ELECTRONIC SUPPLEMENTARY INFORMATION (ESI-2)

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

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LCA impacts assessment midpoint results

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Impact assessment and interpretation

The impact assessment was performed using SimaPro 9.1.1.7 software[1] (PRé Consultants 2022). The impact categories were defined considering the most relevant life-cycle environmental aspects in chemicals production:[2,3] global warming potential, ozone formation affecting human health, ozone formation affecting terrestrial ecosystems, terrestrial acidification, freshwater eutrophication, terrestrial ecotoxicity, freshwater ecotoxicity, human carcinogenic toxicity, human non-carcinogenic toxicity, and fossil resource scarcity. Given the usage of iodine and metallic chemicals extracted from ores, the impact category of mineral resource scarcity was also included. For the scope of the present study, the impact assessment method Recipe 2016 was used given that it includes the 11 selected impact categories for this study. Midpoint impact categories and endpoint damage areas (human health, ecosystems, and resources) under the hierarchical perspective were analysed. Long-term emissions, which affect scenarios beyond 100 years, were included due to the usage of organometallic compounds in the evaluated reactions, such as the palladium-based homogeneous catalysts, relevant to the long-term toxicity effects on human health and ecosystems. For example, the impacts on freshwater ecotoxicity of palladium extraction can increase about 20,000% when long-term emissions are included.

Given the important contribution of solvents and catalysts to the total environmental impacts of the halobenzenes and the CCR, respectively, sensitivity analyses were performed by considering higher and completely recovery rates of these compounds.

[1] PRé Consultants. 2022. SimaPro v9. *About SimaPro*. Amersfoort. www.pre.nl/content/simapro-lca-software. Accessed January 16, 2022

[2] Maranghi, S. and C. Brondi. 2020. *Life Cycle Assessment in the Chemical Product Chain*. *Life Cycle Assessment in the Chemical Product Chain*. Siena: Springer

[3] Osorio-Tejada, J., F. Ferlin, L. Vaccaro, and V. Hessel. 2022a. Life cycle assessment of multistep benzoxazole synthesis: from batch to waste-minimised continuous flow systems. *Green Chemistry* 24(1): 325–337

Chlorine-based halobenzenes

Table S1 *Chlorobenzene production – midpoints characterization results, ReCiPe 2016*

Impact category	Unit	Total	Process emissions	Benzene	Chlorine	Sodium hydroxide	Water	Chemicals factory	Electricity
Global warming	kg CO_2 eq	**3.96E+00**	8.31E-01	1.67E+00	3.53E-01	6.81E-01	4.39E-05	5.35E-02	3.66E-01
Ozone formation, human health	kg NO_x eq	**7.75E-03**	5.81E-05	4.29E-03	7.91E-04	1.77E-03	1.02E-07	1.78E-04	6.66E-04
Ozone formation, ecosystems	kg NO_x eq	**8.54E-03**	9.36E-05	5.00E-03	8.00E-04	1.79E-03	1.04E-07	1.82E-04	6.72E-04
Terrestrial acidification	kg SO_2 eq	**1.15E-02**	0.00E+00	5.48E-03	1.52E-03	2.65E-03	3.02E-07	4.93E-04	1.40E-03
Freshwater eutrophication	kg P eq	**1.74E-03**	0.00E+00	6.47E-04	3.09E-04	3.51E-04	1.74E-08	7.93E-05	3.58E-04
Terrestrial ecotoxicity	kg 1,4-DCB	**8.93E+00**	2.48E-03	1.21E+00	1.95E+00	2.79E+00	2.29E-04	2.56E+00	4.08E-01
Freshwater ecotoxicity	kg 1,4-DCB	**1.74E-01**	2.37E-03	2.33E-02	3.65E-02	4.78E-02	3.52E-06	4.77E-02	1.60E-02
Human carcinogenic toxicity	kg 1,4-DCB	**1.59E-01**	1.20E-02	5.88E-02	2.32E-02	3.24E-02	3.39E-06	1.15E-02	2.13E-02
Human non-carcinogenic toxicity	kg 1,4-DCB	**3.62E+00**	1.02E-02	8.91E-01	6.99E-01	9.21E-01	6.43E-05	6.27E-01	4.73E-01
Mineral resource scarcity	kg Cu eq	**8.95E-03**	0.00E+00	5.58E-04	2.04E-03	2.82E-03	3.48E-07	3.06E-03	4.66E-04
Fossil resource scarcity	kg oil eq	**1.64E+00**	0.00E+00	1.27E+00	9.12E-02	1.69E-01	1.21E-05	1.29E-02	9.67E-02

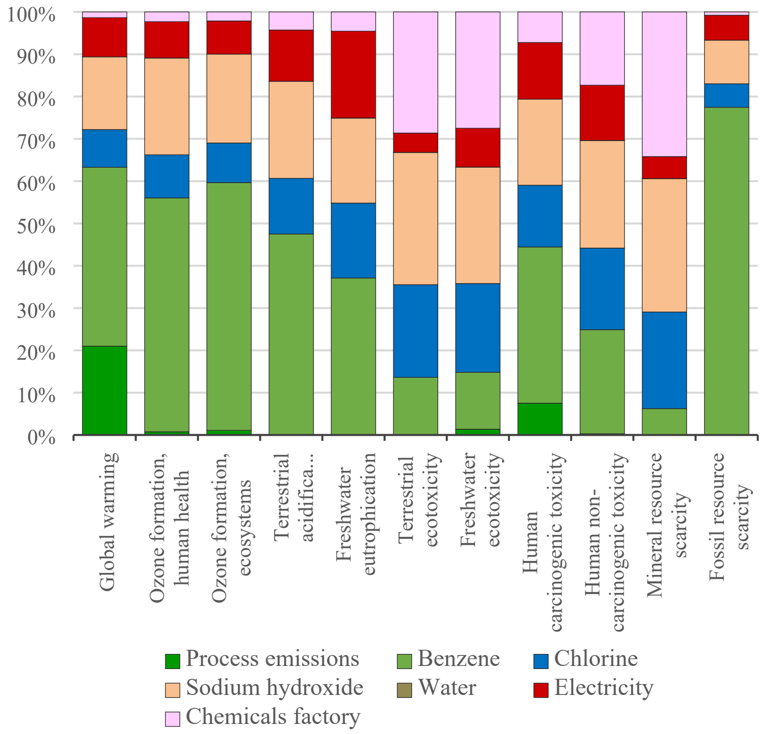

Fig. S1 *Chlorobenzene production – characterization shares - ReCiPe 2016 midpoints*

Table S2 *4-chloroanisole production – midpoints characterization results, ReCiPe 2016*

Impact category	Unit	Total	Process emissions	Anisole	Water	Dichloro-methane	Chemicals factory	Chlorine	Dimethyl sulphide	Sodium bicarbonate	Sodium chloride	Electricity
Global warming	kg CO_2 eq	**9.63E+01**	7.45E+00	6.10E+00	1.38E-03	4.00E+01	5.35E-02	4.97E-01	1.47E+00	5.82E+00	1.37E+00	3.35E+01
Ozone formation, human health	kg NO_x eq	**2.55E-01**	8.27E-04	1.16E-02	3.22E-06	1.58E-01	1.78E-04	1.11E-03	3.30E-03	1.61E-02	3.58E-03	6.09E-02
Ozone formation, ecosystems	kg NO_x eq	**2.59E-01**	1.33E-03	1.22E-02	3.27E-06	1.60E-01	1.82E-04	1.13E-03	3.49E-03	1.63E-02	3.64E-03	6.15E-02
Terrestrial acidification	kg SO_2 eq	**4.23E-01**	0.00E+00	2.37E-02	9.52E-06	1.99E-01	4.92E-04	2.14E-03	9.32E-03	5.19E-02	8.26E-03	1.28E-01
Freshwater eutrophication	kg P eq	**4.54E-03**	0.00E+00	2.51E-04	5.86E-08	2.83E-05	6.96E-06	4.72E-05	4.74E-05	5.26E-04	1.11E-04	3.52E-03
Terrestrial ecotoxicity	kg 1,4-DCB	**1.54E+02**	2.95E-01	2.08E+01	7.17E-03	9.46E+00	2.55E+00	2.71E+00	5.89E+00	5.08E+01	2.82E+01	3.31E+01
Freshwater ecotoxicity	kg 1,4-DCB	**1.95E-01**	1.12E-01	3.37E-02	4.51E-06	2.59E-02	2.30E-04	3.75E-04	2.20E-03	8.13E-03	2.71E-03	1.02E-02
Human carcinogenic toxicity	kg 1,4-DCB	**9.97E-01**	1.98E-01	5.78E-02	2.93E-05	3.88E-01	3.59E-03	5.71E-03	1.01E-02	8.48E-02	4.20E-02	2.07E-01
Human non-carcinogenic toxicity	kg 1,4-DCB	**2.45E+01**	7.42E+00	1.41E+00	6.88E-04	3.17E+00	1.42E-01	2.07E-01	3.70E-01	3.08E+00	1.65E+00	7.03E+00
Mineral resource scarcity	kg Cu eq	**2.36E-01**	0.00E+00	2.09E-02	1.10E-05	5.45E-03	3.06E-03	2.88E-03	6.84E-03	1.20E-01	3.35E-02	4.26E-02
Fossil resource scarcity	kg oil eq	**2.20E+01**	0.00E+00	2.95E+00	3.81E-04	7.41E+00	1.29E-02	1.29E-01	1.09E+00	1.22E+00	3.33E-01	8.85E+00

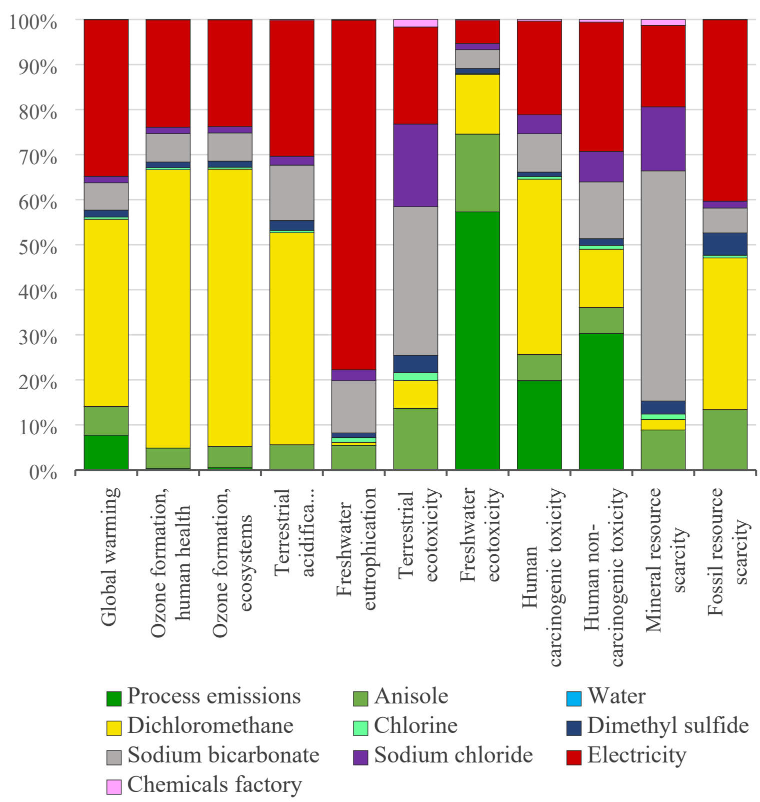

Fig. S2 *4-chloroanisole production – characterization shares - ReCiPe 2016 midpoints*

Table S3 *4-chlorotoluene production – midpoints characterization results, ReCiPe 2016*

Impact category	**Unit**	**Total**	**Process emissions**	**Toluene**	**Dichloro-methane**	**Diethyl ether**	**t-butyl hypochlorite**	**Methanol**	**Chemicals factory**	**Electricity**
Global warming	kg CO_2 eq	**6.65E+01**	1.20E+01	1.21E+00	2.22E+01	1.21E+01	1.91E+00	6.28E-01	5.35E-02	1.65E+01
Ozone formation, human health	kg NO_x eq	**1.56E-01**	4.43E-03	1.86E-03	8.73E-02	2.60E-02	5.30E-03	1.29E-03	1.78E-04	3.00E-02
Ozone formation, ecosystems	kg NO_x eq	**1.65E-01**	7.14E-03	2.02E-03	8.84E-02	3.03E-02	5.54E-03	1.37E-03	1.82E-04	3.02E-02
Terrestrial acidification	kg SO_2 eq	**2.17E-01**	0.00E+00	2.27E-03	1.10E-01	3.03E-02	9.27E-03	1.69E-03	4.92E-04	6.29E-02
Freshwater eutrophication	kg P eq	**5.55E-03**	0.00E+00	5.27E-07	1.57E-05	3.65E-03	1.32E-04	1.65E-05	6.96E-06	1.73E-03
Terrestrial ecotoxicity	kg 1,4-DCB	**6.16E+01**	1.27E-02	7.28E-01	5.24E+00	2.74E+01	8.55E+00	7.60E-01	2.55E+00	1.63E+01
Freshwater ecotoxicity	kg 1,4-DCB	**3.79E-02**	4.16E-03	2.86E-04	1.43E-02	5.04E-03	7.72E-03	1.15E-03	2.30E-04	5.00E-03
Human carcinogenic toxicity	kg 1,4-DCB	**4.30E-01**	1.86E-02	3.62E-03	2.15E-01	6.77E-02	1.77E-02	2.29E-03	3.59E-03	1.02E-01
Human non-carcinogenic toxicity	kg 1,4-DCB	**8.65E+00**	7.17E-01	1.37E-02	1.75E+00	1.68E+00	8.07E-01	8.00E-02	1.42E-01	3.46E+00
Mineral resource scarcity	kg Cu eq	**7.11E-02**	0.00E+00	1.40E-04	3.02E-03	3.29E-02	9.55E-03	1.49E-03	3.06E-03	2.10E-02
Fossil resource scarcity	kg oil eq	**2.06E+01**	0.00E+00	9.92E-01	4.10E+00	9.53E+00	9.43E-01	6.85E-01	1.29E-02	4.35E+00

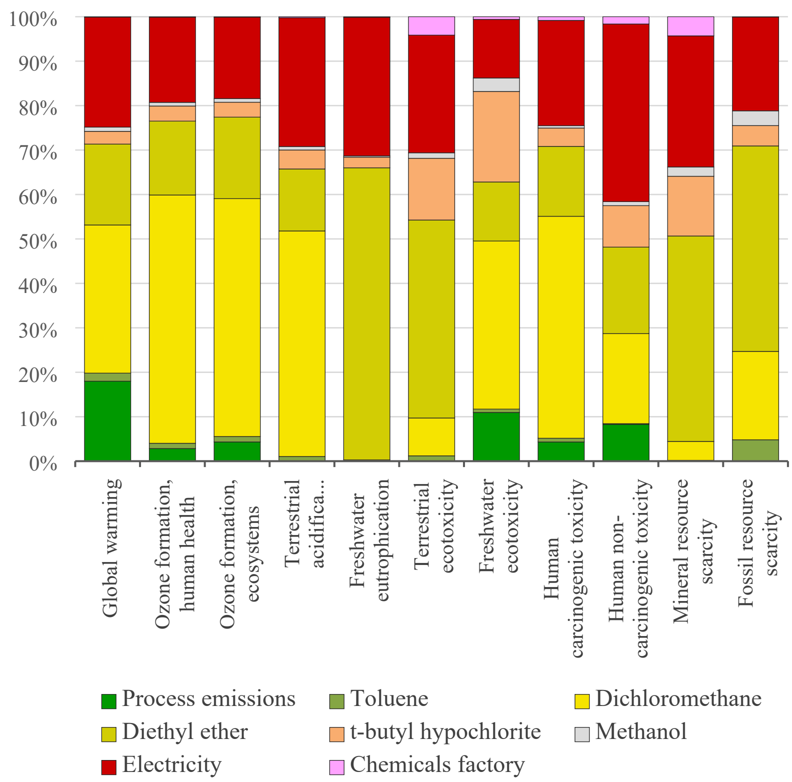

Fig. S3 *4-chlorotoluene production – characterization shares - ReCiPe 2016 midpoints*

Table S4 *4-chloronitrobenzene production – midpoints characterization results, ReCiPe 2016*

Impact category	Unit	Total	Process emissions	Chlorobenzene	Nitric acid	Water	Sodium hydroxide	Chemicals factory	Electricity
Global warming	kg CO_2 eq	**2.33E+01**	2.77E-02	2.88E+00	1.41E+01	5.27E-04	3.38E+00	5.35E-02	2.84E+00
Ozone formation, human health	kg NO_x eq	**4.91E-02**	0.00E+00	5.65E-03	2.93E-02	1.23E-06	8.81E-03	1.78E-04	5.17E-03
Ozone formation, ecosystems	kg NO_x eq	**5.00E-02**	0.00E+00	6.23E-03	2.95E-02	1.25E-06	8.89E-03	1.82E-04	5.21E-03
Terrestrial acidification	kg SO_2 eq	**8.63E-02**	0.00E+00	8.41E-03	5.35E-02	3.63E-06	1.31E-02	4.93E-04	1.08E-02
Freshwater eutrophication	kg P eq	**6.83E-03**	0.00E+00	1.27E-03	9.59E-04	2.09E-07	1.74E-03	7.93E-05	2.78E-03
Terrestrial ecotoxicity	kg 1,4-DCB	**5.31E+01**	2.71E-03	6.51E+00	2.70E+01	2.75E-03	1.38E+01	2.56E+00	3.17E+00
Freshwater ecotoxicity	kg 1,4-DCB	**9.85E-01**	9.81E-04	1.27E-01	4.48E-01	4.23E-05	2.37E-01	4.77E-02	1.24E-01
Human carcinogenic toxicity	kg 1,4-DCB	**5.80E-01**	9.21E-04	1.16E-01	1.26E-01	4.08E-05	1.60E-01	1.15E-02	1.65E-01
Human non-carcinogenic toxicity	kg 1,4-DCB	**2.22E+01**	3.20E-03	2.64E+00	1.07E+01	7.73E-04	4.57E+00	6.27E-01	3.67E+00
Mineral resource scarcity	kg Cu eq	**8.58E-02**	0.00E+00	6.52E-03	5.86E-02	4.18E-06	1.40E-02	3.06E-03	3.62E-03
Fossil resource scarcity	kg oil eq	**4.03E+00**	0.00E+00	1.19E+00	1.23E+00	1.45E-04	8.37E-01	1.29E-02	7.51E-01

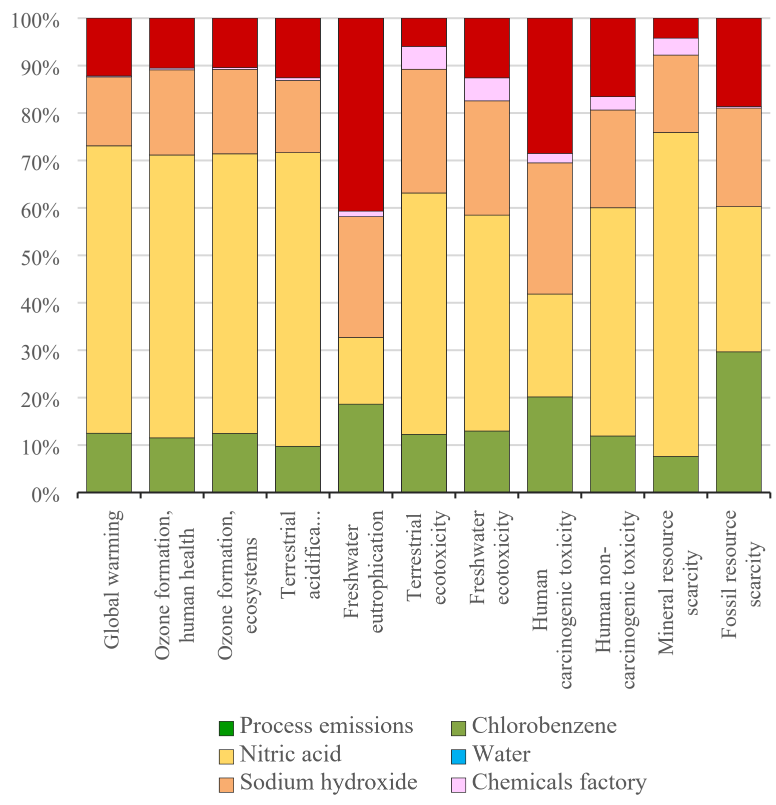

Fig. S4 *4-chloronitrobenzene production – characterization shares - ReCiPe 2016 midpoints*

Bromine-based halobenzenes

Table S5 *Bromobenzene production – midpoints characterization results, ReCiPe 2016*

Impact category	Unit	Total	Process emissions	Benzene	Pyridine	Bromine	Sodium hydroxide	Water	Chemicals factory	Electricity
Global warming	kg CO_2 eq	**1.25E+01**	6.71E-01	1.15E+00	8.77E-05	7.25E+00	1.53E-01	4.46E-04	5.35E-02	3.22E+00
Ozone formation, human health	kg NO_x eq	**1.99E-02**	3.99E-05	2.95E-03	1.80E-07	1.05E-02	3.99E-04	1.04E-06	1.78E-04	5.86E-03
Ozone formation, ecosystems	kg NO_x eq	**2.07E-02**	6.44E-05	3.44E-03	1.94E-07	1.07E-02	4.03E-04	1.05E-06	1.82E-04	5.92E-03
Terrestrial acidification	kg SO_2 eq	**3.75E-02**	0.00E+00	3.77E-03	2.59E-07	2.03E-02	5.94E-04	3.07E-06	4.93E-04	1.23E-02
Freshwater eutrophication	kg P eq	**5.03E-03**	0.00E+00	4.45E-04	1.85E-08	1.27E-03	7.88E-05	1.77E-07	7.93E-05	3.15E-03
Terrestrial ecotoxicity	kg 1,4-DCB	**3.29E+01**	2.04E-03	8.36E-01	2.44E-04	2.53E+01	6.27E-01	2.33E-03	2.56E+00	3.59E+00
Freshwater ecotoxicity	kg 1,4-DCB	**3.85E-01**	1.92E-03	1.61E-02	3.76E-06	1.68E-01	1.07E-02	3.58E-05	4.77E-02	1.40E-01
Human carcinogenic toxicity	kg 1,4-DCB	**3.78E-01**	9.49E-03	4.04E-02	3.04E-06	1.21E-01	7.27E-03	3.45E-05	1.15E-02	1.88E-01
Human non-carcinogenic toxicity	kg 1,4-DCB	**9.42E+00**	8.82E-03	6.13E-01	6.56E-05	3.80E+00	2.07E-01	6.54E-04	6.27E-01	4.16E+00
Mineral resource scarcity	kg Cu eq	**1.92E-02**	0.00E+00	3.84E-04	2.21E-07	1.10E-02	6.34E-04	3.54E-06	3.06E-03	4.10E-03
Fossil resource scarcity	kg oil eq	**3.91E+00**	0.00E+00	8.74E-01	4.23E-05	2.14E+00	3.79E-02	1.23E-04	1.29E-02	8.52E-01

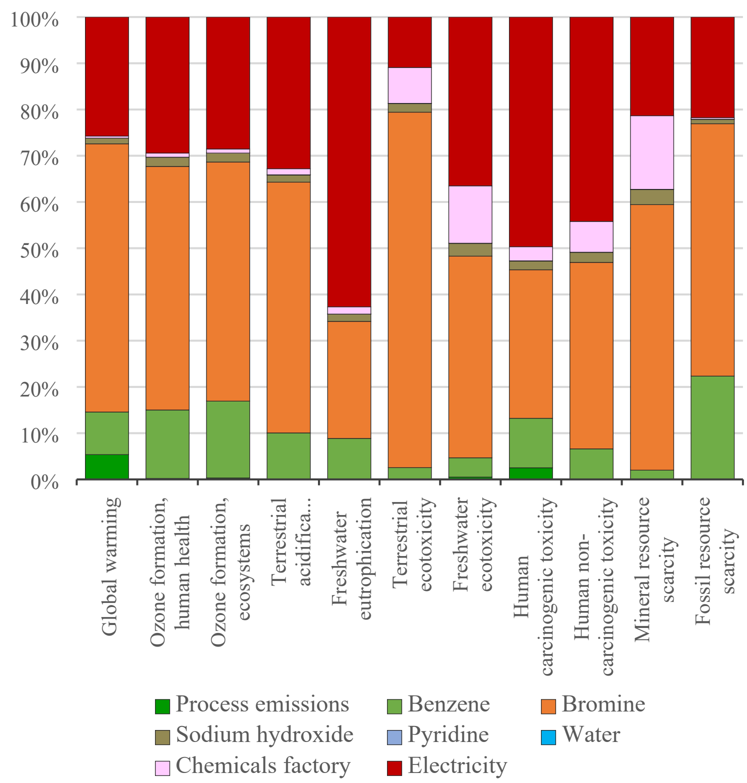

Fig. S5 *Bromobenzene production – characterization shares - ReCiPe 2016 midpoints*

Table S6 *4-Bromoanisole production – midpoints characterization results, ReCiPe 2016*

Impact category	Unit	Total	Process emissions	Anisole	Acetic acid	Bromine	Water	Chemicals factory	Electricity
Global warming	kg CO_2 eq	**1.38E+01**	2.09E-01	3.13E+00	8.93E-01	3.99E+00	4.38E-04	5.35E-02	5.55E+00
Ozone formation, human health	kg NO_x eq	**2.44E-02**	1.19E-04	5.96E-03	2.23E-03	5.78E-03	1.02E-06	1.78E-04	1.01E-02
Ozone formation, ecosystems	kg NO_x eq	**2.51E-02**	1.92E-04	6.27E-03	2.38E-03	5.90E-03	1.04E-06	1.82E-04	1.02E-02
Terrestrial acidification	kg SO_2 eq	**4.83E-02**	0.00E+00	1.21E-02	3.31E-03	1.12E-02	3.01E-06	4.93E-04	2.12E-02
Freshwater eutrophication	kg P eq	**7.66E-03**	0.00E+00	1.16E-03	3.06E-04	7.01E-04	1.74E-07	7.93E-05	5.42E-03
Terrestrial ecotoxicity	kg 1,4-DCB	**3.71E+01**	4.43E-01	1.07E+01	3.27E+00	1.39E+01	2.28E-03	2.56E+00	6.18E+00
Freshwater ecotoxicity	kg 1,4-DCB	**7.39E-01**	1.01E-01	2.01E-01	5.58E-02	9.23E-02	3.52E-05	4.77E-02	2.42E-01
Human carcinogenic toxicity	kg 1,4-DCB	**5.52E-01**	0.00E+00	1.20E-01	3.05E-02	6.68E-02	3.39E-05	1.15E-02	3.23E-01
Human non-carcinogenic toxicity	kg 1,4-DCB	**1.41E+01**	0.00E+00	3.28E+00	9.59E-01	2.09E+00	6.42E-04	6.27E-01	7.16E+00
Mineral resource scarcity	kg Cu eq	**3.02E-02**	0.00E+00	1.07E-02	3.26E-03	6.07E-03	3.47E-06	3.06E-03	7.06E-03
Fossil resource scarcity	kg oil eq	**4.69E+00**	0.00E+00	1.51E+00	5.30E-01	1.18E+00	1.21E-04	1.29E-02	1.47E+00

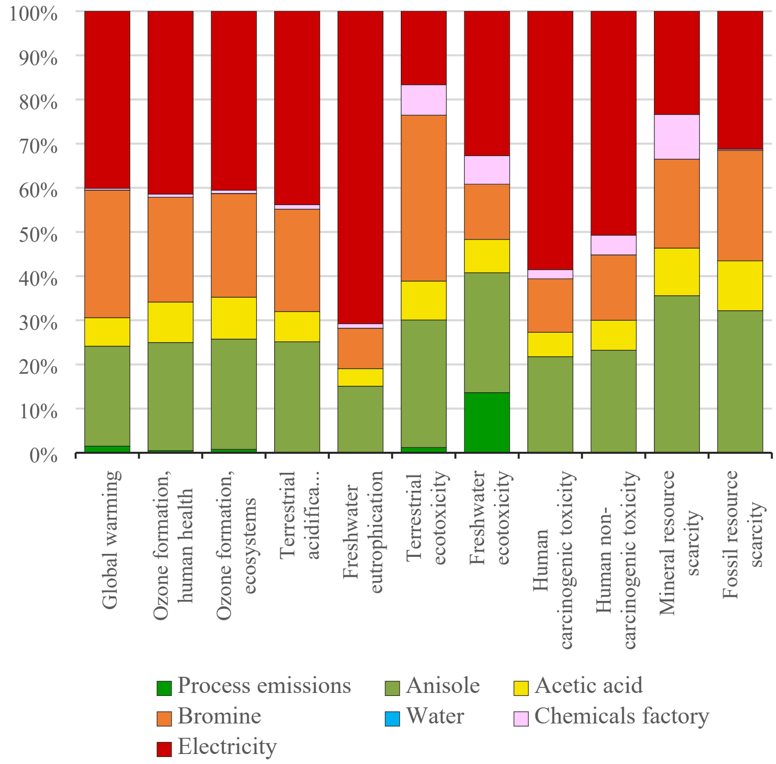

Fig. S6 *4-Bromoanisole production – characterization shares - ReCiPe 2016 midpoints*

Table S7 *4-bromotoluene production – midpoints characterization results, ReCiPe 2016*

Impact	Unit	Total	Process	4-	Water	Sulfuric	Hydrochlo	Sodium	Copper(I)	Sodium	Chemicals	Electricity

category			emissions	toluidine		acid	-ric acid	nitrite	bromide	hydroxide	factory	
Global warming	kg CO_2 eq	**2.19E+01**	6.80E-01	6.21E+00	1.99E-03	2.53E-01	1.64E+00	1.69E+00	2.99E+00	1.33E+00	5.35E-02	7.02E+00
Ozone formation, human health	kg NO_x eq	**6.67E-02**	0.00E+00	1.19E-02	4.62E-06	1.92E-03	3.95E-03	4.46E-03	2.80E-02	3.47E-03	1.78E-04	1.28E-02
Ozone formation, ecosystems	kg NO_x eq	**6.80E-02**	0.00E+00	1.24E-02	4.70E-06	1.96E-03	4.02E-03	4.51E-03	2.85E-02	3.50E-03	1.82E-04	1.29E-02
Terrestrial acidification	kg SO_2 eq	**2.55E-01**	0.00E+00	1.82E-02	1.37E-05	1.88E-02	1.07E-02	6.83E-03	1.68E-01	5.17E-03	4.93E-04	2.68E-02
Freshwater eutrophication	kg P eq	**3.69E-02**	0.00E+00	1.02E-03	7.89E-07	1.45E-04	1.28E-03	6.85E-04	2.61E-02	6.85E-04	7.93E-05	6.86E-03
Terrestrial ecotoxicity	kg 1,4-DCB	**1.27E+03**	4.86E-02	1.71E+01	1.04E-02	7.99E+00	1.35E+01	8.16E+00	1.20E+03	5.45E+00	2.56E+00	7.82E+00
Freshwater ecotoxicity	kg 1,4-DCB	**2.35E+01**	1.75E-01	2.47E-01	1.59E-04	7.44E-02	2.35E-01	1.11E-01	2.22E+01	9.34E-02	4.77E-02	3.06E-01
Human carcinogenic toxicity	kg 1,4-DCB	**2.12E+00**	0.00E+00	1.29E-01	1.54E-04	2.06E-02	1.11E-01	6.41E-02	1.31E+00	6.32E-02	1.15E-02	4.09E-01
Human non-carcinogenic toxicity	kg 1,4-DCB	**2.93E+02**	0.00E+00	4.45E+00	2.91E-03	1.27E+00	3.95E+00	1.99E+00	2.70E+02	1.80E+00	6.27E-01	9.06E+00
Mineral resource scarcity	kg Cu eq	**5.31E-01**	0.00E+00	1.85E-02	1.58E-05	5.41E-03	1.42E-02	6.68E-03	4.68E-01	5.51E-03	3.06E-03	8.93E-03
Fossil resource scarcity	kg oil eq	**6.74E+00**	0.00E+00	2.54E+00	5.47E-04	2.27E-01	5.14E-01	4.99E-01	7.65E-01	3.30E-01	1.29E-02	1.85E+00

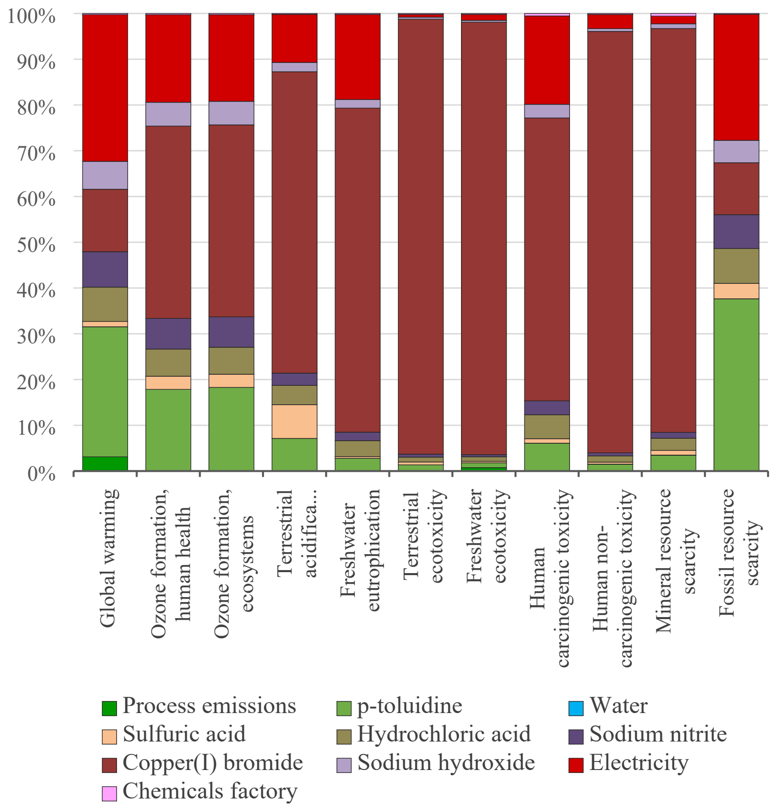

Fig. S7 *4-bromotoluene production – characterization shares - ReCiPe 2016 midpoints*

Table S8 *4-bromonitrobenzene production – midpoints characterization results, ReCiPe 2016*

Impact category	Unit	Total	Process emissions	Bromo-benzene	Nitric acid	Sulfuric acid	Water	Ethanol	Sodium hydroxide	Chemicals factory	Electricity
Global warming	kg CO_2 eq	**4.32E+01**	3.35E+00	1.43E+01	6.53E+00	2.97E-01	3.02E-03	2.03E+00	4.32E+00	5.35E-02	1.24E+01
Ozone formation, human health	kg NO_x eq	**7.70E-02**	0.00E+00	2.27E-02	1.35E-02	2.25E-03	7.02E-06	4.51E-03	1.13E-02	1.78E-04	2.25E-02
Ozone formation, ecosystems	kg NO_x eq	**7.91E-02**	0.00E+00	2.36E-02	1.36E-02	2.29E-03	7.14E-06	5.22E-03	1.14E-02	1.82E-04	2.28E-02
Terrestrial acidification	kg SO_2 eq	**1.59E-01**	0.00E+00	4.28E-02	2.47E-02	2.21E-02	2.08E-05	5.12E-03	1.68E-02	4.93E-04	4.73E-02
Freshwater eutrophication	kg P eq	**2.16E-02**	0.00E+00	5.73E-03	4.44E-04	1.70E-04	1.20E-06	8.07E-04	2.23E-03	7.93E-05	1.21E-02
Terrestrial ecotoxicity	kg 1,4-DCB	**9.89E+01**	1.50E-01	3.75E+01	1.25E+01	9.37E+00	1.57E-02	5.20E+00	1.77E+01	2.56E+00	1.38E+01
Freshwater ecotoxicity	kg 1,4-DCB	**1.81E+00**	9.65E-02	4.39E-01	2.07E-01	8.73E-02	2.42E-04	8.49E-02	3.04E-01	4.77E-02	5.40E-01
Human carcinogenic toxicity	kg 1,4-DCB	**1.50E+00**	1.94E-04	4.31E-01	5.82E-02	2.42E-02	2.33E-04	4.45E-02	2.05E-01	1.15E-02	7.22E-01
Human non-carcinogenic toxicity	kg 1,4-DCB	**4.09E+01**	0.00E+00	1.07E+01	4.94E+00	1.50E+00	4.43E-03	1.24E+00	5.85E+00	6.27E-01	1.60E+01
Mineral resource scarcity	kg Cu eq	**9.77E-02**	0.00E+00	2.19E-02	2.71E-02	6.34E-03	2.39E-05	5.57E-03	1.79E-02	3.06E-03	1.58E-02
Fossil resource scarcity	kg oil eq	**1.12E+01**	0.00E+00	4.46E+00	5.70E-01	2.66E-01	8.31E-04	1.59E+00	1.07E+00	1.29E-02	3.28E+00

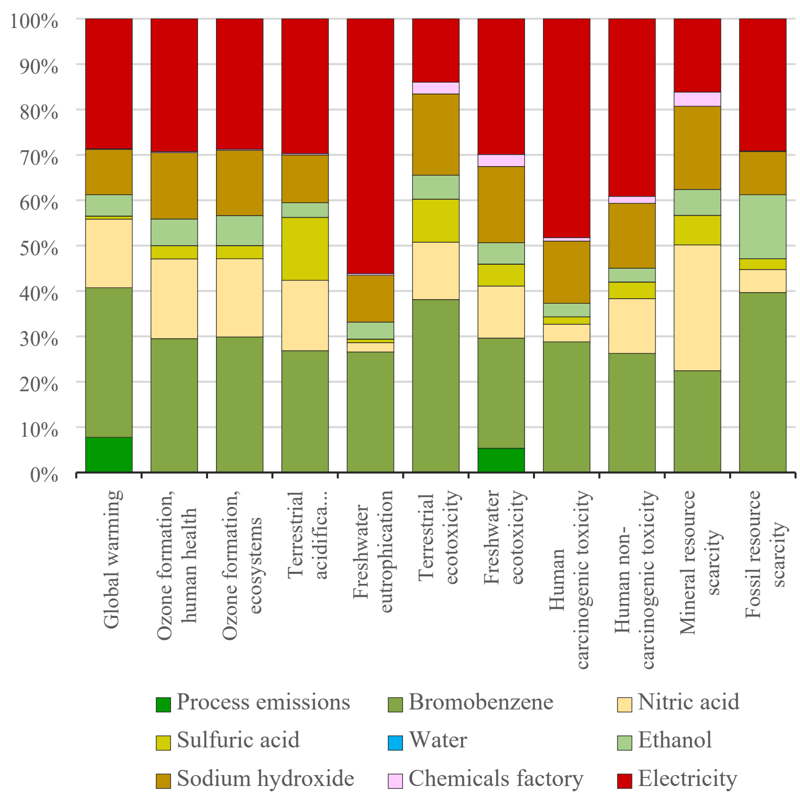

Fig. S8 *4-bromonitrobenzene production – characterization shares - ReCiPe 2016 midpoints*

Iodine-based halobenzenes

Table S9 *Iodobenzene production – midpoints characterization results, ReCiPe 2016*

Impact category	Unit	Total	Process emissions	Benzene	Iodine	Nitric acid	Sodium hydroxide	Water	Hydrochloric acid	Chemicals factory	Electricity
Global warming	kg CO_2 eq	**9.74E+00**	7.33E-01	1.04E+00	2.52E+00	1.64E+00	4.73E-01	1.68E-05	1.57E-02	5.35E-02	3.26E+00
Ozone formation, human health	kg NO_x eq	**1.72E-02**	3.62E-05	2.67E-03	3.75E-03	3.40E-03	1.23E-03	3.90E-08	3.78E-05	1.78E-04	5.93E-03
Ozone formation, ecosystems	kg NO_x eq	**1.79E-02**	5.83E-05	3.12E-03	3.83E-03	3.43E-03	1.25E-03	3.96E-08	3.84E-05	1.82E-04	5.98E-03
Terrestrial acidification	kg SO_2 eq	**3.15E-02**	0.00E+00	3.41E-03	6.94E-03	6.22E-03	1.84E-03	1.15E-07	1.02E-04	4.93E-04	1.25E-02
Freshwater eutrophication	kg P eq	**4.48E-03**	0.00E+00	4.03E-04	4.39E-04	1.12E-04	2.44E-04	6.66E-09	1.22E-05	7.93E-05	3.19E-03
Terrestrial ecotoxicity	kg 1,4-DCB	**2.10E+01**	2.16E-03	7.57E-01	8.86E+00	3.14E+00	1.94E+00	8.74E-05	1.29E-01	2.56E+00	3.64E+00
Freshwater ecotoxicity	kg 1,4-DCB	**3.51E-01**	2.09E-03	1.45E-02	5.67E-02	5.21E-02	3.33E-02	1.35E-06	2.25E-03	4.77E-02	1.42E-01
Human carcinogenic toxicity	kg 1,4-DCB	**3.28E-01**	9.97E-03	3.66E-02	4.22E-02	1.46E-02	2.25E-02	1.30E-06	1.06E-03	1.15E-02	1.90E-01
Human non-carcinogenic toxicity	kg 1,4-DCB	**8.62E+00**	8.47E-03	5.55E-01	1.29E+00	1.24E+00	6.41E-01	2.46E-05	3.78E-02	6.27E-01	4.21E+00
Mineral resource scarcity	kg Cu eq	**3.37E+00**	0.00E+00	3.48E-04	3.35E+00	6.81E-03	1.96E-03	1.33E-07	1.36E-04	3.06E-03	4.15E-03
Fossil resource scarcity	kg oil eq	**2.67E+00**	0.00E+00	7.91E-01	7.39E-01	1.43E-01	1.17E-01	4.61E-06	4.91E-03	1.29E-02	8.62E-01

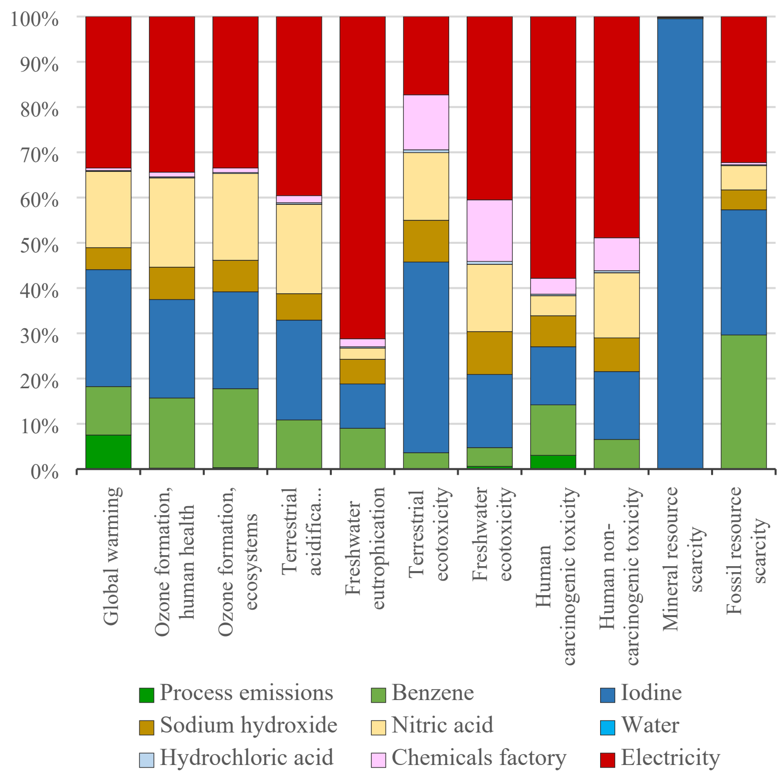

Fig. S9 *Iodobenzene production – characterization shares - ReCiPe 2016 midpoints*

Table S10 *4-iodoanisole production – midpoints characterization results, ReCiPe 2016*

Impact category	Unit	Total	Process emissions	Anisole	Hydrogen peroxide	Water	Iodine	Ethanol	Sulfuric acid	Diethyl ether	Sodium hydro-xide	Chemicals factory	Electricity
Global warming	kg CO_2 eq	**3.35E+01**	9.17E+00	3.75E+00	5.01E-01	3.19E-04	3.65E+00	3.32E+00	2.02E-02	7.54E+00	5.65E-02	5.35E-02	5.46E+00
Ozone formation, h. health	kg NO_x eq	**5.20E-02**	4.58E-03	7.15E-03	8.25E-04	7.41E-07	5.45E-03	7.37E-03	1.54E-04	1.62E-02	1.47E-04	1.78E-04	9.93E-03
Ozone formation, ecosystems	kg NO_x eq	**5.93E-02**	7.40E-03	7.52E-03	8.77E-04	7.53E-07	5.56E-03	8.53E-03	1.56E-04	1.89E-02	1.49E-04	1.82E-04	1.00E-02
Terrestrial acidification	kg SO_2 eq	**7.64E-02**	0.00E+00	1.46E-02	1.39E-03	2.19E-06	1.01E-02	8.37E-03	1.51E-03	1.89E-02	2.20E-04	4.93E-04	2.09E-02
Freshwater eutrophic-cation	kg P eq	**1.20E-02**	0.00E+00	1.39E-03	1.86E-04	1.27E-07	6.37E-04	1.32E-03	1.16E-05	3.04E-03	2.91E-05	7.93E-05	5.34E-03
Terrestrial ecotoxicity	kg 1,4-DCB	**6.28E+01**	8.55E-02	1.28E+01	1.84E+00	1.66E-03	1.29E+01	8.50E+00	6.39E-01	1.71E+01	2.32E-01	2.56E+00	6.09E+00
Freshwater ecotoxicity	kg 1,4-DCB	**1.15E+00**	2.85E-02	2.41E-01	4.29E-02	2.56E-05	8.23E-02	1.39E-01	5.96E-03	3.17E-01	3.97E-03	4.77E-02	2.38E-01
Human carcinogenic toxicity	kg 1,4-DCB	**8.50E-01**	5.05E-04	1.44E-01	7.31E-02	2.46E-05	6.12E-02	7.28E-02	1.65E-03	1.64E-01	2.69E-03	1.15E-02	3.18E-01
Human non-carcinogenic toxicity	kg 1,4-DCB	**2.11E+01**	3.28E-03	3.93E+00	7.82E-01	4.67E-04	1.88E+00	2.03E+00	1.02E-01	4.59E+00	7.65E-02	6.27E-01	7.06E+00
Mineral resource scarcity	kg Cu eq	**4.92E+00**	0.00E+00	1.29E-02	2.17E-03	2.53E-06	4.86E+00	9.10E-03	4.32E-04	2.05E-02	2.34E-04	3.06E-03	6.95E-03
Fossil resource scarcity	kg oil eq	**1.31E+01**	0.00E+00	1.81E+00	1.76E-01	8.77E-05	1.07E+00	2.59E+00	1.81E-02	5.94E+00	1.40E-02	1.29E-02	1.44E+00

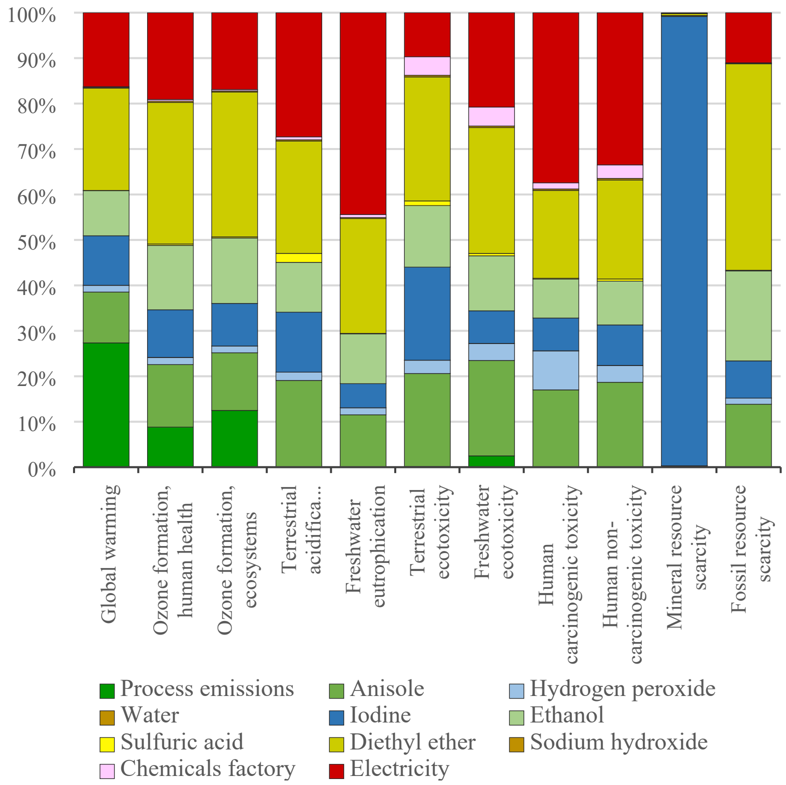

Fig. S10 *4-iodoanisole production – characterization shares - ReCiPe 2016 midpoints*

***Table S11** 4-iodotoluene production – midpoints characterization results, ReCiPe 2016*

Impact category	Unit	Total	Process emissions	4-toluidine	Water	Hydro-chloric acid	Sodium nitrite	Pota-ssium iodide	Sodium sulfite	Sodium hydroxide	Ethanol	Chemicals factory	Electricity
Global warming	kg CO_2 eq	**1.82E+01**	8.29E-01	3.76E+00	5.72E-04	9.93E-01	1.07E+00	6.08E+00	5.95E-02	7.96E-01	5.13E-01	5.35E-02	4.04E+00
Ozone formation, h. health	kg NO_x eq	**3.70E-02**	3.49E-03	7.20E-03	1.33E-06	2.39E-03	2.83E-03	1.02E-02	1.43E-04	2.08E-03	1.14E-03	1.78E-04	7.34E-03
Ozone formation, ecosystems	kg NO_x eq	**4.00E-02**	5.65E-03	7.52E-03	1.35E-06	2.43E-03	2.86E-03	1.04E-02	1.45E-04	2.10E-03	1.32E-03	1.82E-04	7.41E-03
Terrestrial acidification	kg SO_2 eq	**6.16E-02**	0.00E+00	1.10E-02	3.94E-06	6.48E-03	4.33E-03	1.81E-02	1.39E-03	3.09E-03	1.29E-03	4.93E-04	1.54E-02
Freshwater eutrophic-cation	kg P eq	**7.99E-03**	0.00E+00	6.20E-04	2.27E-07	7.75E-04	4.34E-04	1.48E-03	3.49E-05	4.10E-04	2.04E-04	7.93E-05	3.95E-03
Terrestrial ecotoxicity	kg 1,4-DCB	**5.97E+01**	8.78E-02	1.03E+01	2.98E-03	8.18E+00	5.18E+00	2.40E+01	3.49E-01	3.27E+00	1.31E+00	2.56E+00	4.50E+00
Freshwater ecotoxicity	kg 1,4-DCB	**1.23E+00**	3.15E-01	1.50E-01	4.59E-05	1.42E-01	7.04E-02	2.41E-01	6.09E-03	5.60E-02	2.14E-02	4.77E-02	1.76E-01
Human carcinogenic toxicity	kg 1,4-DCB	**6.29E-01**	3.36E-04	7.79E-02	4.42E-05	6.71E-02	4.07E-02	1.43E-01	3.18E-03	3.78E-02	1.12E-02	1.15E-02	2.35E-01
Human non-carcinogenic toxicity	kg 1,4-DCB	**1.83E+01**	0.00E+00	2.69E+00	8.39E-04	2.39E+00	1.26E+00	4.59E+00	1.05E-01	1.08E+00	3.13E-01	6.27E-01	5.22E+00
Mineral resource scarcity	kg Cu eq	**6.42E+00**	0.00E+00	1.12E-02	4.54E-06	8.60E-03	4.24E-03	6.38E+00	3.81E-04	3.30E-03	1.41E-03	3.06E-03	5.14E-03
Fossil resource scarcity	kg oil eq	**5.62E+00**	0.00E+00	1.53E+00	1.57E-04	3.11E-01	3.16E-01	1.76E+00	1.97E-02	1.97E-01	4.00E-01	1.29E-02	1.07E+00

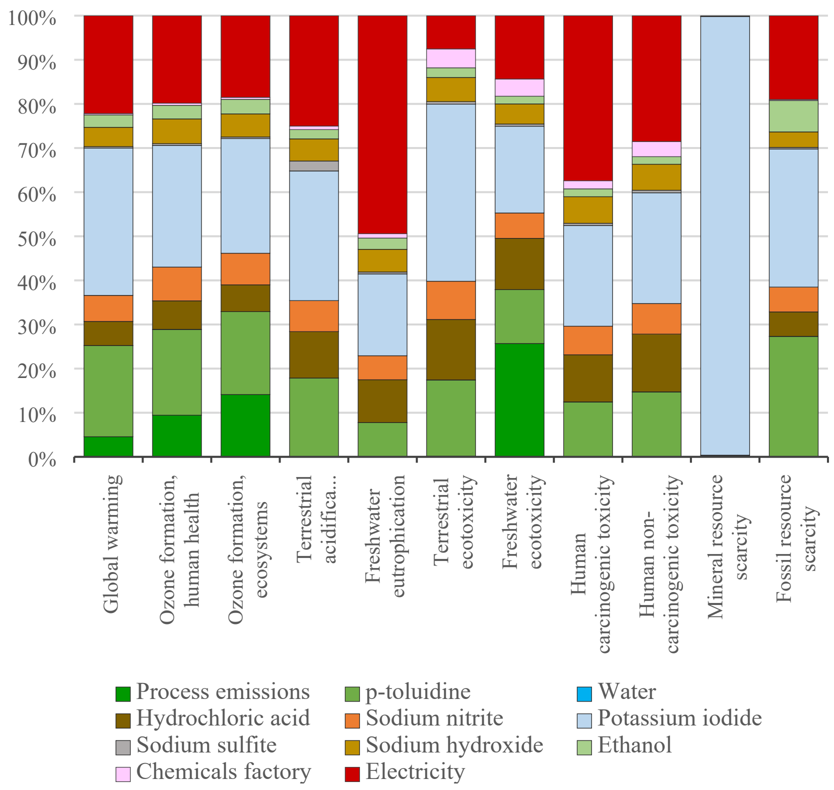

Fig. S11 *4-iodotoluene production – characterization shares - ReCiPe 2016 midpoints*

Table S12 *4-iodonitrobenzene production – midpoints characterization results, ReCiPe 2016*

Impact category	**Unit**	**Total**	**Process emissions**	**p-nitroani-line**	**Water**	**Sulfuric acid**	**Sodium nitrite**	**Potassium iodide**	**Ethanol**	**Sodium hydroxide**	**Chemicals factory**	**Electricity**
Global warming	kg CO_2 eq	**3.77E+01**	7.06E-01	1.89E+01	1.51E-03	1.16E-01	9.93E-01	9.46E+00	3.52E-01	6.87E-01	5.35E-02	6.49E+00
Ozone formation, human health	kg NO_x eq	**8.31E-02**	2.40E-04	4.86E-02	3.50E-06	8.79E-04	2.62E-03	1.59E-02	7.81E-04	1.79E-03	1.78E-04	1.21E-02
Ozone formation, ecosystems	kg NO_x eq	**8.54E-02**	3.88E-04	5.01E-02	3.56E-06	8.95E-04	2.65E-03	1.62E-02	9.04E-04	1.81E-03	1.82E-04	1.22E-02
Terrestrial acidification	kg SO_2 eq	**2.28E-01**	0.00E+00	1.57E-01	1.04E-05	8.62E-03	4.01E-03	2.82E-02	8.87E-04	2.67E-03	4.93E-04	2.61E-02
Freshwater eutrophication	kg P eq	**1.63E-02**	0.00E+00	6.54E-03	5.98E-07	6.62E-05	4.02E-04	2.31E-03	1.40E-04	3.54E-04	7.93E-05	6.46E-03
Terrestrial ecotoxicity	kg 1,4-DCB	**1.72E+02**	1.97E+00	1.01E+02	7.85E-03	3.66E+00	4.79E+00	3.73E+01	9.01E-01	2.82E+00	2.56E+00	1.70E+01
Freshwater ecotoxicity	kg 1,4-DCB	**2.83E+00**	8.07E-02	1.44E+00	1.21E-04	3.41E-02	6.51E-02	3.75E-01	1.47E-02	4.83E-02	4.77E-02	7.29E-01
Human carcinogenic toxicity	kg 1,4-DCB	**1.44E+00**	5.35E-05	6.90E-01	1.16E-04	9.43E-03	3.76E-02	2.23E-01	7.71E-03	3.27E-02	1.15E-02	4.27E-01
Human non-carcinogenic toxicity	kg 1,4-DCB	**4.69E+01**	0.00E+00	2.59E+01	2.21E-03	5.84E-01	1.17E+00	7.15E+00	2.15E-01	9.30E-01	6.27E-01	1.03E+01
Mineral resource scarcity	kg Cu eq	**1.01E+01**	0.00E+00	1.14E-01	1.19E-05	2.47E-03	3.92E-03	9.93E+00	9.65E-04	2.85E-03	3.06E-03	1.35E-02
Fossil resource scarcity	kg oil eq	**1.11E+01**	0.00E+00	5.83E+00	4.14E-04	1.04E-01	2.92E-01	2.74E+00	2.75E-01	1.70E-01	1.29E-02	1.71E+00

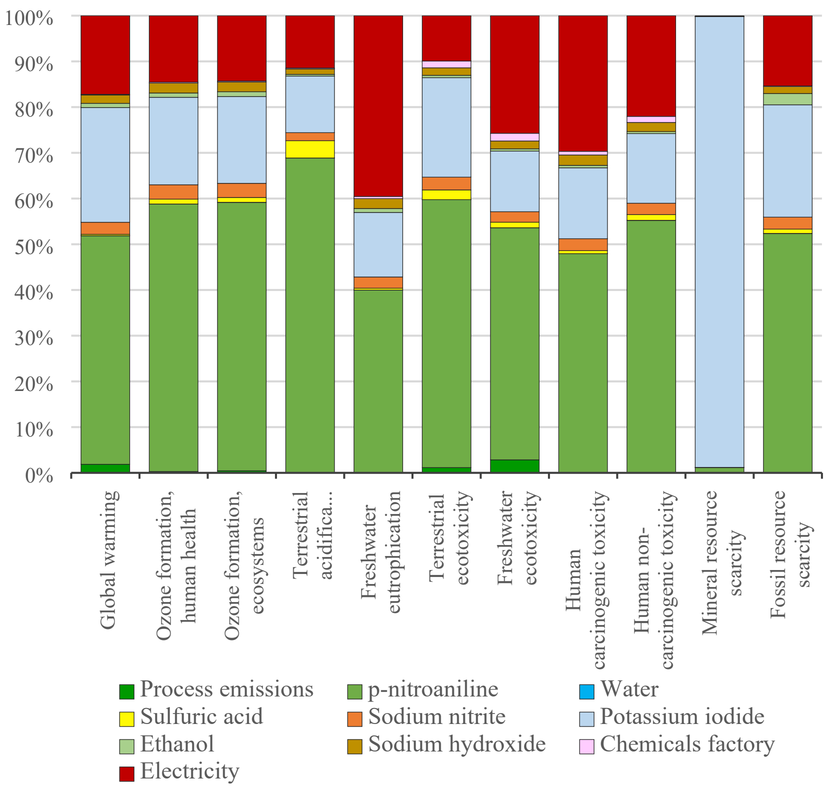

Fig. S12 *4-iodonitrobenzene production – characterization shares - ReCiPe 2016 midpoints*

Palladium-based catalysts

Table S13 *Palladium acetate production – midpoints characterization results, ReCiPe 2016*

Impact category	Unit	Total	Process emissions	Palladium	Acetic acid	Nitric acid	Chemicals factory	Sodium hydroxide	Electricity
Global warming	kg CO_2 eq	**5.96E+00**	1.38E-03	5.94E+00	1.77E-02	1.22E-04	5.35E-05	2.94E-05	1.21E-03
Ozone formation, human health	kg NO_x eq	**7.69E-02**	6.85E-07	7.69E-02	4.42E-05	2.30E-07	1.78E-07	7.75E-08	2.20E-06
Ozone formation, ecosystems	kg NO_x eq	**7.86E-02**	1.10E-06	7.86E-02	4.71E-05	2.31E-07	1.82E-07	7.83E-08	2.22E-06
Terrestrial acidification	kg SO_2 eq	**8.55E-01**	0.00E+00	8.55E-01	6.55E-05	4.21E-07	4.93E-07	1.27E-07	4.62E-06
Freshwater eutrophication	kg P eq	**7.00E-03**	0.00E+00	6.99E-03	6.04E-06	9.49E-09	7.93E-08	1.51E-08	1.18E-06
Terrestrial ecotoxicity	kg 1,4-DCB	**2.61E+01**	1.83E-03	2.60E+01	6.46E-02	2.10E-04	2.56E-03	1.33E-04	1.35E-03
Freshwater ecotoxicity	kg 1,4-DCB	**2.90E+00**	1.85E-05	2.90E+00	1.10E-03	1.46E-06	4.77E-05	2.27E-06	5.28E-05
Human carcinogenic toxicity	kg 1,4-DCB	**7.83E-01**	0.00E+00	7.82E-01	6.03E-04	1.04E-06	1.15E-05	1.42E-06	7.05E-05
Human non-carcinogenic toxicity	kg 1,4-DCB	**1.19E+02**	0.00E+00	1.19E+02	1.90E-02	6.83E-05	6.27E-04	4.28E-05	1.56E-03
Mineral resource scarcity	kg Cu eq	**9.99E-01**	0.00E+00	9.99E-01	6.44E-05	4.74E-07	3.06E-06	1.63E-07	1.54E-06
Fossil resource scarcity	kg oil eq	**1.92E+00**	0.00E+00	1.91E+00	1.05E-02	1.09E-05	1.29E-05	7.20E-06	3.20E-04

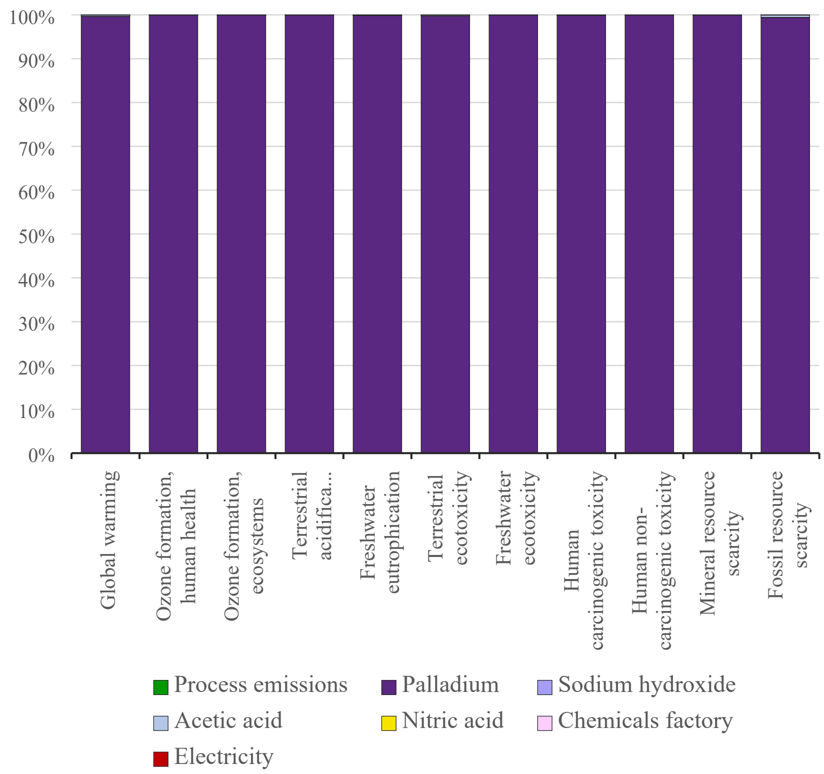

Fig. S13 *Palladium acetate production – characterization shares - ReCiPe 2016 midpoints*

__Table S14__ Palladium tetrakis production – midpoints characterization results, ReCiPe 2016

Impact category	Unit	Total	Process emissions	Palladium dichloride	Triphenylp-hosphine	Dimethyl sulfoxide	Hydrazine	Ethanol	Chemicals factory	Diethyl ether	Electricity
Global warming	kg CO_2 eq	**1.21E+00**	5.31E-03	1.18E+00	1.24E-02	5.15E-03	2.19E-03	2.89E-04	5.35E-05	1.06E-03	4.24E-03
Ozone formation, human health	kg NO_x eq	**1.53E-02**	4.05E-07	1.52E-02	2.61E-05	1.17E-05	4.75E-06	6.62E-07	1.78E-07	2.61E-06	7.72E-06
Ozone formation, ecosystems	kg NO_x eq	**1.56E-02**	6.54E-07	1.55E-02	2.77E-05	1.23E-05	4.82E-06	7.57E-07	1.82E-07	2.84E-06	7.79E-06
Terrestrial acidification	kg SO_2 eq	**1.69E-01**	0.00E+00	1.69E-01	3.93E-05	3.33E-05	9.37E-06	7.90E-07	4.93E-07	5.66E-06	1.62E-05
Freshwater eutrophication	kg P eq	**1.40E-03**	0.00E+00	1.38E-03	1.46E-05	1.47E-06	1.11E-06	1.15E-07	7.93E-08	5.19E-07	4.15E-06
Terrestrial ecotoxicity	kg 1,4-DCB	**5.39E+00**	3.21E-02	5.14E+00	3.49E-02	2.17E-02	1.51E-01	5.79E-04	2.56E-03	4.82E-03	4.73E-03
Freshwater ecotoxicity	kg 1,4-DCB	**5.78E-01**	7.08E-04	5.74E-01	6.65E-04	3.98E-04	1.44E-03	4.54E-06	4.77E-05	3.45E-05	1.85E-04
Human carcinogenic toxicity	kg 1,4-DCB	**1.57E-01**	9.15E-04	1.55E-01	5.22E-04	1.66E-04	1.01E-04	6.76E-06	1.15E-05	3.85E-05	2.47E-04
Human non-carcinogenic toxicity	kg 1,4-DCB	**2.36E+01**	3.13E-07	2.36E+01	1.31E-02	6.05E-03	3.29E-03	2.03E-04	6.27E-04	1.56E-03	5.48E-03
Mineral resource scarcity	kg Cu eq	**1.98E-01**	0.00E+00	1.98E-01	1.72E-04	2.69E-05	1.15E-05	5.83E-07	3.06E-06	3.70E-06	5.40E-06
Fossil resource scarcity	kg oil eq	**3.89E-01**	0.00E+00	3.78E-01	4.32E-03	3.92E-03	6.47E-04	2.12E-04	1.29E-05	5.78E-04	1.12E-03

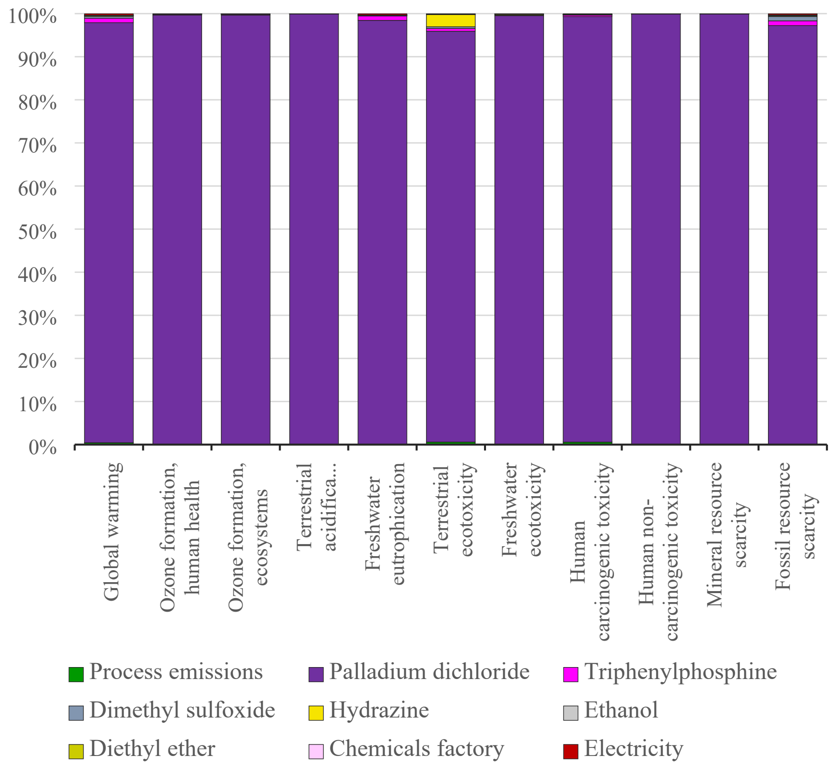

Fig. S14 *Palladium tetrakis production – characterization shares - ReCiPe 2016 midpoints*

Ligand

Table S15 *Triphenylphosphine production – midpoints characterization results, ReCiPe 2016*

Impact category	Unit	Total	Process emissions	Phosphorus trichloride	Chlorobenzene	Sodium	Chemicals factory	Electricity	Heat
Global warming	kg CO_2 eq	**9.94E+00**	2.96E-01	2.54E+00	5.66E+00	1.15E+00	5.35E-02	1.42E-01	1.04E-01
Ozone formation, human health	kg NO_x eq	**2.08E-02**	0.00E+00	6.40E-03	1.11E-02	2.77E-03	1.78E-04	2.65E-04	7.47E-05
Ozone formation, ecosystems	kg NO_x eq	**2.20E-02**	0.00E+00	6.46E-03	1.22E-02	2.81E-03	1.82E-04	2.67E-04	7.74E-05
Terrestrial acidification	kg SO_2 eq	**3.15E-02**	0.00E+00	9.61E-03	1.65E-02	4.31E-03	4.93E-04	5.71E-04	5.81E-05
Freshwater eutrophication	kg P eq	**1.18E-02**	0.00E+00	8.53E-03	2.49E-03	5.02E-04	7.93E-05	1.42E-04	1.34E-06
Terrestrial ecotoxicity	kg 1,4-DCB	**2.78E+01**	1.29E-02	5.87E+00	1.28E+01	6.20E+00	2.56E+00	3.73E-01	1.17E-02
Freshwater ecotoxicity	kg 1,4-DCB	**5.35E-01**	1.05E-02	1.24E-01	2.48E-01	8.85E-02	4.77E-02	1.60E-02	2.42E-04
Human carcinogenic toxicity	kg 1,4-DCB	**4.19E-01**	2.03E-03	1.18E-01	2.28E-01	4.95E-02	1.15E-02	9.36E-03	3.54E-04
Human non-carcinogenic toxicity	kg 1,4-DCB	**1.05E+01**	7.07E-03	2.86E+00	5.18E+00	1.59E+00	6.27E-01	2.26E-01	3.88E-03
Mineral resource scarcity	kg Cu eq	**1.38E-01**	0.00E+00	1.17E-01	1.28E-02	5.49E-03	3.06E-03	2.95E-04	2.98E-05
Fossil resource scarcity	kg oil eq	**3.47E+00**	0.00E+00	7.31E-01	2.34E+00	3.03E-01	1.29E-02	3.75E-02	4.05E-02

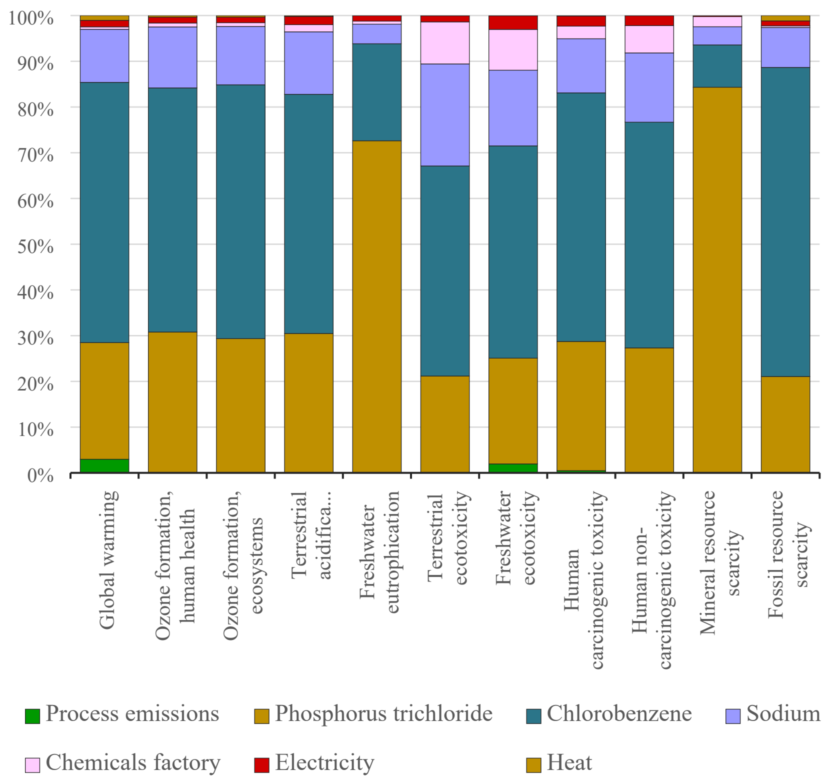

Fig. S15 *Triphenylphosphine production – characterization shares - ReCiPe 2016 midpoints*

Cross-coupling reactions protocols

Table S16 *Biphenyl production via the standard Suzuki protocol using bromobenzene – midpoints characterization results, ReCiPe 2016*

Impact category	Unit	Total	Process emissions	Bromobenzene	Benzene	Sodium hydroxide	Water	Palladium tetrakis	Phenylboronic acid	Hydrogen peroxide	Chemicals factory	Electricity
Global warming	kg CO_2 eq	**4.92E+02**	1.51E+01	1.68E+01	9.08E+00	9.08E-01	6.72E-04	3.57E+02	4.21E+01	7.27E-01	5.35E-02	5.00E+01
Ozone formation, human health	kg NO_x eq	**4.74E+00**	3.15E-04	2.71E-02	2.33E-02	2.37E-03	1.56E-06	4.52E+00	7.87E-02	1.20E-03	1.78E-04	9.09E-02
Ozone formation, ecosystems	kg NO_x eq	**4.85E+00**	5.08E-04	2.82E-02	2.72E-02	2.39E-03	1.59E-06	4.62E+00	8.31E-02	1.27E-03	1.82E-04	9.18E-02
Terrestrial acidification	kg SO_2 eq	**5.05E+01**	0.00E+00	5.05E-02	2.98E-02	3.53E-03	4.62E-06	5.01E+01	1.28E-01	2.02E-03	4.93E-04	1.91E-01
Freshwater eutrophication	kg P eq	**4.92E-01**	0.00E+00	6.75E-03	3.51E-03	4.68E-04	2.67E-07	4.16E-01	1.59E-02	2.70E-04	7.93E-05	4.89E-02
Terrestrial ecotoxicity	kg 1,4-DCB	**1.82E+03**	3.80E-02	4.46E+01	6.59E+00	3.72E+00	3.50E-03	1.60E+03	1.05E+02	2.67E+00	2.56E+00	5.57E+01
Freshwater ecotoxicity	kg 1,4-DCB	**1.76E+02**	3.76E-02	5.18E-01	1.27E-01	6.38E-02	5.39E-05	1.71E+02	1.65E+00	6.22E-02	4.77E-02	2.18E+00
Human carcinogenic toxicity	kg 1,4-DCB	**5.18E+01**	1.66E-01	5.10E-01	3.19E-01	4.32E-02	5.19E-05	4.64E+01	1.30E+00	1.06E-01	1.15E-02	2.91E+00
Human non-carcinogenic toxicity	kg 1,4-DCB	**7.11E+03**	1.41E-01	1.27E+01	4.84E+00	1.23E+00	9.85E-04	6.99E+03	3.61E+01	1.13E+00	6.27E-01	6.46E+01
Mineral resource scarcity	kg Cu eq	**5.88E+01**	0.00E+00	2.61E-02	3.03E-03	3.76E-03	5.32E-06	5.86E+01	1.06E-01	3.15E-03	3.06E-03	6.37E-02
Fossil resource scarcity	kg oil eq	**1.54E+02**	0.00E+00	5.26E+00	6.90E+00	2.25E-01	1.85E-04	1.15E+02	1.32E+01	2.55E-01	1.29E-02	1.32E+01

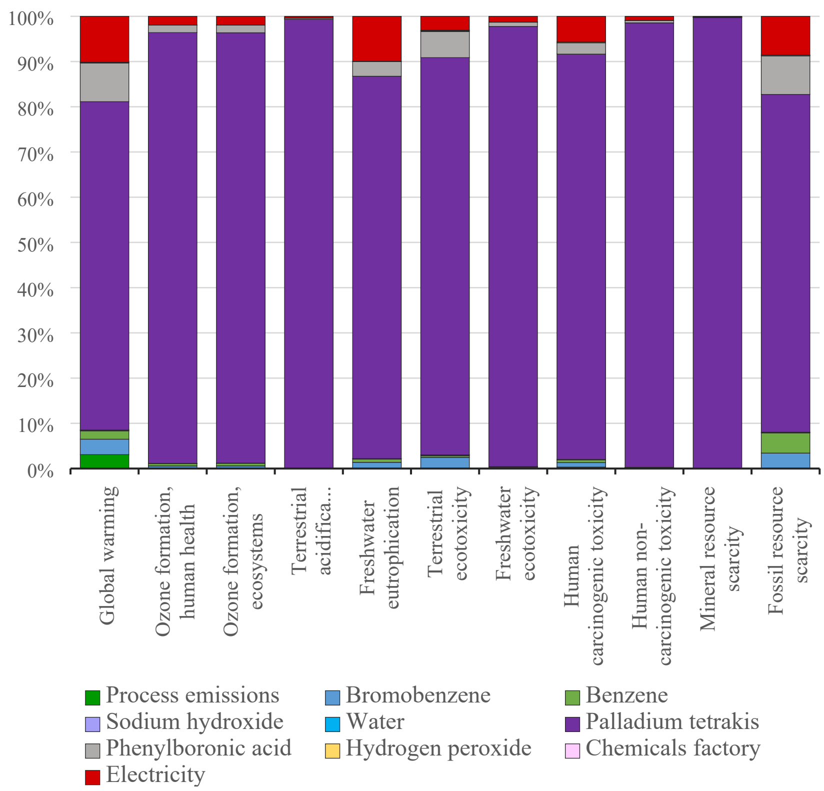

Fig. S16 *Biphenyl production via the standard Suzuki protocol using bromobenzene – characterization shares - ReCiPe 2016 midpoints*

Table S17 *Biphenyl production via the standard Suzuki protocol using iodobenzene – midpoints characterization results, ReCiPe 2016*

Impact category	Unit	Total	Process emissions	Iodobenzene	Benzene	Sodium hydroxide	Water	Phenylboronic acid	Hydrogen peroxide	Chemicals factory	Palladium tetrakis	Electricity
Global warming	kg CO_2 eq	**6.05E+02**	1.92E+01	2.08E+01	1.11E+01	1.11E+00	4.36E-04	5.17E+01	8.90E-01	5.35E-02	4.38E+02	6.18E+01
Ozone formation, human health	kg NO_x eq	**5.82E+00**	3.85E-04	3.73E-02	2.85E-02	2.90E-03	1.01E-06	9.66E-02	1.46E-03	1.78E-04	5.54E+00	1.12E-01
Ozone formation, ecosystems	kg NO_x eq	**5.95E+00**	6.20E-04	3.87E-02	3.33E-02	2.93E-03	1.03E-06	1.02E-01	1.56E-03	1.82E-04	5.66E+00	1.13E-01
Terrestrial acidification	kg SO_2 eq	**6.19E+01**	0.00E+00	6.74E-02	3.65E-02	4.32E-03	3.00E-06	1.57E-01	2.47E-03	4.93E-04	6.14E+01	2.36E-01
Freshwater eutrophication	kg P eq	**6.05E-01**	0.00E+00	9.56E-03	4.31E-03	5.73E-04	1.73E-07	1.95E-02	3.31E-04	7.93E-05	5.10E-01	6.04E-02
Terrestrial ecotoxicity	kg 1,4-DCB	**2.22E+03**	4.65E-02	4.55E+01	8.08E+00	4.56E+00	2.27E-03	1.29E+02	3.27E+00	2.56E+00	1.96E+03	6.89E+01
Freshwater ecotoxicity	kg 1,4-DCB	**2.16E+02**	4.61E-02	7.51E-01	1.55E-01	7.82E-02	3.50E-05	2.03E+00	7.62E-02	4.77E-02	2.10E+02	2.69E+00
Human carcinogenic toxicity	kg 1,4-DCB	**6.36E+01**	2.03E-01	7.05E-01	3.91E-01	5.29E-02	3.37E-05	1.59E+00	1.30E-01	1.15E-02	5.69E+01	3.60E+00
Human non-carcinogenic toxicity	kg 1,4-DCB	**8.72E+03**	1.73E-01	1.84E+01	5.93E+00	1.51E+00	6.39E-04	4.43E+01	1.39E+00	6.27E-01	8.57E+03	7.98E+01
Mineral resource scarcity	kg Cu eq	**7.92E+01**	0.00E+00	7.17E+00	3.72E-03	4.61E-03	3.46E-06	1.30E-01	3.86E-03	3.06E-03	7.18E+01	7.86E-02
Fossil resource scarcity	kg oil eq	**1.88E+02**	0.00E+00	5.71E+00	8.45E+00	2.76E-01	1.20E-04	1.62E+01	3.12E-01	1.29E-02	1.41E+02	1.63E+01

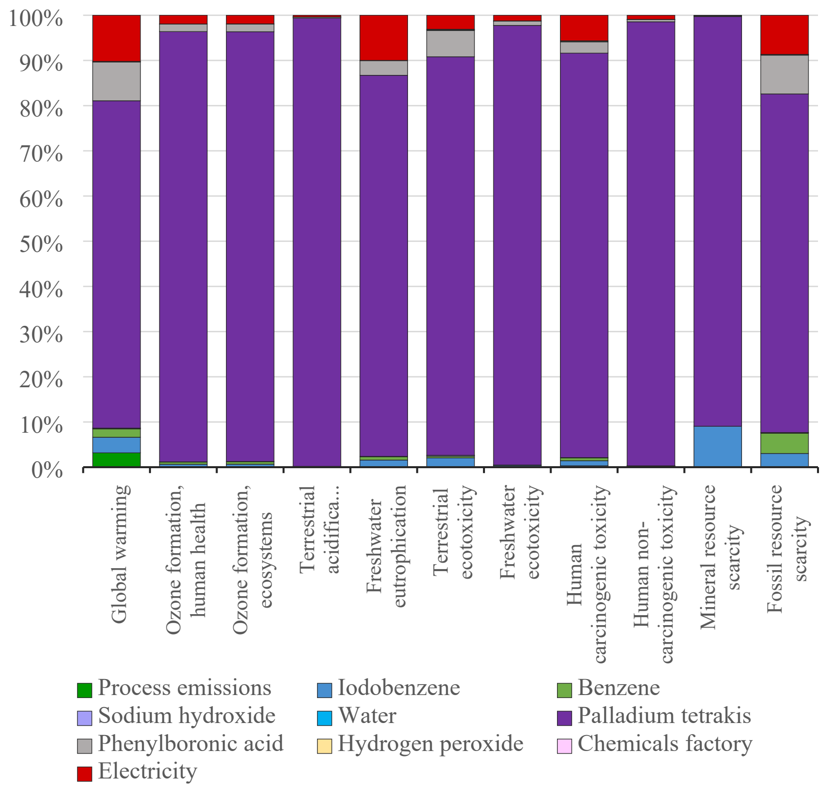

Fig. S17 *Biphenyl production via the standard Suzuki protocol using iodobenzene – characterization shares - ReCiPe 2016 midpoints*

***Table S18** Diphenylacetylene production via the standard Heck protocol using bromobenzene (variant Dieck and Heck, 1975) – midpoints characterization results, ReCiPe 2016*

Impact category	Unit	Total	Process emissions	Bromobenzene	Phenylacetylene	Triethylamine	Palladium(II) acetate	Chemicals factory	Electricity
Global warming	kg CO_2 eq	**2.01E+02**	9.72E+00	2.17E+01	9.06E+00	8.37E+00	1.47E+02	5.35E-02	4.50E+00
Ozone formation, human health	kg NO_x eq	**1.97E+00**	0.00E+00	3.50E-02	7.50E-03	1.98E-02	1.90E+00	1.78E-04	8.18E-03
Ozone formation, ecosystems	kg NO_x eq	**2.02E+00**	0.00E+00	3.64E-02	8.07E-03	2.18E-02	1.94E+00	1.82E-04	8.25E-03
Terrestrial acidification	kg SO_2 eq	**2.12E+01**	0.00E+00	6.52E-02	1.04E-02	2.83E-02	2.11E+01	4.93E-04	1.72E-02
Freshwater eutrophication	kg P eq	**1.91E-01**	0.00E+00	8.72E-03	1.18E-03	3.51E-03	1.73E-01	7.93E-05	4.40E-03
Terrestrial ecotoxicity	kg 1,4-DCB	**7.49E+02**	1.30E+00	5.76E+01	1.35E+01	2.56E+01	6.43E+02	2.56E+00	5.01E+00
Freshwater ecotoxicity	kg 1,4-DCB	**7.36E+01**	1.62E-01	6.68E-01	4.03E-01	3.76E-01	7.17E+01	4.77E-02	1.96E-01
Human carcinogenic toxicity	kg 1,4-DCB	**2.08E+01**	0.00E+00	6.58E-01	2.28E-01	2.90E-01	1.93E+01	1.15E-02	2.62E-01
Human non-carcinogenic toxicity	kg 1,4-DCB	**2.98E+03**	3.22E-01	1.64E+01	4.20E+00	7.24E+00	2.95E+03	6.27E-01	5.81E+00
Mineral resource scarcity	kg Cu eq	**2.48E+01**	0.00E+00	3.36E-02	1.59E-02	2.86E-02	2.47E+01	3.06E-03	5.72E-03
Fossil resource scarcity	kg oil eq	**6.17E+01**	0.00E+00	6.79E+00	1.92E+00	4.29E+00	4.75E+01	1.29E-02	1.19E+00

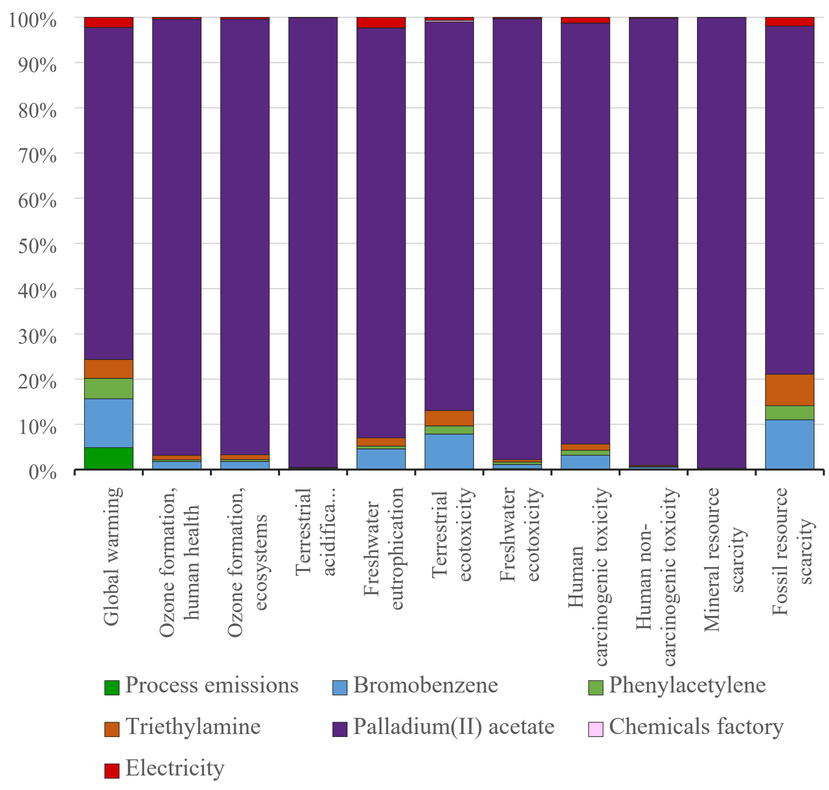

Fig. S18 *Diphenylacetylene production via the standard Heck protocol using bromobenzene (variant Dieck and Heck, 1975) – characterization shares - ReCiPe 2016 midpoints*

Table S19 *Diphenylacetylene production via the standard Heck protocol using iodobenzene (variant Dieck and Heck, 1975) – midpoints characterization results, ReCiPe 2016*

Impact category	Unit	Total	Process emissions	Iodobenzene	Phenylacetylene	Triethylamine	Palladium(II) acetate	Chemicals factory	Electricity
Global warming	kg CO_2 eq	**1.35E+02**	4.61E+00	1.54E+01	3.95E+00	5.85E+00	1.03E+02	5.35E-02	1.83E+00
Ozone formation, human health	kg NO_x eq	**1.38E+00**	0.00E+00	2.75E-02	3.27E-03	1.39E-02	1.33E+00	1.78E-04	3.32E-03
Ozone formation, ecosystems	kg NO_x eq	**1.41E+00**	0.00E+00	2.85E-02	3.52E-03	1.53E-02	1.36E+00	1.82E-04	3.35E-03
Terrestrial acidification	kg SO_2 eq	**1.49E+01**	0.00E+00	4.97E-02	4.54E-03	1.98E-02	1.48E+01	4.93E-04	6.98E-03
Freshwater eutrophication	kg P eq	**1.33E-01**	0.00E+00	7.05E-03	5.12E-04	2.46E-03	1.21E-01	7.93E-05	1.79E-03
Terrestrial ecotoxicity	kg 1,4-DCB	**5.13E+02**	3.45E-01	3.35E+01	5.89E+00	1.79E+01	4.51E+02	2.56E+00	2.04E+00
Freshwater ecotoxicity	kg 1,4-DCB	**5.14E+01**	7.06E-02	5.53E-01	1.76E-01	2.63E-01	5.02E+01	4.77E-02	7.97E-02
Human carcinogenic toxicity	kg 1,4-DCB	**1.45E+01**	0.00E+00	5.20E-01	9.95E-02	2.03E-01	1.35E+01	1.15E-02	1.06E-01
Human non-carcinogenic toxicity	kg 1,4-DCB	**2.09E+03**	1.92E-01	1.36E+01	1.83E+00	5.07E+00	2.06E+03	6.27E-01	2.36E+00
Mineral resource scarcity	kg Cu eq	**2.26E+01**	0.00E+00	5.29E+00	6.95E-03	2.00E-02	1.73E+01	3.06E-03	2.33E-03
Fossil resource scarcity	kg oil eq	**4.18E+01**	0.00E+00	4.21E+00	8.38E-01	3.00E+00	3.32E+01	1.29E-02	4.83E-01

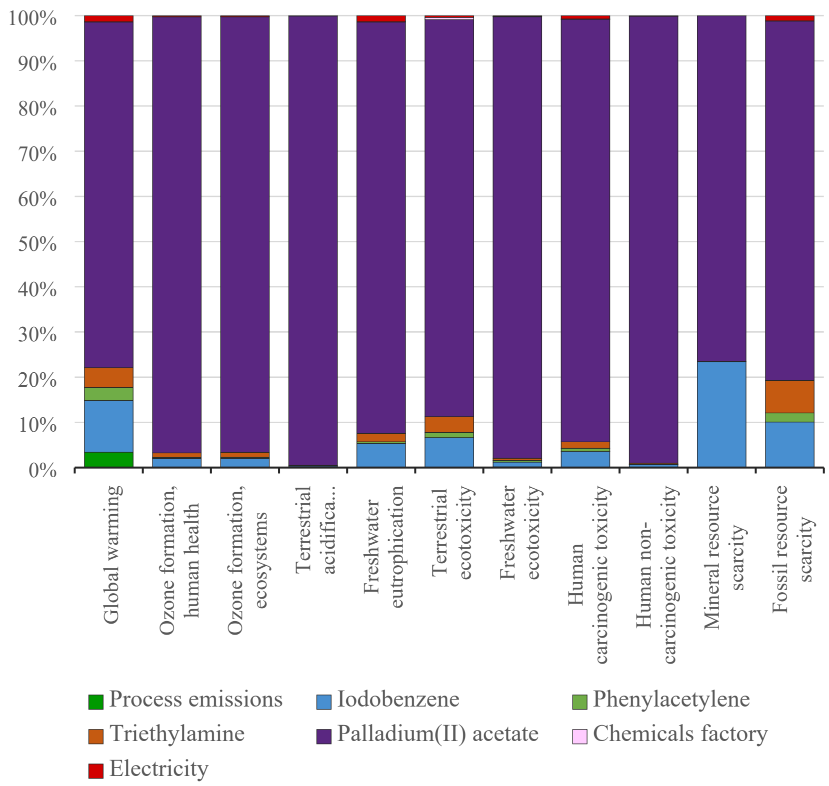

Fig. S19 *Diphenylacetylene production via the standard Heck protocol using iodobenzene (variant Dieck and Heck, 1975) – characterization shares - ReCiPe 2016 midpoints*

Table S20 *Diphenylacetylene production via the standard Heck protocol using bromobenzene (variant Cassar, 1975) – midpoints characterization results, ReCiPe 2016*

Impact category	Unit	Total	Process emissions	Bromobenzene	Phenylacetylene	Sodium methoxide	N,N-dimethylformamide	Palladium-tetrakis	Chemicals factory	Electricity
Global warming	kg CO_2 eq	**6.09E+02**	1.55E+01	1.25E+01	2.62E+00	6.93E-01	1.91E+01	5.33E+02	5.35E-02	2.53E+01
Ozone formation, human health	kg NO_x eq	**6.86E+00**	0.00E+00	2.02E-02	2.17E-03	1.75E-03	4.09E-02	6.75E+00	1.78E-04	4.61E-02
Ozone formation, ecosystems	kg NO_x eq	**7.01E+00**	0.00E+00	2.10E-02	2.34E-03	1.80E-03	4.26E-02	6.89E+00	1.82E-04	4.65E-02
Terrestrial acidification	kg SO_2 eq	**7.50E+01**	0.00E+00	3.77E-02	3.01E-03	2.48E-03	7.16E-02	7.48E+01	4.93E-04	9.67E-02
Freshwater eutrophication	kg P eq	**6.57E-01**	0.00E+00	5.04E-03	3.40E-04	2.86E-04	5.70E-03	6.21E-01	7.93E-05	2.48E-02
Terrestrial ecotoxicity	kg 1,4-DCB	**2.54E+03**	8.62E-02	3.33E+01	3.91E+00	2.87E+00	8.69E+01	2.38E+03	2.56E+00	2.82E+01
Freshwater ecotoxicity	kg 1,4-DCB	**2.58E+02**	7.13E-03	3.86E-01	1.16E-01	5.09E-02	1.22E+00	2.55E+02	4.77E-02	1.10E+00
Human carcinogenic toxicity	kg 1,4-DCB	**7.18E+01**	0.00E+00	3.81E-01	6.60E-02	2.82E-02	5.86E-01	6.93E+01	1.15E-02	1.48E+00
Human non-carcinogenic toxicity	kg 1,4-DCB	**1.05E+04**	2.88E+00	9.45E+00	1.22E+00	8.80E-01	1.96E+01	1.04E+04	6.27E-01	3.27E+01
Mineral resource scarcity	kg Cu eq	**8.76E+01**	0.00E+00	1.94E-02	4.61E-03	3.12E-03	7.28E-02	8.75E+01	3.06E-03	3.23E-02
Fossil resource scarcity	kg oil eq	**1.94E+02**	0.00E+00	3.92E+00	5.56E-01	2.97E-01	1.10E+01	1.72E+02	1.29E-02	6.70E+00

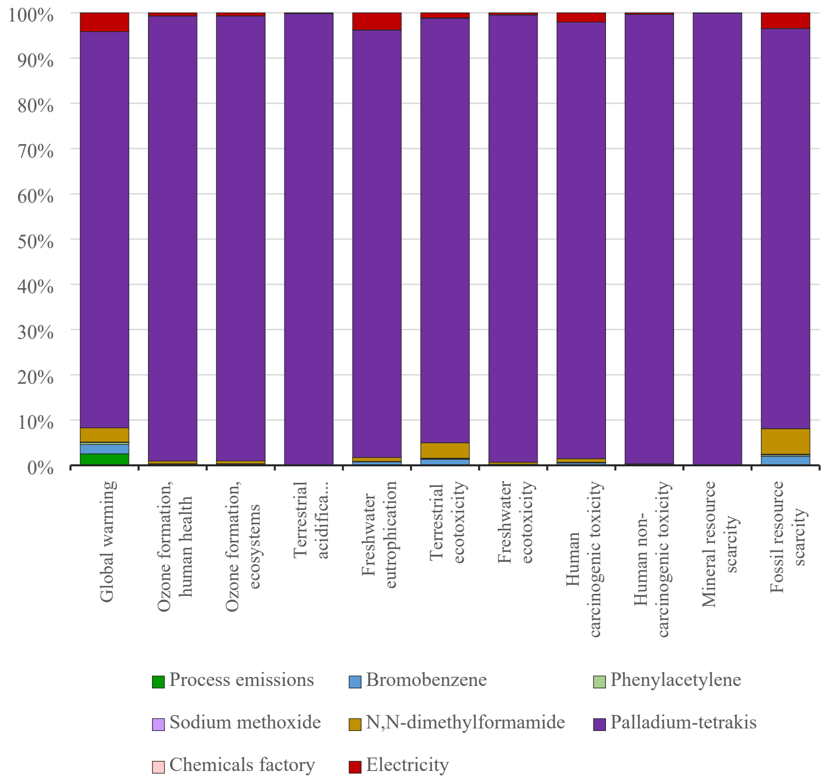

Fig. S20 *Diphenylacetylene production via the standard Heck protocol using bromobenzene (variant Cassar, 1975) – characterization shares - ReCiPe 2016 midpoints*

Table S21 *Diphenylacetylene production via the standard Heck protocol using iodobenzene (variant Cassar, 1975) – midpoints characterization results, ReCiPe 2016*

Impact category	**Unit**	**Total**	**Process emissions**	**Iodobenzene**	**Phenylacetylene**	**Sodium methoxide**	**N,N-dimethylformamide**	**Palladium-tetrakis**	**Chemicals factory**	**Electricity**
Global warming	kg CO_2 eq	**2.02E+02**	6.04E+00	1.17E+01	2.43E+00	5.89E-01	8.87E+00	1.64E+02	5.35E-02	8.40E+00
Ozone formation, human health	kg NO_x eq	**2.13E+00**	0.00E+00	2.10E-02	2.01E-03	1.49E-03	1.90E-02	2.08E+00	1.78E-04	1.53E-02
Ozone formation, ecosystems	kg NO_x eq	**2.18E+00**	0.00E+00	2.18E-02	2.16E-03	1.53E-03	1.97E-02	2.12E+00	1.82E-04	1.54E-02
Terrestrial acidification	kg SO_2 eq	**2.31E+01**	0.00E+00	3.80E-02	2.79E-03	2.11E-03	3.32E-02	2.30E+01	4.93E-04	3.21E-02
Freshwater eutrophication	kg P eq	**2.08E-01**	0.00E+00	5.39E-03	3.15E-04	2.43E-04	2.64E-03	1.91E-01	7.93E-05	8.22E-03
Terrestrial ecotoxicity	kg 1,4-DCB	**8.18E+02**	4.21E-02	2.56E+01	3.62E+00	2.44E+00	4.03E+01	7.34E+02	2.56E+00	9.37E+00
Freshwater ecotoxicity	kg 1,4-DCB	**8.01E+01**	3.02E-03	4.23E-01	1.08E-01	4.33E-02	5.64E-01	7.86E+01	4.77E-02	3.66E-01
Human carcinogenic toxicity	kg 1,4-DCB	**2.26E+01**	0.00E+00	3.97E-01	6.12E-02	2.39E-02	2.72E-01	2.13E+01	1.15E-02	4.89E-01
Human non-carcinogenic toxicity	kg 1,4-DCB	**3.25E+03**	1.34E+00	1.04E+01	1.13E+00	7.48E-01	9.09E+00	3.21E+03	6.27E-01	1.09E+01
Mineral resource scarcity	kg Cu eq	**3.10E+01**	0.00E+00	4.04E+00	4.27E-03	2.65E-03	3.37E-02	2.69E+01	3.06E-03	1.07E-02
Fossil resource scarcity	kg oil eq	**6.42E+01**	0.00E+00	3.22E+00	5.15E-01	2.52E-01	5.08E+00	5.29E+01	1.29E-02	2.22E+00

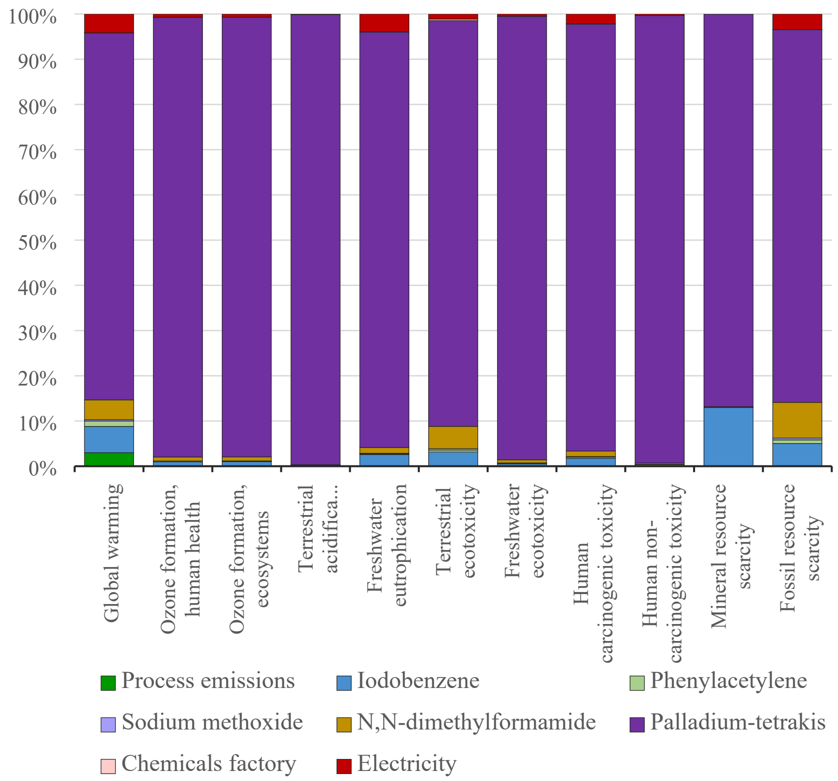

Fig. S21 *Diphenylacetylene production via the standard Heck protocol using iodobenzene (variant Cassar, 1975) – characterization shares - ReCiPe 2016 midpoints*

Table S22 *Trans-methyl cinnamate production via the standard Heck protocol using bromobenzene (variant Dieck and Heck, 1974) – midpoints characterization results, ReCiPe 2016*

Impact category	Unit	Total	Process emissions	Bromobenzene	Methyl acrylate	Tetramethylethylenediamine	Palladium(II) acetate	Triphenylphosphine	Chemicals factory	Electricity
Global warming	kg CO_2 eq	1.42E+02	3.41E+00	1.43E+01	3.56E+00	3.87E+00	9.72E+01	3.80E-01	5.35E-02	1.94E+01
Ozone formation, human health	kg NO_x eq	1.33E+00	0.00E+00	2.30E-02	5.59E-03	6.88E-03	1.25E+00	8.02E-04	1.78E-04	3.52E-02
Ozone formation, ecosystems	kg NO_x eq	1.35E+00	0.00E+00	2.40E-02	5.88E-03	7.18E-03	1.28E+00	8.50E-04	1.82E-04	3.56E-02
Terrestrial acidification	kg SO_2 eq	1.41E+01	0.00E+00	4.30E-02	7.36E-03	1.33E-02	1.39E+01	1.21E-03	4.93E-04	7.40E-02
Freshwater eutrophication	kg P eq	1.41E-01	0.00E+00	5.75E-03	5.61E-04	1.26E-03	1.14E-01	4.48E-04	7.93E-05	1.89E-02
Terrestrial ecotoxicity	kg 1,4-DCB	5.13E+02	4.11E-01	3.79E+01	8.59E+00	1.67E+01	4.25E+02	1.07E+00	2.56E+00	2.16E+01
Freshwater ecotoxicity	kg 1,4-DCB	4.93E+01	1.84E-01	4.40E-01	1.49E-01	2.29E-01	4.73E+01	2.04E-02	4.77E-02	8.44E-01
Human carcinogenic toxicity	kg 1,4-DCB	1.46E+01	0.00E+00	4.34E-01	7.70E-02	1.44E-01	1.28E+01	1.61E-02	1.15E-02	1.13E+00
Human non-carcinogenic toxicity	kg 1,4-DCB	1.99E+03	0.00E+00	1.08E+01	3.88E+00	3.87E+00	1.94E+03	4.01E-01	6.27E-01	2.50E+01
Mineral resource scarcity	kg Cu eq	1.64E+01	0.00E+00	2.22E-02	9.78E-03	1.41E-02	1.63E+01	5.28E-03	3.06E-03	2.47E-02
Fossil resource scarcity	kg oil eq	4.46E+01	0.00E+00	4.47E+00	1.76E+00	1.82E+00	3.13E+01	1.33E-01	1.29E-02	5.12E+00

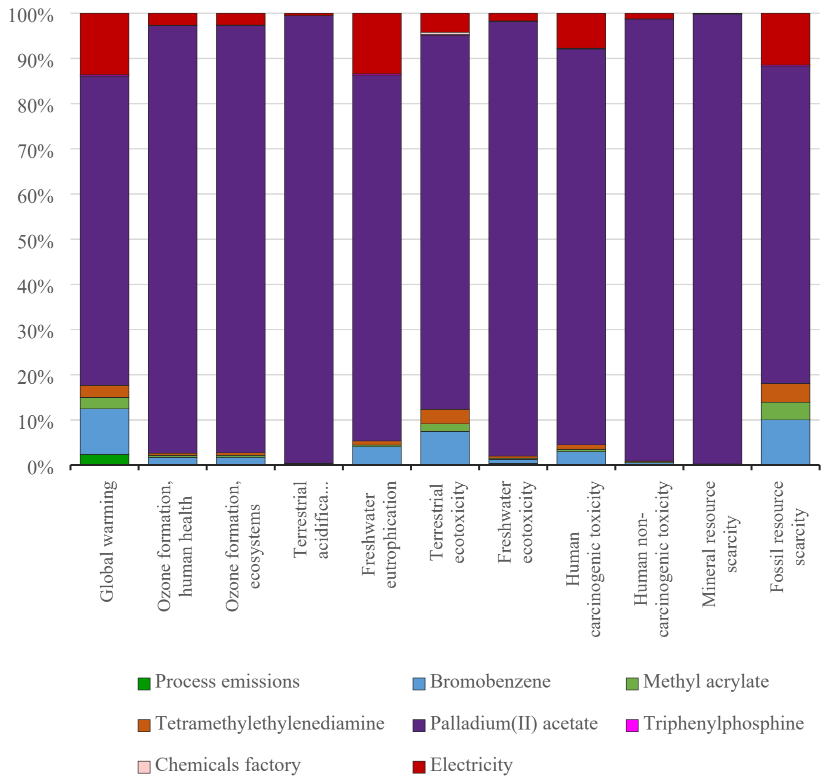

Fig. S22 *Trans-methyl cinnamate production via the standard Heck protocol using bromobenzene (variant Dieck and Heck, 1974) – characterization shares - ReCiPe 2016 midpoints*

Table S23 *Trans-methyl cinnamate production via the standard Heck protocol using iodobenzene (variant Heck and Nolley, 1972) – midpoints characterization results, ReCiPe 2016*

Impact category	Unit	Total	Process emissions	Iodobenzene	Methyl acrylate	Tripropylamine	Palladium(II) acetate	N-methyl-2-pyrrolidone	Chemicals factory	Electricity
Global warming	kg CO_2 eq	1.71E+02	1.21E+01	1.52E+01	3.74E+00	2.10E+01	1.02E+02	1.31E+01	5.35E-02	3.74E+00
Ozone formation, human health	kg NO_x eq	1.45E+00	0.00E+00	2.72E-02	5.85E-03	6.89E-02	1.32E+00	2.84E-02	1.78E-04	6.81E-03
Ozone formation, ecosystems	kg NO_x eq	1.50E+00	0.00E+00	2.82E-02	6.16E-03	8.03E-02	1.34E+00	2.94E-02	1.82E-04	6.87E-03
Terrestrial acidification	kg SO_2 eq	1.48E+01	0.00E+00	4.90E-02	7.71E-03	8.97E-02	1.46E+01	4.81E-02	4.93E-04	1.43E-02
Freshwater eutrophication	kg P eq	1.46E-01	0.00E+00	6.96E-03	5.88E-04	1.02E-02	1.20E-01	4.48E-03	7.93E-05	3.66E-03
Terrestrial ecotoxicity	kg 1,4-DCB	5.87E+02	4.00E-01	3.31E+01	9.00E+00	4.49E+01	4.45E+02	4.75E+01	2.56E+00	4.17E+00
Freshwater ecotoxicity	kg 1,4-DCB	5.26E+01	4.77E-01	5.46E-01	1.56E-01	8.95E-01	4.97E+01	6.95E-01	4.77E-02	1.63E-01
Human carcinogenic toxicity	kg 1,4-DCB	1.56E+01	2.90E-03	5.13E-01	8.07E-02	1.01E+00	1.34E+01	4.21E-01	1.15E-02	2.18E-01
Human non-carcinogenic toxicity	kg 1,4-DCB	2.10E+03	0.00E+00	1.34E+01	4.06E+00	2.25E+01	2.04E+03	1.30E+01	6.27E-01	4.84E+00
Mineral resource scarcity	kg Cu eq	2.24E+01	0.00E+00	5.22E+00	1.02E-02	6.98E-02	1.71E+01	3.95E-02	3.06E-03	4.77E-03
Fossil resource scarcity	kg oil eq	5.26E+01	0.00E+00	4.16E+00	1.84E+00	8.06E+00	3.29E+01	4.71E+00	1.29E-02	9.90E-01

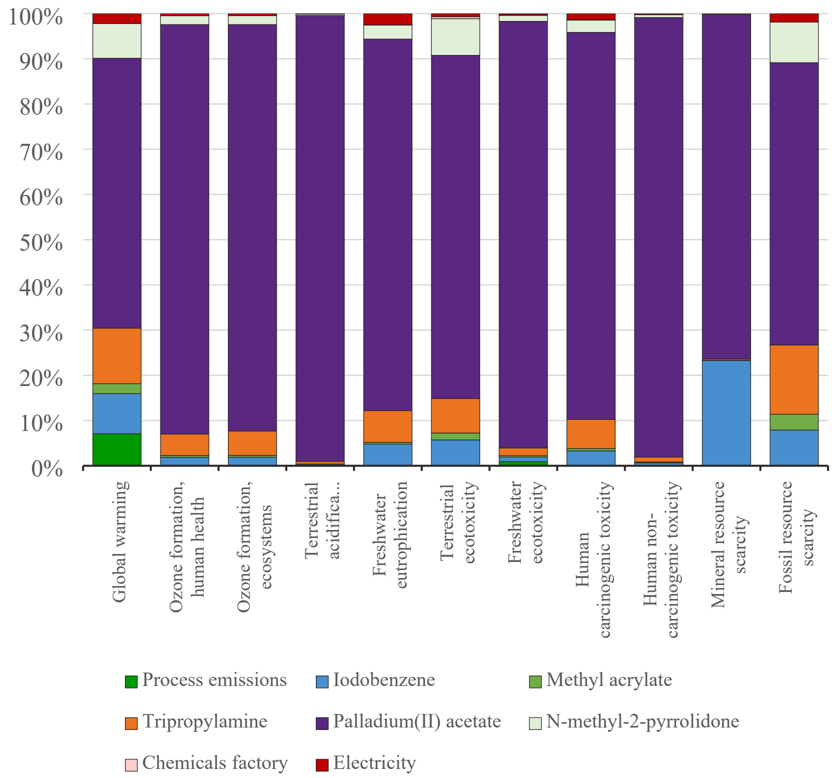

Fig. S23 *Trans-methyl cinnamate production via the standard Heck protocol using iodobenzene (variant Heck and Nolley, 1972) – characterization shares - ReCiPe 2016 midpoints*

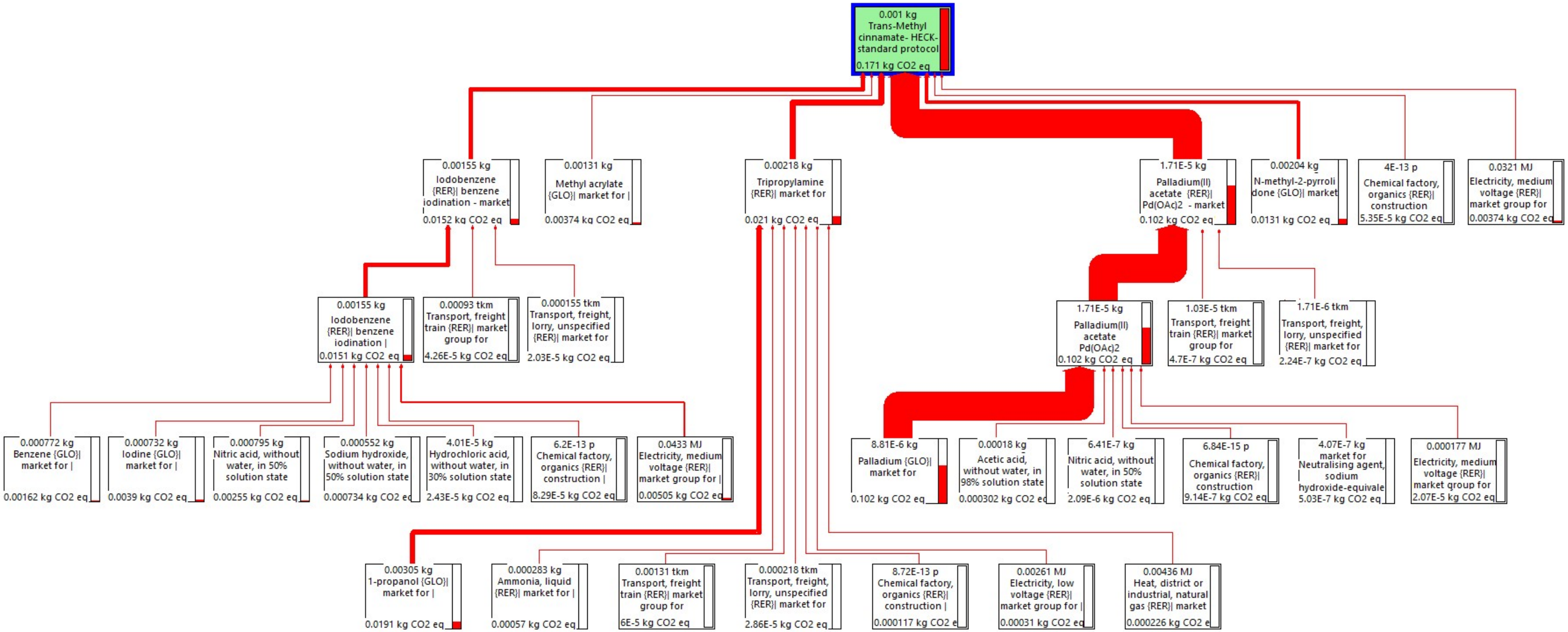

Fig. S24 Global warming impacts for 1 g of Trans methyl cinnamate from iodobenzene via Heck protocol – Midpoint Impacts contribution tree, Cut-off: 0.01%.
Source: SimaPro 9.1.1.7

Note: This tree only shows the materials and energy that have contributions higher than 0.01% of the total impact of 0.171 kg CO_2 eq per gram of Trans methyl cinnamate