

# Reaction Planning and Analysis

Excel File Edit View Insert Format Tools Data Window Help

Reaction Planning and Analysis

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Paragraph: Wrap Text, Merge & Center

Number: General, Currency, Percentage, Date, Time, Text, Fraction, Decimals

Conditional Formatting, Format as Table

Styles: 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													
10	C													
11	D													
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

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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)	Density (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		<u>There is 1μmol of ligand in each vial</u>													
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															

Ready

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

120%

- 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

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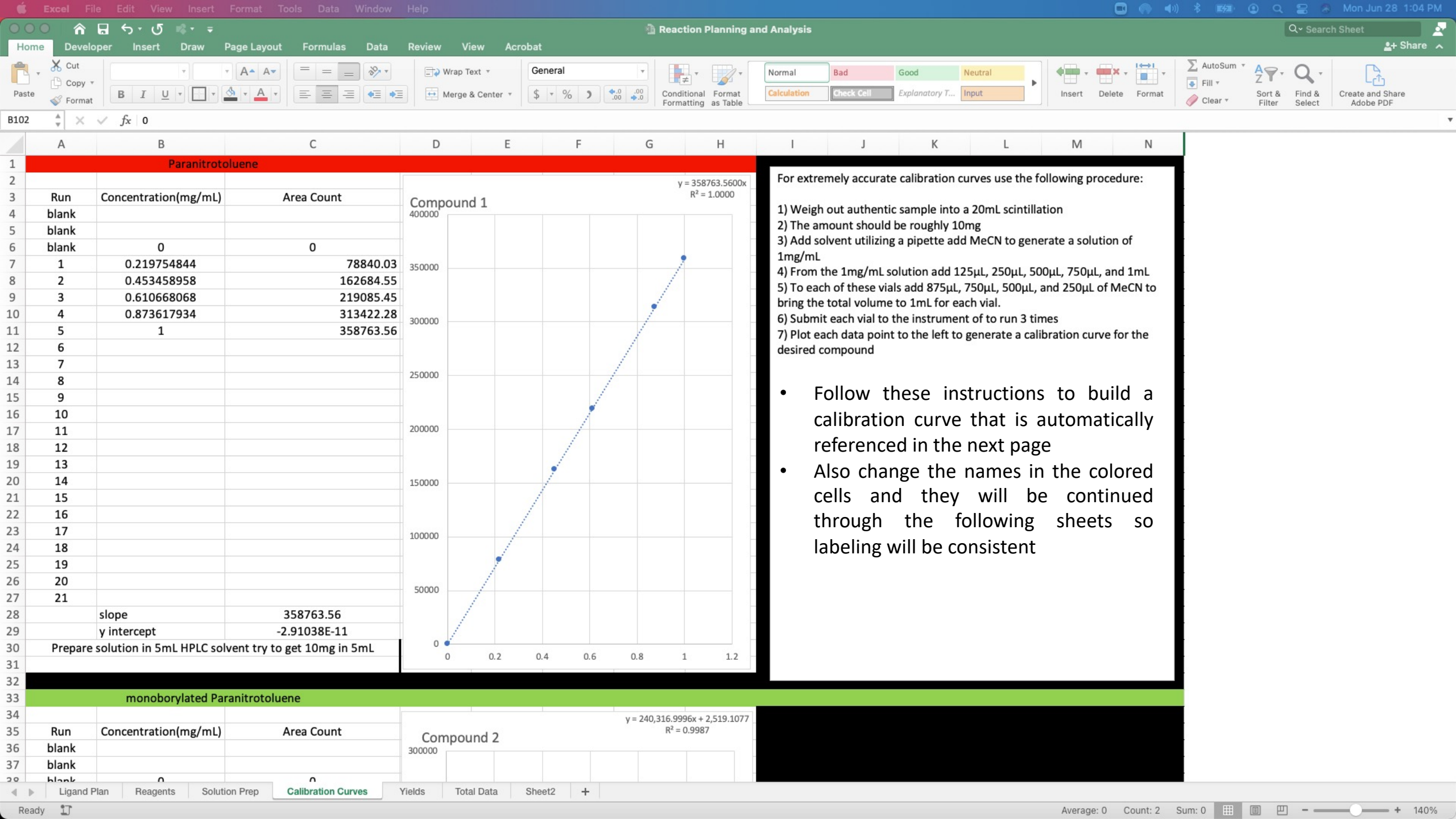
B17 fx Solution 6 Preparation

	A	B	C
1			
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!	
25			

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  $\mu\text{L}$





Reaction Planning and Analysis

Search Sheet

Share

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B32.74276

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V
				Plate Well	Area Count	Product (mg)	Yield %		Plate Well	Area Count	Product (mg)	Yield %		Plate Well	Area Count	Product (mg)	Yield %		Plate Well	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													114.06		10	225.24	0.002	0.13
11	Injection Volume (µL):	10		11													50.30		11	38658.39	0.945	53.85
12	absorbance of injection (100% yield):	328000.7806		12													75.63		12	1144.78	0.025	1.42
13	monoborylated Paranitrotoluene			13													87.14		13	26750.5	0.653	37.20
14	100% Yield Mass (mg):	5.2626		14													-0.88		14	35521.51	0.868	49.46
15	Final Volume of Vial (µL):	600		15													84.40		15	27228.77	0.664	37.87
16	theoretical mg/µL:	8.77100		16													81.63		16	24923.73	0.608	34.65
17	Amount taken from crude (µL):	100		17													78.76		17	16298.64	0.396	22.60
18	Fraction taken from crude:	0.166666667		18													73.28		18	4582.79	0.109	6.22
19	Mass taken from cude(mg):	0.8771		19													83.74		19	27177.06	0.663	37.80
20	Volume in Final Well (µL):	500		20													123.94		20	20.63	-0.003	-0.16
21	(mg/mL) in Final Well:	1.75		21													98.25		21	16139.18	0.392	22.37
22	Calibration Injection Volume (µL):	10		22													131.32		22	3024.35	0.071	4.04
23	Injection Volume (µL):	10		23													115.59		23	212.96	0.002	0.11
24	absorbance of injection (100% yield):	107910.128		24													132.69		24	1262.59	0.028	1.58
25	metanitrotoluene			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

Ligand PlanReagentsSolution PrepCalibration CurvesYieldsTotal DataSheet2+

Ready

80%

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

3

4

5

6

7

8

9

10

11

12

13

14

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:0.16666667

Mass taken from crude(mg):0.45712667

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:0.16666667

Mass taken from crude(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):

391113.450.0030.34

407913.020.0222.41

41245642.020.68574.89

42311506.060.86894.97

4370899.340.19821.62

443644.280.0101.11

453147.920.0090.96

46359771.781.003109.69

471049.790.0030.32

48364922.631.017111.26

490.0000.00

500.0000.00

510.0000.00

3991555.231.482

40162137.732.657

41632.69-0.031-1.79

423767.830.0211.18

4363116.251.00957.50

446157.690.0613.45

45100227.531.62692.71

46341.62-0.036-2.07

47534.32-0.033-1.88

48409.94-0.035-2.00

49-0.042-2.39

50-0.042-2.39

51-0.042-2.39

Yield %

6.96

4.34

24.28

-1.85

62.28

-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

84.48

151.45

-1.79

1.18

57.50

3.45

92.71

-2.07

-1.88

-2.00

-2.39

-2.39

-2.39

21202234.250.89898.25

22269662.561.201131.32

23237578.331.057115.59

242724501.213132.69

25316579.51.411154.33

26305273.381.360148.79

27-0.009-0.93

28242849.751.080118.17

29213253.30.948103.66

30231314.521.029112.52

31233041.831.036113.36

32214781.970.955104.41

33105633.090.46550.88

34208733.330.927101.44

35457.49-0.006-0.71

36241994.841.077117.75

37274305.881.221133.60

38-0.009-0.93

39205181.910.91299.70

40198559.560.88296.45

41212583.090.945103.33

42254128.031.131123.70

43183569.940.81589.10

44159440.840.70677.27

45181928.920.80788.30

46295178.471.315143.84

47511.57-0.006-0.68

48297781.311.327145.11

49-0.009-0.93

50-0.009-0.93

51-0.009-0.93

2116139.180.39222.37

223024.350.0714.04

23212.960.0020.11

241262.590.0281.58

2537.23-0.002-0.13

26115.960.000-0.02

27-0.003-0.18

289496.950.23013.09

295401.160.1297.36

30493.760.0090.51

3119154.250.46626.59

3224775.40.60434.44

3323493.150.57332.65

3425758.780.62835.82

3536.76-0.002-0.13

3611890.290.28816.43

37515.510.0090.54

38-0.003-0.18

3919450.060.47427.00

4026204.190.63936.44

4168.92-0.002-0.09

421484.670.0331.89

437750.010.18710.65

4429064.890.70940.44

4524713.210.60334.36

46162.330.0010.04

4757040.291.39579.54

48160.160.0010.04

49-0.003-0.18

50-0.003-0.18

51-0.003-0.18

Reaction Planning and Analysis

Search Sheet

Ready

Ligand Plan

Reagents

Solution Prep

Calibration Curves

Yields

Total Data

Sheet2

+

98%

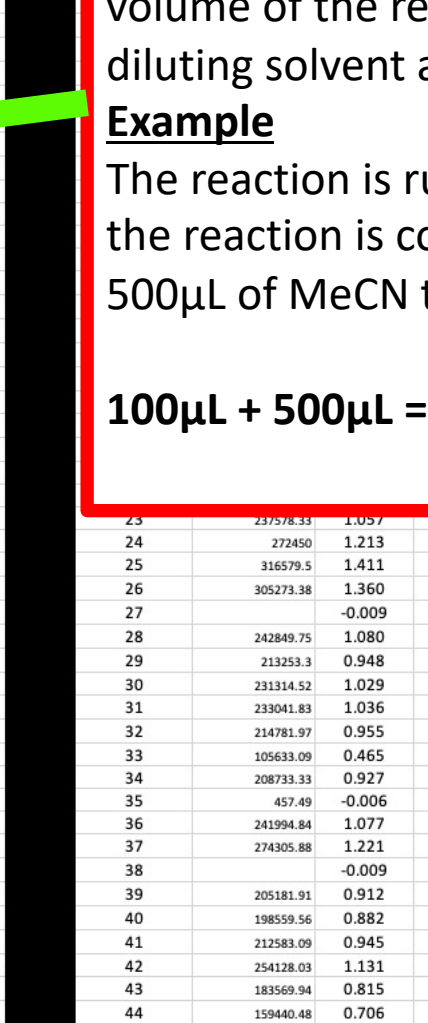
- ### Consumption of Starting Material

  - 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





The screenshot shows a spreadsheet with column L highlighted in green. The values in column L are: 6.96, 4.34, 24.28, 7.84, -1.83, -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, 84.48, 151.45, -1.79, 1.18, 57.50, 3.45, 92.71, -2.07, -1.88, -2.00, -2.39, -2.39, 2.39. A green arrow points to the value -1.83 in row 12.

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.

**Example**

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**

## Example

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		39	1113.45	0.003	0.34		39	91555.23	1.482	84.48		38	-0.009	-0.93		38	-0.003	-0.18		
41	theoretical mg/µL:	8.77100		40	7913.02	0.022	2.41		40	162137.73	2.657	151.45		39	0.912	96.70		39	19450.06	0.474	27.00	
42	Amount taken from crude (µL):	100		41	245642.02	0.685	74.89		41	632.69	-0.031	-1.79		40	198559.56	0.882	96.45		40	26204.19	0.639	36.44
43	Fraction taken from crude:	0.166666667		42	311506.06	0.868	94.97		42	3767.83	0.021	1.18		41	212583.09	0.945	103.33		41	68.92	-0.002	-0.09
44	Mass taken from crude(mg):	0.8771		43	70899.34	0.198	21.62		43	63116.25	1.009	57.50		42	254128.03	1.131	123.70		42	1484.67	0.033	1.89
45	Volume in Final Well (µL):	500		44	3644.28	0.010	1.11		44	6157.69	0.061	3.45		43	183569.94	0.815	89.10		43	7750.01	0.187	10.65
46	(mg/mL) in Final Well:	1.75		45	3147.92	0.009	0.96		45	100227.53	1.626	92.71		44	159440.48	0.706	77.27		44	29064.89	0.709	40.44
47	Calibration Injection Volume (µL):	10		46	359771.78	1.003	109.69		46	341.62	-0.036	-2.07		45	181928.92	0.807	88.30		45	24713.21	0.603	34.36
48	Injection Volume (µL):	10		47	1049.79	0.003	0.32		47	534.32	-0.033	-1.88		46	295178.47	1.315	143.84		46	162.33	0.001	0.04
49	absorbance of injection (100% yield):	35905.824		48	364922.63	1.017	111.26		48	409.94	-0.035	-2.00		47	511.57	-0.006	-0.68		47	57040.29	1.395	79.54
50	Compound 5			49		0.000	0.00		49		-0.042	-2.39		48	297781.31	1.327	145.11		48	160.16	0.001	0.04
51	100% Yield Mass (mg):			50		0.000	0.00		50		-0.042	-2.39		49		-0.009	-0.93		49		-0.003	-0.18
52	Final Volume of Vial (µL):			51		0.000	0.00		51		-0.042	-2.39		50		-0.009	-0.93		50		-0.003	-0.18



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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

Yield %

6.96

4.34

24.28

7.84

-1.83

62.28

-1.90

-0.69

-1.85

5.78

12.48

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

84.48

151.45

-1.79

1.18

57.50

3.45

92.71

-2.07

-1.88

-2.00

-2.39

-2.39

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202234.25

269662.56

237578.33

272450

316579.5

305273.38

-0.009

242849.75

213253.3

231314.52

233041.83

214781.97

105633.09

208733.33

457.49

241994.84

274305.88

-0.009

205181.91

198559.56

212583.09

254128.03

183569.94

159440.88

181928.92

295178.47

511.57

297781.31

-0.009

-0.93

98.25

131.32

115.59

132.69

154.33

148.79

-0.93

118.17

103.66

112.52

113.36

104.41

50.88

101.44

-0.71

117.75

133.60

99.70

96.45

103.33

123.70

89.10

77.27

88.30

143.84

-0.68

145.11

-0.93

-0.93

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16139.18

3024.35

212.96

1262.59

37.23

115.96

-0.003

9496.95

5401.16

493.76

19154.25

24775.4

23493.15

25758.78

36.76

11890.29

515.51

-0.003

19450.06

26204.19

68.92

1484.67

7750.01

29064.89

24713.21

162.33

57040.29

160.16

-0.003

-0.003

0.392

0.071

0.002

0.028

-0.002

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-0.003

0.230

0.129

0.009

0.466

0.604

0.573

0.628

-0.002

0.288

0.009

0.474

0.639

-0.002

0.033

0.187

0.709

0.603

0.001

1.395

0.001

-0.003

-0.003

22.37

4.04

0.11

1.58

-0.13

-0.02

-0.18

13.09

7.36

0.51

26.59

34.44

32.65

35.82

-0.13

16.43

0.54

27.00

36.44

-0.09

1.89

10.65

40.44

34.36

0.04

79.54

0.04

-0.18

-0.18

Ready

Ligand Plan

Reagents

Solution Prep

Calibration Curves

Yields

Total Data

Sheet2

+

• 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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Paranitrotoluene

100% Yield Mass (mg):2.74276

Final Volume of Vial (µL):600

theoretical mg/mL:4.57127

Amount taken from crude (µL):100

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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

Yield %

6.96

4.34

24.28

7.84

-1.83

62.28

-1.90

-0.69

-1.88

-1.40

66.78

102.48

100.12

11.22

90.50

51.76

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

84.48

151.45

-1.79

1.18

57.50

3.45

92.71

-2.07

-1.88

-2.00

-2.39

-2.39

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172633.98

254604.66

202234.25

269662.56

237578.33

272450

316579.5

305273.38

-0.009

242849.75

213253.3

231314.52

233041.83

214781.97

105633.09

208733.33

457.49

241994.84

274305.88

-0.009

205181.91

198559.56

212583.09

254128.03

183569.94

159440.48

181928.92

295178.47

511.57

297781.31

-0.009

-0.93

99.70

96.45

103.33

123.70

89.10

77.27

88.30

143.84

-0.68

145.11

-0.93

-0.93

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27177.06

20.63

16139.18

3024.35

212.96

1262.59

37.23

115.96

-0.003

9496.95

5401.16

493.76

19154.25

24775.4

23493.15

25758.78

36.76

11890.29

515.51

-0.003

19450.06

26204.19

68.92

1484.67

7750.01

29064.89

24713.21

162.33

57040.29

160.16

-0.003

-0.003

0.663

-0.003

0.392

0.071

0.002

0.028

-0.002

0.000

-0.003

0.230

0.129

0.009

0.466

0.604

0.573

0.628

-0.002

0.288

0.009

-0.003

0.474

0.639

-0.002

0.033

0.187

0.709

0.603

0.001

1.395

0.001

-0.003

-0.003

37.80

-0.16

22.37

4.04

0.11

1.58

-0.13

-0.02

-0.18

13.09

7.36

0.51

26.59

34.44

32.65

35.82

-0.13

16.43

0.54

-0.18

27.00

36.44

-0.09

1.89

10.65

40.44

34.36

0.04

79.54

0.04

-0.18

-0.18

Reaction Planning and Analysis

Search Sheet

Ready

100%

- 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



+ Share										
L	M	N	O	P	Q	R	S	T	U	V
		metanitrotoluene					monoborylated metanitrotoluene			
Yield %		Plate Well	Area Count	Product (mg)	Yield %		Plate Well	Area Count	Product (mg)	Yield %
6.96		1	185101.27	0.821	89.85		1	3857.35	0.091	5.21
4.34		2	191022.67	0.848	92.76		2	1869.76	0.043	2.43
24.28		3	175766.25	0.780	85.27		3	10501.81	0.254	14.49
7.84		4	162671.8	0.721	78.85		4	8935.55	0.216	12.30
-1.83		5	480.12	-0.006	-0.70		5	214.69	0.002	0.12
62.28		6	137995.13	0.610	66.75		6	21068.75	0.513	29.26

- |  |       |
|--|-------|
|  | 37.57 |
|  | 5.71  |
|  | -2.07 |
|  | 5.26  |
|  | -1.46 |
|  | 2.39  |
|  | 61.90 |
|  | 13.28 |

Ready Ligand Plan Reagents Solution Prep Calibration Curves **Yields** Total Data Sheet2 + 80%

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		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