Supporting Information for:

Design and Evolution of the BMS Process Greenness Scorecard

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### Step Greenness Score – Parameter Weighting and Scoring

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Weight</th>
<th>4</th>
<th>3</th>
<th>2</th>
<th>1</th>
<th>0</th>
</tr>
</thead>
<tbody>
<tr>
<td>Class of Solvents Used</td>
<td>4</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Number of Unique Solvents Used</td>
<td>1</td>
<td>1</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Solvent Recovery Percentage</td>
<td>1</td>
<td>100 to 90</td>
<td>89 to 75</td>
<td>74 to 60</td>
<td>59 to 30</td>
<td>&gt;4</td>
</tr>
<tr>
<td>Liquid Process Waste (kg/kg output)</td>
<td>4</td>
<td>-2.1 ln (kg liquid waste /kg output) + 9 (score capped between 4 and -2)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Solid Process Waste (kg/kg output)</td>
<td>1</td>
<td>&lt;1</td>
<td>1 to 2</td>
<td>2 to 3</td>
<td>3 to 5</td>
<td>&gt;5</td>
</tr>
<tr>
<td>Gaseous/Highly Volatile By-products/Excess Reagent Gases</td>
<td>1</td>
<td>None, CO₂, N₂</td>
<td>Butane, isobutylene, ethylene</td>
<td>Sulfur oxides, nitrogen oxides</td>
<td>CO₂, H₂, O₂, NH₃, HCl, HBr, HI, MeX</td>
<td>MeSH, H₂S, HCN, chloramine</td>
</tr>
<tr>
<td>Number of Chemical Transformations</td>
<td>0.5</td>
<td>1 to 2</td>
<td>3 to 4</td>
<td>5 to 6</td>
<td>7 to 8</td>
<td>9+</td>
</tr>
<tr>
<td>Number of Isolations</td>
<td>1</td>
<td>1</td>
<td>2</td>
<td>3</td>
<td>4</td>
<td>&gt;4</td>
</tr>
<tr>
<td>Step Yield</td>
<td>2</td>
<td>(8*Yield)-4 (if &lt;50%, 0)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Number of Hazardious Reagents Used</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>2</td>
<td>3</td>
<td>4+</td>
</tr>
<tr>
<td>Dust Explosion Potential</td>
<td>0.5</td>
<td>Calculated from 4 individual sub-scores</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Process Hazards</td>
<td>1</td>
<td>Inherently safe process (≤10 °C T_ad no gas generation)</td>
<td>Moderate heat (&gt;10 °C to ≤50 °C T_ad OR gas generation)</td>
<td>Moderate heat (&gt;10 °C to ≤50 °C T_ad AND gas generation)</td>
<td>High heat (&gt;50 °C T_ad) AND/OR high gas generation</td>
<td>Runaway potential</td>
</tr>
<tr>
<td>Environmental issues/ Biopersistent Materials</td>
<td>1</td>
<td>None, Na, K, Ca, Mg</td>
<td>SiO₂, activated carbon, S, P, halogens</td>
<td>Li, Fe, Pd, Pt</td>
<td>Cu, Sn, Zn, Ce</td>
<td>As, Hg, Pb, Cr, Ni, Cd</td>
</tr>
<tr>
<td>Worker Exposure Issues</td>
<td>1</td>
<td>≥ 100 µg/m³</td>
<td>10-100 µg/m³</td>
<td>1.1 µg/m³</td>
<td>0.1-1 µg/m³</td>
<td>&lt;0.1 µg/m³</td>
</tr>
</tbody>
</table>

### Calculation of Dust Explosion Potential Score

<table>
<thead>
<tr>
<th>Sub-score Parameter</th>
<th>4</th>
<th>3</th>
<th>2</th>
<th>1</th>
<th>0</th>
</tr>
</thead>
<tbody>
<tr>
<td>Charge Dissipation Time</td>
<td>&lt; 1 ms</td>
<td>1 ms to 1 s</td>
<td>1 s to 1 min</td>
<td>1 min to 5 min</td>
<td>&gt;5 min</td>
</tr>
<tr>
<td>Pressure Rise Rate (bar/sec)</td>
<td>0 bar/s</td>
<td>&lt;50 bar/s</td>
<td>50 to 200 bar/s</td>
<td>200 to 500 bar/s</td>
<td>&gt;500 bar/s</td>
</tr>
<tr>
<td>Minimum Ignition Energy (mJ)</td>
<td>&gt;500 mJ</td>
<td>500 to 50 mJ</td>
<td>50 to 25 mJ</td>
<td>25 to 10 mJ</td>
<td>&lt;10 mJ</td>
</tr>
<tr>
<td>Kst Explosion Energy value (ST)</td>
<td>0 (St 0)</td>
<td>-</td>
<td>&lt;200 (St 1)</td>
<td>201-300 (St 2)</td>
<td>&gt; 300 (St 3)</td>
</tr>
<tr>
<td>Overall Dust Explosion Potential Score</td>
<td>(2/3 * Max Sub-score) + (1/2 * Min Sub-score) (Capped at 4)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Solvent Classification

**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

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

Acetaldehyde
Acetone cyanohydrin
Acetone thiosemicarbazide
Acetylene
Acrolein (2-Propanal)
Acrylamide
Acrylonitrile (2-Propanenitrile)
Acryl Chloride (2-Propanoyl chloride)
Adiponitrile
Aldicarb
Aldrin
Allyl alcohol (2-Propan-1-ol)
Allyl Chloride
Allylamine (2-Propan-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
ANTSU
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
Benzy1 chloride
Benzy1 cyanide
Benzy1 cyanide
beta-Propiolactone
Bicyclo(2.2.1)heptane-2-carbonitrile, 5-chloro-6-(((methylamino)carbonyl)oxy)imino)-(1-
alpa,2-bet4,4-alpaha,5-alpaha,6E))-
Bis (Chloromethyl) Ether
Bis (chloromethyl) ketone

SI-6
<table>
<thead>
<tr>
<th>Compound</th>
</tr>
</thead>
<tbody>
<tr>
<td>Biscanate</td>
</tr>
<tr>
<td>Boron Trichloride (Borane, trichloro-)</td>
</tr>
<tr>
<td>Boron Trifluoride (Borane, trifluoro-)</td>
</tr>
<tr>
<td>Boron trifluoride compound with methyl ether (1:1)</td>
</tr>
<tr>
<td>Bromadiolone</td>
</tr>
<tr>
<td>Bromine</td>
</tr>
<tr>
<td>Bromine Chloride</td>
</tr>
<tr>
<td>Bromine Pentrafluoride</td>
</tr>
<tr>
<td>Bromine Trifluoride</td>
</tr>
<tr>
<td>3-Bromopropyne (also called Propargyl Bromide)</td>
</tr>
<tr>
<td>Bromotrifluorethylene</td>
</tr>
<tr>
<td>1,3-Butadiene</td>
</tr>
<tr>
<td>Butane</td>
</tr>
<tr>
<td>1-Butene</td>
</tr>
<tr>
<td>2-Butene</td>
</tr>
<tr>
<td>Butene</td>
</tr>
<tr>
<td>2-Butene-cis</td>
</tr>
<tr>
<td>2-Butene-trans</td>
</tr>
<tr>
<td>Butyl Hydroperoxide (Tertiary)</td>
</tr>
<tr>
<td>Butyl Perbenzoate (Tertiary)</td>
</tr>
<tr>
<td>Cadmium stearate</td>
</tr>
<tr>
<td>Cadmium oxide</td>
</tr>
<tr>
<td>Calcium arsenate</td>
</tr>
<tr>
<td>Camphenechlor</td>
</tr>
<tr>
<td>Cantharidin</td>
</tr>
<tr>
<td>Carbachol chloride</td>
</tr>
<tr>
<td>Carbamic acid, methyl-, O-((2,4-dimethyl-1,3-dithiolan-2-yl)methylene)amino)-Carbofuran</td>
</tr>
<tr>
<td>Carbonyl Chloride (see Phosgene)</td>
</tr>
<tr>
<td>Carbon disulfide</td>
</tr>
<tr>
<td>Carbon oxysulfide</td>
</tr>
<tr>
<td>Carbophenothion</td>
</tr>
<tr>
<td>Carbonyl Fluoride</td>
</tr>
<tr>
<td>Cellulose Nitrate</td>
</tr>
<tr>
<td>Chlordane</td>
</tr>
<tr>
<td>Chlorfenvinfos</td>
</tr>
<tr>
<td>Chlorine</td>
</tr>
<tr>
<td>Chlorine Dioxide (Chlorine oxide (ClO2))</td>
</tr>
<tr>
<td>Chlorine monoxide</td>
</tr>
<tr>
<td>Chlorine Pentrafluoride</td>
</tr>
<tr>
<td>Chlorine Trifluoride</td>
</tr>
<tr>
<td>Chlormephos</td>
</tr>
<tr>
<td>Chlormequat chloride</td>
</tr>
<tr>
<td>Chloroacetic acid</td>
</tr>
<tr>
<td>Chloroethanol</td>
</tr>
<tr>
<td>Chlorodiethylaluminum (also called Diethylaluminum Chloride)</td>
</tr>
<tr>
<td>Chloroethyl chloroformate</td>
</tr>
<tr>
<td>1-Chloro-2,4-Dinitrobenzene</td>
</tr>
<tr>
<td>Chloroform (Methane, trichloro-)</td>
</tr>
<tr>
<td>Chloromethyl Methyl Ether (Methane, chloromethoxy-)</td>
</tr>
</tbody>
</table>
Chloromethyl ether
Chlorophacinone
Chloropicrin
Chloropicrin and Methyl Bromide mixture
Chloropicrin and Methyl Chloride mixture
2-Chloropropylene
2-Chloropropyline
Chloroxuron
Chlordithiophos
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
Dicophos
Diethyl chlorophosphate
Diethylzinc
Difluoroethane
Digitoxicin
Diglycidyl ether
Digoxin
Diisopropyl Peroxydicarbonate
Dilauroyl Peroxide
Dimefox
Dimethoate
Dimethylamine, Anhydrous
Dimethylidichlorosilane (Silane, dichlorodimethyl-)
Dimethylhydrazine, 1,1- (Hydrazine, 1,1-dimethyl-)
Dimethylamine, Anhydrous
Dimethyl phosphorochloridothioate
Dimethyl-p-phenylenediamine
Dimethylidichlorosilane
Dimethylhydrazine
Dimetilan
2,2-Dimethylpropane
Dimethyl sulfate
2,4-Dinitroaniline
Dinitroresol
dinoseb
dinoterb
dioxathion
diphascinone
diphasoramide, oxtamethyl-
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
Fluenetil
Fluorine
Fluroacetamide
Fluroacetic acid
Flyoroacetyl 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
Isobutynitrile
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
Methyacrylonitrile
Methacryloyl Chloride
Methacryloyloxyethyl Isocyanate
Methamidophos
Methanesulfonyl fluoride
Methidathion
Methiocarb
Methomyl
Methoxyethylmercuric acetate
Methyl Acrylonitrile
Methyamine, 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
Norbornide
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
Phenylsilatrace
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
Propadiene
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, Dimethyl dichloro
Silane, Trimethyl chloro
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
Sulfitopen
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
Thiocarbamide
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
Triethoxyethane
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

**Product:** HOAt

**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**

**Category:** Ring Formation  
**Type:** Other Ring Formation

![Chemical Reaction](image)

- **N2H4**  
  - 46%  
  - Molecular Weight: 136.11

**Molecular Weight:** 154.13  
**Cost:** ~$100/mol
Charges Input – Substrates

Charges Input – Reagents
**Charges Input – Solvents**

<table>
<thead>
<tr>
<th>Name</th>
<th>Category</th>
<th>Recovery</th>
<th>vol</th>
<th>kg/kg</th>
<th>L</th>
<th>kg</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water</td>
<td>4</td>
<td></td>
<td></td>
<td>10.4</td>
<td></td>
<td>10.4</td>
</tr>
<tr>
<td>Dimethylformamide</td>
<td>1</td>
<td></td>
<td></td>
<td>15.3</td>
<td></td>
<td>14.4</td>
</tr>
<tr>
<td>Water</td>
<td>4</td>
<td></td>
<td></td>
<td></td>
<td>50.0</td>
<td>50.0</td>
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<tr>
<td>Water</td>
<td>4</td>
<td>1.0</td>
<td>1.0</td>
<td>13.6</td>
<td></td>
<td>13.6</td>
</tr>
<tr>
<td>Water</td>
<td>4</td>
<td></td>
<td></td>
<td></td>
<td>75.0</td>
<td>75.0</td>
</tr>
</tbody>
</table>

**Charges Input – Aqueous**

<table>
<thead>
<tr>
<th>Name</th>
<th>dens</th>
<th>vol</th>
<th>kg/kg</th>
<th>L</th>
<th>kg</th>
</tr>
</thead>
<tbody>
<tr>
<td>conc HCl</td>
<td>1.000</td>
<td></td>
<td></td>
<td>17.0</td>
<td>17.0</td>
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</tbody>
</table>

S120
**Product Input**

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Charges</th>
<th><strong>Product</strong></th>
<th>Greenness</th>
<th>Results</th>
<th>Metrics</th>
<th>Cost</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Product Name</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>HOAt</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Product MW</td>
<td>136.11 g/mol</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Theoretical Output</td>
<td>11.992 kg</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Actual Output</td>
<td>5.46 kg</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Step Yield</td>
<td>45.5%</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>40.11 mol</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Assay (optional)</td>
<td>wt%</td>
<td></td>
<td></td>
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<td></td>
</tr>
</tbody>
</table>

Molecular Weight: 136.11
**Greenness Input – Waste**

<table>
<thead>
<tr>
<th>Waste</th>
<th>Hazardous reagents</th>
<th>Safety</th>
</tr>
</thead>
<tbody>
<tr>
<td>Solid Waste</td>
<td>0.15 kg/kg input</td>
<td>0.17 kg/kg output</td>
</tr>
<tr>
<td>Liquid Waste</td>
<td>41.5 kg/kg input</td>
<td>47.8 kg/kg output</td>
</tr>
<tr>
<td>Solvent Recovery Percentage</td>
<td>0.0%</td>
<td></td>
</tr>
<tr>
<td>Number of Solvents</td>
<td>3</td>
<td></td>
</tr>
<tr>
<td>Gaseous By-products</td>
<td>4 - Carbon Dioxide</td>
<td></td>
</tr>
<tr>
<td># Chemical Transformations</td>
<td>2</td>
<td></td>
</tr>
<tr>
<td># Isolations</td>
<td>1</td>
<td></td>
</tr>
</tbody>
</table>

**Greenness Input – Hazardous Reagents**

-A hazardous (listed) reagent is any reagent included in the drop-down list below.
-This is NOT the same as the DEA List 1 Reagent classification, which is a significantly smaller list.

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
### Greenness Input – Safety

**Dust Explosion Potential:**
- Charge Dissipation Time: 3 - 1 millisecond to 1 sec
- Pressure Rise Rate (bar/sec): 2 - 50 to 200 bar/sec
- Minimum Ignition Energy (mJ): 4 - >500 millijoules
- 'Kst Explosion Energy value (ST): 2 - <200 (St 1)

**Process Hazards:** 4 - Inherently Safe Process (≤10 °C T adiabatic, no gas generation)

**Environmental Issues:** 3 - Activated Carbon

**Worker Exposure Issues:** 3 - Band 3
## Results – Step Greenness

<table>
<thead>
<tr>
<th>Step Greenness</th>
<th>Cumulative Greenness</th>
<th>PMI</th>
<th>Cumulative Metrics</th>
</tr>
</thead>
<tbody>
<tr>
<td>Solvent Recovery</td>
<td>0.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Solid Process Waste</td>
<td>4.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Liquid Process Waste</td>
<td>0.9</td>
<td>4.0</td>
<td></td>
</tr>
<tr>
<td>Hazardous Reagents</td>
<td>3.0</td>
<td></td>
<td>1.1</td>
</tr>
<tr>
<td>Process Hazards</td>
<td>4.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Environmental Issues</td>
<td>3.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Worker Exposure Issues</td>
<td>3.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Gaseous By-products</td>
<td>4.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Dust Explosion Potential</td>
<td>3.7</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Chemical Transformations</td>
<td>4.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Isolations</td>
<td>4.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Class of Solvents</td>
<td>1.1</td>
<td></td>
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</tr>
<tr>
<td>Number of Solvents</td>
<td>2.0</td>
<td></td>
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</tr>
</tbody>
</table>

## Results – Cumulative Greenness

<table>
<thead>
<tr>
<th>Step Greenness</th>
<th>Cumulative Greenness</th>
<th>PMI</th>
<th>Cumulative Metrics</th>
</tr>
</thead>
<tbody>
<tr>
<td>Solvent Recovery</td>
<td>0.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Solid Process Waste</td>
<td>4.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Liquid Process Waste</td>
<td>1.5</td>
<td></td>
<td>0.4</td>
</tr>
<tr>
<td>Hazardous Reagents</td>
<td>1.0</td>
<td></td>
<td>1.3</td>
</tr>
<tr>
<td>Process Hazards</td>
<td>4.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Environmental Issues</td>
<td>3.3</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Worker Exposure Issues</td>
<td>3.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Gaseous By-products</td>
<td>2.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Dust Explosion Potential</td>
<td>3.7</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Chemical Transformations</td>
<td>3.7</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Isolations</td>
<td>4.0</td>
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<td></td>
</tr>
<tr>
<td>Class of Solvents</td>
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<td></td>
</tr>
<tr>
<td>Number of Solvents</td>
<td>1.3</td>
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</tr>
<tr>
<td>Steps</td>
<td>3.7</td>
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<tr>
<td>Intermediates</td>
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</tr>
<tr>
<td>Average Yield</td>
<td>3.3</td>
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</tr>
<tr>
<td>Overall Greenness Score</td>
<td>59</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Percent Complete</td>
<td>93%</td>
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