ELECTRONIC SUPPLEMENTARY INFORMATION (ESI-1)

The Sustainability Impact of Nobel Prize Chemistry: Life Cycle Assessment of C-C Cross-Coupling reactions

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LCA inventory datasets

Note: All input materials correspond to datasets for Market products, that is, they already include average transport.

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Catalysts

Table S1 *Palladium(II) acetate – Inventory dataset based on Richard F. Heck (1985) and Zang et al. (2017)*

Inputs	Quantity per 1 g of $Pd(OAc)_2$	Unit	Process air emissions		Wastewater treatment emissions (g)			
			Output	Unit	CO_2 to air	Compound to river	COD, BOD to river	TOC, DOC to river
Palladium powder	5.15E-01	g		g		2.06E-02		
Acetic acid	1.05E+01	g	2.10E-02	g	1.38E+00	1.05E-01	1.12E-02	4.19E-02
Nitric acid	3.75E-02	g	7.50E-05	g		[a]5.05E-02		
Energy to warm the mixture at 118 °C for 30 min	2.88E-03	kWh	1.04E-02	MJ				
Sodium hydroxide to neutralize residues of nitric and sulfuric acid	2.38E-02	g		g				
Chemicals factory	4.00E-13	unit						

[a]Neutralized to $NaNO_3$

Table S2 *Palladium tetrakis – Inventory dataset based on Cotton (1972)*

Inputs	Quantity per 1 g of $Pd(PPh_3)_4$	Unit	Process air emissions		Wastewater treatment emissions (g)			
			Output	Unit	CO_2 to air	Compound to river	COD, BOD to river	TOC, DOC to river
Palladium dichloride - PdCl2	1.67E-01	g		g		6.86E-03		
Triphenylphosphine - PPh3	1.24E+00	g		g	8.91E-01	3.28E-02	8.83E-02	2.70E-02
Dimethyl sulfoxide - DMSO	3.63E+00	g	2.49E-02	g	3.65E+00	3.60E-01	5.67E-01	1.11E-01
Energy to warm the mixture at 140 °C during an assumed period of 30 min	3.88E-03	kWh	1.40E-02	MJ				
Energy for stirring for 15 min	1.11E-03	kWh	3.99E-03	MJ				
Hydrazine hydrate	1.89E-01	g	3.77E-04	g		1.88E-01		
Ethanol	2.17E-01	g	1.49E-03	g	3.70E-01	2.15E-02	4.31E-02	1.12E-02
Diethyl ether	1.94E-01	g	1.33E-03	g	4.12E-01	1.93E-02	4.79E-02	1.25E-02
Energy to recover solvents	5.15E-03	kWh	1.85E-02	MJ				
Chemicals factory	4.00E-13	unit						

Halobenzenes (chlorine based)

Table S*3* *Chlorobenzene– Inventory dataset based on Fierz-David and Blangley (1949)*

Inputs	Quantity per 1 g of C_6H_5Cl	Unit	Process air emissions		Wastewater treatment emissions (g)			
			Output	Unit	CO_2 to air	Compound to river	COD, BOD to river	TOC, DOC to river
Benzene	7.99E-01	g	1.60E-03	g	8.31E-01	2.73E-02	8.05E-02	2.52E-02
Chlorine	5.29E-01	g	1.06E-03	g		[a]5.18E-02		
Iron powder (used catalyst is not consumed)	0.00E+00	g		g				
Energy to cool down the reaction	4.01E-05	kWh	1.44E-04	MJ				
Sodium hydroxide	5.12E-01	g		g				
Water	1.49E-01	g	1.02E-03	g		5.12E-01		
Energy for fractional distillation	2.30E-04	kWh	8.28E-04	MJ		1.33E-01		
Energy to recover water	6.66E-04	kWh	2.40E-03	MJ				
Chemicals factory	4.00E-13	unit						

[a]Unreacted chlorine leaves the process as chloride emission. Adsorbable Organic Halogen (AOX) as Cl is also generated and released into wastewater (the same amount of the chloride emission)

Table S4 *4-chloroanisole– Inventory dataset based on Olah et al. (1986)*

Inputs	Quantity per 1 g of C_7H_7ClO	Unit	Process air emissions		Wastewater treatment emissions (g)			
			Output	Unit	CO_2 to air	Compound to river	COD, BOD to river	TOC, DOC to river
Chlorine	7.45E-01	g	1.49E-03	g		[a]2.46E-01		
Dichloromethane	3.39E+00	g	2.32E-02	g	1.57E+00	[b]2.81E+00	1.52E+00	3.97E-01
Dimethylsulfide	8.15E-01	g	1.63E-03	g	1.04E+00	[c]8.39E-01	1.87E+00	3.24E-01
Dichloromethane	9.02E-01	g	6.19E-03	g	4.18E-01	[b]7.48E-01	4.06E-01	1.06E-01
Anisole	9.48E-01	g	1.90E-03	g	4.81E-01	1.88E-02	4.72E-03	1.46E-02
Dichloromethane	3.39E+00	g	2.32E-02	g	1.57E+00	2.81E+00	1.52E+00	3.97E-01
Energy to cool down the mixture at -25 °C	7.93E-04	kWh	2.86E-03	MJ				
Energy to stir the mixture for 4 hours	3.69E-02	kWh	1.33E-01	MJ				
Water	3.83E+00	g	2.63E-02	g		3.43E+00		
Dichloromethane	3.37E+00	g	2.32E-02	g	1.56E+00	2.80E+00	1.52E+00	3.95E-01
Sodium carbonate	4.38E+00	g		g		4.38E+00		
Water	5.11E+00	g	3.51E-02	g		4.57E+00		
Brine	1.08E+01	g		g		1.08E+01		
Energy to distil and recover DCM and water	4.59E-02	kWh	1.65E-01	MJ				
Chemicals factory	4.00E-13	unit						

[a]Unreacted chlorine leaves the process as chloride emission. Adsorbable Organic Halogen (AOX) as Cl is also generated and released into wastewater (the same amount of the chloride emission). [b]Generated chloride after oxidation of dichlorometane goes also to water as chloride and AOX + 10% unoxidized dichloromethane. [c]The oxidation of dimethylsulfide releases sulfur dioxide + 10% unoxidized dimethylsufide

Table S5 *4-chlorotoluene– Inventory dataset based on Smith and Butters (1985)*

Inputs	Quantity per 1 g of C_7H_7Cl	Unit	Process air emissions		Wastewater treatment emissions (g)			
			Output	Unit	CO_2 to air	Compound to river	COD, BOD to river	TOC, DOC to river
Proton-exchanged sodium faujasite (not consumed)	0.00E+00	g						
Dichloromethane	6.12E+00	g	4.20E-02	g	2.83E+00	[a]5.07E+00	2.75E+00	7.17E-01
Diethyl ether	3.26E+00	g	2.24E-02	g	6.92E+00	3.24E-01	8.05E-01	2.10E-01
Toluene	7.28E-01	g	1.46E-03	g	2.15E-01	7.14E-03	2.14E-02	6.51E-03
t-butyl hypochlorite	3.23E-01	g	2.22E-03	g	4.68E-01	[b]1.05E-01	1.70E-01	4.63E-02
Energy to stir for 1 hour at 25 °C	2.07E-02	kWh	7.44E-02	MJ				
Methanol	9.13E-01	g			1.12E+00	9.06E-02	1.30E-01	3.39E-02
Energy to distil dichloromethane, diethyl ether, and methanol	1.85E-02	kWh	6.66E-02	MJ				
Chemicals factory	4.00E-13	unit						

[a]Generated chloride after oxidation of dichlorometane goes also to water as chloride and AOX + 10% unoxidized dichloromethane. [b]The oxidation of t-butyl hypochlorite releases chloride and AOX + 10% unoxidized t-butyl hypochlorite

Table S6 *4-chloronitrobenzene– Inventory dataset based on M. Howe-Grant (1993) and IARC (1996)*

Inputs	Quantity per 1 g of $ClC_6H_4NO_2$	Unit	Process air emissions		Wastewater treatment emissions (g)			
			Output	Unit	CO_2 to air	Compound to river	COD, BOD to river	TOC, DOC to river
Chlorobenzene	7.29E-01	g	1.46E-03	g	2.77E-02	1.31E-03	2.51E-03	8.39E-04
Energy to heat chlorobenzene to 40 °C	9.00E-06	kWh	3.24E-05	MJ				
Sulfuric acid	3.93E-01	g		g		[a]5.70E-01		
Nitric acid	4.41E+00	g	8.82E-03	g		[b]5.40E+00		
Energy to stir for 2 hours	5.90E-03	kWh	2.12E-02	MJ				
Energy to create ice bath	5.01E-04	kWh	1.80E-03	MJ				
Water	9.44E-01	g	6.48E-03	g		8.44E-01		
Energy for the fractional distillation	3.51E-04	kWh	1.26E-03	MJ	2.77E-02	1.31E-03	2.51E-03	8.39E-04
Sodium hydroxide to neutralize residues of nitric and sulfuric acid	2.86E+00	g						
Chemicals factory	4.00E-13	unit						

[a]Neutralized to Na_2SO_4. [b]Neutralized to $NaNO_3$.

Halobenzenes (bromine based)

Table S7 *Bromobenzene– Inventory dataset based on Vogel (1989)*

Inputs	Quantity per 1 g of C_6H_5Br	Unit	Process air emissions		Wastewater treatment emissions (g)			
			Output	Unit	CO_2 to air	Compound to river	COD, BOD to river	TOC, DOC to river
Benzene	5.50E-01	g	1.10E-03	g	6.71E-01	2.21E-02	6.50E-02	2.03E-02
Pyridine (assumed completely recovered)		g		g				
bromine	1.37E+00	g	2.75E-03	g		7.00E-01		
Energy to cool down the water bath to 0 °C	2.98E-04	kWh	1.07E-03	MJ				
Energy to warm the mixture at 30° C for 1 hour	1.03E-03	kWh	3.71E-03	MJ				
Energy to warm the mixture at 70 °C for 45 min	4.05E-03	kWh	1.46E-02	MJ				
Energy to stir for assumed 2 hours	2.06E-03	kWh	7.41E-03	MJ				
Sodium hydroxide	1.15E-01	g				1.15E-01		
Water	9.90E-01	g	1.98E-03	g		8.89E-01		
Magnesium sulphate								
Energy to heat at 156 °C to distil bromobenzene (twice)	2.30E-04	kWh	8.29E-04	MJ				
Chemicals factory	4.00E-13	unit						

Table S8 *4-bromoanisole– Inventory dataset based on Hilgetag and Martini (1972)*

Inputs	Quantity per 1 g of $CH_3OC_6H_4Br$	Unit	Process air emissions		Wastewater treatment emissions (g)			
			Output	Unit	CO_2 to air	Compound to river	COD, BOD to river	TOC, DOC to river
Anisole	4.86E-01	g	9.72E-04	g	2.09E-01	8.17E-03	1.97E-02	6.35E-03
Glacial acetic acid	5.31E-01	g	3.65E-03	g	6.96E-01	5.28E-02	5.40E-02	2.11E-02
bromine	7.54E-01	g	1.51E-03	g		1.56E-01		
Water	2.83E+00	g	1.94E-02	g		2.53E+00		
Energy to heat at 120 cC to distil the 4-bromoanisole	2.69E-04	kWh	9.67E-04	MJ				
Energy to recover water and acetic acid	1.31E-02	kWh	4.70E-02	MJ				
Chemicals factory	4.00E-13	unit						

Table S9 *4-bromotoluene– Inventory dataset based on Vogel (1989)*

Inputs	Quantity per 1 g of C_7H_7Br	Unit	Process air emissions		Wastewater treatment emissions (g)			
			Output	Unit	CO_2 to air	Compound to river	COD, BOD to river	TOC, DOC to river
4-Toluidine	8.92E-01	g	1.78E-03	g	6.80E-01	2.63E-02	7.73E-02	2.06E-02
Water	1.94E+00	g	1.33E-02	g		1.74E+00		
Sulfuric acid	1.63E+00	g		g		[a]1.53E+00		
Energy to warm the mixture at 100 °C for 10 min	1.55E-03	kWh	5.57E-03	MJ				
Energy to cool down the mixture to 0 °C	1.42E-03	kWh	5.12E-03	MJ				
Water (frozen)	4.86E-01	g	3.33E-03	g		4.34E-01		
Energy to freeze the water	2.58E-04	kWh	9.28E-04	MJ				
Sodium nitrite	5.83E-01	g	1.17E-03	g		1.79E-01		
Water	1.00E+00	g	2.00E-03	g		8.98E-01		
Energy to stir for assumed 10 min	9.58E-04	kWh	3.45E-03	MJ				
Copper(I) bromide	8.49E-01	g		g		2.65E-03		
Energy to heat at 100 °C the copper(I) bromide solution	2.58E-03	kWh	9.28E-03	MJ				
Energy to distil 4-bromotoluene	2.04E-04	kWh	7.35E-04	MJ				
Sodium hydroxide	1.04E-01	g		g		1.04E-01		
Water	4.00E-01	g	8.00E-04	g		3.59E-01		
Sulfuric acid	6.13E-01	g		g		[a]5.78E-02		
Sodium hydroxide to neutralize sulfuric acid	8.97E-01	g		g				
Energy to recover water	1.08E-02	kWh	3.87E-02	MJ				
Chemicals factory	4.00E-13	unit						

[a]Neutralized to Na_2SO_4

Table S10 *4-bromonitrobenzene – Inventory dataset based on Vogel (1989)*

Inputs	Quantity per 1 g of $C_6H_4BrNO_2$	Unit	Process air emissions		Wastewater treatment emissions (g)			
			Output	Unit	CO_2 to air	Compound to river	COD, BOD to river	TOC, DOC to river
Nitric acid	2.04E+00	g	4.07E-03	g		[a]2.32E+00		
Sulfuric acid	2.64E+00	g		g		[b]3.83E+00		
Energy to cool down the reaction	2.98E-05	kWh	1.07E-04	MJ				
Bromobenzene	1.14E+00	g	2.29E-03	g	5.44E-01	3.59E-02	4.92E-02	4.12E-03
Energy to warm the mixture at 100 °C for 30 min	1.34E-03	kWh	4.81E-03	MJ				
Energy to cool the mixture to room temp	2.21E-04	kWh	7.97E-04	MJ				
Water	4.16E+00	g	2.86E-02	g		3.72E+00		
Ethanol	1.64E+00	g	1.13E-02	g	2.80E+00	1.63E-01	3.26E-01	8.50E-02
Energy to recrystallize	3.70E-04	kWh	0.00E+00	MJ				
Water	1.25E+00	g	8.57E-03	g		1.12E+00		
Energy to stir for 15 + 5 min	1.03E-03	kWh	3.73E-03	MJ				
Energy to recover water and ethanol	2.65E-02	kWh	9.55E-02	MJ				
Sodium hydroxide to neutralize residues of nitric and sulfuric acid	3.25E+00	g						
Chemicals factory	4.00E-13	unit						

[a]Neutralized to $NaNO_3$. [b]Neutralized to Na_2SO_4.

Halobenzenes (iodine based)

Table S11 *Iodobenzene – Inventory dataset based on Vogel (1989)*

Inputs	Quantity per 1 g of C_6H_5I	Unit	Process air emissions		Wastewater treatment emissions (g)			
			Output	Unit	CO_2 to air	Compound to river	COD, BOD to river	TOC, DOC to river
Benzene	4.98E-01	g	9.97E-04	g	7.33E-01	2.41E-02	7.11E-02	2.22E-02
Iodine	4.72E-01	g	9.45E-04	g		5.49E-02		
Energy to heat at 50 °C the mixture	7.84E-04	kWh	2.82E-03	MJ				
Nitric acid	5.13E-01	g	1.03E-03	g		[a]8.05E-02		
Energy to warm the mixture at 80 °C for 15 min	2.37E-03	kWh	8.53E-03	MJ				
Sodium hydroxide	3.10E-01	g		g		3.10E-01		
Energy to distil the mixture	1.66E-03	g	5.96E-03	MJ				
Hydrochloric acid	2.59E-02	g	1.55E-05	g		[b]1.24E-02		
Water	1.08E-01	g	7.44E-04	g		9.69E-02		
Iron filings (assumed recovered)		g		g				
Energy to stir for 3 hours	3.92E-03	kWh	1.41E-02	MJ				
Magnesium sulphate								
Energy to heat at 186 °C to distil iodobenzene	2.05E-04	kWh	7.37E-04	MJ				
Sodium hydroxide to neutralize residues of nitric and hydrochloric acid	4.64E-02	g						
Energy to recover water	4.82E-04	kWh	1.73E-03	MJ				
Chemicals factory	4.00E-13	unit						

[a]Neutralized to $NaNO_3$. [b]Neutralized to NaCl.

Table S12 *4-iodoanisole – Inventory dataset based on Hilgetag and Martini (1972)*

Inputs	Quantity per 1 g of C_7H_7IO	Unit	Process air emissions		Wastewater treatment emissions (g)			
			Output	Unit	CO_2 to air	Compound to river	COD, BOD to river	TOC, DOC to river
Anisole	5.83E-01	g	1.17E-03	g	3.06E-01	1.19E-02	2.88E-02	9.27E-03
Hydrogen peroxide	4.27E-01	g	8.55E-04	g		2.81E-01		
Water	2.00E-01	g	1.38E-03	g		1.79E-01		
iodine	6.85E-01	g	1.37E-03	g		1.41E-01		
Ethanol	6.44E-01	g	4.42E-03	g	1.10E+00	6.39E-02	1.28E-01	3.33E-02
Water	4.29E-01	g	2.95E-03	g		3.84E-01		
Sulfuric acid	1.80E-01	g		g		[a]2.60E-01		
Energy to stir for 20 min	1.11E-03	kWh	4.00E-03	MJ				
Diethyl ether	2.02E+00	g	1.39E-02	g	4.29E+00	2.01E-01	4.99E-01	1.30E-01
Thiosulfate solution (assumed recovered)		g		g				
Calcium chloride (assumed recovered)		g		g				
Ethanol	2.03E+00	g	1.40E-02	g	3.47E+00	2.02E-01	4.04E-01	1.05E-01
Energy to recrystallize	4.58E-04	kWh	1.65E-03	MJ				
water	1.43E+00	g	9.82E-03	g		1.28E+00		
Energy to recover water, ethanol, and diethyl ether	1.14E-02	kWh	4.11E-02	MJ				
Sodium hydroxide to neutralize residues of sulfuric acid	1.47E-01	g						
Chemicals factory	4.00E-13	unit						

[a]Neutralized to Na_2SO_4.

Table S13 *4-iodotoluene – Inventory dataset based on Vogel (1989)*

Inputs	Quantity per 1 g of C_7H_7I	Unit	Process air emissions		Wastewater treatment emissions (g)			
			Output	Unit	CO_2 to air	Compound to river	COD, BOD to river	TOC, DOC to river
4-Toluidine	5.40E-01	g	1.08E-03	g	1.22E-01	4.73E-03	1.39E-02	3.70E-03
Water	3.67E-01	g	2.52E-03	g		3.28E-01		
Hydrochloric acid	1.64E+00	g	9.82E-04	g		[a]7.85E-01		
Energy to warm the mixture at 100 °C for 10 min	6.81E-04	kWh	2.45E-03	MJ				
Energy to cool the mixture to 0 °C	5.31E-04	kWh	1.91E-03	MJ				
Water (frozen)	5.83E-01	g	4.00E-03	g		5.21E-01		
Energy to freeze the water	3.09E-04	kWh	1.11E-03	MJ				
Sodium nitrite	3.70E-01	g	7.40E-04	g		3.69E-01		
Water	8.00E-01	g	1.60E-03	g		7.19E-01		
Energy to stir for assumed 10 min	4.09E-04	kWh	1.47E-03	MJ				
Potassium iodide	8.80E-01	g		g		1.19E-01		
Water	2.56E-01	g	1.76E-03	g		2.29E-01		
Energy to stir for assumed 10 min	5.66E-04	kWh	2.04E-03	MJ				
Sodium metabisulphite	4.00E-02	g	0.00E+00	0		4.00E-02		
Sodium hydroxide	6.25E-02	g	0.00E+00	g		6.25E-02		
Water	1.57E-01	g	1.08E-03	g		1.41E-01		
Energy to recrystallize	9.33E-05	kWh	3.36E-04	MJ				
Ethanol	4.14E-01	g	2.84E-03	g	7.07E-01	4.11E-02	8.22E-02	2.14E-02
energy to recover water and ethanol	7.71E-03	kWh	2.78E-02	MJ				
Sodium hydroxide to neutralize residues of hydrochloric acid	5.37E-01	g						
Chemicals factory	4.00E-13	unit						

[a]*Neutralized to NaCl.*

Table S14 *4-iodonitrobenzene – Inventory dataset based on Vogel (1989)*

Inputs	Quantity per 1 g of $C_6H_4INO_2$	Unit	Process air emissions		Wastewater treatment emissions (g)			
			Output	Unit	CO_2 to air	Compound to river	COD, BOD to river	TOC, DOC to river
4-nitroaniline	6.85E-01	g	1.37E-03	g	2.22E-01	1.29E-02	2.01E-02	6.72E-03
Water	1.20E+00	g	8.22E-03	g		1.07E+00		
Sulfuric acid	1.03E+00	g		g		[a]9.17E-01		
Energy to stir for 1 hour	3.11E-03	kWh	1.12E-02	MJ				
Energy to cool the mixture to 0 °C	9.00E-04	kWh	3.24E-03	MJ				
Sodium nitrite	3.42E-01	g	6.85E-04	g		3.42E-01		
Water	2.99E-01	g	2.05E-03	g		2.68E-01		
Potassium iodide	1.37E+00	g				7.03E-01		
Water	1.20E+00	g	8.22E-03	g		1.07E+00		
Ethanol	2.84E-01	g	1.95E-03	g	4.84E-01	2.82E-02	5.63E-02	1.47E-02
Energy to recrystalize	6.39E-05	g	2.30E-04	MJ				
Energy to recover water and ethanol	1.24E-02	kWh	4.45E-02	MJ				
Sodium hydroxide to neutralize residues of sulfuric acid	5.17E-01	g						
Chemicals factory	4.00E-13	unit						

[a]*Neutralized to Na_2SO_4.*

Ligand

Table S15 *Triphenylphosphine – Inventory dataset based on Corbridge (1995)*

Inputs	Quantity per 1 g of [a]PPh_3	Unit	Process air emissions		Wastewater treatment emissions (g)			
			Output	Unit	CO_2 to air	Compound to river	COD, BOD to river	TOC, DOC to river
Phosphorus trichloride	5.82E-01	g	1.16E-03	g		5.70E-02		
Chlorobenzene	1.43E+00	g	2.86E-03	g	2.96E-01	1.40E-02	2.68E-02	8.97E-03
Sodium	5.84E-01	g		g		5.84E-02		
Heating steam	2.00E-03	MJ						
Electricity	3.33E-04	kWh	1.20E-03	MJ				
Chemicals factory	4.00E-13	unit						

[a]*Assumed yield 90%*

Protocols for cross-coupling reactions

Table S16 *Biphenyl from bromobenzene via Suzuki protocol – Inventory dataset based on Miyaura et al. (1981)*

Inputs	Quantity per 1 g of $C_{12}H_{10}$	Unit	Process air emissions		Wastewater treatment emissions (g)			
			Output	Unit	CO_2 to air	Compound to river	COD, BOD to river	TOC, DOC to river
Bromobenzene	1.34E+00	g	2.68E-03	g	4.82E-01	3.19E-02	4.68E-02	1.46E-02
Benzene	4.34E+00	g	8.68E-03	g	1.32E+01	4.33E-01	1.28E+00	3.99E-01
Sodium hydroxide	6.83E-01	g		g		6.83E-01		
Water	2.29E+00	g	1.57E-02	g		2.04E+00		
$Pd(PPh_3)_4$	2.96E-01	g		g	7.30E-01	2.96E-02	7.23E-02	2.21E-02
Phenylboronic acid	1.14E+00	g		g	6.89E-01	3.54E-02	1.34E-02	2.09E-02
Energy to reflux during 6 h	2.26E-02	kWh	8.12E-02	MJ				
Energy to stir for 6 h	8.31E-02	kWh	2.99E-01	MJ				
Hydrogen peroxide	6.19E-01	g		g				
Energy to recover benzene and water	1.38E-02	kWh	4.98E-02	MJ				
Chemicals factory	4.00E-13	unit						

Table S17 *Biphenyl from iodobenzene via Suzuki protocol – Inventory dataset based on Miyaura et al. (1981)*

Inputs	Quantity per 1 g of $C_{12}H_{10}$	Unit	Process air emissions		Wastewater treatment emissions (g)			
			Output	Unit	CO_2 to air	Compound to river	COD, BOD to river	TOC, DOC to river
Iodobenzene	2.13E+00	g	4.27E-03	g	9.39E-01	8.07E-02	9.11E-02	2.85E-02
Benzene	5.32E+00	g	1.06E-02	g	1.62E+01	5.31E-01	1.57E+00	4.89E-01
Sodium hydroxide	8.37E-01	g		g		8.37E-01		
Water	2.80E+00	g	1.92E-02	g		2.51E+00		
$Pd(PPh_3)_4$	3.63E-01	g		g	8.95E-01	3.63E-02	8.87E-02	2.71E-02
Phenylboronic acid	1.40E+00	g		g	1.19E+00	6.12E-02	2.31E-02	3.61E-02
Energy to reflux during 6 h	2.77E-02	kWh	9.96E-02	MJ				
Energy to stir for 6 h	1.03E-01	kWh	3.73E-01	MJ				
Hydrogen peroxide	7.58E-01	g		g				
Energy to recover benzene and water	1.70E-02	kWh	6.11E-02	MJ				
Chemicals factory	4.00E-13	unit						

Table S18 *Diphenylacetylene from bromobenzene via Heck protocol – Inventory dataset based on Dieck and Heck (1975)*

Inputs	Quantity per 1 g of $C_{14}H_{10}$	Unit	Process air emissions		Wastewater treatment emissions (g)			
			Output	Unit	CO_2 to air	Compound to river	COD, BOD to river	TOC, DOC to river
Bromobenzene	1.73E+00	g	3.45E-03	g	1.28E+00	8.43E-02	1.24E-01	3.87E-02
Phenylacetylene	2.25E+00	g	4.49E-03	g	2.59E+00	1.67E-01	2.26E-01	7.85E-02
Triethyl amine	2.23E+00	g		g	5.84E+00	1.66E-01	7.30E-01	1.77E-01
$Pd(OAc)_2$	2.47E-02	g		g	1.74E-02	2.47E-03	1.18E-03	5.28E-04
Energy to reflux and stir for 2.5 h at 100°C	1.07E-02	kWh	3.85E-02	MJ				
Chemicals factory	4.00E-13	unit						

Table S19 *Diphenylacetylene from iodobenzene via Heck protocol – Inventory dataset based on Dieck and Heck (1975)*

Inputs	Quantity per 1 g of $C_{14}H_{10}$	Unit	Process air emissions		Wastewater treatment emissions (g)			
			Output	Unit	CO_2 to air	Compound to river	COD, BOD to river	TOC, DOC to river
Iodobenzene	1.57E+00	g	3.14E-03	g	4.89E-01	4.20E-02	4.75E-02	1.48E-02
Phenylacetylene	9.81E-01	g	1.96E-03	g	6.30E-01	4.06E-02	5.50E-02	1.91E-02
Triethyl amine	1.56E+00	g		g	3.48E+00	9.88E-02	4.35E-01	1.05E-01
$Pd(OAc)_2$	1.73E-02	g		g	1.22E-02	1.73E-03	8.26E-04	3.69E-04
Energy to reflux and stir for 2.5 h at 100°C	4.35E-03	kWh	1.57E-02	MJ				
Chemicals factory	4.00E-13	unit						

Table S20 *Diphenylacetylene from bromobenzene via Heck protocol – Inventory dataset based on Cassar (1975)*

Inputs	Quantity per 1 g of $C_{14}H_{10}$	Unit	Process air emissions		Wastewater treatment emissions (g)			
			Output	Unit	CO_2 to air	Compound to river	COD, BOD to river	TOC, DOC to river
Bromobenzene	1.00E+00	g	2.00E-03	g	1.79E-01	1.18E-02	1.73E-02	5.42E-03
Phenylacetylene	6.51E-01	g	1.30E-03	g	1.19E-01	7.68E-03	1.04E-02	3.61E-03
Sodium methoxide	4.13E-01	g		g	2.73E+00	4.13E-02	3.41E-01	8.26E-02
Dimethylformamide	7.01E+00	g		g	1.14E+01	7.01E-01	1.33E+00	3.45E-01
$Pd(PPh_3)_4$	4.42E-01	g		g	1.09E+00	4.42E-02	1.08E-01	3.31E-02
Energy to reflux and stir for 4 h at 80°C	5.08E-02	kWh	1.83E-01	MJ				
Energy to recover dimethylformamide	9.44E-03	kWh	3.40E-02	MJ				
Chemicals factory	4.00E-13	unit						

Table S21 *Diphenylacetylene from iodobenzene via Heck protocol – Inventory dataset based on Cassar (1975)*

Inputs	Quantity per 1 g of $C_{14}H_{10}$	Unit	Process air emissions		Wastewater treatment emissions (g)			
			Output	Unit	CO_2 to air	Compound to river	COD, BOD to river	TOC, DOC to river
Iodobenzene	1.20E+00	g	2.41E-03	g	6.74E-02	5.78E-03	6.53E-03	2.04E-03
Phenylacetylene	6.03E-01	g	1.21E-03	g	4.49E-02	2.90E-03	3.92E-03	1.36E-03
Sodium methoxide	3.51E-01	g	0.00E+00	g	3.16E-01	4.79E-03	3.95E-02	9.57E-03
Dimethylformamide	3.25E+00	g	0.00E+00	g	5.28E+00	3.25E-01	6.14E-01	1.60E-01
$Pd(PPh_3)_4$	1.36E-01	g		g	3.37E-01	1.36E-02	3.34E-02	1.02E-02
Energy to reflux and stir for 3 h at 50°C	1.56E-02	kWh	5.62E-02	MJ				
Energy to recover dimethylformamide	4.37E-03	kWh	1.57E-02	MJ				
Chemicals factory	4.00E-13	unit						

Table S22 *Trans-Methyl cinnamate from bromobenzene via Heck protocol – Inventory dataset based on Dieck and Heck (1974)*

Inputs	Quantity per 1 g of $C_{10}H_{10}O_2$	Unit	Process air emissions		Wastewater treatment emissions (g)			
			Output	Unit	CO_2 to air	Compound to river	COD, BOD to river	TOC, DOC to river
Bromobenzene	1.14E+00	g	2.28E-03	g	2.55E-01	1.69E-02	2.47E-02	7.73E-03
Methyl acrylate	1.25E+00	g	2.50E-03	g	1.32E+00	7.16E-02	1.15E-01	3.99E-02
Tetramethylethylenediamine	8.43E-01	g	1.69E-03	g	2.55E-01	1.25E-02	3.46E-02	7.73E-03
$Pd(OAc)_2$	1.63E-02	g		g	1.15E-02	1.63E-03	7.80E-04	3.48E-04
Triphenylphosphine	3.81E-02	g		g	1.03E-01	3.81E-03	1.03E-02	3.13E-03
Energy to reflux during 28 h at 125 °C	4.61E-02	kWh	1.66E-01	MJ				
Chemicals factory	4.00E-13	unit						

Table S23 *Trans-Methyl cinnamate from iodobenzene via Heck protocol – Inventory dataset based on Heck and Nolley (1972)*

Inputs	Quantity per 1 g of $C_{10}H_{10}O_2$	Unit	Process air emissions		Wastewater treatment emissions (g)			
			Output	Unit	CO_2 to air	Compound to river	COD, BOD to river	TOC, DOC to river
Iodobenzene	1.55E+00	g	3.11E-03	g	3.40E-01	2.92E-02	3.30E-02	1.03E-02
Methyl acrylate	1.31E+00	g	2.62E-03	g	1.43E+00	7.77E-02	1.25E-01	4.33E-02
Tripropylamine	2.18E+00	g		g	3.23E+00	1.30E-01	4.03E-01	9.78E-02
$Pd(OAc)_2$	1.71E-02	g		g	1.21E-02	1.71E-03	8.18E-04	3.65E-04
l-methyl-2-pyrrolidinone	2.04E+00	g		g	4.90E+00	2.04E-01	9.49E-02	1.48E-01
Energy to reflux and stir for 1 h at 100 °C	6.18E-03	kWh	2.23E-02	MJ				
Energy to recover l-methyl-2-pyrrolidinone	2.73E-03	kWh	9.82E-03	MJ				
Chemicals factory	4.00E-13	unit						

Table S24 *Trans-Methyl 4-methoxycinnamate from 4-bromoanisole via Heck protocol – Inventory dataset based on Dieck and Heck (1974)*

Inputs	Quantity per 1 g of $C_{11}H_{12}O_3$	Unit	Process air emissions		Wastewater treatment emissions (g)			
			Output	Unit	CO_2 to air	Compound to river	COD, BOD to river	TOC, DOC to river
4-bromoanisole	1.64E+00	g	3.27E-03	g	1.17E+00	7.50E-02	1.11E-01	3.56E-02
Methyl acrylate	1.59E+00	g	3.18E-03	g	2.13E+00	1.16E-01	1.86E-01	6.46E-02
Tetramethylethylenediamine	1.08E+00	g	2.15E-03	g	1.01E+00	4.92E-02	1.37E-01	3.05E-02
$Pd(OAc)_2$	2.08E-02	g		g	1.46E-02	2.08E-03	9.94E-04	4.44E-04
Triphenylphosphine	4.85E-02	g		g	1.32E-01	4.85E-03	1.31E-02	4.00E-03
Energy to reflux during 36 h at 135 °C	8.67E-02	kWh	3.12E-01	MJ				
Chemicals factory	4.00E-13	unit						

Table S25 *Trans-Methyl 4-methoxycinnamate from 4-iodoanisole via Heck protocol – Inventory dataset based on Heck and Nolley (1972)*

Inputs	Quantity per 1 g of $C_{11}H_{12}O_3$	Unit	Process air emissions		Wastewater treatment emissions (g)			
			Output	Unit	CO_2 to air	Compound to river	COD, BOD to river	TOC, DOC to river
4-iodoanisole	1.72E+00	g	3.44E-03	g	5.55E-01	5.47E-02	5.38E-02	1.68E-02
Methyl acrylate	7.90E-01	g	1.58E-03	g	6.60E-01	3.59E-02	5.76E-02	2.00E-02
Tributylamine	1.36E+00	g		g	8.38E-01	4.36E-02	1.05E-01	2.54E-02
$Pd(OAc)_2$	1.65E-02	g		g	1.16E-02	1.65E-03	7.90E-04	3.53E-04
Energy to reflux and stir for 5 h at 100 °C	1.21E-02	kWh	4.35E-02	MJ				
Chemicals factory	4.00E-13	unit						

Other precursor and ancillary compounds

The inventories for the preparation of compounds not available in the database, such as palladium chloride and triphenylphosphine, needed for catalysts; anisole, t-butyl hypochlorite, copper(I) bromide, 4-toluidine, potassium iodide, 4-nitroaniline, and 4-nitroacetanilide, needed for halobenzenes; and phenylboronic acid, tetramethylethylenediamine, tripropylamine, tributylamine, phenylacetylene, and styrene dibromide, needed for the CCR, are detailed below:

Note: These inventory datasets include transport because the products were created to emulate the production of these chemicals at industrial scales in a similar way as the Ecoinvent datasets for Market products. This is because they are not final products but intermediate input materials for the catalysts, halobenzenes, ligands, or products made via de CCR protocols.

Table S26 *Palladium Chloride – Inventory dataset based on Heck (1985)*

Inputs	Quantity per 1 g of $PdCl_2$	Unit	Process air emissions		Wastewater treatment emissions (g)			
			Output	Unit	CO_2 to air	Compound to river	COD, BOD to river	TOC, DOC to river
Palladium powder	6.06E-01	g		g		3.03E-03		
Nitric acid	3.59E-01	g	7.18E-04	g				
Hydrochloric acid	6.23E-01	g	1.25E-03	g				
Heating steam	2.00E-03	MJ						
Electricity	3.33E-04	kWh	1.20E-03	MJ				
Transport lorry	1.00E-04	tkm						
Transport train	6.00E-04	tkm						
Chemicals factory	4.00E-13	unit						

Table S27 *Anisole – Inventory dataset based on Hilgetag and Martini (1972)*

Inputs	Quantity per 1 g of C_7H_8O	Unit	Process air emissions		Wastewater treatment emissions (g)			
			Output	Unit	CO_2 to air	Compound to river	COD, BOD to river	TOC, DOC to river
Phenol	1.16E+00	g	2.32E-03	g	7.27E-01	2.88E-02	6.58E-02	2.20E-02
Sodium hydroxide[a]	4.94E-01	g		g				
Dimethyl sulfate[a]	7.78E-01	g	1.56E-03	g				
Water[a]	2.47E+00	g	4.94E-03	g				
Heating steam	2.00E-03	MJ						
Electricity	3.33E-04	kWh	1.20E-03	MJ				
Transport lorry	1.00E-04	tkm						
Transport train	6.00E-04	tkm						
Chemicals factory	4.00E-13	unit						

[a]The reference assumed that no residues of the system because all is recycled and reused

Table S28 *t-butyl hypochlorite – Inventory dataset based on Mintz and Walling (1969)*

Inputs	Quantity per 1 g of C_4H_9ClO	Unit	Process air emissions		Wastewater treatment emissions (g)			
			Output	Unit	CO_2 to air	Compound to river	COD, BOD to river	TOC, DOC to river
Sodium hypochlorite	8.82E-01	g		g		8.82E-01		
Water	4.01E+00	g	8.02E-03	g		3.60E+00		
t-butyl alcohol	8.50E-01	g	1.70E-03	g	3.54E-01	1.66E-02	4.12E-02	1.07E-02
Acetic acid	7.59E-01	g		g	1.00E+00	7.59E-02	7.77E-02	3.04E-02
Heating steam	2.00E-03	MJ						
Electricity	3.33E-04	kWh	1.20E-03	MJ				
Transport lorry	1.00E-04	tkm						
Transport train	6.00E-04	tkm						
Chemicals factory	4.00E-13	unit						

Table S29 *Copper(I) bromide – Inventory dataset based on Vogel (1989)*

Inputs	Quantity per 1 g of CuBr	Unit	Process air emissions		Wastewater treatment emissions (g)			
			Output	Unit	CO_2 to air	Compound to river	COD, BOD to river	TOC, DOC to river
Copper(II) sulphate	6.18E-01	g		g		1.55E-02		
Copper turnings (not consumed)	0	g		g				
Sodium bromide	1.51E+00	g		g		7.94E-01		
Sulfuric acid	2.94E-01	g		g		[a]4.26E-01		
Water	5.72E+00	g	3.92E-02	g		5.68E+00		
Sodium hydroxide to neutralize sulfuric acid	1.20E-01	g		g				
Heating steam	2.00E-03	MJ						
Electricity	3.33E-04	kWh	1.20E-03	MJ				
Transport lorry	1.00E-04	tkm						
Transport train	6.00E-04	tkm						
Chemicals factory	4.00E-13	unit						

[a]Neutralized to Na_2SO_4

Table S30 *4-toluidine – Inventory dataset based on* Zhengqi and Guidong (2011)

Inputs	Quantity per 1 g of C_7H_9N	Unit	Process air emissions		Wastewater treatment emissions (g)			
			Output	Unit	CO_2 to air	Compound to river	COD, BOD to river	TOC, DOC to river
p-nitrotoluene	1.30E+00	g	2.60E-03	g	3.68E-02	1.82E-03	3.57E-03	1.11E-03
Palladium-carbon catalyst	0.00E+00	g		g				
Water	6.50E-03	g	1.30E-05	g		[a]3.42E-01		
Hydrogen	5.12E-01	g	1.02E-03	g				
Heating steam	2.00E-03	MJ						
Electricity	3.33E-04	kWh	1.20E-03	MJ				
Transport lorry	1.00E-04	tkm						
Transport train	6.00E-04	tkm						
Chemicals factory	4.00E-13	unit						

[a]90% of wastewater plus the water generated in the synthesis

Table S31 *Potassium iodide– Inventory dataset based on stoichiometric balance ($3I_2 + 6KOH = 5KI + KIO_3 + 3H_2O$)*

Inputs	Quantity per 1 g of [a]KI	Unit	Process air emissions		Wastewater treatment emissions (g)			
			Output	Unit	CO_2 to air	Compound to river	COD, BOD to river	TOC, DOC to river
Iodine	1.02E+00	g		g		1.02E-01		
Potassium hydroxide	4.51E-01	g		g		4.51E-02		
Water	2.91E+00	g	2.00E-02	g		2.60E+00		
Heating steam	2.00E-03	MJ						
Electricity	3.33E-04	kWh	1.20E-03	MJ				
Transport lorry	1.00E-04	tkm						
Transport train	6.00E-04	tkm						
Chemicals factory	4.00E-13	unit						

[a]Assumed yield 90%

Table S32 *4-nitroaniline– Inventory dataset based on Vogel (1989)*

Inputs	Quantity per 1 g of $C_6H_6N_2O_2$	Unit	Process air emissions		Wastewater treatment emissions (g)			
			Output	Unit	CO_2 to air	Compound to river	COD, BOD to river	TOC, DOC to river
p-nitroacetanilide	1.36E+00	g	2.73E-03	g	9.95E-02	5.66E-03	8.68E-03	3.02E-03
Sulfuric acid	8.78E+00	g	0.00E+00	g		[a]1.27E+01		
Water	5.96E-01	g	4.09E-03	g		5.33E-01		
Water	1.32E+01	g	9.09E-02	g		1.18E+01		
Sodium hydroxide	2.84E-01	g		g		2.84E-01		
Water	8.86E-01	g	2.45E-01	g		5.77E-01		
Sodium hydroxide to neutralize sulfuric acid	7.16E+00	g		g				
Heating steam	2.00E-03	MJ						
Electricity	3.33E-04	kWh	1.20E-03	MJ				
Transport lorry	1.00E-04	tkm						
Transport train	6.00E-04	tkm						
Chemicals factory	4.00E-13	unit						

[a]Neutralized to Na_2SO_4

Table S33 *4- nitroacetanilide– Inventory dataset based on Vogel (1989)*

Inputs	Quantity per 1 g of $C_8H_8N_2O_3$	Unit	Process air emissions		Wastewater treatment emissions (g)			
			Output	Unit	CO_2 to air	Compound to river	COD, BOD to river	TOC, DOC to river
Acetanilide	1.25E+00	g	2.50E-03	g	1.17E+00	4.97E-02	1.13E-01	3.53E-02
Glacial acetic acid	3.82E-01	g	2.63E-03	g	5.01E-01	3.80E-02	3.89E-02	1.52E-02
Sulfuric acid	4.60E+00	g		g		[a]6.66E+00		
Nitric acid	7.75E-01	g	1.55E-03	g		[b]5.72E-01		
Sulfuric acid	6.25E-01	g		g		[a]1.48E+00		
Water	7.29E+00	g	5.00E-02	g		6.51E+00		
Sodium hydroxide to neutralize nitric and sulfuric acid	4.85E+00	g		g				
Heating steam	2.00E-03	MJ						
Electricity	3.33E-04	kWh	1.20E-03	MJ				
Transport lorry	1.00E-04	tkm						
Transport train	6.00E-04	tkm						
Chemicals factory	4.00E-13	unit						

[a]Neutralized to Na_2SO_4. [b]Neutralized to $NaNO_3$

Table S34 *Phenylboronic acid – Inventory dataset based on Washburn et al. (1959)*

Inputs	Quantity per 1 g of $C_6H_7BO_2$	Unit	Process air emissions		Wastewater treatment emissions (g)			
			Output	Unit	CO_2 to air	Compound to river	COD, BOD to river	TOC, DOC to river
Methyl borate	1.09E+00	g	2.19E-03	g	2.73E-01	2.39E-02	3.00E-02	8.28E-03
Phenylmagnesium bromide	1.91E+00	g	3.81E-03	g	5.45E-01	4.16E-02	5.81E-02	1.65E-02
Diethyl ether	1.65E-01	g	1.14E-03	g	3.50E-01	1.64E-02	4.07E-02	1.06E-02
Water	1.73E+00	g	1.19E-02	g		1.54E+00		
Sulfuric acid	5.42E-01	g		g				
Heating steam	2.00E-03	MJ						
Electricity	3.33E-04	kWh	1.20E-03	MJ				
Transport lorry	1.00E-04	tkm						
Transport train	6.00E-04	tkm						
Chemicals factory	4.00E-13	unit						

Table S35 *Tetramethylethylenediamine – Inventory dataset based on Hammerstrom and Spielberger (1975)*

Inputs	Quantity per 1 g of $^{a}C_6H_{16}N_2$	Unit	Process air emissions		Wastewater treatment emissions (g)			
			Output	Unit	CO_2 to air	Compound to river	COD, BOD to river	TOC, DOC to river
Ethylene dichloride	9.46E-01	g	1.89E-03	g	7.42E-02	9.27E-03	7.19E-03	2.25E-03
Dimethylamine	8.62E-01	g	1.72E-03	g	1.48E-01	8.44E-03	2.30E-02	4.50E-03
Heating steam	2.00E-03	MJ						
Electricity	3.33E-04	kWh	1.20E-03	MJ				
Transport lorry	1.00E-04	tkm						
Transport train	6.00E-04	tkm						
Chemicals factory	4.00E-13	unit						

[a]Assumed yield 90%

Table S36 *Tripropylamine – Inventory dataset based on Huyghe et al. (2011)*

Inputs	Quantity per 1 g of $^{a}C_9H_{21}N$	Unit	Process air emissions		Wastewater treatment emissions (g)			
			Output	Unit	CO_2 to air	Compound to river	COD, BOD to river	TOC, DOC to river
1-Propanol	1.40E+00	g	2.80E-03	g	2.71E-01	1.37E-02	3.15E-02	8.21E-03
Ammonia	1.32E-01	g	2.64E-04	g	0.00E+00	4.66E-02		
Heating steam	2.00E-03	MJ						
Electricity	3.33E-04	kWh	1.20E-03	MJ				
Transport lorry	1.00E-04	tkm						
Transport train	6.00E-04	tkm						
Chemicals factory	4.00E-13	unit						

[a]Assumed yield 90%

Table S37 *Tributylamine – Inventory dataset based on* Lewis (2007)

Inputs	Quantity per 1 g of [a]$C_{12}H_{27}N$	Unit	Process air emissions		Wastewater treatment emissions (g)			
			Output	Unit	CO_2 to air	Compound to river	COD, BOD to river	TOC, DOC to river
1-Butanol	1.08E+00	g	2.16E-03	g	2.79E-01	1.06E-02	3.25E-02	8.46E-03
Ammonia	4.44E-01	g	8.89E-04	g	0.00E+00	1.57E-01		
Heating steam	2.00E-03	MJ						
Electricity	3.33E-04	kWh	1.20E-03	MJ				
Transport lorry	1.00E-04	tkm						
Transport train	6.00E-04	tkm						
Chemicals factory	4.00E-13	unit						

[a]*Assumed yield 90%*

Table S38 *Phenylacetylene – Inventory dataset based on Franke et al. (1960)*

Inputs	Quantity per 1 g of C_8H_6	Unit	Process air emissions		Wastewater treatment emissions (g)			
			Output	Unit	CO_2 to air	Compound to river	COD, BOD to river	TOC, DOC to river
Potassium hydroxide	1.79E-01	g		g		1.79E-01		
Methanol	8.22E-01	g	1.64E-03	g	1.01E+00	8.20E-02	1.18E-01	3.07E-02
Styrene dibromide	3.94E+00	g	7.88E-03	g	1.62E+00	1.35E-01	1.49E-01	4.90E-02
Heating steam	2.00E-03	MJ						
Electricity	3.33E-04	kWh	1.20E-03	MJ				
Transport lorry	1.00E-04	tkm						
Transport train	6.00E-04	tkm						
Chemicals factory	4.00E-13	unit						

Table S39 *Styrene dibromide – Inventory dataset based on Franke et al. (1960)*

Inputs	Quantity per 1 g of [a]$C_8H_8Br_2$	Unit	Process air emissions		Wastewater treatment emissions (g)			
			Output	Unit	CO_2 to air	Compound to river	COD, BOD to river	TOC, DOC to river
Bromine	6.28E-01	g		g		2.13E-02		
Chloroform	1.32E-01	g	2.65E-04	g	4.38E-02	1.32E-02	4.25E-03	1.33E-03
Styrene	4.78E-01	g	9.56E-04	g	2.50E-01	8.23E-03	2.43E-02	7.59E-03
Heating steam	2.00E-03	MJ						
Electricity	3.33E-04	kWh	1.20E-03	MJ				

[a]*no chemicals factory neither transport because it is assumed produced in the same place for phenylacetylene*

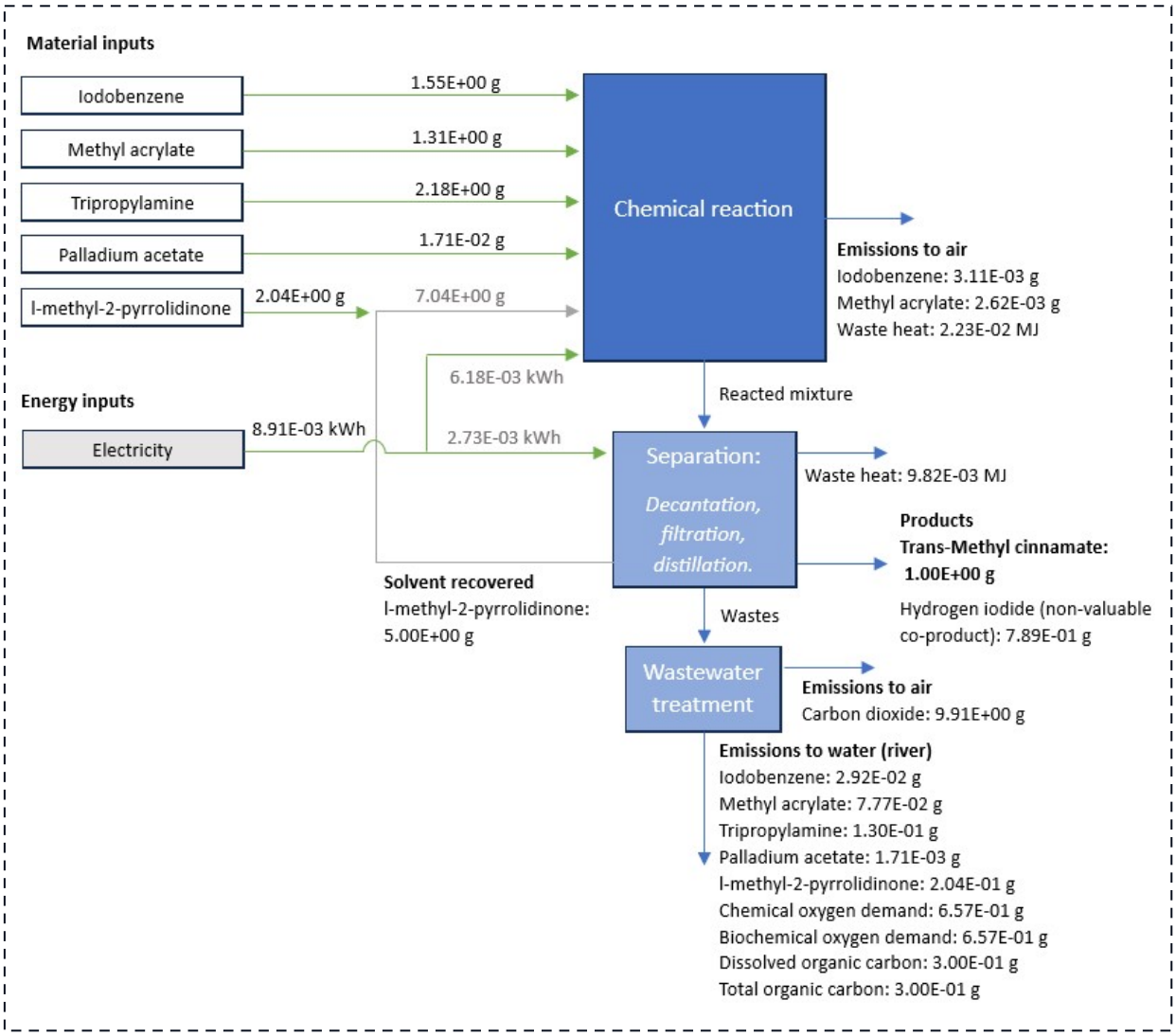

Fig. S1. *Gate-to-gate inventory flows to produce 1 g of Trans-Methyl cinnamate from iodobenzene via Heck protocol. Data based on table S23 and process description on Heck and Nolley (1972)*

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