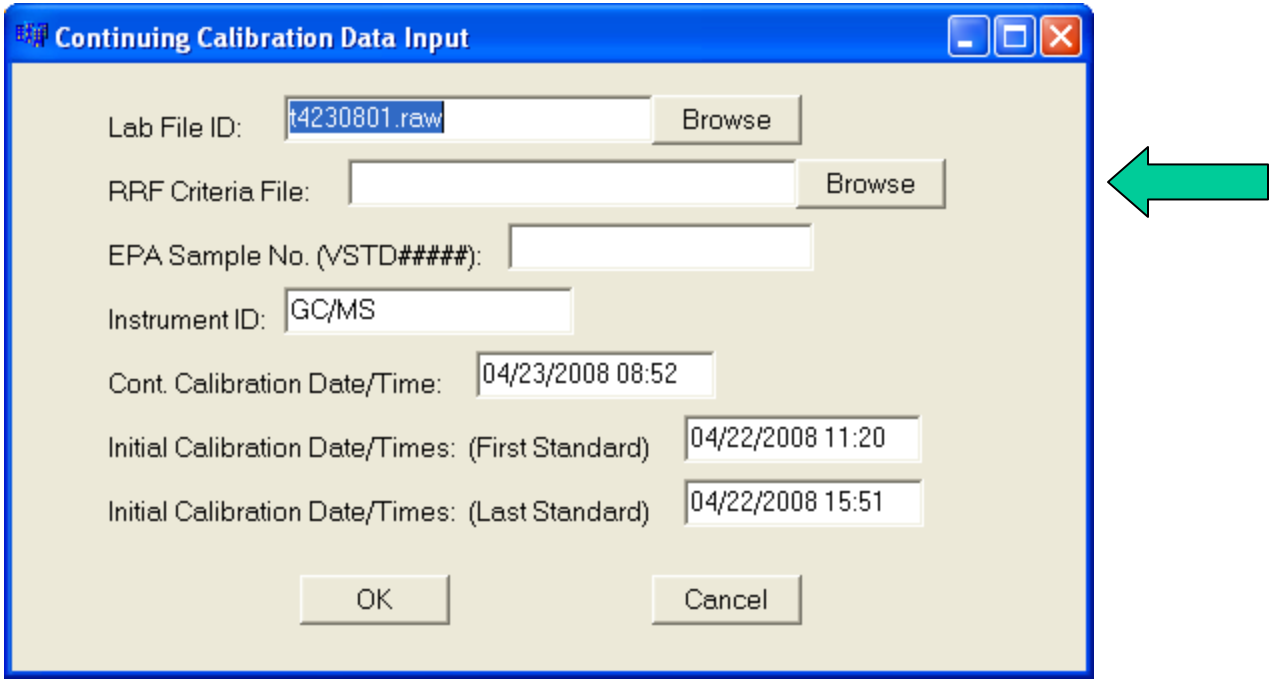
Form 7

Select Form 7. You will be prompted for some additional information



Form 7 Data Entry

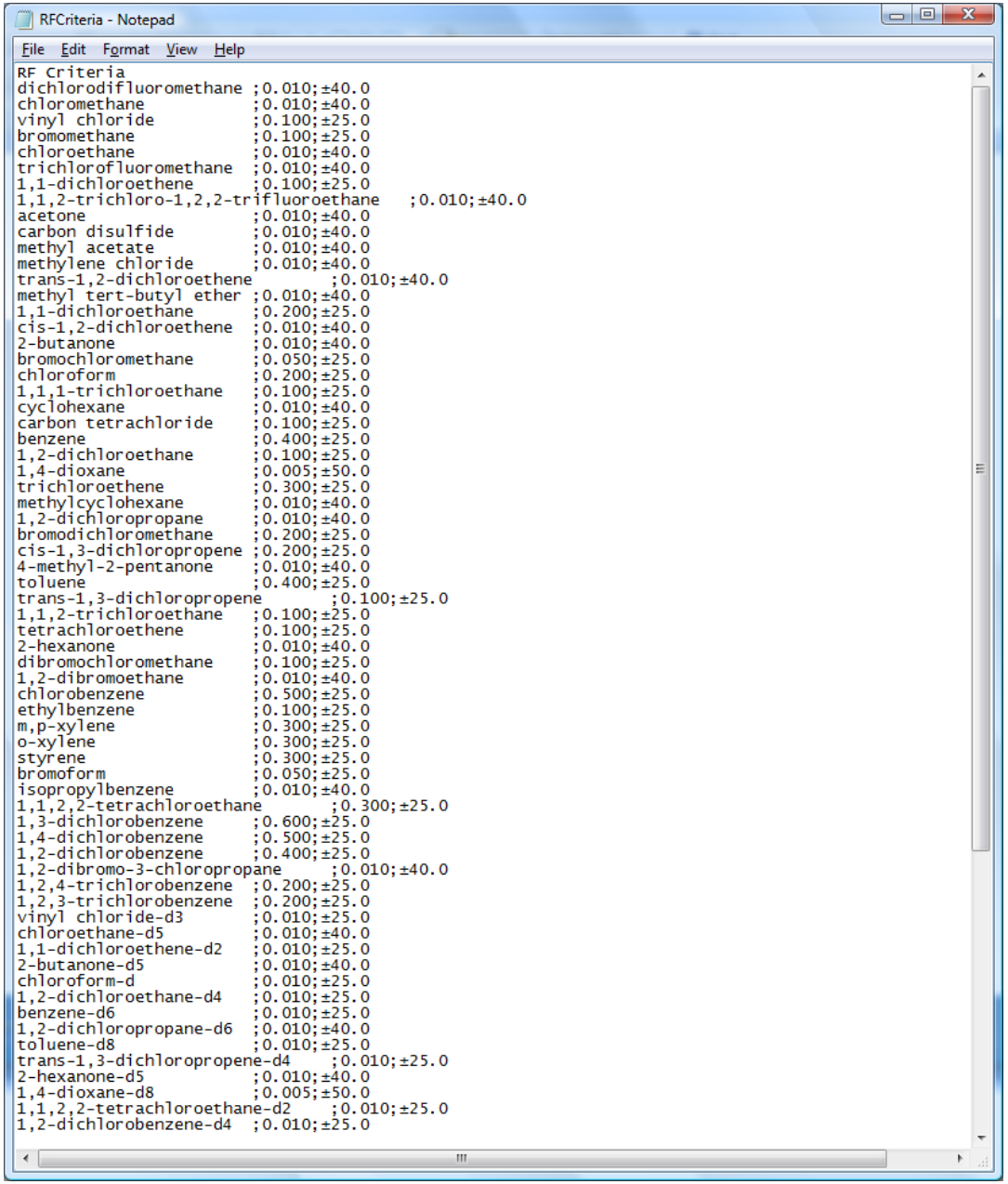
Much of this data should be automatically completed. The response factor criteria file must be selected. Select “Browse” to find the criteria file, rfcriteria.txt (its in c:\SMCReporter\CLP folder). Next select “OK” to print file.



Response Factor Criteria File

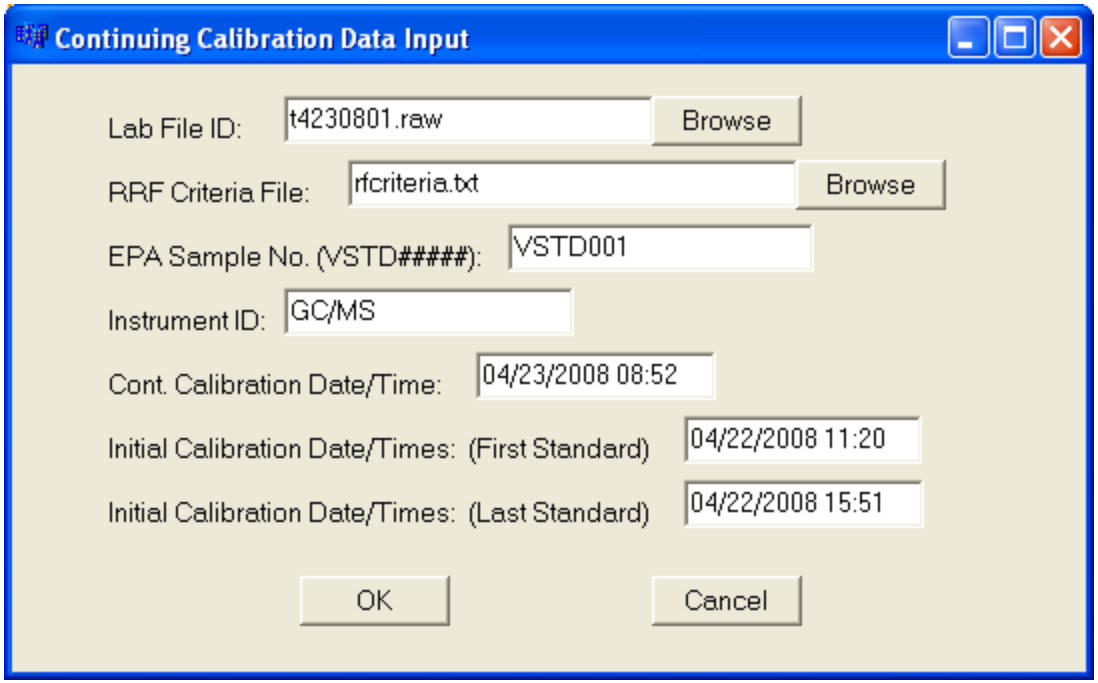
File is simple text file. Compounds listed are used to verify continuing calibration curve.

First number is for minimum response factor (cts/ng) second number is limit for deviation from calibration (as percent).



Form 7

Type in VSTD001 for EPA Sample No. and then select “OK”



Form 7

Generated report should look like this for page 1

7A - FORM VII VOA-1
VOLATILE CONTINUING CALIBRATION DATA

Lab Name: My Lab Contract: 001
Lab Code: 007 Case No.: 001 Mod. Ref No.: 0.1 SDG No.: gc01
Instrument ID: GC/MS Calibration Date: 04/23/2008 Time: 08:52
Lab File ID: t4230801.raw Init. Calib. Date(s): 04/22/2008 04/22/2008
EPA Sample No. (VSTD#####): VSTD001 Init. Calib. Time(s): 11:20 15:51
Heated Purge: (Y/N) N GC Column: vocol ID: .25 (mm) Length: 30 (m)
Purge Volume: 5 (ml)

COMPOUND	$\overline{RF}$	RF_50	MIN RF	%D	MAX %D
diethyl_ether-d10	1500	1587		5.8	
acetone-13c	1086	1130		4.1	
methylene_chloride-d2	2443	2361		-3.3	
nitromethane-13c	1492	1465		-1.8	
hexafluorobenzene	4195	4308		2.7	
tetrahydrofuran-d8	2180	2031		-6.8	
ethylacetate-13c	1065	1046		-1.8	
pentafluorobenzene	5762	5951		3.3	
benzene-d6	17307	17284	0.010	-0.1	±25.0
1,2-dichloroethane-d4	2878	2661	0.010	-7.5	±25.0
fluorobenzene	17594	17787		1.1	
1,4-difluorobenzene	15250	15323		0.5	
1,2-dichloropropane-d6	8047	7766	0.010	-3.5	±40.0
1,4-dioxane-d8	775	770	0.005	-0.7	±50.0
toluene-d8	16552	16500	0.010	-0.3	±25.0
pyridine-d5	359	108		-70.0	
1,1,2-trichloroethane-d3	6109	5636		-7.7	
1,2-dibromoethane-d4	4281	4079		-4.7	
chlorobenzene-d5	6847	6778		-1.0	
o-xylene-d10	15068	15254		1.2	
4-bromofluorobenzene	3898	4002		2.7	
bromobenzene-d5	4138	4146		0.2	
1,2-dichlorobenzene-d4	4977	4958	0.010	-0.4	±25.0
decafluorobiphenyl	490	633		29.2	
nitrobenzene-d5	4957	4335		-12.5	
acetophenone-d5	1337	1099		-17.8	
1,2,4-trichlorobenzene-d3	5470	5102		-6.7	

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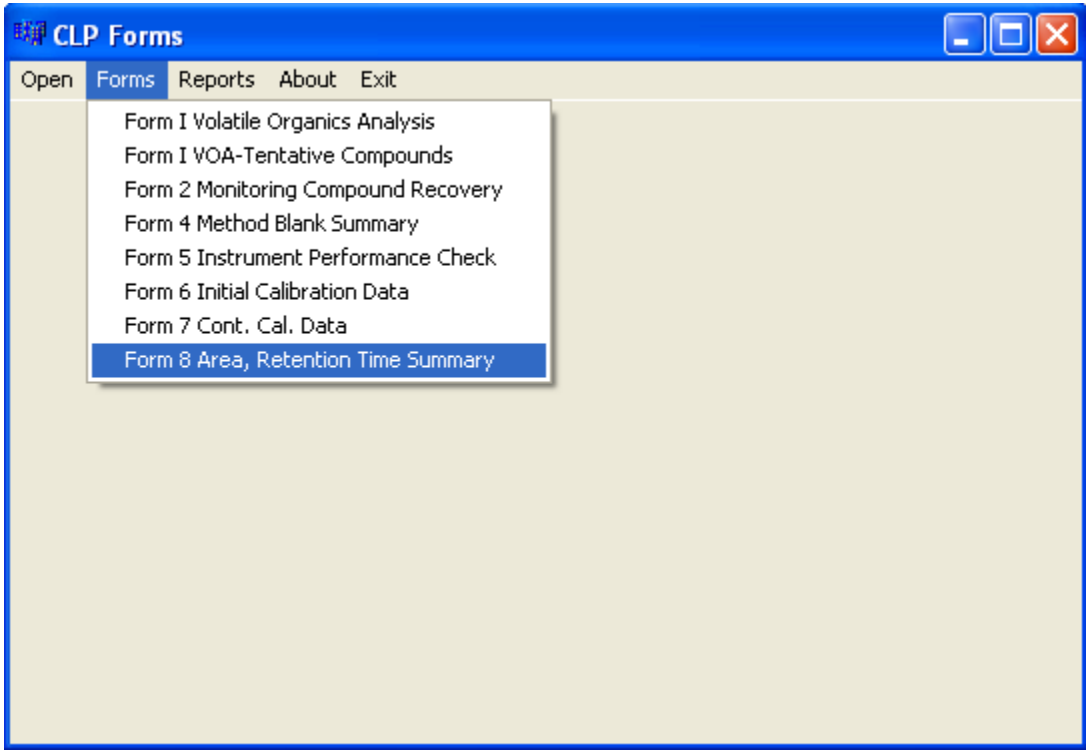
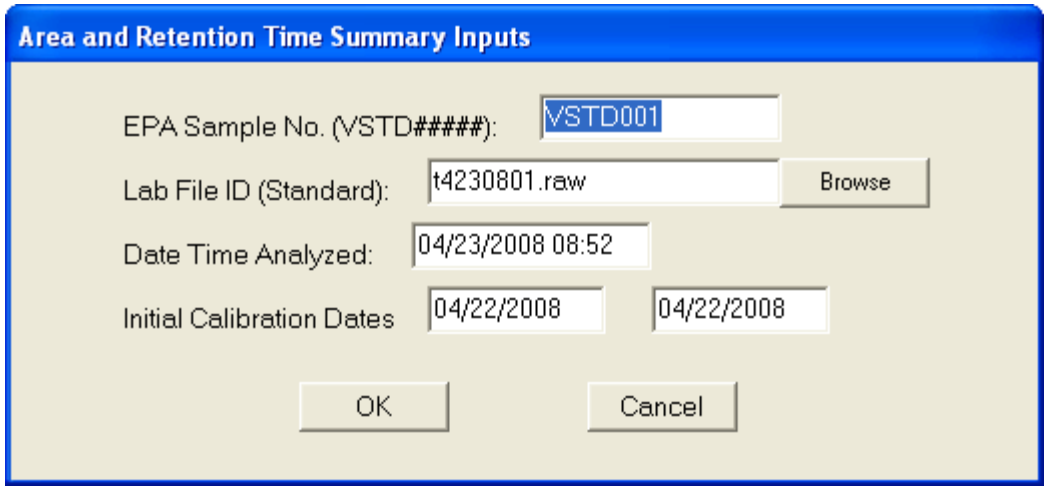
Form 8

Select Form 8



Form 8

You will be prompted for any missing or inaccurate data. If correct, select “OK” to generate report.



Form 8

The generated report should look like this.

8A - FORM VIII VOA
VOLATILE INTERNAL STANDARD AREA AND RETENTION TIME SUMMARY

Lab Name: My Lab
Contract: 001
Lab Code: 007 Case No.: 001 Mod. Ref No.: 0.1 SDG No.: gc01
GC Column: vocol ID: .25 (mm) Init. Calib. Date(s): 04/22/2008 04/22/2008
EPA Sample No. (VSTD#####): VSTD001
Date Analyzed: 04/23/2008
Lab File ID (Standard) t4230801.raw
Time Analyzed: 08:52
Instrument ID: GC/MS
Heated Purge: (Y/N) N

		IS1 AREA	#	RT	#	IS2 AREA	#	RT	#	IS3 AREA	#	RT	#
	12 HOUR STD	2143011		13.92		4944239		8.73		1629447		20.00	
	UPPER LIMIT	4286022		14.42		9888478		9.23		3258894		20.50	
	LOWER LIMIT	1071506		13.42		2472120		8.23		814724		19.50	
	EPA SAMPLE NO.												
1	blank ep01	2325475		13.92		5278917		8.73		1676887		20.00	
2	GC01	2568393		13.92		5600077		8.73		1731146		20.00	
3													
4													
5													
6													
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22													

IS1 = Chlorobenzene-d5
IS2 = 1,4-Difluorobenzene
IS3 = 1,2-Dichlorobenzene-d4

AREA UPPER LIMIT = 200% (Low-Medium Volatiles) of internal standard area
AREA LOWER LIMIT = 50% (Low-Medium Volatiles) of internal standard area
RT UPPER LIMIT = + 0.50 (Low-Medium Volatiles) minutes of internal standard RT
RT LOWER LIMIT = - 0.50 (Low-Medium Volatiles) minutes of internal standard RT

Column used to flag values outside QC limits with an asterisk

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Summary

- CLPForms requires data files generated from SMCReporter 4.2.
- Forms can be generated as pdf or printed depending on user-selected printer.
- Forms can be changed to meet changing criteria and analyte lists.