

Reaction Planning and Analysis

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Reaction Planning and Analysis

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Normal Bad Good Neutral Calculation Check Cell Explanatory T... Input

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Search Sheet

Share

	A	B	C	D	E	F	G	H	I	J	K	L	M	N
6														
7		1	2	3	4	5	6	7	8	9	10	11	12	
8	A													
9	B													
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12	E													
13	F													
14	G													
15	H													
16														

- 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

Excel File Edit View Insert Format Tools Data Window Help

Reaction Planning and Analysis

Home Developer Insert Draw Page Layout Formulas Data Review View Acrobat

fx =IFERROR((H5/K5),"")

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
		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 #	
1															
2				-	-	-	-	-	-	-	-	-	-	-	
3				-	-	-	-	-	-	-	-	-	-	-	
4				-	-	-	-	-	-	-	-	-	-	-	
5				-	-	-	-	-	-	-	-	-	-	-	
6				-	-	-	-	-	-	-	-	-	-	-	
7				-	-	-	-	-	-	-	-	-	-	-	
8				-	-	-	-	-	-	-	-	-	-	-	
9				-	-	-	-	-	-	-	-	-	-	-	
10				-	-	-	-	-	-	-	-	-	-	-	
11		Ligand Loading (%)	10												
12															
13		There is 1 μmol of ligand in each vial													
14		number of solutions	2												
15		solvent	THF												
16		Desired Reaction Concentration (M)	0.100												
17		Total Solvent	-												
18		Amount of Solvent added to each Solution	#VALUE!												
19		μL of each solution added to each vial	#VALUE!												
20															

- 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 (1 μmol 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

The screenshot shows the Microsoft Excel interface with the 'Reaction Planning and Analysis' title bar. The active sheet is 'Solution 6 Preparation'. The spreadsheet has columns A, B, and C, and rows 1 through 25. Column B contains the following text from row 2 to row 24:

	B
2	Solution 1 Preparation
3	#VALUE!
4	
5	Solution 2 Preparation
6	#VALUE!
7	
8	Solution 3 Preparation
9	#VALUE!
10	
11	Solution 4 Preparation
12	#VALUE!
13	
14	Solution 5 Preparation
15	#VALUE!
16	
17	Solution 6 Preparation
18	#VALUE!
19	
20	Solution 7 Preparation
21	#VALUE!
22	
23	Solution 8 Preparation
24	#VALUE!

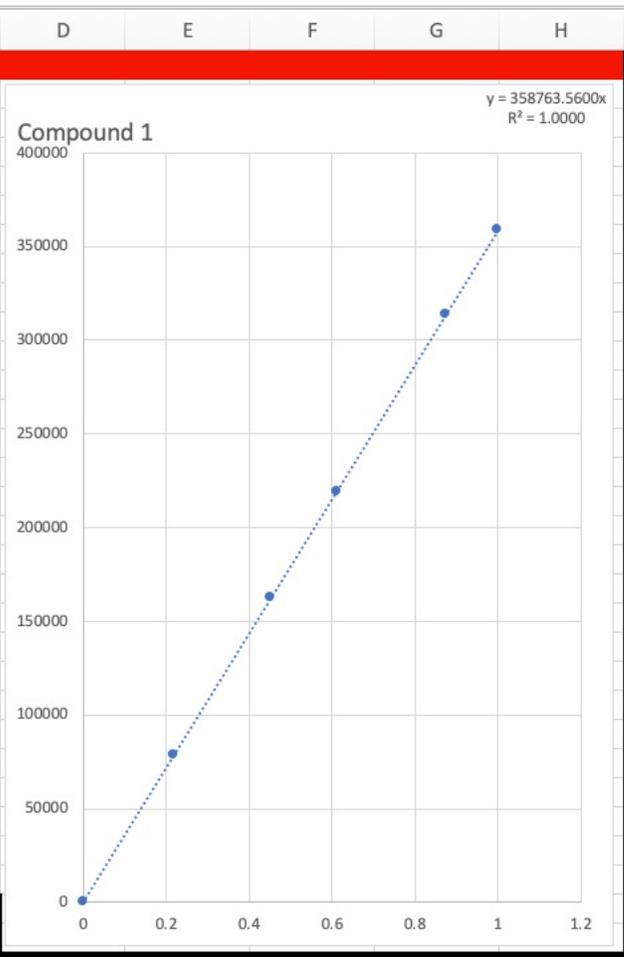
Column C contains a text box with the following text:

This will display how to prepare each of the solutions from the Reagents sheet.

This page isn't perfect but in most cases should provide accurate procedures for your solutions.

- 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

Paranitrotoluene		
Run	Concentration(mg/mL)	Area Count
blank		
blank		
blank	0	0
1	0.219754844	78840.03
2	0.453458958	162684.55
3	0.610668068	219085.45
4	0.873617934	313422.28
5	1	358763.56
6		
7		
8		
9		
10		
11		
12		
13		
14		
15		
16		
17		
18		
19		
20		
21		
28	slope	358763.56
29	y intercept	-2.91038E-11
30	Prepare solution in 5mL HPLC solvent try to get 10mg in 5mL	



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

monoborylated Paranitrotoluene		
Run	Concentration(mg/mL)	Area Count
blank		
blank		
blank	0	0



	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V		
				Plate Well	Paranitrotoluene					Plate Well	monoborylated Paranitrotoluene					metanitrotoluene					Plate Well	monoborylated metanitrotoluene		
					Area Count	Product (mg)	Yield %			Area Count	Product (mg)	Yield %			Area Count	Product (mg)	Yield %			Area Count	Product (mg)	Yield %		
1	Paranitrotoluene			1	309766.09	0.863	94.44		1	9858.06	0.122	6.96		1	185101.27	0.821	89.85		1	3857.35	0.091	5.21		
2	100% Yield Mass (mg):	2.74276		2	319772.44	0.891	97.49		2	7093.4	0.076	4.34		2	191022.67	0.848	92.76		2	1869.76	0.043	2.43		
3	Final Volume of Vial (µL):	600		3	274842.81	0.766	83.79		3	28109.01	0.426	24.28		3	175766.25	0.780	85.27		3	10501.81	0.254	14.49		
4	theoretical mg/mL:	4.57127		4	316143.22	0.881	96.38		4	10782.79	0.138	7.84		4	162671.8	0.721	78.85		4	8935.55	0.216	12.30		
5	Amount taken from crude (µL):	100		5	759.39	0.002	0.23		5	586.8	-0.032	-1.83		5	480.12	-0.006	-0.70		5	214.69	0.002	0.12		
6	Fraction taken from crude:	0.166666667		6	218196.11	0.608	66.52		6	68157.59	1.093	62.28		6	137995.13	0.610	66.75		6	21068.75	0.513	29.26		
7	Mass taken from cude(mg):	0.457126667		7	340184.34	0.948	103.71		7	514.39	-0.033	-1.90		7	222001.48	0.987	107.95		7	569.47	0.011	0.61		
8	Volume in Final Well (µL):	500		8	2187.45	0.006	0.67		8	1794.4	-0.012	-0.69		8	245895.16	1.094	119.67		8	1700.68	0.038	2.19		
9	(mg/mL) in Final Well:	0.91		9	2291.55	0.006	0.70		9	536.63	-0.033	-1.88		9	233206.81	1.037	113.44		9	513.56	0.009	0.53		
10	Calibration Injection Volume (µL):	10		10					10					10			114.06		10	225.24	0.002	0.13		
11	Injection Volume (µL):	10		11					11					11			50.30		11	38658.39	0.945	53.85		
12	absorbance of injection (100% yield):	328000.7806		12					12					12			75.63		12	1144.78	0.025	1.42		
13	monoborylated Paranitrotoluene			13					13					13			87.14		13	26750.5	0.653	37.20		
14	100% Yield Mass (mg):	5.2626		14					14					14			-0.88		14	35521.51	0.868	49.46		
15	Final Volume of Vial (µL):	600		15					15					15			84.40		15	27228.77	0.664	37.87		
16	theoretical mg/µL:	8.77100		16					16					16			81.63		16	24923.73	0.608	34.65		
17	Amount taken from crude (µL):	100		17					17					17			78.76		17	16298.64	0.396	22.60		
18	Fraction taken from crude:	0.166666667		18					18					18			73.28		18	4582.79	0.109	6.22		
19	Mass taken from cude(mg):	0.8771		19					19					19			83.74		19	27177.06	0.663	37.80		
20	Volume in Final Well (µL):	500		20					20					20			123.94		20	20.63	-0.003	-0.16		
21	(mg/mL) in Final Well:	1.75		21					21					21			98.25		21	16139.18	0.392	22.37		
22	Calibration Injection Volume (µL):	10		22					22					22			131.32		22	3024.35	0.071	4.04		
23	Injection Volume (µL):	10		23					23					23			115.59		23	212.96	0.002	0.11		
24	absorbance of injection (100% yield):	107910.128		24					24					24			132.69		24	1262.59	0.028	1.58		
25	metanitrotoluene			25					25					25			154.33		25	37.23	-0.002	-0.13		
26	100% Yield Mass (mg):	2.74276		26	329430.47	0.918	100.44		26	6697.51	0.070	3.96		26	305273.38	1.360	148.79		26	115.96	0.000	-0.02		
27	Final Volume of Vial (µL):	600		27		0.000	0.00		27		-0.042	-2.39		27		-0.009	-0.93		27		-0.003	-0.18		
28	theoretical mg/µL:	4.57127		28	191562.77	0.534	58.40		28	67751.47	1.086	61.90		28	242849.75	1.080	118.17		28	9496.95	0.230	13.09		
29	Amount taken from crude (µL):	100		29	247685.42	0.690	75.51		29	16516.03	0.233	13.28		29	213253.3	0.948	103.66		29	5401.16	0.129	7.36		
30	Fraction taken from crude:	0.166666667		30	184838.56	0.515	56.35		30	44651.76	0.701	39.98		30	231314.52	1.029	112.52		30	493.76	0.009	0.51		
31	Mass taken from cude(mg):	0.457126667		31	4126.49	0.012	1.26		31	84528.16	1.365	77.81		31	233041.83	1.036	113.36		31	19154.25	0.466	26.59		
32	Volume in Final Well (µL):	500		32	3691.65	0.010	1.13		32	92826.06	1.503	85.69		32	214781.97	0.955	104.41		32	24775.4	0.604	34.44		
33	(mg/mL) in Final Well:	0.91		33	1884.59	0.005	0.57		33	110840.31	1.803	102.78		33	105633.09	0.465	50.88		33	23493.15	0.573	32.65		
34	Calibration Injection Volume (µL):	10		34	4830.91	0.013	1.47		34	88061.16	1.424	81.17		34	208733.33	0.927	101.44		34	25758.78	0.628	35.82		
35	Injection Volume (µL):	10		35	712.46	0.002	0.22		35	694.81	-0.030	-1.73		35	457.49	-0.006	-0.71		35	36.76	-0.002	-0.13		
36	absorbance of injection (100% yield):	328000.7806		36	256525.92	0.715	78.21		36	30232.28	0.461	26.30		36	241994.84	1.077	117.75		36	11890.29	0.288	16.43		
37	monoborylated metanitrotoluene			37	1744.94	0.005	0.53		37	1462.08	-0.018	-1.00		37	274305.88	1.221	133.60		37	515.51	0.009	0.54		
38	100% Yield Mass (mg):	5.2626		38		0.000	0.00		38		-0.042	-2.39		38		-0.009	-0.93		38		-0.003	-0.18		
39	Final Volume of Vial (µL):	600		39	1113.45	0.003	0.34		39	91555.23	1.482	84.48		39	205181.91	0.912	99.70		39	19450.06	0.474	27.00		
40	theoretical mg/µL:	8.77100		40	7913.02	0.022	2.41		40	162137.73	2.657	151.45		40	198559.56	0.882	96.45		40	26204.19	0.639	36.44		
41	Amount taken from crude (µL):	100		41	245642.02	0.685	74.89		41	632.69	-0.031	-1.79		41	212583.09	0.945	103.33		41	68.92	-0.002	-0.09		
42	Fraction taken from crude:	0.166666667		42	311506.06	0.868	94.97		42	3767.83	0.021	1.18		42	254128.03	1.131	123.70		42	1484.67	0.033	1.89		
43	Mass taken from cude(mg):	0.8771		43	70899.34	0.198	21.62		43	63116.25	1.009	57.50		43	183569.94	0.815	89.10		43	7750.01	0.187	10.65		
44	Volume in Final Well (µL):	500		44	3644.28	0.010	1.11		44	6157.69	0.061	3.45		44	159440.48	0.706	77.27		44	29064.89	0.709	40.44		
45	(mg/mL) in Final Well:	1.75		45	3147.92	0.009	0.96		45	100227.53	1.626	92.71		45	181928.92	0.807	88.30		45	24713.21	0.603	34.36		
46	Calibration Injection Volume (µL):	10		46	359771.78	1.003	109.69		46	341.62	-0.036	-2.07		46	295178.47	1.315	143.84		46	162.33	0.001	0.04		
47	Injection Volume (µL):	10		47	1049.79	0.003	0.32		47	534.32	-0.033	-1.88		47	511.57	-0.006	-0.68		47	57040.29	1.395	79.54		
48	absorbance of injection (100% yield):	35905.824		48	364922.63	1.017	111.26		48	409.94	-0.035	-2.00		48	297781.31	1.327	145.11		48	160.16	0.001	0.04		
49	Compound 5			49		0.000	0.00		49		-0.042	-2.39		49		-0.009	-0.93		49		-0.003	-0.18		
50	100% Yield Mass (mg):			50		0.000	0.00		50		-0.042	-2.39		50		-0.009	-0.93		50		-0.003	-0.18		
51	Final Volume of Vial (µL):			51		0.000	0.00		51		-0.042	-2.39		51		-0.009	-0.93		51		-0.003	-0.18		

- 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

1		
2	Paranitrotoluene	
3	100% Yield Mass (mg):	2.74276
4	Final Volume of Vial (μL):	600
5	theoretical mg/mL:	4.57127
6	Amount taken from crude (μL):	100
7	Fraction taken from crude:	0.166666667
8	Mass taken from crude(mg):	0.457126667
9	Volume in Final Well (μL):	500
10	(mg/mL) in Final Well:	0.91
11	Calibration Injection Volume (μL):	10
12	Injection Volume (μL):	10
13	absorbance of injection (100% yield):	328000.7806
14	monoborylated Paranitrotoluene	

40	Final Volume of Vial (μL):	600	39	1113.45	0.003	0.34	39	91555.23	1.482	84.48
41	theoretical mg/μL:	8.77100	40	7913.02	0.022	2.41	40	162137.73	2.657	151.45
42	Amount taken from crude (μL):	100	41	245642.02	0.685	74.89	41	632.69	-0.031	-1.79
43	Fraction taken from crude:	0.166666667	42	311506.06	0.868	94.97	42	3767.83	0.021	1.18
44	Mass taken from crude(mg):	0.8771	43	70899.34	0.198	21.62	43	63116.25	1.009	57.50
45	Volume in Final Well (μL):	500	44	3644.28	0.010	1.11	44	6157.69	0.061	3.45
46	(mg/mL) in Final Well:	1.75	45	3147.92	0.009	0.96	45	100227.53	1.626	92.71
47	Calibration Injection Volume (μL):	10	46	359771.78	1.003	109.69	46	341.62	-0.036	-2.07
48	Injection Volume (μL):	10	47	1049.79	0.003	0.32	47	534.32	-0.033	-1.88
49	absorbance of injection (100% yield):	35905.824	48	364922.63	1.017	111.26	48	409.94	-0.035	-2.00
50	Compound 5		49		0.000	0.00	49		-0.042	-2.39
51	100% Yield Mass (mg):		50		0.000	0.00	50		-0.042	-2.39
51	Final Volume of Vial (μL):		51		0.000	0.00	51		-0.042	-2.39

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

21	202234.25	0.898	98.25	21	16139.18	0.392	22.37
22	269662.56	1.201	131.32	22	3024.35	0.071	4.04
23	237578.33	1.057	115.59	23	212.96	0.002	0.11
24	272450	1.213	132.69	24	1262.59	0.028	1.58
25	316579.5	1.411	154.33	25	37.23	-0.002	-0.13
26	305273.38	1.360	148.79	26	115.96	0.000	-0.02
27		-0.009	-0.93	27		-0.003	-0.18
28	242849.75	1.080	118.17	28	9496.95	0.230	13.09
29	213253.3	0.948	103.66	29	5401.16	0.129	7.36
30	231314.52	1.029	112.52	30	493.76	0.009	0.51
31	233041.83	1.036	113.36	31	19154.25	0.466	26.59
32	214781.97	0.955	104.41	32	24775.4	0.604	34.44
33	105633.09	0.465	50.88	33	23493.15	0.573	32.65
34	208733.33	0.927	101.44	34	25758.78	0.628	35.82
35	457.49	-0.006	-0.71	35	36.76	-0.002	-0.13
36	241994.84	1.077	117.75	36	11890.29	0.288	16.43
37	274305.88	1.221	133.60	37	515.51	0.009	0.54
38		-0.009	-0.93	38		-0.003	-0.18
39	205181.91	0.912	99.70	39	19450.06	0.474	27.00
40	198559.56	0.882	96.45	40	26204.19	0.639	36.44
41	212583.09	0.945	103.33	41	68.92	-0.002	-0.09
42	254128.03	1.131	123.70	42	1484.67	0.033	1.89
43	183569.94	0.815	89.10	43	7750.01	0.187	10.65
44	159440.48	0.706	77.27	44	29064.89	0.709	40.44
45	181928.92	0.807	88.30	45	24713.21	0.603	34.36
46	295178.47	1.315	143.84	46	162.33	0.001	0.04
47	511.57	-0.006	-0.68	47	57040.29	1.395	79.54
48	297781.31	1.327	145.11	48	160.16	0.001	0.04
49		-0.009	-0.93	49		-0.003	-0.18
50		-0.009	-0.93	50		-0.003	-0.18
51		-0.009	-0.93	51		-0.003	-0.18

1		
2	Paranitrotoluene	
3	100% Yield Mass (mg):	2.74276
4	Final Volume of Vial (µL):	600
5	theoretical mg/mL:	4.57127
6	Amount taken from crude (µL):	100
7	Fraction taken from crude:	0.166666667
8	Mass taken from crude(mg):	0.457126667
9	Volume in Final Well (µL):	500
10	(mg/mL) in Final Well:	0.91
11	Calibration Injection Volume (µL):	10
12	Injection Volume (µL):	10
13	absorbance of injection (100% yield):	328000.7806
14	monoborylated Paranitrotoluene	

	L	M					
21	202234.25	0.898	98.25	21	16139.18	0.392	22.37
22	269662.56	1.201	131.32	22	3024.35	0.071	4.04
23	237578.33	1.057	115.59	23	212.96	0.002	0.11
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25	316579.5	1.411	154.33	25	37.23	-0.002	-0.13
26	305273.38	1.360	148.79	26	115.96	0.000	-0.02
27		-0.009	-0.93	27		-0.003	-0.18
28	242849.75	1.080	118.17	28	9496.95	0.230	13.09
29	213253.3	0.948	103.66	29	5401.16	0.129	7.36
30	231314.52	1.029	112.52	30	493.76	0.009	0.51
31	233041.83	1.036	113.36	31	19154.25	0.466	26.59
32	214781.97	0.955	104.41	32	24775.4	0.604	34.44
33	105633.09	0.465	50.88	33	23493.15	0.573	32.65
34	208733.33	0.927	101.44	34	25758.78	0.628	35.82
35	457.49	-0.006	-0.71	35	36.76	-0.002	-0.13
36	241994.84	1.077	117.75	36	11890.29	0.288	16.43
37	274305.88	1.221	133.60	37	515.51	0.009	0.54
38		-0.009	-0.93	38		-0.003	-0.18
39	205181.91	0.912	99.70	39	19450.06	0.474	27.00
40	198559.56	0.882	96.45	40	26204.19	0.639	36.44
41	212583.09	0.945	103.33	41	68.92	-0.002	-0.09
42	254128.03	1.131	123.70	42	1484.67	0.033	1.89
43	183569.94	0.815	89.10	43	7750.01	0.187	10.65
44	159440.48	0.706	77.27	44	29064.89	0.709	40.44
45	181928.92	0.807	88.30	45	24713.21	0.603	34.36
46	295178.47	1.315	143.84	46	162.33	0.001	0.04
47	511.57	-0.006	-0.68	47	57040.29	1.395	79.54
48	297781.31	1.327	145.11	48	160.16	0.001	0.04
49		-0.009	-0.93	49		-0.003	-0.18
50		-0.009	-0.93	50		-0.003	-0.18
51		-0.009	-0.93	51		-0.003	-0.18

- 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

	39	40	41	42	43	44	45	46	47	48	49	50	51
Final Volume of Vial (µL):	600	1113.45	0.003	0.34	39	91555.23	1.482	84.48	39	205181.91	0.912	99.70	39
theoretical mg/µL:	8.77100	7913.02	0.022	2.41	40	162137.73	2.657	151.45	40	198559.56	0.882	96.45	40
Amount taken from crude (µL):	100	245642.02	0.685	74.89	41	632.69	-0.031	-1.79	41	212583.09	0.945	103.33	41
Fraction taken from crude:	0.166666667	311506.06	0.868	94.97	42	3767.83	0.021	1.18	42	254128.03	1.131	123.70	42
Mass taken from crude(mg):	0.8771	70899.34	0.198	21.62	43	63116.25	1.009	57.50	43	183569.94	0.815	89.10	43
Volume in Final Well (µL):	500	3644.28	0.010	1.11	44	6157.69	0.061	3.45	44	159440.48	0.706	77.27	44
(mg/mL) in Final Well:	1.75	3147.92	0.009	0.96	45	100227.53	1.626	92.71	45	181928.92	0.807	88.30	45
Calibration Injection Volume (µL):	10	359771.78	1.003	109.69	46	341.62	-0.036	-2.07	46	295178.47	1.315	143.84	46
Injection Volume (µL):	10	1049.79	0.003	0.32	47	534.32	-0.033	-1.88	47	511.57	-0.006	-0.68	47
absorbance of injection (100% yield):	35905.824	364922.63	1.017	111.26	48	409.94	-0.035	-2.00	48	297781.31	1.327	145.11	48
Compound 5			0.000	0.00	49		-0.042	-2.39	49		-0.009	-0.93	49
100% Yield Mass (mg):			0.000	0.00	50		-0.042	-2.39	50		-0.009	-0.93	50
Final Volume of Vial (µL):			0.000	0.00	51		-0.042	-2.39	51		-0.009	-0.93	51

1		
2	Paranitrotoluene	
3	100% Yield Mass (mg):	2.74276
4	Final Volume of Vial (μL):	600
5	theoretical mg/mL:	4.57127
6	Amount taken from crude (μL):	100
7	Fraction taken from crude:	0.166666667
8	Mass taken from crude(mg):	0.457126667
9	Volume in Final Well (μL):	500
10	(mg/mL) in Final Well:	0.91
11	Calibration Injection Volume (μL):	10
12	Injection Volume (μL):	10
13	absorbance of injection (100% yield):	328000.7806
14	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

40	Final Volume of Vial (μL):	600	39	1113.45	0.003	0.34	39	91555.23	1.482	84.48	39	19450.06	0.474	27.00
41	theoretical mg/μL:	8.77100	40	7913.02	0.022	2.41	40	162137.73	2.657	151.45	40	26204.19	0.639	36.44
42	Amount taken from crude (μL):	100	41	245642.02	0.685	74.89	41	632.69	-0.031	-1.79	41	68.92	-0.002	-0.09
43	Fraction taken from crude:	0.166666667	42	311506.06	0.868	94.97	42	3767.83	0.021	1.18	42	1484.67	0.033	1.89
44	Mass taken from crude(mg):	0.8771	43	70899.34	0.198	21.62	43	63116.25	1.009	57.50	43	7750.01	0.187	10.65
45	Volume in Final Well (μL):	500	44	3644.28	0.010	1.11	44	6157.69	0.061	3.45	44	29064.89	0.709	40.44
46	(mg/mL) in Final Well:	1.75	45	3147.92	0.009	0.96	45	100227.53	1.626	92.71	45	24713.21	0.603	34.36
47	Calibration Injection Volume (μL):	10	46	359771.78	1.003	109.69	46	341.62	-0.036	-2.07	46	162.33	0.001	0.04
48	Injection Volume (μL):	10	47	1049.79	0.003	0.32	47	534.32	-0.033	-1.88	47	57040.29	1.395	79.54
49	absorbance of injection (100% yield):	35905.824	48	364922.63	1.017	111.26	48	409.94	-0.035	-2.00	48	160.16	0.001	0.04
50	Compound 5		49		0.000	0.00	49		-0.042	-2.39	49		-0.003	-0.18
51	100% Yield Mass (mg):		50		0.000	0.00	50		-0.042	-2.39	50		-0.003	-0.18
51	Final Volume of Vial (μL):		51		0.000	0.00	51		-0.042	-2.39	51		-0.003	-0.18

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	85.77	14.49	-
4	-		96.38	7.84	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	-
44	-		-	-	-	-	-

- 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