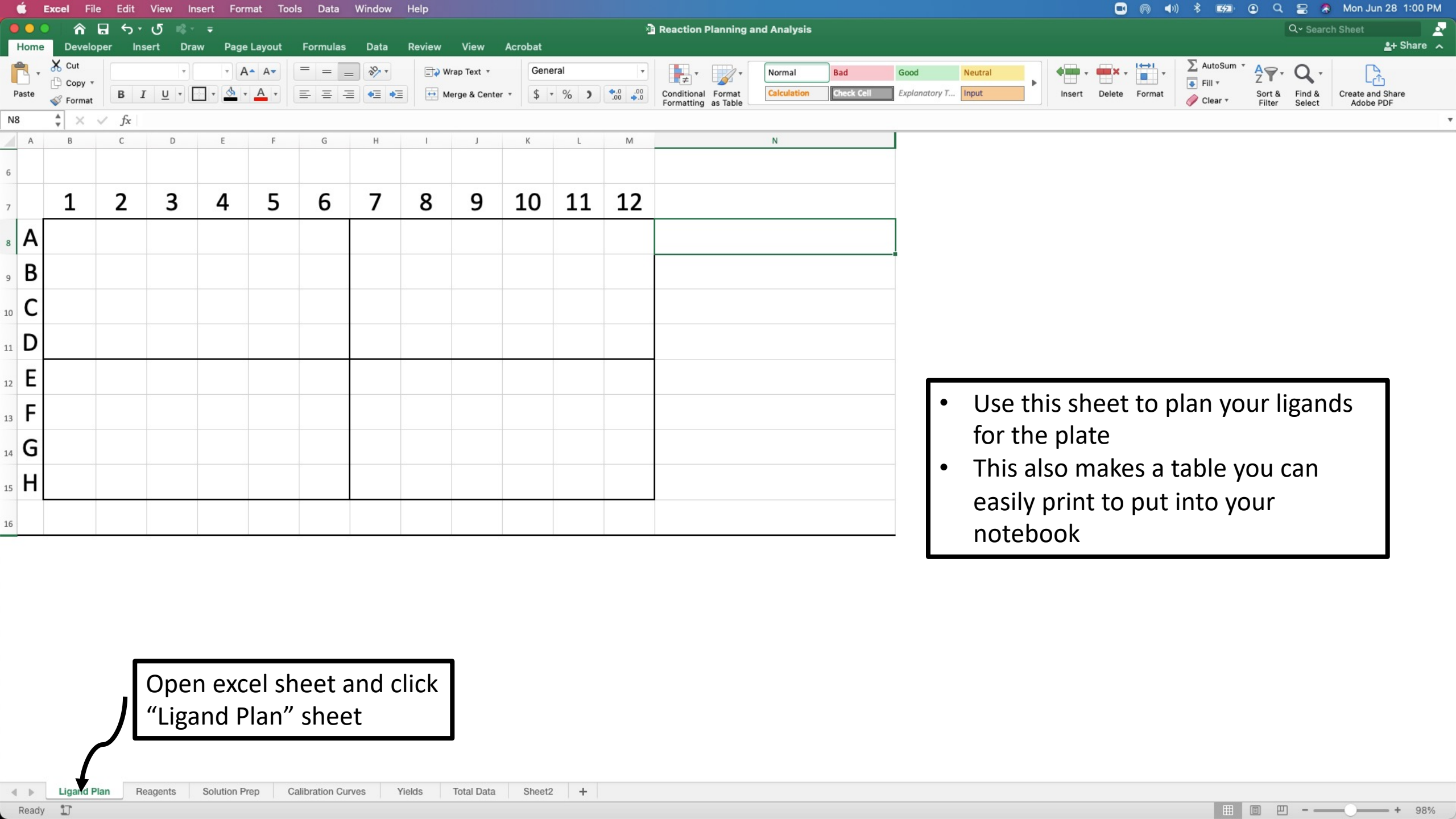
Reaction Planning and Analysis


Excel File Edit View Insert Format Tools Data Window Help
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Reaction Planning and Analysis
Search Sheet
Home Developer Insert Draw Page Layout Formulas Data Review View Acrobat
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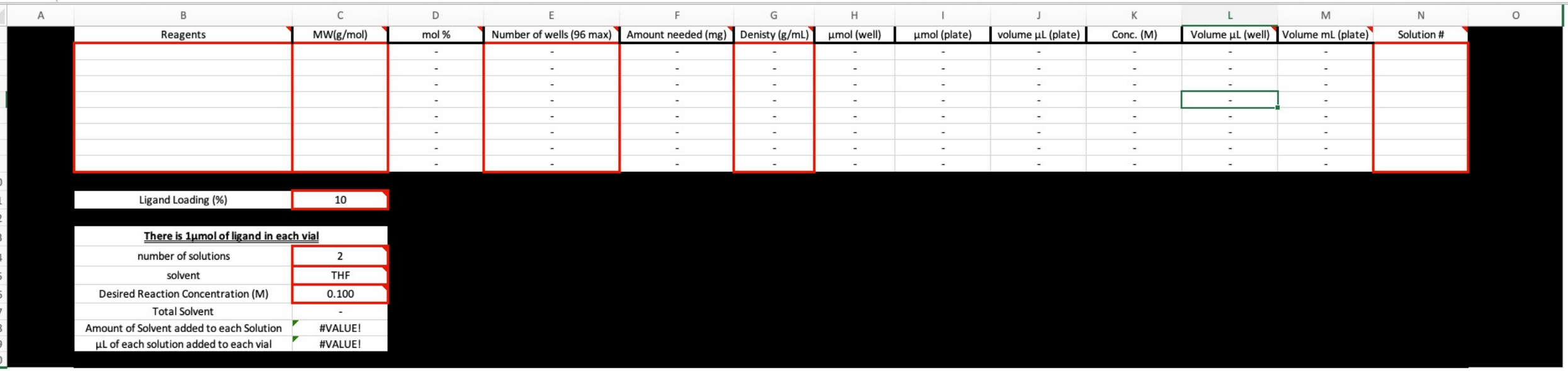
N8
1 2 3 4 5 6 7 8 9 10 11 12
A B C D E F G H
Use this sheet to plan your ligands for the plate
This also makes a table you can easily print to put into your notebook
Open excel sheet and click “Ligand Plan” sheet
Ligand Plan Reagents Solution Prep Calibration Curves Yields Total Data Sheet2
Ready
98%

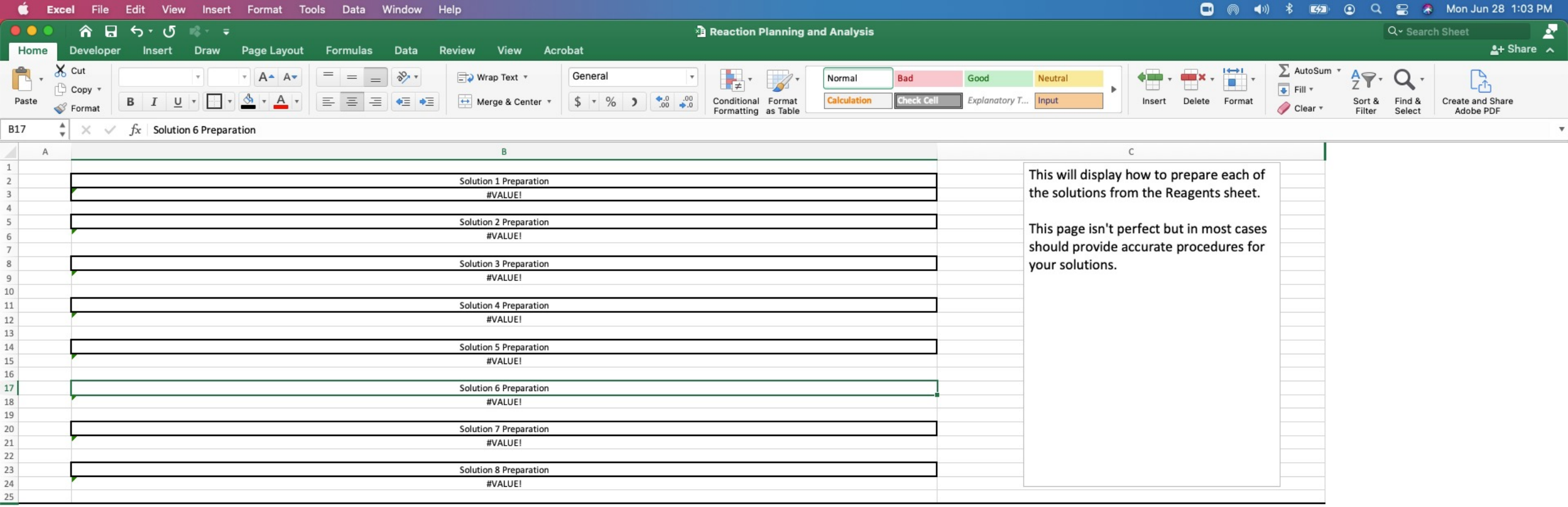


	Reagents	MW(g/mol)	mol %	Number of wells (96 max)	Amount needed (mg)	Denisty (g/mL)	µmol (well)	µmol (plate)	volume µL (plate)	Conc. (M)	Volume µL (well)	Volume mL (plate)	Solution #
2			-	-	-	-	-	-	-	-	-	-	
3			-	-	-	-	-	-	-	-	-	-	
4			-	-	-	-	-	-	-	-	-	-	
5			-	-	-	-	-	-	-	-	-	-	
6			-	-	-	-	-	-	-	-	-	-	
7			-	-	-	-	-	-	-	-	-	-	
8			-	-	-	-	-	-	-	-	-	-	
9			-	-	-	-	-	-	-	-	-	-	

Ligand Loading (%)	10

There is 1µmol of ligand in each vial	
number of solutions	2
solvent	THF
Desired Reaction Concentration (M)	0.100
Total Solvent	-
Amount of Solvent added to each Solution	#VALUE!
µL of each solution added to each vial	#VALUE!

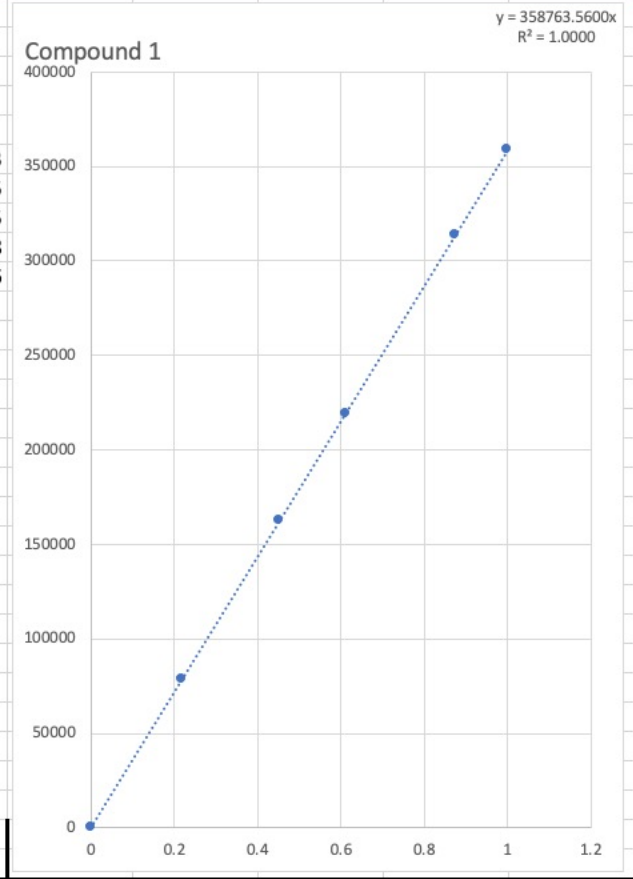
- This sheet allows for automated calculation of the amount of each reagent you will need for your plate
  - Please only change the cells that are highlighted in red
- Place your reagents names, molecular weights, number of wells it will appear in, the density if applicable, and finally which number solution it will appear in
- Second change the ligand loading to the appropriate value. This will change everything on the plate as everything is in relation to the pre-plated ligand (1µmol of ligand per vial)
- Next the number of solutions you would like to add to your vials (important for incompatible reagents)
- Put which solvent you will be using
- Put the desired reaction concentration in as well
- Notice the amount of solvent to added to each solution and then the amount of each solution to add to each vial



- This page is not perfect but will work in most cases
- This will give instructions for the preparation of each solution designated
- It does not round so round to the near µL

Reaction Planning and Analysis

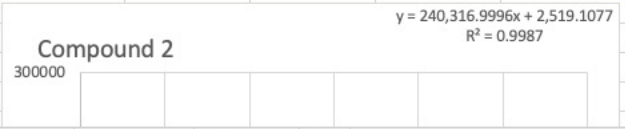
	A	B	C
1	Paranitrotoluene		
2			
3	Run	Concentration(mg/mL)	Area Count
4	blank		
5	blank		
6	blank	0	0
7	1	0.219754844	78840.03
8	2	0.453458958	162684.55
9	3	0.610668068	219085.45
10	4	0.873617934	313422.28
11	5	1	358763.56
12	6		
13	7		
14	8		
15	9		
16	10		
17	11		
18	12		
19	13		
20	14		
21	15		
22	16		
23	17		
24	18		
25	19		
26	20		
27	21		
28		slope	358763.56
29		y intercept	-2.91038E-11
30	Prepare solution in 5mL HPLC solvent try to get 10mg in 5mL		
31			
32			
33	monoborylated Paranitrotoluene		
34			
35	Run	Concentration(mg/mL)	Area Count
36	blank		
37	blank		



For extremely accurate calibration curves use the following procedure:

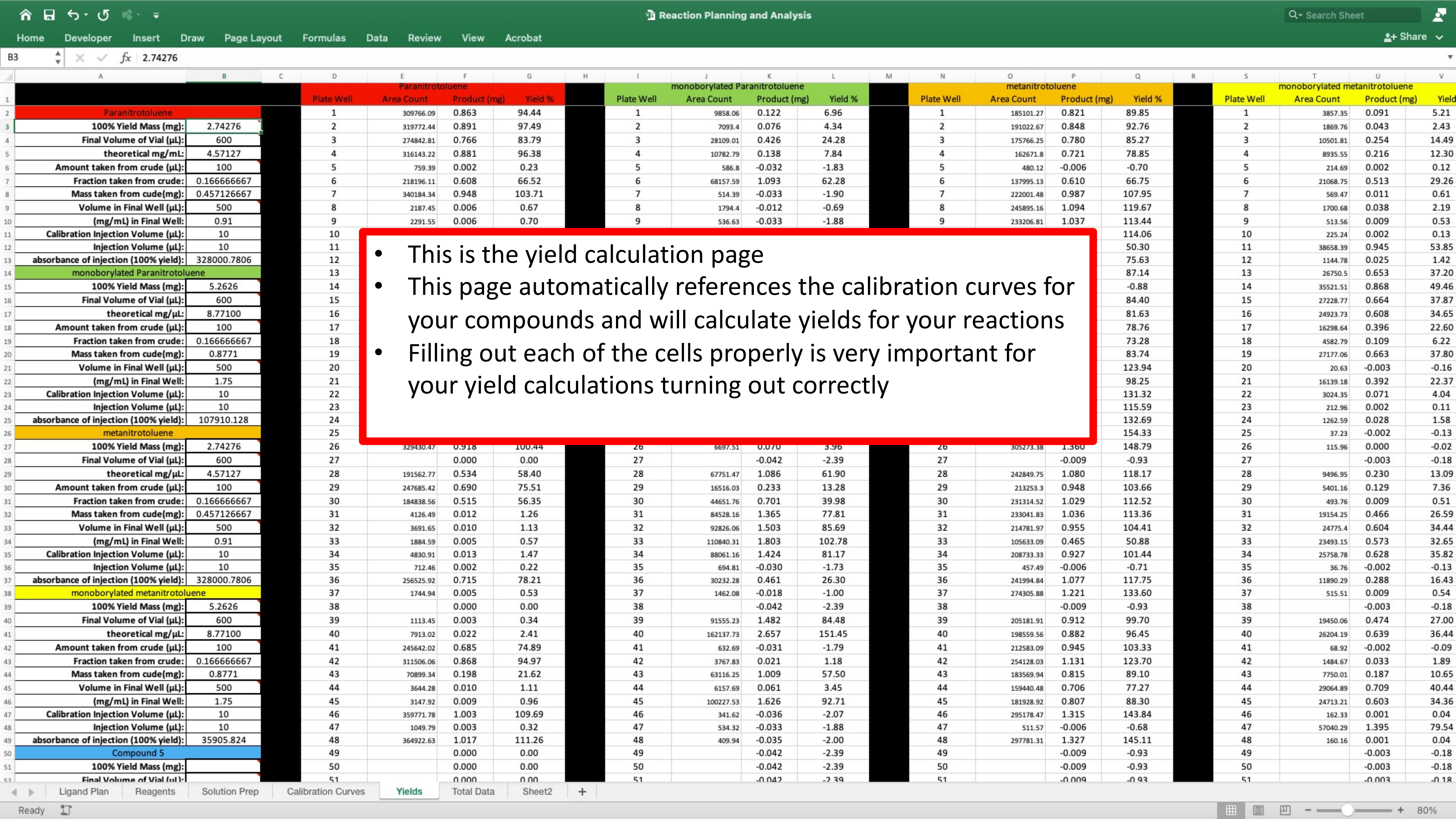
1) Weigh out authentic sample into a 20mL scintillation
2) The amount should be roughly 10mg
3) Add solvent utilizing a pipette add MeCN to generate a solution of 1mg/mL
4) From the 1mg/mL solution add 125µL, 250µL, 500µL, 750µL, and 1mL
5) To each of these vials add 875µL, 750µL, 500µL, and 250µL of MeCN to bring the total volume to 1mL for each vial.
6) Submit each vial to the instrument of to run 3 times
7) Plot each data point to the left to generate a calibration curve for the desired compound

- Follow these instructions to build a calibration curve that is automatically referenced in the next page
- Also change the names in the colored cells and they will be continued through the following sheets so labeling will be consistent



Ligand Plan | Reagents | Solution Prep | Calibration Curves | Yields | Total Data | Sheet2

Ready | Average: 0 | Count: 2 | Sum: 0 | 140%



- This is the yield calculation page
- This page automatically references the calibration curves for your compounds and will calculate yields for your reactions
- Filling out each of the cells properly is very important for your yield calculations turning out correctly

Paranitrotoluene	
100% Yield Mass (mg):	2.74276
Final Volume of Vial (µL):	600
theoretical mg/mL:	4.57127
Amount taken from crude (µL):	100
Fraction taken from crude:	0.166666667
Mass taken from cude(mg):	0.457126667
Volume in Final Well (µL):	500
(mg/mL) in Final Well:	0.91
Calibration Injection Volume (µL):	10
Injection Volume (µL):	10
absorbance of injection (100% yield):	328000.7806
monoborylated Paranitrotoluene	

Final Volume of Vial (µL):	600
theoretical mg/µL:	8.77100
Amount taken from crude (µL):	100
Fraction taken from crude:	0.166666667
Mass taken from cude(mg):	0.8771
Volume in Final Well (µL):	500
(mg/mL) in Final Well:	1.75
Calibration Injection Volume (µL):	10
Injection Volume (µL):	10
absorbance of injection (100% yield):	35905.824
Compound 5	
100% Yield Mass (mg):	
Final Volume of Vial (µL):	

Consumption of Starting Material

- Using the Reagents page determine the mass of the compound in a well and place in this cell

Determination of Yield

- If you are trying to determine yield calculate the mass of a reaction that yields 100% for a well and place in this cell

Reaction Planning and Analysis

Search Sheet

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monoborylated Paranitrotoluene	

When you complete the plate you will dilute the reaction. This cell should contain the volume of the reaction plus amount of diluting solvent added to each vial.

<u>Example</u>

The reaction is run in 100µL of THF. When the reaction is completed the user adds 500µL of MeCN to each vial.

100µL + 500µL = 600µL goes into the cell

Final Volume of Vial (µL):	600
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absorbance of injection (100% yield):	35905.824
Compound 5	
100% Yield Mass (mg):	
Final Volume of Vial (µL):	

39	1113.45	0.003	0.34
40	7913.02	0.022	2.41
41	245642.02	0.685	74.89
42	311506.06	0.868	94.97
43	70899.34	0.198	21.62
44	3644.28	0.010	1.11
45	3147.92	0.009	0.96
46	359771.78	1.003	109.69
47	1049.79	0.003	0.32
48	364922.63	1.017	111.26
49		0.000	0.00
50		0.000	0.00
51		0.000	0.00

L			
			Yield %
			6.96
			4.34
			24.28
			7.84
			-1.83
			[illegible]
			-1.90
			-0.69
			-1.88
			-1.40
			66.78
			102.48
			100.12
			11.22
			90.50
			51.13
			37.76
			8.96
			94.80
			-2.18
			37.57
			5.71
			-2.07
			5.26
			-1.40
			3.96
			-2.39
			61.90
			13.28
			39.98
			77.81
			85.69
			102.78
			81.17
			-1.73
			26.30
			-1.00
			-2.39
39	91555.23	1.482	84.48
40	162137.73	2.657	151.45
41	632.69	-0.031	-1.79
42	3767.83	0.021	1.18
43	63116.25	1.009	57.50
44	6157.69	0.061	3.45
45	100227.53	1.626	92.71
46	341.62	-0.036	-2.07
47	534.32	-0.033	-1.88
48	409.94	-0.035	-2.00
49		-0.042	-2.39
50		-0.042	-2.39
51		-0.042	-2.39

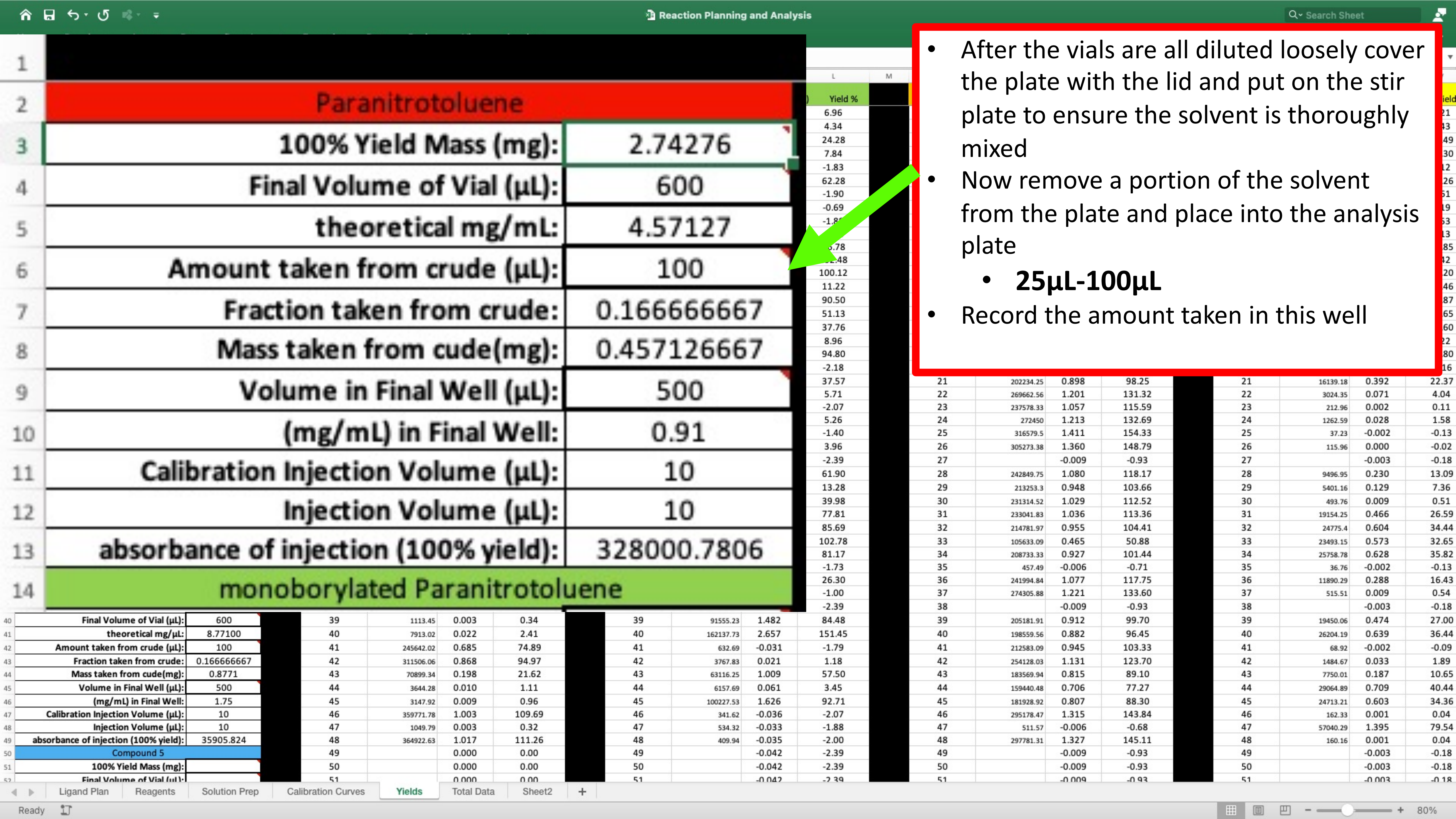
M			
23	237578.33	1.057	115.59
24	272450	1.213	132.69
25	316579.5	1.411	154.33
26	305273.38	1.360	148.79
27		-0.009	-0.93
28	242849.75	1.080	118.17
29	213253.3	0.948	103.66
30	231314.52	1.029	112.52
31	233041.83	1.036	113.36
32	214781.97	0.955	104.41
33	105633.09	0.465	50.88
34	208733.33	0.927	101.44
35	457.49	-0.006	-0.71
36	241994.84	1.077	117.75
37	274305.88	1.221	133.60
38		-0.009	-0.93
39	205181.91	0.912	99.70
40	198559.56	0.882	96.45
41	212583.09	0.945	103.33
42	254128.03	1.131	123.70
43	183569.94	0.815	89.10
44	159440.48	0.706	77.27
45	181928.92	0.807	88.30
46	295178.47	1.315	143.84
47	511.57	-0.006	-0.68
48	297781.31	1.327	145.11
49		-0.009	-0.93
50		-0.009	-0.93
51		-0.009	-0.93

			ield
			21
			43
			49
			30
			12
			26
			51
			19
			53
			13
			85
			42
			20
			46
			87
			65
			60
			22
			80
			16
			37
			04
23	212.96	0.002	0.11
24	1262.59	0.028	1.58
25	37.23	-0.002	-0.13
26	115.96	0.000	-0.02
27		-0.003	-0.18
28	9496.95	0.230	13.09
29	5401.16	0.129	7.36
30	493.76	0.009	0.51
31	19154.25	0.466	26.59
32	24775.4	0.604	34.44
33	23493.15	0.573	32.65
34	25758.78	0.628	35.82
35	36.76	-0.002	-0.13
36	11890.29	0.288	16.43
37	515.51	0.009	0.54
38		-0.003	-0.18
39	19450.06	0.474	27.00
40	26204.19	0.639	36.44
41	68.92	-0.002	-0.09
42	1484.67	0.033	1.89
43	7750.01	0.187	10.65
44	29064.89	0.709	40.44
45	24713.21	0.603	34.36
46	162.33	0.001	0.04
47	57040.29	1.395	79.54
48	160.16	0.001	0.04
49		-0.003	-0.18
50		-0.003	-0.18
51		-0.003	-0.18

Ligand Plan | Reagents | Solution Prep | Calibration Curves | Yields | Total Data | Sheet2 | +

Ready

80%



- After the vials are all diluted loosely cover the plate with the lid and put on the stir plate to ensure the solvent is thoroughly mixed
- Now remove a portion of the solvent from the plate and place into the analysis plate
    - **25µL-100µL**
- Record the amount taken in this well

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Injection Volume (µL):	10
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monoborylated Paranitrotoluene	

- Each well in the analysis plate now contains 100µL
- Each well must be diluted further with more solvent
- In this case an addition 400µL of MeCN was added to each well giving a total of 500µL

Example

100µL + 400µL = 500µL goes into the cell

Final Volume of Vial (µL):	600
theoretical mg/µL:	8.77100
Amount taken from crude (µL):	100
Fraction taken from crude:	0.166666667
Mass taken from cude(mg):	0.8771
Volume in Final Well (µL):	500
(mg/mL) in Final Well:	1.75
Calibration Injection Volume (µL):	10
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absorbance of injection (100% yield):	35905.824
Compound 5	
100% Yield Mass (mg):	
Final Volume of Vial (µL):	

Reaction Planning and Analysis

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Compound 5	
100% Yield Mass (mg):	

- These two cells are you to account for different injection volumes
  - Calibration Injection Volume
  - Injection Volume
- If your calibration standards are injected at 10µL place a 10 in the cell "Calibration Injection Volume (µL)"
- If your plate injections are 10µL place a 10 in the cell "Injection Volume (µL)"

Ligand Plan | Reagents | Solution Prep | Calibration Curves | Yields | Total Data | Sheet2

Reaction Planning and Analysis

=IF(ISBLANK(Yields!J2),"-",Yields!L2)

Well	Ligand #	Notes	Paranitrotoluene	monoborylated Paranitrotoluene	metanitrotoluene	monoborylated metanitrotoluene	Compound 5
1	-		-	6.96	89.85	5.21	-
2	-		97.49	4.34	92.76	2.43	-
3	-		83.79	24.28	85.27	14.49	-
4	-		96.38	7.84	[illegible]	12.30	-
5	-		0.23	-1.83	-0.70	0.12	-
6	-		66.52	62.28	66.75	29.26	-
7	-		103.71	-1.90	107.95	0.61	-
8	-		0.67	-0.69	119.67	2.19	-
9	-		0.70	-1.88	113.44	0.53	-
10	-		106.53	-1.40	114.06	0.13	-
11	-		64.56	66.78	50.30	53.85	-
12	-		2.30	102.48	75.63	1.42	-
13	-		3.87	100.12	87.14	37.20	-
14	-		0.15	11.22	-0.88	49.46	-
15	-		2.27	90.50	84.40	37.87	-
16	-		71.36	51.13	81.63	34.65	-
17	-		73.87	37.76	78.76	22.60	-
18	-		67.27	8.96	73.28	6.22	-
19	-		26.45	94.80	83.74	37.80	-
20	-		102.56	-2.18	123.94	-0.16	-
21	-		89.11	37.57	98.25	22.37	-
22	-		105.59	5.71	131.32	4.04	-
23	-		99.95	-2.07	115.59	0.11	-
24	-		101.46	5.26	132.69	1.58	-
25	-		106.48	-1.40	154.33	-0.13	-
26	-		100.44	3.96	148.79	-0.02	-
27	-		-	-	-	-	-
28	-		58.40	61.90	118.17	13.09	-
29	-		75.51	13.28	103.66	7.36	-
30	-		56.35	39.98	112.52	0.51	-
31	-		1.26	77.81	113.36	26.59	-
32	-		1.13	85.69	104.41	34.44	-
33	-		0.57	102.78	50.88	32.65	-
34	-		1.47	81.17	101.44	35.82	-
35	-		0.22	-1.73	-0.71	-0.13	-
36	-		78.21	26.30	117.75	16.43	-
37	-		0.53	-1.00	133.60	0.54	-
38	-		-	-	-	-	-
39	-		0.34	84.48	99.70	27.00	-
40	-		2.41	151.45	96.45	36.44	-
41	-		74.89	-1.79	103.33	-0.09	-
42	-		94.97	1.18	123.70	1.89	-
43	-		21.62	57.50	89.10	10.65	-

Ligand Plan | Reagents | Solution Prep | Calibration Curves | Yields | Total Data | Notes

- This is all the total data from each the “Yields” sheet
- The “Ligand #” cell is automatically filled in from the corresponding cell on the ”Ligand Plan” sheet so do not alter the formulas in these cells
- The Notes cells are empty and are their for you to add notes or comments on the data in the row
- Cells that contain yield <0 are automatically colored coded as red
  - This is due to slight errors in the calibration curve and is normal in many cases