"How To" Review, Blank Correct and Calculate Total PCB

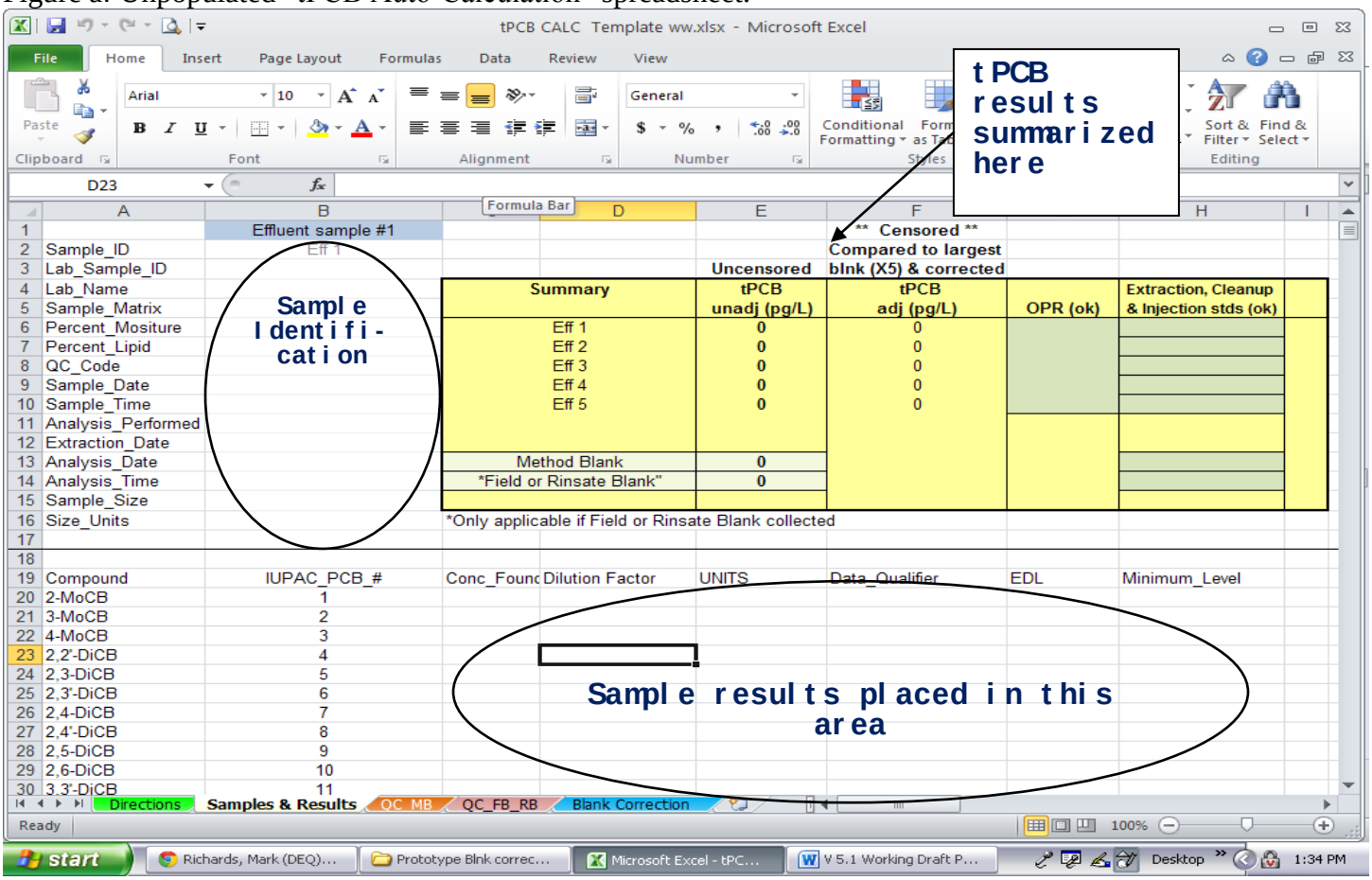
(Supplemental document to TMDL GM14-2004)

Note - Basic knowledge of Microsoft Excel is necessary to perform these tasks.

Automated Excel Spreadsheet Used to Calculate Total PCB (tPCB)

An Excel "tPCB Auto-Calculation" spreadsheet has been developed to automatically compute "uncensored" and "censored" (i.e., blank corrected) tPCB concentrations. The spreadsheet is comprised of a worksheet that includes directions as well as four interactive worksheets: 1) "Directions" provides an overview of the spreadsheet, 2) "Samples & Results" is the worksheet where effluent (i.e., field sample) data are uploaded yielding a summary of computed "uncensored" and "censored" tPCB results, 3) "QC_MB" is the worksheet where method blank data are uploaded, 4) the worksheet "QC_FB_RB" receives field and/or rinsate blanks, and 5) "Blank Correction" is where an automatic comparative analysis for the blank correction process occurs with the calculated results transferred to the "Samples & Results" worksheet. Information is taken directly from the "Analytical Results" EDD .csv spreadsheet (provided by the laboratory) by copying and pasting the appropriate data into the "Samples & Results", "QC_MB", and "QC_FB_RB" worksheets. The formatting of the EDD .csv file is defined in Appendix E of **TMDL GM No. 09-2001, Amendment No. 1** and the PCB data should be delivered by the laboratory in this format. An example of the "tPCB Calculation" spreadsheet is found in Figure a. below with instructions for populating the spreadsheet. **Note: When dual computer screens are available, do not open Excel software twice and show on both screens as the copy and paste functions become disabled.**

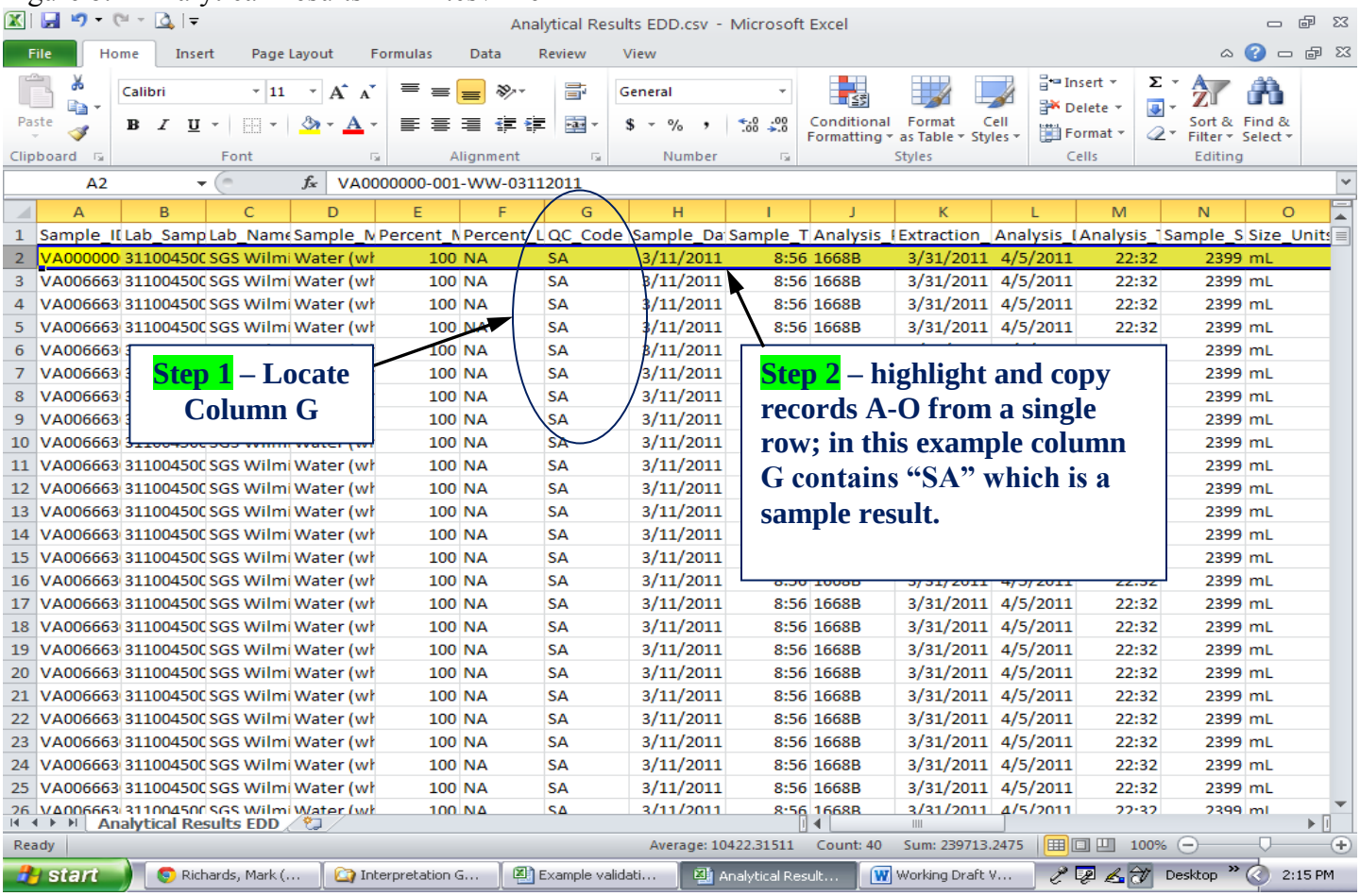
Figure a. Unpopulated "tPCB Auto-Calculation" spreadsheet.



Steps required to populate the PCB spreadsheet:

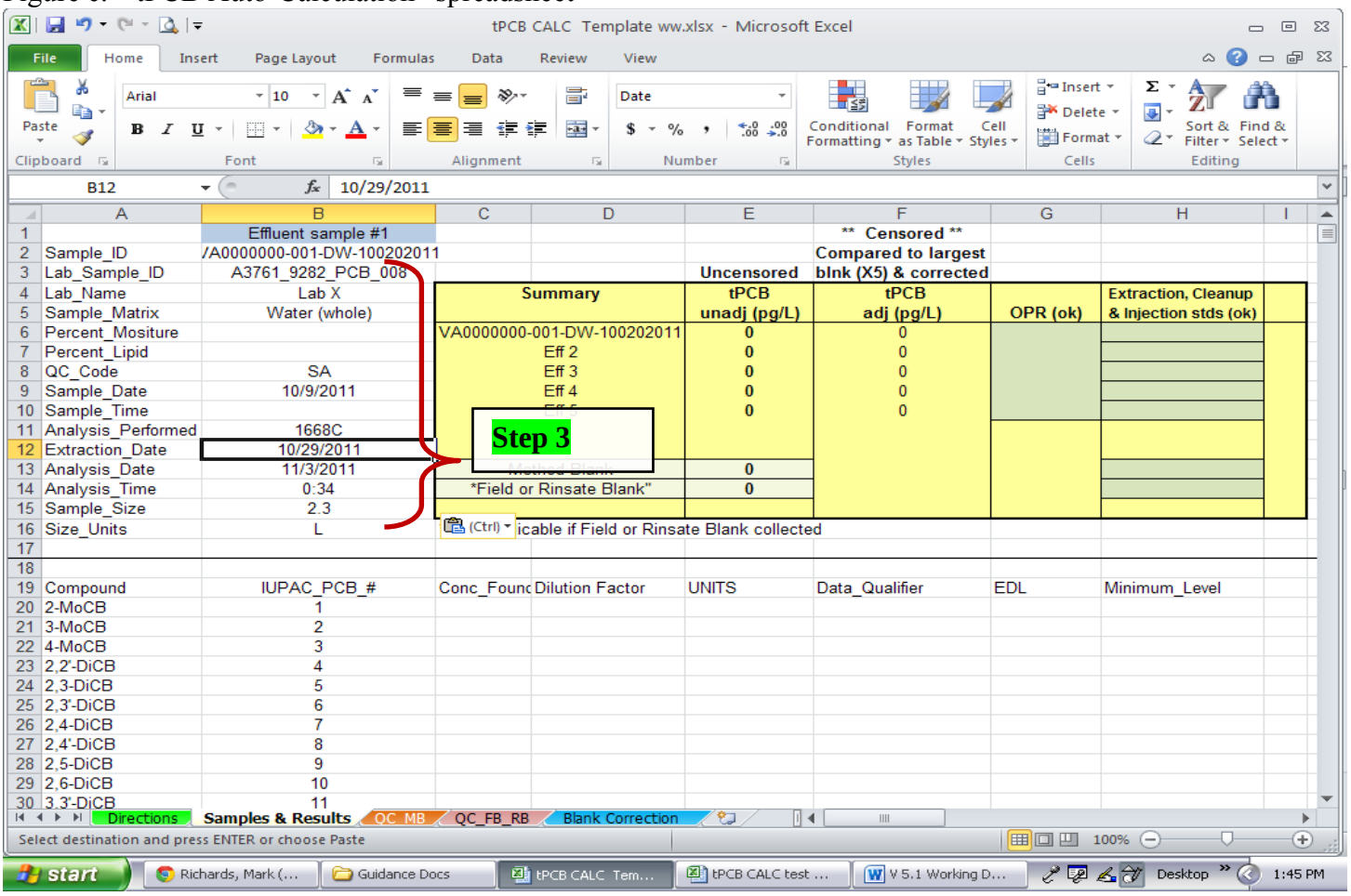
1) Open an unpopulated "tPCB Auto-Calculation" spreadsheet. A functional copy of the spreadsheet is available at: (http://www.deq.state.va.us/Programs/Water/WaterQualityInformationTMDLs/TMDL/PCBTMDLs.aspx). Next open the "Analytical Results" EDD .csv file of interest and locate column G (labeled as QC_Code, see Figure b.). This field ("QC-Code") identifies the different type of samples included in the EDD .csv file (i.e., "MB" = Method Blank, "OPR" = On-going Precision and Recovery, "SA" = Sample).
    a. Three of the worksheets included inThe "tPCB Auto-Calculation " spreadsheet are set-up to receive imported data. These are identified as "Samples & Results", "QC_MB", and "QC_FB_RB". Up to 5 effluent sample results associated with the "SA" identifier in column G of the EDD can be copied into the "Samples & Results" worksheet (scroll right to include additional samples). Field blanks and rinsate blanks, also identified in column G with an "SA", are imported to the "QC_FB_RB" worksheet. These can be separated from the effluent samples by referring to column A (Sample ID) of the EDD .csv spreadsheet. Lastly, results associated with the "MB" identifier in column G will be copied into "QC_MB" worksheet. Specific directions follow.
2) From the "Analytical Results" EDD .csv file, find and select records from a single row in columns A through O from the first targeted sample (QC_code = "SA"). Highlight and copy (see Figure b).

Figure b. "Analytical Results" EDD.csv file



3) Records A-O are pasted into cell B2 of the "Sample & Results" spreadsheet (or "QC_MB" or "QC_FB_RB") using the Paste Special - transpose function. The information fits into cell array B2:B16 (Figure c).

Figure c. "tPCB Auto-Calculation" spreadsheet



	A	B	C	D	E	F	G	H
1		Effluent sample #1				** Censored **		
2	Sample_ID	/A0000000-001-DW-100202011				Compared to largest		
3	Lab_Sample_ID	A3761_9282_PCB_008			Uncensored	blnk (X5) & corrected		
4	Lab_Name	Lab X	Summary		tPCB	tPCB		Extraction, Cleanup
5	Sample_Matrix	Water (whole)			unadj (pg/L)	adj (pg/L)	OPR (ok)	& Injection stds (ok)
6	Percent_Mositure		VA0000000-001-DW-100202011		0	0		
7	Percent_Lipid		Eff 2		0	0		
8	QC_Code	SA	Eff 3		0	0		
9	Sample_Date	10/9/2011	Eff 4		0	0		
10	Sample_Time		[illegible]		0	0		
11	Analysis_Performed	1668C						
12	Extraction_Date	10/29/2011						
13	Analysis_Date	11/3/2011	[illegible]		0			
14	Analysis_Time	0:34	"Field or Rinsate Blank"		0			
15	Sample_Size	2.3						
16	Size_Units	L	(Ctrl) icable if Field or Rinsate Blank collected					
17								
18								
19	Compound	IUPAC_PCB_#	Conc_Founc	Dilution Factor	UNITS	Data_Qualifier	EDL	Minimum_Level
20	2-MoCB	1						
21	3-MoCB	2						
22	4-MoCB	3						
23	2,2'-DiCB	4						
24	2,3-DiCB	5						
25	2,3'-DiCB	6						
26	2,4-DiCB	7						
27	2,4'-DiCB	8						
28	2,5-DiCB	9						
29	2,6-DiCB	10						
30	3,3'-DiCB	11						

4) The next step is to copy the PCB congener data set from the targeted sample in the Analytical Results EDD .csv to the "tPCB Auto-Calculation " spreadsheet.

a. Referring to the example presented in Figure d below, use PCB congener numbers 1-209 in column Y from the "Analytical Results" EDD .csv file as a guide in determining what should be copied from columns AA through AF. Congeners 1-209 are provided for each sample result.

i. ***IMPORTANT:*** For the "tPCB Auto-Calculation " spreadsheet to work properly, all PCB congeners found in column Y must be in numeric rank order (1-209). If one or more PCBs are out of rank order, highlight all rows (i.e., PCB records 1-209) for that sample beginning at column A and extending to the far right to include all fields for that sample. Next, using column Y as a guide, go to the DATA Tab and click on the "Sort" function. Sort in asscending order 1-209.

ii. Occasionly, a single congener from a sample may be errantly located within the labeled PCB surrogates from the same sample. In this situation, insert a blank row in the numerically ordered spot, then cut and paste the out-of-order record in the newly created row.

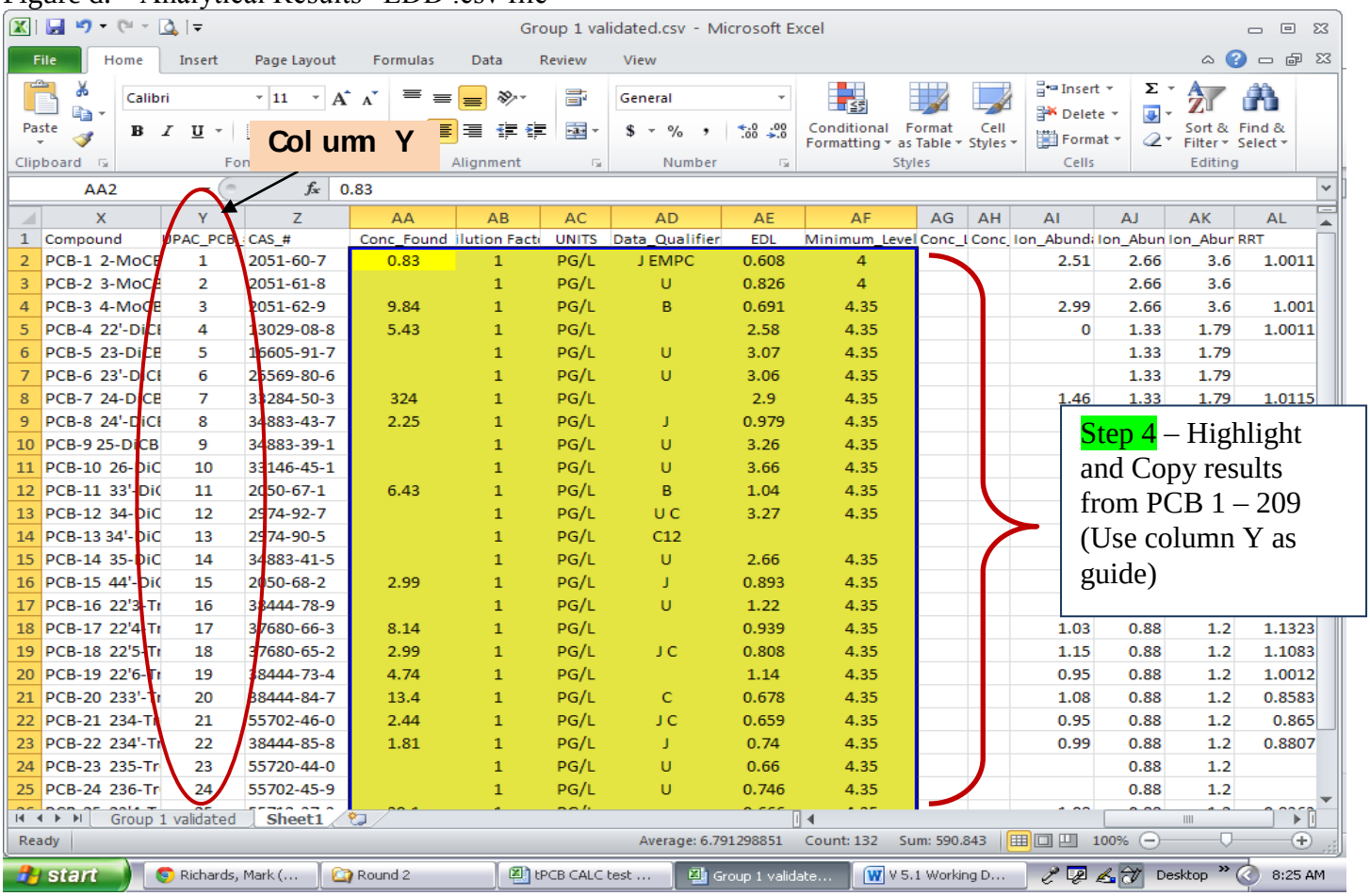
b. Records from columns AA through AF, including 209 rows to capture all PCB congeners from a

specific sample, are highlighted in the "Analytical Results" EDD.csv and copied to the predetermined worksheet file (see Figure d).

c. Columns AA - AF in the "Analytical Results" EDD .csv file are labeled as follows:

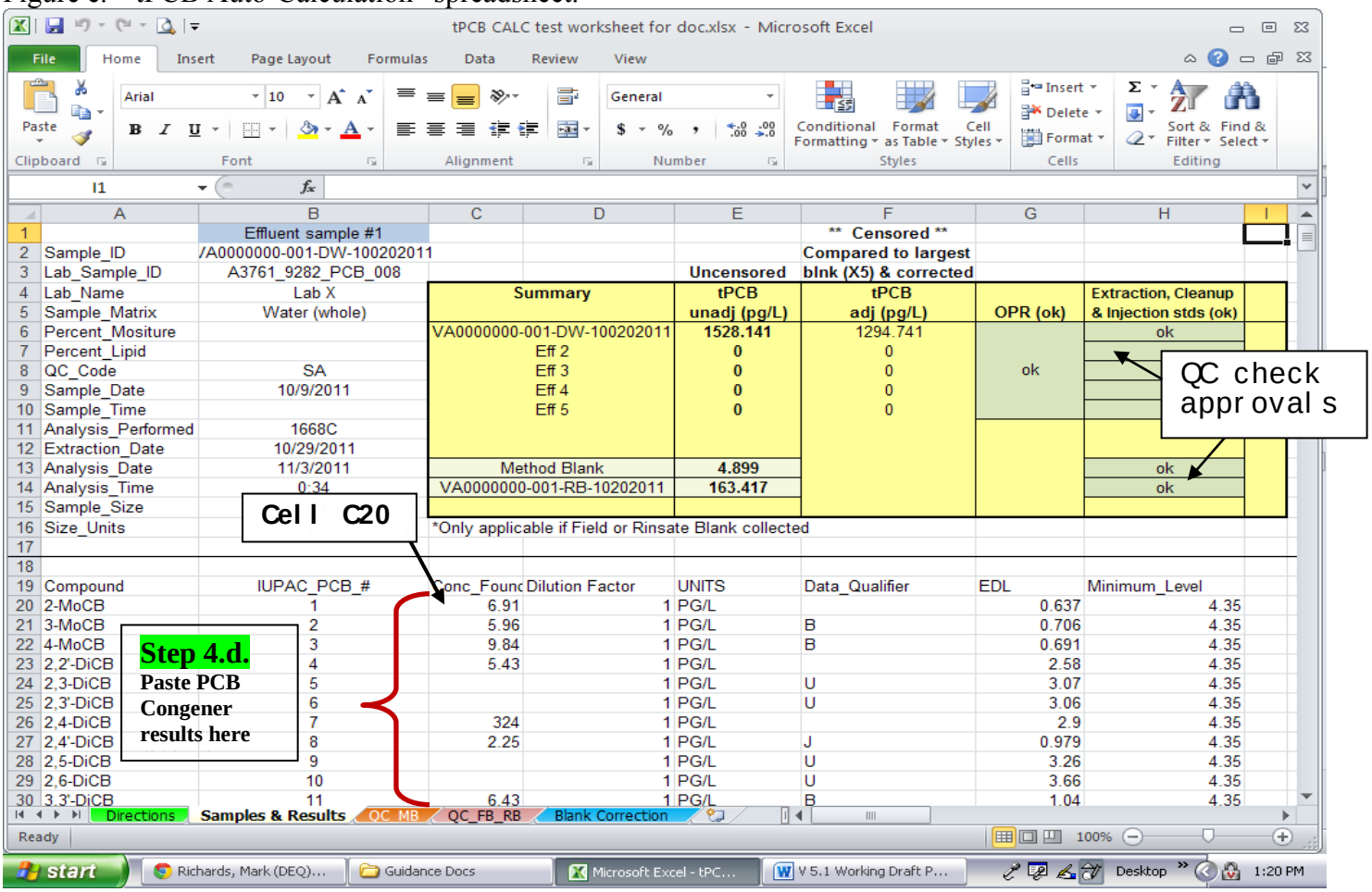
"Analytical Results"EDD .csv file Column Heading	Field Name
AA	*Conc_Found*
AB	*Dilution Factor*
AC	*UNITS*
AD	*Data_Qualifier*
AE	*EDL*
AF	*Minimum_Level*

Figure d. "Analytical Results" EDD .csv file



d. The 209 records are pasted into the applicable worksheet of the "tPCB Auto-Calculation" spreadsheet beginning at cell C20 (see Figure e.). For additional samples, move within the spreadsheet to the right and find cells M20, W20, etc. for data placement.

Figure e. "tPCB Auto-Calculation" spreadsheet.



Note: For simplicity, only the first 11 PCB congeners are presented (altogether there are 209).

5) The next step is to a perform a QC review of the PCB C^{13} labeled congener results including surrogates, extraction, cleanup, and injection standards (this step does not involve copying QC data to the spreadsheet).

a. Following the example provided in Figure f., locate the PCB C^{13} labeled congeners in the "Analytical Results" EDD .csv file immediately below the final PCB congener result from the sample of interest (i.e., use column Y as a guide and look immediately below PCB 209). Note that PCB C^{13} labeled congeners are identified with a "L" (e.g., 104L).

i. In addition to the "Analytical Results" EDD .csv file, it is necessary to locate these results in the "hardcopy" .pdf document also provided as a laboratory deliverable. This serves as a cursory check of the overall results as well as providing information on the PCB C^{13} labeled congeners.

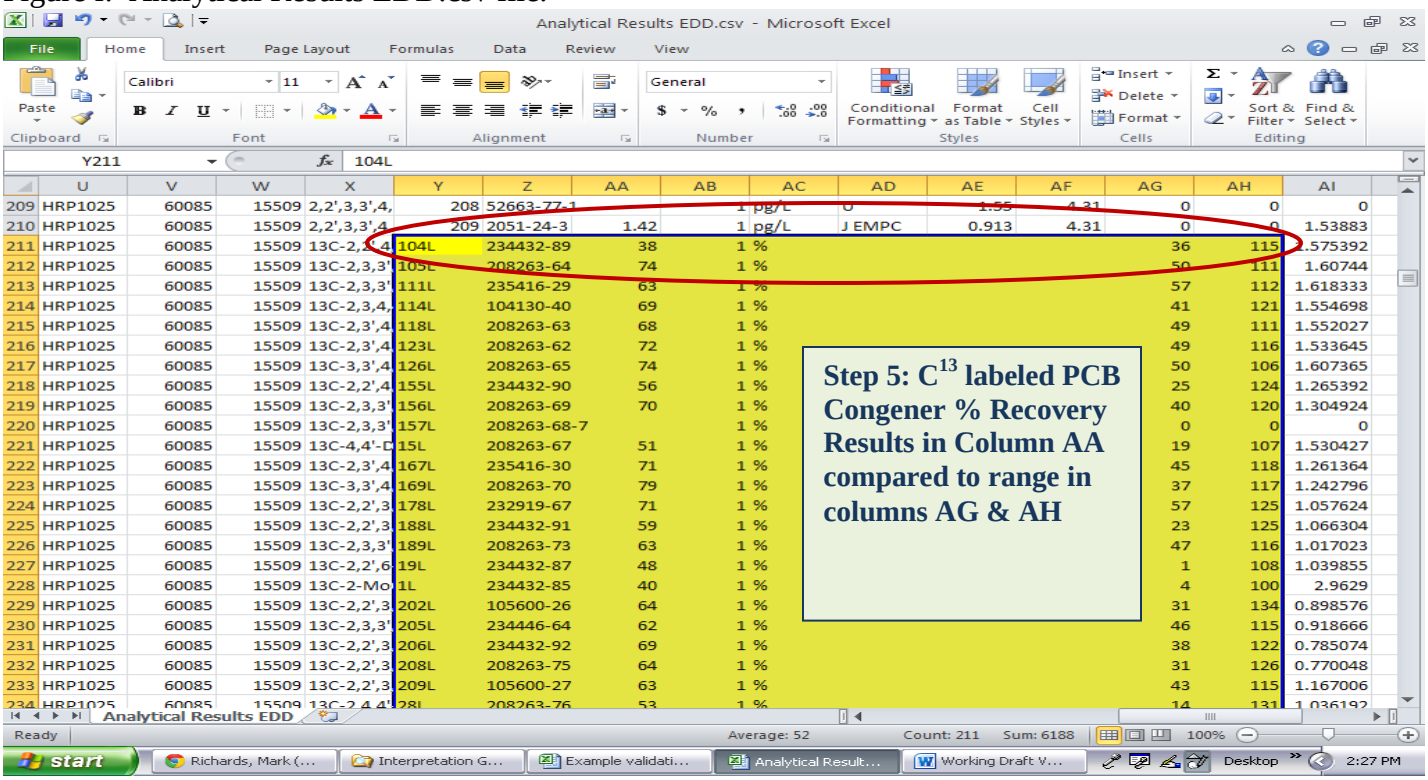
b. Percent recovery results found in column AA are reviewed to ensure the data are within the lab specific range in columns AG and AH. Column AC includes units which are identified as "%".

i. If percent recoveries cannot be found in the EDD .csv file, refer to the "hardcopy" .pdf file.

c. If the PCB C^{13} labeled congener recoveries are in the acceptable range (i.e., columns AG and AH), place "ok" in the specified slot for Surrogates, Clean-up and Extraction Stds found in the "Samples & Results" worksheet tPCB summary table (see Figure e). If the recoveries are out of range, refer to Section III.B.3.c. of the guidance.

d. The OPR and OPR (duplicate) samples are reviewed (not copied) similarly to the labeled surrogates (i.e., percent recovery results in column AA are reviewed to ensure the results are within the lab specific range included in columns AG and AH). If the OPR sample recoveries are in the acceptable range, place "ok" in the "Samples & Results" worksheet tPCB summary table (see Figure e). If the data are out of range, refer to Section III.B.3.b. of the guidance. OPR data are not copied to the spreadsheet.

Figure f. Analytical Results EDD.csv file.

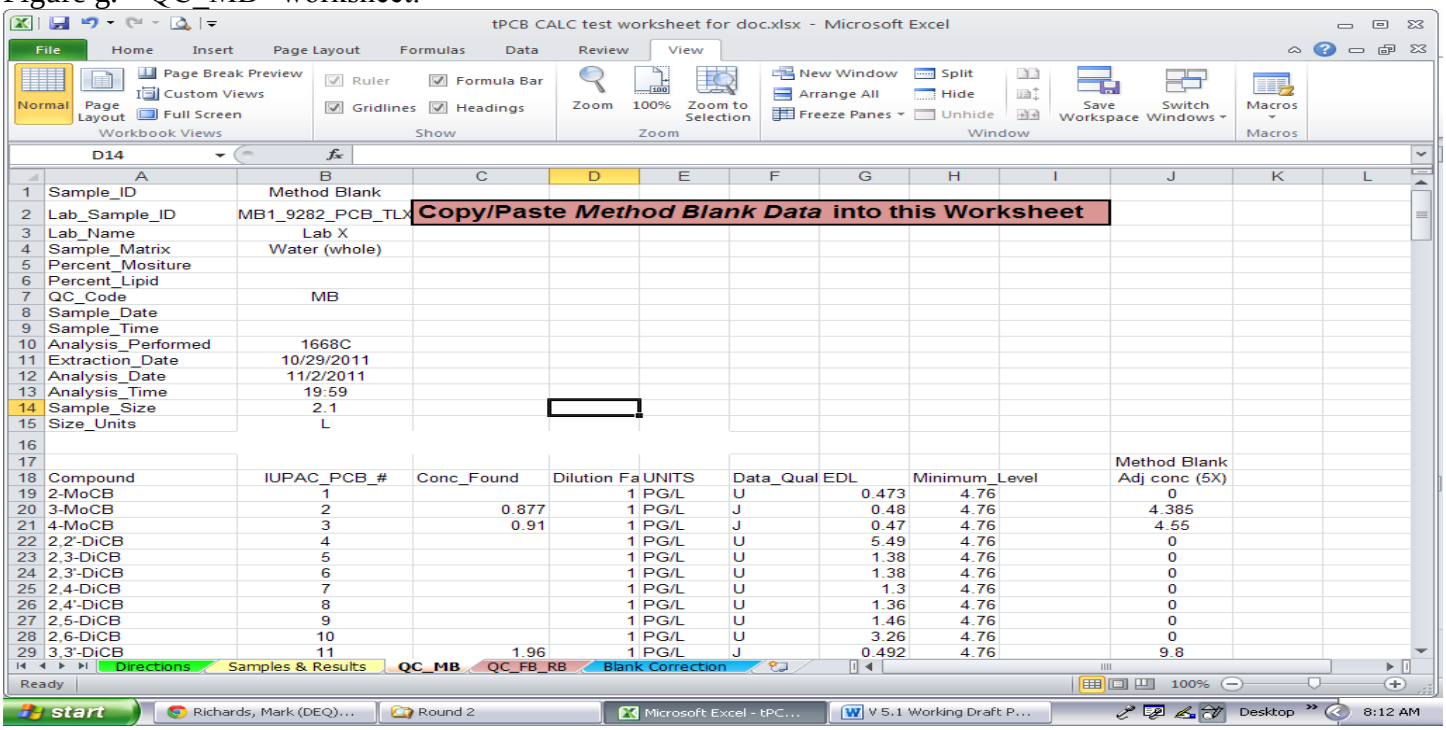


6) Steps 1-5 are followed for all "SA" and "MB" samples types.

a. "MB" data are copied and pasted to the "QC_MB" worksheet (see figure g. below).

b. Similarly, data originating from a field blank or rinsate blank, also notated with an "SA" but differentiated by looking in column A of the Analytical Results EDD.csv file, are copied and pasted into the "QC_FB_RB" worksheet (see figure h. below).

Figure g. "QC_MB" worksheet.

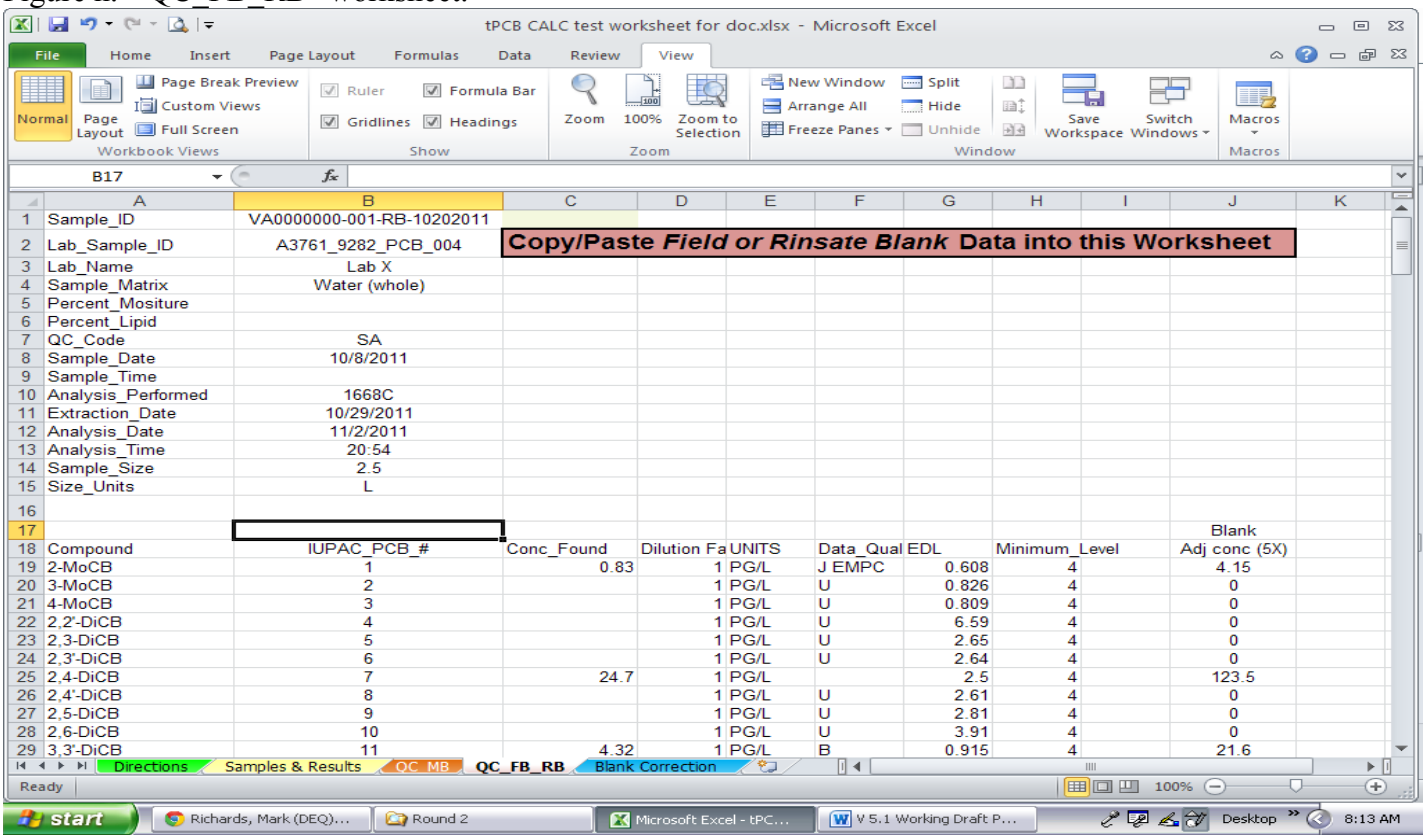


tPCB CALC test worksheet for doc.xlsx - Microsoft Excel

Copy/Paste *Method Blank Data* into this Worksheet

	A	B	C	D	E	F	G	H	I	J
1	Sample_ID	Method Blank								
2	Lab_Sample_ID	MB1_9282_PCB_TLX								
3	Lab_Name	Lab X								
4	Sample_Matrix	Water (whole)								
5	Percent_Mositure									
6	Percent_Lipid									
7	QC_Code	MB								
8	Sample_Date									
9	Sample_Time									
10	Analysis_Performed	1668C								
11	Extraction_Date	10/29/2011								
12	Analysis_Date	11/2/2011								
13	Analysis_Time	19:59								
14	Sample_Size	2.1								
15	Size_Units	L								
16										
17										Method Blank
18	Compound	IUPAC_PCB_#	Conc_Found	Dilution Fa	UNITS	Data_Qual	EDL	Minimum_Level		Adj conc (5X)
19	2-MoCB	1		1	PG/L	U	0.473	4.76		0
20	3-MoCB	2	0.877	1	PG/L	J	0.48	4.76		4.385
21	4-MoCB	3	0.91	1	PG/L	J	0.47	4.76		4.55
22	2,2'-DiCB	4		1	PG/L	U	5.49	4.76		0
23	2,3-DiCB	5		1	PG/L	U	1.38	4.76		0
24	2,3'-DiCB	6		1	PG/L	U	1.38	4.76		0
25	2,4-DiCB	7		1	PG/L	U	1.3	4.76		0
26	2,4'-DiCB	8		1	PG/L	U	1.36	4.76		0
27	2,5-DiCB	9		1	PG/L	U	1.46	4.76		0
28	2,6-DiCB	10		1	PG/L	U	3.26	4.76		0
29	3,3'-DiCB	11	1.96	1	PG/L	J	0.492	4.76		9.8

Figure h. "QC_FB_RB" worksheet.



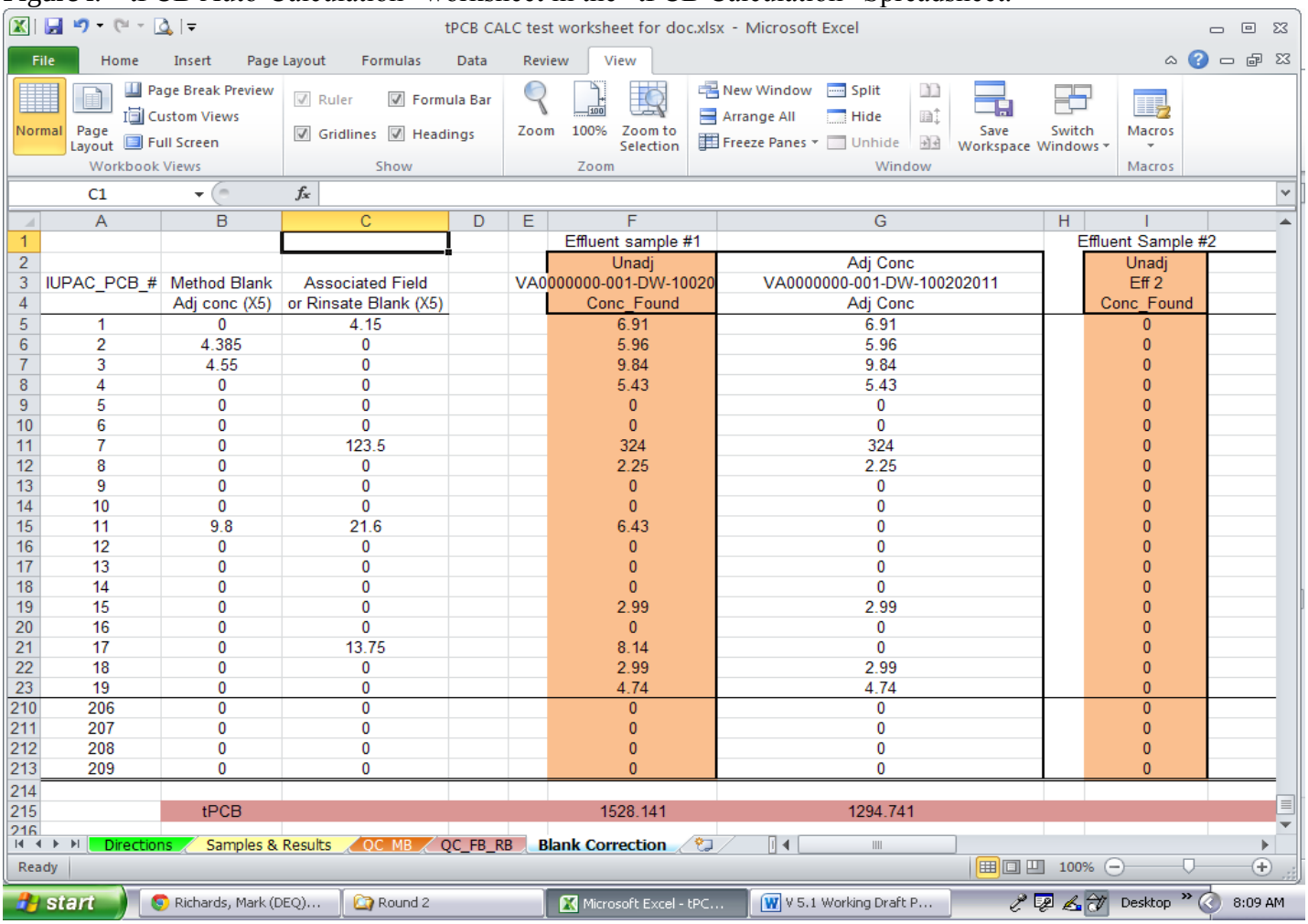
tPCB CALC test worksheet for doc.xlsx - Microsoft Excel

Copy/Paste *Field or Rinsate Blank* Data into this Worksheet

	A	B	C	D	E	F	G	H	I	J
1	Sample_ID	VA0000000-001-RB-10202011								
2	Lab_Sample_ID	A3761_9282_PCB_004								
3	Lab_Name	Lab X								
4	Sample_Matrix	Water (whole)								
5	Percent_Mositure									
6	Percent_Lipid									
7	QC_Code	SA								
8	Sample_Date	10/8/2011								
9	Sample_Time									
10	Analysis_Performed	1668C								
11	Extraction_Date	10/29/2011								
12	Analysis_Date	11/2/2011								
13	Analysis_Time	20:54								
14	Sample_Size	2.5								
15	Size_Units	L								
16										
17										Blank
18	Compound	IUPAC_PCB_#	Conc_Found	Dilution Fa	UNITS	Data_Qual	EDL	Minimum_Level		Adj conc (5X)
19	2-MoCB	1	0.83	1	PG/L	J EMPC	0.608	4		4.15
20	3-MoCB	2		1	PG/L	U	0.826	4		0
21	4-MoCB	3		1	PG/L	U	0.809	4		0
22	2,2'-DiCB	4		1	PG/L	U	6.59	4		0
23	2,3-DiCB	5		1	PG/L	U	2.65	4		0
24	2,3'-DiCB	6		1	PG/L	U	2.64	4		0
25	2,4-DiCB	7	24.7	1	PG/L		2.5	4		123.5
26	2,4'-DiCB	8		1	PG/L	U	2.61	4		0
27	2,5-DiCB	9		1	PG/L	U	2.81	4		0
28	2,6-DiCB	10		1	PG/L	U	3.91	4		0
29	3,3'-DiCB	11	4.32	1	PG/L	B	0.915	4		21.6

7) Figure i. provides an example of the "Blank Correction" worksheet. The sheet is automatically populated with data transferred from the Analytical Results EDD into the "Samples & Results", "QC_MB", and QC_FB_RB" worksheets. Upon entering the PCB results into the aforementioned worksheets the data are autocorrected for laboratory background and/or field contamination. The tPCB results are auto linked to the "Samples & Results" worksheet data summary (see Figure e.).

Figure i. "tPCB Auto-Calculation" worksheet in the "tPCB Calculation" Spreadsheet.



	A	B	C	D	E	F	G	H	I
1						Effluent sample #1			Effluent Sample #2
2						Unadj	Adj Conc		Unadj
3	IUPAC_PCB_#	Method Blank	Associated Field			VA0000000-001-DW-10020	VA0000000-001-DW-100202011		Eff 2
4		Adj conc (X5)	or Rinsate Blank (X5)			Conc_Found	Adj Conc		Conc_Found
5	1	0	4.15			6.91	6.91		0
6	2	4.385	0			5.96	5.96		0
7	3	4.55	0			9.84	9.84		0
8	4	0	0			5.43	5.43		0
9	5	0	0			0	0		0
10	6	0	0			0	0		0
11	7	0	123.5			324	324		0
12	8	0	0			2.25	2.25		0
13	9	0	0			0	0		0
14	10	0	0			0	0		0
15	11	9.8	21.6			6.43	0		0
16	12	0	0			0	0		0
17	13	0	0			0	0		0
18	14	0	0			0	0		0
19	15	0	0			2.99	2.99		0
20	16	0	0			0	0		0
21	17	0	13.75			8.14	0		0
22	18	0	0			2.99	2.99		0
23	19	0	0			4.74	4.74		0
210	206	0	0			0	0		0
211	207	0	0			0	0		0
212	208	0	0			0	0		0
213	209	0	0			0	0		0
214									
215		tPCB				1528.141	1294.741		
216									