Electronic Supplementary Material (ESI) for Green Chemistry.

Electronic Supporting Information

The need to integrate mass- and energy-based metrics with life cycle impacts for sustainable chemicals manufacture

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S1. Detailed methodology

Stage 1: Compiling data on chemical production processes

Process level and life cycle inventory data for chemical production processes were first compiled from the ecoinvent v3.9 life cycle inventory (LCI) database.[1] The ecoinvent database contains a wide variety of datasets on the production of chemical products such as agrochemicals (fertilisers, pesticides, plant growth regulators, etc.), ink and paints, bulk, and specialised chemicals. Data on each chemical production process covers mass and energy flows in and out of all synthesis and processing steps to reach final product.

For this analysis, we selected chemical processes, representing production globally, in the ecoinvent database with sufficient data to compute all metrics of interest. Using Brightway2[2] to manage ecoinvent's life-cycle inventory datasets, we started selecting chemical production activities based on their international standard industrial classification (ISIC) revision 4.[3] More specifically, we initially included all activities with ISIC starting with "20" (Manufacture of chemicals and chemical products) or "21" (Manufacture of pharmaceuticals, medicinal chemical and botanical products), resulting in around 1407 datasets. Then, the chemical corresponding to the reference product (or the CAS number if available) of each activity was identified using the Chemical Identifier Resolver, leading to 795 datasets of unique, unambiguous chemicals production with an associated SMILE structure. Additionally, in order to comply with complete datasets only, we filtered out system process (*i.e.*, cradle-to-gate aggregated of life-cycle environmental flows and no technosphere inputs), resulting in 762 datasets. Also, we removed activities with no waste streams or emission data, leading to 731 datasets. Two activities were also dropped from our analysis as they did not include energy inputs. Finally, we eliminated activities for which mass balance did not hold, resulting in the final 711 chemical production datasets.

The final dataset is comprised of 711 chemical processes, producing a range of organic (70% of the dataset) and inorganic (30% of the dataset) compounds (see **Table S2** for a complete list). Notable structural types of organic compounds constituting considerable portions of the dataset include benzenoids (*e.g.*, simpler compounds such as phenol (C_6H_5OH) and aniline ($C_6H_5NH_2$), and larger molecules such as aclonifen ($C_{12}H_9ClN_2O_3$) and dioctyl terephthalate ($C_{24}H_{38}O_4$)) and organic acids and their derivatives (*e.g.*, formic acid (CH_2O_2), mancozeb ($C_{40}H_{60}Mn_9N_{20}S_{40}Zn$)). For inorganic compounds, the dataset mostly covers structures of mixed metal/non-metal compounds (*e.g.*, lithium fluoride (LiF), sodium tripolyphosphate ($Na_5P_3O_{10}$)) and homogeneous non-metal compounds (*e.g.*, ammonium nitrate (NH_4NO_3), phosphorus pentachloride (PCl_5)). The production data in the ecoinvent LCI database typically represent business-as-usual synthesis and manufacturing routes.

Stage 2: Calculating environmental performance metrics

Various mass- and energy-based metrics and life cycle impacts were then calculated for each chemical process. We used process-level (*i.e.*, process input and output mass flows) and LCI data to compute process E-factor (including and excluding water), PMI, Mass Intensity (MI), Process Energy Intensity (PEI) and life cycle impacts for 16 environmental impact categories.

The E-factor,[4] PMI,[4] and MI[5,6] of each process were calculated using its associated process-level data in ecoinvent v3.9 on mass outputs (*e.g.*, emissions to air and water, wastewater, or solid waste streams from system) as in **Equation (S1)** and inputs (*e.g.*, reactants and reagents into system) as in **Equation (S2)**. Two variants of the E-factor metric were evaluated – one in which water and wastewater streams are accounted for in the numerator of **Equation (S1)** ('complete'; henceforth referred to E-factor including water and abbreviated as cEF) and the other in which water and wastewater streams are excluded ('partial'; henceforth referred to as E-factor excluding water and abbreviated as pEF). Similarly, PMI and MI both represent input resource efficiency but differ by the inclusion of water inputs in the numerator of **Equation (S2)** – *i.e.*, water is included in the calculation of PMI and excluded for MI.

$$\text{E-factor} = \text{Mass of waste and environmental emissions [kg]} / \text{Mass of product [kg]} \quad \textbf{(S1)}$$

$$\text{(P)MI} = \text{Mass of all inputs [kg]} / \text{Mass of product [kg]} \quad \textbf{(S2)}$$

Energy intensities were also computed using foreground data in ecoinvent v3.9 by summing the amounts of input electricity and heating into each process [**Equation (S3)**].

$$\text{PEI} = \text{Amount of energy inputs into process [MJ]} / \text{Mass of product [kg]} \quad \textbf{(S3)}$$

The attributional life cycle impacts of each chemical production process (per kg of product) were calculated in Brightway2[2] using the Environmental Footprint (EF) v3 life cycle impact assessment (LCIA) method as recommended by the European Commission.[7] The 'Allocation, cut-off by classification' system model[1] of the ecoinvent v3.9 database was used. **Section S2** briefly describes the methodology adopted in this study to calculate the life cycle impact-based metrics using Life Cycle Assessments (LCAs).

The EF LCIA method characterises life cycle data into 16 environmental impact categories spanning a broad range of environmental levels: climate change, pollution (ozone depletion, particulate matter formation, ionising radiation, photochemical ozone formation, acidification, freshwater/marine/terrestrial eutrophication), resources (land use, water use, minerals and metals use, fossil resource use) and toxicity (carcinogenic and non-carcinogenic human toxicity, freshwater ecotoxicity). In a European context, the EF method is the European

Commission's recommended LCIA method for assessing the environmental impact of products.[7] It is also the adopted method for executing the environmental sustainability assessment step in the European Commission's Safe and Sustainable by Design chemicals and materials framework as it is considered to cover the most basic set of impacts for any LCA study.[8] Moreover, in a recent study, these life cycle impact metrics were linked to a number of Sustainable Development Goals, providing a framework to quantify the progress made towards wider global sustainability.[9]

The mass- and energy-based metrics we calculate in this analysis relate to the performance of only the process system (*i.e.*, process gate-to-gate), while life cycle impacts account for impacts embedded in all material and energy inputs to the process, from the process itself, as well as from the treatment or disposal of waste streams (*i.e.*, cradle-to-gate). The expansion of system boundaries for mass-based metrics has been previously proposed, *e.g.*, the inclusion of 'intrinsic' E-factors which incorporate the embedded waste intensities of procured raw materials.[10,11] Accounting for the inherent resource or waste intensities of input materials could lead to appreciable worsening of the environmental score of a process, especially if input materials are advanced intermediates with multiple complex synthesis steps. In this analysis, however, we consider only 'traditional' gate-to-gate system boundaries for the E-factor, PMI, MI and PEI as there is no agreed standard on the cut-off criterion for the starting point of raw materials. Consequently, there is great uncertainty on whether 'intrinsic' mass-based metrics are commonly utilised in practice given this lack of standardisation and the additional data needed regarding procured materials.

Stage 3: Analysing scores to uncover trends in mass-, energy- and life cycle impact-based metrics

Following the computation of all metrics, we sought to investigate (i) if and to what extent mass- and energy-based metrics correlate with life cycle impacts, and (ii) what the main contributing factors are to the life cycle impact of a chemical process and how they relate to the scope of mass- and energy-based process metrics.

Spearman's Rank correlation analysis was used to measure the strength and direction of association between each mass- or energy-based metric and life cycle impact score of all chemical processes in our dataset. Spearman's Rank tests for a monotonic relationship between metrics, *i.e.*, testing whether when the value of one variable increases, the value of the other increases or decreases regardless of the type of relationship between the variables (*e.g.*, linear or nonlinear). More specifically, the strength of association between the *ranks* of metric and impact scores is measured. Additionally, this correlation testing technique does not assume that the relationship between the variables being investigated are linear and this flexibility is a key factor in why it was selected for this analysis.

To delve deeper into the presence or absence of any correlation between metrics, the contributions from various process aspects (*e.g.*, material inputs, energy, waste treatment) to life cycle impacts were examined. The life cycle impacts of each chemical production process were disaggregated to contributions from every process input and output, allowing for the major contributors, or hotspots, to be identified.

Table S1. Definitions of terminology.

Term	Definition
Mass- or energy-based process metric	Metric measuring the amount of material (mass-based with unit of kilogram) or amount of electricity, heat, and fuel (energy-based with unit of megajoule of energy) directly into or out of a chemical process (all synthesis and processing steps in production system).
Process Mass Intensity (PMI)	Mass (kilograms) of all input materials including water into a chemical process (all synthesis and processing steps in production system) per kilogram of product.
Mass Intensity (MI)	Mass (kilograms) of all input materials excluding water into a chemical process (all synthesis and processing steps in production system) per kilogram of product.
E-factor including water	Mass (kilograms) of all waste streams including water and wastewater from a chemical process (all synthesis and processing steps in production system).
E-factor excluding water	Mass (kilograms) of all waste streams excluding water and wastewater from a chemical process (all synthesis and processing steps in production system).
Life Cycle Assessment (LCA)	Method to estimate the overall environmental impacts associated with the wider life cycle (production, distribution, use and end-of-life phases) of a chosen system of interest (*e.g.*, a product, activity, or process).
Life Cycle Inventory (LCI)	Data on amounts of all inputs (material, resource, and energy) and outputs (products, waste streams, emissions).
System boundary	Activities in the product/process' life cycle that are included and analysed.
Cradle-to-gate	A type of system boundary considering only inputs/outputs from resource extraction (cradle) to factory gate (before distribution and supply).
Gate-to-gate	A type of system boundary considering only inputs/outputs from reception of resources and energy (entry factory gate) to final product at factory exit gate.

S2. Life cycle assessment method and data

Life cycle assessment methodology

We investigate the environmental impacts of chemical production processes available in the ecoinvent v3.9 database. We conduct an attributional LCA of all the chemical processes following the four different phases outlined in ISO 14040 and 14044 standards.[12,13] In the first phase of the analysis, we define the goal and scope of our study. In this work, we consider the functional unit as the production of 1 kg of a chemical (as shown in **Table S2**) *via* a specific production technology as defined in the ecoinvent database, the details of which are described below. We follow a cradle-to-gate approach, encompassing all the upstream flows from the technosphere (A) matrix (*e.g.*, electricity) and biosphere (B) matrix (*e.g.*, emissions and inputs from nature) required for the production of the chemical under consideration. We choose the cradle-to-gate approach to avoid assumptions regarding the use of the chemical later downstream due to uncertainties in performing such an analysis. We quantify the global average impact of the chemical production process. For this, we rely on 'global' or 'rest of the world' inventories in the ecoinvent database. In cases where the global datasets are not available, we rely on European (RER) inventories for our analysis.

In phase 2 of our LCA, which involves the inventory analysis, we compiled datasets from the ecoinvent v3.9 database. The ecoinvent database consists of numerous datasets across various sectors. For this analysis, we selected chemical processes with sufficient data to compute all metrics considered in this study, as thoroughly explained in **Section S1**.

Phase 3 encompasses the LCIA, where we used Brightway2 to assess multiple impact categories and discover potential hidden trade-offs. Given a final demand vector (f) defined from the functional unit, the inventory vector (g) is calculated with the following equation:

$$g = B\,A^{-1}\,f \qquad \textbf{(S4)}$$

where A and B are the technosphere and biosphere matrices.[14] We utilise the Environmental Footprint (EF) v3 methods to quantify 16 impact categories.[7] The impact assessment vector (h) is calculated using the following equation:

$$h = Q\,g \qquad \textbf{(S5)}$$

where Q represents the characterisation factors.[14] These factors assign numerical values to the impact depending on the method employed, thereby representing the environmental impact potential of each flow. Therefore, **Equation (S5)** provides a quantification of the overall environmental impacts associated with a chemical production process, in terms of the chosen

impact category. In the final phase of the LCA, we interpret the results by analysing impacts to discover correlations among mass, energy, and life cycle impact-based metrics.

Database details

The 'Allocation, cut-off classification' system model of the ecoinvent v3.9 database[1] was used to generate process-level mass- and energy-based metrics and Environmental Footprint life cycle impacts. The 'cut-off' nature of this system model relates to the consideration of recycled and recyclable materials.[1]

For multi-product systems, ecoinvent applies economic allocation - *i.e.*, attributing process input and emission flows to each co-product based on economic price. Such allocation is maintained for the calculation of life cycle environmental impacts via the Environmental Footprint method. In other words, for processes with multiple products, the 'burden' of environmental impacts is shared among the products according to their economic value.

To calculate process metrics (E-factor, Process Mass Intensity, Mass Intensity and Process Energy Intensity), unallocated (*i.e.*, the values of input and emission flows prior to economic allocation) inventory data was used in which process input and emission flows maintain material and energy balances.

The inventories of the 711 chemical production processes extracted from the ecoinvent v3.9 database encompass different sources from both industry and literature,[1] providing detailed insights into the production processes of these chemicals. The ecoinvent database is typically used as a 'background' database, containing numerous background processes, including waste treatment, electricity, heating, cooling, and the manufacturing of chemicals. Despite the valuable information and robust datasets available in the ecoinvent database, there are still data gaps. For example, in Europe alone, approximately 20,000 chemicals are traded commercially.[15] These data gaps act as limitations of our study.

List of chemical processes

Table S2. Activity name, product compound name and geographical context for each chemical production process from the ecoinvent v3.9 database that was analysed in this study.

ecoinvent v3.9 activity name	Product	Location
barium sulfide production	barium sulfide	Global
sodium dithionite production, anhydrous	sodium dithionite, anhydrous	Europe
methyl-3-methoxypropionate production	methyl-3-methoxypropionate	Global
anthranilic acid production	anthranilic acid	Europe
dichlobenil production	dichlobenil	Global
aniline production	aniline	Europe
resorcinol production, hydroperoxidation of meta-diisopropylbenzene	resorcinol	Global
4-tert-butylbenzaldehyde production	4-tert-butylbenzaldehyde	Europe
trichloroacetic acid production	trichloroacetic acid	Europe
phosphorus oxychloride production, from phosphorus trichloride	phosphorus oxychloride	Rest of World
acetanilide production	acetanilide	Rest of World
pentaerythritol production in sodium hydroxide solution	sodium formate	Europe
calcium ammonium nitrate production	calcium ammonium nitrate	China
isoproturon production	isoproturon	Europe
sodium cyanide production	sodium cyanide	Europe
Sohio process	acrylonitrile	Europe
lactic acid production	lactic acid	Rest of World
chlorpropham production	chlorpropham	Global
sodium phenolate production	sodium phenolate	Europe
2-nitroaniline production	2-nitroaniline	Rest of World
carbon disulfide production, from natural gas	carbon disulfide	Global
Sohio process	hydrogen cyanide	Europe
trichloroethylene production	trichloroethylene	Rest of World
chlorosulfonic acid production	chlorosulfonic acid	Europe
phosphorus trichloride production	phosphorus trichloride	Global
dichloromethane production	dichloromethane	Rest of World
benzyl alcohol production	benzyl alcohol	Europe
lithium hexafluorophosphate production	lithium hexafluorophosphate	Rest of World
carbon tetrachloride production	carbon tetrachloride	Europe
phenol production, from cumene	phenol	Rest of World
tetrahydrofuran production	tetrahydrofuran	Rest of World
lithium iron phosphate production, solid state process	lithium iron phosphate	China
potassium hydroxide production	chlorine, gaseous	Europe
Sohio process	hydrogen cyanide	Rest of World
hydroxylamine production	hydroxylamine	Europe
chloropropionic acid production	chloropropionic acid	Europe
isohexane production	isohexane	Rest of World
ethylene bromide production	ethylene bromide	Rest of World
sulfur dichloride production	sulfur dichloride	Rest of World
nitrous oxide production	nitrous oxide	Europe
methylcyclohexane production	methylcyclohexane	Europe
tetrahydrofuran production	tetrahydrofuran	Europe
ethanolamine production	diethanolamine	Rest of World
2-methyl-2-butanol production	2-methyl-2-butanol	Rest of World
ethanolamine production	diethanolamine	Europe
dimethyl malonate production	dimethyl malonate	Europe
adipic acid production	succinic acid	Rest of World
chichibabin amination	aminopyridine	Europe

manganese sulfate production	manganese sulfate	Global
acrylonitrile-butadiene-styrene copolymer production	acrylonitrile-butadiene-styrene copolymer	Europe
ethanolamine production	triethanolamine	Europe
napropamide production	napropamide	Europe
trimethylamine production	trimethylamine	Europe
azodicarbonamide production	azodicarbonamide	Europe
butyldiglycol acetate production	butyldiglycol acetate	Global
barium hydroxide production	barium hydroxide	Global
acetaldehyde production	acetaldehyde	Rest of World
tert-butyl amine production	tert-butyl amine	Rest of World
chlorodifluoromethane production	chlorodifluoromethane	Netherlands
propanal production	propanal	Europe
benzal chloride production	benzal chloride	Rest of World
benzyl chloride production	benzyl chloride	Rest of World
azodicarbonamide production	azodicarbonamide	Rest of World
ethyl tert-butyl ether production, from bioethanol	ethyl tert-butyl ether	Rest of World
boron trifluoride production	boron trifluoride	Global
aluminium hydroxide production	aluminium hydroxide	North America
phosphorus oxychloride production, from phosphorus pentachloride	phosphorus oxychloride	Global
vinyl chloride production	vinyl chloride	Rest of World
cobalt sulfate production	cobalt sulfate	China
adipic acid production	adipic acid	Europe
butyl acetate production	butyl acetate	Rest of World
soda production, solvay process	sodium bicarbonate	Europe
o-aminophenol production	o-aminophenol	Europe
oxalic acid production	oxalic acid	China
lithium fluoride production	lithium fluoride	Rest of World
lithium hydroxide production	lithium hydroxide	Global
2-nitroaniline production	2-nitroaniline	Europe
dodecanol production, ziegler process	dodecanol	Global
aluminium hydroxide production	aluminium hydroxide	Rest of World
methylcyclohexane production	methylcyclohexane	Rest of World
acrolein production	acrolein	Rest of World
chlorine dioxide production	chlorine dioxide	Europe
benzene chlorination	o-dichlorobenzene	Rest of World
butane-1,4-diol production	butane-1,4-diol	Rest of World
phenyl acetic acid production	phenyl acetic acid	Rest of World
strontium carbonate production	strontium carbonate	Global
aluminium fluoride production	aluminium fluoride	Rest of World
benzyl chloride production	benzyl chloride	Europe
1-propanol production	1-propanol	Rest of World
calcium ammonium nitrate production	calcium ammonium nitrate	Rest of World
zinc monosulfate production	zinc monosulfate	Europe
maleic anhydride production by catalytic oxidation of benzene	maleic anhydride	Europe
ethylene glycol production	triethylene glycol	Rest of World
epichlorohydrin production from allyl chloride	epichlorohydrin	Europe
ethephon production	ethylene dichloride	Global
phenolic resin production	phenolic resin	Rest of World
sodium amide production	sodium amide	Rest of World
ethyl acetate production	ethyl acetate	Rest of World
silicon production, solar grade, modified Siemens process	silicon, solar grade	Rest of World
soda production, solvay process	soda ash, light	Rest of World
4-tert-butylbenzaldehyde production	4-tert-butylbenzaldehyde	Rest of World

lauric diethanolamide production	lauric diethanolamide	Global
cyanogen chloride production	cyanogen chloride	Rest of World
bromopropane production	bromopropane	Europe
sodium amide production	sodium amide	Europe
tetrafluoroethylene production	tetrafluoroethylene	Rest of World
sodium dithionite production, anhydrous	sodium dithionite, anhydrous	Rest of World
sodium perchlorate production	sodium perchlorate	Global
cyanogen chloride production	cyanogen chloride	Europe
butyl acrylate production	butyl acrylate	Europe
sodium chloroacetate production	sodium chloroacetate	Global
prosulfocarb production	prosulfocarb	Rest of World
chichibabin amination	aminopyridine	Rest of World
ethylenediamine production, from ethylene dichloride	ethylenediamine	Rest of World
vinyl acetate production	vinyl acetate	Europe
sodium sulfate production, from natural sources	sodium sulfate, anhydrite	Rest of World
ammonium nitrite production	ammonium nitrite	Rest of World
titanium dioxide production, sulfate process	titanium dioxide	Europe
glyphosate production	glyphosate	Europe
polysulfone production, for membrane filtration production	polysulfone	Global
styrene production	styrene	Rest of World
Sohio process	acetonitrile	Europe
Brown-Schlesinger process	sodium tetrahydridoborate	Global
ethanolamine production	monoethanolamine	Europe
resorcinol production, benzene disulfonation	resorcinol	Germany
metolachlor production	metolachlor	Europe
glyphosate production	glyphosate	Rest of World
dipropylene glycol monomethyl ether production	dipropylene glycol monomethyl ether	Europe
hydroformylation of butene	3-methyl-1-butanol	Rest of World
hydroformylation of propylene	isobutanol	Rest of World
hydroquinone production	hydroquinone	Rest of World
calcium nitrate production	calcium nitrate	Rest of World
diammonium phosphate production	diammonium phosphate	China
phenyl isocyanate production	phenyl isocyanate	Europe
hexamethylenediamine production	hexamethylenediamine	Rest of World
isopropyl acetate production	isopropyl acetate	Europe
manganese dioxide production	manganese dioxide	Global
vinyl acetate production	vinyl acetate	Rest of World
aluminium hydroxide production	aluminium hydroxide	China
titanium dioxide production, chloride process	titanium dioxide	Rest of World
potassium perchlorate production	potassium perchlorate	Global
aluminium hydroxide production	aluminium hydroxide	International Aluminium Institute producing area, EU27 and EFTA countries
phosphorus pentachloride production	phosphorus pentachloride	Rest of World
ethanolamine production	monoethanolamine	Rest of World
EDTA, ethylenediaminetetraacetic acid production	EDTA, ethylenediaminetetraacetic acid	Rest of World
2-butanol production by hydration of butene	butane	Europe
orbencarb production	orbencarb	Rest of World
sodium silver thiosulfate production	sodium silver thiosulfate	Global

acetone cyanohydrin production	acetone cyanohydrin	Europe
napropamide production	napropamide	Rest of World
dipropyl amine production	dipropyl amine	Europe
sodium pyrophosphate production	sodium pyrophosphate	Global
sodium oxide production	sodium oxide	Europe
methylchloride production	methylchloride	Western Europe
sodium hydrogen sulfite production	sodium hydrogen sulfite	Rest of World
methylamine production	methylamine	Rest of World
metaldehyde production	metaldehyde	Rest of World
fosetyl-Al production	fosetyl-Al	Rest of World
trimethyl borate production	trimethyl borate	Global
benzaldehyde production	benzaldehyde	Rest of World
xylene production	xylene	Europe
chloromethyl methyl ether production	chloromethyl methyl ether	Europe
alpha-naphthol production	alpha-naphthol	Europe
silicon production, single crystal, Czochralski process, photovoltaics	silicon, single crystal, Czochralski process, photovoltaics	Rest of World
lithium fluoride production	lithium fluoride	China
sulfuryl chloride production	sulfuryl chloride	Global
strontium carbonate production	sodium sulfide	Global
ascorbic acid production	ascorbic acid	Rest of World
hydroformylation of propylene	1-butanol	Europe
silicon tetrachloride production	silicon tetrachloride	Global
methallylchloride production	methallylchloride	Global
alpha-picoline production	alpha-picoline	Rest of World
toluene diisocyanate production	toluene diisocyanate	Rest of World
metolachlor production	metolachlor	Rest of World
fluorination of sodium tetrahydridoborate	sodium tetrafluoroborate	Global
4-methyl-2-pentanone production	4-methyl-2-pentanone	Europe
2-butanol production by hydration of butene	2-butanol	Rest of World
piperidine production	piperidine	Rest of World
phosphorus pentachloride production	phosphorus pentachloride	China
zirconium oxide production	zirconium oxide	Australia
stearic acid production	stearic acid	Global
Sohio process	acrylonitrile	Rest of World
lithium hexafluorophosphate production	lithium hexafluorophosphate	China
acrylic acid production	acrylic acid	Europe
daminozide production	daminozide	Global
lithium iron phosphate production, solid state process	lithium iron phosphate	Rest of World
methyl acrylate production	methyl acrylate	Global
sodium hydrosulfide production	sodium hydrosulfide	Europe
glycine production	glycine	Rest of World
methylene diphenyl diisocyanate production	methylene diphenyl diisocyanate	Rest of World
ethanolamine production	triethanolamine	Rest of World
3-methylpyridine production	3-methylpyridine	Europe
lithium chloride production	lithium chloride	Global
1-propanol production	1-propanol	Europe
sodium oxide production	sodium oxide	Rest of World
4-tert-butyltoluene production	4-tert-butyltoluene	Europe
vinyl carbonate production	vinyl carbonate	Global
urea production	urea	North America
dipropylene glycol monomethyl ether production	dipropylene glycol monomethyl ether	Rest of World
cyanuric chloride production	cyanuric chloride	Global
polycarbonate production	polycarbonate	Europe

chloromethyl methyl ether production	chloromethyl methyl ether	Rest of World
vinyl chloride production	vinyl chloride	Europe
allyl chloride production, reaction of propylene and chlorine	dichloropropene	Europe
ascorbic acid production	ascorbic acid	Europe
lithium carbonate production, from spodumene	lithium carbonate	Rest of World
propanal production	propanal	Rest of World
resorcinol production, hydrolysis of meta-phenylene diamine	resorcinol	Global
hydroxylamine production	hydroxylamine	Rest of World
chloridazon production	chloridazon	Global
melamine production	melamine	Europe
potassium hydroxide production	hydrogen, liquid	Europe
potassium sulfate production	potassium sulfate	Europe
zineb production	zineb	Global
decabromodiphenyl ether production	decabromodiphenyl ether	Europe
isopropanol production	isopropanol	Rest of World
ammonium nitrite production	ammonium nitrite	Europe
dioctyl adipate production	dioctyl adipate	Global
dimethyl sulfate production	dimethyl sulfate	Rest of World
sodium hydrogen sulfate production	sodium hydrogen sulfate	Global
aluminium hydroxide production	aluminium hydroxide	United Nations region Oceania
methyl methacrylate production	methyl methacrylate	Rest of World
ethylene glycol monoethyl ether production	ethylene glycol monoethyl ether	Rest of World
decabromodiphenyl ether production	decabromodiphenyl ether	Rest of World
ammonium carbonate production	ammonium carbonate	Europe
prochloraz production	prochloraz	Global
ammonium chloride production	ammonium chloride	Global
Mannheim process	sodium sulfate, anhydrite	Europe
benzal chloride production	benzal chloride	Europe
propyl amine production	propyl amine	Europe
aniline production	aniline	Rest of World
heavy water production	heavy water	Canada
dimethyl ether production	dimethyl ether	Rest of World
chlorothalonil production	chlorothalonil	Europe
sulfur trioxide production	sulfur trioxide	Rest of World
monoammonium phosphate production	monoammonium phosphate	Europe
captan production	captan	Europe
iodine production	iodine	Rest of World
copper carbonate production	copper carbonate	Europe
dimethylamine production	dimethylamine	Europe
urea production	urea	China
aluminium chloride production	aluminium chloride	Global
dioxane production	dioxane	Europe
methacrylic acid production	methacrylic acid	Europe
cumene production	cumene	Rest of World
p-nitrotoluene production	p-nitrotoluene	Europe
epichlorohydrin production from allyl chloride	trichloropropane	Europe
Mannheim process	sodium sulfate, anhydrite	Rest of World
decarboxylative cyclization of adipic acid	formic acid	Rest of World
disodium disulphite production	disodium disulphite	Global
paclobutrazol production	paclobutrazol	Global
phenyl isocyanate production	phenyl isocyanate	Rest of World
propyl amine production	propyl amine	Rest of World
2,4-dichlorotoluene production	2,4-dichlorotoluene	Europe

ethyl tert-butyl ether production, from bioethanol	ethyl tert-butyl ether	Europe
phthalimide production	phthalimide	Rest of World
trichloroborane production	trichloroborane	Global
phenyl acetic acid production	phenyl acetic acid	Europe
chloroacetic acid production	chloroacetic acid	Europe
butyl acetate production	butyl acetate	Europe
triethyl amine production	triethyl amine	Europe
benzaldehyde production	benzaldehyde	Europe
polybutadiene production	polybutadiene	Rest of World
ammonium sulfate production	ammonium sulfate	Rest of World
octabenzone production	octabenzone	Global
ethylene glycol production	diethylene glycol	Europe
isopropanol production	isopropanol	Europe
p-nitrophenol production	p-nitrophenol	Europe
acetyl chloride production	acetyl chloride	Europe
chloroacetyl chloride production	chloroacetyl chloride	Rest of World
dioctyl terephthalate production	dioctyl terephthalate	Global
o-nitrophenol production	o-nitrophenol	Europe
dimethyl carbonate production	dimethyl carbonate	Rest of World
ethyl benzene production	ethyl benzene	Europe
fosetyl-Al production	sodium nitrate	Rest of World
cumene production	cumene	Europe
dimethyl sulfide production	dimethyl sulfide	Europe
p-chlorophenol production	p-chlorophenol	Europe
titanium dioxide production, chloride process	titanium dioxide	Europe
soda production, solvay process	soda ash, light	Europe
sodium phosphate production	sodium phosphate	Europe
carbon disulfide production, from charcoal	carbon disulfide	Global
boric oxide production	boric oxide	Global
potassium hydroxide production	potassium hydroxide	Europe
cyclohexanol production	cyclohexanol	Rest of World
ethylene glycol diethyl ether production	ethylene glycol diethyl ether	Europe
ethephon production	ethephon	Global
sodium dichromate production	sodium dichromate	Europe
benzene chlorination	p-dichlorobenzene	Europe
sodium tripolyphosphate production	sodium tripolyphosphate	Rest of World
dimethylaminopropylamine production	dimethylaminopropylamine	Europe
ethyl acetate production	ethyl acetate	Europe
isoproturon production	isoproturon	Rest of World
styrene production	styrene	Europe
boron carbide production	boron carbide	Global
copper oxide production	copper oxide	Europe
chlorine dioxide production	chlorine dioxide	Rest of World
benzene chlorination	o-dichlorobenzene	Europe
methyl iodide production	methyl iodide	Europe
lithium carbonate production, from spodumene	lithium carbonate	China
hydrogen cyanide production	hydrogen cyanide	Rest of World
pentaerythritol production in sodium hydroxide solution	sodium formate	Rest of World
polybutadiene production	polybutadiene	Europe
triethyl amine production	triethyl amine	Rest of World
toluene oxidation	benzoic acid	Europe
amidosulfuron production	amidosulfuron	Global
metamitron production	metamitron	Rest of World
2,4-dichlorophenol production	2,4-dichlorophenol	Rest of World
ammonium nitrate phosphate production	ammonium nitrate phosphate	Europe

acetone cyanohydrin production	acetone cyanohydrin	Rest of World
dehydrogenation of butan-1,4-diol	butyrolactone	Rest of World
dimethyl carbonate production	formaldehyde	Rest of World
potassium mining and benefication	potassium chloride	Canada-Saskatchewan
hydroformylation of butene	1-pentanol	Europe
hydroformylation of butene	2-methyl-1-butanol	Europe
lithium carbonate production, from concentrated brine	lithium carbonate	Global
fibre production, viscose	sulfuric acid	Global
indium production	indium	Europe
2,6-di-tert-butylphenol production	2,6-di-tert-butylphenol	Global
vinyl fluoride production	vinyl fluoride	Rest of World
maleic hydrazide production	maleic hydrazide	Global
hydroquinone production	hydroquinone	Europe
aluminium hydroxide production	aluminium hydroxide	International Aluminium Institute producing area, Russia and Europe outside EU27 and EFTA
hydroformylation of butene	1-pentanol	Rest of World
propyl acetate production	isopropyl acetate	Rest of World
isohexane production	isohexane	Europe
sulfamic acid production	sulfamic acid	Global
urea formaldehyde resin production	urea formaldehyde resin	Rest of World
pentaerythritol production in sodium hydroxide solution	pentaerythritol	Rest of World
isopropylamine production	isopropylamine	Rest of World
dimethylamine production	dimethylamine	Rest of World
nylon 6 production	nylon 6	Europe
helium purification	helium	Global
calcium carbonate production, precipitated	calcium carbonate, precipitated	Rest of World
vinyl fluoride production	vinyl fluoride	United States of America
silicon production, solar grade, modified Siemens process	silicon, solar grade	Europe
ethylene glycol production	ethylene glycol	Europe
glycerine production, from epichlorohydrin	glycerine	Europe
sulfur dichloride production	sulfur dichloride	Europe
naphthalene sulfonic acid production	naphthalene sulfonic acid	Europe
urea formaldehyde resin production	urea formaldehyde resin	Europe
dimethyl sulfoxide production	dimethyl sulfoxide	Europe
phosphorous chloride production	phosphorous chloride	Rest of World
salicylic acid production	salicylic acid	Global
silicon hydrochloration	silicon tetrahydride	Global
4-tert-butyltoluene production	4-tert-butyltoluene	Rest of World
chloronitrobenzene production	chloronitrobenzene	Rest of World
monoammonium phosphate production	monoammonium phosphate	North America
aluminium hydroxide production	aluminium hydroxide	International Aluminium Institute producing area, South America
benzene chlorination	p-dichlorobenzene	Rest of World
calcium carbonate production, precipitated	calcium carbonate, precipitated	Europe
mecoprop production	mecoprop	Rest of World
acrolein production	acrolein	Europe

Mannheim process	hydrochloric acid, without water, in 30% solution state	Rest of World
alkyl sulphate (C12-14) production	alkyl sulphate (C12-14)	Global
sodium nitrite production	sodium nitrite	Europe
diammonium phosphate production	diammonium phosphate	North America
acetoacetic acid production	acetoacetic acid	Rest of World
zinc monosulfate production	zinc monosulfate	Rest of World
tebuconazole production	tebuconazole	Global
dimethyl carbonate production	dimethyl carbonate	Europe
barium carbonate production	barium carbonate	Global
sodium chlorate production, powder	sodium chlorate, powder	Rest of World
chlorofluorination of ethylene	monochloropentafluoroethane	Global
nylon 6 production	nylon 6	Rest of World
silicon production, electronics grade	silicon tetrachloride	Germany
aclonifen production	aclonifen	Rest of World
acetaldehyde production	acetaldehyde	Europe
N-methyl-2-pyrrolidone production	N-methyl-2-pyrrolidone	Rest of World
mancozeb production	mancozeb	Rest of World
acetaldehyde oxidation	acetic anhydride	Rest of World
ethylene glycol monoethyl ether production	ethylene glycol monoethyl ether	Europe
phenol production, from cumene	phenol	Europe
sodium cumenesulphonate production	sodium cumenesulphonate	Rest of World
tetrafluoroethylene production	tetrafluoroethylene	Europe
acetanilide production	acetanilide	Europe
chloroacetic acid production	chloroacetic acid	Rest of World
copper oxide production	copper oxide	Rest of World
xylene production	xylene	Rest of World
sodium sulfite production	sodium sulfite	Rest of World
trichloroacetic acid production	trichloroacetic acid	Rest of World
methyl methacrylate production	methyl methacrylate	Europe
potassium chloride production	potassium chloride	Rest of World
fosetyl-Al production	fosetyl-Al	Europe
adipic acid production	succinic acid	Europe
6-benzyladenine production	6-benzyladenine	Global
dimethylacetamide production	dimethylacetamide	Global
ammonium nitrate phosphate production	ammonium nitrate phosphate	China
melamine production	melamine	Rest of World
methyl iodide production	methyl iodide	Rest of World
chloronitrobenzene production	chloronitrobenzene	Europe
captan production	captan	Rest of World
metazachlor production	metazachlor	Global
barium oxide production	barium oxide	Global
hydrochloric acid production, from the reaction of hydrogen with chlorine	hydrochloric acid, without water, in 30% solution state	Rest of World
sodium chlorate production, powder	sodium chlorate, powder	Europe
allyl chloride production, reaction of propylene and chlorine	allyl chloride	Europe
glycerine production, from epichlorohydrin	glycerine	Rest of World
sodium sulfide production	sodium sulfide	Global
N-methyl-2-pyrrolidone production	N-methyl-2-pyrrolidone	Europe
oxidation of methanol	formaldehyde	Rest of World
bromine production	bromine	Europe
epichlorohydrin production from allyl chloride	trichloropropane	Rest of World
sodium nitrate production	sodium nitrate	Europe
methyl ethyl ketone production	methyl ethyl ketone	Rest of World
potassium chloride production	potassium chloride	Europe

succinic acid production	succinic acid	Global
phosphorous chloride production	phosphorous chloride	Europe
chichibabin pyridine synthesis	pyridine	Europe
mepiquat chloride production	mepiquat chloride	Global
naphthalene sulfonic acid production	naphthalene sulfonic acid	Rest of World
modified Solvay process, Hou's process	ammonium chloride	Global
propyl acetate production	isopropyl acetate	Europe
benzene chlorination	monochlorobenzene	Rest of World
propionic acid production	propionic acid	Rest of World
oxalic acid production	oxalic acid	Rest of World
indium production	indium	Rest of World
vinyl fluoride production	hydrogen fluoride	Rest of World
styrene-acrylonitrile copolymer production	styrene-acrylonitrile copolymer	Europe
Sohio process	acetonitrile	Rest of World
tetrachloroethylene production	tetrachloroethylene	Western Europe
o-chlorotoluene production	o-chlorotoluene	Europe
oxidation of methanol	formaldehyde	Europe
isopropylamine production	isopropylamine	Europe
soda production, solvay process	sodium bicarbonate	Rest of World
acetoacetic acid production	acetoacetic acid	Europe
o-chlorobenzaldehyde production	o-chlorobenzaldehyde	Rest of World
trimesoyl chloride production, for membrane filtration production	trimesoyl chloride	Global
nickel sulfate production	nickel sulfate	Global
sulfur trioxide production	sulfur trioxide	Europe
dimethylaminopropylamine production	dimethylaminopropylamine	Rest of World
toluene diisocyanate production	toluene diisocyanate	Europe
amination of chlorosilane	ammonium chloride	Global
isopropyl acetate production	isopropyl acetate	Rest of World
morpholine production	morpholine	Global
o-cresol production	o-cresol	Rest of World
ethylene glycol production	triethylene glycol	Europe
selenium production	selenium	Rest of World
purification of wet-process phosphoric acid to industrial grade, product in 85% solution state	phosphoric acid, industrial grade, without water, in 85% solution state	Rest of World
formic acid production, methyl formate route	formic acid	Europe
p-chlorophenol production	p-chlorophenol	Rest of World
chlorodifluoromethane production	chlorodifluoromethane	Rest of World
4-methyl-2-pentanone production	4-methyl-2-pentanone	Rest of World
calcium nitrate production	ammonium nitrate	Rest of World
hydrazine production	hydrazine	Europe
electrolysis of lithium chloride	lithium	Global
sodium ethyl xanthate production	sodium ethyl xanthate	Rest of World
hydroformylation of butene	3-methyl-1-butanol	Europe
cadmium telluride production, semiconductor-grade	cadmium telluride, semiconductor-grade	United States of America
sodium cumenesulphonate production	sodium cumenesulphonate	Europe
2-pyridinol production	2-pyridinol	Rest of World
chlorothalonil production	chlorothalonil	Rest of World
prosulfocarb production	prosulfocarb	Europe
resorcinol production, benzene disulfonation	sodium sulfite	Germany
cobalt sulfate production	cobalt sulfate	Rest of World
sodium hypochlorite production, product in 15% solution state	sodium hypochlorite, without water, in 15% solution state	Canada-Quebec
ethylene carbonate production	ethylene carbonate	Rest of World

cyclohexanol production	cyclohexanol	Europe
hydrogen fluoride production	hydrogen fluoride	Rest of World
dimethyldichlorosilane production	dimethyldichlorosilane	Global
epichlorohydrin production from allyl chloride	calcium chloride	Europe
hydrazine production	hydrazine	Rest of World
formic acid production, methyl formate route	formic acid	Rest of World
ethylene glycol dimethyl ether production	ethylene glycol dimethyl ether	Europe
1-methoxy-2-propanol production	1-methoxy-2-propanol	Global
ammonium carbonate production	ammonium carbonate	Rest of World
hexamethylenediamine production	hexamethylenediamine	Europe
sodium phosphate production	sodium phosphate	Rest of World
atrazine production	atrazine	Europe
carbon tetrachloride production	carbon tetrachloride	Rest of World
monoammonium phosphate production	monoammonium phosphate	Rest of World
acetyl chloride production	acetyl chloride	Rest of World
sodium hydrosulfide production	sodium hydrosulfide	Rest of World
mecoprop production	mecoprop	Europe
2,4-dichlorotoluene production	2,4-dichlorotoluene	Rest of World
trichloroethylene production	hydrochloric acid, without water, in 30% solution state	Rest of World
methyl formate production	methyl formate	Europe
ethylene carbonate production	ethylene carbonate	China
o-aminophenol production	o-aminophenol	Rest of World
vinyl fluoride production	hydrogen fluoride	United States of America
phthalimide production	phthalimide	Europe
p-nitrotoluene production	p-nitrotoluene	Rest of World
aluminium hydroxide production	aluminium hydroxide	International Aluminium Institute producing area, South and East Asia, without China
2-butanol production by hydration of butene	butane	Rest of World
selenium production	selenium	Europe
lithium sulfate production	lithium sulfate	Global
ethylene oxide production	ethylene oxide	Europe
bromine production	bromine	Rest of World
urea production	urea	Europe
imidazole production	imidazole	Rest of World
2,4-dinitrotoluene production	2,4-dinitrotoluene	Europe
copper carbonate production	copper carbonate	Rest of World
glyoxal production	glyoxal	Rest of World
2,4-dinitrotoluene production	2,4-dinitrotoluene	Rest of World
imidazole production	imidazole	Europe
dinitrogen tetroxide production	dinitrogen tetroxide	Global
trifluoromethane production	trifluoromethane	Global
dimethyl sulfate production	dimethyl sulfate	Europe
ethylenediamine production, from ethylene dichloride	ethylenediamine	Europe
o-nitrophenol production	o-nitrophenol	Rest of World
ammonium nitrate phosphate production	ammonium nitrate phosphate	Rest of World
silicon production, single crystal, Czochralski process, photovoltaics	silicon, single crystal, Czochralski process, photovoltaics	Europe
manganese(III) oxide production	manganese(III) oxide	China
p-nitrophenol production	p-nitrophenol	Rest of World

ethylamine production	ethylamine	Europe
manganese dioxide production	manganese sulfate	Global
sodium ethyl xanthate production	sodium ethyl xanthate	South Africa
2-butanol production by hydration of butene	2-butanol	Europe
dimethyl ether production	dimethyl ether	Europe
ammonium nitrate phosphate production	ammonium nitrate phosphate	North America
potassium sulfate production	potassium sulfate	Rest of World
ethylene glycol production	diethylene glycol	Rest of World
piperidine production	piperidine	Europe
cyclohexanone production	cyclohexanone	Rest of World
sodium hypochlorite production, product in 15% solution state	sodium hypochlorite, without water, in 15% solution state	Rest of World
allyl chloride production, reaction of propylene and chlorine	allyl chloride	Rest of World
amination of chlorosilane	hexamethyldisilazane	Global
folpet production	folpet	Rest of World
anthranilic acid production	anthranilic acid	Rest of World
nitrobenzene production	nitrobenzene	Rest of World
isobutyl acetate production	isobutyl acetate	Rest of World
manganese(III) oxide production	manganese(III) oxide	Rest of World
polycarbonate production	polycarbonate	Rest of World
ethylene glycol diethyl ether production	ethylene glycol diethyl ether	Rest of World
cyclohexane production	cyclohexane	Rest of World
cyclohexane production	cyclohexane	Europe
cadmium telluride production, semiconductor-grade	cadmium telluride, semiconductor-grade	Rest of World
silicon production, electronics grade	silicon, solar grade	Germany
maneb production	maneb	Global
soda production, solvay process	calcium chloride	Rest of World
epichlorohydrin production from allyl chloride	calcium chloride	Rest of World
fosetyl-Al production	sodium nitrate	Europe
alpha-picoline production	alpha-picoline	Europe
chloroacetyl chloride production	chloroacetyl chloride	Europe
methylene diphenyl diisocyanate production	methylene diphenyl diisocyanate	Europe
dimethyl sulfide production	dimethyl sulfide	Rest of World
methyl formate production	methyl formate	Rest of World
adipic acid production	adipic acid	Rest of World
2-pyridinol production	2-pyridinol	Europe
dimethyl carbonate production	formaldehyde	Europe
copper sulfate production	copper sulfate	Global
pyrazole production	pyrazole	Rest of World
metamitron production	metamitron	Europe
hydroformylation of butene	2-methyl-1-butanol	Rest of World
cyanoacetic acid production	cyanoacetic acid	Europe
calcium nitrate production	ammonium nitrate	Europe
hydrogen fluoride production	hydrogen fluoride	Europe
methyl ethyl ketone production	methyl ethyl ketone	Europe
benzyl alcohol production	benzyl alcohol	Rest of World
iodine production	iodine	Europe
dipropyl amine production	dipropyl amine	Rest of World
hydrochloric acid production, from the reaction of hydrogen with chlorine	hydrochloric acid, without water, in 30% solution state	Canada-Quebec
sodium chlorate production, powder	sodium chlorate, powder	Canada-Quebec
sodium fluoride production	sodium fluoride	Global
acrylonitrile-butadiene-styrene copolymer production	acrylonitrile-butadiene-styrene copolymer	Rest of World

Brown-Schlesinger process	sodium methoxide	Global
phosphorus oxychloride production, from phosphorus trichloride	phosphorus oxychloride	Europe
hydrogen cyanide production	hydrogen cyanide	Europe
silicon production, electronics grade	silicon, solar grade	Rest of World
trichloroethylene production	trichloroethylene	Europe
lactic acid production	lactic acid	Europe
dodecanol production, from coconut oil	dodecanol	Global
potassium hydroxide production	chlorine, gaseous	Rest of World
metaldehyde production	metaldehyde	Europe
stearic acid production	glycerine	Global
acrylic acid production	acrylic acid	Rest of World
bromoxynil production	bromoxynil	Global
acetylene production	acetylene	Europe
sodium cyanide production	sodium cyanide	Rest of World
calcium nitrate production	calcium nitrate	Europe
o-chlorobenzaldehyde production	o-chlorobenzaldehyde	Europe
triphenyl phosphate production	triphenyl phosphate	Global
diammonium phosphate production	diammonium phosphate	Europe
dimethyl hexynediol production	dimethyl hexynediol	Global
salicylic acid production	phenol	Global
atrazine production	atrazine	Rest of World
sodium tripolyphosphate production	sodium tripolyphosphate	Europe
fluazifop-butyl production	fluazifop-butyl	Global
dioxane production	dioxane	Rest of World
potassium hydroxide production	potassium hydroxide	Rest of World
diammonium phosphate production	diammonium phosphate	Rest of World
chlorotoluron production	chlorotoluron	Europe
monoammonium phosphate production	monoammonium phosphate	China
2,4-di-tert-butylphenol production	2,4-di-tert-butylphenol	Global
trifluoroacetic acid production	trifluoroacetic acid	Europe
dimethylamine borane production	dimethylamine borane	Global
methylchloride production	methylchloride	Rest of World
ethylene oxide production	ethylene oxide	Rest of World
chloropropionic acid production	chloropropionic acid	Rest of World
soda production, solvay process	calcium chloride	Europe
chlormequat chloride production	chlormequat chloride	Global
hydrazine sulfate production	hydrazine sulfate	Global
o-chlorotoluene production	o-chlorotoluene	Rest of World
dichloromethane production	dichloromethane	Europe
nitrous oxide production	nitrous oxide	Rest of World
pyrazole production	pyrazole	Europe
thionyl chloride production	thionyl chloride	Europe
2-methyl-2-butanol production	2-methyl-2-butanol	Europe
adiponitrile production	adiponitrile	Rest of World
sodium sulfate production, from natural sources	sodium sulfate, anhydrite	Europe
sodium hypochlorite production, product in 15% solution state	sodium hypochlorite, without water, in 15% solution state	Europe
sodium sulfite production	sodium sulfite	Europe
silicon production, electronics grade	silicon, electronics grade	Rest of World
styrene-acrylonitrile copolymer production	styrene-acrylonitrile copolymer	Rest of World
tetrachloroethylene production	tetrachloroethylene	Rest of World
phosphane production	phosphane	Global
tris(2,4-ditert-butylphenyl) phosphite production	tris(2,4-ditert-butylphenyl) phosphite	Global
refrigerant R134a production	refrigerant R134a	Rest of World
chichibabin pyridine synthesis	pyridine	Rest of World

silicon hydrochloration	silicon tetrachloride	Global
butyl acrylate production	butyl acrylate	Rest of World
methacrylic acid production	methacrylic acid	Rest of World
propionic acid production	propionic acid	Europe
silicon production, electronics grade	silicon tetrachloride	Rest of World
sodium chloride electrolysis	sodium	Europe
N,N-dimethylformamide production	N,N-dimethylformamide	Europe
sodium phenolate production	sodium phenolate	Rest of World
ethylamine production	ethylamine	Rest of World
dehydrogenation of butan-1,4-diol	butyrolactone	Europe
chlorofluorination of ethylene	hexafluoroethane	Global
trisodium phosphate production	trisodium phosphate	Global
sodium formate production	sodium formate	Global
sodium dichromate production	sodium dichromate	Rest of World
maleic anhydride production by catalytic oxidation of benzene	maleic anhydride	Rest of World
pendimethalin production	pendimethalin	Rest of World
nitrobenzene production	nitrobenzene	Europe
adiponitrile production	adiponitrile	Europe
silicon tetrachloride production	carbon monoxide	Global
epichlorohydrin production from allyl chloride	epichlorohydrin	Rest of World
N,N-dimethylformamide production	N,N-dimethylformamide	Rest of World
sodium methoxide production	sodium methoxide	Global
phenolic resin production	phenolic resin	Europe
cyanoacetic acid production	cyanoacetic acid	Rest of World
butadiene production	butadiene	Rest of World
aluminium fluoride production	aluminium fluoride	Europe
Mannheim process	hydrochloric acid, without water, in 30% solution state	Europe
zinc sulfide production	sulfuric acid	Rest of World
2,4-dichlorophenol production	2,4-dichlorophenol	Europe
ethyl benzene production	ethyl benzene	Rest of World
chlorotoluron production	chlorotoluron	Rest of World
acetylene production	acetylene	Rest of World
butadiene production	butadiene	Europe
tetraethyl orthosilicate production	tetraethyl orthosilicate	Global
benzene chlorination	monochlorobenzene	Europe
zinc sulfide production	sulfuric acid	Europe
arsine production	arsine	Global
potassium hydroxide production	hydrogen, liquid	Rest of World
allyl chloride production, reaction of propylene and chlorine	dichloropropene	Rest of World
acetaldehyde oxidation	acetic anhydride	Europe
ethylenediamine production, from ethanolamine	ethylenediamine	Europe
3-methylpyridine production	3-methylpyridine	Rest of World
1-methylcyclopropene production	1-methylcyclopropene	Global
cyclohexanone production	cyclohexanone	Europe
pentaerythritol production in sodium hydroxide solution	pentaerythritol	Europe
hydrochloric acid production, from the reaction of hydrogen with chlorine	hydrochloric acid, without water, in 30% solution state	Europe
sodium chloride electrolysis	sodium	Rest of World
refrigerant R134a production	refrigerant R134a	Europe
aclonifen production	aclonifen	Europe
alpha-naphthol production	alpha-naphthol	Rest of World
trifluoroacetic acid production	trifluoroacetic acid	Rest of World
ioxynil production	ioxynil	Global

dimethyl sulfoxide production	dimethyl sulfoxide	Rest of World
hydroformylation of propylene	1-butanol	Rest of World
isobutyl acetate production	isobutyl acetate	Europe
3-methyl-1-butyl acetate production	3-methyl-1-butyl acetate	Europe
silicon production, electronics grade	silicon, electronics grade	Germany
trimethylamine production	trimethylamine	Rest of World
ethylenediamine production, from ethanolamine	ethylenediamine	Rest of World
orbencarb production	orbencarb	Europe
glycine production	glycine	Europe
purification of wet-process phosphoric acid to industrial grade, product in 85% solution state	phosphoric acid, industrial grade, without water, in 85% solution state	Europe
sodium nitrite production	sodium nitrite	Rest of World
dimethyl malonate production	dimethyl malonate	Rest of World
polydimethylsiloxane production	polydimethylsiloxane	Global
sodium nitrate production	sodium nitrate	Rest of World
EDTA, ethylenediaminetetraacetic acid production	EDTA, ethylenediaminetetraacetic acid	Europe
o-cresol production	o-cresol	Europe
decarboxylative cyclization of adipic acid	formic acid	Europe
heavy water production	heavy water	Rest of World
ethylene bromide production	ethylene bromide	Europe
trichloropropane production	trichloropropane	Global
3-methyl-1-butyl acetate production	3-methyl-1-butyl acetate	Rest of World
sodium persulfate production	sodium persulfate	Global
glyoxal production	glyoxal	Europe
fluorination of sodium tetrahydridoborate	diborane	Global
ethylene glycol production	ethylene glycol	Rest of World
ammonium sulfate production	ammonium sulfate	Europe
calcium ammonium nitrate production	calcium ammonium nitrate	North America
hydroformylation of propylene	isobutanol	Europe
trichloroethylene production	hydrochloric acid, without water, in 30% solution state	Europe
calcium ammonium nitrate production	calcium ammonium nitrate	Europe
butane-1,4-diol production	butane-1,4-diol	Europe
thionyl chloride production	thionyl chloride	Rest of World
triclopyr production	triclopyr	Global
potassium carbonate production, from potassium hydroxide	potassium carbonate	Global
ethylene glycol dimethyl ether production	ethylene glycol dimethyl ether	Rest of World
sodium hydrogen sulfite production	sodium hydrogen sulfite	Europe
dimethyl hexanediol production	dimethyl hexanediol	Global
toluene oxidation	benzoic acid	Rest of World
pendimethalin production	pendimethalin	Europe
urea production	urea	Rest of World
chlorosulfonic acid production	chlorosulfonic acid	Rest of World
tert-butyl amine production	tert-butyl amine	Europe
indolylbutyric acid production	indolylbutyric acid	Global
mancozeb production	mancozeb	Europe
1-naphthylacetic acid production	1-naphthylacetic acid	Global
folpet production	folpet	Europe
titanium dioxide production, sulfate process	titanium dioxide	Rest of World
methylamine production	methylamine	Europe
bromopropane production	bromopropane	Rest of World
zirconium oxide production	zirconium oxide	Rest of World

S3. Scatter plots – process mass- and energy-based metric scores *vs.* Environmental Footprint life cycle impacts

Figures S1 to **S16** present the scatter plots between each process-level mass- and energy-based metric (E-factor incl. water, E-factor excl. water, Process Mass Intensity, Mass Intensity and Process Energy Intensity) and life cycle impact category of the Environmental Footprint method. The following scatter plots serve as a visual of the correlation strengths presented in **Figure 2** of the main text – *i.e.*, higher correlation coefficients correspond to a stronger relationship between the process-level metric and life cycle impact (an increase in one corresponds to an increase in the other). Scatter plot points are colour coded according to whether product compounds are organic or inorganic to visualise the composition of our analysed dataset.

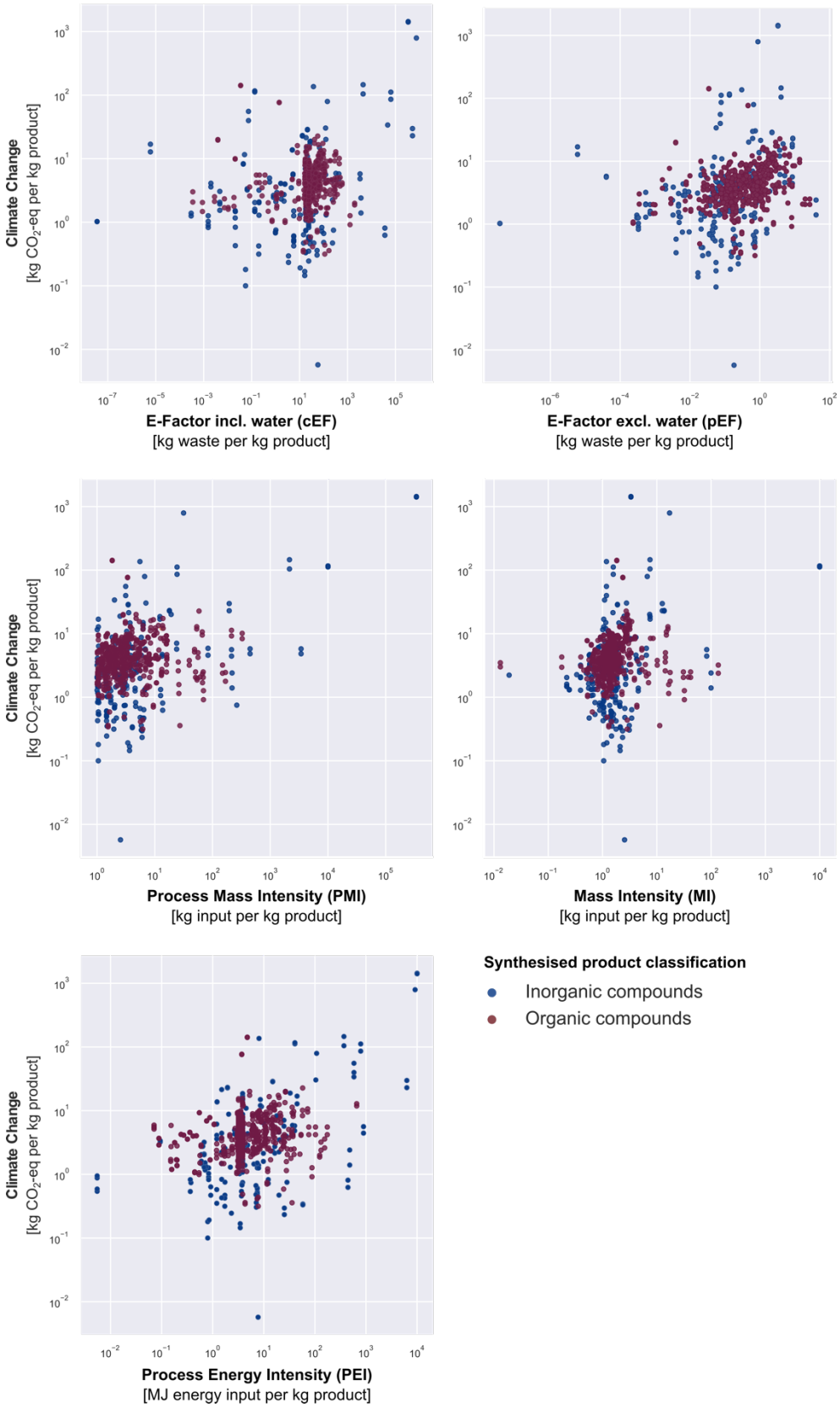

Figure S1. Scatter plots for life cycle climate change impacts (y-axis) *vs.* process-level metrics (x-axis) (*N* = 711 processes). Each data point corresponds to the impact and metric score of a chemical production process. Colour of data points correspond to the organic/inorganic classification of the product.

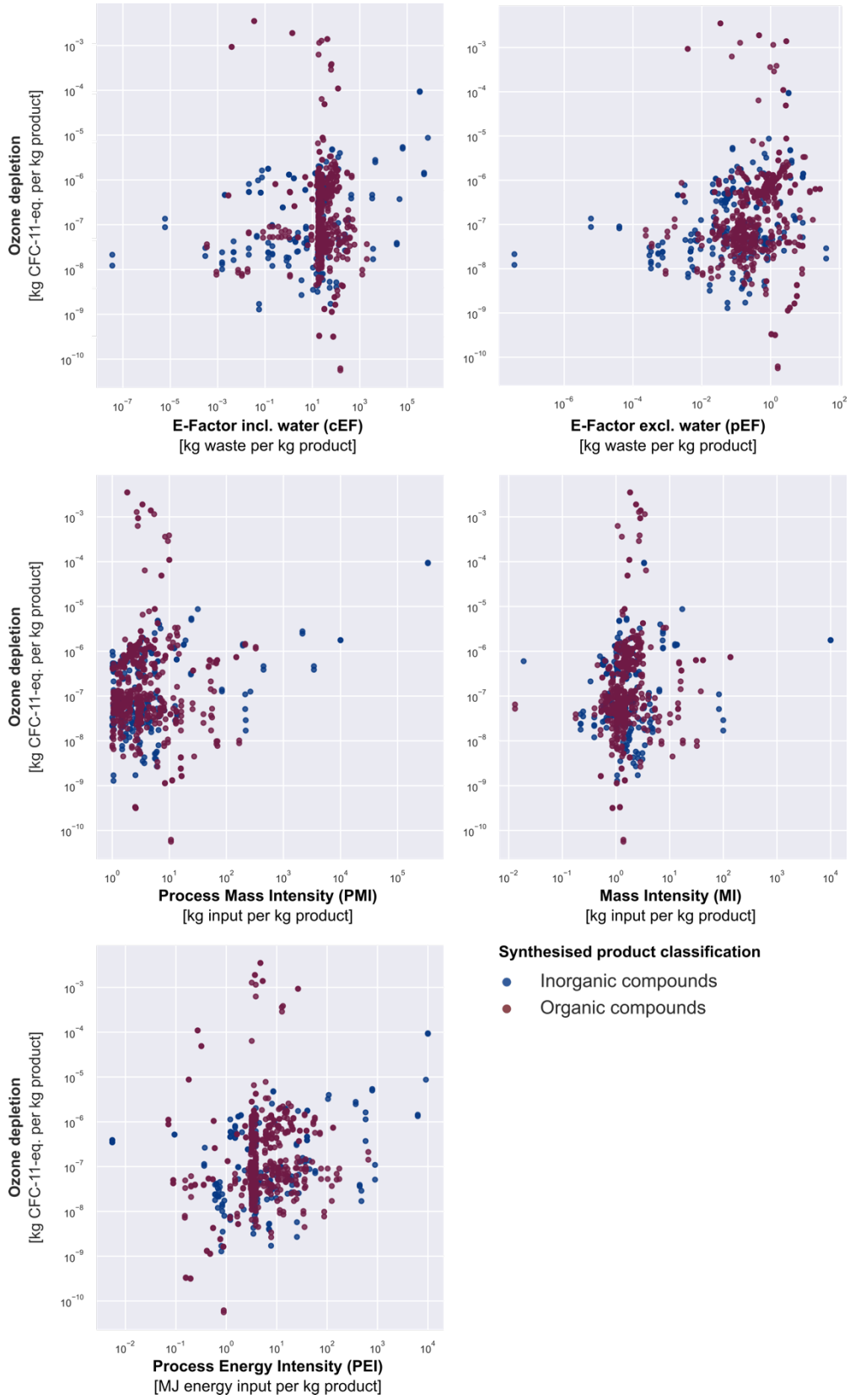

Figure S2. Scatter plots for life cycle ozone depletion impacts (y-axis) *vs.* process-level metrics (x-axis) (*N* = 711 processes). Each data point corresponds to the impact and metric score of a chemical production process. Colour of data points correspond to the organic/inorganic classification of the product.

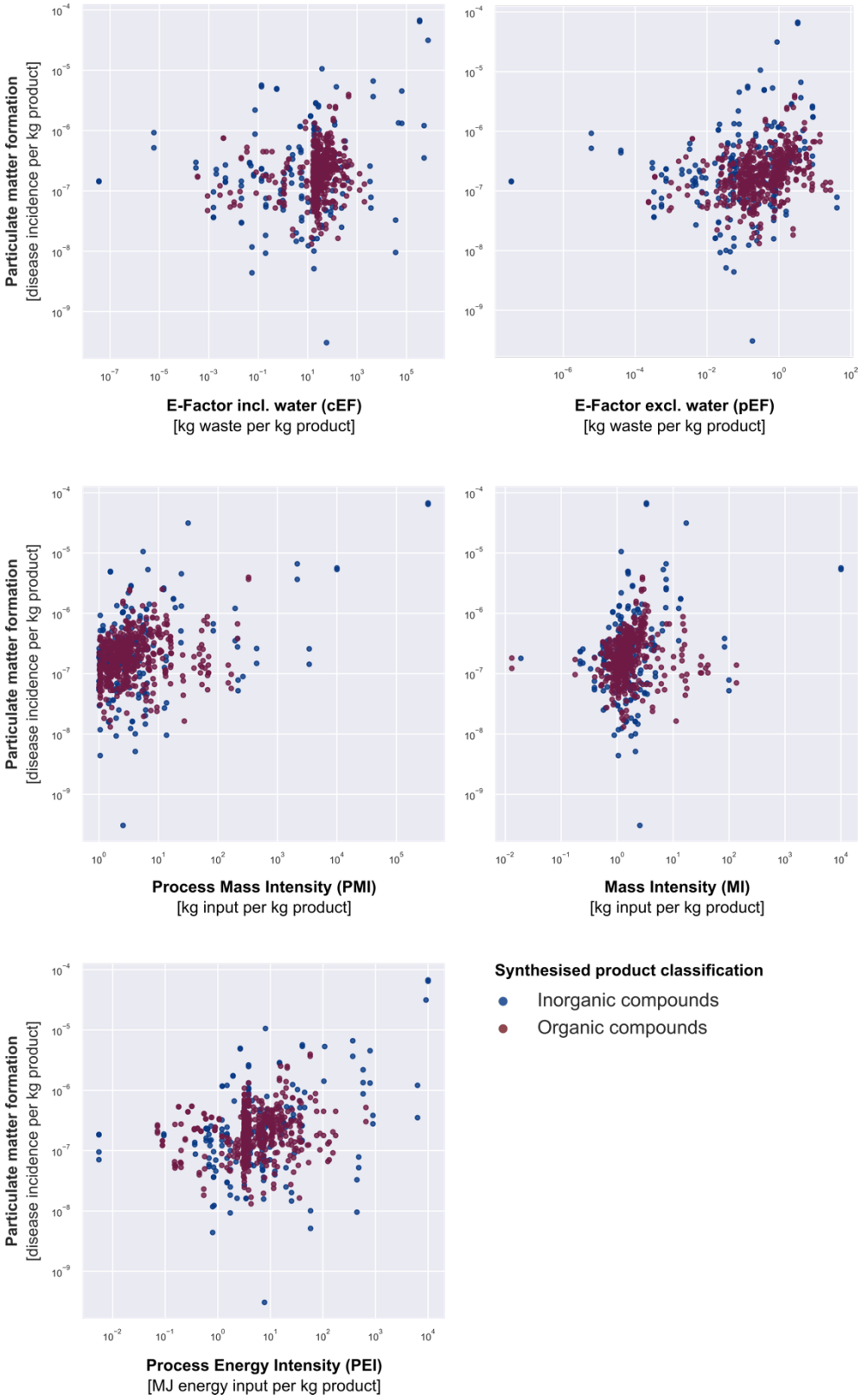

Figure S3. Scatter plots for life cycle particulate matter formation impacts (y-axis) vs. process-level metrics (x-axis) (*N* = 711 processes). Each data point corresponds to the impact and metric score of a chemical production process. Colour of data points correspond to the organic/inorganic classification of the product.

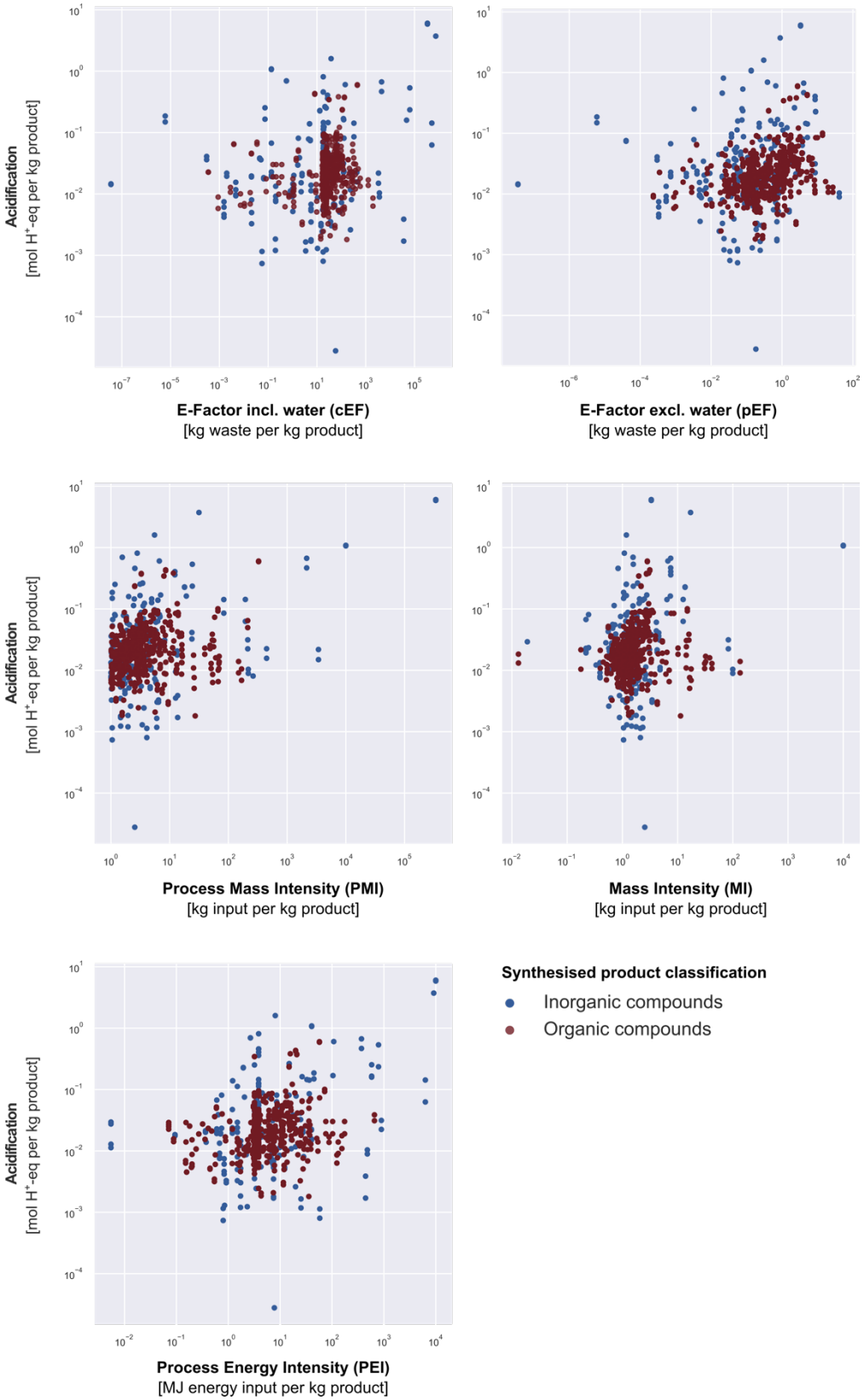

Figure S4. Scatter plots for life cycle acidification impacts (y-axis) *vs.* process-level metrics (x-axis) (*N* = 711 processes). Each data point corresponds to the impact and metric score of a chemical production process. Colour of data points correspond to the organic/inorganic classification of the product.

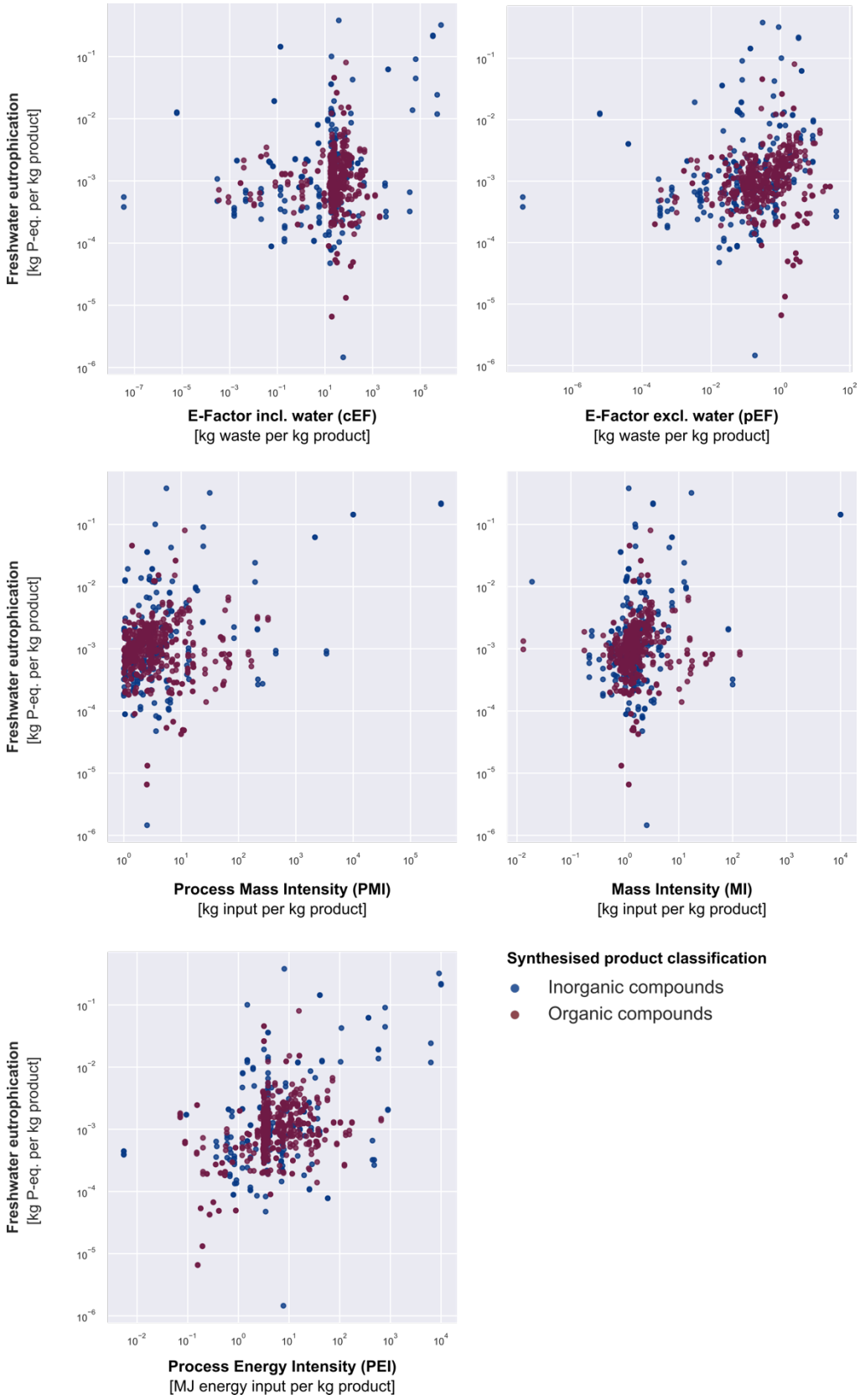

Figure S5. Scatter plots for life cycle freshwater eutrophication impacts (y-axis) *vs.* process-level metrics (x-axis) (*N* = 711 processes). Each data point corresponds to the impact and metric score of a chemical production process. Colour of data points correspond to the organic/inorganic classification of the product.

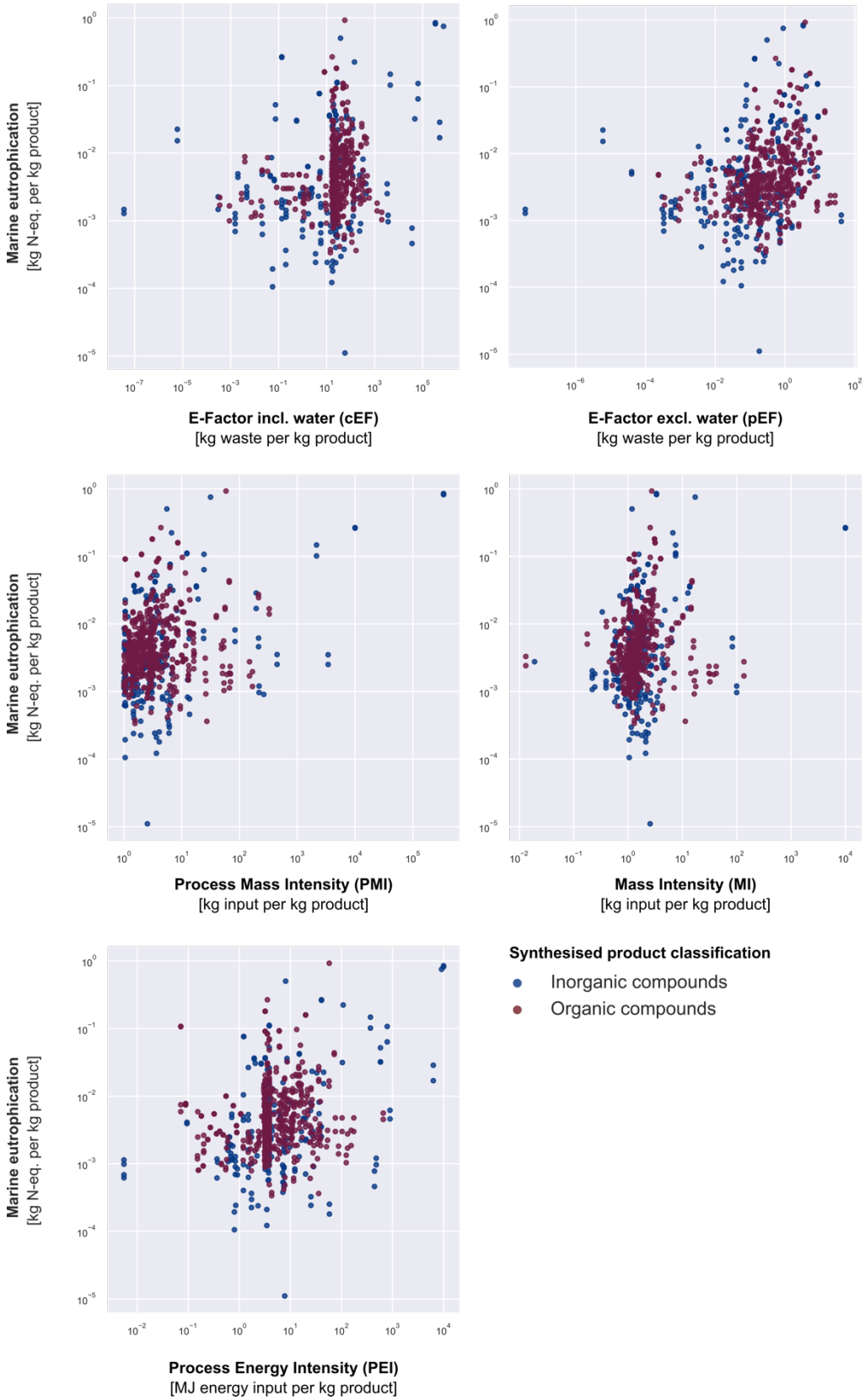

Figure S6. Scatter plots for life cycle marine eutrophication impacts (y-axis) *vs.* process-level metrics (x-axis) (N = 711 processes). Each data point corresponds to the impact and metric score of a chemical production process. Colour of data points correspond to the organic/inorganic classification of the product.

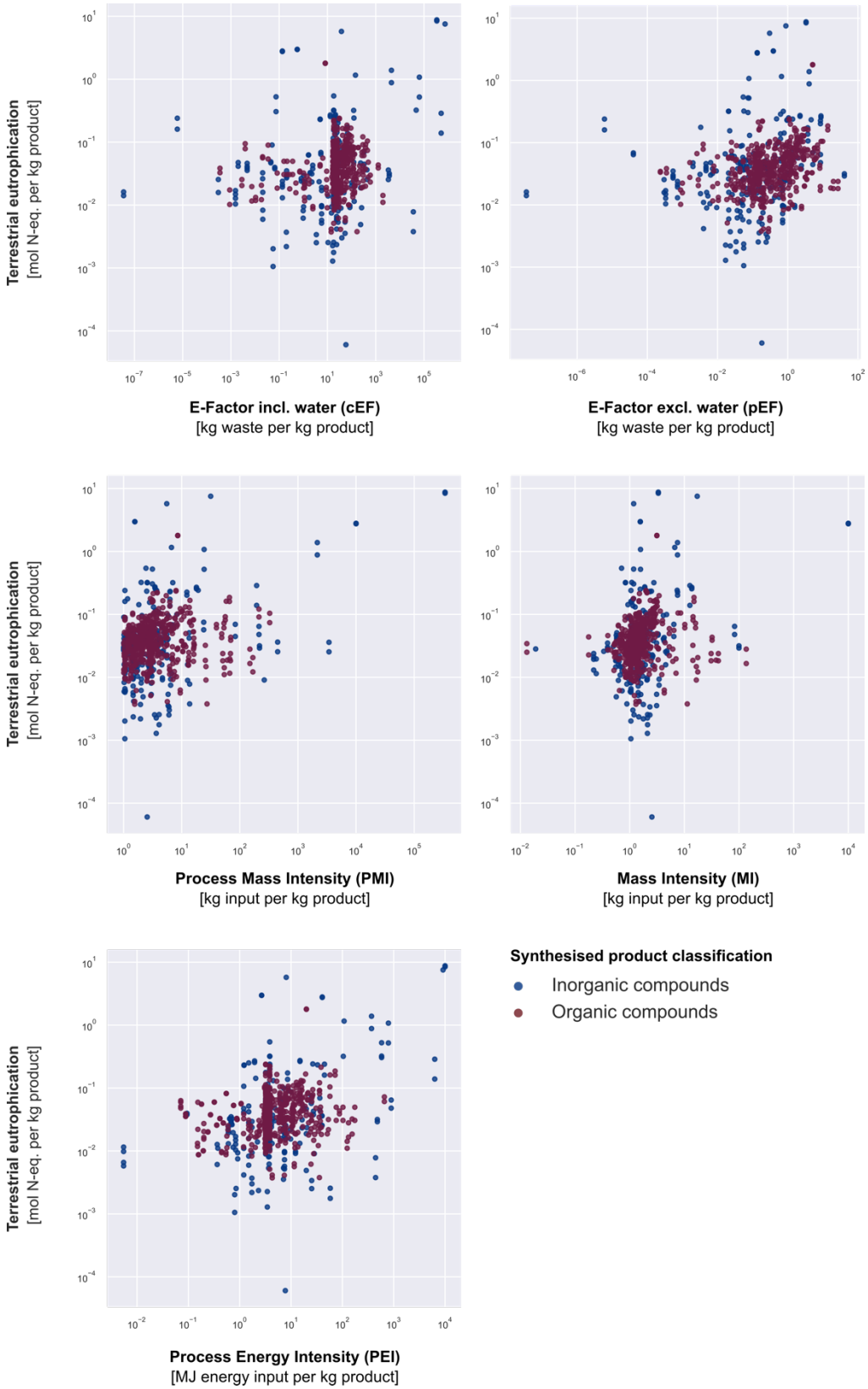

Figure S7. Scatter plots for life cycle terrestrial eutrophication impacts (y-axis) *vs.* process-level metrics (x-axis) (*N* = 711 processes). Each data point corresponds to the impact and metric score of a chemical production process. Colour of data points correspond to the organic/inorganic classification of the product.

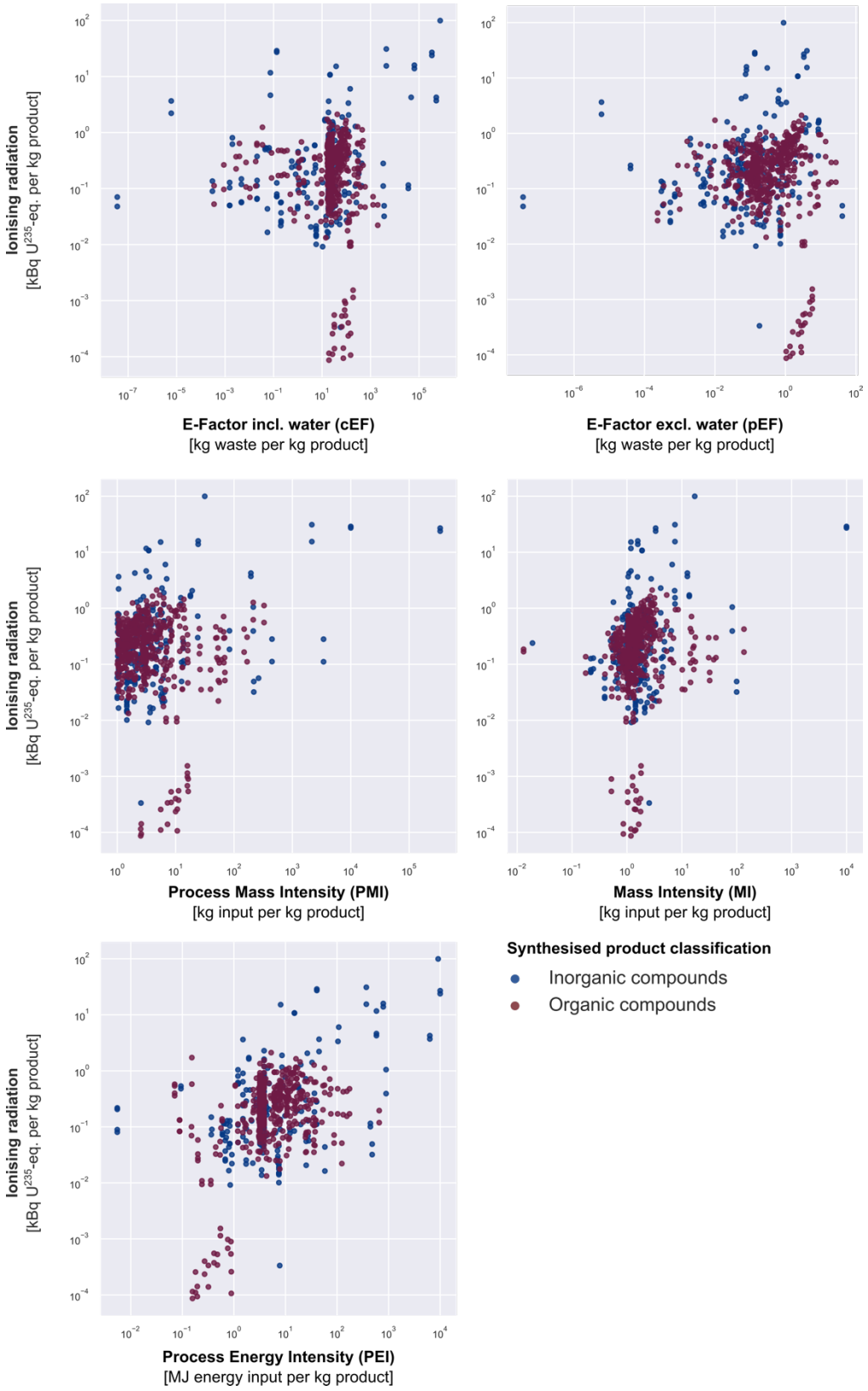

Figure S8. Scatter plots for life cycle ionising radiation impacts (y-axis) *vs.* process-level metrics (x-axis) (*N* = 711 processes). Each data point corresponds to the impact and metric score of a chemical production process. Colour of data points correspond to the organic/inorganic classification of the product.

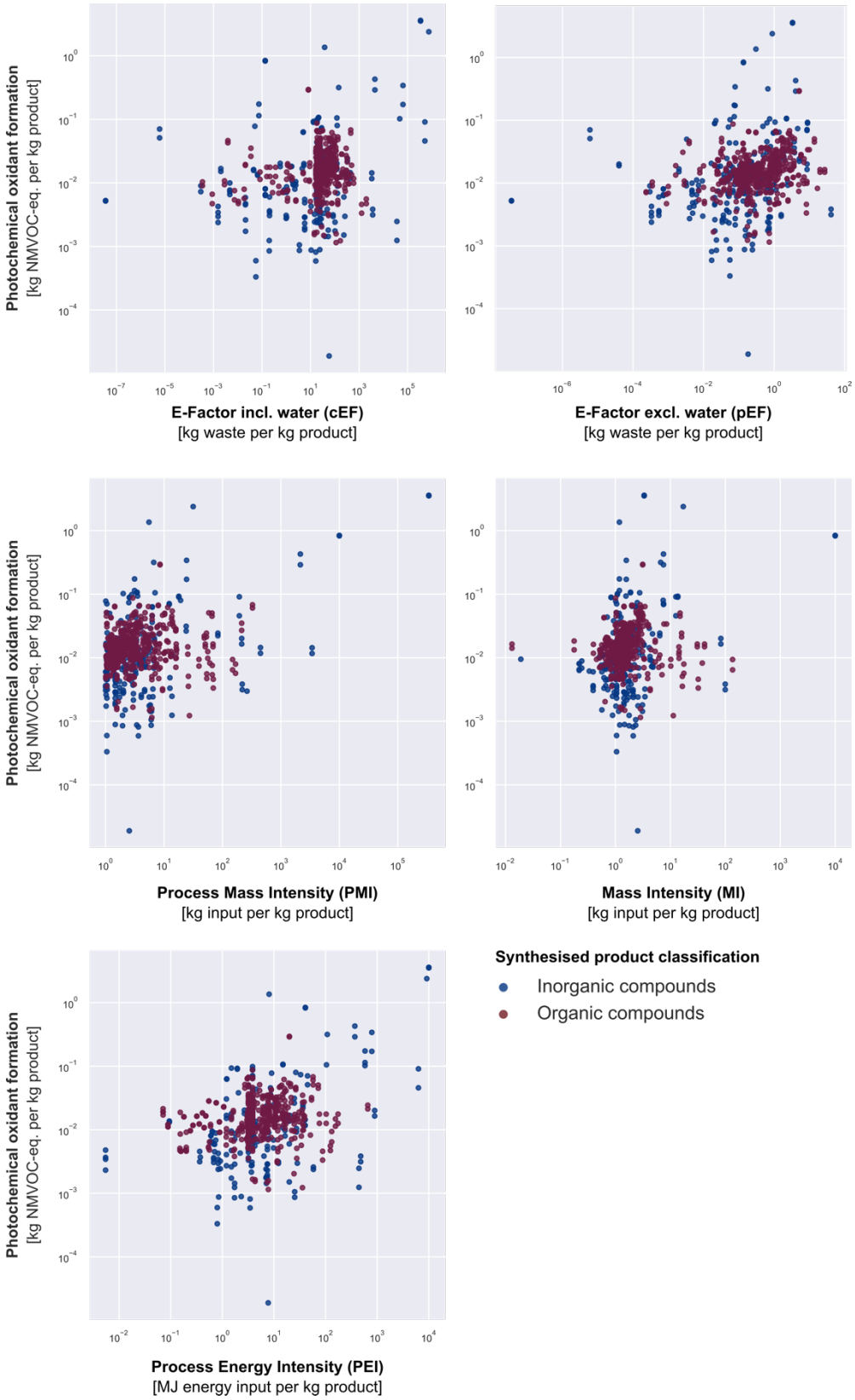

Figure S9. Scatter plots for life cycle photochemical ozone formation impacts (y-axis) *vs.* process-level metrics (x-axis) (*N* = 711 processes). Each data point corresponds to the impact and metric score of a chemical production process. Colour of data points correspond to the organic/inorganic classification of the product. Unit of NMVOC-eq. refers to Non-Methane Volatile Organic Compound equivalents.

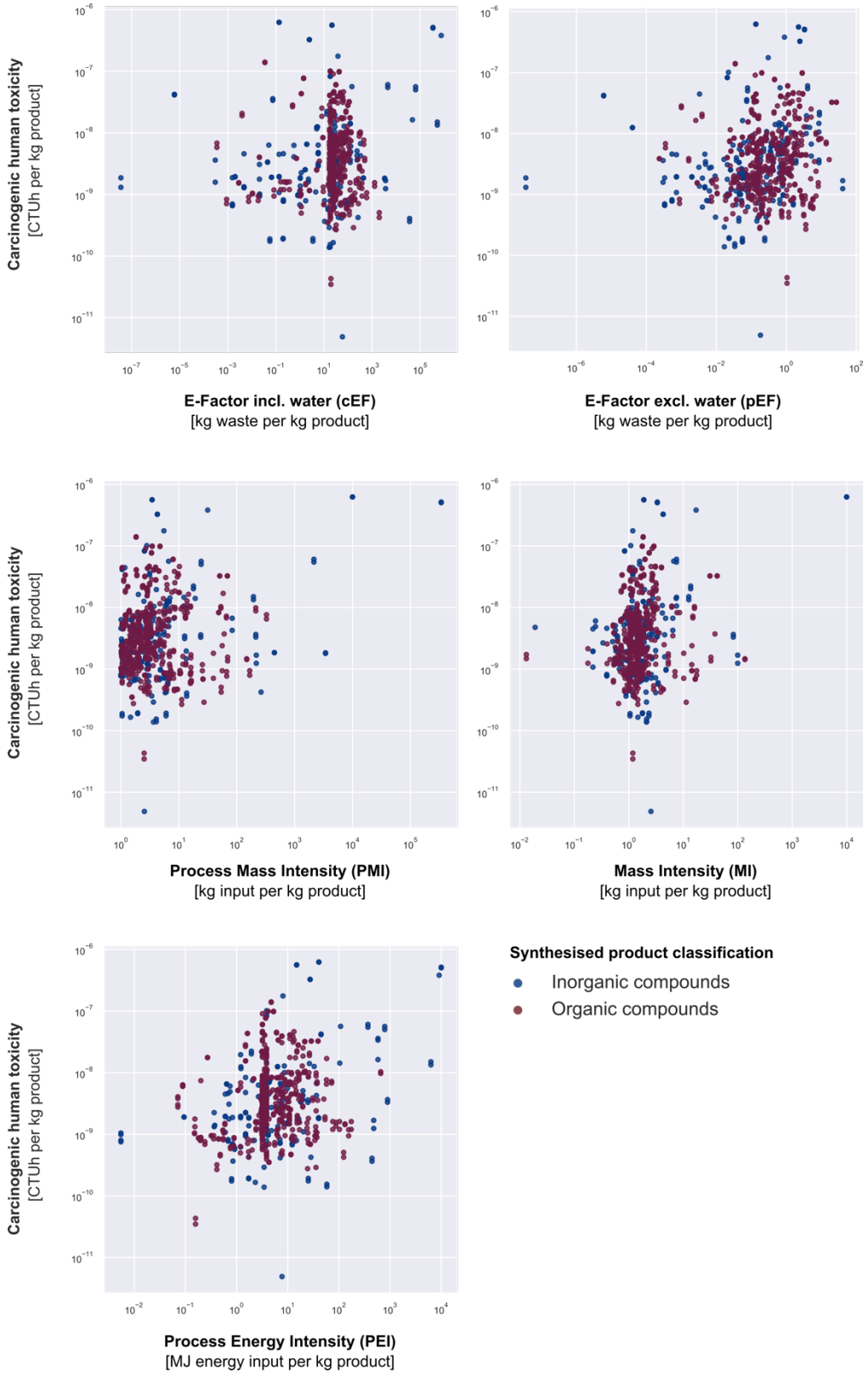

Figure S10. Scatter plots for life cycle carcinogenic human toxicity impacts (y-axis) *vs.* process-level metrics (x-axis) (*N* = 711 processes). Each data point corresponds to the impact and metric score of a chemical production process. Colour of data points correspond to the organic/inorganic classification of the product. Unit of CTUh refers to Comparative Toxic Unit, human health.

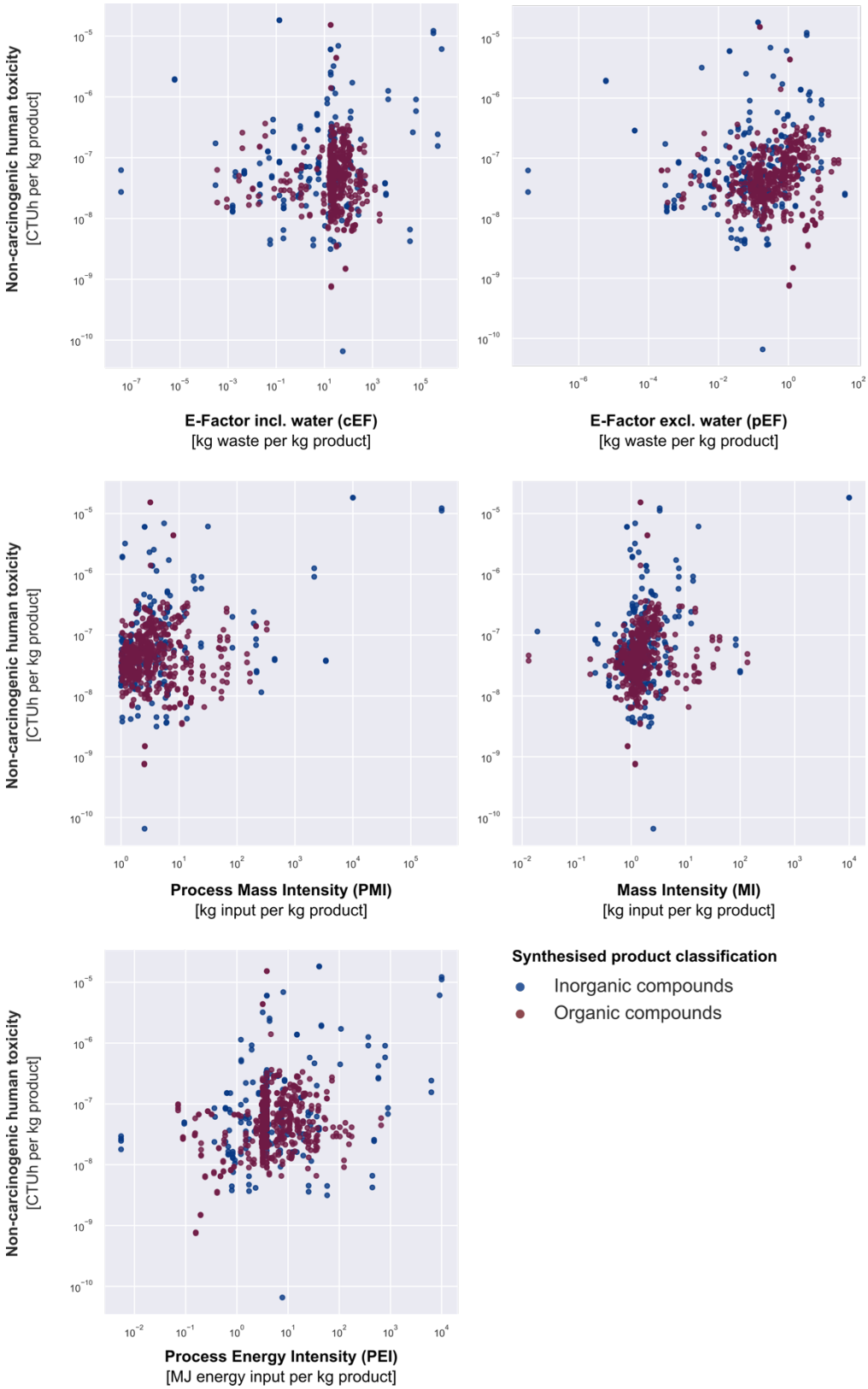

Figure S11. Scatter plots for life cycle non-carcinogenic human toxicity impacts (y-axis) *vs.* process-level metrics (x-axis) (*N* = 711 processes). Each data point corresponds to the impact and metric score of a chemical production process. Colour of data points correspond to the organic/inorganic classification of the product. Unit of CTUh refers to Comparative Toxic Unit, human health.

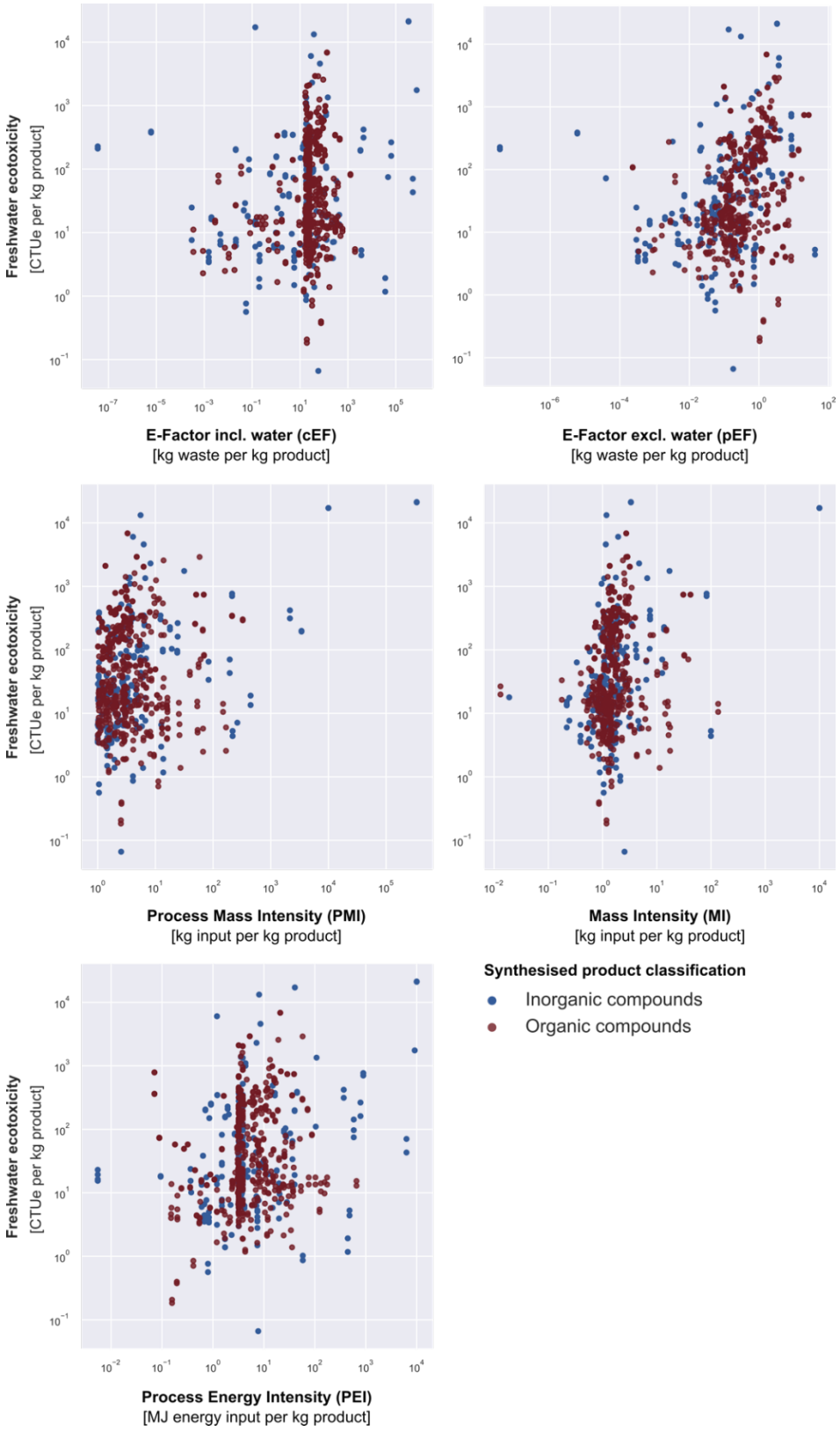

Figure S12. Scatter plots for life cycle freshwater ecotoxicity impacts (y-axis) *vs.* process-level metrics (x-axis) (*N* = 711 processes). Each data point corresponds to the impact and metric score of a chemical production process. Colour of data points correspond to the organic/inorganic classification of the product. Unit of CTUe refers to Comparative Toxic Unit, ecotoxicity.

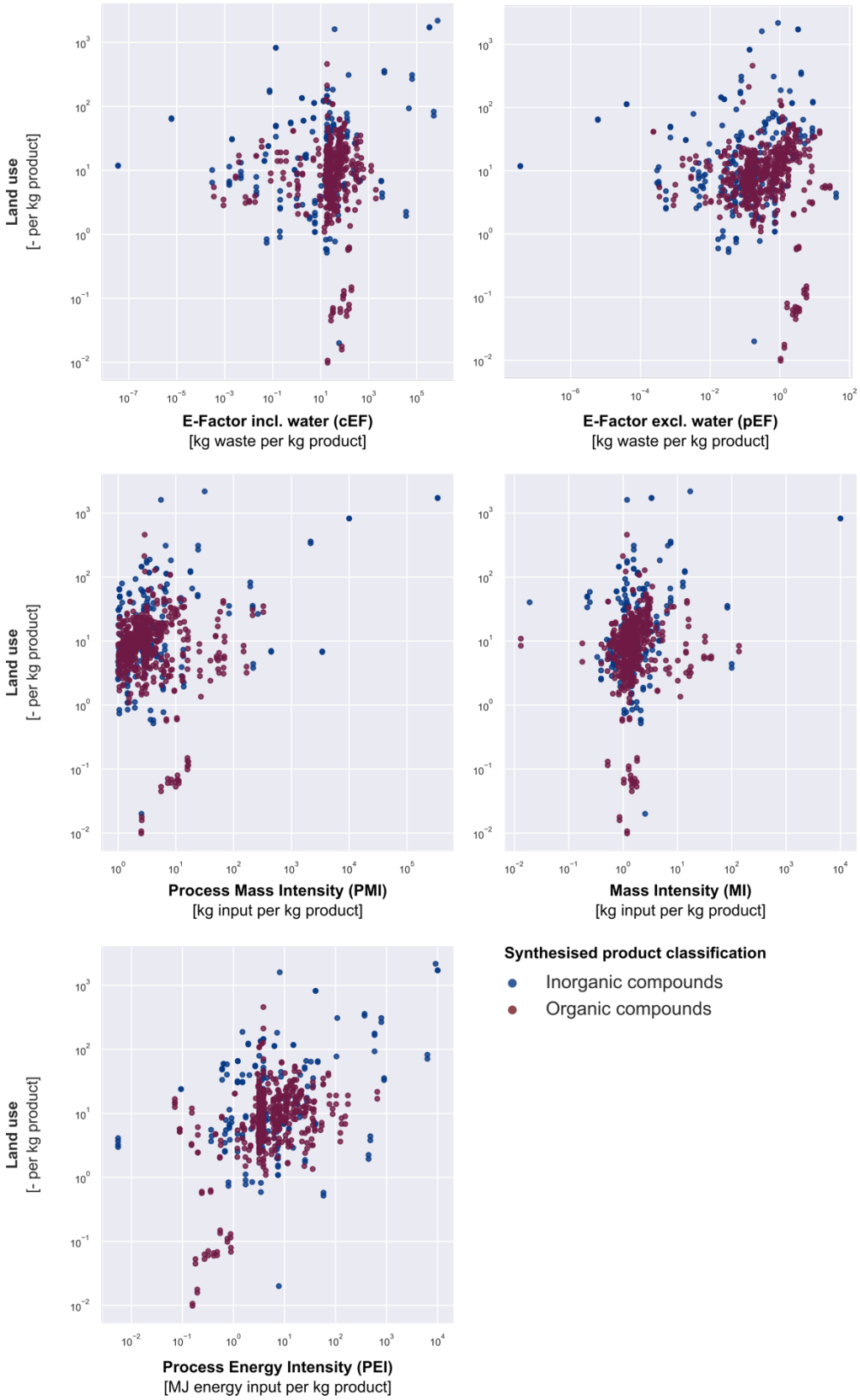

Figure S13. Scatter plots for life cycle land use impacts (y-axis) *vs.* process-level metrics (x-axis) (*N* = 711 processes). Each data point corresponds to the impact and metric score of a chemical production process. Colour of data points correspond to the organic/inorganic classification of the product. Unit for land use is dimensionless, based on a soil quality index.

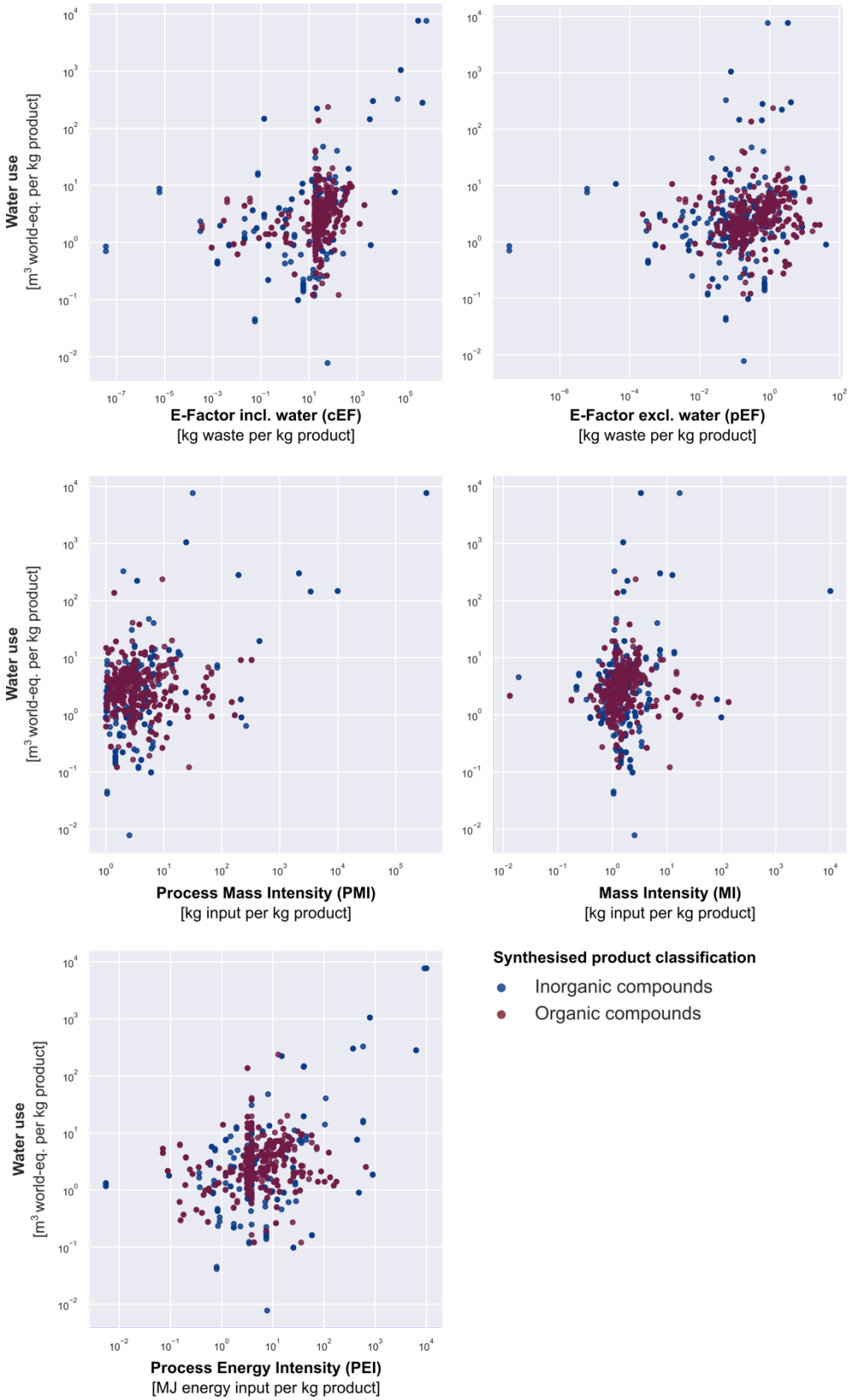

Figure S14. Scatter plots for life cycle water use impacts (y-axis) *vs.* process-level metrics (x-axis) (*N* = 711 processes). Each data point corresponds to the impact and metric score of a chemical production process. Colour of data points correspond to the organic/inorganic classification of the product.

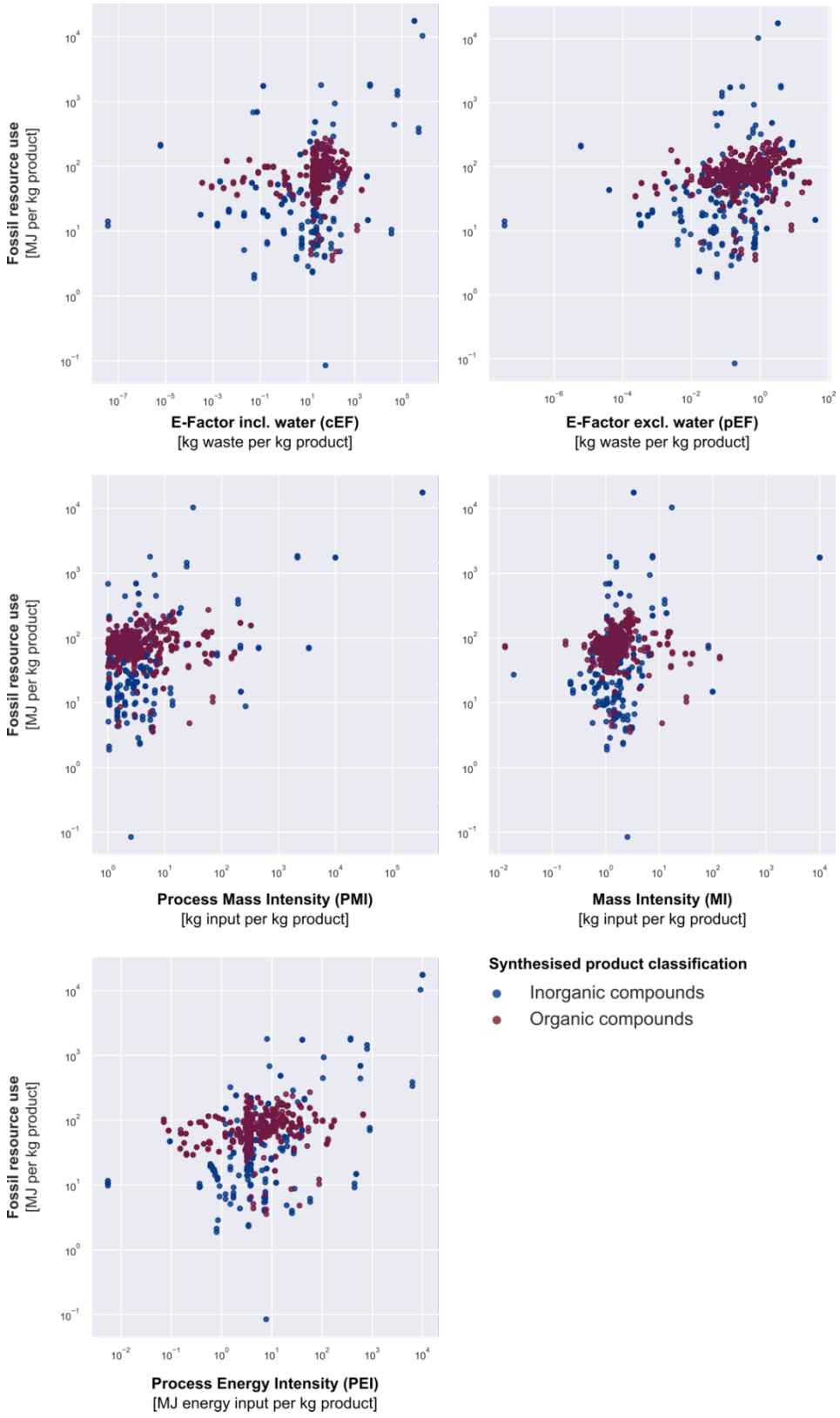

Figure S15. Scatter plots for life cycle fossil resource use impacts (y-axis) *vs.* process-level metrics (x-axis) (*N* = 711 processes). Each data point corresponds to the impact and metric score of a chemical production process. Colour of data points correspond to the organic/inorganic classification of the product.

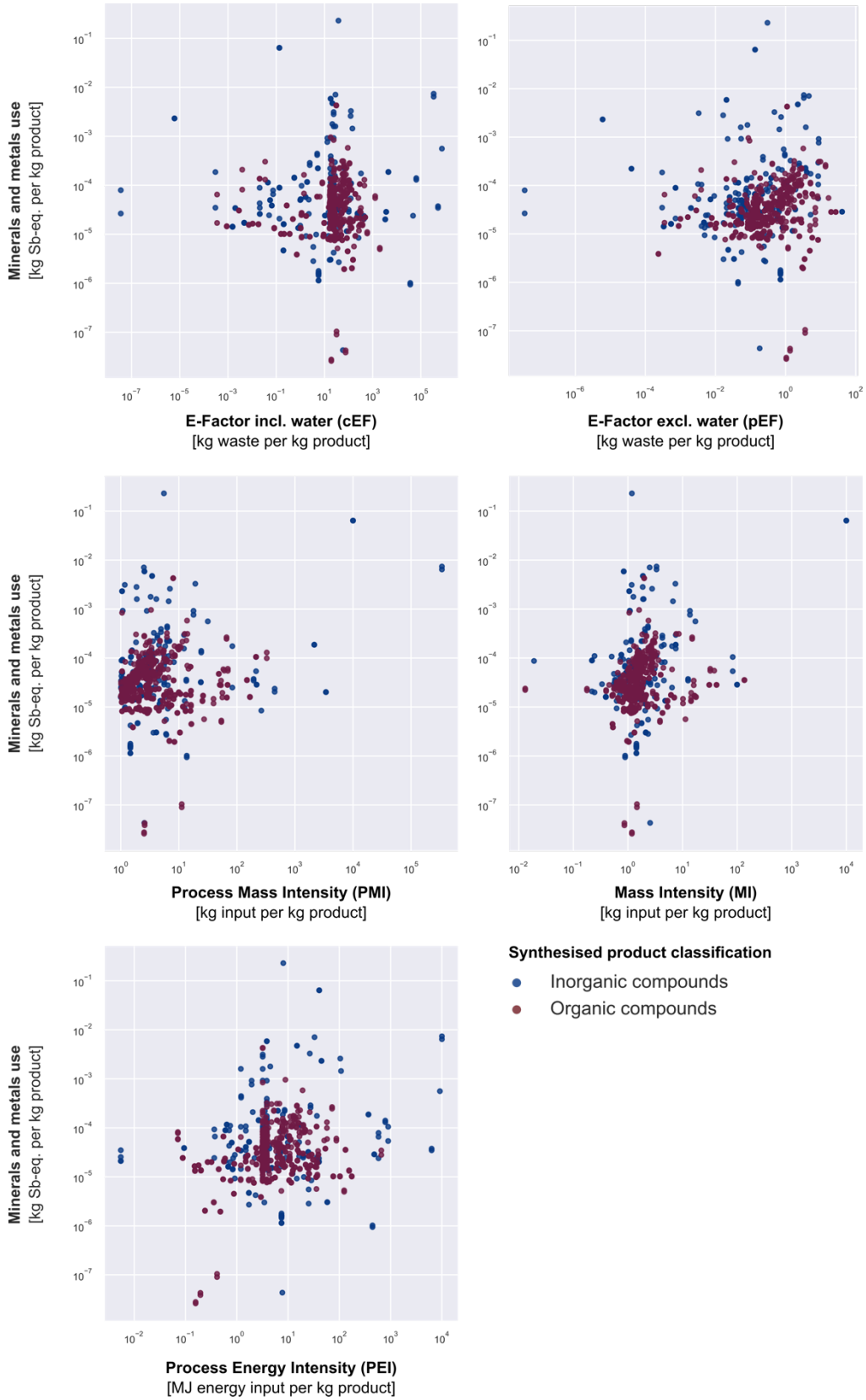

Figure S16. Scatter plots for life cycle minerals and metals use impacts (y-axis) *vs.* process-level metrics (x-axis) (*N* = 711 processes). Each data point corresponds to the impact and metric score of a chemical production process. Colour of data points correspond to the organic/inorganic classification of the product.

S4. Mean and degree of variation of life cycle impact contributions from main process drivers

Figure 4 in the main text shows the average percentage contributions to the total life cycle impacts of a chemical process. Coefficients of variation, presented in **Table S3**, are a measure of the distribution of contributions across all 711 chemical processes analysed. Coefficients of variation are a ratio of the standard deviation to the mean and expressed as a percentage. Raw material contributions have the lowest coefficients of variation across all life cycle impact categories meaning that contributions are most narrowly distributed and vary from the mean value the least.

Table S3: Mean and coefficient of variation values for contributions to life cycle impacts of chemical processes (N = 711). For example, the mean contribution to climate change impacts from raw materials is 70% and has a 37% level of dispersion around this mean value. Contributions from raw materials refer to the life cycle impacts associated with the activities to produce and distribute each input material until entering the chemical process. Similarly, contributions from energy correspond to the impacts associated with the generation and distribution of electricity, heating from steam or natural gas, etc. Contributions from other utilities refer to impacts from cooling water, liquid nitrogen, and compressed air. Chemical plant contributions are the impacts from the construction of the chemical plant, including required materials (*e.g.*, steel and concrete), energy, and water. Waste treatment or disposal refers to the impacts from incinerating spent solvent or hazardous waste from the production process, while wastewater contributions cover impacts from treating the amount of wastewater generated by the process.

Source of impact contribution	**Raw material**		**Energy**		**Infrastructure**		**Other utilities**		**Waste treatment or disposal**		**Wastewater treatment**	
Environmental Footprint life cycle impact category	Mean	Coefficient of variation (%)	Mean	Coefficient of variation (%)	Mean	Coefficient of variation (%)	Mean	Coefficient of variation (%)	Mean	Coefficient of variation (%)	Mean	Coefficient of variation (%)
Climate change	0.70	37	0.19	106	0.02	123	0.01	487	0.00	496	0.00	933
Ozone depletion	0.79	34	0.13	143	0.02	189	0.01	582	0.03	531	0.00	1293
Particulate matter formation	0.72	38	0.15	126	0.04	116	0.01	468	0.00	594	0.00	1151
Acidification	0.71	37	0.14	121	0.05	108	0.01	418	0.00	840	0.00	986
Freshwater eutrophication	0.64	44	0.20	100	0.08	108	0.01	377	0.04	431	0.00	872
Marine eutrophication	0.65	45	0.14	124	0.03	118	0.01	510	0.00	667	0.00	993
Terrestrial eutrophication	0.71	36	0.15	116	0.04	103	0.01	465	0.00	555	0.00	973
Ionising radiation	0.63	46	0.26	89	0.06	137	0.01	371	0.04	498	0.00	965
Photochemical ozone formation	0.72	35	0.14	118	0.03	124	0.01	455	0.00	577	0.00	960
Carcinogenic human toxicity	0.63	47	0.08	164	0.15	102	0.01	365	0.04	431	0.00	1023
Non-carcinogenic human toxicity	0.61	44	0.10	137	0.17	89	0.02	361	0.02	467	0.00	1126
Freshwater ecotoxicity	0.51	64	0.07	177	0.05	164	0.01	552	0.02	491	0.00	1118
Land use	0.68	61	0.15	150	0.12	187	0.01	424	0.05	411	0.00	1171
Water use	0.74	38	0.05	166	0.01	156	0.01	633	0.00	600	0.00	931

Fossil resource use	0.76	34	0.17	120	0.02	149	0.01	500	0.00	611	0.00	1004
Minerals and metals use	0.63	43	0.02	224	0.29	81	0.02	410	0.01	758	0.00	1100

Table S3: (continued) Mean and coefficient of variation values for contributions to life cycle impacts of chemical processes (*N* = 711). Hyphens indicate a null value due to a mean of zero. Impacts due to inputs from the environment and emissions to the environment are caused by the natural resources consumed (e.g., water from natural bodies such as rivers) or emissions released directly (e.g., carbon dioxide) by the chemical process, respectively.

Source of impact contribution	**Inputs to process directly from environment**		**Outputs from process directly to environment**	
Environmental Footprint life cycle impact category	Mean	Coefficient of variation (%)	Mean	Coefficient of variation (%)
Climate change	0.00	-	0.07	279
Ozone depletion	0.00	-	0.02	755
Particulate matter formation	0.00	-	0.08	268
Acidification	0.00	-	0.09	262
Freshwater eutrophication	0.00	-	0.03	506
Marine eutrophication	0.00	-	0.16	184
Terrestrial eutrophication	0.00	-	0.09	246
Ionising radiation	0.00	-	0.00	1989
Photochemical ozone formation	0.00	-	0.09	230
Carcinogenic human toxicity	0.00	-	0.09	250
Non-carcinogenic human toxicity	0.00	-	0.07	269
Freshwater ecotoxicity	0.00	-	0.34	104
Land use	0.00	1273	0.00	-
Water use	0.00	-	0.19	140
Fossil resource use	0.04	513	0.00	-
Minerals and metals use	0.03	508	0.00	-

S5. Life cycle impact contributions along a supply chain

Figure 5 in the main manuscript shows the evolution of the life cycle impact contributions for the agrochemical triclopyr and its precursors at various points in its upstream supply chain. For the building blocks, *i.e.*, ammonia and methanol, we found that the impacts of raw material inputs represent relatively minor shares, whereas energy, direct emissions, and infrastructure/construction have a more critical impact on the overall life cycle. On the contrary, for more complex products downstream, the raw material inputs constitute the major share towards the climate change impacts. To delve further into the contributions for triclopyr, **Figure S17** shows the evolution of the life cycle impact contributions along a supply chain, by aggregating the process contributions along the life cycle by their reference product of each activity as in the ecoinvent v3.9 database.

In **Figure S17**, we consider two main categories: life cycle emissions and direct emissions throughout the life cycle, aggregated by their reference product as in the ecoinvent database. The primary feedstock (in blue) encompasses the raw materials required for the production of the chemical (*e.g.*, natural gas or coal) throughout the life cycle. Other intermediates (in light blue, *e.g.*, ethylene, propylene, etc.) are not shown as their primary feedstock equivalents because these processes are included as system processes in the ecoinvent v3.9 database, leading to a lack of data for representation. The life cycle emissions of heat (orange) and electricity (light orange) account for the extraction, transport, and combustion of energy sources (*i.e.*, cradle-to-grave) emissions. Other life cycle emissions, such as transport, wastewater treatment, etc. are categorised as 'others' (in green). Further, the contributions of direct emissions are categorised for each chemical production activity.

From **Figure S17**, we find that for ammonia, the largest impact on climate change is from direct emissions. Heat also contributes a large portion, indicating high energy requirements for production. Similarly, for methanol, the major contributions are heat, electricity, and direct emissions. Primary feedstock (*i.e.*, natural gas) is also one of the major contributors to methanol production impacts, especially because of natural gas leakages during extraction and transportation. Moving further downstream, for the production of triclopyr, around 60% of the impacts are due to heat and electricity throughout the life cycle. Furthermore, other intermediates contribute to pyridine and triclopyr as life cycle emissions from using these raw materials in the production route. Conversely, we identified a reduction in the environmental impact contribution downstream from primary feedstock (*e.g.*, natural gas and coal), as they are mostly employed in the production of the chemical value chain's building blocks.

In summary, all chemicals exhibit significant impacts from energy use (heat and electricity) and direct emissions. Therefore, these impacts accumulate throughout the life cycle, resulting in

higher impacts of chemical production downstream. Furthermore, the life cycle impacts become increasingly varied, implying that each step of the process adds complexity, thereby increasing the environmental impacts, while the impacts of primary feedstock tend to have reduced importance.

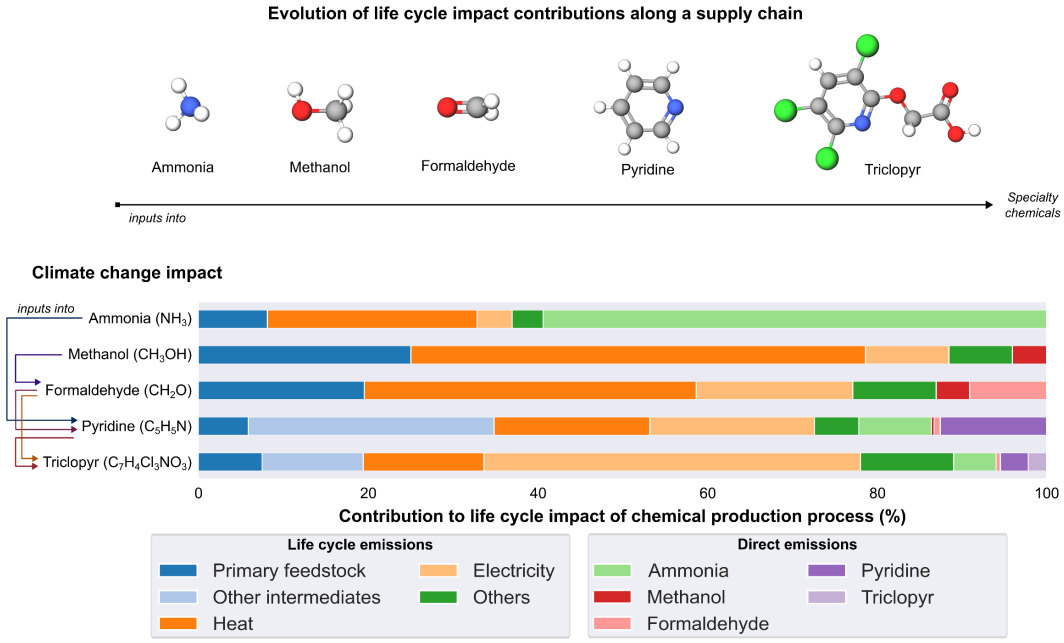

Figure S17. Climate change life cycle impact contribution profiles for the agrochemical product triclopyr and its precursors at various points of its upstream supply chain. These contributions are categorised into life cycle emissions (left side of the legend) of primary feedstock (*e.g.*, natural gas and coal), other intermediates (*e.g.*, ethylene, propylene, etc.), heat, electricity, others (*i.e.*, transport, wastewater treatment), and direct emissions (right side of the legend) of individual processes throughout the supply chain. Squares represent feedstock material into the process producing the compound indicated with an arrow.

S6. Assumptions and limitations

This analysis was subject to sources of uncertainty and limitations that affect LCA-based studies in general – namely, aspects related to environmental impact characterisation methods, as well as data availability and quality.

The underlying uncertainty in the characterisation factors that translate natural resource input and emission flows to environmental impacts (*e.g.*, characterising the toxicity effects of emitting a particular substance) means that life cycle impact assessment methods have higher levels of methodological uncertainty than others. Due to challenges in modelling their underlying cause-and-effect mechanisms, environmental categories related to toxicity and resource use are estimated with methods that are currently classified as in need of further improvement and numerical results should be interpreted with caution. However, we sought to consider as many environmental dimensions as possible and deemed it important to include toxicity and resource use related life cycle impacts as these methods are sufficiently fit for the purpose of providing directional insights.

Regarding data on chemical processes, data availability constrained the product and technological coverage of this analysis, while quantitative uncertainty was an important factor to consider when translating our findings. First, there is lower data coverage of more complex, fine chemical products in life cycle inventory databases, such as ecoinvent. Although the inclusion of more processes producing more complex compounds would be greatly beneficial to increasing sample representativeness, we can assume that it would not strengthen the correlation between life cycle impacts and mass- or energy-based process metrics as these compounds require more advanced intermediate inputs with a wider distribution of embedded upstream impacts.

Second, potential measurement errors in life cycle inventory data for the modelling of each chemical process (*i.e.*, uncertain values of material and energy inputs, as well as direct inputs/emissions to/from the environment) introduce uncertainty in the calculated process metrics and life cycle impact values. Additionally, life cycle impact values are subject to uncertainty from other technological activities to which a process is linked throughout its supply chain (*e.g.*, infrastructure activities, which are acknowledged to be uncertain since they are roughly estimated in the ecoinvent database), as well as the uncertainty of impact characterisation methods, as previously noted. Given these various complex sources of uncertainty, we can expect that mass- or energy-based metrics and life cycle impacts are likely to be more weakly correlated compared to the deterministic results we present in the main text. With respect to the central aim of this study, therefore, we do not expect that accounting for the underlying uncertainty of life cycle inventory data would overturn the trends observed and the main conclusions of the analysis.

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