General notes:

Macros need to be enabled for the template to work as intended.
The general concept is that areas with blue or green coloration will require your data entry; everything else is calculated from your data entry or pulled from a table somewhere else.

Do not forget that IOMs need to be analyzed before and after each sequence, meaning you will need to provide current IOM sheets (provided during Phase One) for every batch of samples you run as well as *each batch of calibrations you perform*.

The following is a tab-by-tab guide with examples of each table.

Compounds Enter purity, manufacturer name and lot # for each of the compounds to be used for the test

Compound	CAS #	Density	Purity	MFG	Lot #
IPA	67-63-0	0.79	1.000	Aldrich	Example Lot
Triethylamine	121-44-8	0.73	1.000	Aldrich	Example Lot
Heptane	142-82-5	0.68	1.000	Aldrich	Example Lot
Toluene	108-88-3	0.87	1.000	Aldrich	Example Lot
EGDE	629-14-1	0.84	0.994	Aldrich	Example Lot
2-Butanone Oxime	96-29-7	0.90	1.000	Aldrich	Example Lot
Propylene Glycol	57-55-6	1.04	1.000	Aldrich	Example Lot
p-Xylene	106-42-3	0.86	1.000	Aldrich	Example Lot
Nonane	111-84-2	0.72	1.000	Aldrich	Example Lot
2-Heptanone	110-43-0	0.82	1.000	Aldrich	Example Lot
Mesitylene	108-67-8	0.86	1.000	Aldrich	Example Lot
Decane	124-18-5	0.74	1.000	Aldrich	Example Lot
Dipropylene Glycol Methyl Ether	34590-94-8	0.96	1.000	Aldrich	Example Lot
Undecane	1120-21-4	0.74	1.000	Aldrich	Example Lot
Dipropylene Glycol	106-62-7	1.03	1.000	Aldrich	Example Lot
NMP	872-50-4	1.03	1.000	Aldrich	Example Lot
Dodecane	112-40-3	0.75	1.000	Aldrich	Example Lot
Triglyme	112-49-2	0.99	1.000	Aldrich	Example Lot
Dipropylene Glycol Butyl Ether	29911-28-2	0.91	0.985	Aldrich	Example Lot
Texanol	25265-77-4	0.95	1.000	Aldrich	Example Lot
Tetraethylene Glycol	112-60-7	1.13	1.000	Aldrich	Example Lot
TXIB	6846-50-0	0.94	1.000	Aldrich	Example Lot
DIIBA	141-04-8	0.95	1.000	Aldrich	Example Lot
Benzophenone	119-61-9	1.00	1.000	Aldrich	Example Lot
Pentaethylene Glycol	4792-15-8	1.13	1.000	Aldrich	Example Lot
BFB	460-00-4	1.59	1.000	Aldrich	Example Lot
THF	109-99-9	0.89	0.990	Aldrich	Example Lot
Methanol	67-56-1	0.79	1.000	Aldrich	Example Lot

CalInfo Enter calibration levels in top table

- 15,10,1,0.1 for IPA/DIIBA/Heptane/Triglyme
- 0.5, 0.2 for Tetraethylene glycol and pentaethylene glycol
- 15, 0.1 for all other compounds

Standards below 1 g/L will require a stepdown “Dilution Standard”. 5 g/L is recommended since other concentrations have not been tested in the template.

The solvent and the internal standard must be specified in the “Compound Information” table. **Select the compound you want to calibrate FROM THE PICK LIST**. *If you don’t use the picklist then all of the downstream logic may be broken.*

Calibration Standards		
Cal Levels (g/L)	Volume (mL)	Made with Dilution?
15	25	
5	25	
0.1	25	Yes

Dilution Standard	
Standard Level (g/L)	Volume (mL)
5	25

Compound Information		
CMPD Assignment	Compound	CAS
Solvent	THF	109-99-9
Internal Standard	EGDE	629-14-1
	Dipropylene Glycol Butyl Ether	29911-28-2

This example is using irrelevant cal levels, but it’s the only example I had handy.

Cal Prep

The amount of the compound is calculated for you based upon your inputs on the CalInfo table. The concentration of each compound is calculated based upon the mass of each compound that you will measured during addition. Be aware that standards below 1 g/L will default to using the dilution standard during prep inseatd of individual injections of compounds.

	Dilution Preparation		
	Amount	Mass (g)	g/L
25 mL Vol Flask	-	50.9771	-
THF	~10 mL	63.3527	-
Dipropylene Glycol Butyl Ether	140 uL	63.4786	4.96
QS to Volume	To 25 mL	73.0088	-

	15 g/L Preparation			5 g/L Preparation			0.1 g/L Preparation		
	Amount	Mass (g)	g/L	Amount	Mass (g)	g/L	Amount	Mass (g)	g/L
25 mL Vol Flask	-	47.3523	-	-	46.7484	-	-	50.3619	-
THF	~10 mL	59.5697	-	~10 mL	62.8516	-	~10 mL	61.9579	-
EGDE	150 uL	59.6989	5.137	150 uL	62.9808	5.137	150 uL	62.0866	5.117
Dilution Prep	-	59.6989	-	-	62.9808	-	500 uL	62.5482	-
Dipropylene Glycol Butyl Ether	335 uL	60.0923	15.500	110 uL	63.1079	5.008	-	62.5482	0.104
QS to Volume	To 25 mL	69.2868	-	To 25 mL	68.8236	-	To 25 mL	72.4010	-

Cal Data

Provide the raw file name for each cal file at the top of the page

Paste in Retention times and area counts for each peak in the chromatogram for the specified cal levels in black. Assign the appropriate peak names for each peak in the third column. Do this for each calibrated level. Compounds with multiple peaks will be summed together during the cal curve generation.

STD Level	15		STD Level	15		STD Level	5		STD Level	5		STD Level	0.1		STD Level	0.1	
Filename	16MFD0301C1404.D		Filename	16MFD0301C1406.D		Filename	16MFD0301C1408.D		Filename	16MFD0301C1410.D		Filename	16MFD0301C1412.D		Filename	16MFD0301C1414.D	
Retention Time	Area Counts	Assignment	Retention Time	Area Counts	Assignment	Retention Time	Area Counts	Assignment	Retention Time	Area Counts	Assignment	Retention Time	Area Counts	Assignment	Retention Time	Area Counts	Assignment
1.242	178819		1.244	156206		1.388	222265		1.389	213712		1.388	213872		1.389	211425	
1.389	299383		1.389	291058		2.619	962483		2.62	938667		4.289	654682		4.291	650296	
1.818	220984		1.816	214624		4.285	654919		4.287	656339		4.553	601486		4.554	609437	
2.619	2796656		2.614	2770046		4.551	648427		4.549	606804		6.147	89195246538	THF	6.148	89363149382	THF
3.036	211978		3.031	220634		6.144	91394602620	THF	6.142	88729867408	THF	7.175	2888159		7.176	2873000	
3.473	279904		3.466	280811		7.169	2953901		7.171	2844289		8.191	917490		8.192	920734	
4.294	715846		4.288	714849		8.183	1000502		8.186	966252		8.463	598367		8.464	605602	
4.562	643585		4.554	625177		8.456	624922		8.458	602201		9.409	451858		9.41	452000	
6.156	92308814677	THF	6.147	91265470919	THF	9.401	456281		9.404	446786		9.632	3149089		9.633	3153747	
7.18	2941410		7.172	2920128		9.624	3180081		9.627	3071701		12.256	403296664	EGDE	12.257	403999039	EGDE
7.468	478157		7.463	473481		12.249	413831592	EGDE	12.251	400021976	EGDE	13.653	304497		13.654	333174	
8.193	1123622		8.185	1124518		13.645	457630		13.649	345578		17.237	189870		17.237	225979	
8.467	623147		8.459	619468		13.757	242816		16.825	548494		17.609	208664		17.61	408437	
9.412	451919		9.404	449468		16.823	553723		17.239	467844		19.784	239892		19.785	242727	
9.636	3182889		9.627	3181038		17.238	523174		17.61	192598		20.777	8515173		20.778	8528804	
12.259	421015159	EGDE	12.252	418553848	EGDE	17.608	223523		19.388	606187		21.252	401436		21.252	404044	
13.655	387687		13.647	357895		19.388	623934		19.796	348138		22.136	4322340	Dipropylene Gl	22.136	4326270	Dipropylene Glycol
13.765	243701		16.824	1705590		19.795	327671		20.547	644595		22.206	5278690	Dipropylene Gl	22.207	5282225	Dipropylene Glycol
16.828	1727686		17.274	892477		20.546	654605		20.796	401758218		25.743	40534047		25.743	40572786	
17.279	869380		19.282	407138		20.795	411631841		21.069	1169889							
19.285	377585		19.448	1883241		21.068	1189772		21.251	17231634							
19.452	1900323		19.835	378597		21.249	1759158		21.484	1687197							
19.839	394051		20.592	2132813		21.483	1747417		21.83	2902809							
20.596	2160379		20.826	1215030187	1-Ethyl-Pyrrolid	21.836	3042371		22.145	205863594	Dipropylene Glycol Butyl Ether						
20.829	1233140343		21.071	3856821		22.143	210795218	Dipropylene Gl	22.217	243345851	Dipropylene Glycol Butyl Ether						
21.074	3920356		21.255	51298569		22.216	249259583	Dipropylene Gl	22.543	7077181							
21.258	52040036		21.409	1077771		22.542	7222148		24.087	3522273							
21.412	1148232		21.485	3101729		24.085	3448770		24.579	309341							
21.488	3131204		21.829	6813629		24.579	290625		25.742	38936197							
21.828	7006658		22.161	637797005	Dipropylene Gl	25.741	39806911										
22.164	648554187	Dipropylene Gl	22.239	736705090	Dipropylene Glycol Butyl Ether												
22.242	746878264	Dipropylene Gl	22.545	23119841													
22.548	23555565		22.807	1150671													
22.809	1255007		23.343	386204													
23.346	421180		24.091	10776966													
24.093	11725171		24.355	1457894													
24.357	1896723		24.587	1269423													
24.589	1313804		24.747	506896													
24.748	520527		25.568	804624													
25.57	630856		25.742	37100511													
25.743	37620567		28.449	254848													
28.45	230310		28.744	214576													
28.746	216024																

CalSummary Nothing needs to be done on this page; it simply summarizes the RRF and the % recoveries for each level. Nominal RRF values were provided via email in the past as a point of comparison for your determinations. Calibrations will need to be repeated for compounds with divergent RRFs and/or poor recoveries (> 15% difference or 0.02 g/L absolute, whichever is larger)

	Dipropylene Glycol Butyl Ether		Internal Standard				
STD Level	Prep g/L	Area Counts	Prep g/L	Area Counts	% Recovery	ABS. Diff	RRF/RF 1.0984
15	15.5000	1395432451	5.1370	421015159	100.0	0.00	R2/RSD 0.9998
15	15.5000	1374502095	5.1370	418553848	99.1	0.14	Levels 15/15/5/5/0.1/0.1
5	5.0077	460054801	5.1370	413831592	103.8	0.19	% R 100.0/99.1/103.8/104.9/106.7/106.6
5	5.0077	449209445	5.1370	400021976	104.9	0.24	ABS D 0.00/0.14/0.19/0.24/0.01/0.01
0.1	0.1039	9601030	5.1171	403296664	106.7	0.01	
0.1	0.1039	9608495	5.1171	403999039	106.6	0.01	

	EGDE		Internal Standard				
STD Level	Prep g/L	Area Counts	Prep g/L	Area Counts	% Recovery	ABS. Diff	RRF/RF 79939670
15	5.1370	421015159	5.1370	421015159	102.5	0.13	R2/RSD 2.2
15	5.1370	418553848	5.1370	418553848	101.9	0.10	Levels 15/15/5/5/0.1/0.1
5	5.1370	413831592	5.1370	413831592	100.8	0.04	% R 102.5/101.9/100.8/97.4/98.6/98.8
5	5.1370	400021976	5.1370	400021976	97.4	0.13	ABS D 0.13/0.10/0.04/0.13/0.07/0.06
0.1	5.1171	403296664	5.1171	403296664	98.6	0.07	
0.1	5.1171	403999039	5.1171	403999039	98.8	0.06	

CalExport If the calibrations are considered acceptable, they should be stored with this tab by pressing the “Save Calibrations Button”. If “Set Internal Standard RF” is set to “Yes” then the IS cal factor will be collected as well. Do this during the first calibration and then do not do it again. The internal standard cal factor and all RRFS are stored in the RRF tab at the end of the workbook.

Calibration Summary

Set Internal Standard RF?	Yes	Save Calibrations				
Compound	CAS #	CAS #	RF/RRF	R2/RSD	MFG	Lot #
Dipropylene Glycol Butyl Ether	29911282	29911-28-2	1.0984	0.9998	Aldrich	Example Lot
EGDE	629141	629-14-1	79939670	2.2	Aldrich	Example Lot

Note: Pressing “Save Calibrations” will also store a copy of the current CalSummary page as a hidden page in the workbook.

CSV Prep

This page is where all the prep data for the CSVs is stored. Only 2 CSVs need to be prepared if Samples 1-3 are analyzed in the same batch. If each sample is prepared and analyzed on different days then all 4 CSV prep slots will require completion.

Indicate the prep date, and volumetric flask size.

The table will indicate how the standard should be prepared. Enter in the measured mass of each component in the standard and the concentration of each component will be calculated.

Once masses have been added to the prep table, click “Create Table” to build a new tab in the workbook where the retention times and area counts can be entered.

CSV Prep	CSV 1		Create Table
Prep Date:	10/22/16		
Flask Volume (mL):	25		
	To Add	**Mass (g)**	**g/L**
25 mL Flask	-	47.3960	-
THF	10 mL	60.5280	520.03
EGDE	150 uL	60.6561	5.09
Triglyme	26 uL	60.6815	1.00
IPA	31 uL	60.7052	0.95
DIIBA	26 uL	60.7299	0.98
Heptane	36 uL	60.7537	0.94
QS w/ THF to 25 mL	To 25 mL	69.3103	-

Note: Clicking “Create Table” after data has been entered will clear all data entered for that standard in the new (CSV X Data) tab.

CSV X Data Similar to the Cal Data sheet—add the filenames, retention times, area counts, and then assign each of the CSV constituents. A and B injections should be injected prior to sample injections, with C and D injections afterwards.

ID:	CSV 1 A	
Filename	16MFD0301C1408.D	
RT (min)	Area Counts	Compound ID
1.39	196408	
3.23	10183770	IPA
3.46	74347261	IPA
4.29	650067	
4.55	602077	
6.15	88700003936	
6.90	874538	
7.18	3495127	
7.55	160457650	Heptane
8.19	913985	
8.47	734666	
8.55	921884	
9.41	452699	
9.63	3175341	
12.26	401997314	EGDE
13.65	301560	
17.24	193034	
17.61	217341	
19.78	239623	
21.94	60635382	Triglyme
22.18	275483	
24.60	507061	
25.74	39621846	
26.46	563712	
28.00	106453301	DIIBA
28.58	338914	

ID:	CSV 1 B	
Filename	16MFD0301C1410.D	
RT (min)	Area Counts	Compound ID
1.39	207262	
3.23	9807102	IPA
3.45	73522073	IPA
4.29	635817	
4.55	598595	
6.14	87398115602	
6.90	859515	
7.17	3320400	
7.54	158154359	Heptane
8.19	904019	
8.47	714568	
8.55	923512	
9.41	446834	
9.63	3139518	
12.26	398037726	EGDE
13.65	290919	
17.24	221861	
17.61	395330	
19.78	232420	
21.94	60253882	Triglyme
22.18	270951	
24.60	531681	
25.74	39384158	
26.46	556646	
28.00	105831006	DIIBA
28.58	339188	

ID:	CSV 1 C	
Filename	16MFD0301C1428.D	
RT (min)	Area Counts	Compound ID
1.40	176202	
3.23	10182811	IPA
3.46	73397521	IPA
4.29	588996	
4.55	605239	
6.15	87881230646	
6.90	872110	
7.18	3349553	
7.55	158174567	Heptane
8.20	935578	
8.47	712962	
8.55	915626	
9.41	450821	
9.64	3091251	
12.26	385312095	EGDE
15.93	284733	
17.62	333136	
21.46	464570	
21.94	54658919	Triglyme
22.18	259233	
24.60	457617	
24.68	409780	
25.75	36036066	
25.99	298994	
26.46	415999	
27.37	1901931	
27.66	5542563	
28.01	96508267	DIIBA
28.58	293690	
33.02	299828	
33.16	2091023	

ID:	CSV 1 D	
Filename	16MFD0301C1430.D	
RT (min)	Area Counts	Compound ID
3.23	10133252	IPA
3.46	73312314	IPA
4.29	598969	
4.55	607272	
6.15	87803348784	
6.90	870284	
7.18	3344011	
7.55	157938772	Heptane
8.20	927944	
8.47	705643	
8.55	923541	
9.42	445425	
9.64	3072739	
12.26	383837225	EGDE
15.93	292582	
17.62	330585	
21.46	454131	
21.94	54230111	Triglyme
22.18	247858	
24.60	453957	
24.68	356809	
25.75	35668321	
25.99	233112	
26.46	410654	
27.37	1549366	
27.66	4734777	
28.01	95757579	DIIBA
28.58	297839	
33.02	300121	
33.16	1651604	

As with everywhere else in this template, peaks with the same ID get summed as with IPA here.

CSV Summary This tab summarizes the results for the CSV injections and requires no action from the user if all QC passes.

CSV 1								
			A + B			C + D		
Compound	Prep g/L	RRF	Avg. AC	g/L	% Recovery	Avg. AC	g/L	% Recovery
EGDE	5.09	6.17E+7	400017520	6.48	127.3	384574660	6.23	122.4
IPA	0.95	1.058626	83930103	1.01	106.5	83512949	1.04	110.2
Heptane	0.94	2.050724	159306004.5	0.99	104.9	158056670	1.02	108.3
Triglyme	1.00	0.757913	60444632	1.02	101.3	54444515	0.95	94.9
DIIBA	0.98	1.400111	106142153.5	0.97	98.5	96132923	0.91	92.8

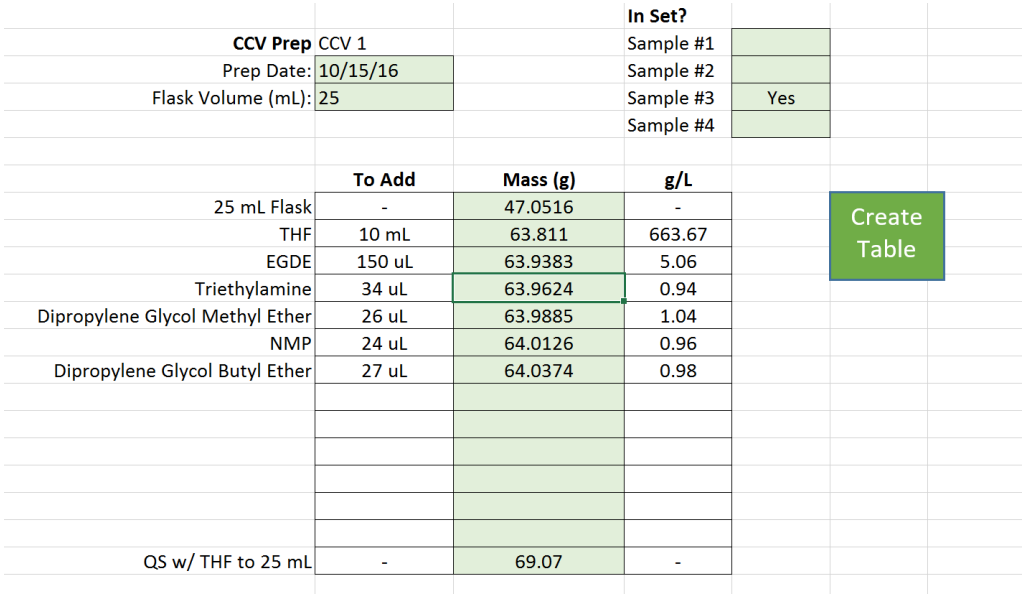
CCV Prep This page is where all the prep data for the CCVs is stored. Only 2 CCVs need to be prepared if Samples 1-3 are analyzed in the same batch. If each sample is prepared and analyzed on different days then all 4 CCV prep slots will require completion.

Indicate the prep date, and volumetric flask size.

The “In Set?” table allows you to create the appropriate standard easily—if you select that you are running Sample #1 and Sample #2 in the same sequence you’ll be given the prep instructions with the 6 compounds that are required. Samples 1-3 can be analyzed in the same sequence, but Sample #4 must be analyzed on its own. To reinforce this concept, Sample #4 fills the entire CCV table.

The table will indicate how the standard should be prepared. Enter in the mass of each component of the standard and the concentration of each component will be calculated.

Once masses have been added to the prep table, click “Create Table” to build a new tab in the workbook where the retention times and area counts can be entered.



				In Set?	
CCV Prep	CCV 1			Sample #1	
Prep Date:	10/15/16			Sample #2	
Flask Volume (mL):	25			Sample #3	Yes
				Sample #4	
	To Add	**Mass (g)**	**g/L**		
25 mL Flask	-	47.0516	-		
THF	10 mL	63.811	663.67		
EGDE	150 uL	63.9383	5.06		
Triethylamine	34 uL	63.9624	0.94		
Dipropylene Glycol Methyl Ether	26 uL	63.9885	1.04		
NMP	24 uL	64.0126	0.96		
Dipropylene Glycol Butyl Ether	27 uL	64.0374	0.98		
QS w/ THF to 25 mL	-	69.07	-		

I didn’t have an example of this specific prep, so the CCV examples are going to be simulated with only the “Sample #3” selection.

Note: Clicking “Create Table” after data has been entered will clear all data entered for that standard on the new (CCV X Data) sheet.

CCV X Data

Similar to the Cal Data sheet—add the filenames, retention times, area counts, and then assign each of the constituents of the CSV. A and B injections should be injected prior to sample injections, with C and D injections afterwards.

ID:	CCV 1 A			ID:	CCV 1 B			ID:	CCV 1 C			ID:	CCV 1 D	
Filename	16MFD0301C1412.D			Filename	16MFD0301C1414.D			Filename	16MFD0301C1424.D			Filename	16MFD0301C1426.D	
RT (min)	Area Counts	Compound ID		RT (min)	Area Counts	Compound ID		RT (min)	Area Counts	Compound ID		RT (min)	Area Counts	Compound ID
1.39	200161			1.38	196146			4.29	600409			4.29	581979	
4.29	688141			4.29	669884			4.55	693176			4.55	679993	
4.55	624395			4.54	604734			6.14	87589277473			6.14	87088466868	
6.14	87702769921			6.14	86053724834			7.20	123270190	Triethylamine		7.20	123105320	Triethylamine
7.20	126304050	Triethylamine		7.20	124066697	Triethylamine		8.04	58446166			8.04	58169136	
8.04	60263783			8.03	59243591			8.19	1317781			8.19	1303658	
8.19	1306699			8.19	1292252			8.46	601085			8.47	592542	
8.46	604650			8.46	590515			9.41	475296			9.41	495958	
9.41	507984			9.41	493120			9.63	3145873			9.63	3133353	
9.63	3234172			9.63	3167034			12.26	380701421	EGDE		12.26	379377696	EGDE
12.25	396286557	EGDE		12.25	389856837	EGDE		15.93	348237			15.93	330319	
16.19	91323318			16.19	89863572			16.19	84874782			16.19	84083304	
17.24	203939			17.61	270524			17.61	369854			17.61	383355	
17.61	311491			18.24	179012			18.24	191478			18.24	185024	
18.24	258474			19.78	238099			21.04	293835			21.56	76829822	
19.78	276288			21.56	83312429			21.56	77488012			22.85	150347	
21.56	84598341			22.85	163593			22.85	156976			23.62	1829488	
22.85	164824			23.62	2002031			23.62	1839093			24.24	44613232	
23.62	2033048			24.24	49113840			24.24	44953475			24.46	55822114	
24.24	49928356			24.46	60929096			24.46	56096173			24.62	572173	
24.46	61926666			24.61	467904			24.68	1879814			24.68	1027352	
24.61	478047			25.74	39042423			24.94	548469			24.94	386138	
25.74	39686204			26.91	677738			25.52	807809			25.52	212643	
26.91	689531							25.74	37106843			25.74	36050593	
								25.99	977502			25.99	374808	
								26.91	698664			26.91	596033	
								27.36	4894546			27.36	2796773	
								27.66	12750097			27.66	8438907	
								32.55	1682955			32.78	1648409	
								32.69	680709			33.02	478322	
								32.80	861046			33.16	4912672	
								33.16	17886755					

This example is just the Triethylamine assignment. You would also add the other 3 compounds onto this page as well if you were performing this part for the study.

CSV Summary This tab summarizes the results for all of the CCV injections and requires no action from the user if all QC passes.

CCV 1								
			A + B			C + D		
Compound	Prep g/L	RRF	Avg. AC	g/L	% Recovery	Avg. AC	g/L	% Recovery
EGDE	5.06	6.17E+7	393071697	6.37	125.9	380039559	6.16	121.7
Triethylamine	0.94	1.556217	125185374	1.04	109.6	123187755	1.05	111.6

Again, this example includes only Triethylamine.

Sample #X This is where the heavy lifting will be performed. Enter the Sample Information for each sample, which will be provided to you on or before 10/28.

Sample Information	
Density (g/mL)	1.3492
Wt% Water	53.5
Wt % Non-Volatiles	45.0
Wt % pCBTF	0.0
Wt % D4	0.0
Wt % D5	0.0

The Sample Spiking table will instruct on preparation depending on your sample starting mass. It's intended that you use 30 g. Alternate values may work, but were not tested in this template. Add your masses to the table to enable g/L calculations downstream.

Sample Spiking

Target Mass (g)	30		
	To Add	**Mass**	**Wt fx**
Vial	-	24.9002	-
Sample #1	30 g	62.0149	0.974
Triglyme	250 uL	62.2649	0.006
IPA	310 uL	62.5234	0.007
DIIBA	250 uL	62.7652	0.006
Heptane	350 uL	63.0114	0.006

The Sample Dilution volume must be entered, after which the table will instruct on how to prep the samples. Add your sample dilution values to the table. Make sure to specify the retention time for methyl palmitate in the bottom-left most portion of the tab.

Sample Dilution

Flask Volume (mL)	25		
	To Add	**Mass**	**g/L**
25 mL Flask	-	49.2075	-
THF	~ 10 mL	61.3285	479.992
EGDE	150 uL	61.4564	5.085
Spiked Sample #1	~ 2.5 g	64.1444	104.709
QS to 25 mL	To 25 mL	72.1859	-
Triglyme			0.70
IPA			0.73
DIIBA			0.68
Heptane			0.69
Methyl Palmitate RT (Min)		32.8	

The next two tables are provided to help decide which peaks in the samples originate from the solvent or spike contaminants. Paste your retention times and area counts into the Pre-Sample Blank table—this blank should be injected immediately prior to the sample in question. The g/L concentration is estimated with an assumed 5 g/L internal

standard with the assumption that the second largest peak is the internal standard peak. If this assumption does not hold, the g/L value should be ignored.

The CSV table allows you to select the CSV from the blue header of the table, which means that you don't need to paste in those values yourself. You can also type in the name of the CSV injection, but it should always be the second, or "B", injection of the CSV that's used in that sample's batch. If you see errors on the CSV table, it's probably because you're pulling from a CSV with no data in it. Switch to the appropriate CSV and it should resolve the issue.

From the Blank and CSV tables, you will determine which peaks in the sample are directly attributable to the solvent and spike contaminants. You will assign those peaks as "solvent" on the Sample tables.

Pre-Sample #1 Blank		
RT (min)	Area Counts	**~ Measured g/L***
1.39	357945	0.01
4.29	730587	0.01
4.55	612694	0.01
6.15	89004224244	1436.08
7.18	2872348	0.05
8.19	919351	0.01
8.46	597098	0.01
9.41	448730	0.01
9.63	3191981	0.05
12.26	408866826	6.60
13.65	627846	0.01
13.76	255410	0.00
17.23	774509	0.01
17.61	395289	0.01
19.78	312640	0.01
25.74	40661936	0.66

CSV 1 B		
RT (min)	Area Counts	**~Measured g/L***
1.39	207262	0.00
3.23	9807102	0.17
3.45	73522073	1.24
4.29	635817	0.01
4.55	598595	0.01
6.14	87398115602	1475.55
6.90	859515	0.01
7.17	3320400	0.06
7.54	158154359	2.67
8.19	904019	0.02
8.47	714568	0.01
8.55	923512	0.02
9.41	446834	0.01
9.63	3139518	0.05
12.26	398037726	6.72
13.65	290919	0.00
17.24	221861	0.00
17.61	395330	0.01
19.78	232420	0.00
21.94	60253882	1.02
22.18	270951	0.00
24.60	531681	0.01
25.74	39384158	0.66
26.46	556646	0.01
28.00	105831006	1.79
28.58	339188	0.01

Paste in each sample's retention times and area counts in the appropriate Sample tables, then assign the ID for each of the 4 surrogate spikes and the internal standard.

Next, assign the IDs for any calibrated compounds you see in the sample. This will automatically calculate the concentration of that peak using a stored RRF. Work through each peak and determine if it originates from the blank and/or the CSV and assign it the "solvent" classification if it does. Make sure that any peaks which elute at or after the

methyl palmitate retention time receive a designation of “After MeP” so they aren’t tallied in the final VOC count.

All unassigned peaks should be left blank in the assignment column and will automatically calculate using the Triglyme RRF. The user should **not** assign Triglyme as an ID for anything but the Triglyme spike as any peaks assigned as Triglyme will count for the Triglyme recovery and not for the total VOC.

The Sample g/L column will factor in the dilution of the sample, whereas the Measured g/L does not. Any cells colored blue in the “Qual ID” column require an ID from the Mass Spectrometer since they exceed 1 g/L and are not already accounted for by the calibrated compounds, spikes, or solvent assignments. *Please don’t forget to do this, especially for sample #4!*

Sample #1 A						
RT (min)	**Area Counts**	**Assignment**	**RF/RRF**	**Measured g/L**	**Sample g/L**	**Qual ID (CAS #)**
2.73	491432		0.758	0.01	0.11	
3.23	2816393	IPA	1.059	0.03		
3.44	56630679	IPA	1.059	0.68		
4.29	589357	Solvent	0.000	0.00	0.00	
4.53	520986	Solvent	0.000	0.00	0.00	
6.11	80179987024	Solvent	0.000	0.00	0.00	
6.90	1021406		0.758	0.02	0.22	
7.18	3557944	Solvent	0.000	0.00	0.00	
7.54	112489318	Heptane	2.051	0.69		
8.19	1129229	Solvent	0.000	0.00	0.00	
8.47	1459080	Solvent	0.000	0.00	0.00	
9.41	423912	Solvent	0.000	0.00	0.00	
9.64	3192364	Solvent	0.000	0.00	0.00	
12.26	401828462	EGDE	6.17E+7	6.51		
12.66	1376411		0.758	0.02	0.30	
16.71	354909		0.758	0.01	0.08	
17.65	742712	Solvent	0.000	0.00	0.00	
18.58	496652		0.758	0.01	0.11	
18.77	2143209		0.758	0.04	0.46	
19.23	698023		0.758	0.01	0.15	
20.43	907125		0.758	0.02	0.20	
20.89	1543441		0.758	0.03	0.33	
21.11	902762		0.758	0.02	0.19	
21.71	700338		0.758	0.01	0.15	
21.94	40062257	Triglyme	0.758	0.67		
22.17	262642		0.758	0.00	0.06	
22.39	1660728		0.758	0.03	0.36	
23.78	559766		0.758	0.01	0.12	
24.61	518021		0.758	0.01	0.11	
25.74	35586301	Solvent	0.000	0.00	0.00	
28.00	69281121	DIIBA	1.400	0.63		
28.58	216448		0.758	0.00	0.05	
37.56	2101195	After MeP	0.000	0.00	0.00	
40.32	13521124	After MeP	0.000	0.00	0.00	

It should be noted that the EGDE peak should be assigned first since a g/L calculation cannot be completed until the spreadsheet is made aware of the EGDE concentration. Not having g/L values as guides makes the table more difficult to work with. Complete both injections of each sample in this manner.

Sample Summary

This tab is a collection of the information for the 4 samples, consisting of the final VOC Material/Coating results and the Spike Recoveries for each sample. If the recoveries are acceptable and if the replicate sample injections are proximal then no action is required by the user.

Sample #1

	Injection #1	Injection #2	Average g/L
VOC Material	2.80	2.37	2.58
VOC Coating	10		
Calculated Water Wt %	54.8		

		Injection #1		Injection #2	
	Prep (gL)	Meas (g/L)	% Recovery	Meas (g/L)	% Recovery
EGDE	5.09	6.51	128.1	6.43	126.4
IPA	0.73	0.71	97.5	0.71	97.2
Heptane	0.69	0.69	101.0	0.69	100.3
Triglyme	0.70	0.67	96.1	0.68	98.1
DIIBA	0.68	0.63	92.5	0.64	95.3

RRFs

This is a collection of the Response Factors and Relative Response Factors accumulated throughout the test, along with the metadata for the calibrations. This tab requires no action from the user.

Thank you again for your participation in this study—I hope the template makes your job much easier than it would be otherwise. If you have any questions about how to use this template, or have any questions about what you are expected to be provide following analysis, please get in touch with me.