

Supporting Information for:

Design and Evolution of the BMS Process Greenness Scorecard

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Table of Contents

Step Greenness Score – Parameter Weighting and Scoring	page	SI-2 – SI-4
Overall Greenness Score – Parameter Weighting and Scoring	page	SI-5 – SI-5
List of Hazardous Reagents	page	SI-6 – SI-16
Screenshots of Web-based Process Greenness Scorecard	page	SI-17 – SI-24
References	page	SI-25

Step Greenness Score – Parameter Weighting and Scoring

Parameter	Weight	4	3	2	1	0
Class of Solvents Used	4	$4 * (\text{mass \% Cat 4}) + 2 * (\text{mass \% Cat 3}) + 0 * (\text{mass \% Cat 2}) - 2 * (\text{mass \% Cat 1})$				
Number of Unique Solvents Used	1	1	2	3	4	>4
Solvent Recovery Percentage	1	100 to 90	89 to 75	74 to 60	59 to 30	29 to 0
Liquid Process Waste (kg/kg output)	4	$-2.1 \ln (\text{kg liquid waste /kg output}) + 9$ (score capped between 4 and -2)				
Solid Process Waste (kg/kg output)	1	<1	1 to 2	2 to 3	3 to 5	>5
Gaseous/Highly Volatile By-products/ Excess Reagent Gases	1	None, CO ₂ , N ₂	Butane, isobutylene, ethylene	Sulfur oxides, nitrogen oxides	CO, H ₂ , O ₂ , NH ₃ , HCl, HBr, HI, MeX	MeSH, H ₂ S, HN ₃ , HCN, chloramine
Number of Chemical Transformations	0.5	1 to 2	3 to 4	5 to 6	7 to 8	9+
Number of Isolations	1	1	2	3	4	>4
Step Yield	2	$(8 * \text{Yield}) - 4$ (if <50%, 0)				
Number of Hazardous Reagents Used	1	0	1	2	3	4+
Dust Explosion Potential	0.5	Calculated from 4 individual sub-scores				
Process Hazards	1	Inherently safe process ($\leq 10^\circ\text{C } T_{\text{ad}}$, no gas generation)	Moderate heat ($>10^\circ\text{C}$ to $\leq 50^\circ\text{C } T_{\text{ad}}$) OR gas generation	Moderate heat ($>10^\circ\text{C}$ to $\leq 50^\circ\text{C } T_{\text{ad}}$) AND gas generation	High heat ($>50^\circ\text{C } T_{\text{ad}}$) AND/OR high gas generation	Runaway potential
Environmental Issues/ Biopersistent Materials	1	None, Na, K, Ca, Mg	SiO ₂ , activated carbon, S, P, halogens	Li, Fe, Pd, Pt	Cu, Sn, Zn, Ce	As, Hg, Pb, Cr, Ni, Cd
Worker Exposure Issues	1	$\geq 100 \mu\text{g}/\text{m}^3$	10-100 $\mu\text{g}/\text{m}^3$	1-10 $\mu\text{g}/\text{m}^3$	0.1-1 $\mu\text{g}/\text{m}^3$	<0.1 $\mu\text{g}/\text{m}^3$

Calculation of Dust Explosion Potential Score

Sub-score Parameter	4	3	2	1	0
Charge Dissipation Time	< 1 ms	1 ms to 1 s	1 s to 1 min	1 min to 5 min	>5 min
Pressure Rise Rate (bar/sec)	0 bar/s	<50 bar/s	50 to 200 bar/s	200 to 500 bar/s	>500 bar/s
Minimum Ignition Energy (mJ)	>500 mJ	500 to 50 mJ	50 to 25 mJ	25 to 10 mJ	<10 mJ
Kst Explosion Energy value (ST)	0 (St 0)	-	<200 (St 1)	201-300 (St 2)	> 300 (St 3)
Overall Dust Explosion Potential Score	$(2/3 * \text{Max Sub-score}) + (1/2 * \text{Min Sub-score})$ (Capped at 4)				

Solvent Classification¹

Category 4 (Recommended)

Acetone
tert-Amyl methyl ether (TAME)
 Anisole
 1-Butanol
tert-Butanol
n-Butyl acetate
 Dimethyl carbonate
 Ethanol
 Ethyl acetate

Ethylene glycol
Isoamyl alcohol
Isobutanol
Isobutyl acetate
Isopropanol
Isopropyl acetate
Methanol
Methyl ethyl ketone
Methyl isobutyl ketone
Water

Category 3 (Problematic)

Acetic acid
Acetic anhydride
Acetonitrile
Benzyl alcohol
Chlorobenzene
Cyclohexane
Cyclohexanone
Cyclopentyl methyl ether (CPME)
Dimethylpropyleneurea (DMPU)
Dimethylsulfoxide (DMSO)
Formic acid
n-Heptane
Methyl acetate
Methylcyclohexane
2-Methyltetrahydrofuran (2-MeTHF)
1,3-Propanediol
Propylene carbonate
Tetrahydrofuran (THF)
Toluene
m-Xylene
o-Xylene
p-Xylene
Xylenes

Category 2 (Hazardous)

tert-Butyl methyl ether (MTBE)
Dichloromethane (DCM)
Diisopropyl ether
1,2-Dimethoxyethane (DME)
Dimethylacetamide (DMAc)
Dimethylformamide (DMF)
1,4-Dioxane
n-Hexane
n-Pentane
2-Methoxyethanol
1-Methyl-2-pyrrolidinone (NMP)

Pyridine
Sulfolane
Triethylamine

Category 1 (Highly Hazardous)

Benzene
Carbon tetrachloride
Chloroform
1,2-Dichloroethane (DCE)
Diethyl ether
Hexamethylphosphoramide (HMPA)
Nitromethane

Overall Greenness Score – Parameter Weighting and Scoring

Parameter	Score Calculation	Weight
Class of Solvents Used	% Over All Processes	16%
Number of Unique Solvents Used	(min value+ave)/2	4%
Solvent Recovery Percentage	Total % (Relative to All solvent Used)	4%
Liquid Process Waste (kg/kg output)	Total kg/kg API	16%
Solid Process Waste (kg/kg output)	Total kg/kg API	4%
Gaseous/Highly Volatile By-products/Excess Reagent Gases	(min value+ave)/2	4%
Number of Chemical Transformations	Sum of All Steps	2%
Number of Isolations	Sum of All Steps	4%
Intermediates (kg/kg API)	Calculated over all steps	4%
Number of Steps	Sum of All Steps	12%
Average Yield	Average over all steps	12%
Number of Hazardous Reagents Used	Sum of All Steps	4%
Dust Explosion Potential	Recalculated based on worst scores	2%
Charge Dissipation Time	Worst Score	
Pressure rise rate (bar/sec)	Worst Score	
Minimum Ignition Energy (millijoules)	Worst Score	
Kst Explosion Energy value (ST)	Worst Score	
Process Hazards	(min value+ave)/2	4%
Environmental Issues/Biopersistent Materials	(min value+ave)/2	4%
Worker Exposure Issues	(min value+ave)/2	4%

List of Hazardous Reagents

Acetaldehyde
Acetone cyanohydrin
Acetone thiosemicarbazide
Acetylene
Acrolein (2-Propenal)
Acrylamide
Acrylonitrile (2-Propenenitrile)
Acrylyl Chloride (2-Propenoyl chloride)
Adiponitrile
Aldicarb
Aldrin
Allyl alcohol (2-Propen-1-ol)
Allyl Chloride
Allylamine (2-Propen-1-amine)
Alkylaluminums
Aluminum phosphide
Aminopterin
Amiton
Amiton oxalate
Ammonia
Ammonia, Anhydrous
Ammonia solutions (20% or greater)
Ammonium Perchlorate
Ammonium Permanganate
Amphetamine
Aniline
Aniline, 2,4,6-trimethyl-
Antimony pentafluoride
Antimycin A
ANTU
Arsenic pentoxide
Arsenous oxide
Arsenous trichloride
Arsine (also called Arsenic Hydride)
Azinphos-ethyl
Azinphos-methyl
Benzenamine, 3-(trifluoromethyl)-
Benzene, 1-(chloromethyl)-4-nitro-
Benzenearsonic acid
Benzimidazole, 4,5-dichloro-2-(trifluoromethyl)-
Benzotrichloride
Benzyl chloride
Benzyl cyanide
beta-Propiolactone
Bicyclo(2.2.1)heptane-2-carbonitrile,5-chloro-6-(((methylamino)carbonyl)oxy)imino)-,(1-alpha,2-beta,4-alpha,5-alpha,6E))-
Bis (Chloromethyl) Ether
Bis (chloromethyl) ketone

Bitoscanate
Boron Trichloride (Borane, trichloro-)
Boron Trifluoride (Borane, trifluoro-)
Boron trifluoride compound with methyl ether (1:1)
Bromadiolone
Bromine
Bromine Chloride
Bromine Pentafluoride
Bromine Trifluoride
3-Bromopropyne (also called Propargyl Bromide)
Bromotrifluorethylene
1,3-Butadiene
Butane
1-Butene
2-Butene
Butene
2-Butene-cis
2-Butene-trans
Butyl Hydroperoxide (Tertiary)
Butyl Perbenzoate (Tertiary)
Cadmium stearate
Cadmium oxide
Calcium arsenate
Camphechlor
Cantharidin
Carbachol chloride
Carbamic acid, methyl-, O-((2,4-dimethyl-1,3-dithiolan-2-yl)methylene)amino)-
Carbofuran
Carbonyl Chloride (see Phosgene)
Carbon disulfide
Carbon oxysulfide
Carbophenothion
Carbonyl Fluoride
Cellulose Nitrate
Chlordane
Chlorfenvinfos
Chlorine
Chlorine Dioxide (Chlorine oxide (ClO₂))
Chlorine monoxide
Chlorine Pentafluoride
Chlorine Trifluoride
Chlormephos
Chlormequat chloride
Chloroacetic acid
Chloroethanol
Chlorodiethylaluminum (also called Diethylaluminum Chloride)
Chloroethyl chloroformate
1-Chloro-2,4-Dinitrobenzene
Chloroform (Methane, trichloro-)
Chloromethyl Methyl Ether (Methane, chloromethoxy-)

Chloromethyl ether
Chlorophacinone
Chloropicrin
Chloropicrin and Methyl Bromide mixture
Chloropicrin and Methyl Chloride mixture
2-Chloropropylene
2-Chloropropylene
Chloroxuron
Chlorthiophos
Chromic chloride
Cobalt carbonyl
Cobalt, ((2,2'-(1,2-ethanediylbis(nitrilomethylidyne))bis(6-fluorophenylato))(2)-N,N',O,O')-
Colchicine
Commune Hydroperoxide
Coumaphos
Coumatetralyl
Crimidine
Crotonaldehyde (2-Butenal, (E)-)
Crontonaldehyde, (E)- (2-Butenal, (E)-)
Cyanogen
Cyanogen bromide
Cyanogen Chloride
Cyanogen iodide
Cyanophos
Cyanuric Fluoride
Cycloheximide
Cyclohexylamine (Cyclohexanamine)
Cyclopropane
Decaborane(14)
Demeton
Demeton-S-methyl
Diacetyl Peroxide
Dialifor
Diazomethane
Dibenzoyl Peroxide
Diborane
Dibutyl Peroxide (Tertiary)
Dichloro Acetylene
Dichloroethyl ether
Dichloromethylphenylsilane
Dichlorosilane
Dichlorvos
Dicrotophos
Diepoxybutane
Diethyl chlorophosphate
Diethylzinc
Difluoroethane
Digitoxin
Diglycidyl ether
Digoxin

Diisopropyl Peroxydicarbonate
 Dilauroyl Peroxide
 Dimefox
 Dimethoate
 Dimethylamine, Anhydrous
 Dimethyldichlorosilane (Silane, dichlorodimethyl-)
 Dimethylhydrazine, 1,1- (Hydrazine, 1,1-dimethyl-)
 Dimethylamine, Anhydrous
 Dimethyl phosphorochloridothioate
 Dimethyl-p-phenylenediamine
 Dimethyldichlorosilane
 Dimethylhydrazine
 Dimetilan
 2,2-Dimethylpropane
 Dimethyl sulfate
 2,4-Dinitroaniline
 Dinitrocresol
 Dinoseb
 Dinoterb
 Dioxathion
 Diphacinone
 Diphosphoramidate, octamethyl-
 Disulfoton
 Dithiazanine iodide
 Dithiobiuret
 Emetine, dihydrochloride
 Endosulfan
 Endothion
 Endrin
 Epichlorohydrin (Oxirane, (chloromethyl)-)
 EPN
 Ergocalciferol
 Ergotamine tartrate
 Ethane
 Ethanesulfonyl chloride, 2-chloro-
 Ethanol, 1,2-dichloro-, acetate
 Ethion
 Ethoprophos
 Ethyl acetylene
 Ethylamine
 Ethylbis(2-chloroethyl)amine
 Ethyl chloride
 Ethyl ether
 Ethyl mercaptan
 Ethyl Methyl Ketone Peroxide (also Methyl Ethyl Ketone Peroxide; concentration greater than 60%)
 Ethyl Nitrite
 Ethylamine
 Ethylene
 Ethylene Fluorohydrin

Ethylene Oxide (Oxirane)
Ethylenediamine (1,2-Ethanediamine)
Ethyleneimine (Aziridine)
Ethylthiocyanate
Fenamiphos
Fensulfothion
Fluometil
Fluorine
Fluoroacetamide
Fluoroacetic acid
Fluoroacetyl chloride
Fluorouracil
Fonofos
Formaldehyde cyanohydrin
Formaldehyde (Formalin)
Formetanate hydrochloride
Formothion
Formparanate
Fosthietan
Fuberidazole
Furan
Gallium trichloride
Hexachlorocyclopentadiene
Hexafluoroacetone
Hexamethylenediamine,N,N'-dibutyl-
Hydrazine
Hydrochloric Acid, Anhydrous
Hydrochloric Acid Solutions (37% or greater)
Hydrocyanic acid
Hydrofluoric Acid, Anhydrous
Hydrofluoric Acid Solutions (50% or greater)
Hydrogen
Hydrogen Bromide
Hydrogen Chloride
Hydrogen Cyanide, Anhydrous
Hydrogen Fluoride/Hydrofluoric acid
Hydrogen Peroxide (52% by weight or greater)
Hydrogen Selenide
Hydrogen Sulfide
Hydroquinone
Hydroxylamine
Iron, Pentacarbonyl
Isobenzan
Isobutane
Isobutyronitrile
Isocyanic acid, 3,4-dichlorophenyl ester
Isodrin
Isofluorphate
Isopentane
Isophorone diisocyanate

Isoprene
Isopropylamine
Isopropyl chloride
Isopropyl chloroformate
Isopropylmethylpyrazolyl dimethylcarbamate
Ketene
Lactonitrile
Leptophos
Lewisite
Lindane
Lithium hydride
Malononitrile
Manganese, tricarbonyl methylcyclopentadienyl
Mechlorethamine
Mephosfolan
Mercuric acetate
Mercuric oxide
Mercuric chloride
Methacrylaldehyde
Methane
Methacrolein diacetate
Methacrylic anhydride
Methacrylonitrile
Methacryloyl Chloride
Methacryloyloxyethyl Isocyanate
Methamidophos
Methanesulfonyl fluoride
Methidathion
Methiocarb
Methomyl
Methoxyethylmercuric acetate
Methyl Acrylonitrile
Methylamine, Anhydrous
3-Methyl-1-butene
2-Methyl-1-butene
Methyl Bromide
Methyl Chloride
Methyl Chloroformate
Methyl ether
Methyl Ethyl Ketone Peroxide
Methyl ether
Methyl Fluoroacetate
Methyl Fluorosulfate
Methyl formate
Methyl Hydrazine
Methyl Iodide
Methyl Isocyanate
Methyl isothiocyanate
Methyl Mercaptan
Methyl phenkapton

Methyl phosphonic dichloride
Methyl thiocyanate
Methyl Vinyl Ketone
Methyl 2-chloroacrylate
2-Methylpropene
Methyltrichlorosilane
Methylmercuric dicyanamide
Metolcarb
Mevinphos
Mexacarbate
Mitomycin C
Monocrotophos
Muscimol
Mustard gas
Nickel Carbonyl (Nickel Tetracarbonyl)
Nicotine sulfate
Nicotine
Nitric Acid (80% or greater)
Nitric Oxide
Nitroaniline (para Nitroaniline)
Nitrobenzene
Nitrocyclohexane
Nitromethane
Nitrogen Dioxide
Nitrogen Oxides (NO; NO (2); N2O4; N2O3)
Nitrosodimethylamine
Nitrogen Tetroxide (also called Nitrogen Peroxide)
Nitrogen Trifluoride
Nitrogen Trioxide
Norbormide
o-Cresol
Oleum (65% to 80% by weight; also called Fuming Sulfuric Acid)
Organorhodium Complex (PMN-82-147)
Osmium Tetroxide
Ouabain
Oxamyl
Oxetane, 3,3-bis(chloromethyl)-
Oxydisulfoton
Oxygen Difluoride (Fluorine Monoxide)
Ozone
Paraquat methosulfate
Paraquat dichloride
Parathion
Parathion-methyl
Paris green
Pentaborane
Pentadecylamine
1,3-Pentadiene
Pentane
1-Pentene

2-Pentene, (E)-
 2-Pentene, (Z)-
 Peracetic Acid (concentration greater 60%) (also called Peroxyacetic Acid)
 Perchloric Acid (concentration greater than 60% by weight)
 Perchloromethyl Mercaptan
 Perchloryl Fluoride
 Peroxyacetic Acid (concentration greater than 60% Acetic Acid; also called Peracetic Acid)
 Phenol
 Phenol, 3-(1-methylethyl)-,methylcarbamate
 Phenol, 2,2'-thiobis[4-chloro-6-methyl-
 Phenoxarsine, 10,10'-oxydi-
 Phenyl dichloroarsine
 Phenylhydrazine hydrochloride
 Phenylmercury acetate
 Phenylsilatrane
 Phenylthiourea
 Phorate
 Phosacetim
 Phosfolan
 Phosgene (also called Carbonyl Chloride)
 Phosmet
 Phosphamidon
 Phosphine (Hydrogen Phosphide)
 Phosphonothioic acid, methyl-, O-ethyl O-(4-(methylthio)phenyl) ester
 Phosphonothioic acid, methyl-, S-(2-(bis(1-methylethyl)amino)ethyl) O-ethyl ester
 Phosphonothioic acid,methyl-, O-(4-nitrophenyl) O-phenyl ester
 Phosphoric acid, dimethyl 4-(methylthio) phenyl ester
 Phosphorothioic acid, O,O-dimethyl-5-(2-(methylthio)ethyl)ester
 Phosphorus Oxychloride (also called Phosphoryl Chloride)
 Phosphorus pentachloride
 Phosphorus Trichloride
 Phosphorus
 Phosphoryl Chloride (also called Phosphorus Oxychloride)
 Physostigmine
 Physostigmine, salicylate (1:1)
 Picrotoxin
 Piperidine
 Pirimifos-ethyl
 Potassium cyanide
 Potassium arsenite
 Potassium silver cyanide
 Promecarb
 Propadiene
 Propane
 Propargyl Bromide
 Propionitrile
 Propionitrile, 3-chloro-
 Propiophenone, 4'-amino
 Propyl chloroformate
 Propyleneimine

Propylene
Propylene oxide
Propyl chloroformate
Propyl Nitrate
Propyne
Prothoate
Pyrene
Pyridine, 4-amino-
Pyridine, 2-methyl-5-vinyl-
Pyridine, 4-nitro-, 1-oxide
Pyriminil
Salcomine
Sarin
Selenious acid
Selenium Hexafluoride
Selenium oxychloride
Semicarbazide hydrochloride
Silane
Silane, Dimethyldichloro
Silane, Trimethylchloro
Silane, Trichloro
Silane, Tetramethyl
Silane, (4-aminobutyl)diethoxymethyl-
Sodium selenate
Sodium arsenite
Sodium fluorocetate
Sodium cacodylate
Sodium cyanide (Na(CN))
Sodium arsenate
Sodium selenite
Sodium azide (Na(N₃))
Sodium tellurite
Stannane, acetoxytriphenyl-
Stibine (Antimony Hydride)
Strychnine
Strychnine, sulfate
Sulfotep
Sulfoxide, 3-chloropropyl octyl
Sulfur Dioxide (liquid)
Sulfur Pentafluoride
Sulfur Tetrafluoride
Sulfur Trioxide (also called Sulfuric Anhydride)
Sulfuric acid
Sulfuric Anhydride (also called Sulfur Trioxide)
Tabun
Tellurium Hexafluoride
Tepp
Terbufos
Tetraethyl lead
Tetraethyltin

Tetramethyllead
Tetrafluoroethylene
Tetrafluorohydrazine
Tetramethyl Lead
Tetramethylsilane
Tetranitromethane
Thallium sulfate
Thallous malonate
Thallous carbonate
Thallous chloride
Thallous sulfate
Thiocarbazide
Thiofanox
Thionazin
Thionyl Chloride
Thiophenol
Thiosemicarbazide
Thiourea, (2-chlorophenyl)-
Thiourea, (2-methylphenyl)-
Titanium tetrachloride
Toluene 2,4-diisocyanate
Toluene 2,6-diisocyanate
Toluene diisocyanate
Trans-1,4-Dichlorobutene
Triamiphos
Triazofos
Trichloro (chloromethyl) Silane
Trichloro (dichlorophenyl) Silane
Trichloroacetyl chloride
Trichloroethylsilane
Trichloronate
Trichlorophenylsilane
Trichlorosilane
Triethoxysilane
Trifluorochloroethylene
Trimethylamine
Trimethylchlorosilane
Trimethylolpropane phosphite
Trimethyltin chloride
Trimethoxysilane
Triphenyltin chloride
Tris(2-chloroethyl)amine
Valinomycin
Vanadium pentoxide
Vinyl acetate monomer
Vinyl acetylene
Vinyl chloride
Vinyl ethyl ether
Vinyl fluoride
Vinylidene chloride

Vinylidene fluoride

Vinyl methyl ether

Warfarin sodium

Warfarin sodium

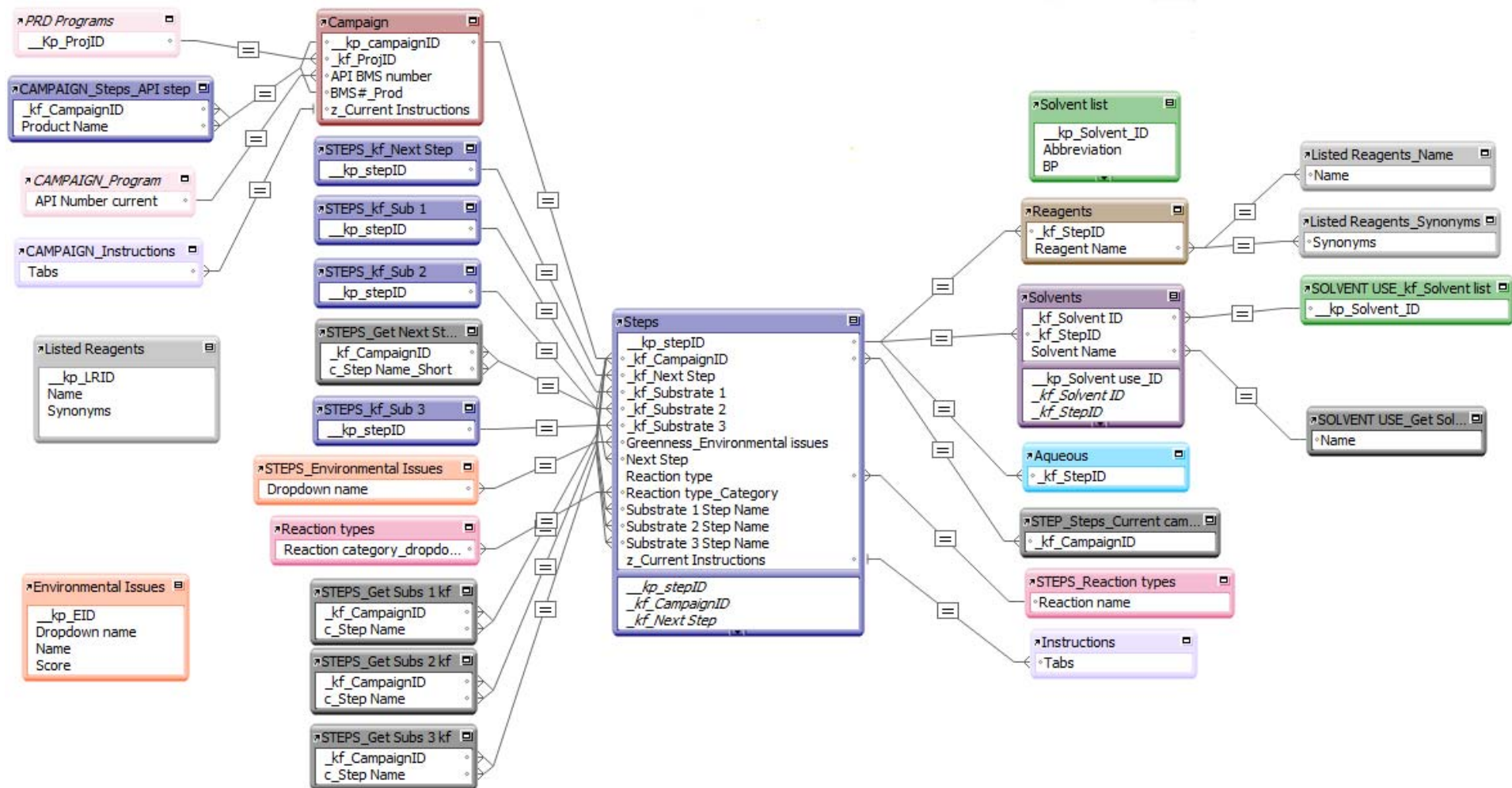
Xylylene dichloride

Zinc phosphide

Zinc, dichloro(4,4-dimethyl-5((((methylamino)carbonyl)oxy)imino)pentanenitrile)-(T-4)-

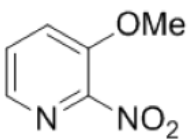
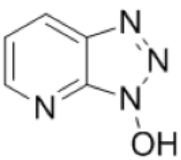
Screenshots of Web-based Process Greenness Scorecard

Database Relationship Diagram



Step Overview

Step Number	2	Reaction Type	Other Ring Formation		
Location		Step Type	Main step	Step List	Campaign Details
Product	HOAt	Recalculate Step	Next Step	Campaign Steps	
Substrate 1					
Substrate 2					
Substrate 3					
Step Yield	45.5%	Step PMI	40.4	Step Greenness	51% % Complete 55%
Overall	45.5%	Cumulative	40	Cumulative	86 % Complete 55%

Reaction	Charges	Product	Greenness	Results	Metrics	Cost	Notes
Category	Ring Formation		Type	Other Ring Formation			
 Molecular Weight: 154.13 ~\$100/mol $\xrightarrow[\text{46\%}]{\text{N}_2\text{H}_4}$  Molecular Weight: 136.11							

Reaction	Charges	Product	Greenness	Results	Metrics	Cost	Notes
Substrates	Reagents	Solvents	Aqueous				
Name	MW	assay	equiv	kg	mol		
2-nitro-3-methoxypyridine	154.13		(1.0)	13.58	88.1		

Reaction	Charges	Product	Greenness	Results	Metrics	Cost	Notes
Substrates Reagents Solvents Aqueous							
Name	CAS	MW	equiv	kg			
95% hydrazine				26.40			

Charges Input – Solvents

Reaction	Charges	Product	Greenness	Results	Metrics	Cost	Notes
Substrates		Reagents		Solvents		Aqueous	
Name	Category	Recovery	vol	kg/kg	L	kg	
Water	4				10.4	10.4	▲
Dimethylformamide	1				15.3	14.4	
Water	4				50.0	50.0	
Water	4		1.0	1.0	13.6	13.6	
Water	4				75.0	75.0	
							▼

Charges Input – Aqueous

Reaction	Charges	Product	Greenness	Results	Metrics	Cost	Notes
Substrates		Reagents		Solvents		Aqueous	
Name	dens	vol	kg/kg	L	kg		
conc HCl	1.000			17.0	17.0	▲	
							▼

Product Input

Reaction	Charges	Product	Greenness	Results	Metrics	Cost	Notes
Product Name HOAt							
Product MW 136.11 g/mol							
Theoretical Output 11.992 kg							
Actual Output 5.46 kg							
Step Yield 45.5%							
40.11 mol							
Assay (optional) wt% AP							

Molecular Weight: 136.11

Greenness Input – Waste

Reaction	Charges	Product	Greenness	Results	Metrics	Cost	Notes
Waste Hazardous reagents Safety							
Solid Waste		0.15	kg/kg input	0.17	kg/kg output		
Liquid Waste		41.5	kg/kg input	47.8	kg/kg output		
Solvent Recovery Percentage		0.0%					
Number of Solvents		3					
Gaseous By-products		4 - Carbon Dioxide					
# Chemical Transformations		2					
# Isolations		1					

Greenness Input – Hazardous Reagents

Reaction	Charges	Product	Greenness	Results	Metrics	Cost	Notes
Waste Hazardous reagents Safety							
<i>-A hazardous (listed) reagent is any reagent included in the drop-down list below.</i> <i>-This is NOT the same as the DEA List 1 Reagent classification, which is a significantly smaller list.</i>							
Are any hazardous (listed) reagents used in this process?				Yes			
If yes, select hazardous (listed) reagents:							
Listed reagent 1		Hydrochloric Acid Solutions (37% or greater)					
Listed reagent 2							
Listed reagent 3							
Listed reagent 4							

Reaction	Charges	Product	Greenness	Results	Metrics	Cost	Notes																											
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Results – Step Greenness

Reaction	Charges	Product	Greenness	Results	Metrics	Cost	Notes
Step Greenness		Cumulative Greenness		PMI	Cumulative Metrics		
Solvent Recovery		0.0		Chemical Transformations		4.0	
Solid Process Waste		4.0		Isolations		4.0	
Liquid Process Waste		0.9		Class of Solvents		1.1	
Hazardous Reagents		3.0		Number of Solvents		2.0	
Process Hazards		4.0					
Environmental Issues		3.0					
Worker Exposure Issues		3.0		Step Yield		3.6	
Gaseous By-products		4.0		Step Greenness Score		57%	
Dust Explosion Potential		3.7		Percent Complete		100%	

Results – Cumulative Greenness

Reaction	Charges	Product	Greenness	Results	Metrics	Cost	Notes
Step Greenness		Cumulative Greenness		PMI	Cumulative Metrics		
Solvent Recovery		0.0		Chemical Transformations		3.7	
Solid Process Waste		4.0		Isolations		4.0	
Liquid Process Waste		1.5		Class of Solvents		0.4	
Hazardous Reagents		1.0		Number of Solvents		1.3	
Process Hazards		4.0		Steps		3.7	
Environmental Issues		3.3		Intermediates		4.0	
Worker Exposure Issues		3.0		Average Yield		3.3	
Gaseous By-products		2.0		Overall Greenness Score		59	
Dust Explosion Potential		3.7		Percent Complete		93%	

References

- (1) Prat, D.; Wells, A.; Hayler, J.; Sneddon, H.; McElroy, C. R.; Abou-Shehada, S.; Dunn, P. *J. Green Chemistry* **2016**, *18*, 288.