On the Use of "Green" Metrics in the Undergraduate Organic Chemistry Lecture and Lab to Assess the Mass Efficiency of Organic Reactions

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Supplementary Material

Derivation of Eq 1 and Eq 4

Given a general chemical transformation given by

$$A + B \rightarrow P + Q$$

where A and B are reagents, P is the target product of interest, and Q is the by-product.

If a, b, p, and q represent the corresponding molecular weights of all chemical species, c, s, and ω represent the masses of reaction solvent, catalyst, and all post-reaction materials, respectively, and x, z, and y represent the number of moles of A, B, and P where A is the limiting reagent so that $z > x$, and the reaction yield is $\varepsilon = y/x$, then we can write a conservation of mass law as

$$ax + bz + c + s + \omega = py + qy + w + c + s + \omega$$

where w is the mass of waste due to unreacted starting materials.

By definition, the atom economy is given by

$$AE = \frac{p}{p+q} = \frac{p}{a+b},$$

the excess moles of B that are used is $\phi = z - x$, the mass of product collected is $m_p = py$, and the stoichometric factor is given by

$$SF = 1 + \frac{b\phi}{x(a+b)}.$$

The environmental impact factor based on mass, E_m, is then

$$\begin{aligned}
E_m &= \frac{\text{total mass of waste}}{\text{mass of target product}} \\
&= \frac{qy + w + c + s + w}{py} \\
&= \frac{ax + bz + c + s + \omega - py}{py} \\
&= \frac{ax + bz + c + s + \omega}{py} - 1 \\
&= \frac{ax + bx + b\phi + c + s + \omega}{py} - 1 \\
&= \frac{a + b + \dfrac{b\phi + c + s + \omega}{x}}{p\left(\dfrac{y}{x}\right)} - 1 \\
&= \frac{a + b + \dfrac{b\phi + c + s + \omega}{x}}{p\varepsilon} - 1 \\
&= \frac{1 + \dfrac{b\phi + c + s + \omega}{x(a+b)}}{\dfrac{p\varepsilon}{a+b}} - 1 \\
&= \frac{\left\lceil 1 + \dfrac{b\phi}{x(a+b)} \right\rceil + \dfrac{c + s + \omega}{x(a+b)}}{(AE)\varepsilon} - 1 \\
&= \frac{(SF) + \dfrac{c + s + \omega}{x(a+b)}}{(AE)\varepsilon} - 1 \\
&= \frac{(SF)\left(1 + \dfrac{c + s + \omega}{x(a+b)(SF)}\right)}{(AE)\varepsilon} - 1
\end{aligned}$$

$$= \frac{(SF)\left(1+\frac{c+s+\omega}{\frac{y}{\varepsilon}\frac{p}{(AE)}(SF)}\right)}{(AE)\varepsilon} - 1$$

$$= \frac{(SF)\left(1+\frac{(AE)\varepsilon(c+s+\omega)}{m_P(SF)}\right)}{(AE)\varepsilon} - 1$$

Define the materials recovery parameter, MRP, as

$$MRP = \frac{1}{1+\frac{(AE)\varepsilon(c+s+\omega)}{m_P(SF)}}.$$

Then,

$$E_m = \frac{(SF)\left(\frac{1}{MRP}\right)}{\varepsilon(AE)} - 1 = \frac{1}{\frac{\varepsilon(AE)(MRP)}{(SF)}} - 1 = \frac{1}{RME} - 1$$

where $RME = \frac{\varepsilon(AE)(MRP)}{(SF)}$.

Cell Definitions and Formulas in Excel template file:

C53 = E53/B53
moles of product = mass of product collected (g)/MW product (g/mol)

D53 = C53/(MIN(E12:E15))
reaction yield = moles of product collected/moles of limiting reagent

F53 = F50/E53
cost of product ($/g) = total cost of input materials ($)/mass of product collected (g)

B58 = MIN(E12:E15)
reaction scale (moles) = moles of limiting reagent

B59 = (B16-B53)/B53
E(mw) = [Total MW reagents – MW product]/MW product

B60 = B53/B16
AE = MW product/Total MW reagents

Under reclaiming reaction solvents, catalysts, and byproducts, and all post-reaction materials:

B63 = F16-E53
Mass of waste (g) = total mass of reagents (g) – mass of product collected (g)

B64 = B63/E53
E(m) = mass of waste (g)/mass of product collected (g)

B65 = 1/(1+B64)
RME = 1/(1 + E(m))

B66 = D53*B60/B65
SF = (reaction yield)*AE/RME

B67 = (1-B65)*(F50-H21-G26-G47)
Wasted input costs ($) = (1 – RME)*(total cost of input materials - sum of cost of retrieved materials)

Under committing all reaction solvents, catalysts, and byproducts, and post-reaction materials to waste:

B70 = E50 - E53
Mass of waste (g) = total mass of input materials (g) – mass of product collected (g)

B71 = B70/E53
E(m) = mass of waste (g)/mass of product collected (g)

B72 = 1/(1+B71)
RME = 1/(1 + E(m))

B73 = (1-B72)*F50
Wasted input costs ($) = (1 – RME)*total cost of input materials

Check formula (see eq 1 in text):

B75 = (D53*B60/B66)*E53/(E53+(D53*B60/B66)*(E47+E26+F21))

where,
D53 = reaction yield
B60 = AE
B66 = SF
E53 = mass of product collected (g)
E47 = mass of post-reaction materials (g)
E26 = mass of reaction solvents (g)
F21 = mass of reaction catalysts (g)

Radial Pentagon Parameters:

Parameter	Complete Reclaiming	Partial Reclaiming	No Reclaiming	Ideal
AE	B60	B60	B60	1
Rxn Yield	D53	D53	D53	1
1/SF	1/B66	1/B66	1/B66	1
MRP	1	M64/(D53*B60/B66)	B75/(D53*B60/B66)	1
RME	B65	B80	B72	1

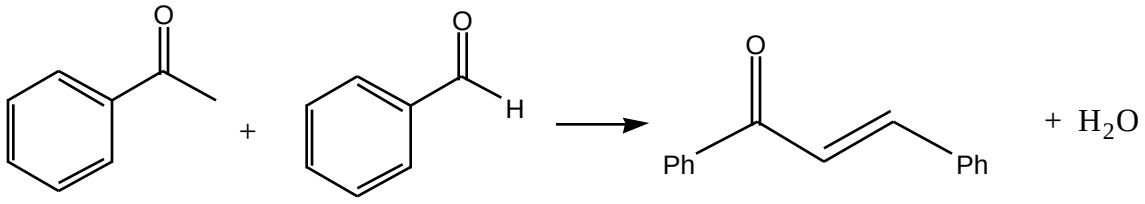
Course Syllabus

Section	Topics
Part 1: Chemistry and Society	- development and chronology of organic chemistry - development and chronology of industrial chemistry - industrial accidents - responsible care - relationship between media and chemical scientists - views from chemical societies (CIC (Chemical Institute of Canada), ACS (American Chemical Society))
Part 2: The Business of Doing Chemistry	- highlights from Chemical and Engineering News articles - career development in the chemical industry - Patents - Markush Structures - Confidentiality Agreements
Part 3: Survey of Modern Concerns	- thalidomide - phthalate esters - insecticides and herbicides - pharmaceuticals in the environment - acrylamide formation in fried and oven-cooked foods - insect repellent (DEET, diethyl-meta-toluidine) - lead emissions in the atmosphere - methyl t-butyl ether as gasoline additive - biodiesel - energy use for chemical processes

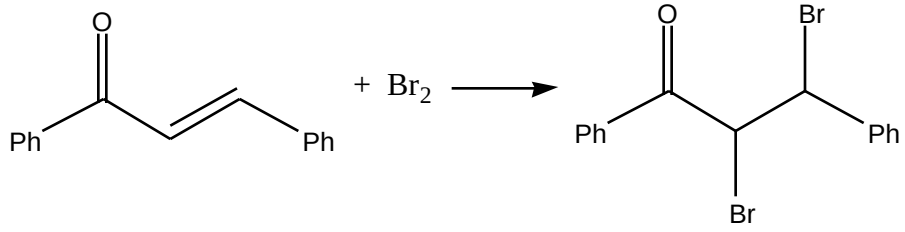
Part 4: Green Chemistry I: Technologies	- general principles - new and emerging technologies: ionic liquids, ultrasound, microwave irradiation, grindstone chemistry, microchannel reactors, biotransformations - application to old reactions: survey of literature
Green Chemistry II: Chemical Accounting	- general paradigm for carrying out organic reactions in the academic laboratory - general paradigm for carrying out industrial reactions - parameters involved in optimization of organic synthesis - chemical processing: unit operations, unit reactions - quantification of "greenness": atom economy, reaction mass efficiency, enviromental impact factor reaction metrics - key relationships between metrics - effect of recycling - concept of minimum atom economy - concept of "golden" atom economy threshold - probability of achieving minimum atom economy and RME thresholds - application of reaction metrics to classic organic reactions: substitutions, redox reactions, rearrangements, carbon-carbon bond forming reactions, non-carbon-carbon forming reactions, multi-component reactions - synthesis trees analysis: degree of convergence, degree of asymmetry, overall RME, overall raw material cost (RMC) - detailed analysis of synthesis plans: ibuprofen, aspirin, methamphetamine, triclosan, nicotine, caffeine, thalidomide, tartrazine, prontosil, quinine (Woodward-Doering-Rabe and Stork)
Part 5: Dyestuffs	- mauveine, indigo, anthraquinone dyes (alizarin), azo dyes, phenolphthalein dyes, triphenylmethane dyes, phthalocyanines, concept of colour
Part 6: Pharmaceuticals	- narcotics - therapeutics - drug action

Part 7: Industrial Feedstocks	- industrial chemical trees - Group I: ethylene, ethylene oxide, propene, acrylonitrile, 1,3-butadiene, vinyl chloride - Group II: cyclohexane, nylon - Group III: benzene, toluene, ethylbenzene, styrene, cumene, phenol, aniline - Group IV: acetone, ammonia, urea, ethyl acetate, acetonitrile, diethyl ether, THF, ethanol, chloroform, carbon tetrachloride
Part 8: Chemistry of "Everyday" Experience (topics for independent research written assignment)	- Petroleum related chemistry (fuels, polymers) - Personal care products and cosmetics - Detergents and cleaners (soaps, surfactants, solvents) - Food additives (preservatives, colourants, dyes) - Agricultural practice (pesticides, natural defense chemicals, fertilizers) - Common and Modern Pharmaceuticals (drugs)

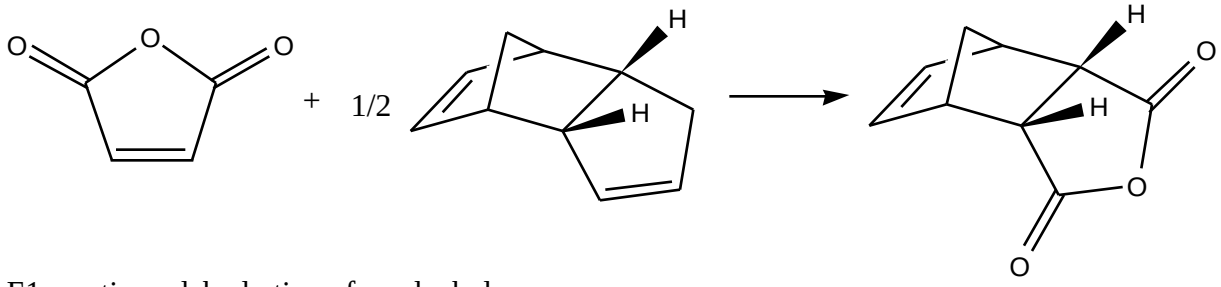
Aldol condensation



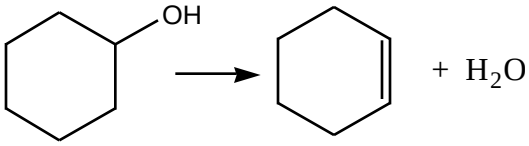
Bromination of an olefin



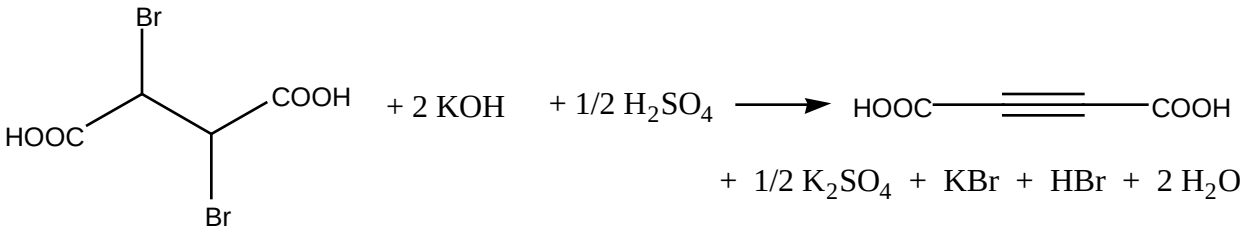
Diels-Alder reaction



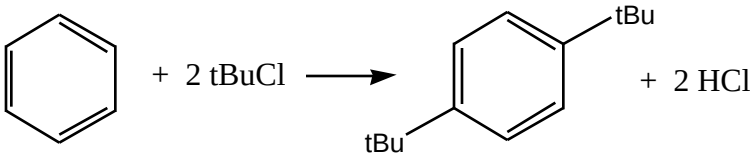
E1 reaction: dehydration of an alcohol



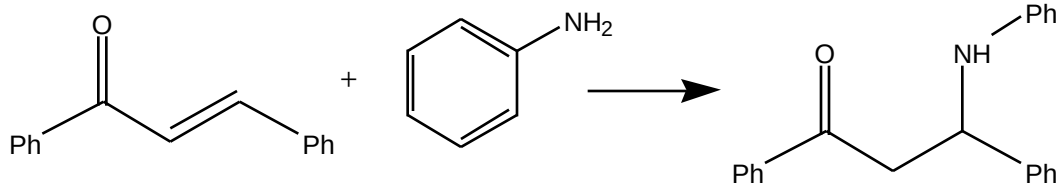
E2 reaction: debromination of an alkyl halide



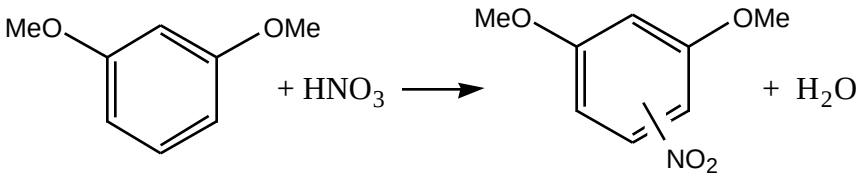
Friedel-Crafts alkylation reaction



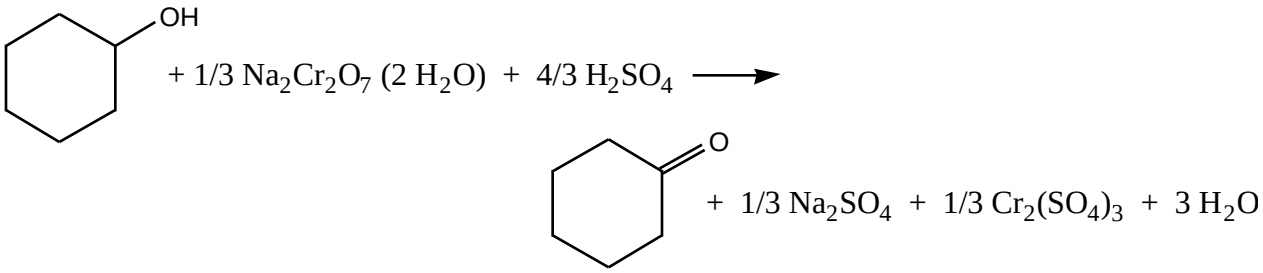
Michael 1,4-addition reaction



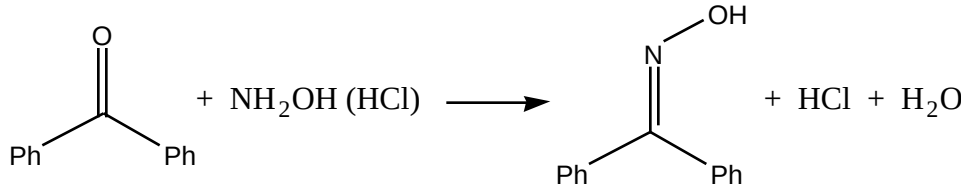
Aromatic nitration



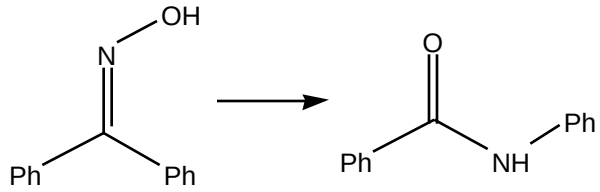
Oxidation of secondary alcohol



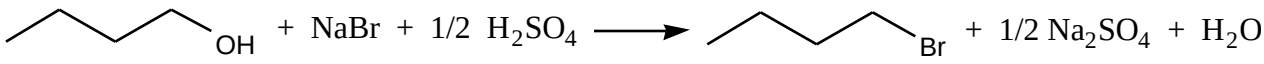
Oximation



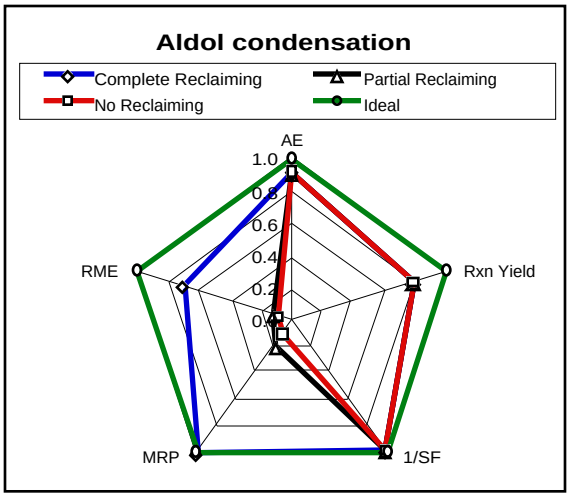
Beckmann rearrangement

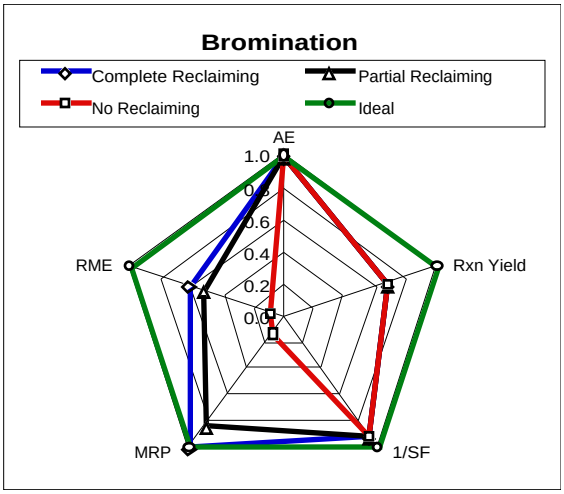


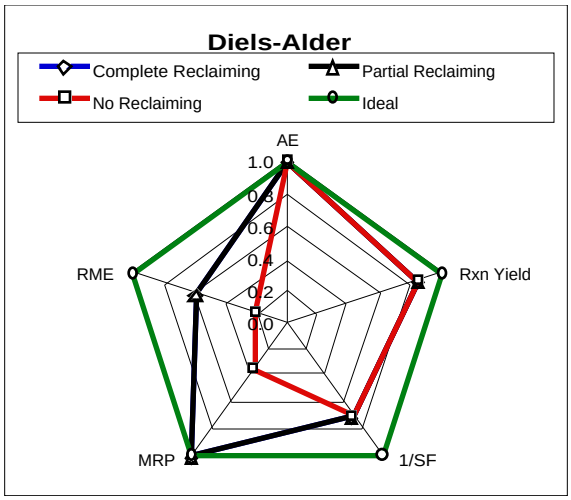
SN2 reaction: bromination of a primary alcohol

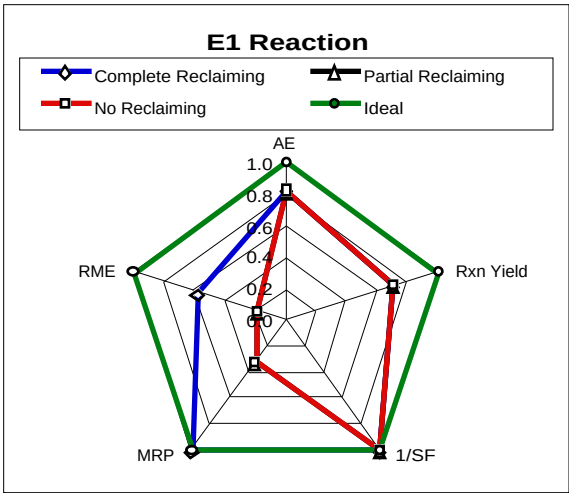


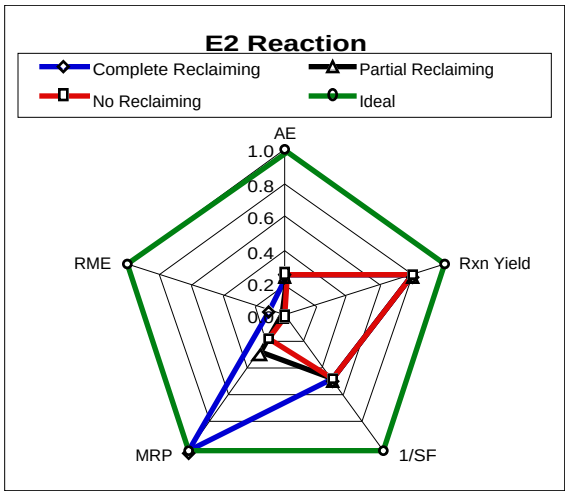
Scheme 2


Aldol condensation
Complete Reclaiming
Partial Reclaiming
No Reclaiming
Ideal
AE
1.0
0.8
0.6
0.4
0.2
0.0
RME
Rxn Yield
MRP
1/SF


Bromination
Complete Reclaiming
Partial Reclaiming
No Reclaiming
Ideal
AE
1.0
0.6
0.4
0.2
0.0
RME
Rxn Yield
MRP
1/SF


Diels-Alder
Complete Reclaiming
Partial Reclaiming
No Reclaiming
Ideal
AE
1.0
0.6
0.4
0.2
0.0
RME
Rxn Yield
MRP
1/SF


E1 Reaction
Complete Reclaiming
Partial Reclaiming
No Reclaiming
Ideal
AE
1.0
0.8
0.6
0.4
0.2
0.0
RME
Rxn Yield
MRP
1/SF


E2 Reaction
Complete Reclaiming
Partial Reclaiming
No Reclaiming
Ideal
AE
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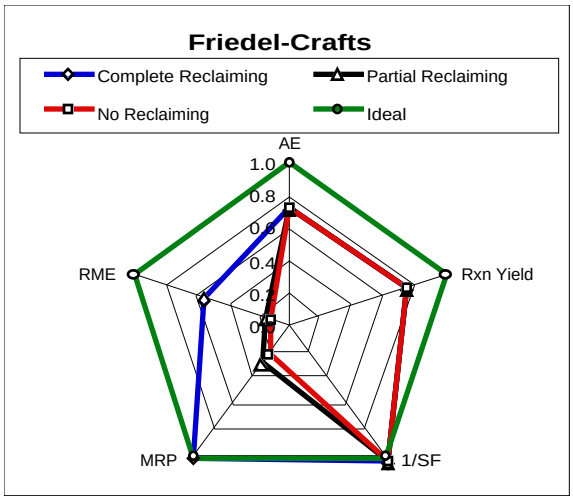
0.8
0.6
0.4
0.2
0.0
RME
Rxn Yield
MRP
1/SF


Friedel-Crafts
Complete Reclaiming
Partial Reclaiming
No Reclaiming
Ideal
AE
1.0
0.8
0.4
RME
Rxn Yield
MRP
1/SF

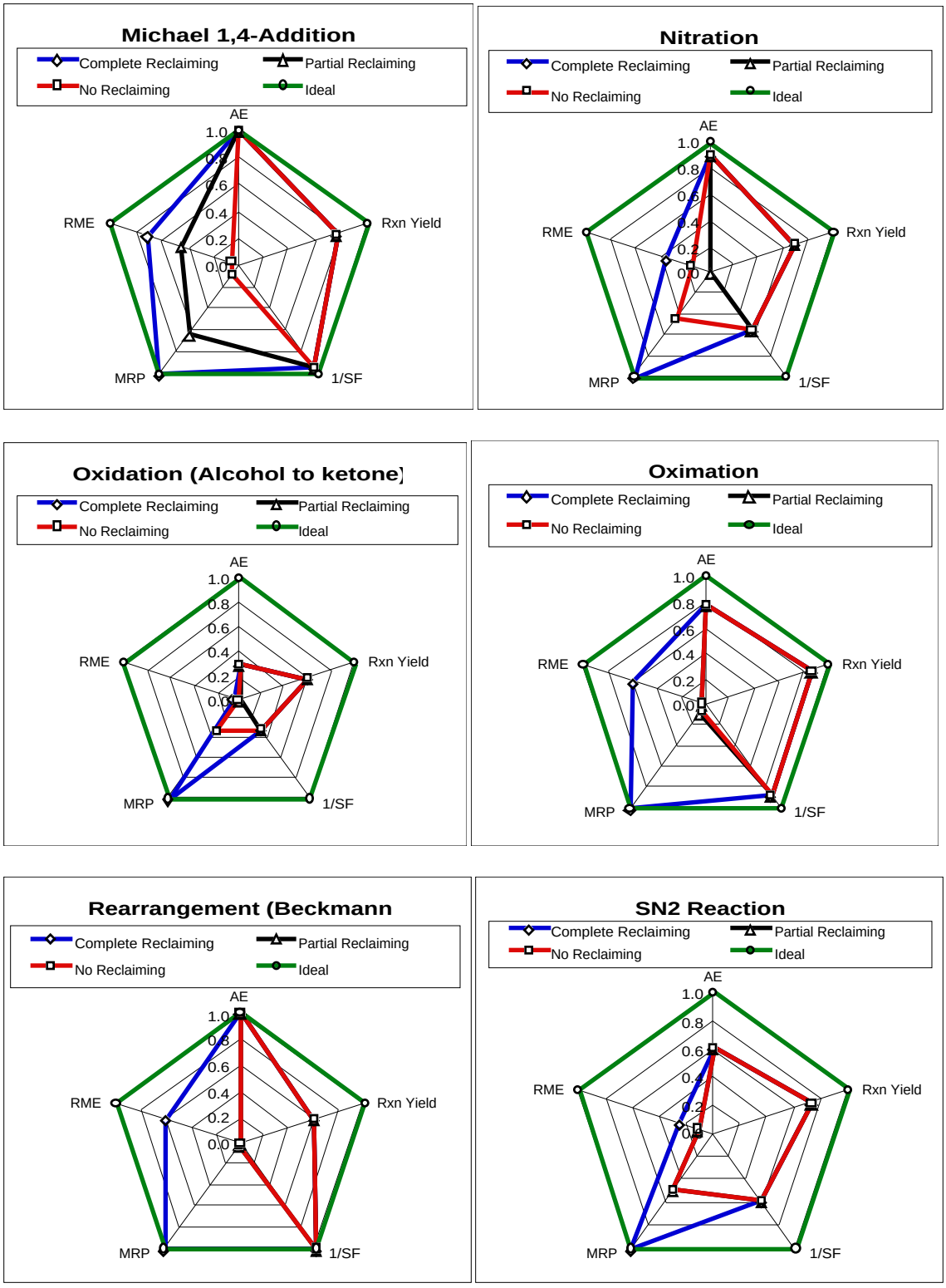


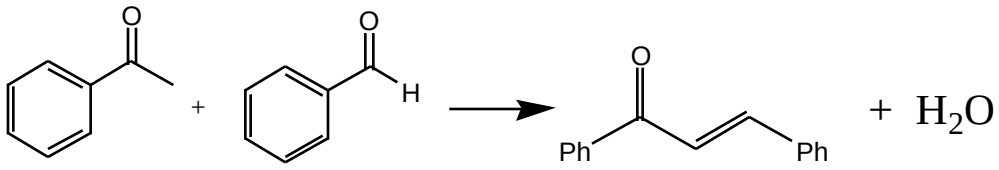
Figure 4. Radial pentagons representing RME values under various scenarios for a variety of reaction types. See **Scheme 2** for balanced chemical reactions.

Example EXCEL Template Outputs:

Aldol Condensation

REACTION METRICS FORM

DATE: May 31, 2005
NAME OF TARGET PRODUCT: trans-Benzal acetophenone
REACTION CLASSIFICATION: Carbon-carbon bond forming



BALANCED CHEMICAL EQUATIONS:

PART 1: RAW MATERIALS USAGE

(A) REACTION STAGE:

(i) REAGENTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
acetophenone	120	1.03	3	0.02575	3.09	0.0321	0.099	12
benzaldehyde	106	1.046	2.5	0.0247	2.615	0.0149	0.039	13
								14
								15
TOTAL REAGENTS	226			Add lines 12 to 15	5.705		0.138	**16**

(ii) CATALYSTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
3 M NaOH (12 %)	40	1.1309	12.5	0.353406 25	14.1362 5	0.0177	0.030	19
							0.000	20
TOTAL CATALYSTS				Add lines 19 to 20	14.1362 5		0.030	**21**

(iii) SOLVENTS	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
95% EtOH	0.816	7.5	6.1200	0.0422	0.258	24
					0.000	25
TOTAL SOLVENTS		Add lines 24 to 25	6.12		0.258	**26**

Reaction Materials Subtotals		Add lines 16, 21, 26	25.96125		0.427	**29**

(B) WORK-UP STAGE:

MATERIAL	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
H2O	1	10	10.000	0	0.000	33
95% EtOH	0.816	10	8.160	0.0422	0.344	34
					0.000	35
					0.000	36
TOTAL WORK-UP MATERIALS		Add lines 33 to 36	18.16		0.344	**37**

(C) PURIFICATION STAGE:

MATERIAL	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
95 % EtOH	0.816	10	8.160	0.0422	0.344	41
					0.000	42
					0.000	43
					0.000	44
TOTAL PURIFICATION MATERIALS		Add lines 41 to 44	8.16		0.344	**45**
Post-reaction Materials Subtotals		Add lines 37, 45	26.32		0.689	**47**

		Mass (g)	Cost ($)	
TOTAL INPUT MATERIALS	Add lines 29, 47	52.28125	1.115	**50**

	MW (g/mol)	Moles	Yield	Mass (g)	Cost ($/g)	
OUTPUT TARGET PRODUCT	208	0.0192	0.7795	4	0.279	**53**

PART 2: GREEN METRICS ANALYSIS

Limiting reagent: benz-aldehyde

PARAMETER	VALUE		
Reaction Scale	0.025	moles	**58**
E(mw)	0.087	MW byproducts/MW product	**59**
AE	0.920	MW product/Σ MW reagents	**60**

(i) Under reclaiming reaction solvents, catalysts, and byproducts, and all post-reaction materials

Mass of waste (line 16 - 53)	1.705	g	**63**
E(m)	0.426	g waste/g product	**64**
RME	0.701	g product/Σ g reagents	**65**
SF	1.023		**66**

Wasted input costs ($)	0.041		

(ii) Under committing all reaction solvents, catalysts, and byproducts, and post-reaction materials to waste

Mass of waste (line 50 - 53)	48.281	g	**69**
E(m)	12.070	g waste/g product	**70**
RME	0.077	g product/Σ g reagents	**71**
Wasted input costs ($)	1.030		
Check formula	0.077		

(iii) Under reclaiming EtOH

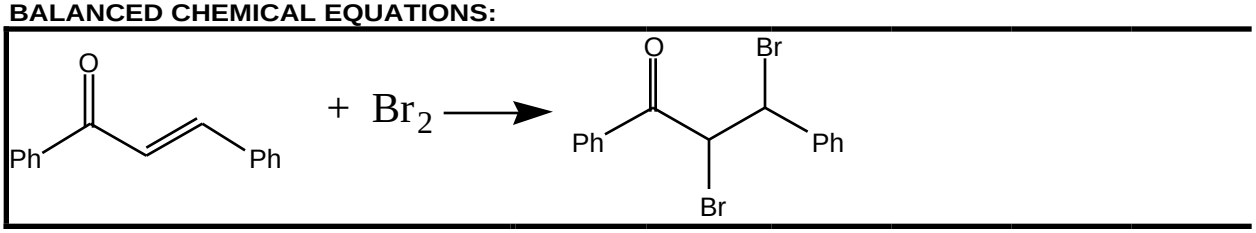
Mass of waste	26.963	g	**76**
E(m)	6.741	g waste/g product	**77**
RME	0.129	g product/Σ g reagents	**78**
Wasted input costs ($)	0.671		

Bromination of an Olefin

REACTION METRICS FORM

DATE: May 31, 2005
NAME OF TARGET PRODUCT: benzalacetophenone dibromide
REACTION CLASSIFICATION: Non-carbon-carbon bond forming

BALANCED CHEMICAL EQUATIONS:



PART 1: RAW MATERIALS USAGE

(A) REACTION STAGE:

(i) REAGENTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
trans-benzal acetophenone	208			0.00240	0.5	0.373	0.187	12
bromine	159.8	3.119	0.15	0.00293	0.468	0.147	0.069	13
							0.000	14
							0.000	15

TOTAL REAGENTS	367.8			Add lines 12 to 15	0.968	0.255	**16**

(ii) CATALYSTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
None	0	0	0	0	0	0	0.000	19
							0.000	20

TOTAL CATALYSTS	Add lines 19 to 20	0	0.000	**21**

(iii) SOLVENTS	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
CH2Cl2	1.336	2	2.672	0.0146	0.039	24
					0.000	25

TOTAL SOLVENTS	Add lines 24 to 25	2.672	0.039	**26**

Reaction Materials Subtotals	Add lines 16, 21, 26	3.63985	0.294	**29**

(B) WORK-UP STAGE:

MATERIAL	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
None	0	0	0	0	0.000	33
					0.000	34
					0.000	35
					0.000	36

TOTAL WORK-UP MATERIALS	Add lines 33 to 36	0	0.000	**37**

(C) PURIFICATION STAGE:

MATERIAL	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
95 % EtOH	0.816	5	4.08	0.0422	0.172	41
					0.000	42
					0.000	43
					0.000	44

TOTAL PURIFICATION MATERIALS	Add lines 41 to 44	4.08	0.172	**45**

Post-reaction Materials Subtotals	Add lines 37, 45	4.08	0.172	**47**

		Mass (g)	**Cost ($)**	
TOTAL INPUT MATERIALS	Add lines 29, 47	7.71985	0.466	**50**

	MW (g/mol)	Moles	Yield	Mass (g)	Cost ($/g)	
OUTPUT TARGET PRODUCT	367.8	0.0016	0.6786	0.6	0.777	**53**

PART 2: GREEN METRICS ANALYSIS

Limiting reagent:

PARAMETER	VALUE		
Reaction Scale	0.0024	moles	**58**
E(mw)	0	MW byproducts/MW product	**59**
AE	1	MW product/Σ MW reagents	**60**

(i) Under reclaiming reaction solvents, catalysts, and byproducts, and all post-reaction materials

Mass of waste (line 16 - 53)	0.368	g	**63**
E(m)	0.613	g waste/g product	**64**
RME	0.620	g product/Σ g reagents	**65**
SF	1.095		**66**
Wasted input costs ($)	0.097		

(ii) Under committing all reaction solvents, catalysts, and byproducts, and post-reaction materials to waste

Mass of waste (line 50 - 53)	7.120	g	**69**
E(m)	11.866	g waste/g product	**70**
RME	0.078	g product/Σ g reagents	**71**
Wasted input costs ($)	0.430		
Check formula	0.078		

(iii) Under reclaiming CH2Cl2 and EtOH

Mass of waste	0.57185	g	**76**
E(m)	0.953	g waste/g product	**77**
RME	0.512	g product/Σ g reagents	**78**
Wasted input costs ($)	0.125		

Diels-Alder Reaction

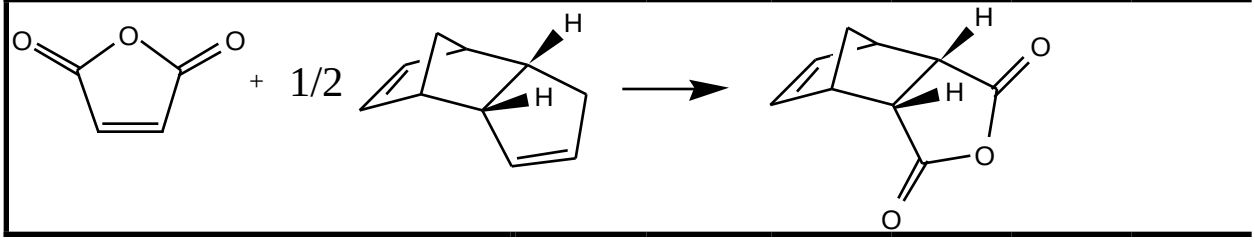
REACTION METRICS FORM

DATE: May 31, 2005

NAME OF TARGET PRODUCT: endo-Norborn-2-ene-(cis)-5,6-dicarboxylic anhydride

REACTION CLASSIFICATION: Carbon-carbon bond forming reaction

BALANCED CHEMICAL EQUATIONS:



PART 1: RAW MATERIALS USAGE

(A) REACTION STAGE:

(i) REAGENTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
dicyclopentadiene	66	0.986	5	0.0373	4.93	0.0646	0.318	12
maleic anhydride	98			0.0357	3.5	0.0114	0.040	13
							0.000	14
							0.000	15
TOTAL REAGENTS	164			Add lines 12 to 15	8.43		0.358	**16**

(ii) CATALYSTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
None	0	0	0	0	0	0	0.000	19
							0.000	20
TOTAL CATALYSTS				Add lines 19 to 20	0		0.000	**21**

(iii) SOLVENTS	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
EtOAc	0.901	10	9.01	0.0167	0.151	24
Et2O	0.708	10	7.08	0.0287	0.203	25
TOTAL SOLVENTS		Add lines 24 to 25	16.09		0.354	**26**

Reaction Materials Subtotals	Add lines 16, 21, 26	24.52	0.712 **29**

(B) WORK-UP STAGE:

MATERIAL	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
None	0	0	0	0	0.000	33
					0.000	34
					0.000	35
					0.000	36
TOTAL WORK-UP MATERIALS		Add lines 33 to 36	0		0.000	**37**

(C) PURIFICATION STAGE:

MATERIAL	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
None	0	0	0	0	0.000	41
					0.000	42
					0.000	43
					0.000	44
TOTAL PURIFICATION MATERIALS		Add lines 41 to 44	0		0.000	**45**
Post-reaction Materials Subtotals		Add lines 37, 45	0		0.000	**47**

		Mass (g)	Cost ($)	
TOTAL INPUT MATERIALS	Add lines 29, 47	24.52	0.712	**50**

	MW (g/mol)	Moles	Yield	Mass (g)	Cost ($/g)	
OUTPUT TARGET PRODUCT	164	0.0305	0.8537	5	0.142	**53**

PART 2: GREEN METRICS ANALYSIS

Limiting reagent: maleic anhydride

PARAMETER	VALUE		
Reaction Scale	0.0357	moles	**58**
E(mw)	0	MW byproducts/MW product	**59**
AE	1	MW product/Σ MW reagents	**60**

(i) Under reclaiming reaction solvents, catalysts, and byproducts, and all post-reaction materials

Mass of waste (line 16 - 53)	3.430	g	**63**
E(m)	0.686	g waste/g product	**64**
RME	0.593	g product/Σ g reagents	**65**
SF	1.439		**66**
Wasted input costs ($)	0.146		

(ii) Under committing all reaction solvents, catalysts, and byproducts, and post-reaction materials to waste

Mass of waste (line 50 - 53)	19.52	g	**69**
E(m)	3.904	g waste/g product	**70**
RME	0.204	g product/Σ g reagents	**71**
Wasted input costs ($)	0.567		

Check formula	0.204		

(iii) Under reclaiming ether and EtOAc

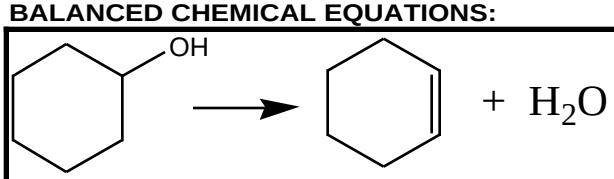
Mass of waste	3.430	g	**76**
E(m)	0.686	g waste/g product	**77**
RME	0.593	g product/Σ g reagents	**78**
Wasted input costs ($)	0.146		

E1-Reaction

REACTION METRICS FORM

DATE: May 31, 2005
NAME OF TARGET PRODUCT: Cyclohexene
REACTION CLASSIFICATION: Elimination

BALANCED CHEMICAL EQUATIONS:



PART 1: RAW MATERIALS USAGE

(A) REACTION STAGE:

(i) REAGENTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
cyclohexanol	100	0.948	11	0.1043	10.428	0.0226	0.236	12
							0.000	13
							0.000	14
							0.000	15
TOTAL REAGENTS	100			Add lines 12 to 15	10.428		0.236	**16**

(ii) CATALYSTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
85% H3PO4	98	1.689	2.5	0.0366	4.2225	0.00959	0.041	19
							0.000	20
TOTAL CATALYSTS				Add lines 19 to 20	4.2225		0.041	**21**

(iii) SOLVENTS	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
None	0	0	0	0	0.000	24
					0.000	25

TOTAL SOLVENTS	Add lines 24 to 25	0	0.000	**26**
Reaction Materials Subtotals	Add lines 16, 21, 26	14.6505	0.276	**29**

(B) WORK-UP STAGE:

MATERIAL	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
sat. NaCl (aq)	1.1804	5	5.902	0.0153	0.090	33
10% Na2CO3	1.1029	10	11.029	0.0280	0.031	34
CaCl2			1	0.0356	0.036	35
					0.000	36

TOTAL WORK-UP MATERIALS	Add lines 33 to 36	17.931	0.157	**37**

(C) PURIFICATION STAGE:

MATERIAL	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
None	0	0	0	0	0.000	41
					0.000	42
					0.000	43
					0.000	44

TOTAL PURIFICATION MATERIALS	Add lines 41 to 44	0	0.000	**45**
Post-reaction Materials Subtotals	Add lines 37, 45	17.931	0.157	**47**

		Mass (g)	**Cost ($)**	
TOTAL INPUT MATERIALS	Add lines 29, 47	32.5815	0.433	**50**

	MW (g/mol)	**Moles**	**Yield**	**Mass (g)**	**Cost ($/g)**	
OUTPUT TARGET PRODUCT	82	0.0732	0.7017	6	0.072	**53**

PART 2: GREEN METRICS ANALYSIS

Limiting reagent: cyclohexanol

PARAMETER	VALUE		
Reaction Scale	0.104	moles	**58**
E(mw)	0.220	MW byproducts/MW product	**59**
AE	0.820	MW product/Σ MW reagents	**60**

(i) Under reclaiming reaction solvents, catalysts, and byproducts, and all post-reaction materials

Mass of waste (line 16 - 53)	4.428	g	**63**
E(m)	0.738	g waste/g product	**64**
RME	0.575	g product/Σ g reagents	**65**
SF	1.000		**66**
Wasted input costs ($)	0.100		

(ii) Under committing all reaction solvents, catalysts, and byproducts, and post-reaction materials to waste

Mass of waste (line 50 - 53)	26.582	g	**69**
E(m)	4.430	g waste/g product	**70**
RME	0.184	g product/Σ g reagents	**71**
Wasted input costs ($)	0.353		
Check formula	0.184		

(iii) Under reclaiming nothing

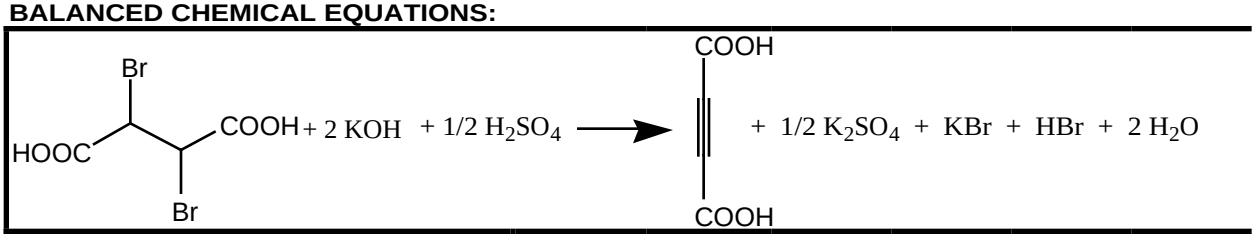
Mass of waste	26.582	g	**76**
E(m)	4.430	g waste/g product	**77**
RME	0.184	g product/Σ g reagents	**78**
Wasted input costs ($)	0.353		

E2-Reaction

REACTION METRICS FORM

DATE: May 31, 2005
NAME OF TARGET PRODUCT: Acetylene dicarboxylic acid
REACTION CLASSIFICATION: Elimination

BALANCED CHEMICAL EQUATIONS:



PART 1: RAW MATERIALS USAGE

(A) REACTION STAGE:

(i) REAGENTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
dibromosuccinic acid	275.8			0.0725	20	0.1736	3.472	12
KOH	112			0.4464	25	0.0158	0.395	13
98 % H2SO4	49	1.8361	12	0.2248	22.0332	0.0112	0.247	14
							0.000	15
TOTAL REAGENTS	436.8			Add lines 12 to 15	67.0332		4.114	**16**

(ii) CATALYSTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
None	0	0	0	0	0	0	0.000	19
							0.000	20
TOTAL CATALYSTS				Add lines 19 to 20	0		0.000	**21**

(iii) SOLVENTS	Density (g/mL)	Volume (mL)		Mass (g)	Cost ($/g)	Cost ($)	
95 % MeOH	0.8062	140		112.868	0.0207	2.337	24
H2O	1	48		48	0	0.000	25
TOTAL SOLVENTS			Add lines 24 to 25	160.868		2.337	**26**

Reaction Materials Subtotals			Add lines 16, 21, 26	227.9012		6.452	**29**

(B) WORK-UP STAGE:

MATERIAL	Density (g/mL)	Volume (mL)		Mass (g)	Cost ($/g)	Cost ($)	
MeOH	0.792	40		31.68	0.0207	0.656	33
H2O	1	61		61	0	0.000	34
98% H2SO4	1.8361	1.6		2.93776	0.0112	0.033	35
Et2O	0.708	100		70.8	0.0287	2.031	36
TOTAL WORK-UP MATERIALS			Add lines 33 to 36	166.41776		2.720	**37**

(C) PURIFICATION STAGE:

MATERIAL	Density (g/mL)	Volume (mL)		Mass (g)	Cost ($/g)	Cost ($)	
None	0	0		0	0	0.000	41
						0.000	42
						0.000	43
						0.000	44
TOTAL PURIFICATION MATERIALS			Add lines 41 to 44	0		0.000	**45**

Post-reaction Materials Subtotals	Add lines 37, 45	166.41776	2.720	**47**

		Mass (g)	**Cost ($)**	
TOTAL INPUT MATERIALS	Add lines 29, 47	394.31896	9.172	**50**

	MW (g/mol)	**Moles**	**Yield**	**Mass (g)**	**Cost ($/g)**	
OUTPUT TARGET PRODUCT	114	0.0579	0.7984	6.6	1.390	**53**

PART 2: GREEN METRICS ANALYSIS

Limiting reagent: dibromosuccinic acid

PARAMETER	VALUE		
Reaction Scale	0.073	moles	**58**
E(mw)	2.832	MW byproducts/MW product	**59**
AE	0.261	MW product/Σ MW reagents	**60**

(i) Under reclaiming reaction solvents, catalysts, and byproducts, and all post-reaction materials

Mass of waste (line 16 - 53)	60.433	g	**63**
E(m)	9.157	g waste/g product	**64**
RME	0.098	g product/Σ g reagents	**65**
SF	2.116		**66**
Wasted input costs ($)	3.709		

(ii) Under committing all reaction solvents, catalysts, and byproducts, and post-reaction materials to waste

Mass of waste (line 50 - 53)	387.719	g	**69**
E(m)	58.745	g waste/g product	**70**
RME	0.017	g product/Σ g reagents	**71**
Wasted input costs ($)	9.018		
Check formula	0.017		

(iii) Under reclaiming MeOH from reaction and workup

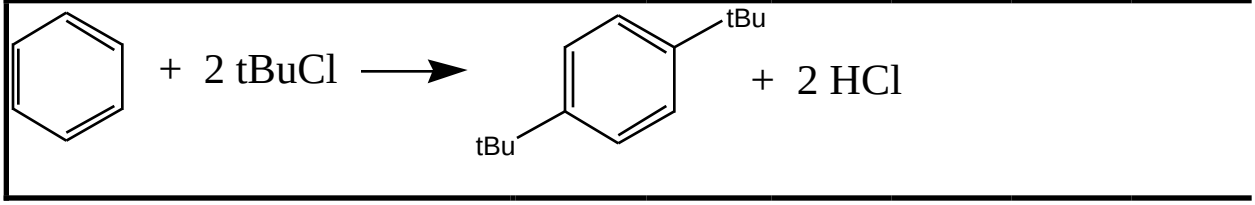
Mass of waste	243.171	g	**76**
E(m)	36.844	g waste/g product	**77**
RME	0.026	g product/Σ g reagents	**78**
Wasted input costs ($)	6.015		

Friedel-Crafts Reaction

REACTION METRICS FORM

DATE: May 31, 2005
NAME OF TARGET PRODUCT: Di-p-t-butylbenzene
REACTION CLASSIFICATION: Carbon-carbon bond forming

BALANCED CHEMICAL EQUATIONS:



PART 1: RAW MATERIALS USAGE

(A) REACTION STAGE:

(i) REAGENTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
benzene	78	0.88	5	0.0564	4.4	0.0263	0.116	12
t-BuCl	184.9	0.847	12	0.1099	10.164	0.0551	0.560	13
							0.000	14
							0.000	15
TOTAL REAGENTS	262.9			Add lines 12 to 15	14.564		0.676	**16**

(ii) CATALYSTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
AlCl3	133.35			0.0037	0.5	0.2286	0.114	19
							0.000	20
TOTAL CATALYSTS				Add lines 19 to 20	0.5		0.114	**21**

(iii) SOLVENTS	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
None	0	0	0	0	0.000	24
					0.000	25
TOTAL SOLVENTS		Add lines 24 to 25	0		0.000	**26**

Reaction Materials Subtotals	Add lines 16, 21, 26	15.064		0.790	**29**

(B) WORK-UP STAGE:

MATERIAL	Density (g/mL)	Volume (mL)		Mass (g)	Cost ($/g)	Cost ($)	
Et2O	0.708	15		10.62	0.0287	0.305	33
H2O	1	30		30	0	0.000	34
MgSO4				5	0.0619	0.309	35
						0.000	36
TOTAL WORK-UP MATERIALS			Add lines 33 to 36	45.62		0.614	**37**

(C) PURIFICATION STAGE:

MATERIAL	Density (g/mL)	Volume (mL)		Mass (g)	Cost ($/g)	Cost ($)	
MeOH	0.792	10		7.92	0.0207	0.164	41
						0.000	42
						0.000	43
						0.000	44
TOTAL PURIFICATION MATERIALS			Add lines 41 to 44	7.92		0.164	**45**
Post-reaction Materials Subtotals			Add lines 37, 45	53.54		0.778	**47**

			Mass (g)	Cost ($)	
TOTAL INPUT MATERIALS		Add lines 29, 47	68.604	1.568	**50**

	MW (g/mol)	Moles	Yield	Mass (g)	Cost ($/g)	
OUTPUT TARGET PRODUCT	190	0.0421	0.7464	8	0.196	**53**

PART 2: GREEN METRICS ANALYSIS

Limiting reagent: benzene

PARAMETER	VALUE		
Reaction Scale	0.056	moles	**58**
E(mw)	0.384	MW byproducts/MW product	**59**
AE	0.723	MW product/Σ MW reagents	**60**

(i) Under reclaiming reaction solvents, catalysts, and byproducts, and all post-reaction materials

Mass of waste (line 16 - 53)	6.564	g	**63**
E(m)	0.821	g waste/g product	**64**
RME	0.549	g product/Σ g reagents	**65**
SF	0.982		**66**
Wasted input costs ($)	0.304		

(ii) Under committing all reaction solvents, catalysts, and byproducts, and post-reaction materials to waste

Mass of waste (line 50 - 53)	60.604	g	**69**
E(m)	7.576	g waste/g product	**70**
RME	0.117	g product/Σ g reagents	**71**
Wasted input costs ($)	1.385		
Check formula	0.117		

(iii) Under reclaiming methanol and ether

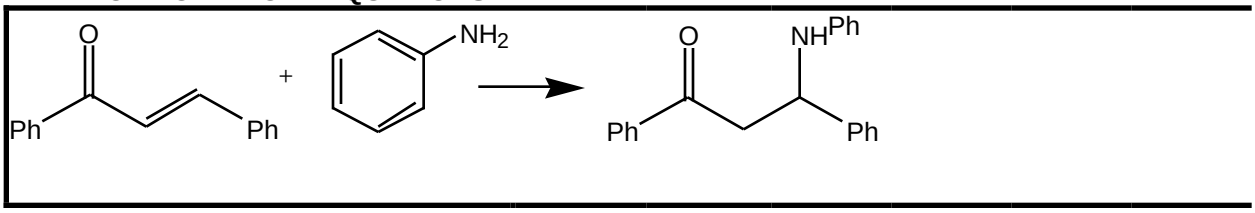
Mass of waste	42.064	g	**76**
E(m)	5.258	g waste/g product	**77**
RME	0.160	g product/Σ g reagents	**78**
Wasted input costs ($)	0.924		

Michael 1,4-Addition

REACTION METRICS FORM

DATE: May 21, 2005
NAME OF TARGET PRODUCT: 1,3-diphenyl-3-phenylamino-propan-1-one
REACTION CLASSIFICATION: non-C-C bond forming

BALANCED CHEMICAL EQUATIONS:



PART 1: RAW MATERIALS USAGE

(A) REACTION STAGE:

(i) REAGENTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
trans-benzal acetophenone	208			0.00240	0.5	0.373	0.187	12
aniline	93	1.022	0.2	0.00220	0.2044	0.0224	0.005	13
								14
								15
TOTAL REAGENTS	301			Add lines 12 to 15	0.7044		0.191	**16**

(ii) CATALYSTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
None	0	0	0	0	0	0	0.000	19
							0.000	20
TOTAL CATALYSTS					Add lines 19 to 20	0	0.000	**21**

(iii) SOLVENTS	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
95 % EtOH	0.816	10	8.160	0.0422	0.344	24
					0.000	25
TOTAL SOLVENTS		Add lines 24 to 25	8.16		0.344	**26**
Reaction Materials Subtotals		Add lines 16, 21, 26	8.8644		0.535	**29**

(B) WORK-UP STAGE:

MATERIAL	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
None	0	0	0	0	0.000	33
					0.000	34
					0.000	35
					0.000	36
TOTAL WORK-UP MATERIALS		Add lines 33 to 36	0		0.000	**37**

(C) PURIFICATION STAGE:

MATERIAL	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
None	0	0	0	0	0.000	41
					0.000	42
					0.000	43
					0.000	44
TOTAL PURIFICATION MATERIALS		Add lines 41 to 44	0		0.000	**45**
Post-reaction Materials Subtotals		Add lines 37, 45	0		0.000	**47**

		Mass (g)	**Cost ($)**	
TOTAL INPUT MATERIALS	Add lines 29, 47	8.8644	0.535	**50**

	MW (g/mol)	**Moles**	**Yield**	**Mass (g)**	**Cost ($/g)**

OUTPUT TARGET PRODUCT	301	0.00166	0.7558	0.5	1.071	**53**

PART 2: GREEN METRICS ANALYSIS

Limiting reagent: aniline

PARAMETER	VALUE		
Reaction Scale	0.002	moles	**58**
E(mw)	0.000	MW byproducts/MW product	**59**
AE	1.000	MW product/Σ MW reagents	**60**

(i) Under reclaiming reaction solvents, catalysts, and byproducts, and all post-reaction materials

Mass of waste (line 16 - 53)	0.204	g	**63**
E(m)	0.409	g waste/g product	**64**
RME	0.710	g product/Σ g reagents	**65**
SF	1.065		**66**
Wasted input costs ($)	0.055		

(ii) Under committing all reaction solvents, catalysts, and byproducts, and post-reaction materials to waste

Mass of waste (line 50 - 53)	8.364	g	**69**
E(m)	16.729	g waste/g product	**70**
RME	0.056	g product/Σ g reagents	**71**
Wasted input costs ($)	0.505		
Check formula	0.056		

(iii) Under reclaiming ethanol

Mass of waste	0.612	g	**76**
E(m)	1.225	g waste/g product	**77**
RME	0.449	g product/Σ g reagents	**78**
Wasted input costs ($)	0.105		

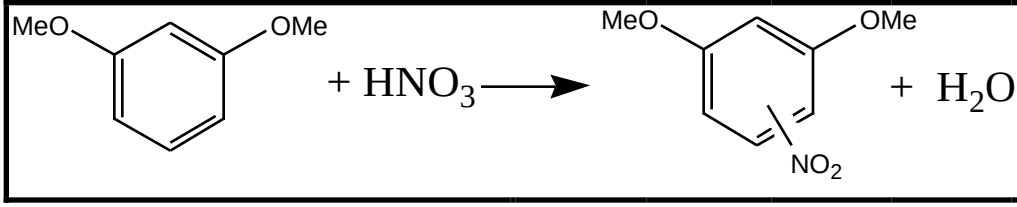
Aromatic Nitration

REACTION METRICS FORM

DATE:	May 31, 2005
NAME OF TARGET PRODUCT:	Nitroveratrole

REACTION CLASSIFICATION: Substitution/Non-carbon-carbon bond forming reaction

BALANCED CHEMICAL EQUATIONS:



PART 1: RAW MATERIALS USAGE

(A) REACTION STAGE:

(i) REAGENTS	MW (g/mol)	Density (g/mL)	Volume (mL)		Moles	Mass (g)	Cost ($/g)	Cost ($)	
veratrole	138	1.084		5	0.0393	5.42	0.1088	0.590	12
nitric acid (fuming)	63	1.5129		6	0.1441	9.0774	0.225	2.042	13
								0.000	14
								0.000	15
TOTAL REAGENTS	201				Add lines 12 to 15	14.4974		2.632	**16**

(ii) CATALYSTS	MW (g/mol)	Density (g/mL)	Volume (mL)		Moles	Mass (g)	Cost ($/g)	Cost ($)	
glacial HOAc	60	1.0498		6	0.1050	6.2988	0.5811	3.660	19
								0.000	20
TOTAL CATALYSTS					Add lines 19 to 20	6.2988		3.660	**21**

(iii) SOLVENTS	Density (g/mL)	Volume (mL)		Mass (g)	Cost ($/g)	Cost ($)	
H2O	1	12.5		12.5	0	0.000	24
						0.000	25
TOTAL SOLVENTS			Add lines 24 to 25	12.5		0.000	**26**

Reaction Materials Subtotals			Add lines 16, 21, 26	33.2962		6.292	**29**

(B) WORK-UP STAGE:

MATERIAL	Density (g/mL)	Volume (mL)		Mass (g)	Cost ($/g)	Cost ($)	
None	0	0		0	0	0.000	33
						0.000	34
						0.000	35
						0.000	36
TOTAL WORK-UP MATERIALS			Add lines 33 to 36	0		0.000	**37**

(C) PURIFICATION STAGE:

MATERIAL	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
None	0	0	0	0	0.000	41
					0.000	42
					0.000	43
					0.000	44
TOTAL PURIFICATION MATERIALS		Add lines 41 to 44	0		0.000	**45**
Post-reaction Materials Subtotals		Add lines 37, 45	0		0.000	**47**

		Mass (g)	Cost ($)	
TOTAL INPUT MATERIALS	Add lines 29, 47	33.2962	6.292	**50**

	MW (g/mol)	Moles	Yield	Mass (g)	Cost ($/g)	
OUTPUT TARGET PRODUCT	183	0.0273	0.6957	5	1.258	**53**

PART 2: GREEN METRICS ANALYSIS

Limiting reagent: veratrole

PARAMETER	VALUE		
Reaction Scale	0.039	moles	**58**
E(mw)	0.098	MW byproducts/MW product	**59**
AE	0.910	MW product/Σ MW reagents	**60**

(i) Under reclaiming reaction solvents, catalysts, and byproducts, and all post-reaction materials

Mass of waste (line 16 - 53)	9.497	g	**63**
E(m)	1.899	g waste/g product	**64**
RME	0.345	g product/Σ g reagents	**65**
SF	1.836		**66**
Wasted input costs ($)	1.724		

(ii) Under committing all reaction solvents, catalysts, and byproducts, and post-reaction materials to waste

Mass of waste (line 50 - 53)	28.296	g	**69**
E(m)	5.659	g waste/g product	**70**
RME	0.150	g product/Σ g reagents	**71**
Wasted input costs ($)	5.347		

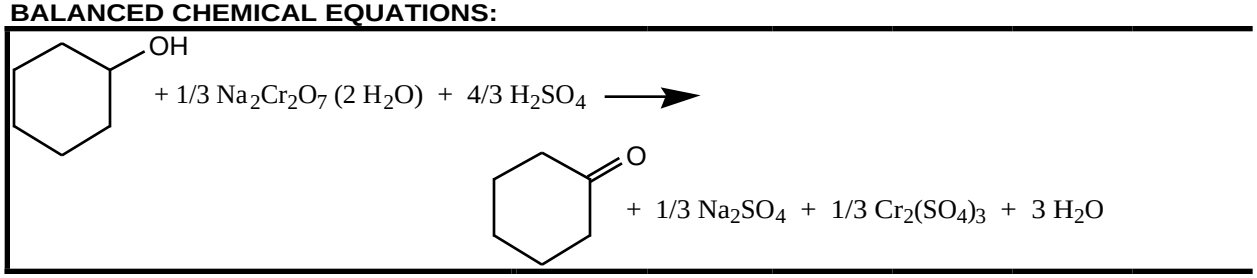
Check formula 0.150

Oxidation of Secondary Alcohol

REACTION METRICS FORM

DATE:
NAME OF TARGET PRODUCT:
REACTION CLASSIFICATION:

BALANCED CHEMICAL EQUATIONS:



PART 1: RAW MATERIALS USAGE

(A) REACTION STAGE:

(i) REAGENTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
cyclohexanol	100	0.948	10.35	0.0981	9.8118	0.0226	0.222	12
sodium dichromate dihydrate	99.333			0.0352	10.5	0.1195	1.255	13
98 % H2SO4	130.667	1.8361	10	0.1874	18.361	0.0112	0.206	14
							0.000	15
TOTAL REAGENTS	330			Add lines 12 to 15	38.6728		1.682	**16**

(ii) CATALYSTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
None	0	0	0	0	0	0	0.000	19
							0.000	20
TOTAL CATALYSTS				Add lines 19 to 20	0		0.000	**21**

(iii) SOLVENTS	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
H2O	1	35	0	0.000	24	
				0.000	25	
TOTAL SOLVENTS		Add lines 24 to 25	35		0.000	**26**

Reaction Materials Subtotals	Add lines 16, 21, 26	73.6728		1.682	**29**

(B) WORK-UP STAGE:

MATERIAL	Density (g/mL)	Volume (mL)		Mass (g)	Cost ($/g)	Cost ($)	
MeOH	0.792	1		0.792	0.0207	0.016	33
H2O	1	30		30	0	0.000	34
NaCl				8	0.0153	0.122	35
MgSO4				10	0.0619	0.619	36
TOTAL WORK-UP MATERIALS			Add lines 33 to 36	48.792		0.758	**37**

(C) PURIFICATION STAGE:

MATERIAL	Density (g/mL)	Volume (mL)		Mass (g)	Cost ($/g)	Cost ($)	
None	0	0		0	0	0.000	41
						0.000	42
						0.000	43
						0.000	44
TOTAL PURIFICATION MATERIALS			Add lines 41 to 44	0		0.000	**45**

Post-reaction Materials Subtotals			Add lines 37, 45	48.792		0.758	**47**

				Mass (g)	**Cost ($)**	
TOTAL INPUT MATERIALS			Add lines 29, 47	122.4648	2.440	**50**

	MW (g/mol)	**Moles**	**Yield**	**Mass (g)**	**Cost ($/g)**	
OUTPUT TARGET PRODUCT	98	0.0204	0.5792	2	1.220	**53**

PART 2: GREEN METRICS ANALYSIS

Limiting reagent: cyclohexanol

PARAMETER	VALUE		
Reaction Scale	0.035	moles	**58**
E(mw)	2.367	MW byproducts/MW product	**59**
AE	0.297	MW product/Σ MW reagents	**60**

(i) Under reclaiming reaction solvents, catalysts, and byproducts, and all post-reaction materials

Mass of waste (line 16 - 53)	36.673	g	**63**
E(m)	18.336	g waste/g product	**64**
RME	0.052	g product/Σ g reagents	**65**
SF	3.326		**66**
Wasted input costs ($)	1.595		

(ii) Under committing all reaction solvents, catalysts, and byproducts, and post-reaction materials to waste

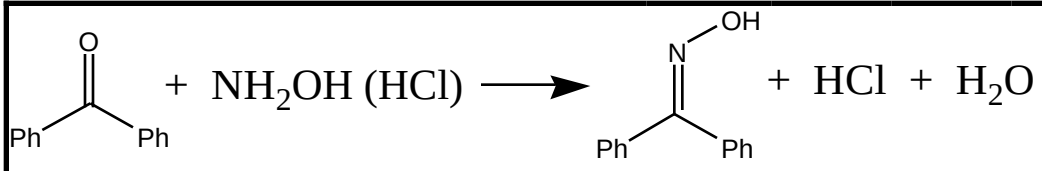
Mass of waste (line 50 - 53)	120.465	g	**69**
E(m)	60.232	g waste/g product	**70**
RME	0.016	g product/Σ g reagents	**71**
Wasted input costs ($)	2.400		
Check formula	0.016		

Oximation

REACTION METRICS FORM

DATE: May 31, 2005
NAME OF TARGET PRODUCT: Benzophenone oxime
REACTION CLASSIFICATION: Non-carbon-carbon bond forming reaction

BALANCED CHEMICAL EQUATIONS:



PART 1: RAW MATERIALS USAGE

(A) REACTION STAGE:

(i) REAGENTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
benzophenone	182			0.0291	5.3	0.0230	0.122	12
hydroxylamine hydrochloride	69.45			0.0461	3.2	0.2296	0.735	13
							0.000	14
							0.000	15
TOTAL REAGENTS	251.45			Add lines 12 to 15	8.5		0.857	**16**

(ii) CATALYSTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
NaOH	40			0.145	5.8	0.0177	0.103	19
							0.000	20
TOTAL CATALYSTS				Add lines 19 to 20	5.8		0.103	**21**

(iii) SOLVENTS	Density (g/mL)	Volume (mL)		Mass (g)	Cost ($/g)	Cost ($)	
95 % EtOH	0.816	15		12.24	0.0422	0.516	24
H2O	1	3		3	0	0.000	25
TOTAL SOLVENTS			Add lines 24 to 25	15.24		0.516	**26**
Reaction Materials Subtotals			Add lines 16, 21, 26	29.54		1.476	**29**

(B) WORK-UP STAGE:

MATERIAL	Density (g/mL)	Volume (mL)		Mass (g)	Cost ($/g)	Cost ($)	
10 % HCl (aq)	1.0474	100		104.74	0.00453	0.475	33
						0.000	34
						0.000	35
						0.000	36
TOTAL WORK-UP MATERIALS			Add lines 33 to 36	104.74		0.475	**37**

(C) PURIFICATION STAGE:

MATERIAL	Density (g/mL)	Volume (mL)		Mass (g)	Cost ($/g)	Cost ($)	
None	0	0		0	0	0.000	41
						0.000	42
						0.000	43
						0.000	44
TOTAL PURIFICATION MATERIALS			Add lines 41 to 44	0		0.000	**45**
Post-reaction Materials Subtotals			Add lines 37, 45	104.74		0.475	**47**

		Mass (g)	**Cost ($)**	
TOTAL INPUT MATERIALS	Add lines 29, 47	134.28	1.950	**50**

	MW (g/mol)	**Moles**	**Yield**	**Mass (g)**	**Cost ($/g)**	
OUTPUT TARGET PRODUCT	197	0.0254	0.8716	5	0.390	**53**

PART 2: GREEN METRICS ANALYSIS

Limiting reagent: benzophenone

PARAMETER	VALUE	
Reaction Scale	0.0291 moles	**58**

E(mw)	0.2764	MW byproducts/MW product	**59**
AE	0.7835	MW product/Σ MW reagents	**60**

(i) Under reclaiming reaction solvents, catalysts, and byproducts, and all post-reaction materials

Mass of waste (line 16 - 53)	3.500	g	**63**
E(m)	0.700	g waste/g product	**64**
RME	0.588	g product/Σ g reagents	**65**
SF	1.161		**66**
Wasted input costs ($)	0.353		

(ii) Under committing all reaction solvents, catalysts, and byproducts, and post-reaction materials to waste

Mass of waste (line 50 - 53)	129.28	g	**69**
E(m)	25.856	g waste/g product	**70**
RME	0.037	g product/Σ g reagents	**71**
Wasted input costs ($)	1.878		
Check formula	0.037		

(iii) Under reclaiming EtOH

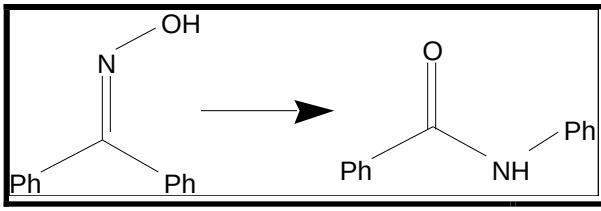
Mass of waste	117.652	g	**76**
E(m)	23.530	g waste/g product	**77**
RME	0.041	g product/Σ g reagents	**78**
Wasted input costs ($)	1.361		

Beckmann Rearrangement

REACTION METRICS FORM

DATE:	May 31, 2005
NAME OF TARGET PRODUCT:	Benzanilide
REACTION CLASSIFICATION:	Rearrangement (Beckmann)

BALANCED CHEMICAL EQUATIONS:



PART 1: RAW MATERIALS USAGE

(A) REACTION STAGE:

(i) REAGENTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
benzophenone oxime	197			0.0254	5	0.295	1.475	12
								13
								14
								15
TOTAL REAGENTS	197			Add lines 12 to 15	5		1.475	**16**

(ii) CATALYSTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
polyphosphoric acid		2.06			60	0.0469	2.814	19
								20
TOTAL CATALYSTS				Add lines 19 to 20	60		2.814	**21**

(iii) SOLVENTS	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
None	0	0	0	0	0.000	24
					0.000	25
TOTAL SOLVENTS		Add lines 24 to 25	0		0.000	**26**

Reaction Materials Subtotals	Add lines 16, 21, 26	65		4.289	**29**

(B) WORK-UP STAGE:

MATERIAL	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
H2O	1	400	400	0	0.000	33
Et2O	0.708	50	35.4	0.0287	1.016	34
EtOAc	0.901	50	45.05	0.0167	0.754	35
sat. NaCl (aq)	1.1804	100	118.04	0.0153	1.806	36a
MgSO4			10	0.0619	0.619	36b
TOTAL WORK-UP MATERIALS		Add lines 33 to 36b	598.49		3.576	**37**

(C) PURIFICATION STAGE:

MATERIAL	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)

None	0	0		0	0	0.000 41
						0.000 42
						0.000 43
						0.000 44
TOTAL PURIFICATION MATERIALS			Add lines 41 to 44	0		0.000 **45**
Post-reaction Materials Subtotals			Add lines 37, 45	598.49		3.576 **47**

				Mass (g)	**Cost ($)**	
TOTAL INPUT MATERIALS			Add lines 29, 47	663.49	7.865	**50**

	MW (g/mol)	**Moles**	**Yield**	**Mass (g)**	**Cost ($/g)**	
OUTPUT TARGET PRODUCT	197	0.0152	0.6000	3	2.622	**53**

PART 2: GREEN METRICS ANALYSIS

Limiting reagent: benzophenone oxime

PARAMETER	VALUE		
Reaction Scale	0.0254	moles	**58**
E(mw)	0	MW byproducts/MW product	**59**
AE	1	MW product/Σ MW reagents	**60**

(i) Under reclaiming reaction solvents, catalysts, and byproducts, and all post-reaction materials

Mass of waste (line 16 - 53)	2	g	**63**
E(m)	0.667	g waste/g product	**64**
RME	0.6	g product/Σ g reagents	**65**
SF	1		**66**
Wasted input costs ($)	1.716		

(ii) Under committing all reaction solvents, catalysts, and byproducts, and post-reaction materials to waste

Mass of waste (line 50 - 53)	660.49	g	**69**
E(m)	220.163	g waste/g product	**70**
RME	0.005	g product/Σ g reagents	**71**
Wasted input costs ($)	7.829		

Check formula 0.0045

(iii) Under reclaiming ether and EtOAc

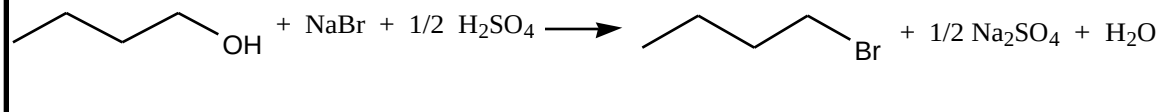
Mass of waste	580.040	g	**76**
E(m)	193.347	g waste/g product	**77**
RME	0.005	g product/Σ g reagents	**78**
Wasted input costs ($)	6.064		

SN2 Reaction

REACTION METRICS FORM

DATE: May 31, 2005
NAME OF TARGET PRODUCT: 1-Bromobutane
REACTION CLASSIFICATION: Substitution

BALANCED CHEMICAL EQUATIONS:



PART 1: RAW MATERIALS USAGE

(A) REACTION STAGE:

(i) REAGENTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
n-BuOH	74	0.8098		0.15	11.1	0.0101	0.112	12
NaBr	102.9			0.15	15.435	0.106	1.636	13
98 % H2SO4	49	1.8361	17.5	0.3279	32.13175	0.0112	0.361	14
							0.000	15
TOTAL REAGENTS	225.9			Add lines 12 to 15	58.667		2.109	**16**

(ii) CATALYSTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
	0	0	0	0	0	0	0.000	19
							0.000	20
TOTAL CATALYSTS				Add lines 19 to 20	0		0.000	**21**

(iii) SOLVENTS	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
H2O	1	18	18	0	0.000	24
					0.000	25
TOTAL SOLVENTS		Add lines 24 to 25	18		0.000	**26**

Reaction Materials Subtotals	Add lines 16, 21, 26	76.66675		2.109	**29**

(B) WORK-UP STAGE:

MATERIAL	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
H2O	1	25	25	0	0.000	33
2 M NaOH (aq) (8 %)	1.08	5	5.4	0.0177	0.008	34
MgSO4			5	0.1124	0.562	35
					0.000	36
TOTAL WORK-UP MATERIALS		Add lines 33 to 36	35.4		0.570	**37**

(C) PURIFICATION STAGE:

MATERIAL	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
H2O	1	10	10	0	0.000	41
					0.000	42
					0.000	43
					0.000	44
TOTAL PURIFICATION MATERIALS		Add lines 41 to 44	10		0.000	**45**

Post-reaction Materials Subtotals	Add lines 37, 45	45.4		0.570	**47**

		Mass (g)	**Cost ($)**	
TOTAL INPUT MATERIALS	Add lines 29, 47	122.067	2.678	**50**

	MW (g/mol)	**Moles**	**Yield**	**Mass (g)**	**Cost ($/g)**	
OUTPUT TARGET PRODUCT	136.9	0.1096	0.7305	15	0.179	**53**

PART 2: GREEN METRICS ANALYSIS

Limiting reagent: nBuOH, NaBr

PARAMETER	VALUE		
Reaction Scale	0.15	moles	**58**
E(mw)	0.650	MW byproducts/MW product	**59**
AE	0.606	MW product/Σ MW reagents	**60**

(i) Under reclaiming reaction solvents, catalysts, and byproducts, and all post-reaction materials

Mass of waste (line 16 - 53)	43.667	g	**63**
E(m)	2.911	g waste/g product	**64**
RME	0.256	g product/Σ g reagents	**65**
SF	1.731		**66**
Wasted input costs ($)	1.570		

(ii) Under committing all reaction solvents, catalysts, and byproducts, and post-reaction materials to waste

Mass of waste (line 50 - 53)	107.067	g	**69**
E(m)	7.138	g waste/g product	**70**
RME	0.123	g product/Σ g reagents	**71**
Wasted input costs ($)	2.349		
Check formula	0.123		

(iii) Under reclaiming nothing

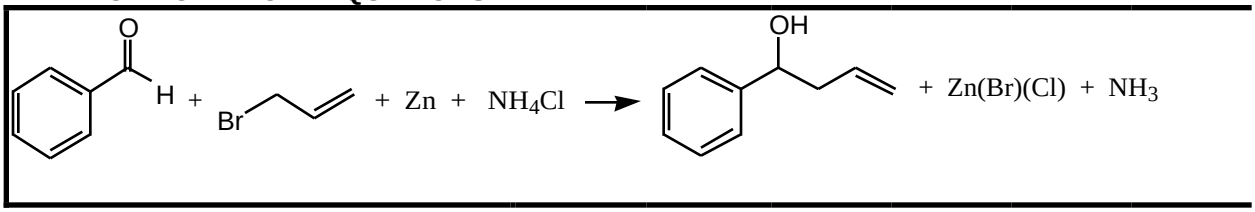
Mass of waste	107.067	g	**76**
E(m)	7.138	g waste/g product	**77**
RME	0.123	g product/Σ g reagents	**78**
Wasted input costs ($)	2.349		

Grignard Reaction (University of Toronto)

REACTION METRICS FORM

DATE: June 1, 2005
NAME OF TARGET PRODUCT: 1-Phenylbut-3-en-1-ol
REACTION CLASSIFICATION: Grignard (Carbon-carbon bond forming)

BALANCED CHEMICAL EQUATIONS:



PART 1: RAW MATERIALS USAGE

(A) REACTION STAGE:

(i) REAGENTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)

benzaldehyde	106	1.044	0.102	0.00100	0.106	0.0149	0.002	12
zinc powder	65.39			0.00119	0.078	0.0458	0.004	13
sat. NH4Cl (aq) (24 %)	53.45	1.0674	1	0.00479	1.067	0.6394	0.164	14
allyl bromide	120.9	1.398	0.104	0.00120	0.145	0.0763	0.011	15
TOTAL REAGENTS	345.74			Add lines 12 to 15	1.39728		0.180	**16**

(ii) CATALYSTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
None	0	0	0	0	0	0	0.000	19
							0.000	20
TOTAL CATALYSTS				Add lines 19 to 20	0		0.000	**21**

(iii) SOLVENTS	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
THF	0.889	0.5	0.4445	0.0206	0.009	24
Et2O	0.708	1	0.708	0.0287	0.020	25
TOTAL SOLVENTS		Add lines 24 to 25	1.1525		0.029	**26**

Reaction Materials Subtotals	Add lines 16, 21, 26	2.54978	0.210	**29**

(B) WORK-UP STAGE:

MATERIAL	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
Et2O	0.708	2	1.416	0.0287	0.041	33
MgSO4			1	0.0619	0.062	34
					0.000	35
					0.000	36
TOTAL WORK-UP MATERIALS		Add lines 33 to 36	2.416		0.103	**37**

(C) PURIFICATION STAGE:

MATERIAL	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
None	0	0	0	0	0.000	41
					0.000	42
					0.000	43
					0.000	44
TOTAL PURIFICATION MATERIALS		Add lines 41 to 44	0		0.000	**45**

Post-reaction Materials Subtotals	Add lines 37, 45	2.416	0.103	**47**

		Mass (g)	Cost ($)	
TOTAL INPUT MATERIALS	Add lines 29, 47	4.96578	0.312	**50**

	MW (g/mol)	Moles	Yield	Mass (g)	Cost ($/g)	
OUTPUT TARGET PRODUCT	148	0.0007	0.7398	0.11	2.837	**53**

PART 2: GREEN METRICS ANALYSIS

Limiting reagent: benzaldehyde

PARAMETER	VALUE		
Reaction Scale	0.001	moles	**58**
E(mw)	1.336	MW byproducts/MW product	**59**
AE	0.428	MW product/Σ MW reagents	**60**

(i) Under reclaiming reaction solvents, catalysts, and byproducts, and all post-reaction materials

Mass of waste (line 16 - 53)	1.287	g	**63**
E(m)	11.703	g waste/g product	**64**
RME	0.079	g product/Σ g reagents	**65**
SF	4.023		**66**
Wasted input costs ($)	0.166		

(ii) Under committing all reaction solvents, catalysts, and byproducts, and post-reaction materials to waste

Mass of waste (line 50 - 53)	4.856	g	**69**
E(m)	44.143	g waste/g product	**70**
RME	0.022	g product/Σ g reagents	**71**
Wasted input costs ($)	0.305		
Check formula	0.022		

(iii) Under reclaiming Et2O and THF

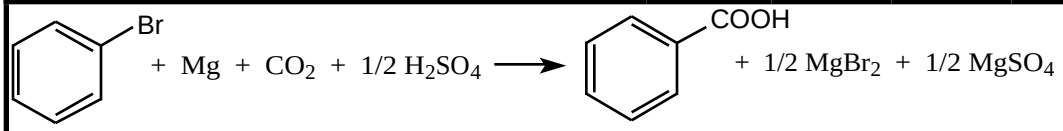
Mass of waste	2.287	g	**76**
E(m)	20.793	g waste/g product	**77**
RME	0.046	g product/Σ g reagents	**78**
Wasted input costs ($)	0.231		

Grignard Reaction (Malaspina University College)

REACTION METRICS FORM

DATE: October 10, 2005
NAME OF TARGET PRODUCT: Benzoic acid
REACTION CLASSIFICATION: Carbon-carbon forming

BALANCED CHEMICAL EQUATIONS:



PART 1: RAW MATERIALS USAGE

(A) REACTION STAGE:

(i) REAGENTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
Mg	24.305			0.1	2.4305	0.0684	0.166	12
Bromobenzene	156.9	1.495	5.00	0.0476	7.475	0.0202	0.151	13
CO2 (dry ice)	44				30		0.000	14
3 M H2SO4	49						0.000	15
TOTAL REAGENTS	274.205			Add lines 12 to 15	39.9055		0.317	**16**

(ii) CATALYSTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
None			0		0		0.000	19
							0.000	20
TOTAL CATALYSTS				Add lines 19 to 20	0		0.000	**21**

(iii) SOLVENTS	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
Diethylether	0.708	155	109.74	0.0287	3.148	24
Ice cubes			10	0	0.000	25
TOTAL SOLVENTS		Add lines 24 to 25	119.74		3.148	**26**

Reaction Materials Subtotals		Add lines 16, 21, 26	159.6455		3.466	**29**

(B) WORK-UP STAGE:

MATERIAL	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
petroleum Et2O	0.708	30	21.24	0.64	13.594	33
2 M NaOH (7.5 %)	1.08	60	64.8	0.0163	1.059	34

6 M HCl (20 %)	1.098	30		32.94	0.00907	0.299	35
				0		0.000	36
TOTAL WORK-UP MATERIALS			Add lines 33 to 36	118.98		14.951	**37**

(C) PURIFICATION STAGE:

MATERIAL	Density (g/mL)	Volume (mL)		Mass (g)	Cost ($/g)	Cost ($)	
None				0		0.000	41
				0		0.000	42
				0		0.000	43
				0		0.000	44
TOTAL PURIFICATION MATERIALS			Add lines 41 to 44	0		0.000	**45**
Post-reaction Materials Subtotals			Add lines 37, 45	118.98		14.951	**47**

			Mass (g)	**Cost ($)**	
TOTAL INPUT MATERIALS		Add lines 29, 47	278.6255	18.417	**50**

	MW (g/mol)	**Moles**	**Yield**	**Mass (g)**	**Cost ($/g)**	
OUTPUT TARGET PRODUCT	122	0.0369	0.7742	4.5	4.093	**53**

PART 2: GREEN METRICS ANALYSIS

Limiting reagent:

PARAMETER	VALUE		
Reaction Scale	0.047641 81	moles	**58**
E(mw)	1.248	MW byproducts/MW product	**59**
AE	0.445	MW product/Σ MW reagents	**60**

(i) Under reclaiming reaction solvents, catalysts, and byproducts, and all post-reaction materials

Mass of waste (line 16 - 53)	35.4055	g	**63**
E(m)	7.867888 889	g waste/g product	**64**
RME	0.112766 411	g product/Σ g reagents	**65**
SF	3.054704		**66**
Wasted input costs ($)	0.281		

(ii) Under committing all reaction solvents, catalysts, and byproducts, and post-reaction materials to waste

Mass of waste (line 50 - 53)	274.1255	g	**69**
E(m)	60.91677778	g waste/g product	**70**
RME	0.016150711	g product/Σ g reagents	**71**
Wasted input costs ($)	18.119		
Check formula	0.016151		

(iii) Under reclaiming ether from reaction and petroleum ether from purification

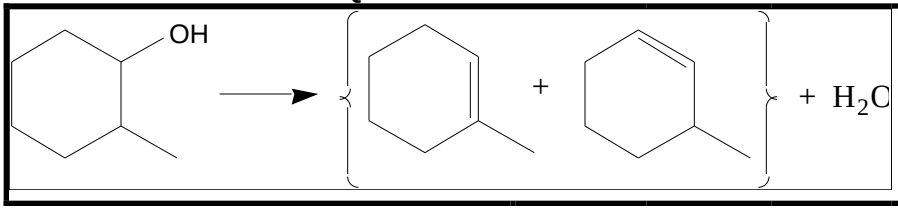
Mass of waste	143.146	g	**76**
E(m)	31.810	g waste/g product	**77**
RME	0.030	g product/Σ g reagents	**78**
Wasted input costs ($)	4.676		

Dehydration

REACTION METRICS FORM

DATE: October 10, 2005
NAME OF TARGET PRODUCT: 1-Methylcyclohex-1-ene
REACTION CLASSIFICATION: Elimination/Fragmentation/Dehydration

BALANCED CHEMICAL EQUATIONS:



PART 1: RAW MATERIALS USAGE

(A) REACTION STAGE:

(i) REAGENTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
2-methylcyclohexanol	114	0.93		0.1	11.4	0.0833	0.950	12
					0		0.000	13
							0.000	14
							0.000	15
TOTAL REAGENTS	114			Add lines 12 to 15	11.4		0.950	**16**

(ii) CATALYSTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
85 % H3PO4	98	1.689	5		8.445	0.00959	0.081	19
							0.000	20
TOTAL CATALYSTS				Add lines 19 to 20	8.445		0.081	**21**

(iii) SOLVENTS	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
None		0	0		0.000	24
			0		0.000	25
TOTAL SOLVENTS			Add lines 24 to 25	0	0.000	**26**

Reaction Materials Subtotals	Add lines 16, 21, 26	19.845		1.031	**29**

(B) WORK-UP STAGE:

MATERIAL	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
1 M NaOH (4 %)	1.04	10	10.4	0.0170	0.177	33
CaCl2			5	0.0356	0.178	34
			0		0.000	35
			0		0.000	36
TOTAL WORK-UP MATERIALS			Add lines 33 to 36	15.4	0.355	**37**

(C) PURIFICATION STAGE:

MATERIAL	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
			0		0.000	41
			0		0.000	42
			0		0.000	43
			0		0.000	44
TOTAL PURIFICATION MATERIALS			Add lines 41 to 44	0	0.000	**45**

Post-reaction Materials Subtotals	Add lines 37, 45	15.4		0.355	**47**

		Mass (g)	**Cost ($)**	
TOTAL INPUT MATERIALS	Add lines 29, 47	35.245	1.386	**50**

	MW (g/mol)	**Moles**	**Yield**	**Mass (g)**	**Cost ($/g)**

OUTPUT TARGET PRODUCT	96	0.0729	0.7292	7	0.198	**53**

PART 2: GREEN METRICS ANALYSIS

Limiting reagent:

PARAMETER	VALUE		
Reaction Scale	0.1	moles	**58**
E(mw)	0.188	MW byproducts/MW product	**59**
AE	0.842	MW product/Σ MW reagents	**60**

(i) Under reclaiming reaction solvents, catalysts, and byproducts, and all post-reaction materials

Mass of waste (line 16 - 53)	4.4	g	**63**
E(m)	0.628571429	g waste/g product	**64**
RME	0.614035088	g product/Σ g reagents	**65**
SF	1		**66**
Wasted input costs ($)	0.367		

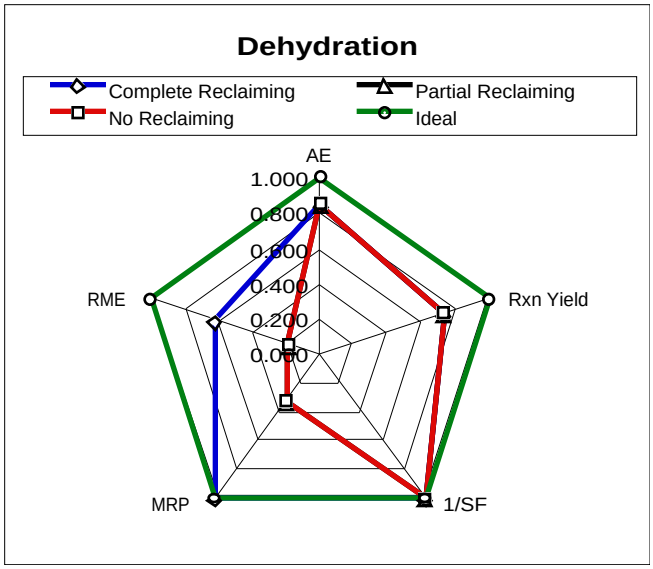
(ii) Under committing all reaction solvents, catalysts, and byproducts, and post-reaction materials to waste

Mass of waste (line 50 - 53)	28.245	g	**69**
E(m)	4.035	g waste/g product	**70**
RME	0.198609732	g product/Σ g reagents	**71**
Wasted input costs ($)	1.110		

Check formula	0.198610

(iii) Under reclaiming nothing

Mass of waste	28.245	g	**76**
E(m)	4.035	g waste/g product	**77**
RME	0.199	g product/Σ g reagents	**78**
Wasted input costs ($)	1.110		

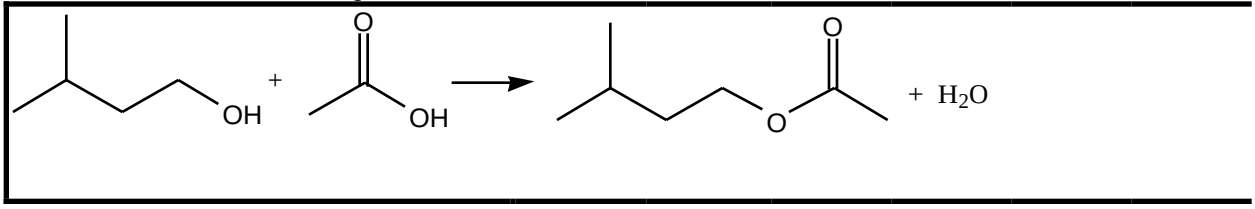


Esterification

REACTION METRICS FORM

DATE: October 10, 2005
NAME OF TARGET PRODUCT: Isoamyl acetate
REACTION CLASSIFICATION: Esterification

BALANCED CHEMICAL EQUATIONS:



PART 1: RAW MATERIALS USAGE

(A) REACTION STAGE:

(i) REAGENTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
Isoamyl alcohol	88	0.809		0.05	4.4	0.0111	0.049	12
Acetic acid (glacial)	60	1.0498		0.2	12	0.5811	6.973	13
							0.000	14
							0.000	15
TOTAL REAGENTS	148			Add lines 12 to 15	16.4		7.022	**16**

(ii) CATALYSTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
98 % H2SO4	98	1.8361	1		1.8361	0.0112	0.021	19
							0.000	20

TOTAL CATALYSTS			Add lines 19 to 20	1.8361	0.021	**21**

(iii) SOLVENTS	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
None			0		0.000	24
			0		0.000	25
TOTAL SOLVENTS		Add lines 24 to 25	0		0.000	**26**
Reaction Materials Subtotals		Add lines 16, 21, 26	18.2361		7.042	**29**

(B) WORK-UP STAGE:

MATERIAL	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
Water	1	50	50	0	0.000	33
5 % NaHCO3	1.0354	10	10.354	0.0003	0.003	34
sat'd NaCl	1.1804	10	11.804	0.0153	0.181	35
MgSO4			10	0.0619	0.619	36
TOTAL WORK-UP MATERIALS		Add lines 33 to 36	82.158		0.802	**37**

(C) PURIFICATION STAGE:

MATERIAL	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
			0		0.000	41
			0		0.000	42
			0		0.000	43
			0		0.000	44
TOTAL PURIFICATION MATERIALS		Add lines 41 to 44	0		0.000	**45**
Post-reaction Materials Subtotals		Add lines 37, 45	82.158		0.802	**47**

		Mass (g)	**Cost ($)**	
TOTAL INPUT MATERIALS	Add lines 29, 47	100.3941	7.844	**50**

	MW (g/mol)	**Moles**	**Yield**	**Mass (g)**	**Cost ($/g)**	
OUTPUT TARGET PRODUCT	130	0.0385	0.7692	5	1.569	**53**

PART 2: GREEN METRICS ANALYSIS

Limiting reagent:

PARAMETER	VALUE		
Reaction Scale	0.05	moles	**58**
E(mw)	0.138	MW byproducts/MW product	**59**
AE	0.878	MW product/Σ MW reagents	**60**

(i) Under reclaiming reaction solvents, catalysts, and byproducts, and all post-reaction materials

Mass of waste (line 16 - 53)	11.4	g	**63**
E(m)	2.28	g waste/g product	**64**
RME	0.304878049	g product/Σ g reagents	**65**
SF	2.216216216		**66**
Wasted input costs ($)	4.881		

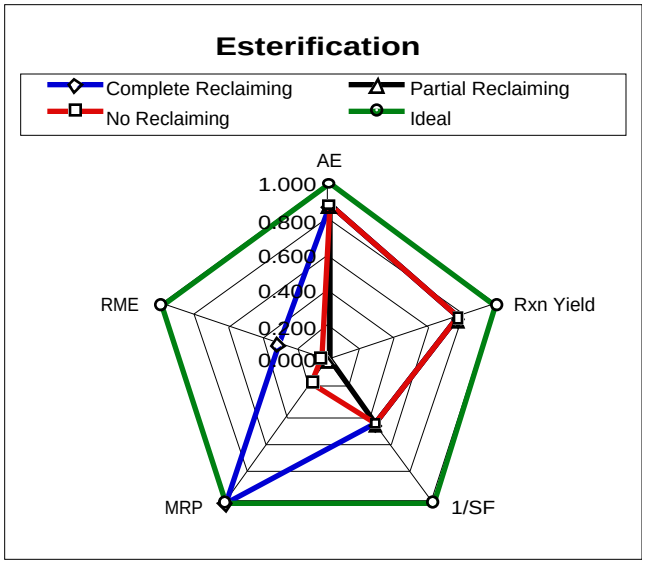
(ii) Under committing all reaction solvents, catalysts, and byproducts, and post-reaction materials to waste

Mass of waste (line 50 - 53)	95.3941	g	**69**
E(m)	19.07882	g waste/g product	**70**
RME	0.049803724	g product/Σ g reagents	**71**
Wasted input costs ($)	7.454		

Check formula	0.049804

(iii) Under reclaiming nothing

Mass of waste	95.394	g	**76**
E(m)	19.079	g waste/g product	**77**
RME	0.050	g product/Σ g reagents	**78**
Wasted input costs ($)	7.454		



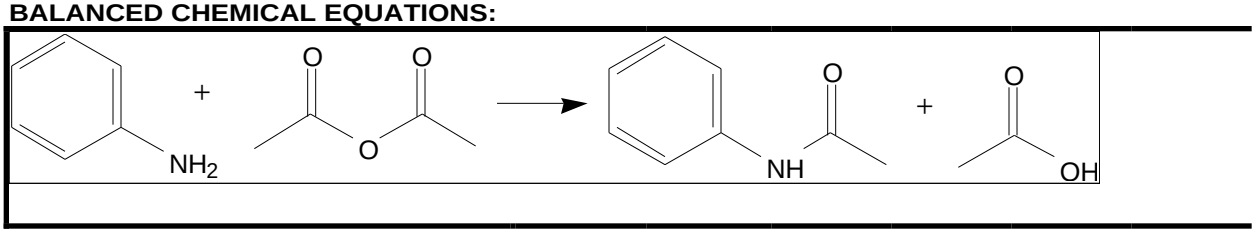
Synthesis of a Sulpha Drug

Step 1: Acetylation

REACTION METRICS FORM

DATE: October 10, 2005
NAME OF TARGET PRODUCT: Acetanilide
REACTION CLASSIFICATION:

BALANCED CHEMICAL EQUATIONS:



PART 1: RAW MATERIALS USAGE

(A) REACTION STAGE:

(i) REAGENTS	MW (g/mol)	Density (g/mL)	Volume (mL)		Moles	Mass (g)	Cost ($/g)	Cost ($)	
Aniline	93	1.022			0.1	9.3	0.0224	0.208	12
Acetic anhydride	102	1.082			0.12	12.24	0.0202	0.248	13
								0.000	14
								0.000	15
TOTAL REAGENTS	195				Add lines 12 to 15	21.54		0.456	**16**

(ii) CATALYSTS	MW (g/mol)	Density (g/mL)	Volume (mL)		Moles	Mass (g)	Cost ($/g)	Cost ($)	
98 % H2SO4	98	1.8361		8	0.1499	14.6888	0.0114	0.168	19
NaOAc	82				0.1195	9.799	0.0512	0.502	20

TOTAL CATALYSTS			Add lines 19 to 20	24.4878		0.670	**21**

(iii) SOLVENTS	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
Water	1	250	250	0	0.000	24
			0		0.000	25
TOTAL SOLVENTS		Add lines 24 to 25	250		0.000	**26**

Reaction Materials Subtotals	Add lines 16, 21, 26	296.0278		1.126	**29**

(B) WORK-UP STAGE:

MATERIAL	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
None		0	0		0.000	33
			0		0.000	34
			0		0.000	35
			0		0.000	36
TOTAL WORK-UP MATERIALS		Add lines 33 to 36	0		0.000	**37**

(C) PURIFICATION STAGE:

MATERIAL	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
None		0	0		0.000	41
			0		0.000	42
			0		0.000	43
			0		0.000	44
TOTAL PURIFICATION MATERIALS		Add lines 41 to 44	0		0.000	**45**

Post-reaction Materials Subtotals	Add lines 37, 45	0		0.000	**47**

		Mass (g)	**Cost ($)**	
TOTAL INPUT MATERIALS	Add lines 29, 47	296.0278	1.126	**50**

	MW (g/mol)	**Moles**	**Yield**	**Mass (g)**	**Cost ($/g)**	
OUTPUT TARGET PRODUCT	135	0.0889	0.8889	12	0.094	**53**

PART 2: GREEN METRICS ANALYSIS

Limiting reagent:

PARAMETER	VALUE		
Reaction Scale	0.1	moles	**58**
E(mw)	0.444	MW byproducts/MW product	**59**
AE	0.692	MW product/Σ MW reagents	**60**

(i) Under reclaiming reaction solvents, catalysts, and byproducts, and all post-reaction materials

Mass of waste (line 16 - 53)	9.54	g	**63**
E(m)	0.795	g waste/g product	**64**
RME	0.557103064	g product/Σ g reagents	**65**
SF	1.104615385		**66**
Wasted input costs ($)	0.202		

(ii) Under committing all reaction solvents, catalysts, and byproducts, and post-reaction materials to waste

Mass of waste (line 50 - 53)	284.0278	g	**69**
E(m)	23.66898333	g waste/g product	**70**
RME	0.040536733	g product/Σ g reagents	**71**
Wasted input costs ($)	1.080		

Check formula 0.040537

(iii) Under reclaiming nothing

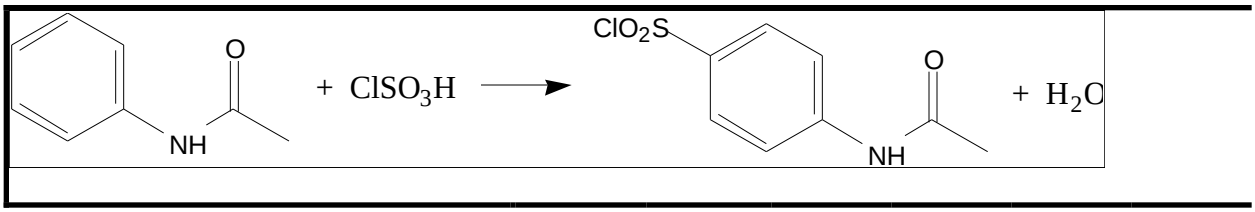
Mass of waste	284.028	g	**76**
E(m)	23.669	g waste/g product	**77**
RME	0.041	g product/Σ g reagents	**78**
Wasted input costs ($)	1.080		

Step 2: Chlorosulfonation

REACTION METRICS FORM

DATE: October 10, 2005
NAME OF TARGET PRODUCT: p-Acetamidobenzenesulfonyl chloride
REACTION CLASSIFICATION:

BALANCED CHEMICAL EQUATIONS:



PART 1: RAW MATERIALS USAGE

(A) REACTION STAGE:

(i) REAGENTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
Acetanilide	135			0.08889	12.00	0.094	1.128	12
Chlorosulfonic acid	116.45			0.45	52.4	0.0571	2.992	13
							0.000	14
							0.000	15
TOTAL REAGENTS	251.45			Add lines 12 to 15	64.40265		4.120	**16**

(ii) CATALYSTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
None			0		0		0.000	19
							0.000	20
TOTAL CATALYSTS				Add lines 19 to 20	0		0.000	**21**

(iii) SOLVENTS	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
None		0	0		0.000	24
			0		0.000	25
TOTAL SOLVENTS		Add lines 24 to 25	0		0.000	**26**

Reaction Materials Subtotals	Add lines 16, 21, 26	64.40265		4.120	**29**	

(B) WORK-UP STAGE:

MATERIAL	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
Water	1	300	300	0	0.000	33
			0		0.000	34
			0		0.000	35
			0		0.000	36
TOTAL WORK-UP MATERIALS		Add lines 33 to 36	300		0.000	**37**

(C) PURIFICATION STAGE:

MATERIAL	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
None		0	0		0.000	41

		0	0.000	42
		0	0.000	43
		0	0.000	44
TOTAL PURIFICATION MATERIALS	Add lines 41 to 44	0	0.000	**45**
Post-reaction Materials Subtotals	Add lines 37, 45	300	0.000	**47**

		Mass (g)	**Cost ($)**	
TOTAL INPUT MATERIALS	Add lines 29, 47	364.40265	4.120	**50**

	MW (g/mol)	**Moles**	**Yield**	**Mass (g)**	**Cost ($/g)**	
OUTPUT TARGET PRODUCT	233.35	0.0643	0.7232	15	0.275	**53**

PART 2: GREEN METRICS ANALYSIS

Limiting reagent:

PARAMETER	VALUE		
Reaction Scale	0.08889	moles	**58**
E(mw)	0.078	MW byproducts/MW product	**59**
AE	0.928	MW product/Σ MW reagents	**60**

(i) Under reclaiming reaction solvents, catalysts, and byproducts, and all post-reaction materials

Mass of waste (line 16 - 53)	49.40265	g	**63**
E(m)	3.29351	g waste/g product	**64**
RME	0.232909671	g product/Σ g reagents	**65**
SF	2.881371072		**66**
Wasted input costs ($)	3.159		

(ii) Under committing all reaction solvents, catalysts, and byproducts, and post-reaction materials to waste

Mass of waste (line 50 - 53)	349.40265	g	**69**
E(m)	23.29351	g waste/g product	**70**
RME	0.041163257	g product/Σ g reagents	**71**
Wasted input costs ($)	3.951		

Check formula 0.041163

(iii) Under reclaiming nothing

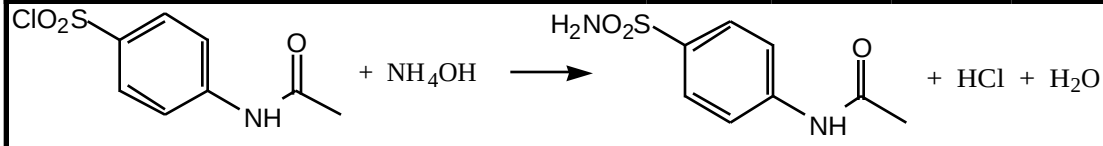
Mass of waste	349.403	g	**76**
E(m)	23.294	g waste/g product	**77**
RME	0.041	g product/Σ g reagents	**78**
Wasted input costs ($)	3.951		

Step 3: Amination

REACTION METRICS FORM

DATE: October 10, 2005
NAME OF TARGET PRODUCT: p-Acetamidobenzenesulfonamide
REACTION CLASSIFICATION:

BALANCED CHEMICAL EQUATIONS:



PART 1: RAW MATERIALS USAGE

(A) REACTION STAGE:

(i) REAGENTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
p-AcetamidobenzenesulfonylCl	233.45			0.06426	15.00	0.271	4.065	12
conc. NH4OH (28 %)	35	0.898	60.00	0.43104	53.88	0.0291	1.566	13
							0.000	14
							0.000	15
TOTAL REAGENTS	268.45			Add lines 12 to 15	68.88149 7		5.631	**16**

(ii) CATALYSTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
None			0		0		0.000	19
							0.000	20
TOTAL CATALYSTS				Add lines 19 to 20	0		0.000	**21**

(iii) SOLVENTS	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
None		0	0	0	0.000	24
			0		0.000	25
TOTAL SOLVENTS		Add lines 24 to 25	0		0.000	**26**

Reaction Materials Subtotals	Add lines 16, 21, 26	68.881497		5.631	**29**

(B) WORK-UP STAGE:

MATERIAL	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
6 M H2SO4 (44 %)	1.3384	10	13.3840	0.0049	0.066	33
			0		0.000	34
			0		0.000	35
			0		0.000	36
TOTAL WORK-UP MATERIALS		Add lines 33 to 36	13.384		0.066	**37**

(C) PURIFICATION STAGE:

MATERIAL	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
None		0	0		0.000	41
			0		0.000	42
			0		0.000	43
			0		0.000	44
TOTAL PURIFICATION MATERIALS		Add lines 41 to 44	0		0.000	**45**

Post-reaction Materials Subtotals	Add lines 37, 45	13.384		0.066	**47**

		Mass (g)	**Cost ($)**	
TOTAL INPUT MATERIALS	Add lines 29, 47	82.265497	5.697	**50**

	MW (g/mol)	**Moles**	**Yield**	**Mass (g)**	**Cost ($/g)**	
OUTPUT TARGET PRODUCT	214	0.0514	0.7999	11	0.518	**53**

PART 2: GREEN METRICS ANALYSIS

Limiting reagent:

PARAMETER	VALUE		
Reaction Scale	0.06426	moles	**58**
E(mw)	0.254	MW byproducts/MW product	**59**
AE	0.797	MW product/Σ MW reagents	**60**

(i) Under reclaiming reaction solvents, catalysts, and byproducts, and all post-reaction materials

Mass of waste (line 16 - 53)	57.881497	g	**63**

E(m)	5.261954273	g waste/g product	**64**
RME	0.159694555	g product/Σ g reagents	**65**
SF	3.992992069		**66**
Wasted input costs ($)	4.777		

(ii) Under committing all reaction solvents, catalysts, and byproducts, and post-reaction materials to waste

Mass of waste (line 50 - 53)	71.265497	g	**69**
E(m)	6.478681545	g waste/g product	**70**
RME	0.133713408	g product/Σ g reagents	**71**
Wasted input costs ($)	4.936		
Check formula	0.133713		

(iii) Under reclaiming nothing

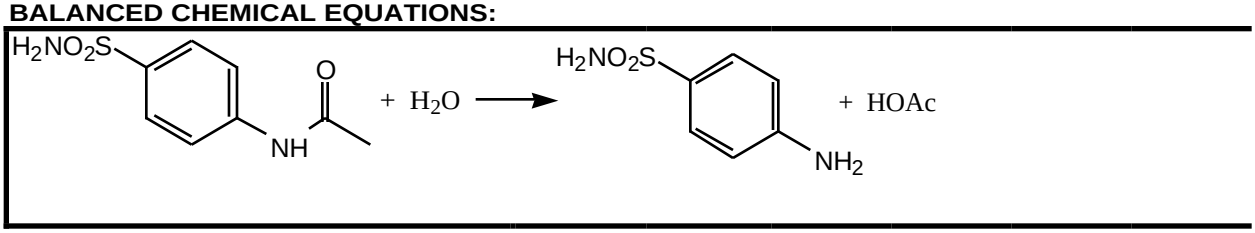
Mass of waste	71.265	g	**76**
E(m)	6.479	g waste/g product	**77**
RME	0.134	g product/Σ g reagents	**78**
Wasted input costs ($)	4.936		

Step 4: Deacetylation

REACTION METRICS FORM

DATE: October 10, 2005
NAME OF TARGET PRODUCT: Sulfanilamide
REACTION CLASSIFICATION:

BALANCED CHEMICAL EQUATIONS:



PART 1: RAW MATERIALS USAGE

(A) REACTION STAGE:

(i) REAGENTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)

p-Acetamidobenzenesulfonamide	214			0.0514	11.0	0.518	5.698	12
water	18	1	60.30	3.35	60.3	0	0.000	13
							0.000	14
							0.000	15
TOTAL REAGENTS	232			Add lines 12 to 15	71.2996		5.698	**16**

(ii) CATALYSTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
3 M HCl (10 %)	36.45	1.047	26.0	0.07468	27.222	0.00453	0.123	19
							0.000	20
TOTAL CATALYSTS				Add lines 19 to 20	27.222		0.123	**21**

(iii) SOLVENTS	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
None		0	0		0.000	24
			0		0.000	25
TOTAL SOLVENTS		Add lines 24 to 25	0		0.000	**26**

Reaction Materials Subtotals	Add lines 16, 21, 26	98.5216		5.821	**29**

(B) WORK-UP STAGE:

MATERIAL	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
6 M NaOH (20 %)	1.2191	15	18.2865	0.0035	0.065	33
sat'd Na2CO3	1.1463	40	45.852	0.0278	1.274	34
			0		0.000	35
			0		0.000	36
TOTAL WORK-UP MATERIALS		Add lines 33 to 36	64.1385		1.339	**37**

(C) PURIFICATION STAGE:

MATERIAL	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
None		0	0		0.000	41
			0		0.000	42
			0		0.000	43
			0		0.000	44
TOTAL PURIFICATION MATERIALS		Add lines 41 to 44	0		0.000	**45**

Post-reaction Materials Subtotals	Add lines 37, 45	64.1385		1.339	**47**

		Mass (g)	Cost ($)	
TOTAL INPUT MATERIALS	Add lines 29, 47	162.6601	7.160	**50**

	MW (g/mol)	Moles	Yield	Mass (g)	Cost ($/g)	
OUTPUT TARGET PRODUCT	172	0.0494	0.9615	8.5	0.842	**53**

PART 2: GREEN METRICS ANALYSIS

Limiting reagent:

PARAMETER	VALUE		
Reaction Scale	0.0514	moles	**58**
E(mw)	0.349	MW byproducts/MW product	**59**
AE	0.741	MW product/Σ MW reagents	**60**

(i) Under reclaiming reaction solvents, catalysts, and byproducts, and all post-reaction materials

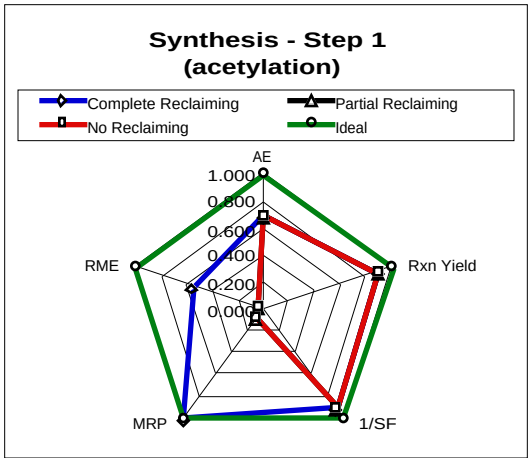
Mass of waste (line 16 - 53)	62.7996	g	**63**
E(m)	7.388188235	g waste/g product	**64**
RME	0.119215255	g product/Σ g reagents	**65**
SF	5.979102375		**66**
Wasted input costs ($)	5.064		

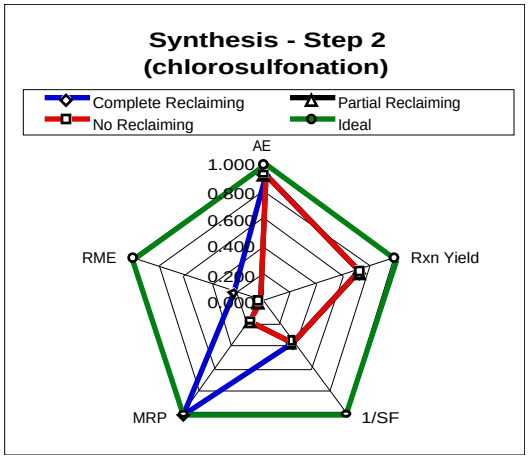
(ii) Under committing all reaction solvents, catalysts, and byproducts, and post-reaction materials to waste

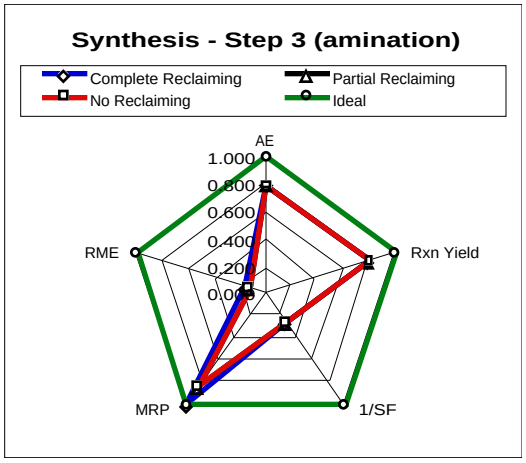
Mass of waste (line 50 - 53)	154.1601	g	**69**
E(m)	18.13648235	g waste/g product	**70**
RME	0.052256208	g product/Σ g reagents	**71**
Wasted input costs ($)	6.786		
Check formula	0.052256		

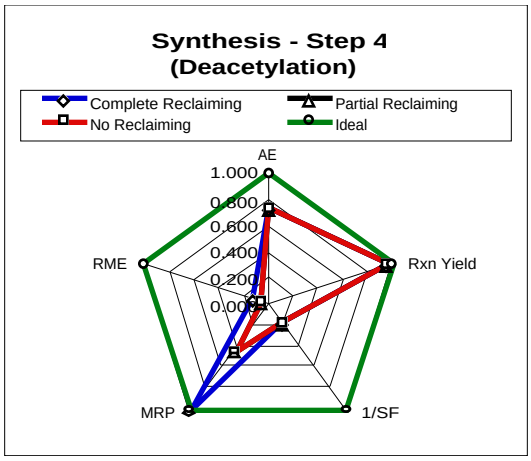
(iii) Under reclaiming ether from reaction and petroleum ether from purification

Mass of waste	154.160	g	**76**
E(m)	18.136	g waste/g product	**77**
RME	0.052	g product/Σ g reagents	**78**
Wasted input costs ($)	6.786		







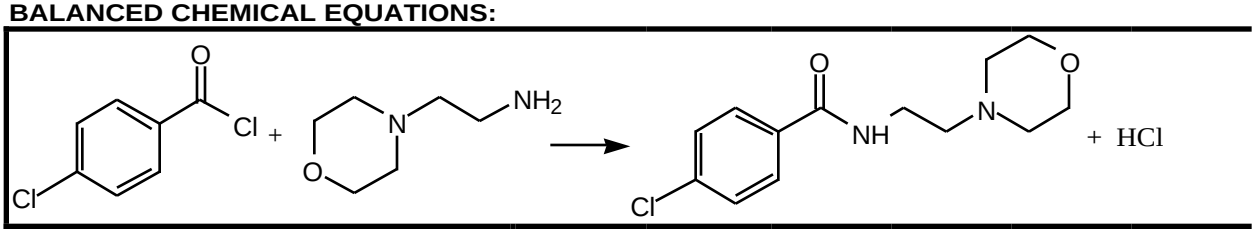


Amidation

REACTION METRICS FORM

DATE: June 1, 2005
NAME OF TARGET PRODUCT: Moclobemide
REACTION CLASSIFICATION: Amidation (Non-carbon-carbon bond forming)

BALANCED CHEMICAL EQUATIONS:



PART 1: RAW MATERIALS USAGE

(A) REACTION STAGE:

(i) REAGENTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
4-chlorobenzoyl chloride	174.9	1.377	0.39	0.00305	0.533	0.0657	0.035	12
4-(2-aminoethyl)morpholine	130	0.992	0.40	0.00307	0.399	1.49	0.595	13
							0.000	14
							0.000	15
TOTAL REAGENTS	304.9			Add lines 12 to 15	0.932545		0.630	**16**

(ii) CATALYSTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
triethylamine	101	0.726	15	0.1078	10.89	0.0362	0.394	19
							0.000	20
TOTAL CATALYSTS				Add lines 19 to 20	10.89		0.394	**21**

(iii) SOLVENTS	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
None	0	0	0	0	0.000	24
					0.000	25
TOTAL SOLVENTS		Add lines 24 to 25	0		0.000	**26**

Reaction Materials Subtotals	Add lines 16, 21, 26	11.822545		1.024	**29**

(B) WORK-UP STAGE:

MATERIAL	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
10% NH3 (aq)	0.9575	10	9.575	0.0372	0.036	33
CH2Cl2	1.336	20	26.725	0.0146	0.390	34
MgSO4				0.0619	0.309	35
					0.000	36
TOTAL WORK-UP MATERIALS		Add lines 33 to 36	41.295		0.735	**37**

(C) PURIFICATION STAGE:

MATERIAL	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
None	0	0	0	0	0.000	41
					0.000	42
					0.000	43
					0.000	44

TOTAL PURIFICATION MATERIALS	Add lines 41 to 44	0	0.000	**45**
Post-reaction Materials Subtotals	Add lines 37, 45	41.295	0.735	**47**

		Mass (g)	**Cost ($)**	
TOTAL INPUT MATERIALS	Add lines 29, 47	53.117545	1.759	**50**

	MW (g/mol)	**Moles**	**Yield**	**Mass (g)**	**Cost ($/g)**	
OUTPUT TARGET PRODUCT	268.45	0.0022	0.7084	0.58	3.032	**53**

PART 2: GREEN METRICS ANALYSIS

Limiting reagent: 4-chlorobenzoyl chloride

PARAMETER	VALUE		
Reaction Scale	0.00305	moles	**58**
E(mw)	0.136	MW byproducts/MW product	**59**
AE	0.880	MW product/Σ MW reagents	**60**

(i) Under reclaiming reaction solvents, catalysts, and byproducts, and all post-reaction materials

Mass of waste (line 16 - 53)	0.353	g	**63**
E(m)	0.608	g waste/g product	**64**
RME	0.622	g product/Σ g reagents	**65**
SF	1.003		**66**
Wasted input costs ($)	0.238		

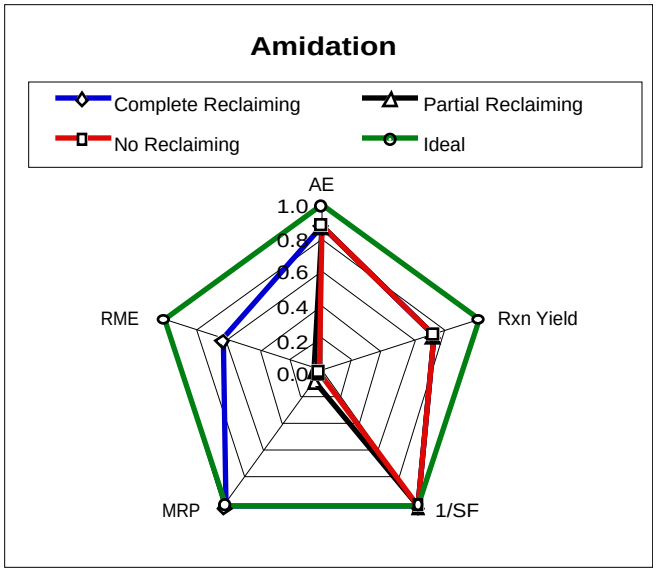
(ii) Under committing all reaction solvents, catalysts, and byproducts, and post-reaction materials to waste

Mass of waste (line 50 - 53)	52.538	g	**69**
E(m)	90.582	g waste/g product	**70**
RME	0.011	g product/Σ g reagents	**71**
Wasted input costs ($)	1.739		
Check formula	0.011		

(iii) Under reclaiming Et3N and CH2Cl2

Mass of waste	14.928	g	**76**
E(m)	25.737	g waste/g product	**77**
RME	0.037	g product/Σ g reagents	**78**

Wasted input costs ($) 0.938

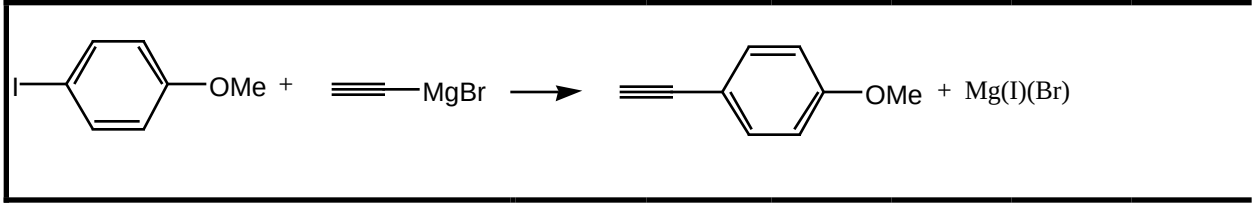


Sonagashira Coupling Reaction

REACTION METRICS FORM

DATE: June 1, 2005
NAME OF TARGET PRODUCT: p-Methoxyphenylacetylene
REACTION CLASSIFICATION: Coupling (Carbon-carbon bond forming)

BALANCED CHEMICAL EQUATIONS:



PART 1: RAW MATERIALS USAGE

(A) REACTION STAGE:

(i) REAGENTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
4-iodoanisole	234			0.00256	0.599	0.802	0.480	12
0.5 M ethynylMgBr (6.9 %)	129.2	0.94	7.6	0.0038	0.491	0.153	0.075	13
							0.000	14
							0.000	15

TOTAL REAGENTS	363.2			Add lines 12 to 15	1.09	0.555	**16**

(ii) CATALYSTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
Pd(PPh3)4	1155.58			0.0001	0.116	12.606	1.457	19
							0.000	20
TOTAL CATALYSTS				Add lines 19 to 20	0.116		1.457	**21**

(iii) SOLVENTS	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
THF	0.889		6.653	0.0206	0.137	24
					0.000	25
TOTAL SOLVENTS		Add lines 24 to 25	6.653		0.137	**26**

Reaction Materials Subtotals	Add lines 16, 21, 26	7.858558		2.149	**29**

(B) WORK-UP STAGE:

MATERIAL	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
sat. NaCl (24 %)	1.1804	50	59.02	0.0153	0.217	33
Et2O	0.708	100	70.8	0.0287	2.031	34
MgSO4			5	0.0619	0.309	35
					0.000	36
TOTAL WORK-UP MATERIALS		Add lines 33 to 36	134.82		2.557	**37**

(C) PURIFICATION STAGE:

MATERIAL	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
CH2Cl2	1.336	20	26.72	0.0146	0.390	41
					0.000	42
					0.000	43
					0.000	44
TOTAL PURIFICATION MATERIALS		Add lines 41 to 44	26.72		0.390	**45**

Post-reaction Materials Subtotals	Add lines 37, 45	161.54		2.947	**47**

		Mass (g)	**Cost ($)**	
TOTAL INPUT MATERIALS	Add lines 29, 47	169.398558	5.097	**50**

	MW (g/mol)	Moles	Yield	Mass (g)	Cost ($/g)	
OUTPUT TARGET PRODUCT	132	0.0018	0.6954	0.235	21.689	**53**

PART 2: GREEN METRICS ANALYSIS

Limiting reagent:

PARAMETER	VALUE		
Reaction Scale	0.00256	moles	**58**
E(mw)	1.752	MW byproducts/MW product	**59**
AE	0.363	MW product/Σ MW reagents	**60**

(i) Under reclaiming reaction solvents, catalysts, and byproducts, and all post-reaction materials

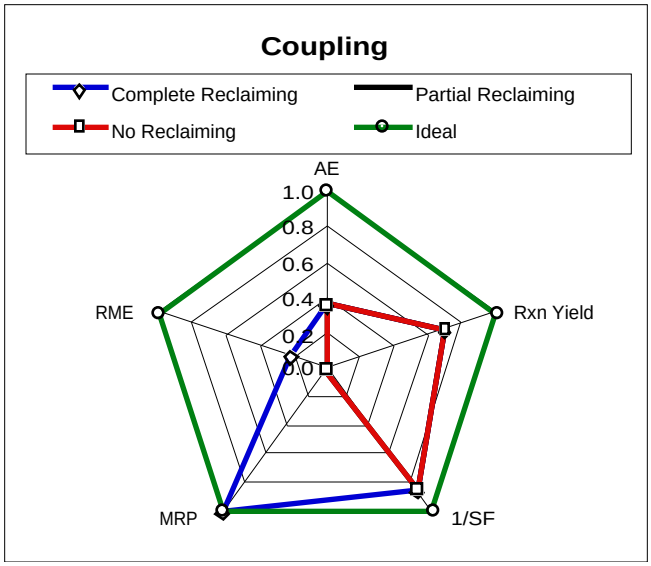
Mass of waste (line 16 - 53)	0.855	g	**63**
E(m)	3.638	g waste/g product	**64**
RME	0.216	g product/Σ g reagents	**65**
SF	1.172		**66**
Wasted input costs ($)	0.436		

(ii) Under committing all reaction solvents, catalysts, and byproducts, and post-reaction materials to waste

Mass of waste (line 50 - 53)	169.164	g	**69**
E(m)	719.845	g waste/g product	**70**
RME	0.00139	g product/Σ g reagents	**71**
Wasted input costs ($)	5.090		
Check formula	0.00139		

(iii) Under reclaiming Pd(PPh3)4 catalyst

Mass of waste	169.048	g	**76**
E(m)	719.351	g waste/g product	**77**
RME	0.001	g product/Σ g reagents	**78**
Wasted input costs ($)	3.635		

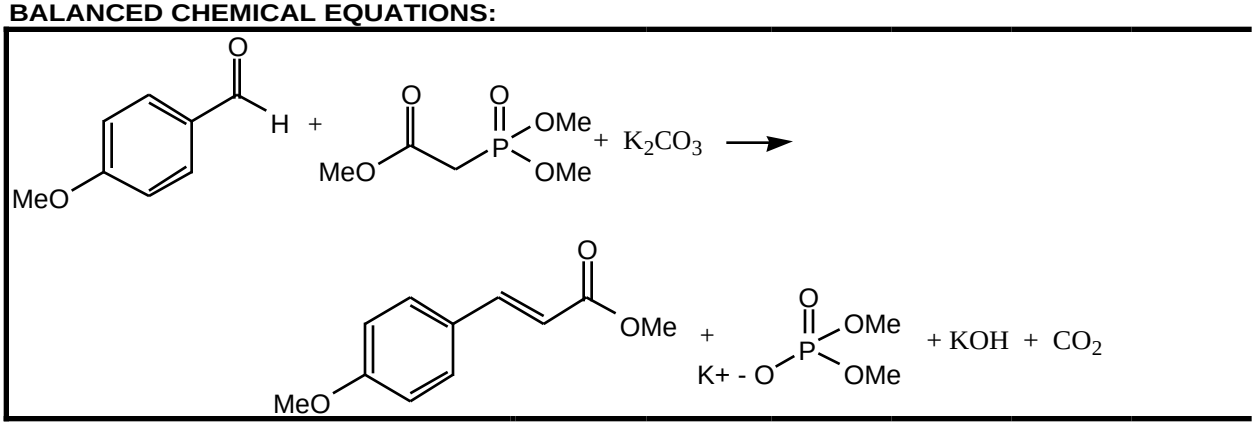


Horner-Emmons-Wadsworth Reaction

REACTION METRICS FORM

DATE: June 1, 2005
NAME OF TARGET PRODUCT: Methyl 4-methoxycinnamate
REACTION CLASSIFICATION: Horner-Wadsworth-Emmons (Carbon-carbon bond forming)

BALANCED CHEMICAL EQUATIONS:



PART 1: RAW MATERIALS USAGE

(A) REACTION STAGE:

(i) REAGENTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
4-methoxybenzaldehyde	136	1.119	0.36	0.003	0.408	0.1157	0.047	12
trimethylphosphonoacetate	182	1.125	1.40	0.00865	1.574	1.22	1.921	13

potassium carbonate	138		0.00796	1.098	0.0241	0.026	14
						0.000	15
TOTAL REAGENTS	456		Add lines 12 to 15	3.08078		1.994	**16**

(ii) CATALYSTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
None	0	0	0	0	0	0	0.000	19
							0.000	20
TOTAL CATALYSTS				Add lines 19 to 20	0		0.000	**21**

(iii) SOLVENTS	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
H2O	1	0.5	0.5	0	0.000	24
					0.000	25
TOTAL SOLVENTS		Add lines 24 to 25	0.5		0.000	**26**

Reaction Materials Subtotals	Add lines 16, 21, 26	3.58078	1.994 **29**

(B) WORK-UP STAGE:

MATERIAL	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
H2O	1	10	10	0	0.000	33
					0.000	34
					0.000	35
					0.000	36
TOTAL WORK-UP MATERIALS		Add lines 33 to 36	10		0.000	**37**

(C) PURIFICATION STAGE:

MATERIAL	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
95 % EtOH	0.816	3	2.448	0.0422	0.103	41
H2O	1	5	5	0	0.000	42
					0.000	43
					0.000	44
TOTAL PURIFICATION MATERIALS		Add lines 41 to 44	7.448		0.103	**45**

Post-reaction Materials Subtotals	Add lines 37, 45	17.448	0.103 **47**

	Mass (g)	**Cost ($)**

TOTAL INPUT MATERIALS			Add lines 29, 47	21.02878	2.098	**50**
	MW (g/mol)	**Moles**	**Yield**	**Mass (g)**	**Cost ($/g)**	
OUTPUT TARGET PRODUCT	192	0.0024	0.8073	0.465	4.511	**53**

PART 2: GREEN METRICS ANALYSIS

Limiting reagent: 4-methoxybenzaldehyde

PARAMETER	VALUE		
Reaction Scale	0.003	moles	**58**
E(mw)	1.375	MW byproducts/MW product	**59**
AE	0.421	MW product/Σ MW reagents	**60**

(i) Under reclaiming reaction solvents, catalysts, and byproducts, and all post-reaction materials

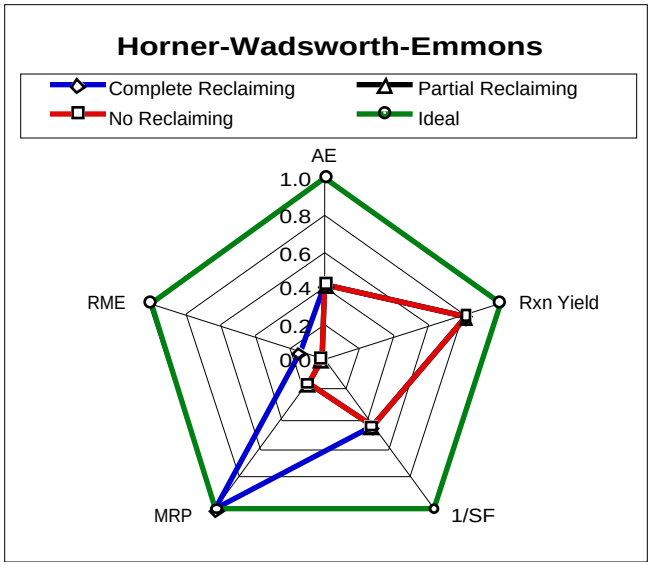
Mass of waste (line 16 - 53)	2.616	g	**63**
E(m)	5.625	g waste/g product	**64**
RME	0.151	g product/Σ g reagents	**65**
SF	2.252		**66**
Wasted input costs ($)	1.693		

(ii) Under committing all reaction solvents, catalysts, and byproducts, and post-reaction materials to waste

Mass of waste (line 50 - 53)	20.564	g	**69**
E(m)	44.223	g waste/g product	**70**
RME	0.022	g product/Σ g reagents	**71**
Wasted input costs ($)	2.051		
Check formula	0.022		

(iii) Under reclaiming ethanol

Mass of waste	18.238	g	**76**
E(m)	39.222	g waste/g product	**77**
RME	0.025	g product/Σ g reagents	**78**
Wasted input costs ($)	1.945		

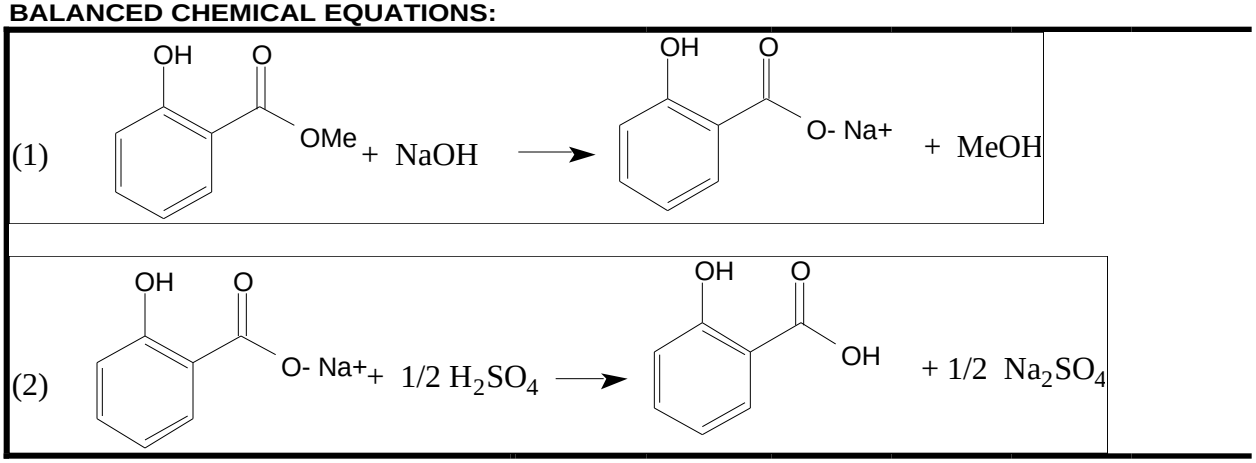


Hydrolysis

REACTION METRICS FORM

DATE: June 1, 2005
NAME OF TARGET PRODUCT: Salicylic acid
REACTION CLASSIFICATION: Substitution (Hydrolysis)

BALANCED CHEMICAL EQUATIONS:



PART 1: RAW MATERIALS USAGE

(A) REACTION STAGE:

(i) REAGENTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
methyl salicylate	152	1.174	0.35	0.00270	0.4109	0.0314	0.013	12
3 M NaOH (12 %)	40	1.1309	1	0.003	1.1309	0.0019	0.002	13
3 M H2SO4 (29.4 %)	49	1.21	2	0.00726	2.42	0.0034	0.008	14

						0.000	15
TOTAL REAGENTS	241		Add lines 12 to 15	3.9618		0.023	**16**

(ii) CATALYSTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
None	0	0	0	0	0	0	0.000	19
							0.000	20
TOTAL CATALYSTS				Add lines 19 to 20	0		0.000	**21**

(iii) SOLVENTS	Density (g/mL)	Volume (mL)		Mass (g)	Cost ($/g)	Cost ($)	
H2O	1	2		2	0	0.000	24
						0.000	25
TOTAL SOLVENTS			Add lines 24 to 25	2		0.000	**26**

Reaction Materials Subtotals			Add lines 16, 21, 26	5.9618		0.023	**29**

(B) WORK-UP STAGE:

MATERIAL	Density (g/mL)	Volume (mL)		Mass (g)	Cost ($/g)	Cost ($)	
None	0	0		0	0	0.000	33
						0.000	34
						0.000	35
						0.000	36
TOTAL WORK-UP MATERIALS			Add lines 33 to 36	0		0.000	**37**

(C) PURIFICATION STAGE:

MATERIAL	Density (g/mL)	Volume (mL)		Mass (g)	Cost ($/g)	Cost ($)	
H2O	1	2		2	0	0.000	41
						0.000	42
						0.000	43
						0.000	44
TOTAL PURIFICATION MATERIALS			Add lines 41 to 44	2		0.000	**45**

Post-reaction Materials Subtotals			Add lines 37, 45	2		0.000	**47**

			Mass (g)	**Cost ($)**	
TOTAL INPUT MATERIALS		Add lines 29, 47	7.9618	0.023	**50**

	MW (g/mol)	Moles	Yield	Mass (g)	Cost ($/g)	
OUTPUT TARGET PRODUCT	138	0.0022	0.8042	0.3	0.077	**53**

PART 2: GREEN METRICS ANALYSIS

Limiting reagent: methyl salicylate

PARAMETER	VALUE		
Reaction Scale	0.003	moles	**58**
E(mw)	0.746	MW byproducts/MW product	**59**
AE	0.573	MW product/Σ MW reagents	**60**

(i) Under reclaiming reaction solvents and catalysts and all post-reaction materials

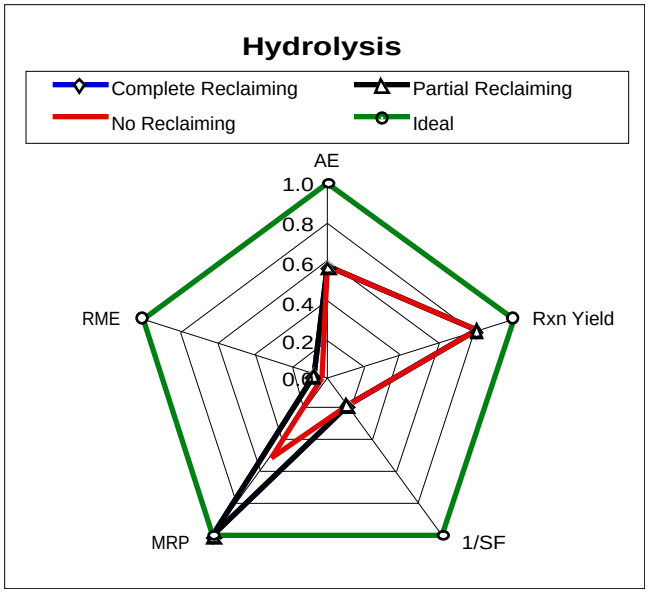
Mass of waste (line 16 - 53)	3.662	g	**63**
E(m)	12.206	g waste/g product	**64**
RME	0.076	g product/Σ g reagents	**65**
SF	6.081		**66**
Wasted input costs ($)	0.021		

(ii) Under committing all reaction solvents and catalysts and post-reaction materials to waste

Mass of waste (line 50 - 53)	7.662	g	**69**
E(m)	25.539	g waste/g product	**70**
RME	0.038	g product/Σ g reagents	**71**
Wasted input costs ($)	0.022		
Check formula	0.038		

(iii) Under reclaiming nothing

Mass of waste	7.662	g	**76**
E(m)	25.539	g waste/g product	**77**
RME	0.038	g product/Σ g reagents	**78**
Wasted input costs ($)	0.022		



Synthesis of Modafinil

Step 1: Sulfur transfer-substitution sequence

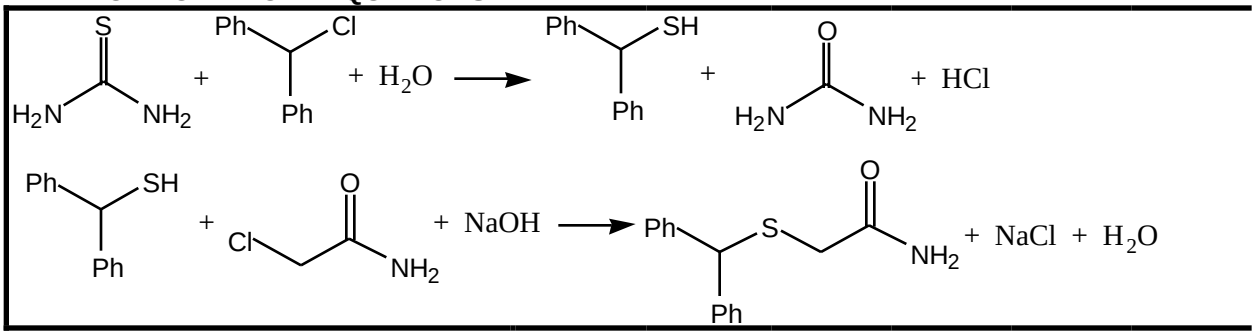
REACTION METRICS FORM

DATE: June 1, 2005

NAME OF TARGET PRODUCT: 2-Benzhydrylsulfanylacetamide

REACTION CLASSIFICATION: Substitution/non-carbon-carbon bond forming reaction sequence

BALANCED CHEMICAL EQUATIONS:



PART 1: RAW MATERIALS USAGE

(A) REACTION STAGE:

(i) REAGENTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
thiourea	76			0.0657	4.993	0.0473	0.236	12
benzhydryl chloride	202.45			0.0543	10.993	0.3704	4.072	13
2-chloroacetamide	93.45			0.0588	5.495	0.0599	0.329	14
NaOH (30 %)	40	1.3279	7.3	0.0727	9.694	0.0053	0.051	15

TOTAL REAGENTS	411.9			Add lines 12 to 15	31.175		4.689	**16**

(ii) CATALYSTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
potassium iodide	166			0.00105	0.174	0.1911	0.033	19
triethylamine	101	0.726	8.3	0.0595	6.010	0.0362	0.217	20
TOTAL CATALYSTS				Add lines 19 to 20	6.1838		0.251	**21**

(iii) SOLVENTS	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
H2O	1	54	54	0	0.000	24
					0.000	25
TOTAL SOLVENTS		Add lines 24 to 25	54		0.000	**26**

Reaction Materials Subtotals	Add lines 16, 21, 26	91.359		4.939	**29**

(B) WORK-UP STAGE:

MATERIAL	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
None	0	0	0	0	0.000	33
					0.000	34
					0.000	35
					0.000	36
TOTAL WORK-UP MATERIALS		Add lines 33 to 36	0		0.000	**37**

(C) PURIFICATION STAGE:

MATERIAL	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
toluene	0.865	20	17.3	0.0099	0.172	41
					0.000	42
					0.000	43
					0.000	44
TOTAL PURIFICATION MATERIALS		Add lines 41 to 44	17.3		0.172	**45**

Post-reaction Materials Subtotals	Add lines 37, 45	17.3		0.172	**47**

		Mass (g)	**Cost ($)**	
TOTAL INPUT MATERIALS	Add lines 29, 47	108.659	5.111	**50**

	MW (g/mol)	Moles	Yield	Mass (g)	Cost ($/g)	
OUTPUT TARGET PRODUCT	257	0.0381	0.7008	9.78	0.523	**53**

PART 2: GREEN METRICS ANALYSIS

Limiting reagent: benzhydryl chloride

PARAMETER	VALUE		
Reaction Scale	0.059	moles	**58**
E(mw)	0.603	MW byproducts/MW product	**59**
AE	0.624	MW product/Σ MW reagents	**60**

(i) Under reclaiming reaction solvents, catalysts, and byproducts, and all post-reaction materials

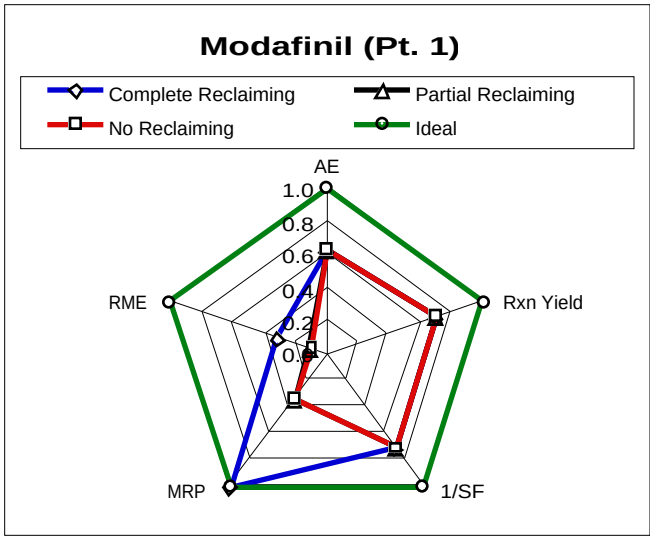
Mass of waste (line 16 - 53)	21.395	g	**63**
E(m)	2.188	g waste/g product	**64**
RME	0.314	g product/Σ g reagents	**65**
SF	1.394		**66**
Wasted input costs ($)	3.218		

(ii) Under committing all reaction solvents, catalysts, and byproducts, and post-reaction materials to waste

Mass of waste (line 50 - 53)	98.879	g	**69**
E(m)	10.110	g waste/g product	**70**
RME	0.090	g product/Σ g reagents	**71**
Wasted input costs ($)	4.651		
Check formula	0.090		

(iii) Under reclaiming toluene

Mass of waste	81.579	g	**76**
E(m)	8.341	g waste/g product	**77**
RME	0.107	g product/Σ g reagents	**78**
Wasted input costs ($)	4.411		

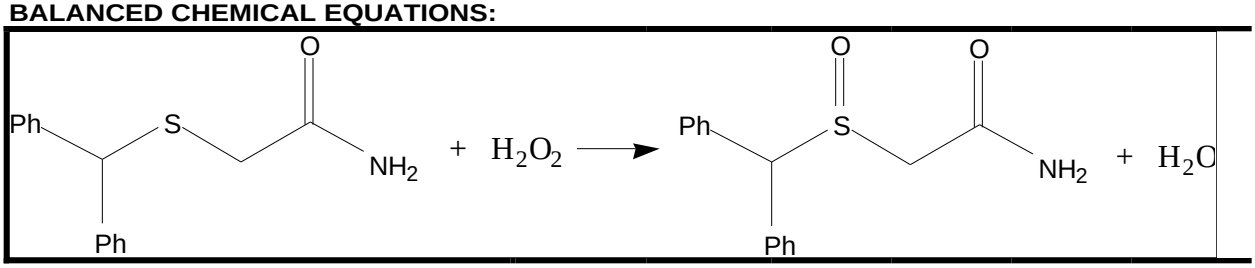


Step 2: Oxidation

REACTION METRICS FORM

DATE: June 1, 2005
NAME OF TARGET PRODUCT: (+/-) Modafinil
REACTION CLASSIFICATION: Oxidation (sulfide to sulfoxide)

BALANCED CHEMICAL EQUATIONS:



PART 1: RAW MATERIALS USAGE

(A) REACTION STAGE:

(i) REAGENTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
2-benzhydrylsulfanyl acetamide	257			0.00194	0.499	0.521	0.260	12
30 % H2O2	34	1.18	0.186	0.00194	0.220	0.0534	0.012	13
							0.000	14
							0.000	15
TOTAL REAGENTS	291			Add lines 12 to 15	0.718		0.271	**16**

(ii) CATALYSTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)

None	0	0	0	0	0	0	0.000	19
							0.000	20
TOTAL CATALYSTS			Add lines 19 to 20	0			0.000	**21**

(iii) SOLVENTS	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
glacial HOAc	1.049	2.5	2.6225	0.02376	0.062	24
					0.000	25
TOTAL SOLVENTS		Add lines 24 to 25	2.6225		0.062	**26**
Reaction Materials Subtotals		Add lines 16, 21, 26	3.3409		0.334	**29**

(B) WORK-UP STAGE:

MATERIAL	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
H2O	1	10	10	0	0.000	33
					0.000	34
					0.000	35
					0.000	36
TOTAL WORK-UP MATERIALS		Add lines 33 to 36	10		0.000	**37**

(C) PURIFICATION STAGE:

MATERIAL	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
MeOH	0.792	5	3.96	0.0207	0.082	41
					0.000	42
					0.000	43
					0.000	44
TOTAL PURIFICATION MATERIALS		Add lines 41 to 44	3.96		0.082	**45**
Post-reaction Materials Subtotals		Add lines 37, 45	13.96		0.082	**47**

			Mass (g)	Cost ($)	
TOTAL INPUT MATERIALS		Add lines 29, 47	17.3009	0.416	**50**

	MW (g/mol)	Moles	Yield	Mass (g)	Cost ($/g)	
OUTPUT TARGET PRODUCT	273	0.0012	0.6004	0.318	1.308	**53**

PART 2: GREEN METRICS ANALYSIS

Limiting reagent: 2-benzhydrylsulfanylacetamide, H2O2

PARAMETER	VALUE		
Reaction Scale	0.002	moles	**58**
E(mw)	0.066	MW byproducts/MW product	**59**
AE	0.938	MW product/Σ MW reagents	**60**

(i) Under reclaiming reaction solvents, catalysts, and byproducts, and all post-reaction materials

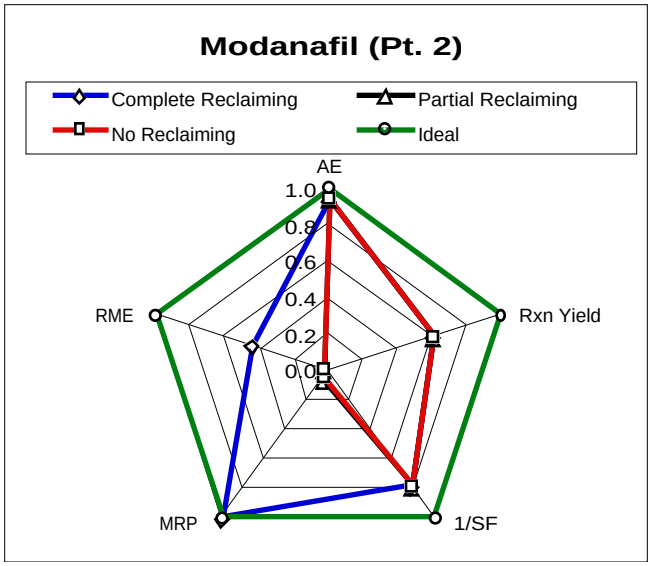
Mass of waste (line 16 - 53)	0.400	g	**63**
E(m)	1.259	g waste/g product	**64**
RME	0.443	g product/Σ g reagents	**65**
SF	1.273		**66**
Wasted input costs ($)	0.151		

(ii) Under committing all reaction solvents, catalysts, and byproducts, and post-reaction materials to waste

Mass of waste (line 50 - 53)	16.983	g	**69**
E(m)	53.405	g waste/g product	**70**
RME	0.018	g product/Σ g reagents	**71**
Wasted input costs ($)	0.408		
Check formula	0.018		

(iii) Under reclaiming methanol

Mass of waste	13.023	g	**76**
E(m)	40.953	g waste/g product	**77**
RME	0.024	g product/Σ g reagents	**78**
Wasted input costs ($)	0.326		

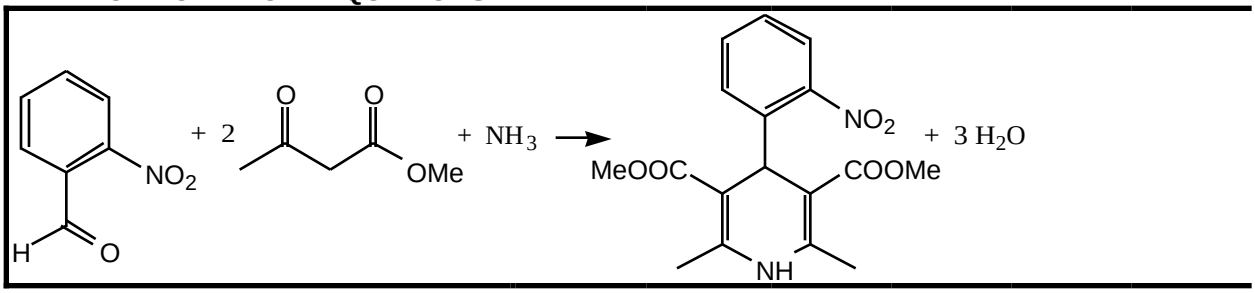


Multicomponent Reaction: Hanzsch Dihydropyridine synthesis of Nifedipine

REACTION METRICS FORM

DATE: June 2, 2005
NAME OF TARGET PRODUCT: Nifedipine
REACTION CLASSIFICATION: MCR (Hanzsch dihydropyridine synthesis)

BALANCED CHEMICAL EQUATIONS:



PART 1: RAW MATERIALS USAGE

(A) REACTION STAGE:

(i) REAGENTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
2-nitrobenzaldehyde	151			0.00336	0.50736	1.5540	0.788	12
methyl acetoacetate	232	1.076	0.90	0.00834	0.96744	0.0303	0.029	13
28 % NH3 (aq)	17	0.9	0.35	0.00519	0.315	0.3182	0.100	14
							0.000	15
TOTAL REAGENTS	400			Add lines 12 to 15	1.7898		0.918	**16**

(ii) CATALYSTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
None	0	0	0	0	0	0	0.000	19
							0.000	20
TOTAL CATALYSTS					Add lines 19 to 20	0	0.000	**21**

(iii) SOLVENTS	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
MeOH	0.79	0.5	0.395	0.0207	0.008	24
			0		0.000	25
TOTAL SOLVENTS		Add lines 24 to 25	0.395		0.008	**26**
Reaction Materials Subtotals		Add lines 16, 21, 26	2.1848		0.926	**29**

(B) WORK-UP STAGE:

MATERIAL	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
MeOH	0.79	2	1.58	0.0207	0.033	33
			0		0.000	34
			0		0.000	35
			0		0.000	36
TOTAL WORK-UP MATERIALS		Add lines 33 to 36	1.58		0.033	**37**

(C) PURIFICATION STAGE:

MATERIAL	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
toluene	0.865	2	1.73	0.0099	0.017	41
			0		0.000	42
			0		0.000	43
			0		0.000	44
TOTAL PURIFICATION MATERIALS		Add lines 41 to 44	1.73		0.017	**45**
Post-reaction Materials Subtotals		Add lines 37, 45	3.31		0.050	**47**

		Mass (g)	**Cost ($)**	
TOTAL INPUT MATERIALS	Add lines 29, 47	5.4948	0.976	**50**

	MW (g/mol)	**Moles**	**Yield**	**Mass (g)**	**Cost ($/g)**

OUTPUT TARGET PRODUCT	346	0.0014	0.4043	0.47	2.077	**53**

PART 2: GREEN METRICS ANALYSIS

Limiting reagent: 2-nitrobenzaldehyde

PARAMETER	VALUE		
Reaction Scale	0.00336	moles	**58**
E(mw)	0.156	MW byproducts/MW product	**59**
AE	0.865	MW product/Σ MW reagents	**60**

(i) Under reclaiming reaction solvents, catalysts, and byproducts, and all post-reaction materials

Mass of waste (line 16 - 53)	1.320	g	**63**
E(m)	2.808	g waste/g product	**64**
RME	0.263	g product/Σ g reagents	**65**
SF	1.332		**66**
Wasted input costs ($)	0.677		

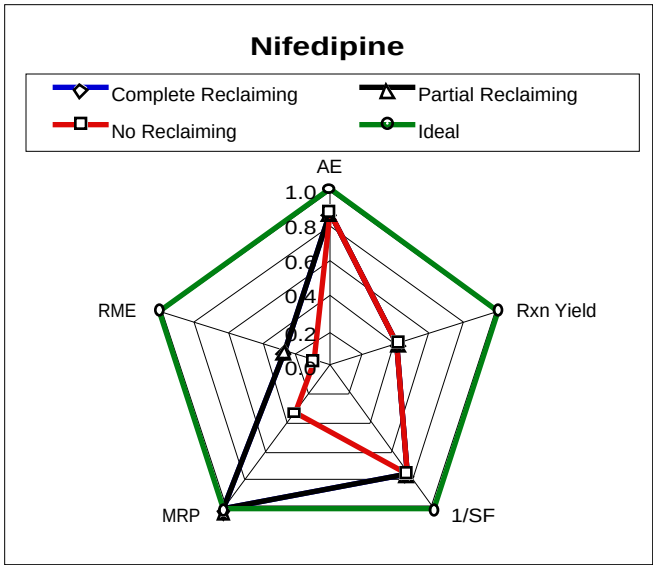
(ii) Under committing all reaction solvents, catalysts, and byproducts, and post-reaction materials to waste

Mass of waste (line 50 - 53)	5.025	g	**69**
E(m)	10.691	g waste/g product	**70**
RME	0.0855	g product/Σ g reagents	**71**
Wasted input costs ($)	0.893		

Check formula 0.0855

(iii) Under reclaiming ether from reaction and petroleum ether from purification

Mass of waste	1.320	g	**76**
E(m)	2.808	g waste/g product	**77**
RME	0.263	g product/Σ g reagents	**78**
Wasted input costs ($)	0.677		

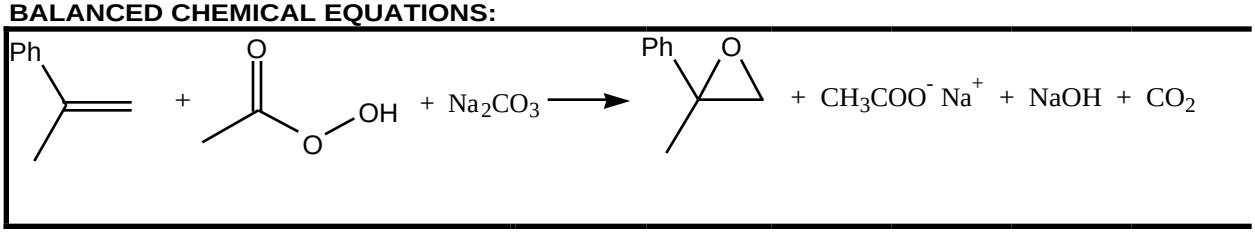


Epoxidation

REACTION METRICS FORM

DATE: June 1, 2005
NAME OF TARGET PRODUCT: 1-Methyl-1-phenyl-oxirane
REACTION CLASSIFICATION: Oxidation (Olefin to epoxide)

BALANCED CHEMICAL EQUATIONS:



PART 1: RAW MATERIALS USAGE

(A) REACTION STAGE:

(i) REAGENTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
alpha-methylstyrene	118	0.909	1.30	0.01	1.18	0.0135	0.016	12
peracetic acid (32 %)	76	1.13	2.73	0.013	3.09	0.1883	0.581	13
Na2CO3	106			0.038	4	0.0354	0.142	14
							0.000	15
TOTAL REAGENTS	300			Add lines 12 to 15	8.2675		0.739	**16**

(ii) CATALYSTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)

None	0	0	0	0	0	0.000	19
						0.000	20
TOTAL CATALYSTS			Add lines 19 to 20	0		0.000	**21**

(iii) SOLVENTS	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
CH2Cl2	1.336	25	33.4	0.0146	0.488	24
					0.000	25
TOTAL SOLVENTS		Add lines 24 to 25	33.4		0.488	**26**
Reaction Materials Subtotals		Add lines 16, 21, 26	41.6675		1.226	**29**

(B) WORK-UP STAGE:

MATERIAL	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
CH2Cl2	1.336	4	5.344	0.0146	0.078	33
					0.000	34
					0.000	35
					0.000	36
TOTAL WORK-UP MATERIALS		Add lines 33 to 36	5.344		0.078	**37**

(C) PURIFICATION STAGE:

MATERIAL	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
alumina			5	1.101	5.505	41
					0.000	42
					0.000	43
					0.000	44
TOTAL PURIFICATION MATERIALS		Add lines 41 to 44	5		5.505	**45**
Post-reaction Materials Subtotals		Add lines 37, 45	10.344		5.583	**47**

			Mass (g)	**Cost ($)**	
TOTAL INPUT MATERIALS		Add lines 29, 47	52.0115	6.809	**50**

	MW (g/mol)	**Moles**	**Yield**	**Mass (g)**	**Cost ($/g)**	
OUTPUT TARGET PRODUCT	134	0.0030	0.2985	0.4	17.024	**53**

PART 2: GREEN METRICS ANALYSIS

Limiting reagent:

PARAMETER	VALUE		
Reaction Scale	0.01	moles	**58**
E(mw)	1.239	MW byproducts/MW product	**59**
AE	0.447	MW product/Σ MW reagents	**60**

(i) Under reclaiming reaction solvents, catalysts, and byproducts, and all post-reaction materials

Mass of waste (line 16 - 53)	7.868	g	**63**
E(m)	19.669	g waste/g product	**64**
RME	0.048	g product/Σ g reagents	**65**
SF	2.756		**66**
Wasted input costs ($)	0.703		

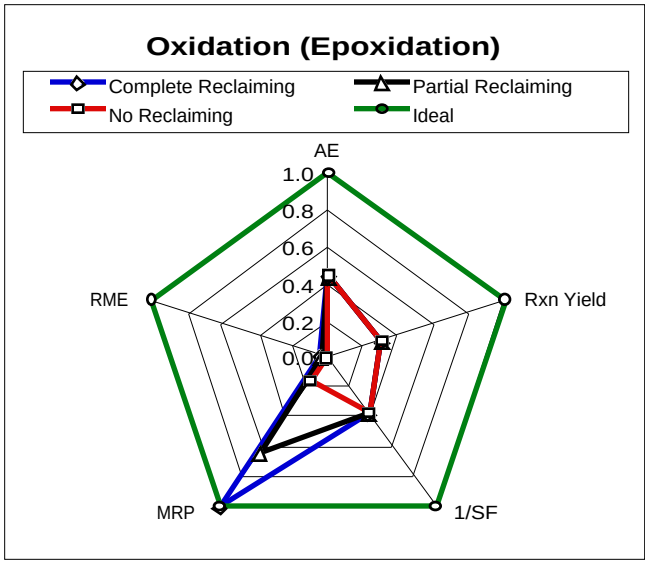
(ii) Under committing all reaction solvents, catalysts, and byproducts, and post-reaction materials to waste

Mass of waste (line 50 - 53)	51.612	g	**69**
E(m)	129.029	g waste/g product	**70**
RME	0.00769	g product/Σ g reagents	**71**
Wasted input costs ($)	6.757		

Check formula 0.00769

(iii) Under reclaiming CH2Cl2

Mass of waste	12.868	g	**76**
E(m)	32.169	g waste/g product	**77**
RME	0.030	g product/Σ g reagents	**78**
Wasted input costs ($)	6.056		

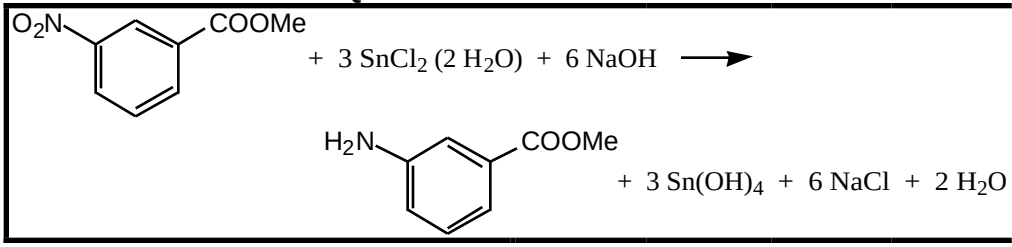


Reduction of Nitro Group

REACTION METRICS FORM

DATE: June 1, 2005
NAME OF TARGET PRODUCT: Methyl 3-aminobenzoate
REACTION CLASSIFICATION: Reduction

BALANCED CHEMICAL EQUATIONS:



PART 1: RAW MATERIALS USAGE

(A) REACTION STAGE:

(i) REAGENTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
methyl 3-nitrobenzoate	181			0.00552	1	0.397	0.397	12
SnCl2 dihydrate	676.89			0.02748	6.2	0.2398	1.487	13
6 M NaOH (aq) (24 %)	240	1.2629	15	0.09	18.9435	0.0177	0.080	14
							0.000	15
TOTAL REAGENTS	1097.89			Add lines 12 to 15	26.1435		1.964	**16**

(ii) CATALYSTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
None	0	0	0	0	0	0	0.000	19
							0.000	20
TOTAL CATALYSTS				Add lines 19 to 20	0		0.000	**21**

(iii) SOLVENTS	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
EtOH (absolute)	0.79	15	11.85	0.0306	0.363	24
ice			30	0	0.000	25
TOTAL SOLVENTS		Add lines 24 to 25	41.85		0.363	**26**

Reaction Materials Subtotals	Add lines 16, 21, 26	67.9935	2.327 **29**

(B) WORK-UP STAGE:

MATERIAL	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
Et2O	0.708	85	60.18	0.0287	1.727	33
MgSO4			5	0.0619	0.309	34
					0.000	35
					0.000	36
TOTAL WORK-UP MATERIALS		Add lines 33 to 36	65.18		2.036	**37**

(C) PURIFICATION STAGE:

MATERIAL	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
CH2Cl2	1.336	60	80.16	0.0146	1.170	41
					0.000	42
					0.000	43
					0.000	44
TOTAL PURIFICATION MATERIALS		Add lines 41 to 44	80.16		1.170	**45**

Post-reaction Materials Subtotals	Add lines 37, 45	145.34	3.206	**47**

		Mass (g)	**Cost ($)**	
TOTAL INPUT MATERIALS	Add lines 29, 47	213.3335	5.533	**50**

	MW (g/mol)	**Moles**	**Yield**	**Mass (g)**	**Cost ($/g)**

OUTPUT TARGET PRODUCT	151	0.00430	0.7791	0.65	8.513	**53**

PART 2: GREEN METRICS ANALYSIS

Limiting reagent: methyl 3-nitrobenzoate

PARAMETER	VALUE		
Reaction Scale	0.006	moles	**58**
E(mw)	6.271	MW byproducts/MW product	**59**
AE	0.138	MW product/Σ MW reagents	**60**

(i) Under reclaiming reaction solvents, catalysts, and byproducts, and all post-reaction materials

Mass of waste (line 16 - 53)	25.494	g	**63**
E(m)	39.221	g waste/g product	**64**
RME	0.025	g product/Σ g reagents	**65**
SF	4.310		**66**
Wasted input costs ($)	1.916		

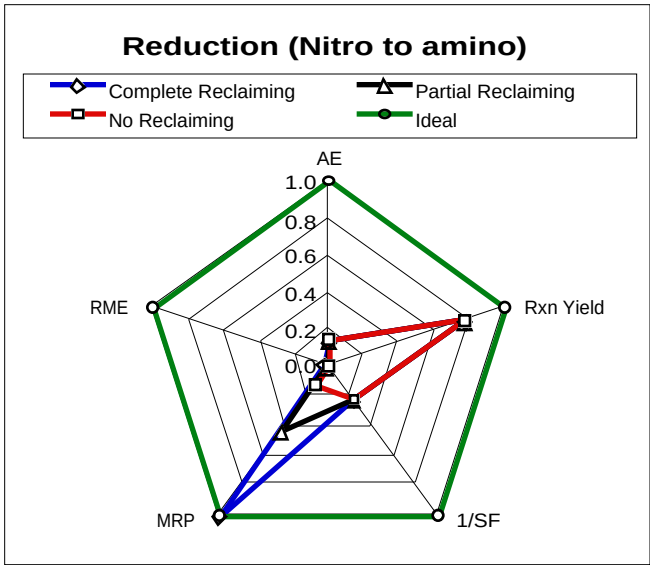
(ii) Under committing all reaction solvents, catalysts, and byproducts, and post-reaction materials to waste

Mass of waste (line 50 - 53)	212.6835	g	**69**
E(m)	327.205	g waste/g product	**70**
RME	0.00305	g product/Σ g reagents	**71**
Wasted input costs ($)	5.517		

Check formula 0.00305

(iii) Under reclaiming ethanol, ether, and dichloromethane

Mass of waste	60.494	g	**76**
E(m)	93.067	g waste/g product	**77**
RME	0.011	g product/Σ g reagents	**78**
Wasted input costs ($)	2.250		

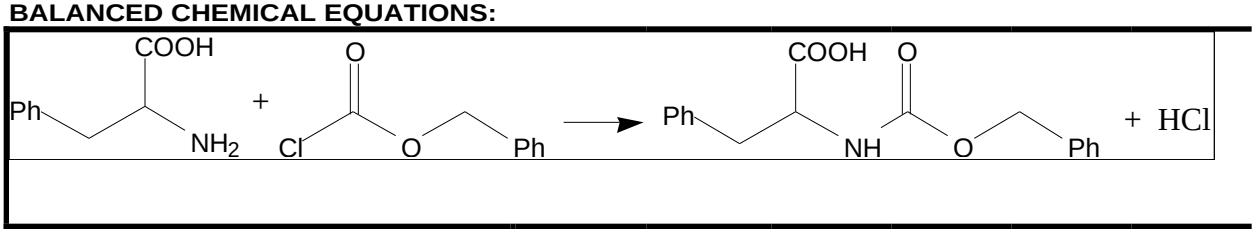


Amino Group Protection

REACTION METRICS FORM

DATE: June 1, 2005
NAME OF TARGET PRODUCT: CBz-Phenylalanine
REACTION CLASSIFICATION: Protection (Non-carbon-carbon bond forming)

BALANCED CHEMICAL EQUATIONS:



PART 1: RAW MATERIALS USAGE

(A) REACTION STAGE:

(i) REAGENTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
L-phenylalanine	165			0.01	1.65	0.555	0.916	12
benzyl chloroformate	170.45	1.195	1.40	0.00981	1.672	0.371	0.620	13
							0.000	14
							0.000	15
TOTAL REAGENTS	335.45			Add lines 12 to 15	3.32211		1.536	**16**

(ii) CATALYSTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
None	0	0	0	0	0	0	0.000	19

					0.000	20
TOTAL CATALYSTS			Add lines 19 to 20	0	0.000	**21**

(iii) SOLVENTS	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
2 M NaOH (aq) (8 %)	1.0869	6.5	7.06485	0.0014	0.010	24
					0.000	25
TOTAL SOLVENTS			Add lines 24 to 25	7.06485	0.010	**26**
Reaction Materials Subtotals			Add lines 16, 21, 26	10.3869645	1.546	**29**

(B) WORK-UP STAGE:

MATERIAL	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
2 M HCl (aq) (7.3 %)	1.03	4	4.12	0.0021	0.009	33
EtOAc	0.902	80	72.16	0.0167	1.208	34
0.1 M HCl (aq) (0.4 %)	1	10	10	0.0001	0.001	35
H2O	1	70	70	0	0.000	36a
Na2SO4			5	0.0255	0.127	36b
TOTAL WORK-UP MATERIALS			Add lines 33 to 36	156.28	1.218	**37**

(C) PURIFICATION STAGE:

MATERIAL	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
EtOAc	0.902	5	4.51	0.0167	0.076	41
hexane	0.672	5	3.36	0.0179	0.060	42
					0.000	43
					0.000	44
TOTAL PURIFICATION MATERIALS			Add lines 41 to 44	7.87	0.136	**45**
Post-reaction Materials Subtotals			Add lines 37, 45	164.15	1.354	**47**

			Mass (g)	**Cost ($)**	
TOTAL INPUT MATERIALS			Add lines 29, 47	174.5369645	2.900	**50**

	MW (g/mol)	**Moles**	**Yield**	**Mass (g)**	**Cost ($/g)**

OUTPUT TARGET PRODUCT	299	0.0067	0.6819	2	1.450	**53**

PART 2: GREEN METRICS ANALYSIS

Limiting reagent: benzyl chloroformate

PARAMETER	VALUE		
Reaction Scale	0.00981	moles	**58**
E(mw)	0.122	MW byproducts/MW product	**59**
AE	0.891	MW product/Σ MW reagents	**60**

(i) Under reclaiming reaction solvents, catalysts, and byproducts, and all post-reaction materials

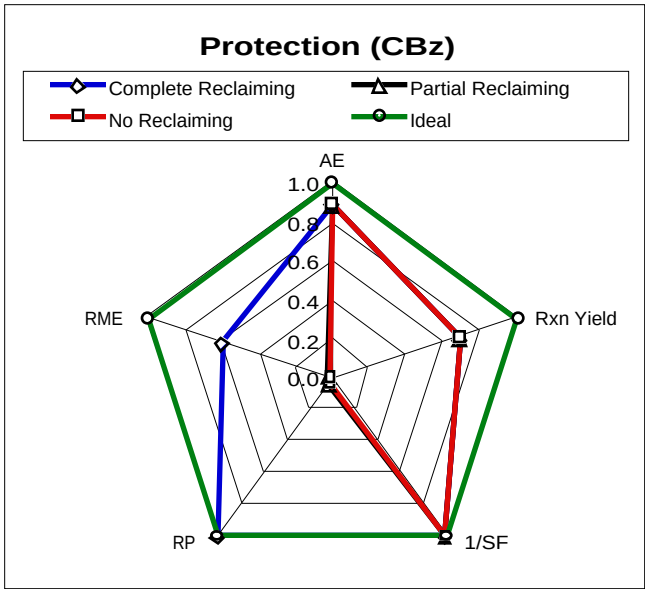
Mass of waste (line 16 - 53)	1.322	g	**63**
E(m)	0.661	g waste/g product	**64**
RME	0.602	g product/Σ g reagents	**65**
SF	1.010		**66**
Wasted input costs ($)	0.615		

(ii) Under committing all reaction solvents, catalysts, and byproducts, and post-reaction materials to waste

Mass of waste (line 50 - 53)	172.537	g	**69**
E(m)	86.268	g waste/g product	**70**
RME	0.011	g product/Σ g reagents	**71**
Wasted input costs ($)	2.866		
Check formula	0.011		

(iii) Under reclaiming ethylacetate and hexane

Mass of waste	92.507	g	**76**
E(m)	46.253	g waste/g product	**77**
RME	0.021	g product/Σ g reagents	**78**
Wasted input costs ($)	1.523		

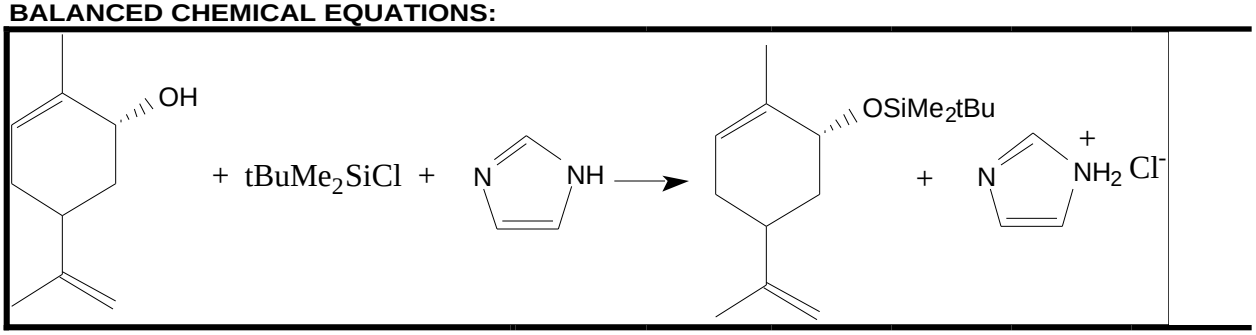


Silylation

REACTION METRICS FORM

DATE: June 1, 2005
NAME OF TARGET PRODUCT: t-Butyldimethylsilylcarveol
REACTION CLASSIFICATION: Protection (Non-carbon-carbon bond forming)

BALANCED CHEMICAL EQUATIONS:



PART 1: RAW MATERIALS USAGE

(A) REACTION STAGE:

(i) REAGENTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
(-)-carveol	152	0.958	0.063	0.00040	0.0608	1.77	0.108	12
tBuMe2SiCl	150.45			0.00111	0.167	0.5965	0.100	13
imidazole	68			0.00120	0.0816	0.1028	0.008	14
							0.000	15
TOTAL REAGENTS	370.45			Add lines 12 to 15	0.3093995		0.216	**16**

(ii) CATALYSTS	MW (g/mol)	Density (g/mL)	Volume (mL)	Moles	Mass (g)	Cost ($/g)	Cost ($)	
None	0	0	0	0	0	0	0.000	19
							0.000	20
TOTAL CATALYSTS					Add lines 19 to 20	0	0.000	**21**

(iii) SOLVENTS	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
dimethylformamide	0.944	2	1.888	0.0231	0.044	24
					0.000	25
TOTAL SOLVENTS			Add lines 24 to 25	1.888	0.044	**26**

Reaction Materials Subtotals			Add lines 16, 21, 26	2.1973995	0.259	**29**

(B) WORK-UP STAGE:

MATERIAL	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
hexane	0.672	202.5	136.08	0.0179	2.432	33
CH2Cl2	1.336	22.5	30.06	0.0146	0.439	34
1 M NaHSO4	1.1	75	82.5	0.0163	0.146	35
					0.000	36
TOTAL WORK-UP MATERIALS			Add lines 33 to 36	248.64	3.017	**37**

(C) PURIFICATION STAGE:

MATERIAL	Density (g/mL)	Volume (mL)	Mass (g)	Cost ($/g)	Cost ($)	
None	0	0	0	0	0.000	41
					0.000	42
					0.000	43
					0.000	44
TOTAL PURIFICATION MATERIALS			Add lines 41 to 44	0	0.000	**45**

Post-reaction Materials Subtotals			Add lines 37, 45	248.64	3.017	**47**

				Mass (g)	**Cost ($)**	
TOTAL INPUT MATERIALS			Add lines 29, 47	250.8374	3.276	**50**

	MW (g/mol)	**Moles**	**Yield**	**Mass (g)**	**Cost ($/g)**

OUTPUT TARGET PRODUCT	266	0.0002	0.5028	0.0535	61.239	**53**

PART 2: GREEN METRICS ANALYSIS

Limiting reagent: (-)-carveol

PARAMETER	VALUE		
Reaction Scale	0.0004	moles	**58**
E(mw)	0.393	MW byproducts/MW product	**59**
AE	0.718	MW product/Σ MW reagents	**60**

(i) Under reclaiming reaction solvents, catalysts, and byproducts, and all post-reaction materials

Mass of waste (line 16 - 53)	0.256	g	**63**
E(m)	4.783	g waste/g product	**64**
RME	0.173	g product/Σ g reagents	**65**
SF	2.088		**66**
Wasted input costs ($)	0.178		

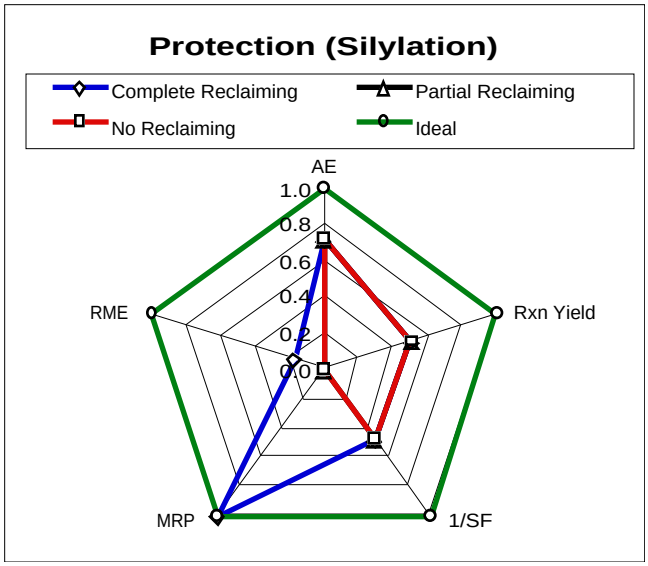
(ii) Under committing all reaction solvents, catalysts, and byproducts, and post-reaction materials to waste

Mass of waste (line 50 - 53)	250.784	g	**69**
E(m)	4687.550	g waste/g product	**70**
RME	0.000213	g product/Σ g reagents	**71**
Wasted input costs ($)	3.276		

Check formula 0.000213

(iii) Under reclaiming DMF, hexane, and CH2Cl2

Mass of waste	82.756	g	**76**
E(m)	1546.839	g waste/g product	**77**
RME	0.001	g product/Σ g reagents	**78**
Wasted input costs ($)	0.362		


Protection (Silylation)
Complete Reclaiming
Partial Reclaiming
No Reclaiming
Ideal
AE
1.0
0.8
0.6
0.4
0.2
0.0
Rxn Yield
1/SF
MRP
RME