Electronic supplementary information
‘Planetary metrics for the absolute environmental sustainability assessment of chemicals’

1. Ecoinvent database filtering criteria

All the inventory data were retrieved from ecoinvent v3.5[1]—using the ‘Allocation at the point of substitution’ (APOS) version of the database—by downloading the individual ecoSpold2 files. Each ecoSpold2 file (XML type file) contains the inventory of one specific activity with a unique reference product and metadata displayed in a standardised form, e.g., the estimated price of the product and its production volume are some of the compulsory and optional fields available in the ecoSpold2, respectively.

Another compulsory field of the ecoSpold2 is the United Nations Central Product Classification (CPC) v2.1[2], information used as filtering criteria, i.e., we only consider products belonging to the divisions 33 to 36 of the CPC (**Table S-1**). For convenience, the products from these four divisions were reorganised, as shown in **Table S-2**.

Table S-1. Reference products from ecoinvent v3.5 (APOS), selected for the study according to the United Nations Central Product Classification v2.1.

Section	Division	Groups
3: Other transportable goods, except metal products, machinery and equipment	33: Coke oven products; refined petroleum products; nuclear fuel	331-337
	34: Basic chemicals	341-348
	35: Other chemical products; man-made fibres	351-355
	36: Rubber and plastics products	361-364, 369

Table S-2. Reorganisation of products from CPC divisions 33-36.

Category	Organic chemical	Inorganic chemical	Other chemical
CPC groups	331-335, 341, 343, 347, 352, 361-364, 369	342, 344	groups not elsewhere attributed

The second filtering step aims to identify reference products (chemicals) with a functional unit (FU) of the type ‘1 kg of chemical *X* generated in a market-type activity with any geographical location’. To this end, keywords ‘market’ and ‘kg’ (as unit) were used.

2. Aggregation into a global production market

Next, the duplicated chemicals from the resulting dataset of section 1—note that duplicates appear due to local markets, i.e., geographical locations other than global (GLO)—were aggregated into one pseudo-GLO market following the mass allocation principle. The impact scores of the duplicated chemicals were allocated according to their contribution to the overall production volume (individual production volumes were gathered from the ecoSpold2 files). This procedure assumes no additional losses and exchanges associated with the transportation, storage, infrastructure, and handling of the chemical product.

The activities containing the keyword ‘market group for’ were removed from the dataset since they present similarly aggregated markets of chemicals generated for convenience in the ecoinvent database, e.g., ‘market group for diesel’.

3. Impact assessment methods

We applied two life-cycle impact assessment (LCIA) methods. The main method, used to quantify the absolute environmental sustainability performance, is based on the Planetary Boundaries (PBs) framework.[3,4] This PB-LCIA method quantifies seven out of nine originally defined PBs. We quantified six PBs—climate change, stratospheric ozone depletion, ocean acidification, biogeochemical flows, land-system change, and freshwater use —, using the characterisation factors (CFs) provided by Ryberg *et al.*[5] To calculate the impacts on the change in biosphere integrity, omitted in Ryberg’s approach, we implemented the CFs proposed by Galán-Martín et al.[6,7] We also applied the IPCC 2013 method to estimate the global warming potential (GWP) in a timeframe of 100 years. These methods were implemented in SimaPro 9.1.[8]

4. Data for the calculation of transgression levels

We calculated the transgression levels (TLs) of chemicals using two alternative sharing principles: equal per capita (EPC) and grandfathering (GF). The latter sharing principle requires information about the total current impact of the anthropogenic activities (IMP_b^{TOT}) and the available safe operating space (SOS_b). Both pieces of information are taken from Galán-Martín *et al.*[6,7]

The EPC sharing principle requires the total world gross value added (GVA^{TOT}), the individual basic prices of each chemical c ($price_c$) and the SOS_b . The global GVA was retrieved from The World Bank database[9] for 2018: 7.38×10^{13} USD$_{2018}$. On the other hand, the basic prices of chemicals—expressed in EUR_{2005}—were retrieved from ecoSpold2 files as part of the ecoinvent v3.5 database.[1] The currency was consequently transformed to USD_{2018} accounting for the inflation rate—adjusted with the Producer Price Index (PPI) from Eurostat[10], PPI=104.5 in 2018 for EU28—and the average exchange rate in 2018[11], i.e., 1.1811 USD_{2018}/EUR_{2018}. Note, however, that in some cases, the ecoinvent prices refer to the cost of raw materials, so they provide a lower bound on the real price.

5. Detection of outliers

To identify the possible outliers, we implemented a robust Mahalanobis-type distance technique following Hubert *et al.*[12] This multivariate detection method employs a highly robust estimator of location, i.e., the minimum covariance determinant (MCD), for which a fast algorithm is implemented in Scikit-learn.[13] In mathematical terms, the robust Mahalanobis-type distances (rMD) are estimated as follows:

$$rMD(x) = d(x, \hat{\mu}_{MCD}, \hat{\Sigma}_{MCD}) = \sqrt{(x - \hat{\mu}_{MCD})^T \hat{\Sigma}_{MCD}^{-1} (x - \hat{\mu}_{MCD})} \tag{1}$$

Where x is an observation (in our case, a chemical), $\hat{\mu}_{MCD}$ is the MCD estimate of location (a robust mean), and $\hat{\Sigma}_{MCD}$ is the MCD covariance estimate. The estimation of rMDs is performed in the nine dimensions of the control variables (CVs) of the PBs.

The square of rMD is assumed to follow a chi-squared distribution with nine degrees of freedom (k=9) and a significance level of 5%. Consequently, each chemical with rMD above the critical value was labelled as an outlier and removed from the dataset. The list of 26 removed activities (outliers) with their scores in the nine dimensions (the TLs of the nine CVs of PBs) is provided in **Table S-3** as reference.

Table S-3. Activities, detected as outliers using the robust Mahalanobis distance method with nine degrees of freedom (k=9) and a significance level of 5%.(α=5%). The degrees of freedom correspond to the transgression levels of the nine control variables of the PBs calculated using the equal per capita (EPC) sharing approach.

Activity name	CC - CO2 conc.	CC - Energy imb.	SOD	OA	BGC flows - P	BGC flows - N	LSC	FWU	CBI - BII loss
Ethanol, without water, in 95% solution state, from fermentation {GLO}| market for | APOS, S	4.7×10^{1}	4.6×10^{1}	8.1×10^{-1}	1.5×10^{1}	8.2×10^{-1}	1.5	4.7×10^{-2}	5.0	1.6×10^{1}
Ethanol, without water, in 99.7% solution state, from fermentation {GLO}| market for | APOS, S	7.5×10^{1}	7.1×10^{1}	9.0×10^{-1}	2.4×10^{1}	1.1	1.2	1.4×10^{-1}	7.1	1.8×10^{1}
Magnetite {GLO}| market for | APOS, S	5.5×10^{2}	5.4×10^{2}	8.1×10^{-1}	1.7×10^{2}	2.7×10^{-1}	1.2×10^{1}	9.4×10^{-3}	9.2×10^{-1}	3.9×10^{1}
Adipic acid {GLO}| market for | APOS, S	7.8×10^{1}	1.5×10^{2}	1.5×10^{1}	2.5×10^{1}	5.7×10^{-3}	1.9×10^{-1}	1.1×10^{-3}	1.2×10^{-1}	1.5×10^{1}
Ammonium nitrate, as N {GLO}| market for | APOS, S	1.3×10^{2}	2.4×10^{2}	2.3×10^{1}	4.3×10^{1}	2.7×10^{-2}	7.0×10^{-1}	5.1×10^{-3}	9.4×10^{-2}	2.3×10^{1}
Charcoal {GLO}| market for | APOS, S	4.9×10^{1}	4.1×10^{1}	2.1×10^{-2}	1.6×10^{1}	2.8×10^{-3}	3.7×10^{-2}	9.7×10^{-4}	2.4×10^{-2}	5.6×10^{1}
Citric acid {GLO}| market for | APOS, S	1.3×10^{2}	1.3×10^{2}	6.9×10^{-1}	4.3×10^{1}	1.4	2.0×10^{1}	5.7×10^{-3}	6.1	1.6×10^{1}
Dimethyldichlorosilane {GLO}| market for dimethyldichlorosilane | APOS, S	5.4×10^{1}	5.2×10^{1}	3.4×10^{1}	1.7×10^{1}	3.5×10^{-3}	6.7×10^{-2}	3.1×10^{-4}	5.4×10^{-2}	4.8
Fluorescent whitening agent, distyrylbiphenyl type {GLO}| market for | APOS, S	2.6×10^{2}	2.5×10^{2}	2.7×10^{-1}	8.3×10^{1}	2.2	3.2×10^{1}	2.3×10^{-5}	7.1×10^{-3}	1.6×10^{1}
Heavy water {GLO}| market for | APOS, S	4.7×10^{1}	4.5×10^{1}	3.3×10^{-2}	1.5×10^{1}	4.5×10^{-3}	1.7×10^{-1}	1.0×10^{-3}	8.0	3.0
Lithium brine, 6.7 % Li {GLO}| market for | APOS, S	3.1×10^{2}	3.0×10^{2}	3.0×10^{-1}	1.0×10^{2}	1.4×10^{-2}	3.7×10^{-1}	1.5×10^{-2}	1.8×10^{-1}	4.3×10^{1}
Phosphane {GLO}| market for | APOS, S	8.9×10^{1}	8.6×10^{1}	1.0×10^{-1}	2.8×10^{1}	9.9×10^{1}	1.0	3.4×10^{-3}	4.5×10^{-1}	6.6
Phosphate rock, as P2O5, beneficiated, wet {GLO}| market for | APOS, S	1.2×10^{2}	1.2×10^{2}	1.7×10^{-1}	3.8×10^{1}	8.2	5.8	3.0×10^{-2}	2.9	1.3×10^{1}
Sodium aluminate, powder {GLO}| market for | APOS, S	6.5×10^{1}	6.2×10^{1}	5.7×10^{-2}	2.1×10^{1}	1.5×10^{-2}	5.8×10^{-1}	8.9×10^{-4}	-6.4	4.2
Sodium nitrate {GLO}| market for | APOS, S	2.3×10^{2}	2.9×10^{2}	1.4×10^{1}	7.4×10^{1}	1.4×10^{-1}	7.7×10^{2}	5.1×10^{-3}	3.5×10^{-1}	2.5×10^{1}
Titanium tetrachloride {GLO}| market for | APOS, S	1.2×10^{2}	1.1×10^{2}	1.2×10^{-1}	3.9×10^{1}	4.5×10^{-2}	2.1	6.1×10^{-3}	9.4×10^{-1}	8.0
Ethanol, without water, in 99.7% solution state, from fermentation, at service station, combined to GLO market	7.0×10^{1}	6.5×10^{1}	8.2×10^{-1}	2.2×10^{1}	9.9×10^{-1}	1.1	1.3×10^{-1}	6.4	1.7×10^{1}
Ammonium carbonate, combined to GLO market	7.8×10^{1}	7.5×10^{1}	6.5×10^{-2}	2.5×10^{1}	1.0×10^{-2}	1.8×10^{2}	2.4×10^{-3}	1.1×10^{-1}	5.6
Chlorodifluoromethane, combined to GLO market	4.7×10^{1}	1.1×10^{2}	3.9×10^{1}	1.5×10^{1}	1.7×10^{-2}	7.3×10^{-1}	1.2×10^{-3}	9.1×10^{-2}	5.1×10^{1}
Glycerine, combined to GLO market	6.5×10^{1}	6.7×10^{1}	1.1	2.1×10^{1}	1.1	1.3	8.6×10^{-2}	8.6×10^{-1}	2.3×10^{1}
Methanol, from biomass, combined to GLO market	5.2×10^{1}	5.1×10^{1}	7.4×10^{-2}	1.7×10^{1}	3.3×10^{-1}	6.4	1.8×10^{-3}	2.1×10^{-1}	7.4×10^{1}
Methyl methacrylate, combined to GLO market	5.9×10^{2}	5.7×10^{2}	3.4×10^{-3}	1.9×10^{2}	5.3	3.5×10^{-1}	-3.9×10^{-5}	5.9×10^{-2}	4.1×10^{1}
Phosphoryl chloride, combined to GLO market	7.1×10^{1}	6.9×10^{1}	8.7×10^{-2}	2.3×10^{1}	4.6×10^{1}	9.3×10^{-1}	2.1×10^{-3}	3.0×10^{-1}	5.2
Sulfur hexafluoride, liquid, combined to GLO market	5.0×10^{1}	5.1×10^{3}	5.3×10^{-2}	1.6×10^{1}	4.0×10^{-3}	1.7×10^{-1}	8.0×10^{-4}	9.6×10^{-2}	4.5×10^{1}
Trichloromethane, combined to GLO market	5.1×10^{1}	5.0×10^{1}	3.7×10^{1}	1.6×10^{1}	2.3×10^{-2}	1.0	9.5×10^{-4}	8.9×10^{-2}	7.9
Sodium formate, combined to GLO market	4.4×10^{1}	4.4×10^{1}	5.8×10^{-2}	1.4×10^{1}	-3.4×10^{-1}	5.3×10^{-1}	1.8×10^{-3}	1.3×10^{-1}	-7.9×10^{1}

The notation for the PBs is as follows: climate change (CC) with control variables of CO_2 concentration (CO_2 conc.) and energy imbalance (Energy imb.), stratospheric ozone depletion (SOD), ocean acidification (OA), biogeochemical (BGC) flows with control variables of phosphorus (P) and nitrogen (N), land-system change (LSC), freshwater use (FWU), change in biosphere integrity (CBI) with control variable of loss of biodiversity intactness index (BII loss).

6. Supplementary results

This section includes additional results supporting the discussions and conclusions drawn in the main manuscript. **Figure S-1** presents the distributions of the chemicals according to the GWP and the seven PBs —climate change and biogeochemical flows PBs are shown with two control variables each—on a series of histogram subplots. Additionally, the correlations between the GWP and the PBs are displayed on scatter plots and complemented with their respective values of Spearman's rank correlation coefficients (r_s). As expected, GWP shows a good correlation with the GHG-related PBs, i.e., climate change (CO_2 concentration and energy imbalance), ocean acidification and biosphere integrity (r_s of 0.99, 0.99 and 0.98, respectively). In contrast, a weaker correlation is observed with the other PBs (at most r_s=0.79 for the stratospheric ozone depletion PB).

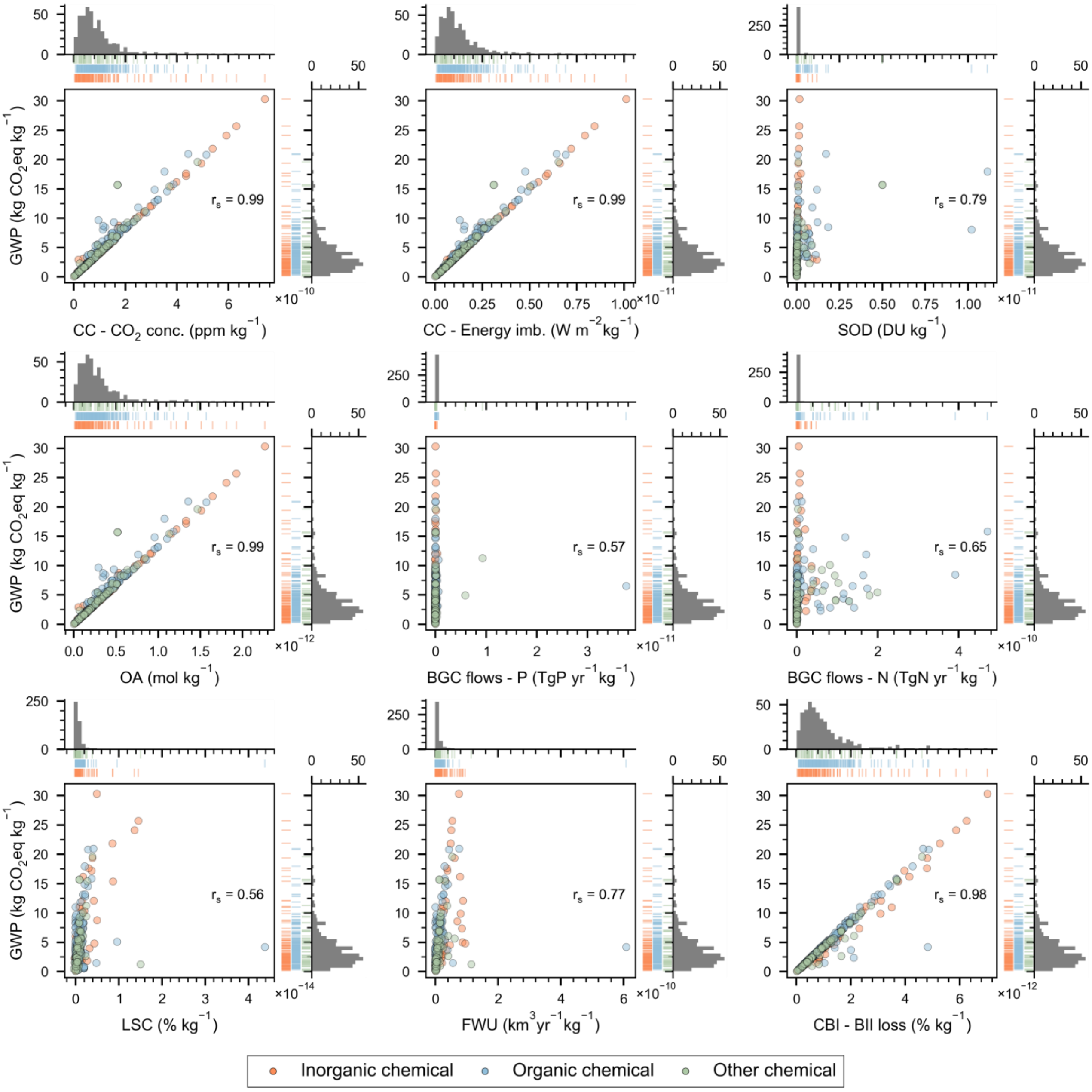

Figure S-1. Global warming potential (GWP) of chemicals versus their impact on the control variables of the PBs. The chemicals, represented by bubbles, are grouped into three categories, 'inorganic' (orange), 'organic' (blue) and 'other' (green). We indicate the Spearman's rank correlation coefficient (r_s) of the impact in a specific PB and GWP scores. Histograms and rug plots on the sides of each scatter plot show the overall and individual distributions of chemicals, respectively. The notation for the PBs is as follows: climate change (CC) with control variables of CO_2 concentration (CO_2 conc.) and energy imbalance (Energy imb.), stratospheric ozone depletion (SOD), ocean acidification (OA), biogeochemical (BGC) flows with control variables of phosphorus (P) and nitrogen (N), land-system change (LSC), freshwater use (FWU), change in biosphere integrity (CBI) with control variable of loss of biodiversity intactness index (BII loss). Note that 21 chemicals with GWP scores ranging from 48 to 3907 kg CO_2eq/kg of chemical are omitted here (for visualisation purposes) but are shown in **Table S-4** for completeness.

Figure S-2 depicts the correlations between the unitary prices and the impact scores in GWP and the PBs, where low Spearman's rank correlation coefficients indicate very weak monotonic relationships between the different variables.

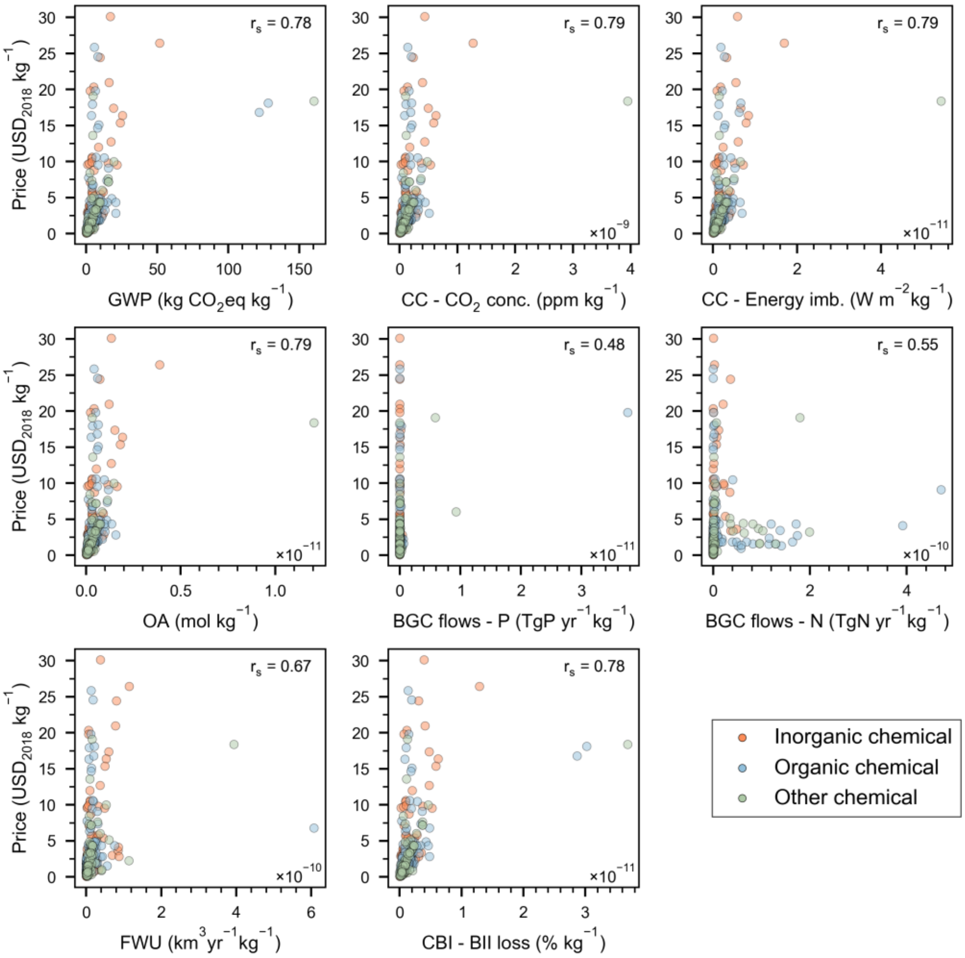

Figure S-2. Unitary prices of chemicals versus their impact scores in global warming potential (GWP) and the PBs. The chemicals, represented by bubbles, are grouped into three categories, 'inorganic' (orange), 'organic' (blue) and 'other' (green). We indicate the Spearman's rank correlation coefficient (r_s) of the prices and the respective impact scores in GWP or PBs on the top right of the scatter plot. The notation for the PBs is as follows: climate change (CC) with control variables of CO$_2$ concentration (CO$_2$ conc.) and energy imbalance (Energy imb.), stratospheric ozone depletion (SOD), ocean acidification (OA), biogeochemical (BGC) flows with control variables of phosphorus (P) and nitrogen (N), land-system change (LSC), freshwater use (FWU), change in biosphere integrity (CBI) with control variable of loss of biodiversity intactness index (BII loss). Note that 23 chemicals with unitary prices ranging from 32.9 to 1421 USD$_{2018}$/kg of chemical are omitted here (for visualisation purposes) but are shown in **Table S-5** for reference.

Table S-4 and **Table S-5** show the activities omitted in **Figure 3** of the main manuscript and **Figure S-1** and **Figure S-2** of the ESI. The prices and/or GWP scores of these activities are very high relative to most of the chemicals studied. Yet, they were considered in the calculations as they were not detected as outliers, e.g., they were accounted for when determining the Spearman's rank correlation coefficients.

Table S-4. Activities, omitted in **Figure 3** and **Figure S-1** for visualisation purposes due to high global warming potential (GWP) scores (ranging from 48 to 3907 kg CO_2eq/kg of chemical), together with their transgression levels in the PBs according to the equal per capita (EPC) sharing approach.

Activity name	**GWP (kg CO_2/kg)**	**Transgression levels in**								
		CC - CO_2 conc.	**CC - Energy imb.**	**SOD**	**OA**	**BGC flows - P**	**BGC flows - N**	**LSC**	**FWU**	**CBI - BII loss**
Lithium {GLO}| market for | APOS, S	4.8×10^{1}	1.8×10^{1}	1.7×10^{1}	1.7×10^{-2}	5.6	2.7×10^{-2}	2.5	9.1×10^{-5}	2.6×10^{-2}	1.3
Silicon, solar grade {GLO}| market for | APOS, S	5.2×10^{1}	4.9×10^{1}	4.8×10^{1}	4.7×10^{-2}	1.6×10^{1}	2.3×10^{-3}	1.3×10^{-1}	6.6×10^{-4}	8.0×10^{-2}	3.6
Silicon, multi-si, casted, combined to GLO market	7.9×10^{1}	4.4×10^{1}	4.3×10^{1}	4.6×10^{-2}	1.4×10^{1}	2.2×10^{-3}	1.3×10^{-1}	5.3×10^{-4}	8.4×10^{-2}	3.2
Aminopyridine, combined to GLO market	9.3×10^{1}	2.7×10^{1}	2.6×10^{1}	1.6×10^{-2}	8.7	4.7×10^{-3}	2.0×10^{-1}	4.4×10^{-4}	3.3×10^{-2}	1.9
Silicon, electronics grade {GLO}| market for | APOS, S	9.5×10^{1}	2.5×10^{1}	2.4×10^{1}	3.1×10^{-2}	7.8	1.8×10^{-3}	9.2×10^{-2}	2.2×10^{-4}	6.4×10^{-2}	1.7
2-pyridinol {GLO}| market for | APOS, S	1.0×10^{2}	2.8×10^{1}	2.7×10^{1}	6.7×10^{-2}	8.9	5.2×10^{-3}	5.4	4.6×10^{-4}	3.5×10^{-2}	1.9
Tetrafluoroethylene {GLO}| market for | APOS, S	1.2×10^{2}	1.2×10^{1}	2.7×10^{1}	9.7	3.7	4.4×10^{-3}	1.8×10^{-1}	2.8×10^{-4}	2.2×10^{-2}	1.3×10^{1}
Tetrafluoroethylene film, on glass {GLO}| market for | APOS, S	1.3×10^{2}	1.2×10^{1}	2.7×10^{1}	9.5	3.8	4.4×10^{-3}	1.8×10^{-1}	2.9×10^{-4}	2.2×10^{-2}	1.2×10^{1}
Gallium, semiconductor-grade {GLO}| market for | APOS, S	1.5×10^{2}	8.1	7.8	1.3×10^{-2}	2.6	2.3×10^{-2}	7.6	1.5×10^{-4}	1.4×10^{-2}	5.8×10^{-1}
Uranium hexafluoride, combined to GLO market	1.5×10^{2}	1.2×10^{2}	1.1×10^{2}	3.5×10^{-1}	3.7×10^{1}	2.6×10^{-2}	5.8	4.0×10^{-3}	2.3	8.1
Silicon, single crystal, czochralski process, photovoltaics, combined to GLO market	1.5×10^{2}	6.7×10^{1}	6.5×10^{1}	7.7×10^{-2}	2.1×10^{1}	2.7×10^{-3}	1.5×10^{-1}	7.8×10^{-4}	8.1×10^{-1}	4.6
Krypton, gaseous {GLO}| market for | APOS, S	1.6×10^{2}	2.2×10^{2}	2.2×10^{2}	2.3×10^{-1}	7.0×10^{1}	5.4×10^{-3}	4.6×10^{-1}	2.4×10^{-3}	4.0×10^{-1}	1.5×10^{1}
Indium {GLO}| market for | APOS, S	2.2×10^{2}	4.4	4.3	6.8×10^{-3}	1.4	2.1×10^{-4}	1.6×10^{-2}	4.3×10^{-5}	4.0×10^{-2}	3.1×10^{-1}
Tantalum, powder, capacitor-grade {GLO}| market for | APOS, S	3.0×10^{2}	1.8×10^{1}	1.8×10^{1}	2.1×10^{-2}	5.8	2.2×10^{-3}	1.3×10^{-1}	5.1×10^{-4}	3.2×10^{-1}	2.1
Silicon, single crystal, czochralski process, electronics, combined to GLO market	3.0×10^{2}	4.2×10^{1}	4.1×10^{1}	5.1×10^{-2}	1.4×10^{1}	2.2×10^{-3}	1.2×10^{-1}	4.4×10^{-4}	3.2×10^{-1}	2.9
Xenon, gaseous, combined to GLO market	1.0×10^{3}	2.2×10^{2}	2.2×10^{2}	2.3×10^{-1}	7.0×10^{1}	5.4×10^{-3}	4.6×10^{-1}	2.4×10^{-3}	4.0×10^{-1}	1.5×10^{1}
Uranium, enriched 3.0%, in fuel element for light water reactor {GLO}| market for | APOS, S	2.5×10^{3}	7.0×10^{1}	7.2×10^{1}	7.8×10^{-1}	2.2×10^{1}	1.4×10^{-2}	1.6	1.3×10^{-3}	9.3×10^{-1}	5.2
Uranium, enriched 3.8%, in fuel element for light water reactor {GLO}| market for | APOS, S	3.5×10^{3}	9.5×10^{1}	9.8×10^{1}	1.1	3.0×10^{1}	1.8×10^{-2}	2.1	1.8×10^{-3}	1.2	7.2
Uranium, enriched 3.9%, in fuel element for light water reactor {GLO}| market for | APOS, S	3.6×10^{3}	9.8×10^{1}	1.0×10^{2}	1.1	3.1×10^{1}	1.8×10^{-2}	2.2	1.8×10^{-3}	1.3	7.4
Uranium, enriched 4%, in fuel element for light water reactor {GLO}| market for | APOS, S	3.7×10^{3}	1.0×10^{2}	1.0×10^{2}	1.2	3.2×10^{1}	1.9×10^{-2}	2.3	1.9×10^{-3}	1.3	7.6
Uranium, enriched 4.2%, in fuel element for light water reactor {GLO}| market for | APOS, S	3.9×10^{3}	1.1×10^{2}	1.1×10^{2}	1.3	3.4×10^{1}	2.0×10^{-2}	2.4	2.0×10^{-3}	1.4	8.1

The notation for the PBs is as follows: climate change (CC) with control variables of CO_2 concentration (CO_2 conc.) and energy imbalance (Energy imb.), stratospheric ozone depletion (SOD), ocean acidification (OA), biogeochemical (BGC) flows with control variables of phosphorus (P) and nitrogen (N), land-system change (LSC), freshwater use (FWU), change in biosphere integrity (CBI) with control variable of loss of biodiversity intactness index (BII loss).

Table S-5. Activities, omitted in **Figure S-2** for visualisation purposes due to high unitary prices (ranging from 32.9 to 1421 $\mathrm{USD_{2018}}$/kg of chemical), together with their impact scores in the global warming potential (GWP) and the PBs.

Activity name	**Price ($\mathrm{USD_{2018}\ kg^{-1}}$)**	**GWP (kg $\mathrm{CO_2\ kg^{-1}}$)**	**CC - CO2 conc. (ppm $\mathrm{kg^{-1}}$)**	**CC - Energy imb. (W $\mathrm{m^{-2}\ kg^{-1}}$)**	**SOD (DU $\mathrm{kg^{-1}}$)**	**OA (mol $\mathrm{kg^{-1}}$)**	**BGC flows – P (TgP $\mathrm{yr^{-1}\ kg^{-1}}$)**	**BGC flows – N (TgN $\mathrm{yr^{-1}\ kg^{-1}}$)**	**LSC (% $\mathrm{kg^{-1}}$)**	**FWU ($\mathrm{km^3\ yr^{-1}\ kg^{-1}}$)**	**CBI - BII loss (% $\mathrm{kg^{-1}}$)**
Uranium hexafluoride, combined to GLO market	3.3×10^{1}	1.5×10^{2}	3.7×10^{-9}	5.0×10^{-11}	2.3×10^{-12}	1.1×10^{-11}	1.1×10^{-13}	1.6×10^{-10}	4.5×10^{-14}	4.0×10^{-9}	3.6×10^{-11}
Zirconium oxide {GLO}| market for | APOS, S	4.3×10^{1}	4.8	1.2×10^{-10}	1.6×10^{-12}	3.5×10^{-14}	3.7×10^{-13}	5.5×10^{-15}	1.6×10^{-12}	4.4×10^{-15}	9.5×10^{-11}	1.3×10^{-12}
Silicon, multi-si, casted, combined to GLO market	4.5×10^{1}	7.9×10^{1}	2.0×10^{-9}	2.6×10^{-11}	4.1×10^{-13}	6.0×10^{-12}	1.3×10^{-14}	4.9×10^{-12}	8.2×10^{-15}	2.1×10^{-10}	2.0×10^{-11}
Hydrazine sulfate {GLO}| market for hydrazine sulfate | APOS, S	5.1×10^{1}	5.7	1.4×10^{-10}	1.9×10^{-12}	4.4×10^{-14}	4.3×10^{-13}	1.0×10^{-14}	3.0×10^{-12}	9.2×10^{-16}	1.4×10^{-11}	1.4×10^{-12}
Sodium tetrahydridoborate {GLO}| market for | APOS, S	5.4×10^{1}	3.0×10^{1}	7.4×10^{-10}	1.0×10^{-11}	1.7×10^{-13}	2.3×10^{-12}	1.7×10^{-14}	5.3×10^{-12}	4.9×10^{-15}	7.5×10^{-11}	7.0×10^{-12}
Silicon, single crystal, czochralski process, photovoltaics, combined to GLO market	5.7×10^{1}	1.5×10^{2}	3.7×10^{-9}	5.0×10^{-11}	8.6×10^{-13}	1.1×10^{-11}	2.0×10^{-14}	7.4×10^{-12}	1.5×10^{-14}	2.5×10^{-9}	3.5×10^{-11}
Lithium {GLO}| market for | APOS, S	7.0×10^{1}	4.8×10^{1}	1.2×10^{-9}	1.6×10^{-11}	2.4×10^{-13}	3.7×10^{-12}	2.5×10^{-13}	1.4×10^{-10}	2.2×10^{-15}	9.8×10^{-11}	1.2×10^{-11}
Selenium {GLO}| market for | APOS, S	7.6×10^{1}	2.6	6.4×10^{-11}	8.7×10^{-13}	1.6×10^{-14}	2.0×10^{-13}	3.1×10^{-14}	1.0×10^{-12}	5.8×10^{-16}	7.9×10^{-12}	7.0×10^{-13}
Aminopyridine, combined to GLO market	8.5×10^{1}	9.3×10^{1}	2.2×10^{-9}	3.0×10^{-11}	2.7×10^{-13}	6.9×10^{-12}	5.3×10^{-14}	1.4×10^{-11}	1.3×10^{-14}	1.5×10^{-10}	2.1×10^{-11}
2-pyridinol {GLO}| market for | APOS, S	8.9×10^{1}	1.0×10^{2}	2.4×10^{-9}	3.3×10^{-11}	1.2×10^{-12}	7.4×10^{-12}	6.2×10^{-14}	4.1×10^{-10}	1.4×10^{-14}	1.7×10^{-10}	2.3×10^{-11}
Silicon, electronics grade {GLO}| market for | APOS, S	9.9×10^{1}	9.5×10^{1}	2.4×10^{-9}	3.2×10^{-11}	6.0×10^{-13}	7.2×10^{-12}	2.4×10^{-14}	7.7×10^{-12}	7.5×10^{-15}	3.4×10^{-10}	2.3×10^{-11}
Xenon, gaseous, combined to GLO market	1.2×10^{2}	1.0×10^{3}	2.5×10^{-8}	3.4×10^{-10}	5.2×10^{-12}	7.6×10^{-11}	8.4×10^{-14}	4.5×10^{-11}	9.6×10^{-14}	2.5×10^{-9}	2.3×10^{-10}
Hexamethyldisilazane {GLO}| market for | APOS, S	1.5×10^{2}	5.8	1.4×10^{-10}	1.9×10^{-12}	3.7×10^{-14}	4.3×10^{-13}	6.9×10^{-15}	6.9×10^{-13}	8.3×10^{-16}	1.3×10^{-11}	1.4×10^{-12}
Silicon, single crystal, czochralski process, electronics, combined to GLO market	1.8×10^{2}	3.0×10^{2}	7.4×10^{-9}	1.0×10^{-10}	1.8×10^{-12}	2.3×10^{-11}	5.2×10^{-14}	1.8×10^{-11}	2.6×10^{-14}	3.1×10^{-9}	7.1×10^{-11}
Tantalum, powder, capacitor-grade {GLO}| market for | APOS, S	4.2×10^{2}	3.0×10^{2}	7.4×10^{-9}	1.0×10^{-10}	1.7×10^{-12}	2.3×10^{-11}	1.2×10^{-13}	4.6×10^{-11}	7.2×10^{-14}	7.3×10^{-9}	1.2×10^{-10}
Gallium, semiconductor-grade {GLO}| market for | APOS, S	4.3×10^{2}	1.5×10^{2}	3.4×10^{-9}	4.6×10^{-11}	1.1×10^{-12}	1.0×10^{-11}	1.3×10^{-12}	2.7×10^{-9}	2.3×10^{-14}	3.4×10^{-10}	3.4×10^{-11}
Uranium, enriched 4.2%, in fuel element for light water reactor {GLO}| market for | APOS, S	8.4×10^{2}	3.9×10^{3}	8.8×10^{-8}	1.3×10^{-9}	2.1×10^{-10}	2.7×10^{-10}	2.2×10^{-12}	1.7×10^{-9}	5.6×10^{-13}	6.4×10^{-8}	9.2×10^{-10}
Uranium, enriched 4%, in fuel element for light water reactor {GLO}| market for | APOS, S	8.4×10^{2}	3.7×10^{3}	8.3×10^{-8}	1.2×10^{-9}	2.0×10^{-10}	2.5×10^{-10}	2.1×10^{-12}	1.6×10^{-9}	5.3×10^{-13}	6.0×10^{-8}	8.6×10^{-10}
Uranium, enriched 3.9%, in fuel element for light water reactor {GLO}| market for | APOS, S	8.4×10^{2}	3.6×10^{3}	8.0×10^{-8}	1.2×10^{-9}	1.9×10^{-10}	2.5×10^{-10}	2.1×10^{-12}	1.6×10^{-9}	5.2×10^{-13}	5.9×10^{-8}	8.4×10^{-10}
Uranium, enriched 3.8%, in fuel element for light water reactor {GLO}| market for | APOS, S	8.4×10^{2}	3.5×10^{3}	7.8×10^{-8}	1.1×10^{-9}	1.8×10^{-10}	2.4×10^{-10}	2.0×10^{-12}	1.5×10^{-9}	5.0×10^{-13}	5.7×10^{-8}	8.2×10^{-10}
Uranium, enriched 3.0%, in fuel element for light water reactor {GLO}| market for | APOS, S	8.4×10^{2}	2.5×10^{3}	5.7×10^{-8}	8.2×10^{-10}	1.3×10^{-10}	1.8×10^{-10}	1.5×10^{-12}	1.1×10^{-9}	3.8×10^{-13}	4.2×10^{-8}	6.0×10^{-10}
Indium {GLO}| market for | APOS, S	1.2×10^{3}	2.2×10^{2}	5.2×10^{-9}	7.2×10^{-11}	1.6×10^{-12}	1.6×10^{-11}	3.5×10^{-14}	1.7×10^{-11}	1.8×10^{-14}	2.7×10^{-9}	5.1×10^{-11}
Trimesoyl chloride {GLO}| market for | APOS, S	1.4×10^{3}	8.3	1.7×10^{-10}	2.4×10^{-12}	6.5×10^{-13}	5.3×10^{-13}	1.4×10^{-14}	4.3×10^{-12}	6.0×10^{-16}	9.0×10^{-12}	1.9×10^{-12}

The notation for the PBs is as follows: climate change (CC) with control variables of CO_2 concentration (CO_2 conc.) and energy imbalance (Energy imb.), stratospheric ozone depletion (SOD), ocean acidification (OA), biogeochemical (BGC) flows with control variables of phosphorus (P) and nitrogen (N), land-system change (LSC), freshwater use (FWU), change in biosphere integrity (CBI) with control variable of loss of biodiversity intactness index (BII loss).

7. Biogeochemical flow of nitrogen PB and cradle-to-gate scope

Following Ryberg *et al.*[5], the characterisation factors (CFs) for nitrogen fixation were calculated via inverse modelling considering the emissions of N-compounds to freshwater. Due to the omission of the gate-to-grave LCA phase, some chemicals containing N may present lower BGC flow – N scores than expected. For example, the nitrate emissions due to ammonia application as fertiliser are not reflected in our results. However, some chemicals still lead to large transgression levels in the BGC flow – N, as nylon 6-6, which contains nitrogen. Indeed, even though we consistently evaluated all the chemicals of the dataset from cradle-to-gate, the amounts of fixated N for 27% of the chemicals exceed the associated share. This percentage would likely increase applying a cradle-to-grave scope. Likewise, considering a cradle-to-grave scope would also increase the impact on all the remaining control variables. Notably, this increment in impact would be more critical in the carbon-related PBs, as the fossil carbon chemically stored in the molecules would be released as CO_2 during their end-use phase due to degradation or incineration.

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